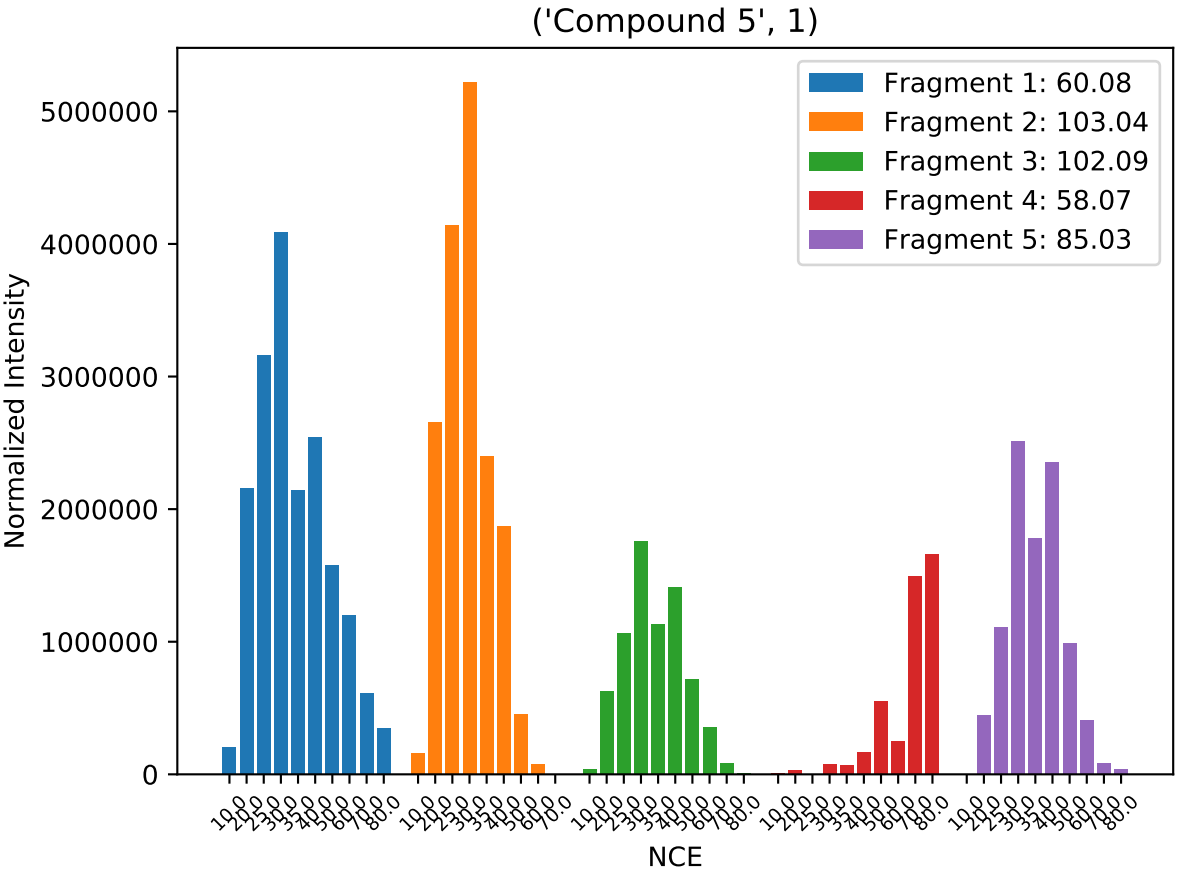
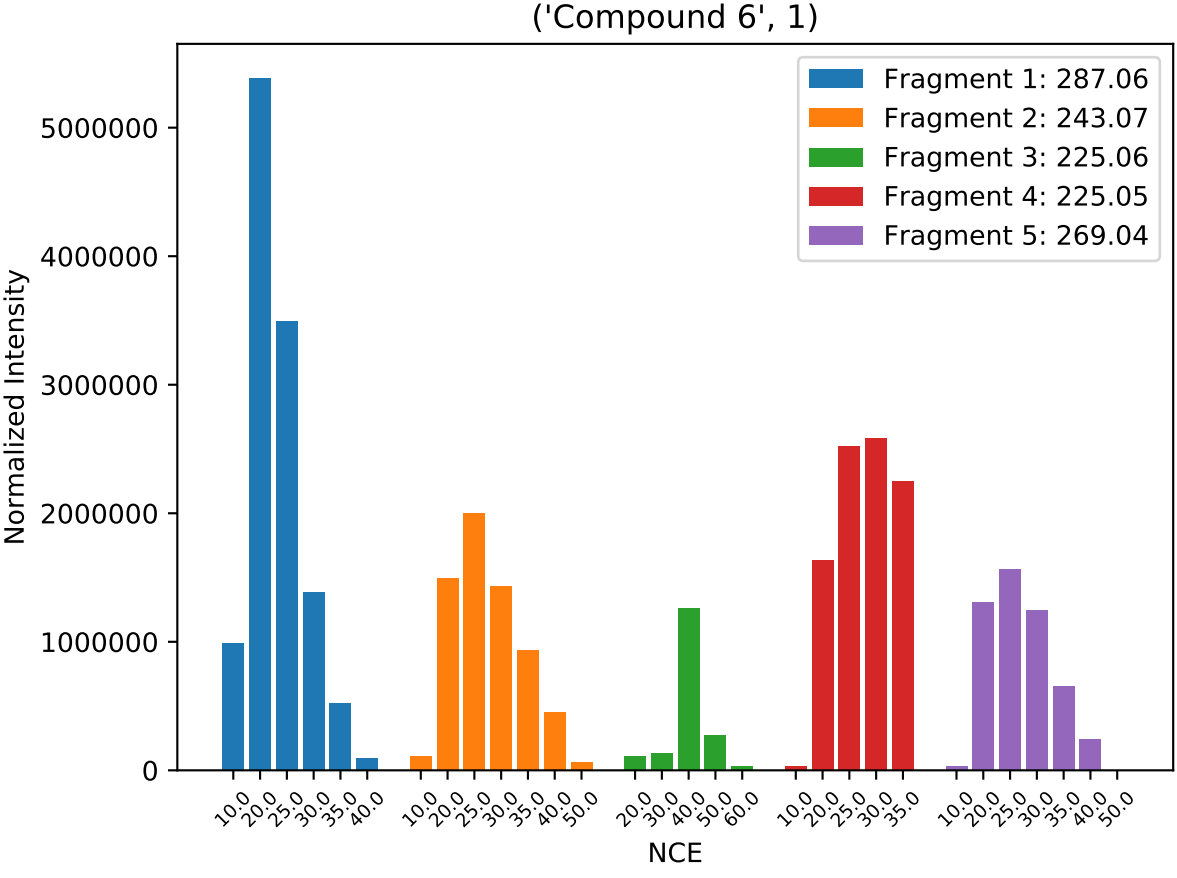
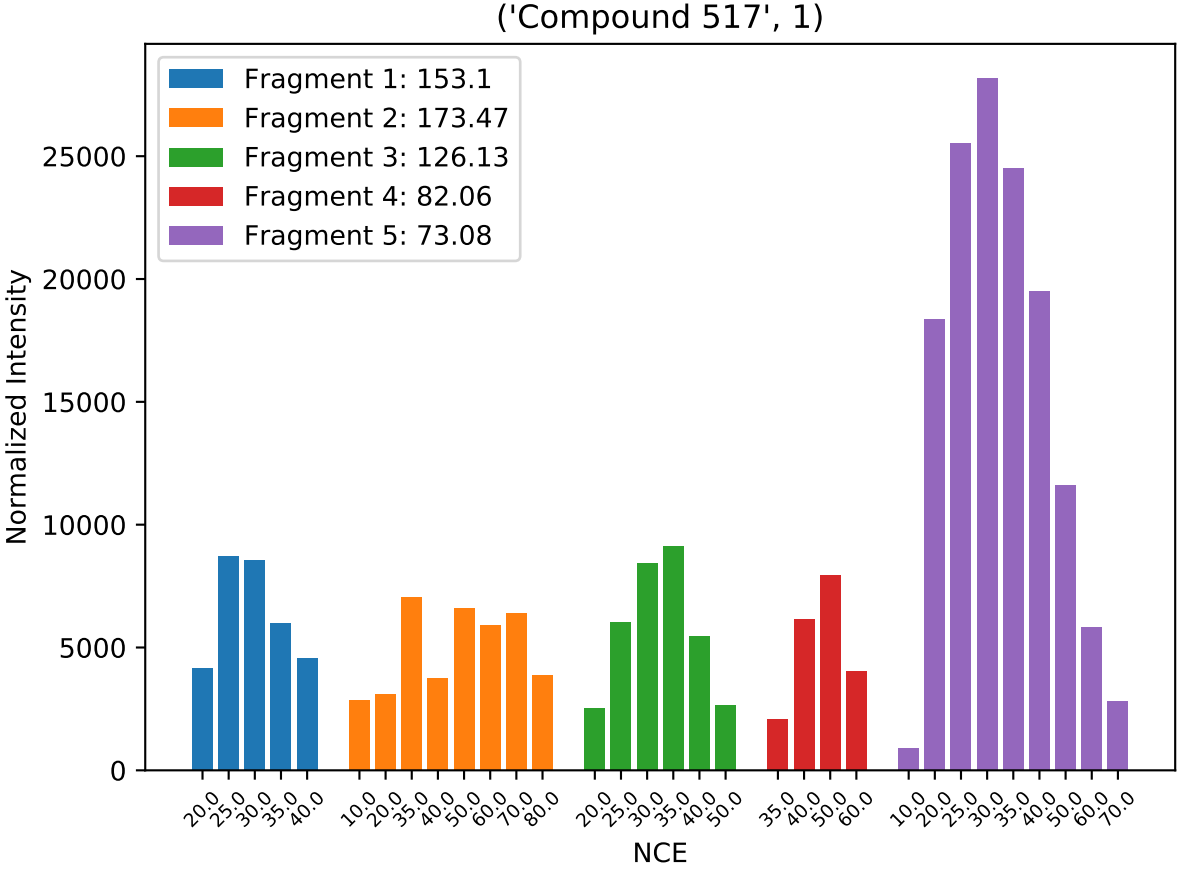
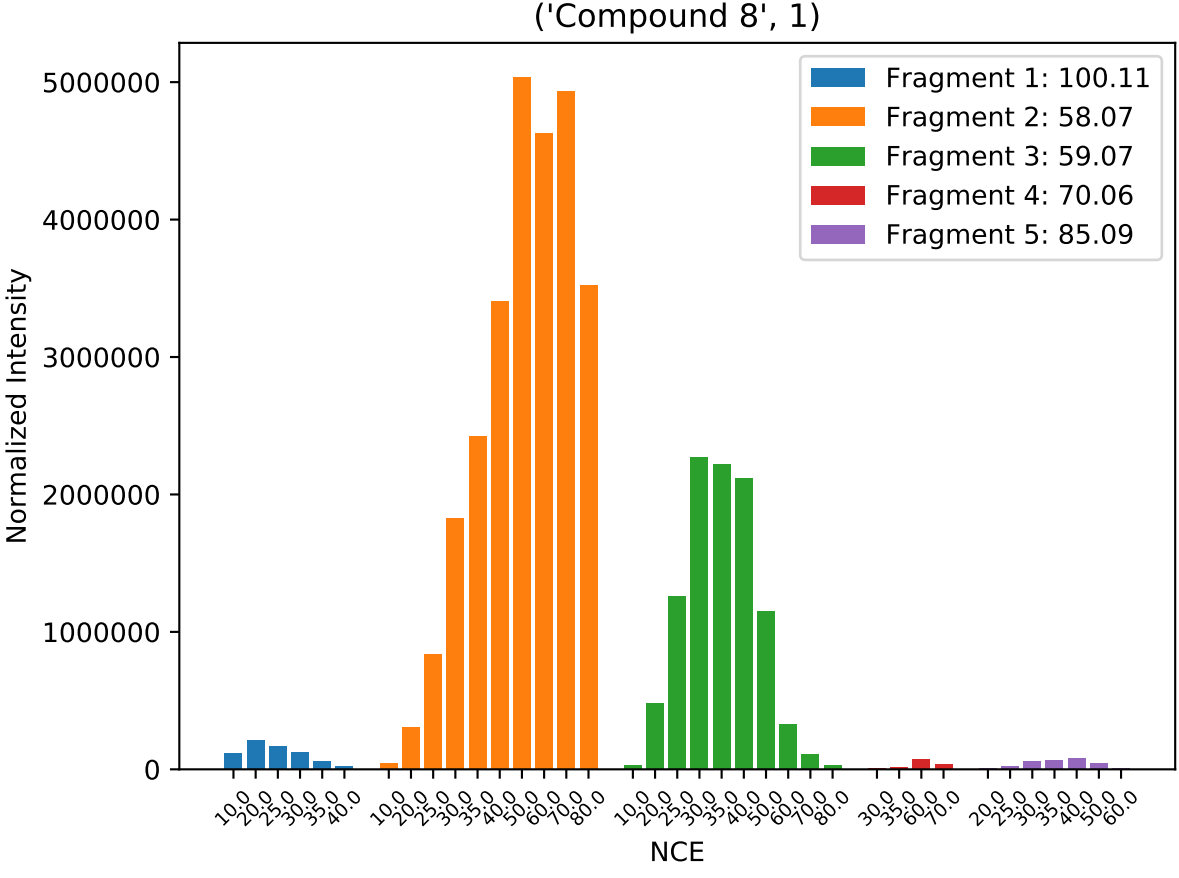
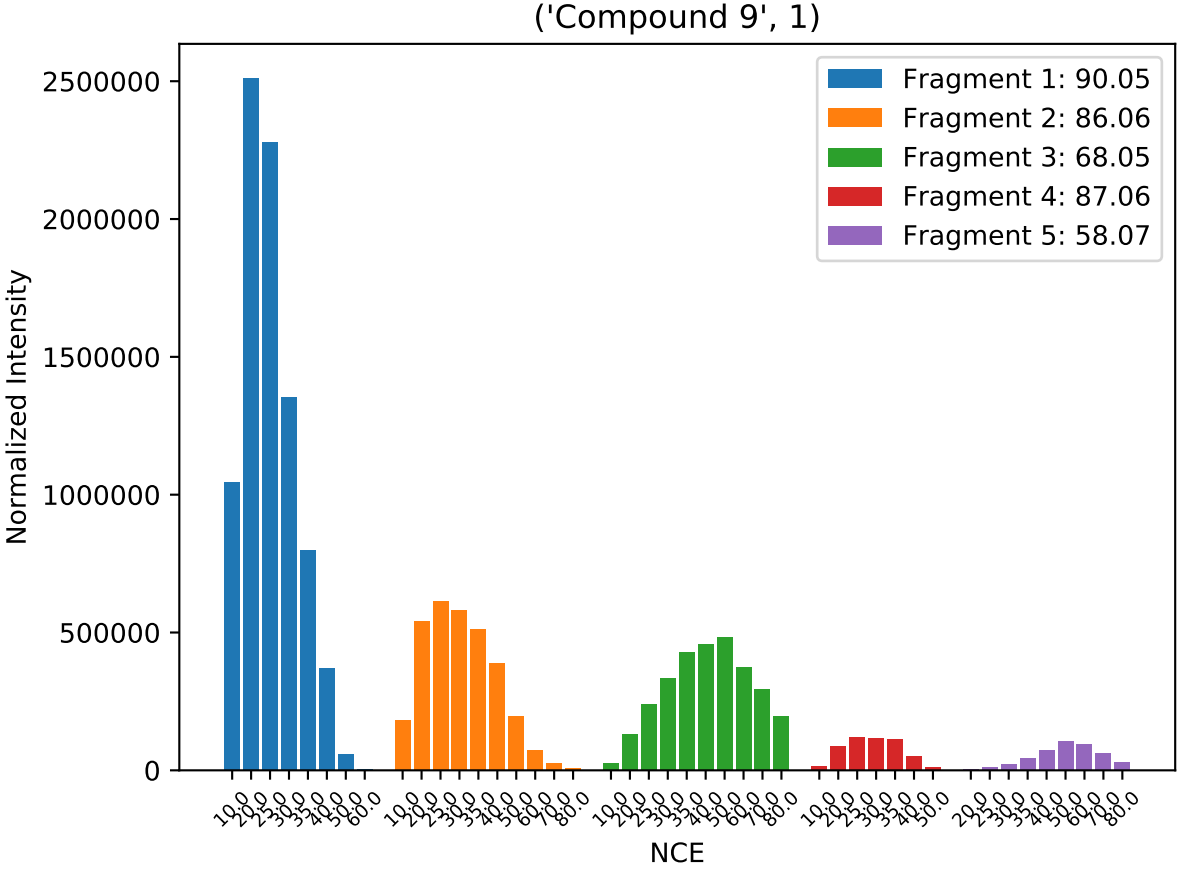
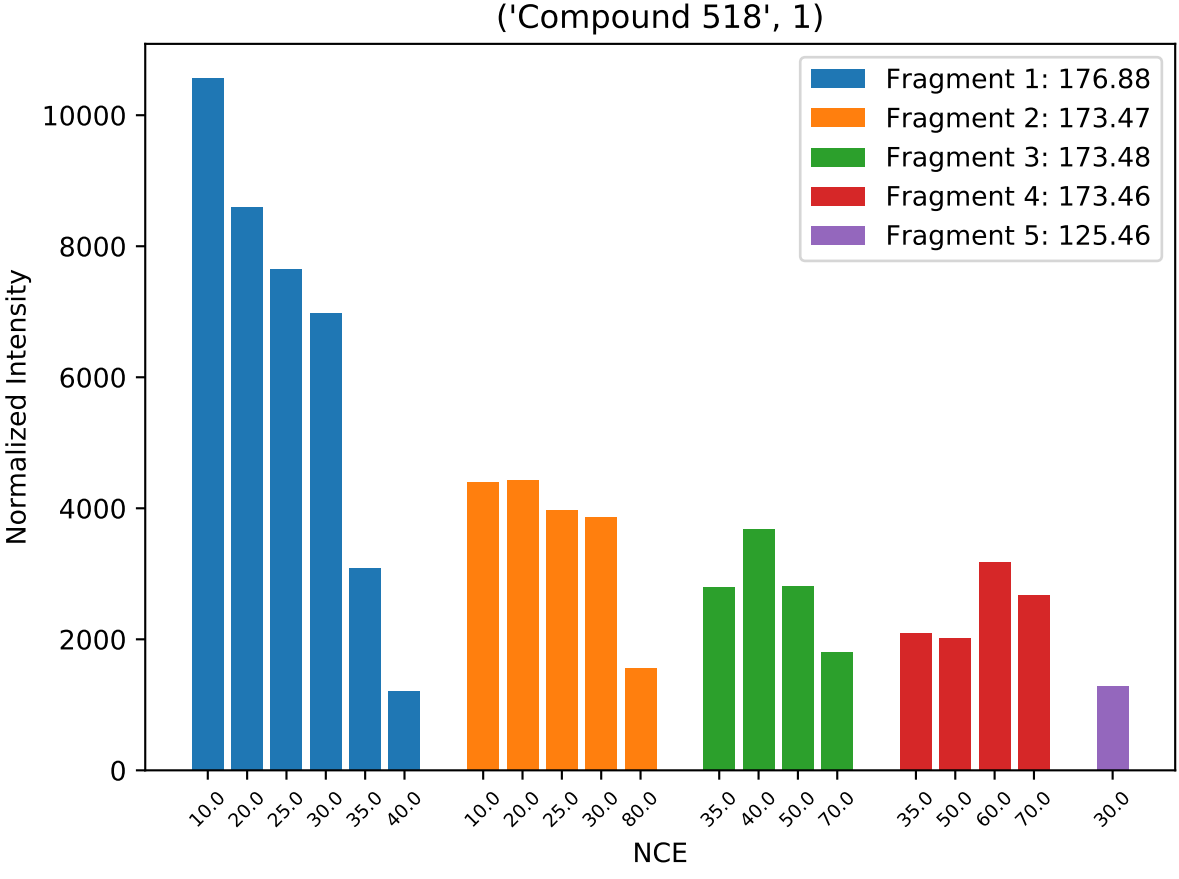

('Compound 5', 1)
Fragment 1: 60.08
Fragment 2: 103.04
Fragment 3: 102.09
Fragment 4: 58.07
Fragment 5: 85.03
Normalized Intensity
5000000
4000000
3000000
2000000
1000000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
80.0
NCE

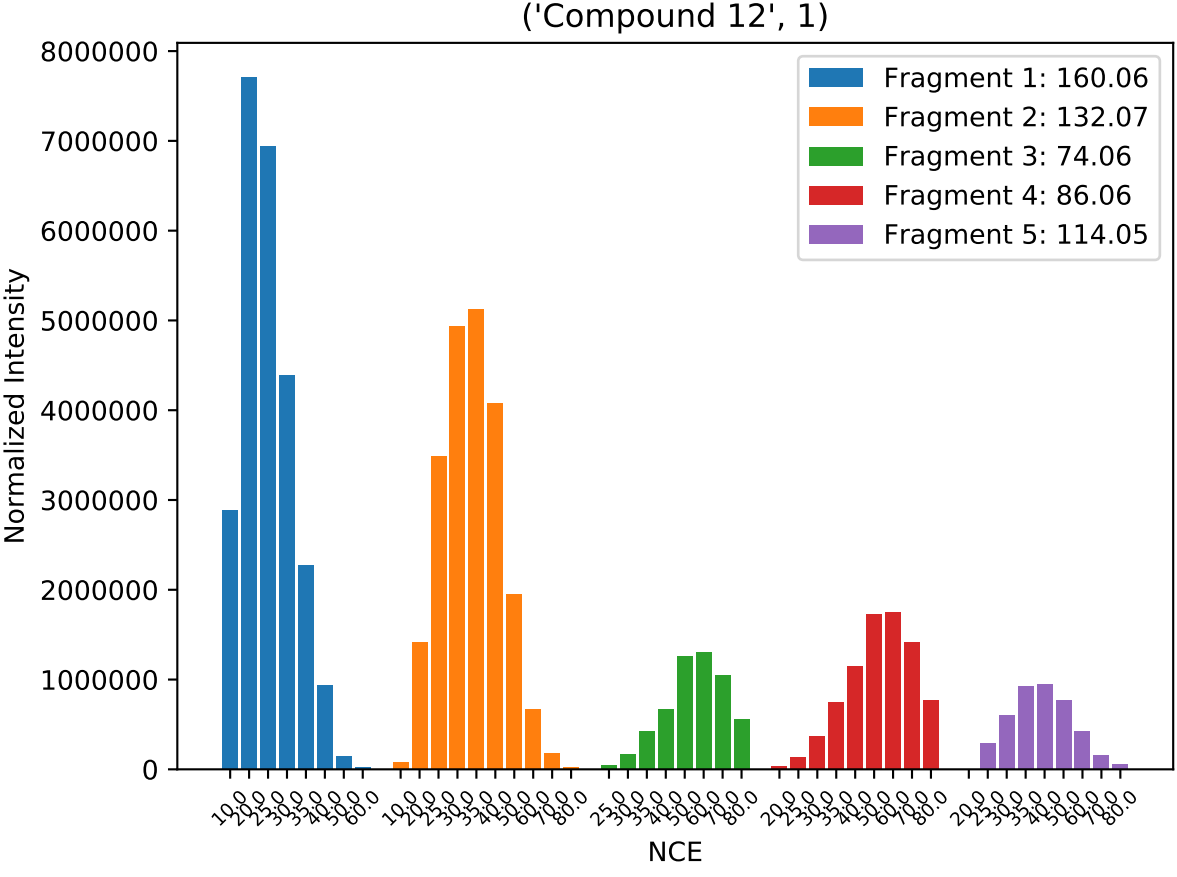

('Compound 6', 1)
Fragment 1: 287.06
Fragment 2: 243.07
Fragment 3: 225.06
Fragment 4: 225.05
Fragment 5: 269.04
Normalized Intensity
0
1000000
2000000
3000000
4000000
5000000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 30.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

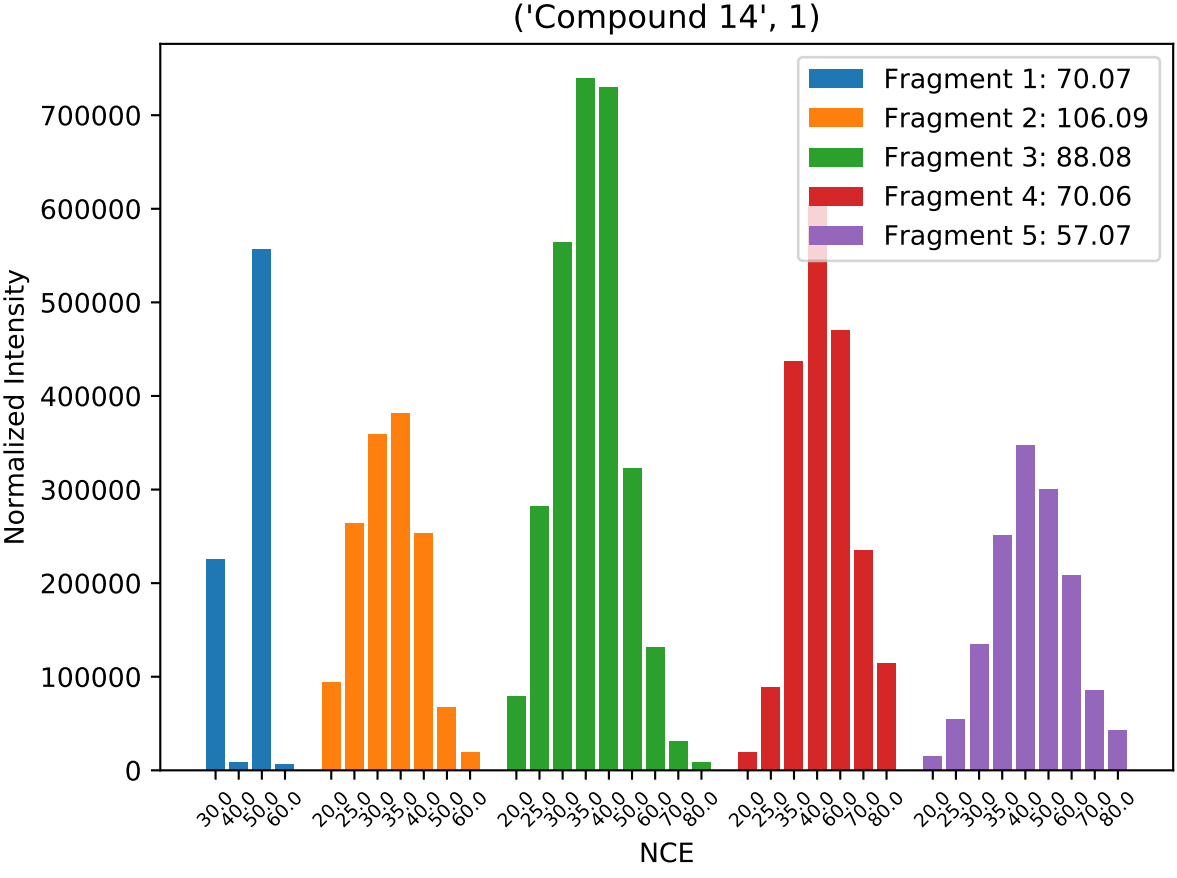

('Compound 517', 1)
Fragment 1: 153.1
Fragment 2: 173.47
Fragment 3: 126.13
Fragment 4: 82.06
Fragment 5: 73.08
Normalized Intensity
0
5000
10000
15000
20000
25000
20.0 25.0 30.0 35.0 40.0
10.0 20.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

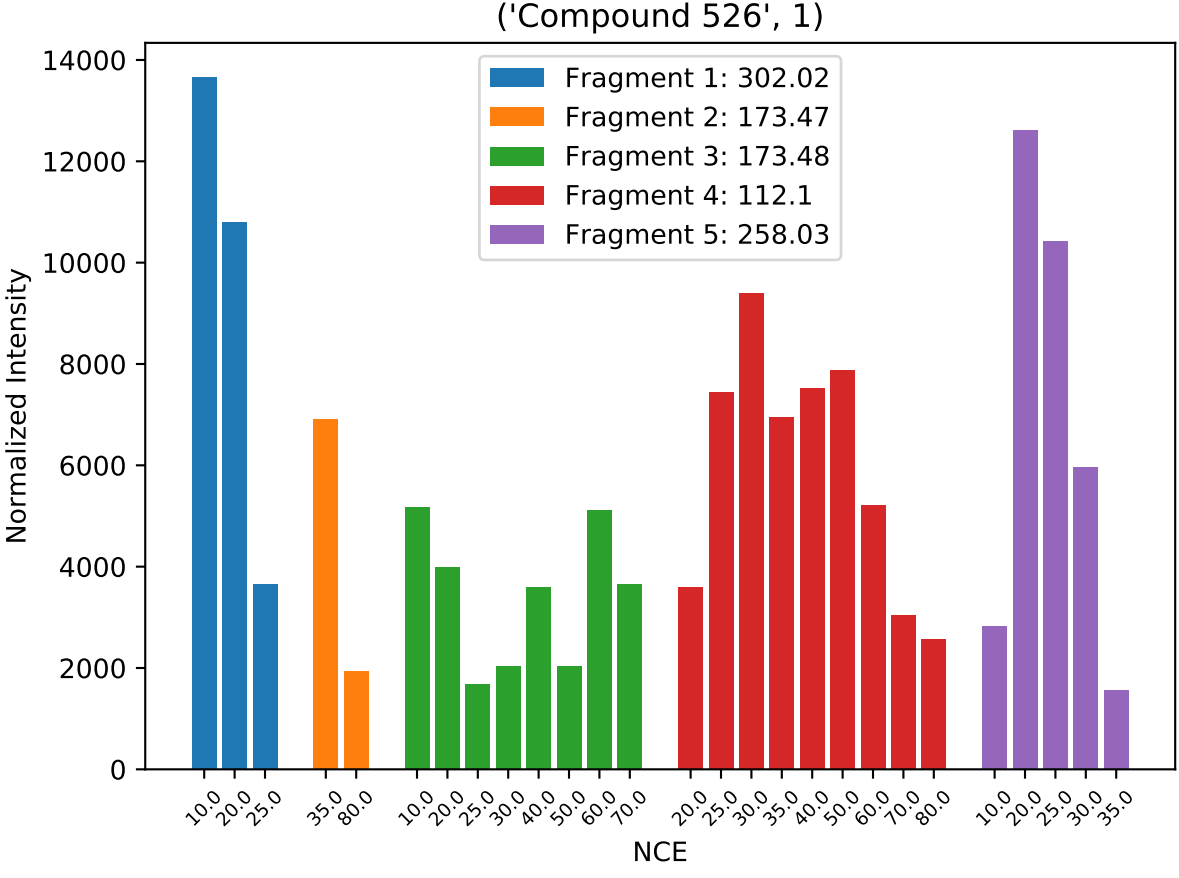

('Compound 8', 1)
Fragment 1: 100.11
Fragment 2: 58.07
Fragment 3: 59.07
Fragment 4: 70.06
Fragment 5: 85.09
Normalized Intensity
5000000
4000000
3000000
2000000
1000000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0

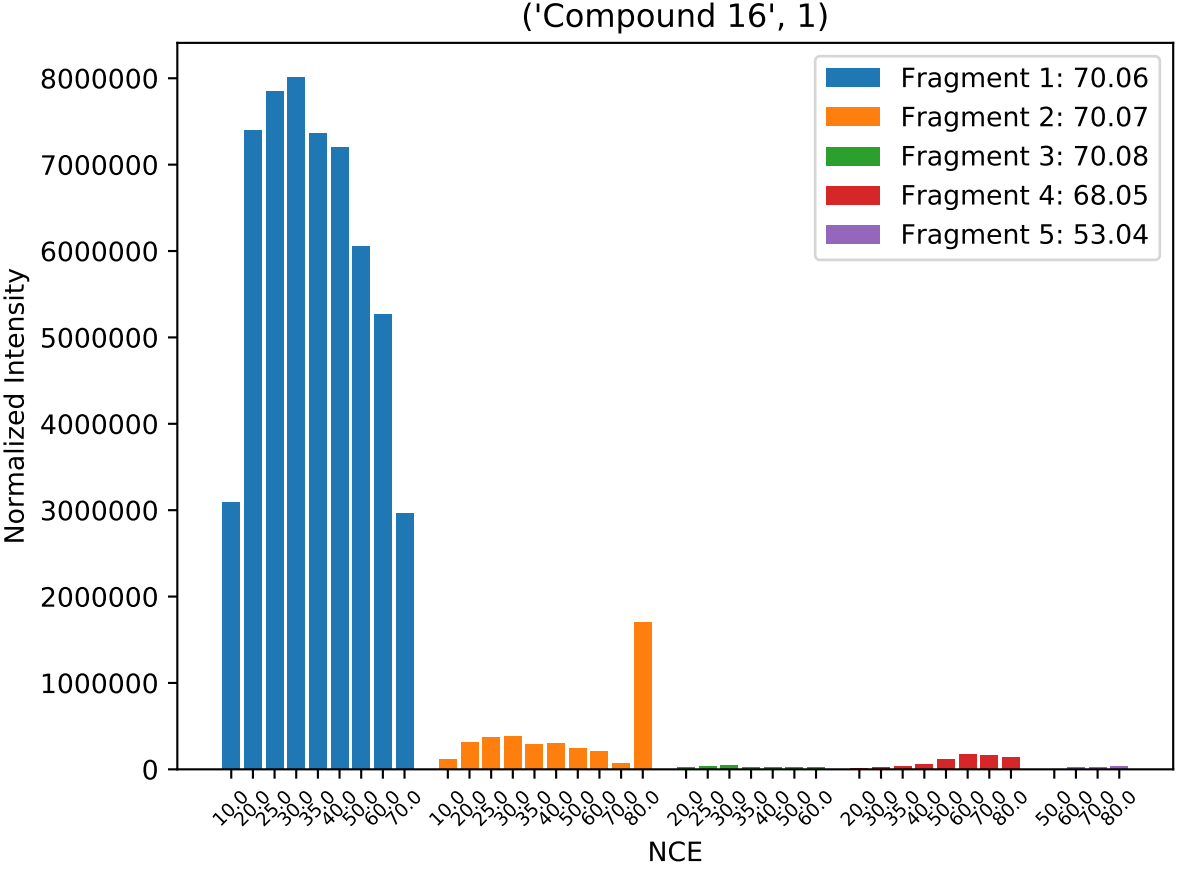

('Compound 9', 1)
Fragment 1: 90.05
Fragment 2: 86.06
Fragment 3: 68.05
Fragment 4: 87.06
Fragment 5: 58.07
Normalized Intensity
2500000
2000000
1500000
1000000
500000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

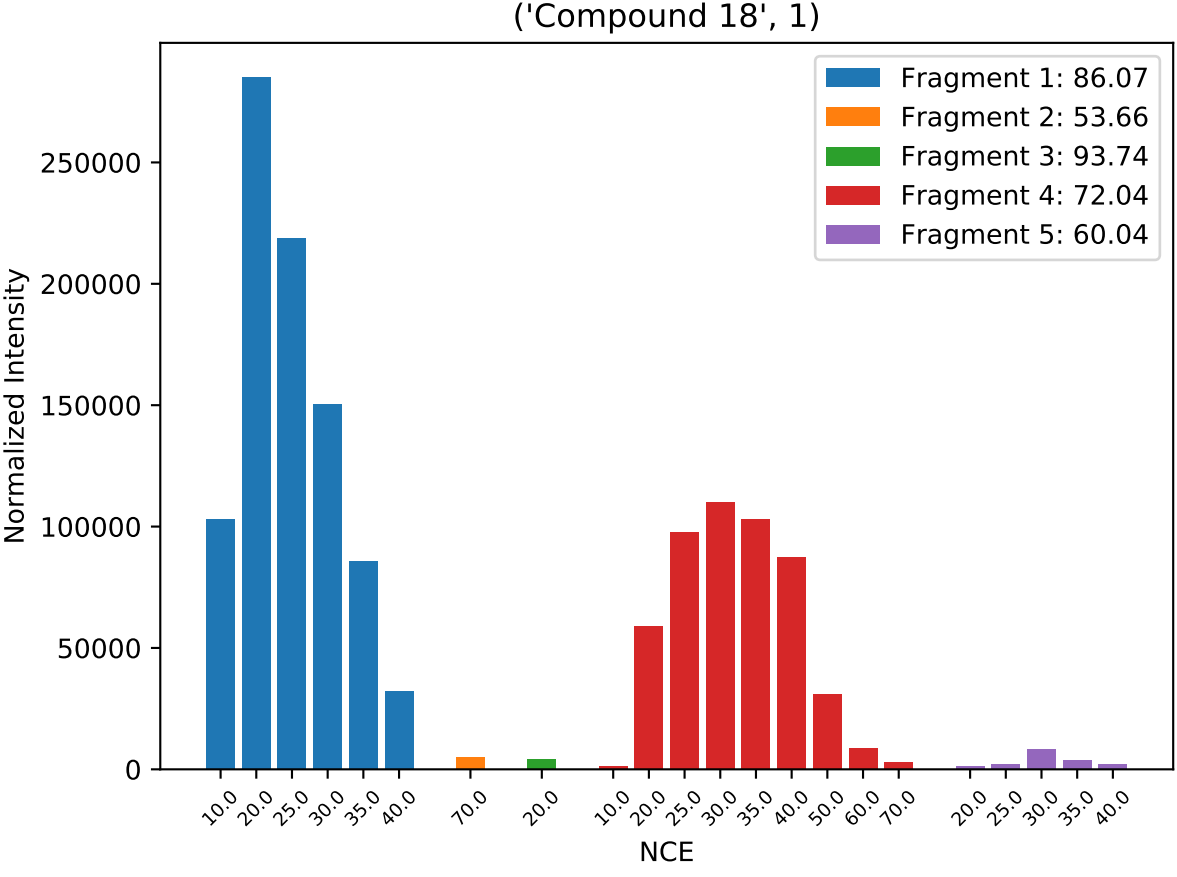

('Compound 518', 1)
Fragment 1: 176.88
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 125.46
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
80.0
35.0
40.0
50.0
70.0
35.0
50.0
60.0
70.0
30.0
NCE

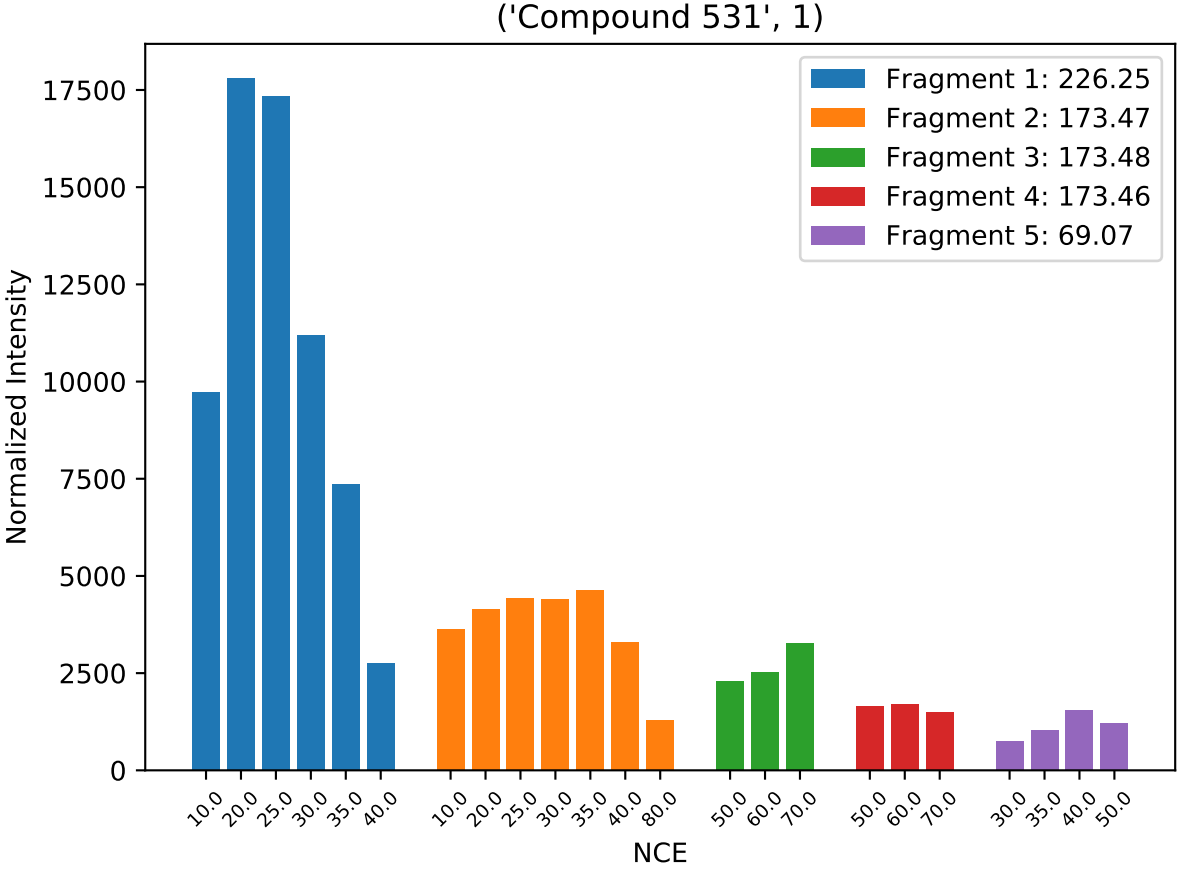

('Compound 12', 1)
Fragment 1: 160.06
Fragment 2: 132.07
Fragment 3: 74.06
Fragment 4: 86.06
Fragment 5: 114.05
Normalized Intensity
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

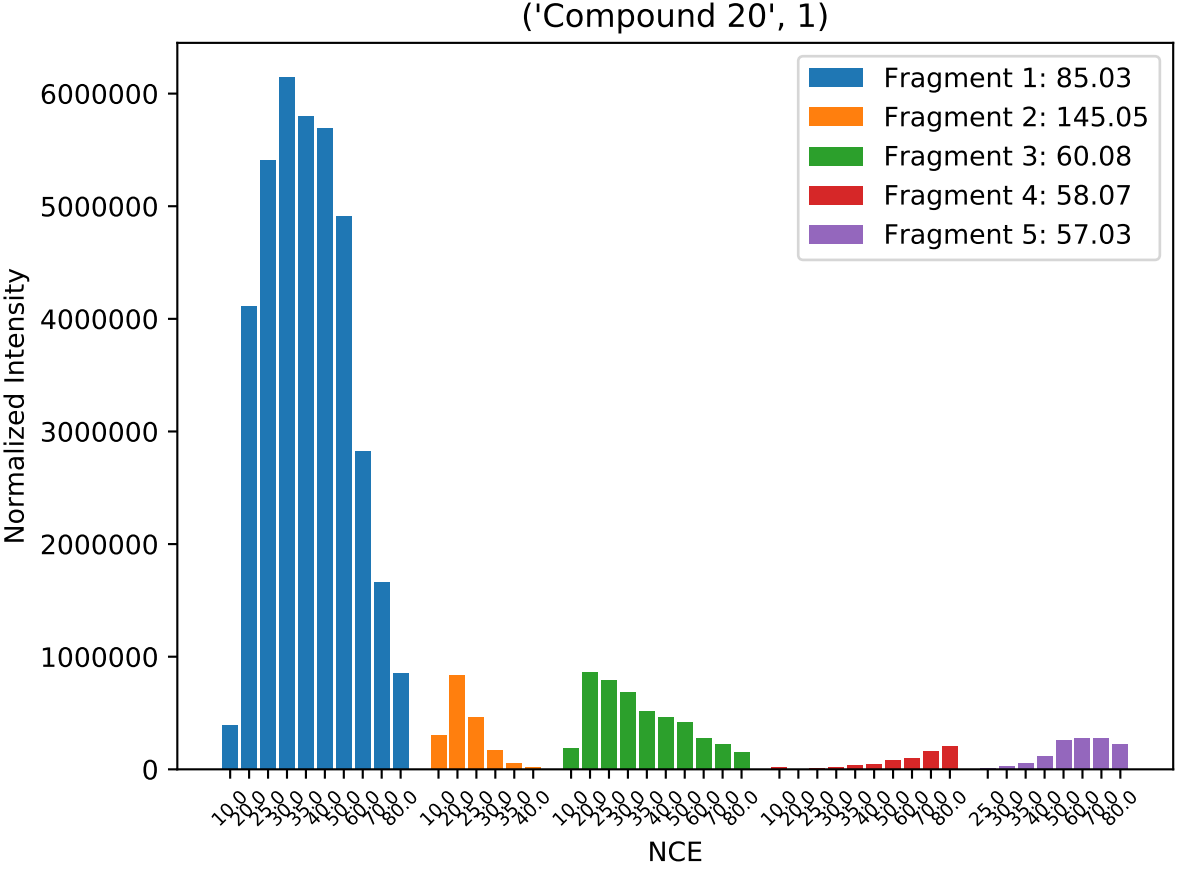

('Compound 14', 1)
Fragment 1: 70.07
Fragment 2: 106.09
Fragment 3: 88.08
Fragment 4: 70.06
Fragment 5: 57.07
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
700000
30.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 35.0 40.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

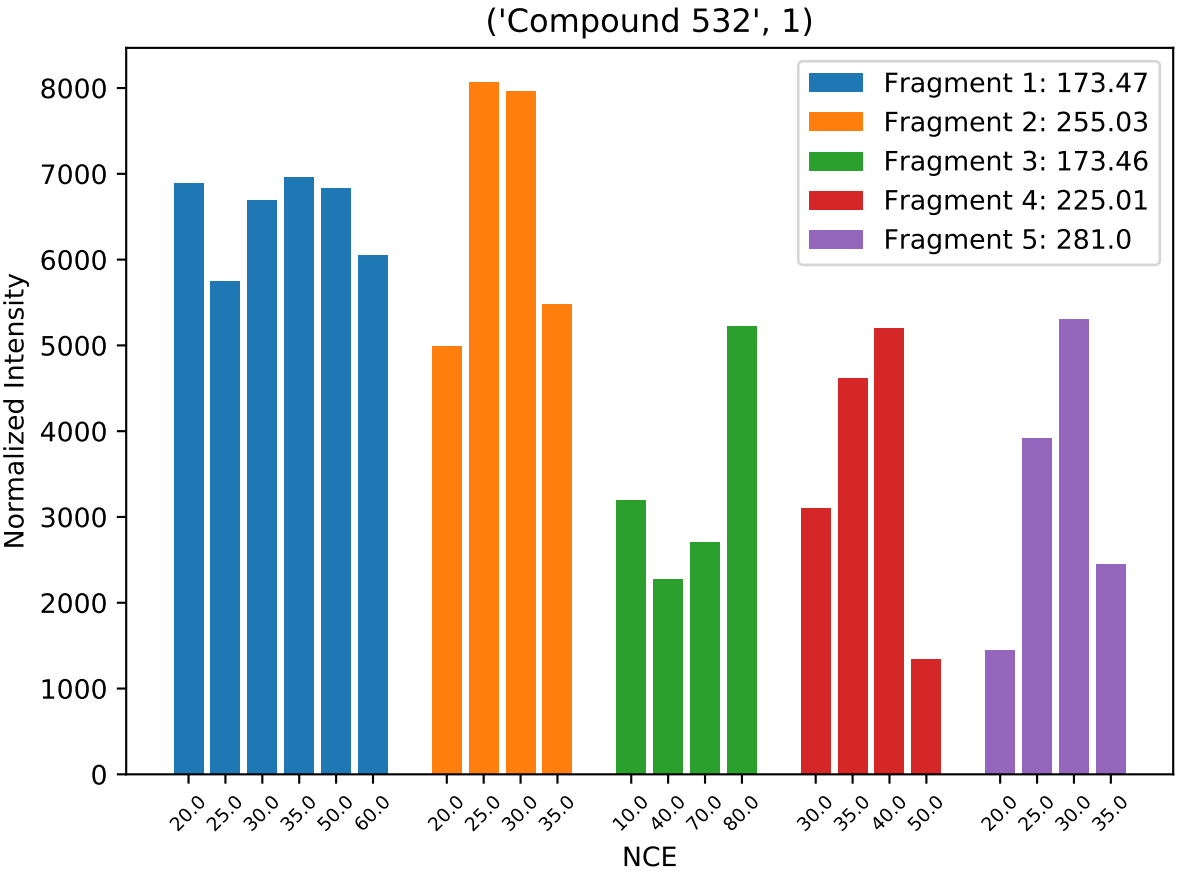

('Compound 526', 1)
Fragment 1: 302.02
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 112.1
Fragment 5: 258.03
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
25.0
35.0
80.0
10.0
20.0
25.0
30.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
NCE

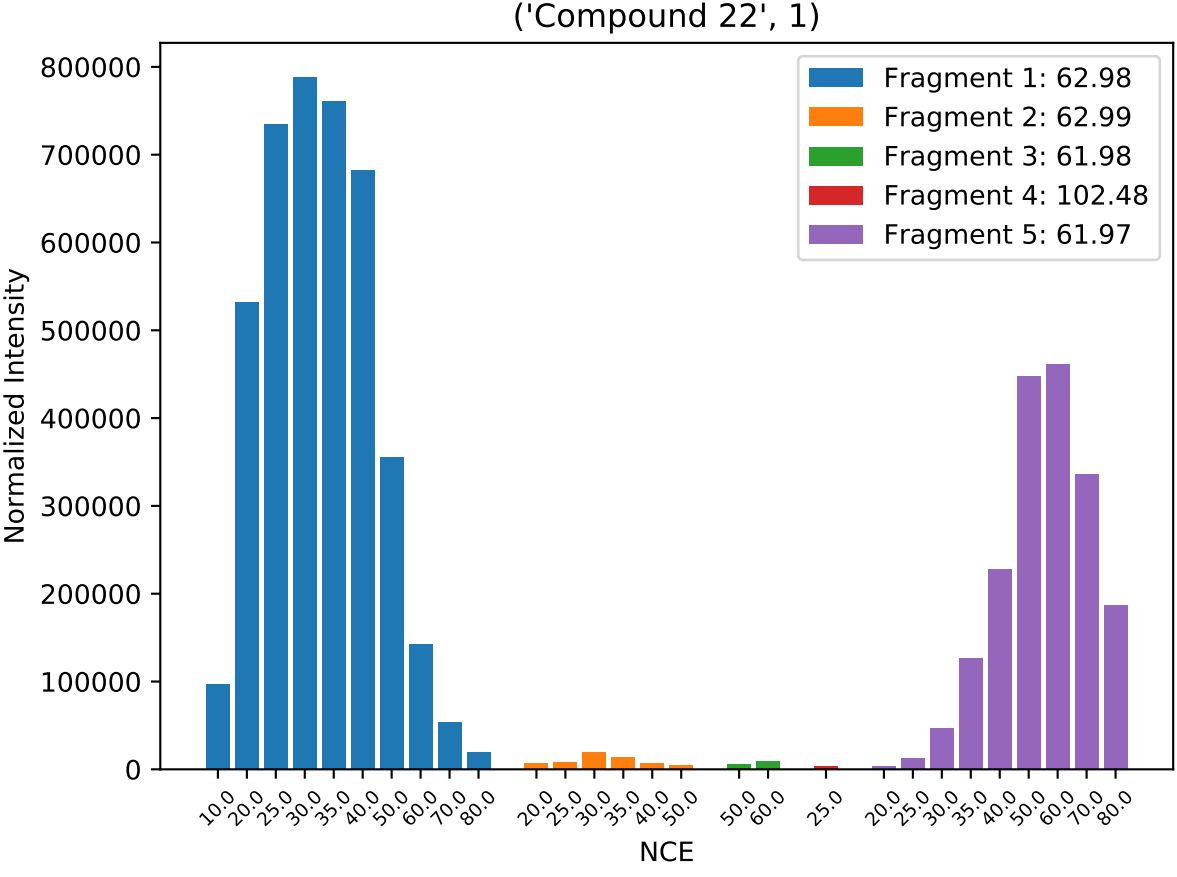

('Compound 16', 1)
Fragment 1: 70.06
Fragment 2: 70.07
Fragment 3: 70.08
Fragment 4: 68.05
Fragment 5: 53.04
Normalized Intensity
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0

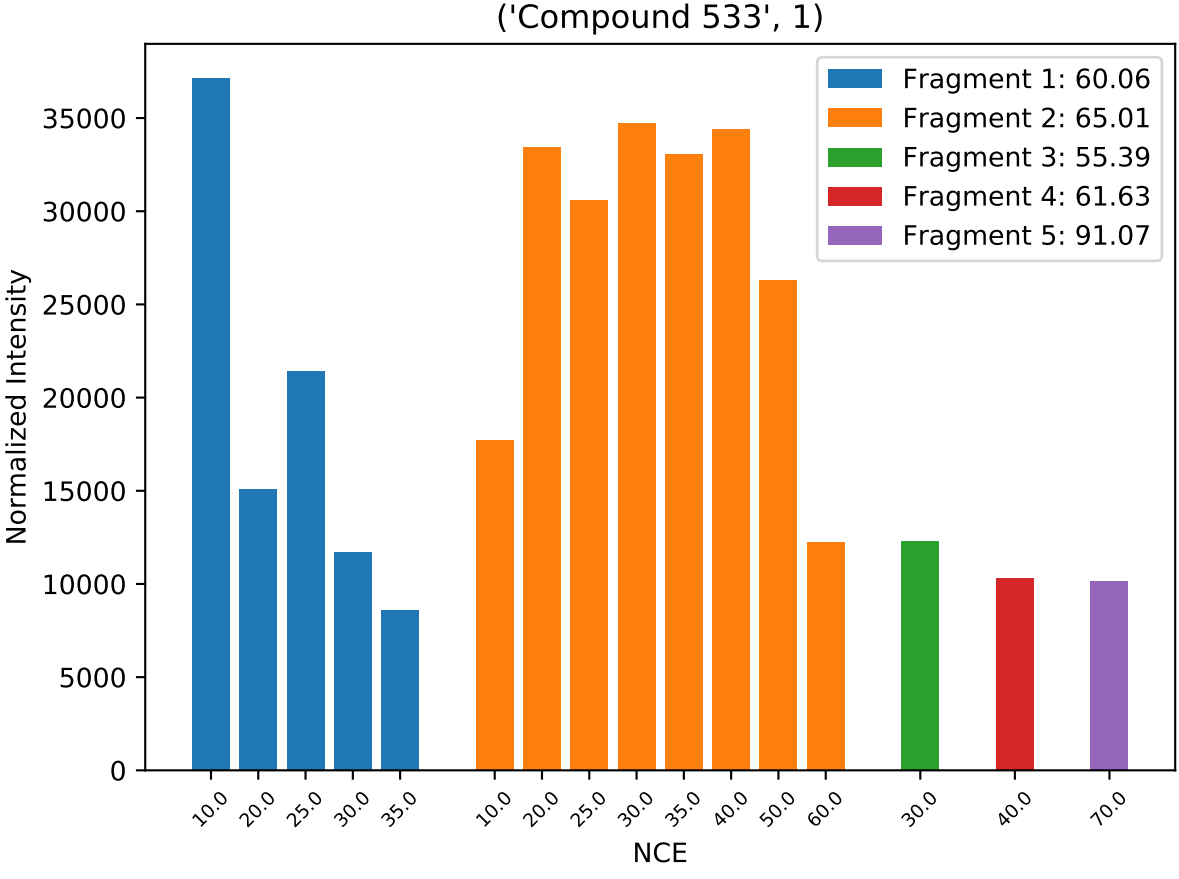

('Compound 18', 1)
Fragment 1: 86.07
Fragment 2: 53.66
Fragment 3: 93.74
Fragment 4: 72.04
Fragment 5: 60.04
Normalized Intensity
0
50000
100000
150000
200000
250000
10.0
20.0
25.0
30.0
35.0
40.0
70.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
NCE

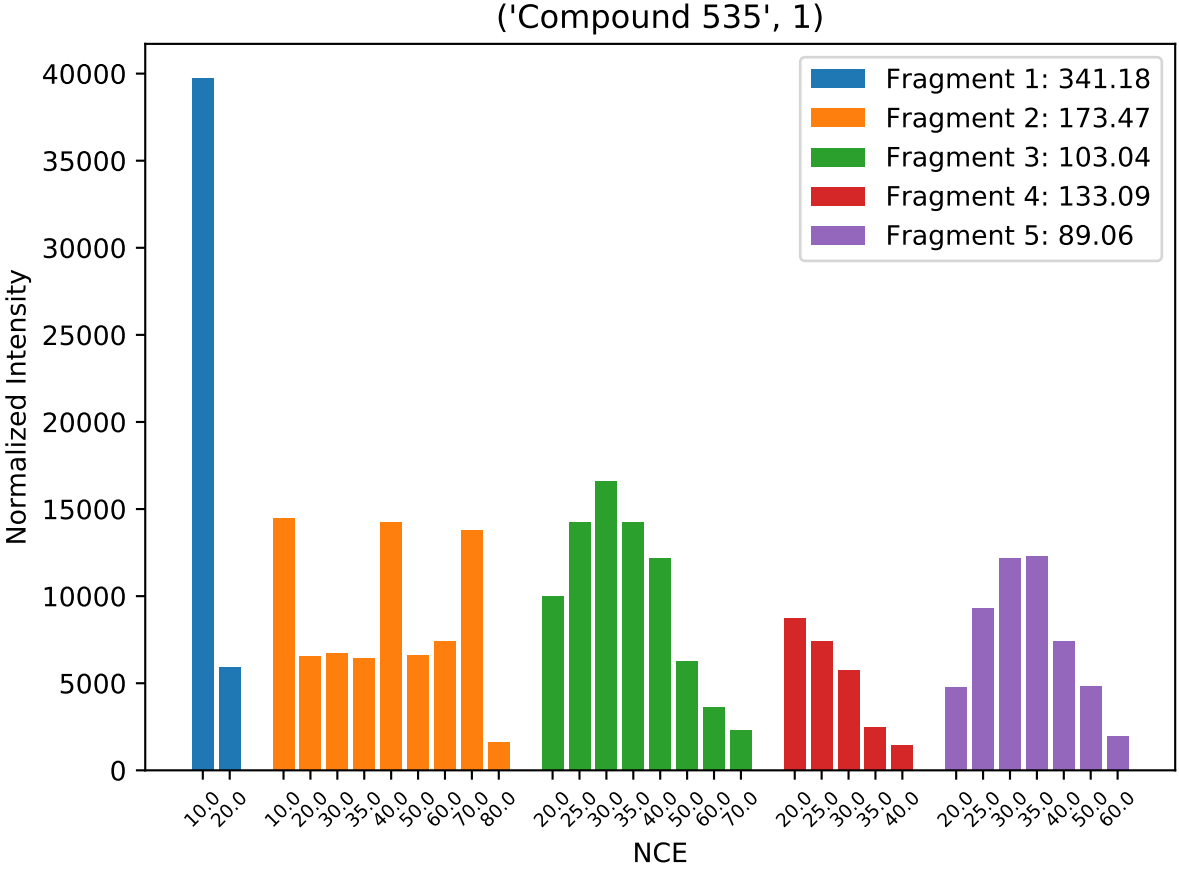

('Compound 531', 1)
Fragment 1: 226.25
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 69.07
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
80.0
50.0
60.0
70.0
50.0
60.0
70.0
30.0
35.0
40.0
50.0
NCE

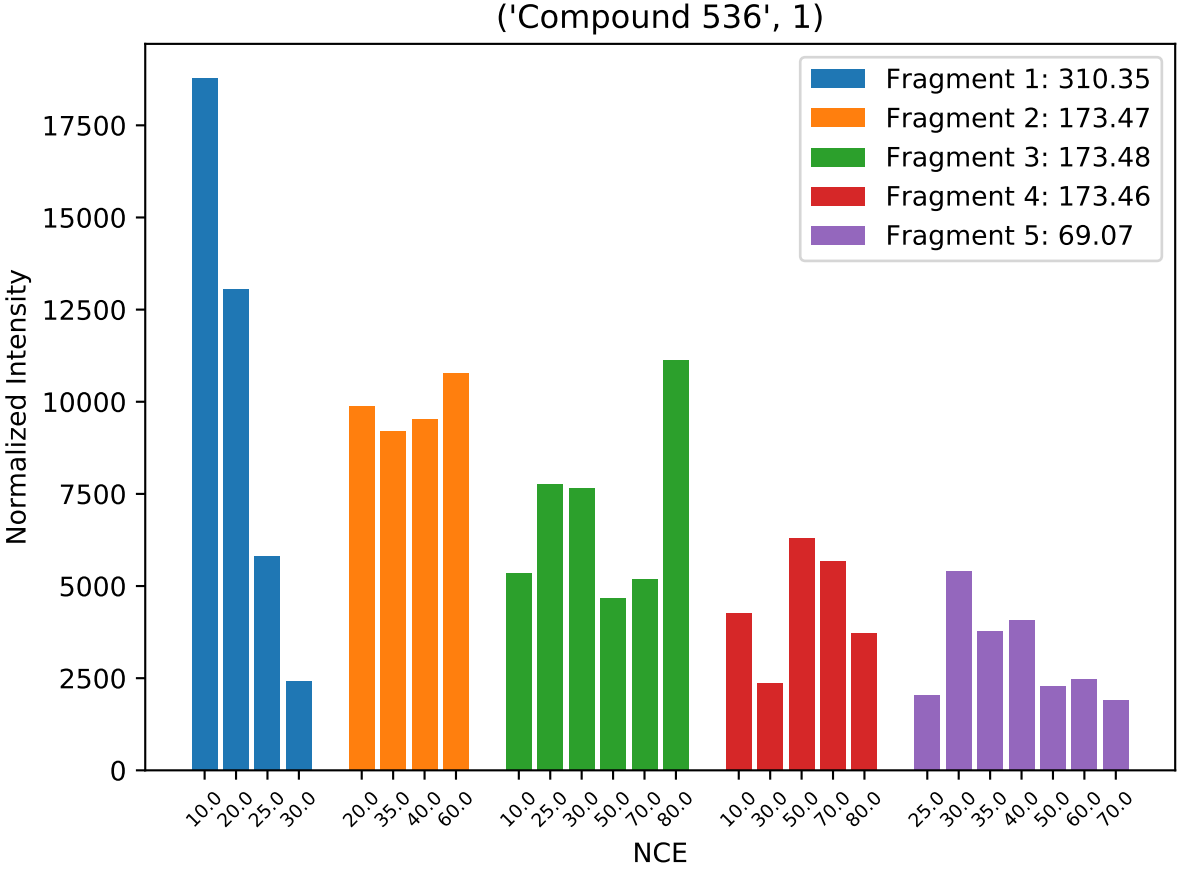

('Compound 20', 1)
Fragment 1: 85.03
Fragment 2: 145.05
Fragment 3: 60.08
Fragment 4: 58.07
Fragment 5: 57.03
Normalized Intensity
0
1000000
2000000
3000000
4000000
5000000
6000000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

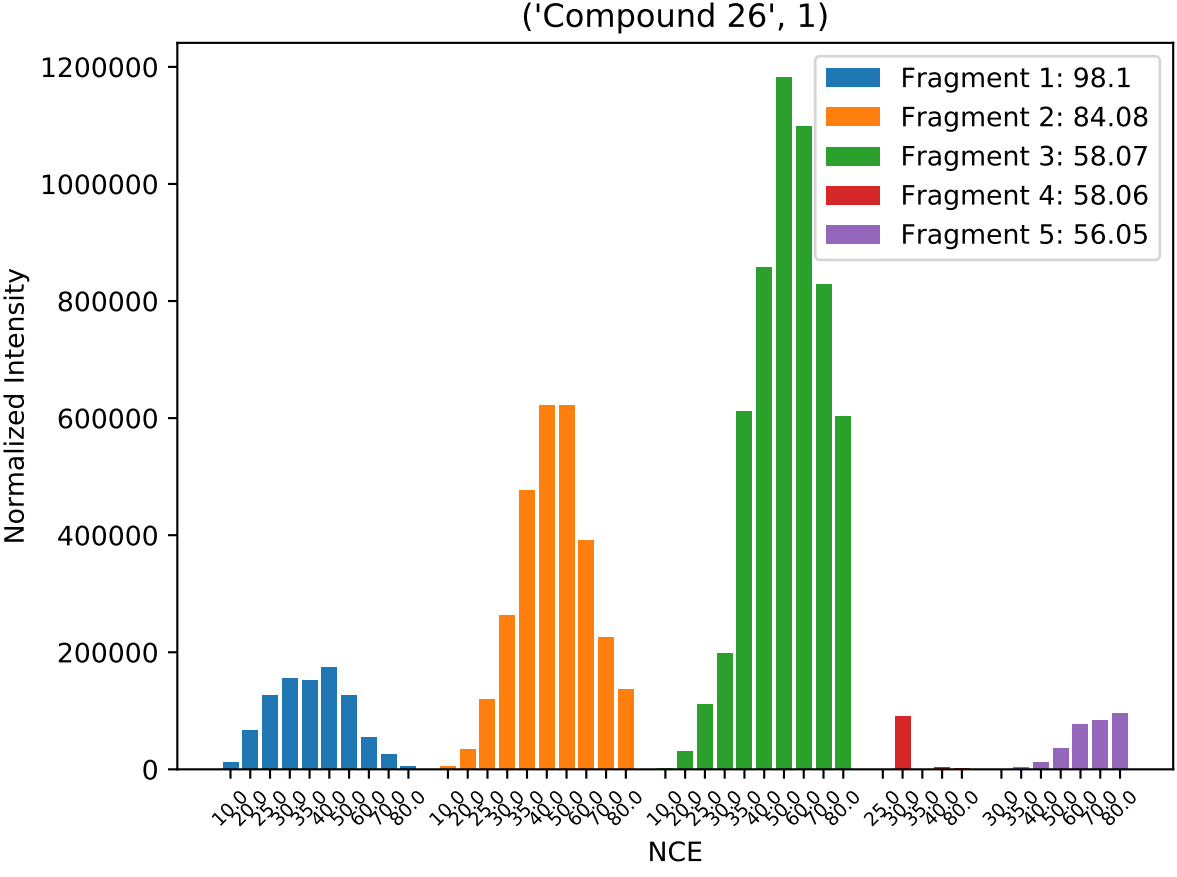

('Compound 532', 1)
Fragment 1: 173.47
Fragment 2: 255.03
Fragment 3: 173.46
Fragment 4: 225.01
Fragment 5: 281.0
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
20.0
25.0
30.0
35.0
50.0
60.0
20.0
25.0
30.0
35.0
10.0
40.0
70.0
80.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
NCE

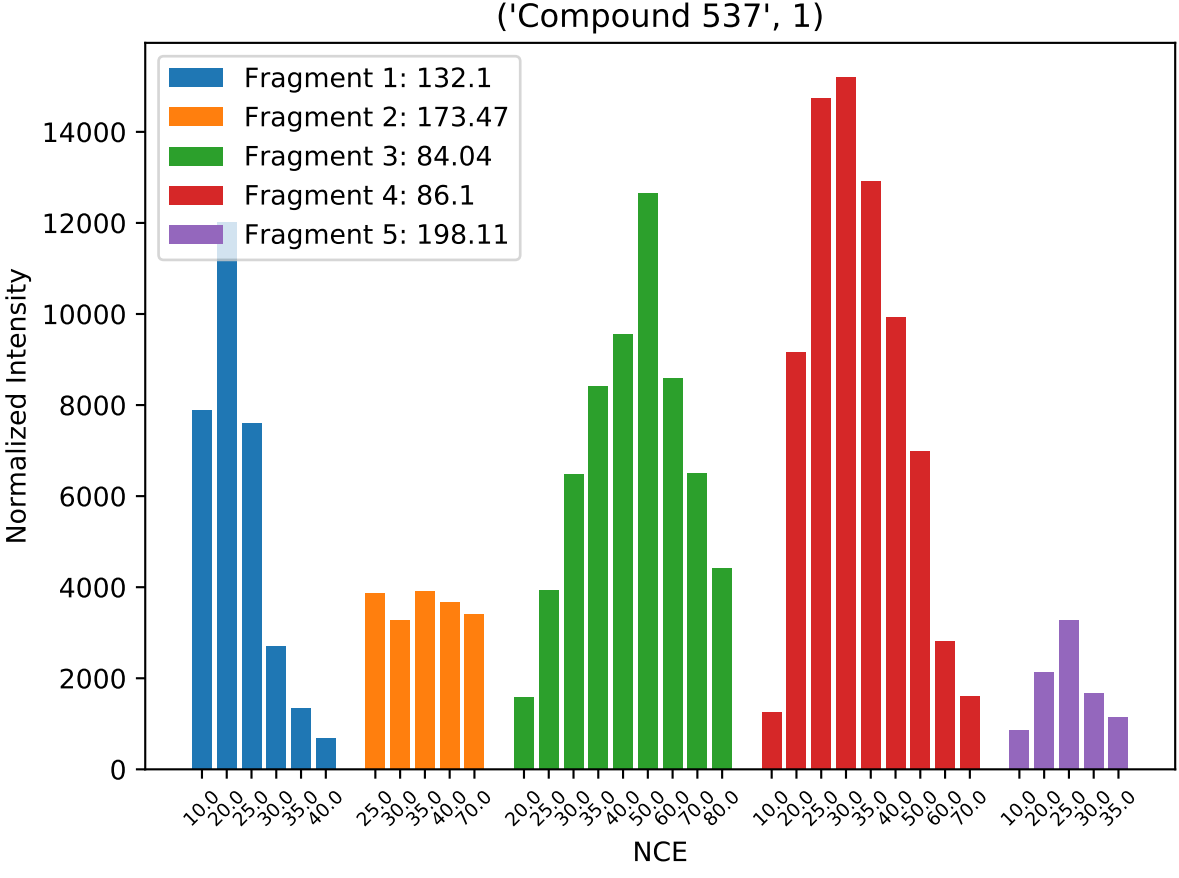

('Compound 22', 1)
Fragment 1: 62.98
Fragment 2: 62.99
Fragment 3: 61.98
Fragment 4: 102.48
Fragment 5: 61.97
Normalized Intensity
800000
700000
600000
500000
400000
300000
200000
100000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
50.0 60.0
25.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

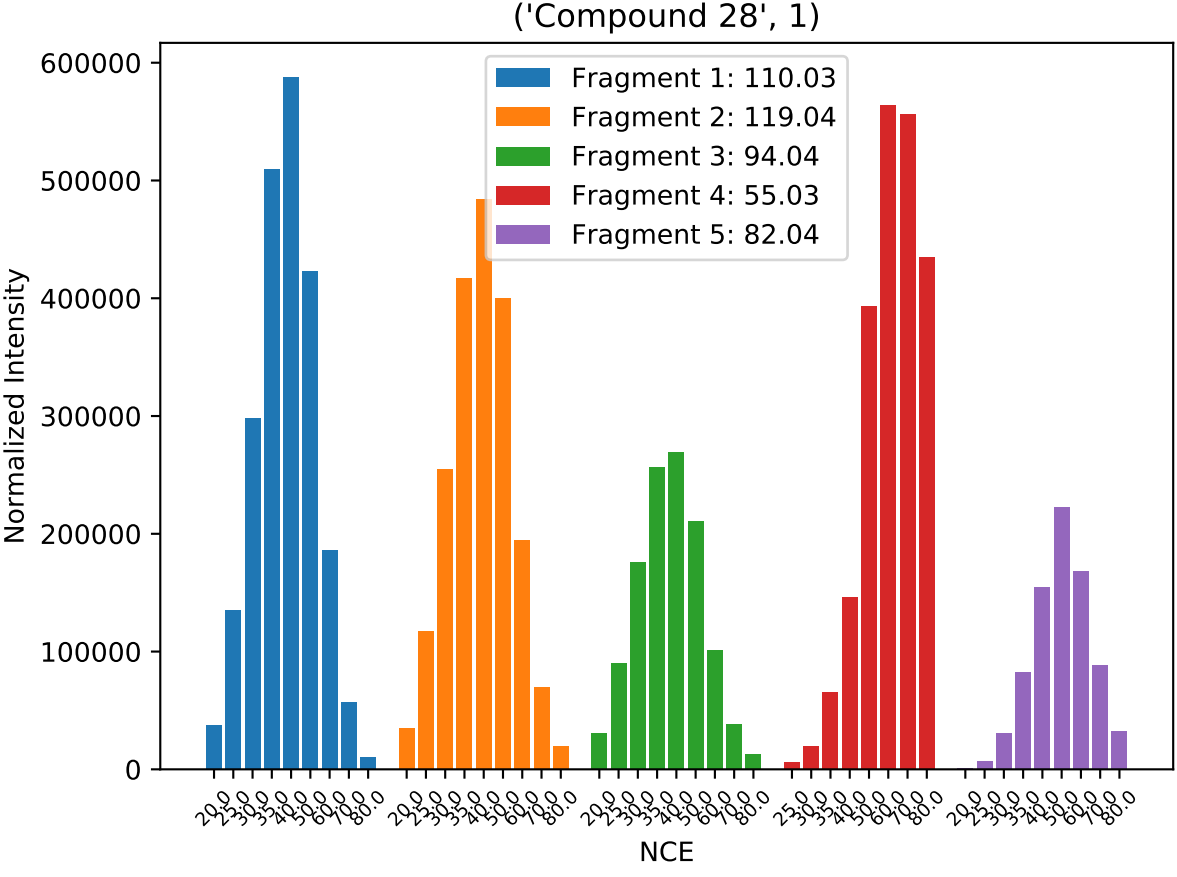

('Compound 533', 1)
Fragment 1: 60.06
Fragment 2: 65.01
Fragment 3: 55.39
Fragment 4: 61.63
Fragment 5: 91.07
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
30.0
40.0
70.0
NCE

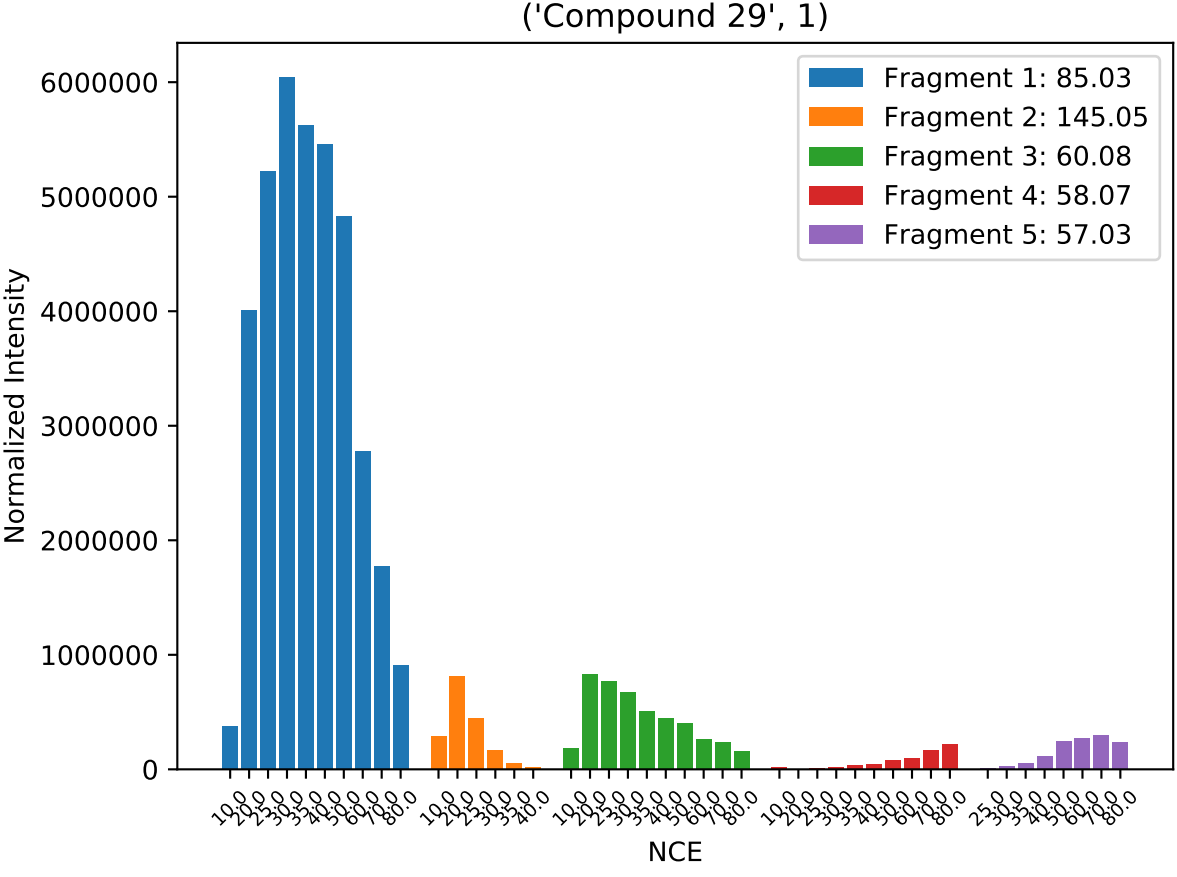

('Compound 535', 1)
Fragment 1: 341.18
Fragment 2: 173.47
Fragment 3: 103.04
Fragment 4: 133.09
Fragment 5: 89.06
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
10.0
20.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

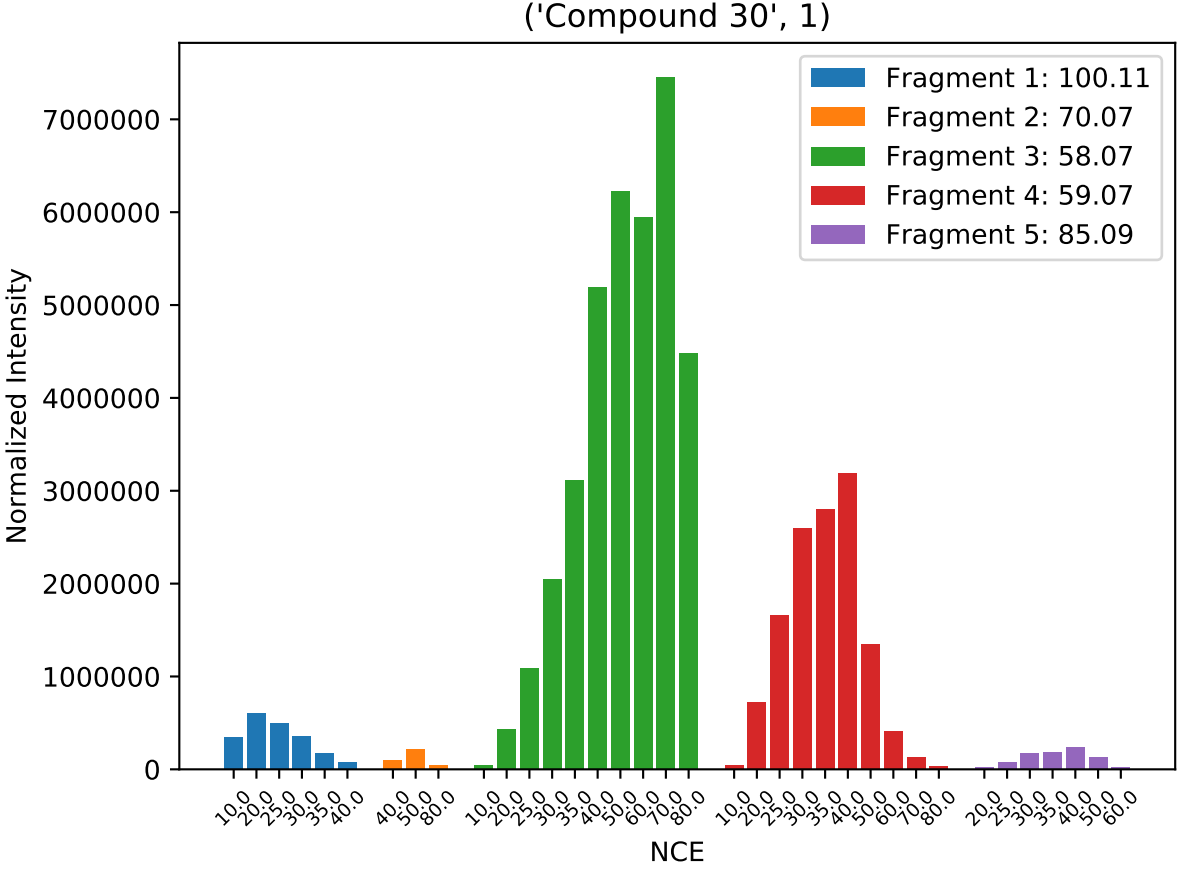

('Compound 536', 1)
Fragment 1: 310.35
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 69.07
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0
20.0
25.0
30.0
20.0
35.0
40.0
60.0
10.0
25.0
30.0
50.0
70.0
80.0
10.0
30.0
50.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

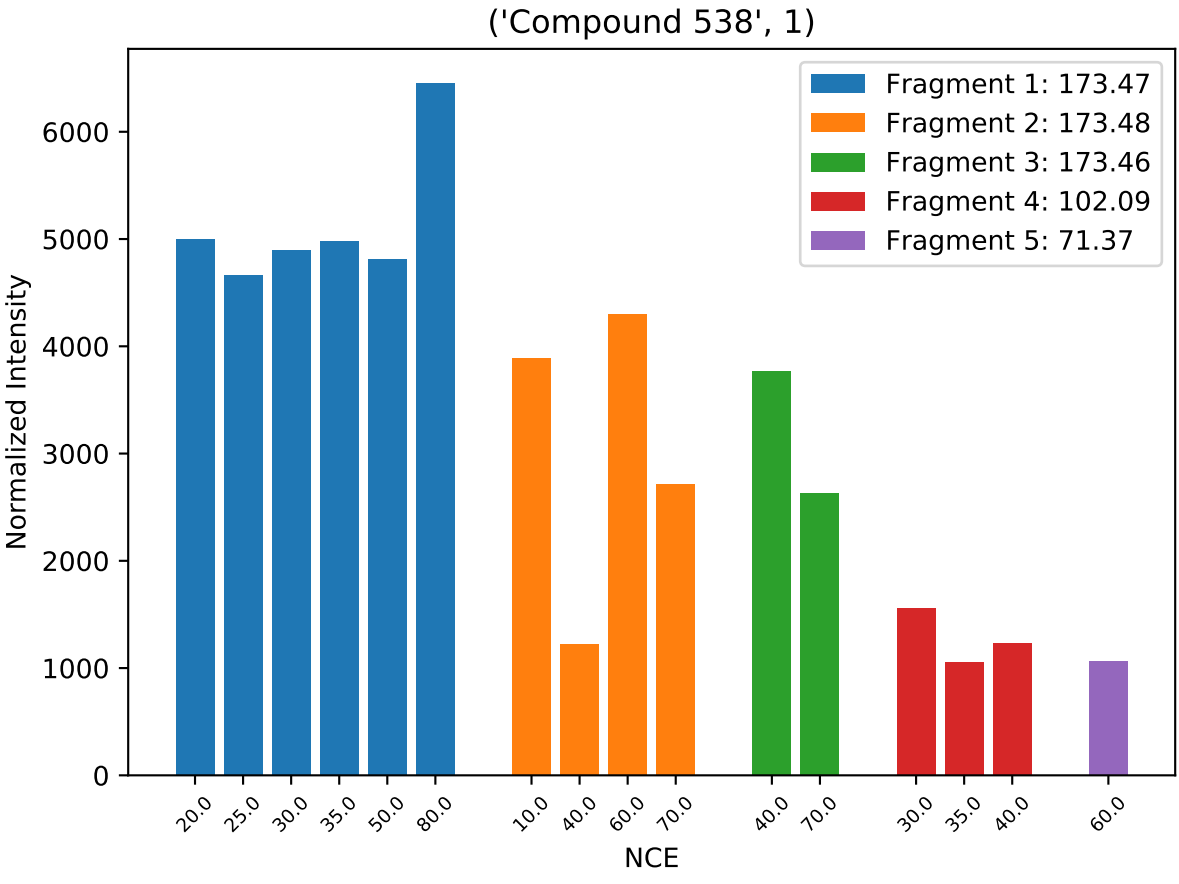

('Compound 26', 1)
Fragment 1: 98.1
Fragment 2: 84.08
Fragment 3: 58.07
Fragment 4: 58.06
Fragment 5: 56.05
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

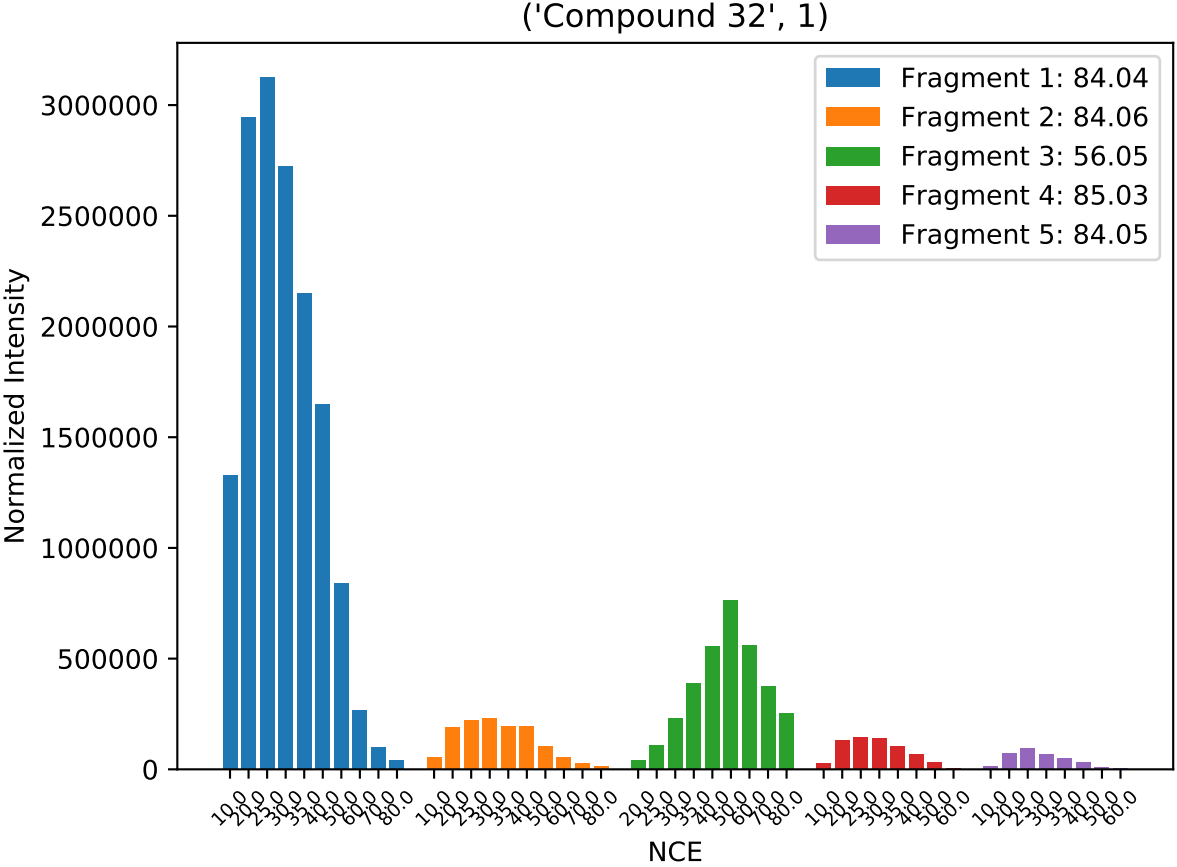

('Compound 537', 1)
Fragment 1: 132.1
Fragment 2: 173.47
Fragment 3: 84.04
Fragment 4: 86.1
Fragment 5: 198.11
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0 20.0 25.0 30.0 35.0 40.0
25.0 30.0 35.0 40.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0
NCE

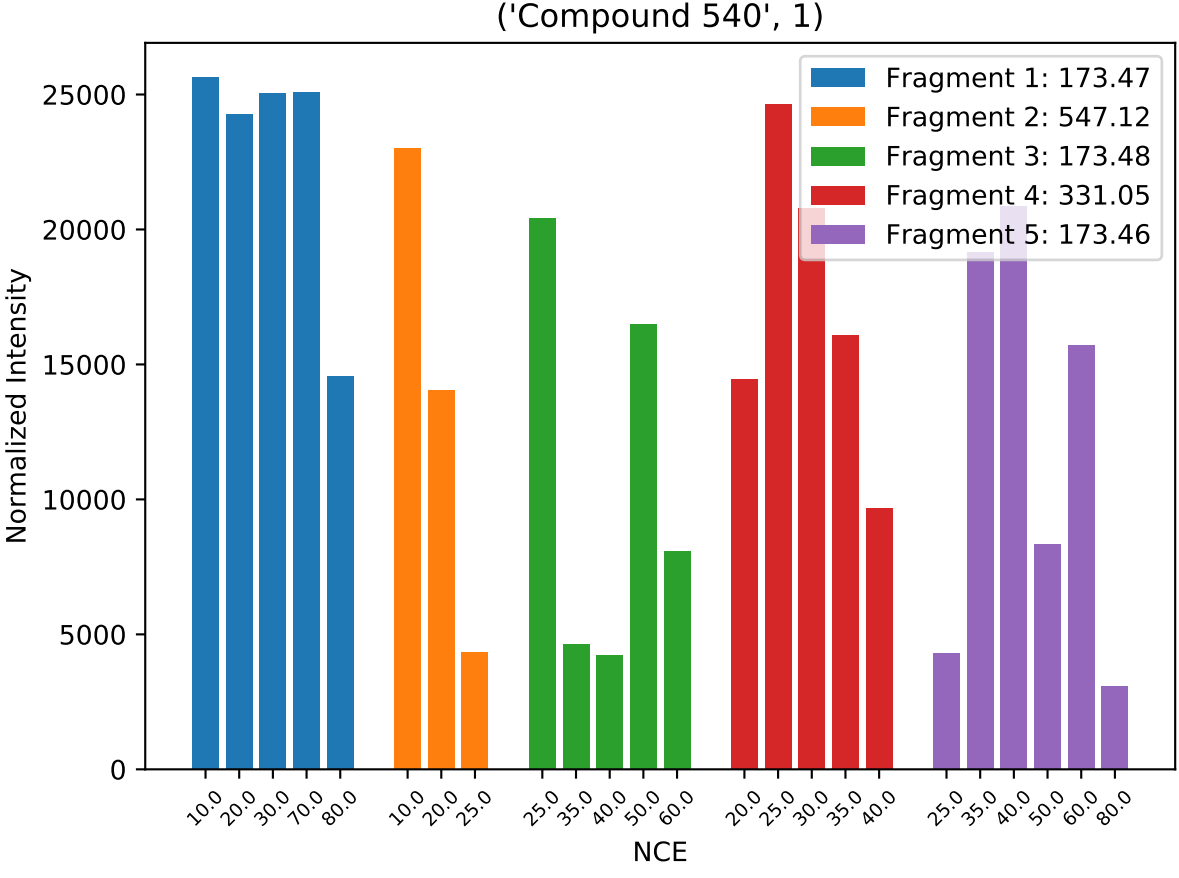

('Compound 28', 1)
Fragment 1: 110.03
Fragment 2: 119.04
Fragment 3: 94.04
Fragment 4: 55.03
Fragment 5: 82.04
Normalized Intensity
600000
500000
400000
300000
200000
100000
0
NCE
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

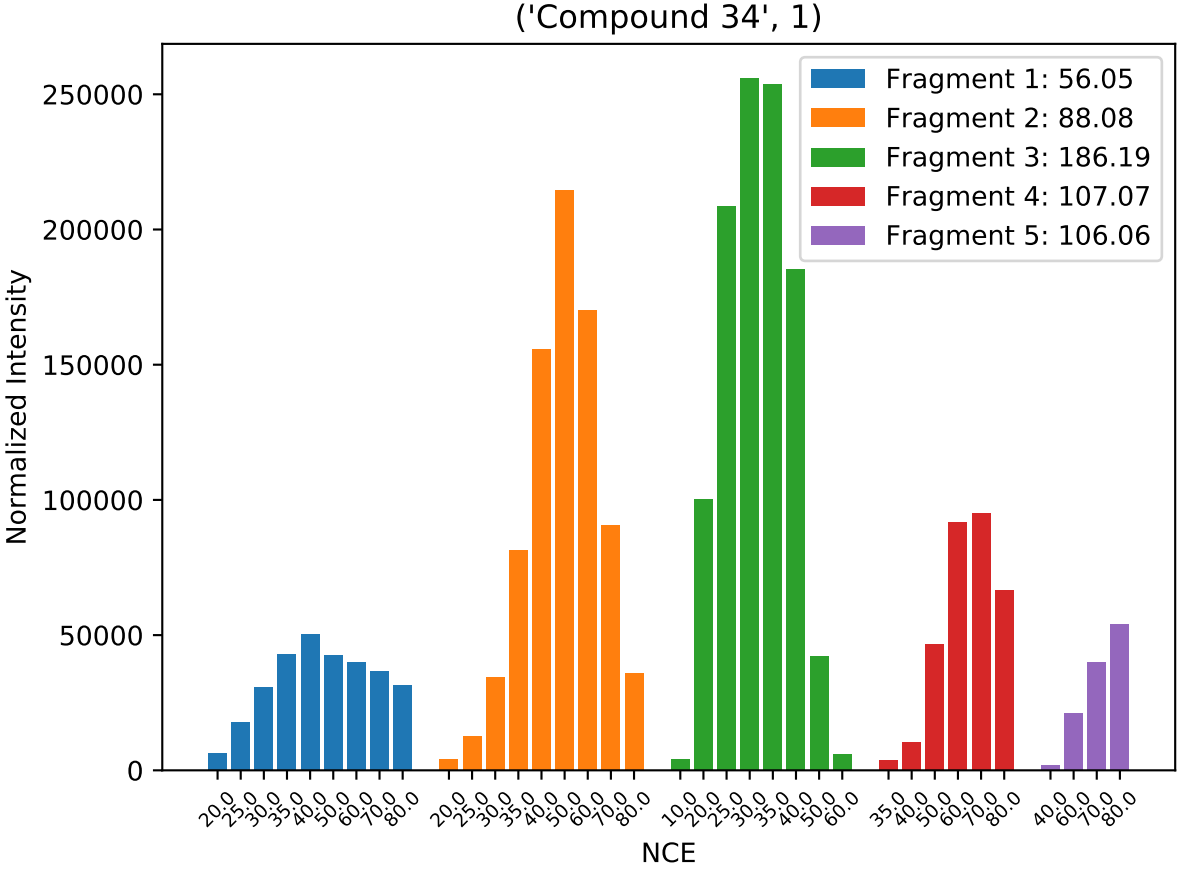

('Compound 29', 1)
Fragment 1: 85.03
Fragment 2: 145.05
Fragment 3: 60.08
Fragment 4: 58.07
Fragment 5: 57.03
Normalized Intensity
6000000
5000000
4000000
3000000
2000000
1000000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

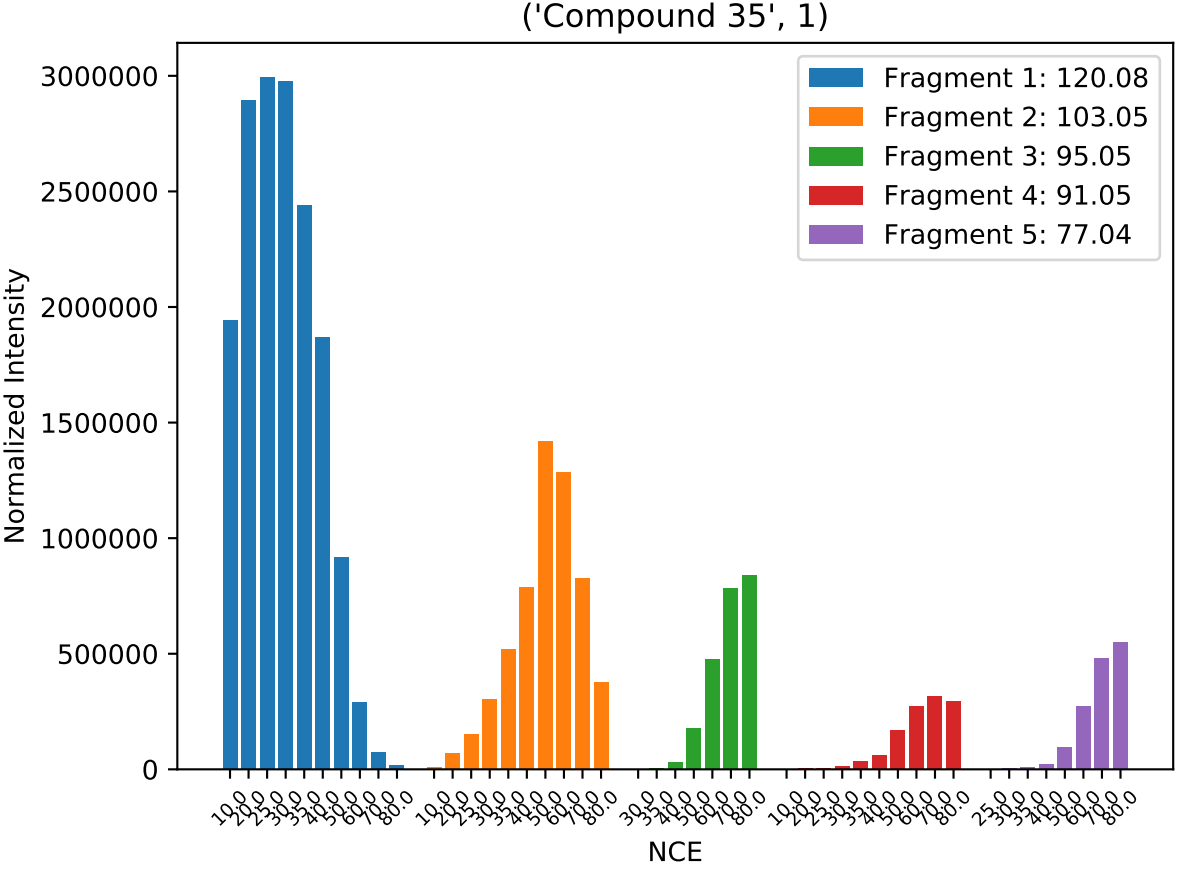

('Compound 30', 1)
Fragment 1: 100.11
Fragment 2: 70.07
Fragment 3: 58.07
Fragment 4: 59.07
Fragment 5: 85.09
Normalized Intensity
0
1000000
2000000
3000000
4000000
5000000
6000000
7000000
10.0 20.0 25.0 30.0 35.0 40.0
40.0 50.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

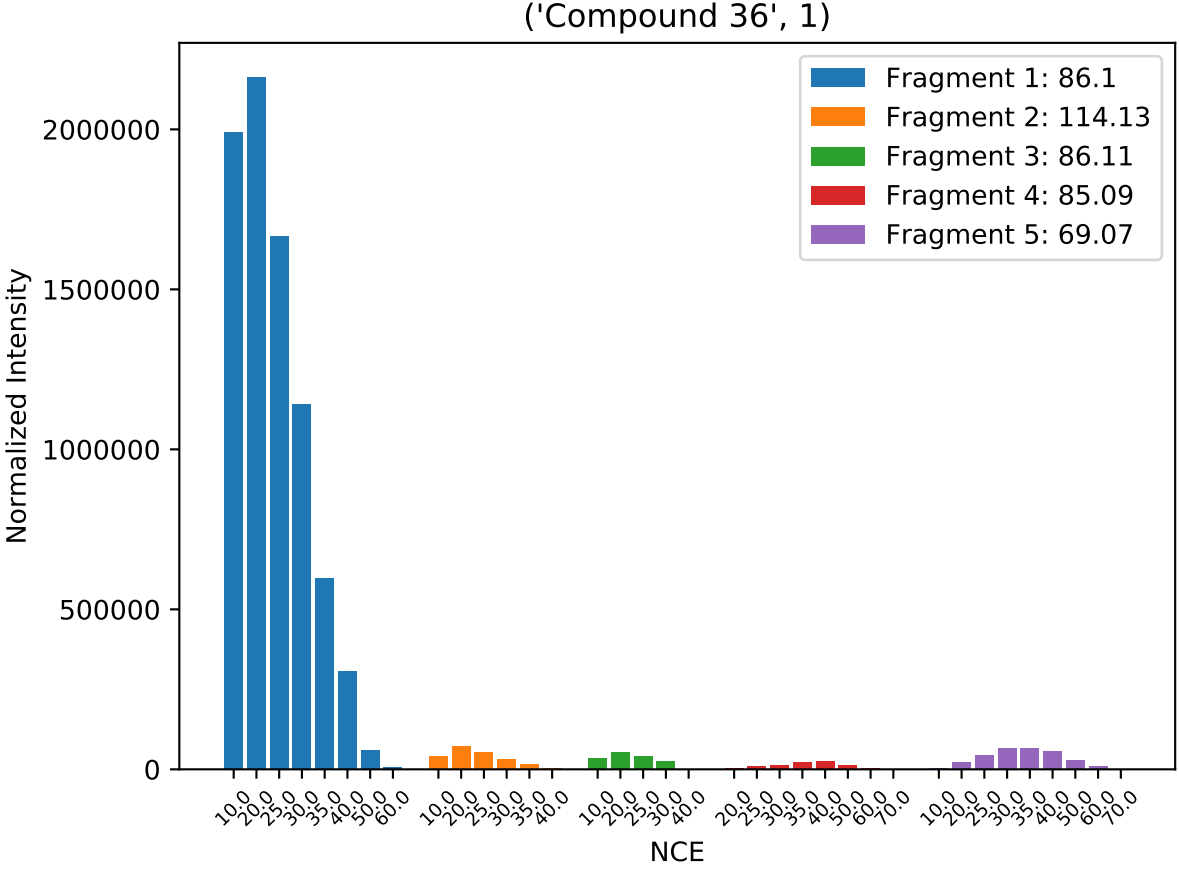

('Compound 538', 1)
Fragment 1: 173.47
Fragment 2: 173.48
Fragment 3: 173.46
Fragment 4: 102.09
Fragment 5: 71.37
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
20.0
25.0
30.0
35.0
50.0
80.0
10.0
40.0
60.0
70.0
40.0
70.0
30.0
35.0
40.0
60.0
NCE

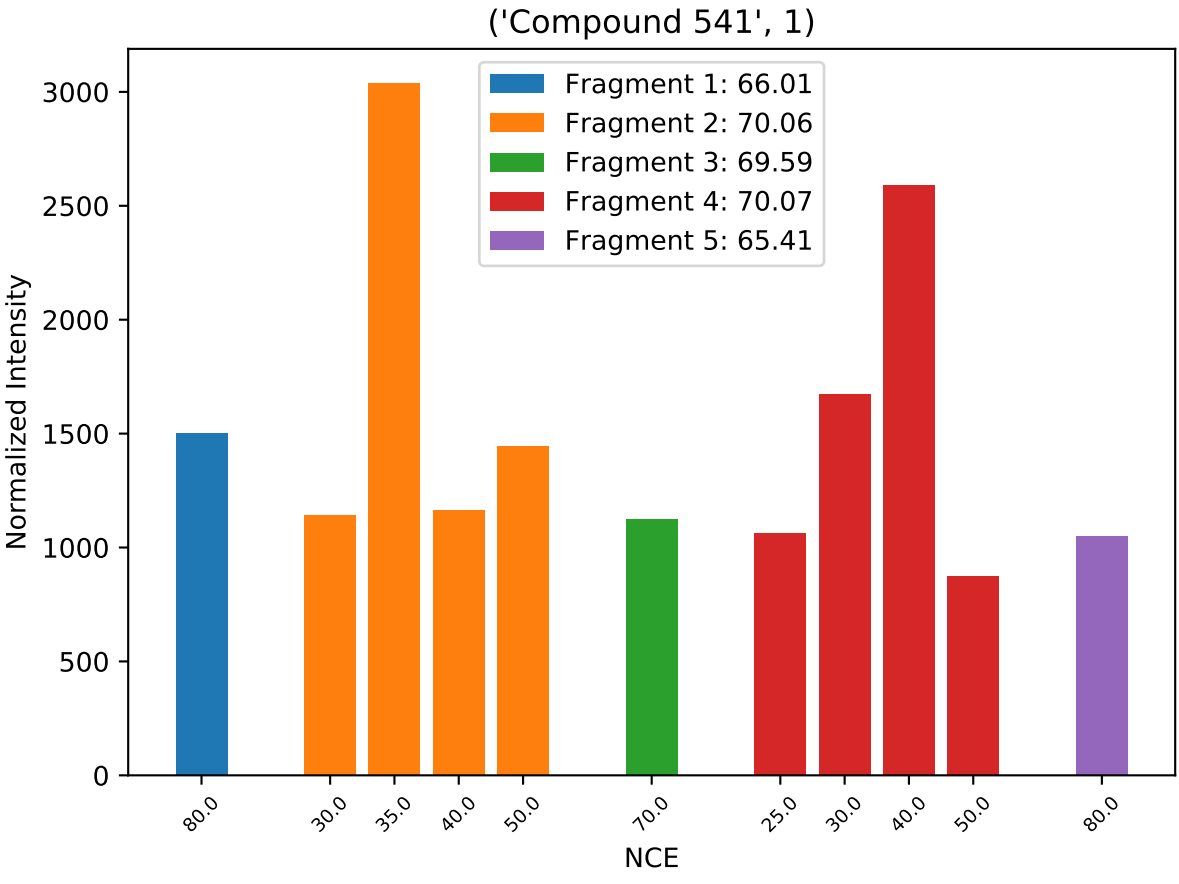

('Compound 32', 1)
Fragment 1: 84.04
Fragment 2: 84.06
Fragment 3: 56.05
Fragment 4: 85.03
Fragment 5: 84.05
Normalized Intensity
3000000
2500000
2000000
1500000
1000000
500000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0

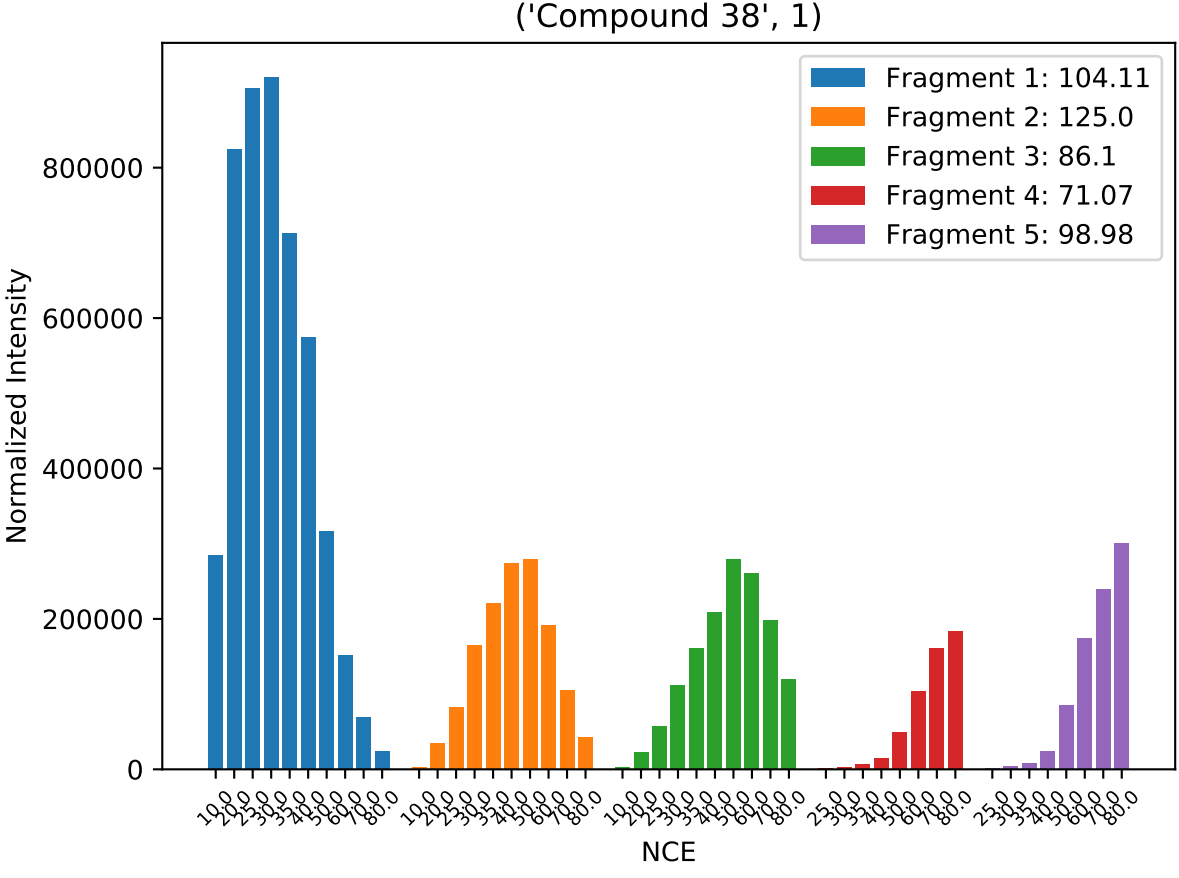

('Compound 540', 1)
Fragment 1: 173.47
Fragment 2: 547.12
Fragment 3: 173.48
Fragment 4: 331.05
Fragment 5: 173.46
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0
20.0
30.0
70.0
80.0
10.0
20.0
25.0
25.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
25.0
35.0
40.0
50.0
60.0
80.0
NCE

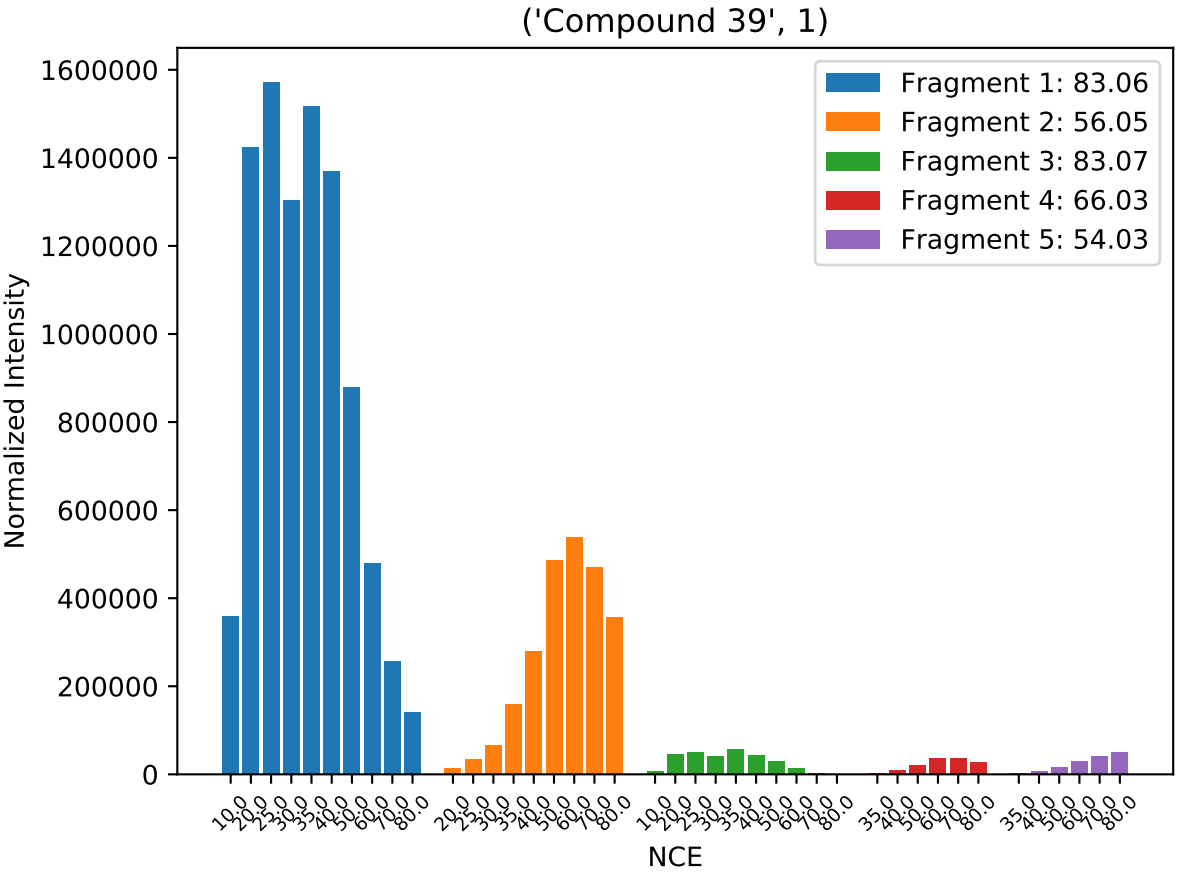

('Compound 34', 1)
Fragment 1: 56.05
Fragment 2: 88.08
Fragment 3: 186.19
Fragment 4: 107.07
Fragment 5: 106.06
Normalized Intensity
0
50000
100000
150000
200000
250000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
35.0 40.0 50.0 60.0 70.0 80.0
40.0 60.0 70.0 80.0

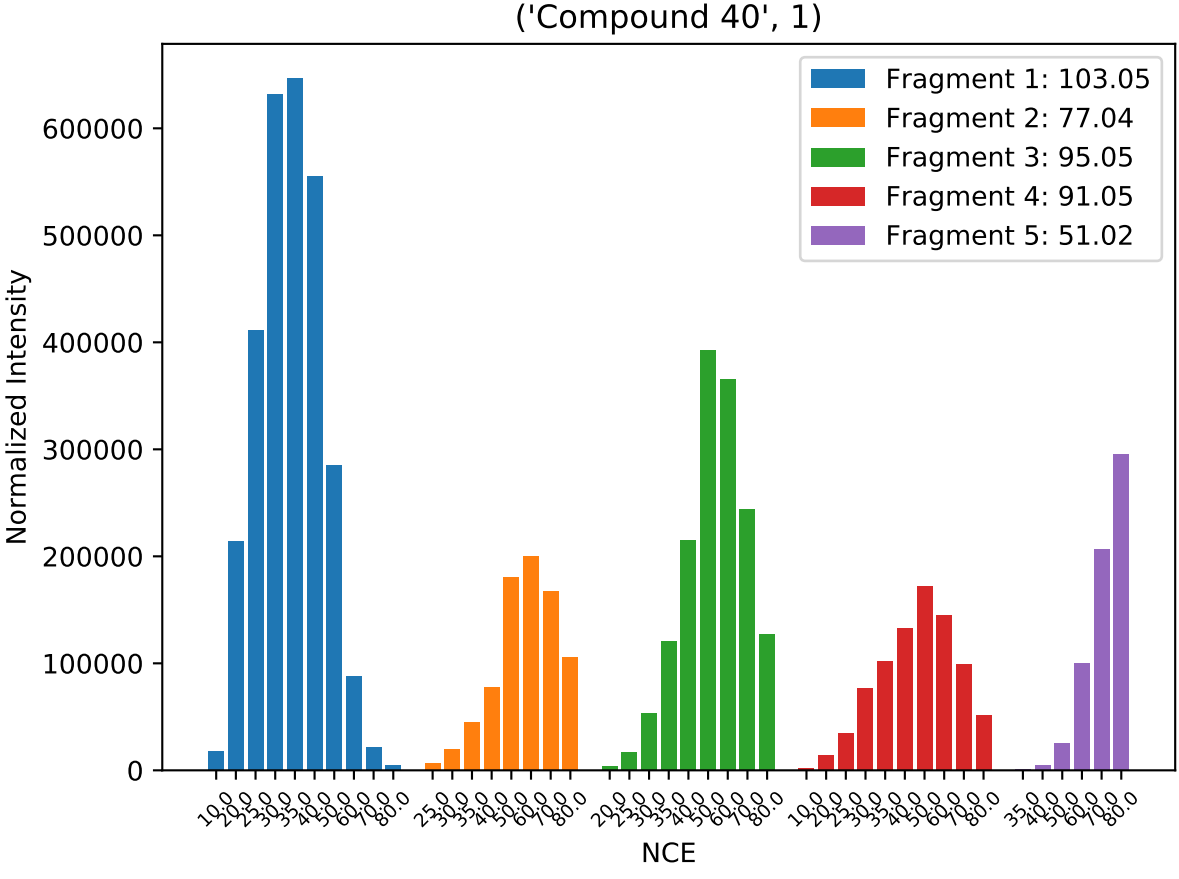

('Compound 35', 1)
Fragment 1: 120.08
Fragment 2: 103.05
Fragment 3: 95.05
Fragment 4: 91.05
Fragment 5: 77.04
Normalized Intensity
3000000
2500000
2000000
1500000
1000000
500000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

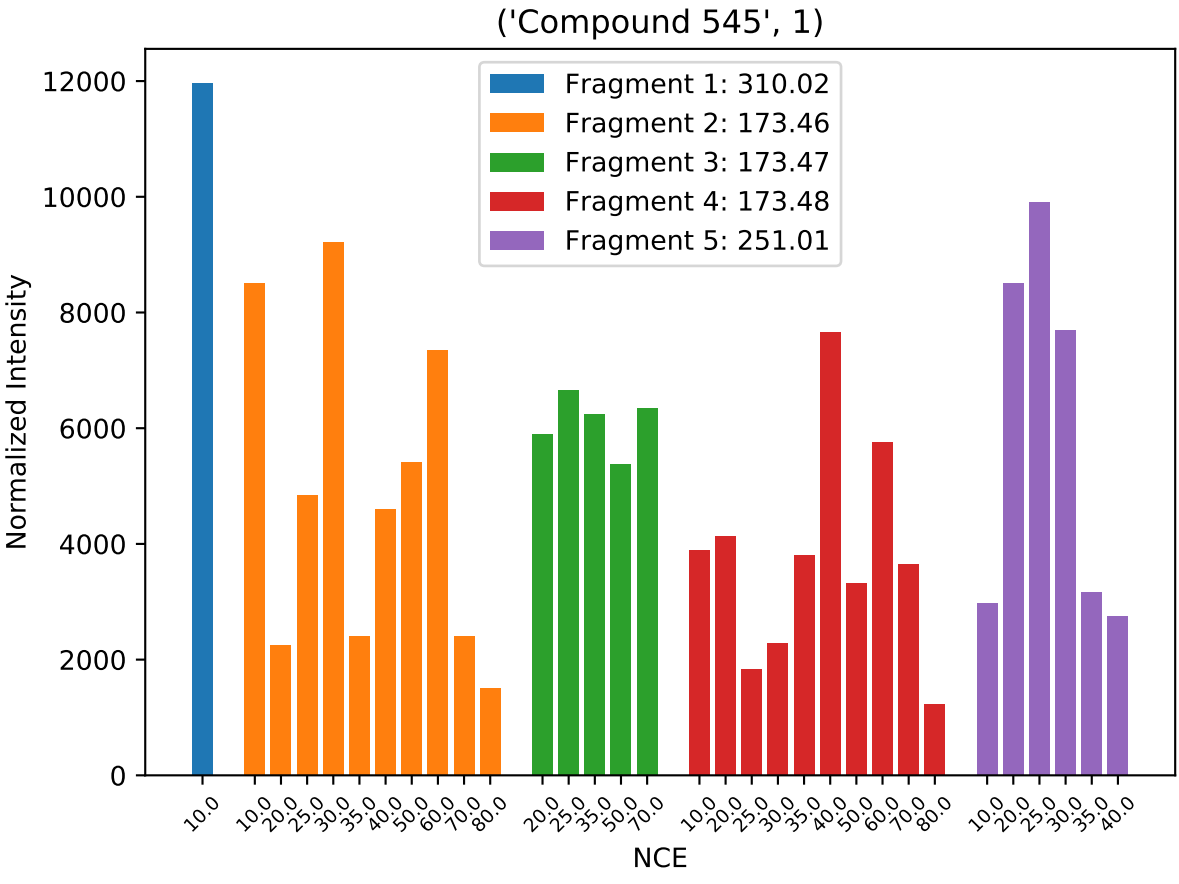

('Compound 36', 1)
Fragment 1: 86.1
Fragment 2: 114.13
Fragment 3: 86.11
Fragment 4: 85.09
Fragment 5: 69.07
Normalized Intensity
2000000
1500000
1000000
500000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

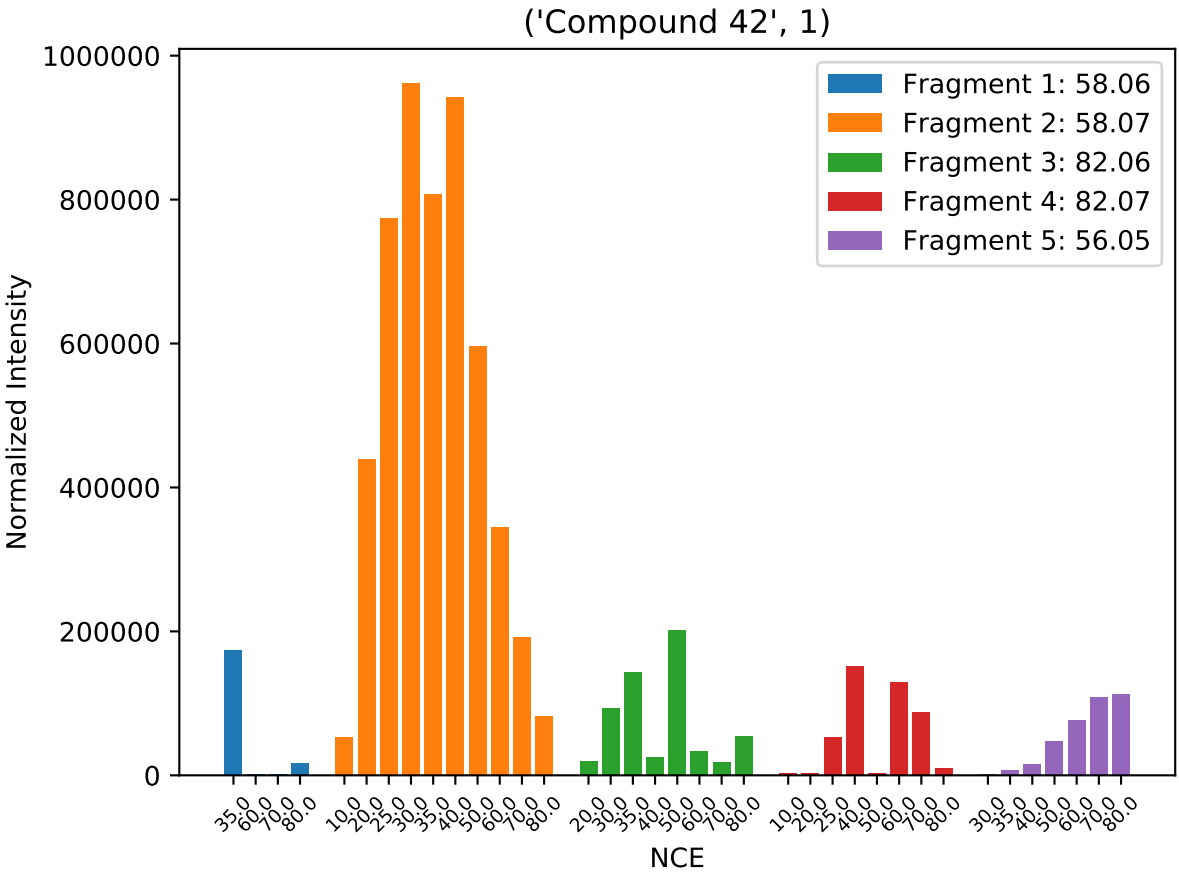

('Compound 541', 1)
Fragment 1: 66.01
Fragment 2: 70.06
Fragment 3: 69.59
Fragment 4: 70.07
Fragment 5: 65.41
Normalized Intensity
0
500
1000
1500
2000
2500
3000
80.0
30.0
35.0
40.0
50.0
70.0
25.0
30.0
40.0
50.0
80.0
NCE

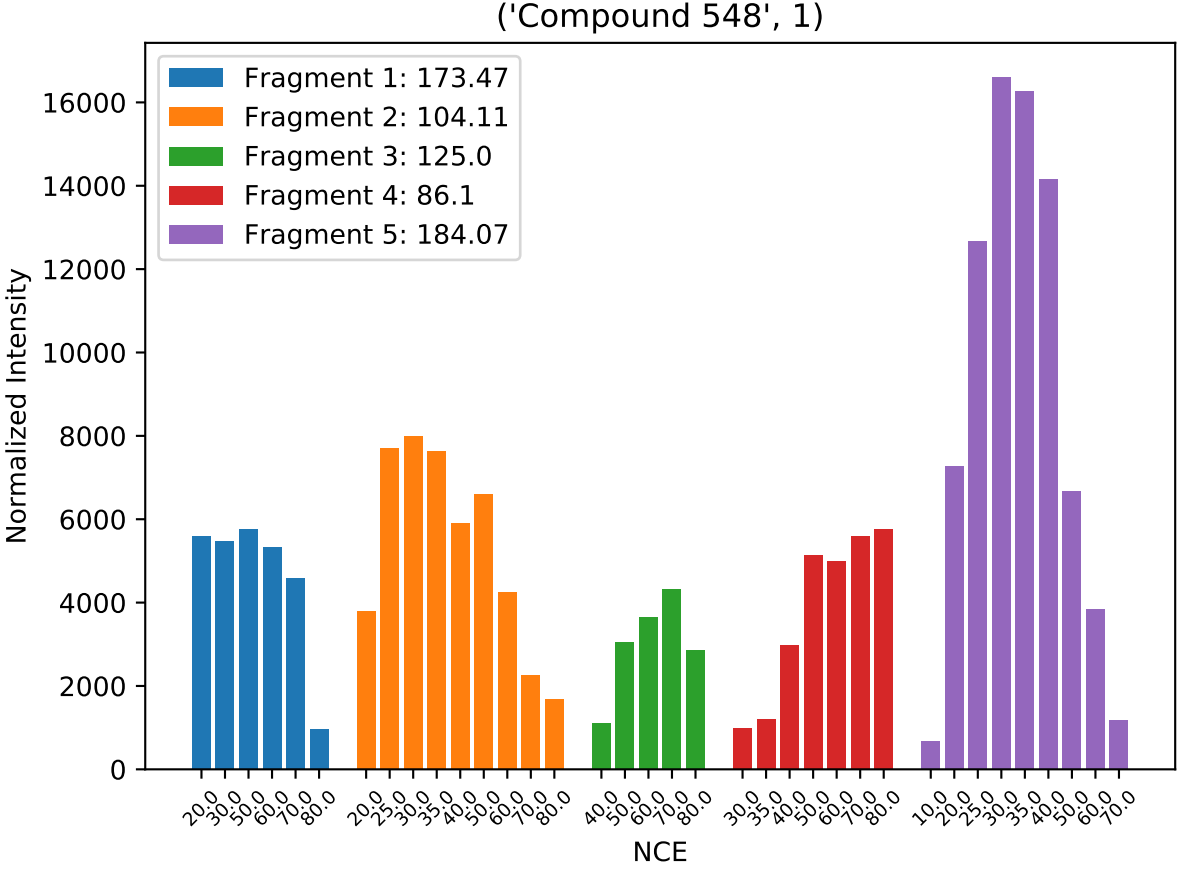

('Compound 38', 1)
Fragment 1: 104.11
Fragment 2: 125.0
Fragment 3: 86.1
Fragment 4: 71.07
Fragment 5: 98.98
Normalized Intensity
0
200000
400000
600000
800000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

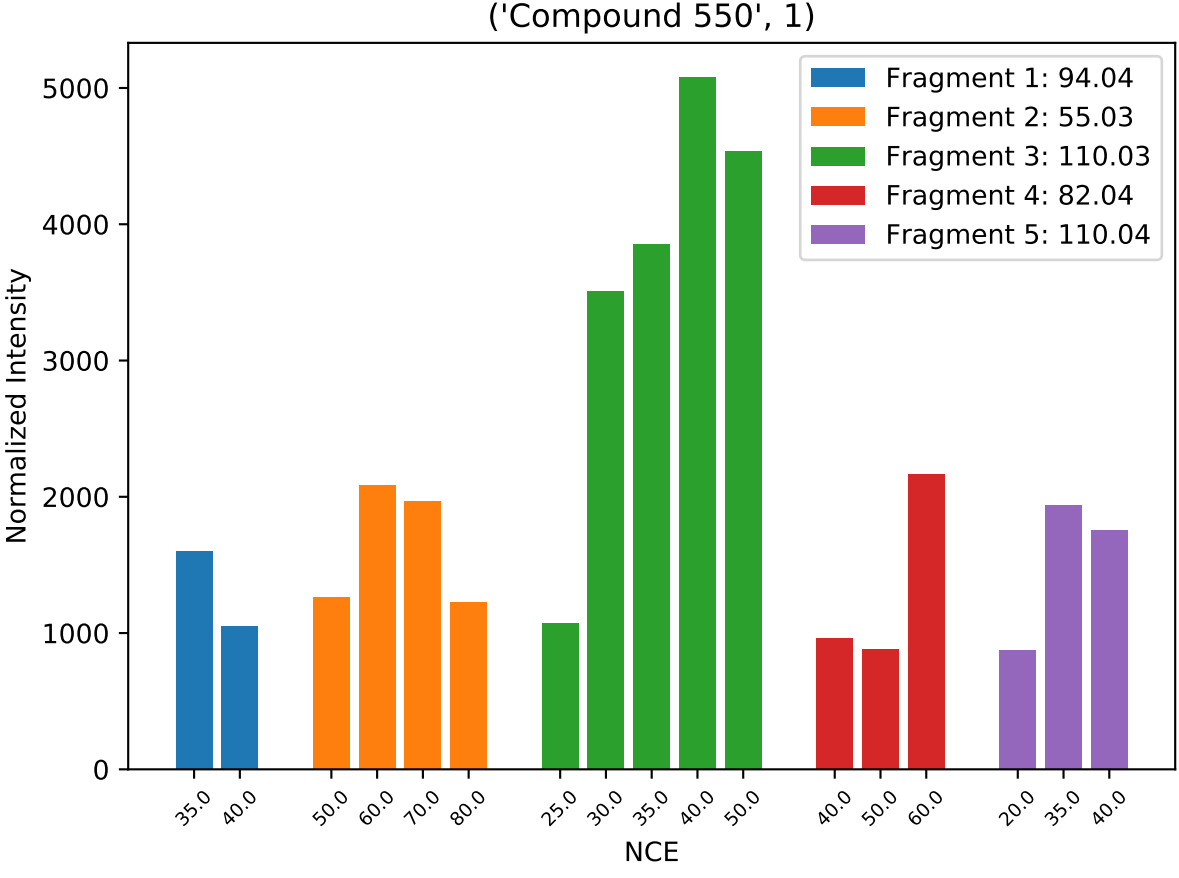

('Compound 39', 1)
Fragment 1: 83.06
Fragment 2: 56.05
Fragment 3: 83.07
Fragment 4: 66.03
Fragment 5: 54.03
Normalized Intensity
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0

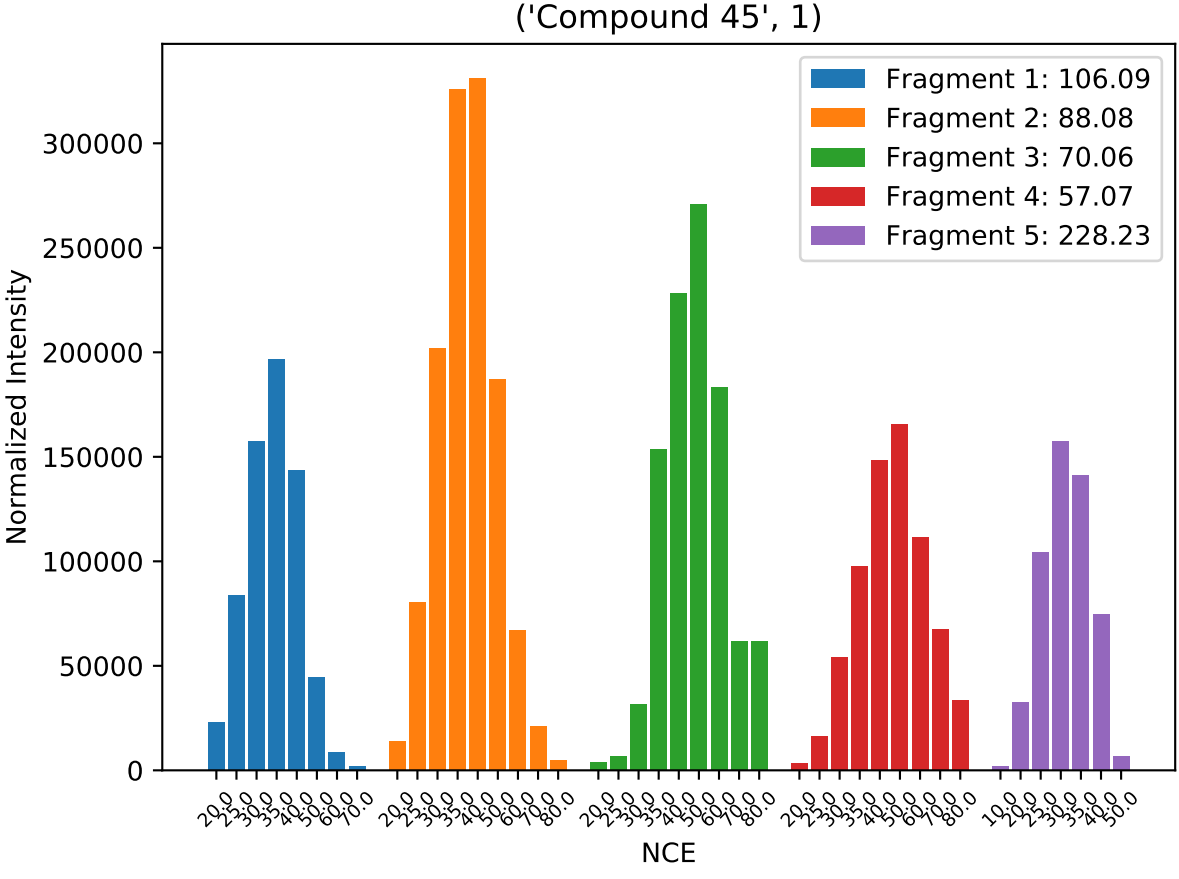

('Compound 40', 1)
Fragment 1: 103.05
Fragment 2: 77.04
Fragment 3: 95.05
Fragment 4: 91.05
Fragment 5: 51.02
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0

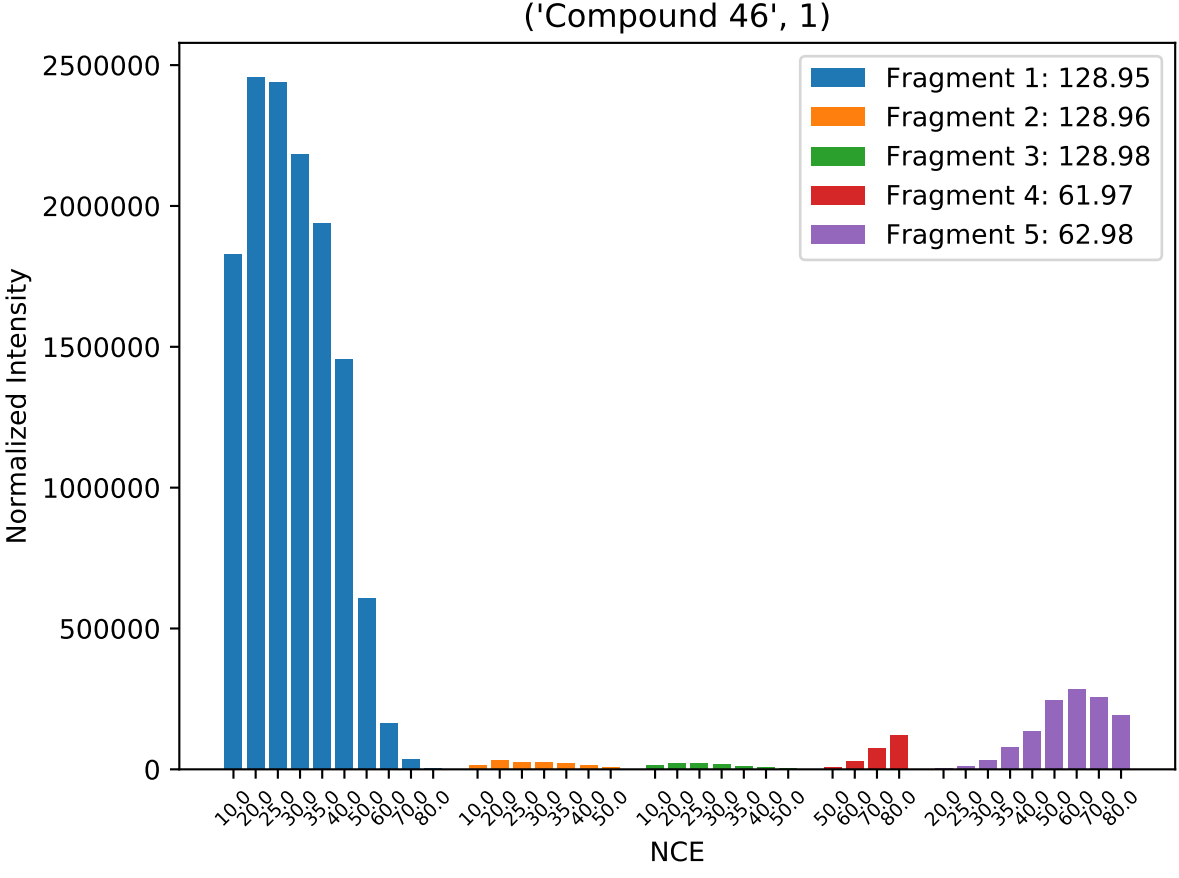

('Compound 545', 1)
Fragment 1: 310.02
Fragment 2: 173.46
Fragment 3: 173.47
Fragment 4: 173.48
Fragment 5: 251.01
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 35.0 50.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

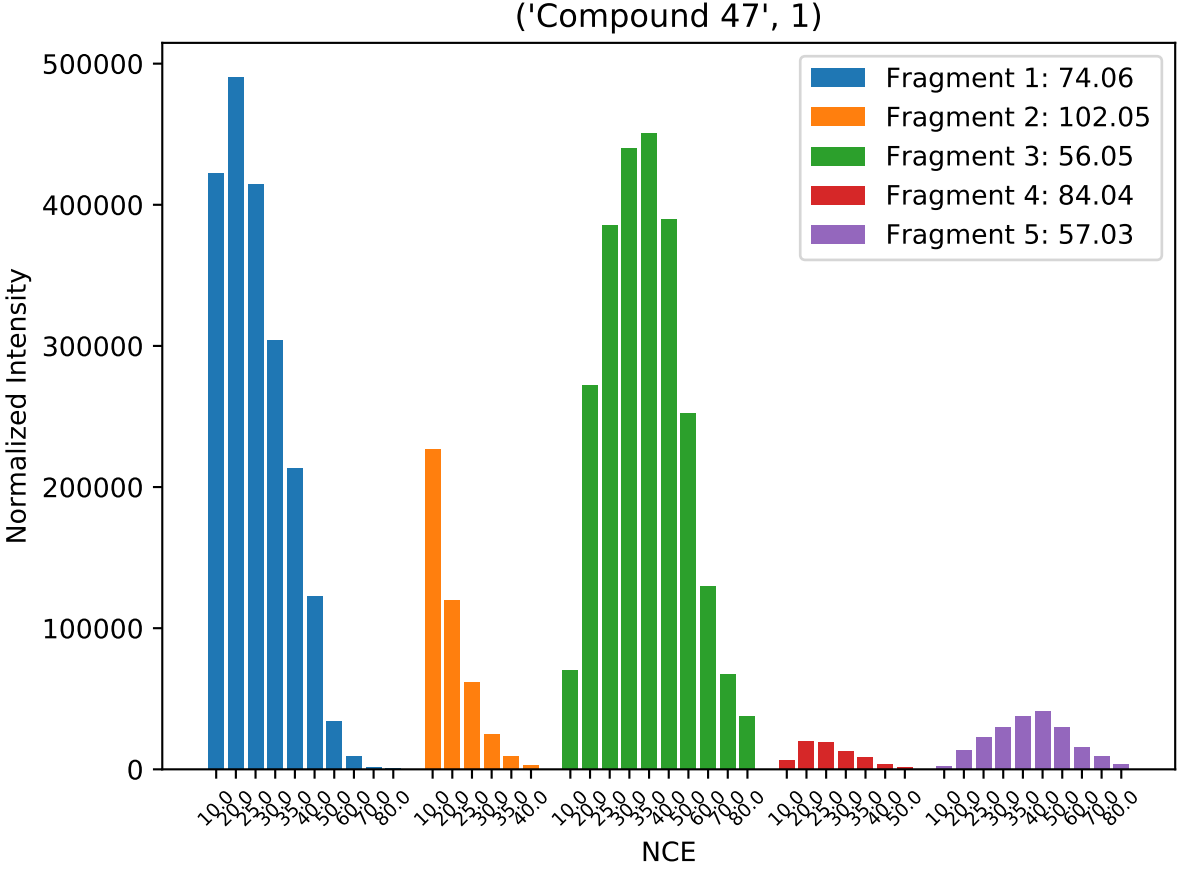

('Compound 42', 1)
Fragment 1: 58.06
Fragment 2: 58.07
Fragment 3: 82.06
Fragment 4: 82.07
Fragment 5: 56.05
Normalized Intensity
1000000
800000
600000
400000
200000
0
NCE
35.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

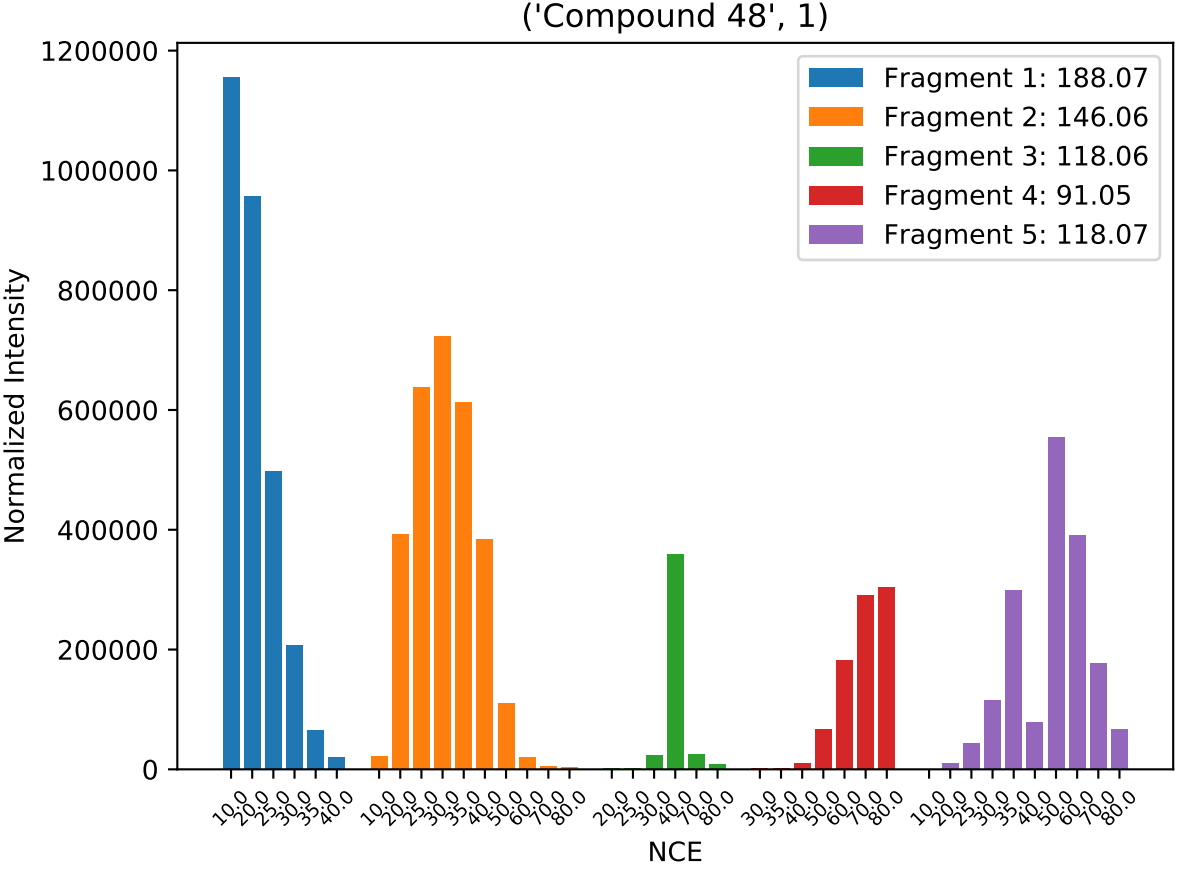

('Compound 548', 1)
Fragment 1: 173.47
Fragment 2: 104.11
Fragment 3: 125.0
Fragment 4: 86.1
Fragment 5: 184.07
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
20.0 30.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

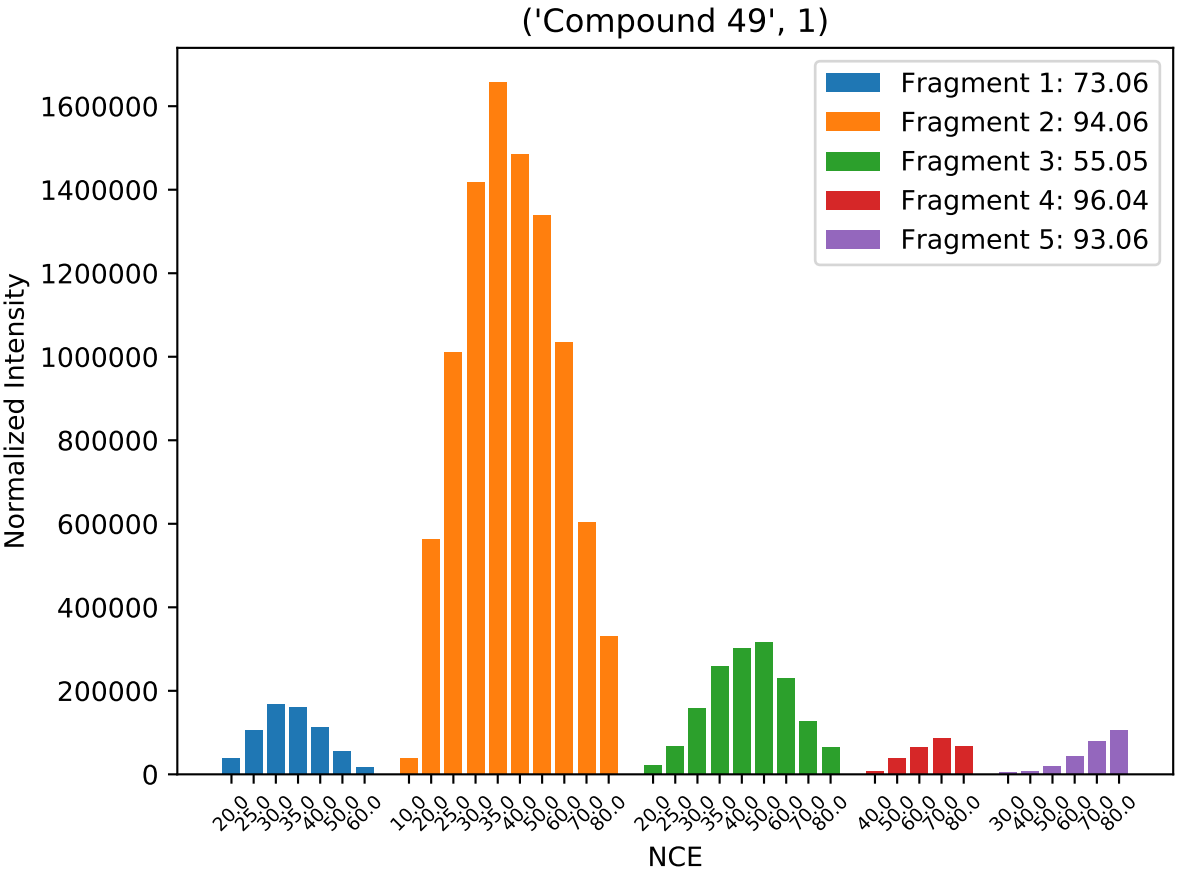

('Compound 550', 1)
Fragment 1: 94.04
Fragment 2: 55.03
Fragment 3: 110.03
Fragment 4: 82.04
Fragment 5: 110.04
Normalized Intensity
0
1000
2000
3000
4000
5000
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
40.0
50.0
60.0
20.0
35.0
40.0
NCE

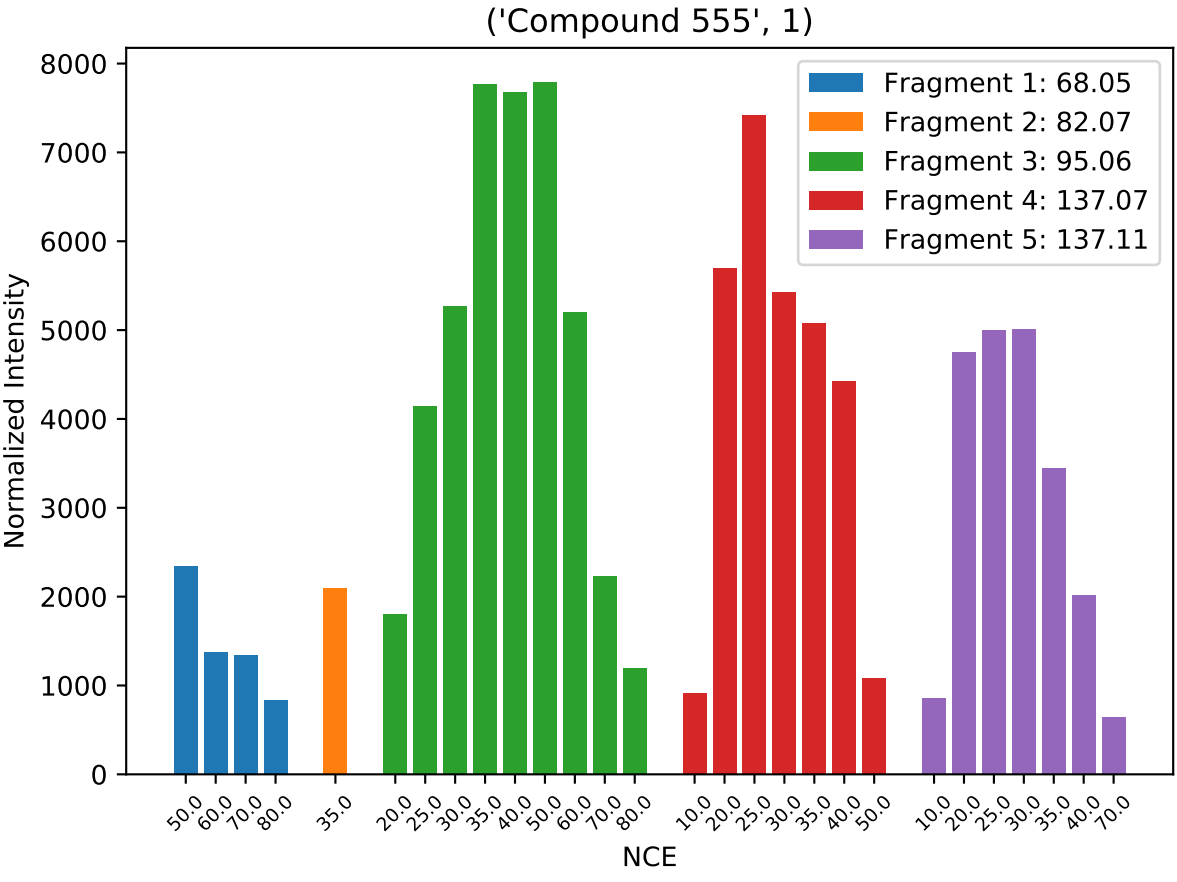

('Compound 45', 1)
Fragment 1: 106.09
Fragment 2: 88.08
Fragment 3: 70.06
Fragment 4: 57.07
Fragment 5: 228.23
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

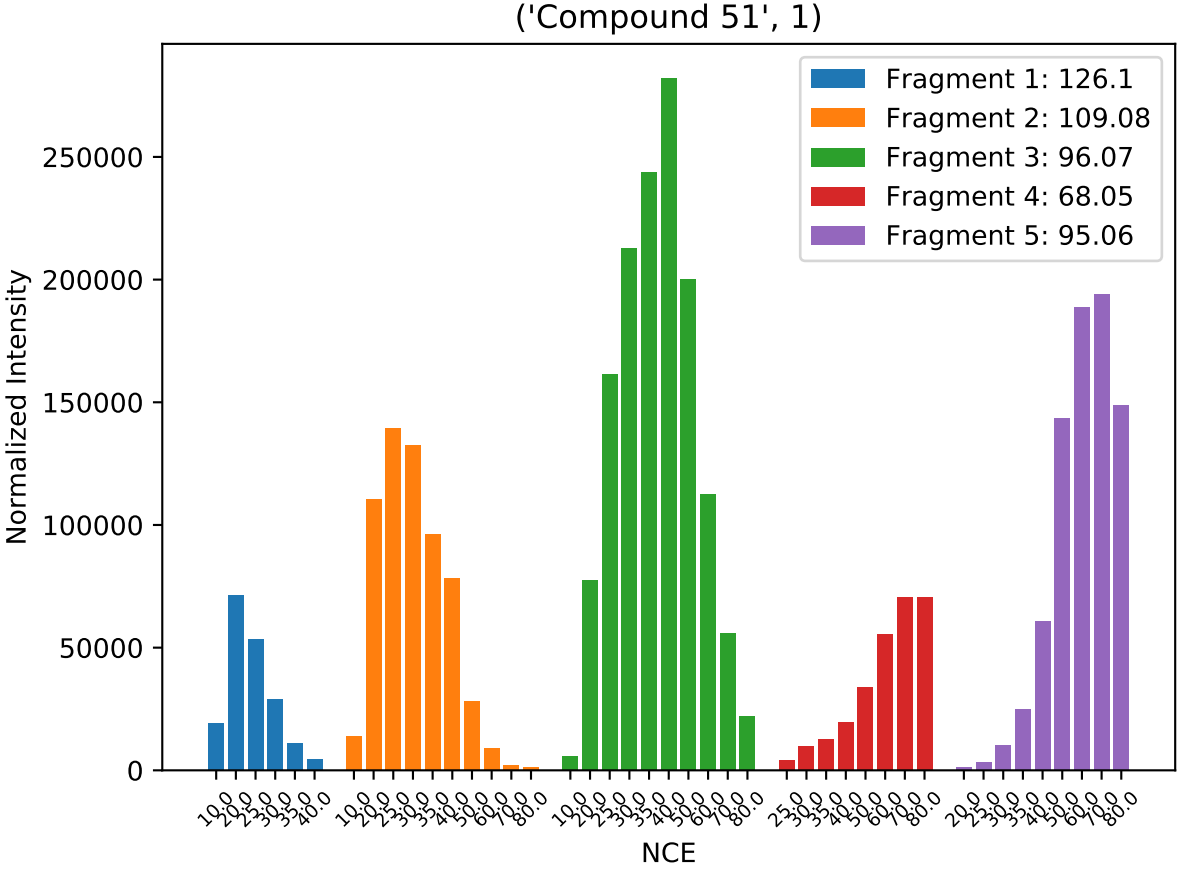

('Compound 46', 1)
Fragment 1: 128.95
Fragment 2: 128.96
Fragment 3: 128.98
Fragment 4: 61.97
Fragment 5: 62.98
Normalized Intensity
2500000
2000000
1500000
1000000
500000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

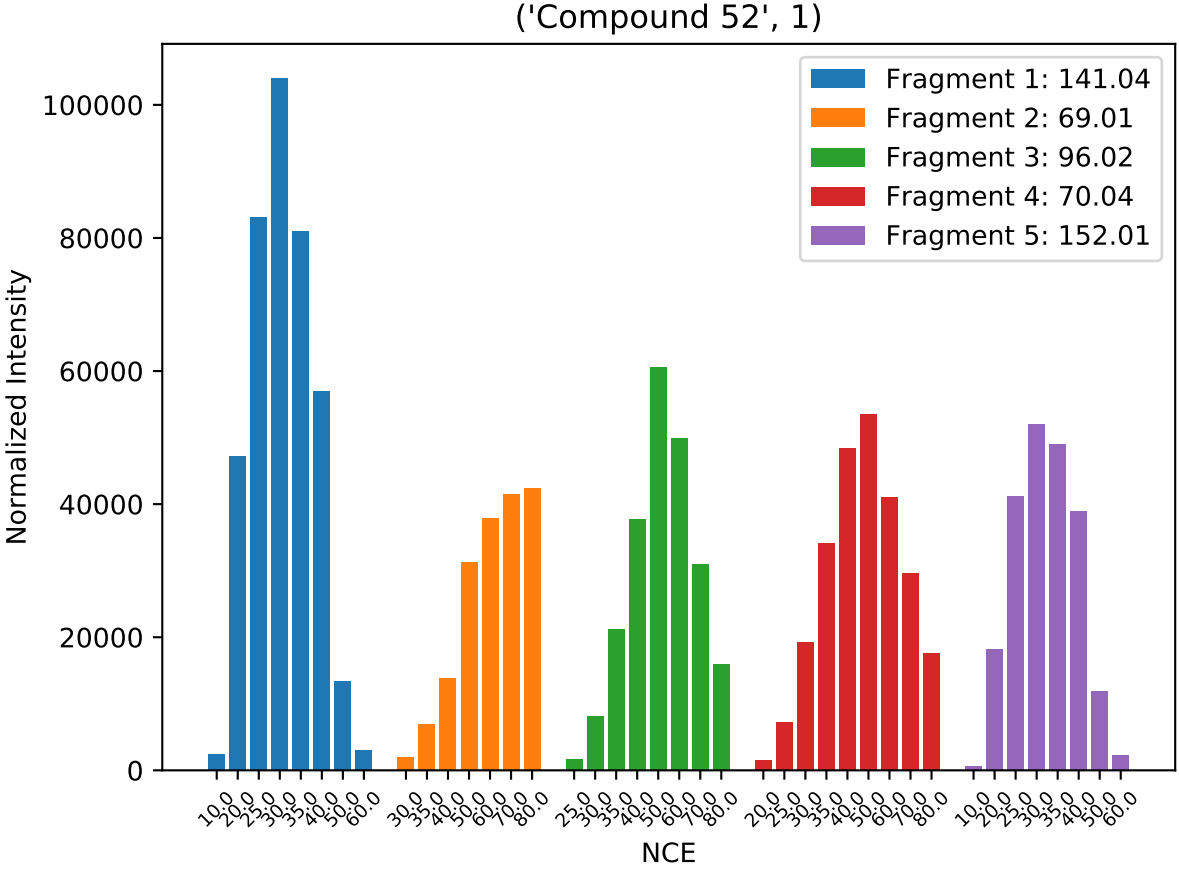

('Compound 47', 1)
Fragment 1: 74.06
Fragment 2: 102.05
Fragment 3: 56.05
Fragment 4: 84.04
Fragment 5: 57.03
Normalized Intensity
500000
400000
300000
200000
100000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

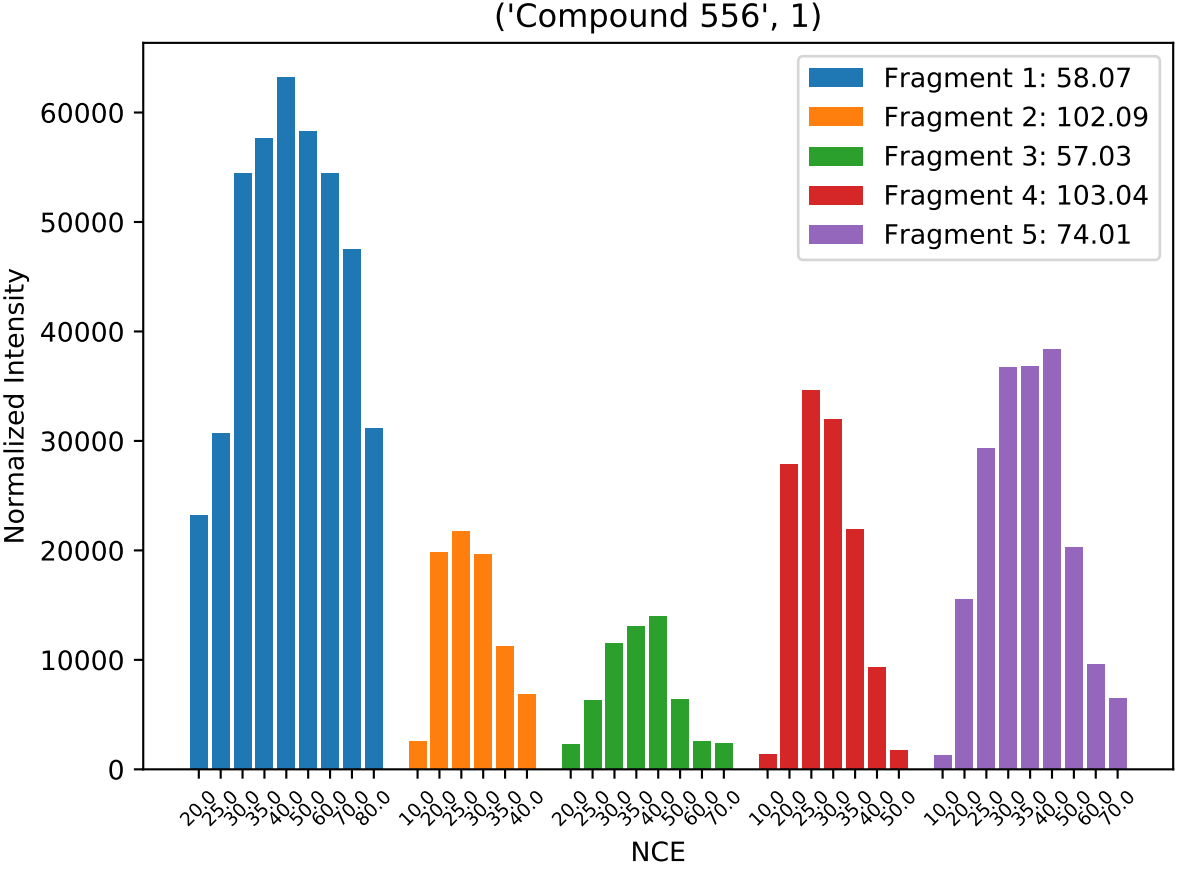

('Compound 48', 1)
Fragment 1: 188.07
Fragment 2: 146.06
Fragment 3: 118.06
Fragment 4: 91.05
Fragment 5: 118.07
Normalized Intensity
1200000
1000000
800000
600000
400000
200000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 40.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

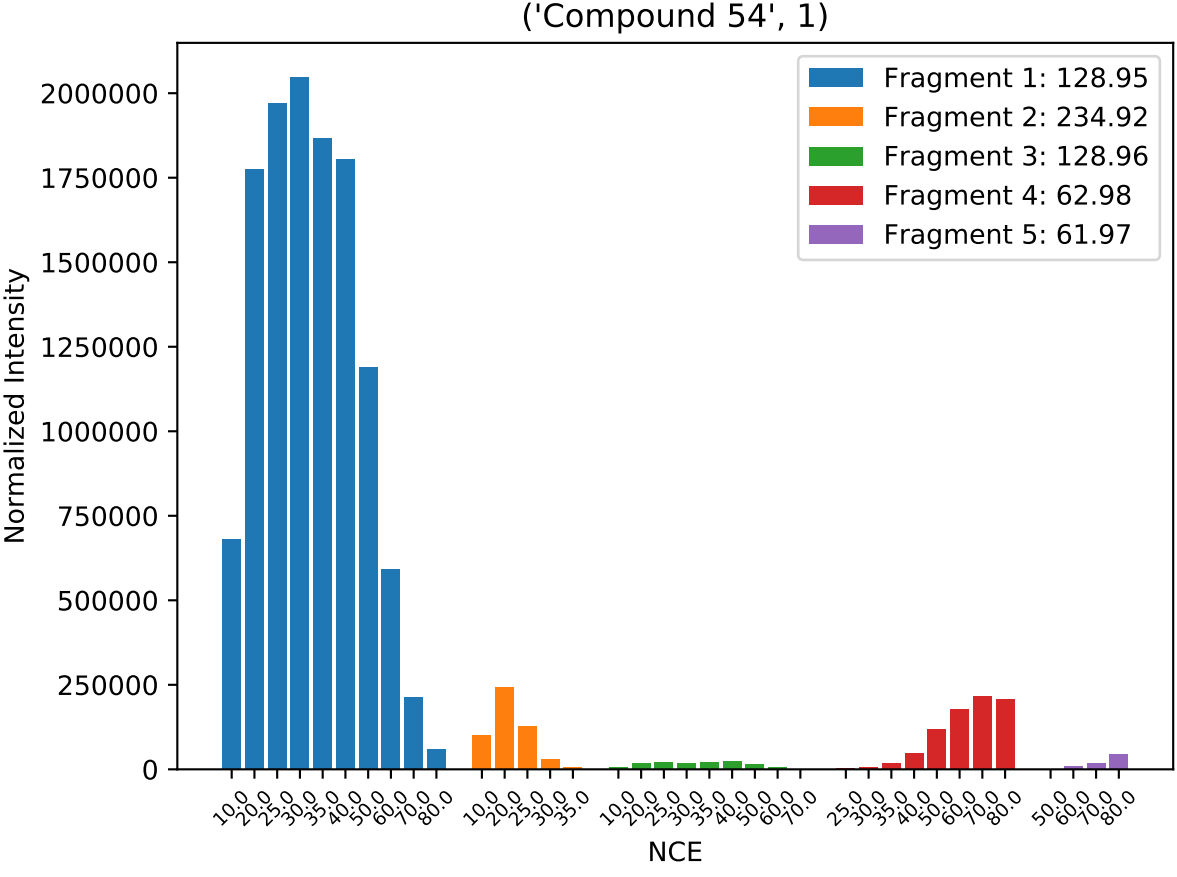

('Compound 49', 1)
Fragment 1: 73.06
Fragment 2: 94.06
Fragment 3: 55.05
Fragment 4: 96.04
Fragment 5: 93.06
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
1400000
1600000
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
30.0 40.0 50.0 60.0 70.0 80.0
NCE

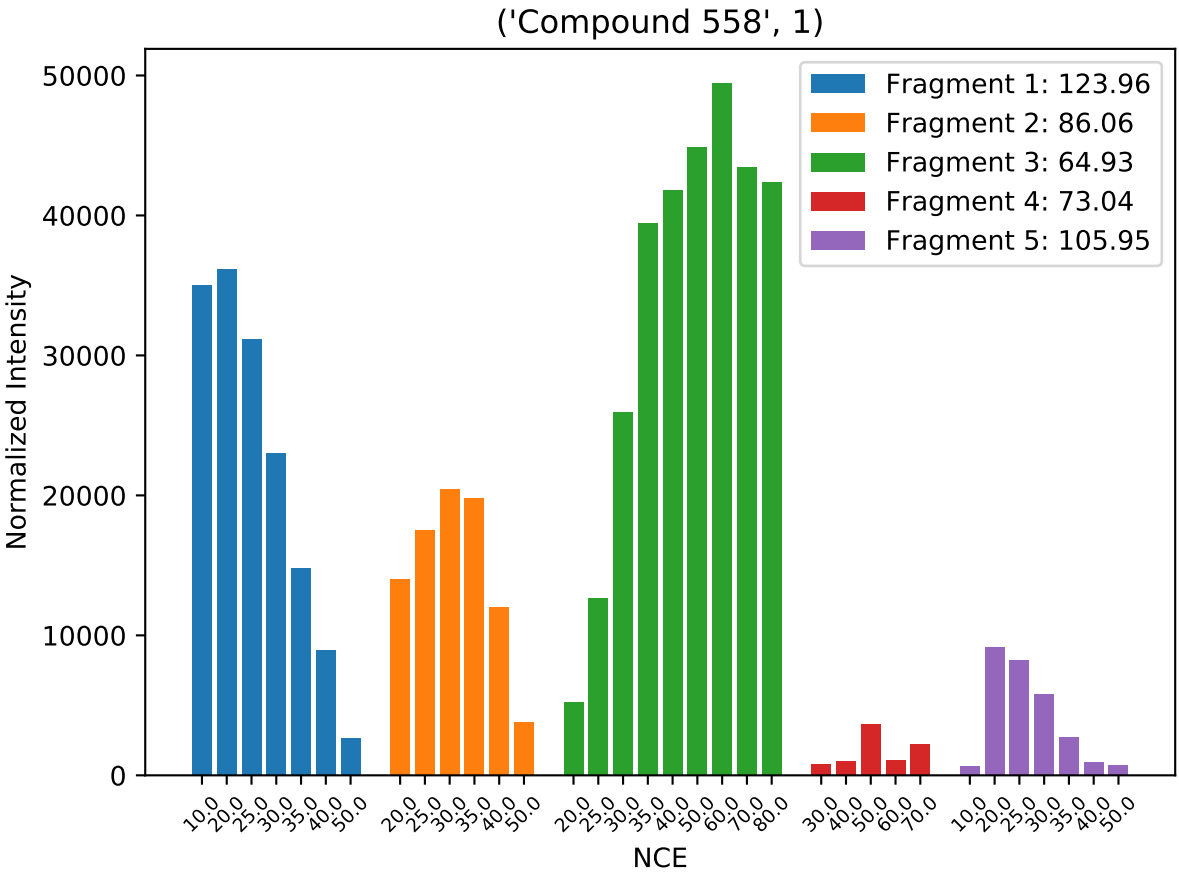

('Compound 555', 1)
Fragment 1: 68.05
Fragment 2: 82.07
Fragment 3: 95.06
Fragment 4: 137.07
Fragment 5: 137.11
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
NCE
50.0
60.0
70.0
80.0
35.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
70.0

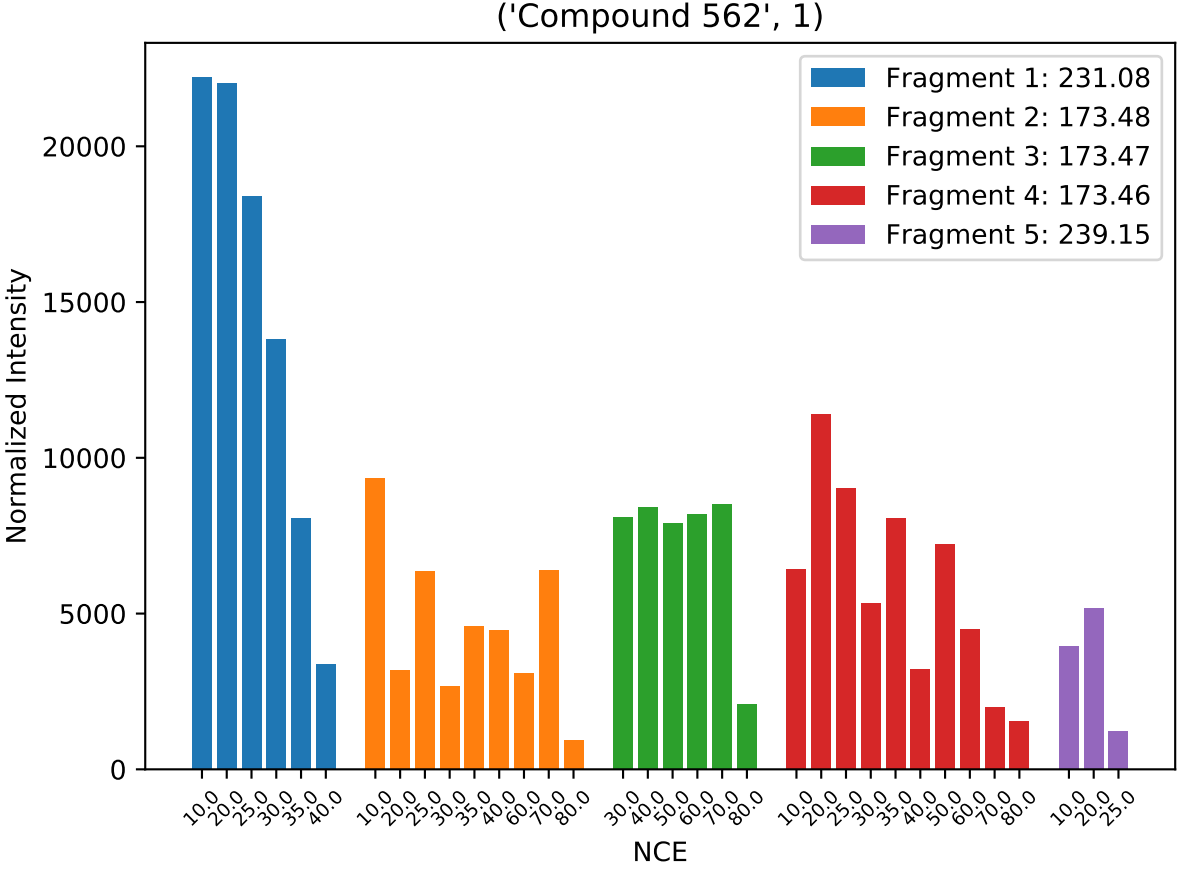

('Compound 51', 1)
Fragment 1: 126.1
Fragment 2: 109.08
Fragment 3: 96.07
Fragment 4: 68.05
Fragment 5: 95.06
Normalized Intensity
0
50000
100000
150000
200000
250000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

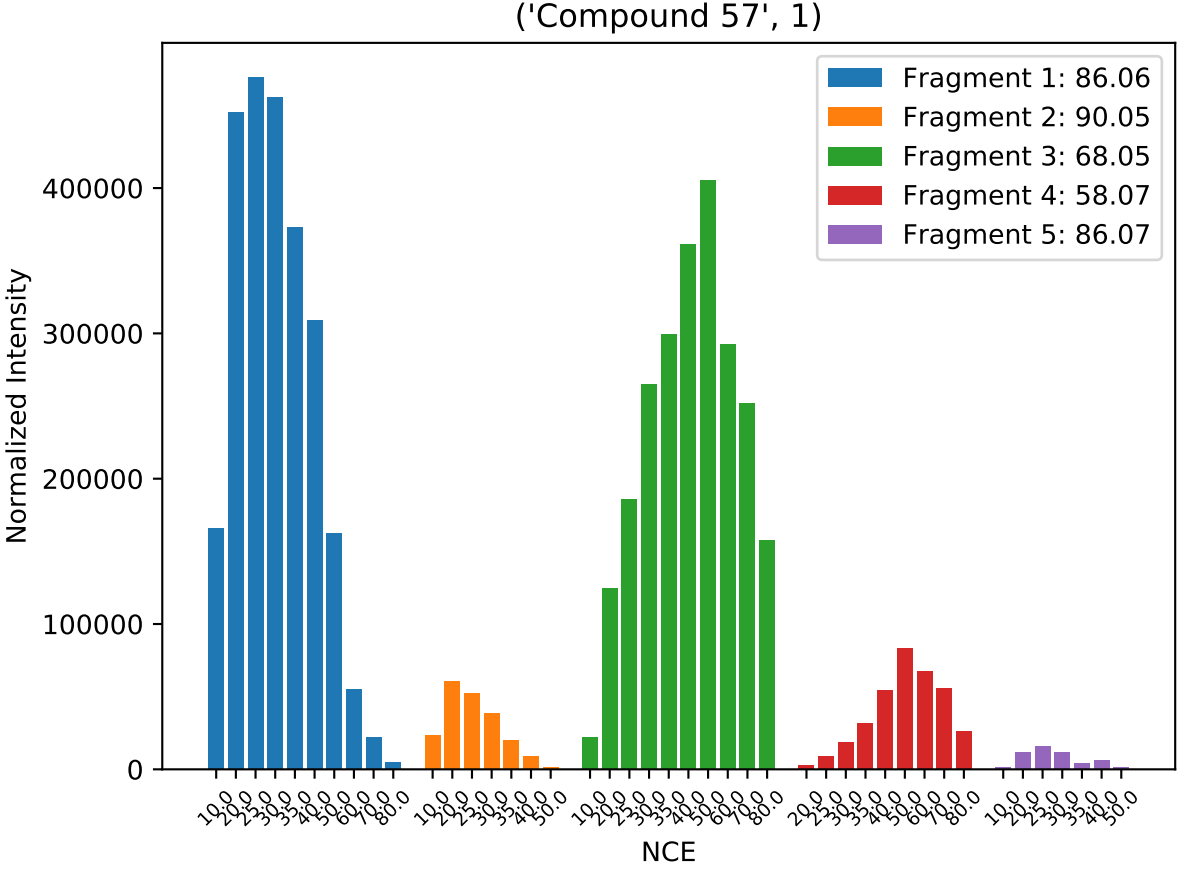

('Compound 52', 1)
Fragment 1: 141.04
Fragment 2: 69.01
Fragment 3: 96.02
Fragment 4: 70.04
Fragment 5: 152.01
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

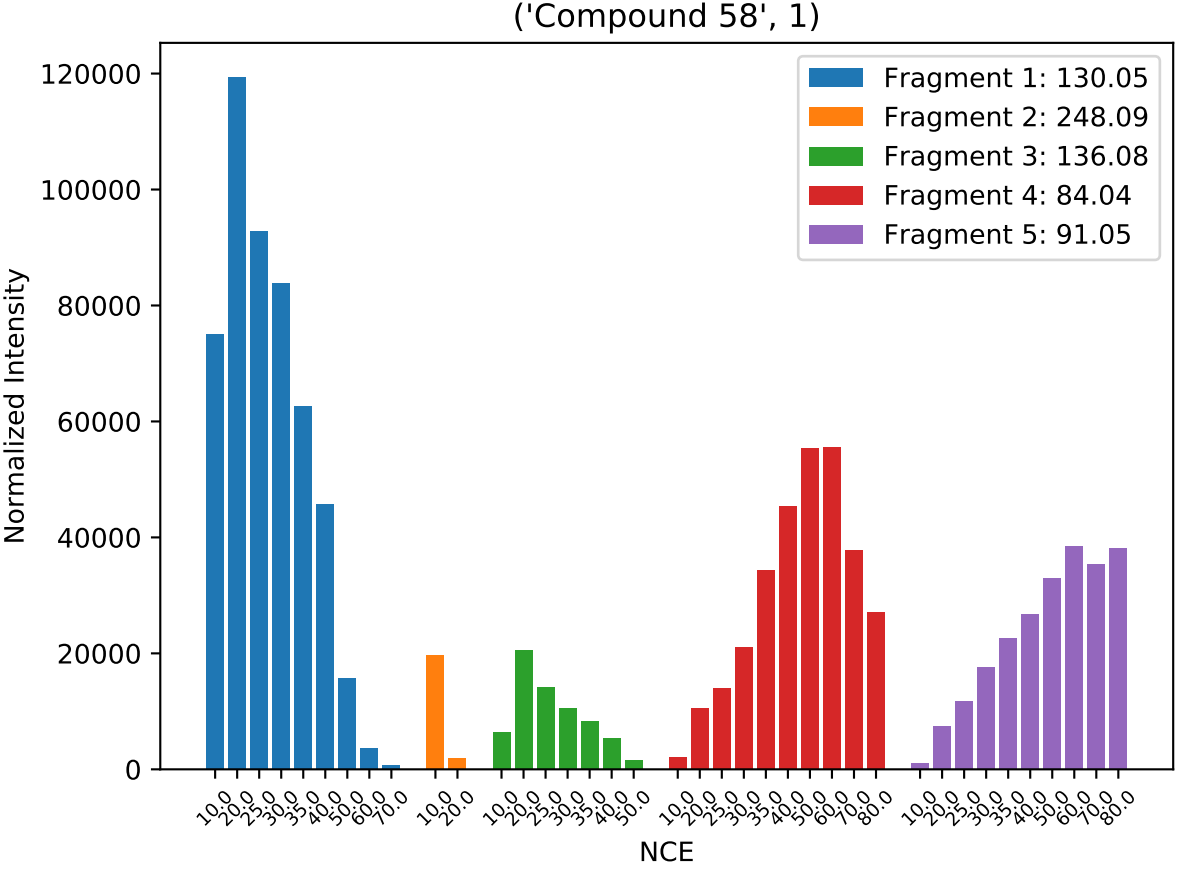

('Compound 556', 1)
Fragment 1: 58.07
Fragment 2: 102.09
Fragment 3: 57.03
Fragment 4: 103.04
Fragment 5: 74.01
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

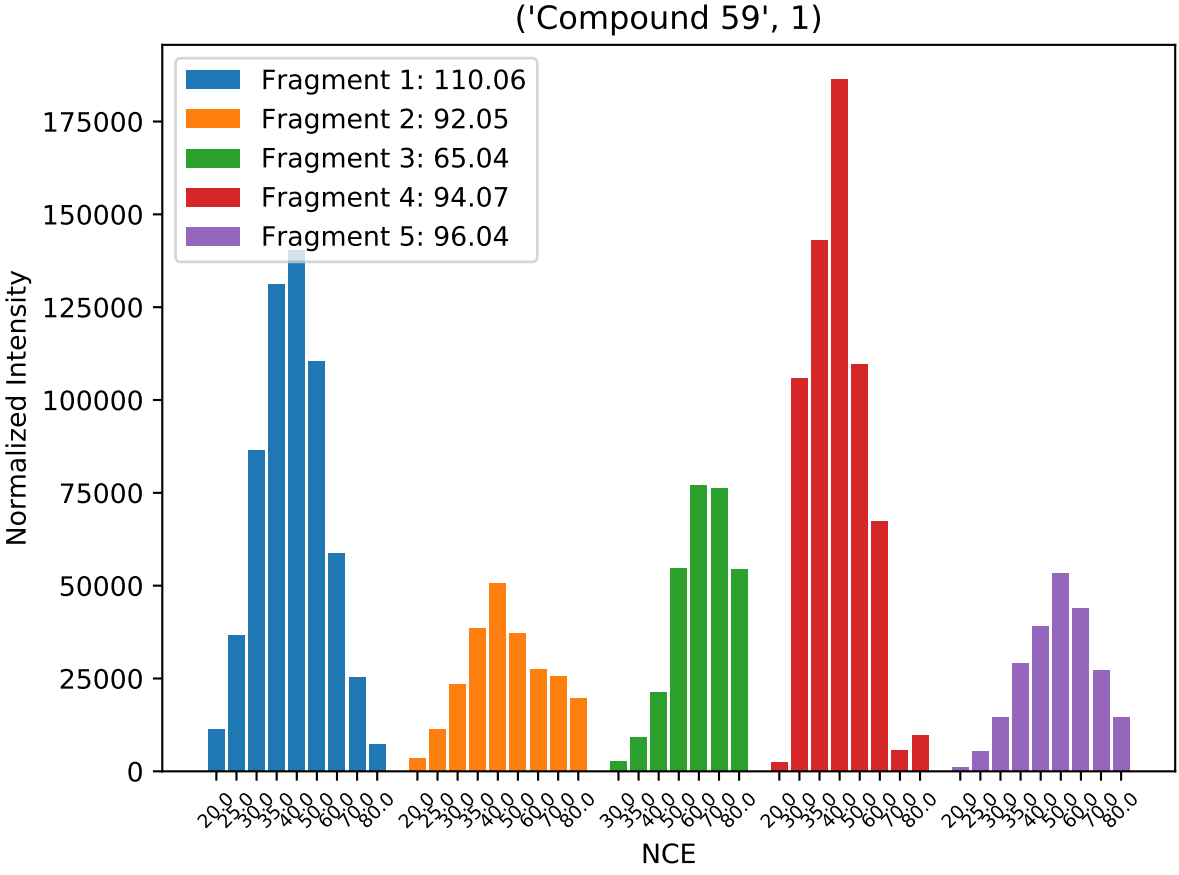

('Compound 54', 1)
Fragment 1: 128.95
Fragment 2: 234.92
Fragment 3: 128.96
Fragment 4: 62.98
Fragment 5: 61.97
Normalized Intensity
2000000
1750000
1500000
1250000
1000000
750000
500000
250000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
NCE

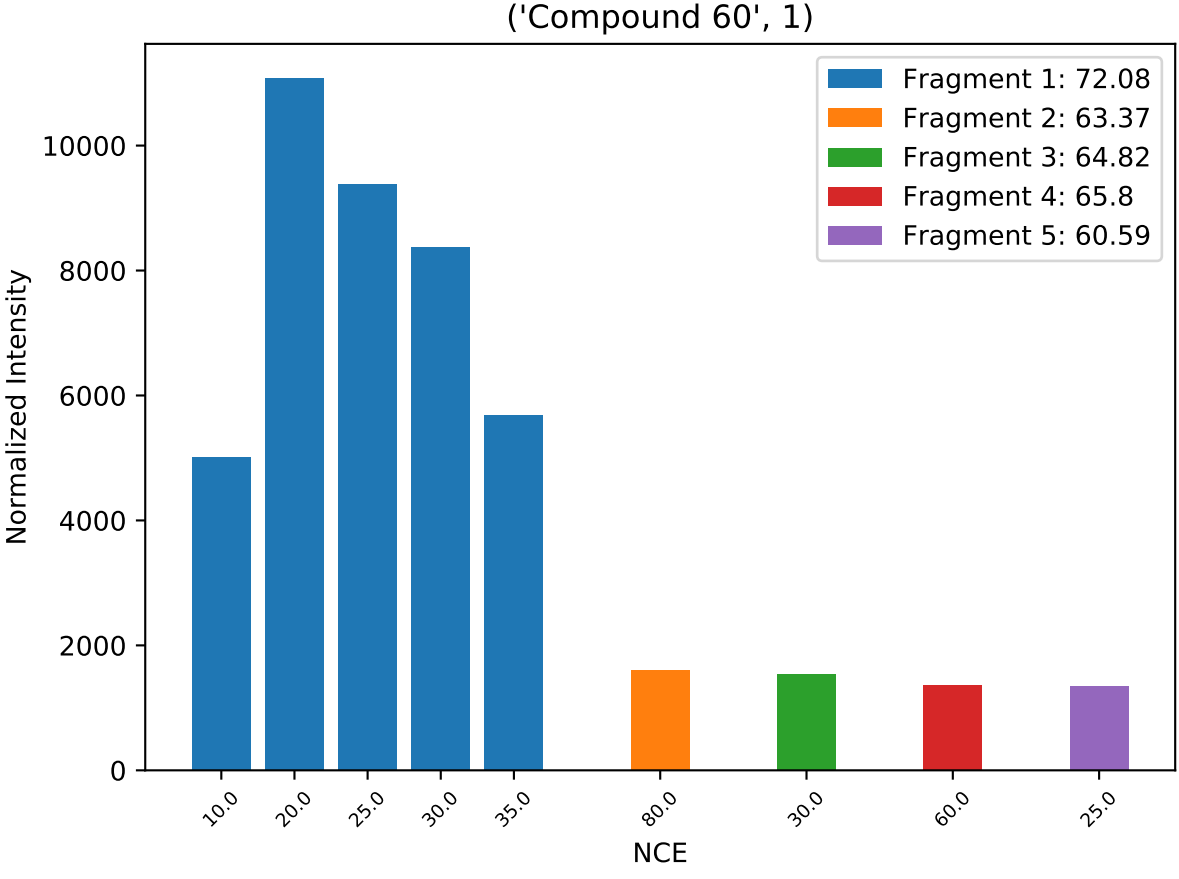

('Compound 558', 1)
Fragment 1: 123.96
Fragment 2: 86.06
Fragment 3: 64.93
Fragment 4: 73.04
Fragment 5: 105.95
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

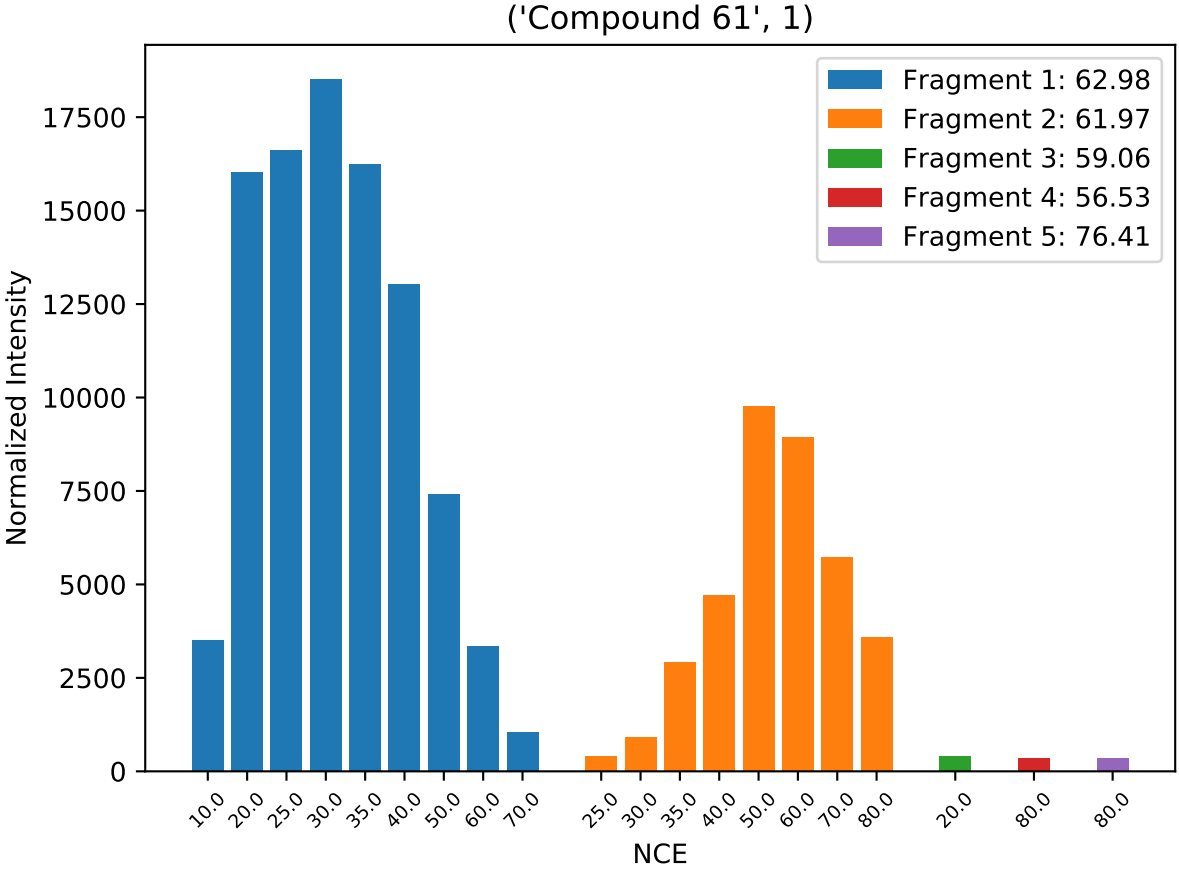

('Compound 562', 1)
Fragment 1: 231.08
Fragment 2: 173.48
Fragment 3: 173.47
Fragment 4: 173.46
Fragment 5: 239.15
Normalized Intensity
0
5000
10000
15000
20000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 60.0 70.0 80.0
30.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0
NCE

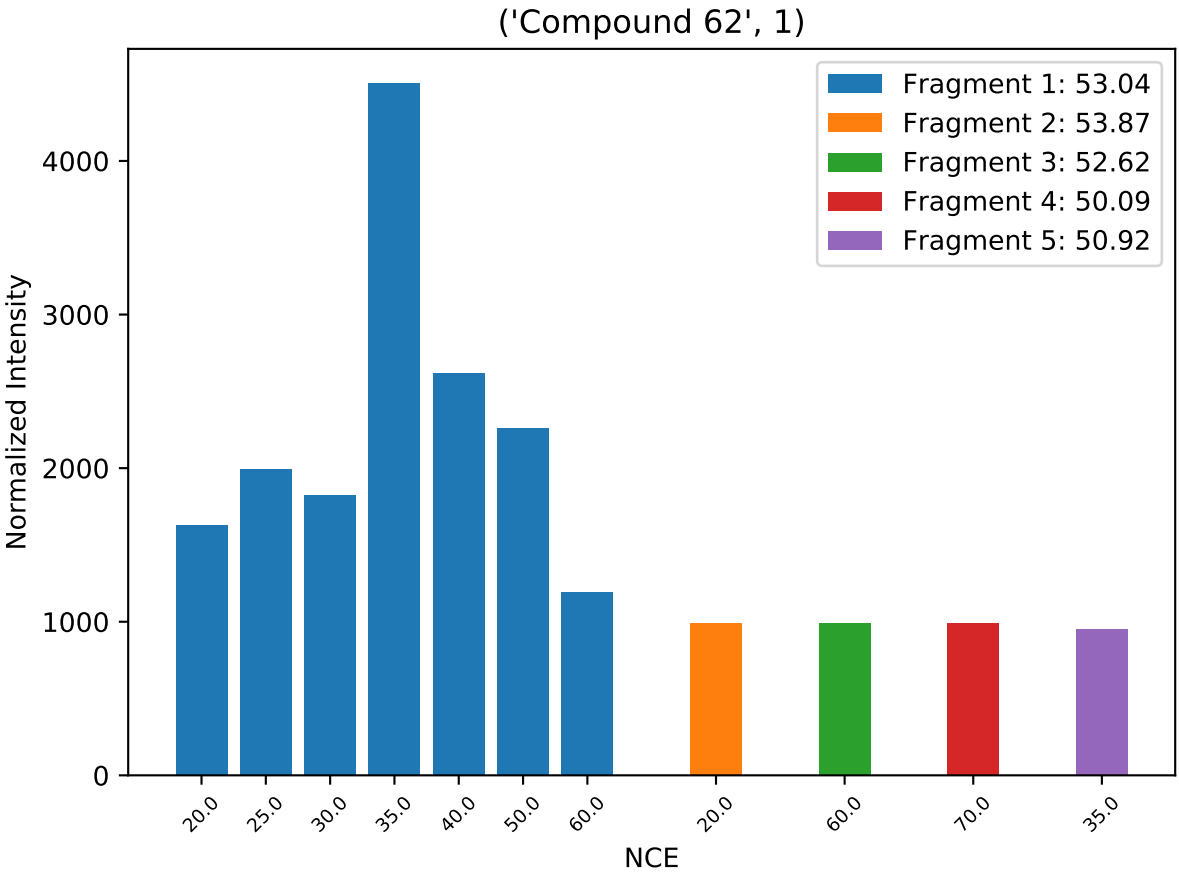

('Compound 57', 1)
Fragment 1: 86.06
Fragment 2: 90.05
Fragment 3: 68.05
Fragment 4: 58.07
Fragment 5: 86.07
Normalized Intensity
0
100000
200000
300000
400000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

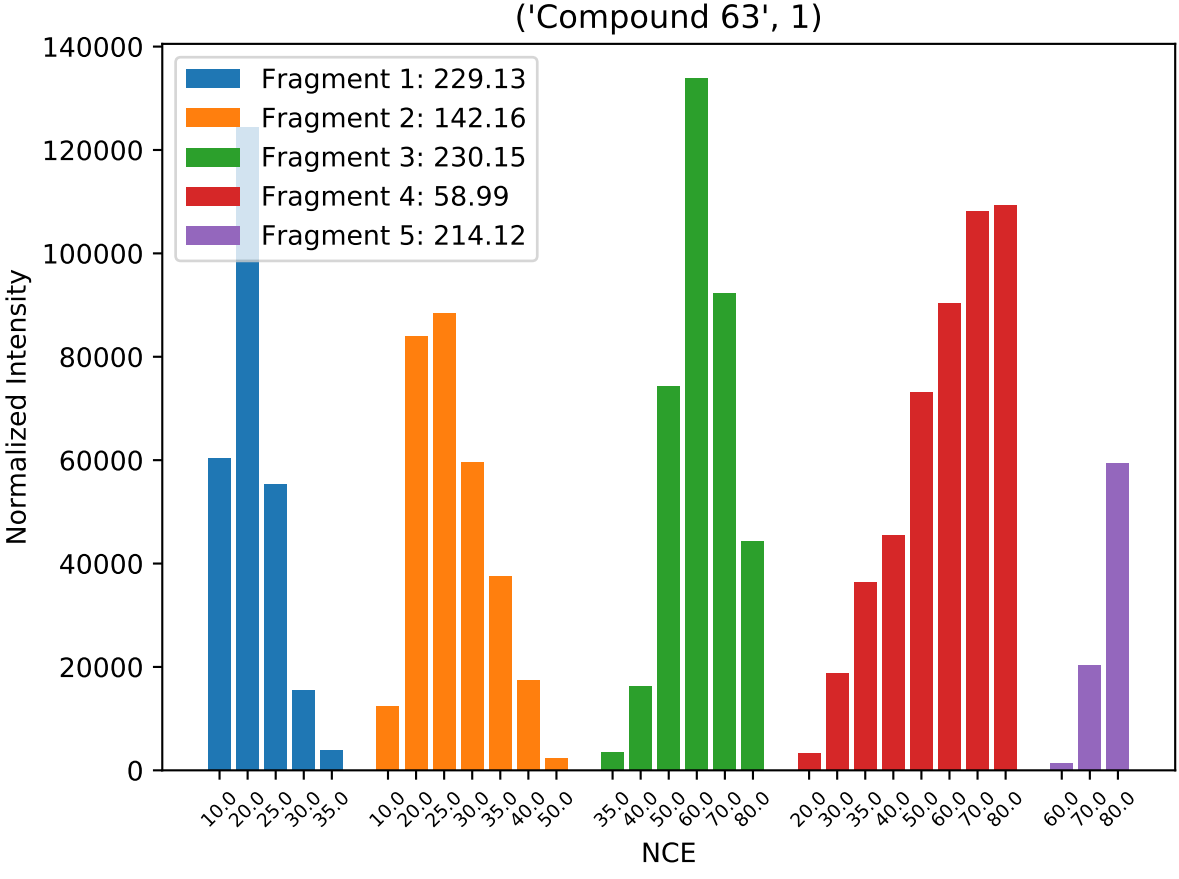

('Compound 58', 1)
Fragment 1: 130.05
Fragment 2: 248.09
Fragment 3: 136.08
Fragment 4: 84.04
Fragment 5: 91.05
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

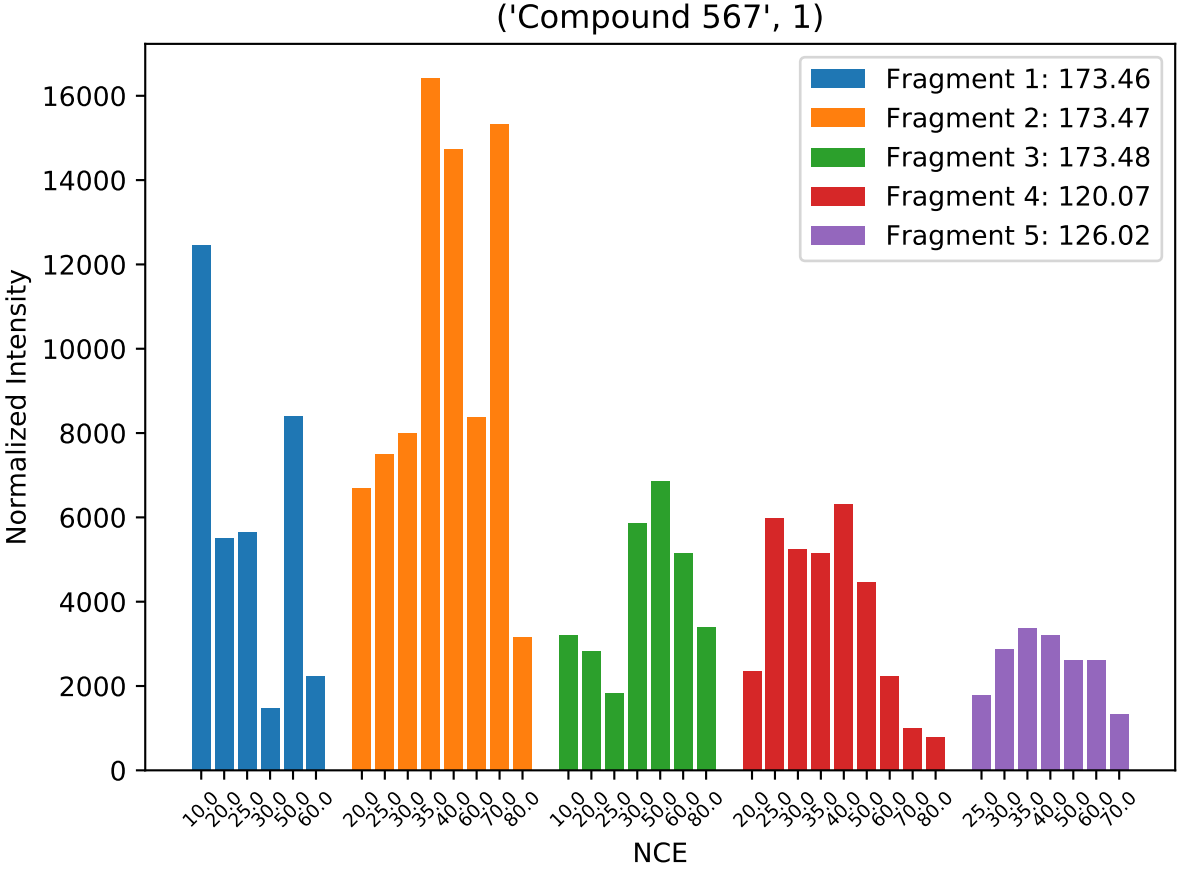

('Compound 59', 1)
Fragment 1: 110.06
Fragment 2: 92.05
Fragment 3: 65.04
Fragment 4: 94.07
Fragment 5: 96.04
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
NCE
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

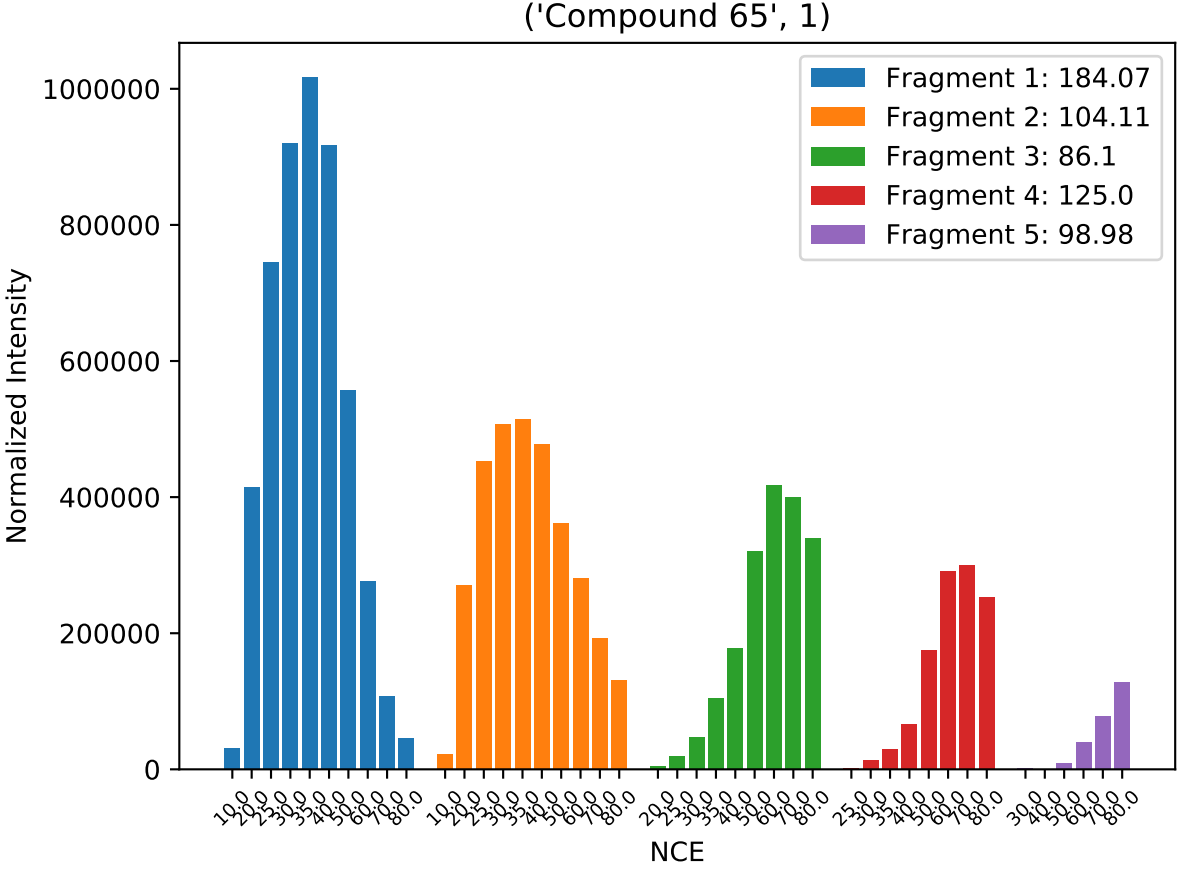

('Compound 60', 1)
Fragment 1: 72.08
Fragment 2: 63.37
Fragment 3: 64.82
Fragment 4: 65.8
Fragment 5: 60.59
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
20.0
25.0
30.0
35.0
80.0
30.0
60.0
25.0
NCE

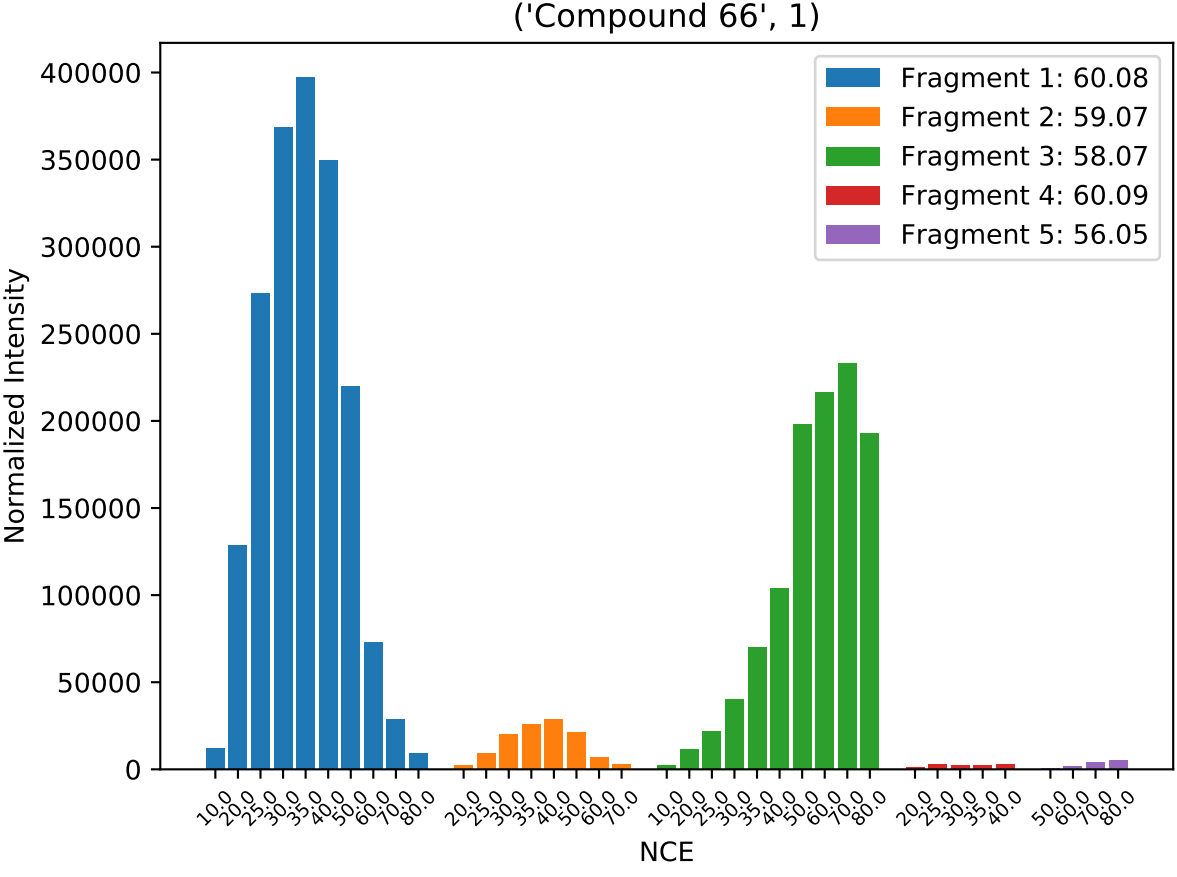

('Compound 61', 1)
Fragment 1: 62.98
Fragment 2: 61.97
Fragment 3: 59.06
Fragment 4: 56.53
Fragment 5: 76.41
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
80.0
80.0
NCE

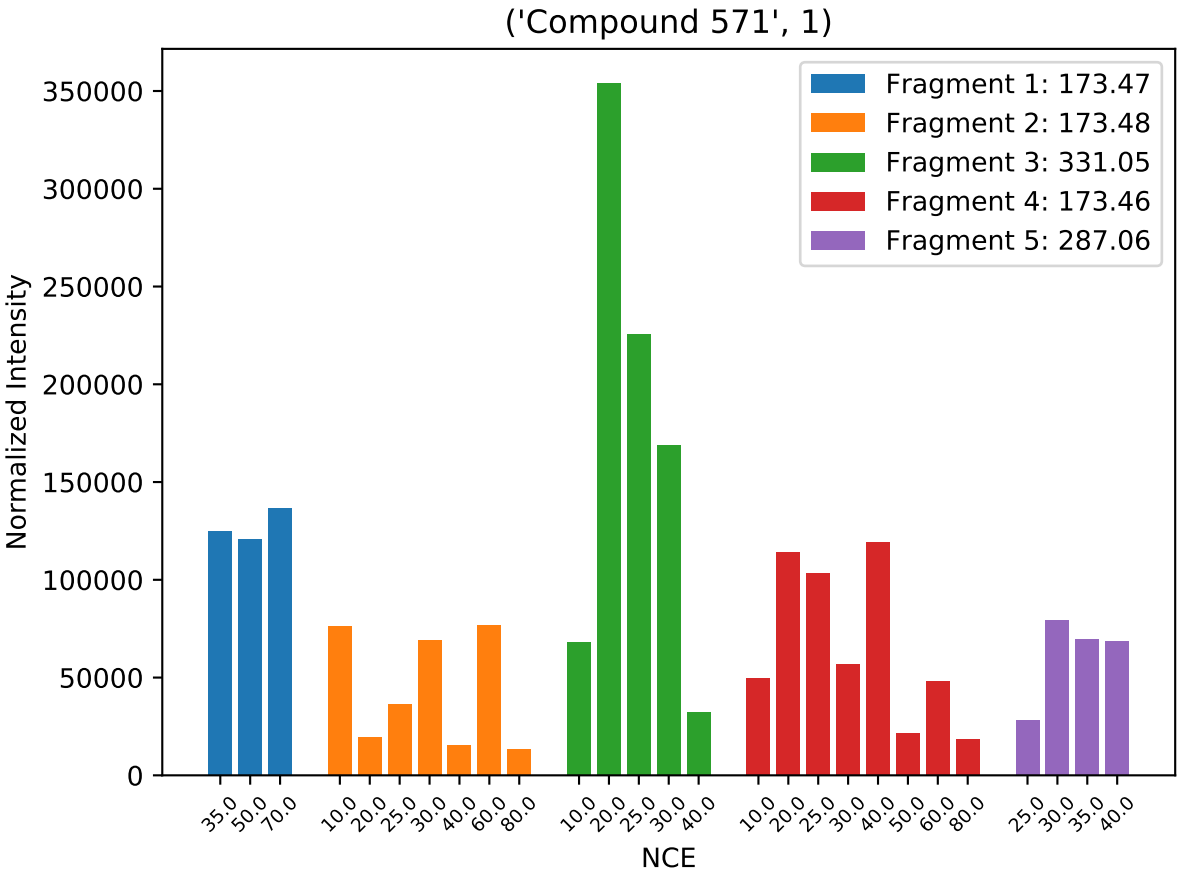

('Compound 62', 1)
Fragment 1: 53.04
Fragment 2: 53.87
Fragment 3: 52.62
Fragment 4: 50.09
Fragment 5: 50.92
Normalized Intensity
0
1000
2000
3000
4000
20.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
60.0
70.0
35.0
NCE

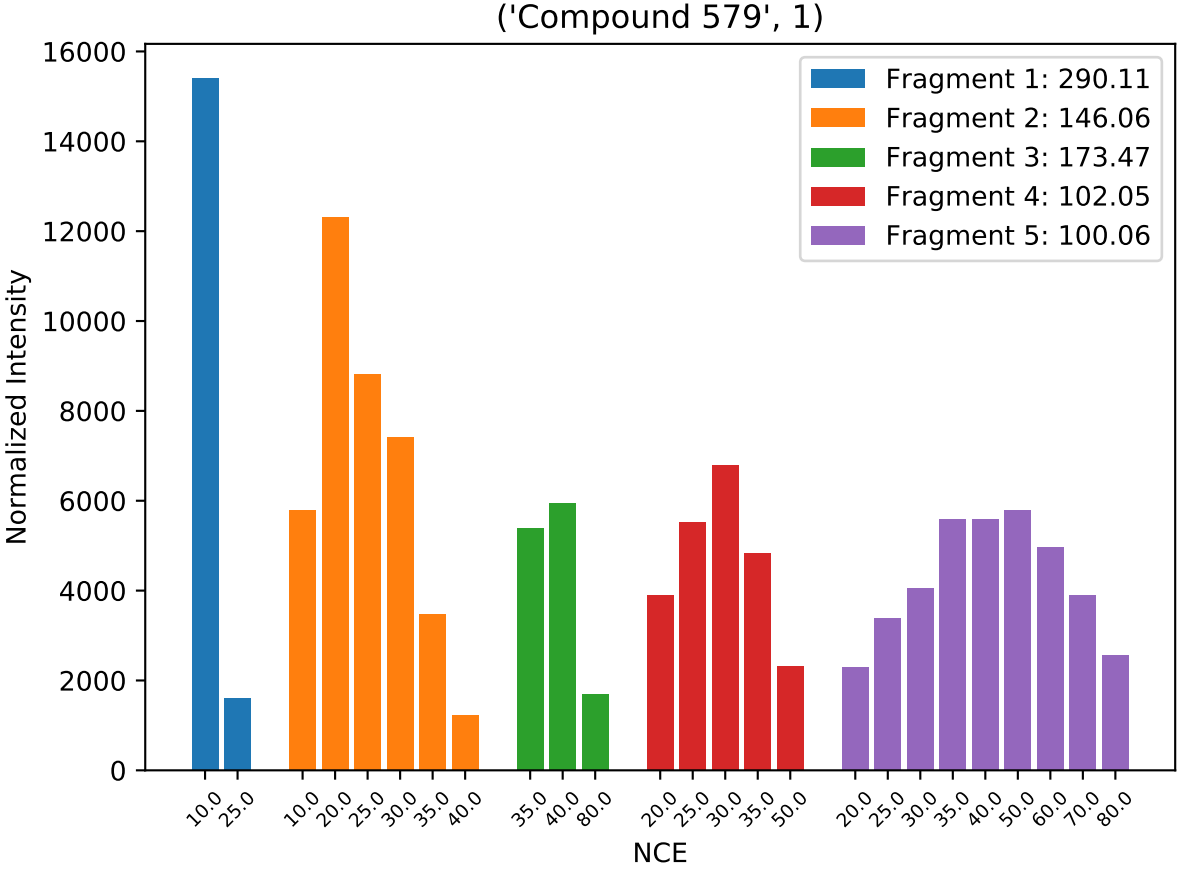

('Compound 63', 1)
Fragment 1: 229.13
Fragment 2: 142.16
Fragment 3: 230.15
Fragment 4: 58.99
Fragment 5: 214.12
Normalized Intensity
NCE
140000
120000
100000
80000
60000
40000
20000
0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
20.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
60.0 70.0 80.0

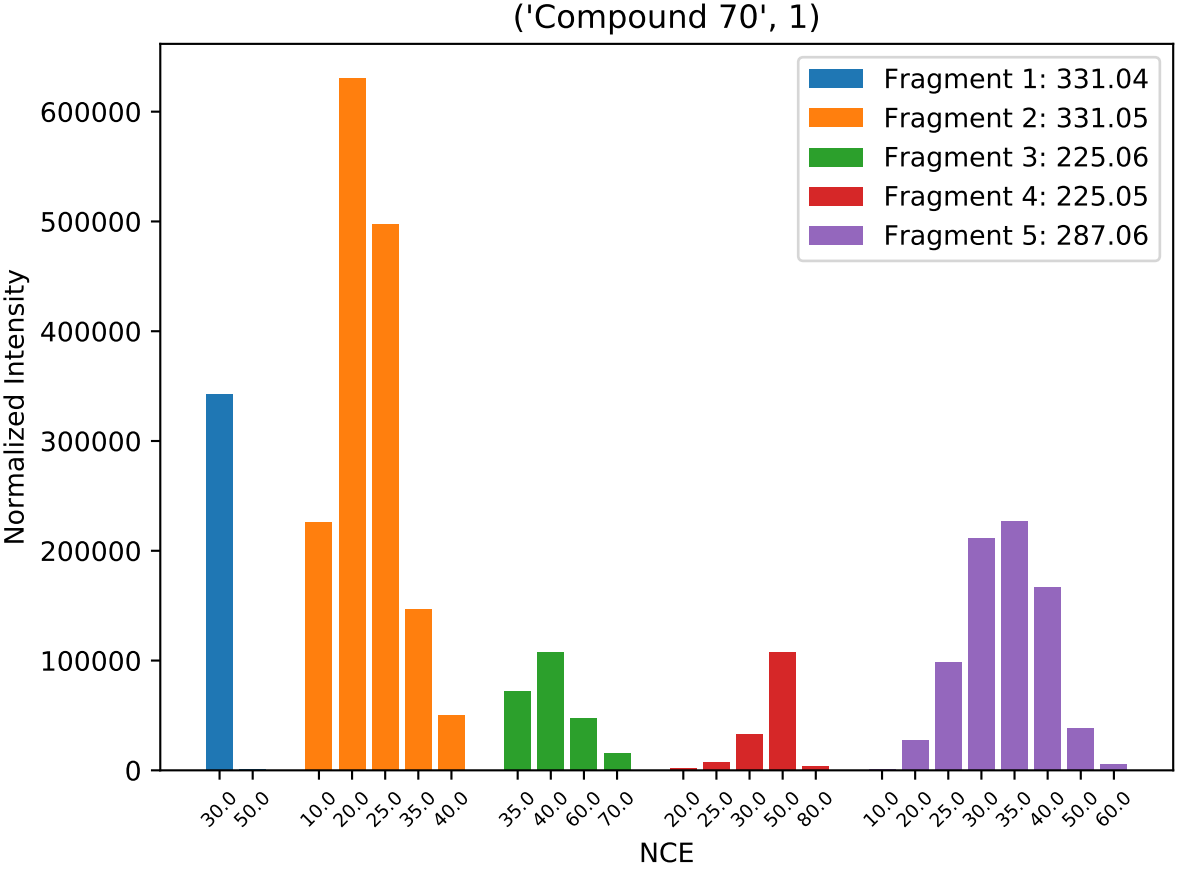

('Compound 567', 1)
Fragment 1: 173.46
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 120.07
Fragment 5: 126.02
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0 20.0 25.0 30.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 50.0 60.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

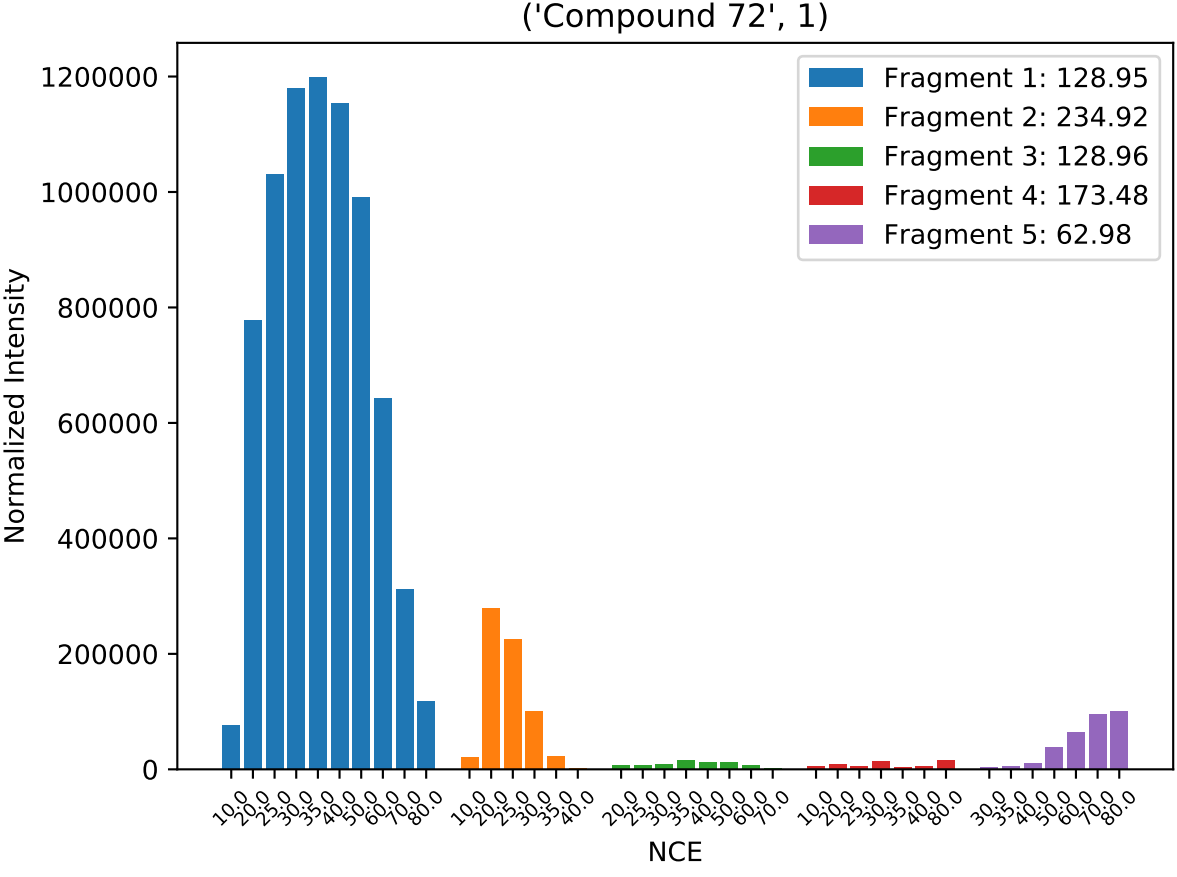

('Compound 65', 1)
Fragment 1: 184.07
Fragment 2: 104.11
Fragment 3: 86.1
Fragment 4: 125.0
Fragment 5: 98.98
Normalized Intensity
1000000
800000
600000
400000
200000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 40.0 50.0 60.0 70.0 80.0

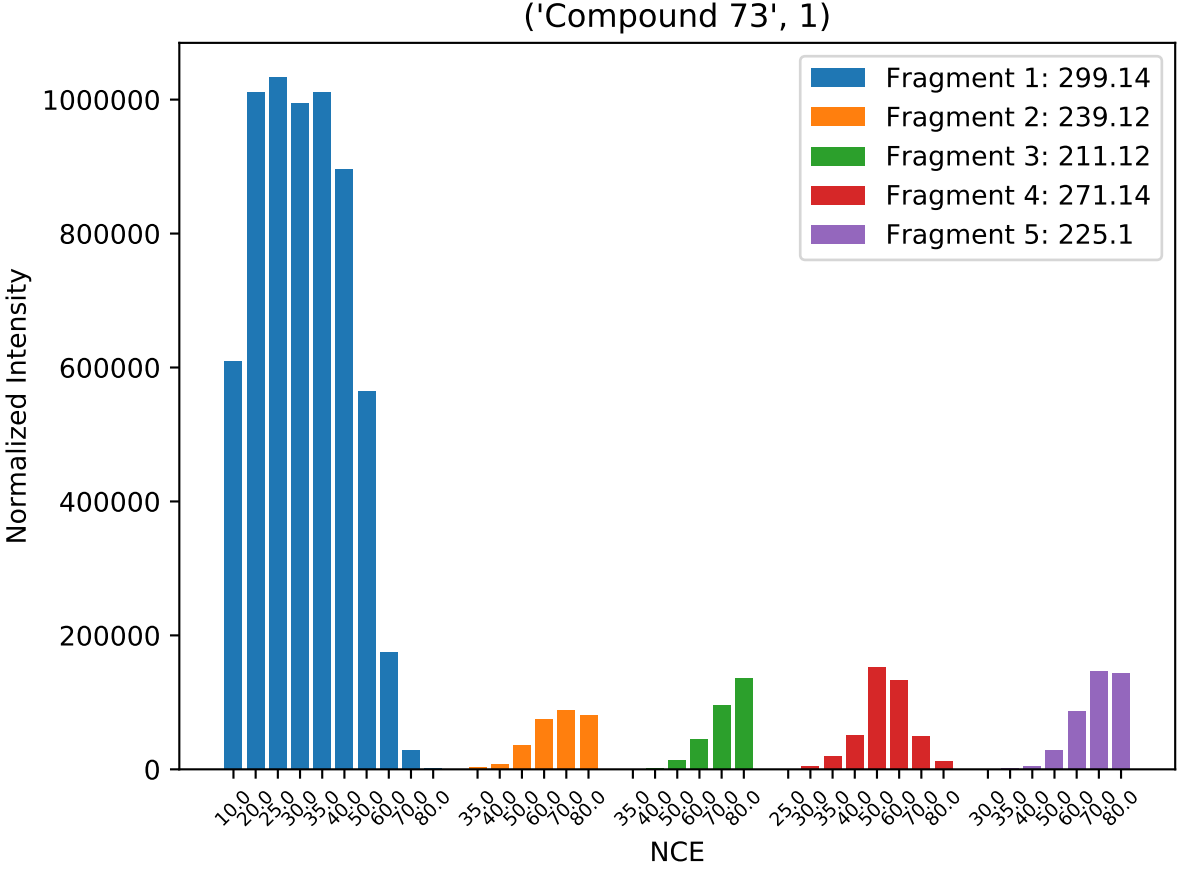

('Compound 66', 1)
Fragment 1: 60.08
Fragment 2: 59.07
Fragment 3: 58.07
Fragment 4: 60.09
Fragment 5: 56.05
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
400000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0
50.0 60.0 70.0 80.0
NCE

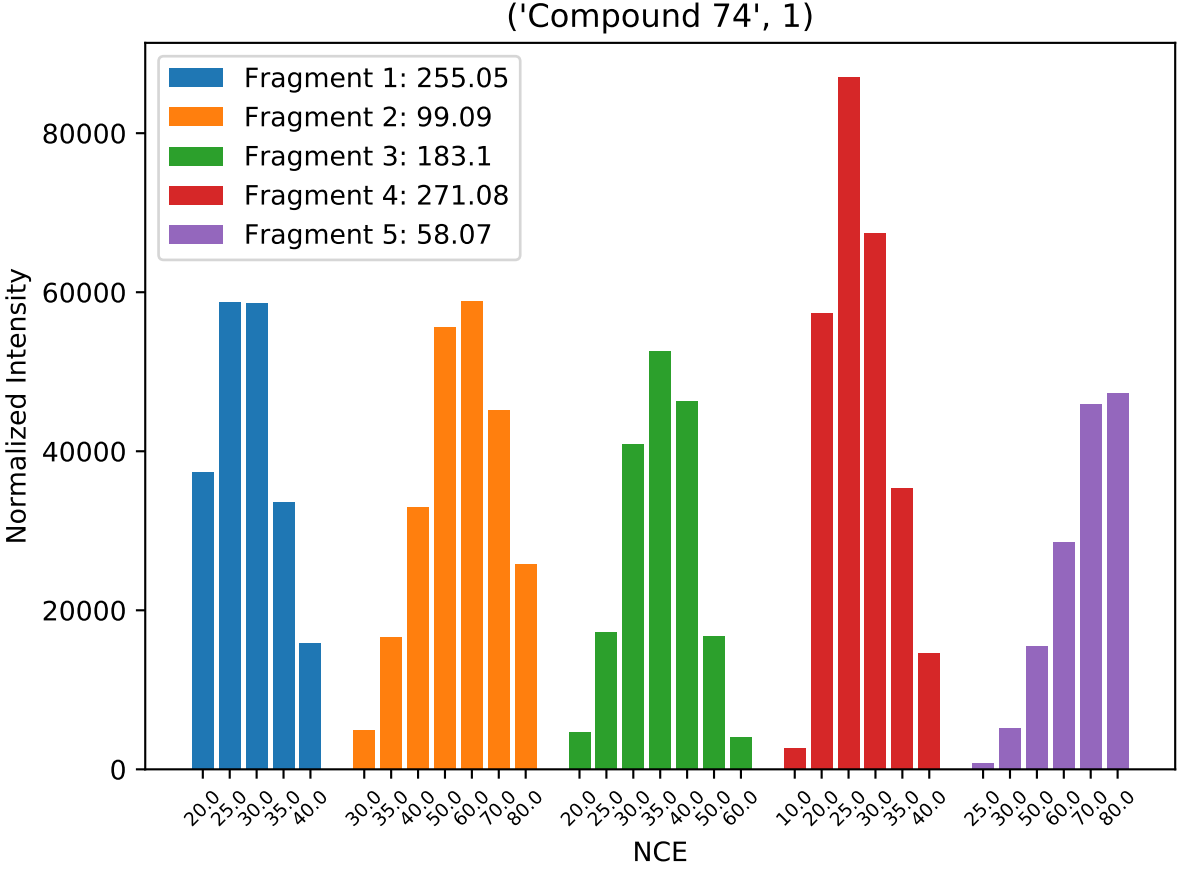

('Compound 571', 1)
Fragment 1: 173.47
Fragment 2: 173.48
Fragment 3: 331.05
Fragment 4: 173.46
Fragment 5: 287.06
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
35.0
50.0
70.0
10.0
20.0
25.0
30.0
40.0
60.0
80.0
10.0
20.0
25.0
30.0
40.0
10.0
20.0
25.0
30.0
40.0
50.0
60.0
80.0
25.0
30.0
35.0
40.0
NCE

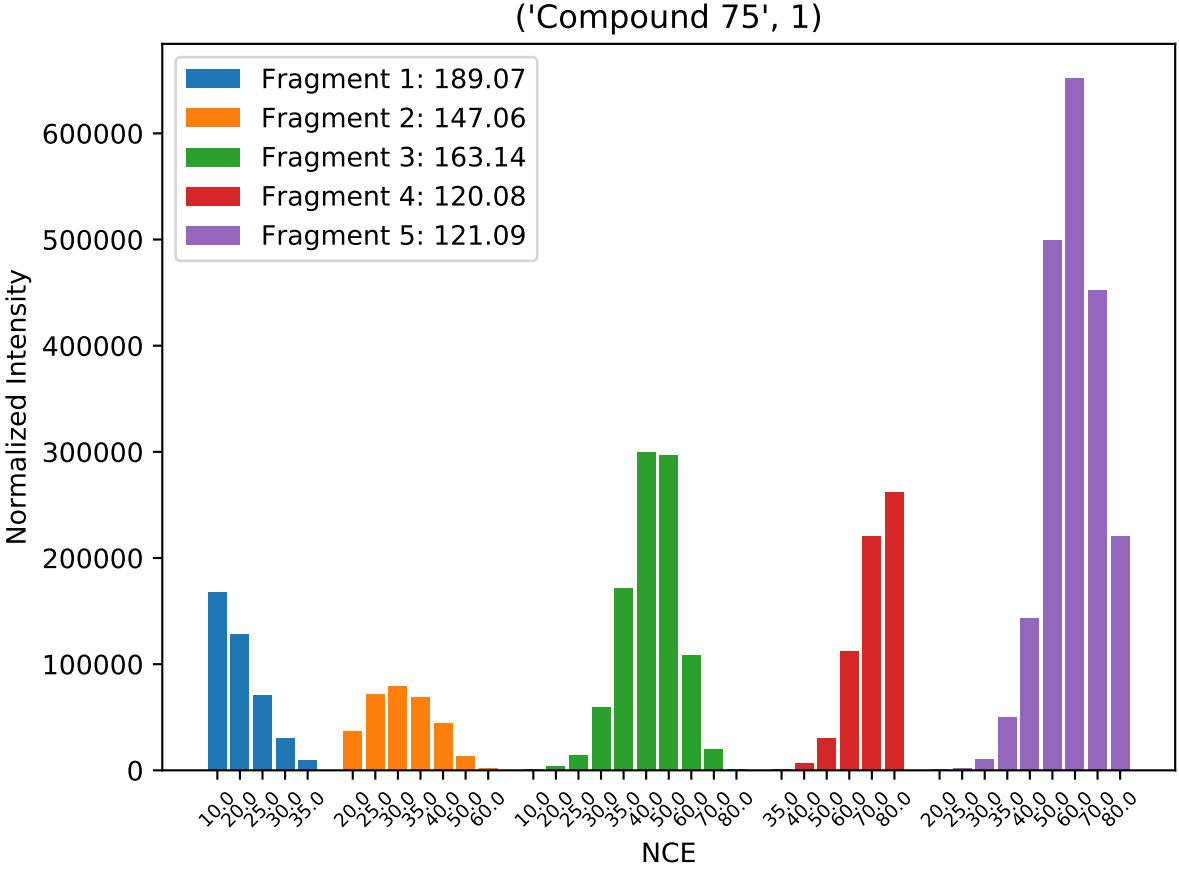

('Compound 579', 1)
Fragment 1: 290.11
Fragment 2: 146.06
Fragment 3: 173.47
Fragment 4: 102.05
Fragment 5: 100.06
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
35.0
40.0
80.0
20.0
25.0
30.0
35.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

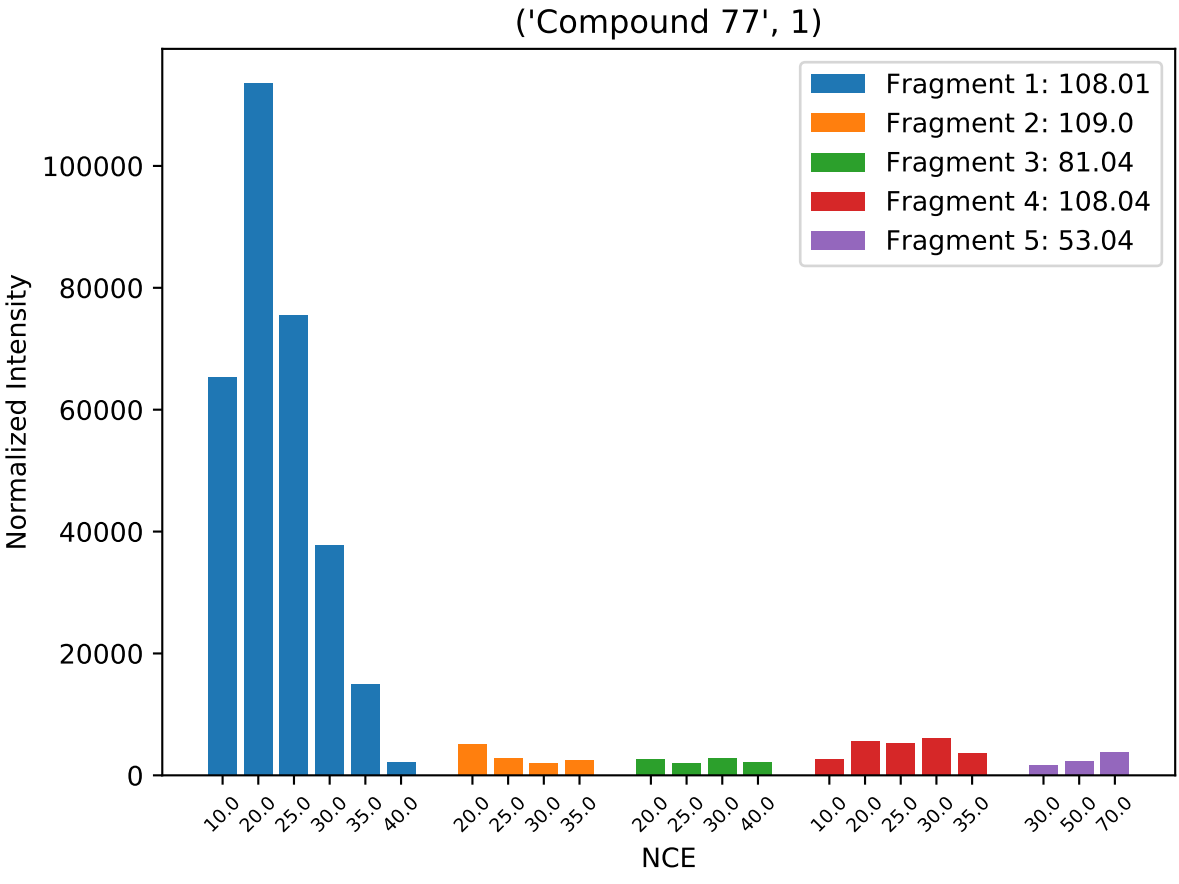

('Compound 70', 1)
Fragment 1: 331.04
Fragment 2: 331.05
Fragment 3: 225.06
Fragment 4: 225.05
Fragment 5: 287.06
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
30.0
50.0
10.0
20.0
25.0
35.0
40.0
35.0
40.0
60.0
70.0
20.0
25.0
30.0
50.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

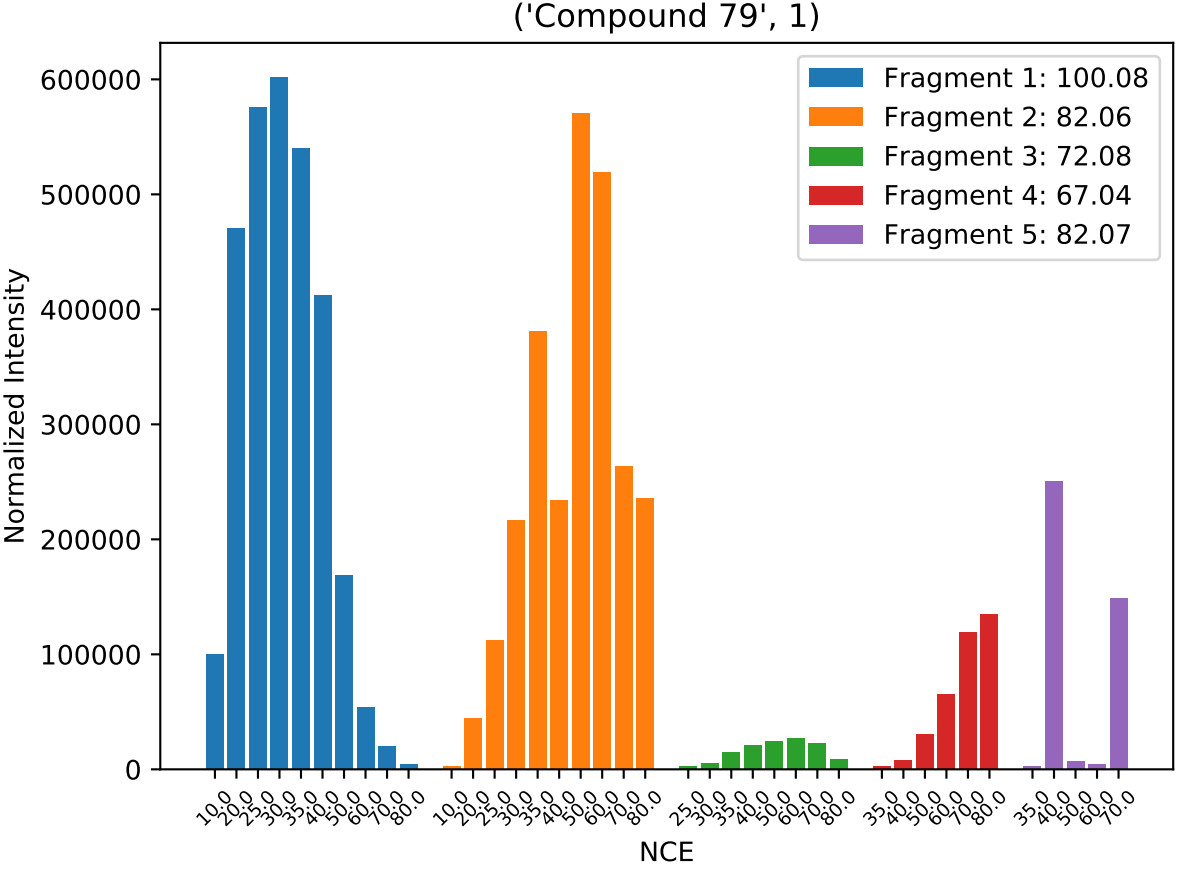

('Compound 72', 1)
Fragment 1: 128.95
Fragment 2: 234.92
Fragment 3: 128.96
Fragment 4: 173.48
Fragment 5: 62.98
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

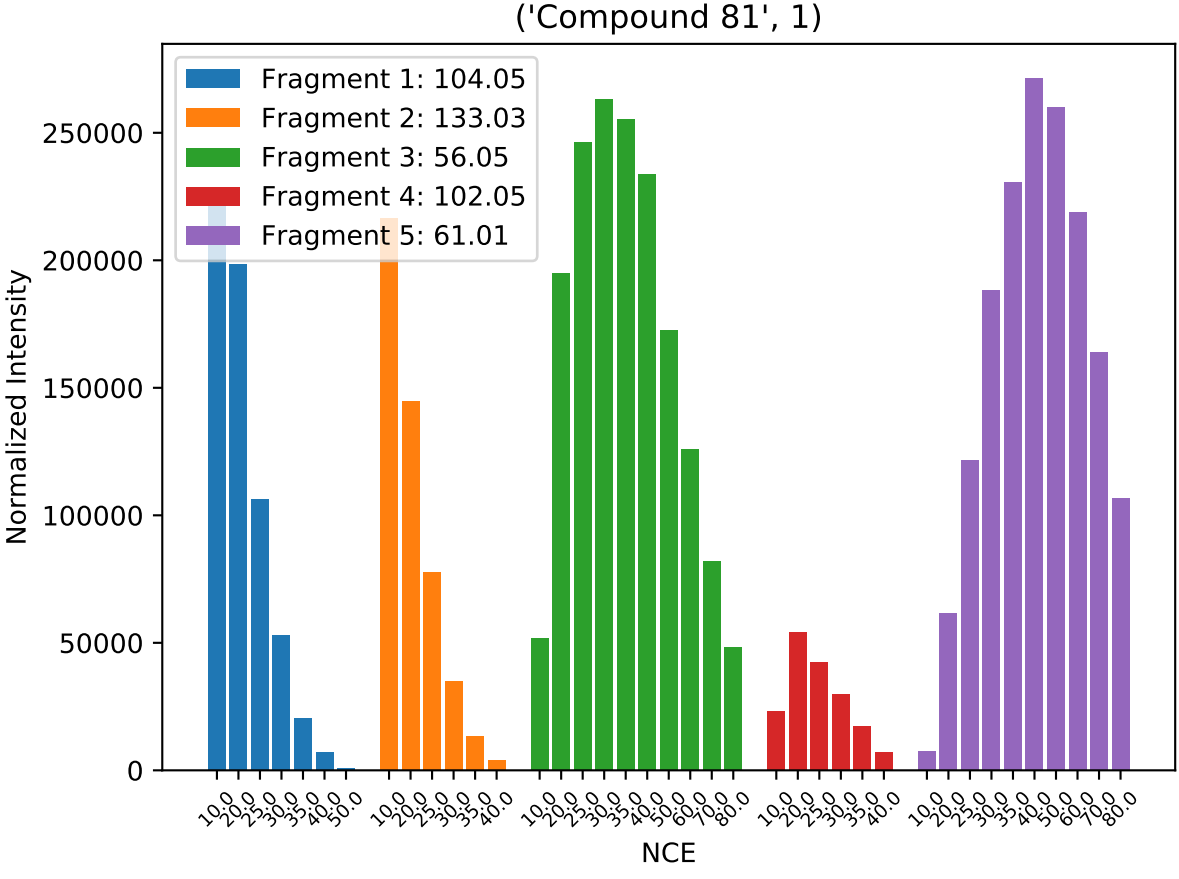

('Compound 73', 1)
Fragment 1: 299.14
Fragment 2: 239.12
Fragment 3: 211.12
Fragment 4: 271.14
Fragment 5: 225.1
Normalized Intensity
0
200000
400000
600000
800000
1000000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

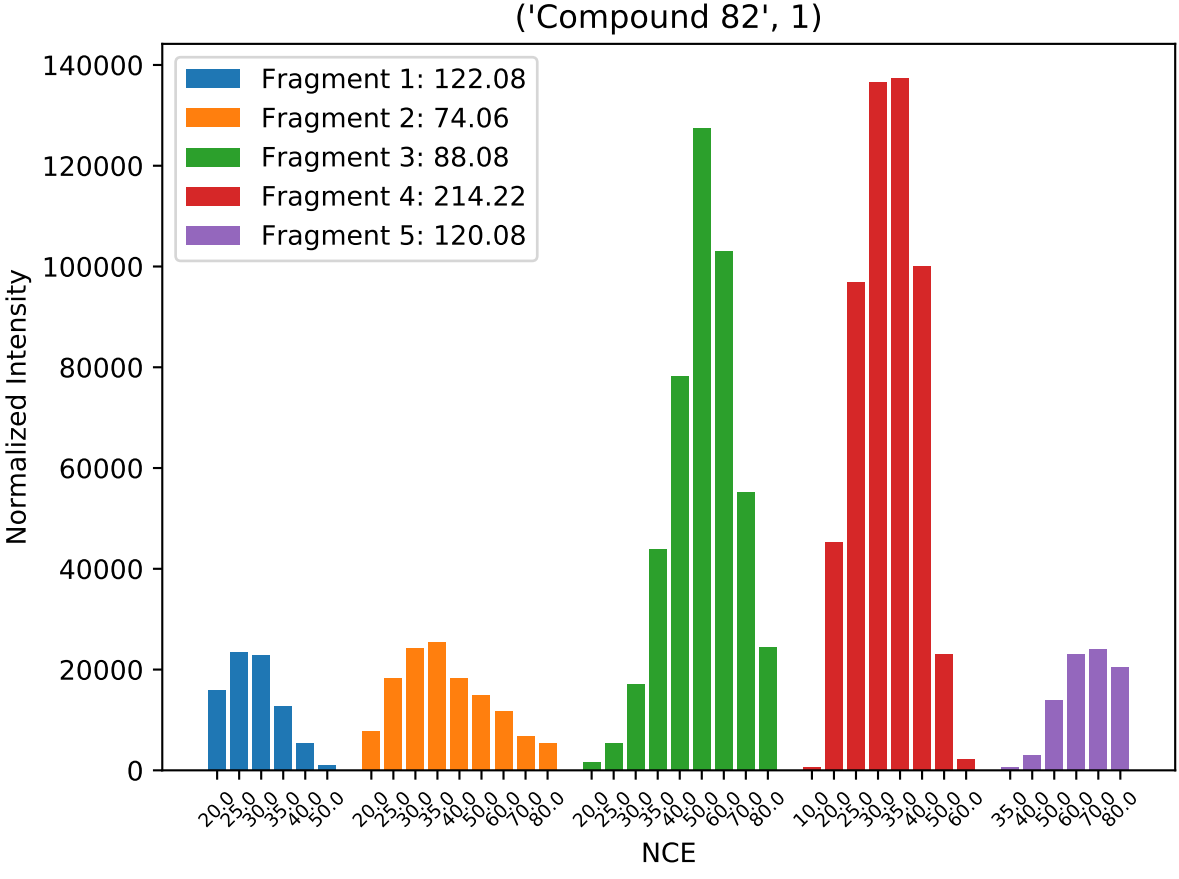

('Compound 74', 1)
Fragment 1: 255.05
Fragment 2: 99.09
Fragment 3: 183.1
Fragment 4: 271.08
Fragment 5: 58.07
Normalized Intensity
0
20000
40000
60000
80000
20.0 25.0 30.0 35.0 40.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
25.0 30.0 50.0 60.0 70.0 80.0
NCE

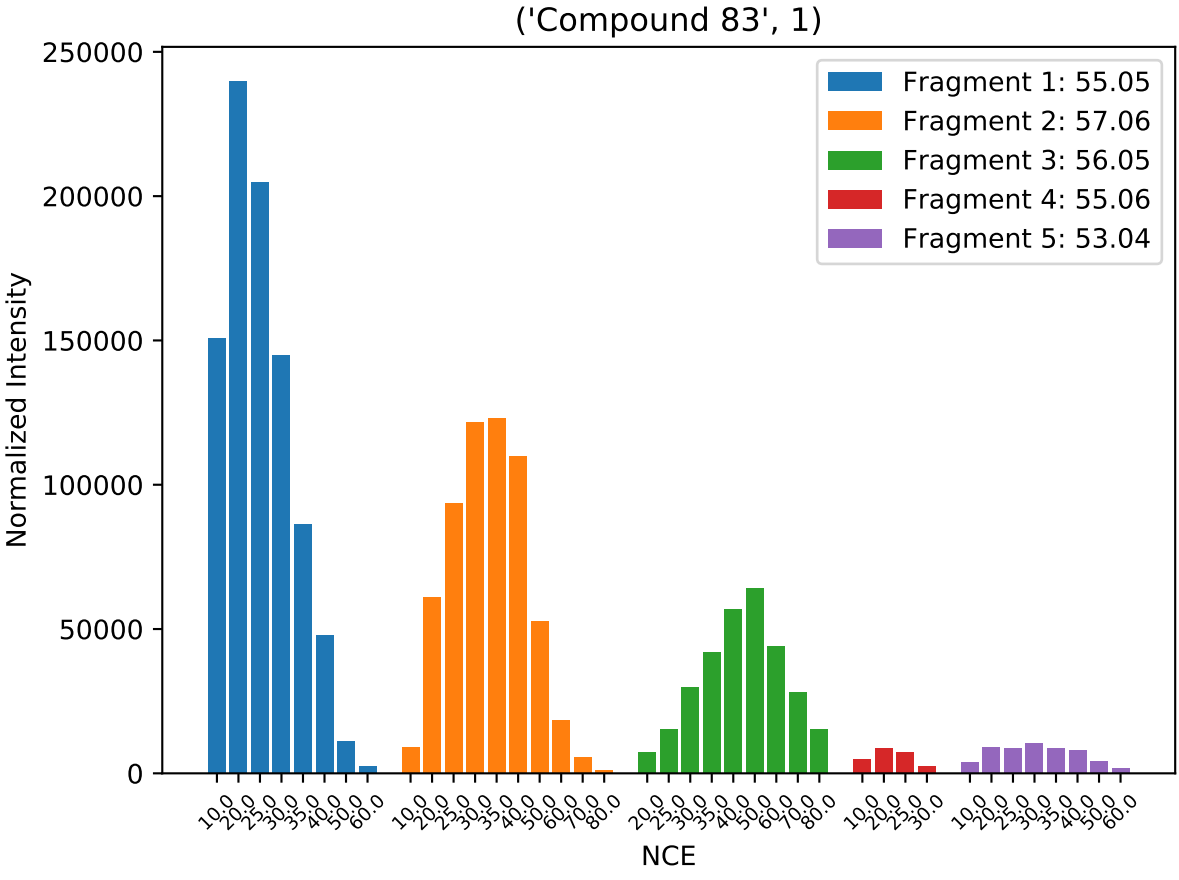

('Compound 75', 1)
Fragment 1: 189.07
Fragment 2: 147.06
Fragment 3: 163.14
Fragment 4: 120.08
Fragment 5: 121.09
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

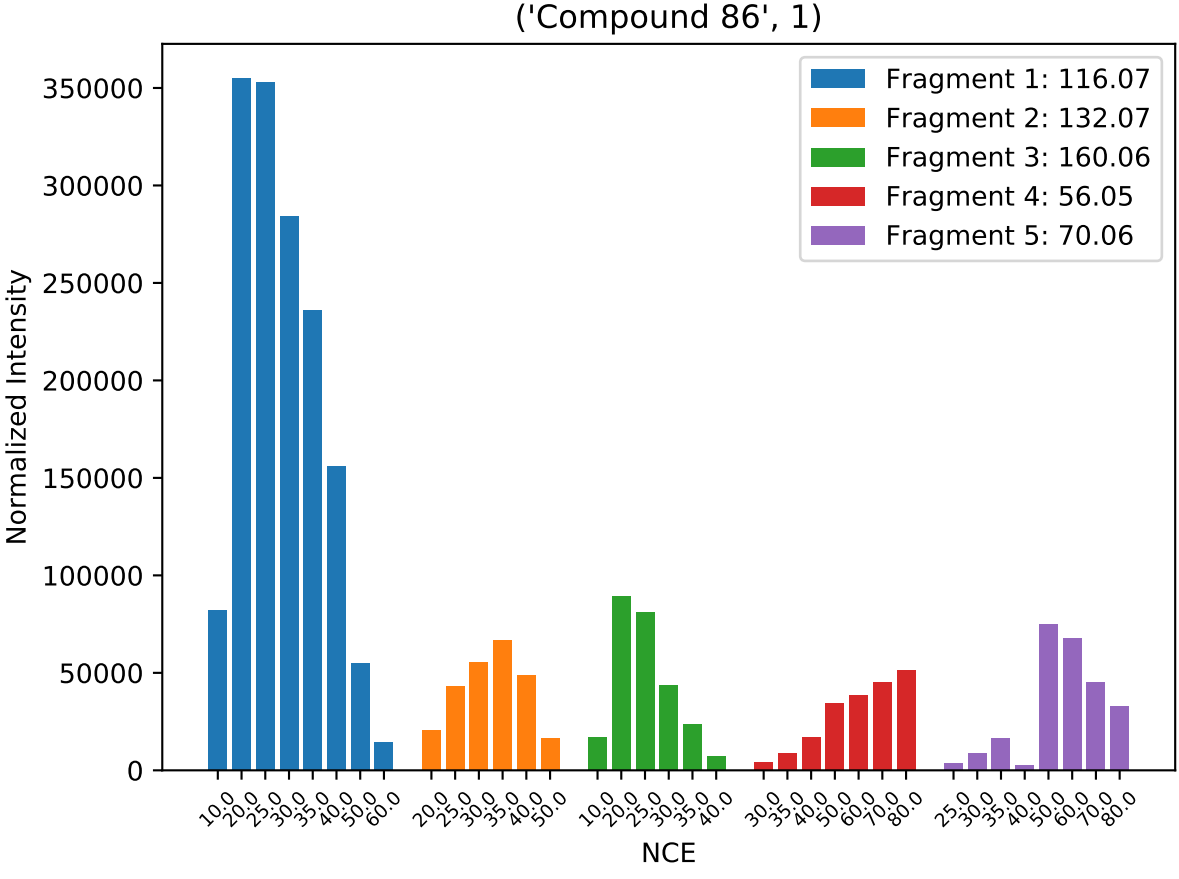

('Compound 77', 1)
Fragment 1: 108.01
Fragment 2: 109.0
Fragment 3: 81.04
Fragment 4: 108.04
Fragment 5: 53.04
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
40.0
10.0
20.0
25.0
30.0
35.0
30.0
50.0
70.0
NCE

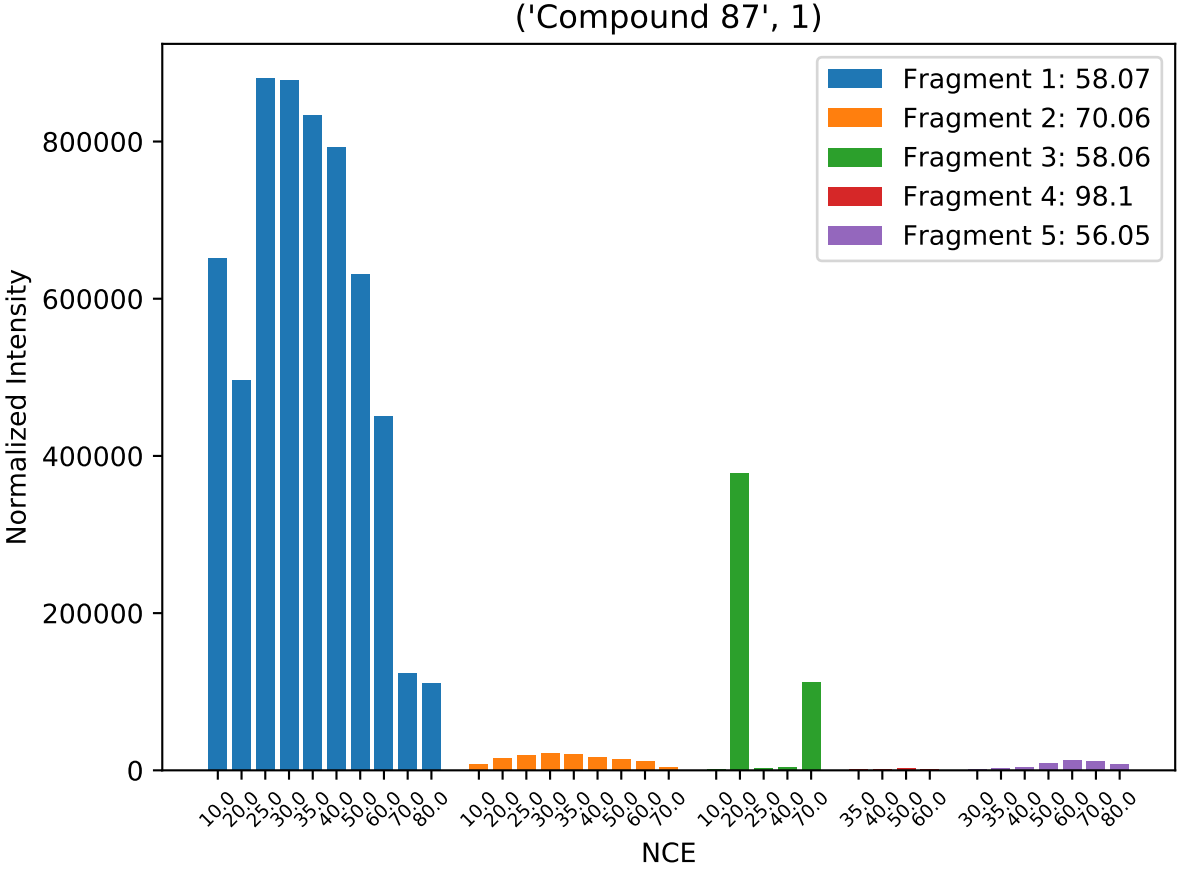

('Compound 79', 1)
Fragment 1: 100.08
Fragment 2: 82.06
Fragment 3: 72.08
Fragment 4: 67.04
Fragment 5: 82.07
Normalized Intensity
600000
500000
400000
300000
200000
100000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0
NCE

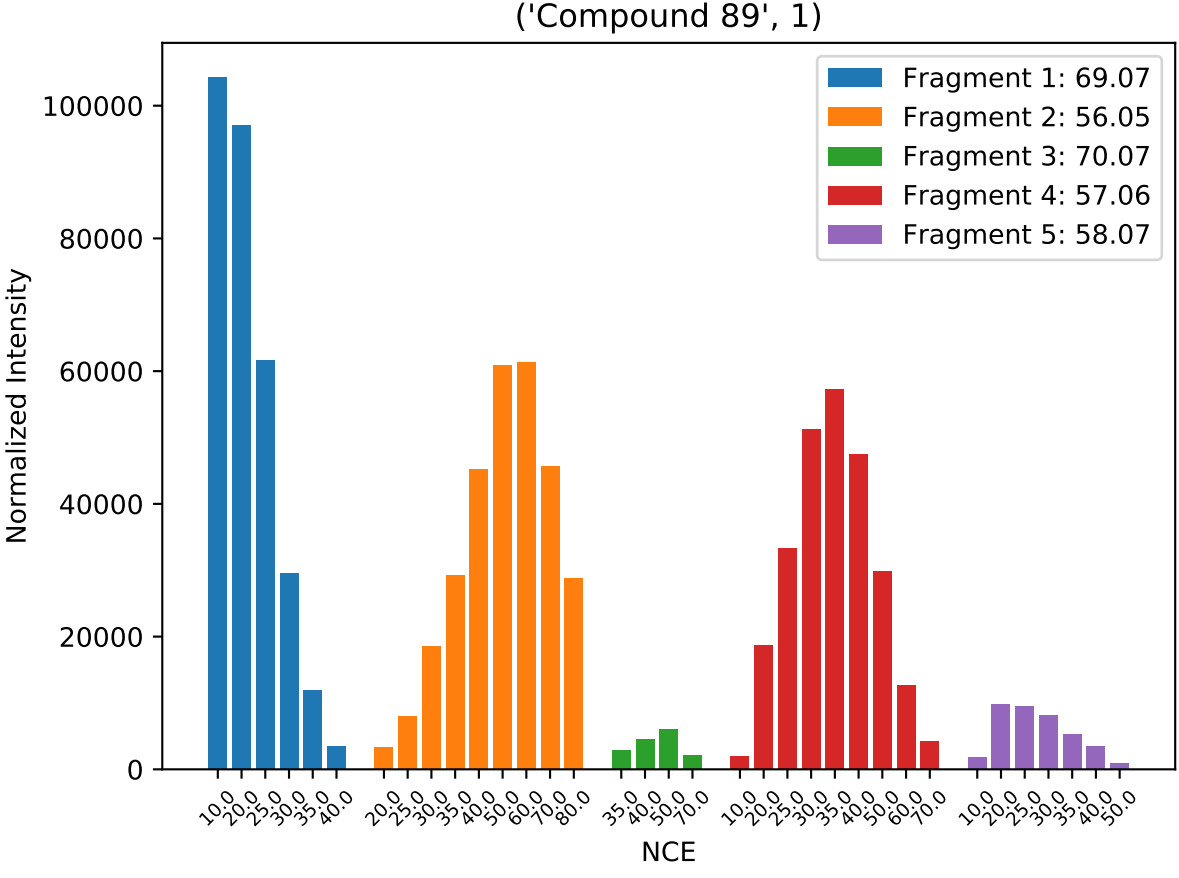

('Compound 81', 1)
Fragment 1: 104.05
Fragment 2: 133.03
Fragment 3: 56.05
Fragment 4: 102.05
Fragment 5: 61.01
Normalized Intensity
0
50000
100000
150000
200000
250000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

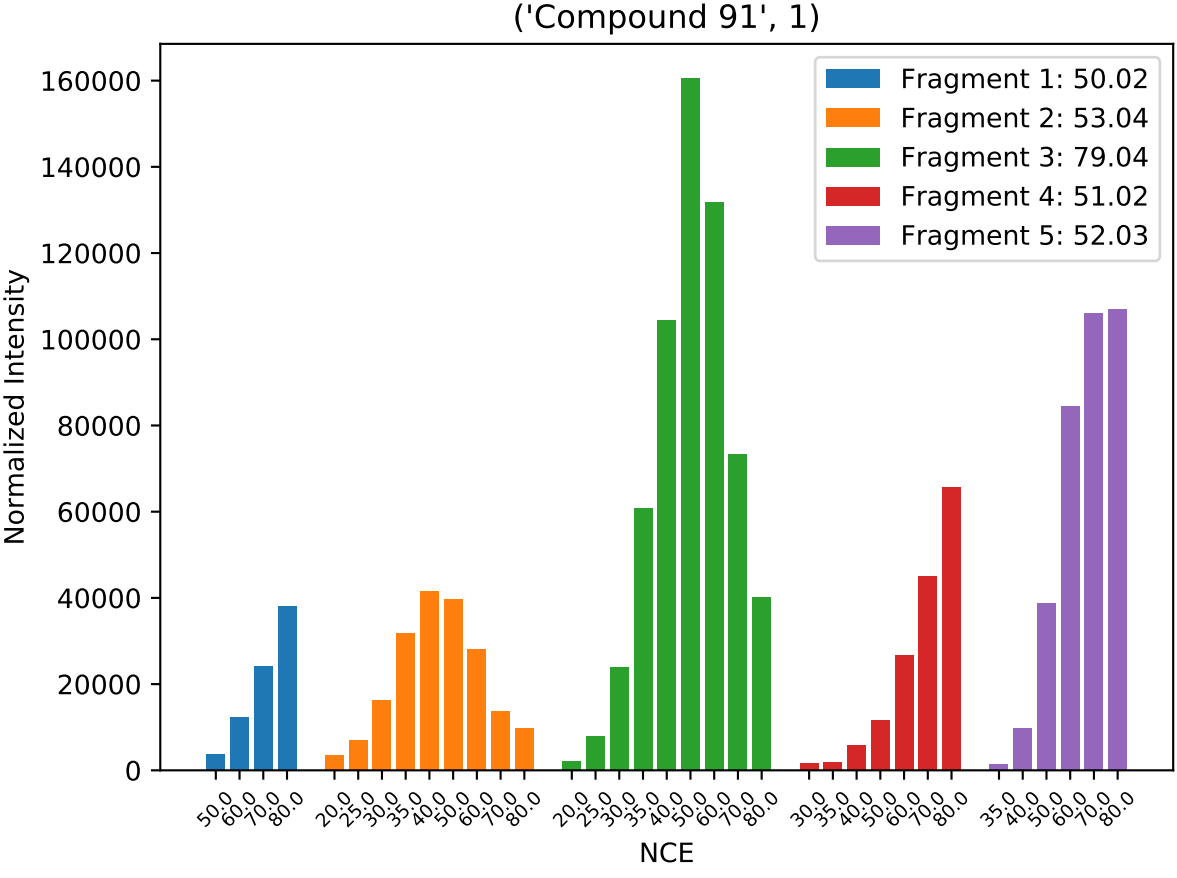

('Compound 82', 1)
Fragment 1: 122.08
Fragment 2: 74.06
Fragment 3: 88.08
Fragment 4: 214.22
Fragment 5: 120.08
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
NCE
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
35.0 40.0 50.0 60.0 70.0 80.0

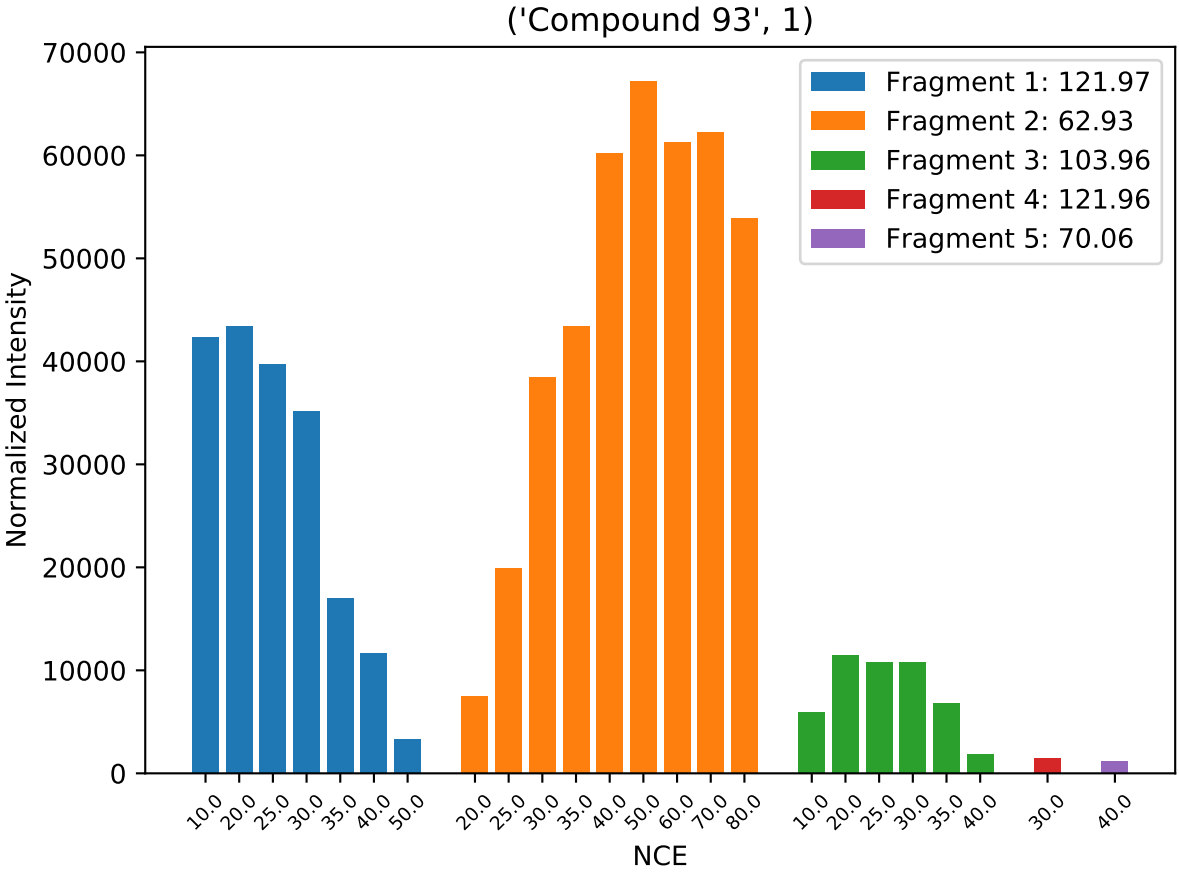

('Compound 83', 1)
Fragment 1: 55.05
Fragment 2: 57.06
Fragment 3: 56.05
Fragment 4: 55.06
Fragment 5: 53.04
Normalized Intensity
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

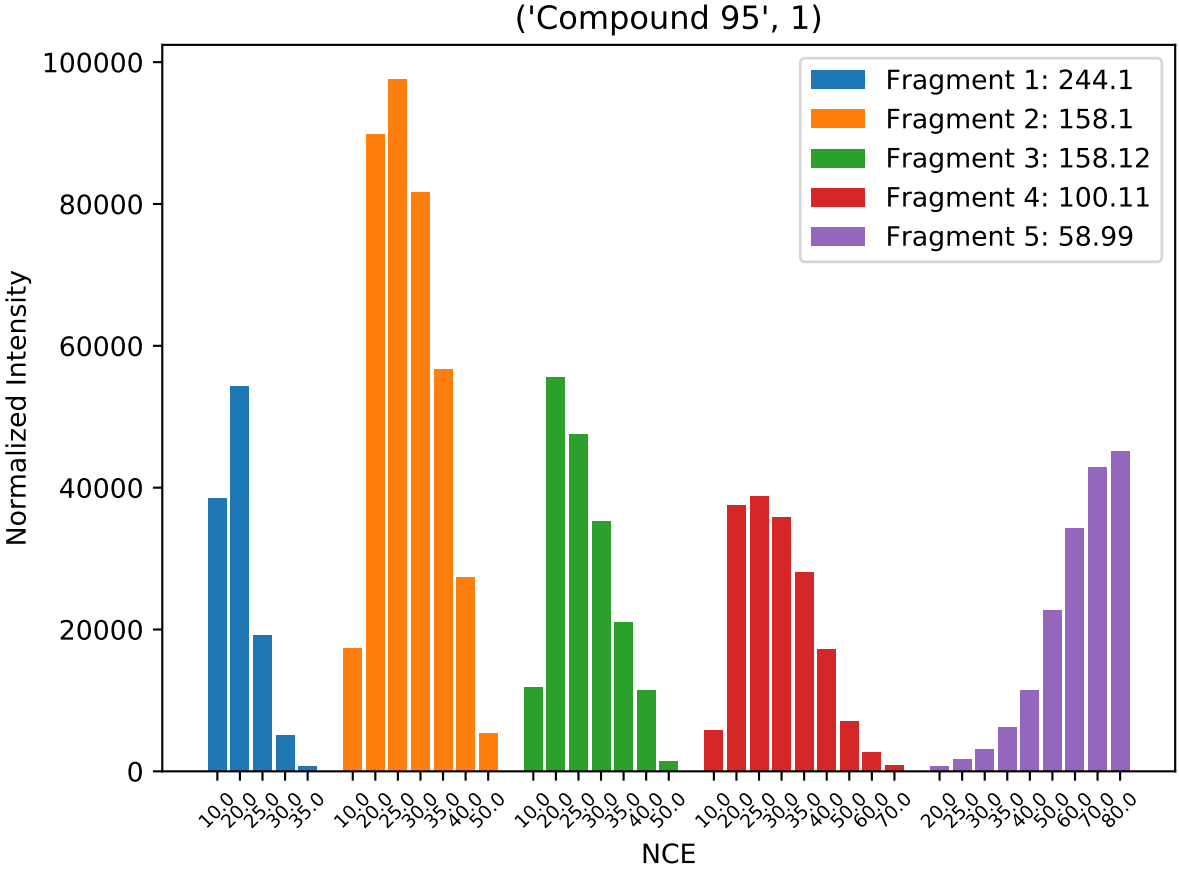

('Compound 86', 1)
Fragment 1: 116.07
Fragment 2: 132.07
Fragment 3: 160.06
Fragment 4: 56.05
Fragment 5: 70.06
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

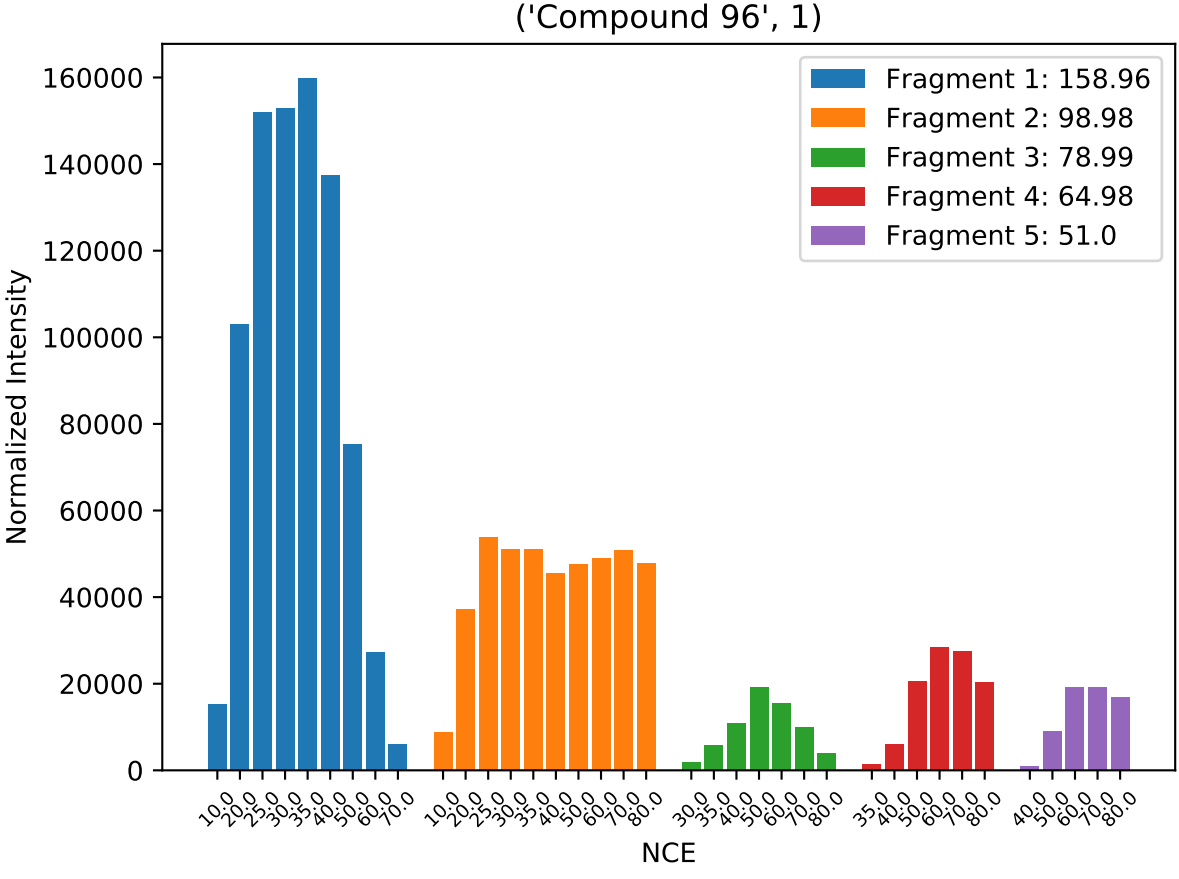

('Compound 87', 1)
Fragment 1: 58.07
Fragment 2: 70.06
Fragment 3: 58.06
Fragment 4: 98.1
Fragment 5: 56.05
Normalized Intensity
0
200000
400000
600000
800000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 40.0 70.0
35.0 40.0 50.0 60.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

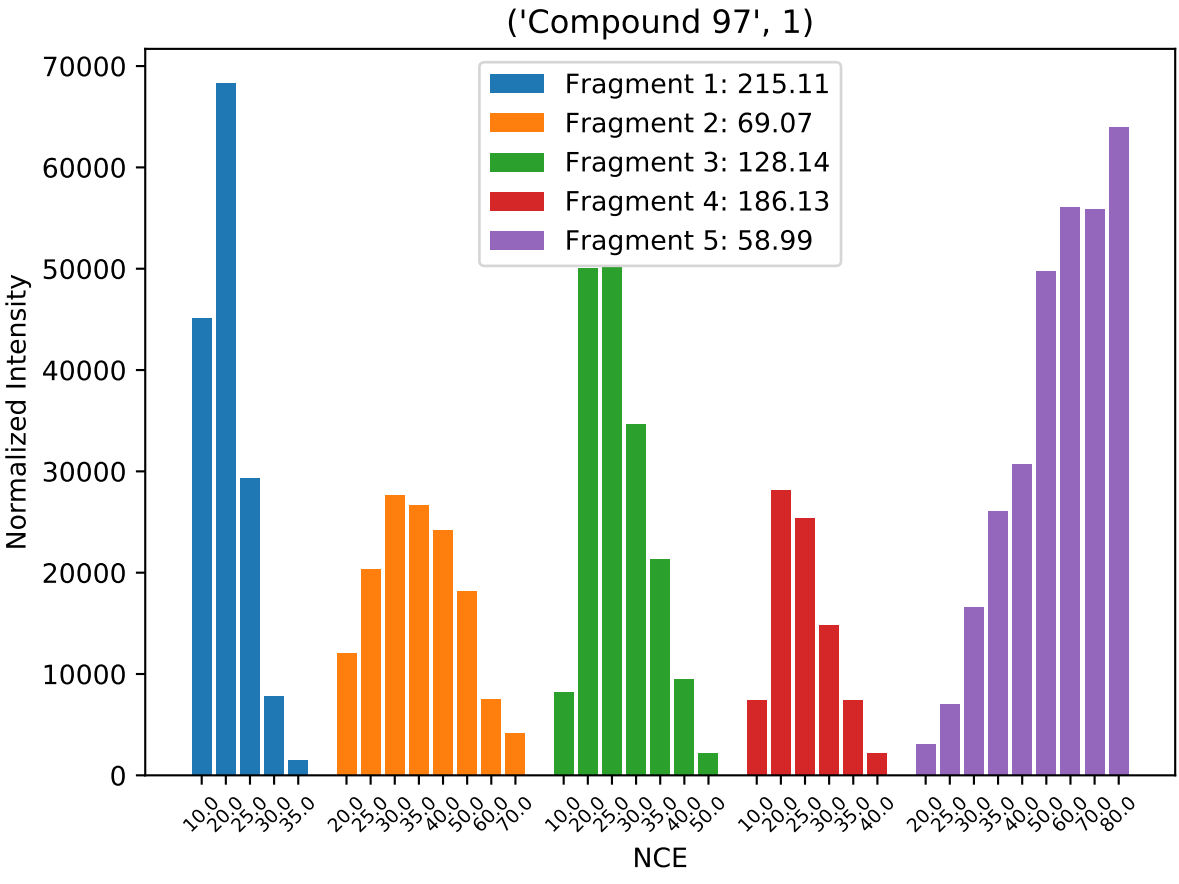

('Compound 89', 1)
Fragment 1: 69.07
Fragment 2: 56.05
Fragment 3: 70.07
Fragment 4: 57.06
Fragment 5: 58.07
Normalized Intensity
0
20000
40000
60000
80000
100000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

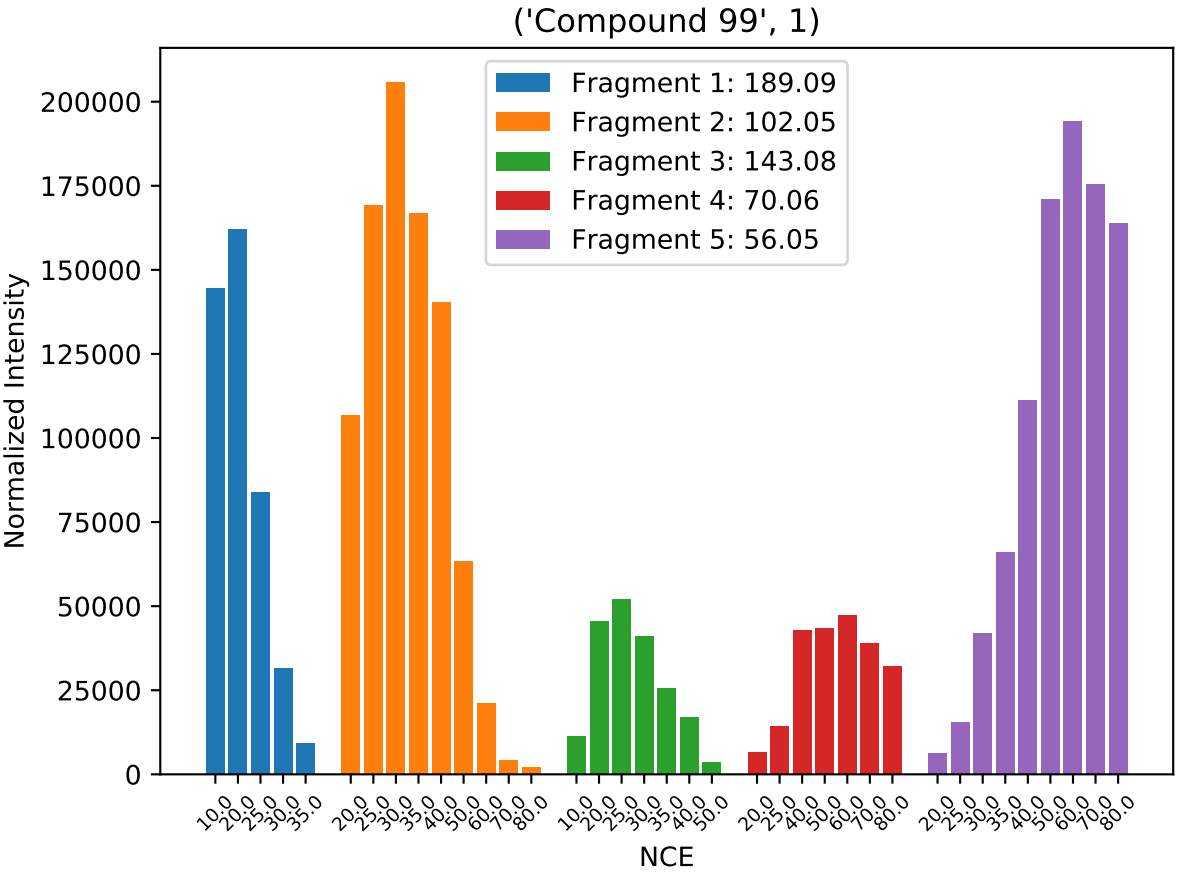

('Compound 91', 1)
Fragment 1: 50.02
Fragment 2: 53.04
Fragment 3: 79.04
Fragment 4: 51.02
Fragment 5: 52.03
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
NCE
50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0

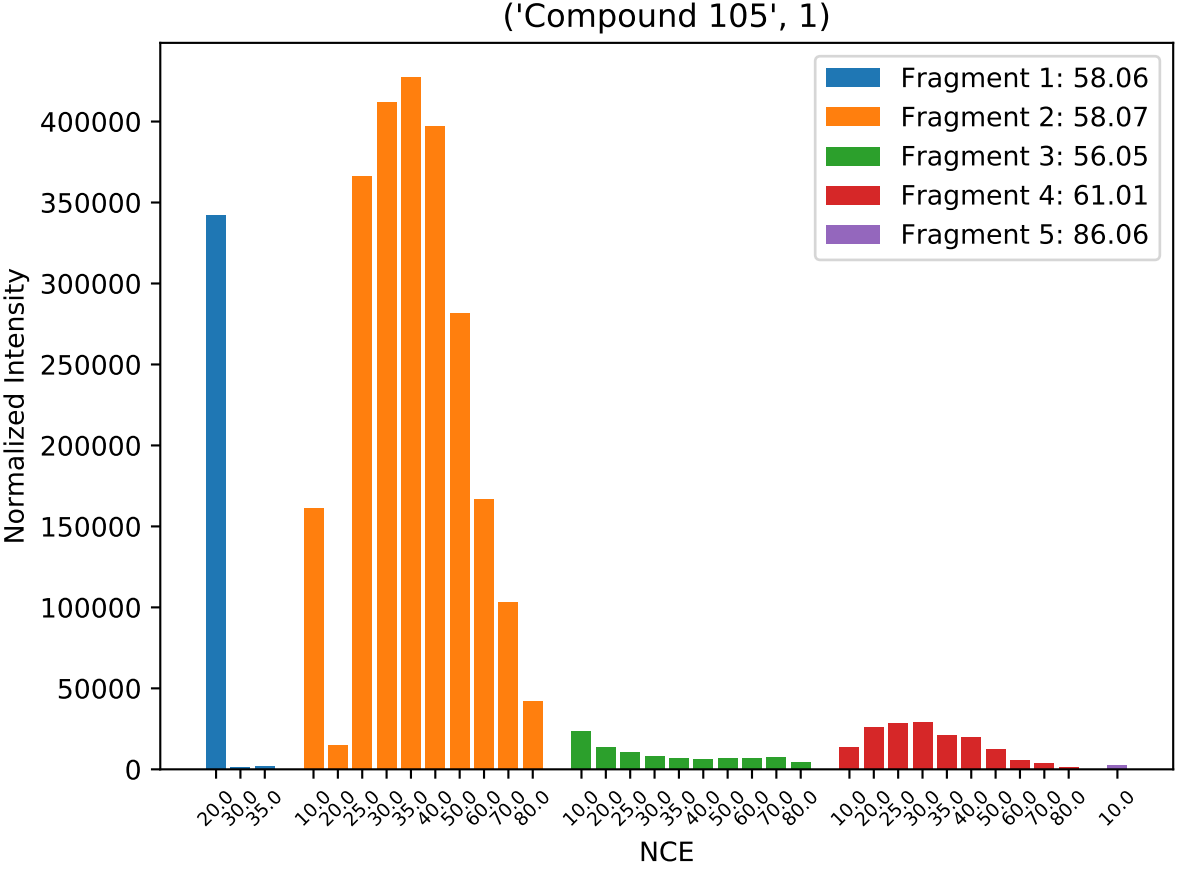

('Compound 93', 1)
Fragment 1: 121.97
Fragment 2: 62.93
Fragment 3: 103.96
Fragment 4: 121.96
Fragment 5: 70.06
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
30.0
40.0
NCE

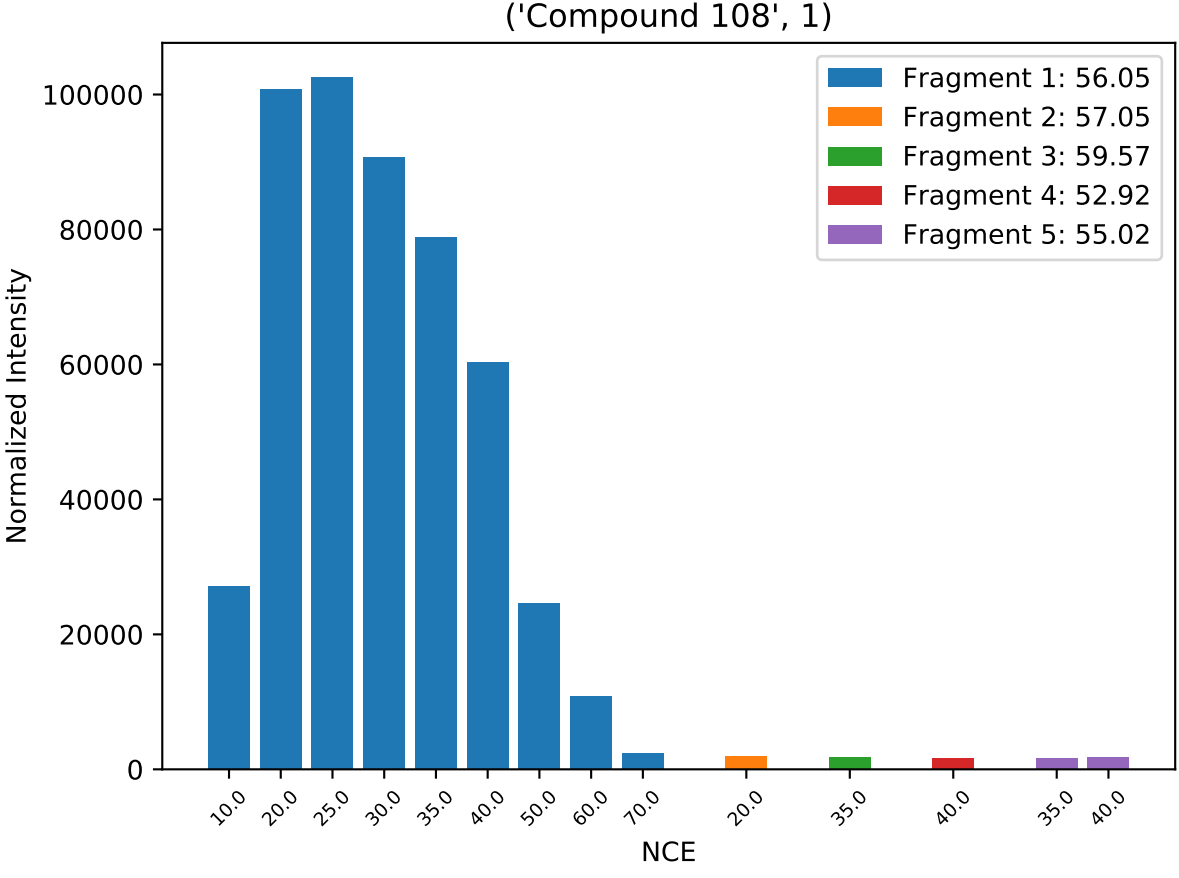

('Compound 95', 1)
Fragment 1: 244.1
Fragment 2: 158.1
Fragment 3: 158.12
Fragment 4: 100.11
Fragment 5: 58.99
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

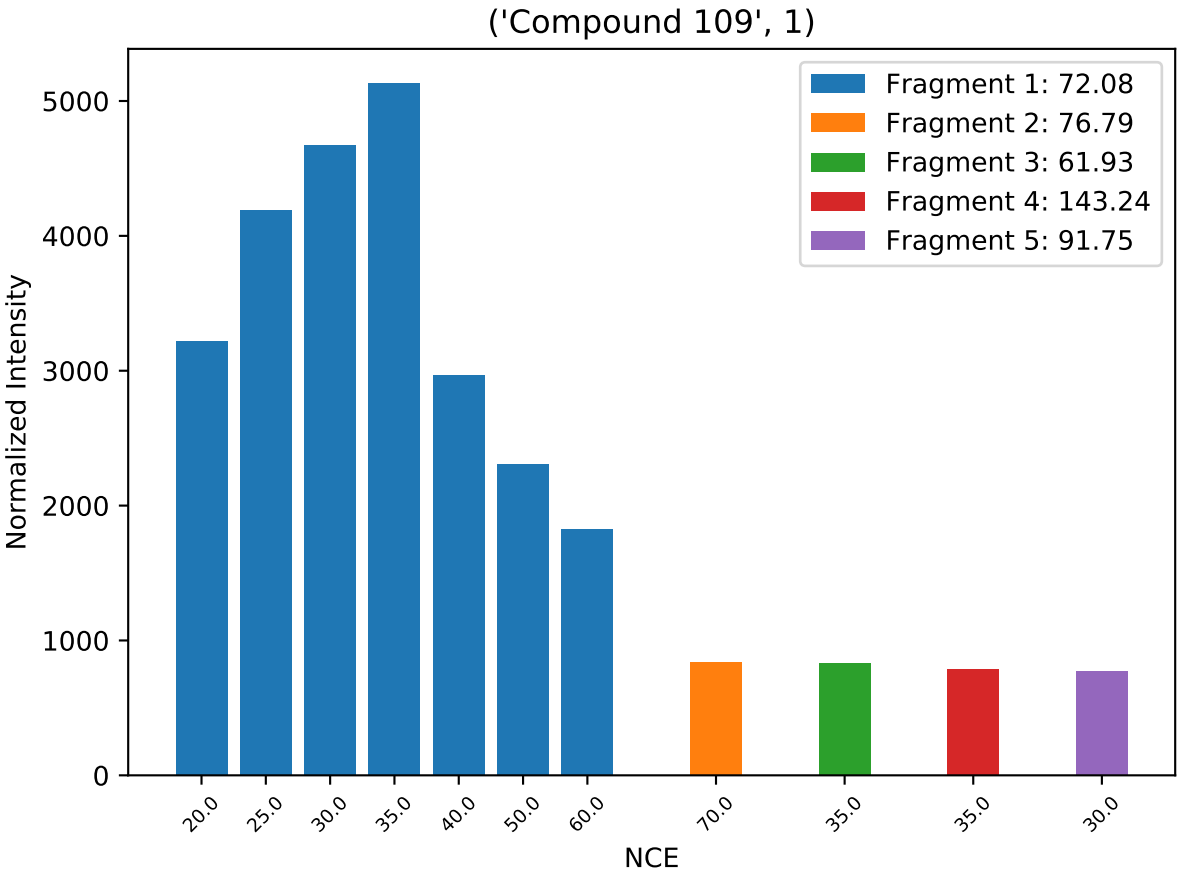

('Compound 96', 1)
Fragment 1: 158.96
Fragment 2: 98.98
Fragment 3: 78.99
Fragment 4: 64.98
Fragment 5: 51.0
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
NCE

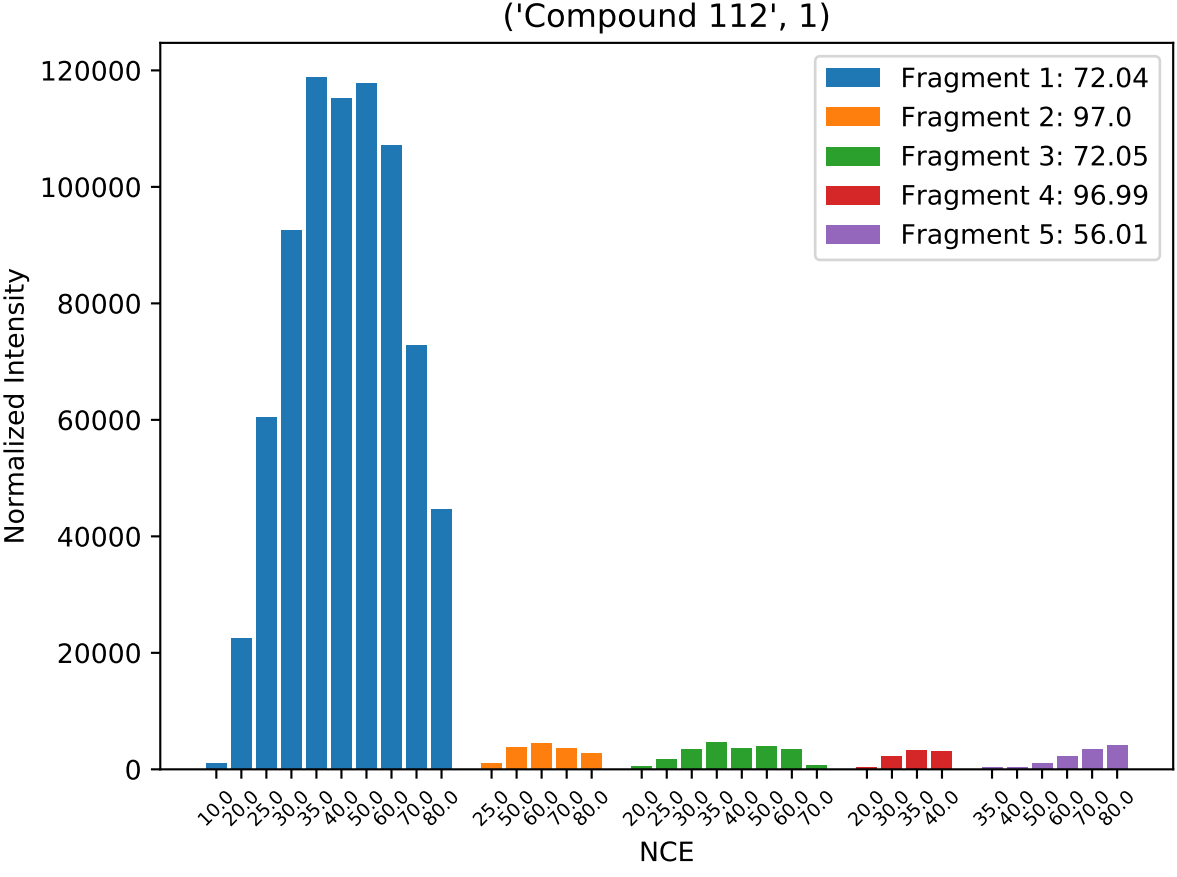

('Compound 97', 1)
Fragment 1: 215.11
Fragment 2: 69.07
Fragment 3: 128.14
Fragment 4: 186.13
Fragment 5: 58.99
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

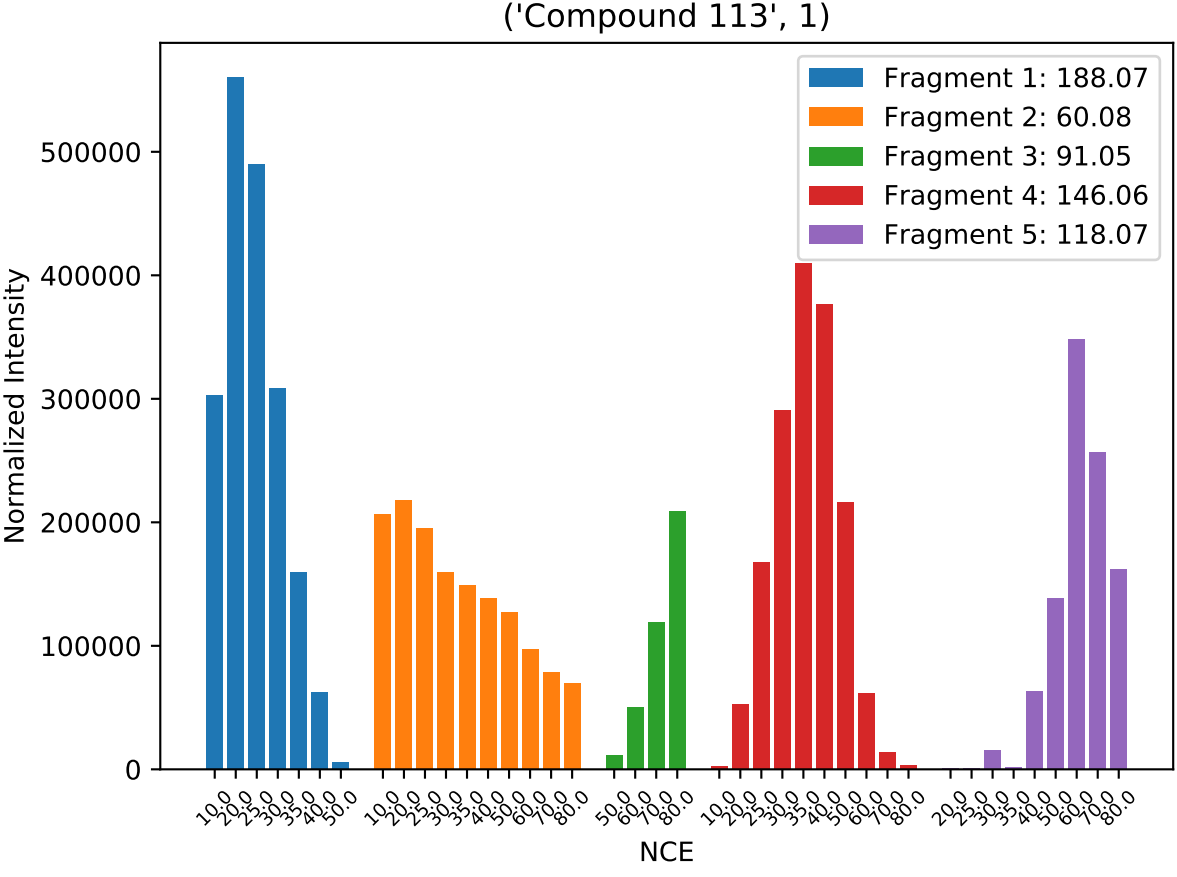

('Compound 99', 1)
Fragment 1: 189.09
Fragment 2: 102.05
Fragment 3: 143.08
Fragment 4: 70.06
Fragment 5: 56.05
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
200000
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

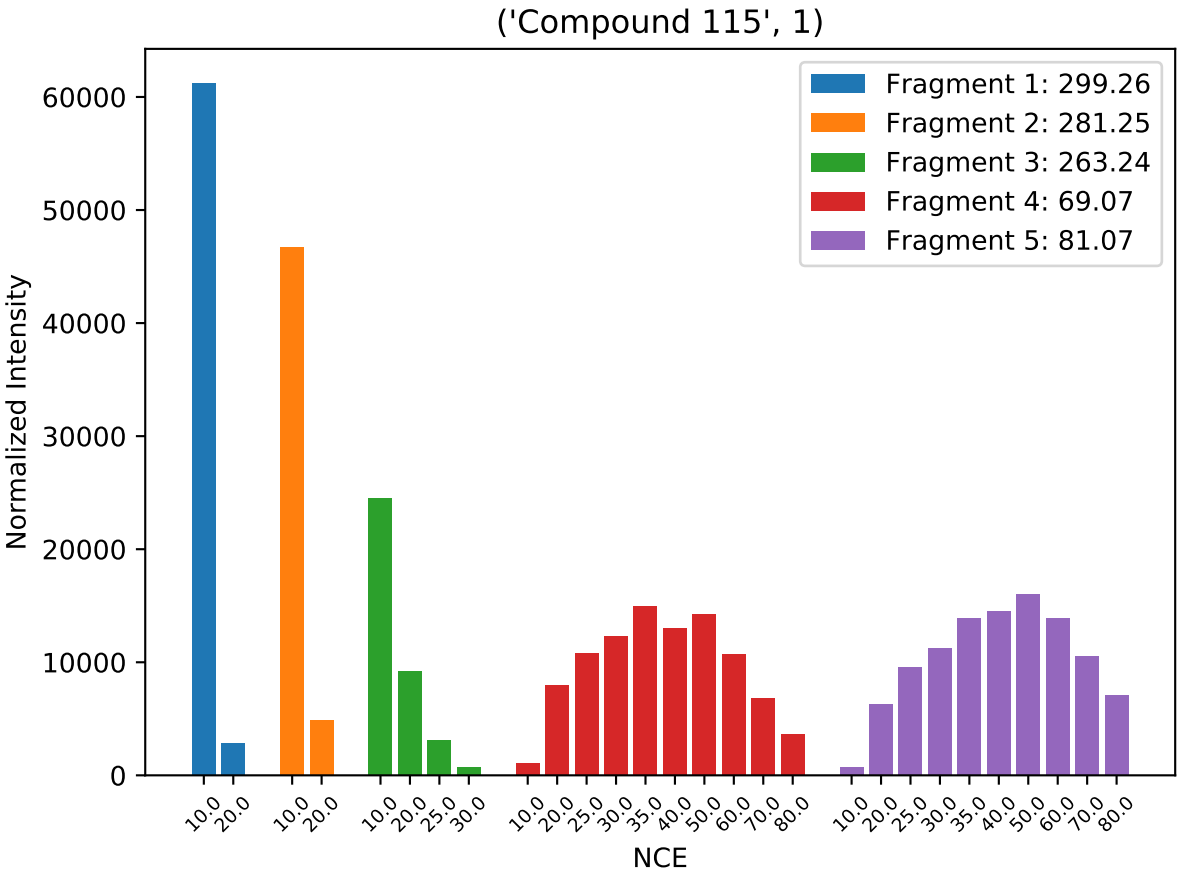

('Compound 105', 1)
Fragment 1: 58.06
Fragment 2: 58.07
Fragment 3: 56.05
Fragment 4: 61.01
Fragment 5: 86.06
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
400000
20.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
NCE

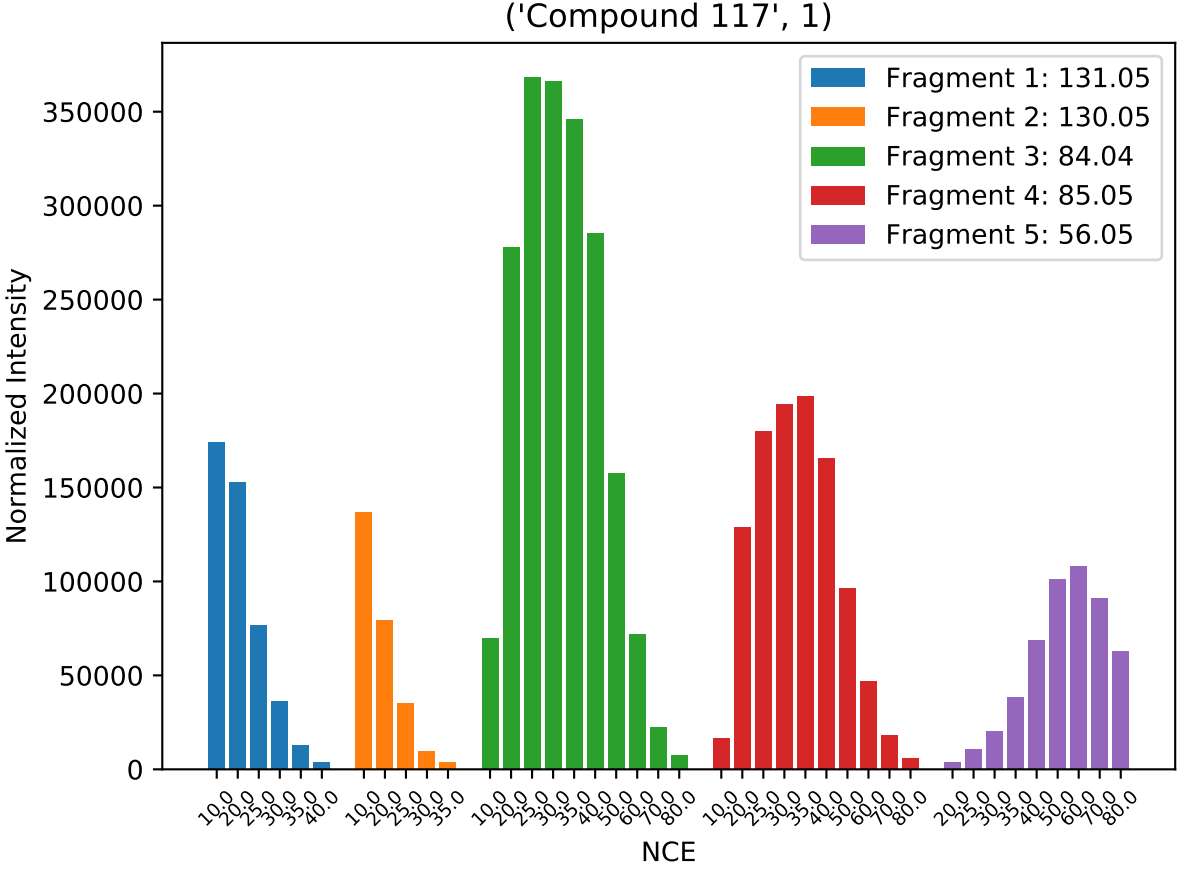

('Compound 108', 1)
Fragment 1: 56.05
Fragment 2: 57.05
Fragment 3: 59.57
Fragment 4: 52.92
Fragment 5: 55.02
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
35.0
40.0
35.0
40.0
NCE

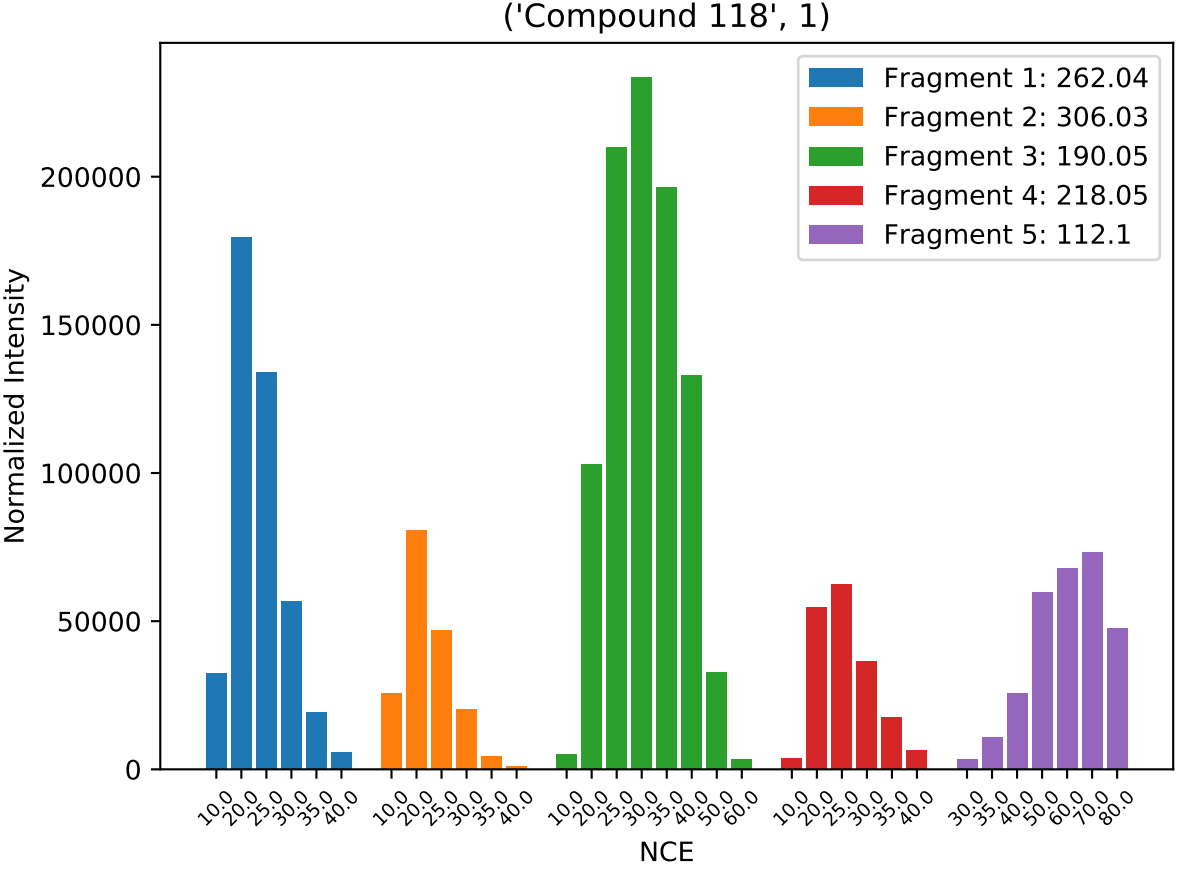

('Compound 109', 1)
Fragment 1: 72.08
Fragment 2: 76.79
Fragment 3: 61.93
Fragment 4: 143.24
Fragment 5: 91.75
Normalized Intensity
0
1000
2000
3000
4000
5000
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
35.0
35.0
30.0
NCE

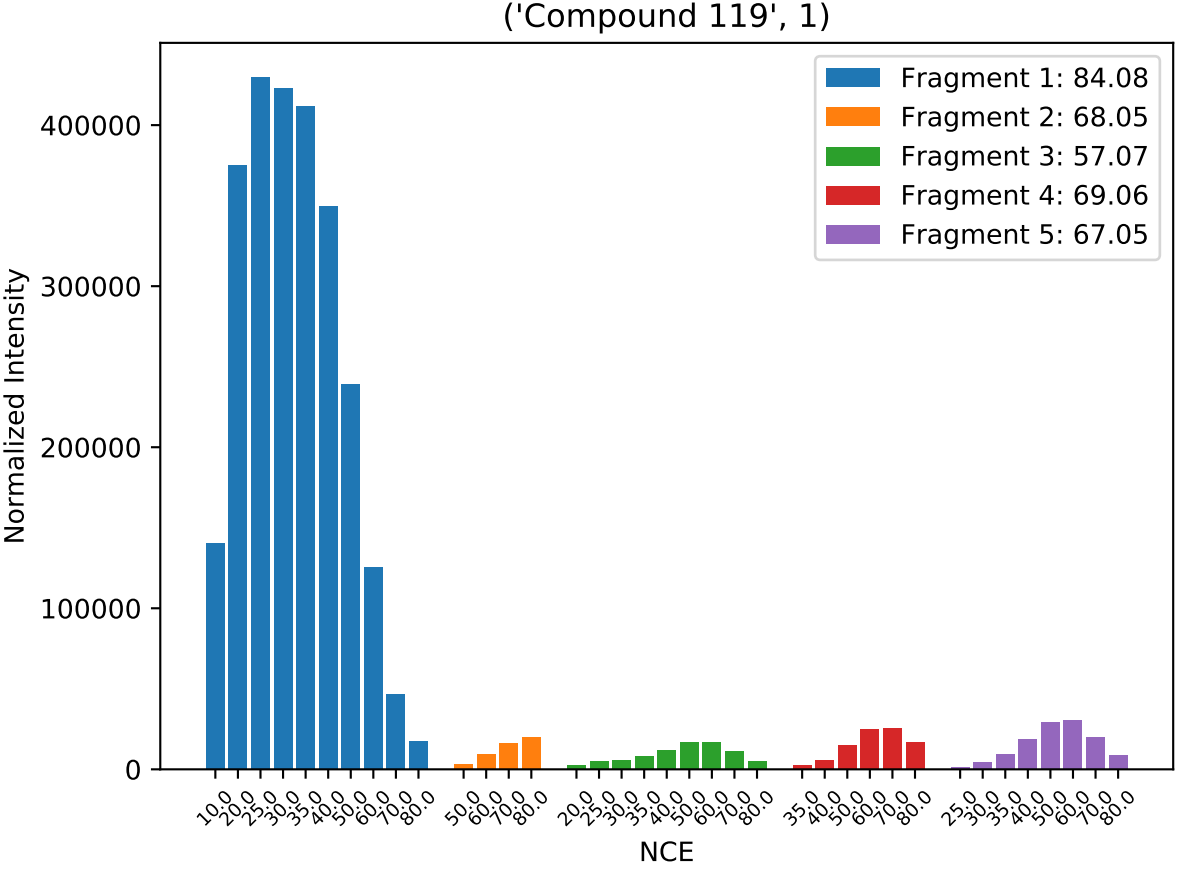

('Compound 112', 1)
Fragment 1: 72.04
Fragment 2: 97.0
Fragment 3: 72.05
Fragment 4: 96.99
Fragment 5: 56.01
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
30.0
35.0
40.0
35.0
40.0
50.0
60.0
70.0
80.0

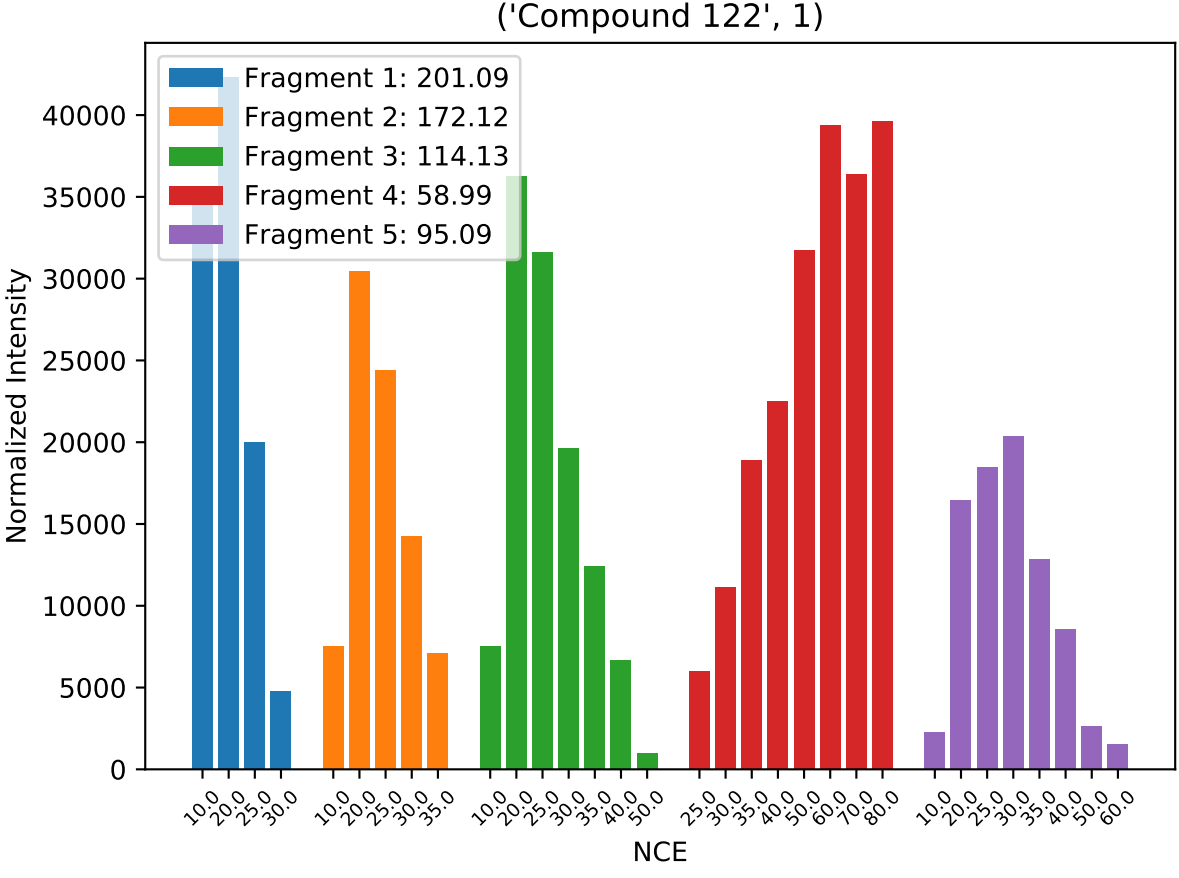

('Compound 113', 1)
Fragment 1: 188.07
Fragment 2: 60.08
Fragment 3: 91.05
Fragment 4: 146.06
Fragment 5: 118.07
Normalized Intensity
0
100000
200000
300000
400000
500000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

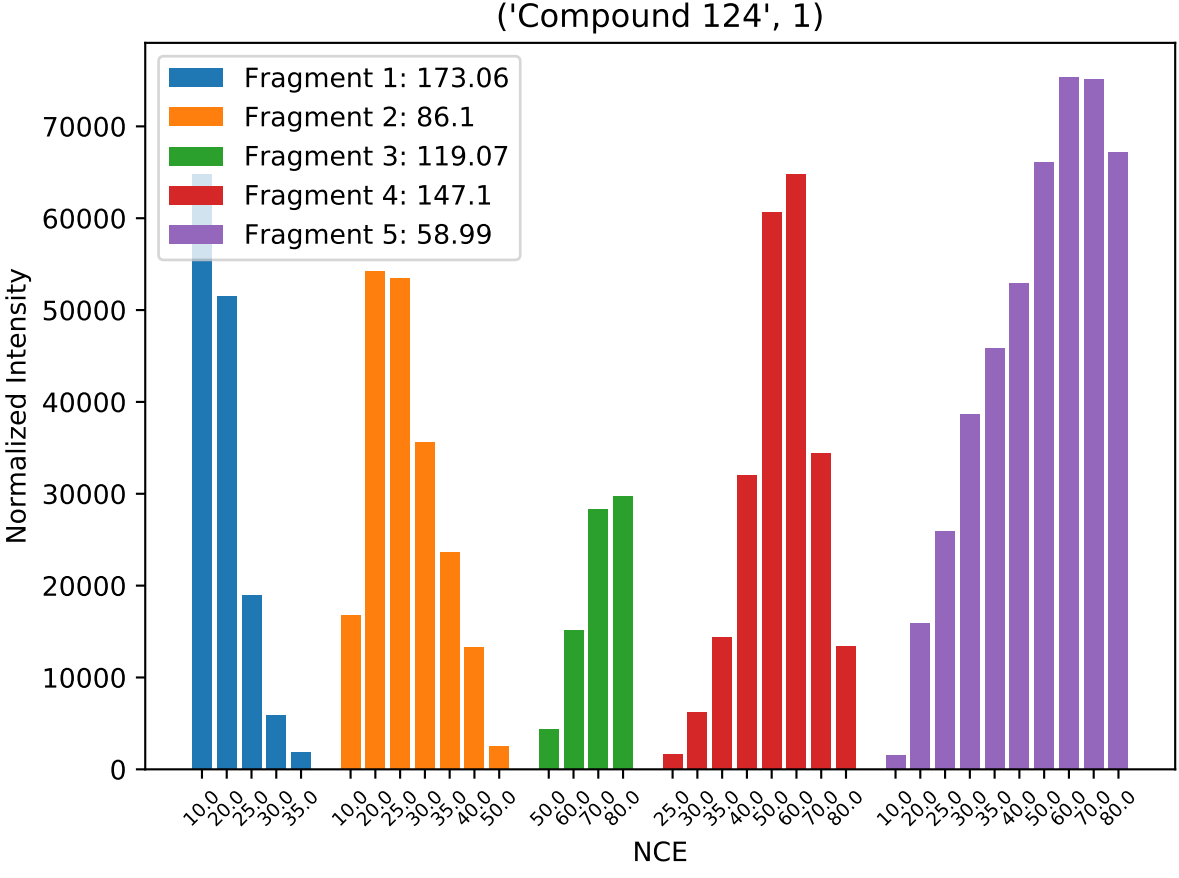

('Compound 115', 1)
Fragment 1: 299.26
Fragment 2: 281.25
Fragment 3: 263.24
Fragment 4: 69.07
Fragment 5: 81.07
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

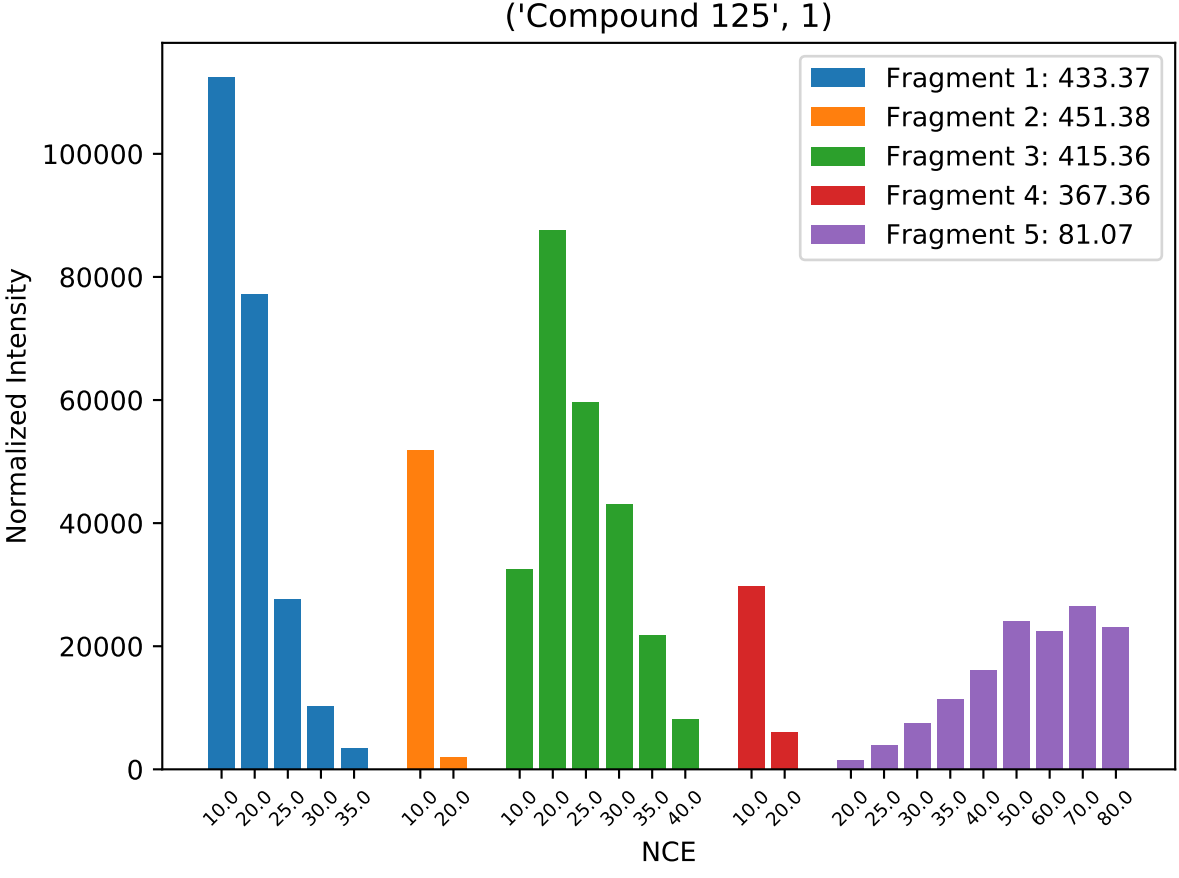

('Compound 117', 1)
Fragment 1: 131.05
Fragment 2: 130.05
Fragment 3: 84.04
Fragment 4: 85.05
Fragment 5: 56.05
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

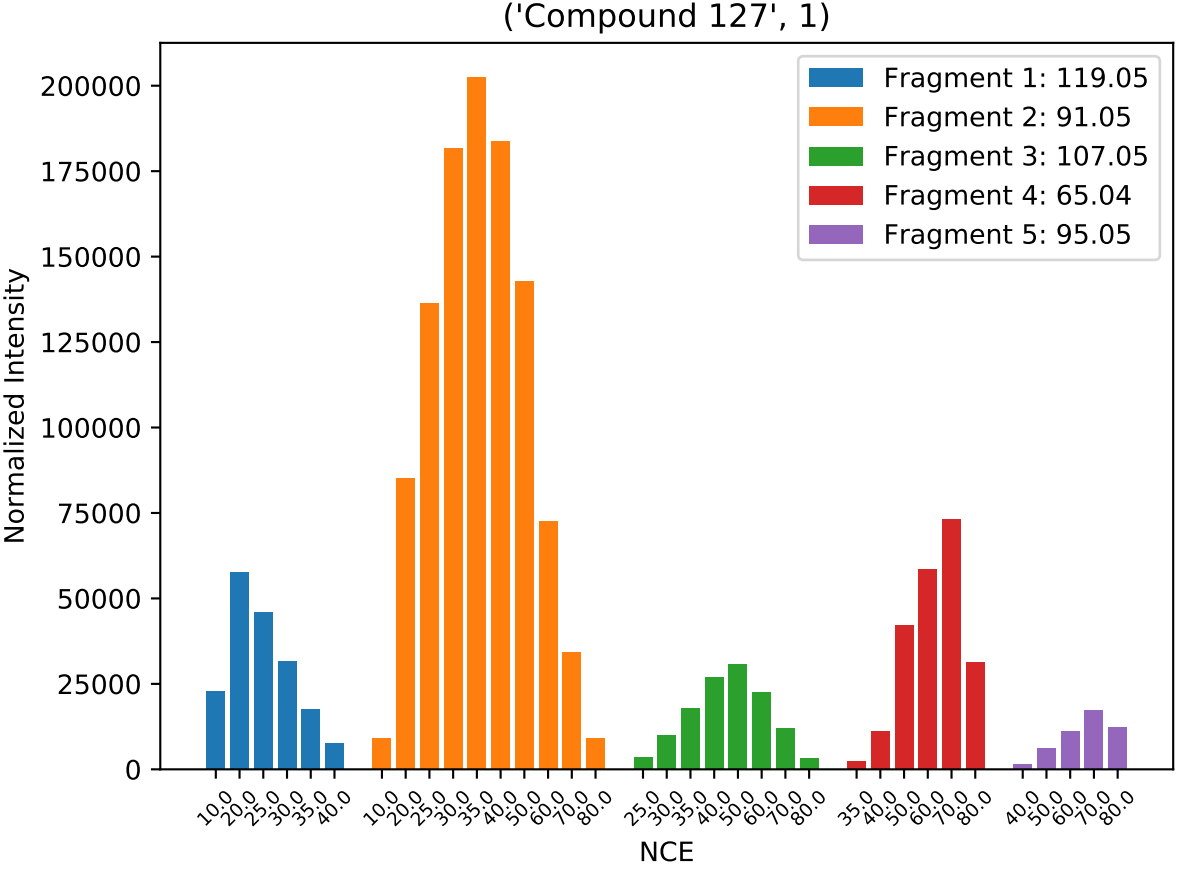

('Compound 118', 1)
Fragment 1: 262.04
Fragment 2: 306.03
Fragment 3: 190.05
Fragment 4: 218.05
Fragment 5: 112.1
Normalized Intensity
0
50000
100000
150000
200000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

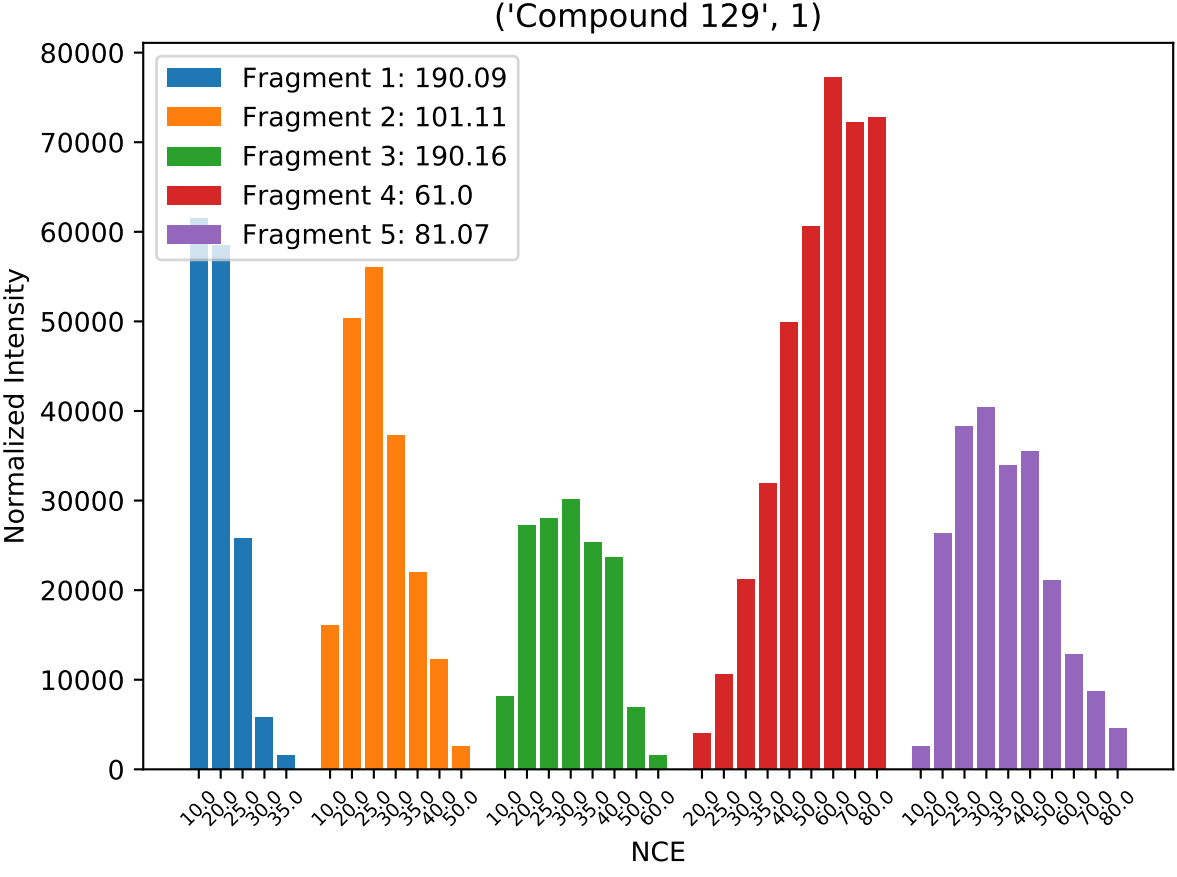

('Compound 119', 1)
Fragment 1: 84.08
Fragment 2: 68.05
Fragment 3: 57.07
Fragment 4: 69.06
Fragment 5: 67.05
Normalized Intensity
0
100000
200000
300000
400000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

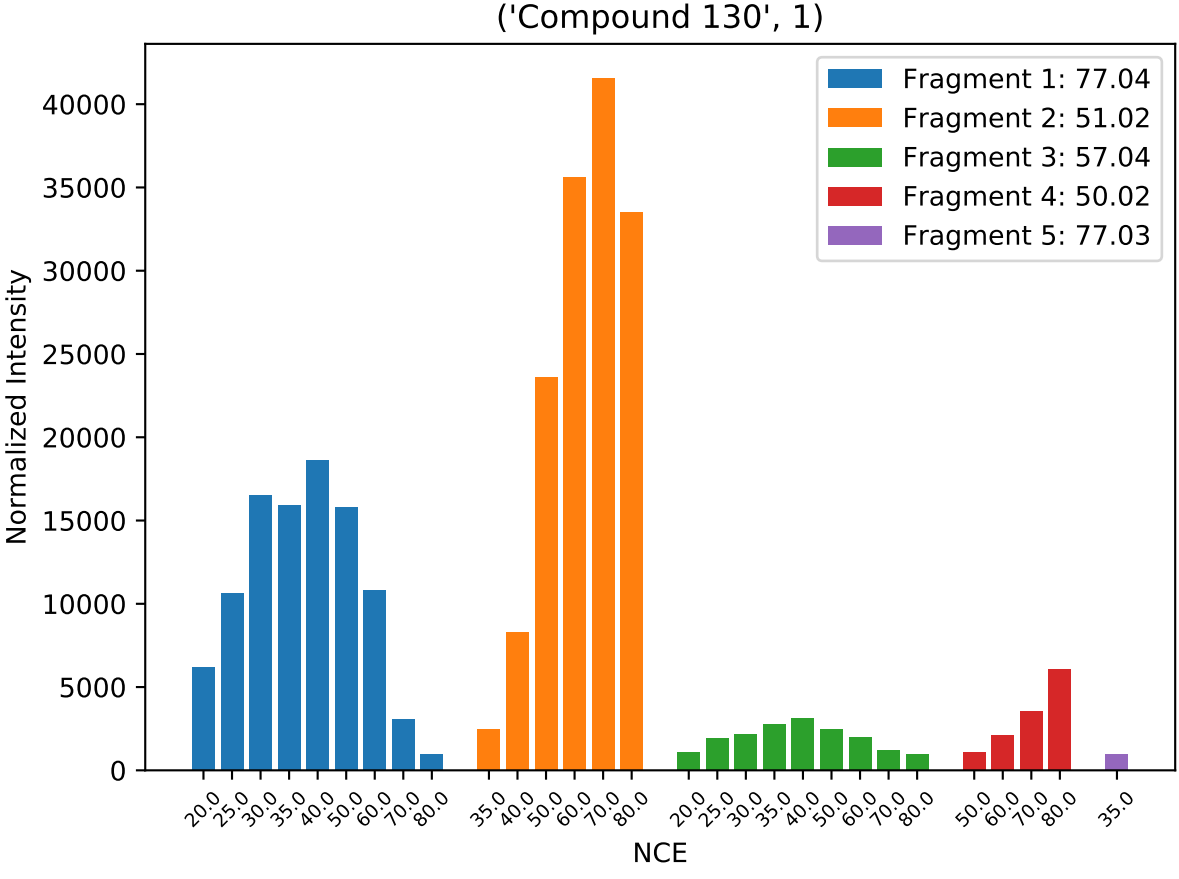

('Compound 122', 1)
Fragment 1: 201.09
Fragment 2: 172.12
Fragment 3: 114.13
Fragment 4: 58.99
Fragment 5: 95.09
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

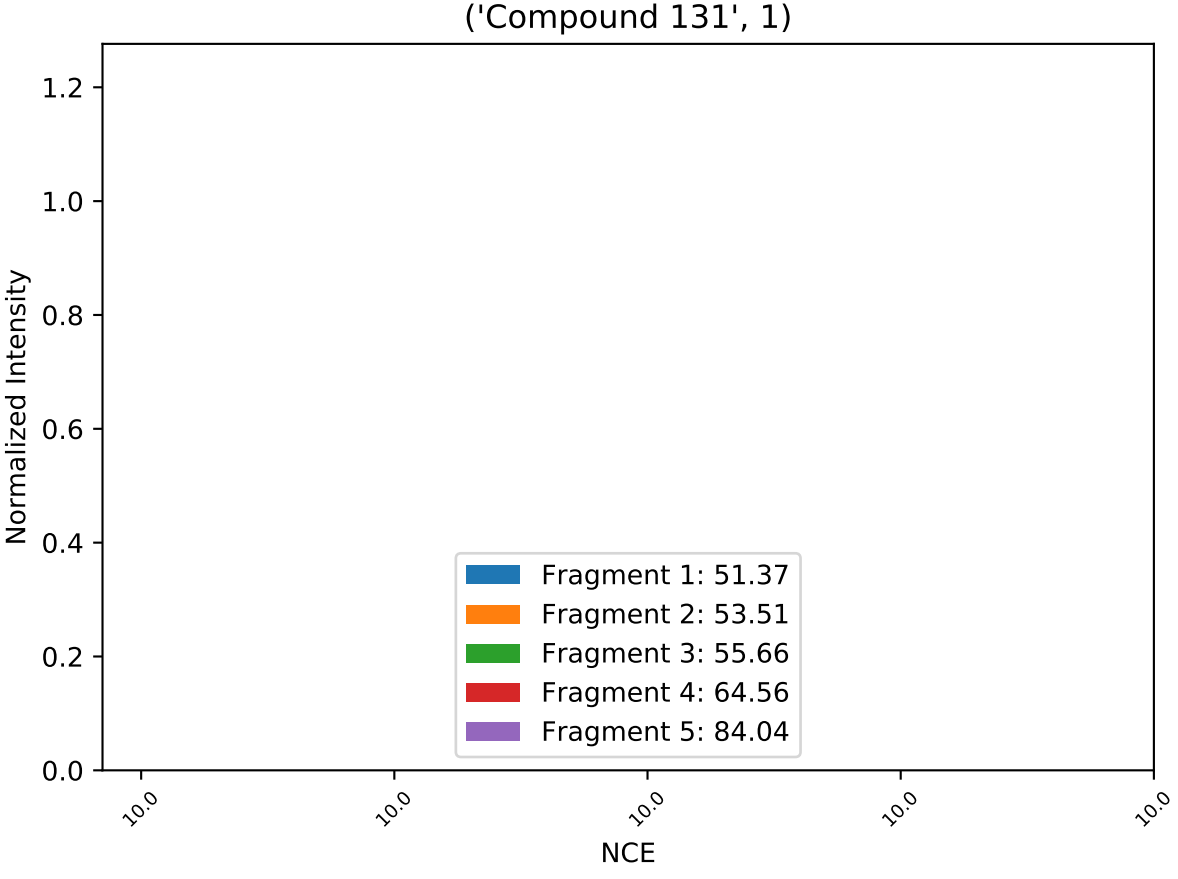

('Compound 124', 1)
Fragment 1: 173.06
Fragment 2: 86.1
Fragment 3: 119.07
Fragment 4: 147.1
Fragment 5: 58.99
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

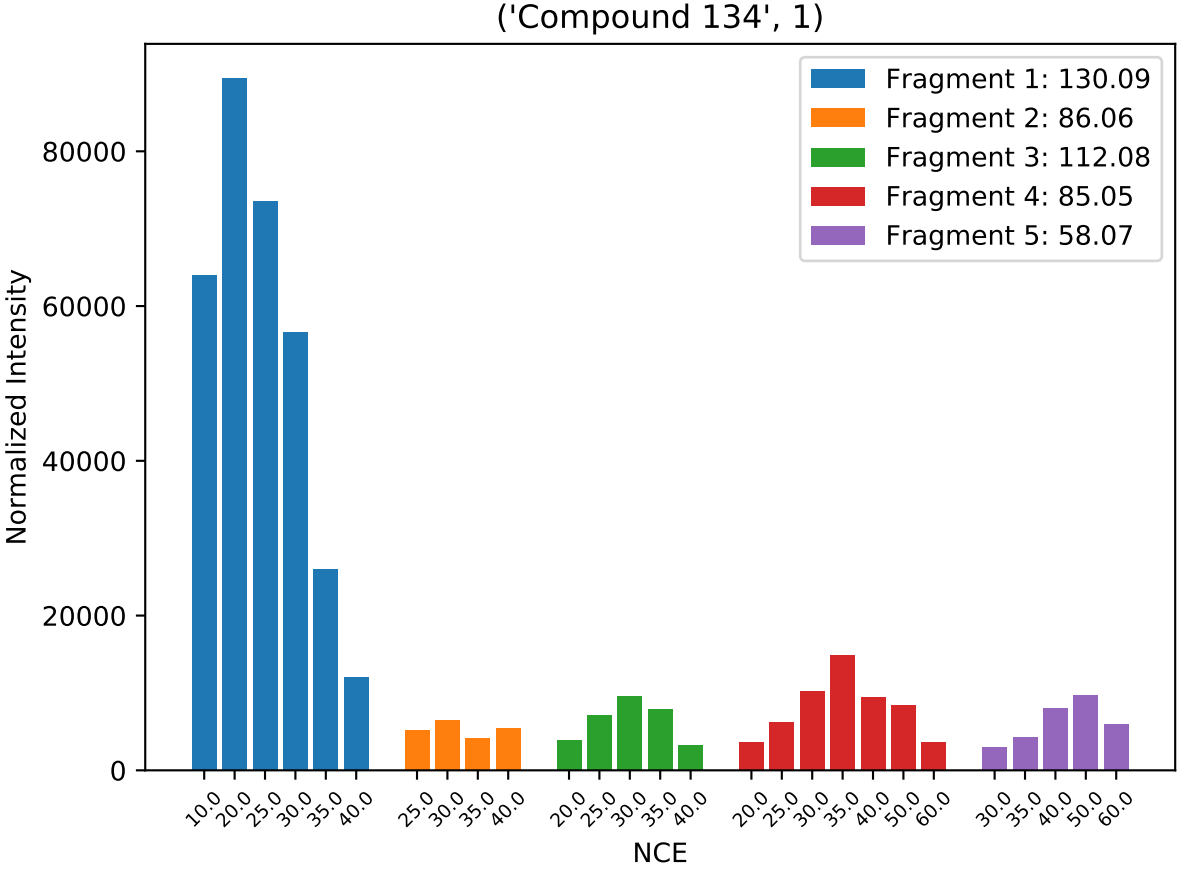

('Compound 125', 1)
Fragment 1: 433.37
Fragment 2: 451.38
Fragment 3: 415.36
Fragment 4: 367.36
Fragment 5: 81.07
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

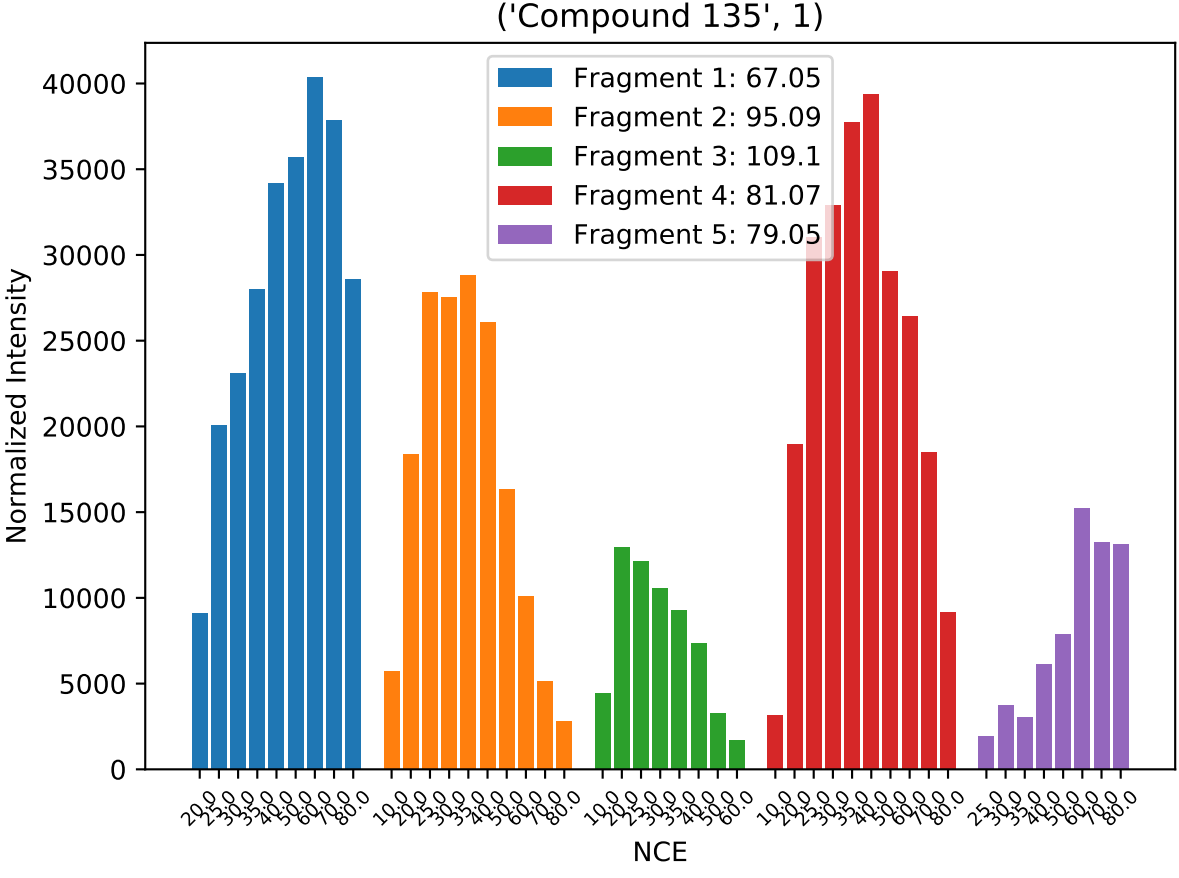

('Compound 127', 1)
Fragment 1: 119.05
Fragment 2: 91.05
Fragment 3: 107.05
Fragment 4: 65.04
Fragment 5: 95.05
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
200000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
NCE

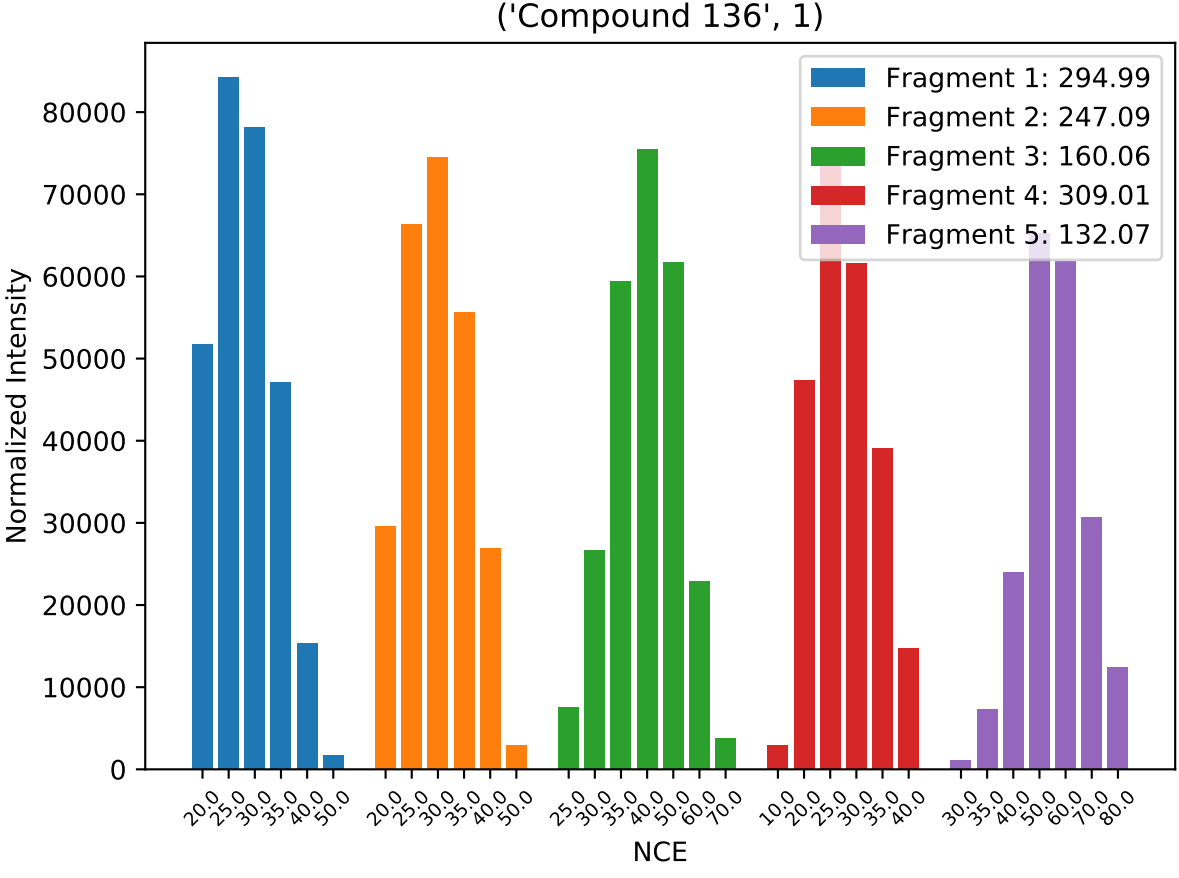

('Compound 129', 1)
Fragment 1: 190.09
Fragment 2: 101.11
Fragment 3: 190.16
Fragment 4: 61.0
Fragment 5: 81.07
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

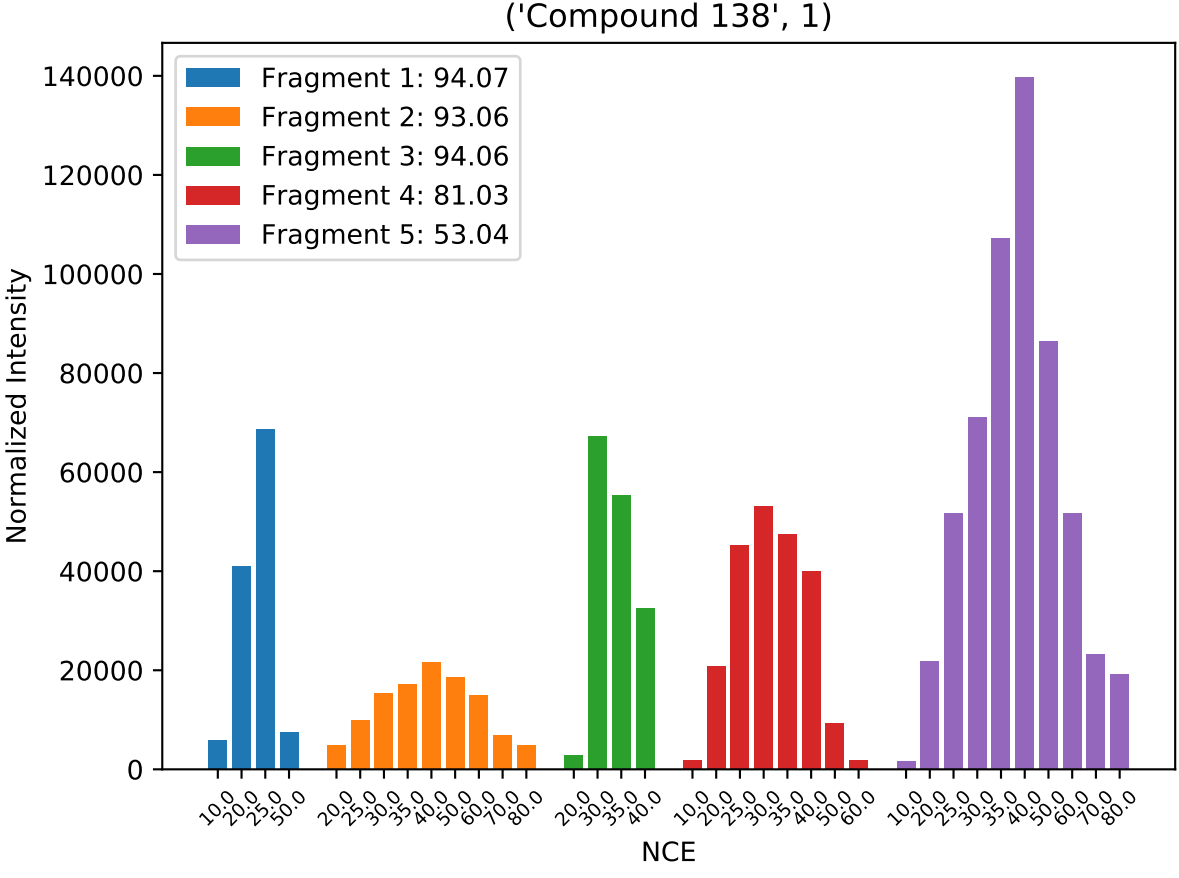

('Compound 130', 1)
Fragment 1: 77.04
Fragment 2: 51.02
Fragment 3: 57.04
Fragment 4: 50.02
Fragment 5: 77.03
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
35.0
NCE

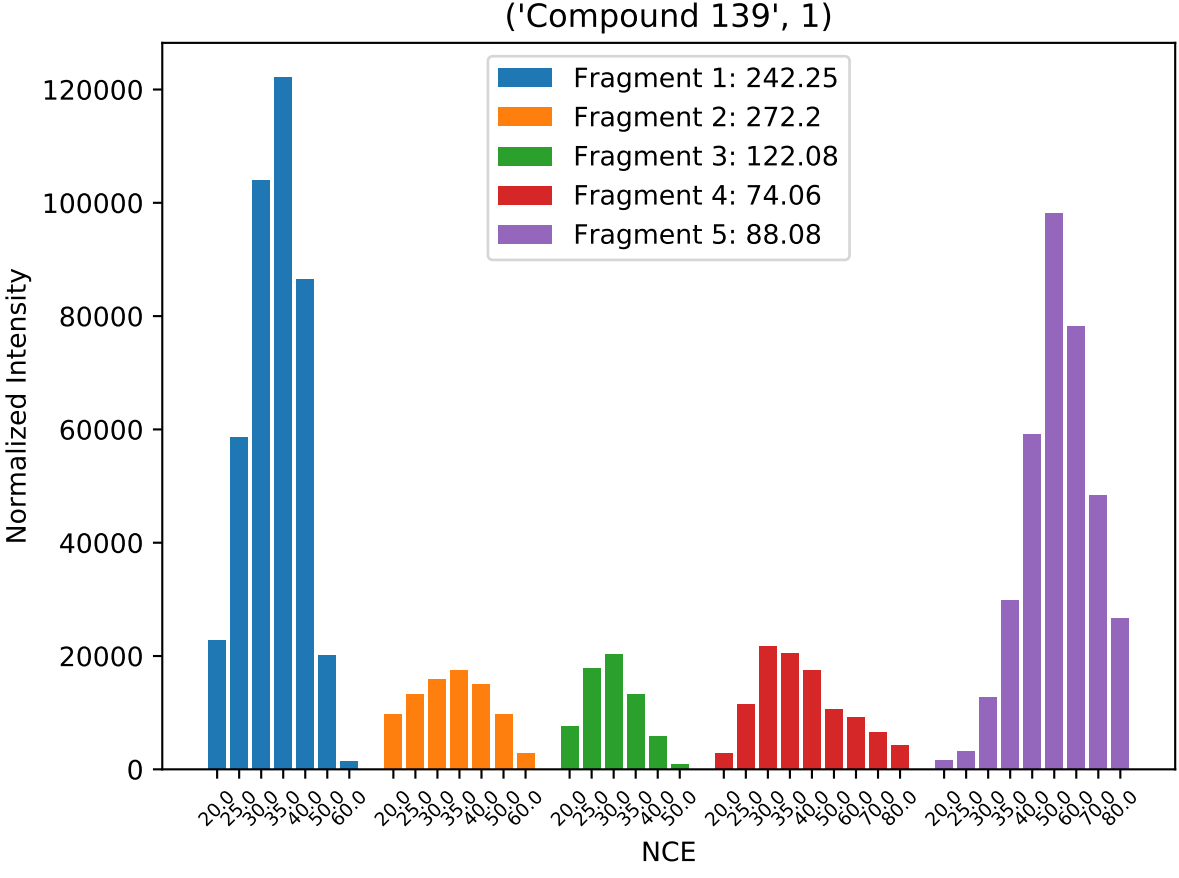

('Compound 131', 1)
Normalized Intensity
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Fragment 1: 51.37
Fragment 2: 53.51
Fragment 3: 55.66
Fragment 4: 64.56
Fragment 5: 84.04
10.0
10.0
10.0
10.0
10.0
NCE

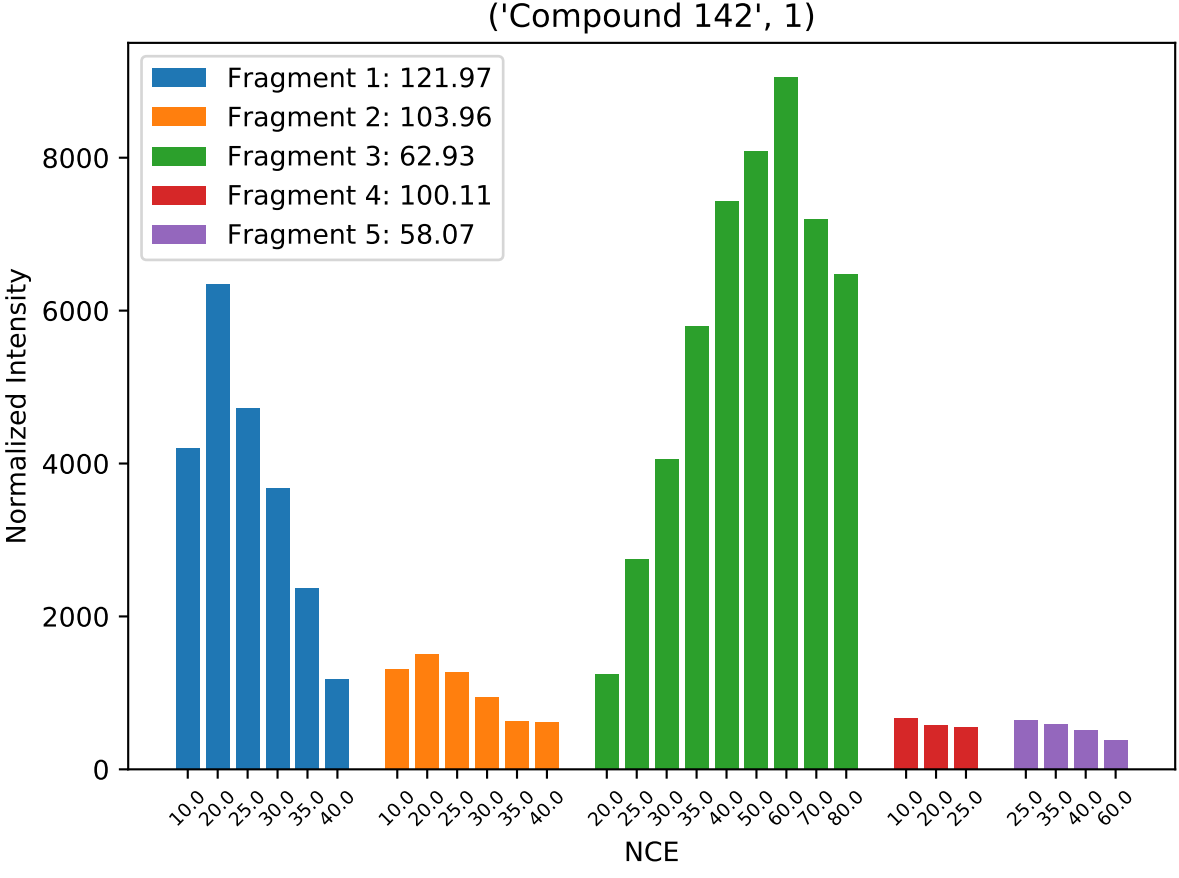

('Compound 134', 1)
Fragment 1: 130.09
Fragment 2: 86.06
Fragment 3: 112.08
Fragment 4: 85.05
Fragment 5: 58.07
Normalized Intensity
0
20000
40000
60000
80000
10.0 20.0 25.0 30.0 35.0 40.0
25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
30.0 35.0 40.0 50.0 60.0
NCE

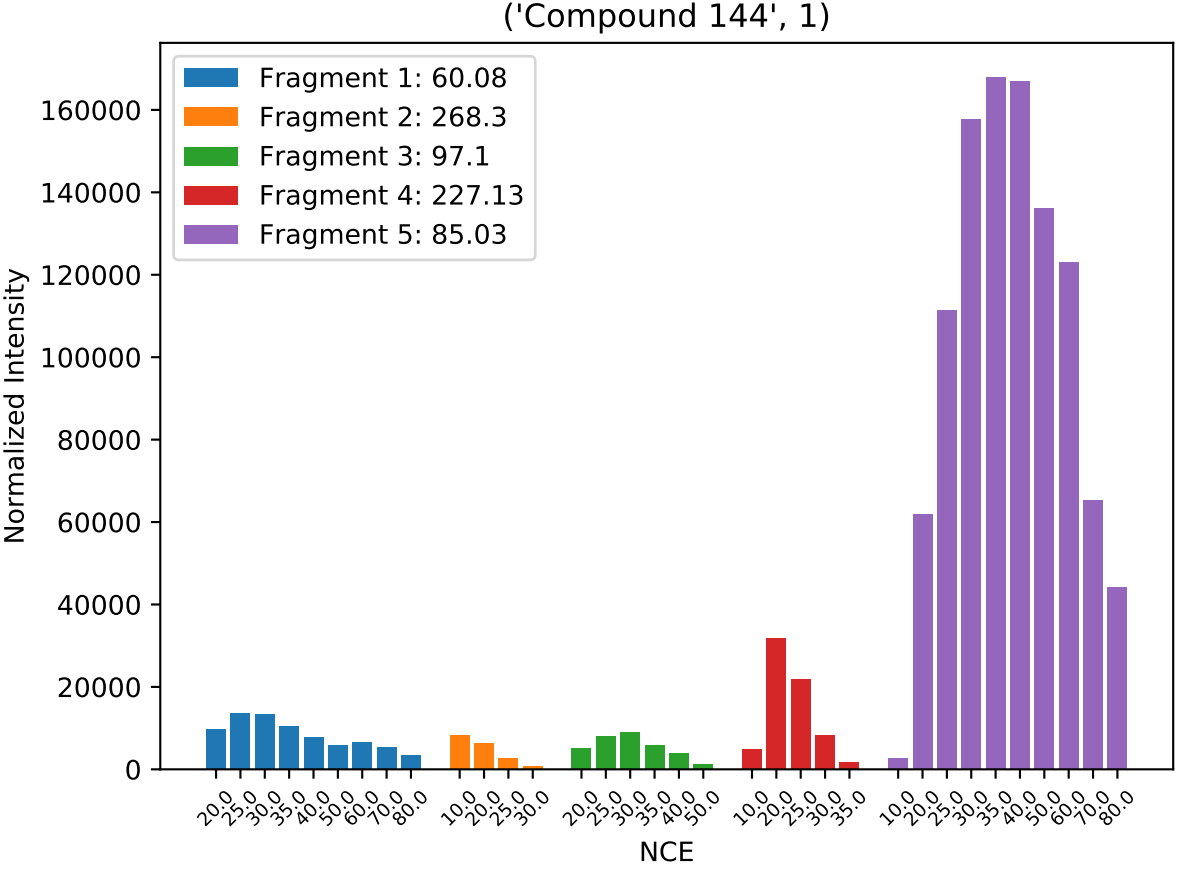

('Compound 135', 1)
Fragment 1: 67.05
Fragment 2: 95.09
Fragment 3: 109.1
Fragment 4: 81.07
Fragment 5: 79.05
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

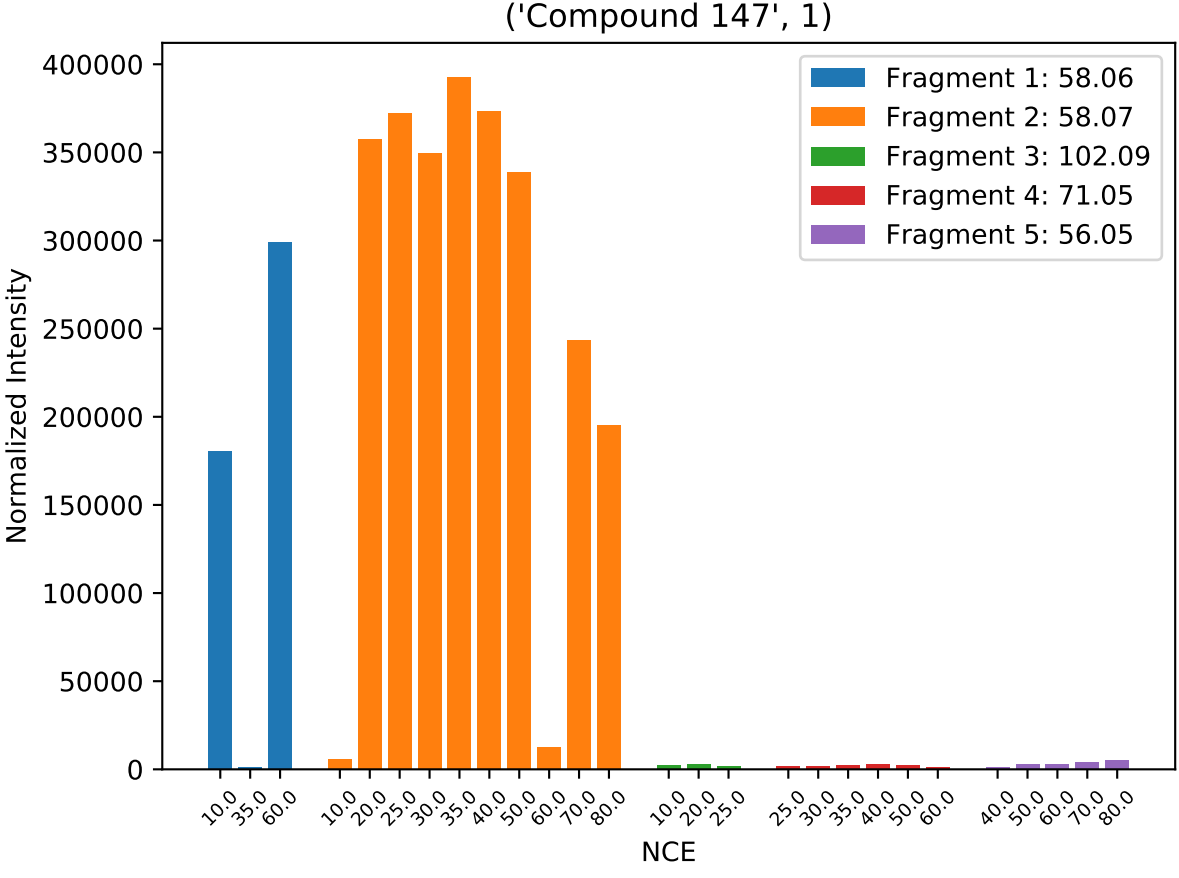

('Compound 136', 1)
Fragment 1: 294.99
Fragment 2: 247.09
Fragment 3: 160.06
Fragment 4: 309.01
Fragment 5: 132.07
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

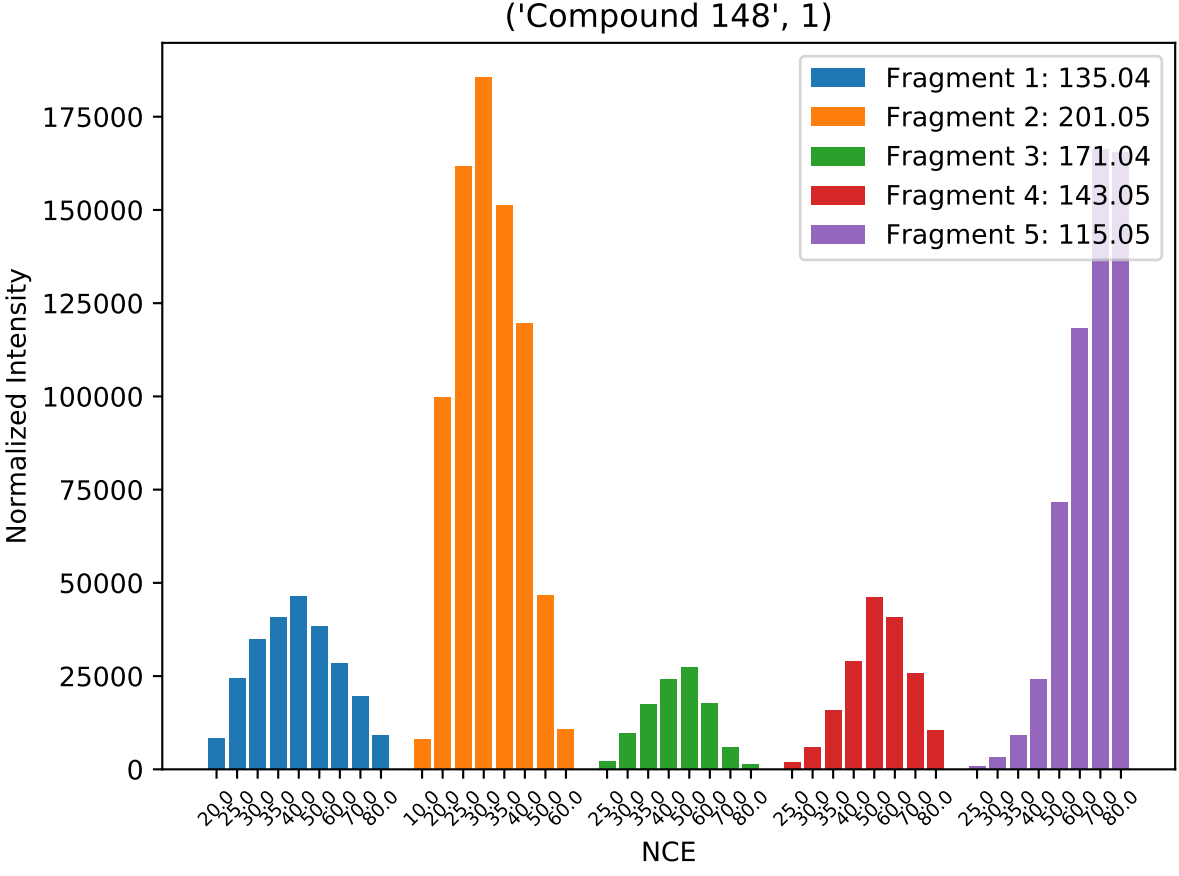

('Compound 138', 1)
Fragment 1: 94.07
Fragment 2: 93.06
Fragment 3: 94.06
Fragment 4: 81.03
Fragment 5: 53.04
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
NCE
10.0 20.0 25.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

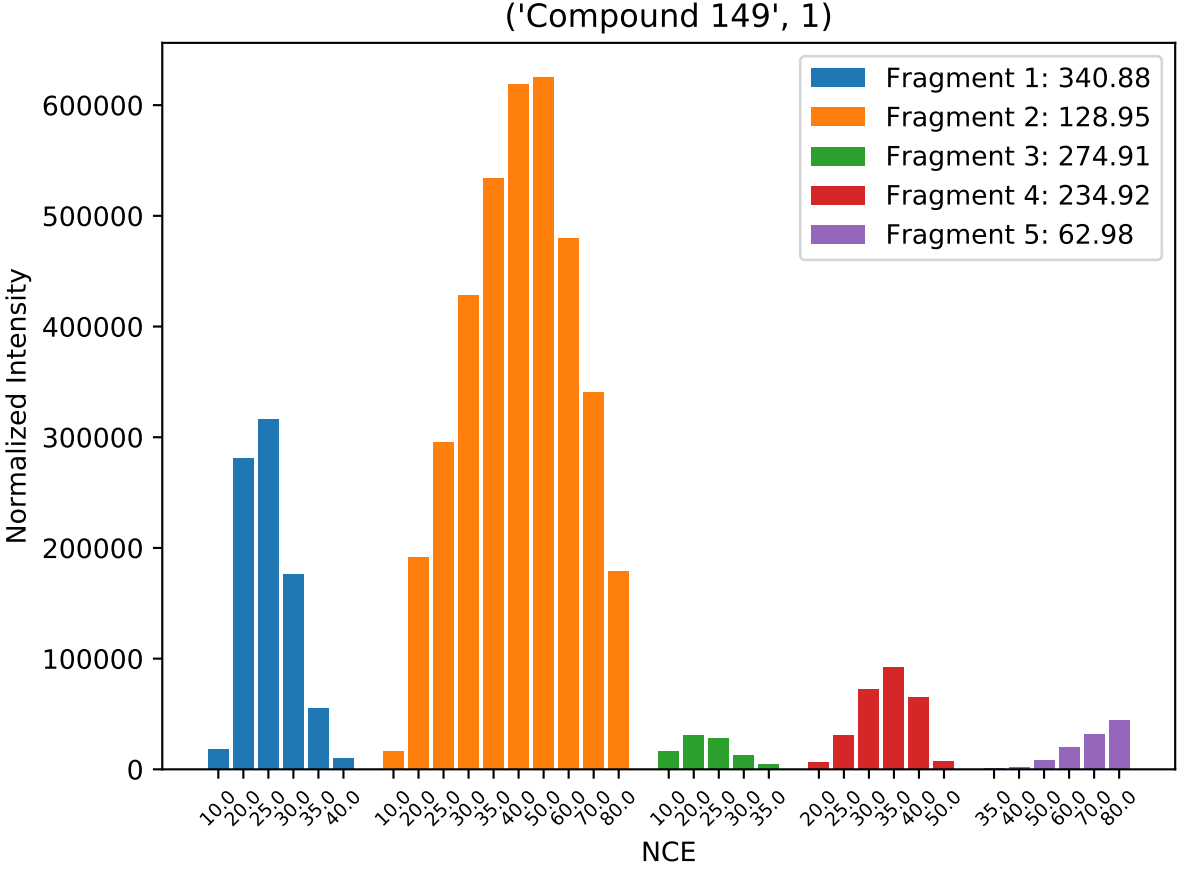

('Compound 139', 1)
Fragment 1: 242.25
Fragment 2: 272.2
Fragment 3: 122.08
Fragment 4: 74.06
Fragment 5: 88.08
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

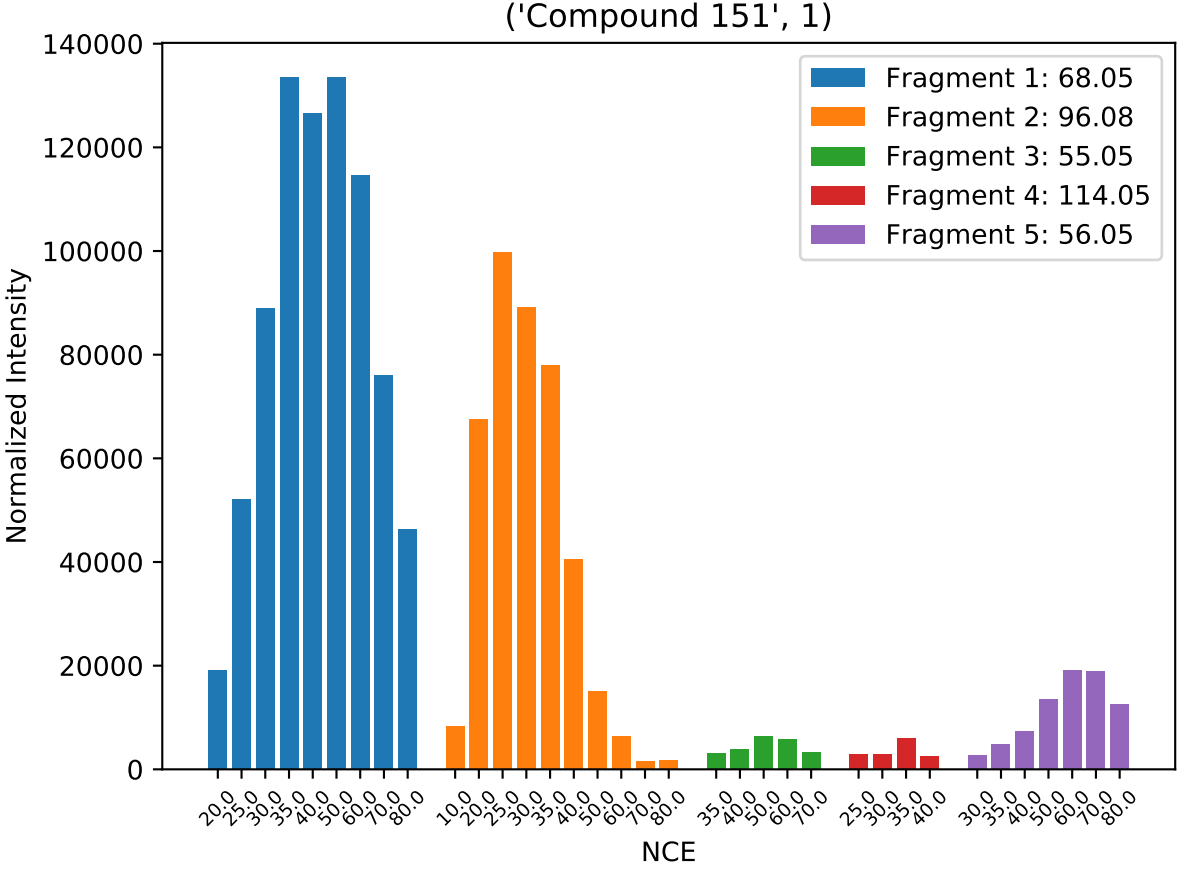

('Compound 142', 1)
Fragment 1: 121.97
Fragment 2: 103.96
Fragment 3: 62.93
Fragment 4: 100.11
Fragment 5: 58.07
Normalized Intensity
0
2000
4000
6000
8000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
25.0
35.0
40.0
60.0
NCE

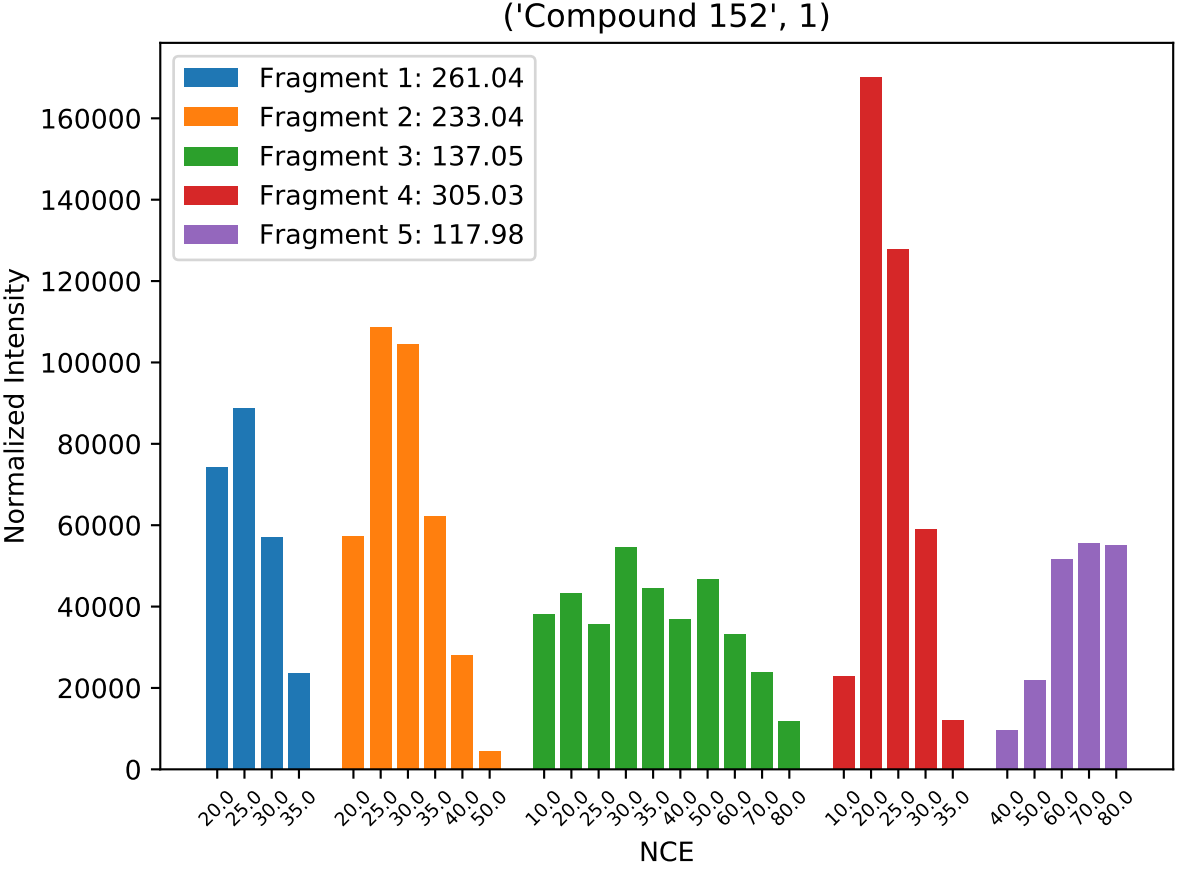

('Compound 144', 1)
Fragment 1: 60.08
Fragment 2: 268.3
Fragment 3: 97.1
Fragment 4: 227.13
Fragment 5: 85.03
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

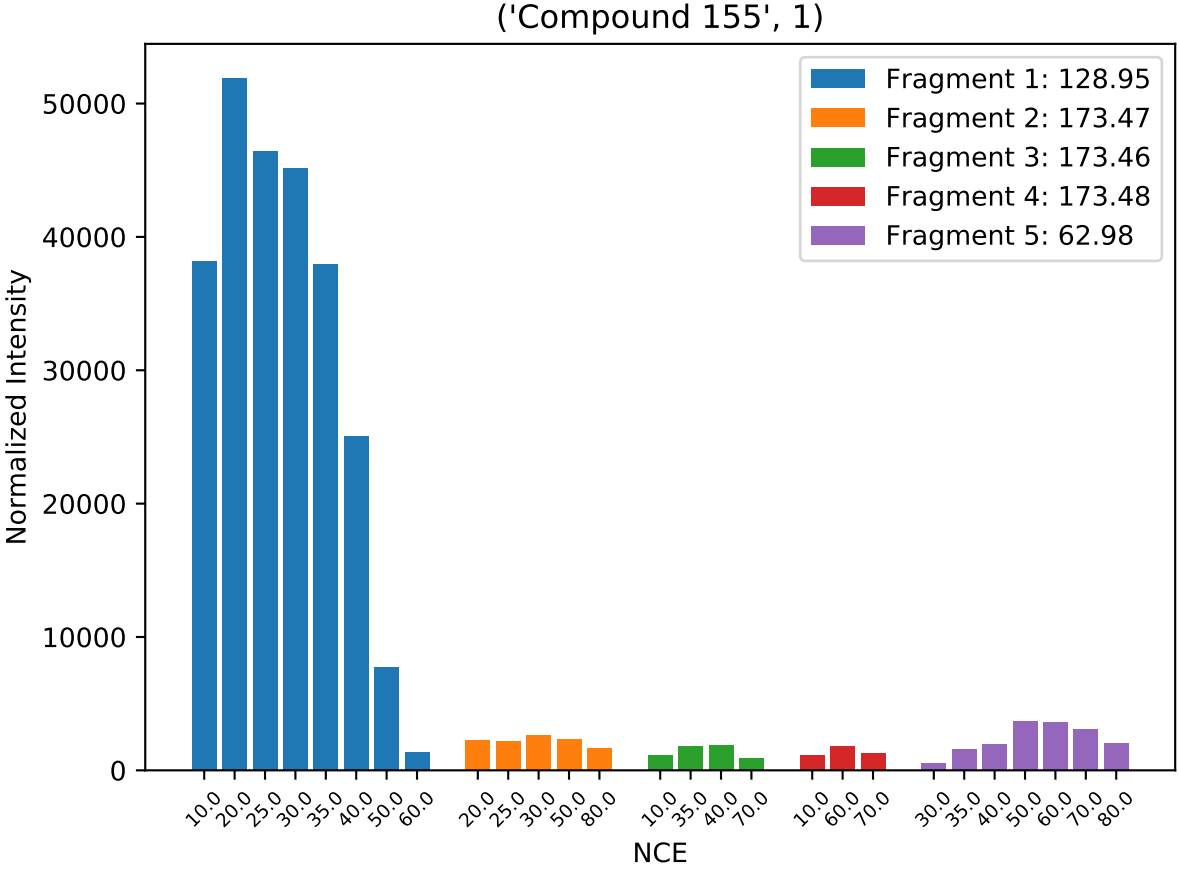

('Compound 147', 1)
Fragment 1: 58.06
Fragment 2: 58.07
Fragment 3: 102.09
Fragment 4: 71.05
Fragment 5: 56.05
Normalized Intensity
400000
350000
300000
250000
200000
150000
100000
50000
0
10.0
35.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
25.0
30.0
35.0
40.0
50.0
60.0
40.0
50.0
60.0
70.0
80.0
NCE

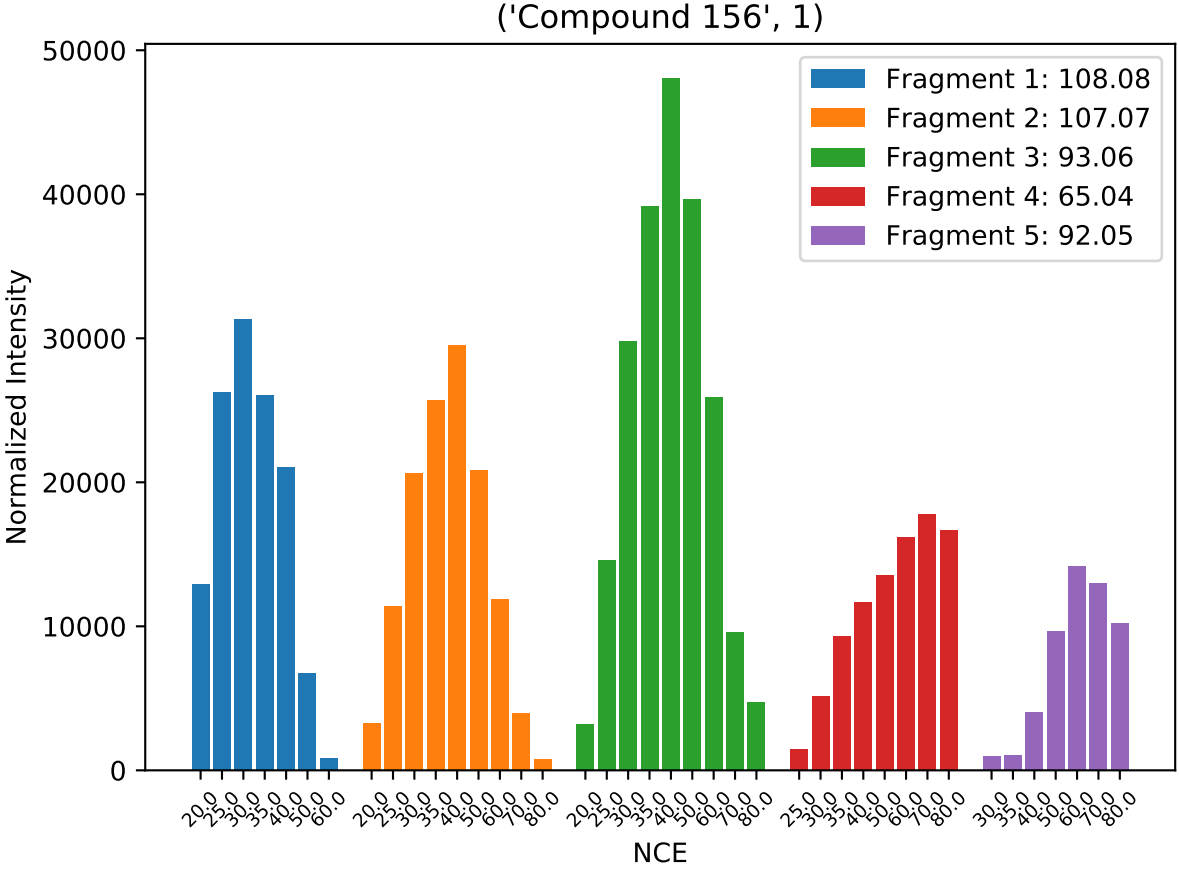

('Compound 148', 1)
Fragment 1: 135.04
Fragment 2: 201.05
Fragment 3: 171.04
Fragment 4: 143.05
Fragment 5: 115.05
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

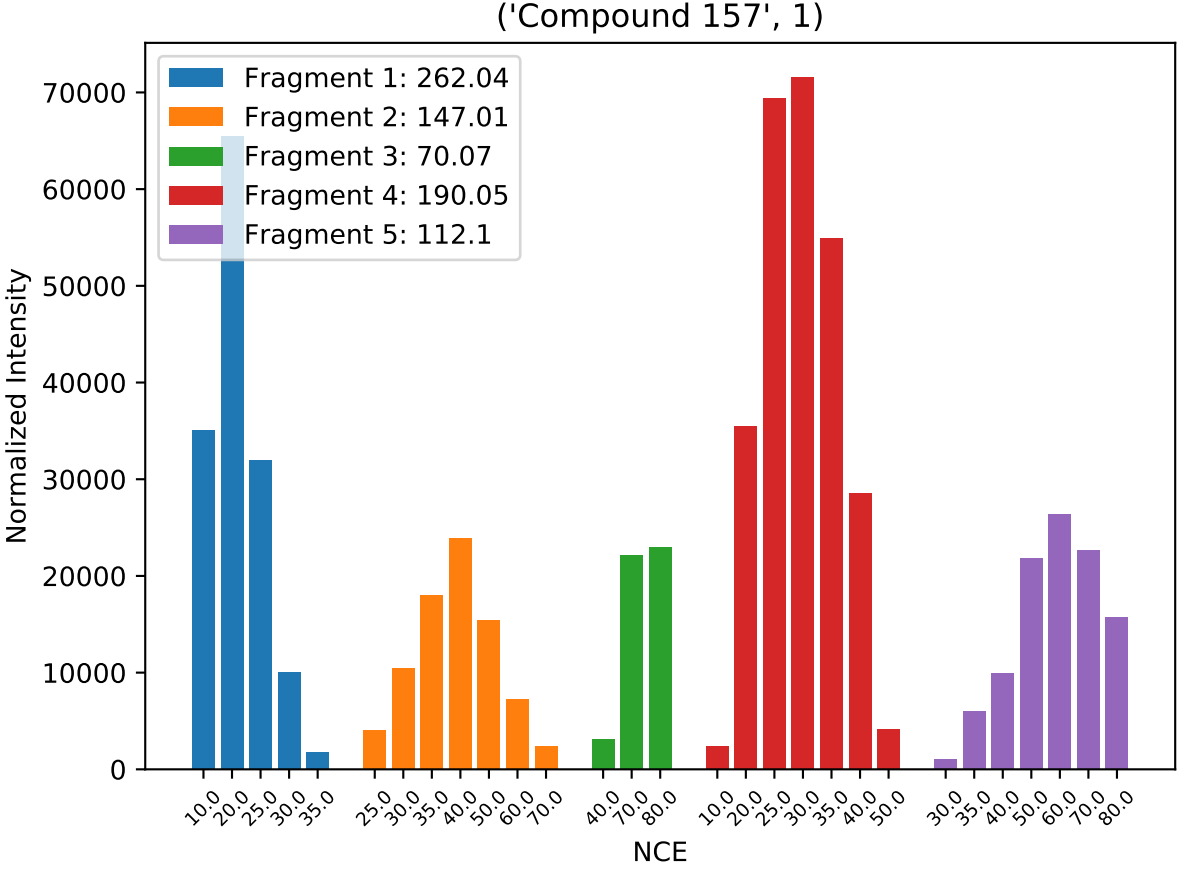

('Compound 149', 1)
Fragment 1: 340.88
Fragment 2: 128.95
Fragment 3: 274.91
Fragment 4: 234.92
Fragment 5: 62.98
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

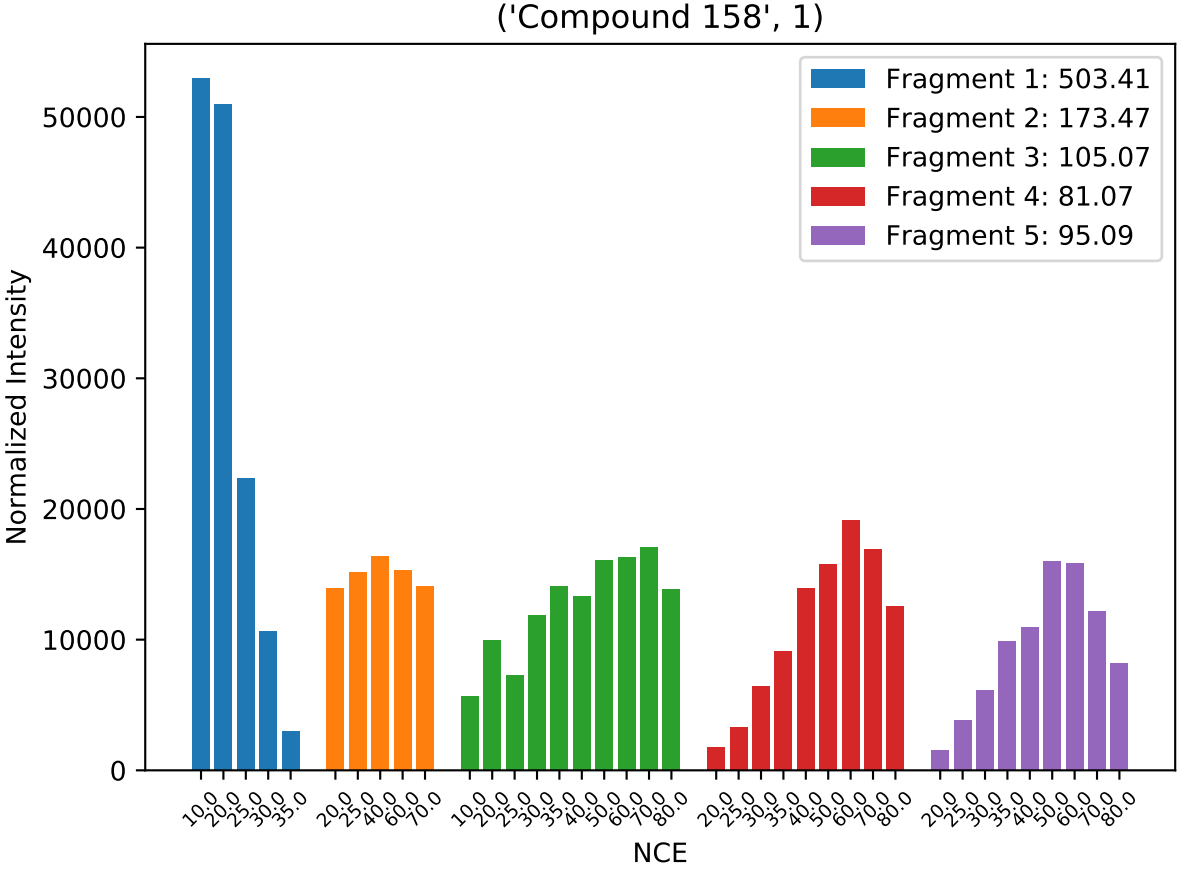

('Compound 151', 1)
Fragment 1: 68.05
Fragment 2: 96.08
Fragment 3: 55.05
Fragment 4: 114.05
Fragment 5: 56.05
Normalized Intensity
NCE
140000
120000
100000
80000
60000
40000
20000
0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

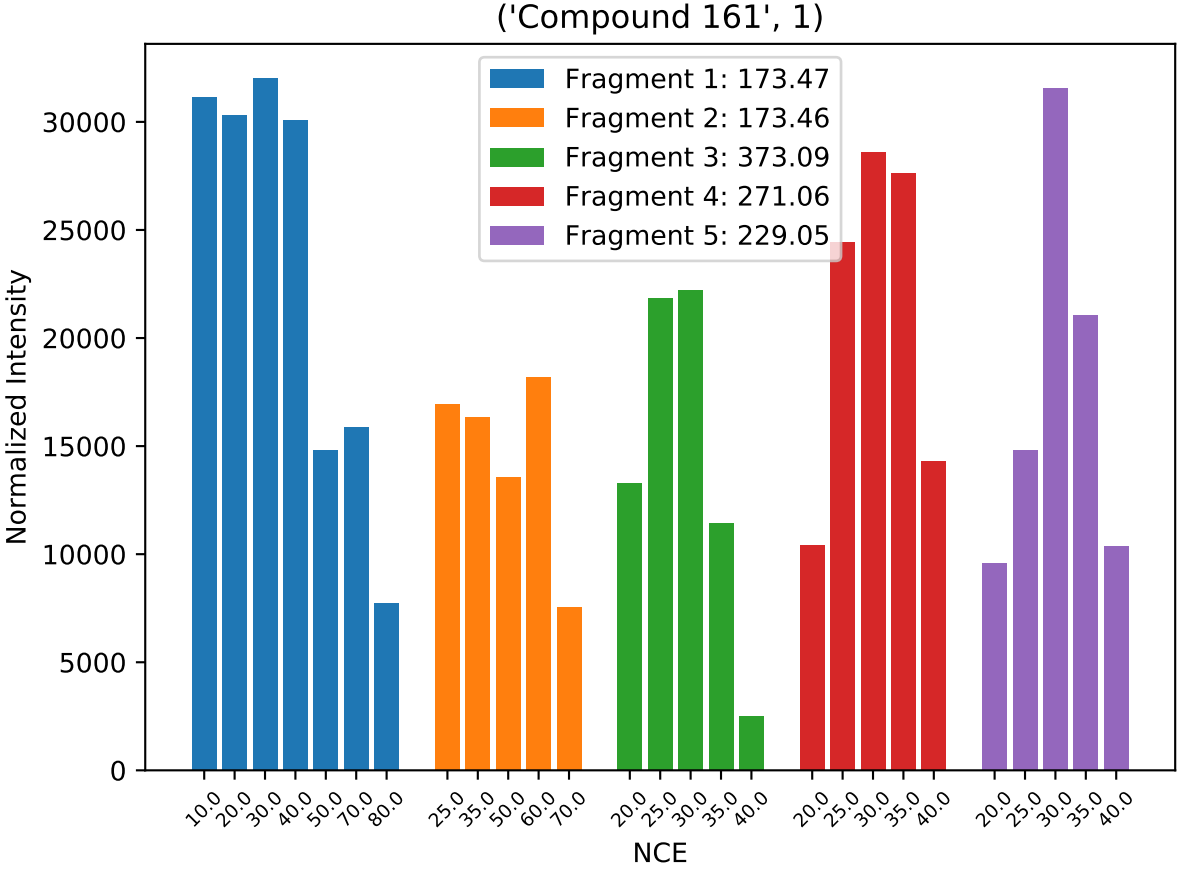

('Compound 152', 1)
Fragment 1: 261.04
Fragment 2: 233.04
Fragment 3: 137.05
Fragment 4: 305.03
Fragment 5: 117.98
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
40.0 50.0 60.0 70.0 80.0
NCE

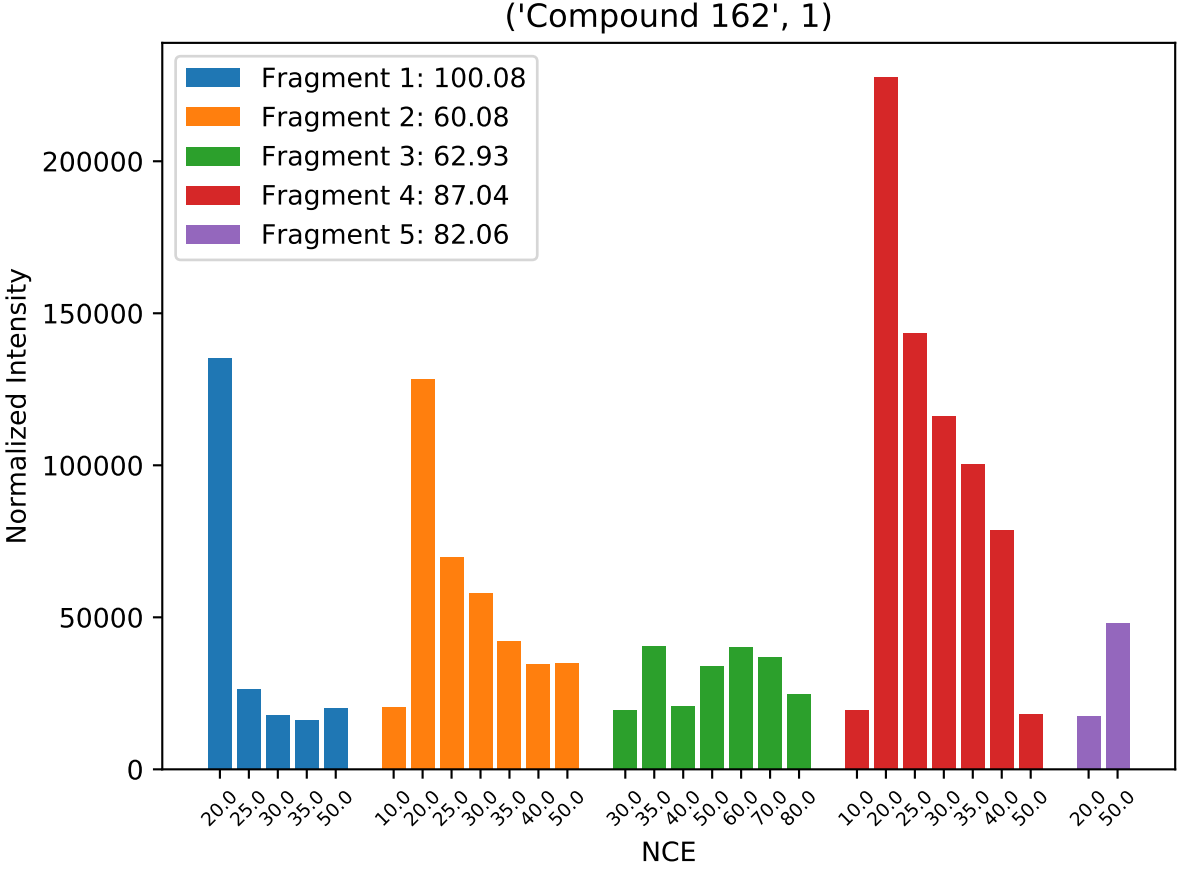

('Compound 155', 1)
Fragment 1: 128.95
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 173.48
Fragment 5: 62.98
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
50.0
80.0
10.0
35.0
40.0
70.0
10.0
60.0
70.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

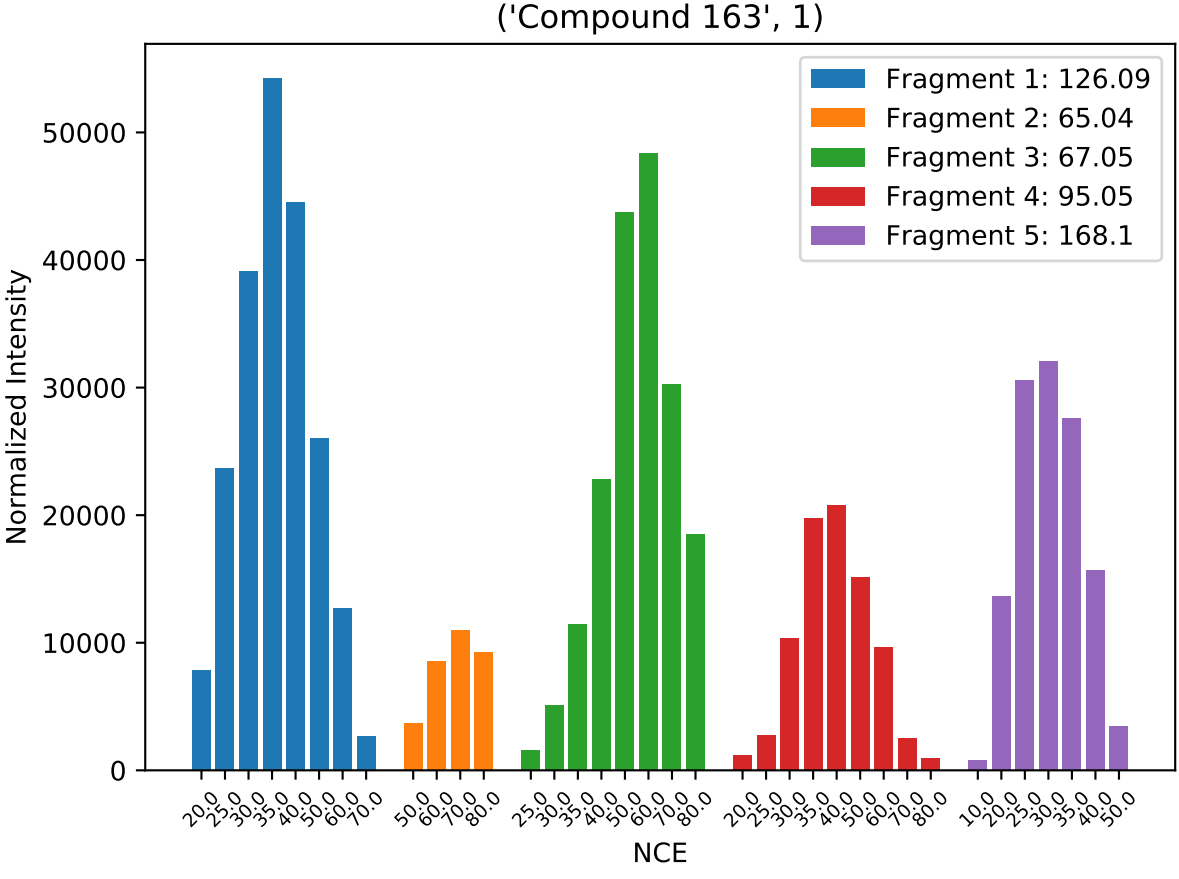

('Compound 156', 1)
Fragment 1: 108.08
Fragment 2: 107.07
Fragment 3: 93.06
Fragment 4: 65.04
Fragment 5: 92.05
Normalized Intensity
NCE
0
10000
20000
30000
40000
50000
20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

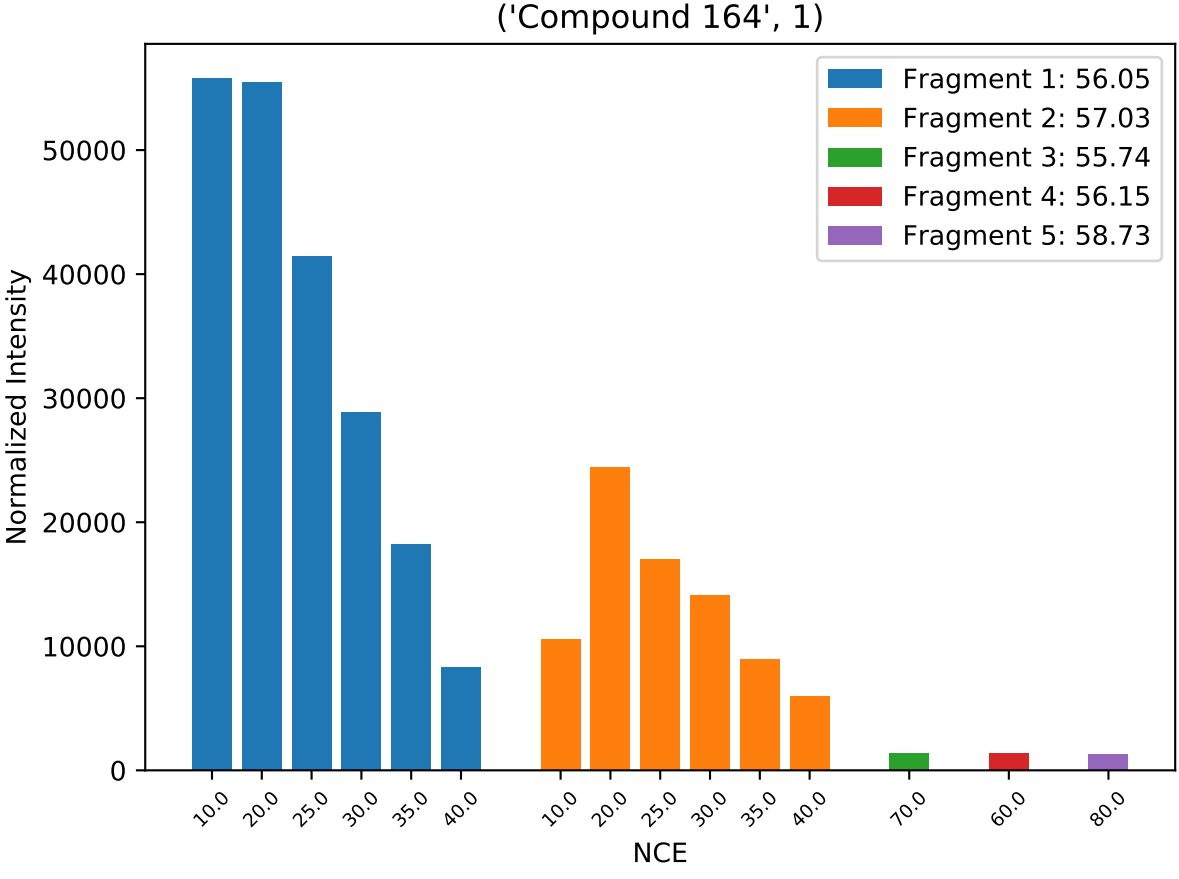

('Compound 157', 1)
Fragment 1: 262.04
Fragment 2: 147.01
Fragment 3: 70.07
Fragment 4: 190.05
Fragment 5: 112.1
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0 20.0 25.0 30.0 35.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
40.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

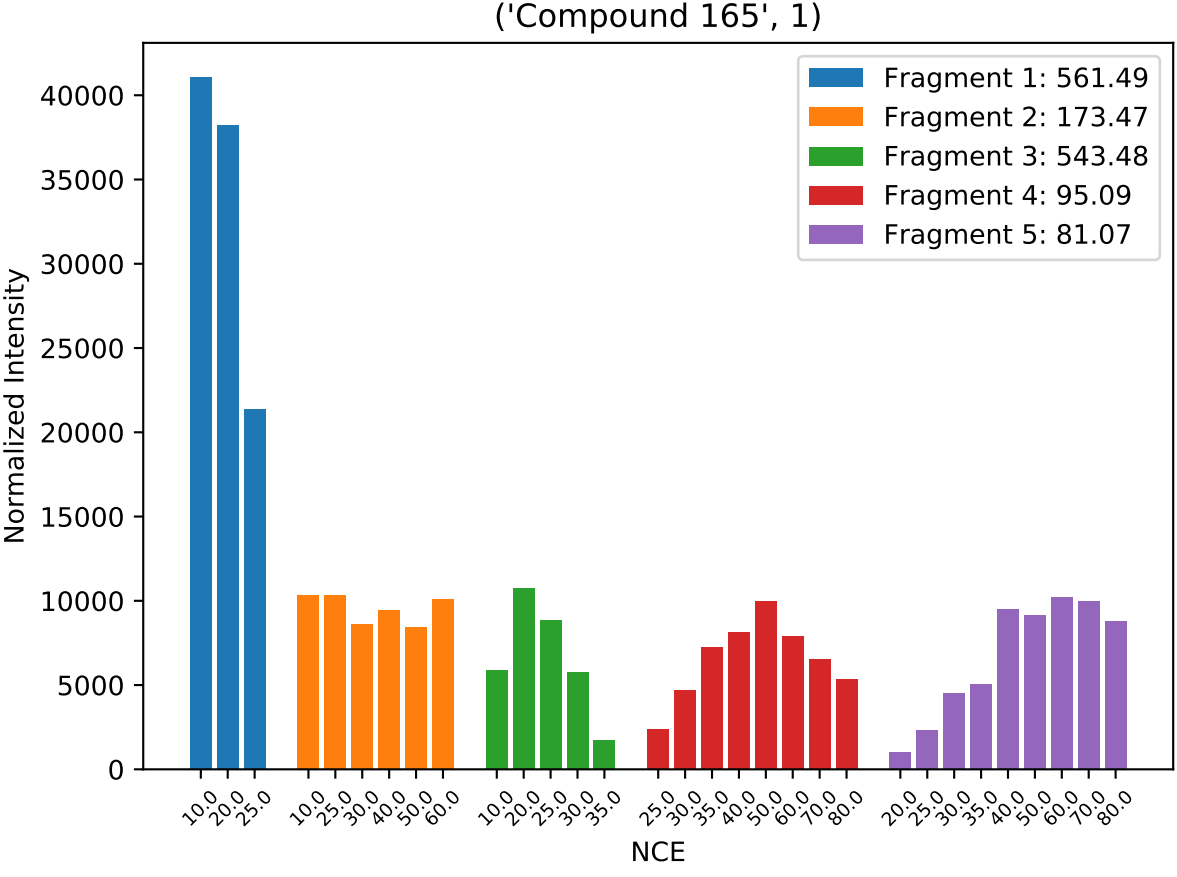

('Compound 158', 1)
Fragment 1: 503.41
Fragment 2: 173.47
Fragment 3: 105.07
Fragment 4: 81.07
Fragment 5: 95.09
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0 20.0 25.0 30.0 35.0
20.0 25.0 40.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

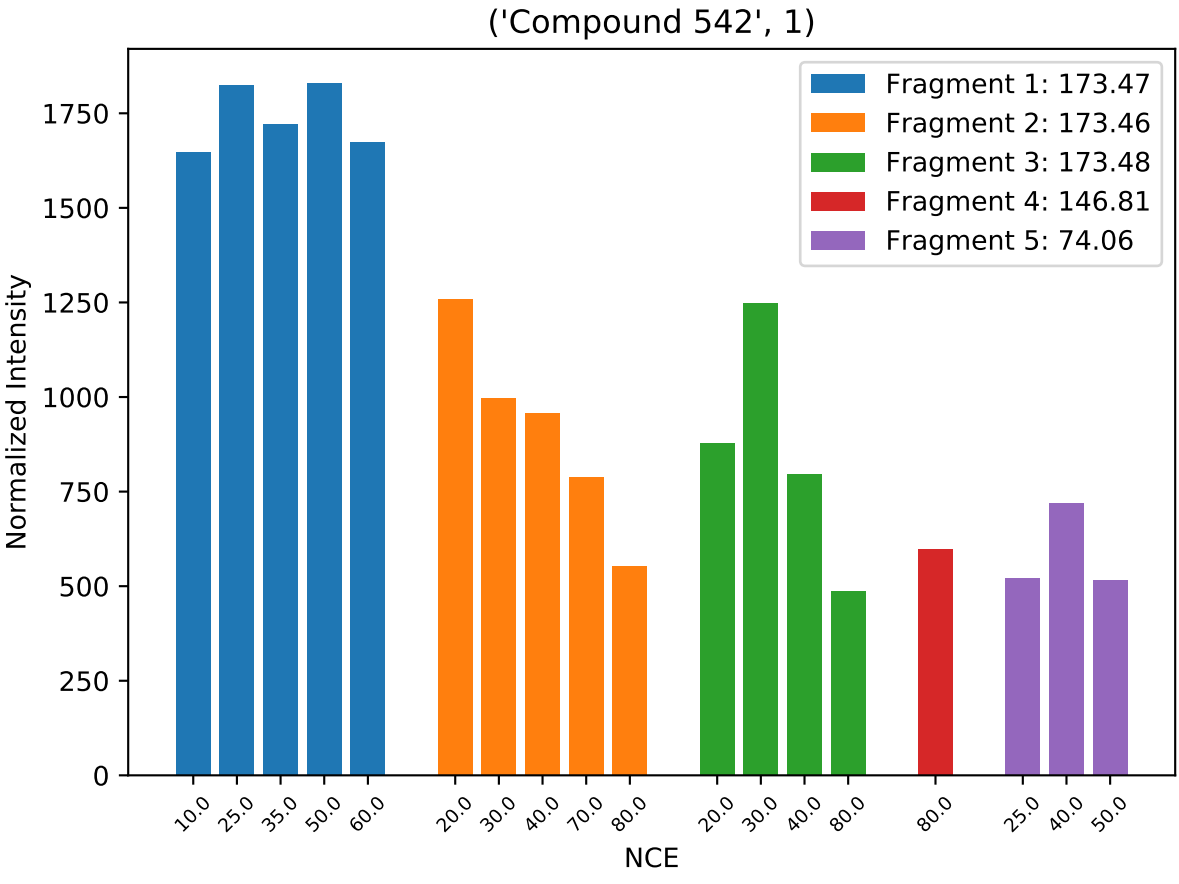

('Compound 161', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 373.09
Fragment 4: 271.06
Fragment 5: 229.05
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0
20.0
30.0
40.0
50.0
70.0
80.0
25.0
35.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
NCE

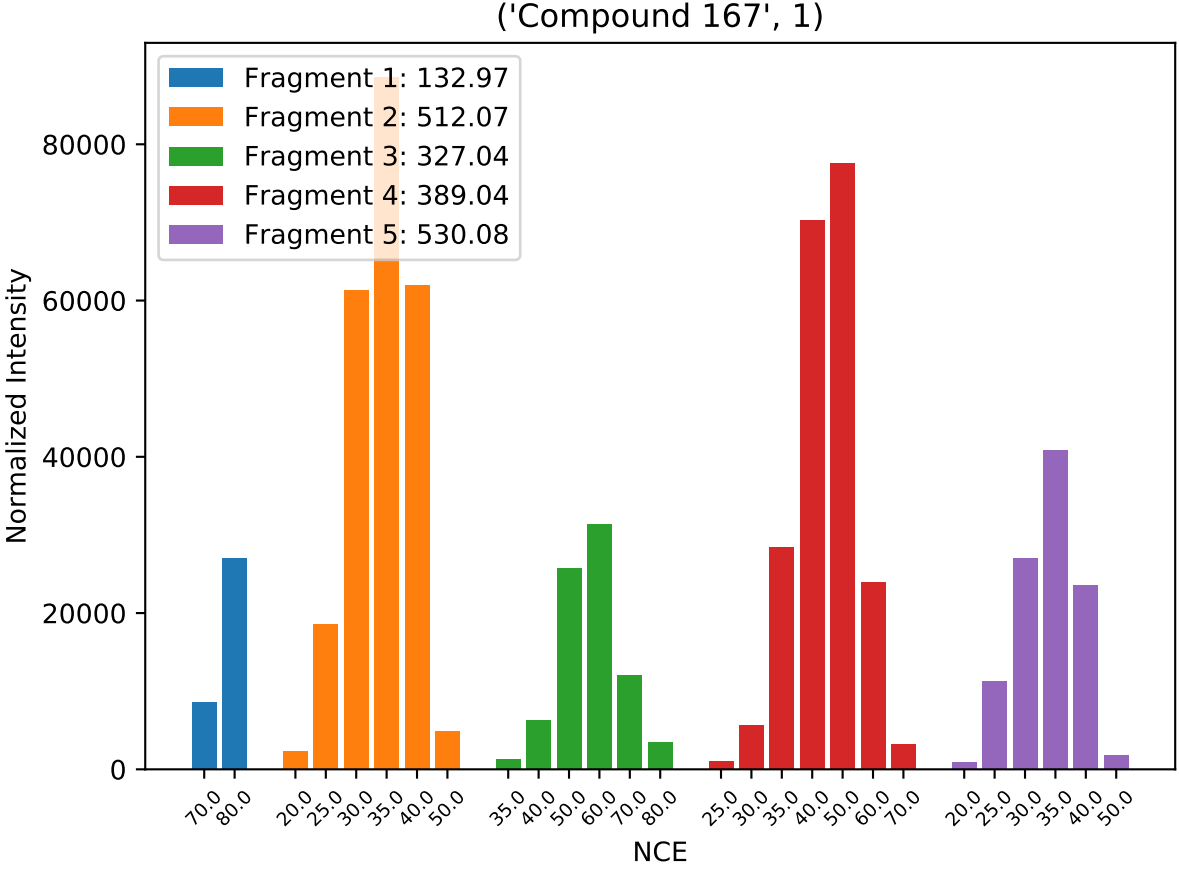

('Compound 162', 1)
Fragment 1: 100.08
Fragment 2: 60.08
Fragment 3: 62.93
Fragment 4: 87.04
Fragment 5: 82.06
Normalized Intensity
0
50000
100000
150000
200000
20.0 25.0 30.0 35.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 50.0
NCE

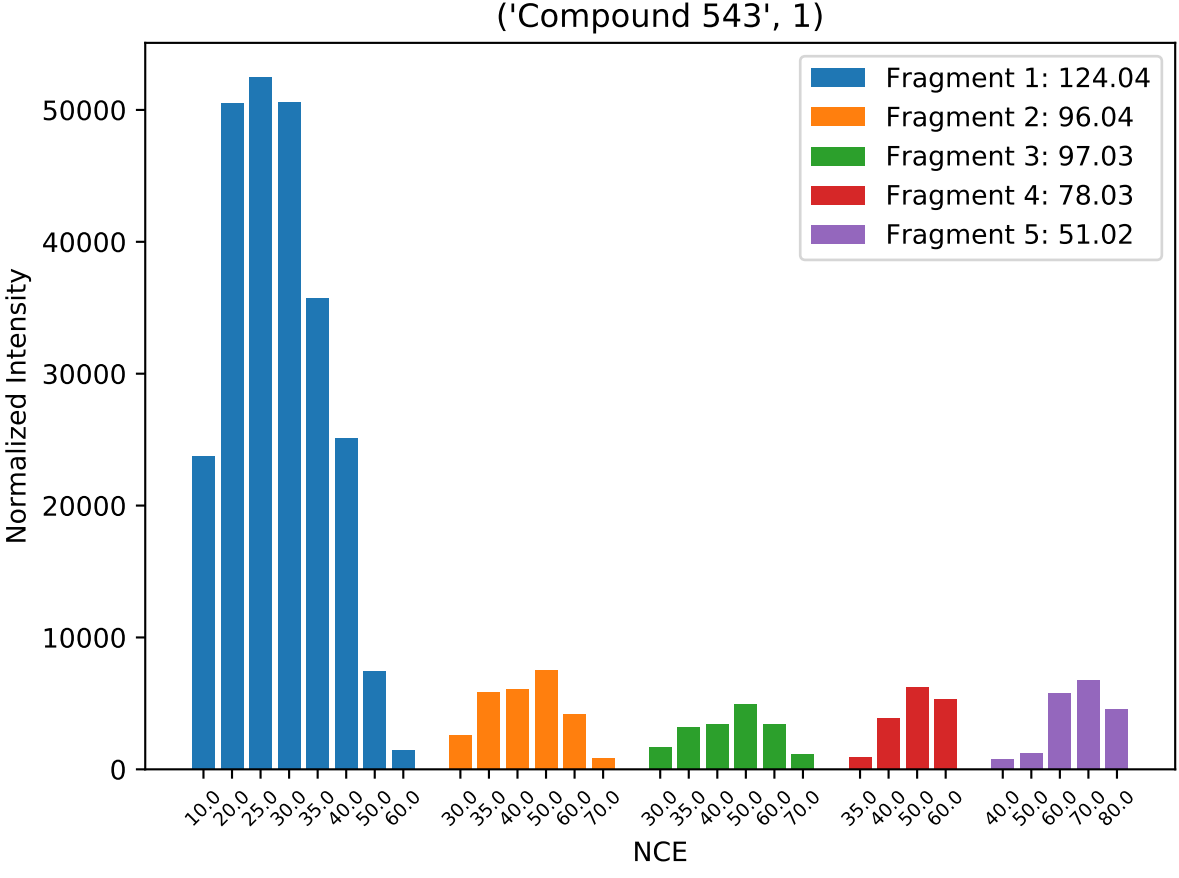

('Compound 163', 1)
Fragment 1: 126.09
Fragment 2: 65.04
Fragment 3: 67.05
Fragment 4: 95.05
Fragment 5: 168.1
Normalized Intensity
0
10000
20000
30000
40000
50000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

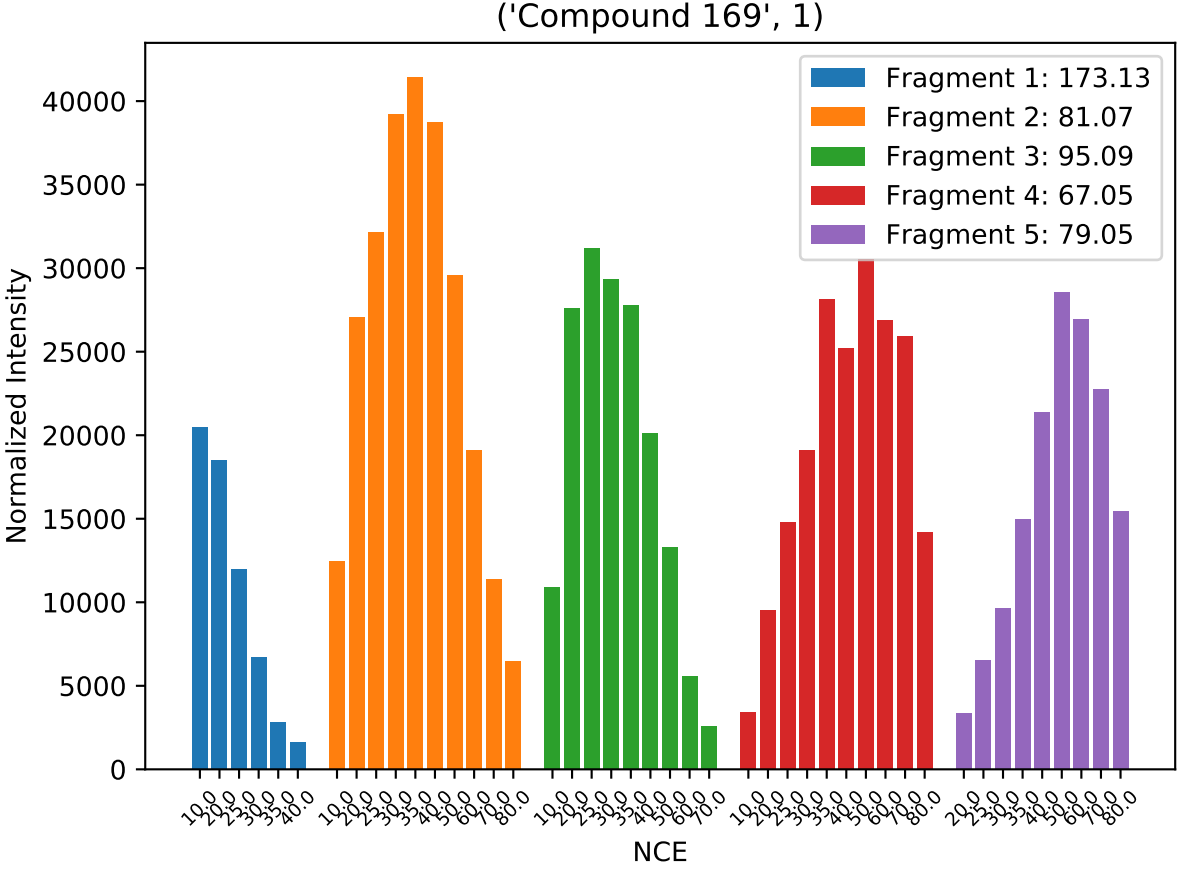

('Compound 164', 1)
Fragment 1: 56.05
Fragment 2: 57.03
Fragment 3: 55.74
Fragment 4: 56.15
Fragment 5: 58.73
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
70.0
60.0
80.0
NCE

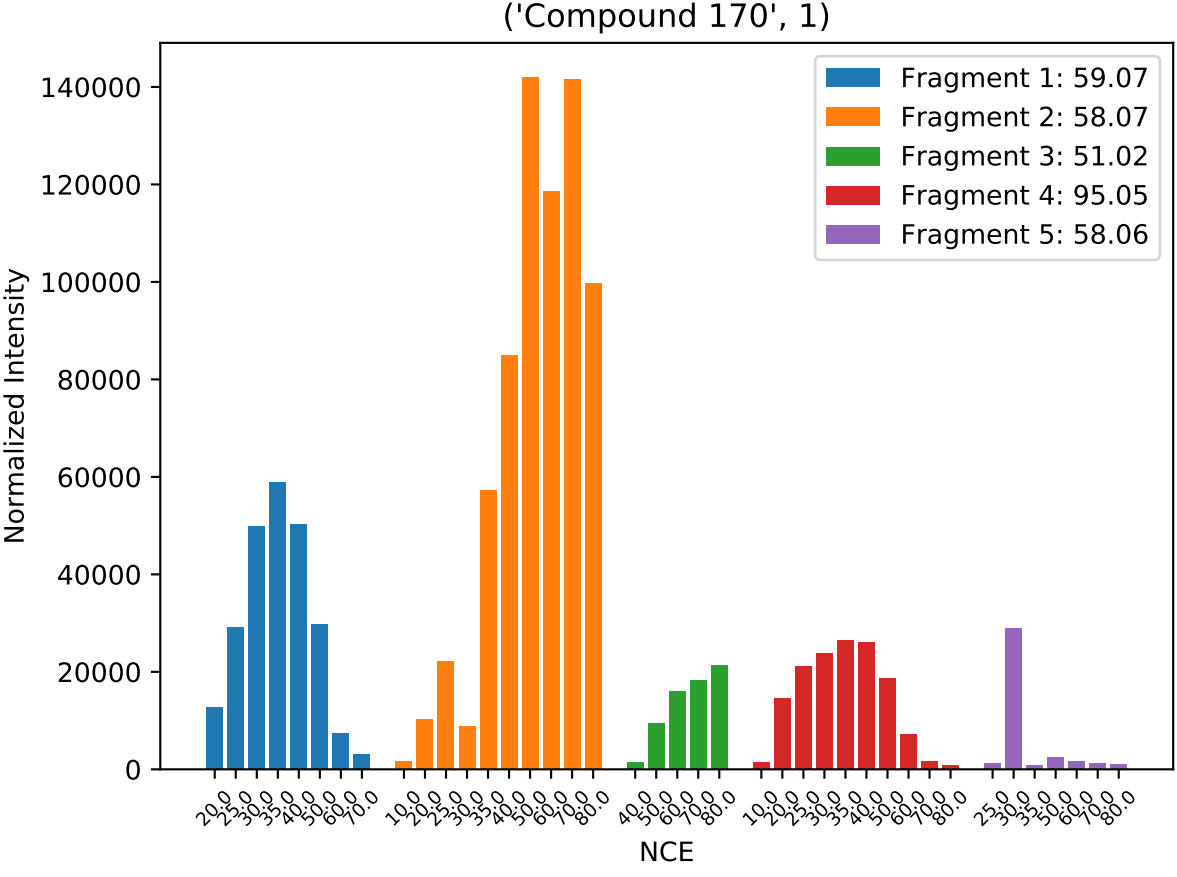

('Compound 165', 1)
Fragment 1: 561.49
Fragment 2: 173.47
Fragment 3: 543.48
Fragment 4: 95.09
Fragment 5: 81.07
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0 20.0 25.0
10.0 25.0 30.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

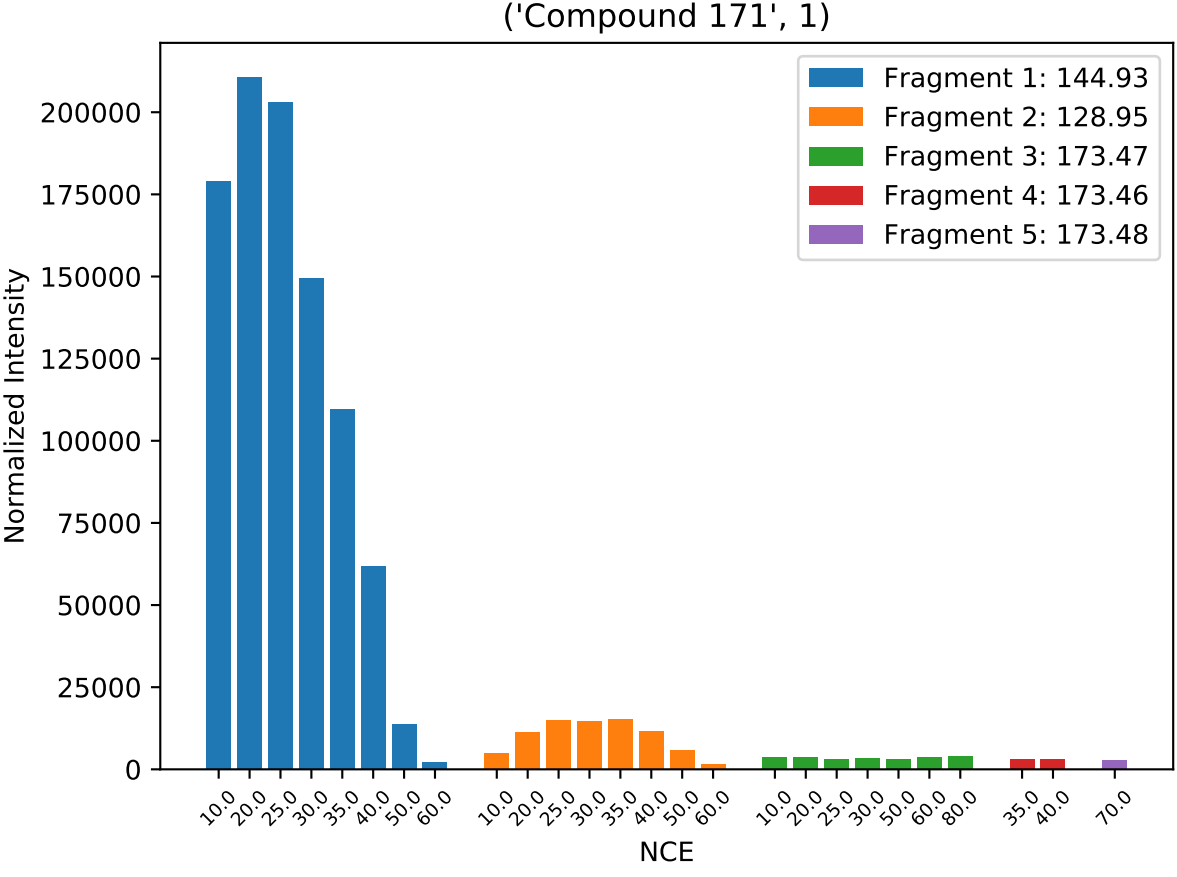

('Compound 542', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 173.48
Fragment 4: 146.81
Fragment 5: 74.06
Normalized Intensity
0
250
500
750
1000
1250
1500
1750
10.0
25.0
35.0
50.0
60.0
20.0
30.0
40.0
70.0
80.0
20.0
30.0
40.0
80.0
80.0
25.0
40.0
50.0
NCE

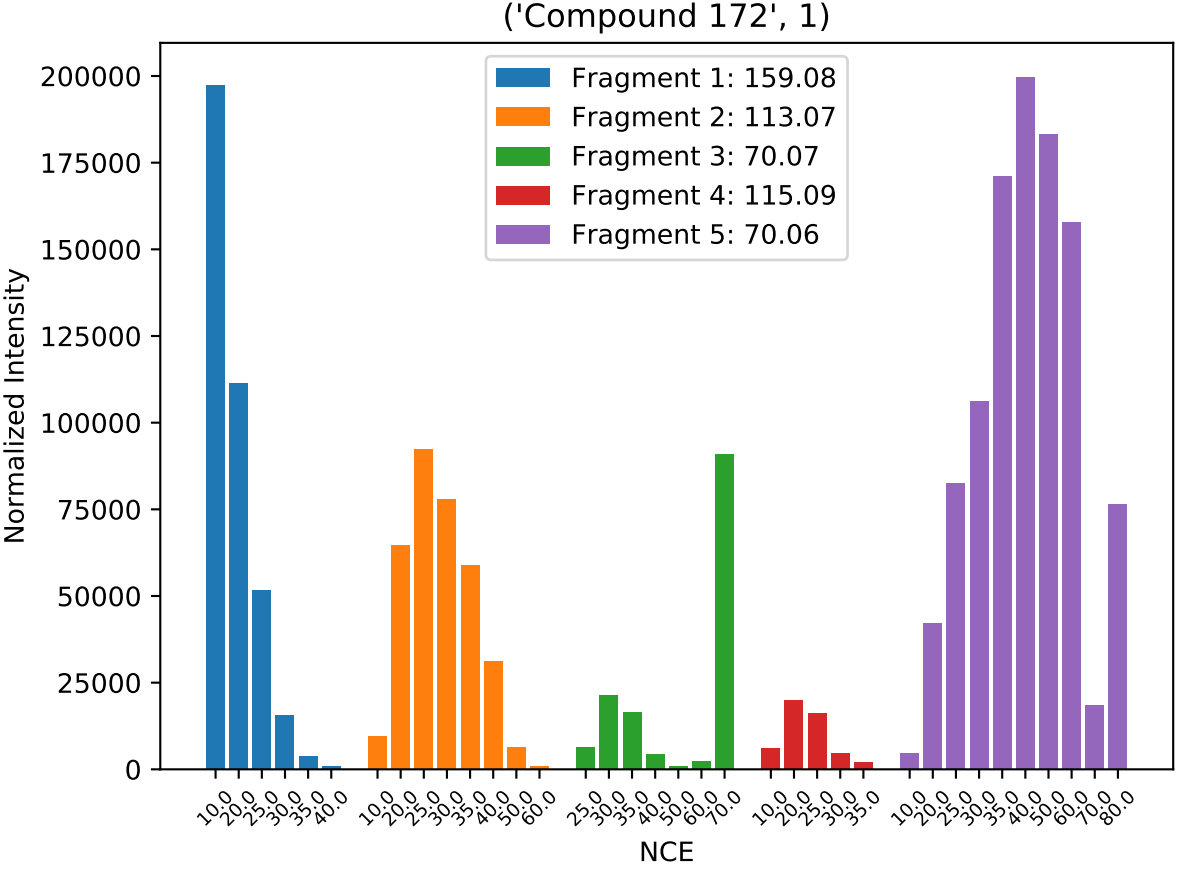

('Compound 167', 1)
Fragment 1: 132.97
Fragment 2: 512.07
Fragment 3: 327.04
Fragment 4: 389.04
Fragment 5: 530.08
Normalized Intensity
0
20000
40000
60000
80000
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

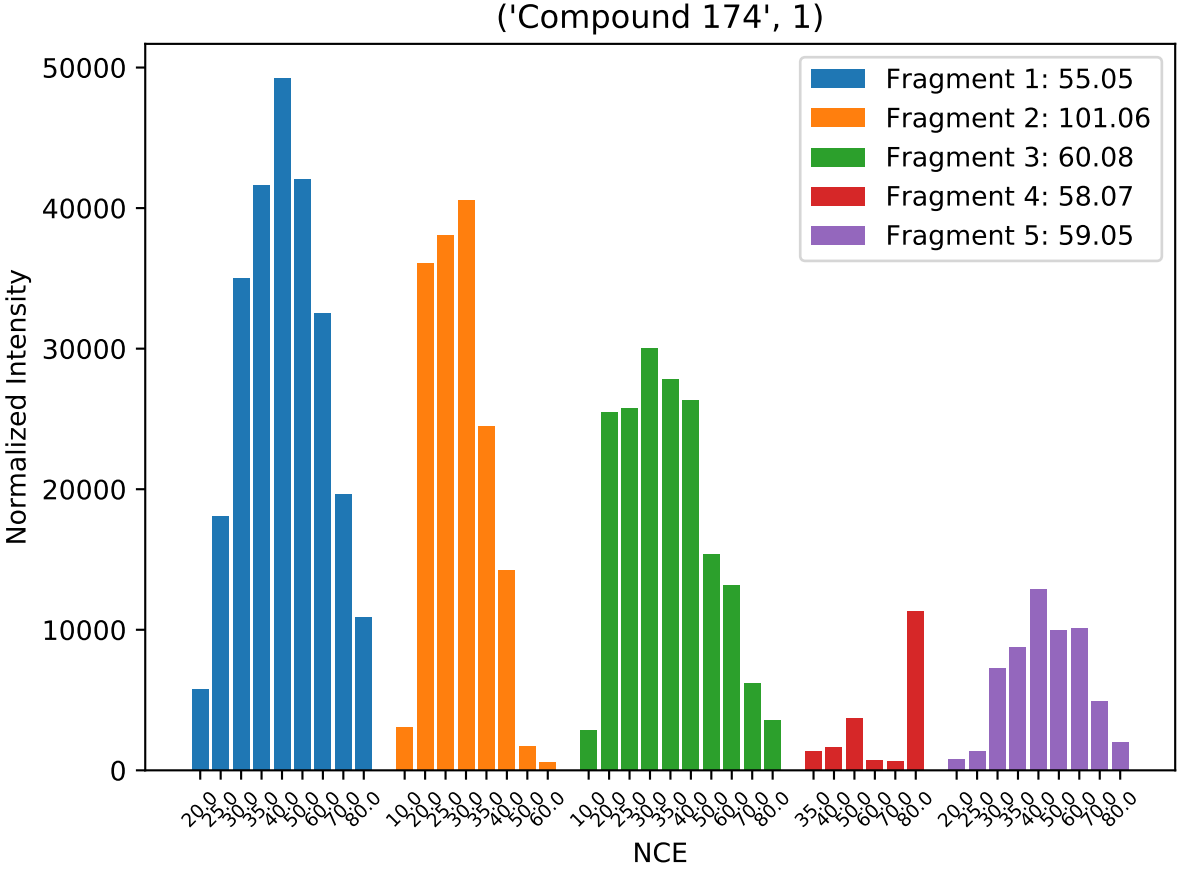

('Compound 543', 1)
Fragment 1: 124.04
Fragment 2: 96.04
Fragment 3: 97.03
Fragment 4: 78.03
Fragment 5: 51.02
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0
35.0 40.0 50.0 60.0
40.0 50.0 60.0 70.0 80.0
NCE

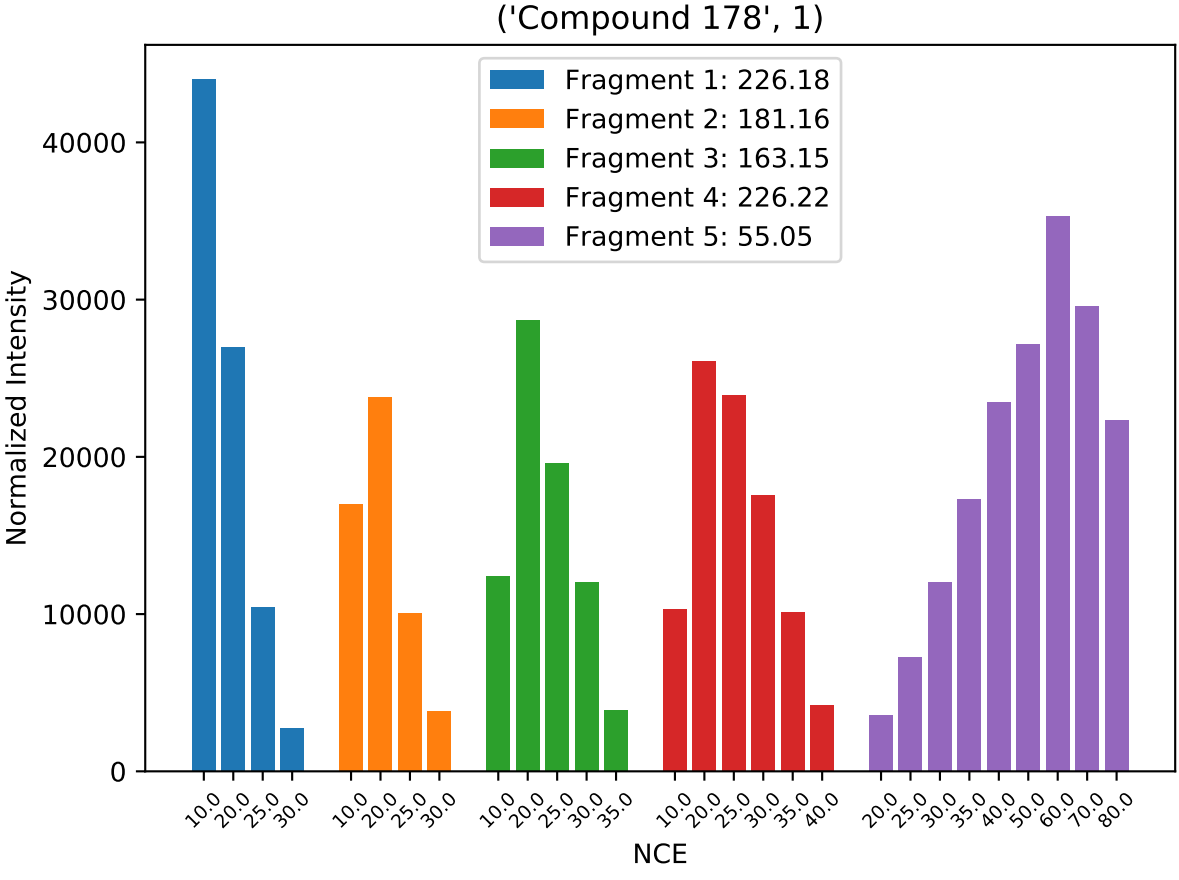

('Compound 169', 1)
Fragment 1: 173.13
Fragment 2: 81.07
Fragment 3: 95.09
Fragment 4: 67.05
Fragment 5: 79.05
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

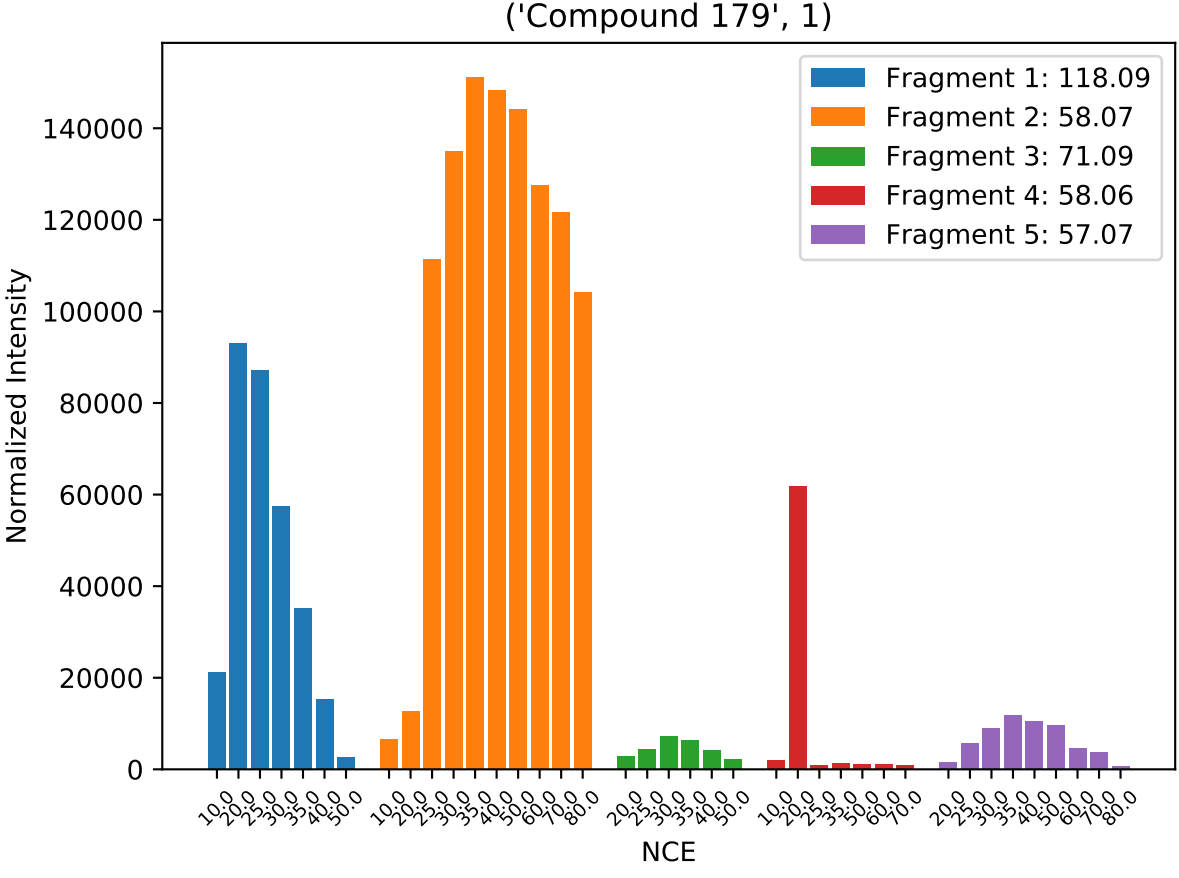

('Compound 170', 1)
Fragment 1: 59.07
Fragment 2: 58.07
Fragment 3: 51.02
Fragment 4: 95.05
Fragment 5: 58.06
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 50.0 60.0 70.0 80.0

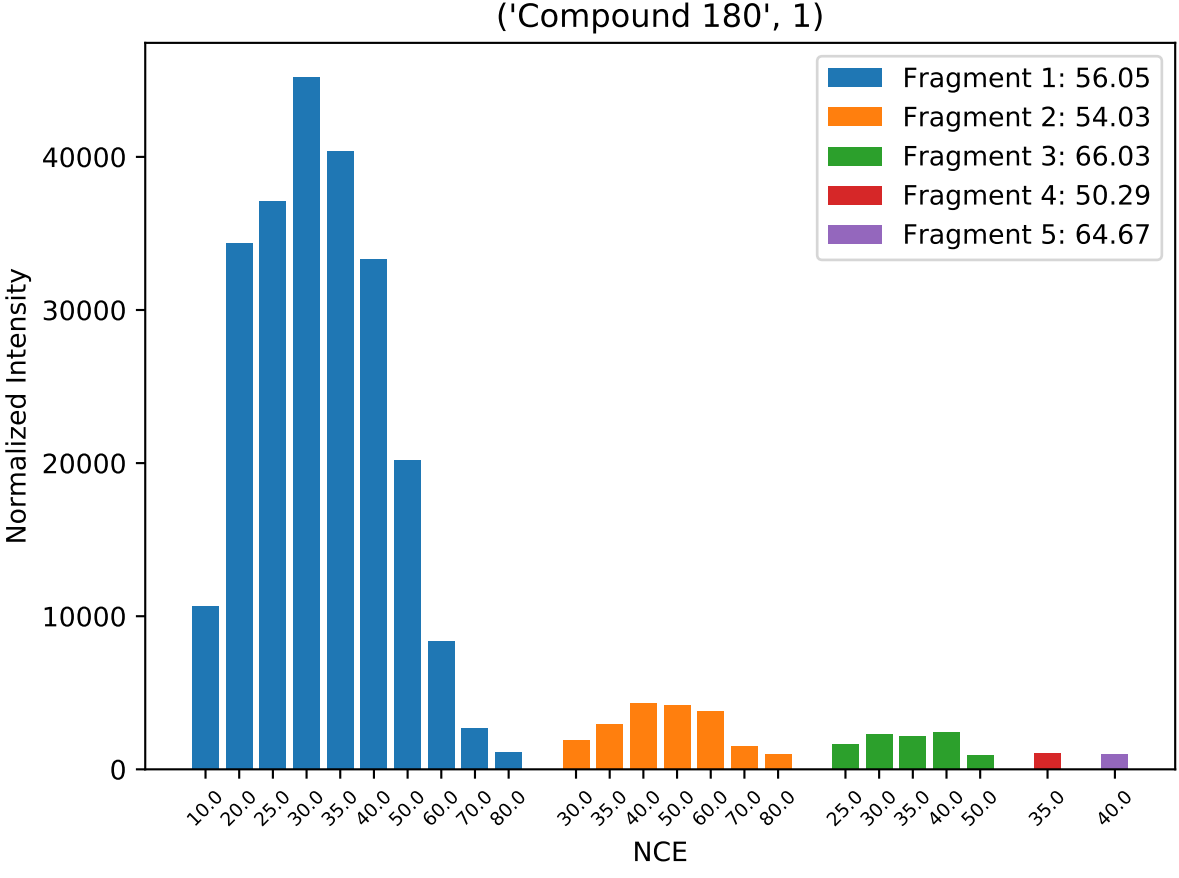

('Compound 171', 1)
Fragment 1: 144.93
Fragment 2: 128.95
Fragment 3: 173.47
Fragment 4: 173.46
Fragment 5: 173.48
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
200000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
50.0
60.0
80.0
35.0
40.0
70.0
NCE

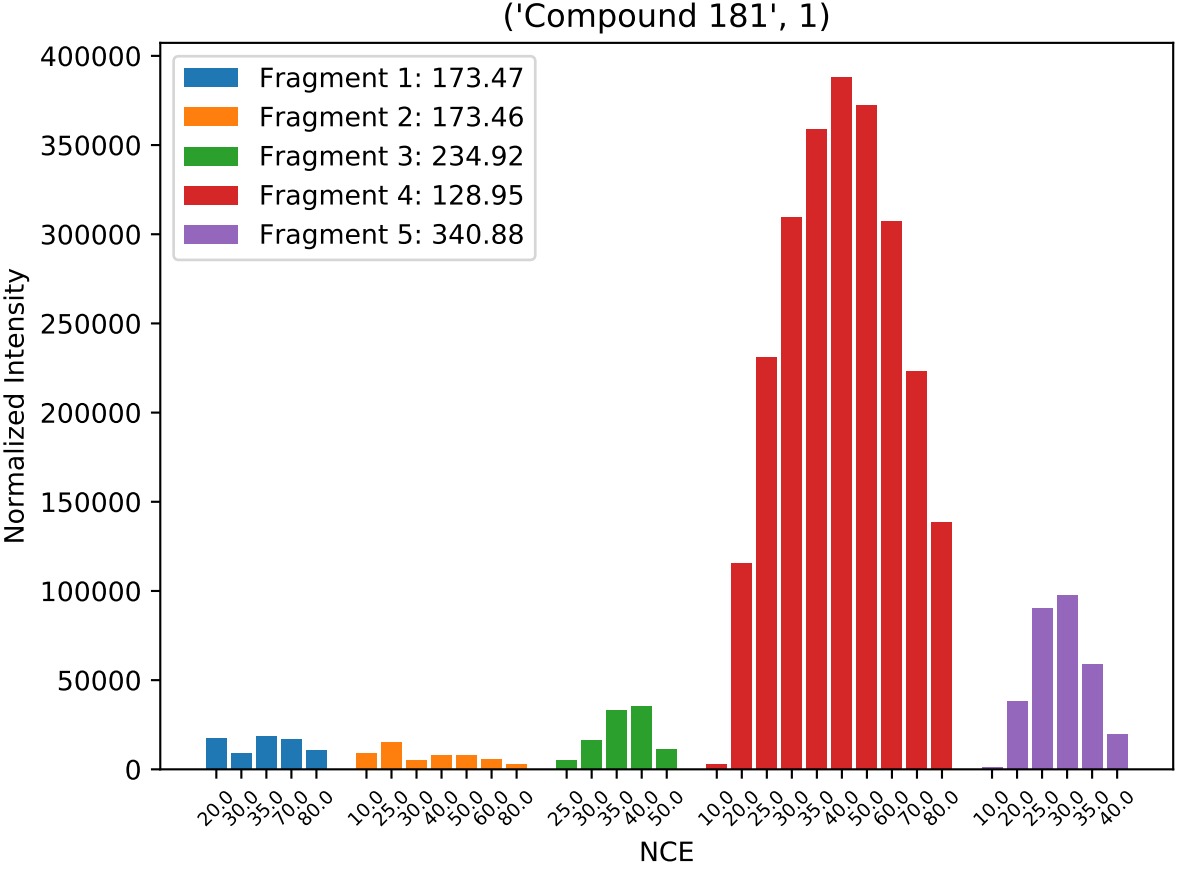

('Compound 172', 1)
Fragment 1: 159.08
Fragment 2: 113.07
Fragment 3: 70.07
Fragment 4: 115.09
Fragment 5: 70.06
Normalized Intensity
200000
175000
150000
125000
100000
75000
50000
25000
0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

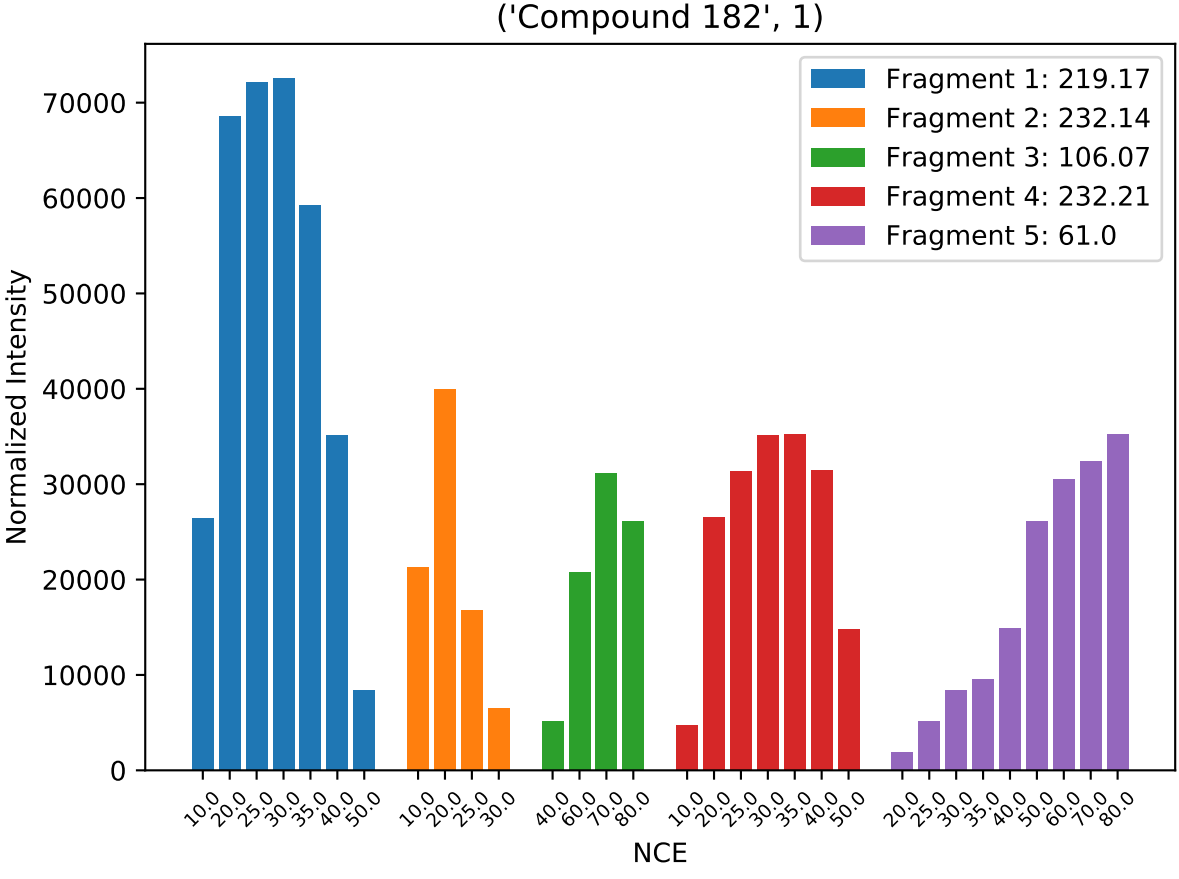

('Compound 174', 1)
Fragment 1: 55.05
Fragment 2: 101.06
Fragment 3: 60.08
Fragment 4: 58.07
Fragment 5: 59.05
Normalized Intensity
0
10000
20000
30000
40000
50000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

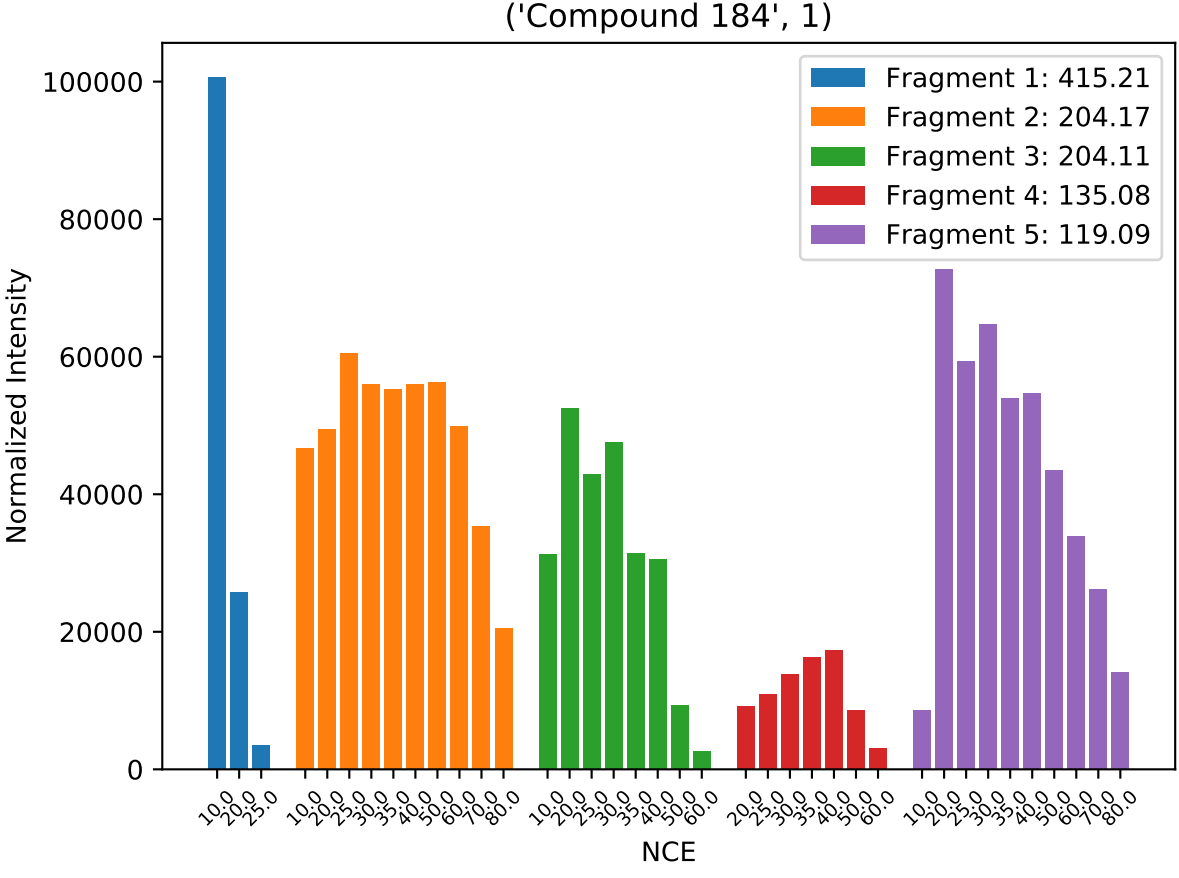

('Compound 178', 1)
Fragment 1: 226.18
Fragment 2: 181.16
Fragment 3: 163.15
Fragment 4: 226.22
Fragment 5: 55.05
Normalized Intensity
0
10000
20000
30000
40000
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

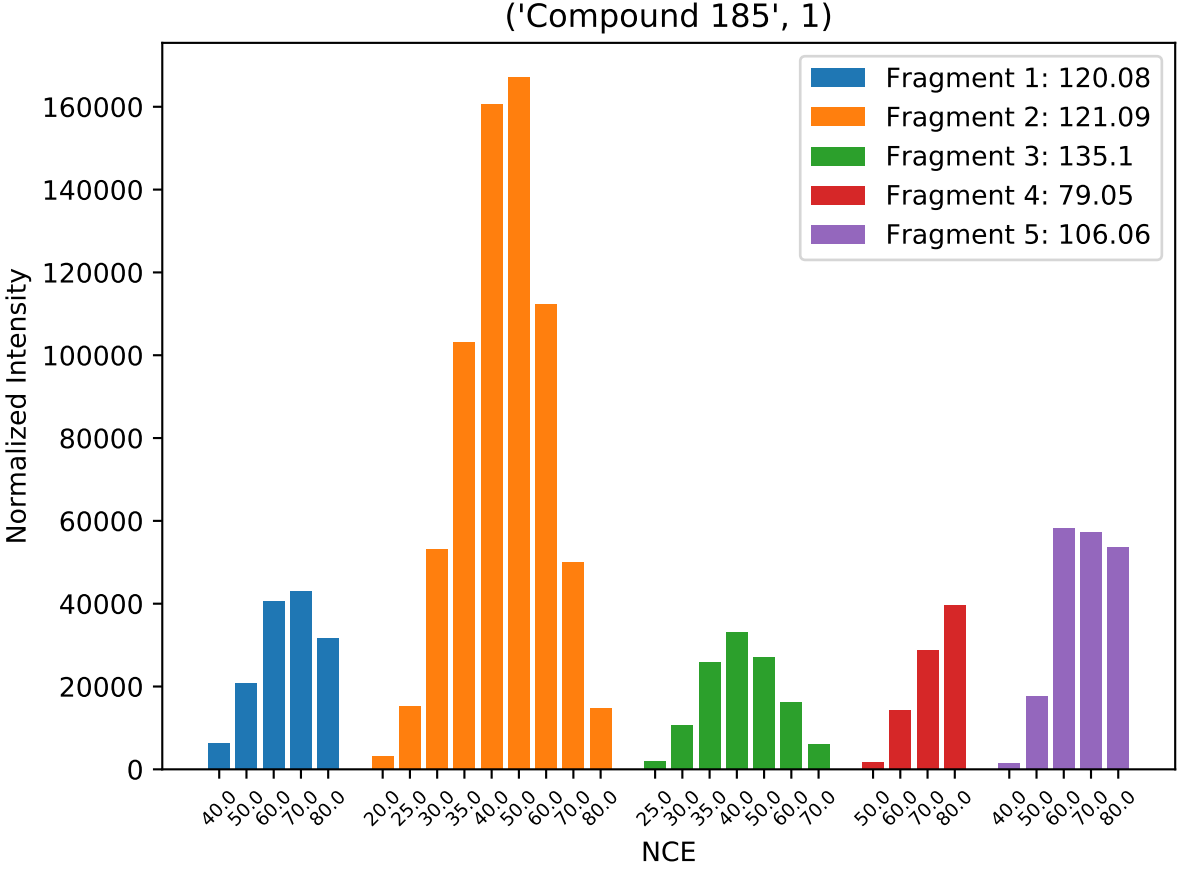

('Compound 179', 1)
Fragment 1: 118.09
Fragment 2: 58.07
Fragment 3: 71.09
Fragment 4: 58.06
Fragment 5: 57.07
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 35.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

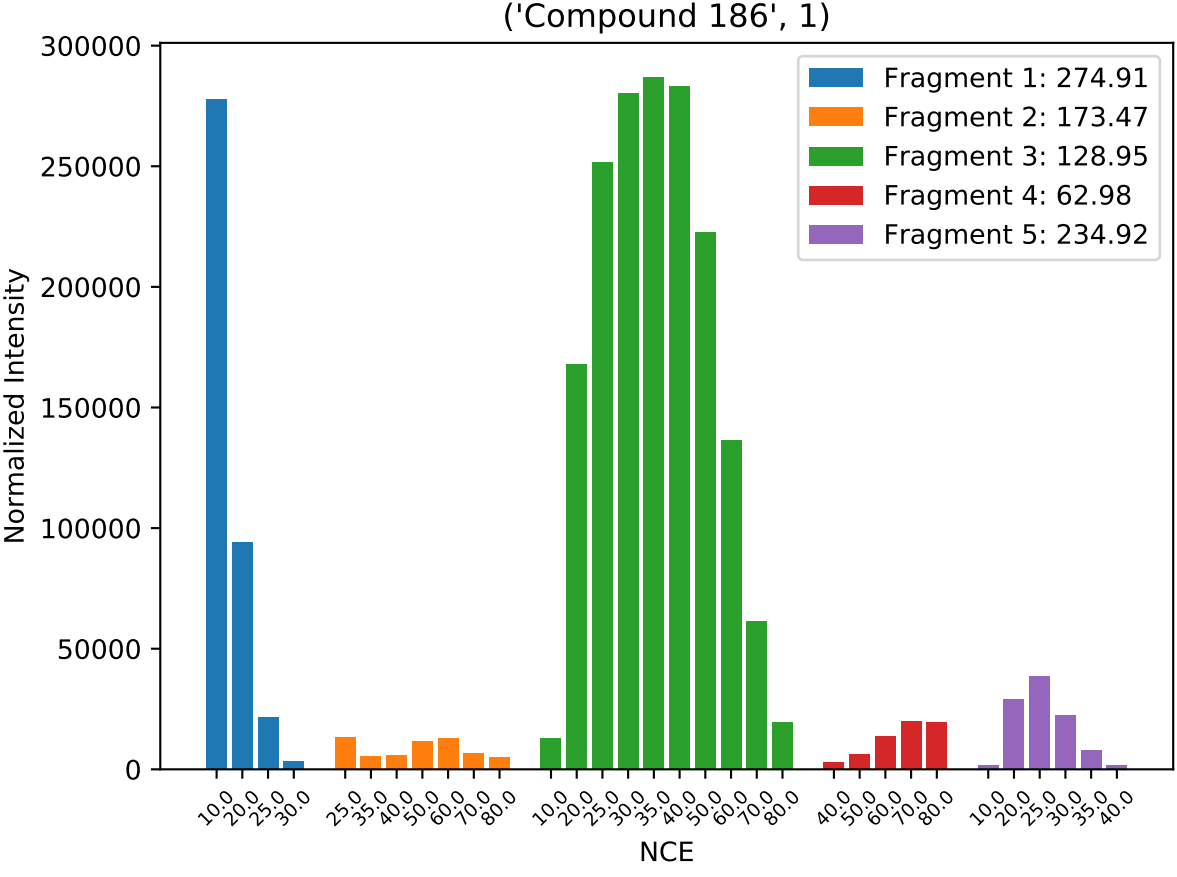

('Compound 180', 1)
Fragment 1: 56.05
Fragment 2: 54.03
Fragment 3: 66.03
Fragment 4: 50.29
Fragment 5: 64.67
Normalized Intensity
0
10000
20000
30000
40000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
35.0
40.0

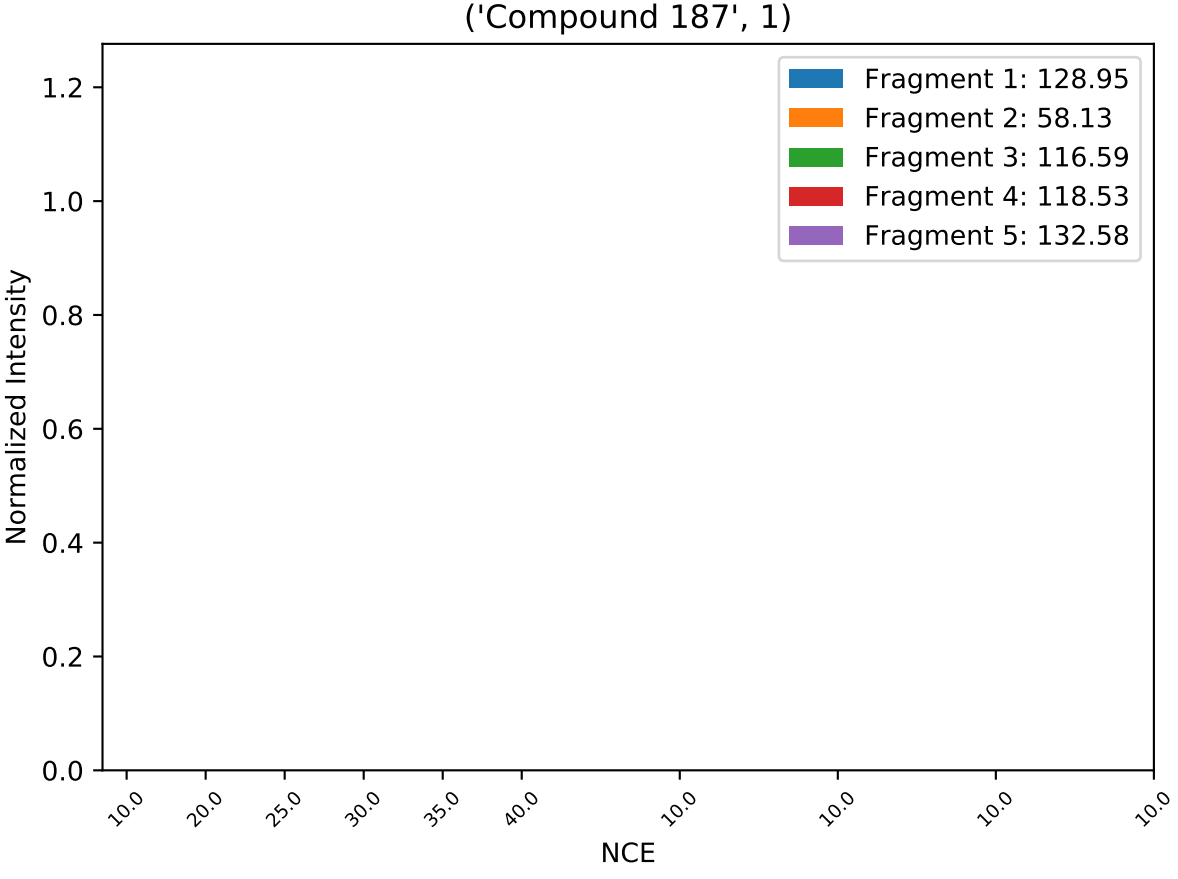

('Compound 181', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 234.92
Fragment 4: 128.95
Fragment 5: 340.88
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
400000
20.0 30.0 35.0 70.0 80.0
10.0 25.0 30.0 40.0 50.0 60.0 80.0
25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

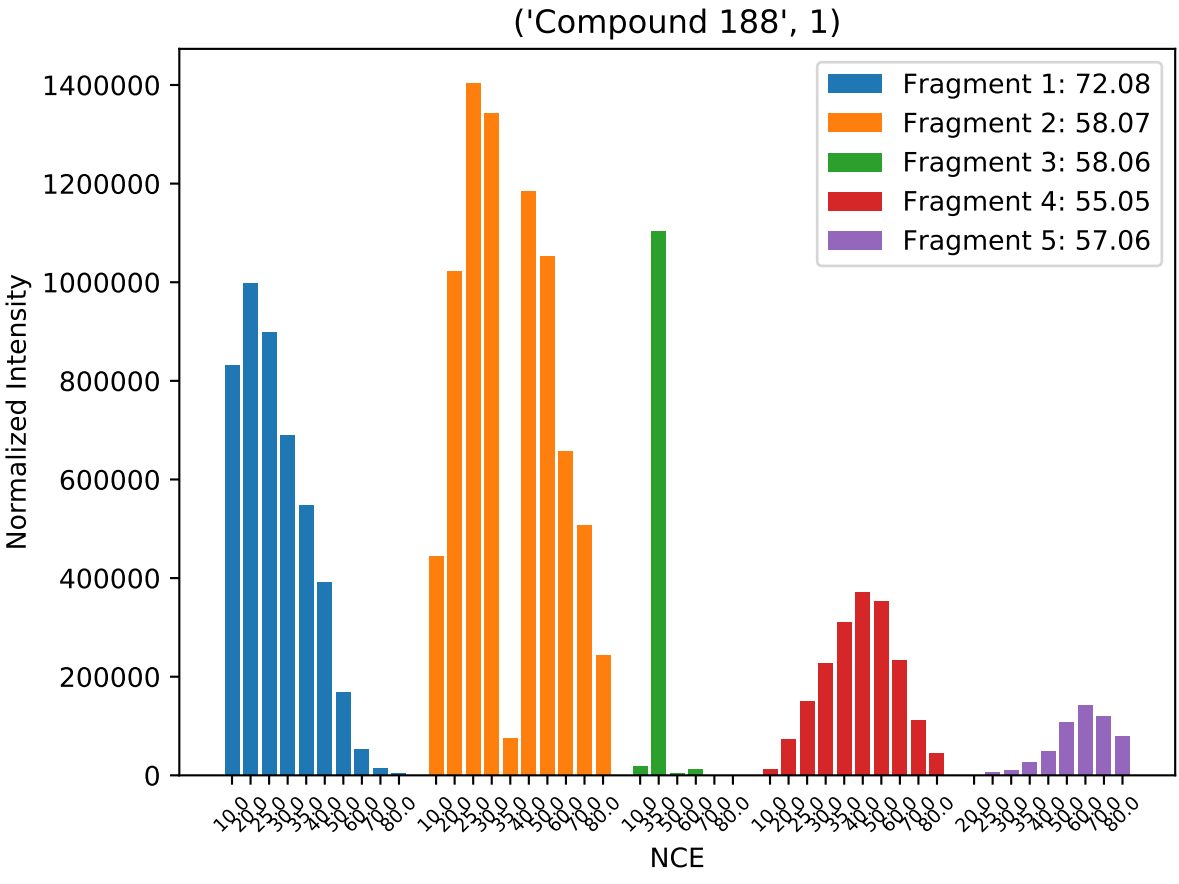

('Compound 182', 1)
Fragment 1: 219.17
Fragment 2: 232.14
Fragment 3: 106.07
Fragment 4: 232.21
Fragment 5: 61.0
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0
40.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

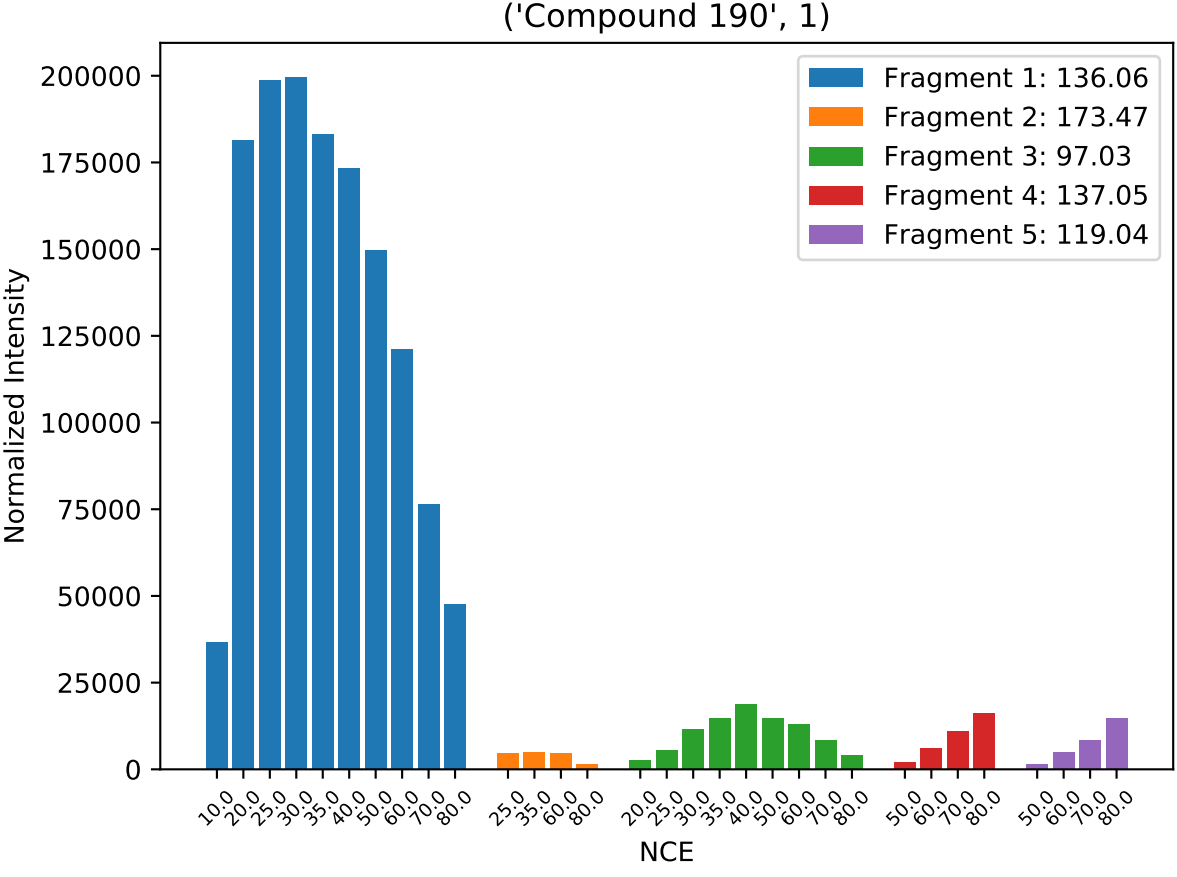

('Compound 184', 1)
Fragment 1: 415.21
Fragment 2: 204.17
Fragment 3: 204.11
Fragment 4: 135.08
Fragment 5: 119.09
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

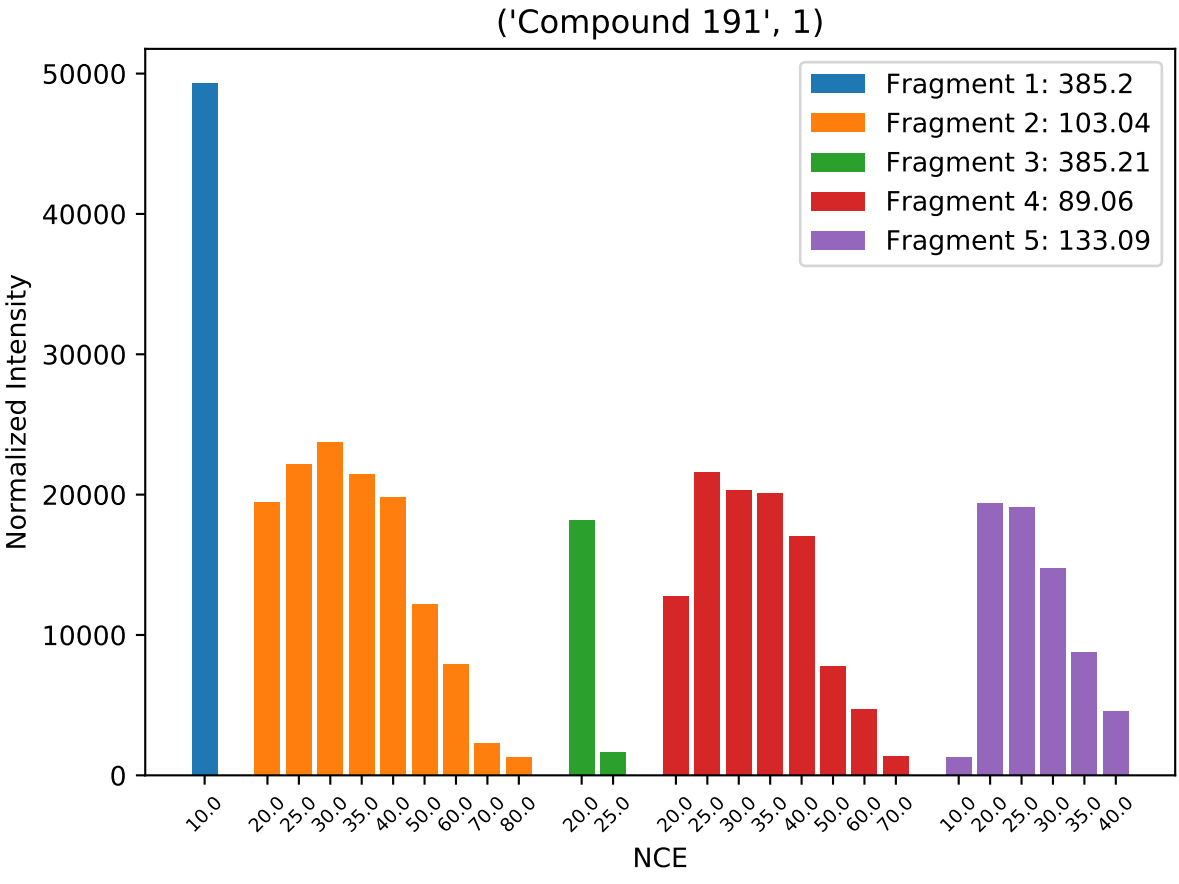

('Compound 185', 1)
Fragment 1: 120.08
Fragment 2: 121.09
Fragment 3: 135.1
Fragment 4: 79.05
Fragment 5: 106.06
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
NCE

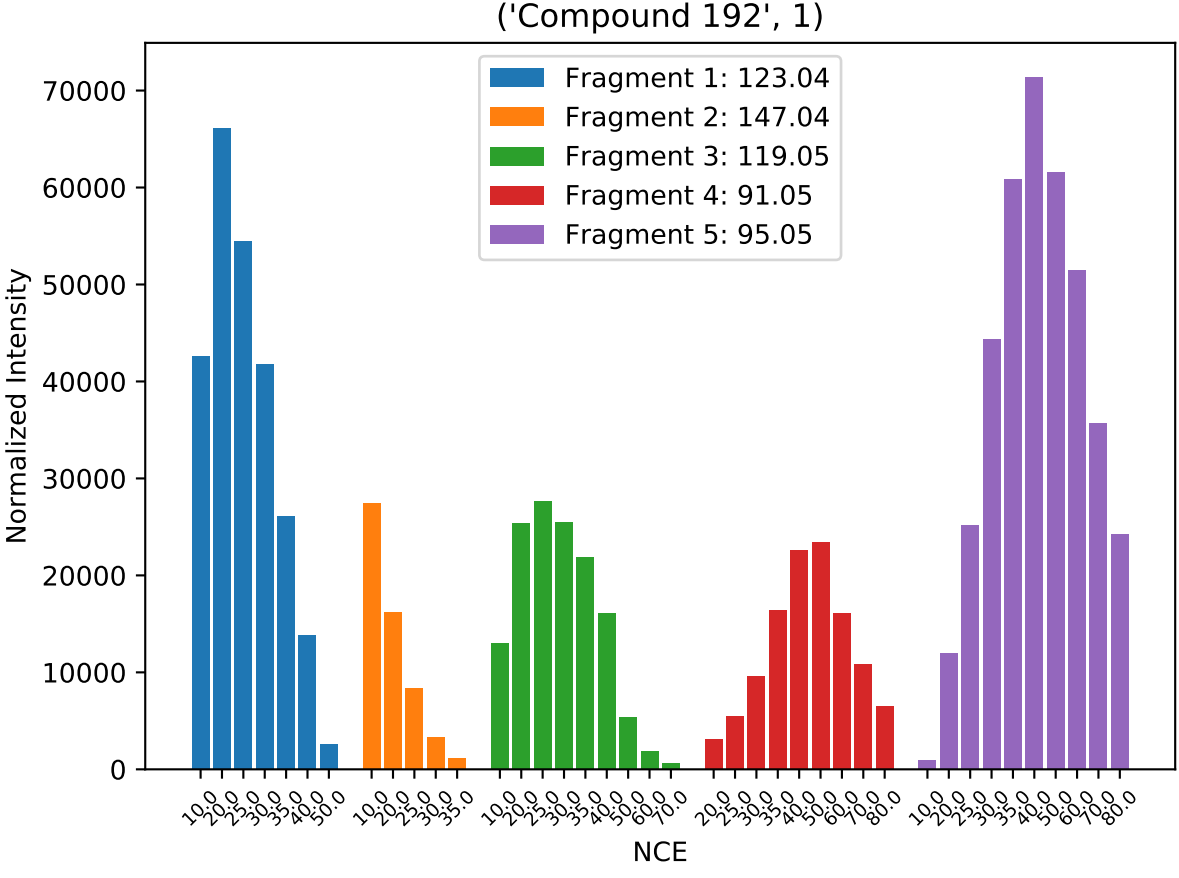

('Compound 186', 1)
Fragment 1: 274.91
Fragment 2: 173.47
Fragment 3: 128.95
Fragment 4: 62.98
Fragment 5: 234.92
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0
25.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

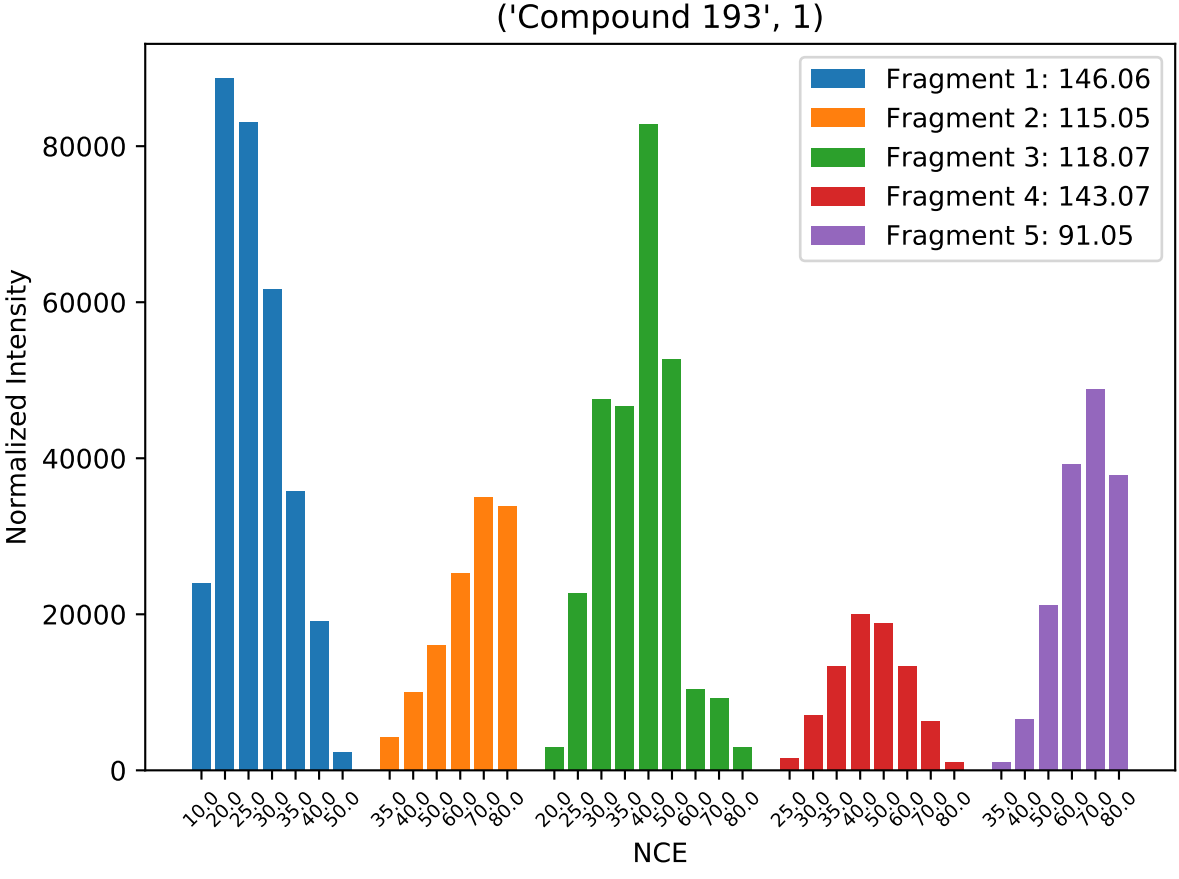

('Compound 187', 1)
Fragment 1: 128.95
Fragment 2: 58.13
Fragment 3: 116.59
Fragment 4: 118.53
Fragment 5: 132.58
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
10.0
10.0
10.0
10.0
NCE

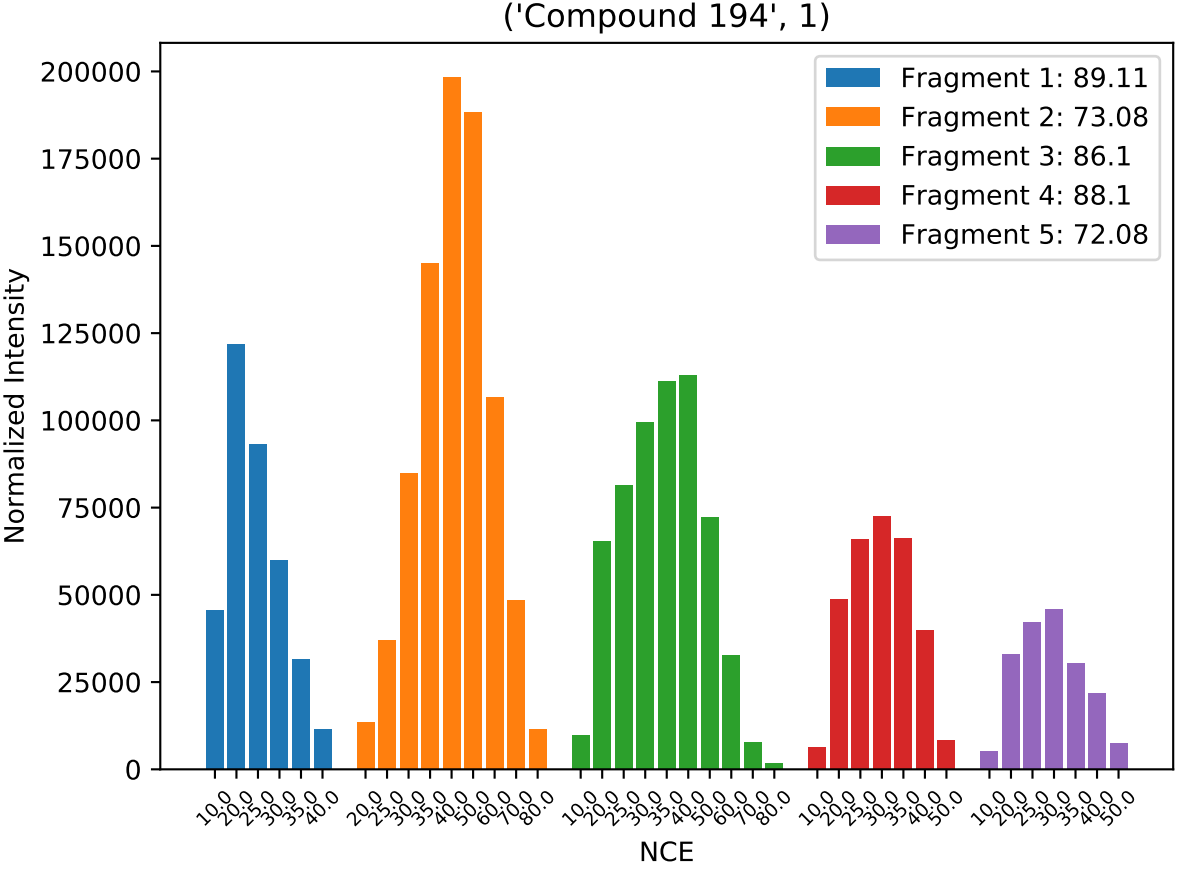

('Compound 188', 1)
Fragment 1: 72.08
Fragment 2: 58.07
Fragment 3: 58.06
Fragment 4: 55.05
Fragment 5: 57.06
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
1400000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

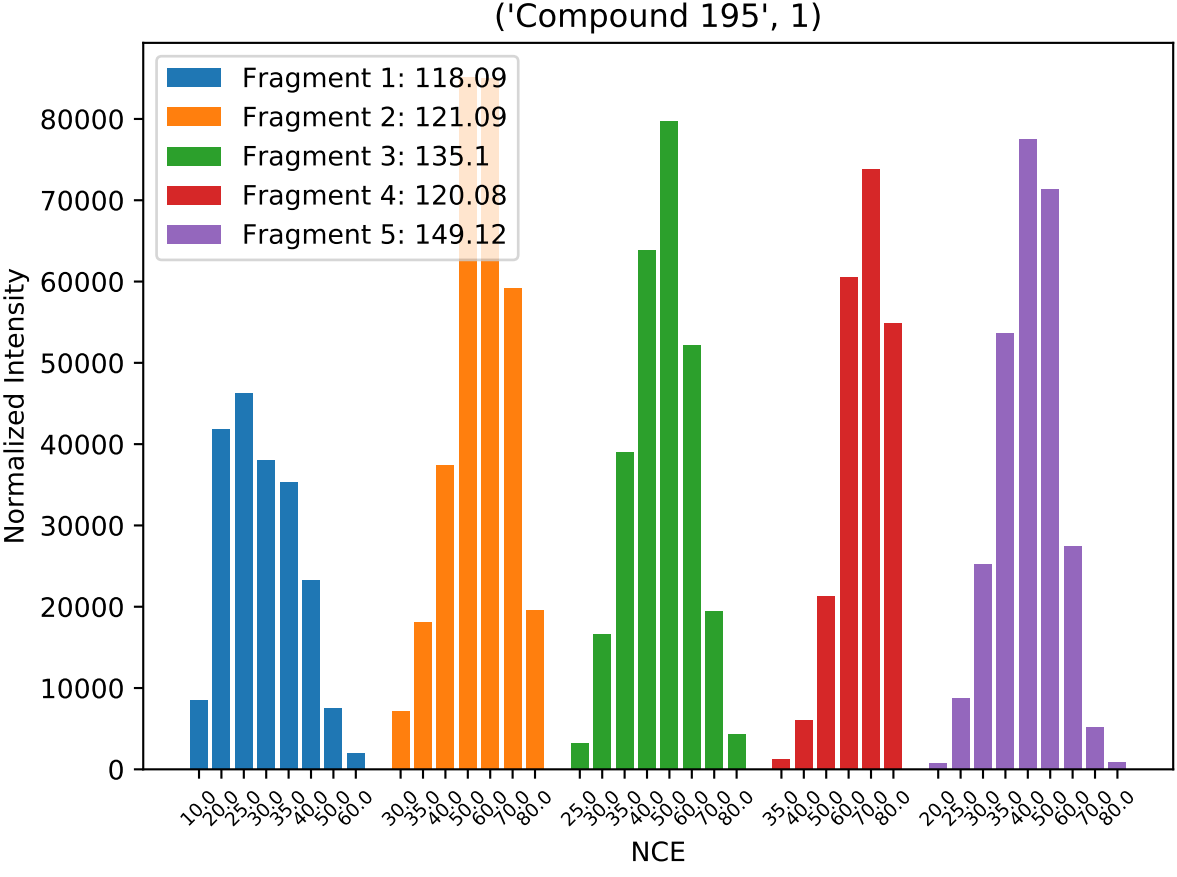

('Compound 190', 1)
Fragment 1: 136.06
Fragment 2: 173.47
Fragment 3: 97.03
Fragment 4: 137.05
Fragment 5: 119.04
Normalized Intensity
200000
175000
150000
125000
100000
75000
50000
25000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
35.0
60.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
50.0
60.0
70.0
80.0
50.0
60.0
70.0
80.0
NCE

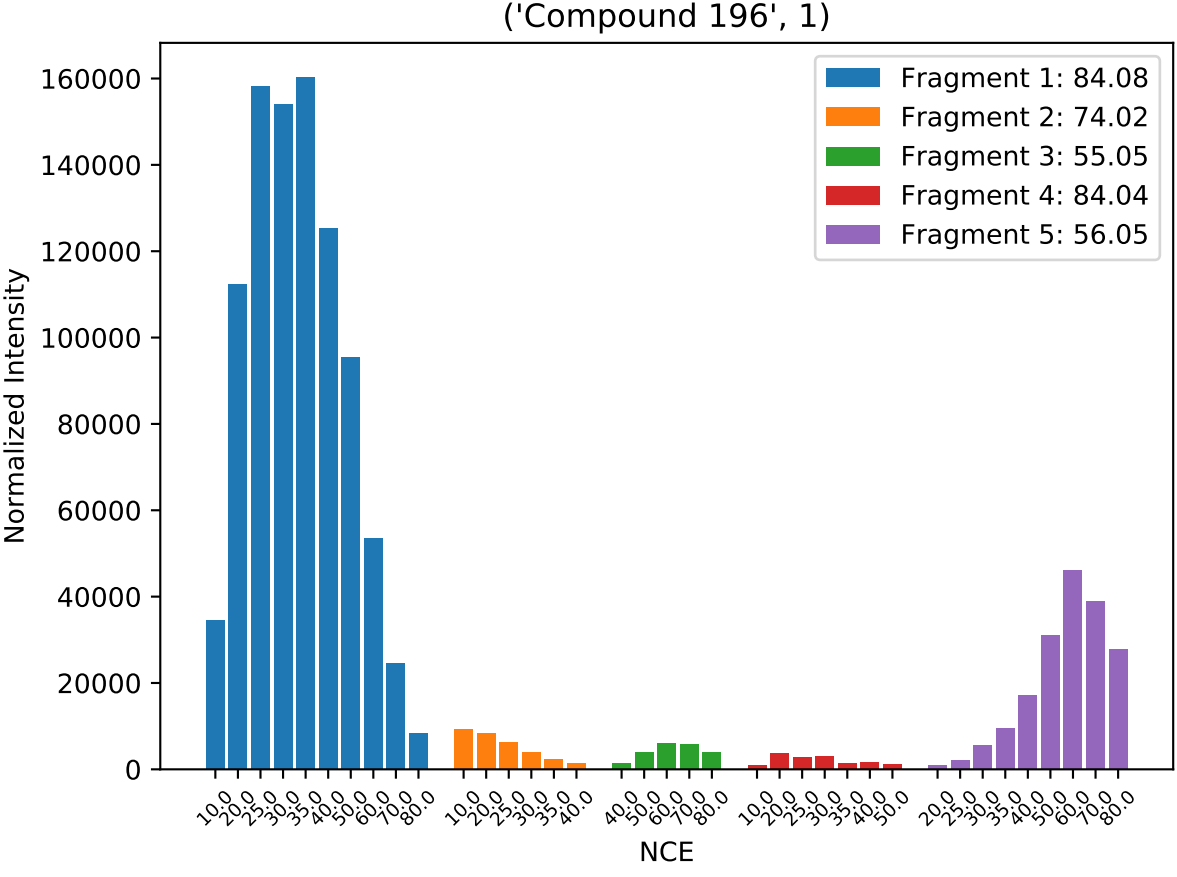

('Compound 191', 1)
Fragment 1: 385.2
Fragment 2: 103.04
Fragment 3: 385.21
Fragment 4: 89.06
Fragment 5: 133.09
Normalized Intensity
0
10000
20000
30000
40000
50000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0

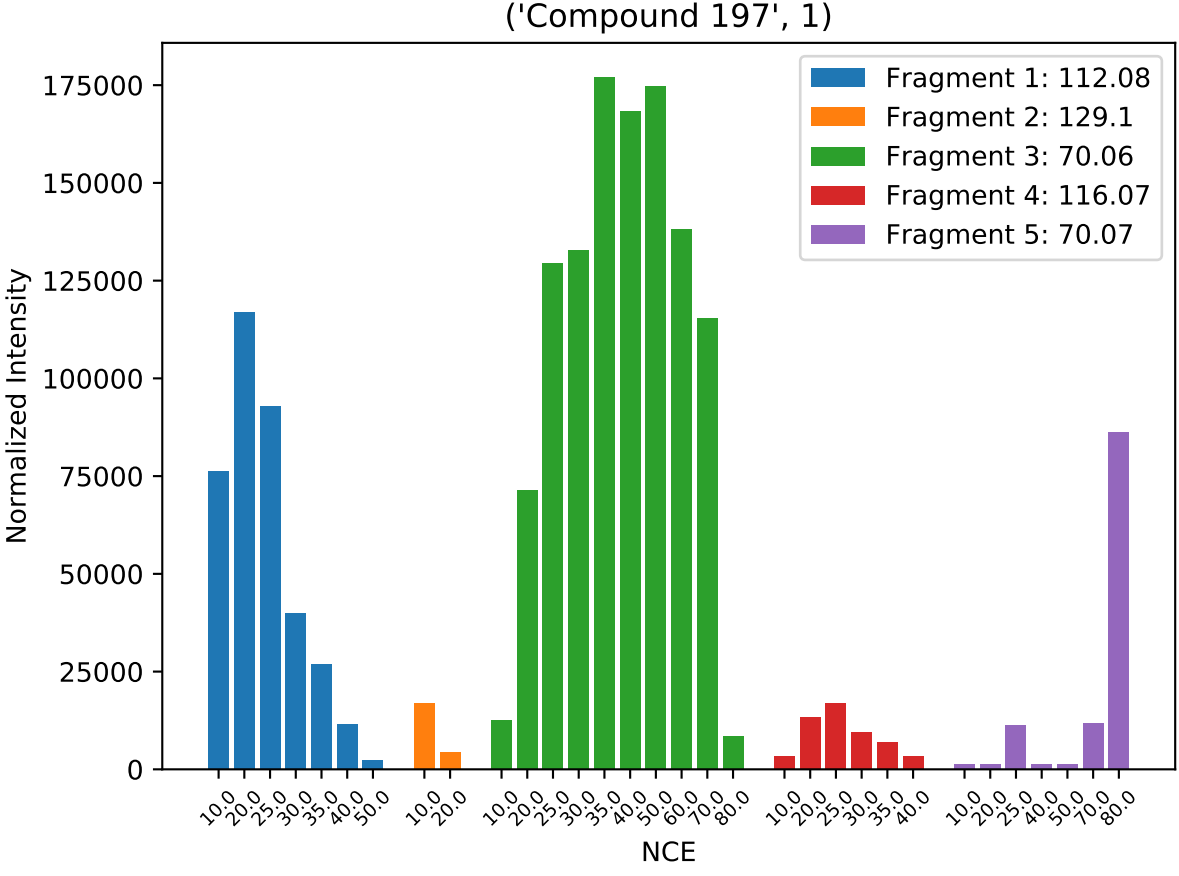

('Compound 192', 1)
Fragment 1: 123.04
Fragment 2: 147.04
Fragment 3: 119.05
Fragment 4: 91.05
Fragment 5: 95.05
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

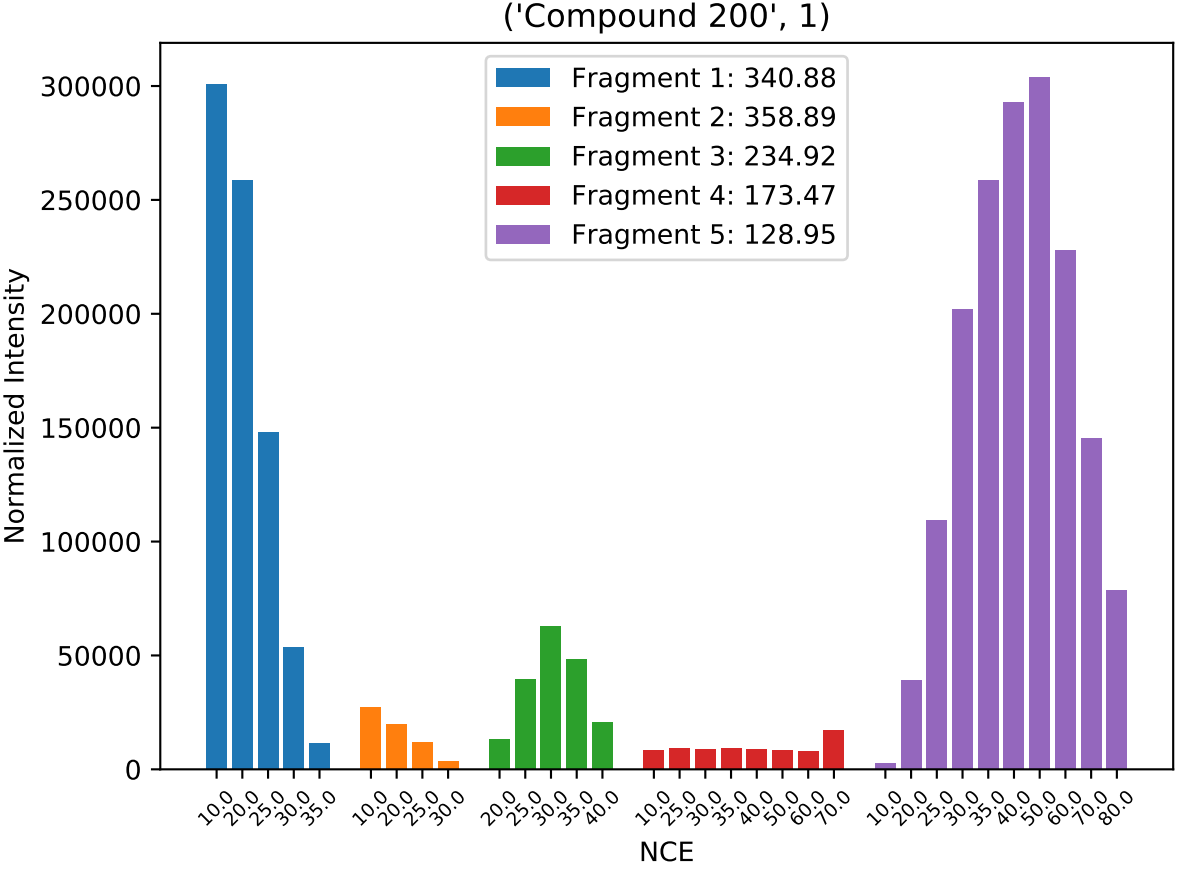

('Compound 193', 1)
Fragment 1: 146.06
Fragment 2: 115.05
Fragment 3: 118.07
Fragment 4: 143.07
Fragment 5: 91.05
Normalized Intensity
0
20000
40000
60000
80000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

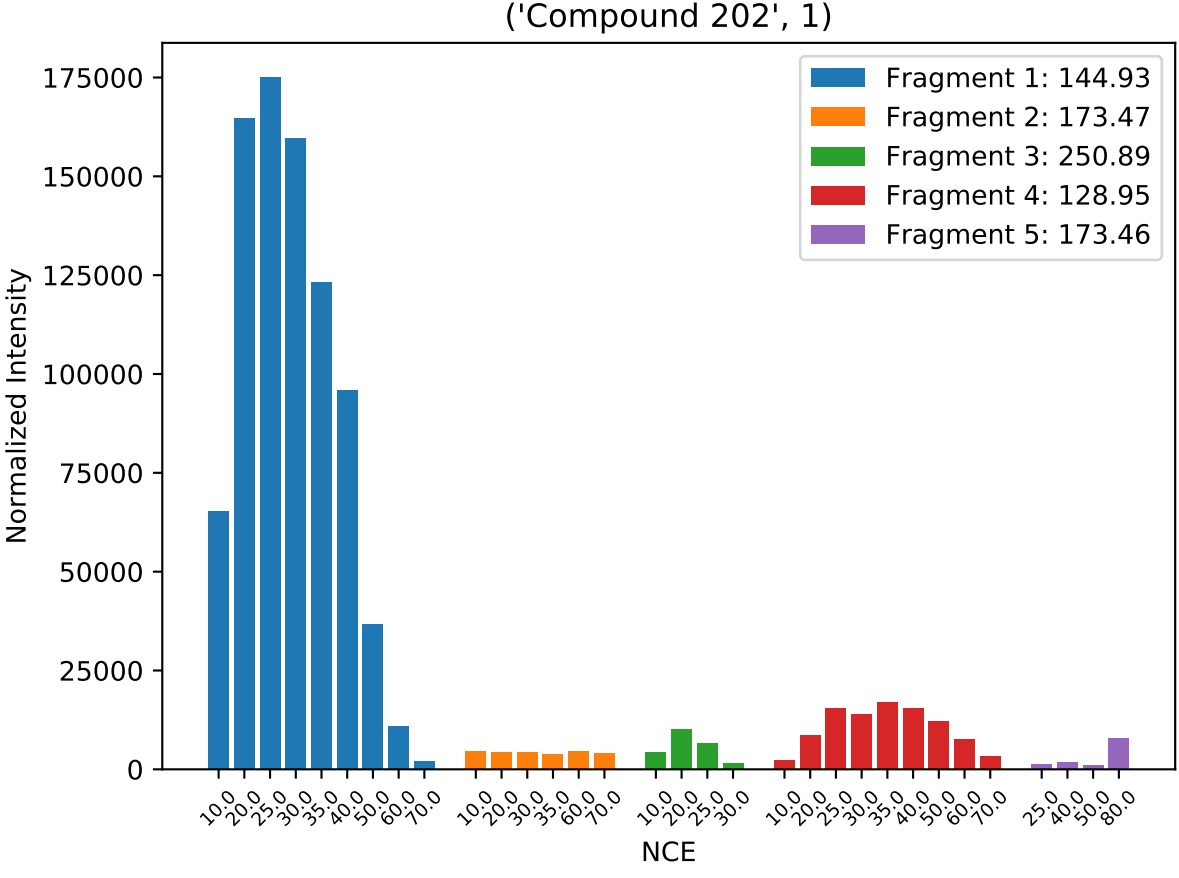

('Compound 194', 1)
Fragment 1: 89.11
Fragment 2: 73.08
Fragment 3: 86.1
Fragment 4: 88.1
Fragment 5: 72.08
Normalized Intensity
200000
175000
150000
125000
100000
75000
50000
25000
0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

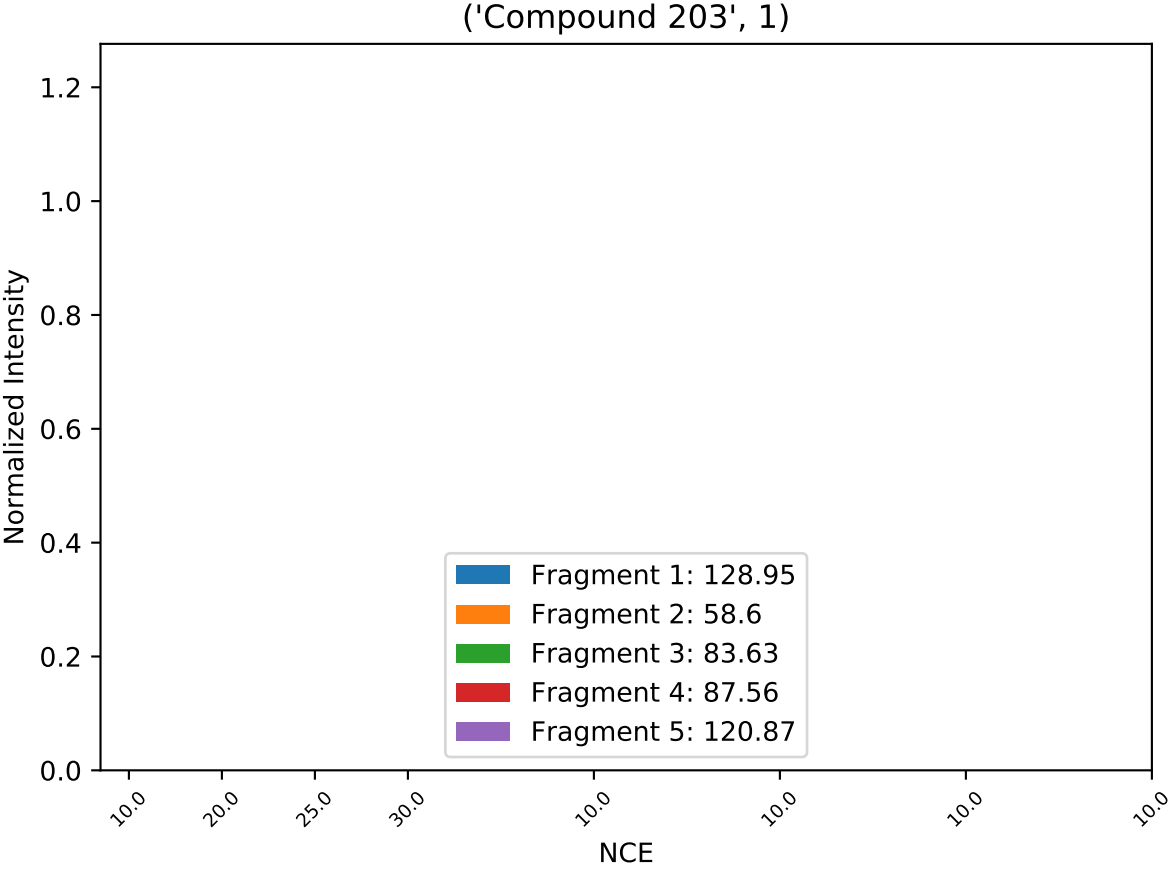

('Compound 195', 1)
Fragment 1: 118.09
Fragment 2: 121.09
Fragment 3: 135.1
Fragment 4: 120.08
Fragment 5: 149.12
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

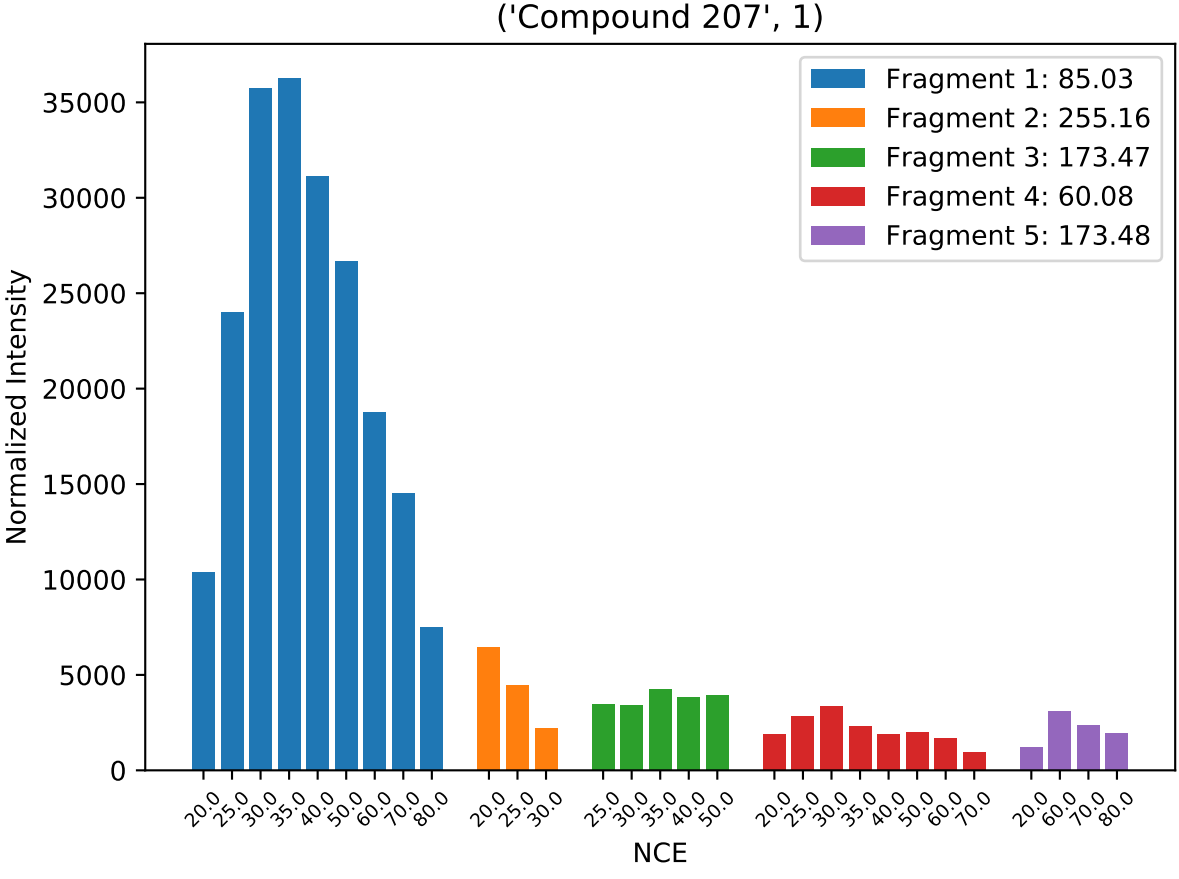

('Compound 196', 1)
Fragment 1: 84.08
Fragment 2: 74.02
Fragment 3: 55.05
Fragment 4: 84.04
Fragment 5: 56.05
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

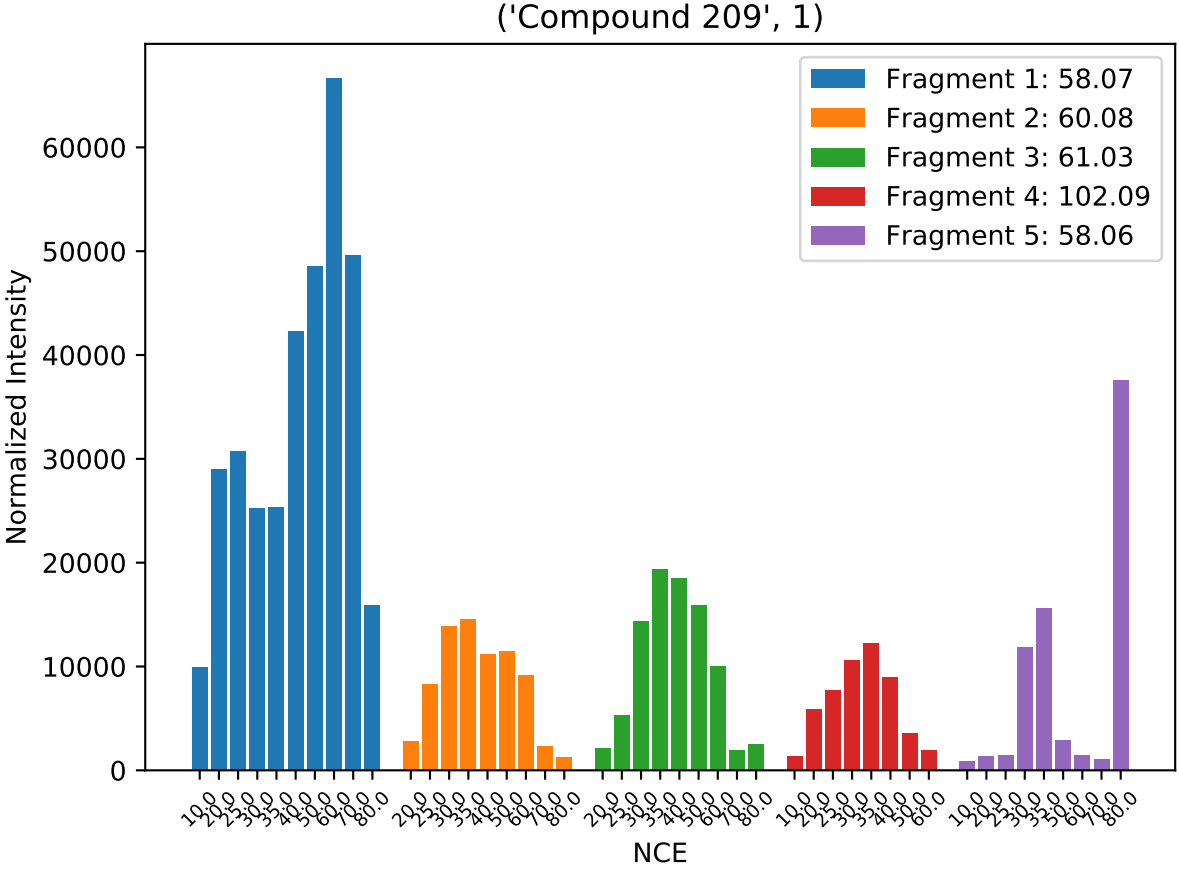

('Compound 197', 1)
Fragment 1: 112.08
Fragment 2: 129.1
Fragment 3: 70.06
Fragment 4: 116.07
Fragment 5: 70.07
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
40.0
50.0
70.0
80.0

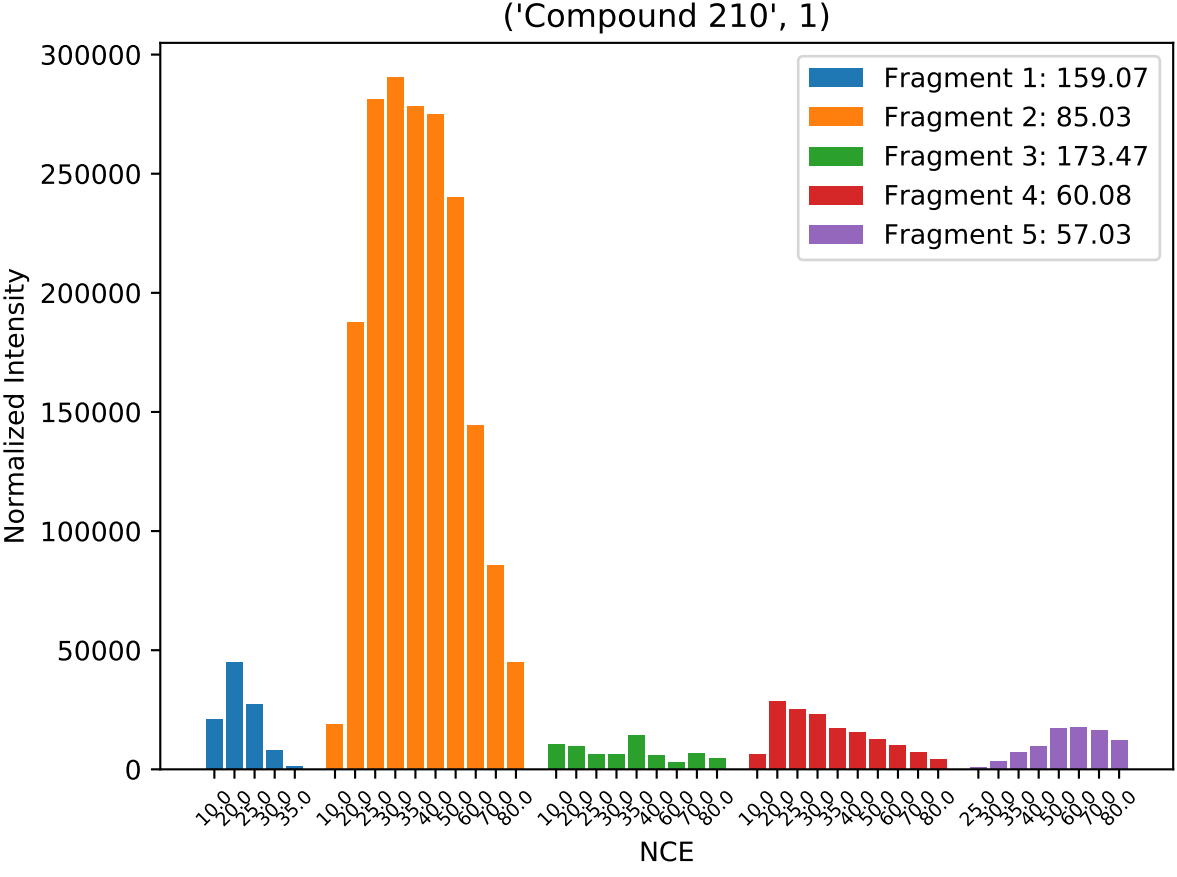

('Compound 200', 1)
Fragment 1: 340.88
Fragment 2: 358.89
Fragment 3: 234.92
Fragment 4: 173.47
Fragment 5: 128.95
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0
20.0 25.0 30.0 35.0 40.0
10.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

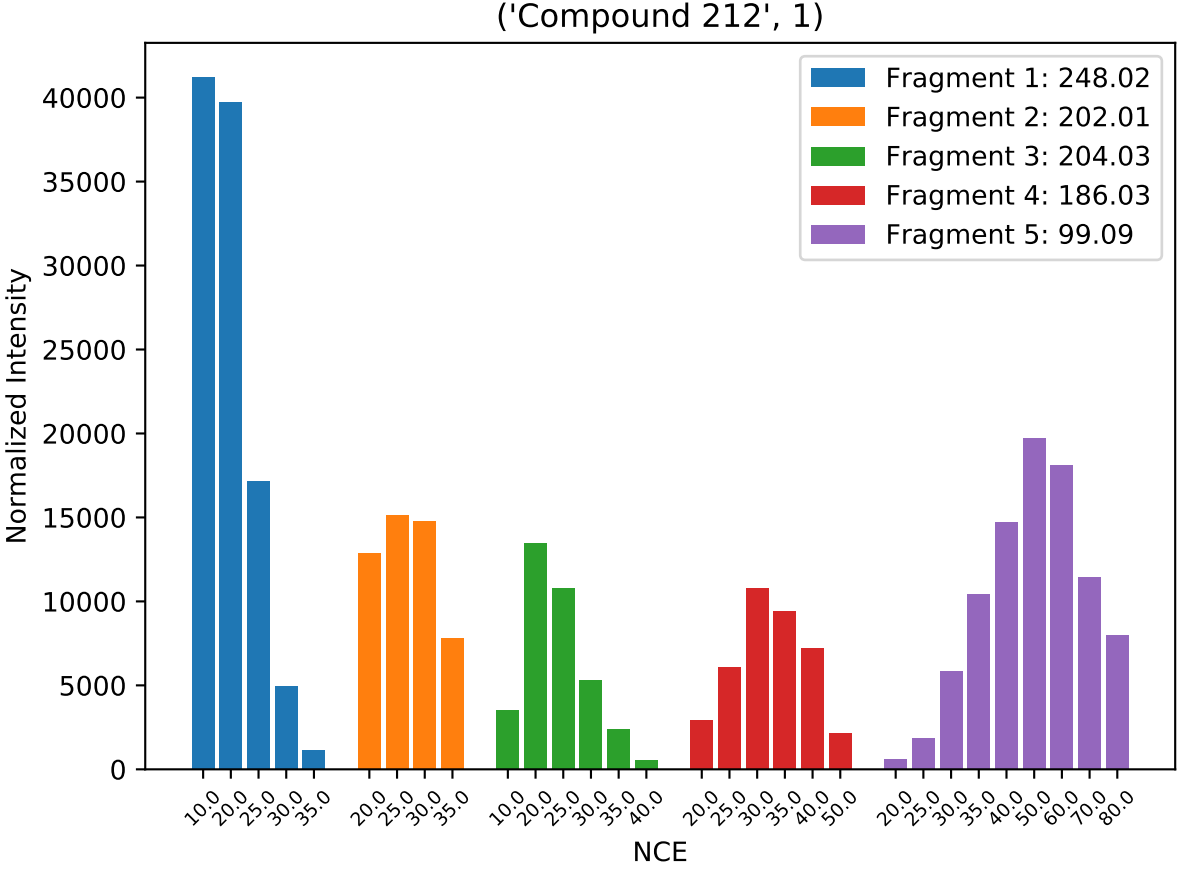

('Compound 202', 1)
Fragment 1: 144.93
Fragment 2: 173.47
Fragment 3: 250.89
Fragment 4: 128.95
Fragment 5: 173.46
Normalized Intensity
175000
150000
125000
100000
75000
50000
25000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 30.0 35.0 60.0 70.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 40.0 50.0 80.0
NCE

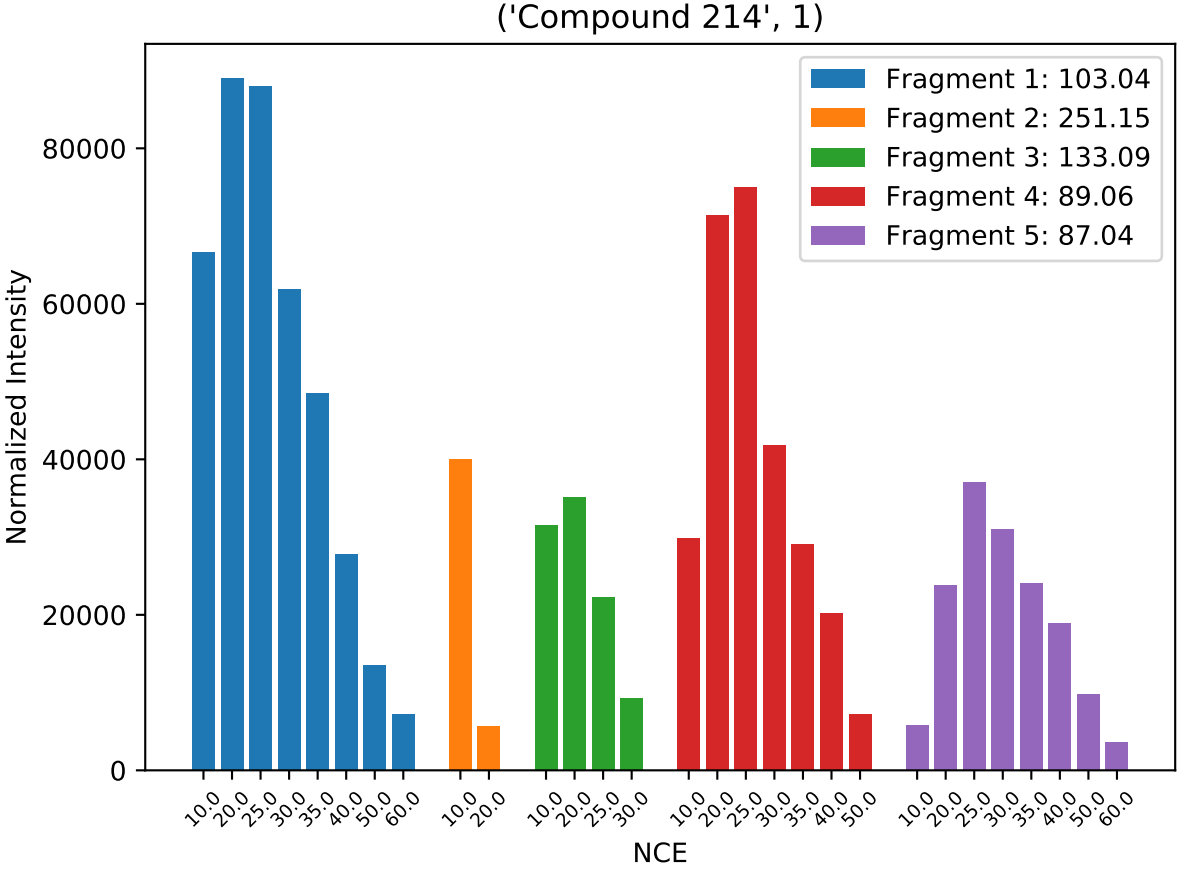

('Compound 203', 1)
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
Fragment 1: 128.95
Fragment 2: 58.6
Fragment 3: 83.63
Fragment 4: 87.56
Fragment 5: 120.87
10.0
20.0
25.0
30.0
10.0
10.0
10.0
10.0
NCE

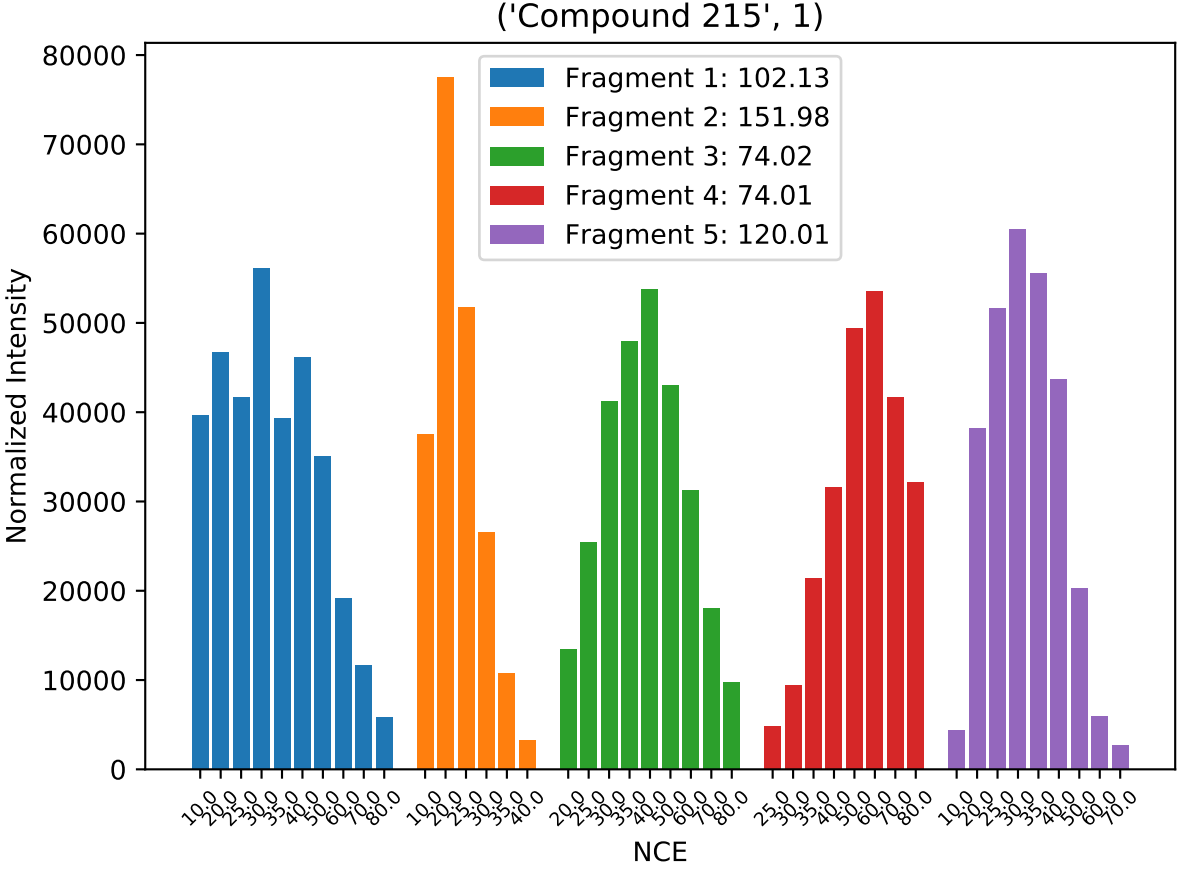

('Compound 207', 1)
Fragment 1: 85.03
Fragment 2: 255.16
Fragment 3: 173.47
Fragment 4: 60.08
Fragment 5: 173.48
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0
25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 60.0 70.0 80.0
NCE

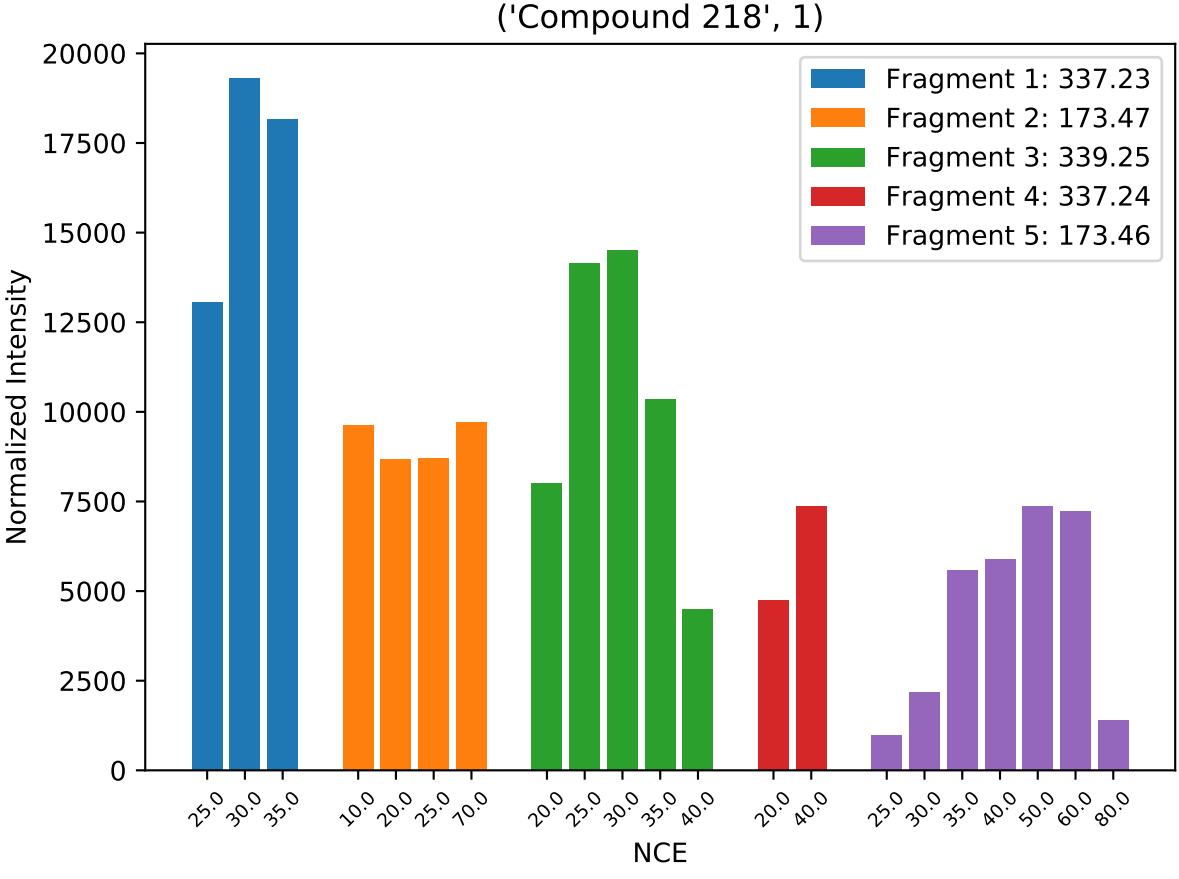

('Compound 209', 1)
Fragment 1: 58.07
Fragment 2: 60.08
Fragment 3: 61.03
Fragment 4: 102.09
Fragment 5: 58.06
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

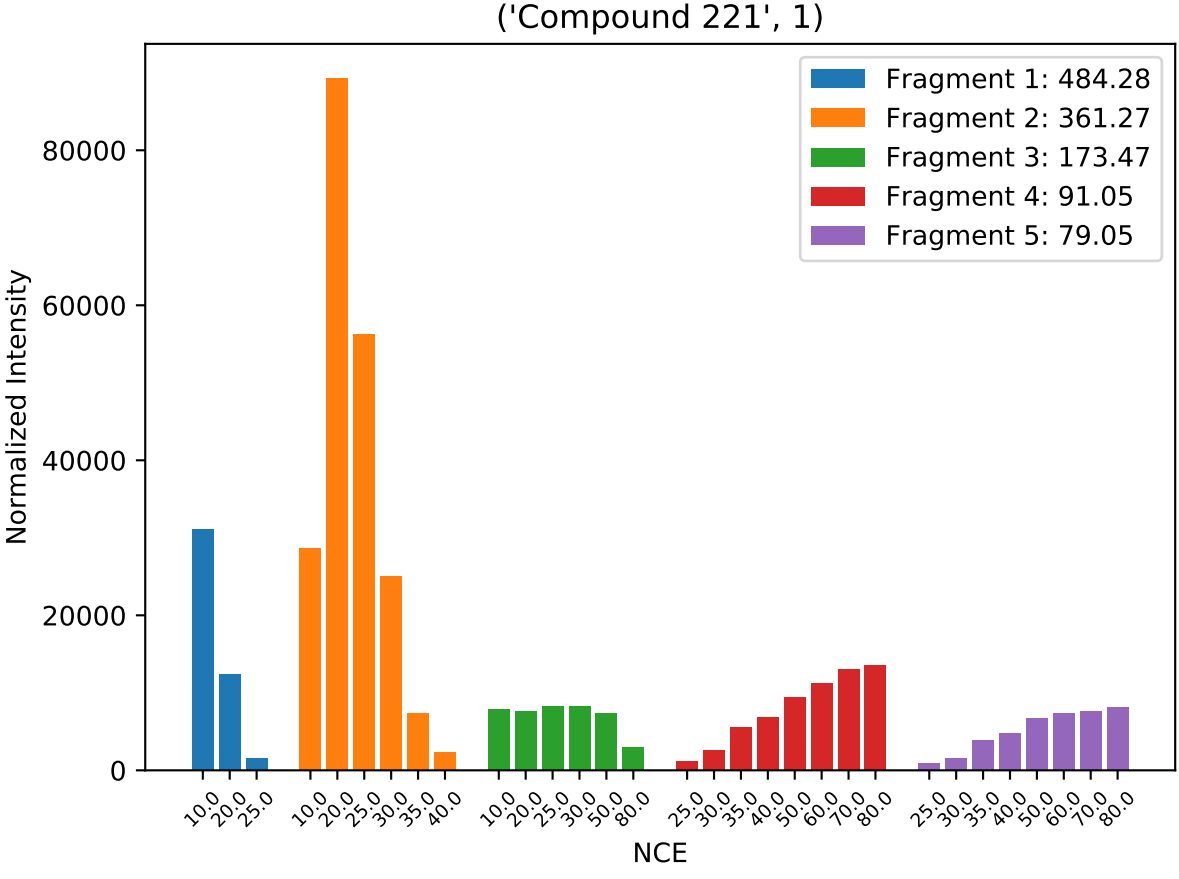

('Compound 210', 1)
Fragment 1: 159.07
Fragment 2: 85.03
Fragment 3: 173.47
Fragment 4: 60.08
Fragment 5: 57.03
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

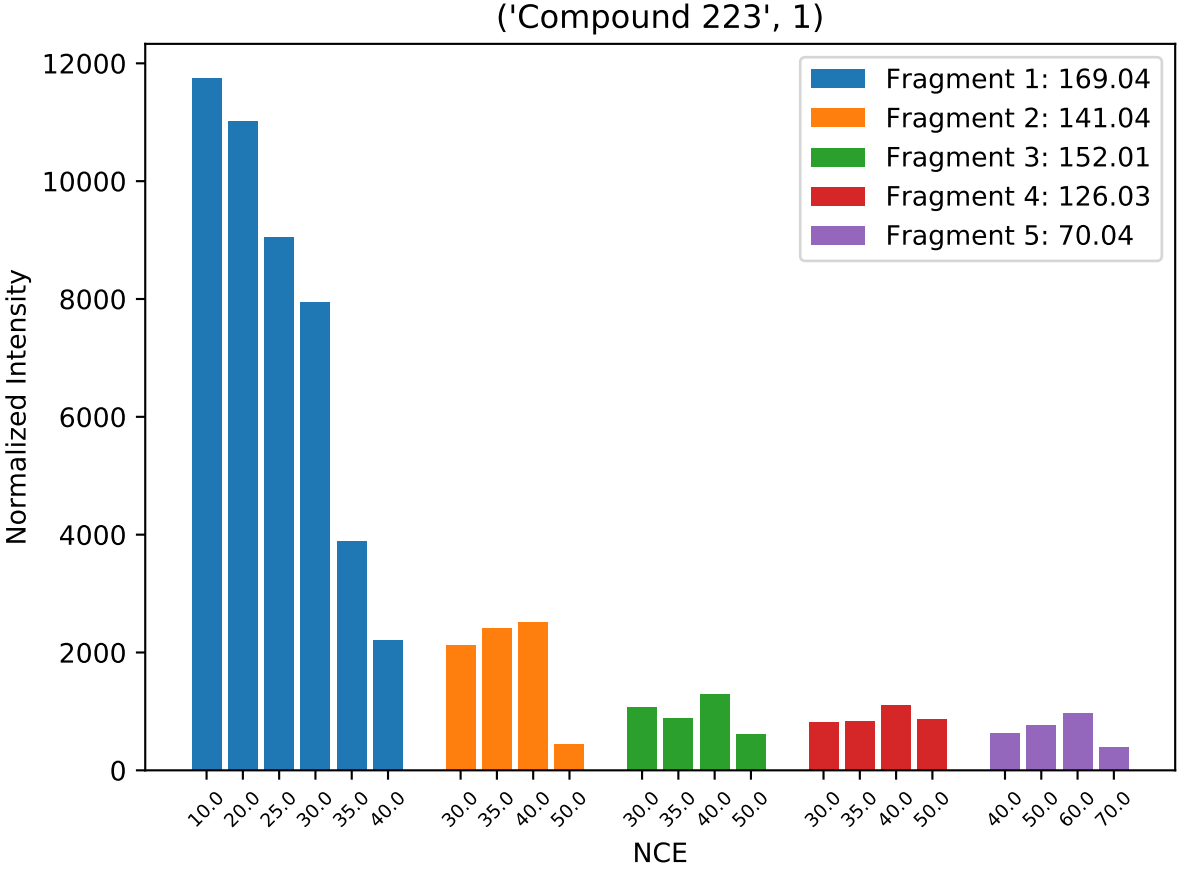

('Compound 212', 1)
Fragment 1: 248.02
Fragment 2: 202.01
Fragment 3: 204.03
Fragment 4: 186.03
Fragment 5: 99.09
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

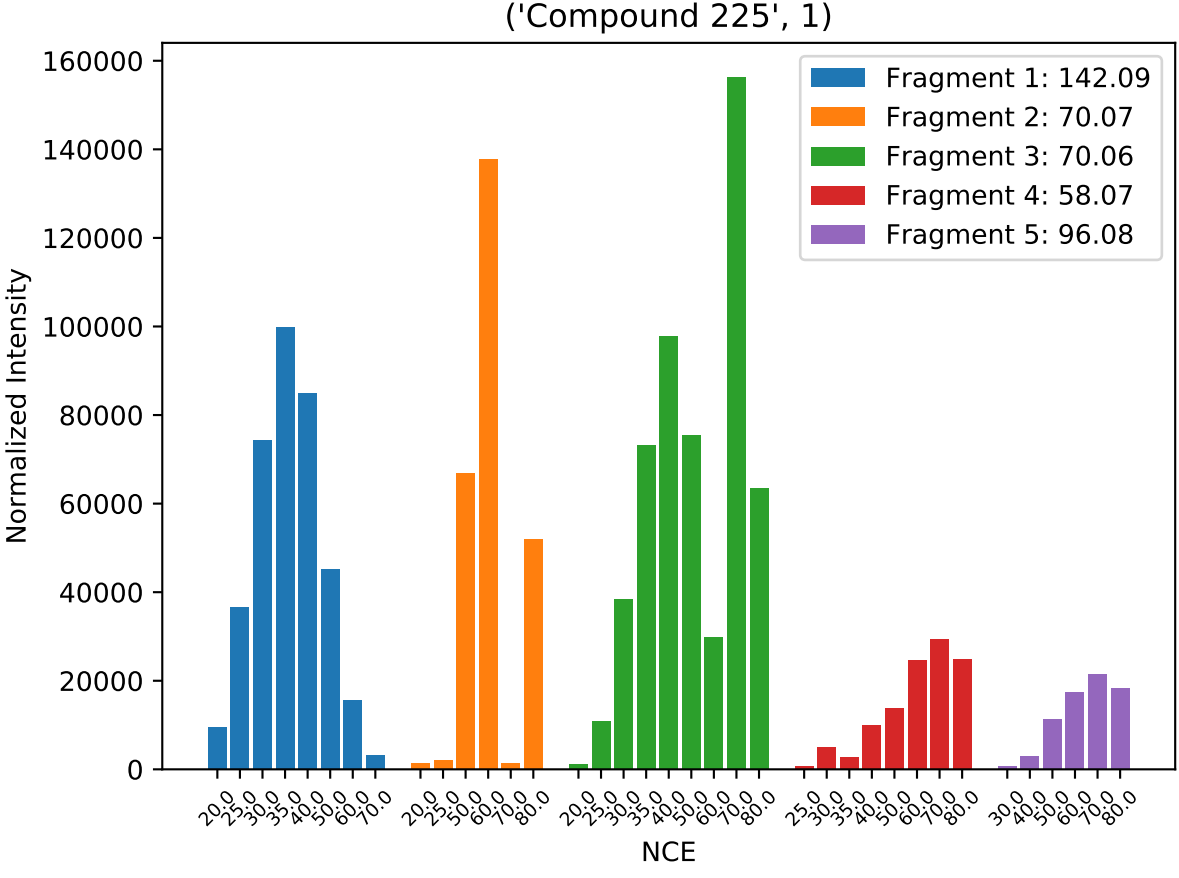

('Compound 214', 1)
Fragment 1: 103.04
Fragment 2: 251.15
Fragment 3: 133.09
Fragment 4: 89.06
Fragment 5: 87.04
Normalized Intensity
0
20000
40000
60000
80000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

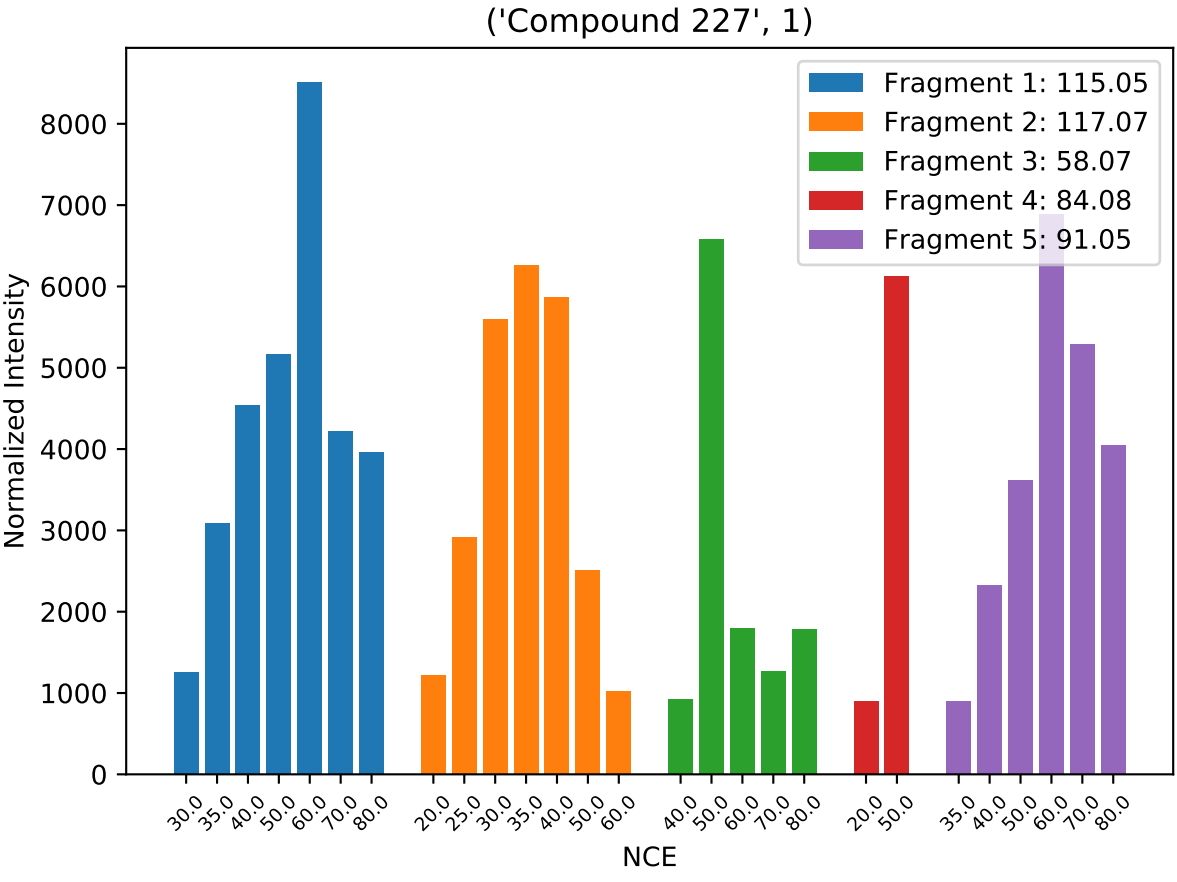

('Compound 215', 1)
Fragment 1: 102.13
Fragment 2: 151.98
Fragment 3: 74.02
Fragment 4: 74.01
Fragment 5: 120.01
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

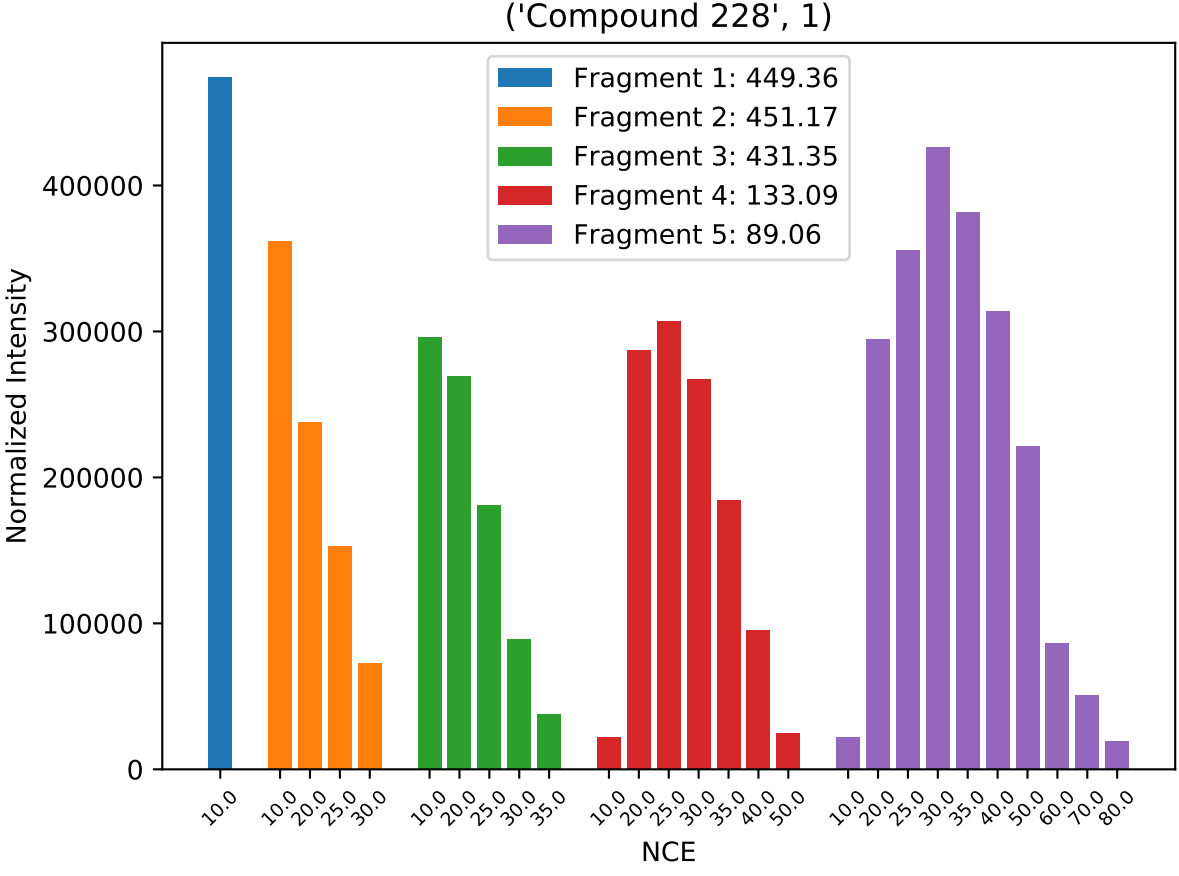

('Compound 218', 1)
Fragment 1: 337.23
Fragment 2: 173.47
Fragment 3: 339.25
Fragment 4: 337.24
Fragment 5: 173.46
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
25.0
30.0
35.0
10.0
20.0
25.0
70.0
20.0
25.0
30.0
35.0
40.0
20.0
40.0
25.0
30.0
35.0
40.0
50.0
60.0
80.0
NCE

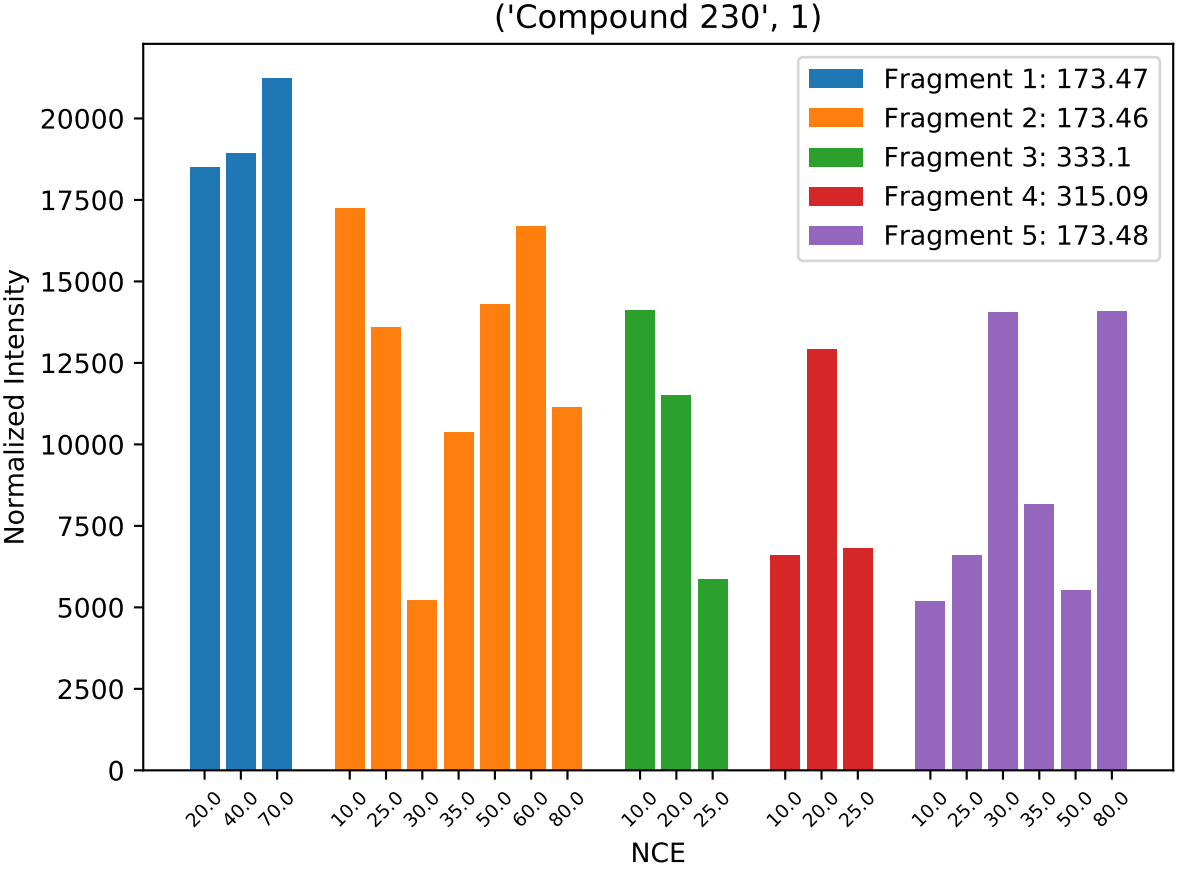

('Compound 221', 1)
Fragment 1: 484.28
Fragment 2: 361.27
Fragment 3: 173.47
Fragment 4: 91.05
Fragment 5: 79.05
Normalized Intensity
0
20000
40000
60000
80000
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
50.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

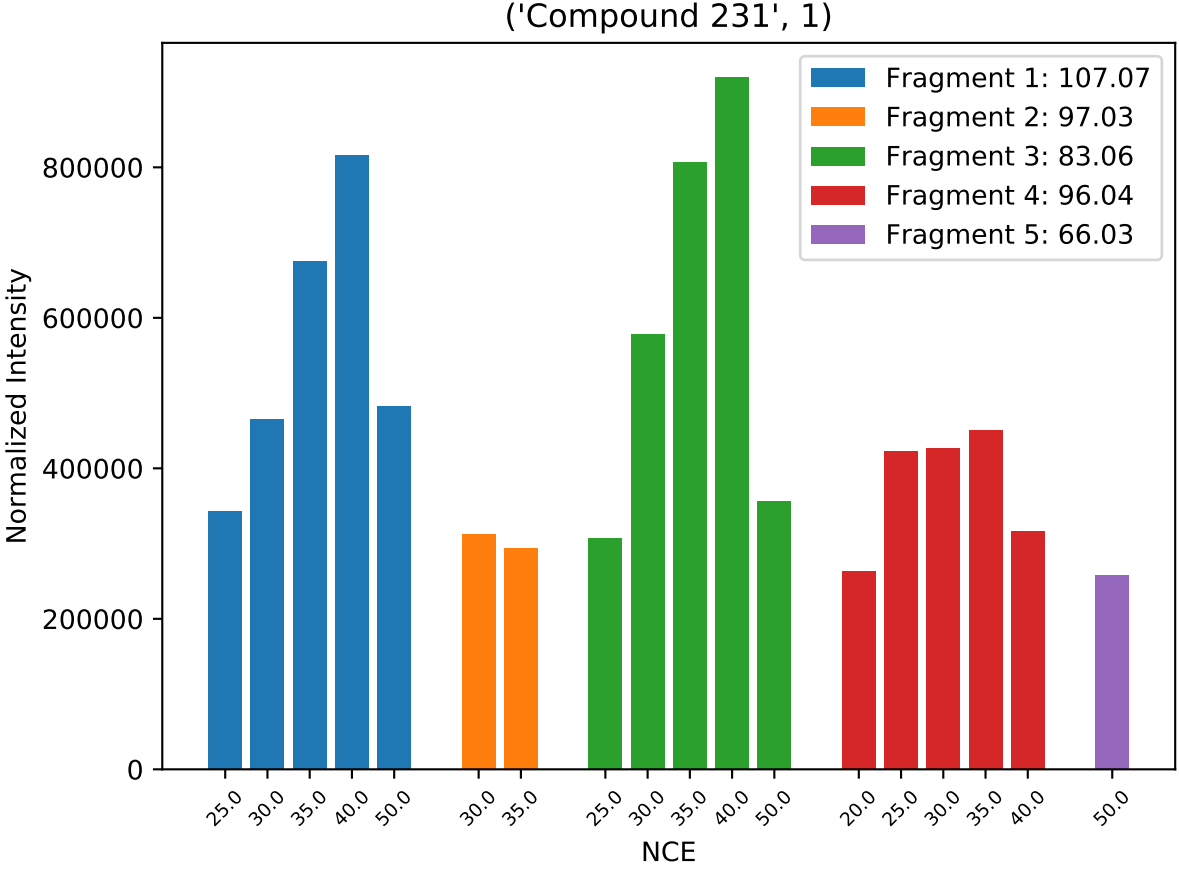

('Compound 223', 1)
Fragment 1: 169.04
Fragment 2: 141.04
Fragment 3: 152.01
Fragment 4: 126.03
Fragment 5: 70.04
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0
20.0
25.0
30.0
35.0
40.0
30.0
35.0
40.0
50.0
30.0
35.0
40.0
50.0
30.0
35.0
40.0
50.0
40.0
50.0
60.0
70.0
NCE

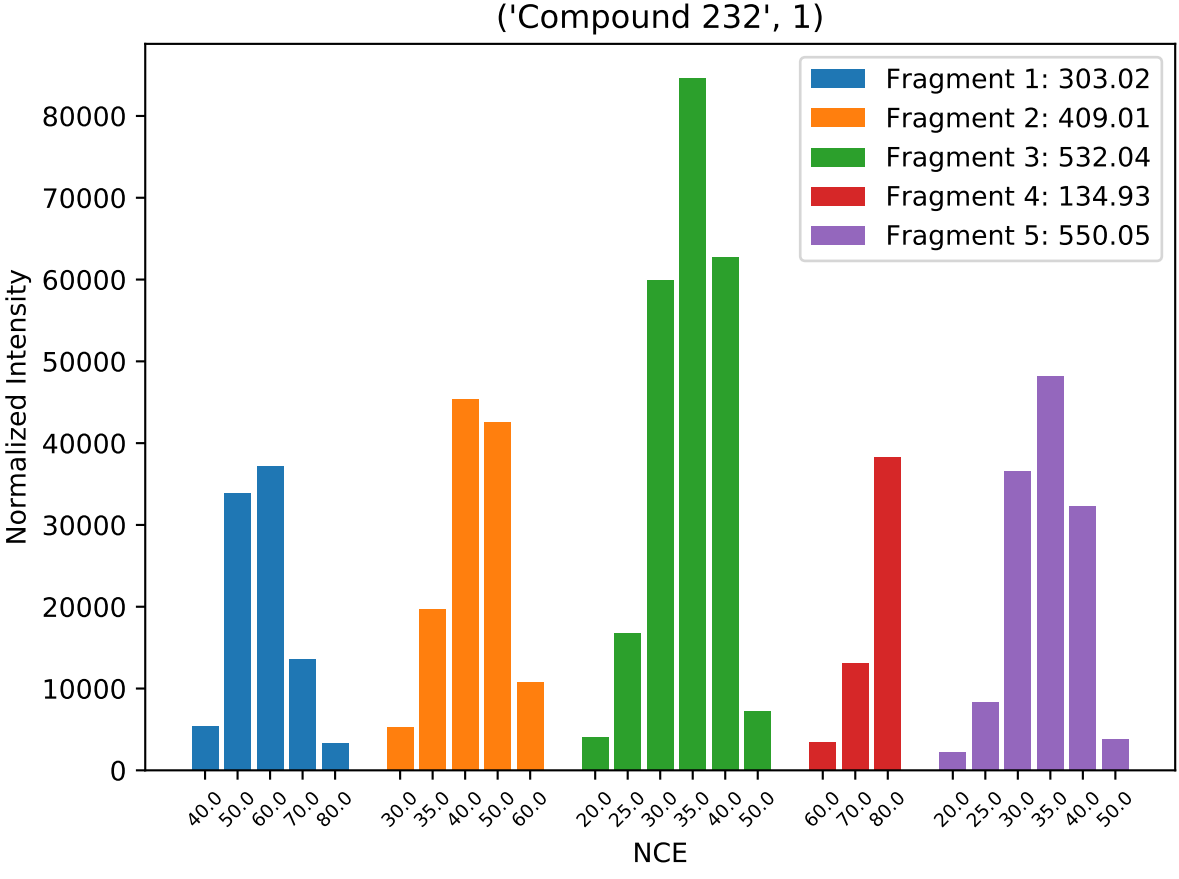

('Compound 225', 1)
Fragment 1: 142.09
Fragment 2: 70.07
Fragment 3: 70.06
Fragment 4: 58.07
Fragment 5: 96.08
Normalized Intensity
NCE
160000
140000
120000
100000
80000
60000
40000
20000
0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 40.0 50.0 60.0 70.0 80.0

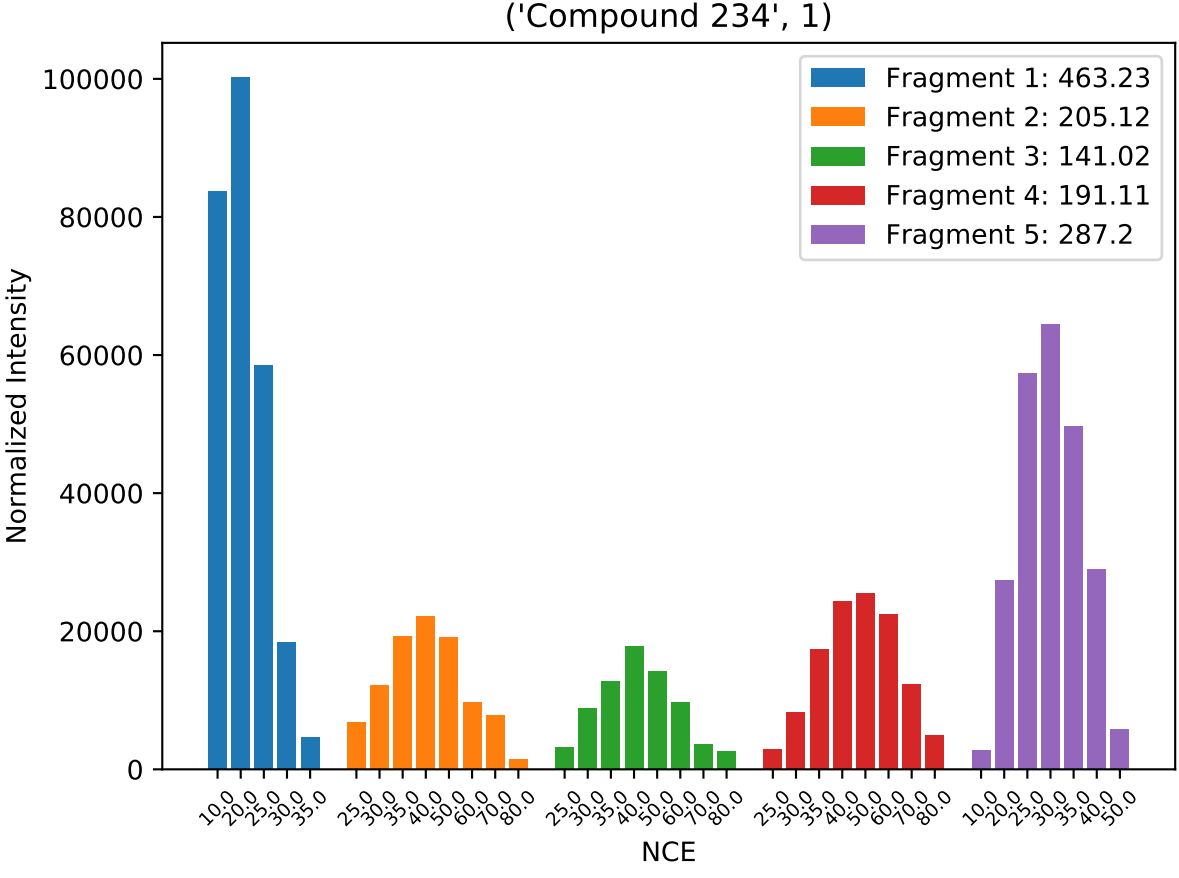

('Compound 227', 1)
Fragment 1: 115.05
Fragment 2: 117.07
Fragment 3: 58.07
Fragment 4: 84.08
Fragment 5: 91.05
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
40.0
50.0
60.0
70.0
80.0
20.0
50.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

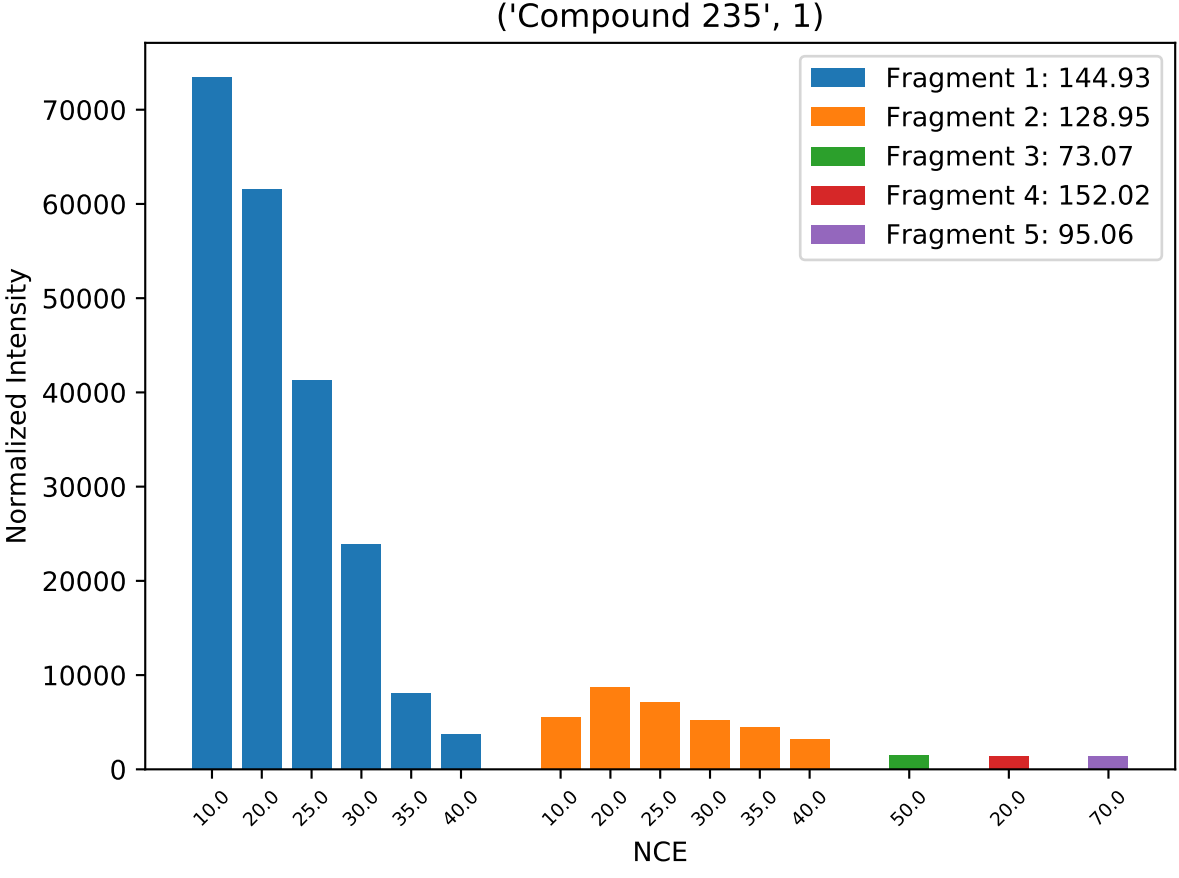

('Compound 228', 1)
Fragment 1: 449.36
Fragment 2: 451.17
Fragment 3: 431.35
Fragment 4: 133.09
Fragment 5: 89.06
Normalized Intensity
0
100000
200000
300000
400000
10.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

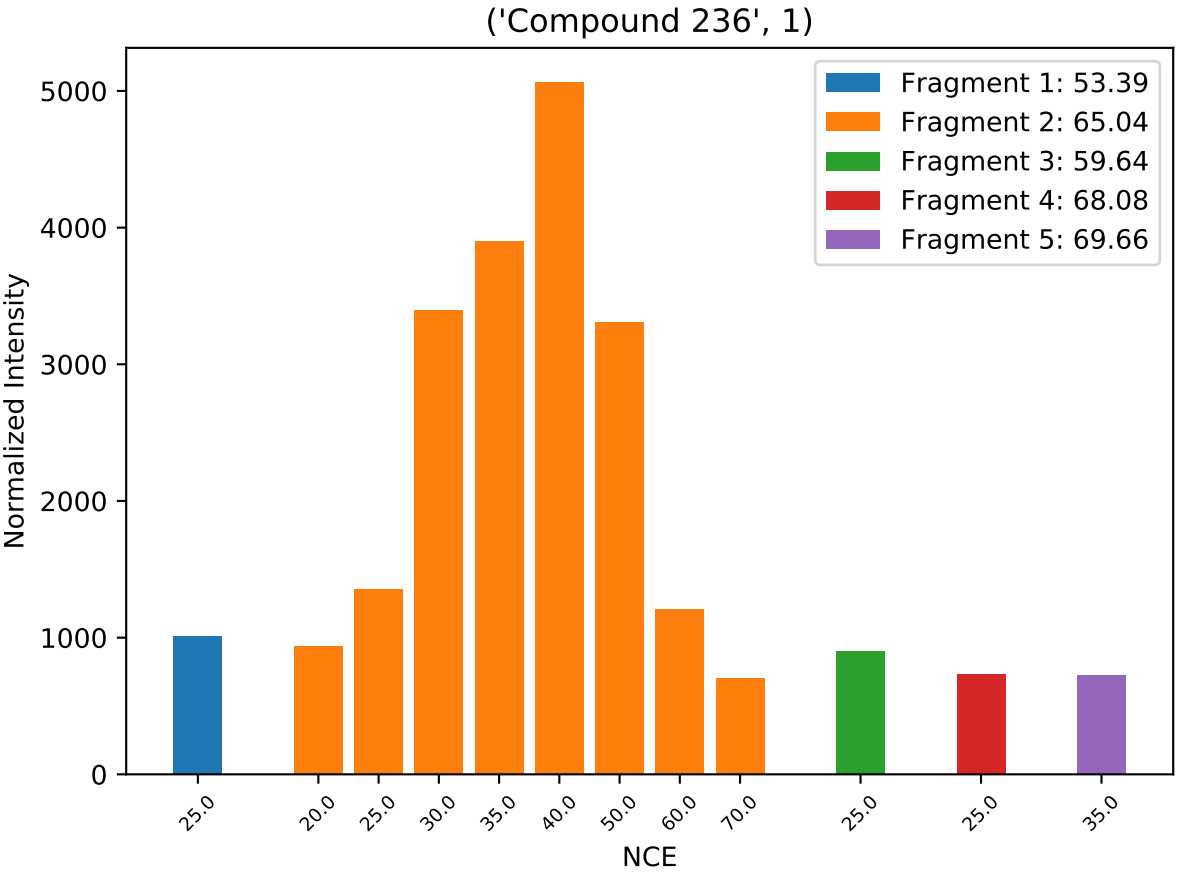

('Compound 230', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 333.1
Fragment 4: 315.09
Fragment 5: 173.48
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
20.0
40.0
70.0
10.0
25.0
30.0
35.0
50.0
60.0
80.0
10.0
20.0
25.0
10.0
20.0
25.0
10.0
25.0
30.0
35.0
50.0
80.0
NCE

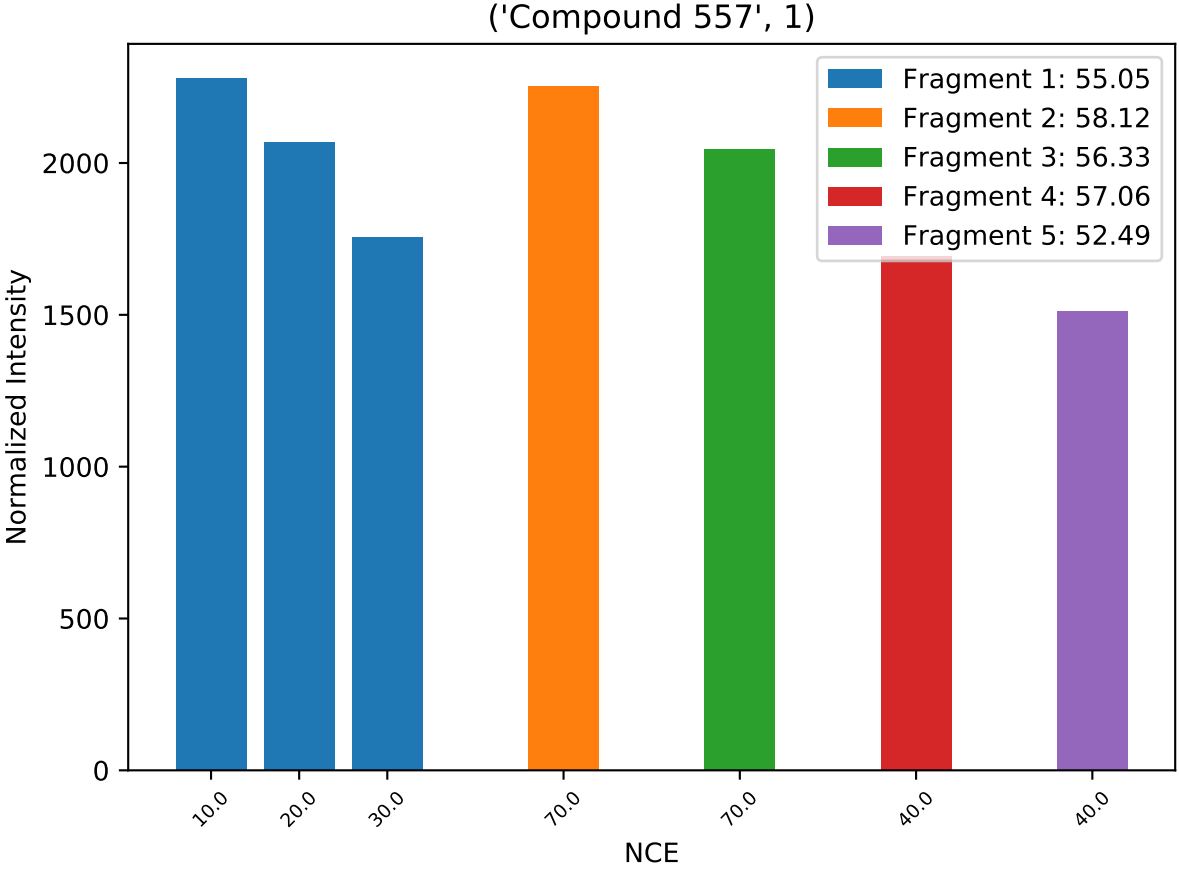

('Compound 231', 1)
Fragment 1: 107.07
Fragment 2: 97.03
Fragment 3: 83.06
Fragment 4: 96.04
Fragment 5: 66.03
Normalized Intensity
0
200000
400000
600000
800000
25.0
30.0
35.0
40.0
50.0
30.0
35.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

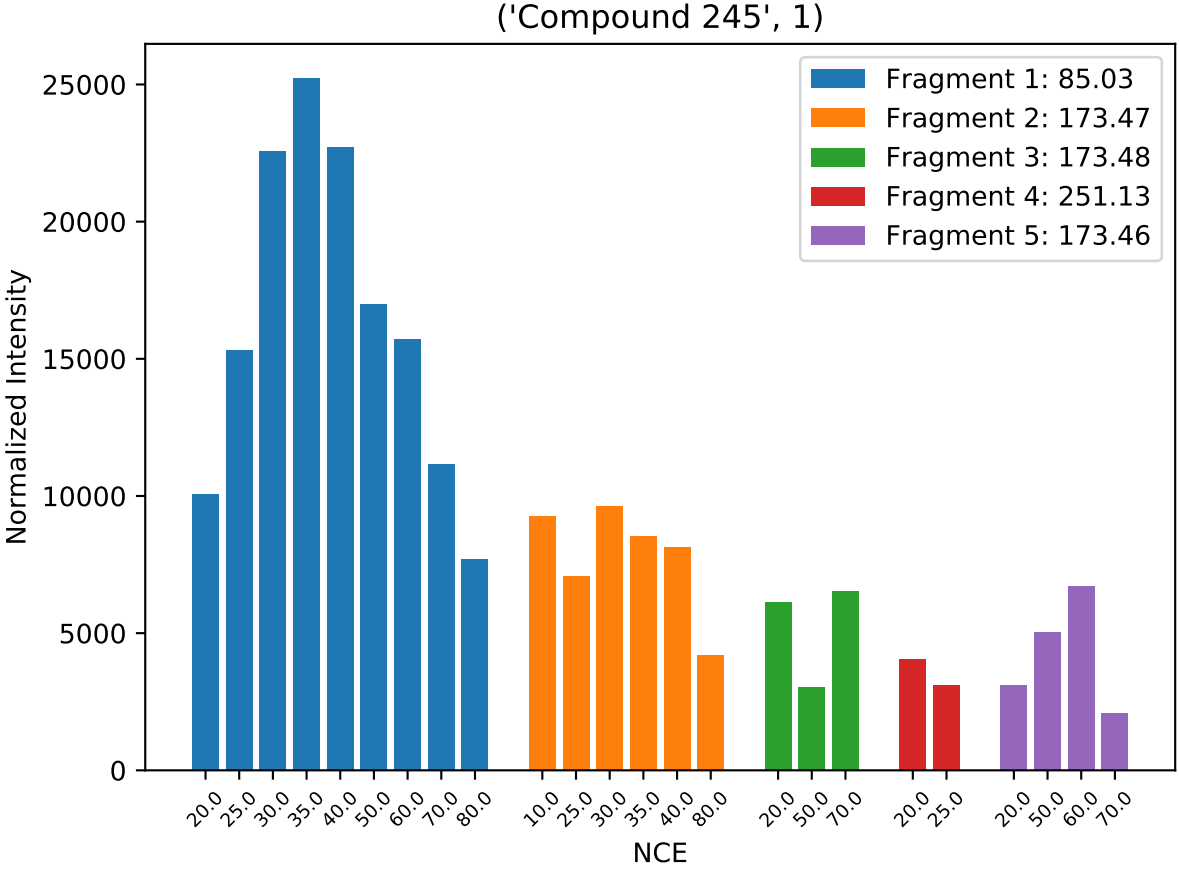

('Compound 232', 1)
Fragment 1: 303.02
Fragment 2: 409.01
Fragment 3: 532.04
Fragment 4: 134.93
Fragment 5: 550.05
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

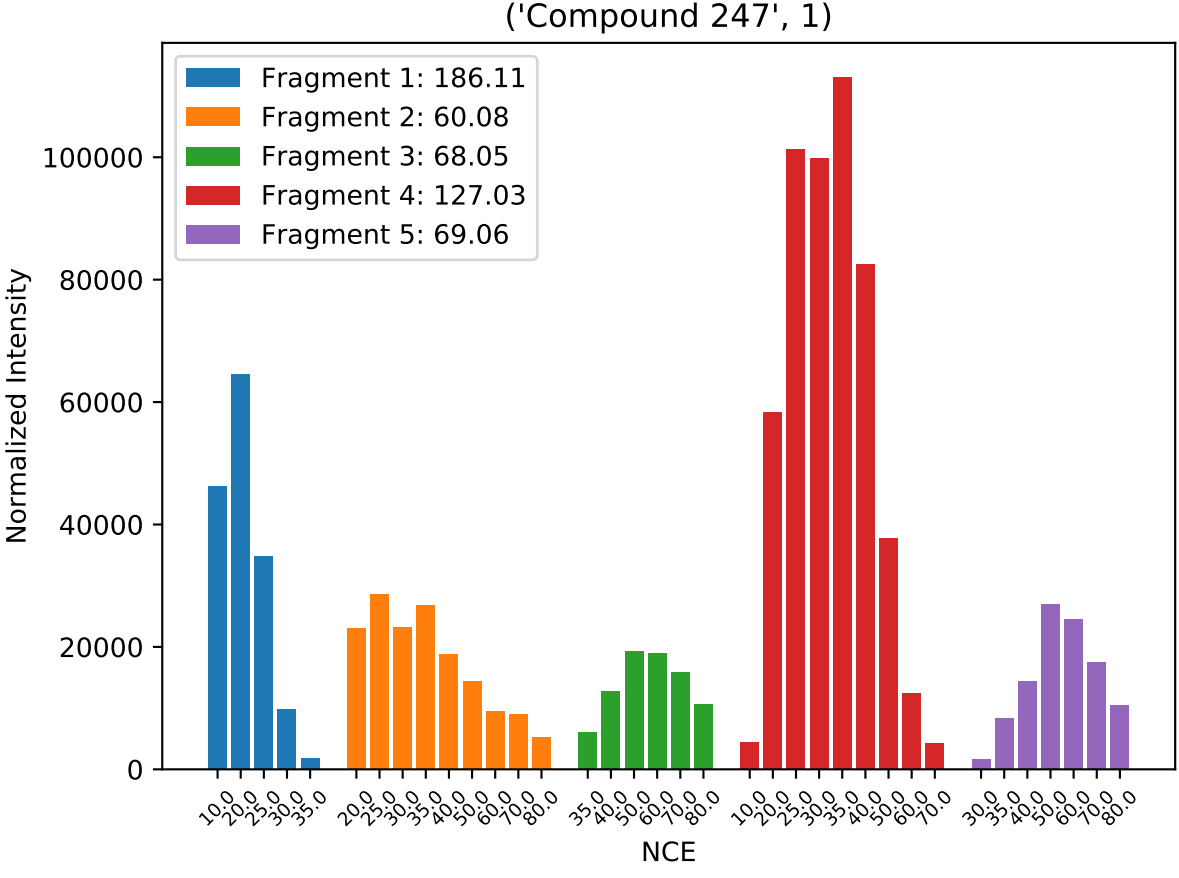

('Compound 234', 1)
Fragment 1: 463.23
Fragment 2: 205.12
Fragment 3: 141.02
Fragment 4: 191.11
Fragment 5: 287.2
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0 20.0 25.0 30.0 35.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

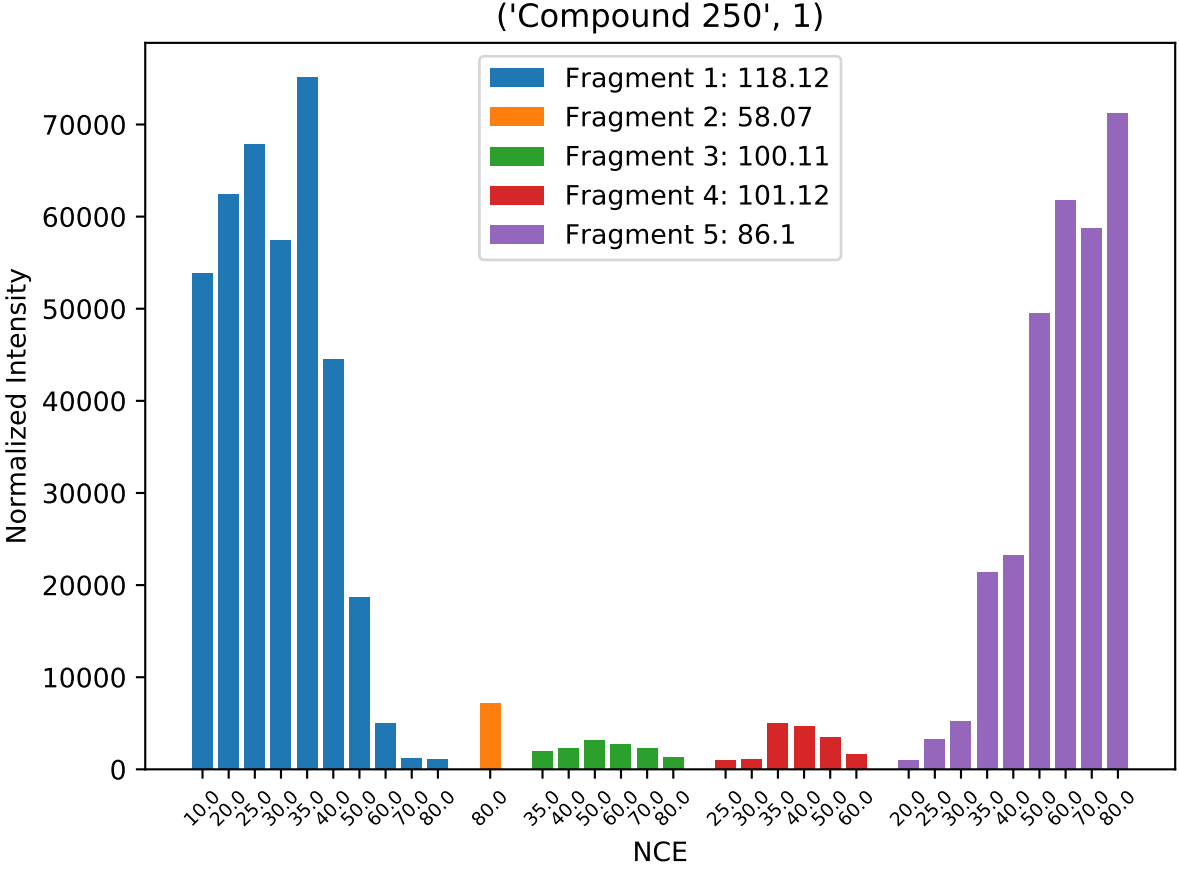

('Compound 235', 1)
Fragment 1: 144.93
Fragment 2: 128.95
Fragment 3: 73.07
Fragment 4: 152.02
Fragment 5: 95.06
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
70.0
NCE

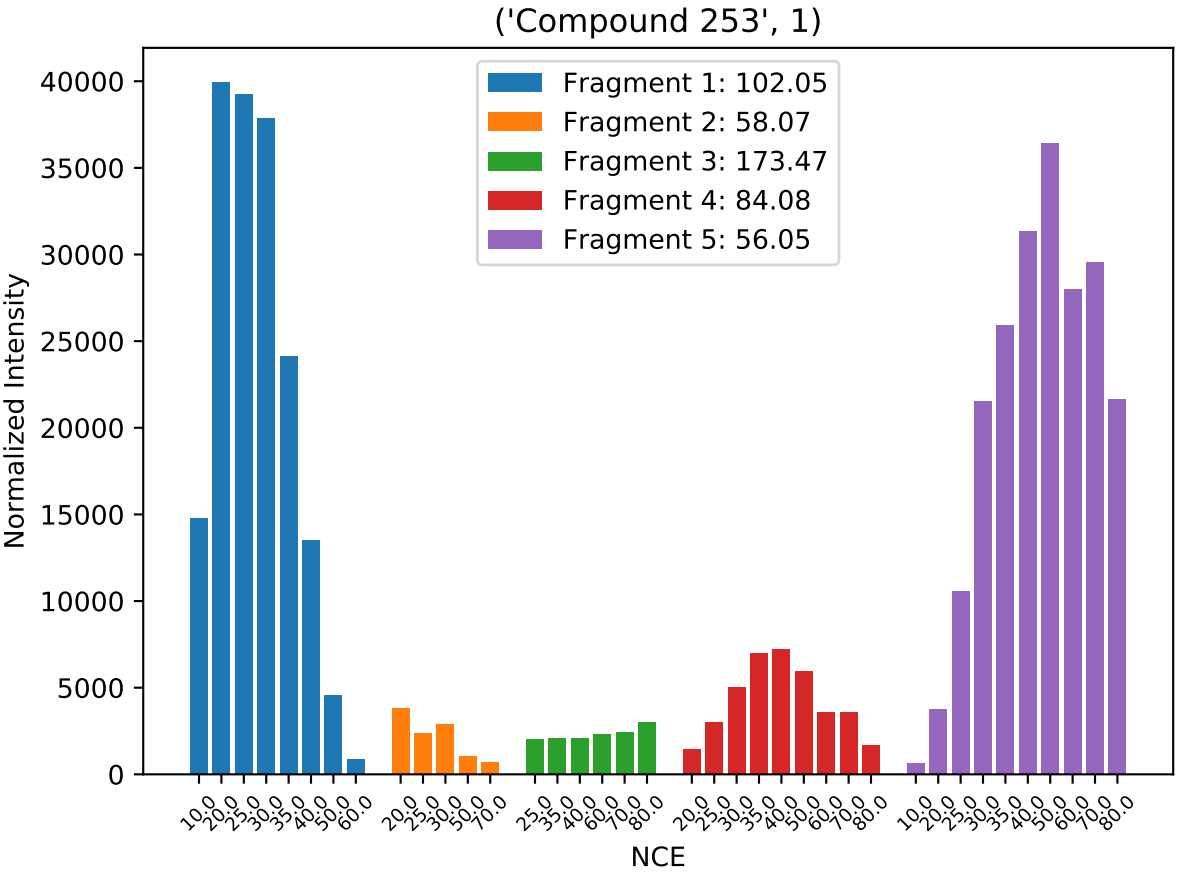

('Compound 236', 1)
Fragment 1: 53.39
Fragment 2: 65.04
Fragment 3: 59.64
Fragment 4: 68.08
Fragment 5: 69.66
Normalized Intensity
0
1000
2000
3000
4000
5000
25.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
25.0
25.0
35.0
NCE

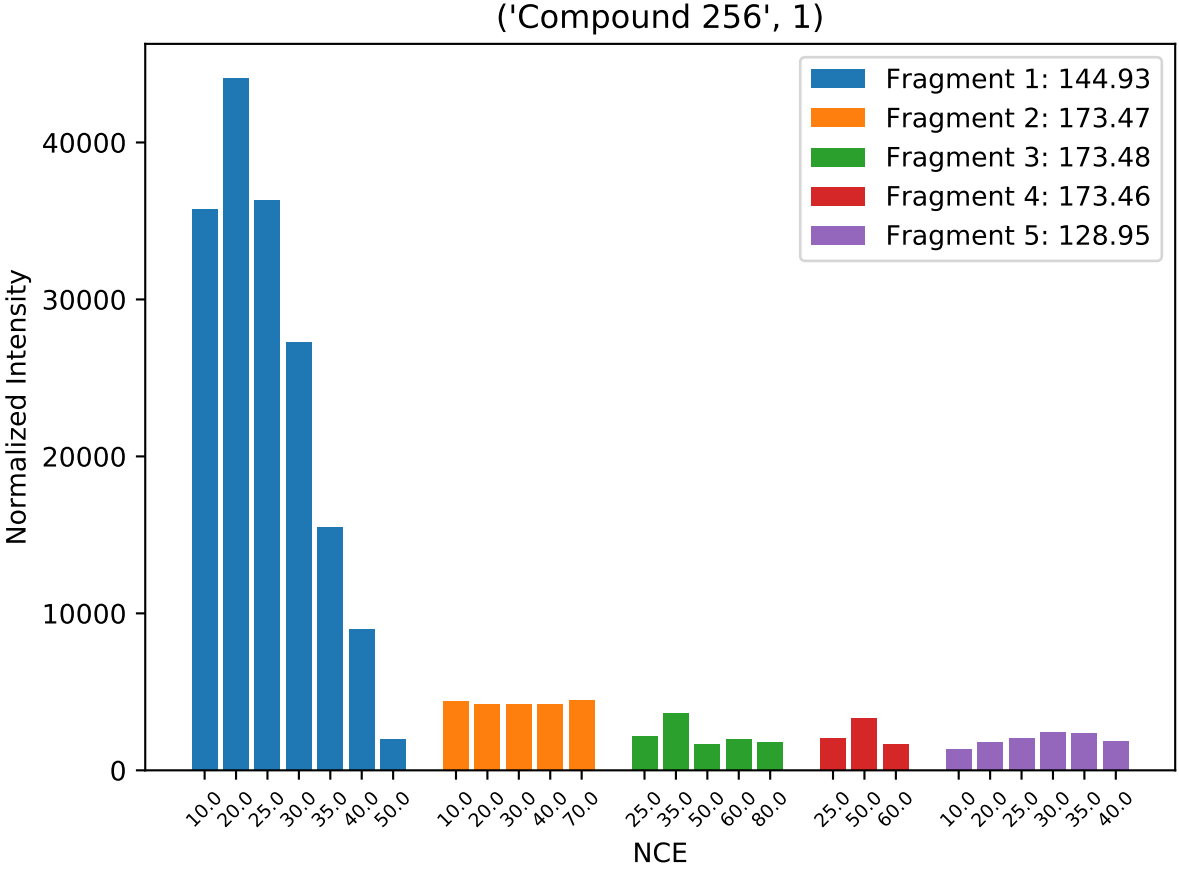

('Compound 557', 1)
Fragment 1: 55.05
Fragment 2: 58.12
Fragment 3: 56.33
Fragment 4: 57.06
Fragment 5: 52.49
Normalized Intensity
0
500
1000
1500
2000
10.0
20.0
30.0
70.0
70.0
40.0
40.0
NCE

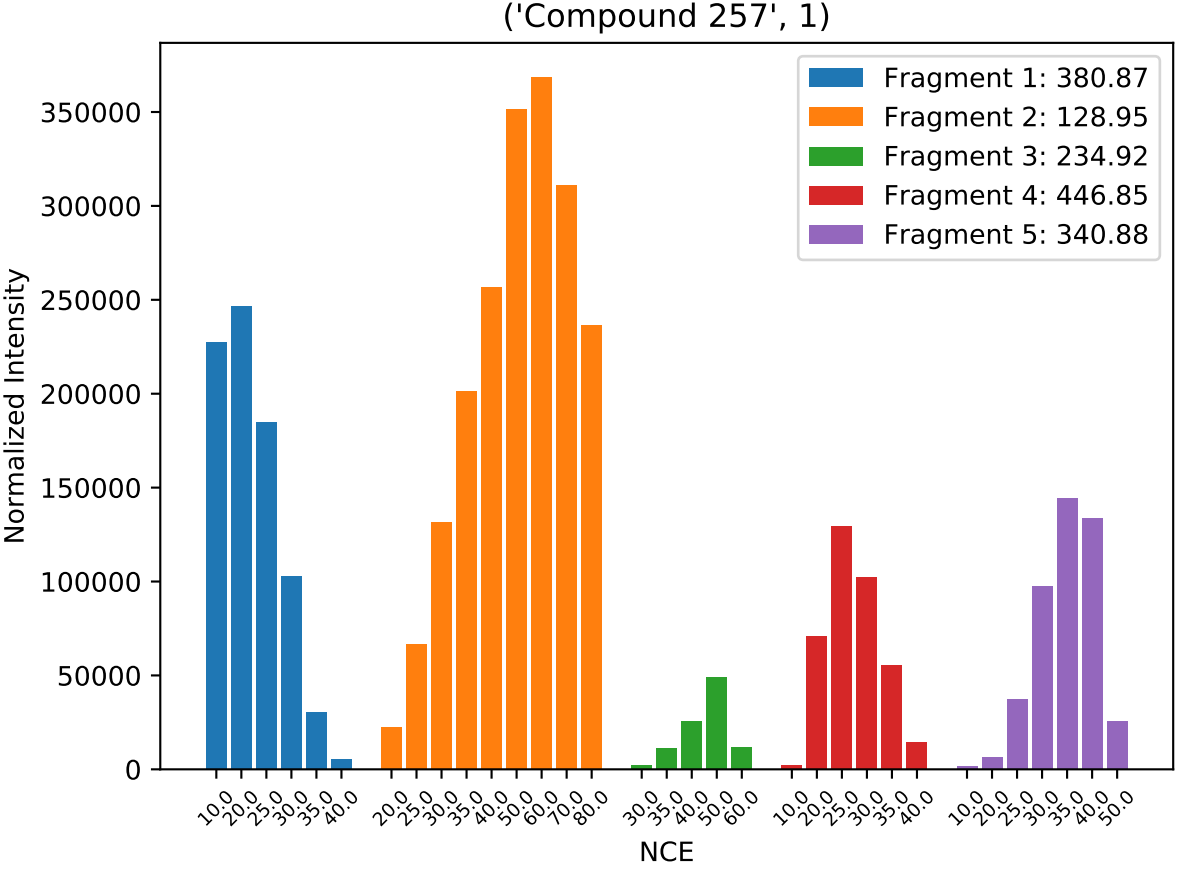

('Compound 245', 1)
Fragment 1: 85.03
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 251.13
Fragment 5: 173.46
Normalized Intensity
0
5000
10000
15000
20000
25000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 25.0 30.0 35.0 40.0 80.0
20.0 50.0 70.0
20.0 25.0
20.0 50.0 60.0 70.0
NCE

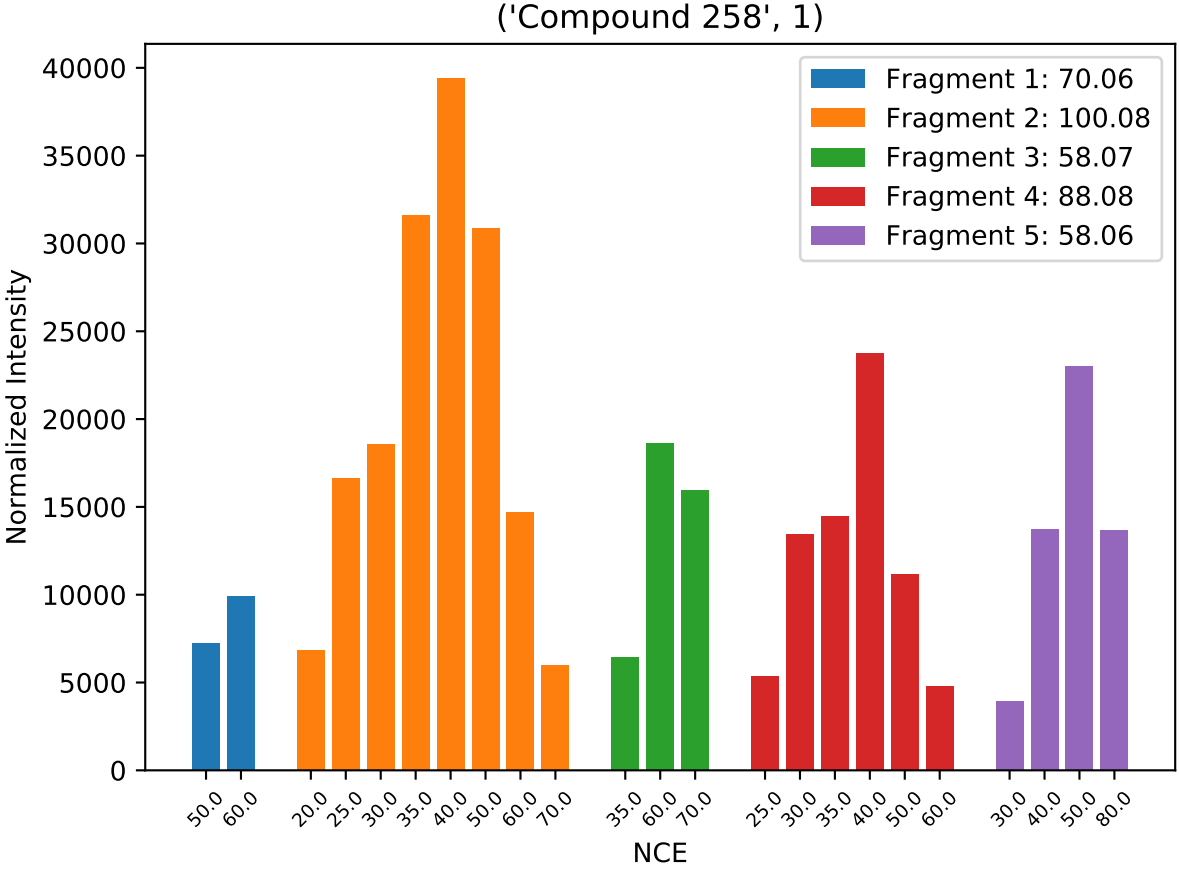

('Compound 247', 1)
Fragment 1: 186.11
Fragment 2: 60.08
Fragment 3: 68.05
Fragment 4: 127.03
Fragment 5: 69.06
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

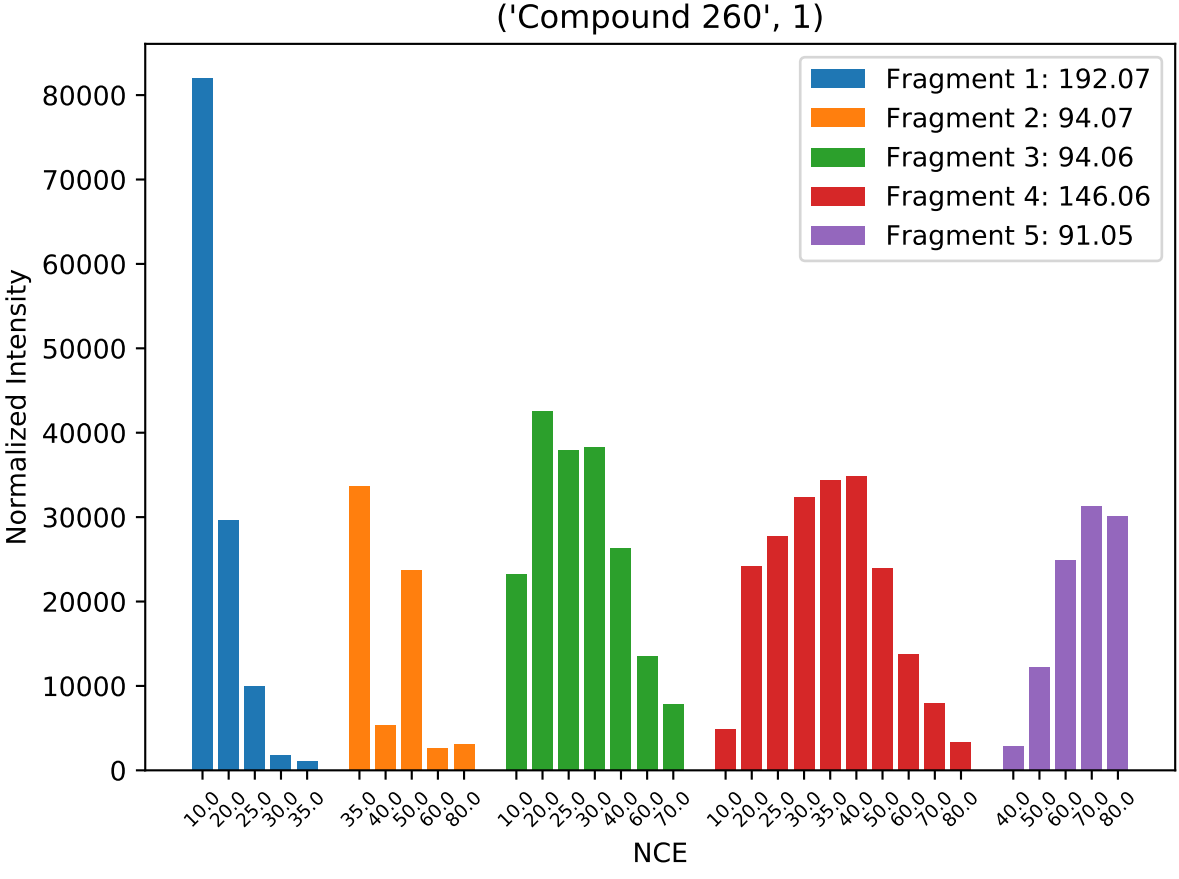

('Compound 250', 1)
Fragment 1: 118.12
Fragment 2: 58.07
Fragment 3: 100.11
Fragment 4: 101.12
Fragment 5: 86.1
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

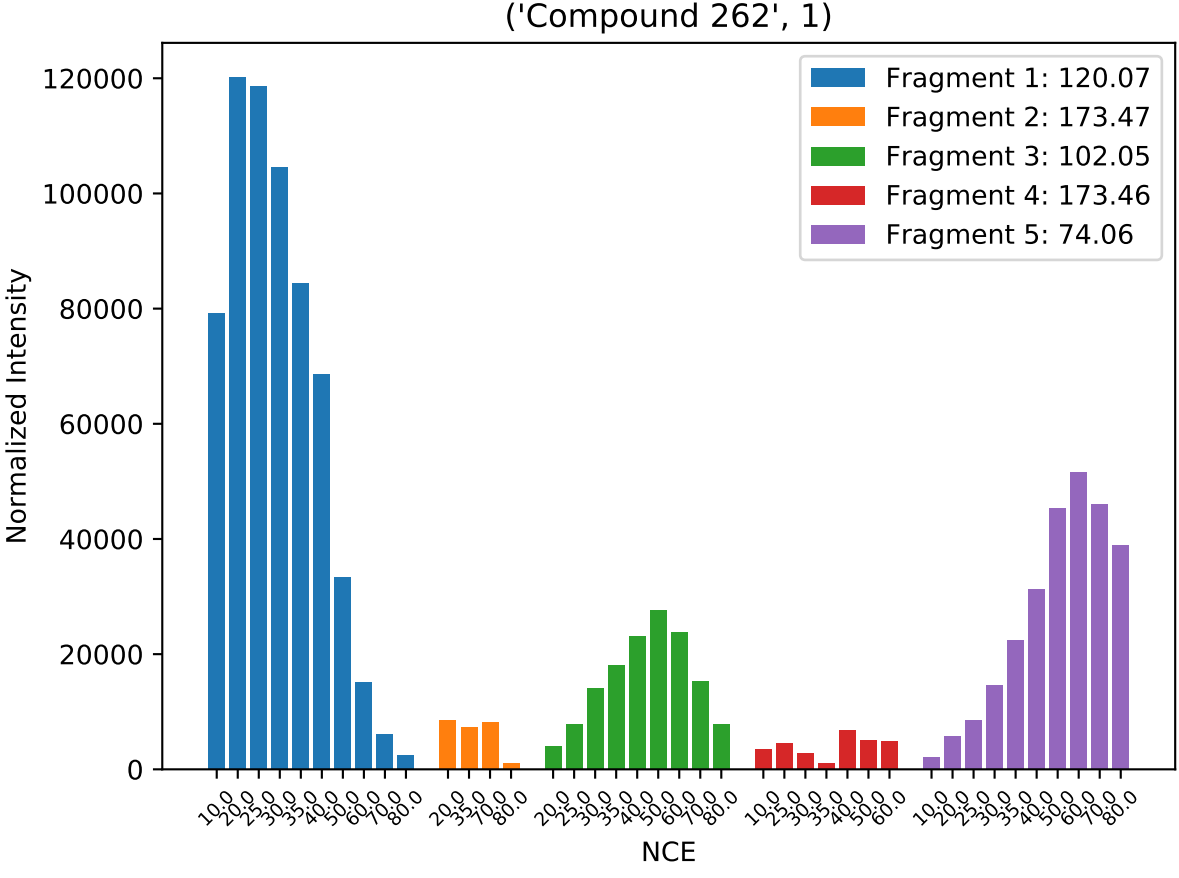

('Compound 253', 1)
Fragment 1: 102.05
Fragment 2: 58.07
Fragment 3: 173.47
Fragment 4: 84.08
Fragment 5: 56.05
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 50.0 70.0
25.0 35.0 40.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

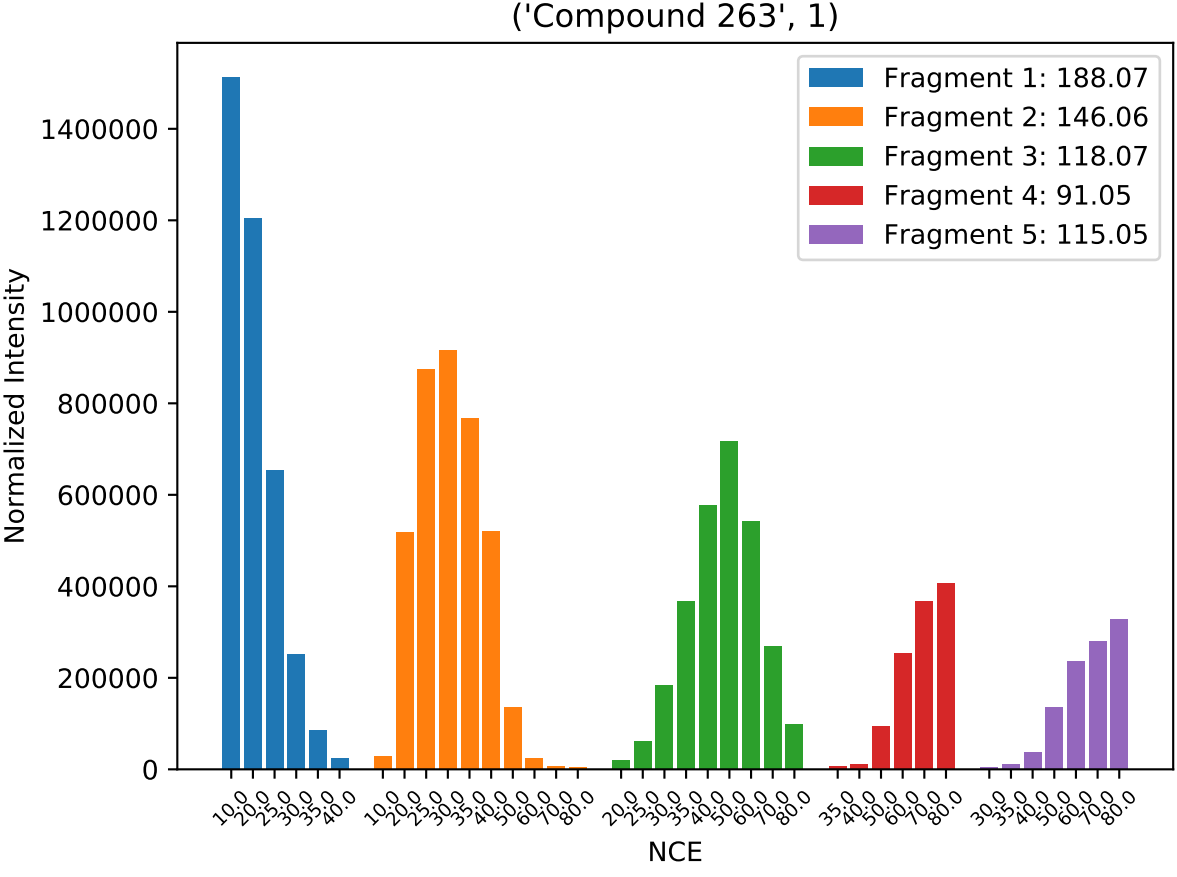

('Compound 256', 1)
Fragment 1: 144.93
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 128.95
Normalized Intensity
0
10000
20000
30000
40000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
30.0
40.0
70.0
25.0
35.0
50.0
60.0
80.0
25.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
NCE

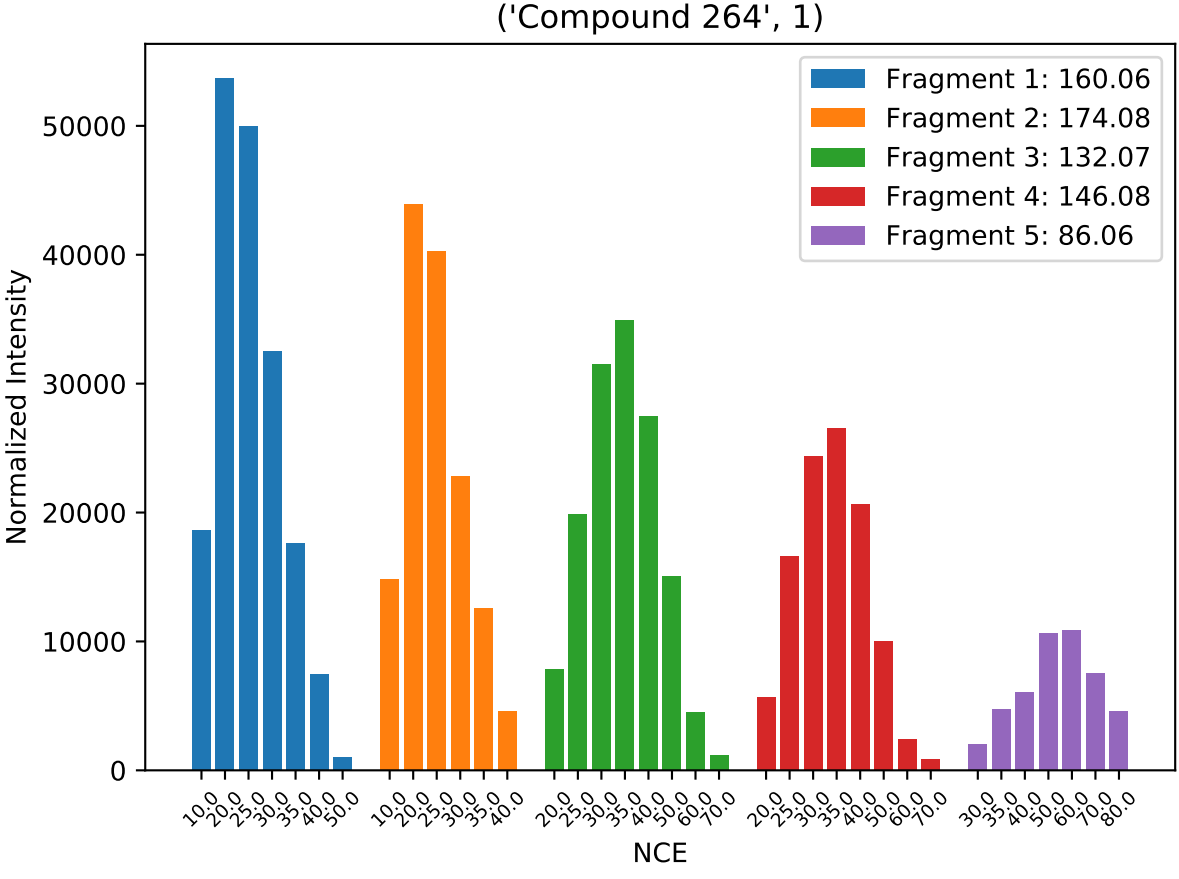

('Compound 257', 1)
Fragment 1: 380.87
Fragment 2: 128.95
Fragment 3: 234.92
Fragment 4: 446.85
Fragment 5: 340.88
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

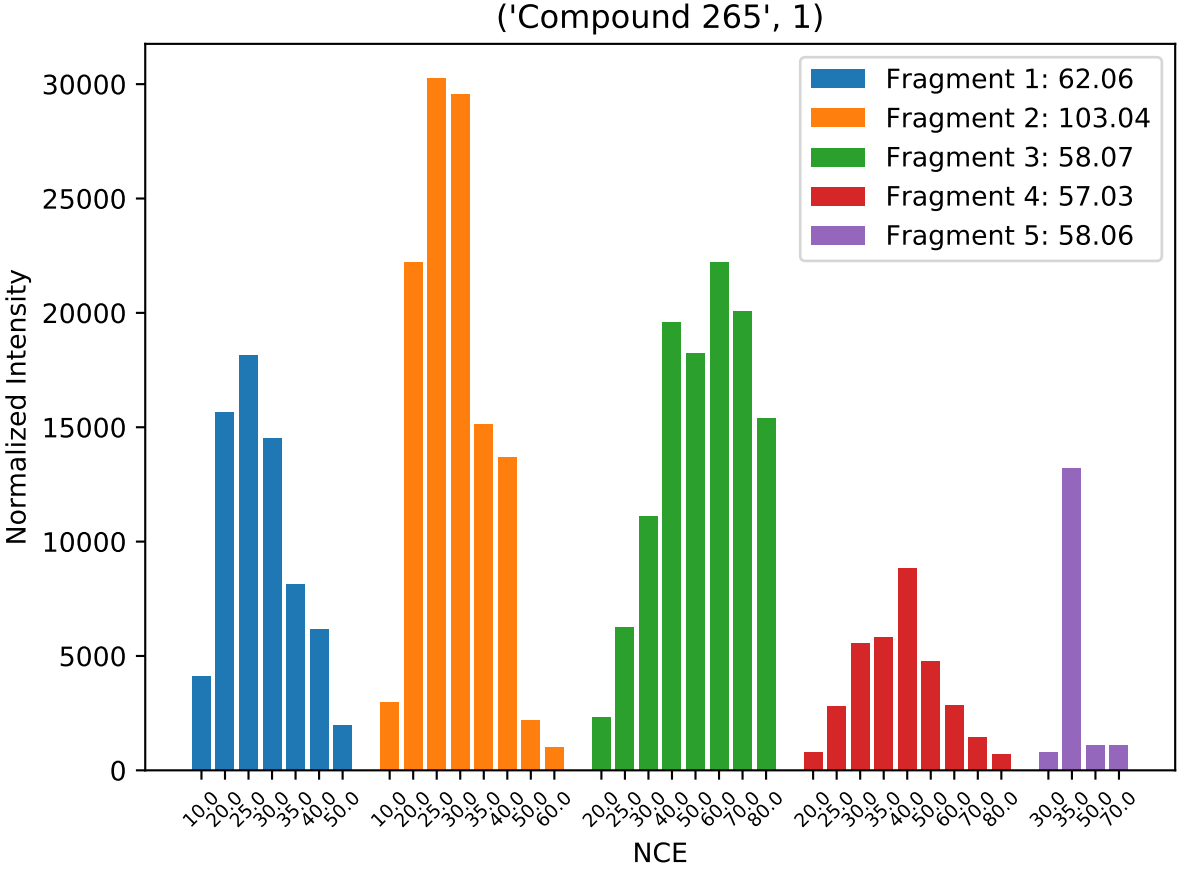

('Compound 258', 1)
Fragment 1: 70.06
Fragment 2: 100.08
Fragment 3: 58.07
Fragment 4: 88.08
Fragment 5: 58.06
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
50.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
35.0
60.0
70.0
25.0
30.0
35.0
40.0
50.0
60.0
30.0
40.0
50.0
80.0
NCE

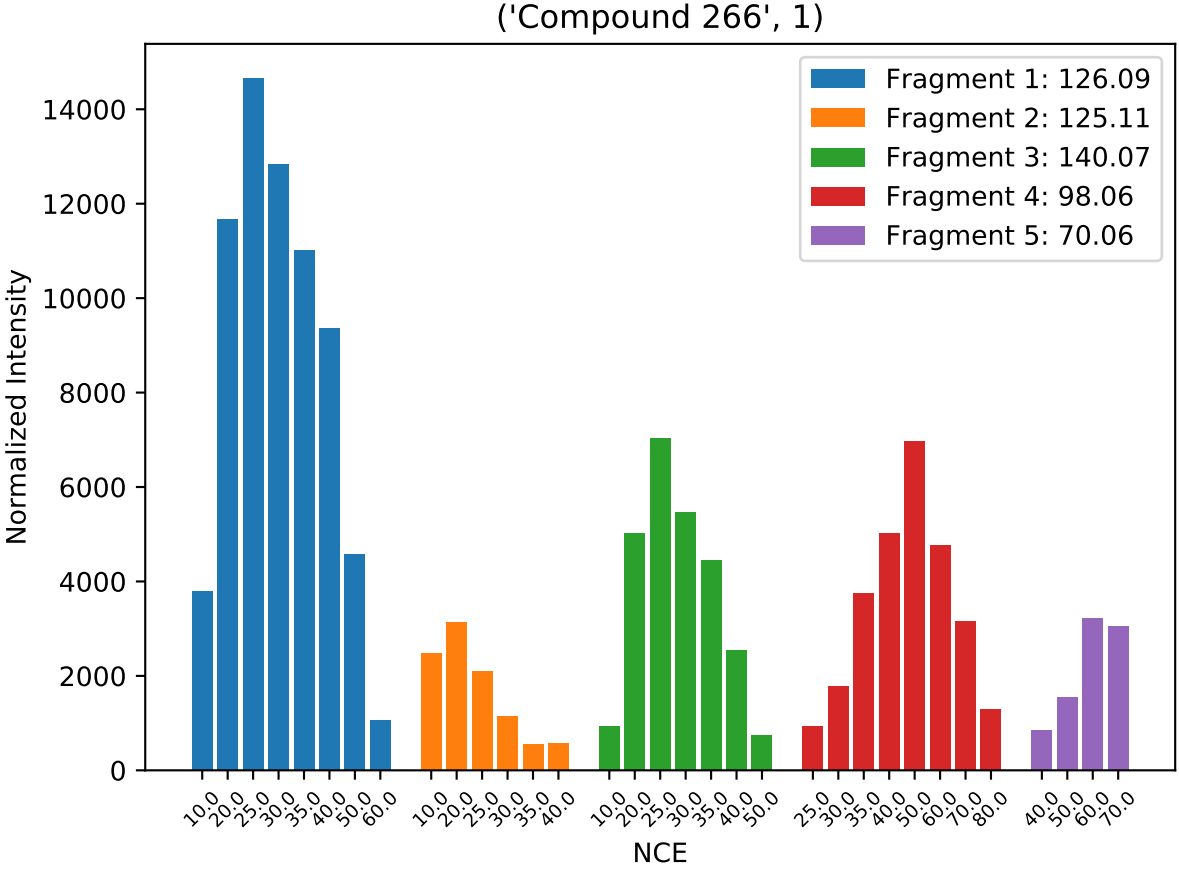

('Compound 260', 1)
Fragment 1: 192.07
Fragment 2: 94.07
Fragment 3: 94.06
Fragment 4: 146.06
Fragment 5: 91.05
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0
20.0
25.0
30.0
35.0
35.0
40.0
50.0
60.0
80.0
10.0
20.0
25.0
30.0
40.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
NCE

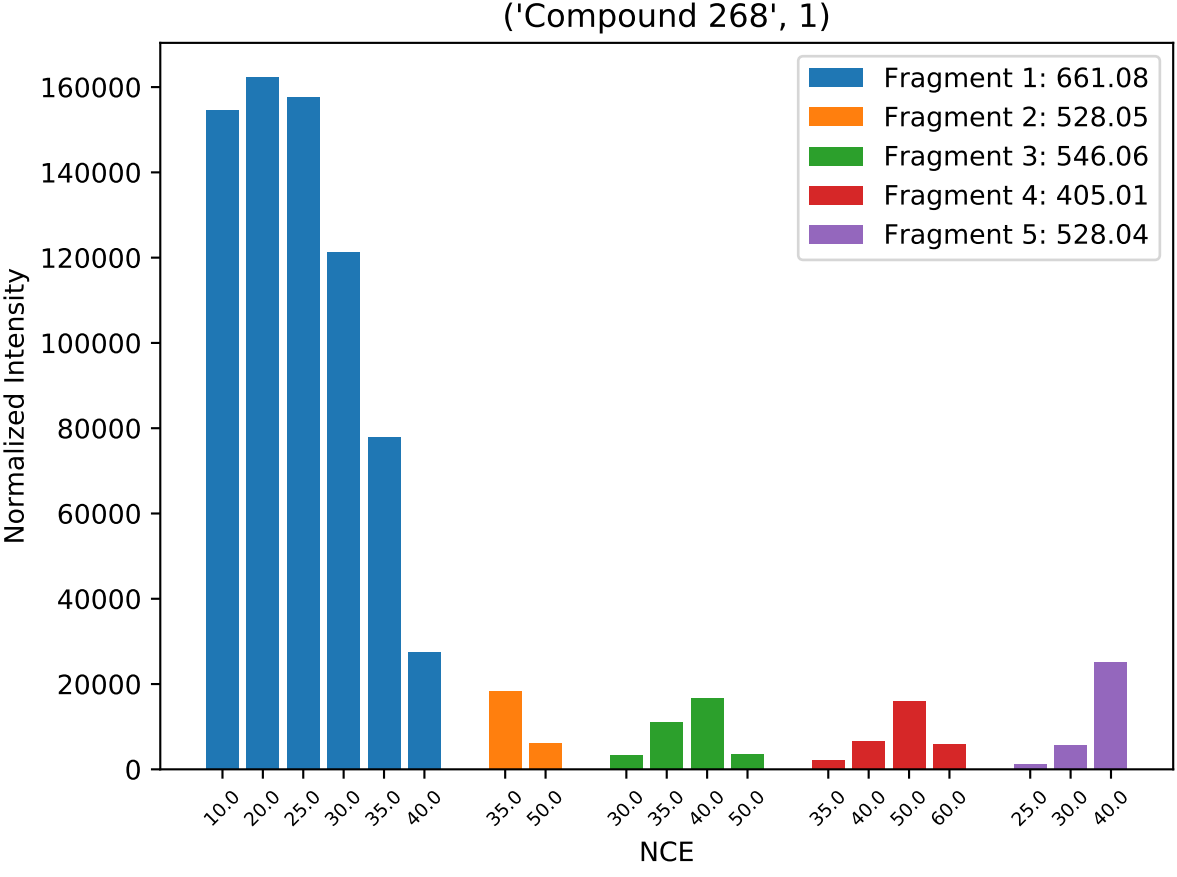

('Compound 262', 1)
Fragment 1: 120.07
Fragment 2: 173.47
Fragment 3: 102.05
Fragment 4: 173.46
Fragment 5: 74.06
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 35.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

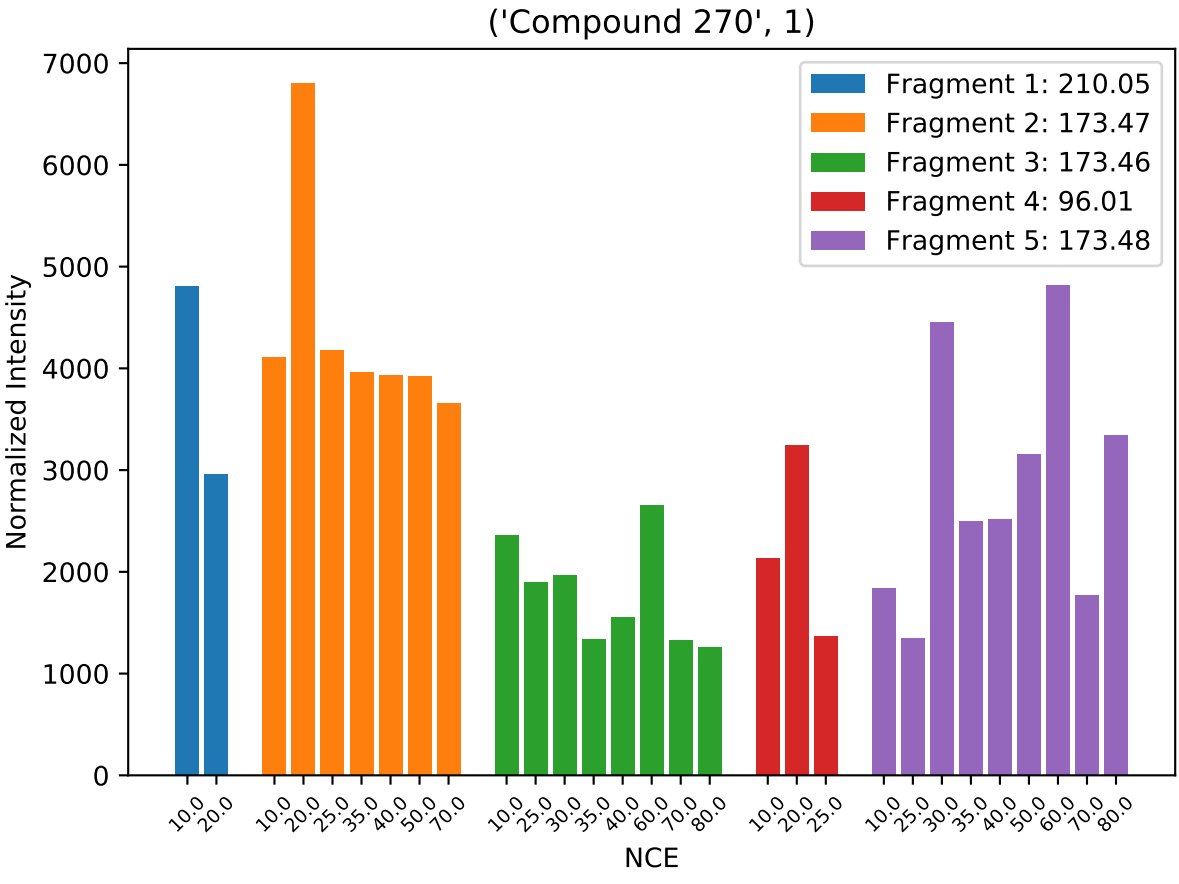

('Compound 263', 1)
Fragment 1: 188.07
Fragment 2: 146.06
Fragment 3: 118.07
Fragment 4: 91.05
Fragment 5: 115.05
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
1400000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

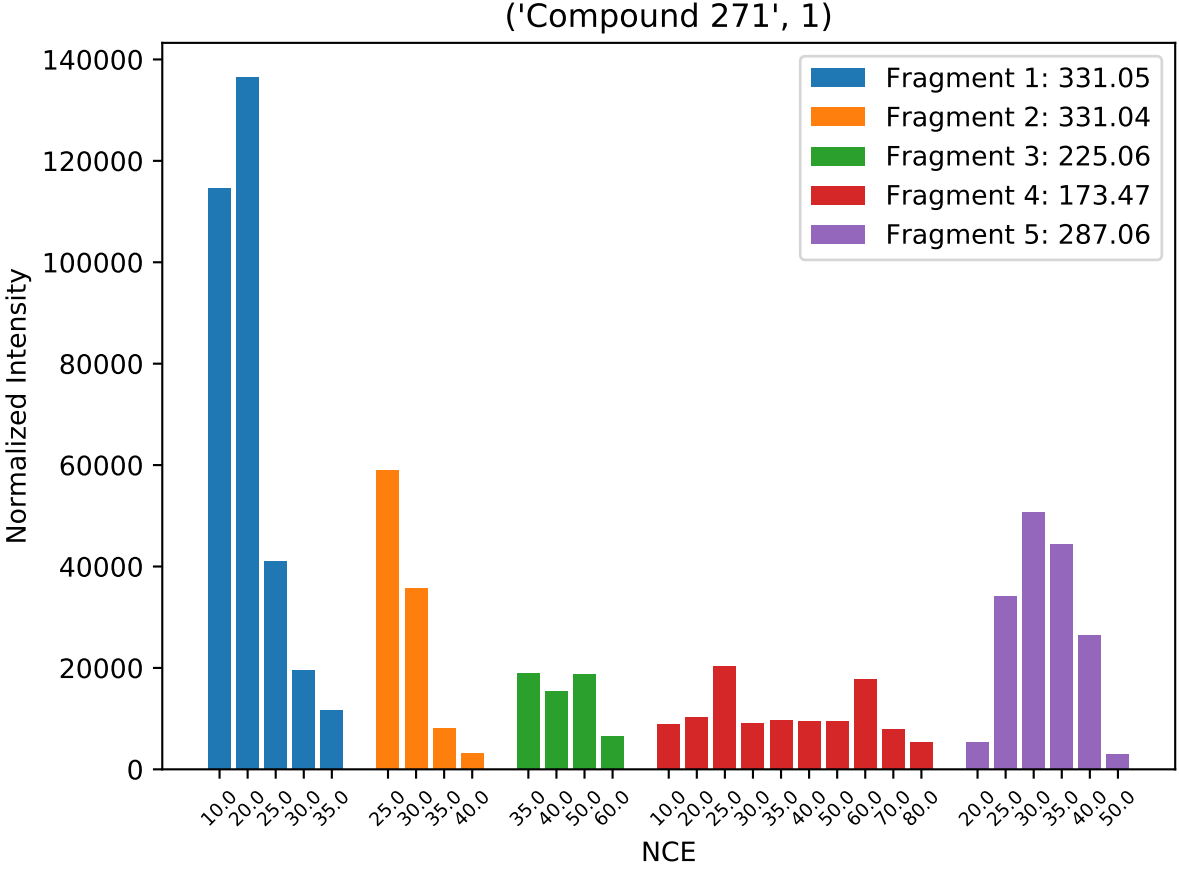

('Compound 264', 1)
Fragment 1: 160.06
Fragment 2: 174.08
Fragment 3: 132.07
Fragment 4: 146.08
Fragment 5: 86.06
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

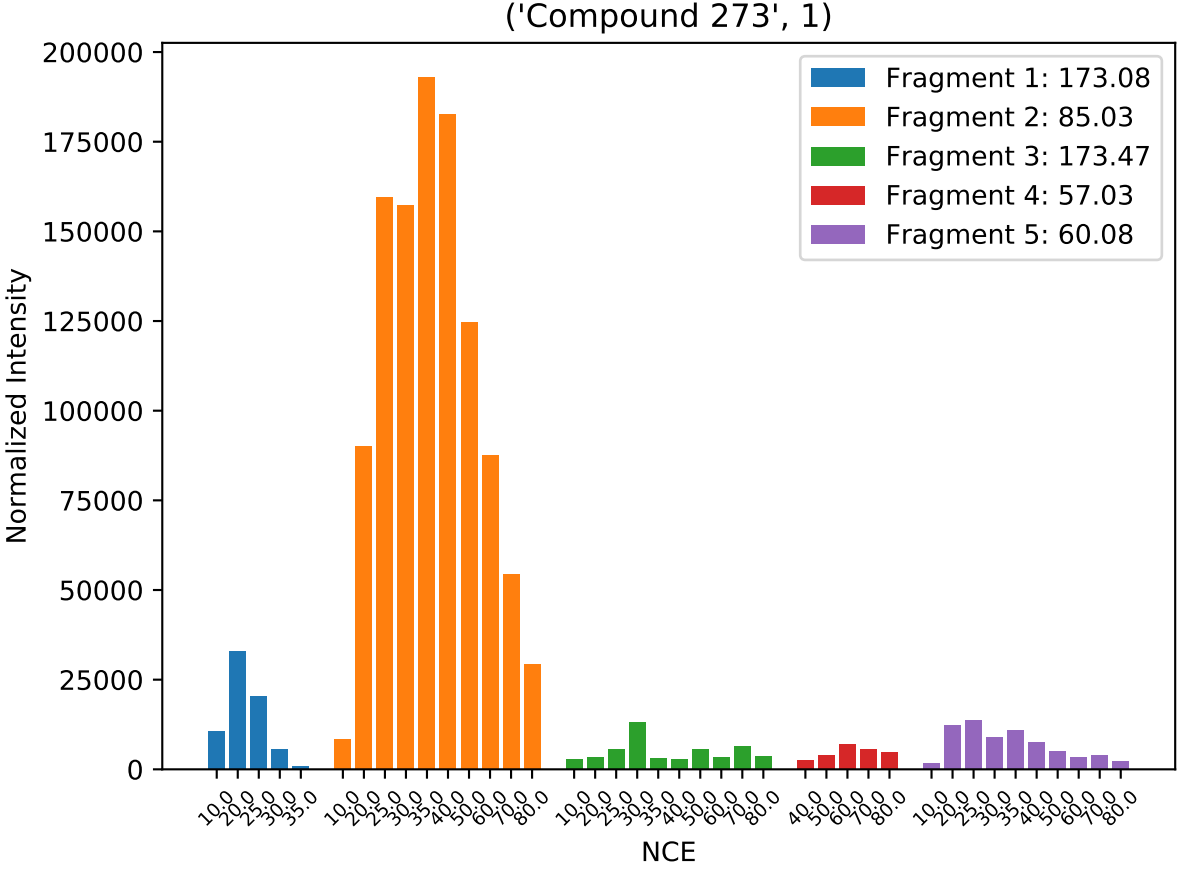

('Compound 265', 1)
Fragment 1: 62.06
Fragment 2: 103.04
Fragment 3: 58.07
Fragment 4: 57.03
Fragment 5: 58.06
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 50.0 70.0
NCE

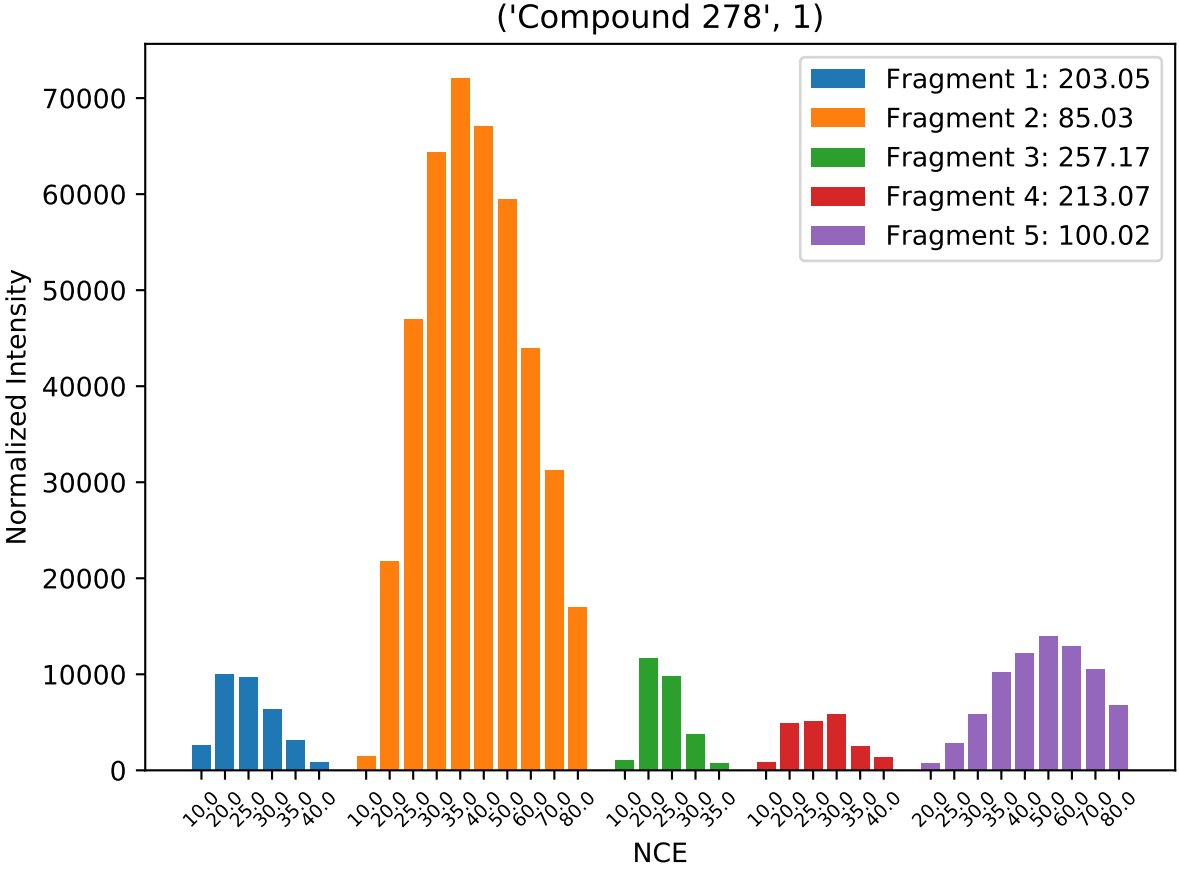

('Compound 266', 1)
Fragment 1: 126.09
Fragment 2: 125.11
Fragment 3: 140.07
Fragment 4: 98.06
Fragment 5: 70.06
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0
NCE

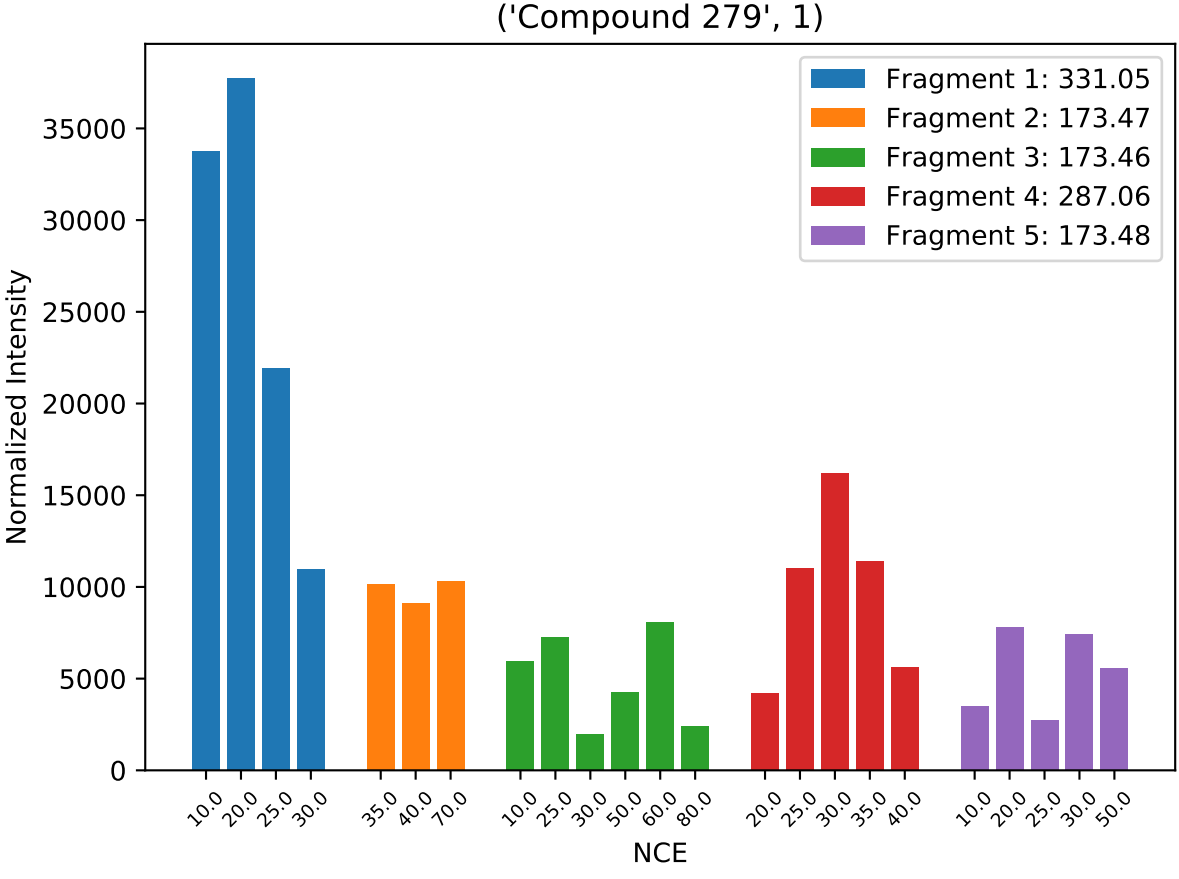

('Compound 268', 1)
Fragment 1: 661.08
Fragment 2: 528.05
Fragment 3: 546.06
Fragment 4: 405.01
Fragment 5: 528.04
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
10.0
20.0
25.0
30.0
35.0
40.0
35.0
50.0
30.0
35.0
40.0
50.0
35.0
40.0
50.0
60.0
25.0
30.0
40.0
NCE

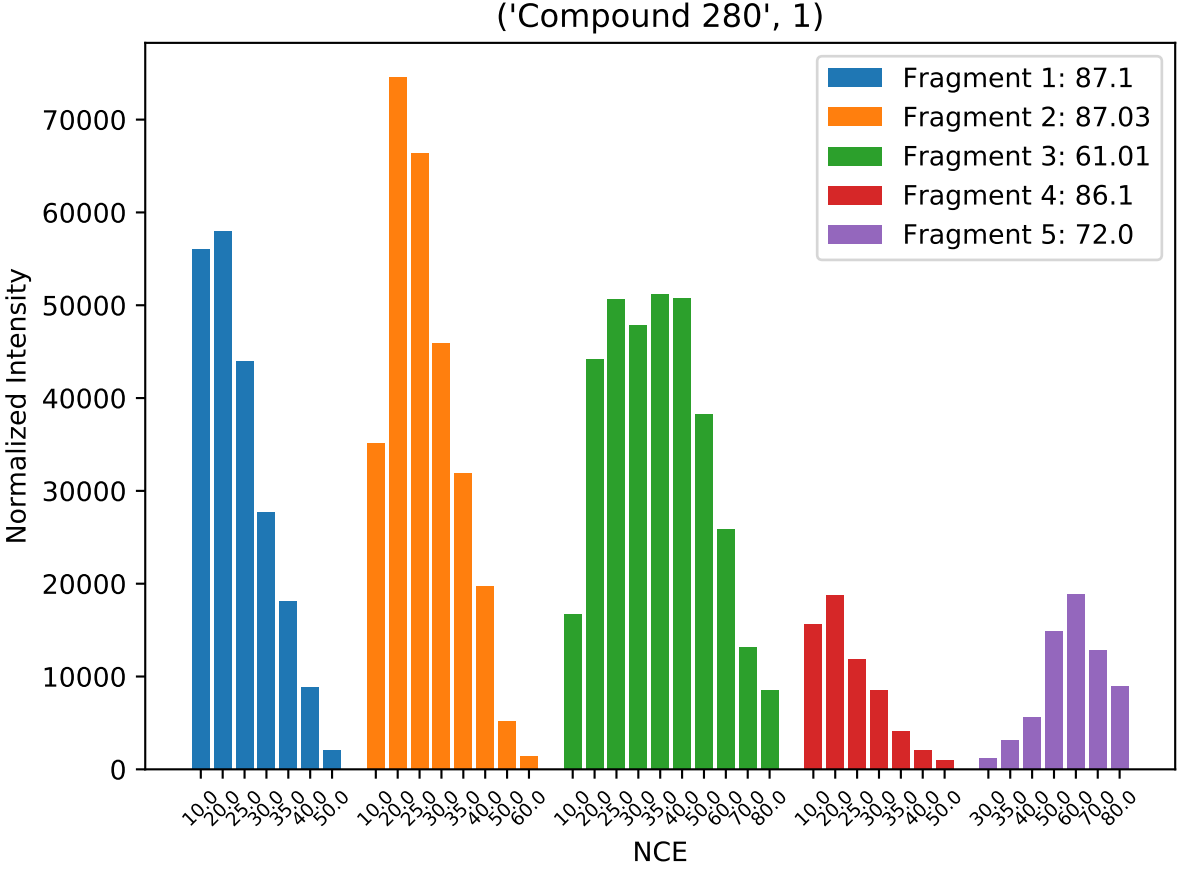

('Compound 270', 1)
Fragment 1: 210.05
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 96.01
Fragment 5: 173.48
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
NCE
10.0
20.0
10.0
20.0
25.0
35.0
40.0
50.0
70.0
10.0
25.0
30.0
35.0
40.0
60.0
70.0
80.0
10.0
20.0
25.0
10.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

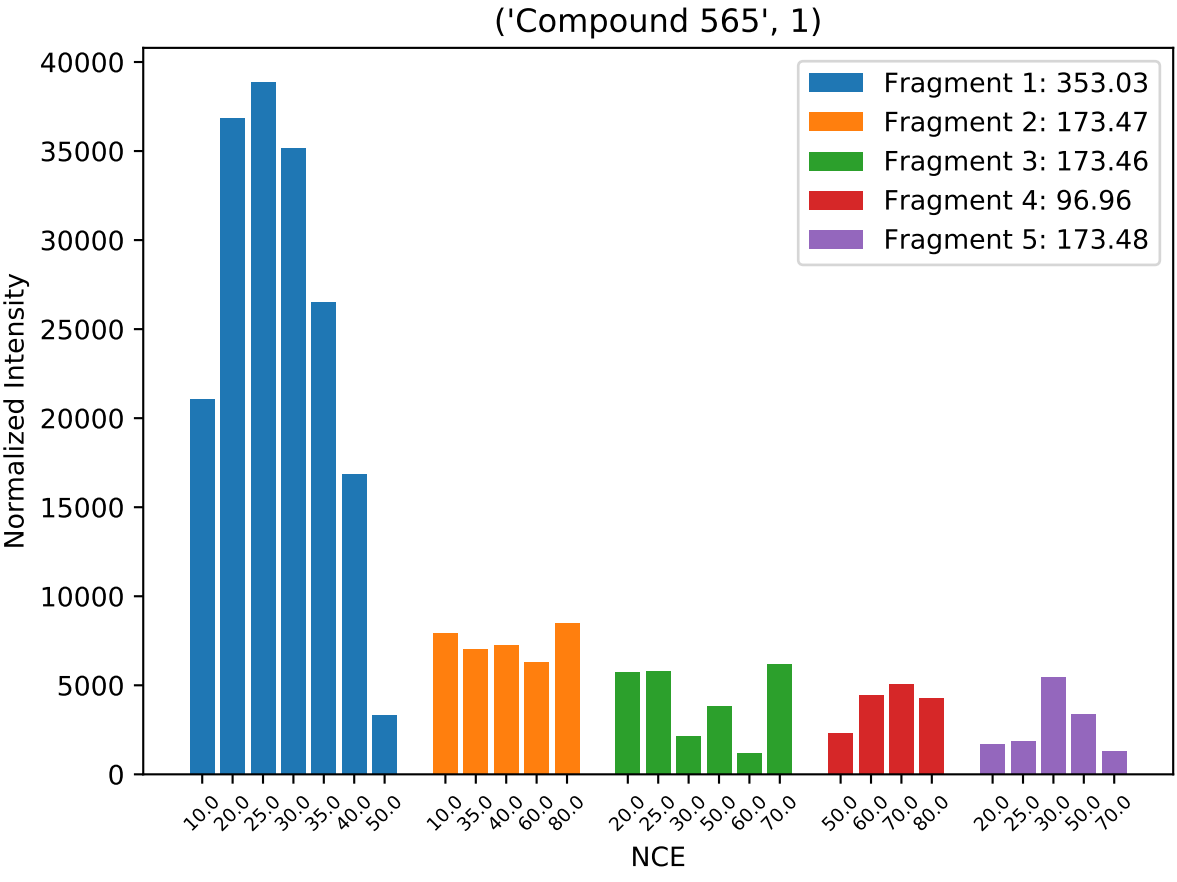

('Compound 271', 1)
Fragment 1: 331.05
Fragment 2: 331.04
Fragment 3: 225.06
Fragment 4: 173.47
Fragment 5: 287.06
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
10.0 20.0 25.0 30.0 35.0
25.0 30.0 35.0 40.0
35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
NCE

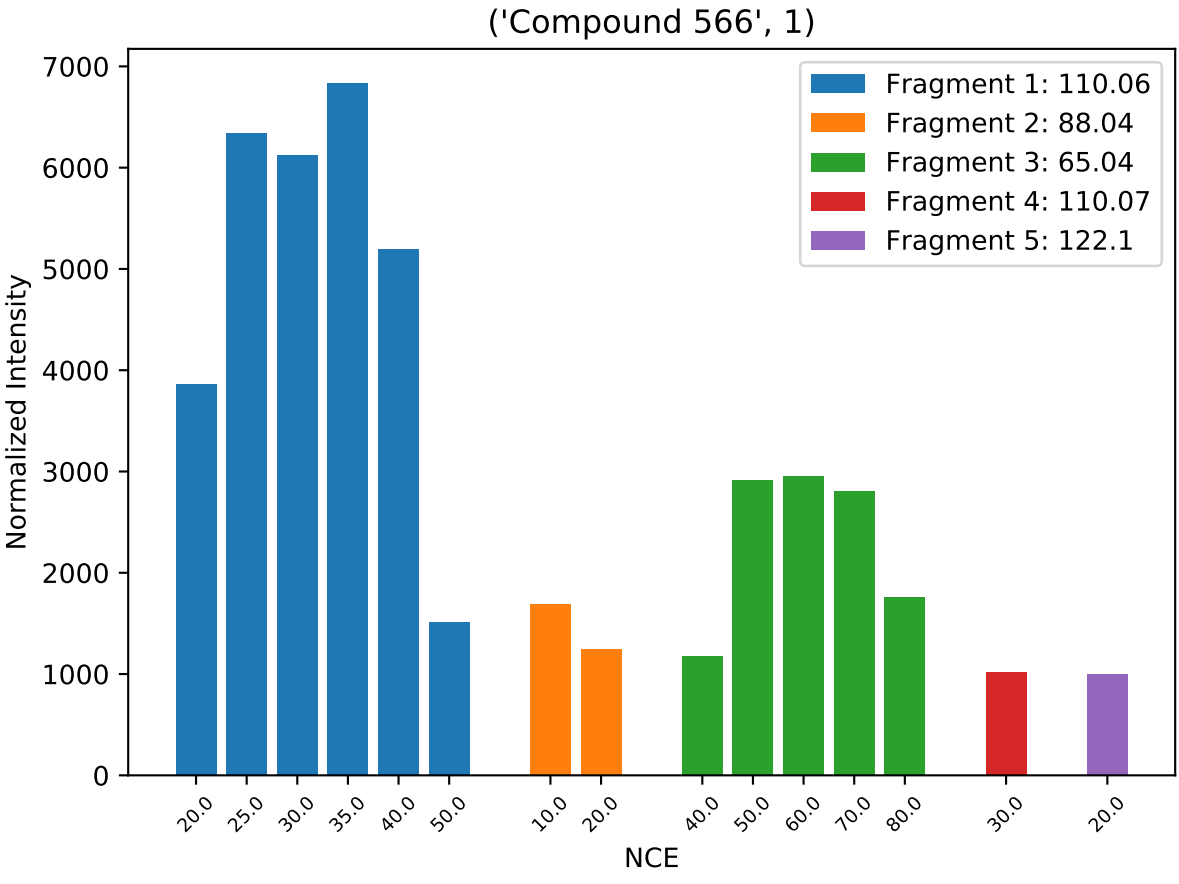

('Compound 273', 1)
Fragment 1: 173.08
Fragment 2: 85.03
Fragment 3: 173.47
Fragment 4: 57.03
Fragment 5: 60.08
Normalized Intensity
200000
175000
150000
125000
100000
75000
50000
25000
0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

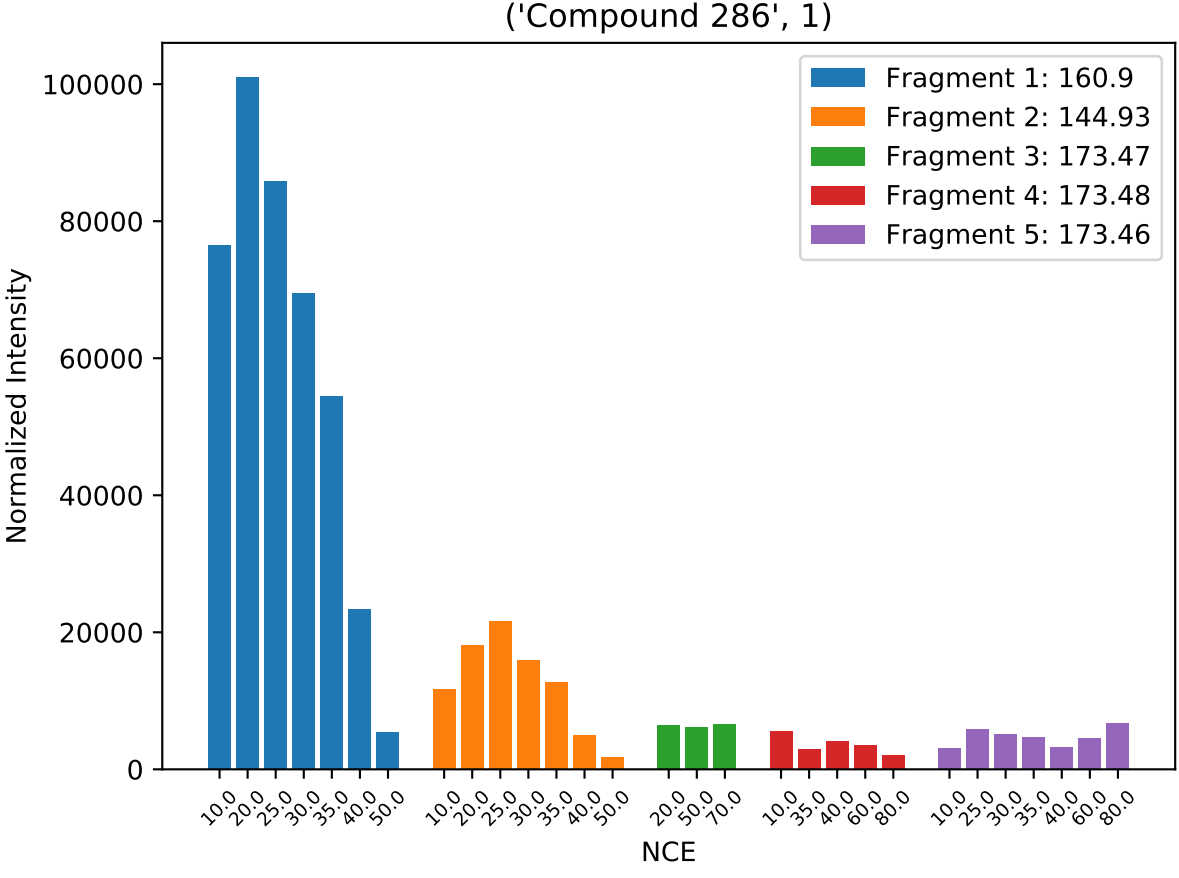

('Compound 278', 1)
Fragment 1: 203.05
Fragment 2: 85.03
Fragment 3: 257.17
Fragment 4: 213.07
Fragment 5: 100.02
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

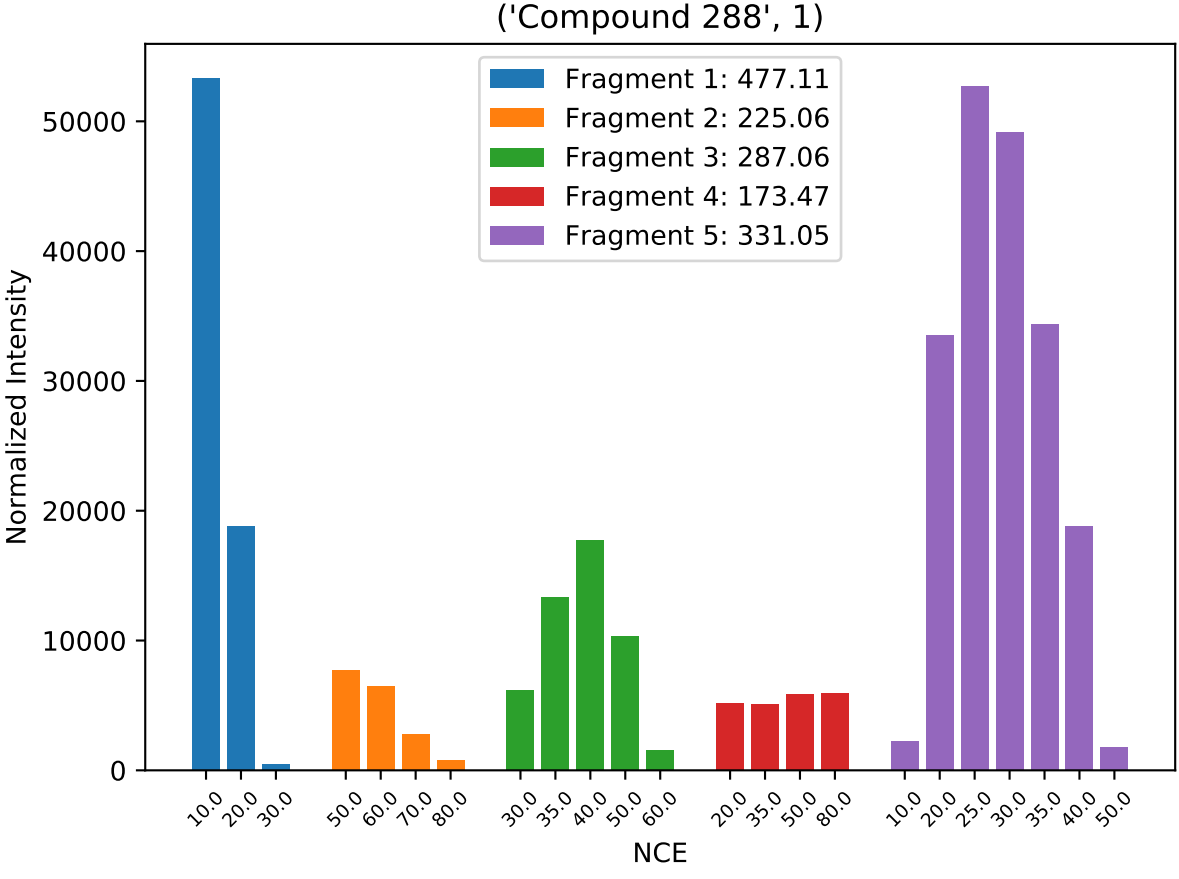

('Compound 279', 1)
Fragment 1: 331.05
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 287.06
Fragment 5: 173.48
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
10.0
20.0
25.0
30.0
35.0
40.0
70.0
10.0
25.0
30.0
50.0
60.0
80.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
50.0
NCE

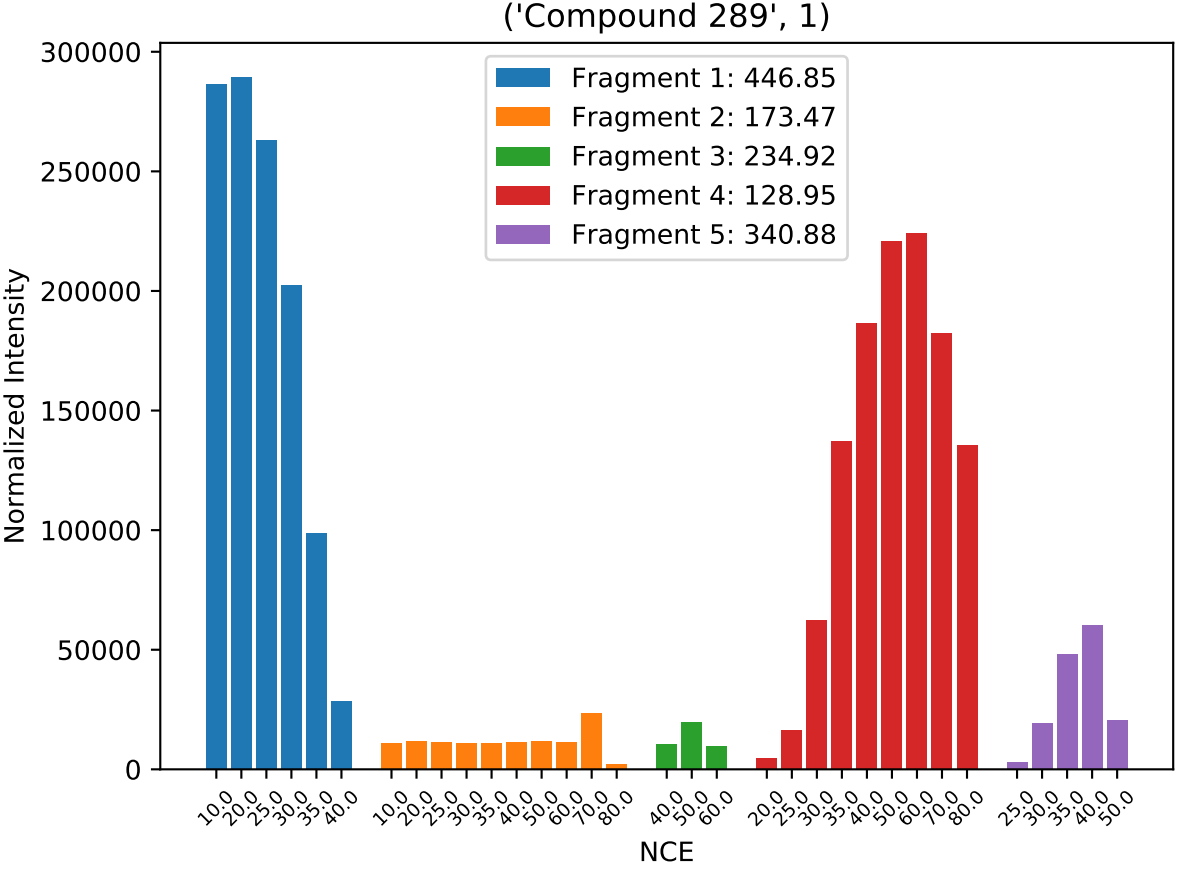

('Compound 280', 1)
Fragment 1: 87.1
Fragment 2: 87.03
Fragment 3: 61.01
Fragment 4: 86.1
Fragment 5: 72.0
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

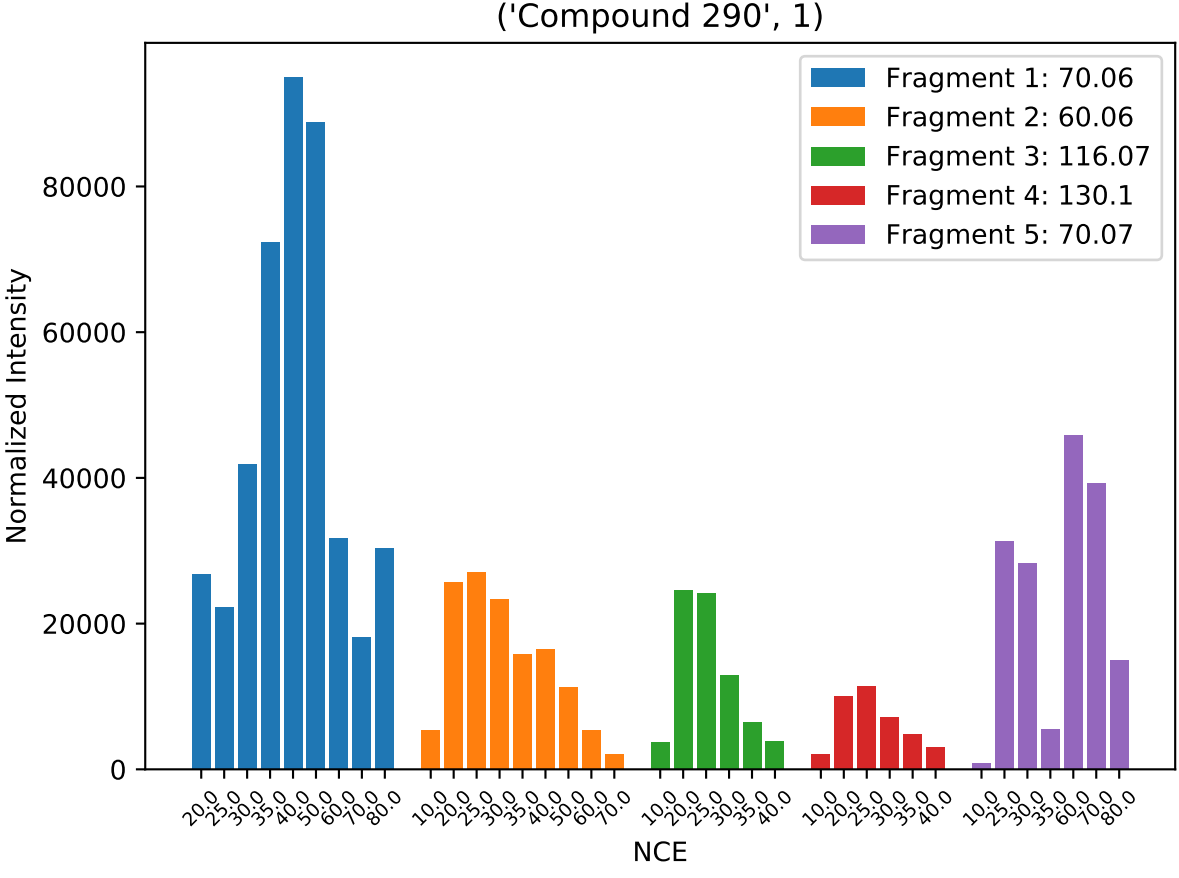

('Compound 565', 1)
Fragment 1: 353.03
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 96.96
Fragment 5: 173.48
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
35.0
40.0
60.0
80.0
20.0
25.0
30.0
50.0
60.0
70.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
50.0
70.0
NCE

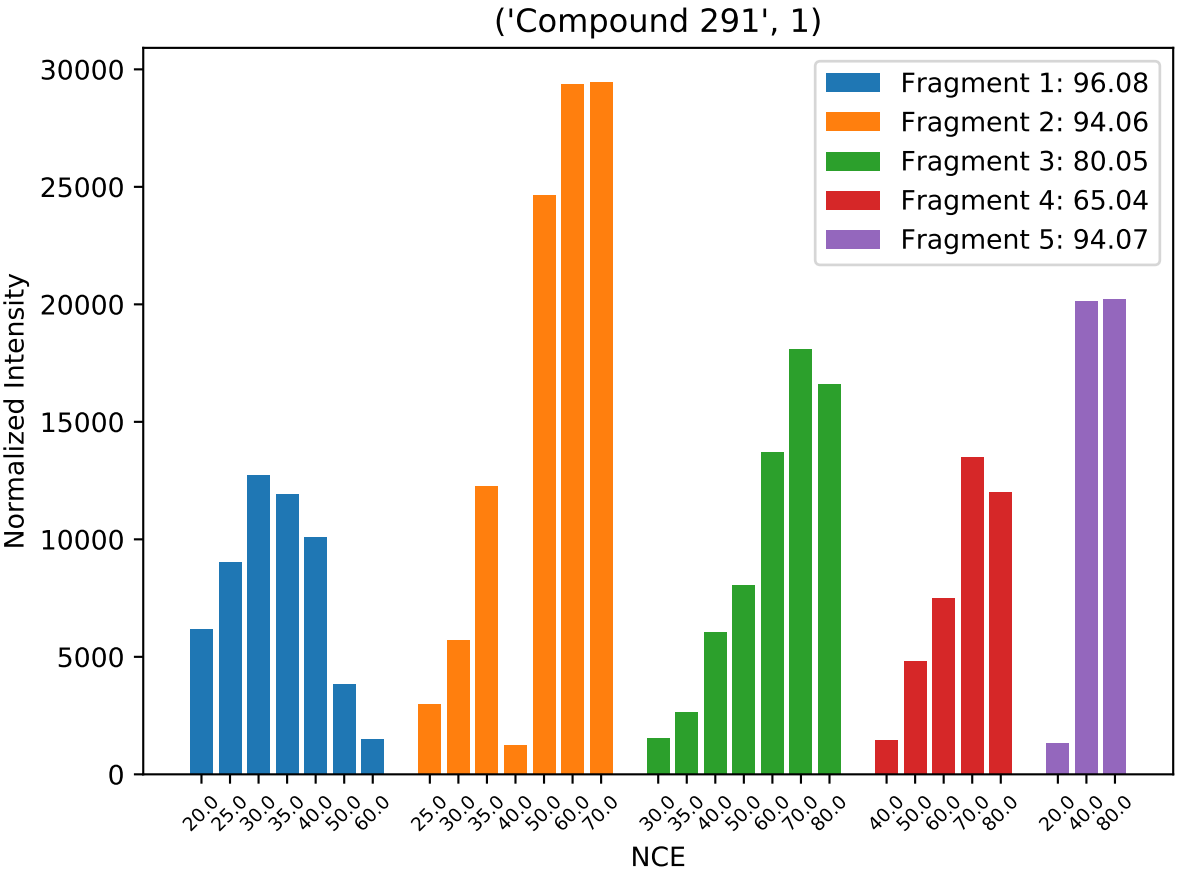

('Compound 566', 1)
Fragment 1: 110.06
Fragment 2: 88.04
Fragment 3: 65.04
Fragment 4: 110.07
Fragment 5: 122.1
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
40.0
50.0
60.0
70.0
80.0
30.0
20.0
NCE

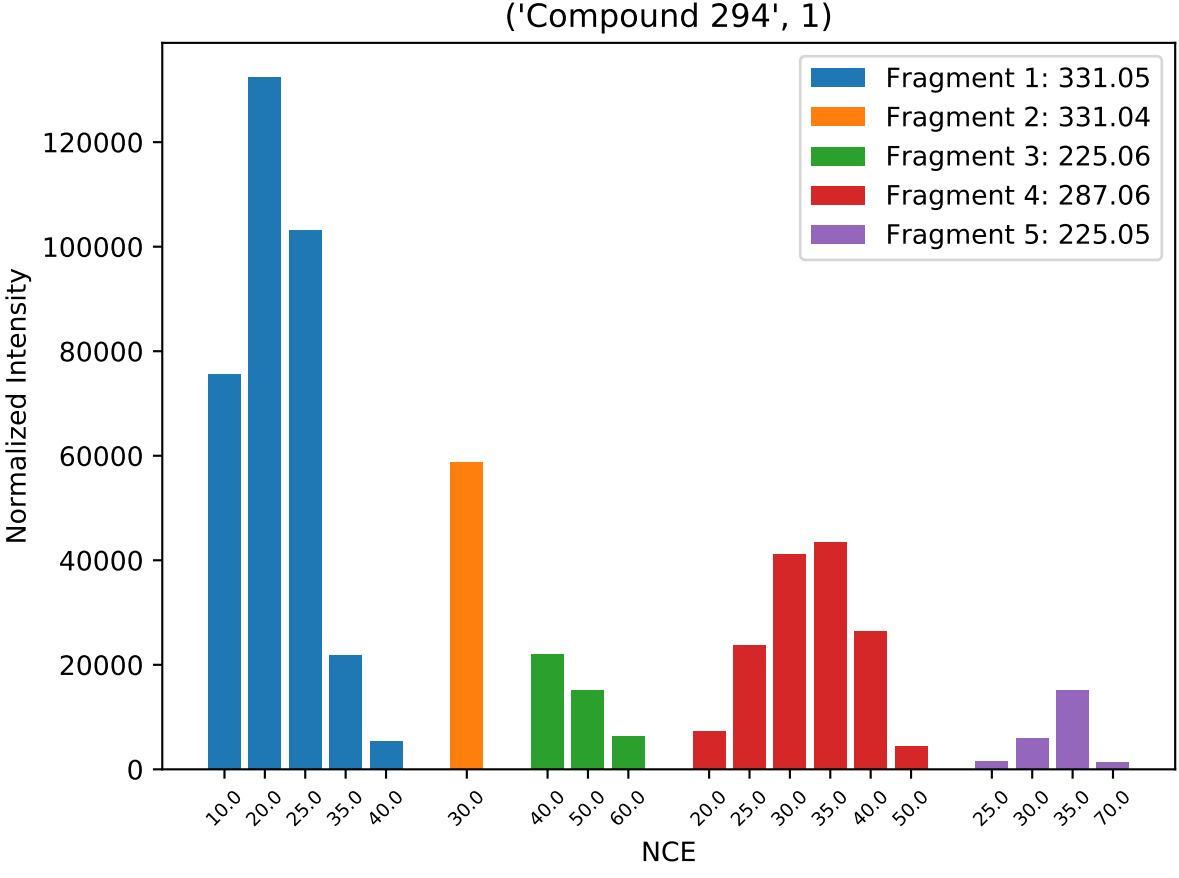

('Compound 286', 1)
Fragment 1: 160.9
Fragment 2: 144.93
Fragment 3: 173.47
Fragment 4: 173.48
Fragment 5: 173.46
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
50.0
70.0
10.0
35.0
40.0
60.0
80.0
10.0
25.0
30.0
35.0
40.0
60.0
80.0
NCE

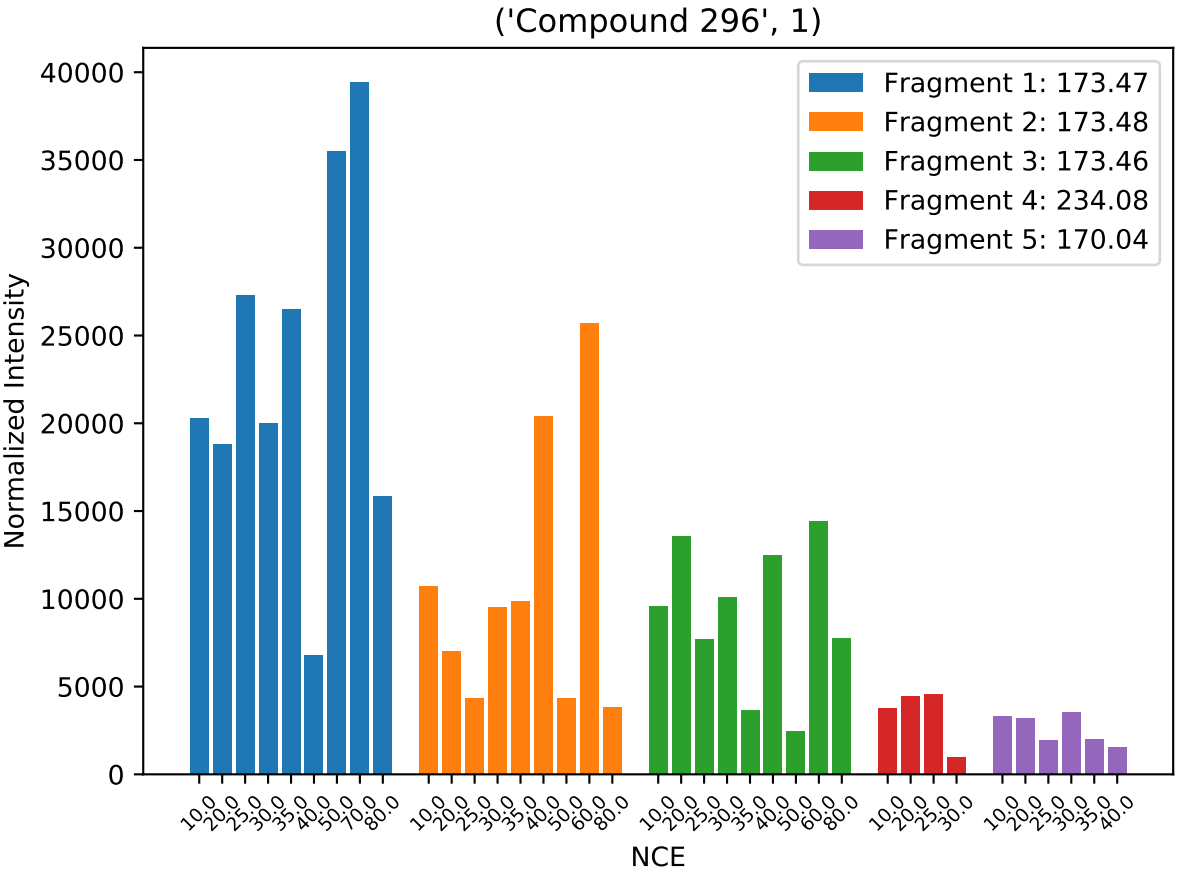

('Compound 288', 1)
Fragment 1: 477.11
Fragment 2: 225.06
Fragment 3: 287.06
Fragment 4: 173.47
Fragment 5: 331.05
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0
20.0
30.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
20.0
35.0
50.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

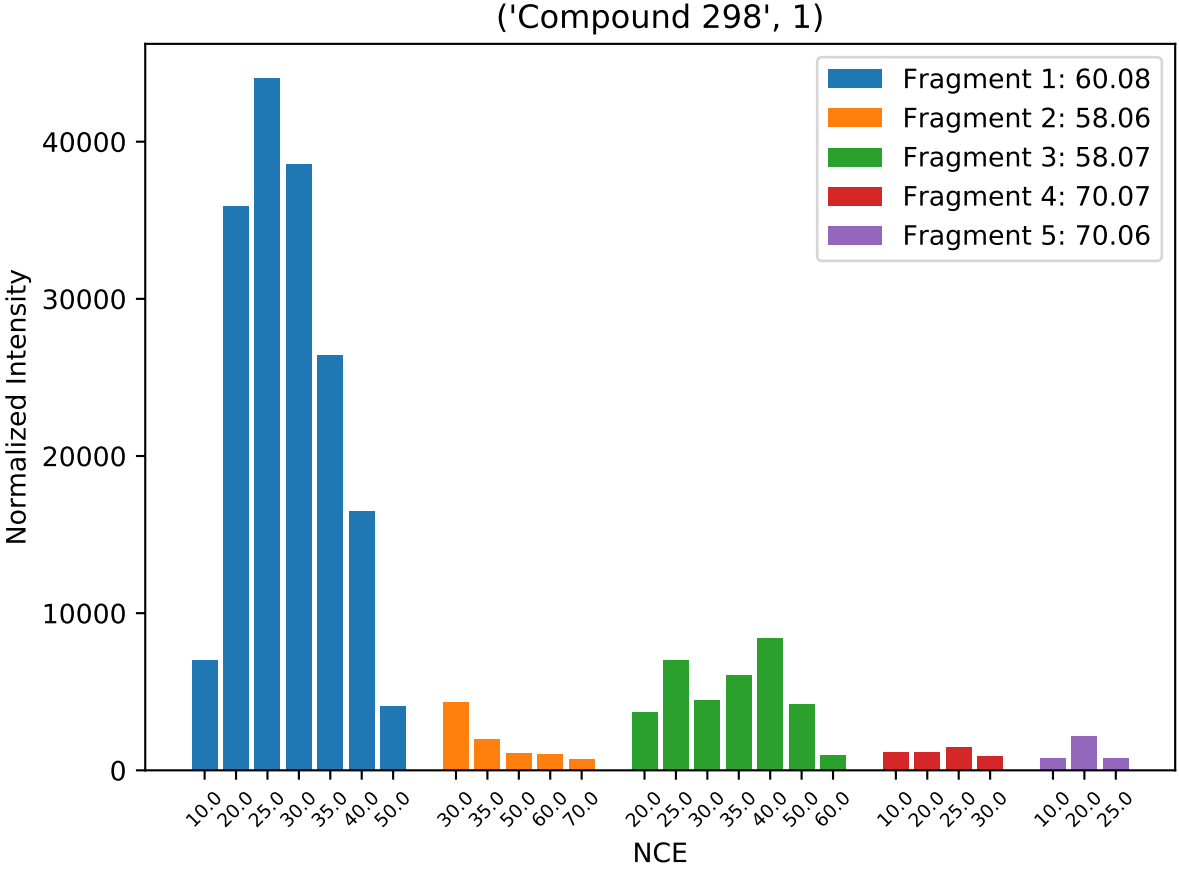

('Compound 289', 1)
Fragment 1: 446.85
Fragment 2: 173.47
Fragment 3: 234.92
Fragment 4: 128.95
Fragment 5: 340.88
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0
NCE

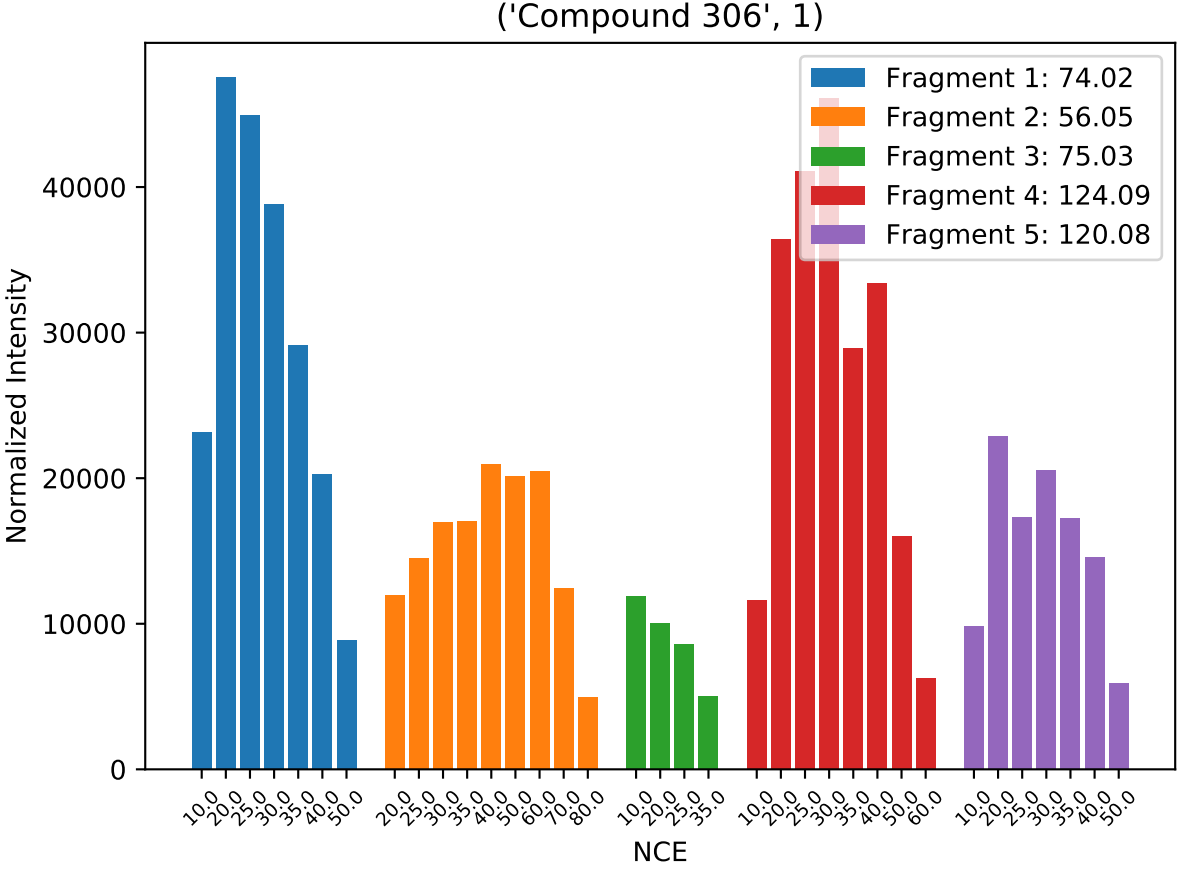

('Compound 290', 1)
Fragment 1: 70.06
Fragment 2: 60.06
Fragment 3: 116.07
Fragment 4: 130.1
Fragment 5: 70.07
Normalized Intensity
0
20000
40000
60000
80000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 25.0 30.0 35.0 60.0 70.0 80.0

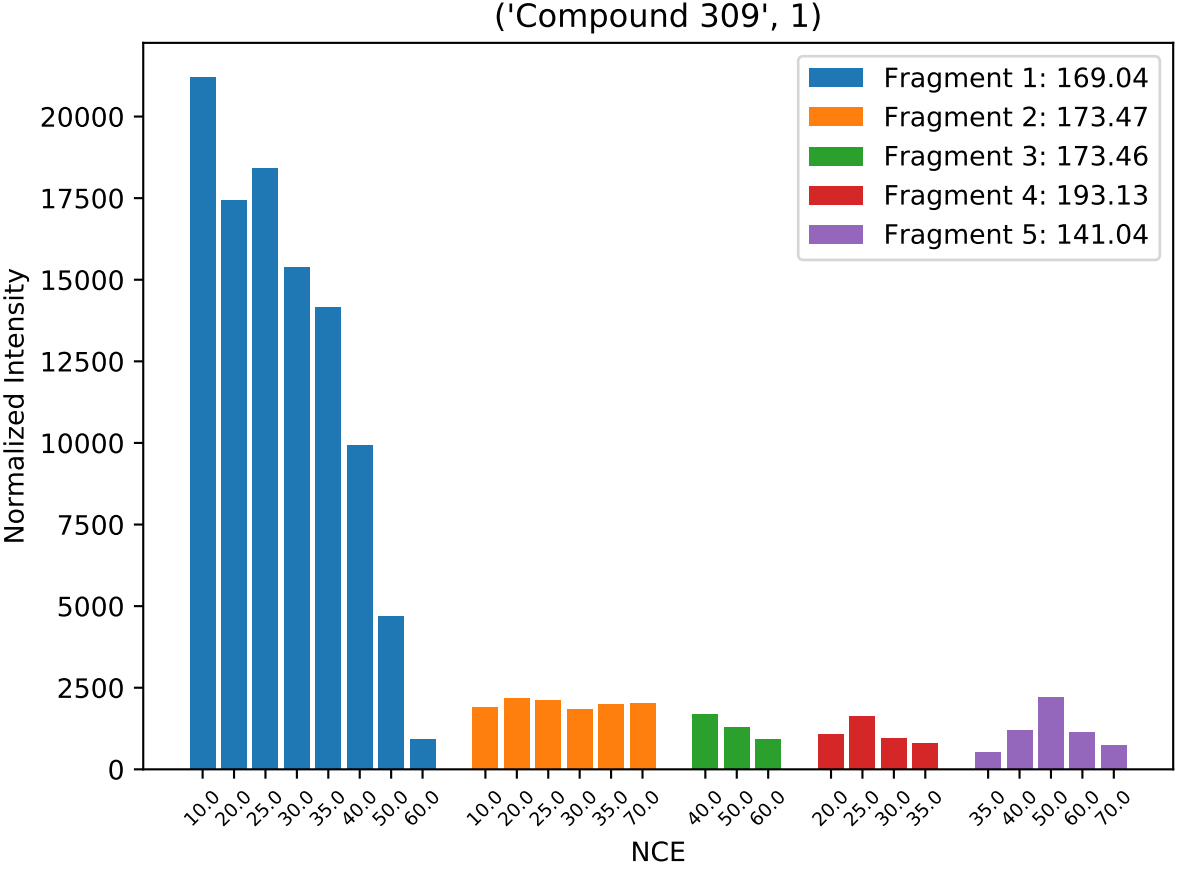

('Compound 291', 1)
Fragment 1: 96.08
Fragment 2: 94.06
Fragment 3: 80.05
Fragment 4: 65.04
Fragment 5: 94.07
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
20.0 40.0 80.0

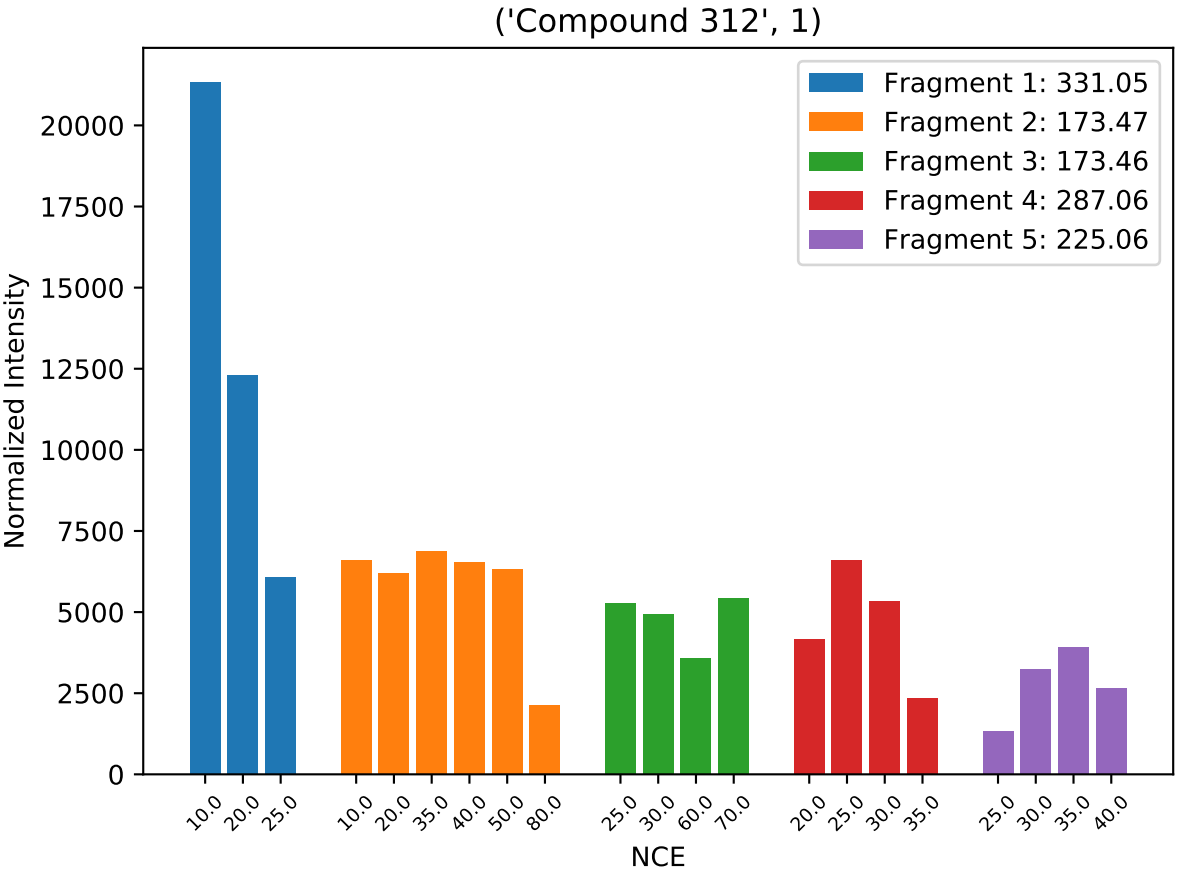

('Compound 294', 1)
Fragment 1: 331.05
Fragment 2: 331.04
Fragment 3: 225.06
Fragment 4: 287.06
Fragment 5: 225.05
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
10.0
20.0
25.0
35.0
40.0
30.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
70.0
NCE

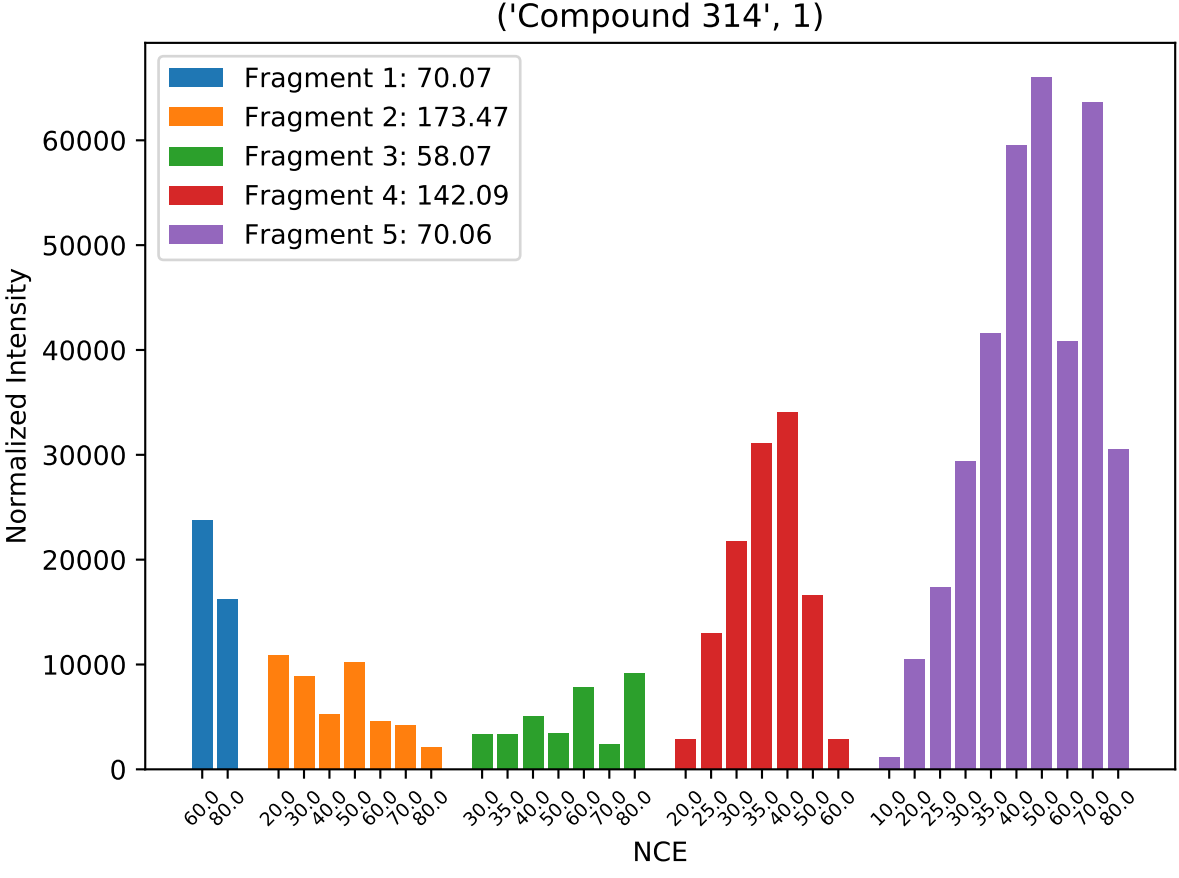

('Compound 296', 1)
Fragment 1: 173.47
Fragment 2: 173.48
Fragment 3: 173.46
Fragment 4: 234.08
Fragment 5: 170.04
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 80.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

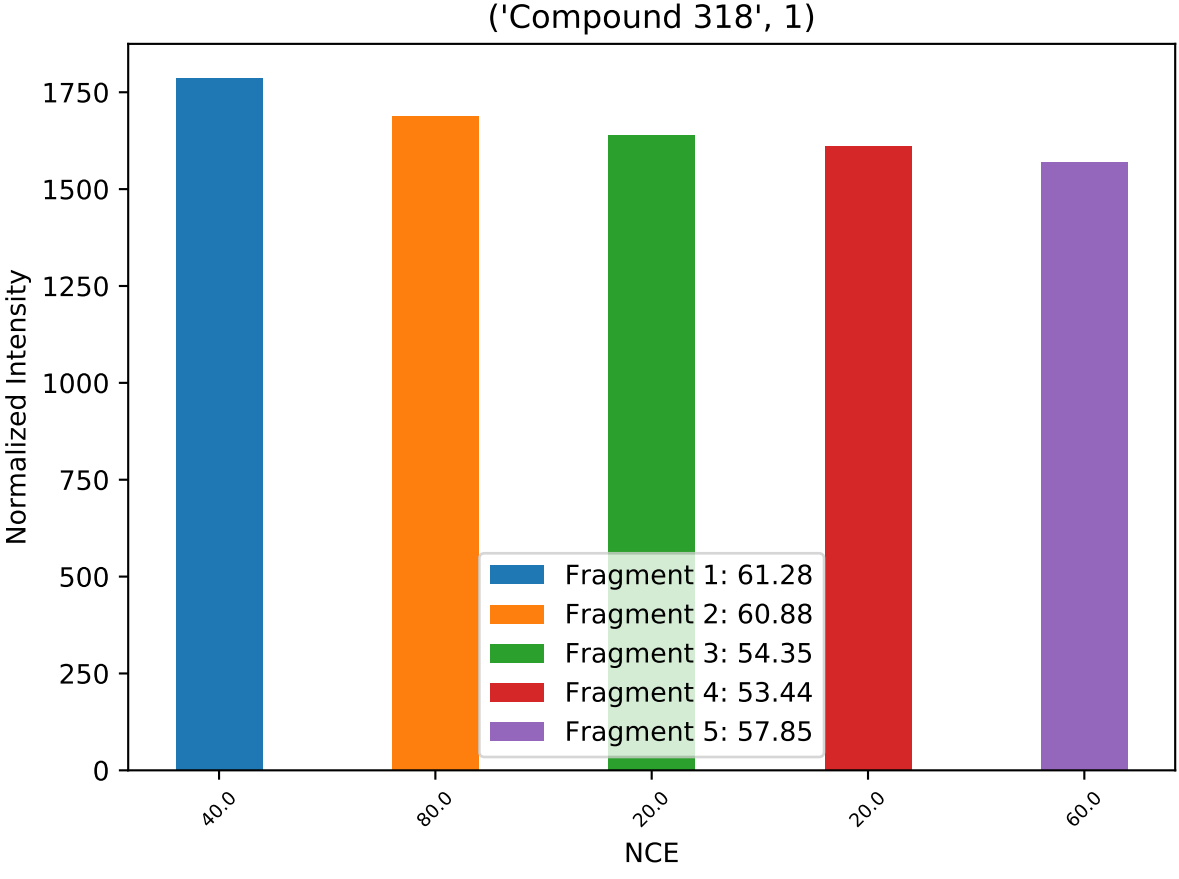

('Compound 298', 1)
Fragment 1: 60.08
Fragment 2: 58.06
Fragment 3: 58.07
Fragment 4: 70.07
Fragment 5: 70.06
Normalized Intensity
0
10000
20000
30000
40000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
30.0
35.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
10.0
20.0
25.0
NCE

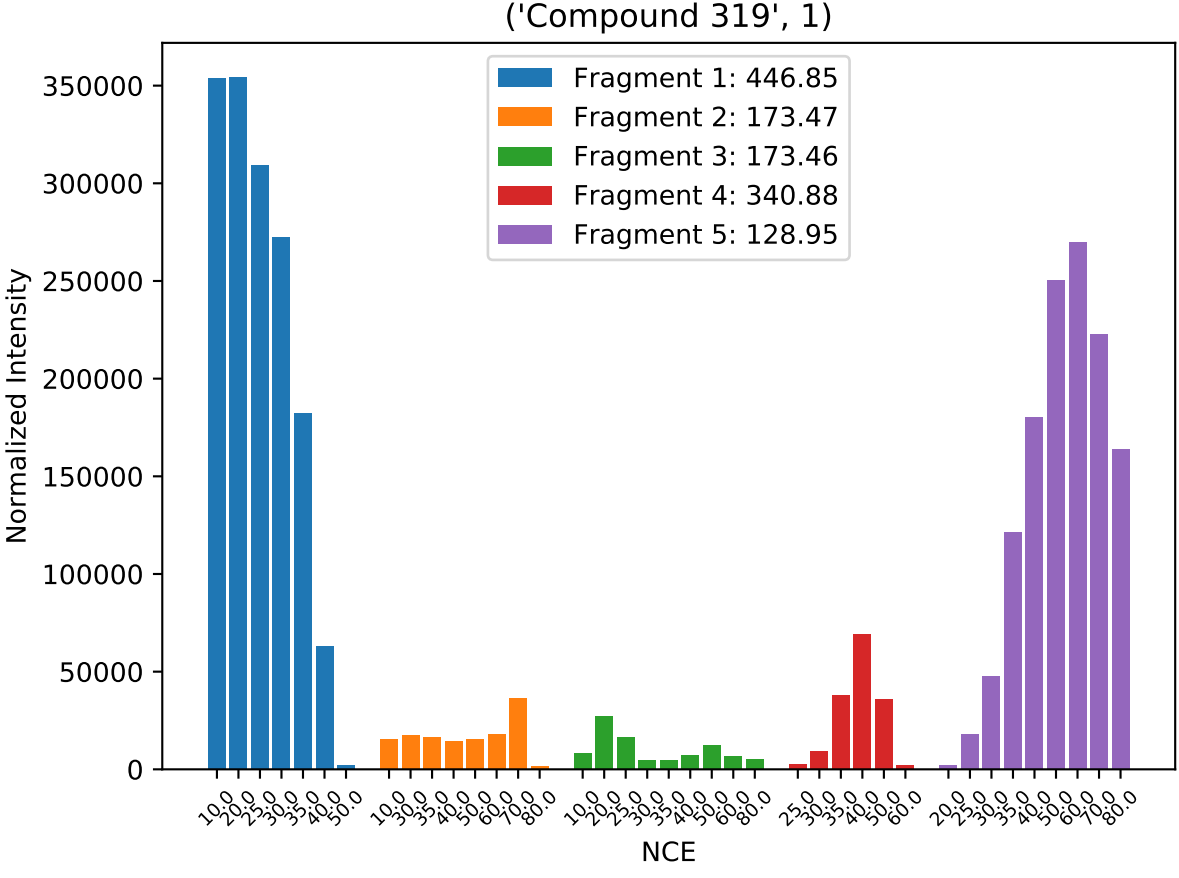

('Compound 306', 1)
Fragment 1: 74.02
Fragment 2: 56.05
Fragment 3: 75.03
Fragment 4: 124.09
Fragment 5: 120.08
Normalized Intensity
0
10000
20000
30000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

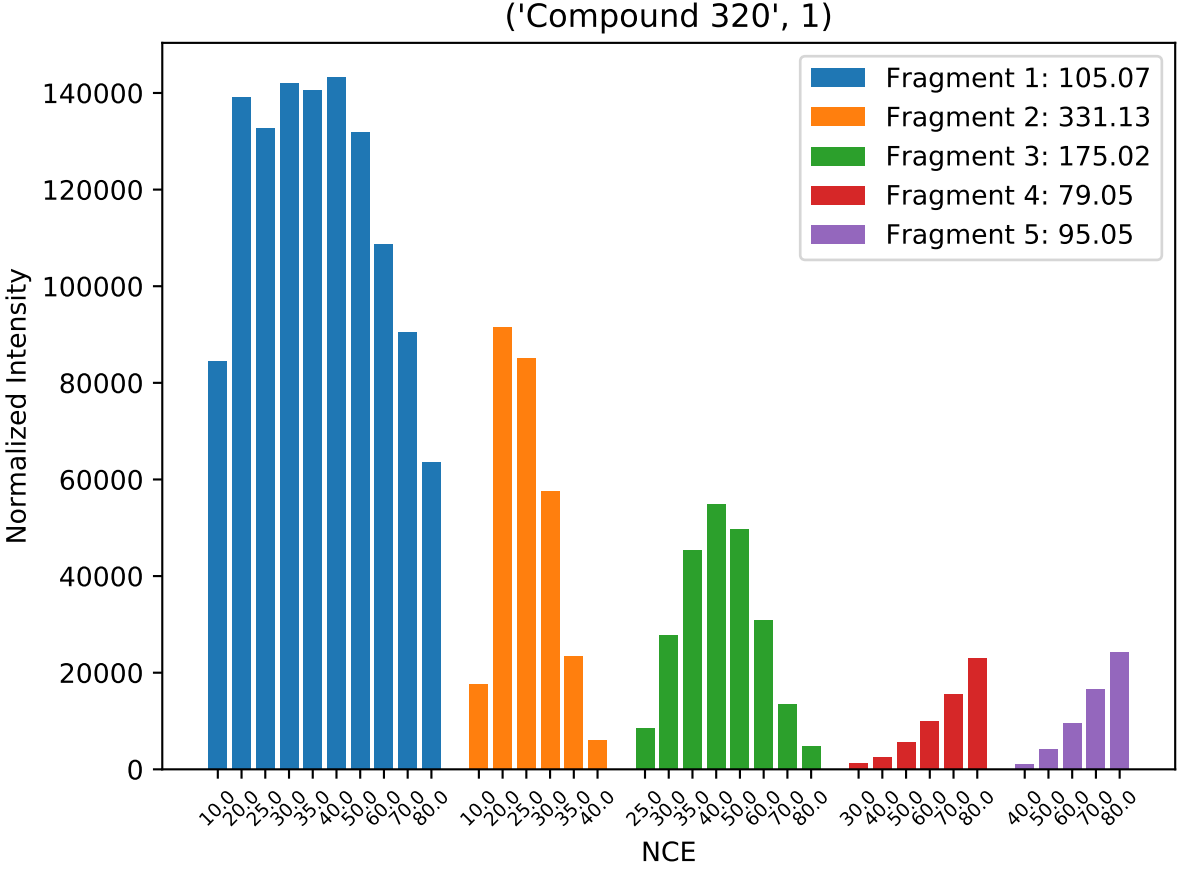

('Compound 309', 1)
Fragment 1: 169.04
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 193.13
Fragment 5: 141.04
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
70.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
35.0
40.0
50.0
60.0
70.0
NCE

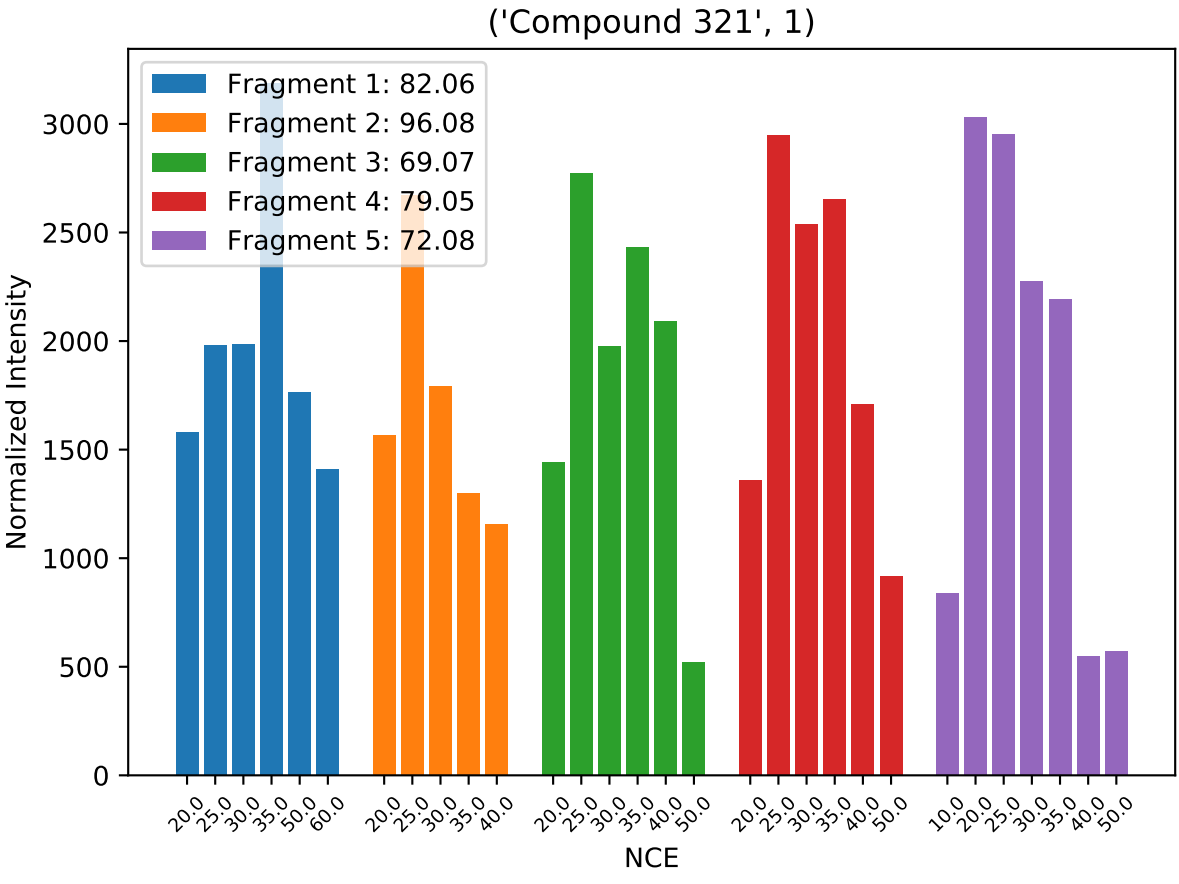

('Compound 312', 1)
Fragment 1: 331.05
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 287.06
Fragment 5: 225.06
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0
20.0
25.0
10.0
20.0
35.0
40.0
50.0
80.0
25.0
30.0
60.0
70.0
20.0
25.0
30.0
35.0
25.0
30.0
35.0
40.0
NCE

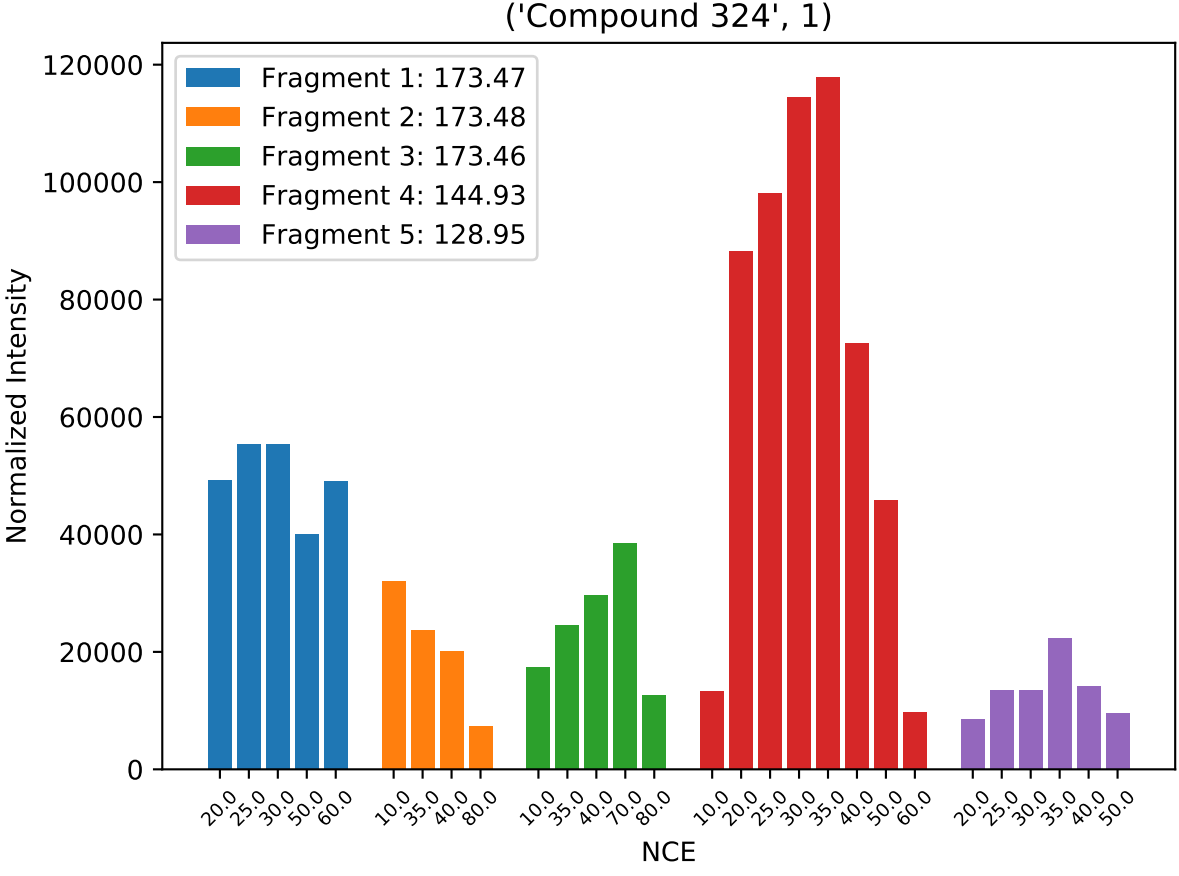

('Compound 314', 1)
Fragment 1: 70.07
Fragment 2: 173.47
Fragment 3: 58.07
Fragment 4: 142.09
Fragment 5: 70.06
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
60.0
80.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

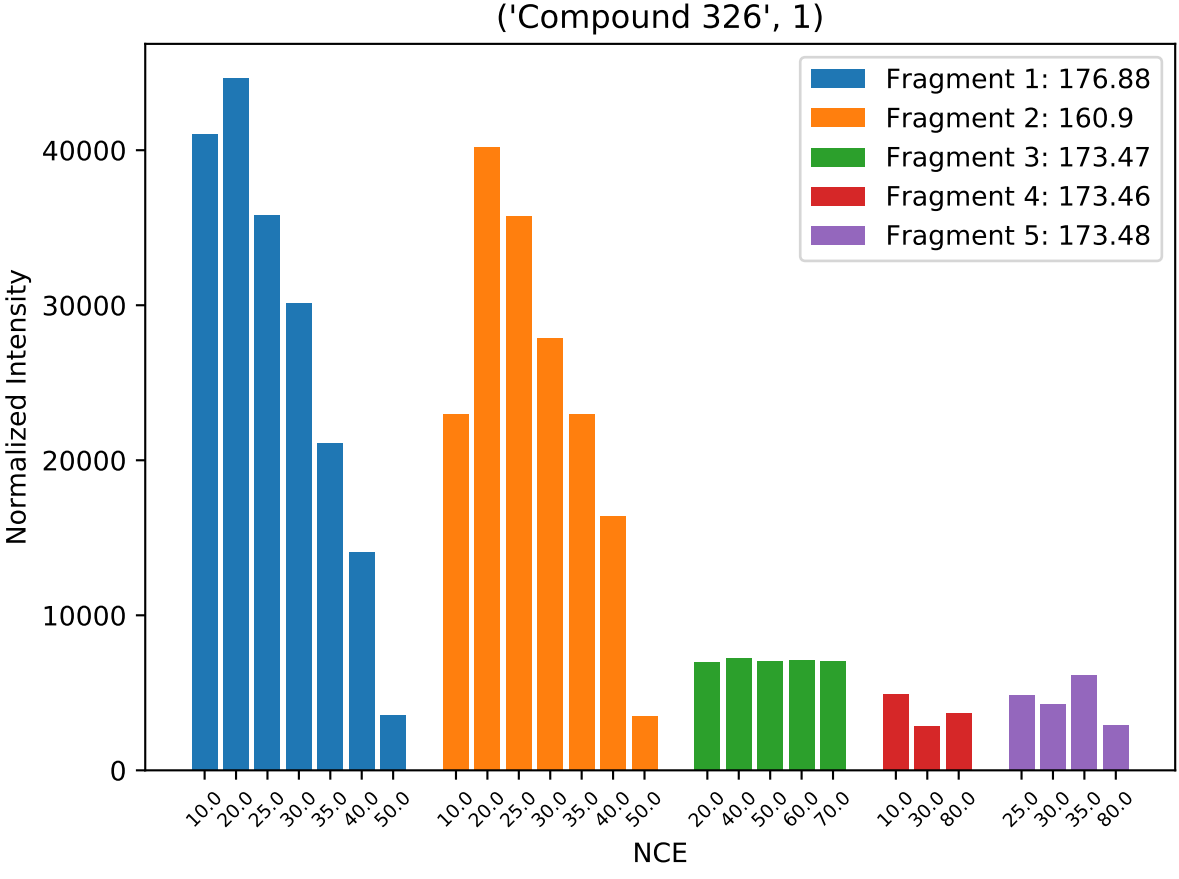

('Compound 318', 1)
Normalized Intensity
1750
1500
1250
1000
750
500
250
0
Fragment 1: 61.28
Fragment 2: 60.88
Fragment 3: 54.35
Fragment 4: 53.44
Fragment 5: 57.85
40.0
80.0
20.0
20.0
60.0
NCE

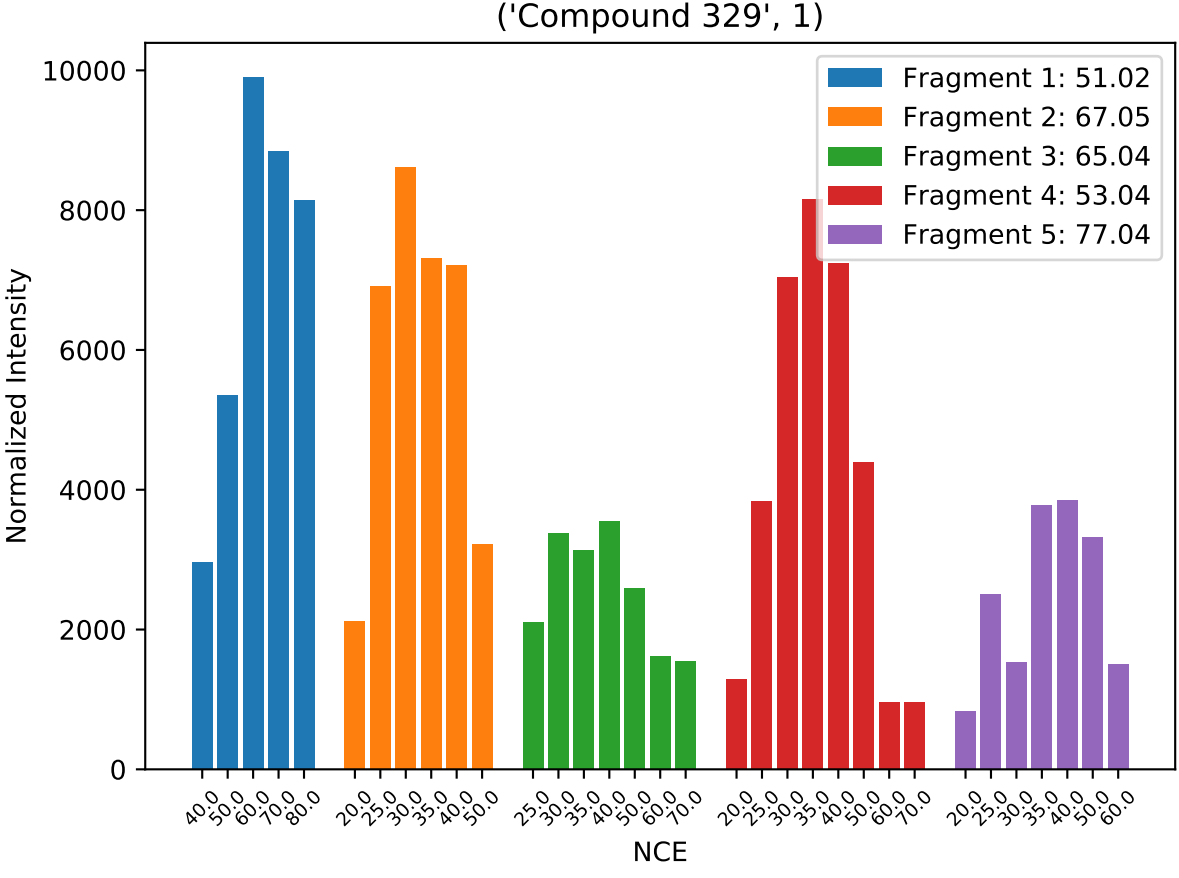

('Compound 319', 1)
Fragment 1: 446.85
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 340.88
Fragment 5: 128.95
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

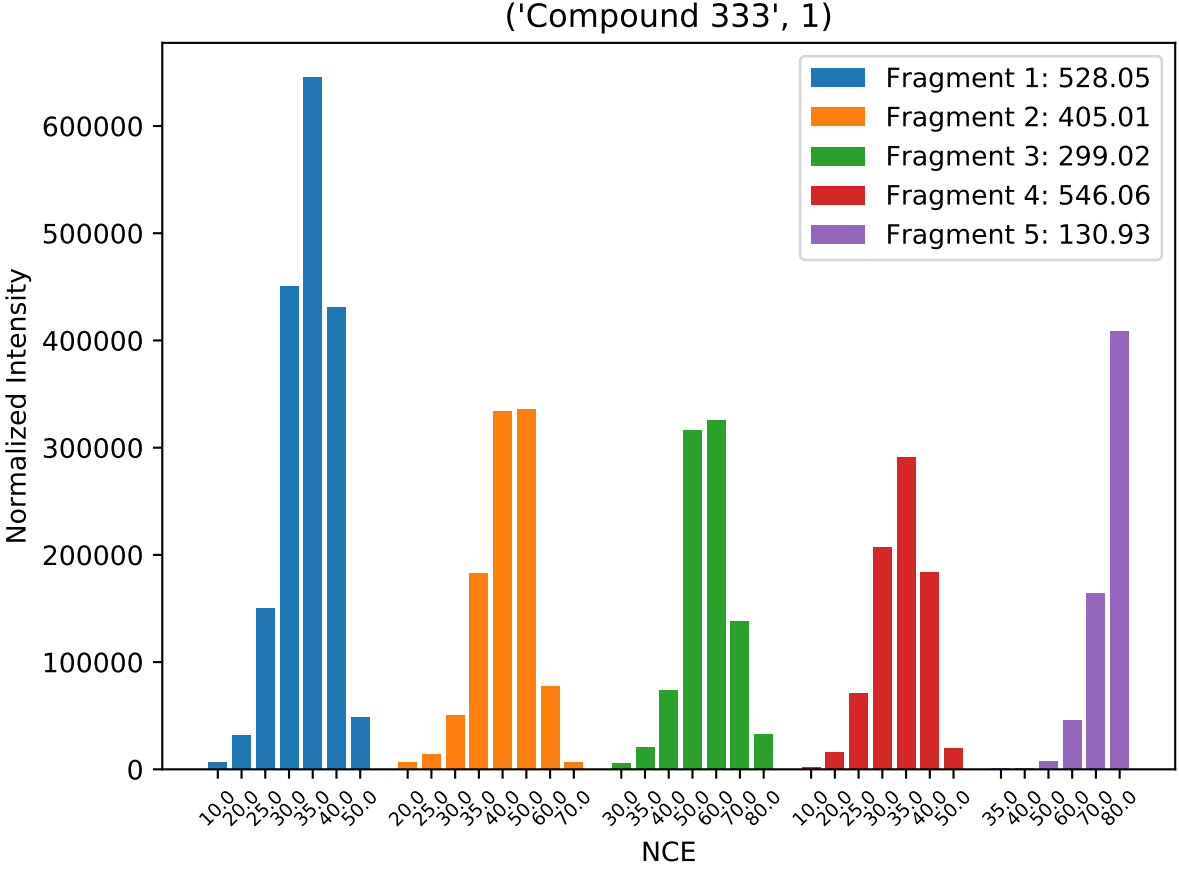

('Compound 320', 1)
Fragment 1: 105.07
Fragment 2: 331.13
Fragment 3: 175.02
Fragment 4: 79.05
Fragment 5: 95.05
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0

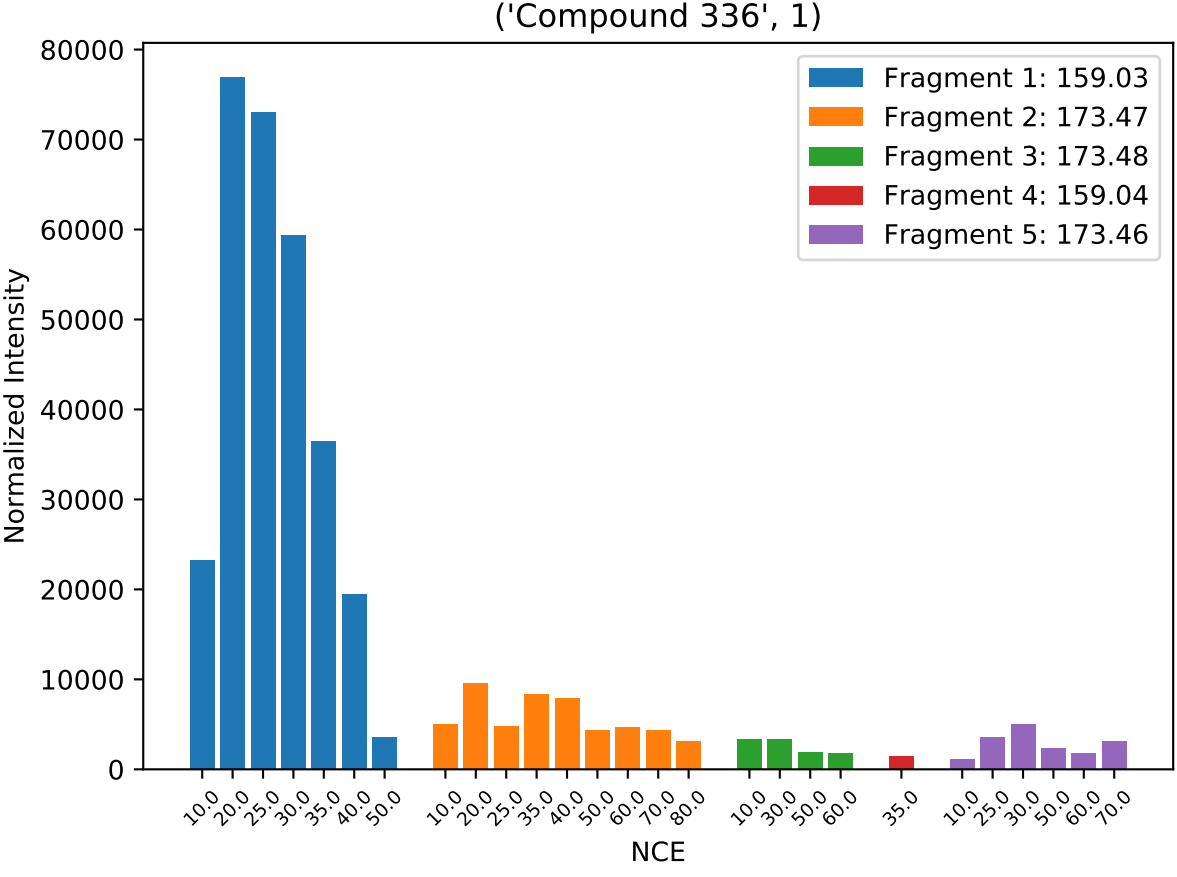

('Compound 321', 1)
Fragment 1: 82.06
Fragment 2: 96.08
Fragment 3: 69.07
Fragment 4: 79.05
Fragment 5: 72.08
Normalized Intensity
0
500
1000
1500
2000
2500
3000
20.0 25.0 30.0 35.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

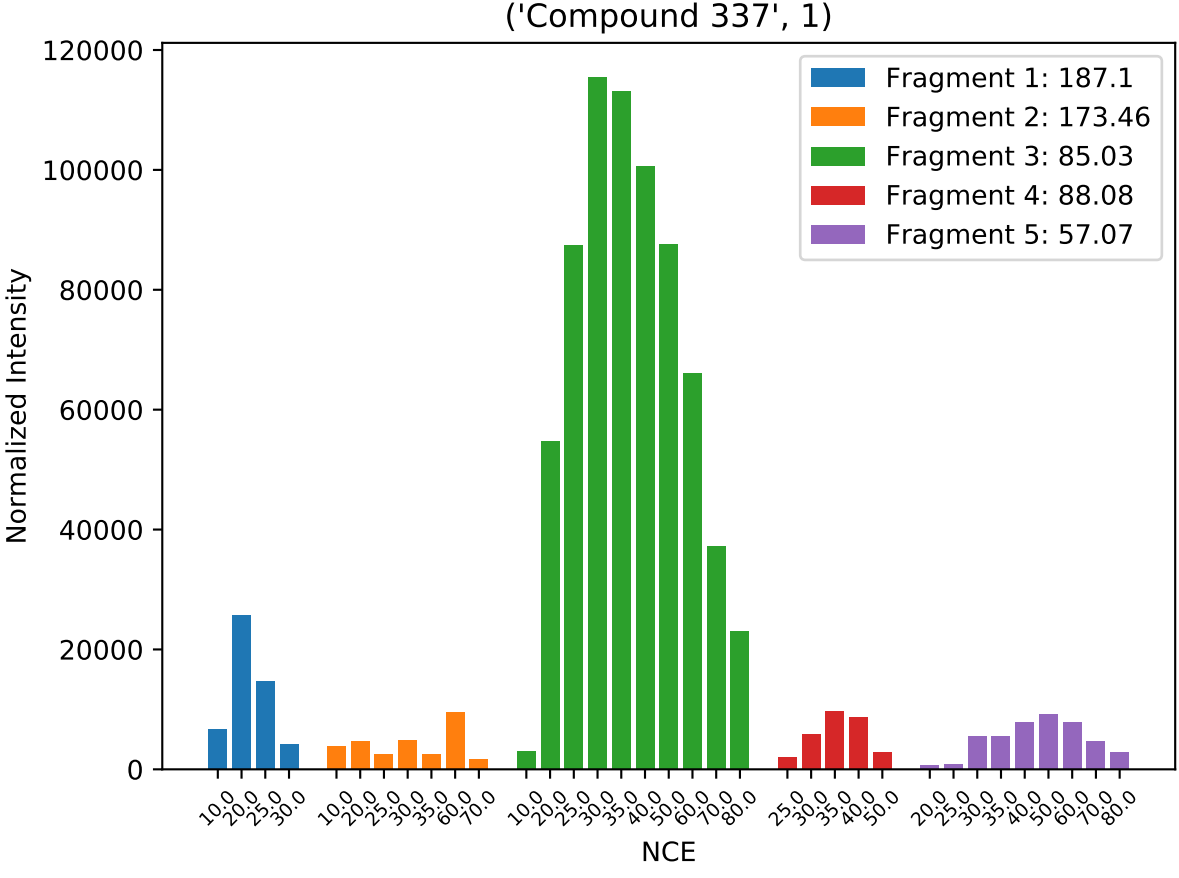

('Compound 324', 1)
Fragment 1: 173.47
Fragment 2: 173.48
Fragment 3: 173.46
Fragment 4: 144.93
Fragment 5: 128.95
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
20.0 25.0 30.0 50.0 60.0
10.0 35.0 40.0 80.0
10.0 35.0 40.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0
NCE

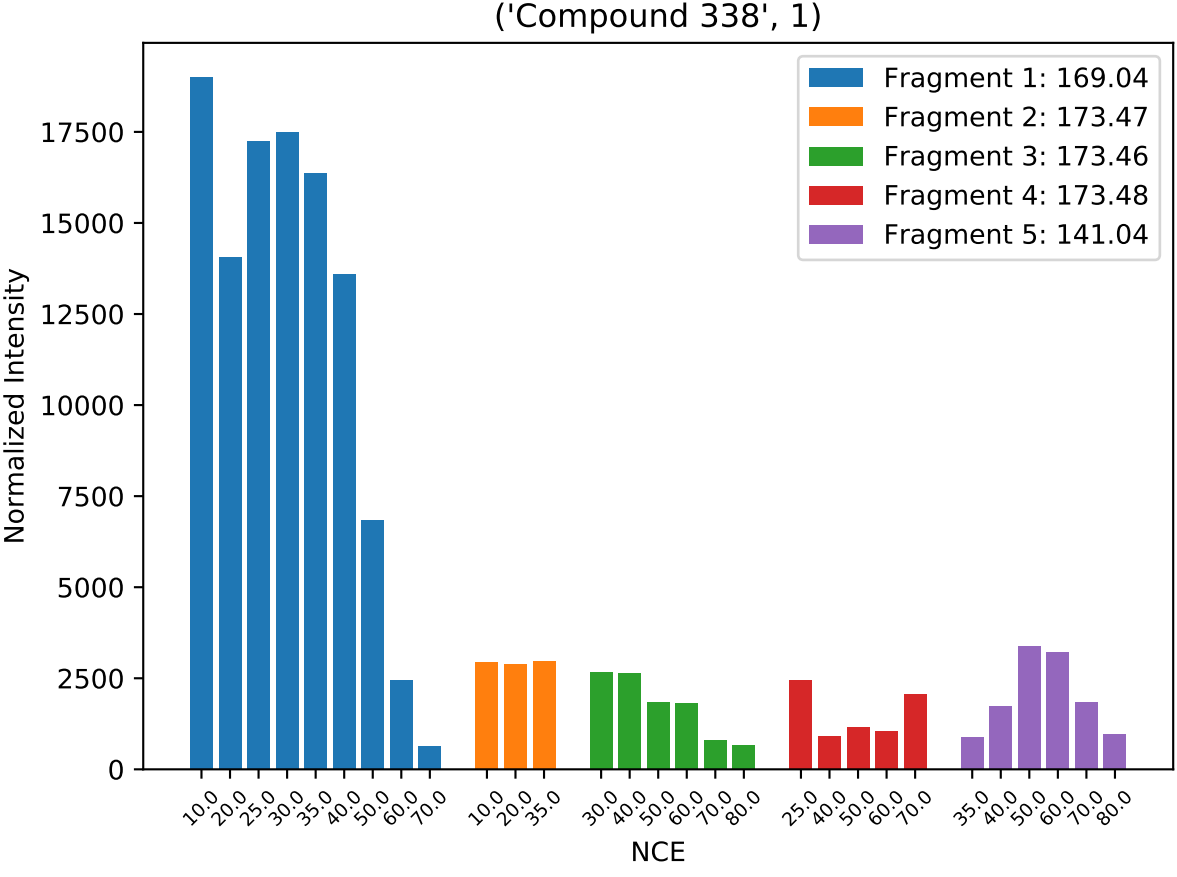

('Compound 326', 1)
Fragment 1: 176.88
Fragment 2: 160.9
Fragment 3: 173.47
Fragment 4: 173.46
Fragment 5: 173.48
Normalized Intensity
0
10000
20000
30000
40000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
40.0
50.0
60.0
70.0
10.0
30.0
80.0
25.0
30.0
35.0
80.0
NCE

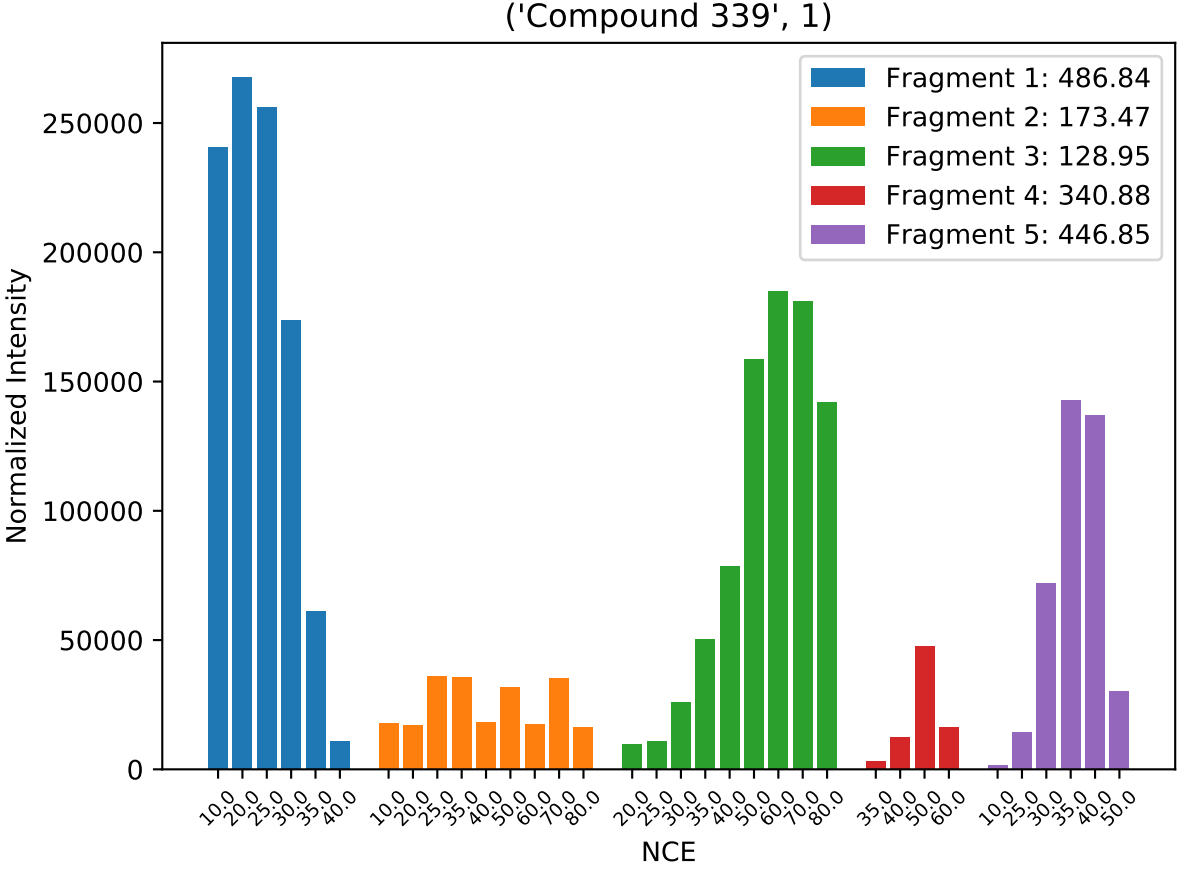

('Compound 329', 1)
Fragment 1: 51.02
Fragment 2: 67.05
Fragment 3: 65.04
Fragment 4: 53.04
Fragment 5: 77.04
Normalized Intensity
0
2000
4000
6000
8000
10000
40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

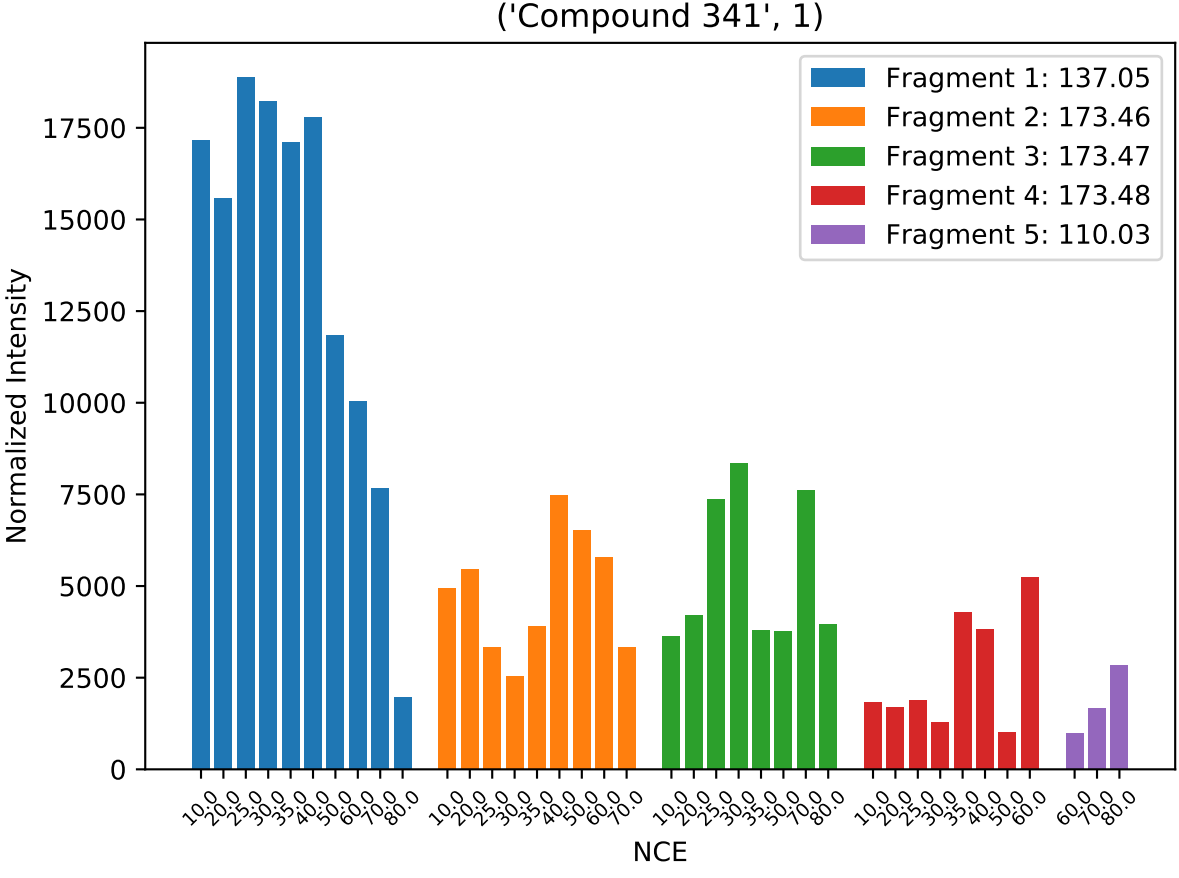

('Compound 333', 1)
Fragment 1: 528.05
Fragment 2: 405.01
Fragment 3: 299.02
Fragment 4: 546.06
Fragment 5: 130.93
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

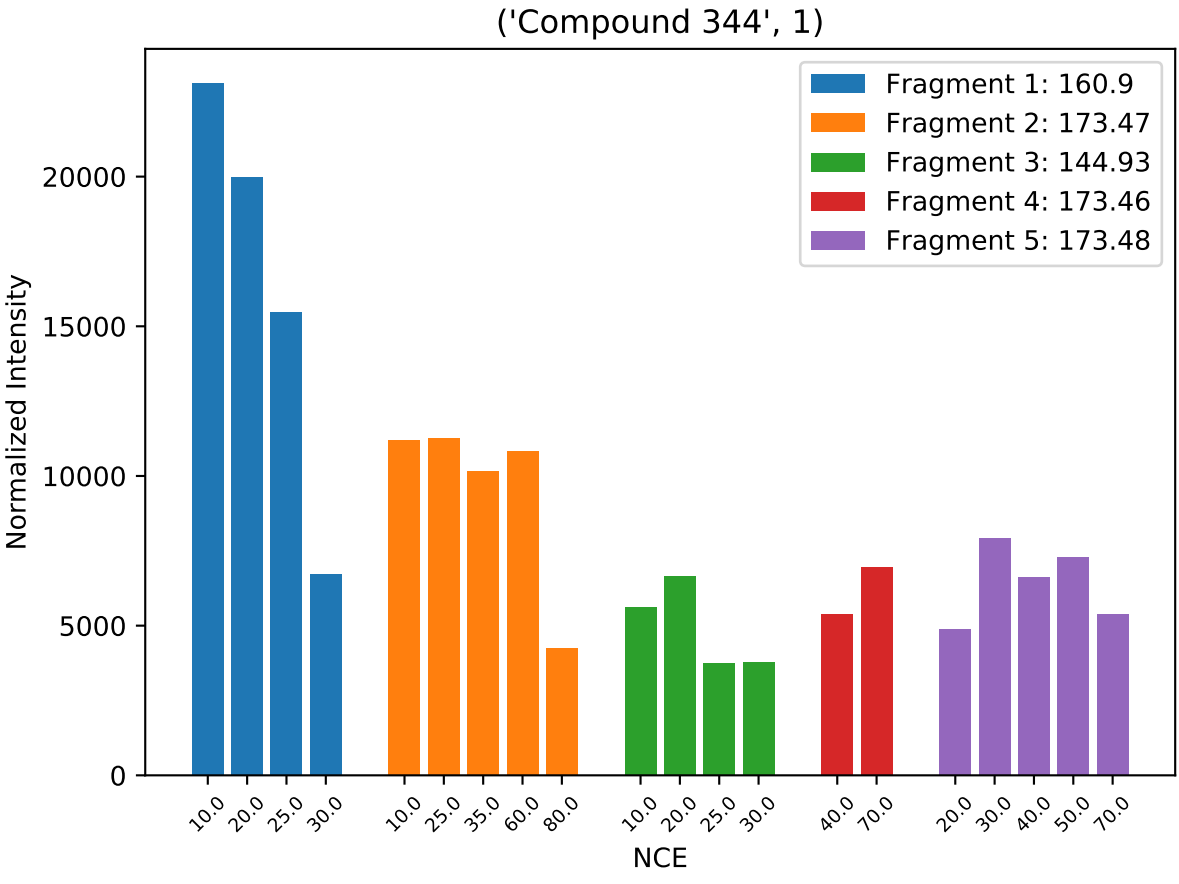

('Compound 336', 1)
Fragment 1: 159.03
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 159.04
Fragment 5: 173.46
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
30.0
50.0
60.0
35.0
10.0
25.0
30.0
50.0
60.0
70.0
NCE

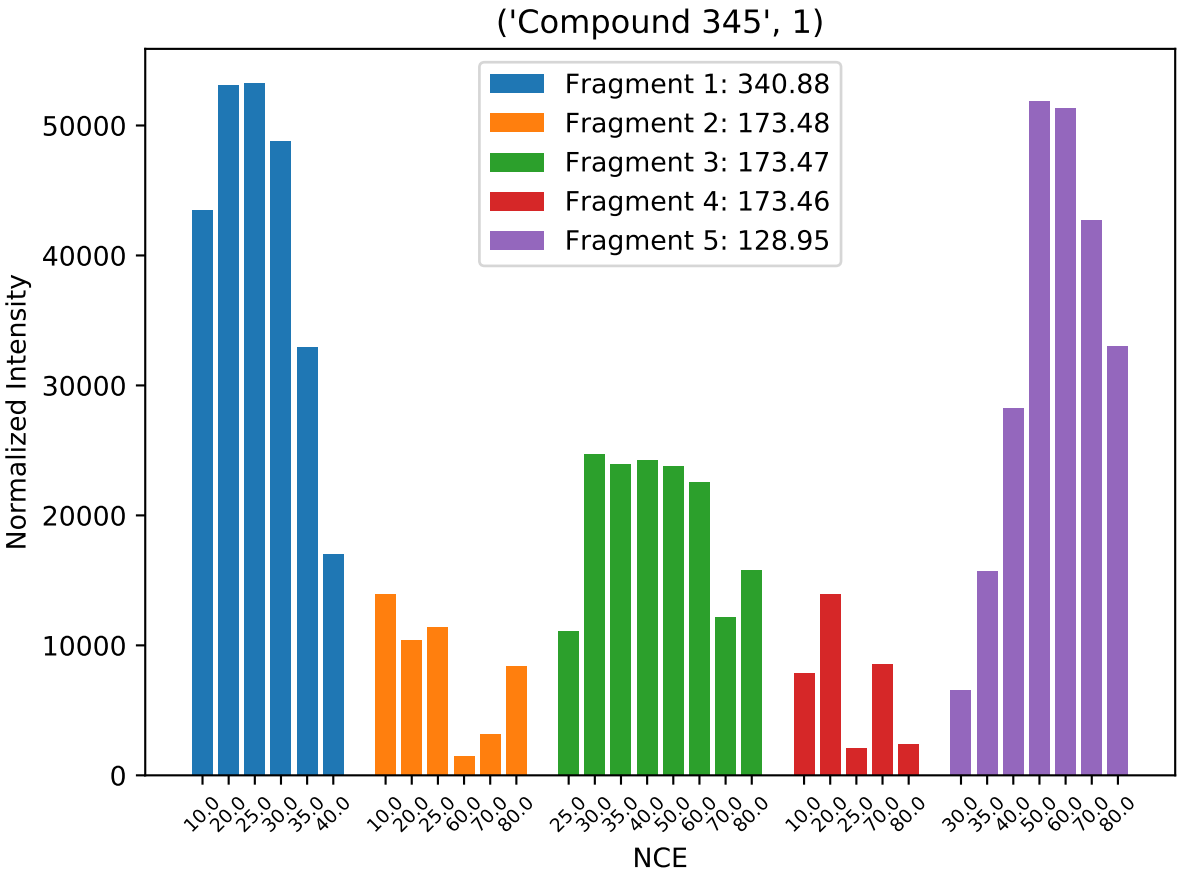

('Compound 337', 1)
Fragment 1: 187.1
Fragment 2: 173.46
Fragment 3: 85.03
Fragment 4: 88.08
Fragment 5: 57.07
Normalized Intensity
120000
100000
80000
60000
40000
20000
0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

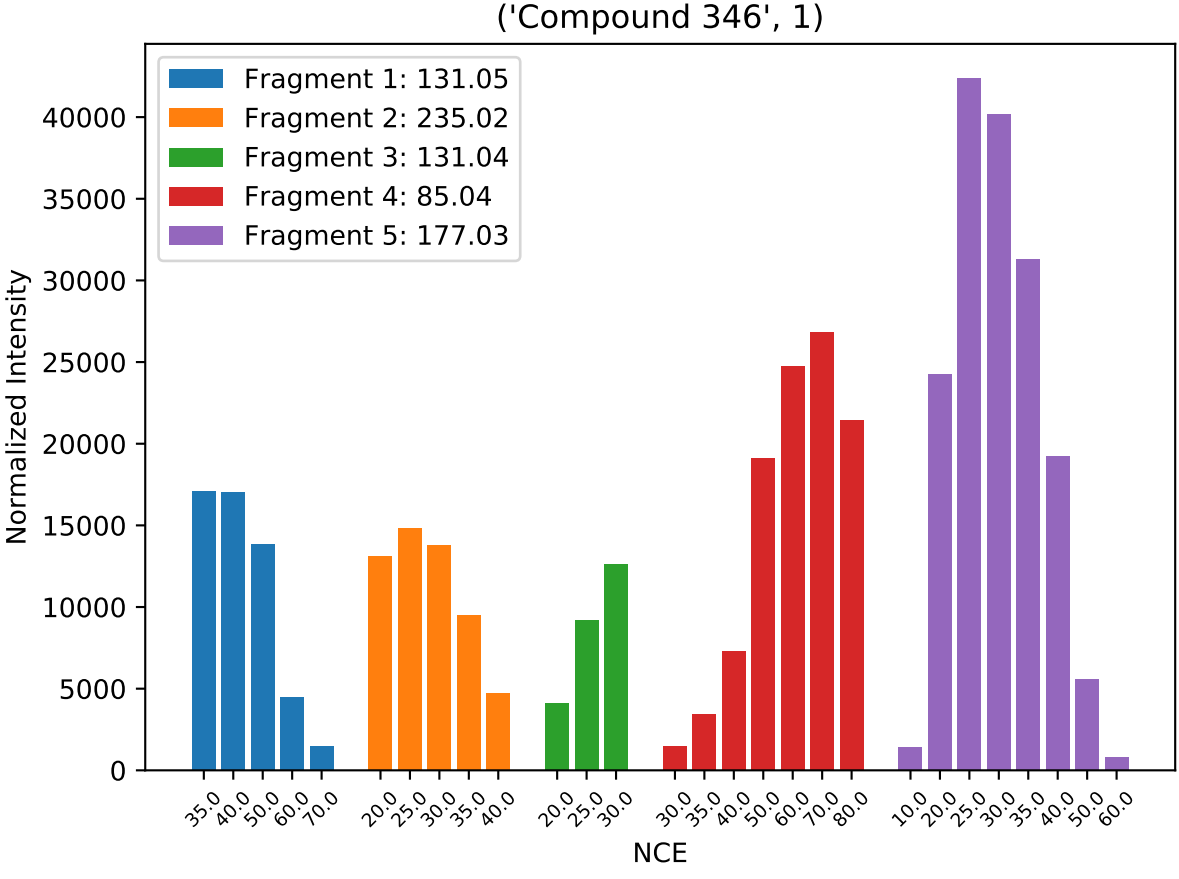

('Compound 338', 1)
Fragment 1: 169.04
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 173.48
Fragment 5: 141.04
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 35.0
30.0 40.0 50.0 60.0 70.0 80.0
25.0 40.0 50.0 60.0 70.0
35.0 40.0 50.0 60.0 70.0 80.0

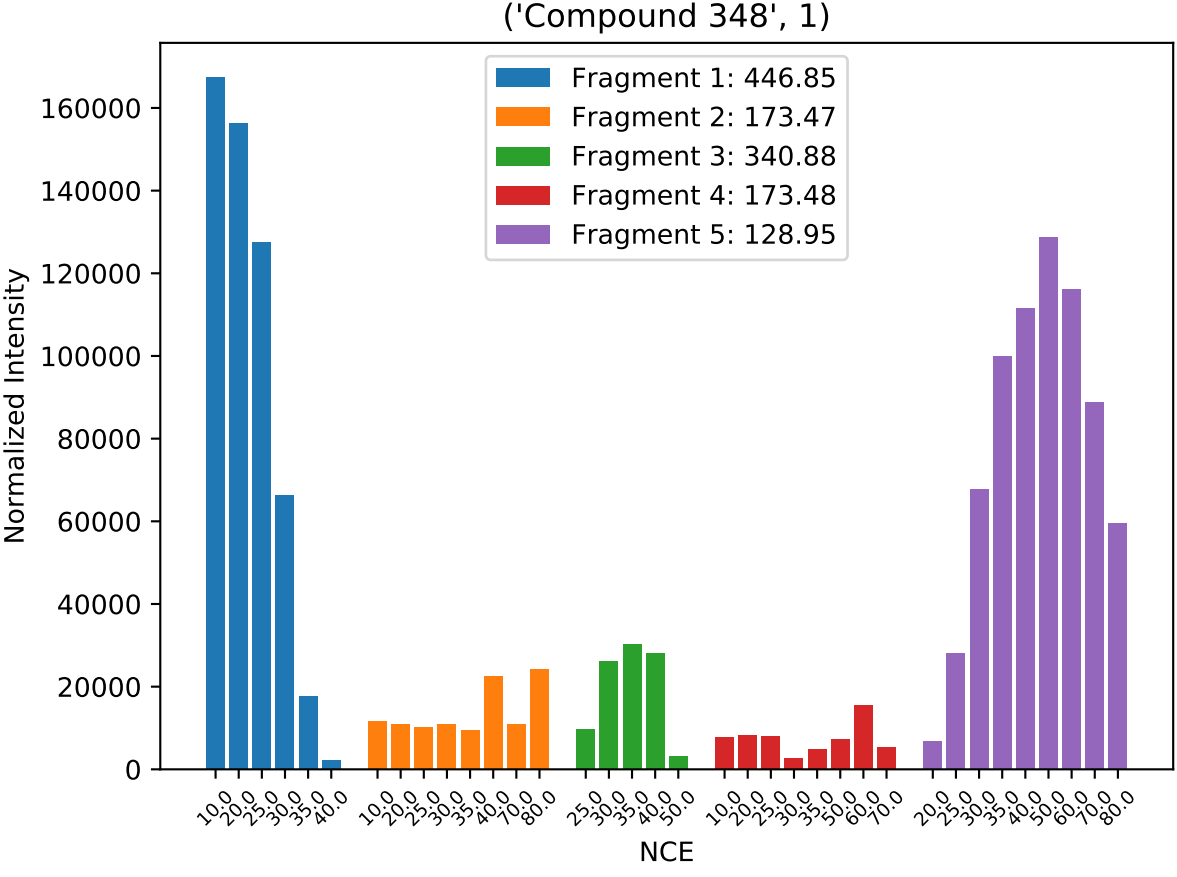

('Compound 339', 1)
Fragment 1: 486.84
Fragment 2: 173.47
Fragment 3: 128.95
Fragment 4: 340.88
Fragment 5: 446.85
Normalized Intensity
0
50000
100000
150000
200000
250000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0
10.0 25.0 30.0 35.0 40.0 50.0

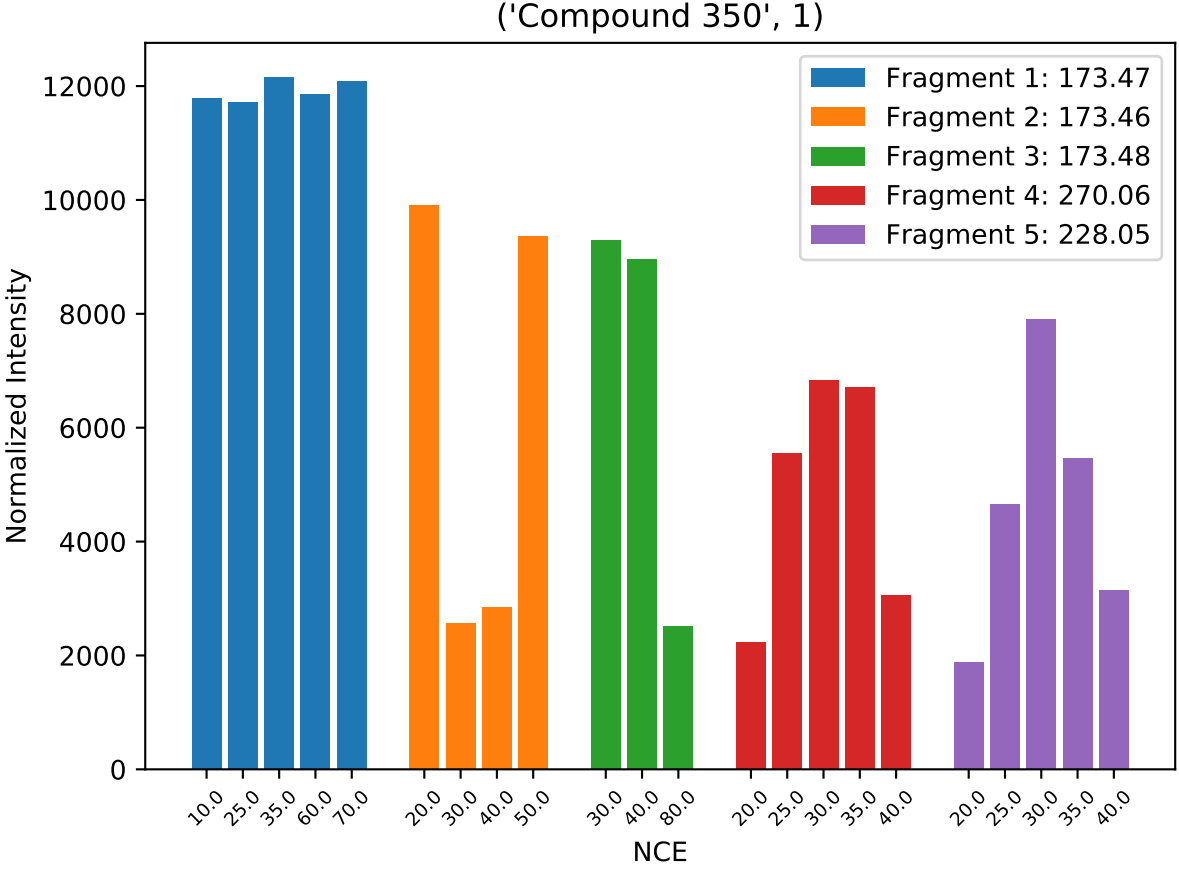

('Compound 341', 1)
Fragment 1: 137.05
Fragment 2: 173.46
Fragment 3: 173.47
Fragment 4: 173.48
Fragment 5: 110.03
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 50.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
60.0 70.0 80.0

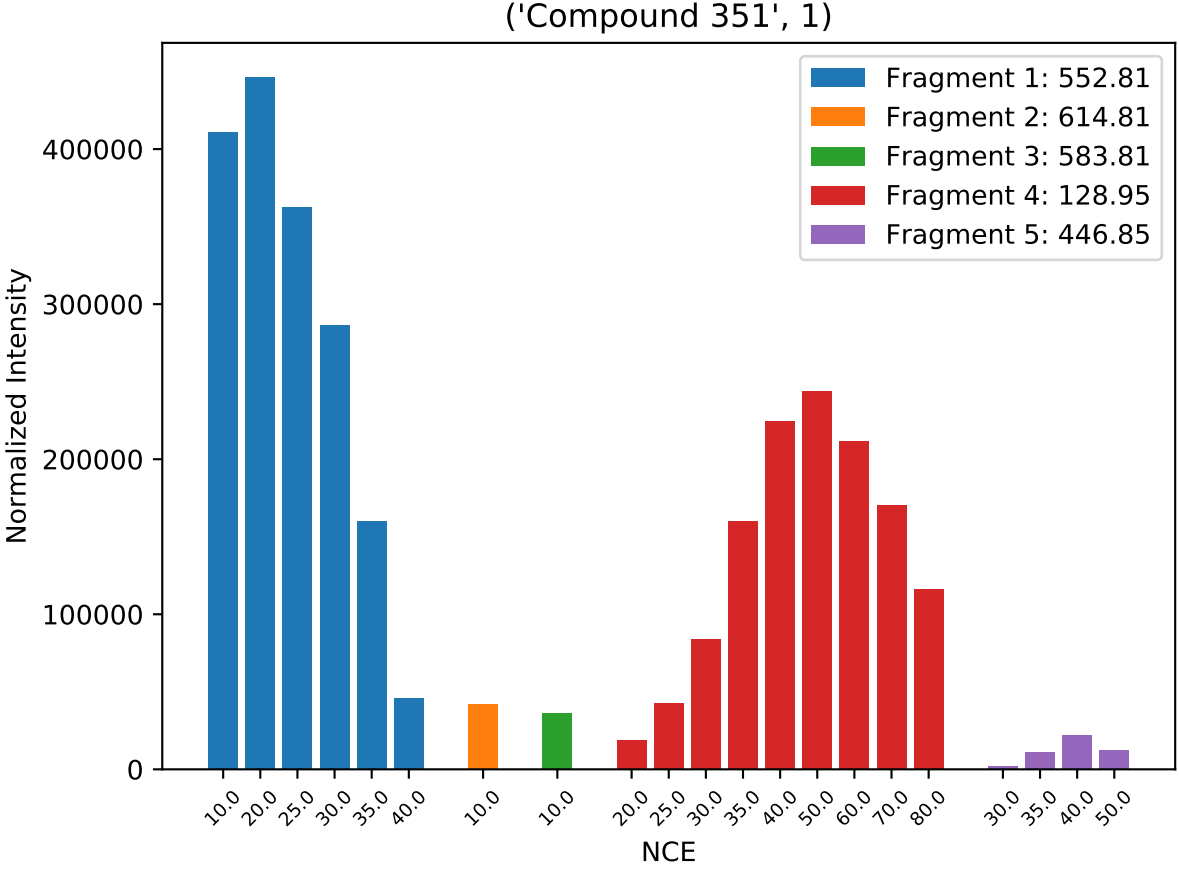

('Compound 344', 1)
Fragment 1: 160.9
Fragment 2: 173.47
Fragment 3: 144.93
Fragment 4: 173.46
Fragment 5: 173.48
Normalized Intensity
0
5000
10000
15000
20000
10.0
20.0
25.0
30.0
10.0
25.0
35.0
60.0
80.0
10.0
20.0
25.0
30.0
40.0
70.0
20.0
30.0
40.0
50.0
70.0
NCE

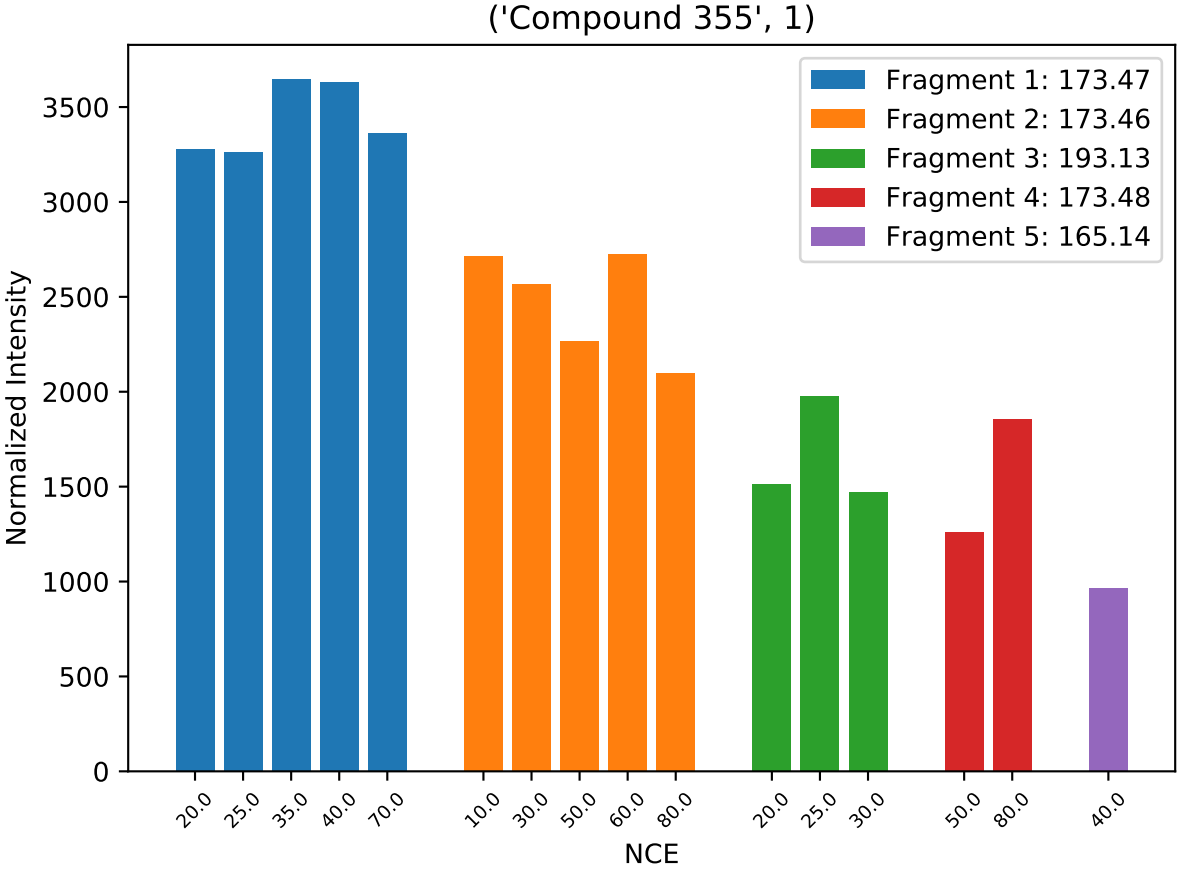

('Compound 345', 1)
Fragment 1: 340.88
Fragment 2: 173.48
Fragment 3: 173.47
Fragment 4: 173.46
Fragment 5: 128.95
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

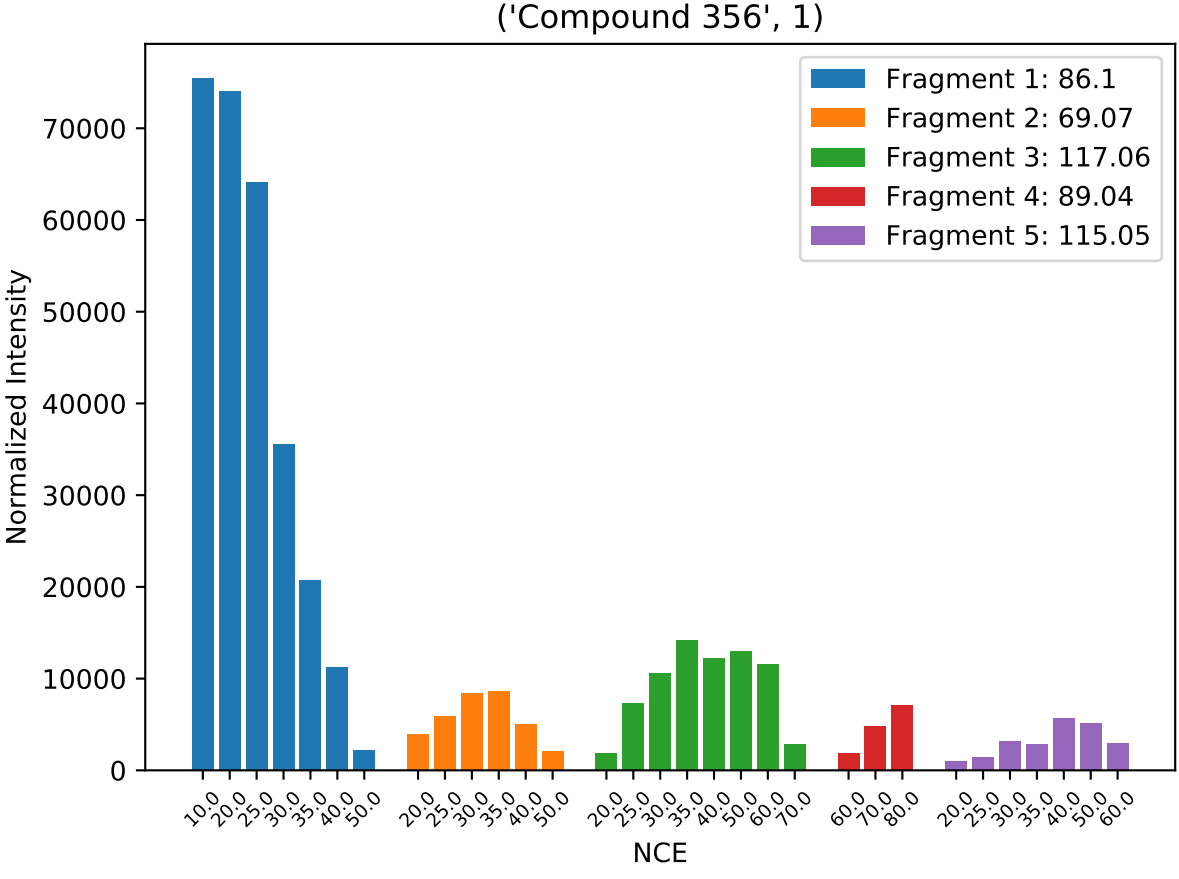

('Compound 346', 1)
Fragment 1: 131.05
Fragment 2: 235.02
Fragment 3: 131.04
Fragment 4: 85.04
Fragment 5: 177.03
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

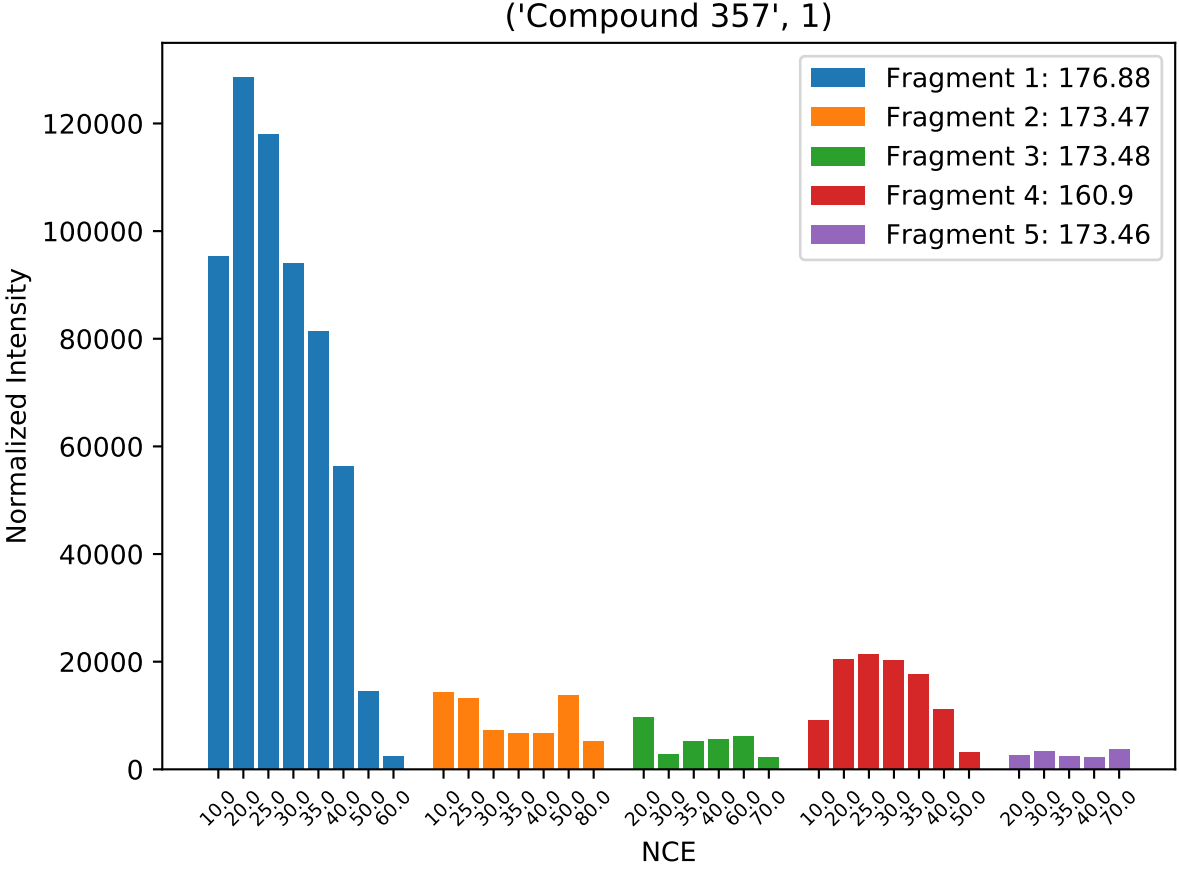

('Compound 348', 1)
Fragment 1: 446.85
Fragment 2: 173.47
Fragment 3: 340.88
Fragment 4: 173.48
Fragment 5: 128.95
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

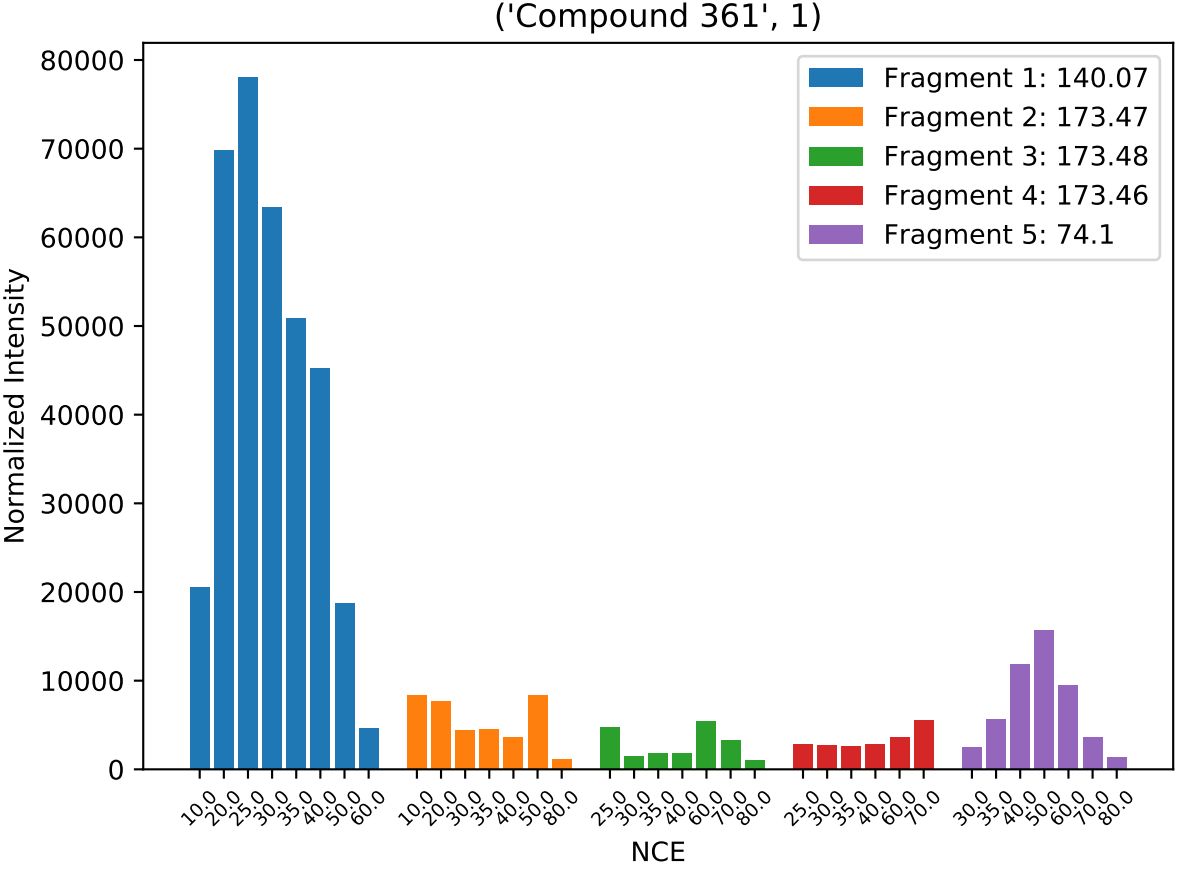

('Compound 350', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 173.48
Fragment 4: 270.06
Fragment 5: 228.05
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0
25.0
35.0
60.0
70.0
20.0
30.0
40.0
50.0
30.0
40.0
80.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
NCE

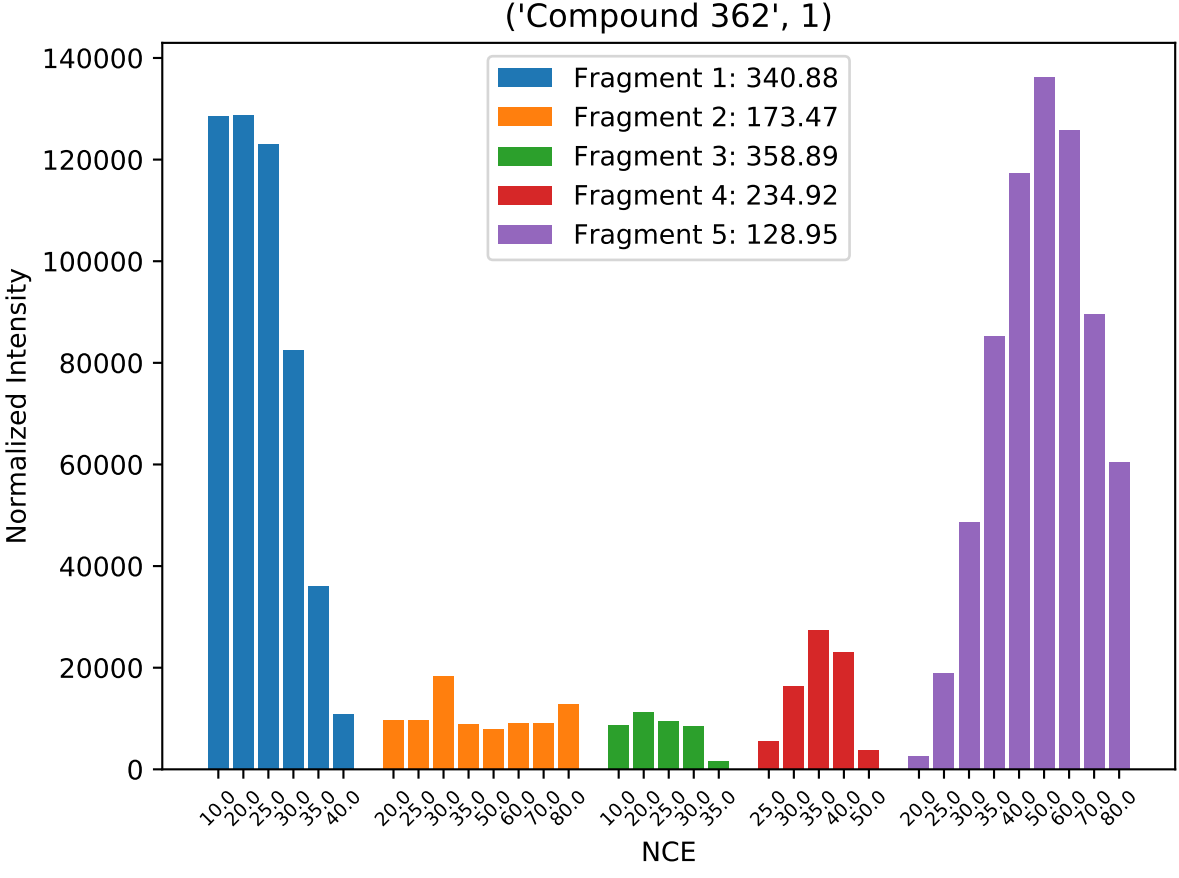

('Compound 351', 1)
Fragment 1: 552.81
Fragment 2: 614.81
Fragment 3: 583.81
Fragment 4: 128.95
Fragment 5: 446.85
Normalized Intensity
0
100000
200000
300000
400000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
NCE

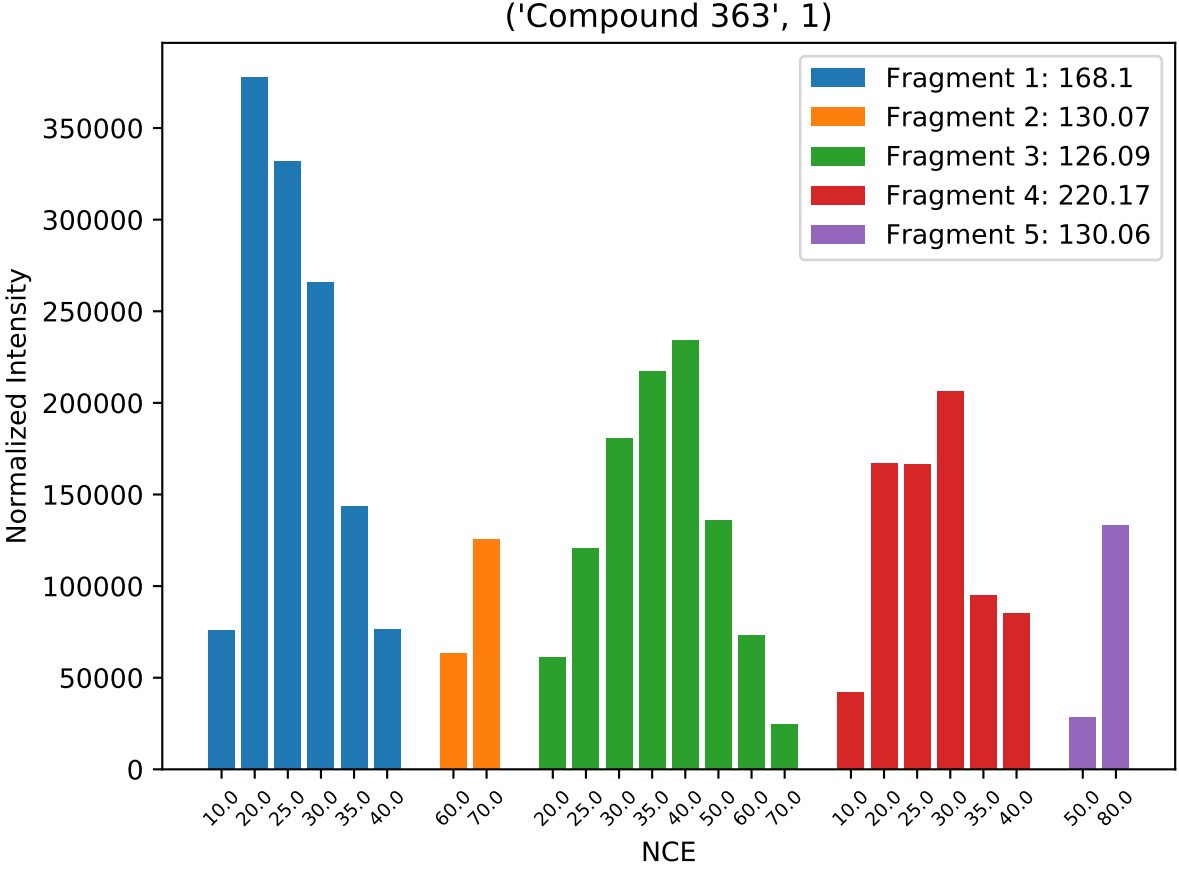

('Compound 355', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 193.13
Fragment 4: 173.48
Fragment 5: 165.14
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
20.0
25.0
35.0
40.0
70.0
10.0
30.0
50.0
60.0
80.0
20.0
25.0
30.0
50.0
80.0
40.0
NCE

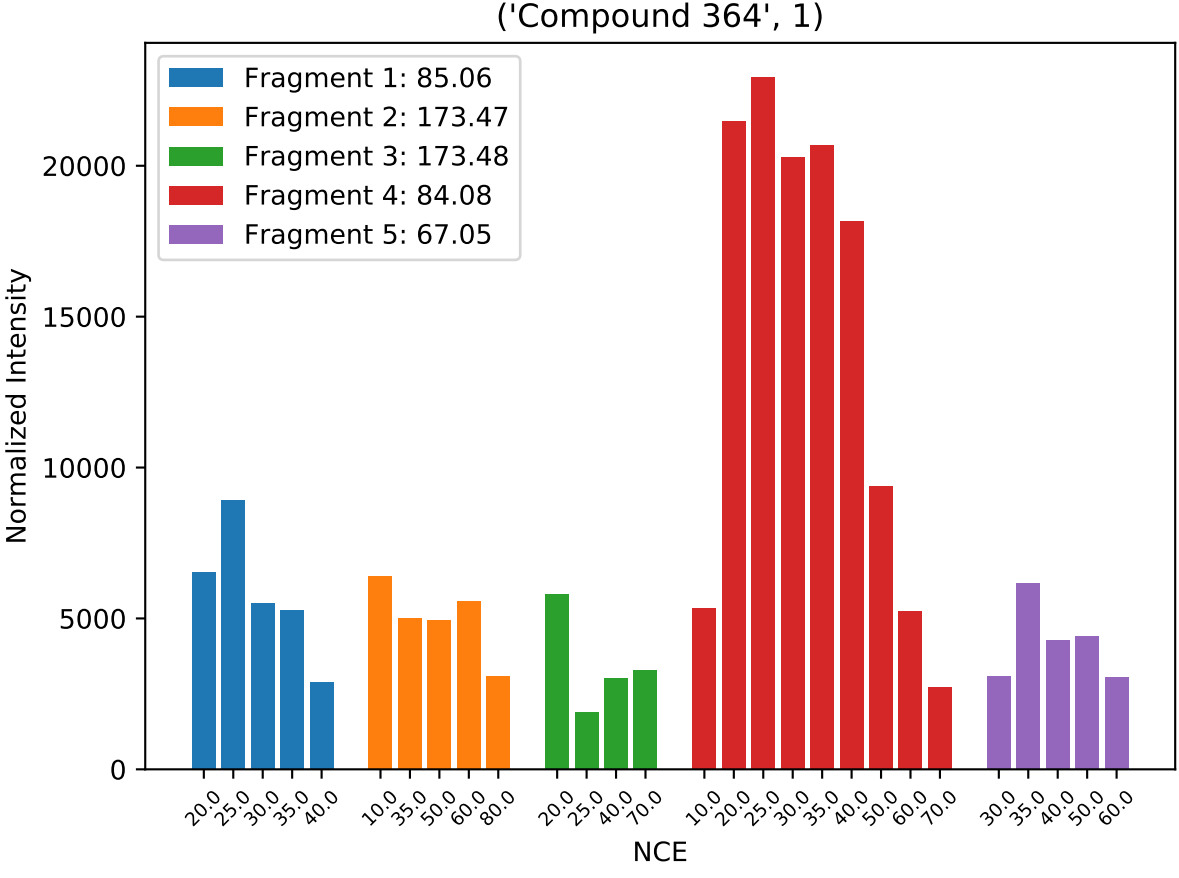

('Compound 356', 1)
Fragment 1: 86.1
Fragment 2: 69.07
Fragment 3: 117.06
Fragment 4: 89.04
Fragment 5: 115.05
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

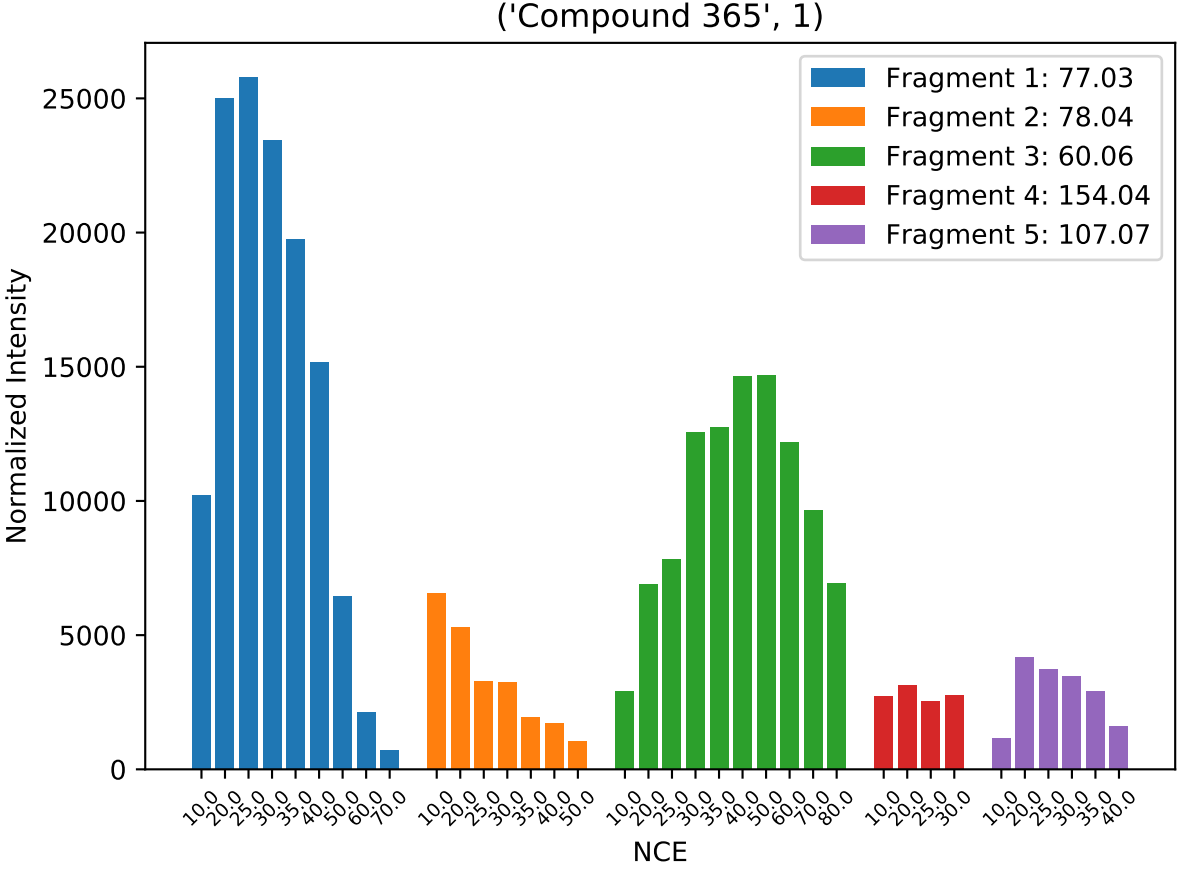

('Compound 357', 1)
Fragment 1: 176.88
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 160.9
Fragment 5: 173.46
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
25.0
30.0
35.0
40.0
50.0
80.0
20.0
30.0
35.0
40.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
30.0
35.0
40.0
70.0
NCE

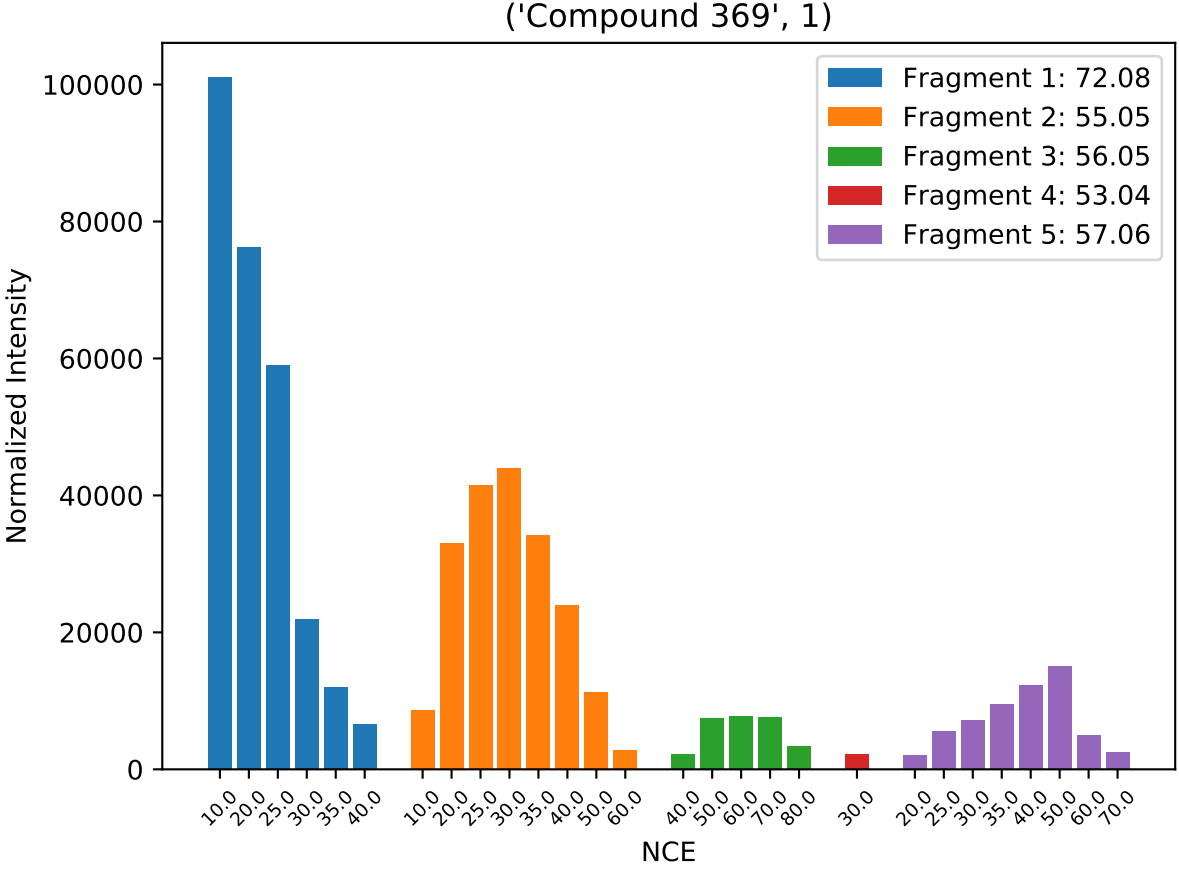

('Compound 361', 1)
Fragment 1: 140.07
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 74.1
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
30.0
35.0
40.0
50.0
80.0
25.0
30.0
35.0
40.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
60.0
70.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

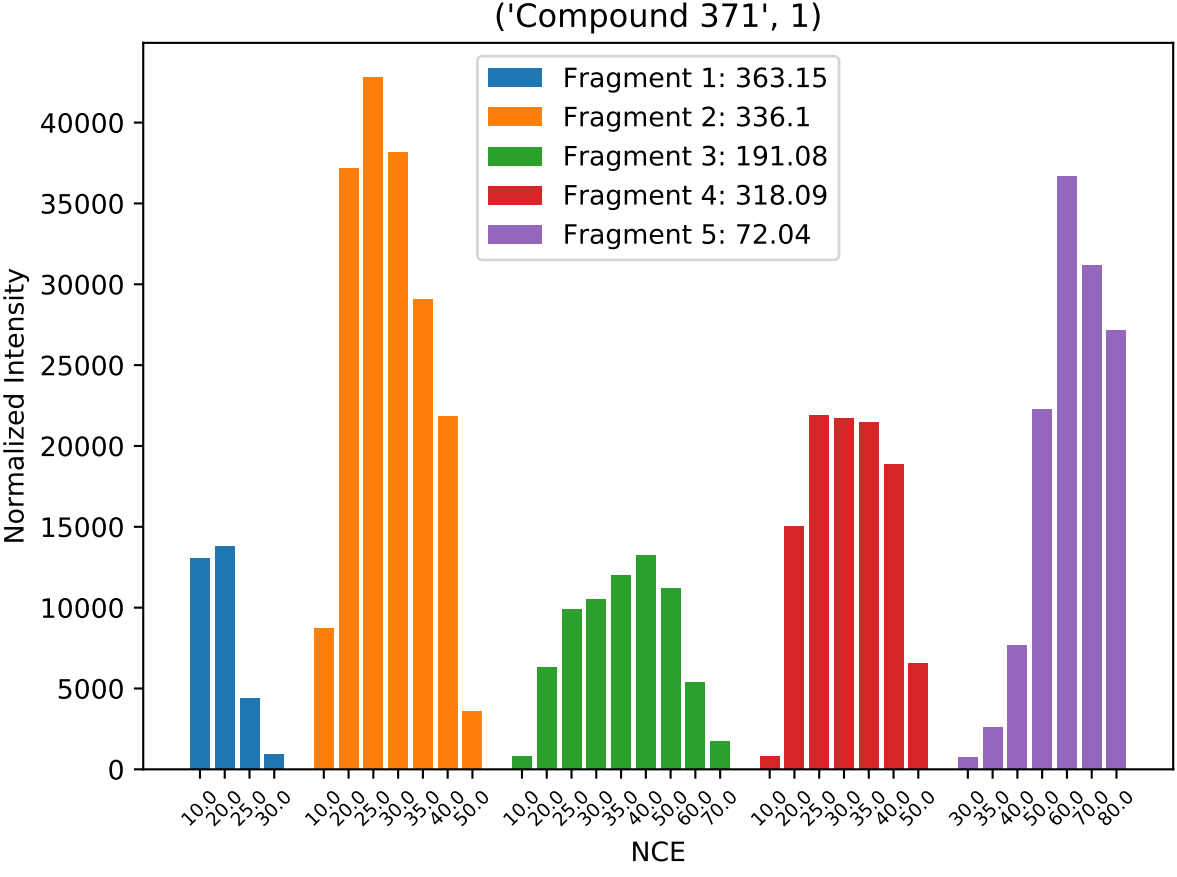

('Compound 362', 1)
Fragment 1: 340.88
Fragment 2: 173.47
Fragment 3: 358.89
Fragment 4: 234.92
Fragment 5: 128.95
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

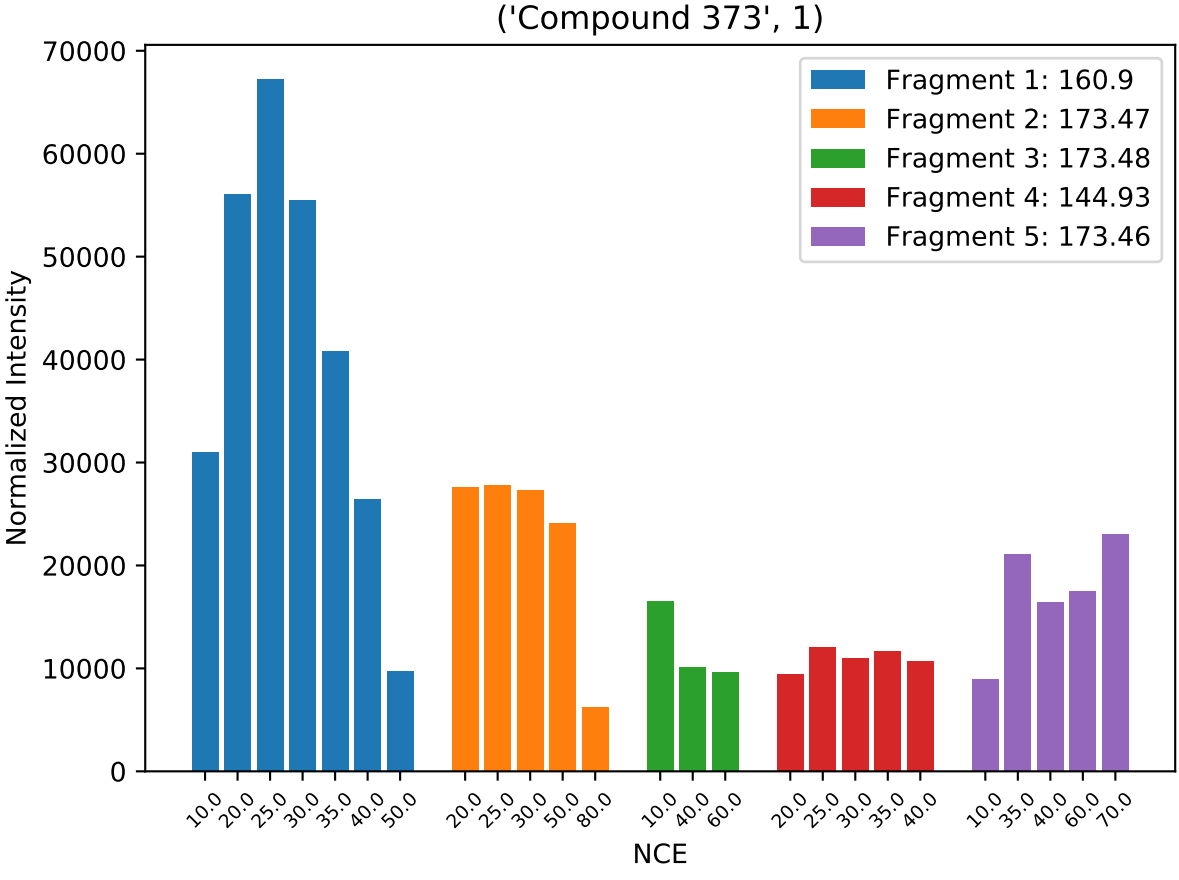

('Compound 363', 1)
Fragment 1: 168.1
Fragment 2: 130.07
Fragment 3: 126.09
Fragment 4: 220.17
Fragment 5: 130.06
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
10.0
20.0
25.0
30.0
35.0
40.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
80.0
NCE

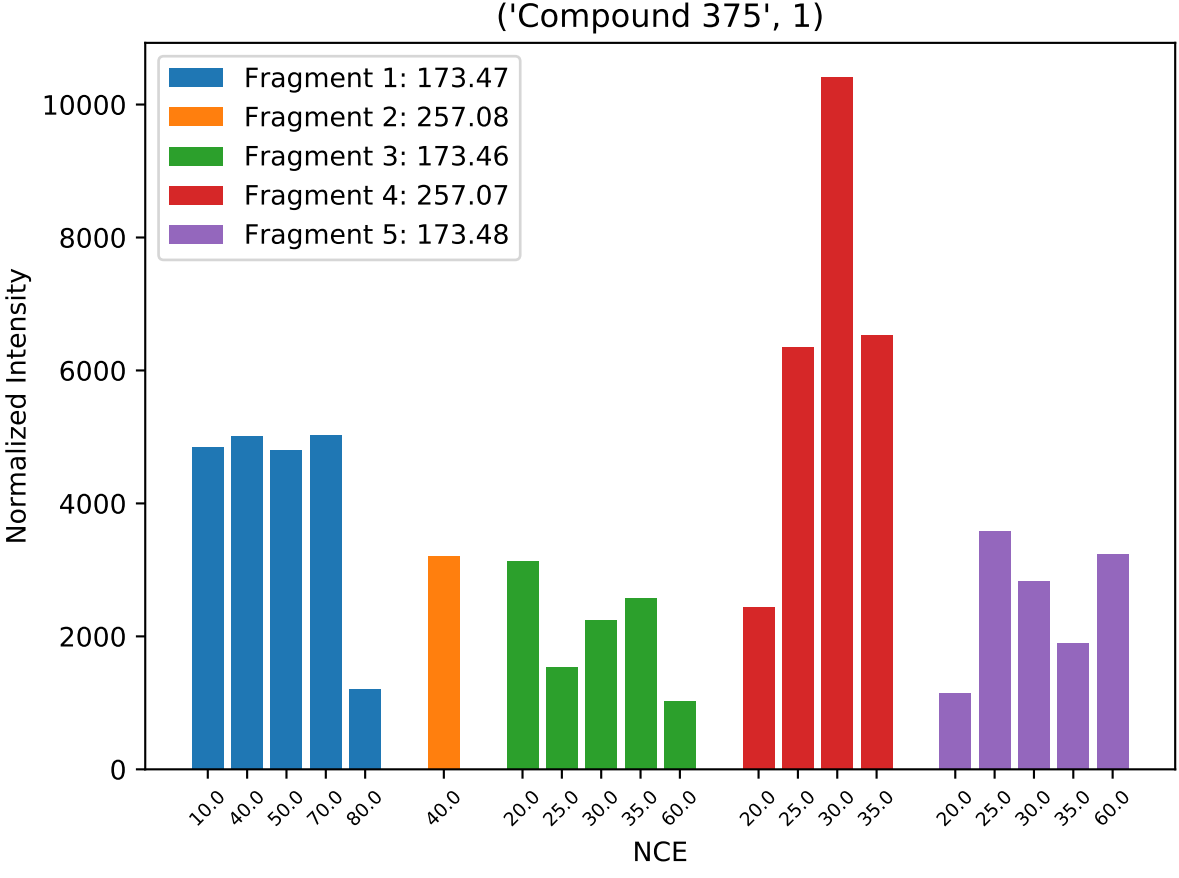

('Compound 364', 1)
Fragment 1: 85.06
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 84.08
Fragment 5: 67.05
Normalized Intensity
0
5000
10000
15000
20000
20.0 25.0 30.0 35.0 40.0
10.0 35.0 50.0 60.0 80.0
20.0 25.0 40.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0
NCE

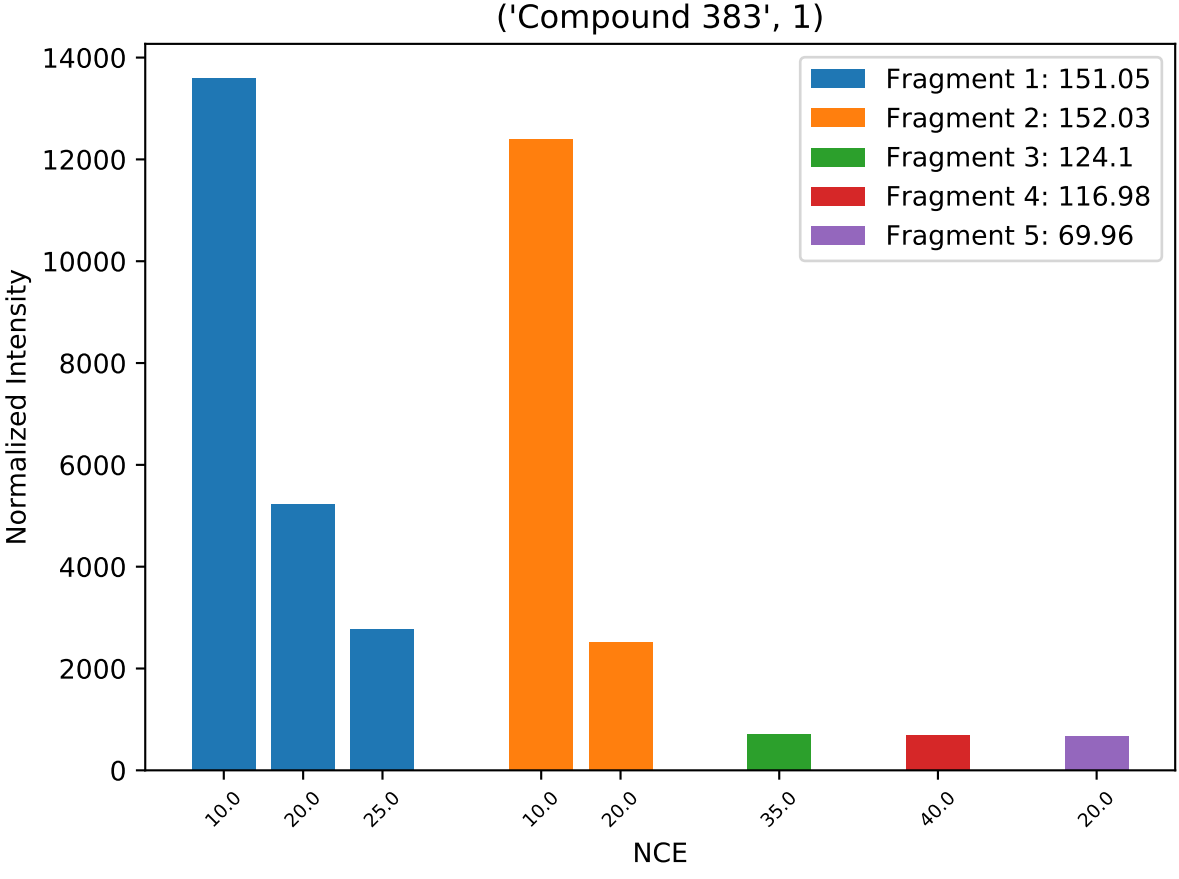

('Compound 365', 1)
Fragment 1: 77.03
Fragment 2: 78.04
Fragment 3: 60.06
Fragment 4: 154.04
Fragment 5: 107.07
Normalized Intensity
0
5000
10000
15000
20000
25000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0

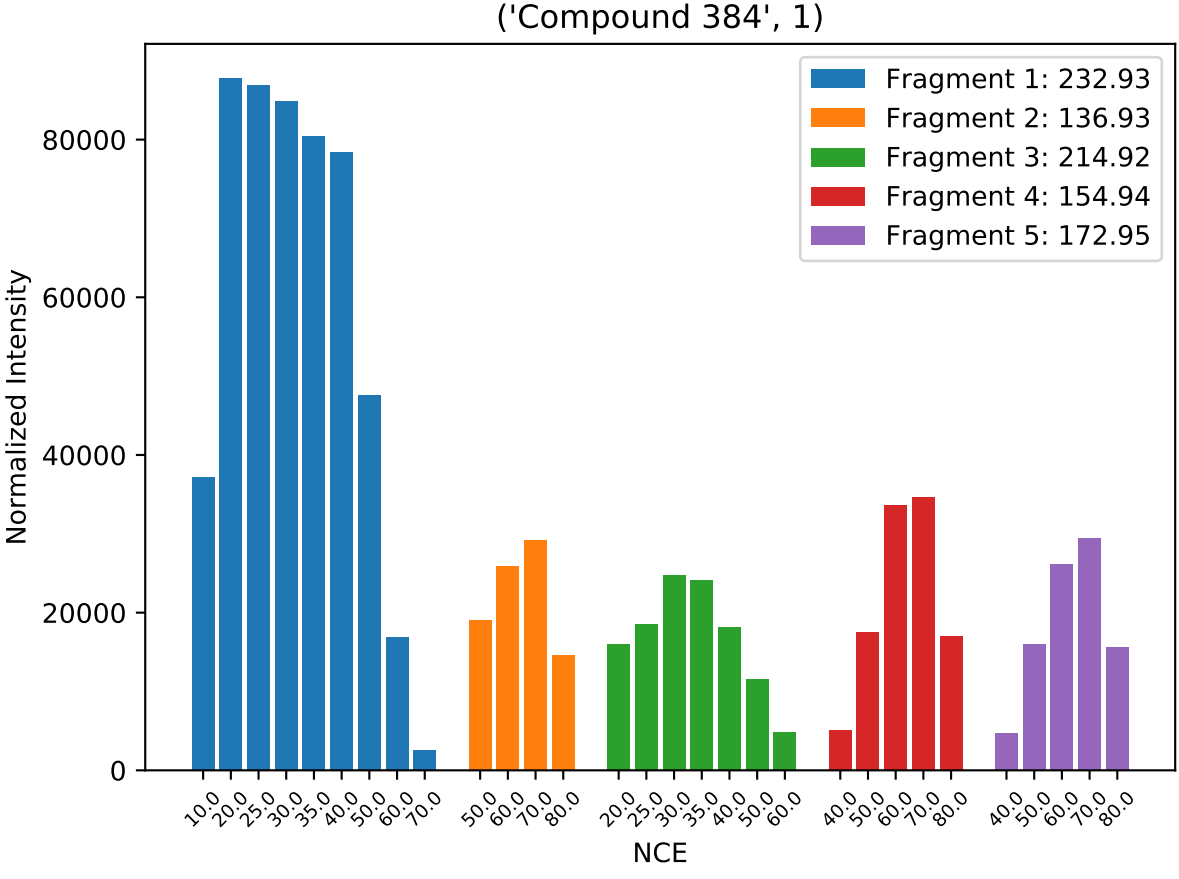

('Compound 369', 1)
Fragment 1: 72.08
Fragment 2: 55.05
Fragment 3: 56.05
Fragment 4: 53.04
Fragment 5: 57.06
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
40.0
50.0
60.0
70.0
80.0
30.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

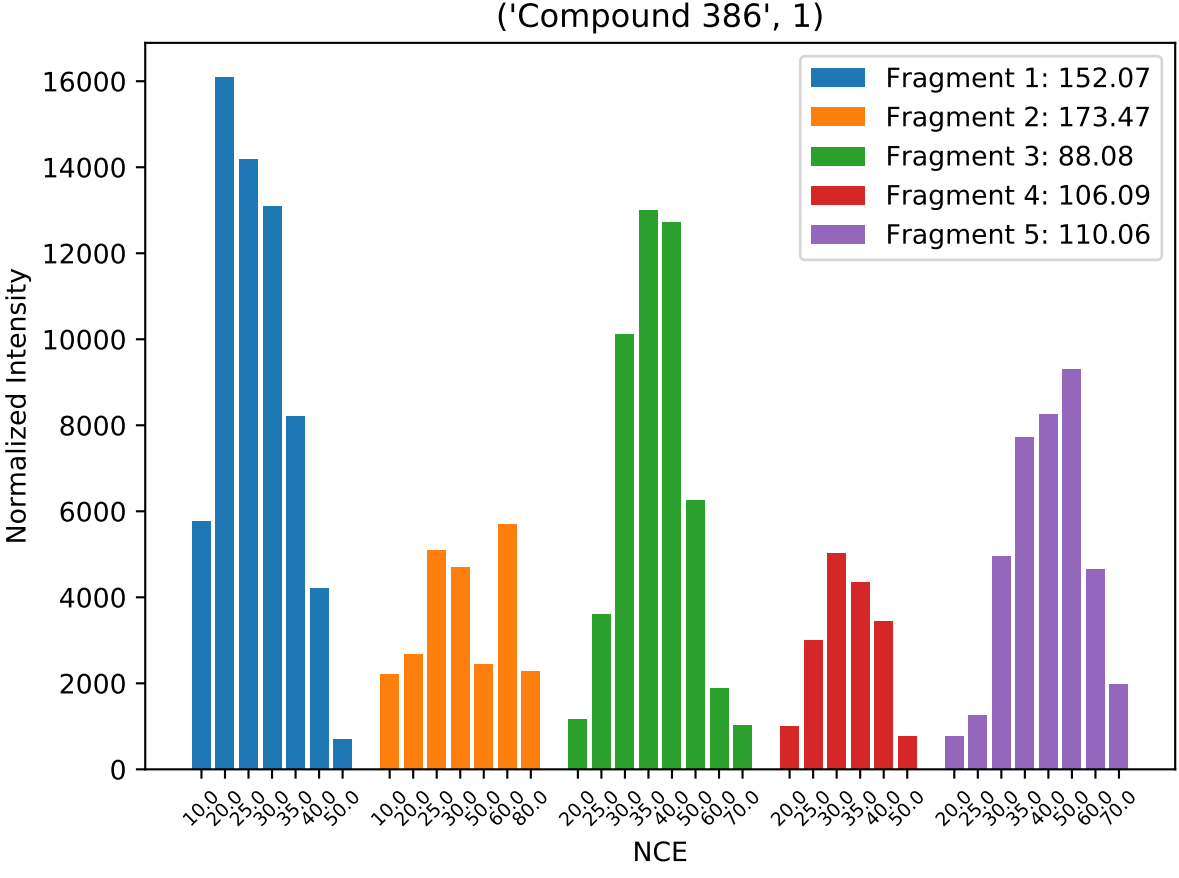

('Compound 371', 1)
Fragment 1: 363.15
Fragment 2: 336.1
Fragment 3: 191.08
Fragment 4: 318.09
Fragment 5: 72.04
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

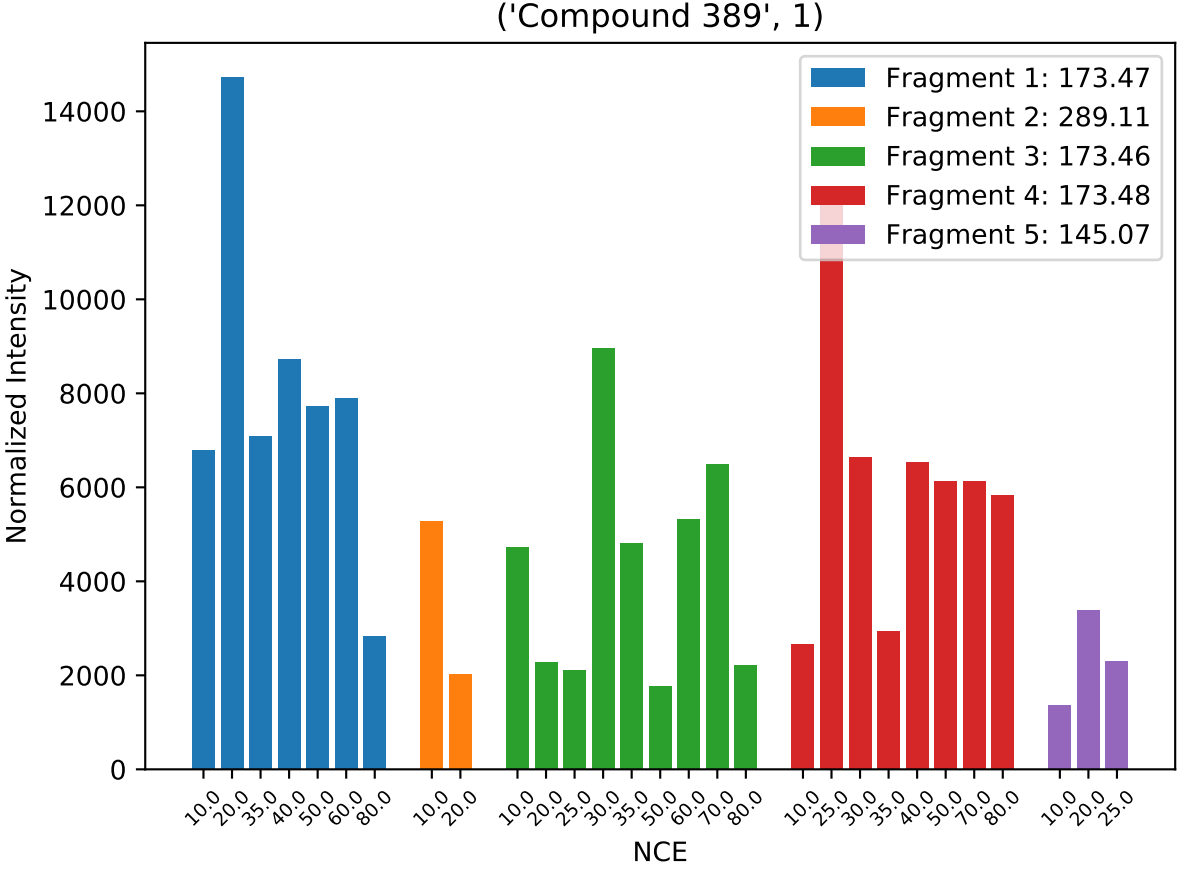

('Compound 373', 1)
Fragment 1: 160.9
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 144.93
Fragment 5: 173.46
Normalized Intensity
70000
60000
50000
40000
30000
20000
10000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
50.0
80.0
10.0
40.0
60.0
20.0
25.0
30.0
35.0
40.0
10.0
35.0
40.0
60.0
70.0
NCE

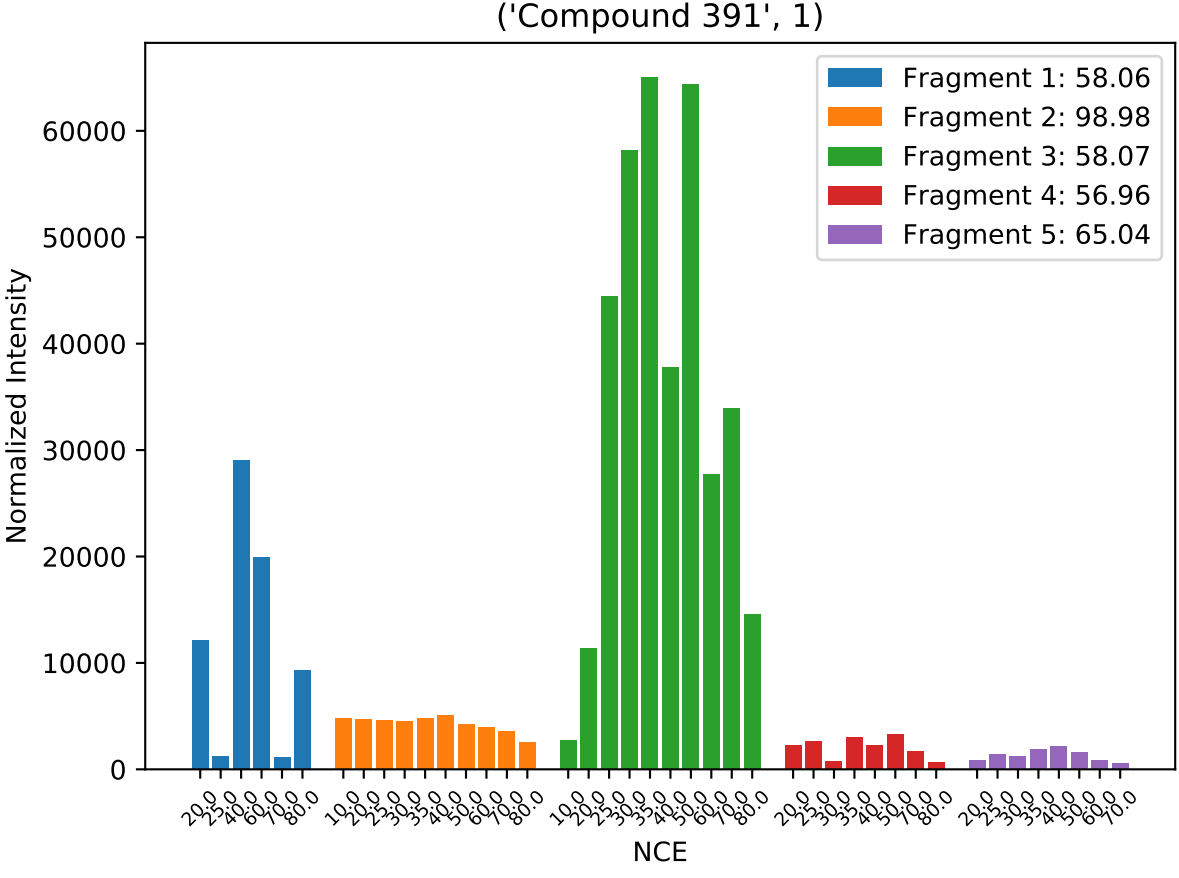

('Compound 375', 1)
Fragment 1: 173.47
Fragment 2: 257.08
Fragment 3: 173.46
Fragment 4: 257.07
Fragment 5: 173.48
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
40.0
50.0
70.0
80.0
40.0
20.0
25.0
30.0
35.0
60.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
35.0
60.0
NCE

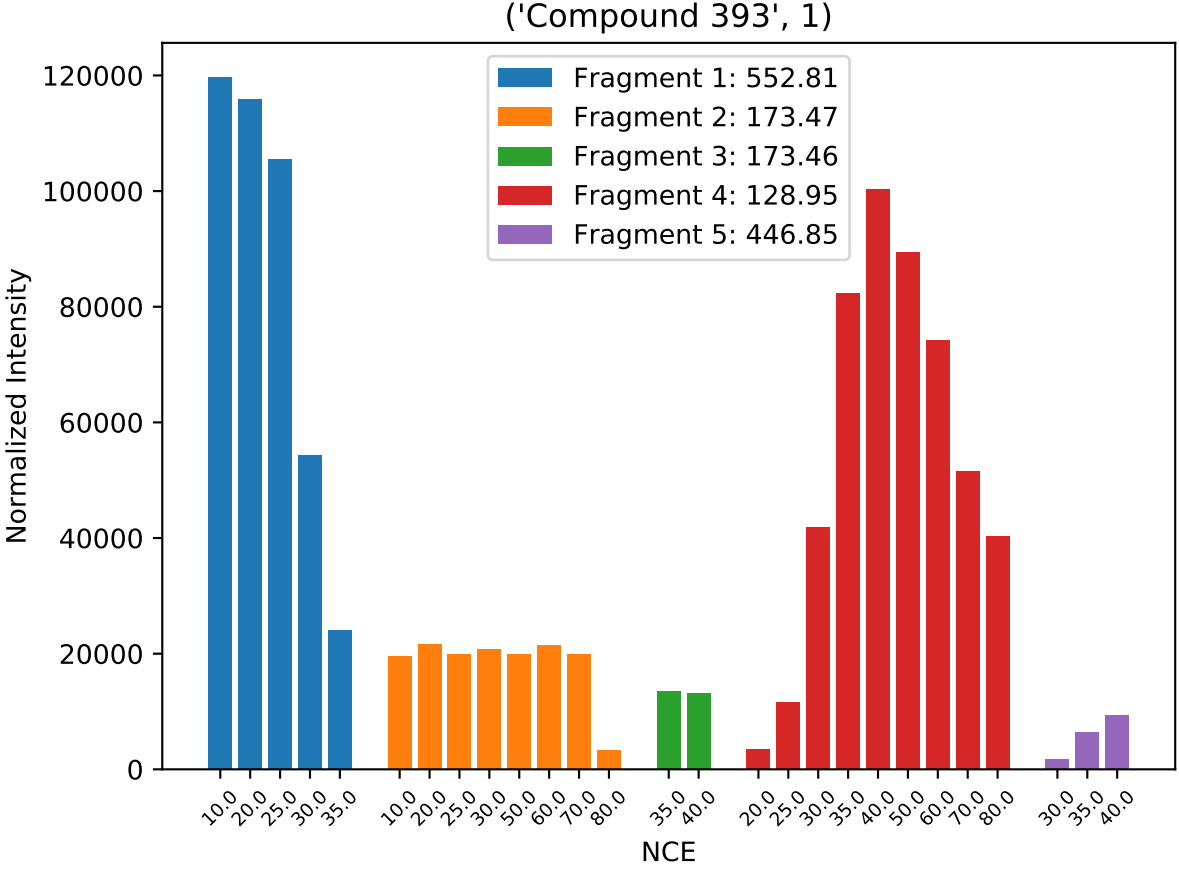

('Compound 383', 1)
Fragment 1: 151.05
Fragment 2: 152.03
Fragment 3: 124.1
Fragment 4: 116.98
Fragment 5: 69.96
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
25.0
10.0
20.0
35.0
40.0
20.0
NCE

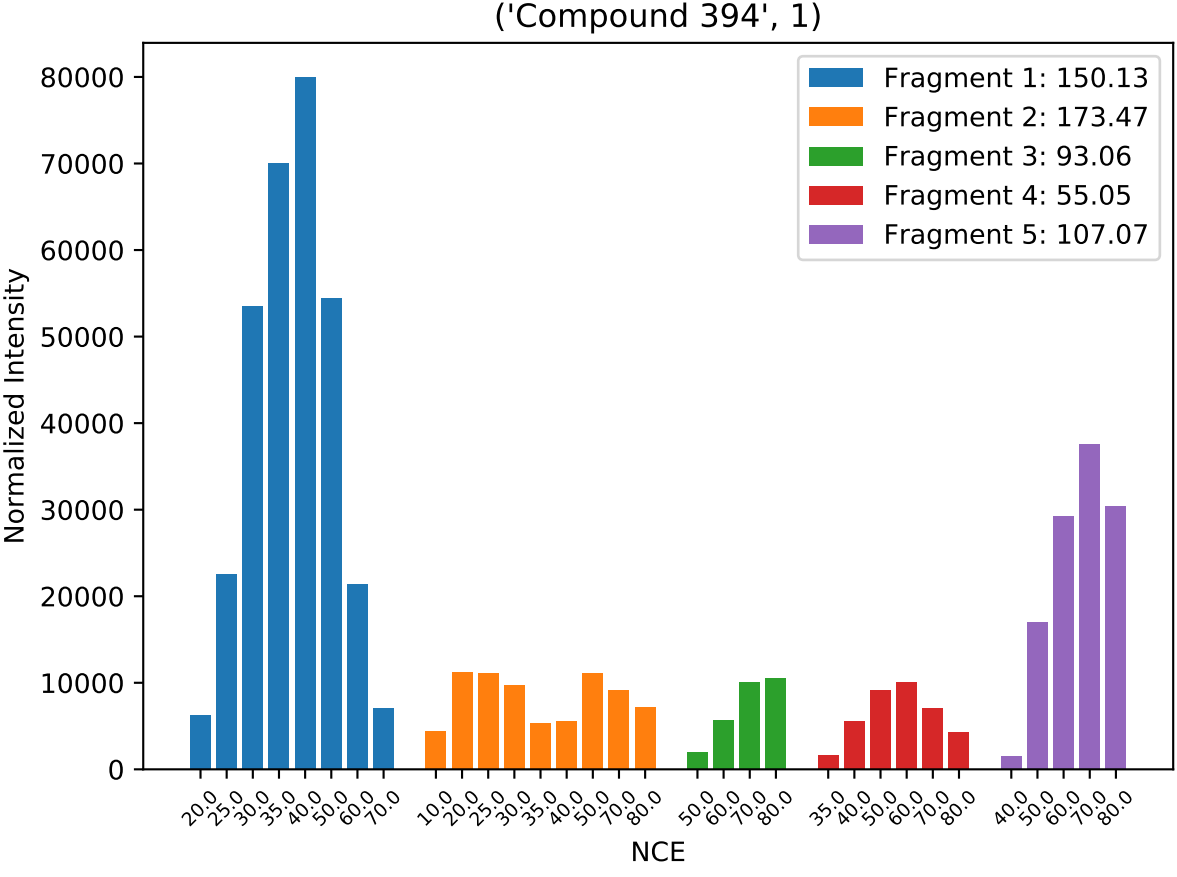

('Compound 384', 1)
Fragment 1: 232.93
Fragment 2: 136.93
Fragment 3: 214.92
Fragment 4: 154.94
Fragment 5: 172.95
Normalized Intensity
0
20000
40000
60000
80000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0

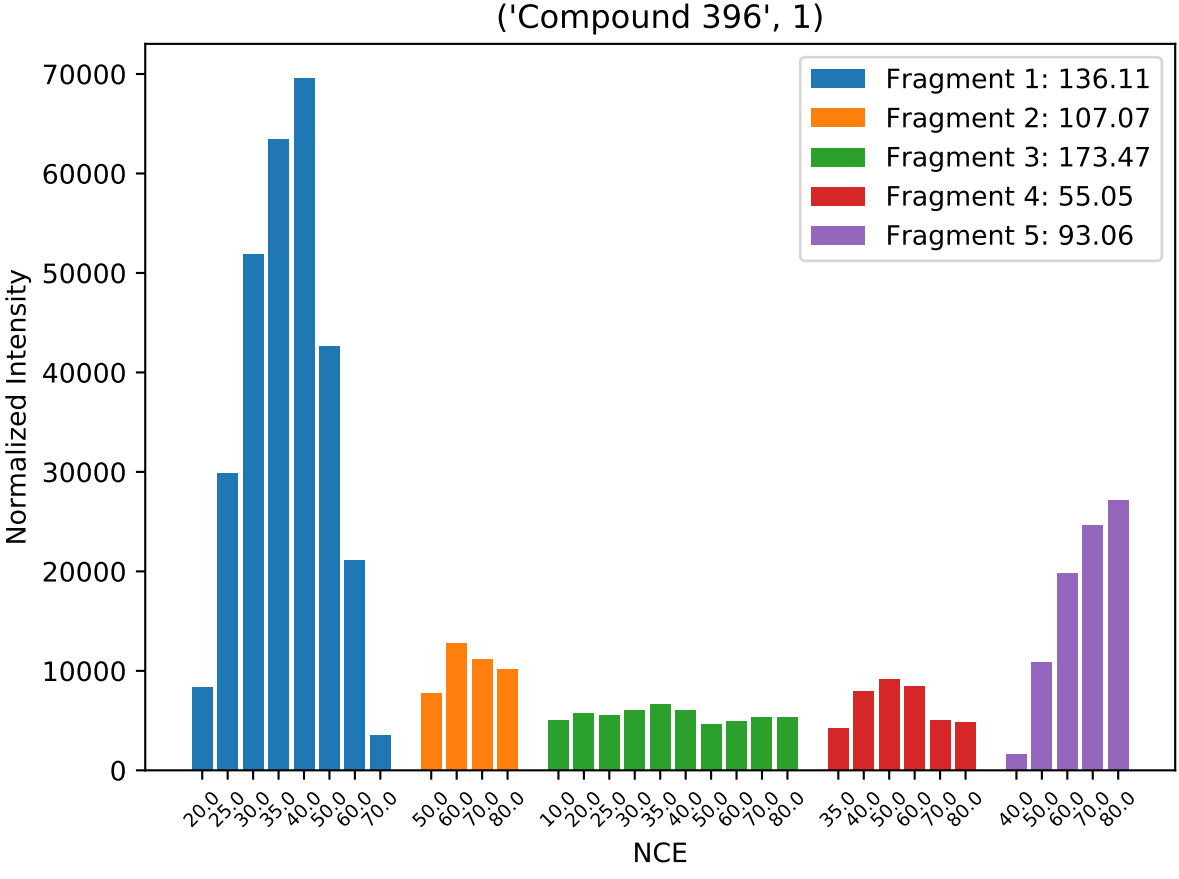

('Compound 386', 1)
Fragment 1: 152.07
Fragment 2: 173.47
Fragment 3: 88.08
Fragment 4: 106.09
Fragment 5: 110.06
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 50.0 60.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

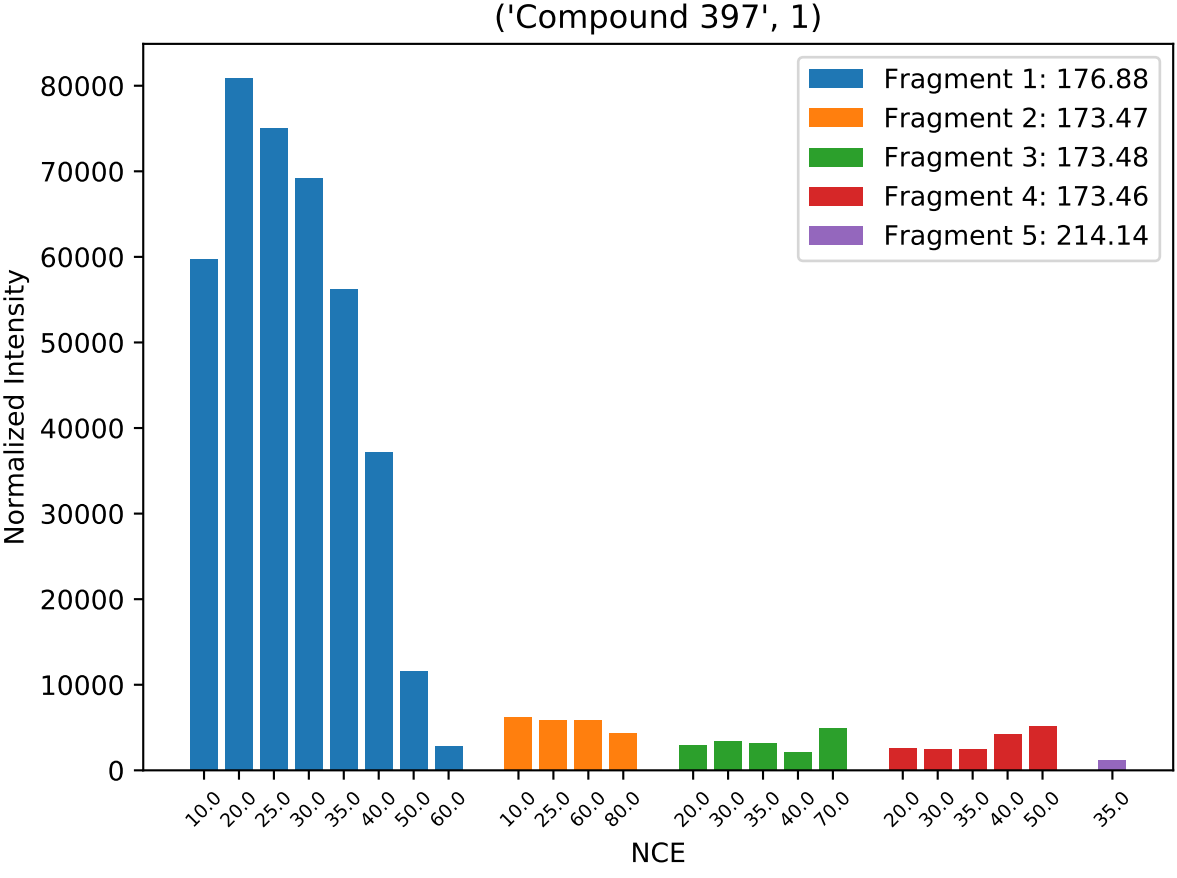

('Compound 389', 1)
Fragment 1: 173.47
Fragment 2: 289.11
Fragment 3: 173.46
Fragment 4: 173.48
Fragment 5: 145.07
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0 20.0 35.0 40.0 50.0 60.0 80.0
10.0 20.0
10.0 20.0 25.0 30.0 35.0 50.0 60.0 70.0 80.0
10.0 25.0 30.0 35.0 40.0 50.0 70.0 80.0
10.0 20.0 25.0
NCE

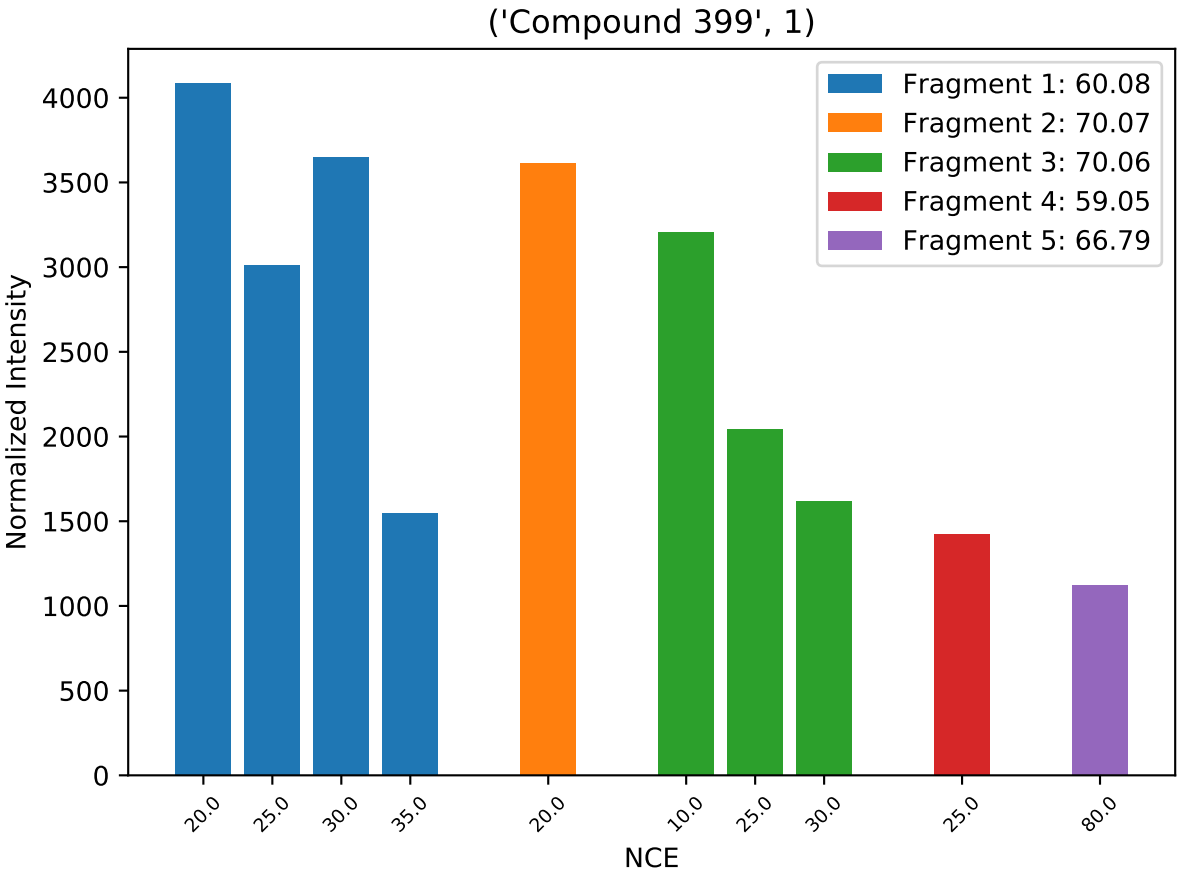

('Compound 391', 1)
Fragment 1: 58.06
Fragment 2: 98.98
Fragment 3: 58.07
Fragment 4: 56.96
Fragment 5: 65.04
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
NCE
20.0 25.0 40.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0

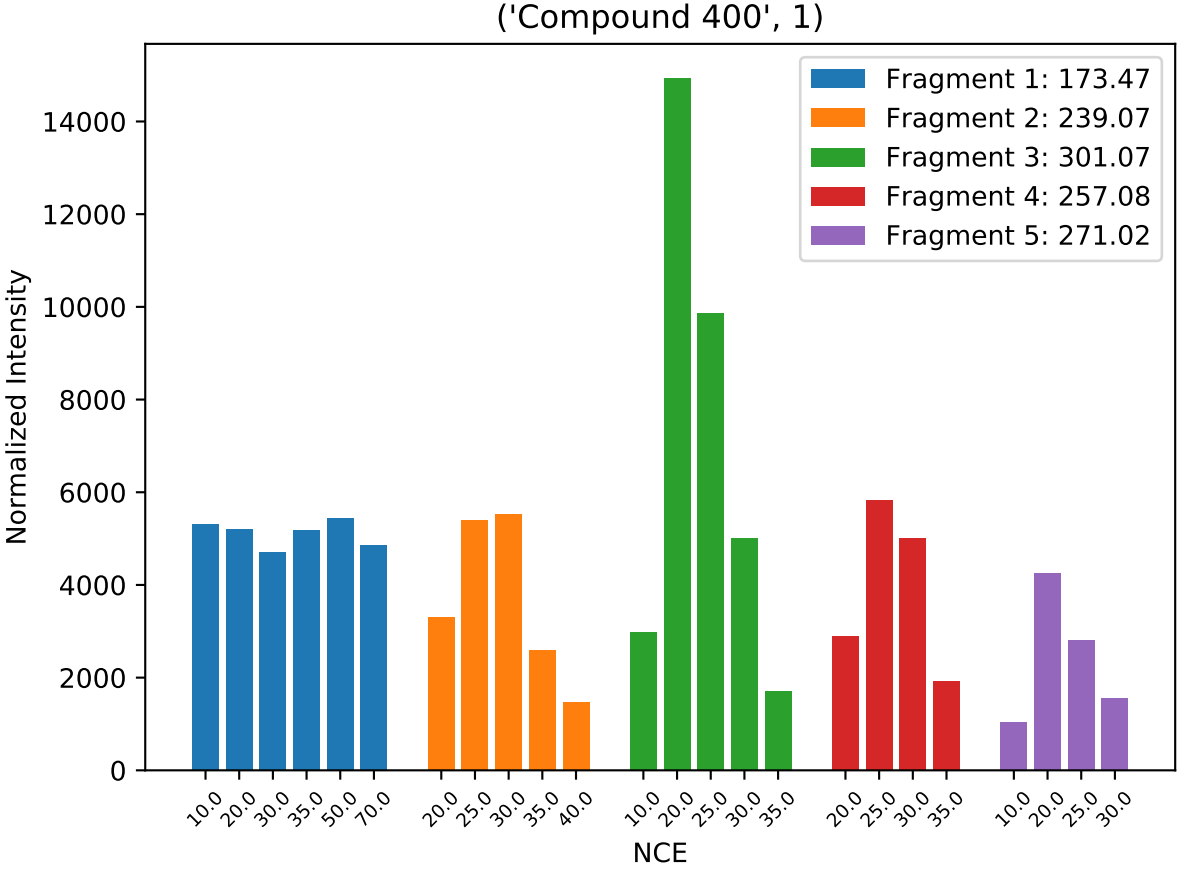

('Compound 393', 1)
Fragment 1: 552.81
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 128.95
Fragment 5: 446.85
Normalized Intensity
120000
100000
80000
60000
40000
20000
0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 50.0 60.0 70.0 80.0
35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0
NCE

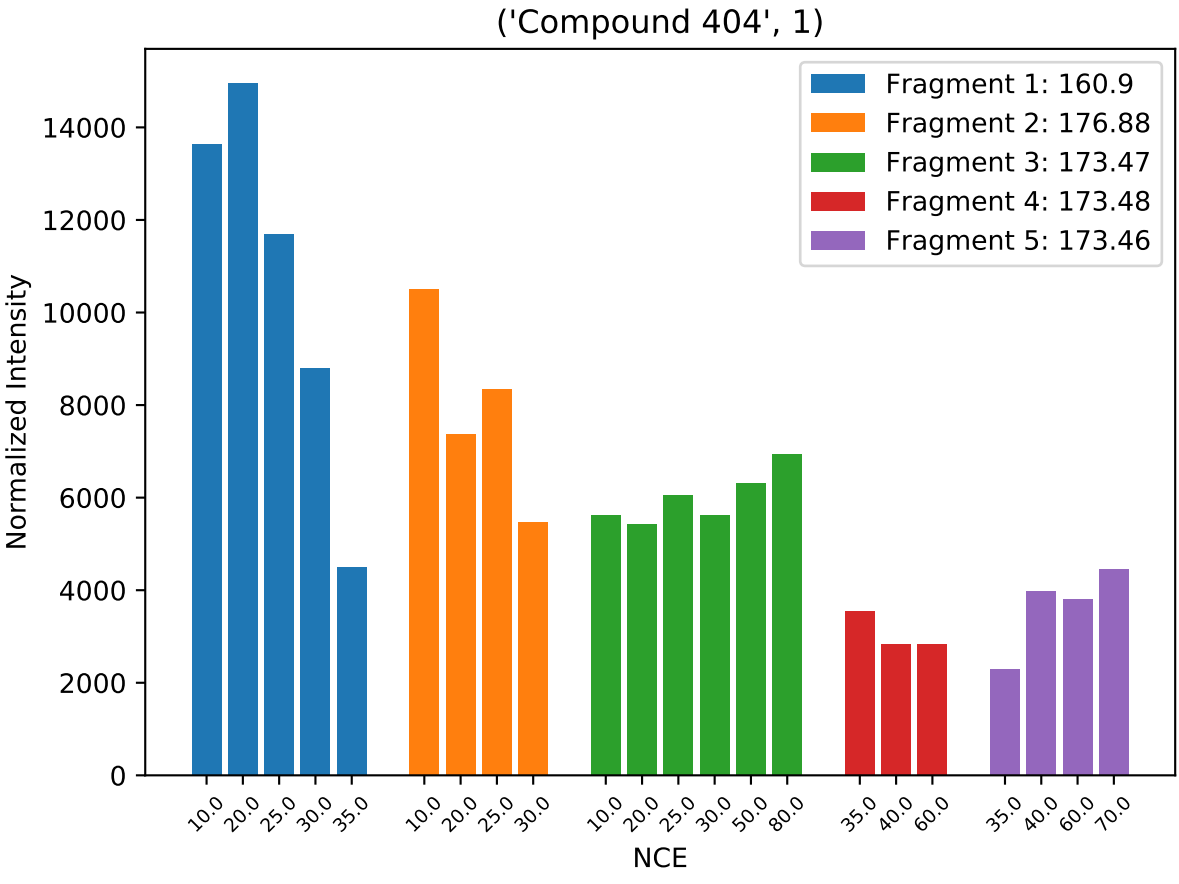

('Compound 394', 1)
Fragment 1: 150.13
Fragment 2: 173.47
Fragment 3: 93.06
Fragment 4: 55.05
Fragment 5: 107.07
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 70.0 80.0
50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
NCE

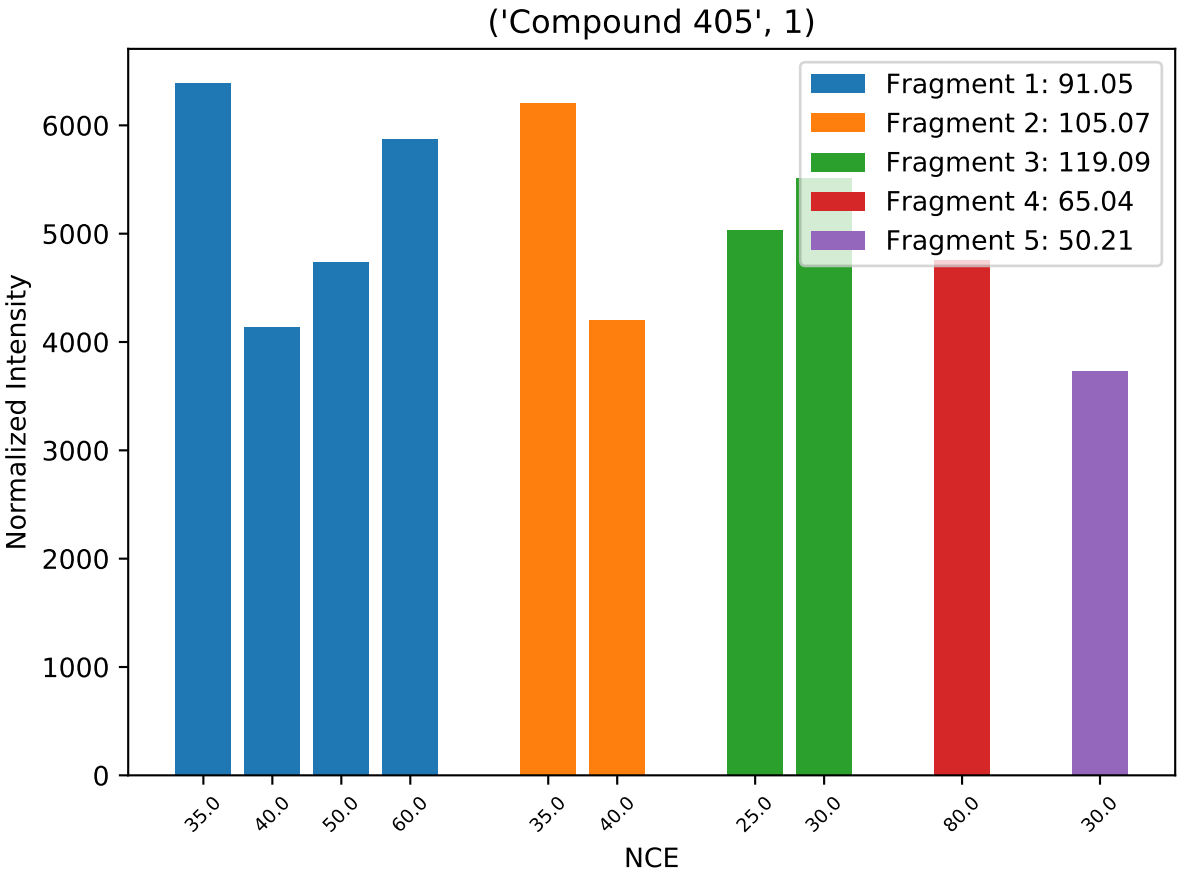

('Compound 396', 1)
Fragment 1: 136.11
Fragment 2: 107.07
Fragment 3: 173.47
Fragment 4: 55.05
Fragment 5: 93.06
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0

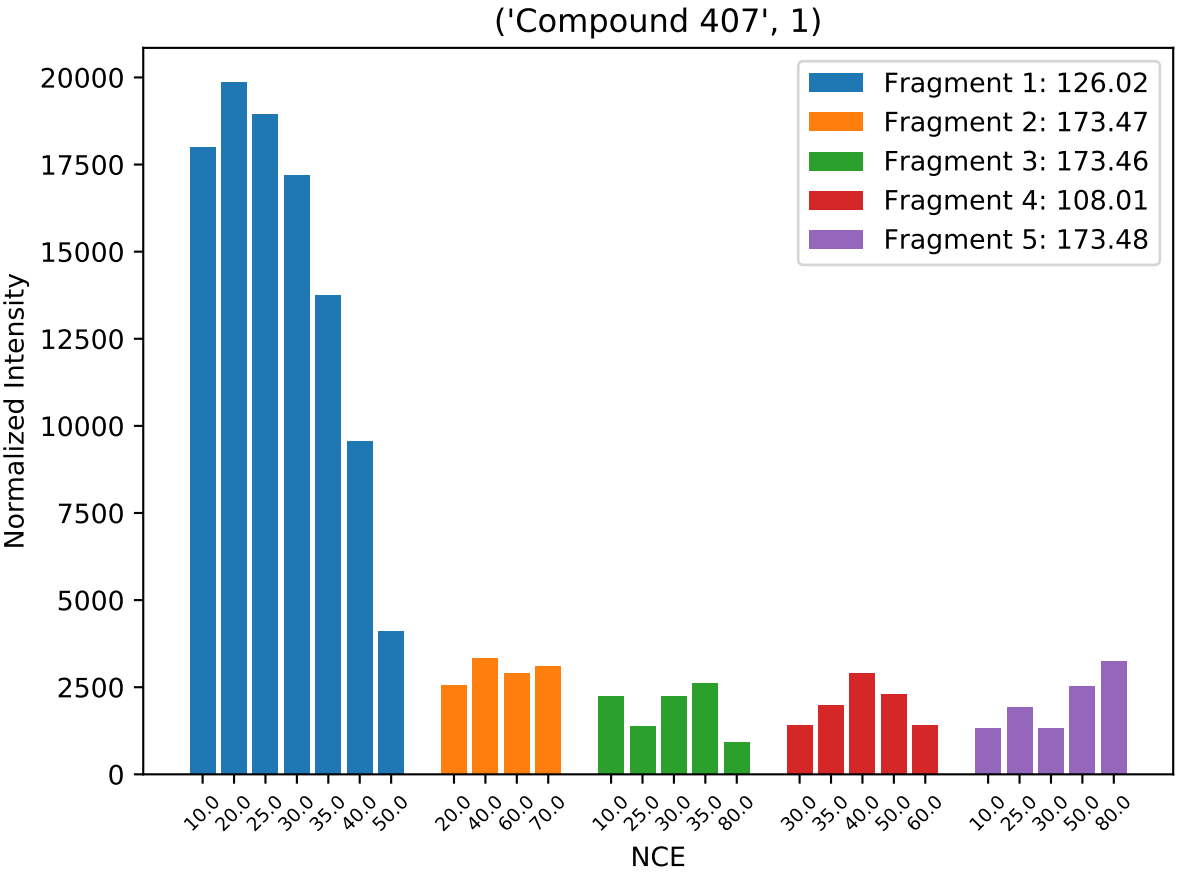

('Compound 397', 1)
Fragment 1: 176.88
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 214.14
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
25.0
60.0
80.0
20.0
30.0
35.0
40.0
70.0
20.0
30.0
35.0
40.0
50.0
35.0
NCE

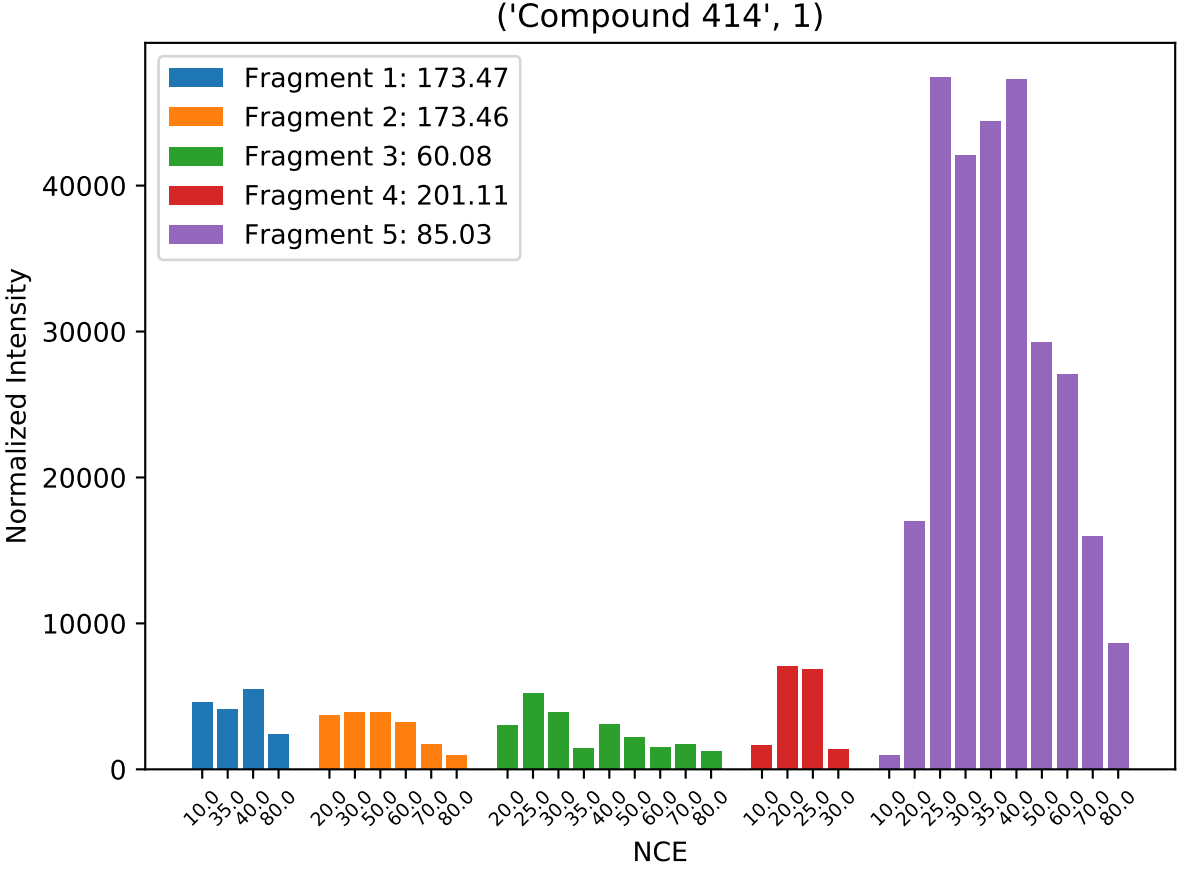

('Compound 399', 1)
Fragment 1: 60.08
Fragment 2: 70.07
Fragment 3: 70.06
Fragment 4: 59.05
Fragment 5: 66.79
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
20.0
25.0
30.0
35.0
20.0
10.0
25.0
30.0
25.0
80.0
NCE

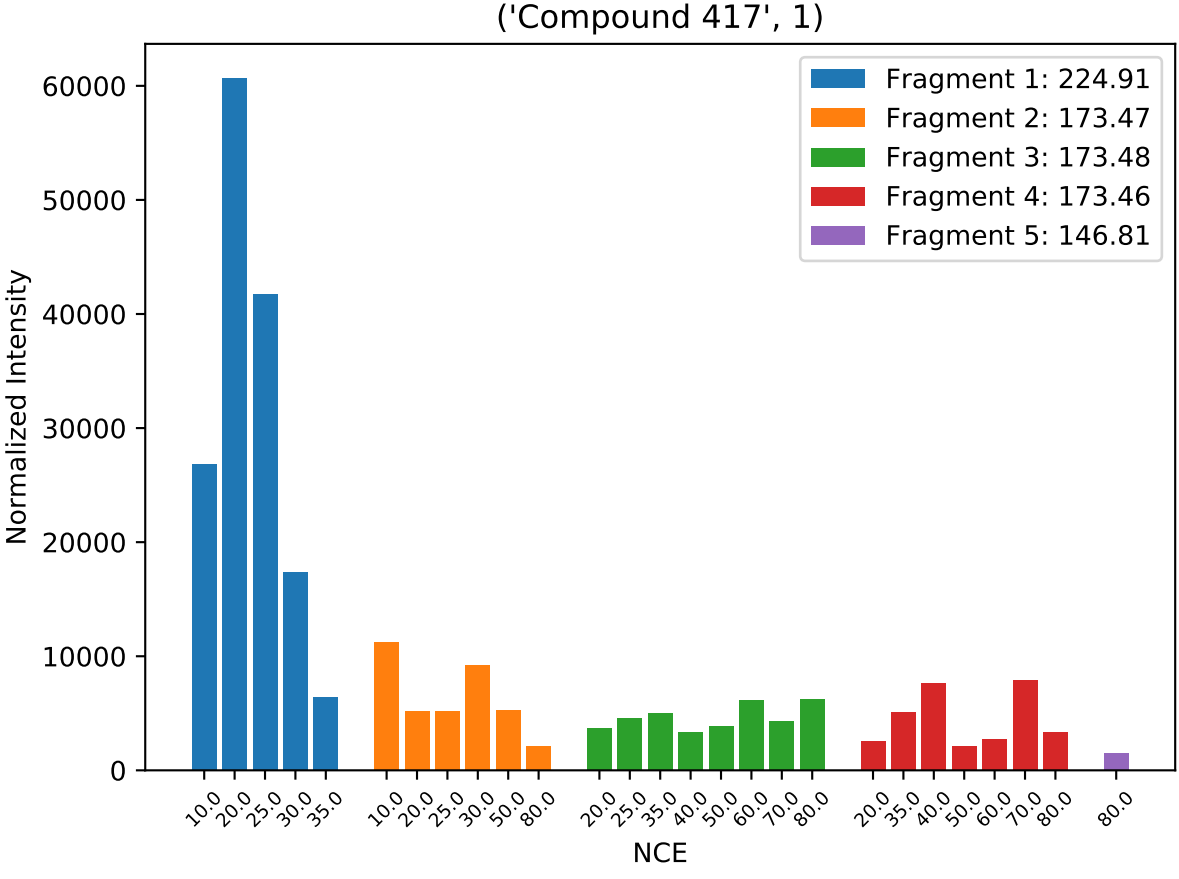

('Compound 400', 1)
Fragment 1: 173.47
Fragment 2: 239.07
Fragment 3: 301.07
Fragment 4: 257.08
Fragment 5: 271.02
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
30.0
35.0
50.0
70.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
NCE

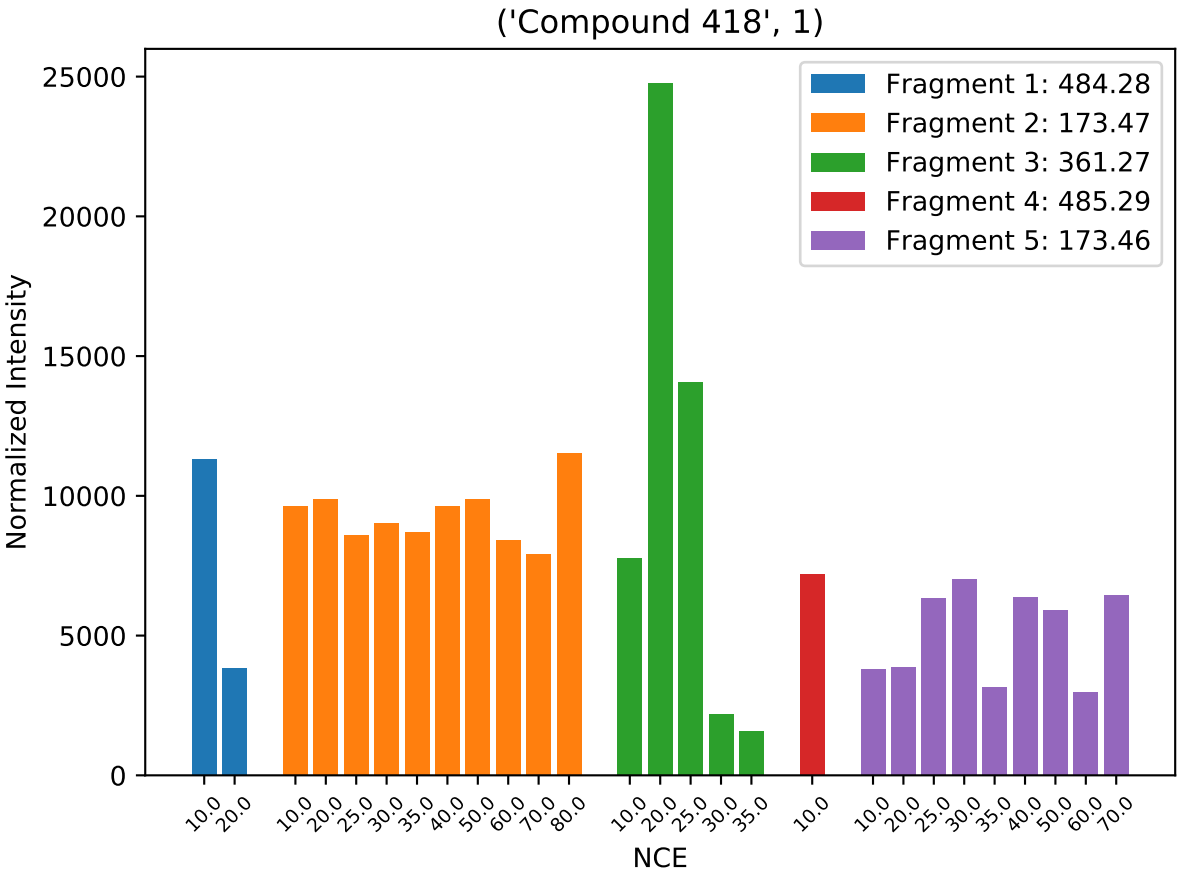

('Compound 404', 1)
Fragment 1: 160.9
Fragment 2: 176.88
Fragment 3: 173.47
Fragment 4: 173.48
Fragment 5: 173.46
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
50.0
80.0
35.0
40.0
60.0
35.0
40.0
60.0
70.0
NCE

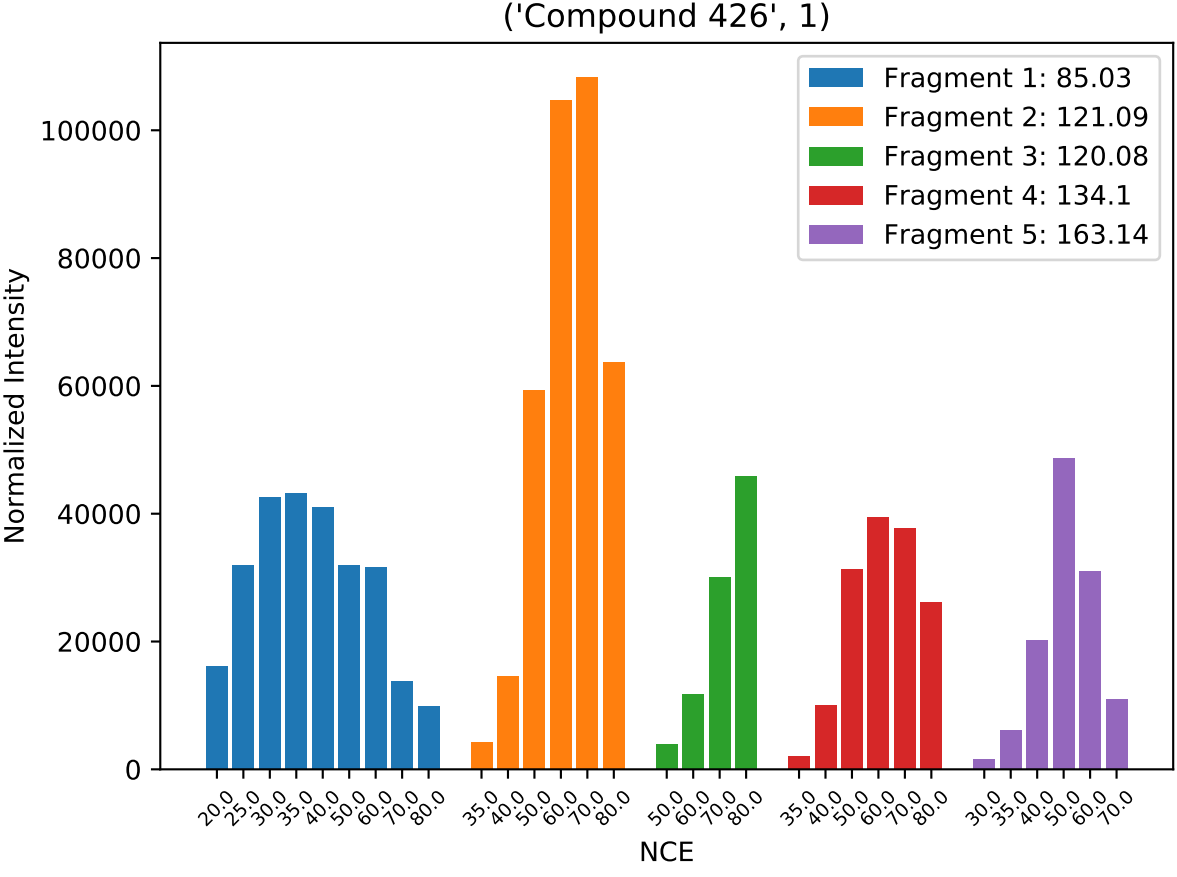

('Compound 405', 1)
Fragment 1: 91.05
Fragment 2: 105.07
Fragment 3: 119.09
Fragment 4: 65.04
Fragment 5: 50.21
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
35.0
40.0
50.0
60.0
35.0
40.0
25.0
30.0
80.0
30.0
NCE

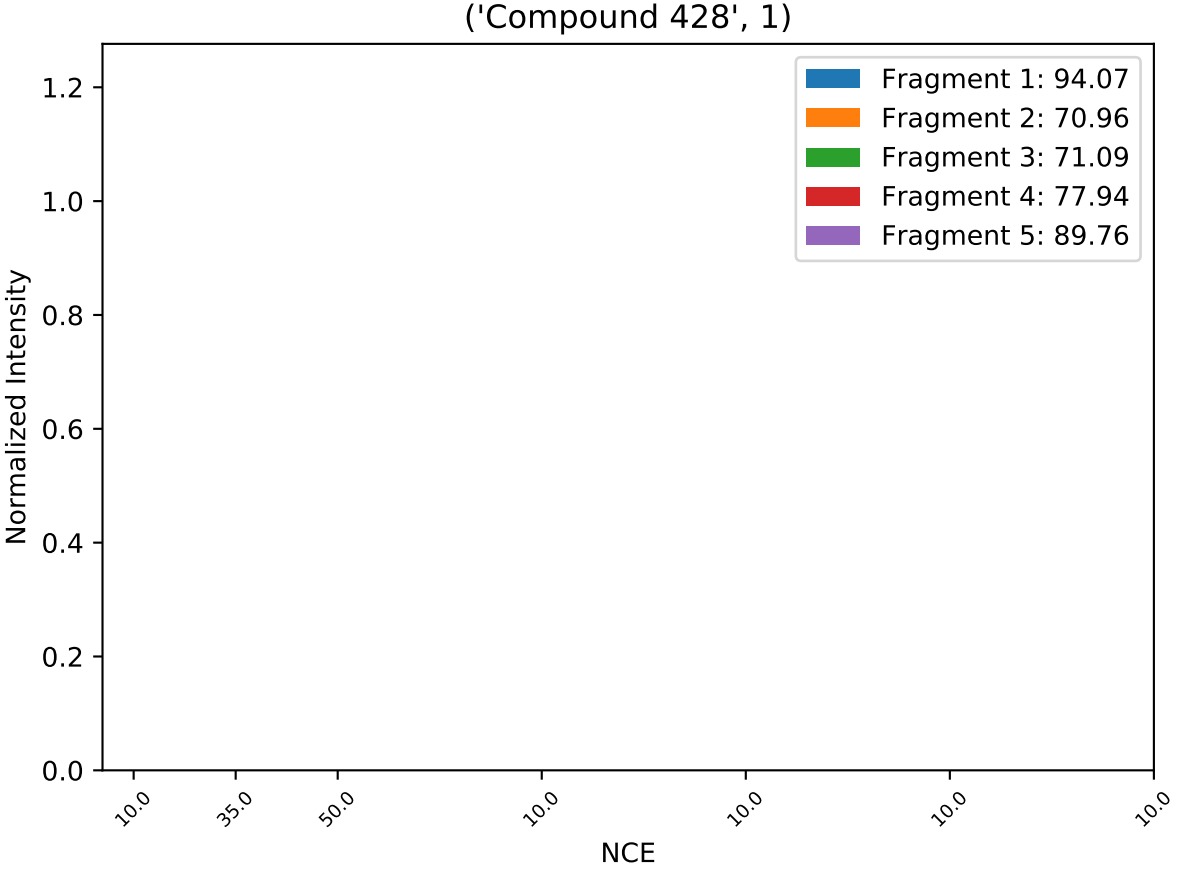

('Compound 407', 1)
Fragment 1: 126.02
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 108.01
Fragment 5: 173.48
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
40.0
60.0
70.0
10.0
25.0
30.0
35.0
80.0
30.0
35.0
40.0
50.0
60.0
10.0
25.0
30.0
50.0
80.0
NCE

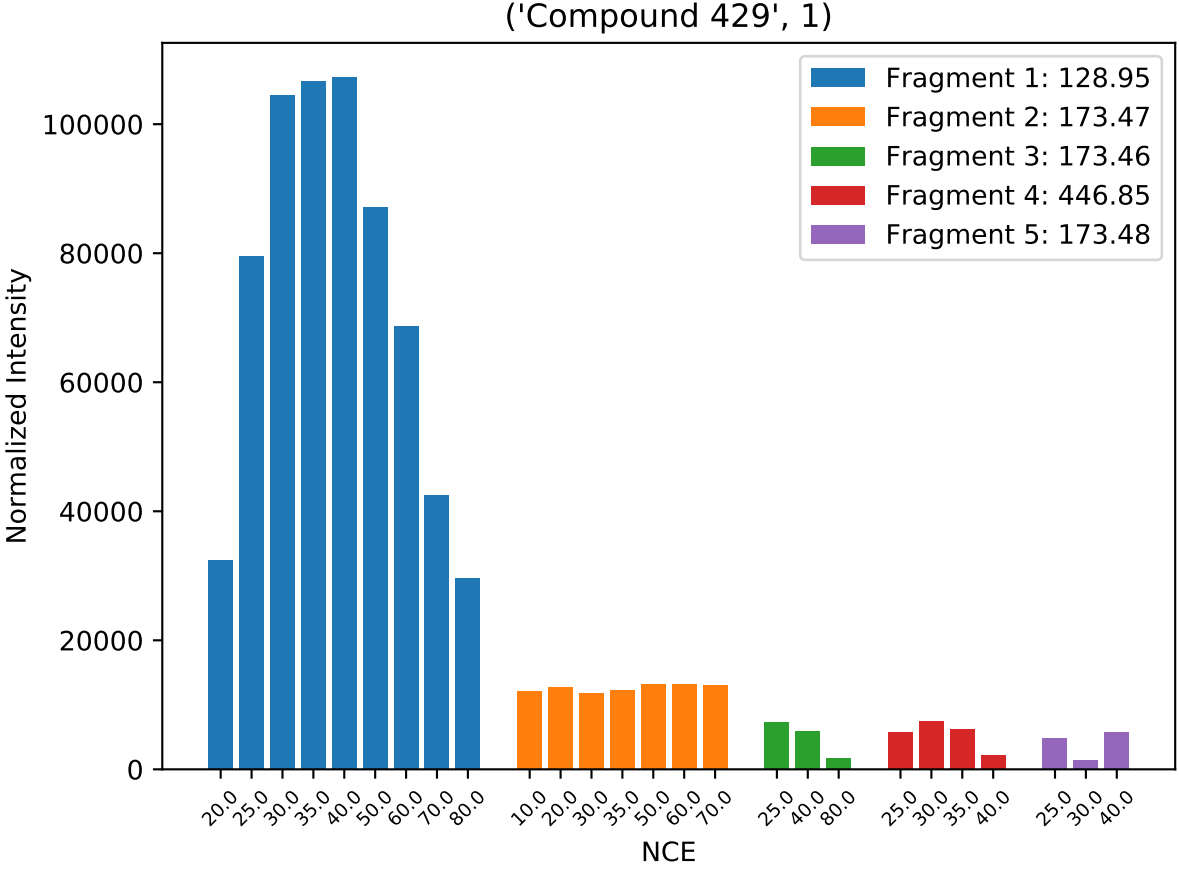

('Compound 414', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 60.08
Fragment 4: 201.11
Fragment 5: 85.03
Normalized Intensity
0
10000
20000
30000
40000
10.0 35.0 40.0 80.0
20.0 30.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

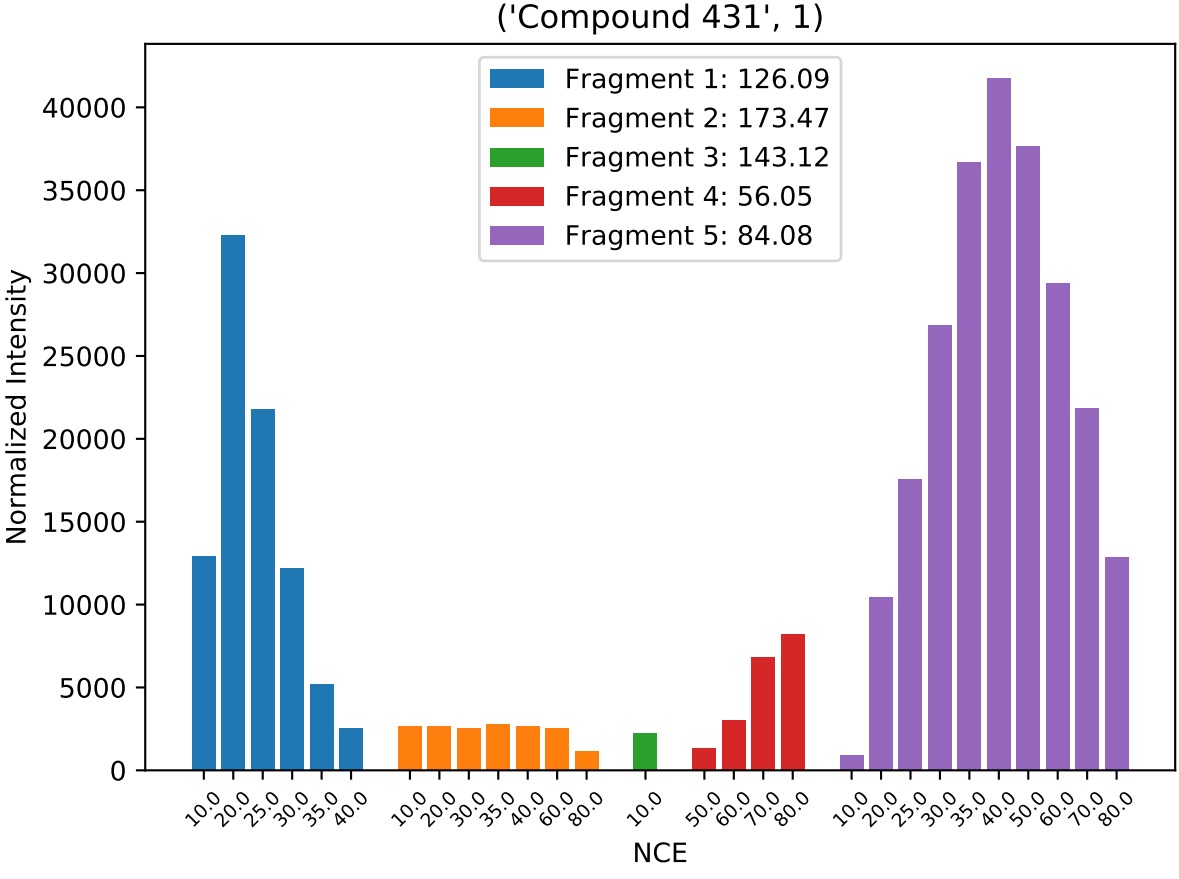

('Compound 417', 1)
Fragment 1: 224.91
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 146.81
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
50.0
80.0
20.0
25.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
35.0
40.0
50.0
60.0
70.0
80.0
80.0
NCE

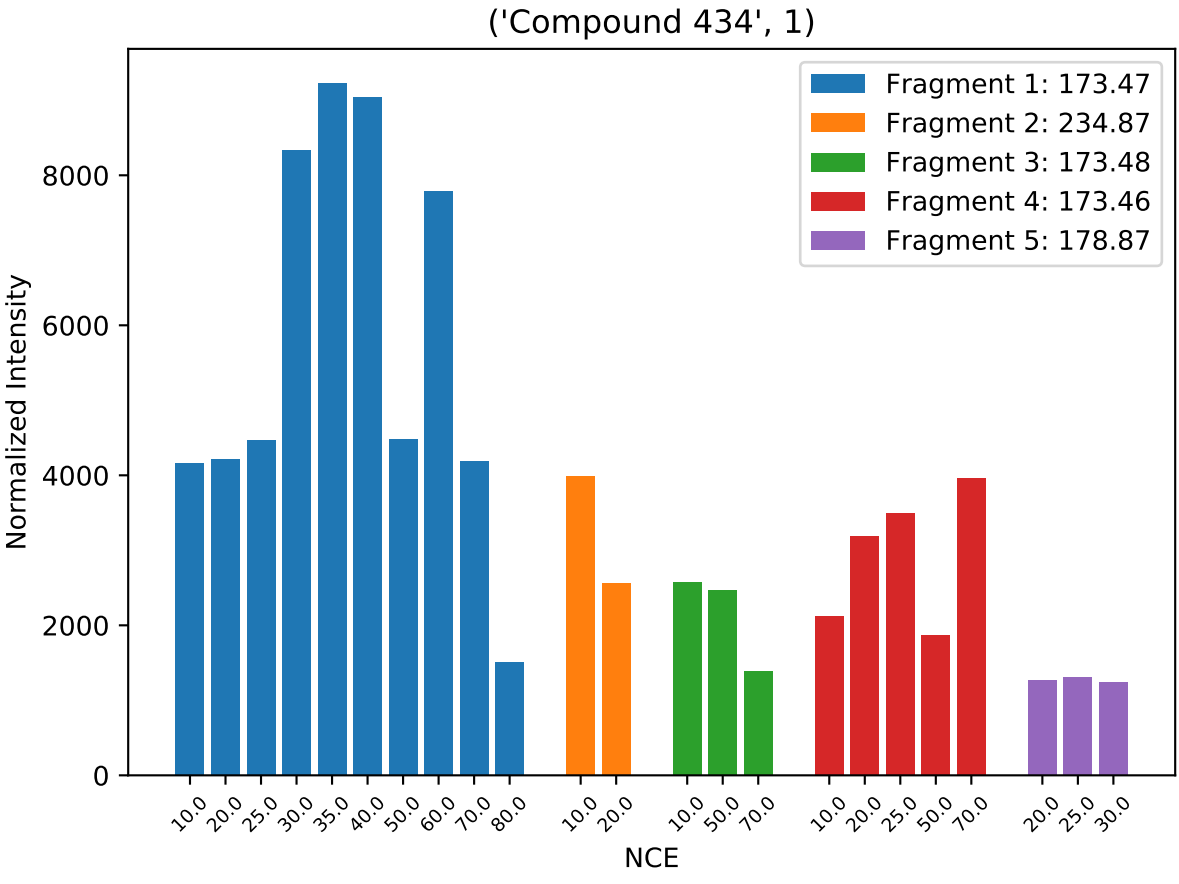

('Compound 418', 1)
Fragment 1: 484.28
Fragment 2: 173.47
Fragment 3: 361.27
Fragment 4: 485.29
Fragment 5: 173.46
Normalized Intensity
25000
20000
15000
10000
5000
0
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
10.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

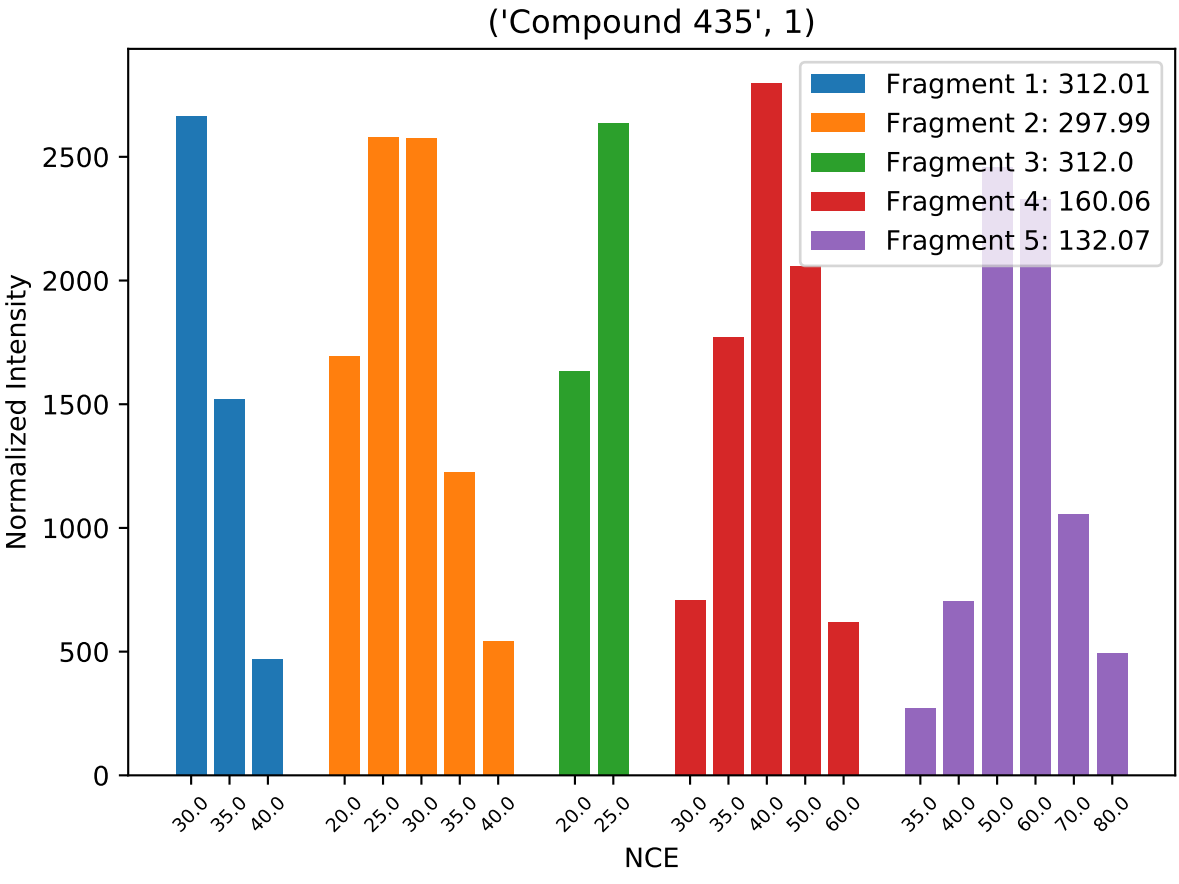

('Compound 426', 1)
Fragment 1: 85.03
Fragment 2: 121.09
Fragment 3: 120.08
Fragment 4: 134.1
Fragment 5: 163.14
Normalized Intensity
0
20000
40000
60000
80000
100000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0

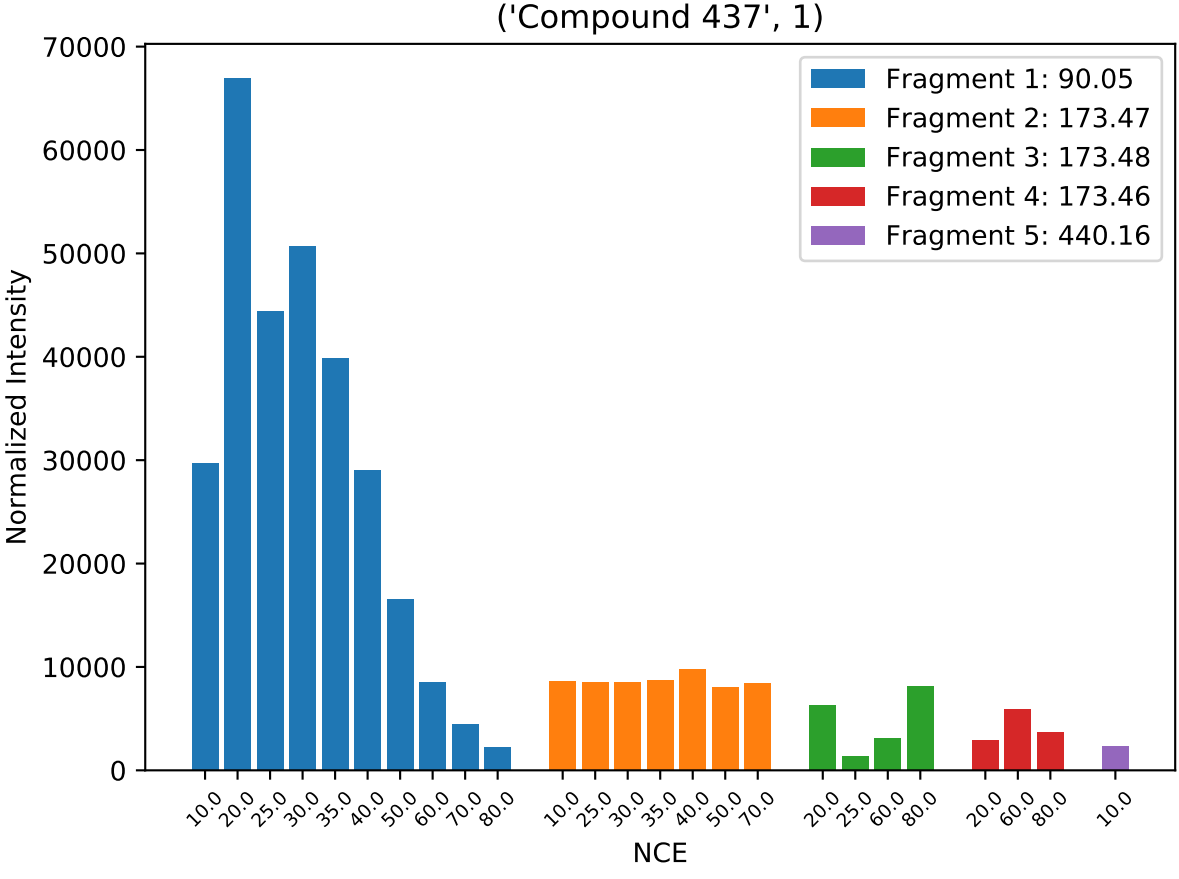

('Compound 428', 1)
Fragment 1: 94.07
Fragment 2: 70.96
Fragment 3: 71.09
Fragment 4: 77.94
Fragment 5: 89.76
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
35.0
50.0
10.0
10.0
10.0
10.0
NCE

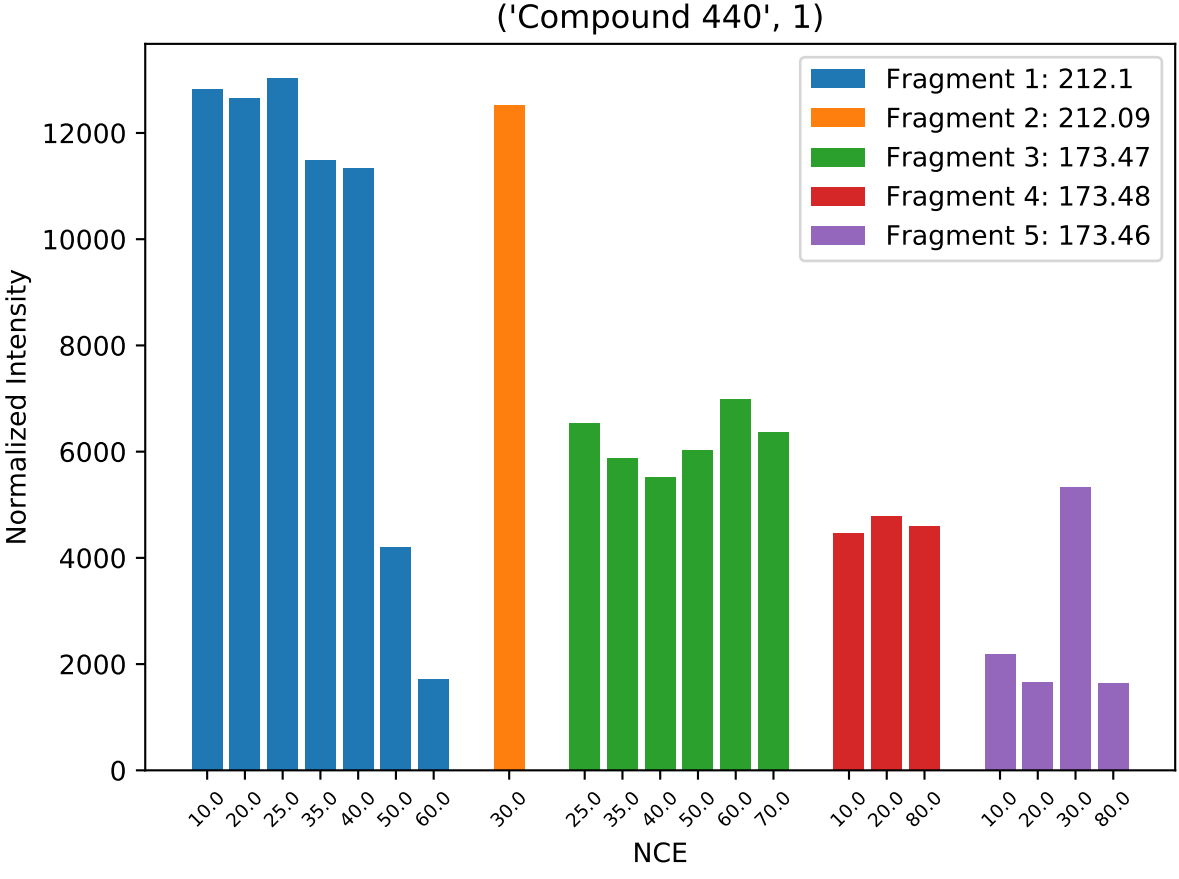

('Compound 429', 1)
Fragment 1: 128.95
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 446.85
Fragment 5: 173.48
Normalized Intensity
0
20000
40000
60000
80000
100000
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
30.0
35.0
50.0
60.0
70.0
25.0
40.0
80.0
25.0
30.0
35.0
40.0
25.0
30.0
40.0
NCE

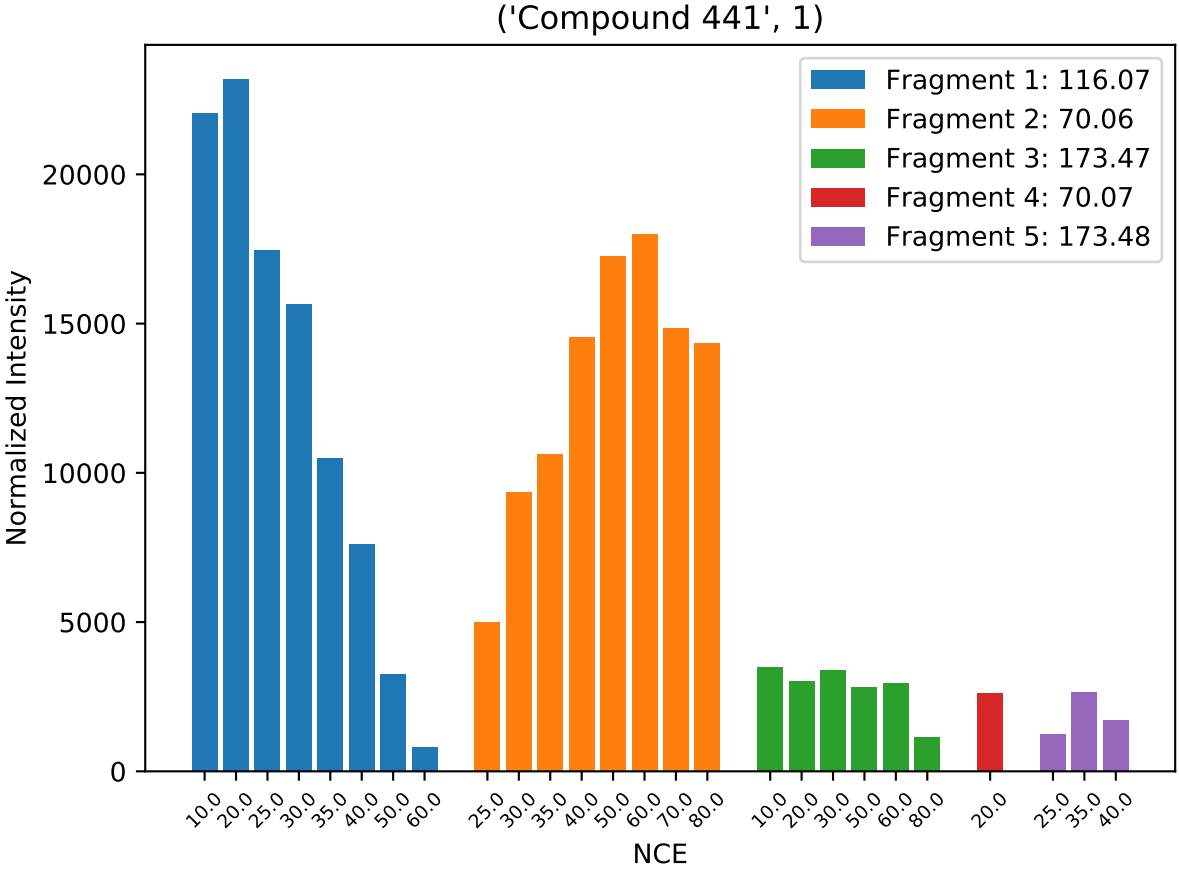

('Compound 431', 1)
Fragment 1: 126.09
Fragment 2: 173.47
Fragment 3: 143.12
Fragment 4: 56.05
Fragment 5: 84.08
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
30.0
35.0
40.0
60.0
80.0
10.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

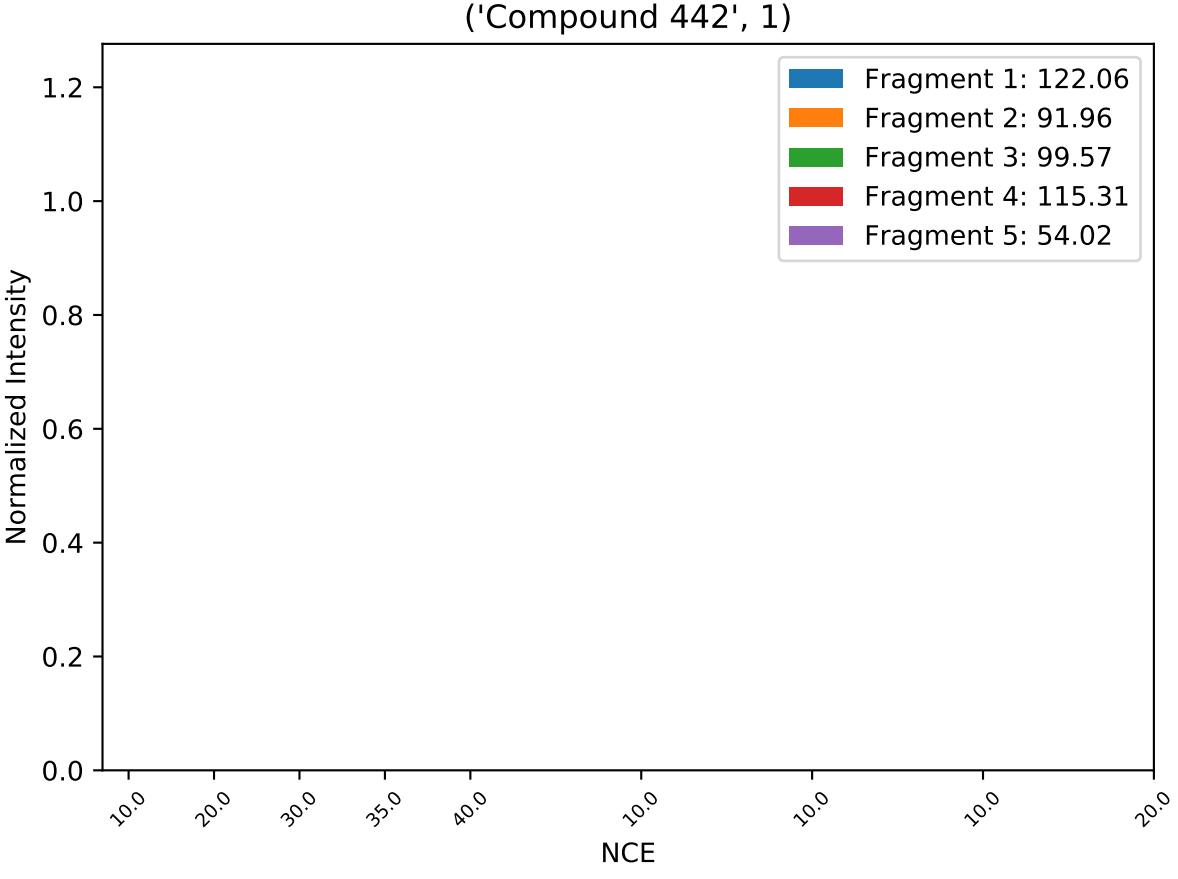

('Compound 434', 1)
Fragment 1: 173.47
Fragment 2: 234.87
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 178.87
Normalized Intensity
0
2000
4000
6000
8000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
10.0
50.0
70.0
10.0
20.0
25.0
50.0
70.0
20.0
25.0
30.0
NCE

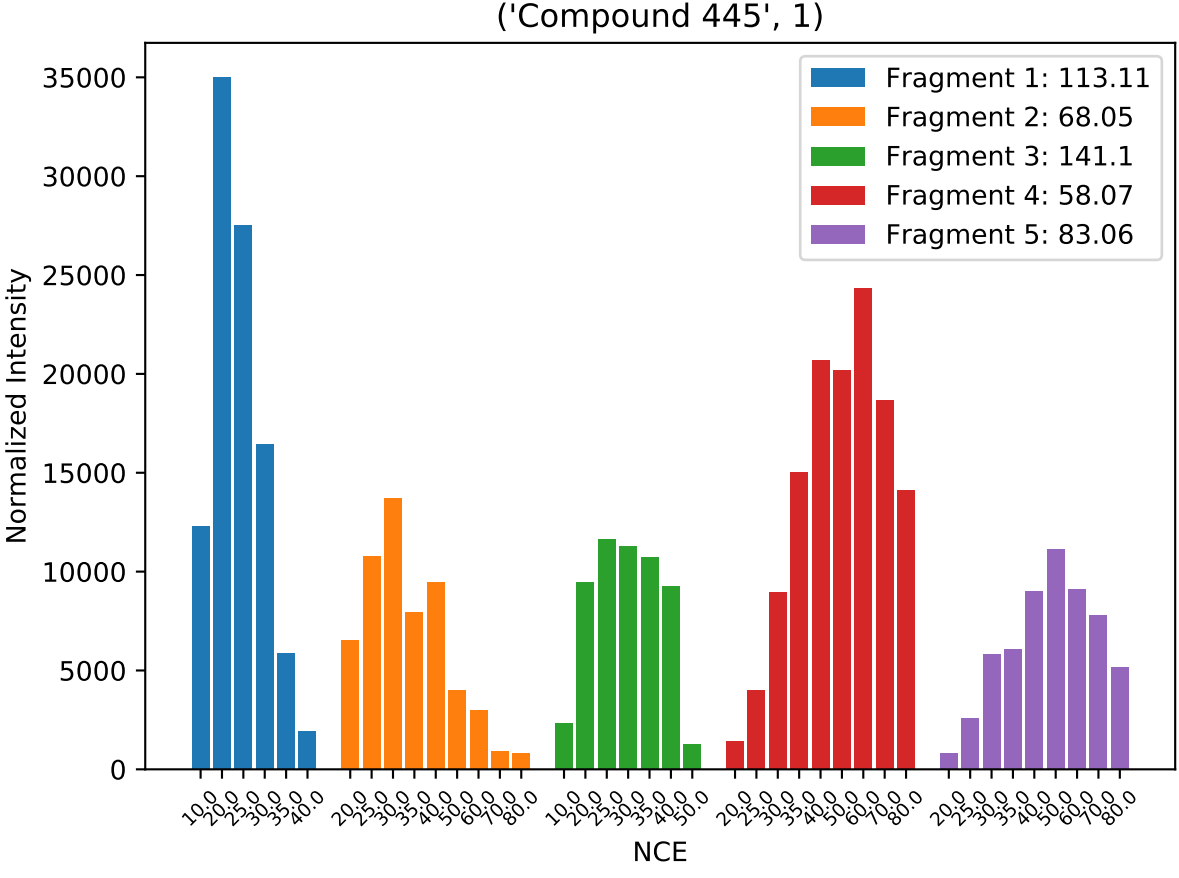

('Compound 435', 1)
Fragment 1: 312.01
Fragment 2: 297.99
Fragment 3: 312.0
Fragment 4: 160.06
Fragment 5: 132.07
Normalized Intensity
0
500
1000
1500
2000
2500
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

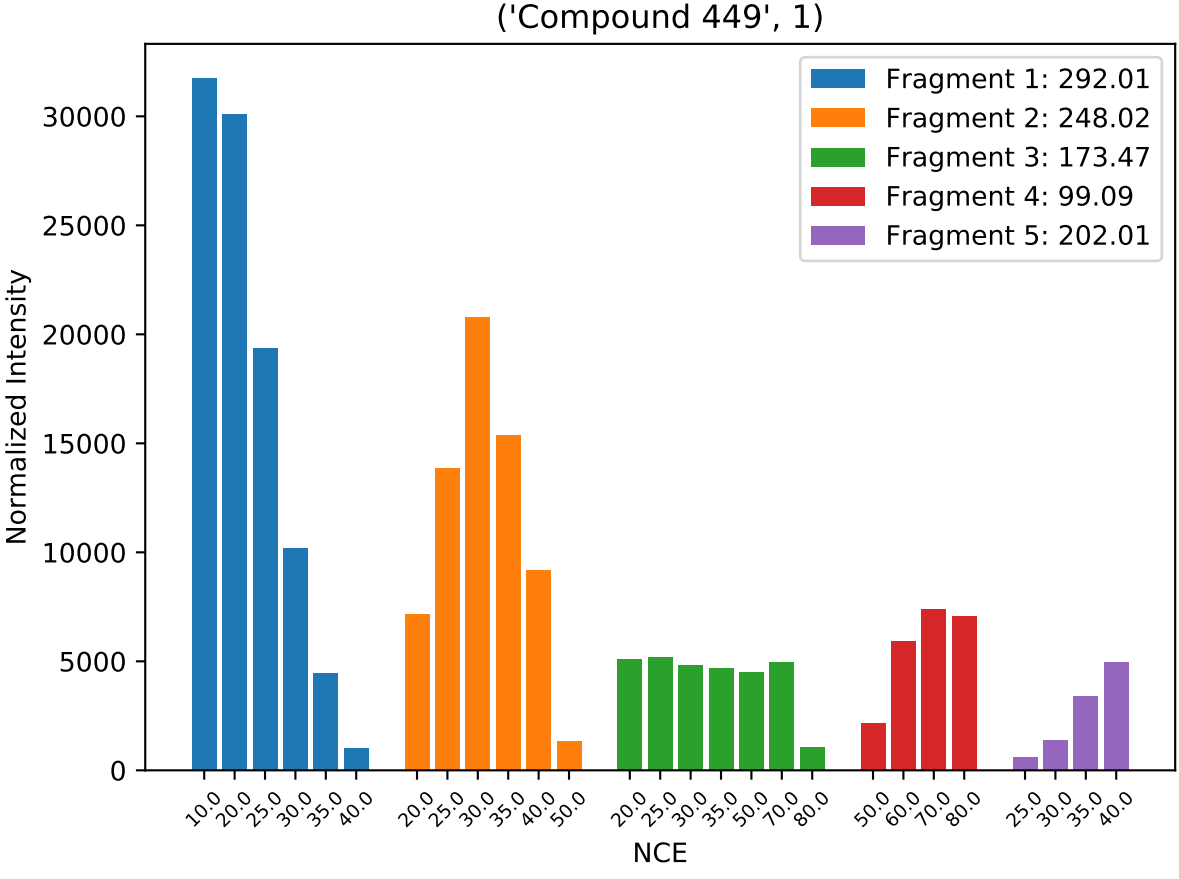

('Compound 437', 1)
Fragment 1: 90.05
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 440.16
Normalized Intensity
70000
60000
50000
40000
30000
20000
10000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
25.0
30.0
35.0
40.0
50.0
70.0
20.0
25.0
60.0
80.0
20.0
60.0
80.0
10.0
NCE

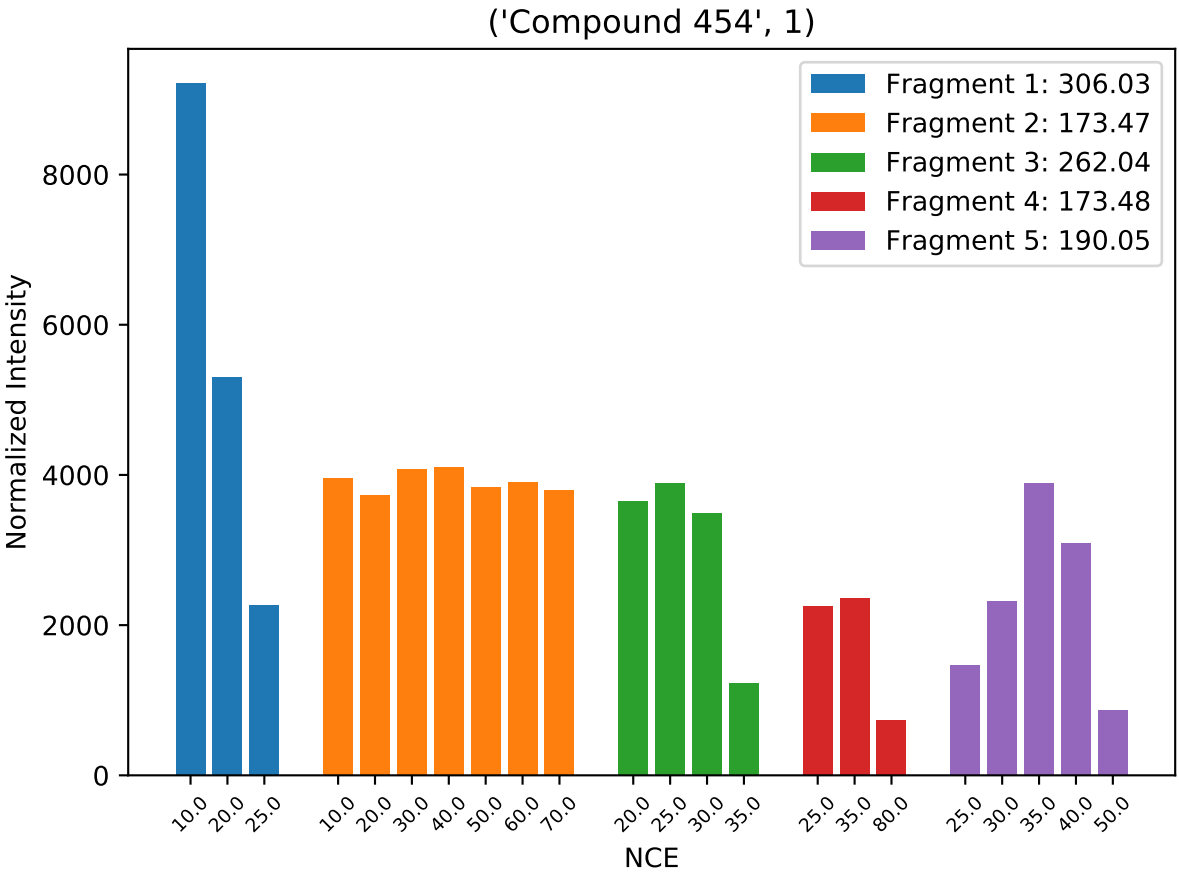

('Compound 440', 1)
Fragment 1: 212.1
Fragment 2: 212.09
Fragment 3: 173.47
Fragment 4: 173.48
Fragment 5: 173.46
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0
20.0
25.0
35.0
40.0
50.0
60.0
30.0
25.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
80.0
10.0
20.0
30.0
80.0
NCE

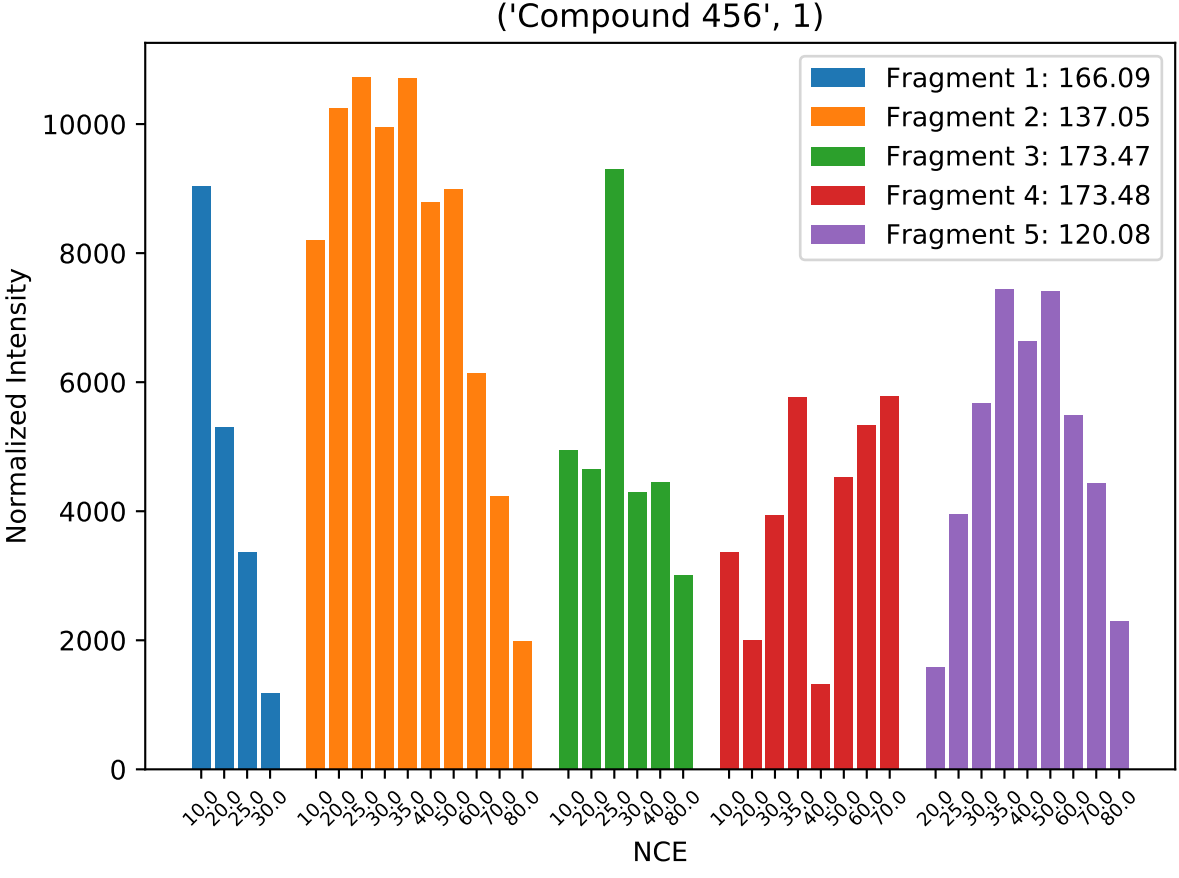

('Compound 441', 1)
Fragment 1: 116.07
Fragment 2: 70.06
Fragment 3: 173.47
Fragment 4: 70.07
Fragment 5: 173.48
Normalized Intensity
0
5000
10000
15000
20000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
30.0
50.0
60.0
80.0
20.0
25.0
35.0
40.0
NCE

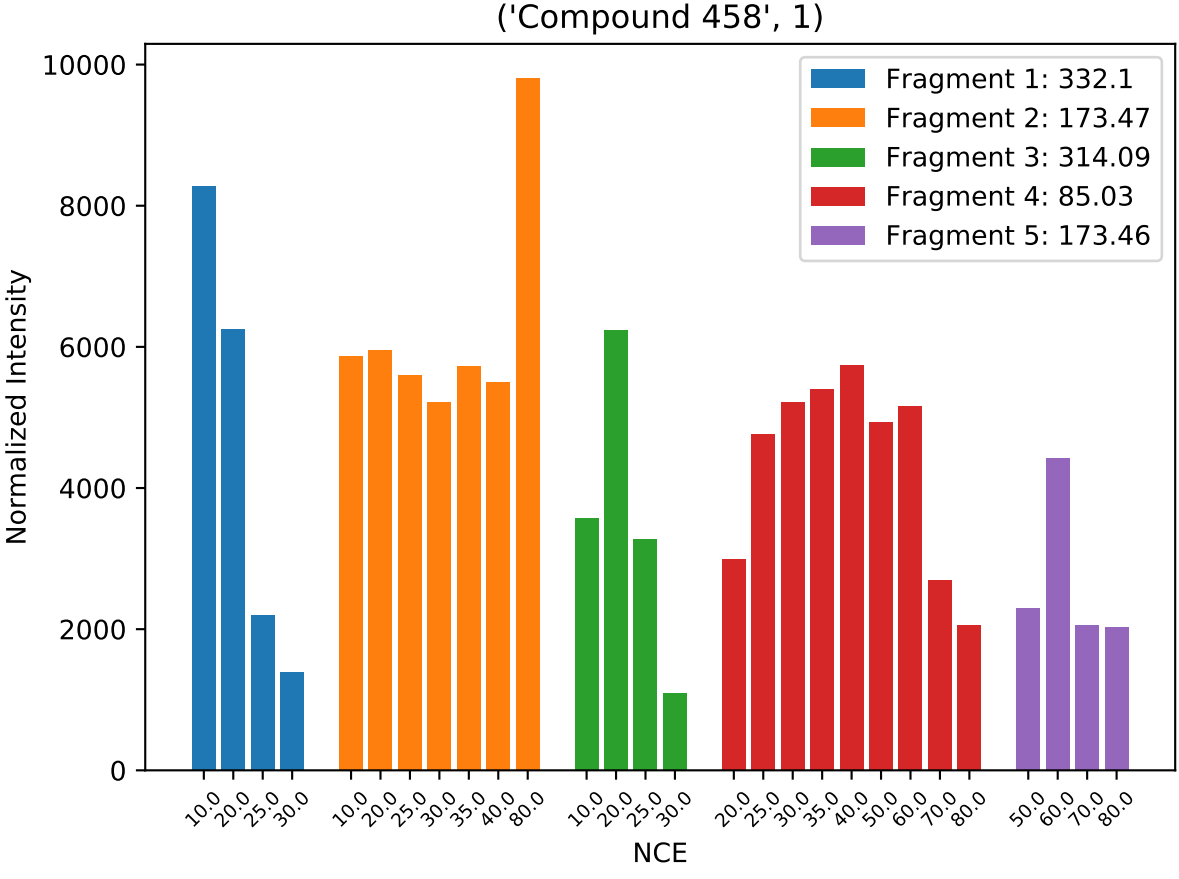

('Compound 442', 1)
Fragment 1: 122.06
Fragment 2: 91.96
Fragment 3: 99.57
Fragment 4: 115.31
Fragment 5: 54.02
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
30.0
35.0
40.0
10.0
10.0
10.0
20.0
NCE

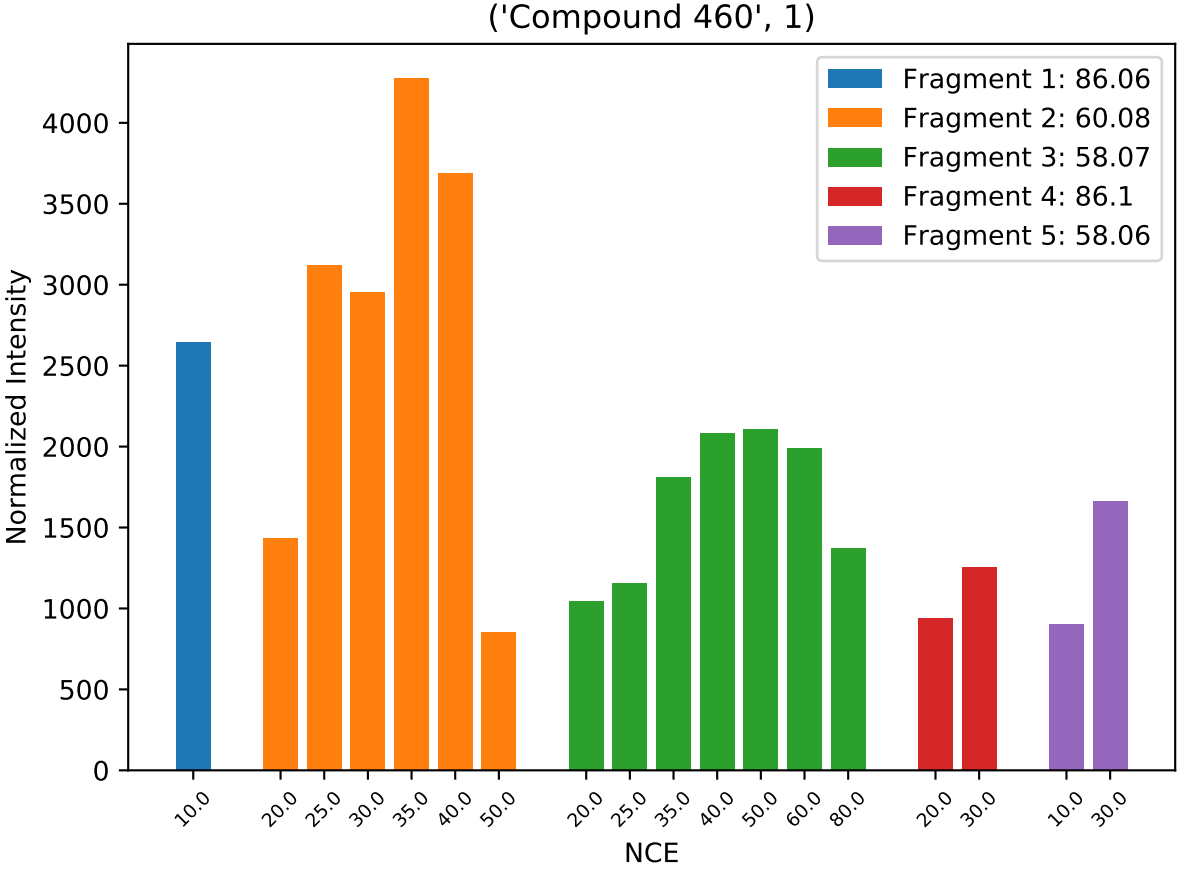

('Compound 445', 1)
Fragment 1: 113.11
Fragment 2: 68.05
Fragment 3: 141.1
Fragment 4: 58.07
Fragment 5: 83.06
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

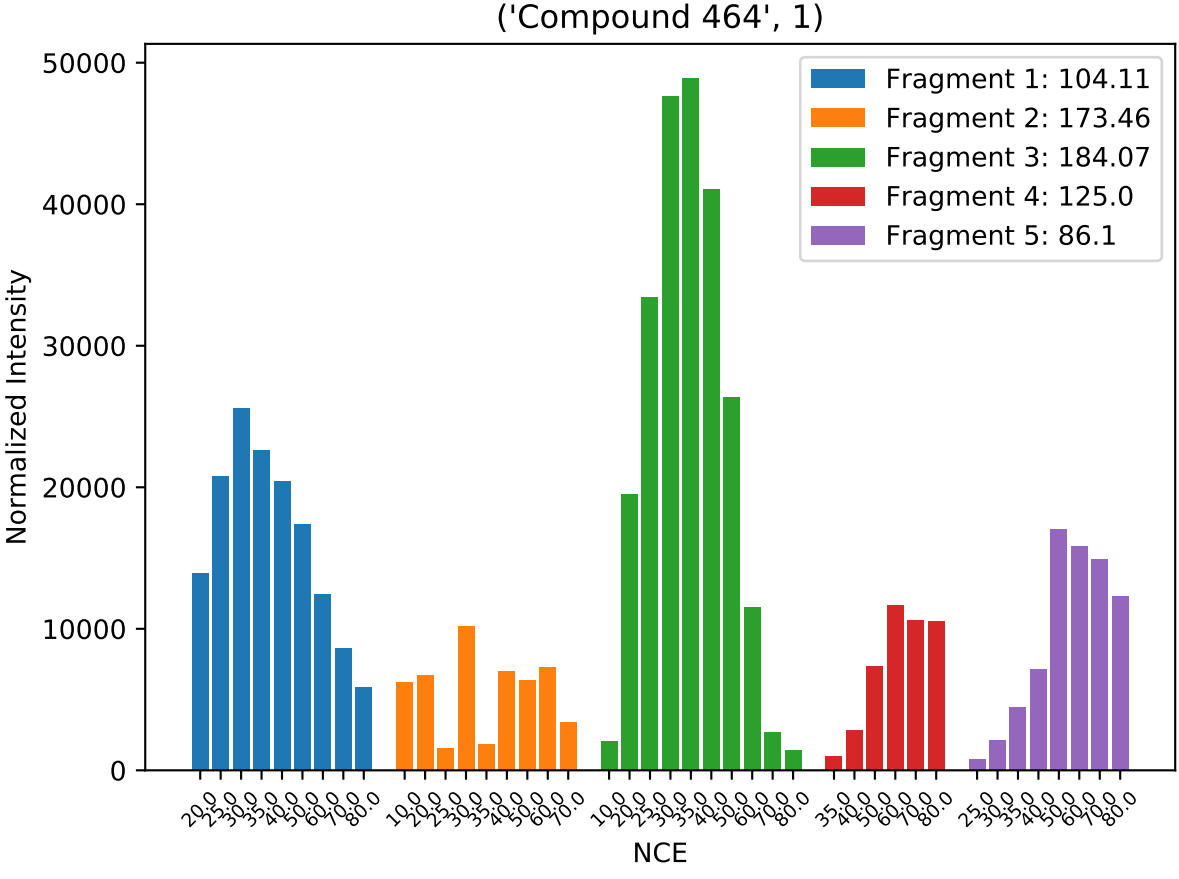

('Compound 449', 1)
Fragment 1: 292.01
Fragment 2: 248.02
Fragment 3: 173.47
Fragment 4: 99.09
Fragment 5: 202.01
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
50.0
70.0
80.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
NCE

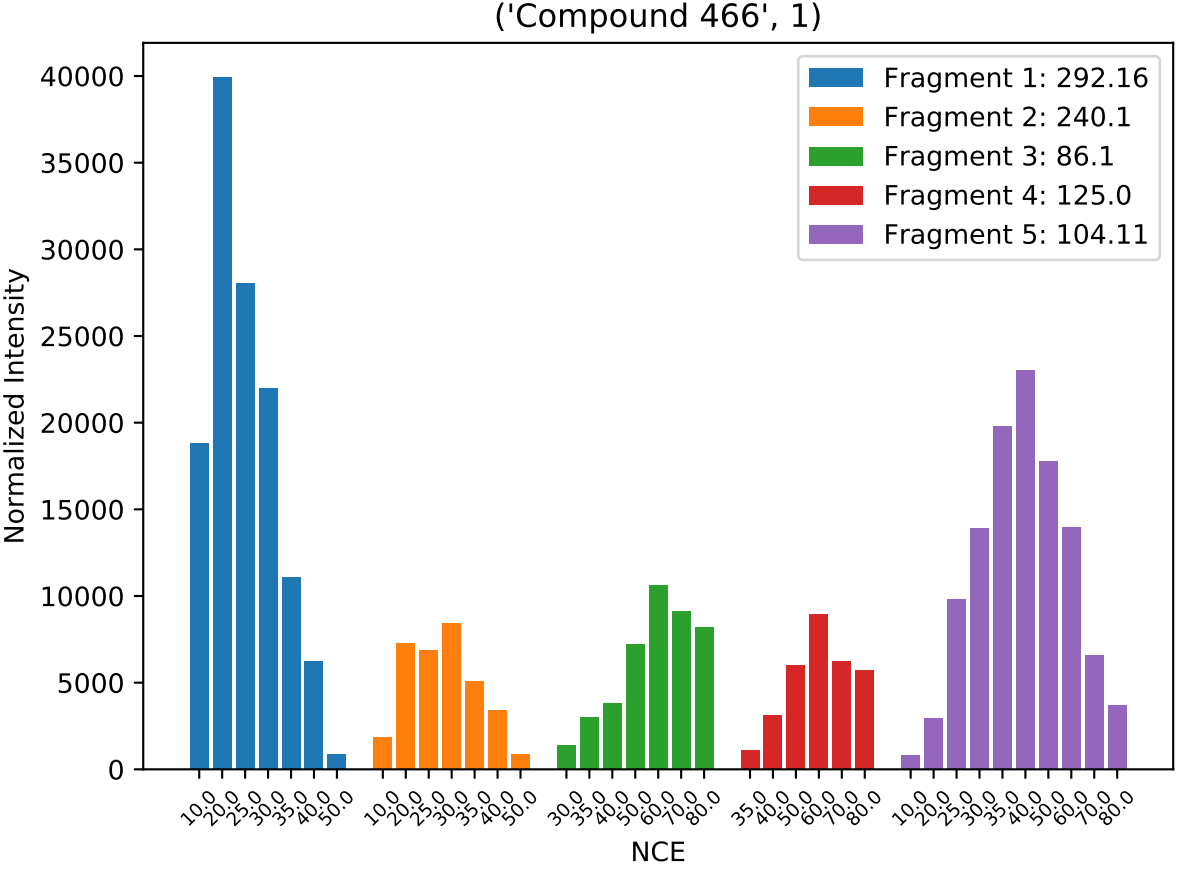

('Compound 454', 1)
Fragment 1: 306.03
Fragment 2: 173.47
Fragment 3: 262.04
Fragment 4: 173.48
Fragment 5: 190.05
Normalized Intensity
0
2000
4000
6000
8000
10.0
20.0
25.0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
25.0
35.0
80.0
25.0
30.0
35.0
40.0
50.0
NCE

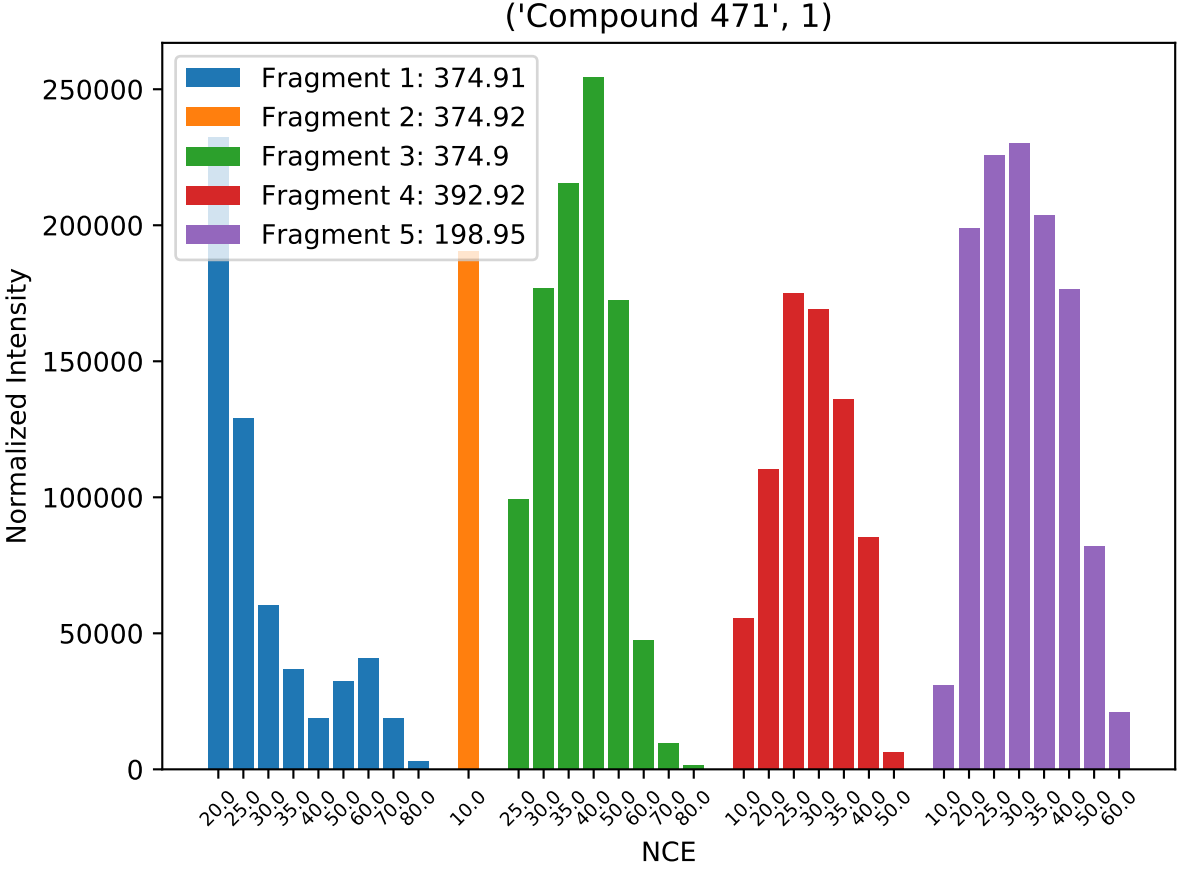

('Compound 456', 1)
Fragment 1: 166.09
Fragment 2: 137.05
Fragment 3: 173.47
Fragment 4: 173.48
Fragment 5: 120.08
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 40.0 80.0
10.0 20.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

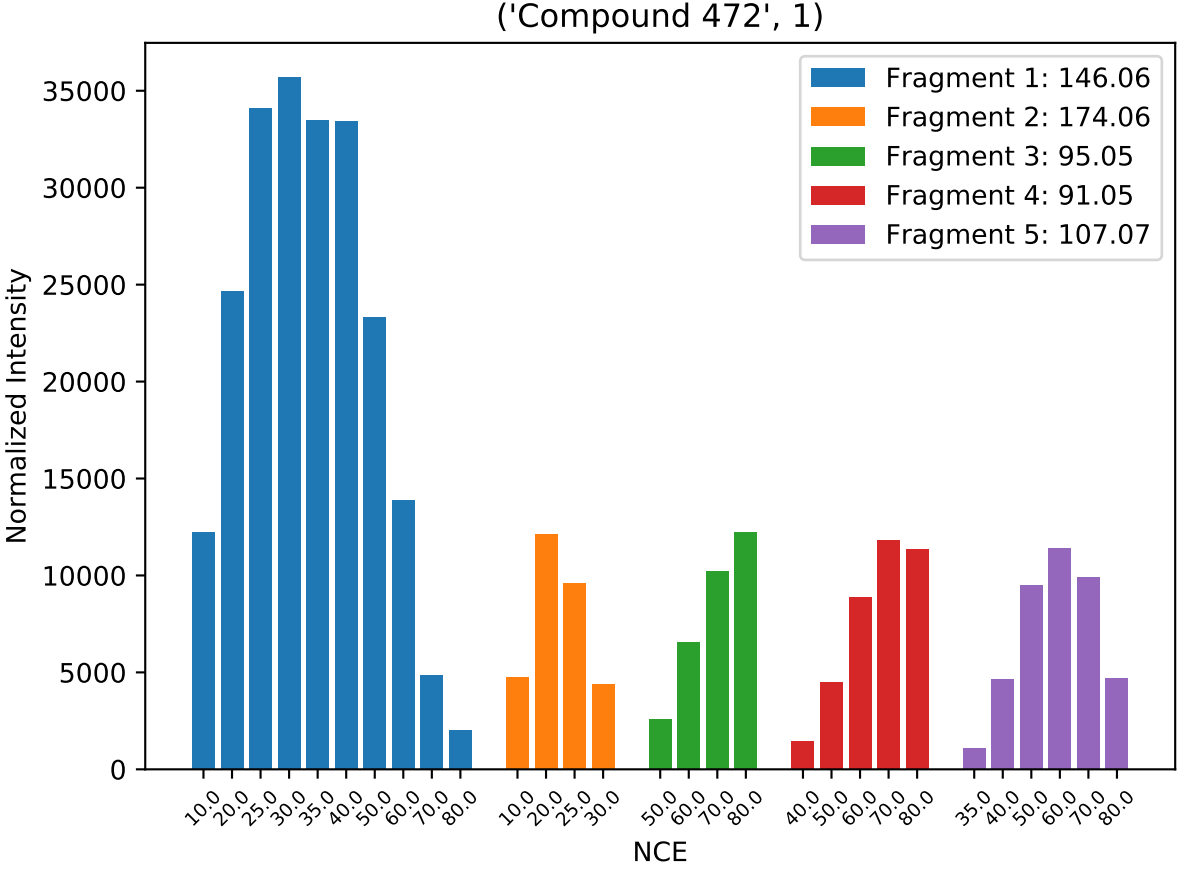

('Compound 458', 1)
Fragment 1: 332.1
Fragment 2: 173.47
Fragment 3: 314.09
Fragment 4: 85.03
Fragment 5: 173.46
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
40.0
80.0
10.0
20.0
25.0
30.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
50.0
60.0
70.0
80.0
NCE

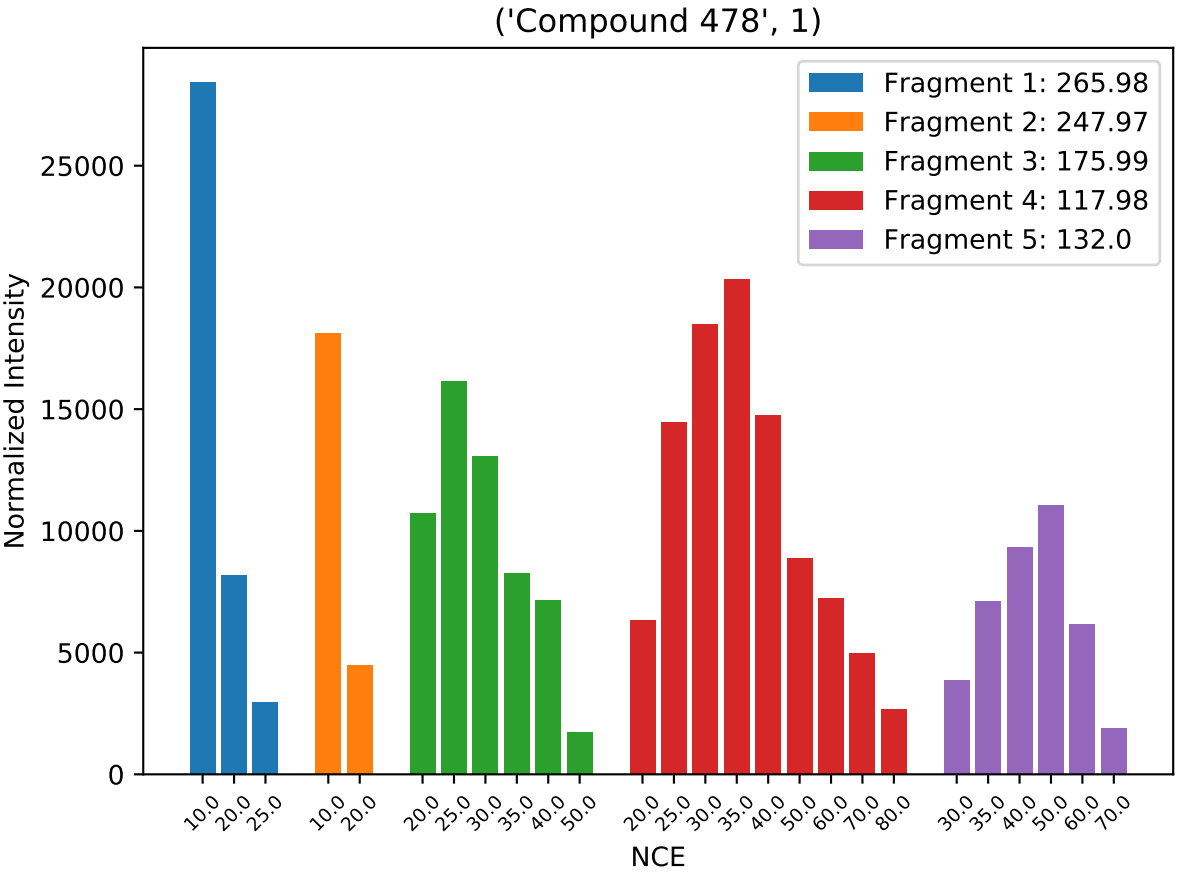

('Compound 460', 1)
Fragment 1: 86.06
Fragment 2: 60.08
Fragment 3: 58.07
Fragment 4: 86.1
Fragment 5: 58.06
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
35.0
40.0
50.0
60.0
80.0
20.0
30.0
10.0
30.0
NCE

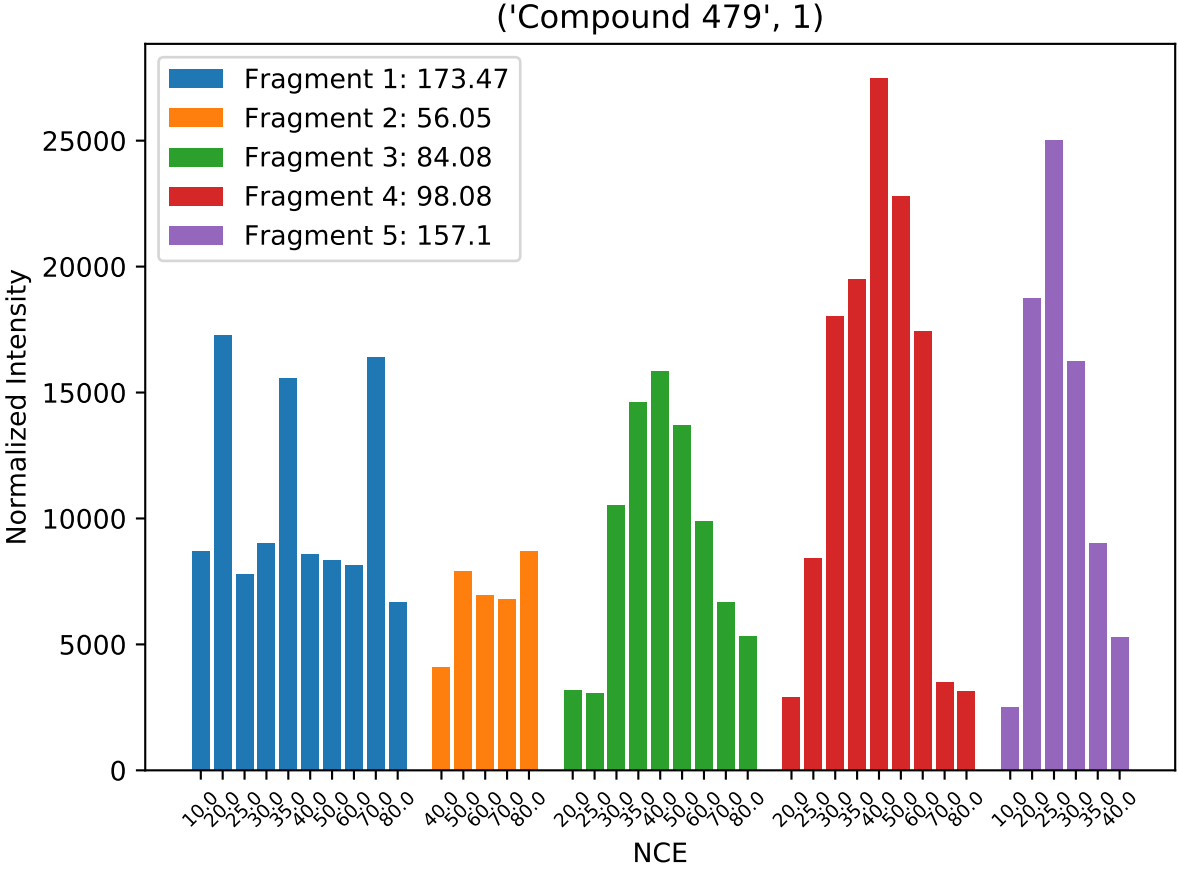

('Compound 464', 1)
Fragment 1: 104.11
Fragment 2: 173.46
Fragment 3: 184.07
Fragment 4: 125.0
Fragment 5: 86.1
Normalized Intensity
0
10000
20000
30000
40000
50000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

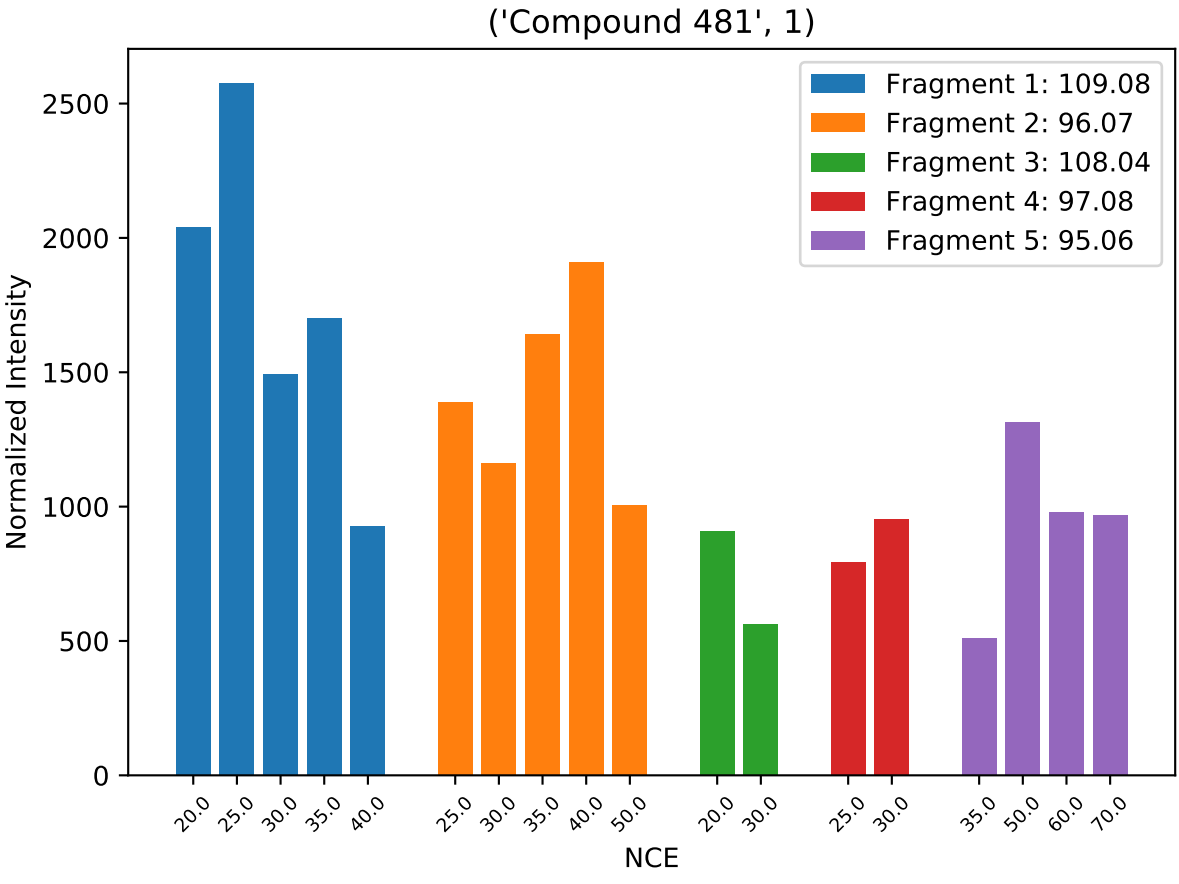

('Compound 466', 1)
Fragment 1: 292.16
Fragment 2: 240.1
Fragment 3: 86.1
Fragment 4: 125.0
Fragment 5: 104.11
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

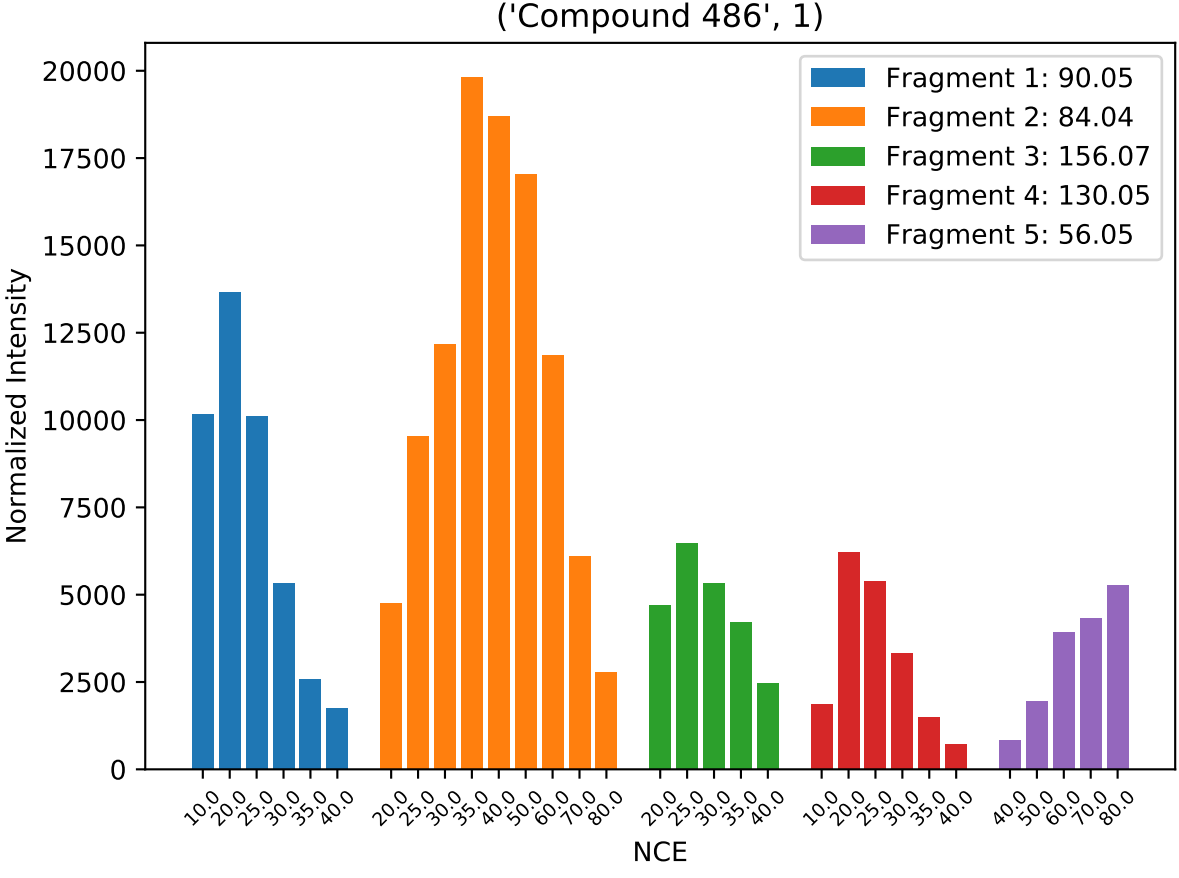

('Compound 471', 1)
Fragment 1: 374.91
Fragment 2: 374.92
Fragment 3: 374.9
Fragment 4: 392.92
Fragment 5: 198.95
Normalized Intensity
250000
200000
150000
100000
50000
0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

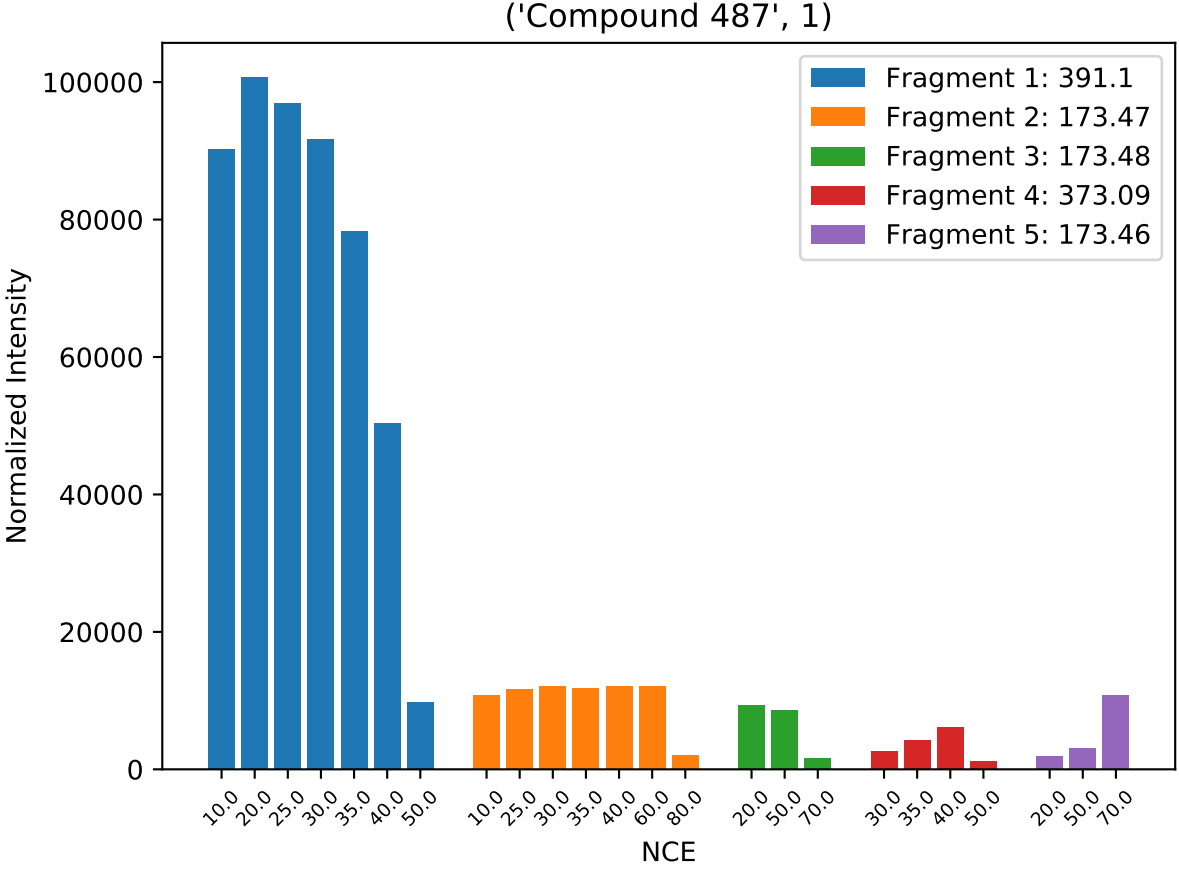

('Compound 472', 1)
Fragment 1: 146.06
Fragment 2: 174.06
Fragment 3: 95.05
Fragment 4: 91.05
Fragment 5: 107.07
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
50.0
60.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

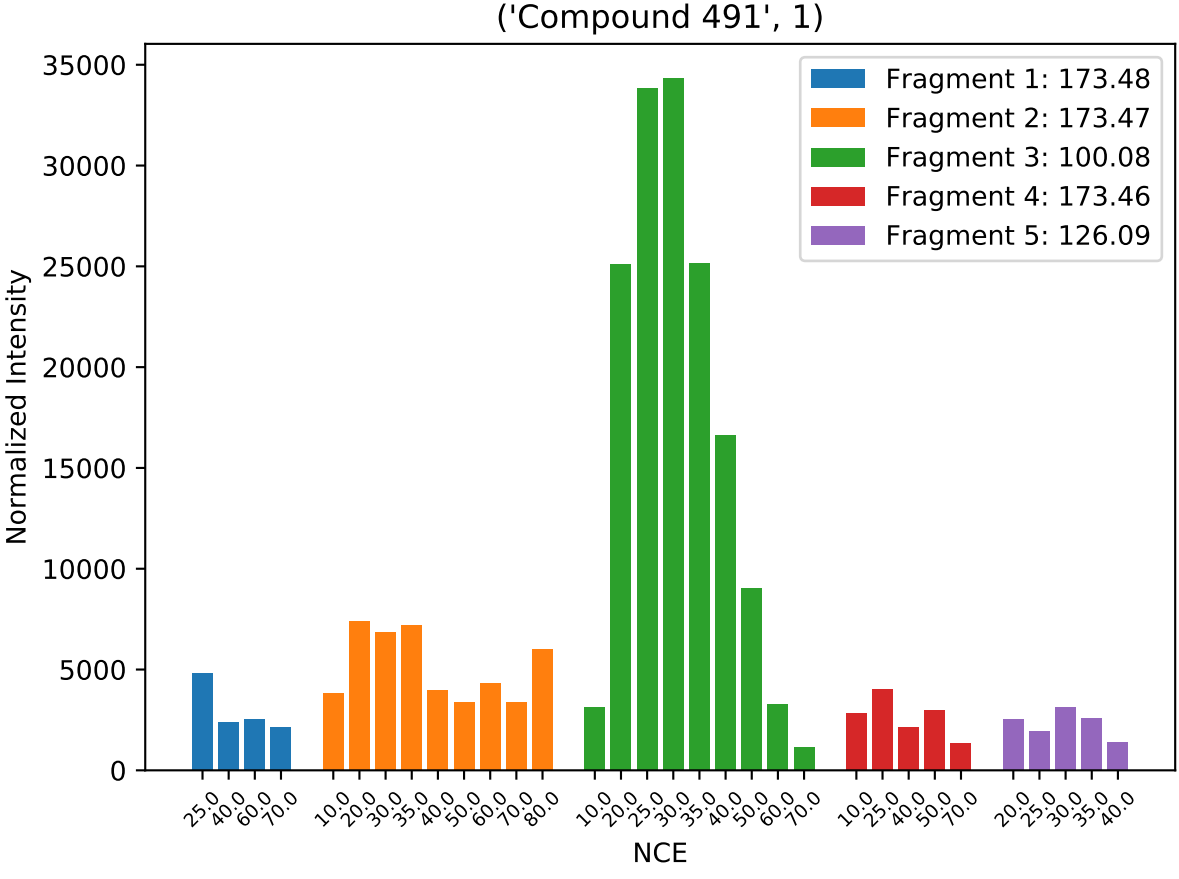

('Compound 478', 1)
Fragment 1: 265.98
Fragment 2: 247.97
Fragment 3: 175.99
Fragment 4: 117.98
Fragment 5: 132.0
Normalized Intensity
0
5000
10000
15000
20000
25000
NCE
10.0 20.0 25.0
10.0 20.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0

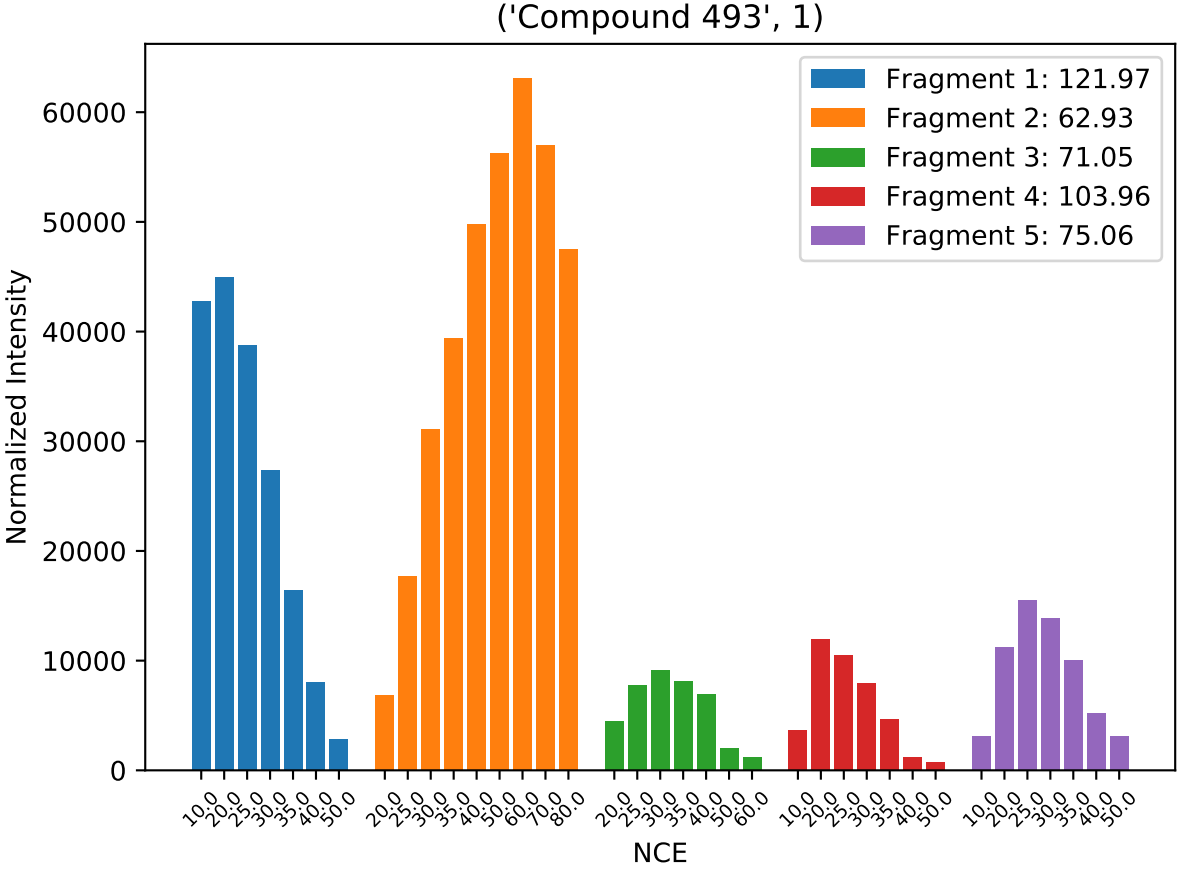

('Compound 479', 1)
Fragment 1: 173.47
Fragment 2: 56.05
Fragment 3: 84.08
Fragment 4: 98.08
Fragment 5: 157.1
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

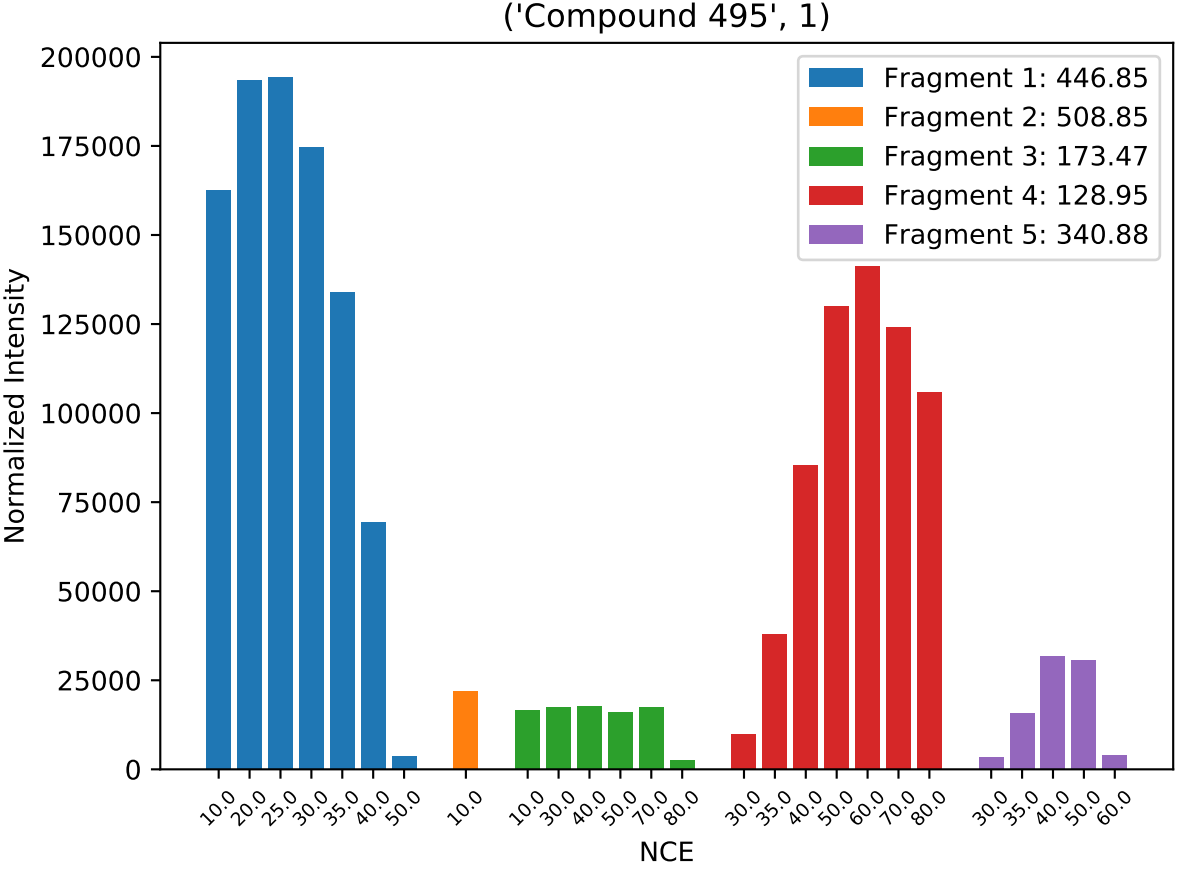

('Compound 481', 1)
Fragment 1: 109.08
Fragment 2: 96.07
Fragment 3: 108.04
Fragment 4: 97.08
Fragment 5: 95.06
Normalized Intensity
0
500
1000
1500
2000
2500
20.0
25.0
30.0
35.0
40.0
25.0
30.0
35.0
40.0
50.0
20.0
30.0
25.0
30.0
35.0
50.0
60.0
70.0
NCE

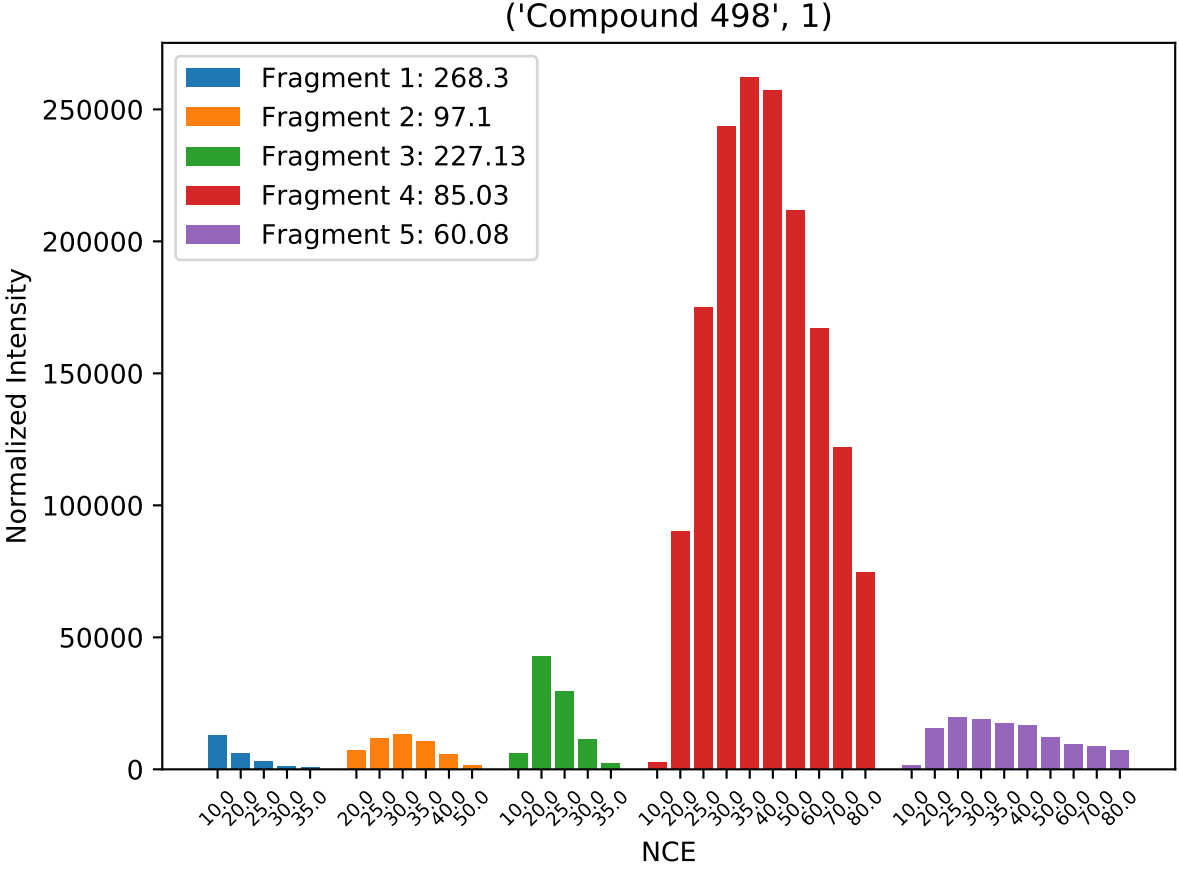

('Compound 486', 1)
Fragment 1: 90.05
Fragment 2: 84.04
Fragment 3: 156.07
Fragment 4: 130.05
Fragment 5: 56.05
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
40.0 50.0 60.0 70.0 80.0
NCE

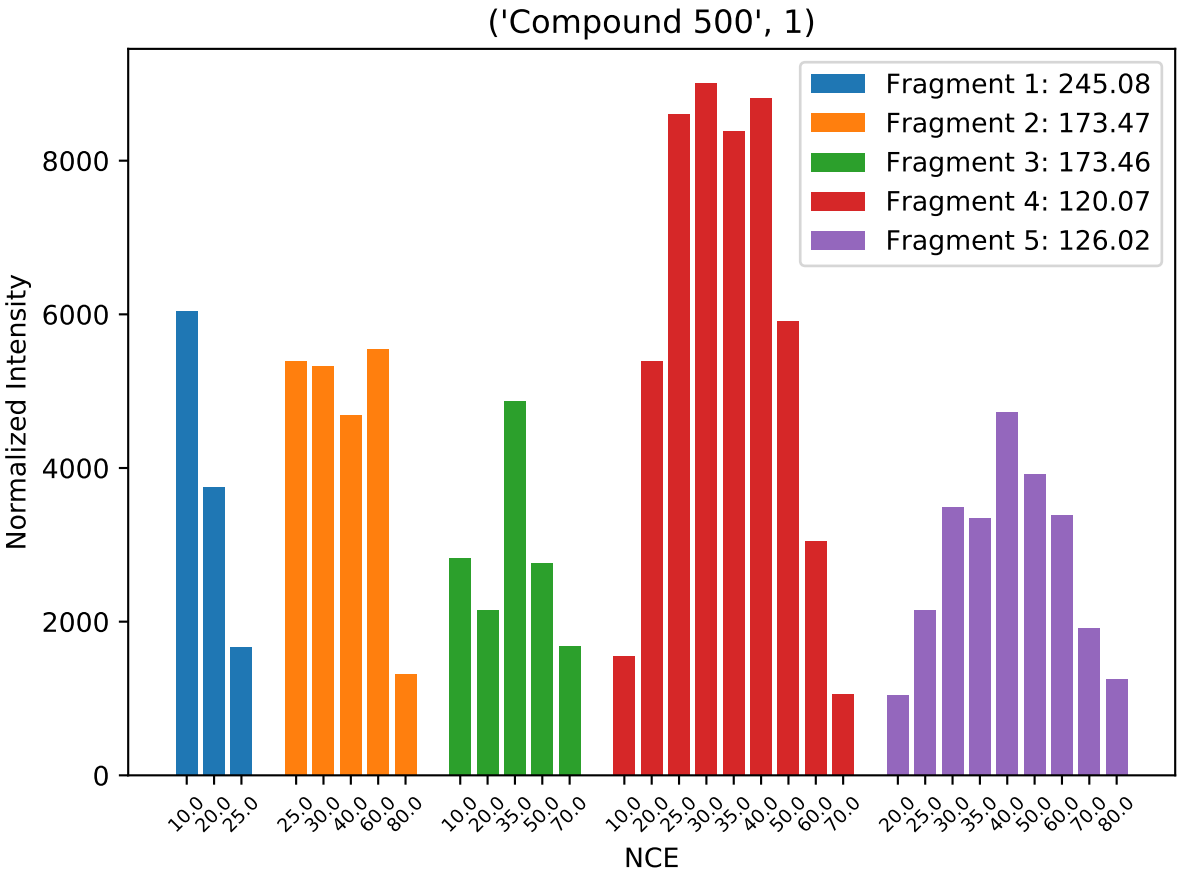

('Compound 487', 1)
Fragment 1: 391.1
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 373.09
Fragment 5: 173.46
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
25.0
30.0
35.0
40.0
60.0
80.0
20.0
50.0
70.0
30.0
35.0
40.0
50.0
20.0
50.0
70.0
NCE

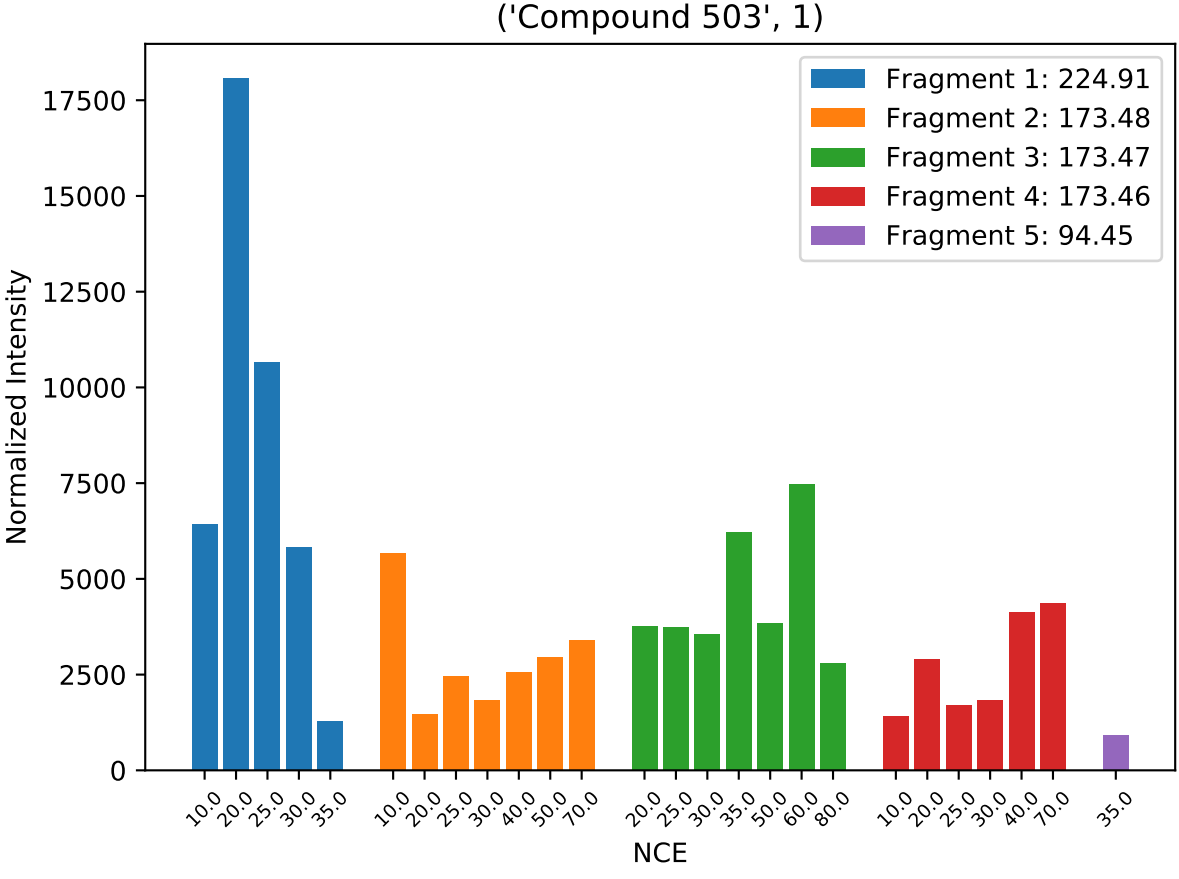

('Compound 491', 1)
Fragment 1: 173.48
Fragment 2: 173.47
Fragment 3: 100.08
Fragment 4: 173.46
Fragment 5: 126.09
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
25.0 40.0 60.0 70.0
10.0 20.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 25.0 40.0 50.0 70.0
20.0 25.0 30.0 35.0 40.0
NCE

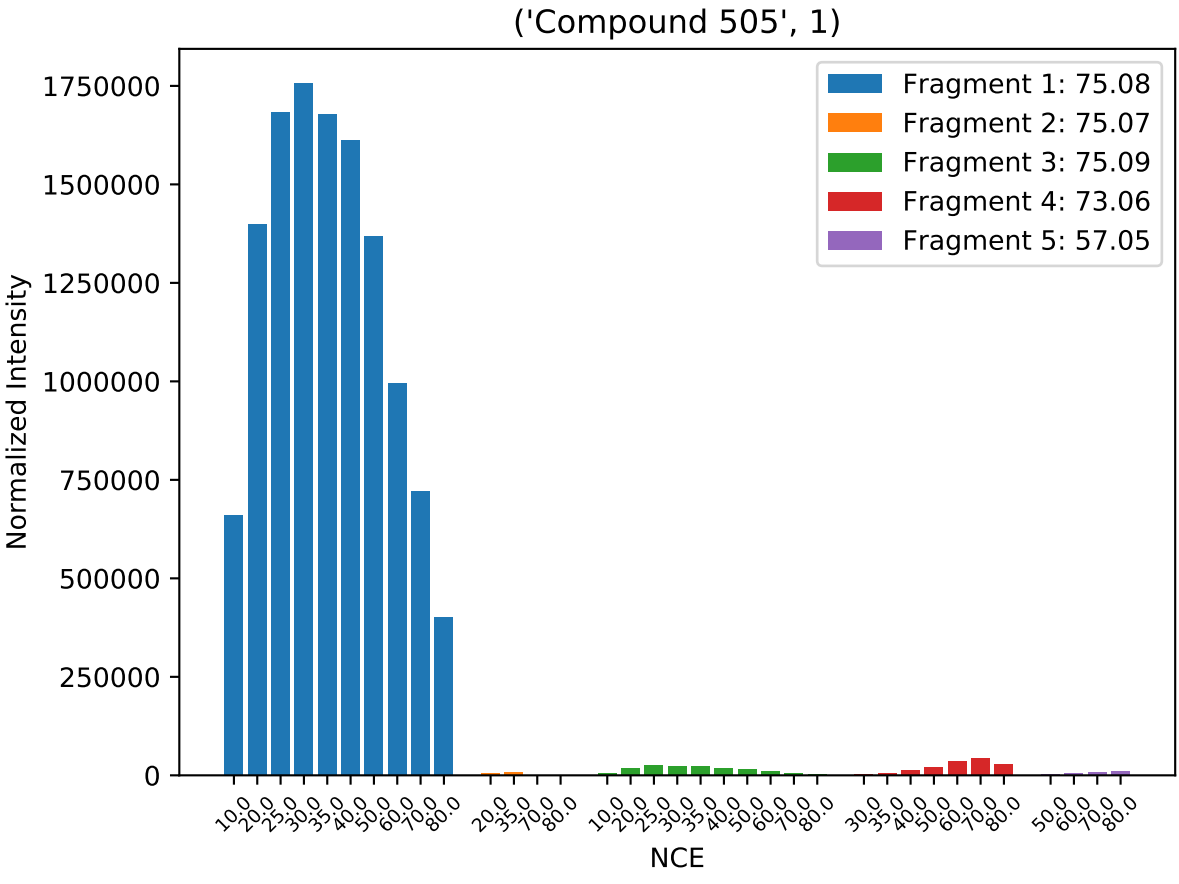

('Compound 493', 1)
Fragment 1: 121.97
Fragment 2: 62.93
Fragment 3: 71.05
Fragment 4: 103.96
Fragment 5: 75.06
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

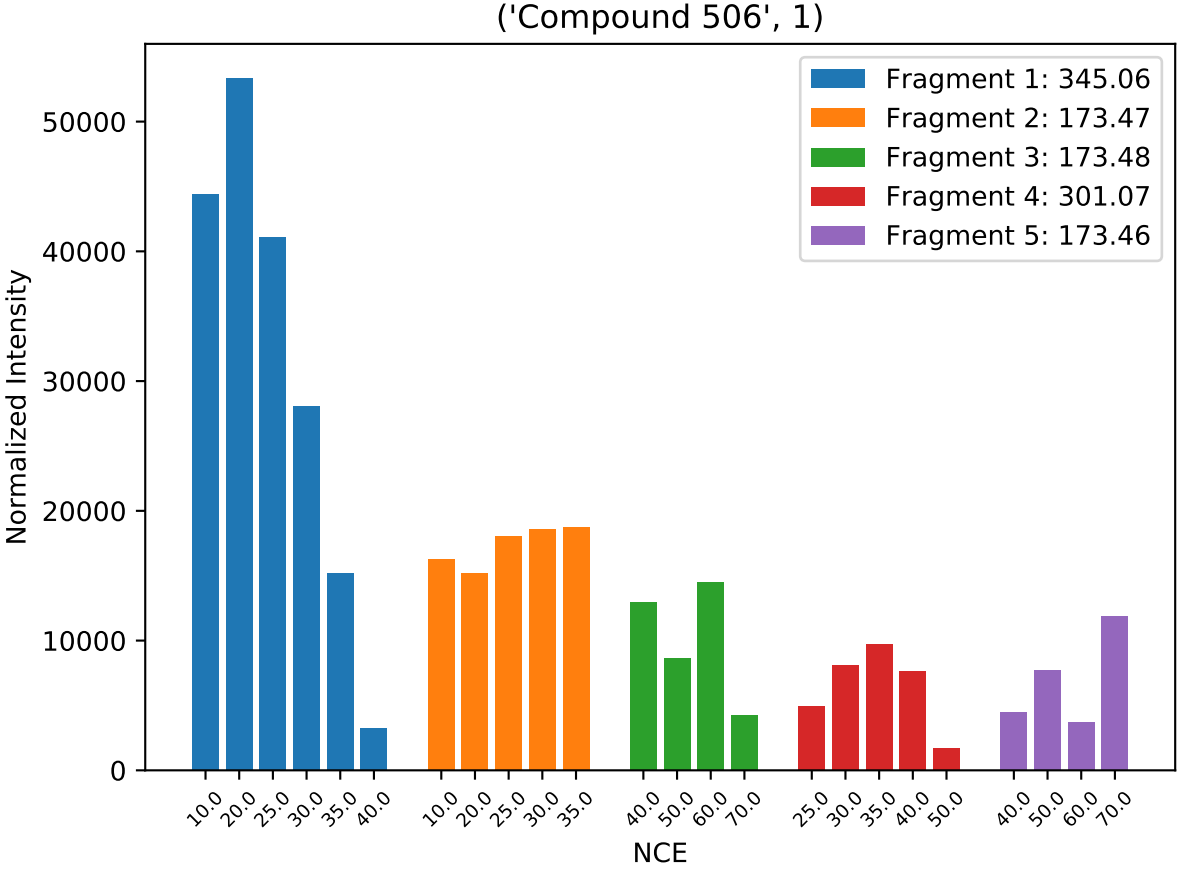

('Compound 495', 1)
Fragment 1: 446.85
Fragment 2: 508.85
Fragment 3: 173.47
Fragment 4: 128.95
Fragment 5: 340.88
Normalized Intensity
200000
175000
150000
125000
100000
75000
50000
25000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0
10.0 30.0 40.0 50.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0
NCE

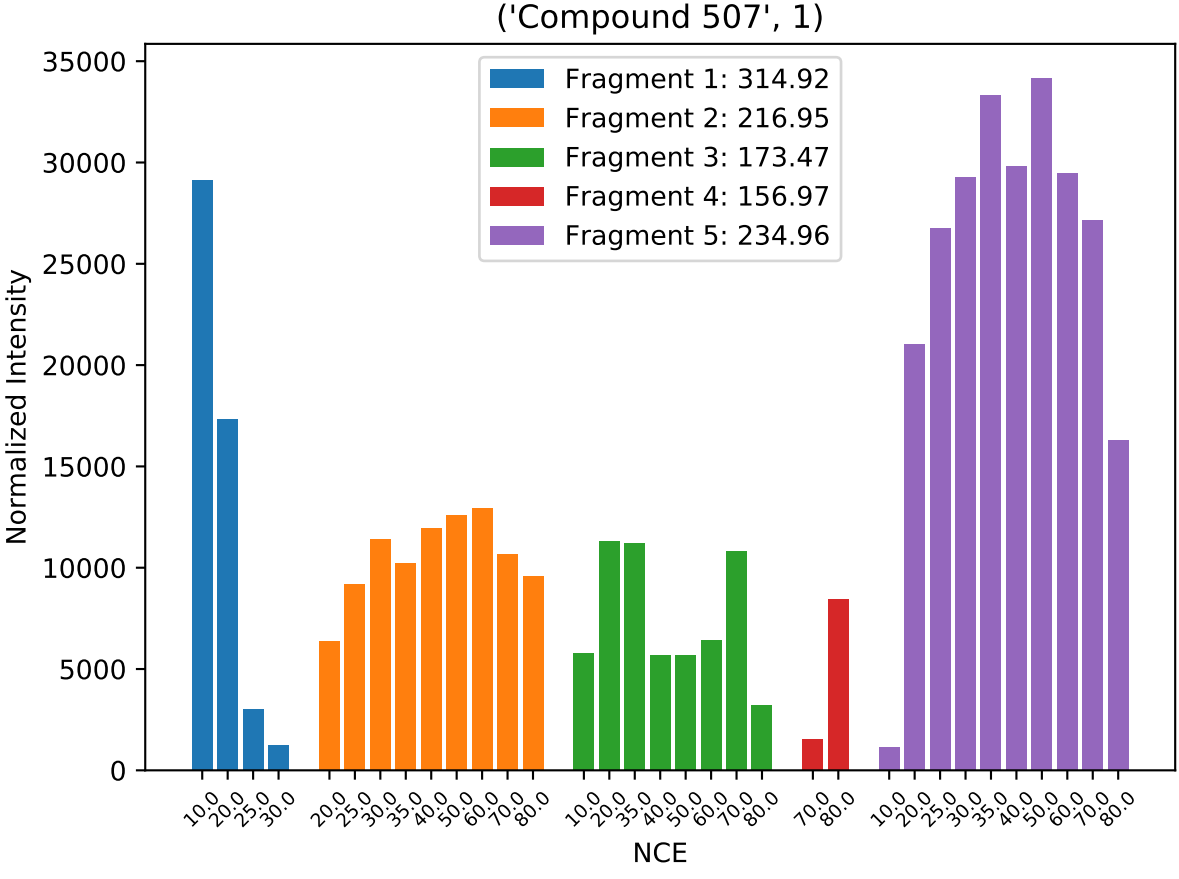

('Compound 498', 1)
Fragment 1: 268.3
Fragment 2: 97.1
Fragment 3: 227.13
Fragment 4: 85.03
Fragment 5: 60.08
Normalized Intensity
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

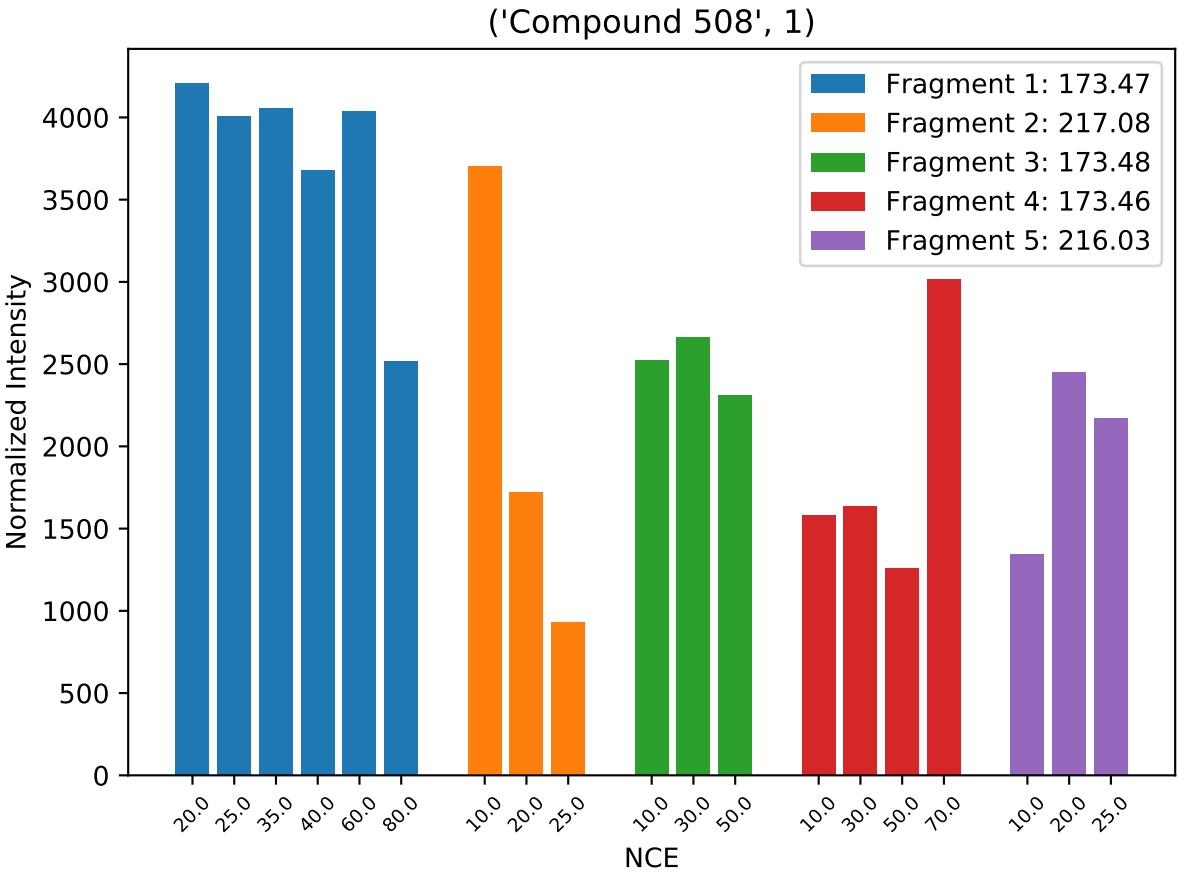

('Compound 500', 1)
Fragment 1: 245.08
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 120.07
Fragment 5: 126.02
Normalized Intensity
0
2000
4000
6000
8000
10.0
20.0
25.0
25.0
30.0
40.0
60.0
80.0
10.0
20.0
35.0
50.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

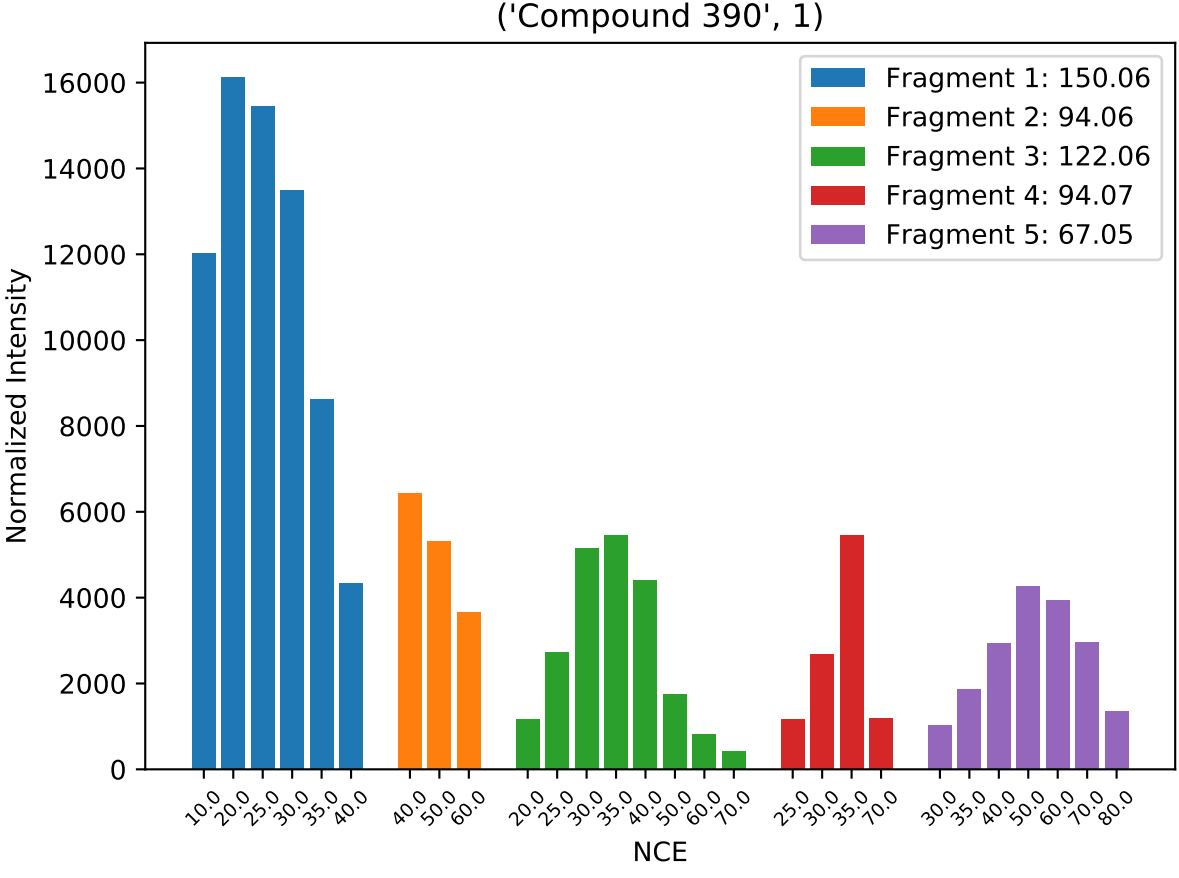

('Compound 503', 1)
Fragment 1: 224.91
Fragment 2: 173.48
Fragment 3: 173.47
Fragment 4: 173.46
Fragment 5: 94.45
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
40.0
50.0
70.0
20.0
25.0
30.0
35.0
50.0
60.0
80.0
10.0
20.0
25.0
30.0
40.0
70.0
35.0
NCE

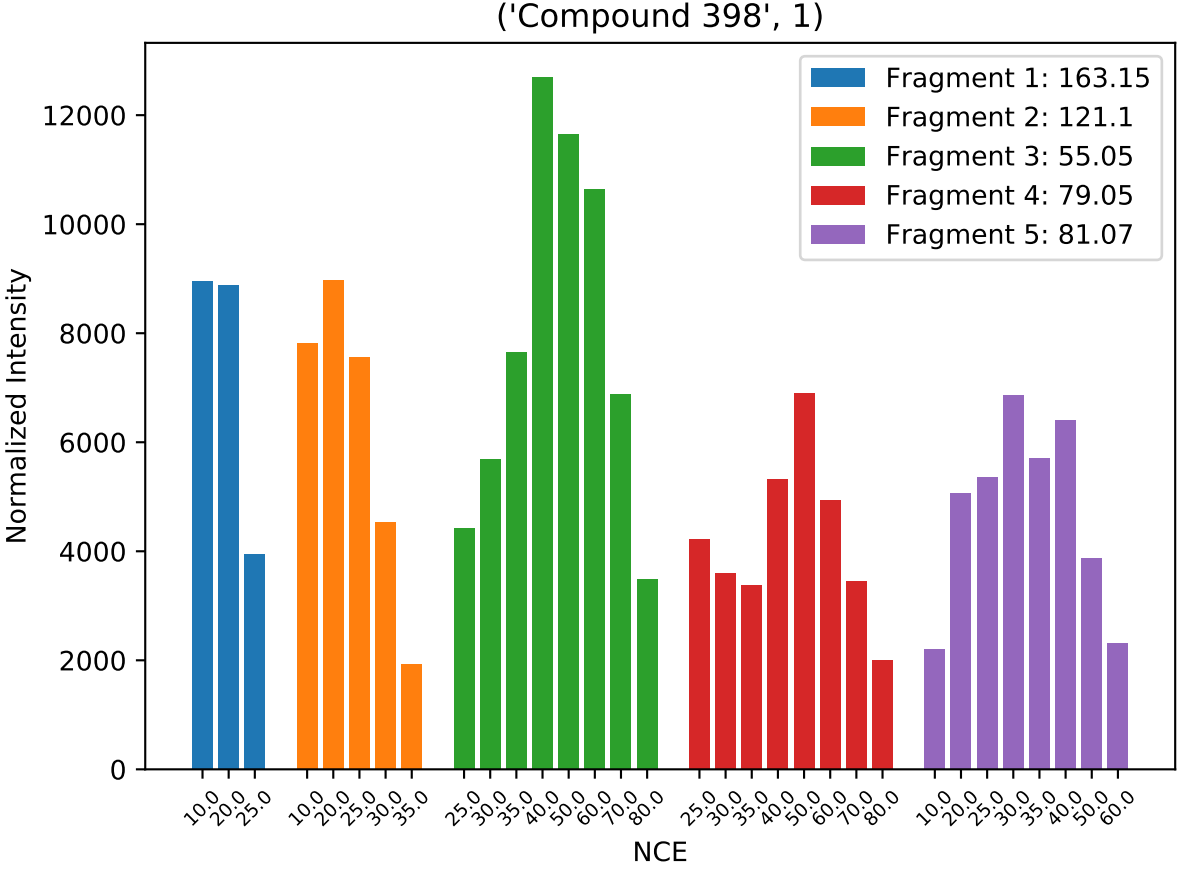

('Compound 505', 1)
Fragment 1: 75.08
Fragment 2: 75.07
Fragment 3: 75.09
Fragment 4: 73.06
Fragment 5: 57.05
Normalized Intensity
1750000
1500000
1250000
1000000
750000
500000
250000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 35.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
NCE

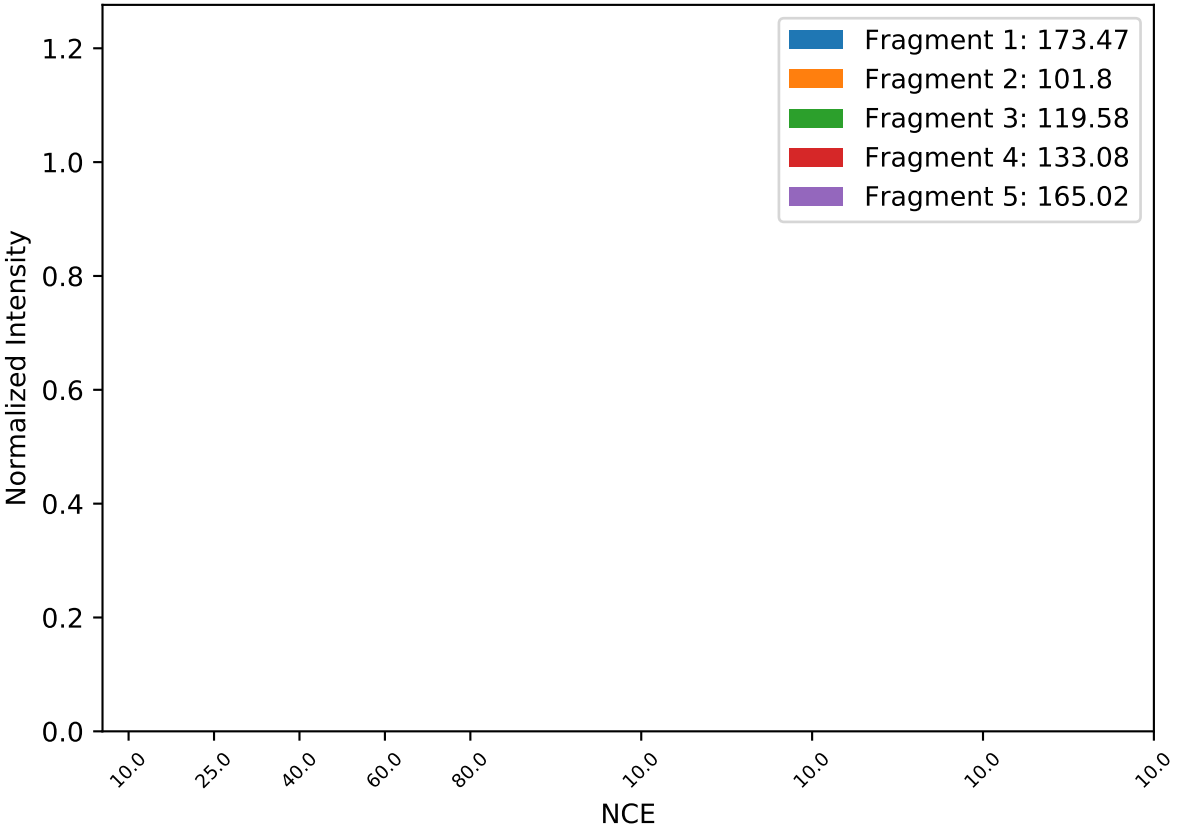

('Compound 506', 1)
Fragment 1: 345.06
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 301.07
Fragment 5: 173.46
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
25.0
30.0
35.0
40.0
50.0
40.0
50.0
60.0
70.0
NCE

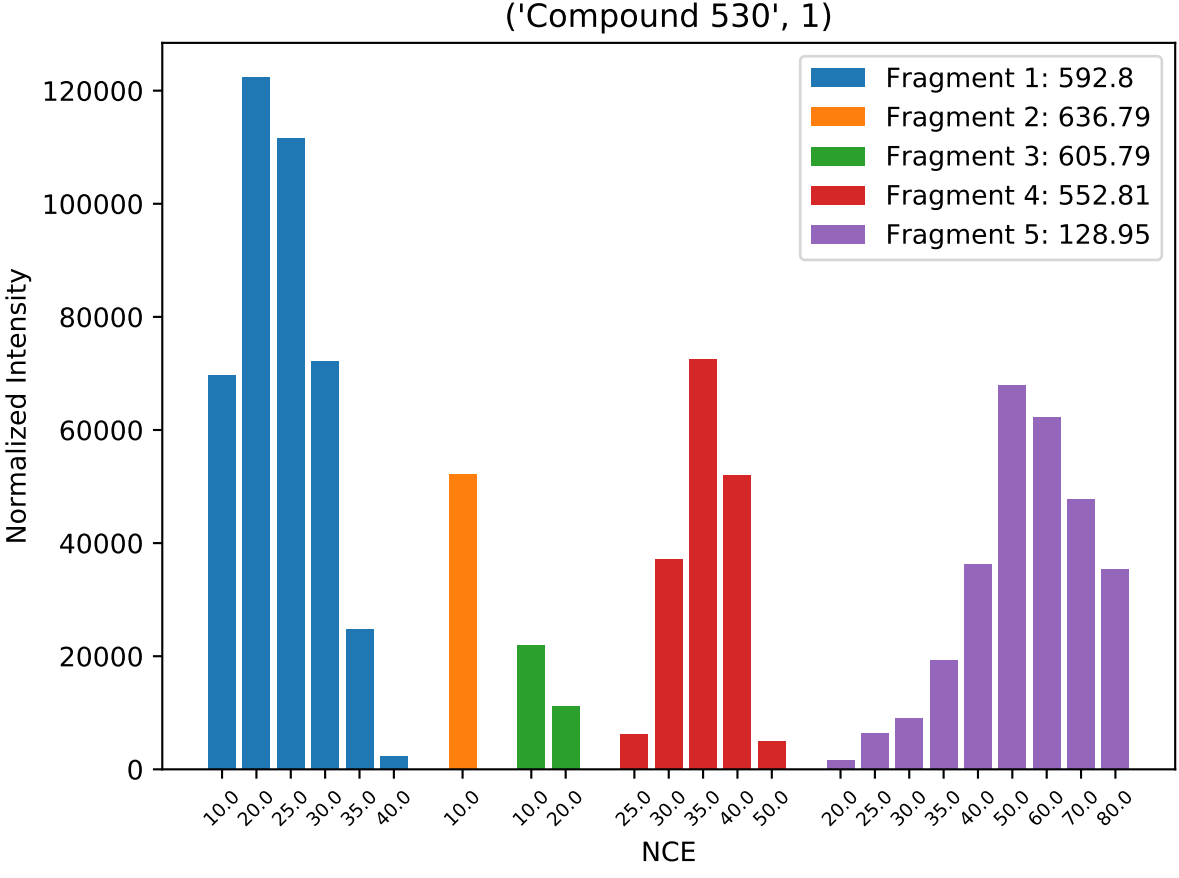

('Compound 507', 1)
Fragment 1: 314.92
Fragment 2: 216.95
Fragment 3: 173.47
Fragment 4: 156.97
Fragment 5: 234.96
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
NCE
10.0 20.0 25.0 30.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 35.0 40.0 50.0 60.0 70.0 80.0
70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

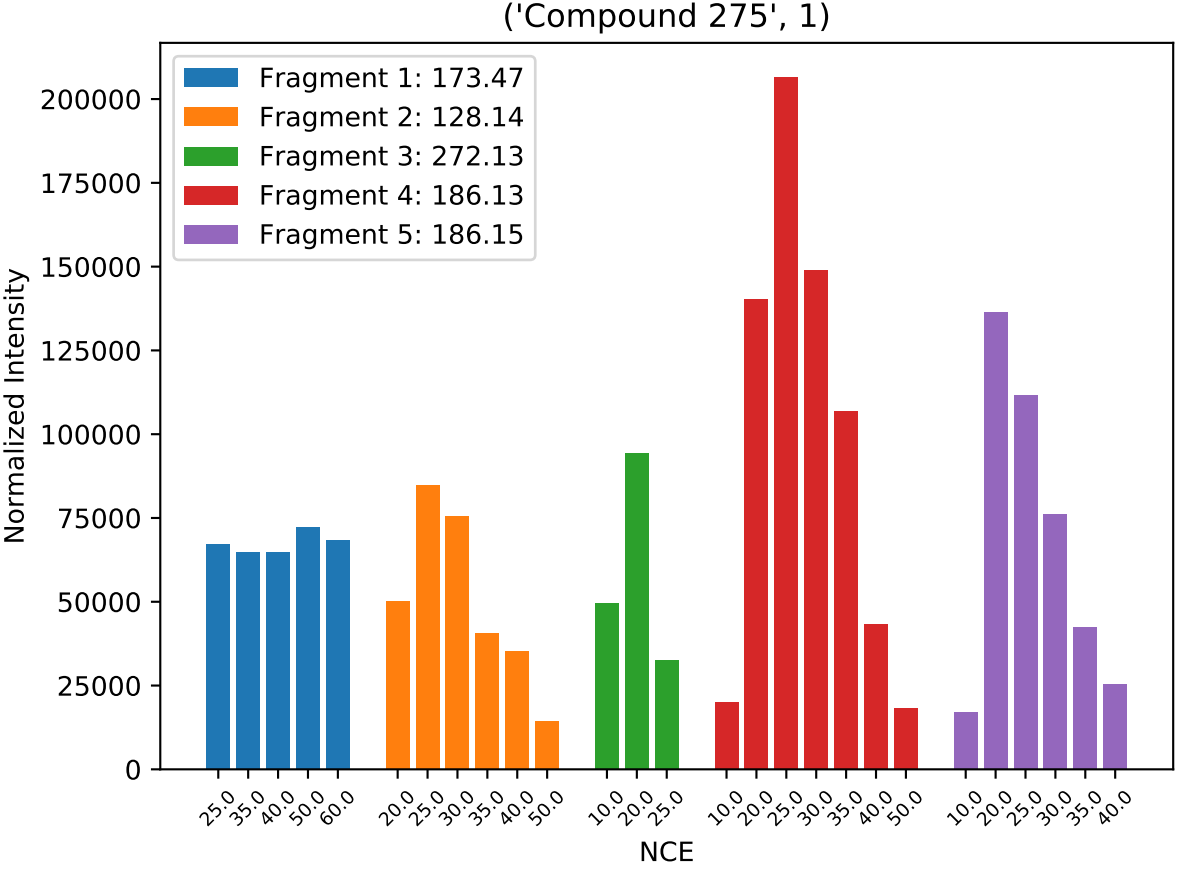

('Compound 508', 1)
Fragment 1: 173.47
Fragment 2: 217.08
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 216.03
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
20.0
25.0
35.0
40.0
60.0
80.0
10.0
20.0
25.0
10.0
30.0
50.0
10.0
30.0
50.0
70.0
10.0
20.0
25.0
NCE

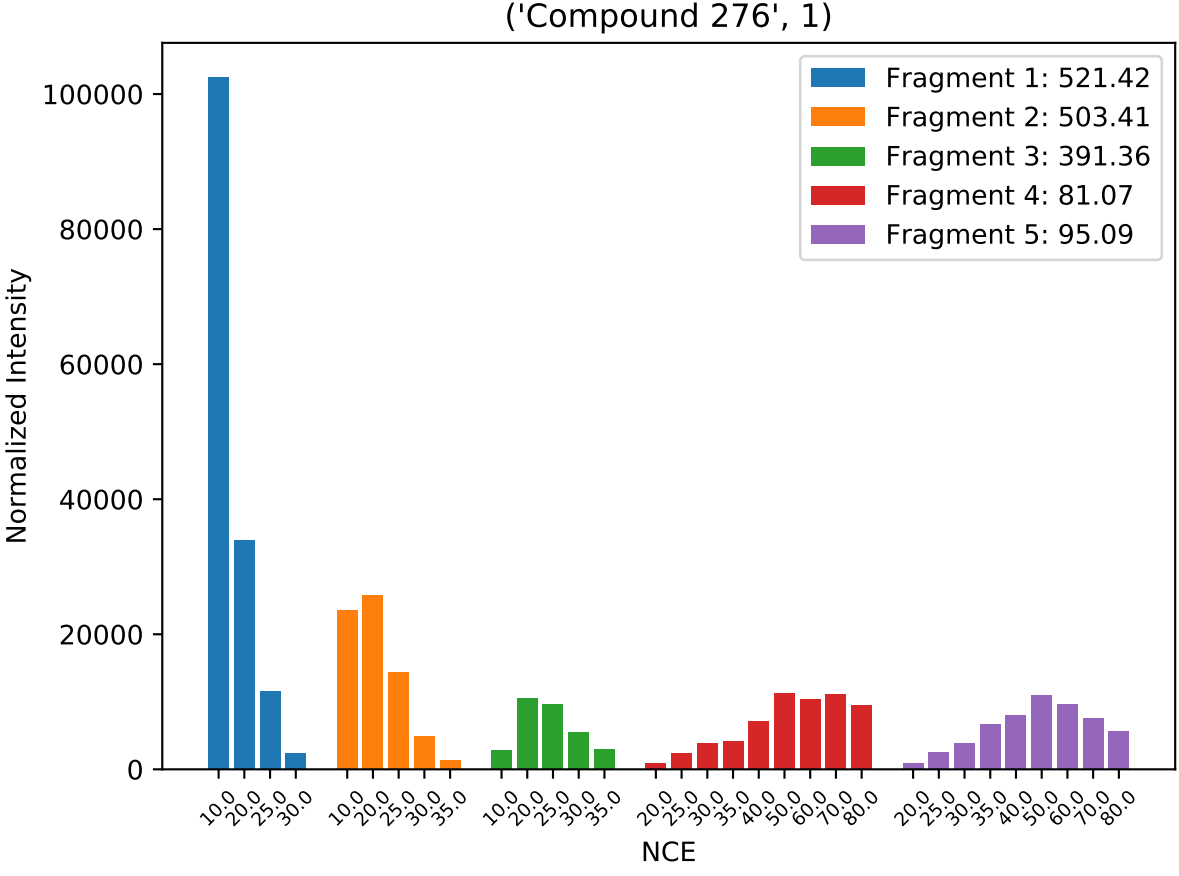

('Compound 390', 1)
Fragment 1: 150.06
Fragment 2: 94.06
Fragment 3: 122.06
Fragment 4: 94.07
Fragment 5: 67.05
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0 20.0 25.0 30.0 35.0 40.0
40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

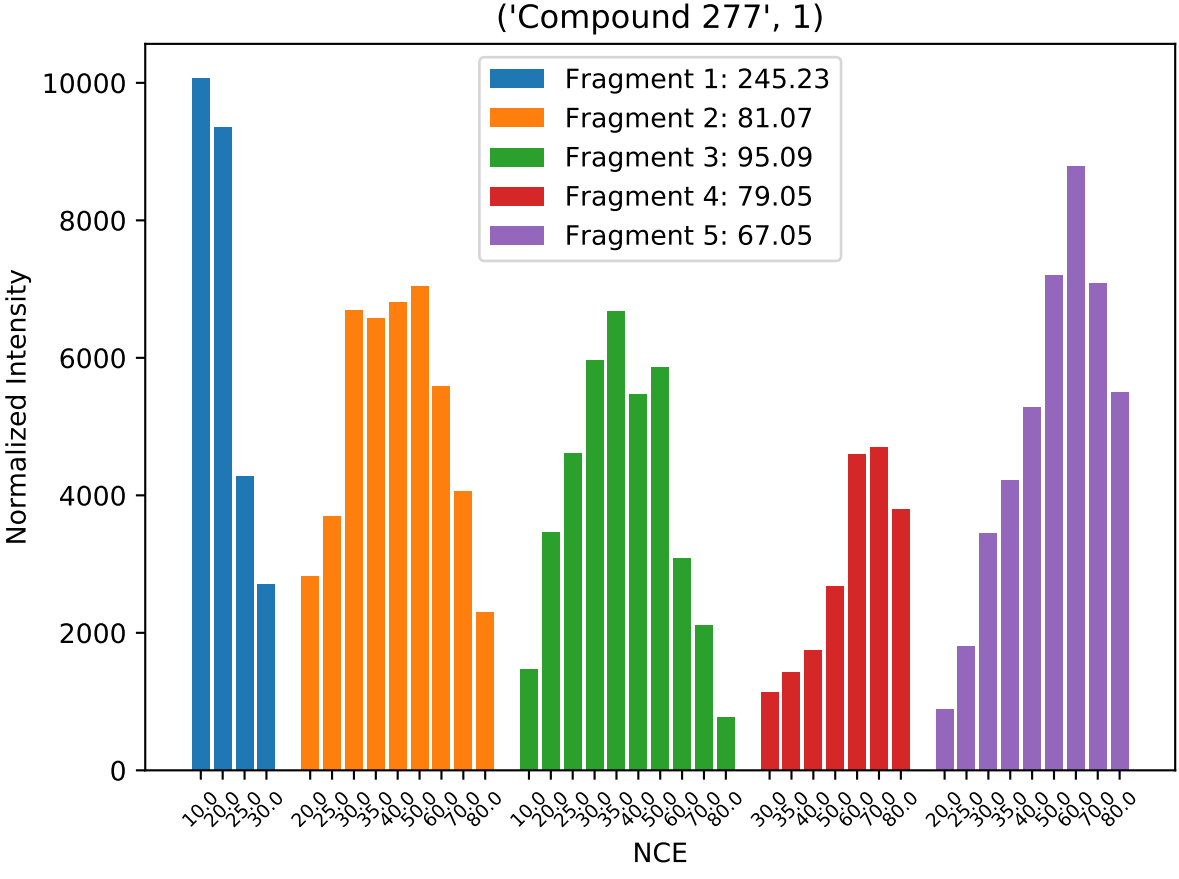

('Compound 398', 1)
Fragment 1: 163.15
Fragment 2: 121.1
Fragment 3: 55.05
Fragment 4: 79.05
Fragment 5: 81.07
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0 20.0 25.0
10.0 20.0 25.0 30.0 35.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

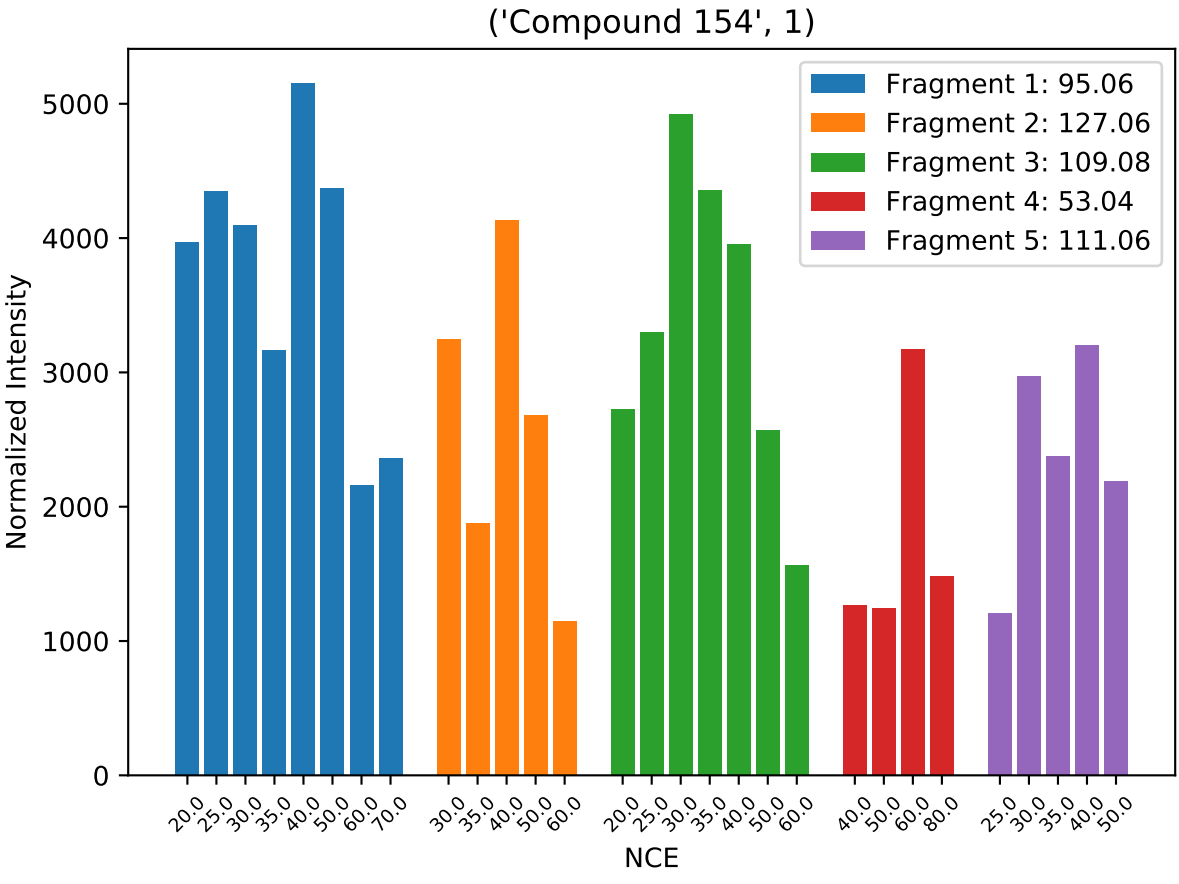

('Compound 272', 1)
Fragment 1: 173.47
Fragment 2: 101.8
Fragment 3: 119.58
Fragment 4: 133.08
Fragment 5: 165.02
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
25.0
40.0
60.0
80.0
10.0
10.0
10.0
10.0
NCE

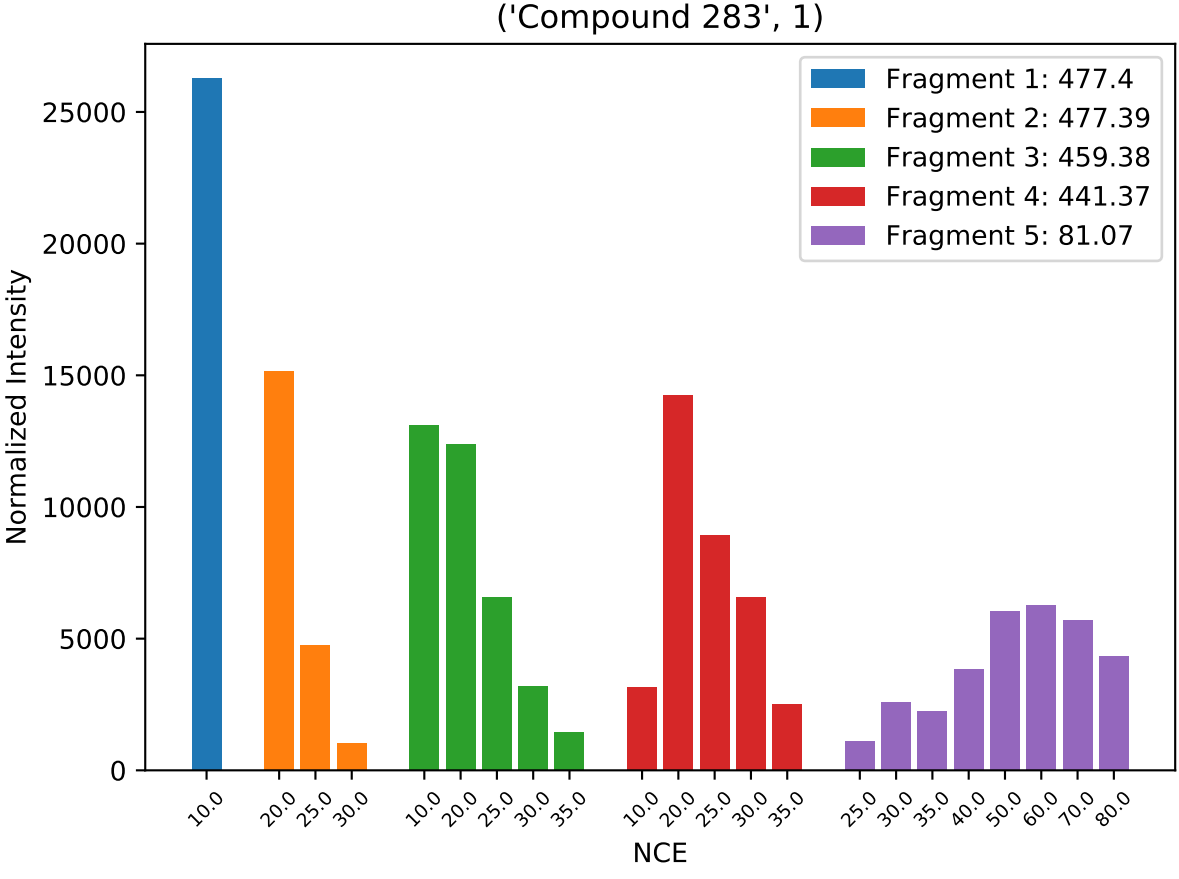

('Compound 530', 1)
Fragment 1: 592.8
Fragment 2: 636.79
Fragment 3: 605.79
Fragment 4: 552.81
Fragment 5: 128.95
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

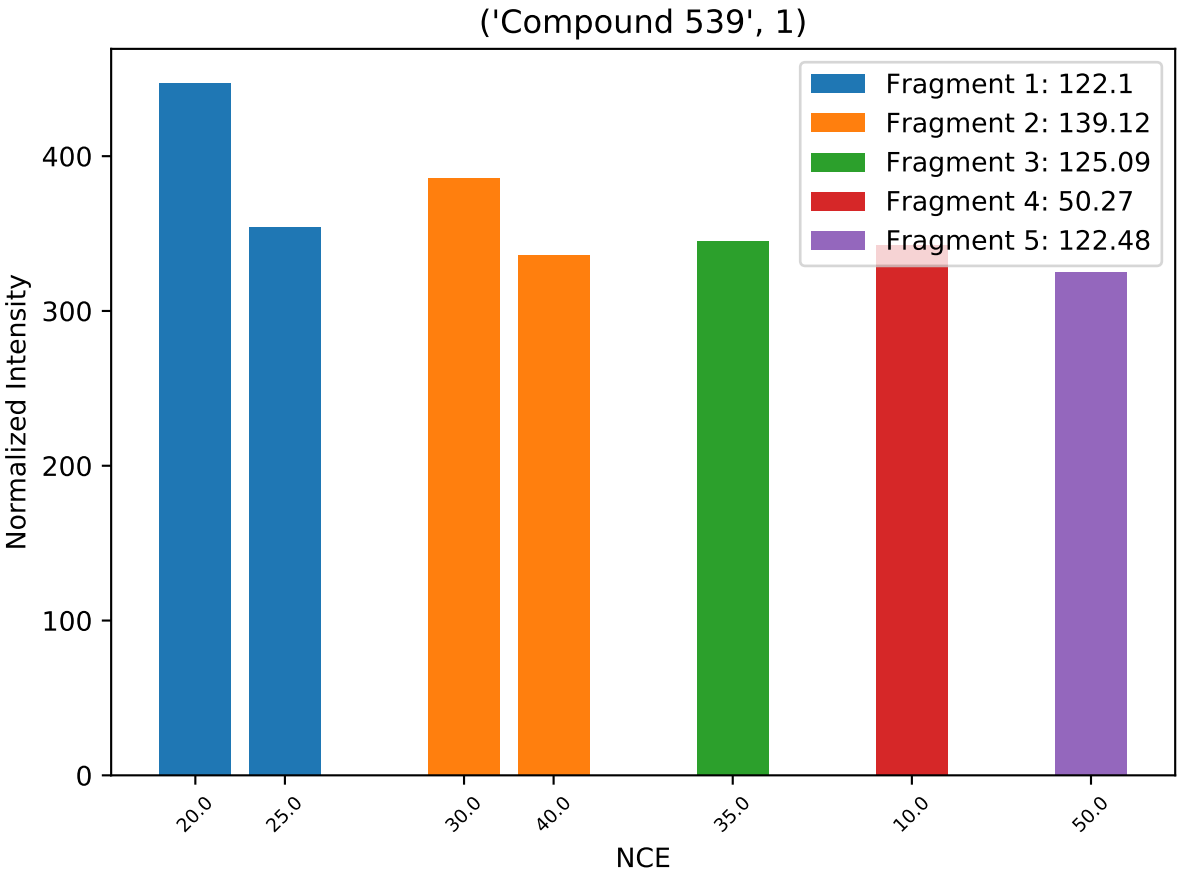

('Compound 275', 1)
Fragment 1: 173.47
Fragment 2: 128.14
Fragment 3: 272.13
Fragment 4: 186.13
Fragment 5: 186.15
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
200000
25.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

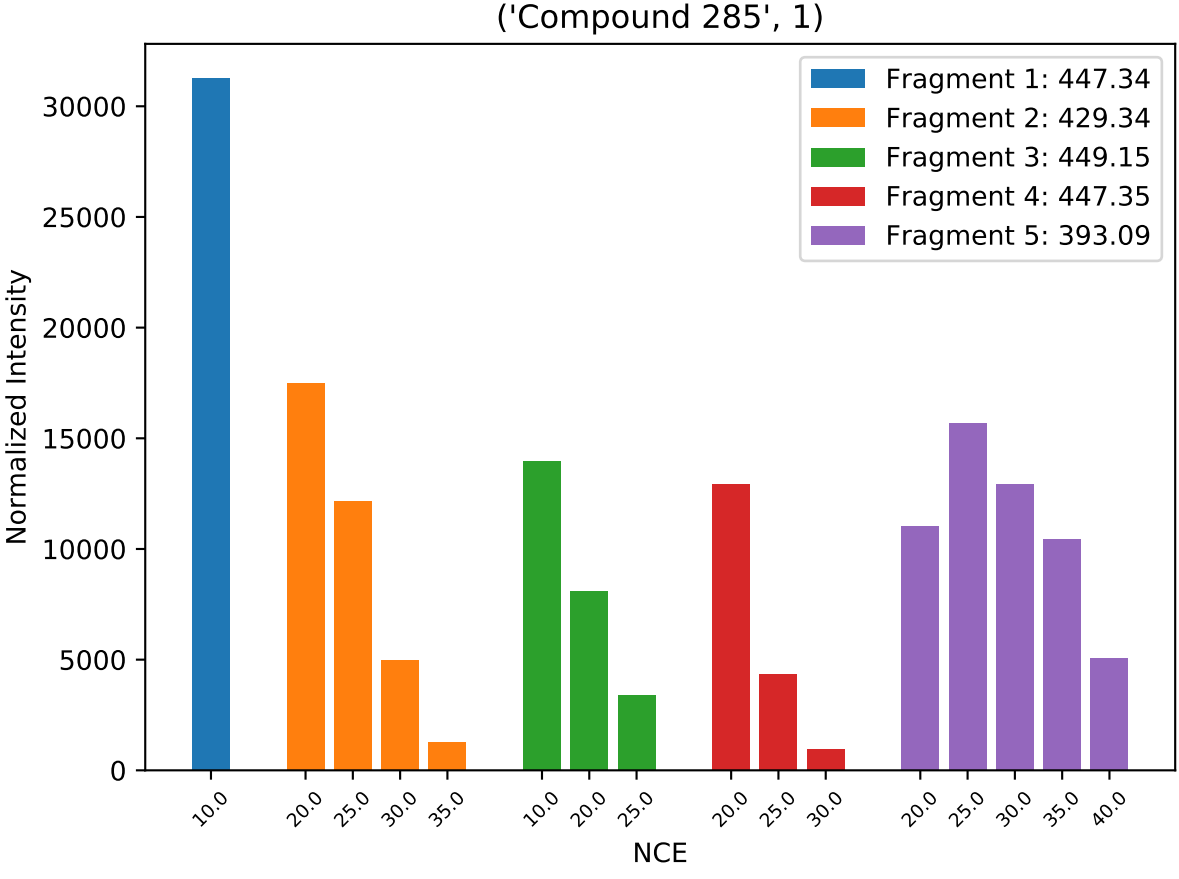

('Compound 276', 1)
Fragment 1: 521.42
Fragment 2: 503.41
Fragment 3: 391.36
Fragment 4: 81.07
Fragment 5: 95.09
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

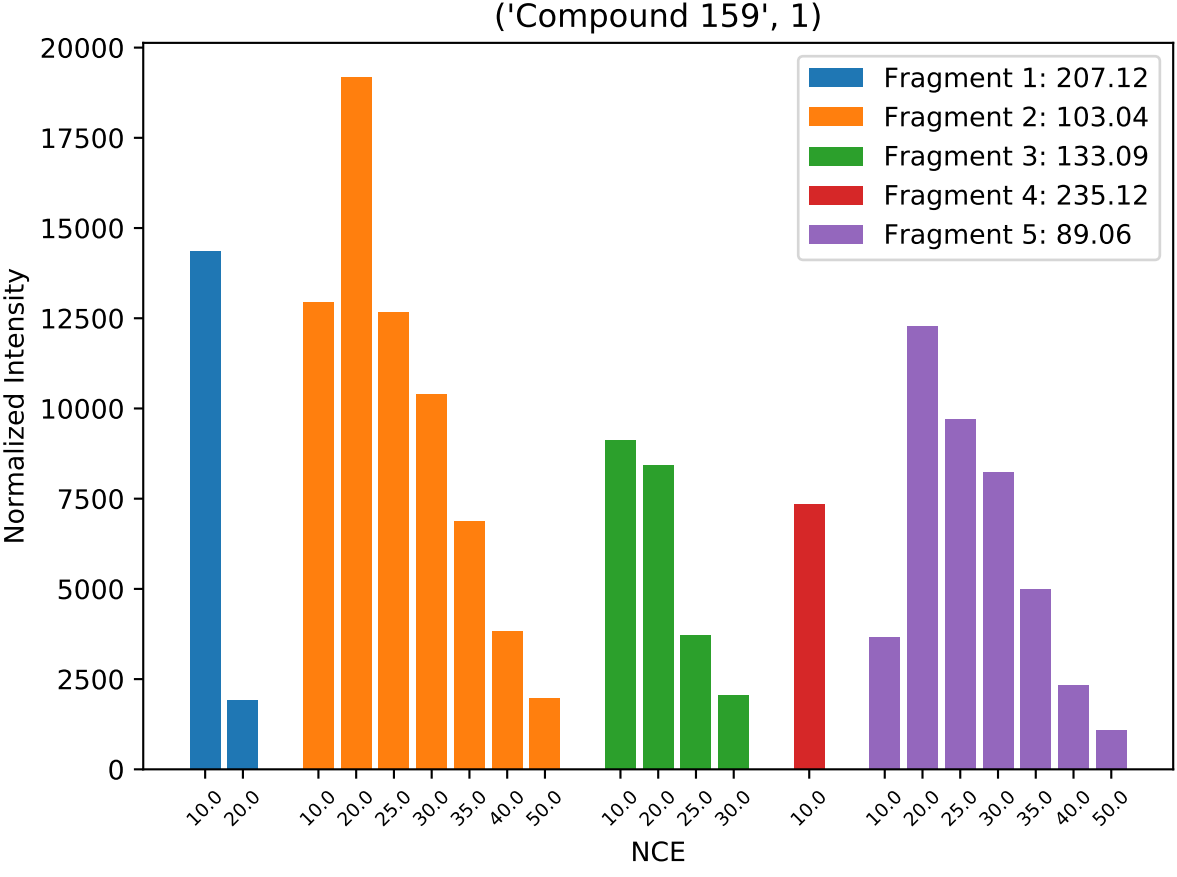

('Compound 277', 1)
Fragment 1: 245.23
Fragment 2: 81.07
Fragment 3: 95.09
Fragment 4: 79.05
Fragment 5: 67.05
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0 20.0 25.0 30.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

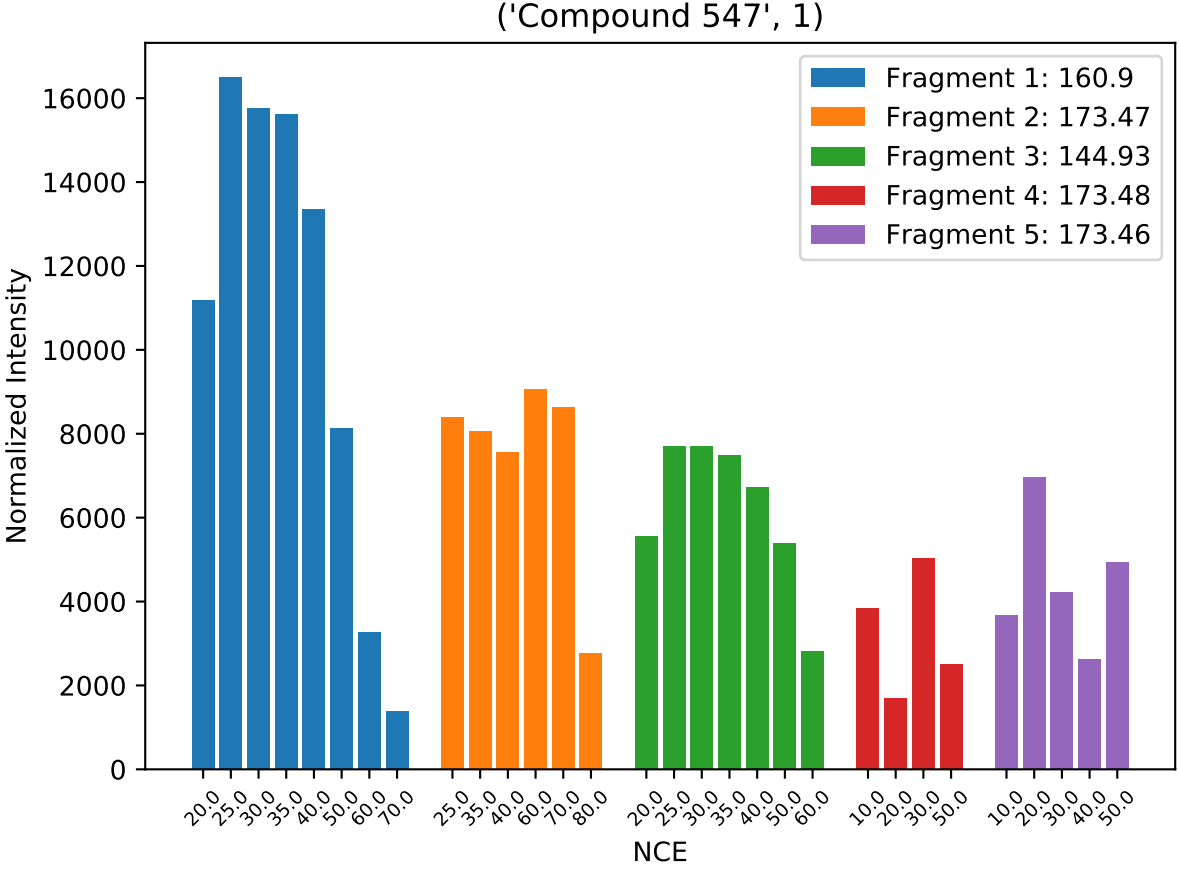

('Compound 154', 1)
Fragment 1: 95.06
Fragment 2: 127.06
Fragment 3: 109.08
Fragment 4: 53.04
Fragment 5: 111.06
Normalized Intensity
0
1000
2000
3000
4000
5000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
40.0 50.0 60.0 80.0
25.0 30.0 35.0 40.0 50.0
NCE

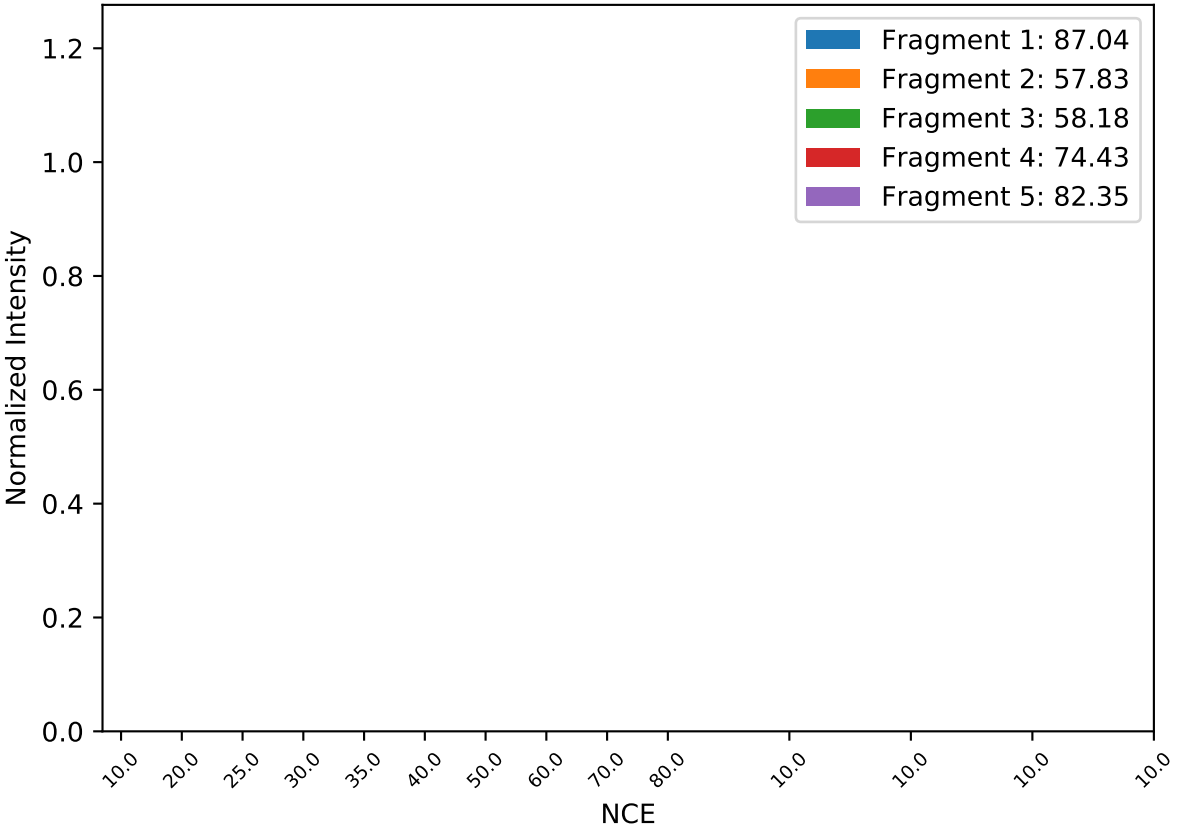

('Compound 283', 1)
Fragment 1: 477.4
Fragment 2: 477.39
Fragment 3: 459.38
Fragment 4: 441.37
Fragment 5: 81.07
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

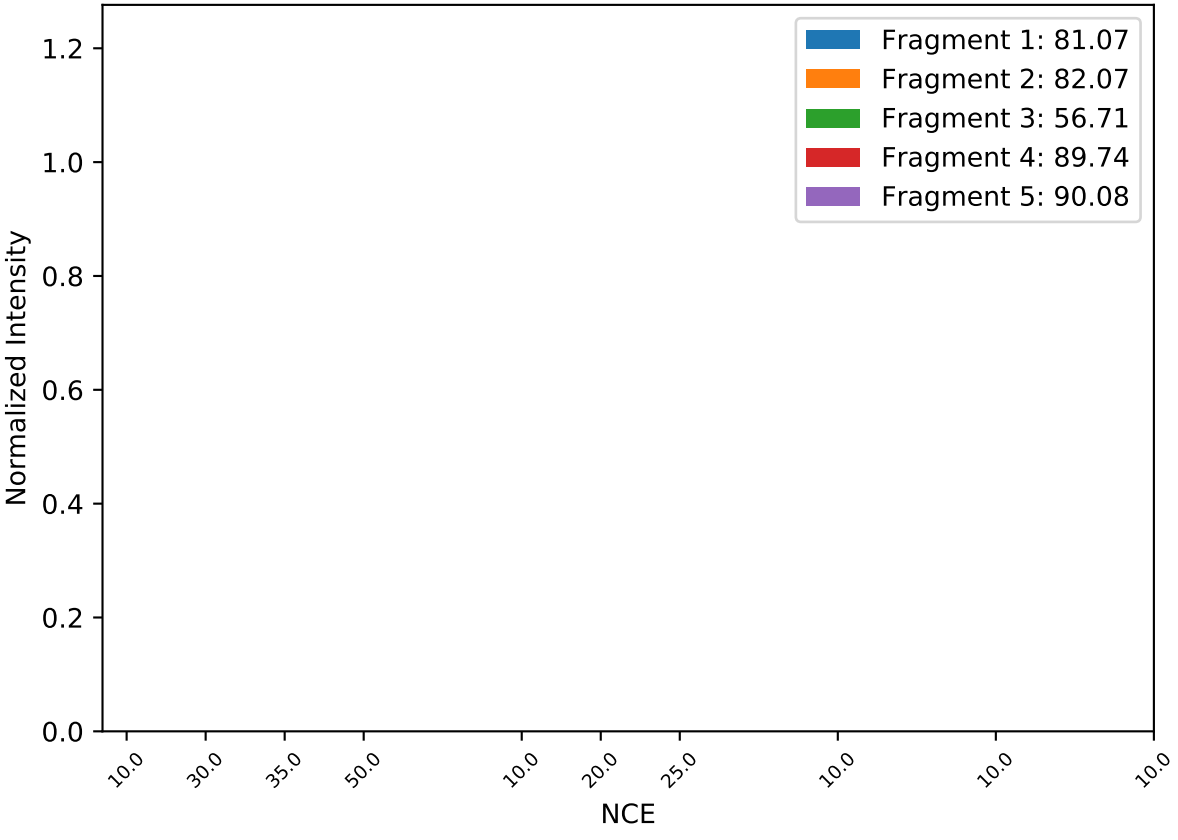

('Compound 539', 1)
Fragment 1: 122.1
Fragment 2: 139.12
Fragment 3: 125.09
Fragment 4: 50.27
Fragment 5: 122.48
Normalized Intensity
0
100
200
300
400
20.0
25.0
30.0
40.0
35.0
10.0
50.0
NCE

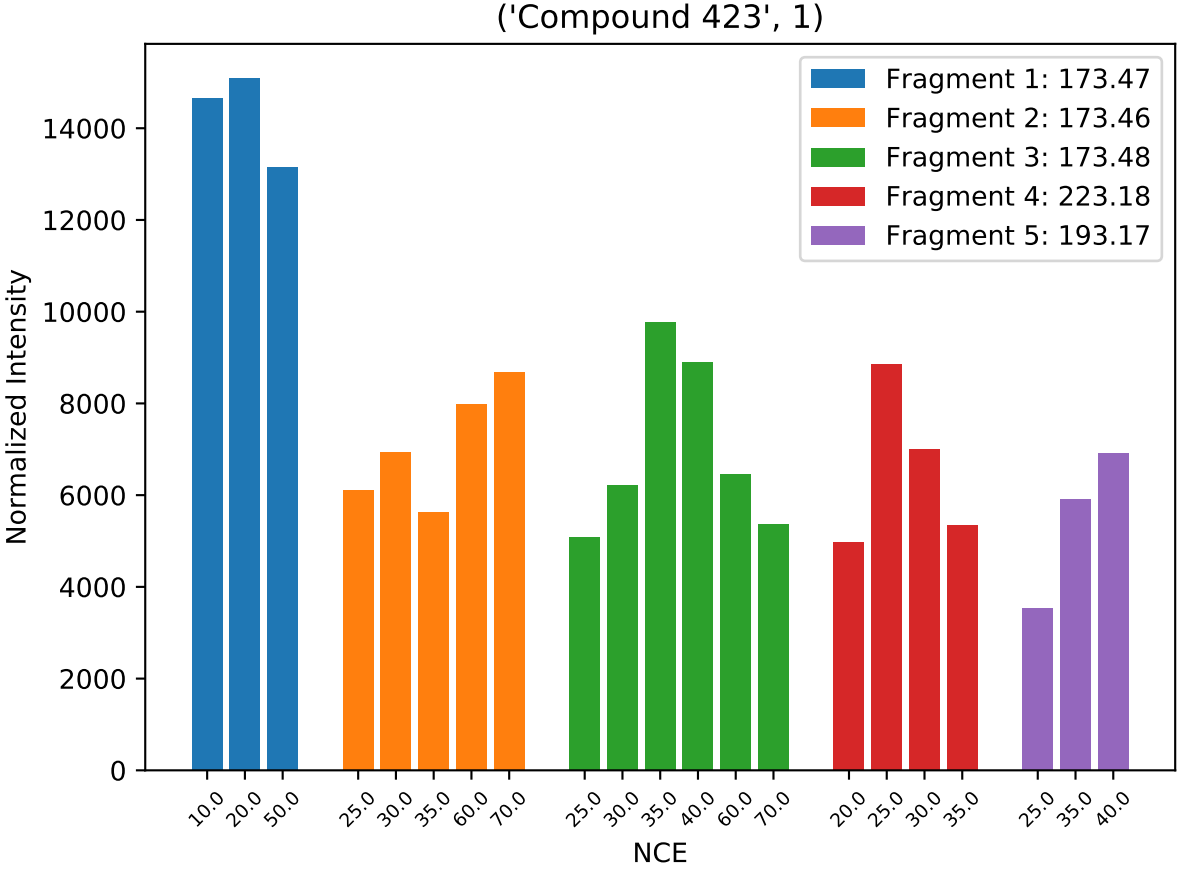

('Compound 285', 1)
Fragment 1: 447.34
Fragment 2: 429.34
Fragment 3: 449.15
Fragment 4: 447.35
Fragment 5: 393.09
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
20.0
25.0
30.0
20.0
25.0
30.0
35.0
40.0
NCE

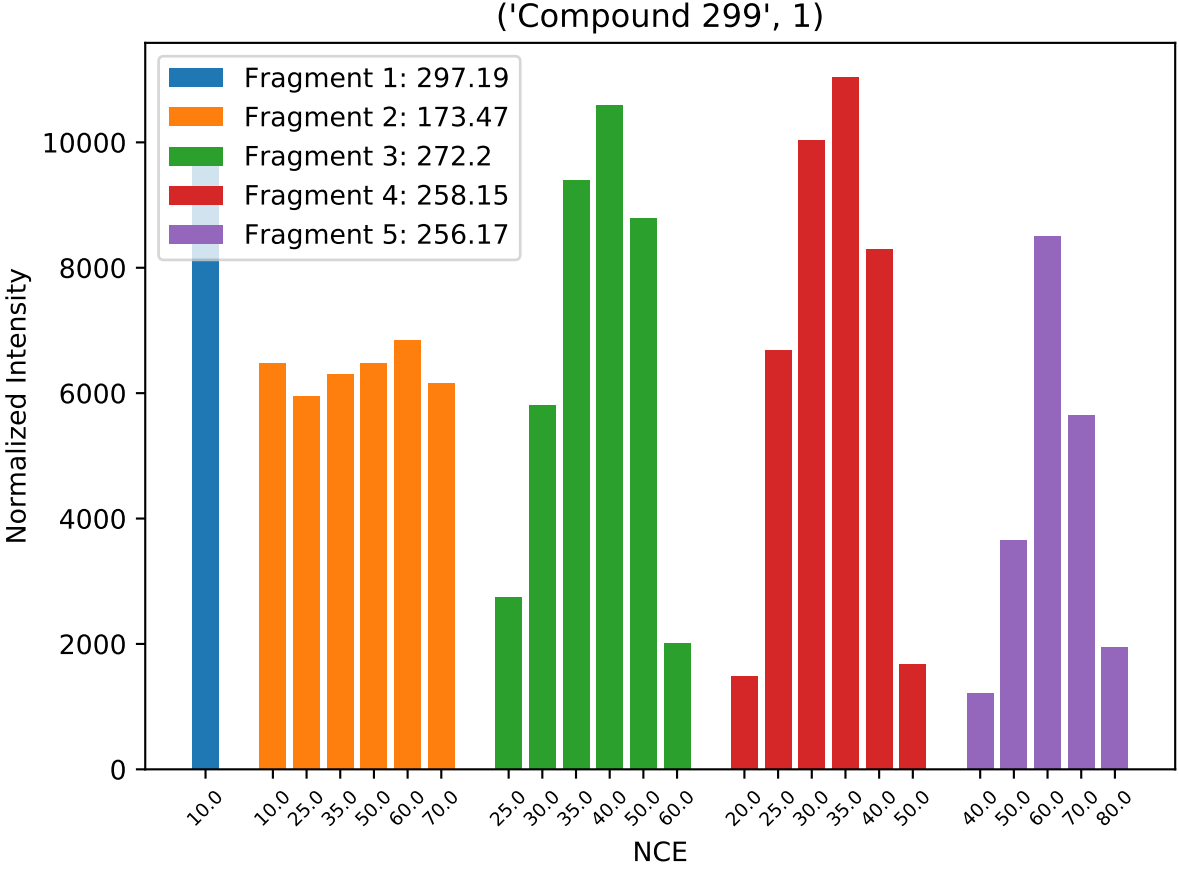

('Compound 159', 1)
Fragment 1: 207.12
Fragment 2: 103.04
Fragment 3: 133.09
Fragment 4: 235.12
Fragment 5: 89.06
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
10.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

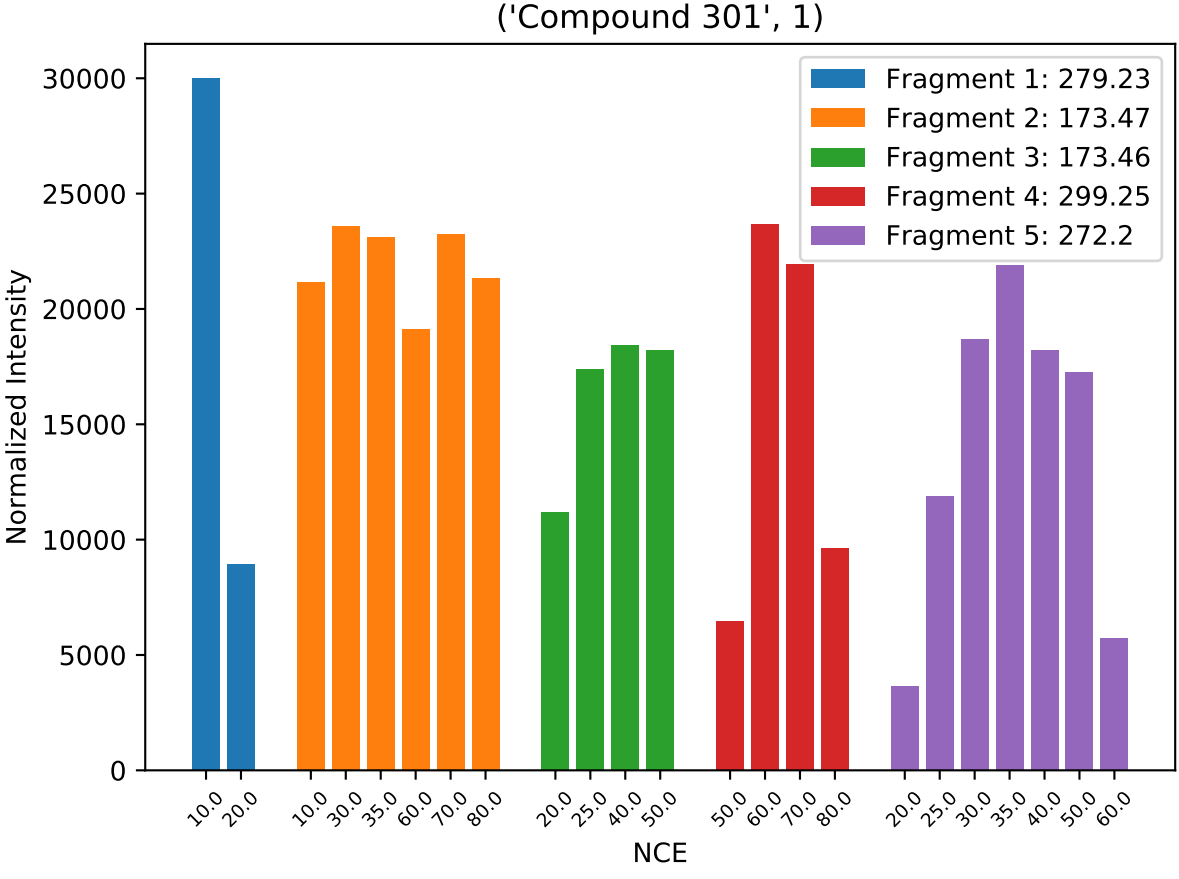

('Compound 547', 1)
Fragment 1: 160.9
Fragment 2: 173.47
Fragment 3: 144.93
Fragment 4: 173.48
Fragment 5: 173.46
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 35.0 40.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 30.0 50.0
10.0 20.0 30.0 40.0 50.0
NCE

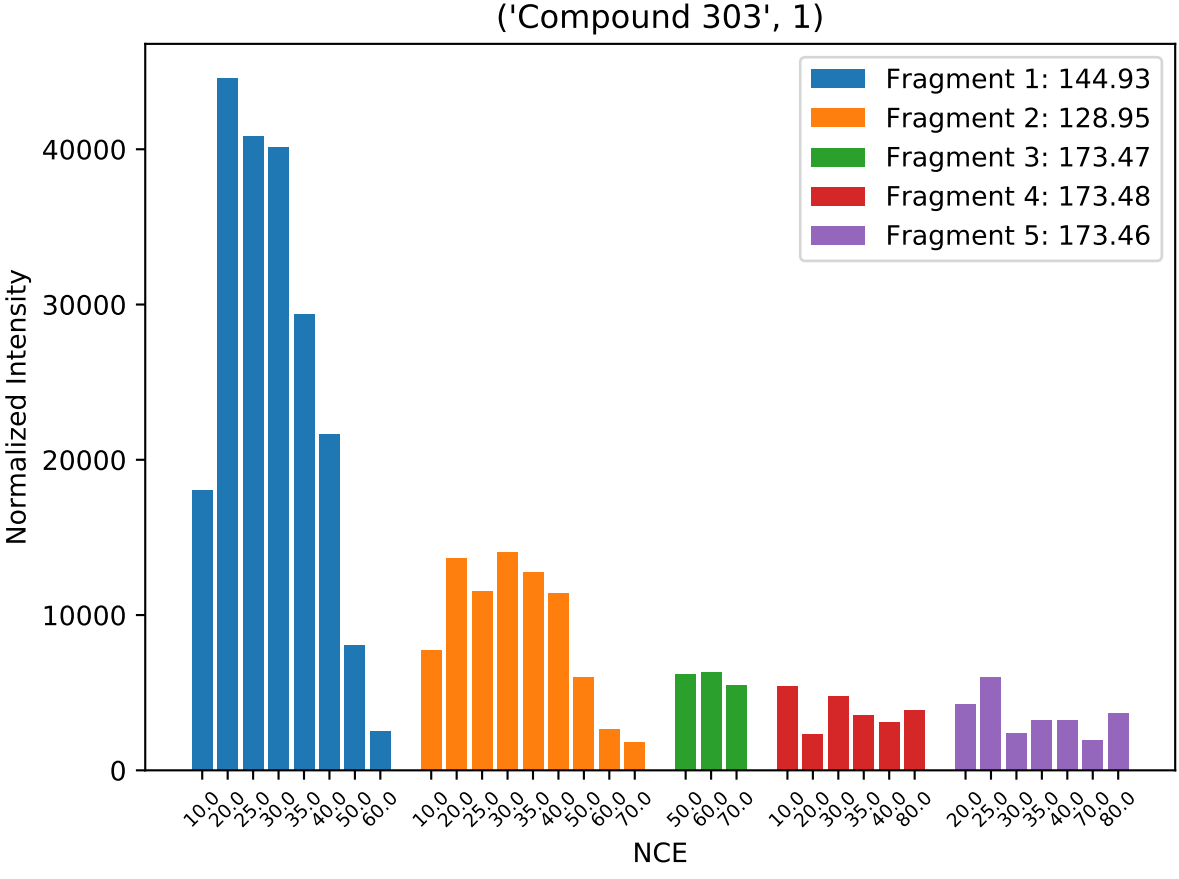

('Compound 420', 1)
Fragment 1: 87.04
Fragment 2: 57.83
Fragment 3: 58.18
Fragment 4: 74.43
Fragment 5: 82.35
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
10.0
10.0
10.0
NCE

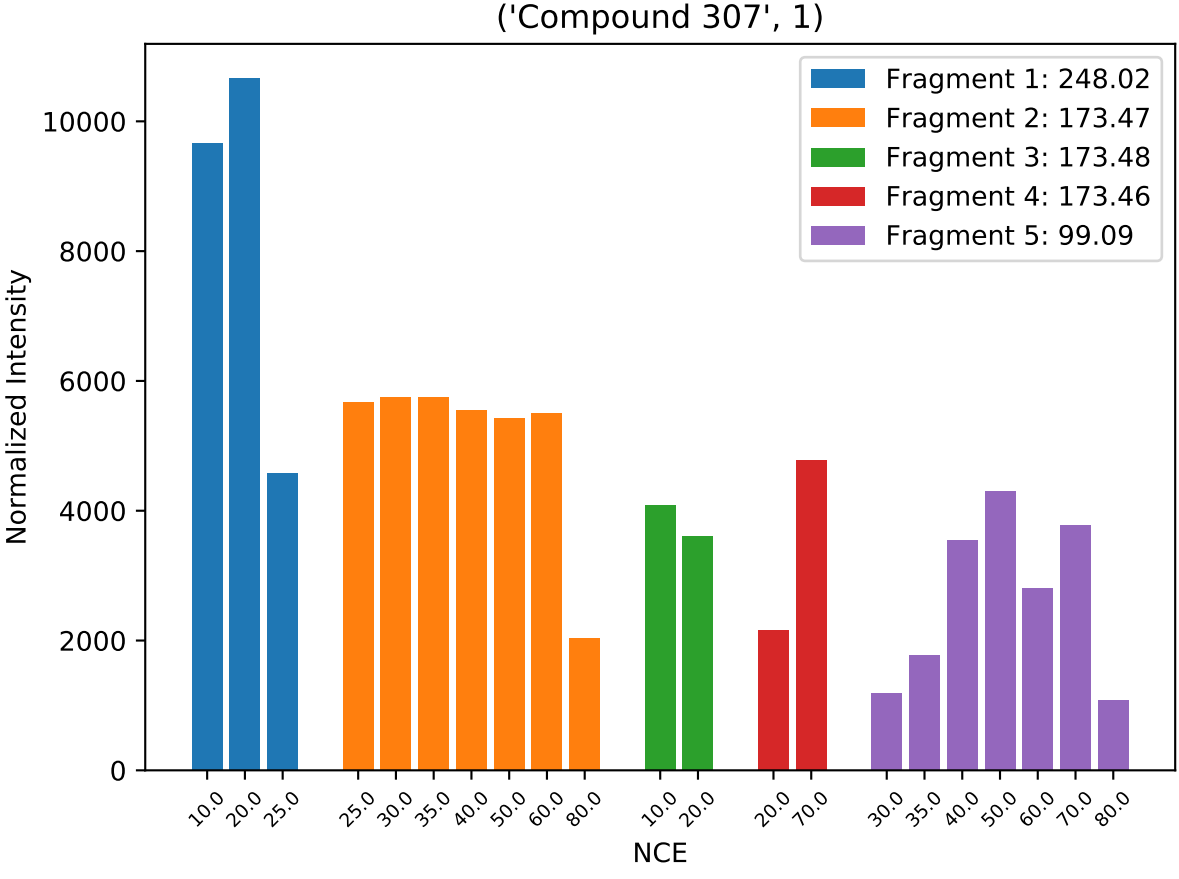

('Compound 422', 1)
Fragment 1: 81.07
Fragment 2: 82.07
Fragment 3: 56.71
Fragment 4: 89.74
Fragment 5: 90.08
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
30.0
35.0
50.0
10.0
20.0
25.0
10.0
10.0
10.0
NCE

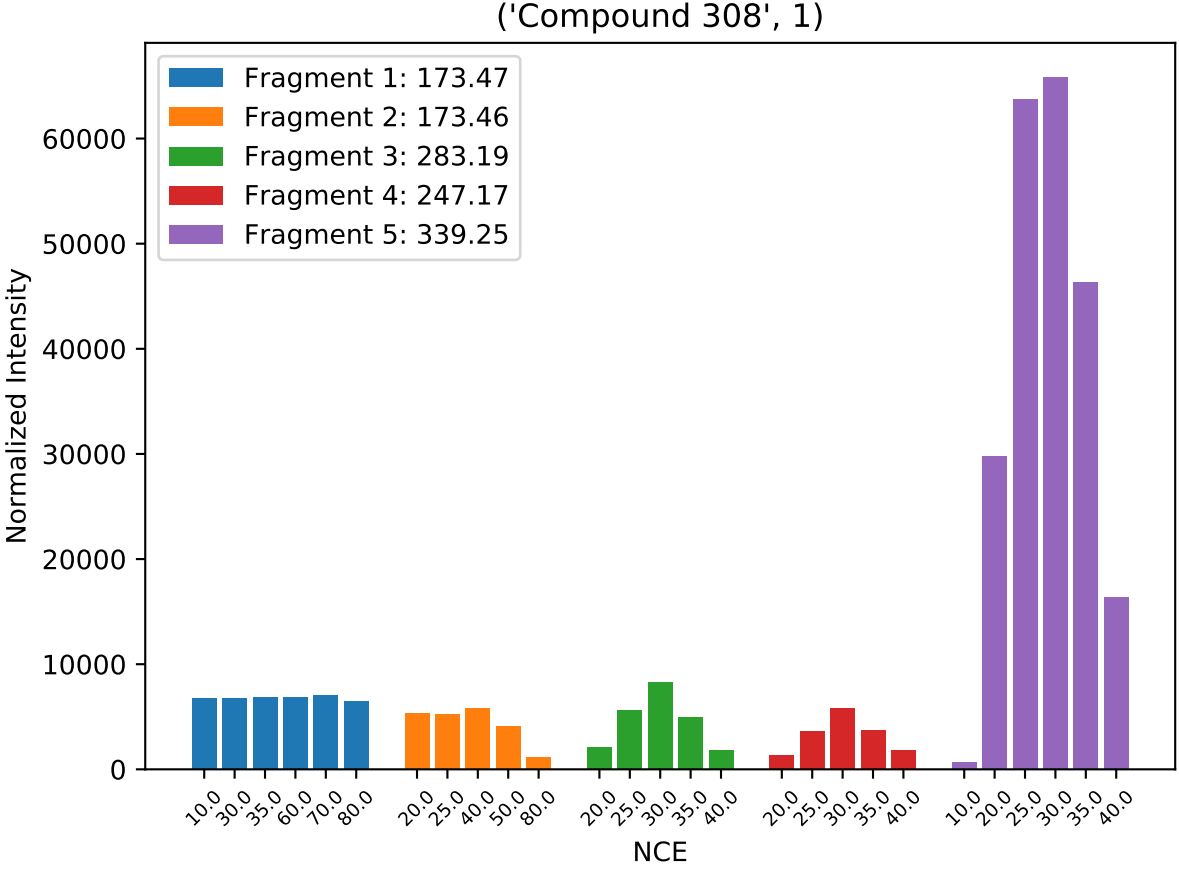

('Compound 423', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 173.48
Fragment 4: 223.18
Fragment 5: 193.17
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
50.0
25.0
30.0
35.0
60.0
70.0
25.0
30.0
35.0
40.0
60.0
70.0
20.0
25.0
30.0
35.0
25.0
35.0
40.0
NCE

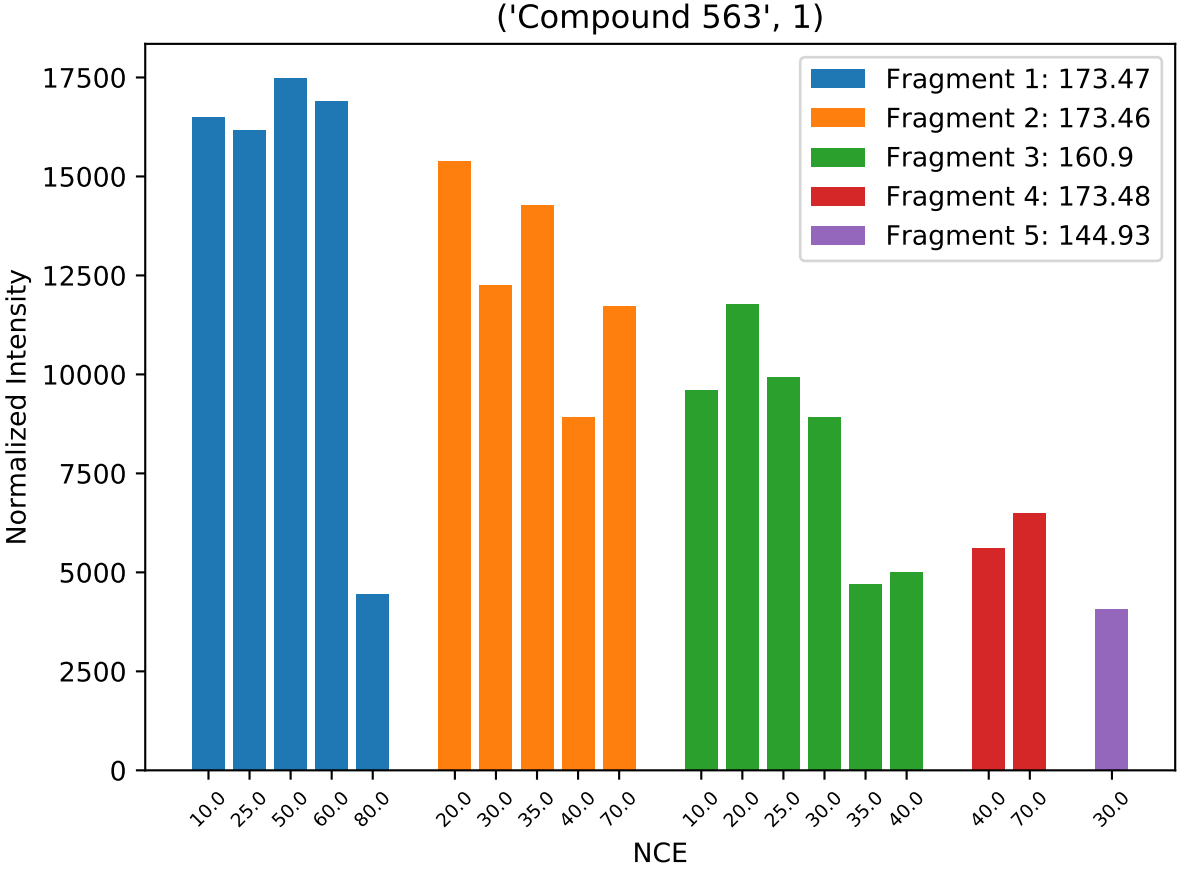

('Compound 299', 1)
Fragment 1: 297.19
Fragment 2: 173.47
Fragment 3: 272.2
Fragment 4: 258.15
Fragment 5: 256.17
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
10.0
25.0
35.0
50.0
60.0
70.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
40.0
50.0
60.0
70.0
80.0
NCE

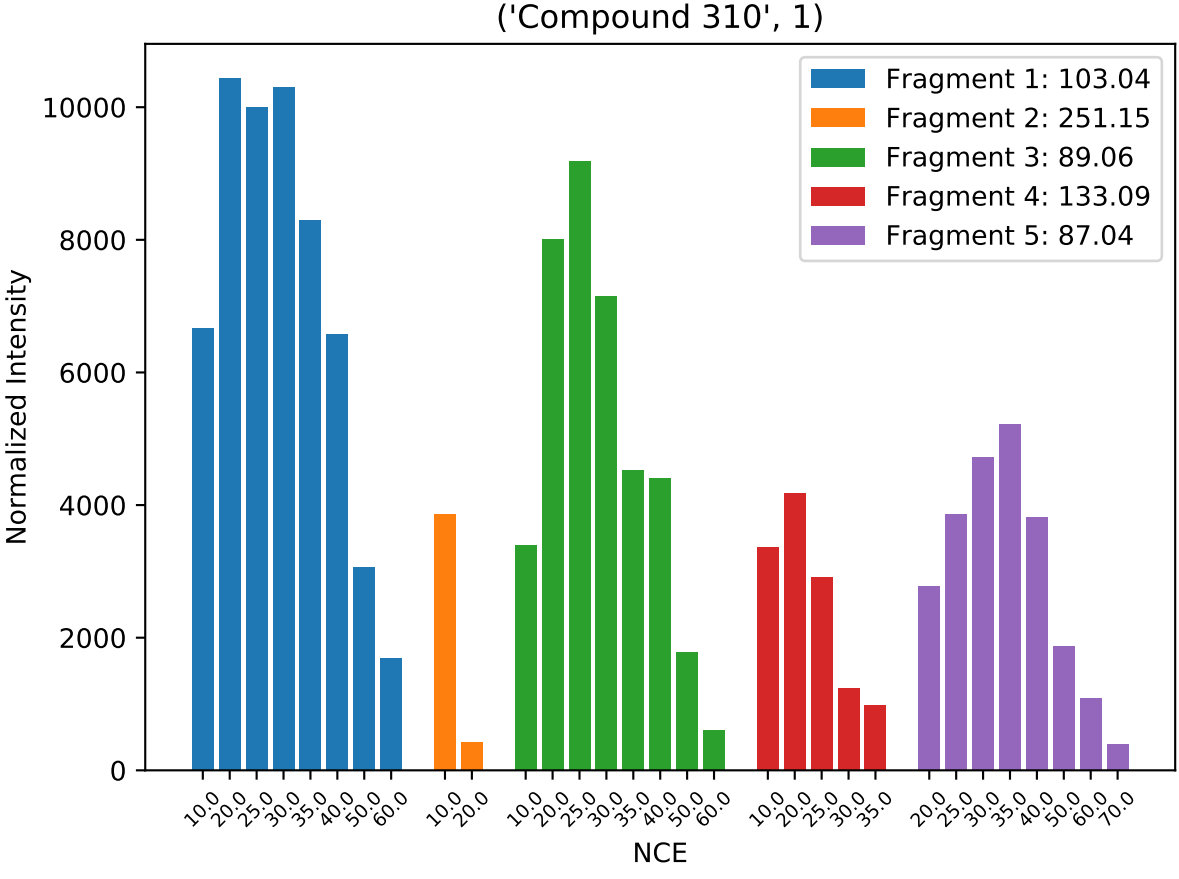

('Compound 301', 1)
Fragment 1: 279.23
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 299.25
Fragment 5: 272.2
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0
20.0
10.0
30.0
35.0
60.0
70.0
80.0
20.0
25.0
40.0
50.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

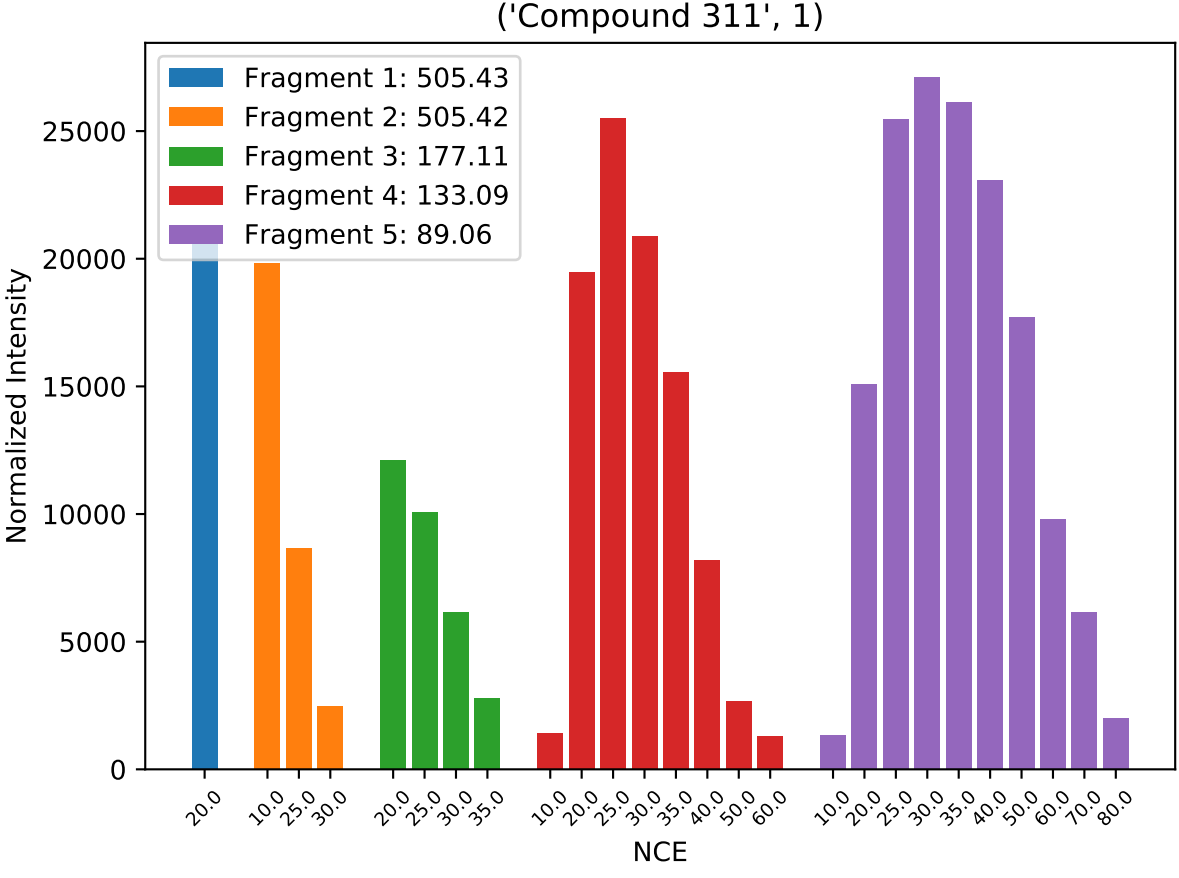

('Compound 303', 1)
Fragment 1: 144.93
Fragment 2: 128.95
Fragment 3: 173.47
Fragment 4: 173.48
Fragment 5: 173.46
Normalized Intensity
0
10000
20000
30000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
50.0 60.0 70.0
10.0 20.0 30.0 35.0 40.0 80.0
20.0 25.0 30.0 35.0 40.0 70.0 80.0
NCE

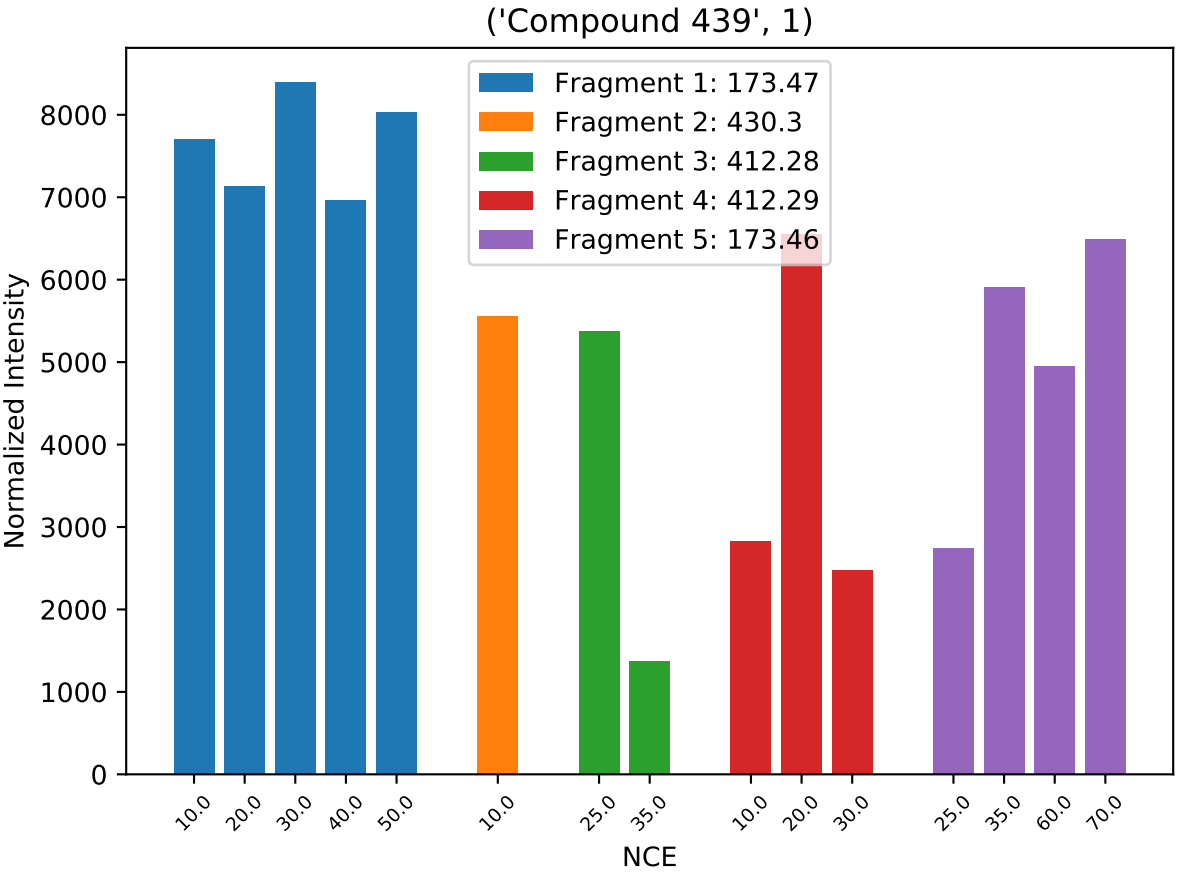

('Compound 307', 1)
Fragment 1: 248.02
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 99.09
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
20.0
25.0
25.0
30.0
35.0
40.0
50.0
60.0
80.0
10.0
20.0
20.0
70.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

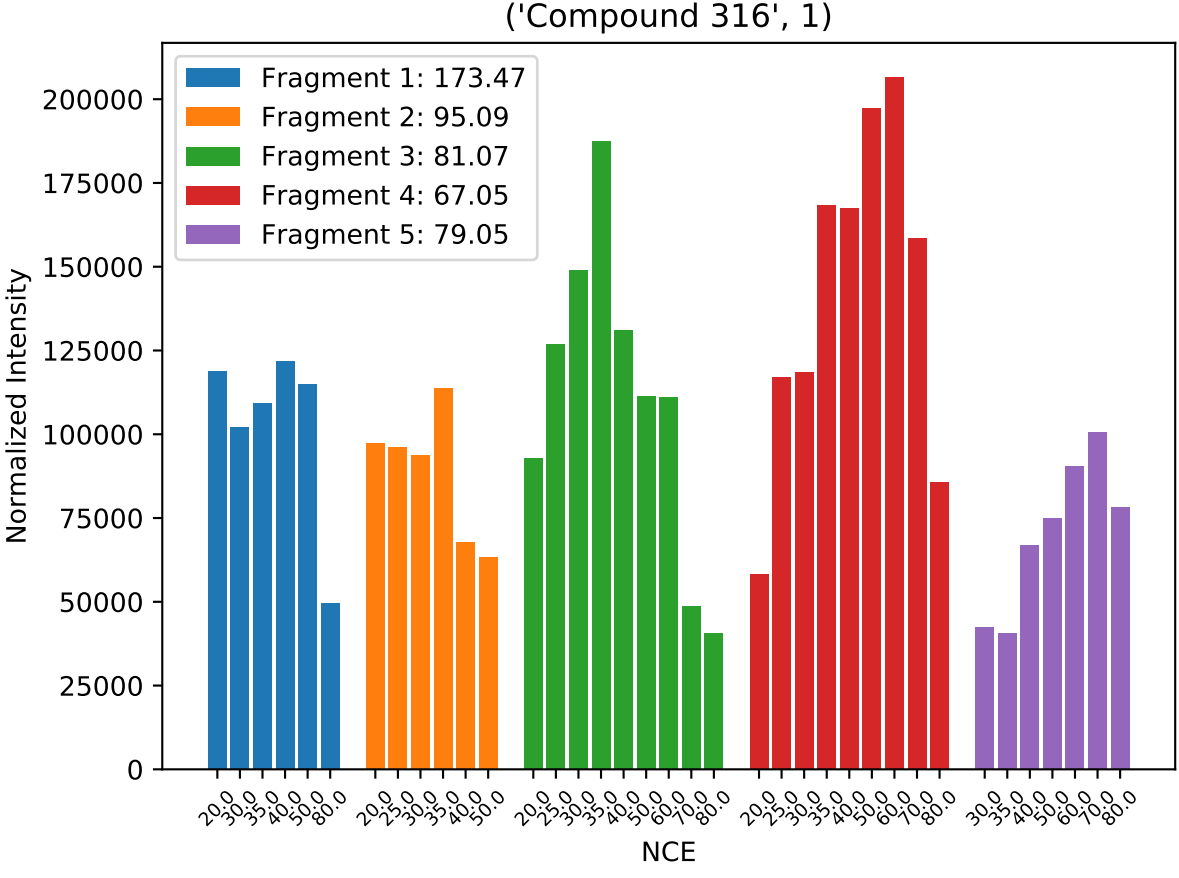

('Compound 308', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 283.19
Fragment 4: 247.17
Fragment 5: 339.25
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
10.0
30.0
35.0
60.0
70.0
80.0
20.0
25.0
40.0
50.0
80.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
NCE

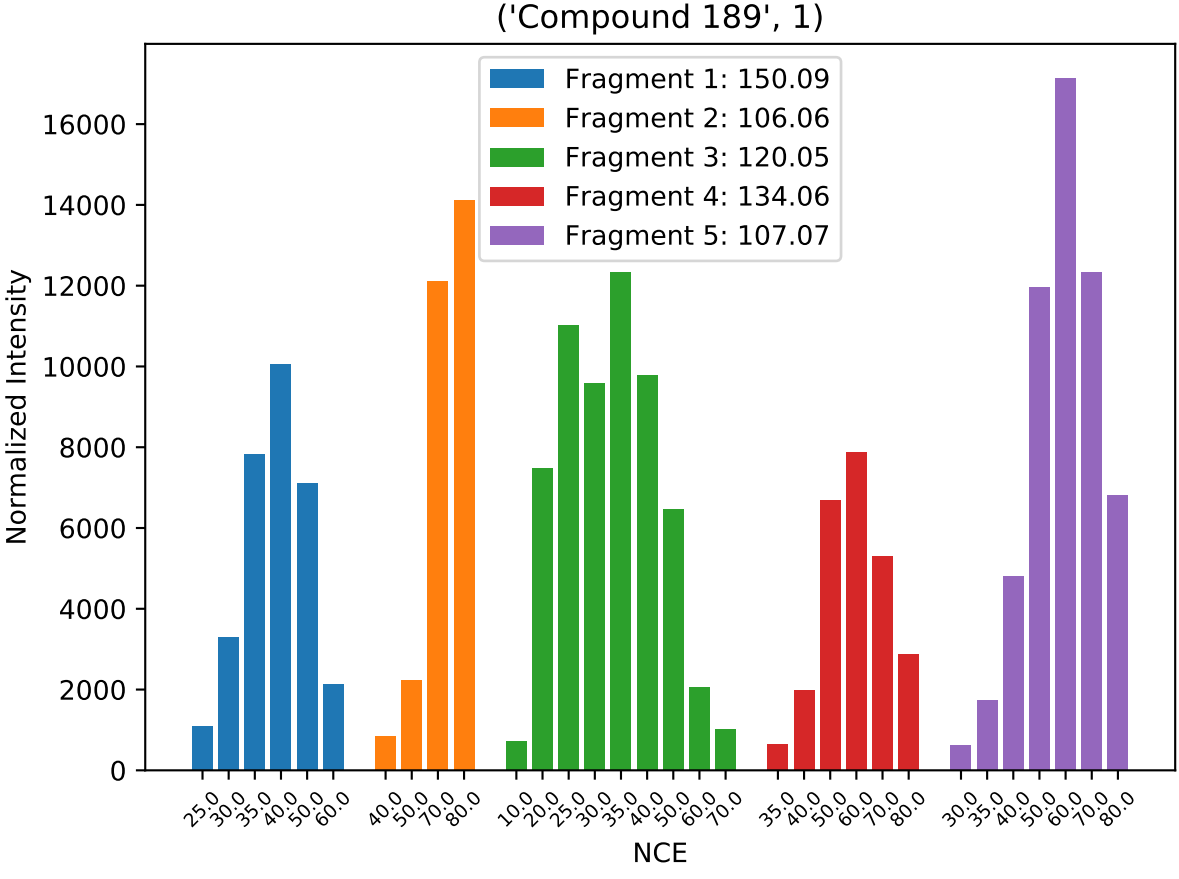

('Compound 563', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 160.9
Fragment 4: 173.48
Fragment 5: 144.93
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0
25.0
50.0
60.0
80.0
20.0
30.0
35.0
40.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
40.0
70.0
30.0
NCE

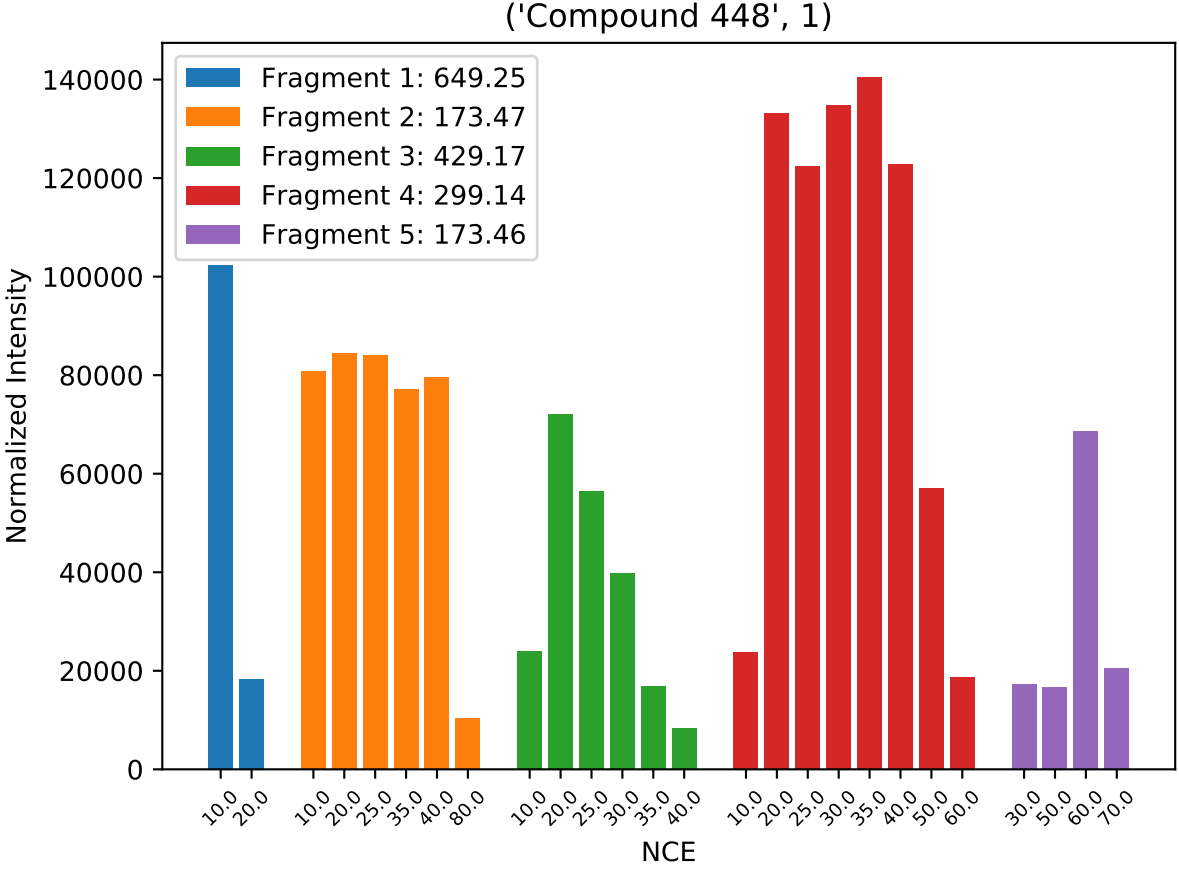

('Compound 310', 1)
Fragment 1: 103.04
Fragment 2: 251.15
Fragment 3: 89.06
Fragment 4: 133.09
Fragment 5: 87.04
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

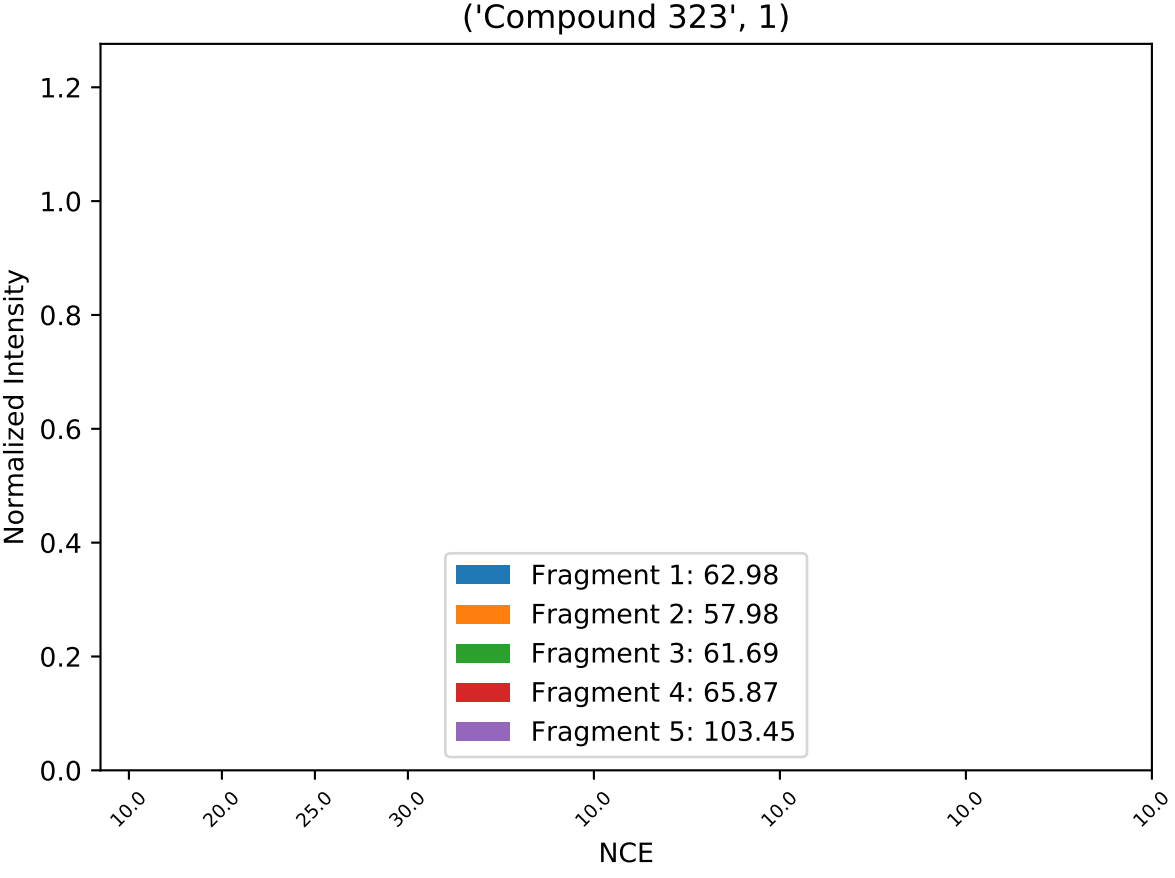

('Compound 311', 1)
Fragment 1: 505.43
Fragment 2: 505.42
Fragment 3: 177.11
Fragment 4: 133.09
Fragment 5: 89.06
Normalized Intensity
0
5000
10000
15000
20000
25000
NCE
20.0
10.0
25.0
30.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

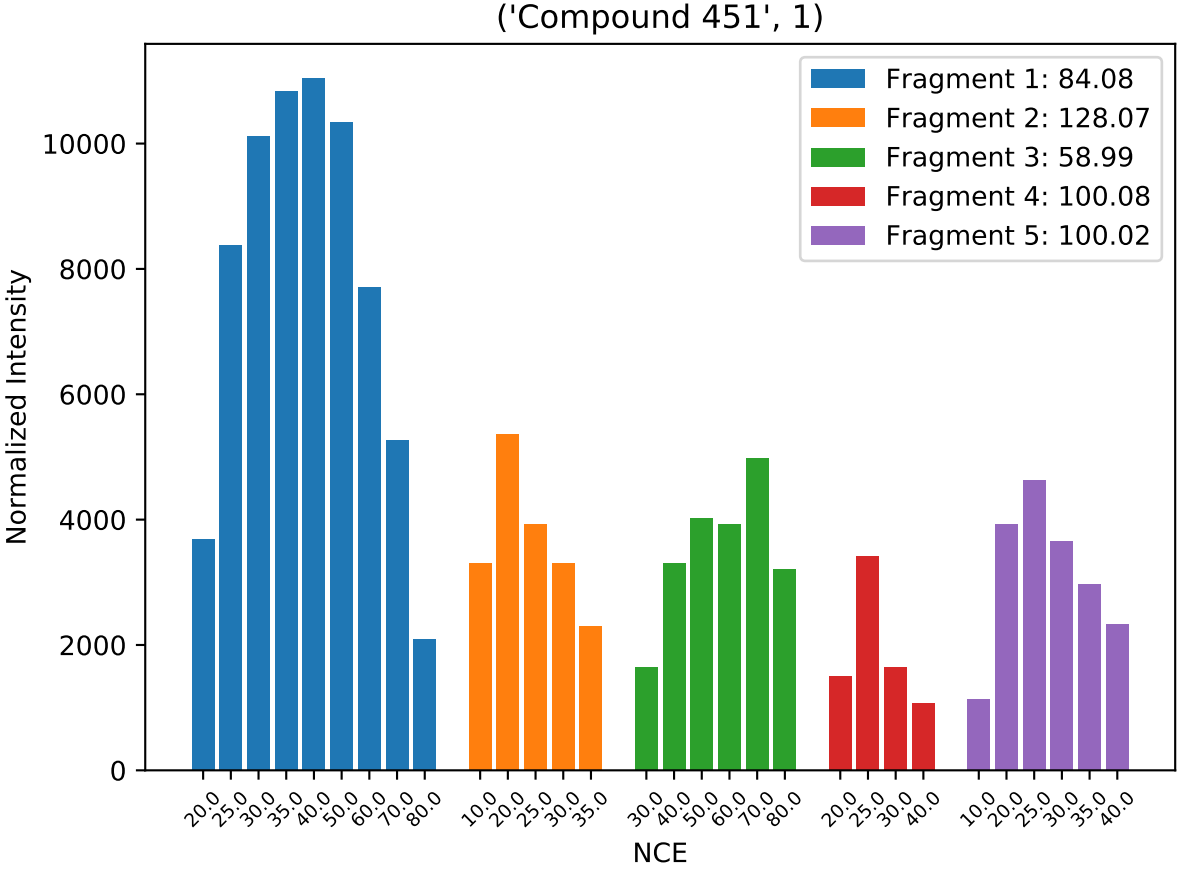

('Compound 439', 1)
Fragment 1: 173.47
Fragment 2: 430.3
Fragment 3: 412.28
Fragment 4: 412.29
Fragment 5: 173.46
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
20.0
30.0
40.0
50.0
10.0
25.0
35.0
10.0
20.0
30.0
25.0
35.0
60.0
70.0
NCE

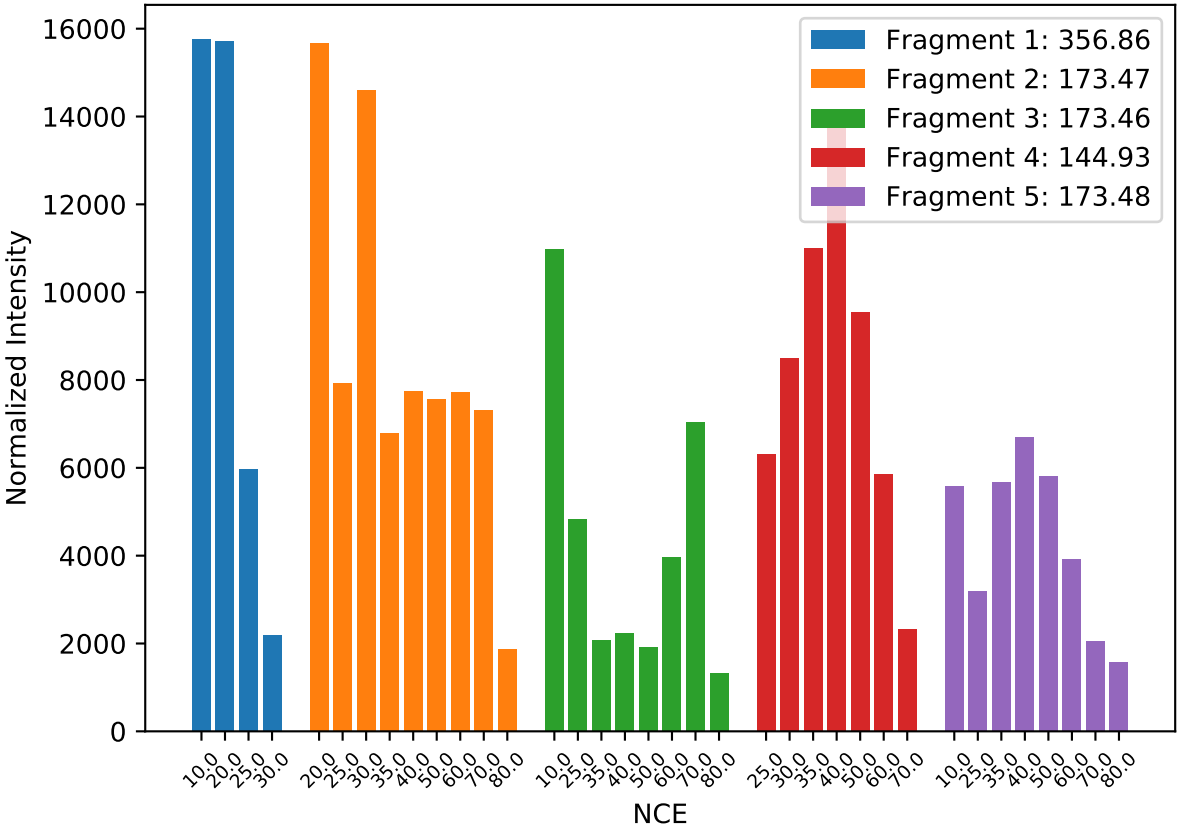

('Compound 316', 1)
Fragment 1: 173.47
Fragment 2: 95.09
Fragment 3: 81.07
Fragment 4: 67.05
Fragment 5: 79.05
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
200000
20.0 30.0 35.0 40.0 50.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

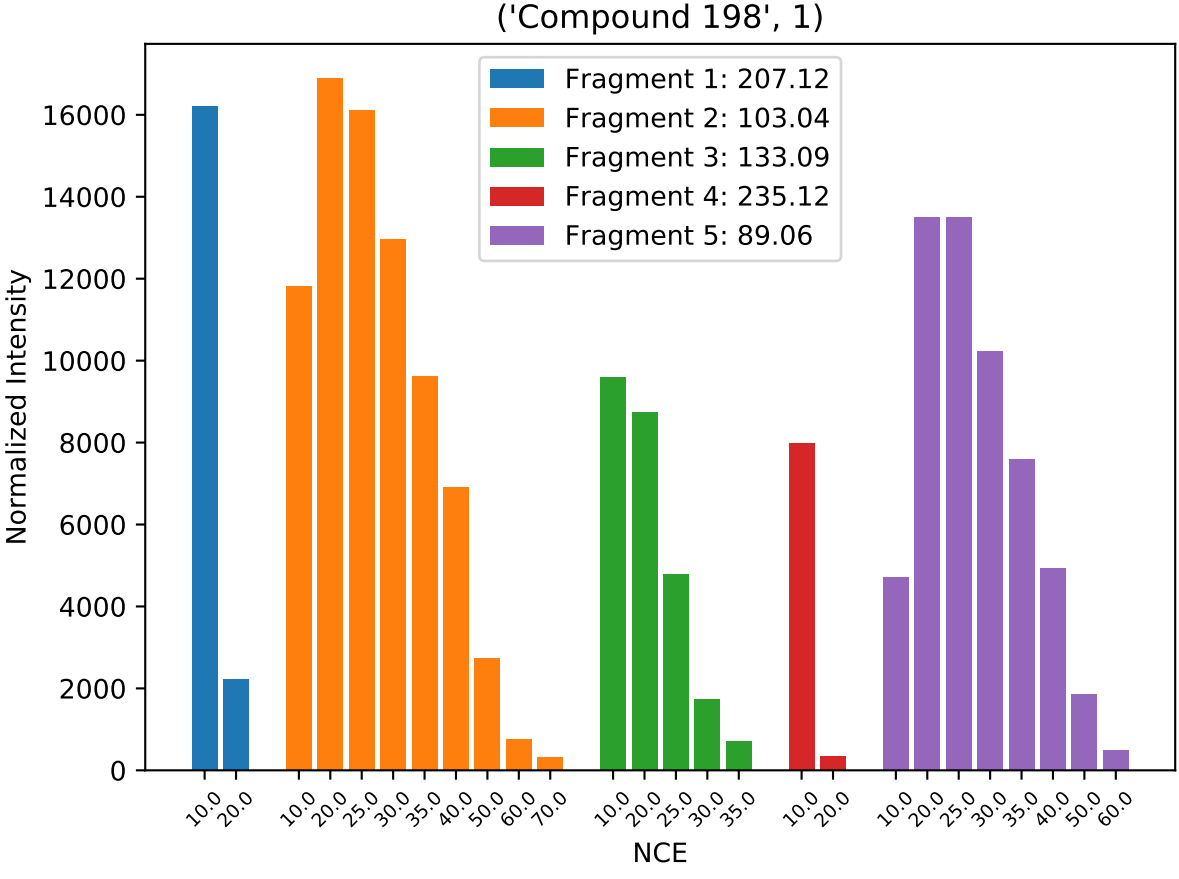

('Compound 189', 1)
Fragment 1: 150.09
Fragment 2: 106.06
Fragment 3: 120.05
Fragment 4: 134.06
Fragment 5: 107.07
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
25.0 30.0 35.0 40.0 50.0 60.0
40.0 50.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

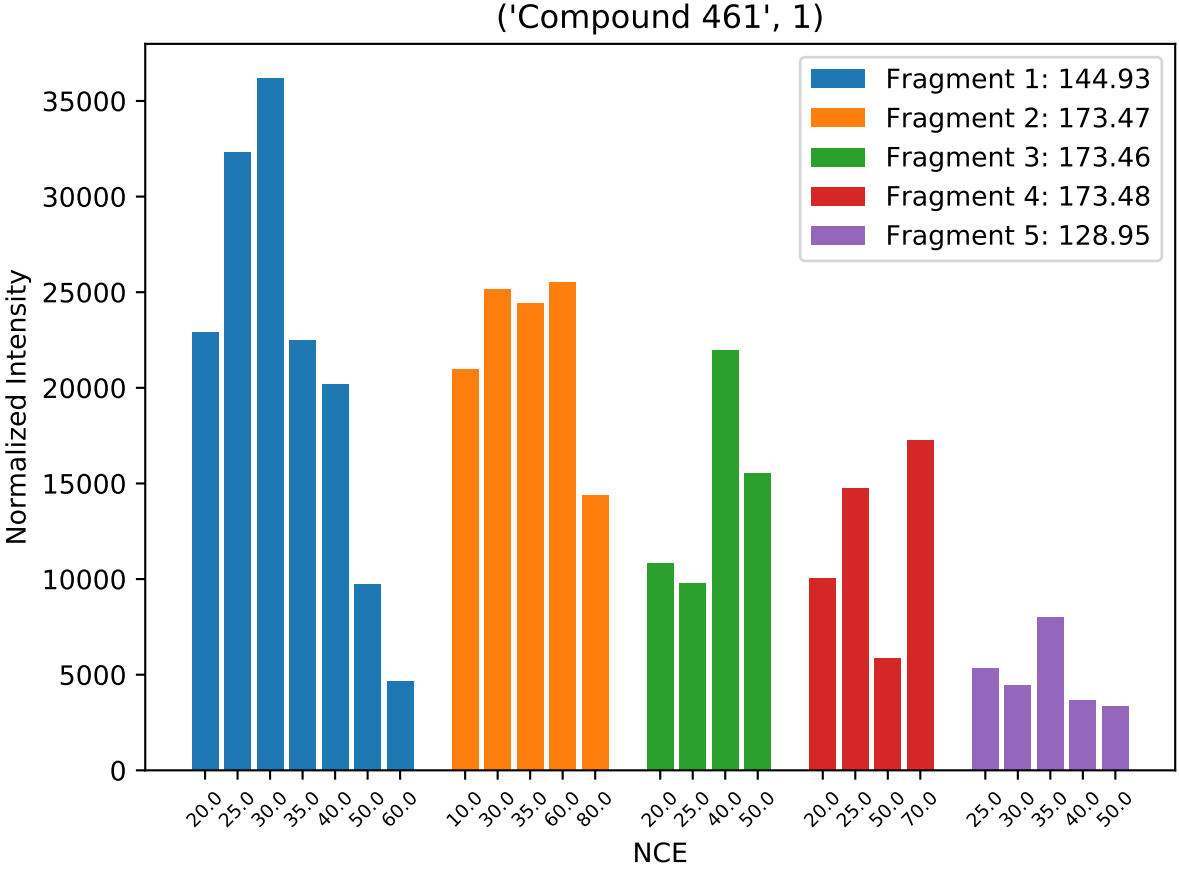

('Compound 448', 1)
Fragment 1: 649.25
Fragment 2: 173.47
Fragment 3: 429.17
Fragment 4: 299.14
Fragment 5: 173.46
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
10.0
20.0
10.0
20.0
25.0
35.0
40.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
30.0
50.0
60.0
70.0
NCE

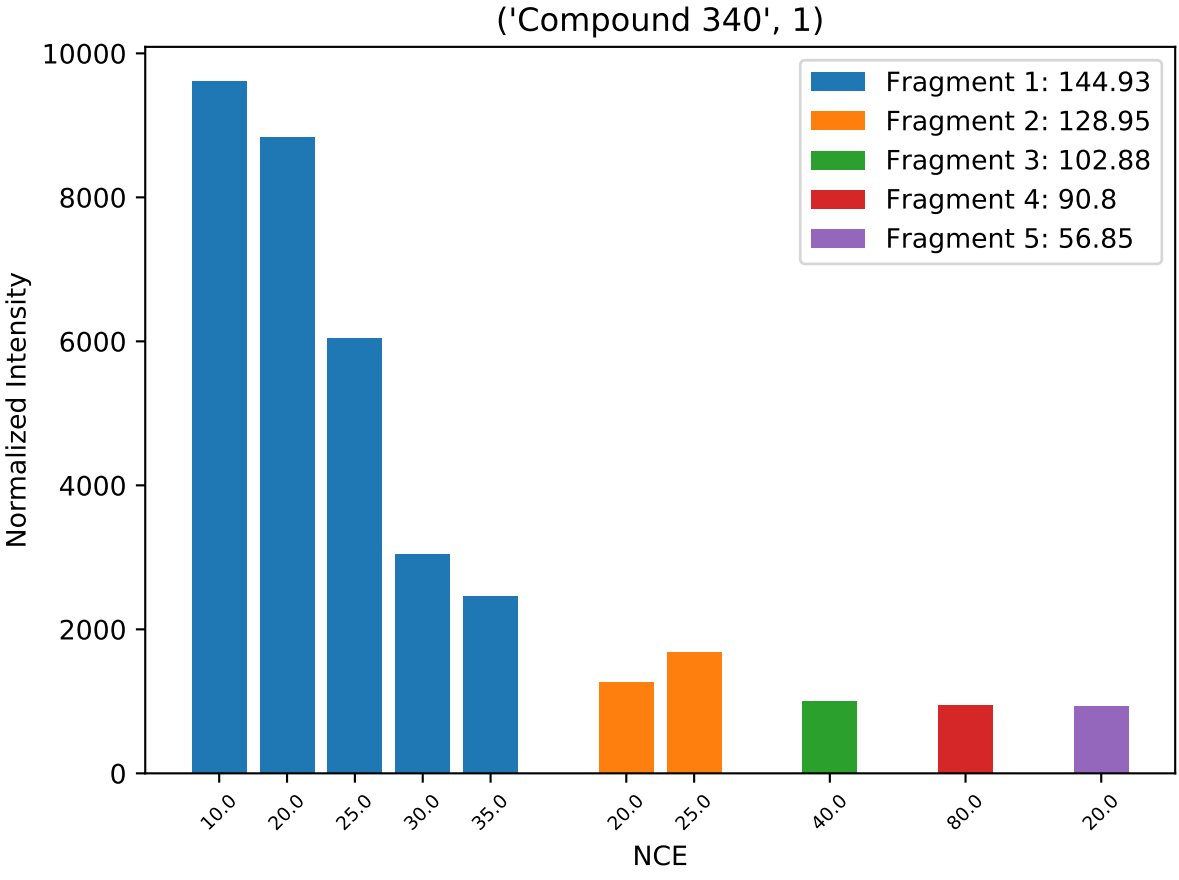

('Compound 323', 1)
Normalized Intensity
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Fragment 1: 62.98
Fragment 2: 57.98
Fragment 3: 61.69
Fragment 4: 65.87
Fragment 5: 103.45
10.0
20.0
25.0
30.0
10.0
10.0
10.0
10.0
NCE

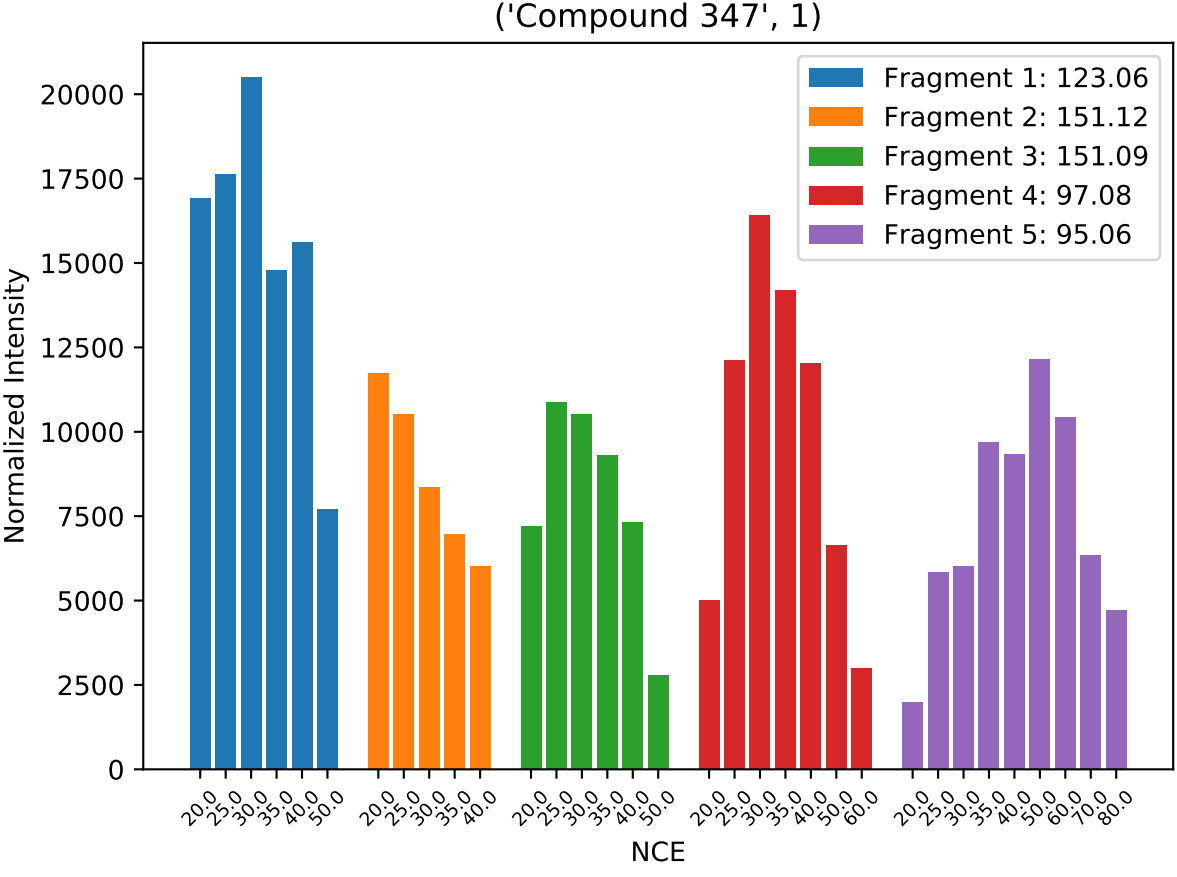

('Compound 451', 1)
Fragment 1: 84.08
Fragment 2: 128.07
Fragment 3: 58.99
Fragment 4: 100.08
Fragment 5: 100.02
Normalized Intensity
0
2000
4000
6000
8000
10000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
30.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

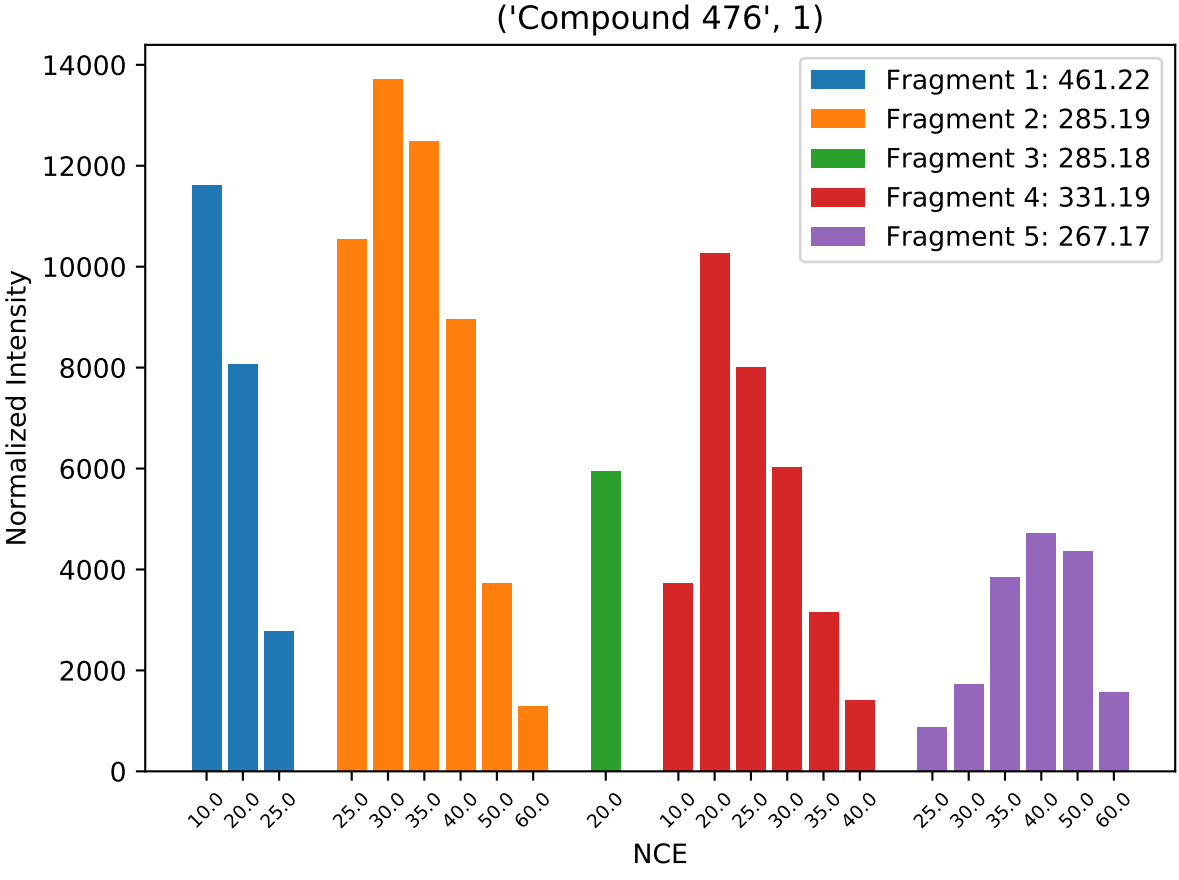

('Compound 580', 1)
Fragment 1: 356.86
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 144.93
Fragment 5: 173.48
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0 20.0 25.0 30.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 25.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 25.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

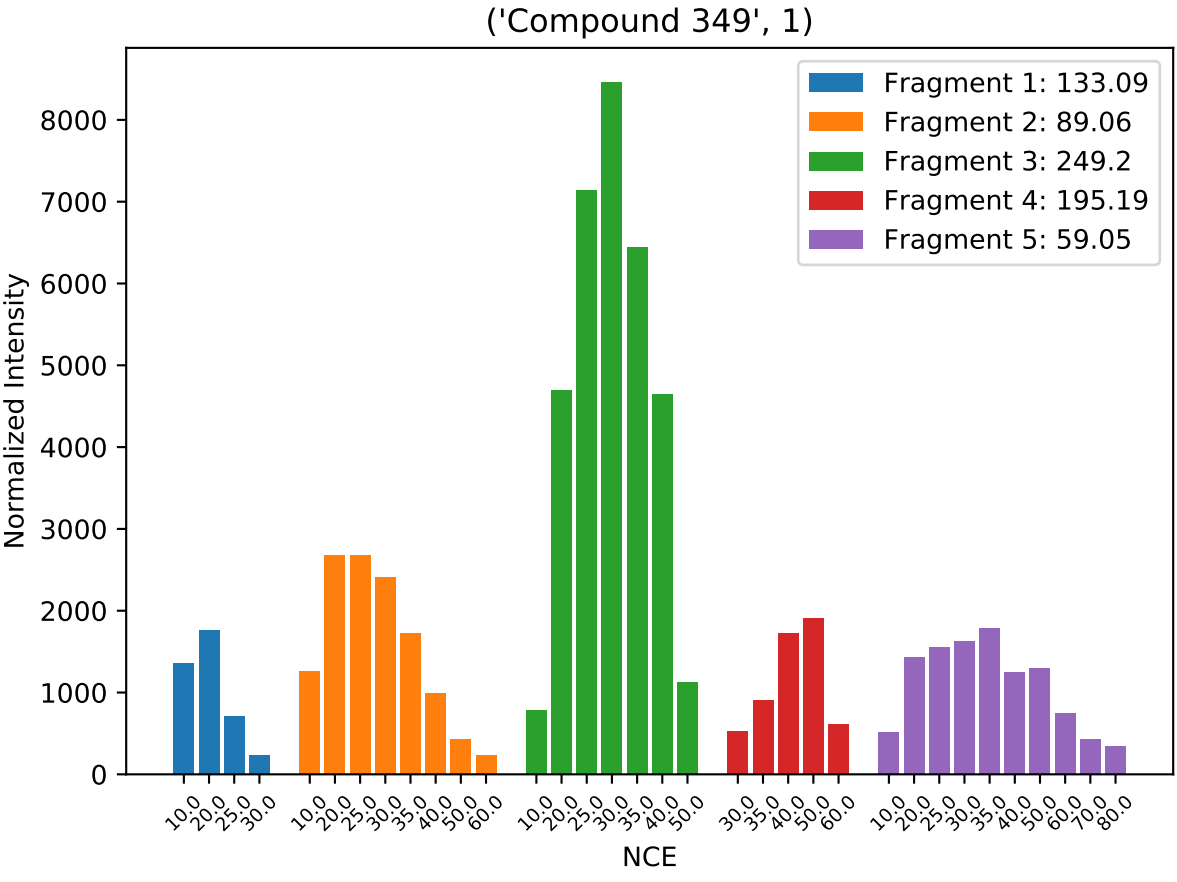

('Compound 198', 1)
Fragment 1: 207.12
Fragment 2: 103.04
Fragment 3: 133.09
Fragment 4: 235.12
Fragment 5: 89.06
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

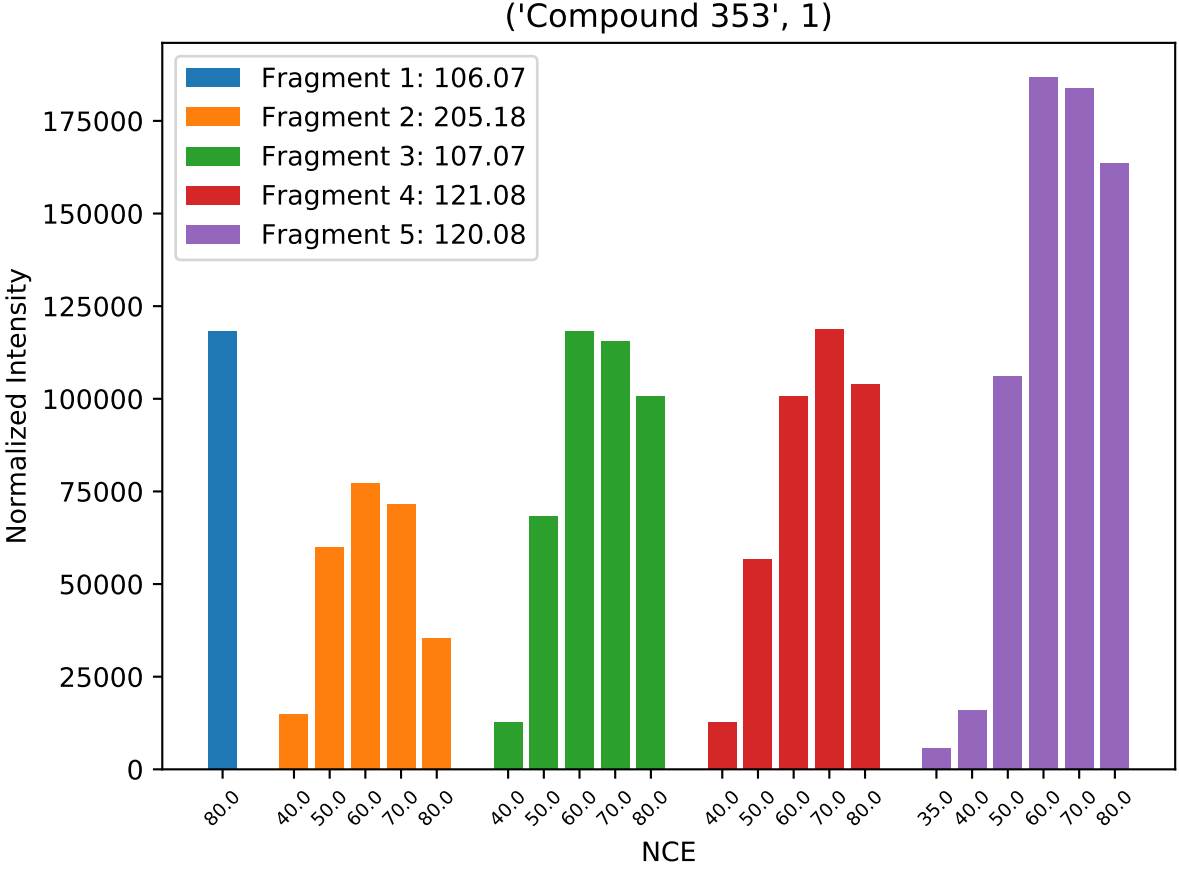

('Compound 461', 1)
Fragment 1: 144.93
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 173.48
Fragment 5: 128.95
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
30.0
35.0
60.0
80.0
20.0
25.0
40.0
50.0
20.0
25.0
50.0
70.0
25.0
30.0
35.0
40.0
50.0
NCE

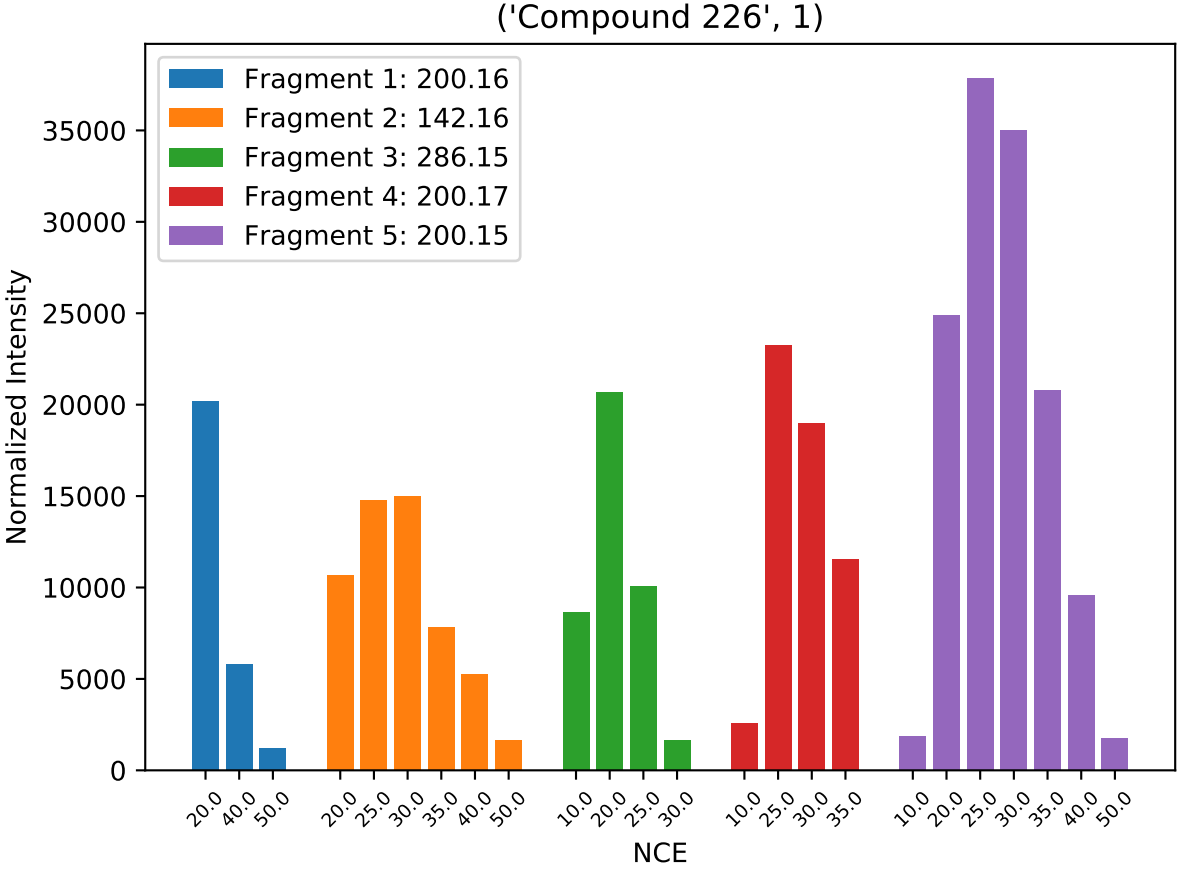

('Compound 340', 1)
Fragment 1: 144.93
Fragment 2: 128.95
Fragment 3: 102.88
Fragment 4: 90.8
Fragment 5: 56.85
Normalized Intensity
10000
8000
6000
4000
2000
0
10.0
20.0
25.0
30.0
35.0
20.0
25.0
40.0
80.0
20.0
NCE

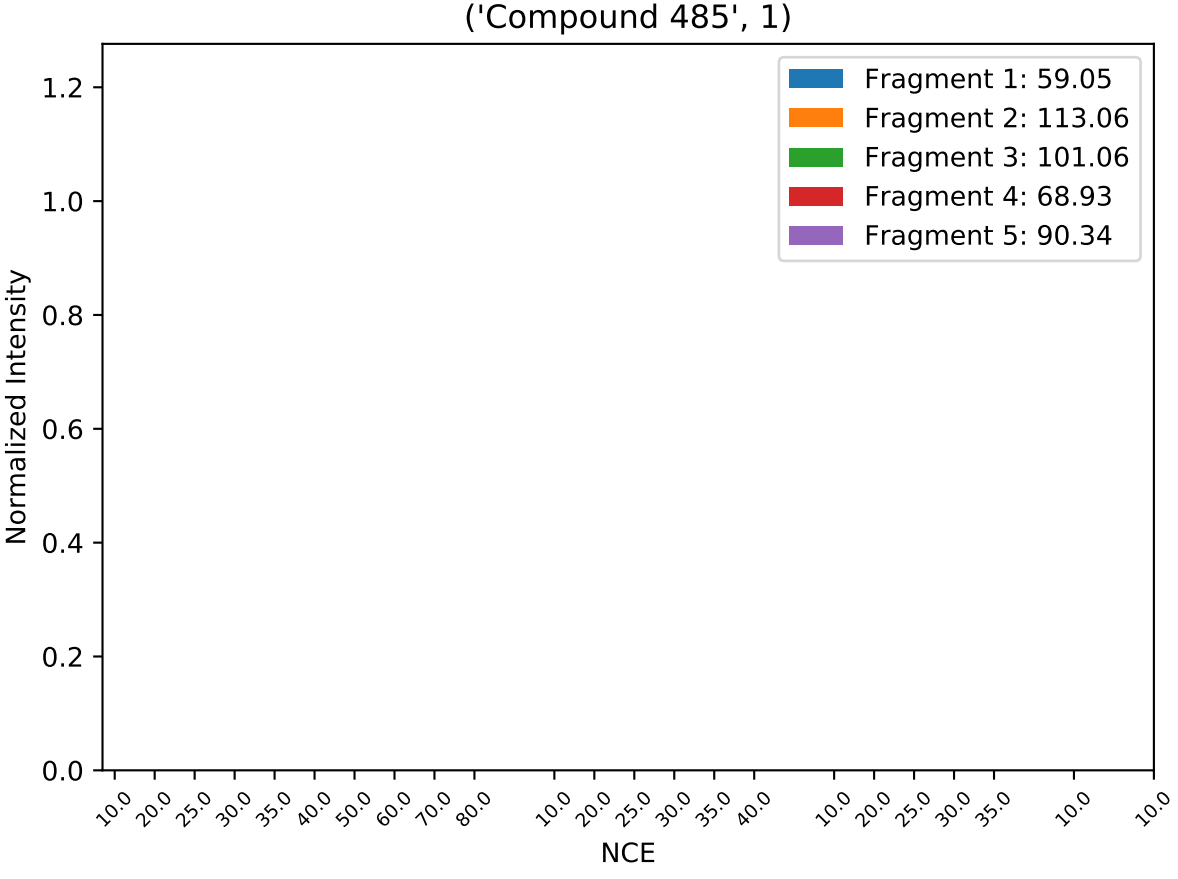

('Compound 347', 1)
Fragment 1: 123.06
Fragment 2: 151.12
Fragment 3: 151.09
Fragment 4: 97.08
Fragment 5: 95.06
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
NCE
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

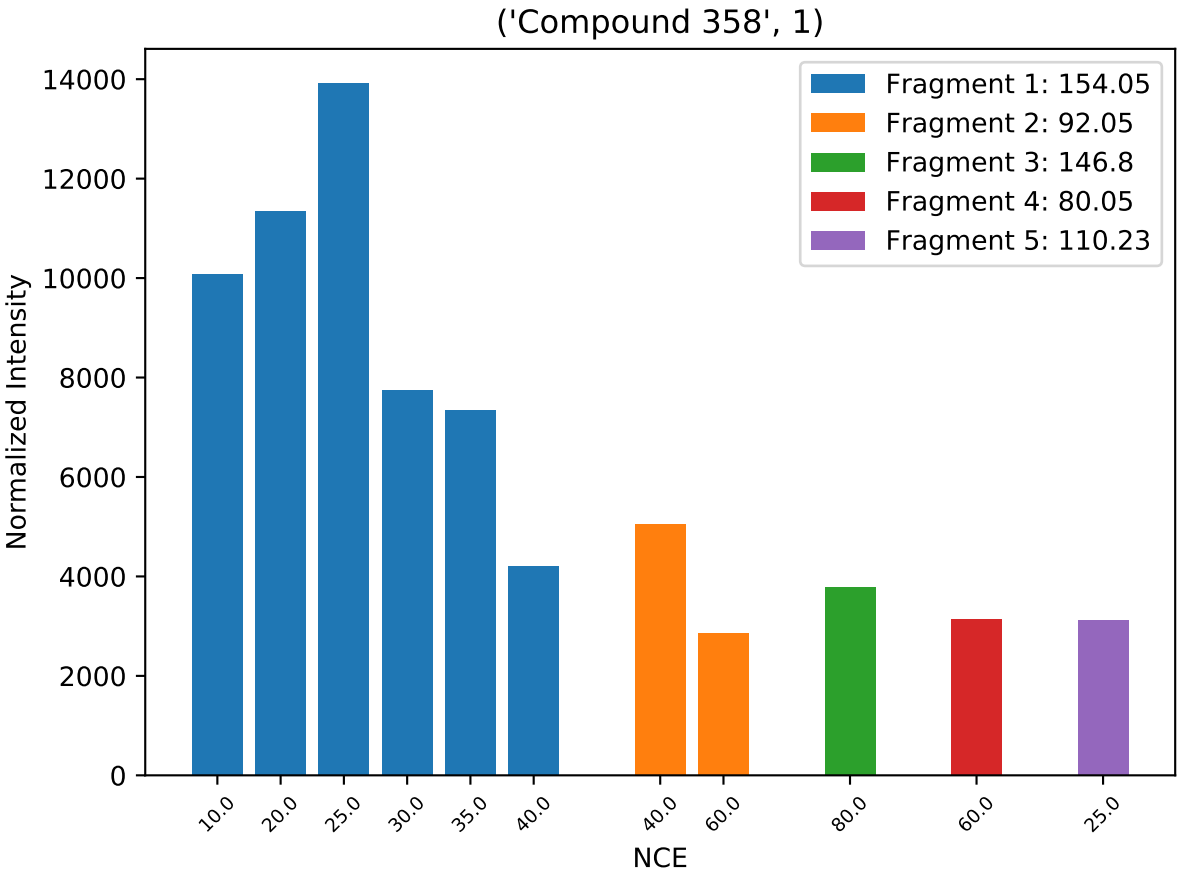

('Compound 476', 1)
Fragment 1: 461.22
Fragment 2: 285.19
Fragment 3: 285.18
Fragment 4: 331.19
Fragment 5: 267.17
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
25.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

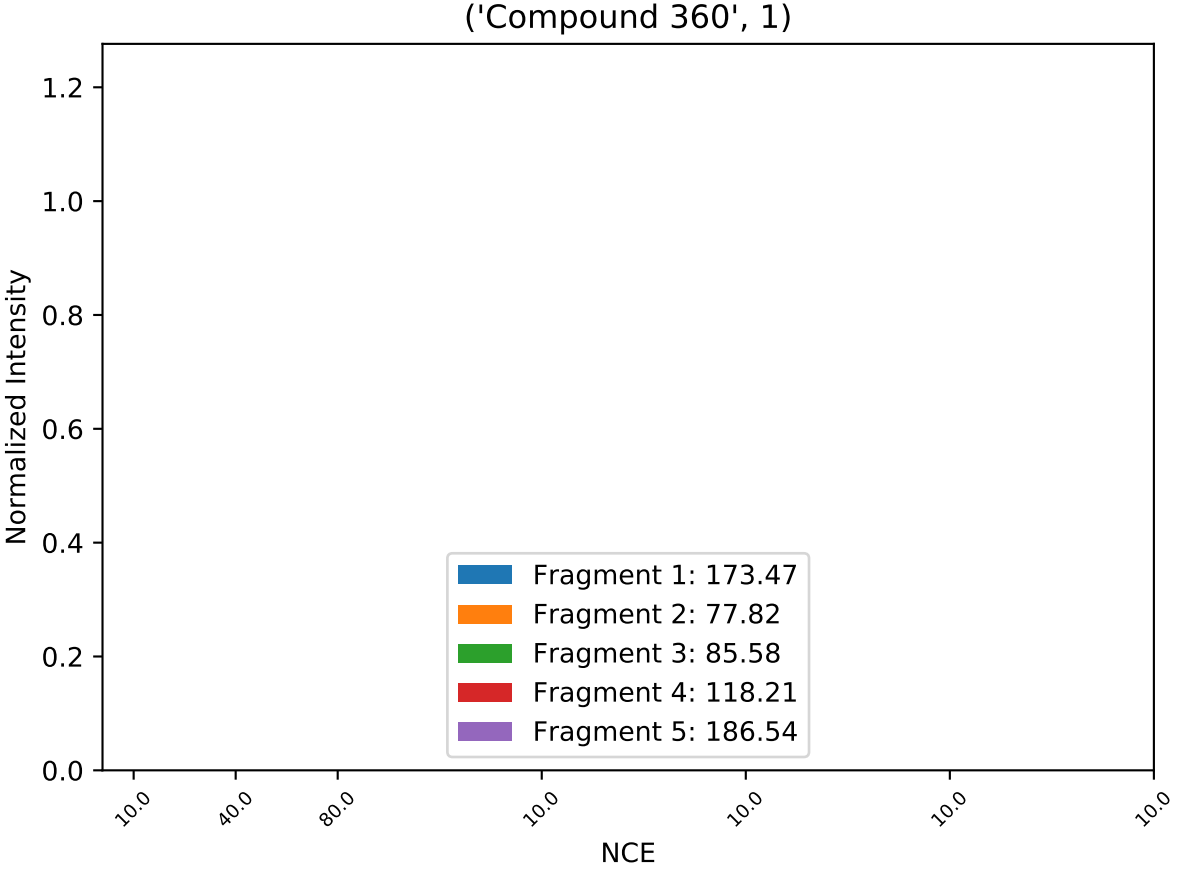

('Compound 349', 1)
Fragment 1: 133.09
Fragment 2: 89.06
Fragment 3: 249.2
Fragment 4: 195.19
Fragment 5: 59.05
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

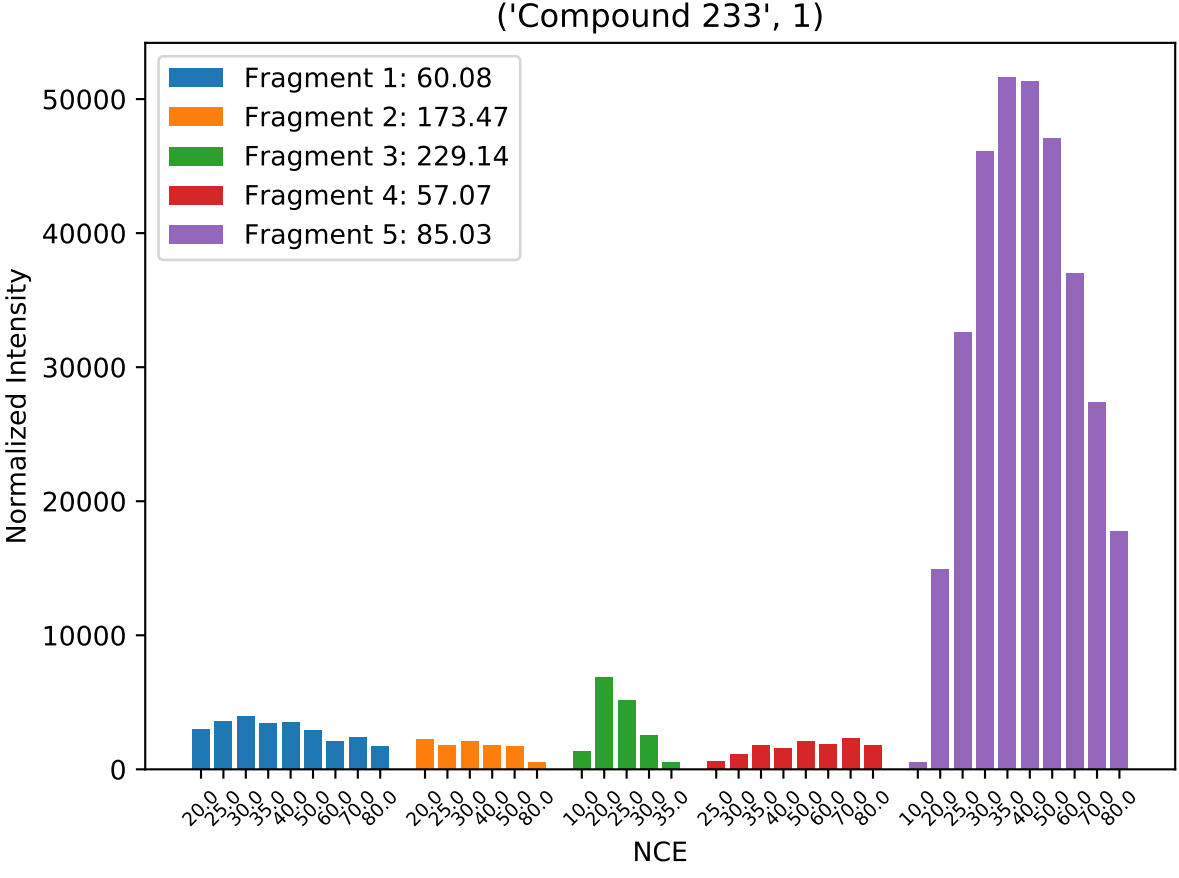

('Compound 353', 1)
Fragment 1: 106.07
Fragment 2: 205.18
Fragment 3: 107.07
Fragment 4: 121.08
Fragment 5: 120.08
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
80.0
40.0
50.0
60.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

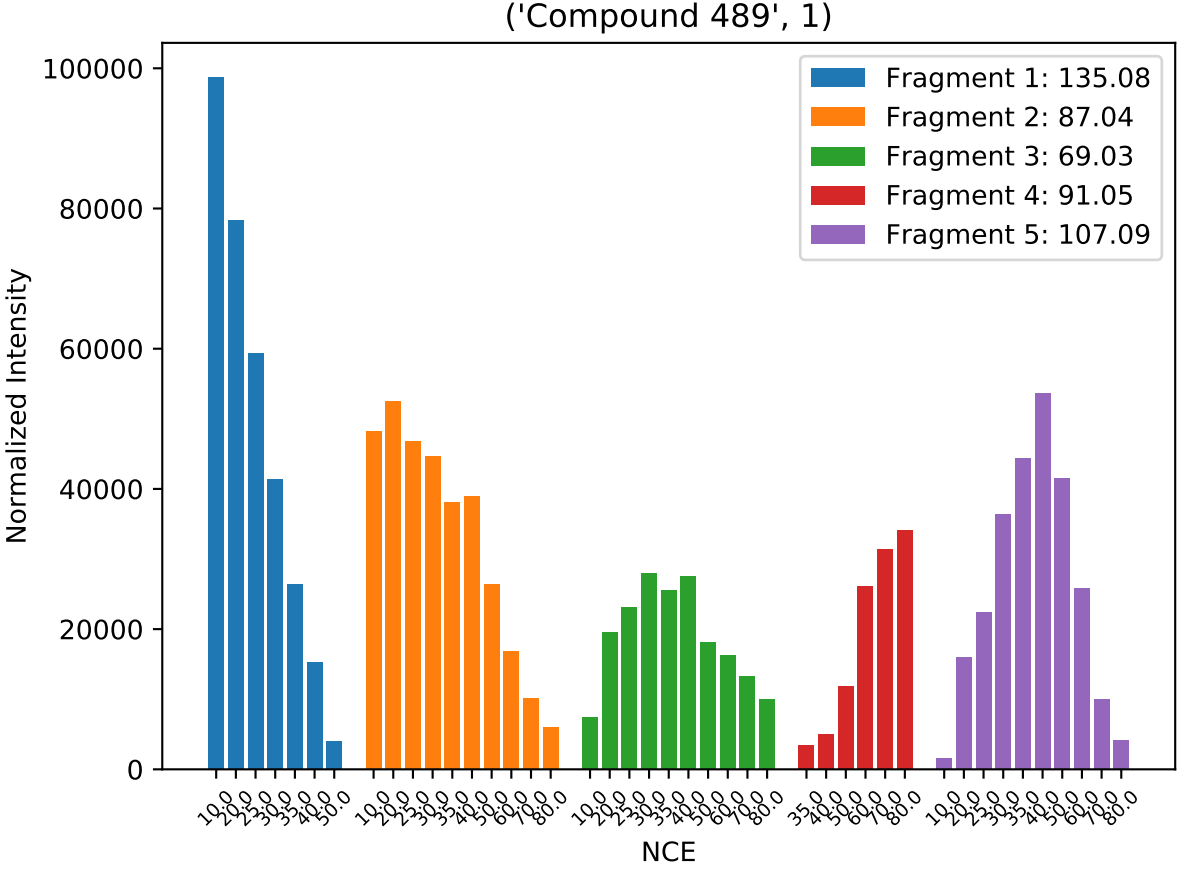

('Compound 226', 1)
Fragment 1: 200.16
Fragment 2: 142.16
Fragment 3: 286.15
Fragment 4: 200.17
Fragment 5: 200.15
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
20.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
10.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

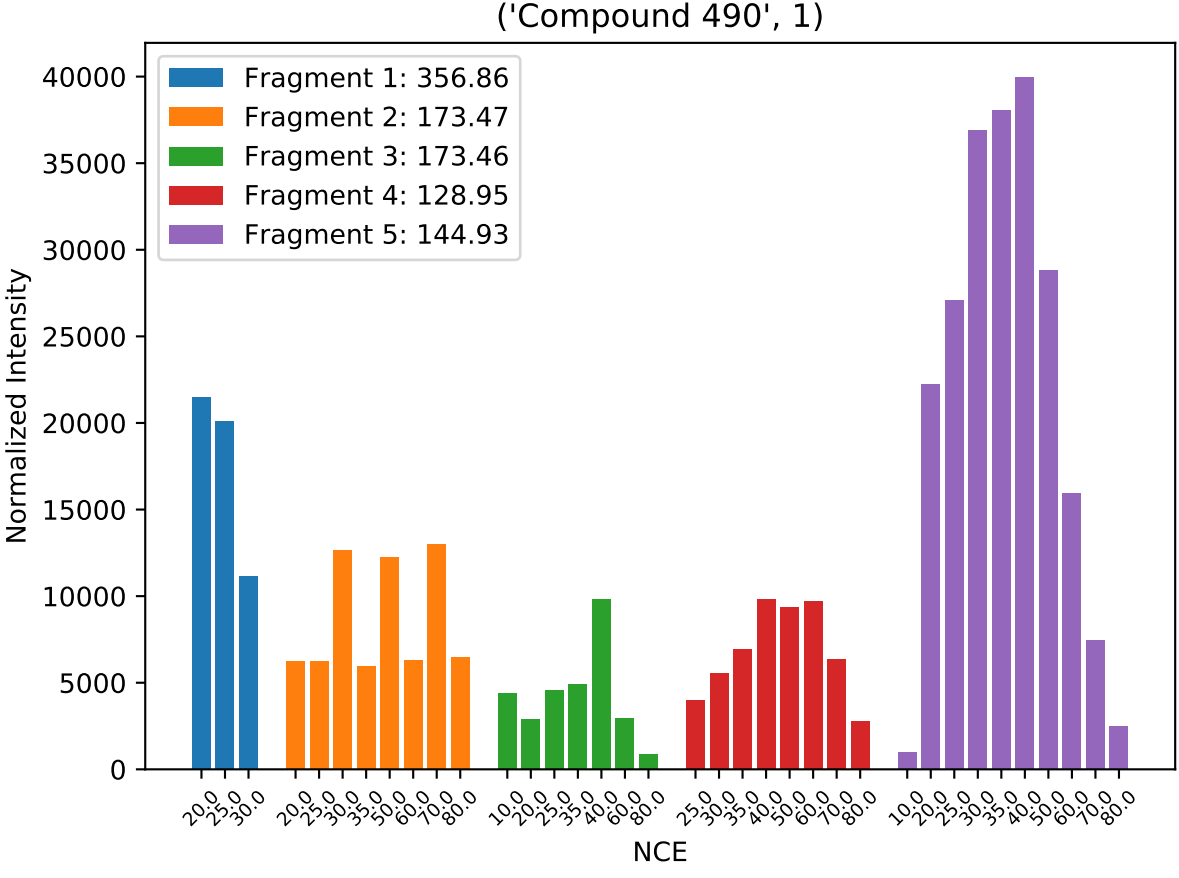

('Compound 485', 1)
Fragment 1: 59.05
Fragment 2: 113.06
Fragment 3: 101.06
Fragment 4: 68.93
Fragment 5: 90.34
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
10.0
10.0
NCE

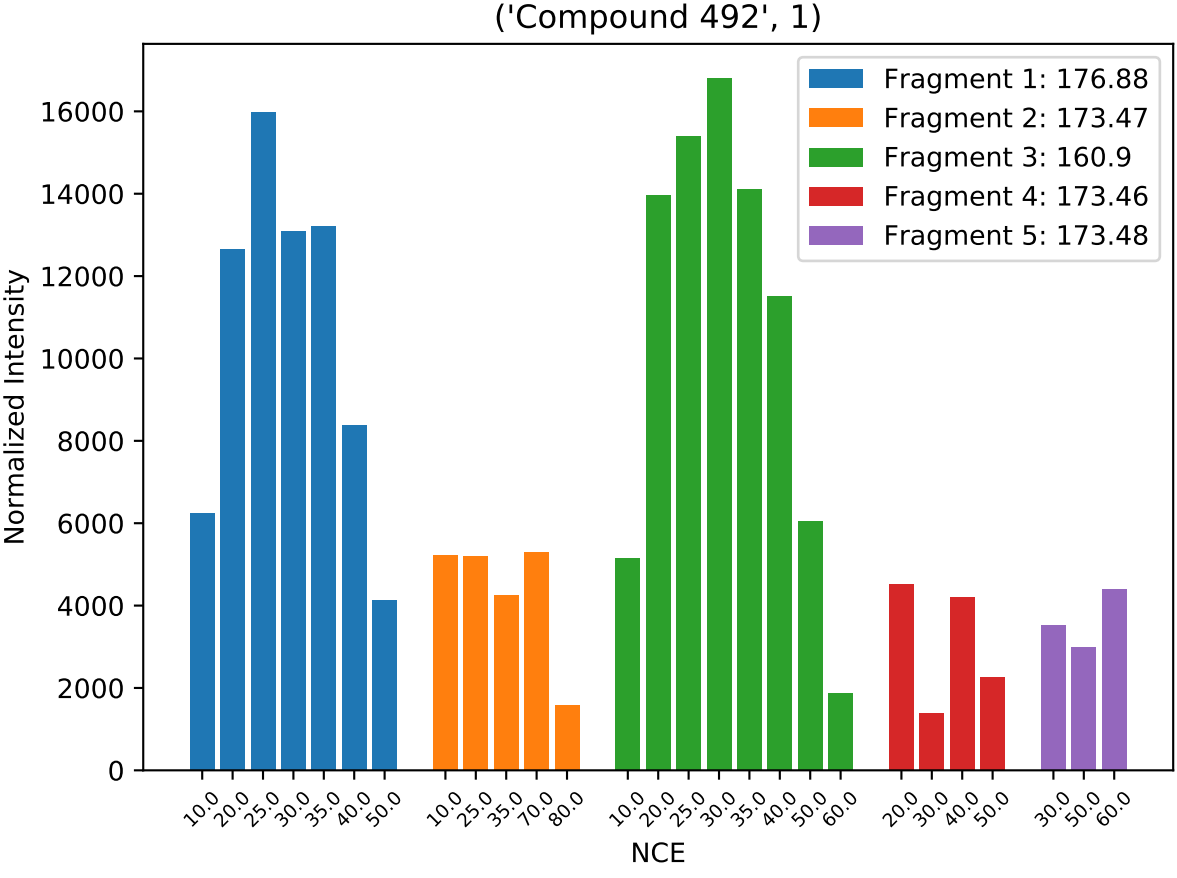

('Compound 358', 1)
Fragment 1: 154.05
Fragment 2: 92.05
Fragment 3: 146.8
Fragment 4: 80.05
Fragment 5: 110.23
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
25.0
30.0
35.0
40.0
40.0
60.0
80.0
60.0
25.0
NCE

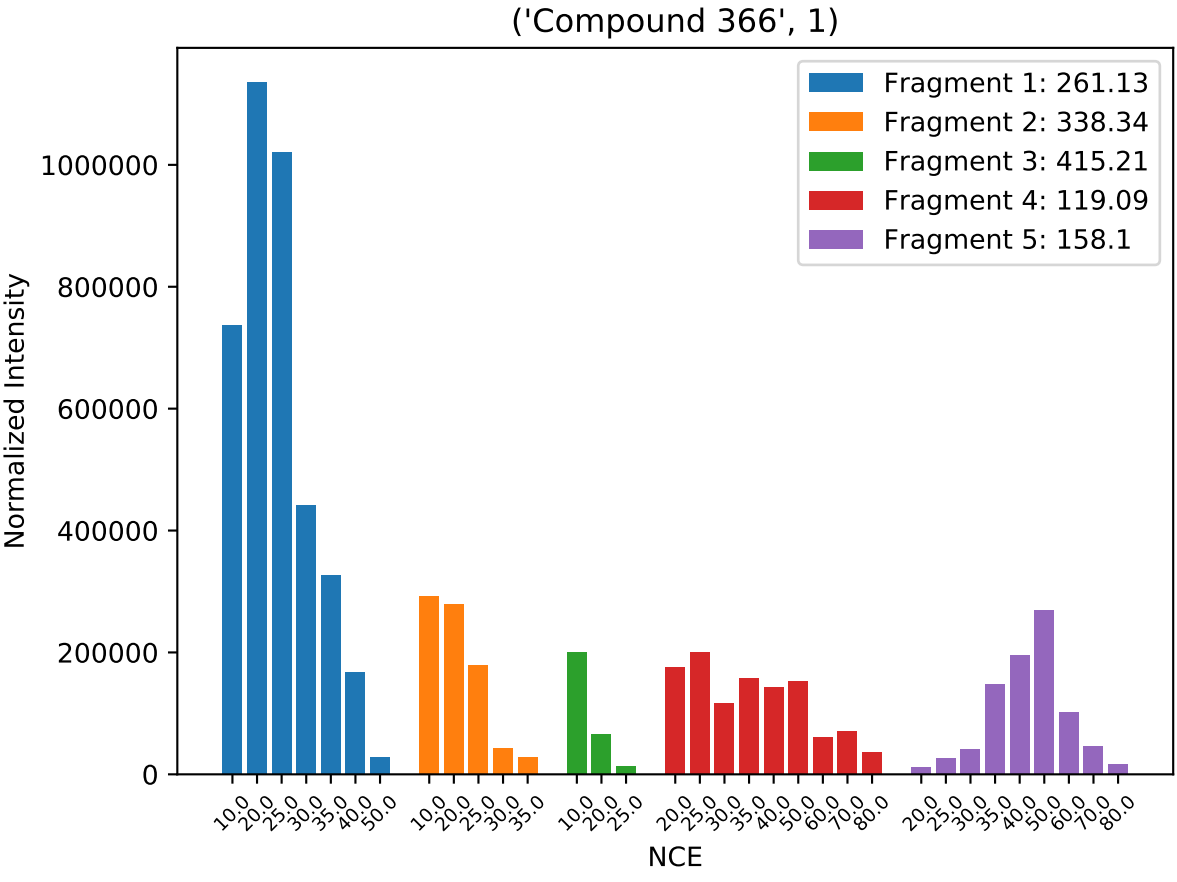

('Compound 360', 1)
Normalized Intensity
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Fragment 1: 173.47
Fragment 2: 77.82
Fragment 3: 85.58
Fragment 4: 118.21
Fragment 5: 186.54
10.0
40.0
80.0
10.0
10.0
10.0
10.0
NCE

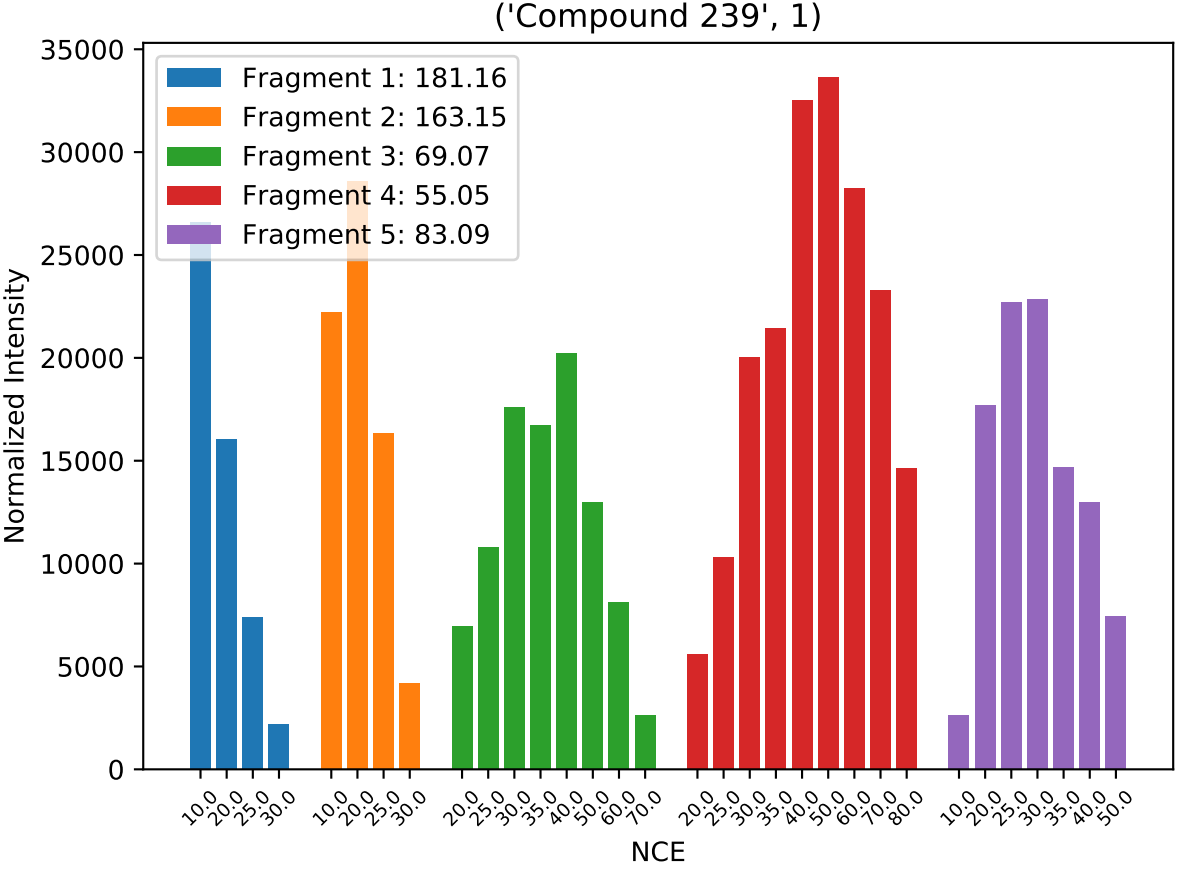

('Compound 233', 1)
Fragment 1: 60.08
Fragment 2: 173.47
Fragment 3: 229.14
Fragment 4: 57.07
Fragment 5: 85.03
Normalized Intensity
0
10000
20000
30000
40000
50000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 40.0 50.0 80.0
10.0 20.0 25.0 30.0 35.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

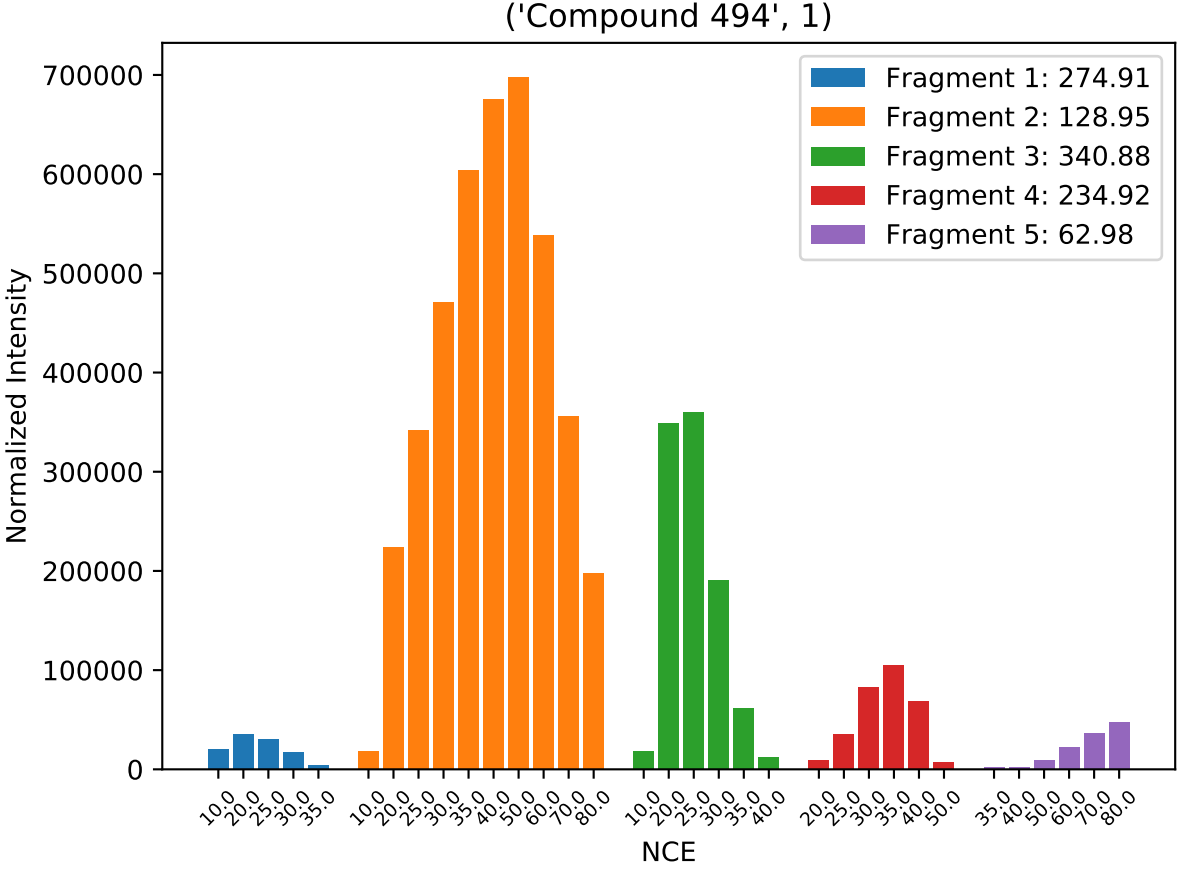

('Compound 489', 1)
Fragment 1: 135.08
Fragment 2: 87.04
Fragment 3: 69.03
Fragment 4: 91.05
Fragment 5: 107.09
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

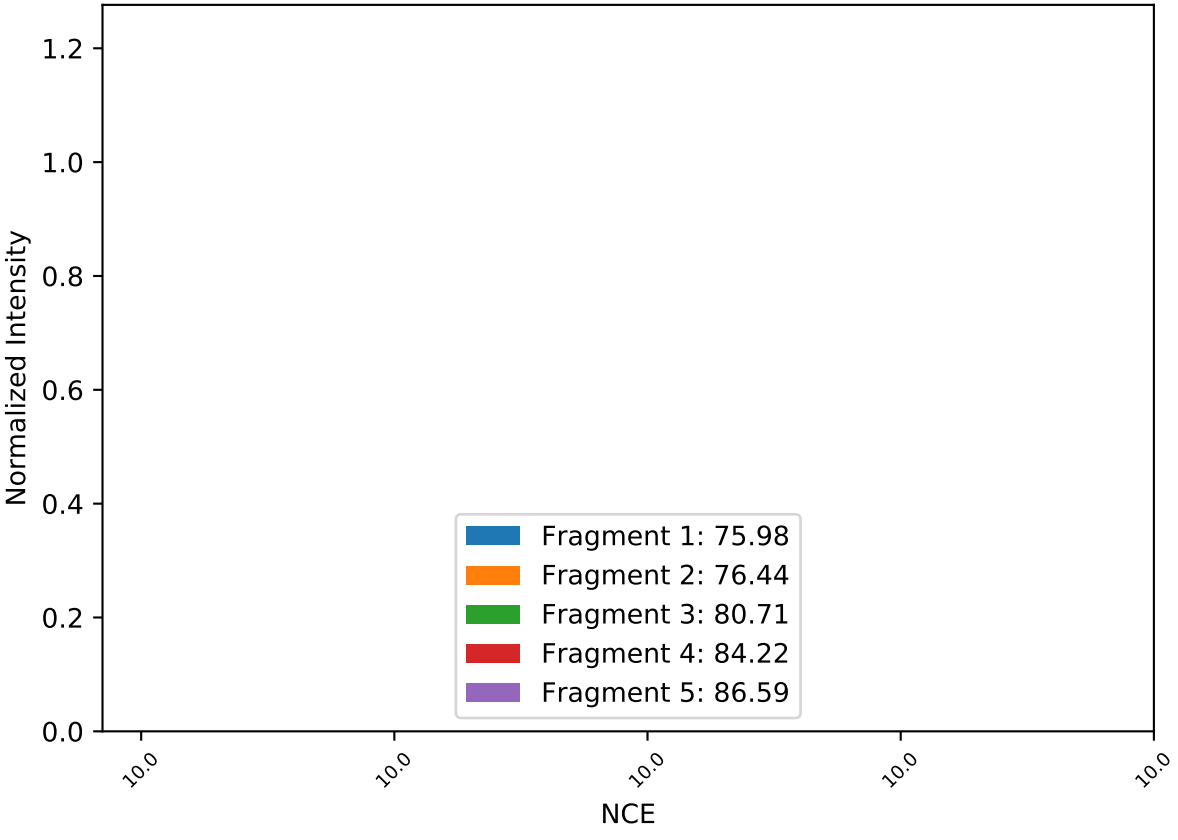

('Compound 490', 1)
Fragment 1: 356.86
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 128.95
Fragment 5: 144.93
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
20.0 25.0 30.0
20.0 25.0 30.0 35.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 35.0 40.0 60.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

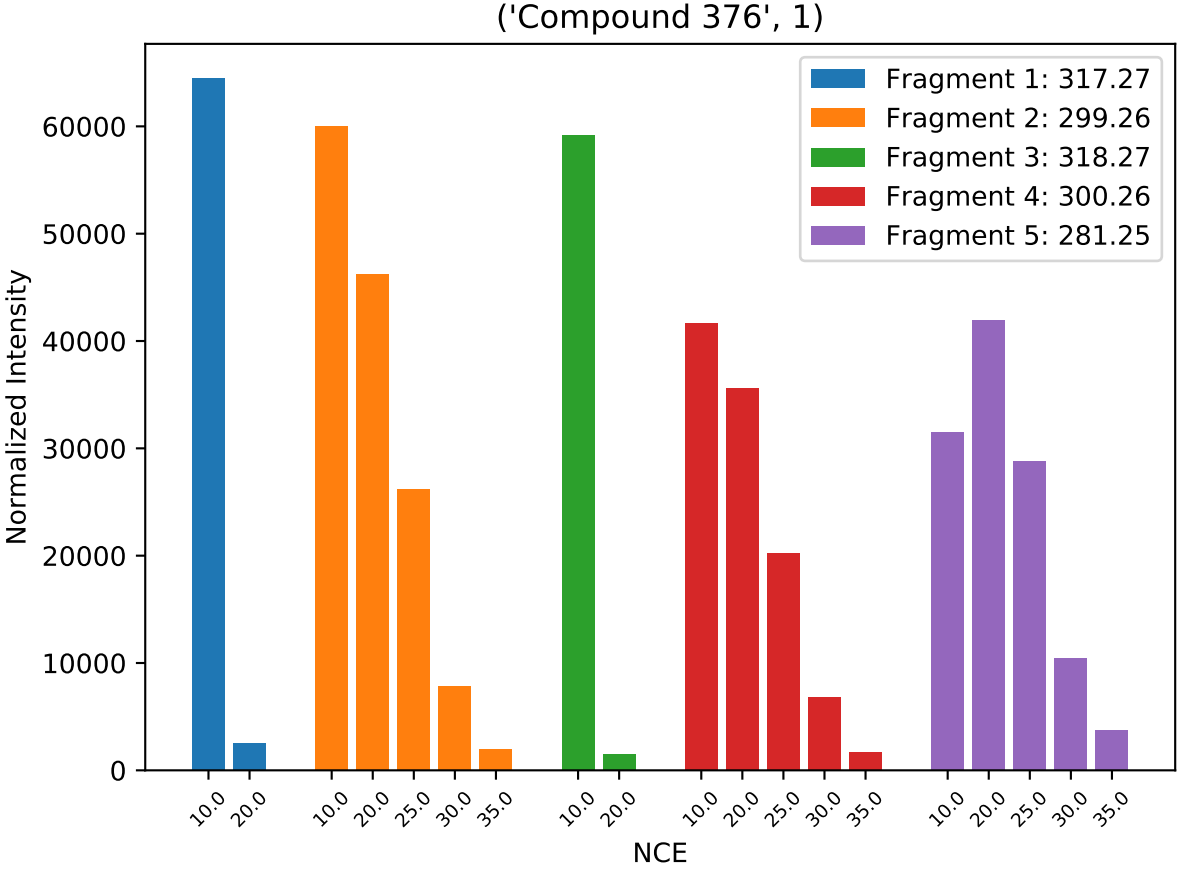

('Compound 492', 1)
Fragment 1: 176.88
Fragment 2: 173.47
Fragment 3: 160.9
Fragment 4: 173.46
Fragment 5: 173.48
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
25.0
35.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
30.0
40.0
50.0
30.0
50.0
60.0
NCE

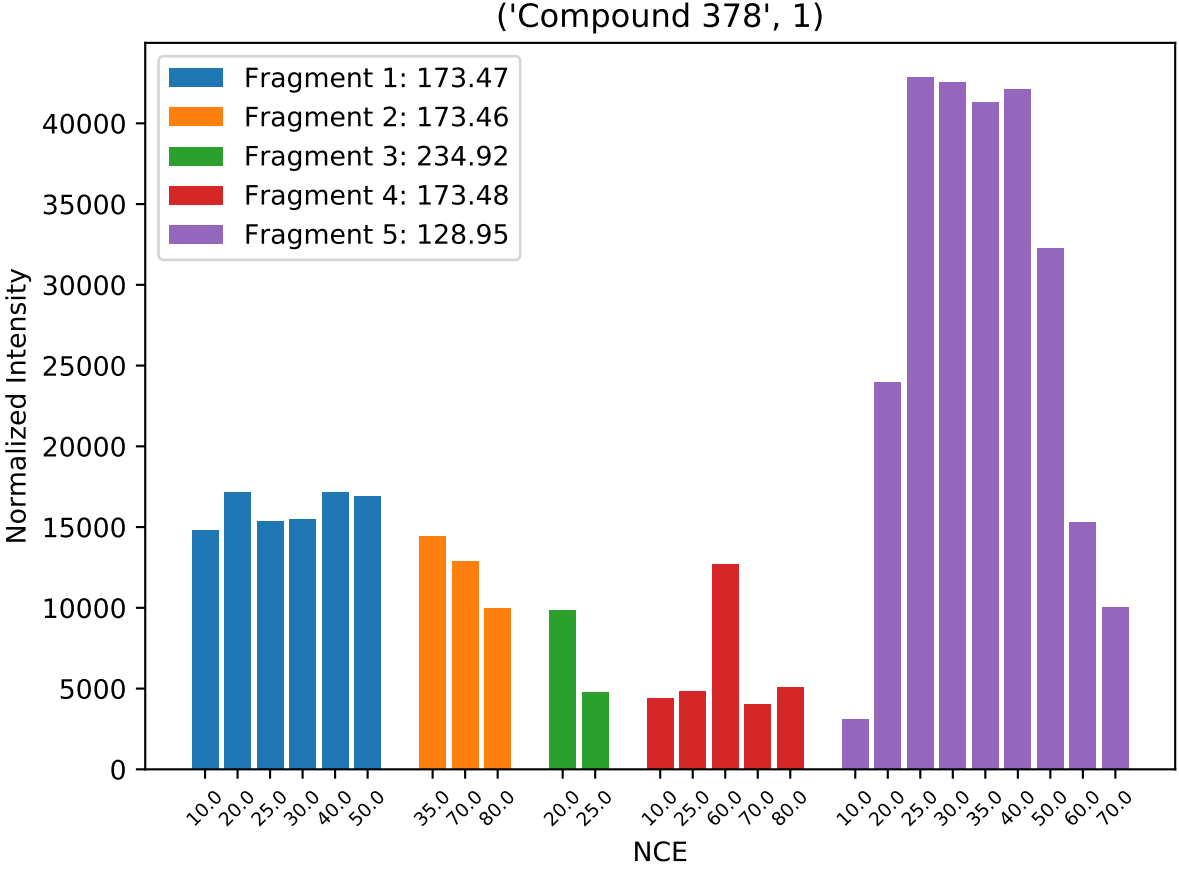

('Compound 366', 1)
Fragment 1: 261.13
Fragment 2: 338.34
Fragment 3: 415.21
Fragment 4: 119.09
Fragment 5: 158.1
Normalized Intensity
0
200000
400000
600000
800000
1000000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

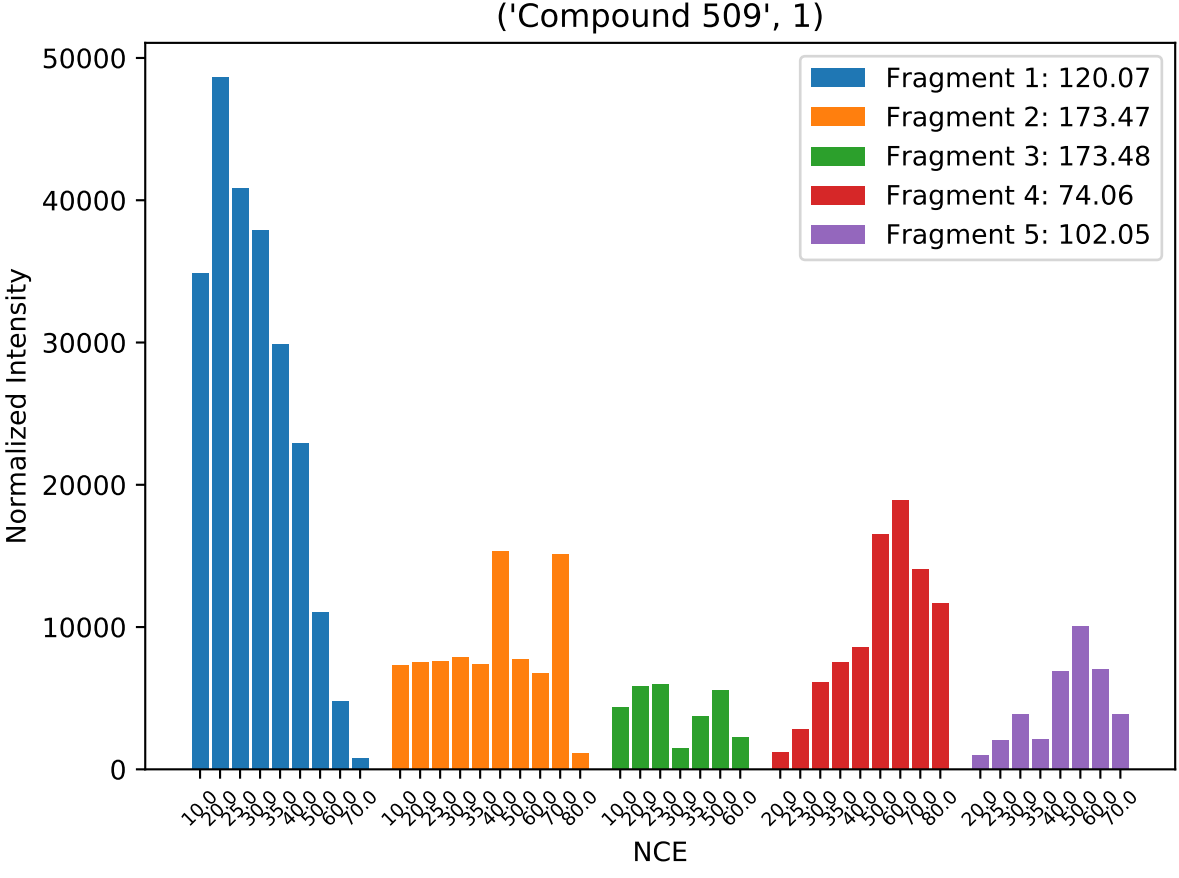

('Compound 239', 1)
Fragment 1: 181.16
Fragment 2: 163.15
Fragment 3: 69.07
Fragment 4: 55.05
Fragment 5: 83.09
Normalized Intensity
NCE
0
5000
10000
15000
20000
25000
30000
35000
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

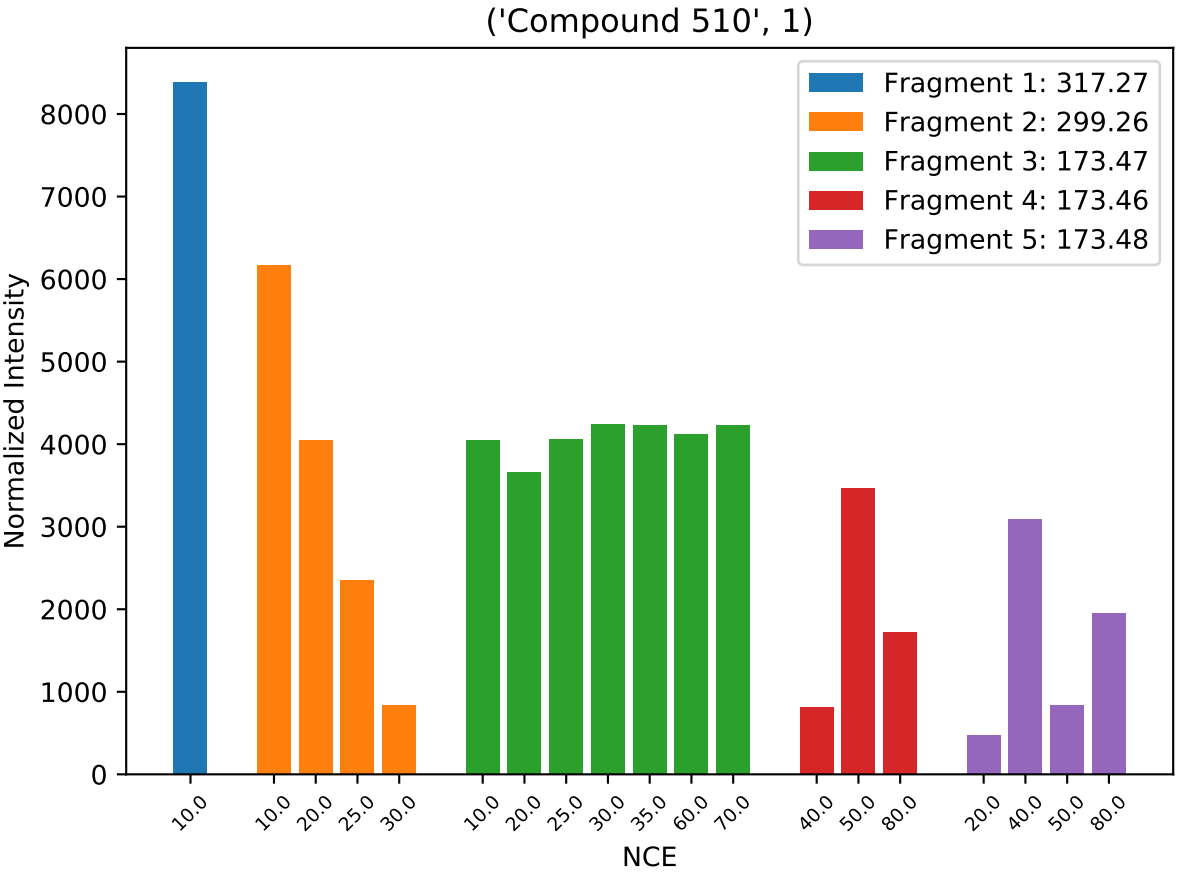

('Compound 494', 1)
Fragment 1: 274.91
Fragment 2: 128.95
Fragment 3: 340.88
Fragment 4: 234.92
Fragment 5: 62.98
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
700000
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

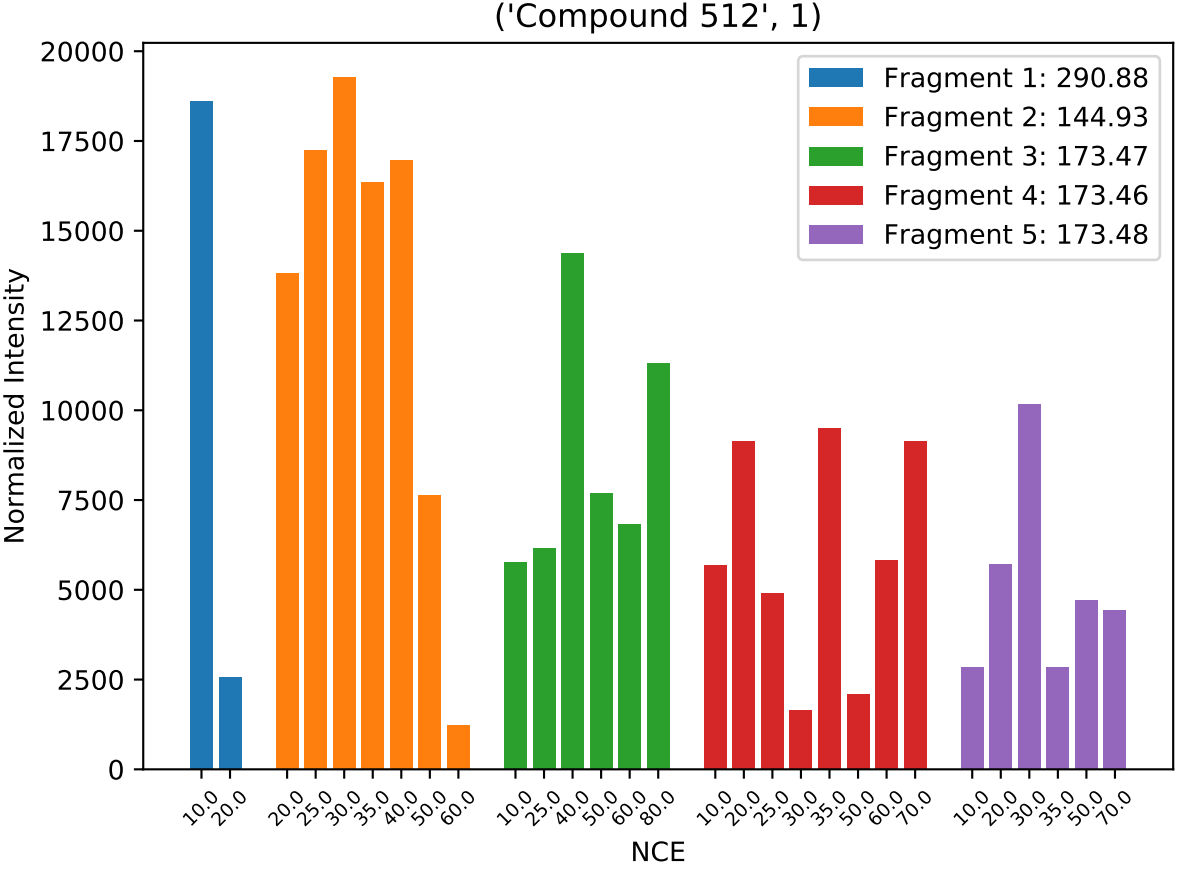

('Compound 502', 1)
Normalized Intensity
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Fragment 1: 75.98
Fragment 2: 76.44
Fragment 3: 80.71
Fragment 4: 84.22
Fragment 5: 86.59
10.0
10.0
10.0
10.0
10.0
NCE

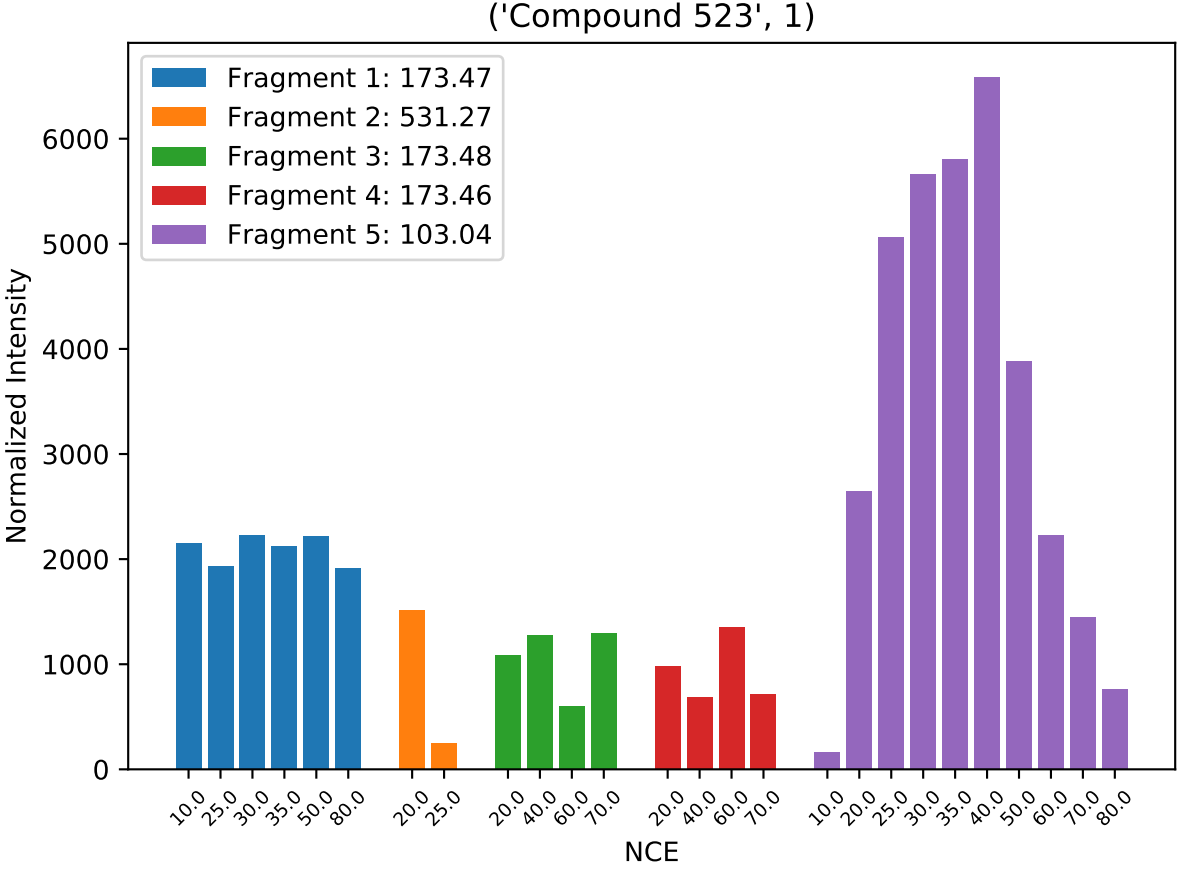

('Compound 376', 1)
Fragment 1: 317.27
Fragment 2: 299.26
Fragment 3: 318.27
Fragment 4: 300.26
Fragment 5: 281.25
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
10.0
20.0
25.0
30.0
35.0
NCE

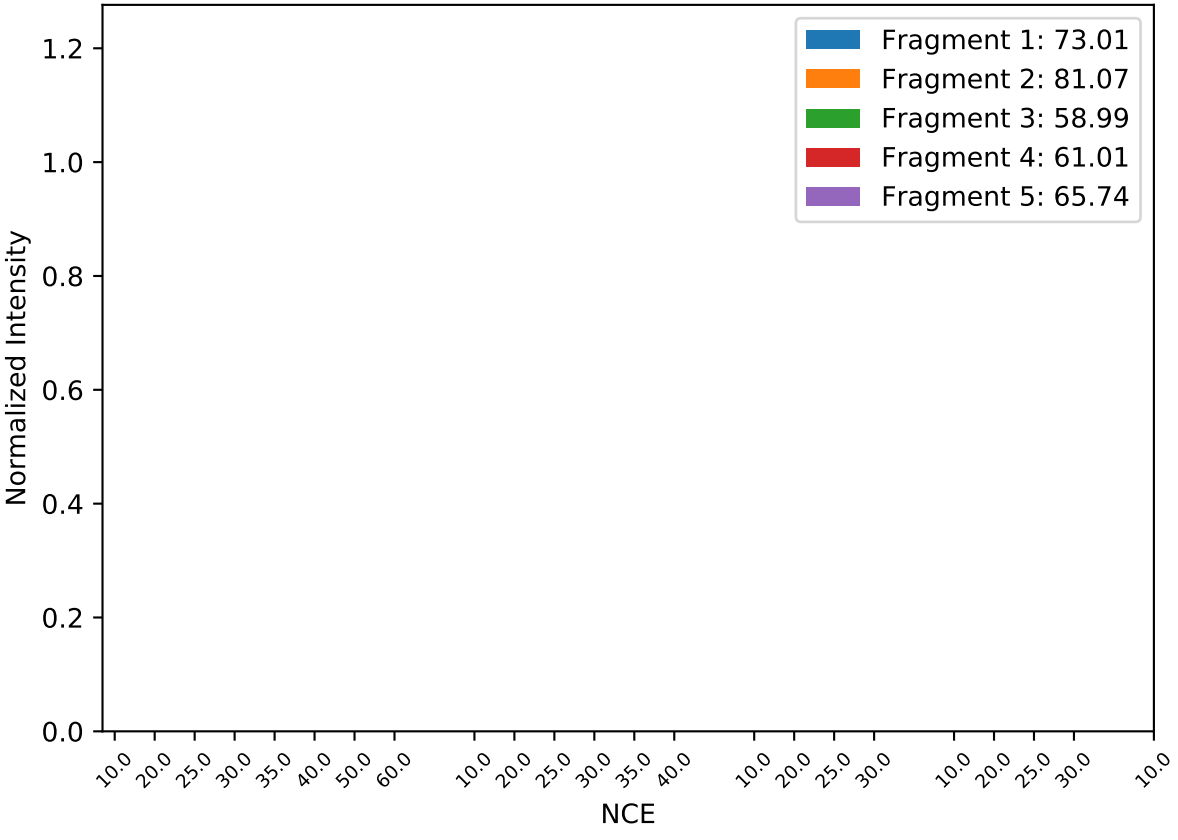

('Compound 378', 1)
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 234.92
Fragment 4: 173.48
Fragment 5: 128.95
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
40.0
50.0
35.0
70.0
80.0
20.0
25.0
10.0
25.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

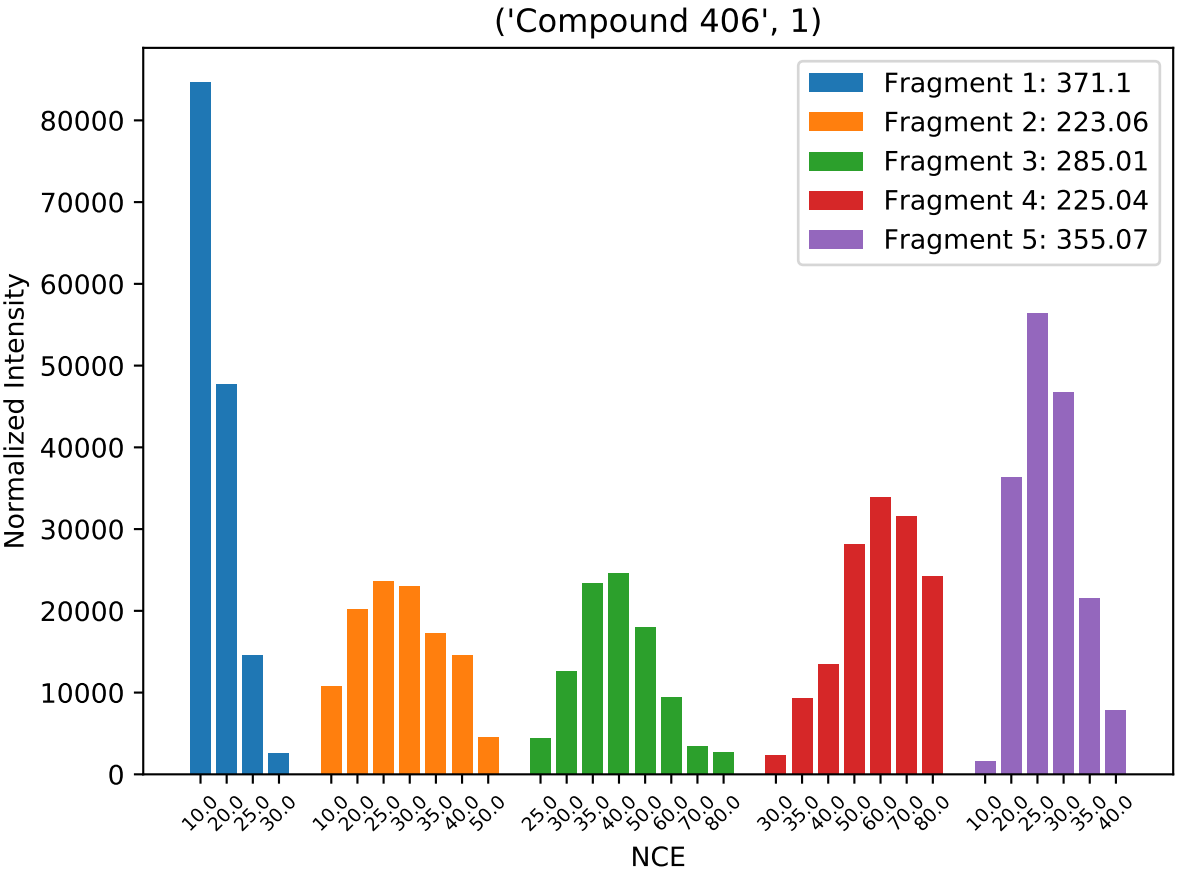

('Compound 509', 1)
Fragment 1: 120.07
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 74.06
Fragment 5: 102.05
Normalized Intensity
0
10000
20000
30000
40000
50000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0

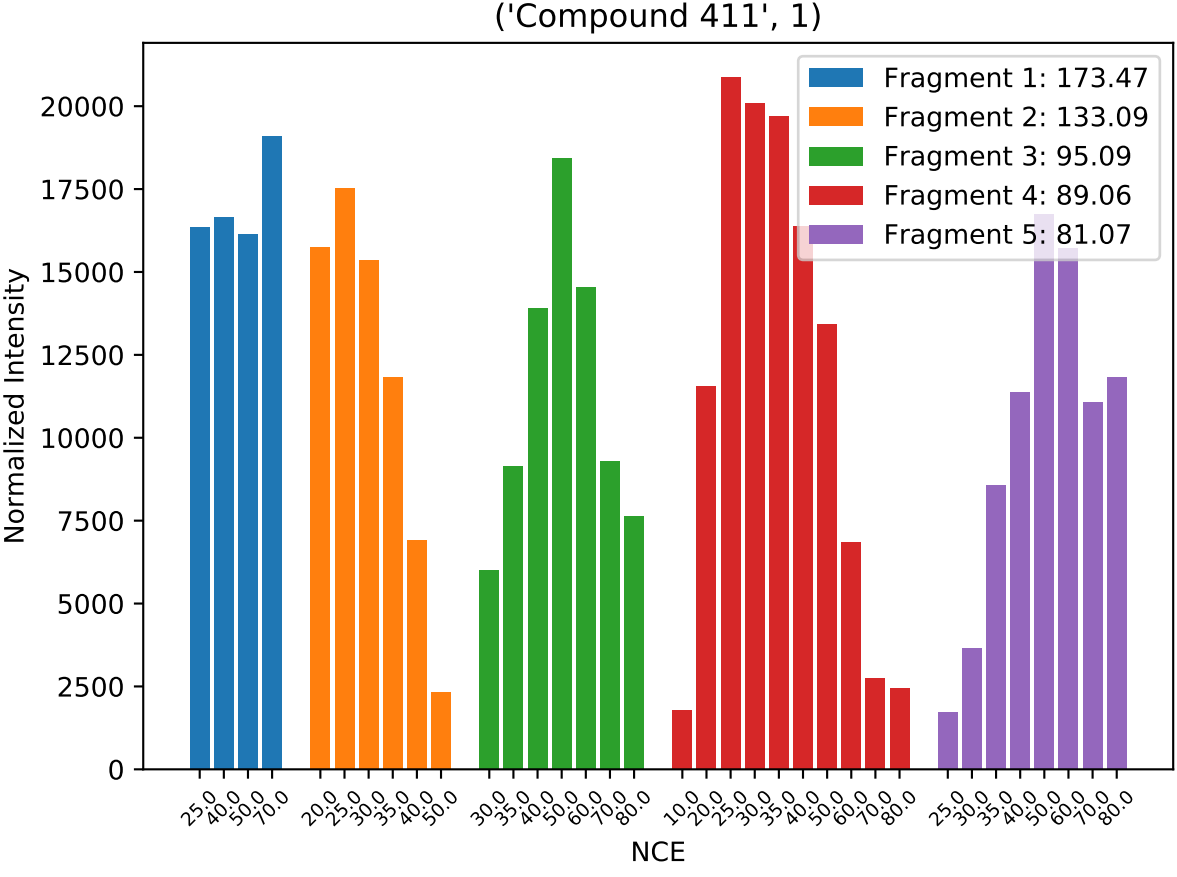

('Compound 510', 1)
Fragment 1: 317.27
Fragment 2: 299.26
Fragment 3: 173.47
Fragment 4: 173.46
Fragment 5: 173.48
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
60.0
70.0
40.0
50.0
80.0
20.0
40.0
50.0
80.0
NCE

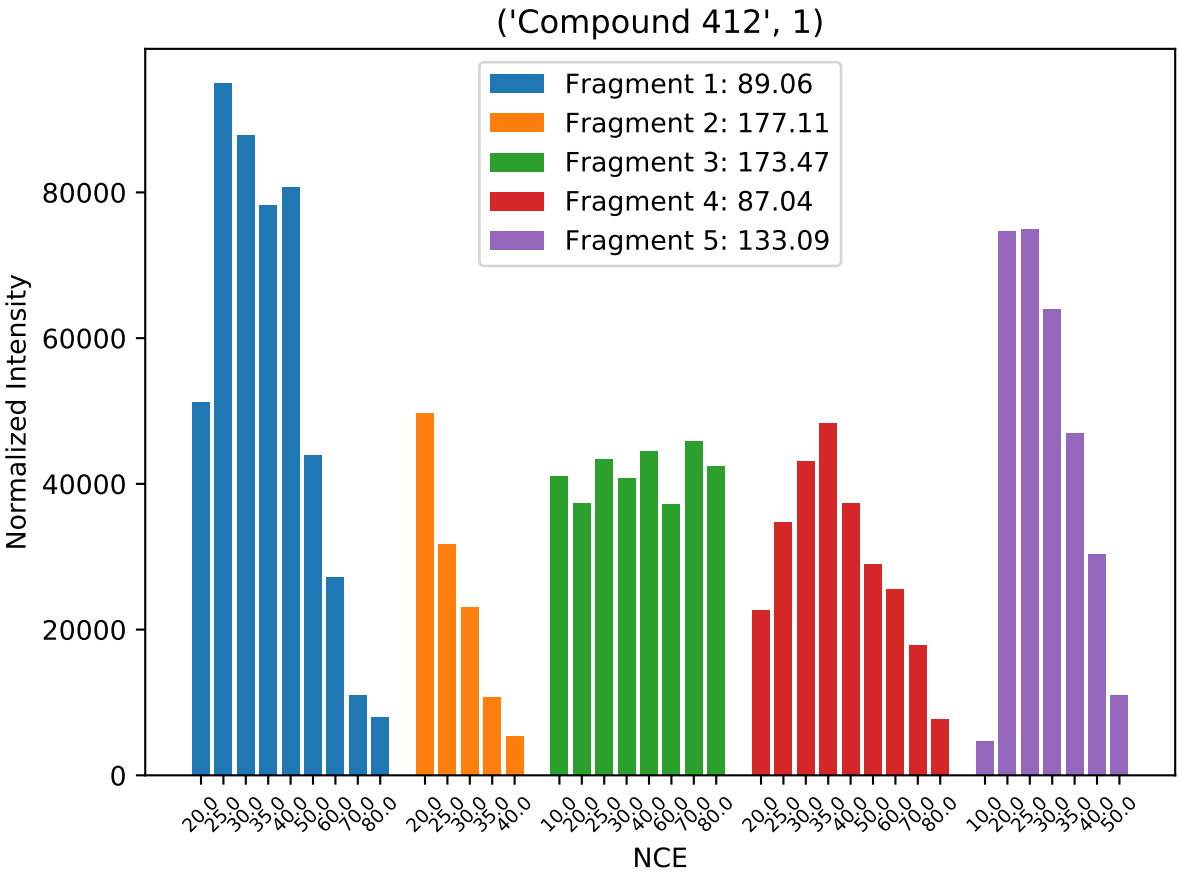

('Compound 512', 1)
Fragment 1: 290.88
Fragment 2: 144.93
Fragment 3: 173.47
Fragment 4: 173.46
Fragment 5: 173.48
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0
20.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
25.0
40.0
50.0
60.0
80.0
10.0
20.0
25.0
30.0
35.0
50.0
60.0
70.0
10.0
20.0
30.0
35.0
50.0
70.0
NCE

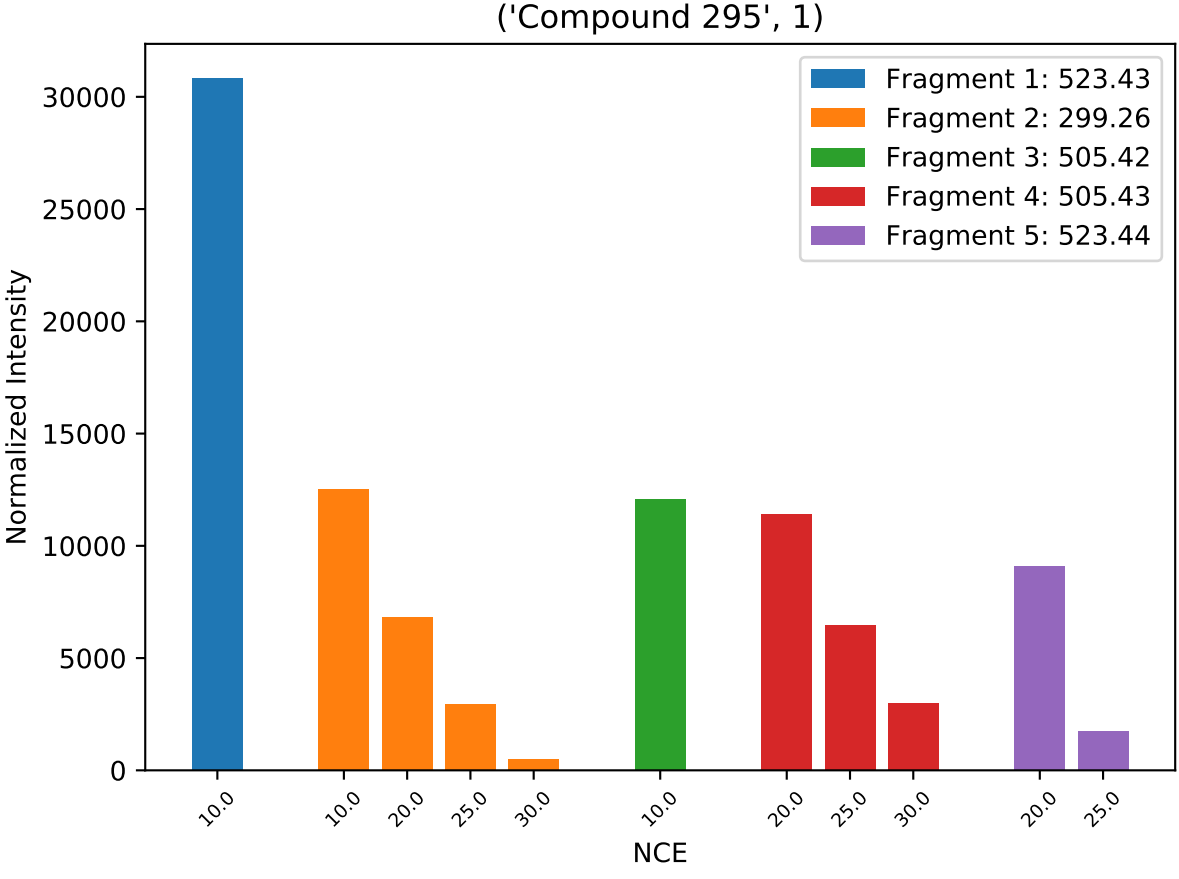

('Compound 523', 1)
Fragment 1: 173.47
Fragment 2: 531.27
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 103.04
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
10.0
25.0
30.0
35.0
50.0
80.0
20.0
25.0
20.0
40.0
60.0
70.0
20.0
40.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

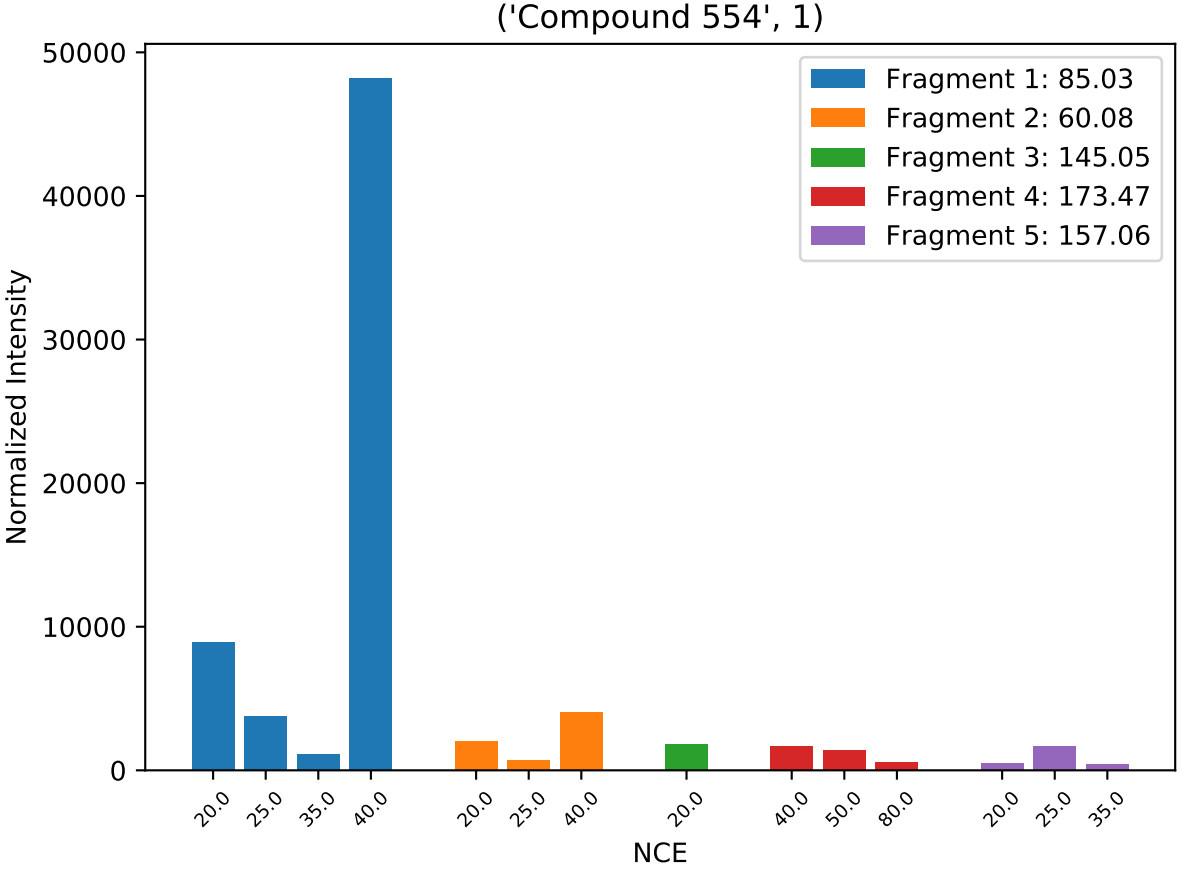

('Compound 402', 1)
Fragment 1: 73.01
Fragment 2: 81.07
Fragment 3: 58.99
Fragment 4: 61.01
Fragment 5: 65.74
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
10.0
NCE

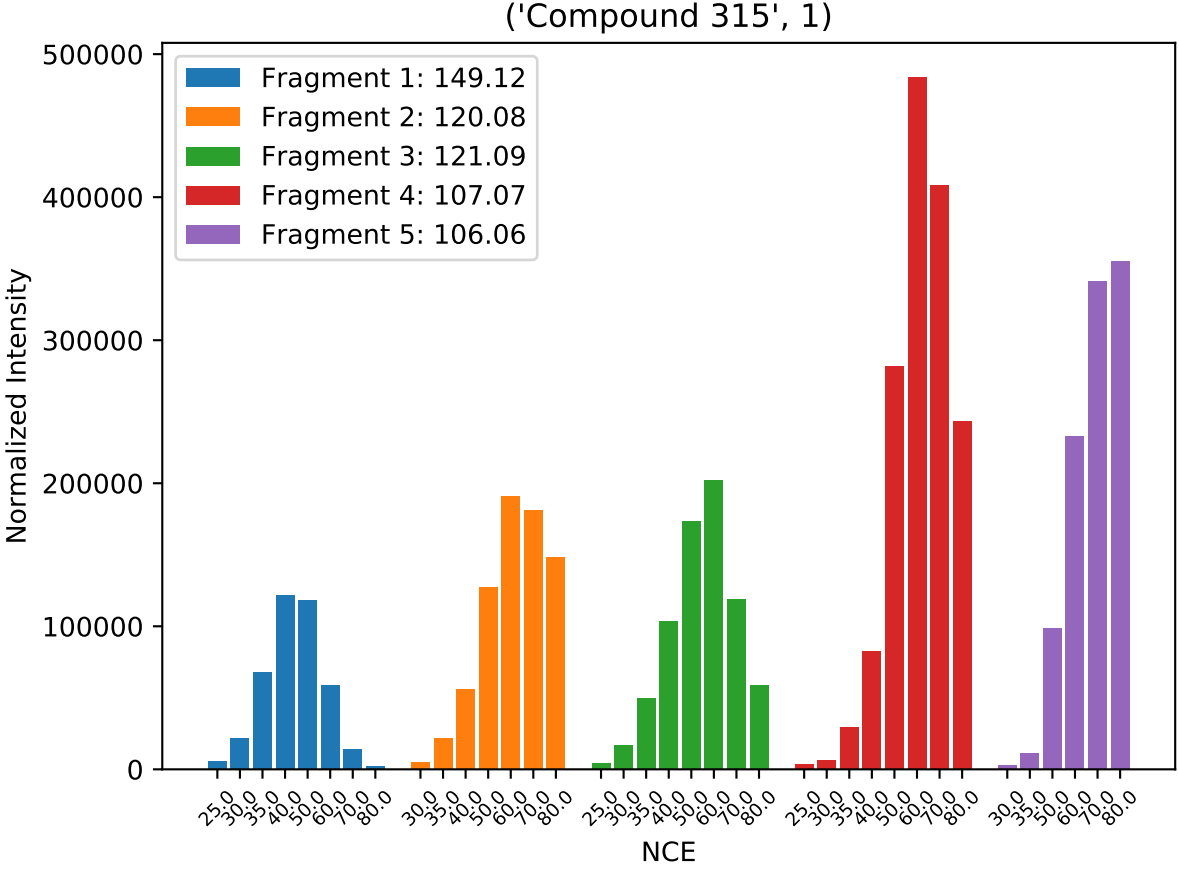

('Compound 406', 1)
Fragment 1: 371.1
Fragment 2: 223.06
Fragment 3: 285.01
Fragment 4: 225.04
Fragment 5: 355.07
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

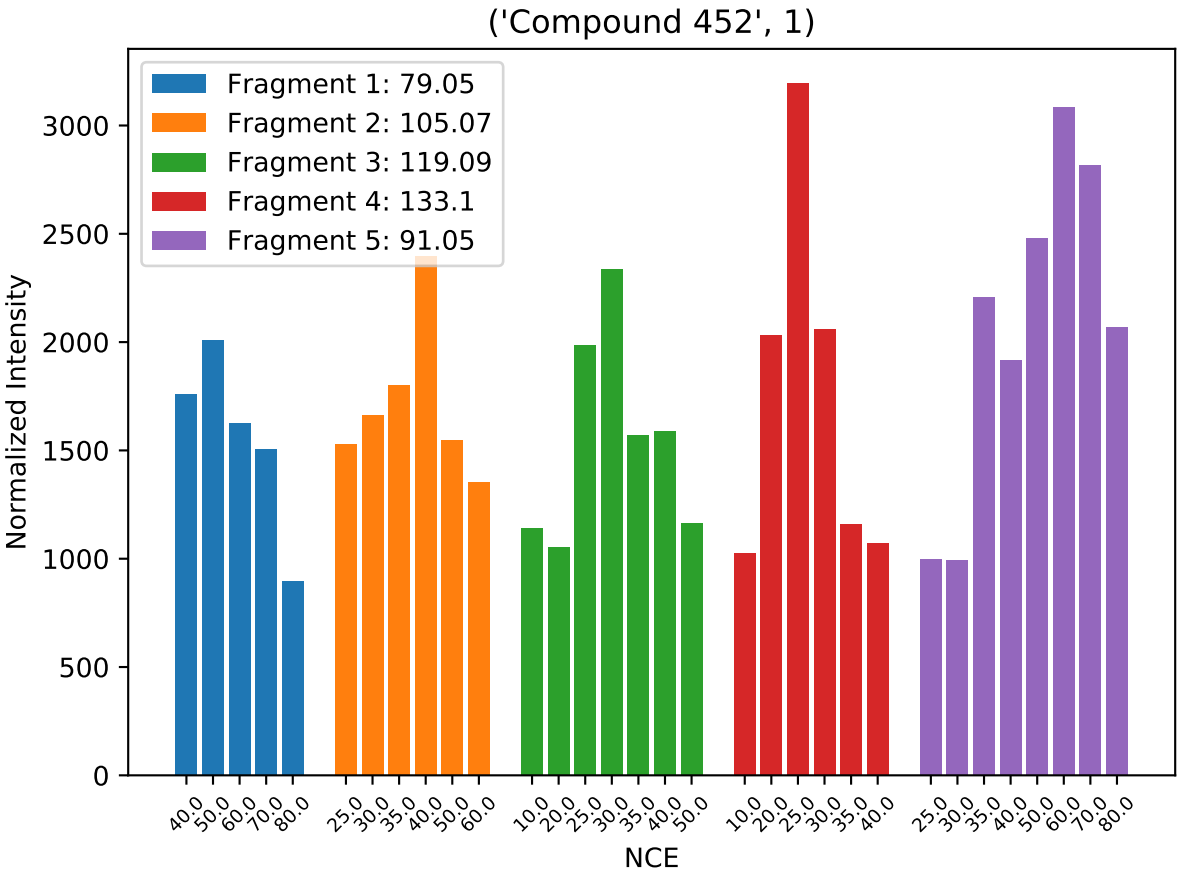

('Compound 411', 1)
Fragment 1: 173.47
Fragment 2: 133.09
Fragment 3: 95.09
Fragment 4: 89.06
Fragment 5: 81.07
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
25.0 40.0 50.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

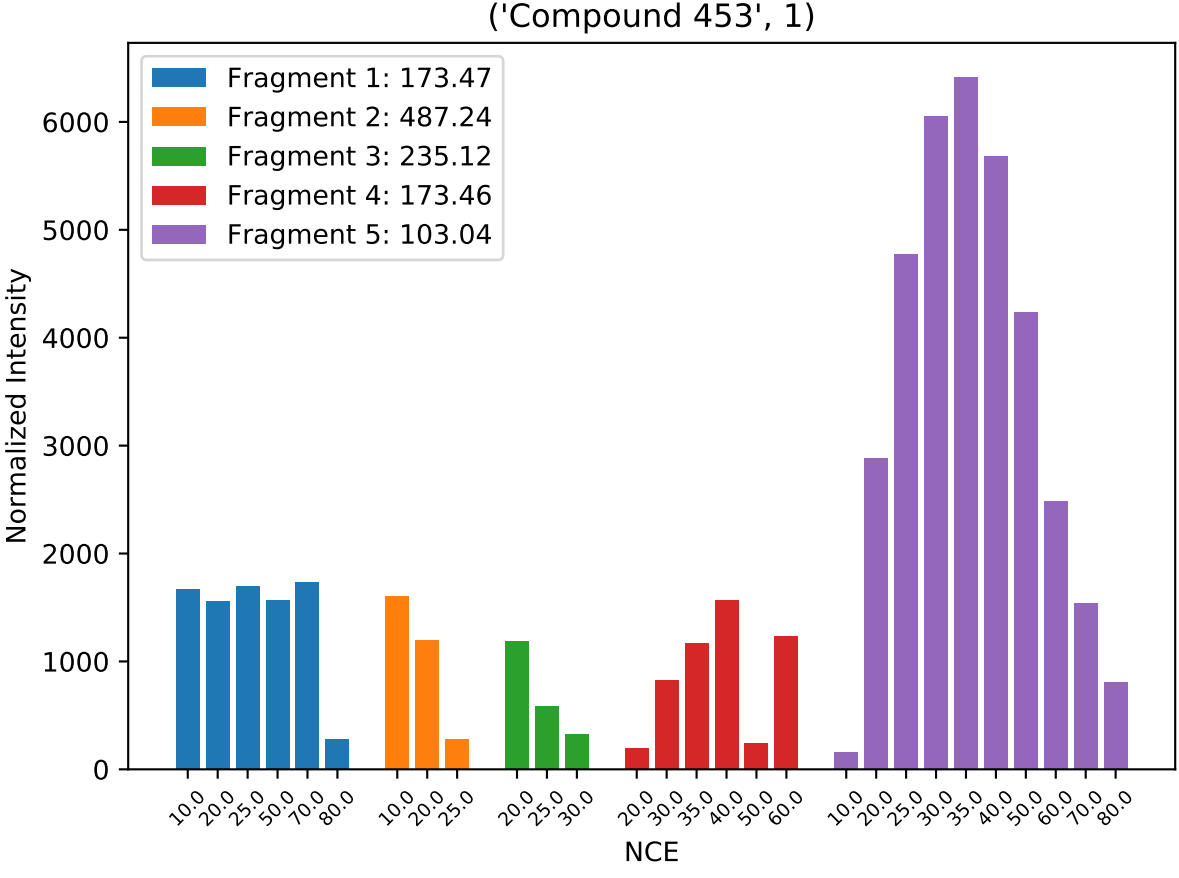

('Compound 412', 1)
Fragment 1: 89.06
Fragment 2: 177.11
Fragment 3: 173.47
Fragment 4: 87.04
Fragment 5: 133.09
Normalized Intensity
0
20000
40000
60000
80000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 40.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

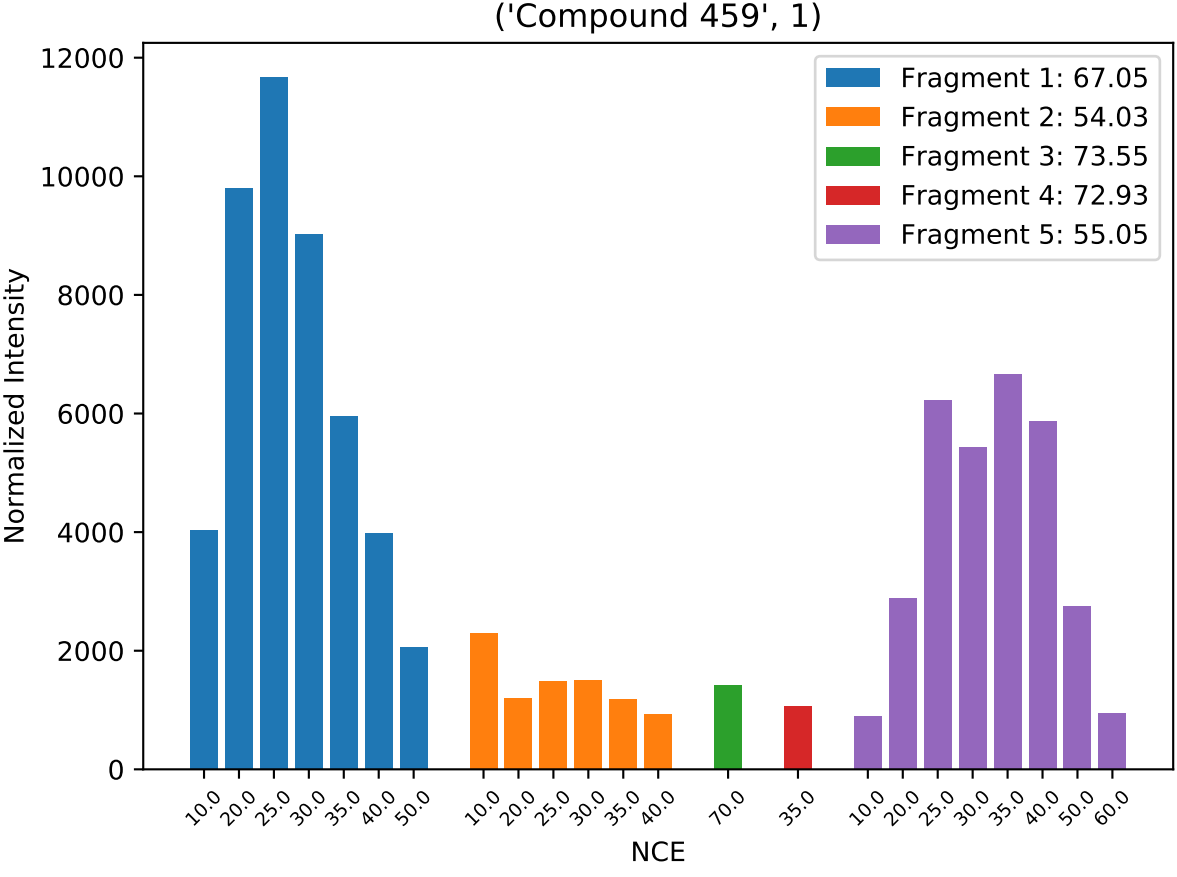

('Compound 295', 1)
Fragment 1: 523.43
Fragment 2: 299.26
Fragment 3: 505.42
Fragment 4: 505.43
Fragment 5: 523.44
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
20.0
25.0
NCE

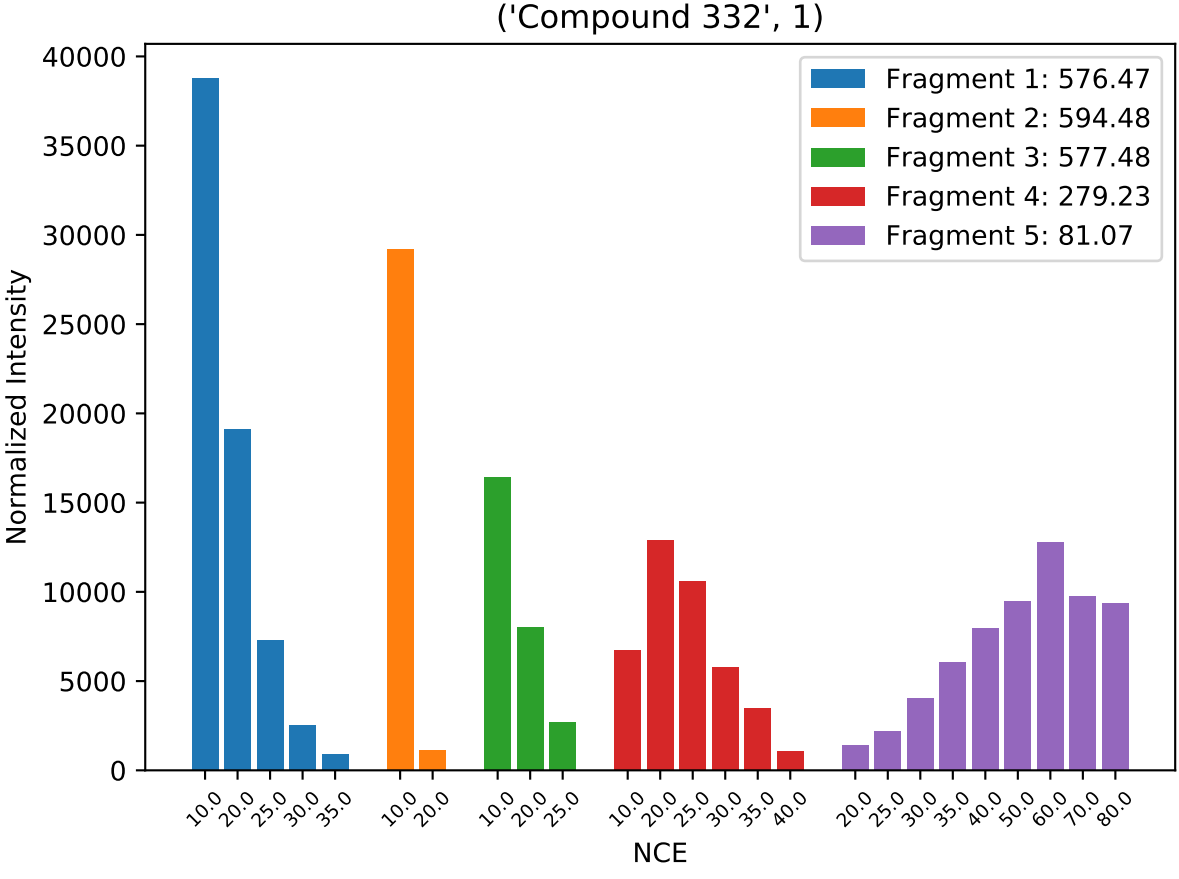

('Compound 554', 1)
Fragment 1: 85.03
Fragment 2: 60.08
Fragment 3: 145.05
Fragment 4: 173.47
Fragment 5: 157.06
Normalized Intensity
50000
40000
30000
20000
10000
0
20.0
25.0
35.0
40.0
20.0
25.0
40.0
20.0
40.0
50.0
80.0
20.0
25.0
35.0
NCE

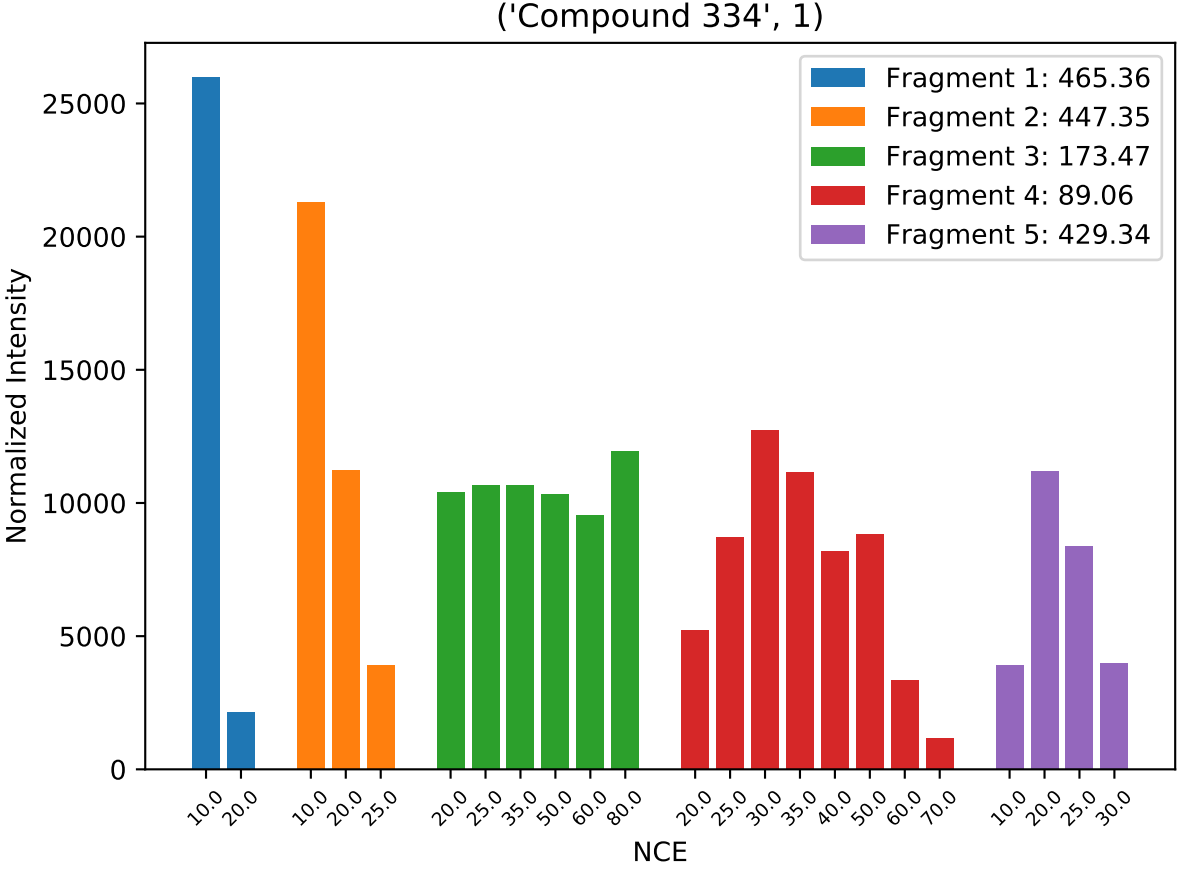

('Compound 315', 1)
Fragment 1: 149.12
Fragment 2: 120.08
Fragment 3: 121.09
Fragment 4: 107.07
Fragment 5: 106.06
Normalized Intensity
500000
400000
300000
200000
100000
0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

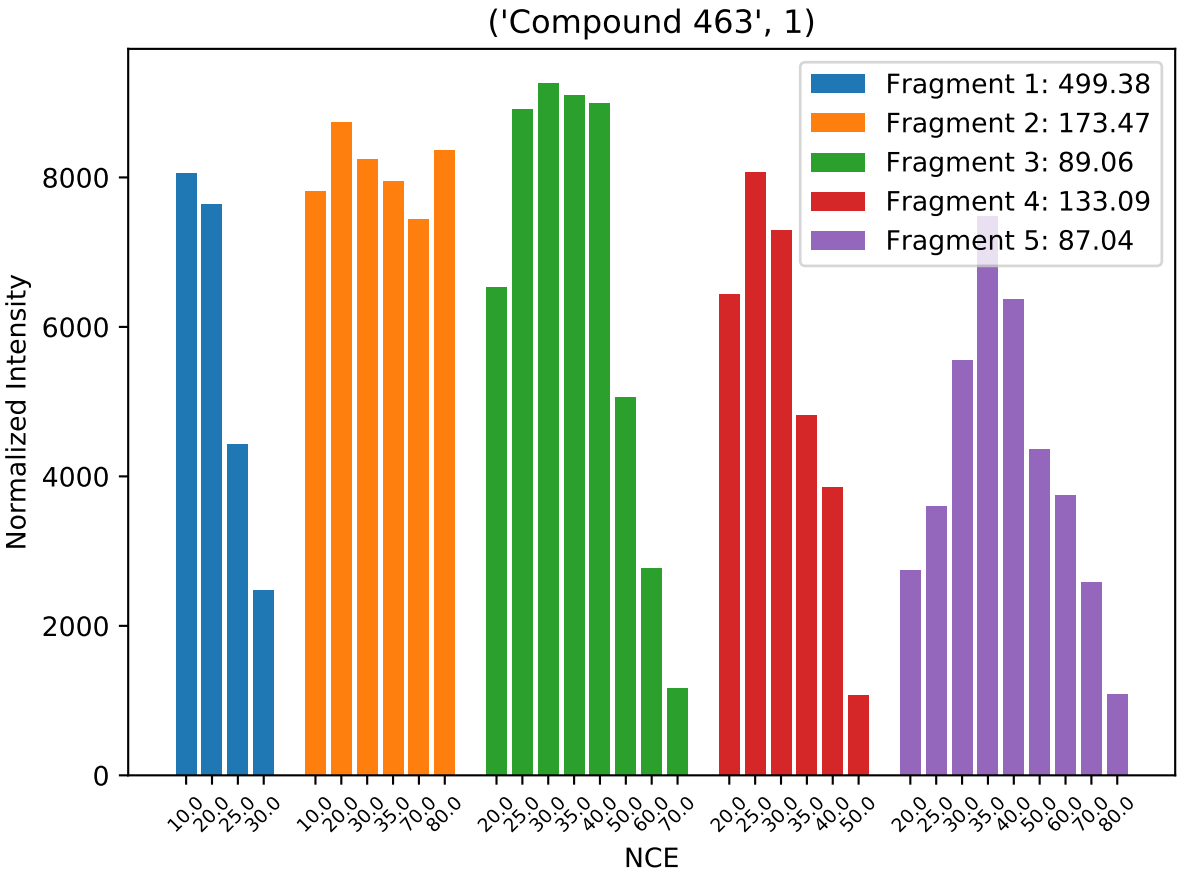

('Compound 452', 1)
Fragment 1: 79.05
Fragment 2: 105.07
Fragment 3: 119.09
Fragment 4: 133.1
Fragment 5: 91.05
Normalized Intensity
0
500
1000
1500
2000
2500
3000
40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

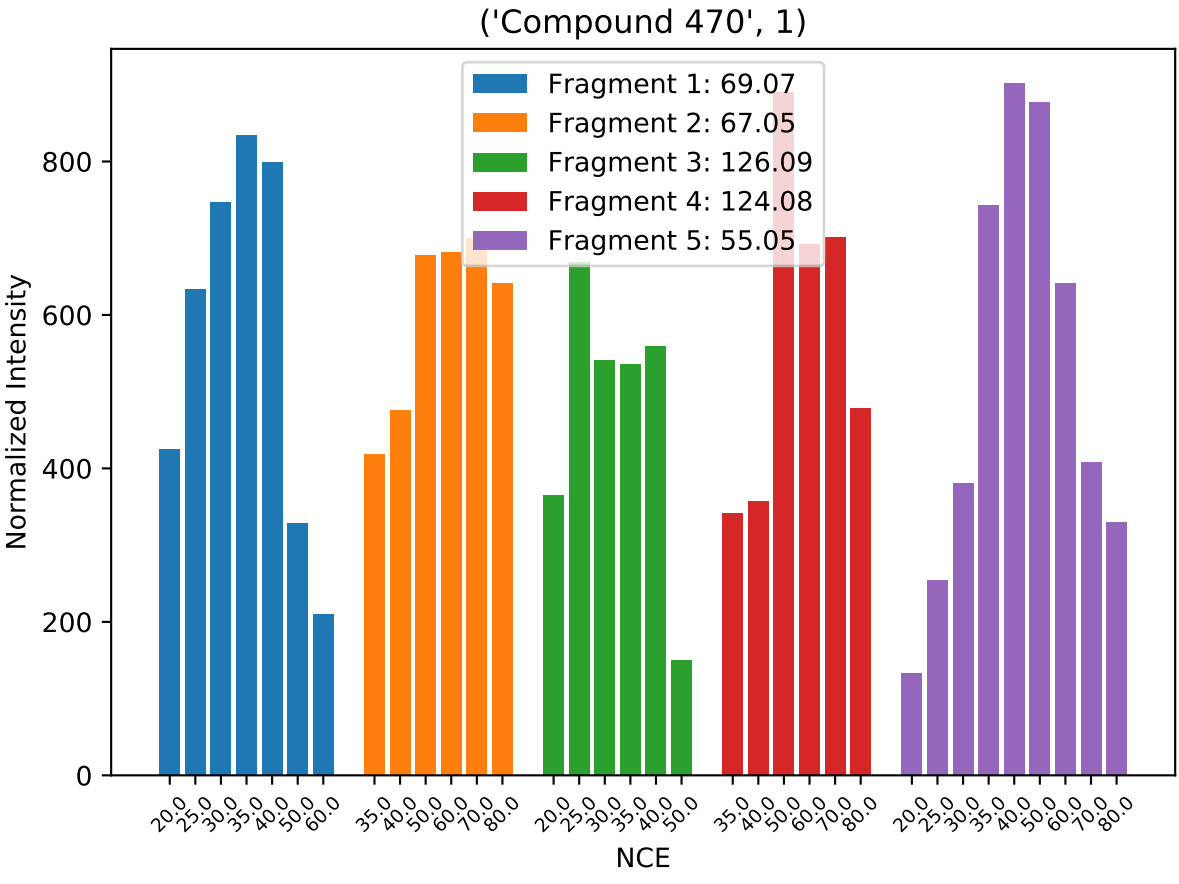

('Compound 453', 1)
Fragment 1: 173.47
Fragment 2: 487.24
Fragment 3: 235.12
Fragment 4: 173.46
Fragment 5: 103.04
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
10.0
20.0
25.0
50.0
70.0
80.0
10.0
20.0
25.0
20.0
25.0
30.0
20.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

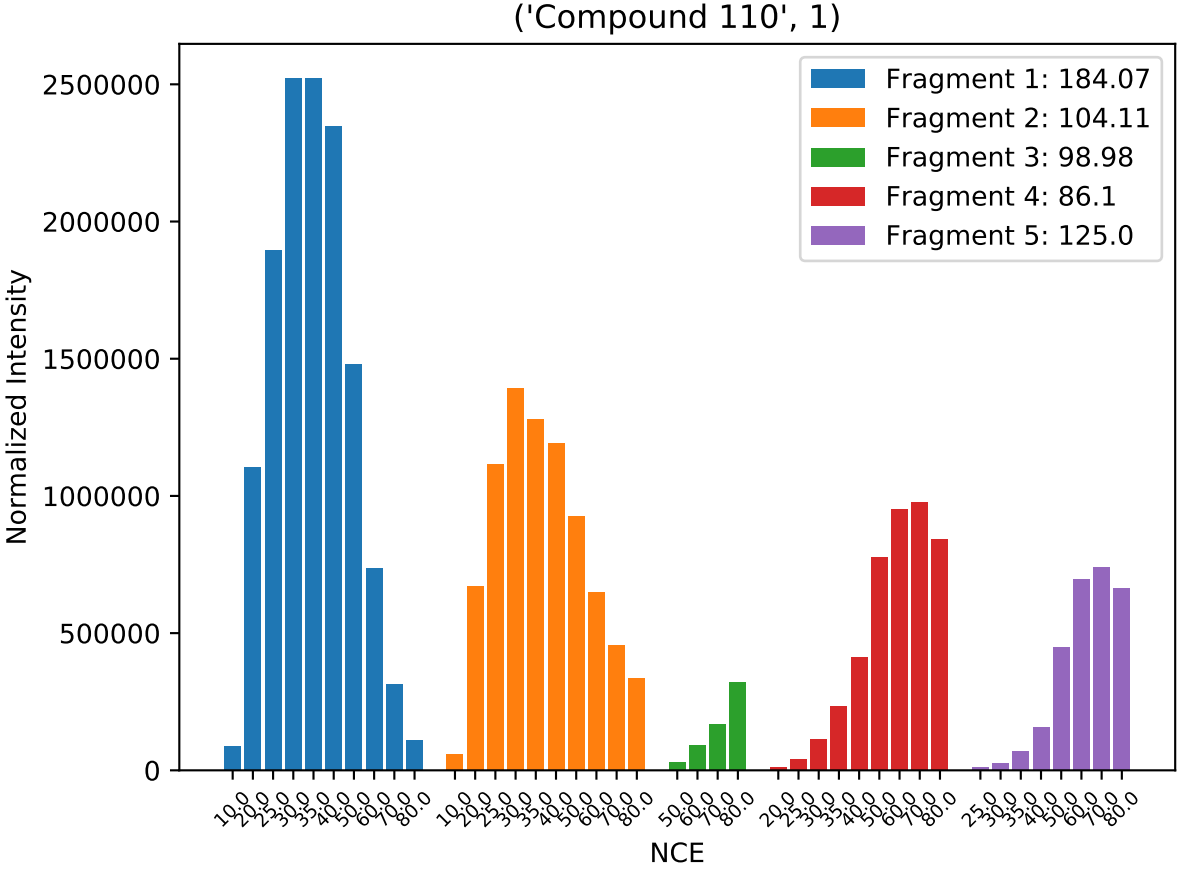

('Compound 459', 1)
Fragment 1: 67.05
Fragment 2: 54.03
Fragment 3: 73.55
Fragment 4: 72.93
Fragment 5: 55.05
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
70.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

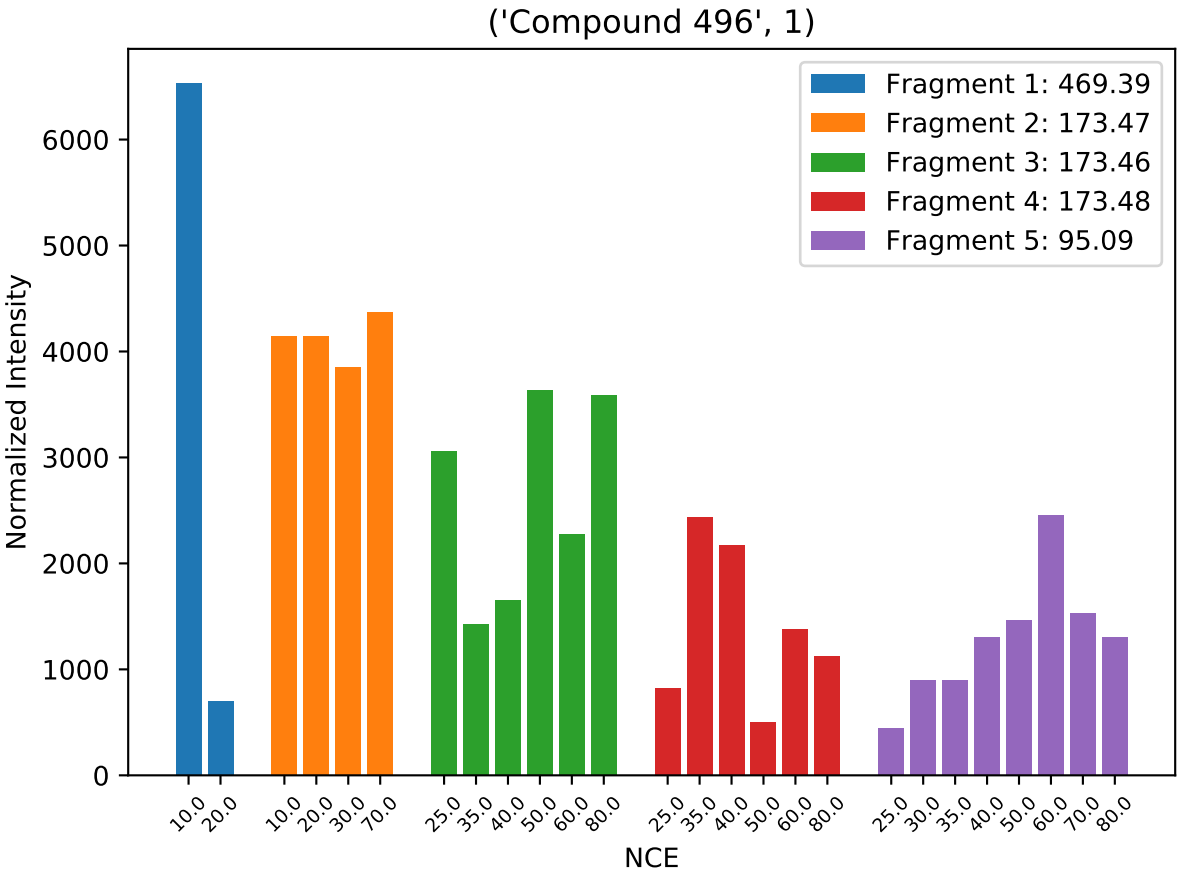

('Compound 332', 1)
Fragment 1: 576.47
Fragment 2: 594.48
Fragment 3: 577.48
Fragment 4: 279.23
Fragment 5: 81.07
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

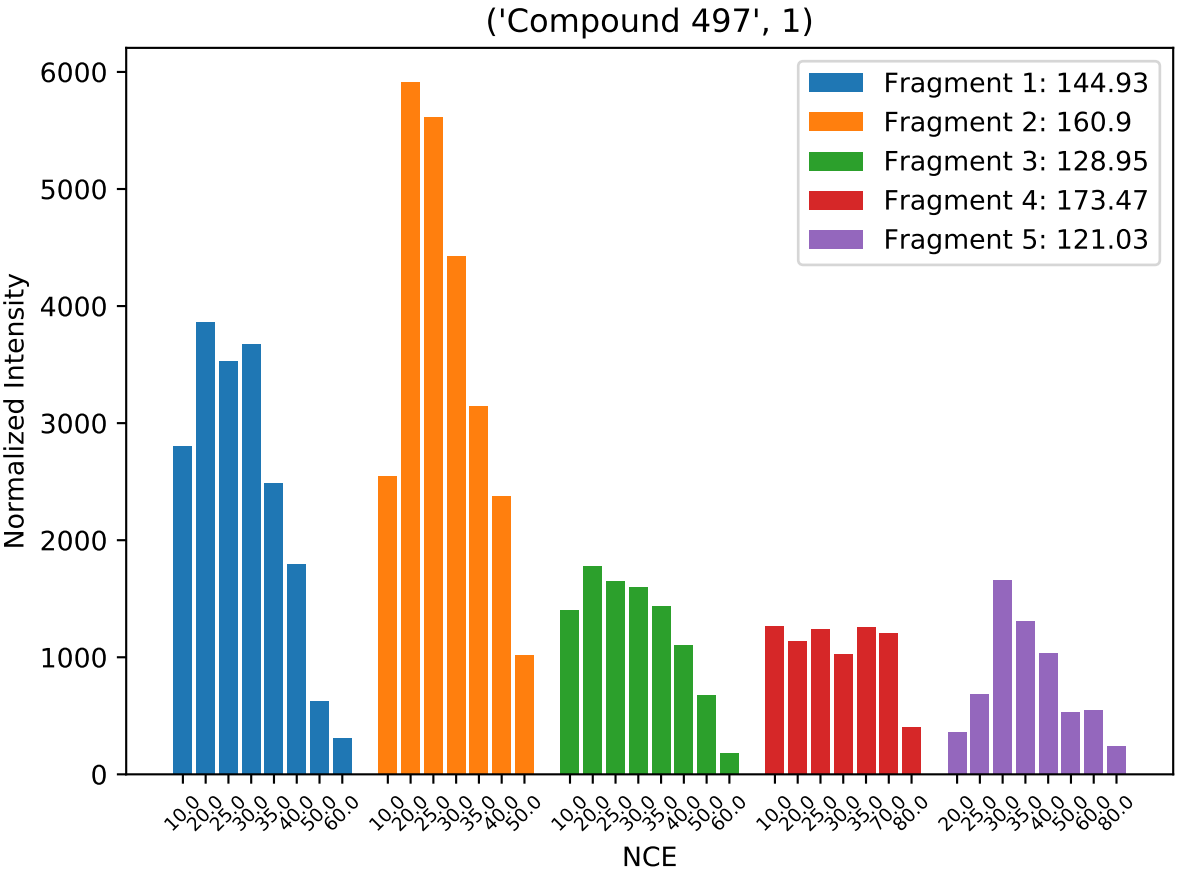

('Compound 334', 1)
Fragment 1: 465.36
Fragment 2: 447.35
Fragment 3: 173.47
Fragment 4: 89.06
Fragment 5: 429.34
Normalized Intensity
0
5000
10000
15000
20000
25000
NCE
10.0
20.0
10.0
20.0
25.0
20.0
25.0
35.0
50.0
60.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0

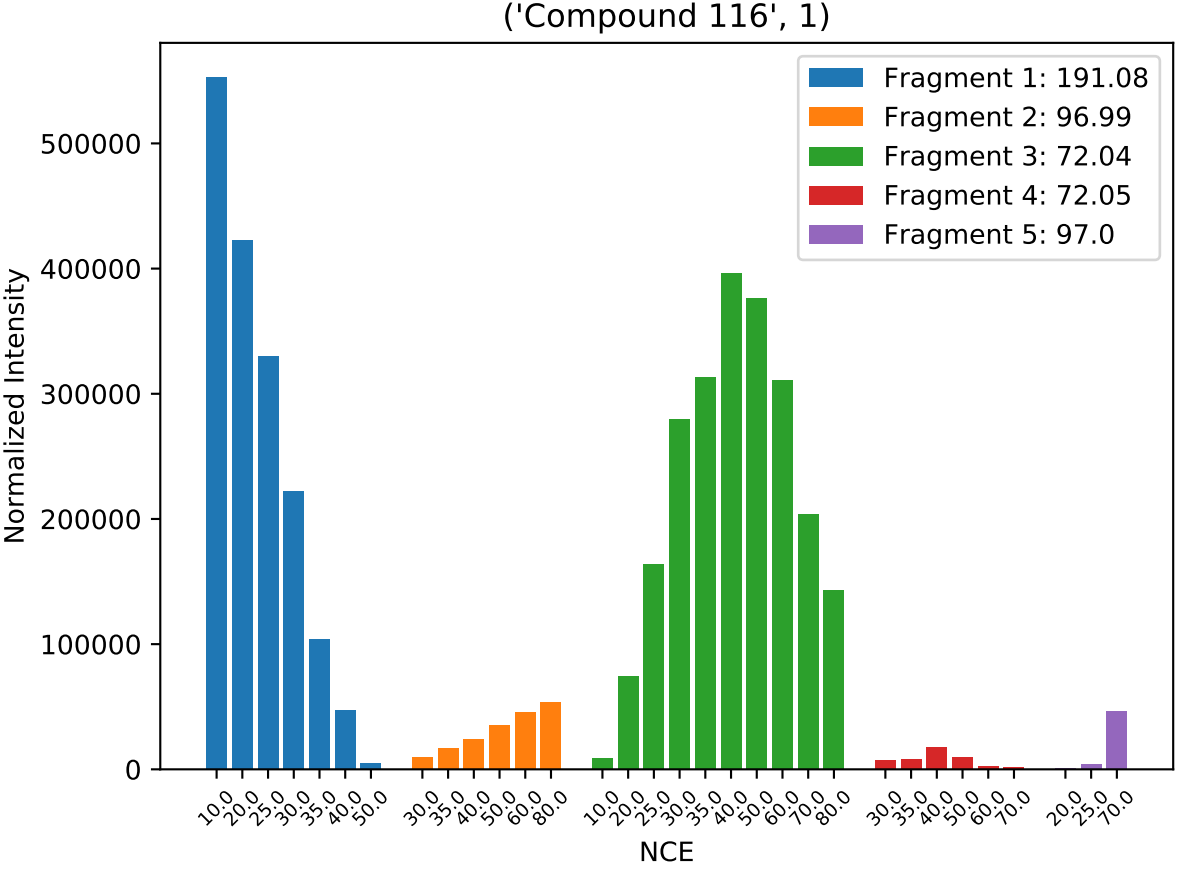

('Compound 463', 1)
Fragment 1: 499.38
Fragment 2: 173.47
Fragment 3: 89.06
Fragment 4: 133.09
Fragment 5: 87.04
Normalized Intensity
0
2000
4000
6000
8000
10.0
20.0
25.0
30.0
10.0
20.0
30.0
35.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

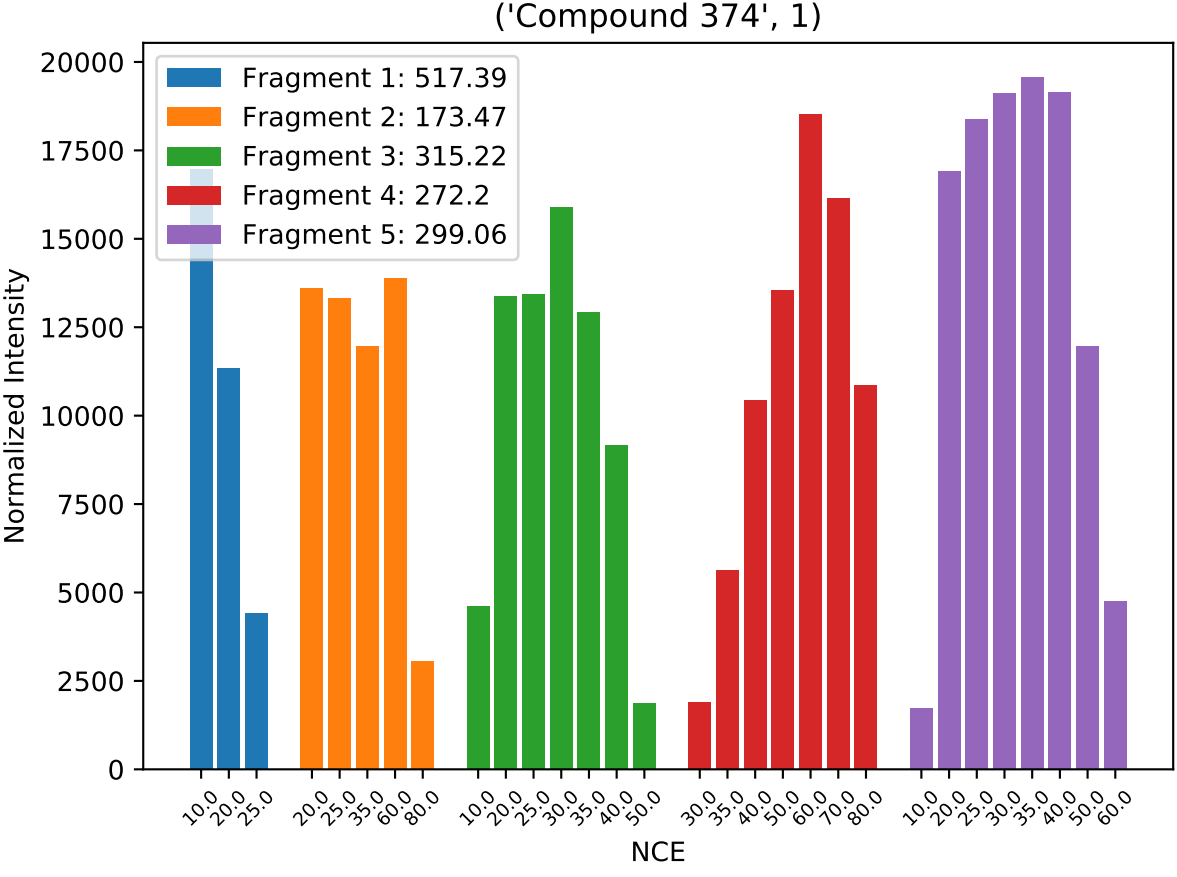

('Compound 470', 1)
Fragment 1: 69.07
Fragment 2: 67.05
Fragment 3: 126.09
Fragment 4: 124.08
Fragment 5: 55.05
Normalized Intensity
0
200
400
600
800
20.0
25.0
30.0
35.0
40.0
50.0
60.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

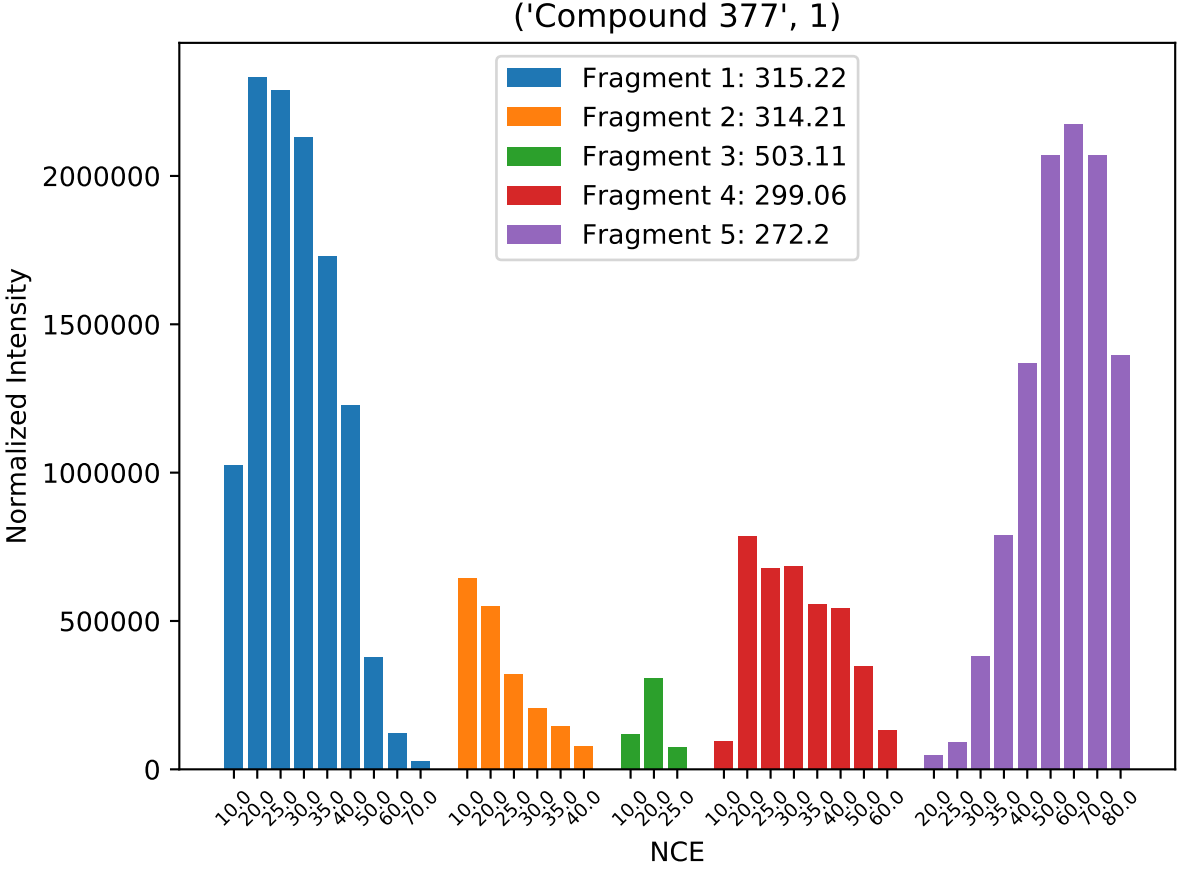

('Compound 110', 1)
Fragment 1: 184.07
Fragment 2: 104.11
Fragment 3: 98.98
Fragment 4: 86.1
Fragment 5: 125.0
Normalized Intensity
2500000
2000000
1500000
1000000
500000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

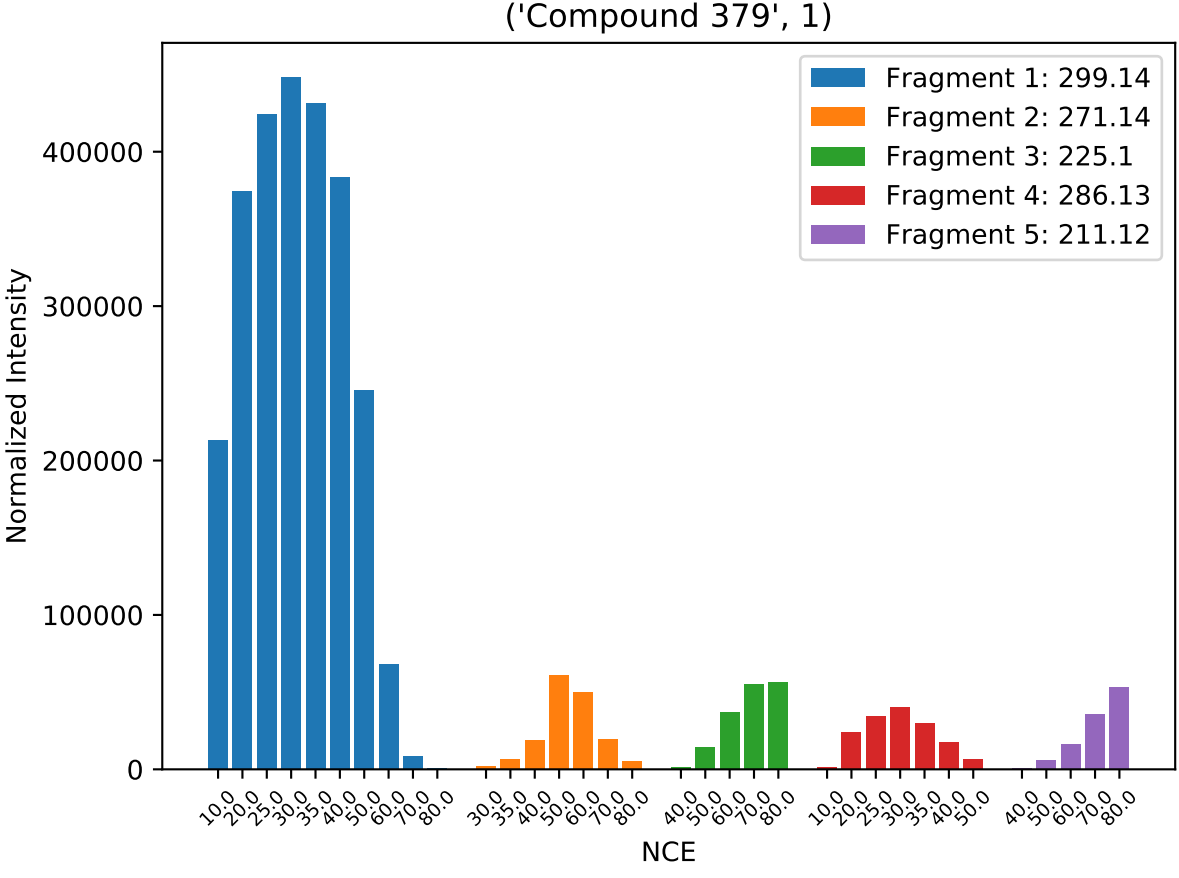

('Compound 496', 1)
Fragment 1: 469.39
Fragment 2: 173.47
Fragment 3: 173.46
Fragment 4: 173.48
Fragment 5: 95.09
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
NCE
10.0
20.0
10.0
20.0
30.0
70.0
25.0
35.0
40.0
50.0
60.0
80.0
25.0
35.0
40.0
50.0
60.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

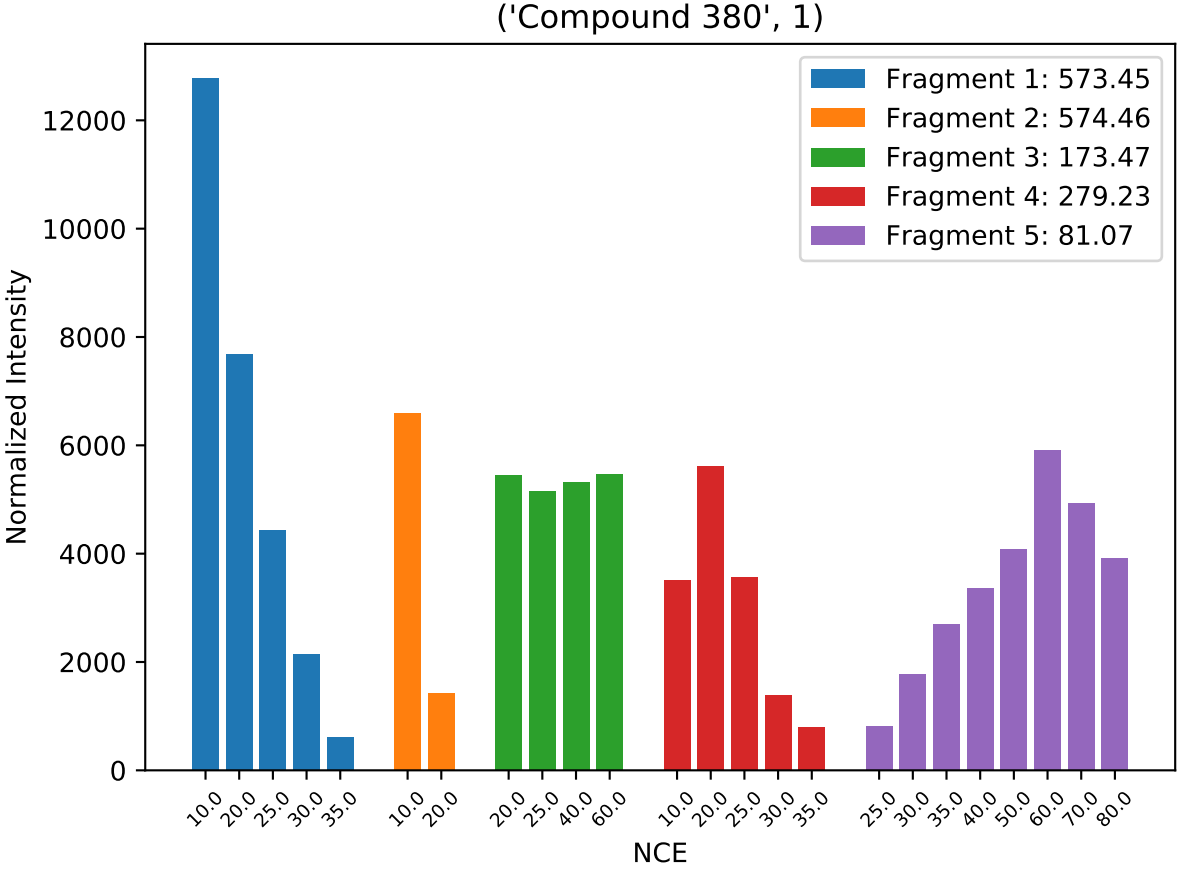

('Compound 497', 1)
Fragment 1: 144.93
Fragment 2: 160.9
Fragment 3: 128.95
Fragment 4: 173.47
Fragment 5: 121.03
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 80.0
NCE

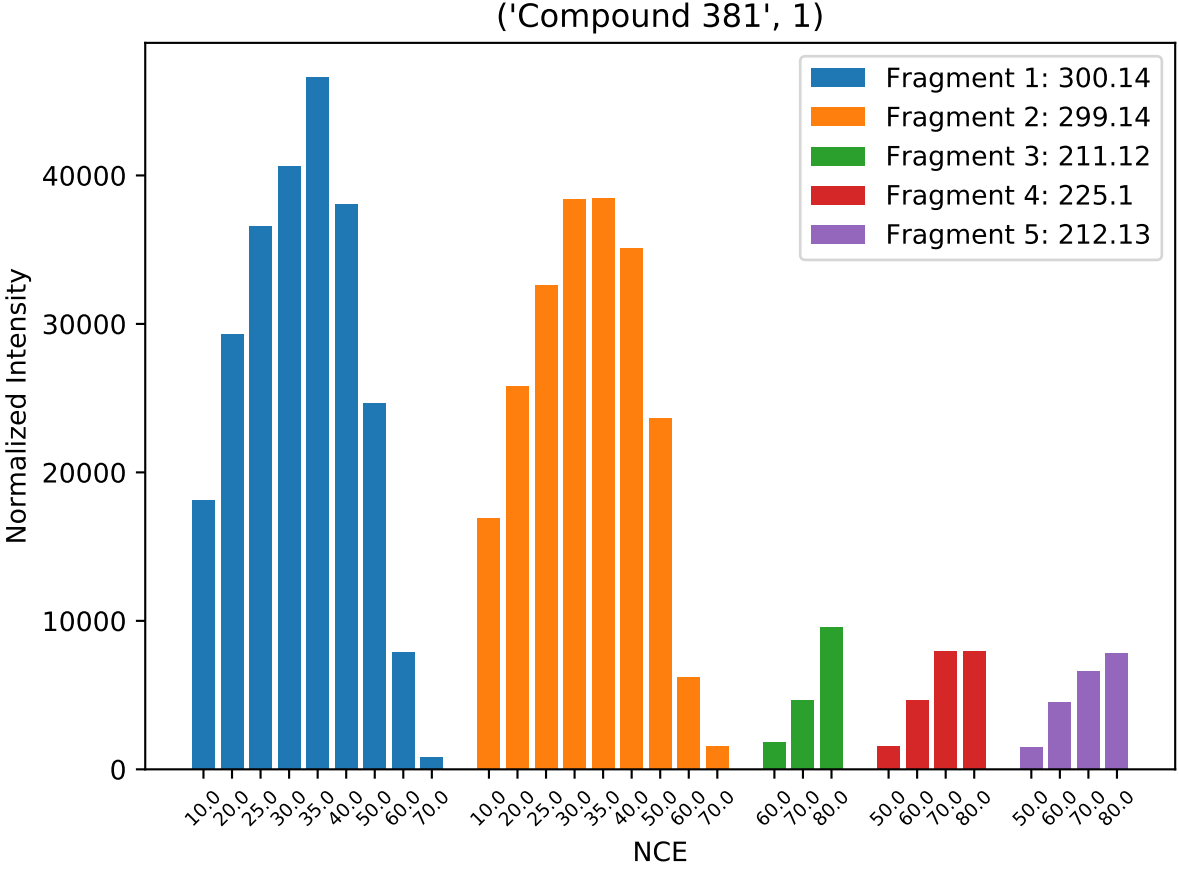

('Compound 116', 1)
Fragment 1: 191.08
Fragment 2: 96.99
Fragment 3: 72.04
Fragment 4: 72.05
Fragment 5: 97.0
Normalized Intensity
0
100000
200000
300000
400000
500000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 70.0
NCE

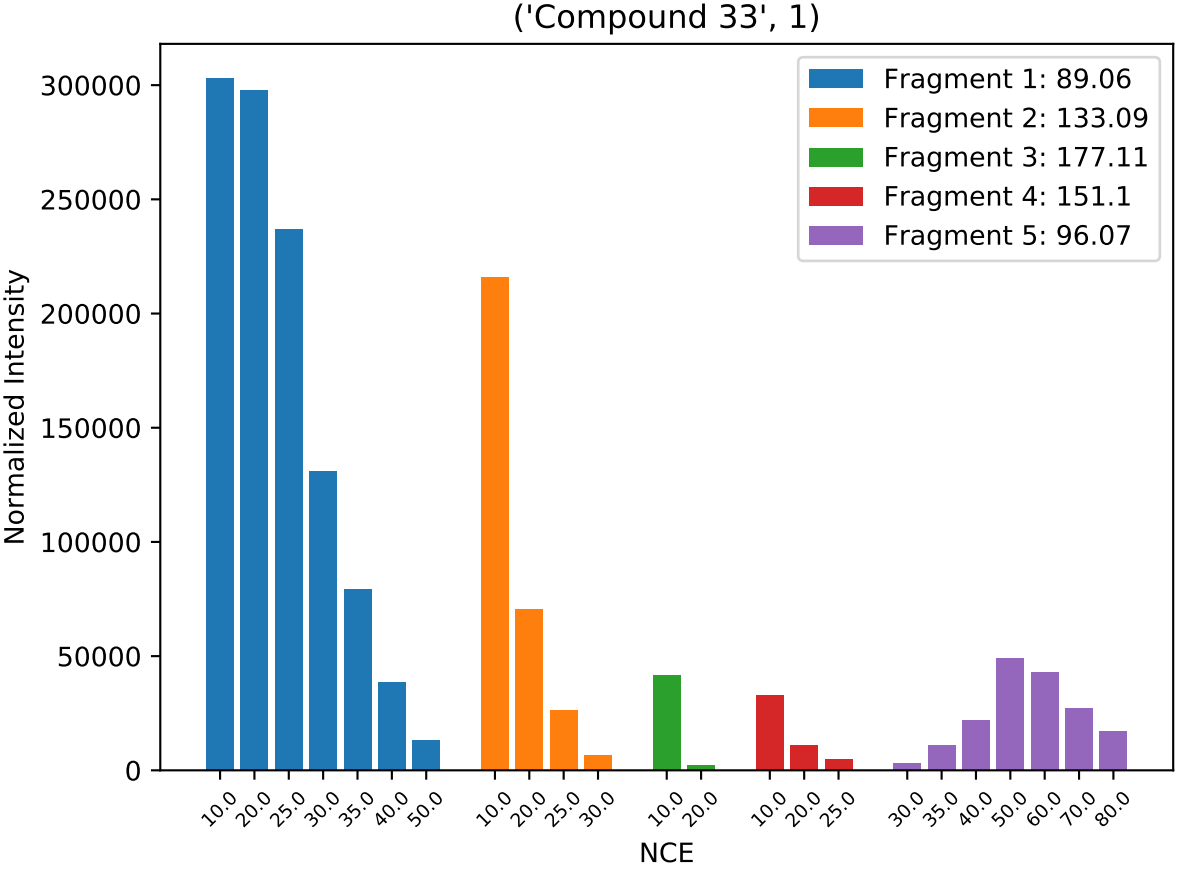

('Compound 374', 1)
Fragment 1: 517.39
Fragment 2: 173.47
Fragment 3: 315.22
Fragment 4: 272.2
Fragment 5: 299.06
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0 20.0 25.0
20.0 25.0 35.0 60.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

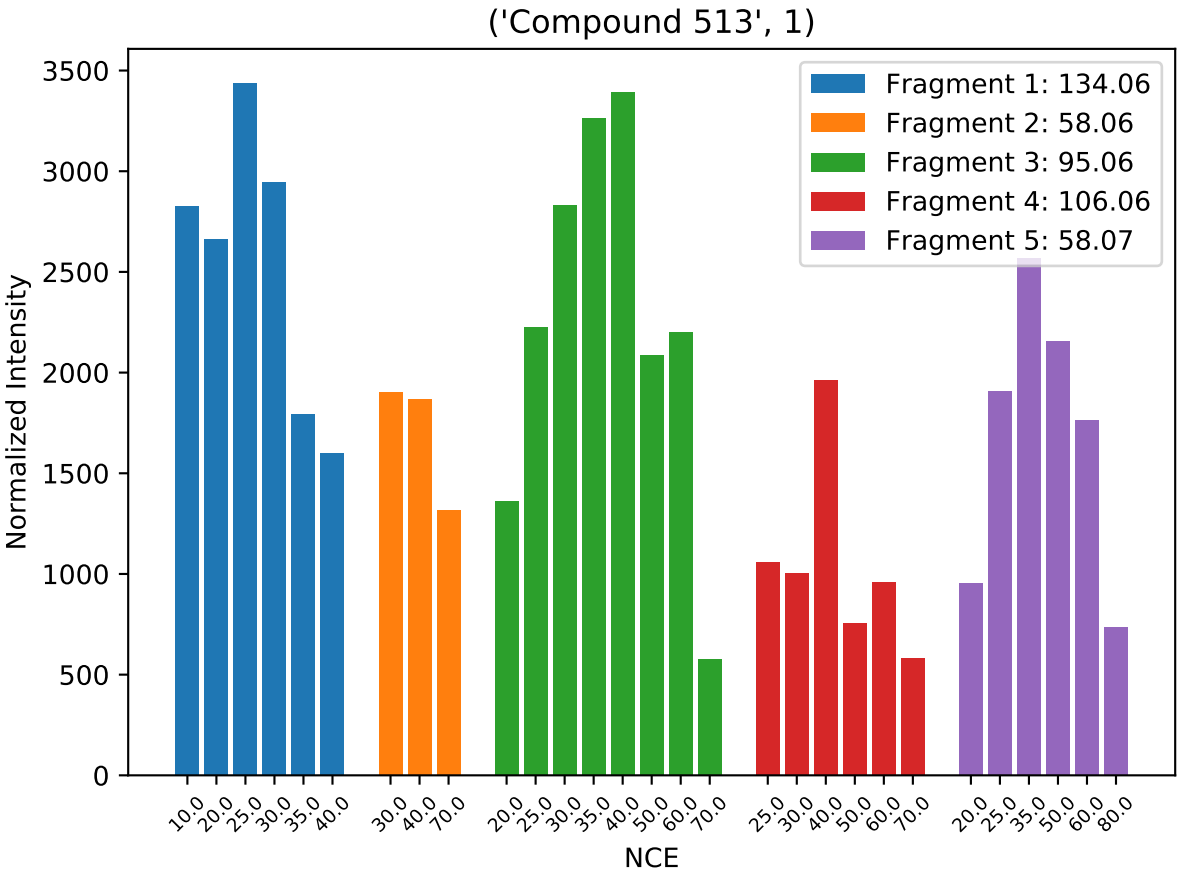

('Compound 377', 1)
Fragment 1: 315.22
Fragment 2: 314.21
Fragment 3: 503.11
Fragment 4: 299.06
Fragment 5: 272.2
Normalized Intensity
0
500000
1000000
1500000
2000000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

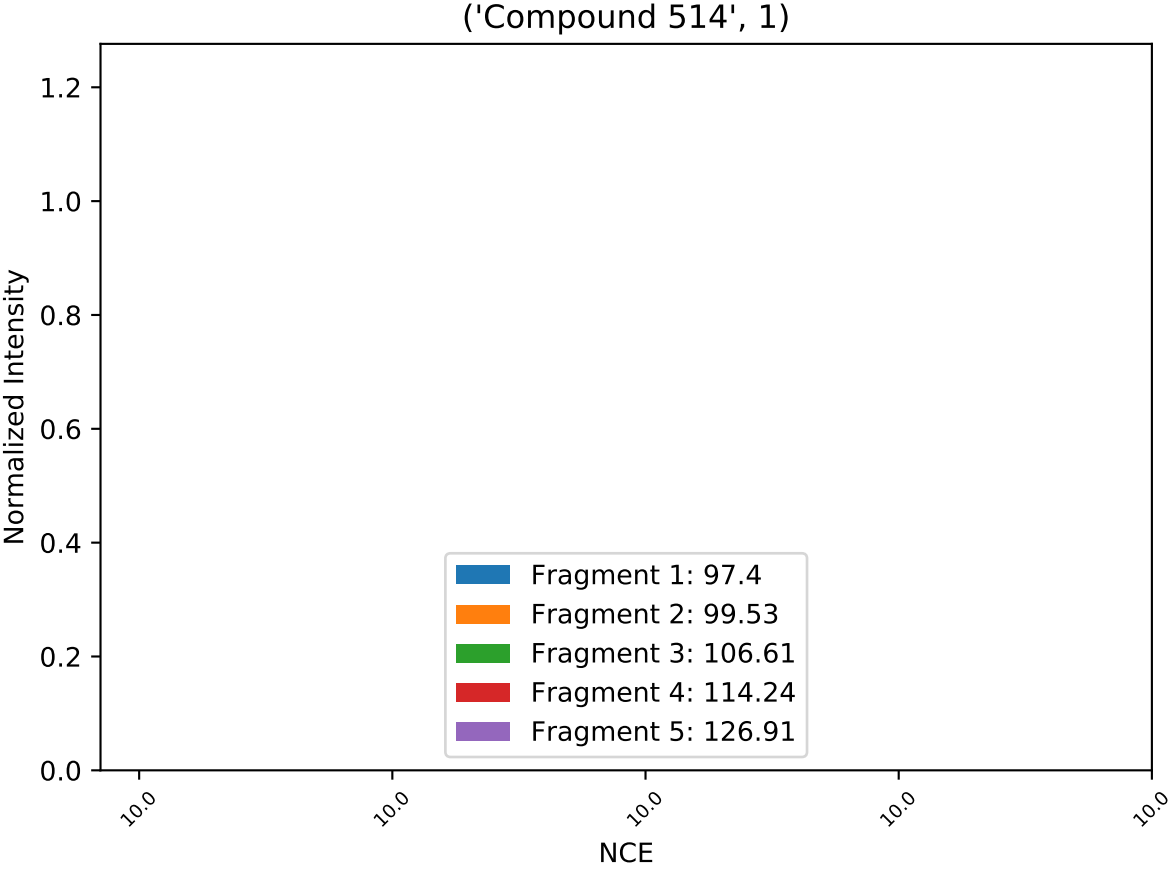

('Compound 379', 1)
Fragment 1: 299.14
Fragment 2: 271.14
Fragment 3: 225.1
Fragment 4: 286.13
Fragment 5: 211.12
Normalized Intensity
0
100000
200000
300000
400000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
40.0 50.0 60.0 70.0 80.0
NCE

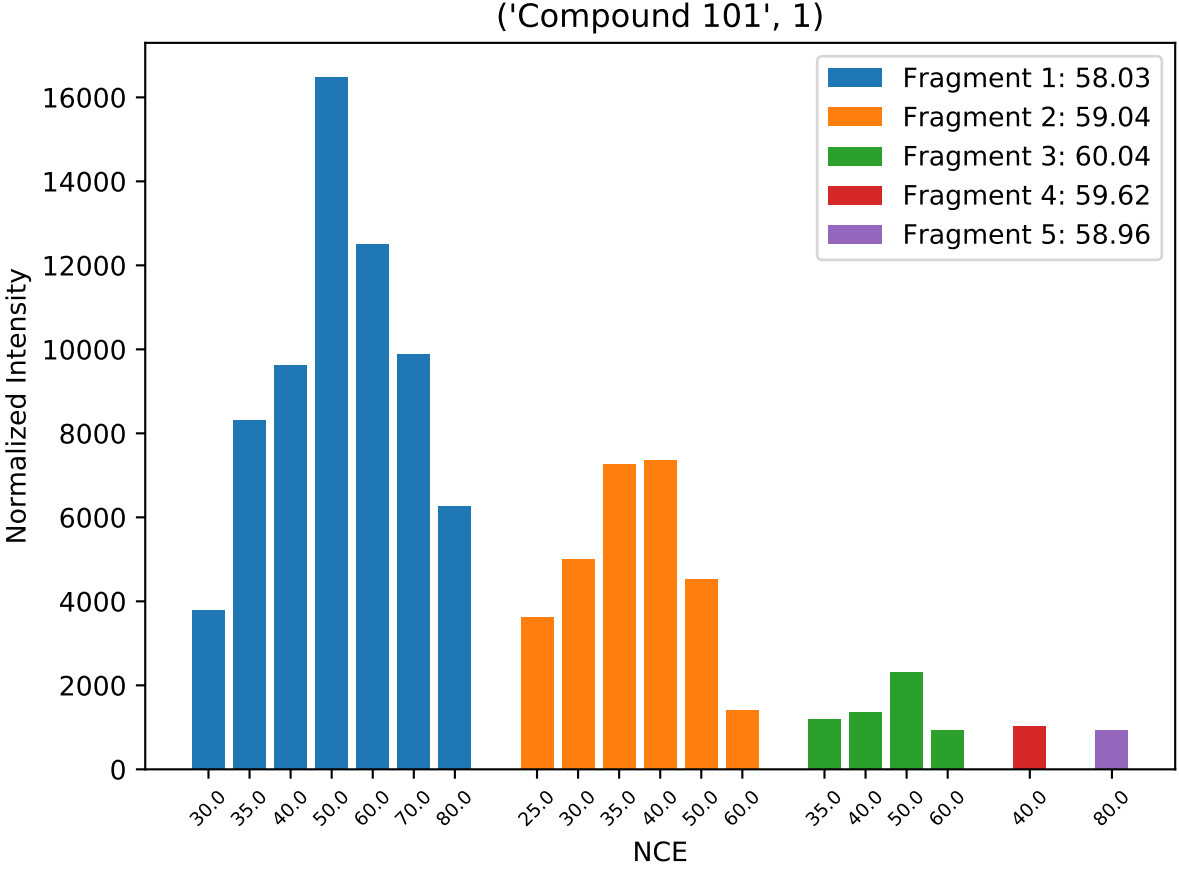

('Compound 380', 1)
Fragment 1: 573.45
Fragment 2: 574.46
Fragment 3: 173.47
Fragment 4: 279.23
Fragment 5: 81.07
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
20.0
25.0
40.0
60.0
10.0
20.0
25.0
30.0
35.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

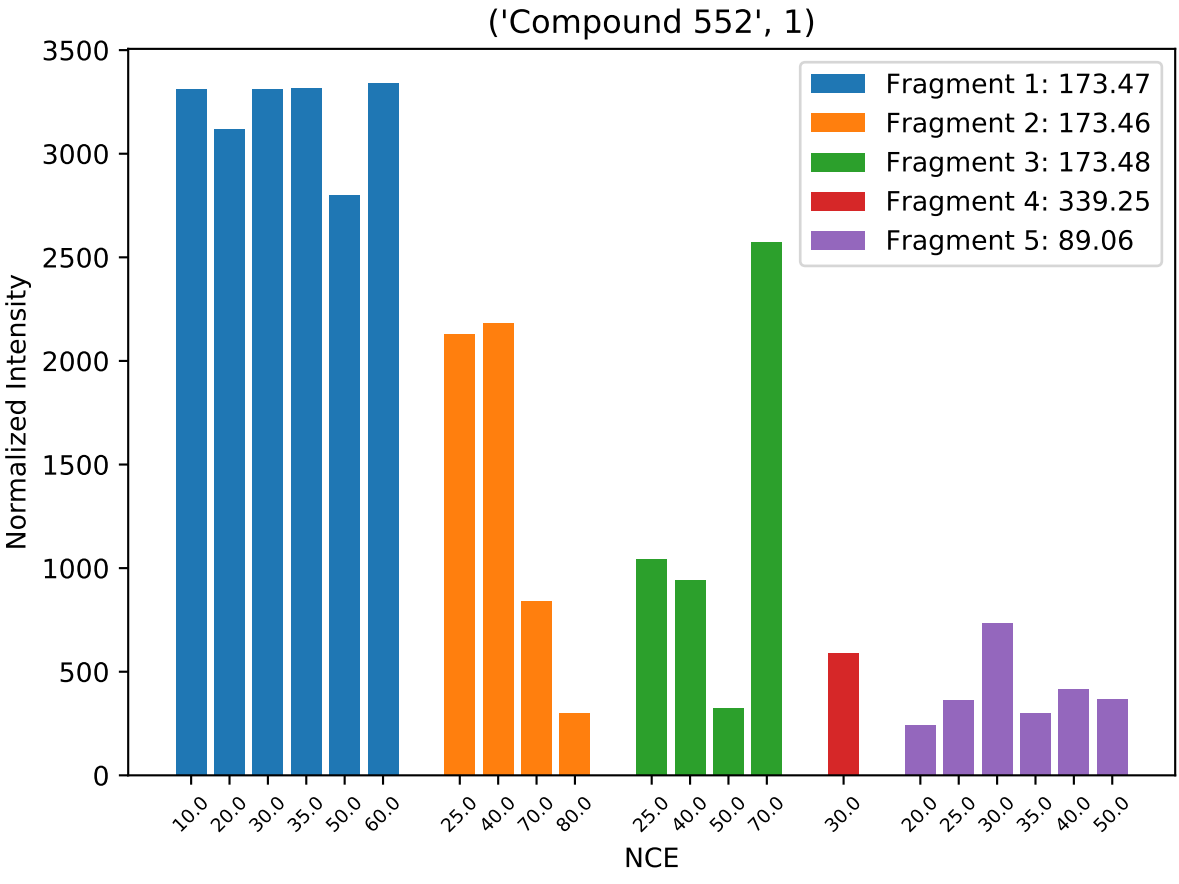

('Compound 381', 1)
Fragment 1: 300.14
Fragment 2: 299.14
Fragment 3: 211.12
Fragment 4: 225.1
Fragment 5: 212.13
Normalized Intensity
0
10000
20000
30000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
60.0 70.0 80.0
50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
NCE

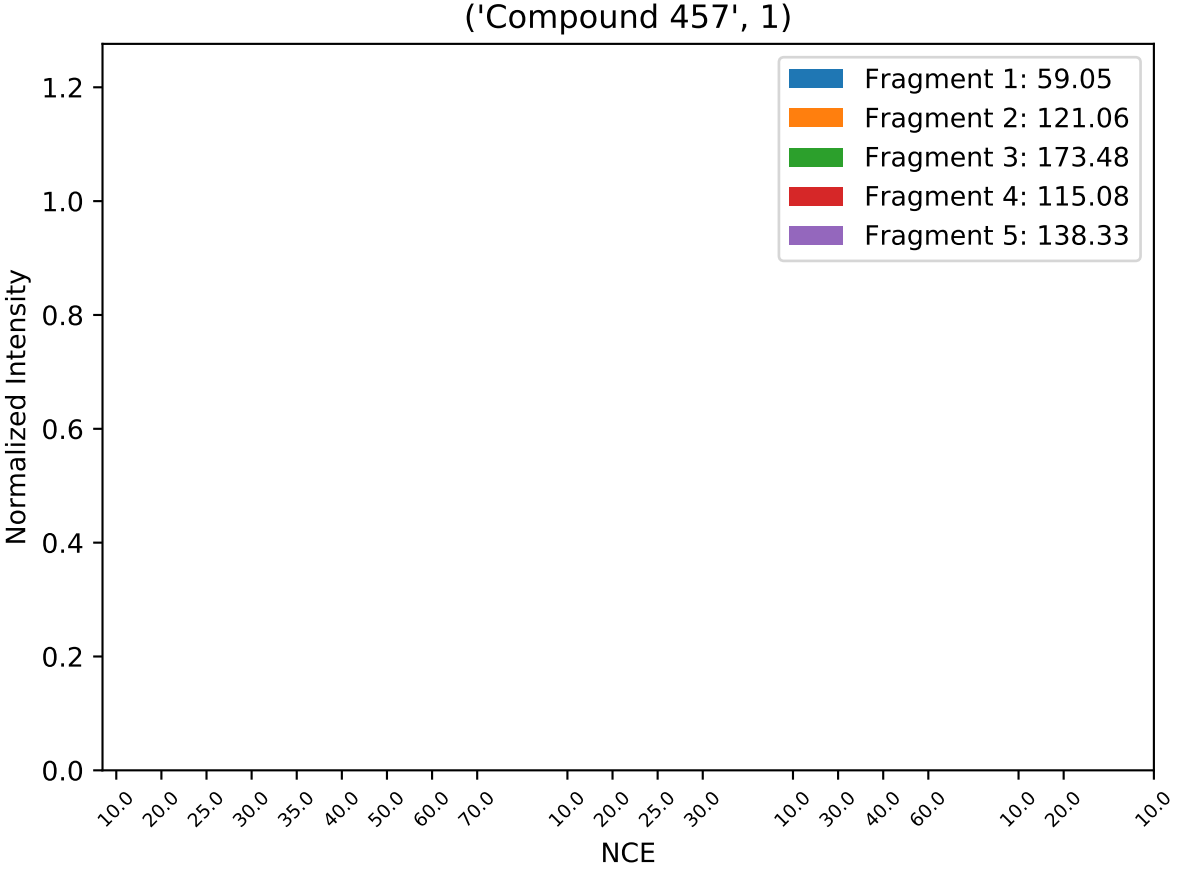

('Compound 33', 1)
Fragment 1: 89.06
Fragment 2: 133.09
Fragment 3: 177.11
Fragment 4: 151.1
Fragment 5: 96.07
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

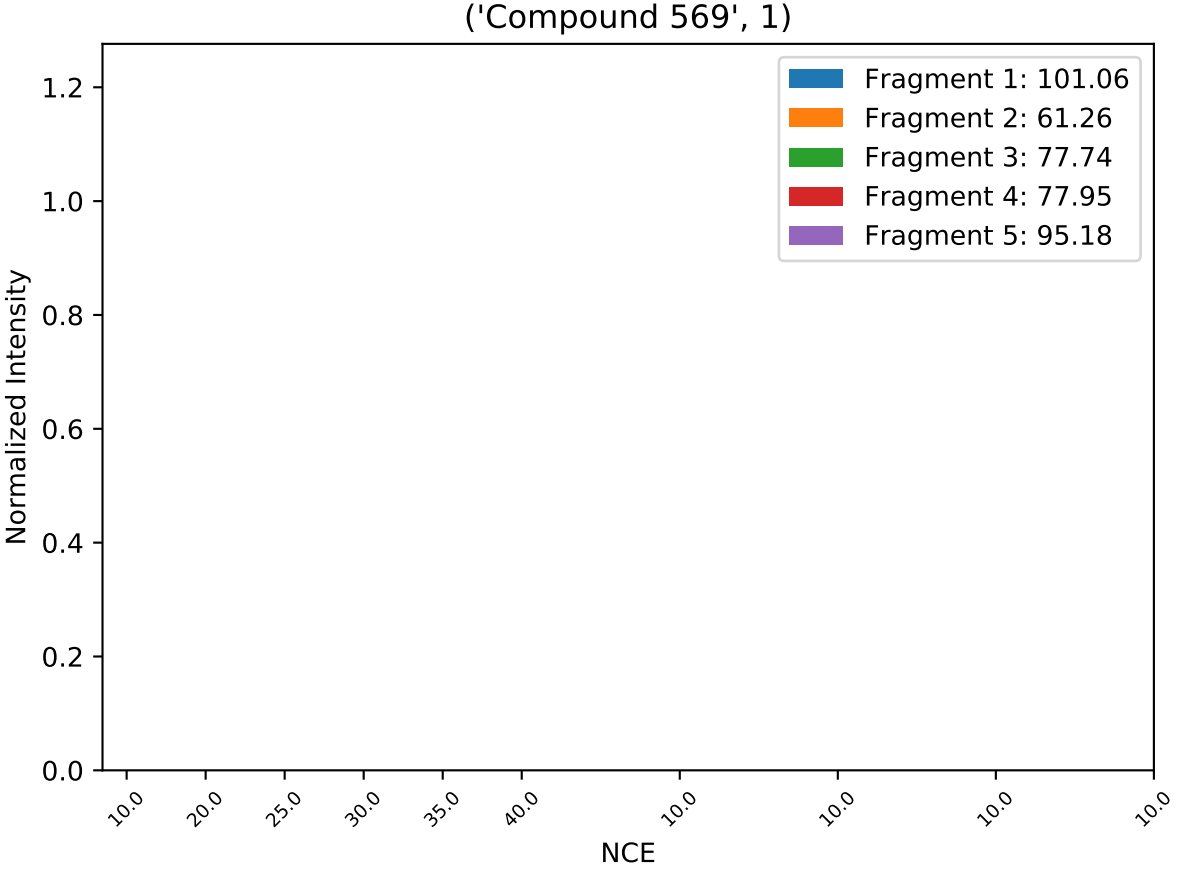

('Compound 513', 1)
Fragment 1: 134.06
Fragment 2: 58.06
Fragment 3: 95.06
Fragment 4: 106.06
Fragment 5: 58.07
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
10.0
20.0
25.0
30.0
35.0
40.0
30.0
40.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
25.0
30.0
40.0
50.0
60.0
70.0
20.0
25.0
35.0
50.0
60.0
80.0
NCE

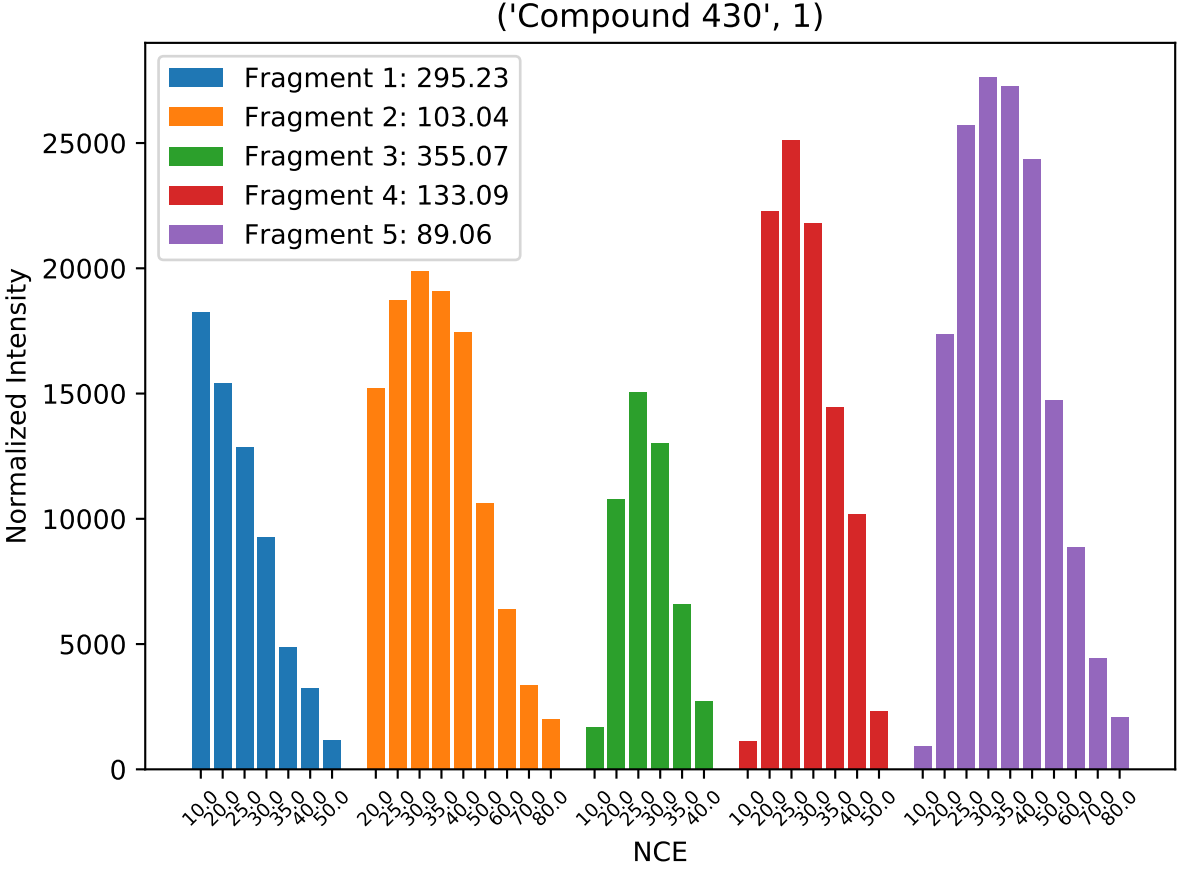

('Compound 514', 1)
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
Fragment 1: 97.4
Fragment 2: 99.53
Fragment 3: 106.61
Fragment 4: 114.24
Fragment 5: 126.91
10.0
10.0
10.0
10.0
10.0
NCE

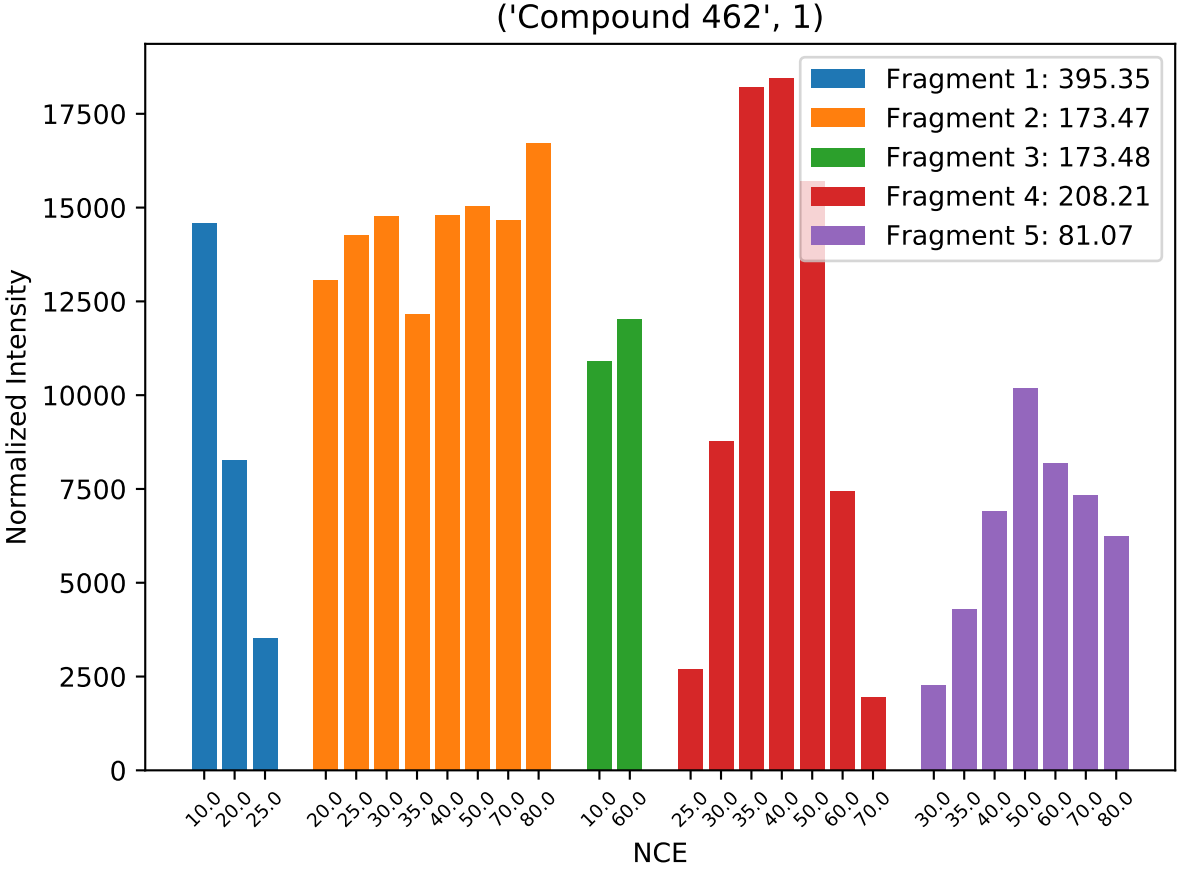

('Compound 101', 1)
Fragment 1: 58.03
Fragment 2: 59.04
Fragment 3: 60.04
Fragment 4: 59.62
Fragment 5: 58.96
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
35.0
40.0
50.0
60.0
40.0
80.0
NCE

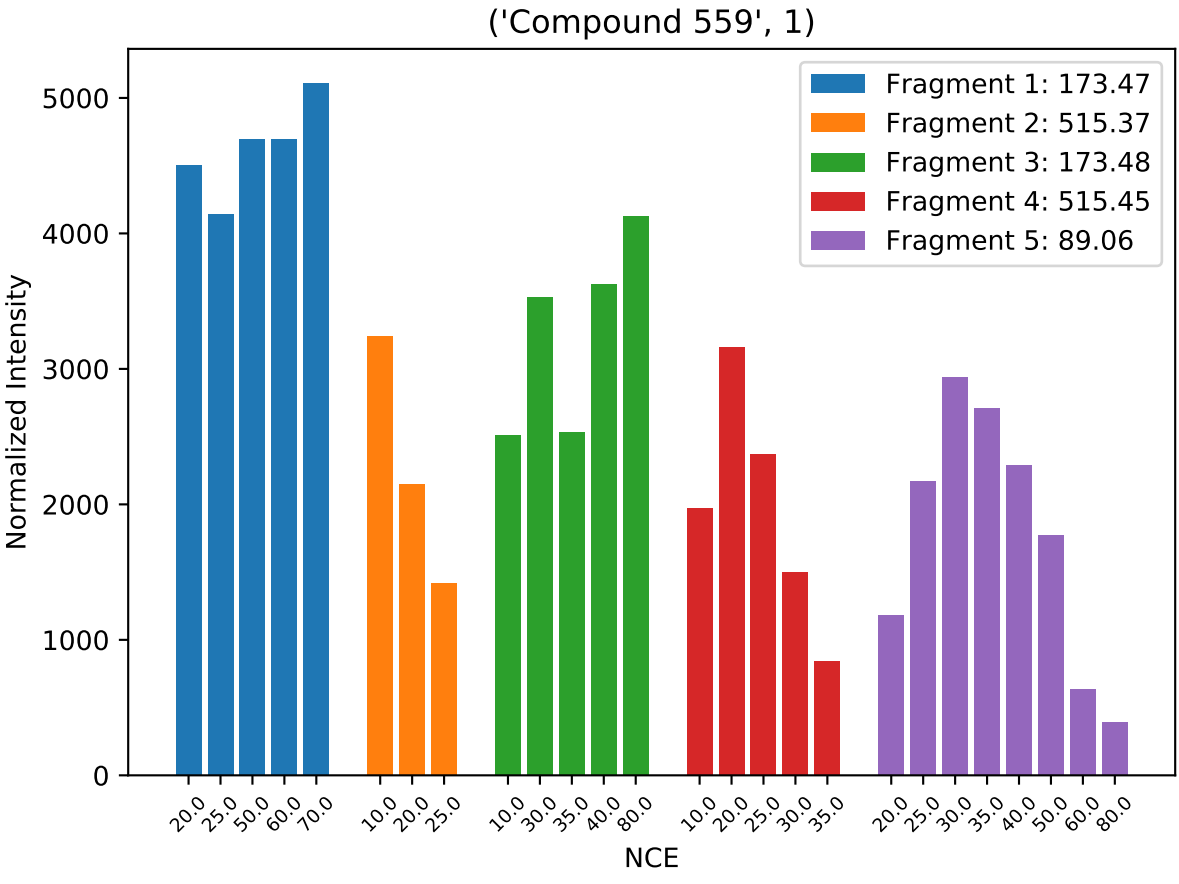

('Compound 552', 1)
Normalized Intensity
NCE
Fragment 1: 173.47
Fragment 2: 173.46
Fragment 3: 173.48
Fragment 4: 339.25
Fragment 5: 89.06
0
500
1000
1500
2000
2500
3000
3500
10.0
20.0
30.0
35.0
50.0
60.0
25.0
40.0
70.0
80.0
25.0
40.0
50.0
70.0
30.0
20.0
25.0
30.0
35.0
40.0
50.0

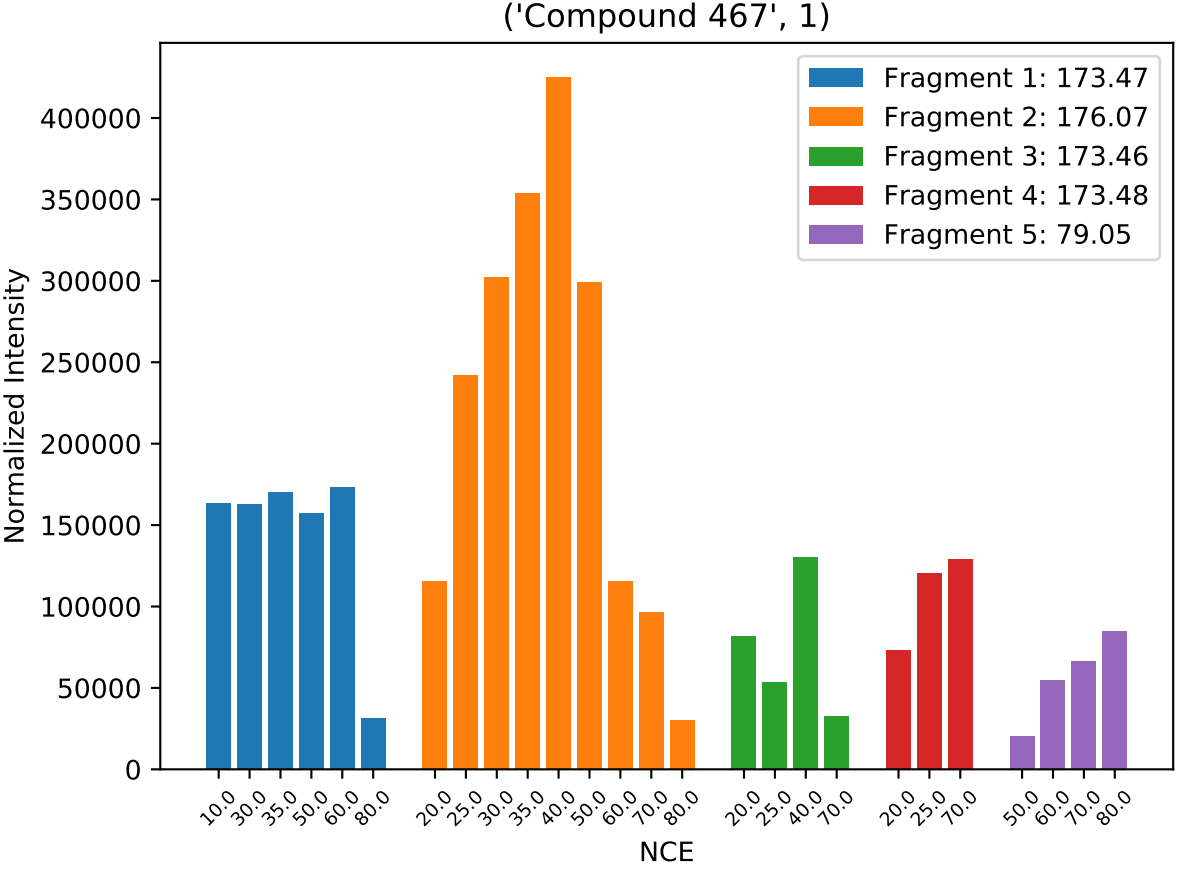

('Compound 457', 1)
Fragment 1: 59.05
Fragment 2: 121.06
Fragment 3: 173.48
Fragment 4: 115.08
Fragment 5: 138.33
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
10.0
30.0
40.0
60.0
10.0
20.0
10.0
NCE

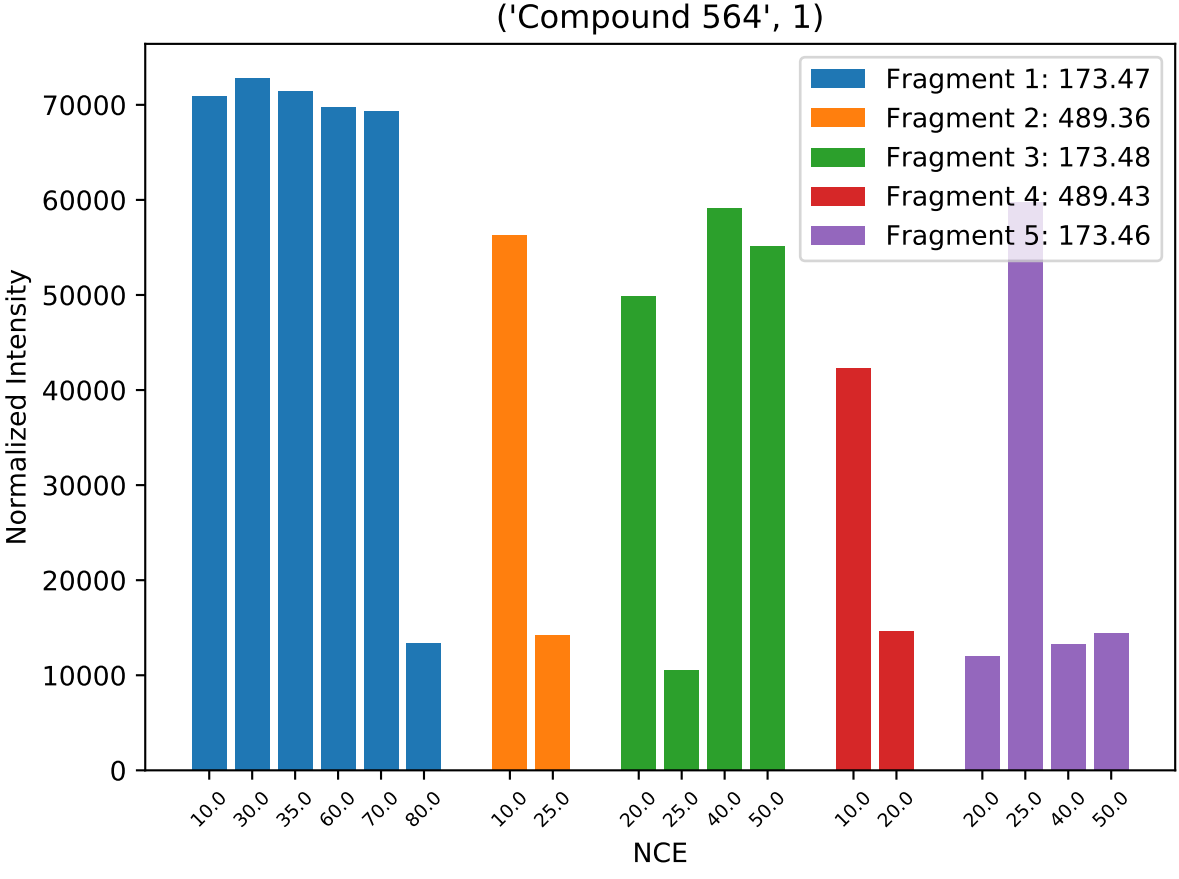

('Compound 569', 1)
Fragment 1: 101.06
Fragment 2: 61.26
Fragment 3: 77.74
Fragment 4: 77.95
Fragment 5: 95.18
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
10.0
10.0
10.0
10.0
NCE

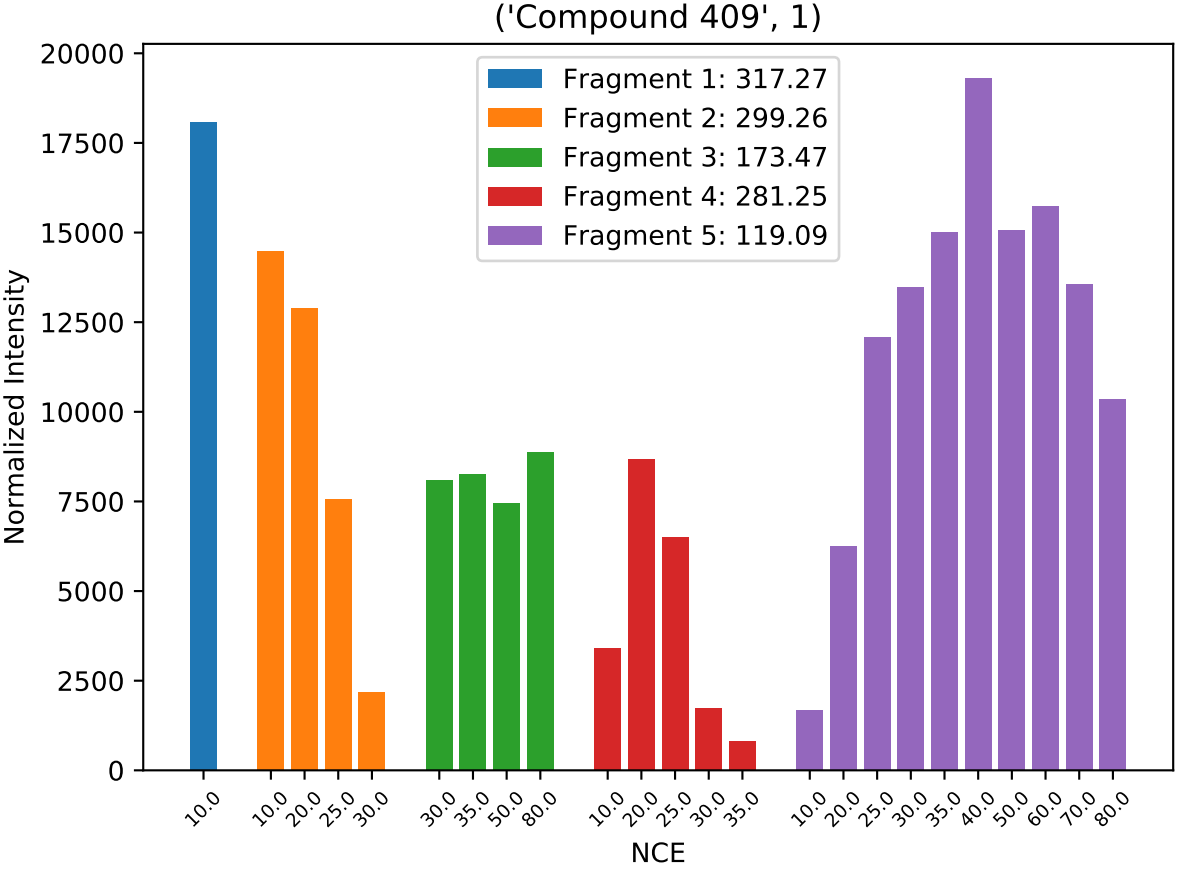

('Compound 430', 1)
Fragment 1: 295.23
Fragment 2: 103.04
Fragment 3: 355.07
Fragment 4: 133.09
Fragment 5: 89.06
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

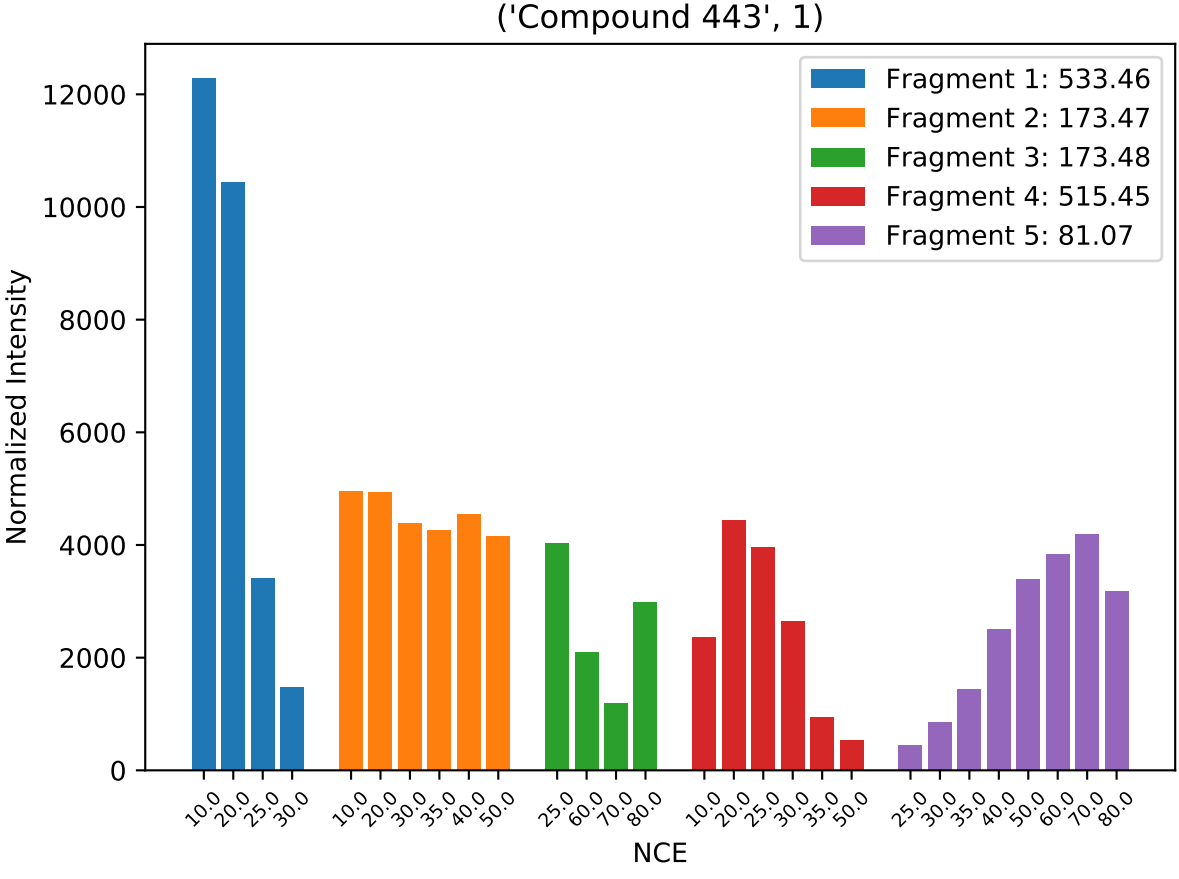

('Compound 462', 1)
Fragment 1: 395.35
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 208.21
Fragment 5: 81.07
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0
20.0
25.0
20.0
25.0
30.0
35.0
40.0
50.0
70.0
80.0
10.0
60.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

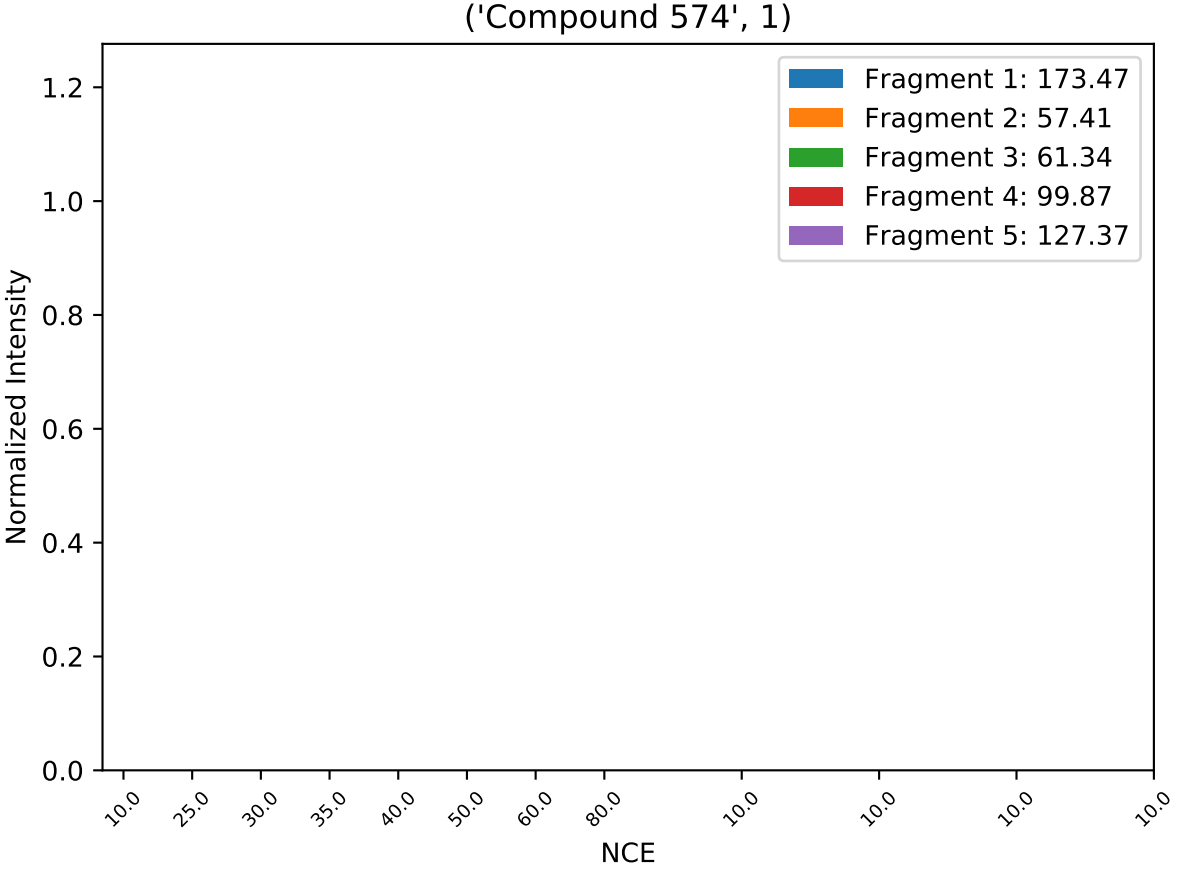

('Compound 559', 1)
Fragment 1: 173.47
Fragment 2: 515.37
Fragment 3: 173.48
Fragment 4: 515.45
Fragment 5: 89.06
Normalized Intensity
0
1000
2000
3000
4000
5000
20.0
25.0
50.0
60.0
70.0
10.0
20.0
25.0
10.0
30.0
35.0
40.0
80.0
10.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
80.0
NCE

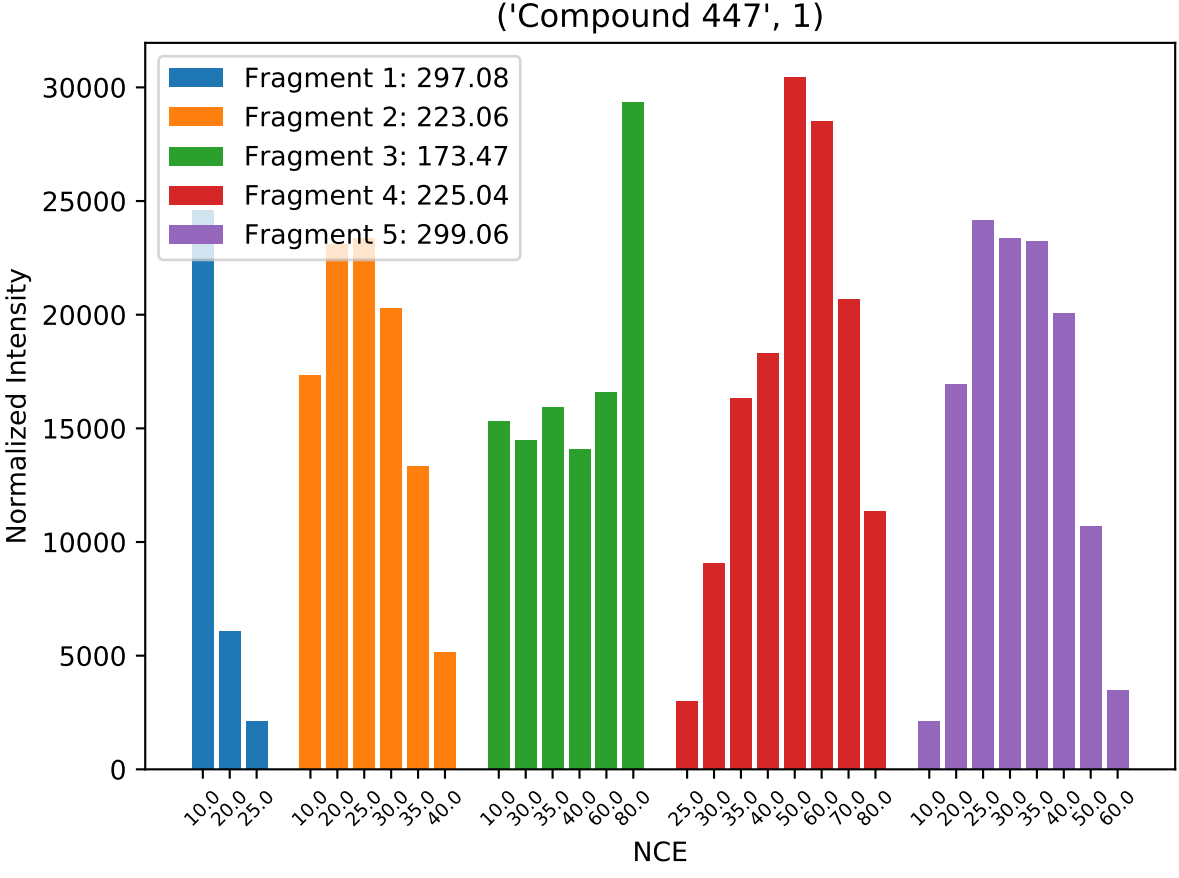

('Compound 467', 1)
Fragment 1: 173.47
Fragment 2: 176.07
Fragment 3: 173.46
Fragment 4: 173.48
Fragment 5: 79.05
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
400000
10.0
30.0
35.0
50.0
60.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
40.0
70.0
20.0
25.0
70.0
50.0
60.0
70.0
80.0
NCE

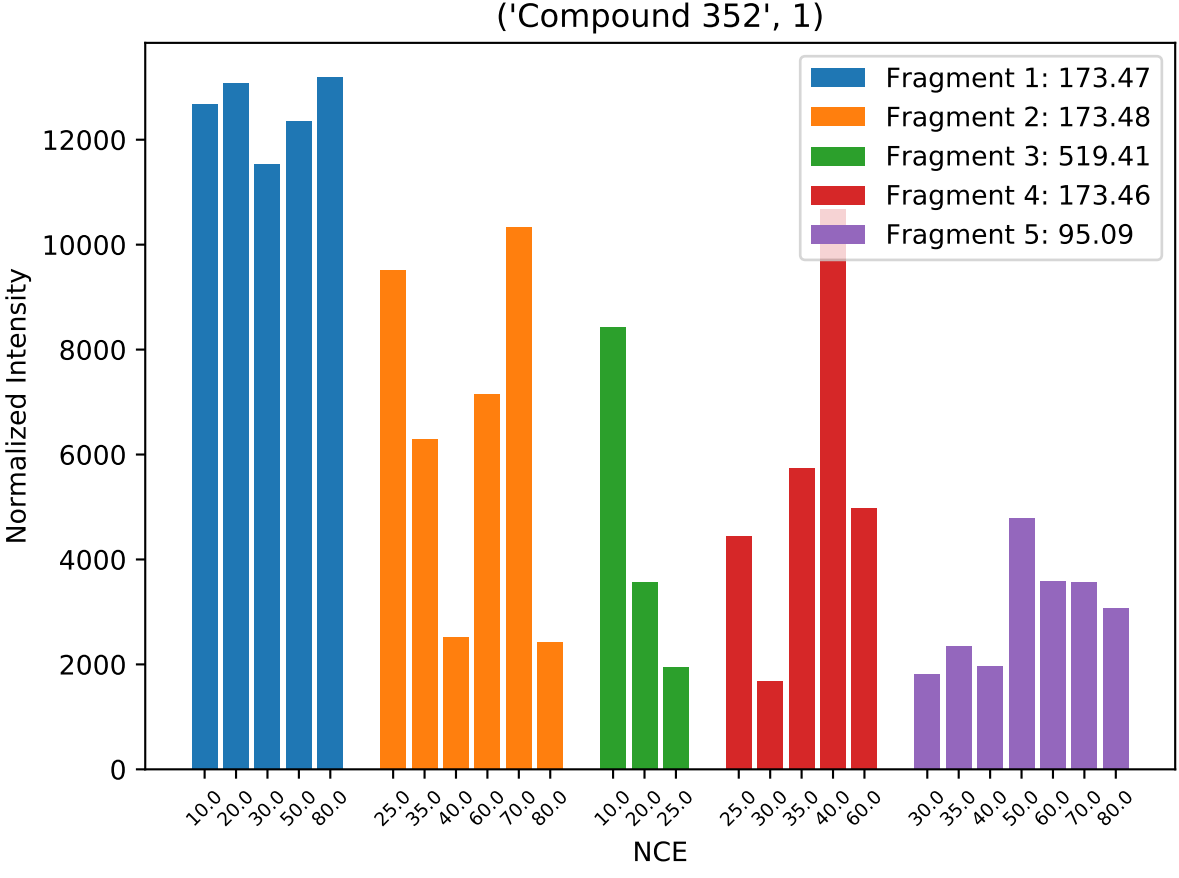

('Compound 564', 1)
Fragment 1: 173.47
Fragment 2: 489.36
Fragment 3: 173.48
Fragment 4: 489.43
Fragment 5: 173.46
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
30.0
35.0
60.0
70.0
80.0
10.0
25.0
20.0
25.0
40.0
50.0
10.0
20.0
20.0
25.0
40.0
50.0
NCE

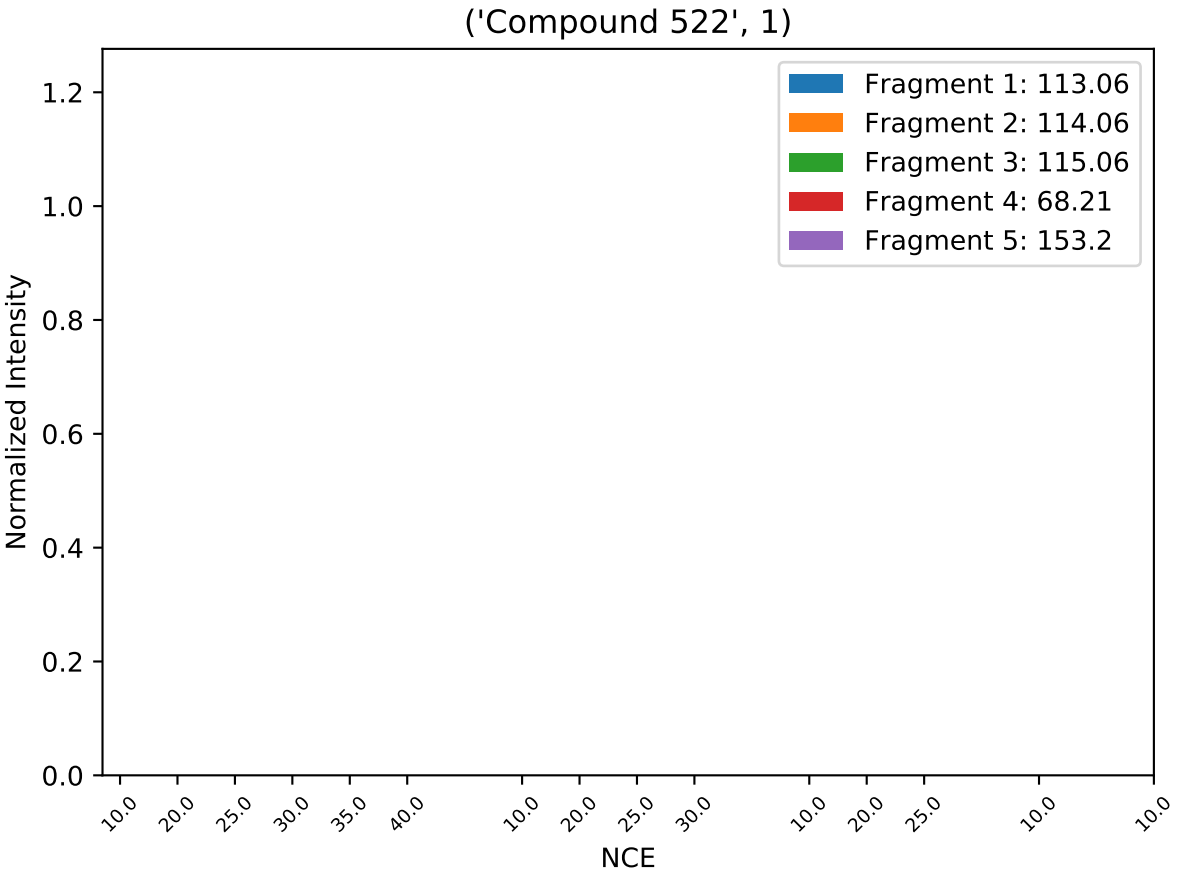

('Compound 409', 1)
Fragment 1: 317.27
Fragment 2: 299.26
Fragment 3: 173.47
Fragment 4: 281.25
Fragment 5: 119.09
Normalized Intensity
20000
17500
15000
12500
10000
7500
5000
2500
0
10.0
10.0 20.0 25.0 30.0
30.0 35.0 50.0 80.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

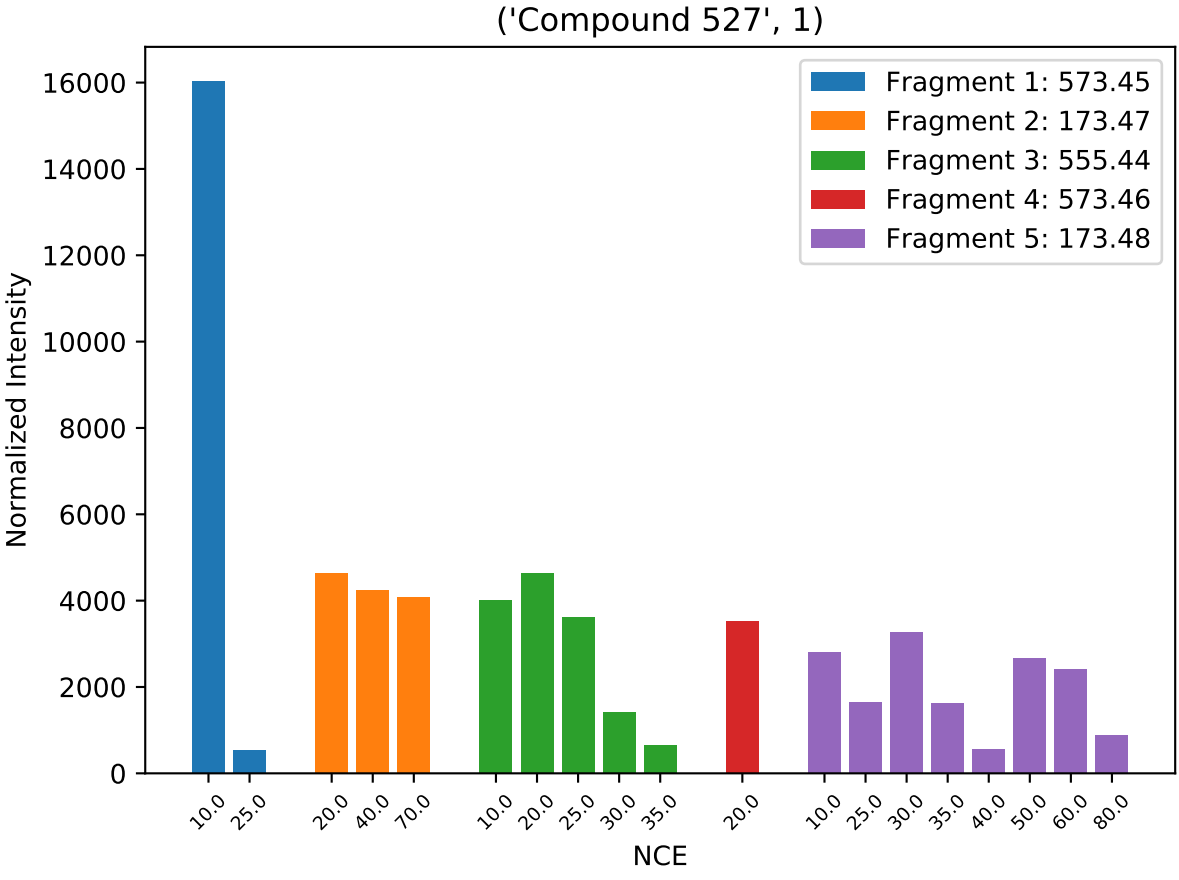

('Compound 443', 1)
Fragment 1: 533.46
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 515.45
Fragment 5: 81.07
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0
20.0
25.0
30.0
10.0
20.0
30.0
35.0
40.0
50.0
25.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
50.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

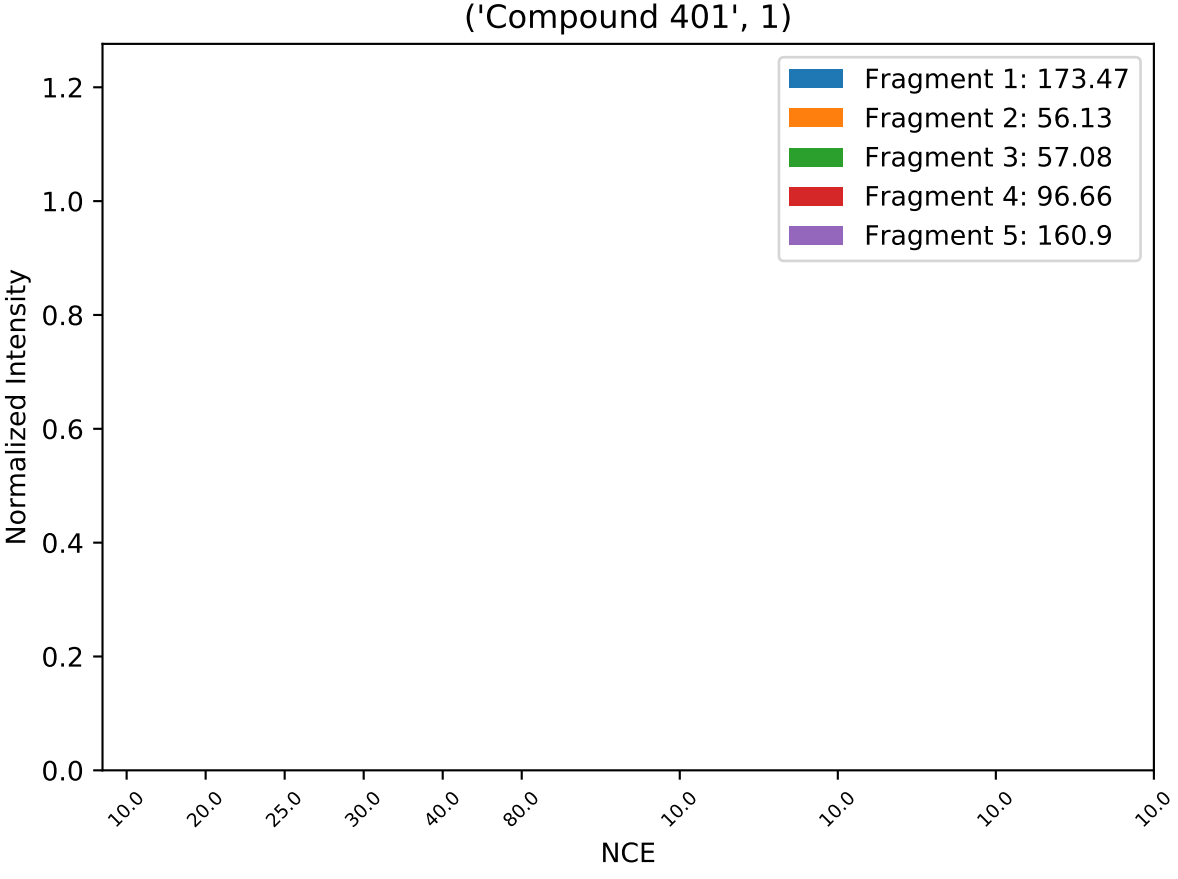

('Compound 574', 1)
Fragment 1: 173.47
Fragment 2: 57.41
Fragment 3: 61.34
Fragment 4: 99.87
Fragment 5: 127.37
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
25.0
30.0
35.0
40.0
50.0
60.0
80.0
10.0
10.0
10.0
10.0
NCE

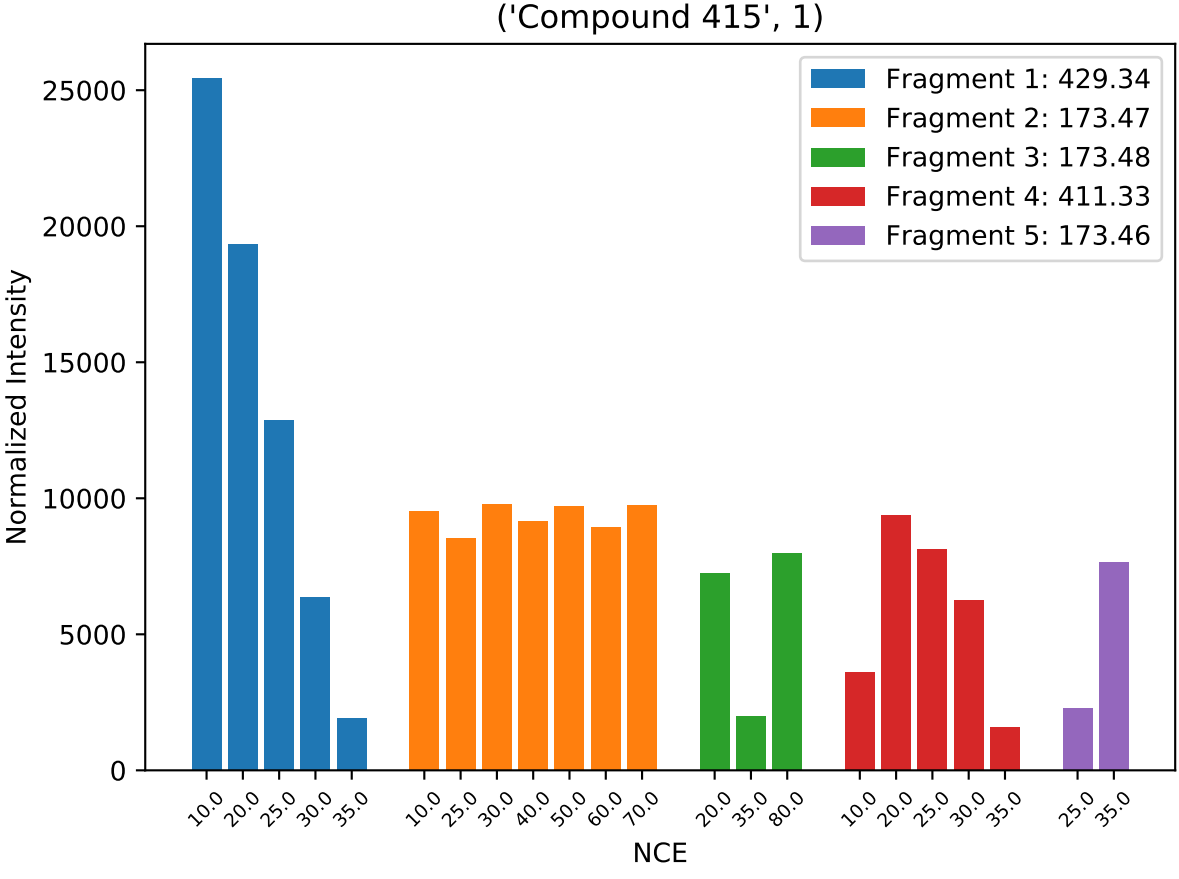

('Compound 447', 1)
Fragment 1: 297.08
Fragment 2: 223.06
Fragment 3: 173.47
Fragment 4: 225.04
Fragment 5: 299.06
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
30.0
35.0
40.0
60.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

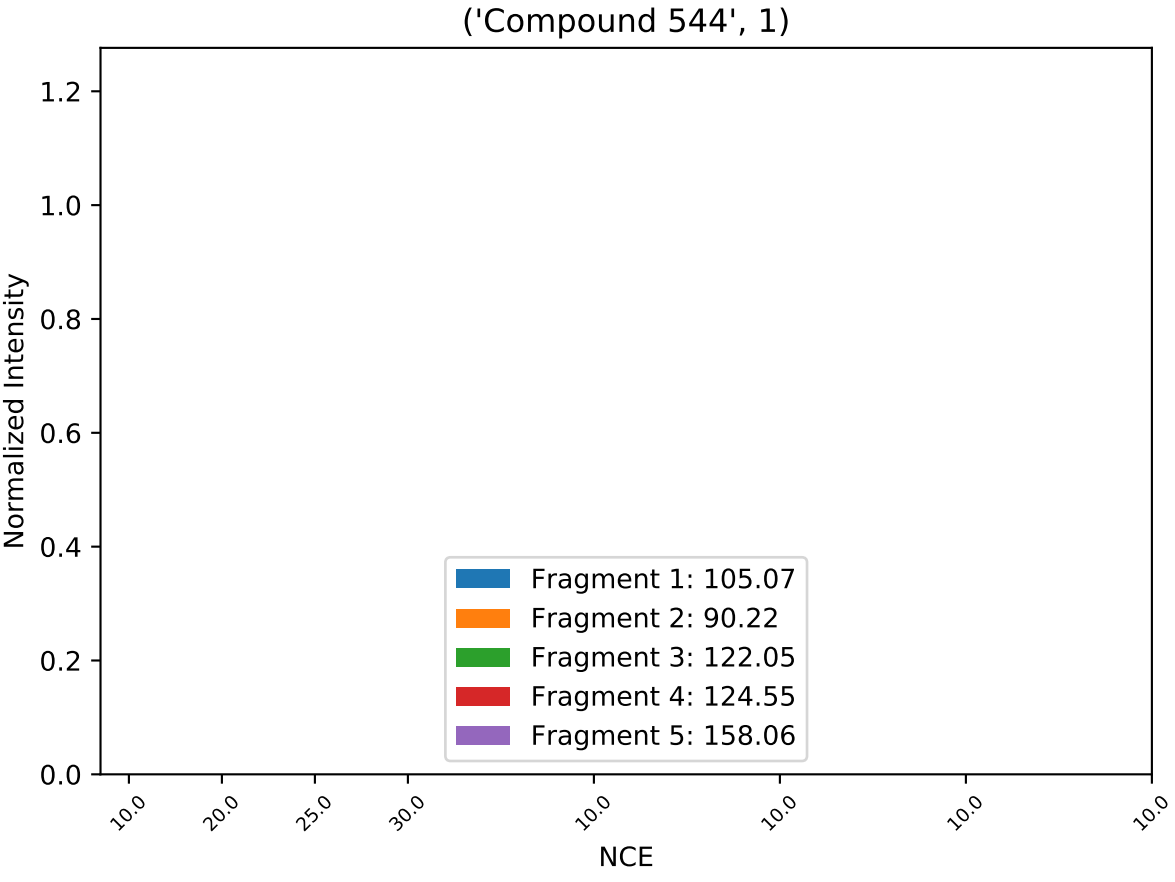

('Compound 352', 1)
Fragment 1: 173.47
Fragment 2: 173.48
Fragment 3: 519.41
Fragment 4: 173.46
Fragment 5: 95.09
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0
20.0
30.0
50.0
80.0
25.0
35.0
40.0
60.0
70.0
80.0
10.0
20.0
25.0
25.0
30.0
35.0
40.0
60.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

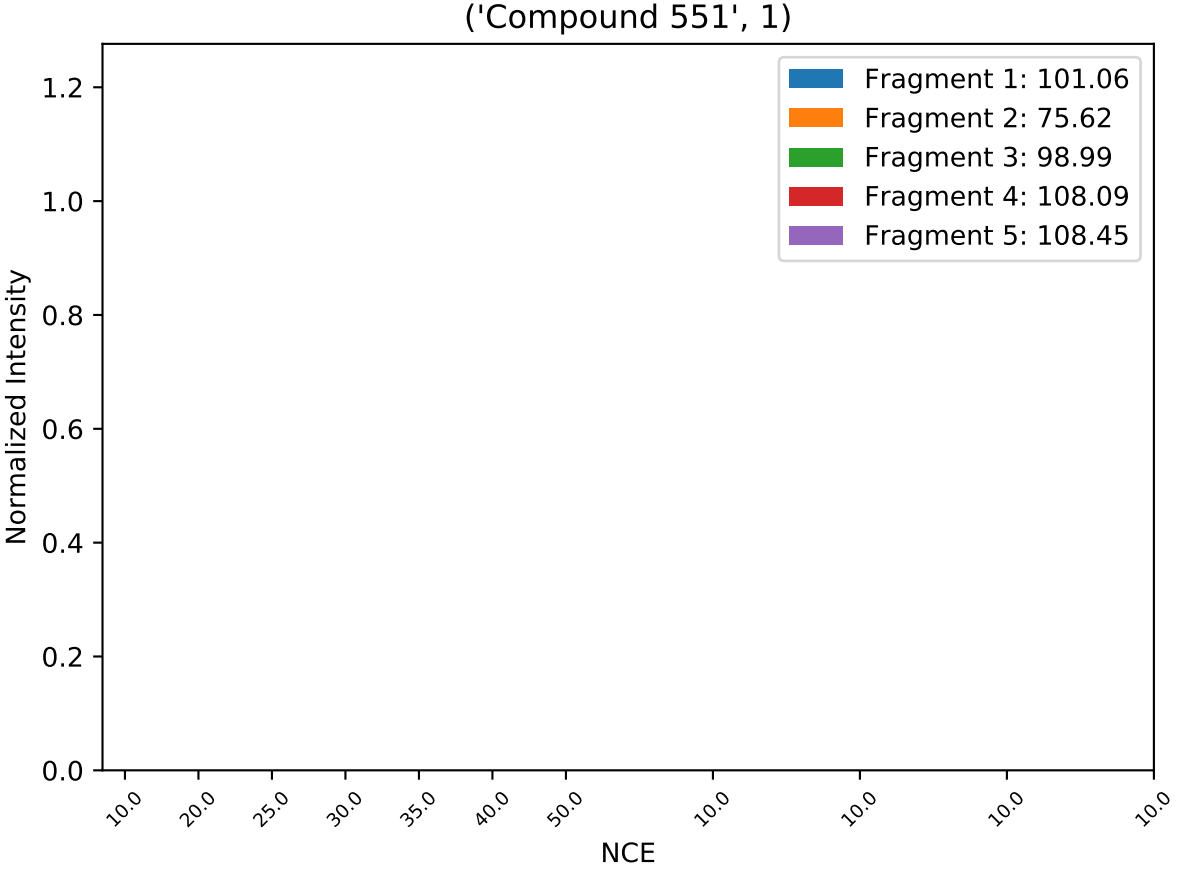

('Compound 522', 1)
Fragment 1: 113.06
Fragment 2: 114.06
Fragment 3: 115.06
Fragment 4: 68.21
Fragment 5: 153.2
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
10.0
20.0
25.0
10.0
10.0
NCE

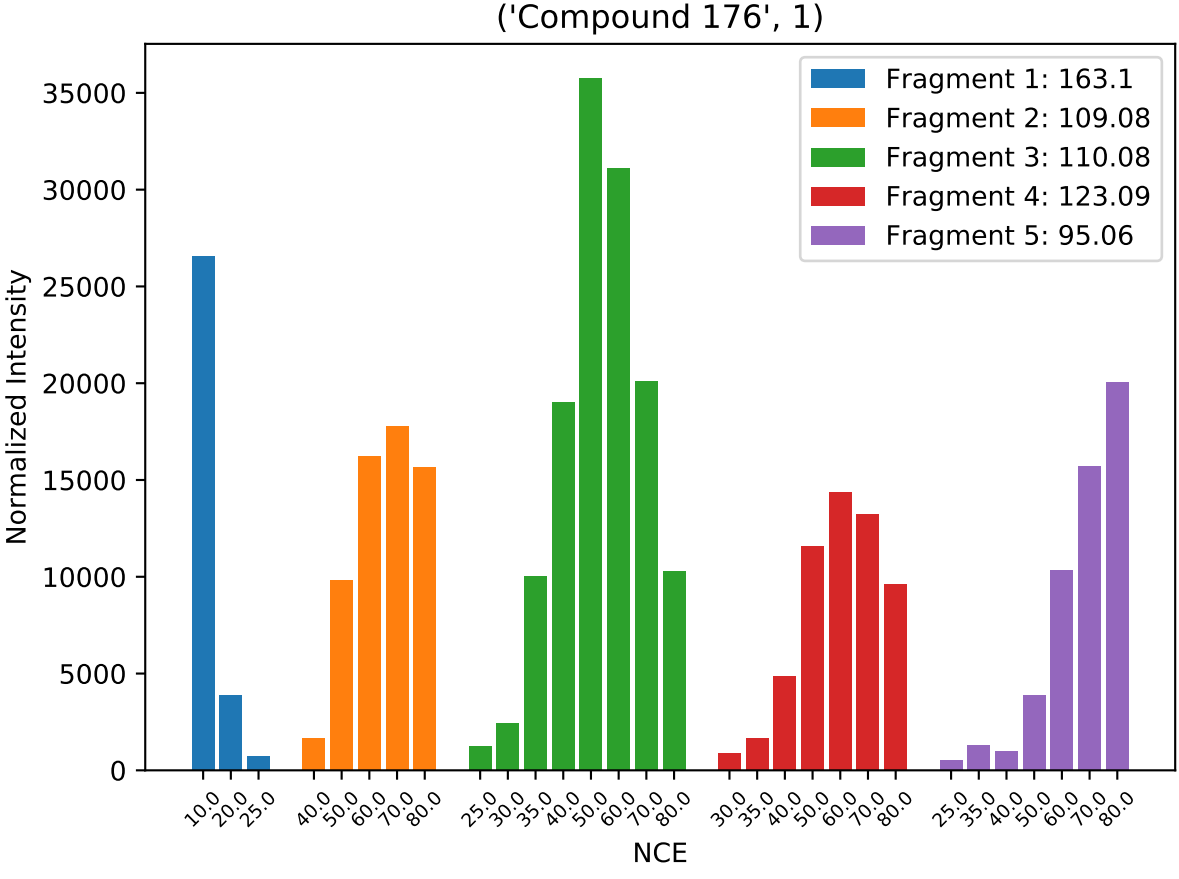

('Compound 527', 1)
Fragment 1: 573.45
Fragment 2: 173.47
Fragment 3: 555.44
Fragment 4: 573.46
Fragment 5: 173.48
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0
25.0
20.0
40.0
70.0
10.0
20.0
25.0
30.0
35.0
20.0
10.0
25.0
30.0
35.0
40.0
50.0
60.0
80.0
NCE

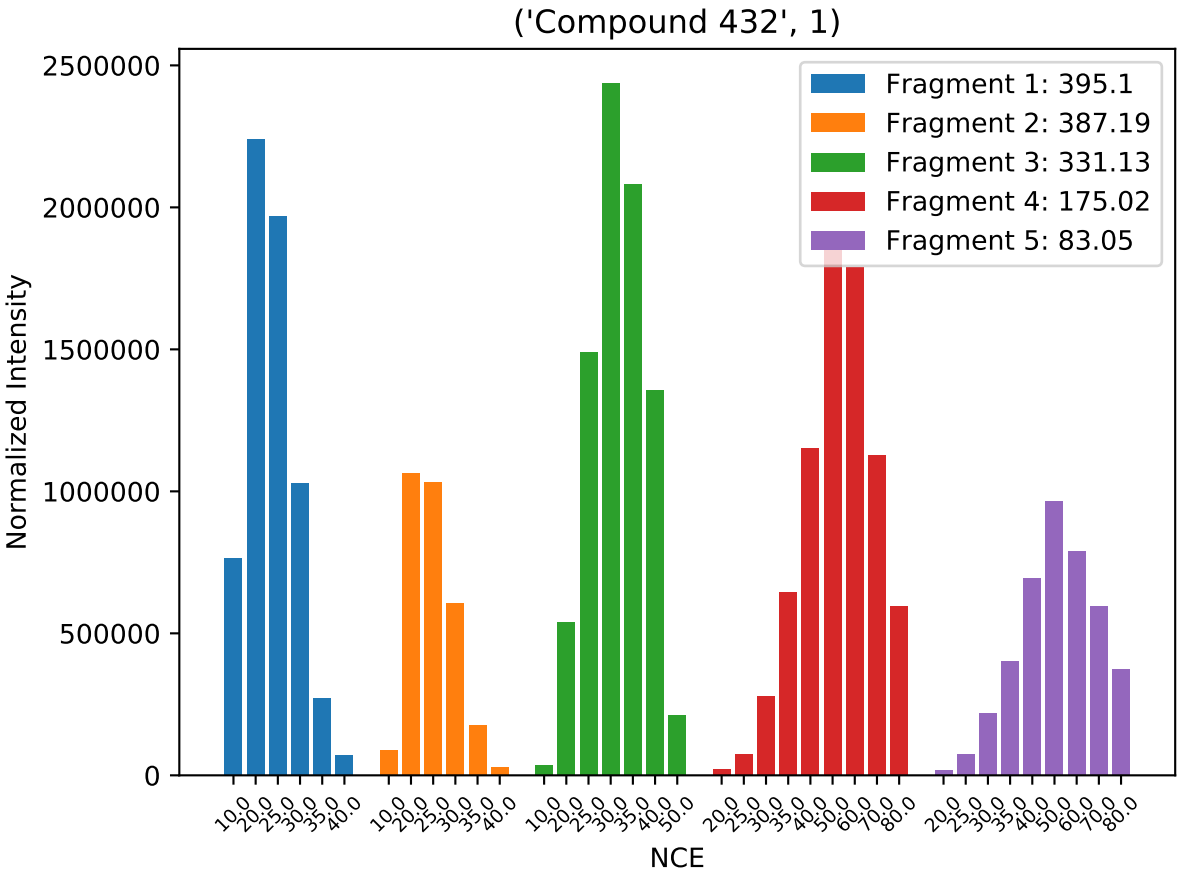

('Compound 401', 1)
Fragment 1: 173.47
Fragment 2: 56.13
Fragment 3: 57.08
Fragment 4: 96.66
Fragment 5: 160.9
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
40.0
80.0
10.0
10.0
10.0
10.0
NCE

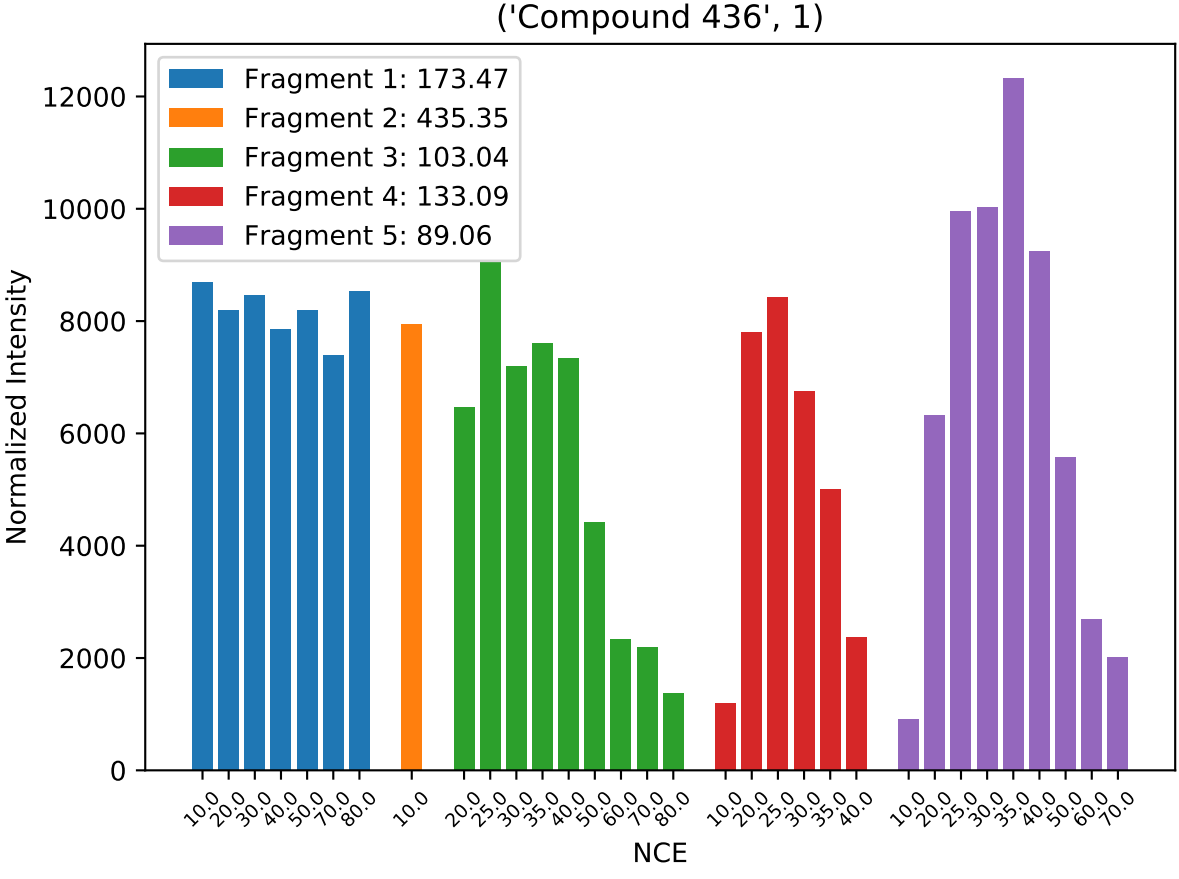

('Compound 415', 1)
Fragment 1: 429.34
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 411.33
Fragment 5: 173.46
Normalized Intensity
25000
20000
15000
10000
5000
0
10.0
20.0
25.0
30.0
35.0
10.0
25.0
30.0
40.0
50.0
60.0
70.0
20.0
35.0
80.0
10.0
20.0
25.0
30.0
35.0
25.0
35.0
NCE

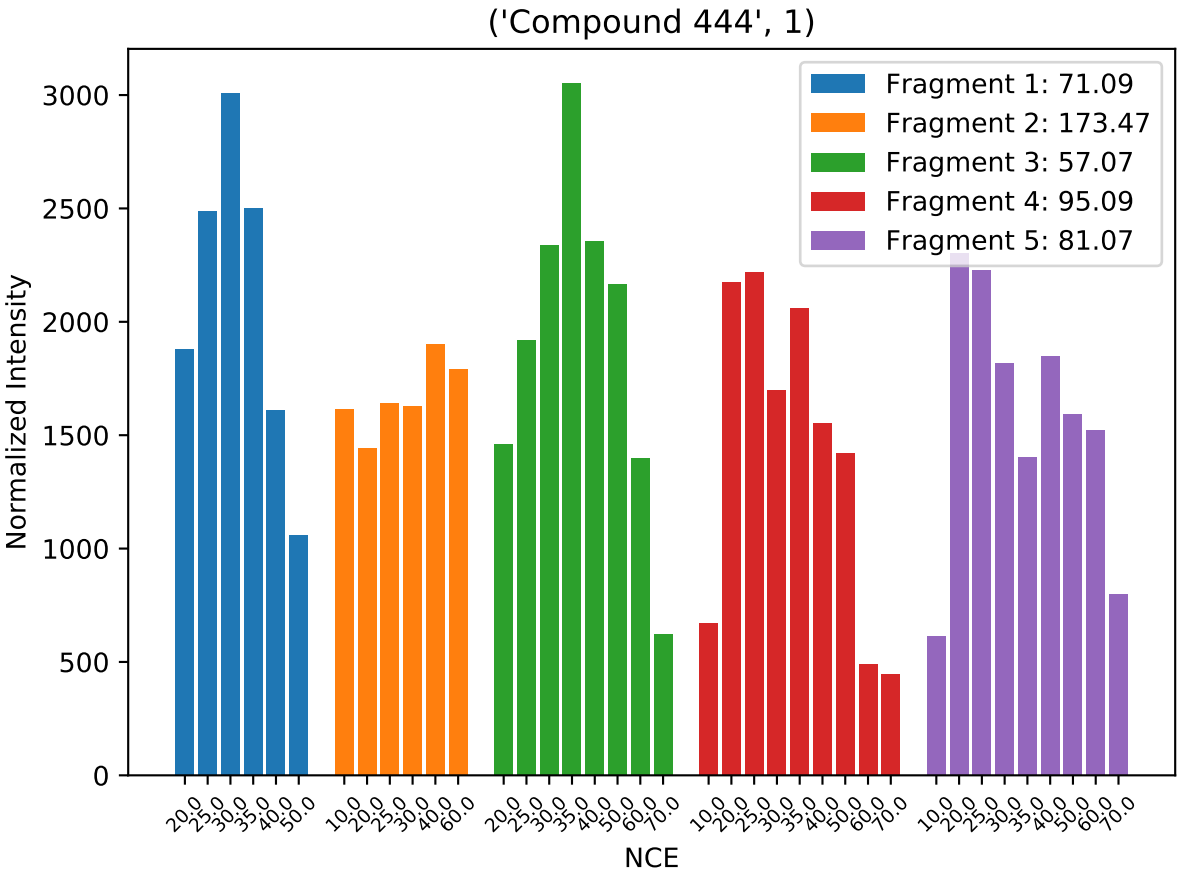

('Compound 544', 1)
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
Fragment 1: 105.07
Fragment 2: 90.22
Fragment 3: 122.05
Fragment 4: 124.55
Fragment 5: 158.06
10.0
20.0
25.0
30.0
10.0
10.0
10.0
10.0
NCE

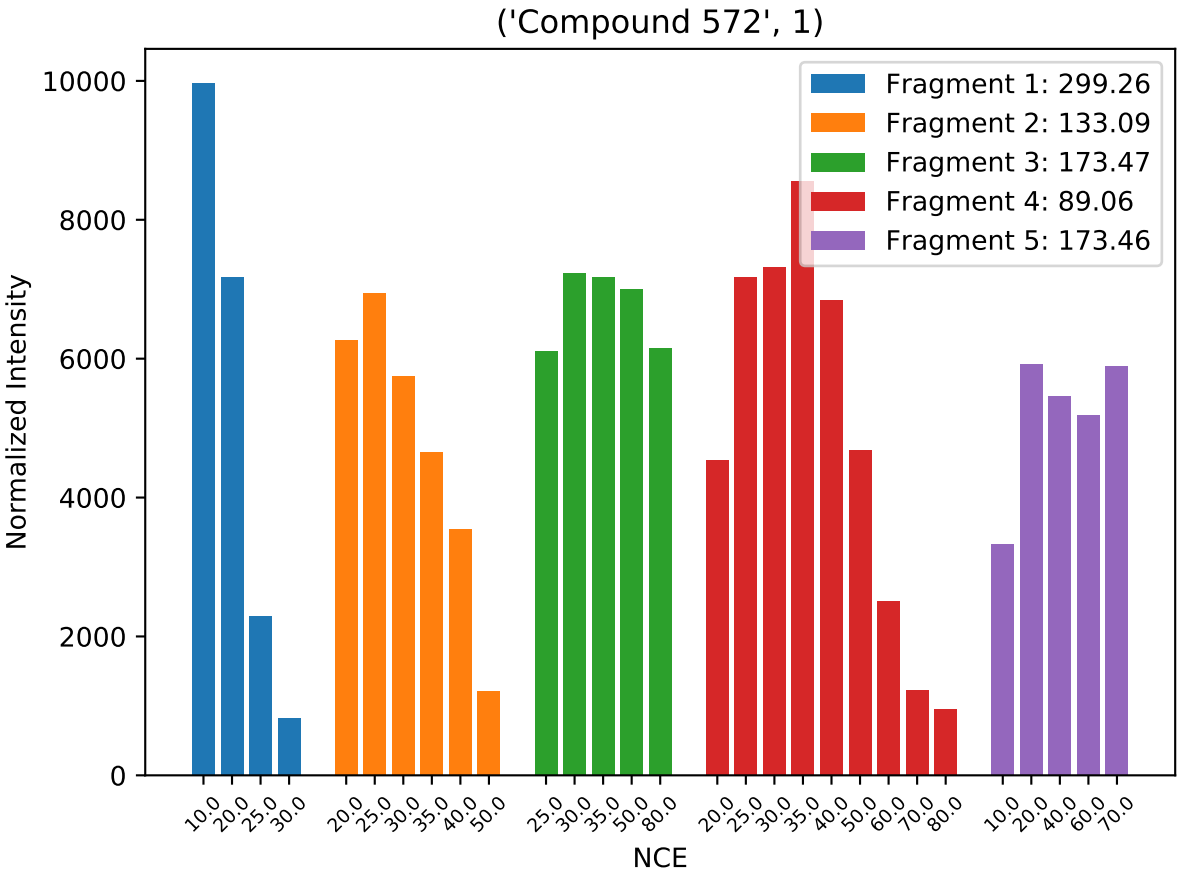

('Compound 551', 1)
Fragment 1: 101.06
Fragment 2: 75.62
Fragment 3: 98.99
Fragment 4: 108.09
Fragment 5: 108.45
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
10.0
10.0
10.0
NCE

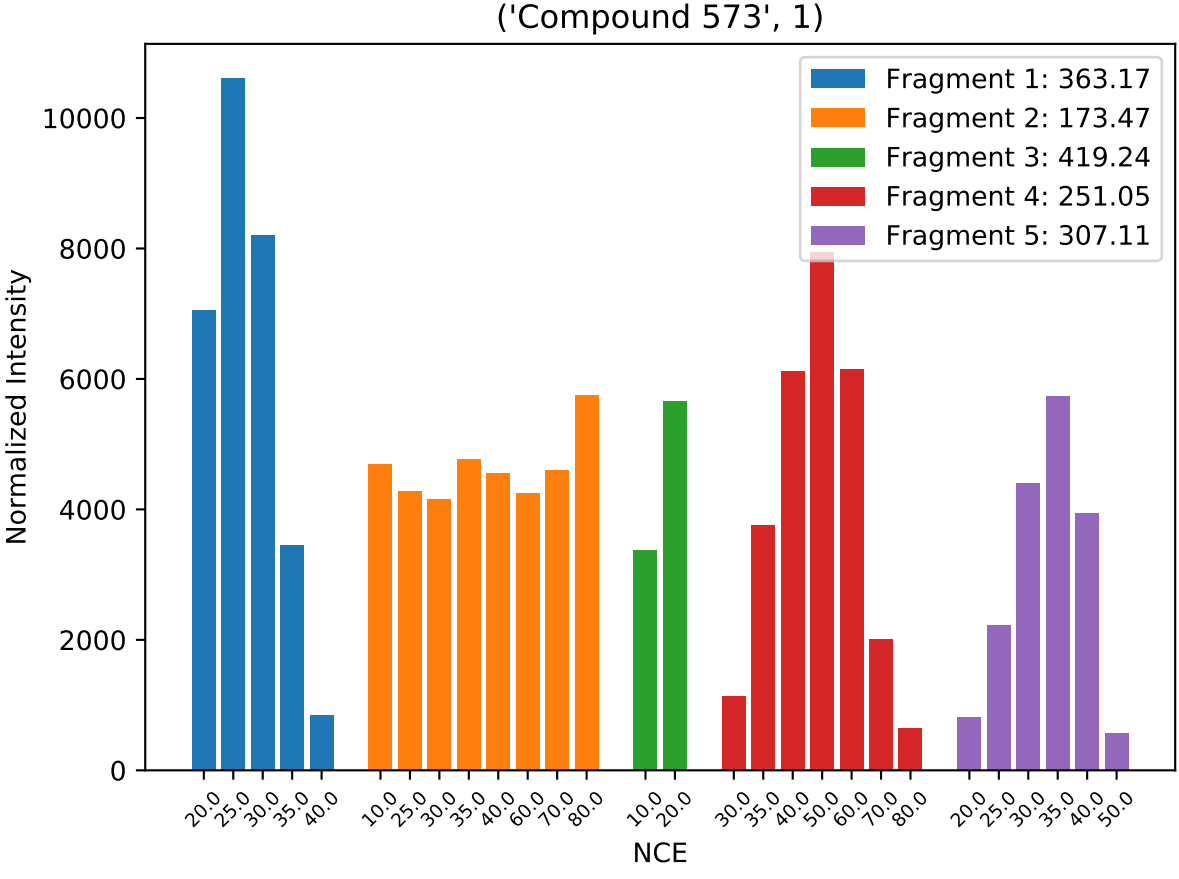

('Compound 176', 1)
Fragment 1: 163.1
Fragment 2: 109.08
Fragment 3: 110.08
Fragment 4: 123.09
Fragment 5: 95.06
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
10.0
20.0
25.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

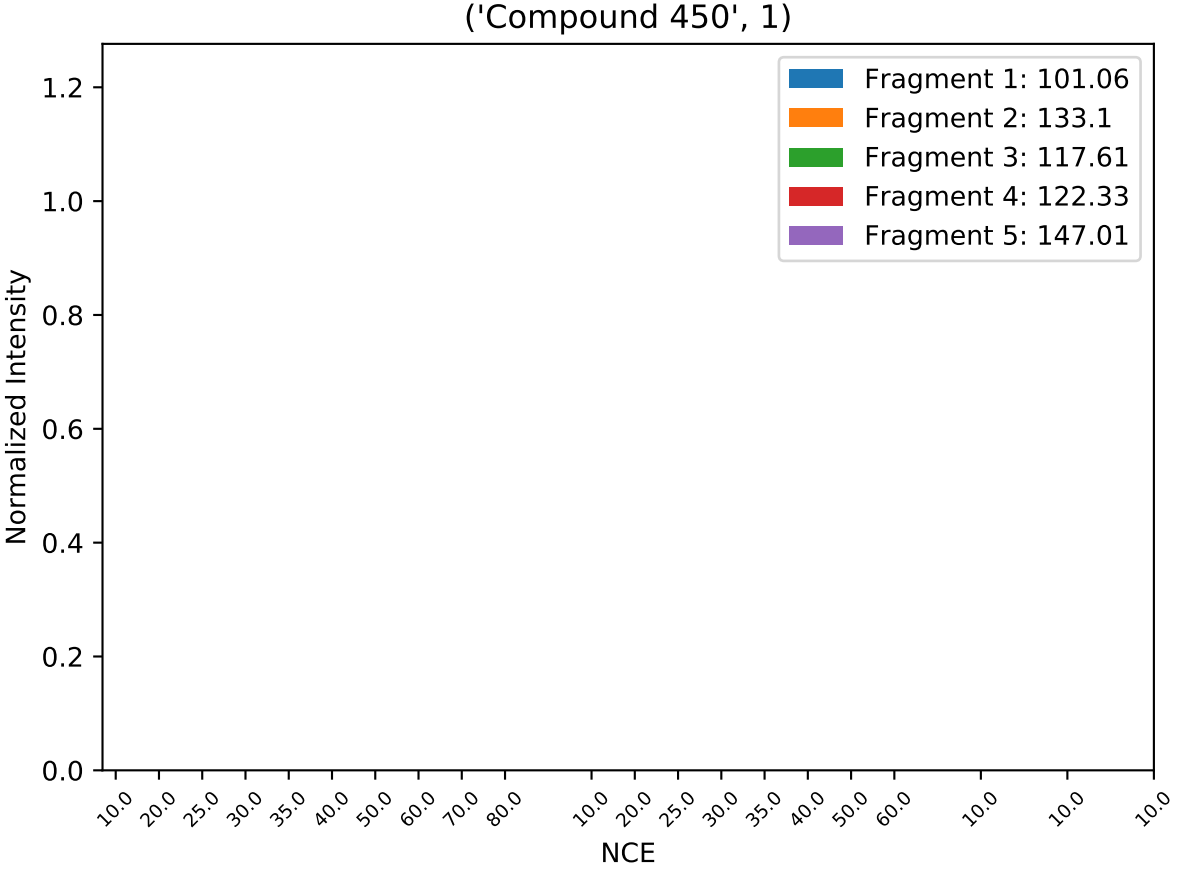

('Compound 432', 1)
Fragment 1: 395.1
Fragment 2: 387.19
Fragment 3: 331.13
Fragment 4: 175.02
Fragment 5: 83.05
Normalized Intensity
2500000
2000000
1500000
1000000
500000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

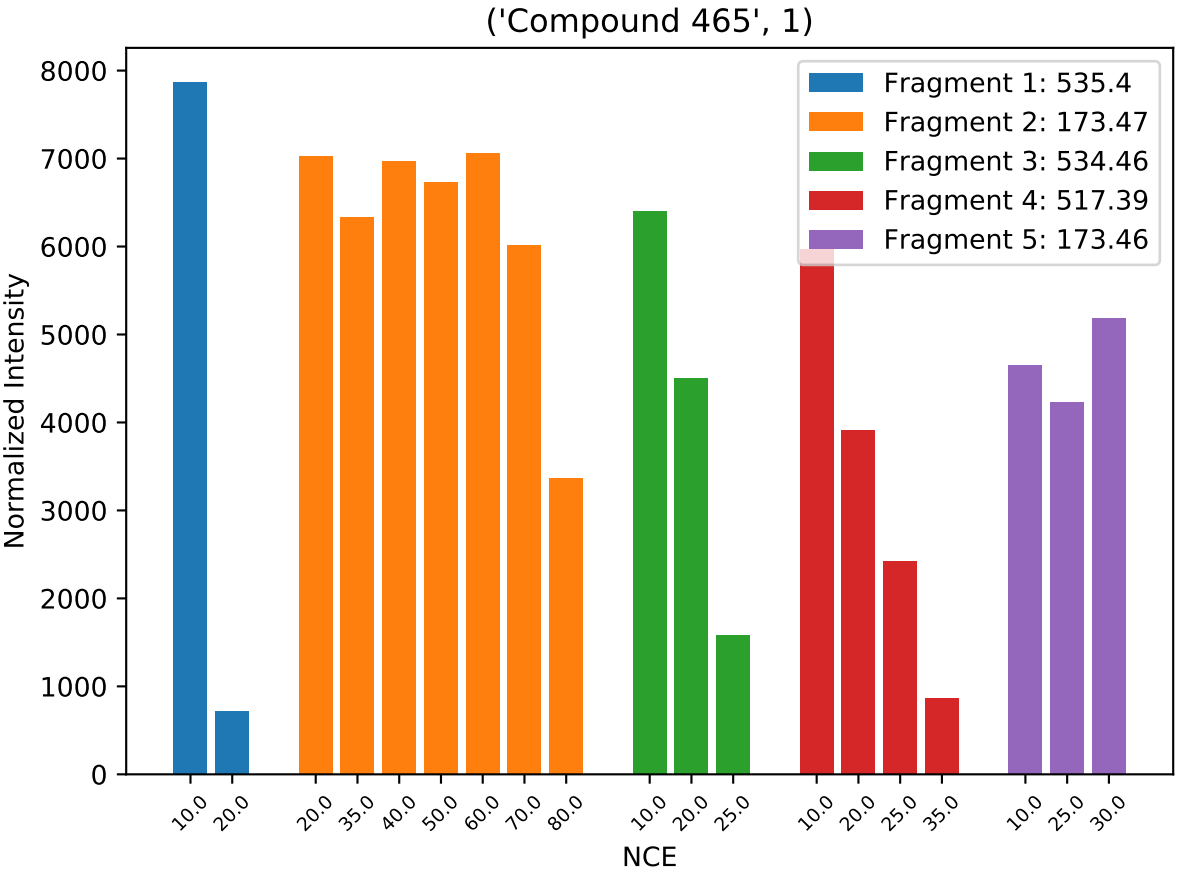

('Compound 436', 1)
Fragment 1: 173.47
Fragment 2: 435.35
Fragment 3: 103.04
Fragment 4: 133.09
Fragment 5: 89.06
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0 20.0 30.0 40.0 50.0 70.0 80.0
10.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

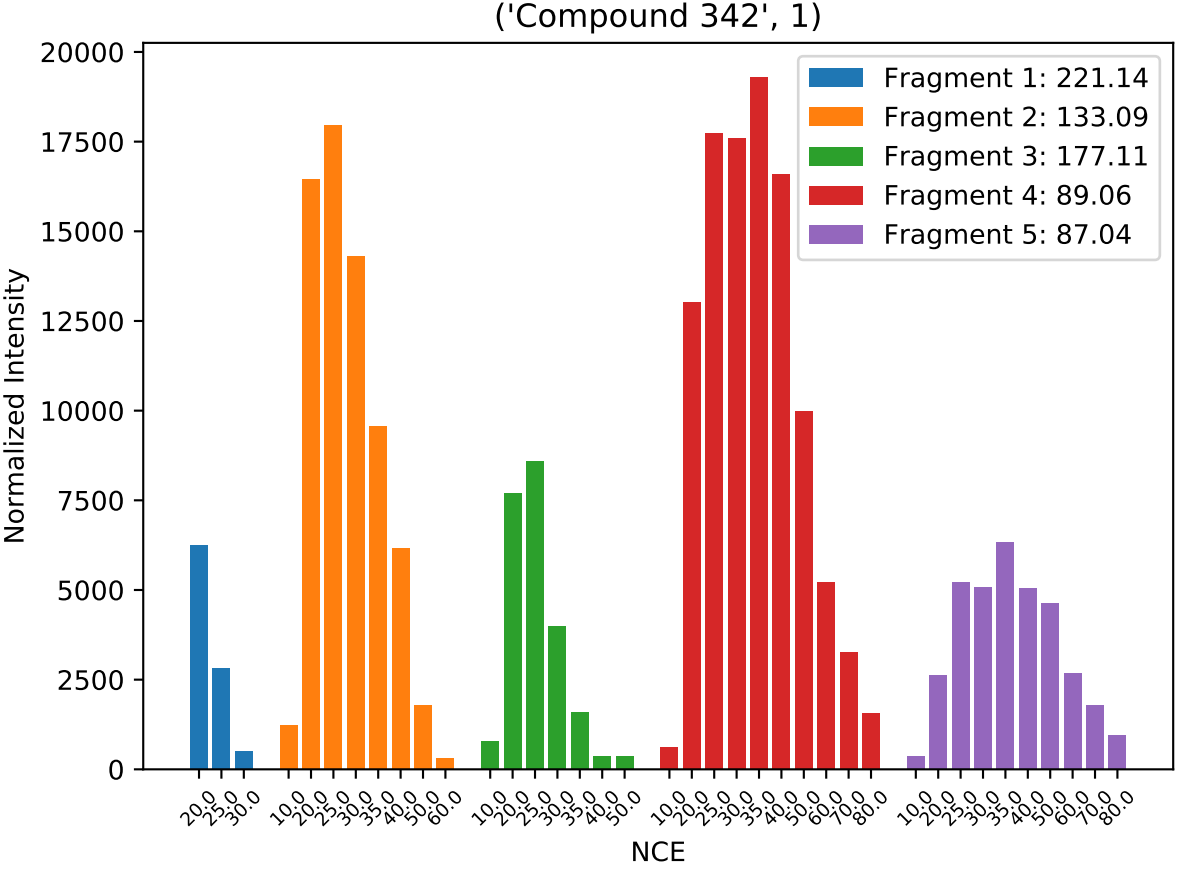

('Compound 444', 1)
Fragment 1: 71.09
Fragment 2: 173.47
Fragment 3: 57.07
Fragment 4: 95.09
Fragment 5: 81.07
Normalized Intensity
0
500
1000
1500
2000
2500
3000
NCE
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 40.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0

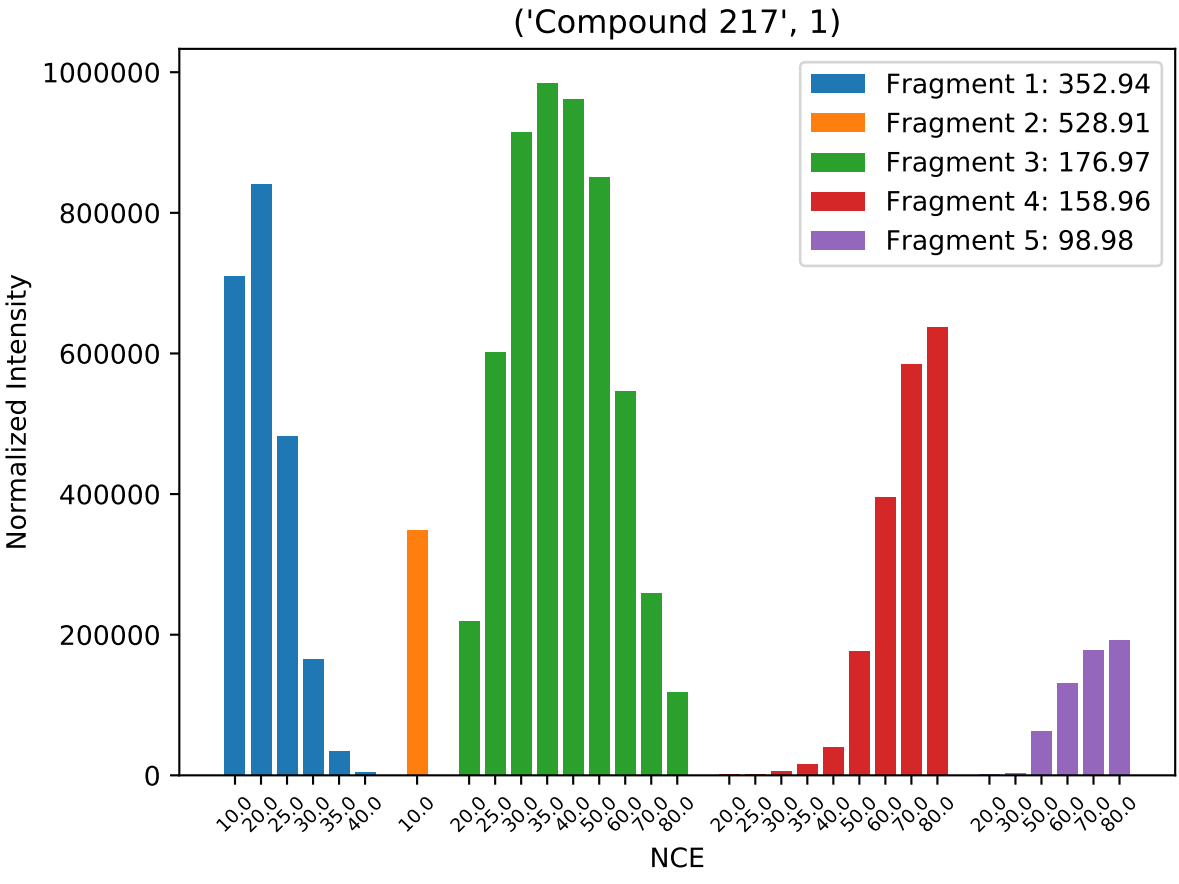

('Compound 572', 1)
Fragment 1: 299.26
Fragment 2: 133.09
Fragment 3: 173.47
Fragment 4: 89.06
Fragment 5: 173.46
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0 20.0 25.0 30.0
20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 50.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 40.0 60.0 70.0
NCE

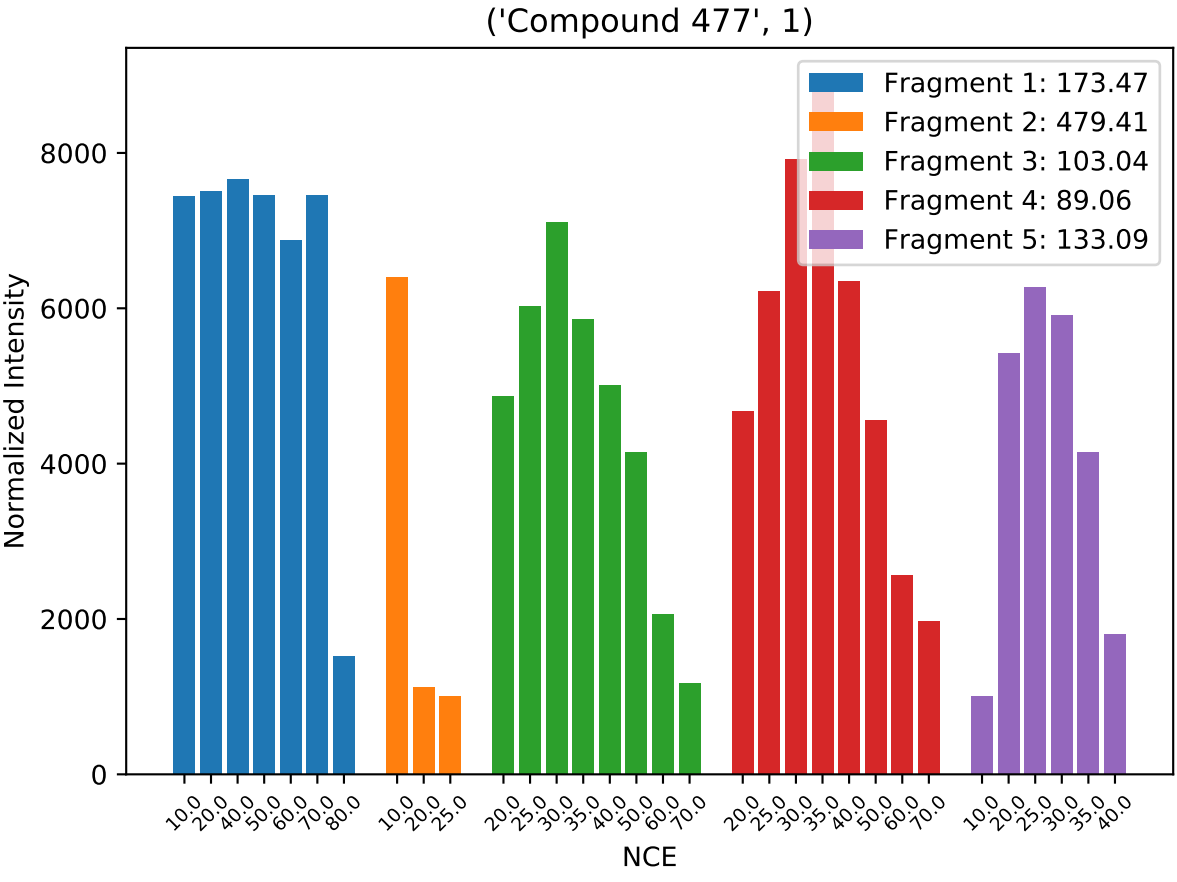

('Compound 573', 1)
Fragment 1: 363.17
Fragment 2: 173.47
Fragment 3: 419.24
Fragment 4: 251.05
Fragment 5: 307.11
Normalized Intensity
0
2000
4000
6000
8000
10000
20.0
25.0
30.0
35.0
40.0
10.0
25.0
30.0
35.0
40.0
60.0
70.0
80.0
10.0
20.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

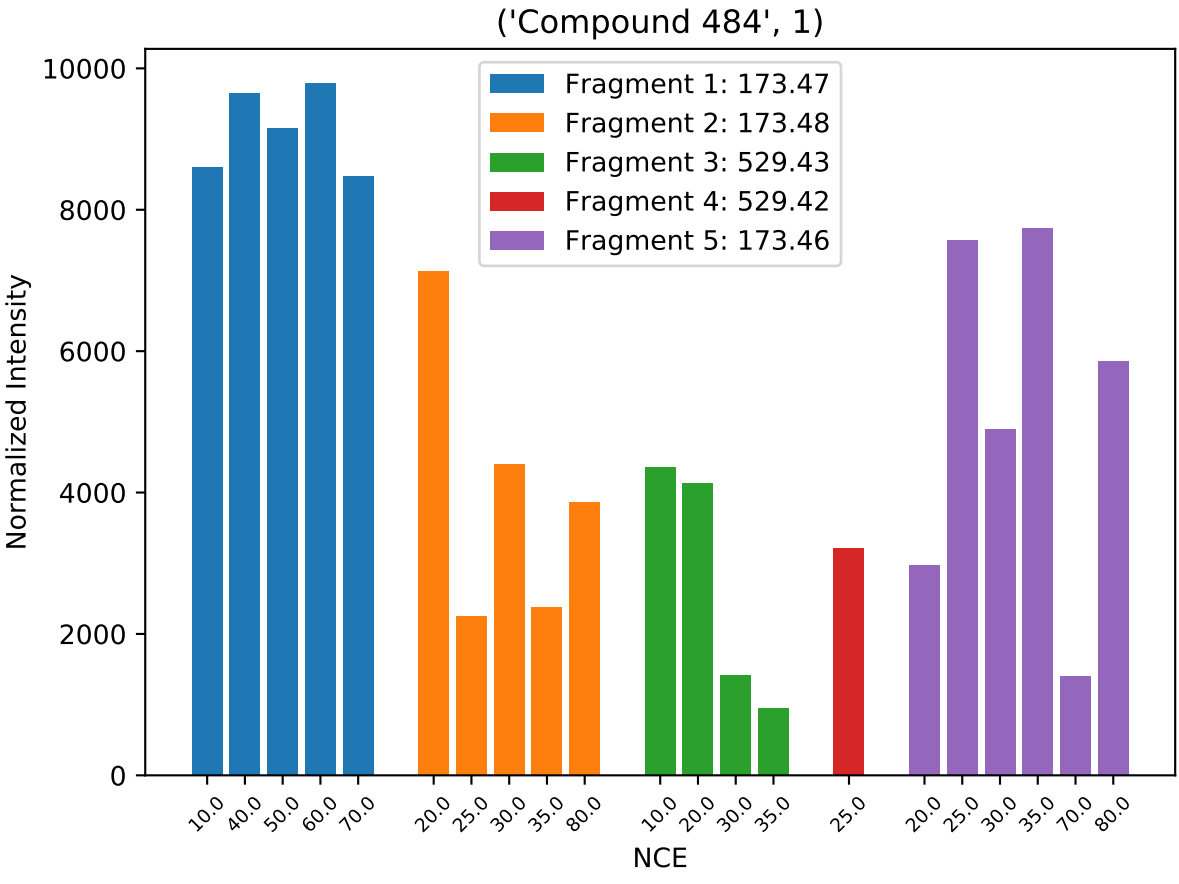

('Compound 450', 1)
Fragment 1: 101.06
Fragment 2: 133.1
Fragment 3: 117.61
Fragment 4: 122.33
Fragment 5: 147.01
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
10.0
10.0
NCE

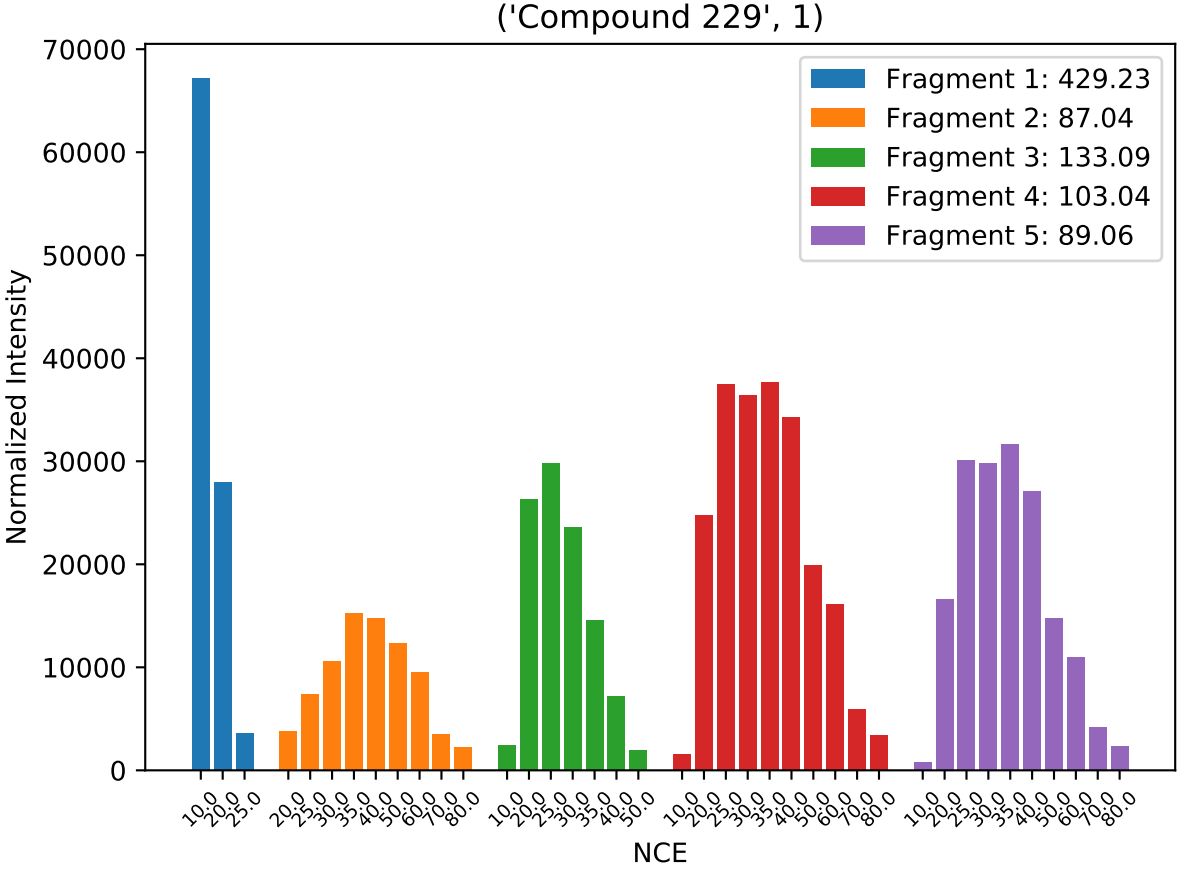

('Compound 465', 1)
Fragment 1: 535.4
Fragment 2: 173.47
Fragment 3: 534.46
Fragment 4: 517.39
Fragment 5: 173.46
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
20.0
20.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
10.0
20.0
25.0
35.0
10.0
25.0
30.0
NCE

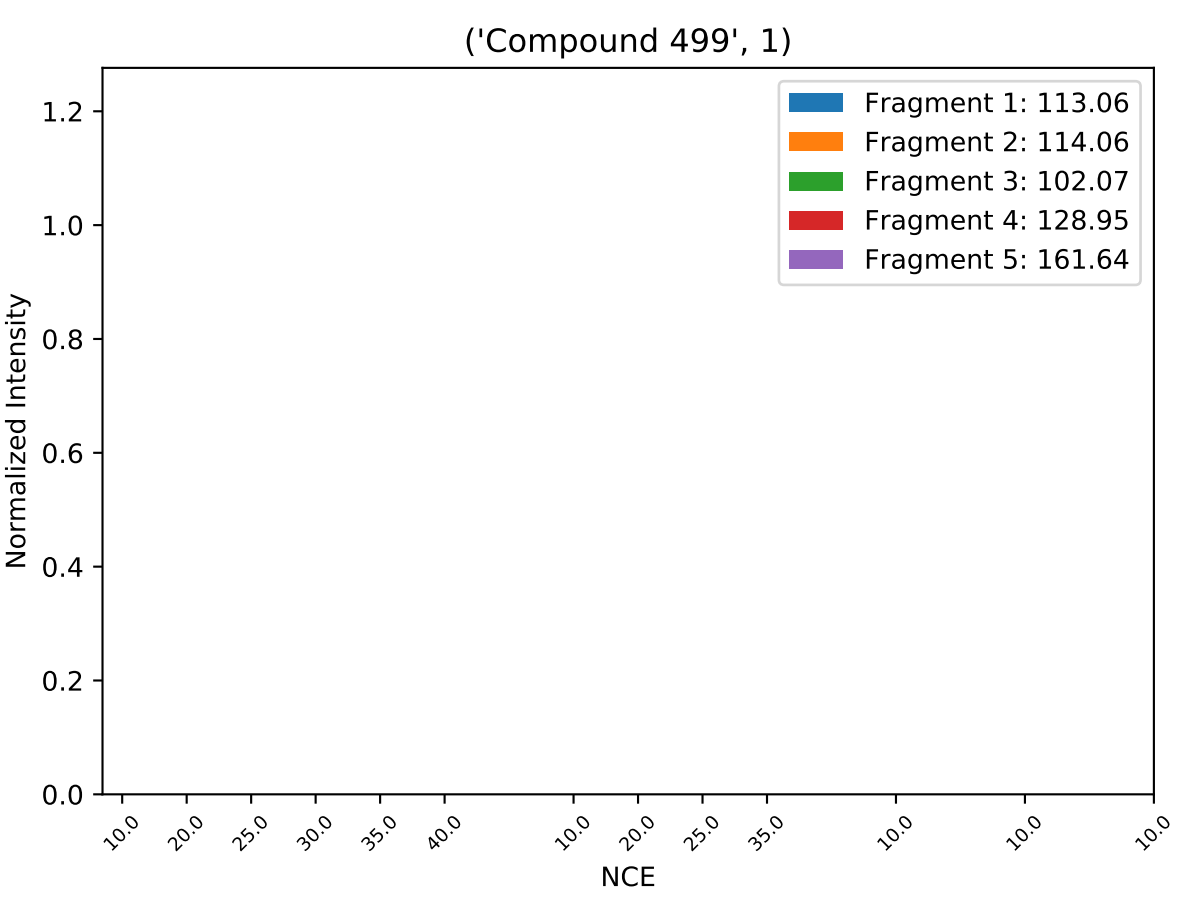

('Compound 342', 1)
Fragment 1: 221.14
Fragment 2: 133.09
Fragment 3: 177.11
Fragment 4: 89.06
Fragment 5: 87.04
Normalized Intensity
NCE
0
2500
5000
7500
10000
12500
15000
17500
20000
20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

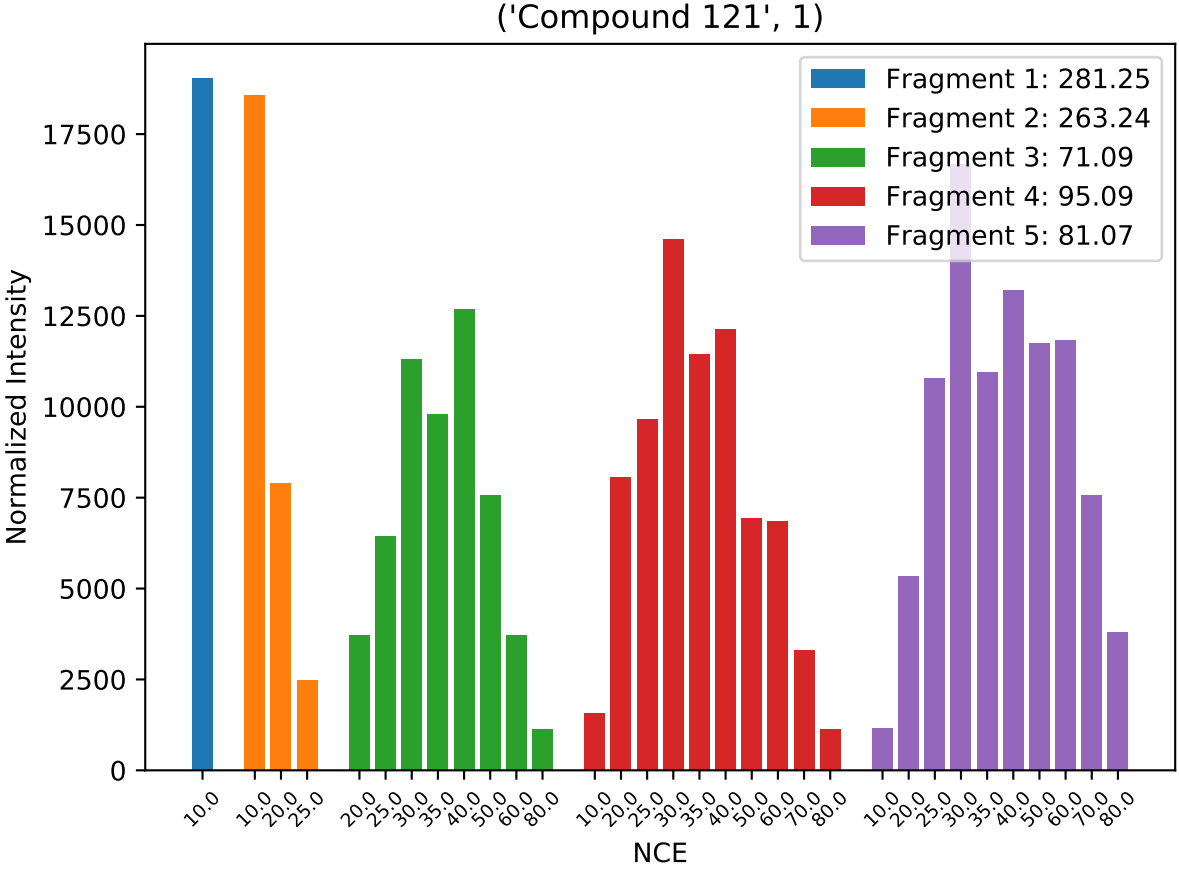

('Compound 217', 1)
Fragment 1: 352.94
Fragment 2: 528.91
Fragment 3: 176.97
Fragment 4: 158.96
Fragment 5: 98.98
Normalized Intensity
1000000
800000
600000
400000
200000
0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
30.0
50.0
60.0
70.0
80.0
NCE

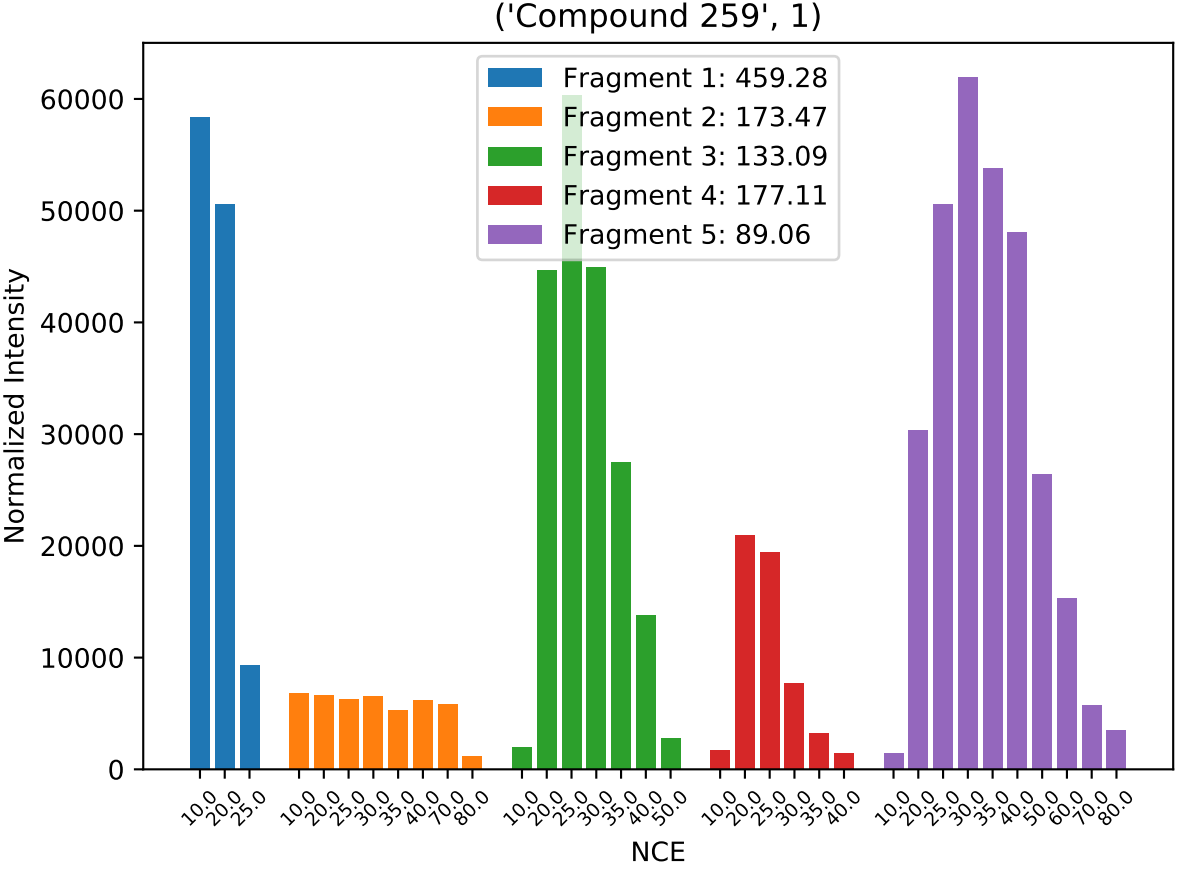

('Compound 477', 1)
Fragment 1: 173.47
Fragment 2: 479.41
Fragment 3: 103.04
Fragment 4: 89.06
Fragment 5: 133.09
Normalized Intensity
0
2000
4000
6000
8000
10.0 20.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

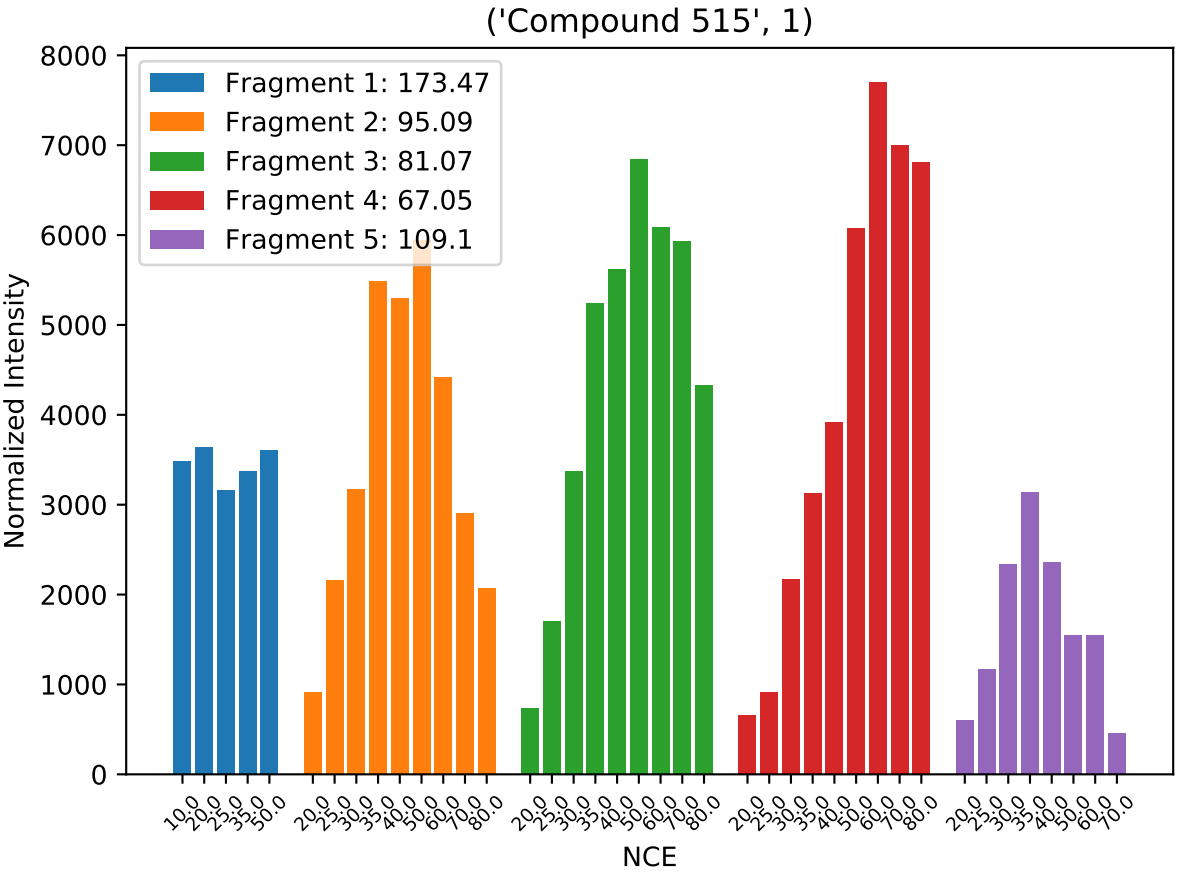

('Compound 484', 1)
Fragment 1: 173.47
Fragment 2: 173.48
Fragment 3: 529.43
Fragment 4: 529.42
Fragment 5: 173.46
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
80.0
10.0
20.0
30.0
35.0
25.0
20.0
25.0
30.0
35.0
70.0
80.0
NCE

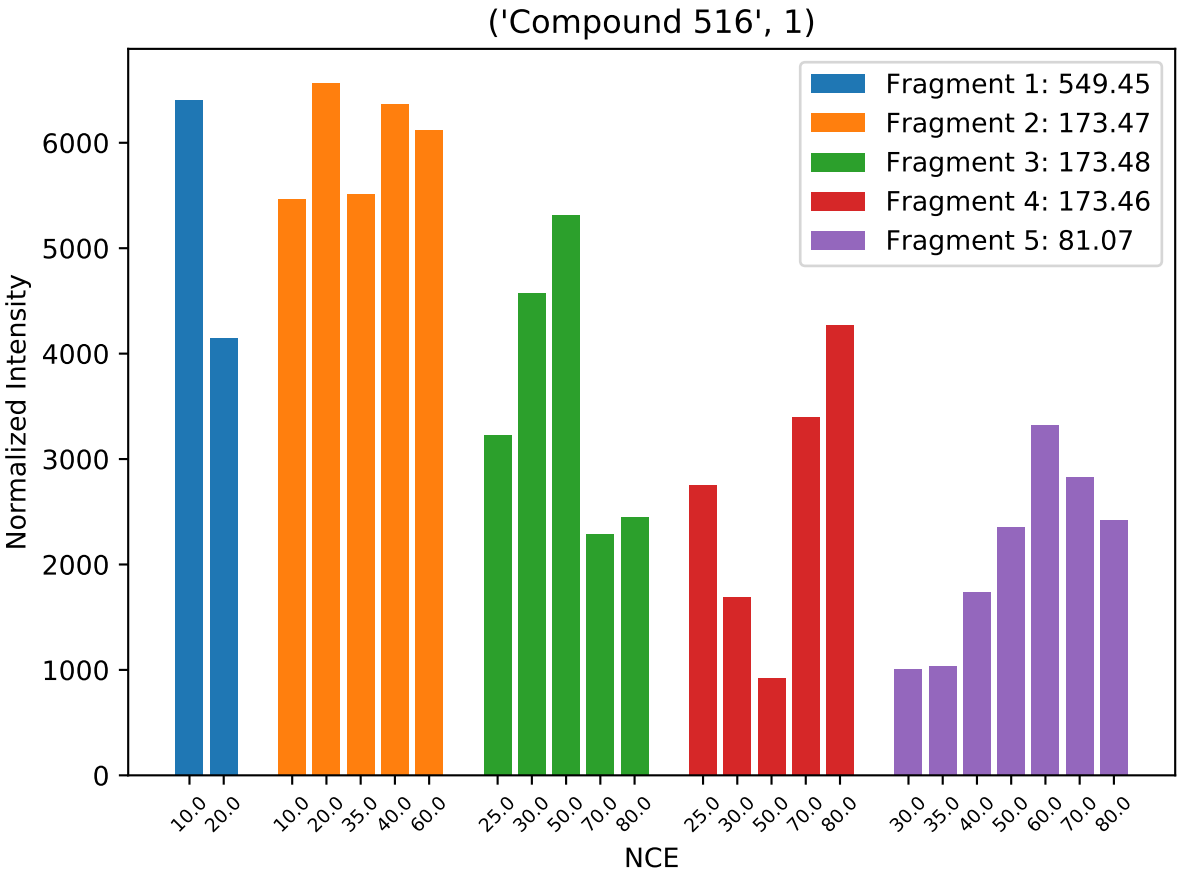

('Compound 229', 1)
Fragment 1: 429.23
Fragment 2: 87.04
Fragment 3: 133.09
Fragment 4: 103.04
Fragment 5: 89.06
Normalized Intensity
NCE
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

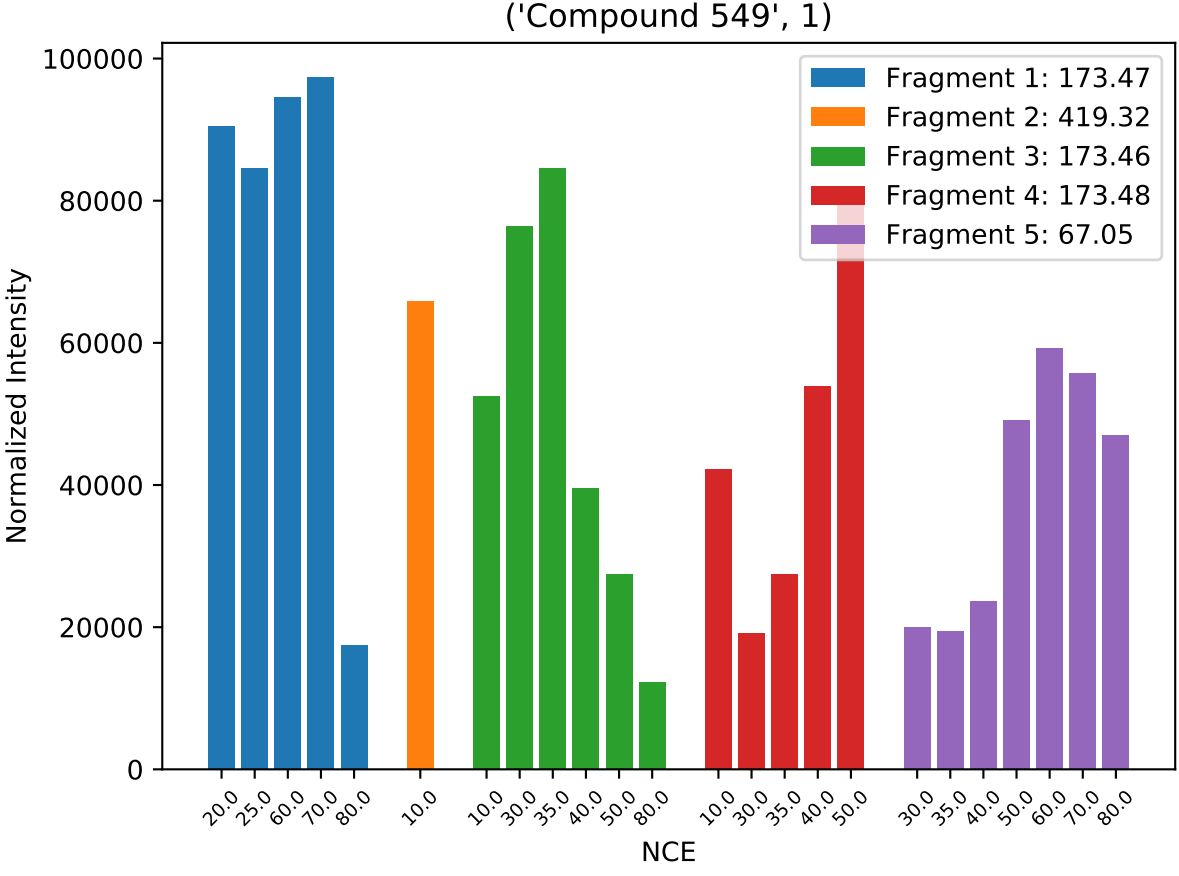

('Compound 499', 1)
Fragment 1: 113.06
Fragment 2: 114.06
Fragment 3: 102.07
Fragment 4: 128.95
Fragment 5: 161.64
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
35.0
10.0
10.0
10.0
NCE

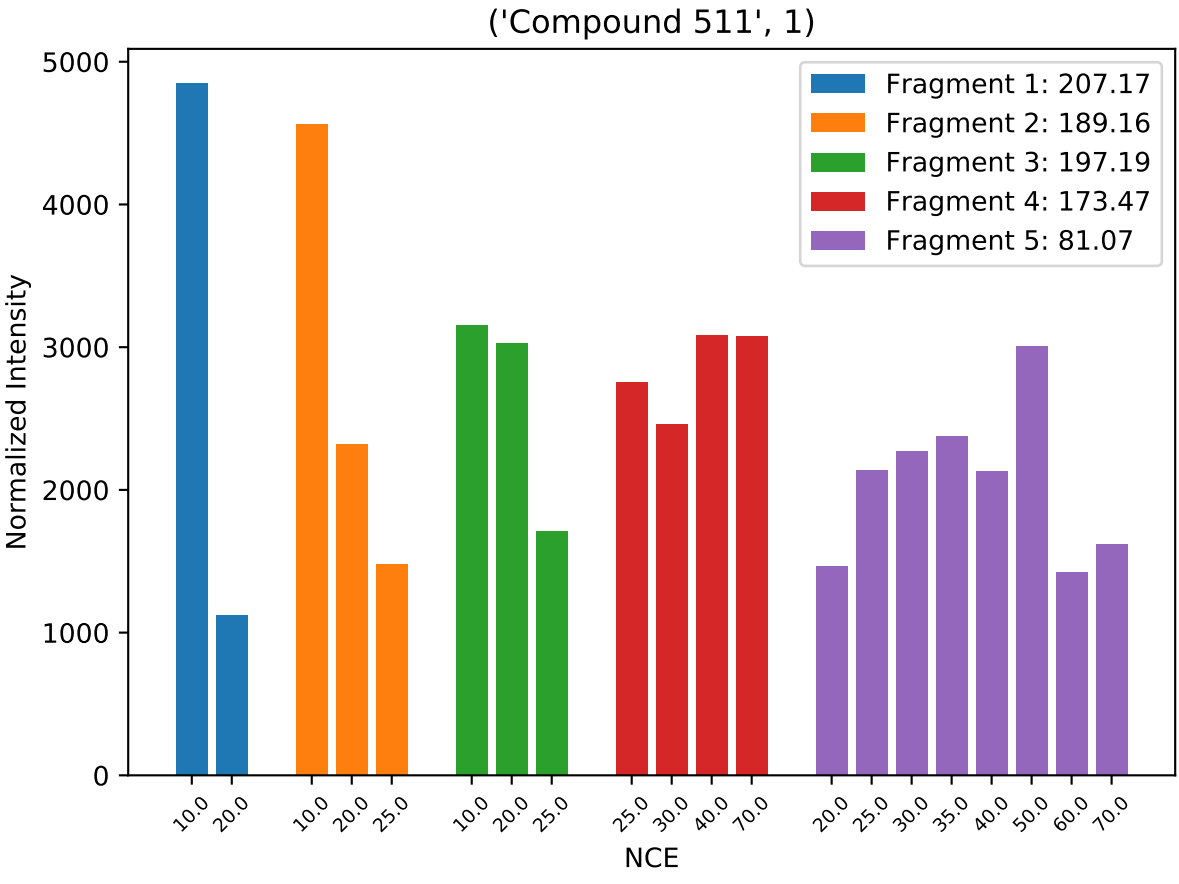

('Compound 121', 1)
Fragment 1: 281.25
Fragment 2: 263.24
Fragment 3: 71.09
Fragment 4: 95.09
Fragment 5: 81.07
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
NCE
10.0
10.0 20.0 25.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

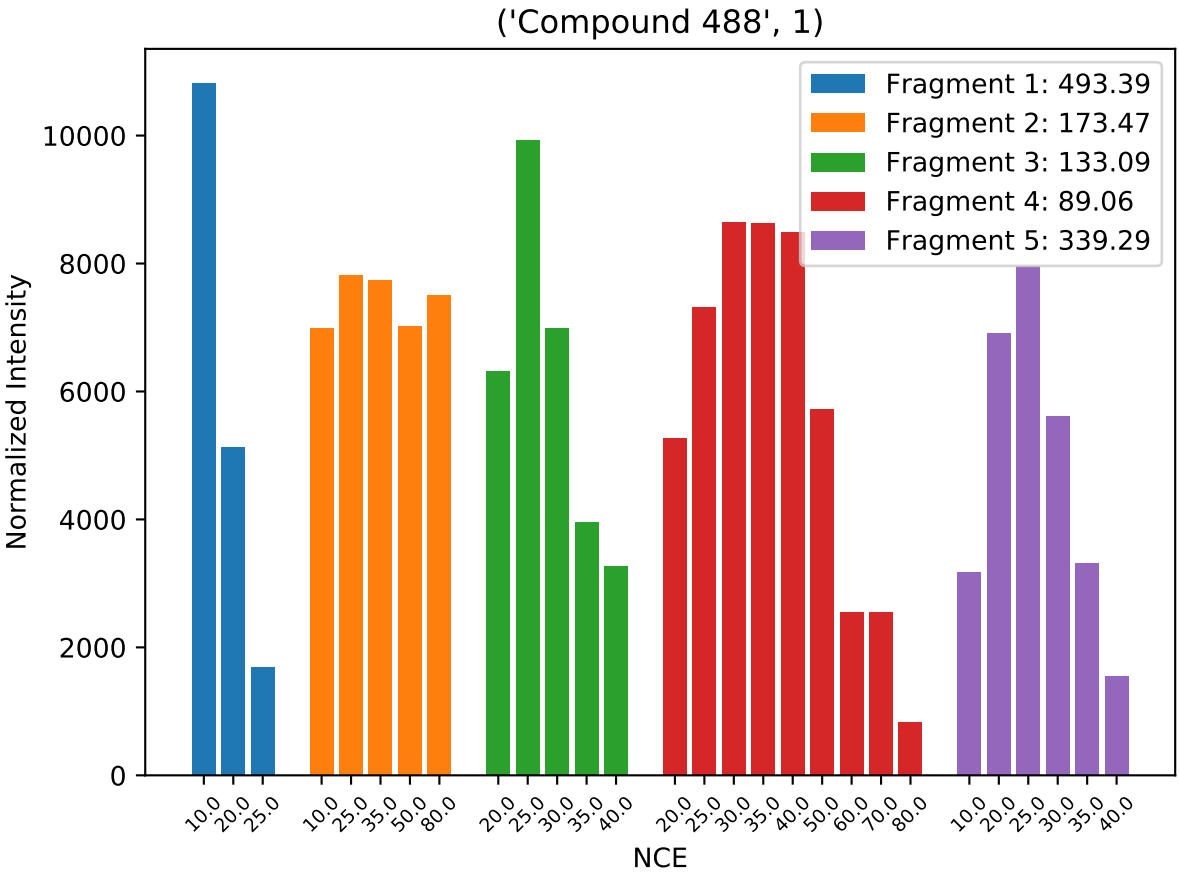

('Compound 259', 1)
Fragment 1: 459.28
Fragment 2: 173.47
Fragment 3: 133.09
Fragment 4: 177.11
Fragment 5: 89.06
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
NCE
10.0 20.0 25.0
10.0 20.0 25.0 30.0 35.0 40.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

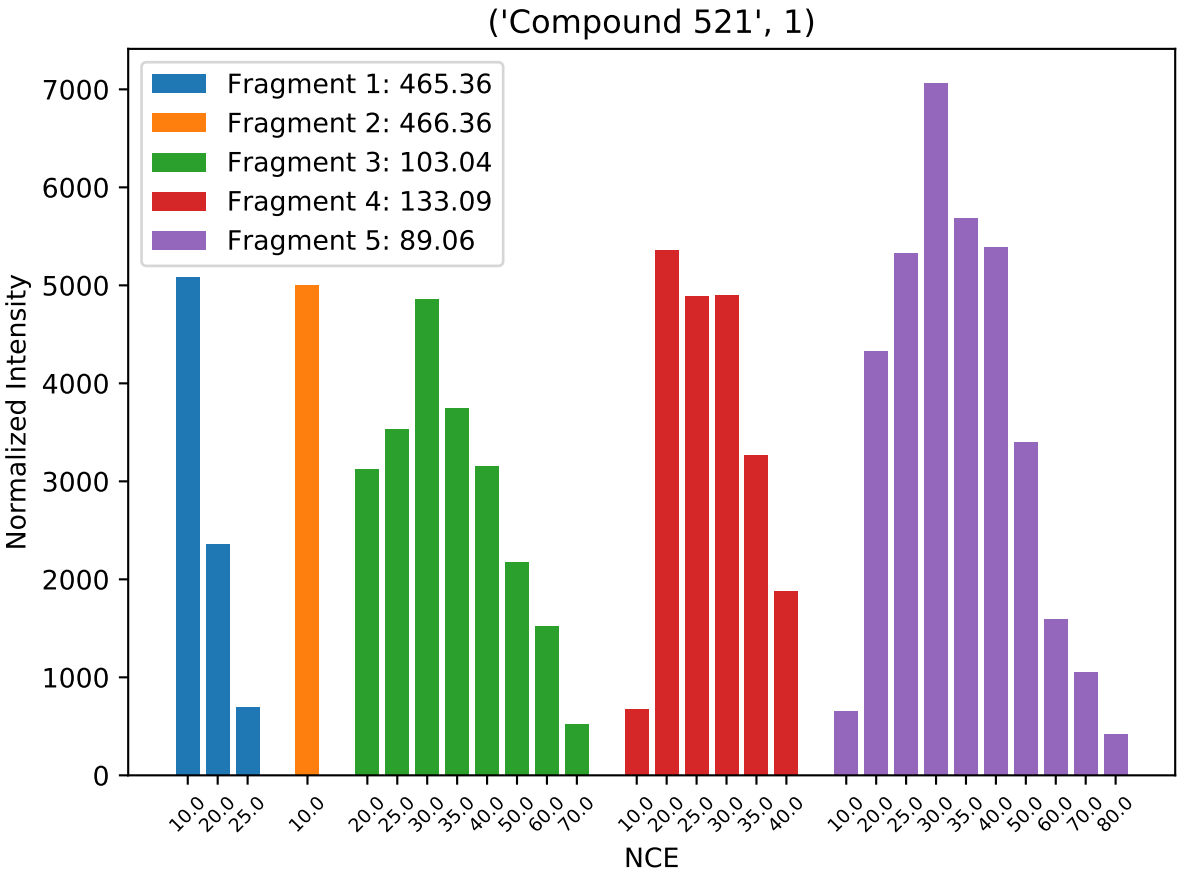

('Compound 515', 1)
Fragment 1: 173.47
Fragment 2: 95.09
Fragment 3: 81.07
Fragment 4: 67.05
Fragment 5: 109.1
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
NCE
10.0 20.0 25.0 35.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0

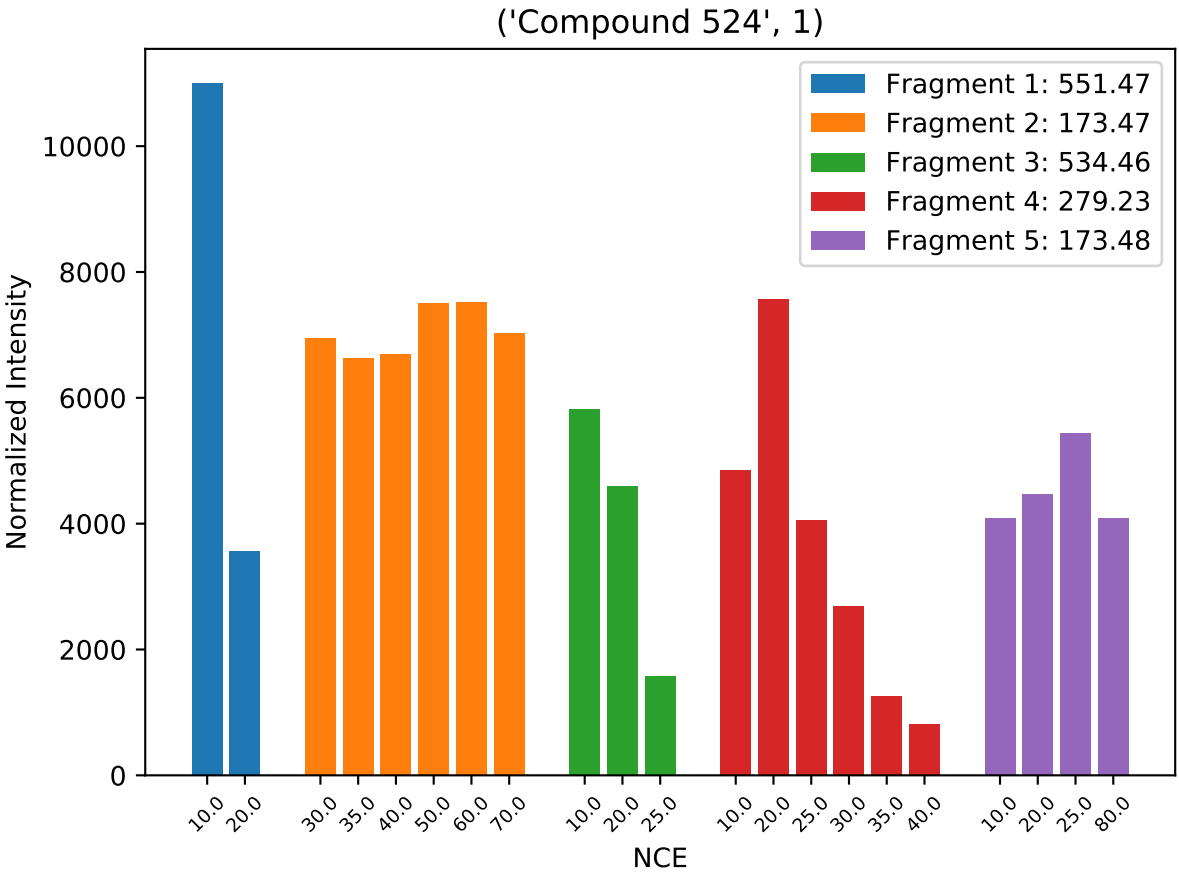

('Compound 516', 1)
Fragment 1: 549.45
Fragment 2: 173.47
Fragment 3: 173.48
Fragment 4: 173.46
Fragment 5: 81.07
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
10.0
20.0
10.0
20.0
35.0
40.0
60.0
25.0
30.0
50.0
70.0
80.0
25.0
30.0
50.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

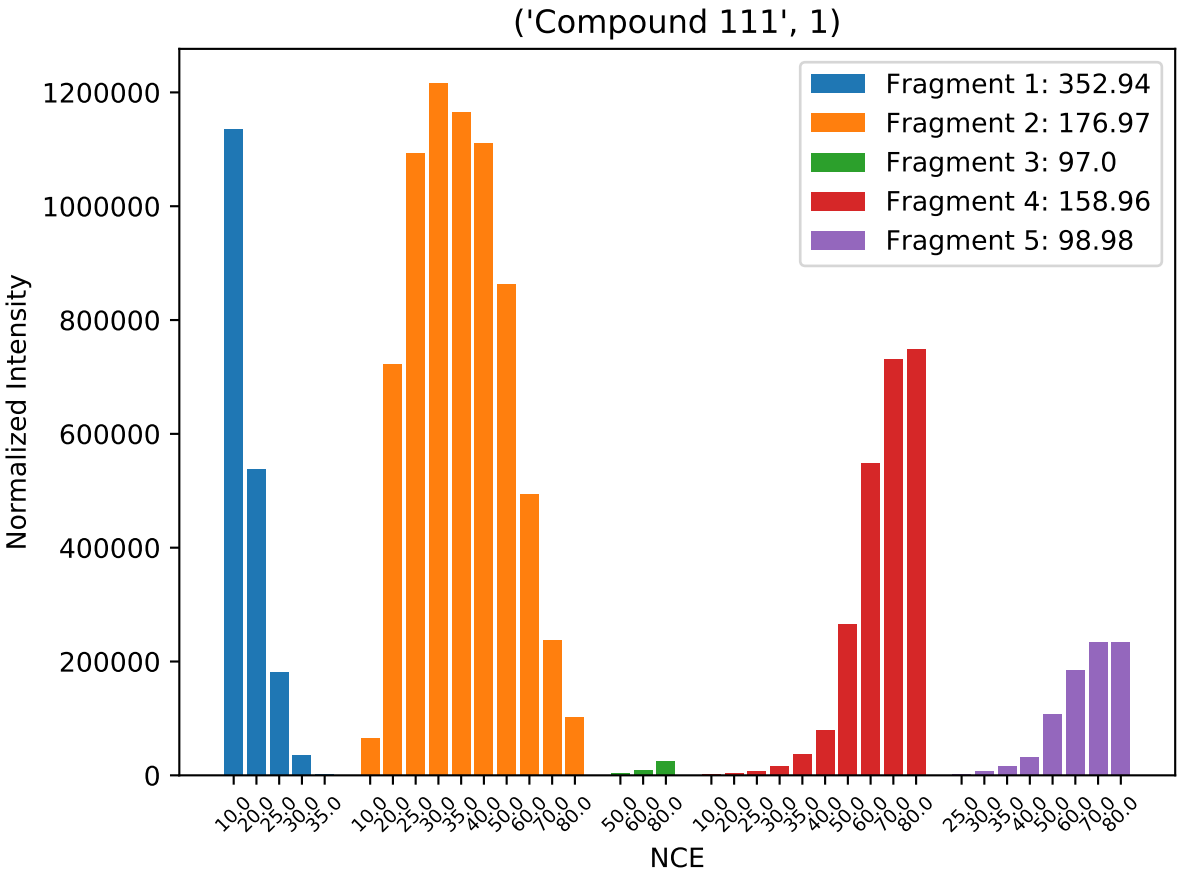

('Compound 549', 1)
Fragment 1: 173.47
Fragment 2: 419.32
Fragment 3: 173.46
Fragment 4: 173.48
Fragment 5: 67.05
Normalized Intensity
100000
80000
60000
40000
20000
0
20.0
25.0
60.0
70.0
80.0
10.0
10.0
30.0
35.0
40.0
50.0
80.0
10.0
30.0
35.0
40.0
50.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

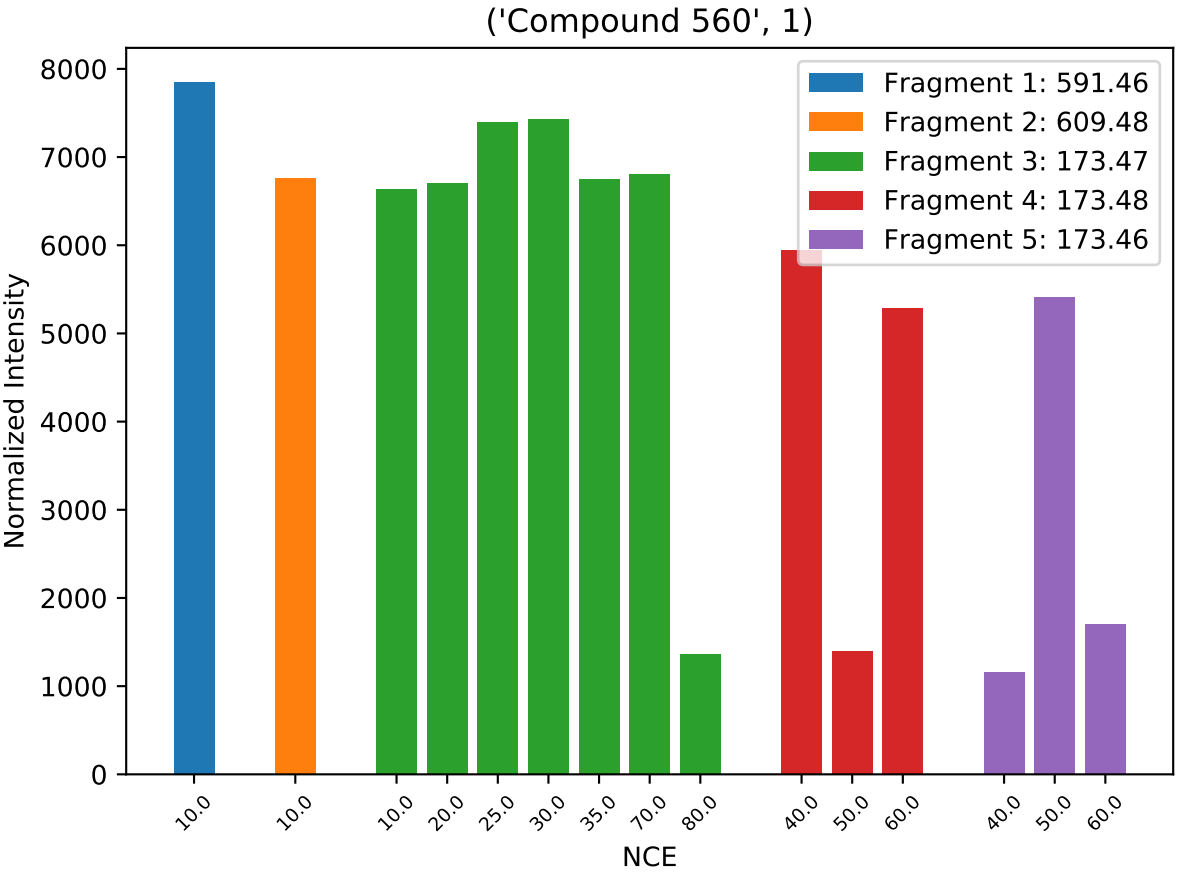

('Compound 511', 1)
Fragment 1: 207.17
Fragment 2: 189.16
Fragment 3: 197.19
Fragment 4: 173.47
Fragment 5: 81.07
Normalized Intensity
0
1000
2000
3000
4000
5000
10.0
20.0
10.0
20.0
25.0
10.0
20.0
25.0
25.0
30.0
40.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

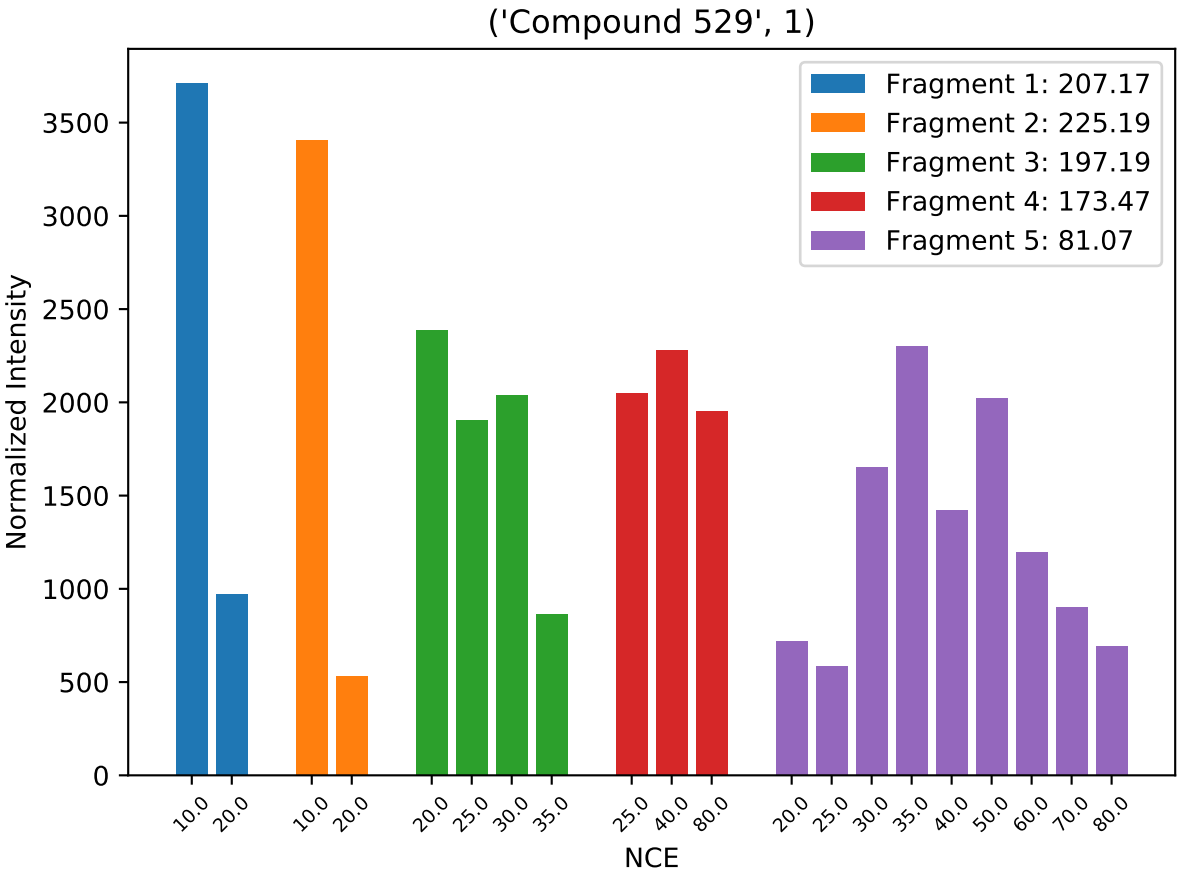

('Compound 488', 1)
Fragment 1: 493.39
Fragment 2: 173.47
Fragment 3: 133.09
Fragment 4: 89.06
Fragment 5: 339.29
Normalized Intensity
0
2000
4000
6000
8000
10000
NCE
10.0 20.0 25.0
10.0 25.0 35.0 50.0 80.0
20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0

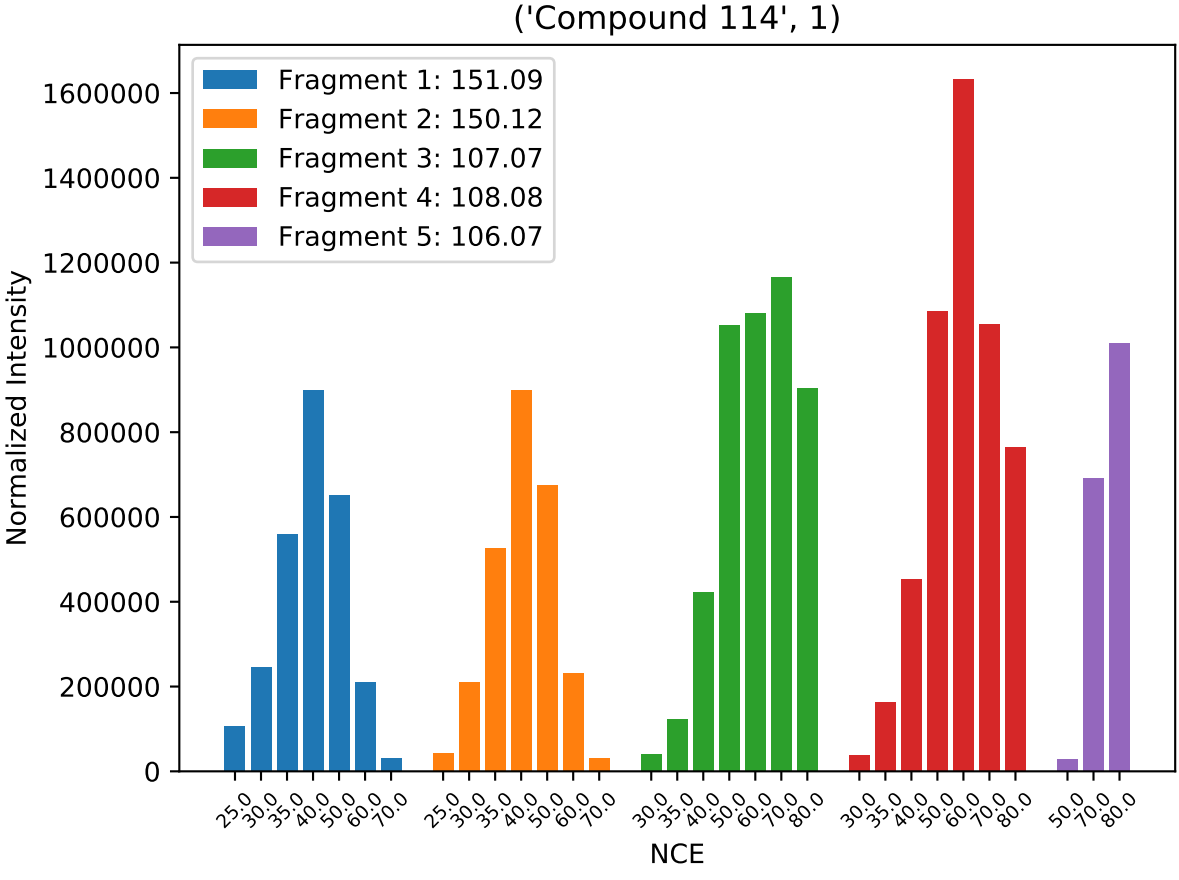

('Compound 521', 1)
Fragment 1: 465.36
Fragment 2: 466.36
Fragment 3: 103.04
Fragment 4: 133.09
Fragment 5: 89.06
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

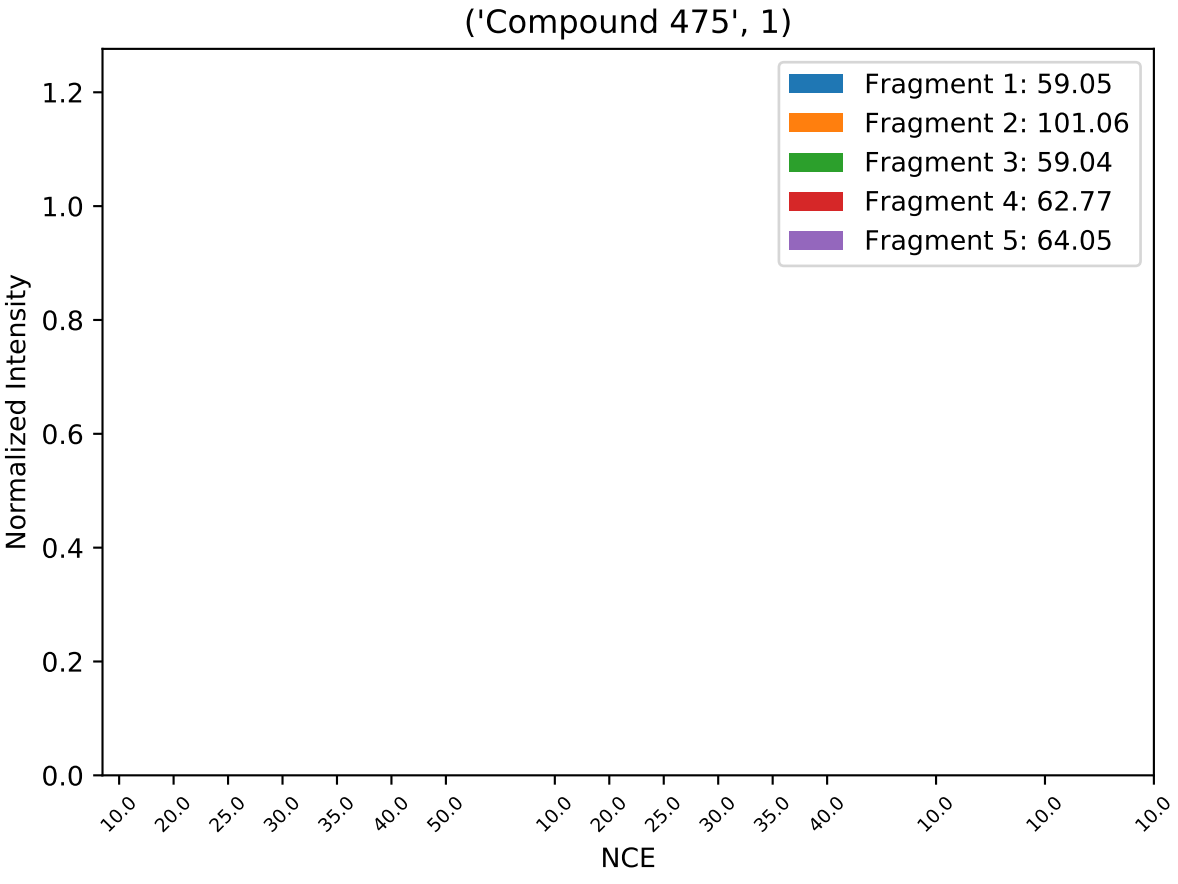

('Compound 524', 1)
Fragment 1: 551.47
Fragment 2: 173.47
Fragment 3: 534.46
Fragment 4: 279.23
Fragment 5: 173.48
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
20.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
80.0
NCE

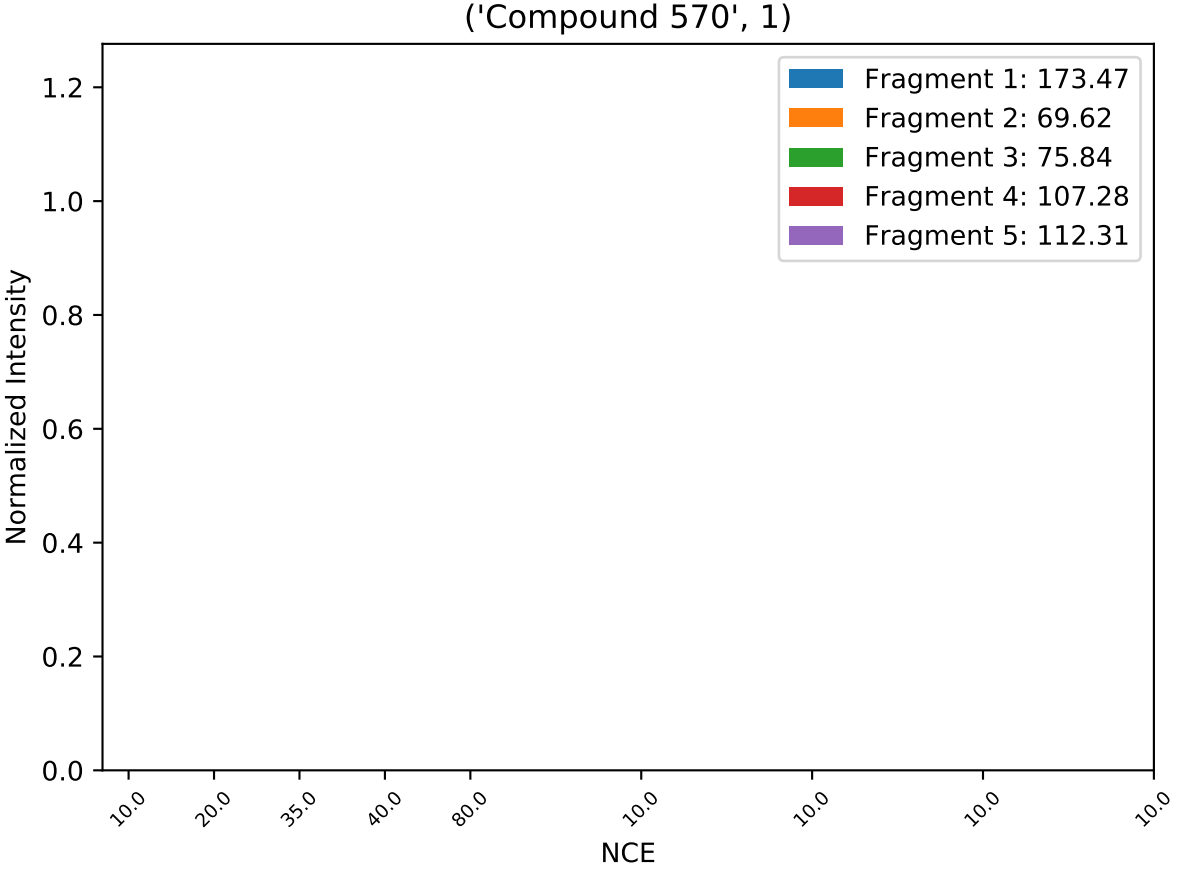

('Compound 111', 1)
Fragment 1: 352.94
Fragment 2: 176.97
Fragment 3: 97.0
Fragment 4: 158.96
Fragment 5: 98.98
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
NCE
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

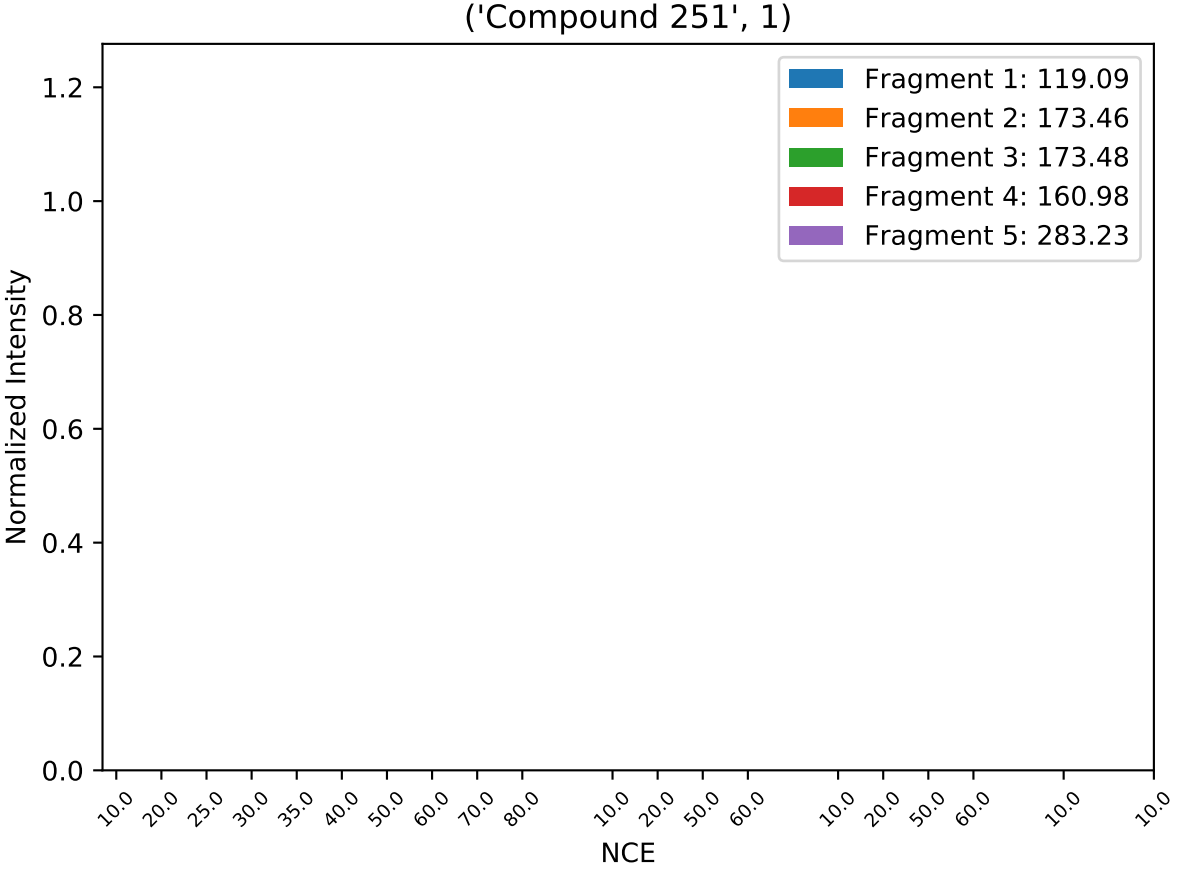

('Compound 560', 1)
Fragment 1: 591.46
Fragment 2: 609.48
Fragment 3: 173.47
Fragment 4: 173.48
Fragment 5: 173.46
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
10.0
10.0
20.0
25.0
30.0
35.0
70.0
80.0
40.0
50.0
60.0
40.0
50.0
60.0
NCE

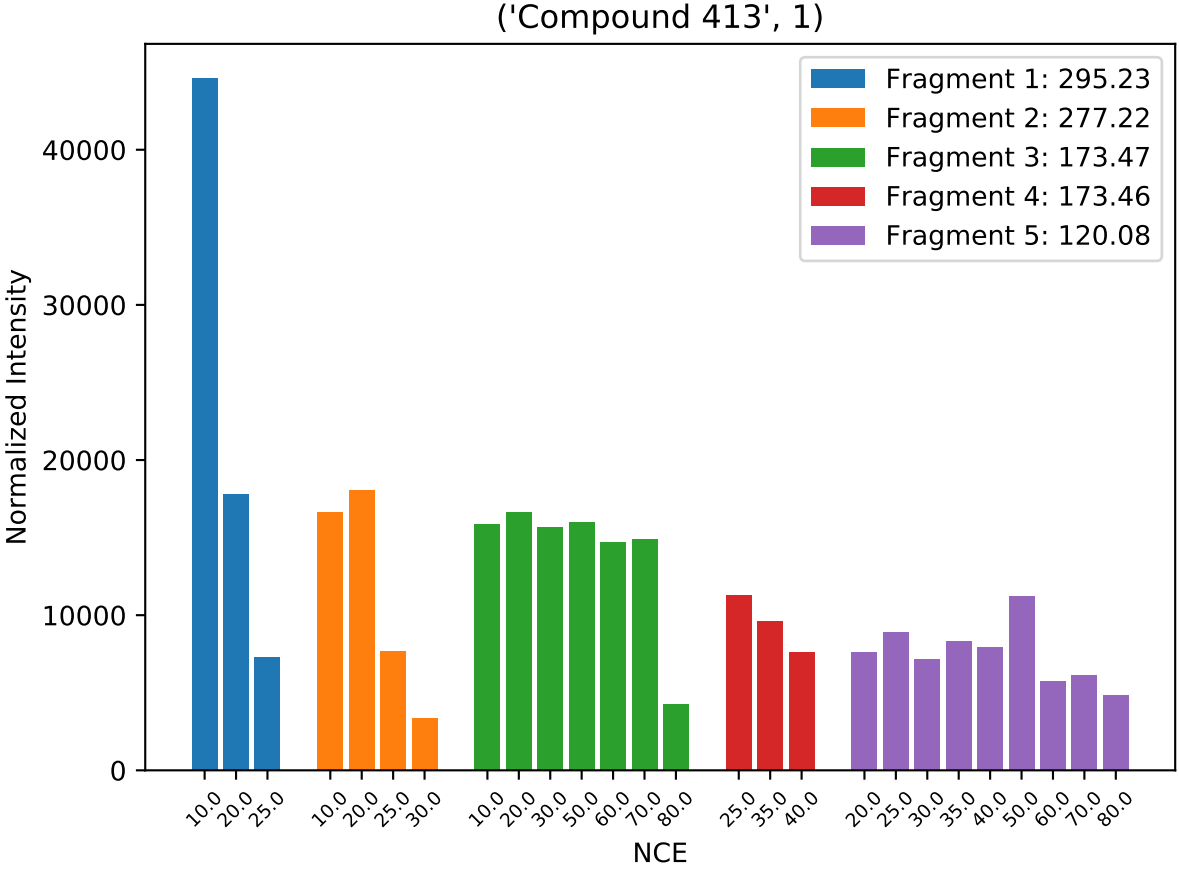

('Compound 529', 1)
Fragment 1: 207.17
Fragment 2: 225.19
Fragment 3: 197.19
Fragment 4: 173.47
Fragment 5: 81.07
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
10.0
20.0
10.0
20.0
20.0
25.0
30.0
35.0
25.0
40.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

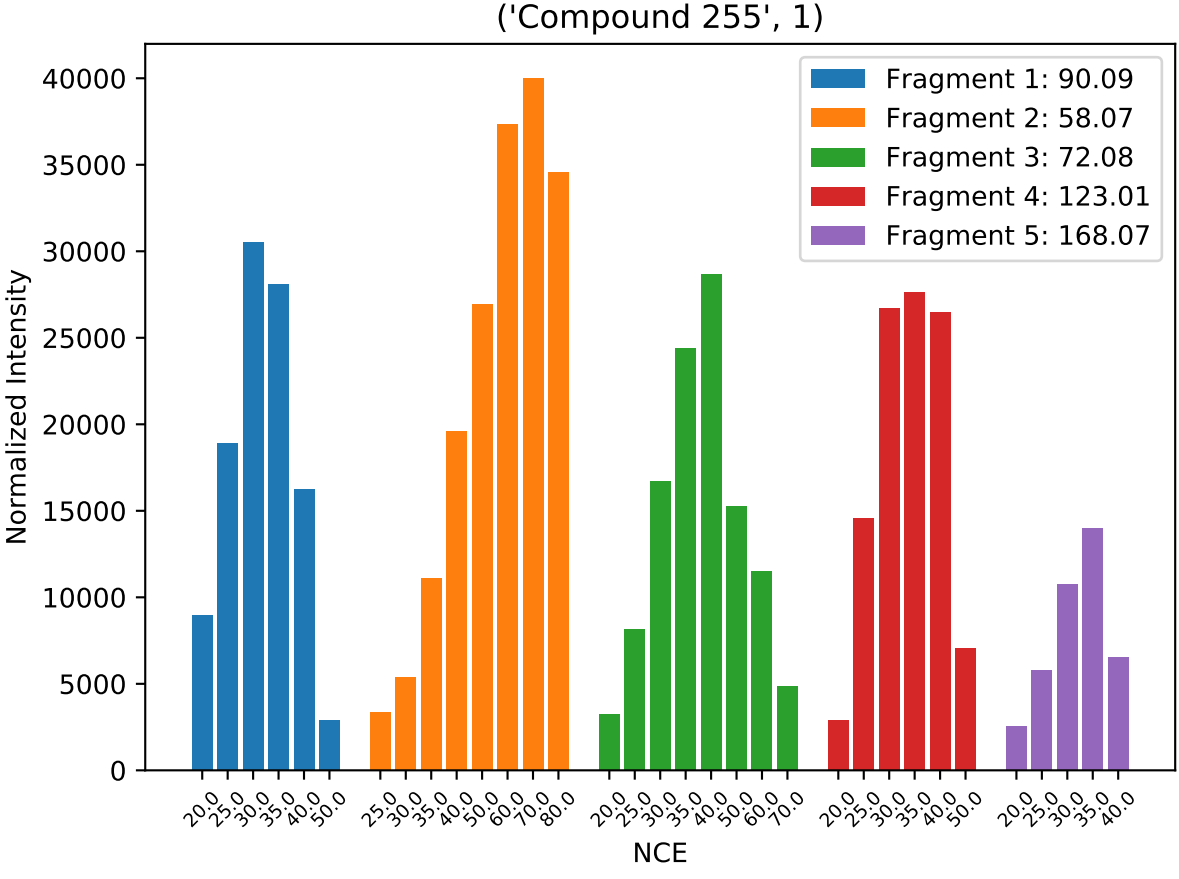

('Compound 114', 1)
Fragment 1: 151.09
Fragment 2: 150.12
Fragment 3: 107.07
Fragment 4: 108.08
Fragment 5: 106.07
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
1400000
1600000
25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
50.0 70.0 80.0
NCE

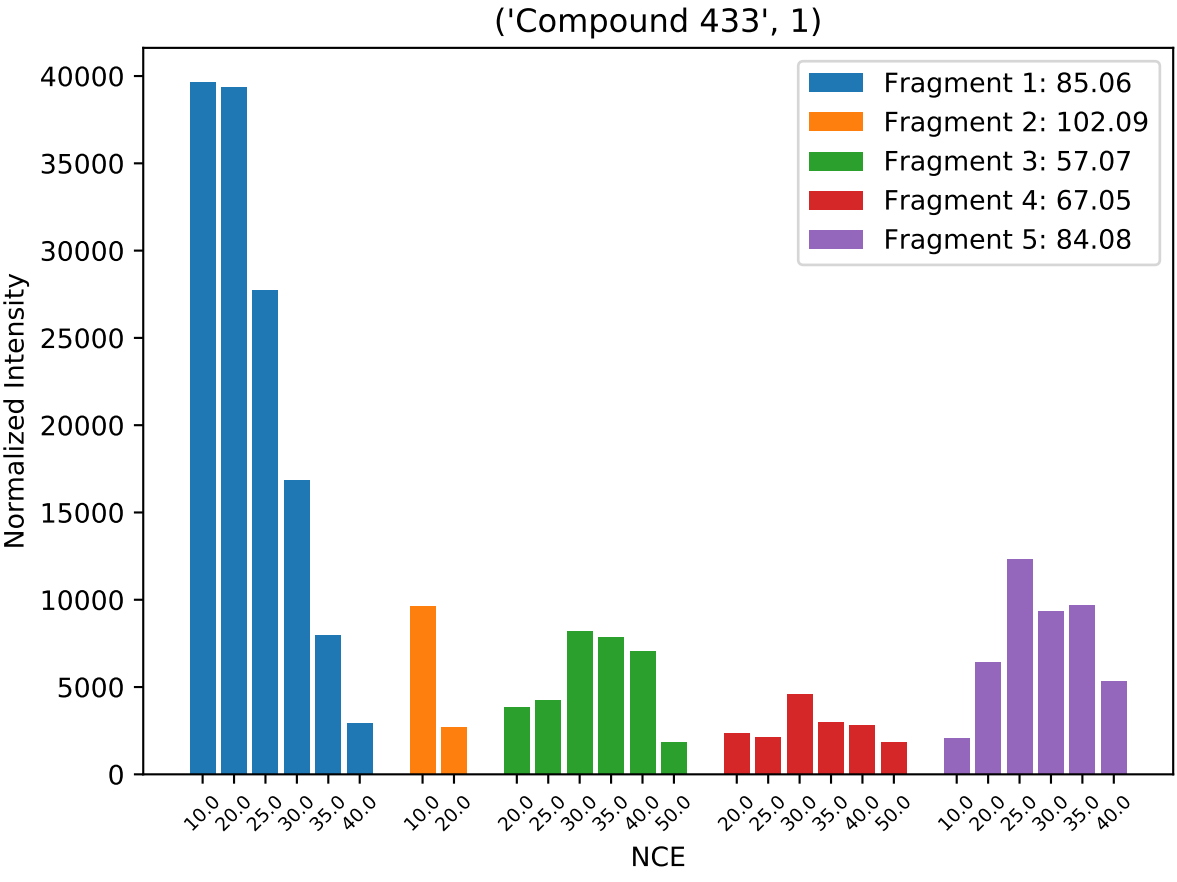

('Compound 475', 1)
Fragment 1: 59.05
Fragment 2: 101.06
Fragment 3: 59.04
Fragment 4: 62.77
Fragment 5: 64.05
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
10.0
10.0
NCE

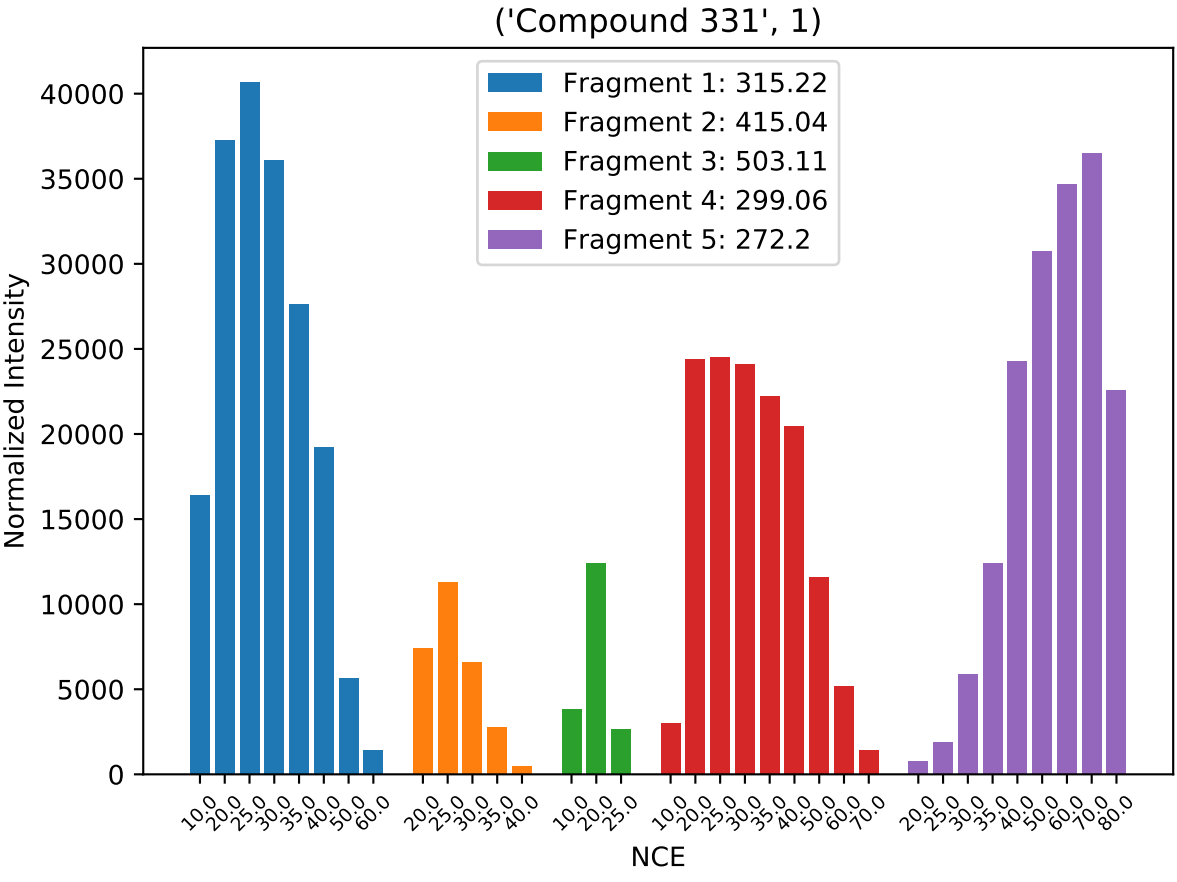

('Compound 570', 1)
Fragment 1: 173.47
Fragment 2: 69.62
Fragment 3: 75.84
Fragment 4: 107.28
Fragment 5: 112.31
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
35.0
40.0
80.0
10.0
10.0
10.0
10.0
NCE

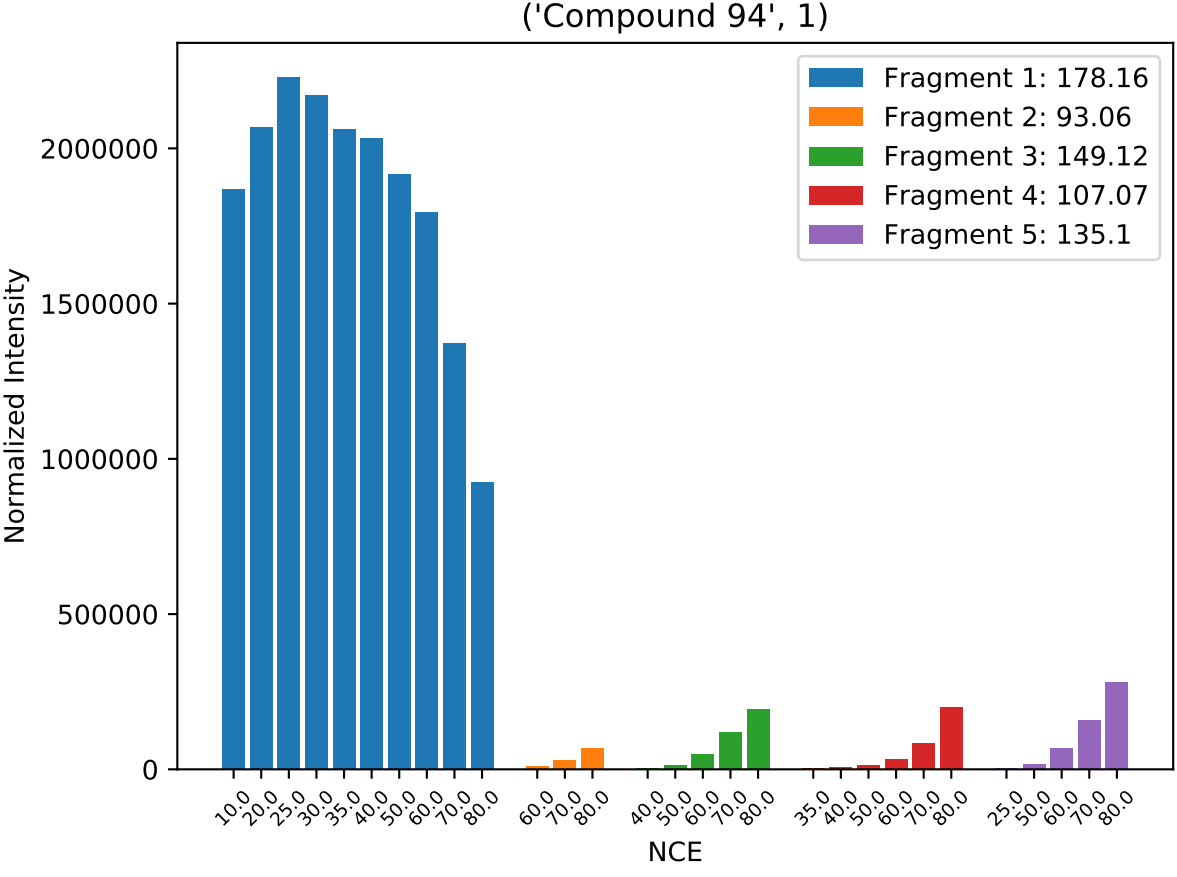

('Compound 251', 1)
Fragment 1: 119.09
Fragment 2: 173.46
Fragment 3: 173.48
Fragment 4: 160.98
Fragment 5: 283.23
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
50.0
60.0
10.0
20.0
50.0
60.0
10.0
10.0
NCE

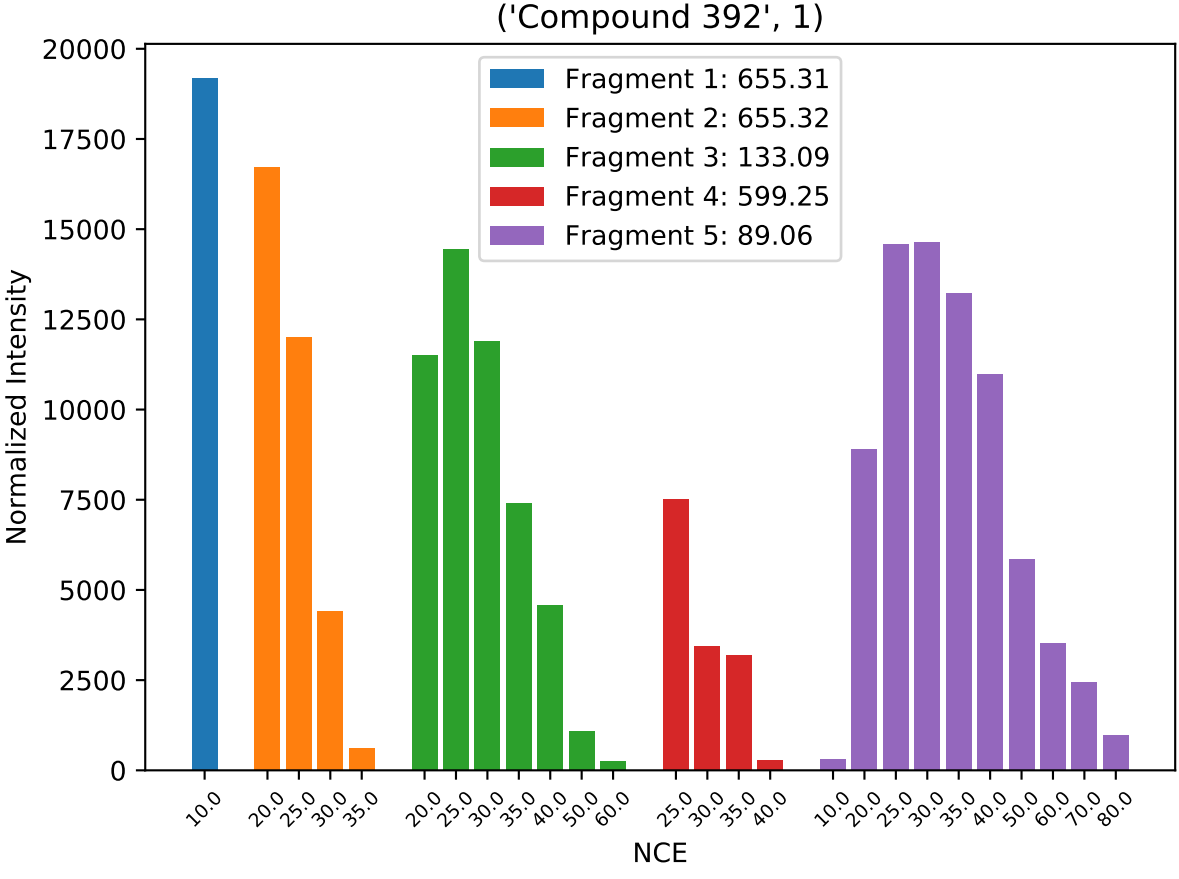

('Compound 413', 1)
Fragment 1: 295.23
Fragment 2: 277.22
Fragment 3: 173.47
Fragment 4: 173.46
Fragment 5: 120.08
Normalized Intensity
0
10000
20000
30000
40000
10.0
20.0
25.0
10.0
20.0
25.0
30.0
10.0
20.0
30.0
50.0
60.0
70.0
80.0
25.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

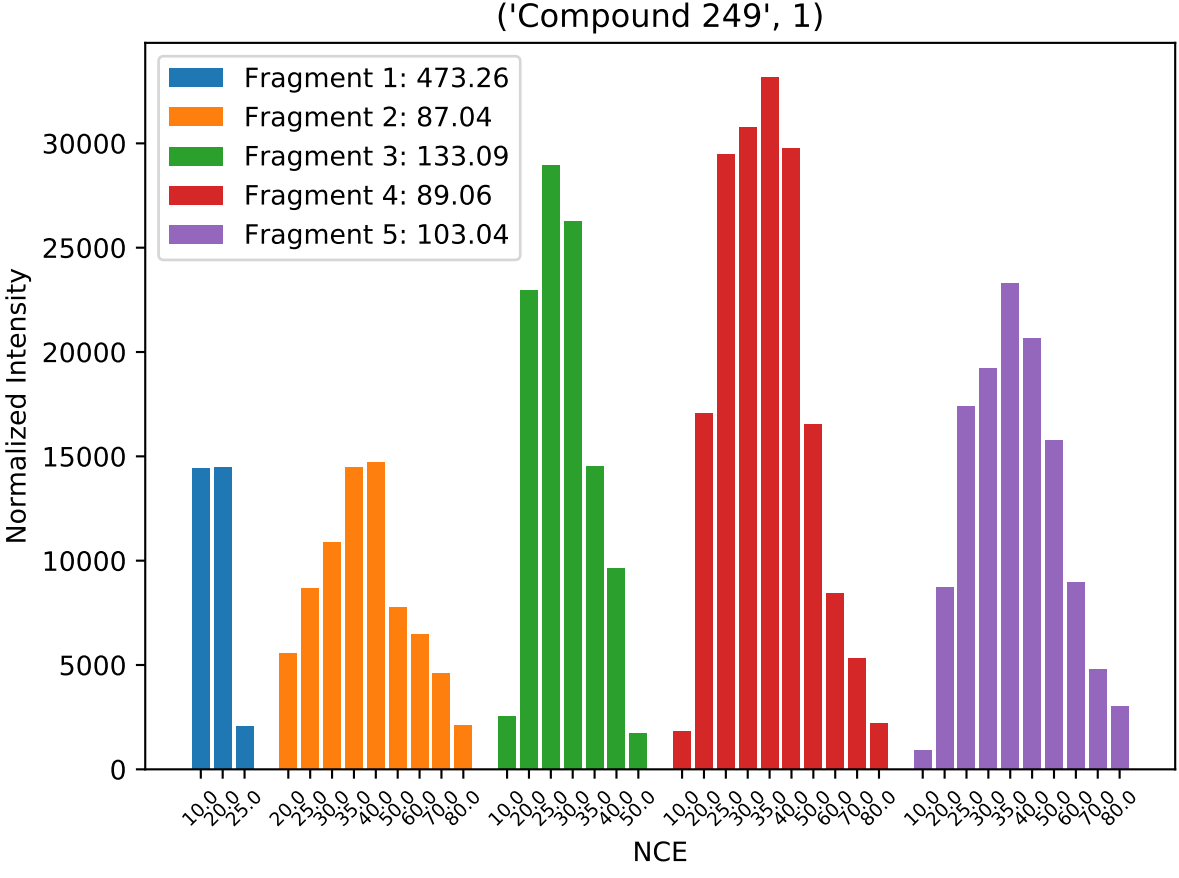

('Compound 255', 1)
Fragment 1: 90.09
Fragment 2: 58.07
Fragment 3: 72.08
Fragment 4: 123.01
Fragment 5: 168.07
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0
NCE

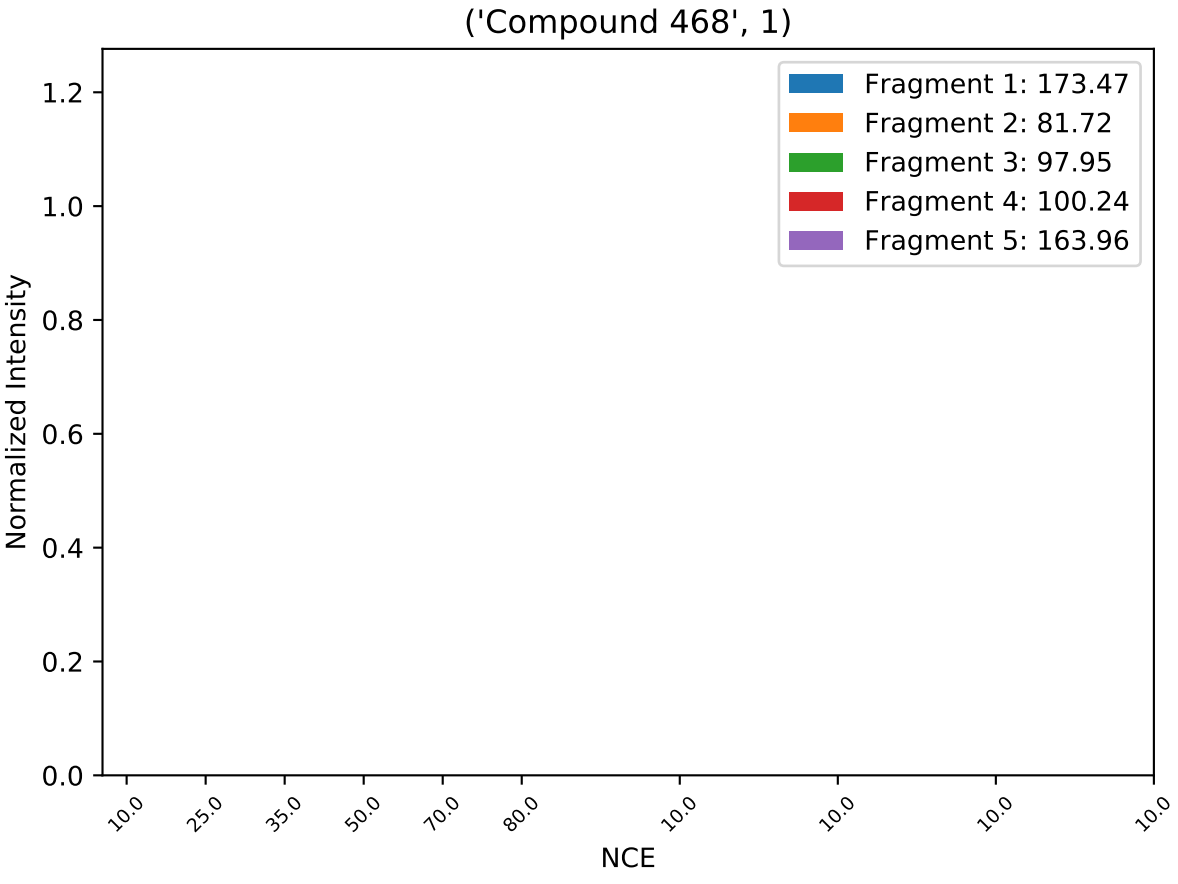

('Compound 433', 1)
Fragment 1: 85.06
Fragment 2: 102.09
Fragment 3: 57.07
Fragment 4: 67.05
Fragment 5: 84.08
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
NCE

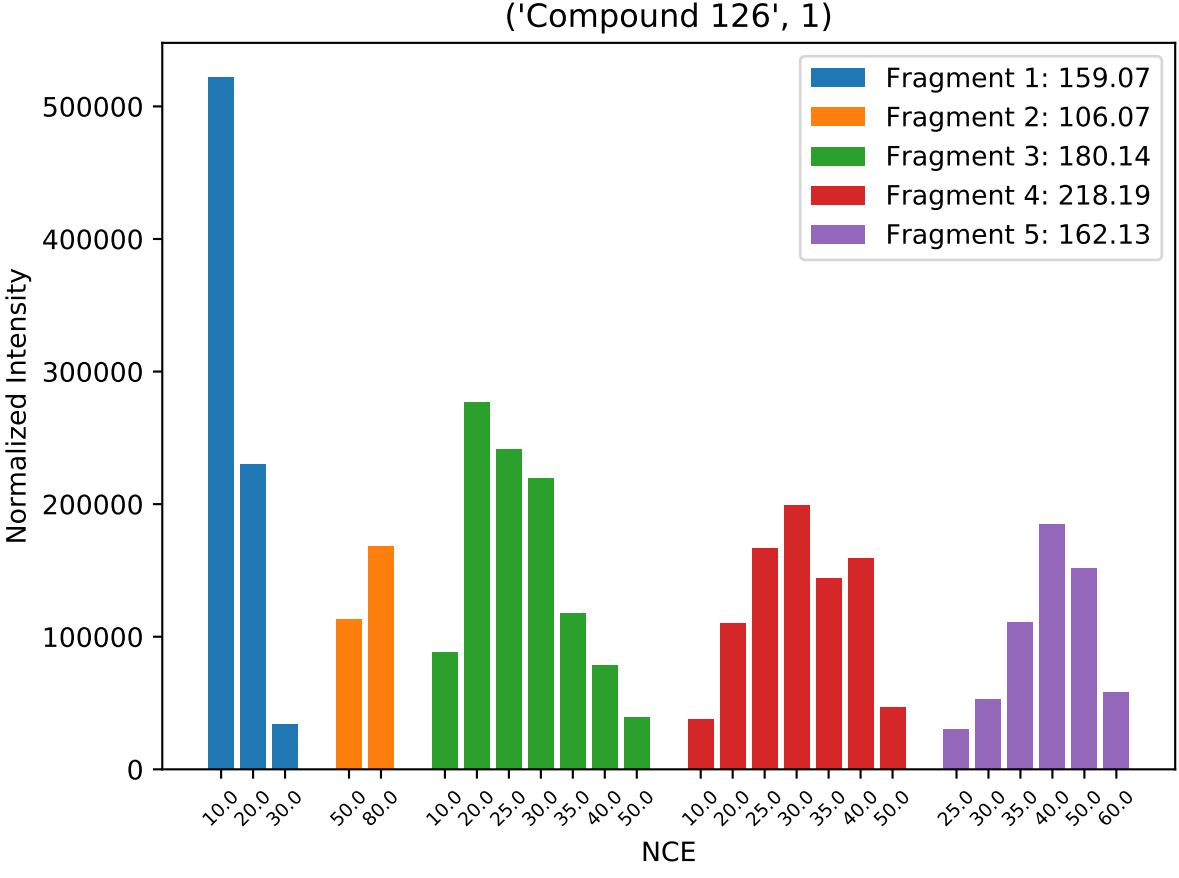

('Compound 331', 1)
Fragment 1: 315.22
Fragment 2: 415.04
Fragment 3: 503.11
Fragment 4: 299.06
Fragment 5: 272.2
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

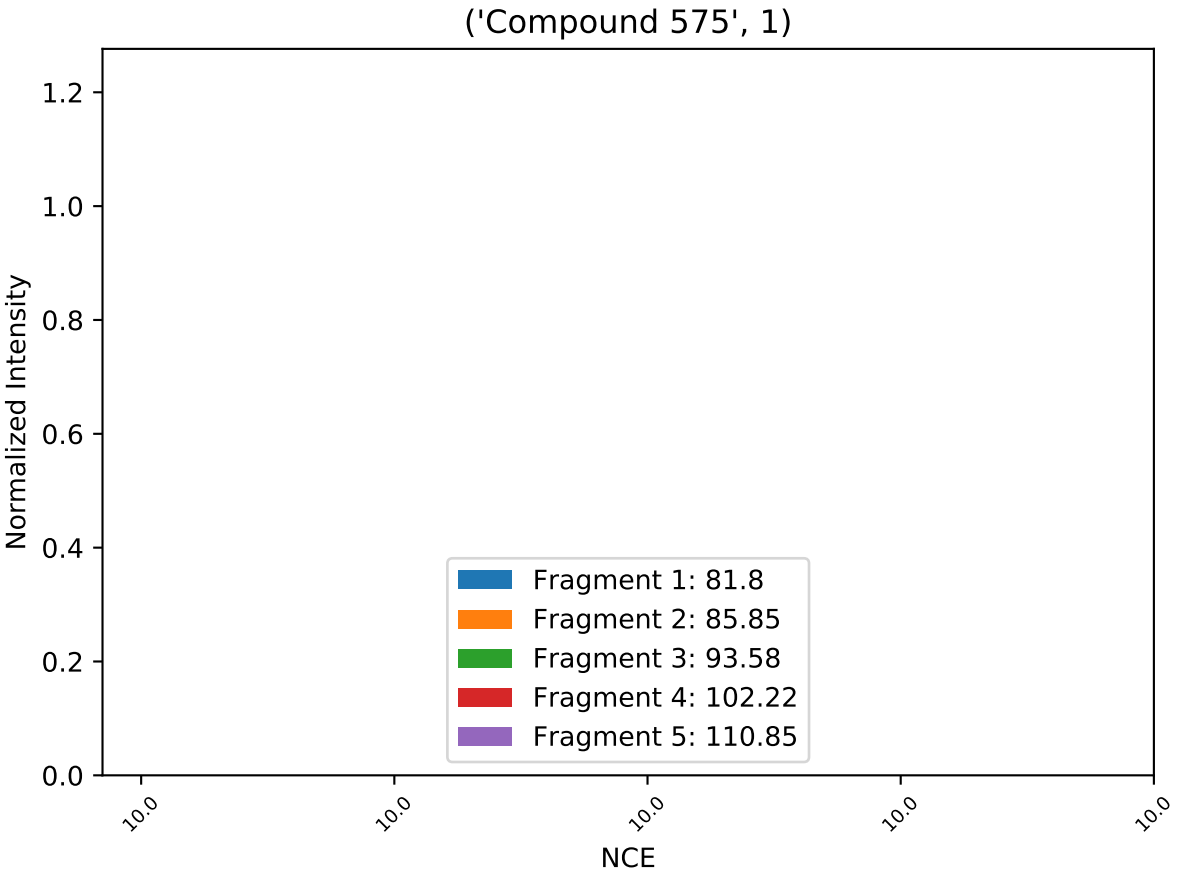

('Compound 94', 1)
Fragment 1: 178.16
Fragment 2: 93.06
Fragment 3: 149.12
Fragment 4: 107.07
Fragment 5: 135.1
Normalized Intensity
2000000
1500000
1000000
500000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
60.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
50.0
60.0
70.0
80.0
NCE

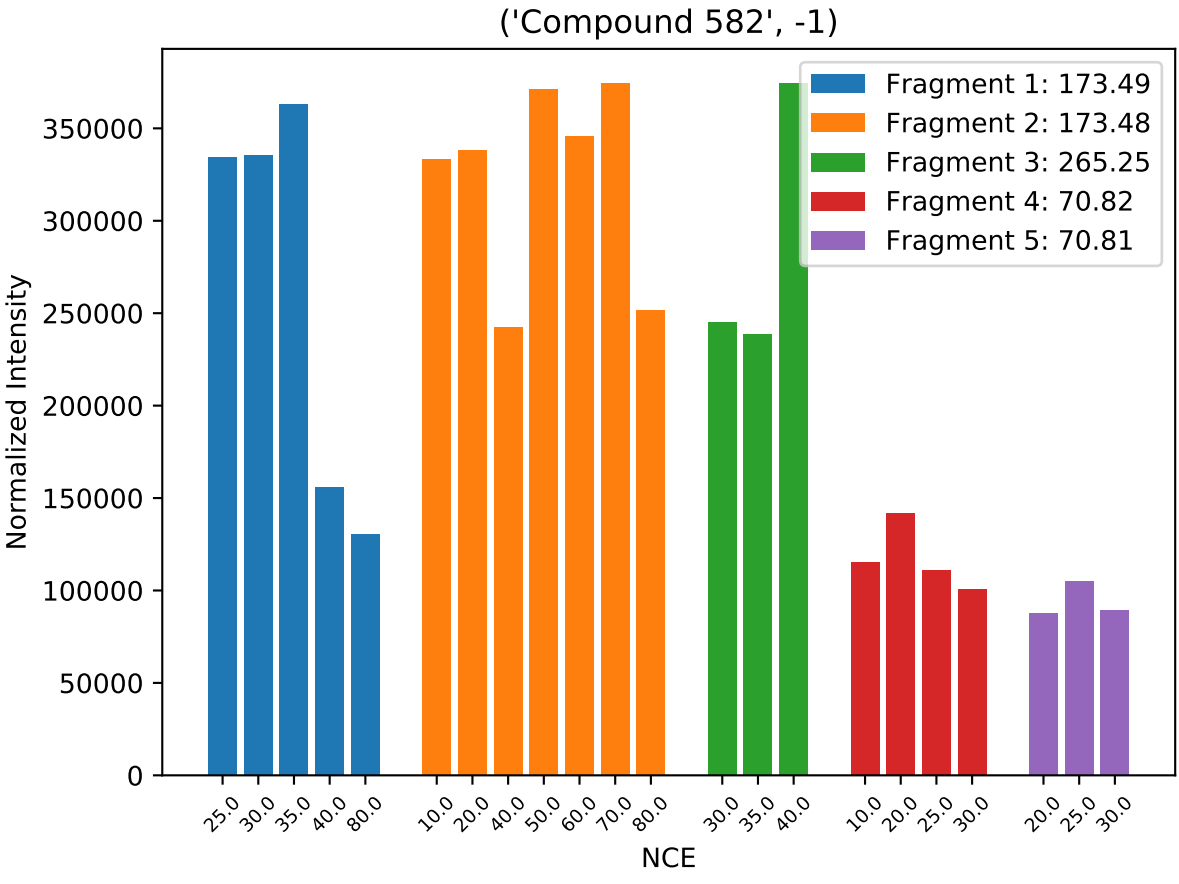

('Compound 392', 1)
Fragment 1: 655.31
Fragment 2: 655.32
Fragment 3: 133.09
Fragment 4: 599.25
Fragment 5: 89.06
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
NCE
10.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

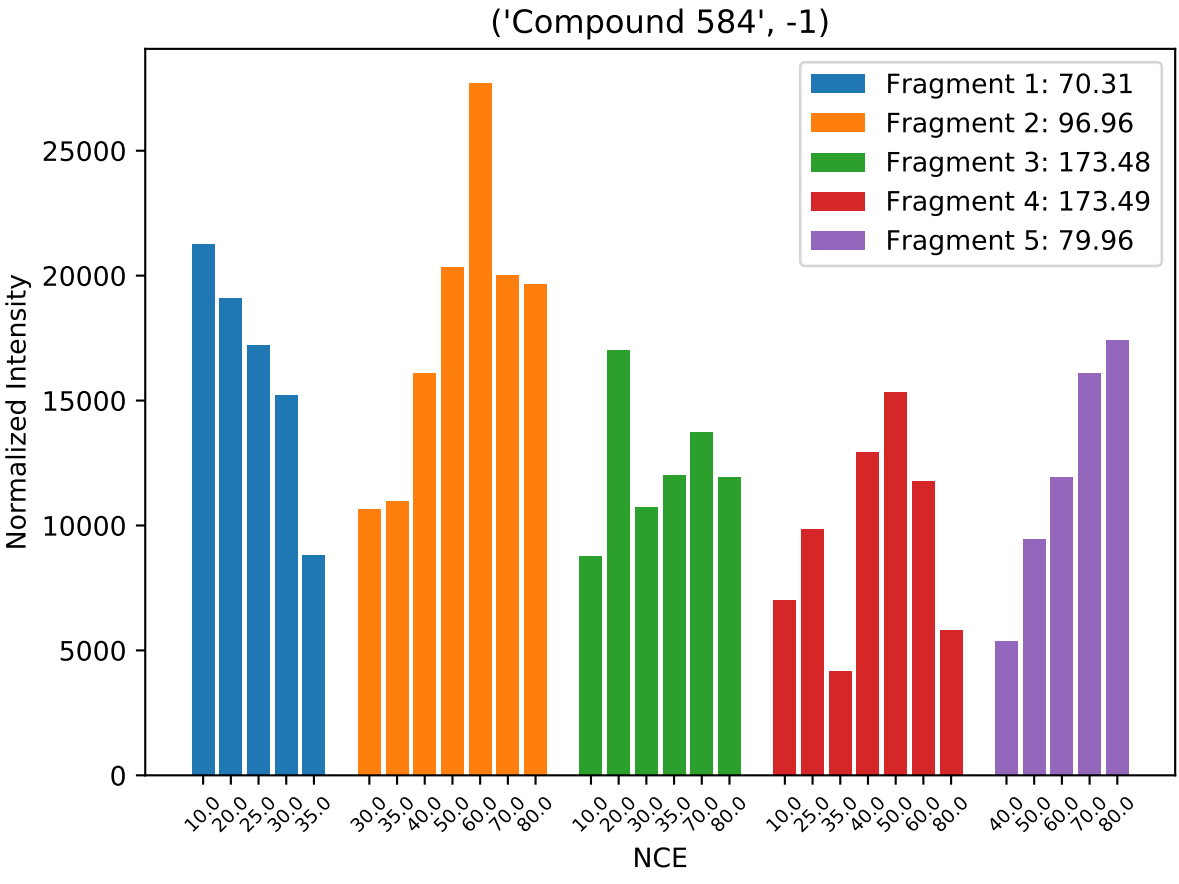

('Compound 249', 1)
Fragment 1: 473.26
Fragment 2: 87.04
Fragment 3: 133.09
Fragment 4: 89.06
Fragment 5: 103.04
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
NCE
10.0 20.0 25.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

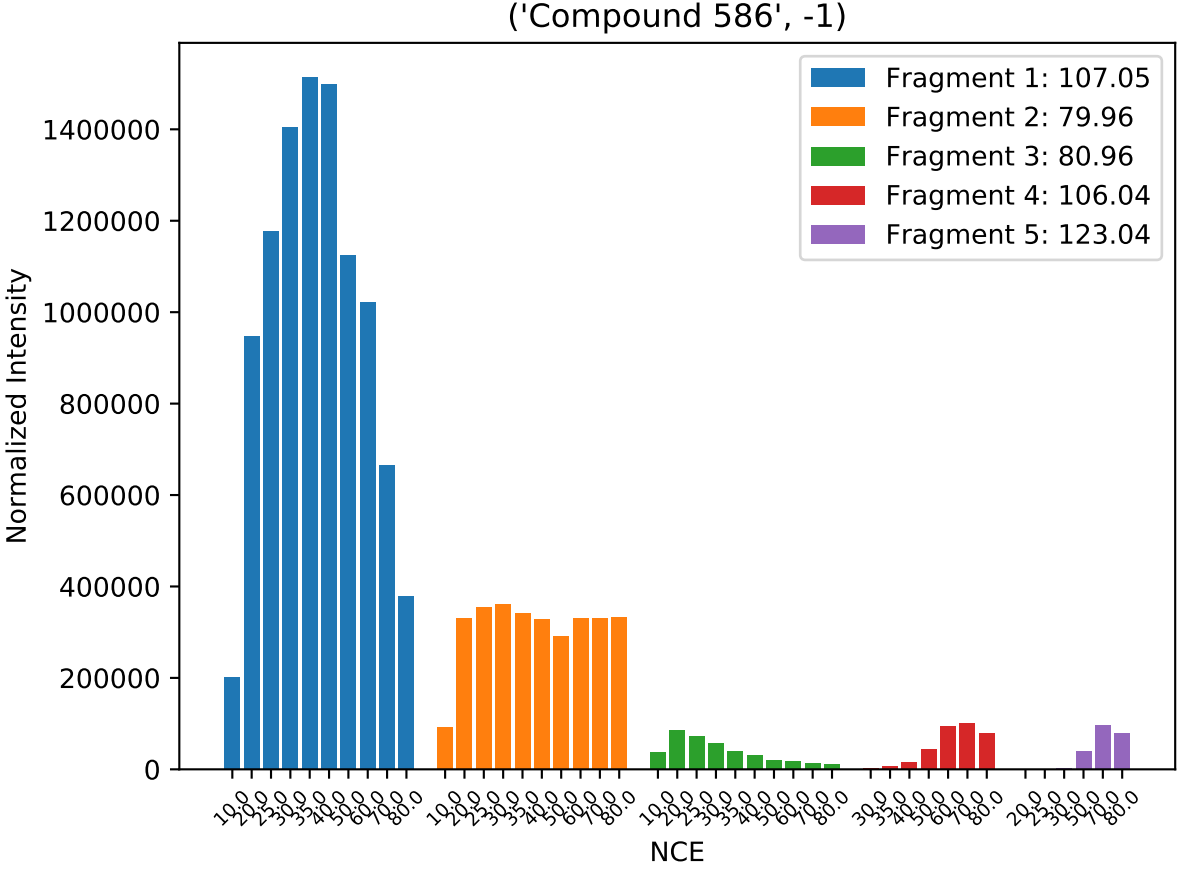

('Compound 468', 1)
Fragment 1: 173.47
Fragment 2: 81.72
Fragment 3: 97.95
Fragment 4: 100.24
Fragment 5: 163.96
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
25.0
35.0
50.0
70.0
80.0
10.0
10.0
10.0
10.0
NCE

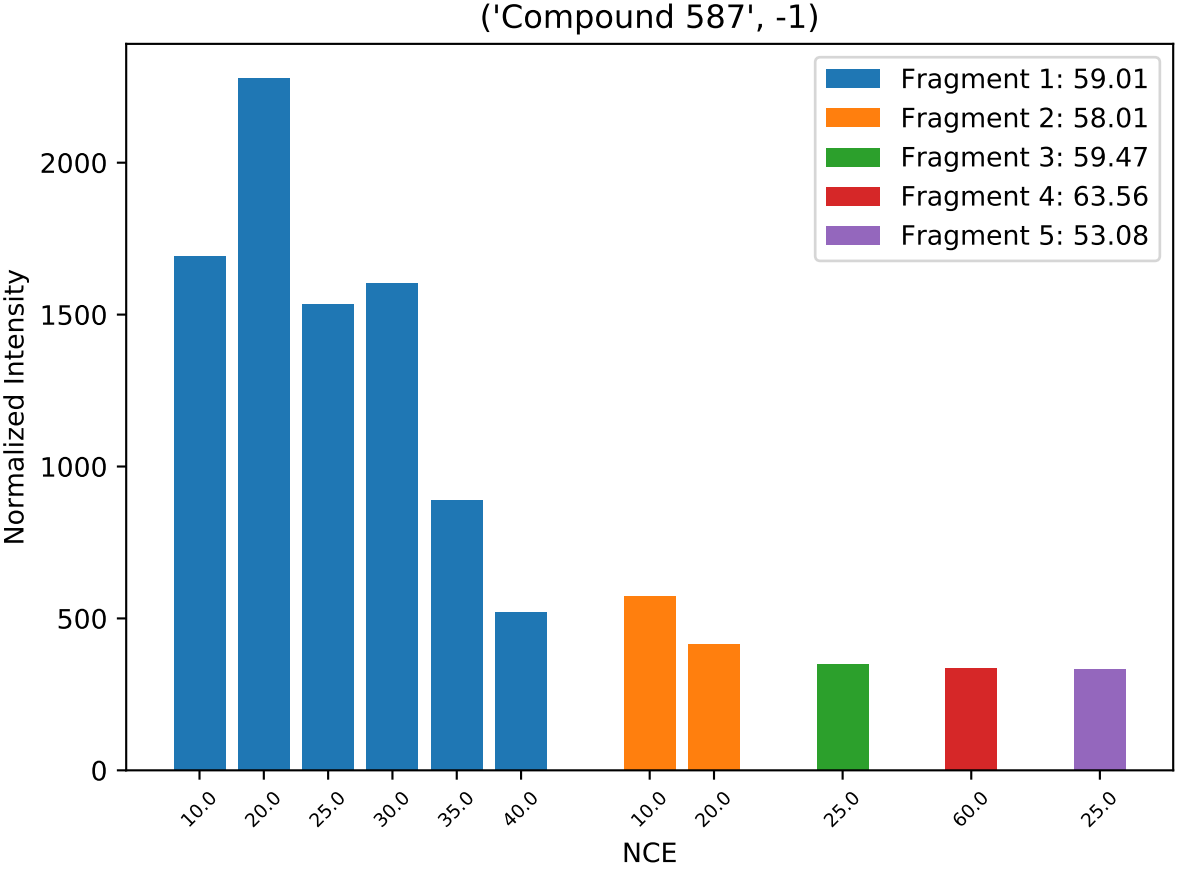

('Compound 126', 1)
Fragment 1: 159.07
Fragment 2: 106.07
Fragment 3: 180.14
Fragment 4: 218.19
Fragment 5: 162.13
Normalized Intensity
0
100000
200000
300000
400000
500000
10.0
20.0
30.0
50.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

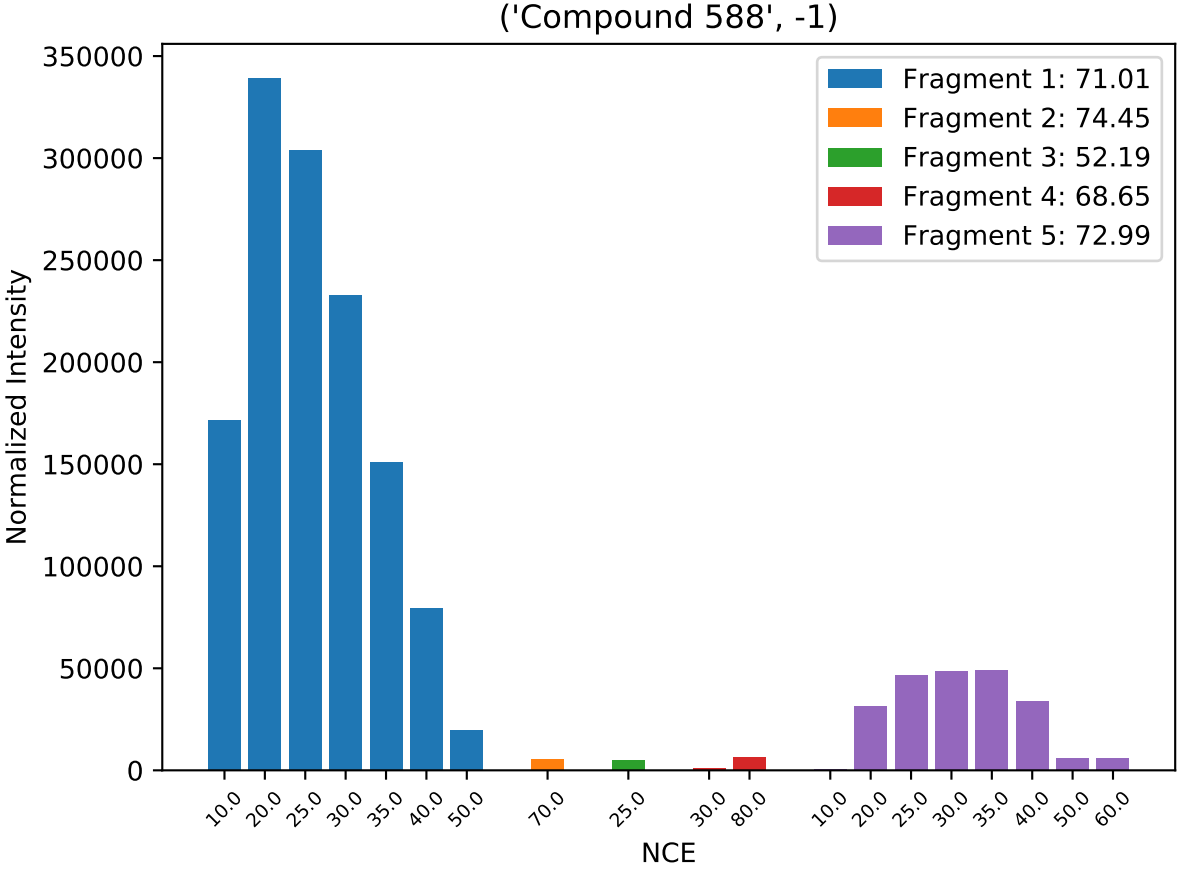

('Compound 575', 1)
Normalized Intensity
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Fragment 1: 81.8
Fragment 2: 85.85
Fragment 3: 93.58
Fragment 4: 102.22
Fragment 5: 110.85
10.0
10.0
10.0
10.0
10.0
NCE

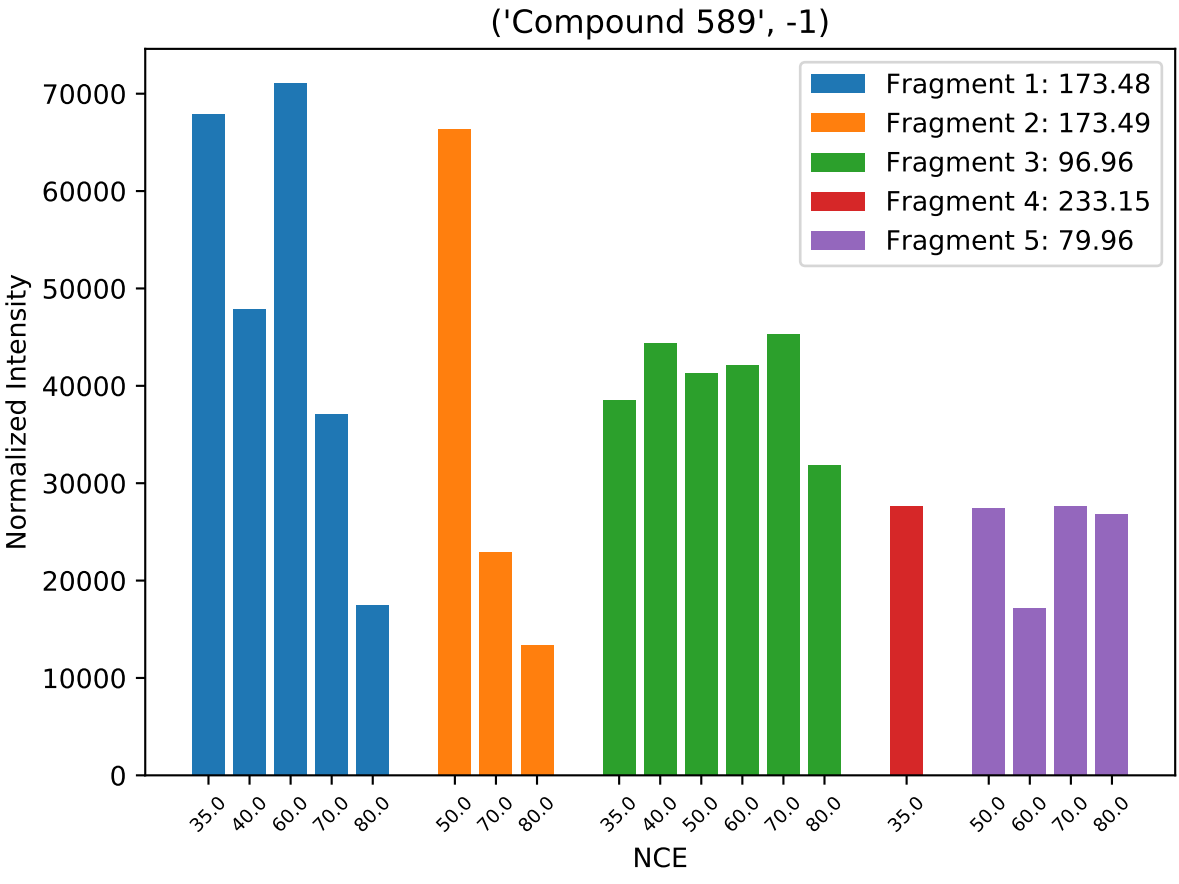

('Compound 582', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 265.25
Fragment 4: 70.82
Fragment 5: 70.81
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
25.0
30.0
35.0
40.0
80.0
10.0
20.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
20.0
25.0
30.0
NCE

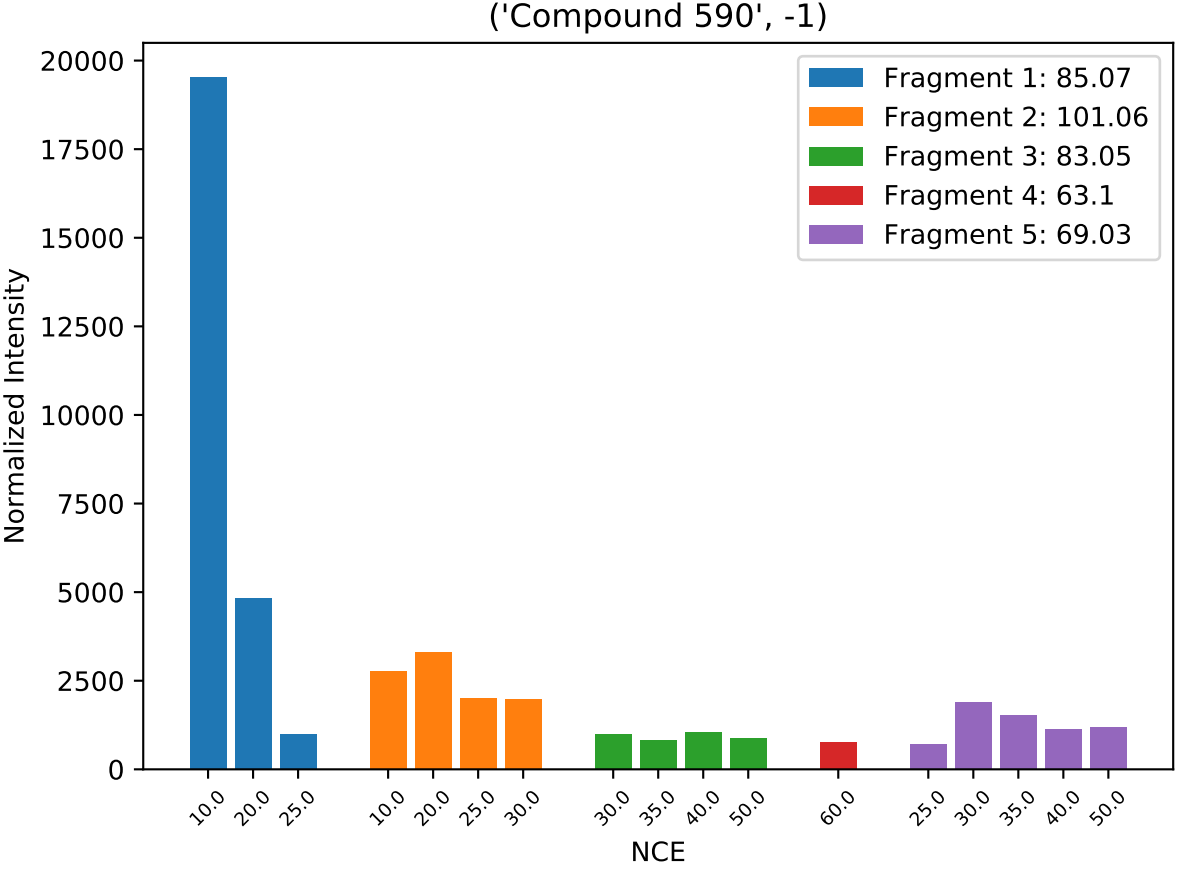

('Compound 584', -1)
Fragment 1: 70.31
Fragment 2: 96.96
Fragment 3: 173.48
Fragment 4: 173.49
Fragment 5: 79.96
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0 20.0 25.0 30.0 35.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 30.0 35.0 70.0 80.0
10.0 25.0 35.0 40.0 50.0 60.0 80.0
40.0 50.0 60.0 70.0 80.0
NCE

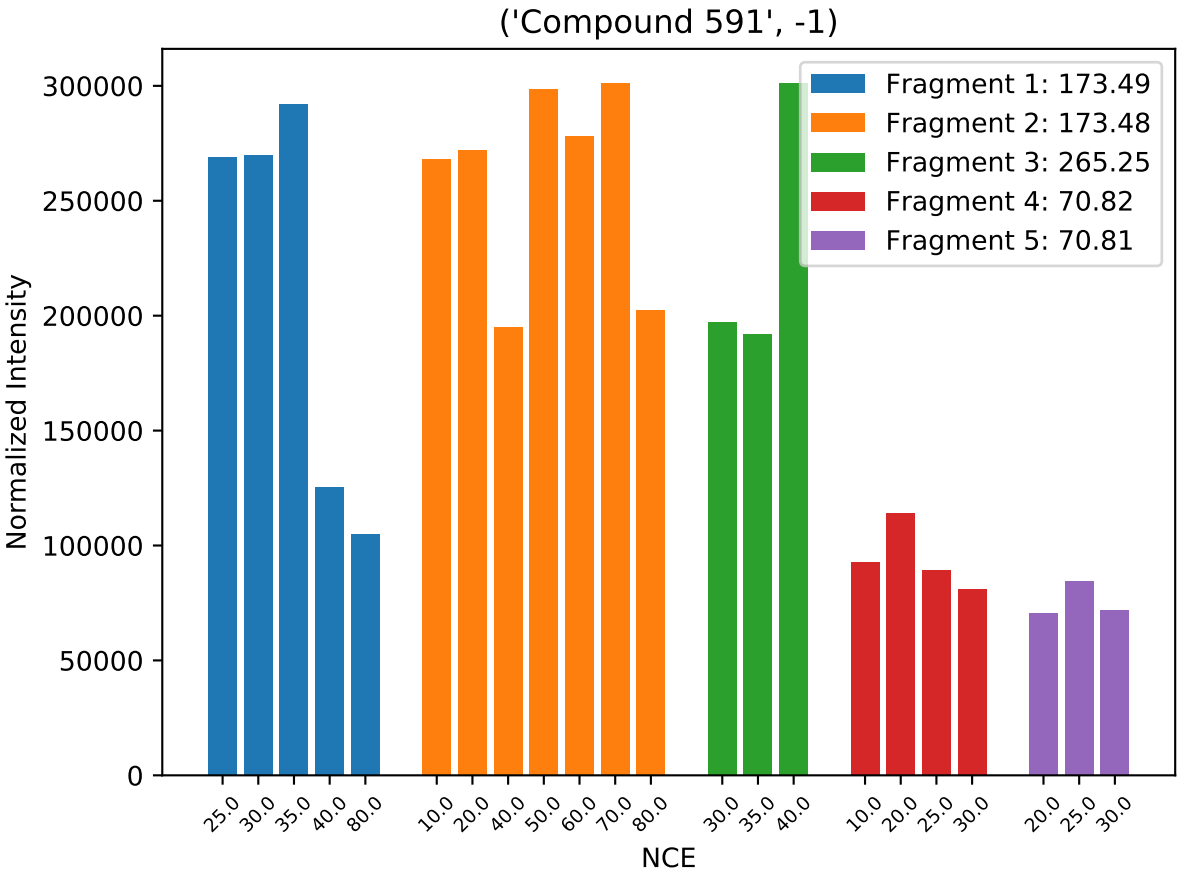

('Compound 586', -1)
Fragment 1: 107.05
Fragment 2: 79.96
Fragment 3: 80.96
Fragment 4: 106.04
Fragment 5: 123.04
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
1400000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 50.0 70.0 80.0

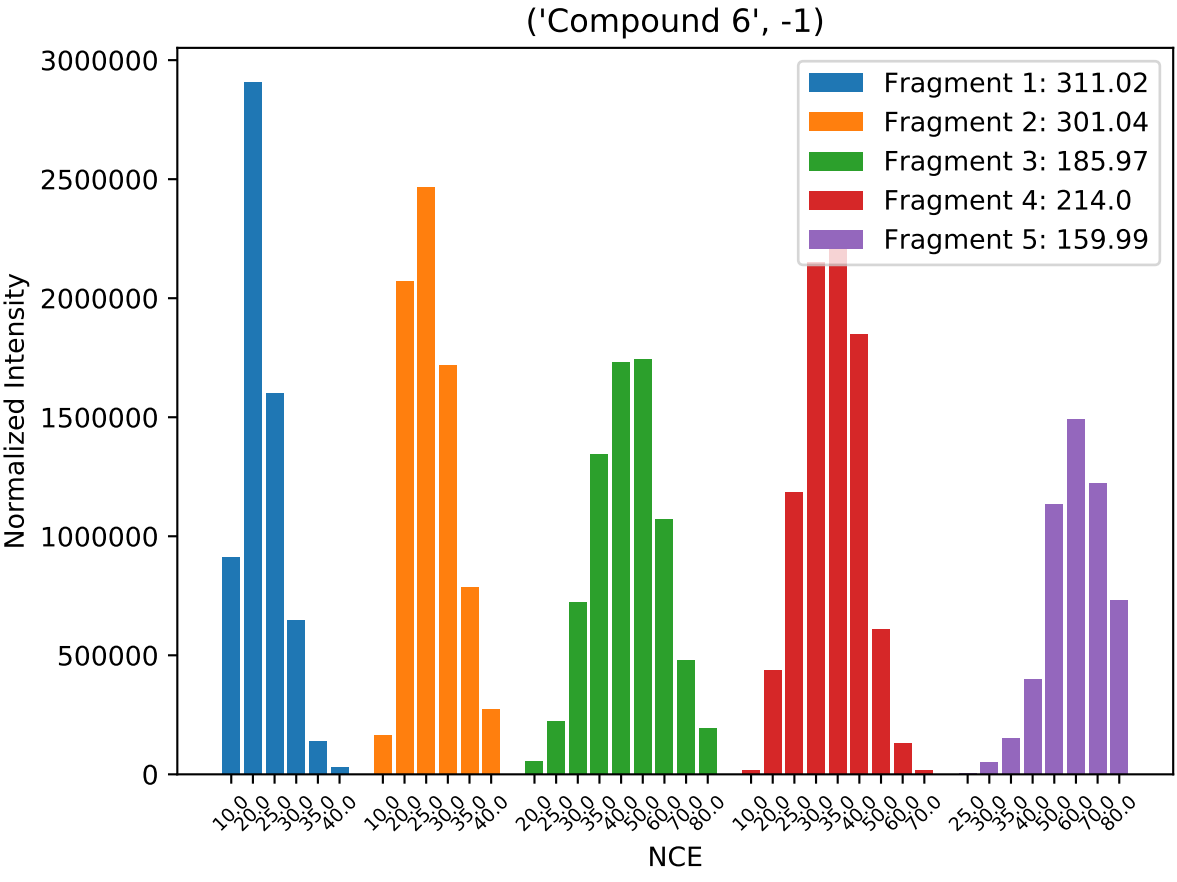

('Compound 587', -1)
Fragment 1: 59.01
Fragment 2: 58.01
Fragment 3: 59.47
Fragment 4: 63.56
Fragment 5: 53.08
Normalized Intensity
0
500
1000
1500
2000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
60.0
25.0
NCE

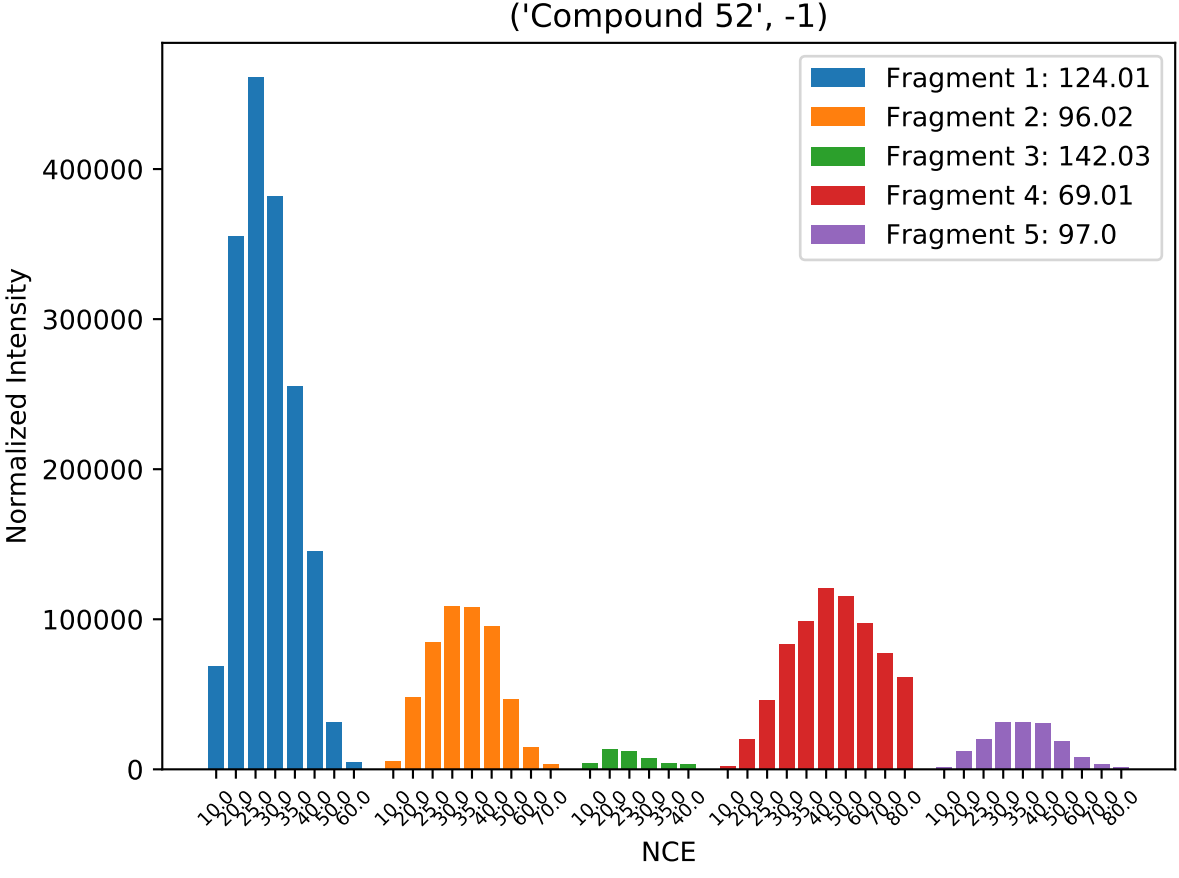

('Compound 588', -1)
Fragment 1: 71.01
Fragment 2: 74.45
Fragment 3: 52.19
Fragment 4: 68.65
Fragment 5: 72.99
Normalized Intensity
350000
300000
250000
200000
150000
100000
50000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
70.0
25.0
30.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

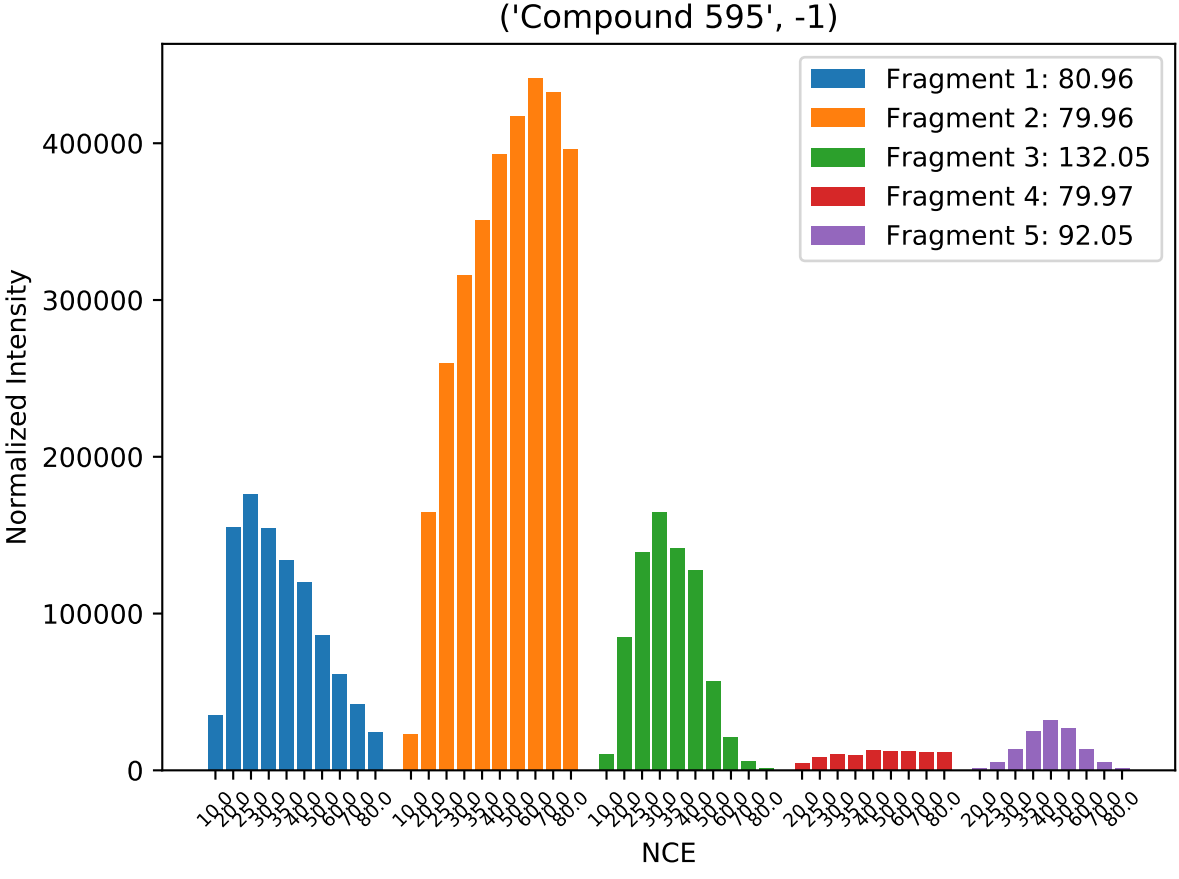

('Compound 589', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 96.96
Fragment 4: 233.15
Fragment 5: 79.96
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
35.0
40.0
60.0
70.0
80.0
50.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
35.0
50.0
60.0
70.0
80.0
NCE

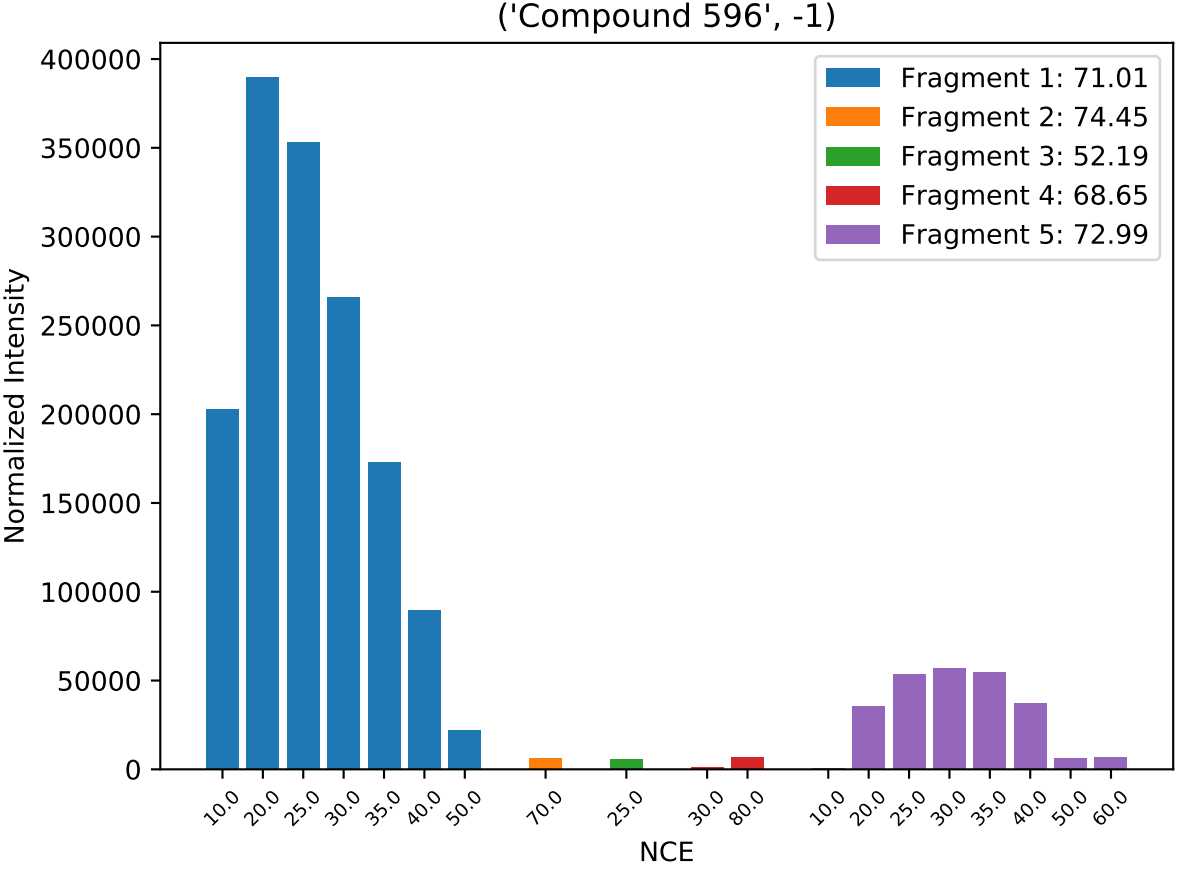

('Compound 590', -1)
Fragment 1: 85.07
Fragment 2: 101.06
Fragment 3: 83.05
Fragment 4: 63.1
Fragment 5: 69.03
Normalized Intensity
20000
17500
15000
12500
10000
7500
5000
2500
0
10.0
20.0
25.0
10.0
20.0
25.0
30.0
30.0
35.0
40.0
50.0
60.0
25.0
30.0
35.0
40.0
50.0
NCE

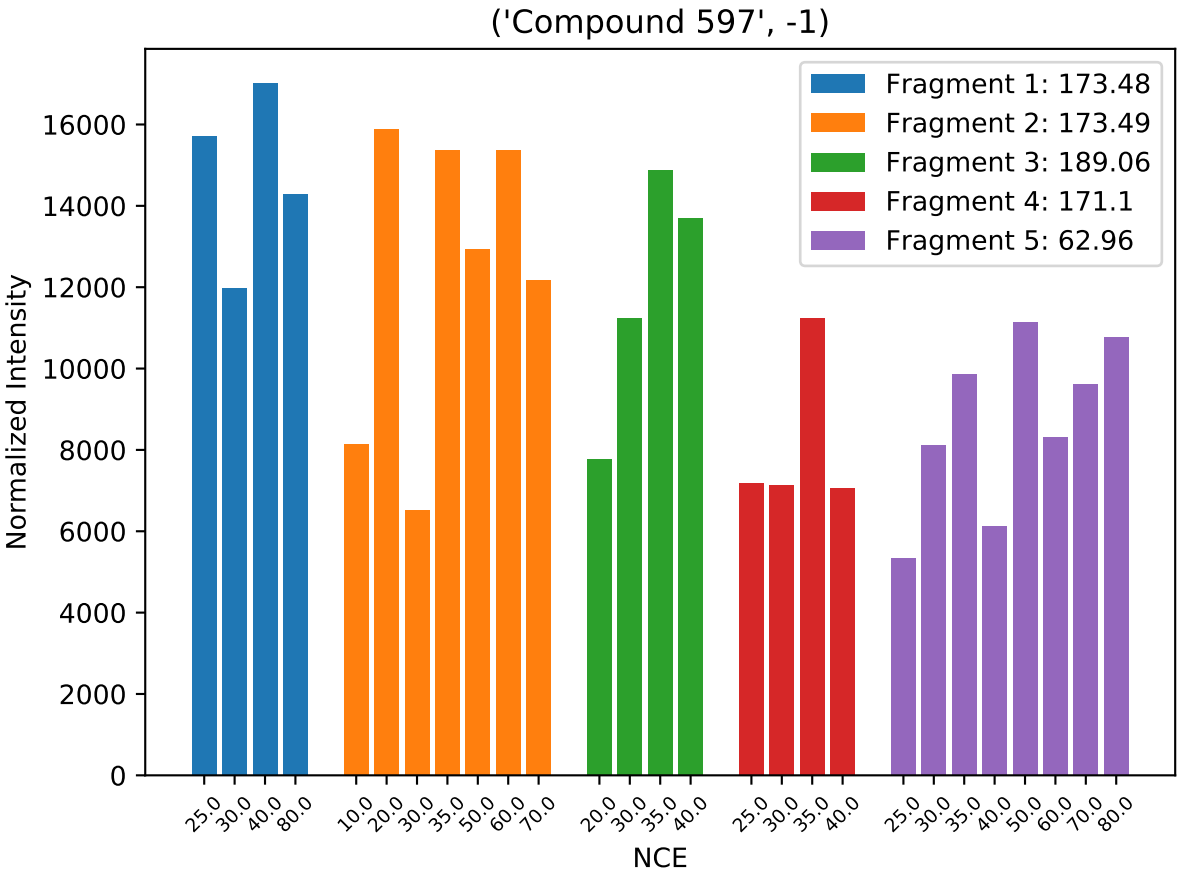

('Compound 591', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 265.25
Fragment 4: 70.82
Fragment 5: 70.81
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
25.0
30.0
35.0
40.0
80.0
10.0
20.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
20.0
25.0
30.0
NCE

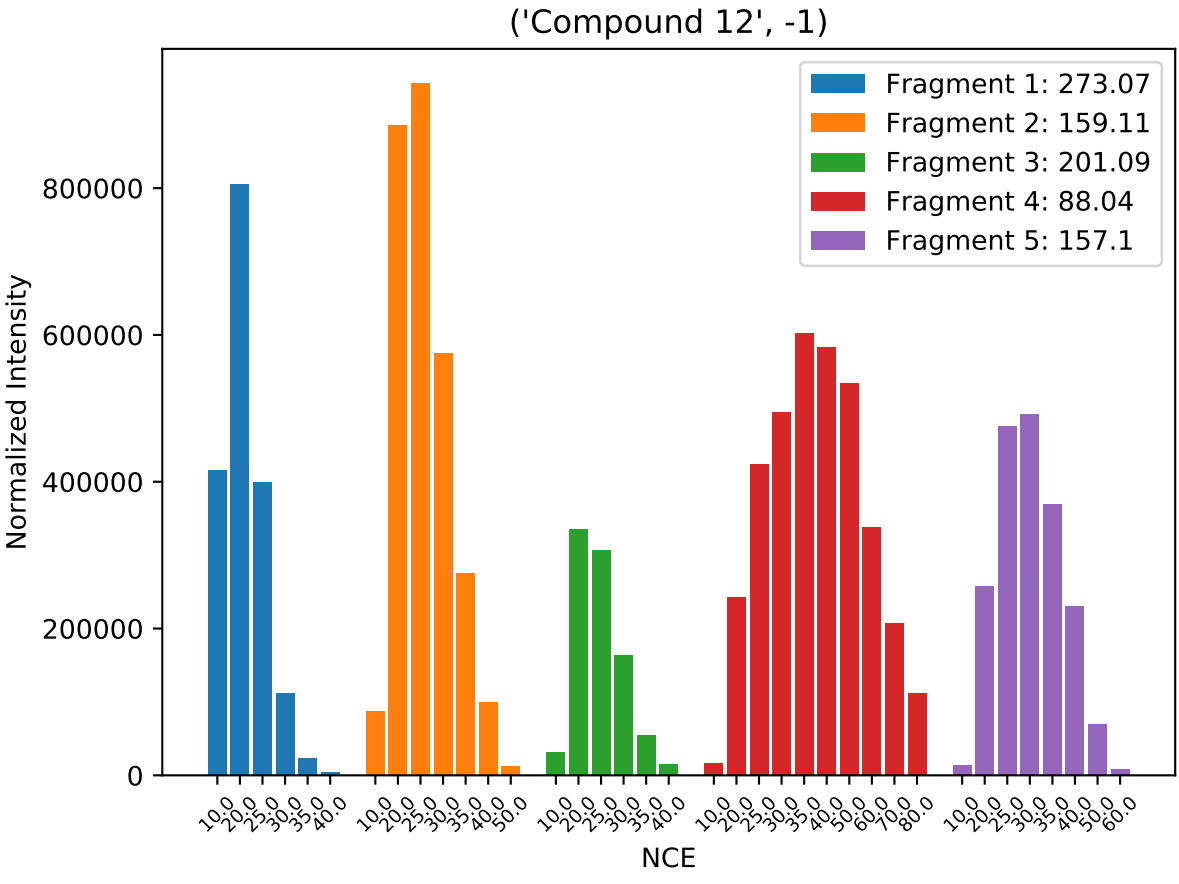

('Compound 6', -1)
Fragment 1: 311.02
Fragment 2: 301.04
Fragment 3: 185.97
Fragment 4: 214.0
Fragment 5: 159.99
Normalized Intensity
3000000
2500000
2000000
1500000
1000000
500000
0
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

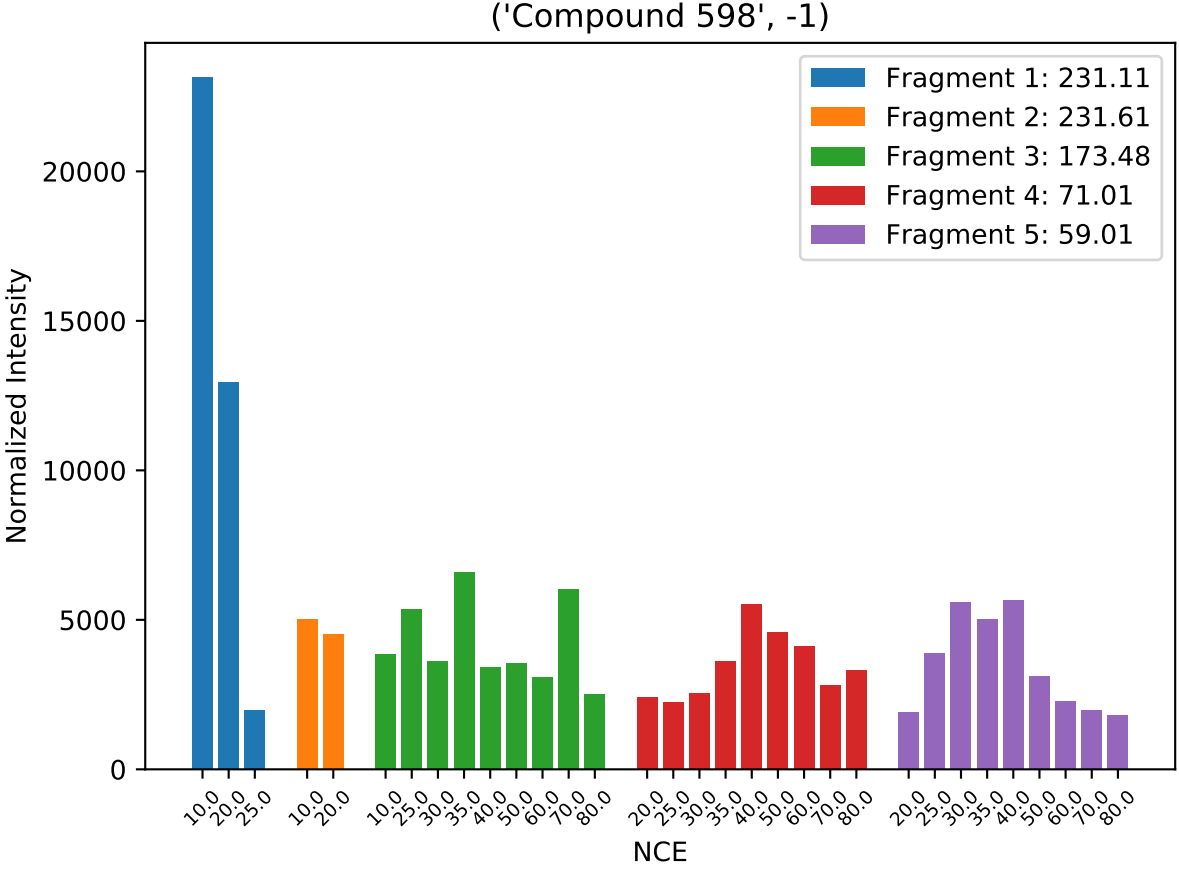

('Compound 52', -1)
Fragment 1: 124.01
Fragment 2: 96.02
Fragment 3: 142.03
Fragment 4: 69.01
Fragment 5: 97.0
Normalized Intensity
0
100000
200000
300000
400000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

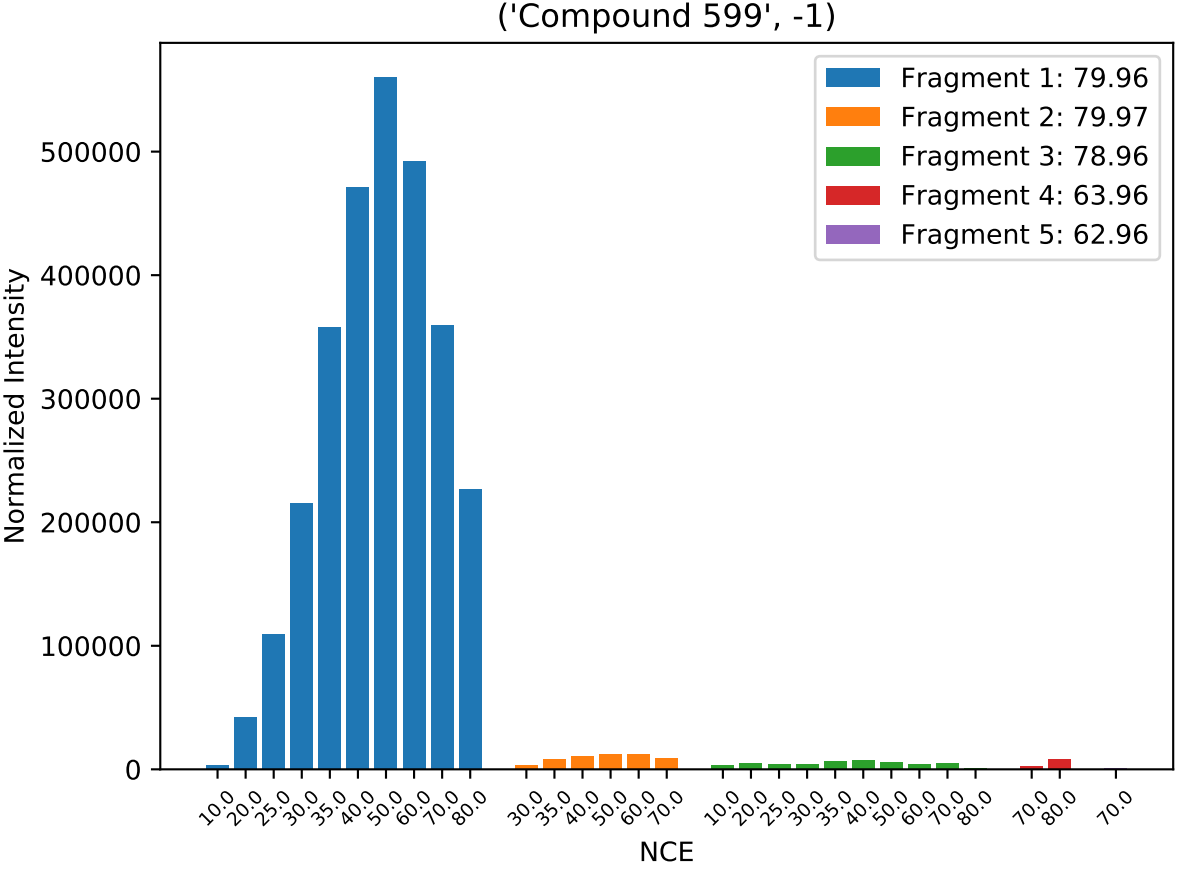

('Compound 595', -1)
Fragment 1: 80.96
Fragment 2: 79.96
Fragment 3: 132.05
Fragment 4: 79.97
Fragment 5: 92.05
Normalized Intensity
0
100000
200000
300000
400000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

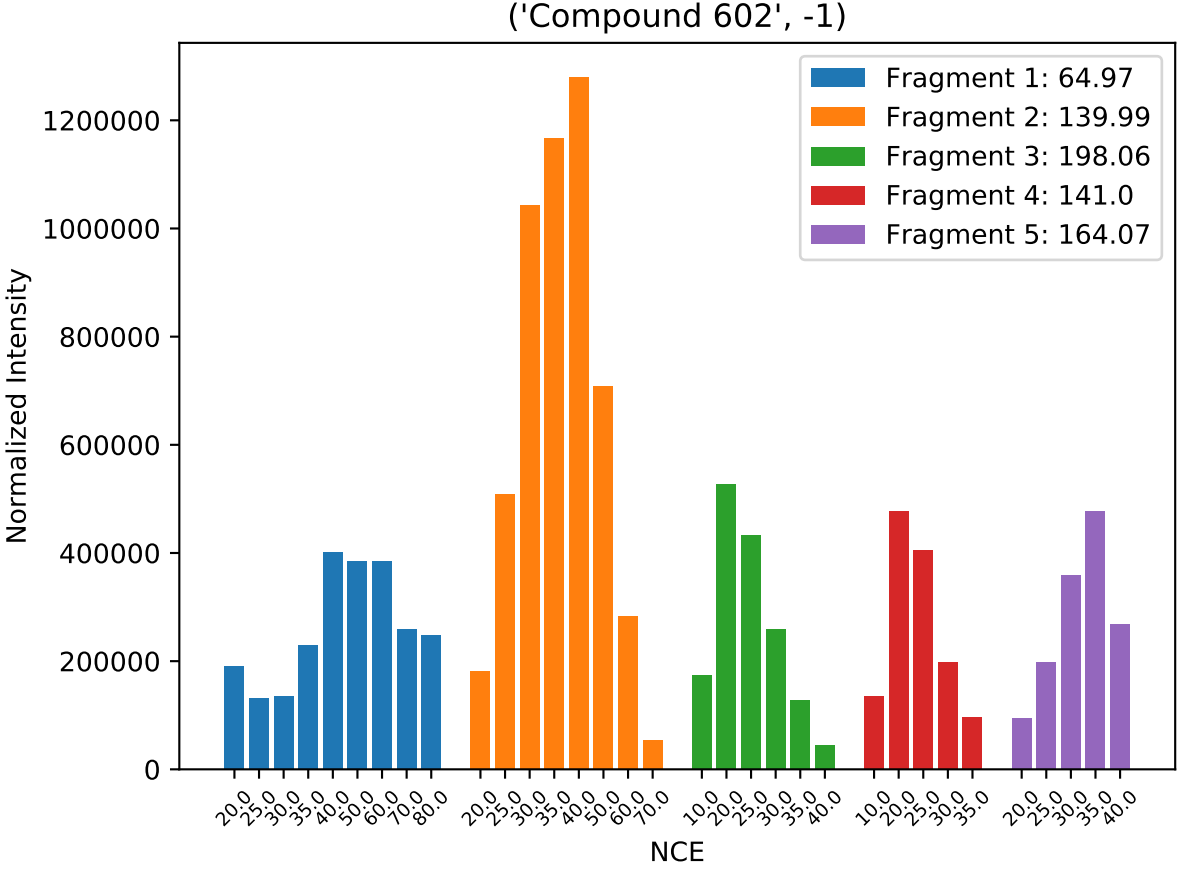

('Compound 596', -1)
Fragment 1: 71.01
Fragment 2: 74.45
Fragment 3: 52.19
Fragment 4: 68.65
Fragment 5: 72.99
Normalized Intensity
400000
350000
300000
250000
200000
150000
100000
50000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
70.0
25.0
30.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

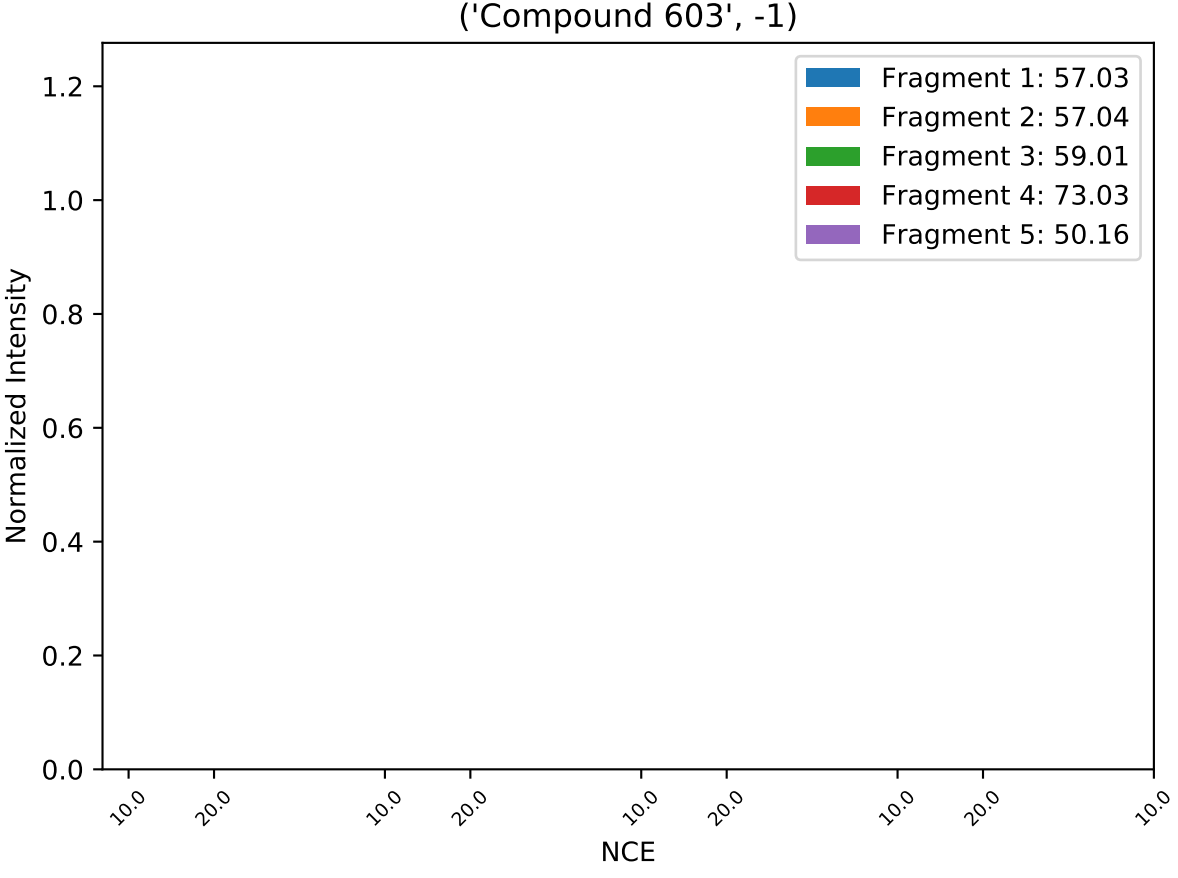

('Compound 597', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 189.06
Fragment 4: 171.1
Fragment 5: 62.96
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
25.0
30.0
40.0
80.0
10.0
20.0
30.0
35.0
50.0
60.0
70.0
20.0
30.0
35.0
40.0
25.0
30.0
35.0
40.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

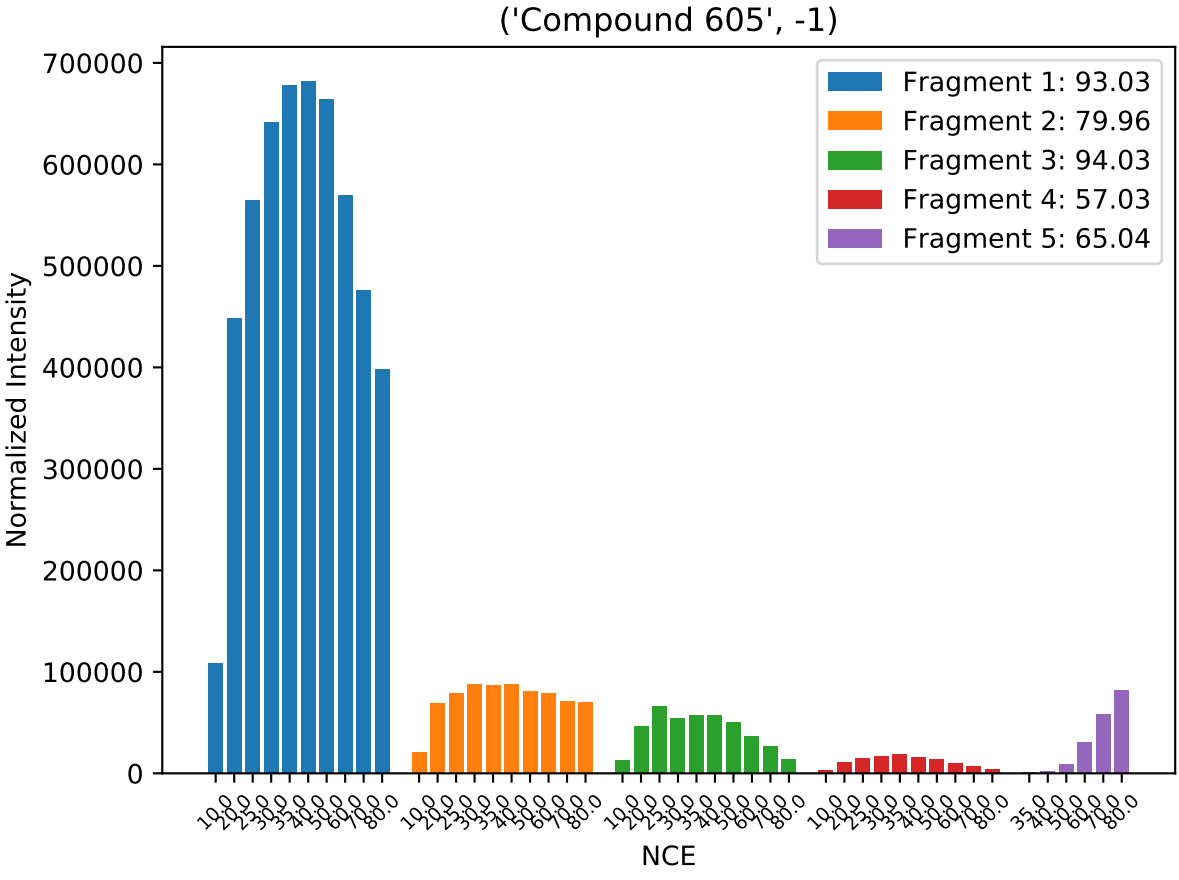

('Compound 12', -1)
Fragment 1: 273.07
Fragment 2: 159.11
Fragment 3: 201.09
Fragment 4: 88.04
Fragment 5: 157.1
Normalized Intensity
0
200000
400000
600000
800000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

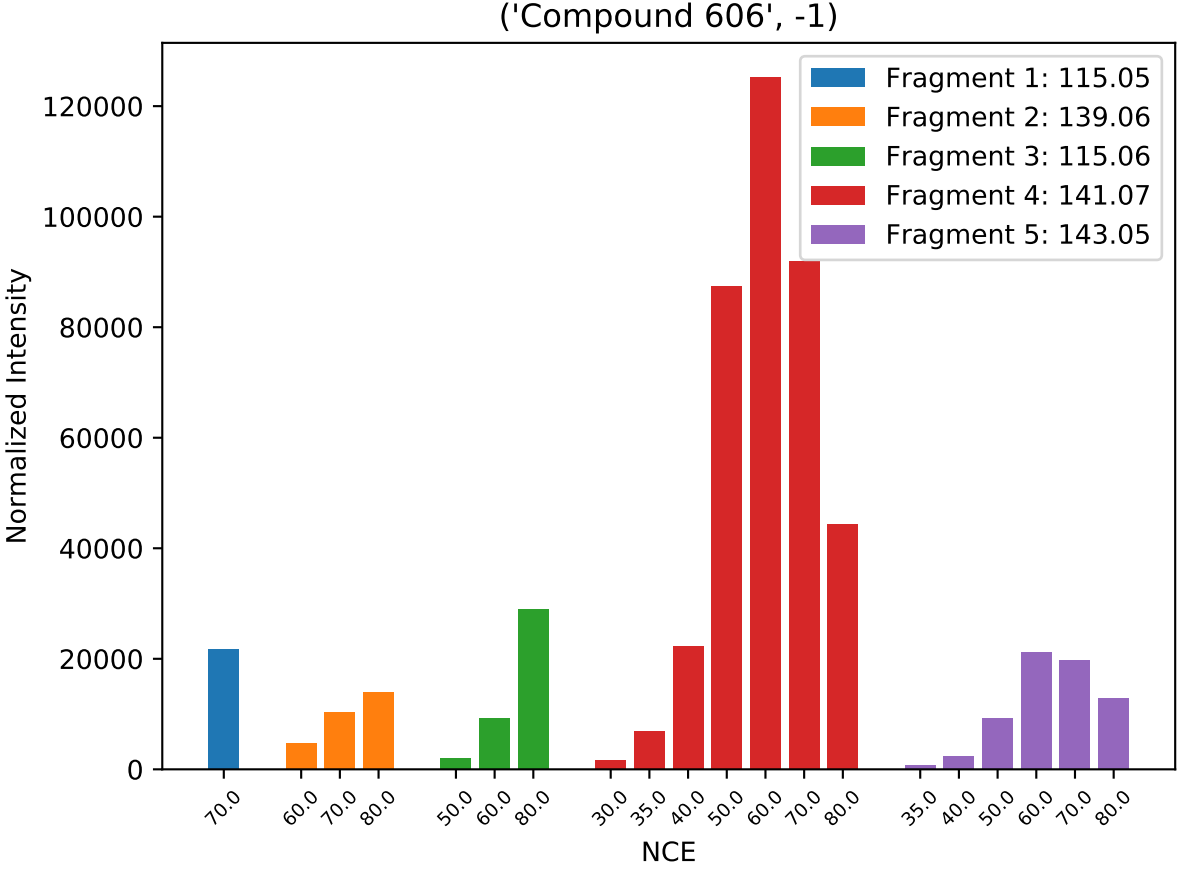

('Compound 598', -1)
Fragment 1: 231.11
Fragment 2: 231.61
Fragment 3: 173.48
Fragment 4: 71.01
Fragment 5: 59.01
Normalized Intensity
0
5000
10000
15000
20000
10.0
20.0
25.0
10.0
20.0
10.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

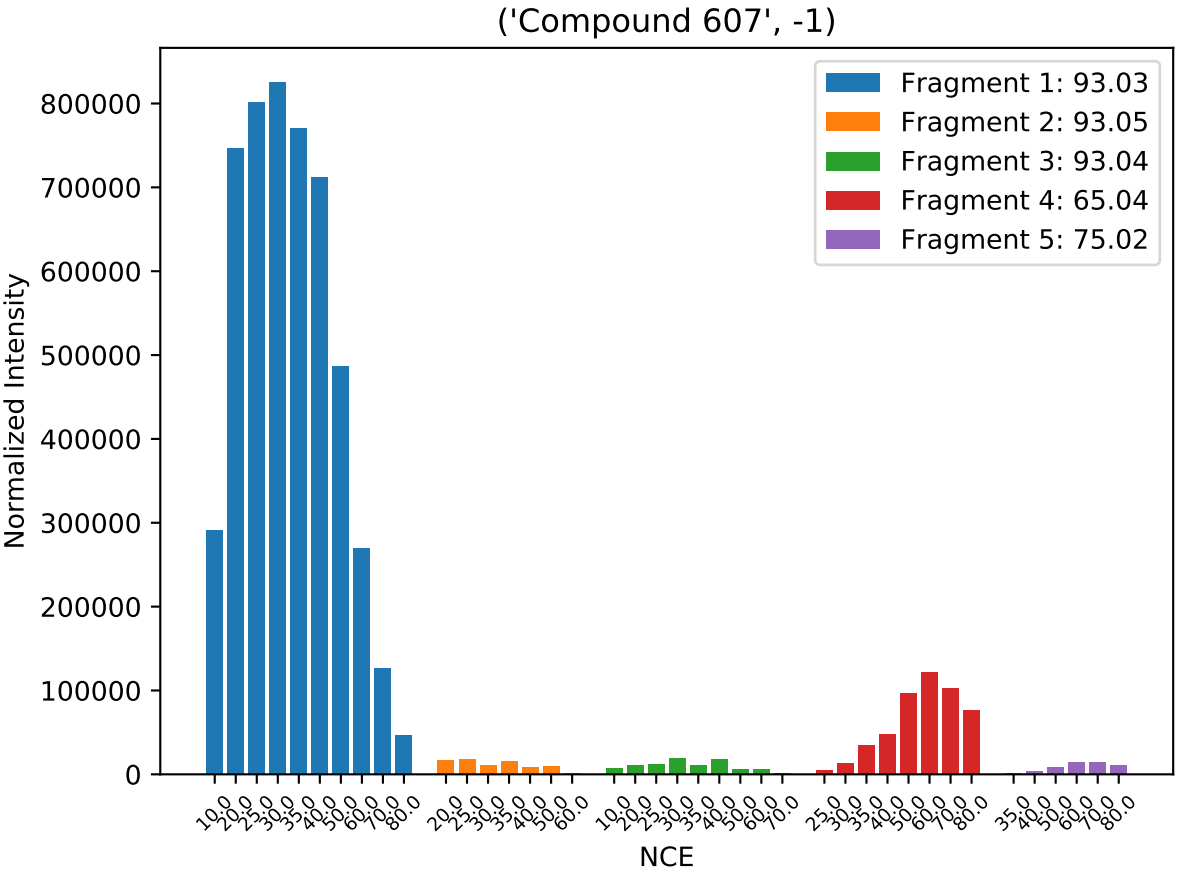

('Compound 599', -1)
Fragment 1: 79.96
Fragment 2: 79.97
Fragment 3: 78.96
Fragment 4: 63.96
Fragment 5: 62.96
Normalized Intensity
0
100000
200000
300000
400000
500000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
70.0
80.0
70.0
NCE

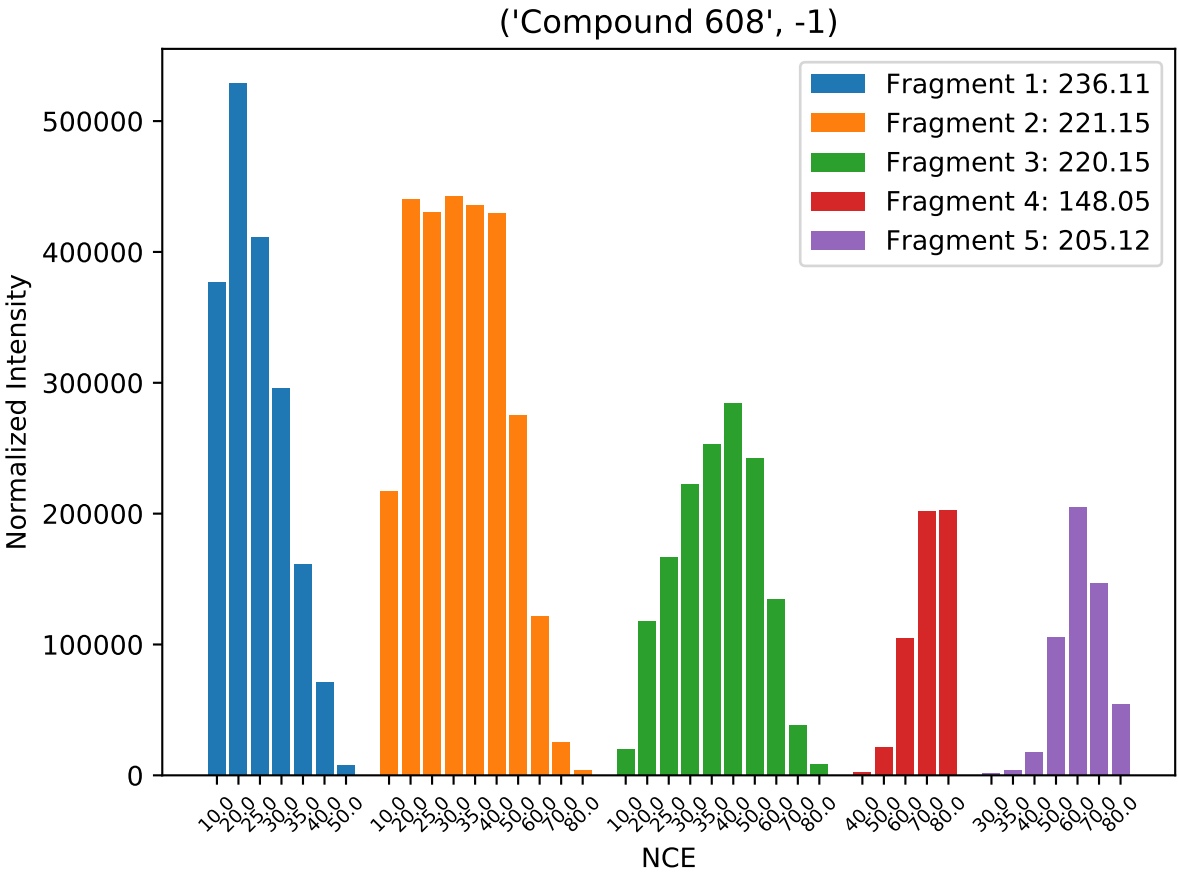

('Compound 602', -1)
Fragment 1: 64.97
Fragment 2: 139.99
Fragment 3: 198.06
Fragment 4: 141.0
Fragment 5: 164.07
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0

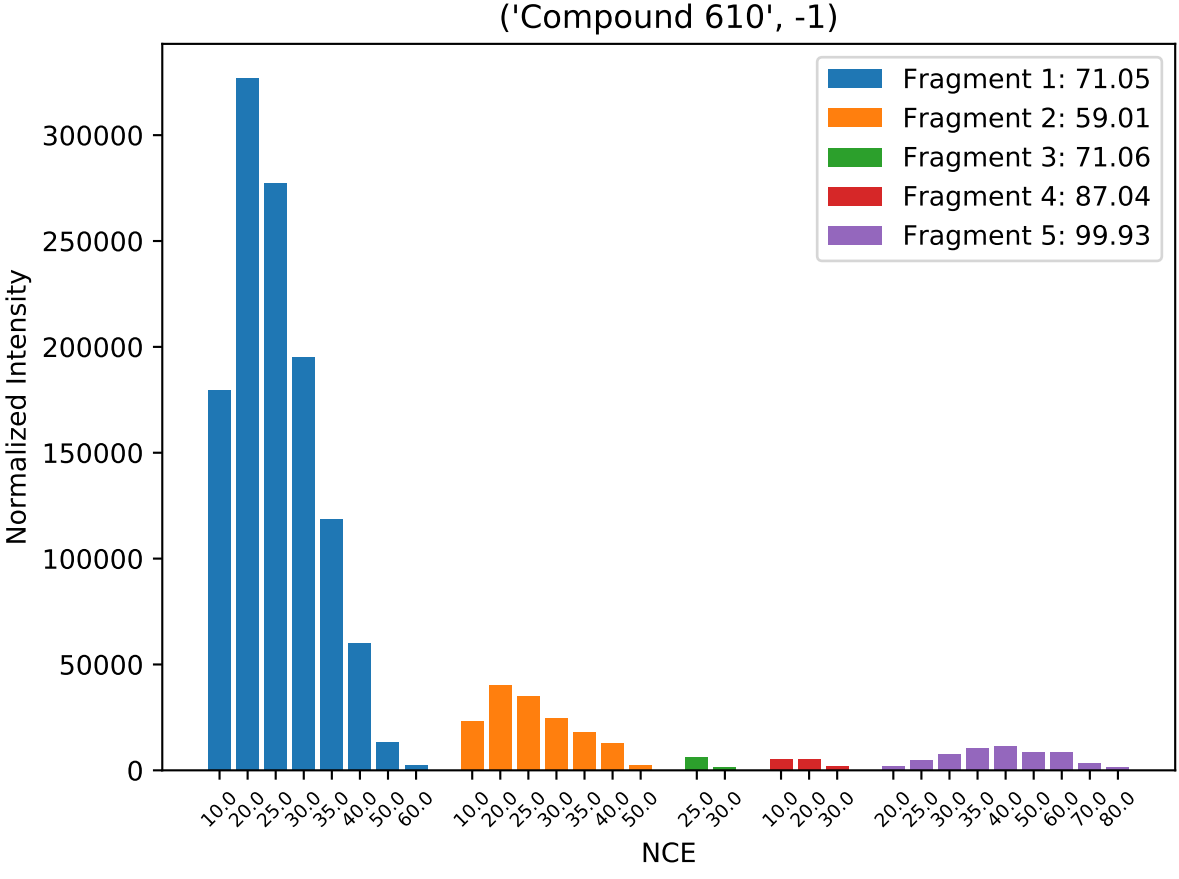

('Compound 603', -1)
Fragment 1: 57.03
Fragment 2: 57.04
Fragment 3: 59.01
Fragment 4: 73.03
Fragment 5: 50.16
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
10.0
20.0
10.0
20.0
10.0
20.0
10.0
NCE

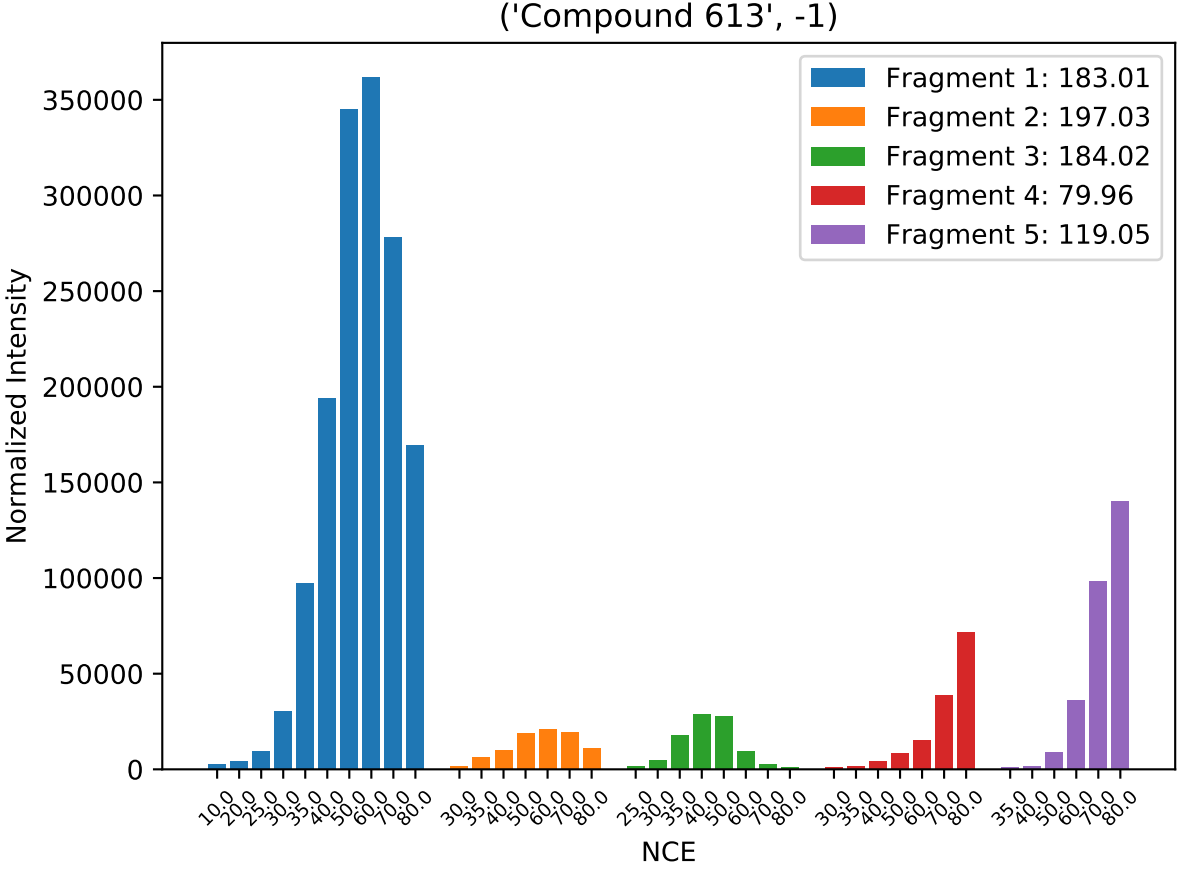

('Compound 605', -1)
Fragment 1: 93.03
Fragment 2: 79.96
Fragment 3: 94.03
Fragment 4: 57.03
Fragment 5: 65.04
Normalized Intensity
700000
600000
500000
400000
300000
200000
100000
0
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

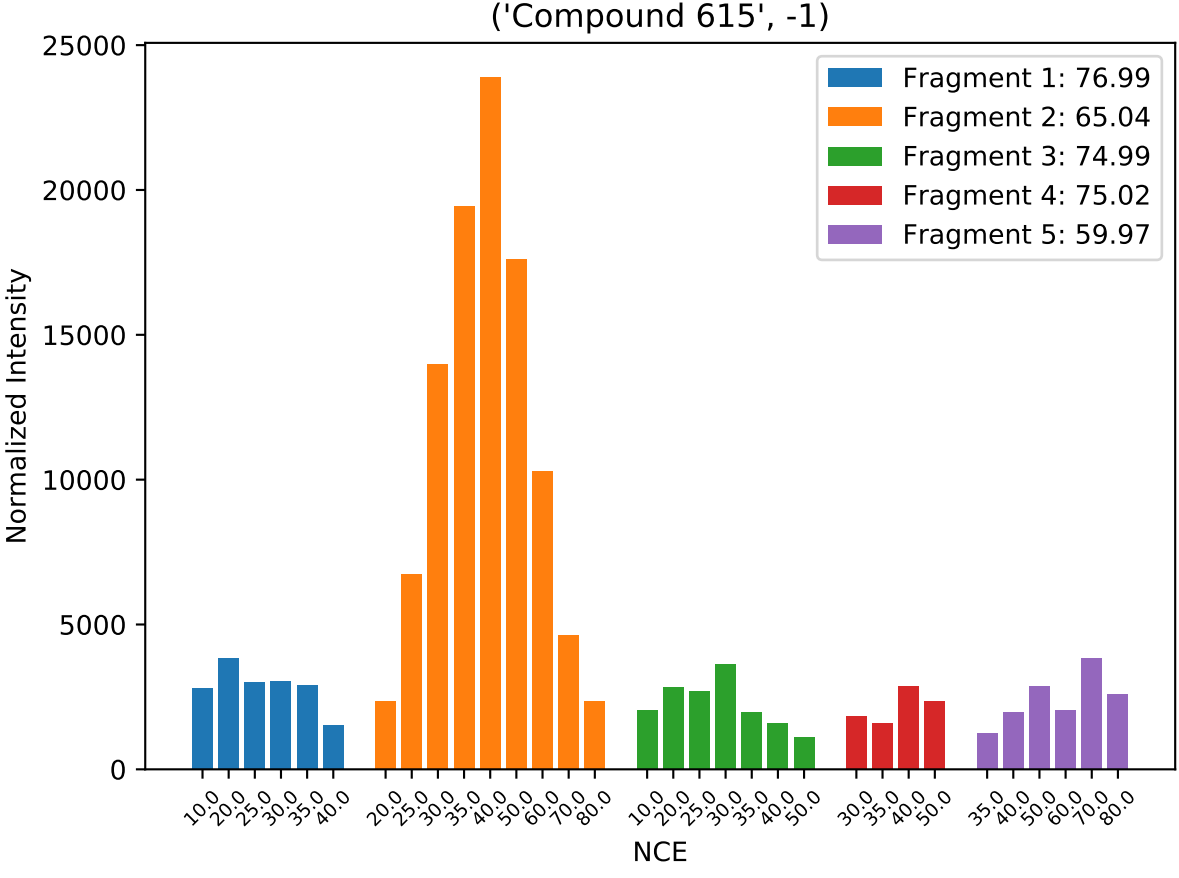

('Compound 606', -1)
Fragment 1: 115.05
Fragment 2: 139.06
Fragment 3: 115.06
Fragment 4: 141.07
Fragment 5: 143.05
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
70.0
60.0
70.0
80.0
50.0
60.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

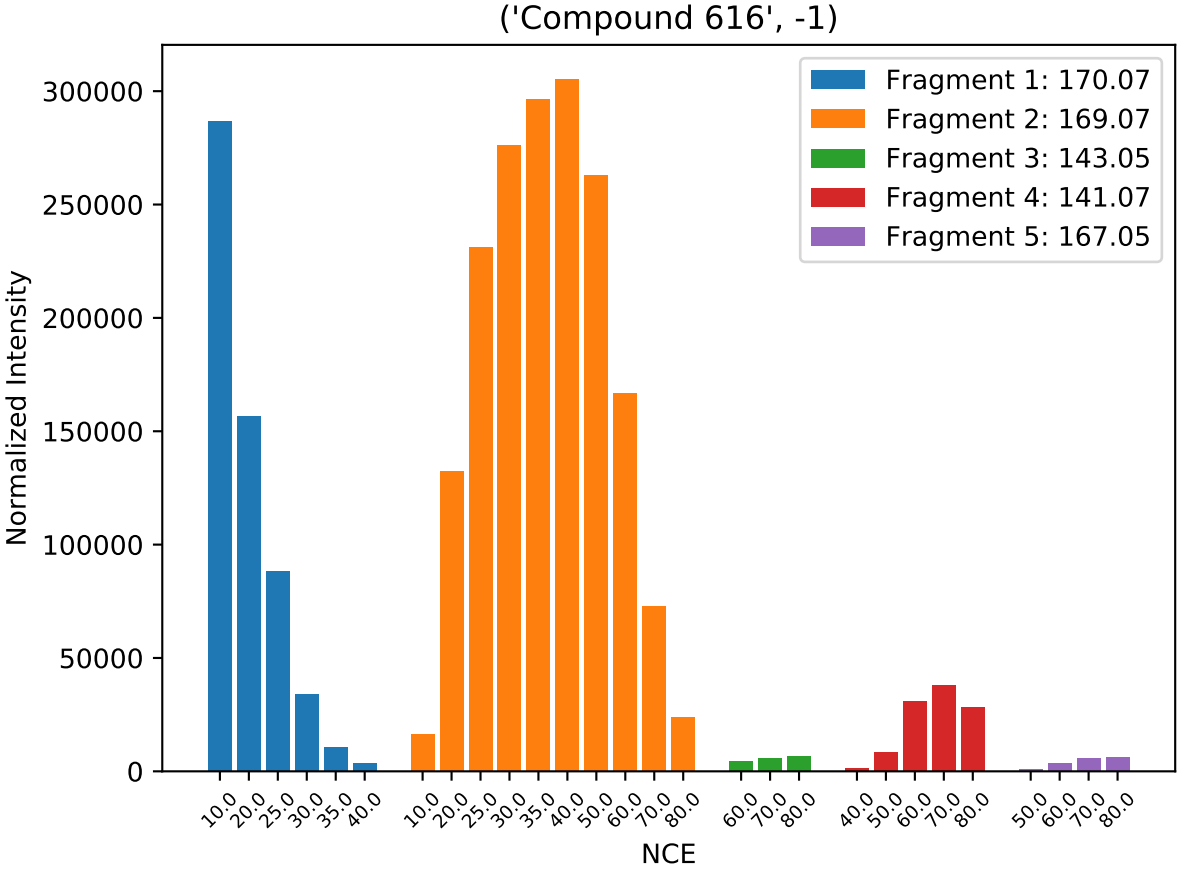

('Compound 607', -1)
Fragment 1: 93.03
Fragment 2: 93.05
Fragment 3: 93.04
Fragment 4: 65.04
Fragment 5: 75.02
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
700000
800000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

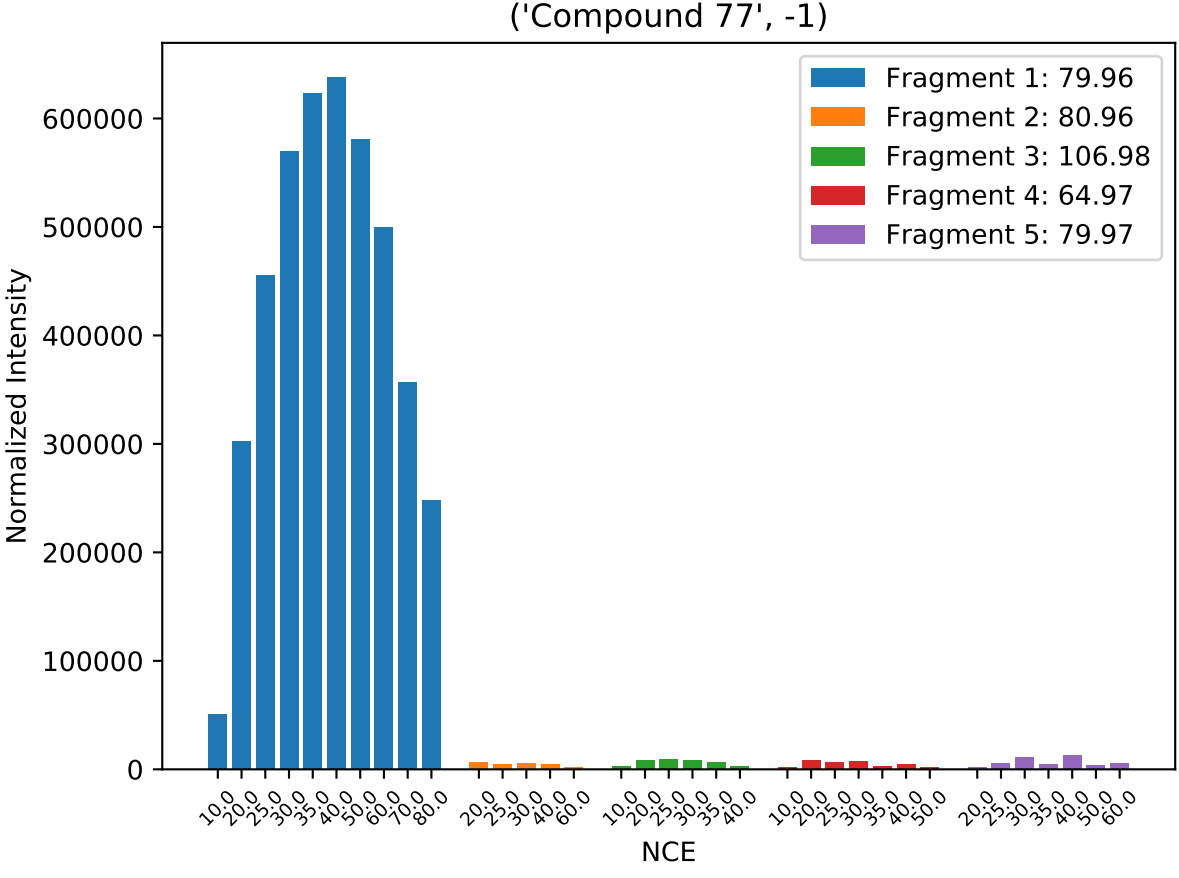

('Compound 608', -1)
Fragment 1: 236.11
Fragment 2: 221.15
Fragment 3: 220.15
Fragment 4: 148.05
Fragment 5: 205.12
Normalized Intensity
0
100000
200000
300000
400000
500000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

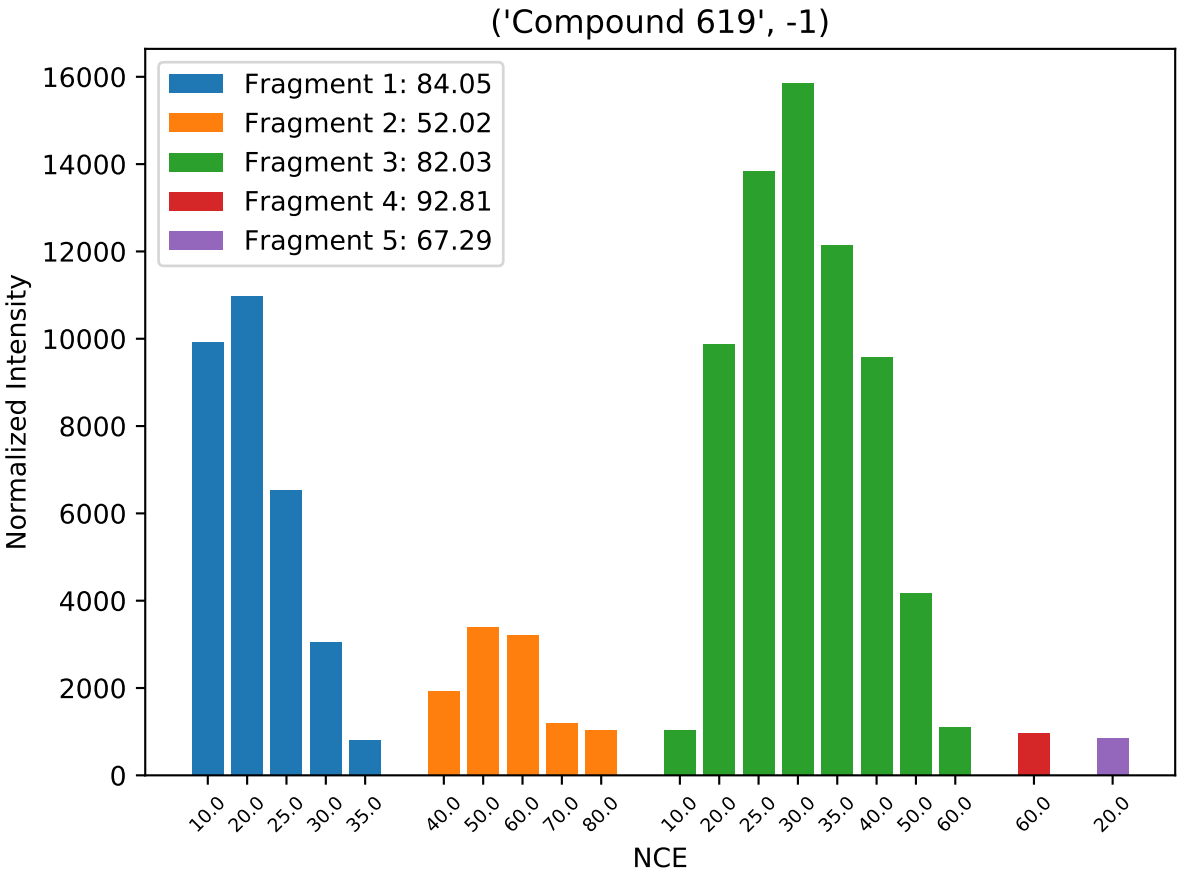

('Compound 610', -1)
Fragment 1: 71.05
Fragment 2: 59.01
Fragment 3: 71.06
Fragment 4: 87.04
Fragment 5: 99.93
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
25.0
30.0
10.0
20.0
30.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

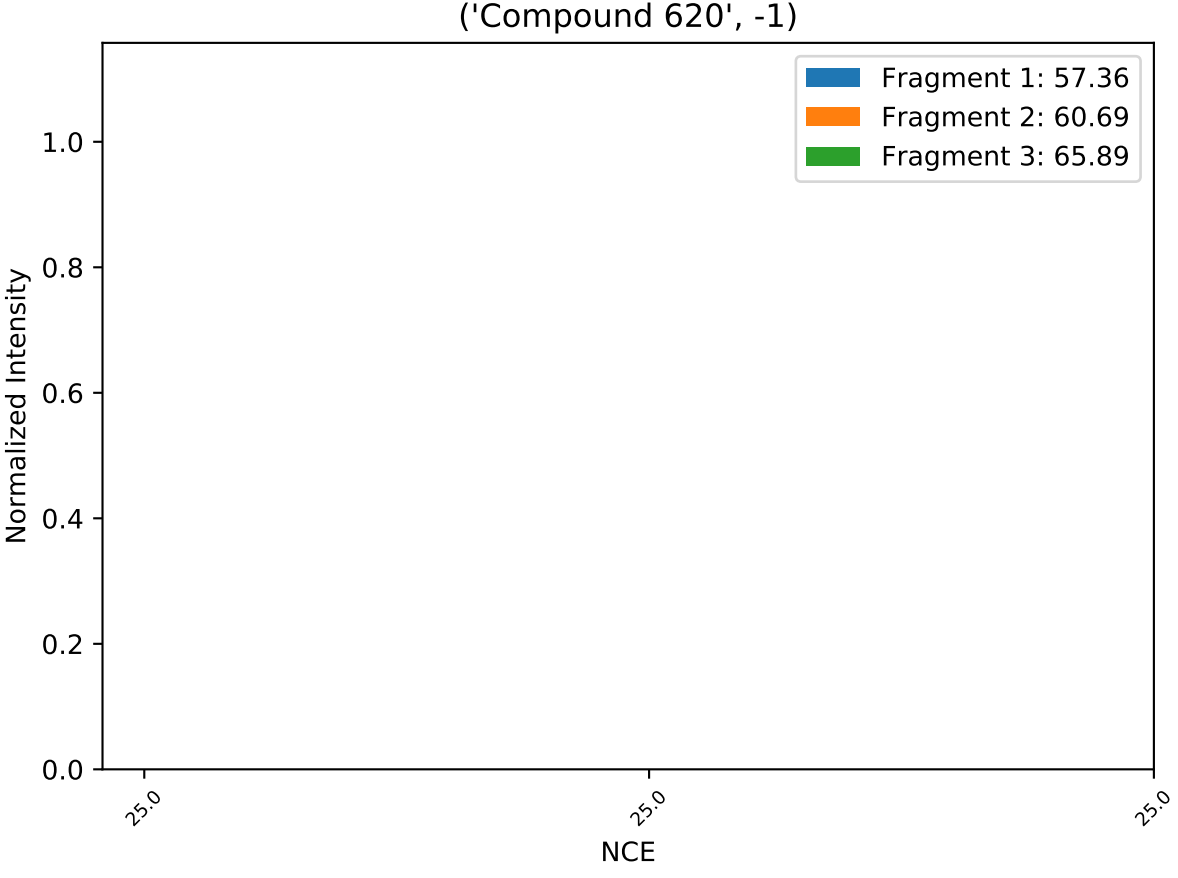

('Compound 613', -1)
Fragment 1: 183.01
Fragment 2: 197.03
Fragment 3: 184.02
Fragment 4: 79.96
Fragment 5: 119.05
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

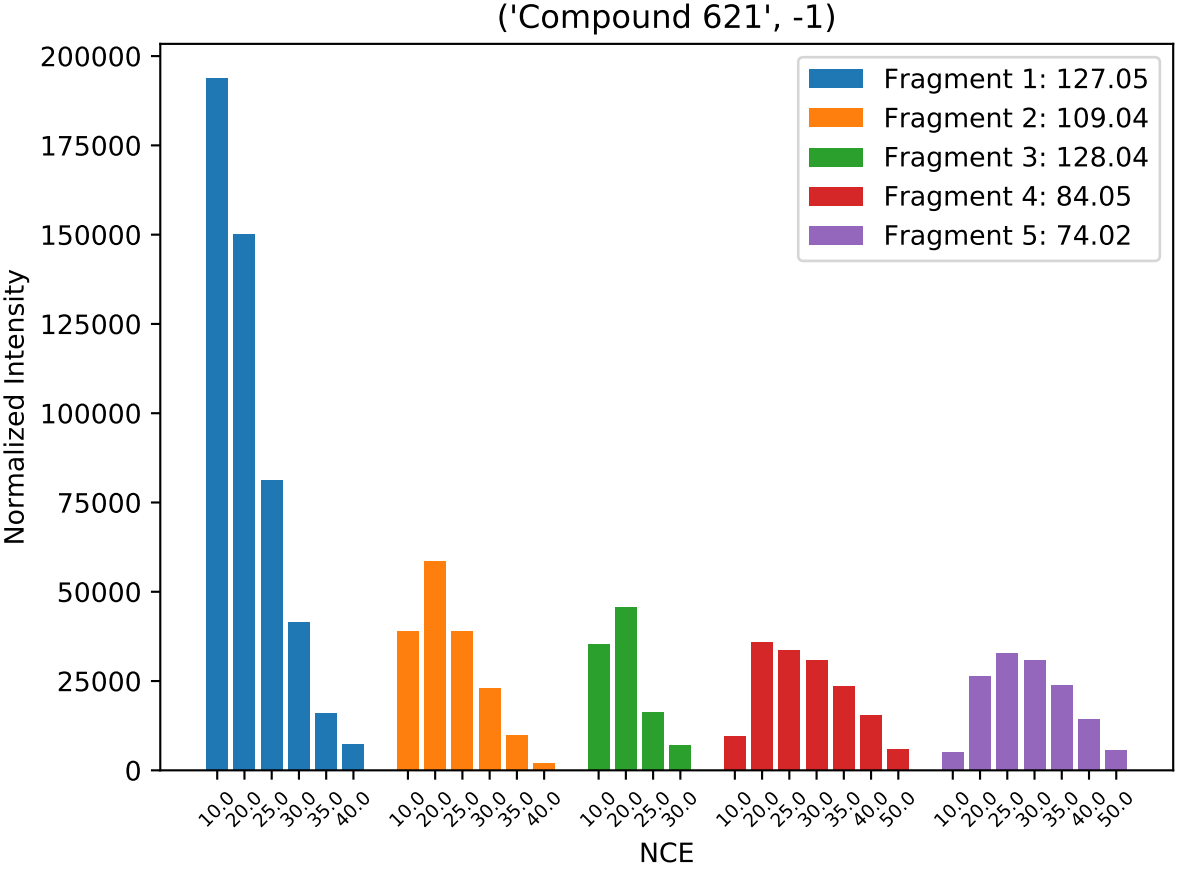

('Compound 615', -1)
Fragment 1: 76.99
Fragment 2: 65.04
Fragment 3: 74.99
Fragment 4: 75.02
Fragment 5: 59.97
Normalized Intensity
25000
20000
15000
10000
5000
0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

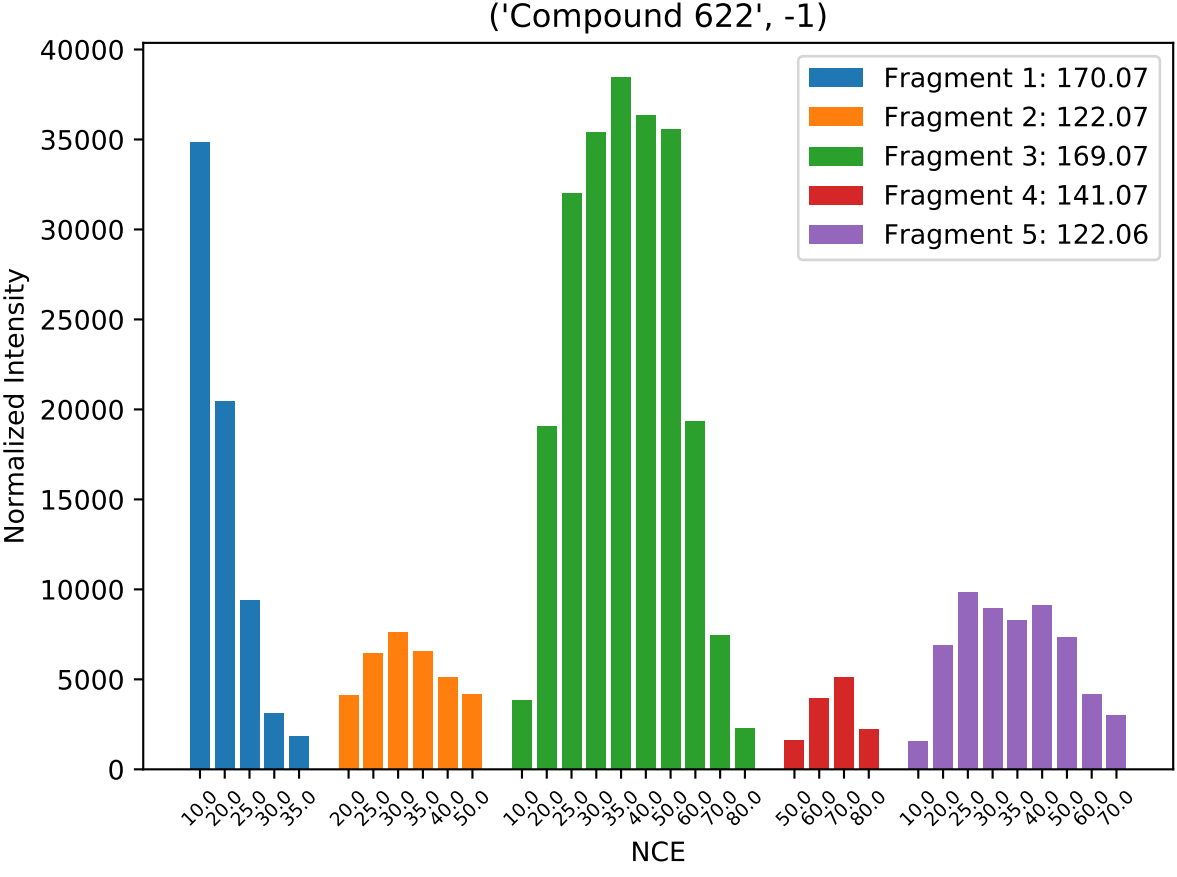

('Compound 616', -1)
Fragment 1: 170.07
Fragment 2: 169.07
Fragment 3: 143.05
Fragment 4: 141.07
Fragment 5: 167.05
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
NCE

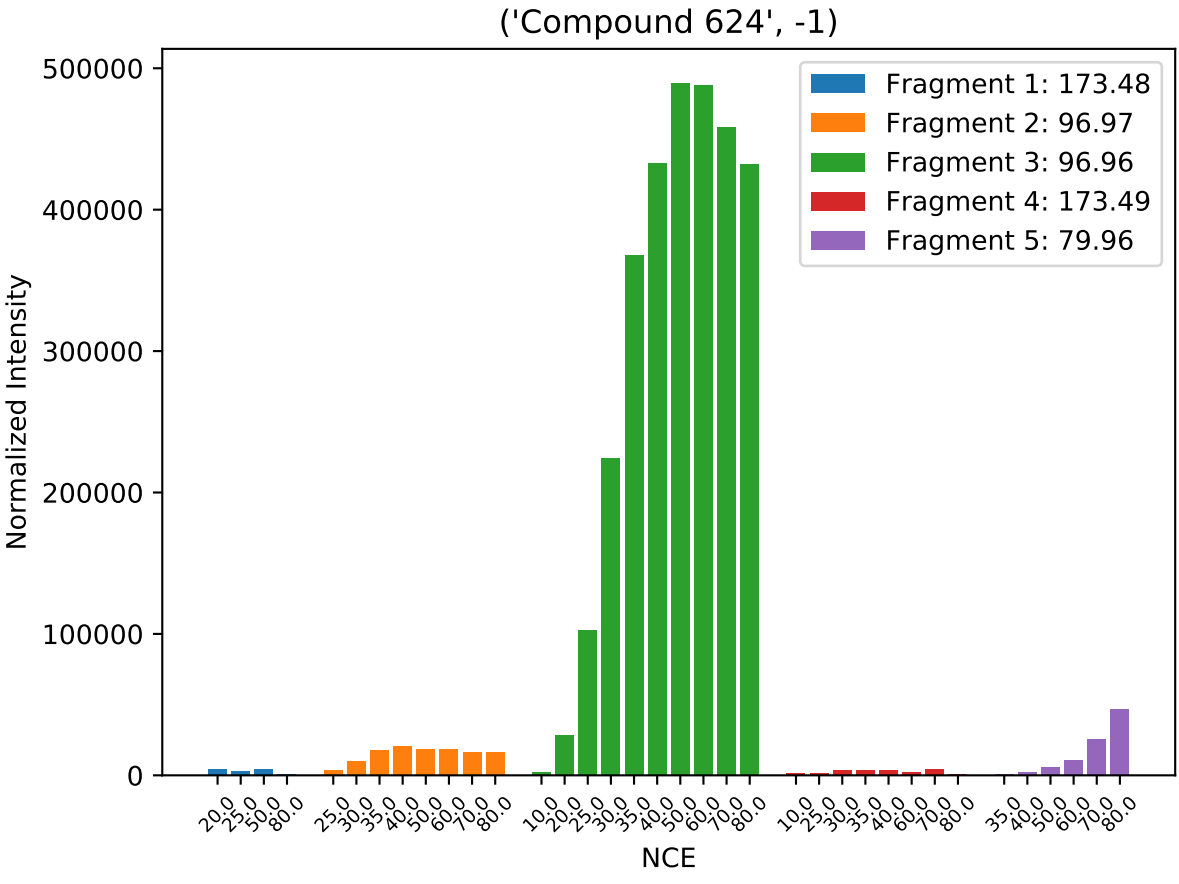

('Compound 77', -1)
Fragment 1: 79.96
Fragment 2: 80.96
Fragment 3: 106.98
Fragment 4: 64.97
Fragment 5: 79.97
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 40.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

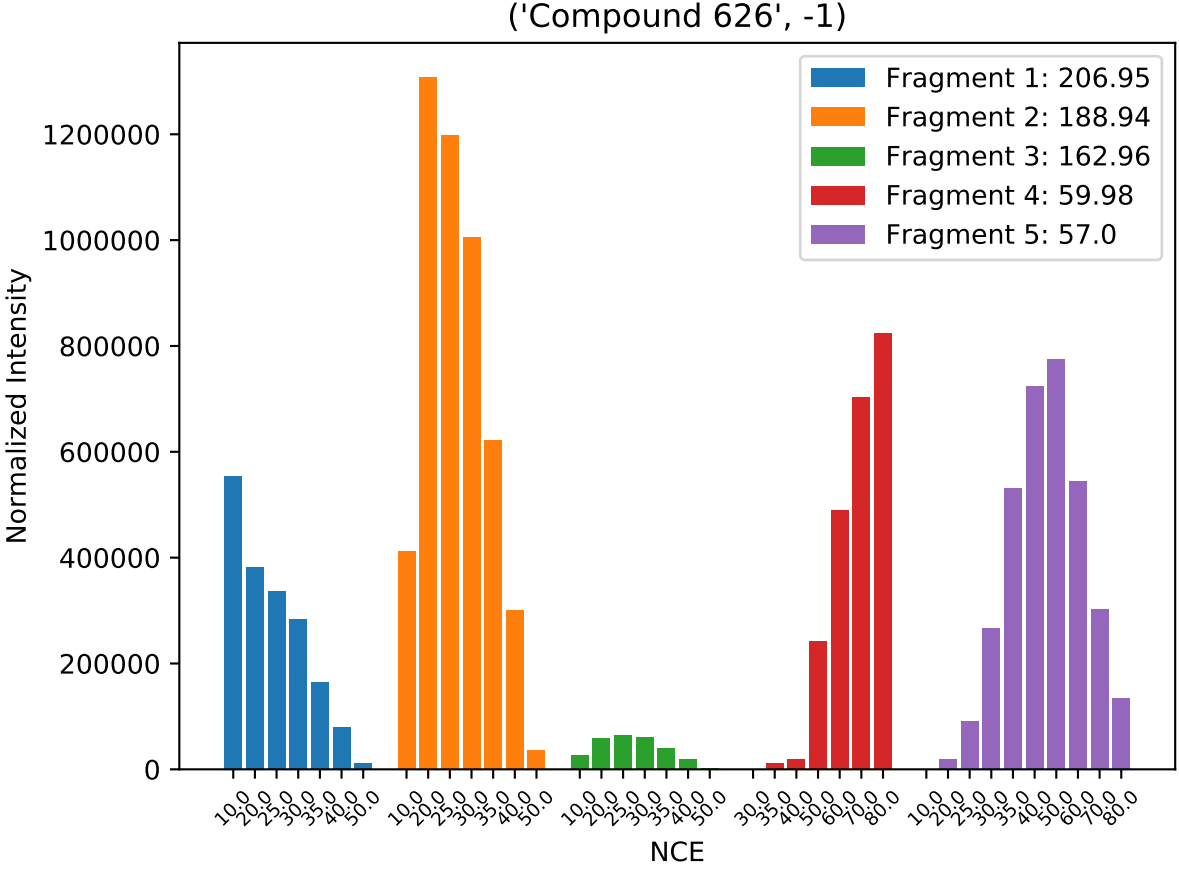

('Compound 619', -1)
Fragment 1: 84.05
Fragment 2: 52.02
Fragment 3: 82.03
Fragment 4: 92.81
Fragment 5: 67.29
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
60.0
20.0
NCE

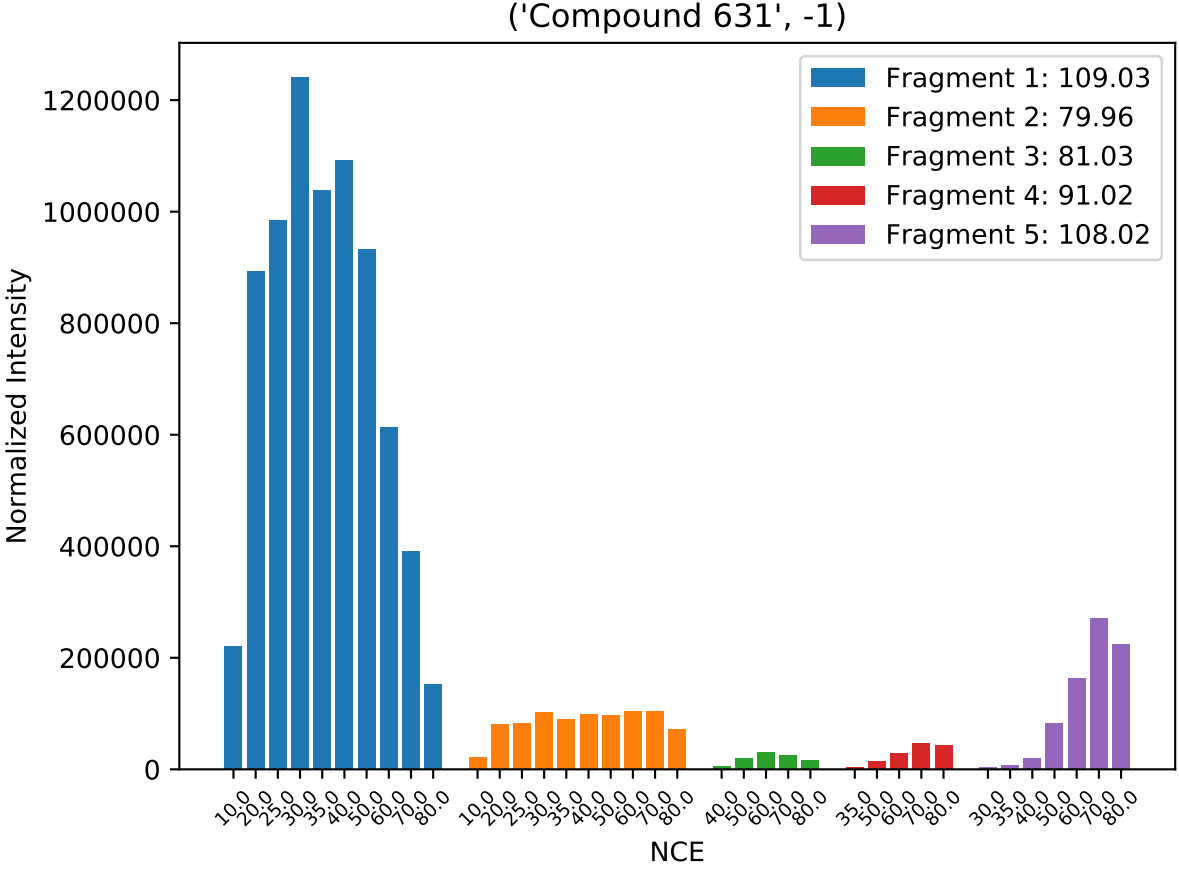

('Compound 620', -1)
Fragment 1: 57.36
Fragment 2: 60.69
Fragment 3: 65.89
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
25.0
25.0
25.0
NCE

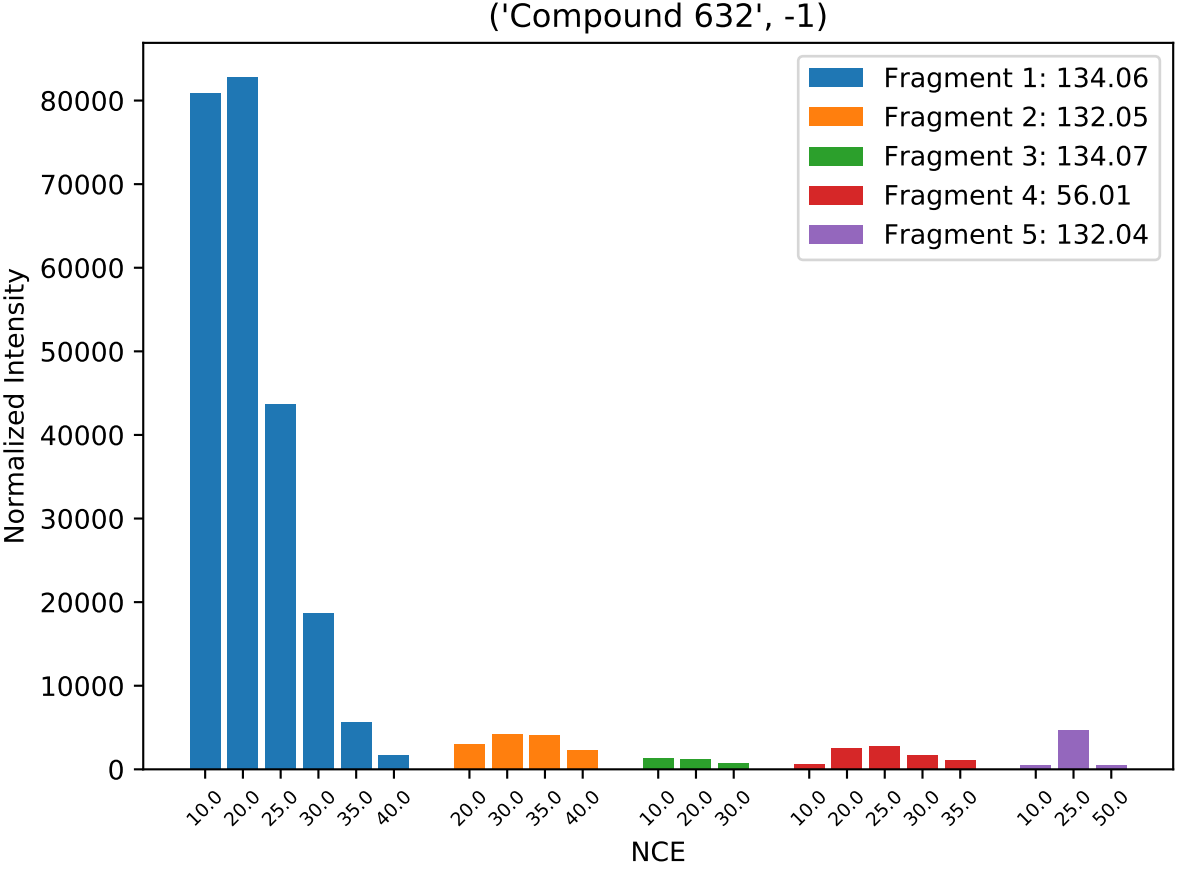

('Compound 621', -1)
Fragment 1: 127.05
Fragment 2: 109.04
Fragment 3: 128.04
Fragment 4: 84.05
Fragment 5: 74.02
Normalized Intensity
200000
175000
150000
125000
100000
75000
50000
25000
0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

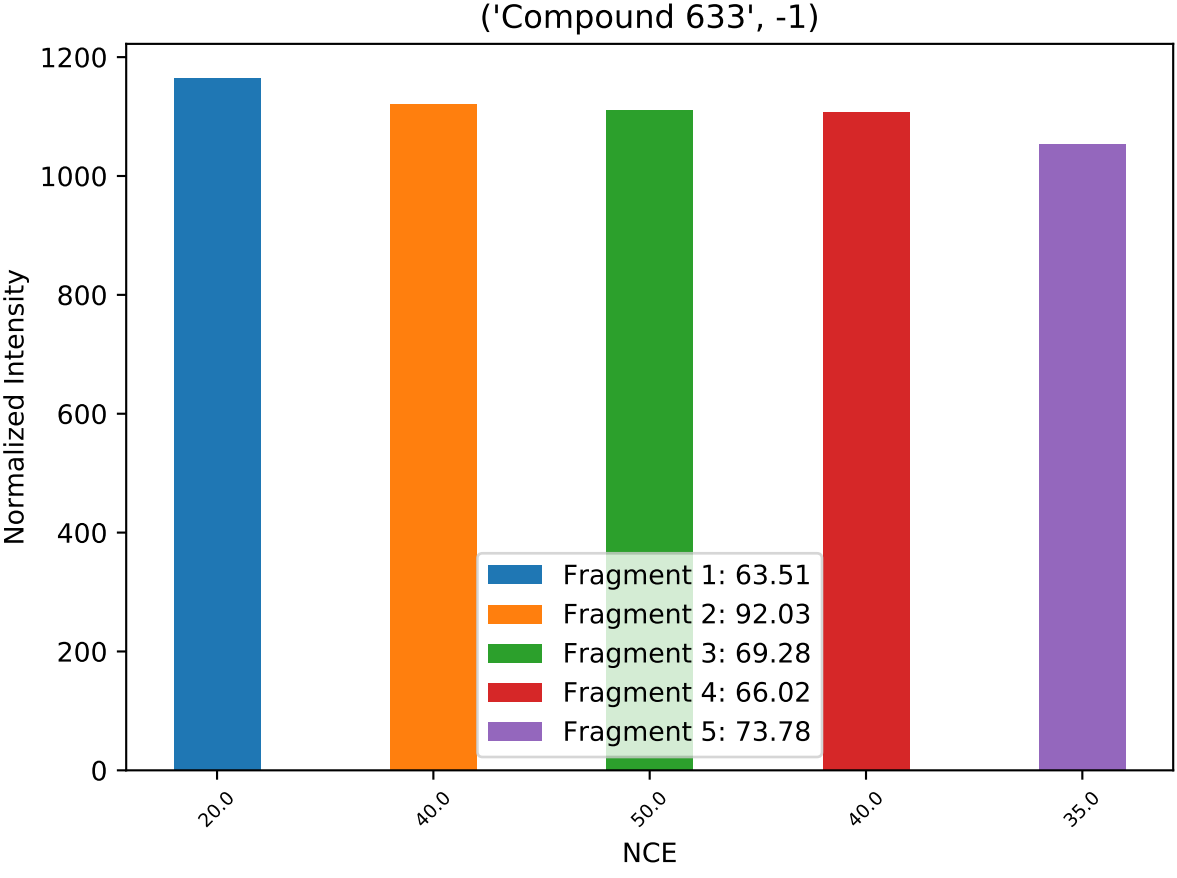

('Compound 622', -1)
Fragment 1: 170.07
Fragment 2: 122.07
Fragment 3: 169.07
Fragment 4: 141.07
Fragment 5: 122.06
Normalized Intensity
NCE
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0

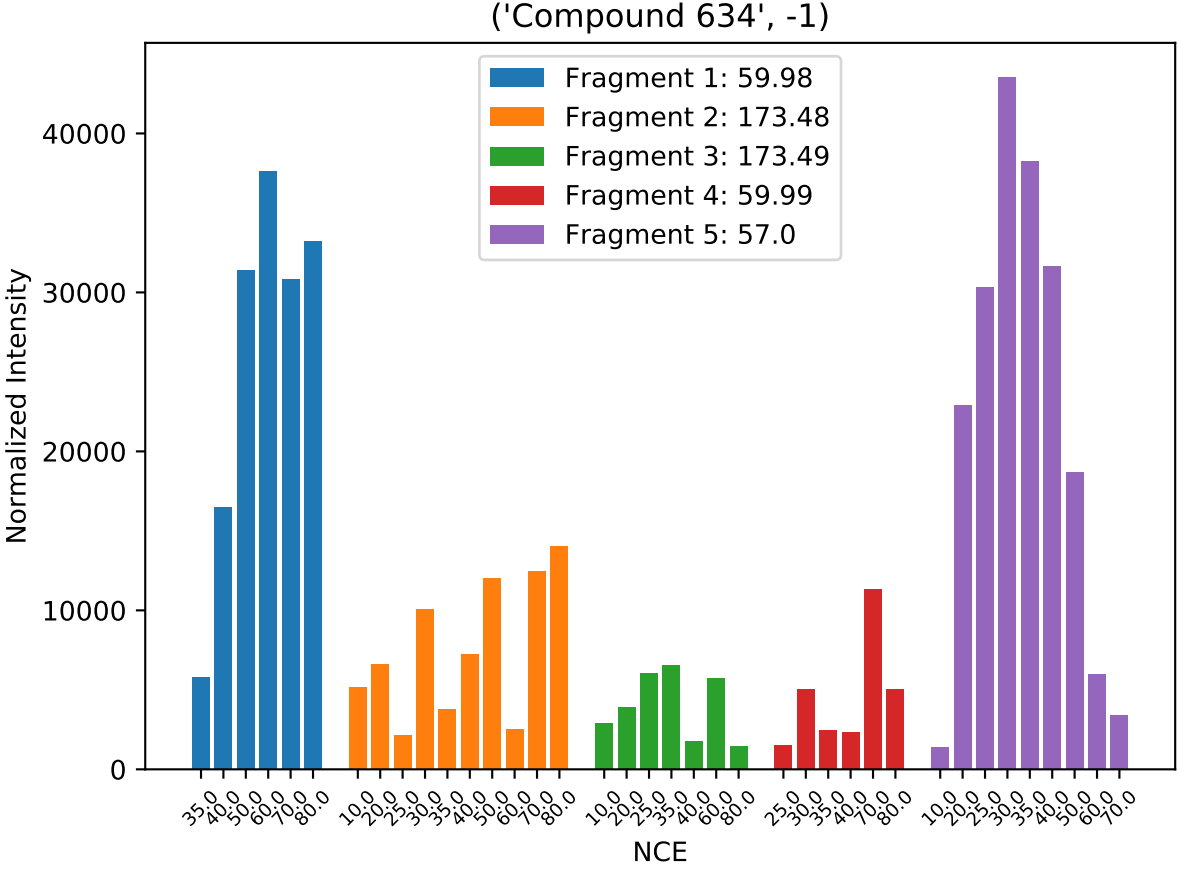

('Compound 624', -1)
Fragment 1: 173.48
Fragment 2: 96.97
Fragment 3: 96.96
Fragment 4: 173.49
Fragment 5: 79.96
Normalized Intensity
500000
400000
300000
200000
100000
0
20.0 25.0 50.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 25.0 30.0 35.0 40.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

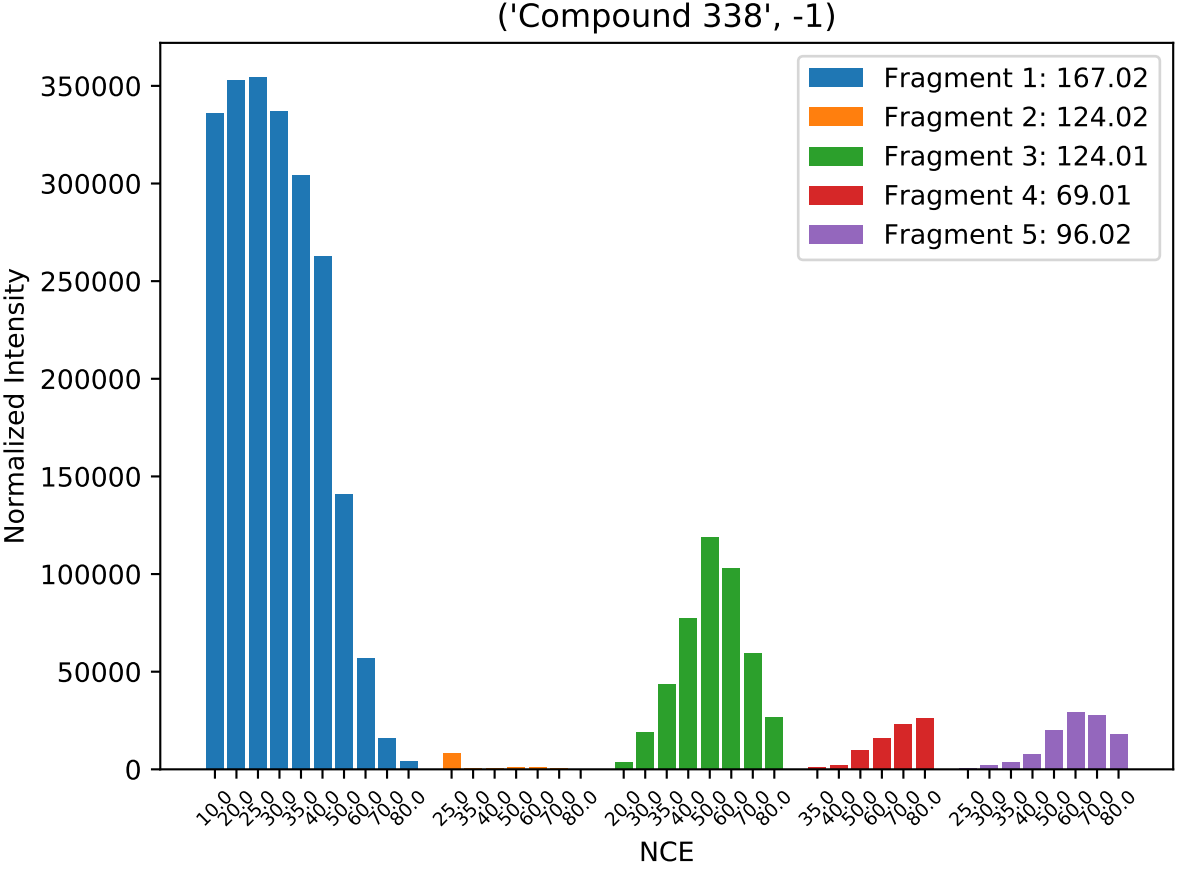

('Compound 626', -1)
Fragment 1: 206.95
Fragment 2: 188.94
Fragment 3: 162.96
Fragment 4: 59.98
Fragment 5: 57.0
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

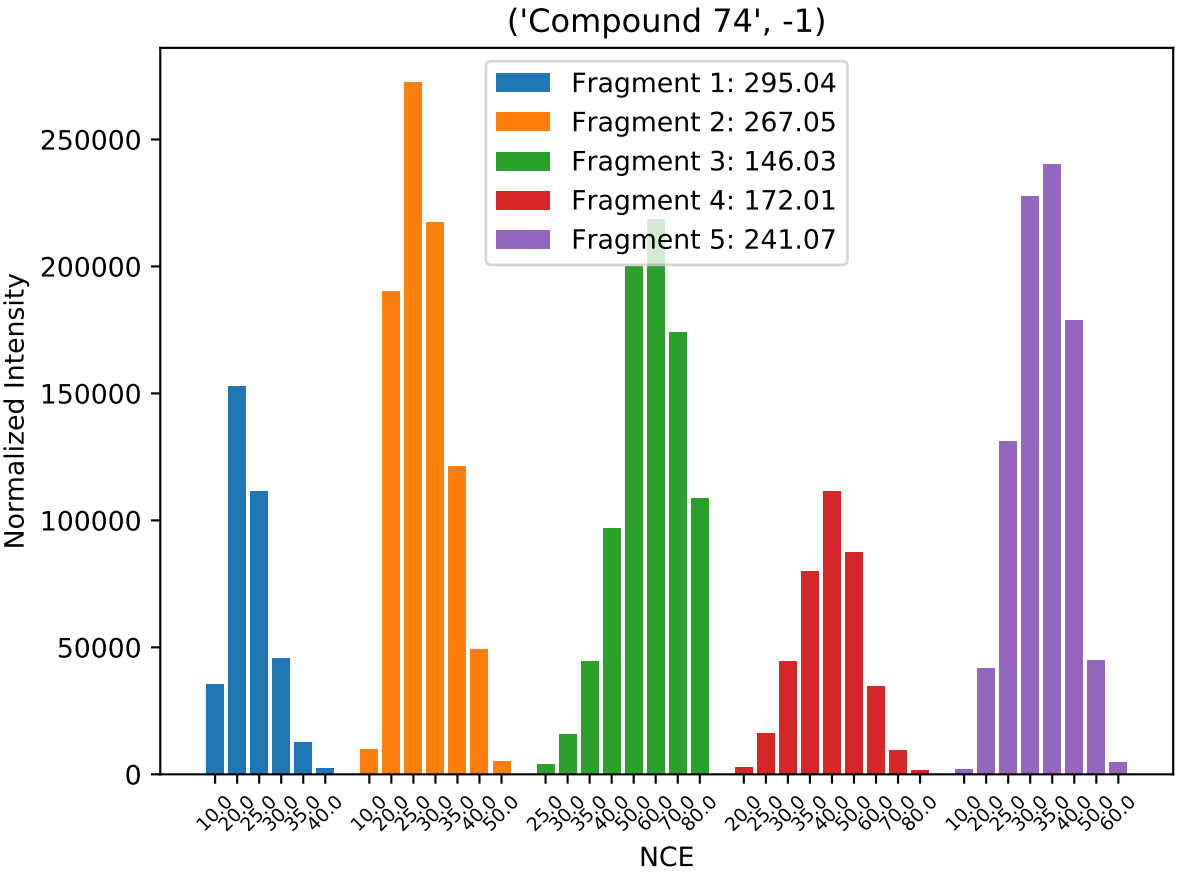

('Compound 631', -1)
Fragment 1: 109.03
Fragment 2: 79.96
Fragment 3: 81.03
Fragment 4: 91.02
Fragment 5: 108.02
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
35.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

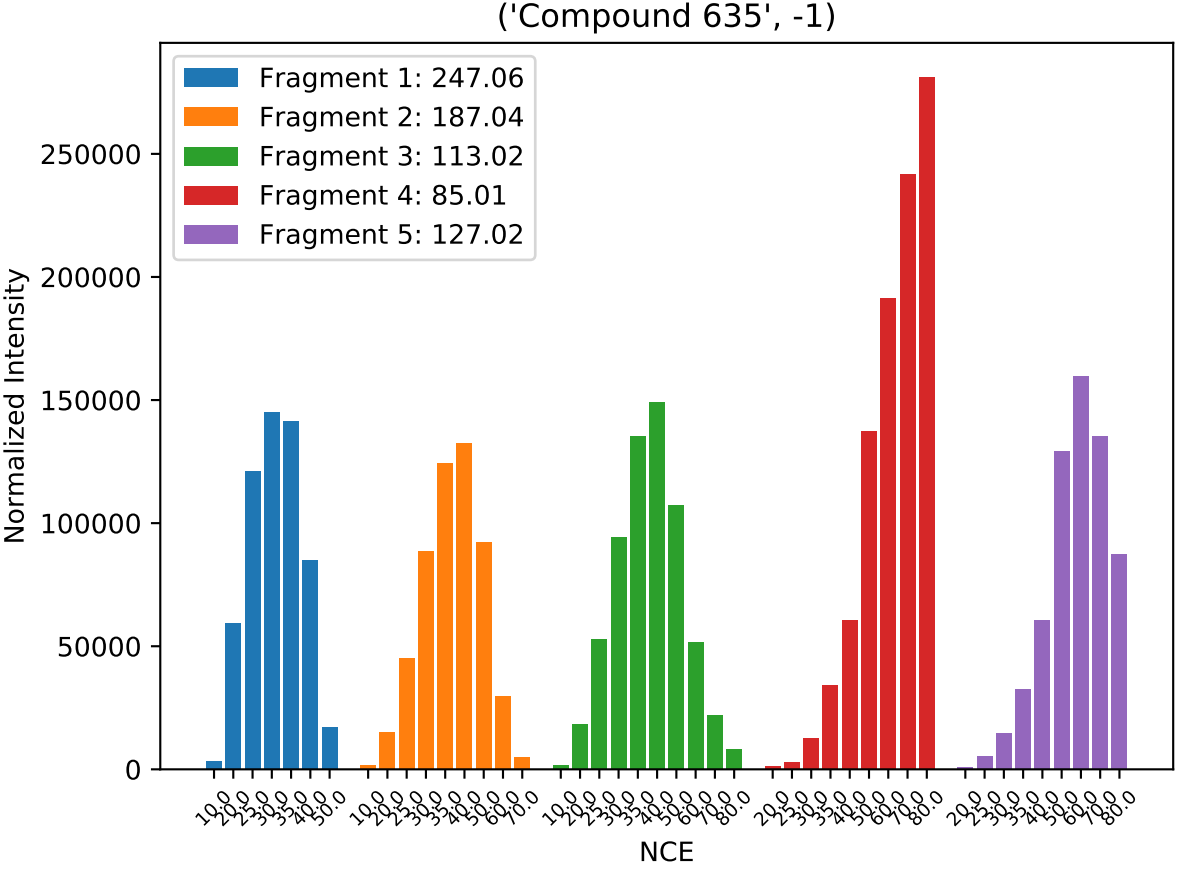

('Compound 632', -1)
Fragment 1: 134.06
Fragment 2: 132.05
Fragment 3: 134.07
Fragment 4: 56.01
Fragment 5: 132.04
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0
20.0
25.0
30.0
35.0
40.0
20.0
30.0
35.0
40.0
10.0
20.0
30.0
10.0
20.0
25.0
30.0
35.0
10.0
25.0
50.0
NCE

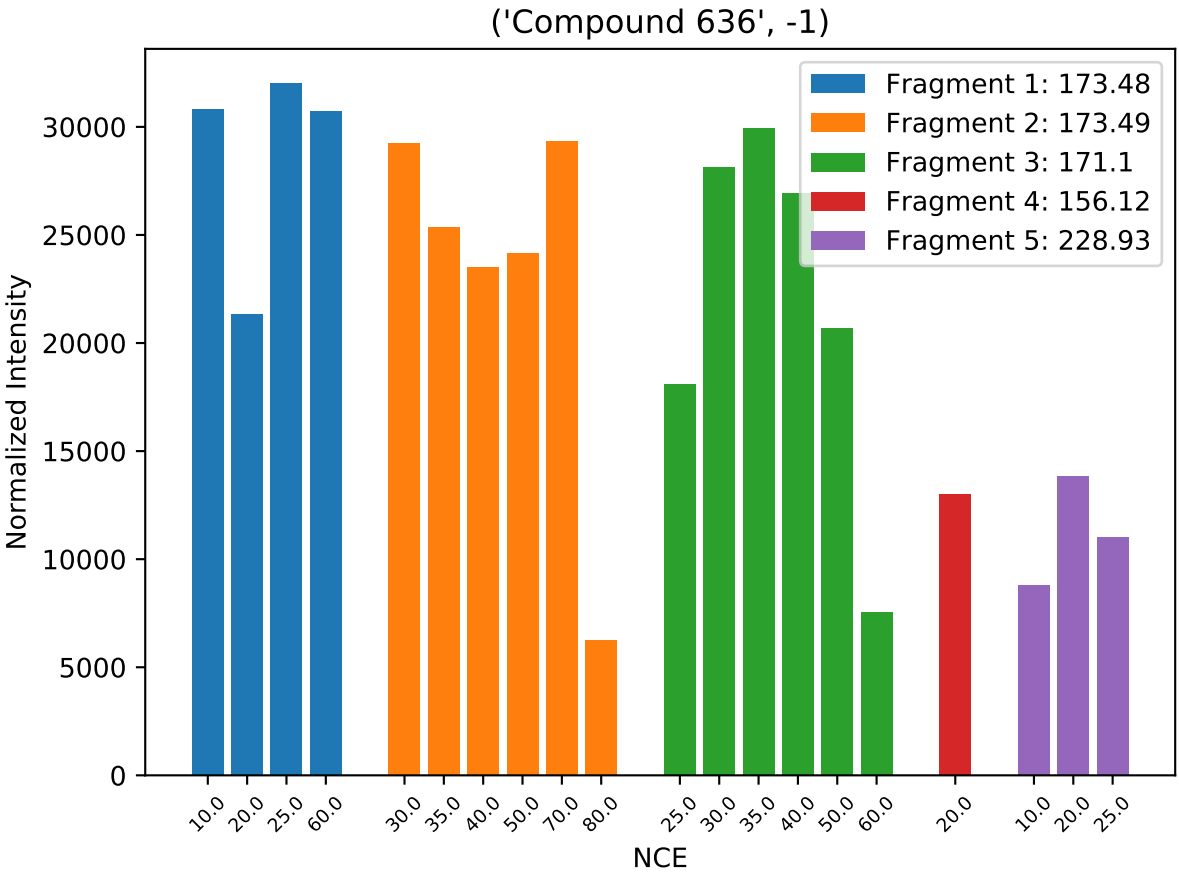

('Compound 633', -1)
Normalized Intensity
0
200
400
600
800
1000
1200
Fragment 1: 63.51
Fragment 2: 92.03
Fragment 3: 69.28
Fragment 4: 66.02
Fragment 5: 73.78
20.0
40.0
50.0
40.0
35.0
NCE

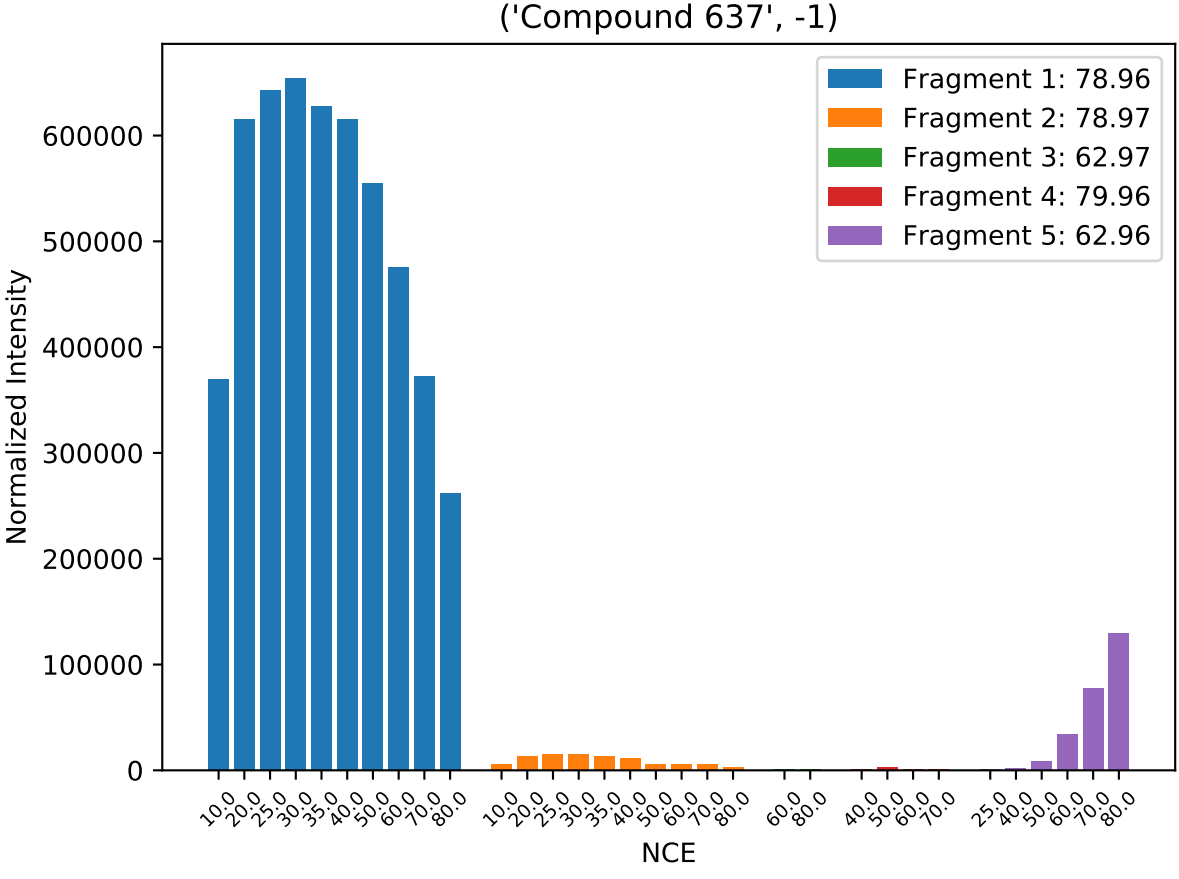

('Compound 634', -1)
Fragment 1: 59.98
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 59.99
Fragment 5: 57.0
Normalized Intensity
0
10000
20000
30000
40000
NCE
35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 35.0 40.0 60.0 80.0
25.0 30.0 35.0 40.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0

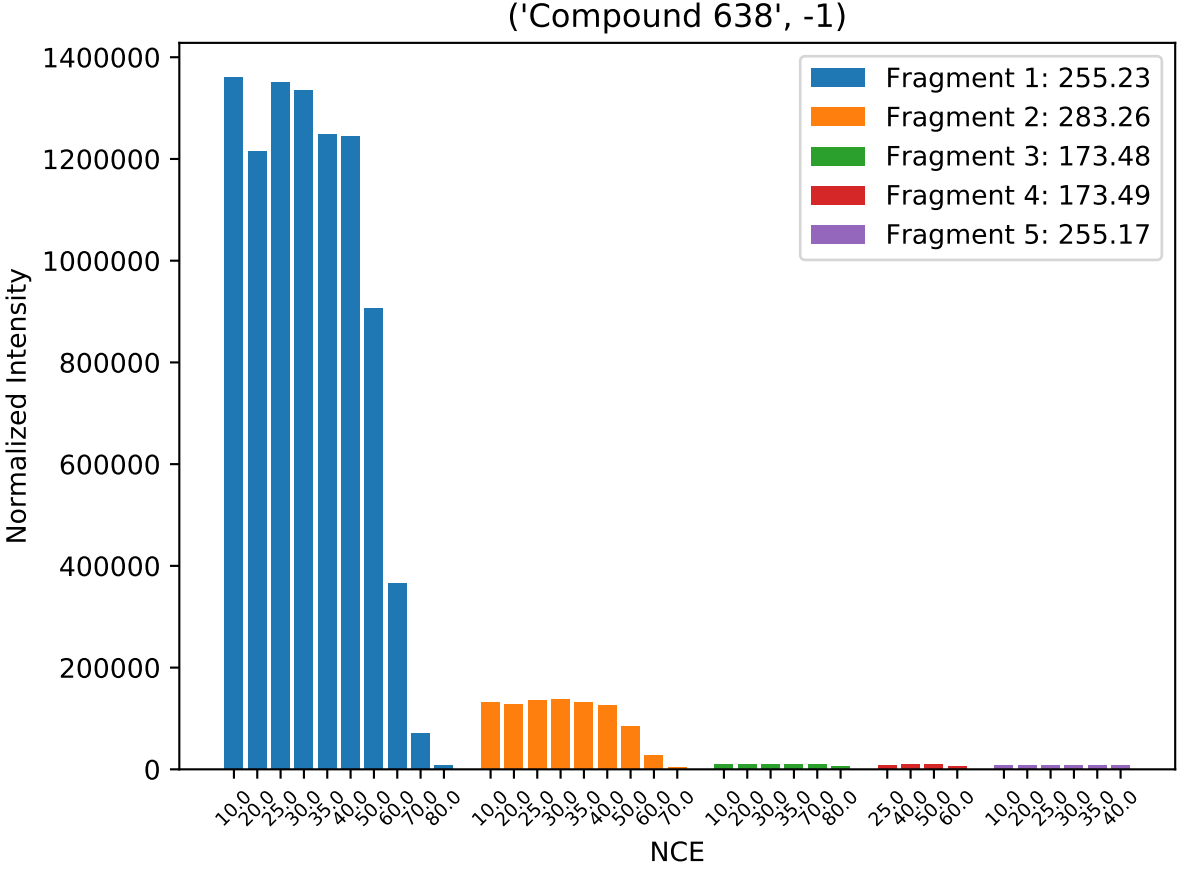

('Compound 338', -1)
Fragment 1: 167.02
Fragment 2: 124.02
Fragment 3: 124.01
Fragment 4: 69.01
Fragment 5: 96.02
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

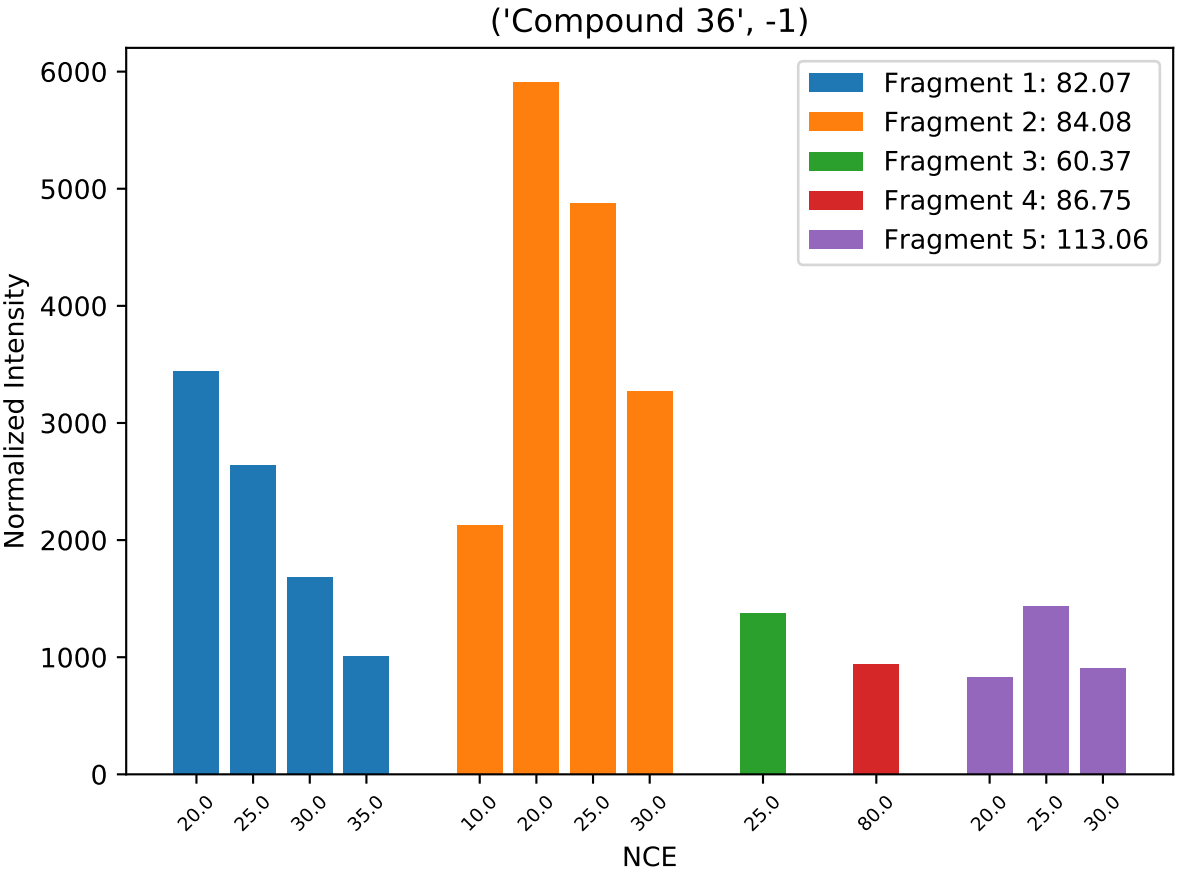

('Compound 74', -1)
Fragment 1: 295.04
Fragment 2: 267.05
Fragment 3: 146.03
Fragment 4: 172.01
Fragment 5: 241.07
Normalized Intensity
0
50000
100000
150000
200000
250000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

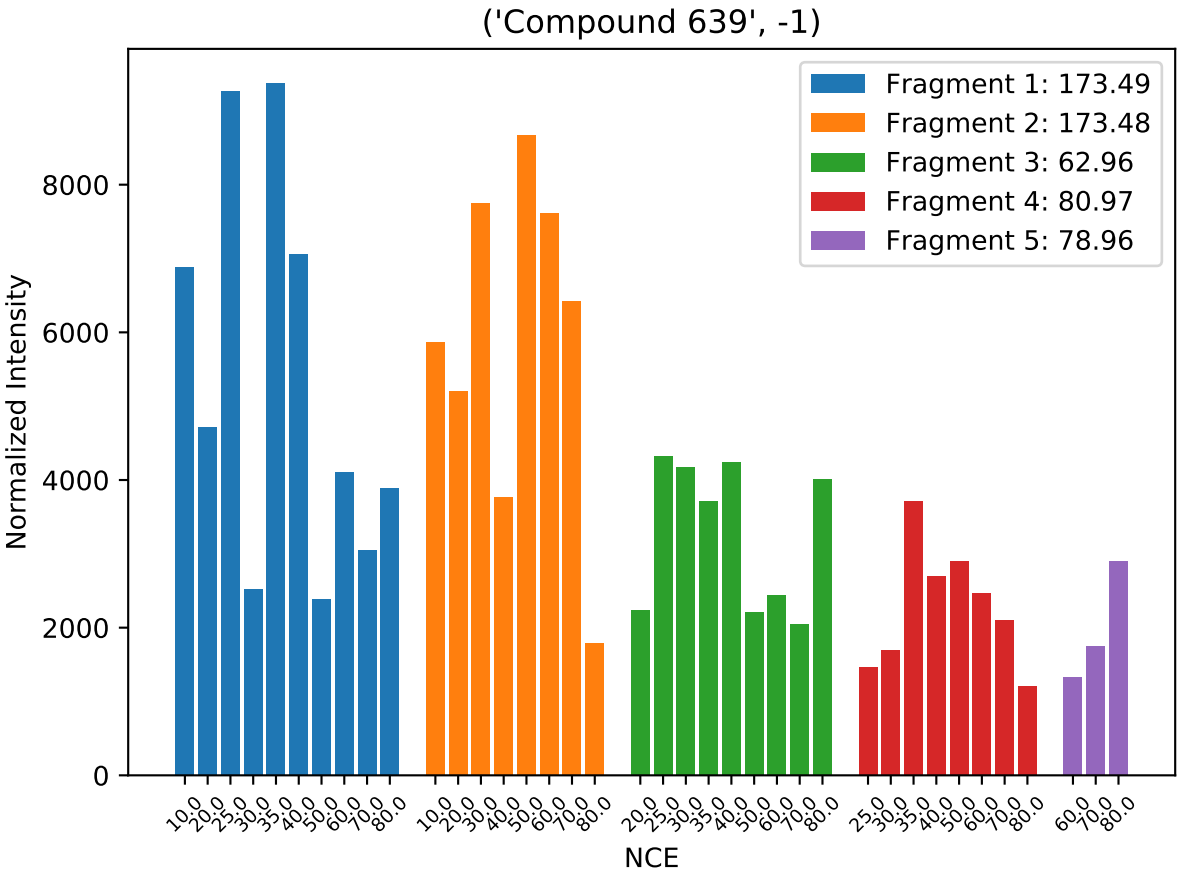

('Compound 635', -1)
Fragment 1: 247.06
Fragment 2: 187.04
Fragment 3: 113.02
Fragment 4: 85.01
Fragment 5: 127.02
Normalized Intensity
0
50000
100000
150000
200000
250000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

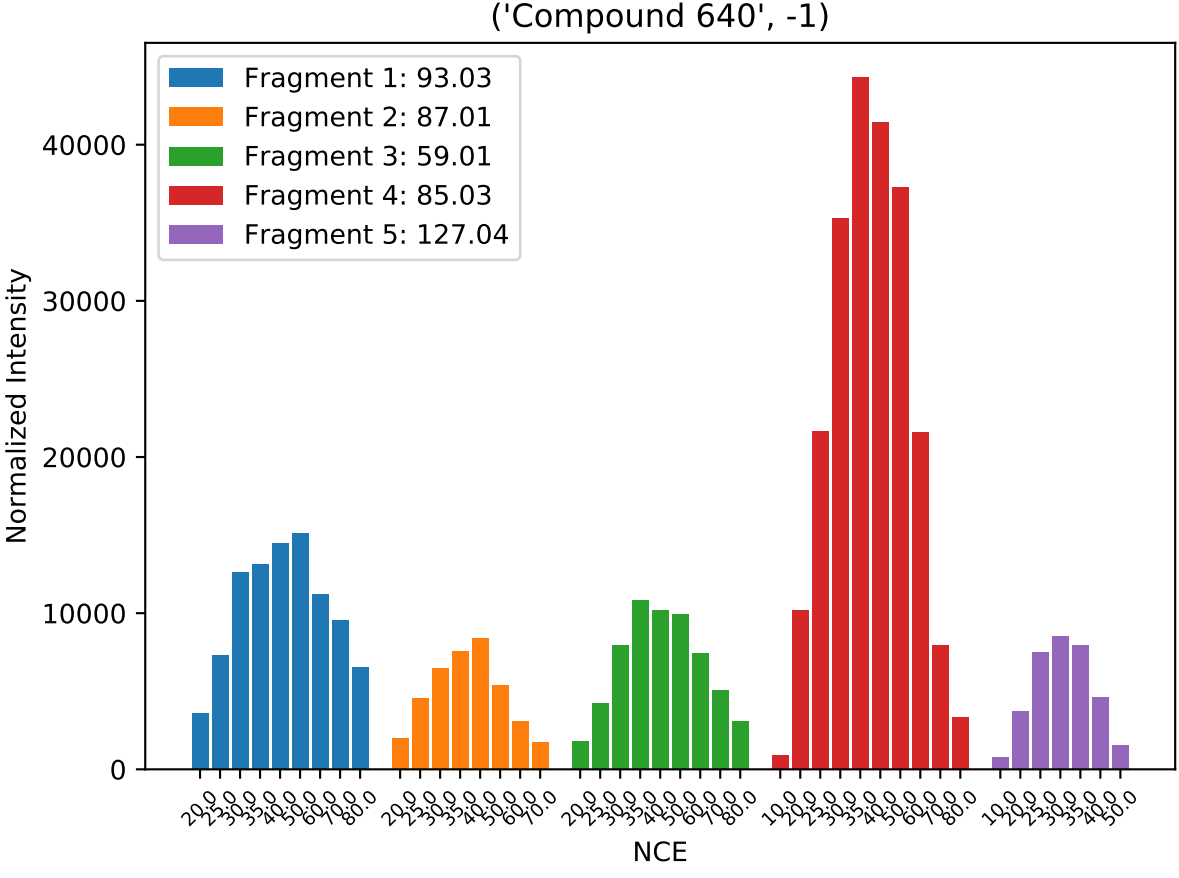

('Compound 636', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 171.1
Fragment 4: 156.12
Fragment 5: 228.93
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0
20.0
25.0
60.0
30.0
35.0
40.0
50.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
10.0
20.0
25.0
NCE

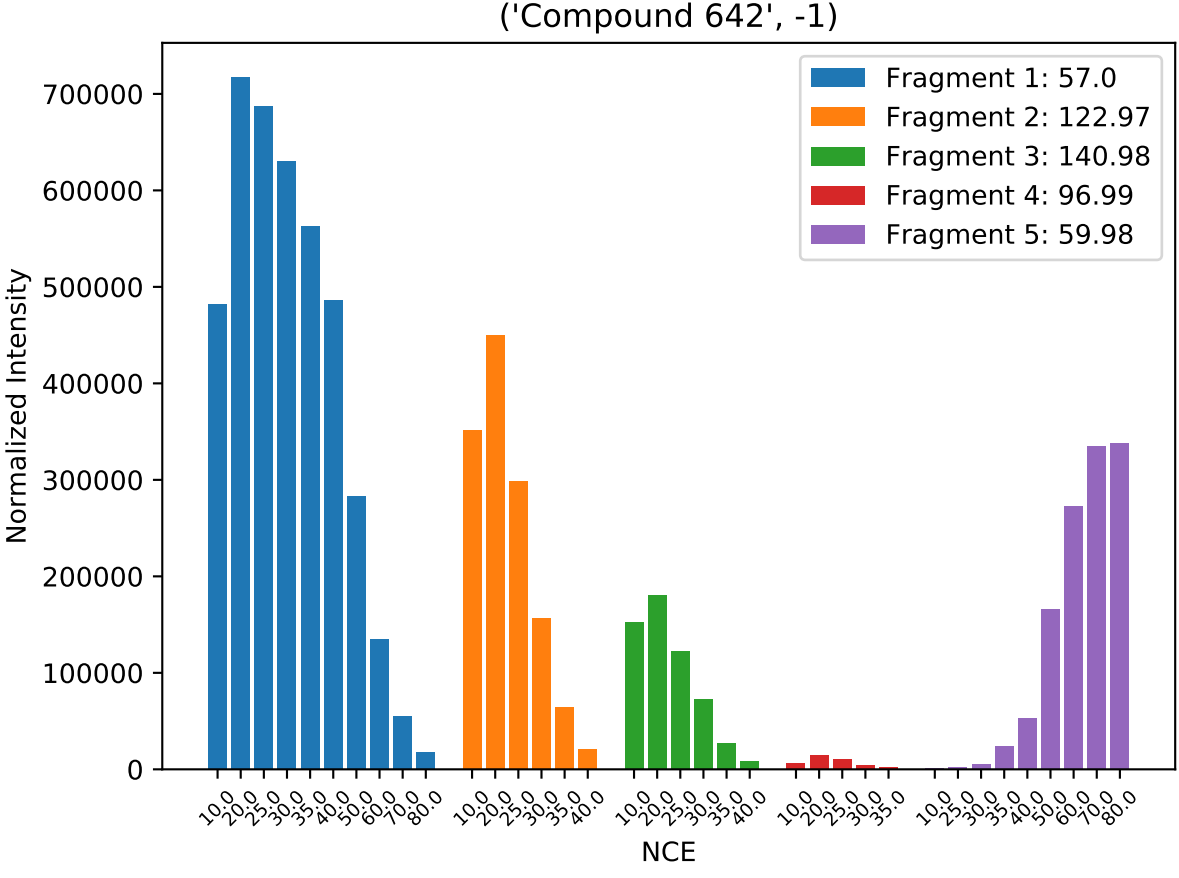

('Compound 637', -1)
Fragment 1: 78.96
Fragment 2: 78.97
Fragment 3: 62.97
Fragment 4: 79.96
Fragment 5: 62.96
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
60.0 80.0
40.0 50.0 60.0 70.0
25.0 40.0 50.0 60.0 70.0 80.0
NCE

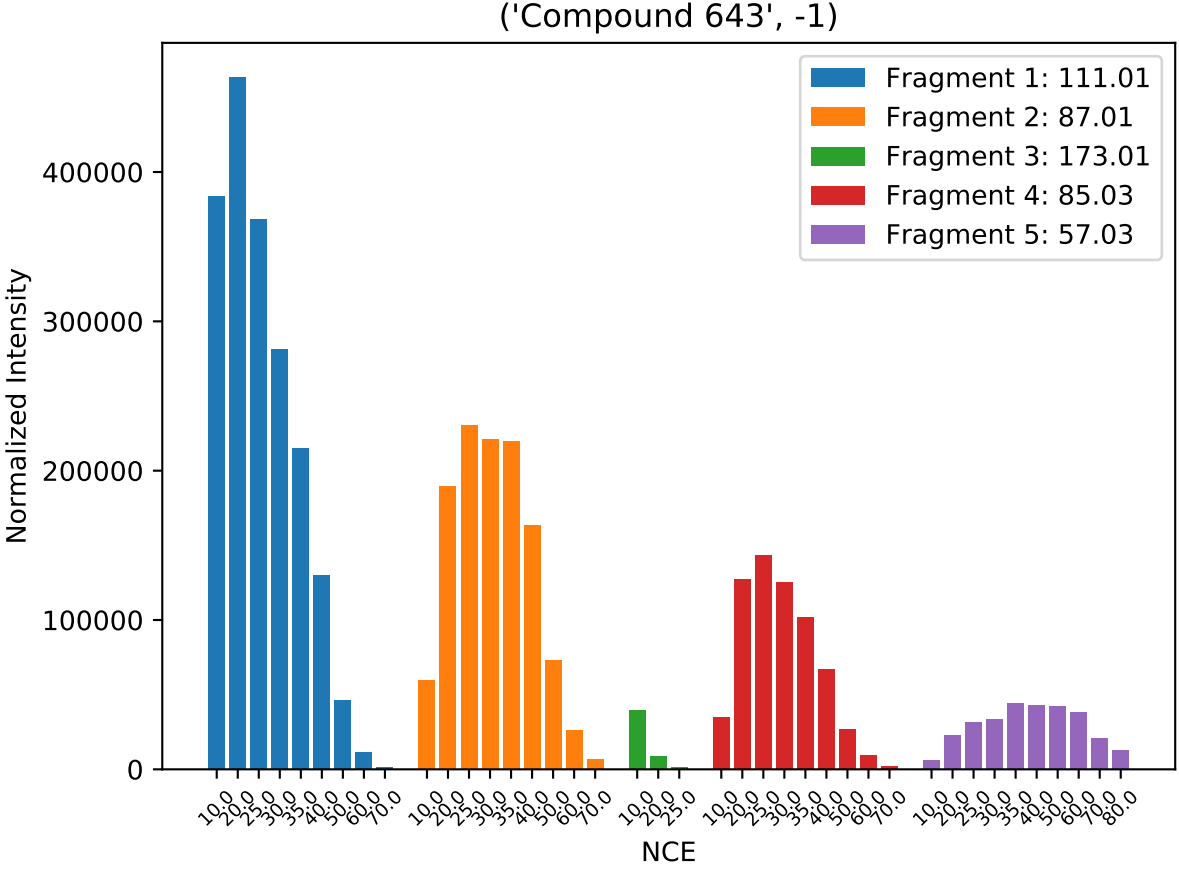

('Compound 638', -1)
Fragment 1: 255.23
Fragment 2: 283.26
Fragment 3: 173.48
Fragment 4: 173.49
Fragment 5: 255.17
Normalized Intensity
0
200000
400000
600000
800000
1000000
1200000
1400000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 30.0 35.0 70.0 80.0
25.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

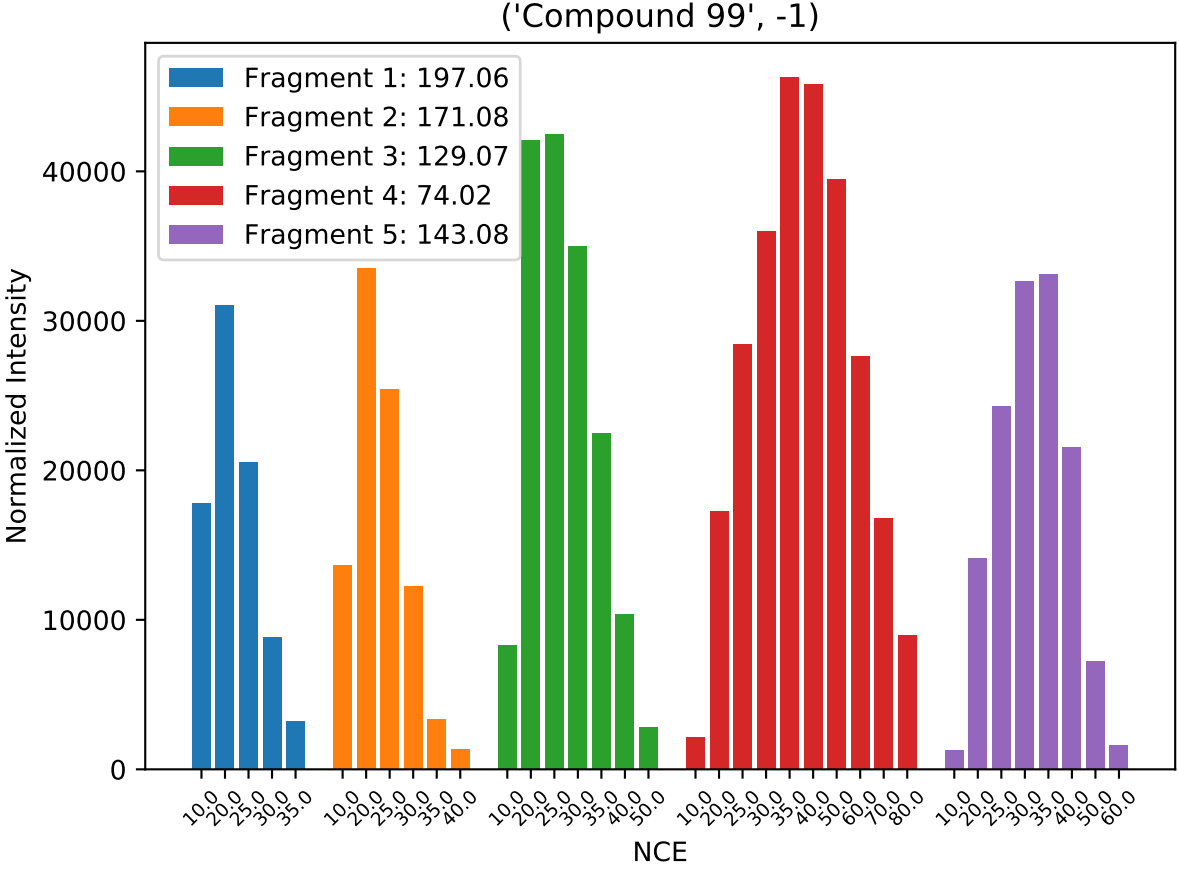

('Compound 36', -1)
Fragment 1: 82.07
Fragment 2: 84.08
Fragment 3: 60.37
Fragment 4: 86.75
Fragment 5: 113.06
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
25.0
80.0
20.0
25.0
30.0
NCE

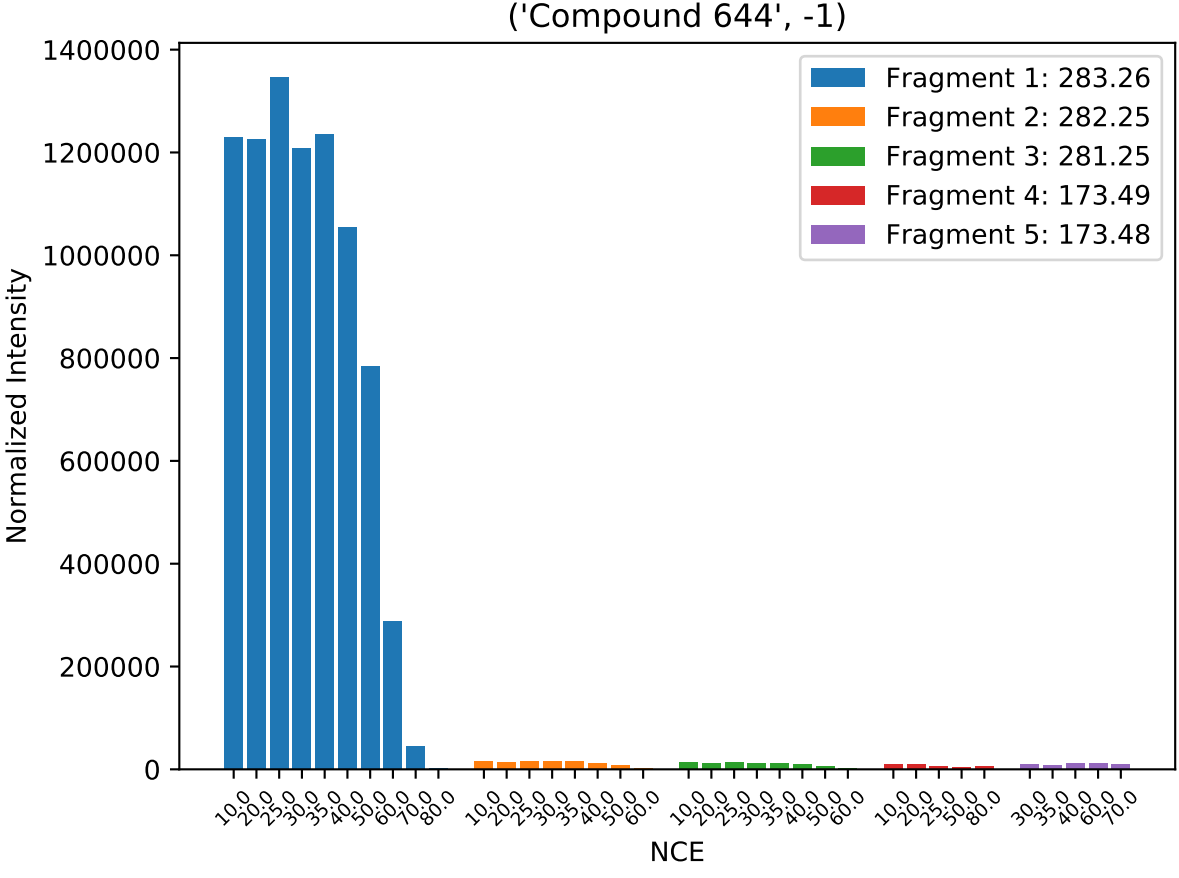

('Compound 639', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 62.96
Fragment 4: 80.97
Fragment 5: 78.96
Normalized Intensity
0
2000
4000
6000
8000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 30.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
60.0 70.0 80.0
NCE

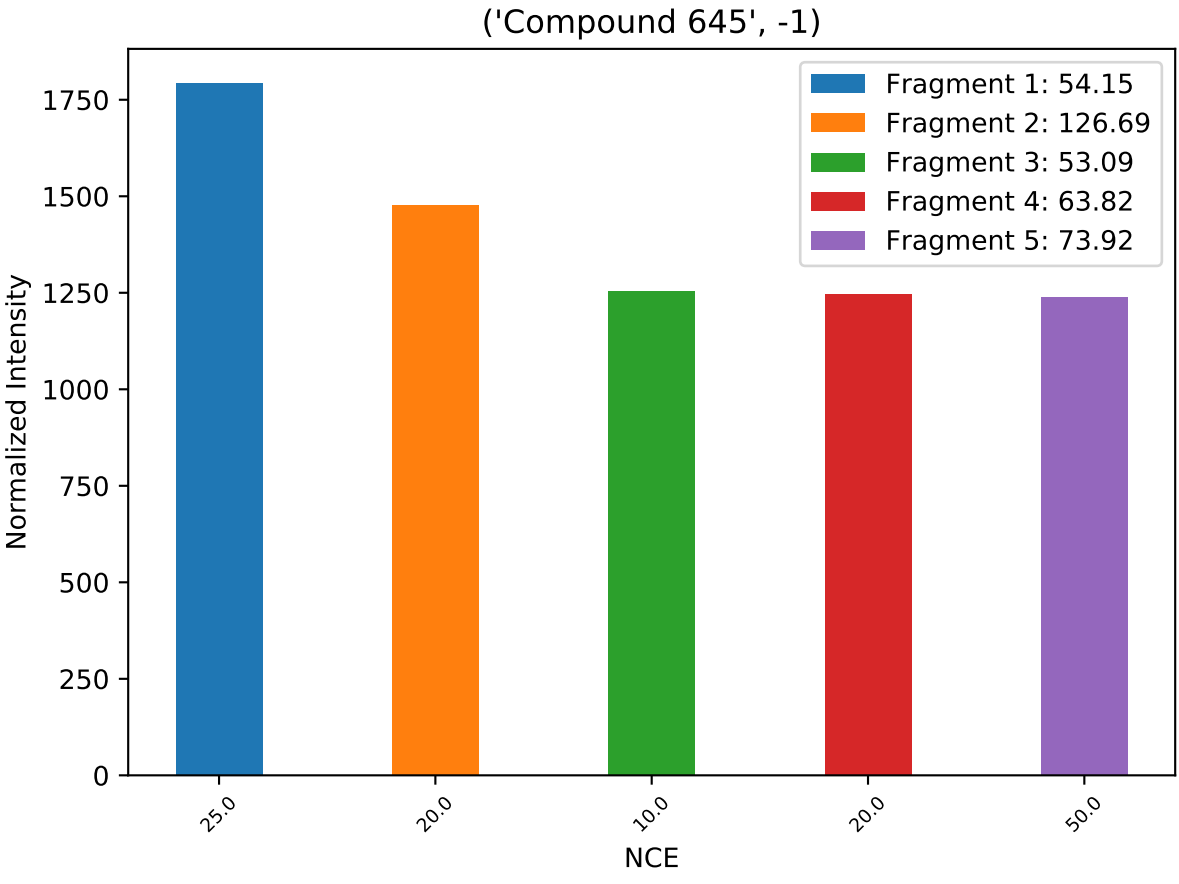

('Compound 640', -1)
Fragment 1: 93.03
Fragment 2: 87.01
Fragment 3: 59.01
Fragment 4: 85.03
Fragment 5: 127.04
Normalized Intensity
0
10000
20000
30000
40000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

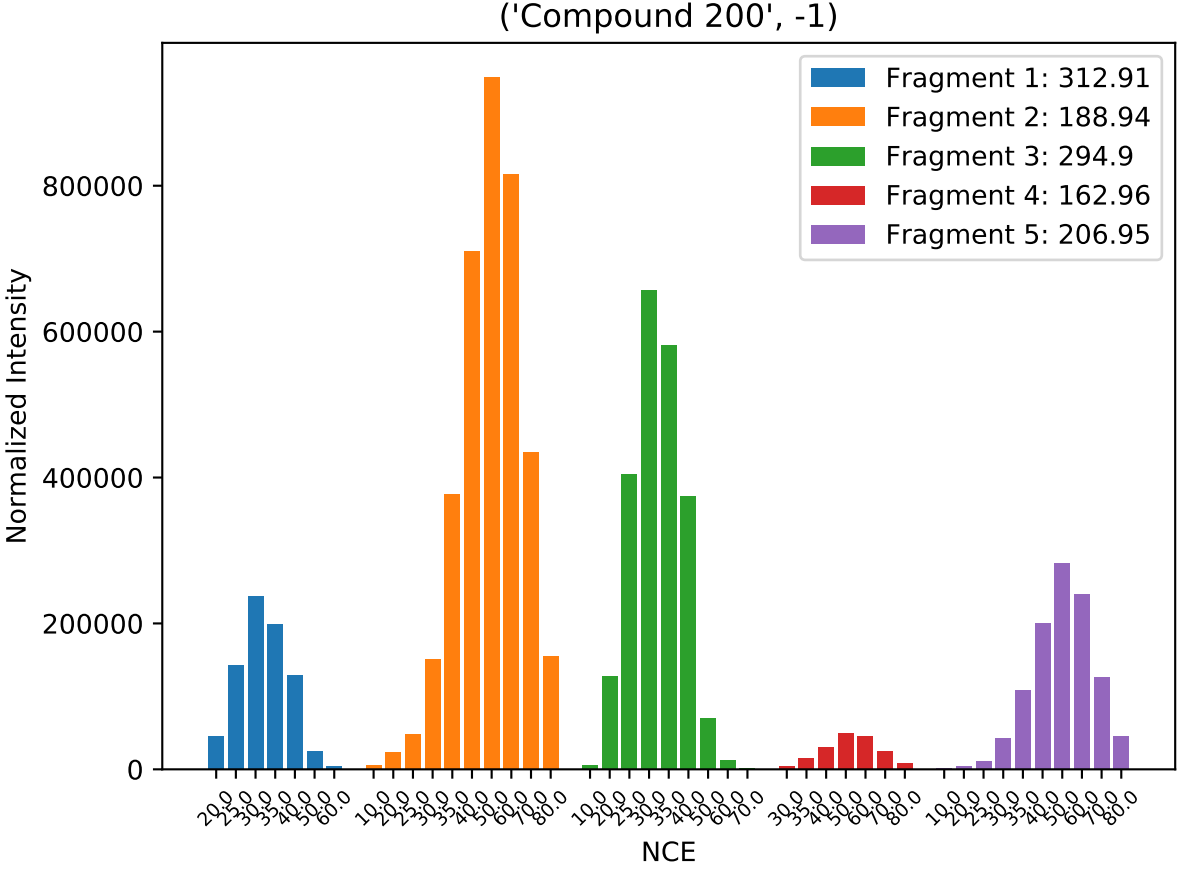

('Compound 642', -1)
Fragment 1: 57.0
Fragment 2: 122.97
Fragment 3: 140.98
Fragment 4: 96.99
Fragment 5: 59.98
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
700000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0
10.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

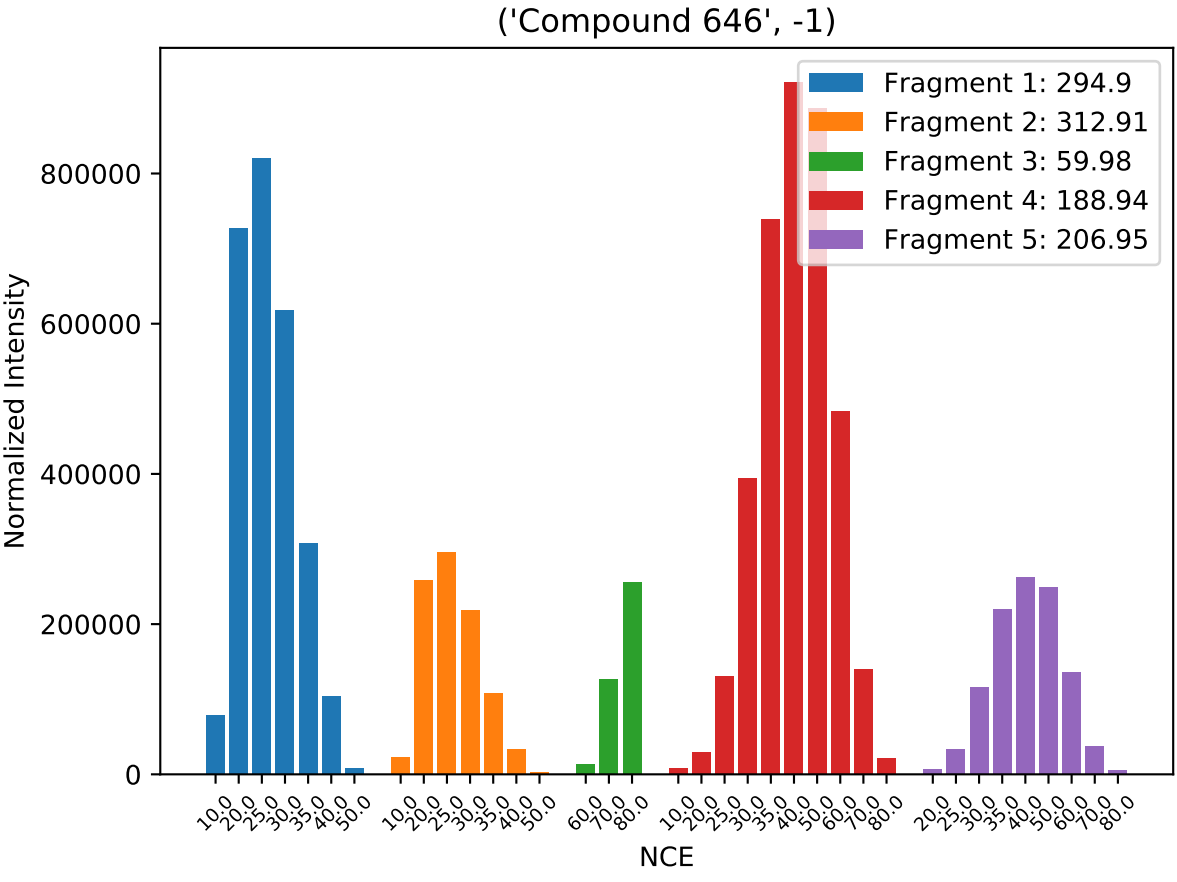

('Compound 643', -1)
Fragment 1: 111.01
Fragment 2: 87.01
Fragment 3: 173.01
Fragment 4: 85.03
Fragment 5: 57.03
Normalized Intensity
0
100000
200000
300000
400000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

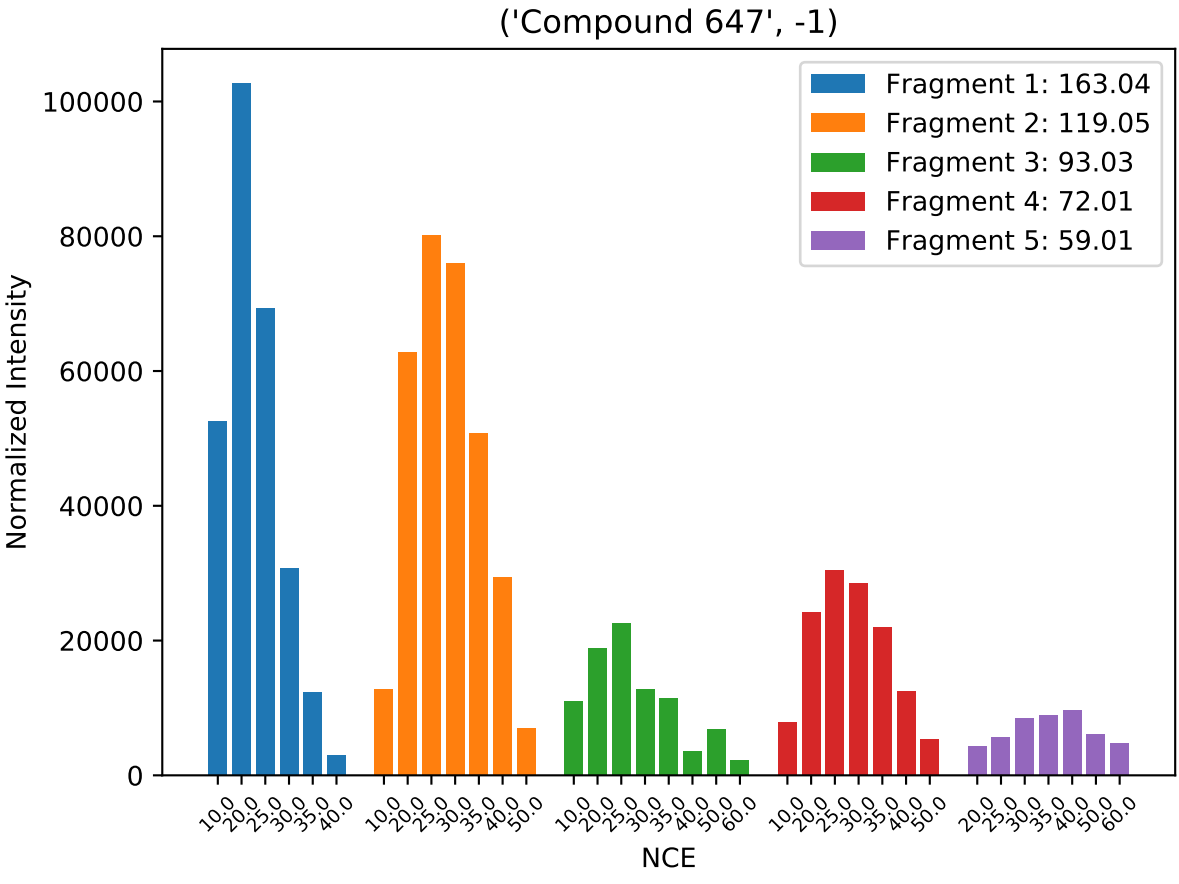

('Compound 99', -1)
Fragment 1: 197.06
Fragment 2: 171.08
Fragment 3: 129.07
Fragment 4: 74.02
Fragment 5: 143.08
Normalized Intensity
0
10000
20000
30000
40000
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

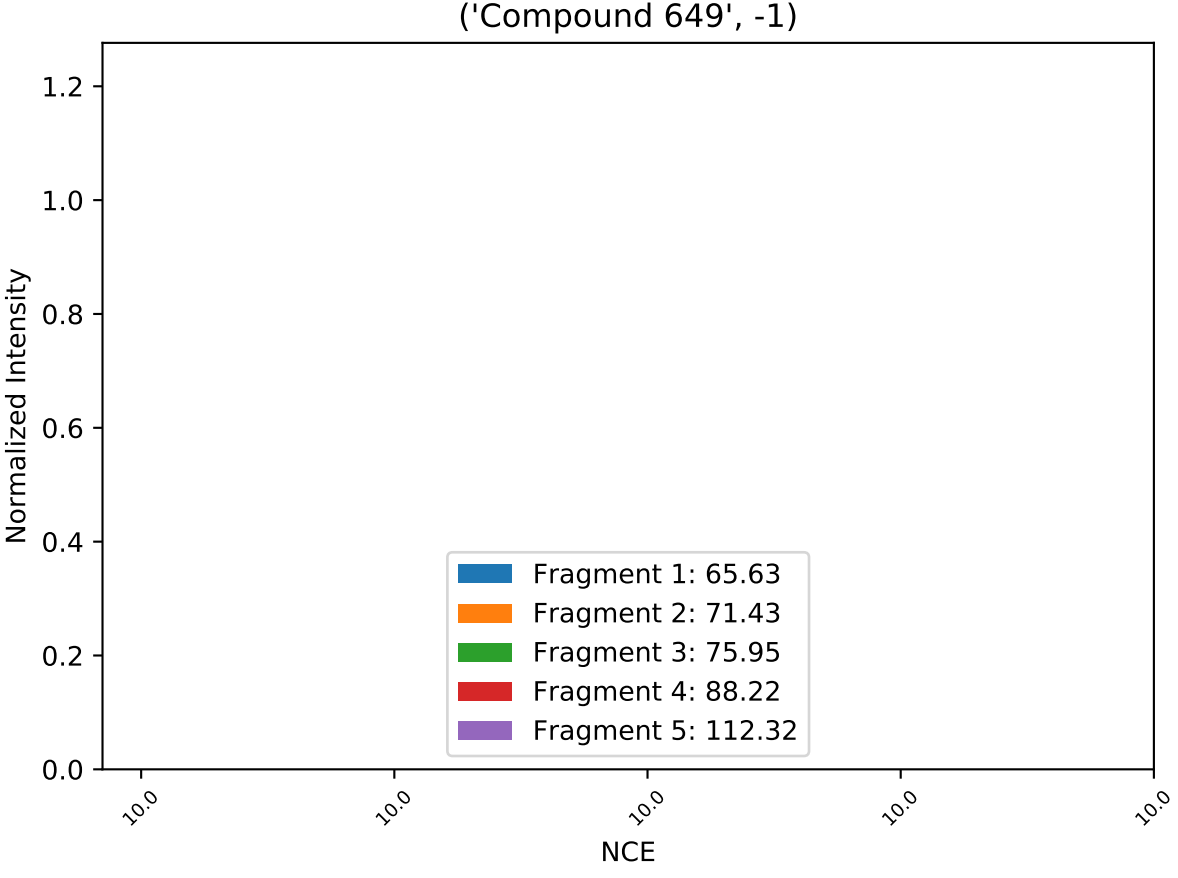

('Compound 644', -1)
Fragment 1: 283.26
Fragment 2: 282.25
Fragment 3: 281.25
Fragment 4: 173.49
Fragment 5: 173.48
Normalized Intensity
1400000
1200000
1000000
800000
600000
400000
200000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 50.0 80.0
30.0 35.0 40.0 60.0 70.0
NCE

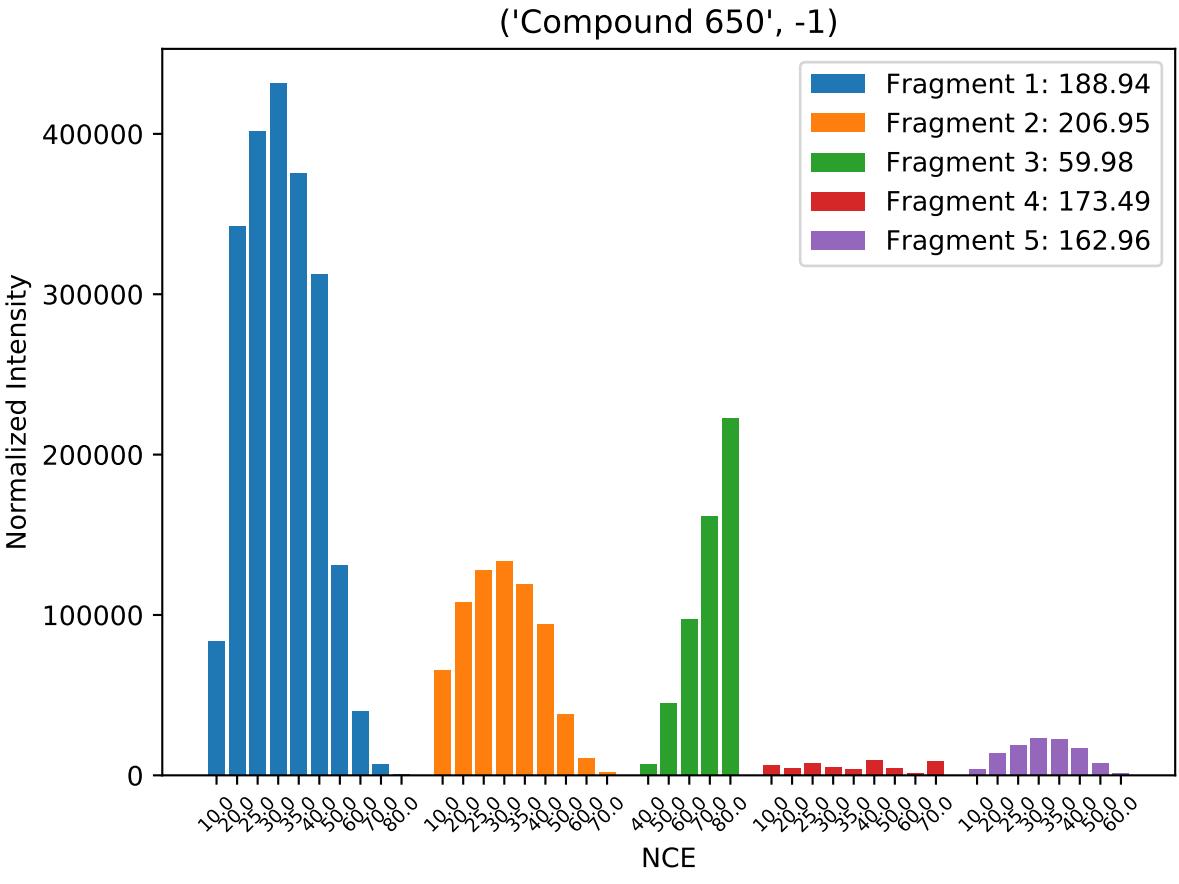

('Compound 645', -1)
Fragment 1: 54.15
Fragment 2: 126.69
Fragment 3: 53.09
Fragment 4: 63.82
Fragment 5: 73.92
Normalized Intensity
0
250
500
750
1000
1250
1500
1750
25.0
20.0
10.0
20.0
50.0
NCE

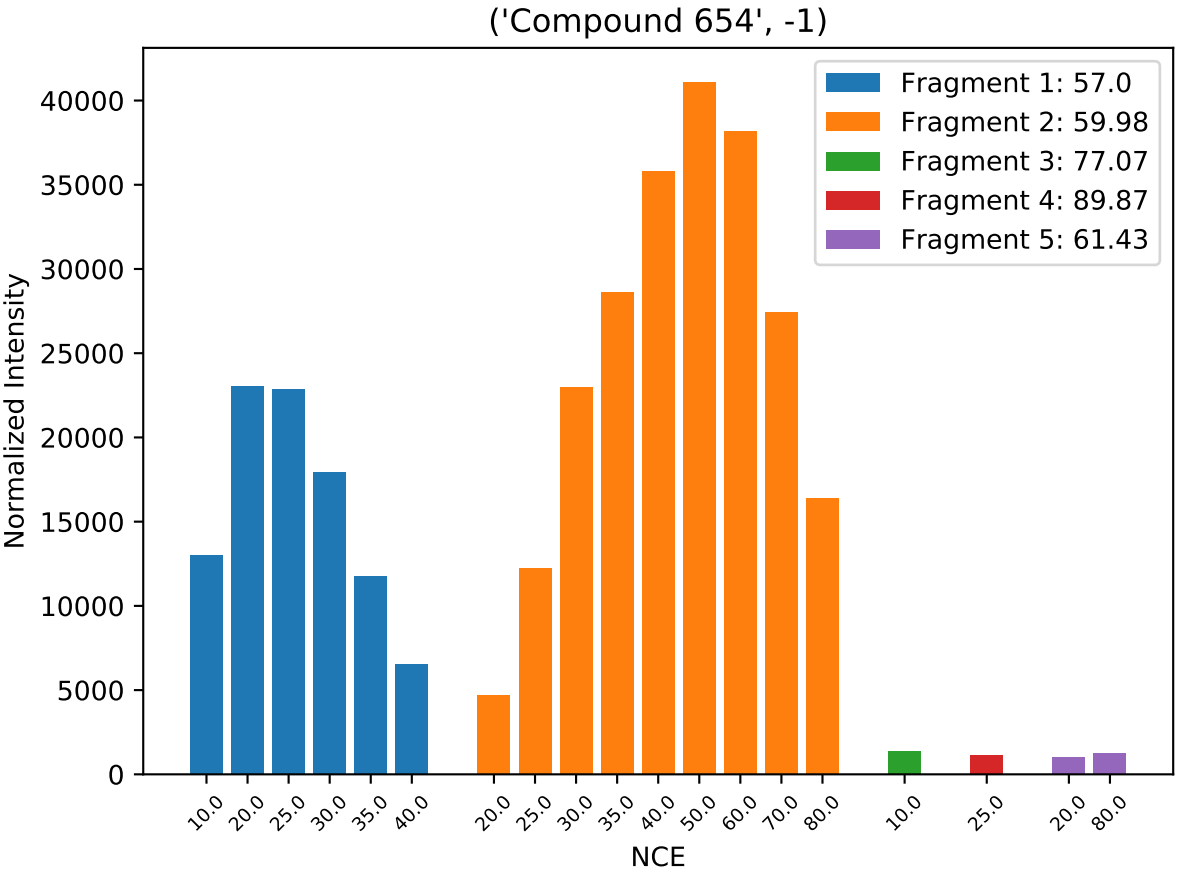

('Compound 200', -1)
Fragment 1: 312.91
Fragment 2: 188.94
Fragment 3: 294.9
Fragment 4: 162.96
Fragment 5: 206.95
Normalized Intensity
0
200000
400000
600000
800000
NCE
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

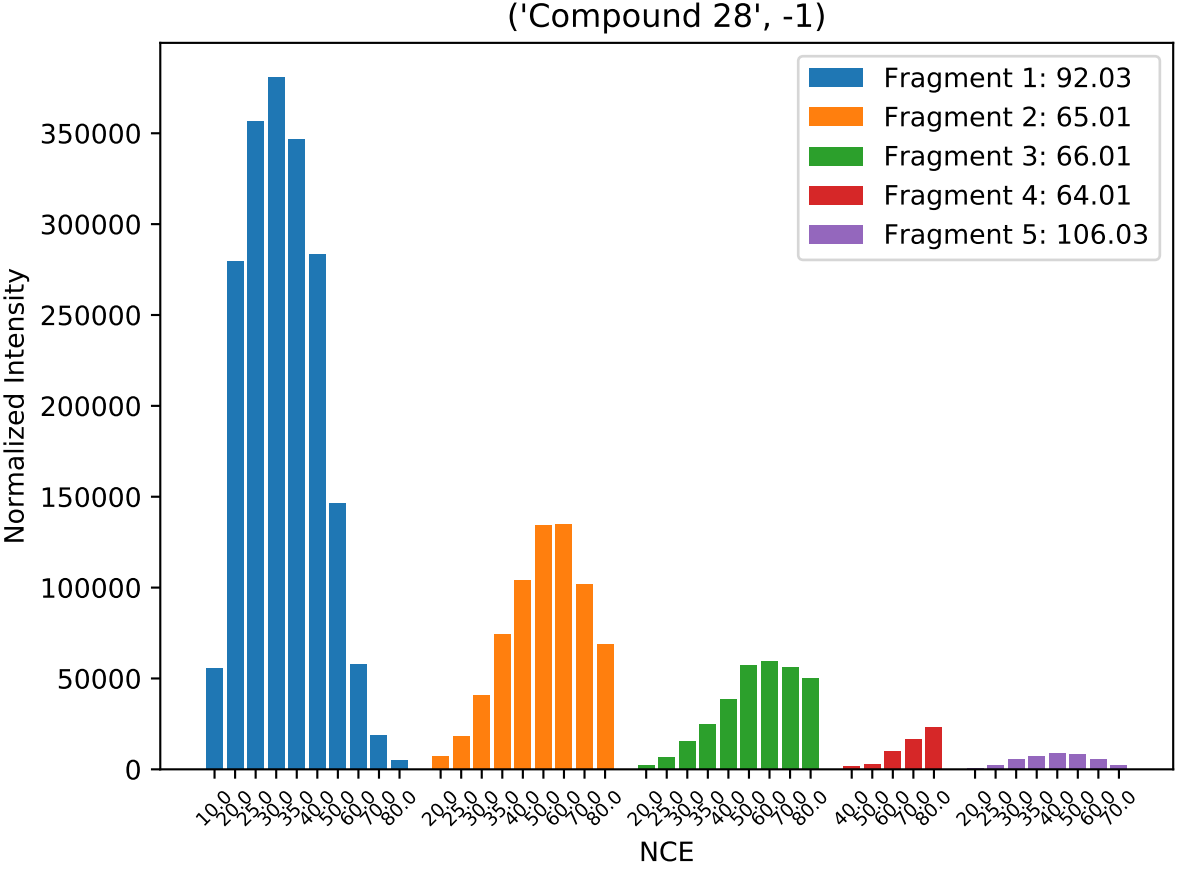

('Compound 646', -1)
Fragment 1: 294.9
Fragment 2: 312.91
Fragment 3: 59.98
Fragment 4: 188.94
Fragment 5: 206.95
Normalized Intensity
0
200000
400000
600000
800000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

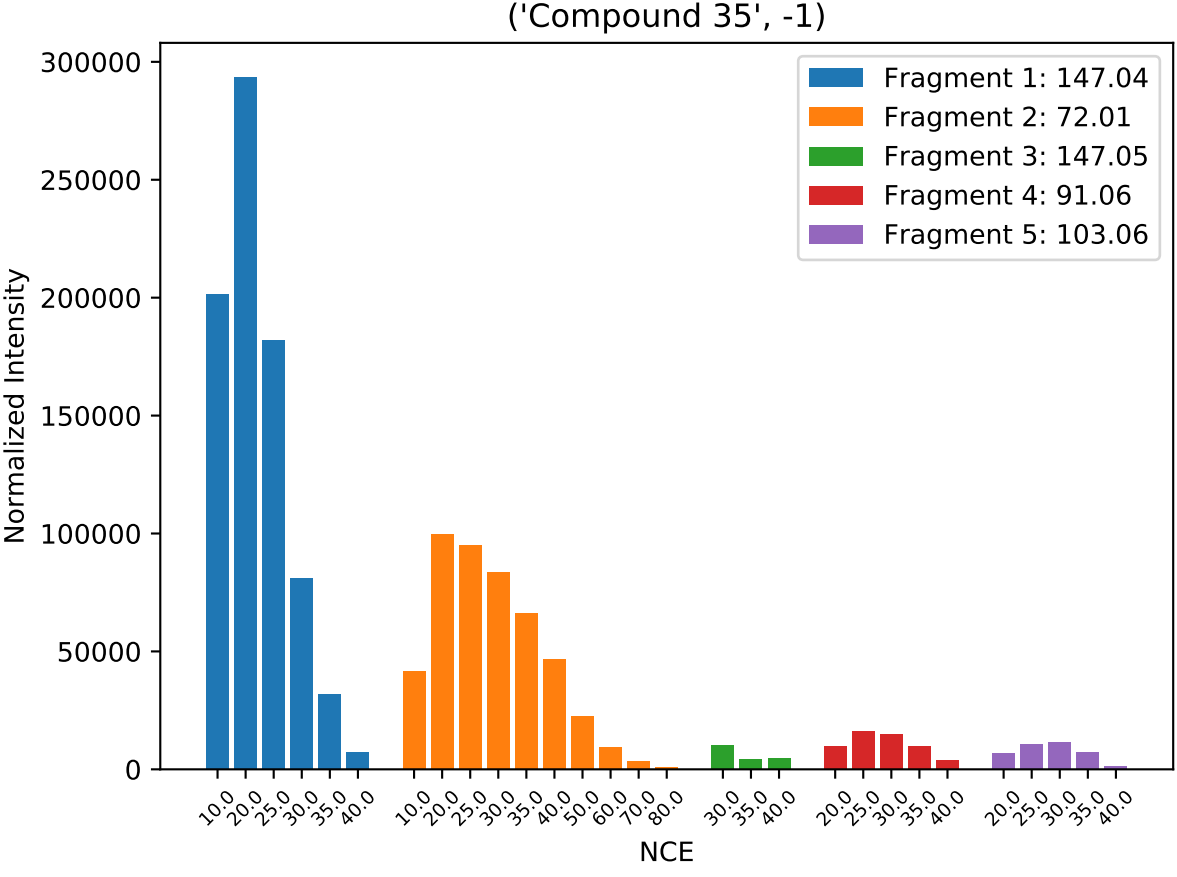

('Compound 647', -1)
Fragment 1: 163.04
Fragment 2: 119.05
Fragment 3: 93.03
Fragment 4: 72.01
Fragment 5: 59.01
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

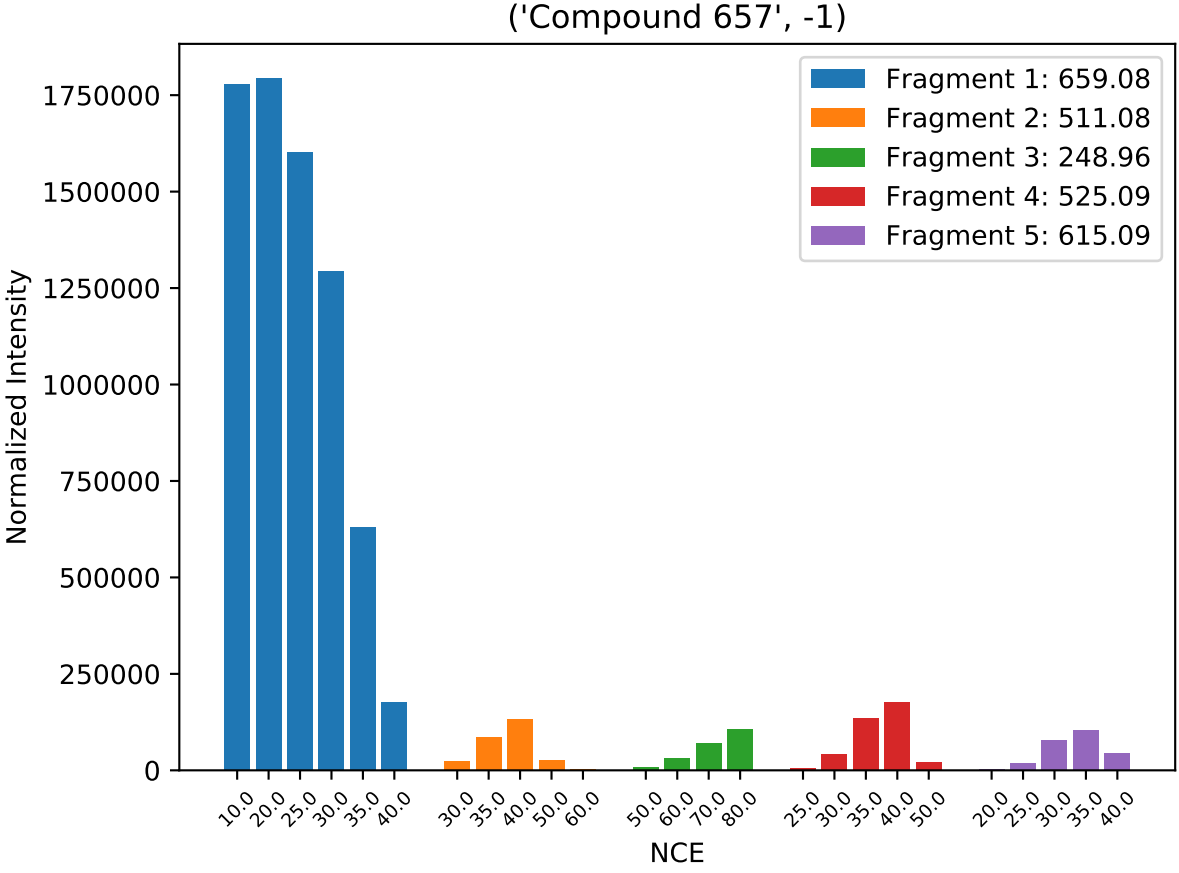

('Compound 649', -1)
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
Fragment 1: 65.63
Fragment 2: 71.43
Fragment 3: 75.95
Fragment 4: 88.22
Fragment 5: 112.32
10.0
10.0
10.0
10.0
10.0
NCE

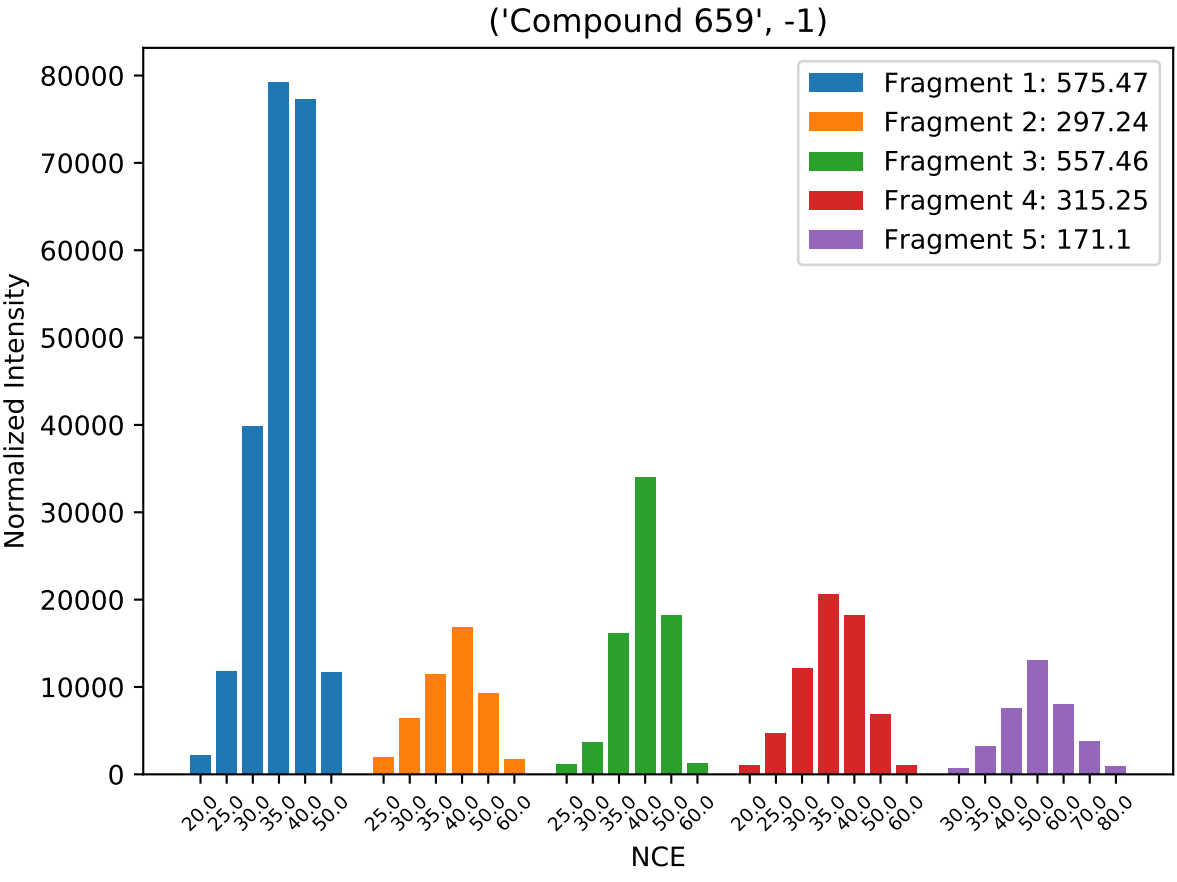

('Compound 650', -1)
Fragment 1: 188.94
Fragment 2: 206.95
Fragment 3: 59.98
Fragment 4: 173.49
Fragment 5: 162.96
Normalized Intensity
400000
300000
200000
100000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

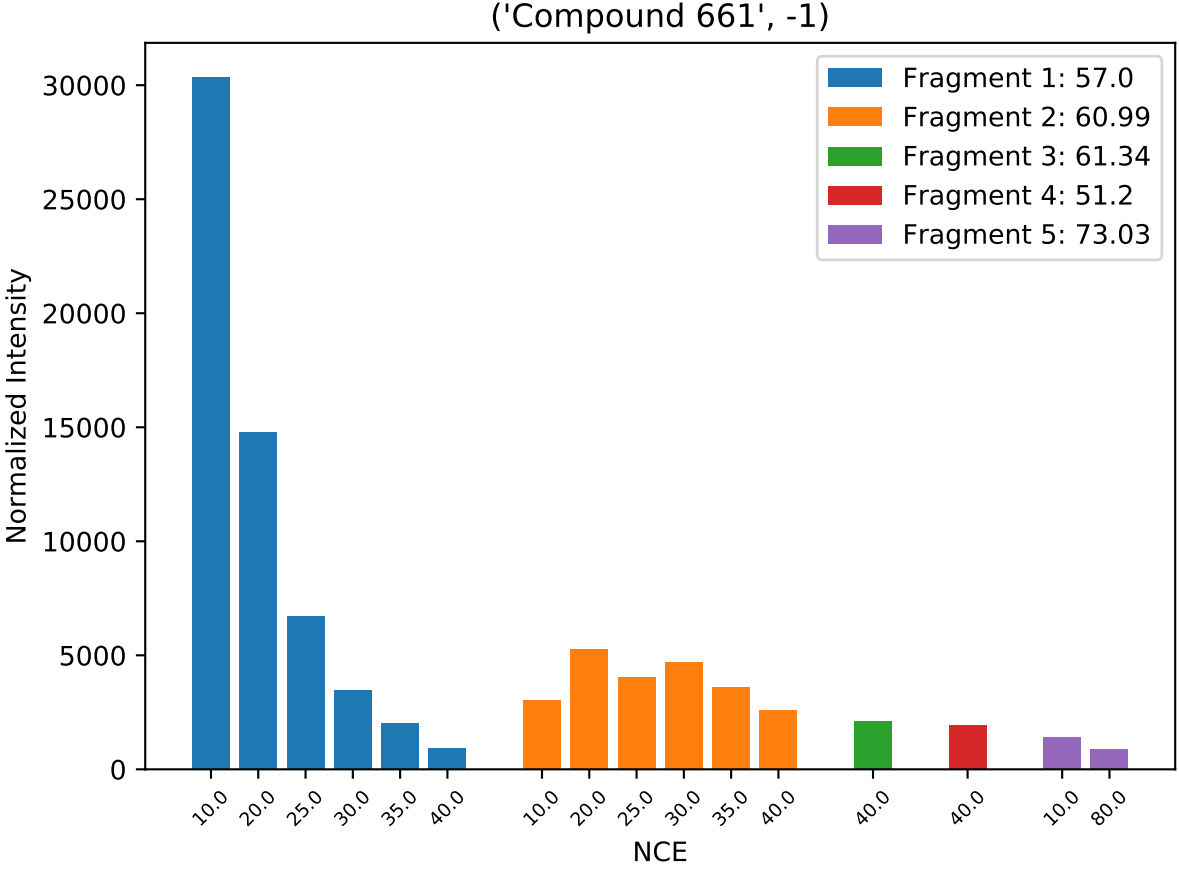

('Compound 654', -1)
Fragment 1: 57.0
Fragment 2: 59.98
Fragment 3: 77.07
Fragment 4: 89.87
Fragment 5: 61.43
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
25.0
20.0
80.0
NCE

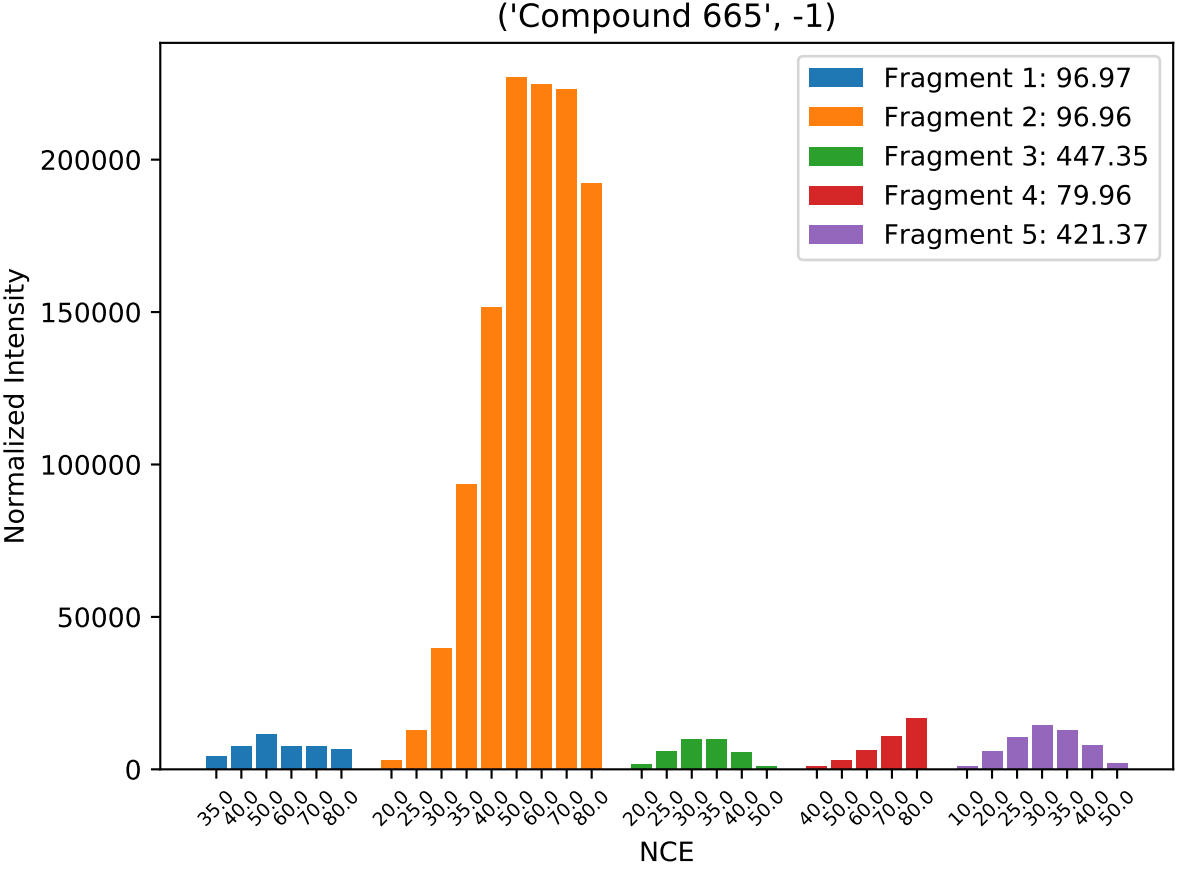

('Compound 28', -1)
Fragment 1: 92.03
Fragment 2: 65.01
Fragment 3: 66.01
Fragment 4: 64.01
Fragment 5: 106.03
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
350000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

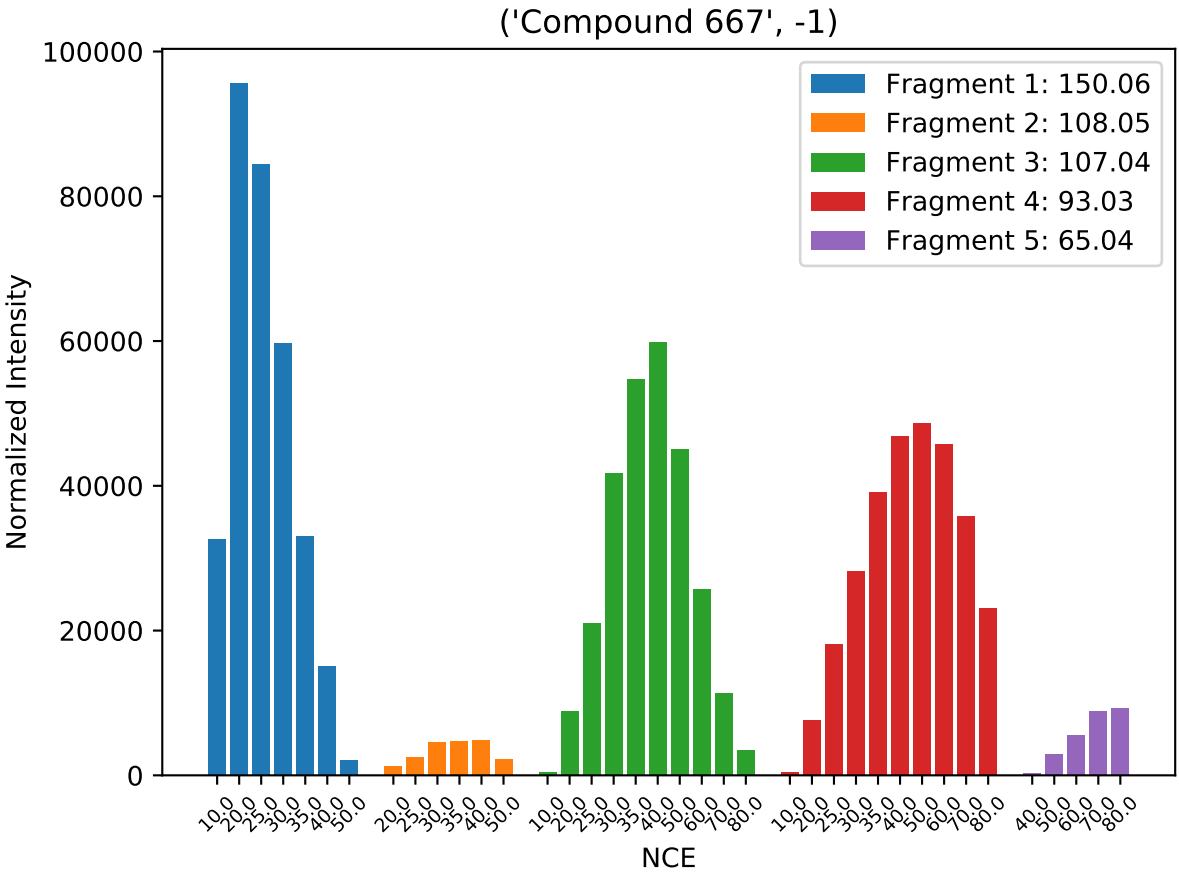

('Compound 35', -1)
Fragment 1: 147.04
Fragment 2: 72.01
Fragment 3: 147.05
Fragment 4: 91.06
Fragment 5: 103.06
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
NCE

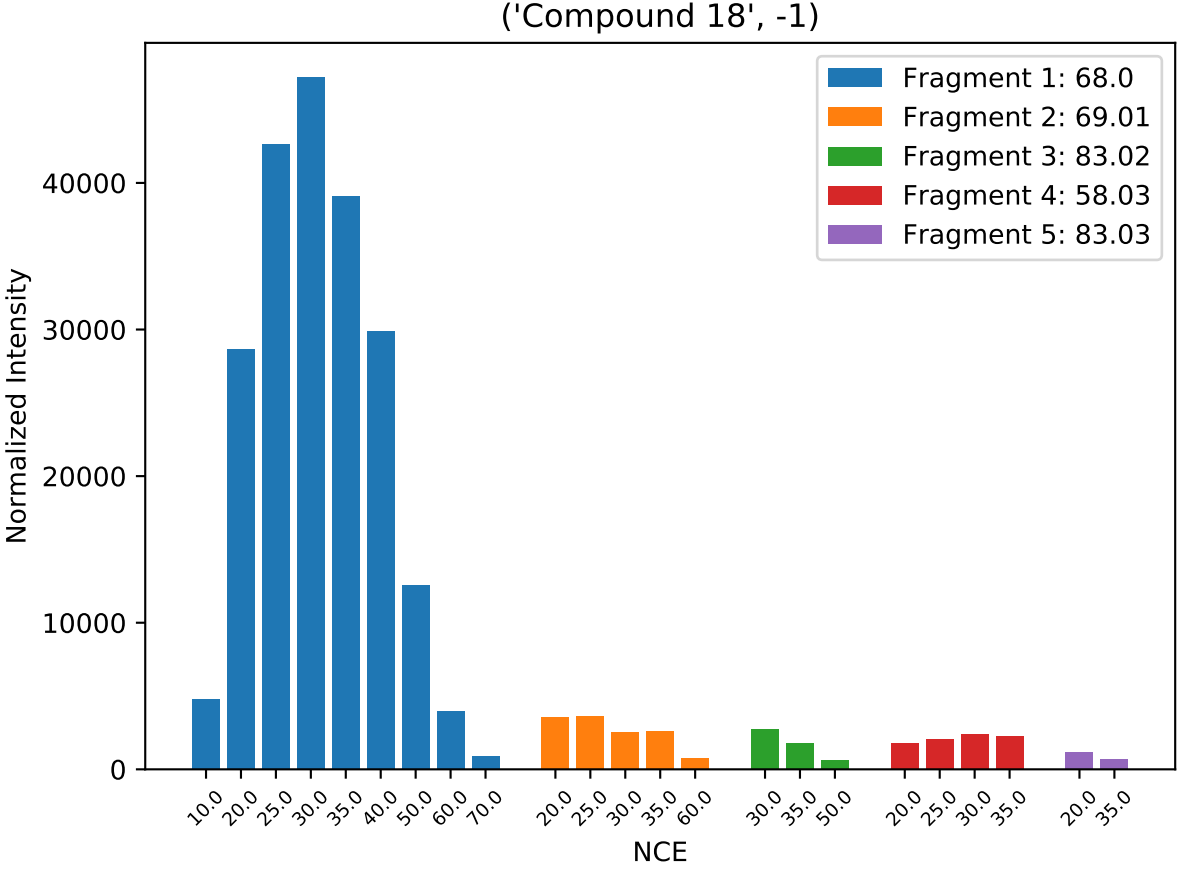

('Compound 657', -1)
Fragment 1: 659.08
Fragment 2: 511.08
Fragment 3: 248.96
Fragment 4: 525.09
Fragment 5: 615.09
Normalized Intensity
1750000
1500000
1250000
1000000
750000
500000
250000
0
10.0
20.0
25.0
30.0
35.0
40.0
30.0
35.0
40.0
50.0
60.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
NCE

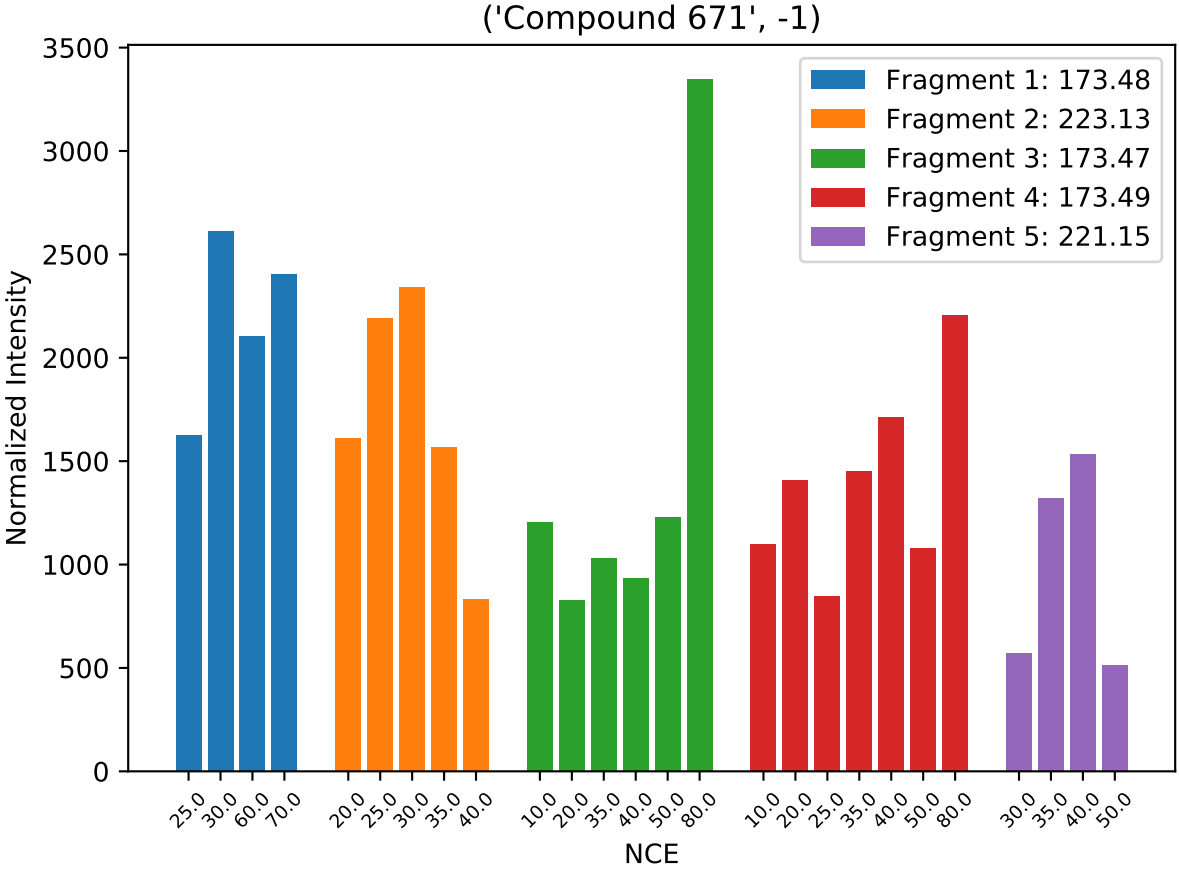

('Compound 659', -1)
Fragment 1: 575.47
Fragment 2: 297.24
Fragment 3: 557.46
Fragment 4: 315.25
Fragment 5: 171.1
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
NCE
20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

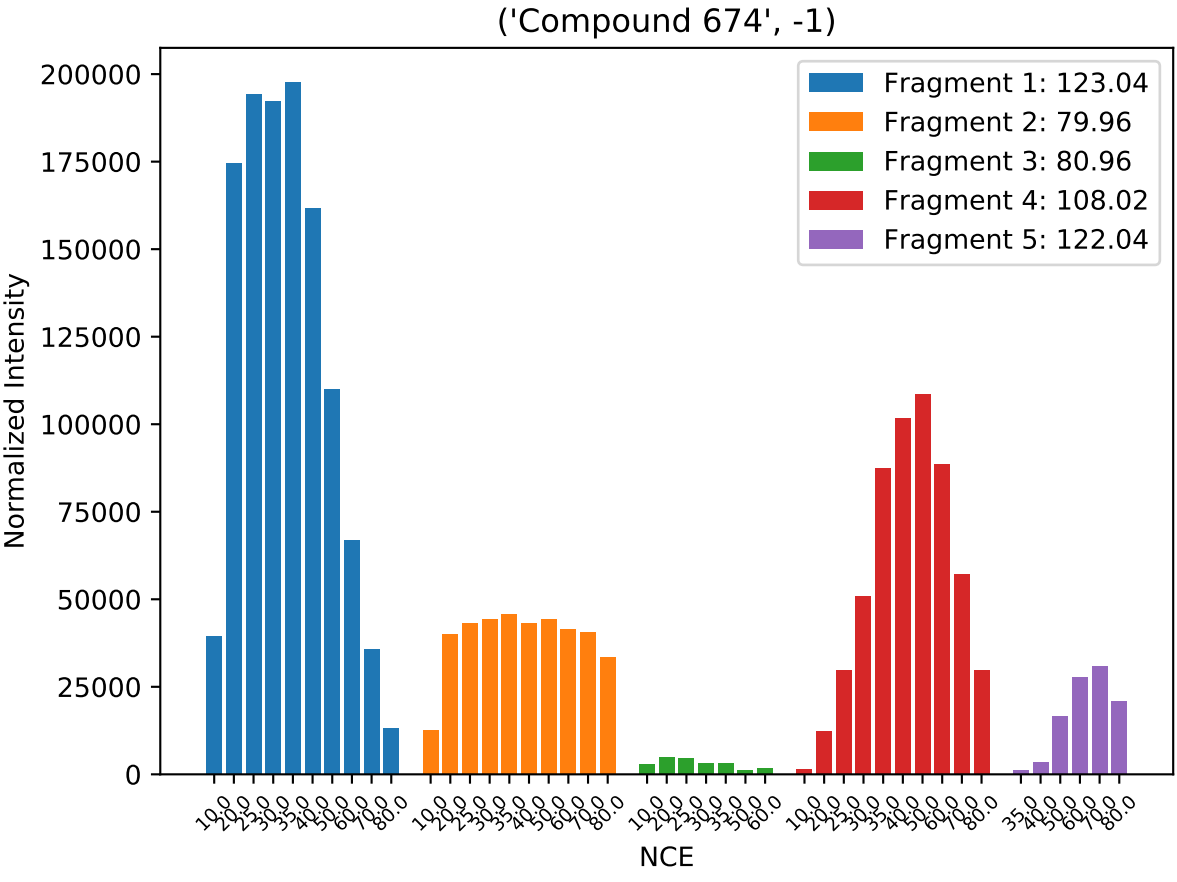

('Compound 661', -1)
Fragment 1: 57.0
Fragment 2: 60.99
Fragment 3: 61.34
Fragment 4: 51.2
Fragment 5: 73.03
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
40.0
40.0
10.0
80.0
NCE

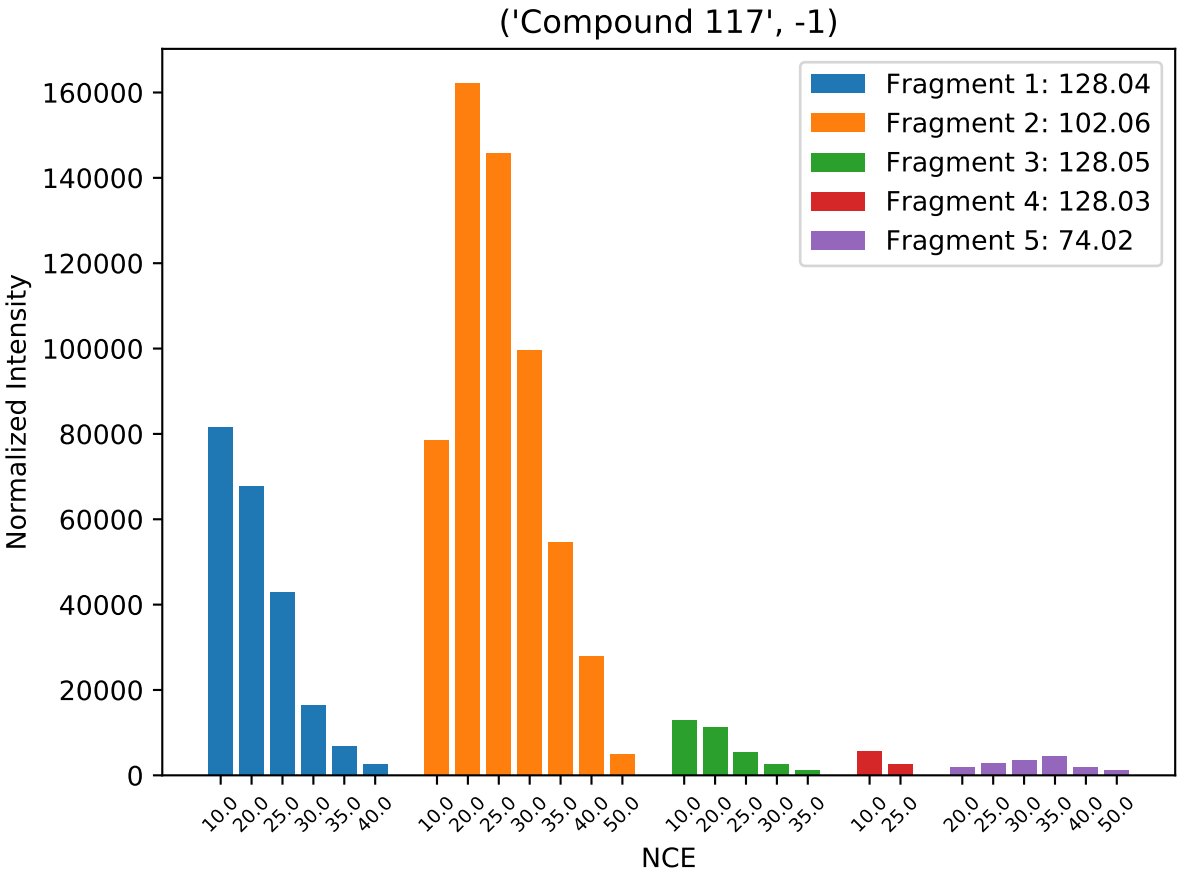

('Compound 665', -1)
Fragment 1: 96.97
Fragment 2: 96.96
Fragment 3: 447.35
Fragment 4: 79.96
Fragment 5: 421.37
Normalized Intensity
0
50000
100000
150000
200000
35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

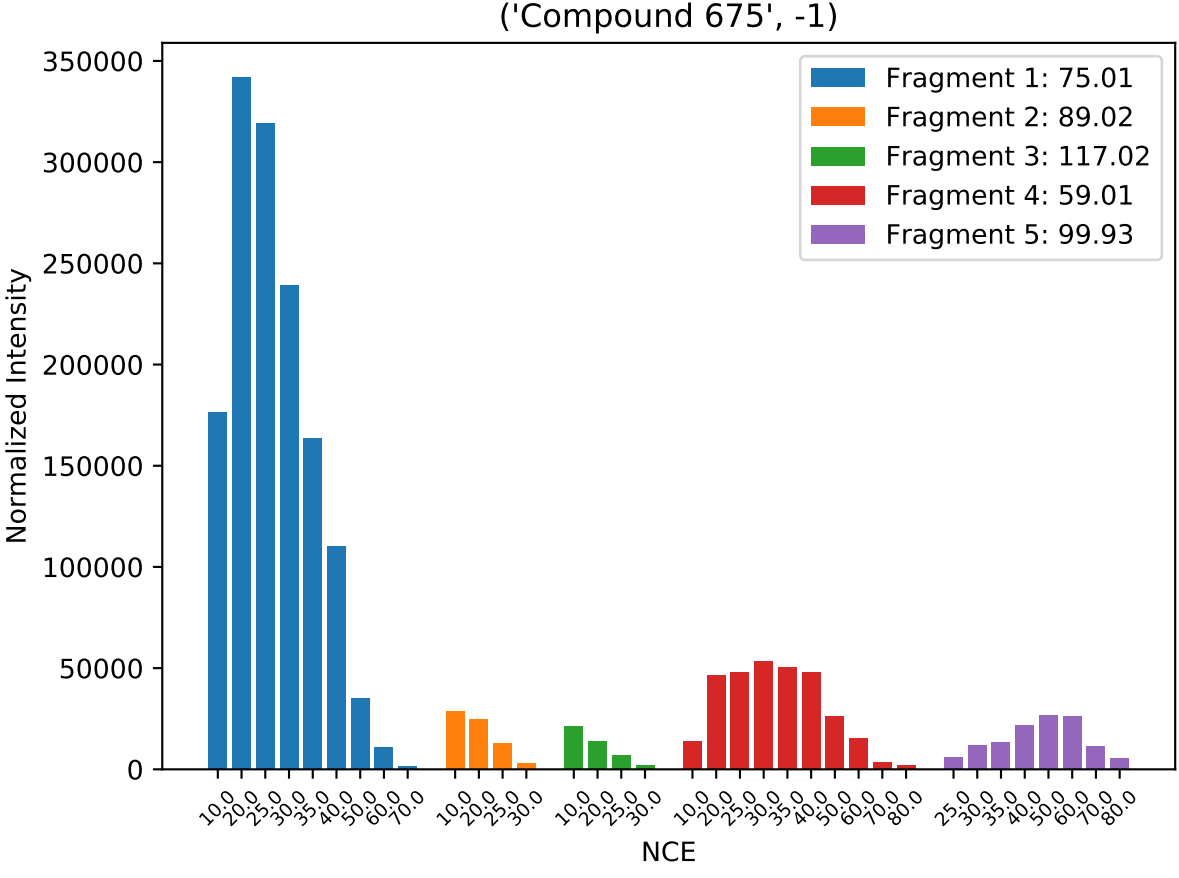

('Compound 667', -1)
Fragment 1: 150.06
Fragment 2: 108.05
Fragment 3: 107.04
Fragment 4: 93.03
Fragment 5: 65.04
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

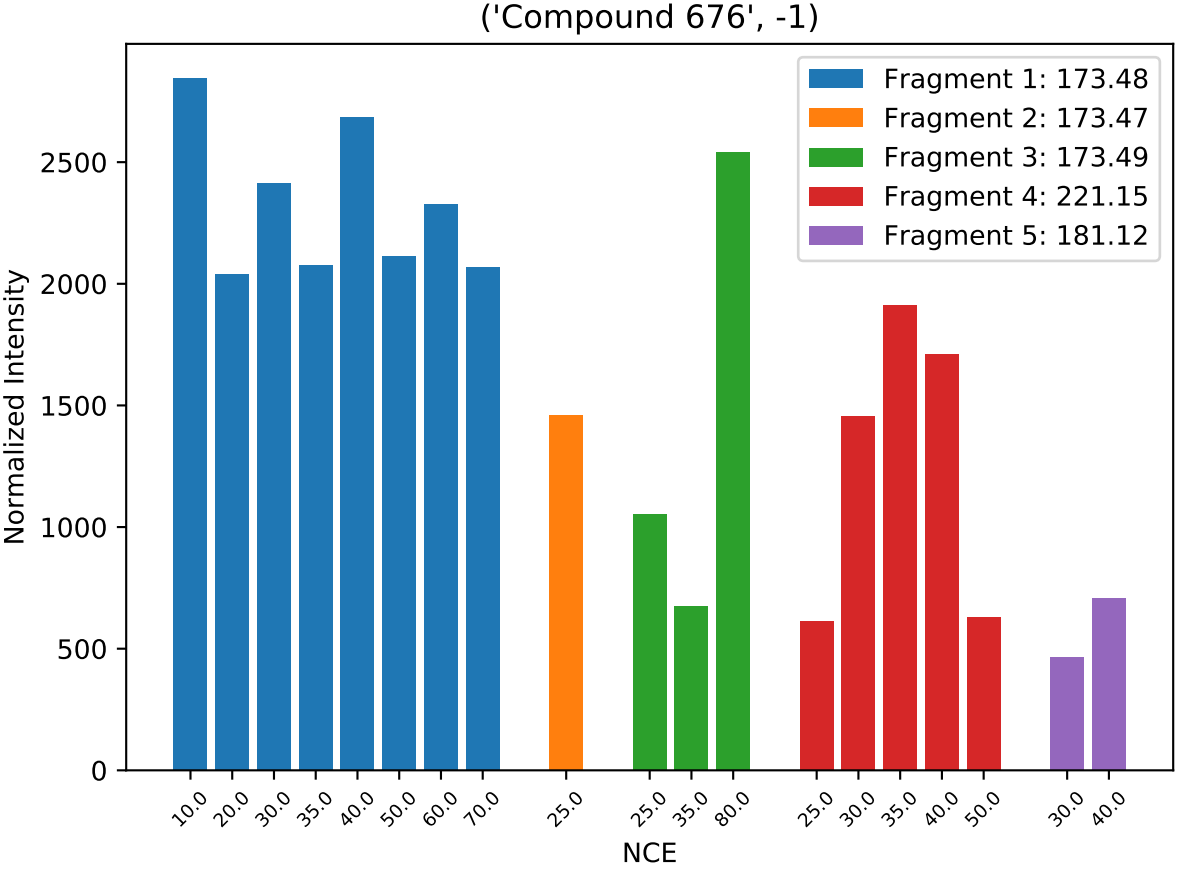

('Compound 18', -1)
Fragment 1: 68.0
Fragment 2: 69.01
Fragment 3: 83.02
Fragment 4: 58.03
Fragment 5: 83.03
Normalized Intensity
0
10000
20000
30000
40000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
60.0
30.0
35.0
50.0
20.0
25.0
30.0
35.0
20.0
35.0
NCE

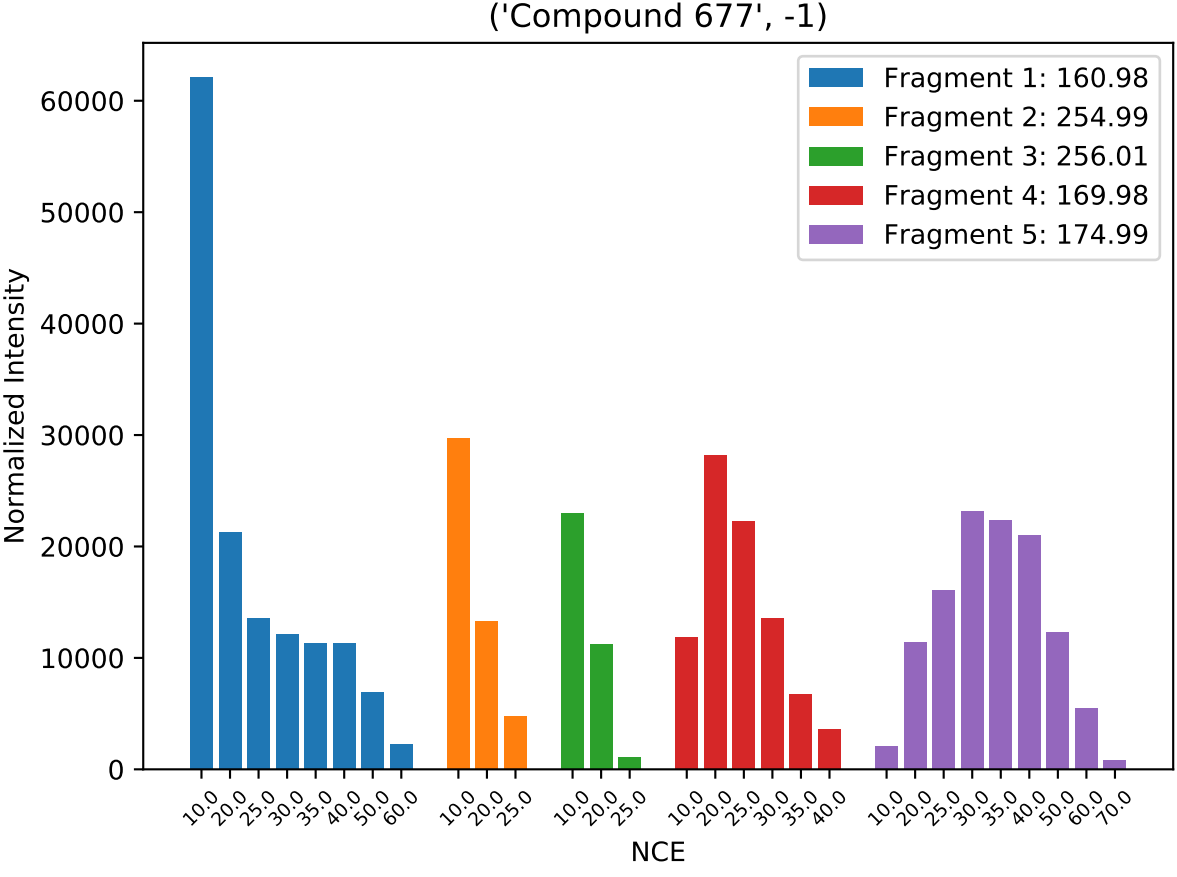

('Compound 671', -1)
Fragment 1: 173.48
Fragment 2: 223.13
Fragment 3: 173.47
Fragment 4: 173.49
Fragment 5: 221.15
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
25.0
30.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
35.0
40.0
50.0
80.0
10.0
20.0
25.0
35.0
40.0
50.0
80.0
30.0
35.0
40.0
50.0
NCE

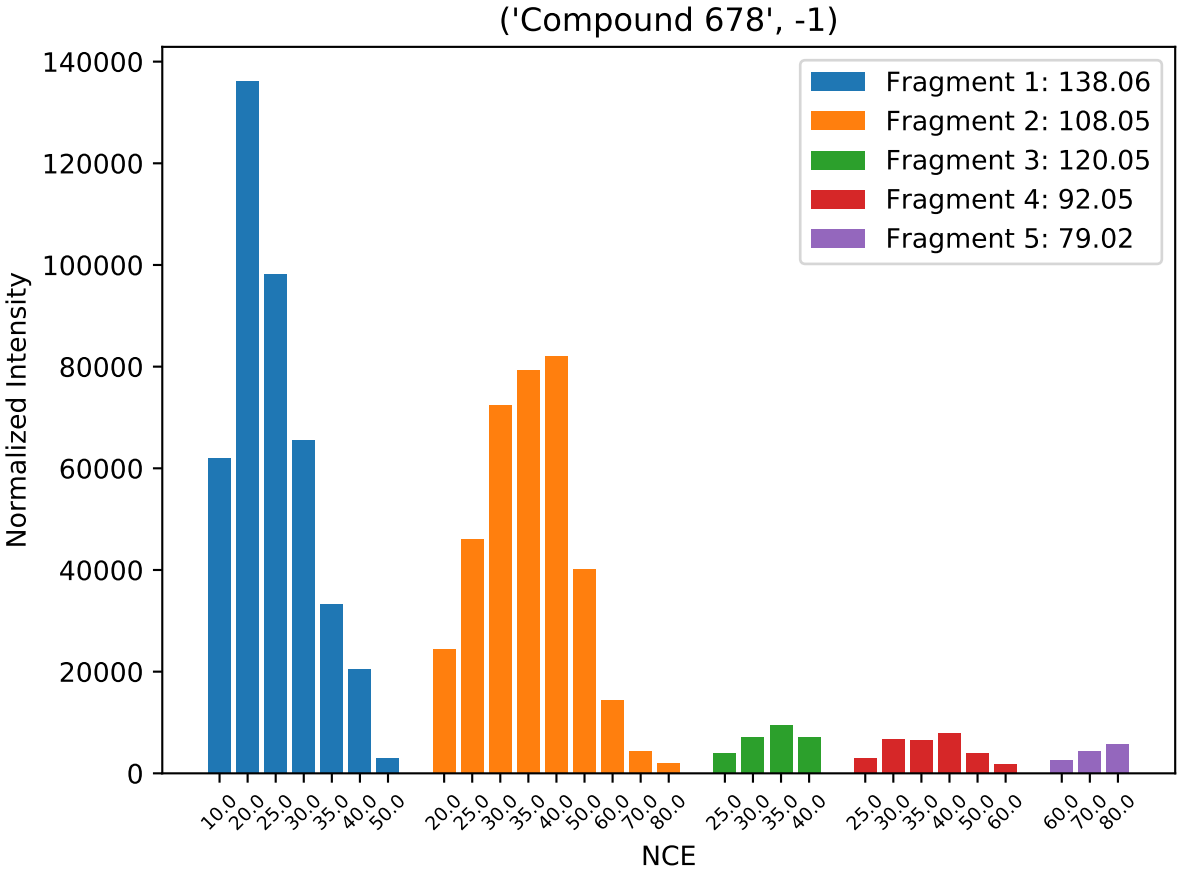

('Compound 674', -1)
Fragment 1: 123.04
Fragment 2: 79.96
Fragment 3: 80.96
Fragment 4: 108.02
Fragment 5: 122.04
Normalized Intensity
200000
175000
150000
125000
100000
75000
50000
25000
0
NCE
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0

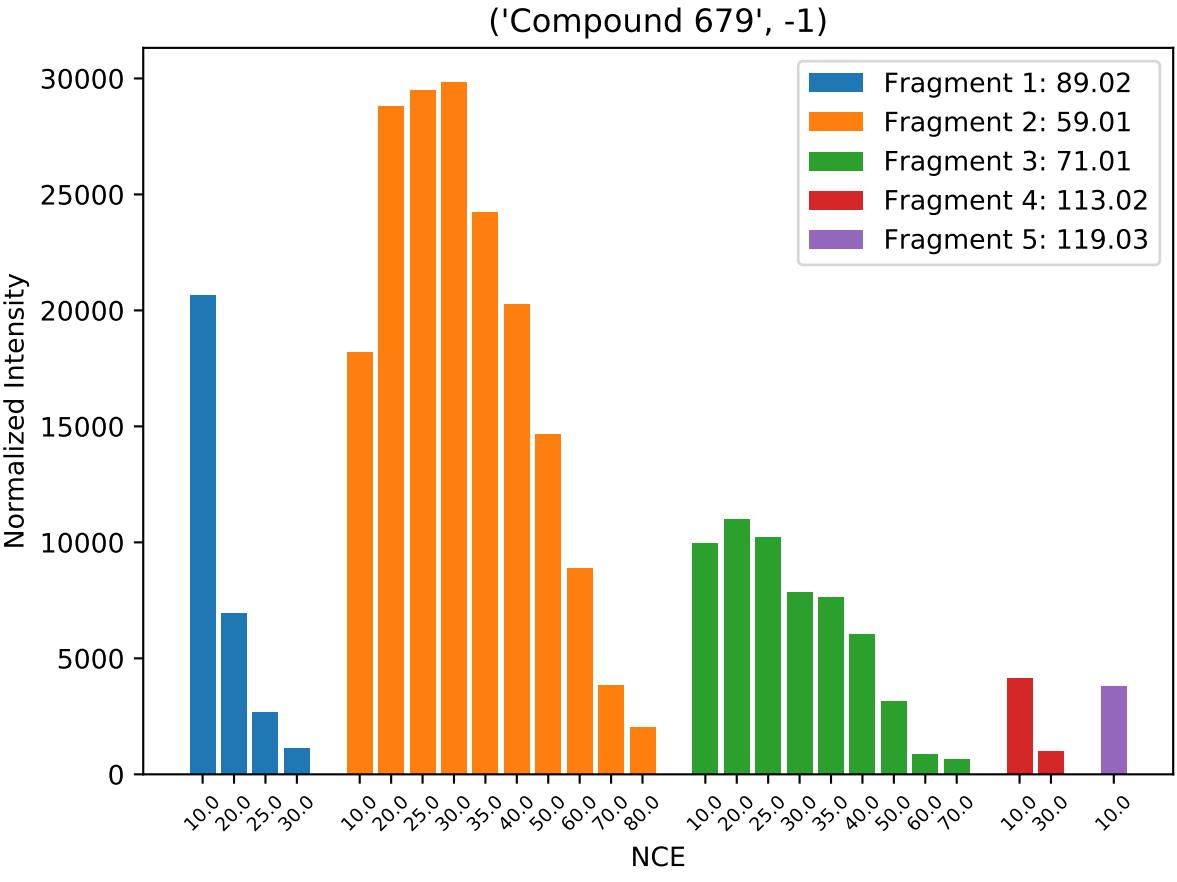

('Compound 117', -1)
Fragment 1: 128.04
Fragment 2: 102.06
Fragment 3: 128.05
Fragment 4: 128.03
Fragment 5: 74.02
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
10.0
25.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

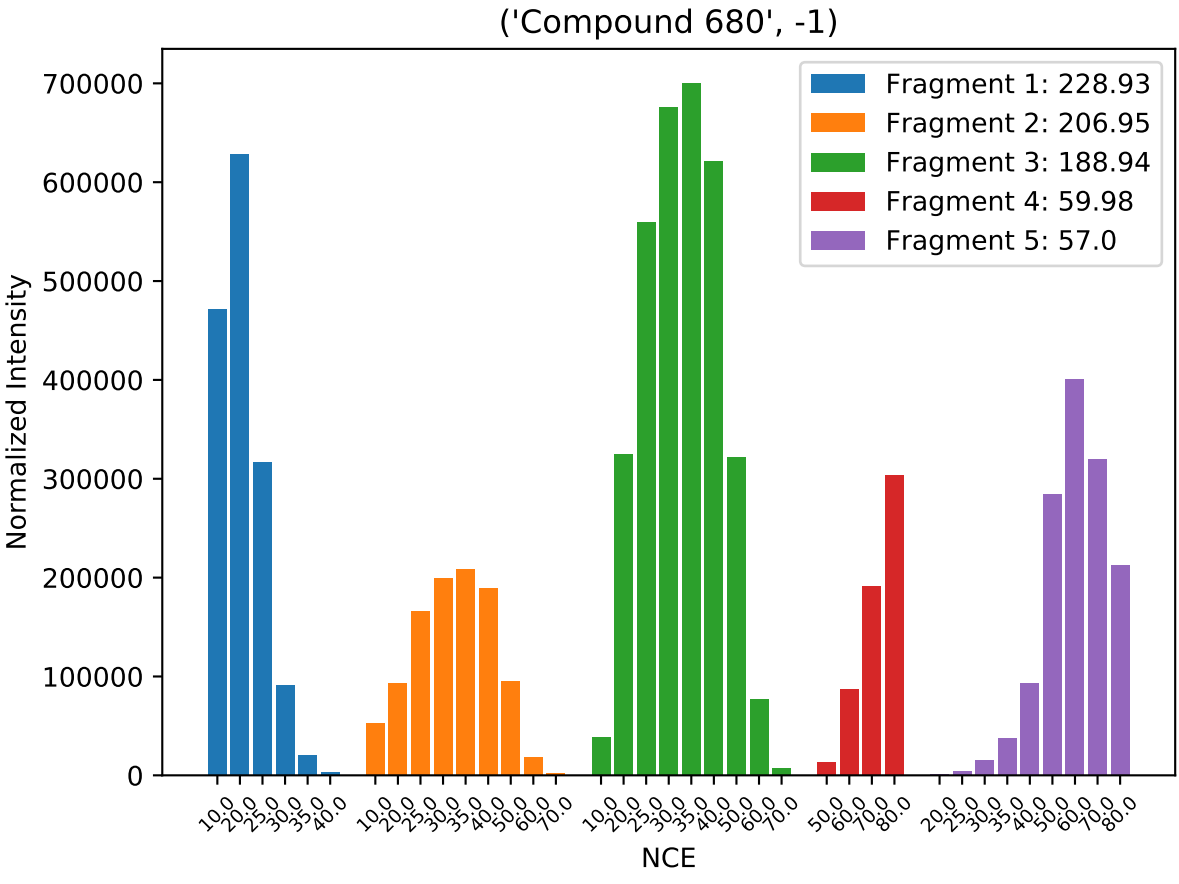

('Compound 675', -1)
Fragment 1: 75.01
Fragment 2: 89.02
Fragment 3: 117.02
Fragment 4: 59.01
Fragment 5: 99.93
Normalized Intensity
350000
300000
250000
200000
150000
100000
50000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

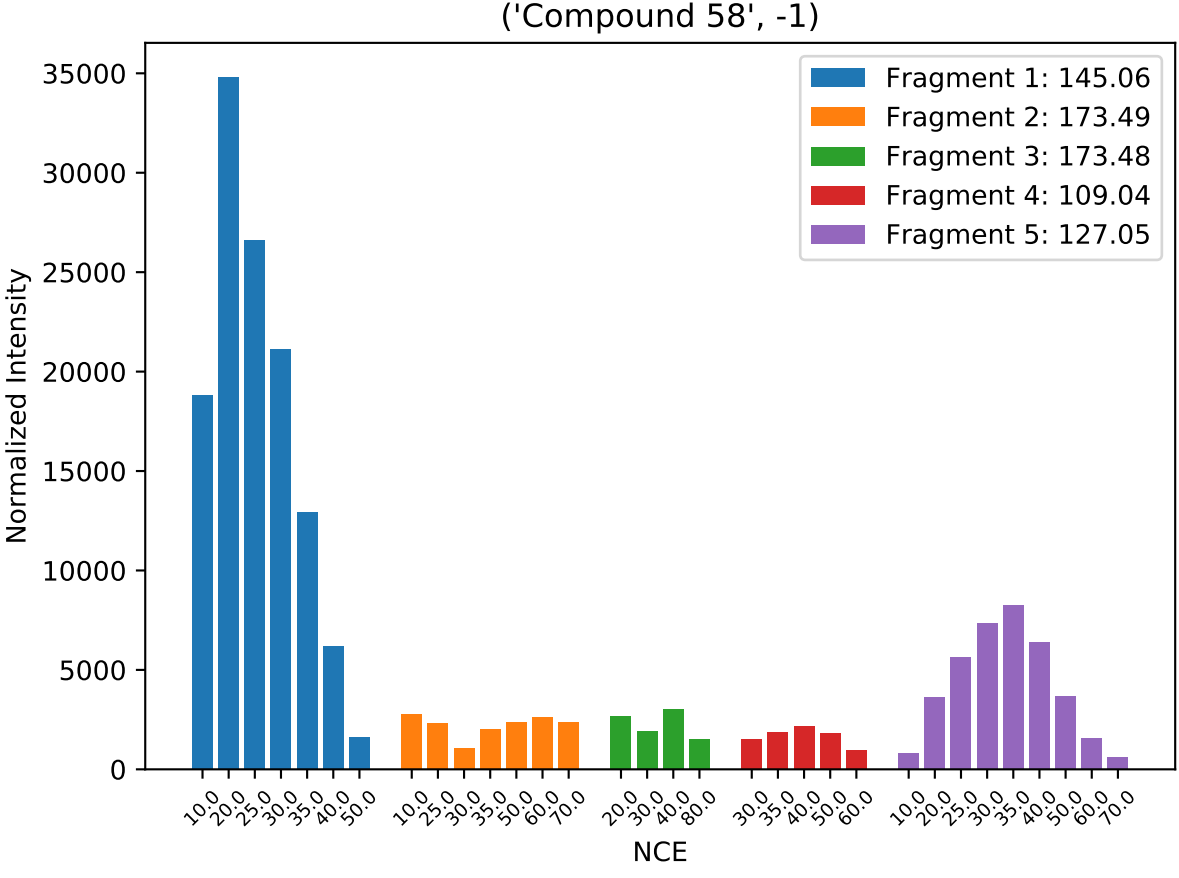

('Compound 676', -1)
Fragment 1: 173.48
Fragment 2: 173.47
Fragment 3: 173.49
Fragment 4: 221.15
Fragment 5: 181.12
Normalized Intensity
0
500
1000
1500
2000
2500
10.0
20.0
30.0
35.0
40.0
50.0
60.0
70.0
25.0
25.0
35.0
80.0
25.0
30.0
35.0
40.0
50.0
30.0
40.0
NCE

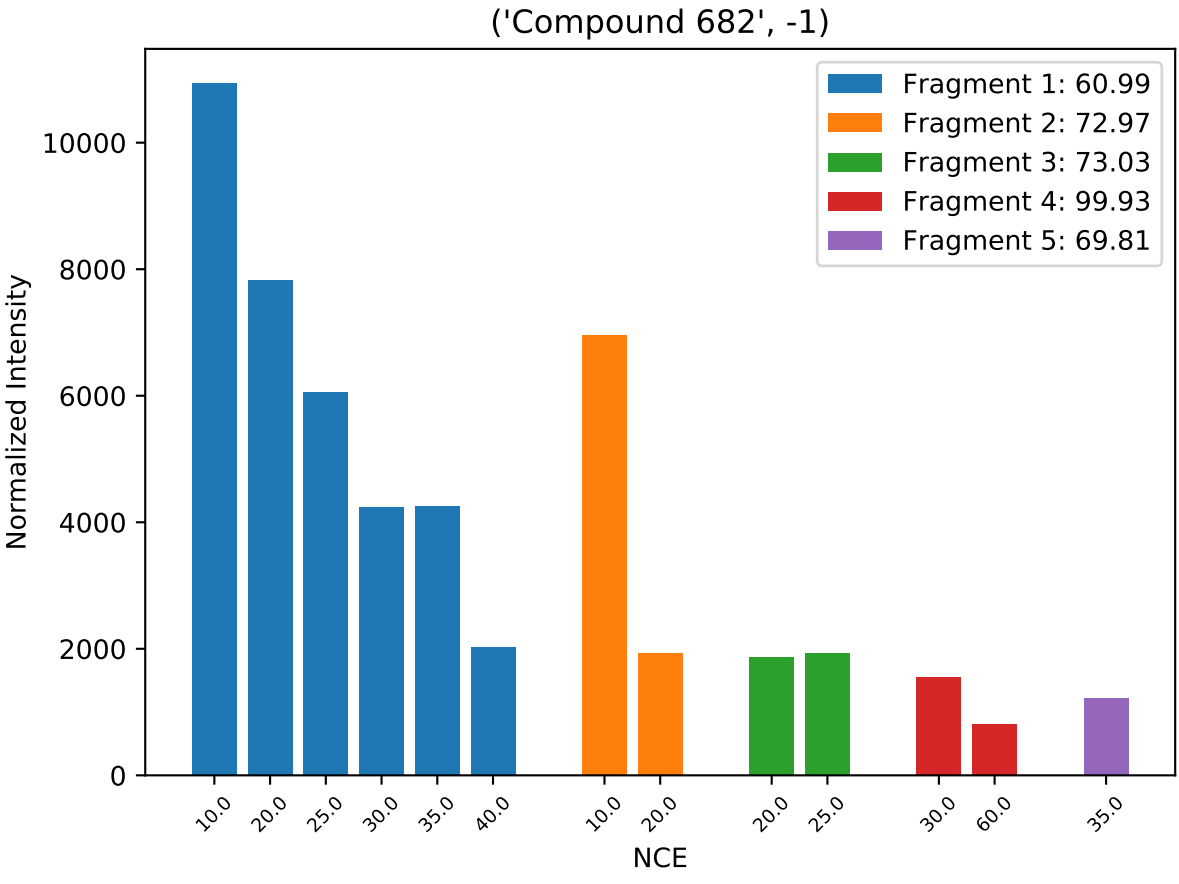

('Compound 677', -1)
Fragment 1: 160.98
Fragment 2: 254.99
Fragment 3: 256.01
Fragment 4: 169.98
Fragment 5: 174.99
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

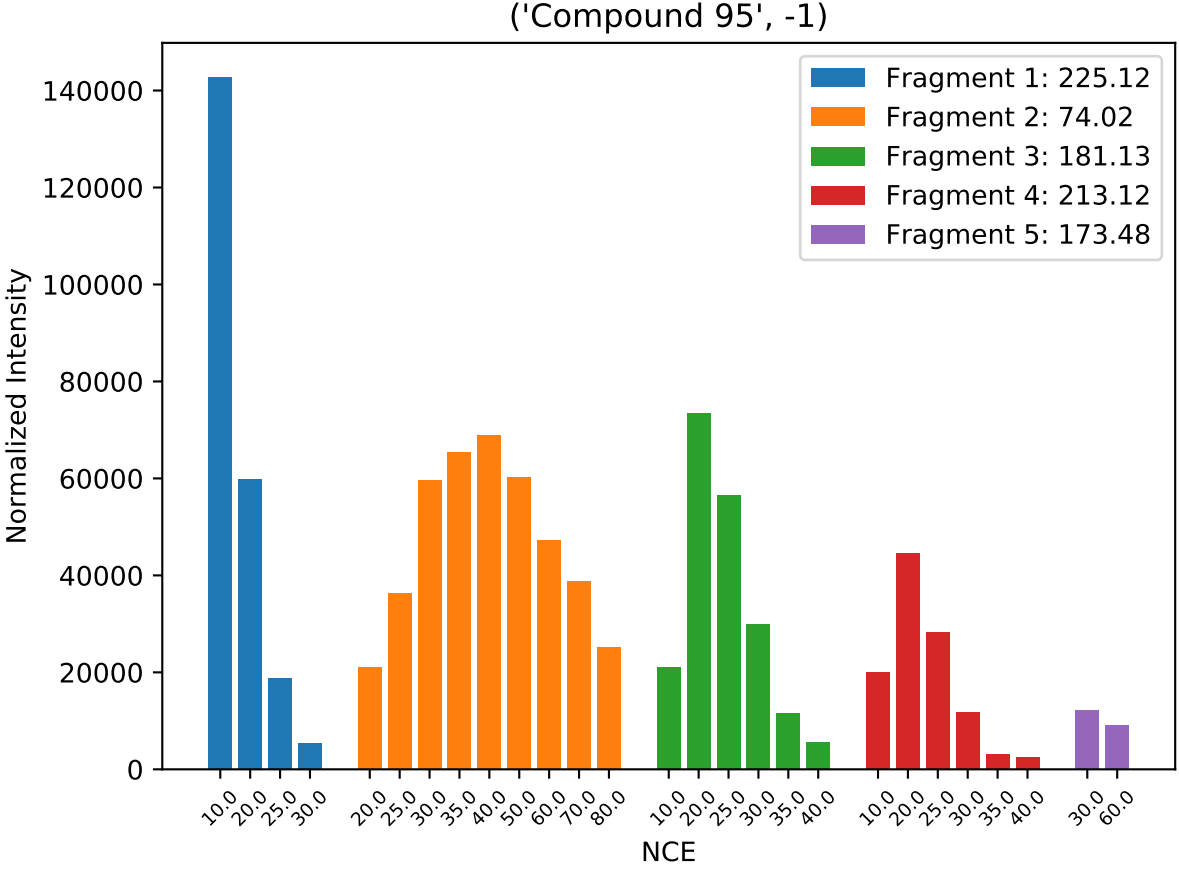

('Compound 678', -1)
Fragment 1: 138.06
Fragment 2: 108.05
Fragment 3: 120.05
Fragment 4: 92.05
Fragment 5: 79.02
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
25.0
30.0
35.0
40.0
50.0
60.0
60.0
70.0
80.0
NCE

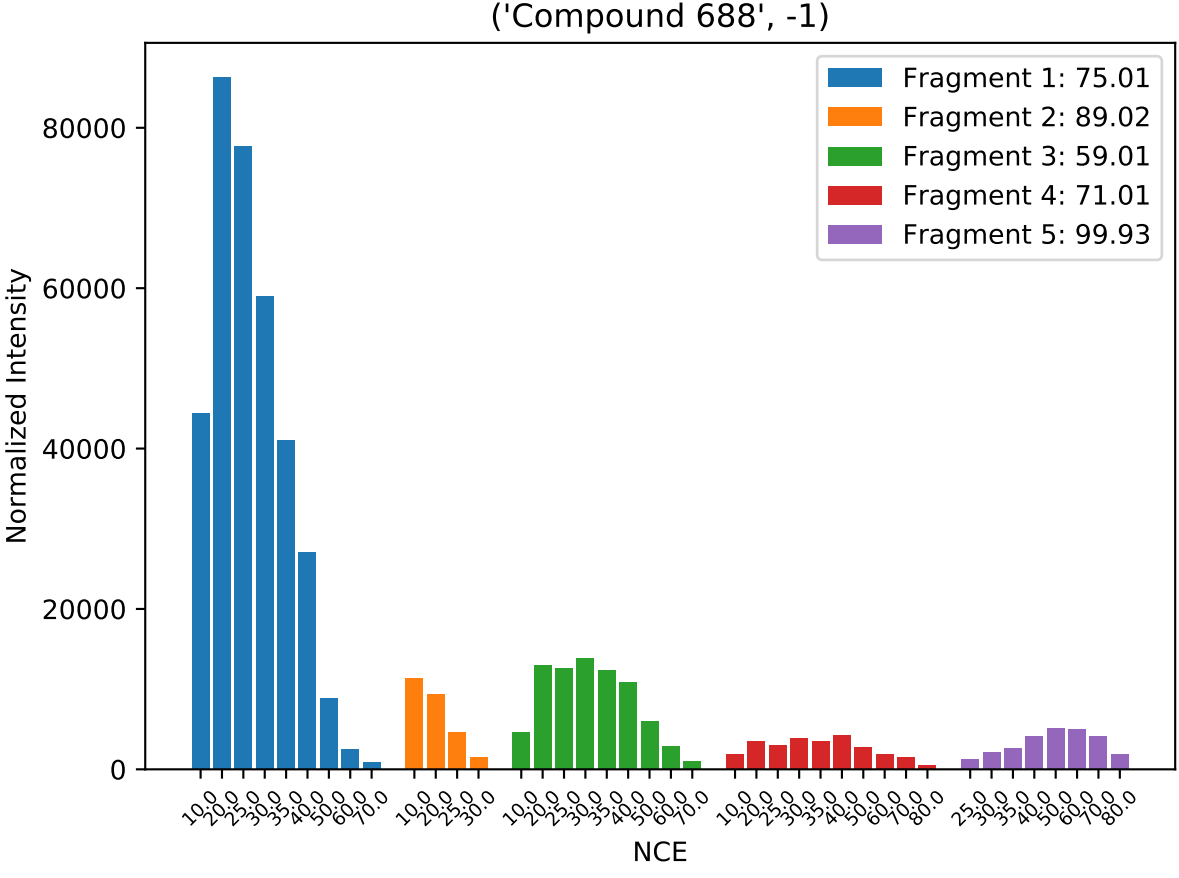

('Compound 679', -1)
Fragment 1: 89.02
Fragment 2: 59.01
Fragment 3: 71.01
Fragment 4: 113.02
Fragment 5: 119.03
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
30.0
10.0
NCE

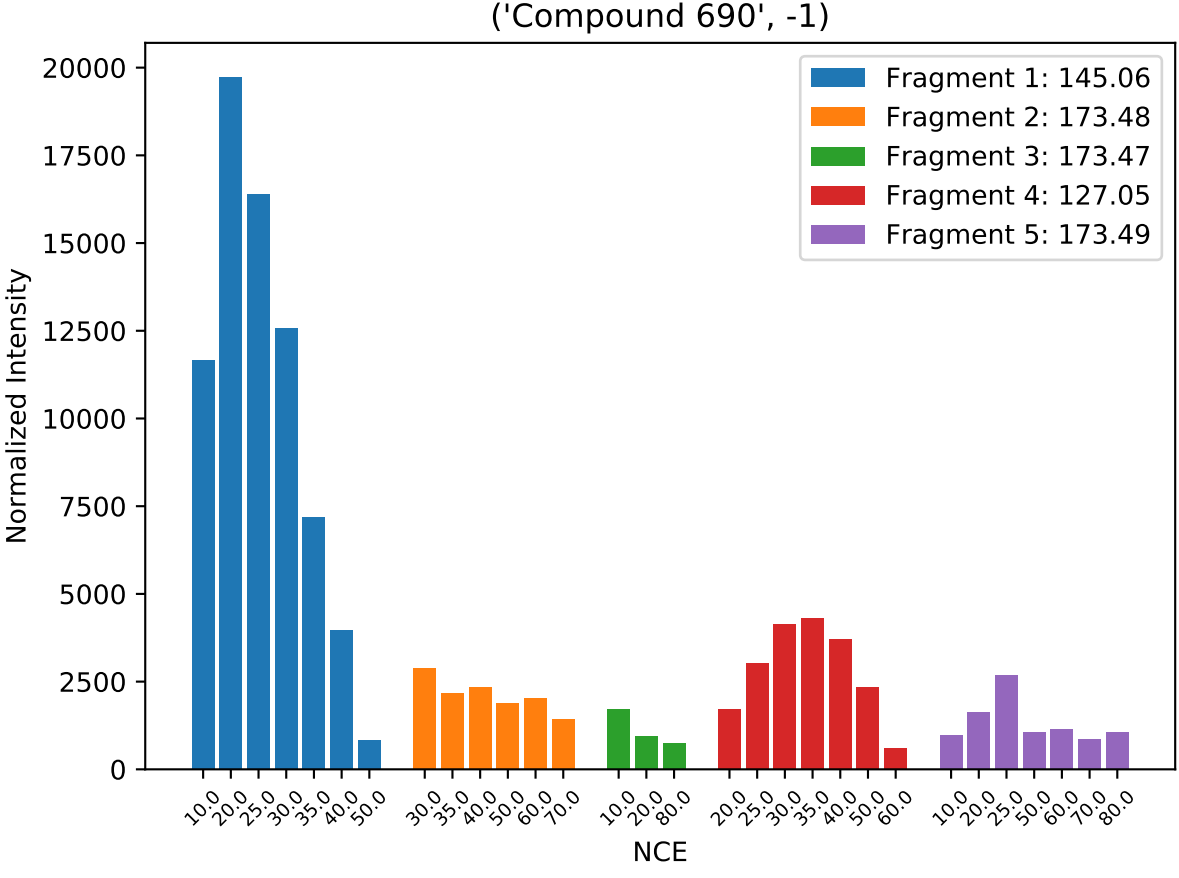

('Compound 680', -1)
Fragment 1: 228.93
Fragment 2: 206.95
Fragment 3: 188.94
Fragment 4: 59.98
Fragment 5: 57.0
Normalized Intensity
NCE
0
100000
200000
300000
400000
500000
600000
700000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

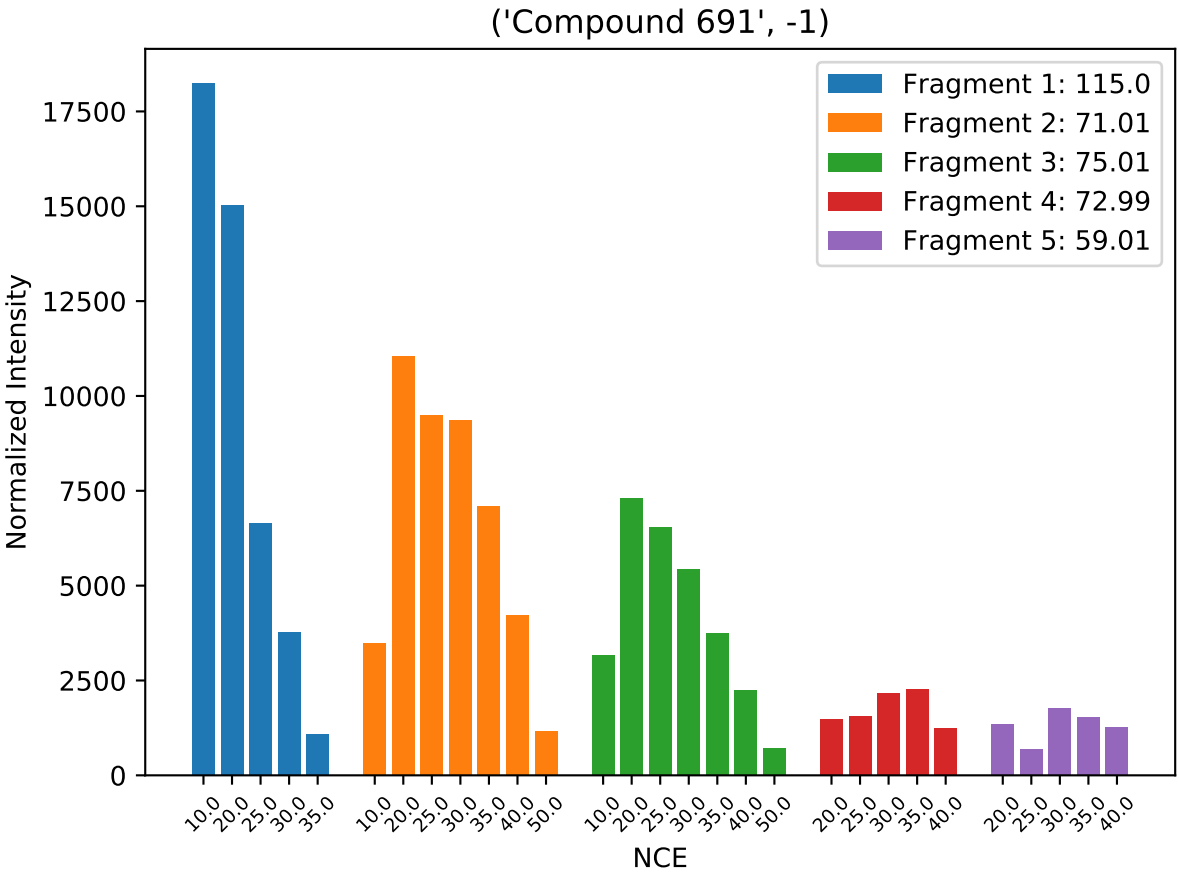

('Compound 58', -1)
Fragment 1: 145.06
Fragment 2: 173.49
Fragment 3: 173.48
Fragment 4: 109.04
Fragment 5: 127.05
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 25.0 30.0 35.0 50.0 60.0 70.0
20.0 30.0 40.0 80.0
30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

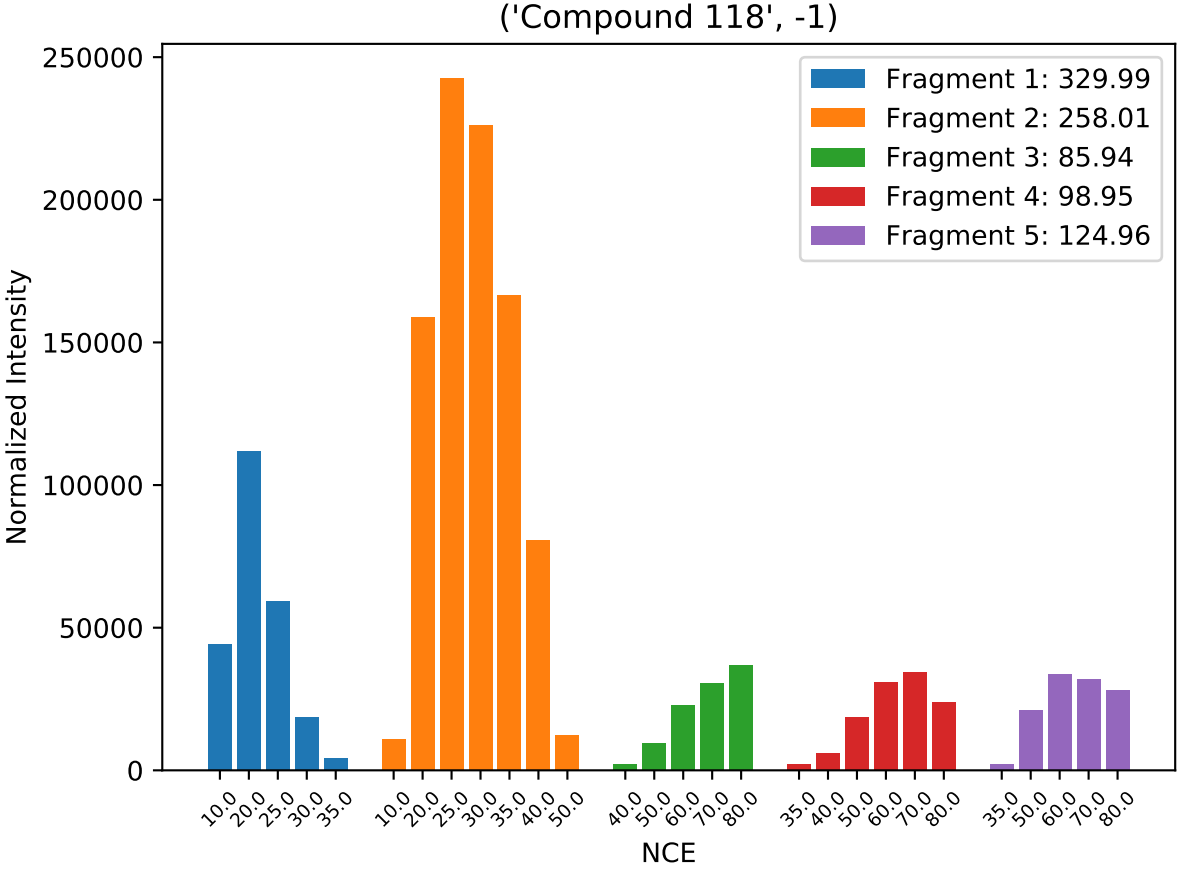

('Compound 682', -1)
Fragment 1: 60.99
Fragment 2: 72.97
Fragment 3: 73.03
Fragment 4: 99.93
Fragment 5: 69.81
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
20.0
25.0
30.0
60.0
35.0
NCE

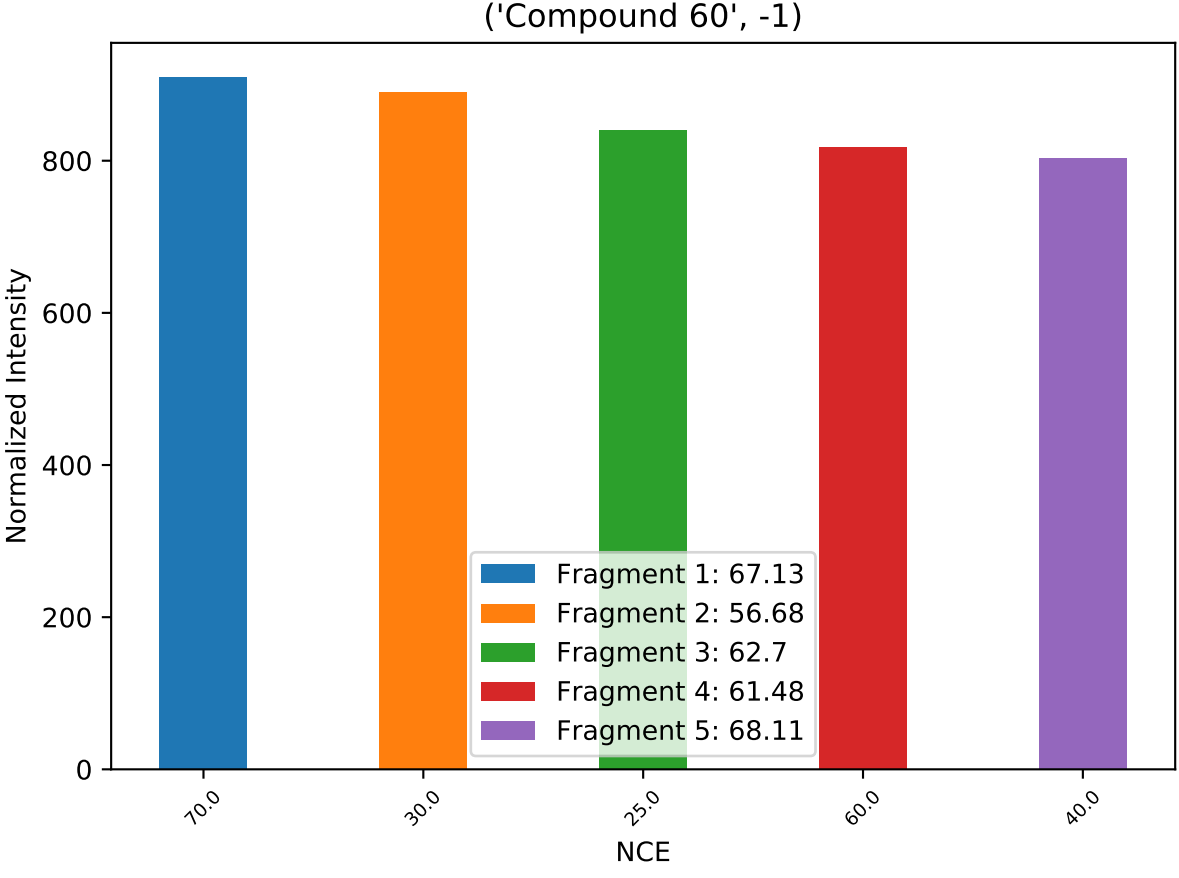

('Compound 95', -1)
Fragment 1: 225.12
Fragment 2: 74.02
Fragment 3: 181.13
Fragment 4: 213.12
Fragment 5: 173.48
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
10.0
20.0
25.0
30.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
30.0
60.0
NCE

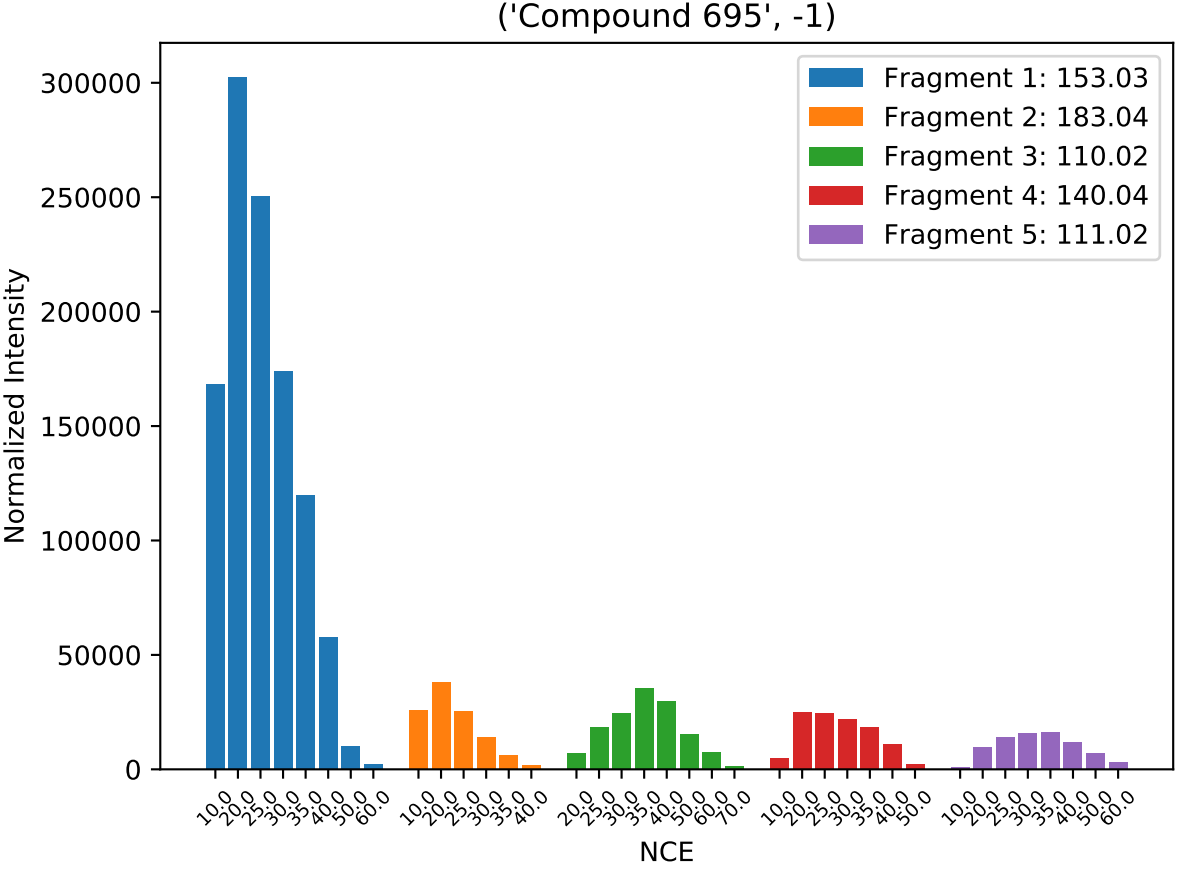

('Compound 688', -1)
Fragment 1: 75.01
Fragment 2: 89.02
Fragment 3: 59.01
Fragment 4: 71.01
Fragment 5: 99.93
Normalized Intensity
0
20000
40000
60000
80000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

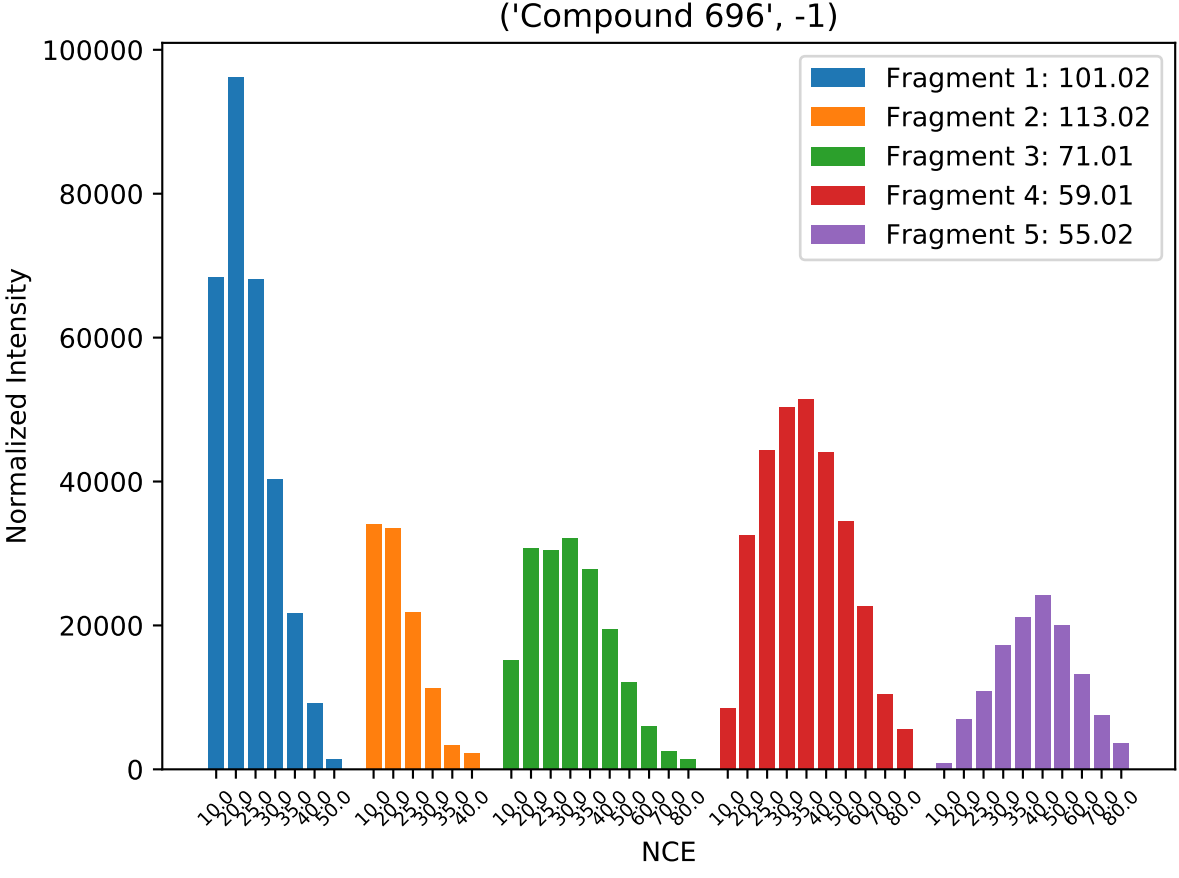

('Compound 690', -1)
Fragment 1: 145.06
Fragment 2: 173.48
Fragment 3: 173.47
Fragment 4: 127.05
Fragment 5: 173.49
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 50.0 60.0 70.0 80.0
NCE

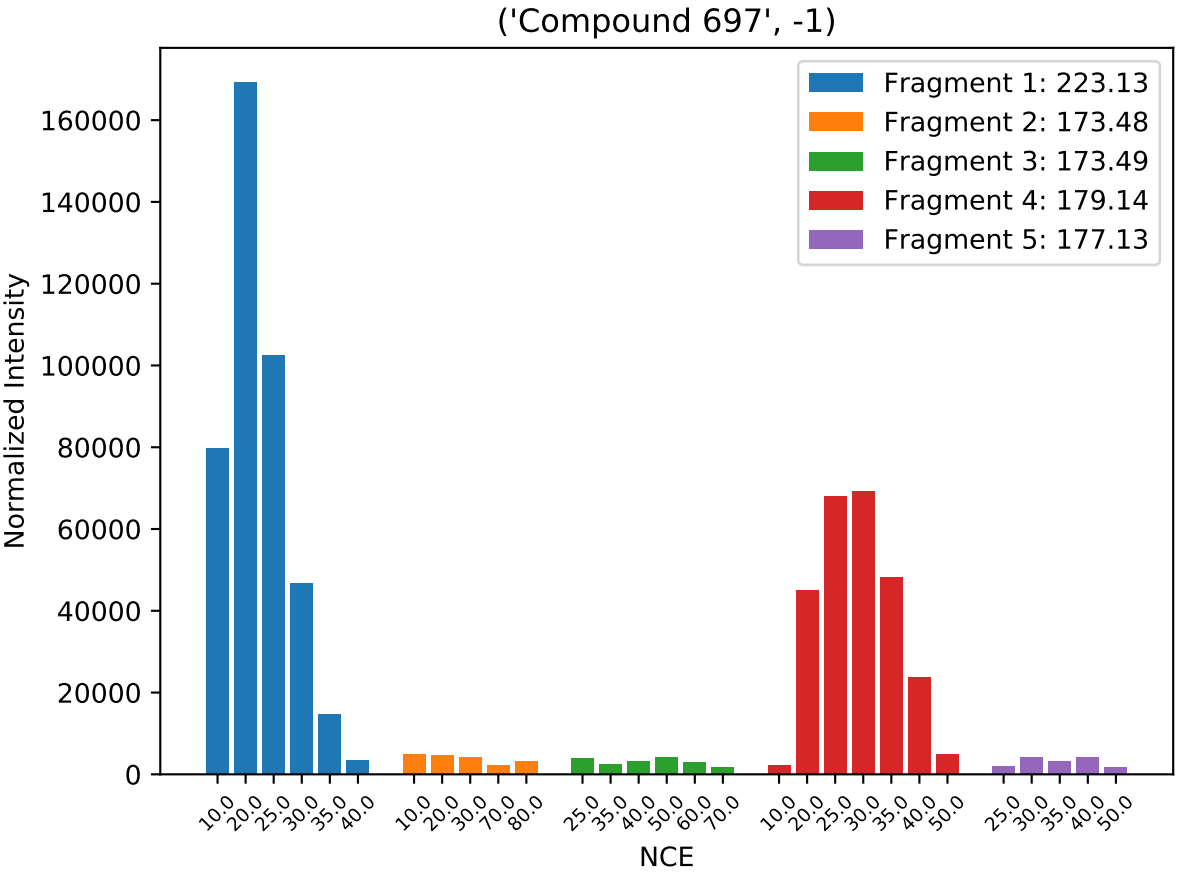

('Compound 691', -1)
Fragment 1: 115.0
Fragment 2: 71.01
Fragment 3: 75.01
Fragment 4: 72.99
Fragment 5: 59.01
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0
NCE

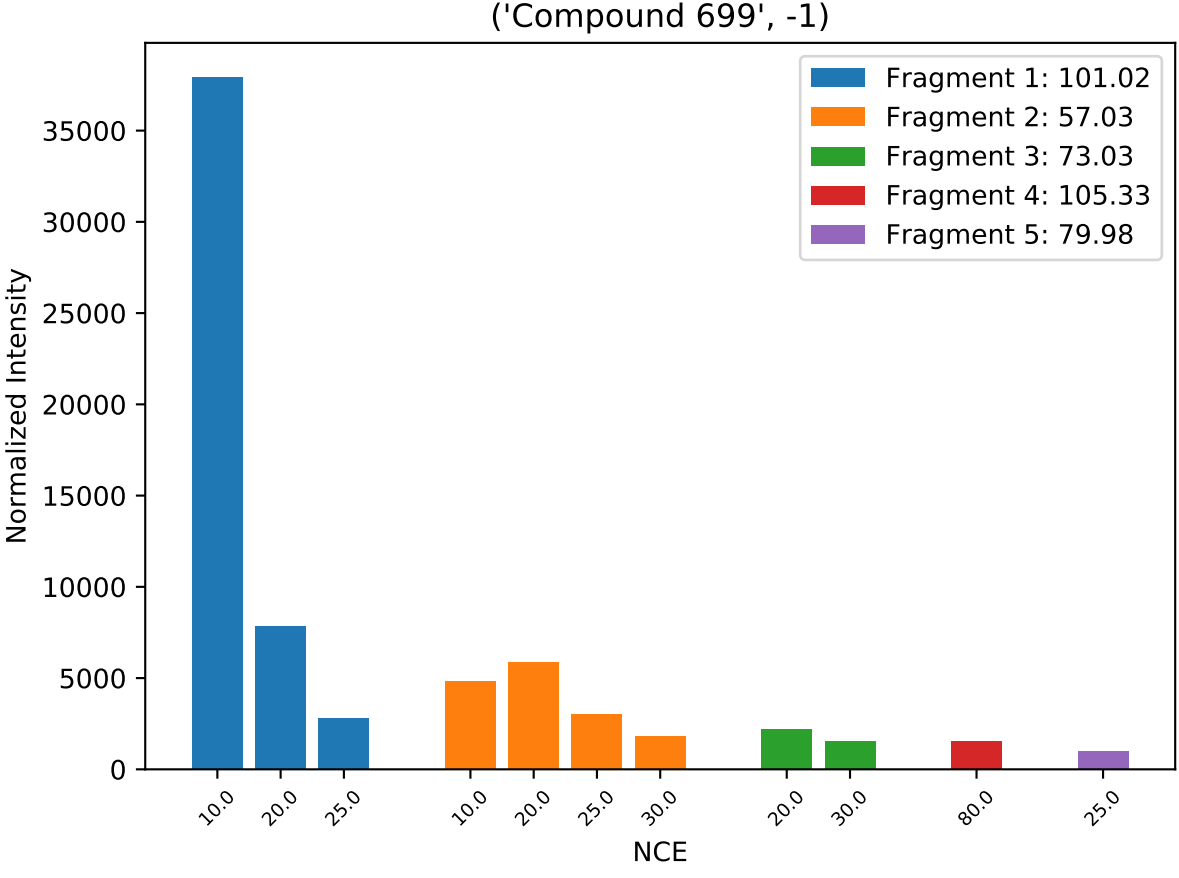

('Compound 118', -1)
Fragment 1: 329.99
Fragment 2: 258.01
Fragment 3: 85.94
Fragment 4: 98.95
Fragment 5: 124.96
Normalized Intensity
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
35.0 50.0 60.0 70.0 80.0
NCE

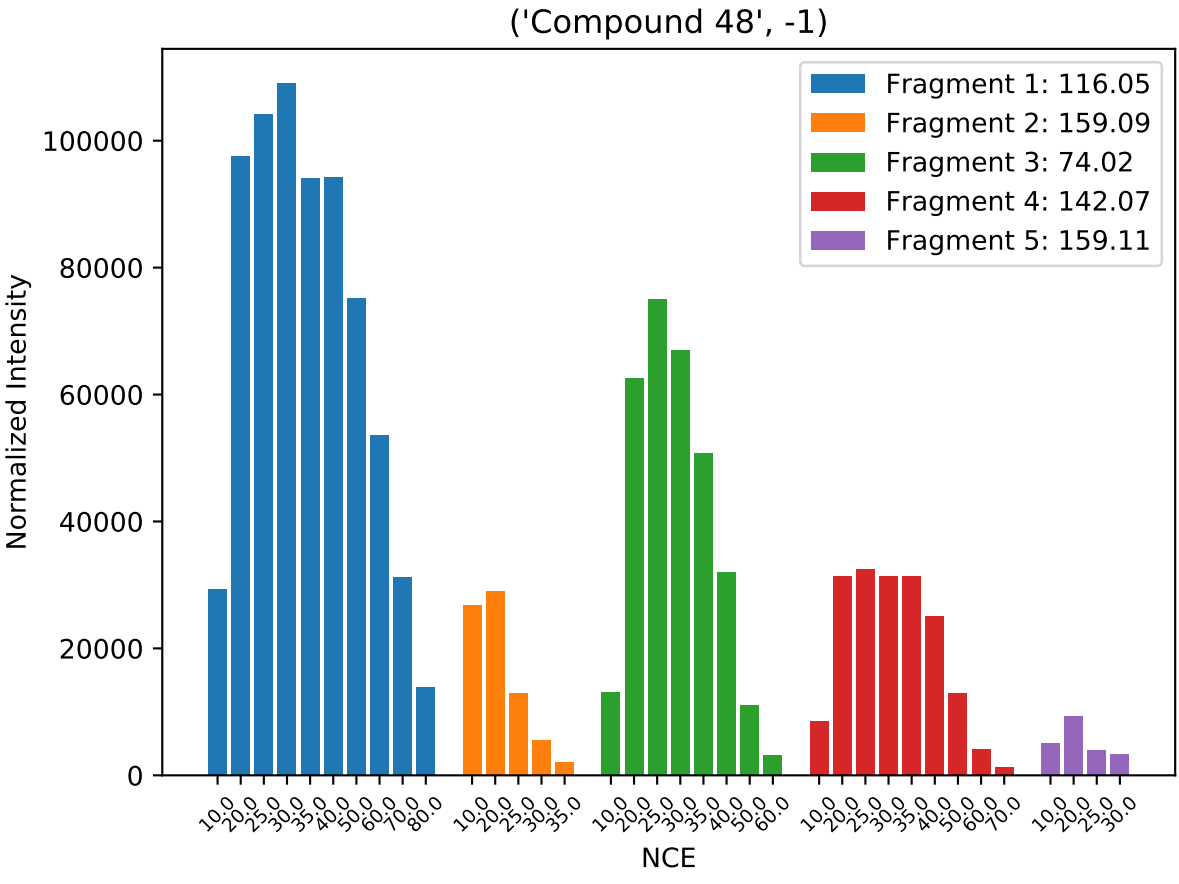

('Compound 60', -1)
Normalized Intensity
0
200
400
600
800
70.0
30.0
25.0
60.0
40.0
NCE
Fragment 1: 67.13
Fragment 2: 56.68
Fragment 3: 62.7
Fragment 4: 61.48
Fragment 5: 68.11

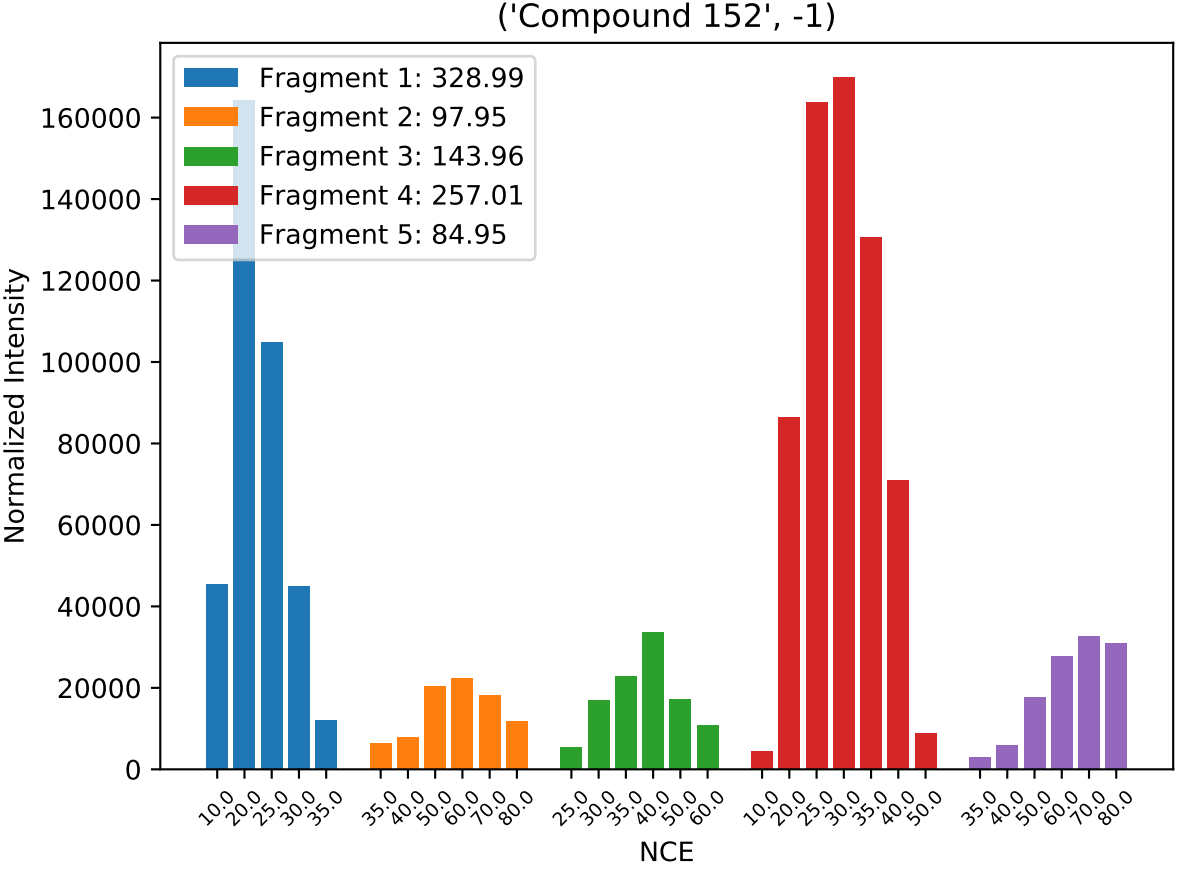

('Compound 695', -1)
Fragment 1: 153.03
Fragment 2: 183.04
Fragment 3: 110.02
Fragment 4: 140.04
Fragment 5: 111.02
Normalized Intensity
300000
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

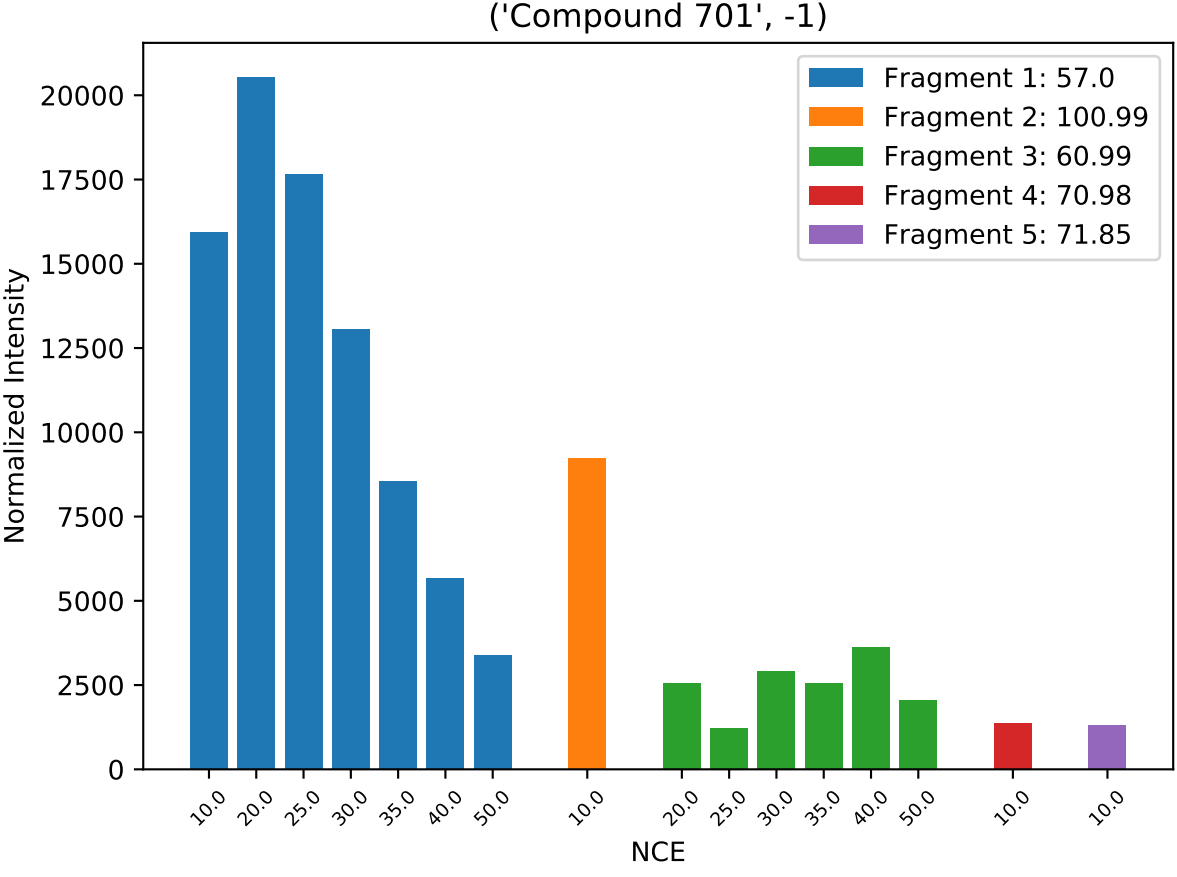

('Compound 696', -1)
Fragment 1: 101.02
Fragment 2: 113.02
Fragment 3: 71.01
Fragment 4: 59.01
Fragment 5: 55.02
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

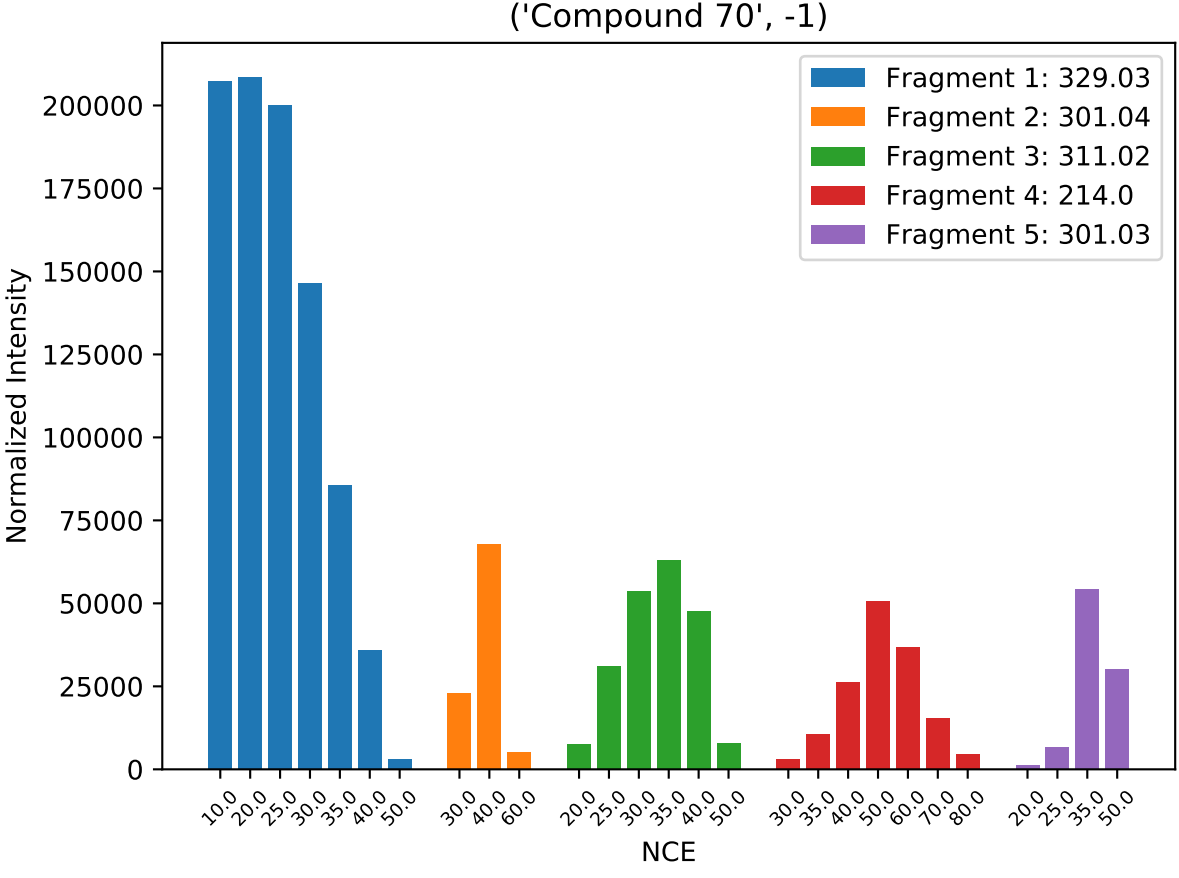

('Compound 697', -1)
Fragment 1: 223.13
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 179.14
Fragment 5: 177.13
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 30.0 70.0 80.0
25.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0
NCE

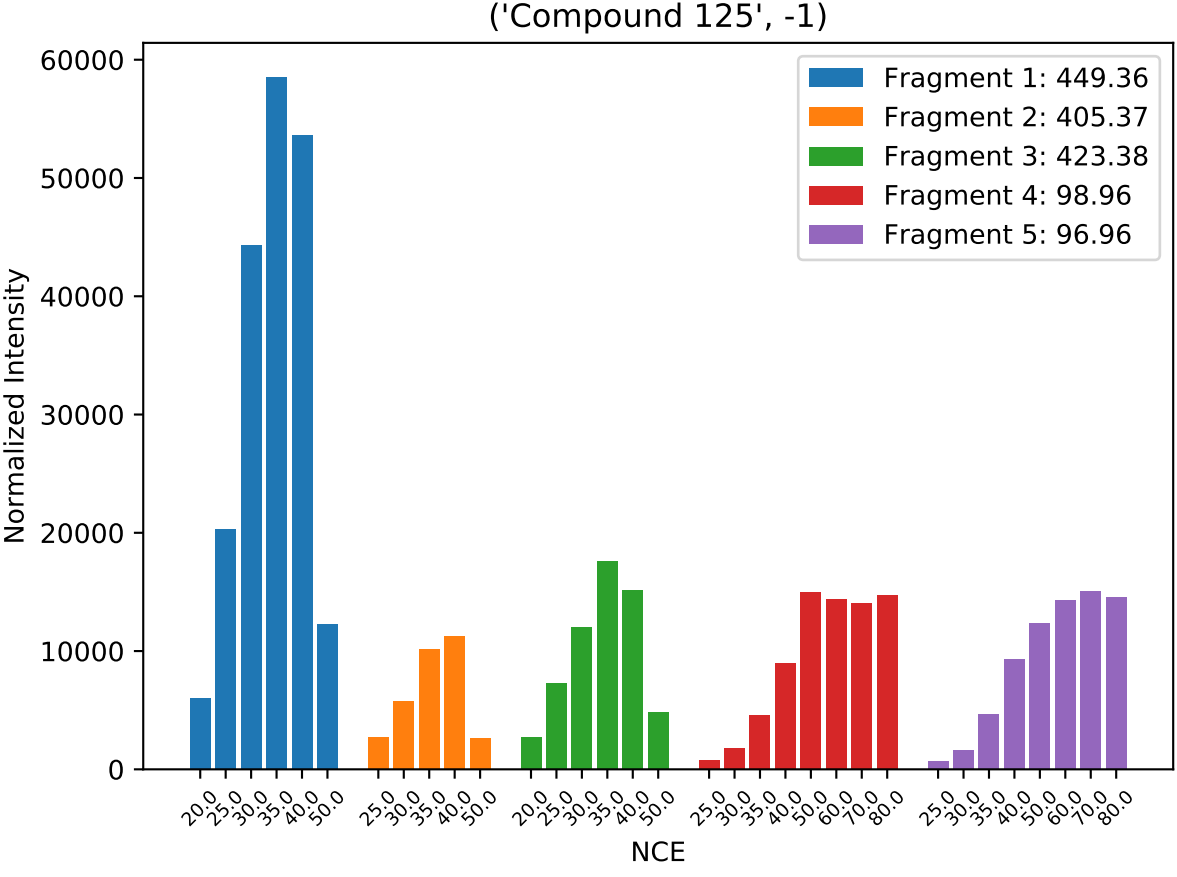

('Compound 699', -1)
Fragment 1: 101.02
Fragment 2: 57.03
Fragment 3: 73.03
Fragment 4: 105.33
Fragment 5: 79.98
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
10.0
20.0
25.0
10.0
20.0
25.0
30.0
20.0
30.0
80.0
25.0
NCE

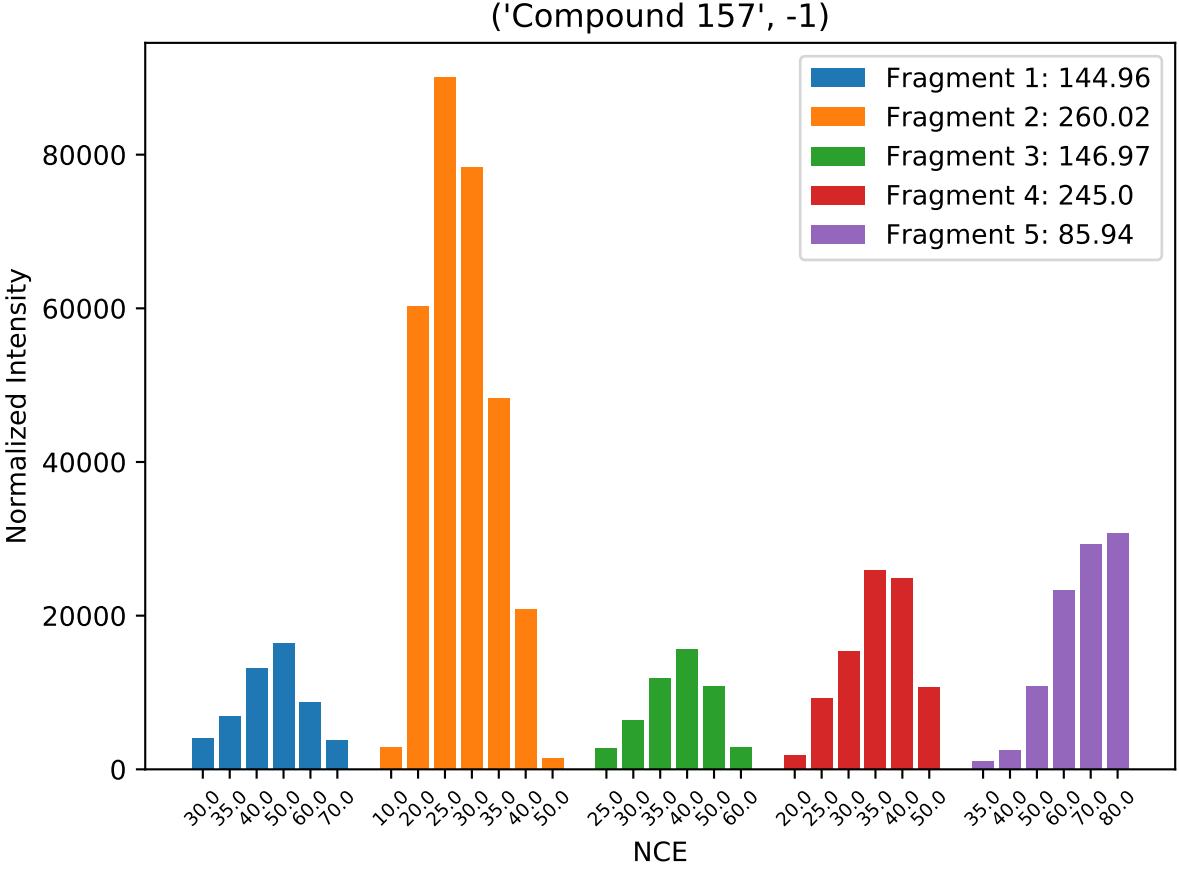

('Compound 48', -1)
Fragment 1: 116.05
Fragment 2: 159.09
Fragment 3: 74.02
Fragment 4: 142.07
Fragment 5: 159.11
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0
NCE

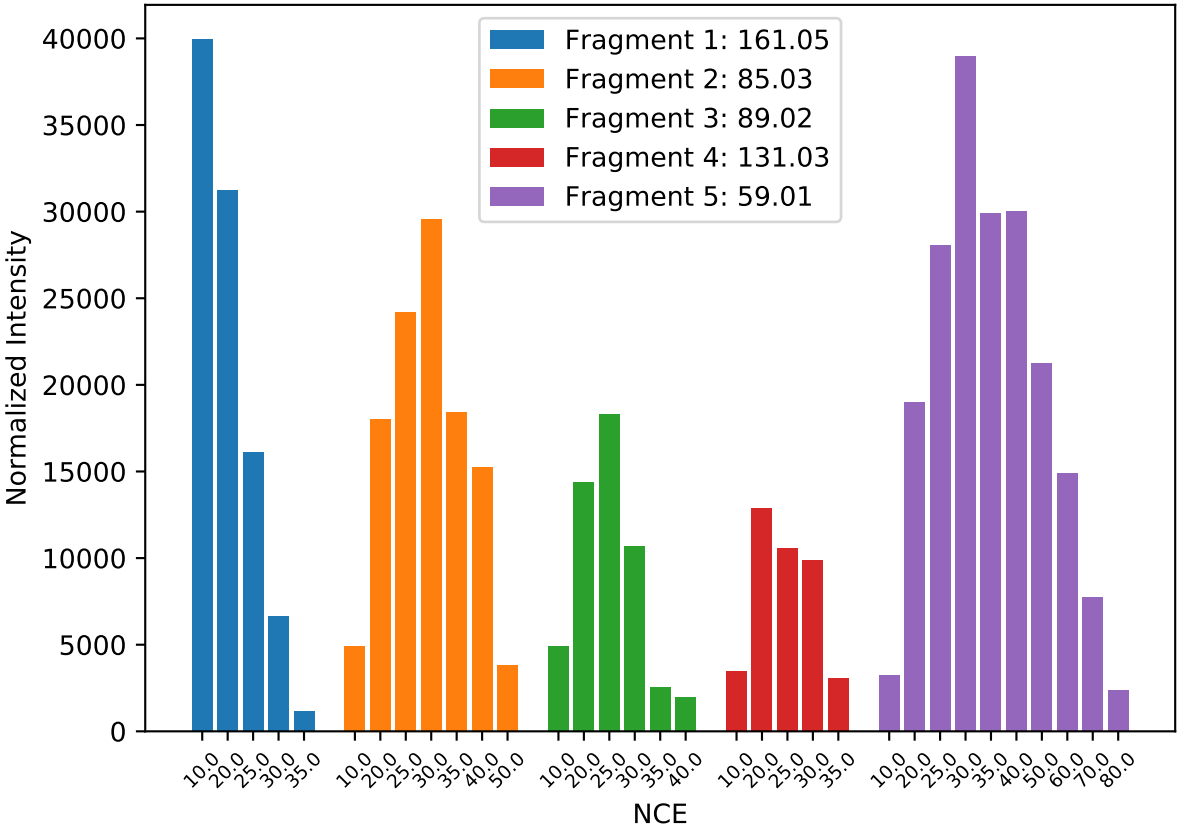

('Compound 152', -1)
Fragment 1: 328.99
Fragment 2: 97.95
Fragment 3: 143.96
Fragment 4: 257.01
Fragment 5: 84.95
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
140000
160000
10.0 20.0 25.0 30.0 35.0
35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

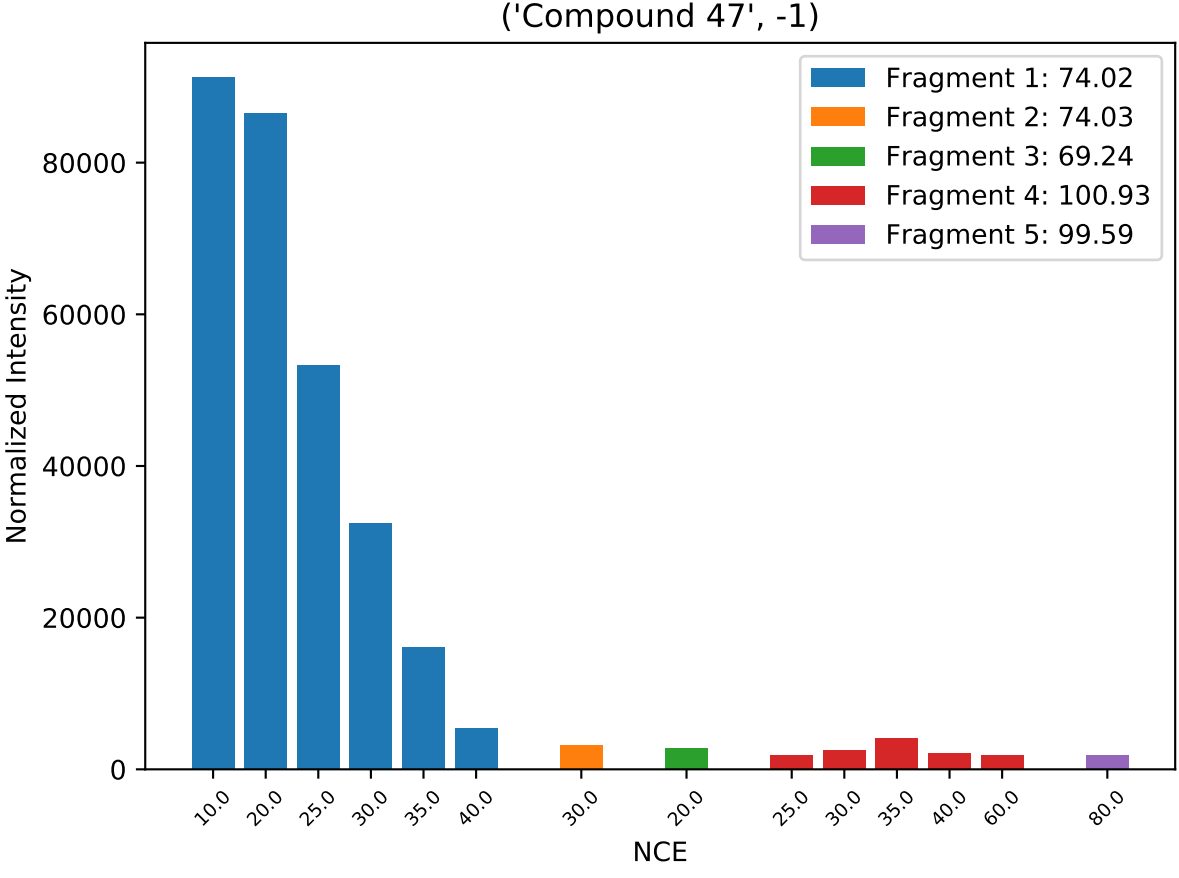

('Compound 701', -1)
Fragment 1: 57.0
Fragment 2: 100.99
Fragment 3: 60.99
Fragment 4: 70.98
Fragment 5: 71.85
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
10.0
NCE

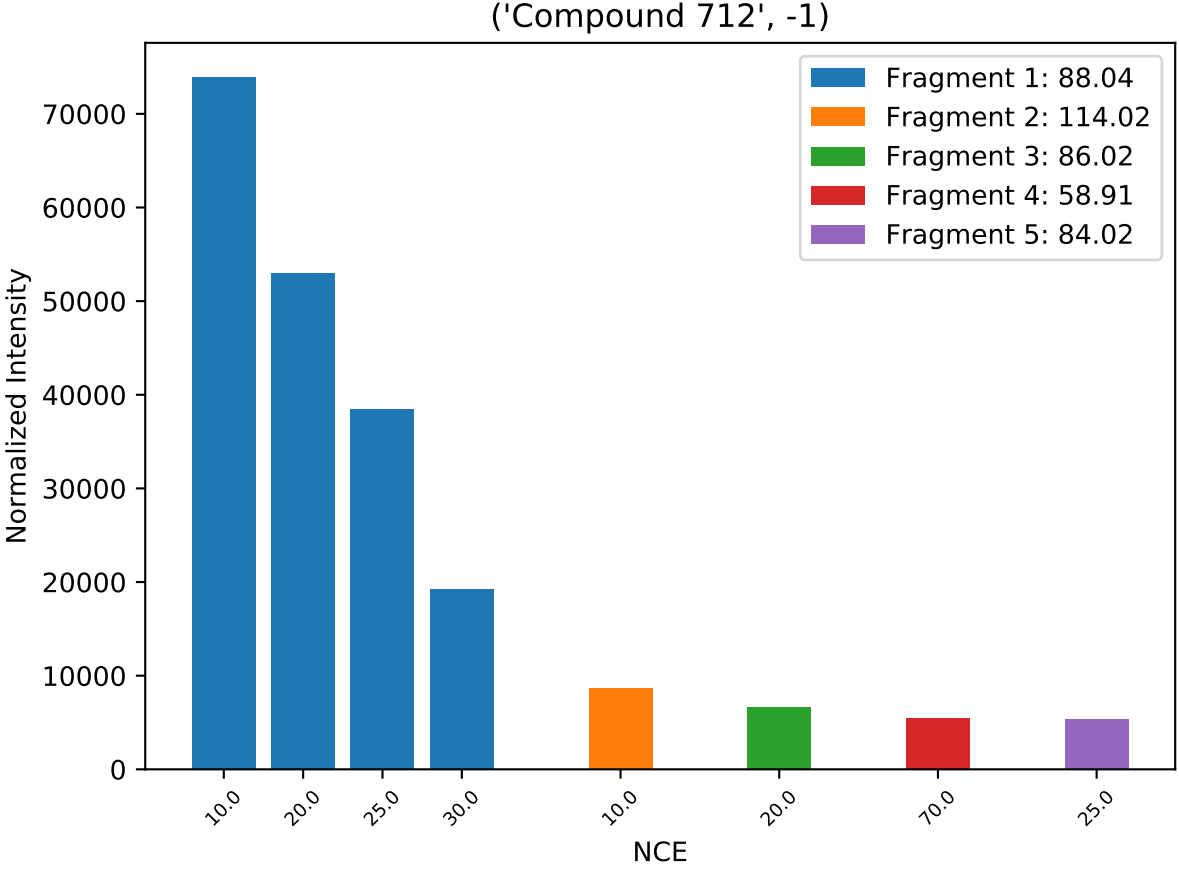

('Compound 70', -1)
Fragment 1: 329.03
Fragment 2: 301.04
Fragment 3: 311.02
Fragment 4: 214.0
Fragment 5: 301.03
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
200000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 40.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 35.0 50.0
NCE

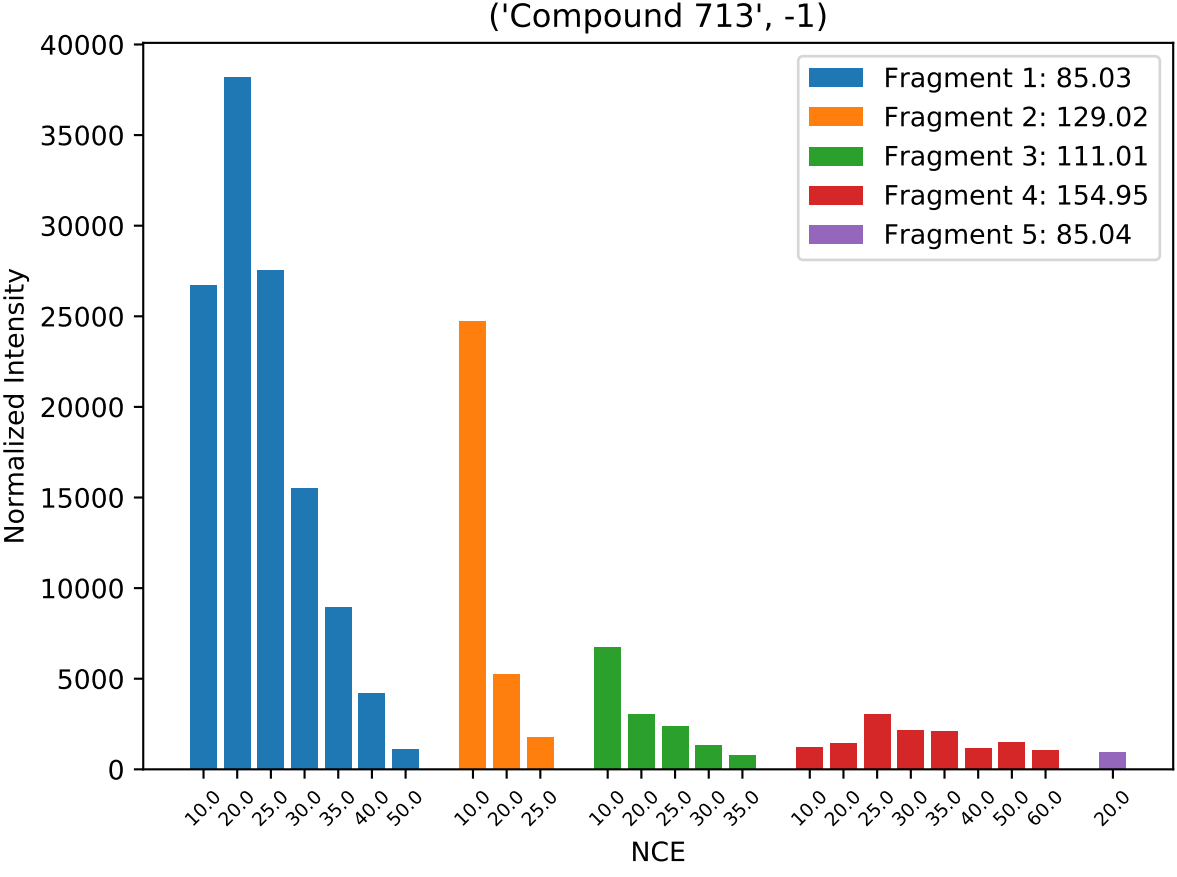

('Compound 125', -1)
Fragment 1: 449.36
Fragment 2: 405.37
Fragment 3: 423.38
Fragment 4: 98.96
Fragment 5: 96.96
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
20.0
25.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

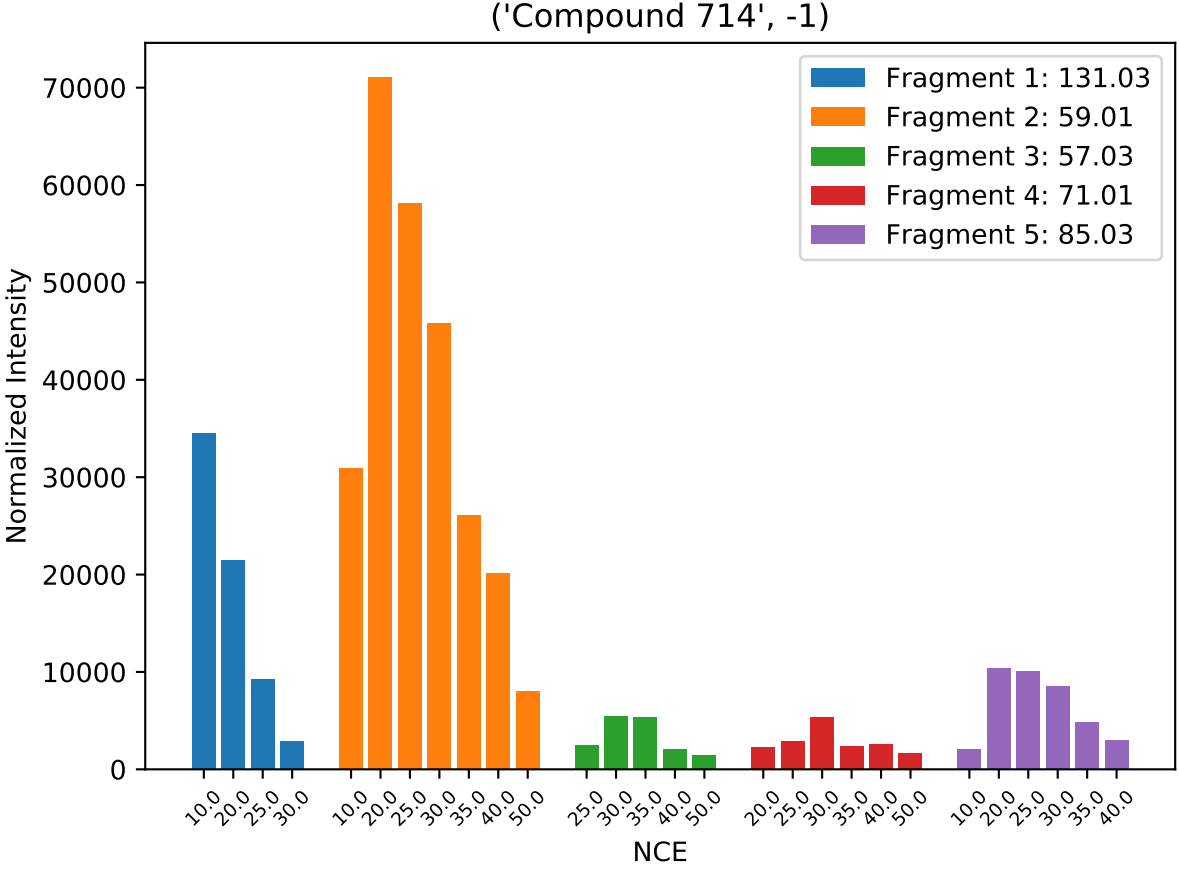

('Compound 157', -1)
Fragment 1: 144.96
Fragment 2: 260.02
Fragment 3: 146.97
Fragment 4: 245.0
Fragment 5: 85.94
Normalized Intensity
0
20000
40000
60000
80000
30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

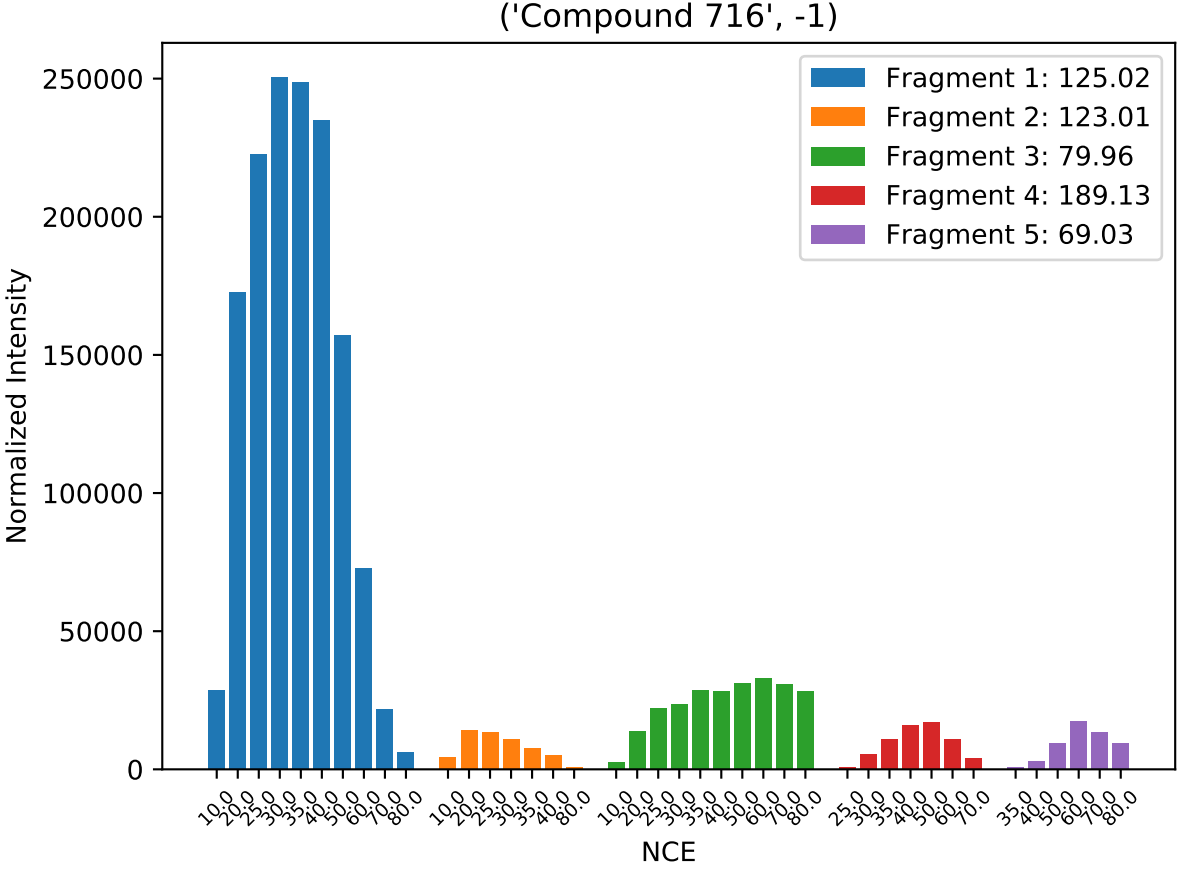

('Compound 707', -1)
Fragment 1: 161.05
Fragment 2: 85.03
Fragment 3: 89.02
Fragment 4: 131.03
Fragment 5: 59.01
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

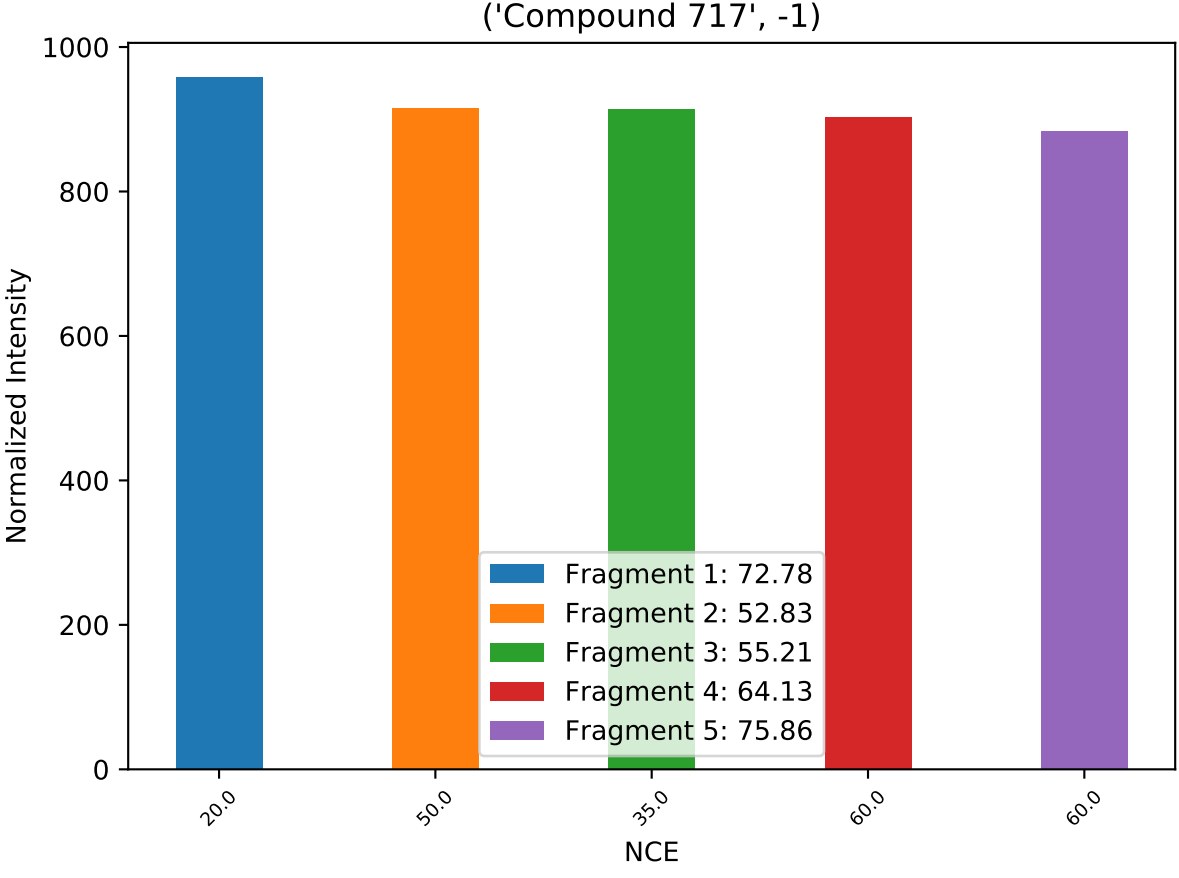

('Compound 47', -1)
Fragment 1: 74.02
Fragment 2: 74.03
Fragment 3: 69.24
Fragment 4: 100.93
Fragment 5: 99.59
Normalized Intensity
0
20000
40000
60000
80000
10.0
20.0
25.0
30.0
35.0
40.0
30.0
20.0
25.0
30.0
35.0
40.0
60.0
80.0
NCE

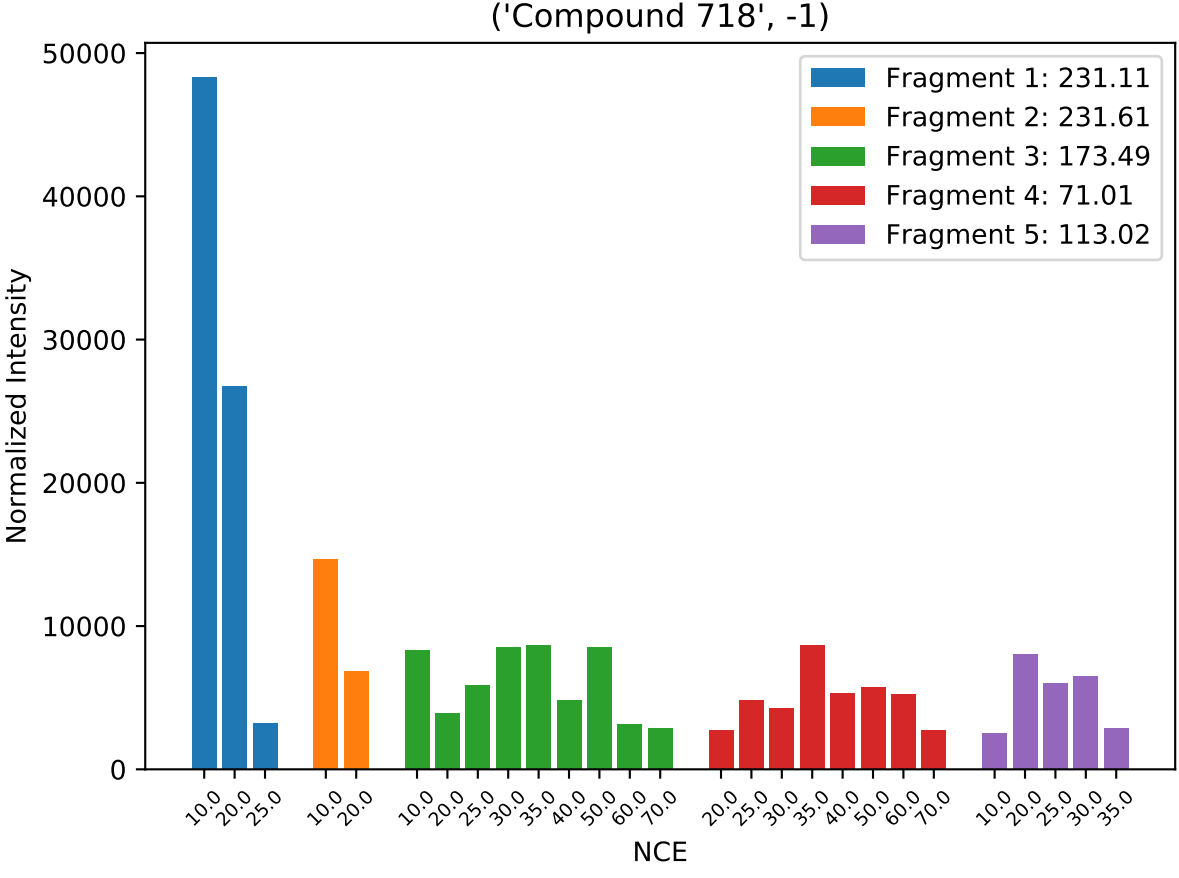

('Compound 712', -1)
Fragment 1: 88.04
Fragment 2: 114.02
Fragment 3: 86.02
Fragment 4: 58.91
Fragment 5: 84.02
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
30.0
10.0
20.0
70.0
25.0
NCE

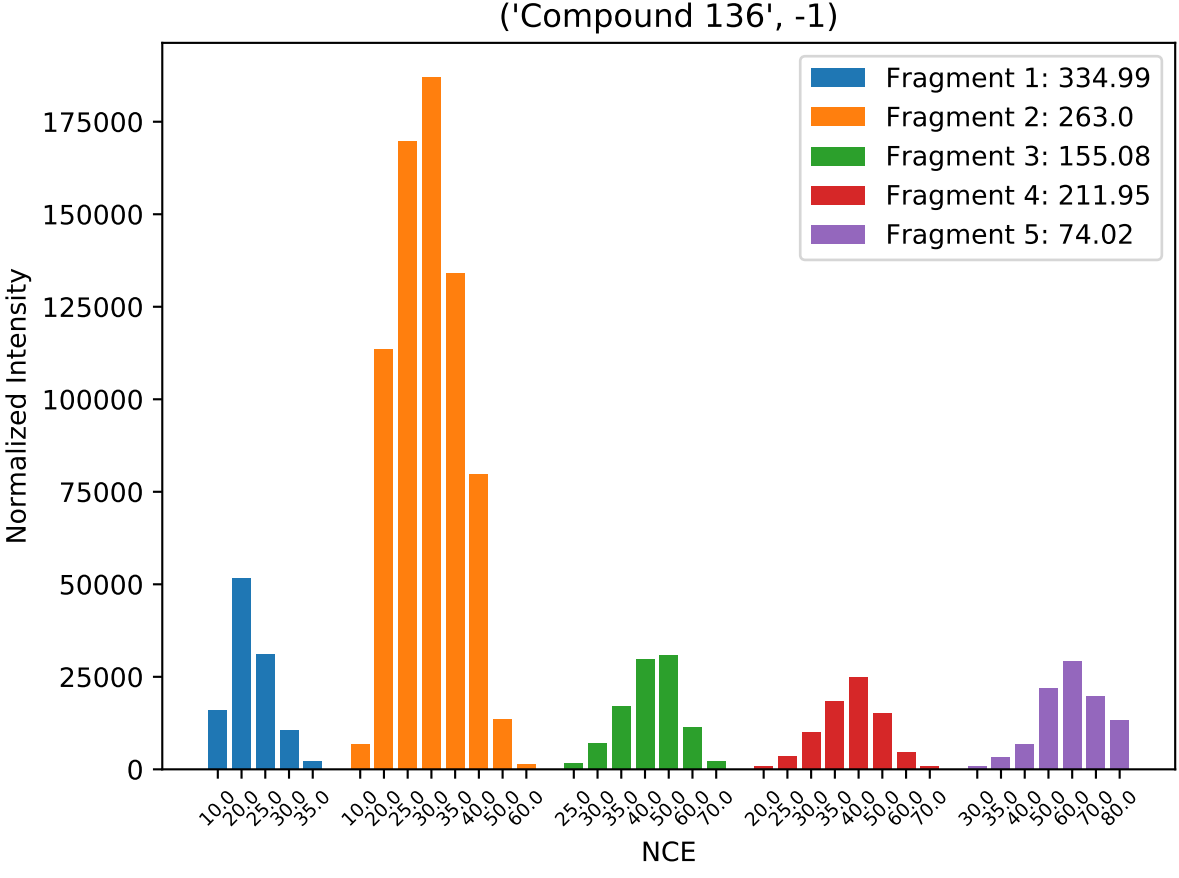

('Compound 713', -1)
Fragment 1: 85.03
Fragment 2: 129.02
Fragment 3: 111.01
Fragment 4: 154.95
Fragment 5: 85.04
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
NCE

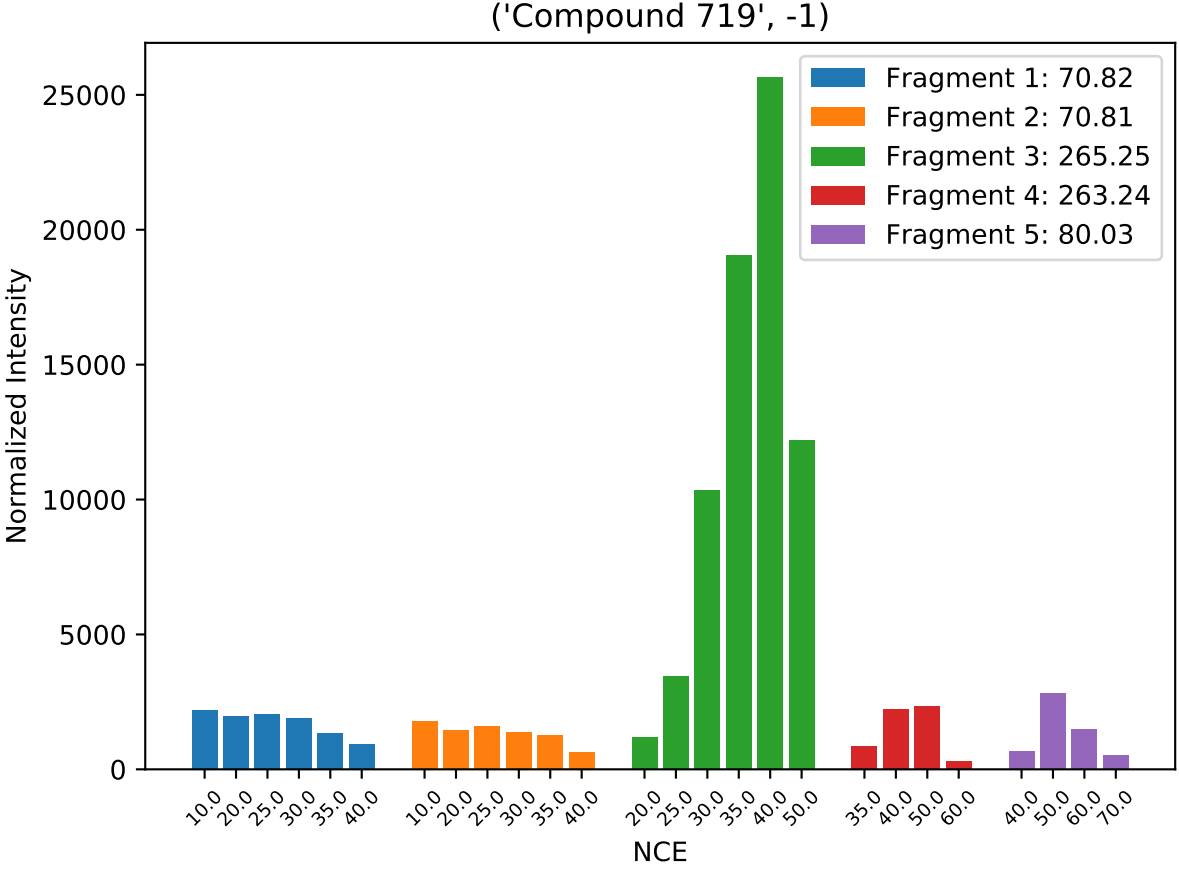

('Compound 714', -1)
Fragment 1: 131.03
Fragment 2: 59.01
Fragment 3: 57.03
Fragment 4: 71.01
Fragment 5: 85.03
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
NCE

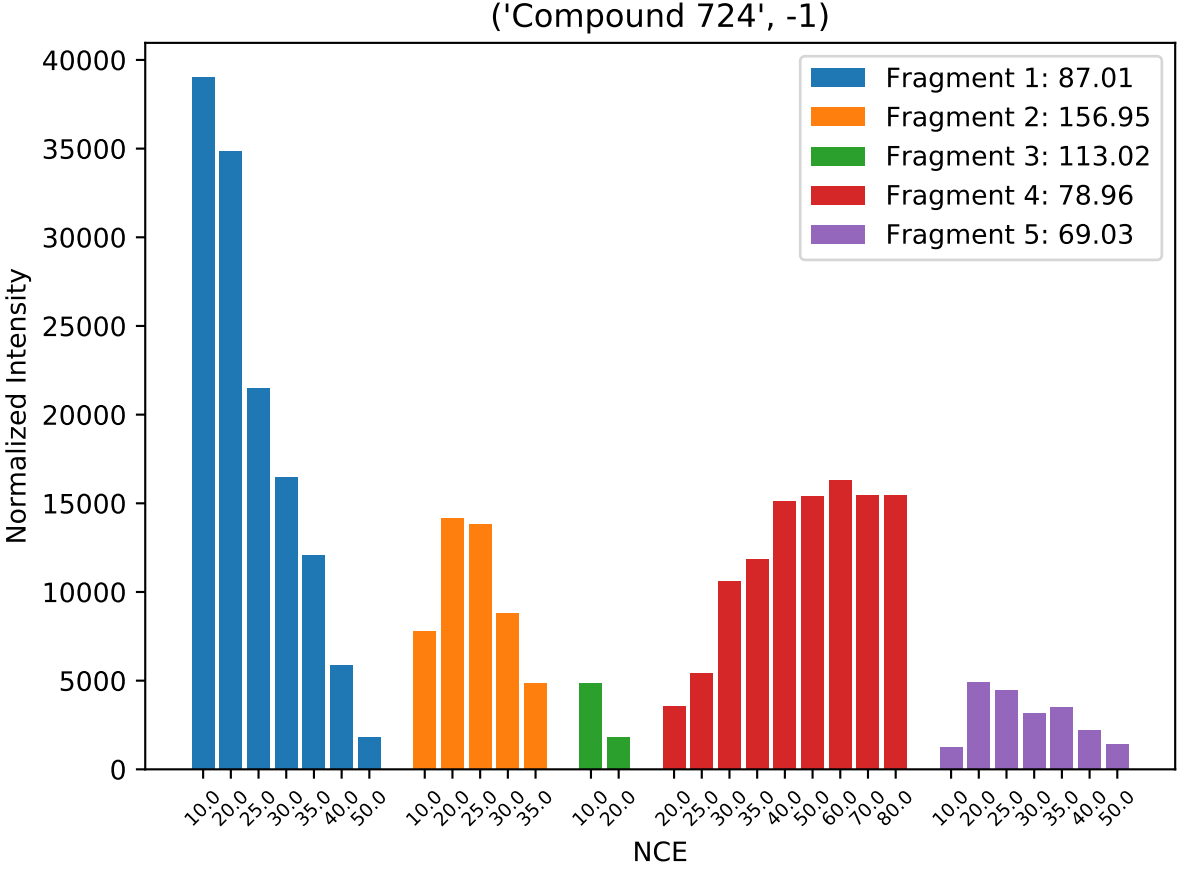

('Compound 716', -1)
Fragment 1: 125.02
Fragment 2: 123.01
Fragment 3: 79.96
Fragment 4: 189.13
Fragment 5: 69.03
Normalized Intensity
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

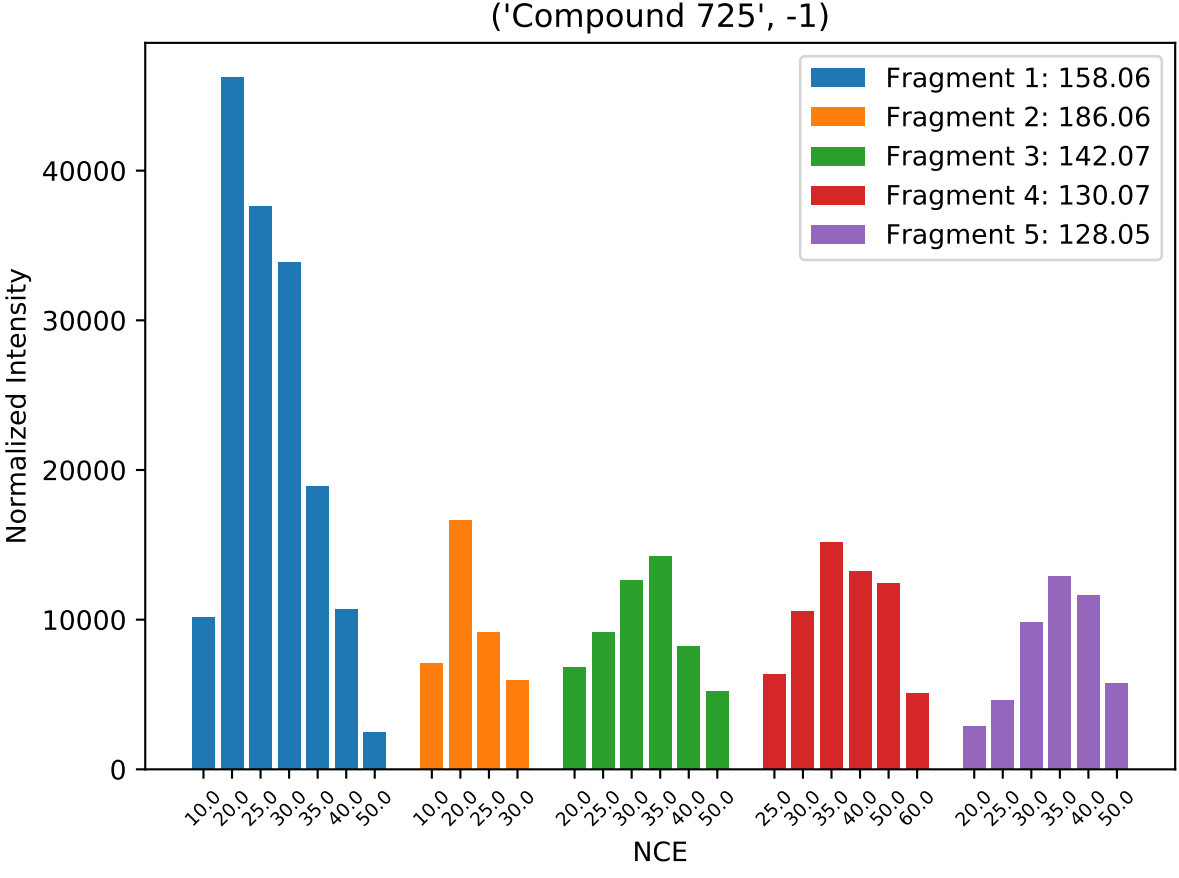

('Compound 717', -1)
Normalized Intensity
1000
800
600
400
200
0
Fragment 1: 72.78
Fragment 2: 52.83
Fragment 3: 55.21
Fragment 4: 64.13
Fragment 5: 75.86
20.0
50.0
35.0
60.0
60.0
NCE

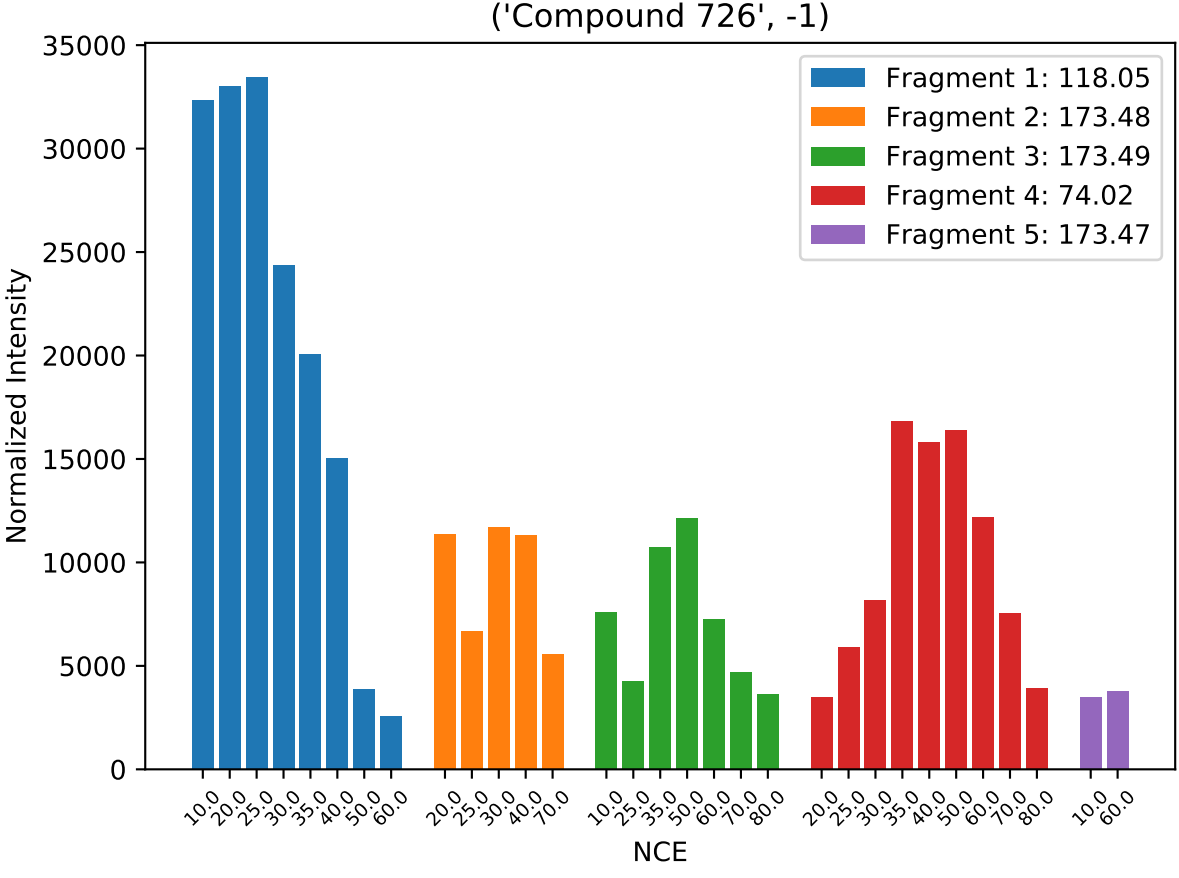

('Compound 718', -1)
Fragment 1: 231.11
Fragment 2: 231.61
Fragment 3: 173.49
Fragment 4: 71.01
Fragment 5: 113.02
Normalized Intensity
50000
40000
30000
20000
10000
0
10.0 20.0 25.0
10.0 20.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0
NCE

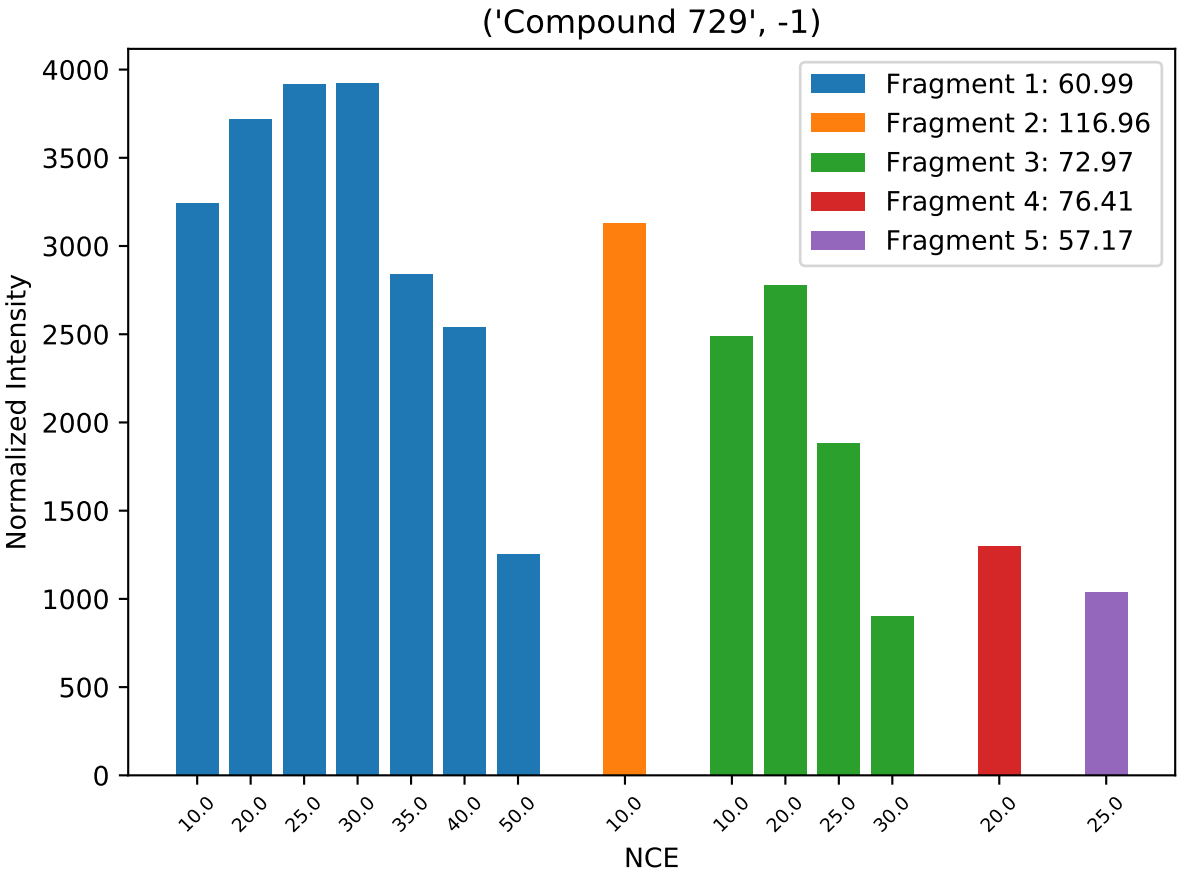

('Compound 136', -1)
Fragment 1: 334.99
Fragment 2: 263.0
Fragment 3: 155.08
Fragment 4: 211.95
Fragment 5: 74.02
Normalized Intensity
0
25000
50000
75000
100000
125000
150000
175000
NCE
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

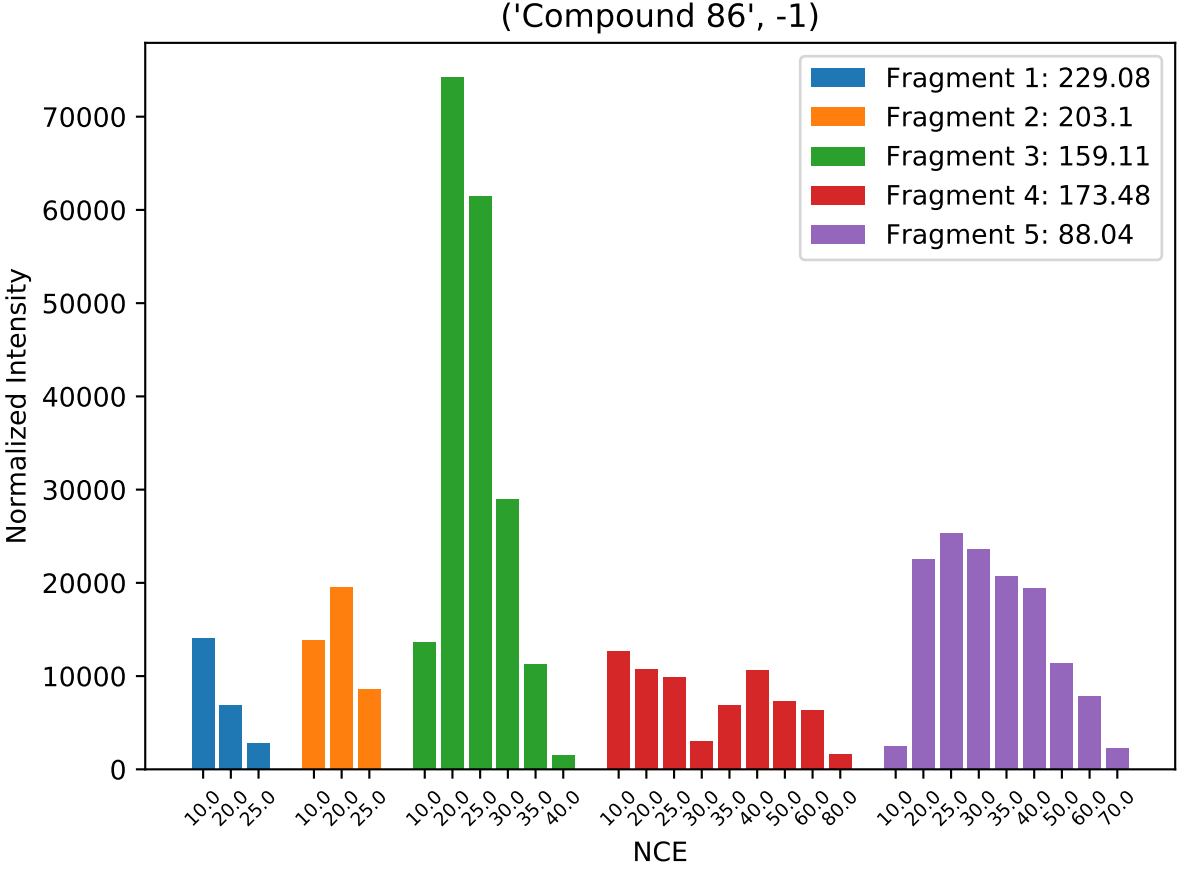

('Compound 719', -1)
Fragment 1: 70.82
Fragment 2: 70.81
Fragment 3: 265.25
Fragment 4: 263.24
Fragment 5: 80.03
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
35.0
40.0
50.0
60.0
40.0
50.0
60.0
70.0
NCE

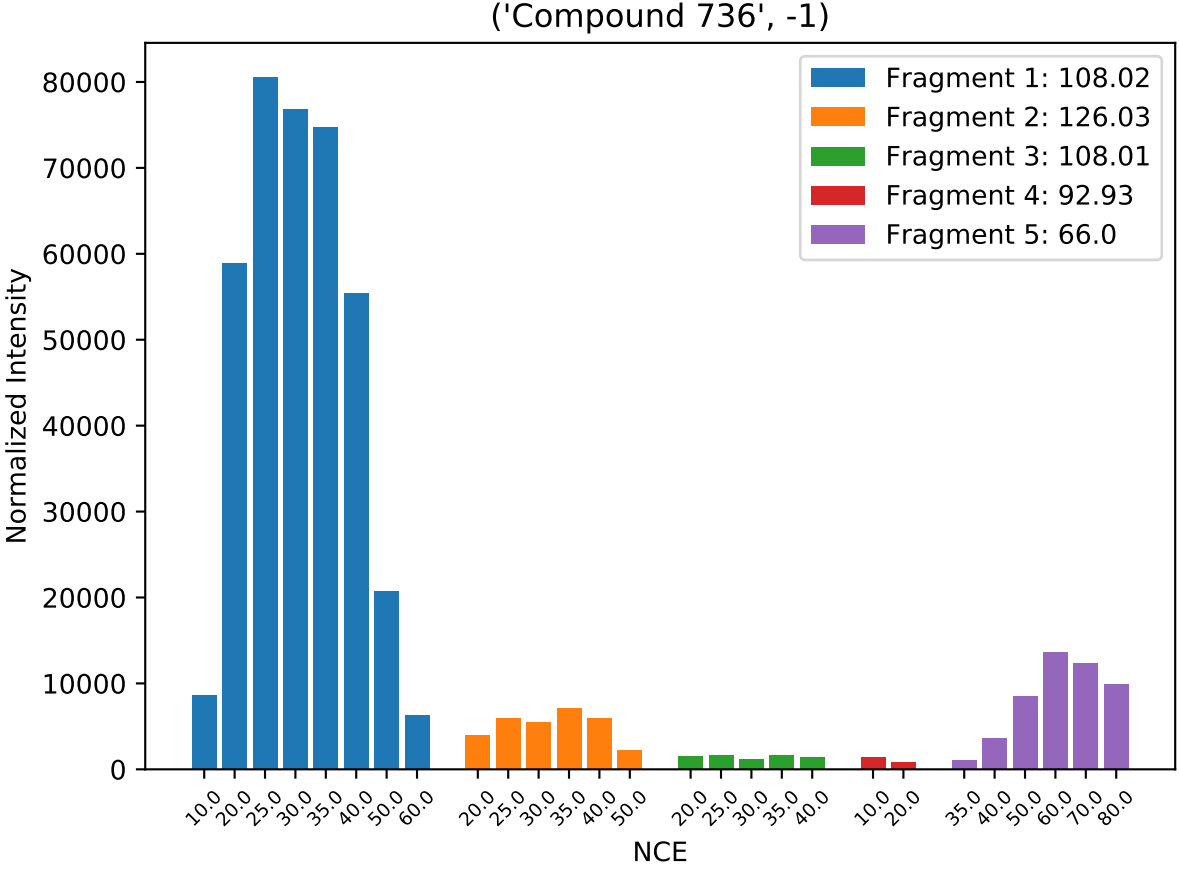

('Compound 724', -1)
Fragment 1: 87.01
Fragment 2: 156.95
Fragment 3: 113.02
Fragment 4: 78.96
Fragment 5: 69.03
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

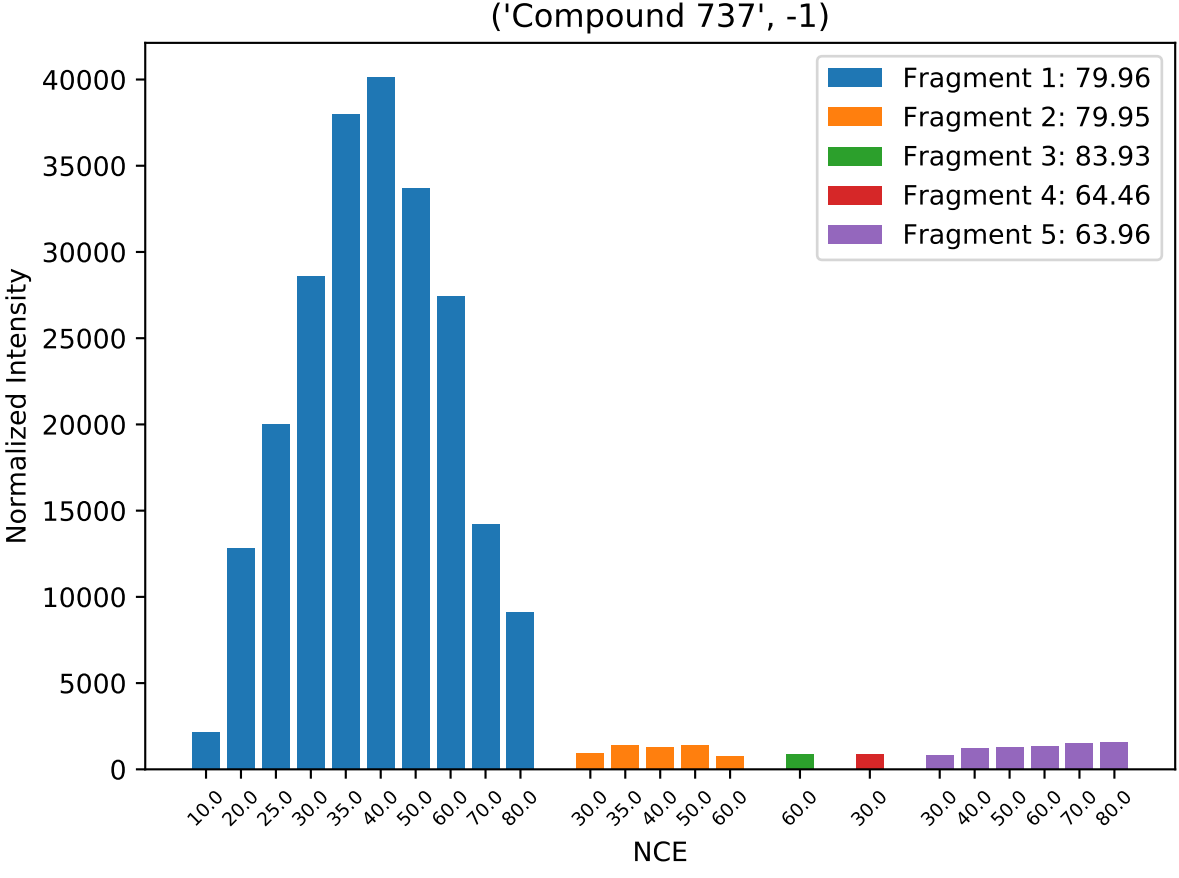

('Compound 725', -1)
Fragment 1: 158.06
Fragment 2: 186.06
Fragment 3: 142.07
Fragment 4: 130.07
Fragment 5: 128.05
Normalized Intensity
0
10000
20000
30000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0
20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0
NCE

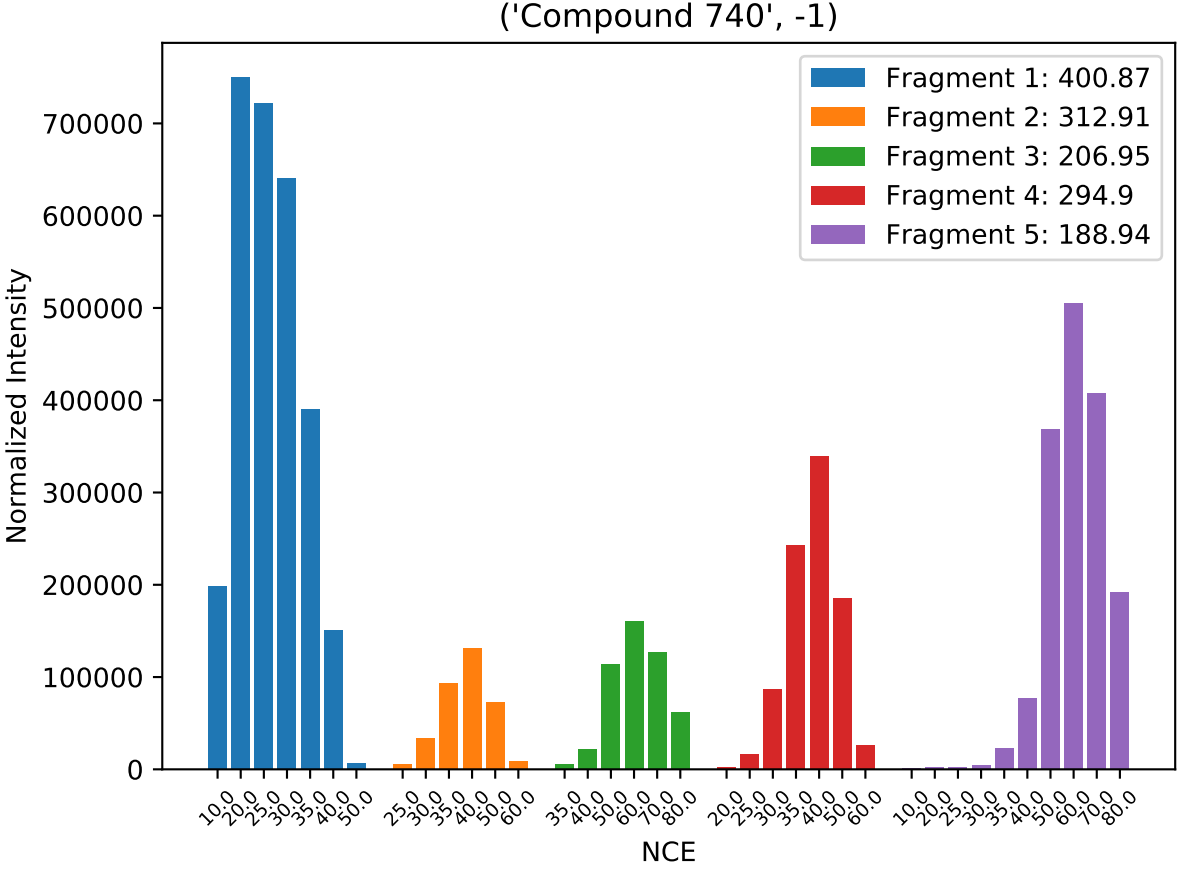

('Compound 726', -1)
Fragment 1: 118.05
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 74.02
Fragment 5: 173.47
Normalized Intensity
35000
30000
25000
20000
15000
10000
5000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 40.0 70.0
10.0 25.0 35.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 60.0
NCE

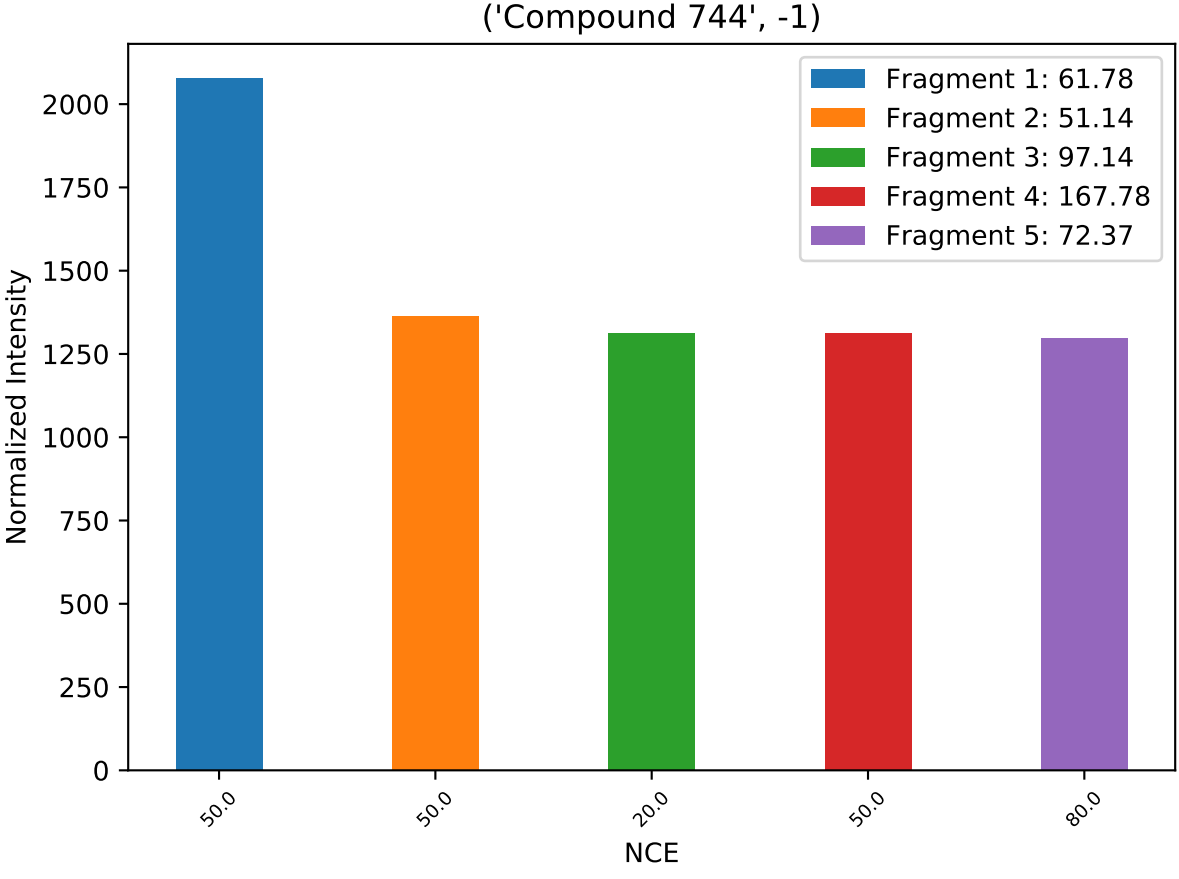

('Compound 729', -1)
Fragment 1: 60.99
Fragment 2: 116.96
Fragment 3: 72.97
Fragment 4: 76.41
Fragment 5: 57.17
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
10.0
20.0
25.0
30.0
20.0
25.0
NCE

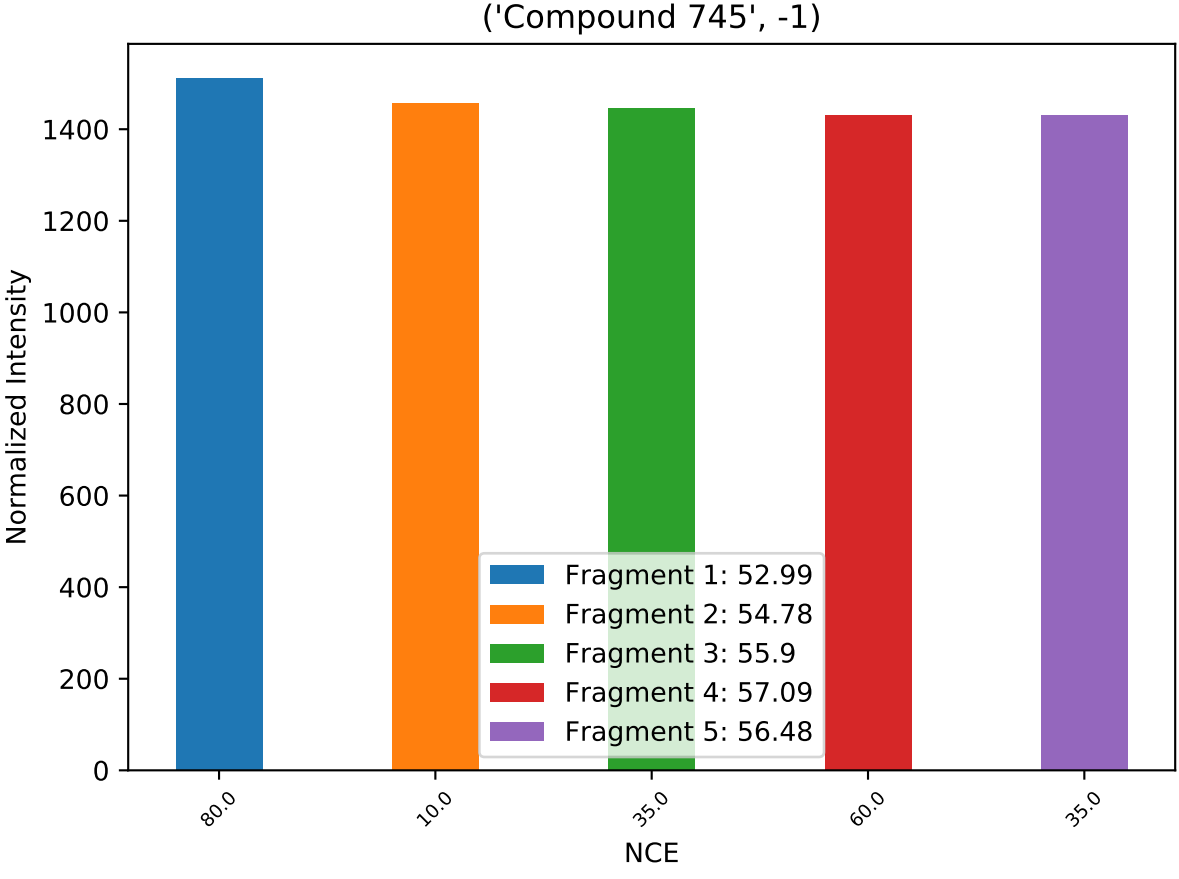

('Compound 86', -1)
Fragment 1: 229.08
Fragment 2: 203.1
Fragment 3: 159.11
Fragment 4: 173.48
Fragment 5: 88.04
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

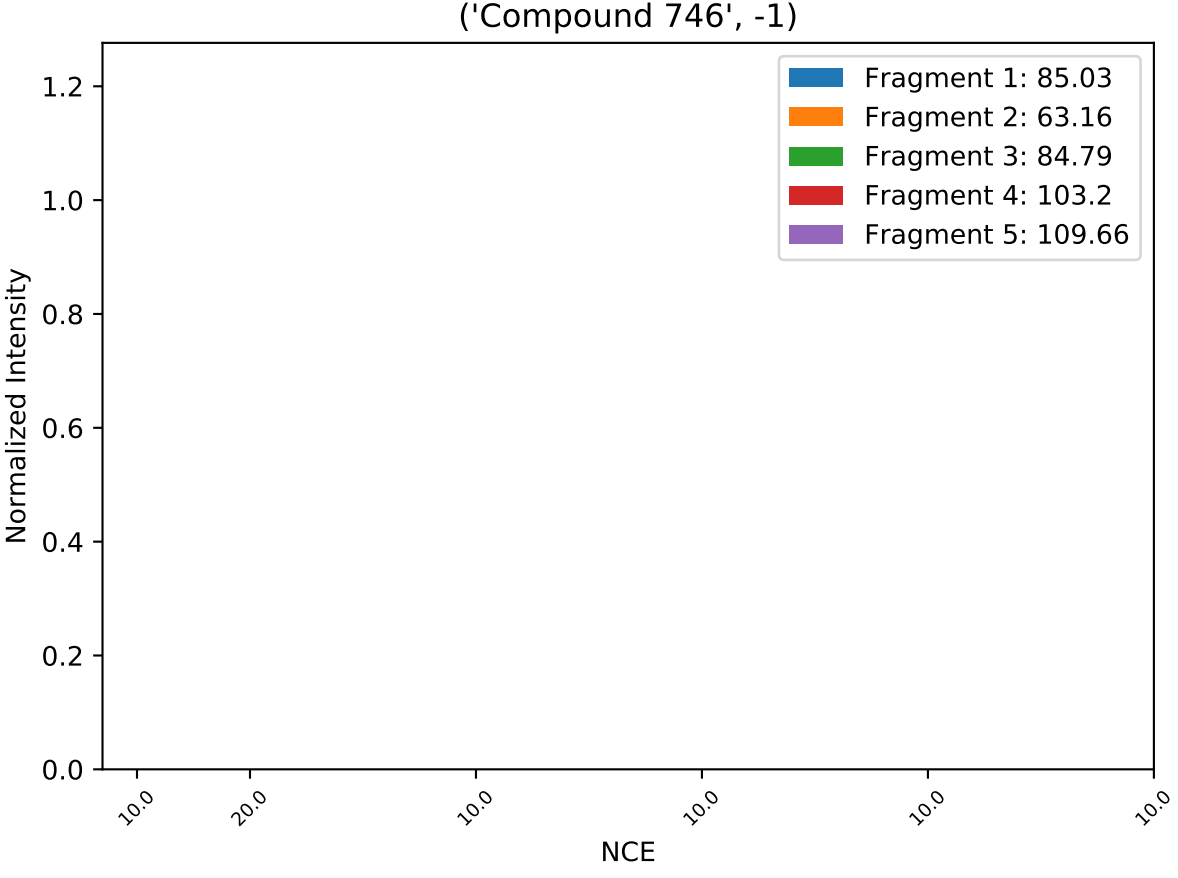

('Compound 736', -1)
Fragment 1: 108.02
Fragment 2: 126.03
Fragment 3: 108.01
Fragment 4: 92.93
Fragment 5: 66.0
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

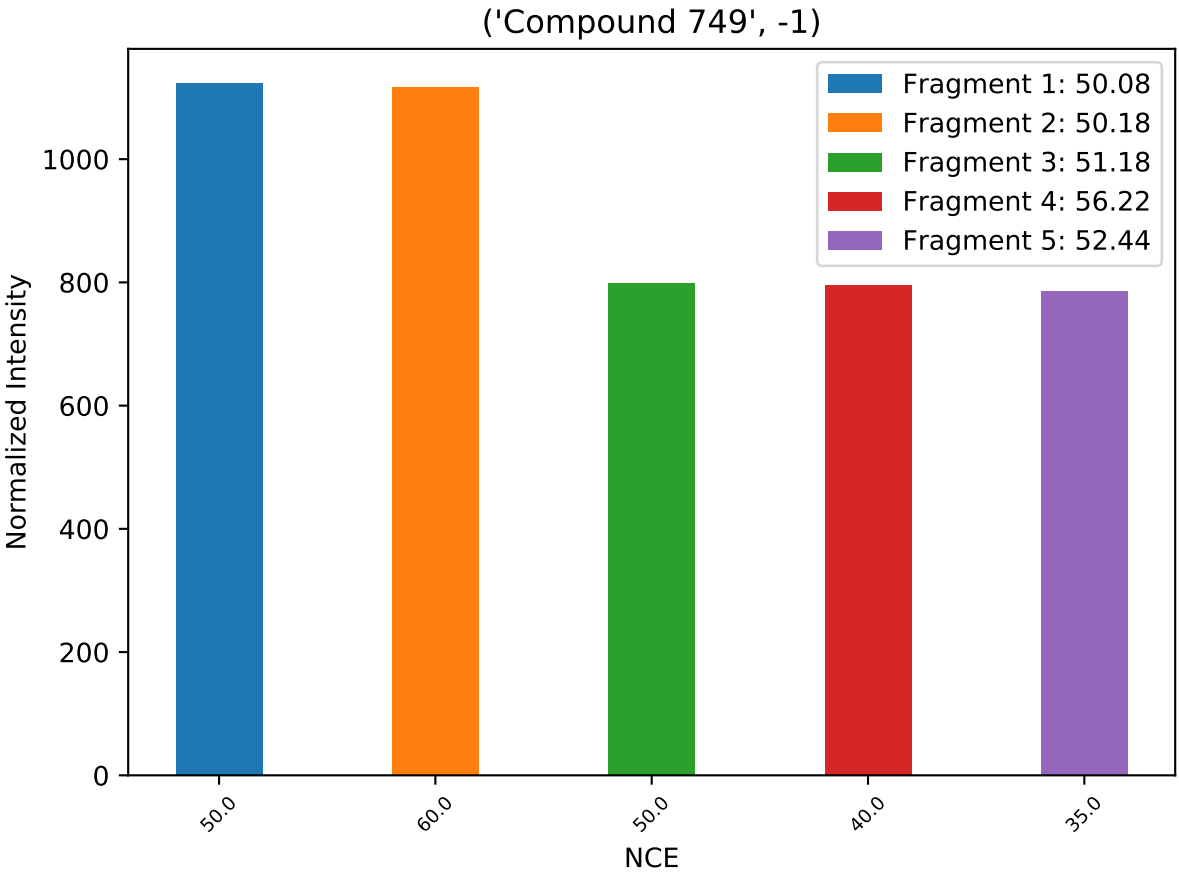

('Compound 737', -1)
Fragment 1: 79.96
Fragment 2: 79.95
Fragment 3: 83.93
Fragment 4: 64.46
Fragment 5: 63.96
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
60.0
30.0
30.0
40.0
50.0
60.0
70.0
80.0
NCE

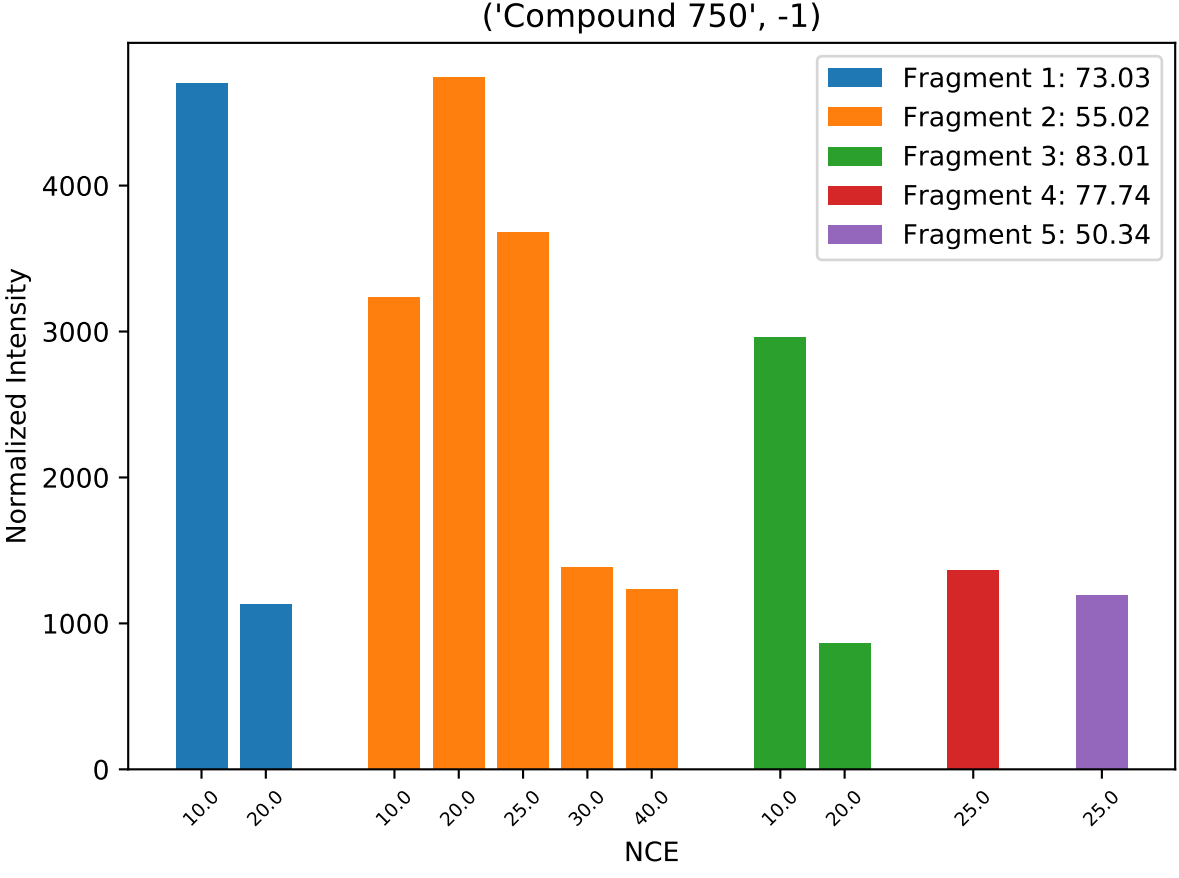

('Compound 740', -1)
Fragment 1: 400.87
Fragment 2: 312.91
Fragment 3: 206.95
Fragment 4: 294.9
Fragment 5: 188.94
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
700000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0
35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

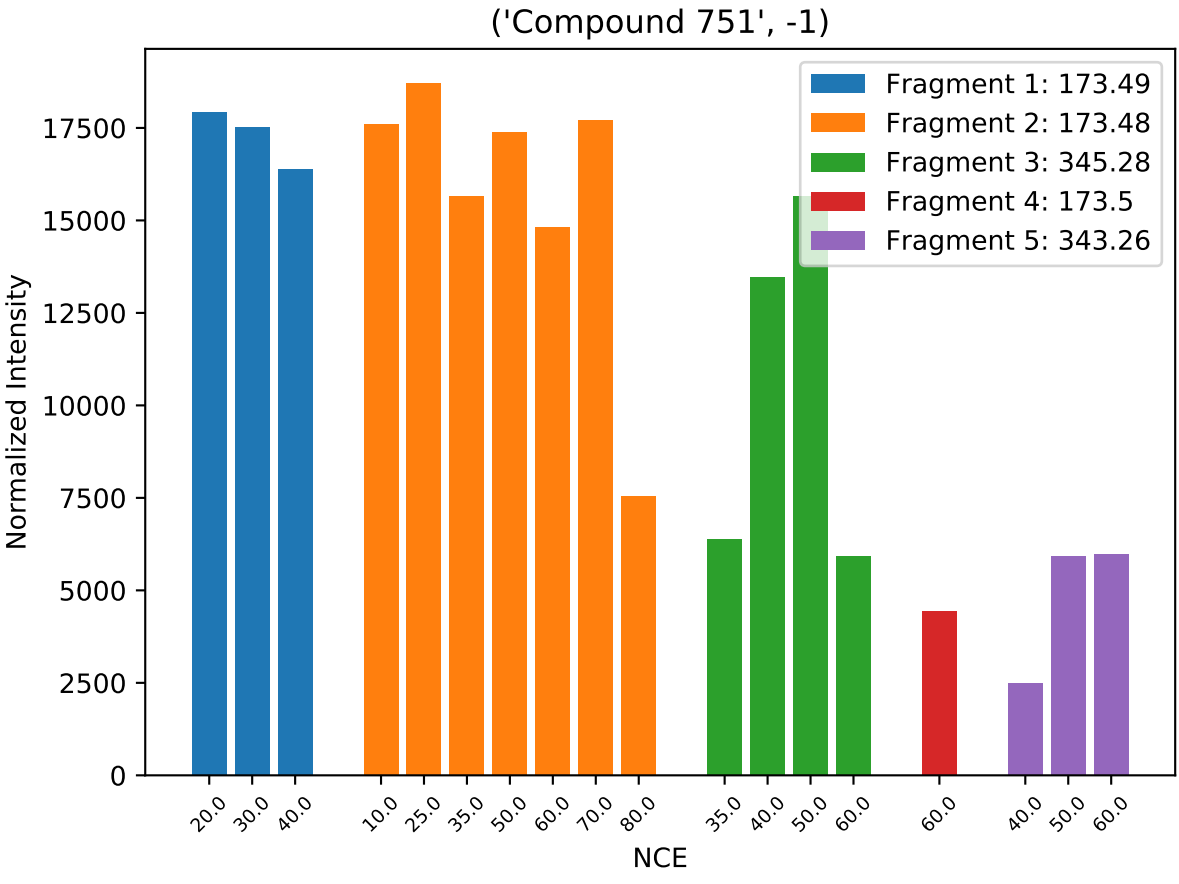

('Compound 744', -1)
Fragment 1: 61.78
Fragment 2: 51.14
Fragment 3: 97.14
Fragment 4: 167.78
Fragment 5: 72.37
Normalized Intensity
0
250
500
750
1000
1250
1500
1750
2000
50.0
50.0
20.0
50.0
80.0
NCE

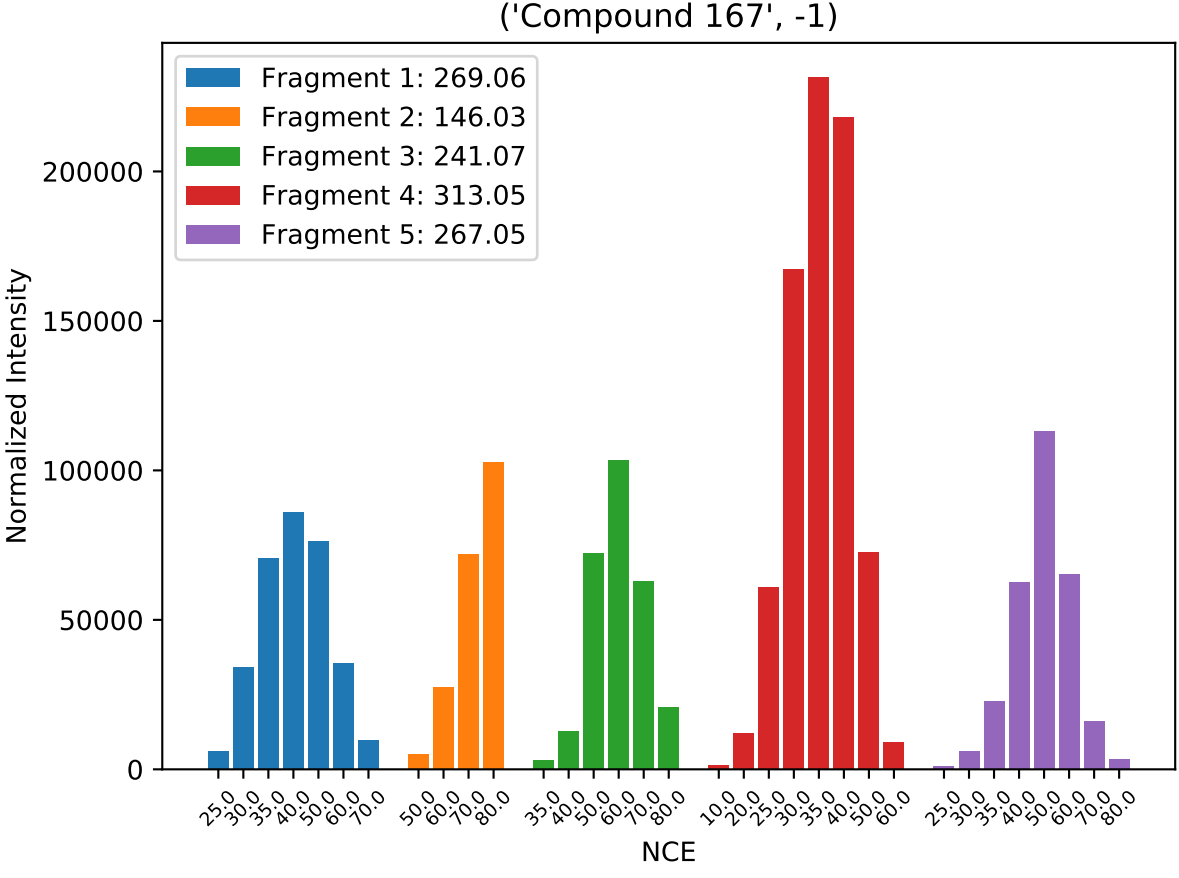

('Compound 745', -1)
Normalized Intensity
0
200
400
600
800
1000
1200
1400
Fragment 1: 52.99
Fragment 2: 54.78
Fragment 3: 55.9
Fragment 4: 57.09
Fragment 5: 56.48
80.0
10.0
35.0
60.0
35.0
NCE

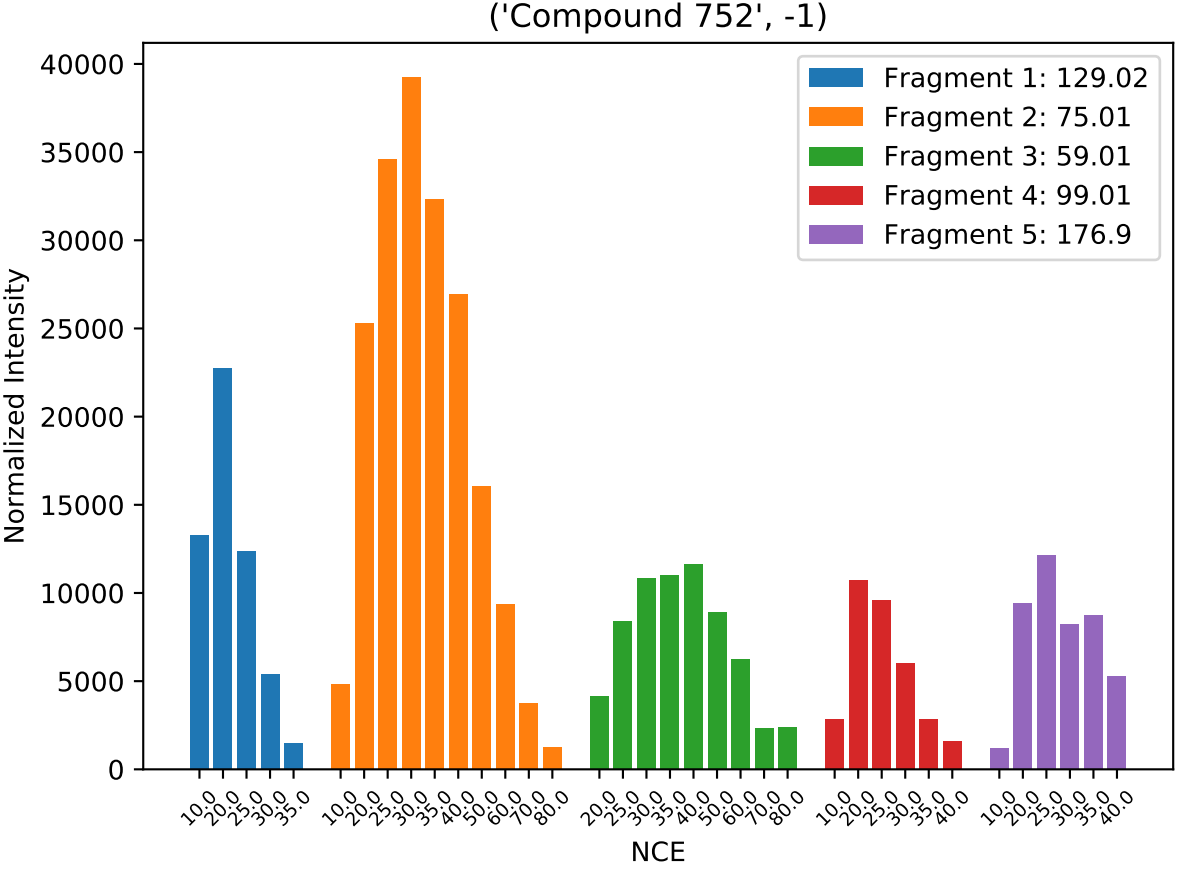

('Compound 746', -1)
Fragment 1: 85.03
Fragment 2: 63.16
Fragment 3: 84.79
Fragment 4: 103.2
Fragment 5: 109.66
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
10.0
10.0
10.0
10.0
NCE

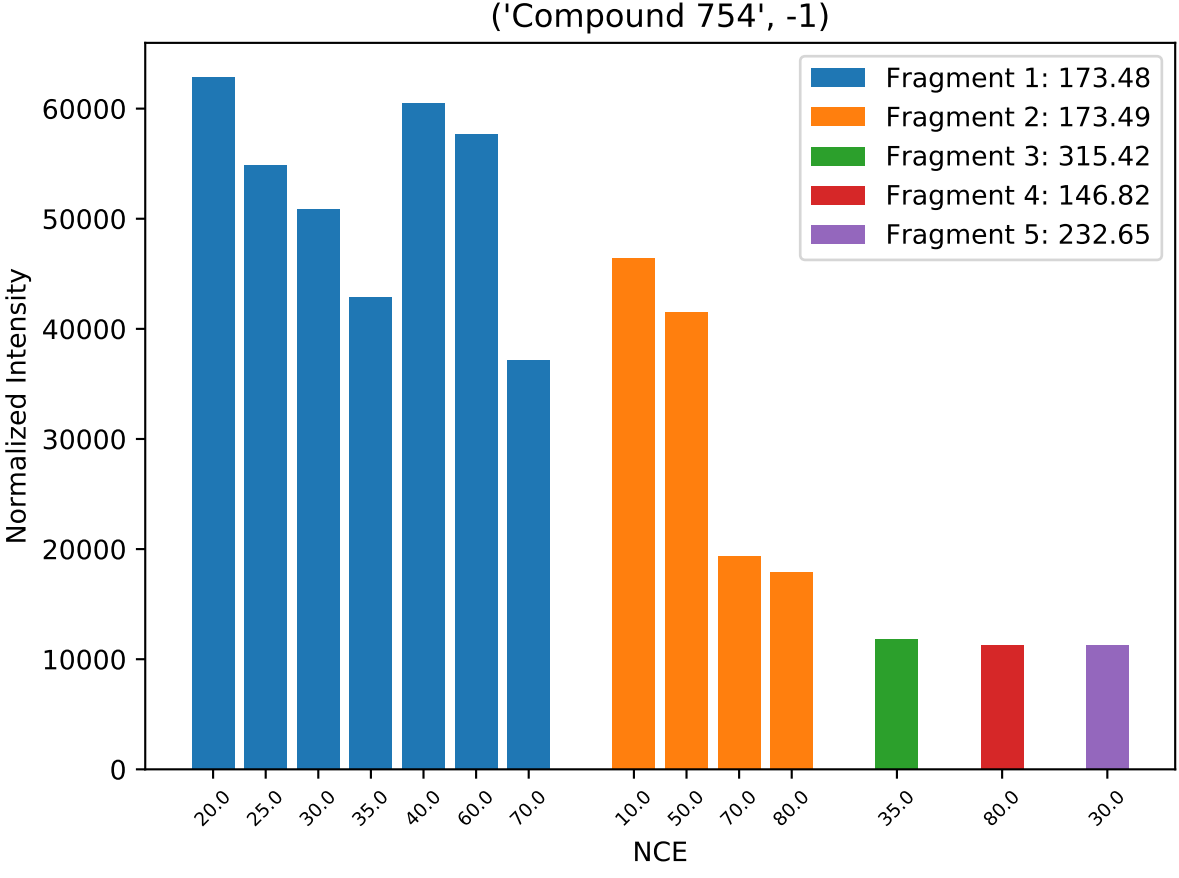

('Compound 749', -1)
Fragment 1: 50.08
Fragment 2: 50.18
Fragment 3: 51.18
Fragment 4: 56.22
Fragment 5: 52.44
Normalized Intensity
0
200
400
600
800
1000
50.0
60.0
50.0
40.0
35.0
NCE

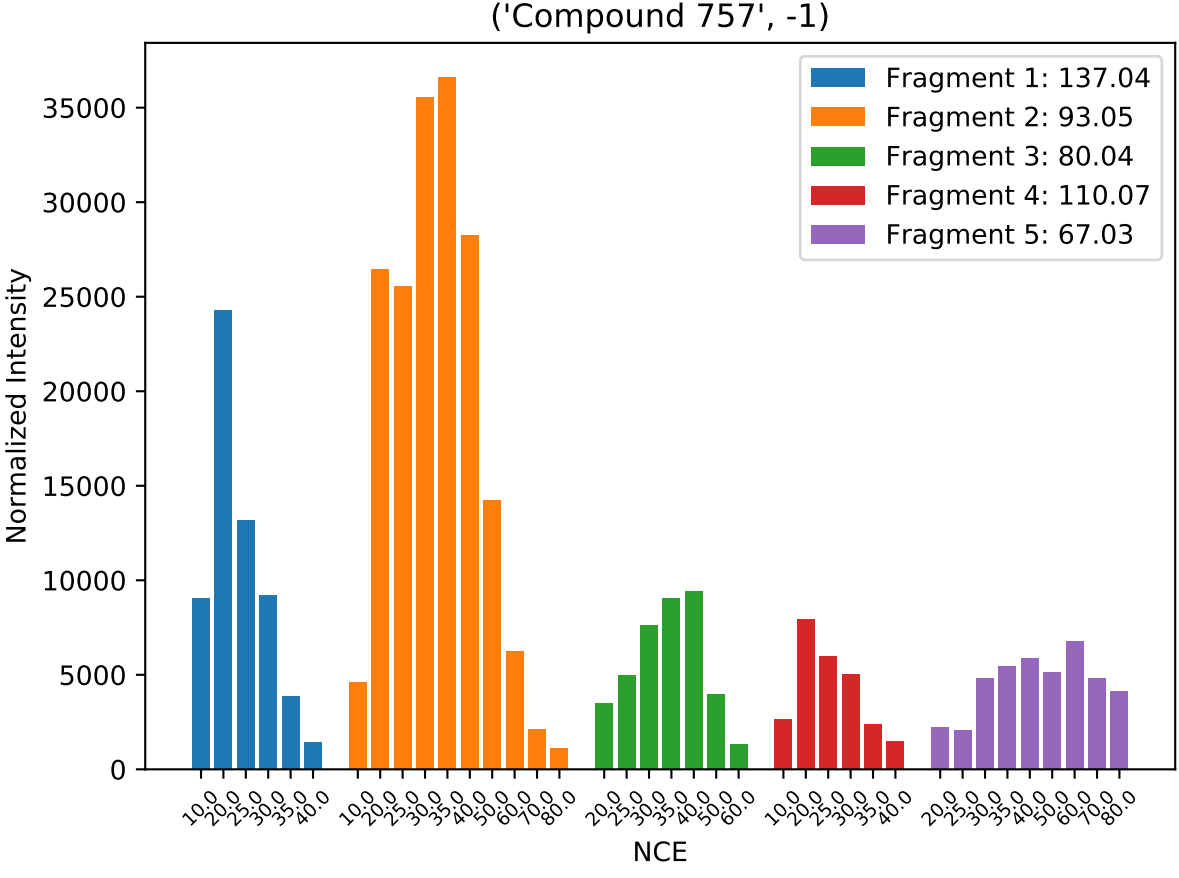

('Compound 750', -1)
Fragment 1: 73.03
Fragment 2: 55.02
Fragment 3: 83.01
Fragment 4: 77.74
Fragment 5: 50.34
Normalized Intensity
0
1000
2000
3000
4000
10.0
20.0
10.0
20.0
25.0
30.0
40.0
10.0
20.0
25.0
25.0
NCE

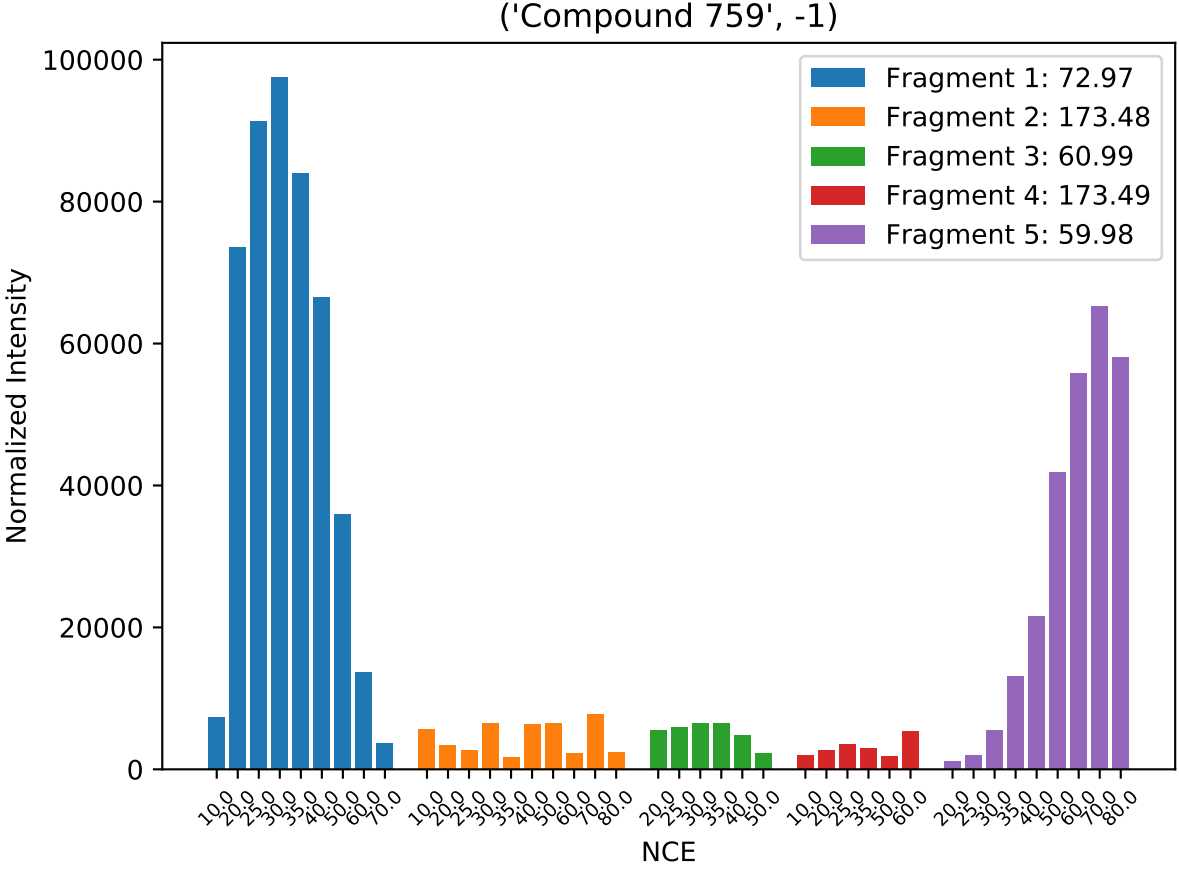

('Compound 751', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 345.28
Fragment 4: 173.5
Fragment 5: 343.26
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20.0
30.0
40.0
10.0
25.0
35.0
50.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
60.0
40.0
50.0
60.0
NCE

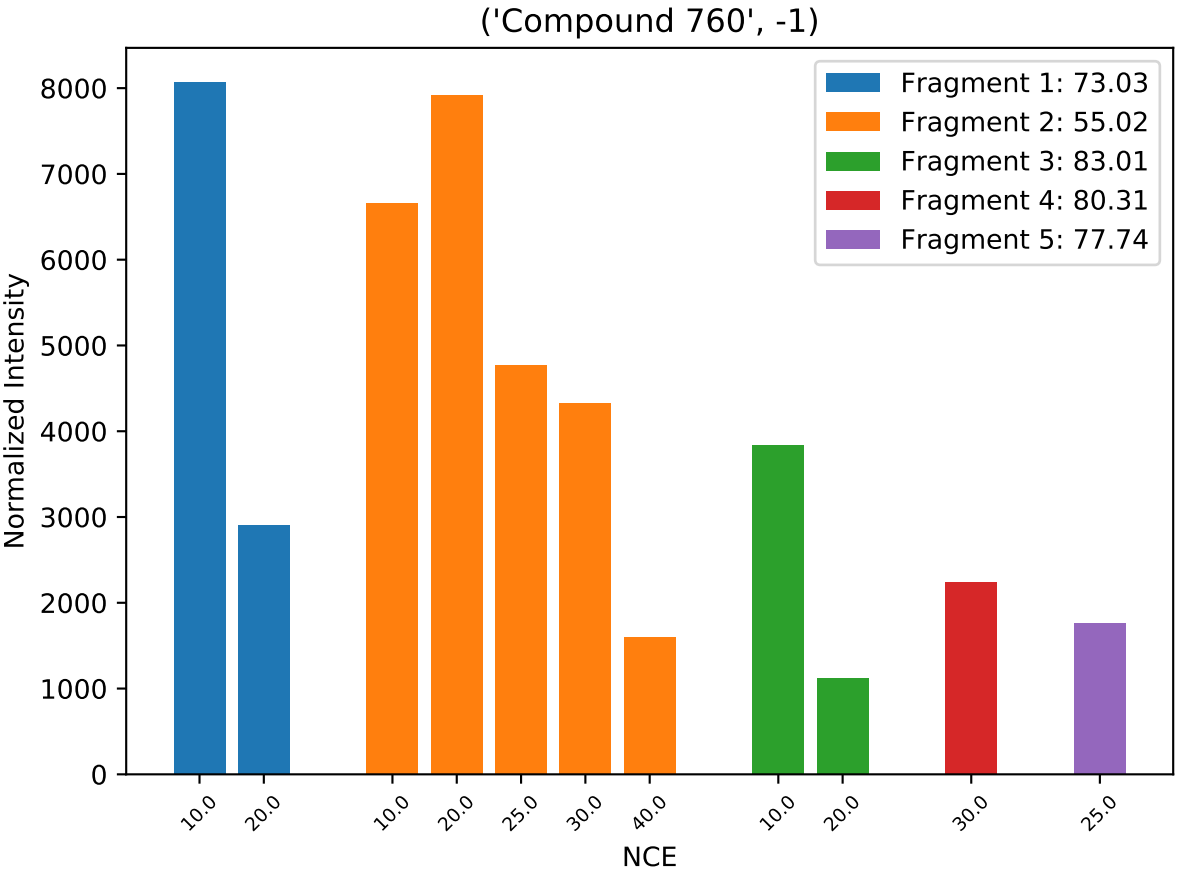

('Compound 167', -1)
Fragment 1: 269.06
Fragment 2: 146.03
Fragment 3: 241.07
Fragment 4: 313.05
Fragment 5: 267.05
Normalized Intensity
0
50000
100000
150000
200000
25.0 30.0 35.0 40.0 50.0 60.0 70.0
50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

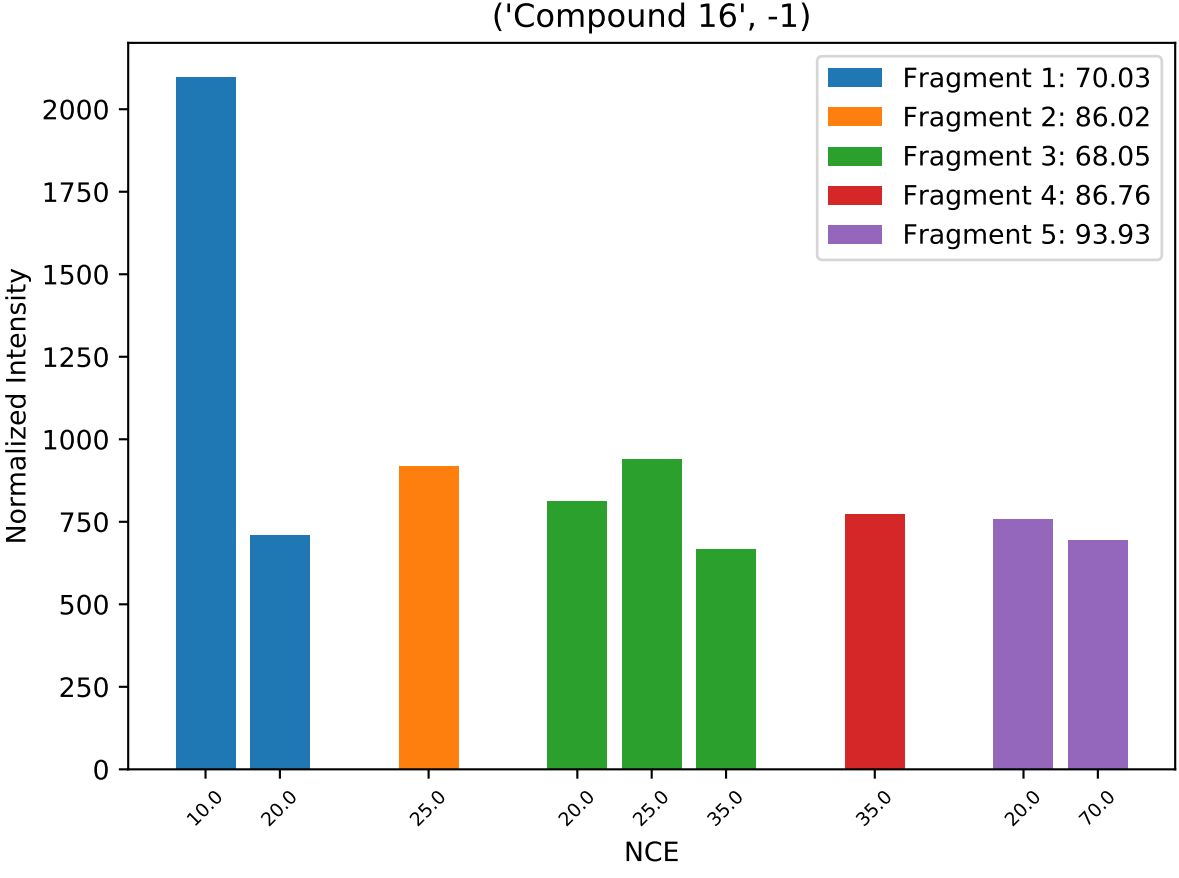

('Compound 752', -1)
Fragment 1: 129.02
Fragment 2: 75.01
Fragment 3: 59.01
Fragment 4: 99.01
Fragment 5: 176.9
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

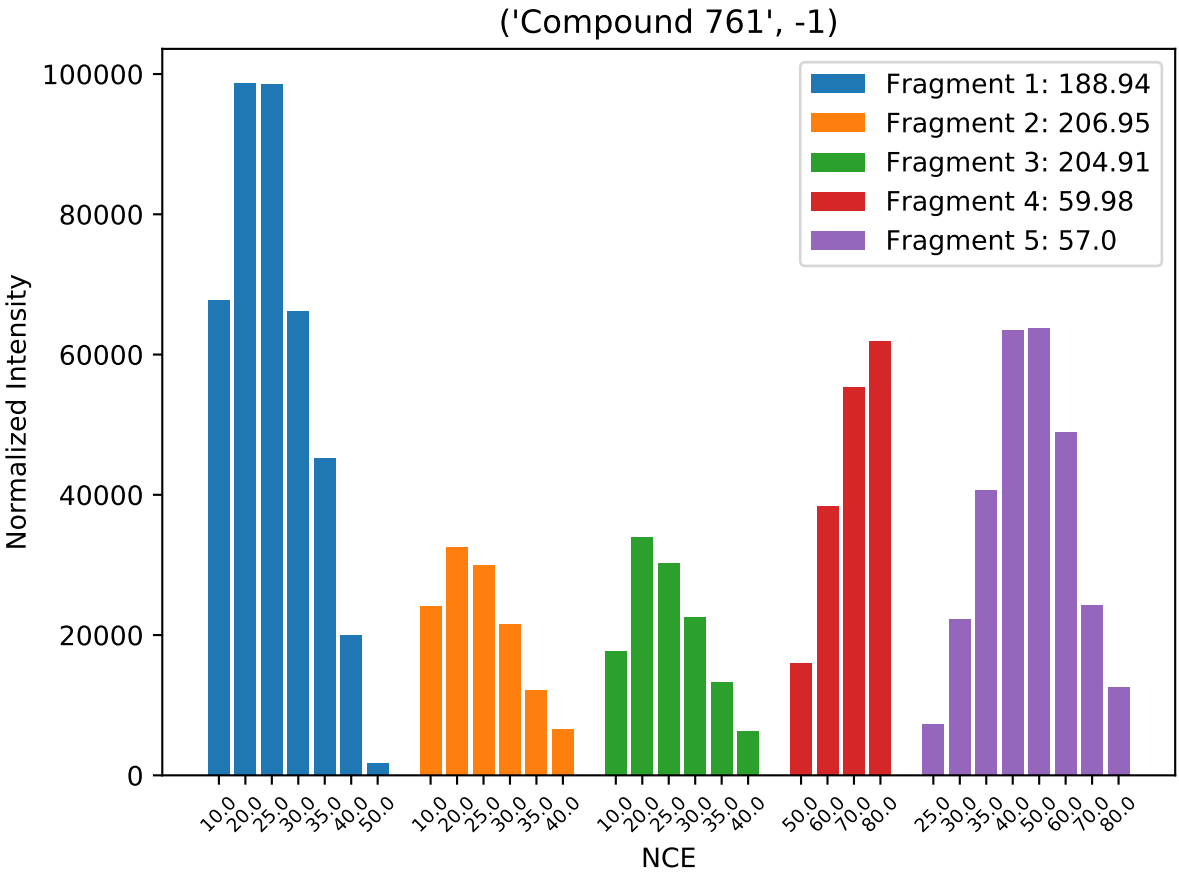

('Compound 754', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 315.42
Fragment 4: 146.82
Fragment 5: 232.65
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
20.0
25.0
30.0
35.0
40.0
60.0
70.0
10.0
50.0
70.0
80.0
35.0
80.0
30.0
NCE

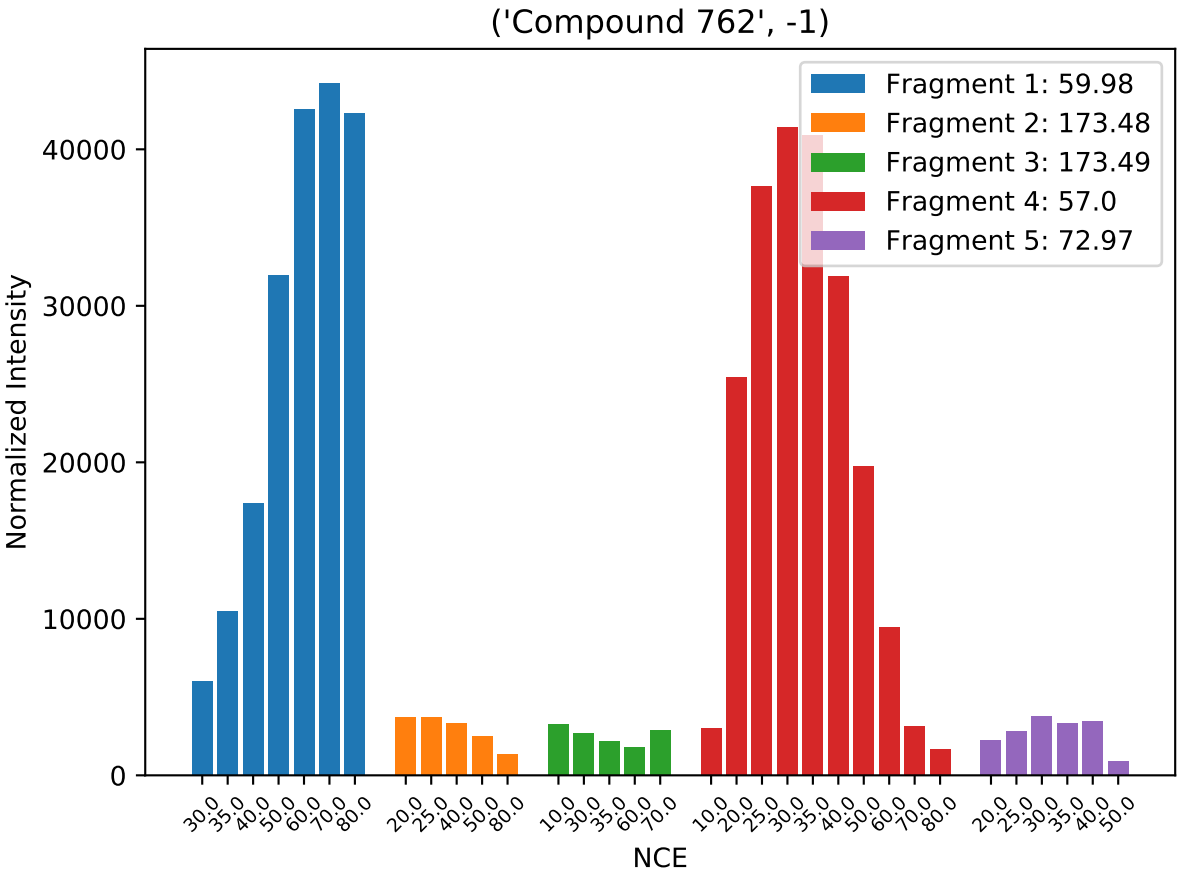

('Compound 757', -1)
Fragment 1: 137.04
Fragment 2: 93.05
Fragment 3: 80.04
Fragment 4: 110.07
Fragment 5: 67.03
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

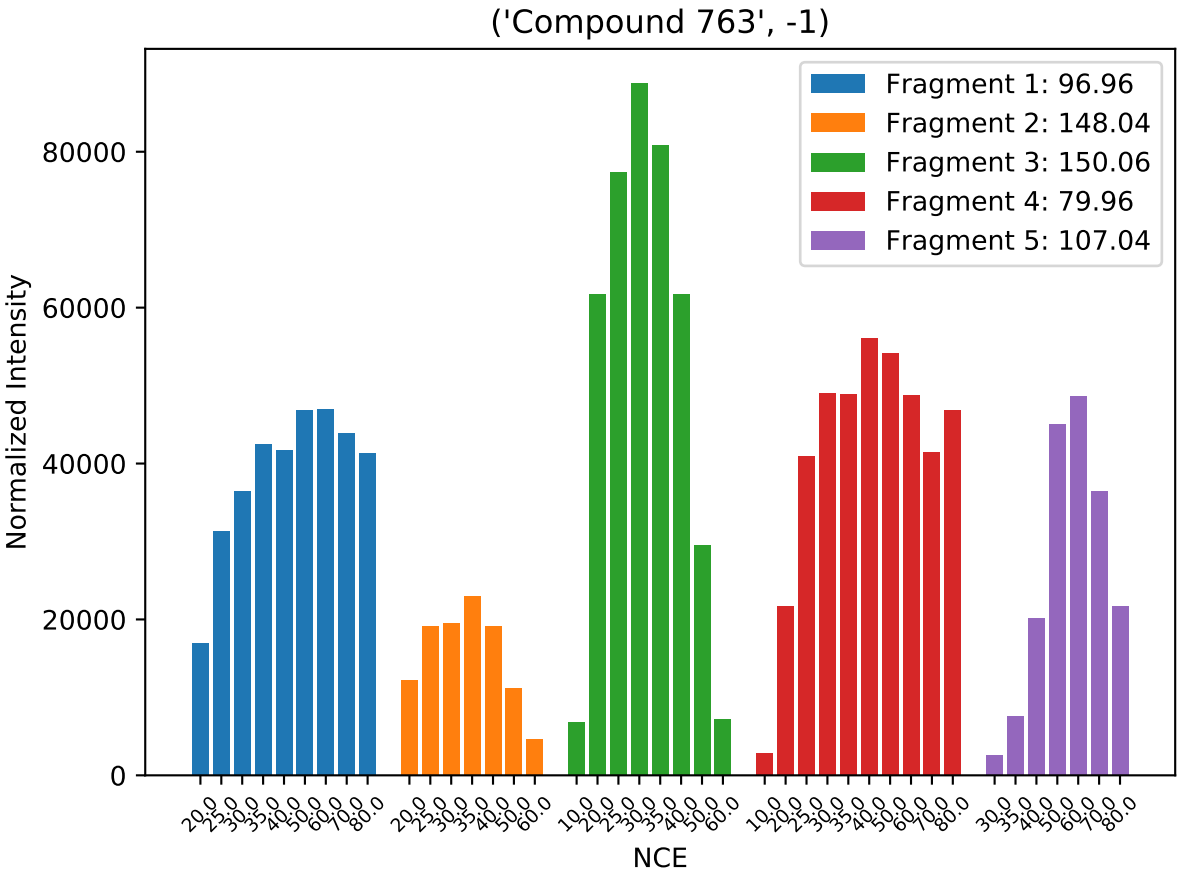

('Compound 759', -1)
Fragment 1: 72.97
Fragment 2: 173.48
Fragment 3: 60.99
Fragment 4: 173.49
Fragment 5: 59.98
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 35.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

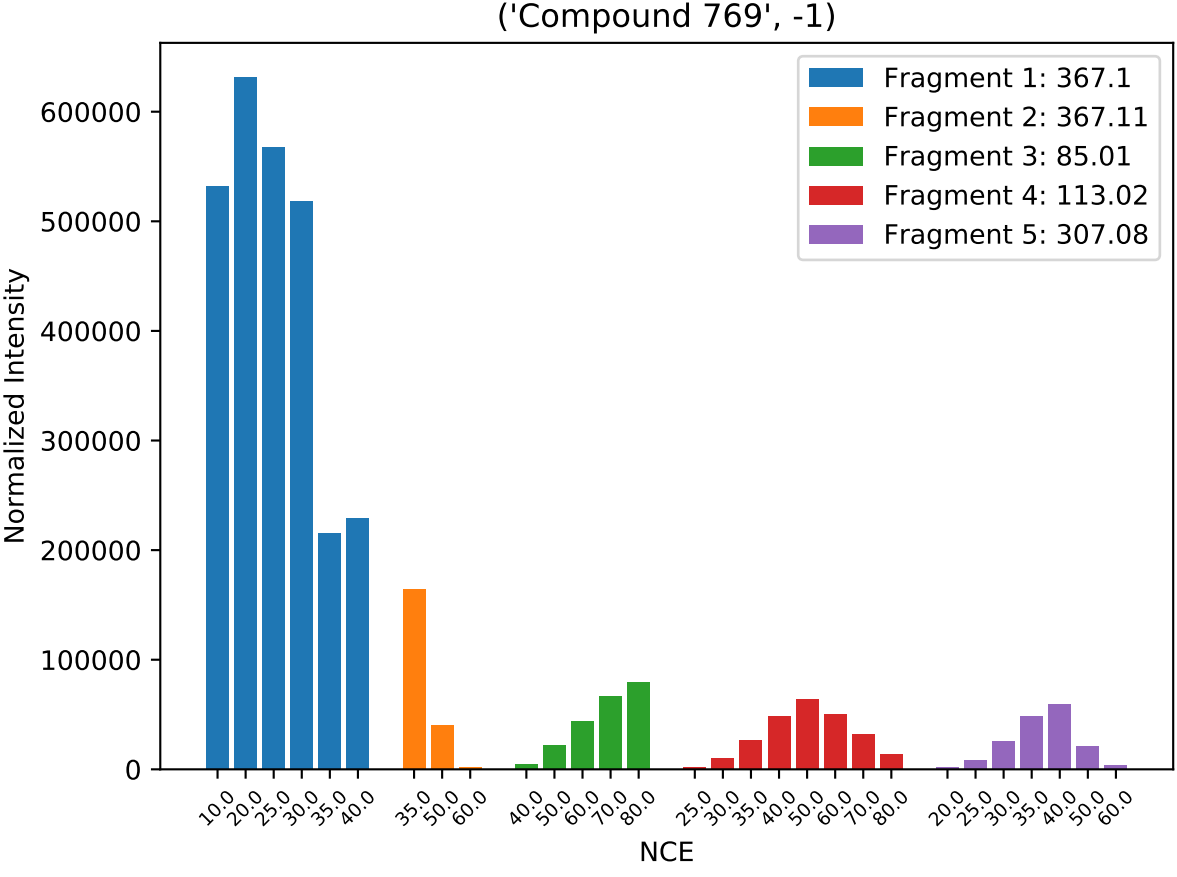

('Compound 760', -1)
Fragment 1: 73.03
Fragment 2: 55.02
Fragment 3: 83.01
Fragment 4: 80.31
Fragment 5: 77.74
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
20.0
10.0
20.0
25.0
30.0
40.0
10.0
20.0
30.0
25.0
NCE

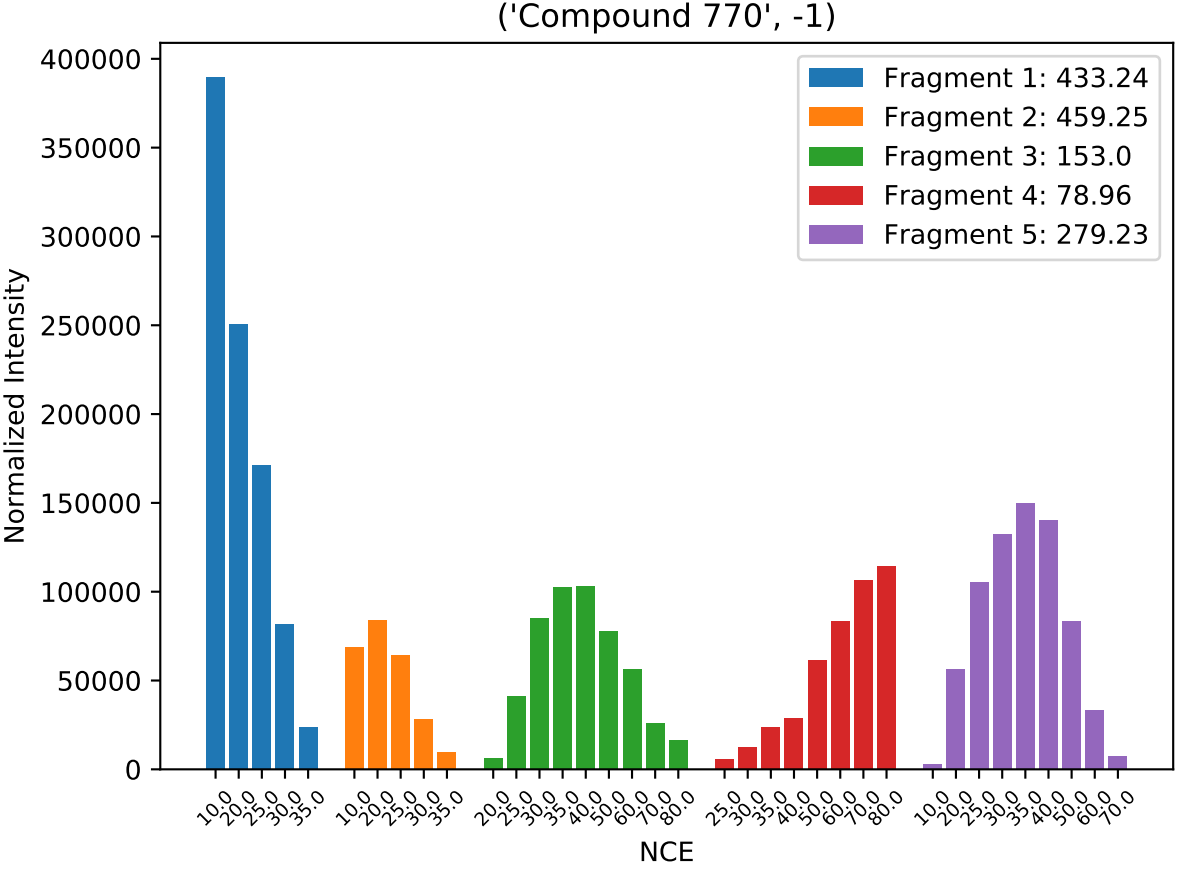

('Compound 16', -1)
Fragment 1: 70.03
Fragment 2: 86.02
Fragment 3: 68.05
Fragment 4: 86.76
Fragment 5: 93.93
Normalized Intensity
0
250
500
750
1000
1250
1500
1750
2000
10.0
20.0
25.0
20.0
25.0
35.0
35.0
20.0
70.0
NCE

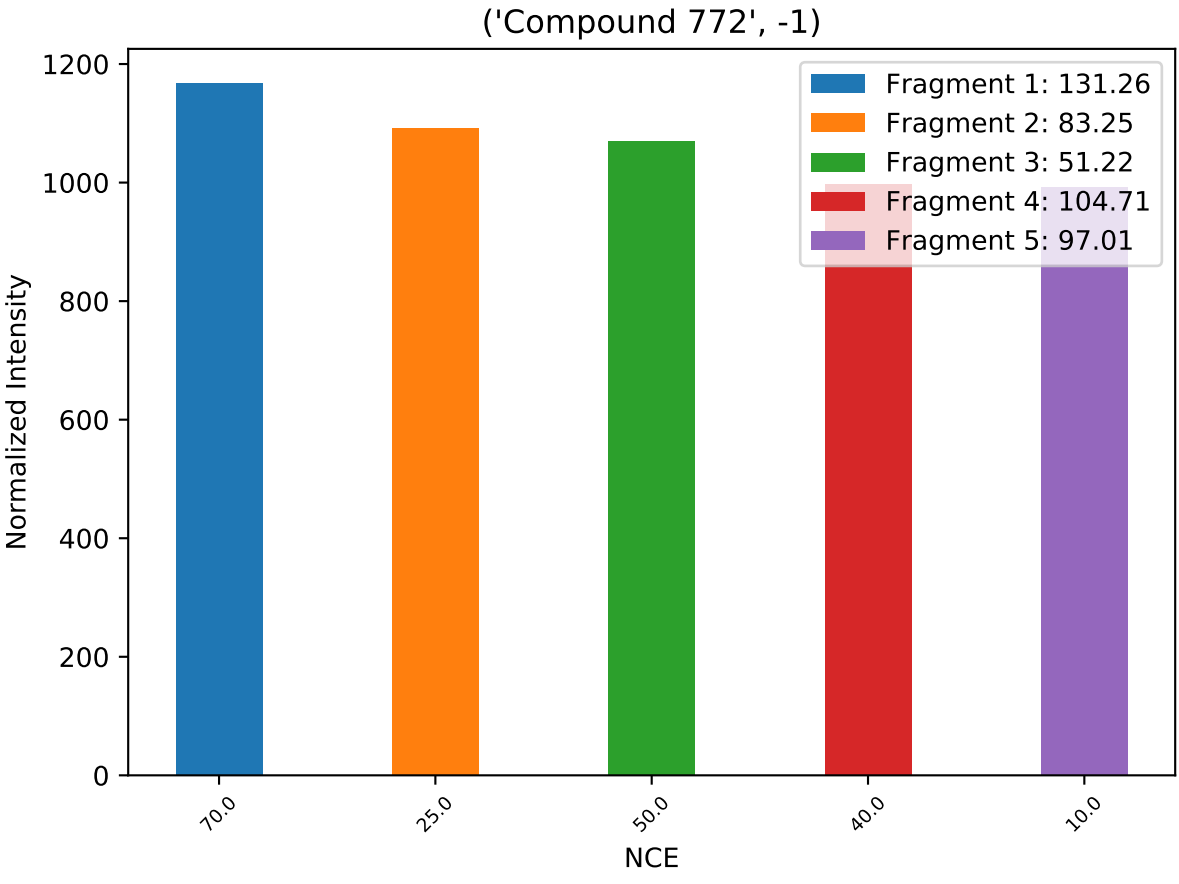

('Compound 761', -1)
Fragment 1: 188.94
Fragment 2: 206.95
Fragment 3: 204.91
Fragment 4: 59.98
Fragment 5: 57.0
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

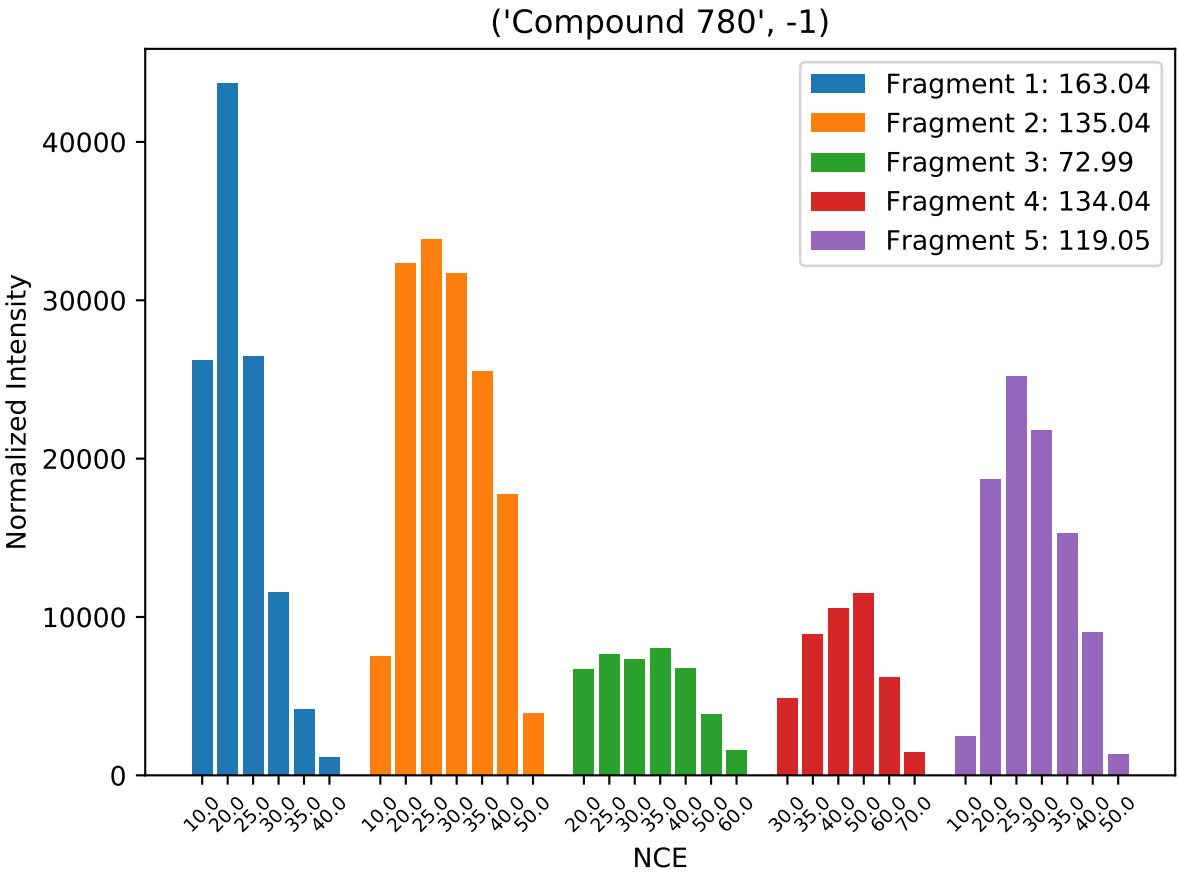

('Compound 762', -1)
Fragment 1: 59.98
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 57.0
Fragment 5: 72.97
Normalized Intensity
0
10000
20000
30000
40000
30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 40.0 50.0 80.0
10.0 30.0 35.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
NCE

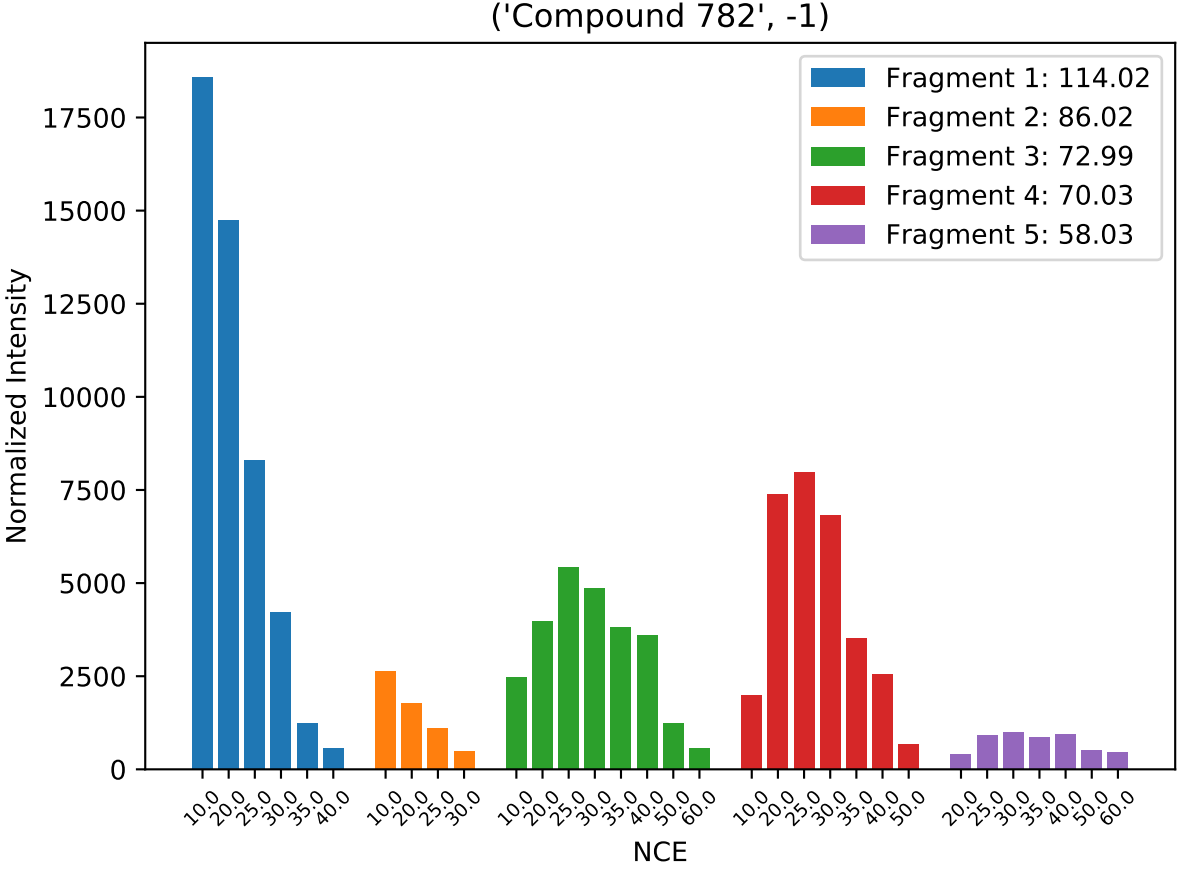

('Compound 763', -1)
Fragment 1: 96.96
Fragment 2: 148.04
Fragment 3: 150.06
Fragment 4: 79.96
Fragment 5: 107.04
Normalized Intensity
0
20000
40000
60000
80000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

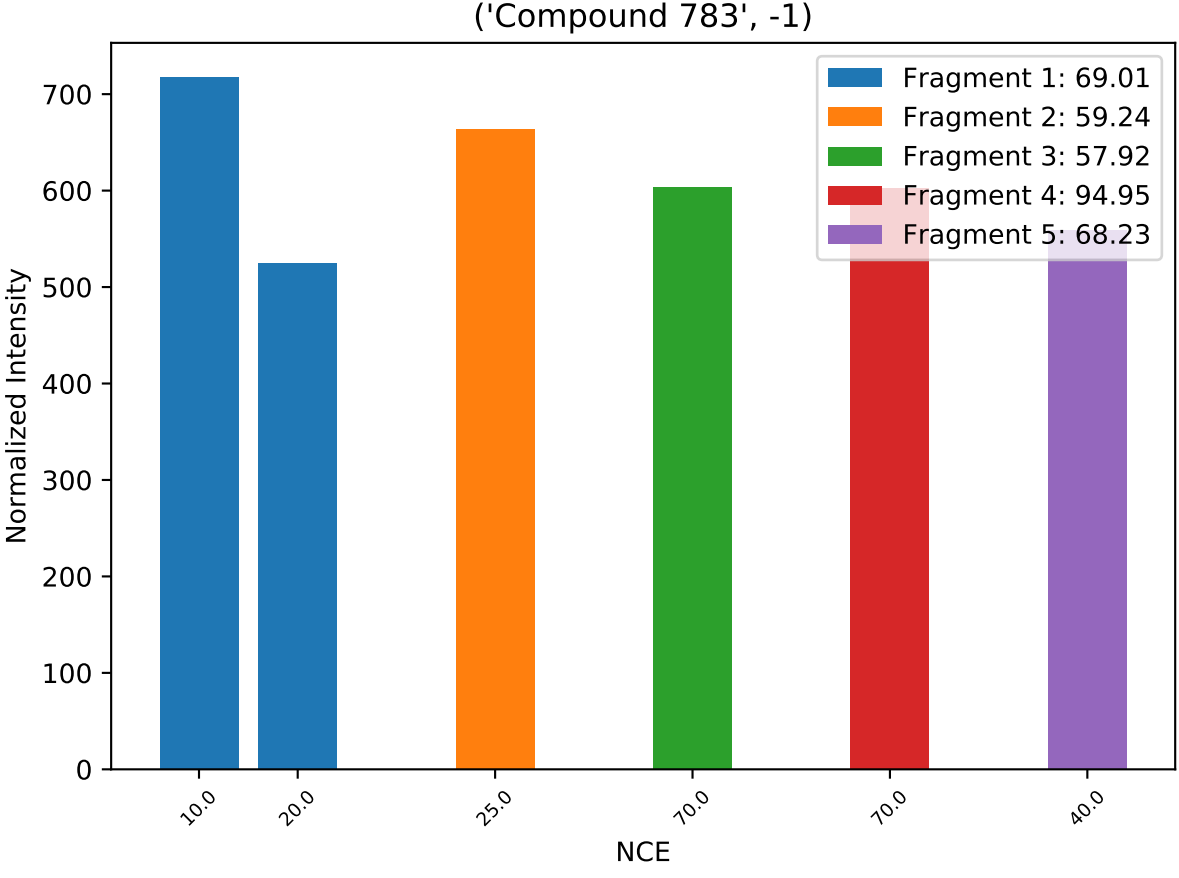

('Compound 769', -1)
Fragment 1: 367.1
Fragment 2: 367.11
Fragment 3: 85.01
Fragment 4: 113.02
Fragment 5: 307.08
Normalized Intensity
0
100000
200000
300000
400000
500000
600000
10.0 20.0 25.0 30.0 35.0 40.0
35.0 50.0 60.0
40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

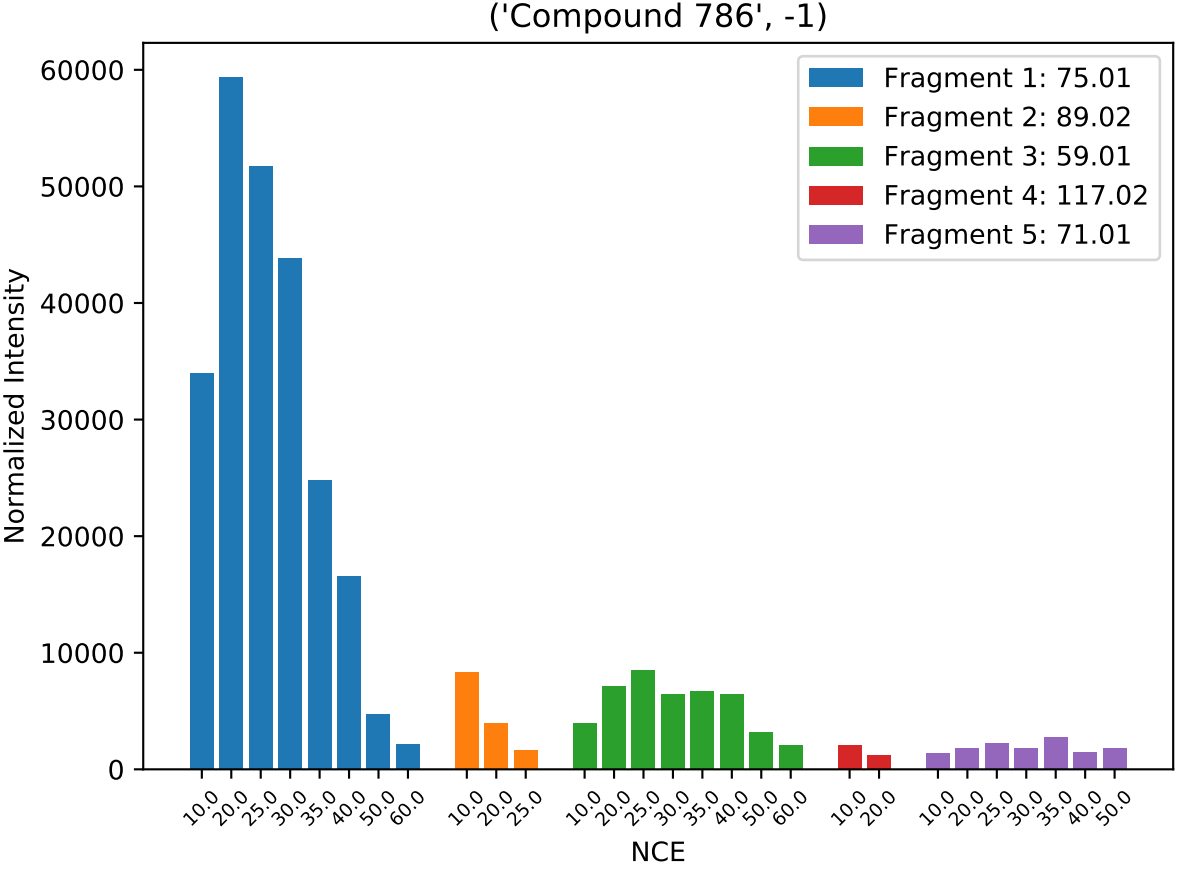

('Compound 770', -1)
Fragment 1: 433.24
Fragment 2: 459.25
Fragment 3: 153.0
Fragment 4: 78.96
Fragment 5: 279.23
Normalized Intensity
400000
350000
300000
250000
200000
150000
100000
50000
0
NCE
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0

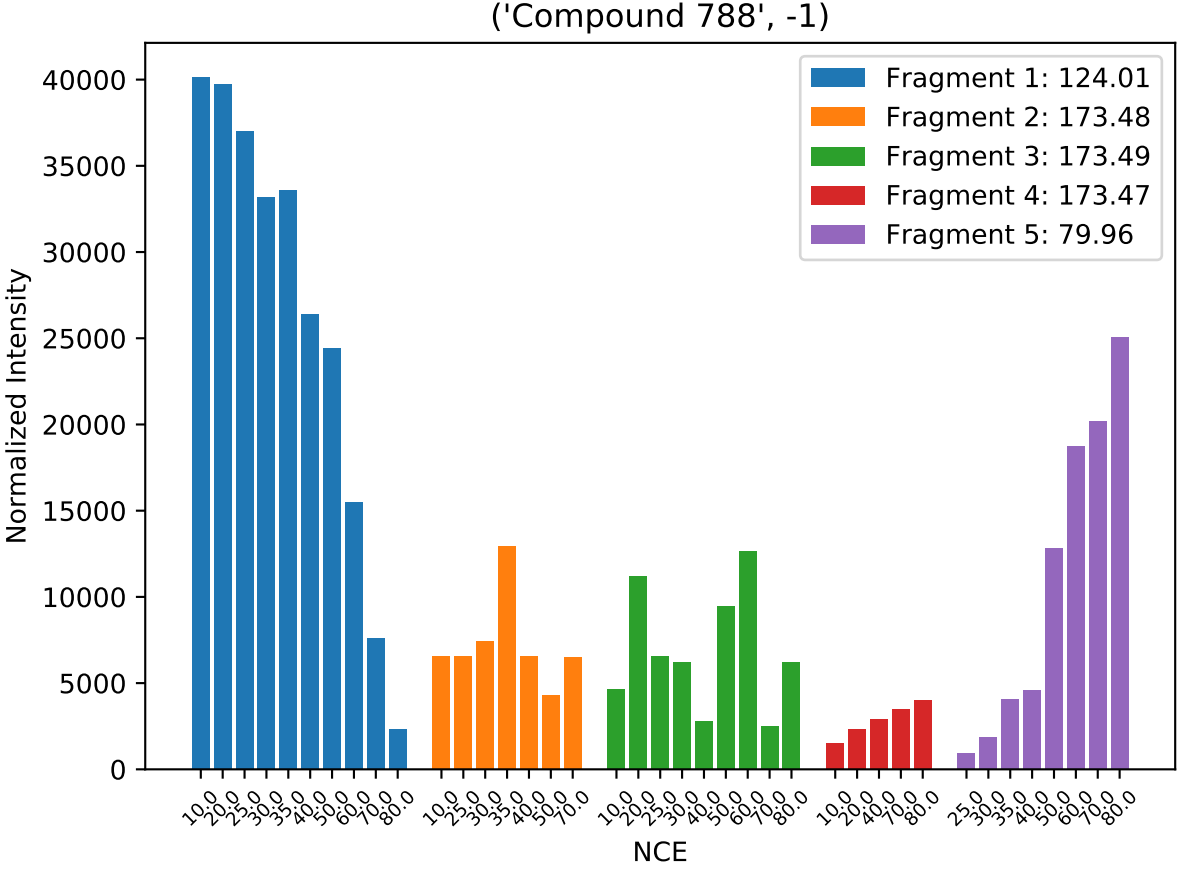

('Compound 772', -1)
Fragment 1: 131.26
Fragment 2: 83.25
Fragment 3: 51.22
Fragment 4: 104.71
Fragment 5: 97.01
Normalized Intensity
0
200
400
600
800
1000
1200
70.0
25.0
50.0
40.0
10.0
NCE

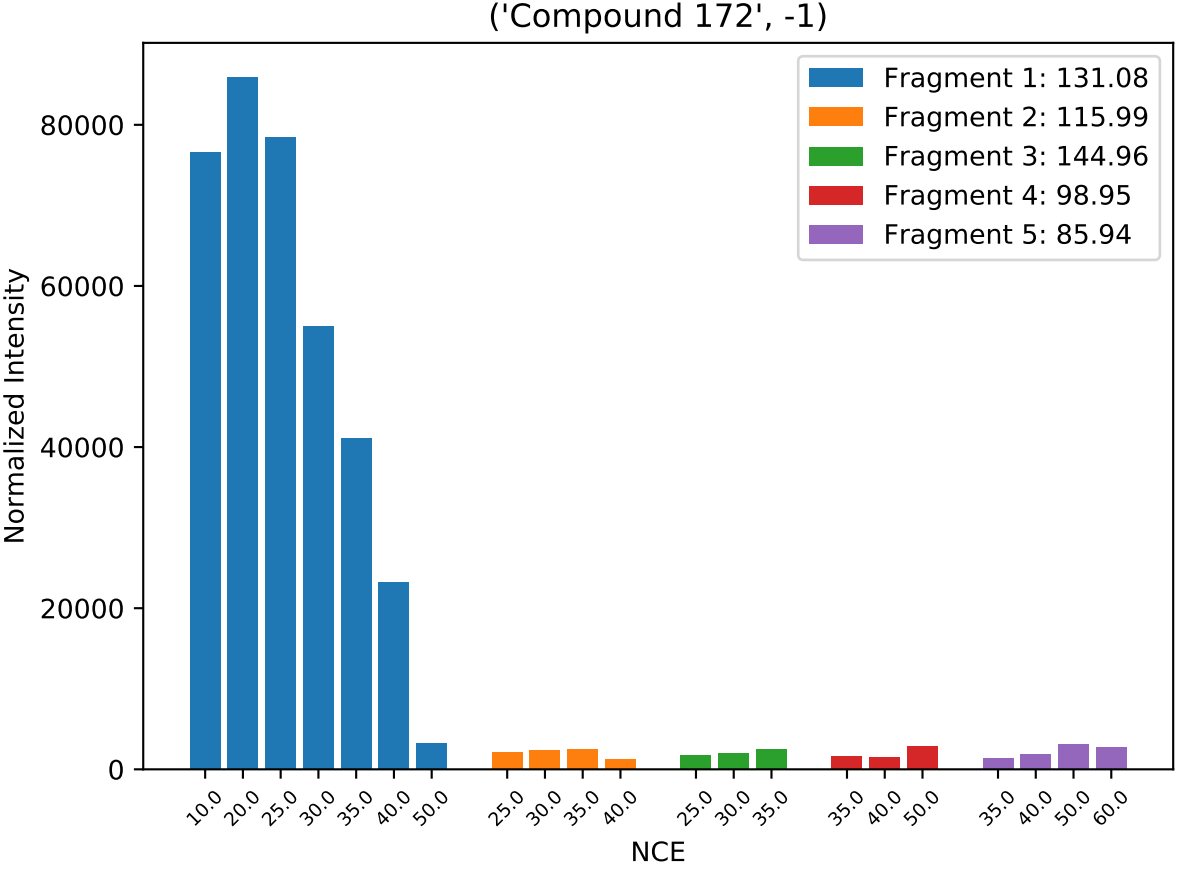

('Compound 780', -1)
Fragment 1: 163.04
Fragment 2: 135.04
Fragment 3: 72.99
Fragment 4: 134.04
Fragment 5: 119.05
Normalized Intensity
0
10000
20000
30000
40000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

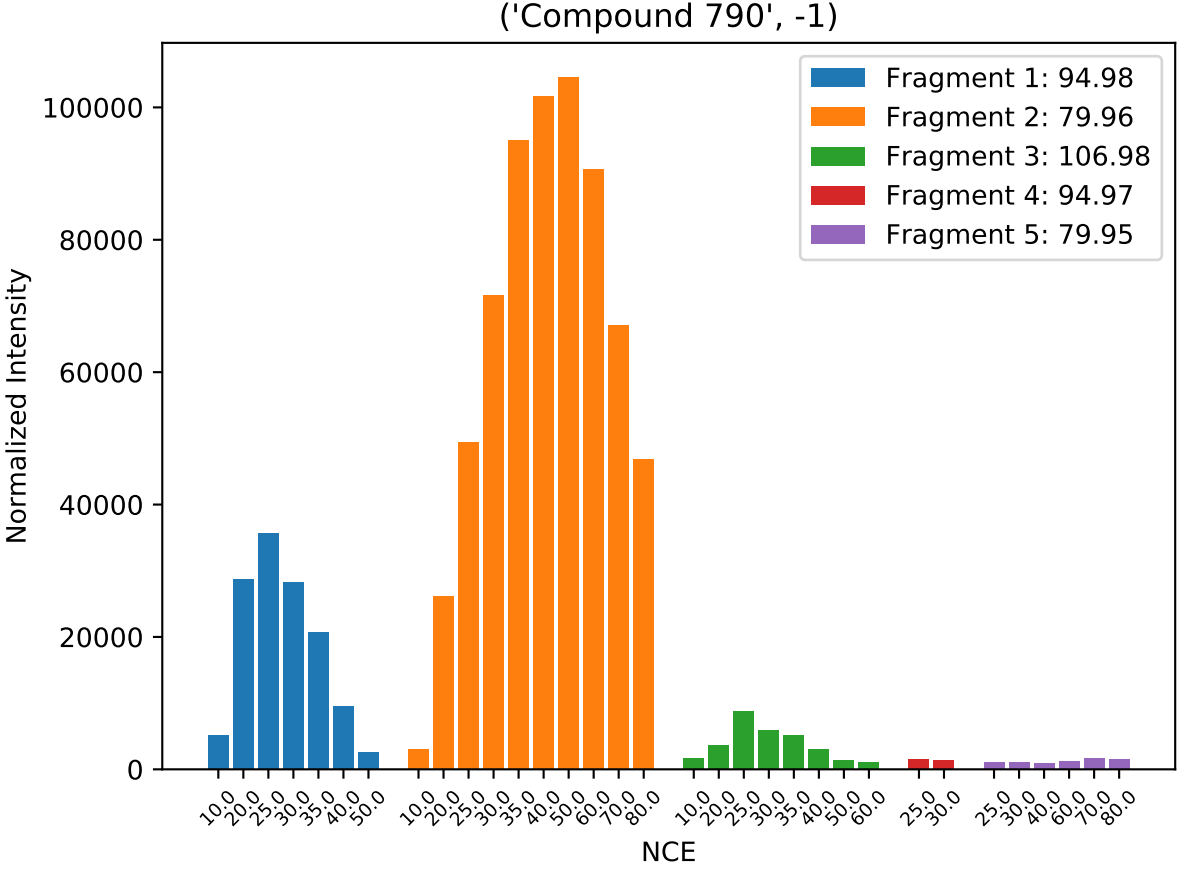

('Compound 782', -1)
Fragment 1: 114.02
Fragment 2: 86.02
Fragment 3: 72.99
Fragment 4: 70.03
Fragment 5: 58.03
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

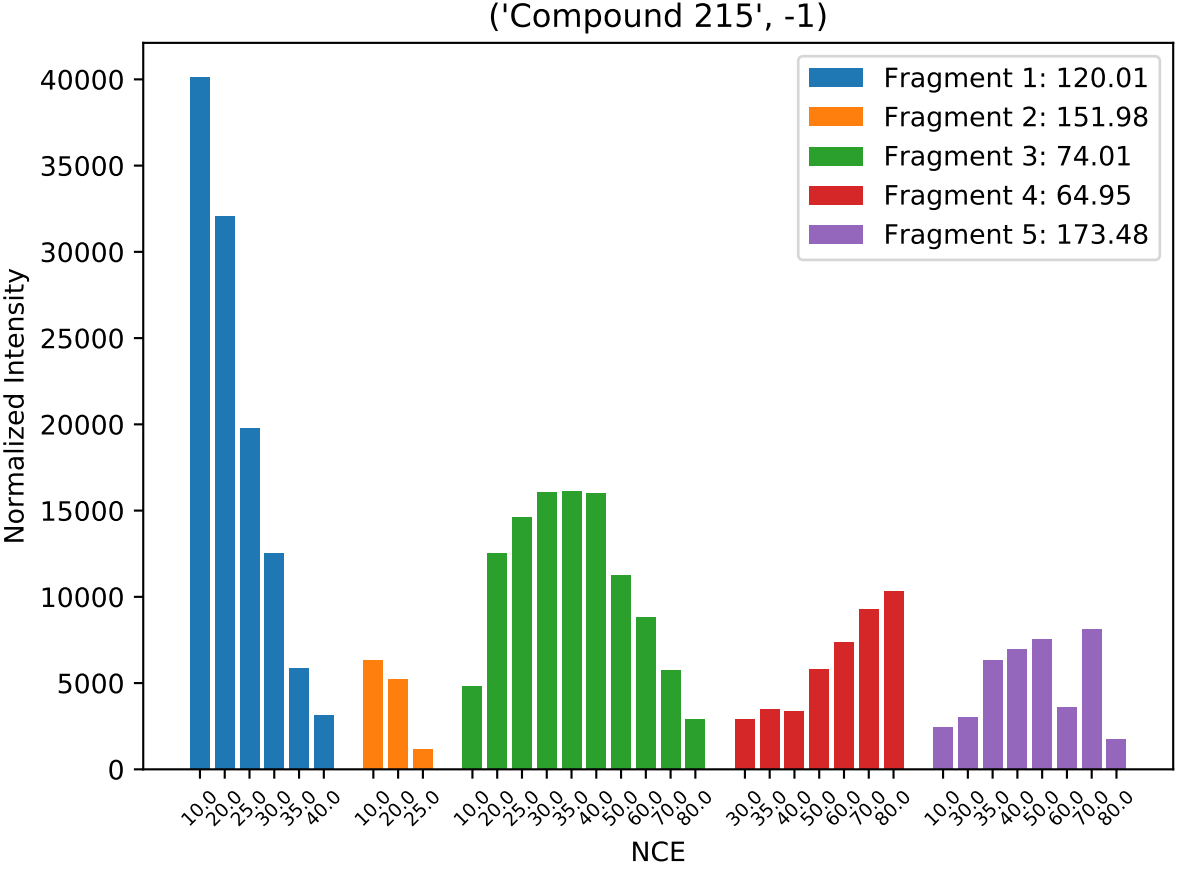

('Compound 783', -1)
Fragment 1: 69.01
Fragment 2: 59.24
Fragment 3: 57.92
Fragment 4: 94.95
Fragment 5: 68.23
Normalized Intensity
0
100
200
300
400
500
600
700
10.0
20.0
25.0
70.0
70.0
40.0
NCE

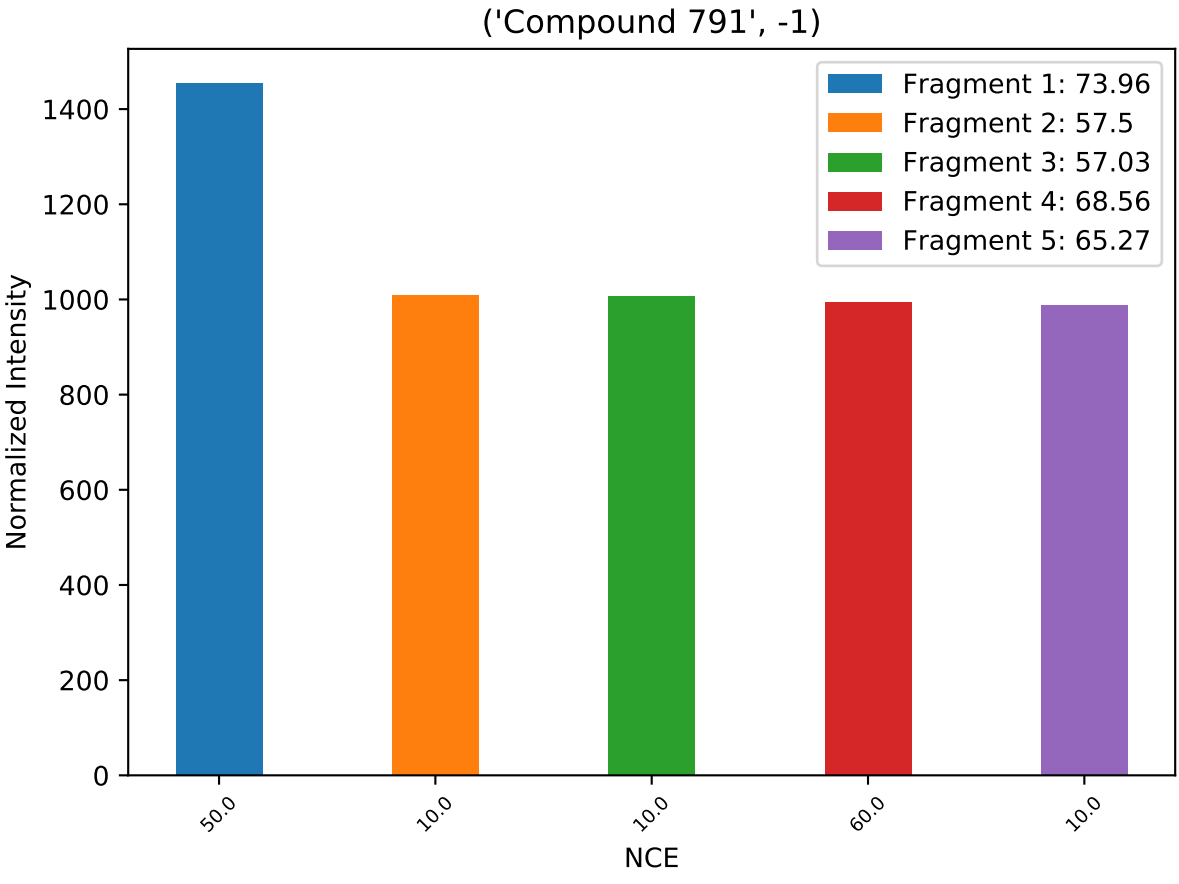

('Compound 786', -1)
Fragment 1: 75.01
Fragment 2: 89.02
Fragment 3: 59.01
Fragment 4: 117.02
Fragment 5: 71.01
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

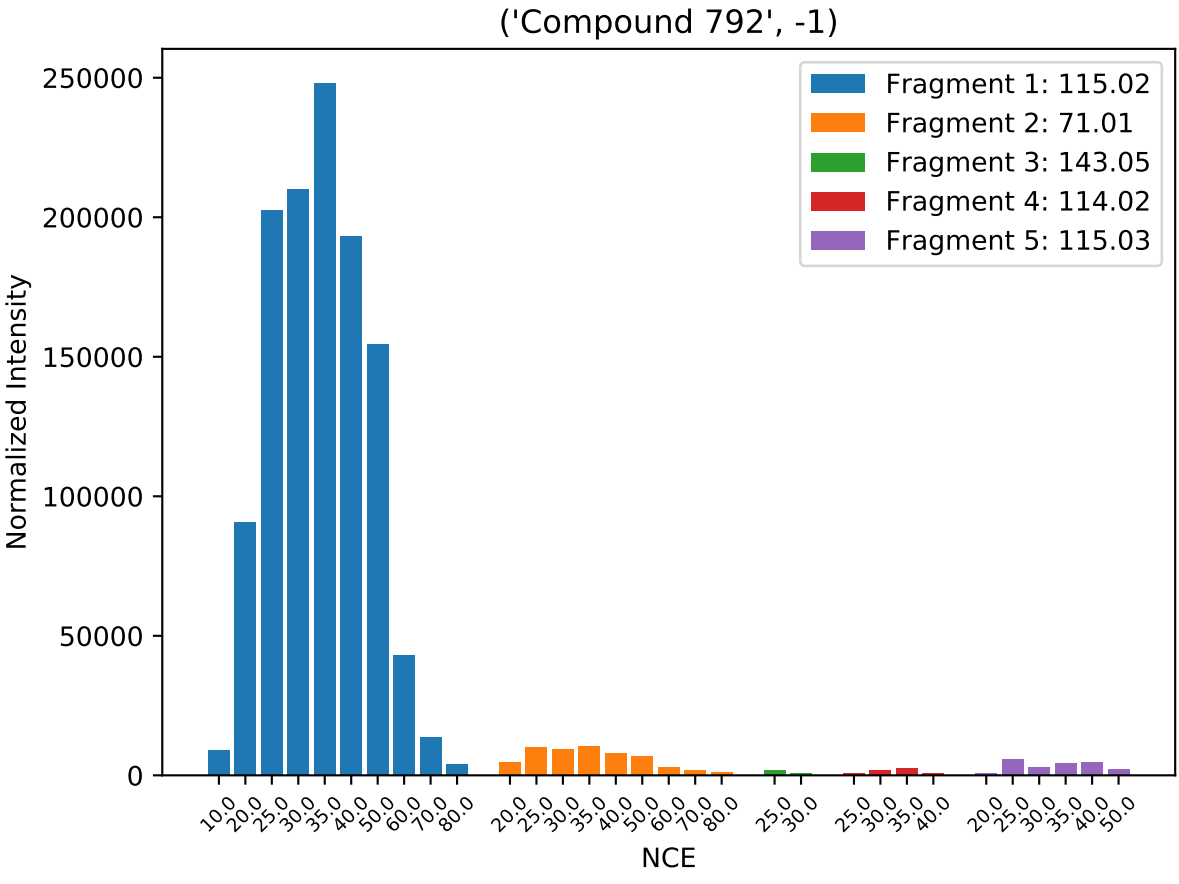

('Compound 788', -1)
Fragment 1: 124.01
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 173.47
Fragment 5: 79.96
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 25.0 30.0 35.0 40.0 50.0 70.0
10.0 20.0 25.0 30.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 40.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

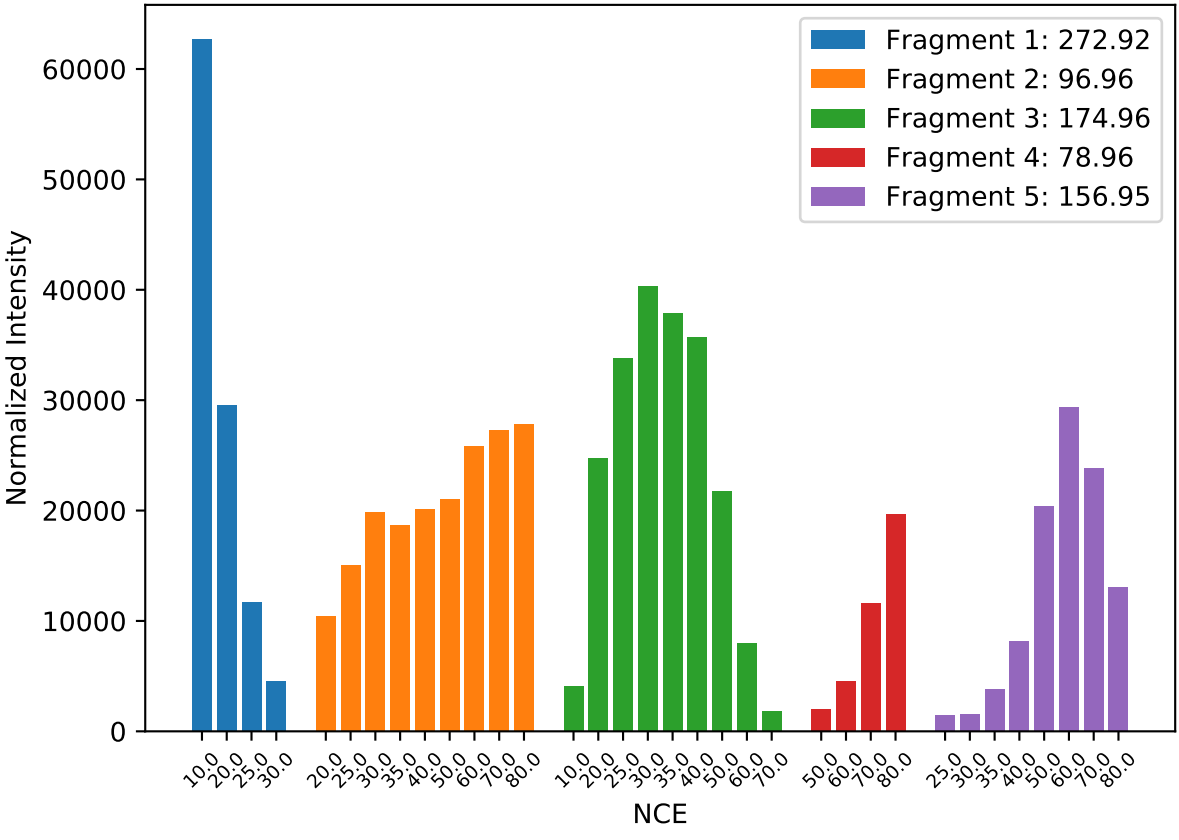

('Compound 172', -1)
Fragment 1: 131.08
Fragment 2: 115.99
Fragment 3: 144.96
Fragment 4: 98.95
Fragment 5: 85.94
Normalized Intensity
0
20000
40000
60000
80000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
40.0
25.0
30.0
35.0
35.0
40.0
50.0
35.0
40.0
50.0
60.0
NCE

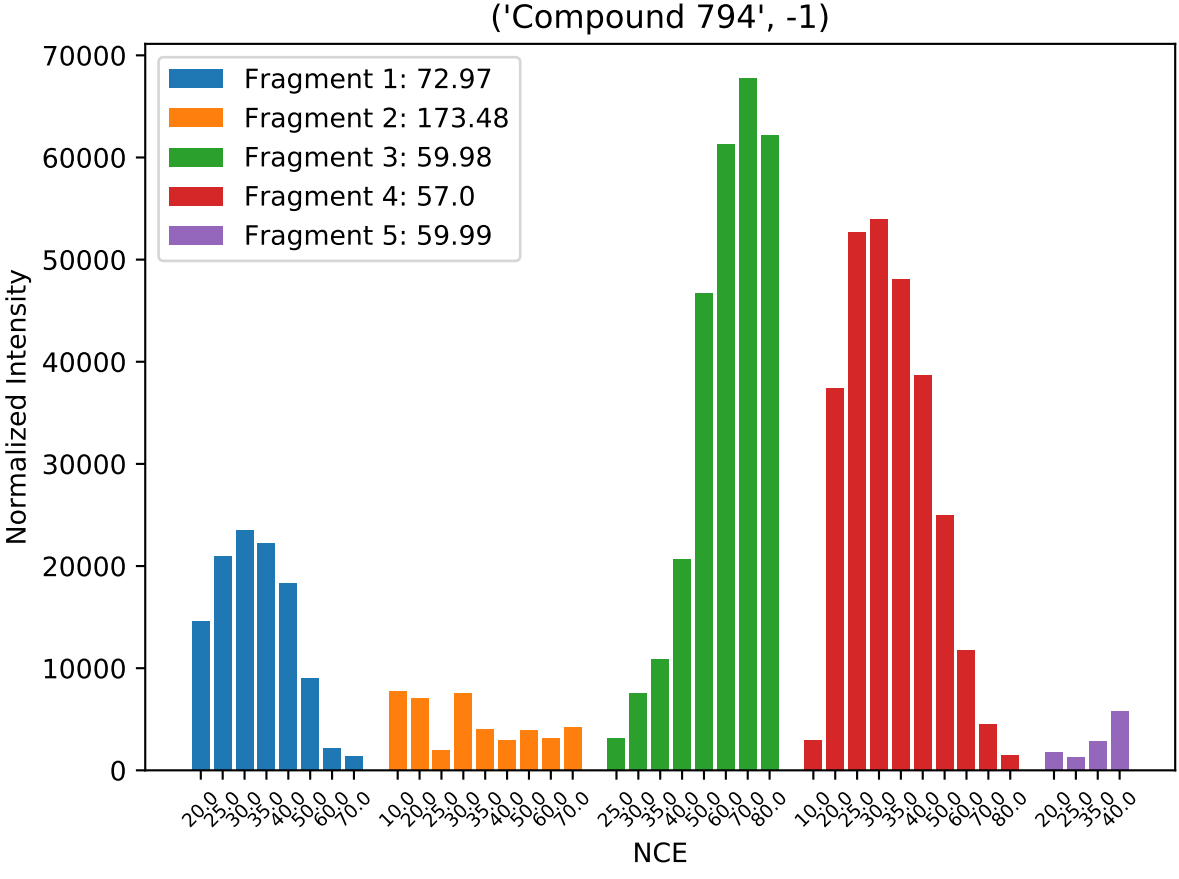

('Compound 790', -1)
Fragment 1: 94.98
Fragment 2: 79.96
Fragment 3: 106.98
Fragment 4: 94.97
Fragment 5: 79.95
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0
25.0 30.0 40.0 60.0 70.0 80.0
NCE

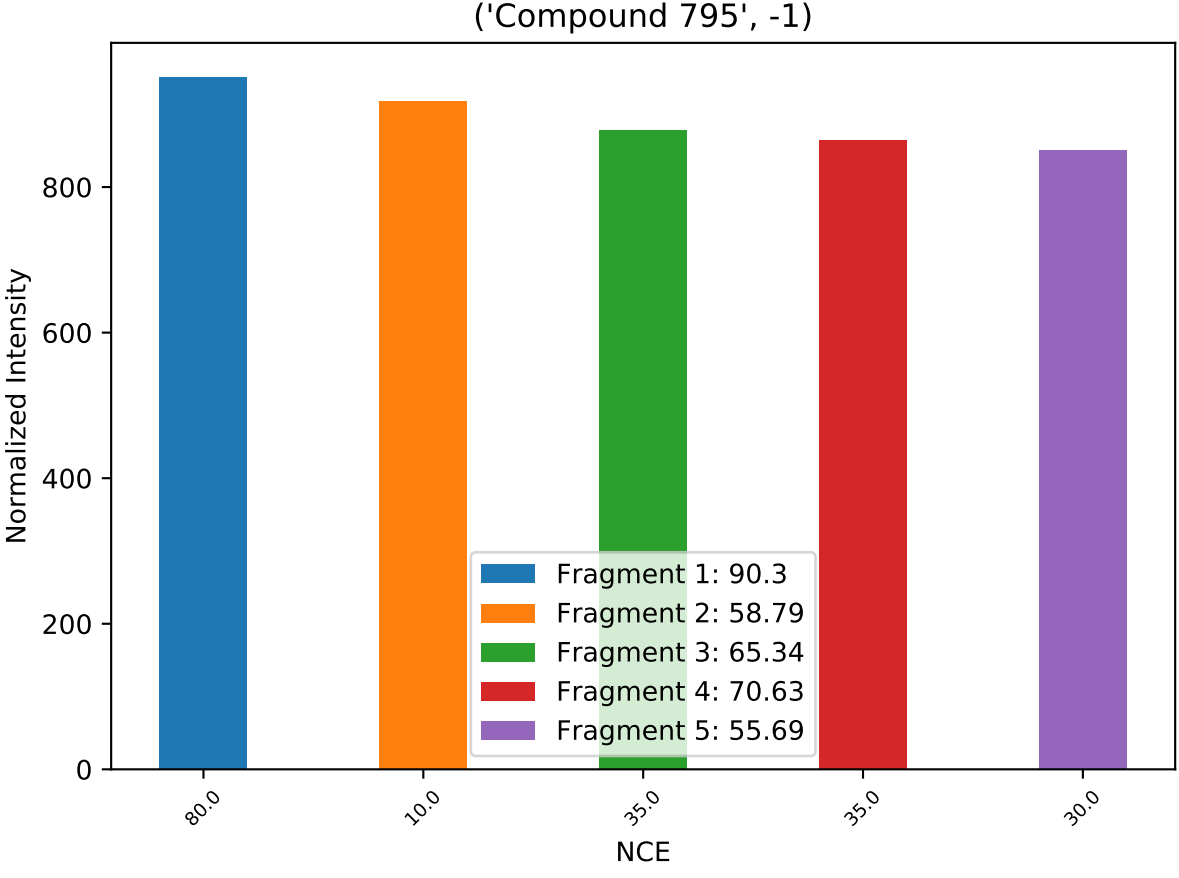

('Compound 215', -1)
Fragment 1: 120.01
Fragment 2: 151.98
Fragment 3: 74.01
Fragment 4: 64.95
Fragment 5: 173.48
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

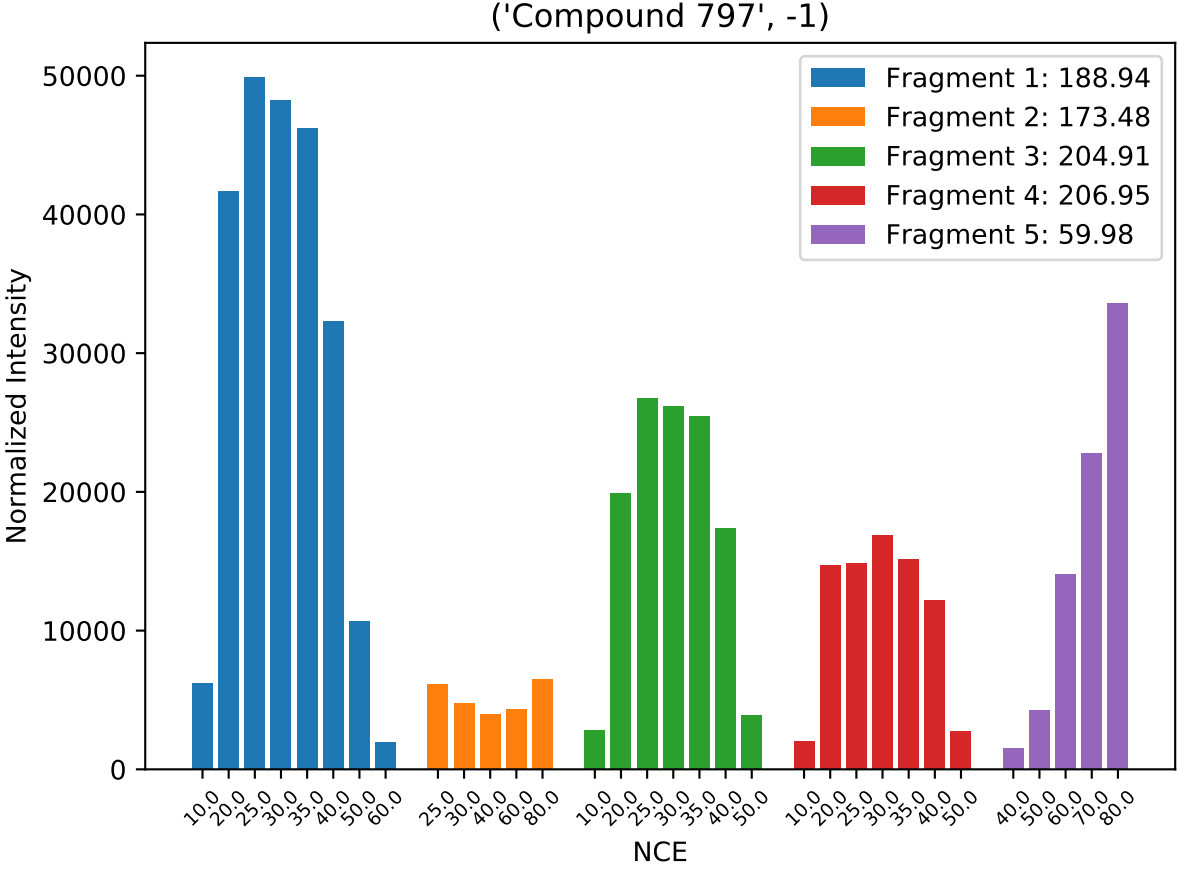

('Compound 791', -1)
Fragment 1: 73.96
Fragment 2: 57.5
Fragment 3: 57.03
Fragment 4: 68.56
Fragment 5: 65.27
Normalized Intensity
0
200
400
600
800
1000
1200
1400
50.0
10.0
10.0
60.0
10.0
NCE

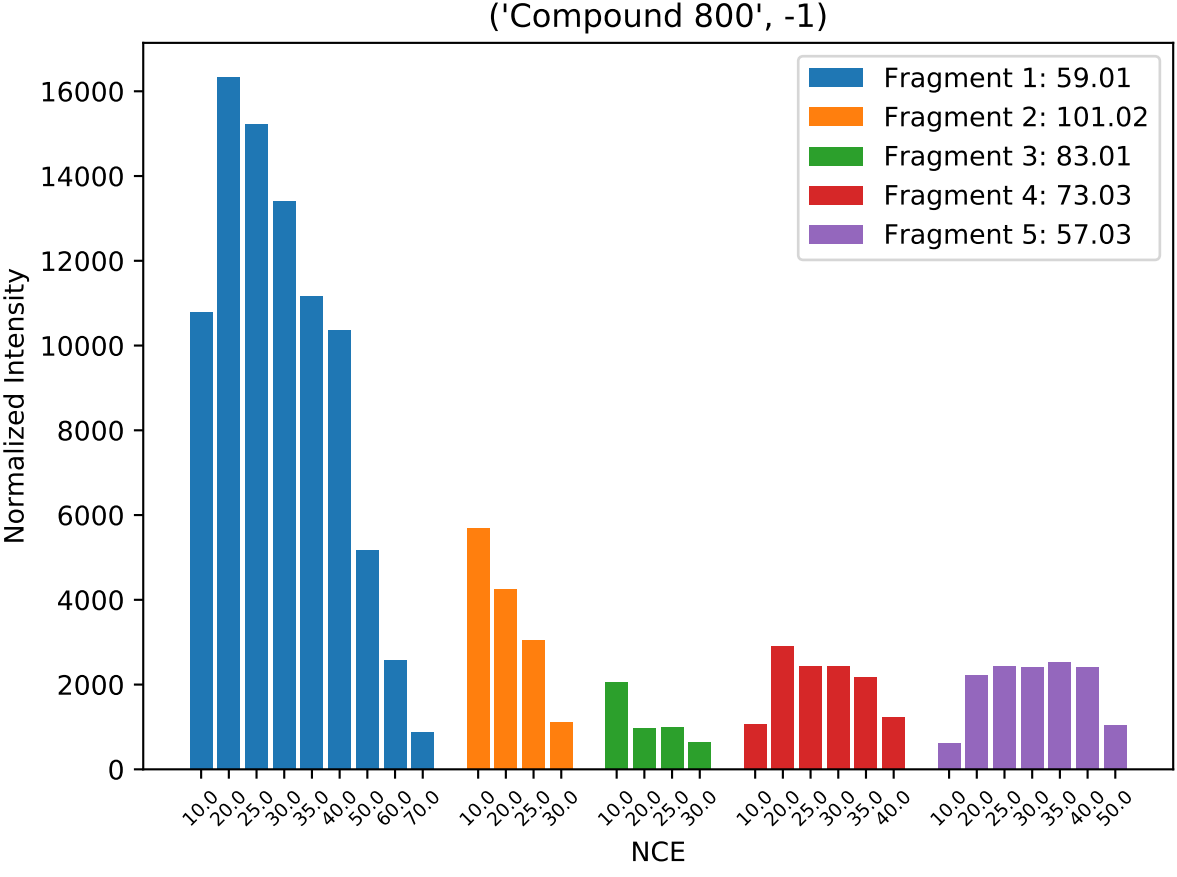

('Compound 792', -1)
Fragment 1: 115.02
Fragment 2: 71.01
Fragment 3: 143.05
Fragment 4: 114.02
Fragment 5: 115.03
Normalized Intensity
250000
200000
150000
100000
50000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

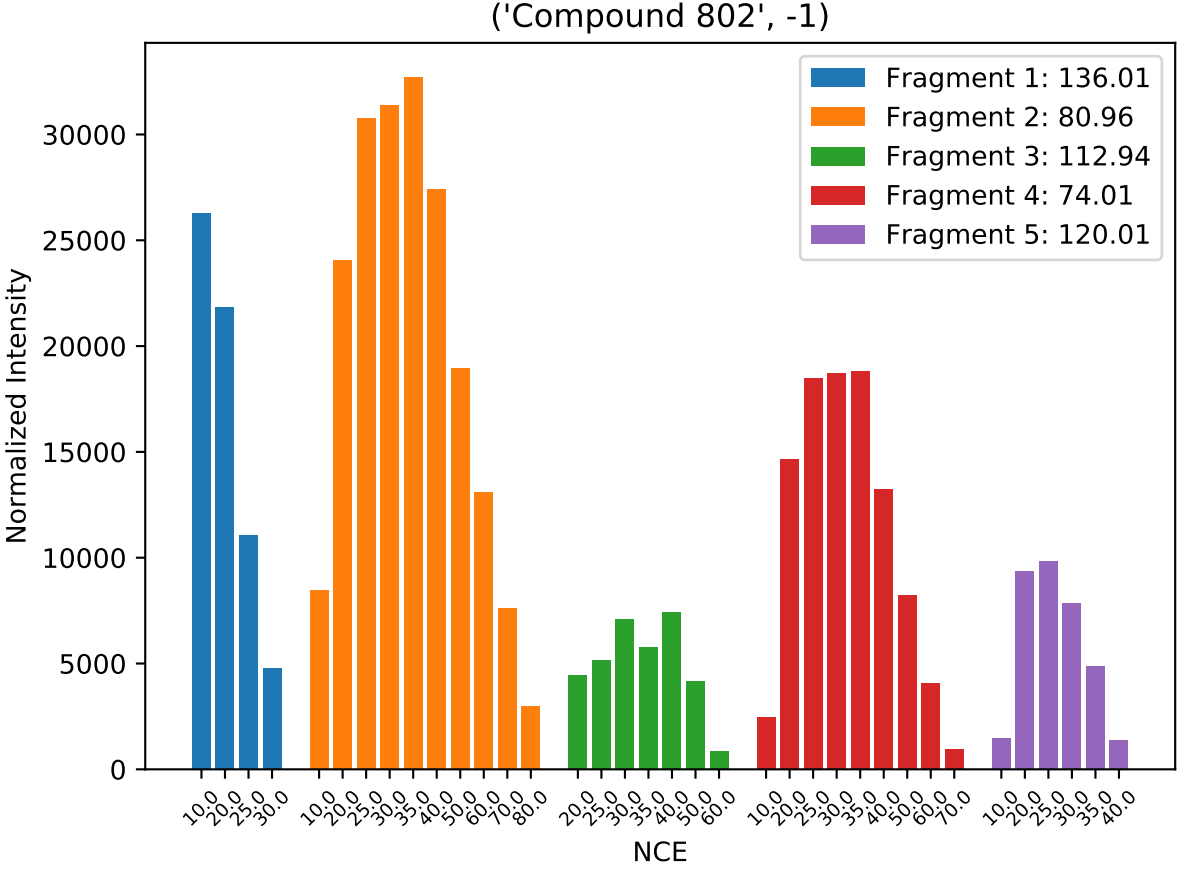

('Compound 793', -1)
Fragment 1: 272.92
Fragment 2: 96.96
Fragment 3: 174.96
Fragment 4: 78.96
Fragment 5: 156.95
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
NCE
10.0 20.0 25.0 30.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

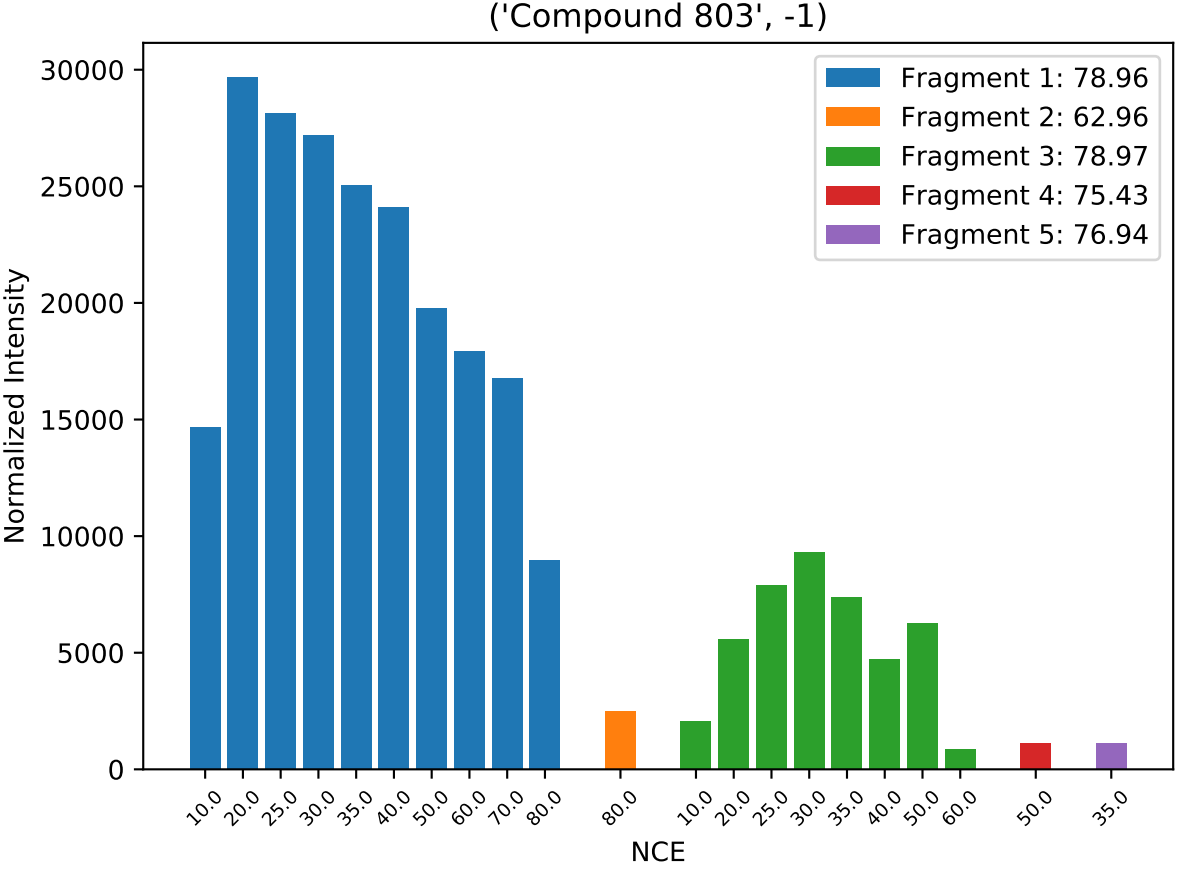

('Compound 794', -1)
Fragment 1: 72.97
Fragment 2: 173.48
Fragment 3: 59.98
Fragment 4: 57.0
Fragment 5: 59.99
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 35.0 40.0
NCE

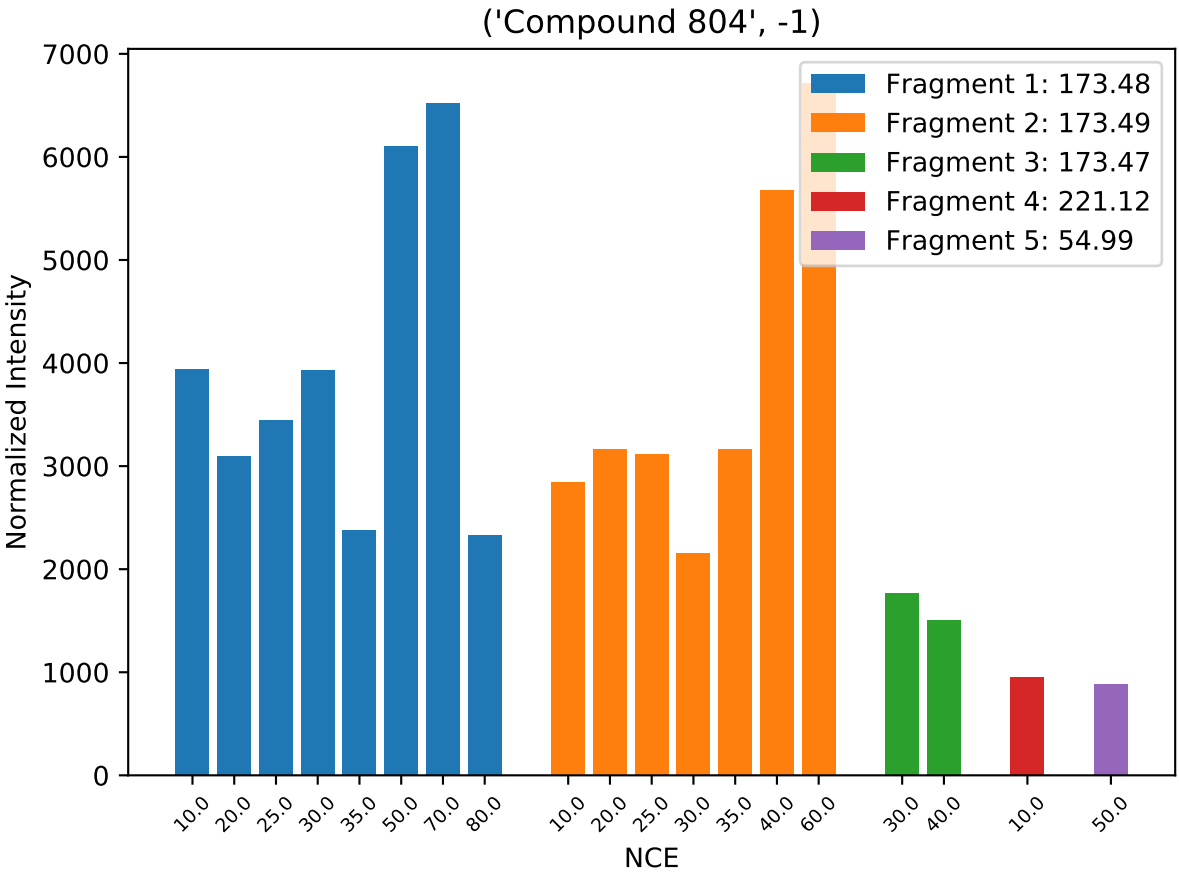

('Compound 795', -1)
Normalized Intensity
0
200
400
600
800
Fragment 1: 90.3
Fragment 2: 58.79
Fragment 3: 65.34
Fragment 4: 70.63
Fragment 5: 55.69
80.0
10.0
35.0
35.0
30.0
NCE

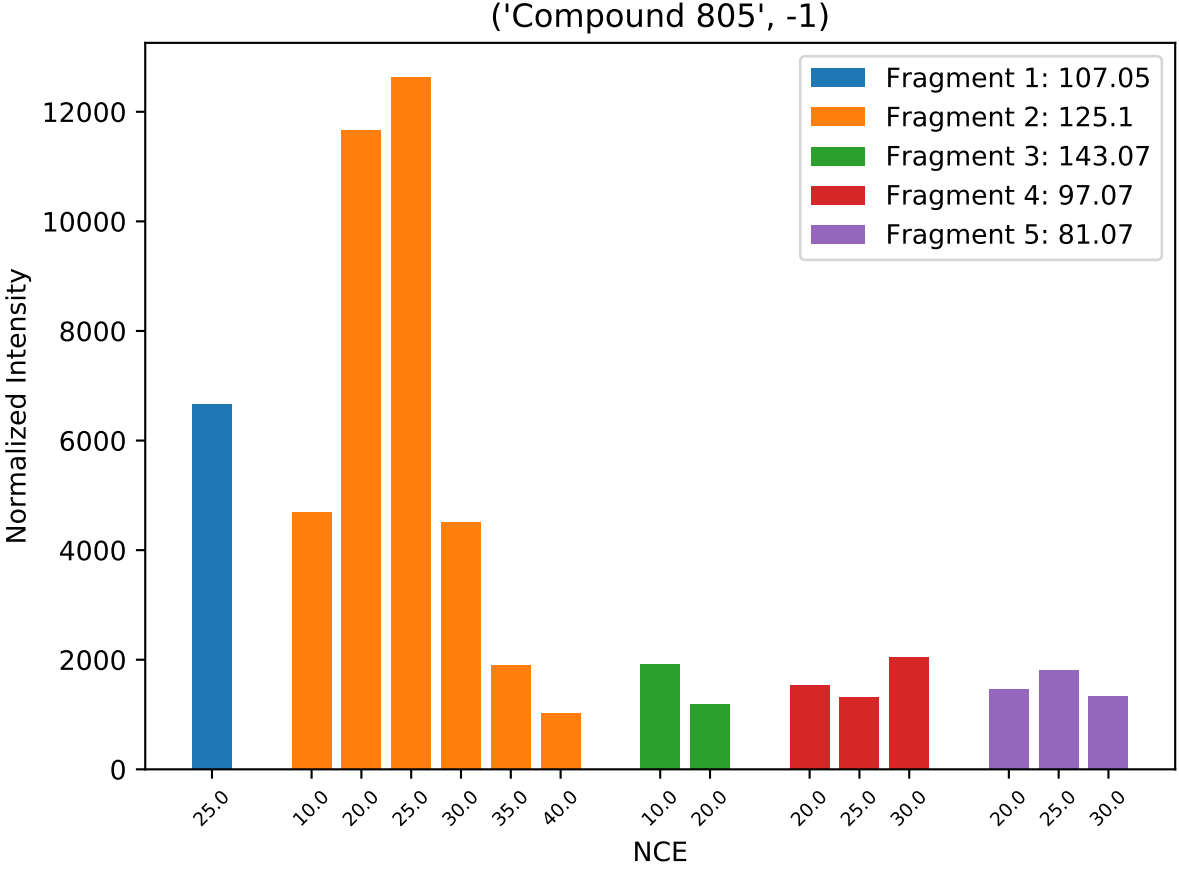

('Compound 797', -1)
Fragment 1: 188.94
Fragment 2: 173.48
Fragment 3: 204.91
Fragment 4: 206.95
Fragment 5: 59.98
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0 40.0 60.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
40.0 50.0 60.0 70.0 80.0
NCE

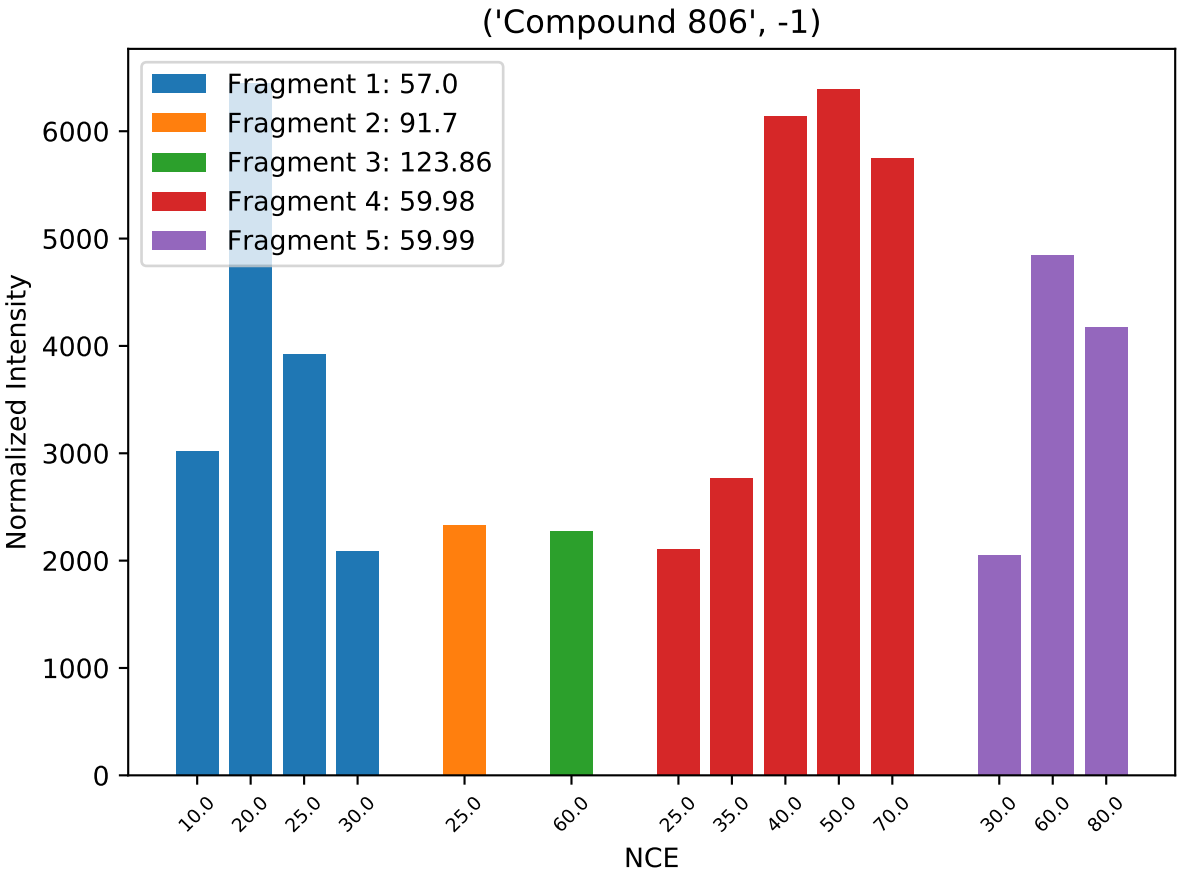

('Compound 800', -1)
Fragment 1: 59.01
Fragment 2: 101.02
Fragment 3: 83.01
Fragment 4: 73.03
Fragment 5: 57.03
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

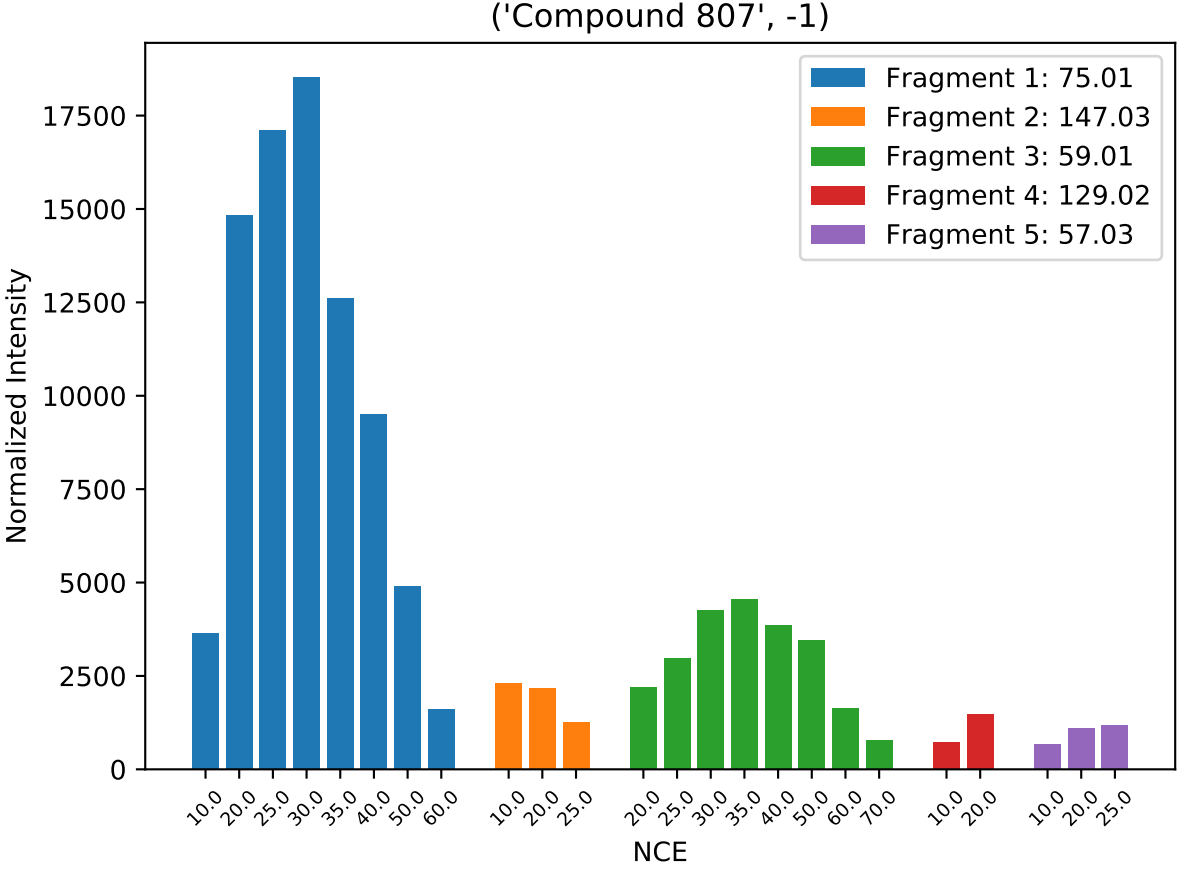

('Compound 802', -1)
Fragment 1: 136.01
Fragment 2: 80.96
Fragment 3: 112.94
Fragment 4: 74.01
Fragment 5: 120.01
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
NCE
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0

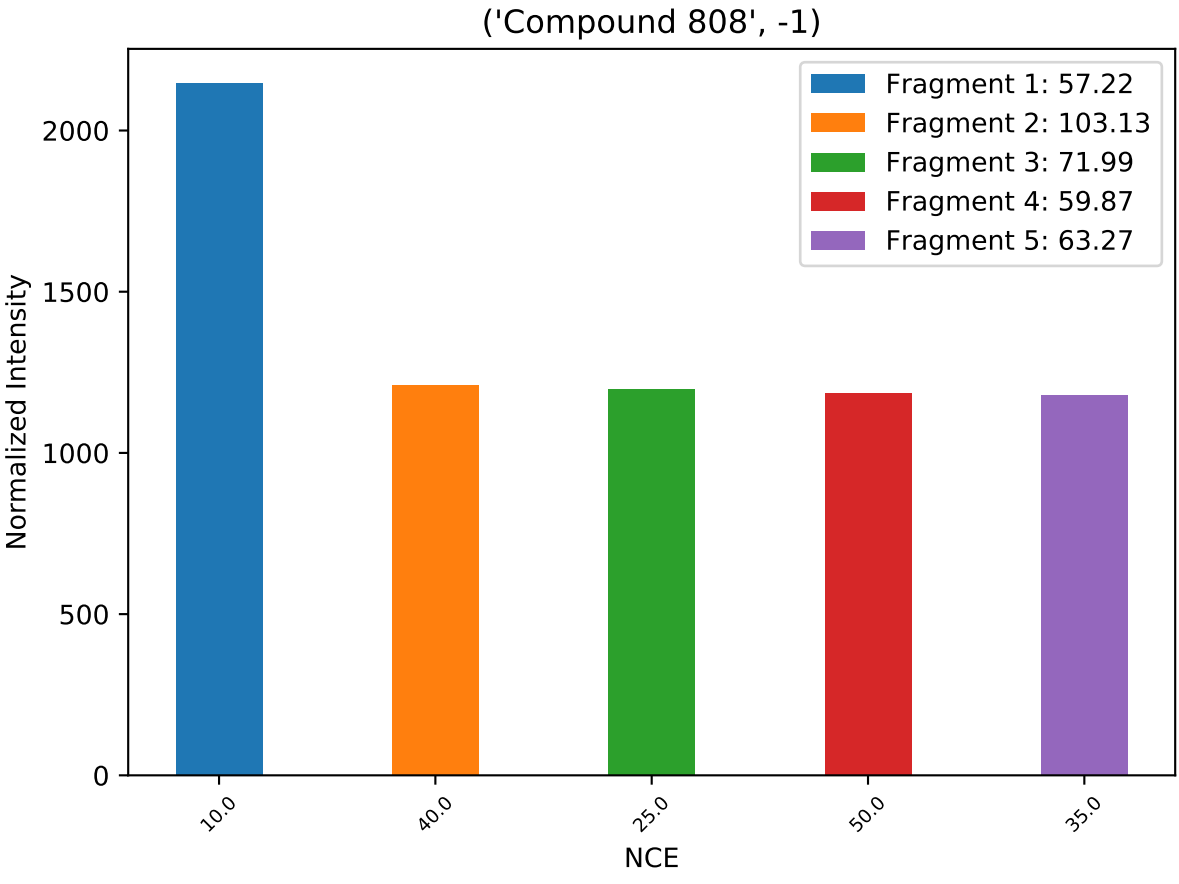

('Compound 803', -1)
Fragment 1: 78.96
Fragment 2: 62.96
Fragment 3: 78.97
Fragment 4: 75.43
Fragment 5: 76.94
Normalized Intensity
30000
25000
20000
15000
10000
5000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
50.0
35.0
NCE

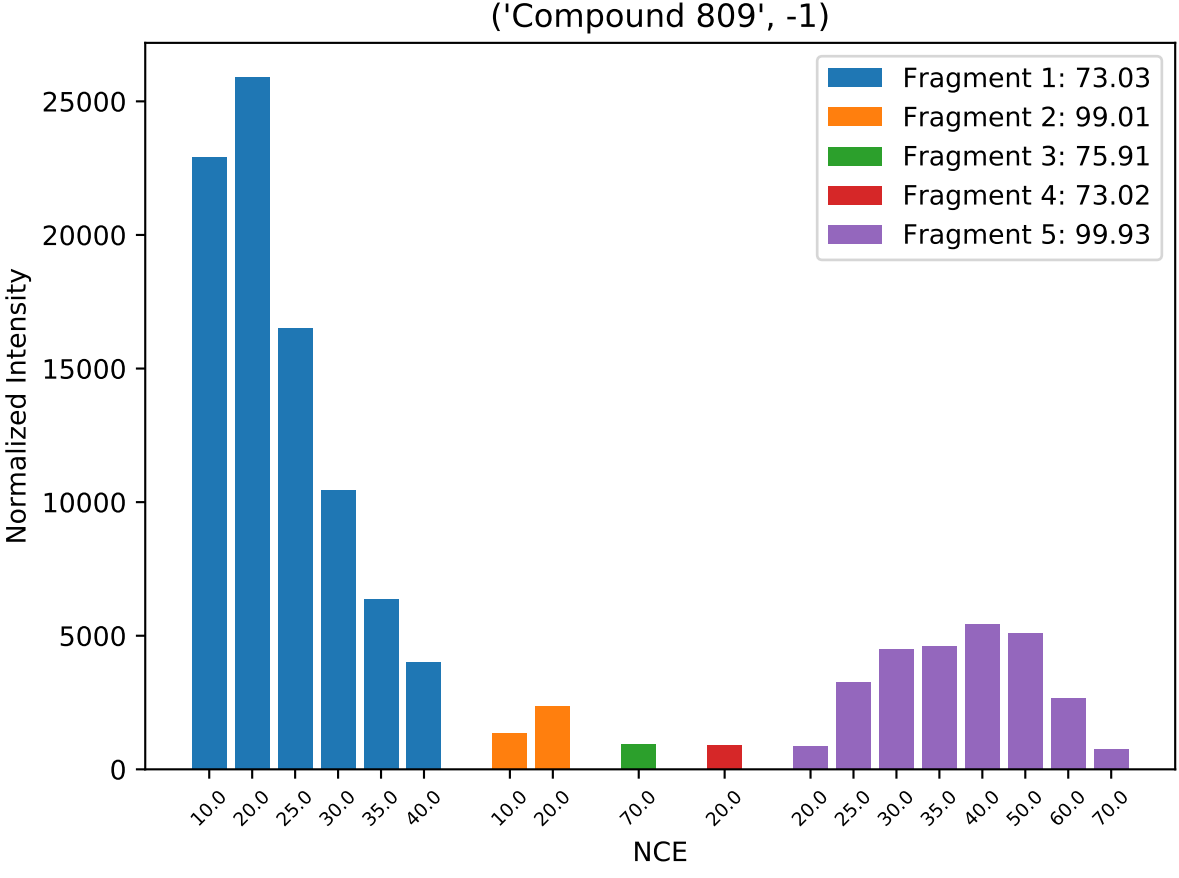

('Compound 804', -1)
Normalized Intensity
NCE
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 173.47
Fragment 4: 221.12
Fragment 5: 54.99
0
1000
2000
3000
4000
5000
6000
7000
10.0
20.0
25.0
30.0
35.0
50.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
60.0
30.0
40.0
10.0
50.0

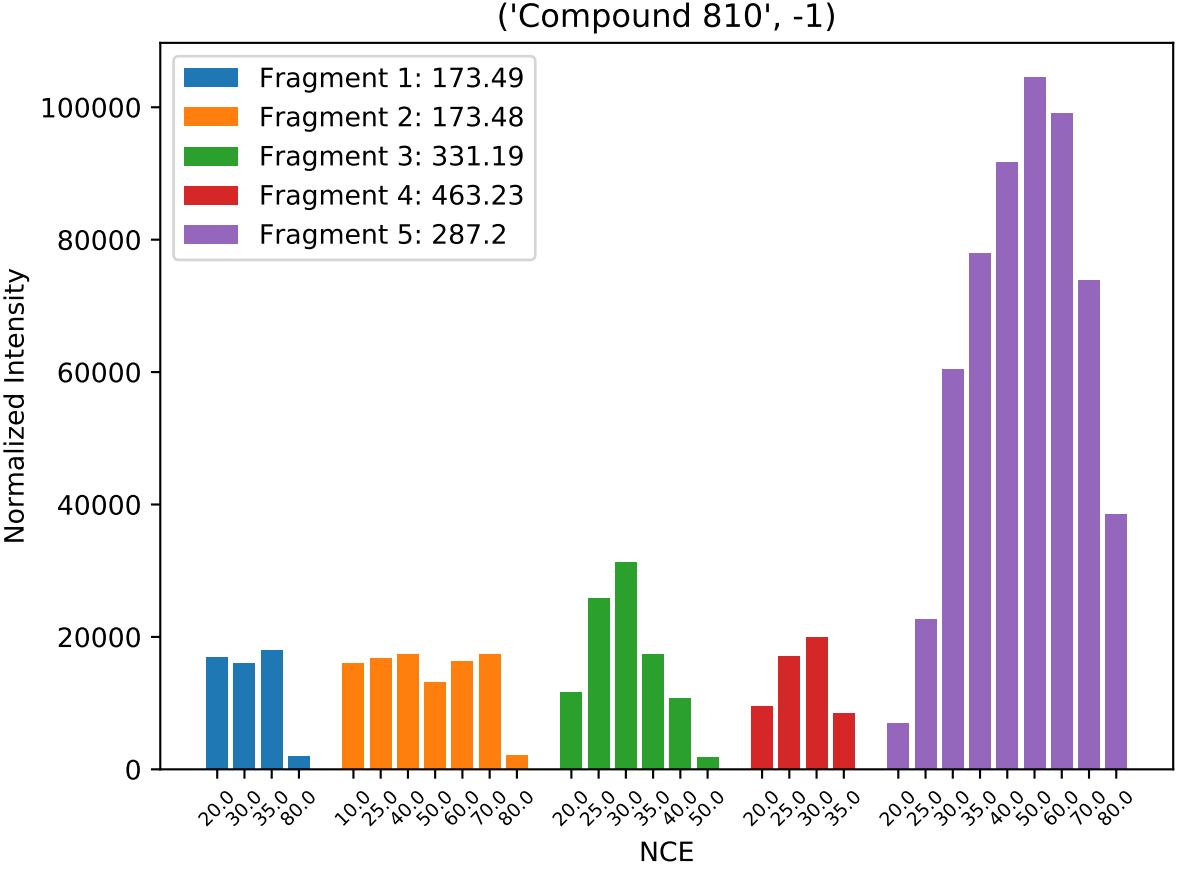

('Compound 805', -1)
Fragment 1: 107.05
Fragment 2: 125.1
Fragment 3: 143.07
Fragment 4: 97.07
Fragment 5: 81.07
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
25.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
20.0
25.0
30.0
20.0
25.0
30.0
NCE

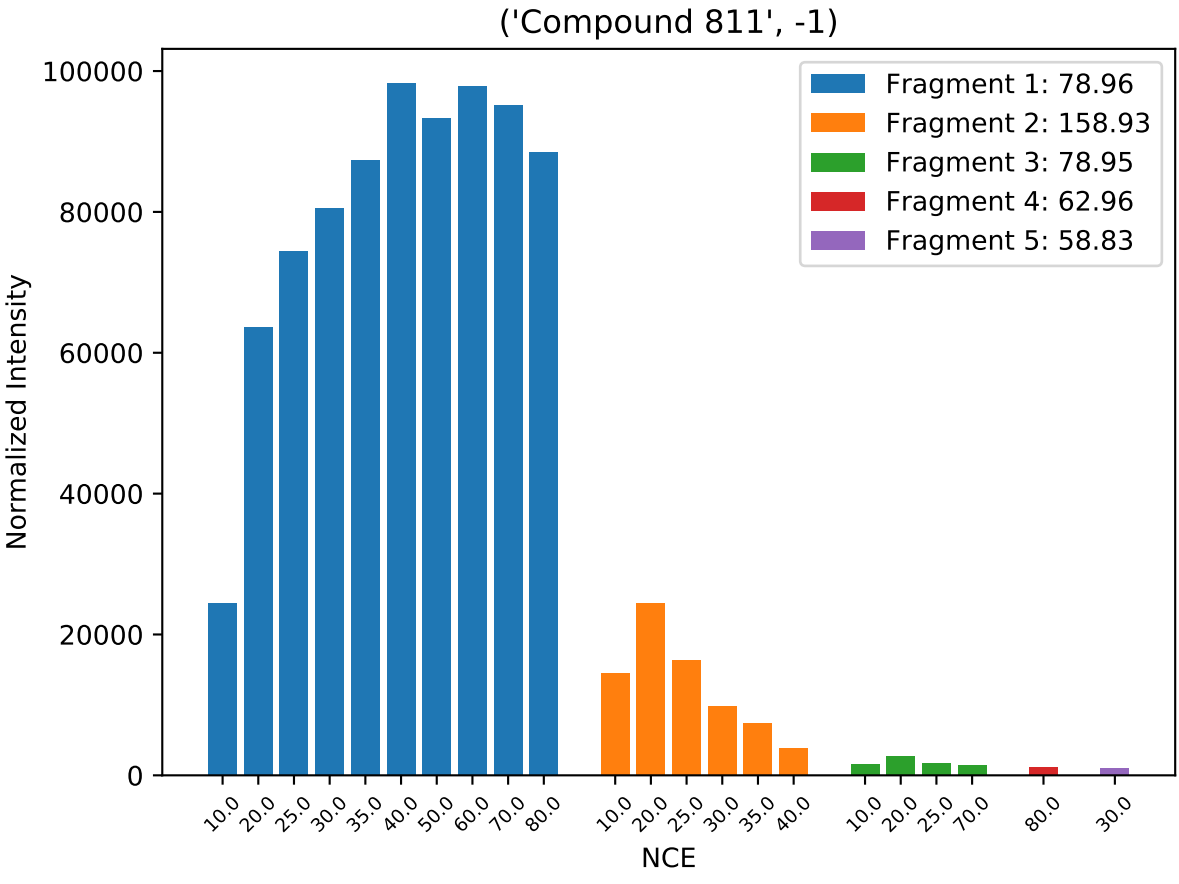

('Compound 806', -1)
Fragment 1: 57.0
Fragment 2: 91.7
Fragment 3: 123.86
Fragment 4: 59.98
Fragment 5: 59.99
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
10.0
20.0
25.0
30.0
25.0
60.0
25.0
35.0
40.0
50.0
70.0
30.0
60.0
80.0
NCE

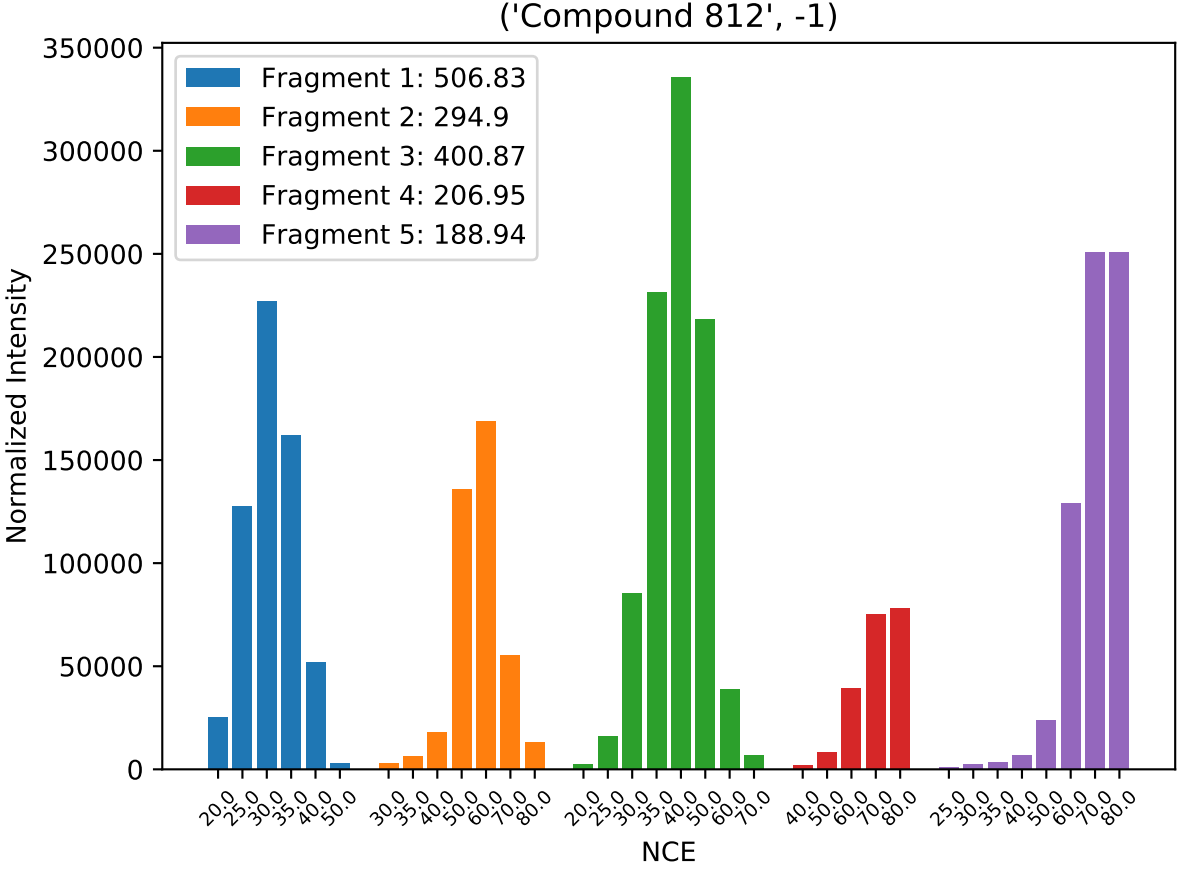

('Compound 807', -1)
Fragment 1: 75.01
Fragment 2: 147.03
Fragment 3: 59.01
Fragment 4: 129.02
Fragment 5: 57.03
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
10.0
20.0
25.0
NCE

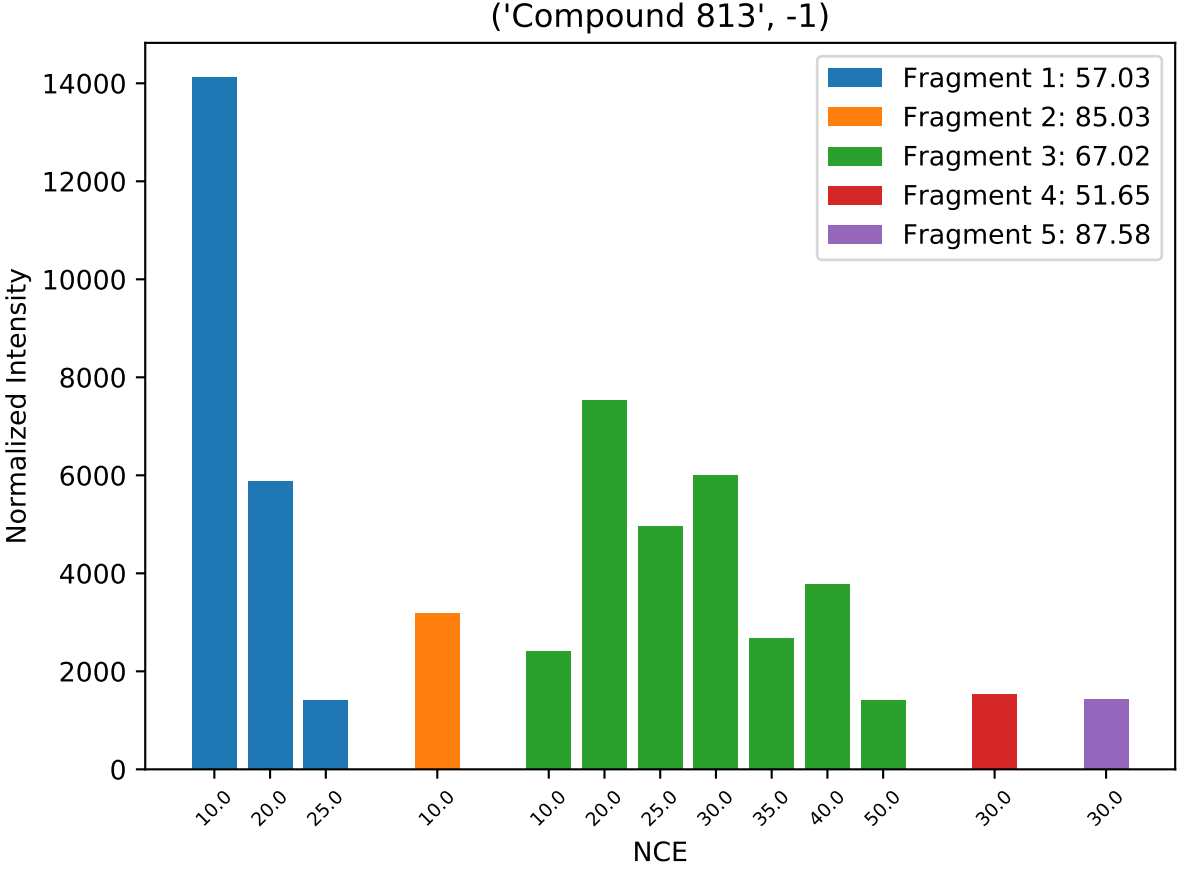

('Compound 808', -1)
Fragment 1: 57.22
Fragment 2: 103.13
Fragment 3: 71.99
Fragment 4: 59.87
Fragment 5: 63.27
Normalized Intensity
0
500
1000
1500
2000
10.0
40.0
25.0
50.0
35.0
NCE

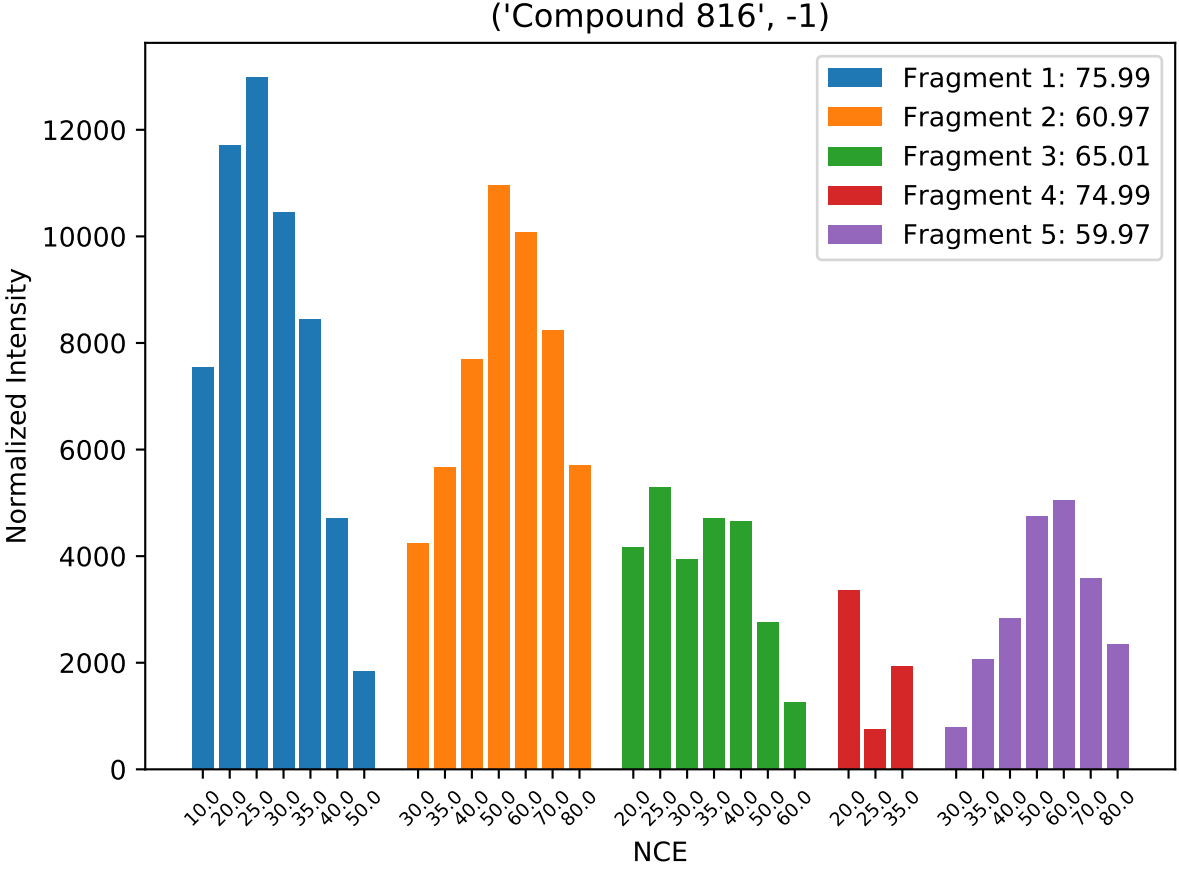

('Compound 809', -1)
Fragment 1: 73.03
Fragment 2: 99.01
Fragment 3: 75.91
Fragment 4: 73.02
Fragment 5: 99.93
Normalized Intensity
25000
20000
15000
10000
5000
0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
70.0
20.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

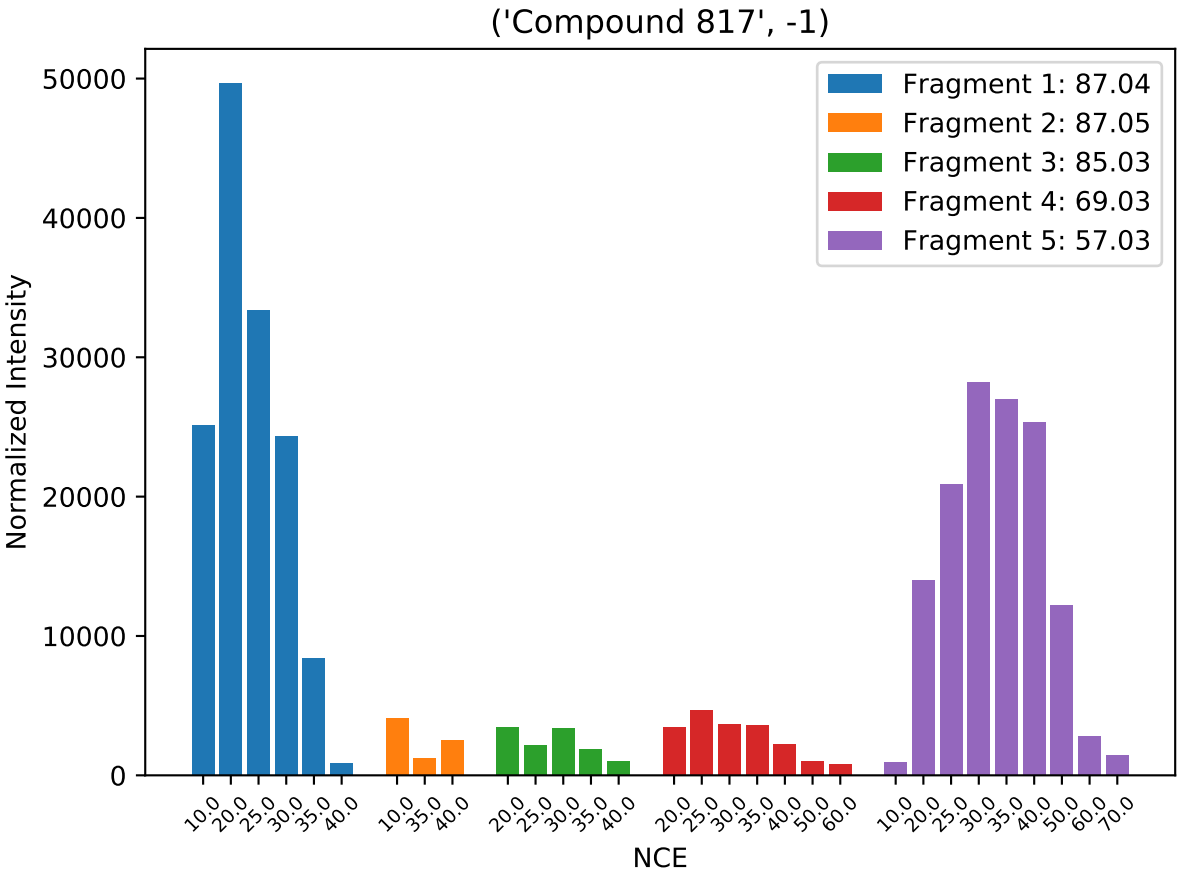

('Compound 810', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 331.19
Fragment 4: 463.23
Fragment 5: 287.2
Normalized Intensity
0
20000
40000
60000
80000
100000
20.0 30.0 35.0 80.0
10.0 25.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

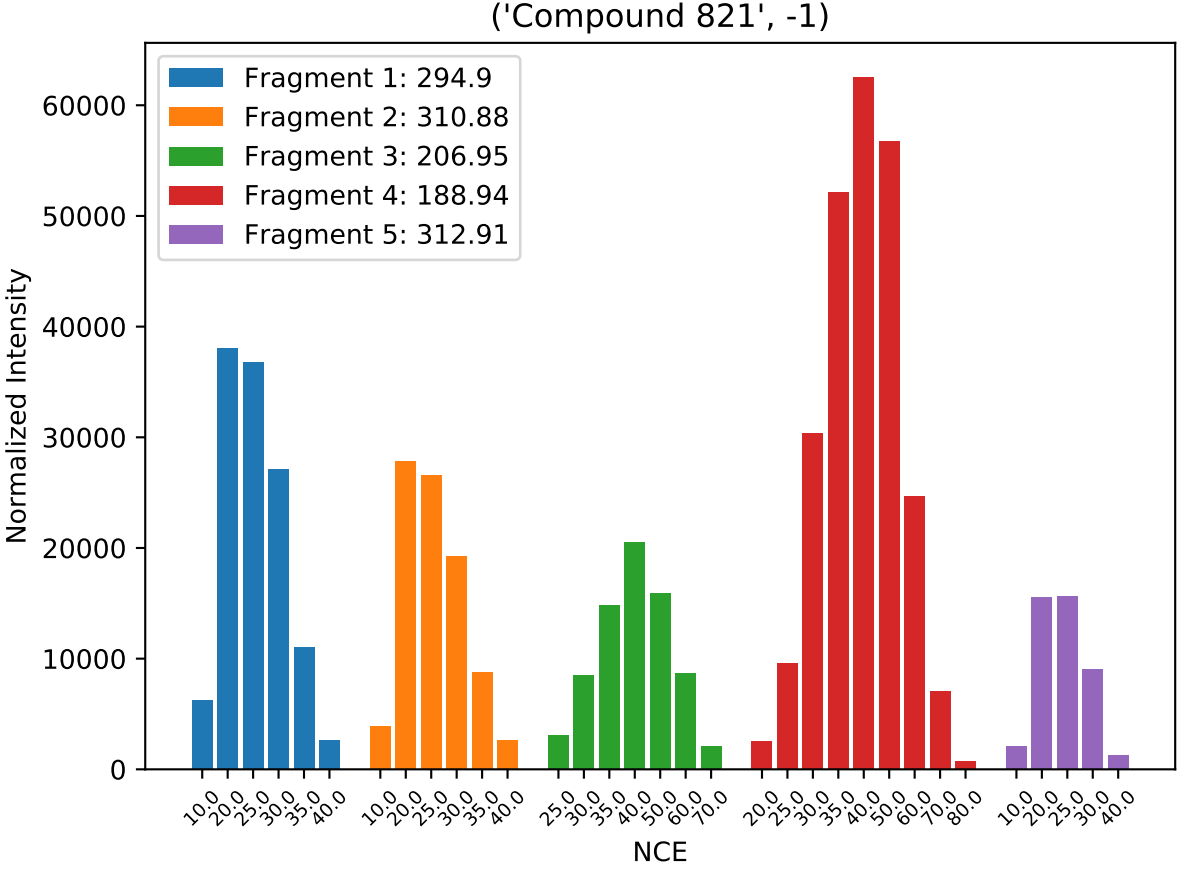

('Compound 811', -1)
Fragment 1: 78.96
Fragment 2: 158.93
Fragment 3: 78.95
Fragment 4: 62.96
Fragment 5: 58.83
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
70.0
80.0
30.0
NCE

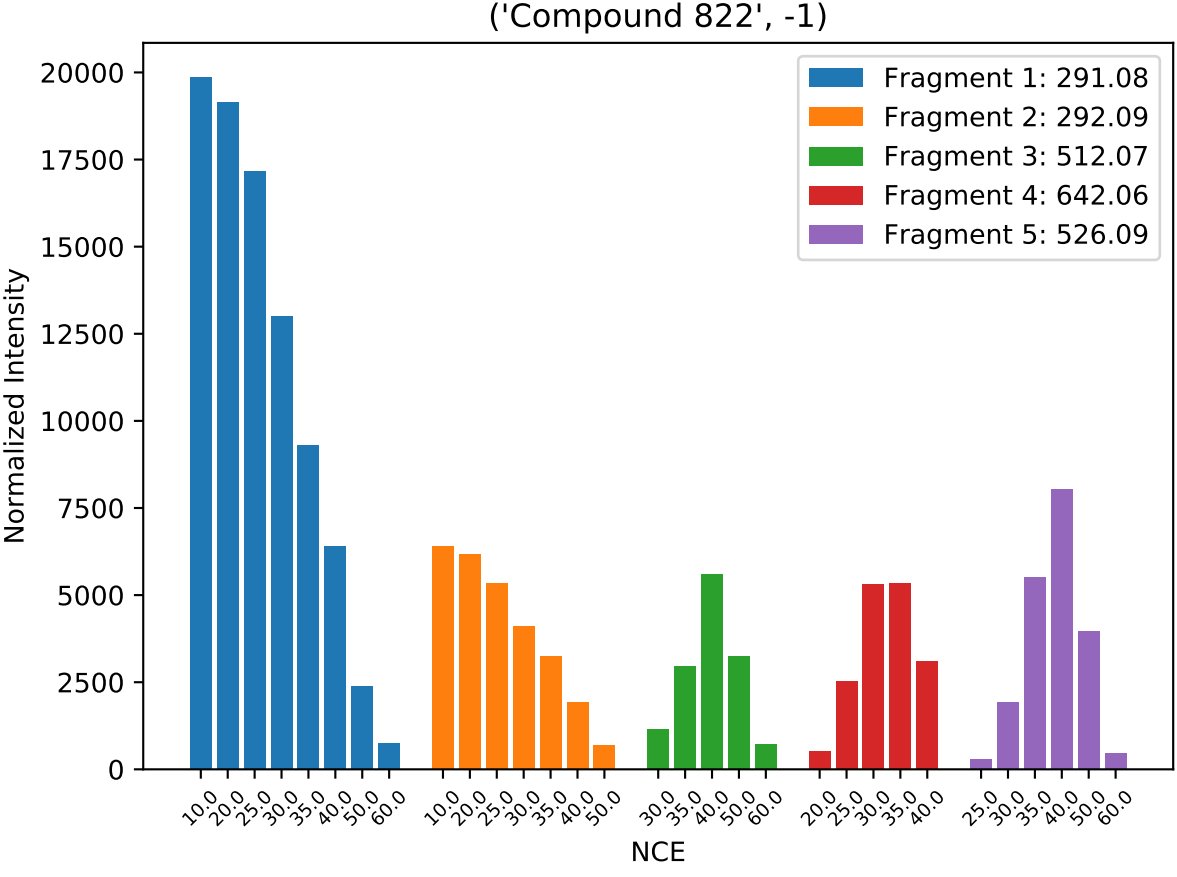

('Compound 812', -1)
Fragment 1: 506.83
Fragment 2: 294.9
Fragment 3: 400.87
Fragment 4: 206.95
Fragment 5: 188.94
Normalized Intensity
350000
300000
250000
200000
150000
100000
50000
0
20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

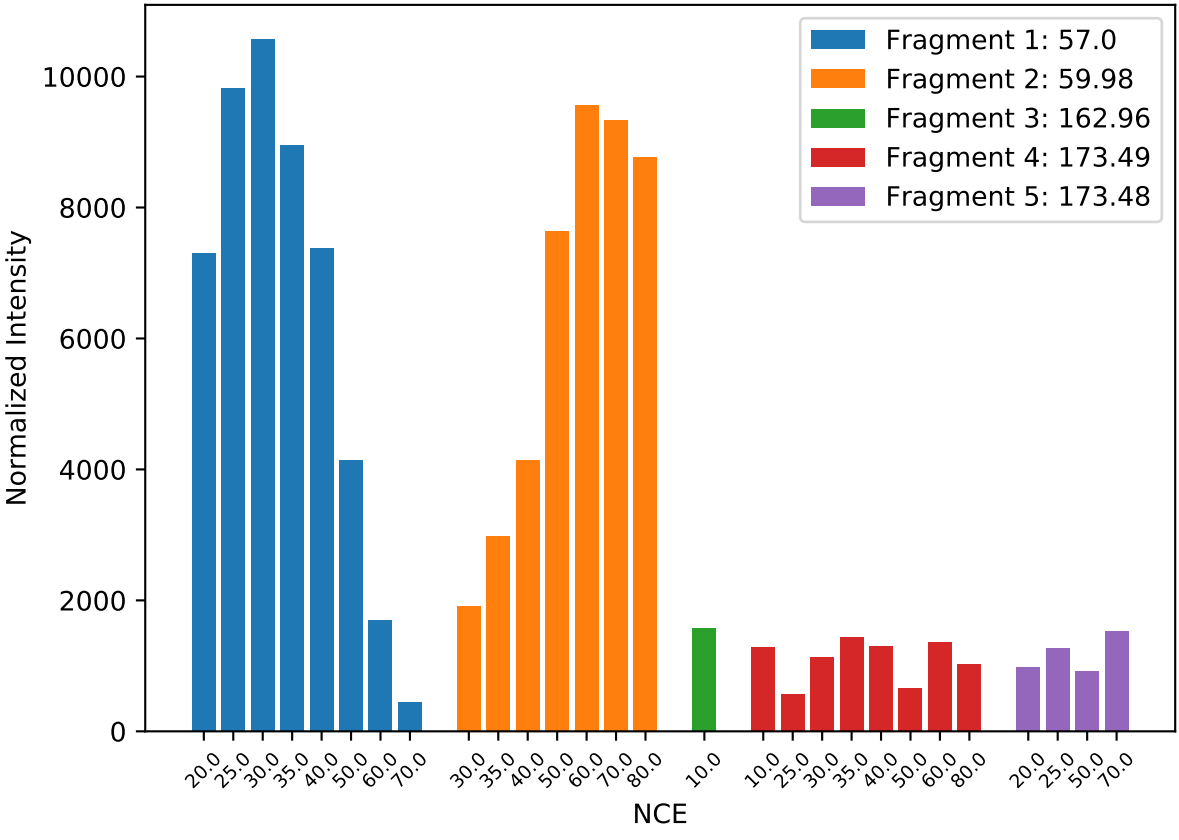

('Compound 813', -1)
Fragment 1: 57.03
Fragment 2: 85.03
Fragment 3: 67.02
Fragment 4: 51.65
Fragment 5: 87.58
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
25.0
10.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
30.0
30.0
NCE

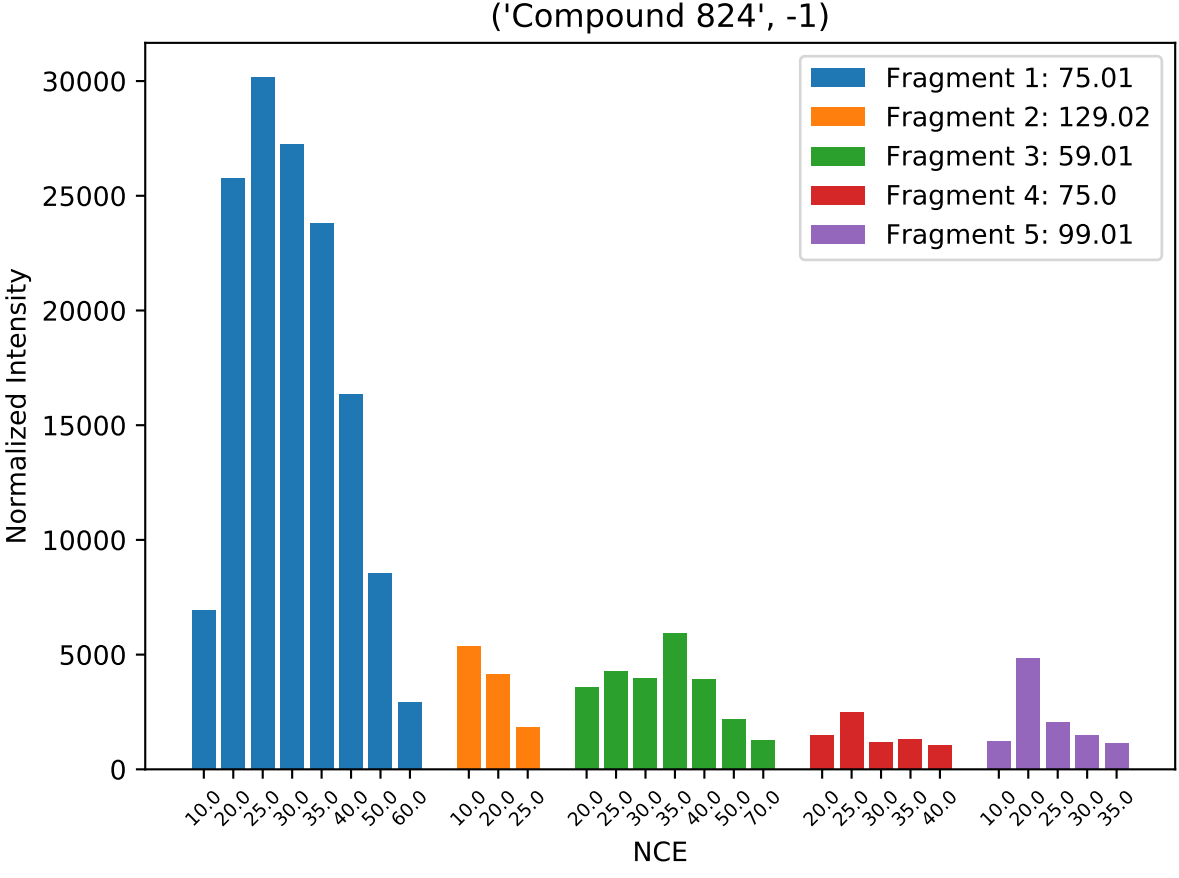

('Compound 816', -1)
Fragment 1: 75.99
Fragment 2: 60.97
Fragment 3: 65.01
Fragment 4: 74.99
Fragment 5: 59.97
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 35.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

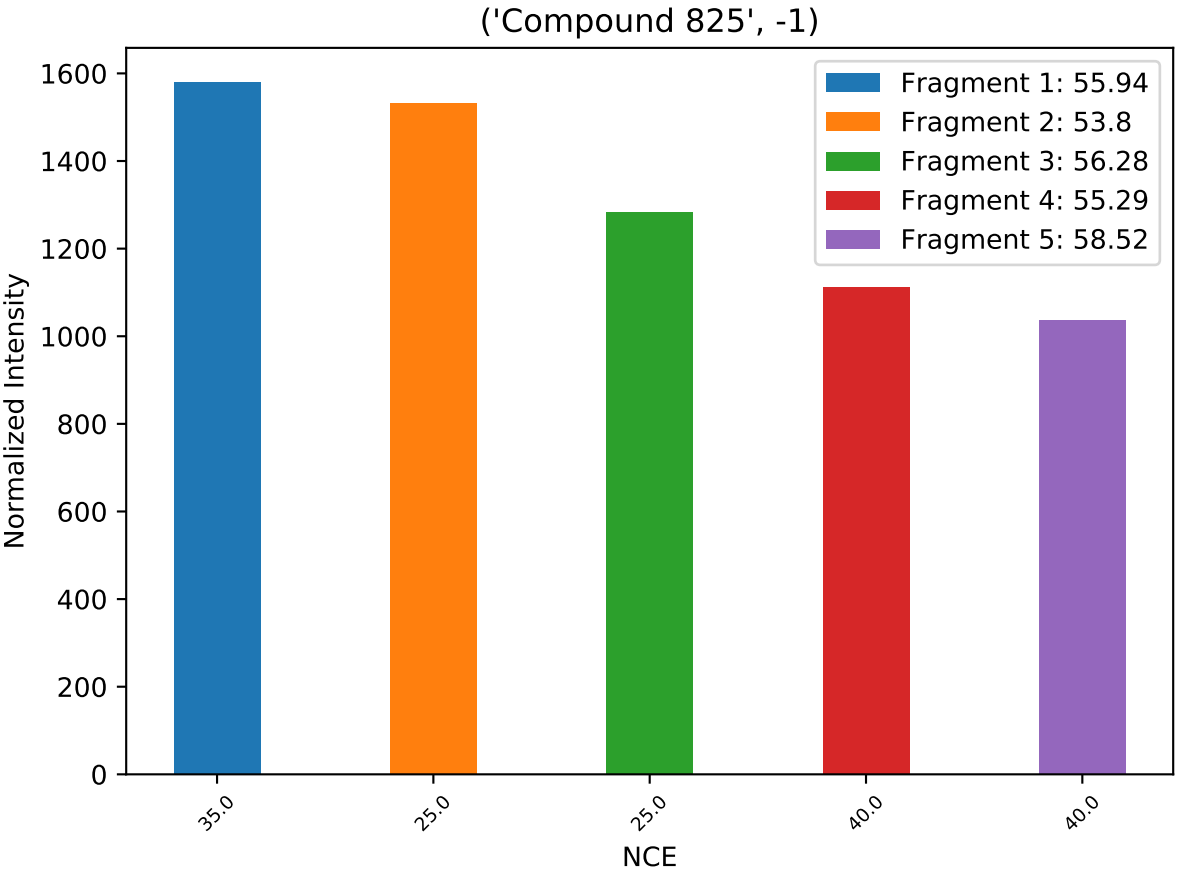

('Compound 817', -1)
Fragment 1: 87.04
Fragment 2: 87.05
Fragment 3: 85.03
Fragment 4: 69.03
Fragment 5: 57.03
Normalized Intensity
0
10000
20000
30000
40000
50000
NCE
10.0
20.0
25.0
30.0
35.0
40.0
10.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0

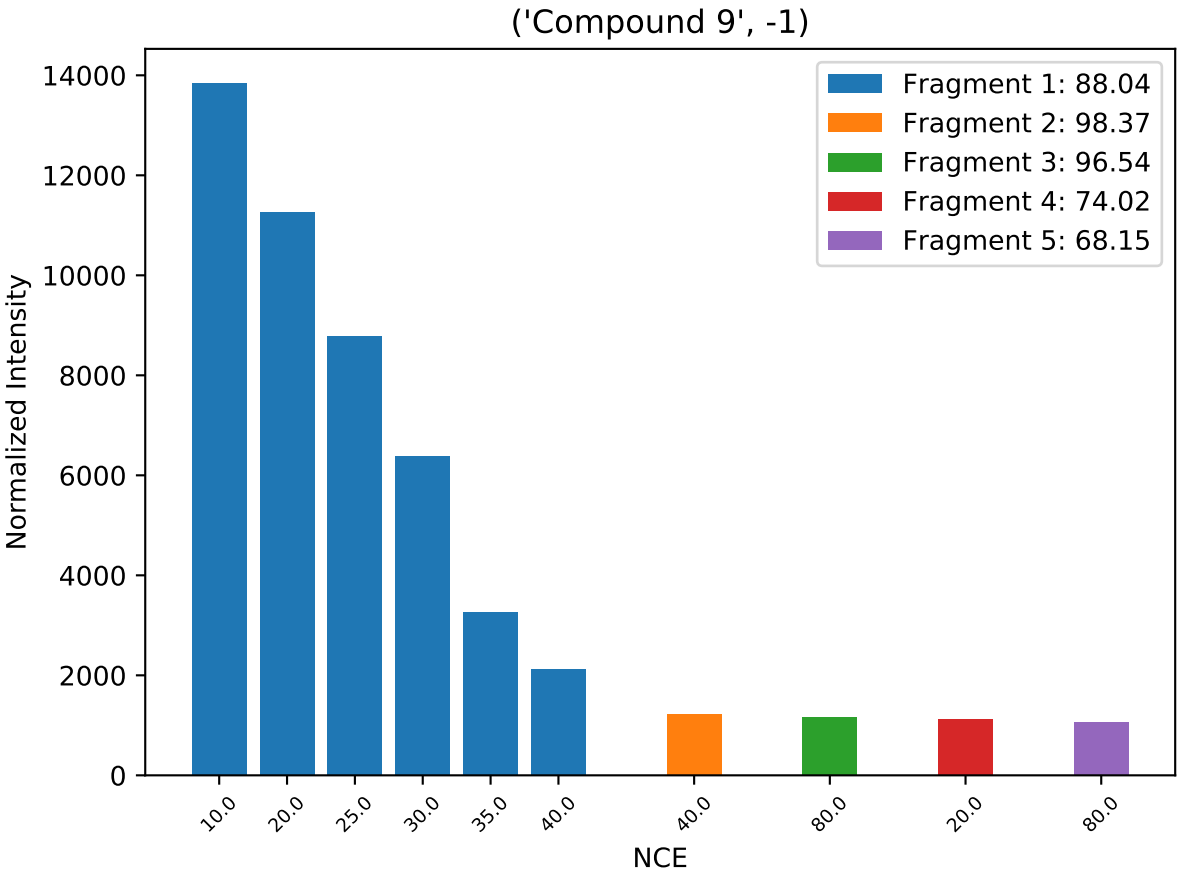

('Compound 821', -1)
Fragment 1: 294.9
Fragment 2: 310.88
Fragment 3: 206.95
Fragment 4: 188.94
Fragment 5: 312.91
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 40.0
NCE

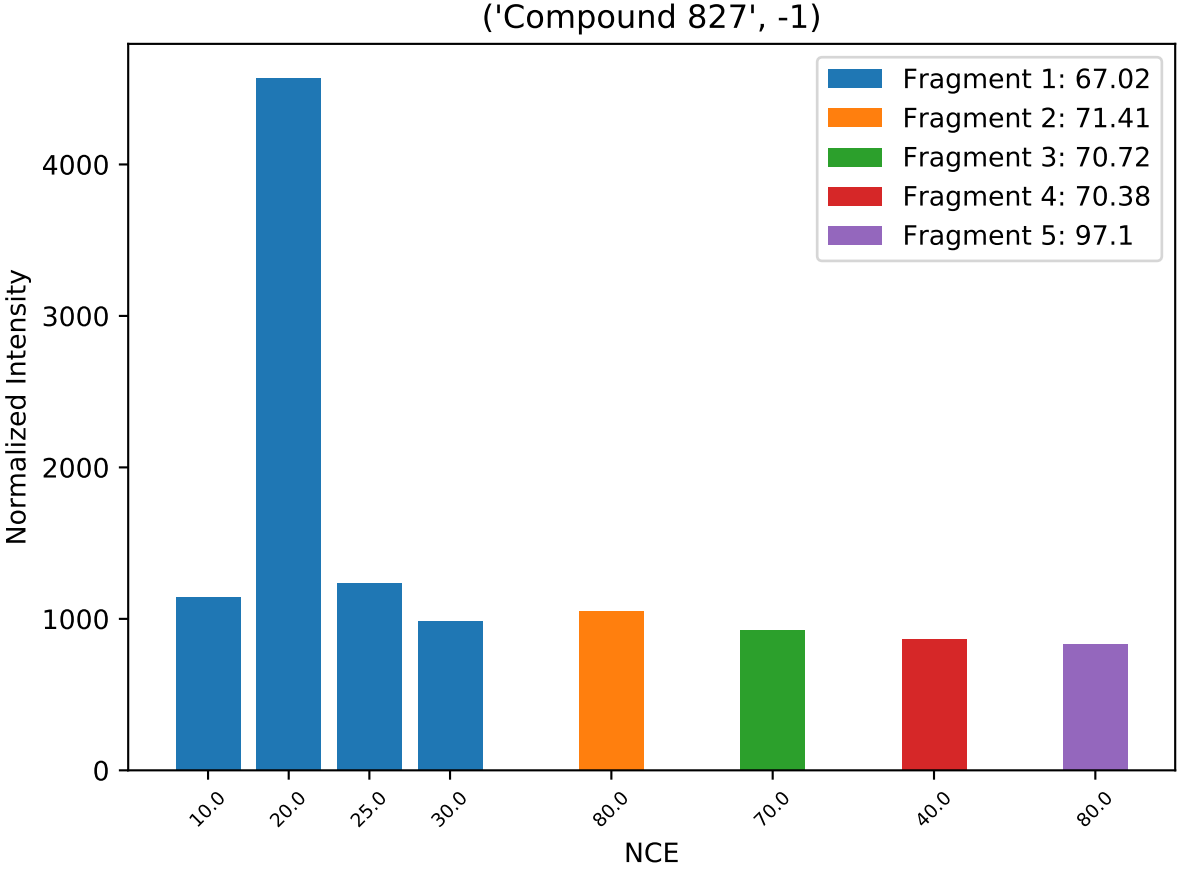

('Compound 822', -1)
Fragment 1: 291.08
Fragment 2: 292.09
Fragment 3: 512.07
Fragment 4: 642.06
Fragment 5: 526.09
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0
25.0 30.0 35.0 40.0 50.0 60.0
NCE

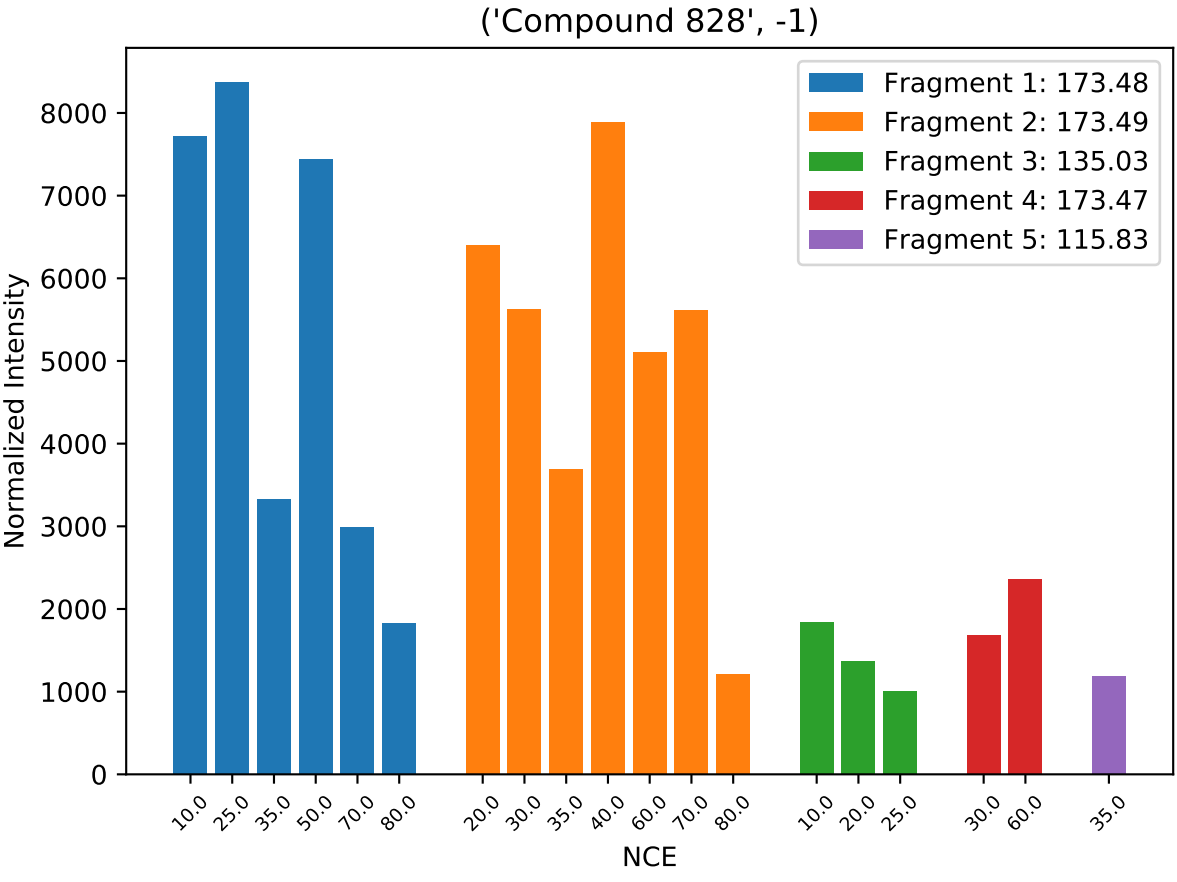

('Compound 823', -1)
Fragment 1: 57.0
Fragment 2: 59.98
Fragment 3: 162.96
Fragment 4: 173.49
Fragment 5: 173.48
Normalized Intensity
0
2000
4000
6000
8000
10000
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
10.0
25.0
30.0
35.0
40.0
50.0
60.0
80.0
20.0
25.0
50.0
70.0
NCE

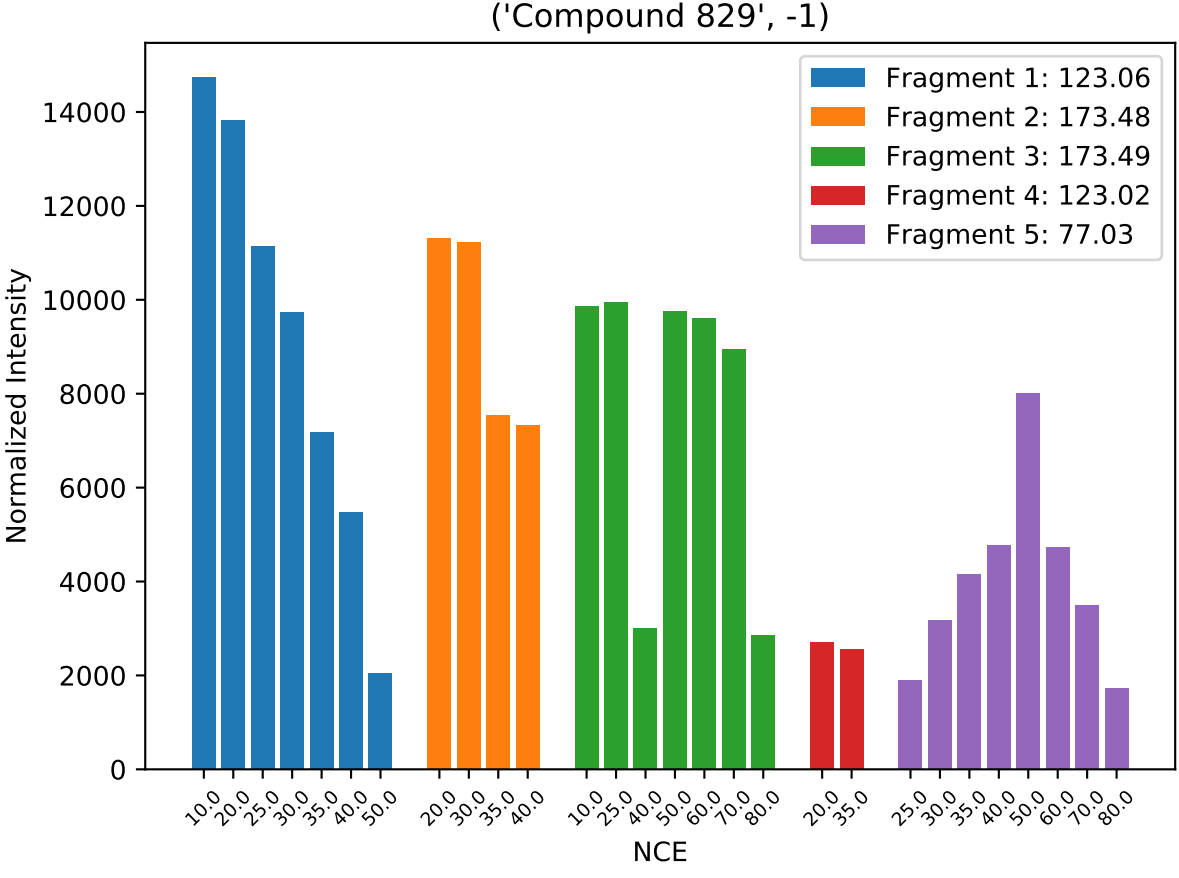

('Compound 824', -1)
Fragment 1: 75.01
Fragment 2: 129.02
Fragment 3: 59.01
Fragment 4: 75.0
Fragment 5: 99.01
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0
20.0 25.0 30.0 35.0 40.0 50.0 70.0
20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0
NCE

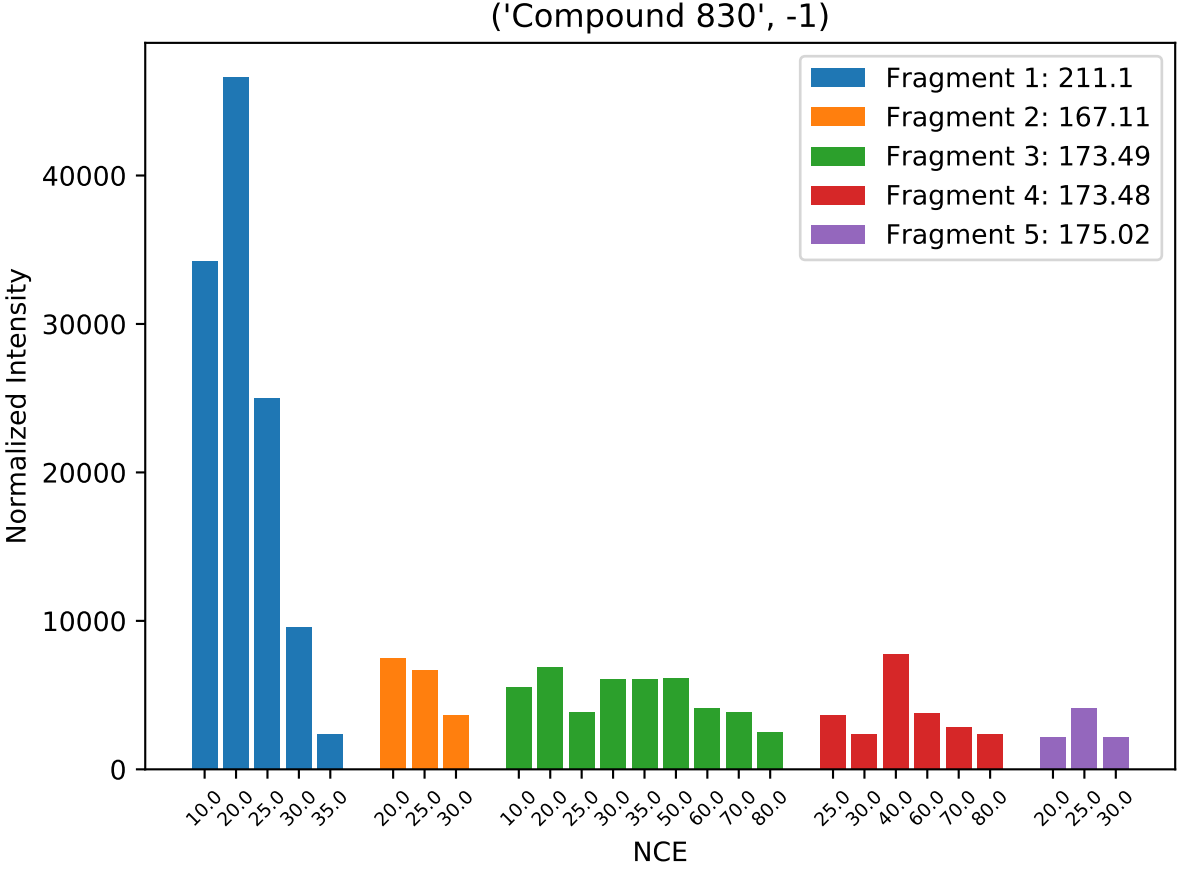

('Compound 825', -1)
Fragment 1: 55.94
Fragment 2: 53.8
Fragment 3: 56.28
Fragment 4: 55.29
Fragment 5: 58.52
Normalized Intensity
0
200
400
600
800
1000
1200
1400
1600
35.0
25.0
25.0
40.0
40.0
NCE

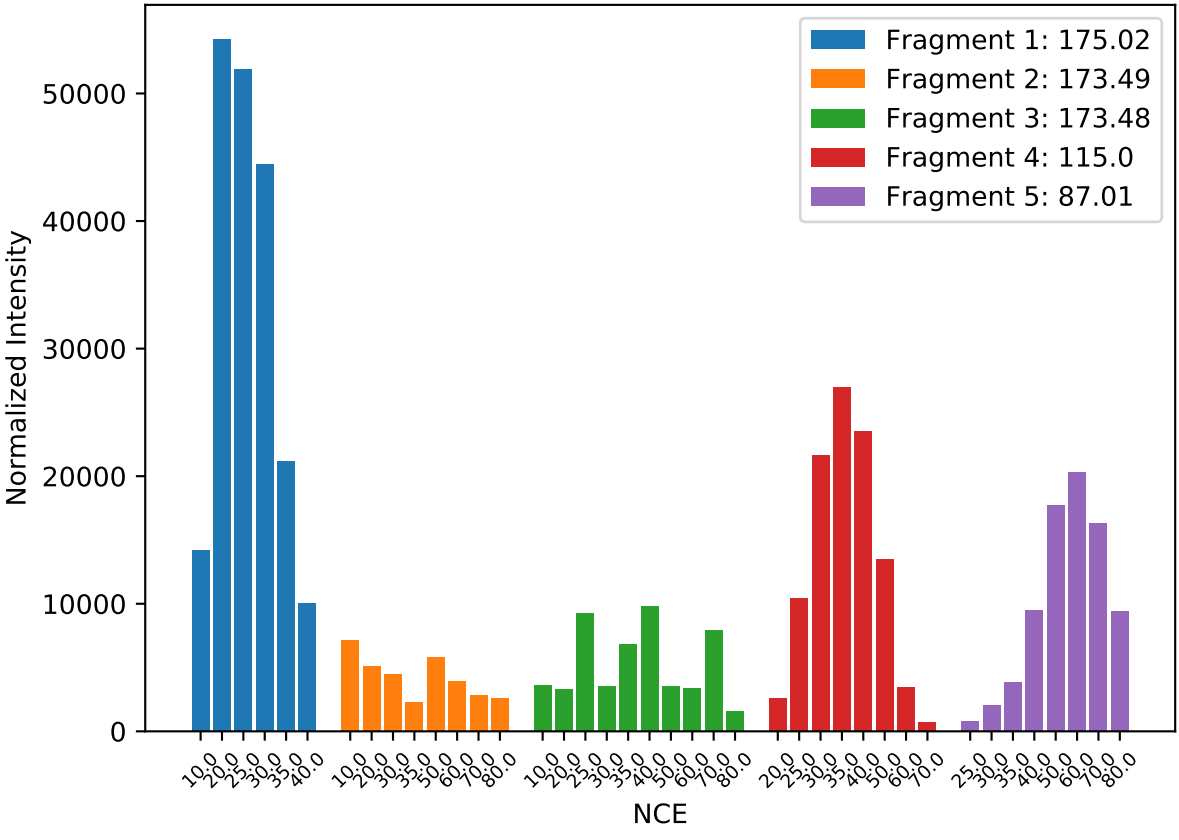

('Compound 9', -1)
Fragment 1: 88.04
Fragment 2: 98.37
Fragment 3: 96.54
Fragment 4: 74.02
Fragment 5: 68.15
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
25.0
30.0
35.0
40.0
40.0
80.0
20.0
80.0
NCE

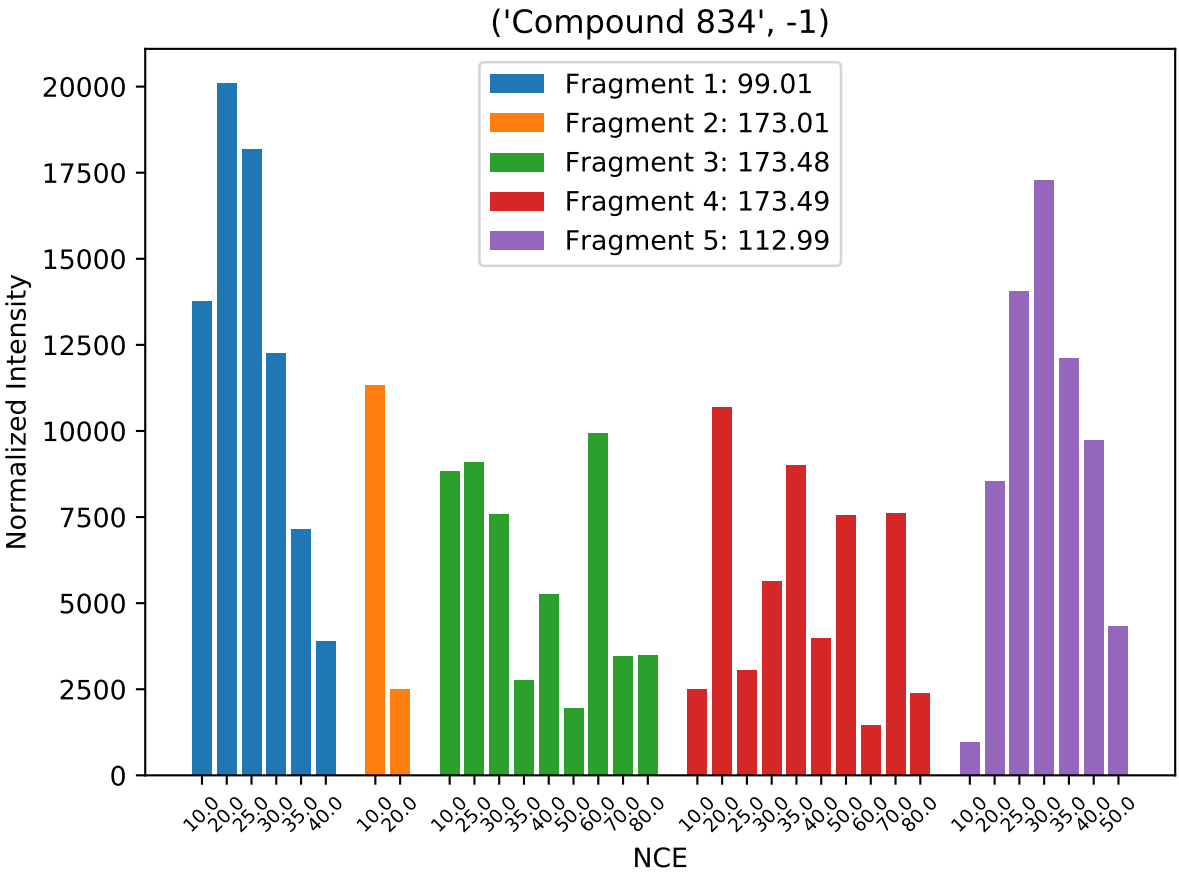

('Compound 827', -1)
Fragment 1: 67.02
Fragment 2: 71.41
Fragment 3: 70.72
Fragment 4: 70.38
Fragment 5: 97.1
Normalized Intensity
0
1000
2000
3000
4000
10.0
20.0
25.0
30.0
80.0
70.0
40.0
80.0
NCE

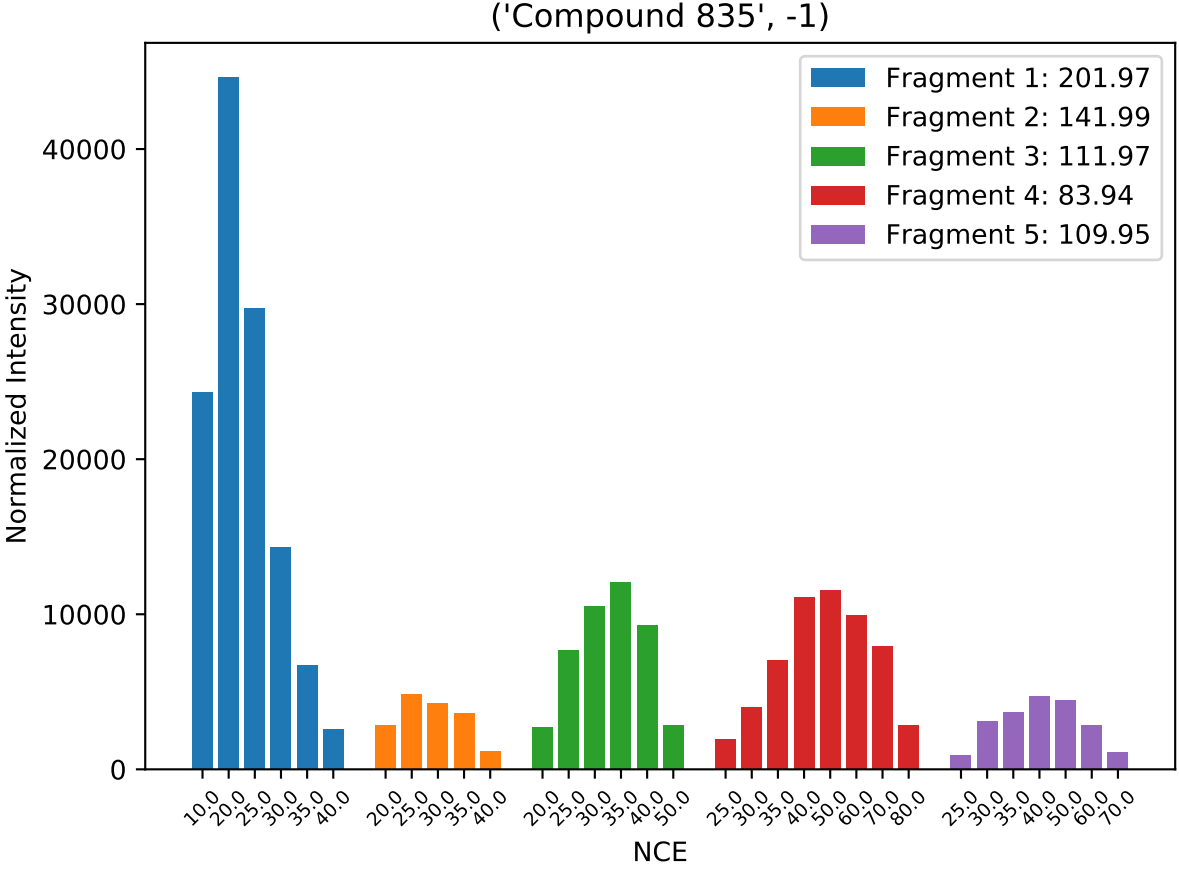

('Compound 828', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 135.03
Fragment 4: 173.47
Fragment 5: 115.83
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
25.0
35.0
50.0
70.0
80.0
20.0
30.0
35.0
40.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
60.0
35.0
NCE

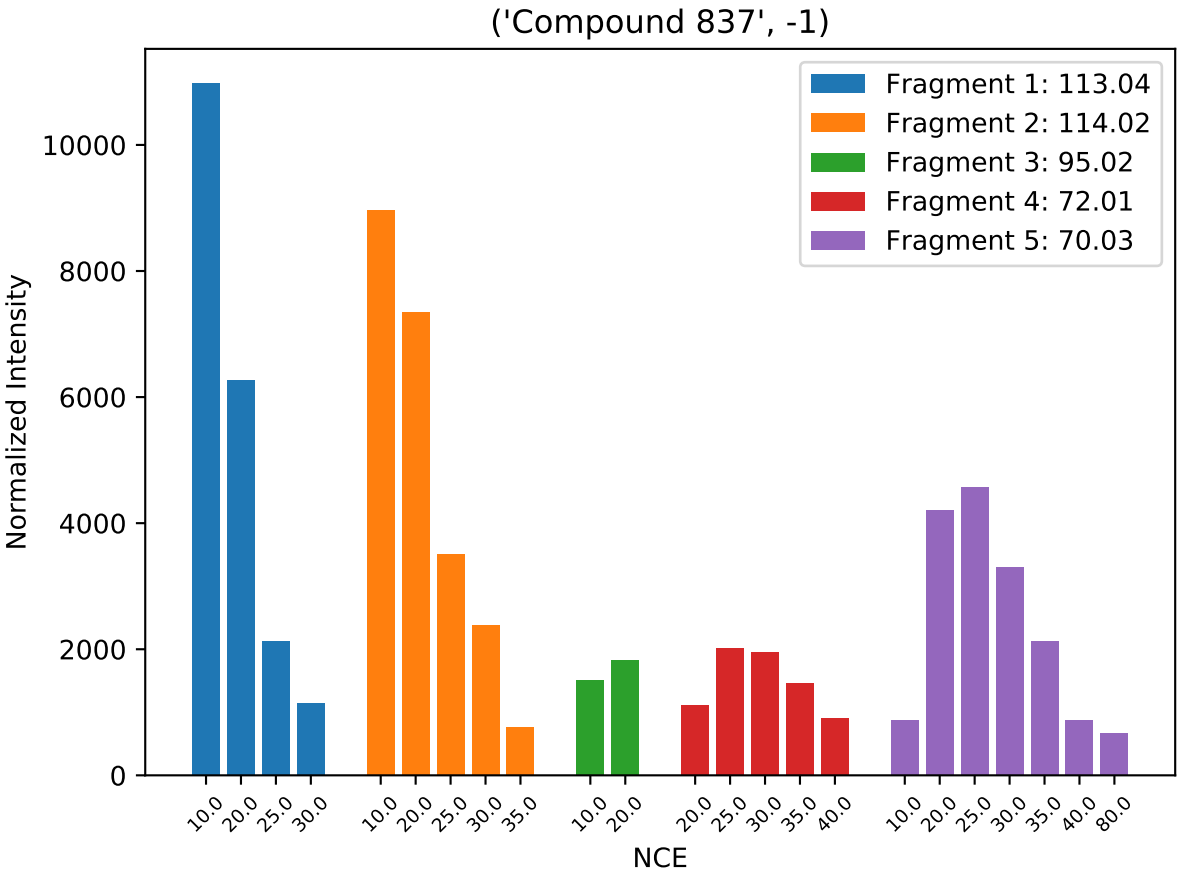

('Compound 829', -1)
Fragment 1: 123.06
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 123.02
Fragment 5: 77.03
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 30.0 35.0 40.0
10.0 25.0 40.0 50.0 60.0 70.0 80.0
20.0 35.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

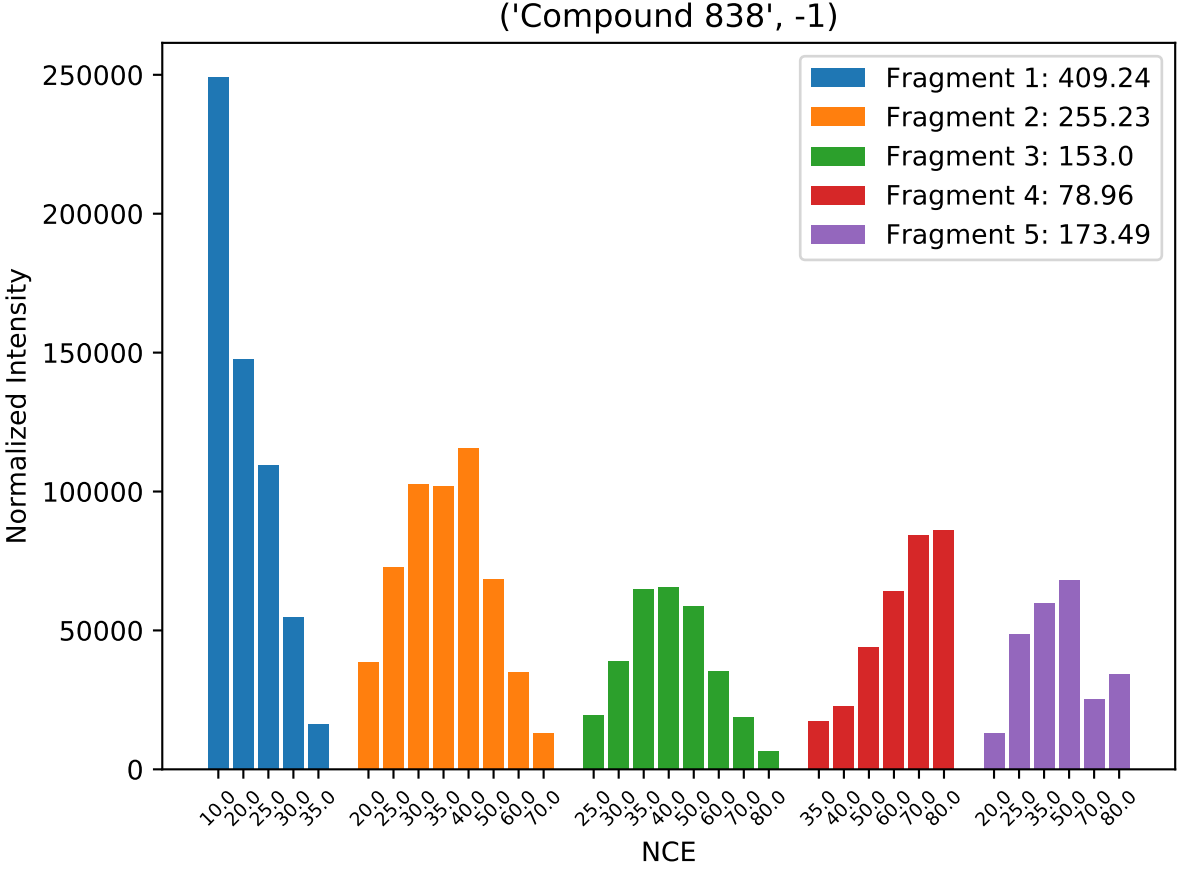

('Compound 830', -1)
Fragment 1: 211.1
Fragment 2: 167.11
Fragment 3: 173.49
Fragment 4: 173.48
Fragment 5: 175.02
Normalized Intensity
0
10000
20000
30000
40000
10.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
50.0
60.0
70.0
80.0
25.0
30.0
40.0
60.0
70.0
80.0
20.0
25.0
30.0
NCE

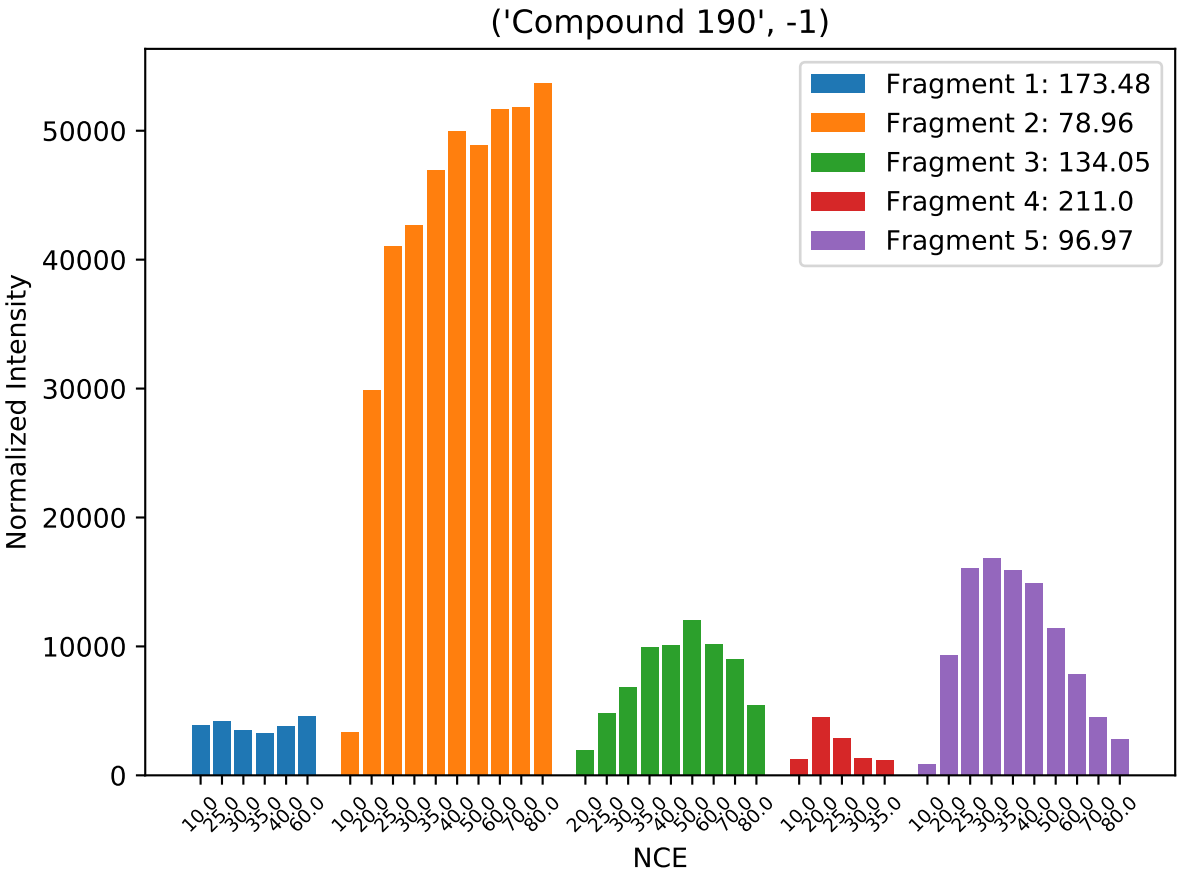

('Compound 832', -1)
Fragment 1: 175.02
Fragment 2: 173.49
Fragment 3: 173.48
Fragment 4: 115.0
Fragment 5: 87.01
Normalized Intensity
0
10000
20000
30000
40000
50000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 30.0 35.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

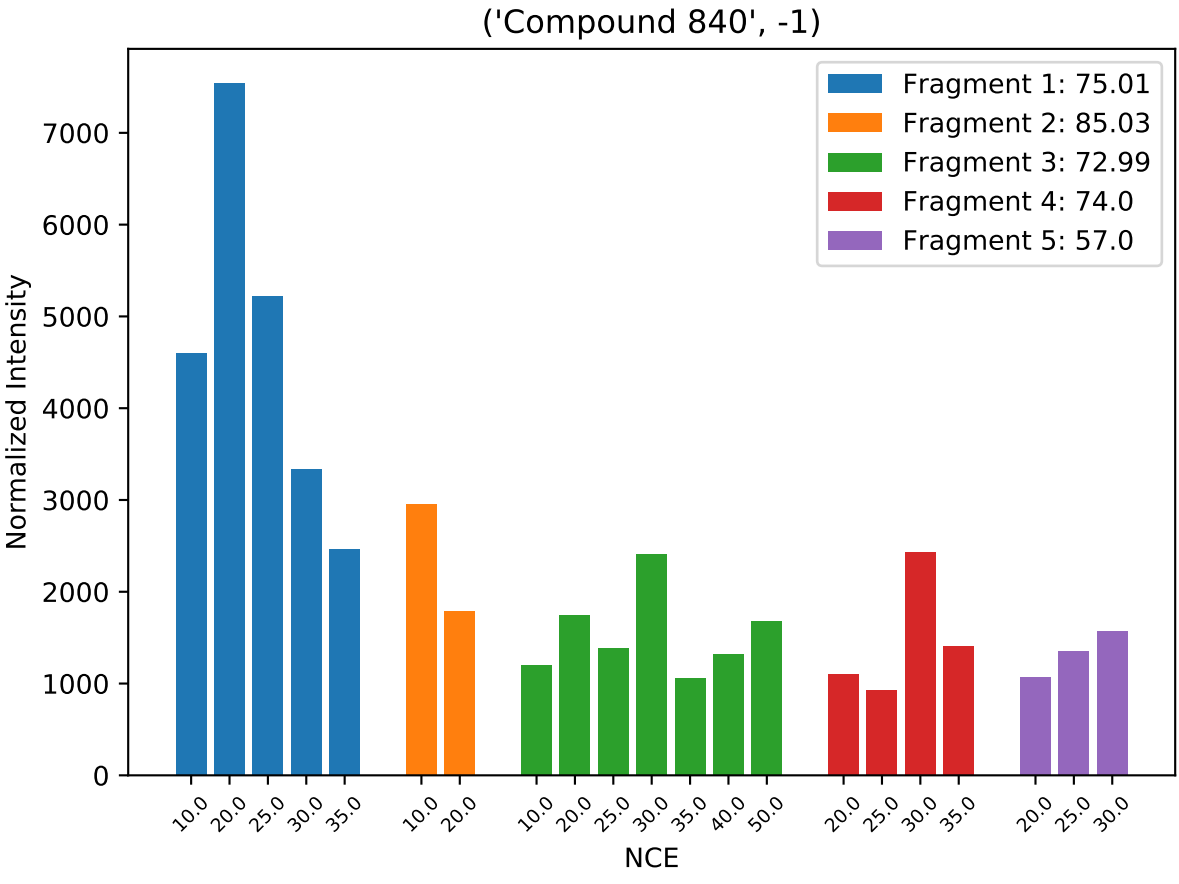

('Compound 834', -1)
Fragment 1: 99.01
Fragment 2: 173.01
Fragment 3: 173.48
Fragment 4: 173.49
Fragment 5: 112.99
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
NCE
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0
10.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0

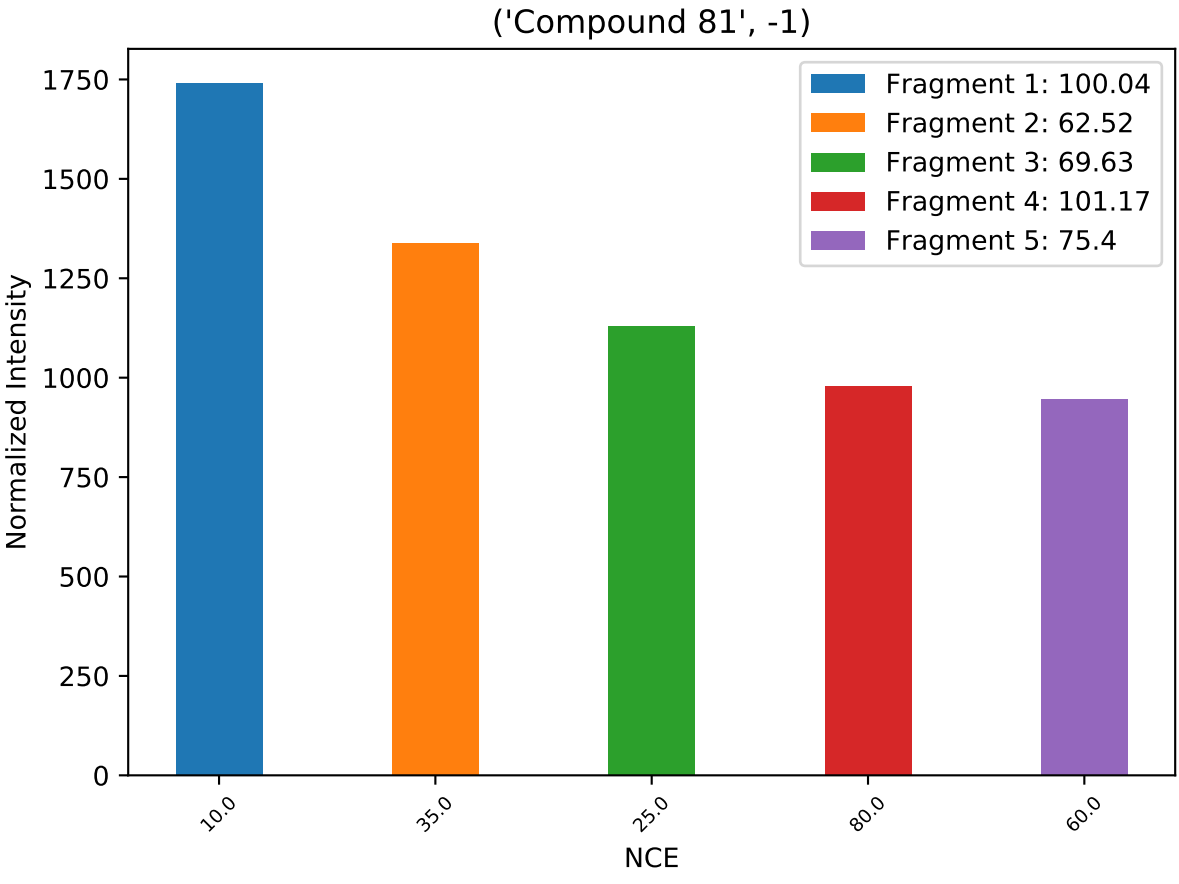

('Compound 835', -1)
Fragment 1: 201.97
Fragment 2: 141.99
Fragment 3: 111.97
Fragment 4: 83.94
Fragment 5: 109.95
Normalized Intensity
0
10000
20000
30000
40000
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

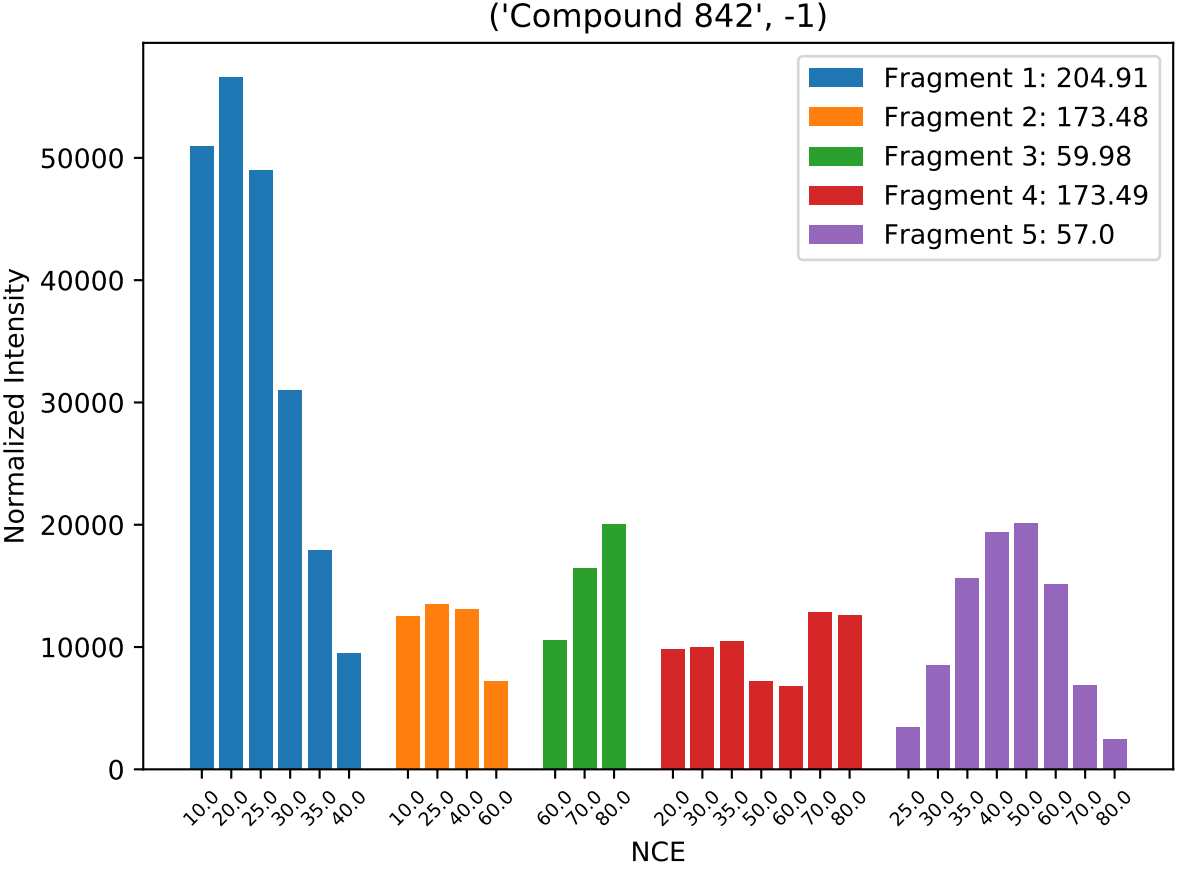

('Compound 837', -1)
Fragment 1: 113.04
Fragment 2: 114.02
Fragment 3: 95.02
Fragment 4: 72.01
Fragment 5: 70.03
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
10.0
20.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
80.0
NCE

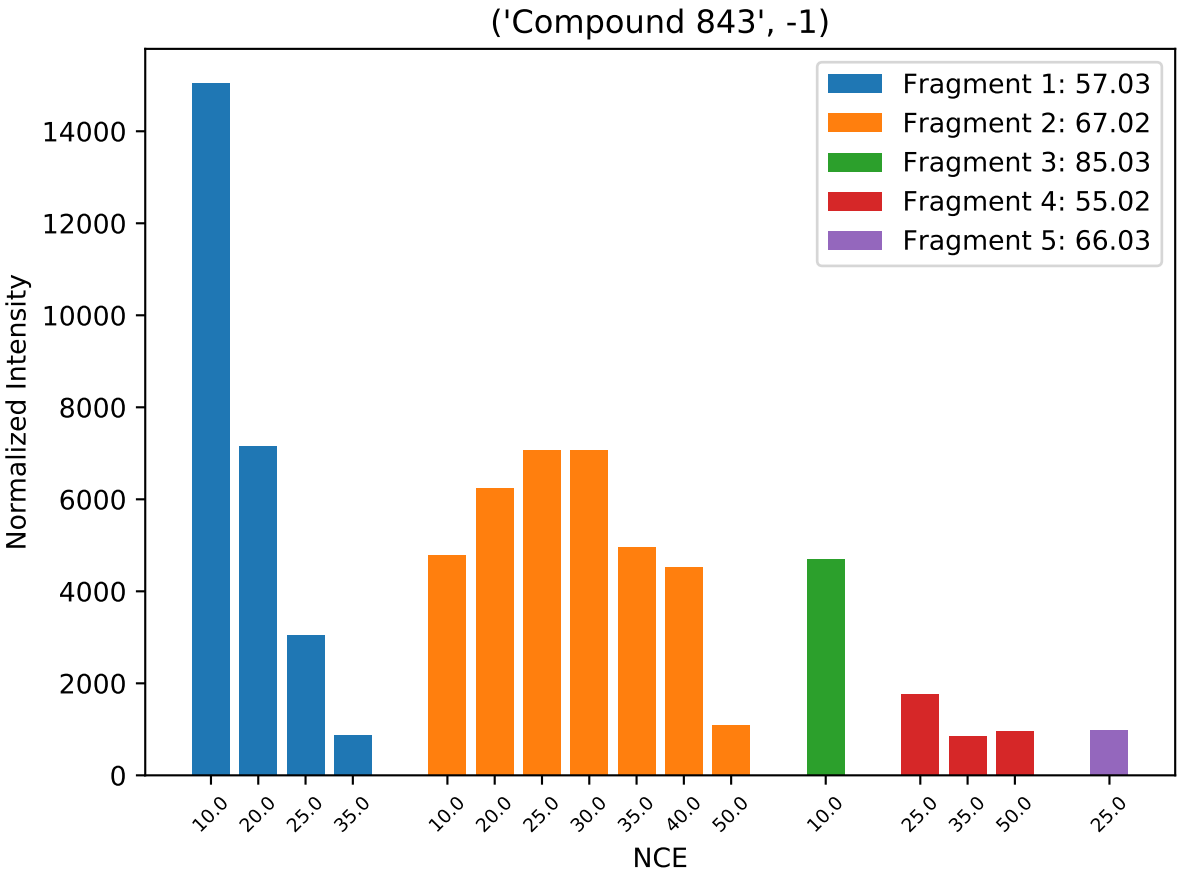

('Compound 838', -1)
Fragment 1: 409.24
Fragment 2: 255.23
Fragment 3: 153.0
Fragment 4: 78.96
Fragment 5: 173.49
Normalized Intensity
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 35.0 50.0 70.0 80.0
NCE

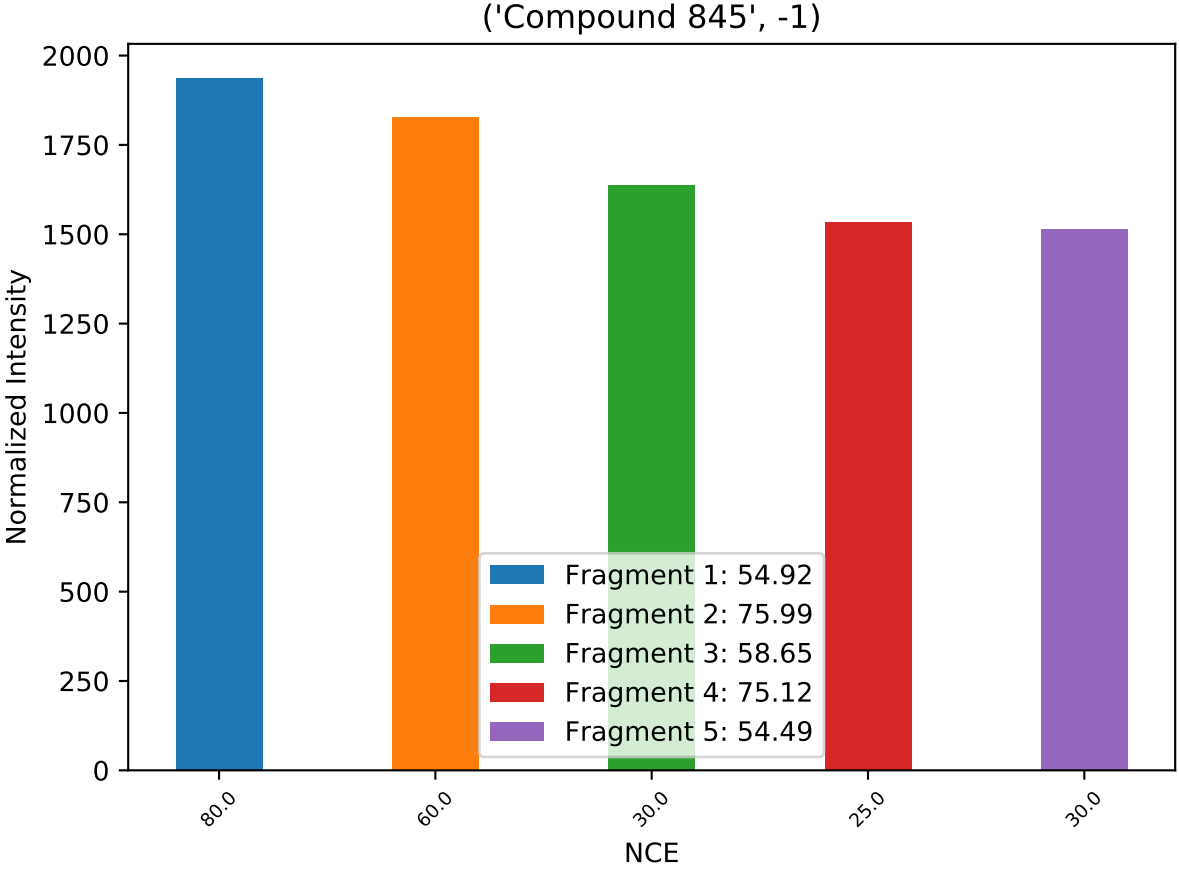

('Compound 190', -1)
Fragment 1: 173.48
Fragment 2: 78.96
Fragment 3: 134.05
Fragment 4: 211.0
Fragment 5: 96.97
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0 25.0 30.0 35.0 40.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

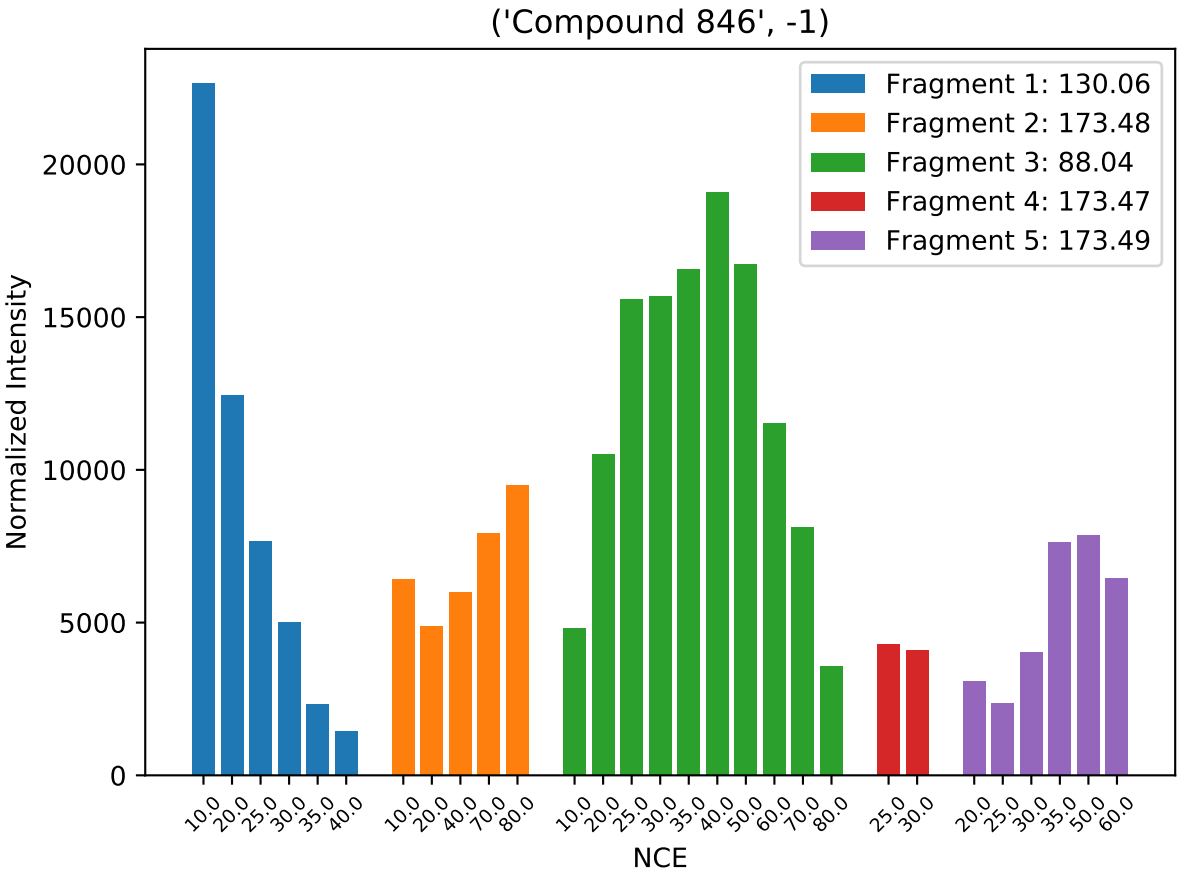

('Compound 840', -1)
Fragment 1: 75.01
Fragment 2: 85.03
Fragment 3: 72.99
Fragment 4: 74.0
Fragment 5: 57.0
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
20.0
25.0
30.0
NCE

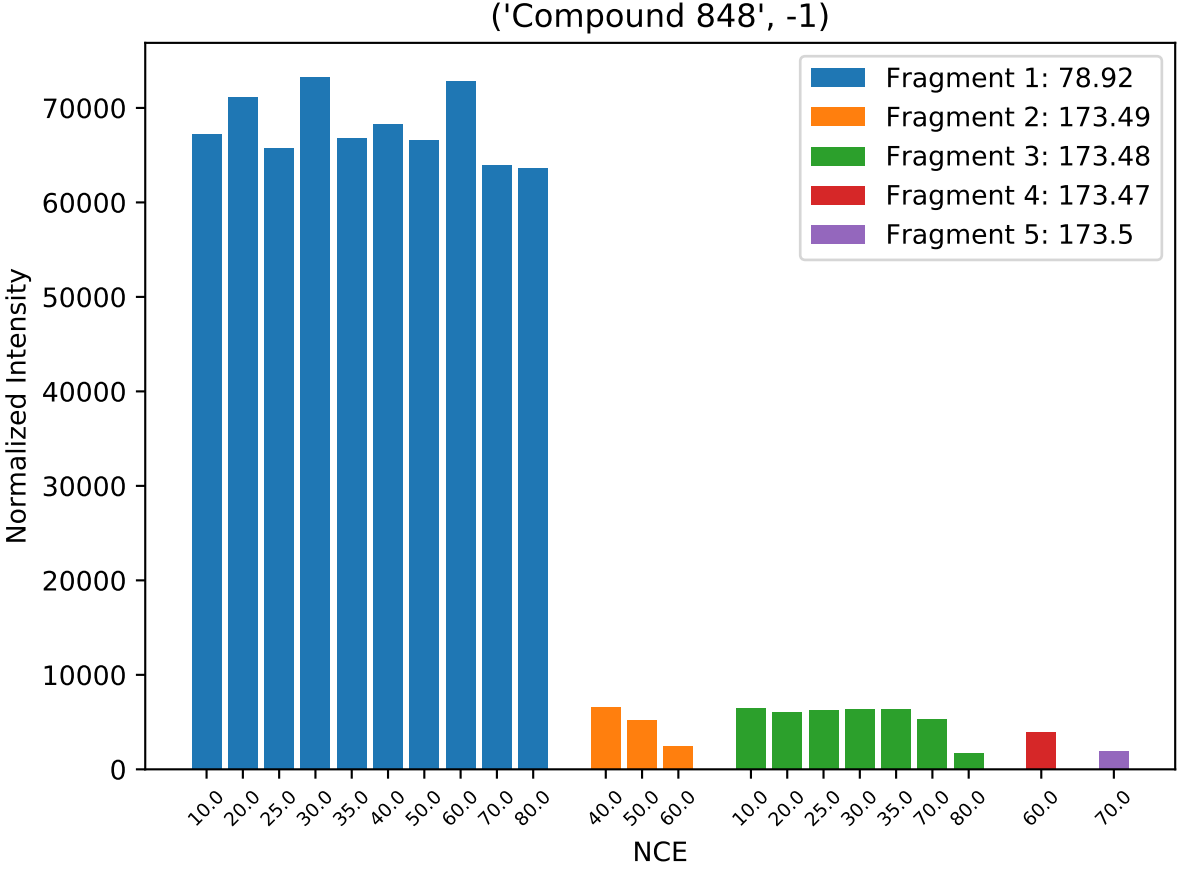

('Compound 81', -1)
Fragment 1: 100.04
Fragment 2: 62.52
Fragment 3: 69.63
Fragment 4: 101.17
Fragment 5: 75.4
Normalized Intensity
1750
1500
1250
1000
750
500
250
0
10.0
35.0
25.0
80.0
60.0
NCE

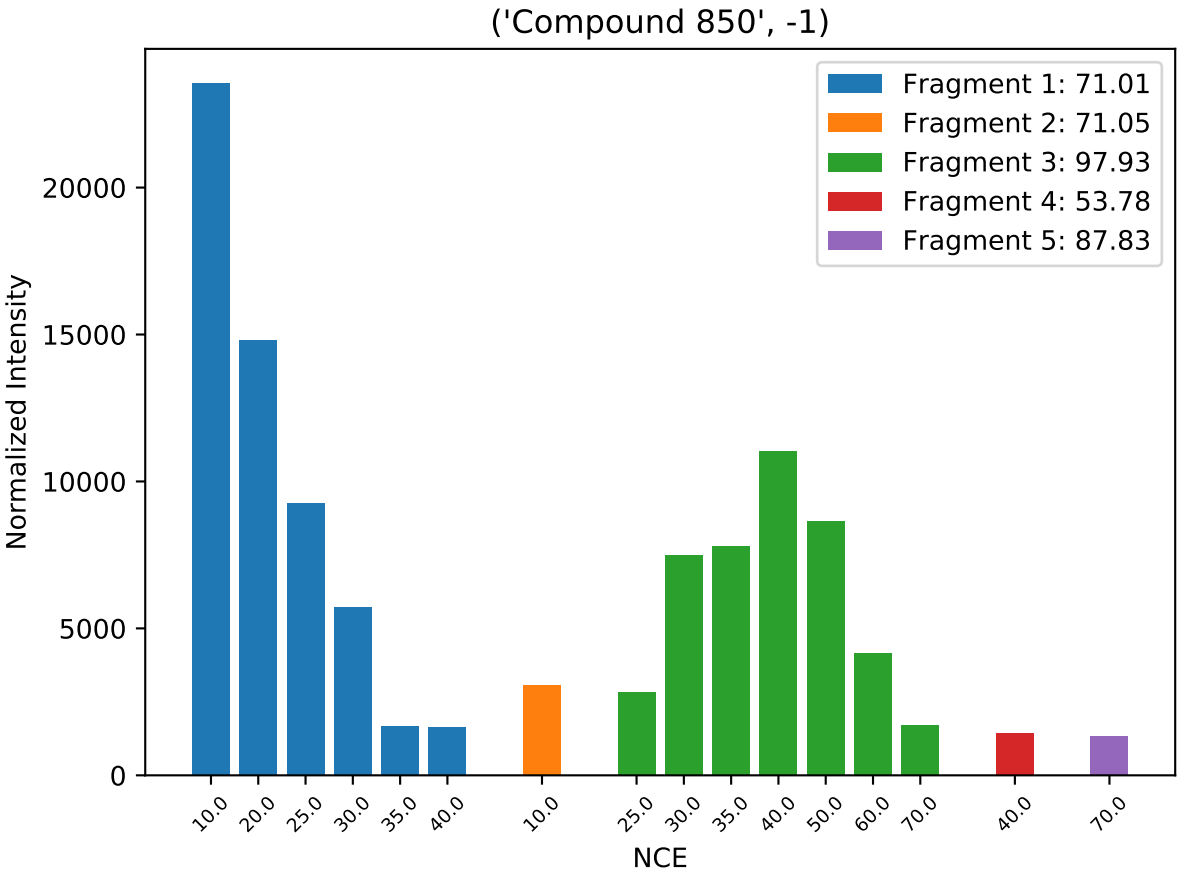

('Compound 842', -1)
Fragment 1: 204.91
Fragment 2: 173.48
Fragment 3: 59.98
Fragment 4: 173.49
Fragment 5: 57.0
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
25.0
40.0
60.0
60.0
70.0
80.0
20.0
30.0
35.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

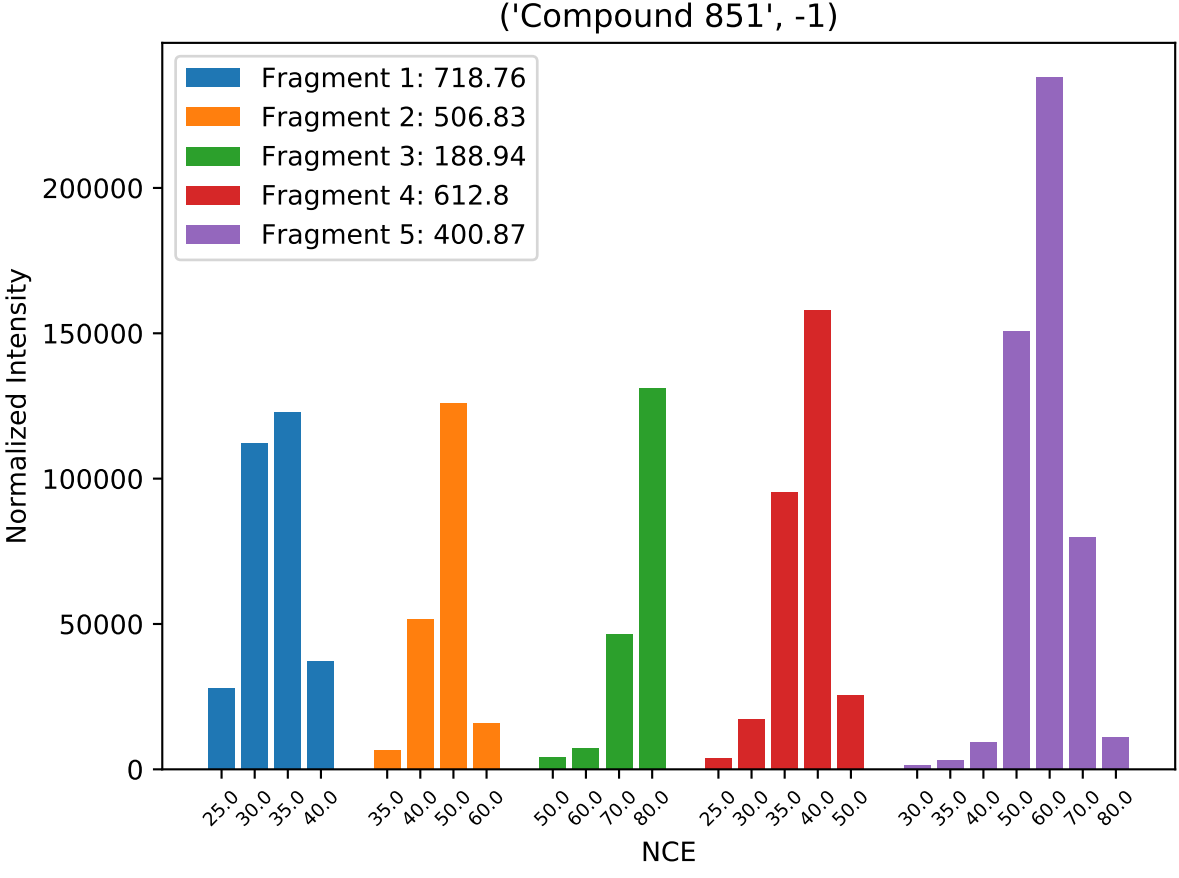

('Compound 843', -1)
Fragment 1: 57.03
Fragment 2: 67.02
Fragment 3: 85.03
Fragment 4: 55.02
Fragment 5: 66.03
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
25.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
25.0
35.0
50.0
25.0
NCE

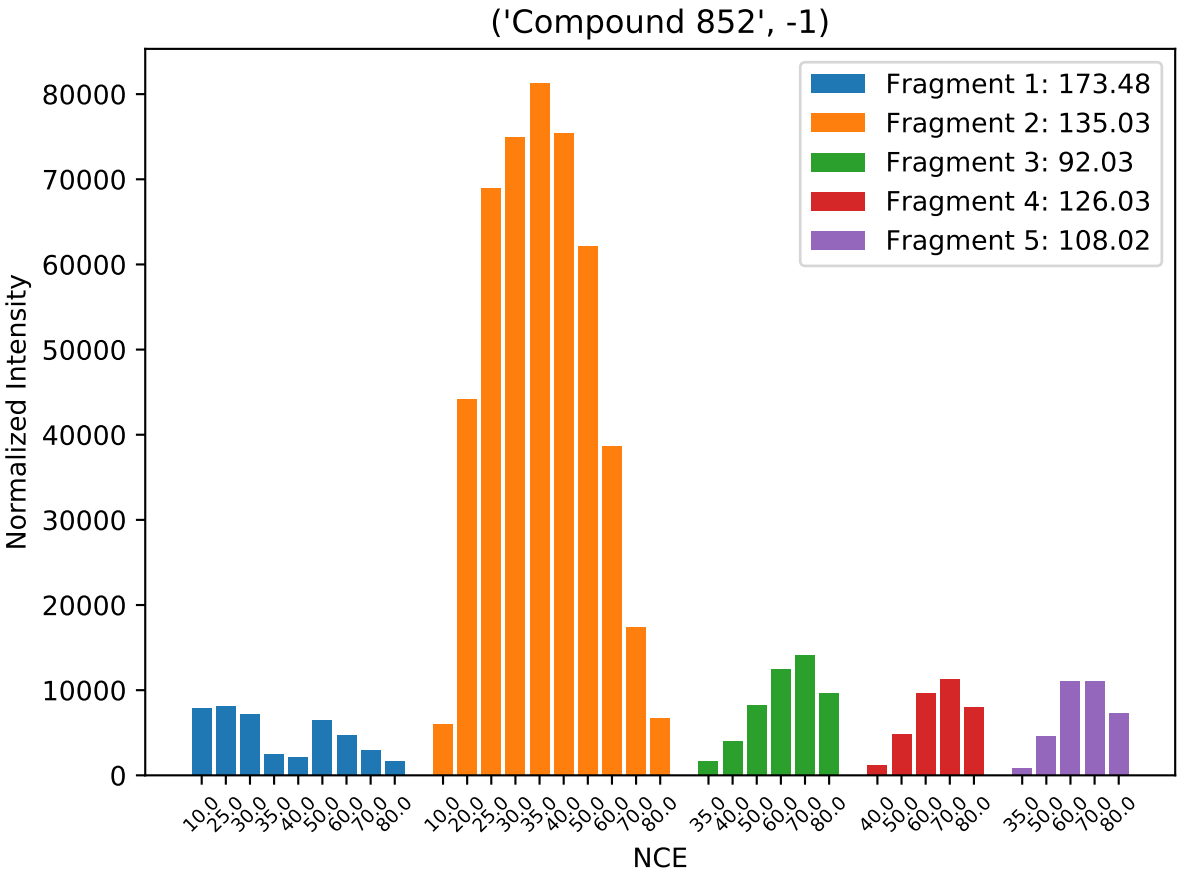

('Compound 845', -1)
Normalized Intensity
2000
1750
1500
1250
1000
750
500
250
0
Fragment 1: 54.92
Fragment 2: 75.99
Fragment 3: 58.65
Fragment 4: 75.12
Fragment 5: 54.49
80.0
60.0
30.0
25.0
30.0
NCE

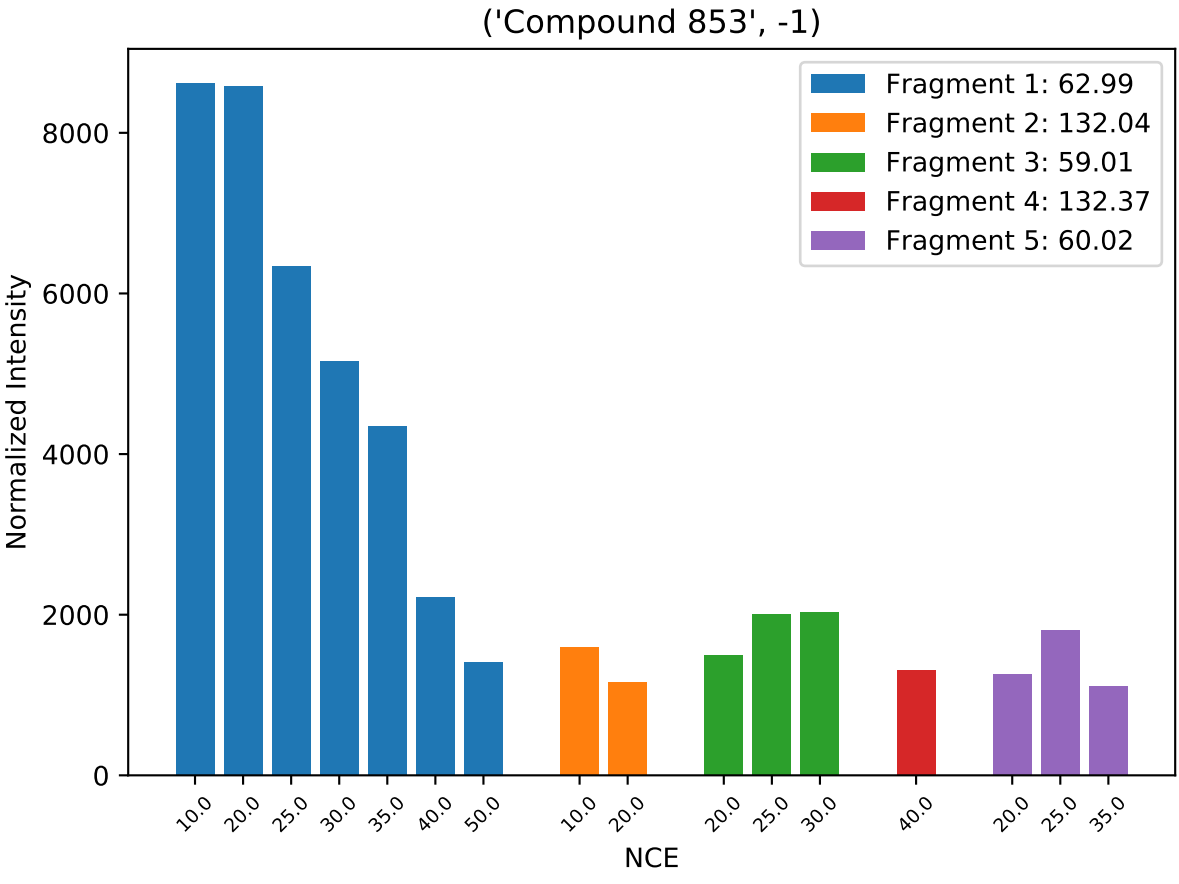

('Compound 846', -1)
Fragment 1: 130.06
Fragment 2: 173.48
Fragment 3: 88.04
Fragment 4: 173.47
Fragment 5: 173.49
Normalized Intensity
0
5000
10000
15000
20000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
40.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
20.0
25.0
30.0
35.0
50.0
60.0
NCE

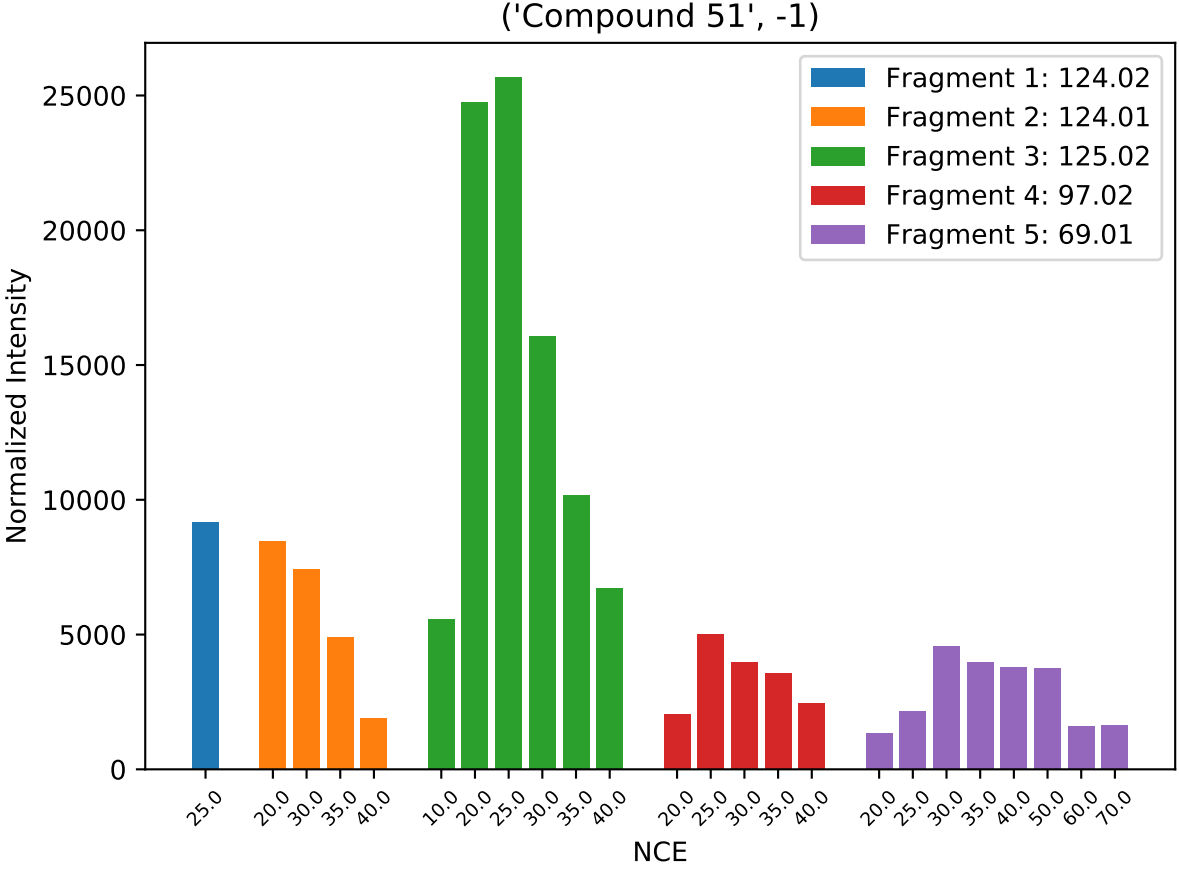

('Compound 848', -1)
Fragment 1: 78.92
Fragment 2: 173.49
Fragment 3: 173.48
Fragment 4: 173.47
Fragment 5: 173.5
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
70.0
80.0
60.0
70.0
NCE

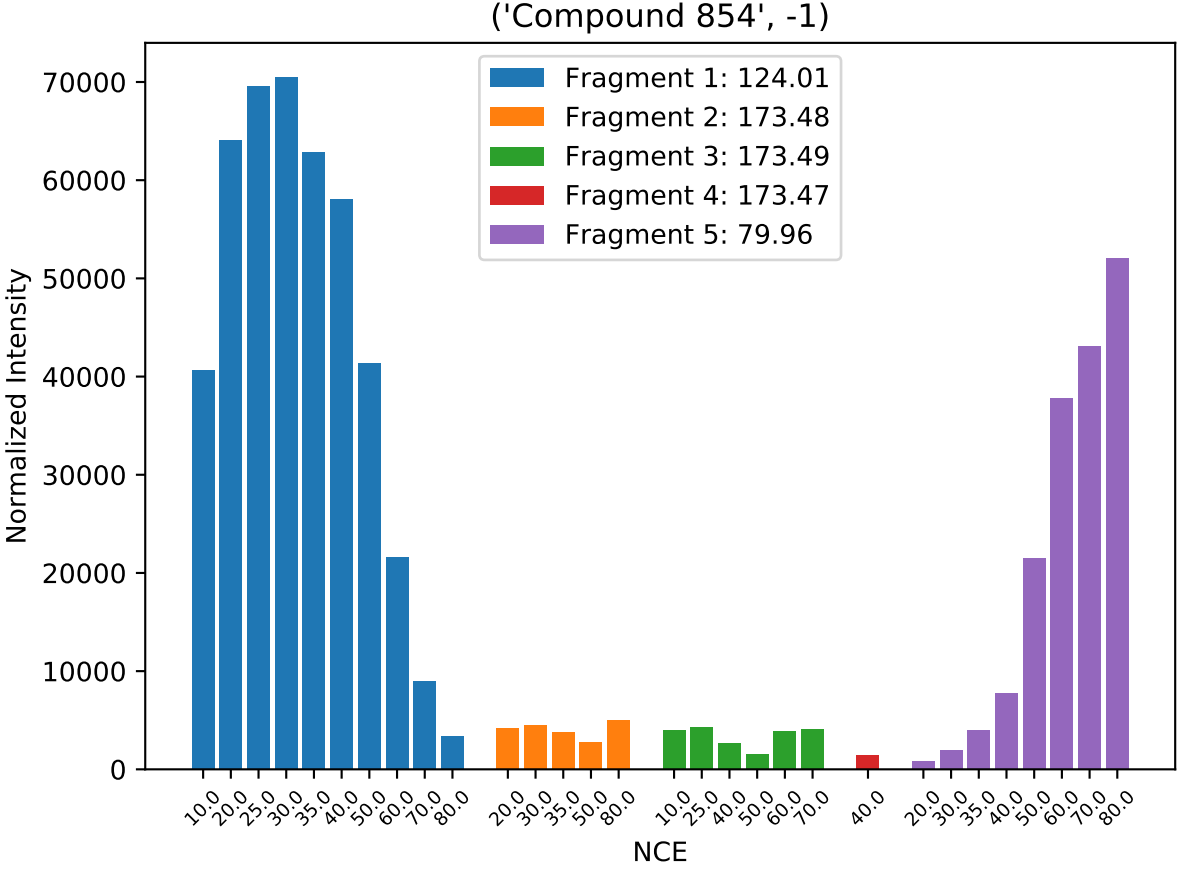

('Compound 850', -1)
Fragment 1: 71.01
Fragment 2: 71.05
Fragment 3: 97.93
Fragment 4: 53.78
Fragment 5: 87.83
Normalized Intensity
0
5000
10000
15000
20000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
40.0
70.0
NCE

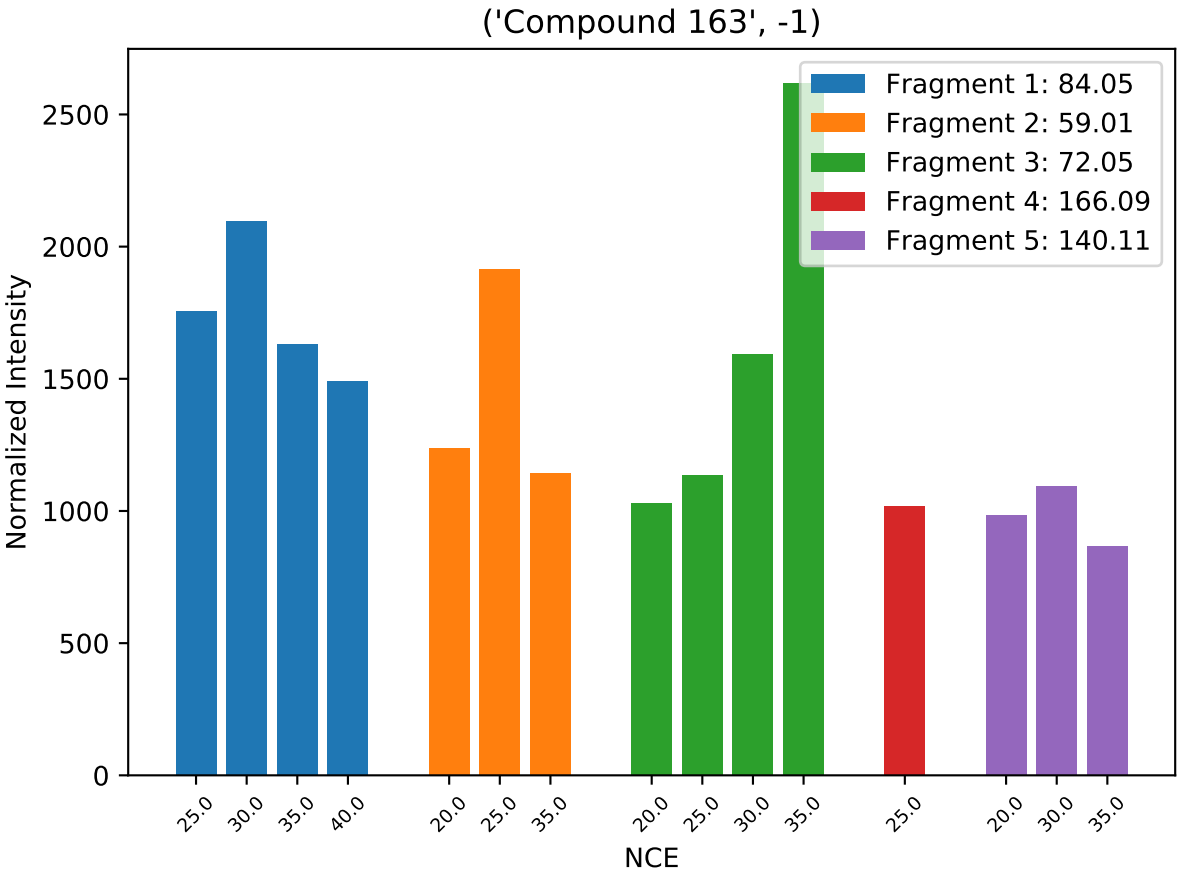

('Compound 851', -1)
Fragment 1: 718.76
Fragment 2: 506.83
Fragment 3: 188.94
Fragment 4: 612.8
Fragment 5: 400.87
Normalized Intensity
0
50000
100000
150000
200000
25.0
30.0
35.0
40.0
35.0
40.0
50.0
60.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

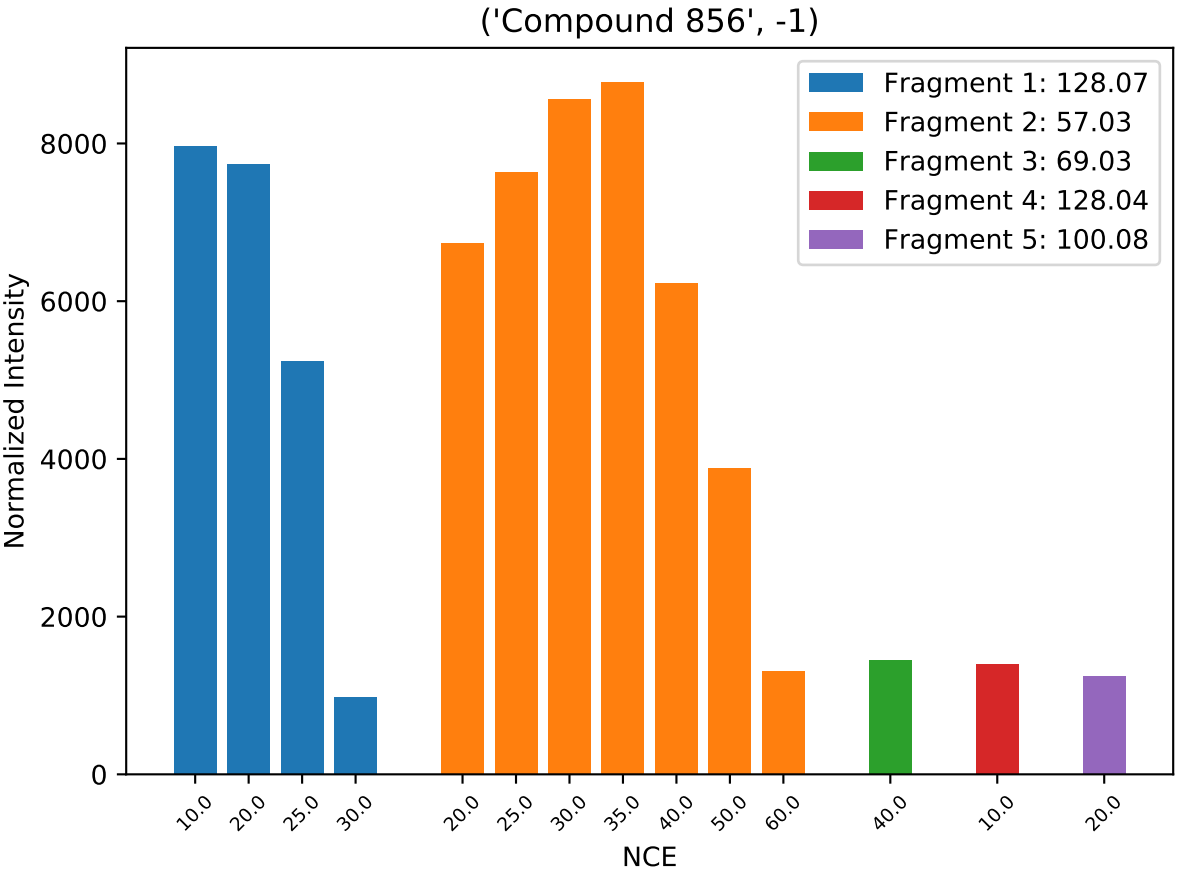

('Compound 852', -1)
Fragment 1: 173.48
Fragment 2: 135.03
Fragment 3: 92.03
Fragment 4: 126.03
Fragment 5: 108.02
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
35.0 50.0 60.0 70.0 80.0
NCE

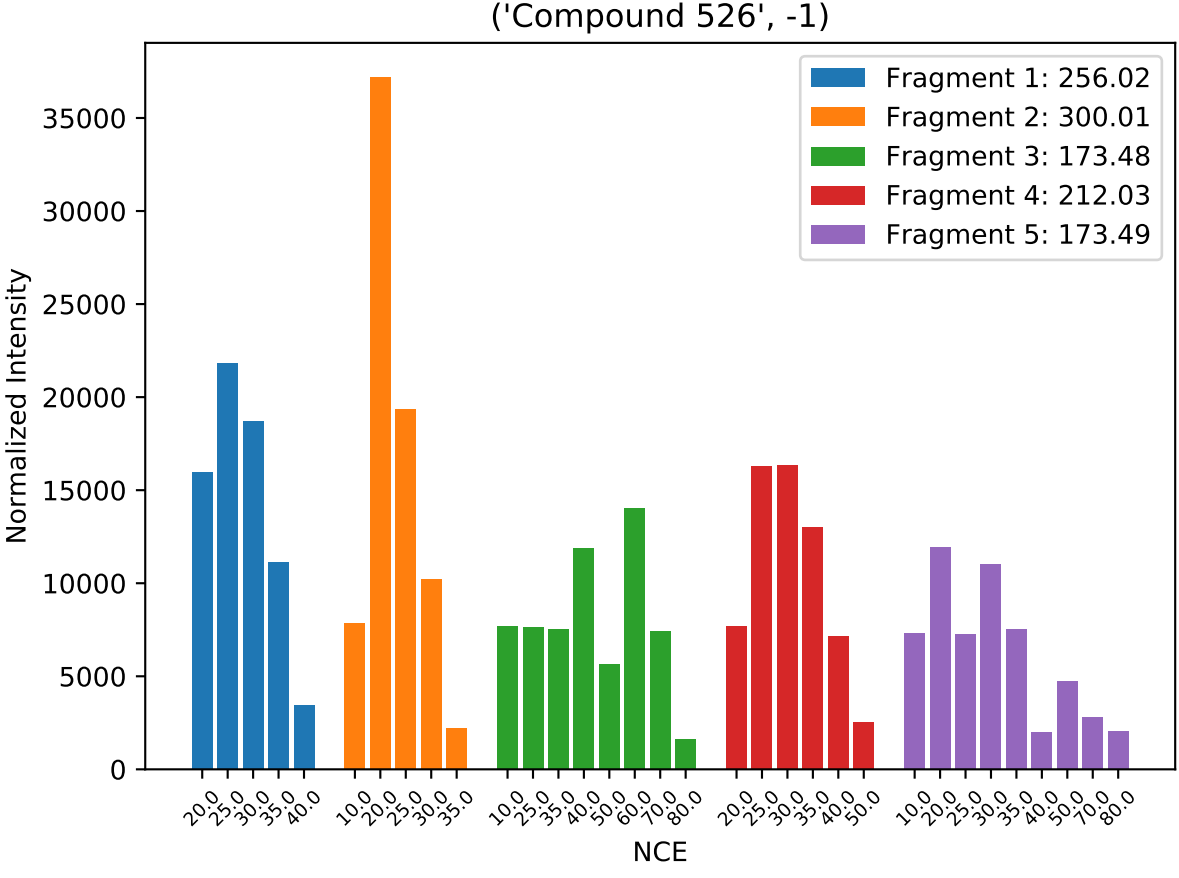

('Compound 853', -1)
Fragment 1: 62.99
Fragment 2: 132.04
Fragment 3: 59.01
Fragment 4: 132.37
Fragment 5: 60.02
Normalized Intensity
0
2000
4000
6000
8000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
20.0
25.0
30.0
40.0
20.0
25.0
35.0
NCE

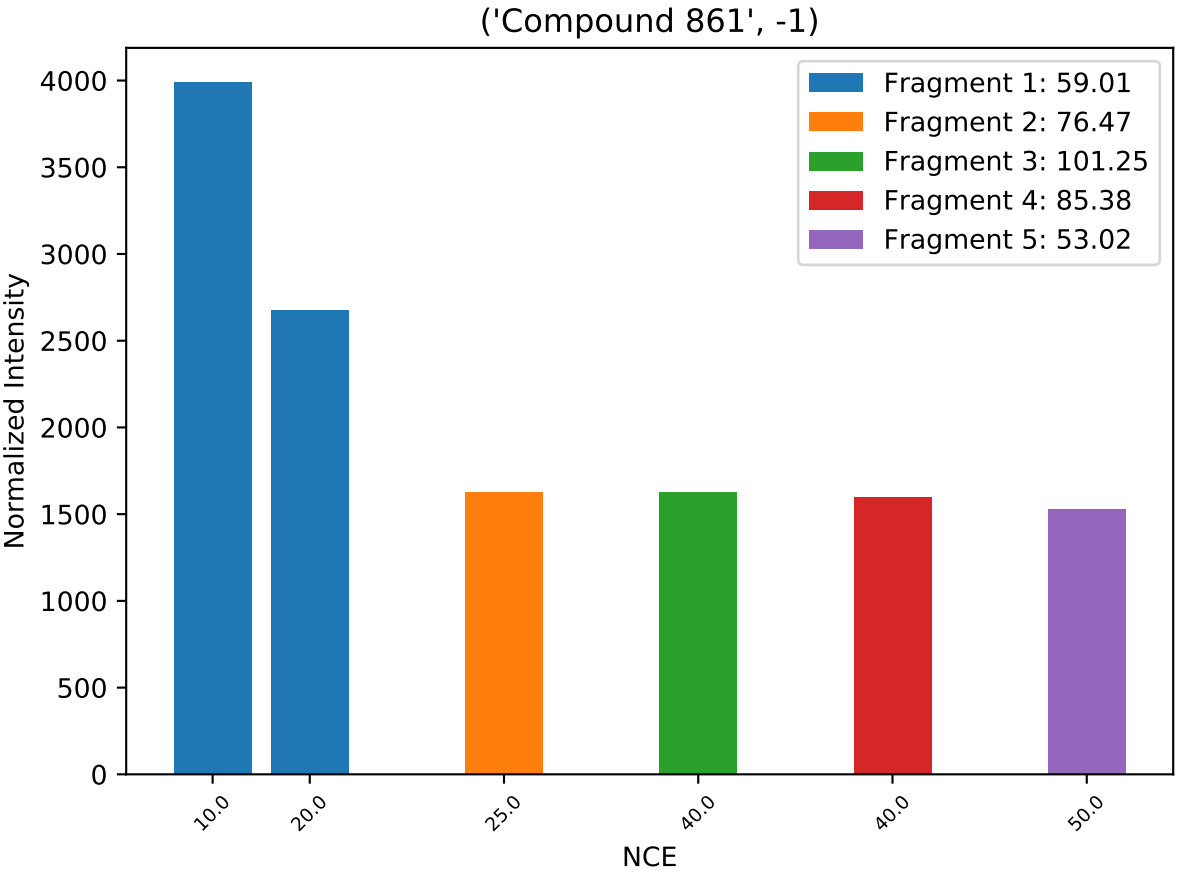

('Compound 51', -1)
Fragment 1: 124.02
Fragment 2: 124.01
Fragment 3: 125.02
Fragment 4: 97.02
Fragment 5: 69.01
Normalized Intensity
0
5000
10000
15000
20000
25000
25.0
20.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

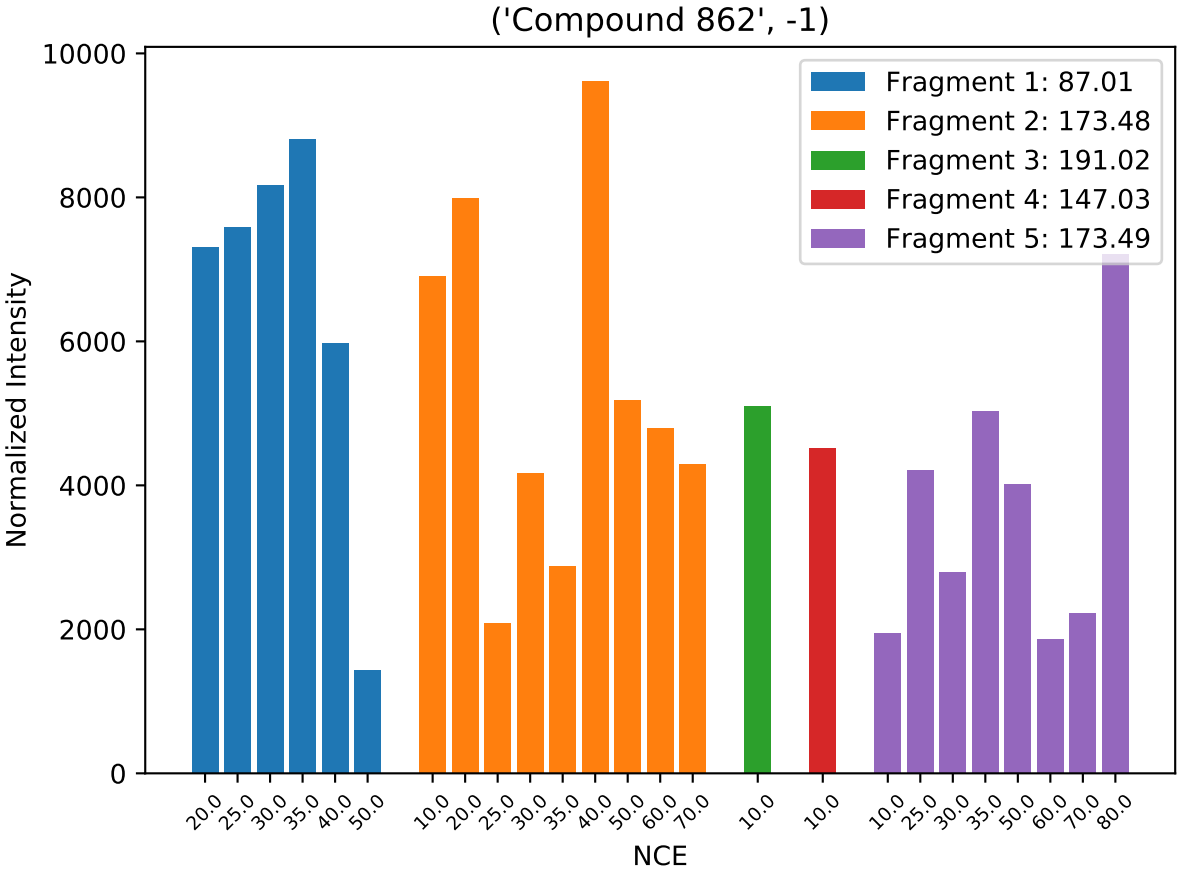

('Compound 854', -1)
Fragment 1: 124.01
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 173.47
Fragment 5: 79.96
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 30.0 35.0 50.0 80.0
10.0 25.0 40.0 50.0 60.0 70.0
40.0
20.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

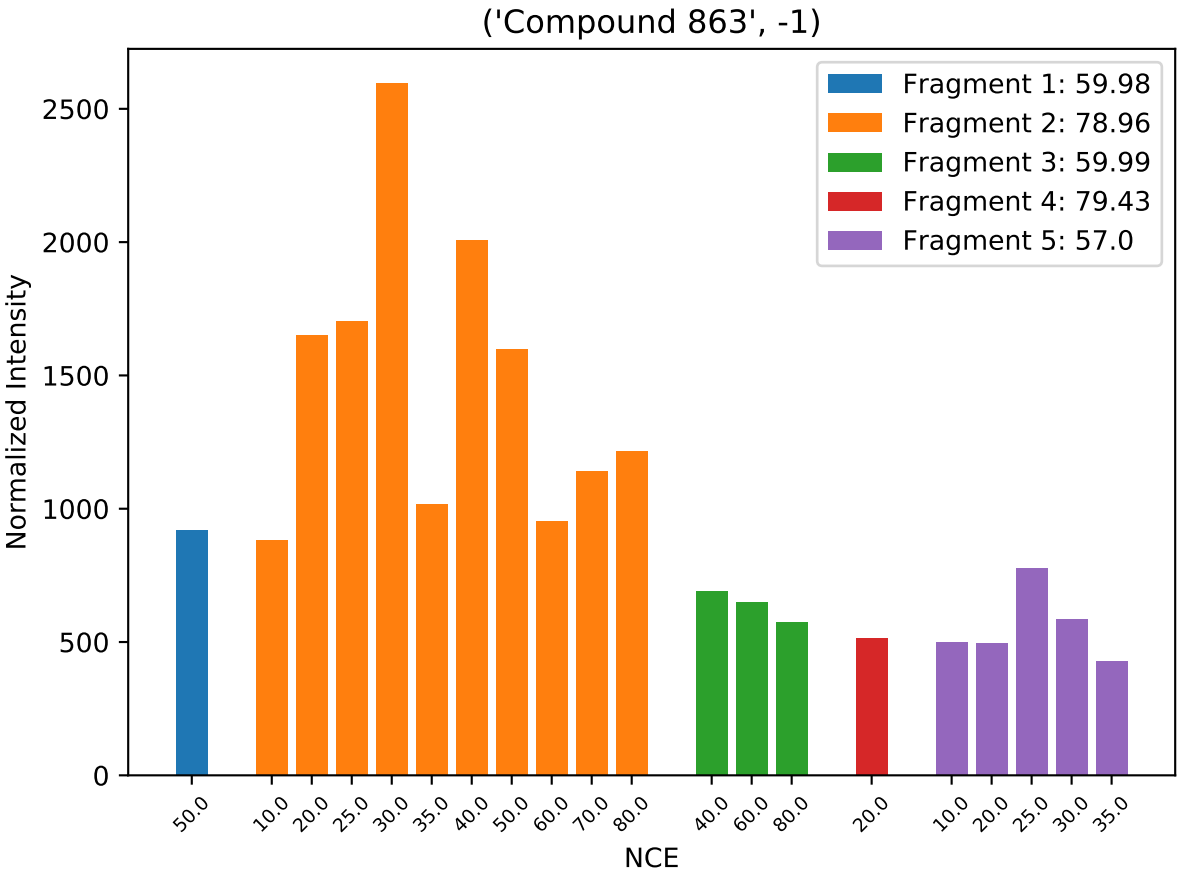

('Compound 163', -1)
Fragment 1: 84.05
Fragment 2: 59.01
Fragment 3: 72.05
Fragment 4: 166.09
Fragment 5: 140.11
Normalized Intensity
0
500
1000
1500
2000
2500
25.0
30.0
35.0
40.0
20.0
25.0
35.0
20.0
25.0
30.0
35.0
25.0
20.0
30.0
35.0
NCE

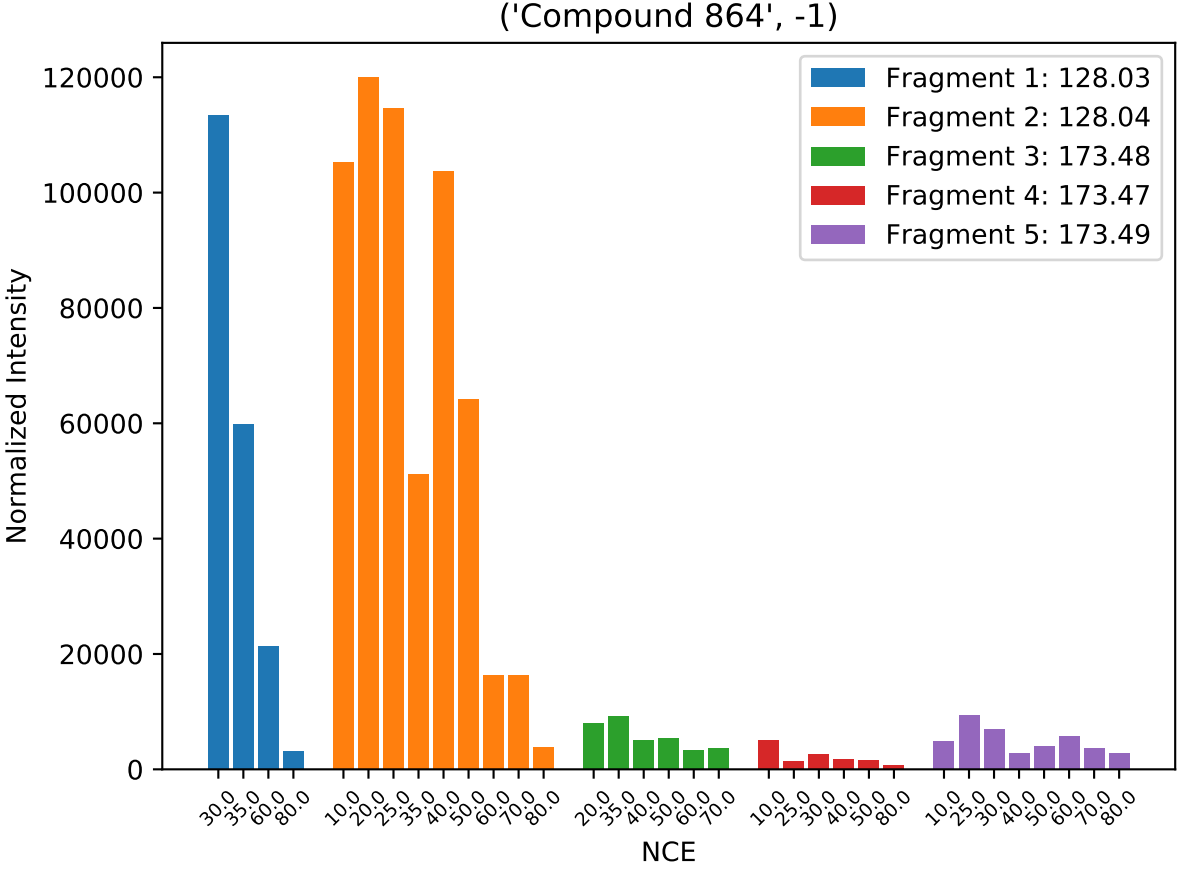

('Compound 856', -1)
Fragment 1: 128.07
Fragment 2: 57.03
Fragment 3: 69.03
Fragment 4: 128.04
Fragment 5: 100.08
Normalized Intensity
0
2000
4000
6000
8000
10.0
20.0
25.0
30.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
40.0
10.0
20.0
NCE

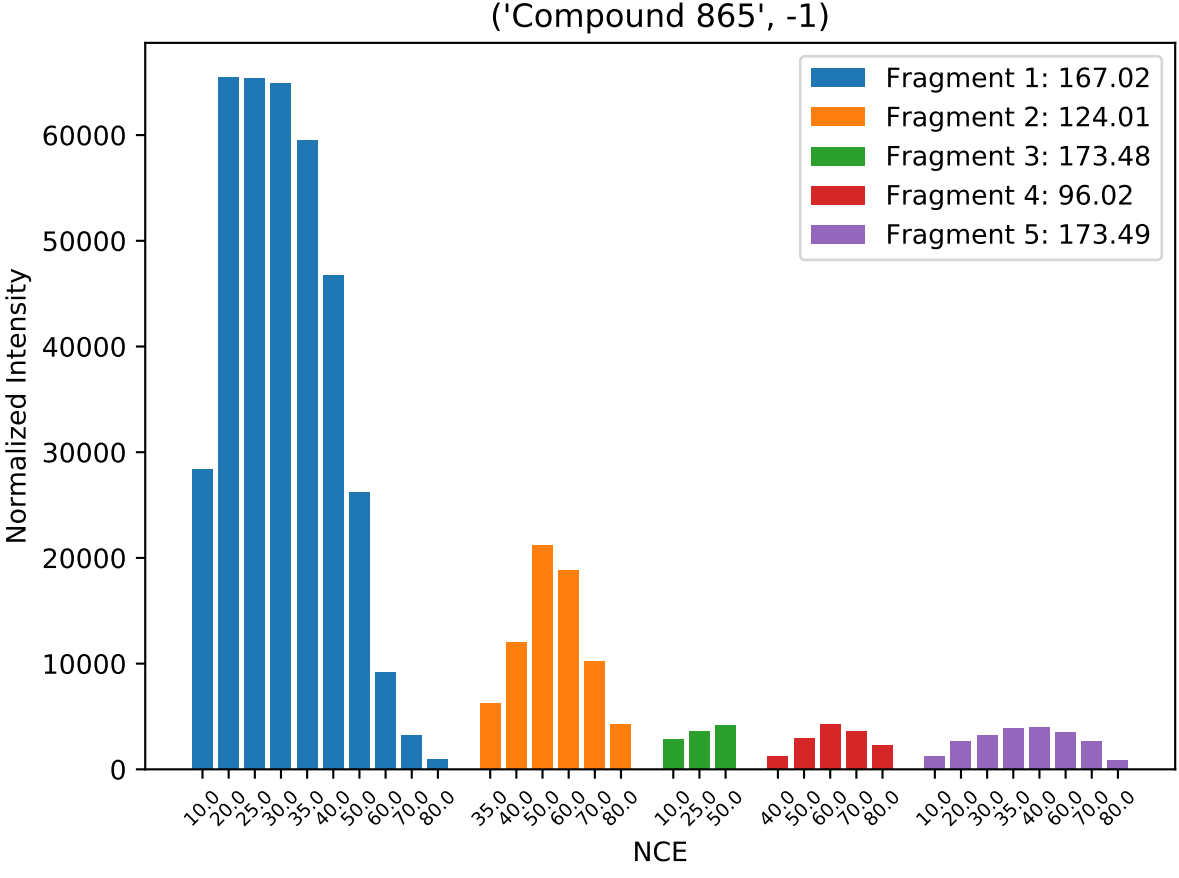

('Compound 526', -1)
Fragment 1: 256.02
Fragment 2: 300.01
Fragment 3: 173.48
Fragment 4: 212.03
Fragment 5: 173.49
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0
10.0 25.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 70.0 80.0
NCE

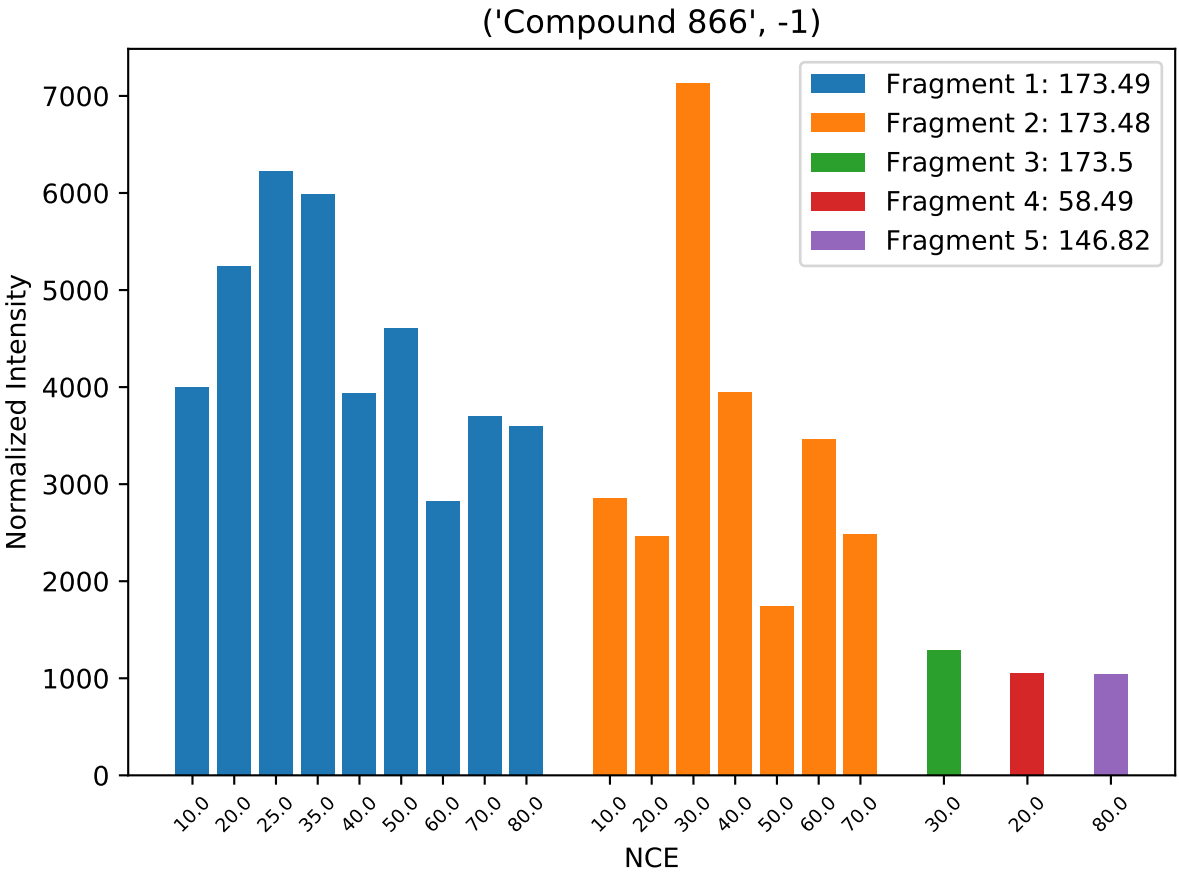

('Compound 861', -1)
Fragment 1: 59.01
Fragment 2: 76.47
Fragment 3: 101.25
Fragment 4: 85.38
Fragment 5: 53.02
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
10.0
20.0
25.0
40.0
40.0
50.0
NCE

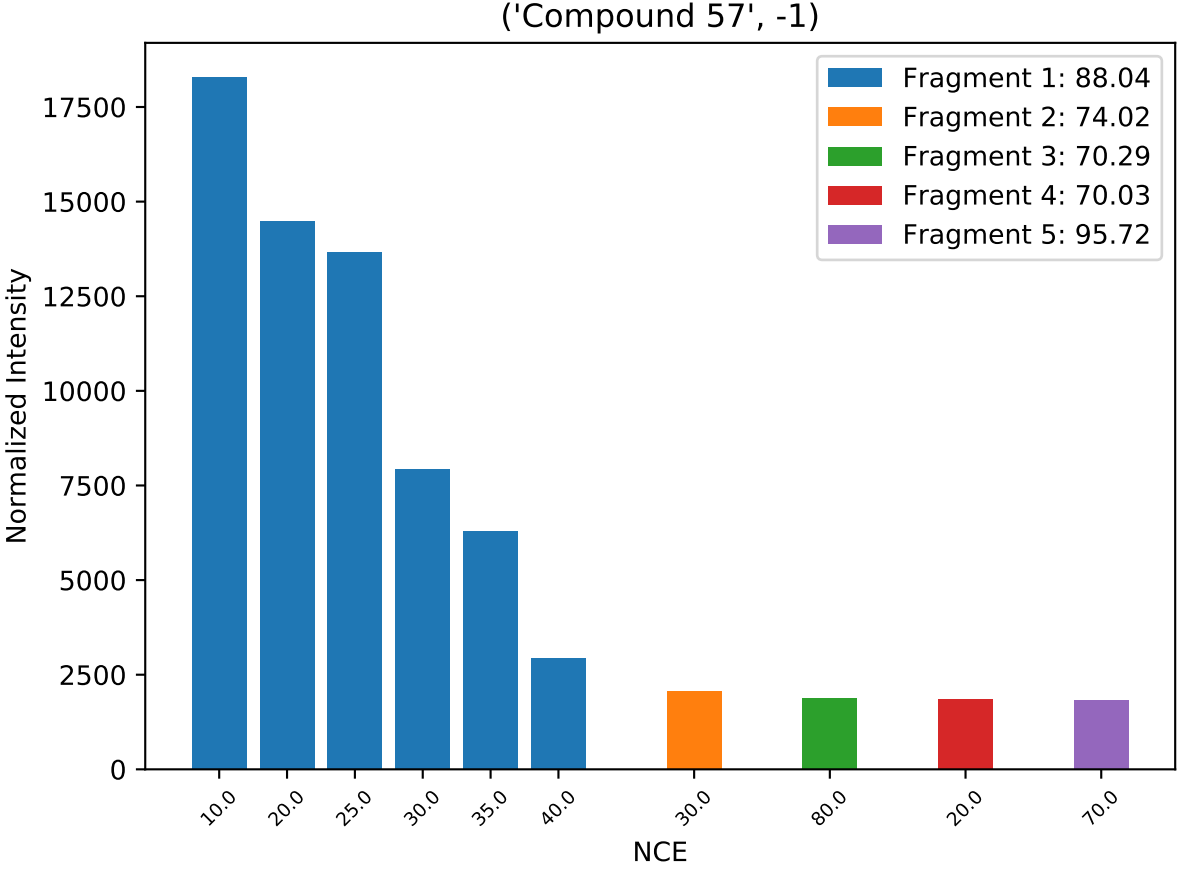

('Compound 862', -1)
Fragment 1: 87.01
Fragment 2: 173.48
Fragment 3: 191.02
Fragment 4: 147.03
Fragment 5: 173.49
Normalized Intensity
10000
8000
6000
4000
2000
0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
10.0
10.0
25.0
30.0
35.0
50.0
60.0
70.0
80.0
NCE

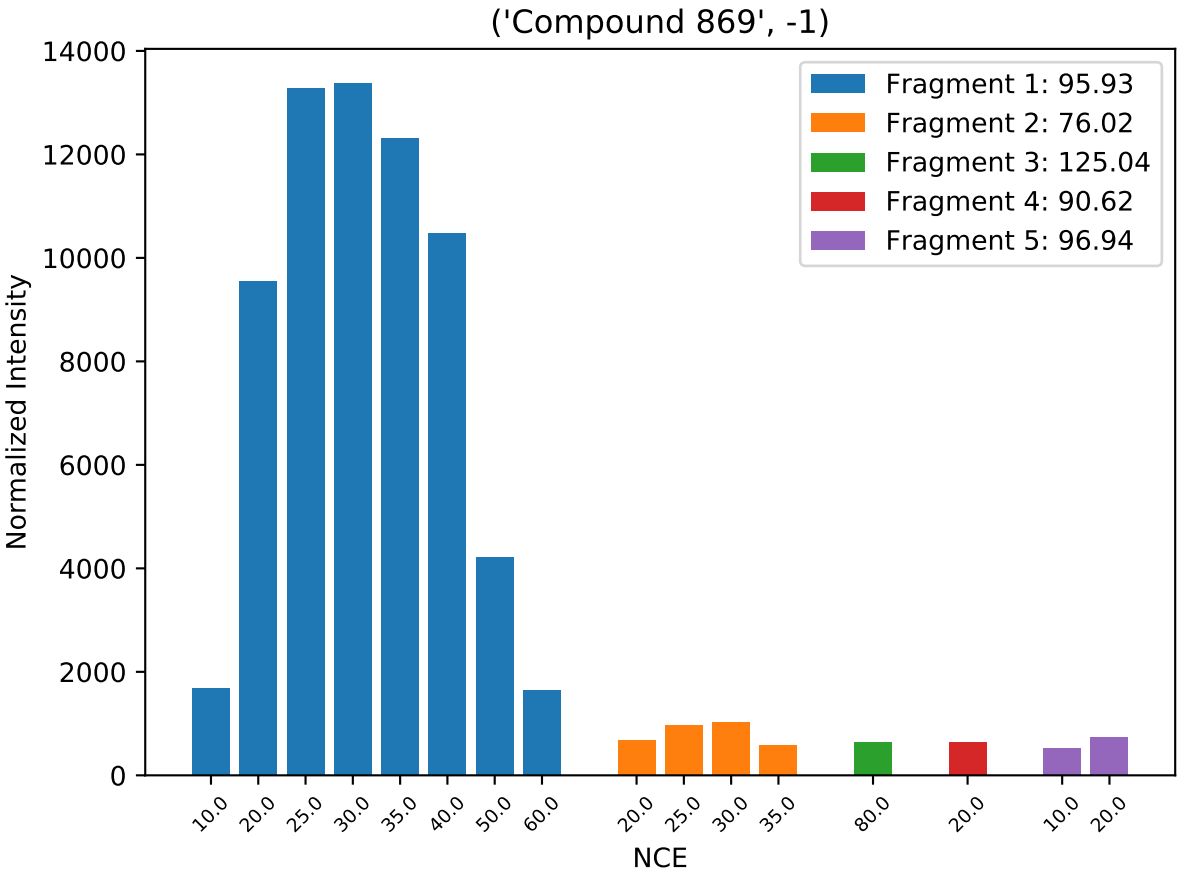

('Compound 863', -1)
Fragment 1: 59.98
Fragment 2: 78.96
Fragment 3: 59.99
Fragment 4: 79.43
Fragment 5: 57.0
Normalized Intensity
0
500
1000
1500
2000
2500
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
40.0
60.0
80.0
20.0
10.0
20.0
25.0
30.0
35.0
NCE

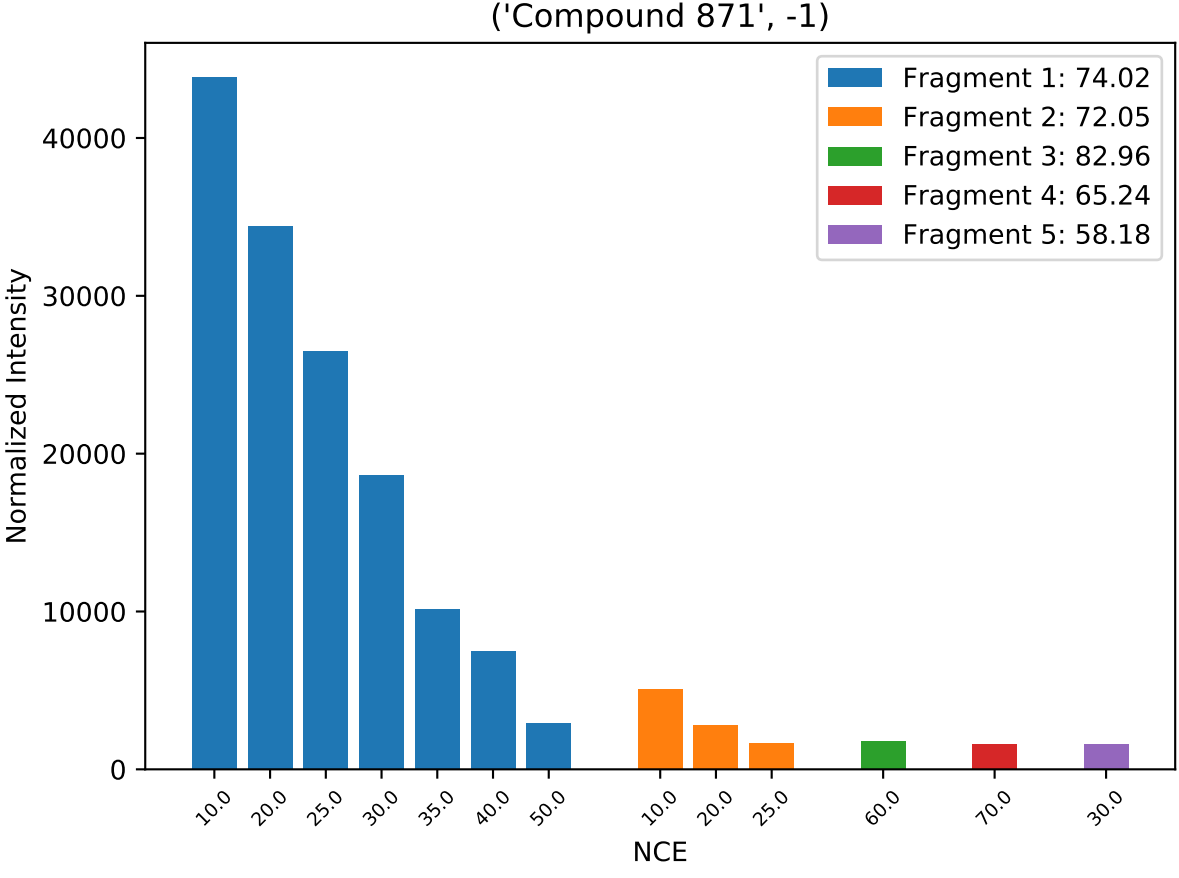

('Compound 864', -1)
Fragment 1: 128.03
Fragment 2: 128.04
Fragment 3: 173.48
Fragment 4: 173.47
Fragment 5: 173.49
Normalized Intensity
120000
100000
80000
60000
40000
20000
0
30.0 35.0 60.0 80.0
10.0 20.0 25.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 35.0 40.0 50.0 60.0 70.0
10.0 25.0 30.0 40.0 50.0 80.0
10.0 25.0 30.0 40.0 50.0 60.0 70.0 80.0
NCE

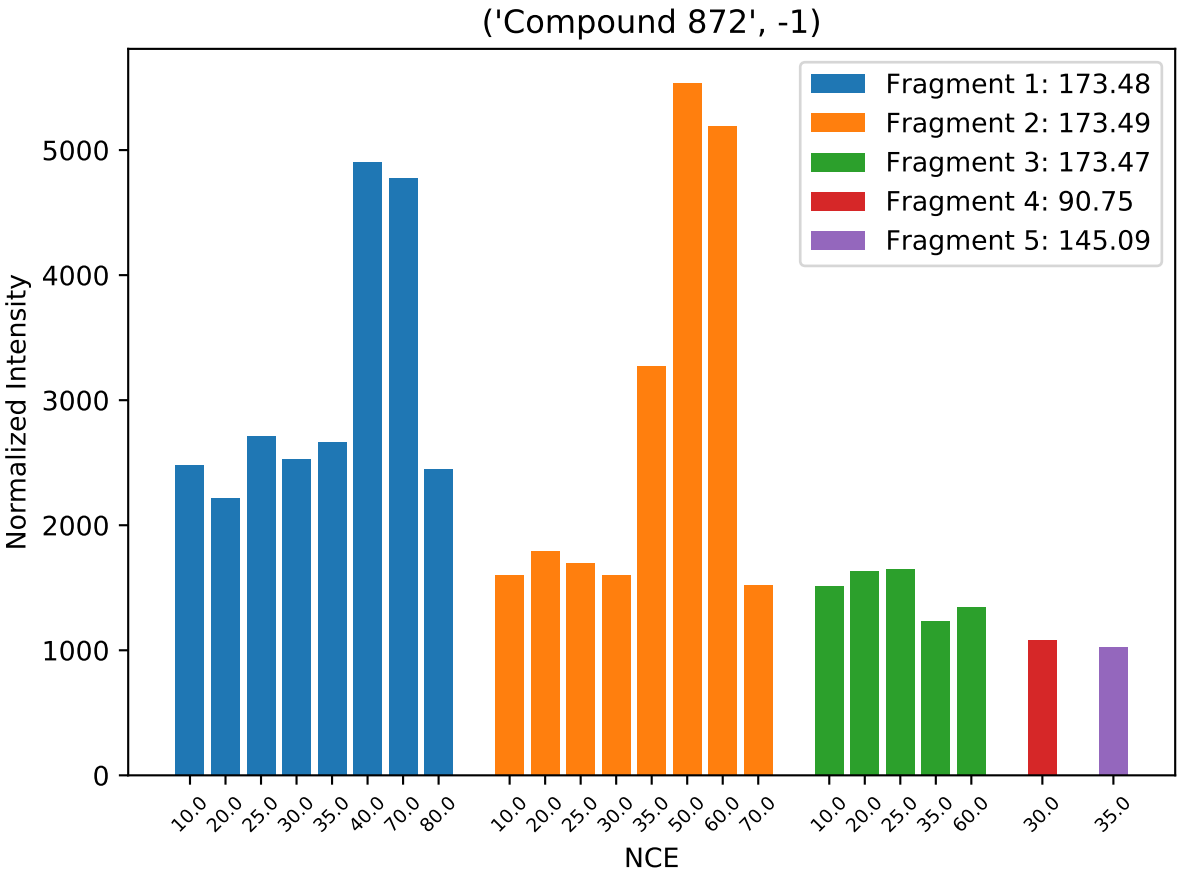

('Compound 865', -1)
Fragment 1: 167.02
Fragment 2: 124.01
Fragment 3: 173.48
Fragment 4: 96.02
Fragment 5: 173.49
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
10.0 25.0 50.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 30.0 35.0 40.0 60.0 70.0 80.0
NCE

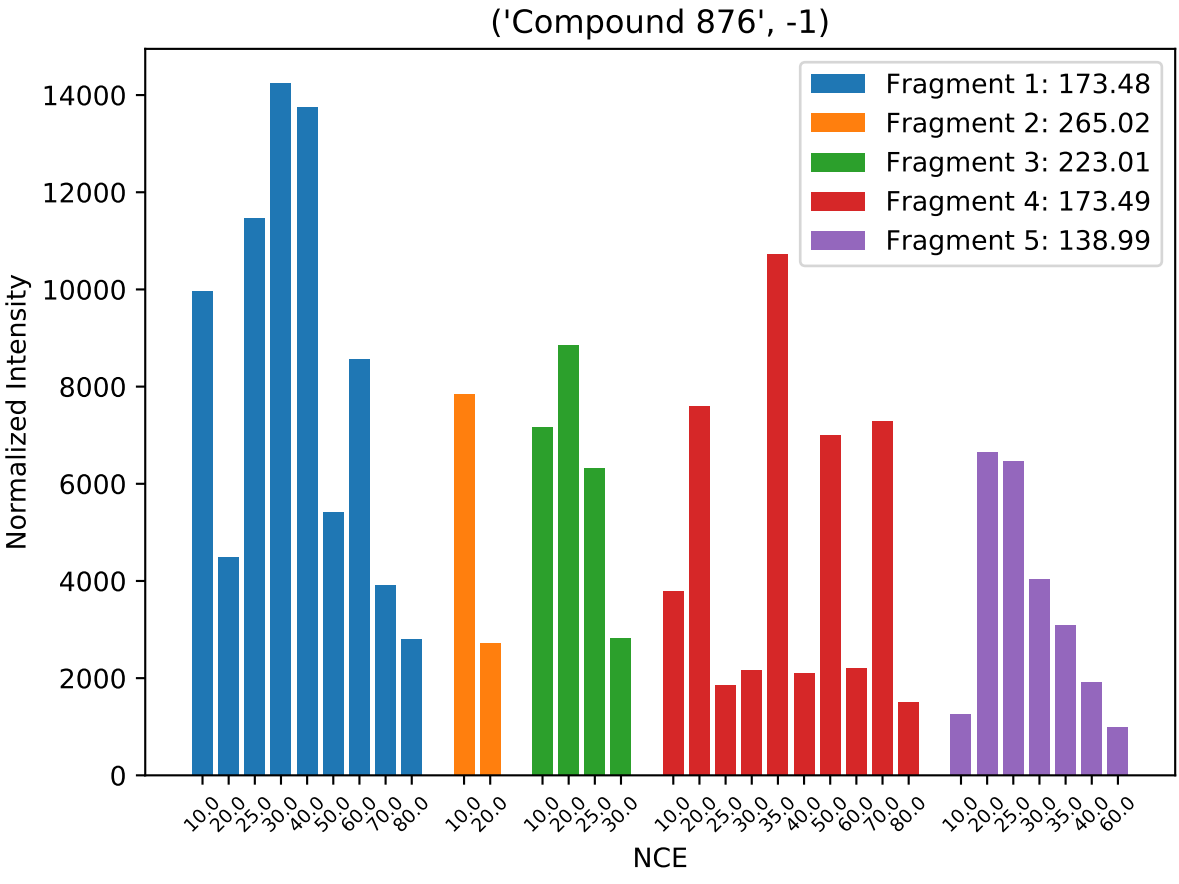

('Compound 866', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 173.5
Fragment 4: 58.49
Fragment 5: 146.82
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
10.0
20.0
25.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
30.0
20.0
80.0
NCE

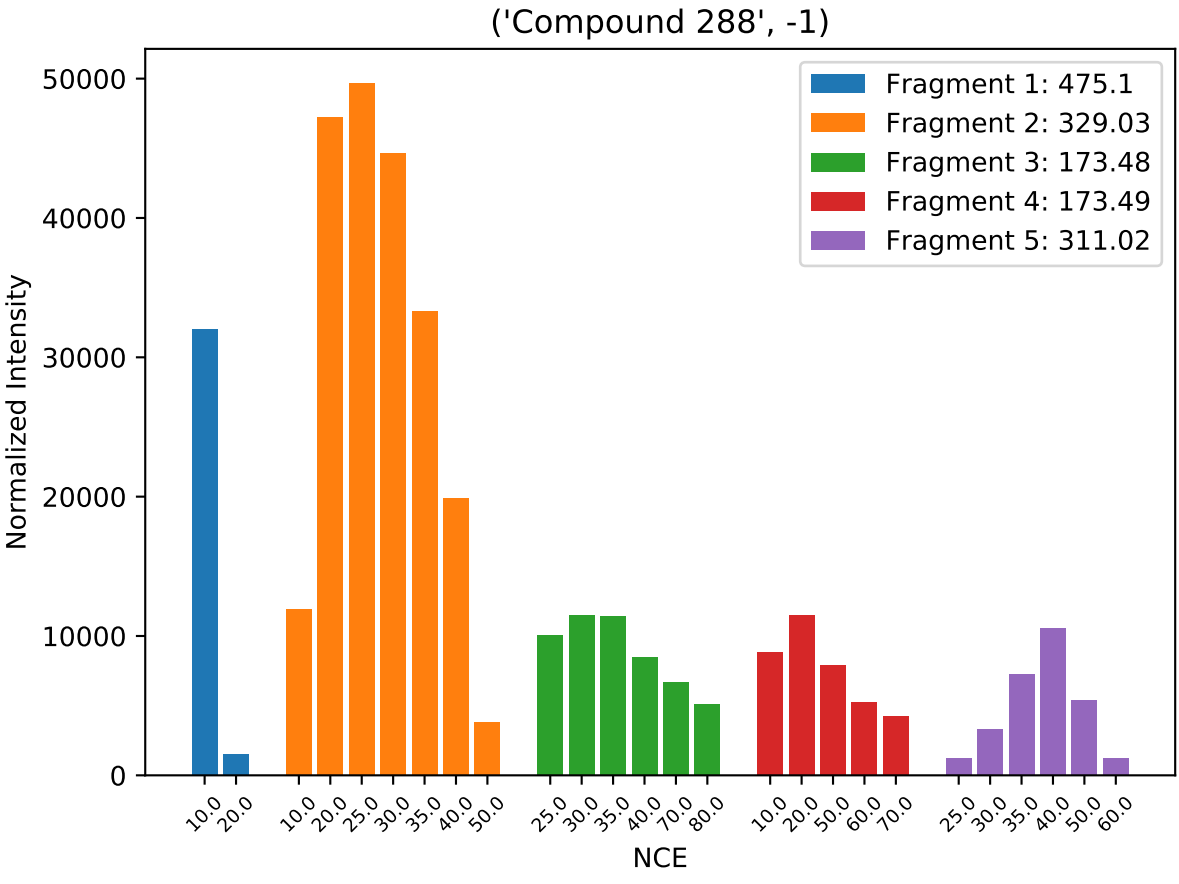

('Compound 57', -1)
Fragment 1: 88.04
Fragment 2: 74.02
Fragment 3: 70.29
Fragment 4: 70.03
Fragment 5: 95.72
Normalized Intensity
17500
15000
12500
10000
7500
5000
2500
0
10.0
20.0
25.0
30.0
35.0
40.0
30.0
80.0
20.0
70.0
NCE

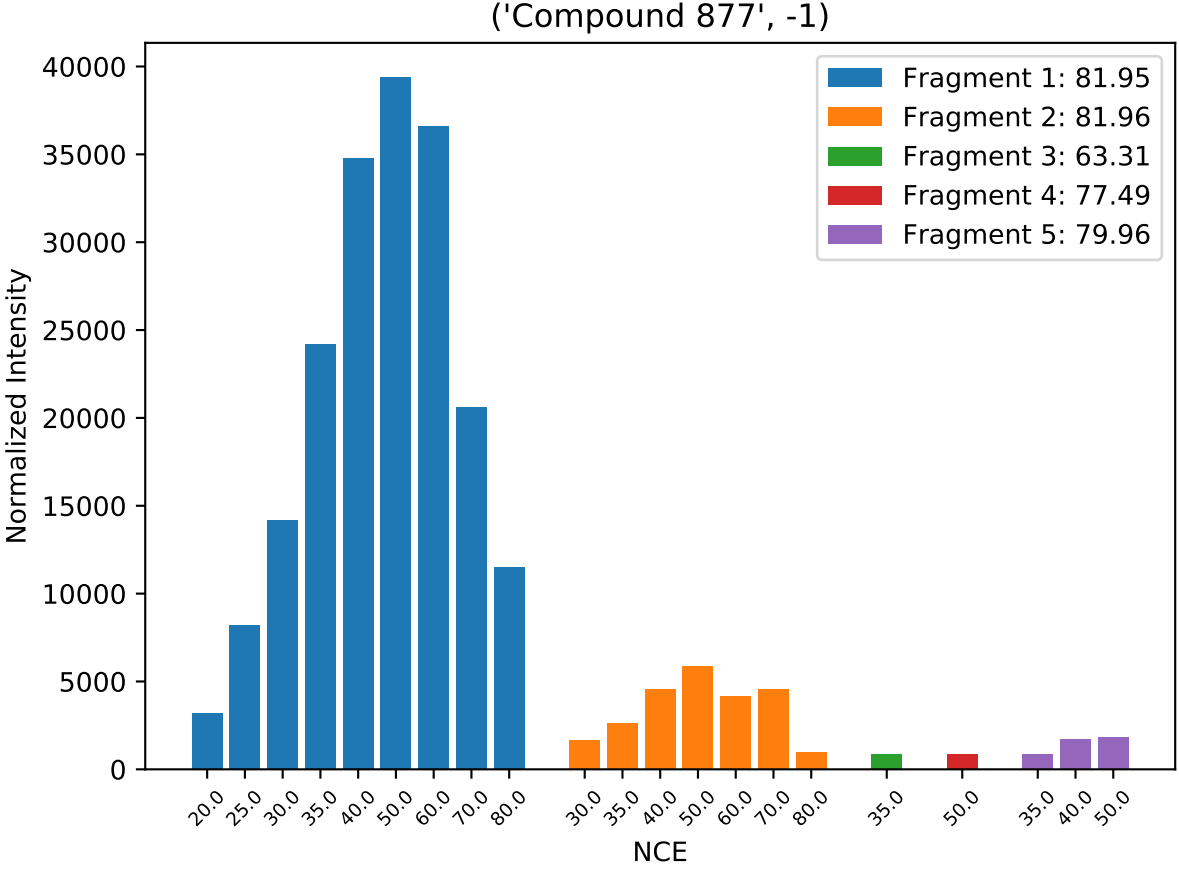

('Compound 869', -1)
Fragment 1: 95.93
Fragment 2: 76.02
Fragment 3: 125.04
Fragment 4: 90.62
Fragment 5: 96.94
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
80.0
20.0
10.0
20.0
NCE

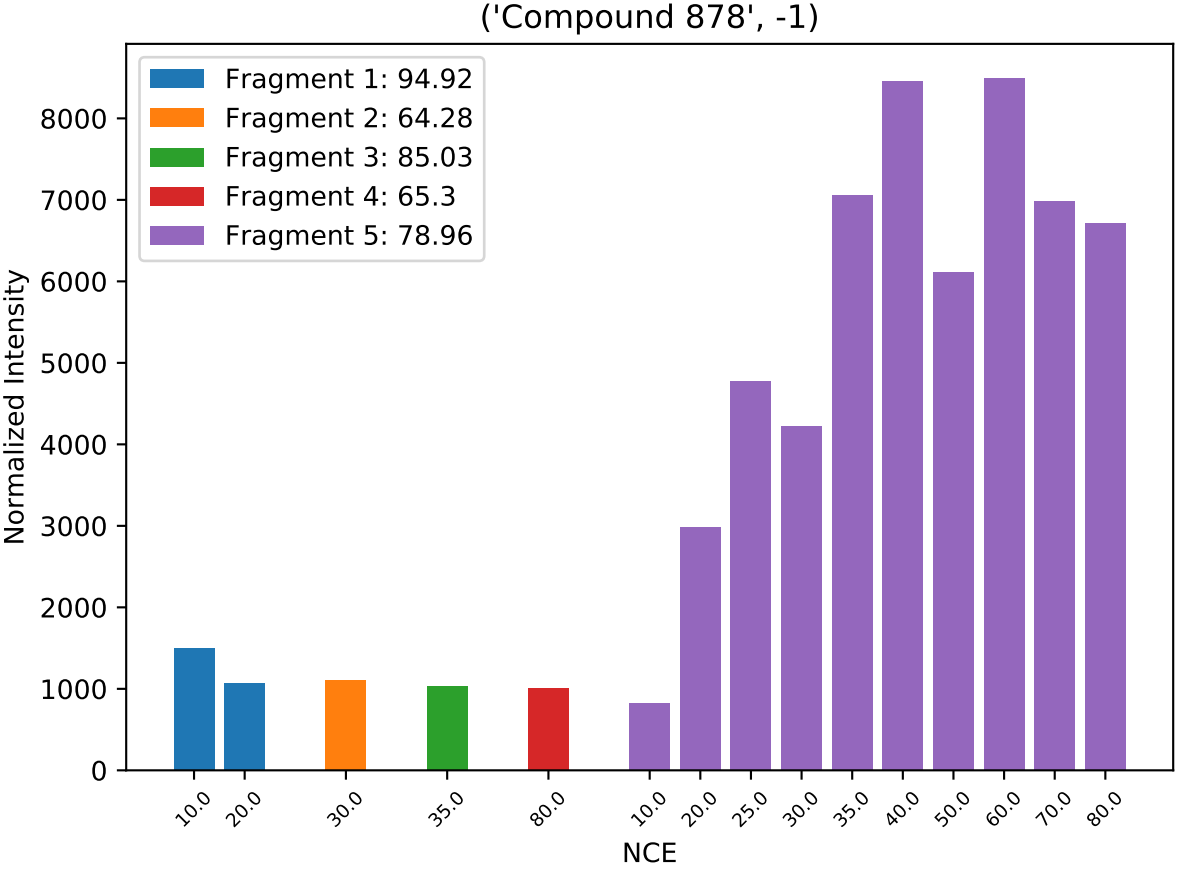

('Compound 871', -1)
Fragment 1: 74.02
Fragment 2: 72.05
Fragment 3: 82.96
Fragment 4: 65.24
Fragment 5: 58.18
Normalized Intensity
0
10000
20000
30000
40000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
60.0
70.0
30.0
NCE

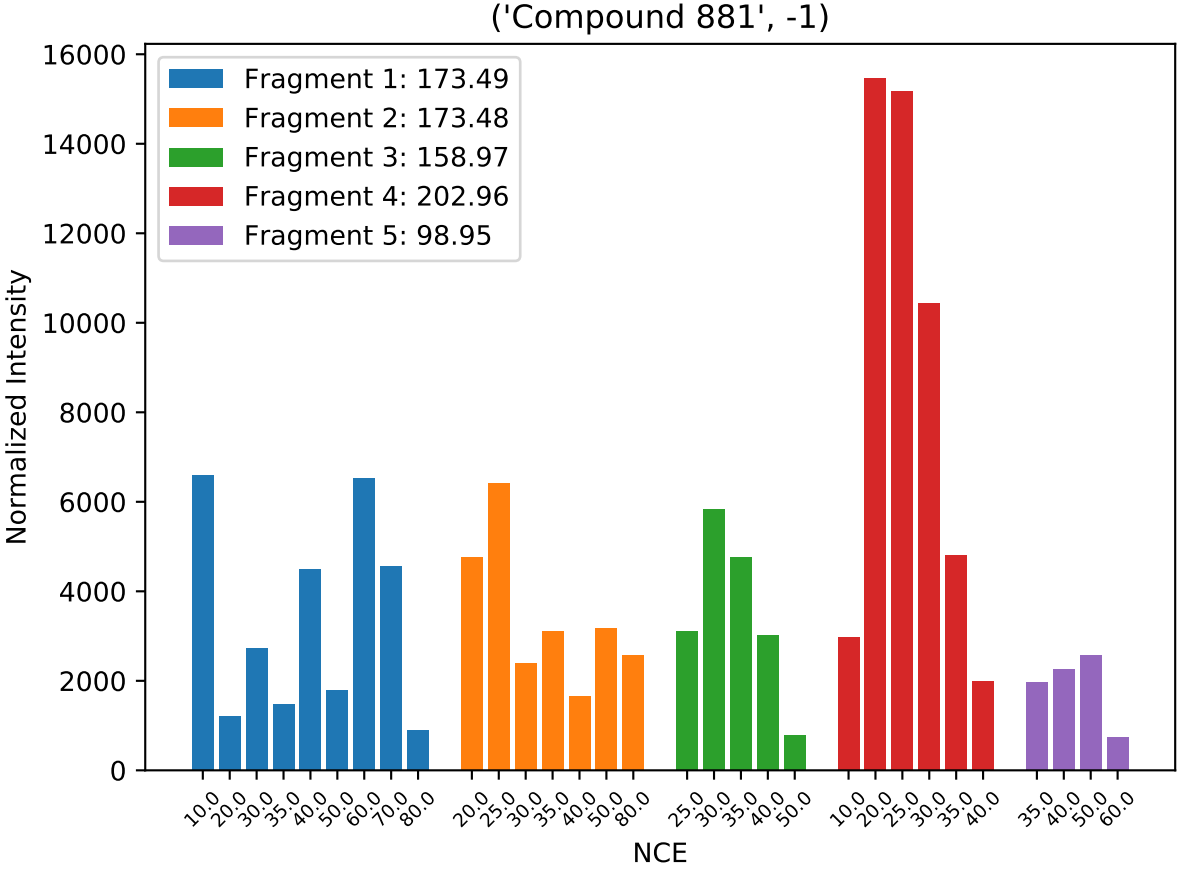

('Compound 872', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 173.47
Fragment 4: 90.75
Fragment 5: 145.09
Normalized Intensity
0
1000
2000
3000
4000
5000
10.0
20.0
25.0
30.0
35.0
40.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
50.0
60.0
70.0
10.0
20.0
25.0
35.0
60.0
30.0
35.0
NCE

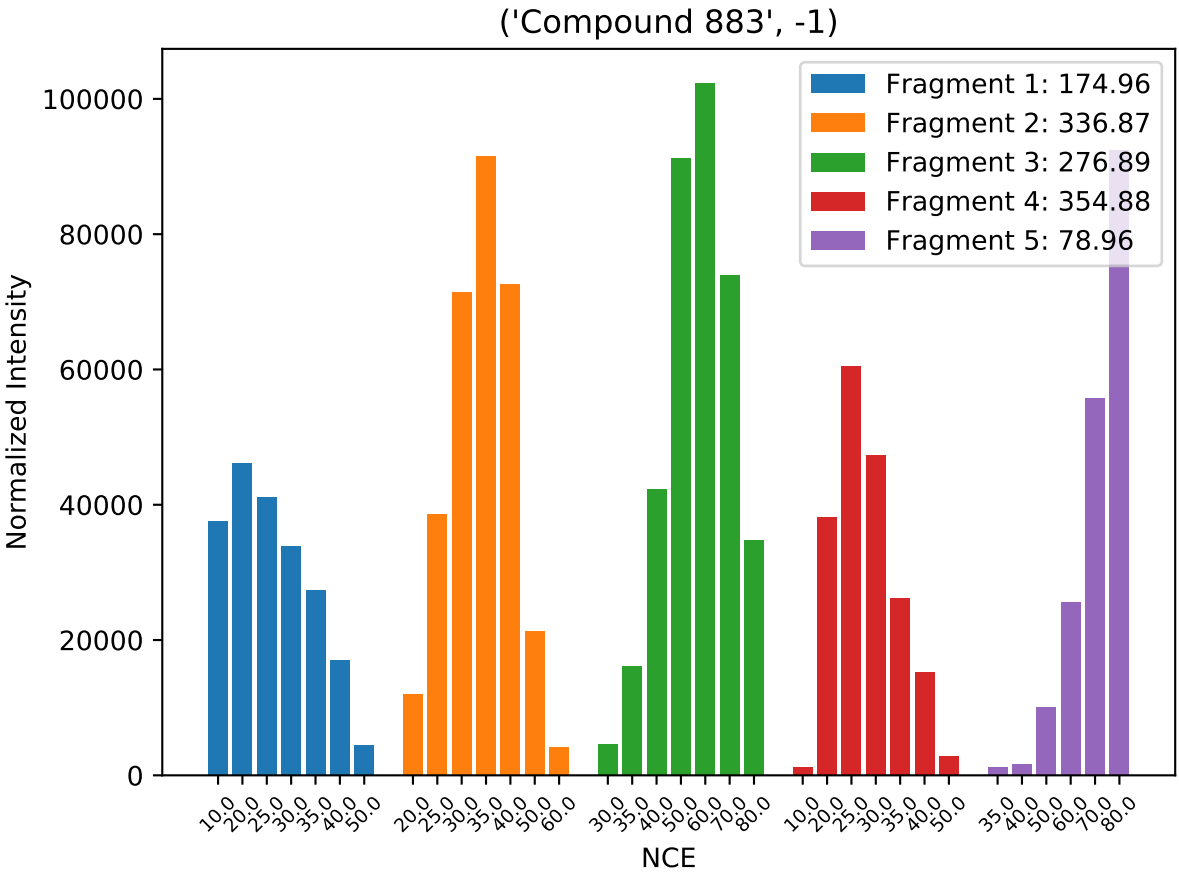

('Compound 876', -1)
Fragment 1: 173.48
Fragment 2: 265.02
Fragment 3: 223.01
Fragment 4: 173.49
Fragment 5: 138.99
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
NCE
10.0 20.0 25.0 30.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 60.0

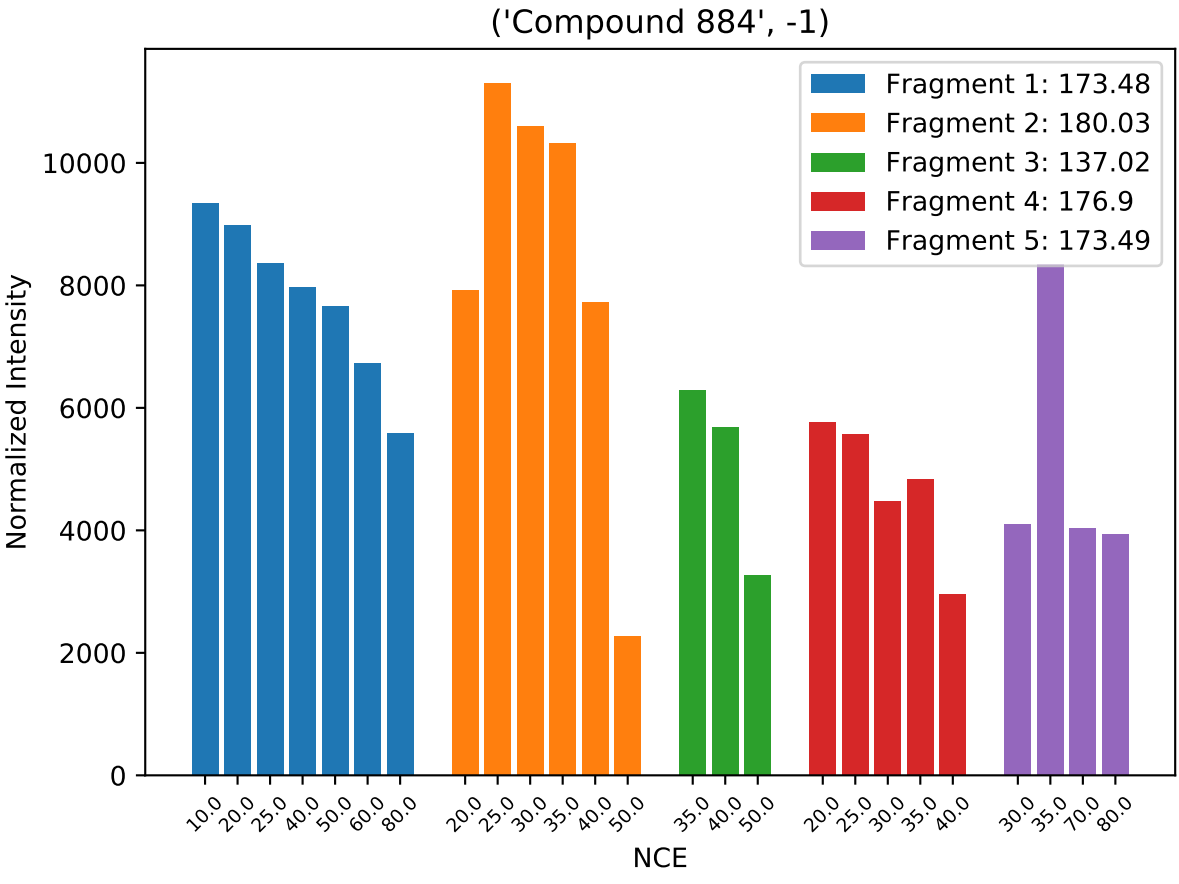

('Compound 288', -1)
Fragment 1: 475.1
Fragment 2: 329.03
Fragment 3: 173.48
Fragment 4: 173.49
Fragment 5: 311.02
Normalized Intensity
0
10000
20000
30000
40000
50000
NCE
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
40.0
70.0
80.0
10.0
20.0
50.0
60.0
70.0
25.0
30.0
35.0
40.0
50.0
60.0

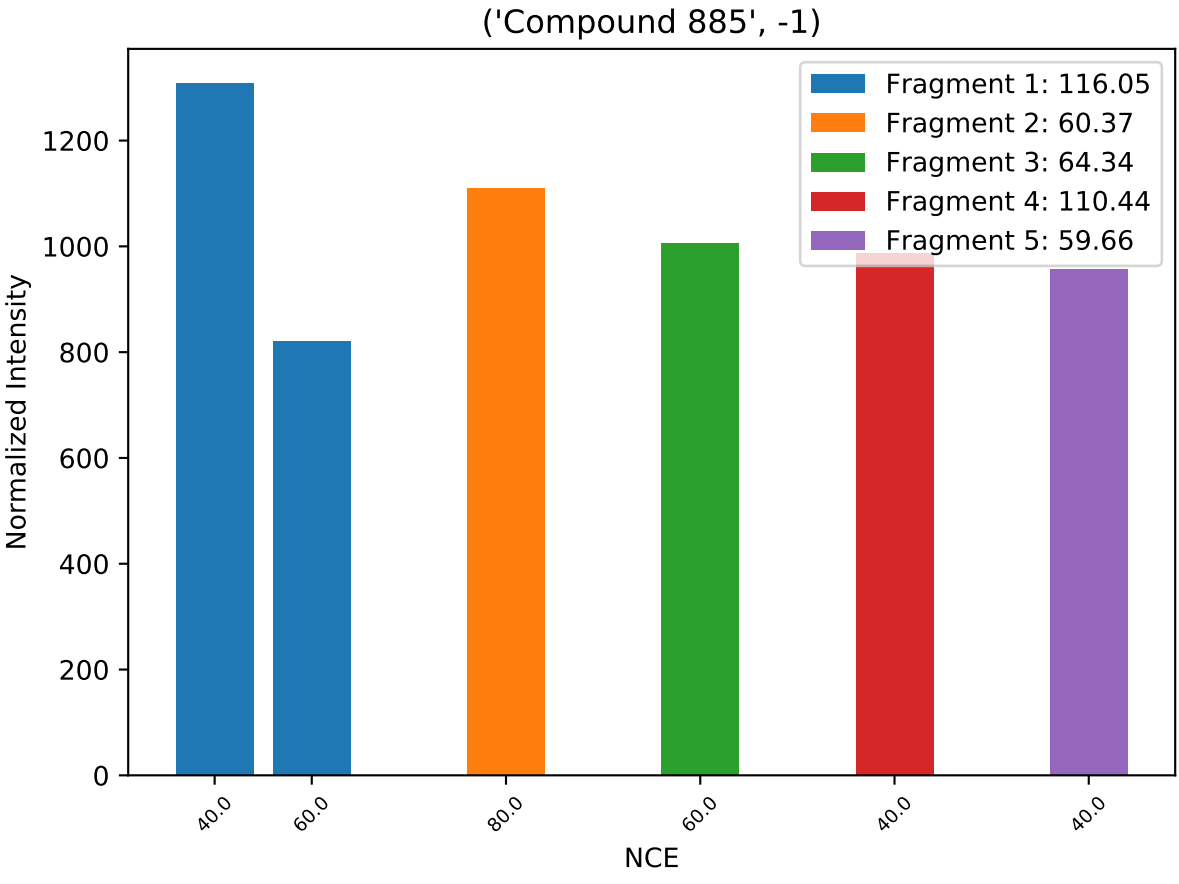

('Compound 877', -1)
Fragment 1: 81.95
Fragment 2: 81.96
Fragment 3: 63.31
Fragment 4: 77.49
Fragment 5: 79.96
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
35.0
50.0
35.0
40.0
50.0
NCE

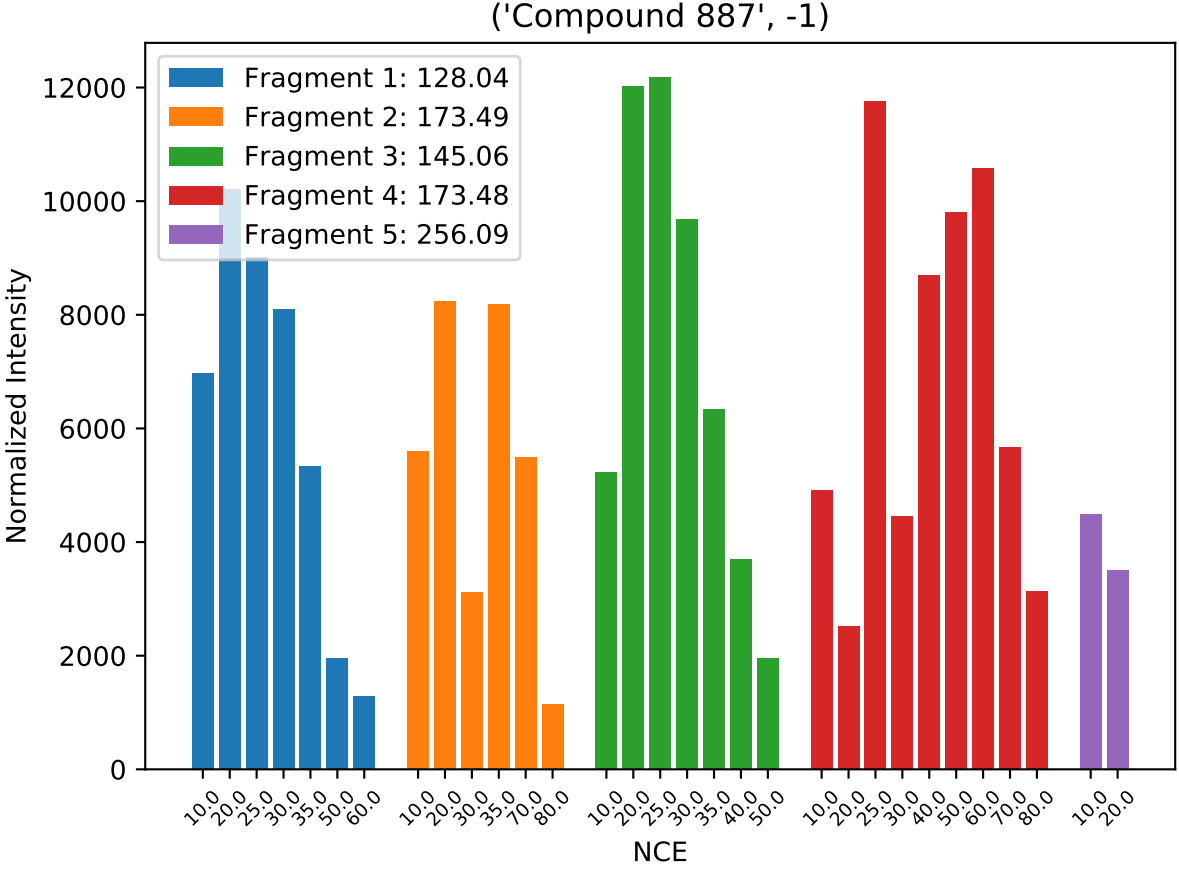

('Compound 878', -1)
Fragment 1: 94.92
Fragment 2: 64.28
Fragment 3: 85.03
Fragment 4: 65.3
Fragment 5: 78.96
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
20.0
30.0
35.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

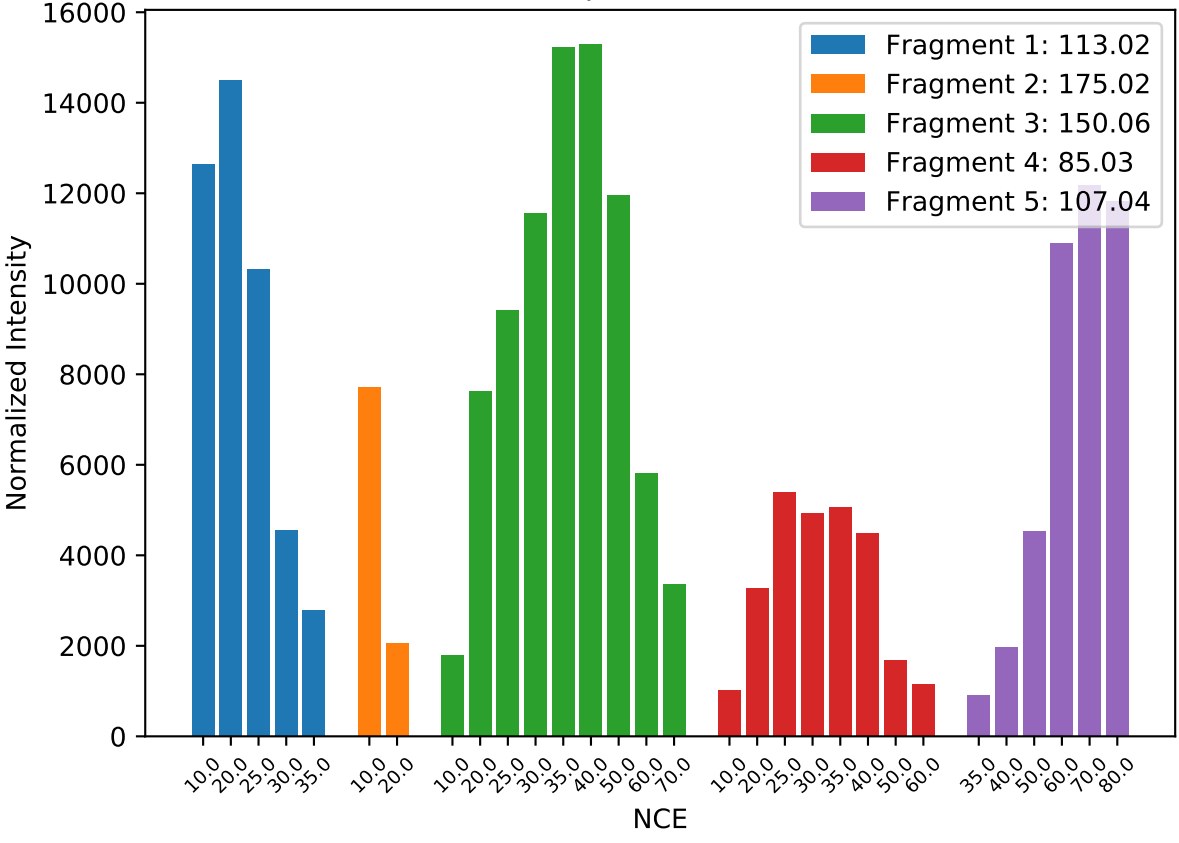

('Compound 881', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 158.97
Fragment 4: 202.96
Fragment 5: 98.95
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0 20.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 80.0
25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0
35.0 40.0 50.0 60.0
NCE

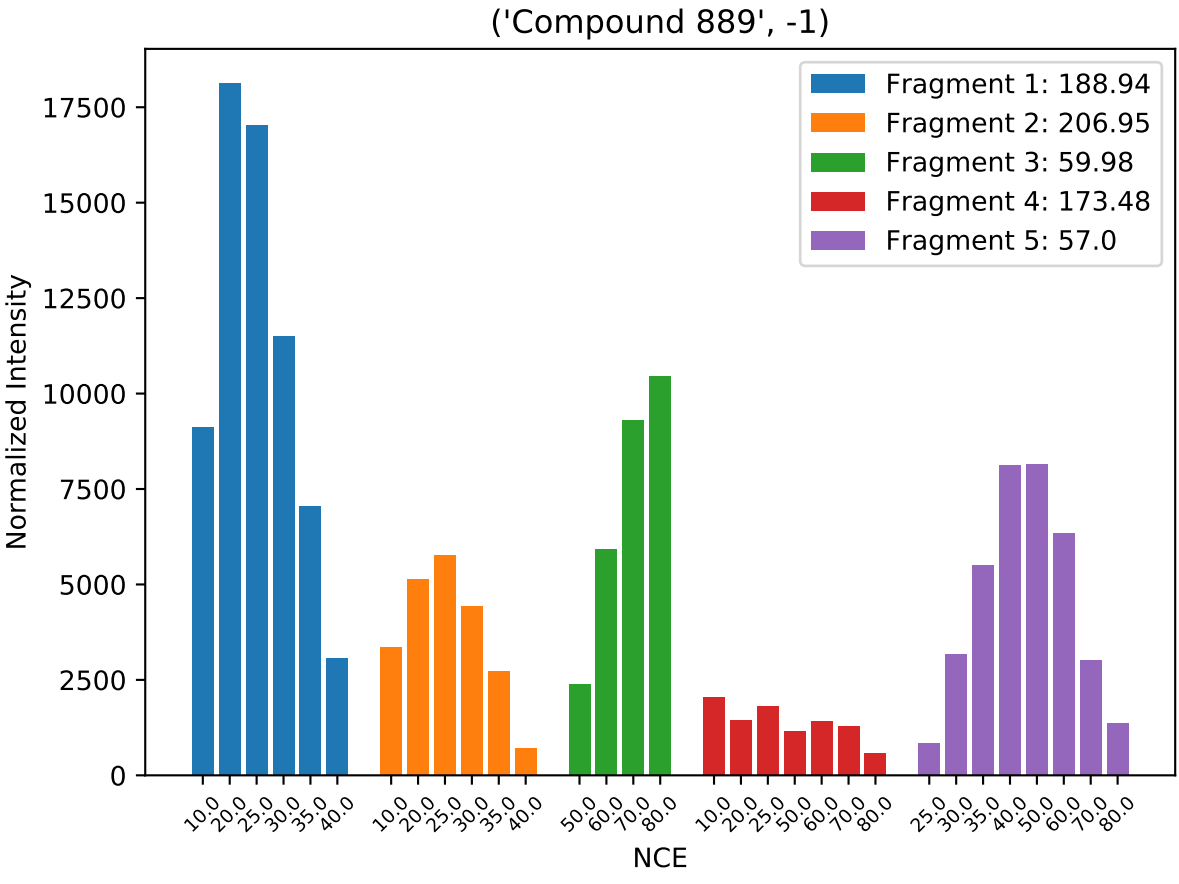

('Compound 883', -1)
Fragment 1: 174.96
Fragment 2: 336.87
Fragment 3: 276.89
Fragment 4: 354.88
Fragment 5: 78.96
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

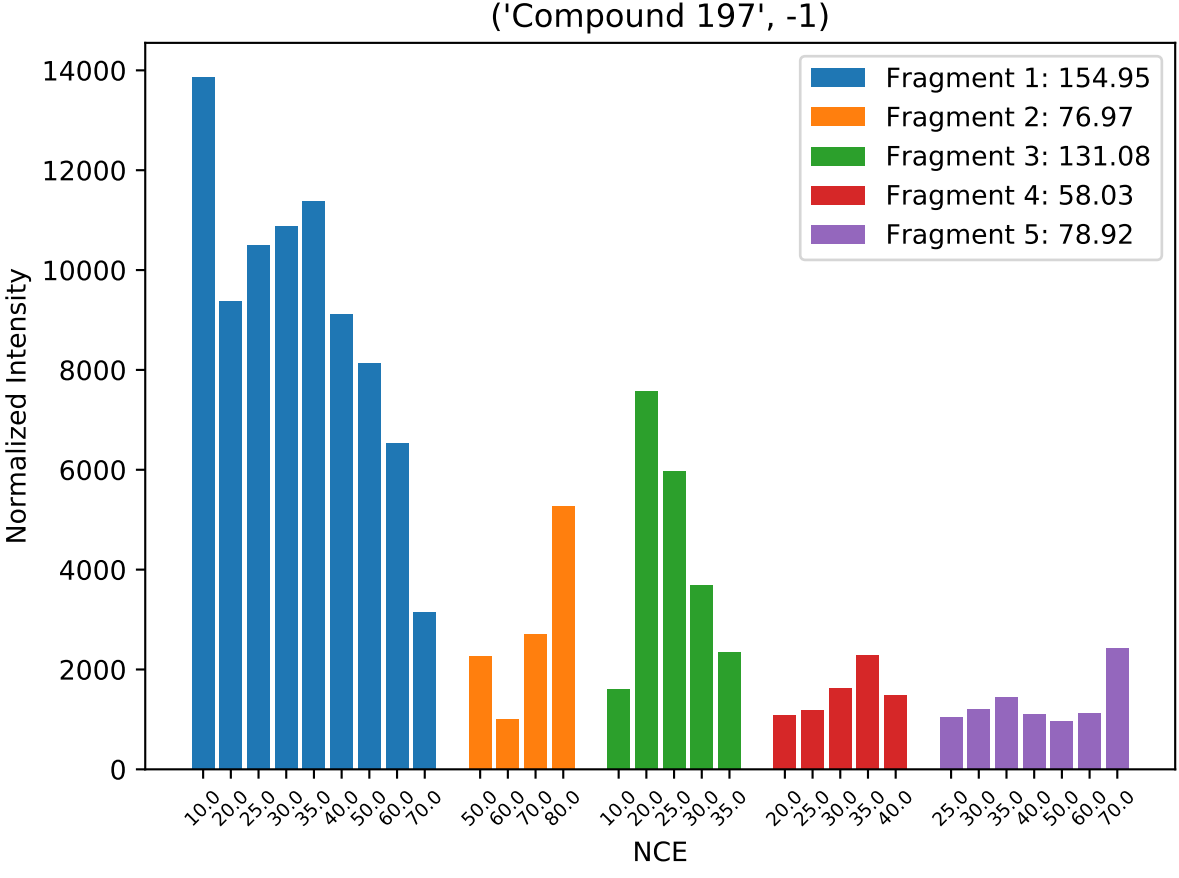

('Compound 884', -1)
Fragment 1: 173.48
Fragment 2: 180.03
Fragment 3: 137.02
Fragment 4: 176.9
Fragment 5: 173.49
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
20.0
25.0
40.0
50.0
60.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
30.0
35.0
70.0
80.0
NCE

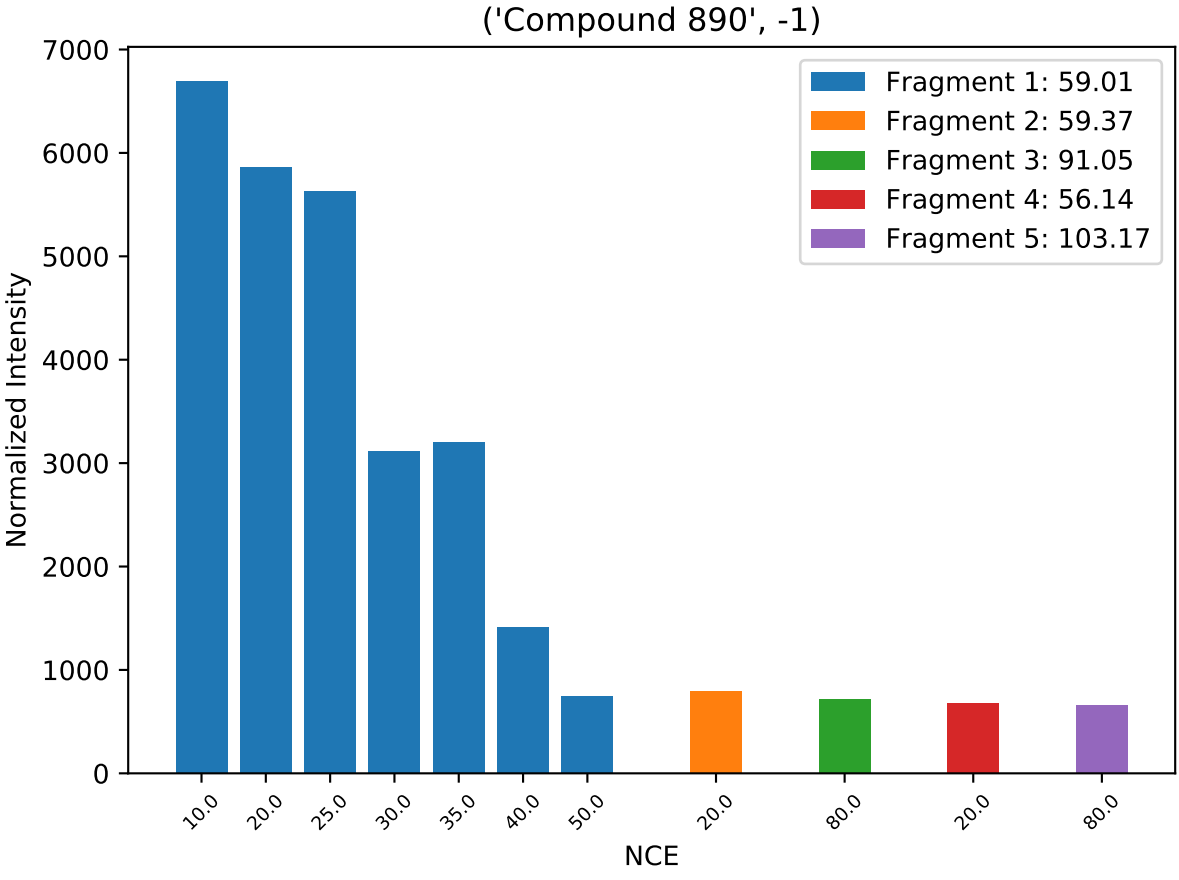

('Compound 885', -1)
Fragment 1: 116.05
Fragment 2: 60.37
Fragment 3: 64.34
Fragment 4: 110.44
Fragment 5: 59.66
Normalized Intensity
0
200
400
600
800
1000
1200
40.0
60.0
80.0
60.0
40.0
40.0
NCE

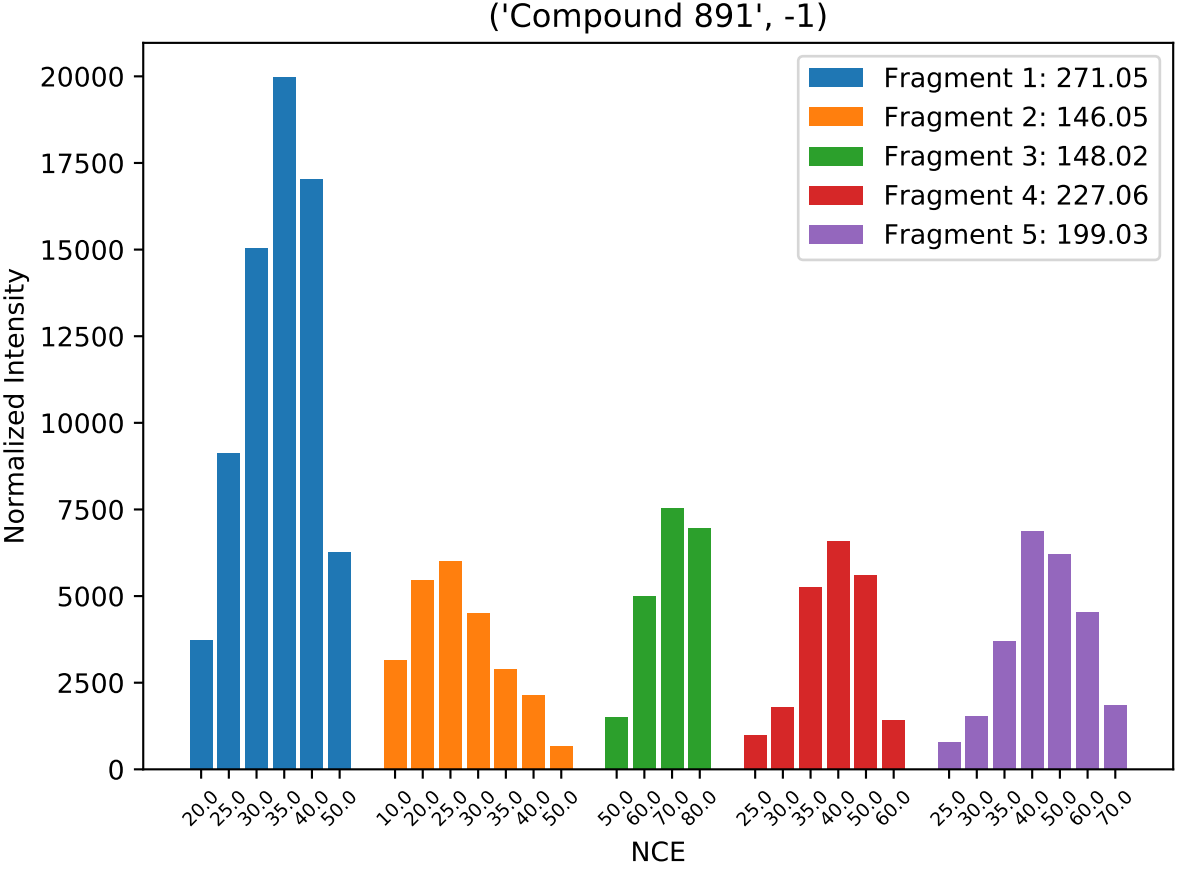

('Compound 887', -1)
Fragment 1: 128.04
Fragment 2: 173.49
Fragment 3: 145.06
Fragment 4: 173.48
Fragment 5: 256.09
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0 20.0 25.0 30.0 35.0 50.0 60.0
10.0 20.0 30.0 35.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0
NCE

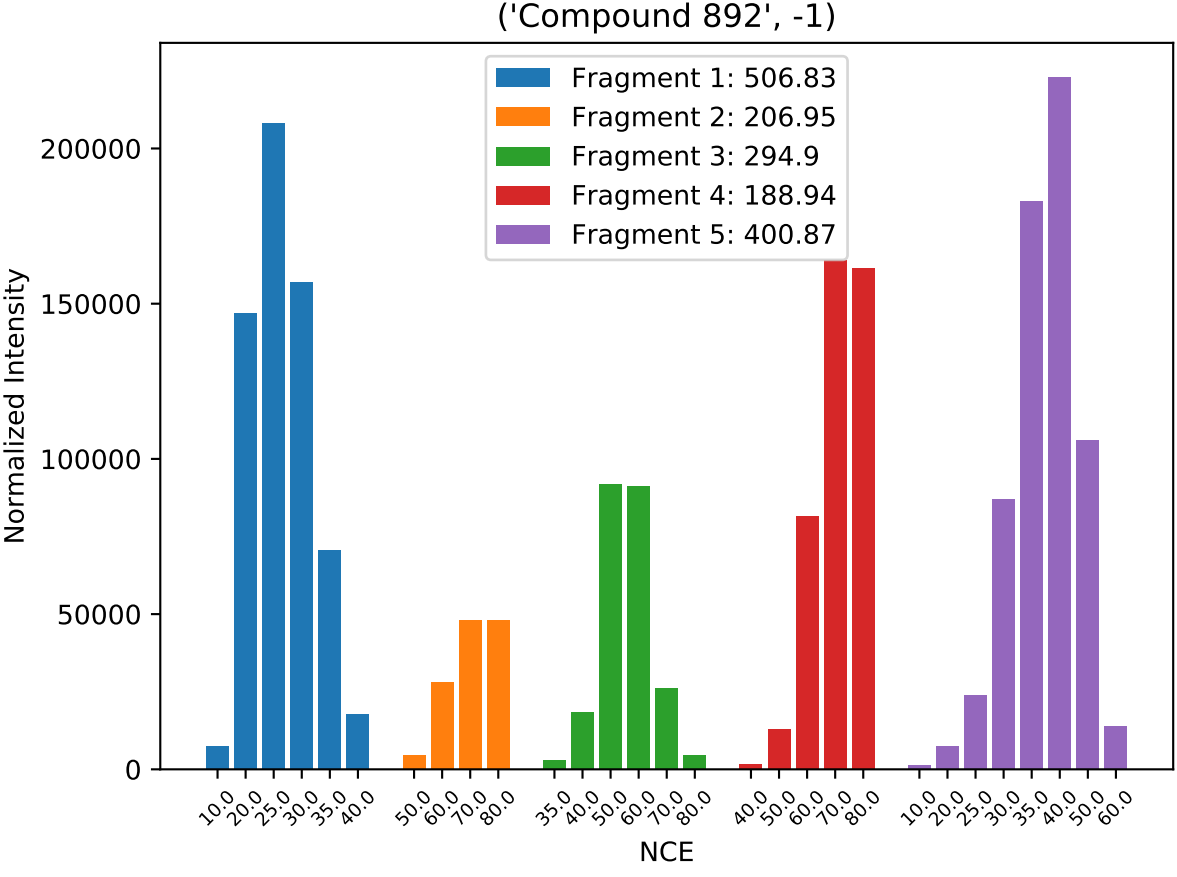

('Compound 888', -1)
Fragment 1: 113.02
Fragment 2: 175.02
Fragment 3: 150.06
Fragment 4: 85.03
Fragment 5: 107.04
Normalized Intensity
NCE
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0 20.0 25.0 30.0 35.0
10.0 20.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
35.0 40.0 50.0 60.0 70.0 80.0

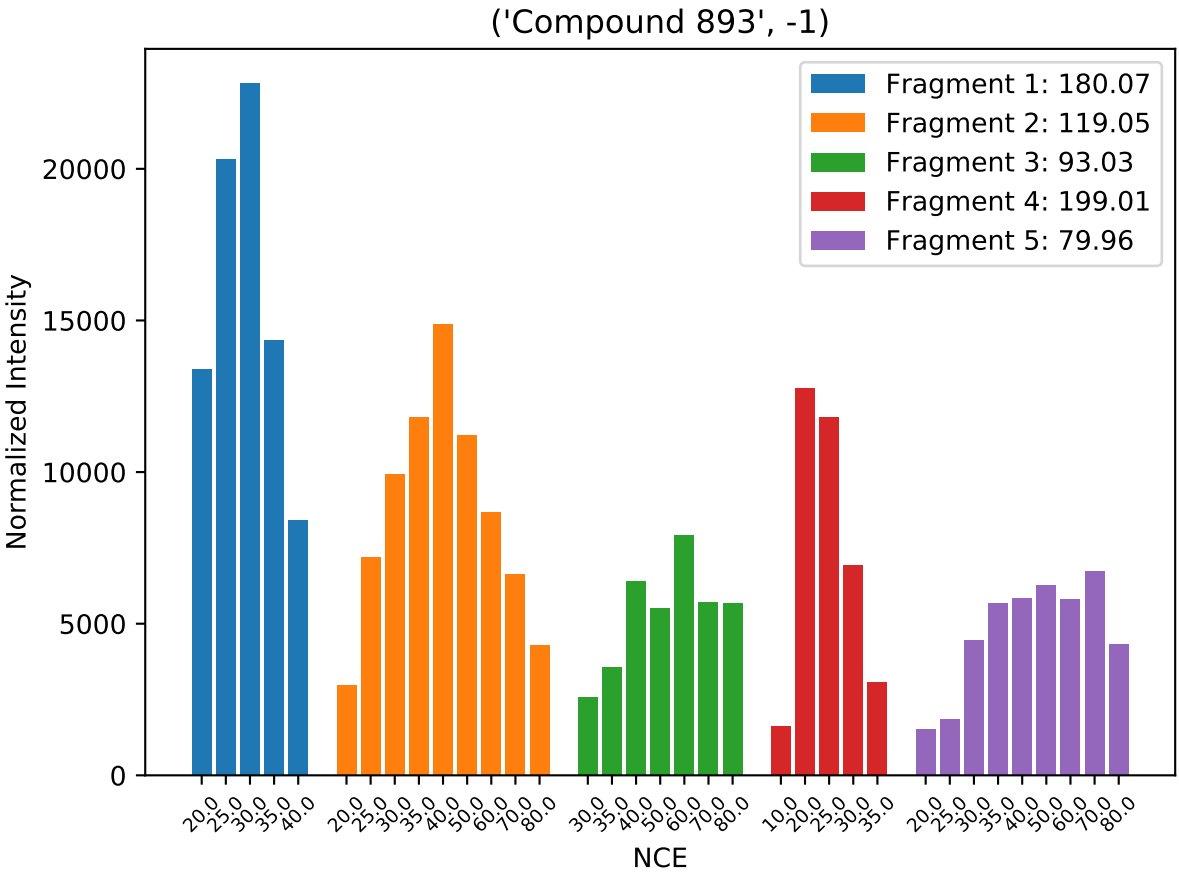

('Compound 889', -1)
Fragment 1: 188.94
Fragment 2: 206.95
Fragment 3: 59.98
Fragment 4: 173.48
Fragment 5: 57.0
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

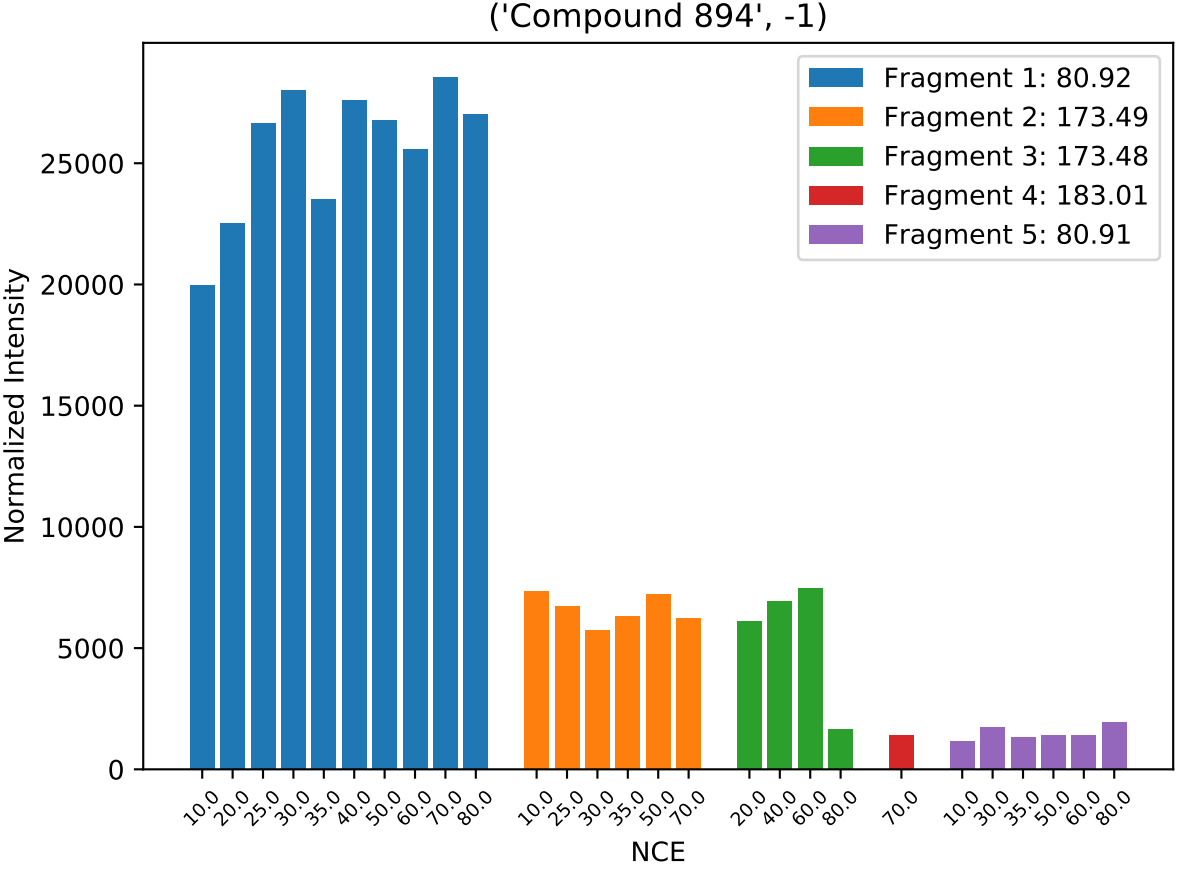

('Compound 197', -1)
Fragment 1: 154.95
Fragment 2: 76.97
Fragment 3: 131.08
Fragment 4: 58.03
Fragment 5: 78.92
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

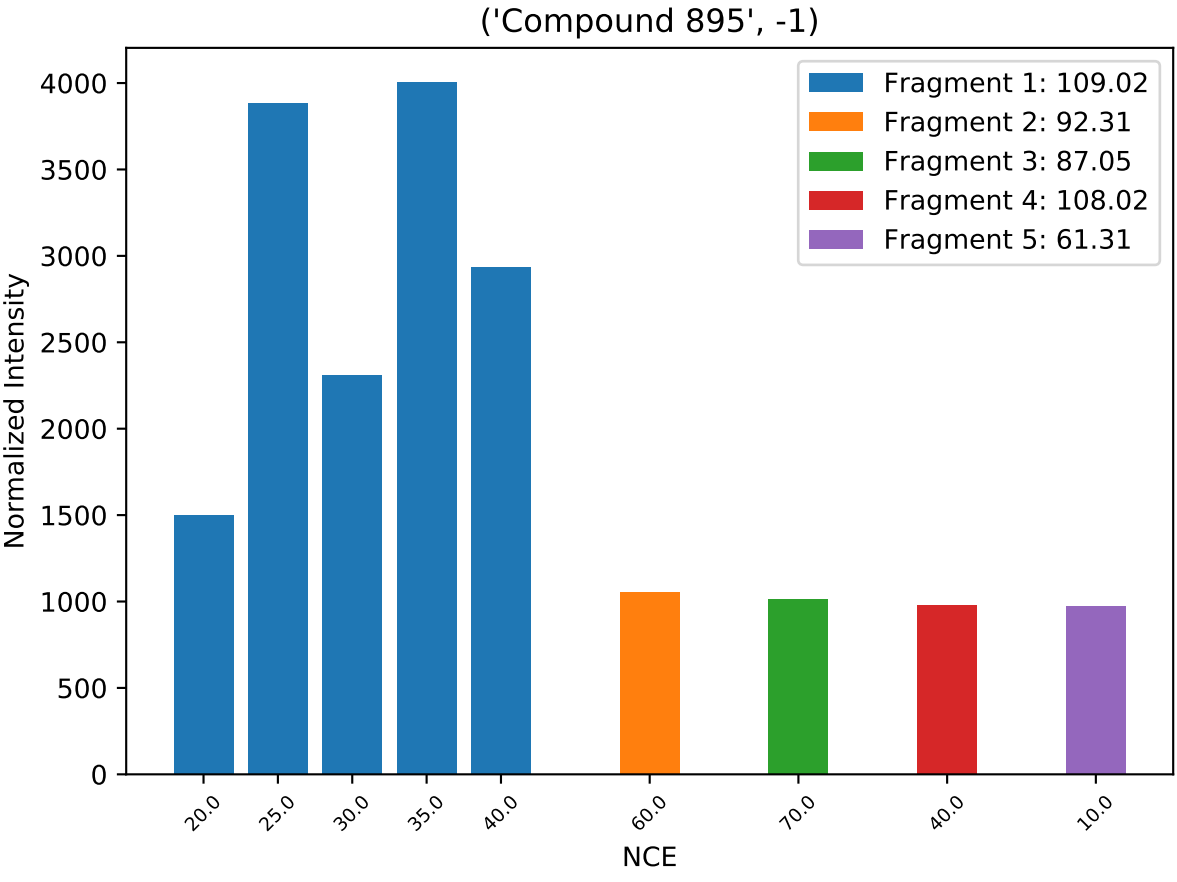

('Compound 890', -1)
Fragment 1: 59.01
Fragment 2: 59.37
Fragment 3: 91.05
Fragment 4: 56.14
Fragment 5: 103.17
Normalized Intensity
7000
6000
5000
4000
3000
2000
1000
0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
80.0
20.0
80.0
NCE

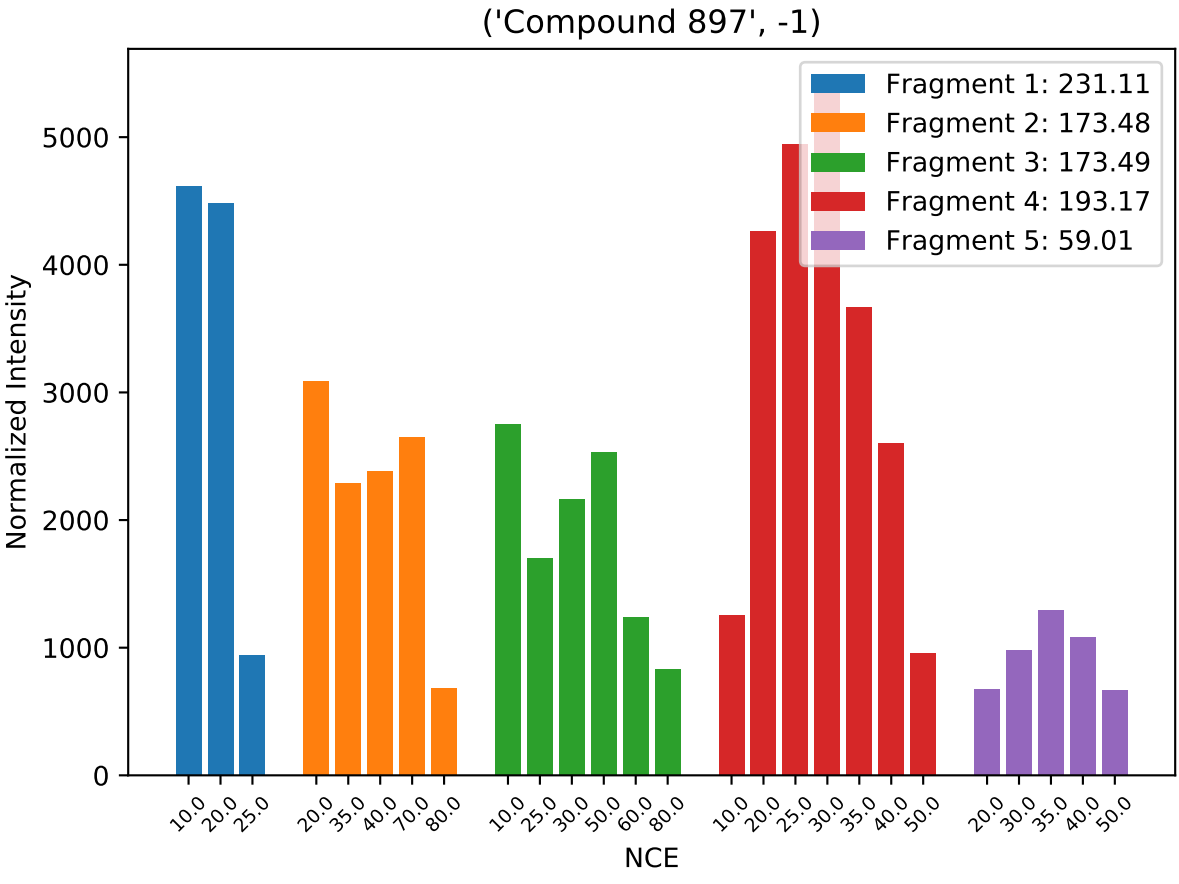

('Compound 891', -1)
Fragment 1: 271.05
Fragment 2: 146.05
Fragment 3: 148.02
Fragment 4: 227.06
Fragment 5: 199.03
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

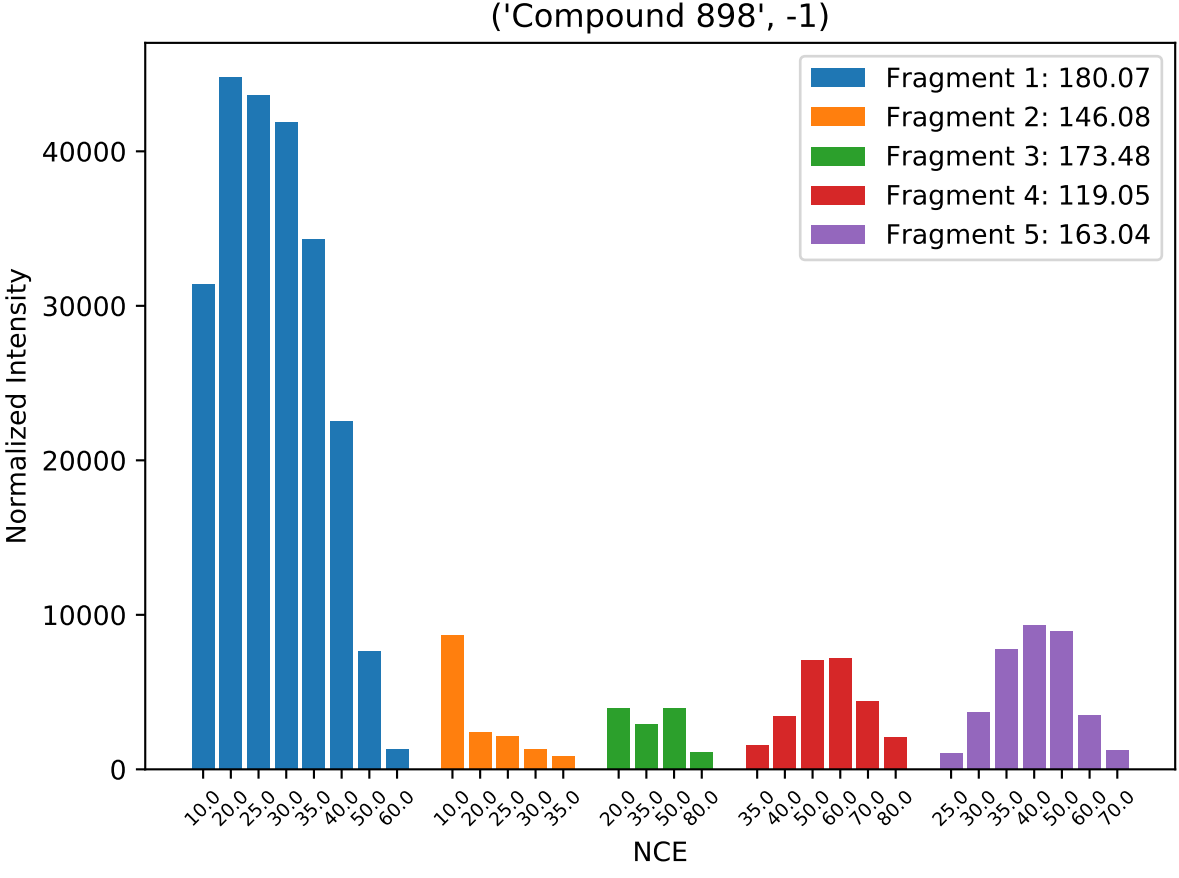

('Compound 892', -1)
Fragment 1: 506.83
Fragment 2: 206.95
Fragment 3: 294.9
Fragment 4: 188.94
Fragment 5: 400.87
Normalized Intensity
0
50000
100000
150000
200000
10.0 20.0 25.0 30.0 35.0 40.0
50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

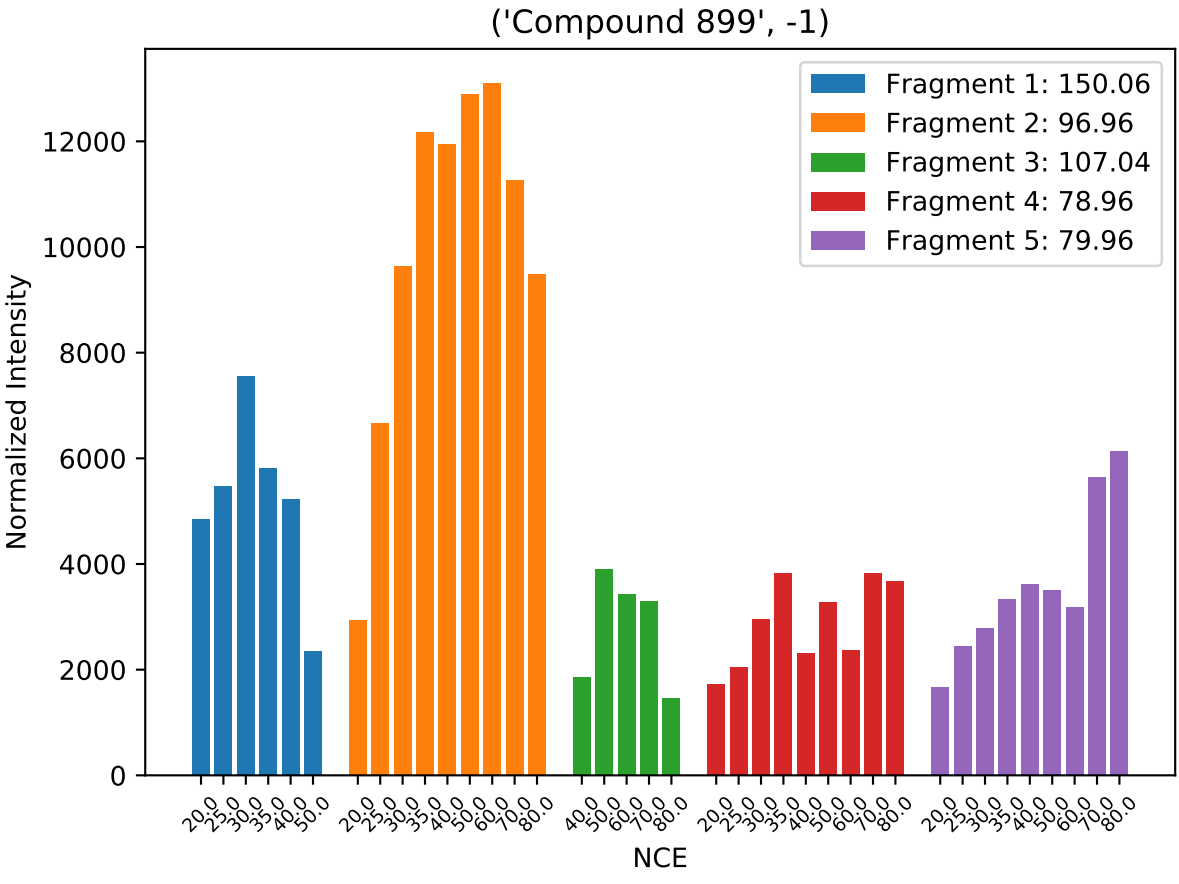

('Compound 893', -1)
Fragment 1: 180.07
Fragment 2: 119.05
Fragment 3: 93.03
Fragment 4: 199.01
Fragment 5: 79.96
Normalized Intensity
0
5000
10000
15000
20000
20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

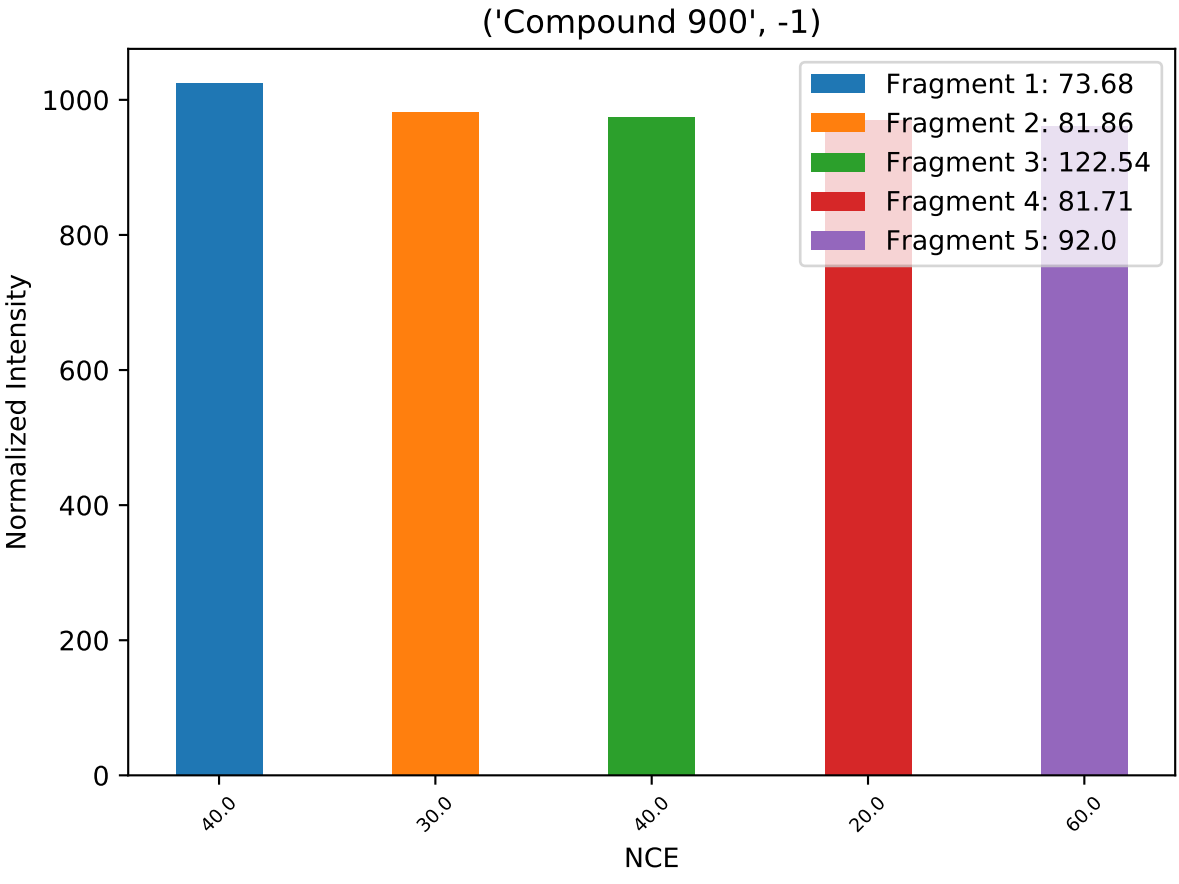

('Compound 894', -1)
Fragment 1: 80.92
Fragment 2: 173.49
Fragment 3: 173.48
Fragment 4: 183.01
Fragment 5: 80.91
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
25.0
30.0
35.0
50.0
70.0
20.0
40.0
60.0
80.0
70.0
10.0
30.0
35.0
50.0
60.0
80.0
NCE

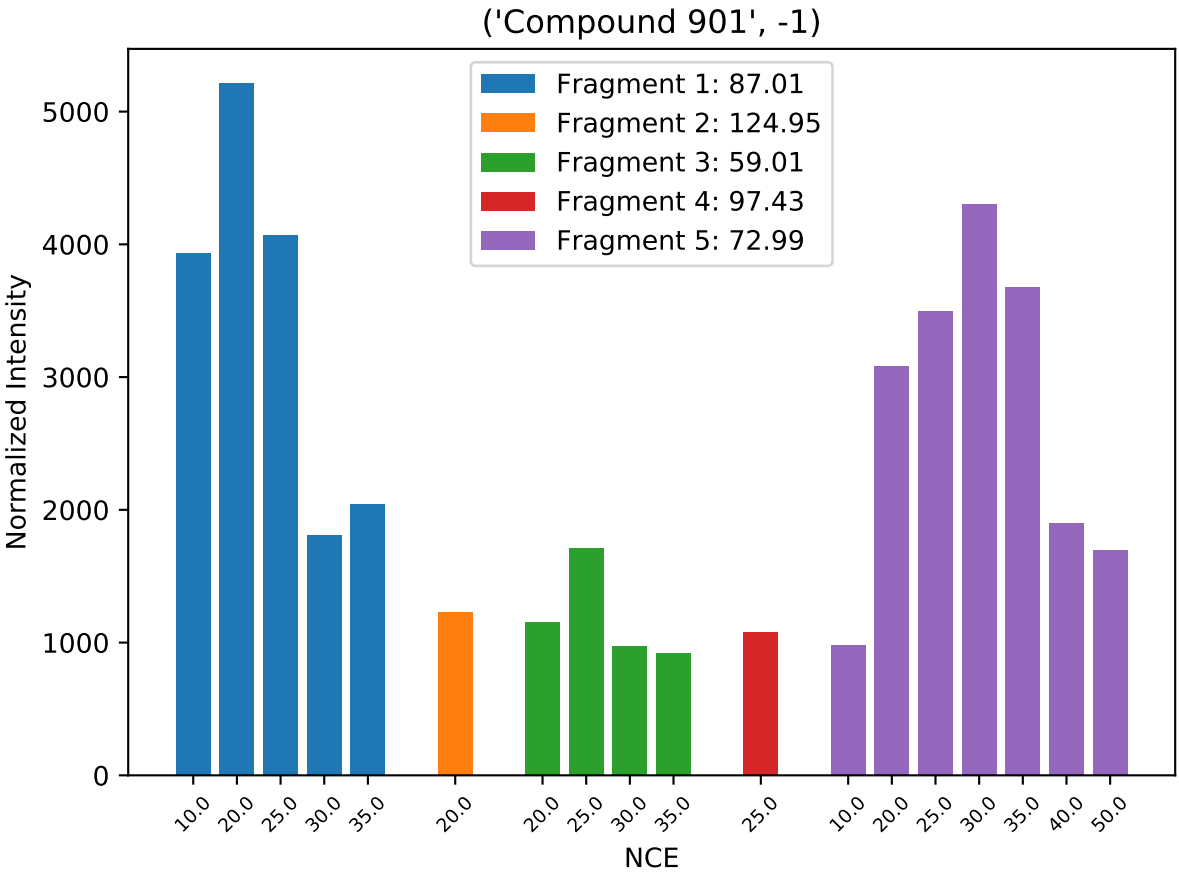

('Compound 895', -1)
Fragment 1: 109.02
Fragment 2: 92.31
Fragment 3: 87.05
Fragment 4: 108.02
Fragment 5: 61.31
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
20.0
25.0
30.0
35.0
40.0
60.0
70.0
40.0
10.0
NCE

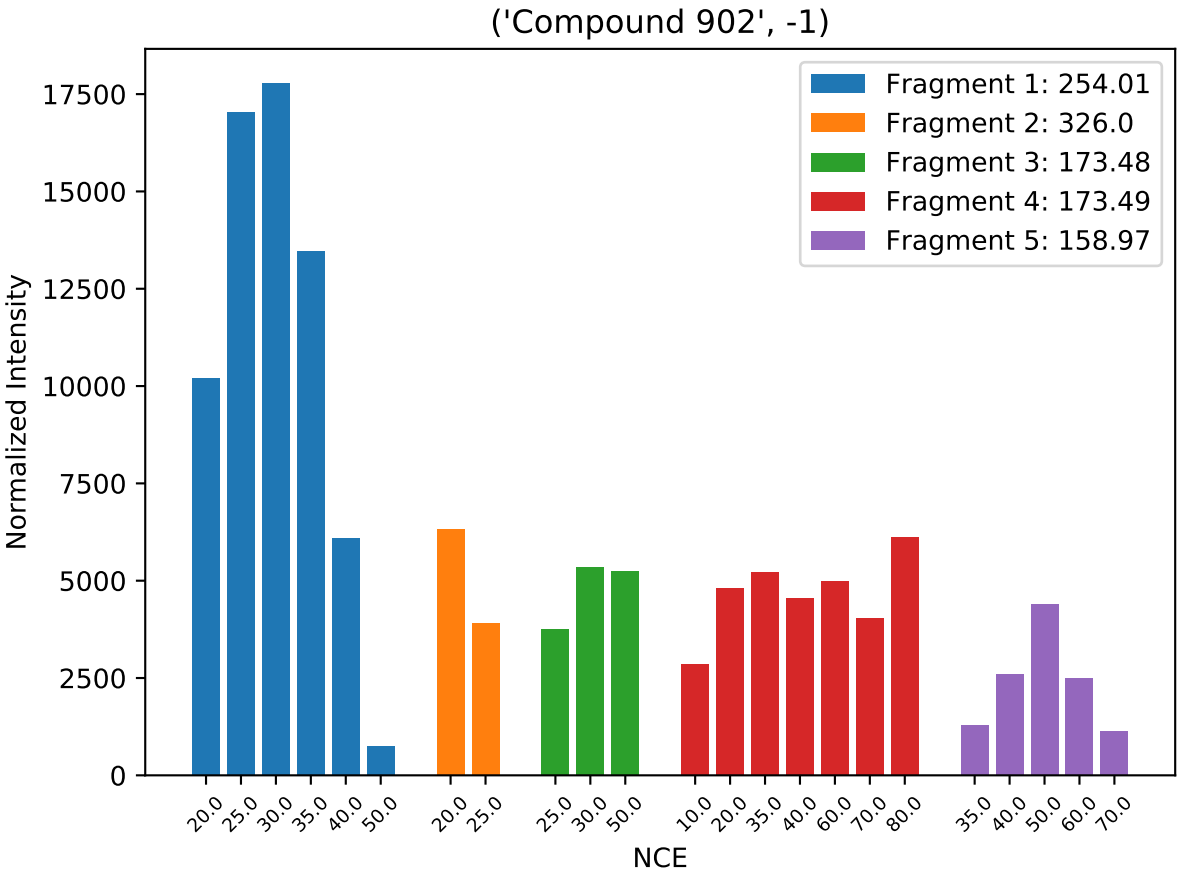

('Compound 897', -1)
Fragment 1: 231.11
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 193.17
Fragment 5: 59.01
Normalized Intensity
0
1000
2000
3000
4000
5000
10.0 20.0 25.0
20.0 35.0 40.0 70.0 80.0
10.0 25.0 30.0 50.0 60.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 30.0 35.0 40.0 50.0
NCE

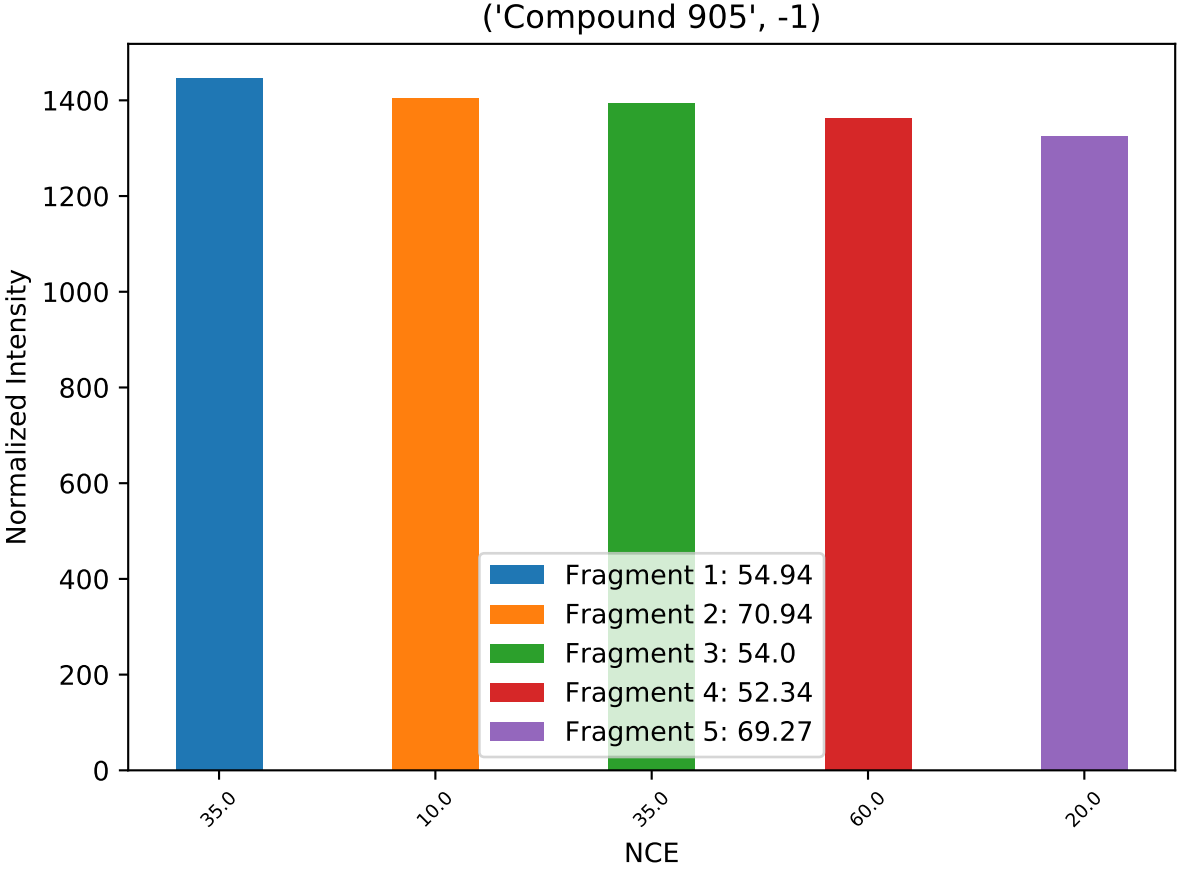

('Compound 898', -1)
Fragment 1: 180.07
Fragment 2: 146.08
Fragment 3: 173.48
Fragment 4: 119.05
Fragment 5: 163.04
Normalized Intensity
0
10000
20000
30000
40000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0
20.0 35.0 50.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
NCE

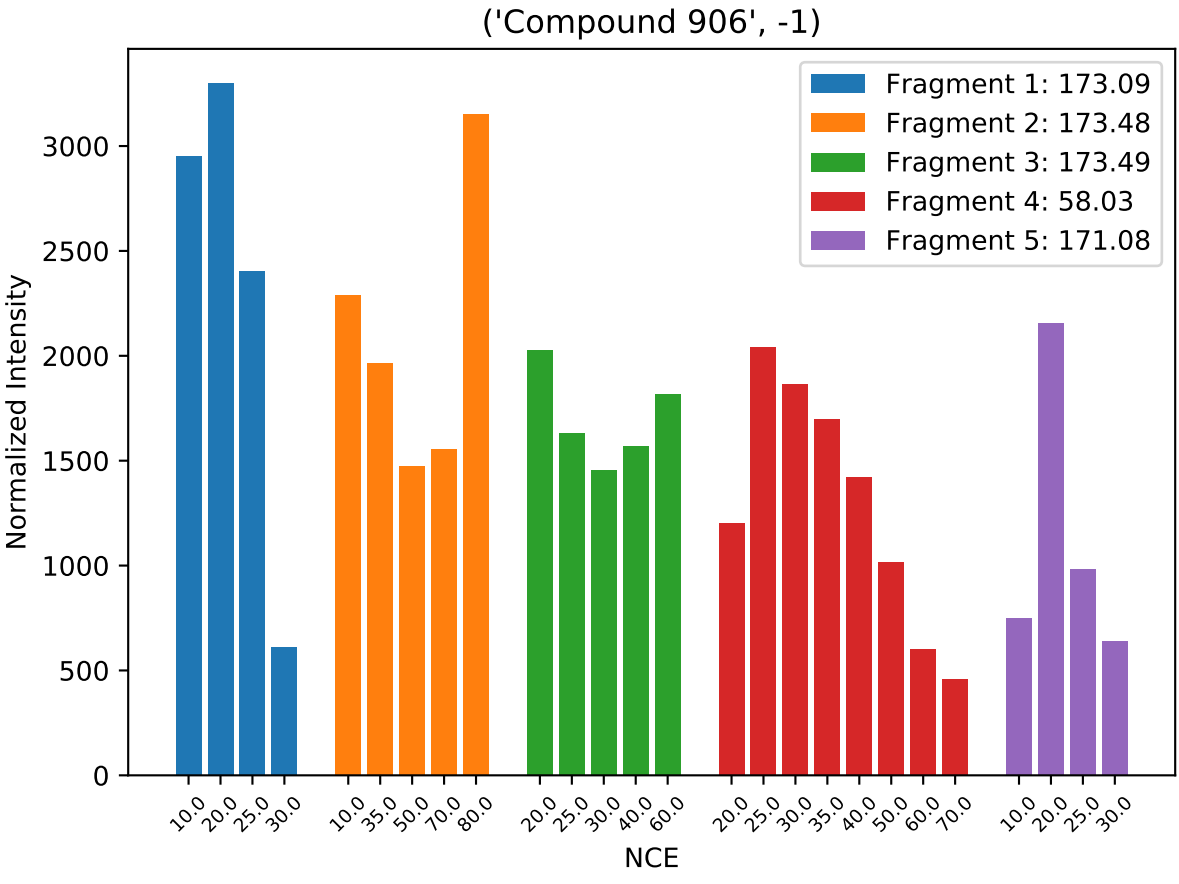

('Compound 899', -1)
Fragment 1: 150.06
Fragment 2: 96.96
Fragment 3: 107.04
Fragment 4: 78.96
Fragment 5: 79.96
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

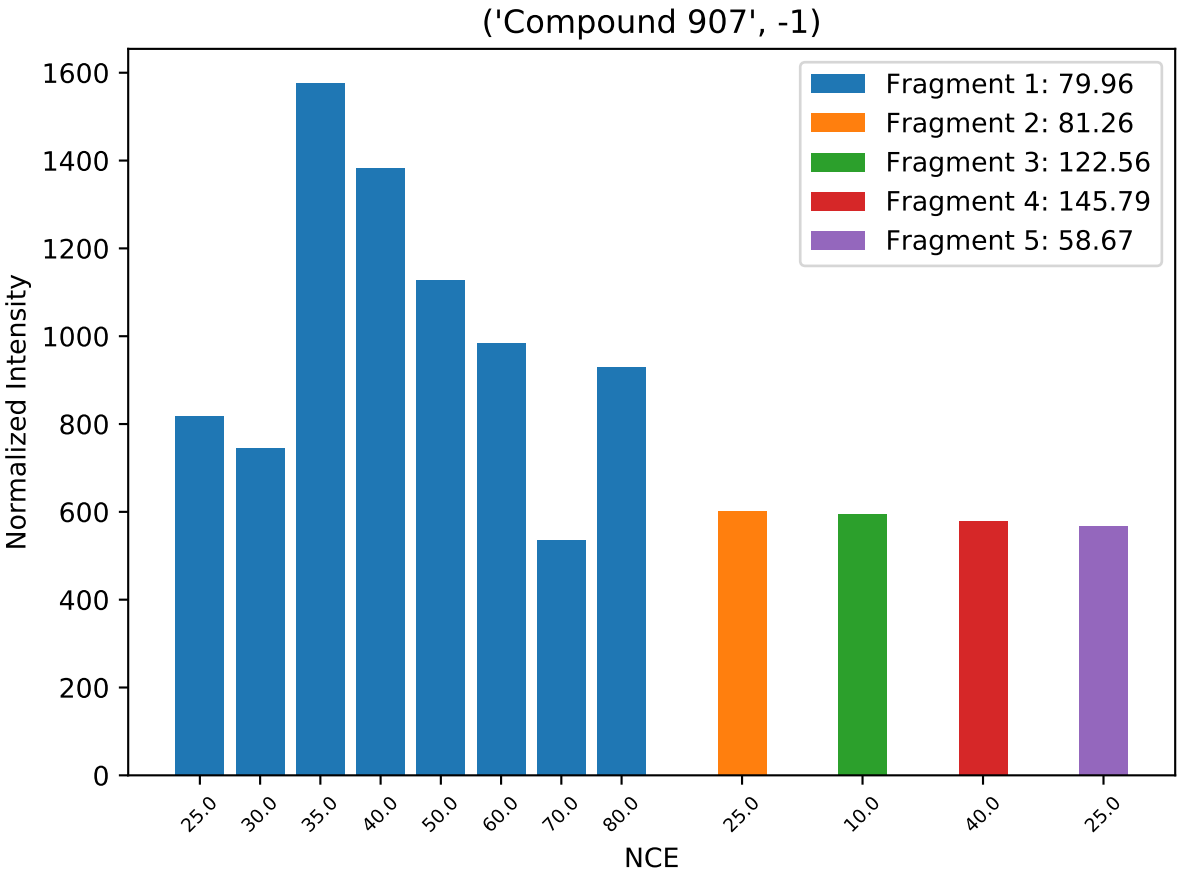

('Compound 900', -1)
Fragment 1: 73.68
Fragment 2: 81.86
Fragment 3: 122.54
Fragment 4: 81.71
Fragment 5: 92.0
Normalized Intensity
0
200
400
600
800
1000
40.0
30.0
40.0
20.0
60.0
NCE

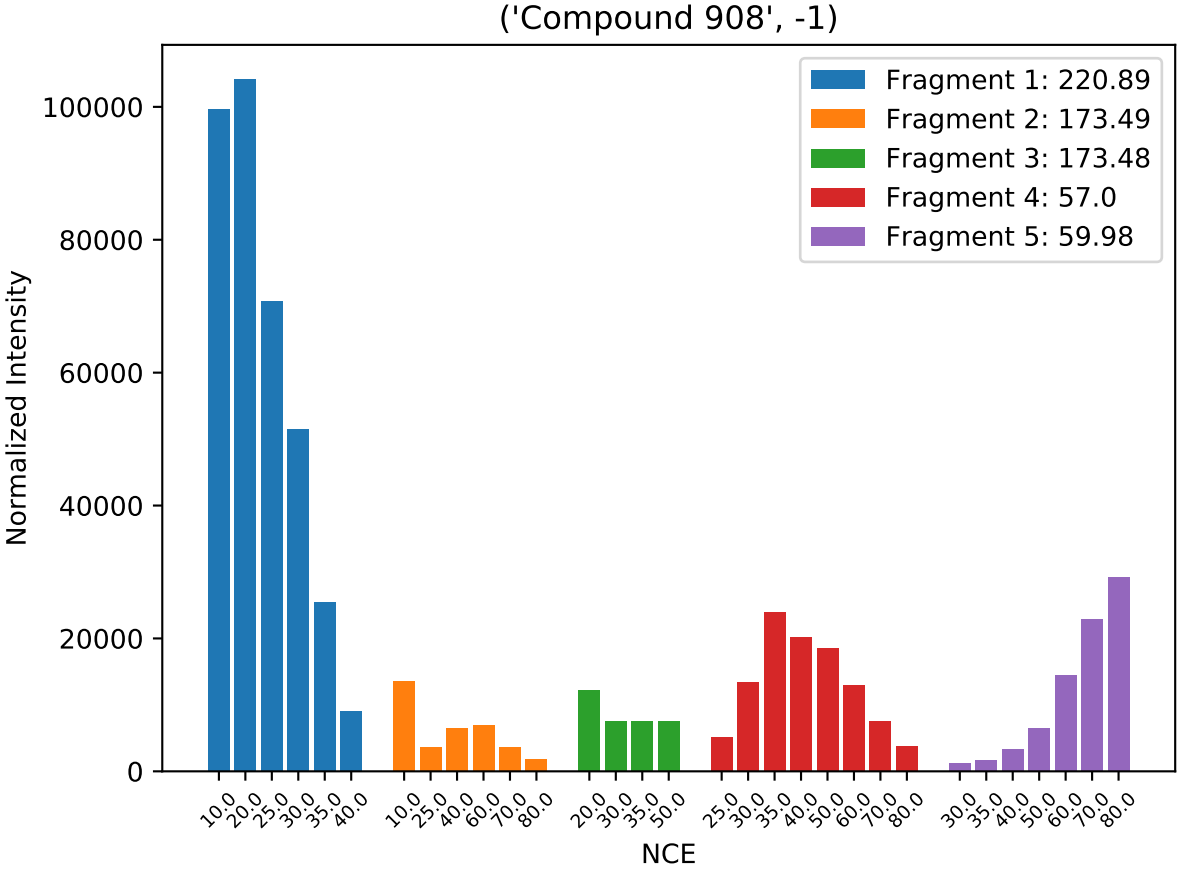

('Compound 901', -1)
Fragment 1: 87.01
Fragment 2: 124.95
Fragment 3: 59.01
Fragment 4: 97.43
Fragment 5: 72.99
Normalized Intensity
0
1000
2000
3000
4000
5000
10.0
20.0
25.0
30.0
35.0
20.0
20.0
25.0
30.0
35.0
25.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
NCE

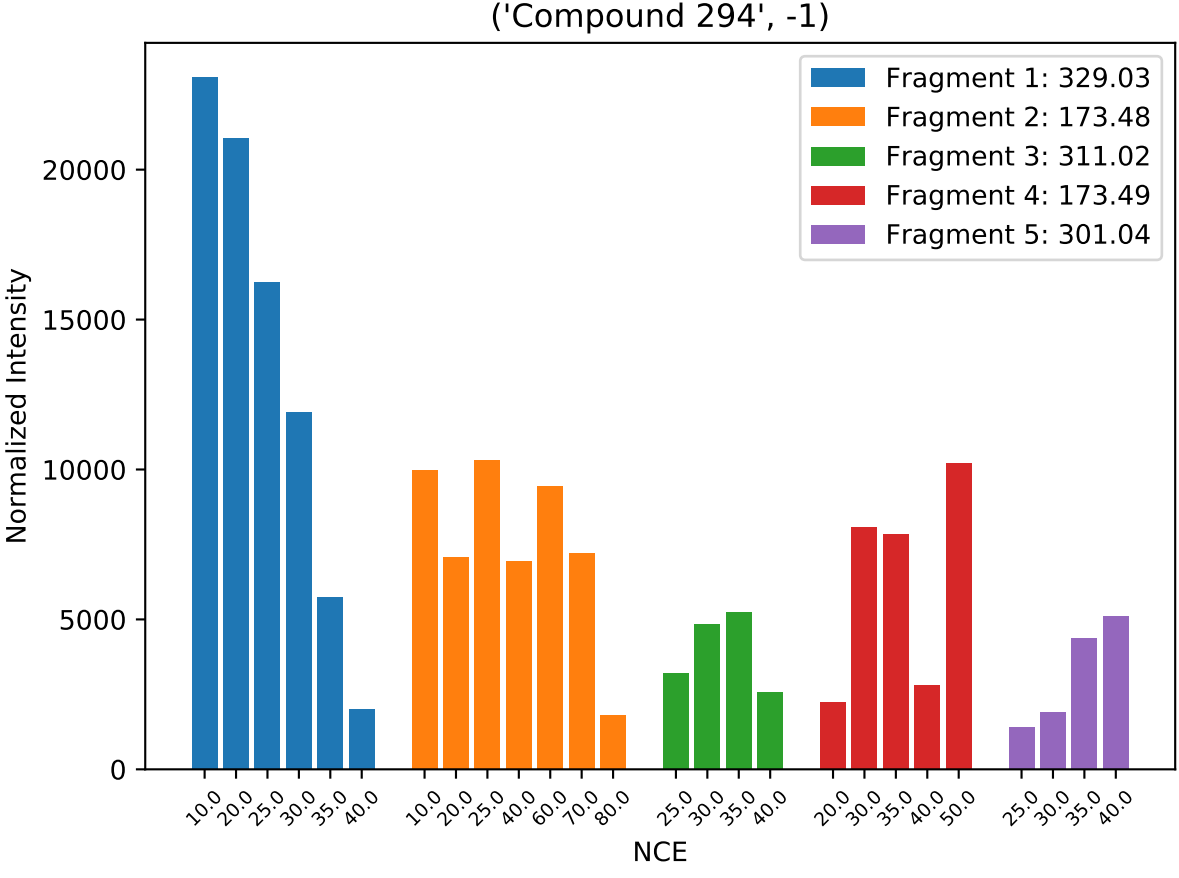

('Compound 902', -1)
Fragment 1: 254.01
Fragment 2: 326.0
Fragment 3: 173.48
Fragment 4: 173.49
Fragment 5: 158.97
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
25.0
30.0
50.0
10.0
20.0
35.0
40.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
NCE

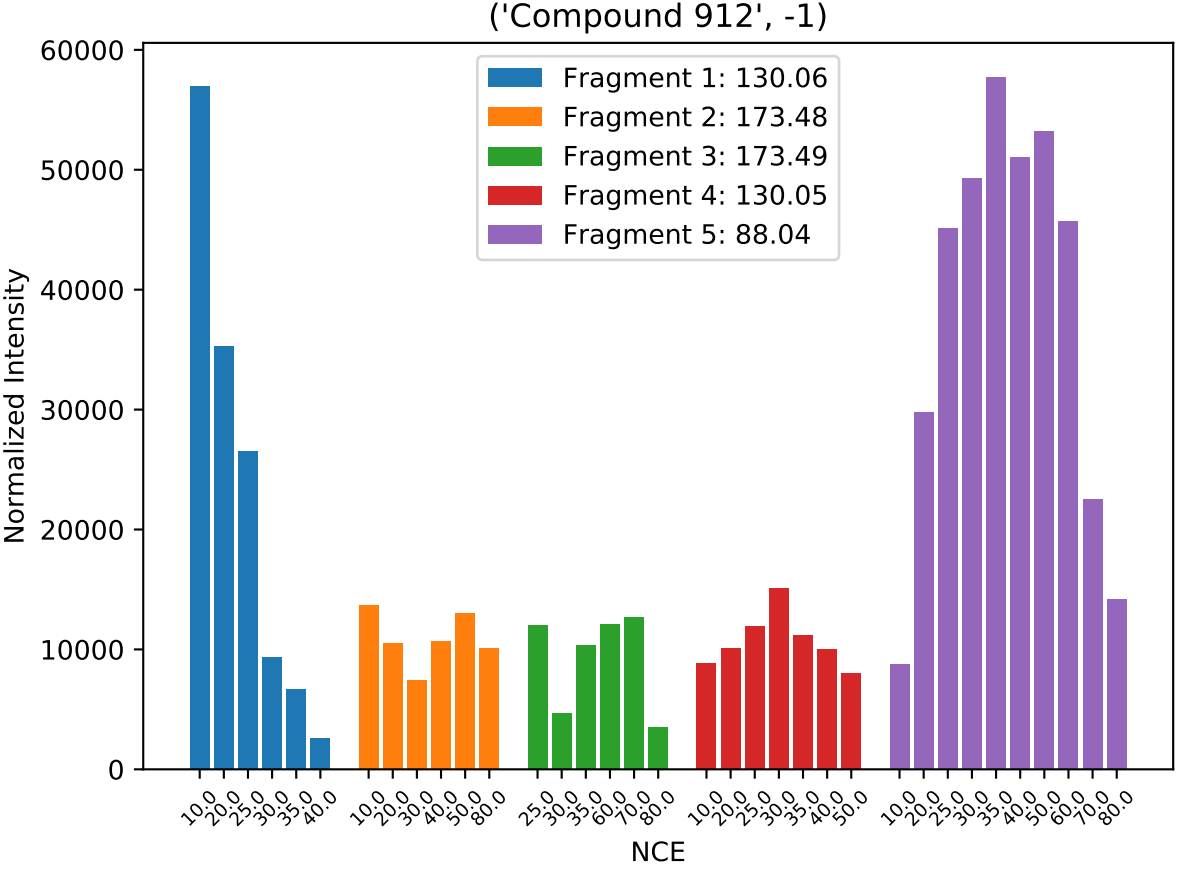

('Compound 905', -1)
Normalized Intensity
0
200
400
600
800
1000
1200
1400
Fragment 1: 54.94
Fragment 2: 70.94
Fragment 3: 54.0
Fragment 4: 52.34
Fragment 5: 69.27
35.0
10.0
35.0
60.0
20.0
NCE

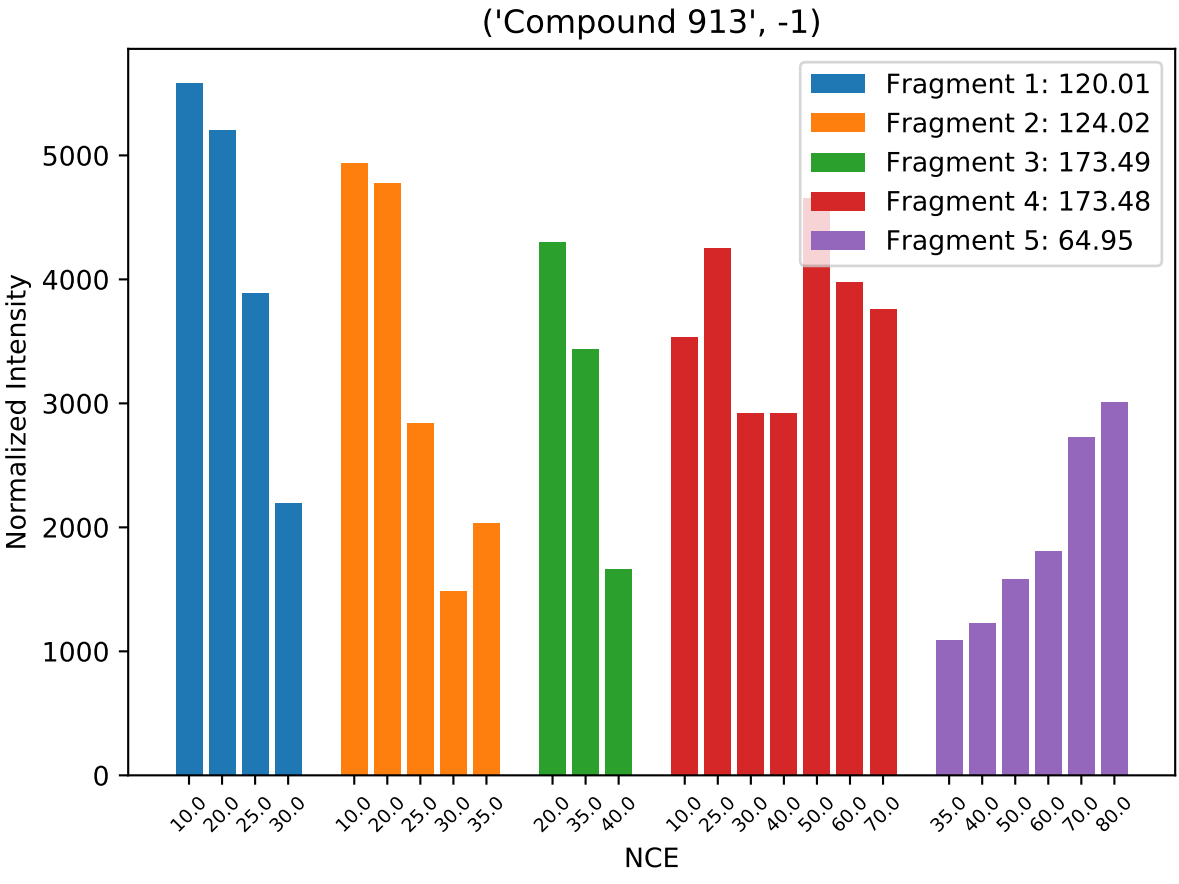

('Compound 906', -1)
Fragment 1: 173.09
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 58.03
Fragment 5: 171.08
Normalized Intensity
0
500
1000
1500
2000
2500
3000
10.0
20.0
25.0
30.0
10.0
35.0
50.0
70.0
80.0
20.0
25.0
30.0
40.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
NCE

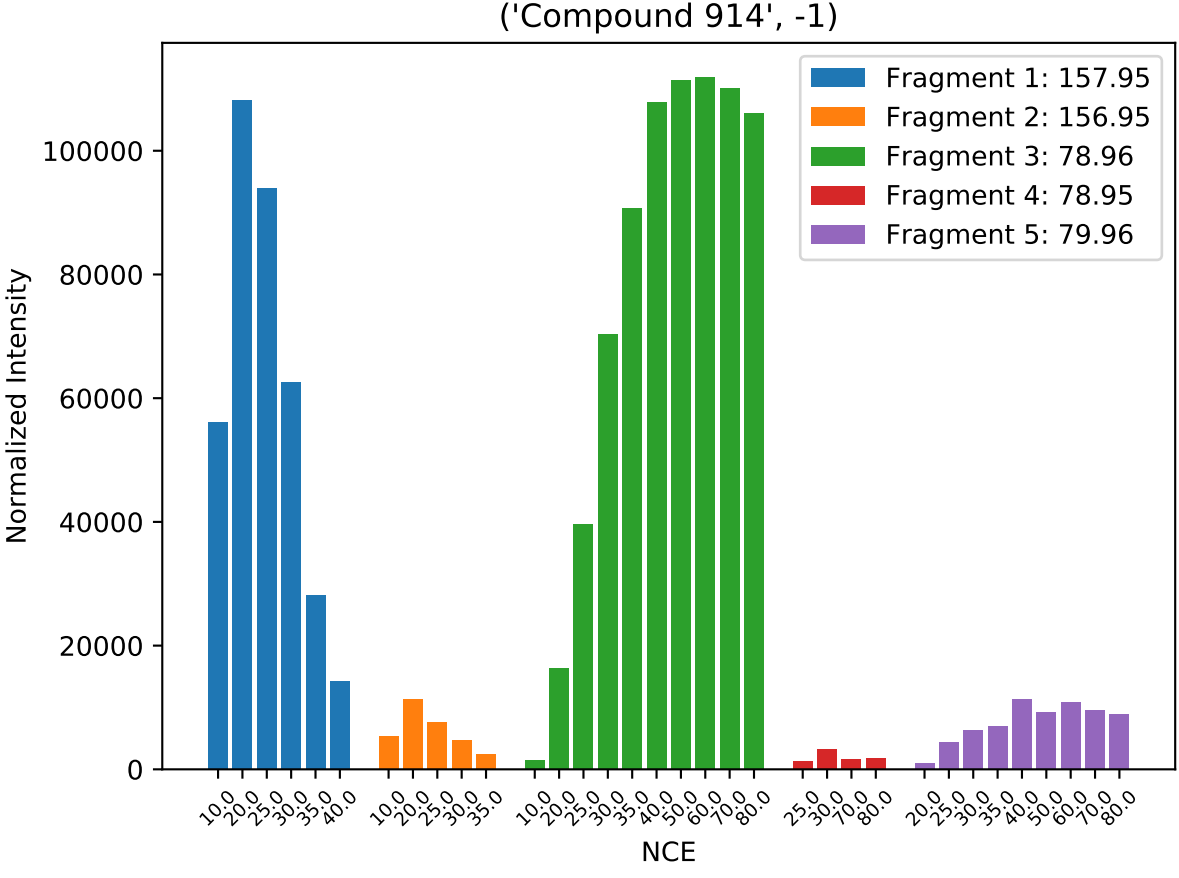

('Compound 907', -1)
Fragment 1: 79.96
Fragment 2: 81.26
Fragment 3: 122.56
Fragment 4: 145.79
Fragment 5: 58.67
Normalized Intensity
0
200
400
600
800
1000
1200
1400
1600
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
10.0
40.0
25.0
NCE

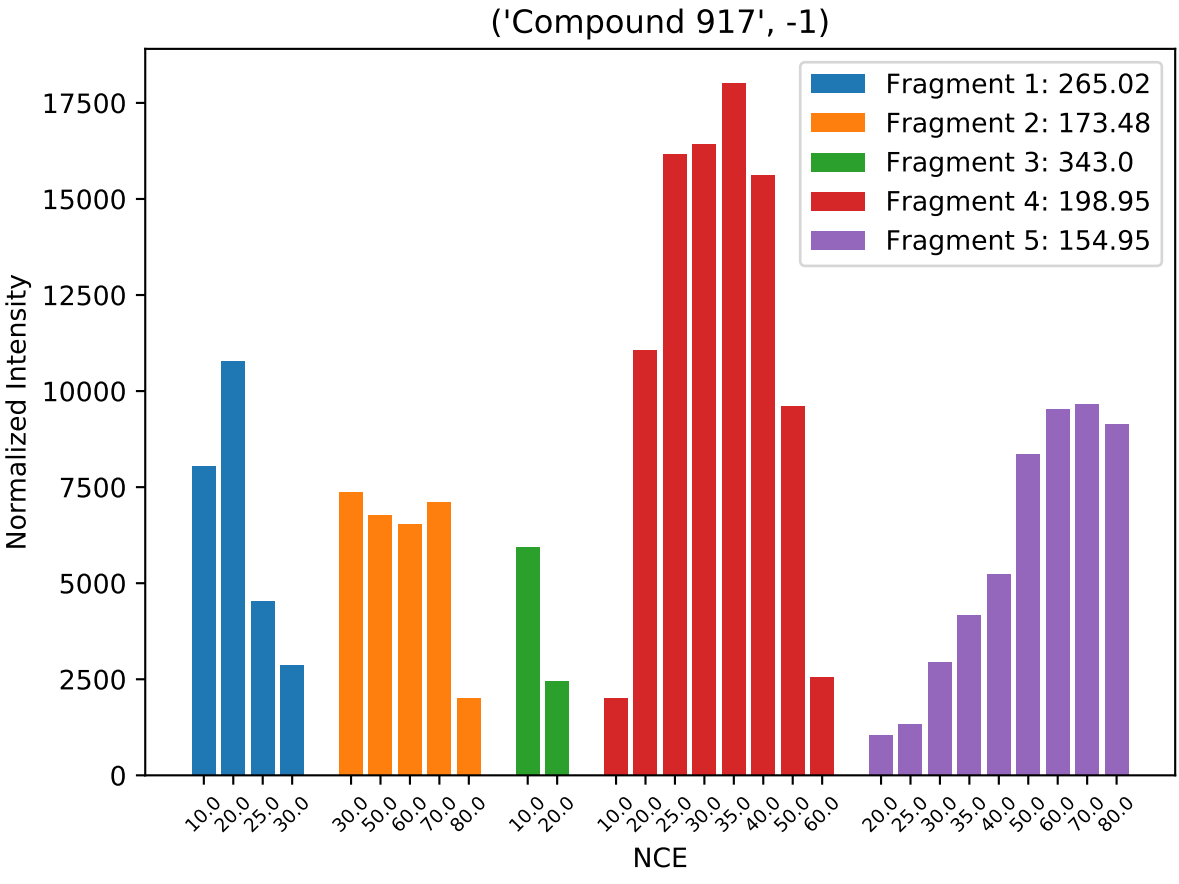

('Compound 908', -1)
Fragment 1: 220.89
Fragment 2: 173.49
Fragment 3: 173.48
Fragment 4: 57.0
Fragment 5: 59.98
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
25.0
40.0
60.0
70.0
80.0
20.0
30.0
35.0
50.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

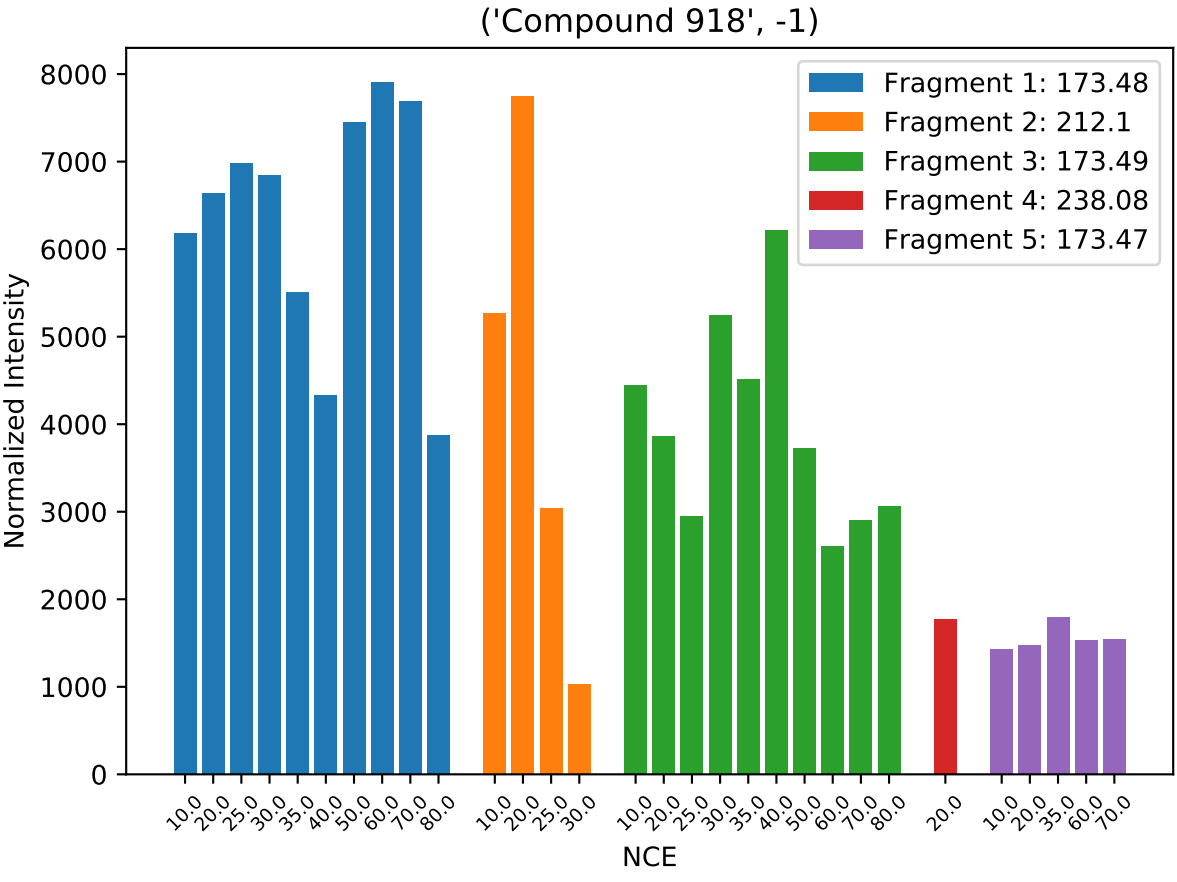

('Compound 294', -1)
Fragment 1: 329.03
Fragment 2: 173.48
Fragment 3: 311.02
Fragment 4: 173.49
Fragment 5: 301.04
Normalized Intensity
0
5000
10000
15000
20000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
40.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
20.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
40.0
NCE

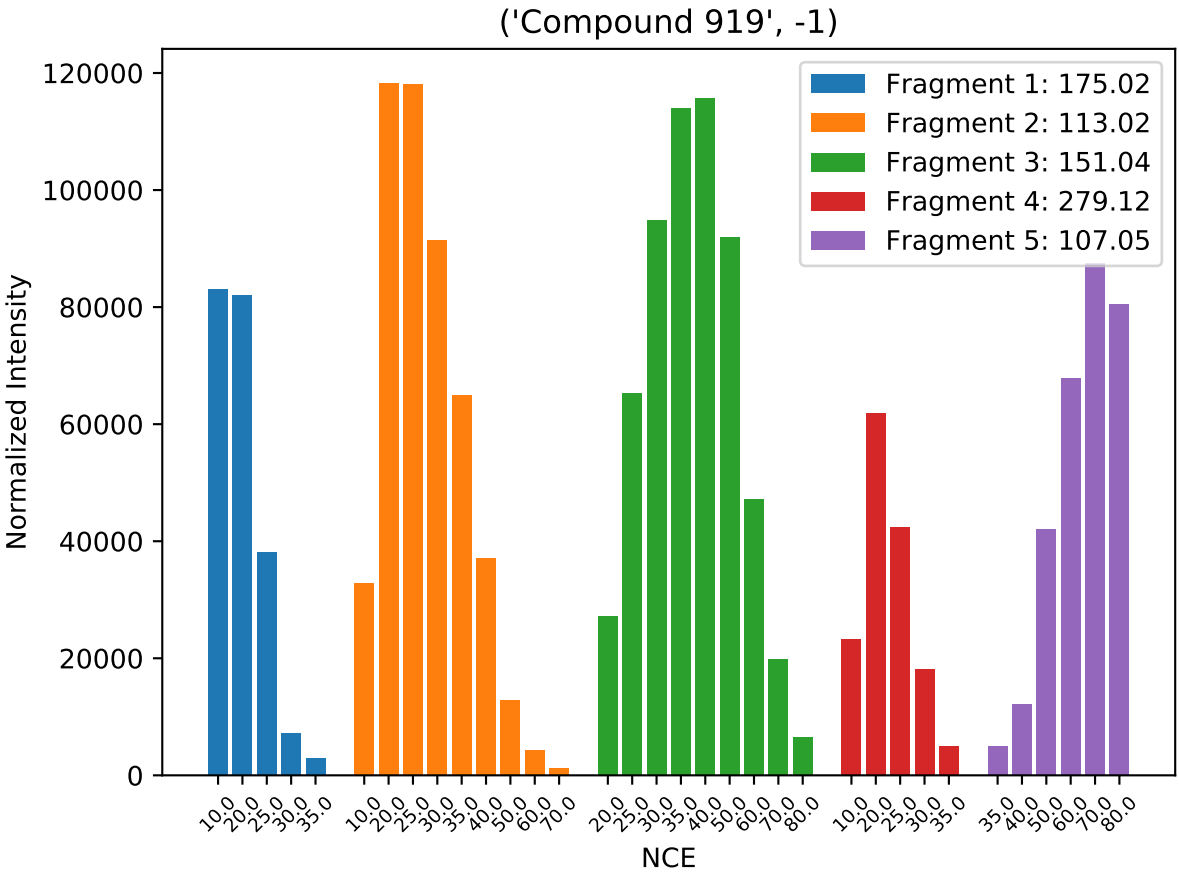

('Compound 912', -1)
Fragment 1: 130.06
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 130.05
Fragment 5: 88.04
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
30.0
40.0
50.0
80.0
25.0
30.0
35.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

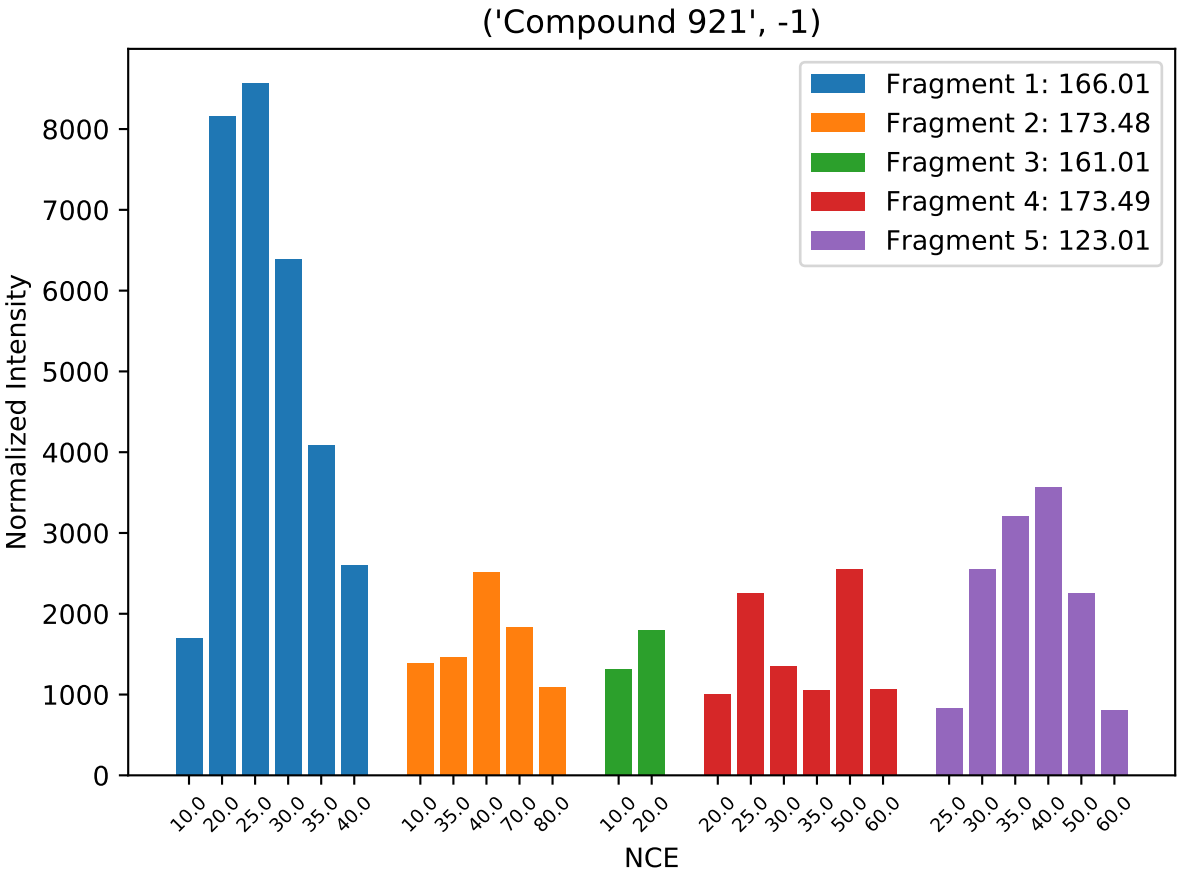

('Compound 913', -1)
Fragment 1: 120.01
Fragment 2: 124.02
Fragment 3: 173.49
Fragment 4: 173.48
Fragment 5: 64.95
Normalized Intensity
0
1000
2000
3000
4000
5000
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
20.0
35.0
40.0
10.0
25.0
30.0
40.0
50.0
60.0
70.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

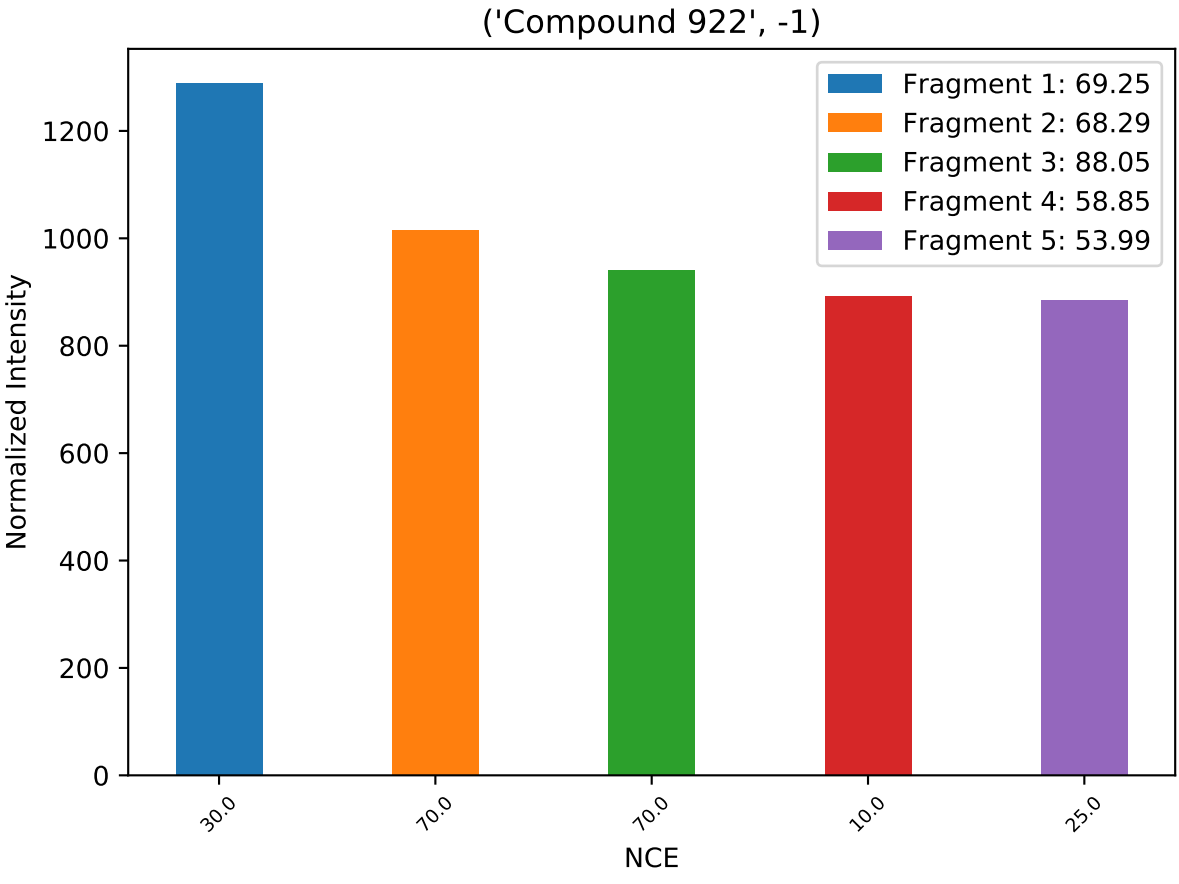

('Compound 914', -1)
Fragment 1: 157.95
Fragment 2: 156.95
Fragment 3: 78.96
Fragment 4: 78.95
Fragment 5: 79.96
Normalized Intensity
0
20000
40000
60000
80000
100000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

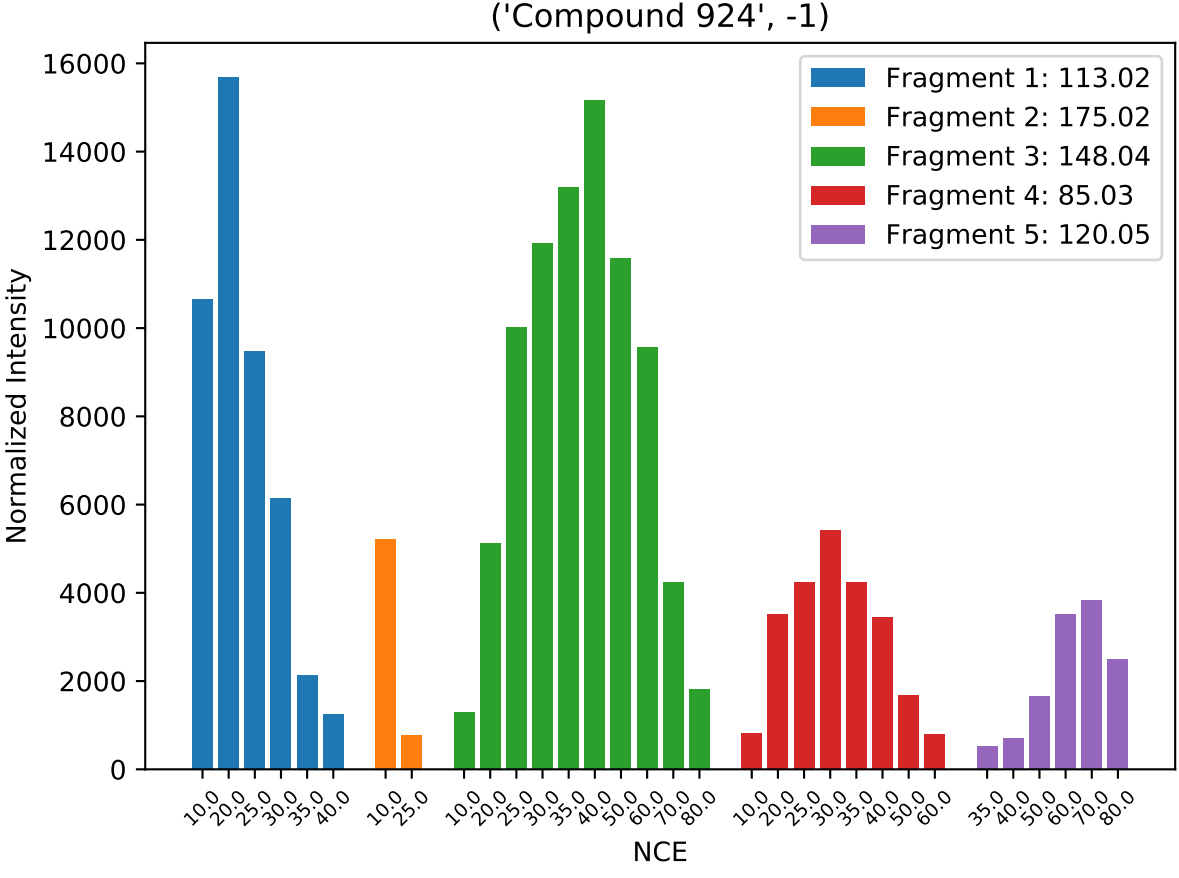

('Compound 917', -1)
Fragment 1: 265.02
Fragment 2: 173.48
Fragment 3: 343.0
Fragment 4: 198.95
Fragment 5: 154.95
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0
20.0
25.0
30.0
30.0
50.0
60.0
70.0
80.0
10.0
20.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

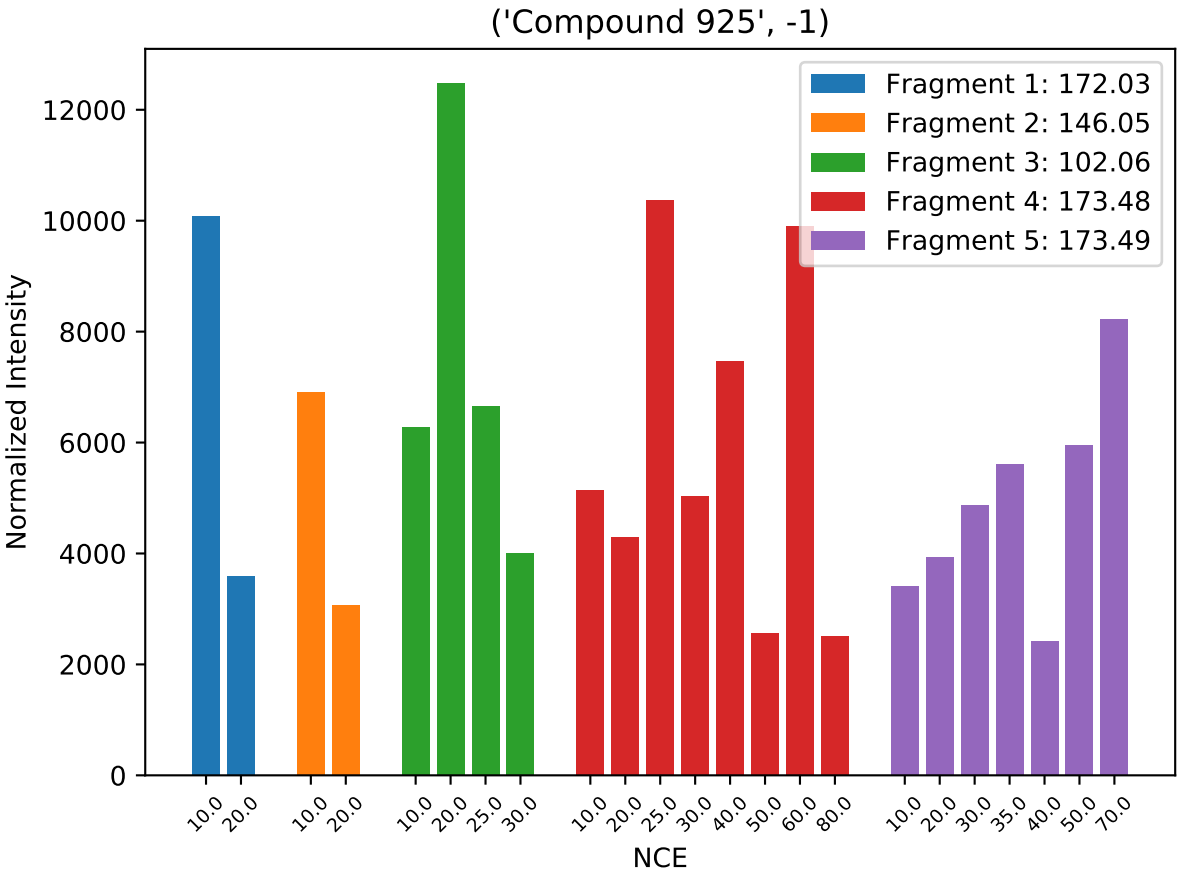

('Compound 918', -1)
Fragment 1: 173.48
Fragment 2: 212.1
Fragment 3: 173.49
Fragment 4: 238.08
Fragment 5: 173.47
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

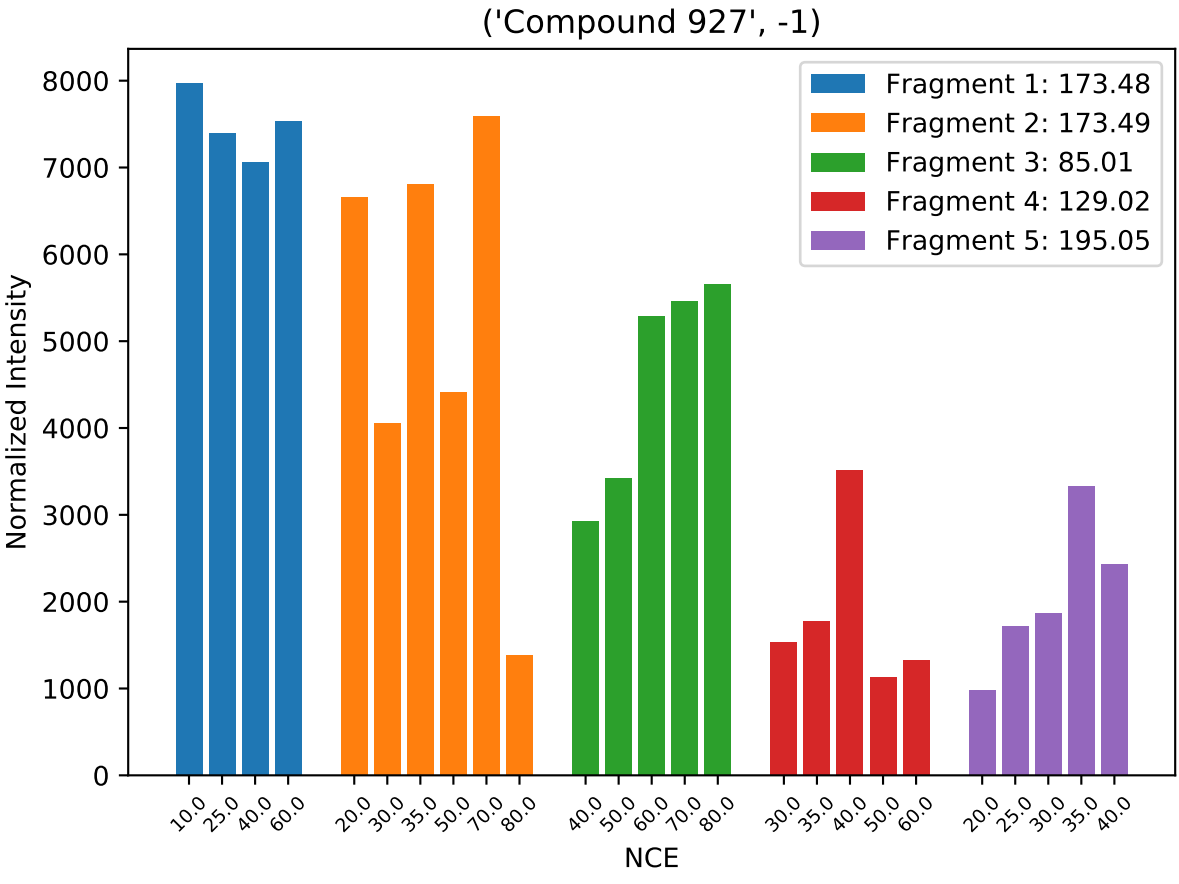

('Compound 919', -1)
Fragment 1: 175.02
Fragment 2: 113.02
Fragment 3: 151.04
Fragment 4: 279.12
Fragment 5: 107.05
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

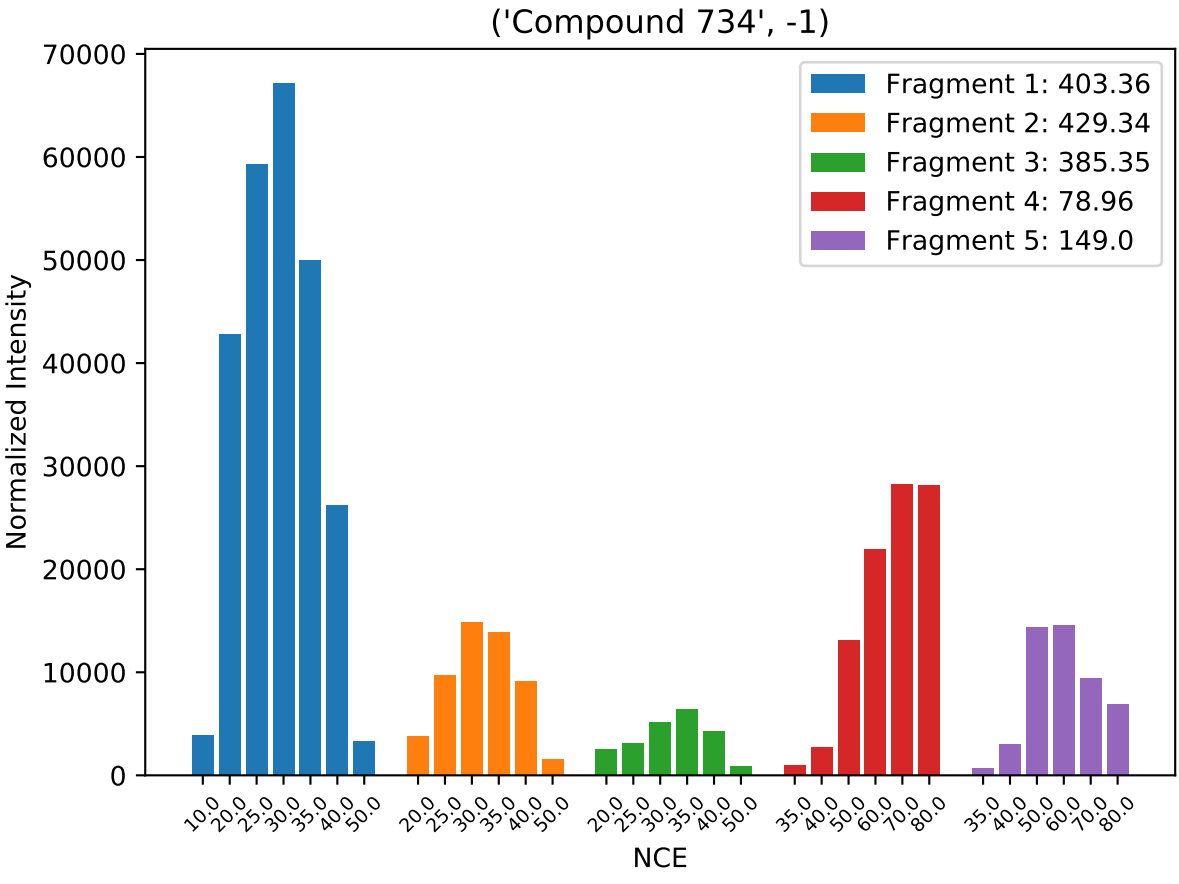

('Compound 921', -1)
Fragment 1: 166.01
Fragment 2: 173.48
Fragment 3: 161.01
Fragment 4: 173.49
Fragment 5: 123.01
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
20.0
25.0
30.0
35.0
40.0
10.0
35.0
40.0
70.0
80.0
10.0
20.0
20.0
25.0
30.0
35.0
50.0
60.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

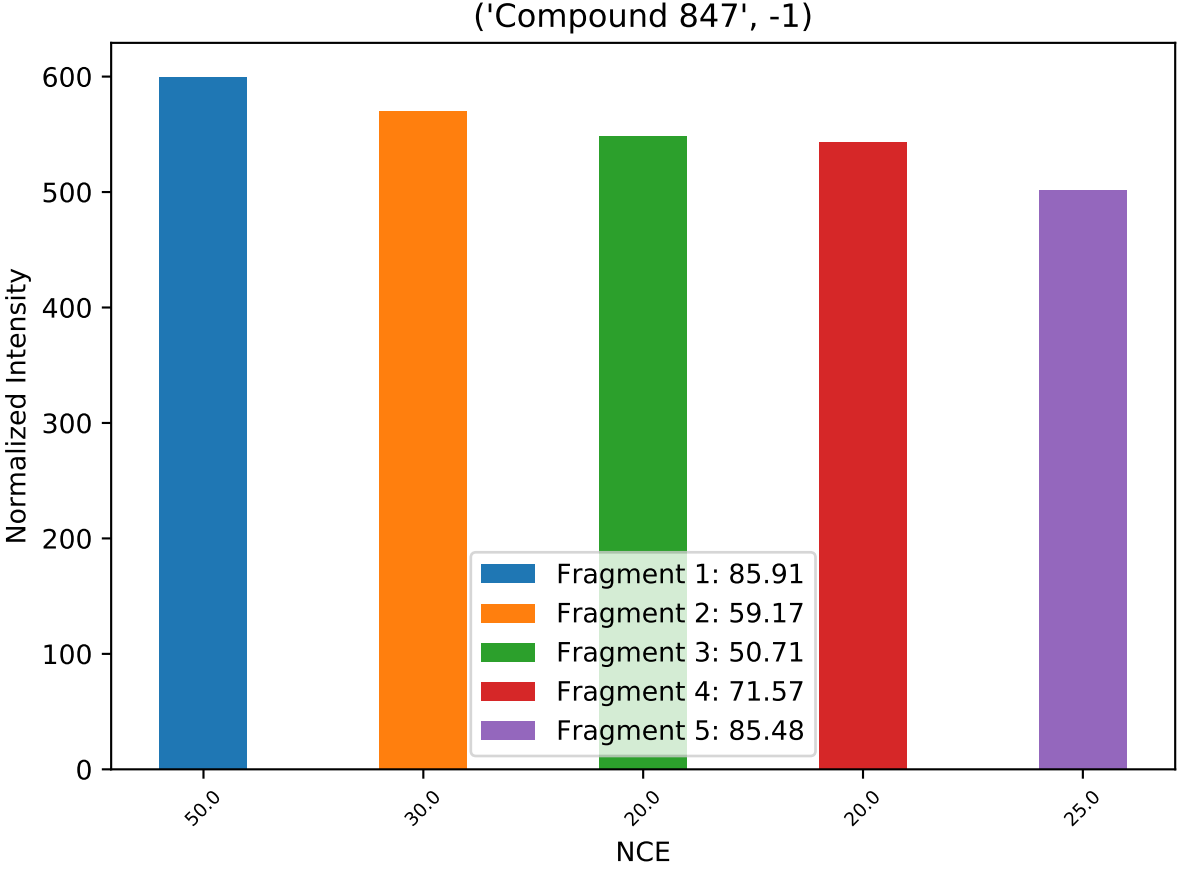

('Compound 922', -1)
Fragment 1: 69.25
Fragment 2: 68.29
Fragment 3: 88.05
Fragment 4: 58.85
Fragment 5: 53.99
Normalized Intensity
0
200
400
600
800
1000
1200
30.0
70.0
70.0
10.0
25.0
NCE

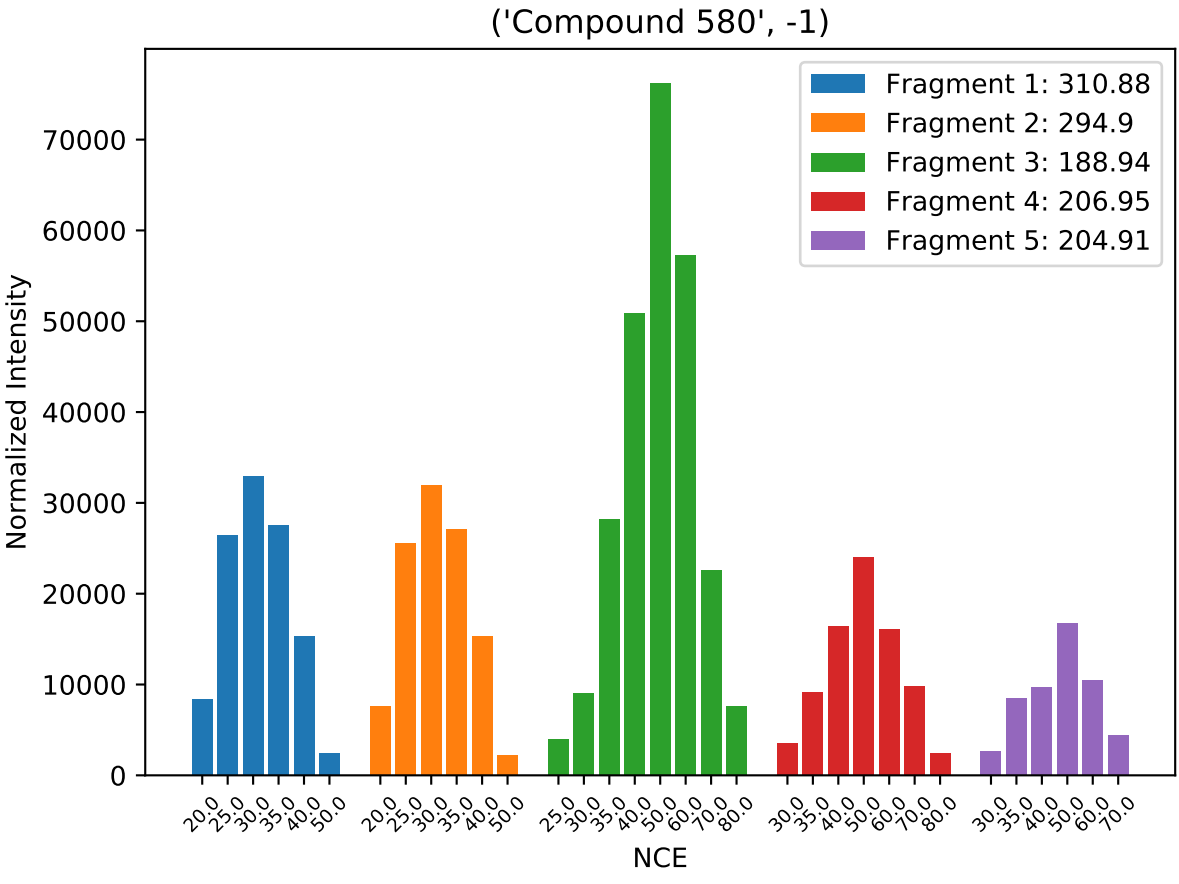

('Compound 924', -1)
Fragment 1: 113.02
Fragment 2: 175.02
Fragment 3: 148.04
Fragment 4: 85.03
Fragment 5: 120.05
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
16000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 25.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

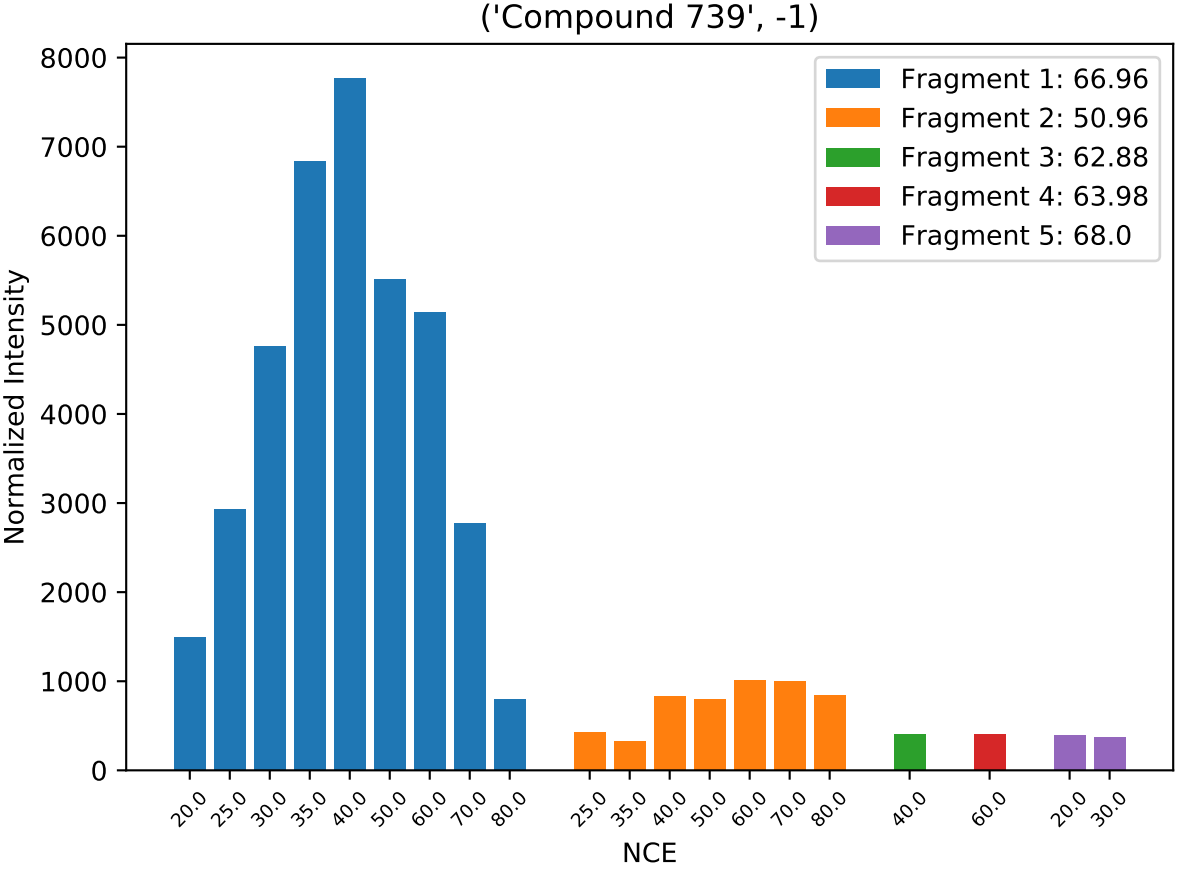

('Compound 925', -1)
Fragment 1: 172.03
Fragment 2: 146.05
Fragment 3: 102.06
Fragment 4: 173.48
Fragment 5: 173.49
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0
20.0
10.0
20.0
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
40.0
50.0
60.0
80.0
10.0
20.0
30.0
35.0
40.0
50.0
70.0
NCE

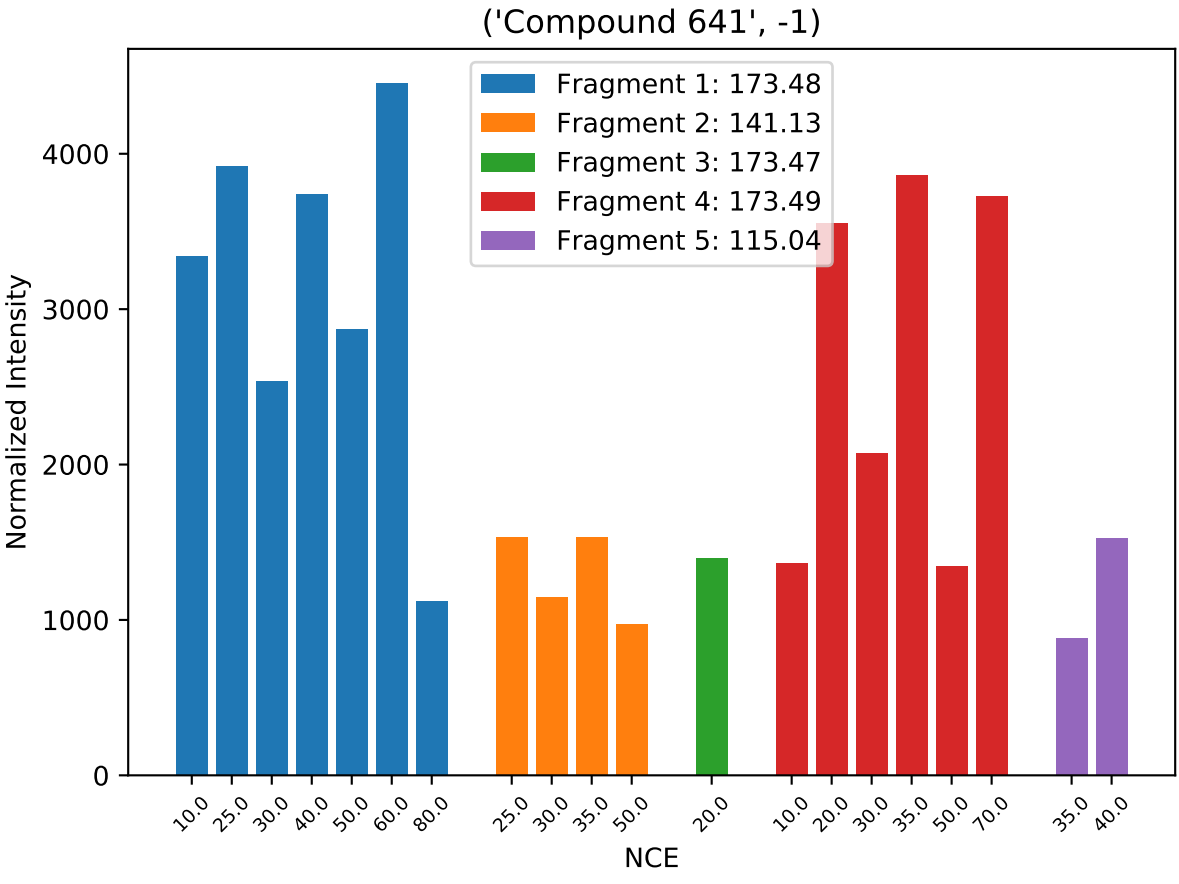

('Compound 927', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 85.01
Fragment 4: 129.02
Fragment 5: 195.05
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
10.0
25.0
40.0
60.0
20.0
30.0
35.0
50.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
NCE

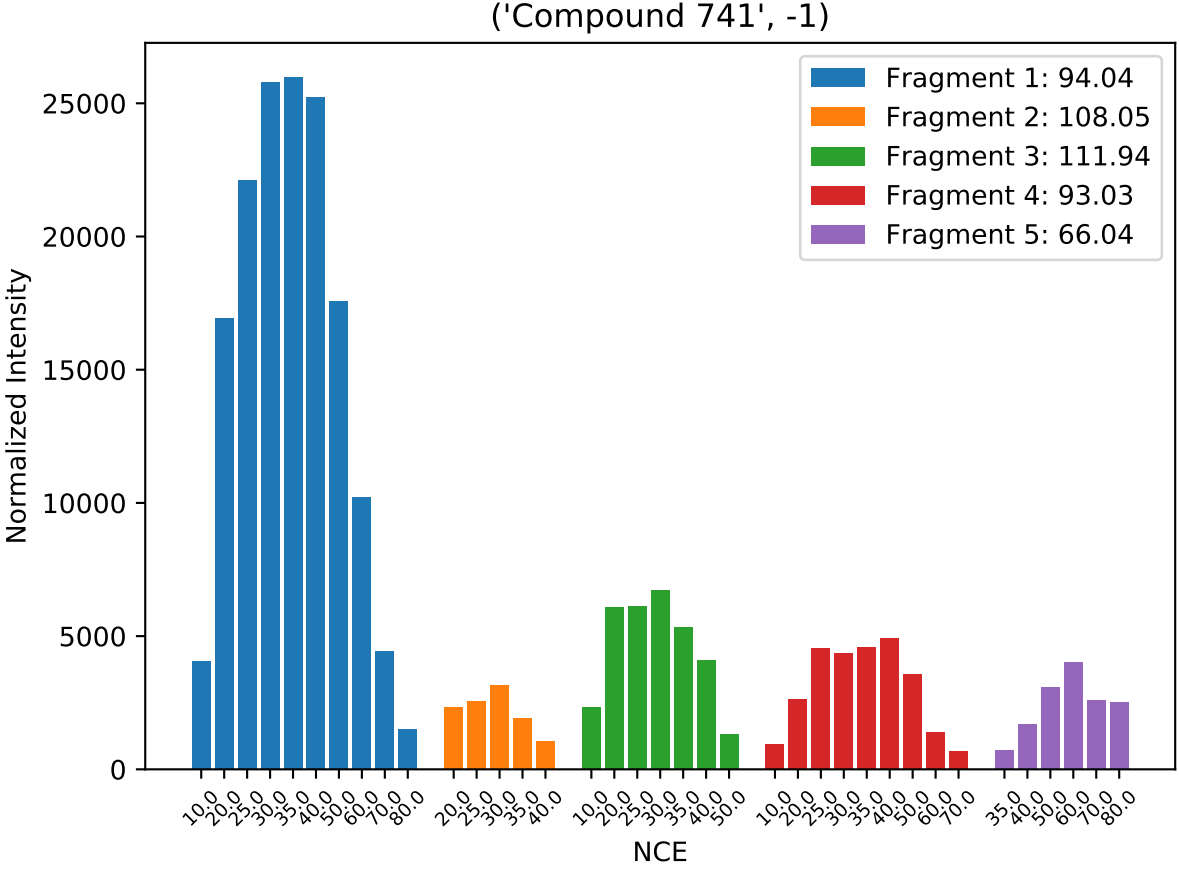

('Compound 734', -1)
Fragment 1: 403.36
Fragment 2: 429.34
Fragment 3: 385.35
Fragment 4: 78.96
Fragment 5: 149.0
Normalized Intensity
NCE
70000
60000
50000
40000
30000
20000
10000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0
35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0

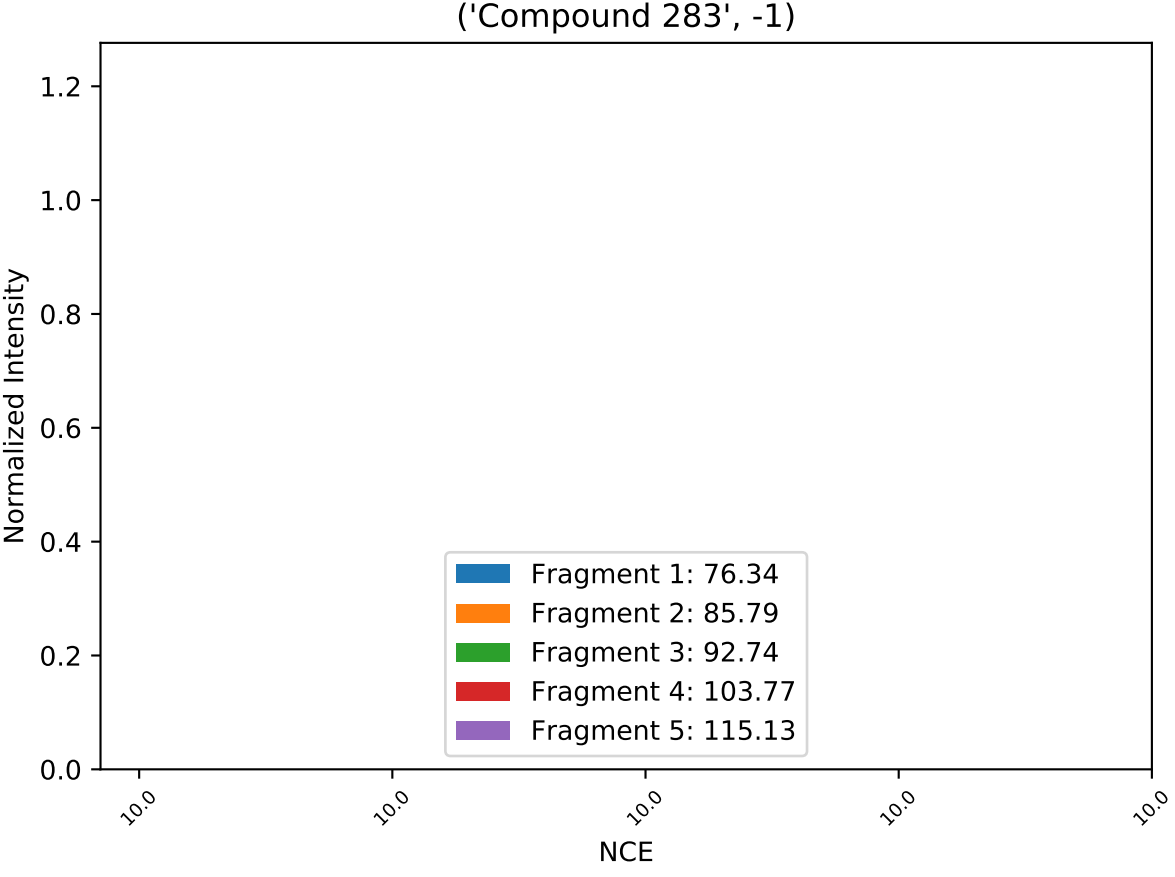

('Compound 847', -1)
Normalized Intensity
0
100
200
300
400
500
600
50.0
30.0
20.0
20.0
25.0
NCE
Fragment 1: 85.91
Fragment 2: 59.17
Fragment 3: 50.71
Fragment 4: 71.57
Fragment 5: 85.48

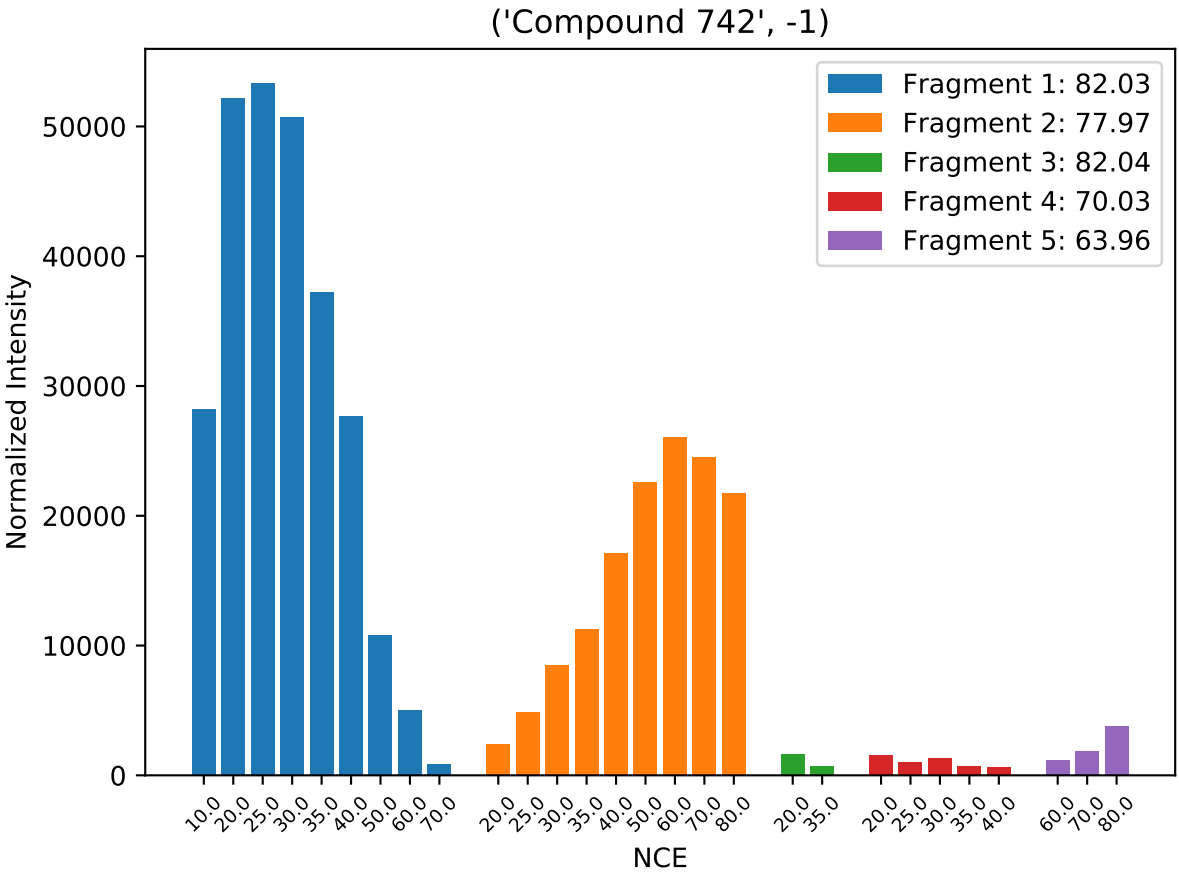

('Compound 580', -1)
Fragment 1: 310.88
Fragment 2: 294.9
Fragment 3: 188.94
Fragment 4: 206.95
Fragment 5: 204.91
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0
NCE

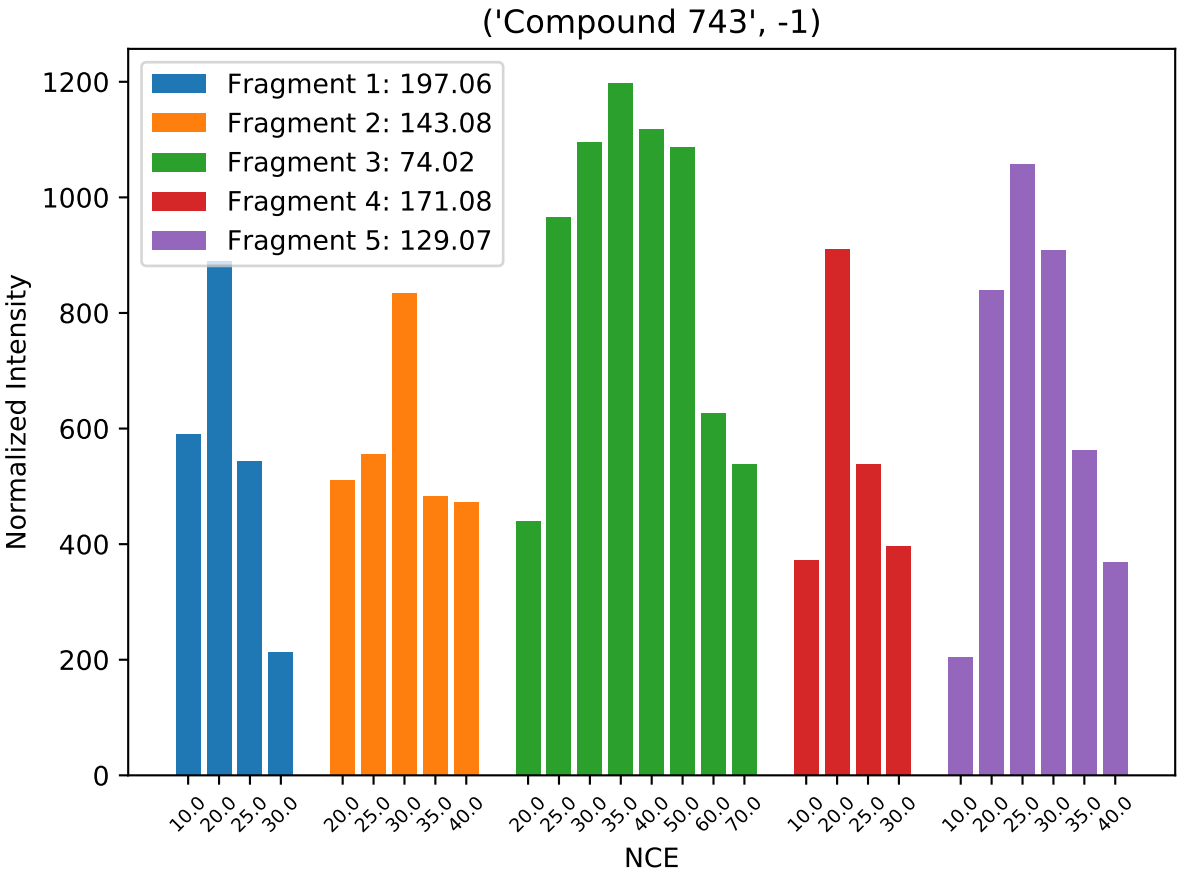

('Compound 739', -1)
Fragment 1: 66.96
Fragment 2: 50.96
Fragment 3: 62.88
Fragment 4: 63.98
Fragment 5: 68.0
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
8000
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
35.0
40.0
50.0
60.0
70.0
80.0
40.0
60.0
20.0
30.0
NCE

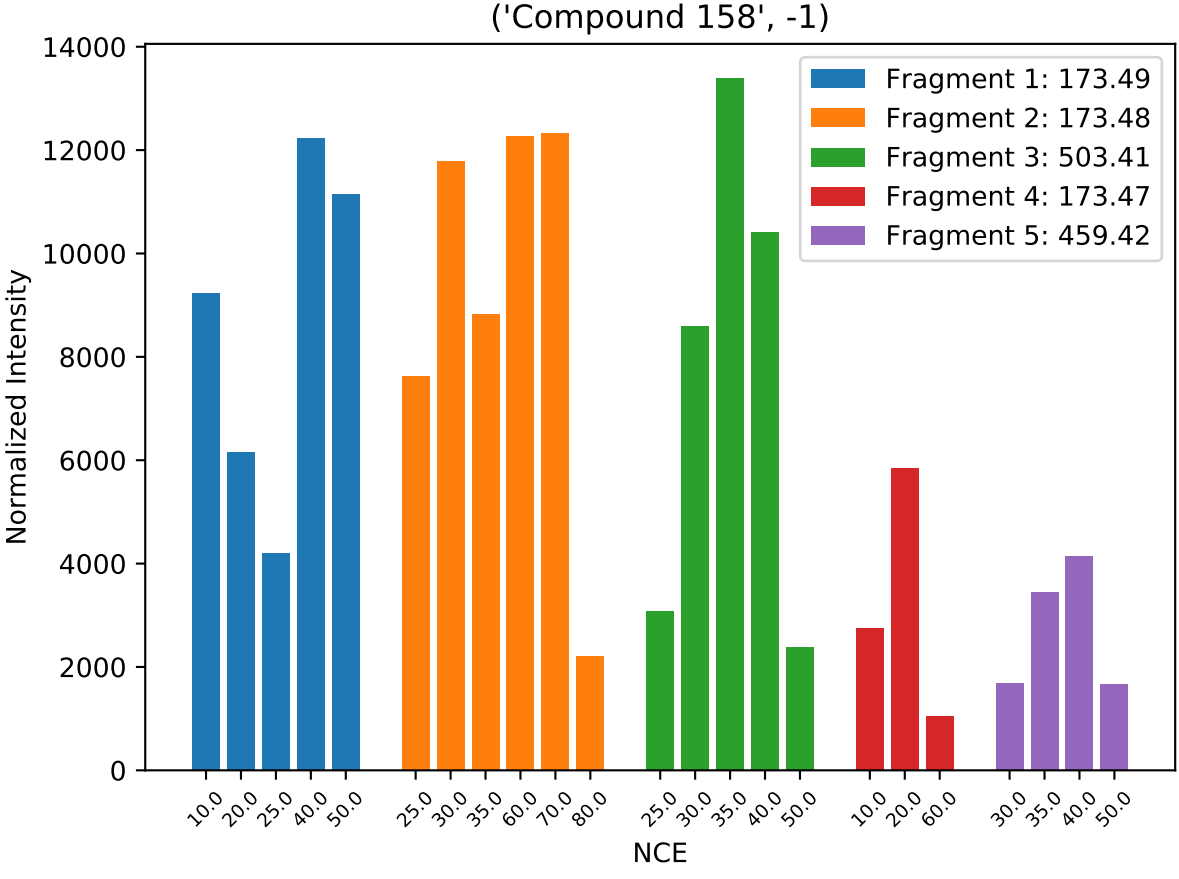

('Compound 641', -1)
Fragment 1: 173.48
Fragment 2: 141.13
Fragment 3: 173.47
Fragment 4: 173.49
Fragment 5: 115.04
Normalized Intensity
0
1000
2000
3000
4000
10.0
25.0
30.0
40.0
50.0
60.0
80.0
25.0
30.0
35.0
50.0
20.0
10.0
20.0
30.0
35.0
50.0
70.0
35.0
40.0
NCE

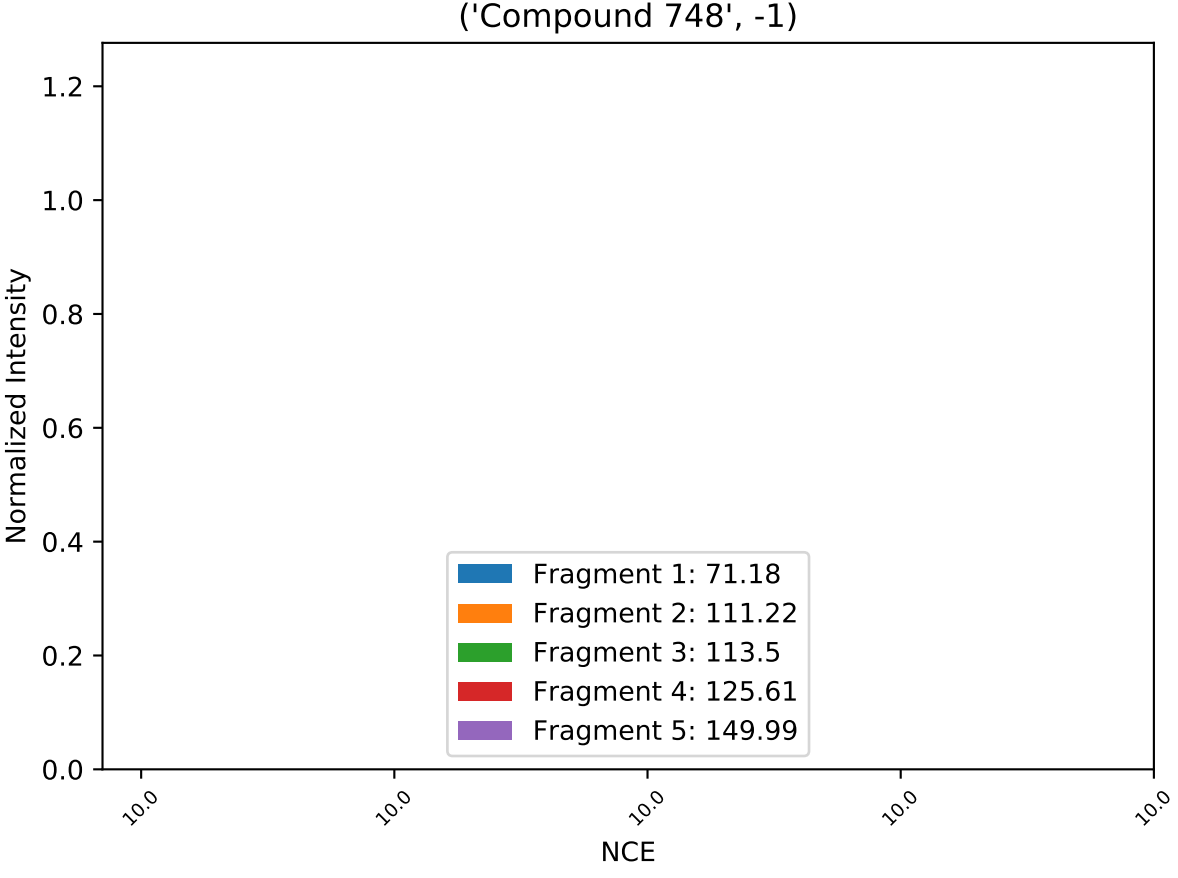

('Compound 741', -1)
Fragment 1: 94.04
Fragment 2: 108.05
Fragment 3: 111.94
Fragment 4: 93.03
Fragment 5: 66.04
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

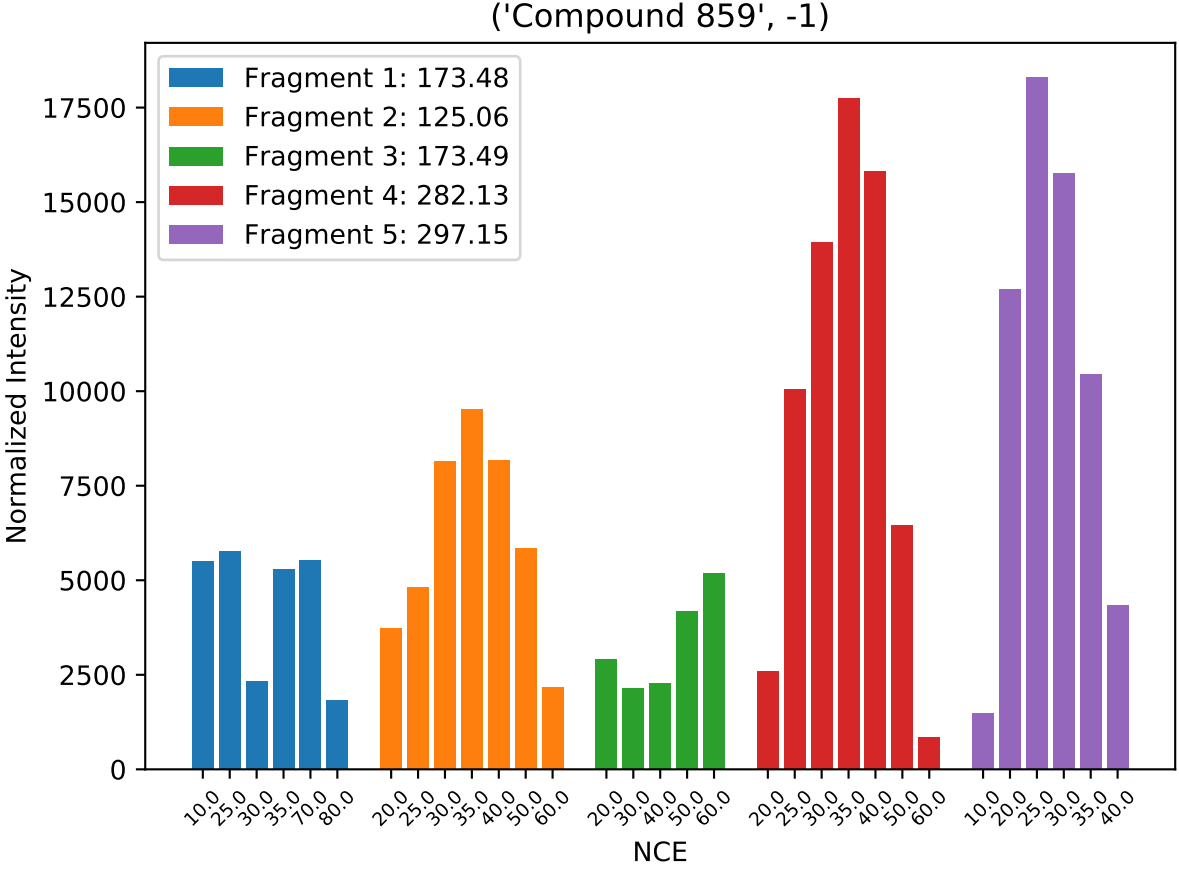

('Compound 283', -1)
Normalized Intensity
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Fragment 1: 76.34
Fragment 2: 85.79
Fragment 3: 92.74
Fragment 4: 103.77
Fragment 5: 115.13
10.0
10.0
10.0
10.0
10.0
NCE

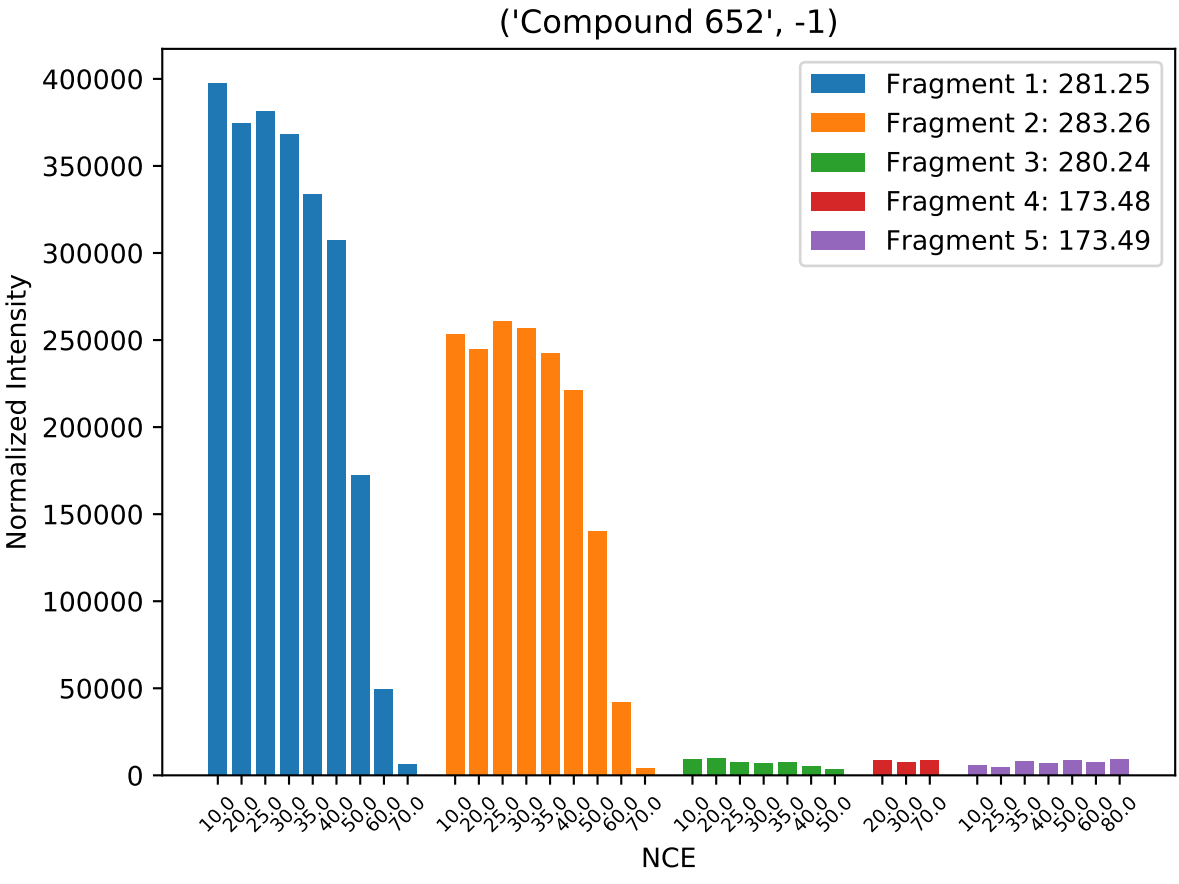

('Compound 742', -1)
Fragment 1: 82.03
Fragment 2: 77.97
Fragment 3: 82.04
Fragment 4: 70.03
Fragment 5: 63.96
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
35.0
20.0
25.0
30.0
35.0
40.0
60.0
70.0
80.0
NCE

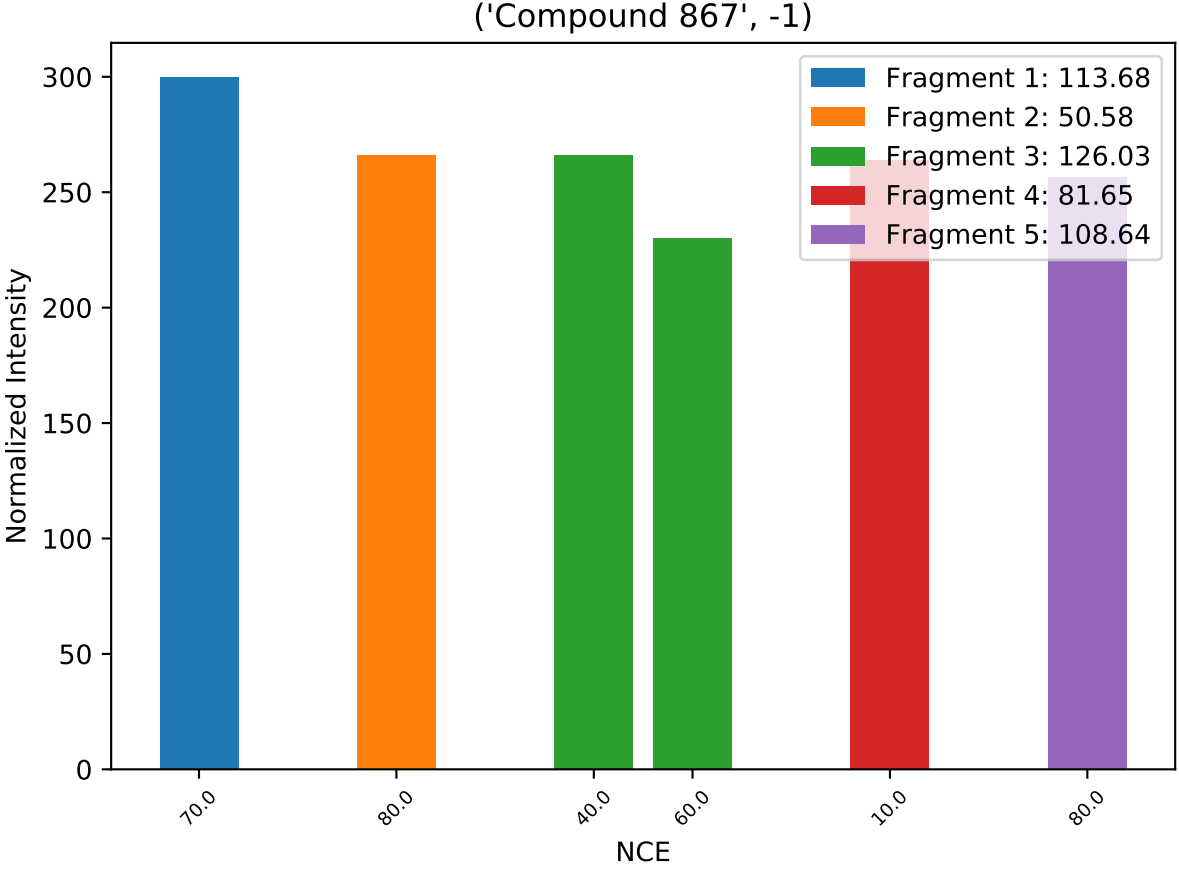

('Compound 743', -1)
Fragment 1: 197.06
Fragment 2: 143.08
Fragment 3: 74.02
Fragment 4: 171.08
Fragment 5: 129.07
Normalized Intensity
0
200
400
600
800
1000
1200
10.0
20.0
25.0
30.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
10.0
20.0
25.0
30.0
35.0
40.0
NCE

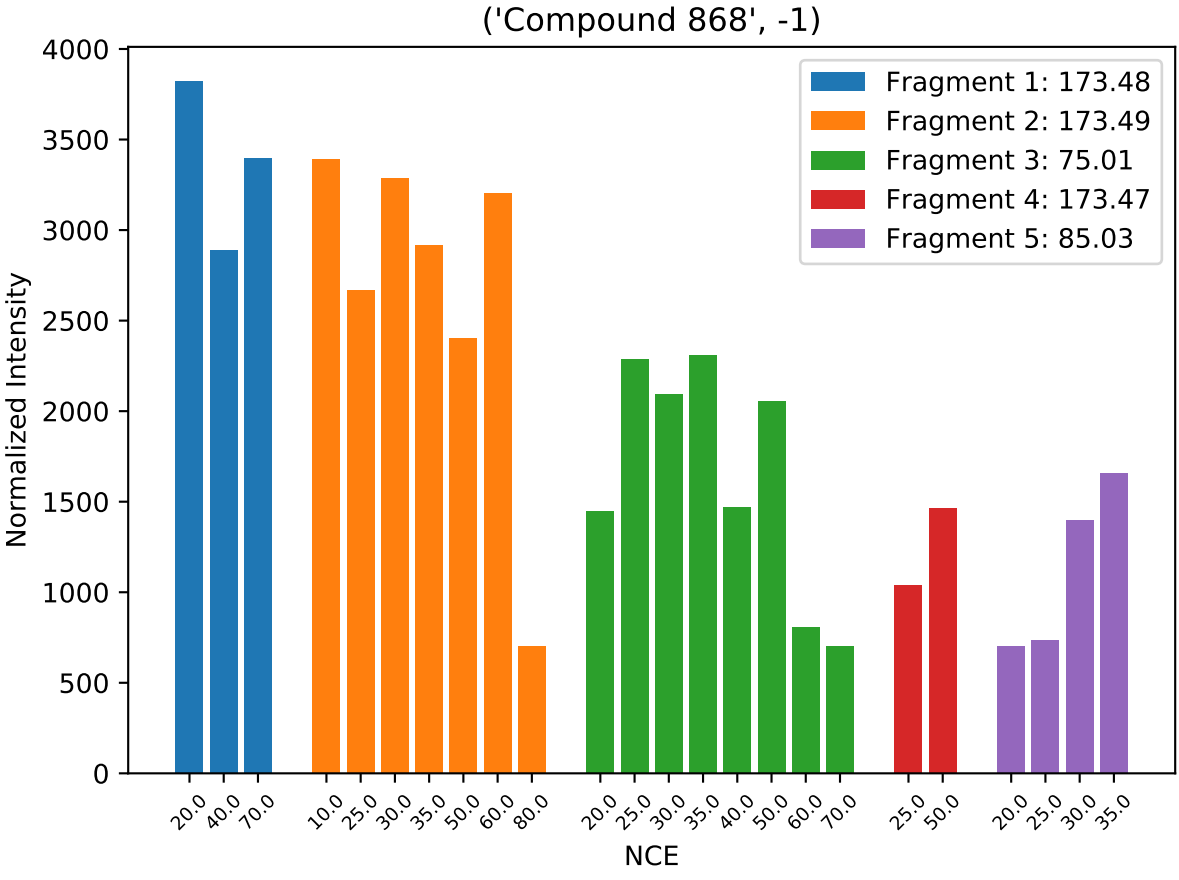

('Compound 158', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 503.41
Fragment 4: 173.47
Fragment 5: 459.42
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
NCE
10.0
20.0
25.0
40.0
50.0
25.0
30.0
35.0
60.0
70.0
80.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
60.0
30.0
35.0
40.0
50.0

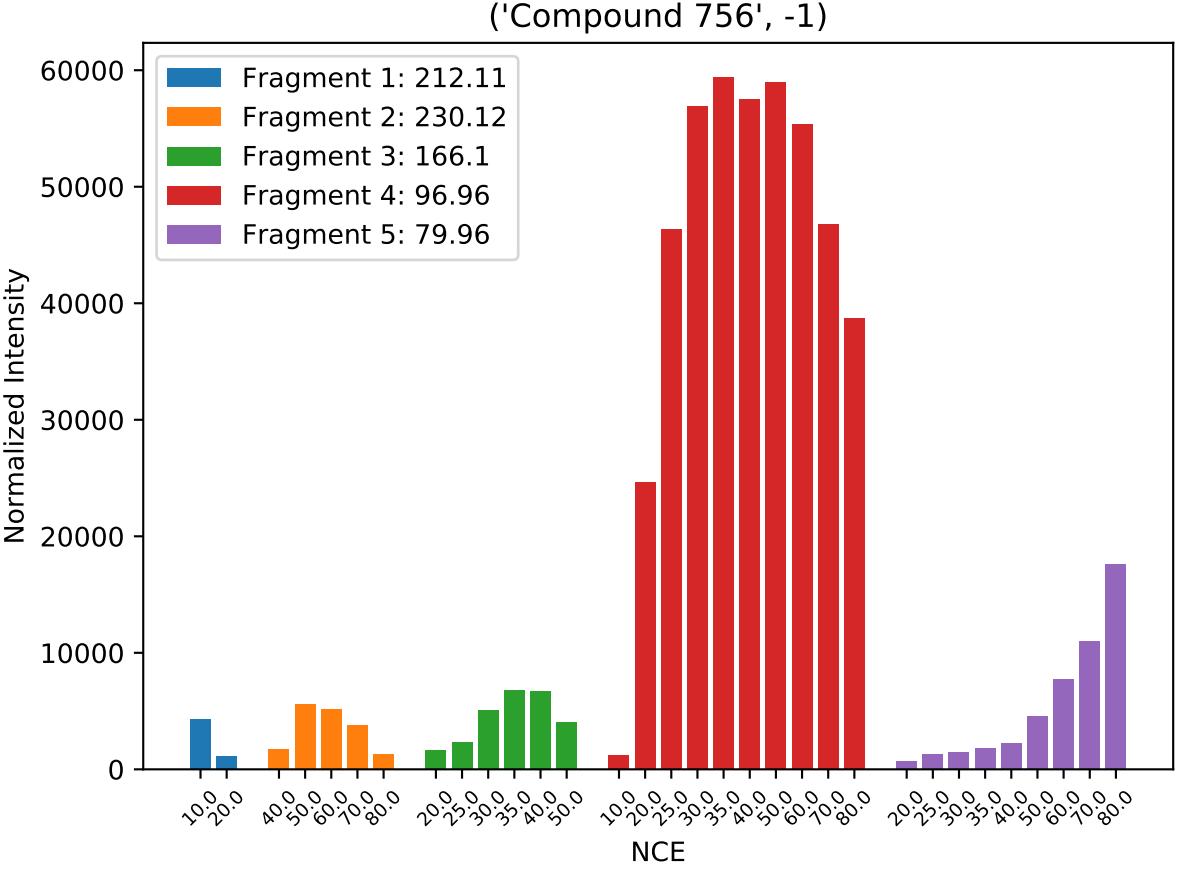

('Compound 748', -1)
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
Fragment 1: 71.18
Fragment 2: 111.22
Fragment 3: 113.5
Fragment 4: 125.61
Fragment 5: 149.99
10.0
10.0
10.0
10.0
10.0
NCE

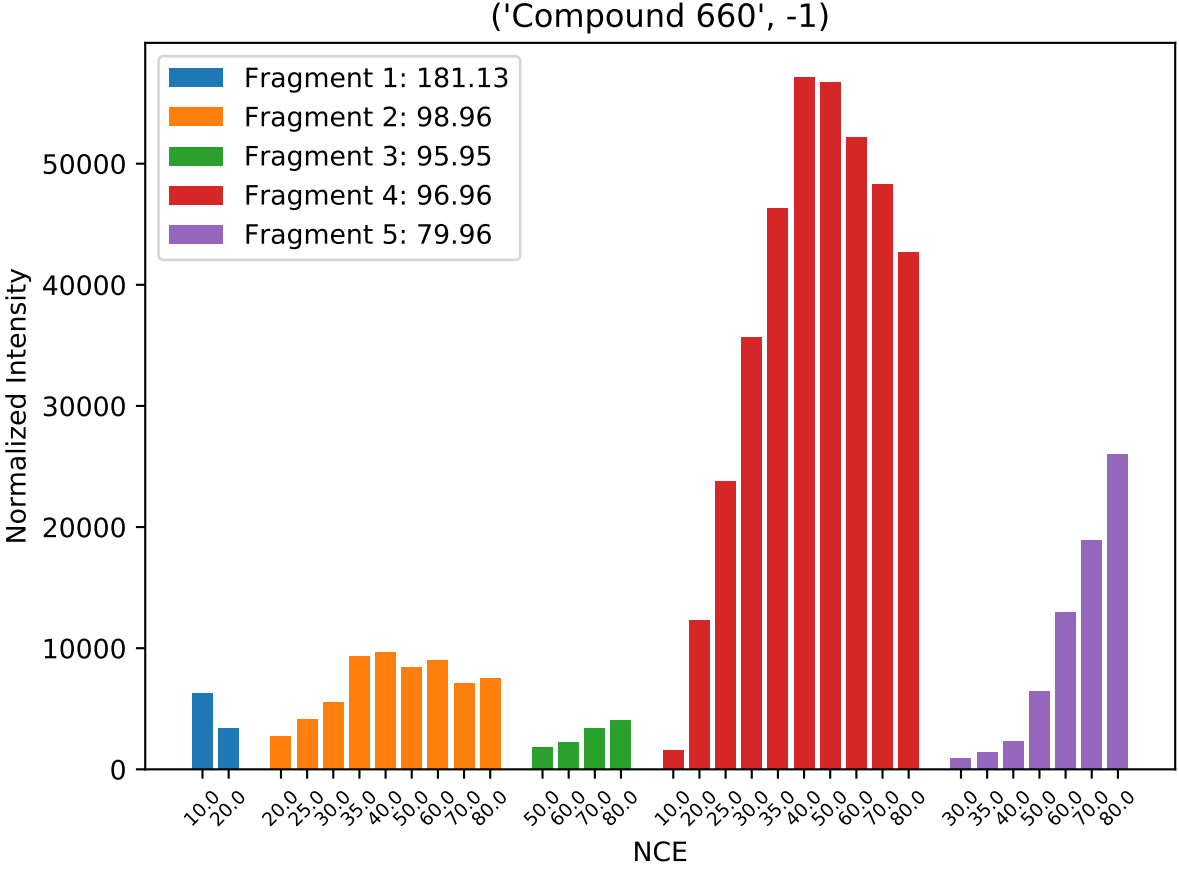

('Compound 859', -1)
Fragment 1: 173.48
Fragment 2: 125.06
Fragment 3: 173.49
Fragment 4: 282.13
Fragment 5: 297.15
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
10.0 25.0 30.0 35.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 30.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0
NCE

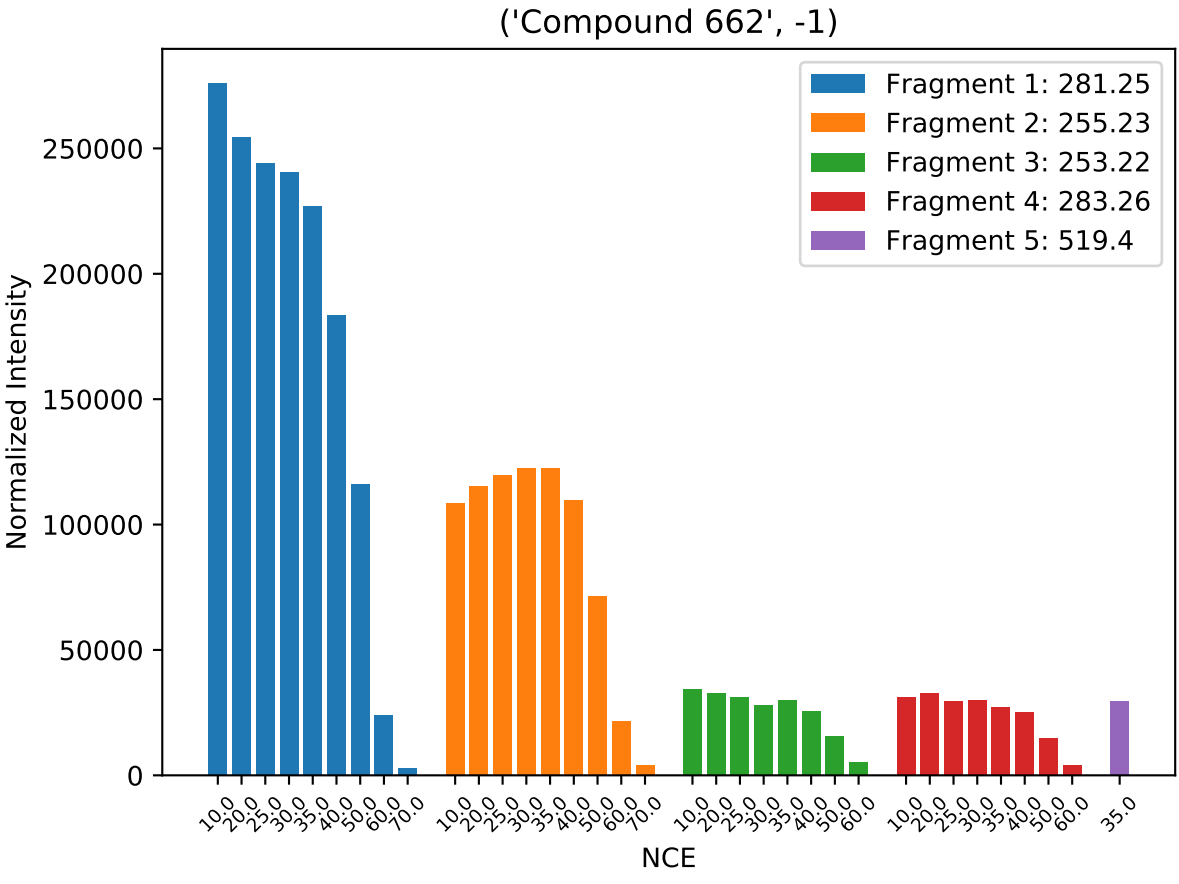

('Compound 652', -1)
Fragment 1: 281.25
Fragment 2: 283.26
Fragment 3: 280.24
Fragment 4: 173.48
Fragment 5: 173.49
Normalized Intensity
400000
350000
300000
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 30.0 70.0
10.0 25.0 35.0 40.0 50.0 60.0 80.0
NCE

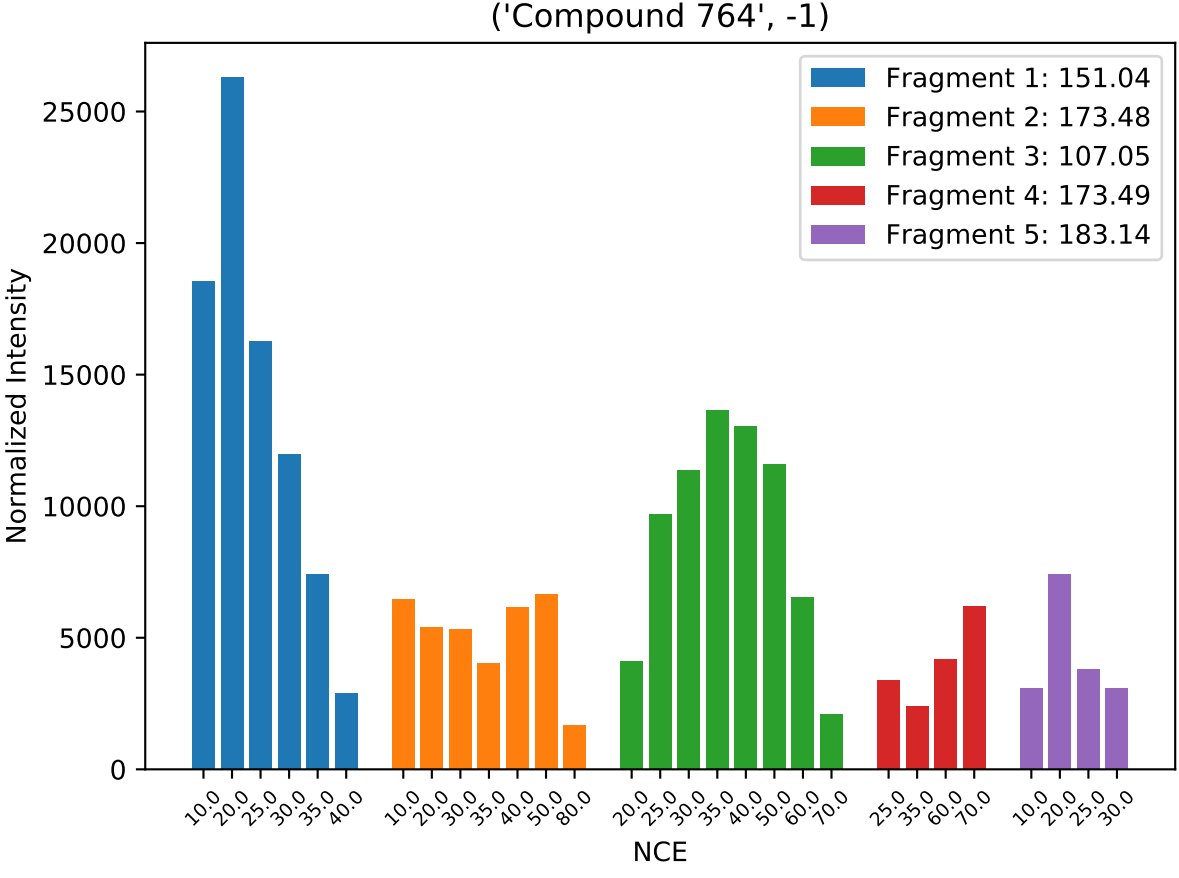

('Compound 867', -1)
Fragment 1: 113.68
Fragment 2: 50.58
Fragment 3: 126.03
Fragment 4: 81.65
Fragment 5: 108.64
Normalized Intensity
0
50
100
150
200
250
300
70.0
80.0
40.0
60.0
10.0
80.0
NCE

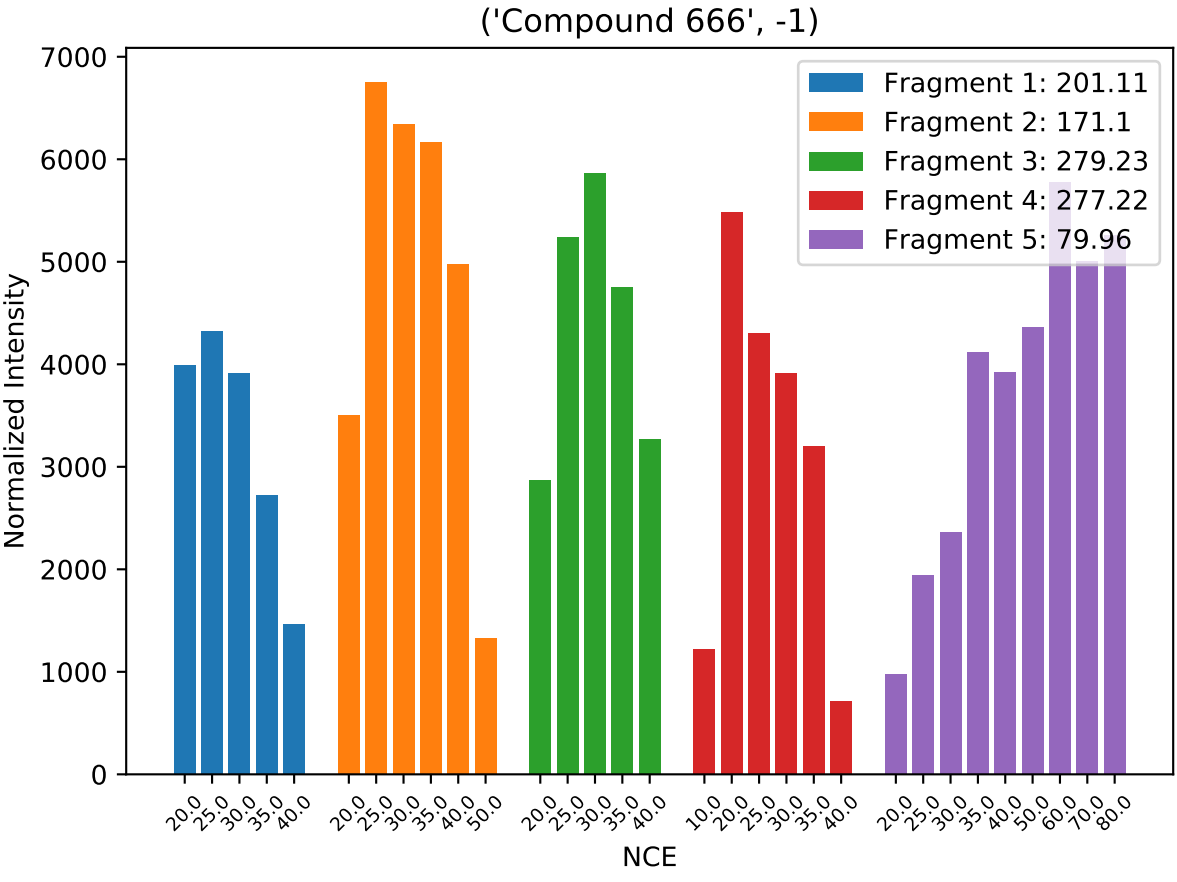

('Compound 868', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 75.01
Fragment 4: 173.47
Fragment 5: 85.03
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
20.0
40.0
70.0
10.0
25.0
30.0
35.0
50.0
60.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
25.0
50.0
20.0
25.0
30.0
35.0
NCE

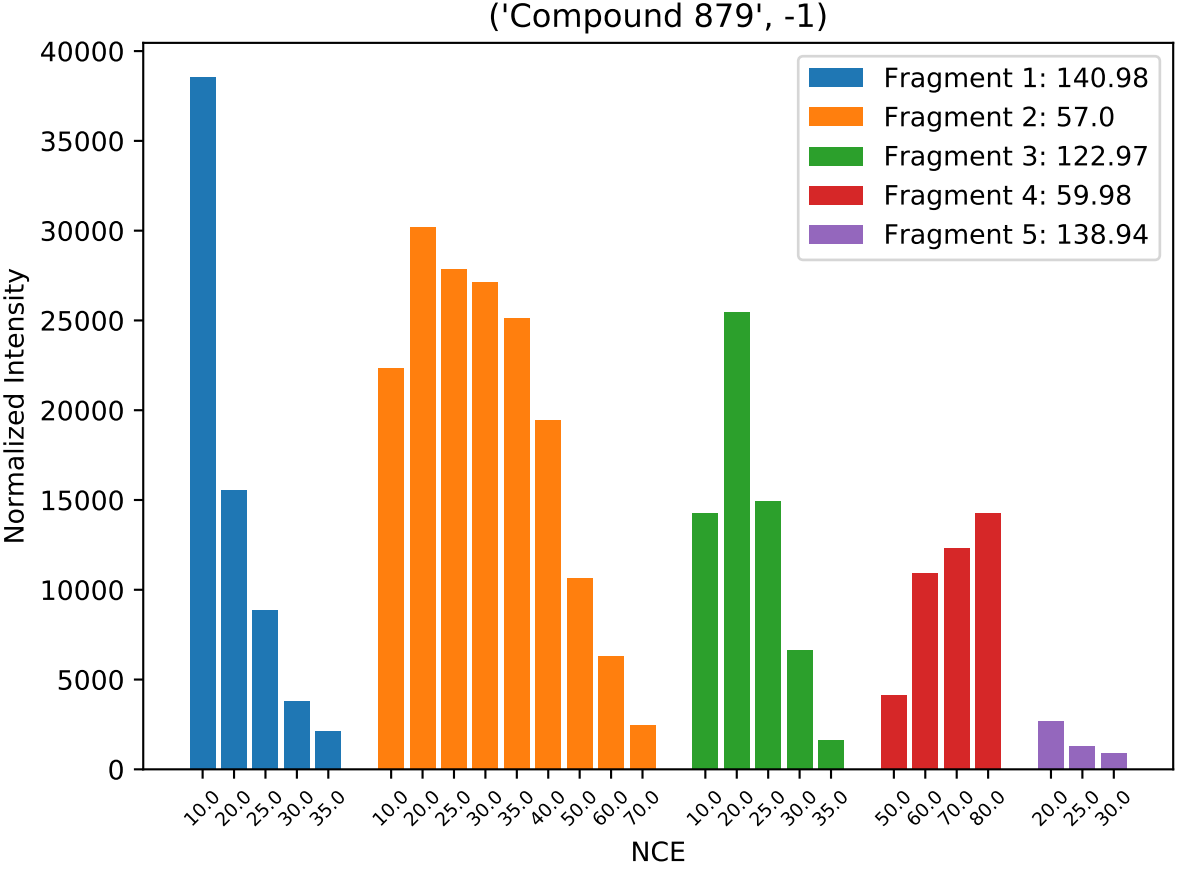

('Compound 756', -1)
Fragment 1: 212.11
Fragment 2: 230.12
Fragment 3: 166.1
Fragment 4: 96.96
Fragment 5: 79.96
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
10.0
20.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

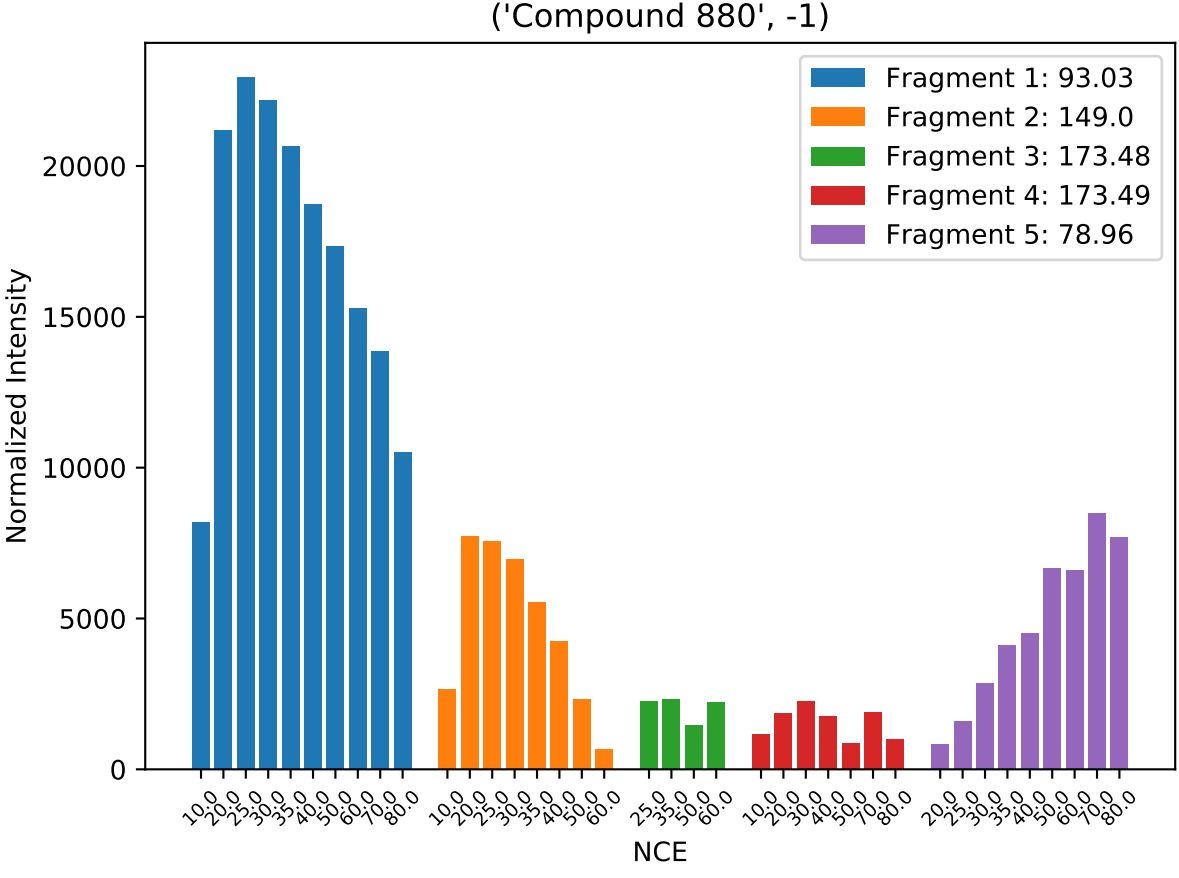

('Compound 660', -1)
Fragment 1: 181.13
Fragment 2: 98.96
Fragment 3: 95.95
Fragment 4: 96.96
Fragment 5: 79.96
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0
20.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

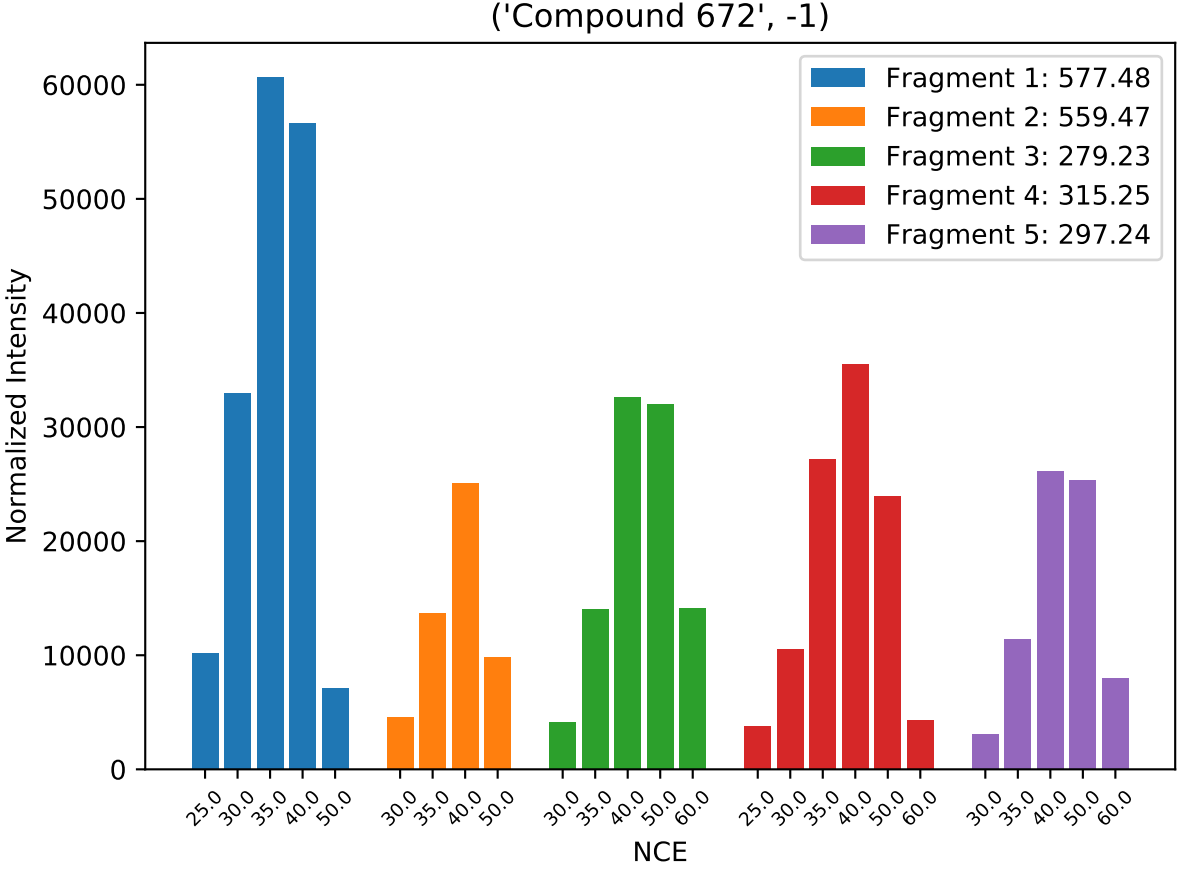

('Compound 662', -1)
Fragment 1: 281.25
Fragment 2: 255.23
Fragment 3: 253.22
Fragment 4: 283.26
Fragment 5: 519.4
Normalized Intensity
250000
200000
150000
100000
50000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
35.0
NCE

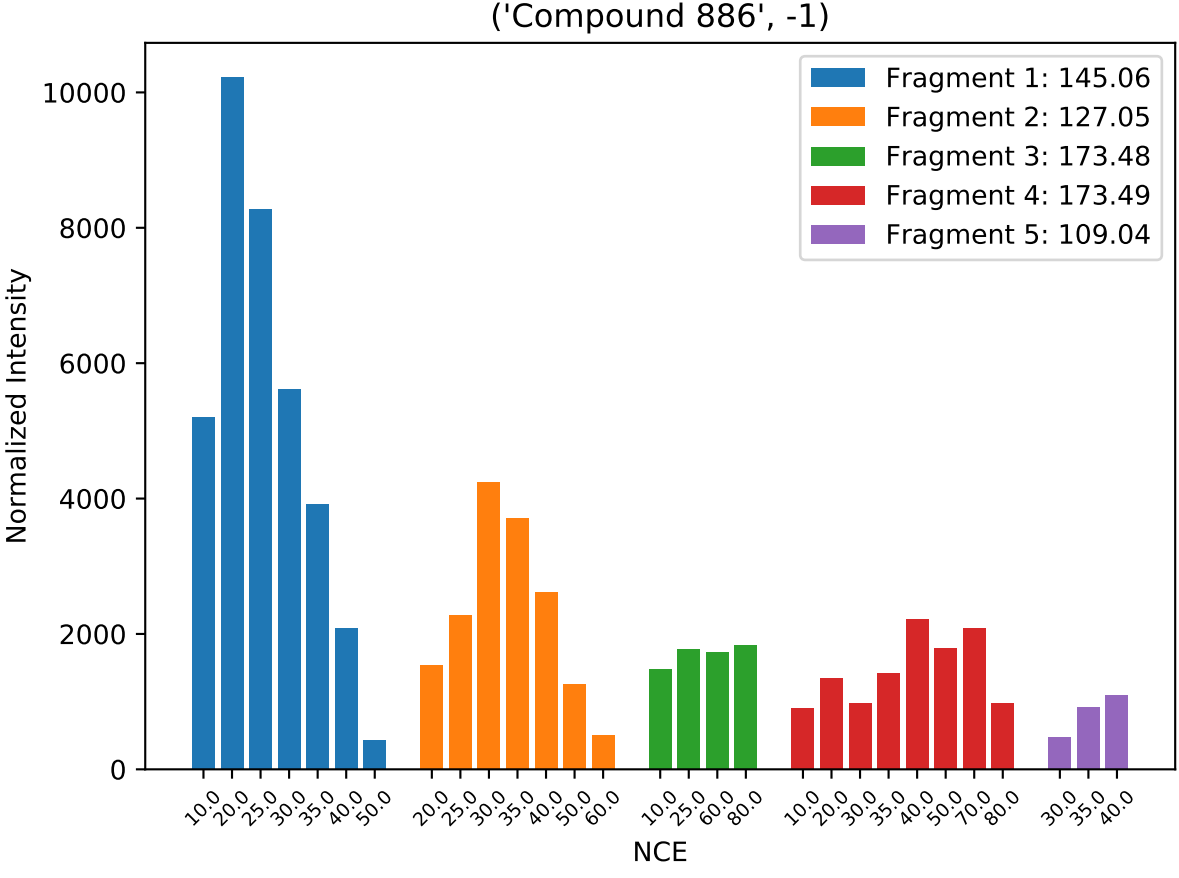

('Compound 764', -1)
Fragment 1: 151.04
Fragment 2: 173.48
Fragment 3: 107.05
Fragment 4: 173.49
Fragment 5: 183.14
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 30.0 35.0 40.0 50.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 35.0 60.0 70.0
10.0 20.0 25.0 30.0
NCE

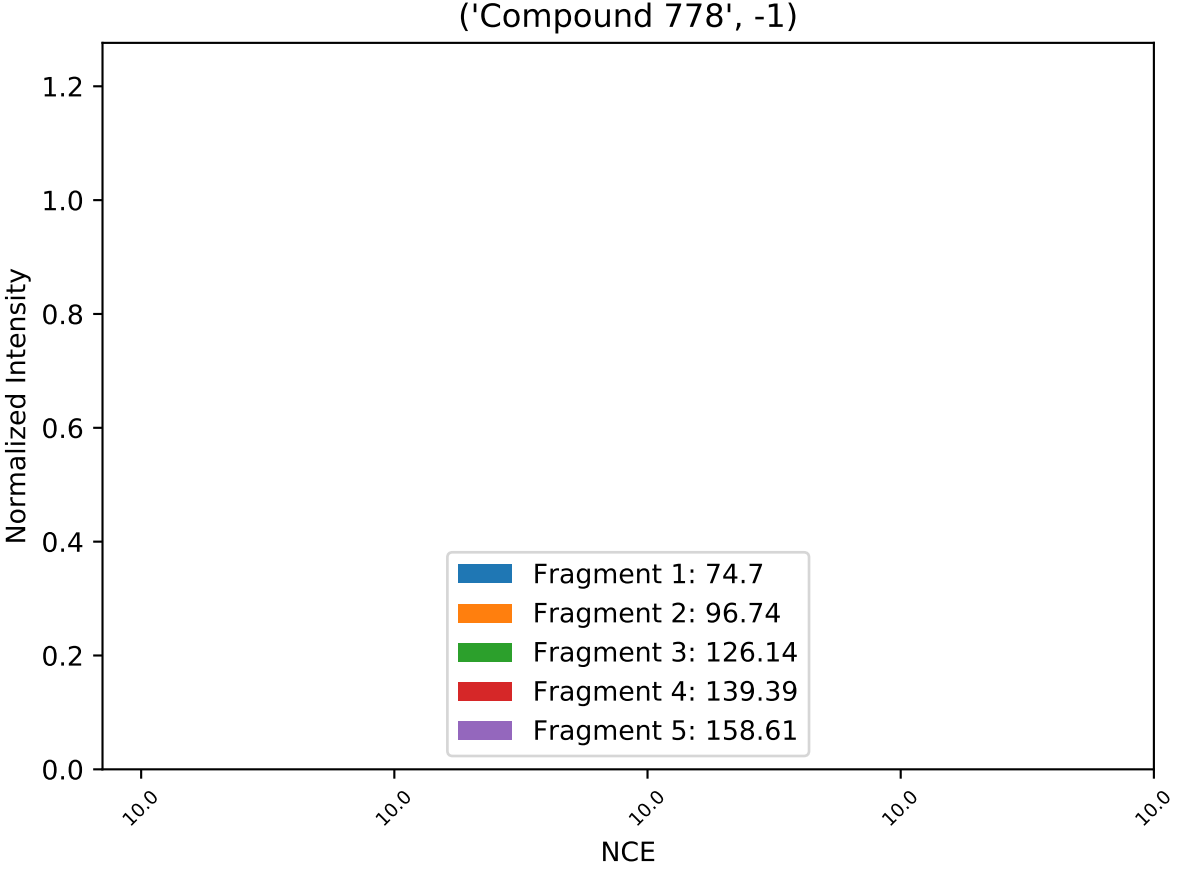

('Compound 666', -1)
Fragment 1: 201.11
Fragment 2: 171.1
Fragment 3: 279.23
Fragment 4: 277.22
Fragment 5: 79.96
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

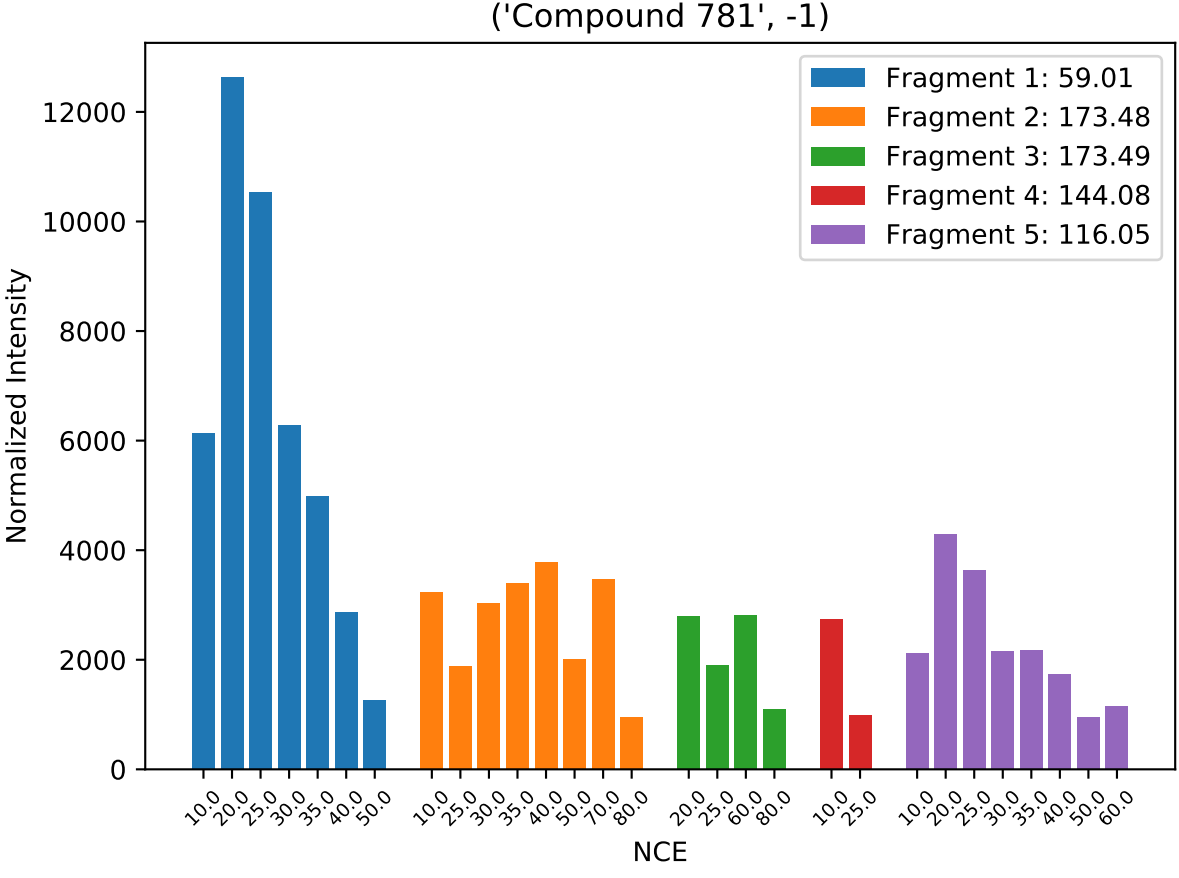

('Compound 879', -1)
Fragment 1: 140.98
Fragment 2: 57.0
Fragment 3: 122.97
Fragment 4: 59.98
Fragment 5: 138.94
Normalized Intensity
0
5000
10000
15000
20000
25000
30000
35000
40000
10.0
20.0
25.0
30.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
10.0
20.0
25.0
30.0
35.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
NCE

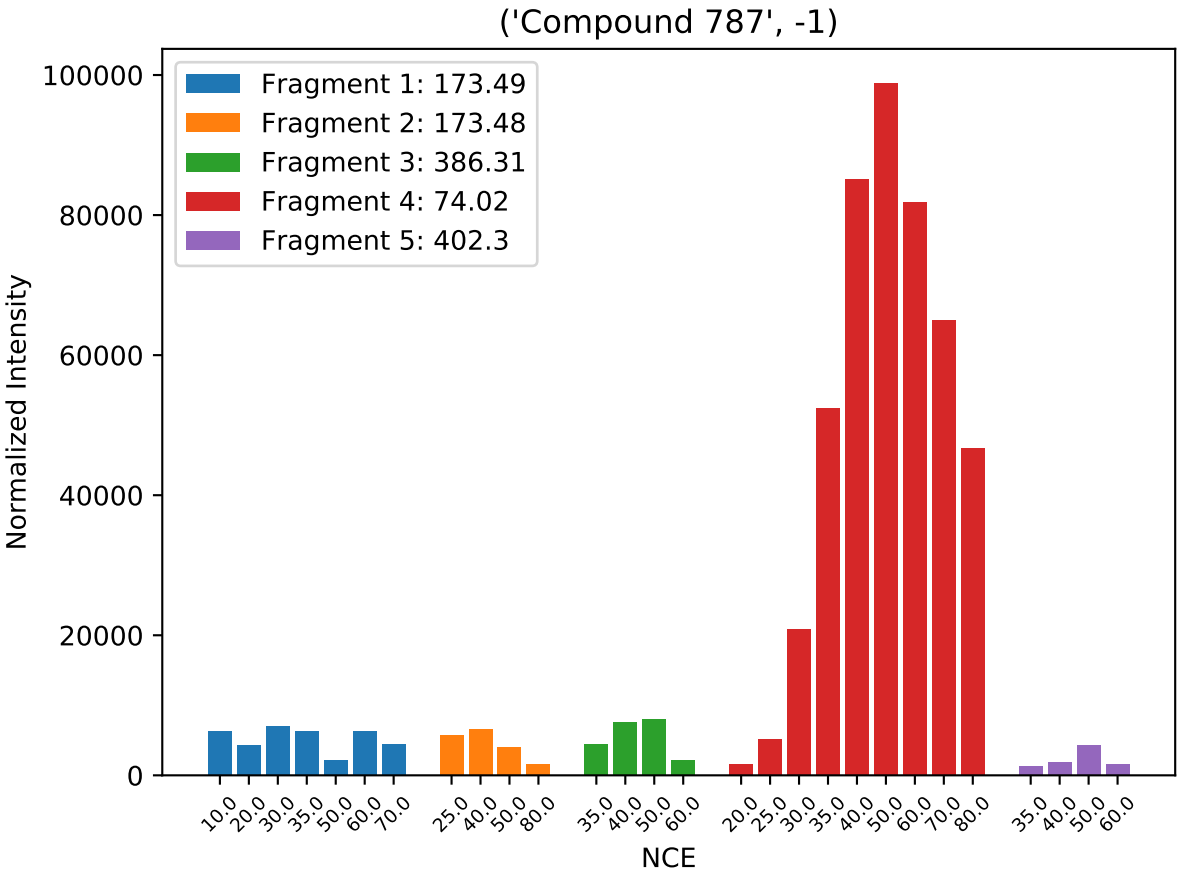

('Compound 880', -1)
Fragment 1: 93.03
Fragment 2: 149.0
Fragment 3: 173.48
Fragment 4: 173.49
Fragment 5: 78.96
Normalized Intensity
0
5000
10000
15000
20000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
25.0 35.0 50.0 60.0
10.0 20.0 30.0 40.0 50.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

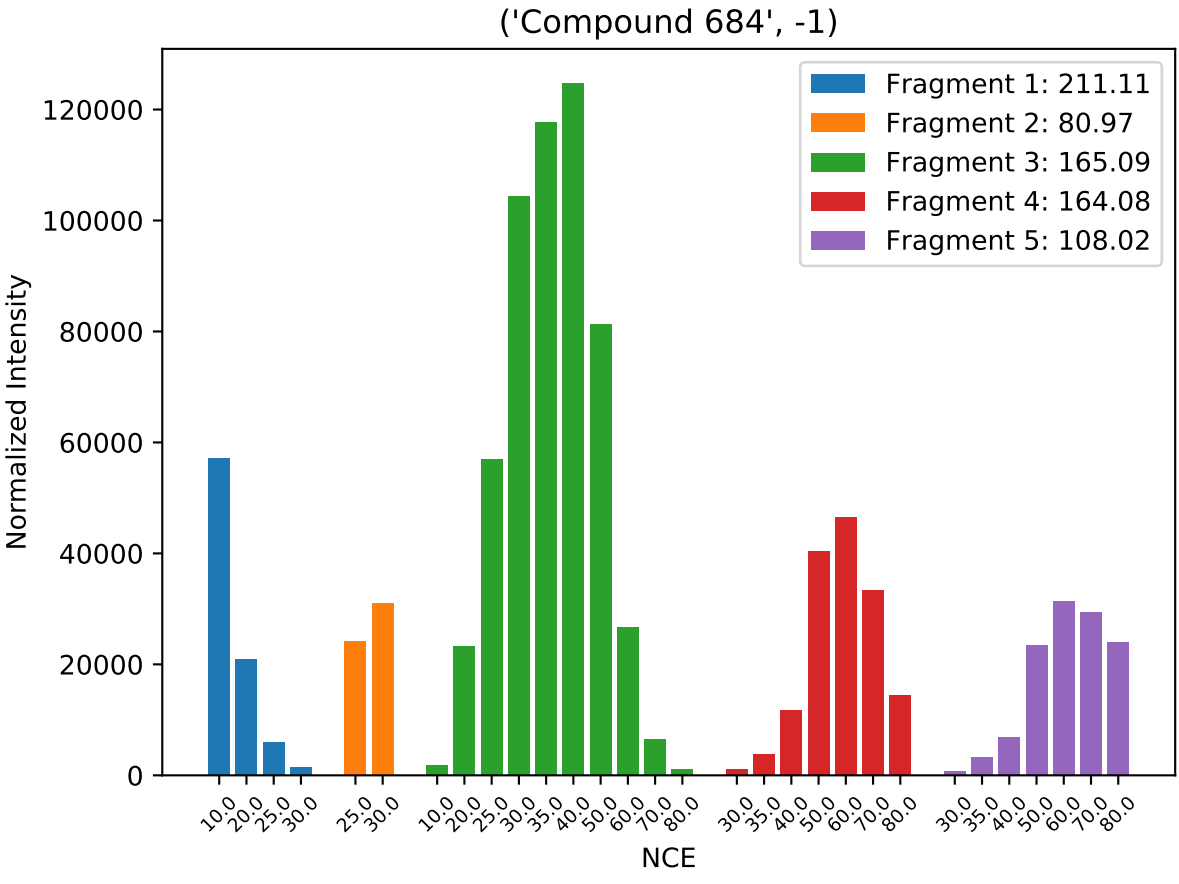

('Compound 672', -1)
Fragment 1: 577.48
Fragment 2: 559.47
Fragment 3: 279.23
Fragment 4: 315.25
Fragment 5: 297.24
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
25.0
30.0
35.0
40.0
50.0
30.0
35.0
40.0
50.0
30.0
35.0
40.0
50.0
60.0
25.0
30.0
35.0
40.0
50.0
60.0
30.0
35.0
40.0
50.0
60.0
NCE

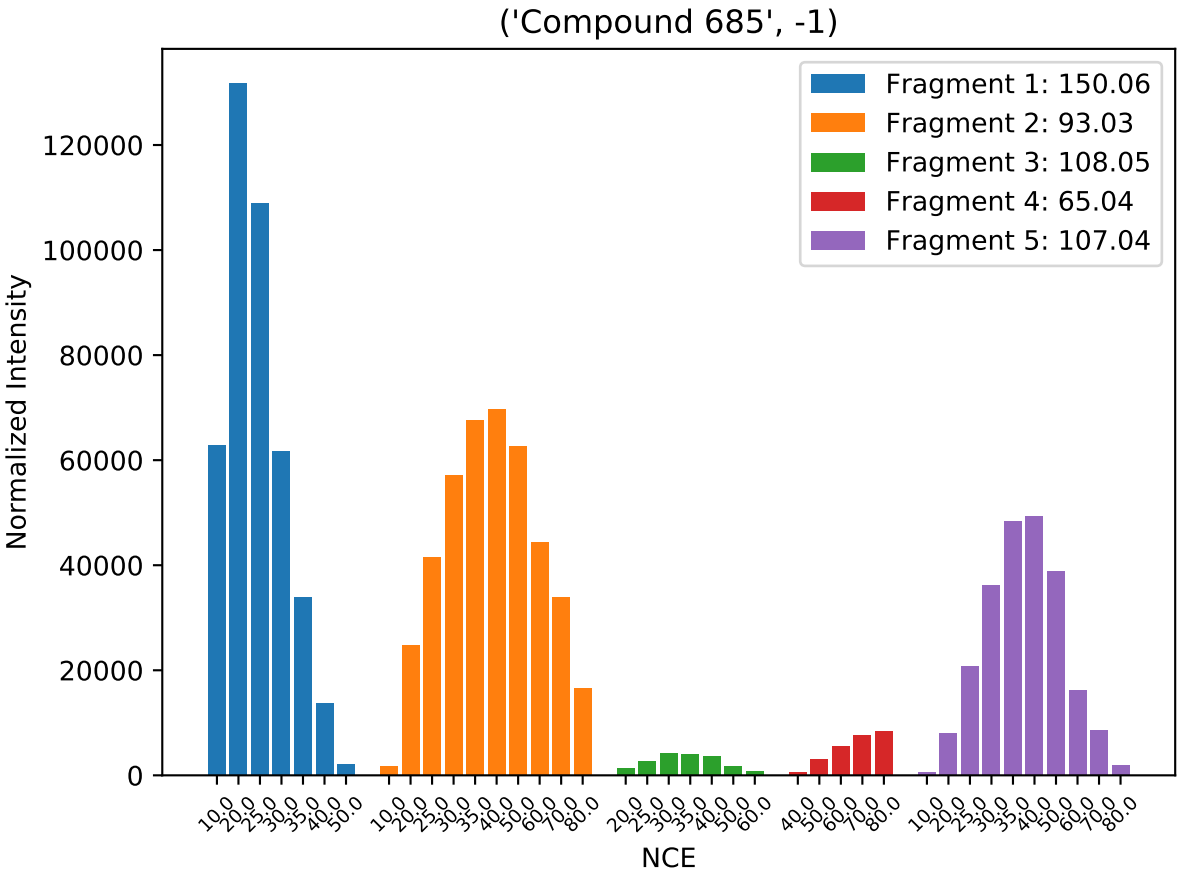

('Compound 886', -1)
Fragment 1: 145.06
Fragment 2: 127.05
Fragment 3: 173.48
Fragment 4: 173.49
Fragment 5: 109.04
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 25.0 60.0 80.0
10.0 20.0 30.0 35.0 40.0 50.0 70.0 80.0
30.0 35.0 40.0
NCE

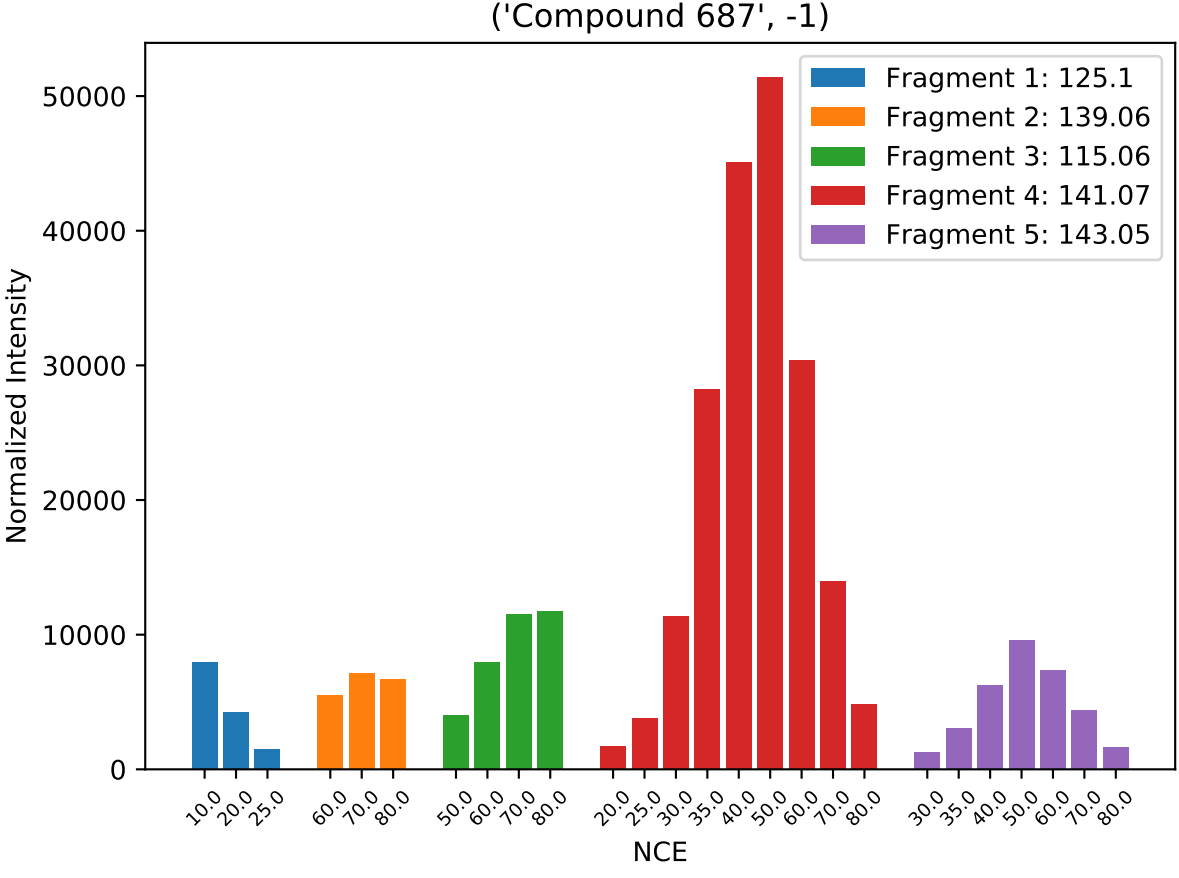

('Compound 778', -1)
Normalized Intensity
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Fragment 1: 74.7
Fragment 2: 96.74
Fragment 3: 126.14
Fragment 4: 139.39
Fragment 5: 158.61
10.0
10.0
10.0
10.0
10.0
NCE

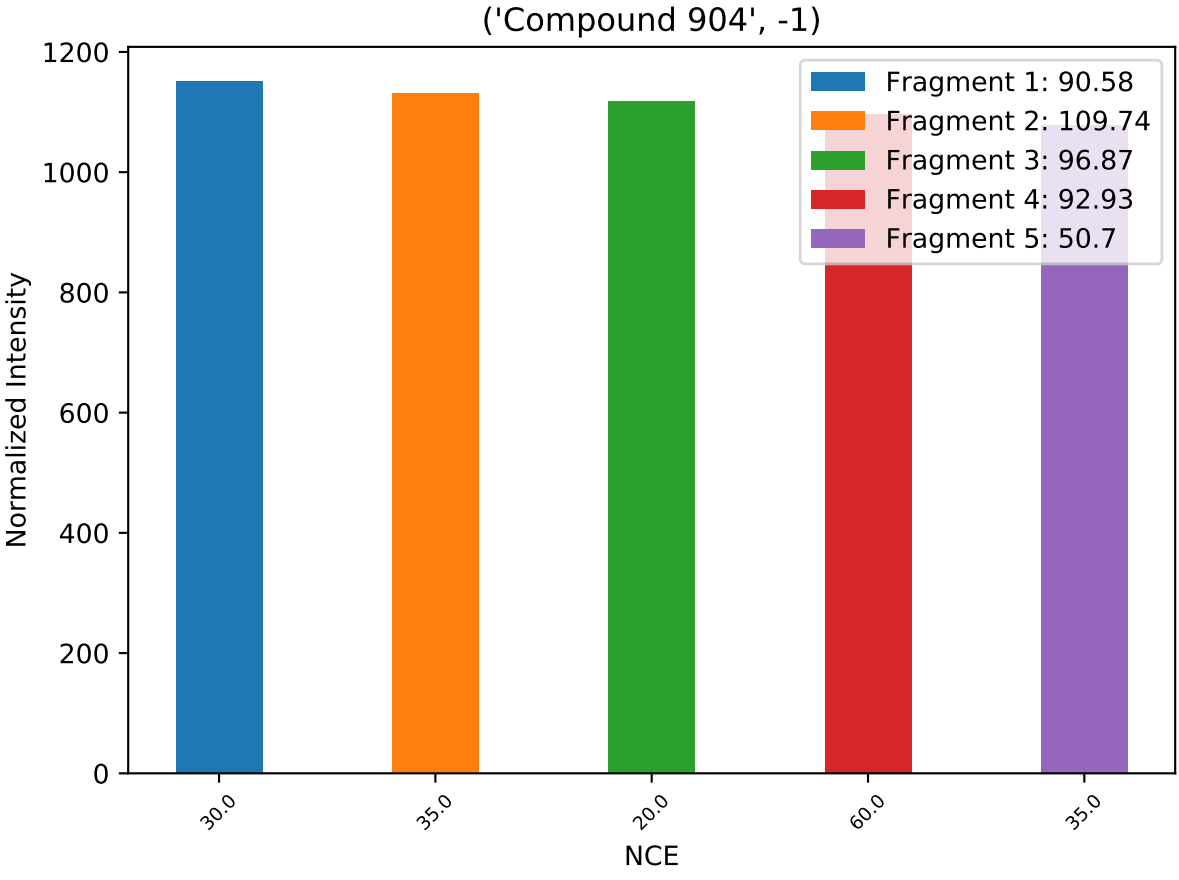

('Compound 781', -1)
Fragment 1: 59.01
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 144.08
Fragment 5: 116.05
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 25.0 30.0 35.0 40.0 50.0 70.0 80.0
20.0 25.0 60.0 80.0
10.0 25.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

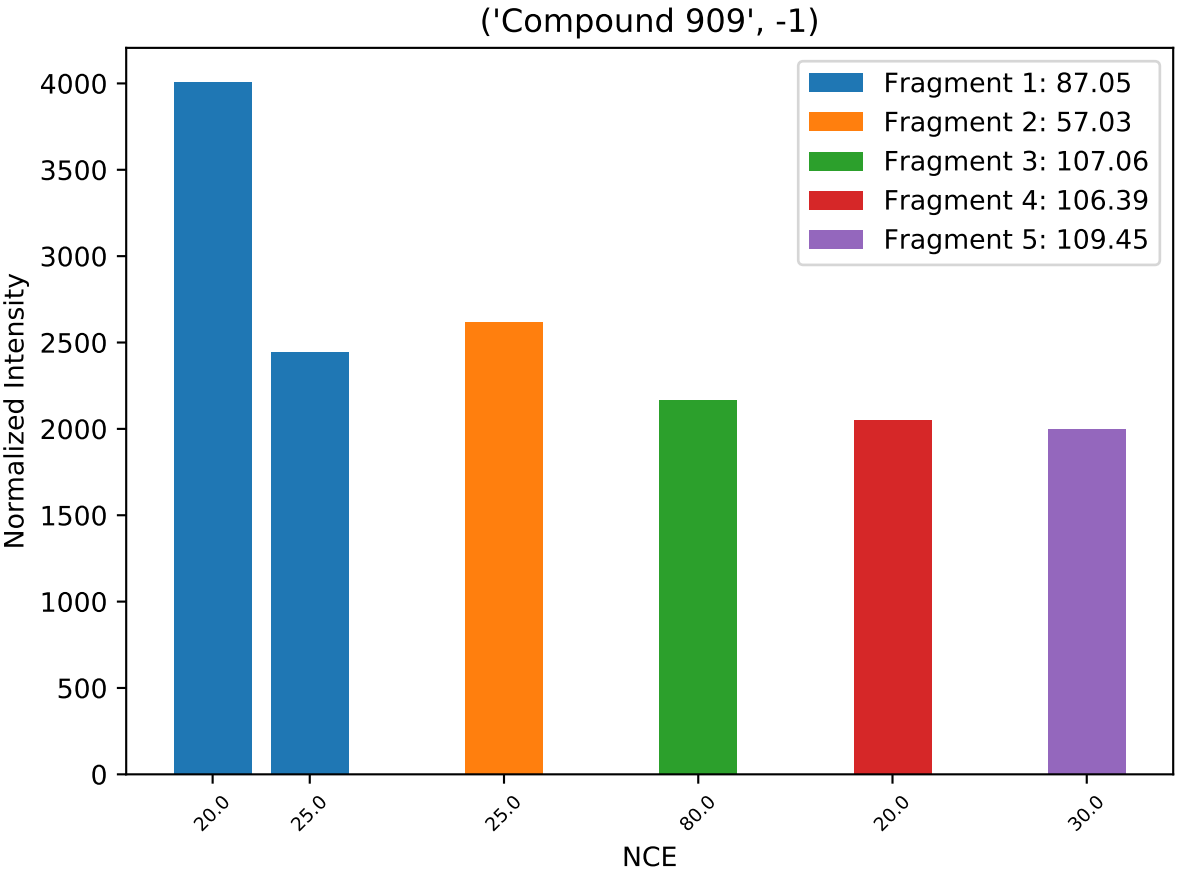

('Compound 787', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 386.31
Fragment 4: 74.02
Fragment 5: 402.3
Normalized Intensity
100000
80000
60000
40000
20000
0
10.0 20.0 30.0 35.0 50.0 60.0 70.0
25.0 40.0 50.0 80.0
35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0
NCE

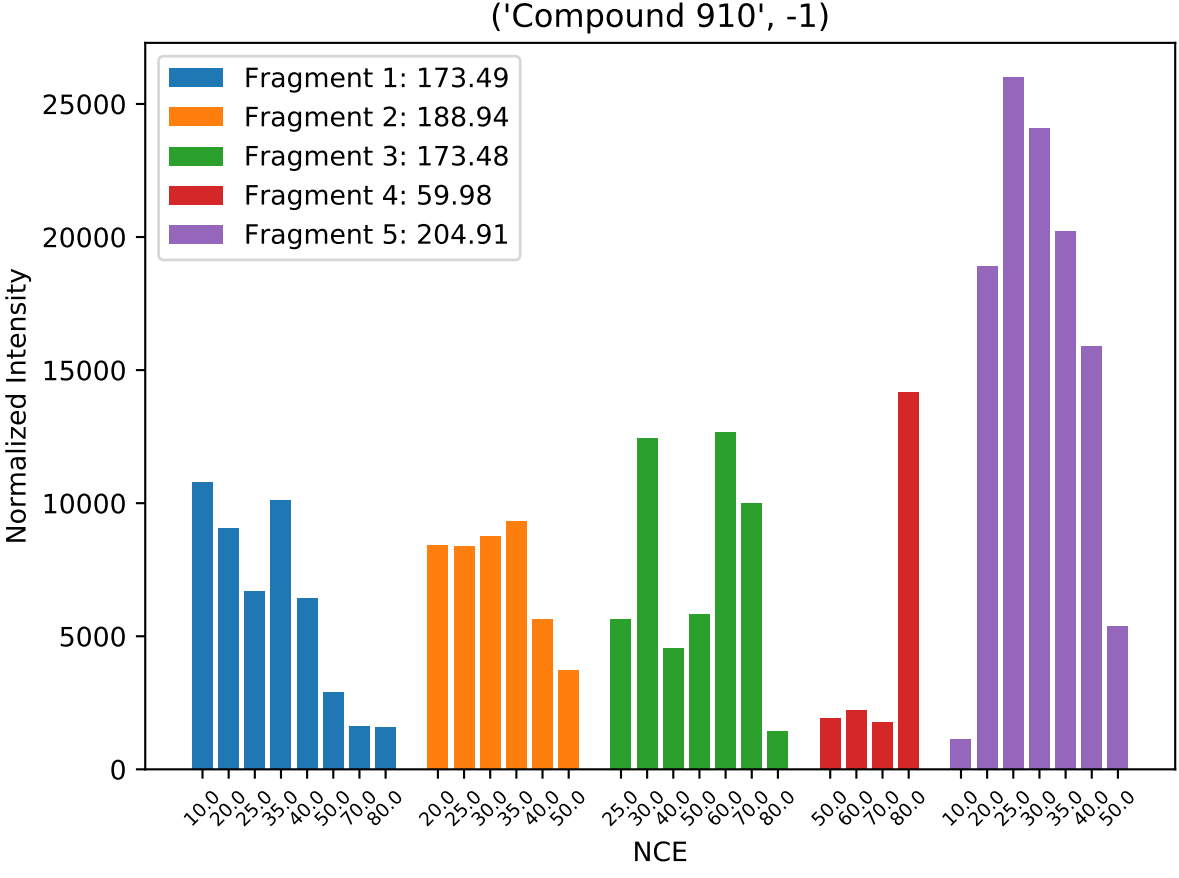

('Compound 684', -1)
Fragment 1: 211.11
Fragment 2: 80.97
Fragment 3: 165.09
Fragment 4: 164.08
Fragment 5: 108.02
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
NCE
10.0 20.0 25.0 30.0
25.0 30.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0

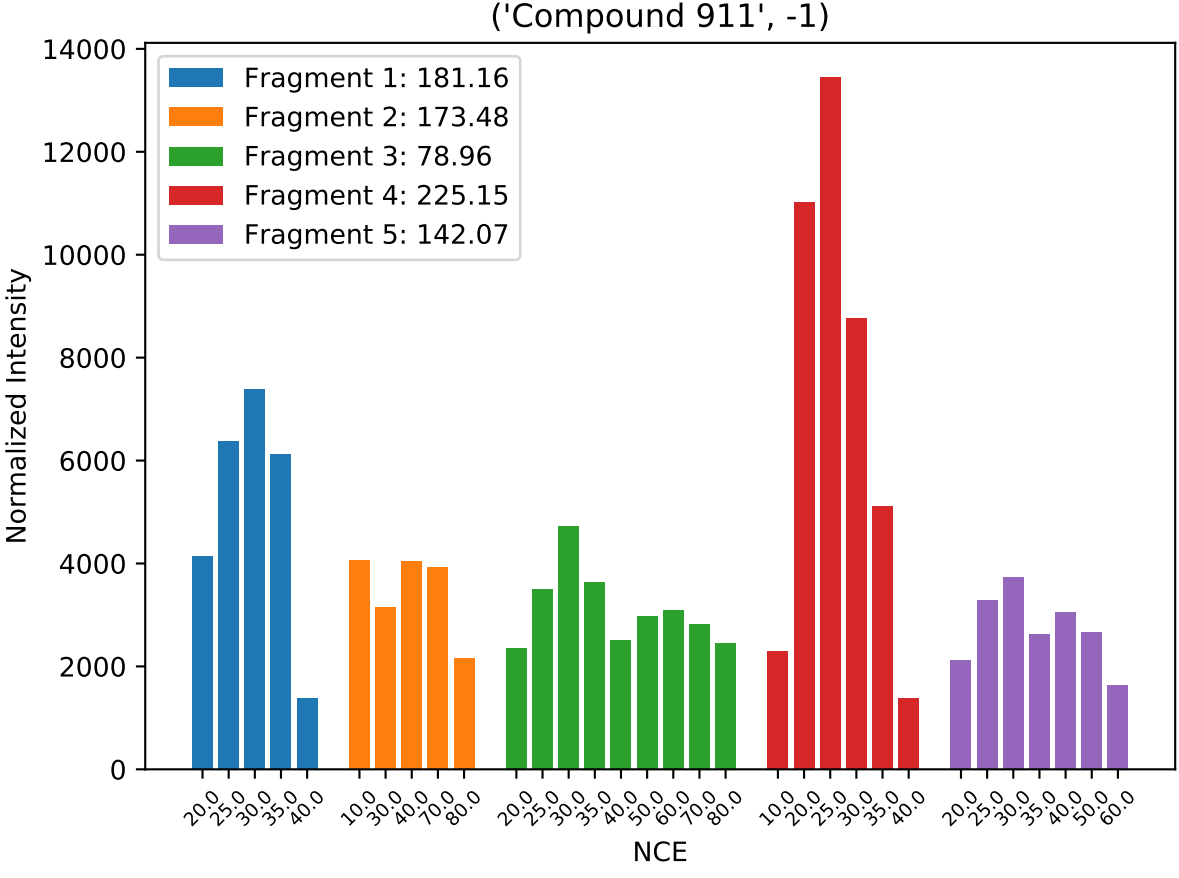

('Compound 685', -1)
Fragment 1: 150.06
Fragment 2: 93.03
Fragment 3: 108.05
Fragment 4: 65.04
Fragment 5: 107.04
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

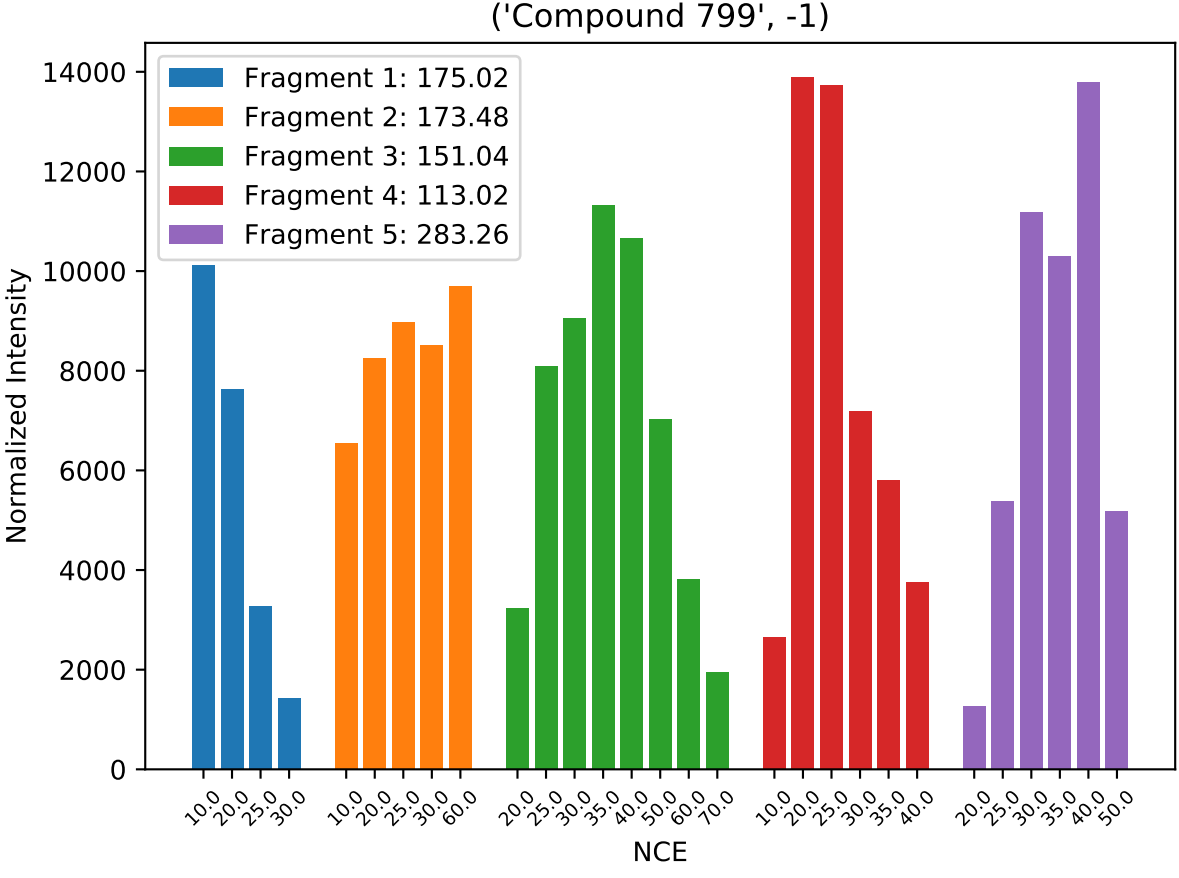

('Compound 687', -1)
Fragment 1: 125.1
Fragment 2: 139.06
Fragment 3: 115.06
Fragment 4: 141.07
Fragment 5: 143.05
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0 20.0 25.0
60.0 70.0 80.0
50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

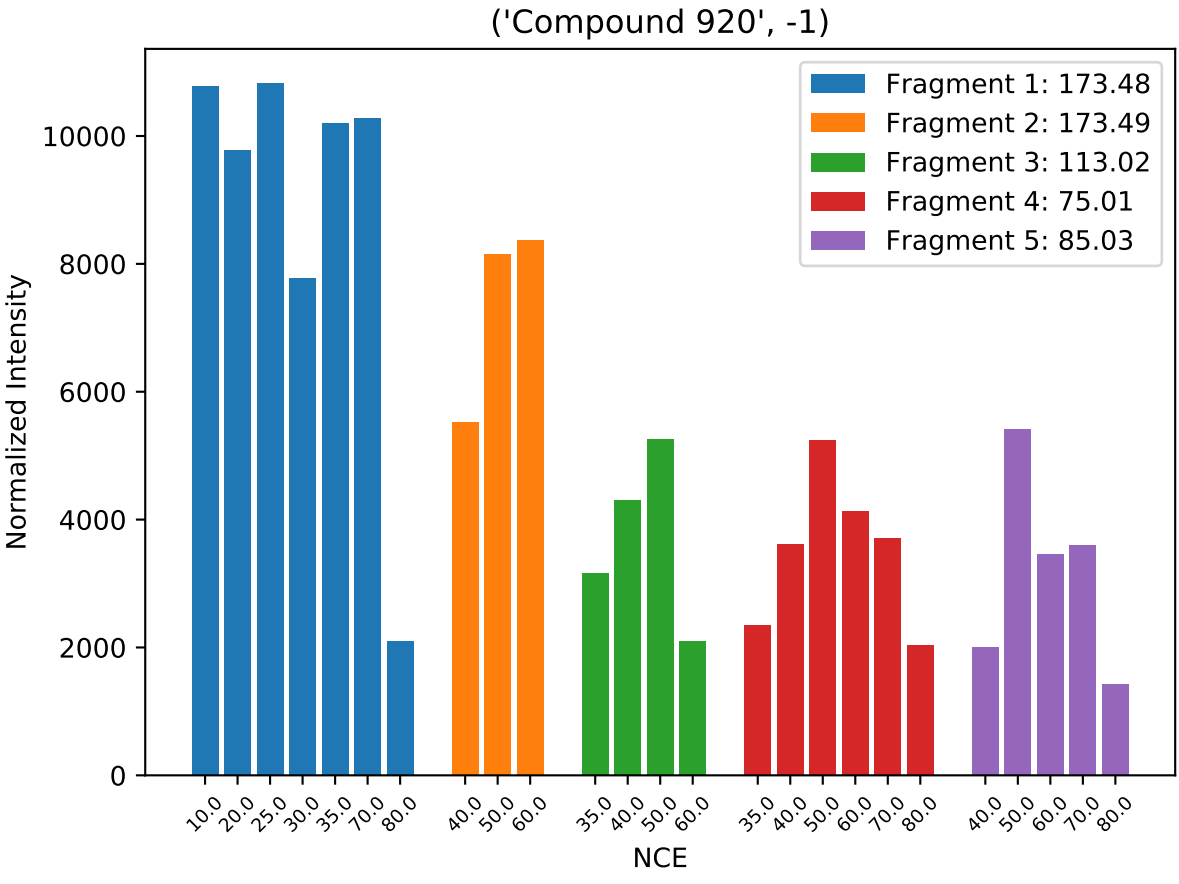

('Compound 904', -1)
Fragment 1: 90.58
Fragment 2: 109.74
Fragment 3: 96.87
Fragment 4: 92.93
Fragment 5: 50.7
Normalized Intensity
0
200
400
600
800
1000
1200
30.0
35.0
20.0
60.0
35.0
NCE

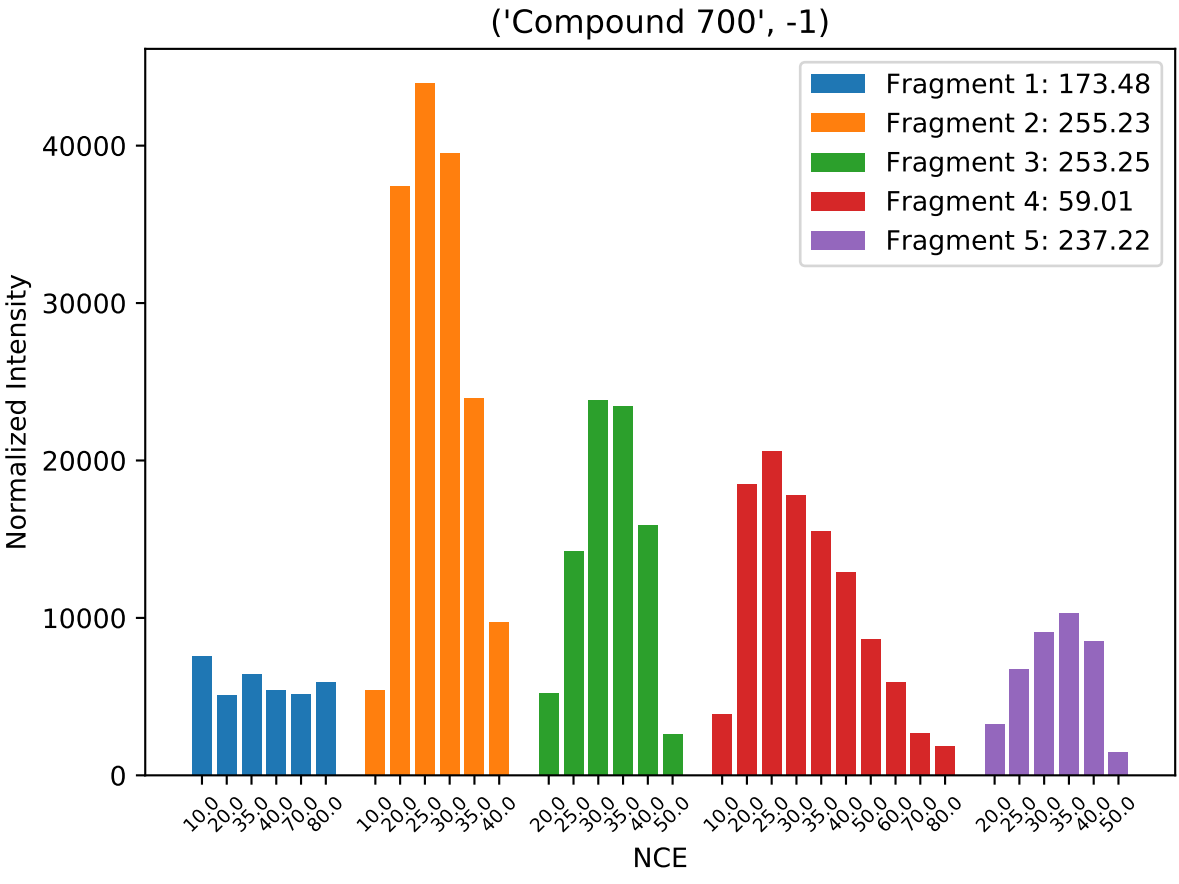

('Compound 909', -1)
Fragment 1: 87.05
Fragment 2: 57.03
Fragment 3: 107.06
Fragment 4: 106.39
Fragment 5: 109.45
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
20.0
25.0
25.0
80.0
20.0
30.0
NCE

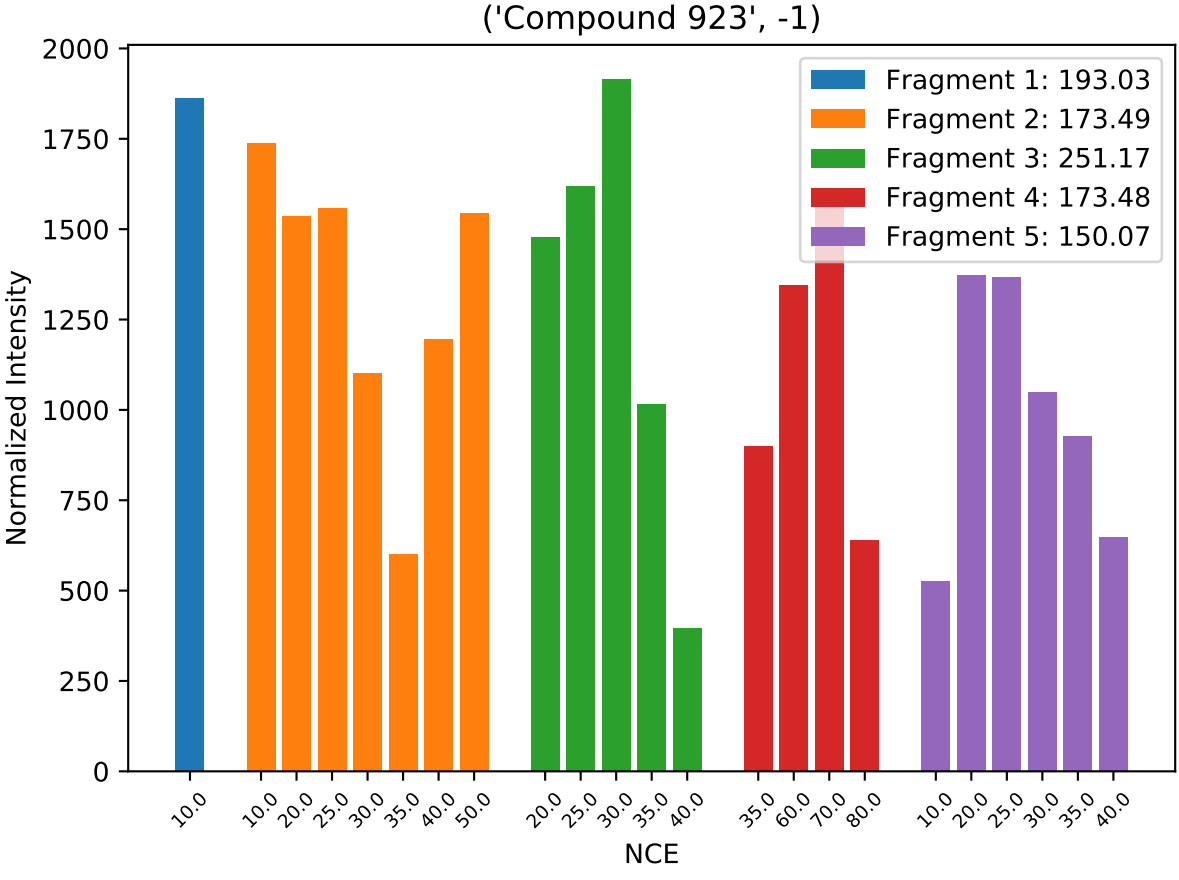

('Compound 910', -1)
Fragment 1: 173.49
Fragment 2: 188.94
Fragment 3: 173.48
Fragment 4: 59.98
Fragment 5: 204.91
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0 20.0 25.0 35.0 40.0 50.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
25.0 30.0 40.0 50.0 60.0 70.0 80.0
50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
NCE

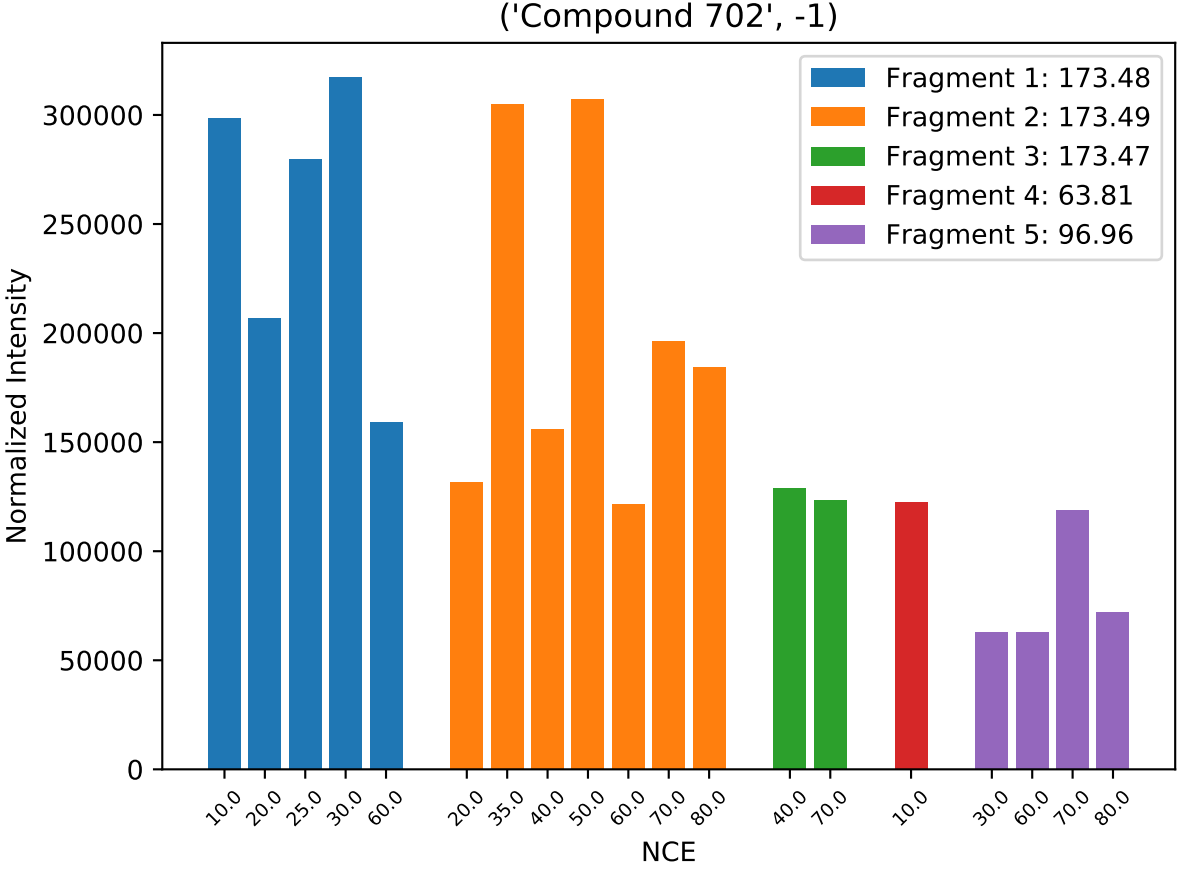

('Compound 911', -1)
Fragment 1: 181.16
Fragment 2: 173.48
Fragment 3: 78.96
Fragment 4: 225.15
Fragment 5: 142.07
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
20.0 25.0 30.0 35.0 40.0
10.0 30.0 40.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

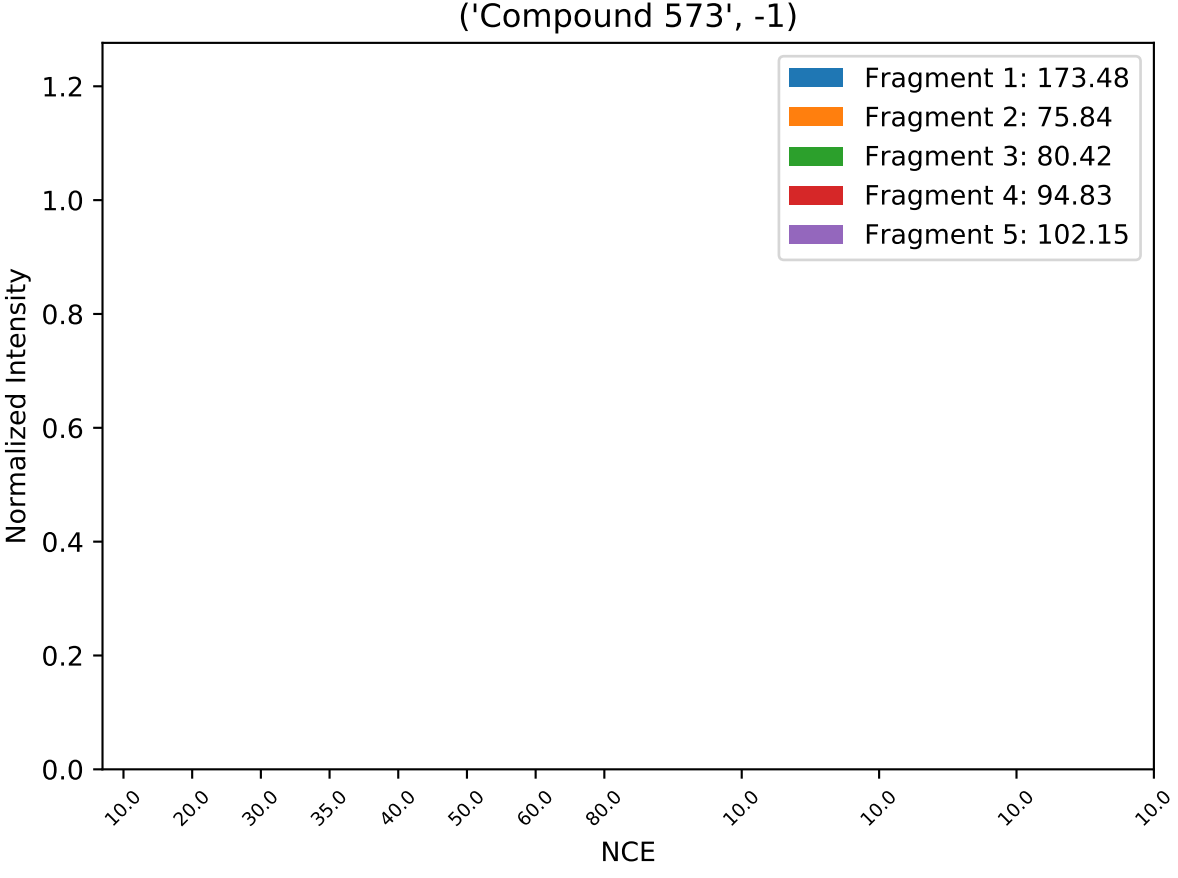

('Compound 799', -1)
Fragment 1: 175.02
Fragment 2: 173.48
Fragment 3: 151.04
Fragment 4: 113.02
Fragment 5: 283.26
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0 20.0 25.0 30.0
10.0 20.0 25.0 30.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0
NCE

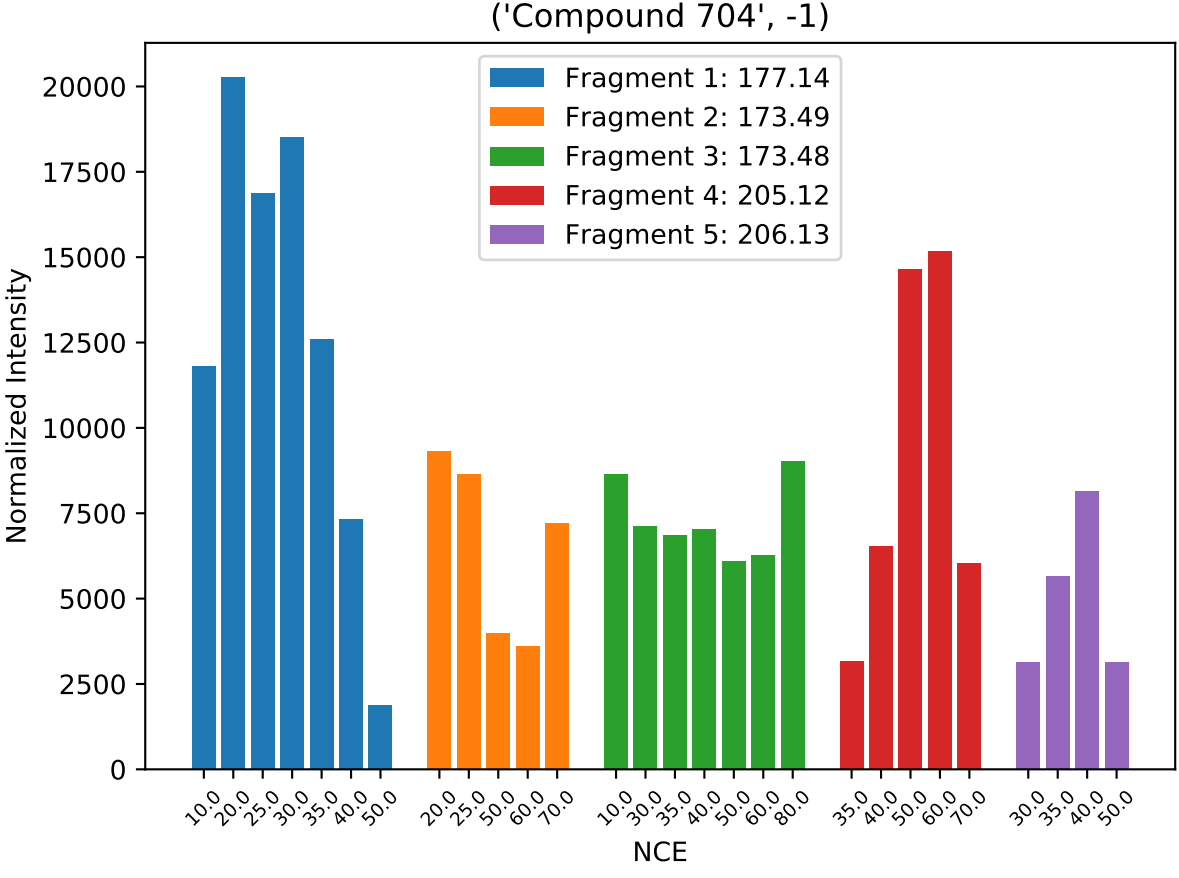

('Compound 920', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 113.02
Fragment 4: 75.01
Fragment 5: 85.03
Normalized Intensity
0
2000
4000
6000
8000
10000
10.0
20.0
25.0
30.0
35.0
70.0
80.0
40.0
50.0
60.0
35.0
40.0
50.0
60.0
35.0
40.0
50.0
60.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
NCE

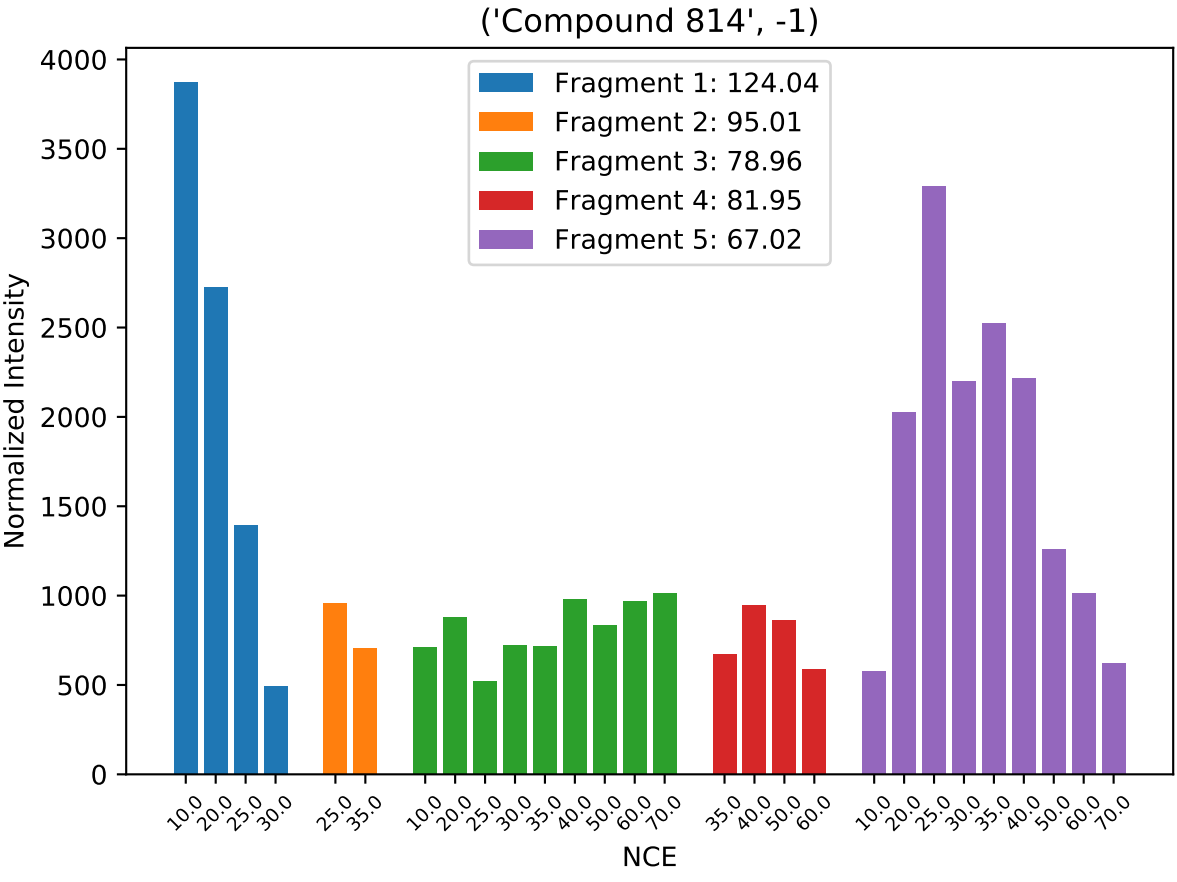

('Compound 700', -1)
Fragment 1: 173.48
Fragment 2: 255.23
Fragment 3: 253.25
Fragment 4: 59.01
Fragment 5: 237.22
Normalized Intensity
0
10000
20000
30000
40000
10.0 20.0 35.0 40.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0
NCE

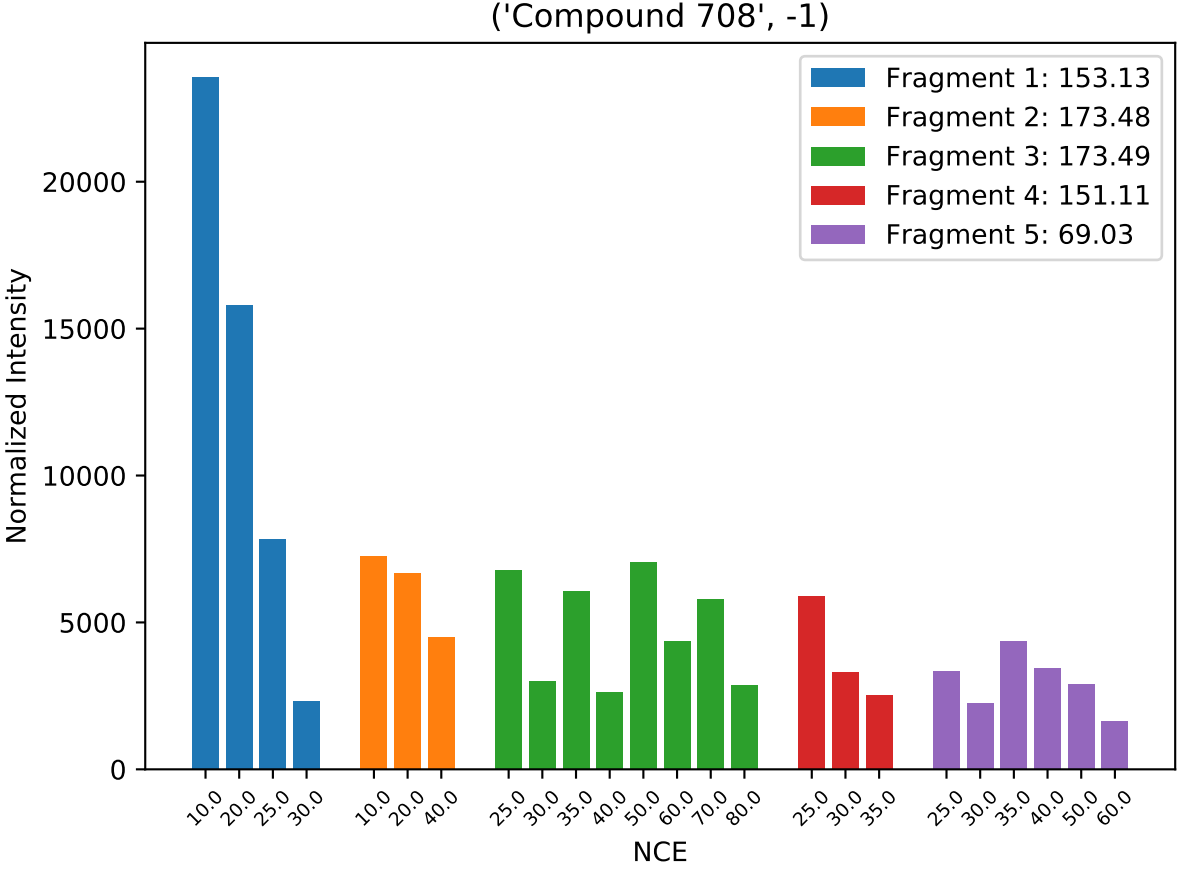

('Compound 923', -1)
Fragment 1: 193.03
Fragment 2: 173.49
Fragment 3: 251.17
Fragment 4: 173.48
Fragment 5: 150.07
Normalized Intensity
NCE
2000
1750
1500
1250
1000
750
500
250
0
10.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
20.0
25.0
30.0
35.0
40.0
35.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0

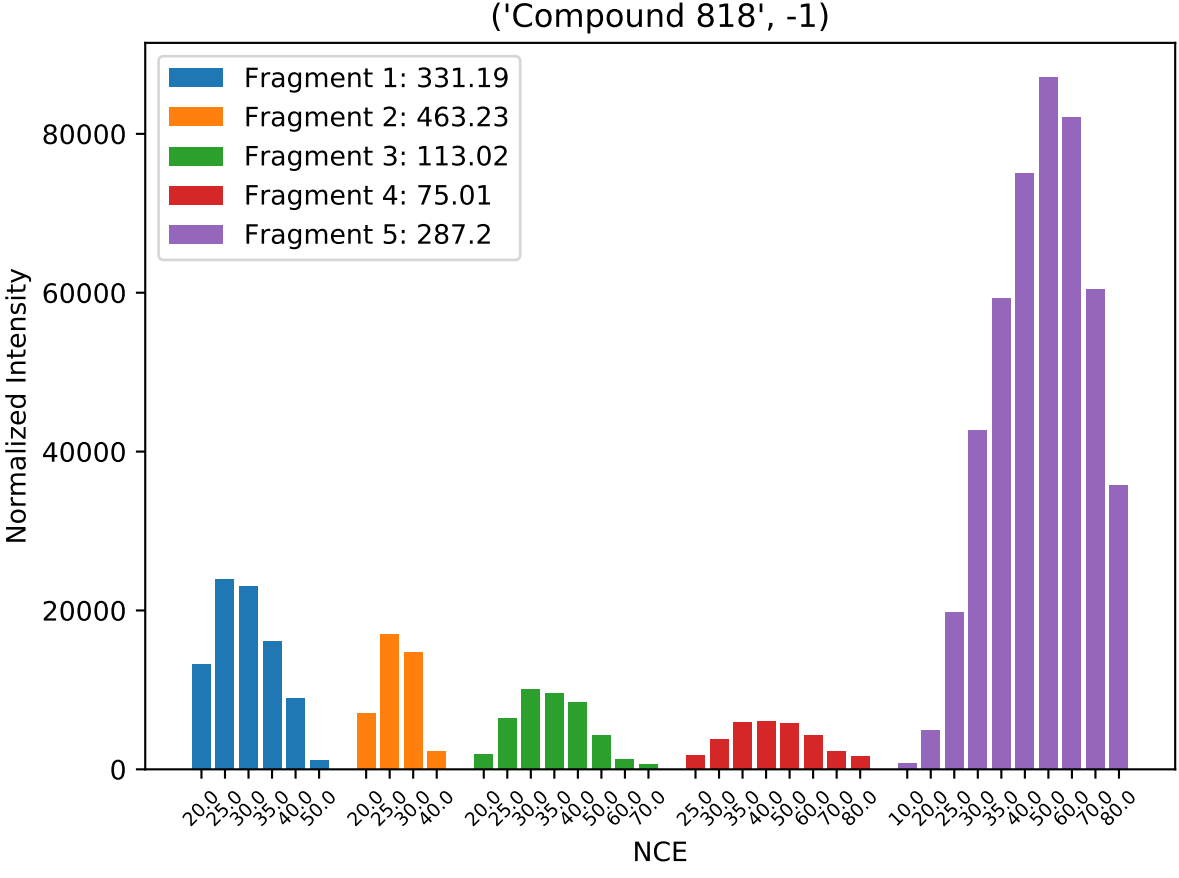

('Compound 702', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 173.47
Fragment 4: 63.81
Fragment 5: 96.96
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
10.0
20.0
25.0
30.0
60.0
20.0
35.0
40.0
50.0
60.0
70.0
80.0
40.0
70.0
10.0
30.0
60.0
70.0
80.0
NCE

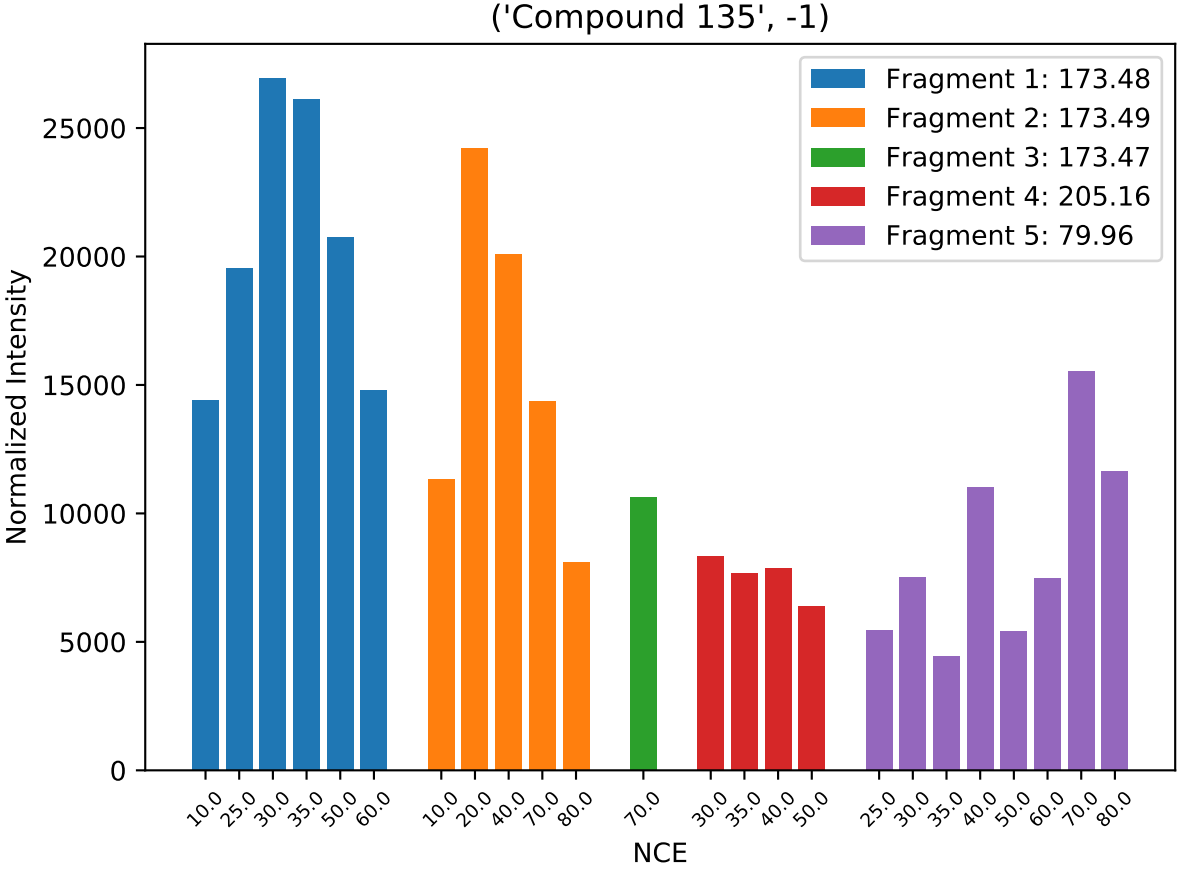

('Compound 573', -1)
Fragment 1: 173.48
Fragment 2: 75.84
Fragment 3: 80.42
Fragment 4: 94.83
Fragment 5: 102.15
Normalized Intensity
0.0
0.2
0.4
0.6
0.8
1.0
1.2
10.0
20.0
30.0
35.0
40.0
50.0
60.0
80.0
10.0
10.0
10.0
10.0
NCE

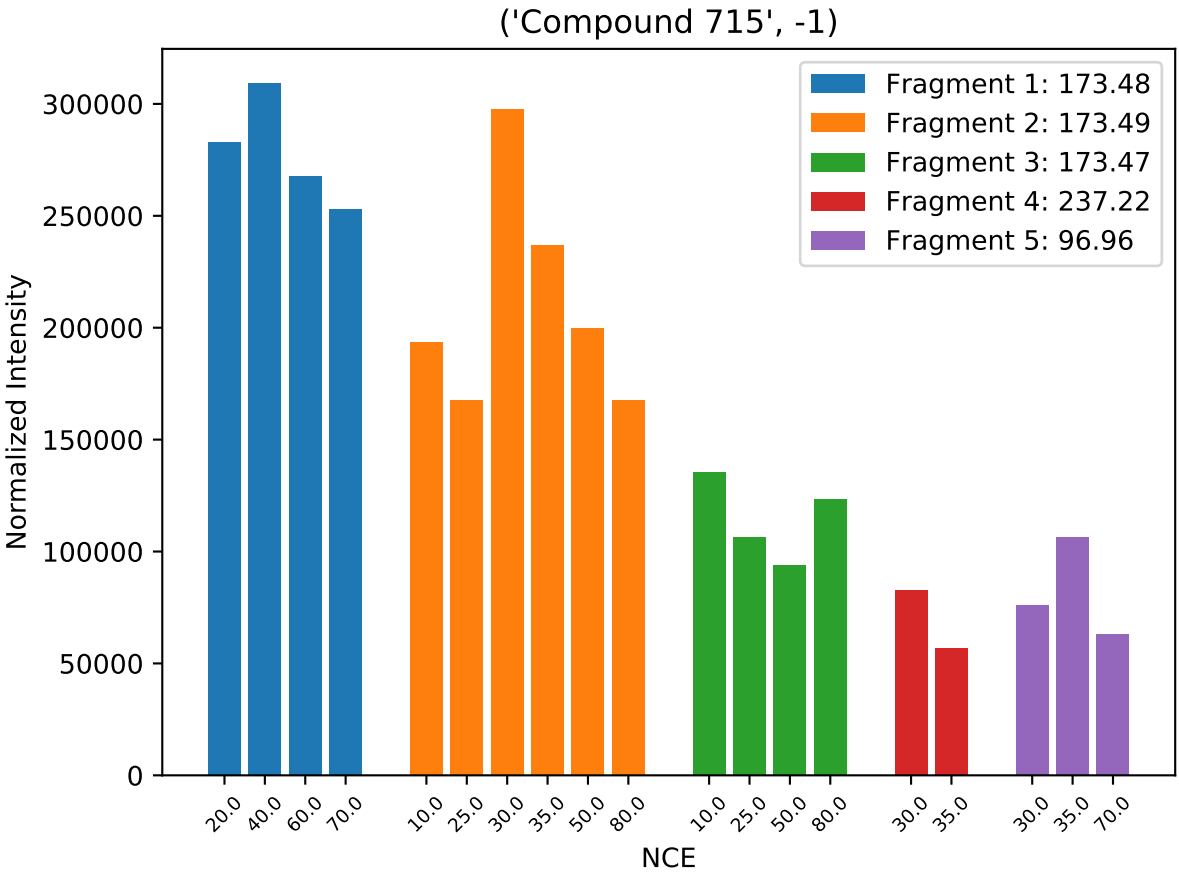

('Compound 704', -1)
Fragment 1: 177.14
Fragment 2: 173.49
Fragment 3: 173.48
Fragment 4: 205.12
Fragment 5: 206.13
Normalized Intensity
0
2500
5000
7500
10000
12500
15000
17500
20000
10.0 20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 50.0 60.0 70.0
10.0 30.0 35.0 40.0 50.0 60.0 80.0
35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0
NCE

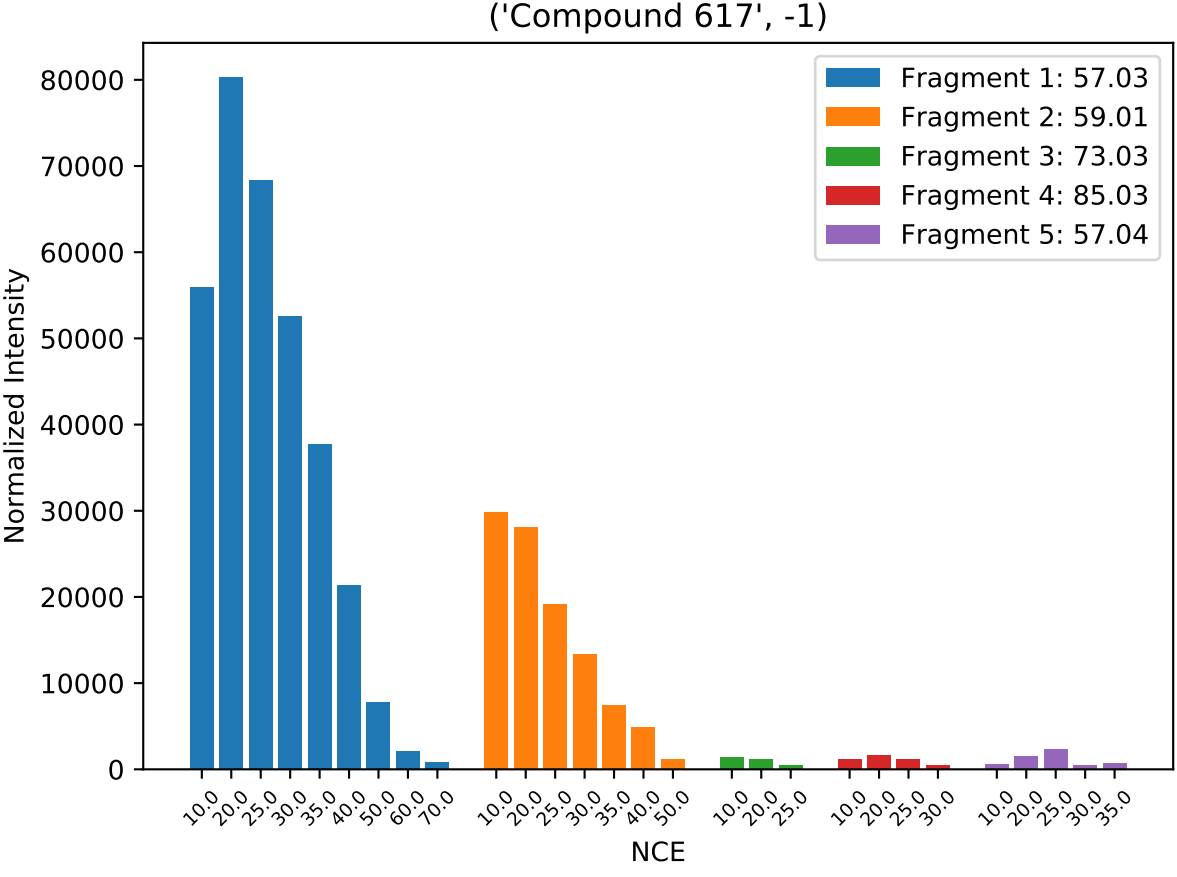

('Compound 814', -1)
Fragment 1: 124.04
Fragment 2: 95.01
Fragment 3: 78.96
Fragment 4: 81.95
Fragment 5: 67.02
Normalized Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
10.0
20.0
25.0
30.0
25.0
35.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
35.0
40.0
50.0
60.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

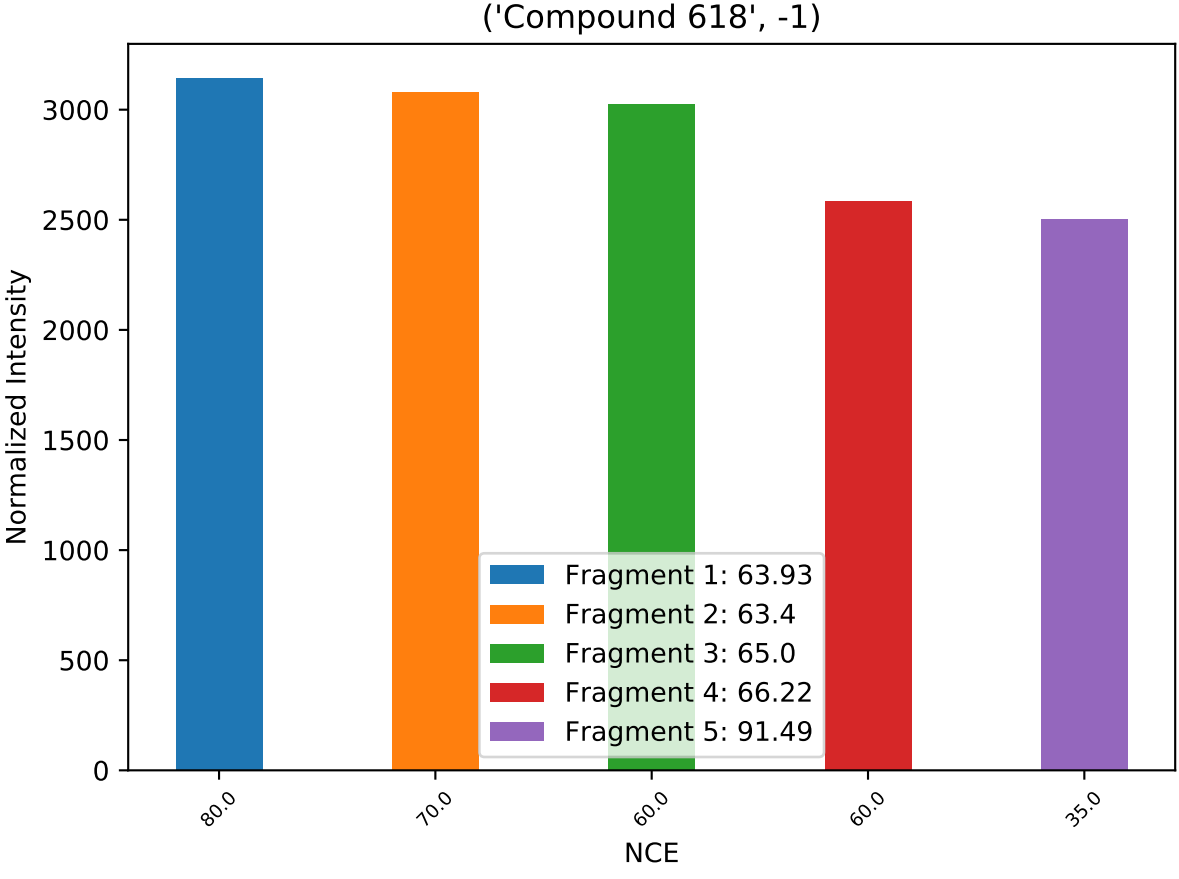

('Compound 708', -1)
Fragment 1: 153.13
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 151.11
Fragment 5: 69.03
Normalized Intensity
0
5000
10000
15000
20000
10.0
20.0
25.0
30.0
10.0
20.0
40.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
30.0
35.0
25.0
30.0
35.0
40.0
50.0
60.0
NCE

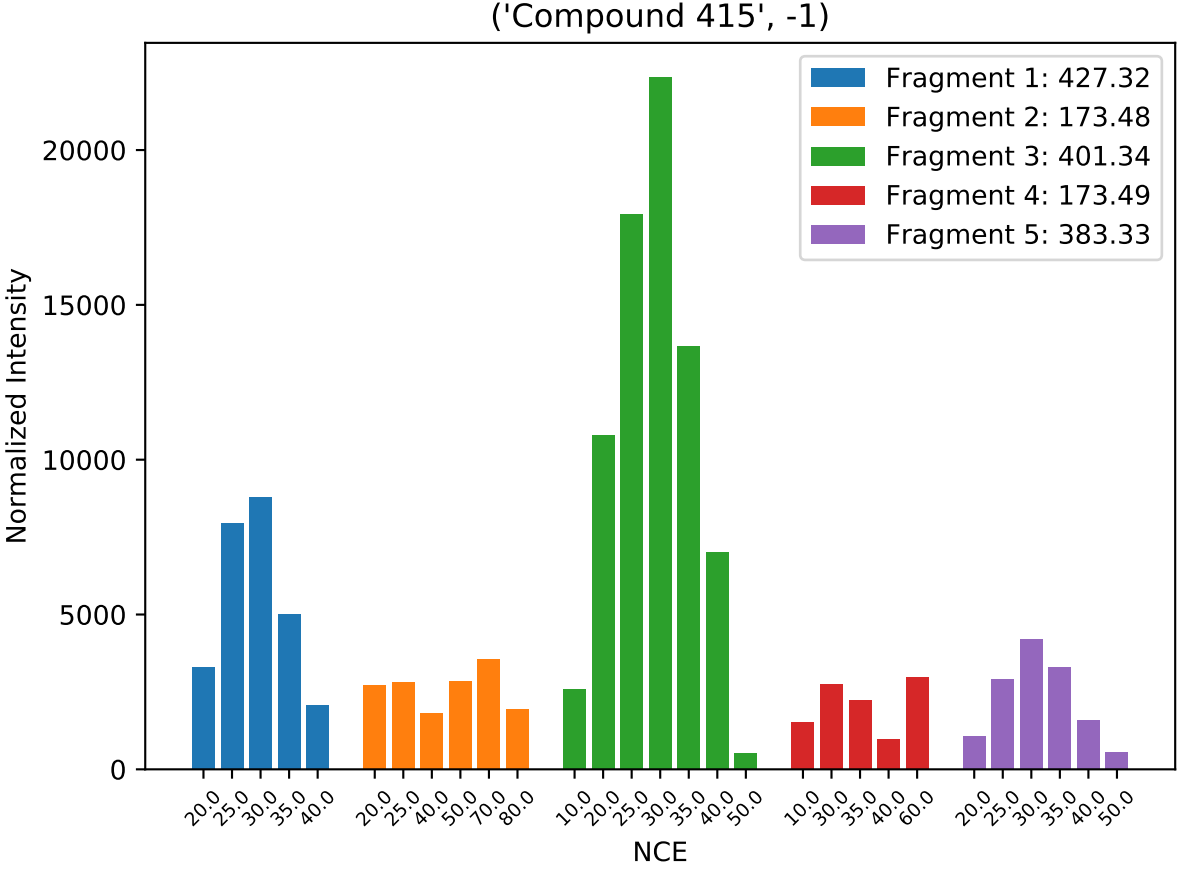

('Compound 818', -1)
Fragment 1: 331.19
Fragment 2: 463.23
Fragment 3: 113.02
Fragment 4: 75.01
Fragment 5: 287.2
Normalized Intensity
0
20000
40000
60000
80000
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 40.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

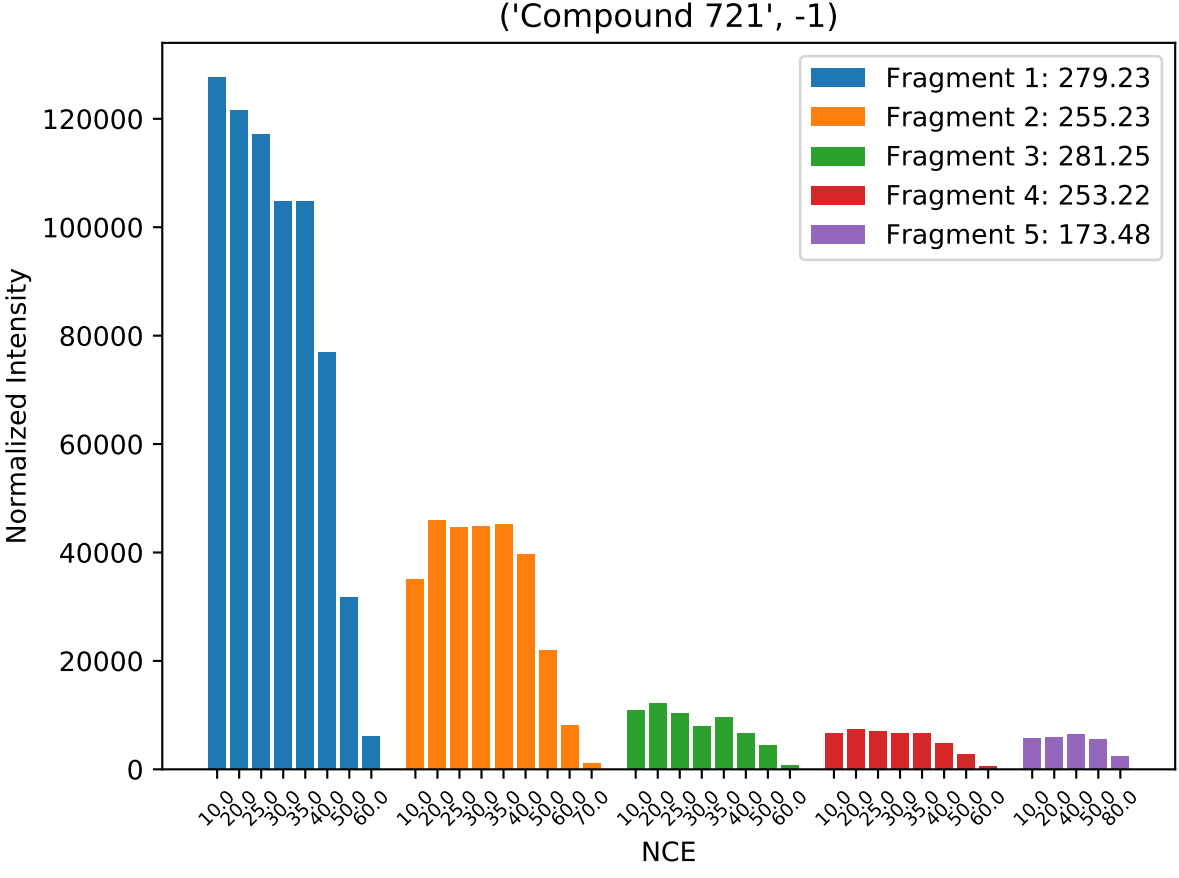

('Compound 135', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 173.47
Fragment 4: 205.16
Fragment 5: 79.96
Normalized Intensity
0
5000
10000
15000
20000
25000
10.0
25.0
30.0
35.0
50.0
60.0
10.0
20.0
40.0
70.0
80.0
70.0
30.0
35.0
40.0
50.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
NCE

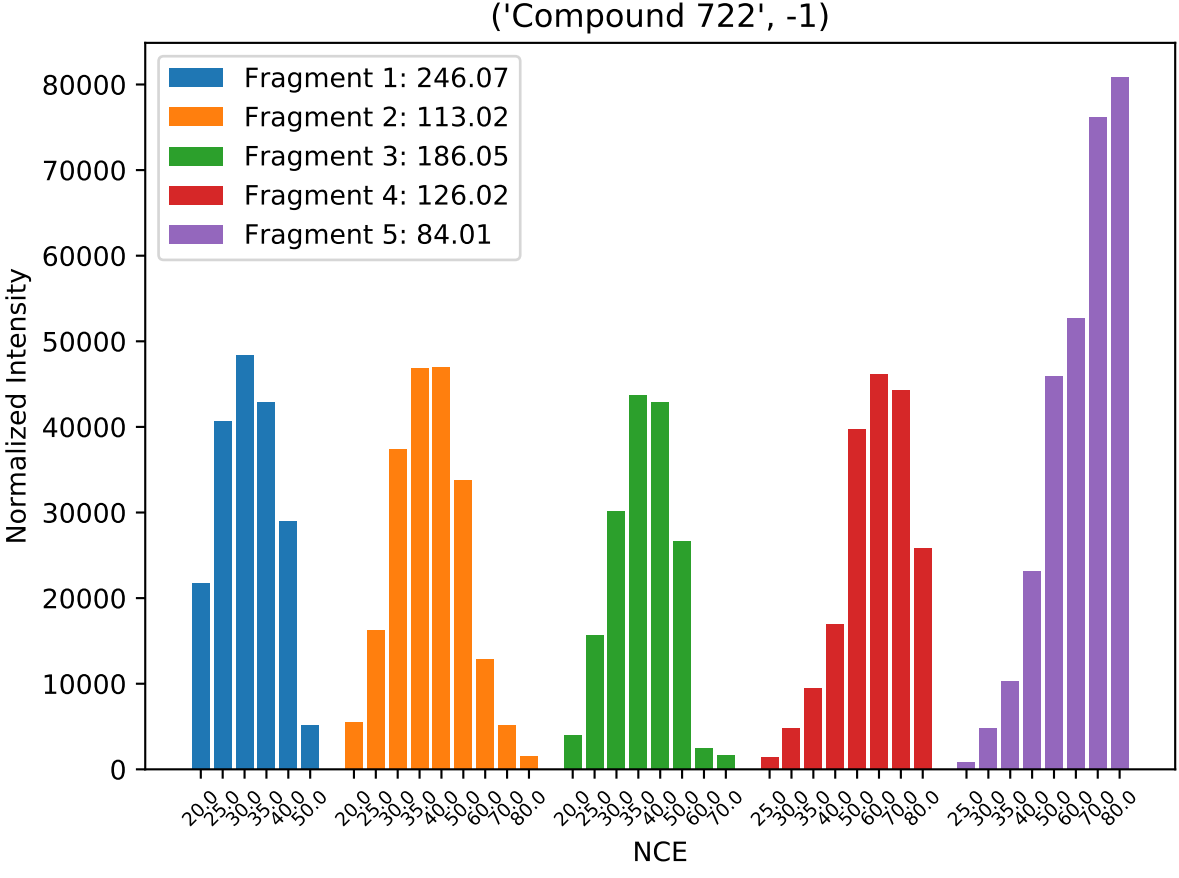

('Compound 715', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 173.47
Fragment 4: 237.22
Fragment 5: 96.96
Normalized Intensity
0
50000
100000
150000
200000
250000
300000
20.0
40.0
60.0
70.0
10.0
25.0
30.0
35.0
50.0
80.0
10.0
25.0
50.0
80.0
30.0
35.0
30.0
35.0
70.0
NCE

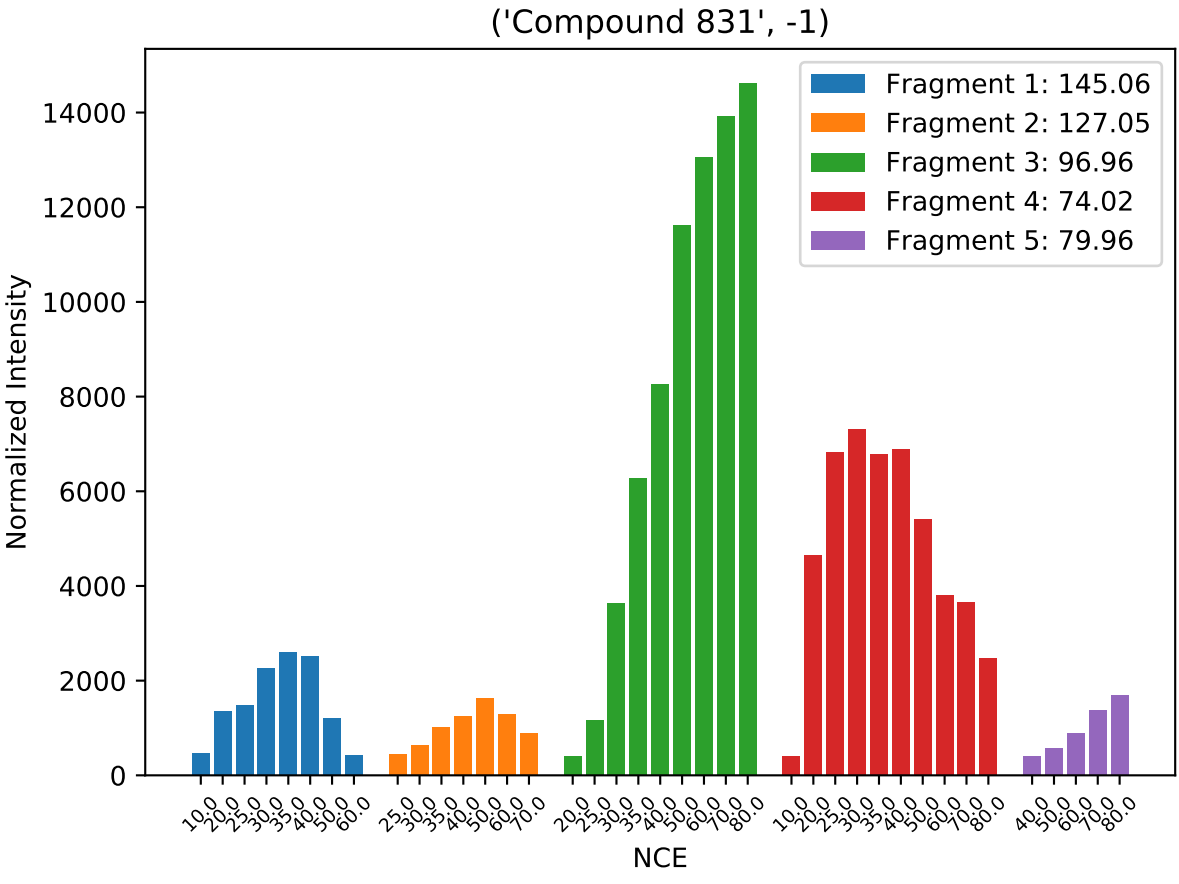

('Compound 617', -1)
Fragment 1: 57.03
Fragment 2: 59.01
Fragment 3: 73.03
Fragment 4: 85.03
Fragment 5: 57.04
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
NCE

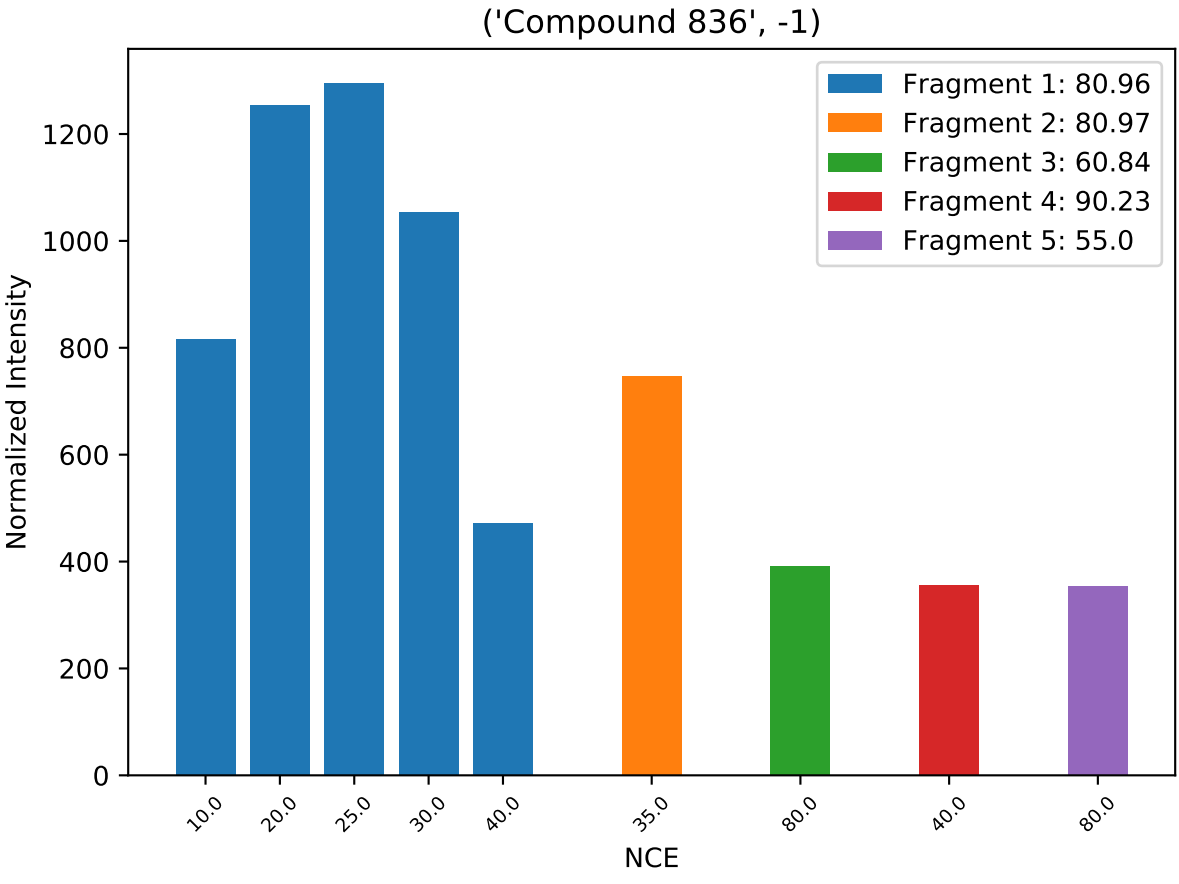

('Compound 618', -1)
Normalized Intensity
0
500
1000
1500
2000
2500
3000
Fragment 1: 63.93
Fragment 2: 63.4
Fragment 3: 65.0
Fragment 4: 66.22
Fragment 5: 91.49
80.0
70.0
60.0
60.0
35.0
NCE

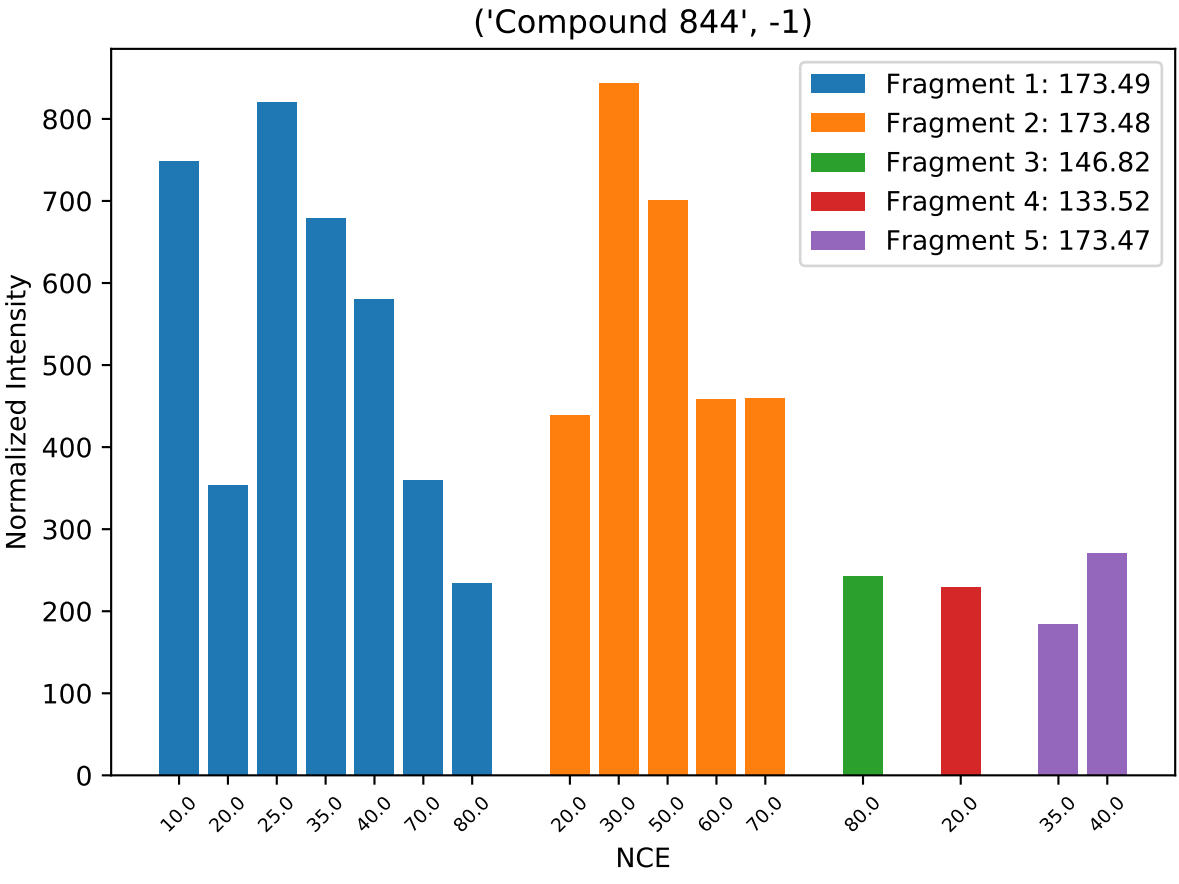

('Compound 415', -1)
Fragment 1: 427.32
Fragment 2: 173.48
Fragment 3: 401.34
Fragment 4: 173.49
Fragment 5: 383.33
Normalized Intensity
0
5000
10000
15000
20000
20.0 25.0 30.0 35.0 40.0
20.0 25.0 40.0 50.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 30.0 35.0 40.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0
NCE

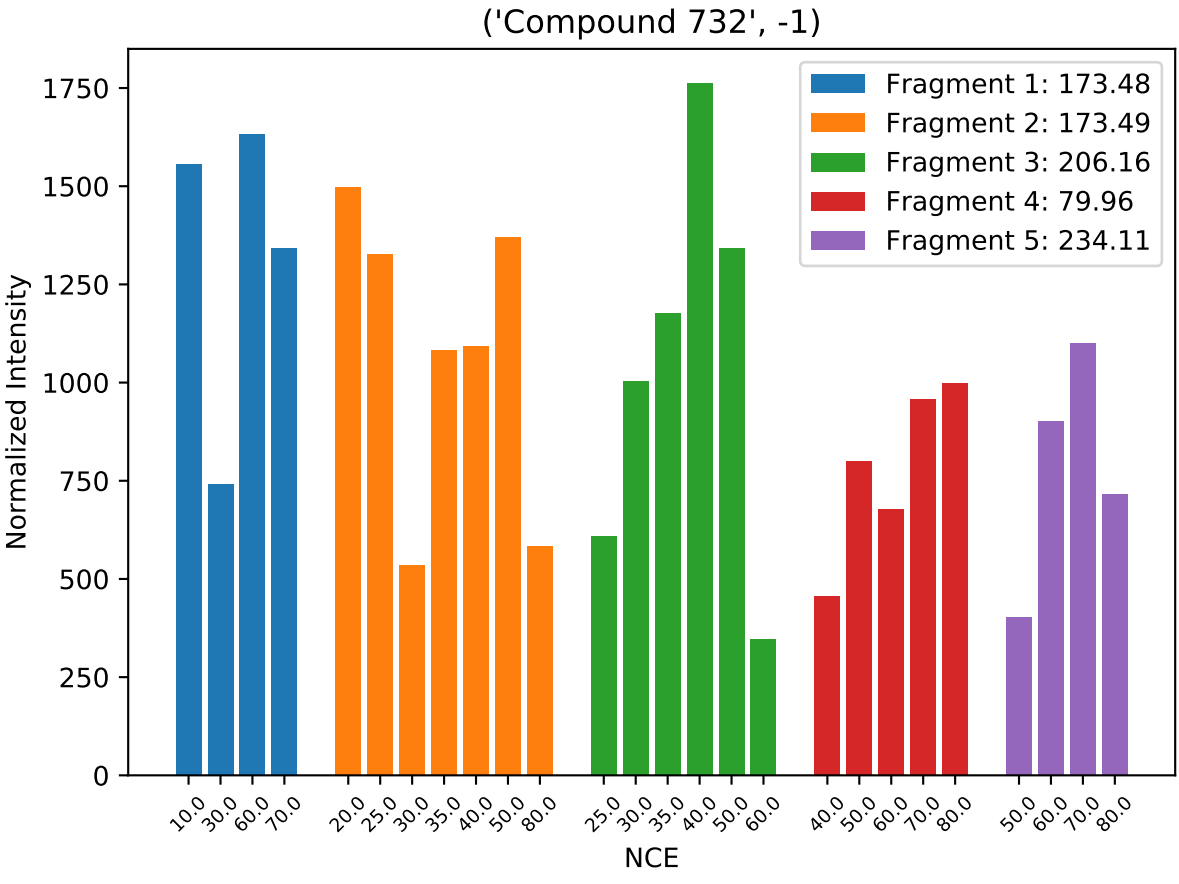

('Compound 721', -1)
Fragment 1: 279.23
Fragment 2: 255.23
Fragment 3: 281.25
Fragment 4: 253.22
Fragment 5: 173.48
Normalized Intensity
0
20000
40000
60000
80000
100000
120000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 40.0 50.0 80.0
NCE

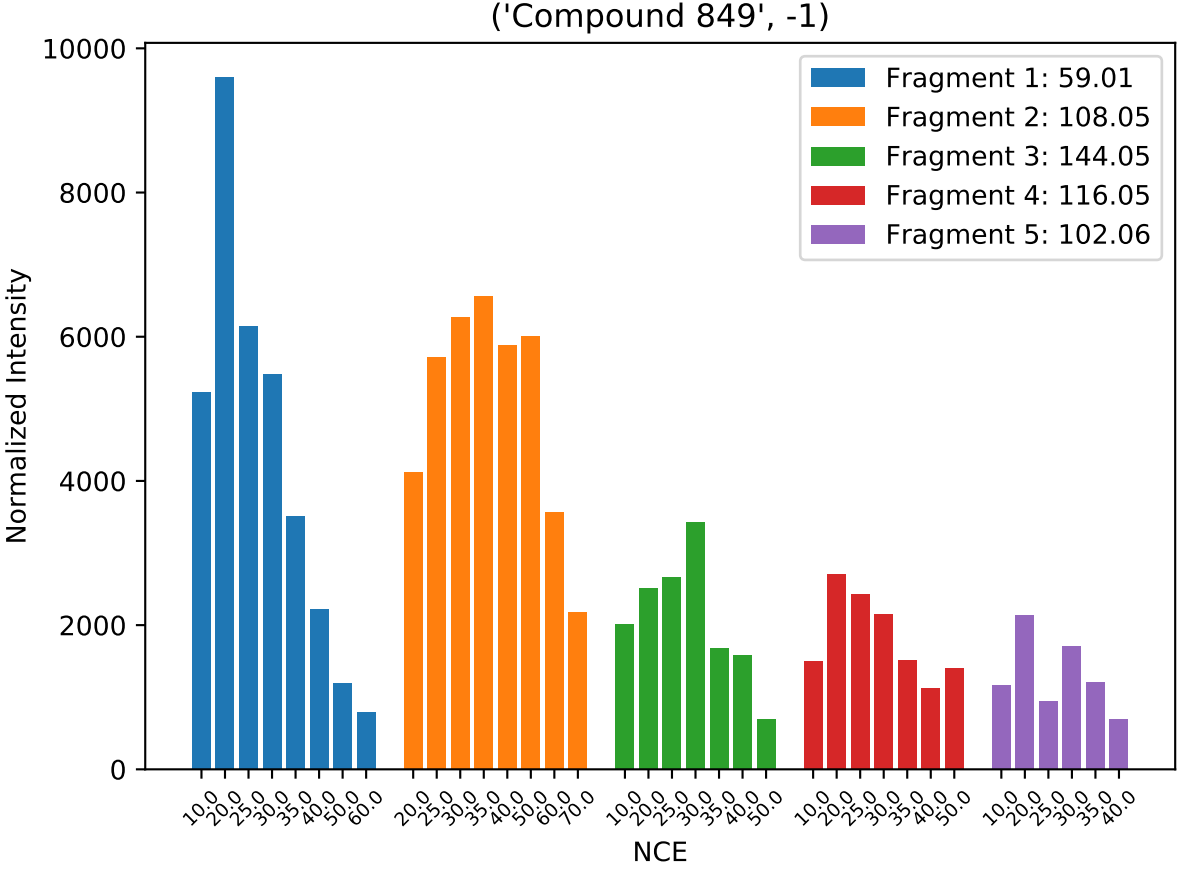

('Compound 722', -1)
Fragment 1: 246.07
Fragment 2: 113.02
Fragment 3: 186.05
Fragment 4: 126.02
Fragment 5: 84.01
Normalized Intensity
0
10000
20000
30000
40000
50000
60000
70000
80000
NCE
20.0 25.0 30.0 35.0 40.0 50.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0

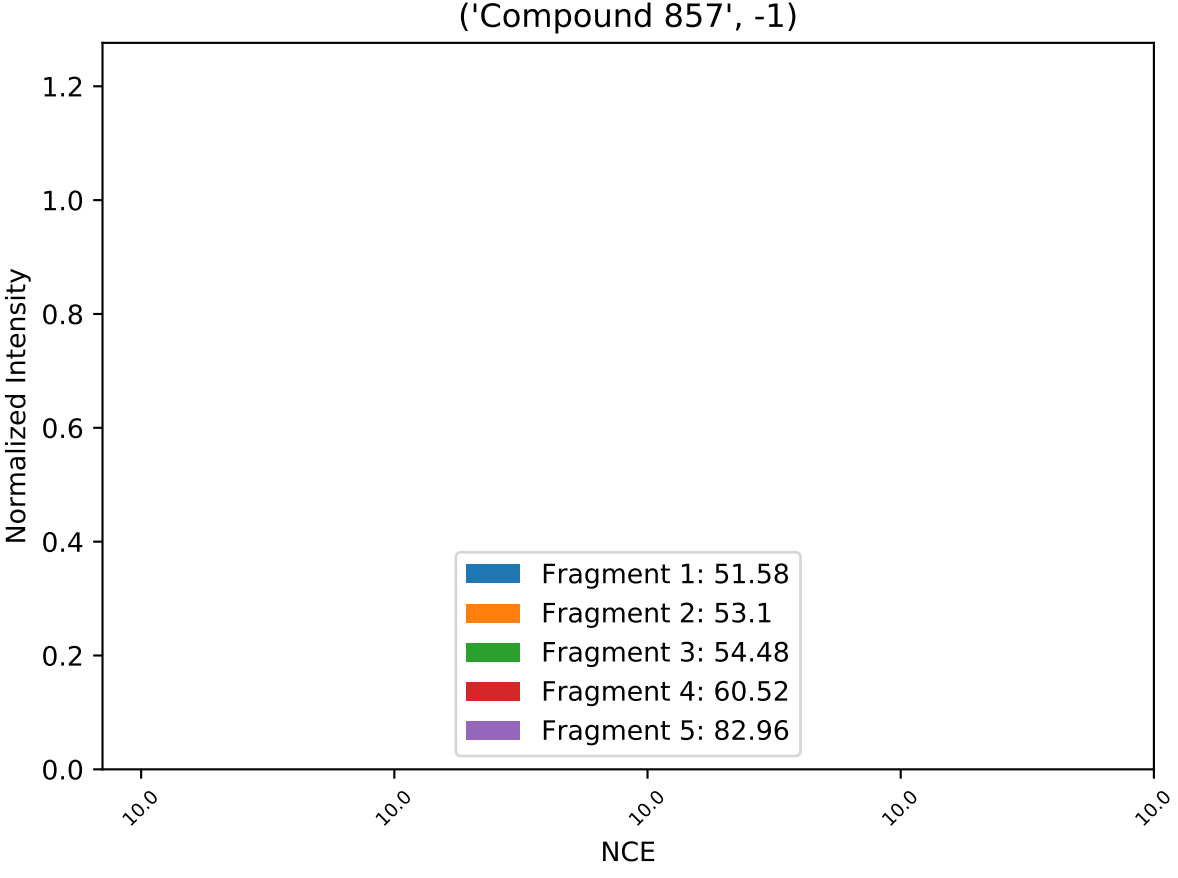

('Compound 831', -1)
Fragment 1: 145.06
Fragment 2: 127.05
Fragment 3: 96.96
Fragment 4: 74.02
Fragment 5: 79.96
Normalized Intensity
0
2000
4000
6000
8000
10000
12000
14000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
40.0 50.0 60.0 70.0 80.0
NCE

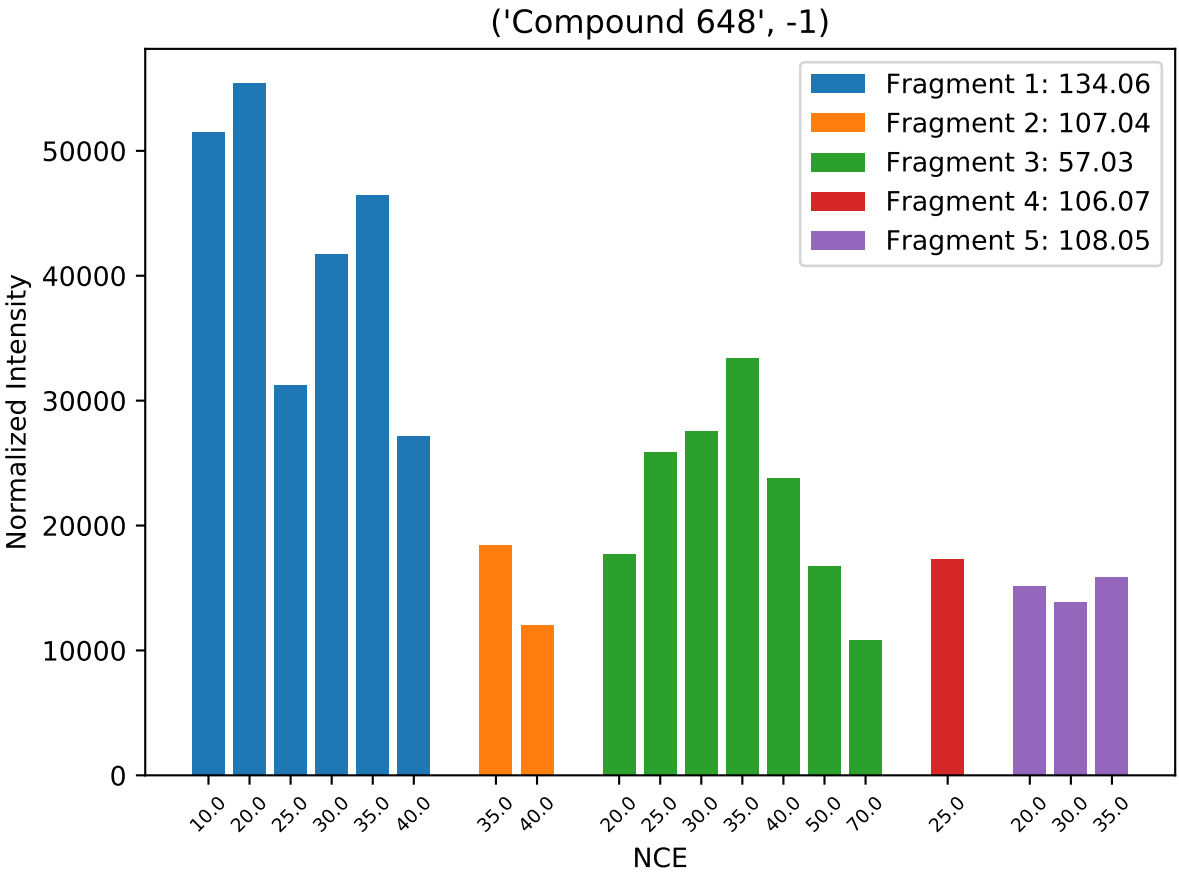

('Compound 836', -1)
Fragment 1: 80.96
Fragment 2: 80.97
Fragment 3: 60.84
Fragment 4: 90.23
Fragment 5: 55.0
Normalized Intensity
0
200
400
600
800
1000
1200
10.0
20.0
25.0
30.0
40.0
35.0
80.0
40.0
80.0
NCE

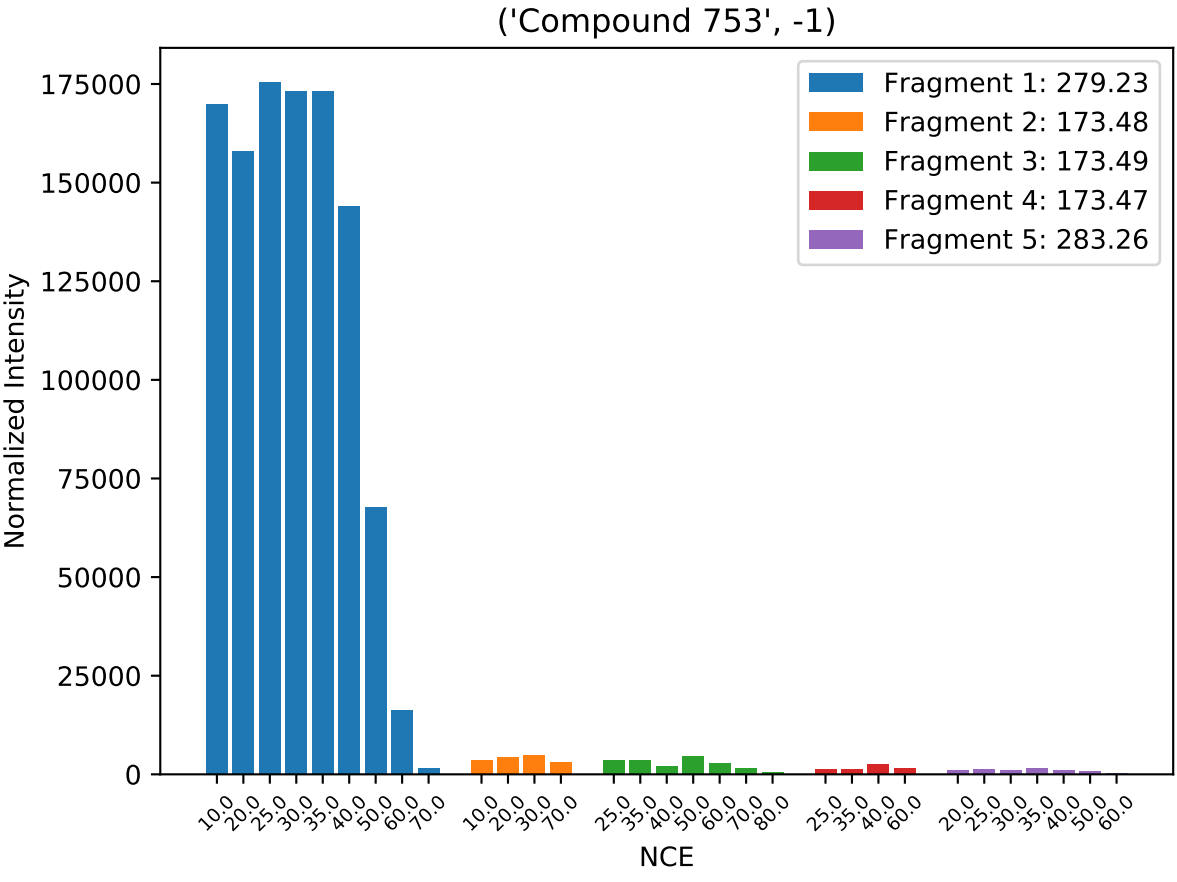

('Compound 844', -1)
Fragment 1: 173.49
Fragment 2: 173.48
Fragment 3: 146.82
Fragment 4: 133.52
Fragment 5: 173.47
Normalized Intensity
0
100
200
300
400
500
600
700
800
10.0
20.0
25.0
35.0
40.0
70.0
80.0
20.0
30.0
50.0
60.0
70.0
80.0
20.0
35.0
40.0
NCE

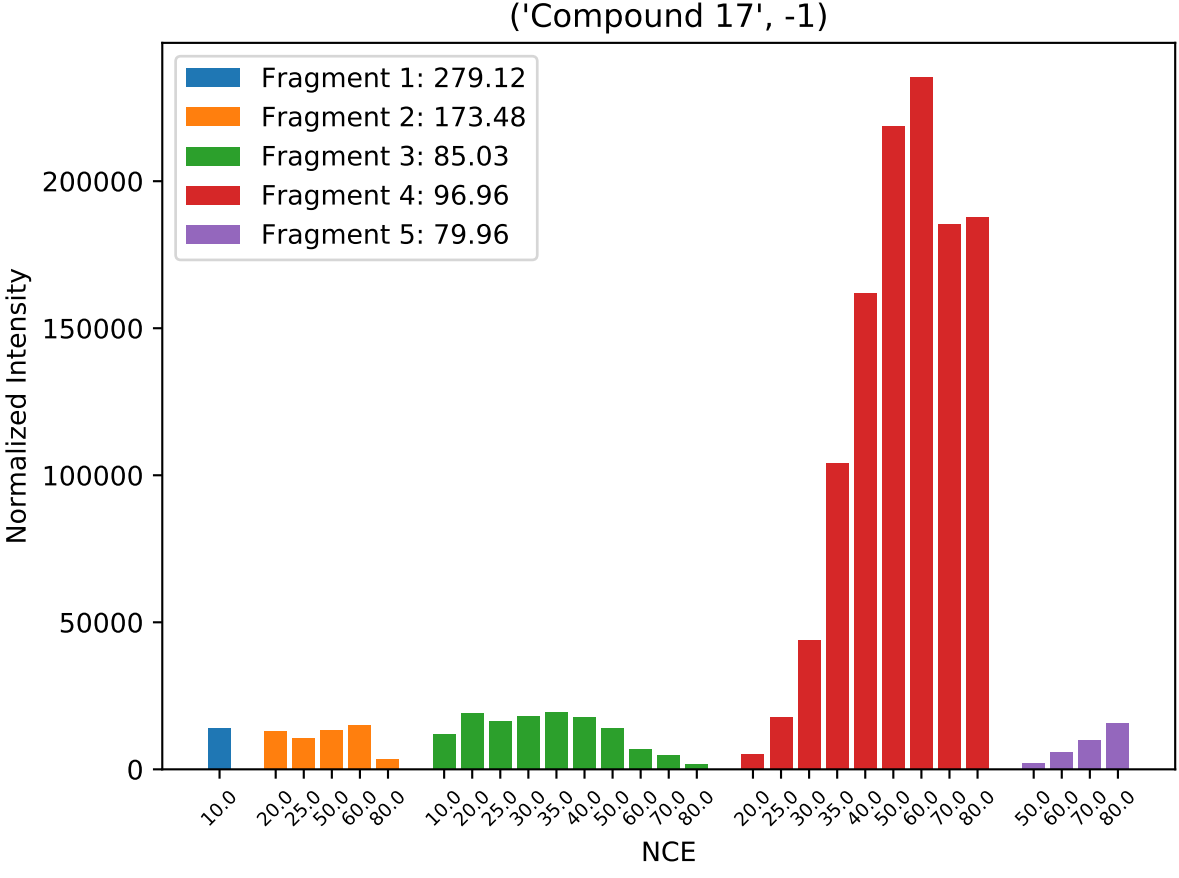

('Compound 732', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 206.16
Fragment 4: 79.96
Fragment 5: 234.11
Normalized Intensity
0
250
500
750
1000
1250
1500
1750
10.0
30.0
60.0
70.0
20.0
25.0
30.0
35.0
40.0
50.0
80.0
25.0
30.0
35.0
40.0
50.0
60.0
40.0
50.0
60.0
70.0
80.0
50.0
60.0
70.0
80.0
NCE

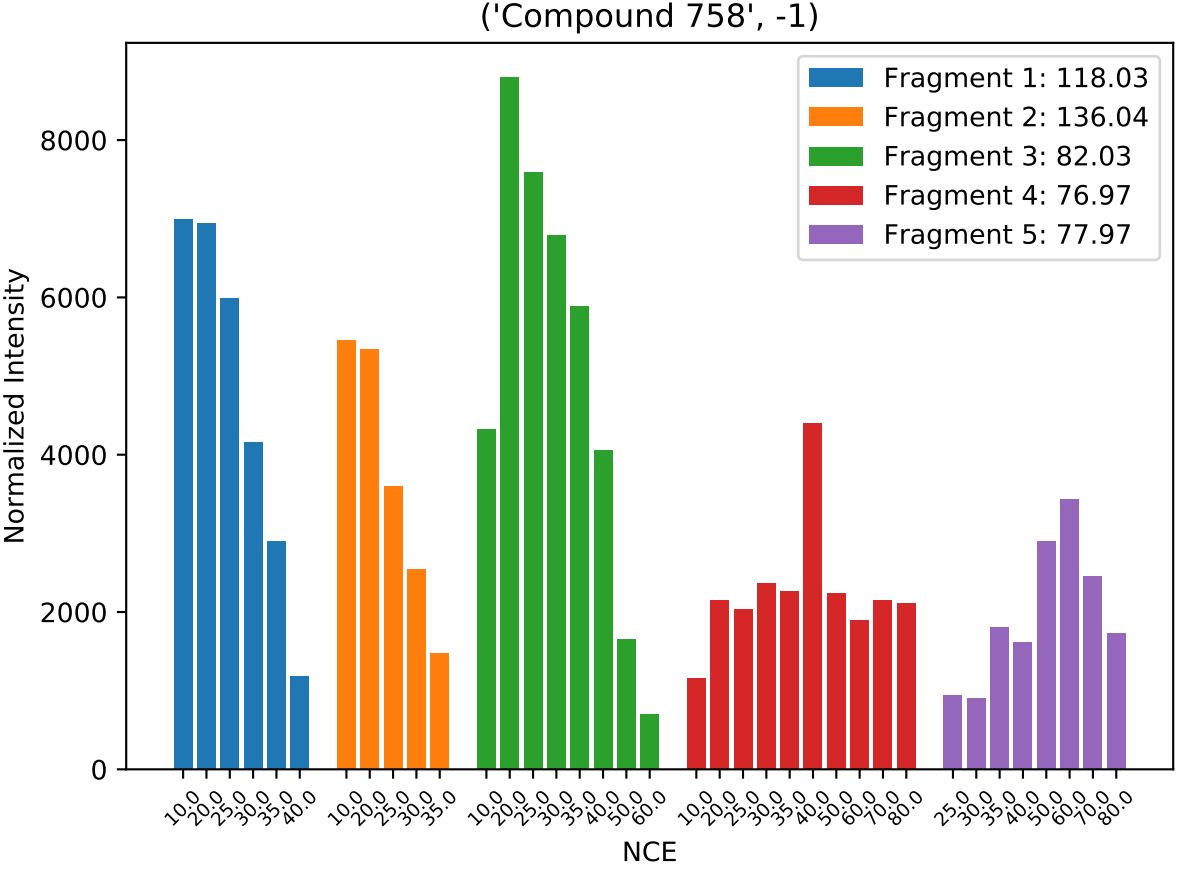

('Compound 849', -1)
Fragment 1: 59.01
Fragment 2: 108.05
Fragment 3: 144.05
Fragment 4: 116.05
Fragment 5: 102.06
Normalized Intensity
NCE
10000
8000
6000
4000
2000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0 40.0

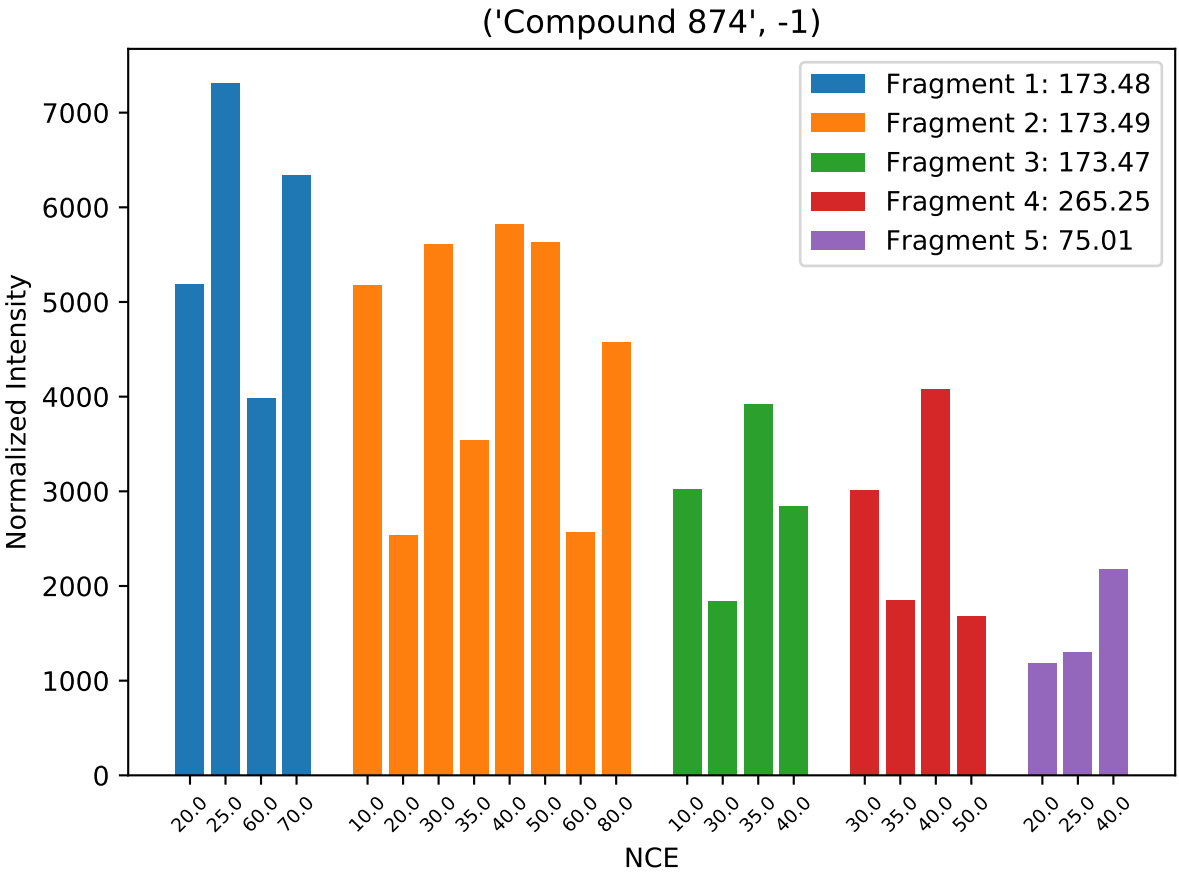

('Compound 857', -1)
Normalized Intensity
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Fragment 1: 51.58
Fragment 2: 53.1
Fragment 3: 54.48
Fragment 4: 60.52
Fragment 5: 82.96
10.0
10.0
10.0
10.0
10.0
NCE

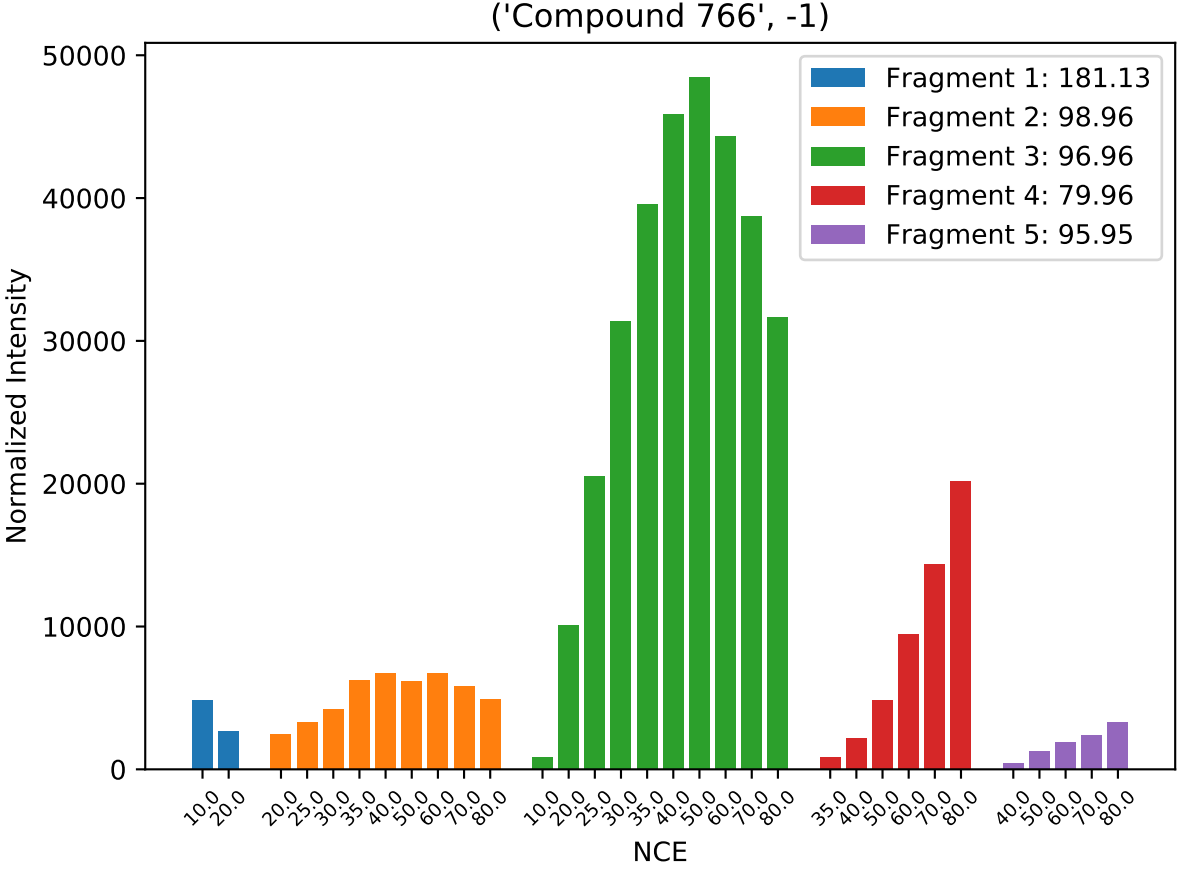

('Compound 648', -1)
Fragment 1: 134.06
Fragment 2: 107.04
Fragment 3: 57.03
Fragment 4: 106.07
Fragment 5: 108.05
Normalized Intensity
0
10000
20000
30000
40000
50000
10.0
20.0
25.0
30.0
35.0
40.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
50.0
70.0
25.0
20.0
30.0
35.0
NCE

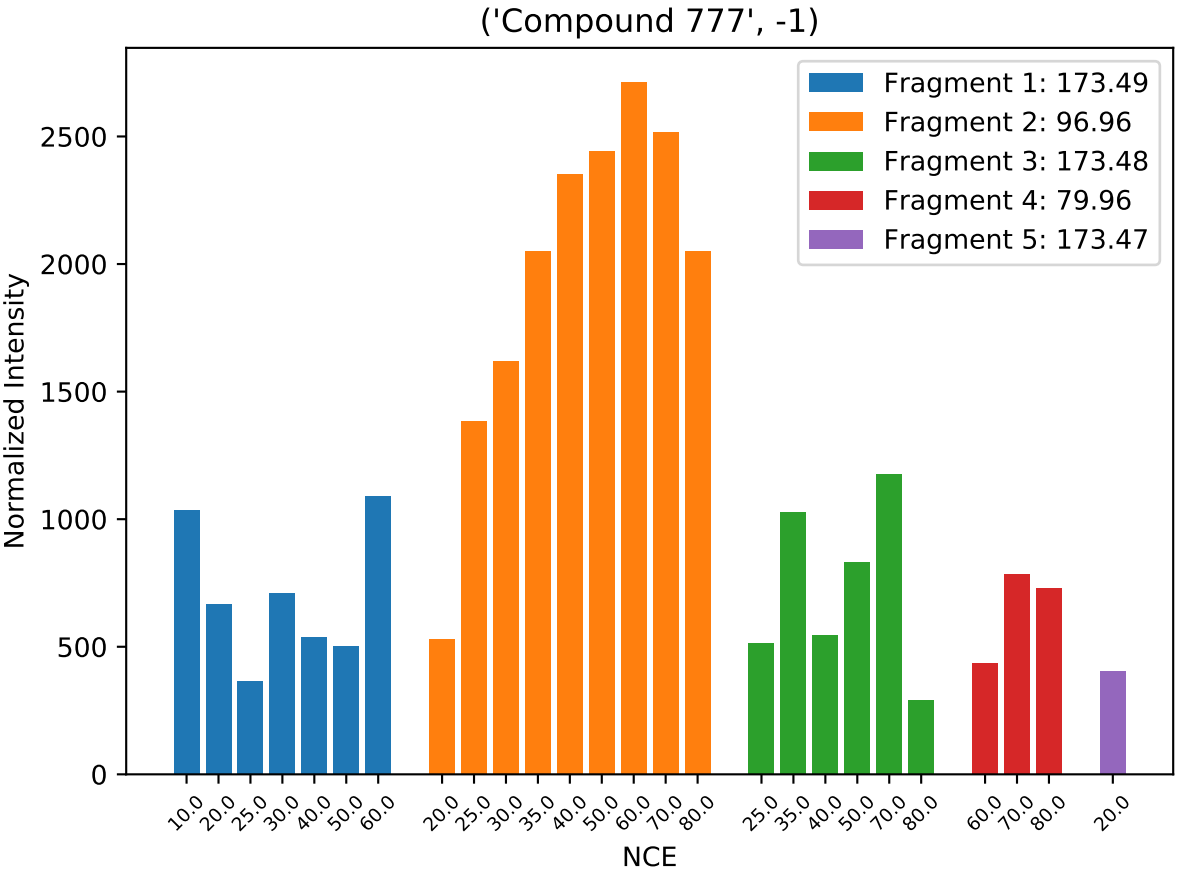

('Compound 753', -1)
Fragment 1: 279.23
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 173.47
Fragment 5: 283.26
Normalized Intensity
175000
150000
125000
100000
75000
50000
25000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 20.0 30.0 70.0
25.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 35.0 40.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

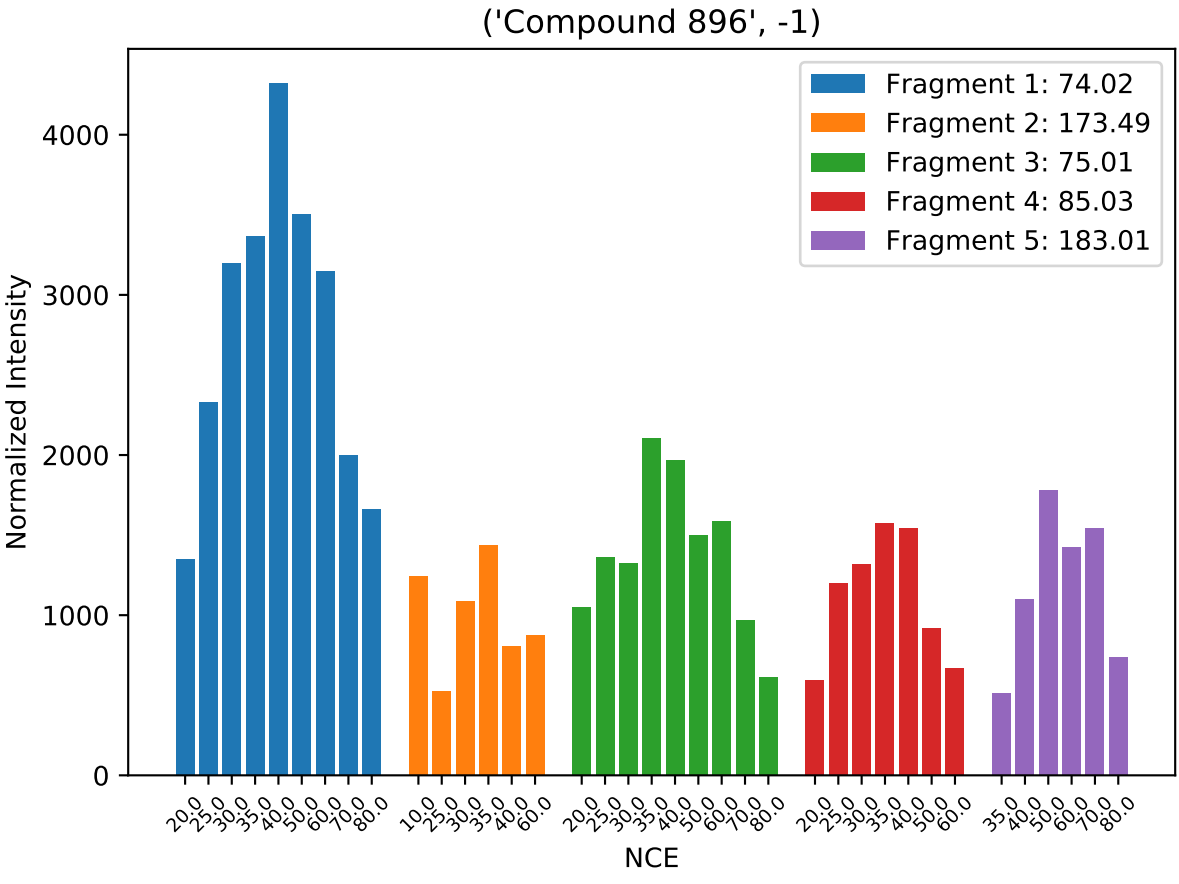

('Compound 17', -1)
Fragment 1: 279.12
Fragment 2: 173.48
Fragment 3: 85.03
Fragment 4: 96.96
Fragment 5: 79.96
Normalized Intensity
0
50000
100000
150000
200000
10.0
20.0
25.0
50.0
60.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
50.0
60.0
70.0
80.0
NCE

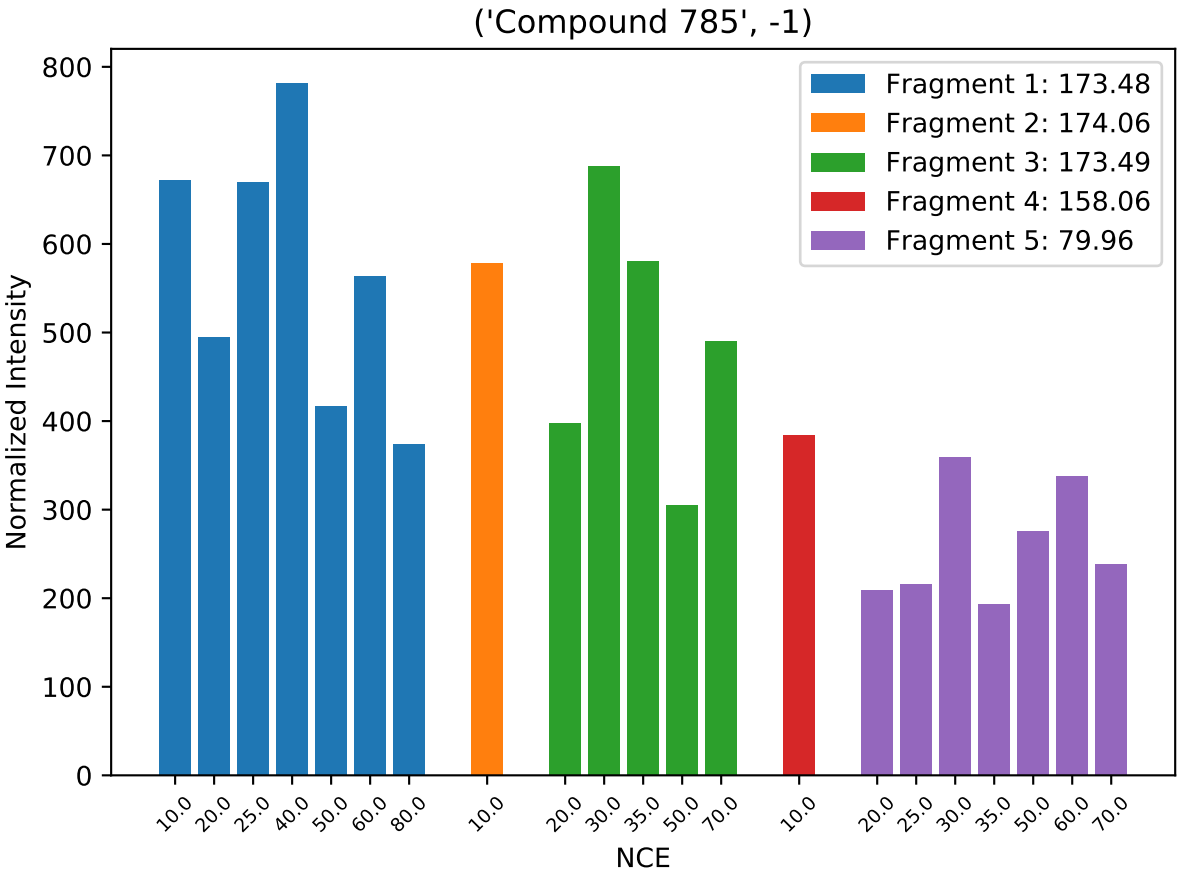

('Compound 758', -1)
Fragment 1: 118.03
Fragment 2: 136.04
Fragment 3: 82.03
Fragment 4: 76.97
Fragment 5: 77.97
Normalized Intensity
0
2000
4000
6000
8000
10.0 20.0 25.0 30.0 35.0 40.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE

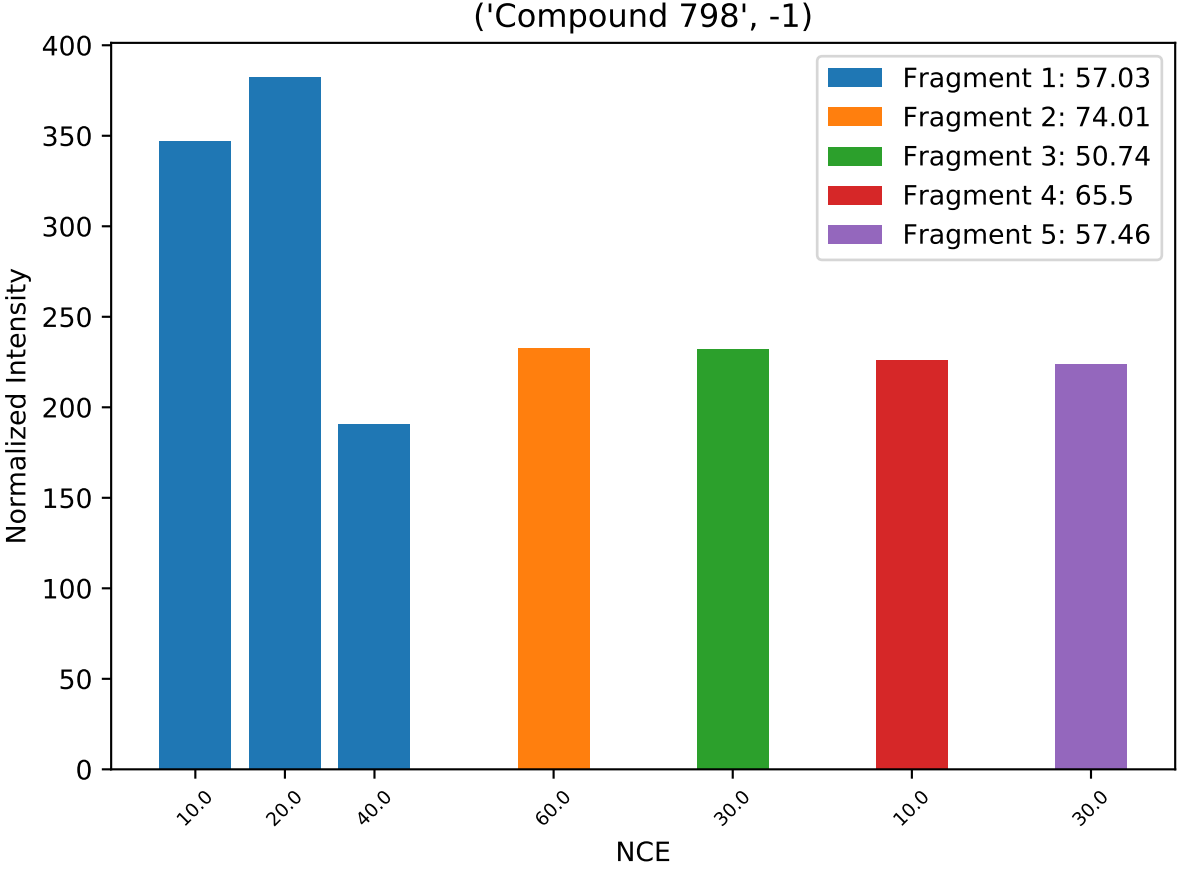

('Compound 874', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 173.47
Fragment 4: 265.25
Fragment 5: 75.01
Normalized Intensity
0
1000
2000
3000
4000
5000
6000
7000
20.0
25.0
60.0
70.0
10.0
20.0
30.0
35.0
40.0
50.0
60.0
80.0
10.0
30.0
35.0
40.0
30.0
35.0
40.0
50.0
20.0
25.0
40.0
NCE

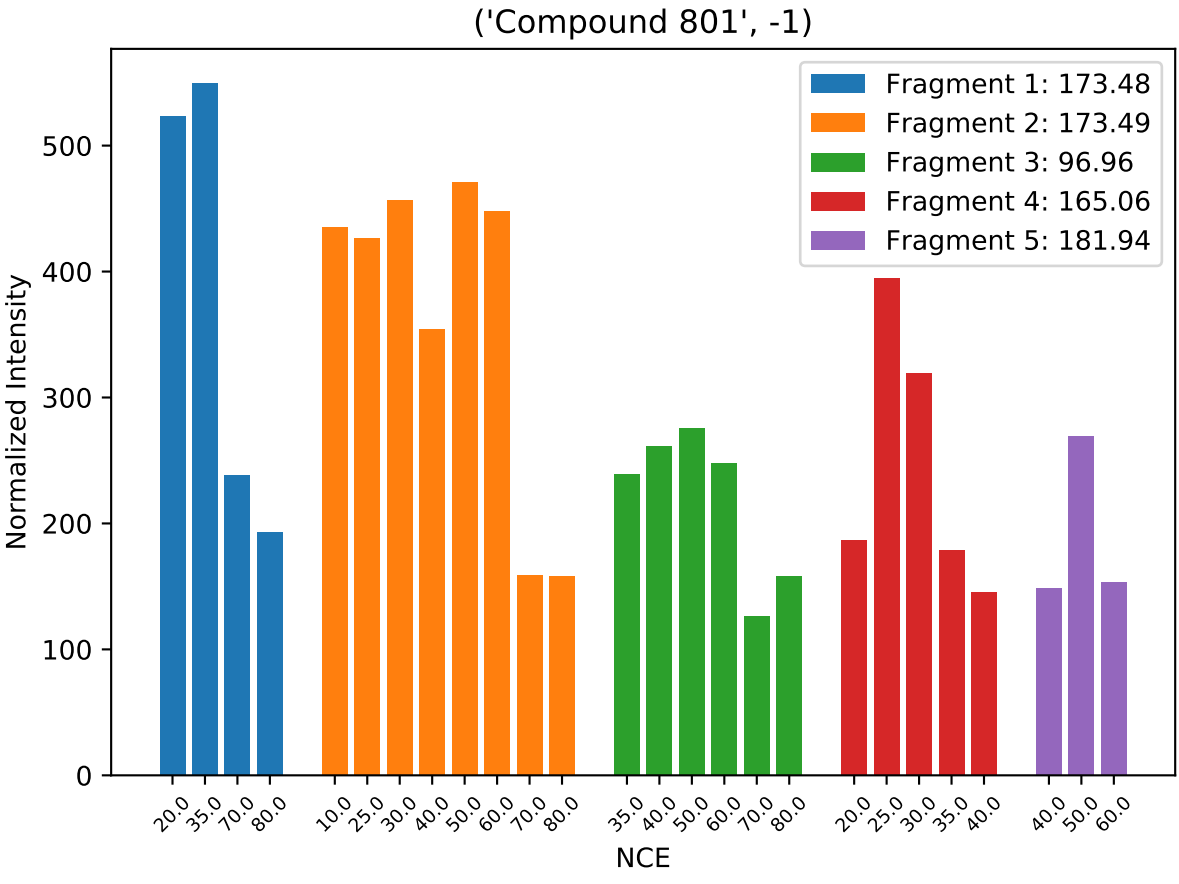

('Compound 766', -1)
Fragment 1: 181.13
Fragment 2: 98.96
Fragment 3: 96.96
Fragment 4: 79.96
Fragment 5: 95.95
Normalized Intensity
50000
40000
30000
20000
10000
0
10.0
20.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
10.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
40.0
50.0
60.0
70.0
80.0
NCE

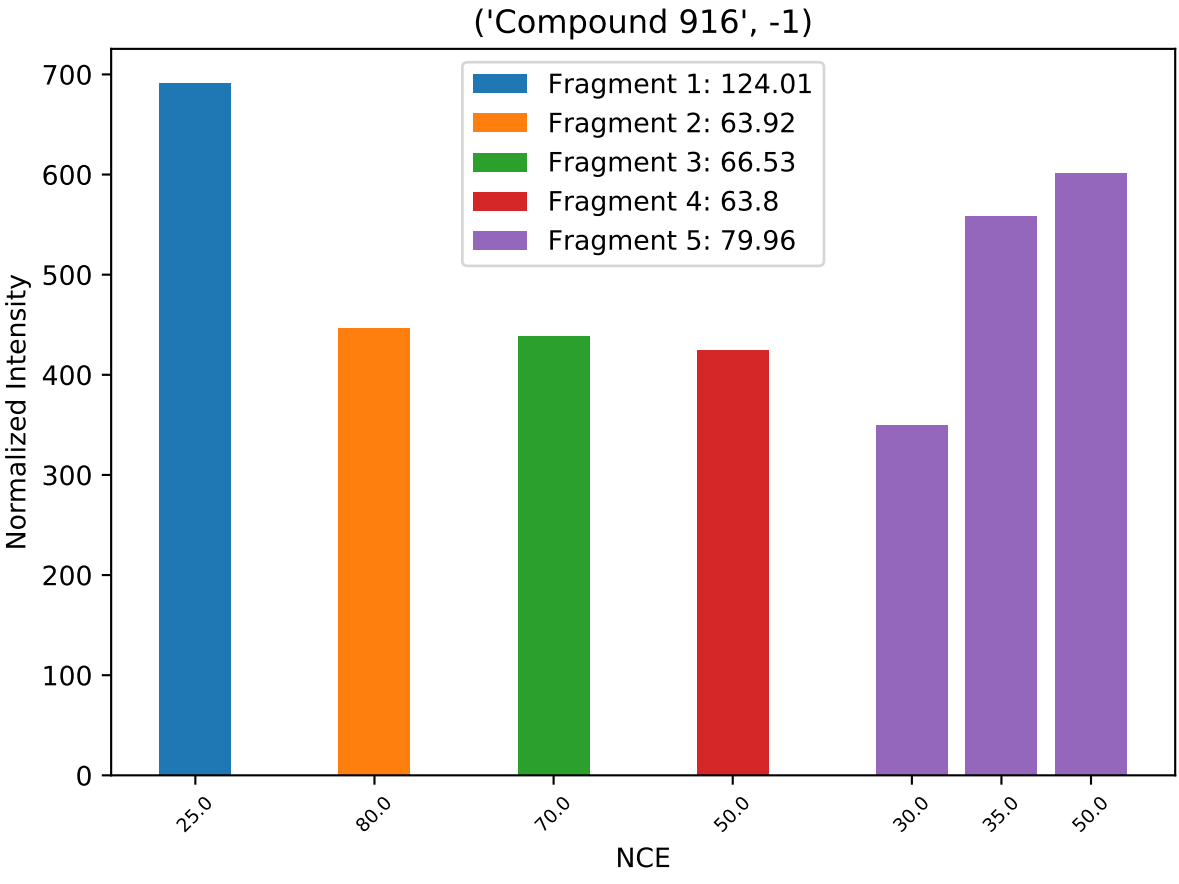

('Compound 777', -1)
Fragment 1: 173.49
Fragment 2: 96.96
Fragment 3: 173.48
Fragment 4: 79.96
Fragment 5: 173.47
Normalized Intensity
0
500
1000
1500
2000
2500
10.0
20.0
25.0
30.0
40.0
50.0
60.0
20.0
25.0
30.0
35.0
40.0
50.0
60.0
70.0
80.0
25.0
35.0
40.0
50.0
70.0
80.0
60.0
70.0
80.0
20.0
NCE

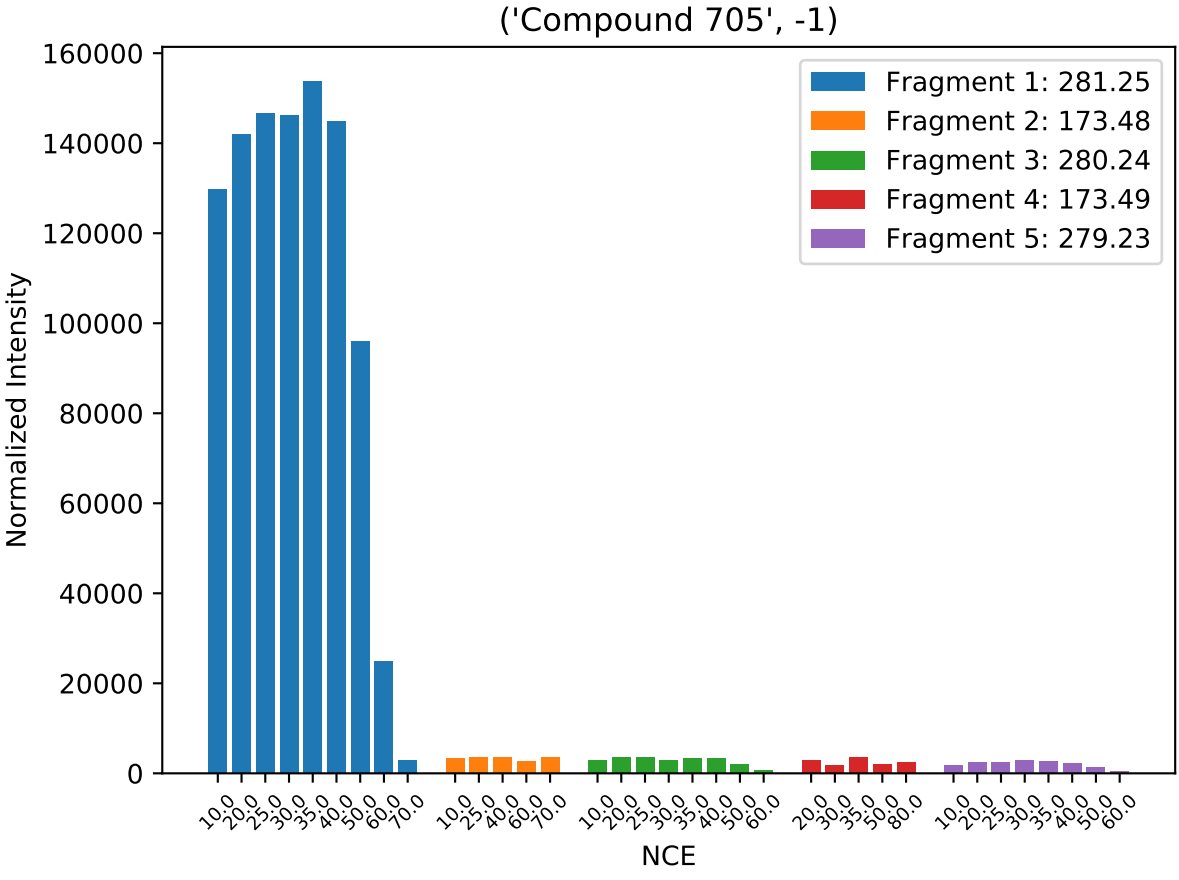

('Compound 896', -1)
Fragment 1: 74.02
Fragment 2: 173.49
Fragment 3: 75.01
Fragment 4: 85.03
Fragment 5: 183.01
Normalized Intensity
0
1000
2000
3000
4000
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 25.0 30.0 35.0 40.0 60.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

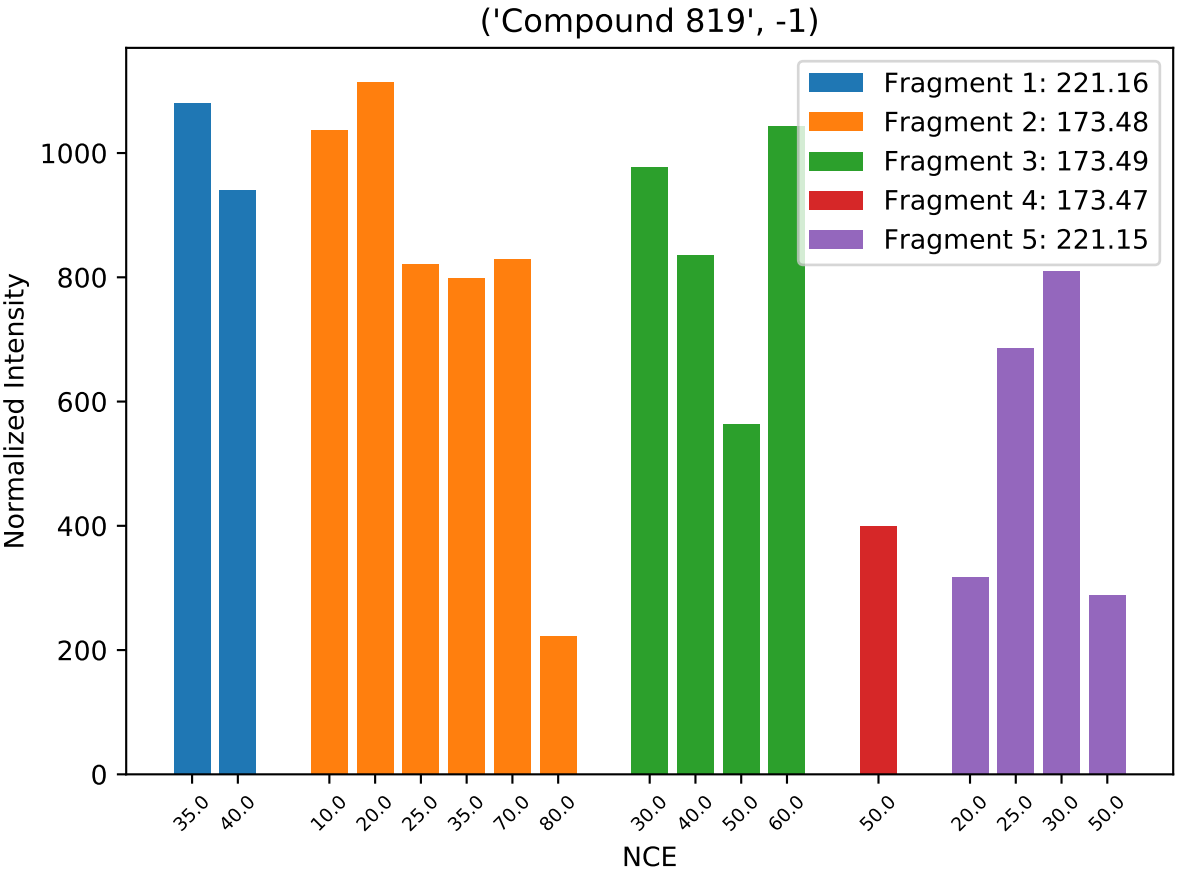

('Compound 785', -1)
Fragment 1: 173.48
Fragment 2: 174.06
Fragment 3: 173.49
Fragment 4: 158.06
Fragment 5: 79.96
Normalized Intensity
0
100
200
300
400
500
600
700
800
10.0
20.0
25.0
40.0
50.0
60.0
80.0
10.0
20.0
30.0
35.0
50.0
70.0
10.0
20.0
25.0
30.0
35.0
50.0
60.0
70.0
NCE

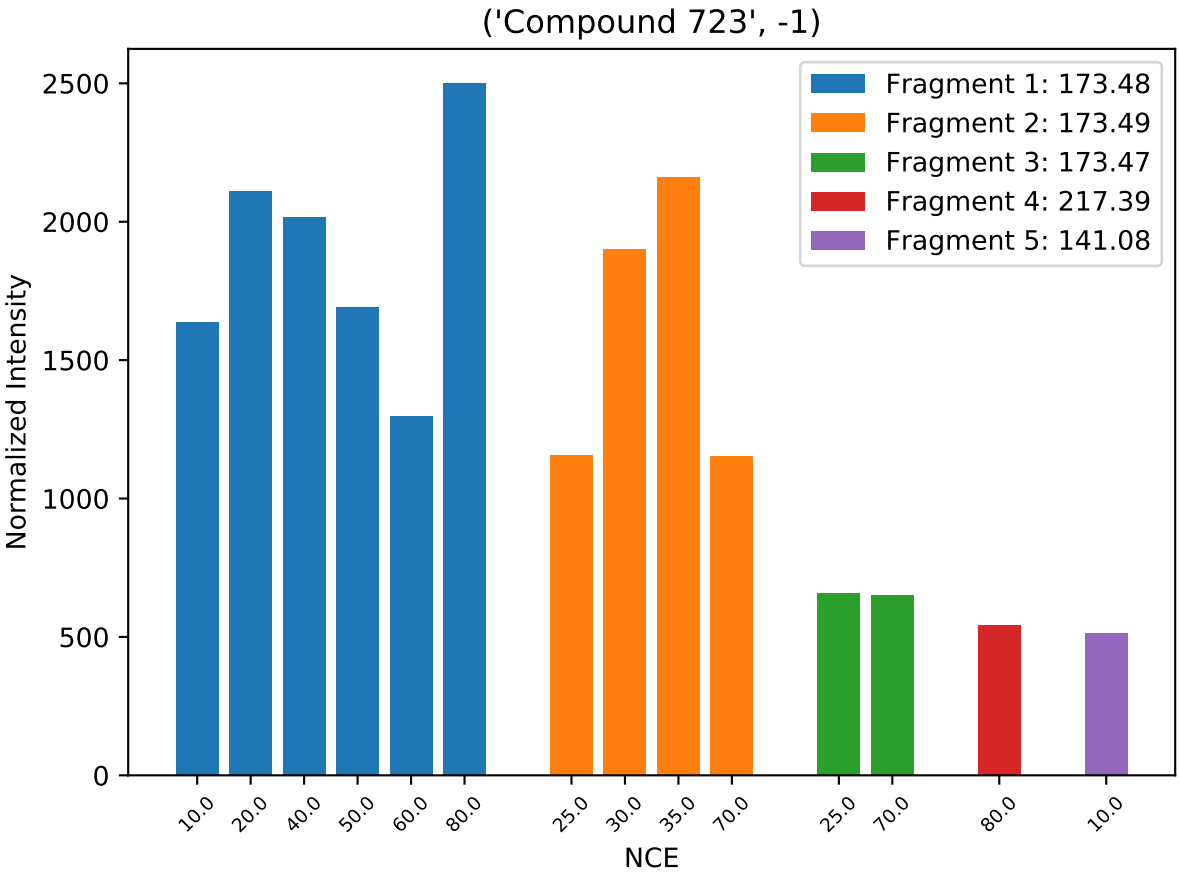

('Compound 798', -1)
Fragment 1: 57.03
Fragment 2: 74.01
Fragment 3: 50.74
Fragment 4: 65.5
Fragment 5: 57.46
Normalized Intensity
0
50
100
150
200
250
300
350
400
10.0
20.0
40.0
60.0
30.0
10.0
30.0
NCE

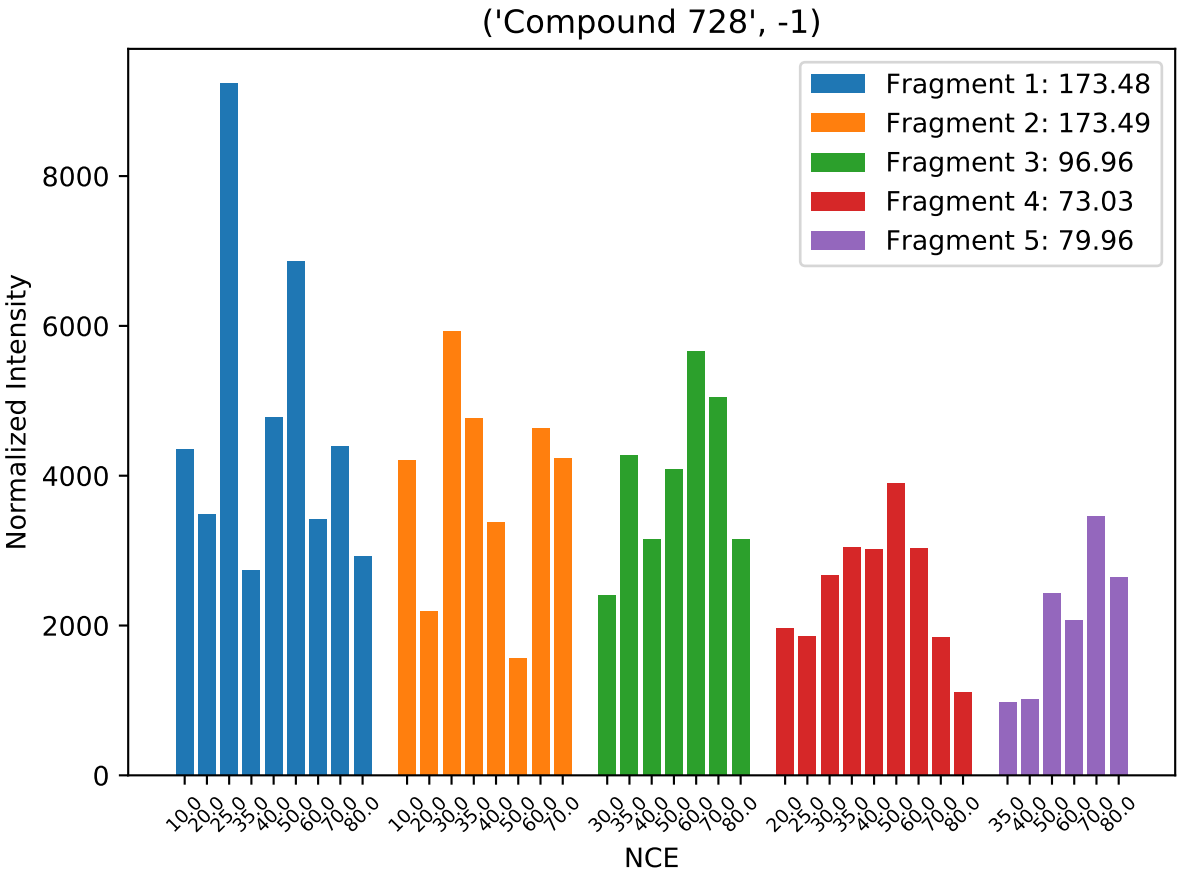

('Compound 801', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 96.96
Fragment 4: 165.06
Fragment 5: 181.94
Normalized Intensity
0
100
200
300
400
500
20.0
35.0
70.0
80.0
10.0
25.0
30.0
40.0
50.0
60.0
70.0
80.0
35.0
40.0
50.0
60.0
70.0
80.0
20.0
25.0
30.0
35.0
40.0
40.0
50.0
60.0
NCE

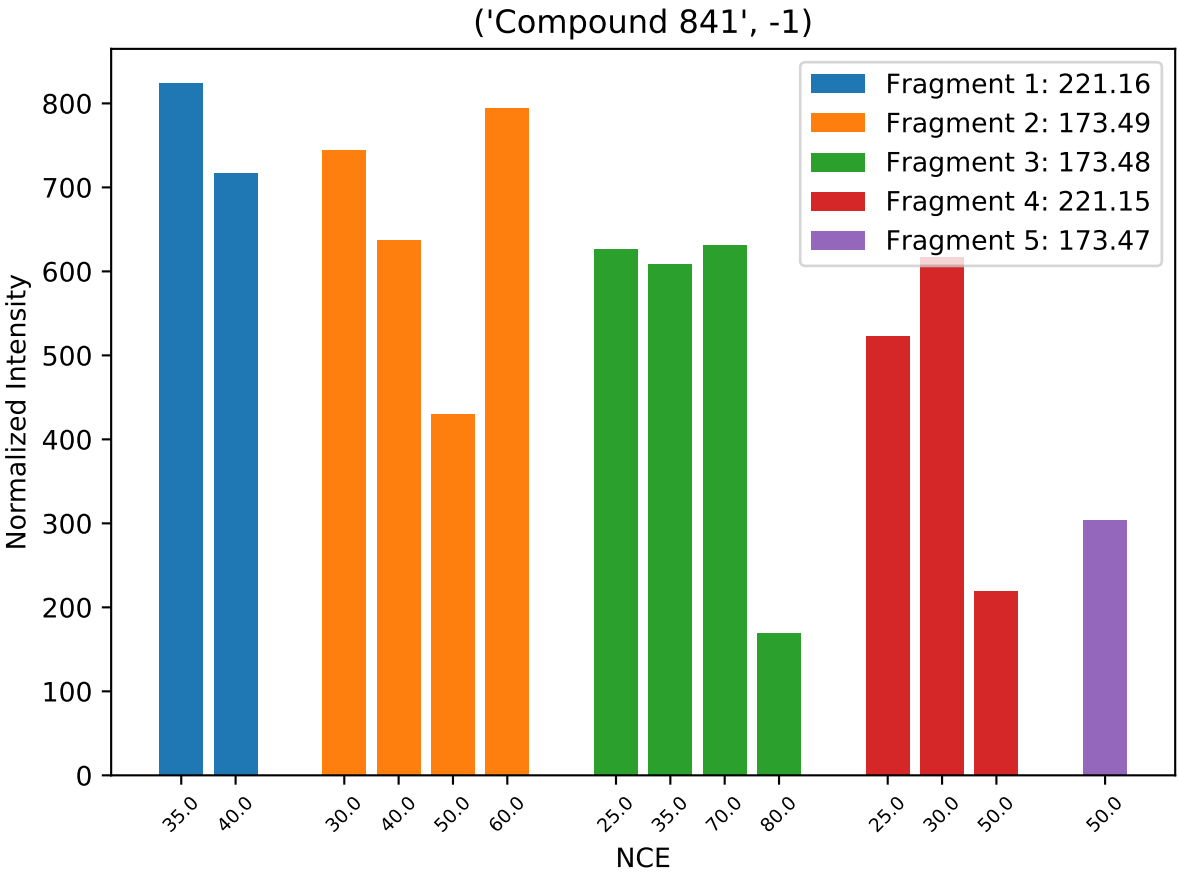

('Compound 916', -1)
Fragment 1: 124.01
Fragment 2: 63.92
Fragment 3: 66.53
Fragment 4: 63.8
Fragment 5: 79.96
Normalized Intensity
0
100
200
300
400
500
600
700
25.0
80.0
70.0
50.0
30.0
35.0
50.0
NCE

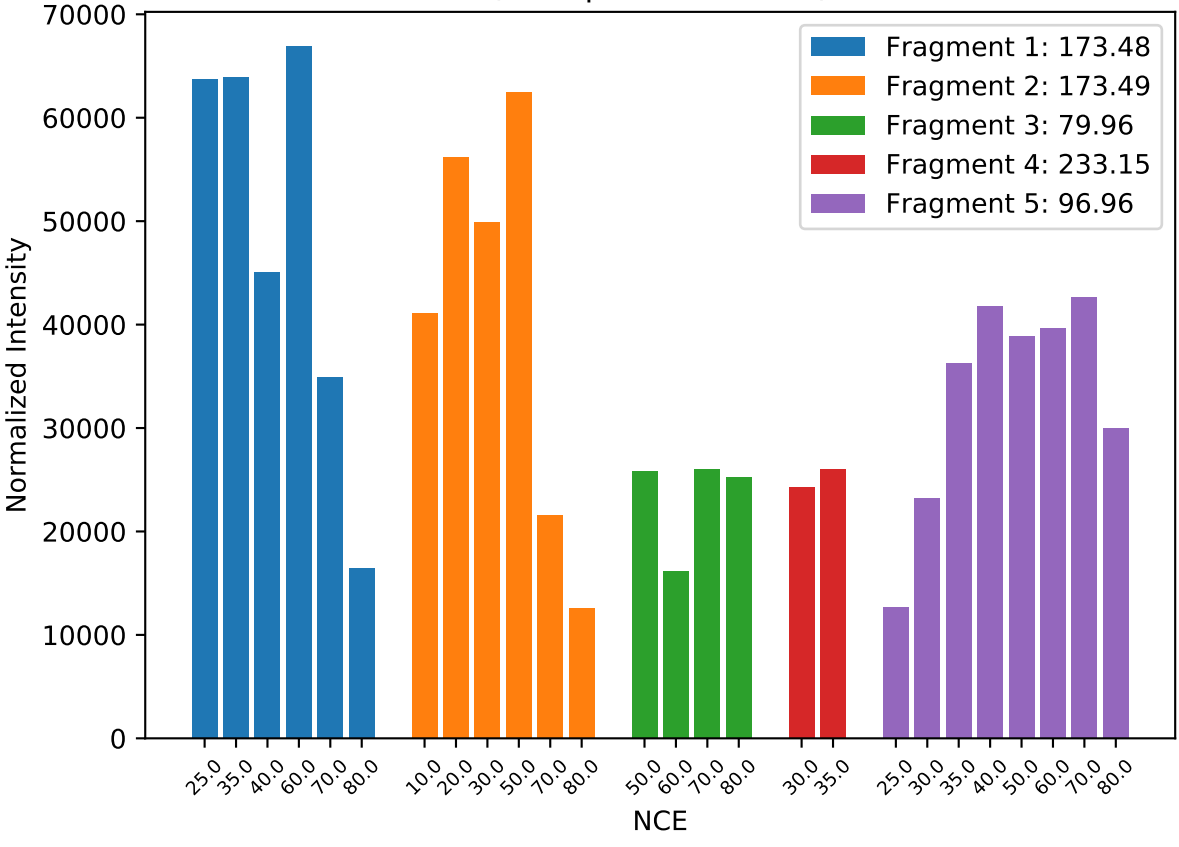

('Compound 705', -1)
Fragment 1: 281.25
Fragment 2: 173.48
Fragment 3: 280.24
Fragment 4: 173.49
Fragment 5: 279.23
Normalized Intensity
160000
140000
120000
100000
80000
60000
40000
20000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
10.0 25.0 40.0 60.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
20.0 30.0 35.0 50.0 80.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0
NCE

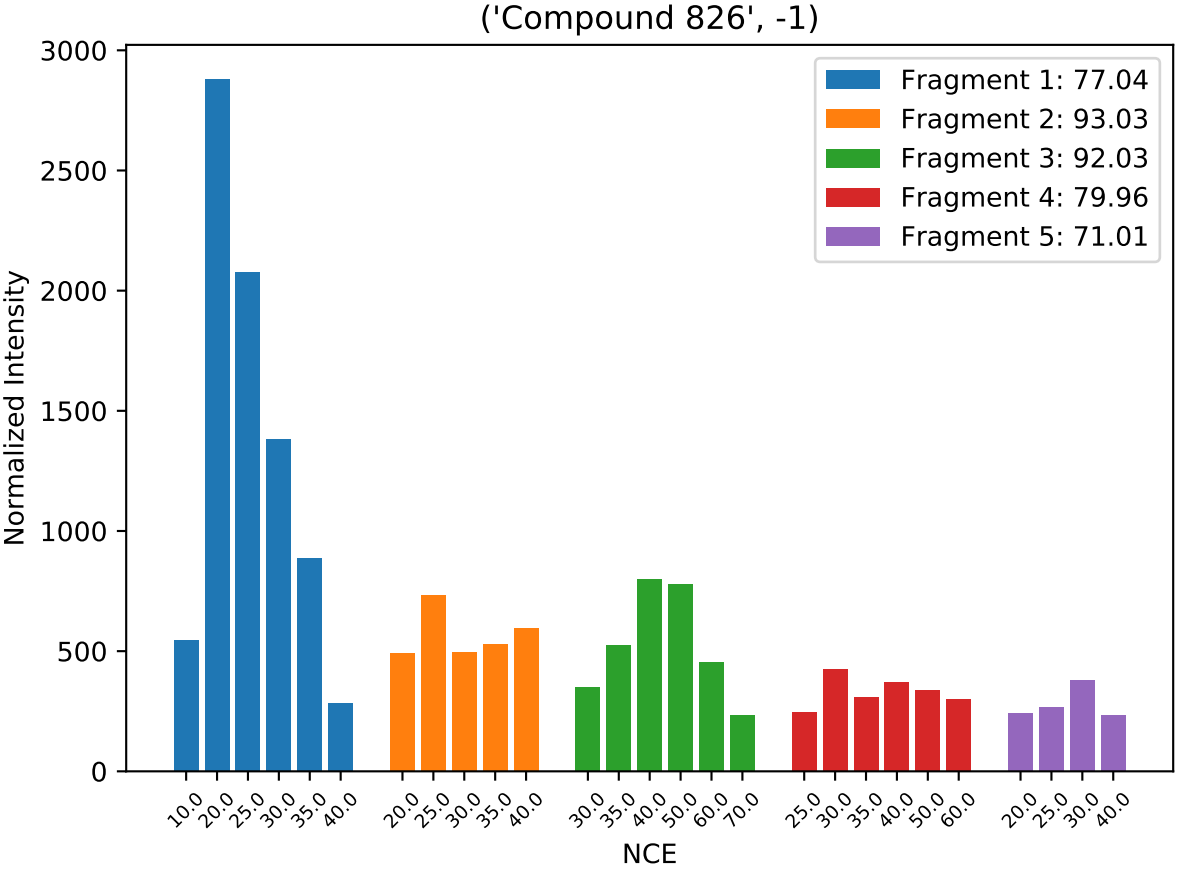

('Compound 819', -1)
Fragment 1: 221.16
Fragment 2: 173.48
Fragment 3: 173.49
Fragment 4: 173.47
Fragment 5: 221.15
Normalized Intensity
0
200
400
600
800
1000
35.0
40.0
10.0
20.0
25.0
35.0
70.0
80.0
30.0
40.0
50.0
60.0
50.0
20.0
25.0
30.0
50.0
NCE

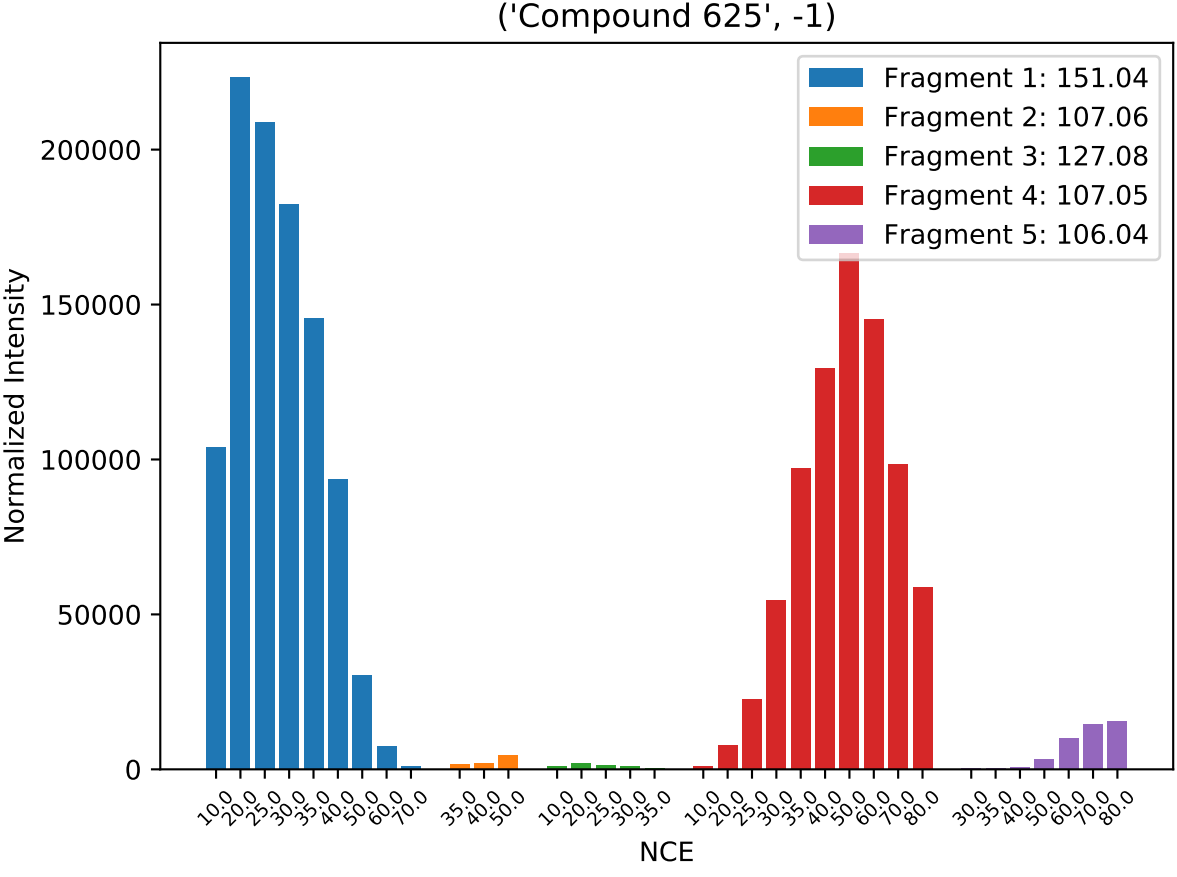

('Compound 723', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 173.47
Fragment 4: 217.39
Fragment 5: 141.08
Normalized Intensity
0
500
1000
1500
2000
2500
10.0
20.0
40.0
50.0
60.0
80.0
25.0
30.0
35.0
70.0
25.0
70.0
80.0
10.0
NCE

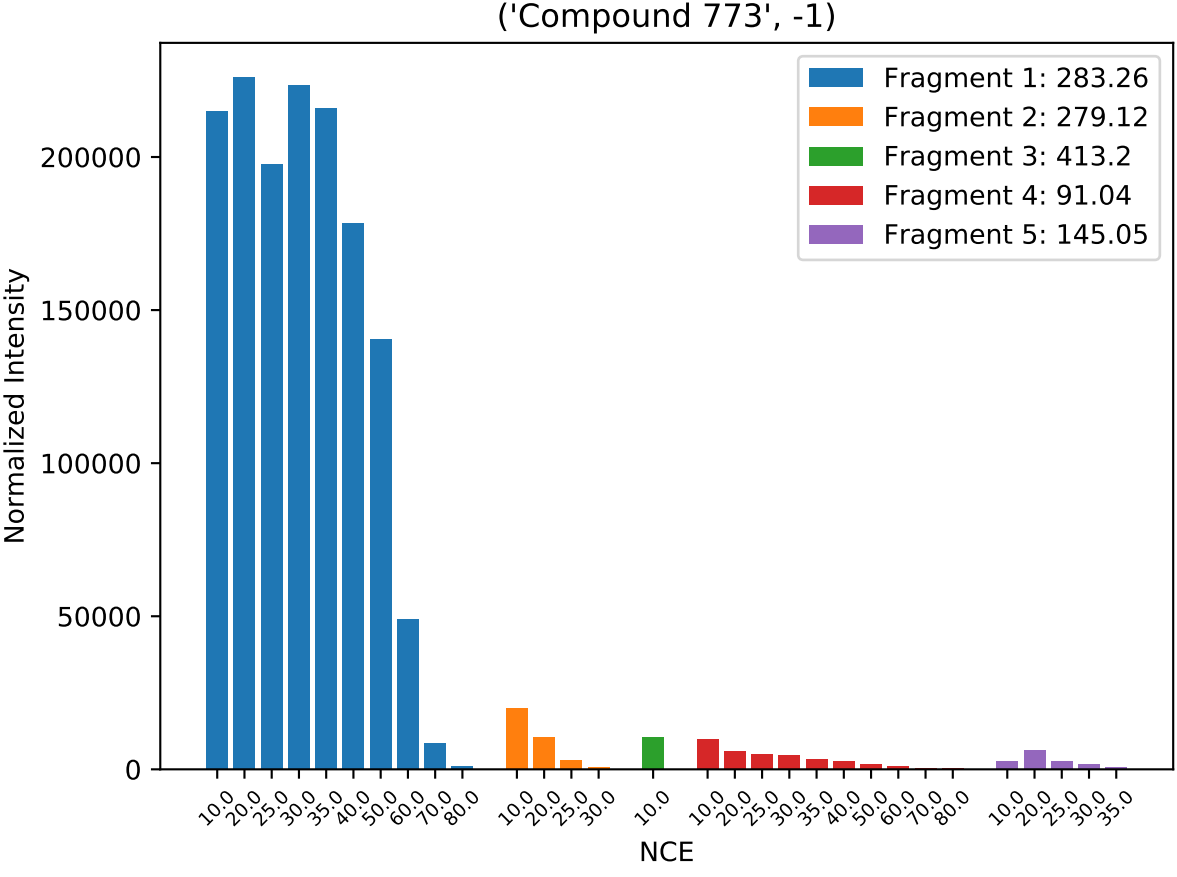

('Compound 728', -1)
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 96.96
Fragment 4: 73.03
Fragment 5: 79.96
Normalized Intensity
0
2000
4000
6000
8000
10.0 20.0 25.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 30.0 35.0 40.0 50.0 60.0 70.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
35.0 40.0 50.0 60.0 70.0 80.0
NCE

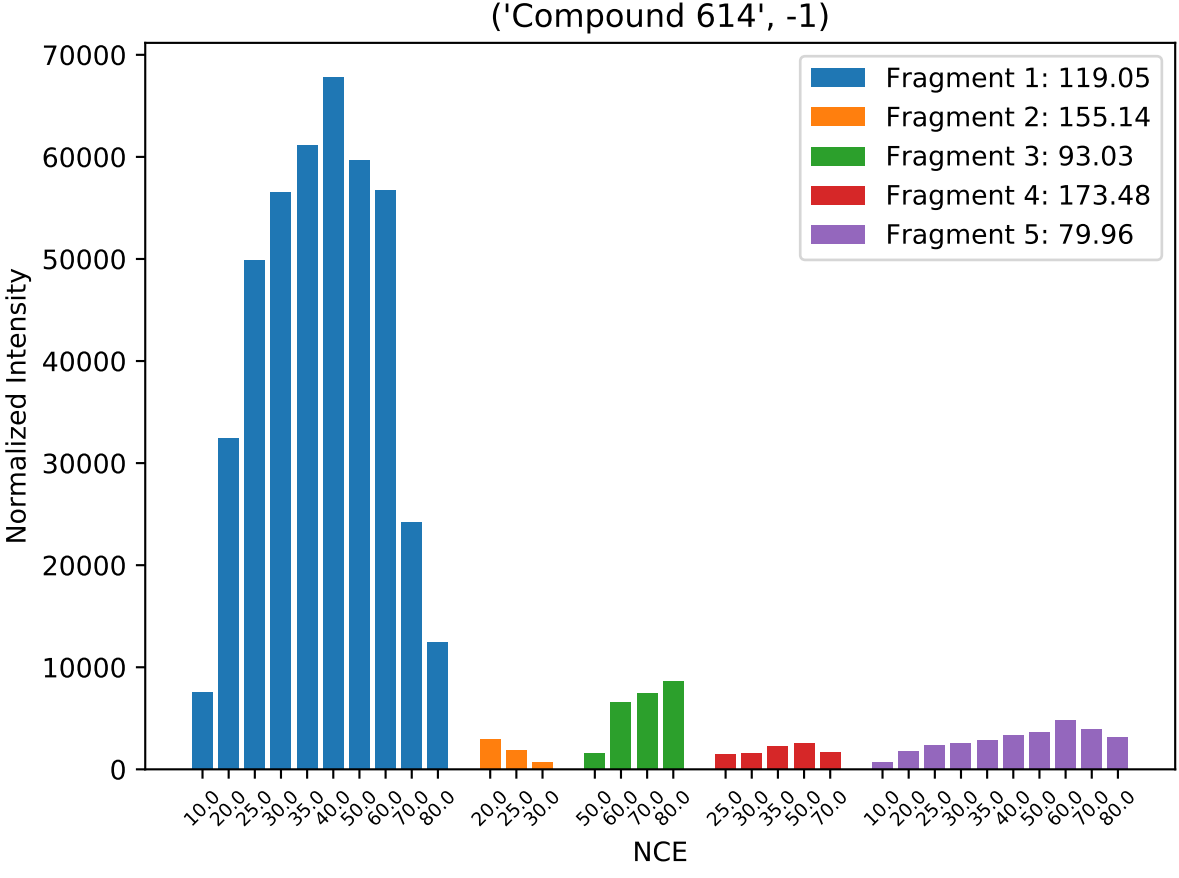

('Compound 841', -1)
Fragment 1: 221.16
Fragment 2: 173.49
Fragment 3: 173.48
Fragment 4: 221.15
Fragment 5: 173.47
Normalized Intensity
0
100
200
300
400
500
600
700
800
35.0
40.0
30.0
40.0
50.0
60.0
25.0
35.0
70.0
80.0
25.0
30.0
50.0
50.0
NCE


('Compound 585', -1)
Normalized Intensity
NCE
Fragment 1: 173.48
Fragment 2: 173.49
Fragment 3: 79.96
Fragment 4: 233.15
Fragment 5: 96.96
0
10000
20000
30000
40000
50000
60000
70000
25.0 35.0 40.0 60.0 70.0 80.0
10.0 20.0 30.0 50.0 70.0 80.0
50.0 60.0 70.0 80.0
30.0 35.0
25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0


('Compound 826', -1)
Fragment 1: 77.04
Fragment 2: 93.03
Fragment 3: 92.03
Fragment 4: 79.96
Fragment 5: 71.01
Normalized Intensity
0
500
1000
1500
2000
2500
3000
10.0
20.0
25.0
30.0
35.0
40.0
20.0
25.0
30.0
35.0
40.0
30.0
35.0
40.0
50.0
60.0
70.0
25.0
30.0
35.0
40.0
50.0
60.0
20.0
25.0
30.0
40.0
NCE


('Compound 625', -1)
Fragment 1: 151.04
Fragment 2: 107.06
Fragment 3: 127.08
Fragment 4: 107.05
Fragment 5: 106.04
Normalized Intensity
0
50000
100000
150000
200000
NCE
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0
35.0 40.0 50.0
10.0 20.0 25.0 30.0 35.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
30.0 35.0 40.0 50.0 60.0 70.0 80.0


('Compound 773', -1)
Fragment 1: 283.26
Fragment 2: 279.12
Fragment 3: 413.2
Fragment 4: 91.04
Fragment 5: 145.05
Normalized Intensity
0
50000
100000
150000
200000
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0
10.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
10.0 20.0 25.0 30.0 35.0
NCE


('Compound 614', -1)
Fragment 1: 119.05
Fragment 2: 155.14
Fragment 3: 93.03
Fragment 4: 173.48
Fragment 5: 79.96
Normalized Intensity
70000
60000
50000
40000
30000
20000
10000
0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
20.0 25.0 30.0
50.0 60.0 70.0 80.0
25.0 30.0 35.0 50.0 70.0
10.0 20.0 25.0 30.0 35.0 40.0 50.0 60.0 70.0 80.0
NCE