# WEB350

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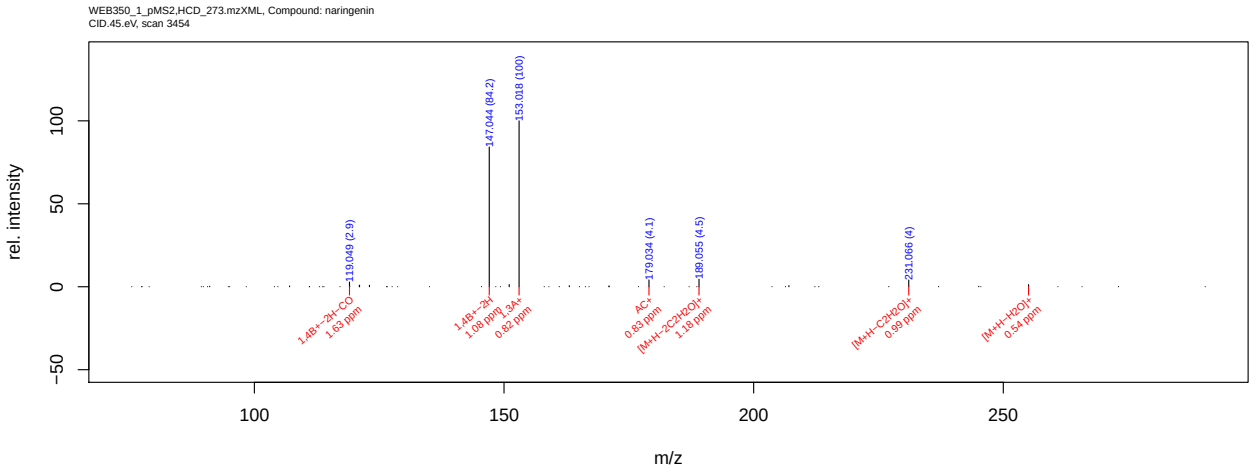
*10/01/2015*

## Contents

| | substance | fragment | formula | MW | mz |
|---|---|---|---|---|---|
| 1 | naringenin | 1,4B+-2H | | | 147.04 |
| 2 | naringenin | 1,4B+-2H-2CO | | | 91.05 |
| 3 | naringenin | 1,4B+-2H-CO | | | 119.05 |
| 4 | naringenin | AC+ | | | 179.03 |
| 5 | naringenin | [M+H]+ | C15H12O5 | 272.07 | 273.08 |
| 6 | naringenin | [M+H-2C2H2O]+ | C15H12O5 | 272.07 | 189.06 |

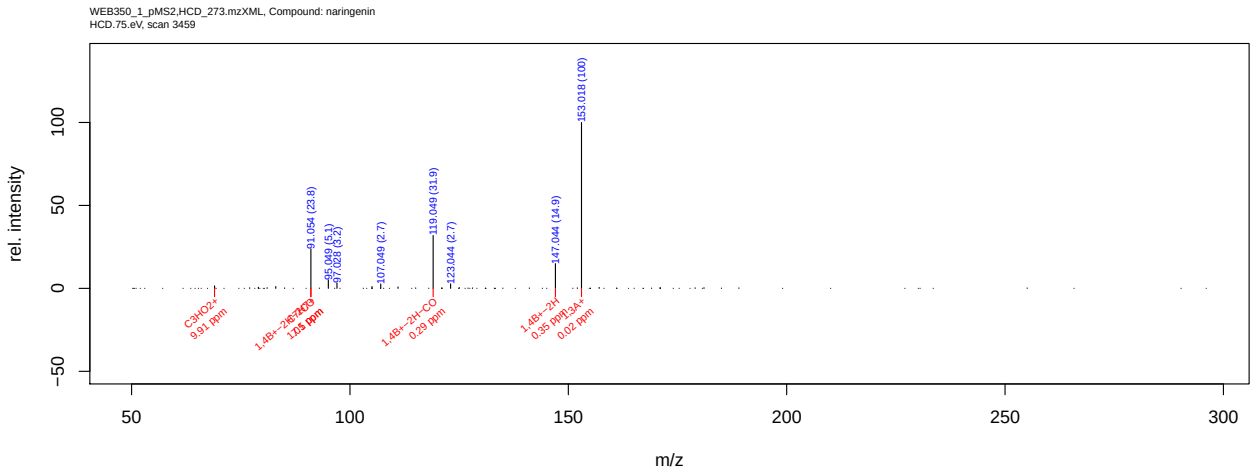
# Automatic annotation of MS spectra

## naringenin.CID.45eV



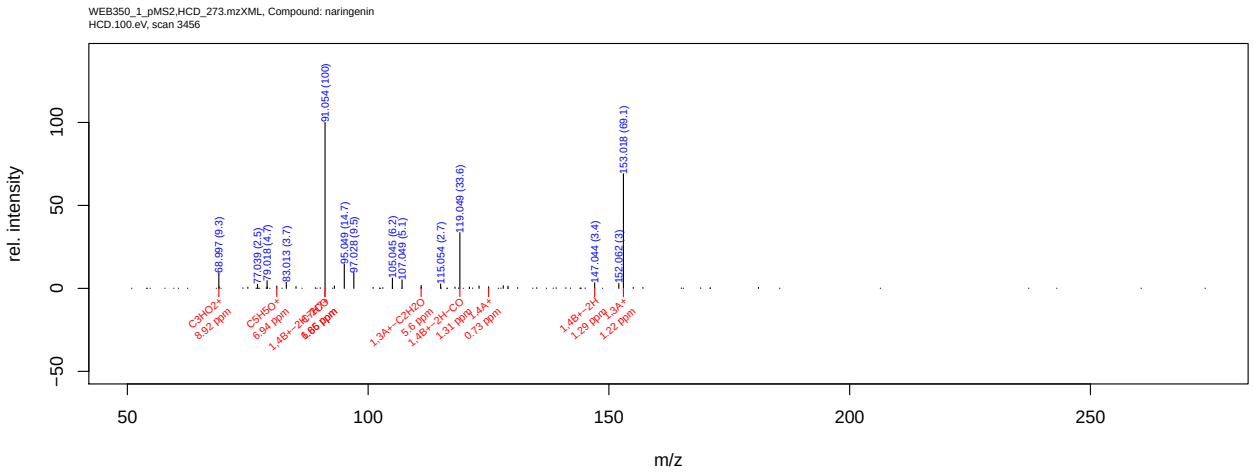

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 119.05 | 2.9 | 1.63 | 1,4B+-2H-CO |
| 2 | 147.04 | 84.2 | 1.08 | 1,4B+-2H |
| 3 | 153.02 | 100.0 | 0.82 | 1,3A+ |
| 4 | 179.03 | 4.1 | 0.83 | AC+ |
| 5 | 189.05 | 4.5 | 1.18 | [M+H-2C2H2O]+ |
| 6 | 231.07 | 4.0 | 0.99 | [M+H-C2H2O]+ |
| 7 | 255.07 | 1.3 | 0.54 | [M+H-H2O]+ |

## naringenin.HCD.75eV



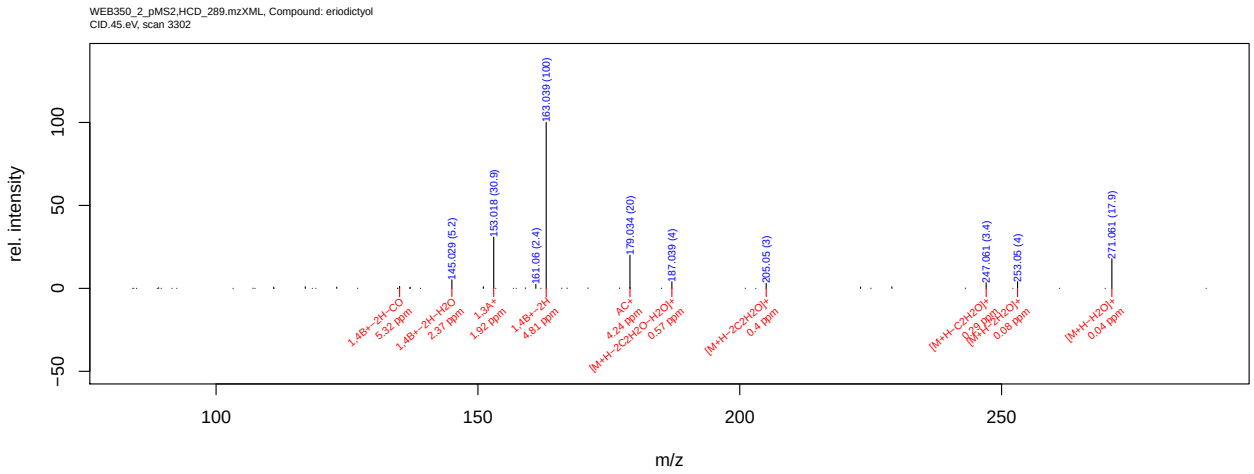

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 1.5 | 9.91 | C3HO2+ |
| 2 | 91.05 | 23.8 | 1.01 | 1,4B+-2H-2CO |
| 3 | 91.05 | 23.8 | 7.50 | C7H7+ |
| 4 | 119.05 | 31.9 | 0.29 | 1,4B+-2H-CO |
| 5 | 147.04 | 14.9 | 0.35 | 1,4B+-2H |
| 6 | 153.02 | 100.0 | 0.02 | 1,3A+ |

## naringenin.HCD.100eV



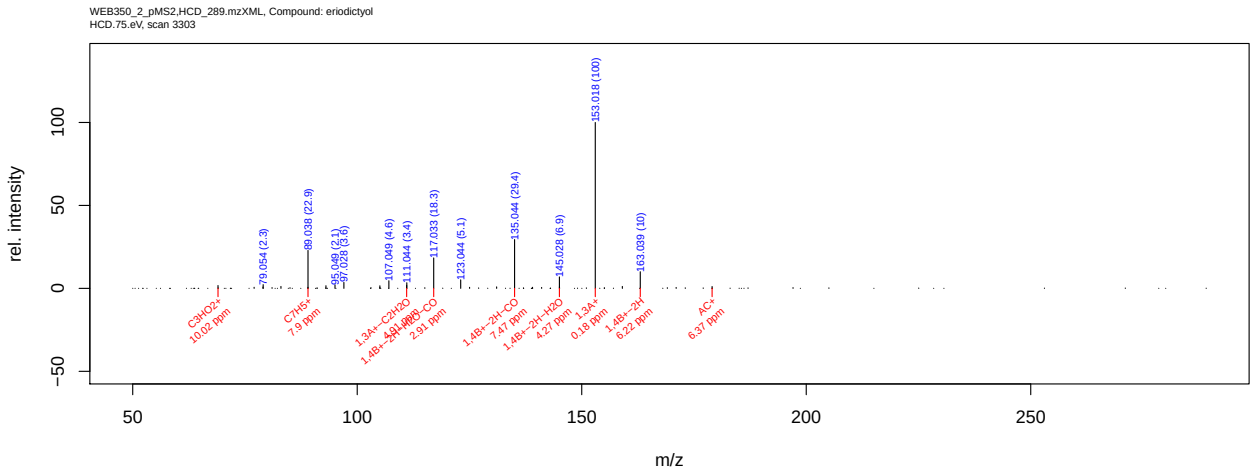

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 9.3 | 8.92 | C3HO2+ |
| 2 | 81.03 | 1.4 | 6.94 | C5H5O+ |
| 3 | 91.05 | 100.0 | 1.85 | 1,4B+-2H-2CO |
| 4 | 91.05 | 100.0 | 6.66 | C7H7+ |
| 5 | 111.01 | 1.8 | 5.60 | 1,3A+-C2H2O |
| 6 | 119.05 | 33.6 | 1.31 | 1,4B+-2H-CO |
| 7 | 125.02 | 1.0 | 0.73 | 1,4A+ |
| 8 | 147.04 | 3.4 | 1.29 | 1,4B+-2H |
| 9 | 153.02 | 69.1 | 1.22 | 1,3A+ |

## eriodictyol.CID.45eV



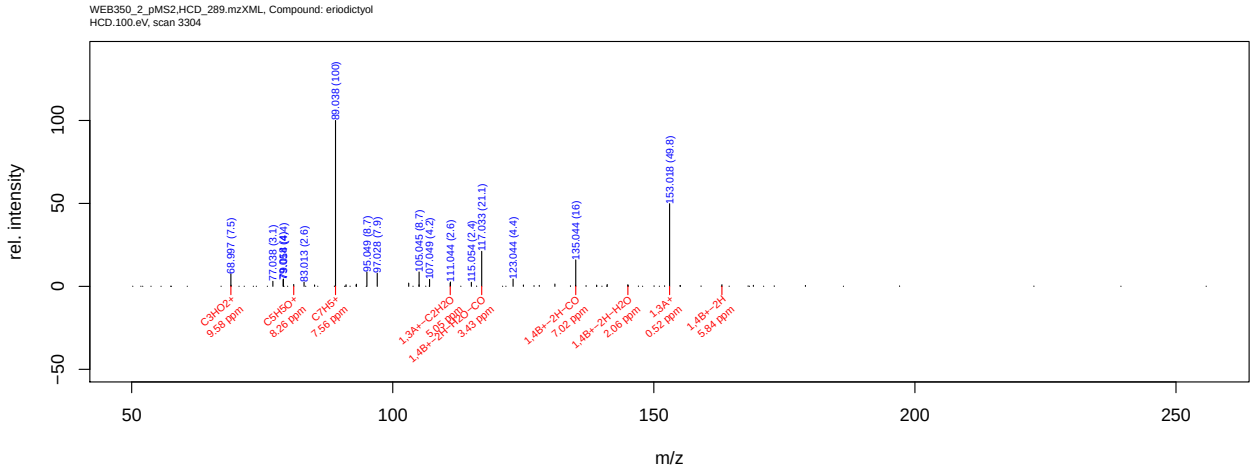

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 135.04 | 1.1 | 5.32 | 1,4B+-2H-CO |
| 2 | 145.03 | 5.2 | 2.37 | 1,4B+-2H-H2O |
| 3 | 153.02 | 30.9 | 1.92 | 1,3A+ |
| 4 | 163.04 | 100.0 | 4.81 | 1,4B+-2H |
| 5 | 179.03 | 20.0 | 4.24 | AC+ |
| 6 | 187.04 | 4.0 | 0.57 | [M+H-2C2H2O-H2O]+ |
| 7 | 205.05 | 3.0 | 0.40 | [M+H-2C2H2O]+ |
| 8 | 247.06 | 3.4 | 0.29 | [M+H-C2H2O]+ |
| 9 | 253.05 | 4.0 | 0.08 | [M+H-2H2O]+ |
| 10 | 271.06 | 17.9 | 0.04 | [M+H-H2O]+ |

## eriodictyol.HCD.75eV



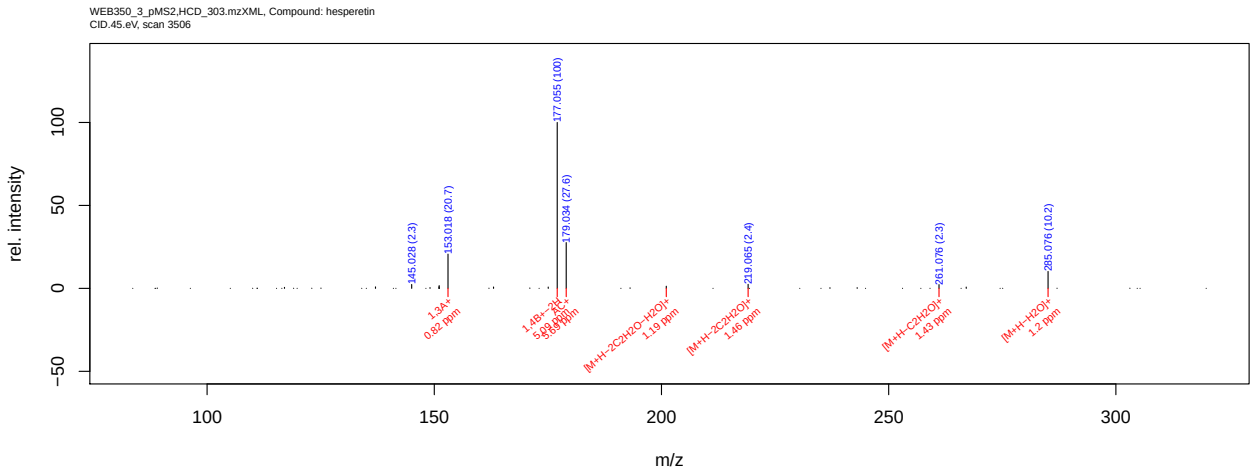

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 1.7 | 10.02 | C3HO2+ |
| 2 | 89.04 | 22.9 | 7.90 | C7H5+ |
| 3 | 111.01 | 1.8 | 4.91 | 1,3A+-C2H2O |
| 4 | 117.03 | 18.3 | 2.91 | 1,4B+-2H-H2O-CO |
| 5 | 135.04 | 29.4 | 7.47 | 1,4B+-2H-CO |
| 6 | 145.03 | 6.9 | 4.27 | 1,4B+-2H-H2O |
| 7 | 153.02 | 100.0 | 0.18 | 1,3A+ |
| 8 | 163.04 | 10.0 | 6.22 | 1,4B+-2H |
| 9 | 179.03 | 1.1 | 6.37 | AC+ |

## eriodictyol.HCD.100eV



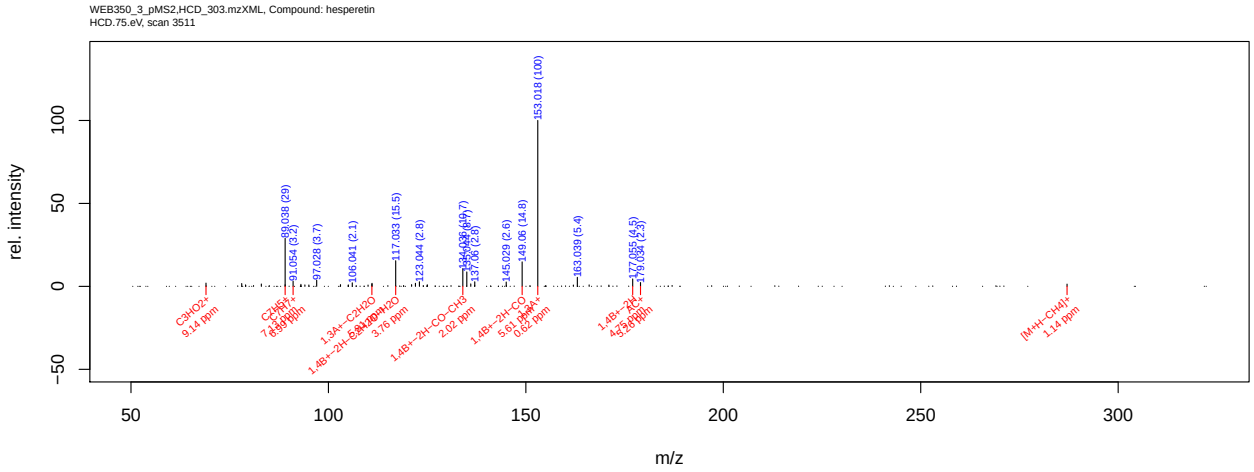

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 7.5 | 9.58 | C3HO2+ |
| 2 | 81.03 | 1.2 | 8.26 | C5H5O+ |
| 3 | 89.04 | 100.0 | 7.56 | C7H5+ |
| 4 | 111.01 | 1.9 | 5.05 | 1,3A+-C2H2O |
| 5 | 117.03 | 21.1 | 3.43 | 1,4B+-2H-H2O-CO |
| 6 | 135.04 | 16.0 | 7.02 | 1,4B+-2H-CO |
| 7 | 145.03 | 1.0 | 2.06 | 1,4B+-2H-H2O |
| 8 | 153.02 | 49.8 | 0.52 | 1,3A+ |
| 9 | 163.04 | 1.0 | 5.84 | 1,4B+-2H |

## hesperetin.CID.45eV



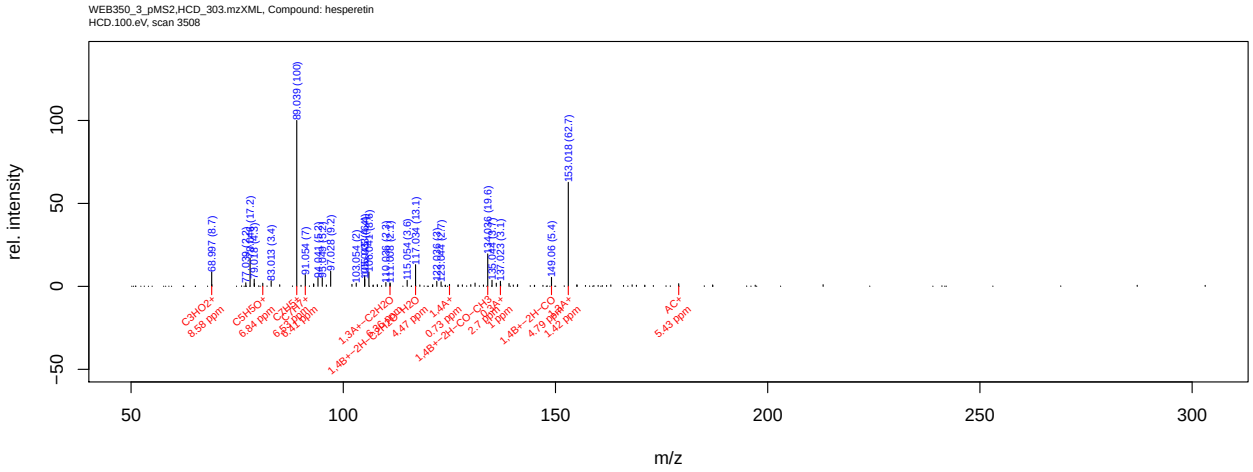

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 153.02 | 20.7 | 0.82 | 1,3A+ |
| 2 | 177.05 | 100.0 | 5.09 | 1,4B+-2H |
| 3 | 179.03 | 27.6 | 5.69 | AC+ |
| 4 | 201.05 | 1.3 | 1.19 | [M+H-2C2H2O-H2O]+ |
| 5 | 219.07 | 2.4 | 1.46 | [M+H-2C2H2O]+ |
| 6 | 261.08 | 2.3 | 1.43 | [M+H-C2H2O]+ |
| 7 | 285.08 | 10.2 | 1.20 | [M+H-H2O]+ |

## hesperetin.HCD.75eV



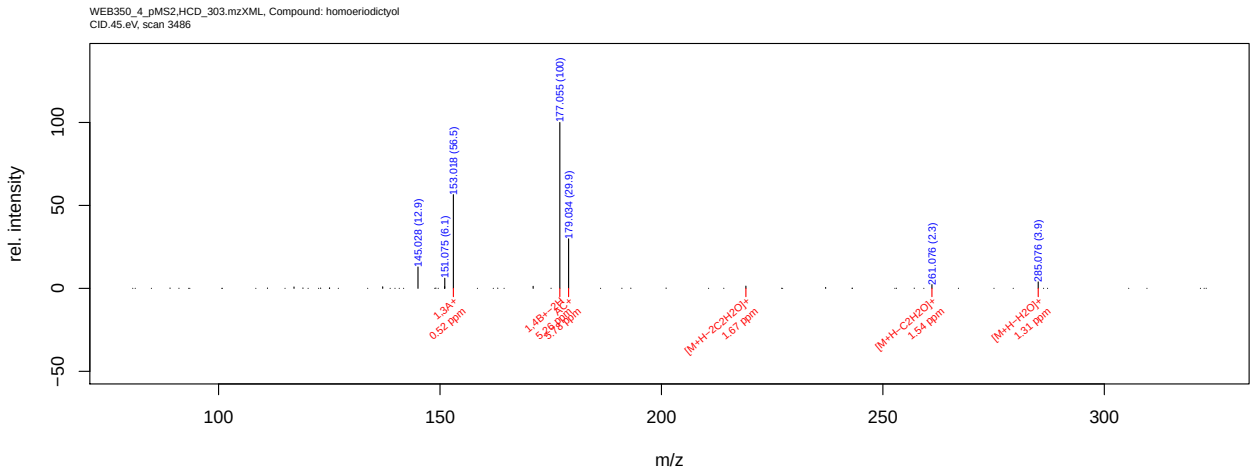

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 2.0 | 9.14 | C3HO2+ |
| 2 | 89.04 | 29.0 | 7.13 | C7H5+ |
| 3 | 91.05 | 3.2 | 6.99 | C7H7+ |
| 4 | 111.01 | 1.4 | 5.81 | 1,3A+-C2H2O |
| 5 | 117.03 | 15.5 | 3.76 | 1,4B+-2H-C2H2O-H2O |
| 6 | 134.04 | 10.7 | 2.02 | 1,4B+-2H-CO-CH3 |
| 7 | 149.06 | 14.8 | 5.61 | 1,4B+-2H-CO |
| 8 | 153.02 | 100.0 | 0.62 | 1,3A+ |
| 9 | 177.05 | 4.5 | 4.75 | 1,4B+-2H |
| 10 | 179.03 | 2.3 | 5.26 | AC+ |
| 11 | 287.06 | 1.4 | 1.14 | [M+H-CH4]+ |

## hesperetin.HCD.100eV



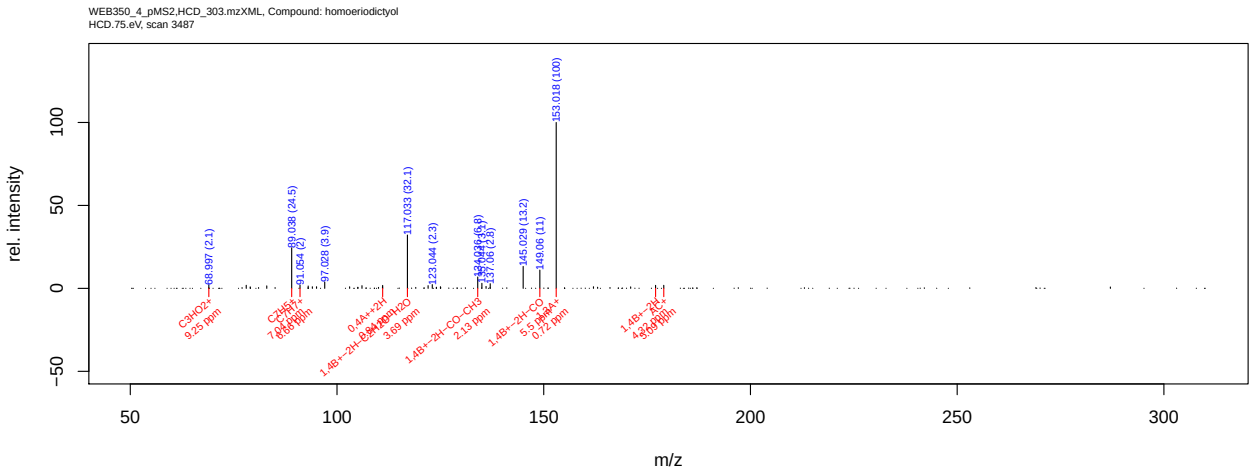

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 8.7 | 8.58 | C3HO2+ |
| 2 | 81.03 | 1.9 | 6.84 | C5H5O+ |
| 3 | 89.04 | 100.0 | 6.53 | C7H5+ |
| 4 | 91.05 | 7.0 | 6.41 | C7H7+ |
| 5 | 111.01 | 2.1 | 6.36 | 1,3A+-C2H2O |
| 6 | 117.03 | 13.1 | 4.47 | 1,4B+-2H-C2H2O-H2O |
| 7 | 125.02 | 1.2 | 0.73 | 1,4A+ |
| 8 | 134.04 | 19.6 | 2.70 | 1,4B+-2H-CO-CH3 |
| 9 | 137.02 | 3.1 | 1.00 | 0,3A+ |
| 10 | 149.06 | 5.4 | 4.79 | 1,4B+-2H-CO |
| 11 | 153.02 | 62.7 | 1.42 | 1,3A+ |
| 12 | 179.03 | 1.6 | 5.43 | AC+ |

## homoeriodictyol.CID.45eV



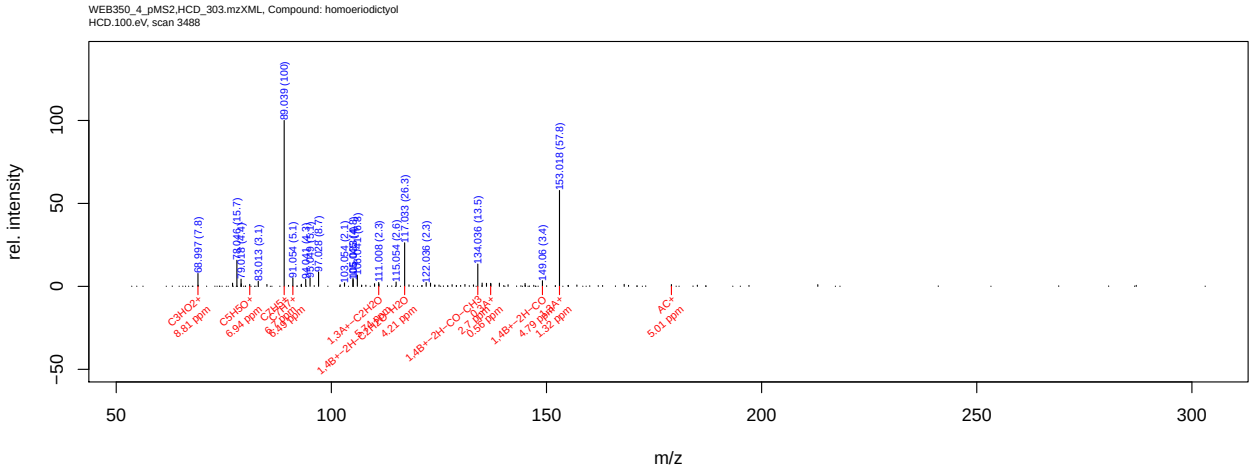

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 153.02 | 56.5 | 0.52 | 1,3A+ |
| 2 | 177.05 | 100.0 | 5.26 | 1,4B+-2H |
| 3 | 179.03 | 29.9 | 5.78 | AC+ |
| 4 | 219.07 | 1.4 | 1.67 | [M+H-2C2H2O]+ |
| 5 | 261.08 | 2.3 | 1.54 | [M+H-C2H2O]+ |
| 6 | 285.08 | 3.9 | 1.31 | [M+H-H2O]+ |

## homoeriodictyol.HCD.75eV



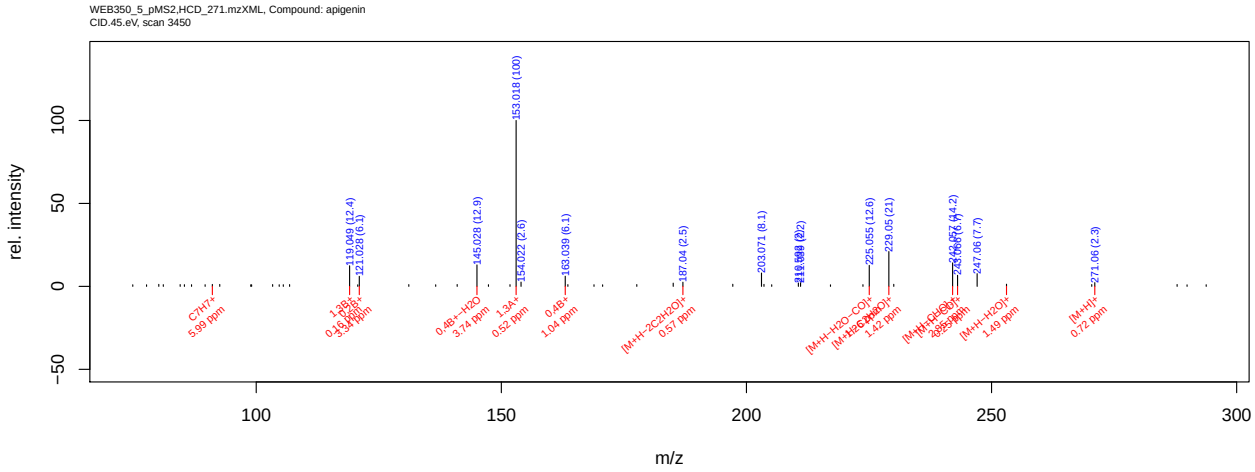

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 2.1 | 9.25 | C3HO2+ |
| 2 | 89.04 | 24.5 | 7.04 | C7H5+ |
| 3 | 91.05 | 2.0 | 6.66 | C7H7+ |
| 4 | 111.04 | 1.8 | 0.84 | 0,4A++2H |
| 5 | 117.03 | 32.1 | 3.69 | 1,4B+-2H-C2H2O-H2O |
| 6 | 134.04 | 6.8 | 2.13 | 1,4B+-2H-CO-CH3 |
| 7 | 149.06 | 11.0 | 5.50 | 1,4B+-2H-CO |
| 8 | 153.02 | 100.0 | 0.72 | 1,3A+ |
| 9 | 177.05 | 1.8 | 4.32 | 1,4B+-2H |
| 10 | 179.03 | 1.8 | 5.09 | AC+ |

## homoeriodictyol.HCD.100eV



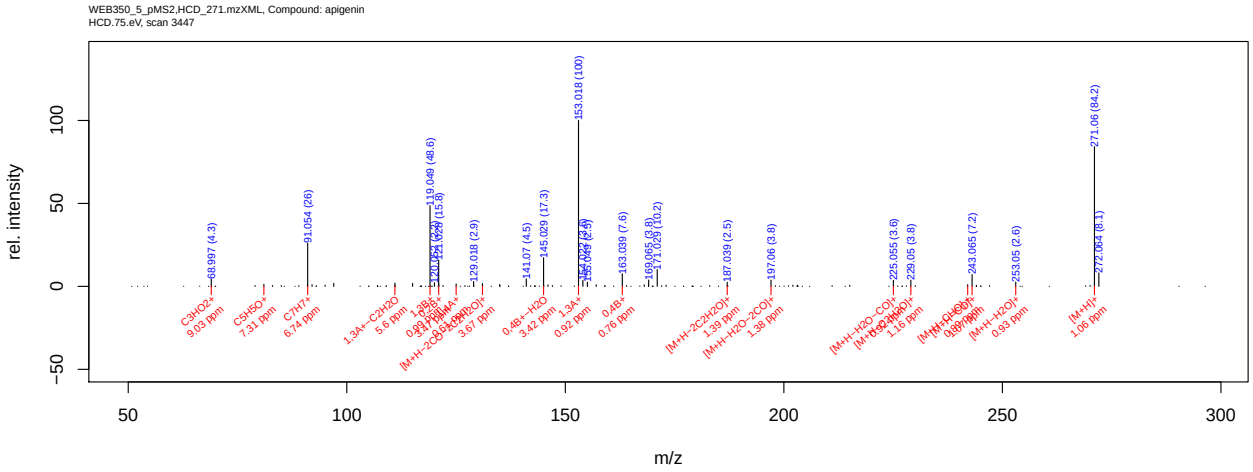

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 7.8 | 8.81 | C3HO2+ |
| 2 | 81.03 | 1.2 | 6.94 | C5H5O+ |
| 3 | 89.04 | 100.0 | 6.70 | C7H5+ |
| 4 | 91.05 | 5.1 | 6.49 | C7H7+ |
| 5 | 111.01 | 2.3 | 5.74 | 1,3A+-C2H2O |
| 6 | 117.03 | 26.3 | 4.21 | 1,4B+-2H-C2H2O-H2O |
| 7 | 134.04 | 13.5 | 2.70 | 1,4B+-2H-CO-CH3 |
| 8 | 137.02 | 1.8 | 0.56 | 0,3A+ |
| 9 | 149.06 | 3.4 | 4.79 | 1,4B+-2H-CO |
| 10 | 153.02 | 57.8 | 1.32 | 1,3A+ |
| 11 | 179.03 | 1.1 | 5.01 | AC+ |

## apigenin.CID.45eV



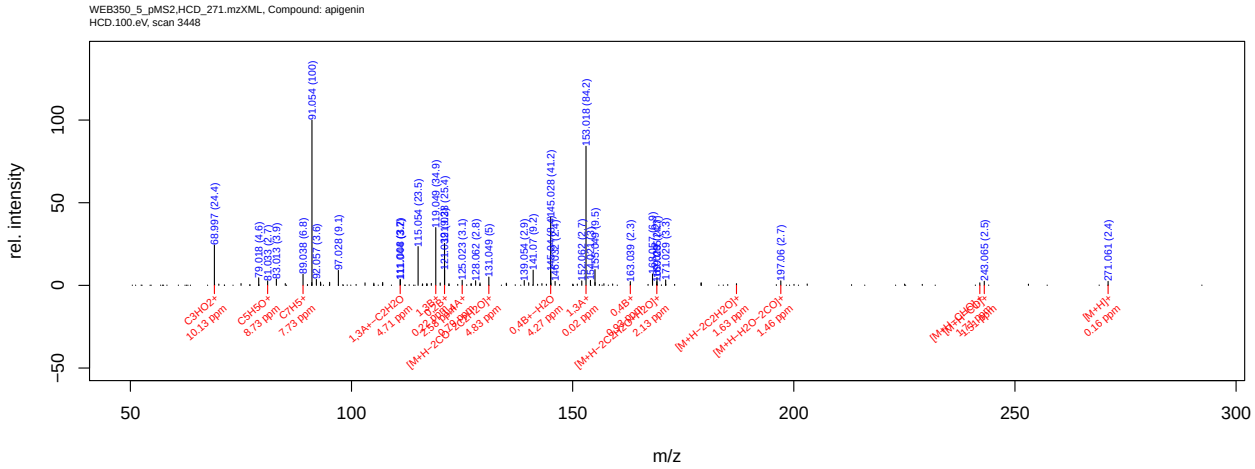

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 91.05 | 1.2 | 5.99 | C7H7+ |
| 2 | 119.05 | 12.4 | 0.16 | 1,3B+ |
| 3 | 121.03 | 6.1 | 3.34 | 0,2B+ |
| 4 | 145.03 | 12.9 | 3.74 | 0,4B+-H2O |
| 5 | 153.02 | 100.0 | 0.52 | 1,3A+ |
| 6 | 163.04 | 6.1 | 1.04 | 0,4B+ |
| 7 | 187.04 | 2.5 | 0.57 | [M+H-2C2H2O]+ |
| 8 | 225.05 | 12.6 | 1.26 | [M+H-H2O-CO]+ |
| 9 | 229.05 | 21.0 | 1.42 | [M+H-C2H2O]+ |
| 10 | 242.06 | 14.2 | 2.85 | [M+H-CHO].+ |
| 11 | 243.07 | 6.7 | 0.25 | [M+H-CO]+ |
| 12 | 253.05 | 1.3 | 1.49 | [M+H-H2O]+ |
| 13 | 271.06 | 2.3 | 0.72 | [M+H]+ |

## apigenin.HCD.75eV



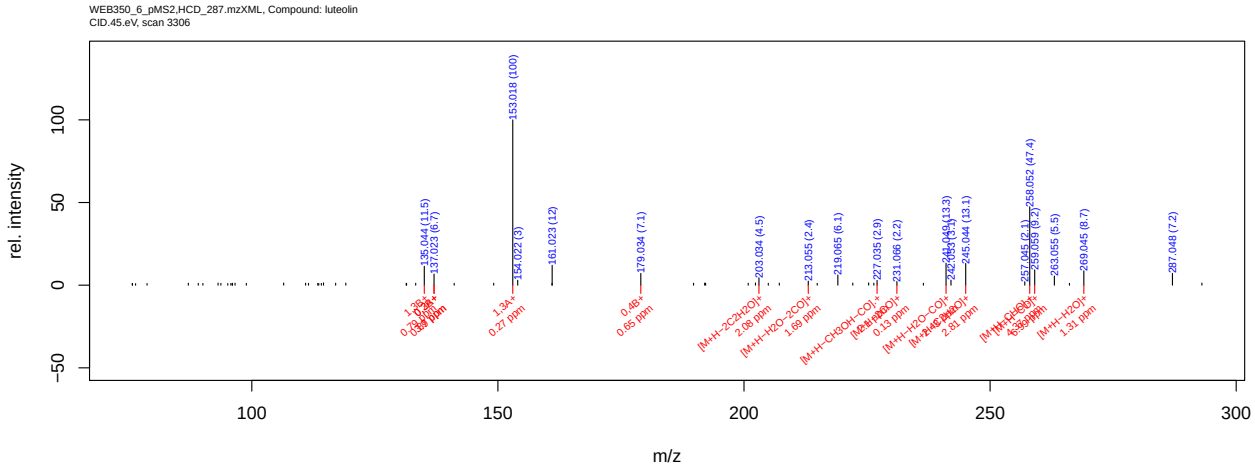

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 4.3 | 9.03 | C3HO2+ |
| 2 | 81.03 | 1.2 | 7.31 | C5H5O+ |
| 3 | 91.05 | 26.0 | 6.74 | C7H7+ |
| 4 | 111.01 | 2.0 | 5.60 | 1,3A+-C2H2O |
| 5 | 119.05 | 48.6 | 0.99 | 1,3B+ |
| 6 | 121.03 | 15.8 | 3.47 | 0,2B+ |
| 7 | 125.02 | 1.5 | 0.61 | 1,4A+ |
| 8 | 131.05 | 1.7 | 3.67 | [M+H-2CO-2C2H2O]+ |
| 9 | 145.03 | 17.3 | 3.42 | 0,4B+-H2O |
| 10 | 153.02 | 100.0 | 0.92 | 1,3A+ |
| 11 | 163.04 | 7.6 | 0.76 | 0,4B+ |
| 12 | 187.04 | 2.5 | 1.39 | [M+H-2C2H2O]+ |
| 13 | 197.06 | 3.8 | 1.38 | [M+H-H2O-2CO]+ |
| 14 | 225.05 | 3.6 | 0.92 | [M+H-H2O-CO]+ |
| 15 | 229.05 | 3.8 | 1.16 | [M+H-C2H2O]+ |
| 16 | 242.06 | 1.0 | 0.89 | [M+H-CHO].+ |
| 17 | 243.07 | 7.2 | 1.07 | [M+H-CO]+ |
| 18 | 253.05 | 2.6 | 0.93 | [M+H-H2O]+ |
| 19 | 271.06 | 84.2 | 1.06 | [M+H]+ |

## apigenin.HCD.100eV



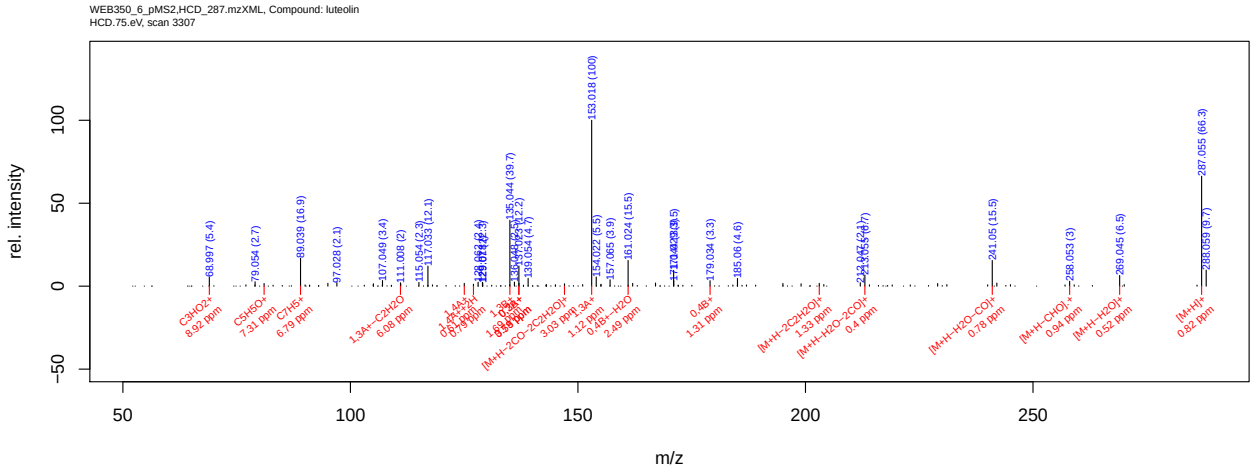

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 24.4 | 10.13 | C3HO2+ |
| 2 | 81.03 | 2.7 | 8.73 | C5H5O+ |
| 3 | 89.04 | 6.8 | 7.73 | C7H5+ |
| 4 | 111.01 | 3.7 | 4.71 | 1,3A+-C2H2O |
| 5 | 119.05 | 34.9 | 0.22 | 1,3B+ |
| 6 | 121.03 | 25.4 | 2.58 | 0,2B+ |
| 7 | 125.02 | 3.1 | 0.79 | 1,4A+ |
| 8 | 131.05 | 5.0 | 4.83 | [M+H-2CO-2C2H2O]+ |
| 9 | 145.03 | 41.2 | 4.27 | 0,4B+-H2O |
| 10 | 153.02 | 84.2 | 0.02 | 1,3A+ |
| 11 | 163.04 | 2.3 | 0.93 | 0,4B+ |
| 12 | 169.03 | 2.2 | 2.13 | [M+H-2C2H2O-H2O]+ |
| 13 | 187.04 | 1.0 | 1.63 | [M+H-2C2H2O]+ |
| 14 | 197.06 | 2.7 | 1.46 | [M+H-H2O-2CO]+ |
| 15 | 242.06 | 1.5 | 1.71 | [M+H-CHO].+ |
| 16 | 243.07 | 2.5 | 1.51 | [M+H-CO]+ |
| 17 | 271.06 | 2.4 | 0.16 | [M+H]+ |

## luteolin.CID.45eV



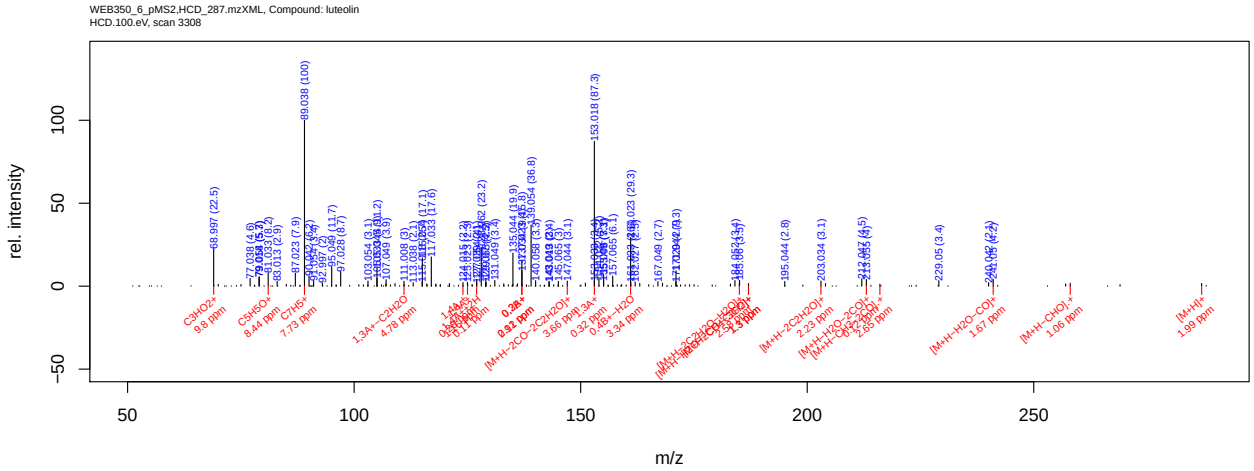

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 135.04 | 11.5 | 0.79 | 1,3B+ |
| 2 | 137.02 | 6.7 | 3.70 | 0,2B+ |
| 3 | 137.02 | 6.7 | 0.89 | 0,3A+ |
| 4 | 153.02 | 100.0 | 0.27 | 1,3A+ |
| 5 | 179.03 | 7.1 | 0.65 | 0,4B+ |
| 6 | 203.03 | 4.5 | 2.08 | [M+H-2C2H2O]+ |
| 7 | 213.05 | 2.4 | 1.69 | [M+H-H2O-2CO]+ |
| 8 | 227.03 | 2.9 | 2.10 | [M+H-CH3OH-CO].+ |
| 9 | 231.07 | 2.2 | 0.13 | [M+H-2CO]+ |
| 10 | 241.05 | 13.3 | 2.43 | [M+H-H2O-CO]+ |
| 11 | 245.04 | 13.1 | 2.81 | [M+H-C2H2O]+ |
| 12 | 258.05 | 47.4 | 4.37 | [M+H-CHO].+ |
| 13 | 259.06 | 9.2 | 6.99 | [M+H-CO]+ |
| 14 | 269.04 | 8.7 | 1.31 | [M+H-H2O]+ |

## luteolin.HCD.75eV



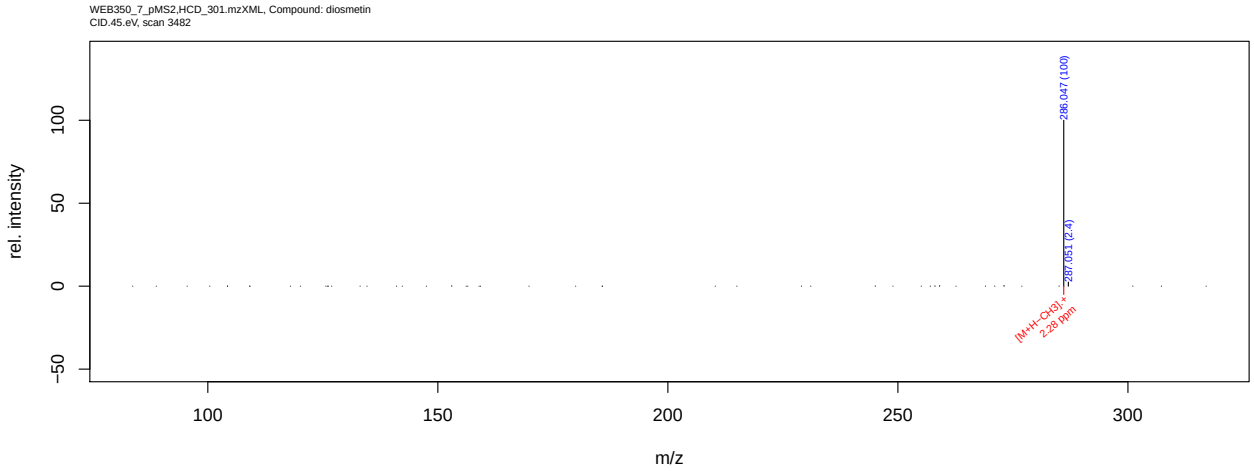

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 5.4 | 8.92 | C3HO2+ |
| 2 | 81.03 | 1.6 | 7.31 | C5H5O+ |
| 3 | 89.04 | 16.9 | 6.79 | C7H5+ |
| 4 | 111.01 | 2.0 | 6.08 | 1,3A+-C2H2O |
| 5 | 125.02 | 1.7 | 0.61 | 1,4A+ |
| 6 | 127.04 | 1.2 | 0.79 | 1,4A++2H |
| 7 | 135.04 | 39.7 | 1.69 | 1,3B+ |
| 8 | 137.02 | 12.2 | 3.59 | 0,2B+ |
| 9 | 137.02 | 12.2 | 0.78 | 0,3A+ |
| 10 | 147.04 | 1.5 | 3.03 | [M+H-2CO-2C2H2O]+ |
| 11 | 153.02 | 100.0 | 1.12 | 1,3A+ |
| 12 | 161.02 | 15.5 | 2.49 | 0,4B+-H2O |
| 13 | 179.03 | 3.3 | 1.31 | 0,4B+ |
| 14 | 203.03 | 1.7 | 1.33 | [M+H-2C2H2O]+ |
| 15 | 213.06 | 6.7 | 0.40 | [M+H-H2O-2CO]+ |
| 16 | 241.05 | 15.5 | 0.78 | [M+H-H2O-CO]+ |
| 17 | 258.05 | 3.0 | 0.94 | [M+H-CHO].+ |
| 18 | 269.04 | 6.5 | 0.52 | [M+H-H2O]+ |
| 19 | 287.06 | 66.3 | 0.82 | [M+H]+ |

## luteolin.HCD.100eV



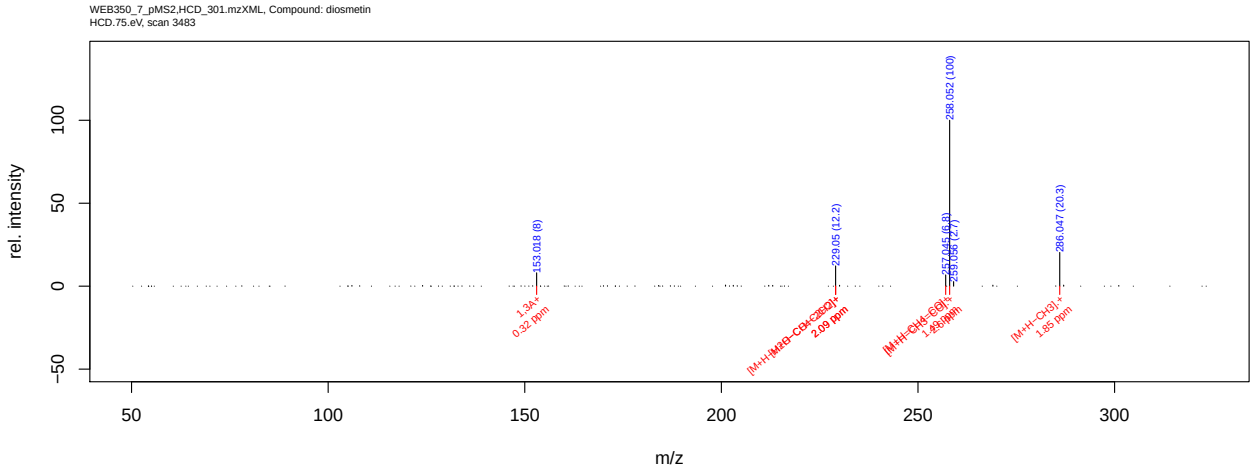

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 22.5 | 9.80 | C3HO2+ |
| 2 | 81.03 | 8.2 | 8.44 | C5H5O+ |
| 3 | 89.04 | 100.0 | 7.73 | C7H5+ |
| 4 | 111.01 | 3.0 | 4.78 | 1,3A+-C2H2O |
| 5 | 124.02 | 2.2 | 0.28 | 1,4A.+ |
| 6 | 125.02 | 2.3 | 1.16 | 1,4A+ |
| 7 | 127.04 | 2.1 | 0.11 | 1,4A++2H |
| 8 | 137.02 | 15.8 | 2.92 | 0,2B+ |
| 9 | 137.02 | 15.8 | 0.11 | 0,3A+ |
| 10 | 147.04 | 3.1 | 3.66 | [M+H-2CO-2C2H2O]+ |
| 11 | 153.02 | 87.3 | 0.32 | 1,3A+ |
| 12 | 161.02 | 29.3 | 3.34 | 0,4B+-H2O |
| 13 | 185.02 | 1.9 | 2.58 | [M+H-2C2H2O-H2O]+ |
| 14 | 187.04 | 1.6 | 1.30 | [M+H-CH4-3CO]+ |
| 15 | 187.04 | 1.6 | 1.30 | [M+H-H2O-2CO-C2H2]+ |
| 16 | 203.03 | 3.1 | 2.23 | [M+H-2C2H2O]+ |
| 17 | 213.06 | 4.0 | 0.12 | [M+H-H2O-2CO]+ |
| 18 | 216.04 | 1.2 | 2.65 | [M+H-CH3-2CO].+ |
| 19 | 241.05 | 4.2 | 1.67 | [M+H-H2O-CO]+ |
| 20 | 258.05 | 1.7 | 1.06 | [M+H-CHO].+ |
| 21 | 287.05 | 1.6 | 1.99 | [M+H]+ |

## diosmetin.CID.45eV



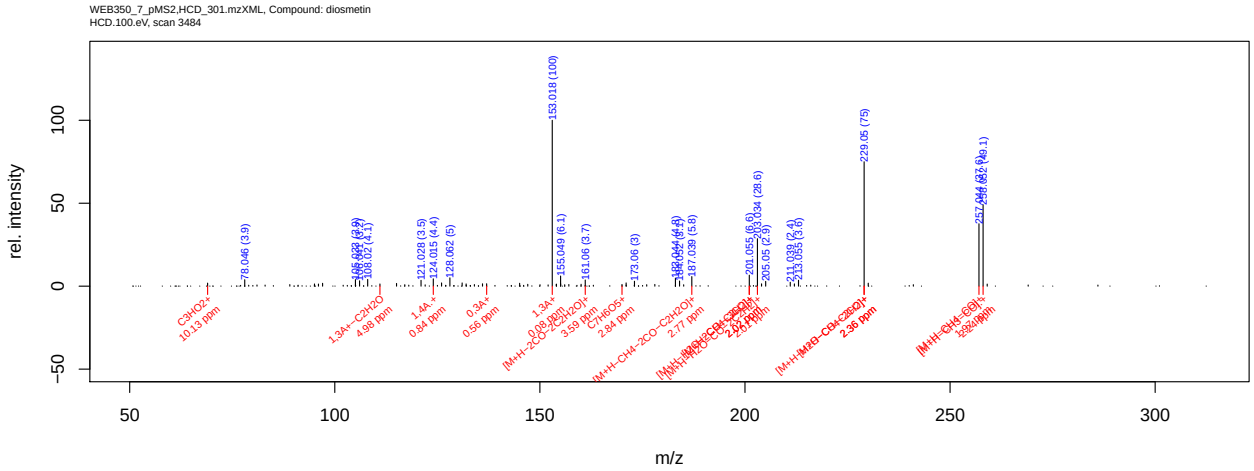

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 286.05 | 100.0 | 2.28 | [M+H-CH3].+ |

## diosmetin.HCD.75eV



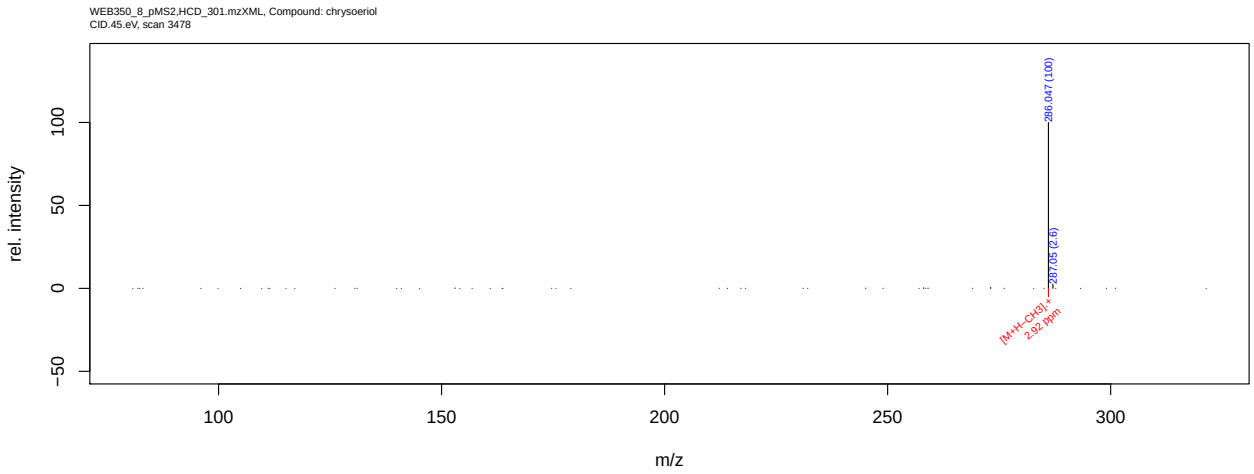

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 153.02 | 8.0 | 0.32 | 1,3A+ |
| 2 | 229.05 | 12.2 | 2.09 | [M+H-CH4-2CO]+ |
| 3 | 229.05 | 12.2 | 2.09 | [M+H-H2O-CO-C2H2]+ |
| 4 | 257.04 | 6.8 | 1.49 | [M+H-CH4-CO]+ |
| 5 | 258.05 | 100.0 | 2.60 | [M+H-CH3-CO].+ |
| 6 | 286.05 | 20.3 | 1.85 | [M+H-CH3].+ |

## diosmetin.HCD.100eV



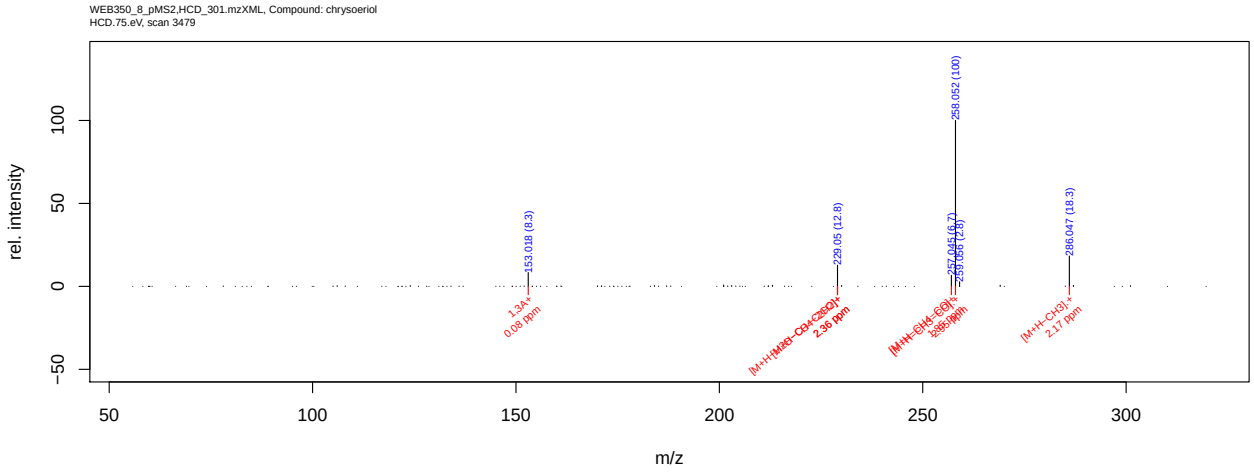

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 1.8 | 10.13 | C3HO2+ |
| 2 | 111.01 | 1.3 | 4.98 | 1,3A+-C2H2O |
| 3 | 124.02 | 4.4 | 0.84 | 1,4A.+ |
| 4 | 137.02 | 1.5 | 0.56 | 0,3A+ |
| 5 | 153.02 | 100.0 | 0.08 | 1,3A+ |
| 6 | 161.06 | 3.7 | 3.59 | [M+H-2CO-2C2H2O]+ |
| 7 | 170.02 | 1.1 | 2.84 | C7H6O5+ |
| 8 | 187.04 | 5.8 | 2.77 | [M+H-CH4-2CO-C2H2O]+ |
| 9 | 201.05 | 6.6 | 2.02 | [M+H-CH4-3CO]+ |
| 10 | 201.05 | 6.6 | 2.02 | [M+H-H2O-2CO-C2H2]+ |
| 11 | 203.03 | 28.6 | 2.01 | [M+H-H2O-CO-2C2H2]+ |
| 12 | 229.05 | 75.0 | 2.36 | [M+H-CH4-2CO]+ |
| 13 | 229.05 | 75.0 | 2.36 | [M+H-H2O-CO-C2H2]+ |
| 14 | 257.04 | 37.6 | 1.97 | [M+H-CH4-CO]+ |
| 15 | 258.05 | 49.1 | 2.24 | [M+H-CH3-CO].+ |

## chrysoeriol.CID.45eV



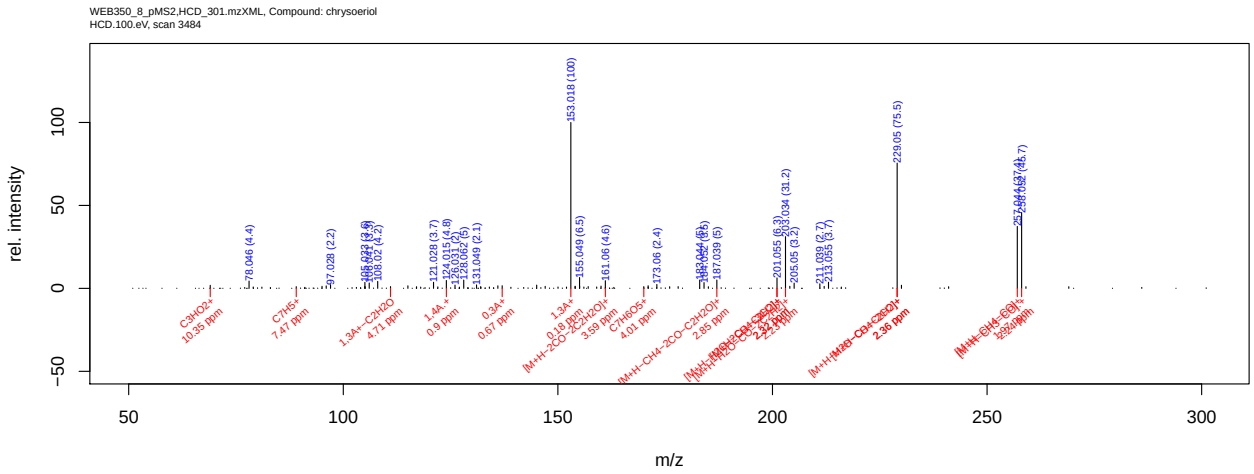

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 286.05 | 100.0 | 2.92 | [M+H-CH3].+ |

## chrysoeriol.HCD.75eV



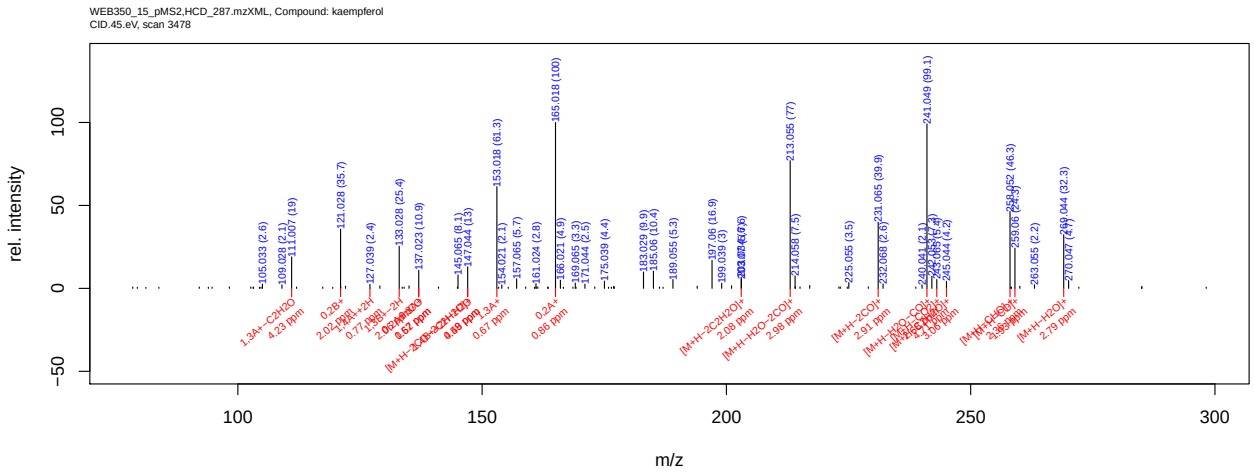

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 153.02 | 8.3 | 0.08 | 1,3A+ |
| 2 | 229.05 | 12.8 | 2.36 | [M+H-CH4-2CO]+ |
| 3 | 229.05 | 12.8 | 2.36 | [M+H-H2O-CO-C2H2]+ |
| 4 | 257.04 | 6.7 | 1.85 | [M+H-CH4-CO]+ |
| 5 | 258.05 | 100.0 | 2.95 | [M+H-CH3-CO].+ |
| 6 | 286.05 | 18.3 | 2.17 | [M+H-CH3].+ |

## chrysoeriol.HCD.100eV



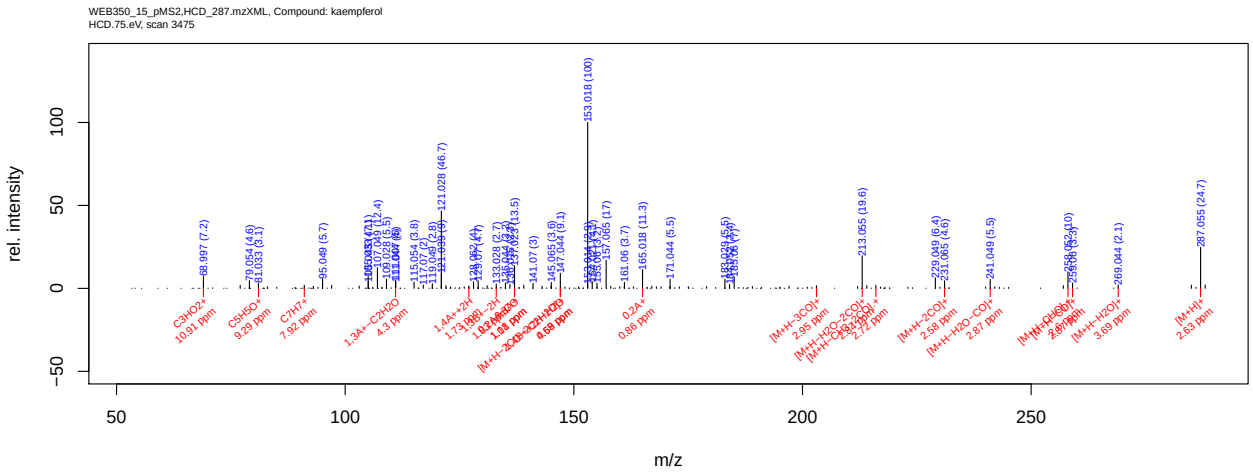

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 1.9 | 10.35 | C3HO2+ |
| 2 | 89.04 | 1.0 | 7.47 | C7H5+ |
| 3 | 111.01 | 1.1 | 4.71 | 1,3A+-C2H2O |
| 4 | 124.02 | 4.8 | 0.90 | 1,4A.+ |
| 5 | 137.02 | 1.6 | 0.67 | 0,3A+ |
| 6 | 153.02 | 100.0 | 0.18 | 1,3A+ |
| 7 | 161.06 | 4.6 | 3.59 | [M+H-2CO-2C2H2O]+ |
| 8 | 170.02 | 1.1 | 4.01 | C7H6O5+ |
| 9 | 187.04 | 5.0 | 2.85 | [M+H-CH4-2CO-C2H2O]+ |
| 10 | 201.05 | 6.3 | 2.32 | [M+H-CH4-3CO]+ |
| 11 | 201.05 | 6.3 | 2.32 | [M+H-H2O-2CO-C2H2]+ |
| 12 | 203.03 | 31.2 | 2.23 | [M+H-H2O-CO-2C2H2]+ |
| 13 | 229.05 | 75.5 | 2.36 | [M+H-CH4-2CO]+ |
| 14 | 229.05 | 75.5 | 2.36 | [M+H-H2O-CO-C2H2]+ |
| 15 | 257.04 | 37.4 | 1.97 | [M+H-CH4-CO]+ |
| 16 | 258.05 | 45.7 | 2.24 | [M+H-CH3-CO].+ |

## kaempferol.CID.45eV



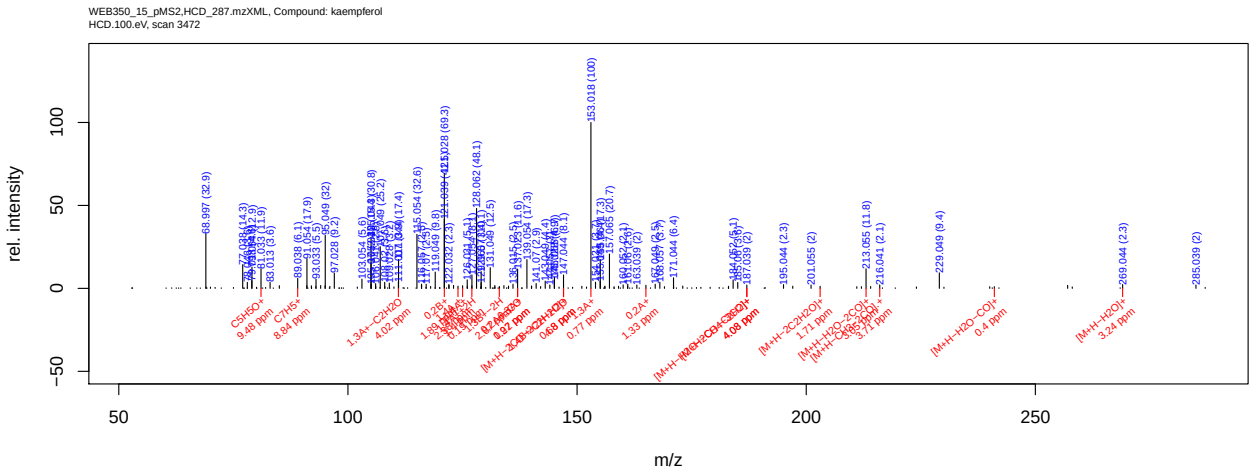

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 111.01 | 19.0 | 4.23 | 1,3A+-C2H2O |
| 2 | 121.03 | 35.7 | 2.02 | 0,2B+ |
| 3 | 127.04 | 2.4 | 0.77 | 1,4A++2H |
| 4 | 133.03 | 25.4 | 2.06 | 1,3B+-2H |
| 5 | 137.02 | 10.9 | 1.52 | 0,2A+-CO |
| 6 | 137.02 | 10.9 | 0.67 | 0,3A+ |
| 7 | 147.04 | 13.0 | 0.48 | 1,4B++2H-H2O |
| 8 | 147.04 | 13.0 | 4.59 | [M+H-2CO-2C2H2O]+ |
| 9 | 153.02 | 61.3 | 0.67 | 1,3A+ |
| 10 | 165.02 | 100.0 | 0.86 | 0,2A+ |
| 11 | 203.03 | 6.6 | 2.08 | [M+H-2C2H2O]+ |
| 12 | 213.05 | 77.0 | 2.98 | [M+H-H2O-2CO]+ |
| 13 | 231.07 | 39.9 | 2.91 | [M+H-2CO]+ |
| 14 | 241.05 | 99.1 | 2.68 | [M+H-H2O-CO]+ |
| 15 | 243.06 | 5.4 | 4.71 | [M+H-CO2]+ |
| 16 | 245.04 | 4.2 | 3.06 | [M+H-C2H2O]+ |
| 17 | 258.05 | 46.3 | 2.36 | [M+H-CHO].+ |
| 18 | 259.06 | 24.3 | 1.93 | [M+H-CO]+ |
| 19 | 269.04 | 32.3 | 2.79 | [M+H-H2O]+ |

## kaempferol.HCD.75eV



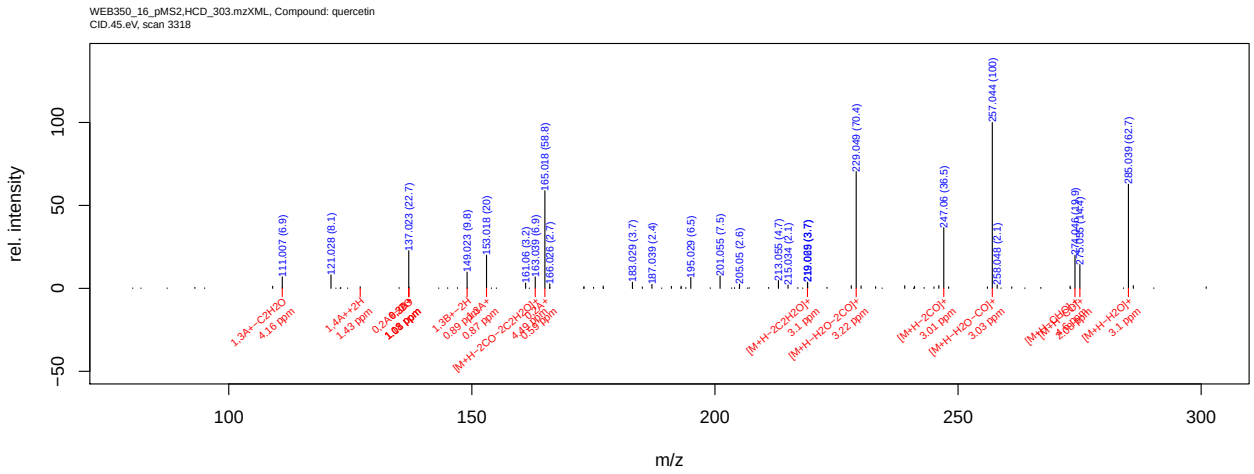

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 7.2 | 10.91 | C3HO2+ |
| 2 | 81.03 | 3.1 | 9.29 | C5H5O+ |
| 3 | 91.05 | 1.9 | 7.92 | C7H7+ |
| 4 | 111.01 | 5.0 | 4.30 | 1,3A+-C2H2O |
| 5 | 127.04 | 1.4 | 1.73 | 1,4A++2H |
| 6 | 133.03 | 2.7 | 1.83 | 1,3B+-2H |
| 7 | 137.02 | 13.5 | 1.08 | 0,2A+-CO |
| 8 | 137.02 | 13.5 | 1.11 | 0,3A+ |
| 9 | 147.04 | 9.1 | 0.58 | 1,4B++2H-H2O |
| 10 | 147.04 | 9.1 | 4.69 | [M+H-2CO-2C2H2O]+ |
| 11 | 165.02 | 11.3 | 0.86 | 0,2A+ |
| 12 | 203.07 | 1.5 | 2.95 | [M+H-3CO]+ |
| 13 | 213.05 | 19.6 | 2.84 | [M+H-H2O-2CO]+ |
| 14 | 216.04 | 1.8 | 2.72 | [M+H-CH3-2CO].+ |
| 15 | 231.07 | 4.6 | 2.58 | [M+H-2CO]+ |
| 16 | 241.05 | 5.5 | 2.87 | [M+H-H2O-CO]+ |
| 17 | 258.05 | 10.0 | 2.60 | [M+H-CHO].+ |
| 18 | 259.06 | 3.3 | 2.87 | [M+H-CO]+ |
| 19 | 269.04 | 2.1 | 3.69 | [M+H-H2O]+ |
| 20 | 287.05 | 24.7 | 2.63 | [M+H]+ |

## kaempferol.HCD.100eV



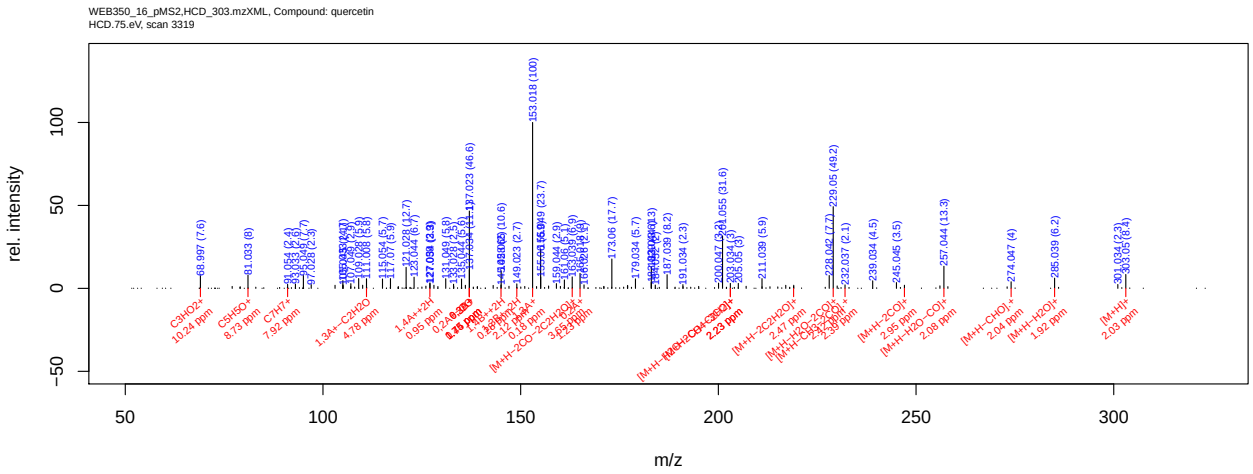

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 81.03 | 11.9 | 9.48 | C5H5O+ |
| 2 | 89.04 | 6.1 | 8.84 | C7H5+ |
| 3 | 111.01 | 3.9 | 4.02 | 1,3A+-C2H2O |
| 4 | 121.03 | 69.3 | 1.89 | 0,2B+ |
| 5 | 124.02 | 1.3 | 2.38 | 1,4A.+ |
| 6 | 125.02 | 1.6 | 1.40 | 1,4A+ |
| 7 | 127.04 | 1.6 | 0.19 | 1,4A++2H |
| 8 | 133.03 | 1.2 | 2.87 | 1,3B+-2H |
| 9 | 137.02 | 11.6 | 0.97 | 0,2A+-CO |
| 10 | 137.02 | 11.6 | 1.22 | 0,3A+ |
| 11 | 147.04 | 8.1 | 0.68 | 1,4B++2H-H2O |
| 12 | 147.04 | 8.1 | 4.80 | [M+H-2CO-2C2H2O]+ |
| 13 | 153.02 | 100.0 | 0.77 | 1,3A+ |
| 14 | 165.02 | 1.9 | 1.33 | 0,2A+ |
| 15 | 187.04 | 2.0 | 4.08 | [M+H-CH4-3CO]+ |
| 16 | 187.04 | 2.0 | 4.08 | [M+H-H2O-2CO-C2H2]+ |
| 17 | 203.03 | 1.3 | 1.71 | [M+H-2C2H2O]+ |
| 18 | 213.05 | 11.8 | 3.05 | [M+H-H2O-2CO]+ |
| 19 | 216.04 | 2.1 | 3.71 | [M+H-CH3-2CO].+ |
| 20 | 241.05 | 1.0 | 0.40 | [M+H-H2O-CO]+ |
| 21 | 269.04 | 2.3 | 3.24 | [M+H-H2O]+ |

## quercetin.CID.45eV



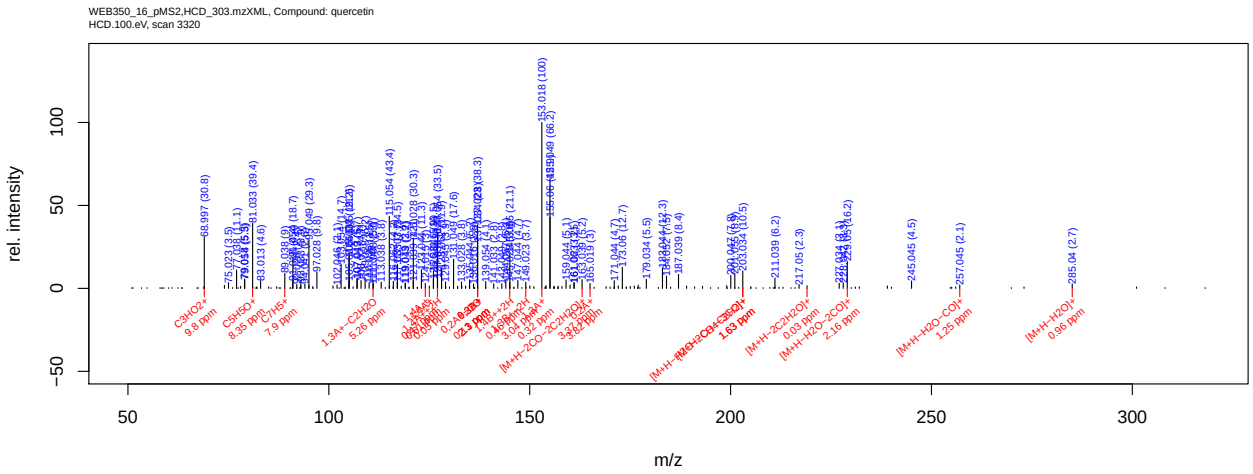

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 111.01 | 6.9 | 4.16 | 1,3A+-C2H2O |
| 2 | 127.04 | 1.0 | 1.43 | 1,4A++2H |
| 3 | 137.02 | 22.7 | 1.08 | 0,2A+-CO |
| 4 | 137.02 | 22.7 | 1.08 | 0,2B+ |
| 5 | 137.02 | 22.7 | 1.11 | 0,3A+ |
| 6 | 149.02 | 9.8 | 0.89 | 1,3B+-2H |
| 7 | 153.02 | 20.0 | 0.87 | 1,3A+ |
| 8 | 163.04 | 6.9 | 4.49 | [M+H-2CO-2C2H2O]+ |
| 9 | 165.02 | 58.8 | 0.59 | 0,2A+ |
| 10 | 219.03 | 3.7 | 3.10 | [M+H-2C2H2O]+ |
| 11 | 229.05 | 70.4 | 3.22 | [M+H-H2O-2CO]+ |
| 12 | 247.06 | 36.5 | 3.01 | [M+H-2CO]+ |
| 13 | 257.04 | 100.0 | 3.03 | [M+H-H2O-CO]+ |
| 14 | 274.05 | 19.9 | 4.60 | [M+H-CHO].+ |
| 15 | 275.05 | 14.4 | 2.08 | [M+H-CO]+ |
| 16 | 285.04 | 62.7 | 3.10 | [M+H-H2O]+ |

## quercetin.HCD.75eV



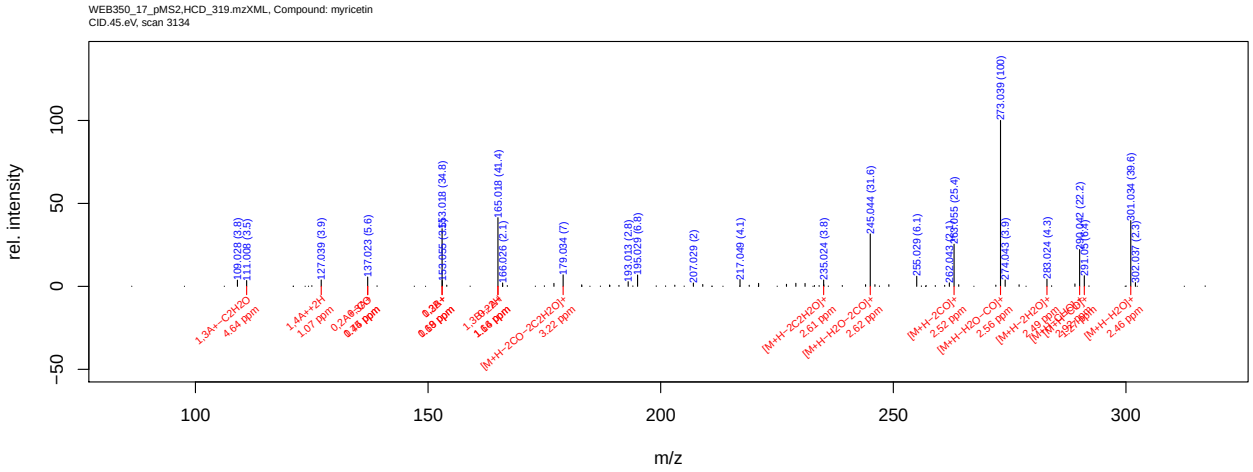

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 7.6 | 10.24 | C3HO2+ |
| 2 | 81.03 | 8.0 | 8.73 | C5H5O+ |
| 3 | 91.05 | 2.4 | 7.92 | C7H7+ |
| 4 | 111.01 | 5.8 | 4.78 | 1,3A+-C2H2O |
| 5 | 127.04 | 2.9 | 0.95 | 1,4A++2H |
| 6 | 137.02 | 46.6 | 1.75 | 0,2A+-CO |
| 7 | 137.02 | 46.6 | 1.75 | 0,2B+ |
| 8 | 137.02 | 46.6 | 0.44 | 0,3A+ |
| 9 | 145.03 | 2.0 | 0.28 | 1,4B++2H |
| 10 | 149.02 | 2.7 | 2.12 | 1,3B+-2H |
| 11 | 153.02 | 100.0 | 0.18 | 1,3A+ |
| 12 | 163.04 | 6.9 | 3.65 | [M+H-2CO-2C2H2O]+ |
| 13 | 165.02 | 9.0 | 1.23 | 0,2A+ |
| 14 | 203.03 | 3.0 | 2.23 | [M+H-CH4-3CO]+ |
| 15 | 203.03 | 3.0 | 2.23 | [M+H-H2O-2CO-C2H2]+ |
| 16 | 219.03 | 1.1 | 2.47 | [M+H-2C2H2O]+ |
| 17 | 229.05 | 49.2 | 2.42 | [M+H-H2O-2CO]+ |
| 18 | 232.04 | 2.1 | 2.39 | [M+H-CH3-2CO].+ |
| 19 | 247.06 | 1.9 | 2.95 | [M+H-2CO]+ |
| 20 | 257.04 | 13.3 | 2.08 | [M+H-H2O-CO]+ |
| 21 | 274.05 | 4.0 | 2.04 | [M+H-CHO].+ |
| 22 | 285.04 | 6.2 | 1.92 | [M+H-H2O]+ |
| 23 | 303.05 | 8.4 | 2.03 | [M+H]+ |

## quercetin.HCD.100eV



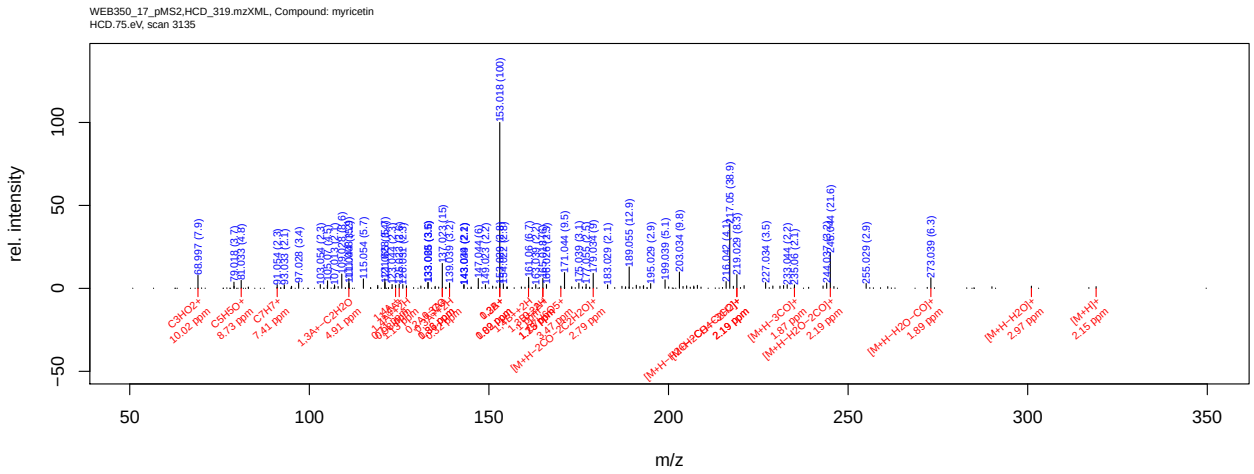

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 30.8 | 9.80 | C3HO2+ |
| 2 | 81.03 | 39.4 | 8.35 | C5H5O+ |
| 3 | 89.04 | 9.0 | 7.90 | C7H5+ |
| 4 | 111.01 | 5.1 | 5.26 | 1,3A+-C2H2O |
| 5 | 124.02 | 3.0 | 0.47 | 1,4A.+ |
| 6 | 125.02 | 1.4 | 0.61 | 1,4A+ |
| 7 | 127.04 | 6.4 | 0.05 | 1,4A++2H |
| 8 | 137.02 | 38.3 | 2.30 | 0,2A+-CO |
| 9 | 137.02 | 38.3 | 2.30 | 0,2B+ |
| 10 | 137.02 | 38.3 | 0.11 | 0,3A+ |
| 11 | 145.03 | 3.6 | 0.46 | 1,4B++2H |
| 12 | 149.02 | 3.7 | 3.04 | 1,3B+-2H |
| 13 | 153.02 | 100.0 | 0.32 | 1,3A+ |
| 14 | 163.04 | 5.2 | 3.37 | [M+H-2CO-2C2H2O]+ |
| 15 | 165.02 | 3.0 | 3.82 | 0,2A+ |
| 16 | 203.03 | 10.5 | 1.63 | [M+H-CH4-3CO]+ |
| 17 | 203.03 | 10.5 | 1.63 | [M+H-H2O-2CO-C2H2]+ |
| 18 | 219.03 | 1.6 | 0.03 | [M+H-2C2H2O]+ |
| 19 | 229.05 | 16.2 | 2.16 | [M+H-H2O-2CO]+ |
| 20 | 257.04 | 2.1 | 1.25 | [M+H-H2O-CO]+ |
| 21 | 285.04 | 2.7 | 0.96 | [M+H-H2O]+ |

## myricetin.CID.45eV



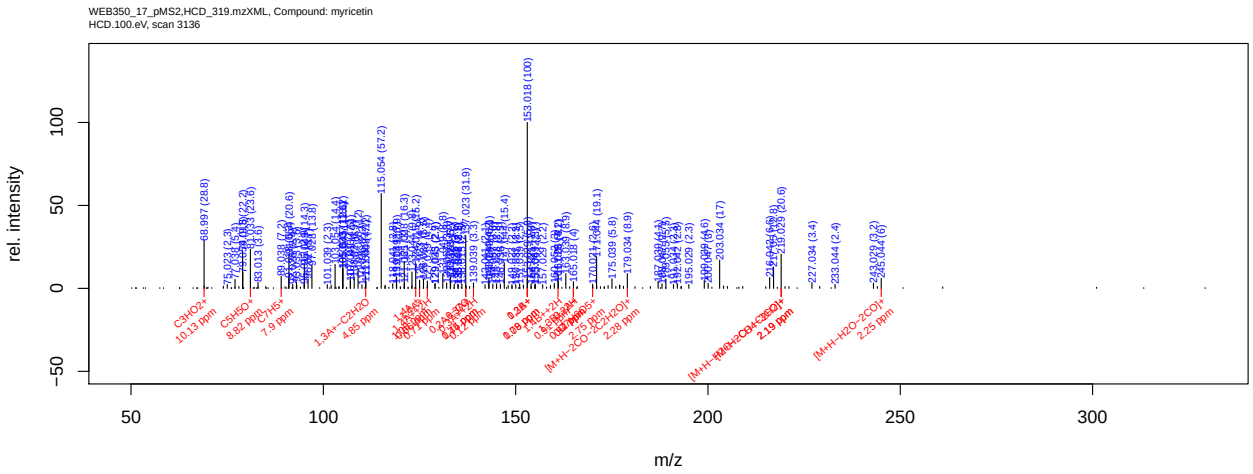

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 111.01 | 3.5 | 4.64 | 1,3A+-C2H2O |
| 2 | 127.04 | 3.9 | 1.07 | 1,4A++2H |
| 3 | 137.02 | 5.6 | 1.75 | 0,2A+-CO |
| 4 | 137.02 | 5.6 | 0.44 | 0,3A+ |
| 5 | 153.02 | 34.8 | 1.69 | 0,2B+ |
| 6 | 153.02 | 34.8 | 0.18 | 1,3A+ |
| 7 | 165.02 | 41.4 | 1.14 | 0,2A+ |
| 8 | 165.02 | 41.4 | 1.66 | 1,3B+-2H |
| 9 | 179.03 | 7.0 | 3.22 | [M+H-2CO-2C2H2O]+ |
| 10 | 235.02 | 3.8 | 2.61 | [M+H-2C2H2O]+ |
| 11 | 245.04 | 31.6 | 2.62 | [M+H-H2O-2CO]+ |
| 12 | 263.05 | 25.4 | 2.52 | [M+H-2CO]+ |
| 13 | 273.04 | 100.0 | 2.56 | [M+H-H2O-CO]+ |
| 14 | 283.02 | 4.3 | 2.49 | [M+H-2H2O]+ |
| 15 | 290.04 | 22.2 | 2.92 | [M+H-CHO].+ |
| 16 | 291.05 | 6.4 | 1.27 | [M+H-CO]+ |
| 17 | 301.03 | 39.6 | 2.46 | [M+H-H2O]+ |

## myricetin.HCD.75eV



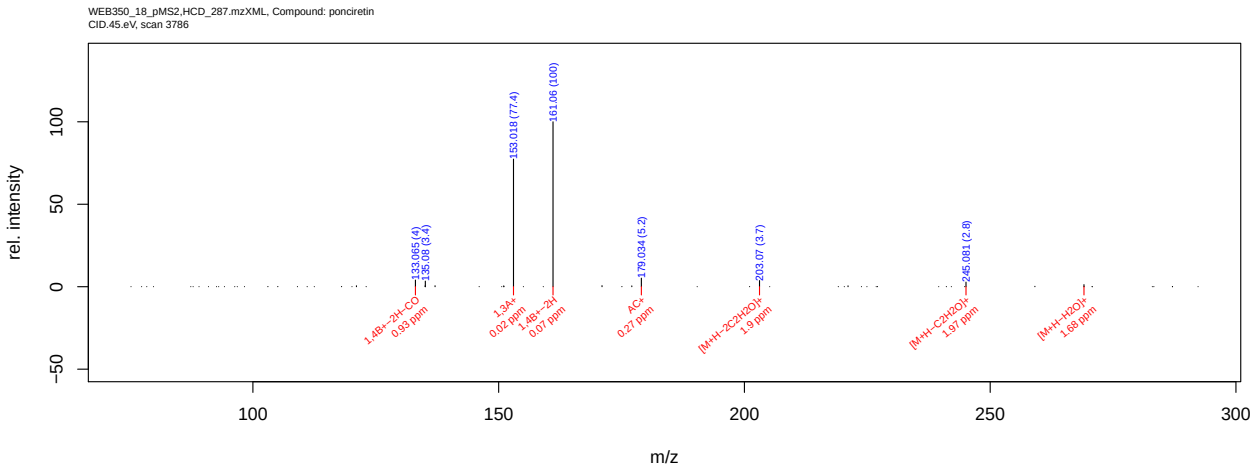

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 7.9 | 10.02 | C3HO2+ |
| 2 | 81.03 | 4.8 | 8.73 | C5H5O+ |
| 3 | 91.05 | 2.3 | 7.41 | C7H7+ |
| 4 | 111.01 | 5.9 | 4.91 | 1,3A+-C2H2O |
| 5 | 124.02 | 2.0 | 0.71 | 1,4A.+ |
| 6 | 125.02 | 2.6 | 0.98 | 1,4A+ |
| 7 | 127.04 | 1.6 | 1.13 | 1,4A++2H |
| 8 | 137.02 | 15.0 | 1.86 | 0,2A+-CO |
| 9 | 137.02 | 15.0 | 0.33 | 0,3A+ |
| 10 | 139.04 | 3.2 | 0.32 | 0,3A++2H |
| 11 | 153.02 | 100.0 | 1.89 | 0,2B+ |
| 12 | 153.02 | 100.0 | 0.02 | 1,3A+ |
| 13 | 161.02 | 1.9 | 1.00 | 1,4B++2H |
| 14 | 165.02 | 6.0 | 1.23 | 0,2A+ |
| 15 | 165.02 | 6.0 | 1.75 | 1,3B+-2H |
| 16 | 170.02 | 1.4 | 3.47 | C7H6O5+ |
| 17 | 179.03 | 9.0 | 2.79 | [M+H-2CO-2C2H2O]+ |
| 18 | 219.03 | 8.3 | 2.19 | [M+H-CH4-3CO]+ |
| 19 | 219.03 | 8.3 | 2.19 | [M+H-H2O-2CO-C2H2]+ |
| 20 | 235.06 | 2.1 | 1.87 | [M+H-3CO]+ |
| 21 | 245.04 | 21.6 | 2.19 | [M+H-H2O-2CO]+ |
| 22 | 273.04 | 6.3 | 1.89 | [M+H-H2O-CO]+ |
| 23 | 301.03 | 1.4 | 2.97 | [M+H-H2O]+ |
| 24 | 319.04 | 1.1 | 2.15 | [M+H]+ |

## myricetin.HCD.100eV



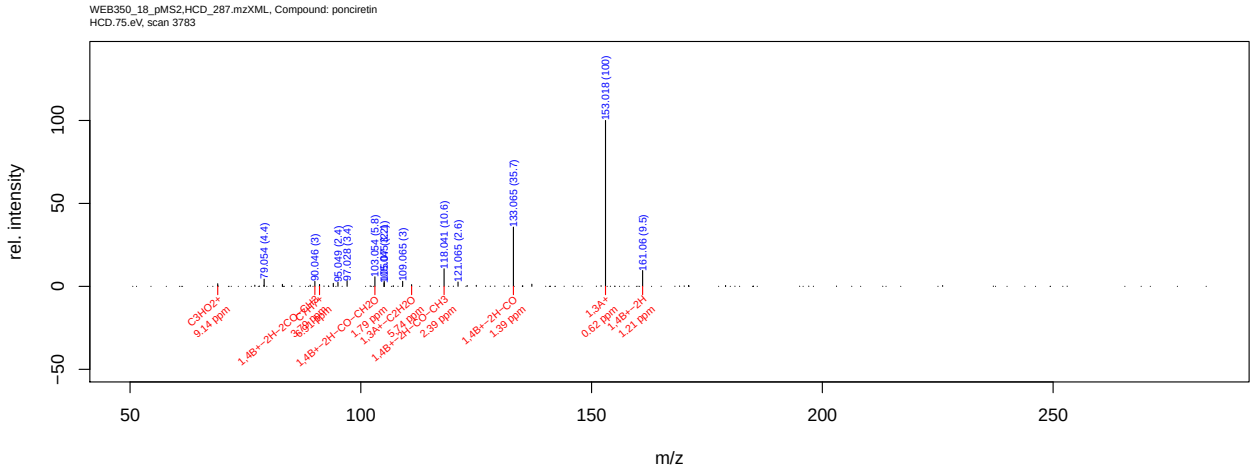

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 28.8 | 10.13 | C3HO2+ |
| 2 | 81.03 | 23.6 | 8.82 | C5H5O+ |
| 3 | 89.04 | 7.2 | 7.90 | C7H5+ |
| 4 | 111.01 | 7.2 | 4.85 | 1,3A+-C2H2O |
| 5 | 124.02 | 15.2 | 1.08 | 1,4A.+ |
| 6 | 125.02 | 4.9 | 0.06 | 1,4A+ |
| 7 | 127.04 | 4.4 | 0.71 | 1,4A++2H |
| 8 | 137.02 | 31.9 | 1.75 | 0,2A+-CO |
| 9 | 137.02 | 31.9 | 0.44 | 0,3A+ |
| 10 | 139.04 | 3.3 | 0.12 | 0,3A++2H |
| 11 | 153.02 | 100.0 | 1.79 | 0,2B+ |
| 12 | 153.02 | 100.0 | 0.08 | 1,3A+ |
| 13 | 161.02 | 4.1 | 0.91 | 1,4B++2H |
| 14 | 165.02 | 4.0 | 0.40 | 0,2A+ |
| 15 | 165.02 | 4.0 | 0.92 | 1,3B+-2H |
| 16 | 170.02 | 2.6 | 2.75 | C7H6O5+ |
| 17 | 179.03 | 8.9 | 2.28 | [M+H-2CO-2C2H2O]+ |
| 18 | 219.03 | 20.6 | 2.19 | [M+H-CH4-3CO]+ |
| 19 | 219.03 | 20.6 | 2.19 | [M+H-H2O-2CO-C2H2]+ |
| 20 | 245.04 | 6.0 | 2.25 | [M+H-H2O-2CO]+ |

## ponciretin.CID.45eV



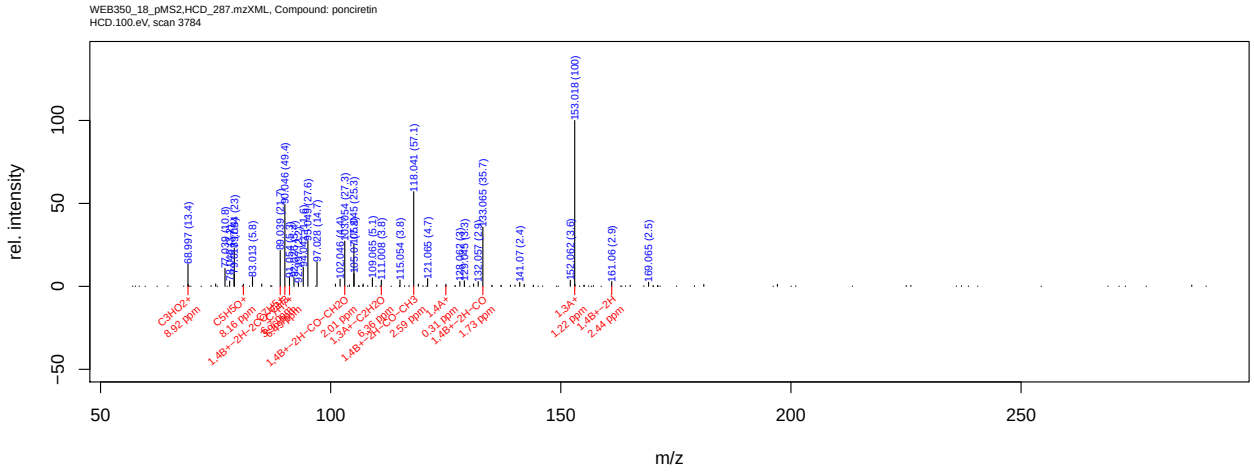

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 133.06 | 4.0 | 0.93 | 1,4B+-2H-CO |
| 2 | 153.02 | 77.4 | 0.02 | 1,3A+ |
| 3 | 161.06 | 100.0 | 0.07 | 1,4B+-2H |
| 4 | 179.03 | 5.2 | 0.27 | AC+ |
| 5 | 203.07 | 3.7 | 1.90 | [M+H-2C2H2O]+ |
| 6 | 245.08 | 2.8 | 1.97 | [M+H-C2H2O]+ |
| 7 | 269.08 | 1.3 | 1.68 | [M+H-H2O]+ |

## ponciretin.HCD.75eV



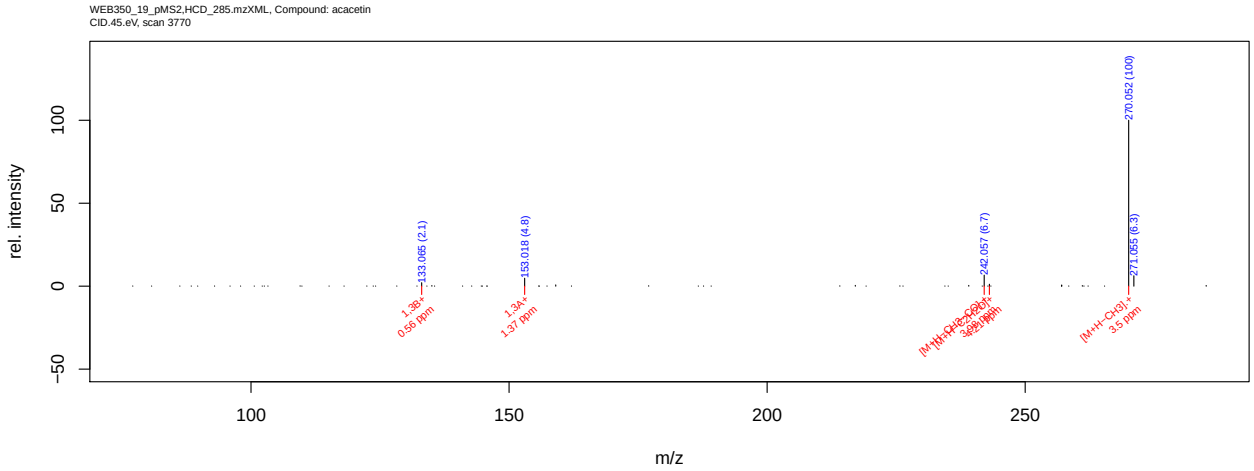

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 1.6 | 9.14 | C3HO2+ |
| 2 | 90.05 | 3.0 | 3.79 | 1,4B+-2H-2CO-CH3 |
| 3 | 91.05 | 1.1 | 6.91 | C7H7+ |
| 4 | 103.05 | 5.8 | 1.79 | 1,4B+-2H-CO-CH2O |
| 5 | 111.01 | 1.1 | 5.74 | 1,3A+-C2H2O |
| 6 | 118.04 | 10.6 | 2.39 | 1,4B+-2H-CO-CH3 |
| 7 | 133.06 | 35.7 | 1.39 | 1,4B+-2H-CO |
| 8 | 153.02 | 100.0 | 0.62 | 1,3A+ |
| 9 | 161.06 | 9.5 | 1.21 | 1,4B+-2H |

## ponciretin.HCD.100eV



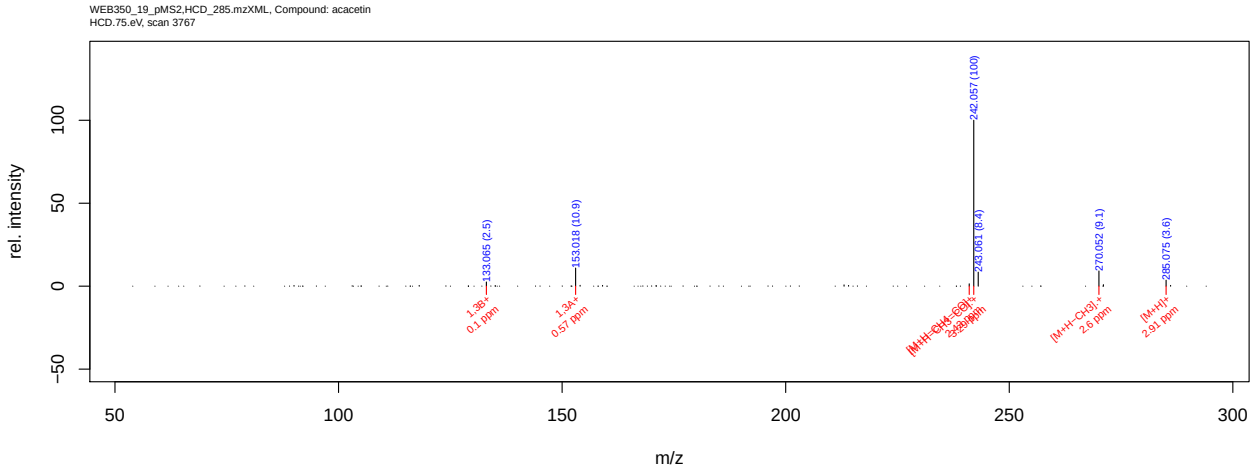

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 13.4 | 8.92 | C3HO2+ |
| 2 | 81.03 | 1.3 | 8.16 | C5H5O+ |
| 3 | 89.04 | 21.7 | 6.70 | C7H5+ |
| 4 | 90.05 | 49.4 | 3.96 | 1,4B+-2H-2CO-CH3 |
| 5 | 91.05 | 5.3 | 6.49 | C7H7+ |
| 6 | 103.05 | 27.3 | 2.01 | 1,4B+-2H-CO-CH2O |
| 7 | 111.01 | 3.8 | 6.36 | 1,3A+-C2H2O |
| 8 | 118.04 | 57.1 | 2.59 | 1,4B+-2H-CO-CH3 |
| 9 | 125.02 | 1.3 | 0.31 | 1,4A+ |
| 10 | 133.06 | 35.7 | 1.73 | 1,4B+-2H-CO |
| 11 | 153.02 | 100.0 | 1.22 | 1,3A+ |
| 12 | 161.06 | 2.9 | 2.44 | 1,4B+-2H |

## acacetin.CID.45eV



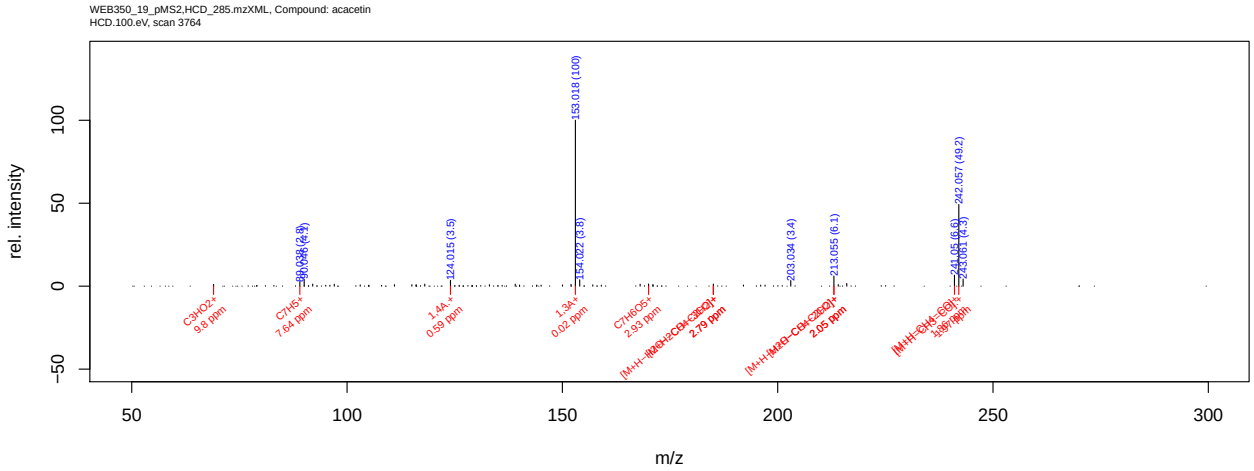

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 133.06 | 2.1 | 0.56 | 1,3B+ |
| 2 | 153.02 | 4.8 | 1.37 | 1,3A+ |
| 3 | 242.06 | 6.7 | 3.98 | [M+H-CH3-CO].+ |
| 4 | 243.06 | 1.2 | 4.21 | [M+H-C2H2O]+ |
| 5 | 270.05 | 100.0 | 3.50 | [M+H-CH3].+ |

## acacetin.HCD.75eV



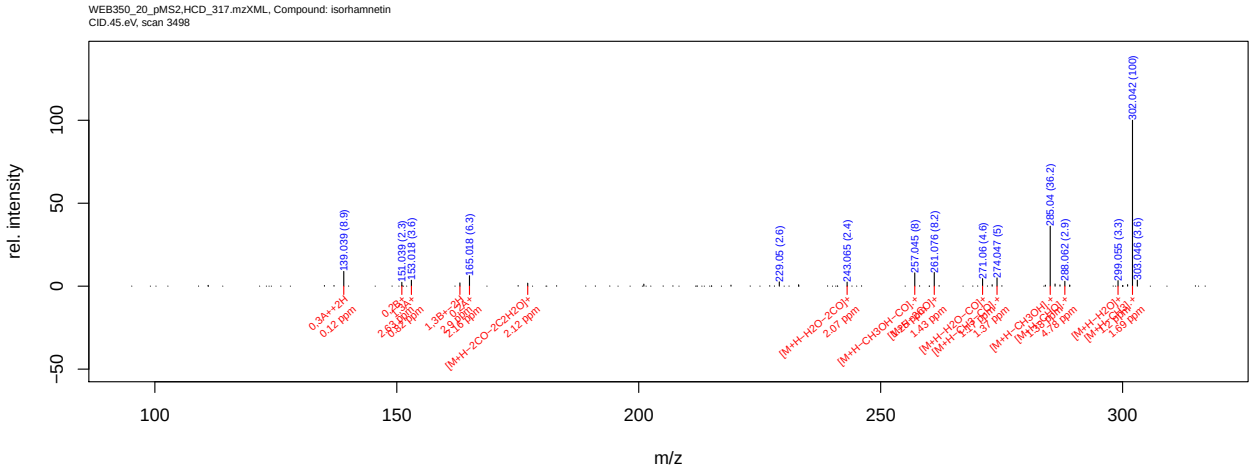

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 133.06 | 2.5 | 0.10 | 1,3B+ |
| 2 | 153.02 | 10.9 | 0.57 | 1,3A+ |
| 3 | 241.05 | 1.4 | 2.43 | [M+H-CH4-CO]+ |
| 4 | 242.06 | 100.0 | 3.29 | [M+H-CH3-CO].+ |
| 5 | 270.05 | 9.1 | 2.60 | [M+H-CH3].+ |
| 6 | 285.08 | 3.6 | 2.91 | [M+H]+ |

## acacetin.HCD.100eV



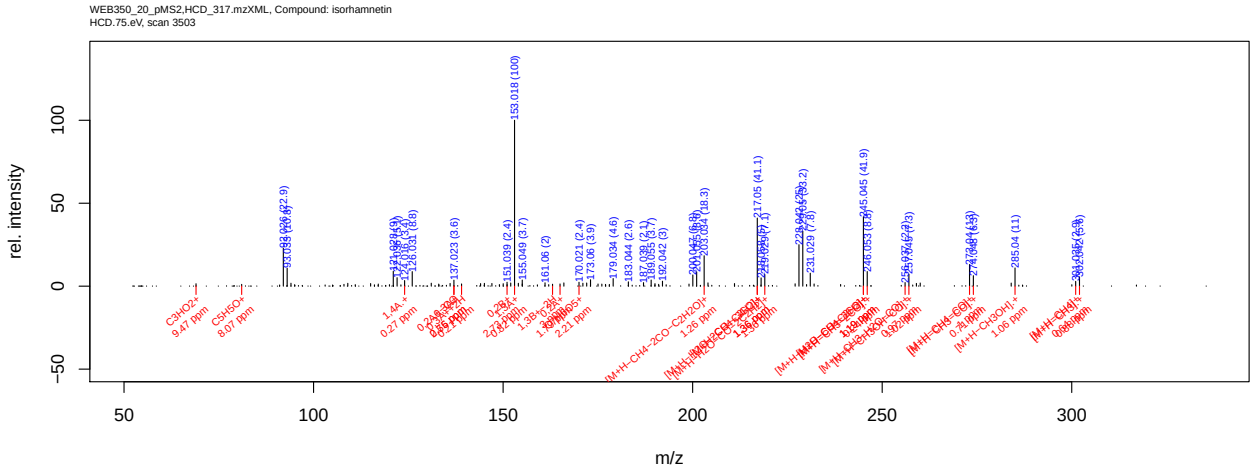

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 1.1 | 9.80 | C3HO2+ |
| 2 | 89.04 | 2.8 | 7.64 | C7H5+ |
| 3 | 124.02 | 3.5 | 0.59 | 1,4A.+ |
| 4 | 153.02 | 100.0 | 0.02 | 1,3A+ |
| 5 | 170.02 | 1.3 | 2.93 | C7H6O5+ |
| 6 | 185.06 | 1.3 | 2.79 | [M+H-CH4-3CO]+ |
| 7 | 185.06 | 1.3 | 2.79 | [M+H-H2O-2CO-C2H2]+ |
| 8 | 213.05 | 6.1 | 2.05 | [M+H-CH4-2CO]+ |
| 9 | 213.05 | 6.1 | 2.05 | [M+H-H2O-CO-C2H2]+ |
| 10 | 241.05 | 6.6 | 1.86 | [M+H-CH4-CO]+ |
| 11 | 242.06 | 49.2 | 1.97 | [M+H-CH3-CO].+ |

## isorhamnetin.CID.45eV



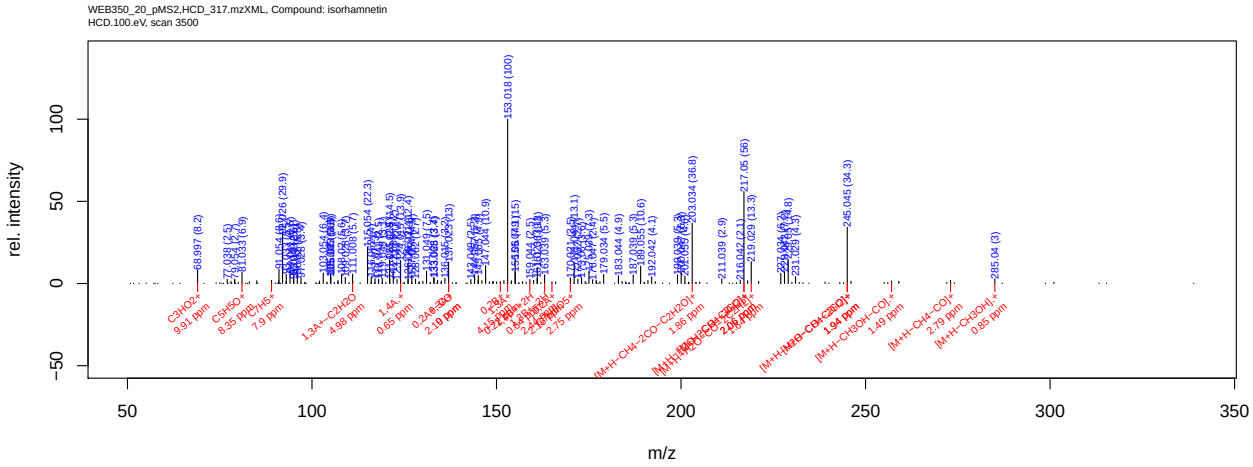

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 139.04 | 8.9 | 0.12 | 0,3A++2H |
| 2 | 151.04 | 2.3 | 2.63 | 0,2B+ |
| 3 | 153.02 | 3.6 | 0.82 | 1,3A+ |
| 4 | 163.04 | 2.0 | 2.90 | 1,3B+-2H |
| 5 | 165.02 | 6.3 | 2.16 | 0,2A+ |
| 6 | 177.05 | 1.8 | 2.12 | [M+H-2CO-2C2H2O]+ |
| 7 | 243.07 | 2.4 | 2.07 | [M+H-H2O-2CO]+ |
| 8 | 257.04 | 8.0 | 1.25 | [M+H-CH3OH-CO].+ |
| 9 | 261.08 | 8.2 | 1.43 | [M+H-2CO]+ |
| 10 | 271.06 | 4.6 | 1.17 | [M+H-H2O-CO]+ |
| 11 | 274.05 | 5.0 | 1.37 | [M+H-CH3-CO].+ |
| 12 | 285.04 | 36.2 | 1.38 | [M+H-CH3OH].+ |
| 13 | 288.06 | 2.9 | 4.78 | [M+H-CHO].+ |
| 14 | 299.06 | 3.3 | 1.20 | [M+H-H2O]+ |
| 15 | 302.04 | 100.0 | 1.69 | [M+H-CH3].+ |

## isorhamnetin.HCD.75eV



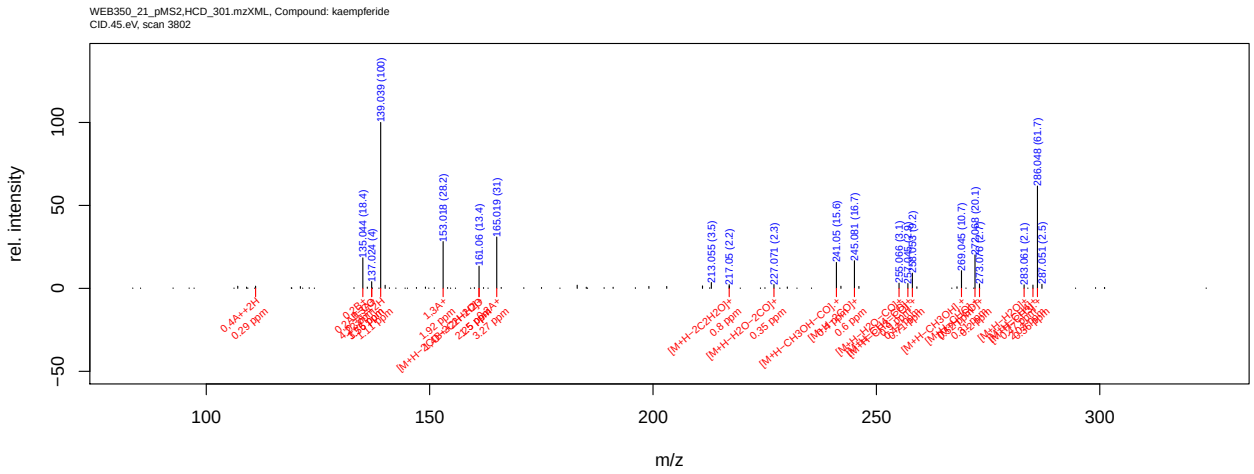

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 1.5 | 9.47 | C3HO2+ |
| 2 | 81.03 | 1.1 | 8.07 | C5H5O+ |
| 3 | 124.02 | 3.4 | 0.27 | 1,4A.+ |
| 4 | 137.02 | 3.6 | 2.75 | 0,2A+-CO |
| 5 | 137.02 | 3.6 | 0.56 | 0,3A+ |
| 6 | 139.04 | 1.3 | 0.21 | 0,3A++2H |
| 7 | 151.04 | 2.4 | 2.73 | 0,2B+ |
| 8 | 153.02 | 100.0 | 0.82 | 1,3A+ |
| 9 | 163.04 | 1.2 | 3.00 | 1,3B+-2H |
| 10 | 165.02 | 1.3 | 1.79 | 0,2A+ |
| 11 | 170.02 | 2.4 | 2.21 | C7H6O5+ |
| 12 | 203.03 | 18.3 | 1.26 | [M+H-CH4-2CO-C2H2O]+ |
| 13 | 217.05 | 41.1 | 1.36 | [M+H-CH4-3CO]+ |
| 14 | 217.05 | 41.1 | 1.36 | [M+H-H2O-2CO-C2H2]+ |
| 15 | 219.03 | 7.1 | 1.36 | [M+H-H2O-CO-2C2H2]+ |
| 16 | 245.04 | 41.9 | 1.19 | [M+H-CH4-2CO]+ |
| 17 | 245.04 | 41.9 | 1.19 | [M+H-H2O-CO-C2H2]+ |
| 18 | 246.05 | 8.8 | 0.24 | [M+H-CH3-2CO].+ |
| 19 | 256.04 | 2.2 | 0.97 | [M+H-CH3-H2O-CO].+ |
| 20 | 257.04 | 7.3 | 1.02 | [M+H-CH3OH-CO].+ |
| 21 | 273.04 | 13.0 | 1.00 | [M+H-CH4-CO]+ |
| 22 | 274.05 | 6.3 | 0.71 | [M+H-CH3-CO].+ |
| 23 | 285.04 | 11.0 | 1.06 | [M+H-CH3OH].+ |
| 24 | 301.03 | 2.9 | 0.64 | [M+H-CH4]+ |
| 25 | 302.04 | 5.6 | 0.88 | [M+H-CH3].+ |

## isorhamnetin.HCD.100eV



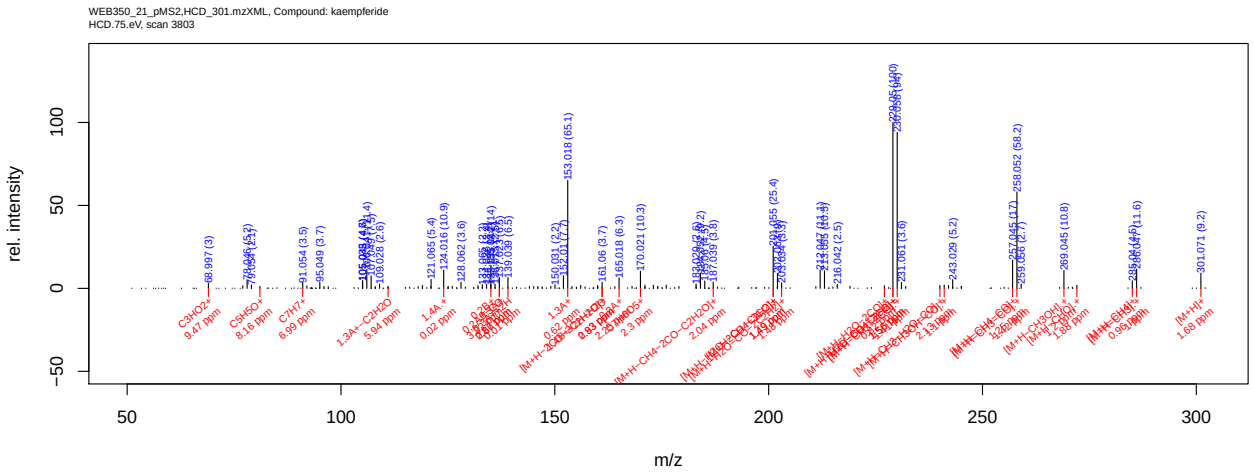

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 8.2 | 9.91 | C3HO2+ |
| 2 | 81.03 | 6.9 | 8.35 | C5H5O+ |
| 3 | 89.04 | 1.9 | 7.90 | C7H5+ |
| 4 | 111.01 | 5.7 | 4.98 | 1,3A+-C2H2O |
| 5 | 124.02 | 13.9 | 0.65 | 1,4A.+ |
| 6 | 137.02 | 13.0 | 2.19 | 0,2A+-CO |
| 7 | 137.02 | 13.0 | 0.00 | 0,3A+ |
| 8 | 151.04 | 1.2 | 4.15 | 0,2B+ |
| 9 | 153.02 | 100.0 | 0.22 | 1,3A+ |
| 10 | 159.04 | 2.5 | 0.64 | 1,4B++2H |
| 11 | 163.04 | 5.3 | 2.44 | 1,3B+-2H |
| 12 | 165.02 | 1.0 | 2.16 | 0,2A+ |
| 13 | 170.02 | 3.5 | 2.75 | C7H6O5+ |
| 14 | 203.03 | 36.8 | 1.86 | [M+H-CH4-2CO-C2H2O]+ |
| 15 | 217.05 | 56.0 | 2.06 | [M+H-CH4-3CO]+ |
| 16 | 217.05 | 56.0 | 2.06 | [M+H-H2O-2CO-C2H2]+ |
| 17 | 219.03 | 13.3 | 1.64 | [M+H-H2O-CO-2C2H2]+ |
| 18 | 245.04 | 34.3 | 1.94 | [M+H-CH4-2CO]+ |
| 19 | 245.04 | 34.3 | 1.94 | [M+H-H2O-CO-C2H2]+ |
| 20 | 257.04 | 1.6 | 1.49 | [M+H-CH3OH-CO].+ |
| 21 | 273.04 | 1.9 | 2.79 | [M+H-CH4-CO]+ |
| 22 | 285.04 | 3.0 | 0.85 | [M+H-CH3OH].+ |

## kaempferide.CID.45eV



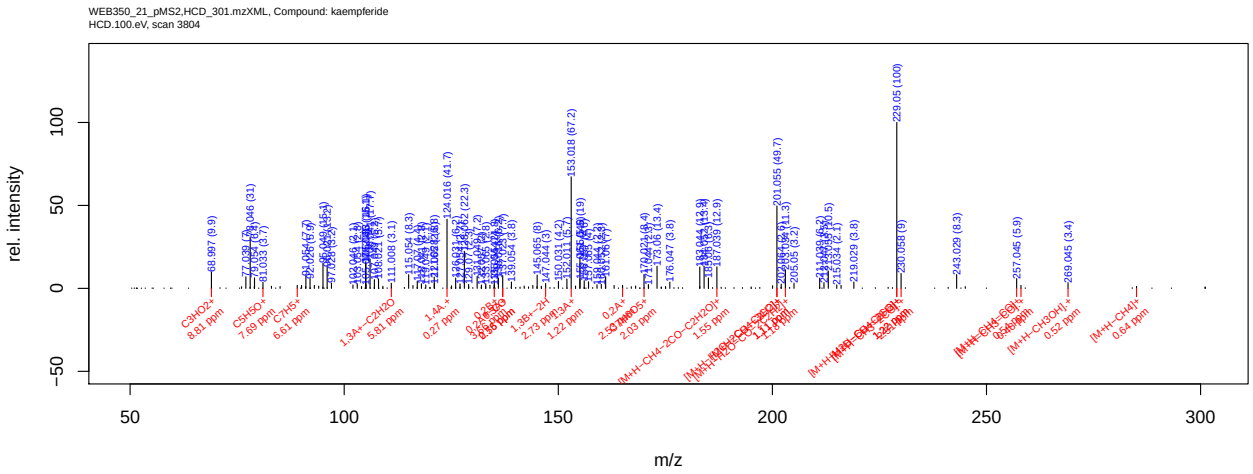

| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 111.04 | 1.3 | 0.29 | 0,4A++2H |
| 2 | 135.04 | 18.4 | 4.22 | 0,2B+ |
| 3 | 137.02 | 4.0 | 3.75 | 0,2A+-CO |
| 4 | 137.02 | 4.0 | 1.56 | 0,3A+ |
| 5 | 139.04 | 100.0 | 1.11 | 0,3A++2H |
| 6 | 153.02 | 28.2 | 1.92 | 1,3A+ |
| 7 | 161.06 | 13.4 | 2.25 | 1,4B++2H-H2O |
| 8 | 161.06 | 13.4 | 1.50 | [M+H-2CO-2C2H2O]+ |
| 9 | 165.02 | 31.0 | 3.27 | 0,2A+ |
| 10 | 217.05 | 2.2 | 0.80 | [M+H-2C2H2O]+ |
| 11 | 227.07 | 2.3 | 0.35 | [M+H-H2O-2CO]+ |
| 12 | 241.05 | 15.6 | 0.40 | [M+H-CH3OH-CO].+ |
| 13 | 245.08 | 16.7 | 0.60 | [M+H-2CO]+ |
| 14 | 255.07 | 3.1 | 0.90 | [M+H-H2O-CO]+ |
| 15 | 257.04 | 2.9 | 0.42 | [M+H-CH4-CO]+ |
| 16 | 258.05 | 9.2 | 0.71 | [M+H-CH3-CO].+ |
| 17 | 269.04 | 10.7 | 0.52 | [M+H-CH3OH].+ |
| 18 | 272.07 | 20.1 | 0.31 | [M+H-CHO].+ |
| 19 | 273.08 | 2.7 | 0.20 | [M+H-CO]+ |
| 20 | 283.06 | 2.1 | 0.47 | [M+H-H2O]+ |
| 21 | 285.04 | 2.0 | 2.03 | [M+H-CH4]+ |
| 22 | 286.05 | 61.7 | 0.36 | [M+H-CH3].+ |

## kaempferide.HCD.75eV




| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 3.0 | 9.47 | C3HO2+ |
| 2 | 81.03 | 1.2 | 8.16 | C5H5O+ |
| 3 | 91.05 | 3.5 | 6.99 | C7H7+ |
| 4 | 111.01 | 1.2 | 5.94 | 1,3A+-C2H2O |
| 5 | 124.02 | 10.9 | 0.02 | 1,4A.+ |
| 6 | 135.04 | 14.0 | 3.32 | 0,2B+ |
| 7 | 137.02 | 6.5 | 2.86 | 0,2A+-CO |
| 8 | 137.02 | 6.5 | 0.67 | 0,3A+ |
| 9 | 139.04 | 6.5 | 0.01 | 0,3A++2H |
| 10 | 153.02 | 65.1 | 0.62 | 1,3A+ |
| 11 | 161.06 | 3.7 | 0.93 | 1,4B++2H-H2O |
| 12 | 161.06 | 3.7 | 2.83 | [M+H-2CO-2C2H2O]+ |
| 13 | 165.02 | 6.3 | 2.25 | 0,2A+ |
| 14 | 170.02 | 10.3 | 2.30 | C7H6O5+ |
| 15 | 187.04 | 3.8 | 2.04 | [M+H-CH4-2CO-C2H2O]+ |
| 16 | 201.05 | 25.4 | 1.49 | [M+H-CH4-3CO]+ |
| 17 | 201.05 | 25.4 | 1.49 | [M+H-H2O-2CO-C2H2]+ |
| 18 | 203.03 | 3.3 | 1.48 | [M+H-H2O-CO-2C2H2]+ |
| 19 | 227.07 | 1.6 | 0.82 | [M+H-H2O-2CO]+ |
| 20 | 229.05 | 100.0 | 1.56 | [M+H-CH4-2CO]+ |
| 21 | 229.05 | 100.0 | 1.56 | [M+H-H2O-CO-C2H2]+ |
| 22 | 230.06 | 94.0 | 1.41 | [M+H-CH3-2CO].+ |
| 23 | 240.04 | 1.8 | 2.13 | [M+H-CH3-H2O-CO].+ |
| 24 | 241.05 | 2.0 | 1.10 | [M+H-CH3OH-CO].+ |
| 25 | 257.04 | 17.0 | 1.25 | [M+H-CH4-CO]+ |
| 26 | 258.05 | 58.2 | 1.42 | [M+H-CH3-CO].+ |
| 27 | 269.04 | 10.8 | 1.20 | [M+H-CH3OH].+ |
| 28 | 272.07 | 1.8 | 1.88 | [M+H-CHO].+ |
| 29 | 285.04 | 4.5 | 0.96 | [M+H-CH4]+ |
| 30 | 286.05 | 11.6 | 1.00 | [M+H-CH3].+ |
| 31 | 301.07 | 9.2 | 1.68 | [M+H]+ |

## kaempferide.HCD.100eV




| | mz | int | ppm | fragment |
|---|---|---|---|---|
| 1 | 69.00 | 9.9 | 8.81 | C3HO2+ |
| 2 | 81.03 | 3.7 | 7.69 | C5H5O+ |
| 3 | 89.04 | 1.8 | 6.61 | C7H5+ |
| 4 | 111.01 | 3.1 | 5.81 | 1,3A+-C2H2O |
| 5 | 124.02 | 41.7 | 0.27 | 1,4A.+ |
| 6 | 135.04 | 4.8 | 3.66 | 0,2B+ |
| 7 | 137.02 | 7.7 | 2.75 | 0,2A+-CO |
| 8 | 137.02 | 7.7 | 0.56 | 0,3A+ |
| 9 | 147.04 | 3.0 | 2.73 | 1,3B+-2H |
| 10 | 153.02 | 67.2 | 1.22 | 1,3A+ |
| 11 | 165.02 | 1.9 | 2.53 | 0,2A+ |
| 12 | 170.02 | 8.4 | 2.03 | C7H6O5+ |
| 13 | 187.04 | 12.9 | 1.55 | [M+H-CH4-2CO-C2H2O]+ |
| 14 | 201.05 | 49.7 | 1.11 | [M+H-CH4-3CO]+ |
| 15 | 201.05 | 49.7 | 1.11 | [M+H-H2O-2CO-C2H2]+ |
| 16 | 203.03 | 11.3 | 1.18 | [M+H-H2O-CO-2C2H2]+ |
| 17 | 229.05 | 100.0 | 1.22 | [M+H-CH4-2CO]+ |
| 18 | 229.05 | 100.0 | 1.22 | [M+H-H2O-CO-C2H2]+ |
| 19 | 230.06 | 9.0 | 2.51 | [M+H-CH3-2CO].+ |
| 20 | 257.04 | 5.9 | 0.54 | [M+H-CH4-CO]+ |
| 21 | 258.05 | 1.8 | 0.48 | [M+H-CH3-CO].+ |
| 22 | 269.04 | 3.4 | 0.52 | [M+H-CH3OH].+ |
| 23 | 285.04 | 1.2 | 0.64 | [M+H-CH4]+ |

Table 1: Fragment table for method *CID.45*

| | fragment | naringenin | eriodictyol | ponciretin | hesperetin | homoeriodictyol | apigenin | luteolin | acacetin | diosmetin | chrysoeriol | kaempferol | quercetin | myricetin | kaempferide | isorhamnetin |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $[M+H]^+$ | | | | | | 271 (2) | | | | | | | | | |
| 2 | $[M+H-CH_3]^{\bullet+}$ | | | | | | | | 270 (100) | 286 (100) | 286 (100) | | | | 286 (62) | 302 (100) |
| 3 | $[M+H-CH_4]^+$ | | | | | | | | | | | | | | 285 (2) | |
| 4 | $[M+H-H_2O]^+$ | 255 (1) | 271 (18) | 269 (1) | 285 (10) | 285 (4) | 253 (1) | 269 (9) | | | | 269 (32) | 285 (63) | 301 (40) | 283 (2) | 299 (3) |
| 5 | $[M+H-CO]^+$ | | | | | | 243 (7) | 259 (9) | | | | 259 (24) | 275 (14) | 291 (6) | 273 (3) | |
| 6 | $[M+H-CHO]^{\bullet+}$ | | | | | | 242 (14) | 258 (47) | | | | 258 (46) | 274 (20) | 290 (22) | 272 (20) | 288 (3) |
| 7 | $[M+H-CH_3OH]^{\bullet+}$ | | | | | | | | | | | | | | 269 (11) | 285 (36) |
| 8 | $[M+H-2H_2O]^+$ | | 253 (4) | | | | | | | | | | | 283 (4) | | |
| 9 | $[M+H-C_2H_2O]^+$ | 231 (4) | 247 (3) | 245 (3) | 261 (2) | 261 (2) | 229 (21) | 245 (13) | 243 (1) | | | 245 (4) | | | | |
| 10 | $[M+H-CH_3-CO]^{\bullet+}$ | | | | | | | | 242 (7) | | | | | | 258 (9) | 274 (5) |
| 11 | $[M+H-CO_2]^+$ | | | | | | | | | | | 243 (5) | | | | |
| 12 | $[M+H-CH_4-CO]^+$ | | | | | | | | | | | | | | 257 (3) | |
| 13 | $[M+H-H_2O-CO]^+$ | | | | | | 225 (13) | 241 (13) | | | | 241 (99) | 257 (100) | 273 (100) | 255 (3) | 271 (5) |
| 14 | $[M+H-2CO]^+$ | | | | | | | 231 (2) | | | | 231 (40) | 247 (37) | 263 (25) | 245 (17) | 261 (8) |
| 15 | $[M+H-CH_3OH-CO]^{\bullet+}$ | | | | | | | 227 (3) | | | | | | | 241 (16) | 257 (8) |
| 16 | $[M+H-H_2O-2CO]^+$ | | | | | | | 213 (2) | | | | 213 (77) | 229 (70) | 245 (32) | 227 (2) | 243 (2) |
| 17 | $[M+H-2C_2H_2O]^+$ | 189 (5) | 205 (3) | 203 (4) | 219 (2) | 219 (1) | 187 (3) | 203 (4) | | | | 203 (7) | 219 (4) | 235 (4) | 217 (2) | |
| 18 | $[M+H-2C_2H_2O-H_2O]^+$ | | 187 (4) | | 201 (1) | | | | | | | | | | | |
| 19 | $[M+H-2CO-2C_2H_2O]^+$ | | | | | | | | | | | 147 (13) | 163 (7) | 179 (7) | 161 (13) | 177 (2) |
| 20 | $AC^+$ | 179 (4) | 179 (20) | 179 (5) | 179 (28) | 179 (30) | | | | | | | | | | |
| 21 | $0,2A^+$ | | | | | | | | | | | 165 (100) | 165 (59) | 165 (41) | 165 (31) | 165 (6) |
| 22 | $0,2A^+-CO$ | | | | | | | | | | | 137 (11) | 137 (23) | 137 (6) | 137 (4) | |
| 23 | $0,2B^+$ | | | | | | 121 (6) | 137 (7) | | | | 121 (36) | 137 (23) | 153 (35) | 135 (18) | 151 (2) |
| 24 | $0,3A^+$ | | | | | | | 137 (7) | | | | 137 (11) | 137 (23) | 137 (6) | 137 (4) | |
| 25 | $0,3A^++2H$ | | | | | | | | | | | | | | 139 (100) | 139 (9) |
| 26 | $0,4A^++2H$ | | | | | | | | | | | | | | 111 (1) | |
| 27 | $0,4B^+$ | | | | | | 163 (6) | 179 (7) | | | | | | | | |
| 28 | $0,4B^+-H_2O$ | | | | | | 145 (13) | | | | | | | | | |
| 29 | $1,3A^+$ | 153 (100) | 153 (31) | 153 (77) | 153 (21) | 153 (57) | 153 (100) | 153 (100) | 153 (5) | | | 153 (61) | 153 (20) | 153 (35) | 153 (28) | 153 (4) |
| 30 | $1,3A^+-C_2H_2O$ | | | | | | | | | | | 111 (19) | 111 (7) | 111 (4) | | |
| 31 | $1,3B^+$ | | | | | | 119 (12) | 135 (11) | 133 (2) | | | | | | | |
| 32 | $1,3B^+-2H$ | | | | | | | | | | | 133 (25) | 149 (10) | 165 (41) | | 163 (2) |
| 33 | $1,4A^++2H$ | | | | | | | | | | | 127 (2) | 127 (1) | 127 (4) | | |
| 34 | $1,4B^+-2H$ | 147 (84) | 163 (100) | 161 (100) | 177 (100) | 177 (100) | | | | | | | | | | |
| 35 | $1,4B^++2H-H_2O$ | | | | | | | | | | | 147 (13) | | | 161 (13) | |
| 36 | $1,4B^+-2H-H_2O$ | | 145 (5) | | | | | | | | | | | | | |
| 37 | $1,4B^+-2H-CO$ | 119 (3) | 135 (1) | 133 (4) | | | | | | | | | | | | |
| 38 | $C_7H_7^+$ | | | | | | 91 (1) | | | | | | | | | |

Table 2: Fragment table for method *HCD.75*

| fragment | naringenin | eriodictyol | ponciretin | hesperetin | homoeriodictyol | apigenin | luteolin | acacetin | diosmetin | chrysoeriol | kaempferol | quercetin | myricetin | kaempferide | isorhamnetin |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 $[M+H]^+$ | | | | | | 271 (84) | 287 (66) | 285 (4) | | | 287 (25) | 303 (8) | 319 (1) | 301 (9) | |
| 2 $[M+H-CH_3]^{\bullet+}$ | | | | | | | | 270 (9) | 286 (20) | 286 (18) | | | | 286 (12) | 302 (6) |
| 3 $[M+H-CH_4]^+$ | | | | 287 (1) | | | | | | | | | | 285 (5) | 301 (3) |
| 4 $[M+H-H_2O]^+$ | | | | | | 253 (3) | 269 (6) | | | | 269 (2) | 285 (6) | 301 (1) | | |
| 5 $[M+H-CO]^+$ | | | | | | 243 (7) | | | | | 259 (3) | | | | |
| 6 $[M+H-CHO]^{\bullet+}$ | | | | | | 242 (1) | 258 (3) | | | | 258 (10) | 274 (4) | | 272 (2) | |
| 7 $[M+H-CH_3OH]^{\bullet+}$ | | | | | | | | | | | | | | 269 (11) | 285 (11) |
| 8 $[M+H-C_2H_2O]^+$ | | | | | | 229 (4) | | | | | | | | | |
| 9 $[M+H-CH_3-CO]^{\bullet+}$ | | | | | | | | 242 (100) | 258 (100) | 258 (100) | | | | 258 (58) | 274 (6) |
| 10 $[M+H-CH_4-CO]^+$ | | | | | | | | 241 (1) | 257 (7) | 257 (7) | | | | 257 (17) | 273 (13) |
| 11 $[M+H-H_2O-CO]^+$ | | | | | | 225 (4) | 241 (16) | | | | 241 (5) | 257 (13) | 273 (6) | | |
| 12 $[M+H-2CO]^+$ | | | | | | | | | | | 231 (5) | 247 (2) | | | |
| 13 $[M+H-CH_3OH-CO]^{\bullet+}$ | | | | | | | | | | | | | | 241 (2) | 257 (7) |
| 14 $[M+H-CH_3-H_2O-CO]^{\bullet+}$ | | | | | | | | | | | | | | 240 (2) | 256 (2) |
| 15 $[M+H-CH_3-2CO]^{\bullet+}$ | | | | | | | | | | | 216 (2) | 232 (2) | | 230 (94) | 246 (9) |
| 16 $[M+H-H_2O-CO-C_2H_2]^+$ | | | | | | | | | 229 (12) | 229 (13) | | | | 229 (100) | 245 (42) |
| 17 $[M+H-CH_4-2CO]^+$ | | | | | | | | | 229 (12) | 229 (13) | | | | 229 (100) | 245 (42) |
| 18 $[M+H-H_2O-2CO]^+$ | | | | | | 197 (4) | 213 (7) | | | | 213 (20) | 229 (49) | 245 (22) | 227 (2) | |
| 19 $[M+H-3CO]^+$ | | | | | | | | | | | 203 (2) | | 235 (2) | | |
| 20 $[M+H-2C_2H_2O]^+$ | | | | | | 187 (2) | 203 (2) | | | | | 219 (1) | | | |
| 21 $[M+H-H_2O-CO-2C_2H_2]^+$ | | | | | | | | | | | | | | 203 (3) | 219 (7) |
| 22 $[M+H-H_2O-2CO-C_2H_2]^+$ | | | | | | | | | | | | 203 (3) | 219 (8) | 201 (25) | 217 (41) |
| 23 $[M+H-CH_4-3CO]^+$ | | | | | | | | | | | | 203 (3) | 219 (8) | 201 (25) | 217 (41) |
| 24 $[M+H-CH_4-2CO-C_2H_2O]^+$ | | | | | | | | | | | | | | 187 (4) | 203 (18) |
| 25 $[M+H-2CO-2C_2H_2O]^+$ | | | | | | 131 (2) | 147 (1) | | | | 147 (9) | 163 (7) | 179 (9) | 161 (4) | |
| 26 $AC^+$ | | 179 (1) | | 179 (2) | 179 (2) | | | | | | | | | | |
| 27 $0,2A^+$ | | | | | | | | | | | 165 (11) | 165 (9) | 165 (6) | 165 (6) | 165 (1) |
| 28 $0,2A^+-CO$ | | | | | | | | | | | 137 (14) | 137 (47) | 137 (15) | 137 (7) | 137 (4) |
| 29 $0,2B^+$ | | | | | | 121 (16) | 137 (12) | | | | | 137 (47) | 153 (100) | 135 (14) | 151 (2) |
| 30 $0,3A^+$ | | | | | | | 137 (12) | | | | 137 (14) | 137 (47) | 137 (15) | 137 (7) | 137 (4) |
| 31 $0,3A^++2H$ | | | | | | | | | | | | | 139 (3) | 139 (7) | 139 (1) |
| 32 $0,4A^++2H$ | | | | | 111 (2) | | | | | | | | | | |
| 33 $0,4B^+$ | | | | | | 163 (8) | 179 (3) | | | | | | | | |
| 34 $0,4B^+-H_2O$ | | | | | | 145 (17) | 161 (16) | | | | | | | | |
| 35 $1,3A^+$ | 153 (100) | 153 (100) | 153 (100) | 153 (100) | 153 (100) | 153 (100) | 153 (100) | 153 (11) | 153 (8) | 153 (8) | | 153 (100) | 153 (100) | 153 (65) | 153 (100) |
| 36 $1,3A^+-C_2H_2O$ | | 111 (2) | 111 (1) | 111 (1) | | 111 (2) | 111 (2) | | | | 111 (5) | 111 (6) | 111 (6) | 111 (1) | |
| 37 $1,3B^+$ | | | | | | 119 (49) | 135 (40) | 133 (3) | | | | | | | |
| 38 $1,3B^+-2H$ | | | | | | | | | | | 133 (3) | 149 (3) | 165 (6) | | 163 (1) |
| 39 $1,4A^++2H$ | | | | | | | 127 (1) | | | | 127 (1) | 127 (3) | 127 (2) | | |
| 40 $1,4A^{\bullet+}$ | | | | | | | | | | | | | 124 (2) | 124 (11) | 124 (3) |
| 41 $1,4A^+$ | | | | | | 125 (1) | 125 (2) | | | | | | 125 (3) | | |
| 42 $1,4B^++2H$ | | | | | | | | | | | | 145 (2) | 161 (2) | | |
| 43 $1,4B^+-2H$ | 147 (15) | 163 (10) | 161 (10) | 177 (4) | 177 (2) | | | | | | | | | | |
| 44 $1,4B^++2H-H_2O$ | | | | | | | | | | | 147 (9) | | | 161 (4) | |
| 45 $1,4B^+-2H-H_2O$ | | 145 (7) | | | | | | | | | | | | | |
| 46 $1,4B^+-2H-CO$ | 119 (32) | 135 (29) | 133 (36) | 149 (15) | 149 (11) | | | | | | | | | | |
| 47 $1,4B^+-2H-CO-CH_3$ | | | 118 (11) | 134 (11) | 134 (7) | | | | | | | | | | |
| 48 $1,4B^+-2H-CO-CH_2O$ | | | 103 (6) | | | | | | | | | | | | |
| 49 $1,4B^+-2H-2CO$ | 91 (24) | | | | | | | | | | | | | | |
| 50 $1,4B^+-2H-2CO-CH_3$ | | | 90 (3) | | | | | | | | | | | | |
| 51 $1,4B^+-2H-C_2H_2O-H_2O$ | | | | 117 (15) | 117 (32) | | | | | | | | | | |
| 52 $1,4B^+-2H-H_2O-CO$ | | 117 (18) | | | | | | | | | | | | | |
| 53 $C_7H_6O_5^+$ | | | | | | | | | | | | | 170 (1) | 170 (10) | 170 (2) |
| 54 $C_7H_7^+$ | 91 (24) | | 91 (1) | 91 (3) | 91 (2) | 91 (26) | | | | | 91 (2) | 91 (2) | 91 (2) | 91 (4) | |
| 55 $C_7H_5^+$ | | 89 (23) | | 89 (29) | 89 (24) | | 89 (17) | | | | | | | | |
| 56 $C_5H_5O^+$ | | | | | | 81 (1) | 81 (2) | | | | 81 (3) | 81 (8) | 81 (5) | 81 (1) | 81 (1) |
| 57 $C_3HO_2^+$ | 69 (2) | 69 (2) | 69 (2) | 69 (2) | 69 (2) | 69 (4) | 69 (5) | | | | 69 (7) | 69 (8) | 69 (8) | 69 (3) | 69 (1) |

Table 3: Fragment table for method *HCD.100*

| | fragment | naringenin | eriodictyol | ponciretin | hesperetin | homoeriodictyol | apigenin | luteolin | acacetin | diosmetin | chrysoeriol | kaempferol | quercetin | myricetin | kaempferide | isorhamnetin |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $[M+H]^+$ | | | | | | 271 (2) | 287 (2) | | | | | | | | |
| 2 | $[M+H-CH_4]^+$ | | | | | | | | | | | | | | 285 (1) | |
| 3 | $[M+H-H_2O]^+$ | | | | | | | | | | | 269 (2) | 285 (3) | | | |
| 4 | $[M+H-CO]^+$ | | | | | | 243 (2) | | | | | | | | | |
| 5 | $[M+H-CHO]^{\bullet+}$ | | | | | | 242 (2) | 258 (2) | | | | | | | | |
| 6 | $[M+H-CH_3OH]^{\bullet+}$ | | | | | | | | | | | | | | 269 (3) | 285 (3) |
| 7 | $[M+H-CH_3-CO]^{\bullet+}$ | | | | | | | | 242 (49) | 258 (49) | 258 (46) | | | | 258 (2) | |
| 8 | $[M+H-CH_4-CO]^+$ | | | | | | | | 241 (7) | 257 (38) | 257 (37) | | | | 257 (6) | 273 (2) |
| 9 | $[M+H-H_2O-CO]^+$ | | | | | | | 241 (4) | | | | 241 (1) | 257 (2) | | | |
| 10 | $[M+H-CH_3OH-CO]^{\bullet+}$ | | | | | | | | | | | | | | | 257 (2) |
| 11 | $[M+H-CH_3-2CO]^{\bullet+}$ | | | | | | | 216 (1) | | | | 216 (2) | | | 230 (9) | |
| 12 | $[M+H-H_2O-CO-C_2H_2]^+$ | | | | | | | | 213 (6) | 229 (75) | 229 (76) | | | | 229 (100) | 245 (34) |
| 13 | $[M+H-CH_4-2CO]^+$ | | | | | | | | 213 (6) | 229 (75) | 229 (76) | | | | 229 (100) | 245 (34) |
| 14 | $[M+H-H_2O-2CO]^+$ | | | | | | 197 (3) | 213 (4) | | | | 213 (12) | 229 (16) | 245 (6) | | |
| 15 | $[M+H-2C_2H_2O]^+$ | | | | | | 187 (1) | 203 (3) | | | | 203 (1) | 219 (2) | | | |
| 16 | $[M+H-H_2O-CO-2C_2H_2]^+$ | | | | | | | | | 203 (29) | 203 (31) | | | | 203 (11) | 219 (13) |
| 17 | $[M+H-H_2O-2CO-C_2H_2]^+$ | | | | | | | 187 (2) | 185 (1) | 201 (7) | 201 (6) | 187 (2) | 203 (10) | 219 (21) | 201 (50) | 217 (56) |
| 18 | $[M+H-CH_4-3CO]^+$ | | | | | | | 187 (2) | 185 (1) | 201 (7) | 201 (6) | 187 (2) | 203 (10) | 219 (21) | 201 (50) | 217 (56) |
| 19 | $[M+H-2C_2H_2O-H_2O]^+$ | | | | | | 169 (2) | 185 (2) | | | | | | | | |
| 20 | $[M+H-CH_4-2CO-C_2H_2O]^+$ | | | | | | | | | 187 (6) | 187 (5) | | | | 187 (13) | 203 (37) |
| 21 | $[M+H-2CO-2C_2H_2O]^+$ | | | | | | 131 (5) | 147 (3) | | 161 (4) | 161 (5) | 147 (8) | 163 (5) | 179 (9) | | |
| 22 | $AC^+$ | | | | 179 (2) | 179 (1) | | | | | | | | | | |
| 23 | $0,2A^+$ | | | | | | | | | | | 165 (2) | 165 (3) | 165 (4) | 165 (2) | 165 (1) |
| 24 | $0,2A^+-CO$ | | | | | | | | | | | 137 (12) | 137 (38) | 137 (32) | 137 (8) | 137 (13) |
| 25 | $0,2B^+$ | | | | | | 121 (25) | 137 (16) | | | | 121 (69) | 137 (38) | 153 (100) | 135 (5) | 151 (1) |
| 26 | $0,3A^+$ | | | | 137 (3) | 137 (2) | | 137 (16) | | 137 (1) | 137 (2) | 137 (12) | 137 (38) | 137 (32) | 137 (8) | 137 (13) |
| 27 | $0,3A^++2H$ | | | | | | | | | | | | | 139 (3) | | |
| 28 | $0,4B^+$ | | | | | | 163 (2) | | | | | | | | | |
| 29 | $0,4B^+-H_2O$ | | | | | | 145 (41) | 161 (29) | | | | | | | | |
| 30 | $1,3A^+$ | 153 (69) | 153 (50) | 153 (100) | 153 (63) | 153 (58) | 153 (84) | 153 (87) | 153 (100) | 153 (100) | 153 (100) | 153 (100) | 153 (100) | 153 (100) | 153 (67) | 153 (100) |
| 31 | $1,3A^+-C_2H_2O$ | 111 (2) | 111 (2) | 111 (4) | 111 (2) | 111 (2) | 111 (4) | 111 (3) | | 111 (1) | 111 (1) | 111 (4) | 111 (5) | 111 (7) | 111 (3) | 111 (6) |
| 32 | $1,3B^+$ | | | | | | 119 (35) | | | | | | | | | |
| 33 | $1,3B^+-2H$ | | | | | | | | | | | 133 (1) | 149 (4) | 165 (4) | 147 (3) | 163 (5) |
| 34 | $1,4A^++2H$ | | | | | | | 127 (2) | | | | 127 (2) | 127 (6) | 127 (4) | | |
| 35 | $1,4A^{\bullet+}$ | | | | | | | 124 (2) | 124 (4) | 124 (4) | 124 (5) | 124 (1) | 124 (3) | 124 (15) | 124 (42) | 124 (14) |
| 36 | $1,4A^+$ | 125 (1) | | 125 (1) | 125 (1) | | 125 (3) | 125 (2) | | | | 125 (2) | 125 (1) | 125 (5) | | |
| 37 | $1,4B^++2H$ | | | | | | | | | | | | 145 (4) | 161 (4) | | 159 (2) |
| 38 | $1,4B^+-2H$ | 147 (3) | 163 (1) | 161 (3) | | | | | | | | | | | | |
| 39 | $1,4B^++2H-H_2O$ | | | | | | | | | | | 147 (8) | | | | |
| 40 | $1,4B^+-2H-H_2O$ | | 145 (1) | | | | | | | | | | | | | |
| 41 | $1,4B^+-2H-CO$ | 119 (34) | 135 (16) | 133 (36) | 149 (5) | 149 (3) | | | | | | | | | | |
| 42 | $1,4B^+-2H-CO-CH_3$ | | | 118 (57) | 134 (20) | 134 (13) | | | | | | | | | | |
| 43 | $1,4B^+-2H-CO-CH_2O$ | | | 103 (27) | | | | | | | | | | | | |
| 44 | $1,4B^+-2H-2CO$ | 91 (100) | | | | | | | | | | | | | | |
| 45 | $1,4B^+-2H-2CO-CH_3$ | | | 90 (49) | | | | | | | | | | | | |
| 46 | $1,4B^+-2H-C_2H_2O-H_2O$ | | | | 117 (13) | 117 (26) | | | | | | | | | | |
| 47 | $1,4B^+-2H-H_2O-CO$ | | 117 (21) | | | | | | | | | | | | | |
| 48 | $C_7H_6O_5^+$ | | | | | | | | 170 (1) | 170 (1) | 170 (1) | | | 170 (3) | 170 (8) | 170 (3) |
| 49 | $C_7H_7^+$ | 91 (100) | | 91 (5) | 91 (7) | 91 (5) | | | | | | | | | | |
| 50 | $C_7H_5^+$ | | 89 (100) | 89 (22) | 89 (100) | 89 (100) | 89 (7) | 89 (100) | 89 (3) | | 89 (1) | 89 (6) | 89 (9) | 89 (7) | 89 (2) | 89 (2) |
| 51 | $C_5H_5O^+$ | 81 (1) | 81 (1) | 81 (1) | 81 (2) | 81 (1) | 81 (3) | 81 (8) | | | | 81 (12) | 81 (39) | 81 (24) | 81 (4) | 81 (7) |
| 52 | $C_3HO_2^+$ | 69 (9) | 69 (8) | 69 (13) | 69 (9) | 69 (8) | 69 (24) | 69 (22) | 69 (1) | 69 (2) | 69 (2) | | 69 (31) | 69 (29) | 69 (10) | 69 (8) |