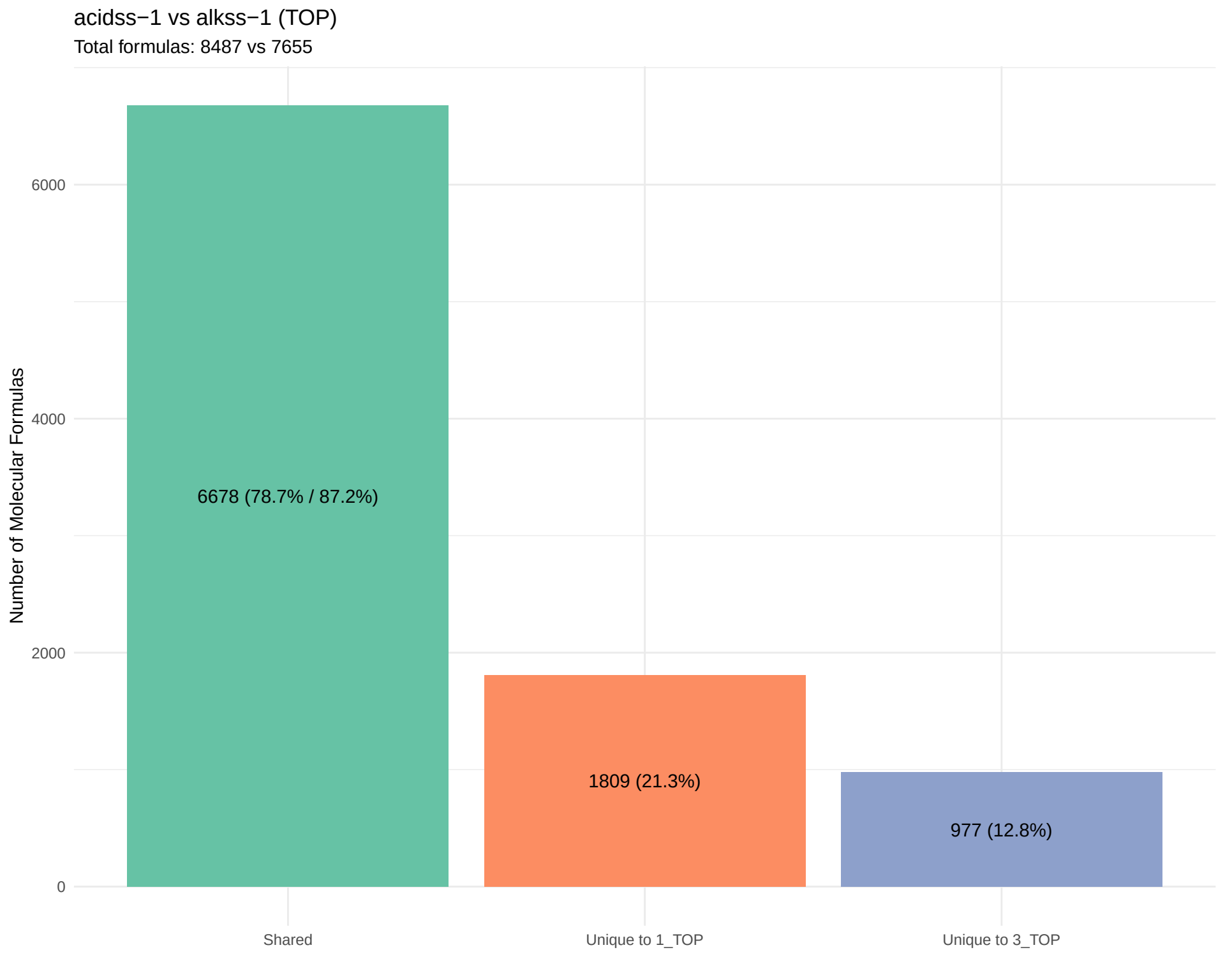
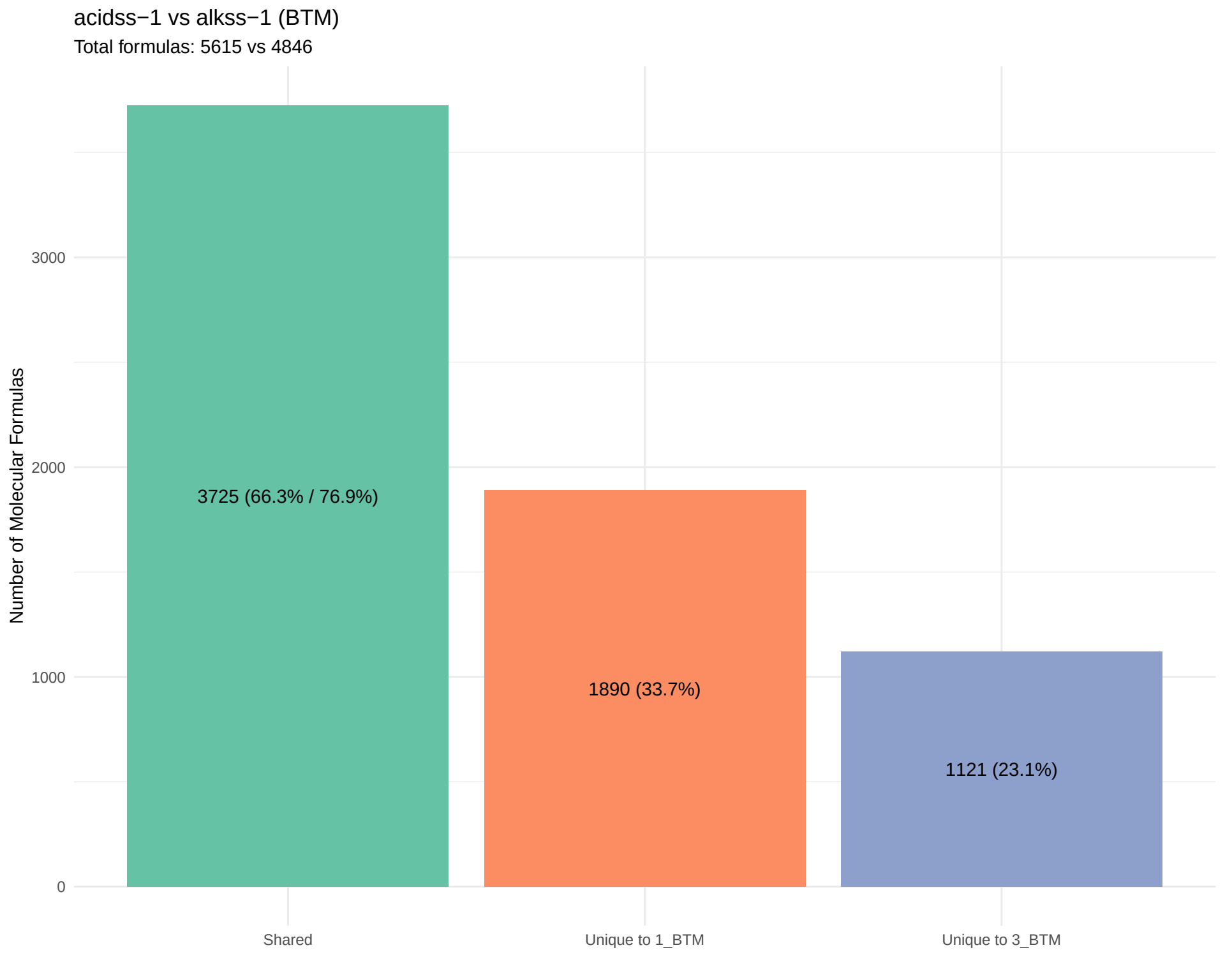
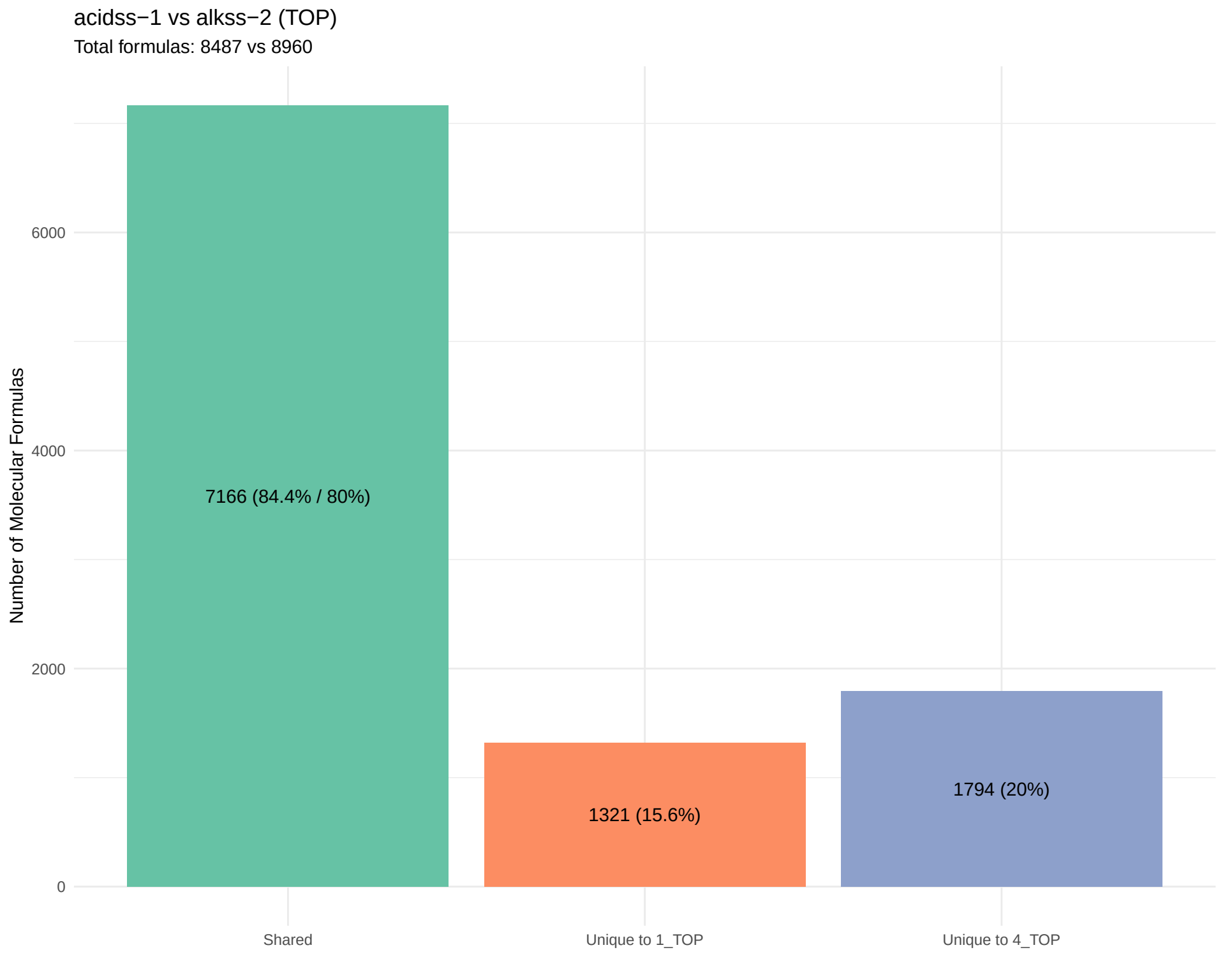
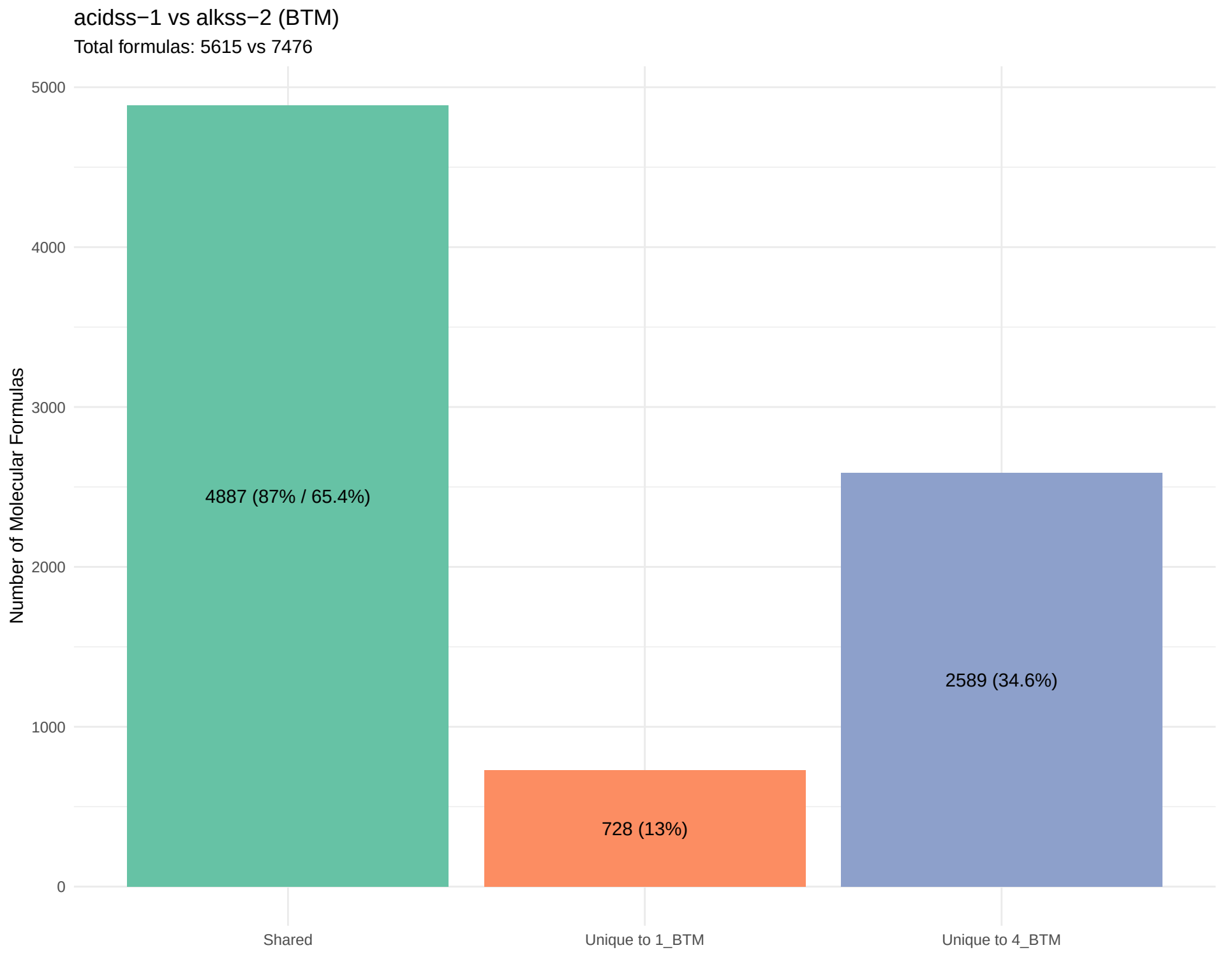
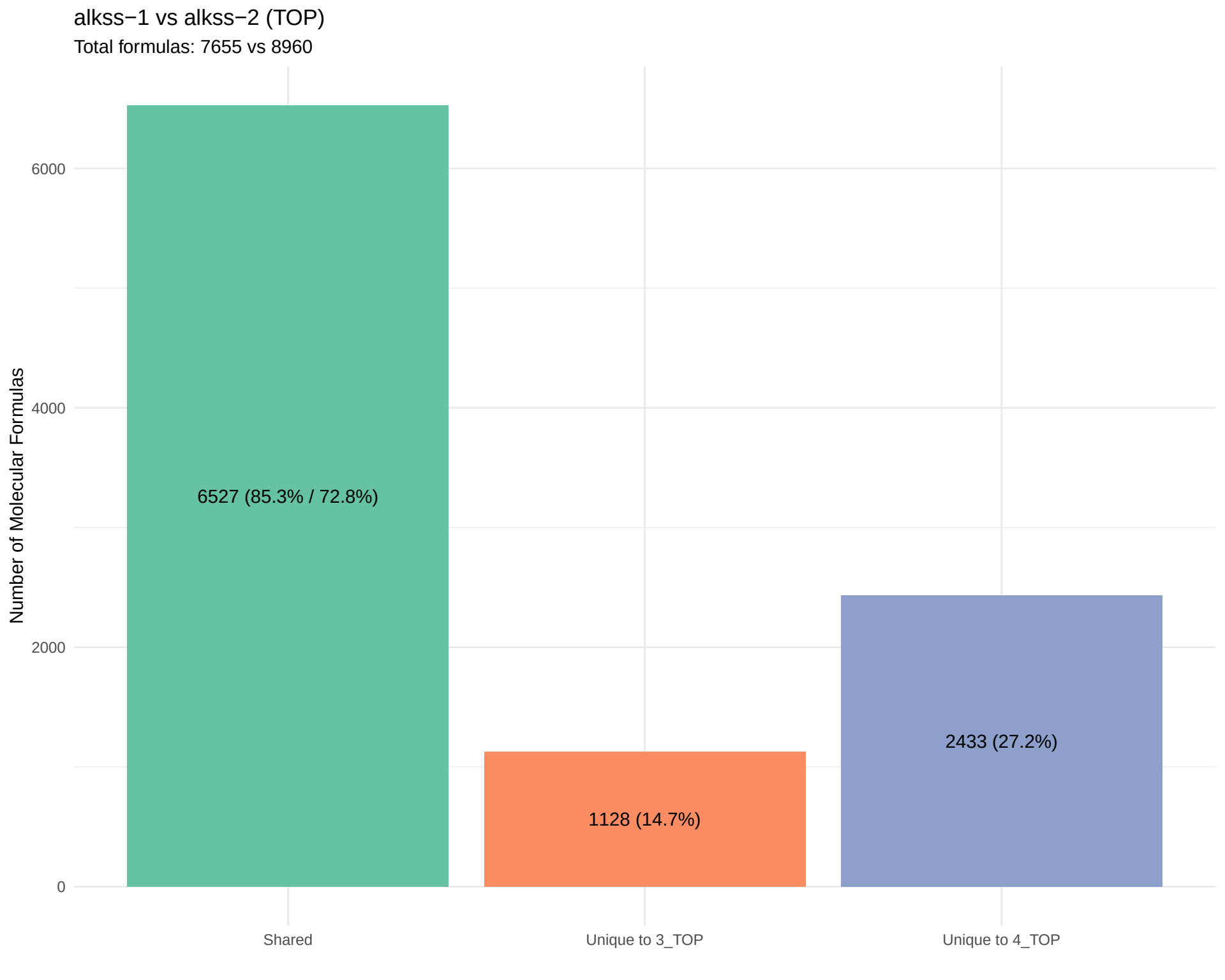
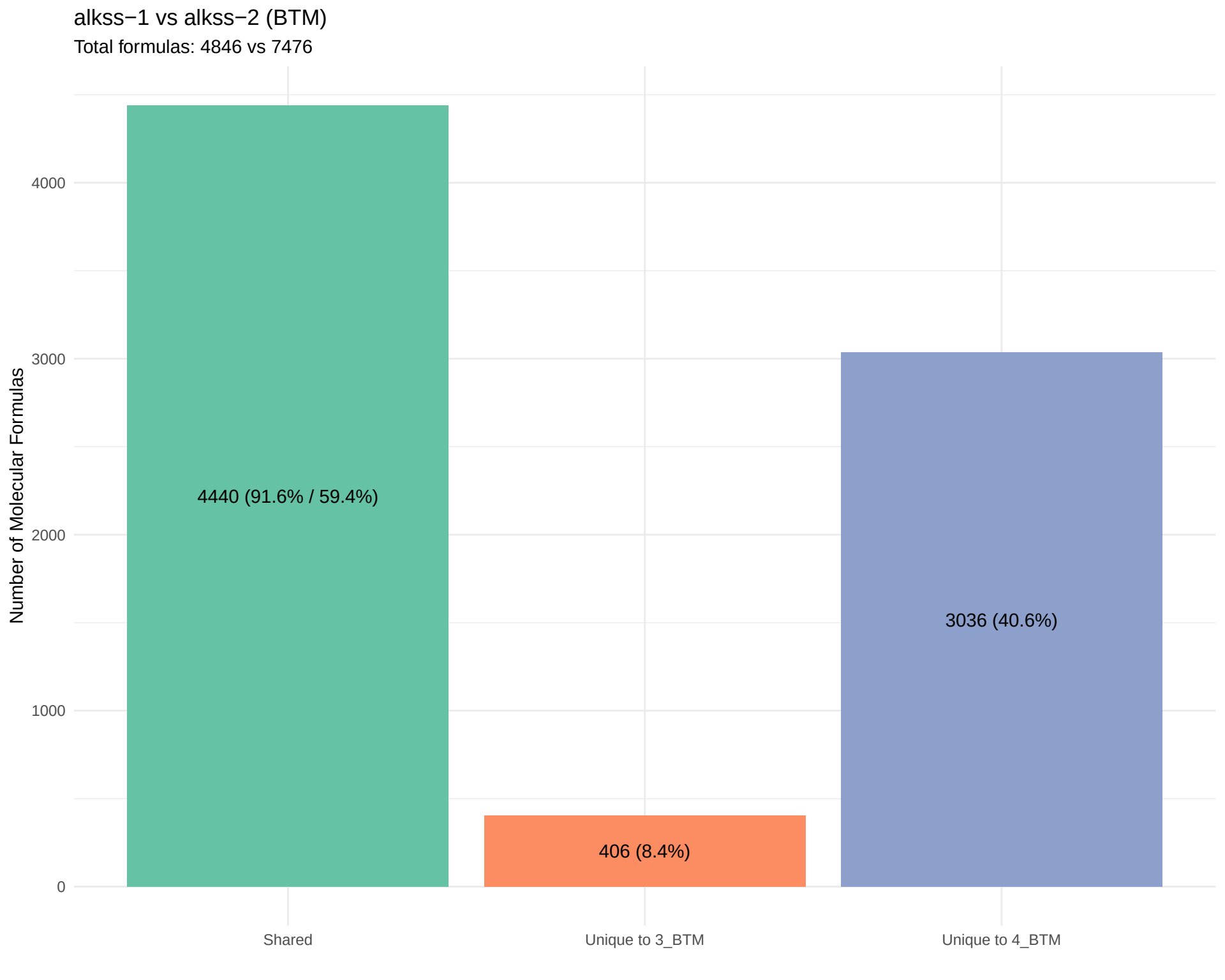

acidss−1 vs alkss−1 (TOP)
Total formulas: 8487 vs 7655
Number of Molecular Formulas
6000
4000
2000
0
6678 (78.7% / 87.2%)
1809 (21.3%)
977 (12.8%)
Shared
Unique to 1_TOP
Unique to 3_TOP

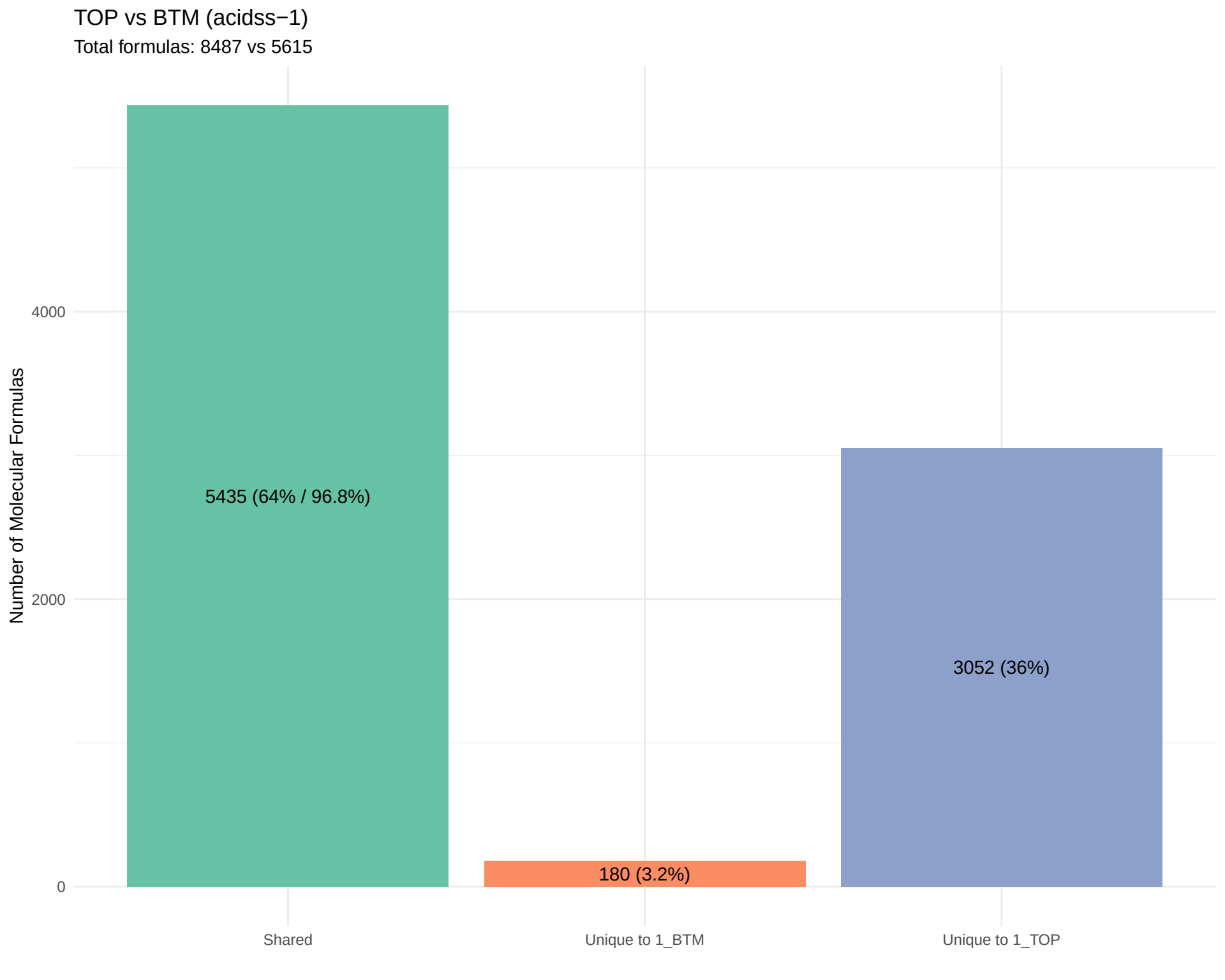

acidss−1 vs alkss−1 (BTM)
Total formulas: 5615 vs 4846
Number of Molecular Formulas
3000
2000
1000
0
3725 (66.3% / 76.9%)
1890 (33.7%)
1121 (23.1%)
Shared
Unique to 1_BTM
Unique to 3_BTM

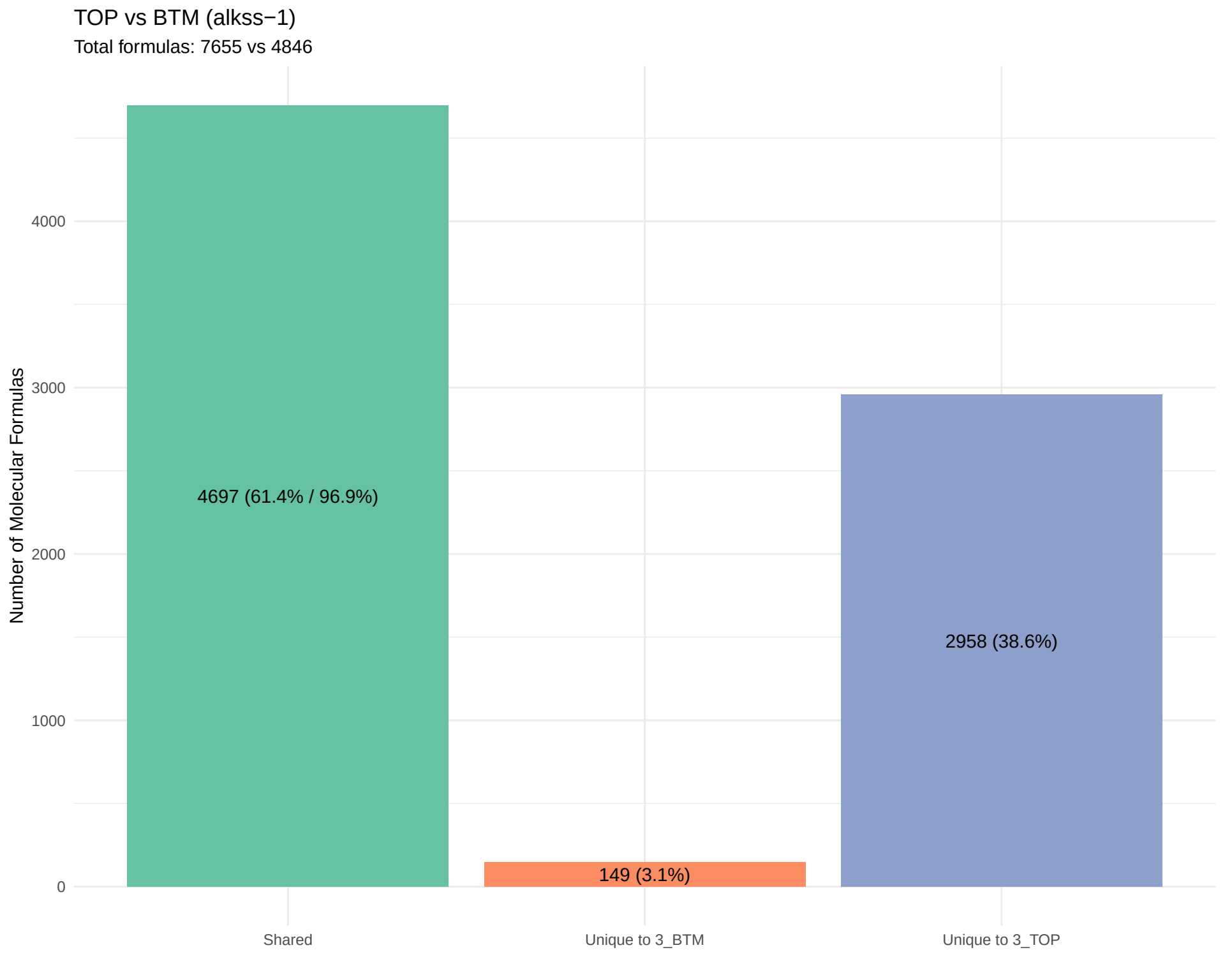

acidss−1 vs alkss−2 (TOP)
Total formulas: 8487 vs 8960
Number of Molecular Formulas
6000
4000
2000
0
7166 (84.4% / 80%)
1321 (15.6%)
1794 (20%)
Shared
Unique to 1_TOP
Unique to 4_TOP

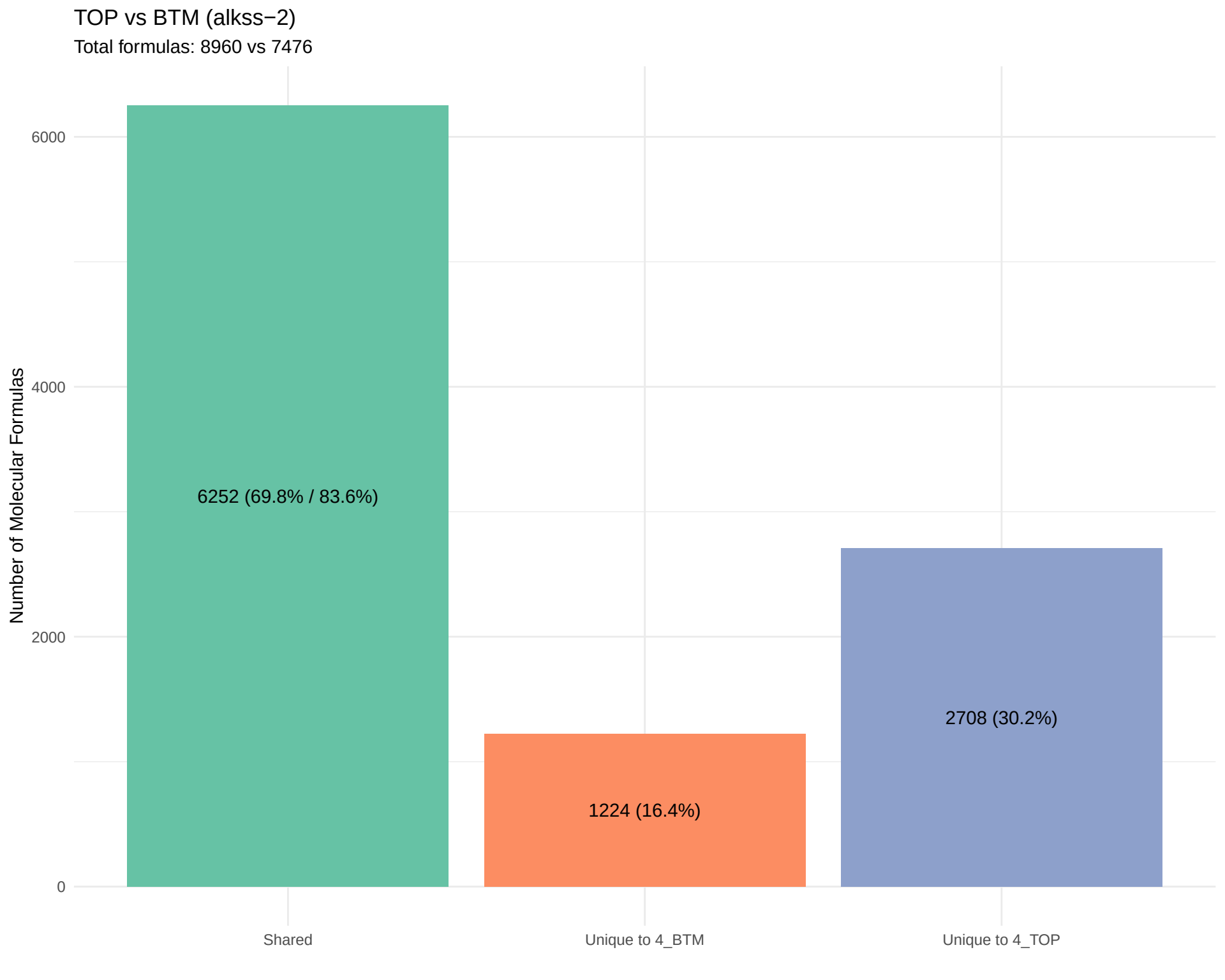

acidss−1 vs alkss−2 (BTM)
Total formulas: 5615 vs 7476
Number of Molecular Formulas
5000
4000
3000
2000
1000
0
4887 (87% / 65.4%)
728 (13%)
2589 (34.6%)
Shared
Unique to 1_BTM
Unique to 4_BTM


alkss−1 vs alkss−2 (TOP)
Total formulas: 7655 vs 8960
Number of Molecular Formulas
6000
4000
2000
0
6527 (85.3% / 72.8%)
1128 (14.7%)
2433 (27.2%)
Shared
Unique to 3_TOP
Unique to 4_TOP


alkss−1 vs alkss−2 (BTM)
Total formulas: 4846 vs 7476
Number of Molecular Formulas
4000
3000
2000
1000
0
4440 (91.6% / 59.4%)
406 (8.4%)
3036 (40.6%)
Shared
Unique to 3_BTM
Unique to 4_BTM


TOP vs BTM (acidss−1)
Total formulas: 8487 vs 5615
Number of Molecular Formulas
4000
2000
0
5435 (64% / 96.8%)
180 (3.2%)
3052 (36%)
Shared
Unique to 1_BTM
Unique to 1_TOP


TOP vs BTM (alkss−1)
Total formulas: 7655 vs 4846
Number of Molecular Formulas
4000
3000
2000
1000
0
4697 (61.4% / 96.9%)
149 (3.1%)
2958 (38.6%)
Shared
Unique to 3_BTM
Unique to 3_TOP


TOP vs BTM (alkss−2)
Total formulas: 8960 vs 7476
Number of Molecular Formulas
6000
4000
2000
0
6252 (69.8% / 83.6%)
1224 (16.4%)
2708 (30.2%)
Shared
Unique to 4_BTM
Unique to 4_TOP