

Compound	Compound ID	Adducts	Formula	Score
31.82_510.1827m/z	HMDB0038329	M+H	C20H31NO14	37.6
31.82_510.1827m/z	HMDB0038329	M+H	C20H31NO14	37.6
31.82_510.1827m/z	HMDB0006592	M+H-2H2O	C20H35NO16	37.5
31.82_510.1827m/z	HMDB0039750	M+H-2H2O	C20H35NO16	37.5
31.82_510.1827m/z	HMDB0041622	M+H-2H2O	C20H35NO16	37.5
31.82_510.1827m/z	HMDB0006592	M+H-2H2O	C20H35NO16	37.5
31.82_510.1827m/z	HMDB0039750	M+H-2H2O	C20H35NO16	37.5
31.82_510.1827m/z	HMDB0041622	M+H-2H2O	C20H35NO16	37.5
7.83_437.0684m/z	HMDB0128725	M+Na	C17H18O12	35.8
7.83_437.0684m/z	HMDB0128726	M+Na	C17H18O12	35.8
7.83_437.0684m/z	HMDB0128727	M+Na	C17H18O12	35.8
7.83_437.0684m/z	HMDB0128728	M+Na	C17H18O12	35.8
7.83_437.0684m/z	HMDB0128725	M+Na	C17H18O12	35.8
7.83_437.0684m/z	HMDB0128726	M+Na	C17H18O12	35.8
7.83_437.0684m/z	HMDB0128727	M+Na	C17H18O12	35.8
7.83_437.0684m/z	HMDB0128728	M+Na	C17H18O12	35.8
7.83_437.0684m/z	HMDB0000797	M+H-H2O	C13H19N4O12P	35.6
7.83_437.0684m/z	HMDB0000797	M+H-H2O	C13H19N4O12P	35.6
42.79_643.2291m/z	HMDB0030112	M+H-2H2O	C40H38O10	35.5
42.79_643.2291m/z	HMDB0035964	M+H-2H2O	C40H38O10	35.5
42.79_643.2291m/z	HMDB0126375	M+H-2H2O	C40H38O10	35.5
38.04_341.1982m/z	HMDB0015075	M+H	C21H26NO3+	35.5
38.04_341.1982m/z	HMDB0015591	M+H	C21H26NO3+	35.5
42.79_643.2291m/z	HMDB0030112	M+H-2H2O	C40H38O10	35.5
42.79_643.2291m/z	HMDB0035964	M+H-2H2O	C40H38O10	35.5
42.79_643.2291m/z	HMDB0126375	M+H-2H2O	C40H38O10	35.5
38.04_341.1982m/z	HMDB0015075	M+H	C21H26NO3+	35.5
38.04_341.1982m/z	HMDB0015591	M+H	C21H26NO3+	35.5
39.00_615.2230m/z	HMDB0006607	M+H-H2O	C23H40N2O18	35.4
39.00_615.2230m/z	HMDB0041621	M+H-H2O	C23H40N2O18	35.4
39.00_615.2230m/z	HMDB0006607	M+H-H2O	C23H40N2O18	35.4
39.00_615.2230m/z	HMDB0041621	M+H-H2O	C23H40N2O18	35.4
38.04_341.1982m/z	HMDB0014876	M+H	C19H24N4O2	35.3
38.04_341.1982m/z	HMDB0014876	M+H	C19H24N4O2	35.3
38.04_341.1982m/z	HMDB0015121	M+Na	C19H28NO3+	34.6
38.04_341.1982m/z	HMDB0015121	M+Na	C19H28NO3+	34.6
2.33_118.0890m/z	HMDB0000043	M+H	C5H11NO2	34.3
2.33_118.0890m/z	HMDB0000883	M+H	C5H11NO2	34.3
2.33_118.0890m/z	HMDB0001382	M+H	C5H11NO2	34.3
2.33_118.0890m/z	HMDB0002141	M+H	C5H11NO2	34.3
2.33_118.0890m/z	HMDB0003355	M+H	C5H11NO2	34.3
2.33_118.0890m/z	HMDB0013716	M+H	C5H11NO2	34.3
2.33_118.0890m/z	HMDB0015550	M+H	C5H11NO2	34.3
2.33_118.0890m/z	HMDB0000043	M+H	C5H11NO2	34.3
2.33_118.0890m/z	HMDB0000883	M+H	C5H11NO2	34.3
2.33_118.0890m/z	HMDB0001382	M+H	C5H11NO2	34.3
28.39_482.1733m/z	HMDB0001396	M+Na	C20H25N7O6	34.2
31.82_510.1827m/z	HMDB0014832	M+H-H2O	C27H29NO10	34.2

31.82_510.1827m/z	HMDB0041884	M+H-2H2O	C27H31NO11	34.2
31.82_510.1827m/z	HMDB0060823	M+H-2H2O	C27H31NO11	34.2
39.04_490.2726m/z	HMDB0011496	M+H-2H2O	C27H44NO7P	34.1
39.04_490.2726m/z	HMDB0011526	M+H-2H2O	C27H44NO7P	34.1
39.04_490.2726m/z	HMDB0011496	M+H-2H2O	C27H44NO7P	34.1
39.04_490.2726m/z	HMDB0011526	M+H-2H2O	C27H44NO7P	34.1
42.79_643.2291m/z	HMDB0130483	M+H-2H2O	C36H38O13	33.8
42.79_643.2291m/z	HMDB0130484	M+H-2H2O	C36H38O13	33.8
42.79_643.2291m/z	HMDB0130485	M+H-2H2O	C36H38O13	33.8
27.53_496.1463m/z	HMDB0029776	M+Na	C20H27NO12	33.8
42.79_643.2291m/z	HMDB0130483	M+H-2H2O	C36H38O13	33.8
42.79_643.2291m/z	HMDB0130484	M+H-2H2O	C36H38O13	33.8
42.79_643.2291m/z	HMDB0130485	M+H-2H2O	C36H38O13	33.8
27.53_496.1463m/z	HMDB0029776	M+Na	C20H27NO12	33.8
31.82_510.1827m/z	HMDB0132953	M+H-H2O	C23H33N3O9S	33.6
31.82_510.1827m/z	HMDB0132954	M+H-H2O	C23H33N3O9S	33.6
31.82_510.1827m/z	HMDB0132953	M+H-H2O	C23H33N3O9S	33.6
31.82_510.1827m/z	HMDB0132954	M+H-H2O	C23H33N3O9S	33.6
28.39_482.1733m/z	HMDB0015230	M+H	C22H28FN3O6S	33.5
38.04_341.1982m/z	HMDB0029850	M+Na	C16H30O6	33.5
38.04_341.1982m/z	HMDB0032368	M+Na	C16H30O6	33.5
43.72_752.1608m/z	HMDB0001197	M+H-2H2O	C27H35N9O15P2	33.3
40.74_629.2282m/z	HMDB0032114	M+H-H2O	C38H34N2O8	32.9
38.94_615.2186m/z	HMDB0006607	M+H-H2O	C23H40N2O18	32.8
38.94_615.2186m/z	HMDB0041621	M+H-H2O	C23H40N2O18	32.8
44.45_779.1615m/z	HMDB0126885	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0126886	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0126887	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0126888	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0127450	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0127451	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0126885	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0126886	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0126887	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0126888	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0127450	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0127451	M+Na	C32H36O21	32.6
44.45_779.1615m/z	HMDB0127452	M+Na	C32H36O21	32.6
7.83_437.0684m/z	HMDB0060316	M+Na	C16H18N2O9S	32.5
39.04_615.2607m/z	HMDB0129666	M+H-2H2O	C36H42O11	32.5
39.04_615.2607m/z	HMDB0129667	M+H-2H2O	C36H42O11	32.5
39.04_615.2607m/z	HMDB0129668	M+H-2H2O	C36H42O11	32.5
7.83_437.0684m/z	HMDB0060316	M+Na	C16H18N2O9S	32.5
39.04_615.2607m/z	HMDB0129666	M+H-2H2O	C36H42O11	32.5
39.04_615.2607m/z	HMDB0129667	M+H-2H2O	C36H42O11	32.5
39.04_615.2607m/z	HMDB0129668	M+H-2H2O	C36H42O11	32.5
35.38_538.2029m/z	HMDB0006595	M+Na	C20H37NO14	32.4
40.66_629.2270m/z	HMDB0032114	M+H-H2O	C38H34N2O8	32.4
40.66_629.2270m/z	HMDB0034634	M+H-H2O	C32H38O14	32.2
43.72_752.1608m/z	HMDB0125188	M+H-2H2O	C36H35O20+	32.1

43.72_752.1608m/z	HMDB0125189	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125190	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125191	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125192	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125193	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125188	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125189	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125190	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125191	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125192	M+H-2H2O	C36H35O20+	32.1
43.72_752.1608m/z	HMDB0125193	M+H-2H2O	C36H35O20+	32.1
40.74_629.2282m/z	HMDB0034634	M+H-H2O	C32H38O14	31.8
38.04_341.1982m/z	HMDB0014469	M+H-2H2O	C22H29FO4	31.8
38.04_341.1982m/z	HMDB0014687	M+H-2H2O	C22H29FO4	31.8
0.29_156.0199m/z	HMDB0033843	M+H-H2O	C6H9NOP2	31.8
40.74_629.2282m/z	HMDB0034634	M+H-H2O	C32H38O14	31.8
44.45_779.1615m/z	HMDB0041730	M+H-H2O	C34H36O22	31.7
27.53_496.1463m/z	HMDB0000972	M+Na	C20H23N7O7	31.7
27.53_496.1463m/z	HMDB0001562	M+Na	C20H23N7O7	31.7
27.53_496.1463m/z	HMDB0002140	M+Na	C20H23N7O7	31.7
27.53_496.1463m/z	HMDB0062757	M+Na	C20H23N7O7	31.7
44.45_779.1615m/z	HMDB0037373	M+Na	C39H32O16	31.6
27.53_496.1463m/z	HMDB0128696	M+H-2H2O	C21H29N3O11S	31.5
38.98_616.2241m/z	HMDB0060139	M+Na	C28H39N3O9S	31.4
38.04_341.1982m/z	HMDB0060574	M+H	C17H28N2O5	31.4
27.53_496.1463m/z	HMDB0031112	M+H-2H2O	C29H25NO9	31.4
27.53_496.1463m/z	HMDB0034788	M+H-2H2O	C29H25NO9	31.4
27.53_496.1463m/z	HMDB0040769	M+H-H2O	C29H23NO8	31.3
27.53_496.1463m/z	HMDB0040769	M+H-H2O	C29H23NO8	31.3
39.28_566.2113m/z	HMDB0040387	M+H	C34H31NO7	31.2
0.29_156.0199m/z	HMDB0000191	M+Na	C4H7NO4	31.2
0.29_156.0199m/z	HMDB0006483	M+Na	C4H7NO4	31.2
0.29_156.0199m/z	HMDB0011753	M+Na	C4H7NO4	31.2
0.29_156.0199m/z	HMDB0062186	M+Na	C4H7NO4	31.2
0.29_156.0199m/z	HMDB0062501	M+Na	C4H7NO4	31.2
39.28_566.2113m/z	HMDB0040387	M+H	C34H31NO7	31.2
28.39_482.1733m/z	HMDB0015481	M+H	C27H23N5O4	30.8
0.28_140.0572m/z	HMDB0000197	M+H-2H2O	C10H9NO2	30.8
0.28_140.0572m/z	HMDB0004073	M+H-2H2O	C10H9NO2	30.8
0.28_140.0572m/z	HMDB0038628	M+H-2H2O	C10H9NO2	30.8
0.28_140.0572m/z	HMDB0040972	M+H-2H2O	C10H9NO2	30.8
28.39_482.1733m/z	HMDB0015481	M+H	C27H23N5O4	30.8
0.28_140.0572m/z	HMDB0000197	M+H-2H2O	C10H9NO2	30.8
0.28_140.0572m/z	HMDB0004073	M+H-2H2O	C10H9NO2	30.8
0.28_140.0572m/z	HMDB0038628	M+H-2H2O	C10H9NO2	30.8
0.28_140.0572m/z	HMDB0040972	M+H-2H2O	C10H9NO2	30.8
35.38_538.2029m/z	HMDB0034773	M+H	C25H31NO12	30.7
35.38_538.2029m/z	HMDB0034774	M+H	C25H31NO12	30.7
43.01_643.2387m/z	HMDB0030112	M+H-2H2O	C40H38O10	30.7
43.01_643.2387m/z	HMDB0035964	M+H-2H2O	C40H38O10	30.7

43.01_643.2387m/z	HMDB0126375	M+H-2H2O	C40H38O10	30.7
27.53_496.1463m/z	HMDB0134078	M+Na	C19H27N3O9S	30.7
35.38_538.2029m/z	HMDB0034773	M+H	C25H31NO12	30.7
35.38_538.2029m/z	HMDB0034774	M+H	C25H31NO12	30.7
43.01_643.2387m/z	HMDB0030112	M+H-2H2O	C40H38O10	30.7
43.01_643.2387m/z	HMDB0035964	M+H-2H2O	C40H38O10	30.7
43.01_643.2387m/z	HMDB0126375	M+H-2H2O	C40H38O10	30.7
27.53_496.1463m/z	HMDB0134078	M+Na	C19H27N3O9S	30.7
38.73_615.2183m/z	HMDB0030627	M+H-2H2O	C31H38O15	30.3
38.73_615.2183m/z	HMDB0034281	M+H-2H2O	C31H38O15	30.3
39.28_566.2113m/z	HMDB0135503	M+H	C27H35NO12	30.3
39.28_566.2113m/z	HMDB0135505	M+H	C27H35NO12	30.3
39.28_566.2113m/z	HMDB0135507	M+H	C27H35NO12	30.3
42.79_643.2291m/z	HMDB0041431	M+H	C38H34N4O6	30.3
0.28_140.0572m/z	HMDB0062189	M+H-H2O	C10H7NO	30.3
38.73_615.2183m/z	HMDB0030627	M+H-2H2O	C31H38O15	30.3
38.73_615.2183m/z	HMDB0034281	M+H-2H2O	C31H38O15	30.3
39.28_566.2113m/z	HMDB0135503	M+H	C27H35NO12	30.3
39.28_566.2113m/z	HMDB0135505	M+H	C27H35NO12	30.3
39.28_566.2113m/z	HMDB0135507	M+H	C27H35NO12	30.3
42.79_643.2291m/z	HMDB0041431	M+H	C38H34N4O6	30.3
0.28_140.0572m/z	HMDB0062189	M+H-H2O	C10H7NO	30.3
38.73_615.2183m/z	HMDB0129415	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0129416	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0129417	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132767	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132768	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132770	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132771	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132772	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132774	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132775	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132776	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132777	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132778	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132779	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132780	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132782	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132783	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132784	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132786	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132787	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132788	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132789	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132791	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132792	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132793	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132811	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132812	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132813	M+H	C31H34O13	30.2

38.73_615.2183m/z	HMDB0132815	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132816	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132817	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132819	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132820	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132821	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132822	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132823	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132824	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132825	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132828	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132831	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132832	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132833	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132835	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132836	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132837	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132838	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132839	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132840	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132841	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132842	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132843	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132844	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132845	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132846	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132847	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132848	M+H	C31H34O13	30.2
40.74_629.2282m/z	HMDB0031149	M+Na	C35H34N4O6	30.2
39.00_615.2230m/z	HMDB0030627	M+H-2H2O	C31H38O15	30.2
39.00_615.2230m/z	HMDB0034281	M+H-2H2O	C31H38O15	30.2
38.94_615.2186m/z	HMDB0030627	M+H-2H2O	C31H38O15	30.2
38.94_615.2186m/z	HMDB0034281	M+H-2H2O	C31H38O15	30.2
38.04_341.1982m/z	HMDB0001337	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0005081	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0006027	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010202	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010205	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010209	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010210	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010212	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010217	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0012534	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0012611	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0013633	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0030101	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0035116	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0035311	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036698	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036706	M+Na	C20H30O3	30.2

38.04_341.1982m/z	HMDB0036712	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036713	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036724	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036752	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036776	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036806	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036839	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036930	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0037523	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0038521	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0039012	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0039716	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0041058	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0060053	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0061114	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0062222	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0062293	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0062296	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0062408	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0137419	M+Na	C20H30O3	30.2
38.73_615.2183m/z	HMDB0129415	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0129416	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0129417	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132767	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132768	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132770	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132771	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132772	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132774	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132775	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132776	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132777	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132778	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132779	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132780	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132782	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132783	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132784	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132786	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132787	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132788	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132789	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132791	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132792	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132793	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132811	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132812	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132813	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132815	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132816	M+H	C31H34O13	30.2

38.73_615.2183m/z	HMDB0132817	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132819	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132820	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132821	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132822	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132823	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132824	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132825	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132828	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132831	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132832	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132833	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132835	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132836	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132837	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132838	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132839	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132840	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132841	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132842	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132843	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132844	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132845	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132846	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132847	M+H	C31H34O13	30.2
38.73_615.2183m/z	HMDB0132848	M+H	C31H34O13	30.2
40.74_629.2282m/z	HMDB0031149	M+Na	C35H34N4O6	30.2
39.00_615.2230m/z	HMDB0030627	M+H-2H2O	C31H38O15	30.2
39.00_615.2230m/z	HMDB0034281	M+H-2H2O	C31H38O15	30.2
38.94_615.2186m/z	HMDB0030627	M+H-2H2O	C31H38O15	30.2
38.94_615.2186m/z	HMDB0034281	M+H-2H2O	C31H38O15	30.2
38.04_341.1982m/z	HMDB0001337	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0005081	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0006027	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010202	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010205	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010209	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010210	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010212	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0010217	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0012534	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0012611	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0013633	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0030101	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0035116	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0035311	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036698	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036706	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036712	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036713	M+Na	C20H30O3	30.2

38.04_341.1982m/z	HMDB0036724	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036752	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036776	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036806	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036839	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0036930	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0037523	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0038521	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0039012	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0039716	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0041058	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0060053	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0061114	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0062222	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0062293	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0062296	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0062408	M+Na	C20H30O3	30.2
38.04_341.1982m/z	HMDB0137419	M+Na	C20H30O3	30.2
38.98_616.2241m/z	HMDB0000825	M+H-H2O	C23H39NO19	30.1
38.98_616.2241m/z	HMDB0006569	M+H-H2O	C23H39NO19	30.1
39.00_615.2230m/z	HMDB0129415	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0129416	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0129417	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132767	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132768	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132770	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132771	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132772	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132774	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132775	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132776	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132777	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132778	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132779	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132780	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132782	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132783	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132784	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132786	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132787	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132788	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132789	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132791	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132792	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132793	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132811	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132812	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132813	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132815	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132816	M+H	C31H34O13	30.1





38.94_615.2186m/z	HMDB0132793	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132811	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132812	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132813	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132815	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132816	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132817	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132819	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132820	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132821	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132822	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132823	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132824	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132825	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132828	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132831	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132832	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132833	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132835	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132836	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132837	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132838	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132839	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132840	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132841	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132842	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132843	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132844	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132845	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132846	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132847	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132848	M+H	C31H34O13	30.1
38.04_341.1982m/z	HMDB0014722	M+H-2H2O	C20H28N2O5	30.1
38.04_341.1982m/z	HMDB0015036	M+H-2H2O	C20H28N2O5	30.1
27.53_496.1463m/z	HMDB0014624	M+Na	C28H27NO4S	30.1
0.29_156.0199m/z	HMDB0002916	M+H	C6H5NO4	30.1
0.29_156.0199m/z	HMDB0006200	M+H	C6H5NO4	30.1
0.29_156.0199m/z	HMDB0062694	M+H	C6H5NO4	30.1
38.98_616.2241m/z	HMDB0000825	M+H-H2O	C23H39NO19	30.1
38.98_616.2241m/z	HMDB0006569	M+H-H2O	C23H39NO19	30.1
39.00_615.2230m/z	HMDB0129415	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0129416	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0129417	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132767	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132768	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132770	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132771	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132772	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132774	M+H	C31H34O13	30.1
39.00_615.2230m/z	HMDB0132775	M+H	C31H34O13	30.1





38.94_615.2186m/z	HMDB0132847	M+H	C31H34O13	30.1
38.94_615.2186m/z	HMDB0132848	M+H	C31H34O13	30.1
38.04_341.1982m/z	HMDB0014722	M+H-2H2O	C20H28N2O5	30.1
38.04_341.1982m/z	HMDB0015036	M+H-2H2O	C20H28N2O5	30.1
27.53_496.1463m/z	HMDB0014624	M+Na	C28H27NO4S	30.1

Mass Error (ppm)	Isotope Similarity	Theoretical Isotope Distribution
1.816.731.948	9.020.664.073	100 - 22.9 - 5.38 - 0.831 - 0.119
1.816.731.948	9.020.664.073	100 - 22.9 - 5.38 - 0.831 - 0.119
1.696.708.715	8.973.038.008	100 - 23 - 5.82 - 0.932 - 0.142
1.696.708.715	8.973.038.008	100 - 23 - 5.82 - 0.932 - 0.142
1.696.708.715	8.973.038.008	100 - 23 - 5.82 - 0.932 - 0.142
1.696.708.715	8.973.038.008	100 - 23 - 5.82 - 0.932 - 0.142
1.696.708.715	8.973.038.008	100 - 23 - 5.82 - 0.932 - 0.142
1.696.708.715	8.973.038.008	100 - 23 - 5.82 - 0.932 - 0.142
-1.565.071.067	8.077.684.174	100 - 19.1 - 4.18 - 0.566
-1.565.071.067	8.077.684.174	100 - 19.1 - 4.18 - 0.566
-1.565.071.067	8.077.684.174	100 - 19.1 - 4.18 - 0.566
-1.565.071.067	8.077.684.174	100 - 19.1 - 4.18 - 0.566
-1.565.071.067	8.077.684.174	100 - 19.1 - 4.18 - 0.566
-1.565.071.067	8.077.684.174	100 - 19.1 - 4.18 - 0.566
-1.565.071.067	8.077.684.174	100 - 19.1 - 4.18 - 0.566
-1.565.071.067	8.077.684.174	100 - 19.1 - 4.18 - 0.566
-1.565.071.067	8.077.684.174	100 - 19.1 - 4.18 - 0.566
-4.452.615.482	8.308.858.912	100 - 16.2 - 3.7 - 0.457
-4.452.615.482	8.308.858.912	100 - 16.2 - 3.7 - 0.457
-5.228.828.358	8.327.628.913	100 - 44.1 - 11.5 - 2.23 - 0.349
-5.228.828.358	8.327.628.913	100 - 44.1 - 11.5 - 2.23 - 0.349
-5.228.828.358	8.327.628.913	100 - 44.1 - 11.5 - 2.23 - 0.349
-1.051.492.245	7.869.278.511	100 - 23.5 - 3.25 - 0.333
-1.051.492.245	7.869.278.511	100 - 23.5 - 3.25 - 0.333
-5.228.828.358	8.327.628.913	100 - 44.1 - 11.5 - 2.23 - 0.349
-5.228.828.358	8.327.628.913	100 - 44.1 - 11.5 - 2.23 - 0.349
-5.228.828.358	8.327.628.913	100 - 44.1 - 11.5 - 2.23 - 0.349
-1.051.492.245	7.869.278.511	100 - 23.5 - 3.25 - 0.333
-1.051.492.245	7.869.278.511	100 - 23.5 - 3.25 - 0.333
-2.084.679.526	7.937.090.878	100 - 26.8 - 7.14 - 1.27 - 0.208
-2.084.679.527	7.937.090.878	100 - 26.8 - 7.14 - 1.27 - 0.208
-2.084.679.526	7.937.090.878	100 - 26.8 - 7.14 - 1.27 - 0.208
-2.084.679.527	7.937.090.878	100 - 26.8 - 7.14 - 1.27 - 0.208
2.895.326.239	7.973.545.924	100 - 22.4 - 2.8 - 0.254
2.895.326.239	7.973.545.924	100 - 22.4 - 2.8 - 0.254
64.359.989	8.038.185.957	100 - 21.4 - 2.78 - 0.271
64.359.989	8.038.185.957	100 - 21.4 - 2.78 - 0.271
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
2.378.515.589	9.386.541.213	100 - 5.98 - 0.56
-5.564.849.437	7.728.332.677	100 - 24.7 - 4.16 - 0.526
1.289.553.642	8.450.122.254	100 - 30.3 - 6.48 - 1.04 - 0.138

1.246.953.867	8.427.802.309	100 - 30.3 - 6.71 - 1.1 - 0.152
1.246.953.867	8.427.802.309	100 - 30.3 - 6.71 - 1.1 - 0.152
1.806.025.151	728.976.974	100 - 30.3 - 5.88 - 0.854 - 0.101
1.806.025.151	728.976.974	100 - 30.3 - 5.88 - 0.854 - 0.101
1.806.025.151	728.976.974	100 - 30.3 - 5.88 - 0.854 - 0.101
1.806.025.151	728.976.974	100 - 30.3 - 5.88 - 0.854 - 0.101
1.726.506.549	8.630.633.261	100 - 39.9 - 10.4 - 2.04 - 0.329
1.726.506.549	8.630.633.261	100 - 39.9 - 10.4 - 2.04 - 0.329
1.726.506.549	8.630.633.261	100 - 39.9 - 10.4 - 2.04 - 0.329
8.022.239.675	7.786.048.389	100 - 22.8 - 4.94 - 0.731
1.726.506.549	8.630.633.261	100 - 39.9 - 10.4 - 2.04 - 0.329
1.726.506.549	8.630.633.261	100 - 39.9 - 10.4 - 2.04 - 0.329
1.726.506.549	8.630.633.261	100 - 39.9 - 10.4 - 2.04 - 0.329
8.022.239.675	7.786.048.389	100 - 22.8 - 4.94 - 0.731
-1.480.719.457	8.332.409.642	100 - 27.5 - 10 - 2.02 - 0.361
-1.480.719.457	8.332.409.642	100 - 27.5 - 10 - 2.02 - 0.361
-1.480.719.457	8.332.409.642	100 - 27.5 - 10 - 2.02 - 0.361
-1.480.719.457	8.332.409.642	100 - 27.5 - 10 - 2.02 - 0.361
-4.705.949.144	728.212.774	100 - 26.2 - 9.06 - 1.74 - 0.28
1.485.857.441	8.270.237.267	100 - 17.9 - 2.74 - 0.299
1.485.857.441	8.270.237.267	100 - 17.9 - 2.74 - 0.299
2.384.745.986	6.952.247.037	100 - 33.5 - 8.52 - 1.6 - 0.255
-0.118742392	6.445.408.393	100 - 42.5 - 10.5 - 1.89 - 0.273
-9.130.519.889	7.386.928.233	100 - 26.8 - 7.14 - 1.27 - 0.208
-9.130.519.889	7.386.928.233	100 - 26.8 - 7.14 - 1.27 - 0.208
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
-3.453.916.598	6.710.130.002	100 - 35.8 - 10.5 - 2.24 - 0.414
141.926.193	7.747.896.643	100 - 19.4 - 8.15 - 1.3 - 0.231
276.353.559	6.579.736.483	100 - 39.8 - 9.99 - 1.87 - 0.287
276.353.559	6.579.736.483	100 - 39.8 - 9.99 - 1.87 - 0.287
276.353.559	6.579.736.483	100 - 39.8 - 9.99 - 1.87 - 0.287
141.926.193	7.747.896.643	100 - 19.4 - 8.15 - 1.3 - 0.231
276.353.559	6.579.736.483	100 - 39.8 - 9.99 - 1.87 - 0.287
276.353.559	6.579.736.483	100 - 39.8 - 9.99 - 1.87 - 0.287
276.353.559	6.579.736.483	100 - 39.8 - 9.99 - 1.87 - 0.287
-1.491.648.852	7.733.729.493	100 - 23 - 5.39 - 0.835 - 0.119
-1.905.963.047	6.445.408.393	100 - 42.5 - 10.5 - 1.89 - 0.273
6.388.584.759	6.822.276.909	100 - 35.6 - 9.02 - 1.71 - 0.27
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493

3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
3.167.556.779	6.444.456.546	100 - 40.1 - 11.9 - 2.64 - 0.493
8.175.820.239	6.822.276.909	100 - 35.6 - 9.02 - 1.71 - 0.27
1.874.704.691	7.792.469.931	100 - 24.3 - 3.64 - 0.408
1.874.704.691	7.792.469.931	100 - 24.3 - 3.64 - 0.408
4.186.559.156	9.310.047.107	100 - 7 - 0.414
8.175.820.239	6.822.276.909	100 - 35.6 - 9.02 - 1.71 - 0.27
-6.301.990.458	6.552.008.835	100 - 38 - 11.6 - 2.56 - 0.488
-1.854.540.535	771.190.327	100 - 24.7 - 4.37 - 0.578
-1.854.540.535	771.190.327	100 - 24.7 - 4.37 - 0.578
-1.854.540.535	771.190.327	100 - 24.7 - 4.37 - 0.578
-1.854.540.535	771.190.327	100 - 24.7 - 4.37 - 0.578
4.313.137.491	630.254.915	100 - 43.2 - 12.4 - 2.66 - 0.473
1.490.140.493	727.205.638	100 - 25.4 - 9.87 - 1.92 - 0.36
-9.839.207.154	6.770.611.539	100 - 33 - 11.6 - 2.61 - 0.484
-2.619.347.796	8.143.883.674	100 - 19.6 - 2.85 - 0.308
1.367.457.802	7.115.846.309	100 - 32.4 - 6.92 - 1.11 - 0.146
1.367.457.802	7.115.846.309	100 - 32.4 - 6.92 - 1.11 - 0.146
1.415.452.391	7.134.694.529	100 - 32.3 - 6.69 - 1.04 - 0.132
1.415.452.391	7.134.694.529	100 - 32.3 - 6.69 - 1.04 - 0.132
-1.061.683.198	6.771.559.477	100 - 37.8 - 8.37 - 1.37 - 0.18
-5.138.438.099	9.447.897.499	100 - 4.92 - 0.919
-5.138.438.099	9.447.897.499	100 - 4.92 - 0.919
-5.138.438.099	9.447.897.499	100 - 4.92 - 0.919
-5.138.438.099	9.447.897.499	100 - 4.92 - 0.919
-5.138.438.099	9.447.897.499	100 - 4.92 - 0.919
-1.061.683.198	6.771.559.477	100 - 37.8 - 8.37 - 1.37 - 0.18
-186.704.287	7.258.062.165	100 - 31.4 - 5.6 - 0.727
4.421.005.008	8.900.129.962	100 - 11.4 - 0.997
4.421.005.008	8.900.129.962	100 - 11.4 - 0.997
4.421.005.008	8.900.129.962	100 - 11.4 - 0.997
4.421.005.008	8.900.129.962	100 - 11.4 - 0.997
-186.704.287	7.258.062.165	100 - 31.4 - 5.6 - 0.727
4.421.005.008	8.900.129.962	100 - 11.4 - 0.997
4.421.005.008	8.900.129.962	100 - 11.4 - 0.997
4.421.005.008	8.900.129.962	100 - 11.4 - 0.997
4.421.005.008	8.900.129.962	100 - 11.4 - 0.997
2.054.858.767	7.369.698.317	100 - 28.2 - 6.3 - 1.03 - 0.143
2.054.858.767	7.369.698.317	100 - 28.2 - 6.3 - 1.03 - 0.143
8.856.224.752	632.120.445	100 - 44.1 - 11.5 - 2.23 - 0.349
8.856.224.752	632.120.445	100 - 44.1 - 11.5 - 2.23 - 0.349























184.533.574	6.915.731.428	100 - 34.4 - 8.41 - 1.54 - 0.234
184.533.574	6.915.731.428	100 - 34.4 - 8.41 - 1.54 - 0.234
3.247.836.587	7.885.945.044	100 - 22.9 - 3.53 - 0.408
3.247.836.587	7.885.945.044	100 - 22.9 - 3.53 - 0.408
-1.893.266.346	6.911.641.802	100 - 31.9 - 10.3 - 2.16 - 0.348



























<a href="http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0132847">http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0132847</a>
---

<a href="http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0132848">http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0132848</a>
---

<a href="http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0014722">http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0014722</a>
---

<a href="http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0015036">http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0015036</a>
---

<a href="http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0014624">http://nonlinear.com/redirect/outbound?p=hmdb&amp;param=HMDB0014624</a>
---

Description
Dide-O-methyl-4-O-alpha-D-glucopyranosylsimmondsin
Dide-O-methyl-4-O-alpha-D-glucopyranosylsimmondsin
Lacto-N-triaose
Lacto-N-triose I
N-Acetylgalactosaminyl lactose
Lacto-N-triaose
Lacto-N-triose I
N-Acetylgalactosaminyl lactose
6-[[6-(2-carboxyeth-1-en-1-yl)-4-methoxy-2H-1,3-benzodioxol-5-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid
3,4,5-trihydroxy-6-[[3-(6-hydroxy-7-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoyl]oxy]oxane-2-carboxylic acid
6-[[6-(2-carboxyeth-1-en-1-yl)-5-methoxy-2H-1,3-benzodioxol-4-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid
3,4,5-trihydroxy-6-[[3-(7-hydroxy-6-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoyl]oxy]oxane-2-carboxylic acid
6-[[6-(2-carboxyeth-1-en-1-yl)-4-methoxy-2H-1,3-benzodioxol-5-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid
3,4,5-trihydroxy-6-[[3-(6-hydroxy-7-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoyl]oxy]oxane-2-carboxylic acid
6-[[6-(2-carboxyeth-1-en-1-yl)-5-methoxy-2H-1,3-benzodioxol-4-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid
3,4,5-trihydroxy-6-[[3-(7-hydroxy-6-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-enoyl]oxy]oxane-2-carboxylic acid
SAICAR
SAICAR
Kuwanon J
Artonin C
3-(2,4-dihydroxyphenyl)-1-{3-[5-(2,4-dihydroxyphenyl)-6-(5-hydroxy-2,2-dimethyl-2H-chromene-6-carbonyl)-3-methoxy]prop-1-en-1-yl}propan-1-one
Methantheline
Mepenzolate
Kuwanon J
Artonin C
3-(2,4-dihydroxyphenyl)-1-{3-[5-(2,4-dihydroxyphenyl)-6-(5-hydroxy-2,2-dimethyl-2H-chromene-6-carbonyl)-3-methoxy]prop-1-en-1-yl}propan-1-one
Methantheline
Mepenzolate
3'-Sialyllactosamine
6'-Sialyllactosamine
3'-Sialyllactosamine
6'-Sialyllactosamine
Pentamidine
Pentamidine
Glycopyrrolate
Glycopyrrolate
Betaine
L-Valine
Vaporole
N-Methyl-alpha-aminoisobutyric acid
5-Aminopentanoic acid
Norvaline
Amyl Nitrite
Betaine
L-Valine
Vaporole
5-Methyltetrahydrofolic acid
Daunorubicin









6-{{6-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-2-(1-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-c
3,4,5-trihydroxy-6-{{5-hydroxy-2-[7-hydroxy-2-(1-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-6-yl]-4-ox
3,4,5-trihydroxy-6-{{7-hydroxy-2-[7-hydroxy-2-(1-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-6-yl]-4-ox
6-{{5,7-dihydroxy-2-[7-hydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromen-6-yl]-4-oxo-3,4-dihydro-2H-1-ben
3,4,5-trihydroxy-6-{{2-methyl-2-(4-methylpent-3-en-1-yl)-6-(5,6,7-trihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-
6-{{5,6-dihydroxy-2-[7-hydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromen-6-yl]-4-oxo-3,4-dihydro-2H-1-ben
6-{{6,7-dihydroxy-2-[7-hydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromen-6-yl]-4-oxo-3,4-dihydro-2H-1-ben
6-{{6-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-2-(5-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-c
3,4,5-trihydroxy-6-{{5-hydroxy-2-[7-hydroxy-2-(5-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-6-yl]-4-ox
3,4,5-trihydroxy-6-{{7-hydroxy-2-[7-hydroxy-2-(5-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-6-yl]-4-ox
3,4,5-trihydroxy-6-{{5-hydroxy-2-[7-hydroxy-2-[(3E)-5-hydroxy-4-methylpent-3-en-1-yl]-2-methyl-2H-chromen-6-yl]-
6-{{6-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-2-(2-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-c
3,4,5-trihydroxy-6-{{5-hydroxy-2-[7-hydroxy-2-(2-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-6-yl]-4-ox
3,4,5-trihydroxy-6-{{7-hydroxy-2-[7-hydroxy-2-(2-hydroxy-4-methylpent-3-en-1-yl)-2-methyl-2H-chromen-6-yl]-4-ox
6-{{6-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-2-[2-(3,3-dimethyloxiran-2-yl)ethyl]-2-methyl-2H-chr
6-[[2-{2-[2-(3,3-dimethyloxiran-2-yl)ethyl]-7-hydroxy-2-methyl-2H-chromen-6-yl]-5-hydroxy-4-oxo-3,4-dihydro-2H-1
6-[[2-{2-[2-(3,3-dimethyloxiran-2-yl)ethyl]-7-hydroxy-2-methyl-2H-chromen-6-yl]-7-hydroxy-4-oxo-3,4-dihydro-2H-1
6-{{10-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-5-methyl-5-(4-methylpent-3-en-1-yl)-3,6-dioxatricyclo
3,4,5-trihydroxy-6-{{5-hydroxy-2-[9-hydroxy-5-methyl-5-(4-methylpent-3-en-1-yl)-3,6-dioxatricyclo[5.4.0.0.0.0]und
3,4,5-trihydroxy-6-{{7-hydroxy-2-[9-hydroxy-5-methyl-5-(4-methylpent-3-en-1-yl)-3,6-dioxatricyclo[5.4.0.0.0.0]und
6-{{6-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-7-hydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-c
6-{{6-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-8-hydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-c
6-{{2-[7,8-dihydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromen-6-yl]-5-hydroxy-4-oxo-3,4-dihydro-2H-1-ben
6-{{2-[7,8-dihydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromen-6-yl]-7-hydroxy-4-oxo-3,4-dihydro-2H-1-ben
6-{{6-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-7-hydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-c
6-{{6-(5,7-dihydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)-5-hydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-c
6-{{2-[5,7-dihydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromen-6-yl]-5-hydroxy-4-oxo-3,4-dihydro-2H-1-ben
6-{{2-[5,7-dihydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromen-6-yl]-7-hydroxy-4-oxo-3,4-dihydro-2H-1-ben
Phaeophorbide b
5-Hydroxy-7,3',4'-trimethoxy-8-methylisoflavone 5-neohesperidoside
Egonol gentiobioside
5-Hydroxy-7,3',4'-trimethoxy-8-methylisoflavone 5-neohesperidoside
Egonol gentiobioside
Leukotriene A4
5-HEPE
Oxymesterone
12-HEPE
14,15-EpETE
15-HEPE
15-KETE
17,18-EpETE
5-KETE
11R-HEPE
18R-HEPE
12-KETE
Methyl [8]-Shogaol
(ent-7alpha)-7-Hydroxy-8(14),15-pimaradien-19-oic acid
Galanal A
Ineketone
Steviol

















6-({2-[5,7-dihydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromen-6-yl]-5-hydroxy-4-oxo-3,4-dihydro-2H-1-benzofuran-3-yl}oxy)propanoic acid
6-({2-[5,7-dihydroxy-2-methyl-2-(4-methylpent-3-en-1-yl)-2H-chromen-6-yl]-7-hydroxy-4-oxo-3,4-dihydro-2H-1-benzofuran-3-yl}oxy)propanoic acid
Enalapril
Remifentanyl
Raloxifene

m/z	Retention time (min)
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
4.370.683.986	7.829.883.333
643.229.098	4.278.953.333
643.229.098	4.278.953.333
643.229.098	4.278.953.333
3.411.981.874	3.803.535
3.411.981.874	3.803.535
643.229.098	4.278.953.333
643.229.098	4.278.953.333
643.229.098	4.278.953.333
3.411.981.874	3.803.535
3.411.981.874	3.803.535
6.152.230.062	3.899.876.667
6.152.230.062	3.899.876.667
6.152.230.062	3.899.876.667
6.152.230.062	3.899.876.667
3.411.981.874	3.803.535
3.411.981.874	3.803.535
3.411.981.874	3.803.535
3.411.981.874	3.803.535
1.180.890.398	232.965
1.180.890.398	232.965
1.180.890.398	232.965
1.180.890.398	232.965
1.180.890.398	232.965
1.180.890.398	232.965
1.180.890.398	232.965
1.180.890.398	232.965
1.180.890.398	232.965
1.180.890.398	232.965
4.821.732.969	2.838.971.667
5.101.826.561	3.181.826.667

5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
4.902.726.351	3.903.501.667
4.902.726.351	3.903.501.667
4.902.726.351	3.903.501.667
4.902.726.351	3.903.501.667
643.229.098	4.278.953.333
643.229.098	4.278.953.333
643.229.098	4.278.953.333
4.961.463.417	275.346
643.229.098	4.278.953.333
643.229.098	4.278.953.333
643.229.098	4.278.953.333
4.961.463.417	275.346
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
5.101.826.561	3.181.826.667
4.821.732.969	2.838.971.667
3.411.981.874	3.803.535
3.411.981.874	3.803.535
752.160.809	4.371.788.333
6.292.281.511	4.074.456.667
6.152.185.516	389.353
6.152.185.516	389.353
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
7.791.615.171	4.444.833.333
4.370.683.986	7.829.883.333
6.152.606.563	3.904.408.333
6.152.606.563	3.904.408.333
6.152.606.563	3.904.408.333
4.370.683.986	7.829.883.333
6.152.606.563	3.904.408.333
6.152.606.563	3.904.408.333
6.152.606.563	3.904.408.333
5.382.029.403	3.538.141.667
6.292.269.961	4.066.476.667
6.292.269.961	4.066.476.667
752.160.809	4.371.788.333

752.160.809	4.371.788.333
752.160.809	4.371.788.333
752.160.809	4.371.788.333
752.160.809	4.371.788.333
752.160.809	4.371.788.333
752.160.809	4.371.788.333
752.160.809	4.371.788.333
752.160.809	4.371.788.333
752.160.809	4.371.788.333
752.160.809	4.371.788.333
6.292.281.511	4.074.456.667
3.411.981.874	3.803.535
3.411.981.874	3.803.535
1.560.198.923	0.286783333
6.292.281.511	4.074.456.667
7.791.615.171	4.444.833.333
4.961.463.417	275.346
4.961.463.417	275.346
4.961.463.417	275.346
4.961.463.417	275.346
7.791.615.171	4.444.833.333
4.961.463.417	275.346
6.162.240.845	3.898.061.667
3.411.981.874	3.803.535
4.961.463.417	275.346
4.961.463.417	275.346
4.961.463.417	275.346
4.961.463.417	275.346
566.211.328	392.778
1.560.198.923	0.286783333
1.560.198.923	0.286783333
1.560.198.923	0.286783333
1.560.198.923	0.286783333
1.560.198.923	0.286783333
566.211.328	392.778
4.821.732.969	2.838.971.667
1.400.572.152	0.277583333
1.400.572.152	0.277583333
1.400.572.152	0.277583333
1.400.572.152	0.277583333
4.821.732.969	2.838.971.667
1.400.572.152	0.277583333
1.400.572.152	0.277583333
1.400.572.152	0.277583333
1.400.572.152	0.277583333
5.382.029.403	3.538.141.667
5.382.029.403	3.538.141.667
6.432.386.512	4.300.743.333
6.432.386.512	4.300.743.333























6.152.185.516	389.353
6.152.185.516	389.353
3.411.981.874	3.803.535
3.411.981.874	3.803.535
4.961.463.417	275.346