

Supplementary Material, Table 1: List of possible HMOs, their masses, retention times, and compositions

Mass (exp/1)	Mass (cal/2)	Mass Error (ppm)	RT (min)	Hex	Hex/Mac	Fuc	Nuc	Intensity	Total Intensity/HMO	% Abundance	Relative % Abundance	
1	635.227	635.227	0.910	31.52	2	0	0	1	15542941			
2	635.227	635.227	0.120	23.31	2	0	0	1	3297373			
3	636.247	636.248	0.750	27.77	2	0	2	0	121555			
4	636.248	636.248	0.500	24.41	2	0	2	0	138076			
5	636.248	636.248	0.810	21.06	2	0	2	0	4467743			
6	709.263	709.264	1.190	31.56	3	1	0	0	383842			
7	709.263	709.264	0.920	30.71	3	1	0	0	71457			
8	709.264	709.264	0.360	18.09	3	1	0	0	83774			
9	709.265	709.264	0.900	21.01	3	1	0	0	2874312			
10	709.265	709.264	1.800	31.51	3	1	0	0	6525444	68649025	22.22	41.87
11	750.290	750.291	0.140	16.84	2	0	0	0	135501			
12	781.285	781.285	0.750	28.88	2	0	1	0	422564			
13	855.322	855.322	1.360	22.22	3	1	1	0	71440			
14	855.321	855.322	0.770	31.02	3	1	1	0	67035			
15	855.322	855.322	0.540	19.78	3	1	1	0	24302818			
16	855.322	855.322	0.070	16.59	3	1	1	0	1761968			
17	855.322	855.322	0.150	15.09	3	1	1	0	251258			
18	855.323	855.322	0.270	24.59	3	1	1	0	25131	42397580	13.72	25.86
19	1000.341	1000.339	1.120	24.56	3	1	0	1	1835422			
20	1000.341	1000.339	2.020	30.66	3	1	0	1	13397574			
21	1001.378	1001.380	1.570	19.74	3	1	2	0	221006			
22	1001.380	1001.380	0.120	16.14	3	1	2	0	5766761			
23	1074.397	1074.396	0.320	27.28	4	2	0	0	3254245			
24	1074.396	1074.396	1.710	26.83	4	2	0	0	259112			
25	1074.399	1074.396	0.180	24.76	4	2	0	0	2144292			
26	1074.400	1074.396	3.850	23.91	4	2	0	0	3124071			
27	1074.400	1074.396	5.330	20.74	4	2	0	0	149504	8933224	2.89	5.45
28	1144.419	1144.417	1.220	32.91	3	1	1	1	162005			
29	1144.419	1144.417	1.580	29.78	3	1	1	1	1730208			
30	1144.419	1144.417	1.660	28.09	3	1	1	1	95741			
31	1144.420	1144.417	2.710	28.94	3	1	1	1	739462			
32	1220.467	1220.454	2.640	19.56	4	2	1	0	132091			
33	1220.468	1220.454	2.980	26.44	4	2	0	0	1234780			
34	1220.458	1220.454	3.140	25.34	4	2	1	0	242071			
35	1220.459	1220.454	4.200	20.76	4	2	1	0	3823837			
36	1220.460	1220.454	4.700	23.69	4	2	0	0	4857376	10272105	3.33	6.27
37	1365.492	1365.492	0.460	33.07	4	2	0	1	2421761			
38	1365.493	1365.492	0.820	31.49	4	2	0	1	12272269			
39	1366.512	1366.512	0.020	18.55	4	2	2	0	1438059			
40	1366.512	1366.512	0.240	26.04	4	2	2	0	375671			
41	1366.513	1366.512	0.600	17.90	4	2	2	0	451349			
42	1366.514	1366.512	1.110	19.62	4	2	2	0	521818			
43	1366.514	1366.512	1.550	26.89	4	2	2	0	174909			
44	1366.515	1366.512	1.990	23.41	4	2	2	0	243830			
45	1366.516	1366.512	2.140	21.64	4	2	2	0	3658893			
46	1366.520	1366.512	5.420	20.69	4	2	2	0	308599	11813876	3.82	7.21
47	1439.529	1439.528	0.520	27.41	5	3	0	0	1541034			
48	1439.530	1439.528	0.790	27.60	5	3	0	0	2394409			
49	1439.531	1439.528	1.560	29.26	5	3	0	0	504490	4444964	1.44	2.71
50	1511.552	1511.550	1.330	29.90	4	2	1	1	799112			
51	1511.552	1511.550	1.330	34.10	4	2	1	1	1649005			
52	1511.552	1511.550	1.450	32.74	4	2	1	1	538658			
53	1511.552	1511.550	1.650	28.90	4	2	1	1	3028840			
54	1511.552	1511.550	1.730	31.61	4	2	1	1	18088512			
55	1512.573	1512.570	1.730	25.46	4	2	3	0	352601			
56	1512.573	1512.570	1.860	18.32	4	2	3	0	539814			
57	1512.573	1512.570	2.060	19.52	4	2	3	0	1665028			
58	1512.574	1512.570	2.770	23.29	4	2	3	0	149446			
59	1585.589	1585.586	1.090	28.71	5	3	1	0	123867			
60	1585.589	1585.586	1.470	27.15	5	3	1	0	1034125			
61	1585.589	1585.586	1.600	26.07	5	3	1	0	2331095			
62	1585.589	1585.586	1.720	29.04	5	3	1	0	84584			
63	1585.589	1585.586	1.850	27.14	5	3	1	0	260977			
64	1585.590	1585.586	2.290	25.44	5	3	1	0	1440343			
65	1585.590	1585.586	2.480	23.34	5	3	1	0	403433			
66	1585.591	1585.586	2.990	24.70	5	3	1	0	3345441			
67	1585.591	1585.586	2.990	26.62	5	3	1	0	521363	9643428	3.12	5.88
68	1627.611	1627.607	1.810	29.44	4	2	2	1	1948912			
69	1627.611	1627.607	1.870	32.44	4	2	2	1	994091			
70	1658.634	1658.628	3.680	24.12	4	2	4	0	293881			
71	1730.626	1730.624	1.390	32.80	5	3	0	1	3094320			
72	1731.643	1731.644	0.840	26.95	5	3	2	0	131952			
73	1731.643	1731.644	0.780	27.49	5	3	2	0	123413			
74	1731.645	1731.644	0.480	21.71	5	3	2	0	184906			
75	1731.646	1731.644	1.050	26.81	5	3	2	0	615407			
76	1731.647	1731.644	1.390	24.89	5	3	2	0	2078025			
77	1731.648	1731.644	2.310	24.66	5	3	2	0	588272			
78	1731.649	1731.644	3.020	23.49	5	3	2	0	3945636			
79	1731.650	1731.644	3.540	20.54	5	3	2	0	124422	7799223	2.52	4.76
80	1804.661	1804.661	0.410	27.62	6	4	0	0	2165661			
81	1804.662	1804.661	1.020	28.98	6	4	0	0	489113			
82	1804.663	1804.661	1.180	29.43	6	4	0	0	200856			
83	1804.665	1804.661	2.560	29.73	6	4	0	0	47958			
84	1876.682	1876.682	0.170	33.60	5	3	1	1	435450			
85	1876.682	1876.682	0.380	29.55	5	3	1	1	137519			
86	1876.683	1876.682	0.590	32.51	5	3	1	1	676508			
87	1876.684	1876.682	1.120	31.12	5	3	1	1	1571989			
88	1877.705	1877.702	1.380	20.12	5	3	3	0	128644			
89	1877.705	1877.702	1.440	21.87	5	3	3	0	162902			
90	1877.705	1877.702	1.500	23.14	5	3	3	0	819140			
91	1877.705	1877.702	1.610	25.39	5	3	3	0	187966			
92	1877.706	1877.702	2.020	24.14	5	3	3	0	622577			
93	1877.706	1877.702	2.180	19.32	5	3	3	0	194413			
94	1877.707	1877.702	2.390	18.76	5	3	3	0	114208			
95	1877.707	1877.702	2.620	21.20	5	3	3	0	904241			
96	1877.712	1877.702	5.160	20.71	5	3	3	0	206536			
97	1877.715	1877.702	6.920	22.76	5	3	3	0	590918			
98	1950.720	1950.719	0.580	27.84	6	4	1	0	1010923			
99	1950.720	1950.719	0.830	27.21	6	4	1	0	1801486			
100	1950.721	1950.719	1.040	27.50	6	4	1	0	1229963			
101	1950.721	1950.719	1.440	27.63	6	4	1	0	168594			
102	1950.723	1950.719	2.220	26.61	6	4	1	0	1906334			
103	2022.741	2022.740	0.650	33.04	5	3	2	1	617970			
104	2022.742	2022.740	0.990	27.88	5	3	2	1	73015			
105	2022.742	2022.740	1.340	30.45	5	3	2	1	990479			
106	2022.743	2022.740	1.380	31.14	5	3	2	1	113477			
107	2022.743	2022.740	1.540	29.07	5	3	2	1	158412			
108	2022.740	2022.740	0.190	19.29	5	3	4	0	109187			
109	2023.763	2023.760	1.380	20.35	5	3	4	0	71895			
110	2023.765	2023.760	2.220	20.99	5	3	4	0	281045			
111	2023.775	2023.760	7.450	22.73	5	3	4	0	638091			
112	2095.757	2095.756	0.440	32.62	6	4	0	1	1274546			
113	2095.760	2095.756	1.970	32.66	6	4	0	1	161712			
114	2096.779	2096.776	1.110	27.89	6	4	2	0	83681			
115	2096.779	2096.776	1.350	27.31	6	4	2	0	410441			
116	2096.780	2096.776	1.670	25.84	6	4	2	0	145179			
117	2096.780	2096.776	1.910	25.41	6	4	2	0	336567			
118	2096.781	2096.776	2.160	26.74	6	4	2	0	152597			
119	2096.784	2096.776	1.850	24.65								