

## Appendix 3

### Tabulated Peak Data from m/z 191, 217 & 218

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-375: 2981.00 m

RT	ION	AREA	HEIGHT	PEAK ID
36.179	191	8107098	481781	23/3
38.350	191	4529121	231561	24/3
42.836	191	4545450	152415	25/3
45.700	191	1412083	79349	24/4
46.386	191	940065	58232	26/3
57.437	191	1340071	71755	27Ts
58.891	191	2877937	154747	27Tm
62.008	191	9596690	409110	28ab
63.387	191	5897756	246413	29ab
64.114	191	526881	27169	30d
65.077	191	618178	26327	29ba
66.143	191	7717813	394345	30ab
66.739	191	387981	19516	30ba
67.492	191	1240317	51819	31abS
69.381	191	3744495	182165	31abR
71.979	191	2069537	87698	32abS
72.494	191	1171053	51943	32abR
75.020	191	1945534	63452	33abS
75.729	191	1252787	42399	33abR
78.220	191	847415	24457	34abS
79.103	191	670129	16780	34abR
81.432	191	1123070	24824	35abS
82.518	191	720247	15246	35abR
49.991	217	19188184	1182597	27dbS
51.147	217	11916362	637483	27dbR
55.900	217	6133321	276014	29dbS
56.689	217	5740920	327992	27aaR
57.150	217	5437387	142423	29dbR
61.459	217	3214024	96653	29aaS
61.996	217	3957713	151916	29bbR
62.306	217	955264	39347	29bbS
63.282	217	4408535	171154	29aaR
55.894	218	1611510	71847	27bbR
56.098	218	2874755	149018	27bbS
59.144	218	1975220	107213	28bbR
59.542	218	1918064	81041	28bbS
61.984	218	2901390	121332	29bbR
62.301	218	1715036	63627	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-377: 2985.00 m

RT	ION	AREA	HEIGHT	PEAK ID
36.069	191	3473772	197440	23/3
38.253	191	1700902	97706	24/3
42.737	191	2124548	67912	25/3
45.618	191	765015	39636	24/4
46.307	191	345680	21690	26/3
57.371	191	568407	31089	27Ts
58.840	191	1230936	60016	27Tm
61.958	191	3929314	154105	28ab
63.360	191	2508839	109971	29ab
64.095	191	193219	11046	30d
65.065	191	259981	11731	29ba
66.116	191	3999478	183397	30ab
67.476	191	570565	24569	30ba
69.368	191	1693579	76006	31abS
69.759	191	1139077	47053	31abR
71.966	191	953978	37379	32abS
72.486	191	612180	23753	32abR
75.008	191	777983	26158	33abS
75.703	191	538082	17290	33abR
78.208	191	308796	9213	34abS
79.090	191	197004	5606	34abR
81.431	191	350609	8659	35abS
82.494	191	243210	5796	35abR
49.915	217	7062798	418015	27dbS
51.065	217	4393467	236486	27dbR
55.847	217	1997995	92369	29dbS
56.630	217	2190663	117169	27aaR
57.126	217	1878708	50418	29dbR
61.415	217	1220595	34777	29aaS
61.964	217	1557976	54603	29bbR
62.268	217	463366	15294	29bbS
63.255	217	1698125	55075	29aaR
55.842	218	524595	23823	27bbR
56.040	218	1108051	52644	27bbS
59.109	218	672344	36703	28bbR
59.500	218	626518	28213	28bbS
61.947	218	1035699	40709	29bbR
62.274	218	703682	23499	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)

Sample H-378: 2986.50 m

RT	ION	AREA	HEIGHT	PEAK ID
36.203	191	11362870	674557	23/3
38.358	191	6436770	322782	24/3
42.831	191	7212995	229247	25/3
45.709	191	2186440	108514	24/4
46.386	191	1323676	78076	26/3
57.463	191	1484232	75626	27Ts
58.899	191	2342368	120832	27Tm
62.023	191	3748043	150273	28ab
63.413	191	5542658	255701	29ab
64.149	191	392054	20970	30d
65.106	191	652144	25132	29ba
66.180	191	7725112	393597	30ab
67.518	191	1275792	54531	30ba
69.409	191	3511527	158151	31abS
69.795	191	2508734	107142	31abR
71.996	191	2056674	87281	32abS
72.510	191	1178613	51344	32abR
75.044	191	1665923	58803	33abS
75.751	191	1167576	39291	33abR
78.250	191	772457	22257	34abS
79.108	191	514164	14648	34abR
81.438	191	1229942	26322	35abS
82.518	191	654749	14365	35abR
50.007	217	19050432	1201032	27dbS
51.151	217	11608875	665206	27dbR
55.927	217	4285900	205592	29dbS
56.710	217	5686160	322178	27aaR
57.218	217	3129628	106896	29dbR
61.451	217	2637964	73905	29aaS
62.011	217	2745666	96803	29bbR
62.321	217	892756	33007	29bbS
63.308	217	3909584	150167	29aaR
55.927	218	1312247	55313	27bbR
56.114	218	2471282	131163	27bbS
59.174	218	1591050	92008	28bbR
59.553	218	1509395	65415	28bbS
62.006	218	2089051	83238	29bbR
62.327	218	1474640	50367	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-380: 2988.55 m

RT	ION	AREA	HEIGHT	PEAK ID
36.145	191	8603646	480630	23/3
38.311	191	3963672	205127	24/3
42.795	191	4432176	139958	25/3
45.674	191	1542321	85576	24/4
46.357	191	811915	47931	26/3
57.434	191	1314514	68801	27Ts
58.893	191	2245096	117262	27Tm
62.011	191	6962577	279616	28ab
63.395	191	5293659	246271	29ab
64.148	191	405623	20694	30d
65.106	191	603179	24513	29ba
66.163	191	8220085	417299	30ab
67.512	191	1209040	54621	30ba
69.404	191	3451200	155426	31abS
69.795	191	2500898	106247	31abR
71.996	191	1856843	77488	32abS
72.516	191	1139912	47405	32abR
75.032	191	1637162	55005	33abS
75.745	191	1107147	37110	33abR
78.232	191	797523	21529	34abS
79.114	191	548386	15072	34abR
81.449	191	1123547	23578	35abS
82.547	191	676088	14356	35abR
49.983	217	12863614	794412	27dbS
51.116	217	7711973	429255	27dbR
55.904	217	3297542	156489	29dbS
56.681	217	4034728	229486	27aaR
57.188	217	3287480	90046	29dbR
61.451	217	2071038	58131	29aaS
62.006	217	2727295	99028	29bbR
62.321	217	825725	31785	29bbS
63.302	217	3230871	117942	29aaR
55.904	218	939288	41606	27bbR
56.097	218	2050862	103981	27bbS
59.150	218	1312159	70647	28bbR
59.536	218	1419219	59705	28bbS
61.988	218	1846348	73987	29bbR
62.321	218	1406649	47318	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-383: 3000.00 m

RT	ION	AREA	HEIGHT	PEAK ID
36.162	191	11815400	688074	23/3
38.323	191	5757412	305011	24/3
42.889	191	8203597	258128	25/3
45.692	191	2156155	115580	24/4
46.375	191	1152107	71848	26/3
57.457	191	2253646	126158	27Ts
58.917	191	4968606	245330	27Tm
62.058	191	21254974	894481	28ab
63.436	191	10503484	466676	29ab
64.172	191	1022492	56080	30d
65.141	191	1241602	48253	29ba
66.210	191	18393072	999022	30ab
67.535	191	2824269	120269	30ba
69.830	191	4769333	216181	31abS
70.513	191	529807	27086	31abR
72.545	191	2665867	106777	32abS
75.062	191	2801536	93780	32abR
75.762	191	1859978	63533	33abS
78.267	191	1595444	46363	33abR
79.143	191	1221348	31927	34abS
81.473	191	1697100	37200	34abR
82.541	191	1081866	22381	35abS
33.009	217	20455300	1217508	35abR
51.151	217	14555747	821718	27dbS
52.114	217	4704206	234523	27dbR
56.108	217	4215321	175306	29dbS
57.212	217	6833698	187507	27aaR
59.174	217	2554912	124673	29dbR
62.052	217	6533484	258792	29aaS
62.350	217	1273585	48739	29bbR
63.331	217	6952390	298429	29bbS
55.933	218	1994797	92158	29aaR
56.120	218	3295888	175695	27bbR
59.174	218	2516150	139574	27bbS
59.565	218	2199951	99632	28bbR
62.035	218	4188373	173520	28bbS
62.356	218	2310974	78308	29bbR
69.439	191	6771428	324267	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-386: 3015.05 m

RT	ION	AREA	HEIGHT	PEAK ID
36.116	191	4593969	250980	23/3
38.270	191	2224545	116669	24/3
42.760	191	2817273	91845	25/3
45.639	191	1144312	61140	24/4
46.322	191	457472	27737	26/3
57.410	191	969458	55154	27Ts
58.876	191	1519896	76461	27Tm
62.017	191	11599582	494302	28ab
63.395	191	4160772	157471	29ab
64.137	191	334671	15535	30d
65.106	191	439081	16762	29ba
66.169	191	6003088	289155	30ab
67.518	191	856821	35663	30ba
69.409	191	2158689	94970	31abS
69.812	191	1613240	64884	31abR
72.025	191	1127656	43877	32abS
72.533	191	878434	31070	32abR
75.067	191	1038044	32347	33abS
75.756	191	658052	21589	33abR
78.255	191	481724	14109	34abS
79.131	191	347084	9623	34abR
81.461	191	556197	13111	35abS
82.512	191	375042	8448	35abR
49.942	217	8028121	458412	27dbS
51.087	217	5154981	288363	27dbR
55.875	217	2920320	131185	29dbS
56.663	217	3148416	163591	27aaR
57.177	217	2977734	75388	29dbR
61.457	217	1642058	48922	29aaS
62.011	217	2977333	119571	29bbR
62.315	217	620161	21759	29bbS
63.290	217	2655308	94680	29aaR
55.881	218	732097	32387	27bbR
56.067	218	1441688	77321	27bbS
59.139	218	1159799	60240	28bbR
59.530	218	1012972	44182	28bbS
61.988	218	1842271	75371	29bbR
62.303	218	1085464	36418	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-388: 3019.50 m

RT	ION	AREA	HEIGHT	PEAK ID
36.122	191	6500718	373954	23/3
38.294	191	3686077	182947	24/3
42.760	191	4729594	148128	25/3
45.651	191	1670572	94328	24/4
46.328	191	781687	42833	26/3
57.428	191	1623357	85494	27Ts
58.876	191	2543605	119984	27Tm
61.994	191	4158105	173882	28ab
63.401	191	5603074	248229	29ab
64.137	191	429360	21286	30d
65.118	191	529594	21932	29ba
66.180	191	9868251	494491	30ab
67.529	191	1357695	58151	30ba
69.421	191	3693310	167440	31abS
69.806	191	2604870	110440	31abR
72.025	191	2085190	83128	32abS
72.533	191	1211649	51638	32abR
75.061	191	2043163	65134	33abS
75.762	191	1434871	47172	33abR
78.279	191	1014455	28045	34abS
79.131	191	694907	17652	34abR
81.461	191	1223578	24864	35abS
82.524	191	708437	15617	35abR
49.960	217	13040248	781893	27dbS
51.098	217	8448656	442375	27dbR
55.898	217	4535086	198803	29dbS
56.675	217	5405368	283928	27aaR
57.194	217	4285764	114316	29dbR
61.457	217	2831161	86319	29aaS
62.006	217	2935089	99599	29bbR
62.327	217	974784	35469	29bbS
63.308	217	4352379	158274	29aaR
55.892	218	1209945	49923	27bbR
56.073	218	2344677	120072	27bbS
59.145	218	2208519	118074	28bbR
59.536	218	1808736	78576	28bbS
61.994	218	2328296	87952	29bbR
62.315	218	1672271	56732	29bbS



Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-390: 3021.90 m

RT	ION	AREA	HEIGHT	PEAK ID
36.174	191	13114404	807945	23/3
38.340	191	7465067	392796	24/3
42.819	191	9319288	280993	25/3
45.686	191	2986943	162935	24/4
46.363	191	1594861	92467	26/3
57.451	191	3023708	170074	27Ts
58.911	191	4451524	213212	27Tm
62.041	191	6641853	282938	28ab
63.430	191	10804019	495089	29ab
64.160	191	733672	36858	30d
65.141	191	1051141	42950	29ba
66.204	191	19734702	1034030	30ab
67.535	191	2458150	111607	30ba
69.439	191	6989486	327952	31abS
69.824	191	5136886	226584	31abR
72.025	191	4190807	176183	32abS
72.539	191	2746485	111957	32abR
75.067	191	3217308	110704	33abS
75.762	191	2260315	76567	33abR
78.261	191	1715626	47869	34abS
79.137	191	1130326	30385	34abR
81.461	191	1702062	38774	35abS
82.518	191	1102506	24209	35abR
50.001	217	24097876	1531818	27dbS
51.139	217	14986578	850376	27dbR
55.933	217	7508985	347891	29dbS
56.721	217	10654811	604111	27aaR
57.200	217	7521128	198778	29dbR
61.468	217	5115384	154108	29aaS
62.035	217	5349618	193875	29bbR
63.331	217	8684279	347723	29bbS
55.916	218	1970691	92225	29aaR
56.114	218	4291755	228401	27bbR
59.174	218	3663864	188458	27bbS
59.565	218	2906511	133491	28bbR
62.023	218	4257551	167097	28bbS
62.333	218	2936709	103855	29bbR
62.338	217	2015929	70662	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-391: 3023.00 m

RT	ION	AREA	HEIGHT	PEAK ID
36.186	191	11778751	667977	23/3
38.370	191	7059465	351092	24/3
42.906	191	7074615	220302	25/3
45.715	191	3250527	164955	24/4
46.410	191	1229326	71499	26/3
57.492	191	3662802	189017	27Ts
58.940	191	5271152	241889	27Tm
62.076	191	10129376	439137	28ab
63.454	191	12699451	553317	29ab
64.184	191	939808	46725	30d
65.159	191	1196815	48150	29ba
66.227	191	23433198	1232811	30ab
67.547	191	3237870	141742	30ba
69.444	191	8705472	404735	31abS
69.847	191	6893260	287138	31abR
72.043	191	5072200	208014	32abS
72.557	191	3547672	138613	32abR
75.073	191	4866032	161073	33abS
75.774	191	3321426	108080	33abR
78.261	191	2551892	68842	34abS
79.131	191	1845840	47475	34abR
81.461	191	3037882	65723	35abS
82.529	191	1994248	41838	35abR
50.030	217	29180362	1965181	27dbS
51.169	217	18261436	1030367	27dbR
55.956	217	10807819	474174	29dbS
56.733	217	11134557	615950	27aaR
57.253	217	11052386	306194	29dbR
61.503	217	6653910	194303	29aaS
62.064	217	6989068	266769	29bbR
62.379	217	2245117	84017	29bbS
63.360	217	11595036	473856	29aaR
55.939	218	3117254	127866	27bbR
56.143	218	5332299	289634	27bbS
59.197	218	4505050	241599	28bbR
59.577	218	3815032	171592	28bbS
62.035	218	5487921	235599	29bbR
62.373	218	3918837	129822	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-396: 3054.00 m

RT	ION	AREA	HEIGHT	PEAK ID
36.127	191	6883328	394209	23/3
38.288	191	3282484	161488	24/3
42.790	191	3017879	95752	25/3
45.651	191	1717475	92765	24/4
46.351	191	550469	31559	26/3
57.428	191	1330655	69572	27Ts
58.876	191	2579393	134268	27Tm
62.017	191	11245097	465684	28ab
63.401	191	7572843	331451	29ab
64.131	191	362817	19999	30d
65.106	191	499869	20132	29ba
66.169	191	10999978	525840	30ab
67.512	191	1073780	42441	30ba
69.404	191	4713821	199332	31abS
69.801	191	3500071	132145	31abR
72.002	191	2932060	103436	32abS
72.516	191	2041295	64630	32abR
75.032	191	2135042	58352	33abS
75.745	191	1230150	37727	33abR
78.232	191	1291138	34946	34abS
79.120	191	1034287	24199	34abR
81.438	191	1487815	30913	35abS
82.459	191	819387	17421	35abR
49.966	217	6958449	392813	27dbS
51.104	217	4743676	234338	27dbR
55.892	217	3293340	146435	29dbS
56.675	217	1996925	97644	27aaR
57.200	217	2906019	85891	29dbR
61.480	217	1677535	49262	29aaS
62.006	217	3171542	126805	29bbR
62.309	217	735349	29784	29bbS
63.302	217	2700067	90101	29aaR
55.892	218	965028	40259	27bbR
56.085	218	1622110	80235	27bbS
59.145	218	1186133	57131	28bbR
59.542	218	898772	39985	28bbS
61.988	218	2303722	95263	29bbR
62.315	218	1636233	51787	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-400: 3069.10 m

RT	ION	AREA	HEIGHT	PEAK ID
35.434	191	3418789	190549	23/3
37.594	191	2215785	102707	24/3
42.055	191	1790282	54536	25/3
44.916	191	2977463	154906	24/4
45.629	191	461604	25180	26/3
56.635	191	2240301	124660	27Ts
58.095	191	3473992	164309	27Tm
61.207	191	830381	34170	28ab
62.602	191	8876554	420693	29ab
63.356	191	464097	23355	30d
64.308	191	659836	29892	29ba
65.365	191	8844700	427777	30ab
66.714	191	1082016	48225	30ba
68.611	191	2817843	133065	31abS
68.997	191	2031953	93125	31abR
71.216	191	1617899	75393	32abS
71.718	191	1051977	48589	32abR
74.234	191	1187013	50826	33abS
74.953	191	853535	34737	33abR
77.434	191	1108896	42113	34abS
78.292	191	736809	28637	34abR
80.611	191	1344655	43609	35abS
81.667	191	815989	25008	35abR
49.214	217	5597645	277285	27dbS
50.358	217	3609122	172474	27dbR
54.609	217	2593297	95060	27aaS
55.105	217	2886177	122649	29dbS
55.911	217	1706361	84728	27aaR
56.431	217	2812486	71194	29dbR
60.646	217	1342886	36346	29aaS
61.213	217	1332819	45344	29bbR
61.545	217	750241	27849	29bbS
62.550	217	2129524	64211	29aaR
55.099	218	853175	36863	27bbR
55.315	218	1340505	62633	27bbS
58.369	218	979654	46961	28bbR
58.766	218	776556	31019	28bbS
61.207	218	1291290	54718	29bbR
61.534	218	1293690	43416	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-402: 3072.05 m

RT	ION	AREA	HEIGHT	PEAK ID
35.414	191	3738020	197774	23/3
37.563	191	1840455	91243	24/3
42.071	191	1702057	54761	25/3
44.902	191	2625853	127062	24/4
45.609	191	476327	21419	26/3
56.633	191	1348753	66813	27Ts
58.063	191	4094312	186276	27Tm
60.428	191	415144	16408	28ab
62.577	191	10668447	361351	29ab
64.282	191	479620	19727	30d
65.339	191	9370373	392916	29ba
65.946	191	496436	21165	30ab
68.573	191	3342344	139996	30ba
68.971	191	2502906	87814	31abS
69.648	191	488203	24301	31abR
71.680	191	889178	39017	32abS
74.196	191	1005160	36594	32abR
74.891	191	650909	23597	33abS
77.367	191	1029583	32050	33abR
78.214	191	714672	21294	34abS
80.508	191	1221699	31562	34abR
81.542	191	681431	17818	35abS
29.044	217	4531078	243131	35abR
50.344	217	4312940	207656	27dbS
51.325	217	1456620	65070	27dbR
54.910	217	773073	38629	27aaS
55.103	217	3628014	150923	29dbS
55.903	217	928811	46496	27aaR
56.417	217	2697788	82981	29dbR
60.656	217	858908	24700	29aaS
61.181	217	1114628	36582	29bbR
61.526	217	727691	26131	29bbS
62.542	217	1566682	43240	29aaR
55.097	218	1318591	47794	27bbR
55.302	218	1435246	64561	27bbS
58.361	218	675215	32073	28bbR
58.764	218	440839	20392	28bbS
61.181	218	1275264	45418	29bbR
61.520	218	1255419	41534	29bbS

Saturated Biomarker Peak Data (m/z 191 & 217/218)  
 Sample H-403: 3073.50 m

RT	ION	AREA	HEIGHT	PEAK ID
35.390	191	1775242	100761	23/3
37.546	191	1210174	55043	24/3
42.044	191	747937	23707	25/3
44.861	191	1475108	73439	24/4
45.580	191	193292	11207	26/3
56.586	191	994608	49341	27Ts
58.029	191	1269308	60854	27Tm
62.555	191	3136232	153877	29ab
63.294	191	124562	6880	30d
64.280	191	256908	11001	29ba
65.310	191	2769601	131188	30ab
66.659	191	333833	15402	30ba
68.560	191	834539	38726	31abS
68.945	191	618118	27417	31abR
71.144	191	448260	21581	32abS
71.659	191	299265	14826	32abR
74.175	191	239614	11859	33abS
74.877	191	201708	8655	33abR
77.346	191	288495	12049	34abS
78.210	191	180194	8270	34abR
80.467	191	370976	13783	35abS
81.486	191	155072	7808	35abR
49.158	217	1557346	77749	27dbS
50.303	217	1069369	51917	27dbR
54.558	217	597135	22608	27aaS
55.066	217	729926	31626	29dbS
55.860	217	370619	19648	27aaR
56.358	217	475321	16778	29dbR
60.642	217	251790	8448	29aaS
61.159	217	314822	11233	29bbR
61.474	217	184682	7216	29bbS
62.502	217	454255	14909	29aaR
55.037	218	219088	9290	27bbR
55.265	218	323964	18441	27bbS
58.332	218	162369	9493	28bbR
58.731	218	157553	6536	28bbS
61.159	218	301311	13140	29bbR
61.486	218	248102	10447	29bbS