LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111547.D
Acq On : 17 Dec 2018 19:03
Operator : JU/SJ
Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.516	67	73	83	rVB	469081	737702	5.26%	0.388%
2	3.152	175	181	190	rBV	154537	296958	2.12%	0.156%
3	4.416	390	396	404	rBV2	440213	619777	4.42%	0.326%
4	5.146	508	520	522	rBV2	668084	2203269	15.72%	1.158%
5	5.822	633	635	637	rVB	6275764	4395283	31.36%	2.311%
6	5.904	638	649	650	rVV	2608905	5998356	42.80%	3.153%
7	5.916	650	651	654	rVV2	1249378	1607018	11.47%	0.845%
8	5.951	655	657	658	rVB	1412179	947420	6.76%	0.498%
9	6.163	666	693	695	rVB	1365186	5502523	39.26%	2.893%
10	6.269	695	711	713	rBV	5479396	14015245	100.00%	7.368%
11	6.545	754	758	763	rBV3	873532	1376889	9.82%	0.724%
12	6.628	763	772	775	rBV4	397653	1085251	7.74%	0.570%
13	6.704	778	785	790	rBV2	1000960	2403730	17.15%	1.264%
14	6.798	794	801	804	rBV	3063518	5230478	37.32%	2.750%
15	6.910	816	820	823	rVB	2125824	2324076	16.58%	1.222%
16	7.016	831	838	840	rBV2	2441815	5332448	38.05%	2.803%
17	7.145	858	860	862	rVB	7575217	5339164	38.10%	2.807%
18	7.228	871	874	876	rVB	729976	819366	5.85%	0.431%
19	7.251	876	878	882	rBV3	464632	566532	4.04%	0.298%
20	7.281	882	883	890	rVB	414799	303246	2.16%	0.159%
21	7.428	894	908	909	rBV4	1589487	4721426	33.69%	2.482%
22	7.475	914	916	918	rVB	2154928	1506592	10.75%	0.792%
23	7.569	928	932	934	rBV	281470	399544	2.85%	0.210%
24	7.592	934	936	940	rVB3	246392	338656	2.42%	0.178%
25	7.763	940	965	967	rBV2	2672847	14000738	99.90%	7.360%
26	7.792	967	970	972	rBV	732802	461269	3.29%	0.242%
27	7.851	976	980	983	rBV3	359389	550208	3.93%	0.289%
28	7.922	986	992	995	rBV	2587523	3088712	22.04%	1.624%
29	7.957	995	998	1000	rBV	1955452	2001663	14.28%	1.052%
30	8.051	1013	1014	1016	rBV	581518	352167	2.51%	0.185%
31	8.081	1016	1019	1020	rVV2	1317722	1346368	9.61%	0.708%
32	8.098	1020	1022	1024	rVB	713323	625305	4.46%	0.329%
33	8.363	1061	1067	1069	rBV4	4287432	8941057	63.80%	4.700%
34	8.381	1069	1070	1074	rVB2	8610550	6925123	49.41%	3.640%

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Misc :
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Instrument : BNA_F
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	8.469	1080	1085	1089	rVB	983199	1618098	11.55%	0.851%
36	8.522	1089	1094	1096	rBV2	1140089	1279706	9.13%	0.673%
37	8.569	1096	1102	1103	rBV2	1071474	1476243	10.53%	0.776%
38	8.598	1103	1107	1109	rVB	1396861	1431086	10.21%	0.752%
39	8.651	1109	1116	1120	rBV2	3501574	5843266	41.69%	3.072%
40	8.751	1126	1133	1135	rVB	1579886	2244792	16.02%	1.180%
41	8.781	1135	1138	1139	rBV	301800	278274	1.99%	0.146%
42	8.810	1139	1143	1148	rVB2	1003043	1245846	8.89%	0.655%
43	8.857	1148	1151	1154	rBV3	1538521	1927336	13.75%	1.013%
44	8.892	1154	1157	1163	rVV2	1051431	1538746	10.98%	0.809%
45	8.963	1166	1169	1173	rVB2	1014626	861891	6.15%	0.453%
46	9.016	1173	1178	1180	rBV2	1035700	1182604	8.44%	0.622%
47	9.075	1185	1188	1190	rVV2	620599	742842	5.30%	0.391%
48	9.104	1190	1193	1194	rVV	1288478	1204135	8.59%	0.633%
49	9.122	1194	1196	1198	rVV	897228	700556	5.00%	0.368%
50	9.157	1198	1202	1205	rVV	2475125	2496204	17.81%	1.312%
51	9.181	1205	1206	1211	rVB3	419529	308312	2.20%	0.162%
52	9.286	1219	1224	1225	rBV3	700310	876926	6.26%	0.461%
53	9.304	1225	1227	1229	rVV2	1291859	1263530	9.02%	0.664%
54	9.328	1229	1231	1232	rVV2	1094340	985369	7.03%	0.518%
55	9.351	1232	1235	1237	rVV2	1831363	2171628	15.49%	1.142%
56	9.386	1239	1241	1245	rVV2	1327682	1734569	12.38%	0.912%
57	9.428	1245	1248	1250	rVV2	768599	1092214	7.79%	0.574%
58	9.469	1251	1255	1259	rVV2	2548975	3496915	24.95%	1.838%
59	9.528	1262	1265	1267	rVV3	281238	338130	2.41%	0.178%
60	9.569	1267	1272	1274	rVV3	1884028	2273657	16.22%	1.195%
61	9.592	1274	1276	1278	rVV	892896	900669	6.43%	0.473%
62	9.628	1278	1282	1284	rVV5	1380776	1884513	13.45%	0.991%
63	9.657	1284	1287	1289	rVV	1717002	1605548	11.46%	0.844%
64	9.686	1289	1292	1293	rVV	1381343	1633839	11.66%	0.859%
65	9.710	1294	1296	1299	rVV2	2139770	2311008	16.49%	1.215%
66	9.757	1301	1304	1306	rVV	1545836	1676043	11.96%	0.881%
67	9.792	1308	1310	1313	rVV2	961857	1173180	8.37%	0.617%
68	9.833	1314	1317	1320	rVB2	1946907	1755715	12.53%	0.923%
69	9.922	1328	1332	1337	rBV5	491205	807427	5.76%	0.424%
70	10.010	1344	1347	1348	rVV2	399544	432729	3.09%	0.227%
71	10.039	1348	1352	1356	rVV	1071847	1371727	9.79%	0.721%

LSC Area Percent Report

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Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	10.086	1358	1360	1363	rVV4	403691	487544	3.48%	0.256%
73	10.139	1366	1369	1371	rVV	301063	274763	1.96%	0.144%
74	10.216	1379	1382	1384	rBV4	400294	512836	3.66%	0.270%
75	10.257	1384	1389	1390	rBV2	1278544	1811334	12.92%	0.952%
76	10.345	1401	1404	1406	rBV3	665226	726114	5.18%	0.382%
77	10.369	1406	1408	1411	rVB2	738118	634449	4.53%	0.334%
78	10.433	1417	1419	1423	rVB	337494	332515	2.37%	0.175%
79	10.622	1448	1451	1455	rVB2	402874	358986	2.56%	0.189%
80	10.698	1460	1464	1471	rVB9	175544	373611	2.67%	0.196%
81	10.957	1496	1508	1512	rBV2	1511526	4526217	32.29%	2.379%
82	11.004	1512	1516	1520	rVB5	309326	415495	2.96%	0.218%
83	11.310	1565	1568	1574	rVB	1648176	1687687	12.04%	0.887%
84	11.857	1656	1661	1670	rVV2	2218897	2392311	17.07%	1.258%
85	11.927	1670	1673	1678	rVB2	209049	257422	1.84%	0.135%
86	12.104	1700	1703	1706	rBV	287918	284328	2.03%	0.149%
87	12.145	1707	1710	1714	rVV5	252457	402610	2.87%	0.212%
88	12.204	1717	1720	1723	rVB	346226	332893	2.38%	0.175%
89	12.633	1790	1793	1810	rVB2	1495730	2022437	14.43%	1.063%
90	13.792	1987	1990	2001	rVB2	664922	859037	6.13%	0.452%
91	13.945	2012	2016	2026	rVB	1285245	1143034	8.16%	0.601%
92	14.116	2042	2045	2048	rBV	533435	438631	3.13%	0.231%
93	14.421	2093	2097	2101	rVB	941806	853252	6.09%	0.449%
94	14.721	2144	2148	2157	rVB	1195050	1155886	8.25%	0.608%
95	15.045	2199	2203	2210	rVB	1055687	1220114	8.71%	0.641%
96	15.380	2256	2260	2263	rBV	886242	1119246	7.99%	0.588%
97	15.415	2263	2266	2272	rVB	1002656	1183192	8.44%	0.622%
98	15.839	2332	2338	2343	rBV	638834	949397	6.77%	0.499%
99	16.327	2415	2421	2434	rVB2	357525	683964	4.88%	0.360%
100	16.892	2512	2517	2526	rVB2	131058	260096	1.86%	0.137%

Sum of corrected areas: 190228233

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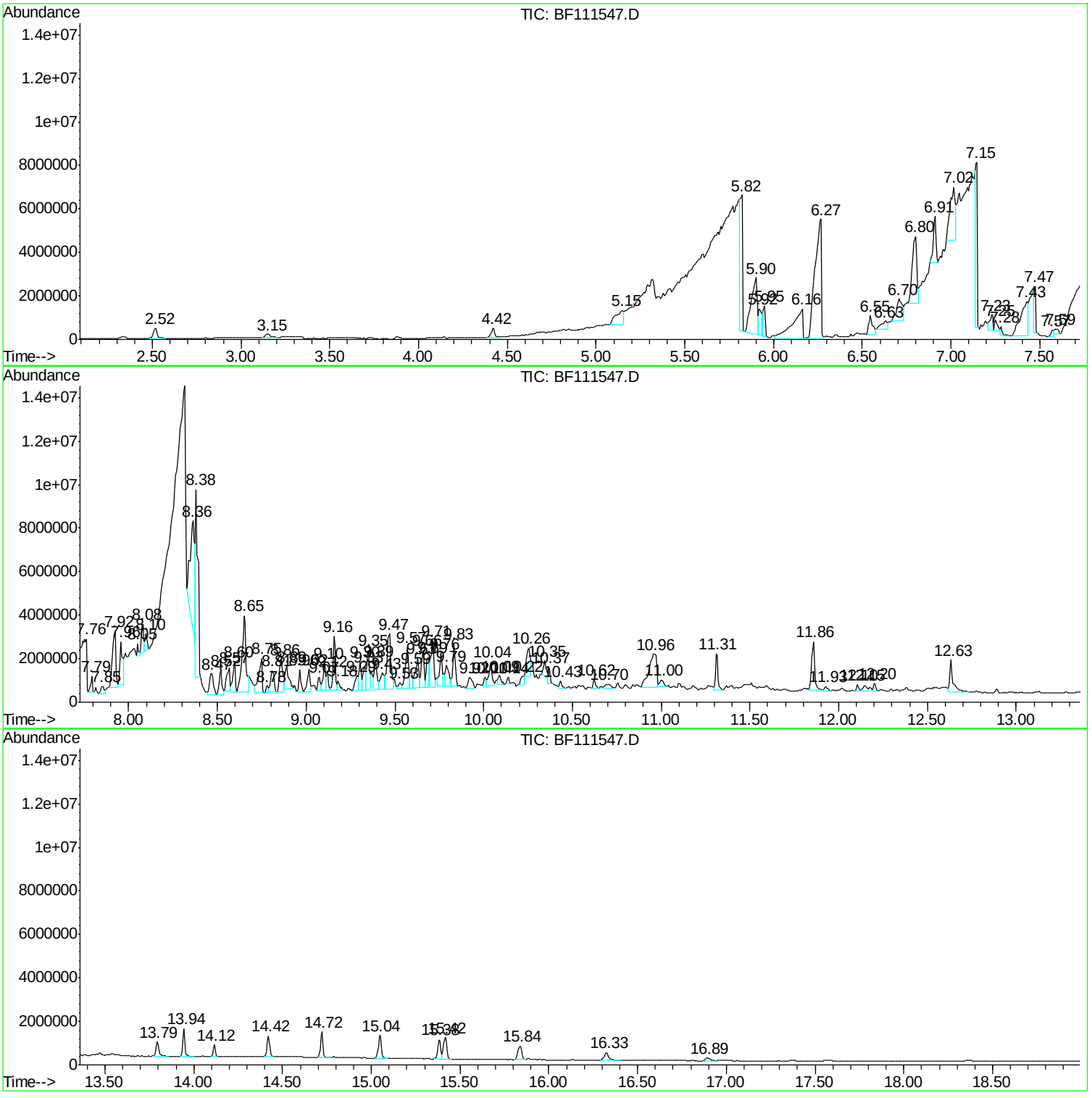
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument : BNA_F
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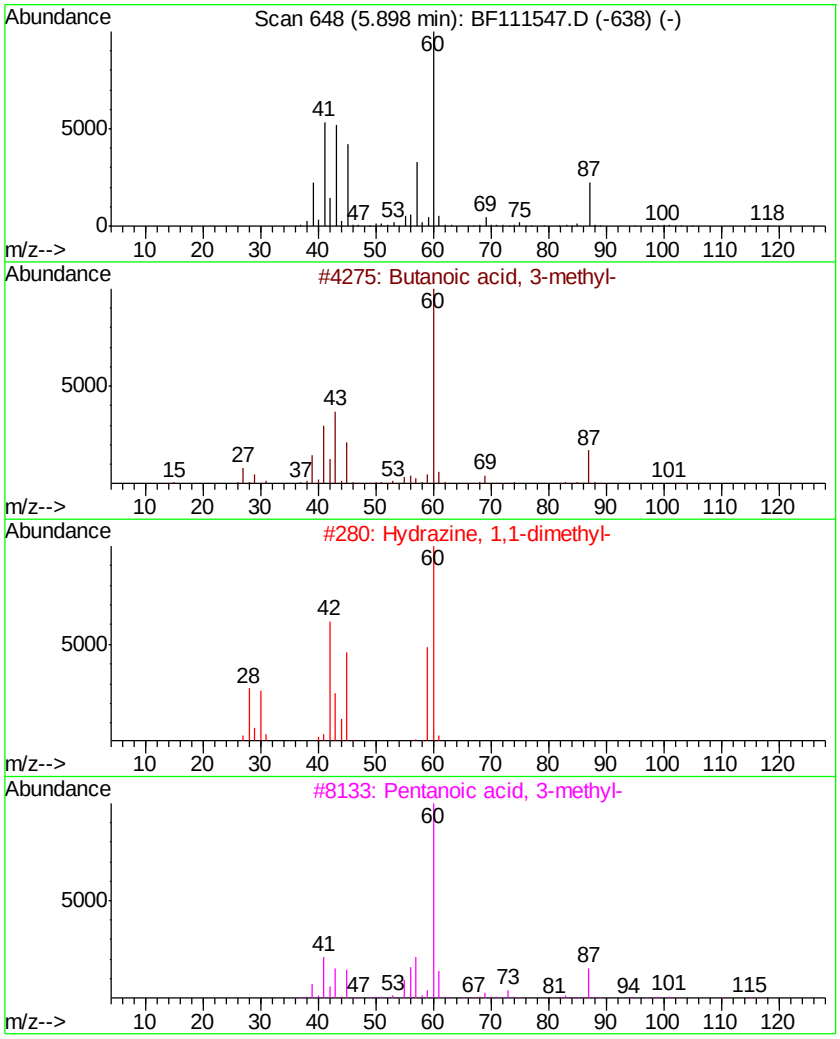
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

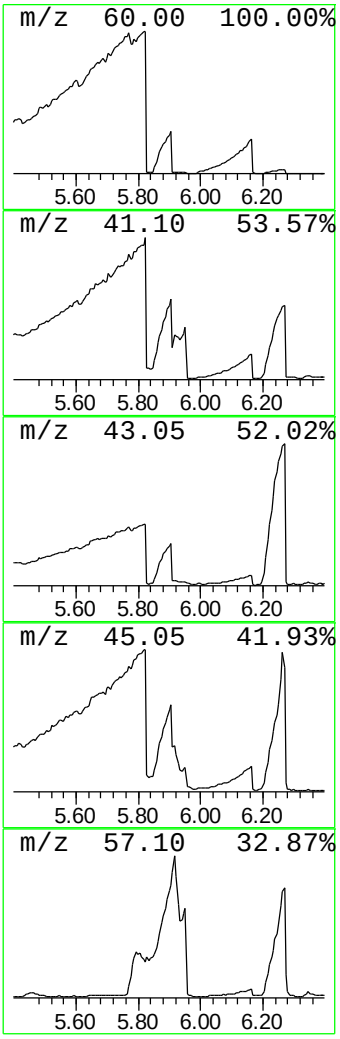
****

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.90	22.94 ng	5998360	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
2	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	53
3	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43
4	Pentanoic acid	102	C5H10O2	000109-52-4	40
5	Heptanoic acid	130	C7H14O2	000111-14-8	33





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

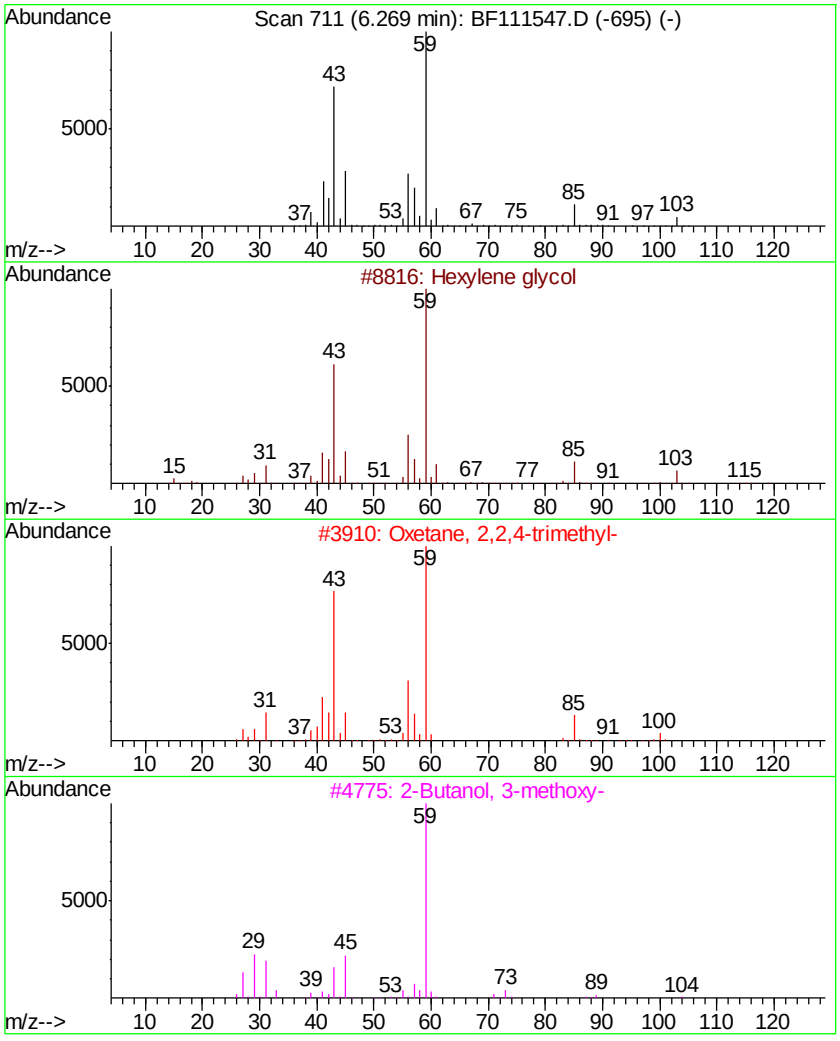
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

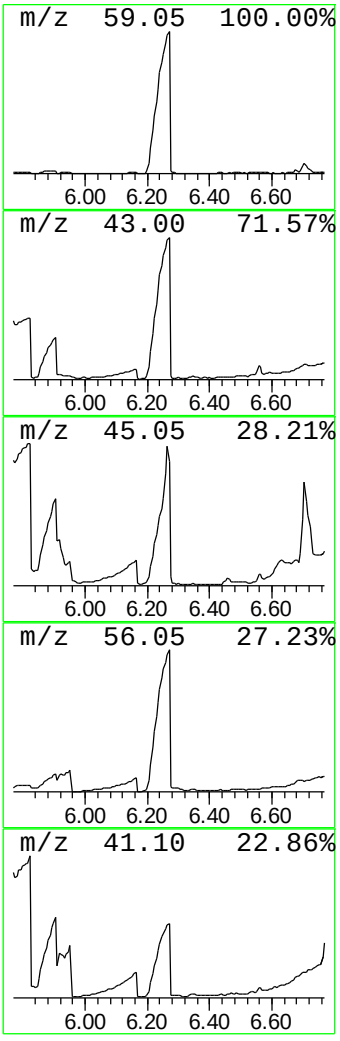
****

Peak Number 2 Hexylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	53.59 ng	14015200	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	83
2	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	72
3	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	50
4	N,N-Dimethylformamide-di-t-butyl...	203	C11H25NO2	036805-97-7	45
5	dl-Erythro-O-methylthreonine	133	C5H11NO3	1000214-70-7	45





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ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
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TIC Library : C:\DATABASE\NIST11.L
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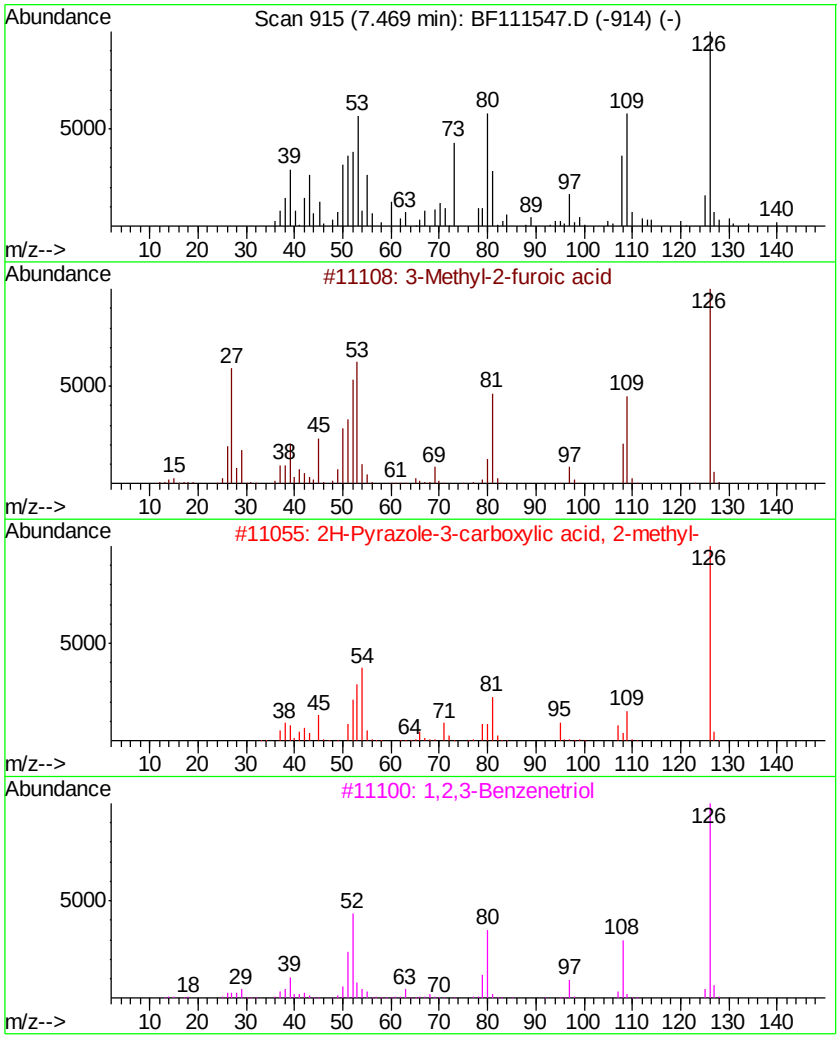
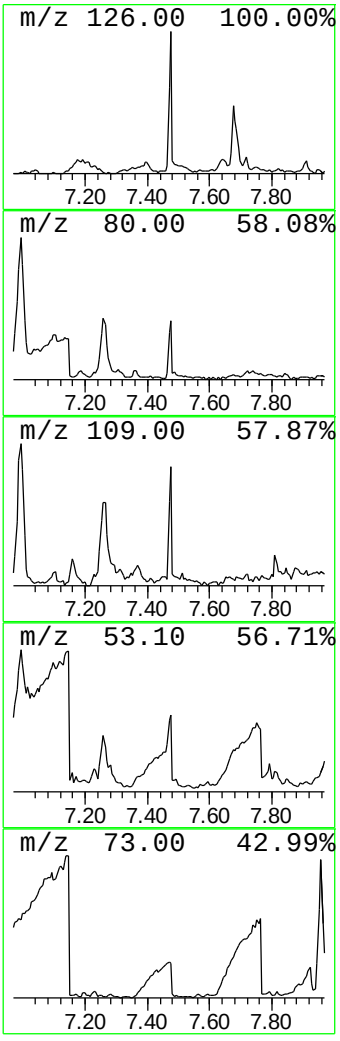
Peak Number 3 3-Methyl-2-furoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	22.38 ng	1506590	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-2-furoic acid	126	C6H6O3	004412-96-8	64
2	2H-Pyrazole-3-carboxylic acid, 2...	126	C5H6N2O2	1000304-39-7	50
3	1,2,3-Benzenetriol	126	C6H6O3	000087-66-1	25
4	1,3,5-Benzenetriol	126	C6H6O3	000108-73-6	22
5	Pyrazine, methoxy-, 4-oxide	126	C5H6N2O2	023902-69-4	12





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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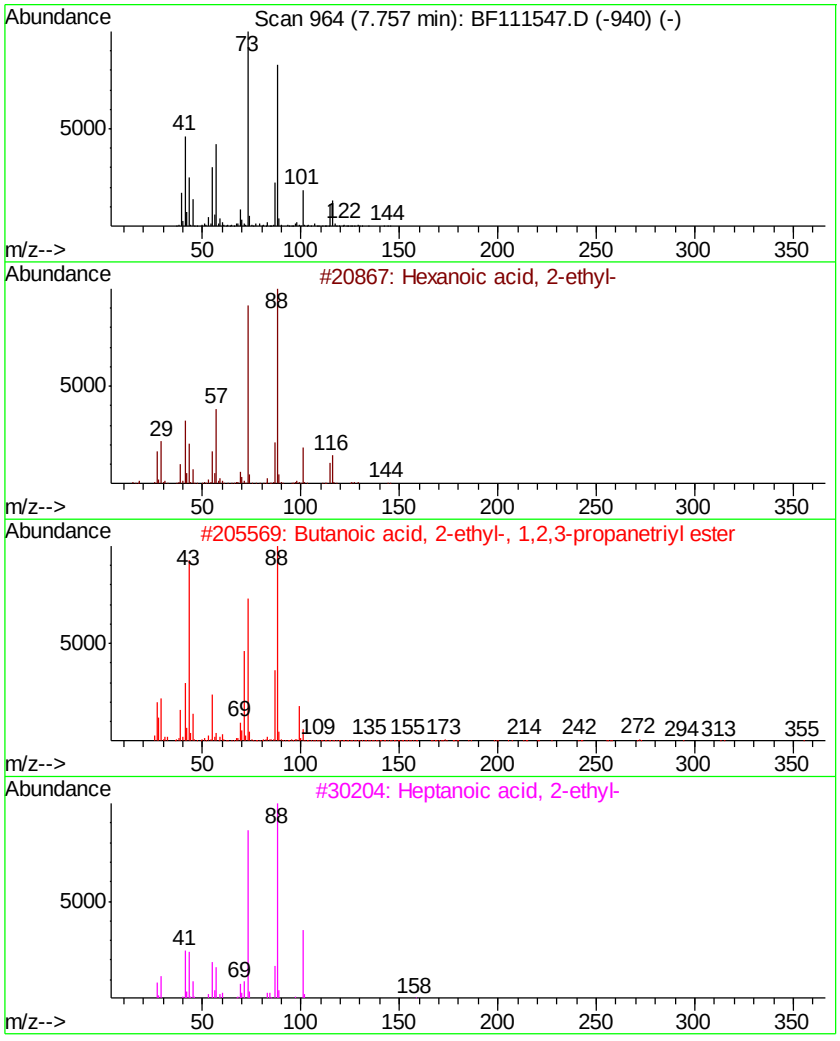
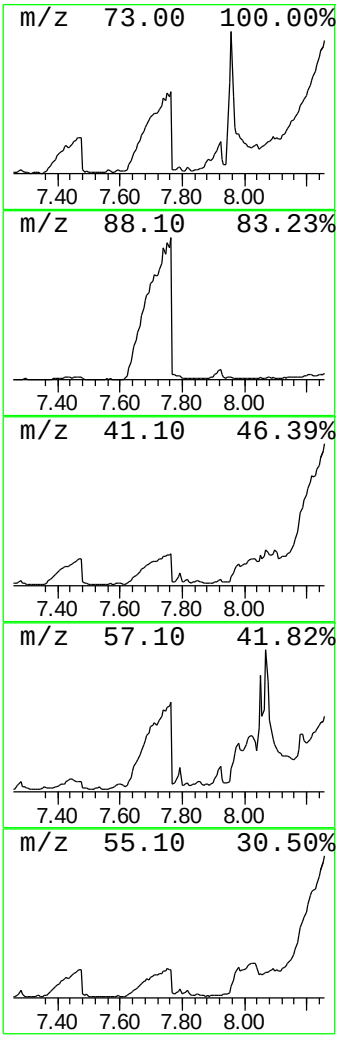
Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.76	207.98 ng	14000700	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
4	1,4-Dioxane	88	C4H8O2	000123-91-1	47
5	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	40





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111547.D
Acq On : 17 Dec 2018 19:03
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Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

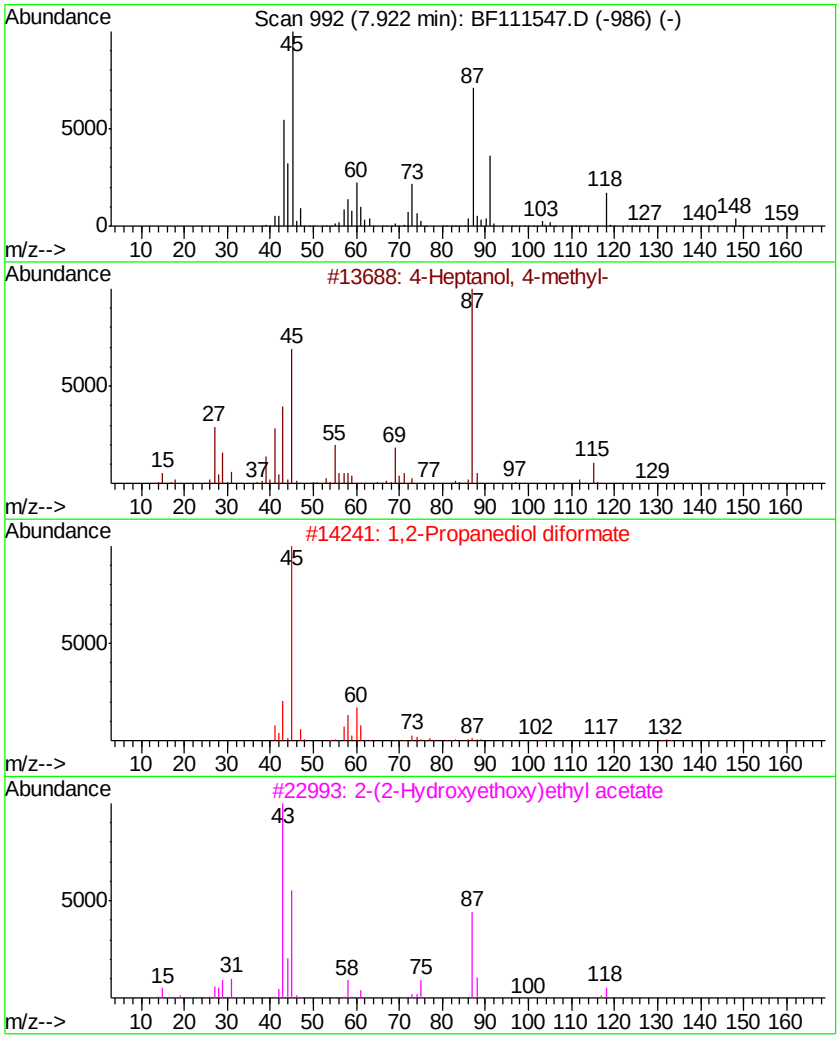
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

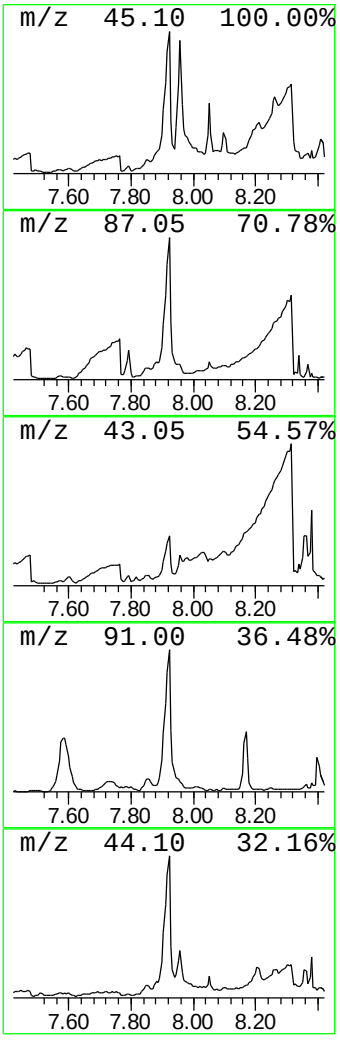
****

Peak Number 5 unknown7.92 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.92	45.88 ng	3088710	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 4-methyl-	130	C8H18O	000598-01-6	43
2	1,2-Propanediol diformate	132	C5H8O4	053818-14-7	43
3	2-(2-Hydroxyethoxy)ethyl acetate	148	C6H12O4	1000351-92-4	42
4	1-(2-Hydroxyethoxy)-2-(vinylthio...	148	C6H12O2S	086241-10-3	38
5	Propane, 1,1'-[ethylidenebis(oxy...	146	C8H18O2	000105-82-8	38





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Acq On : 17 Dec 2018 19:03
Operator : JU/SJ
Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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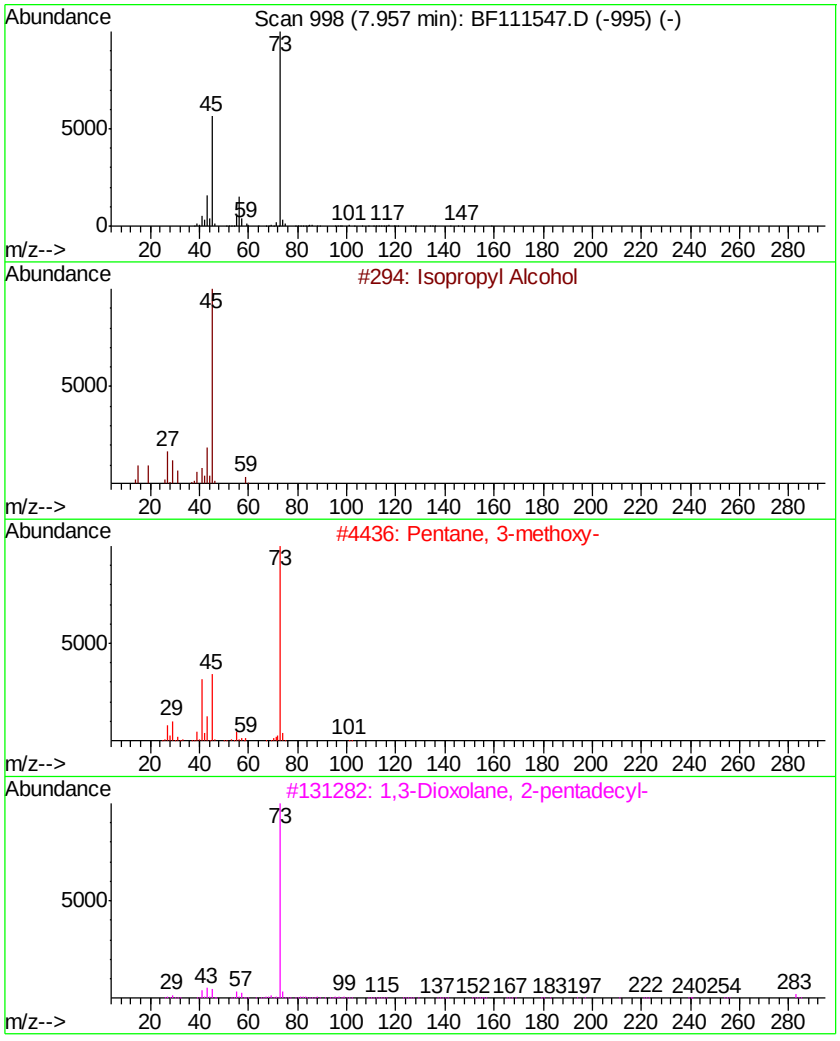
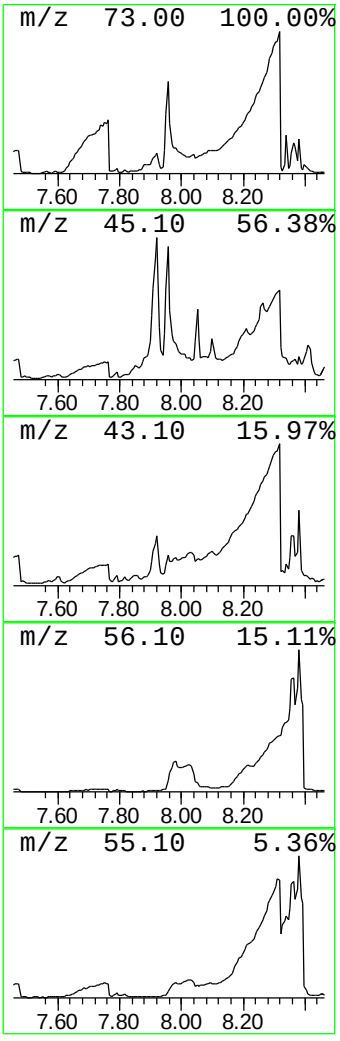
Peak Number 6 unknown7.96 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.96	29.73 ng	2001660	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	38
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
3	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	10
4	Butane, 1-methoxy-	88	C5H12O	000628-28-4	9
5	2-Octanol, (R)-	130	C8H18O	005978-70-1	9





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Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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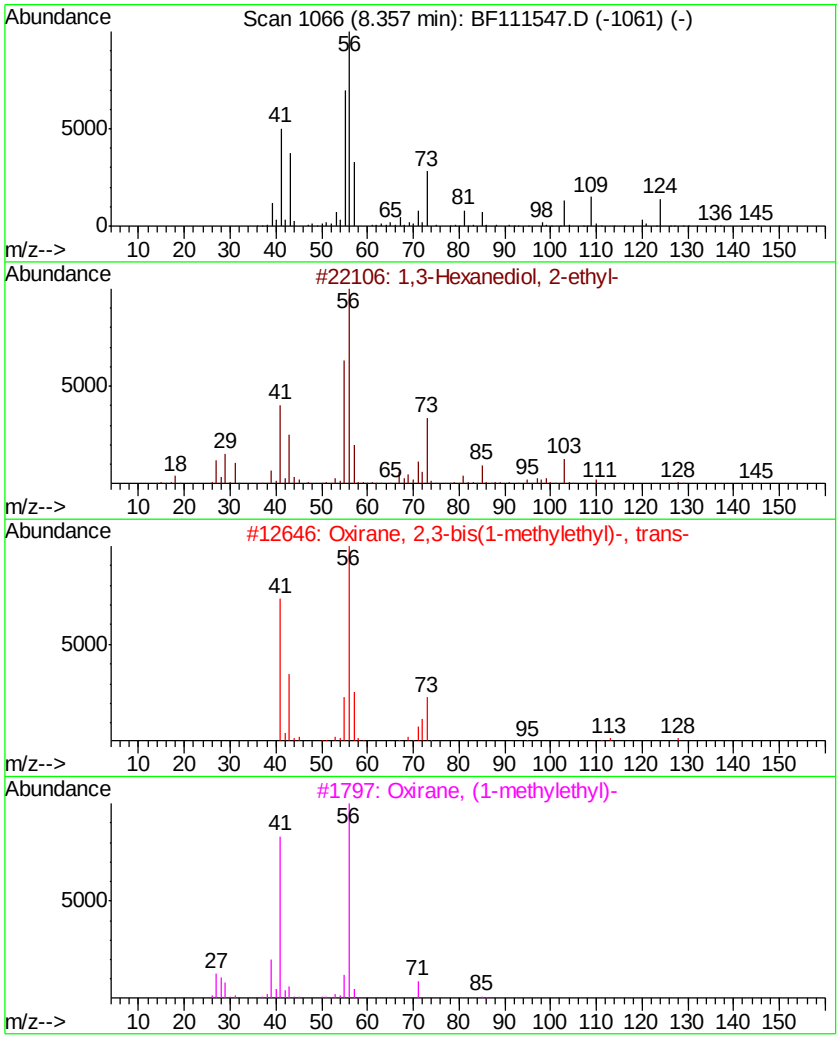
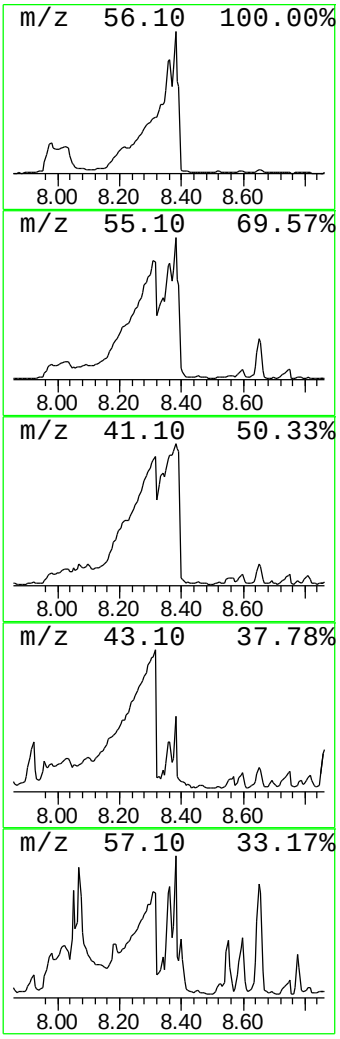
Peak Number 7 1,3-Hexanediol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.36	132.82 ng	8941060	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	56
2	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	53
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	47
4	Neopentyl glycol	104	C5H12O2	000126-30-7	38
5	Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	33





Library Search Compound Report

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Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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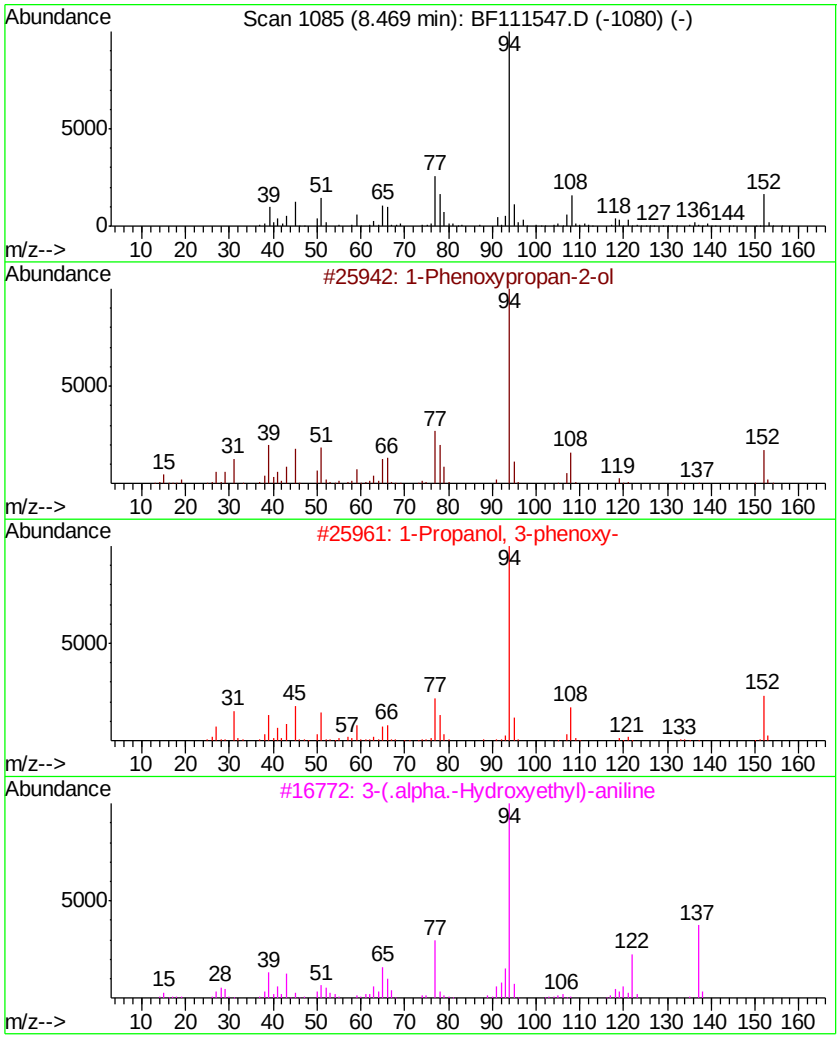
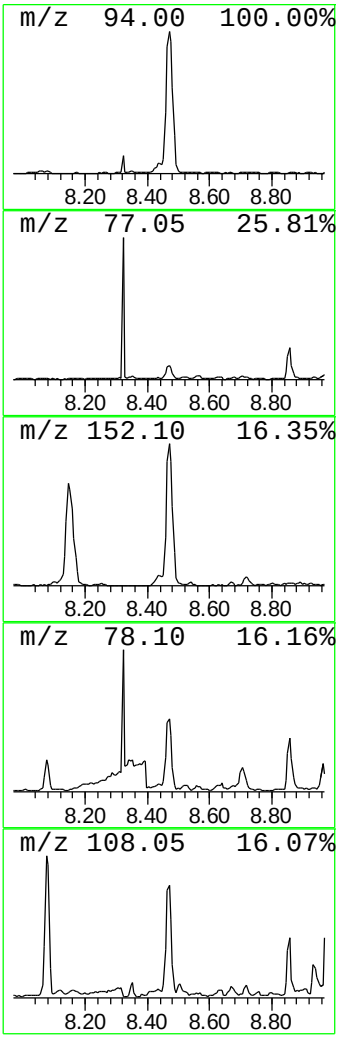
Peak Number 9 1-Phenoxypropan-2-ol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	24.04 ng	1618100	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	90
3	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5	Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	50





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Operator : JU/SJ
Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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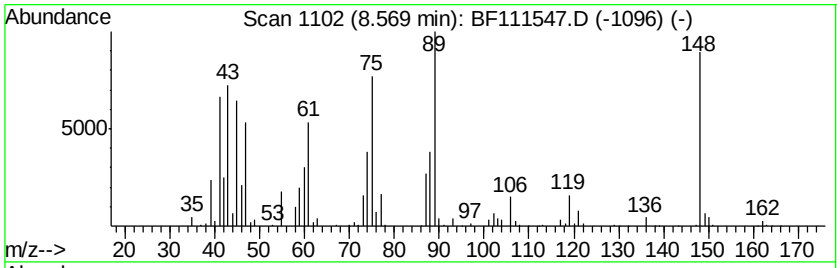
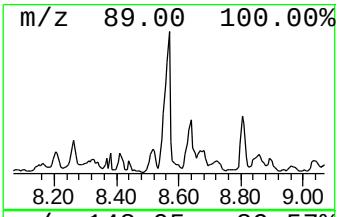
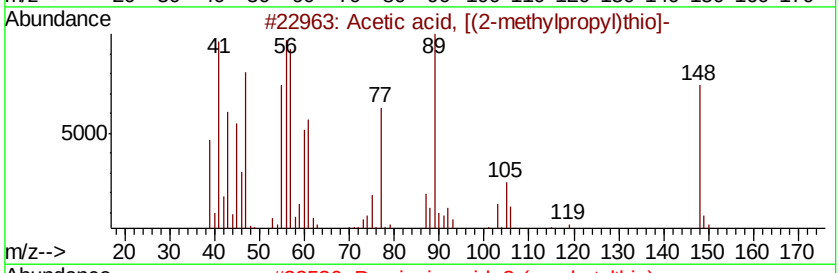
Peak Number 10 Acetic acid, [(2-methylprop... Concentration Rank 20

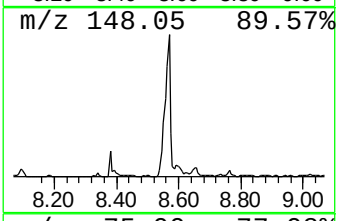
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.57	21.93 ng	1476240	Naphthalene-d8	8.08

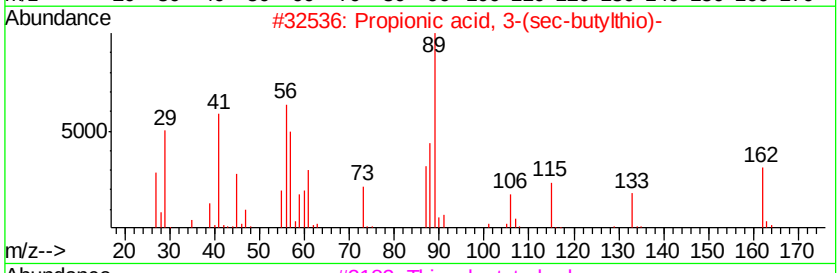
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, [(2-methylpropyl)th...	148	C6H12O2S	020600-62-8	58
2	Propionic acid, 3-(sec-butylthio)-	162	C7H14O2S	024383-15-1	47
3	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	43
4	Acetic acid, (butylthio)-	148	C6H12O2S	020600-61-7	40
5	N-Formyl-beta-alanine	117	C4H7NO3	014565-43-6	37

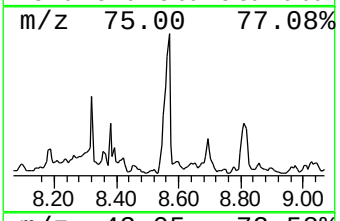


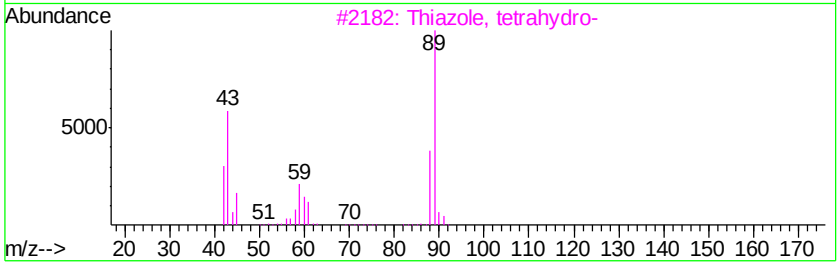


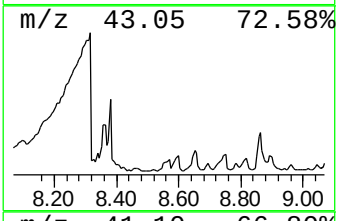


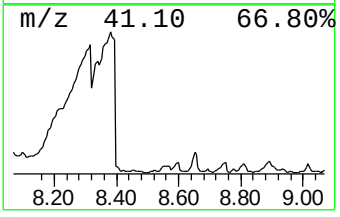












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Acq On : 17 Dec 2018 19:03
Operator : JU/SJ
Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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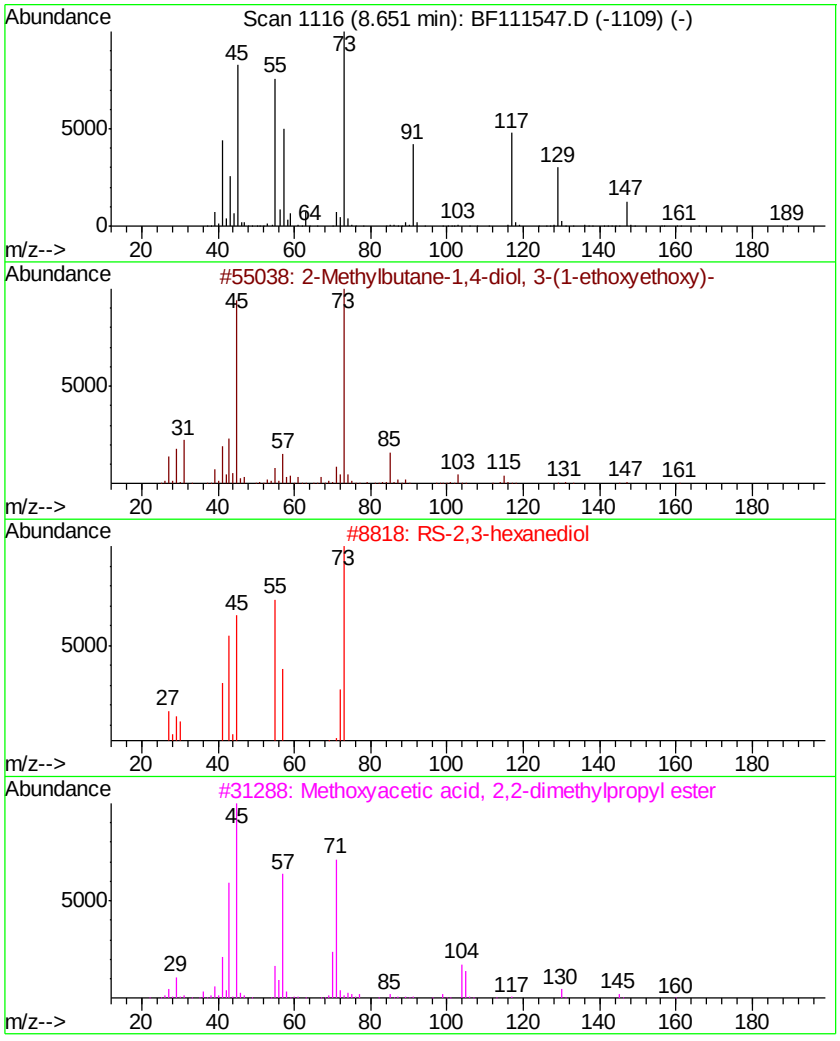
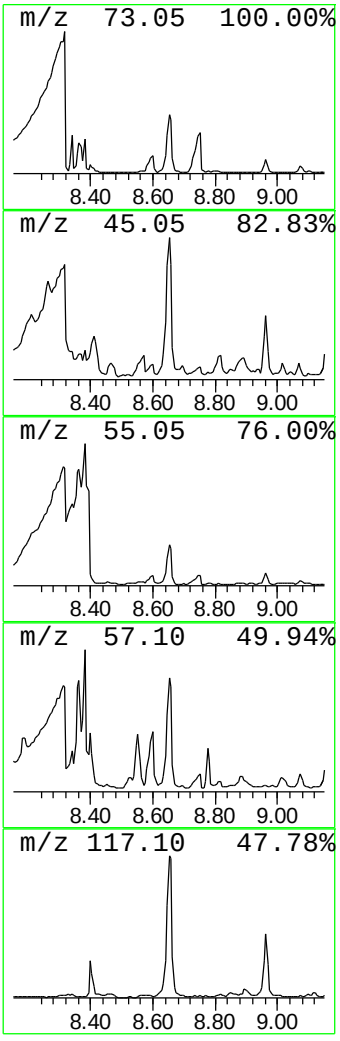
Peak Number 11 unknown8.65 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	86.80 ng	5843270	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylbutane-1,4-diol, 3-(1-et...	192	C9H20O4	088481-54-3	43
2	RS-2,3-hexanediol	118	C6H14O2	082360-67-6	38
3	Methoxyacetic acid, 2,2-dimethyl...	160	C8H16O3	1000282-41-0	27
4	Oxiraneethanol, .beta.-(1-ethoxy...	176	C8H16O4	109613-58-3	25
5	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	22





Library Search Compound Report

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Operator : JU/SJ
Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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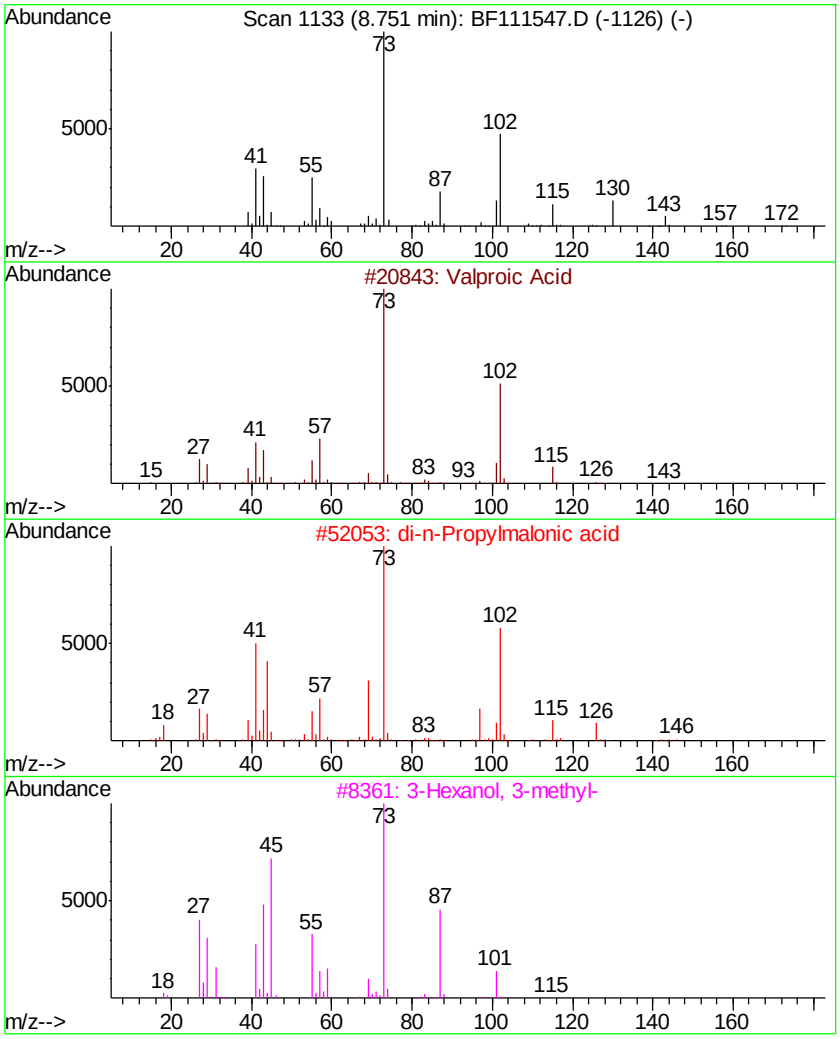
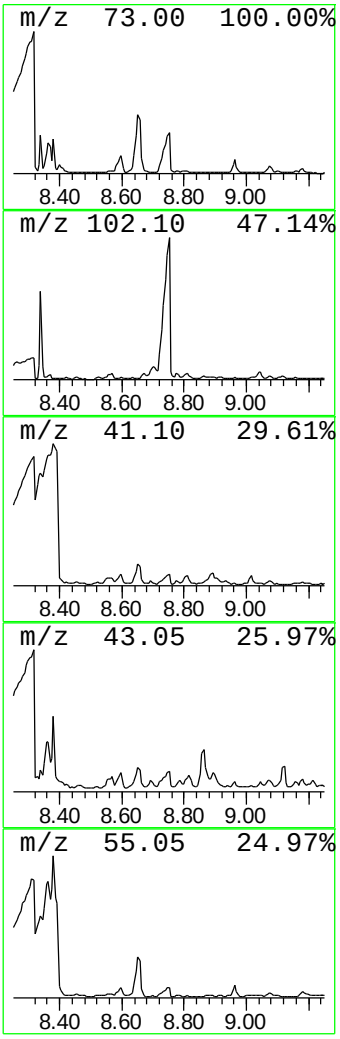
Peak Number 12 Valproic Acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.75	33.35 ng	2244790	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Valproic Acid	144	C8H16O2	000099-66-1	53
2	di-n-Propylmalonic acid	188	C9H16O4	001636-27-7	40
3	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	12
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	10
5	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	10





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Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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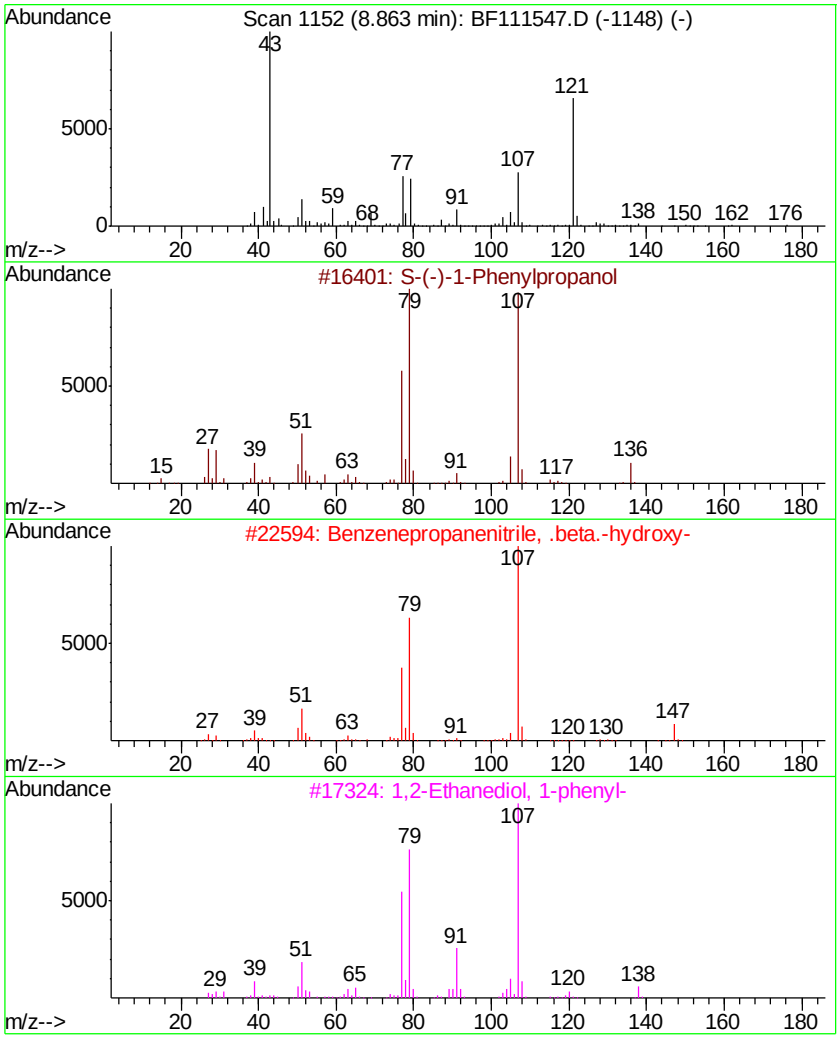
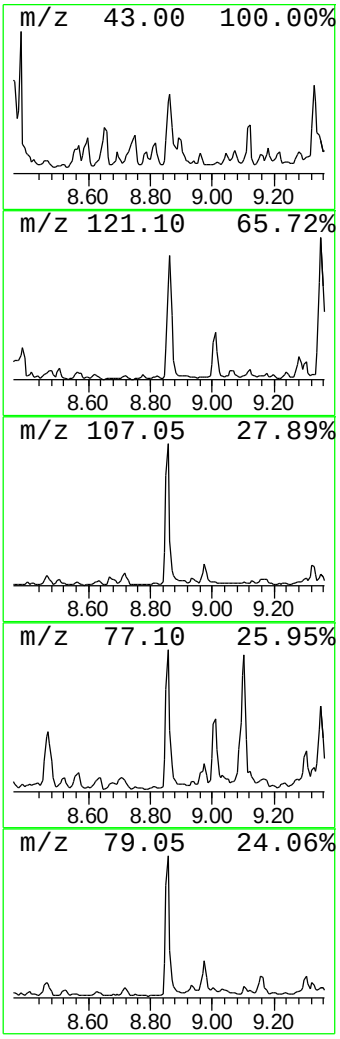
Peak Number 13 S-(-)-1-Phenylpropanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.86	28.63 ng	1927340	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-(-)-1-Phenylpropanol	136	C9H12O	000613-87-6	86
2	Benzenepropanenitrile, .beta.-hy...	147	C9H9NO	017190-29-3	78
3	1,2-Ethanediol, 1-phenyl-	138	C8H10O2	000093-56-1	78
4	Benzenemethanol, .alpha.-propyl-	150	C10H14O	000614-14-2	78
5	Propionic acid, 2,3-dihydroxy-3-...	182	C9H10O4	1000303-10-7	78





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Instrument : BNA_F
ClientSampleId : COMP-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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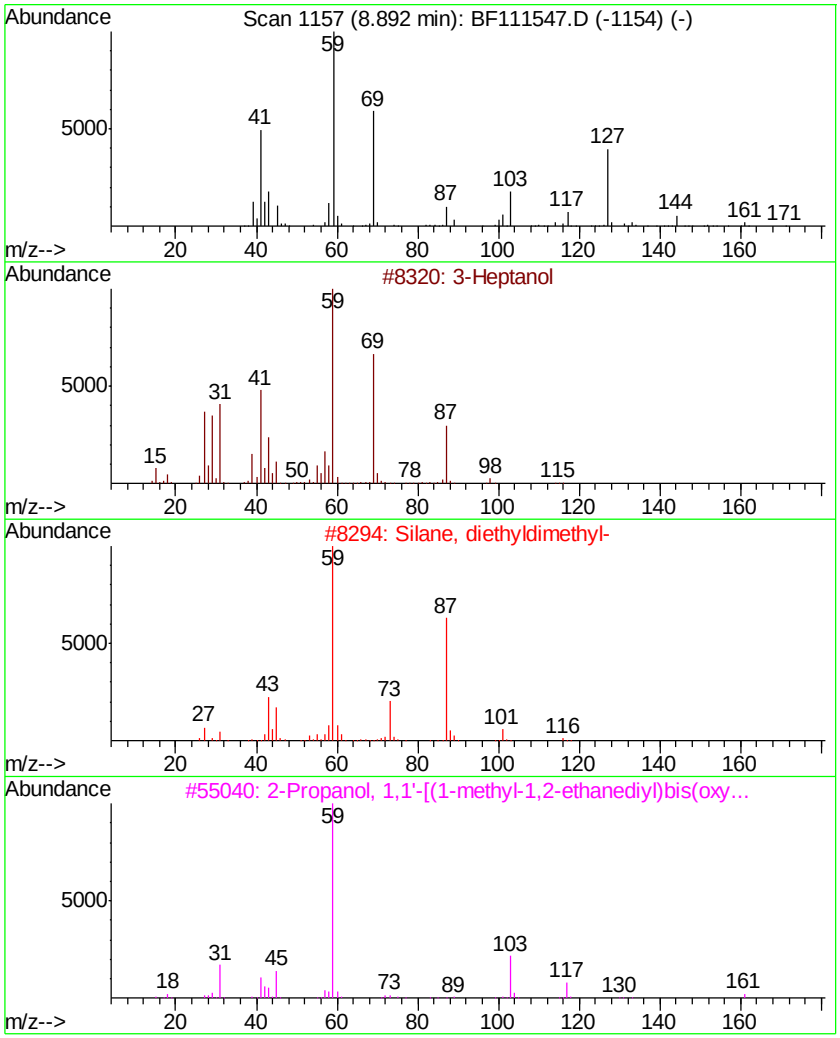
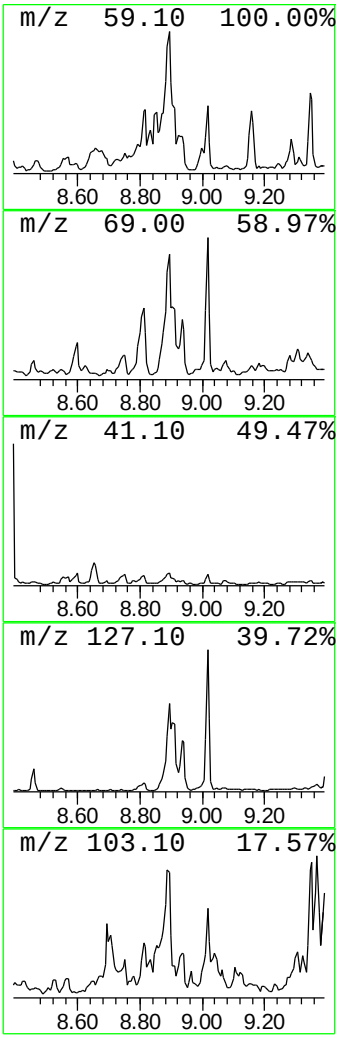
Peak Number 14 unknown8.89 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	22.86 ng	1538750	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanol	116	C7H16O	000589-82-2	43
2	Silane, diethyldimethyl-	116	C6H16Si	000756-81-0	38
3	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	37
4	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	37
5	1-Propanol, 3-[3-(1-methylethoxy...	176	C9H20O3	054518-03-5	37





Library Search Compound Report

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Sample : J6438-13
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ALS Vial : 8 Sample Multiplier: 1

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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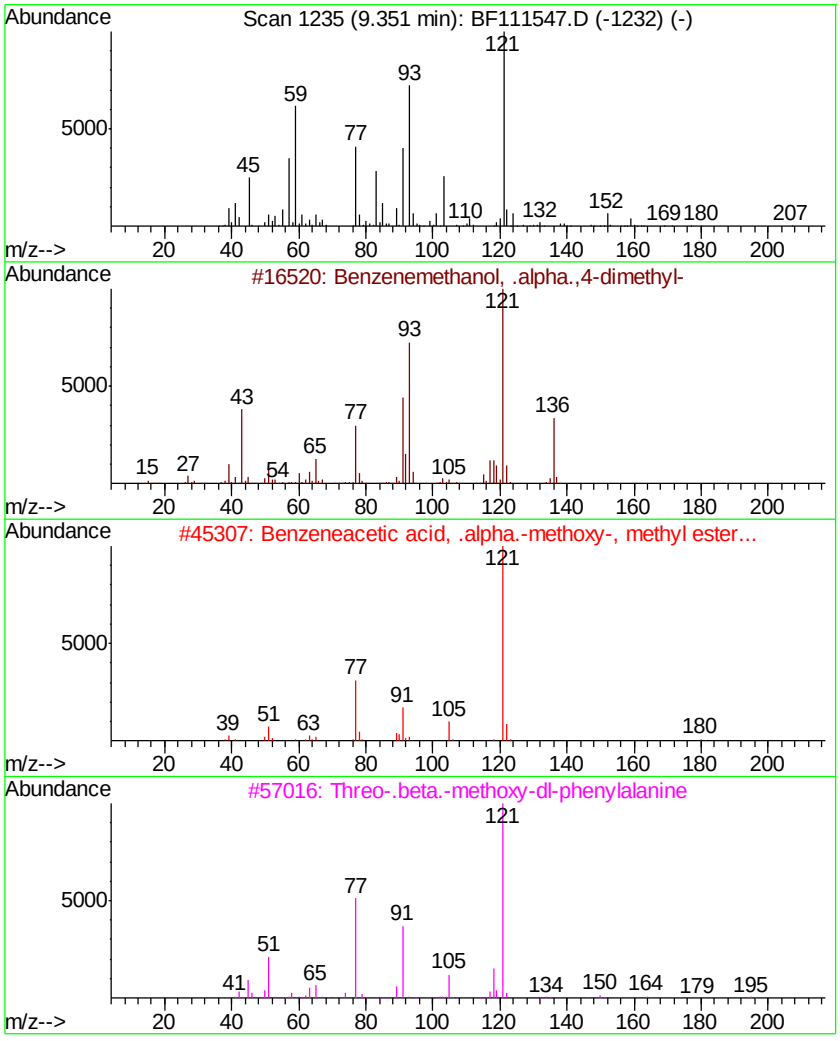
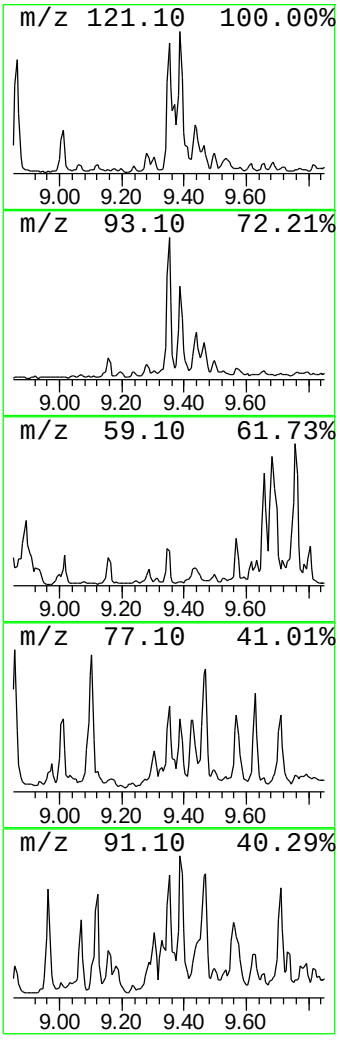
Peak Number 15 unknown9.35 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.35	24.74 ng	2171630	Acenaphthene-d10	9.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, .alpha.,4-dimet...	136	C9H12O	000536-50-5	38
2	Benzeneacetic acid, .alpha.-meth...	180	C10H12O3	056143-21-6	35
3	Threo-.beta.-methoxy-dl-phenylal...	195	C10H13NO3	1000250-97-1	35
4	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	32
5	Acetamide, N-cyclopropyl-2-metho...	205	C12H15NO2	1000305-01-6	25





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ClientSampleId : COMP-3

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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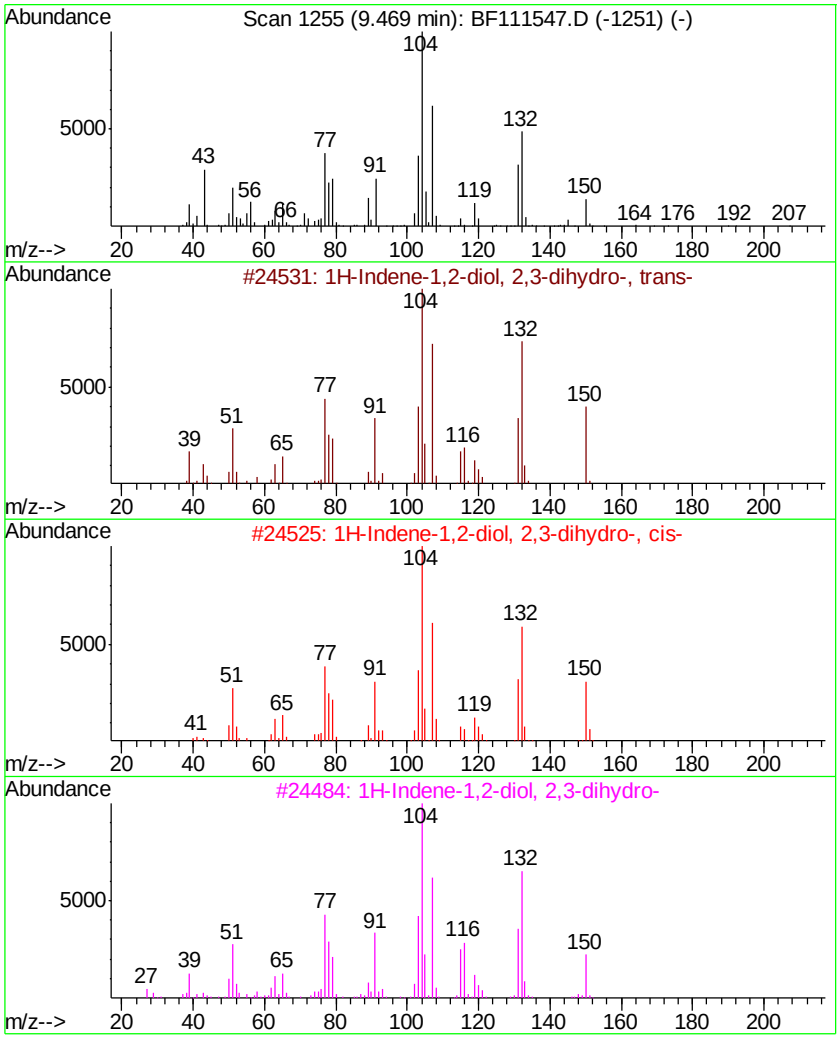
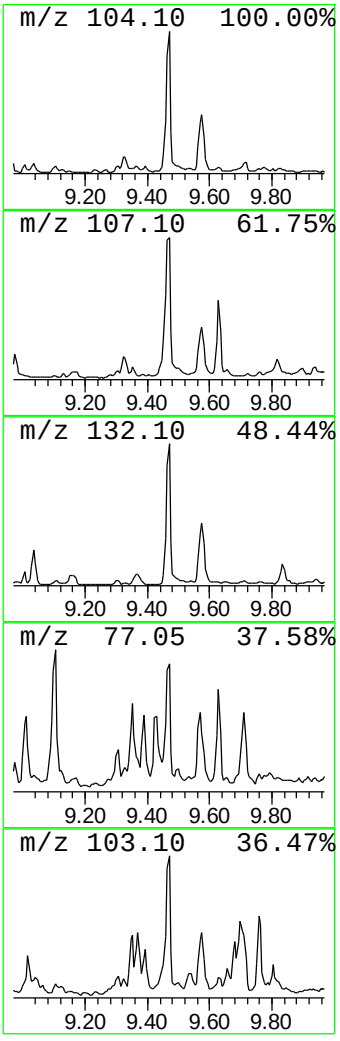
Peak Number 16 1H-Indene-1,2-diol, 2,3-dih... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.47	39.83 ng	3496920	Acenaphthene-d10	9.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene-1,2-diol, 2,3-dihydro-...	150	C9H10O2	004647-43-2	94
2	1H-Indene-1,2-diol, 2,3-dihydro-...	150	C9H10O2	004647-42-1	90
3	1H-Indene-1,2-diol, 2,3-dihydro-	150	C9H10O2	004370-02-9	70
4	Indan, epoxide	132	C9H8O	000768-22-9	60
5	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	60





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Data File : BF111547.D
Acq On : 17 Dec 2018 19:03
Operator : JU/SJ
Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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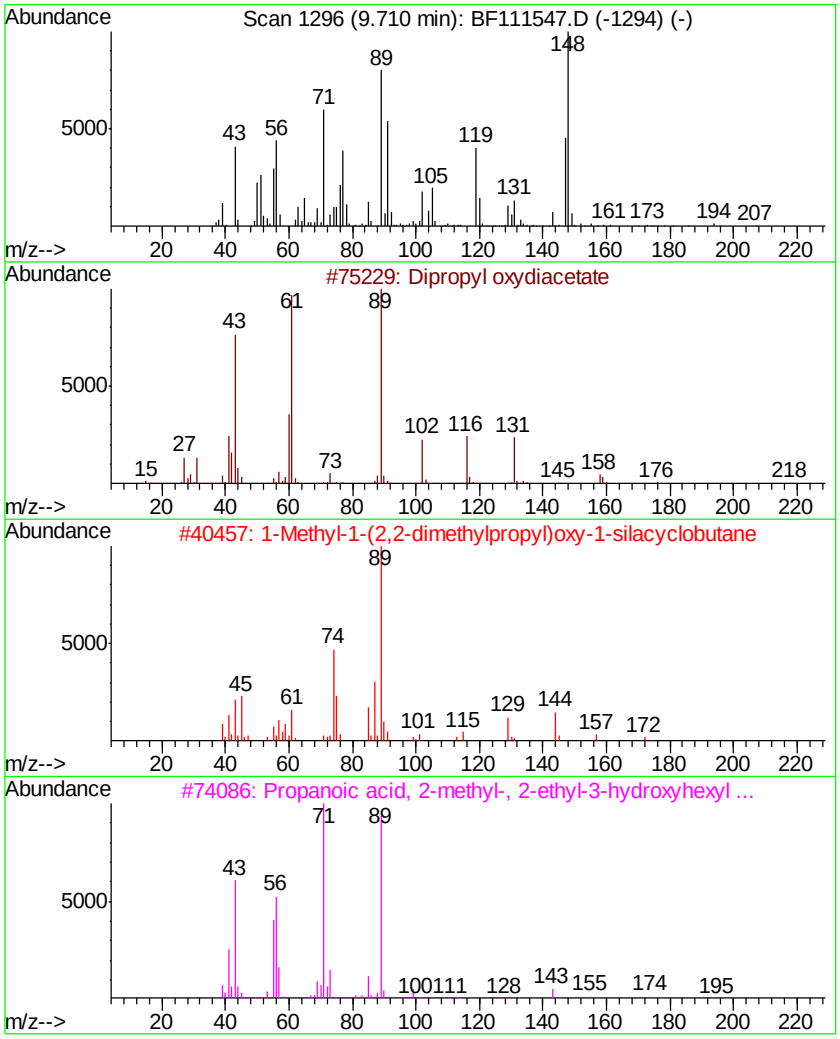
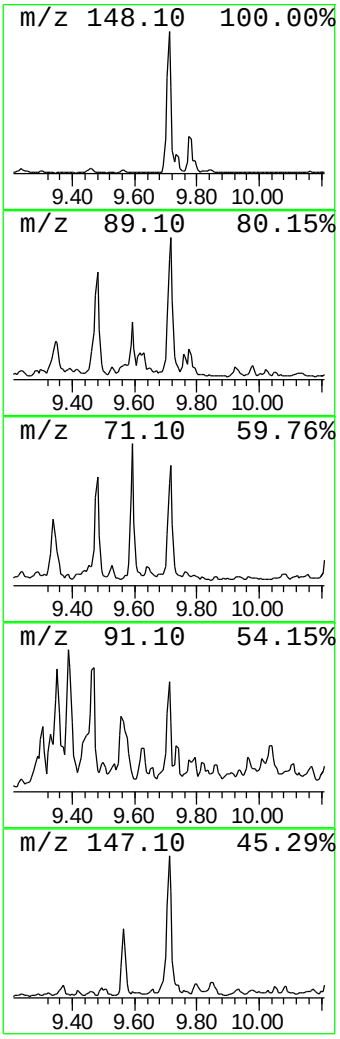
Peak Number 17 unknown9.71 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.71	26.33 ng	2311010	Acenaphthene-d10	9.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dipropyl oxydiacetate	218	C10H18O5	085668-79-7	38
2	1-Methyl-1-(2,2-dimethylpropyl)o...	172	C9H20OSi	1000216-97-6	38
3	Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	38
4	tert-Butyl((1-methoxypropan-2-yl...	204	C10H24O2Si	1000378-33-7	37
5	2,2-Dimethoxypropionamide	133	C5H11NO3	1000237-69-7	32





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Operator : JU/SJ
Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
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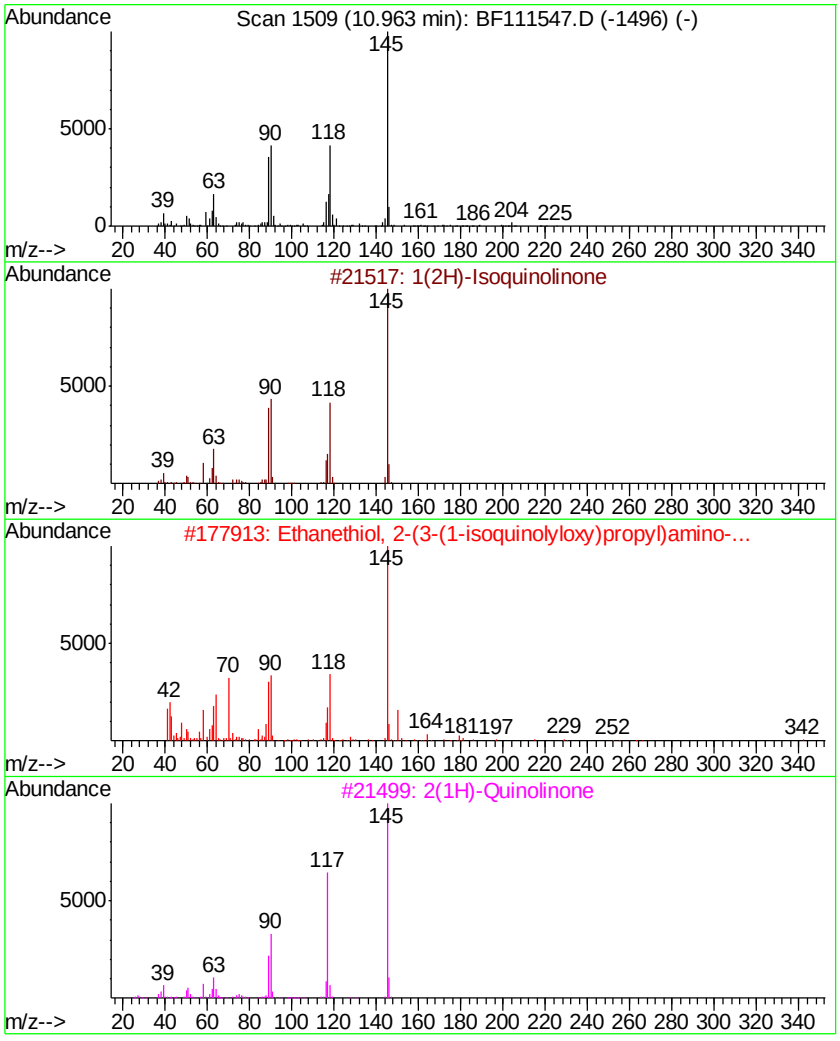
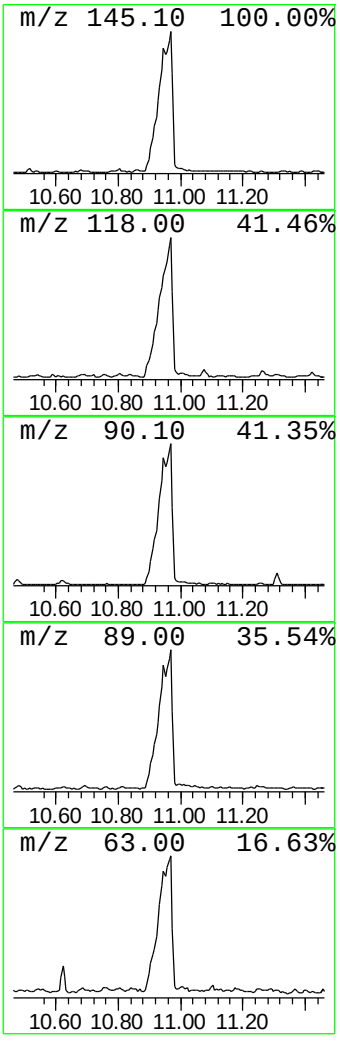
Peak Number 18 1(2H)-Isoquinolinone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	53.64 ng	4526220	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Isoquinolinone	145	C9H7NO	000491-30-5	97
2	Ethanethiol, 2-(3-(1-isoquinolyl...	342	C14H18N2O4S2	041287-44-9	78
3	2(1H)-Quinolinone	145	C9H7NO	000059-31-4	76
4	4-Quinolinol	145	C9H7NO	000611-36-9	70
5	3-Quinolinol	145	C9H7NO	000580-18-7	68





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Acq On : 17 Dec 2018 19:03
Operator : JU/SJ
Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
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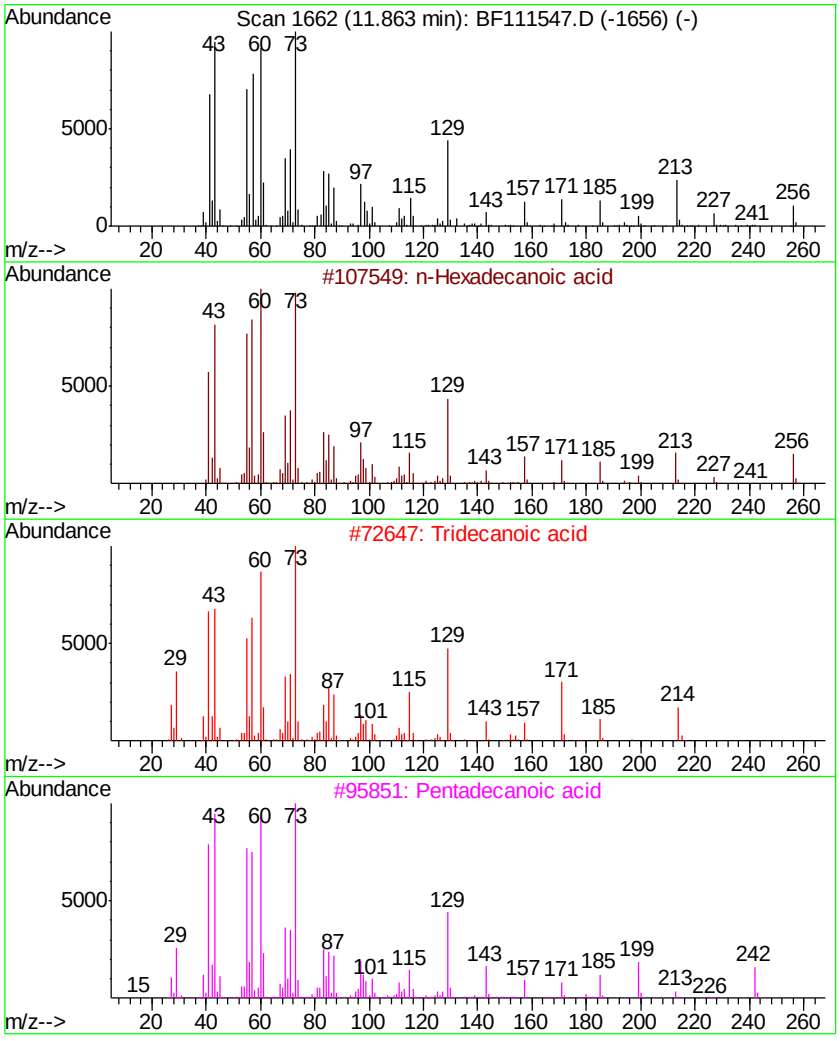
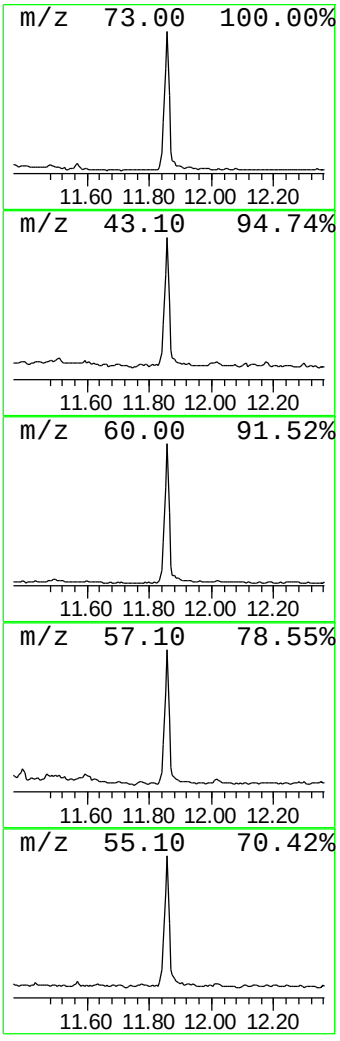
Peak Number 19 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	28.35 ng	2392310	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Sample : J6438-13
Misc :
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Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
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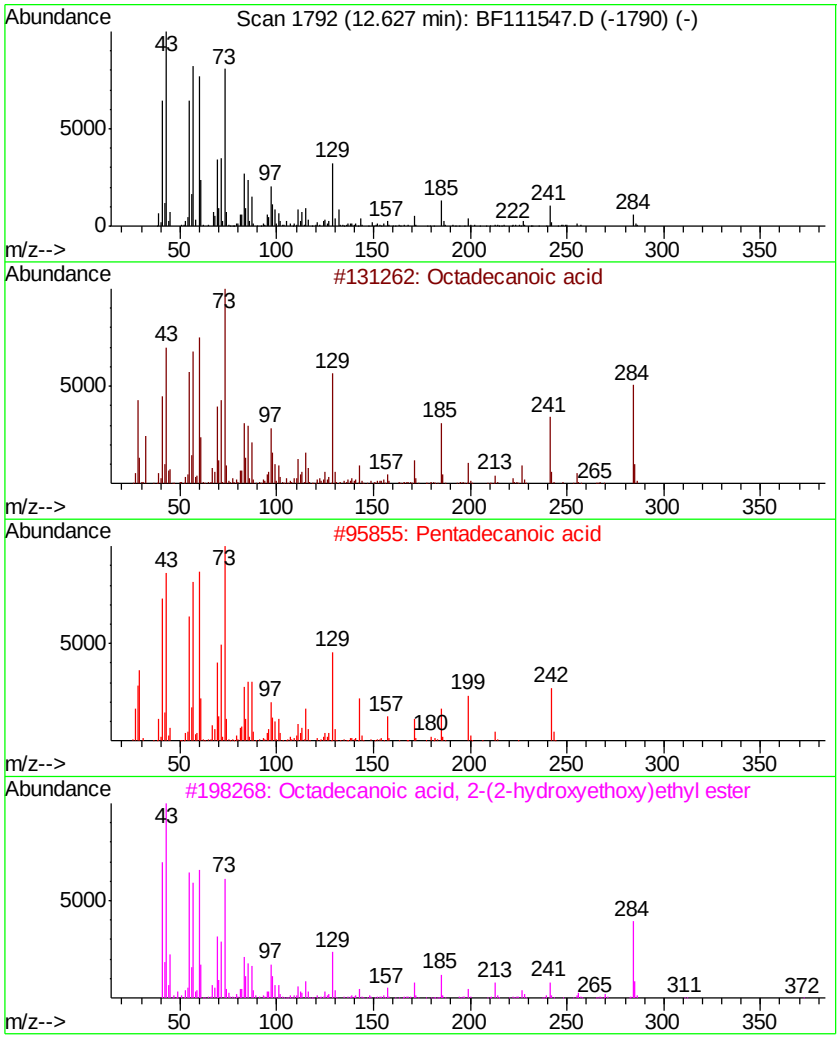
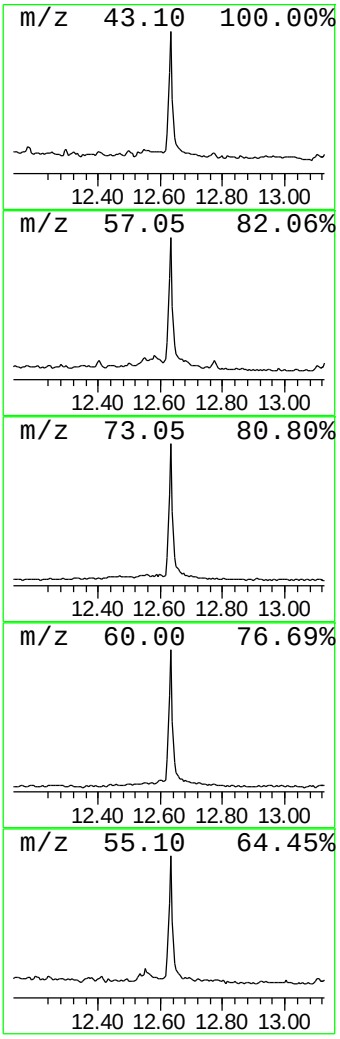
Peak Number 20 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	35.39 ng	2022440	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Tentatively Identified Compound (LSC) summary

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Data File : BF111547.D
Acq On : 17 Dec 2018 19:03
Operator : JU/SJ
Sample : J6438-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanoic acid, 3-...	5.90	22.9	ng	5998360	1	6.80	5230480	20.0
Hexylene glycol	6.27	53.6	ng	14015200	1	6.80	5230480	20.0
3-Methyl-2-furoic...	7.47	22.4	ng	1506590	2	8.08	1346370	20.0
Hexanoic acid, 2-...	7.76	208.0	ng	14000700	2	8.08	1346370	20.0
unknown7.92	7.92	45.9	ng	3088710	2	8.08	1346370	20.0
unknown7.96	7.96	29.7	ng	2001660	2	8.08	1346370	20.0
1,3-Hexanediol, 2...	8.36	132.8	ng	8941060	2	8.08	1346370	20.0
1-Phenoxypropan-2-ol	8.47	24.0	ng	1618100	2	8.08	1346370	20.0
Acetic acid, [(2-...	8.57	21.9	ng	1476240	2	8.08	1346370	20.0
unknown8.65	8.65	86.8	ng	5843270	2	8.08	1346370	20.0
Valproic Acid	8.75	33.4	ng	2244790	2	8.08	1346370	20.0
S-(-)-1-Phenylpro...	8.86	28.6	ng	1927340	2	8.08	1346370	20.0
unknown8.89	8.89	22.9	ng	1538750	2	8.08	1346370	20.0
unknown9.35	9.35	24.7	ng	2171630	3	9.83	1755720	20.0
1H-Indene-1,2-dio...	9.47	39.8	ng	3496920	3	9.83	1755720	20.0
unknown9.71	9.71	26.3	ng	2311010	3	9.83	1755720	20.0
1(2H)-Isoquinolinone	10.96	53.6	ng	4526220	4	11.32	1687690	20.0
n-Hexadecanoic acid	11.86	28.4	ng	2392310	4	11.32	1687690	20.0
Octadecanoic acid	12.63	35.4	ng	2022440	5	13.94	1143030	20.0