LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

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-BF010719.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	2.193	10	18	26	rBV	398958	570076	12.93%	1.286%
2	2.687	97	102	111	rVB	148429	231535	5.25%	0.522%
3	3.799	280	291	296	rBV	52799	98129	2.23%	0.221%
4	4.010	324	327	336	rVB	74677	109479	2.48%	0.247%
5	5.040	496	502	509	rBV	123794	132940	3.02%	0.300%
6	5.104	509	513	520	rBV	276904	331140	7.51%	0.747%
7	5.240	520	536	538	rVV2	69023	210139	4.77%	0.474%
8	5.363	543	557	565	rVB4	68590	232498	5.27%	0.524%
9	5.487	574	578	580	rBV2	64378	68274	1.55%	0.154%
10	5.522	580	584	591	rVB	2100381	1903080	43.17%	4.292%
11	5.651	596	606	607	rBV3	55583	120958	2.74%	0.273%
12	5.716	614	617	620	rBV	201352	179250	4.07%	0.404%
13	5.840	635	638	642	rBV	227193	198635	4.51%	0.448%
14	6.051	666	674	679	rBV	384659	519800	11.79%	1.172%
15	6.204	696	700	704	rVB2	42231	55015	1.25%	0.124%
16	6.434	734	739	741	rBV	60091	62094	1.41%	0.140%
17	6.528	751	755	762	rVB	1468084	1522275	34.53%	3.433%
18	6.663	774	778	783	rBV	3643229	3505366	79.52%	7.905%
19	6.704	783	785	793	rVB3	202238	264129	5.99%	0.596%
20	6.887	811	816	820	rBV	1125500	940841	21.34%	2.122%
21	6.951	823	827	833	rVV	1169948	1099444	24.94%	2.479%
22	6.998	833	835	837	rVV	78922	61553	1.40%	0.139%
23	7.045	837	843	847	rVB2	3514909	3785538	85.87%	8.537%
24	7.298	882	886	889	rVB2	137830	148332	3.36%	0.335%
25	7.445	906	911	914	rVB	2565990	2397740	54.39%	5.407%
26	7.622	922	941	945	rBV2	1078760	2638033	59.84%	5.949%
27	7.675	948	950	953	rVB	116538	101057	2.29%	0.228%
28	7.769	963	966	969	rVB3	57838	63636	1.44%	0.144%
29	7.828	972	976	977	rBV2	54762	62648	1.42%	0.141%
30	7.922	985	992	993	rBV2	313872	482659	10.95%	1.088%
31	7.963	993	999	1008	rVB3	659750	1061240	24.07%	2.393%
32	8.034	1008	1011	1014	rBV3	53262	58779	1.33%	0.133%
33	8.075	1014	1018	1021	rBV	709612	636455	14.44%	1.435%
34	8.139	1024	1029	1031	rBV2	167563	178108	4.04%	0.402%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

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-BF010719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	8.169	1031	1034	1037	rBV	1268107	1013623	22.99%	2.286%
36	8.198	1037	1039	1040	rVV2	114999	79371	1.80%	0.179%
37	8.251	1043	1048	1052	rVB	614460	674954	15.31%	1.522%
38	8.292	1052	1055	1059	rBV3	89455	104190	2.36%	0.235%
39	8.363	1064	1067	1069	rVB	92201	81496	1.85%	0.184%
40	8.392	1069	1072	1074	rBV	64618	51381	1.17%	0.116%
41	8.481	1084	1087	1092	rVB2	190128	285089	6.47%	0.643%
42	8.522	1092	1094	1095	rVV	85697	64809	1.47%	0.146%
43	8.545	1096	1098	1102	rVB	120383	116496	2.64%	0.263%
44	8.604	1105	1108	1111	rVB2	87685	87689	1.99%	0.198%
45	8.681	1117	1121	1122	rBV	143142	159297	3.61%	0.359%
46	8.704	1122	1125	1129	rVB	309894	335629	7.61%	0.757%
47	8.739	1129	1131	1135	rBV	100551	76289	1.73%	0.172%
48	8.804	1139	1142	1145	rVB2	58881	56446	1.28%	0.127%
49	8.851	1145	1150	1154	rBV7	29221	53250	1.21%	0.120%
50	8.916	1157	1161	1165	rBV2	106442	120902	2.74%	0.273%
51	9.010	1174	1177	1181	rBV	78703	85897	1.95%	0.194%
52	9.110	1188	1194	1198	rBV	156982	193609	4.39%	0.437%
53	9.145	1198	1200	1204	rVB2	76542	65073	1.48%	0.147%
54	9.245	1211	1217	1220	rBV	5072928	4408232	100.00%	9.941%
55	9.392	1238	1242	1247	rVB2	164813	196459	4.46%	0.443%
56	9.516	1257	1263	1265	rBV3	87564	117243	2.66%	0.264%
57	9.539	1265	1267	1273	rVB	56517	67289	1.53%	0.152%
58	9.633	1280	1283	1285	rVB	67399	49329	1.12%	0.111%
59	9.692	1290	1293	1296	rVB2	91898	90253	2.05%	0.204%
60	9.739	1296	1301	1304	rBV	241790	226194	5.13%	0.510%
61	9.833	1313	1317	1325	rVB	59670	78057	1.77%	0.176%
62	9.928	1328	1333	1336	rVB	1239311	1137512	25.80%	2.565%
63	10.086	1357	1360	1365	rBV3	50282	56183	1.27%	0.127%
64	10.580	1441	1444	1447	rBV	68537	61064	1.39%	0.138%
65	10.716	1462	1467	1470	rBV	2853678	2572321	58.35%	5.801%
66	11.410	1581	1585	1589	rBV	1171962	974716	22.11%	2.198%
67	11.633	1619	1623	1629	rBV6	44148	59549	1.35%	0.134%
68	11.933	1671	1674	1679	rBV2	202488	224004	5.08%	0.505%
69	12.057	1692	1695	1698	rBV	69897	59711	1.35%	0.135%
70	12.386	1746	1751	1756	rBV2	75659	111860	2.54%	0.252%
71	12.451	1759	1762	1768	rVV	109911	105147	2.39%	0.237%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

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-BF010719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	12.674	1797	1800	1804	rVB	155987	120413	2.73%	0.272%
73	12.722	1804	1808	1812	rBV2	60467	73168	1.66%	0.165%
74	12.998	1850	1855	1858	rBV	3698917	3501857	79.44%	7.897%
75	13.886	2003	2006	2012	rVB2	61582	66697	1.51%	0.150%
76	14.051	2030	2034	2037	rVB	928333	866426	19.65%	1.954%
77	14.863	2168	2172	2175	rVV	140471	143977	3.27%	0.325%
78	14.904	2176	2179	2186	rVB	55488	61586	1.40%	0.139%
79	15.168	2221	2224	2230	rBV	40348	54339	1.23%	0.123%
80	15.533	2280	2286	2296	rVB	832857	1123531	25.49%	2.534%

Sum of corrected areas: 44343482

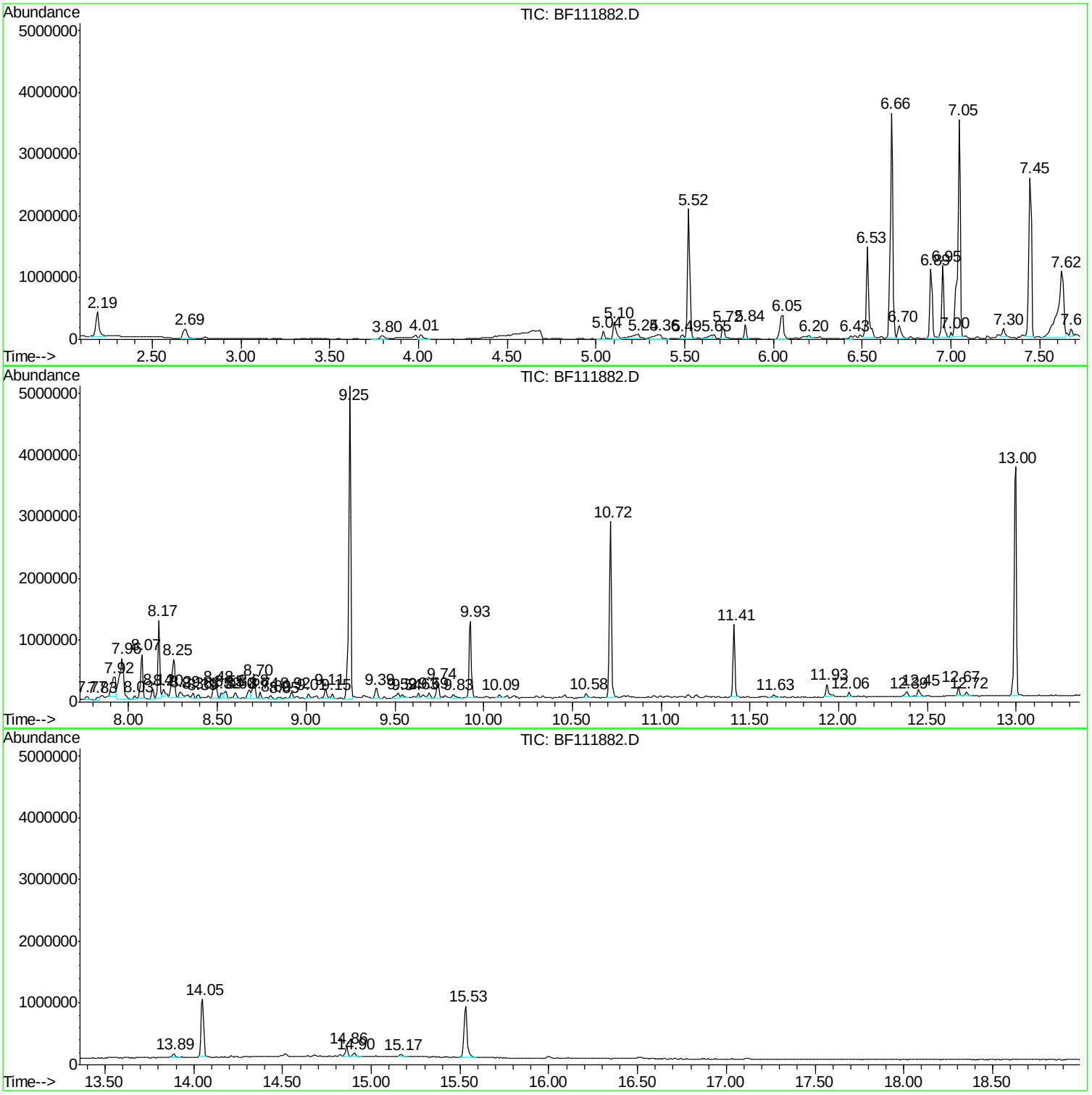
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

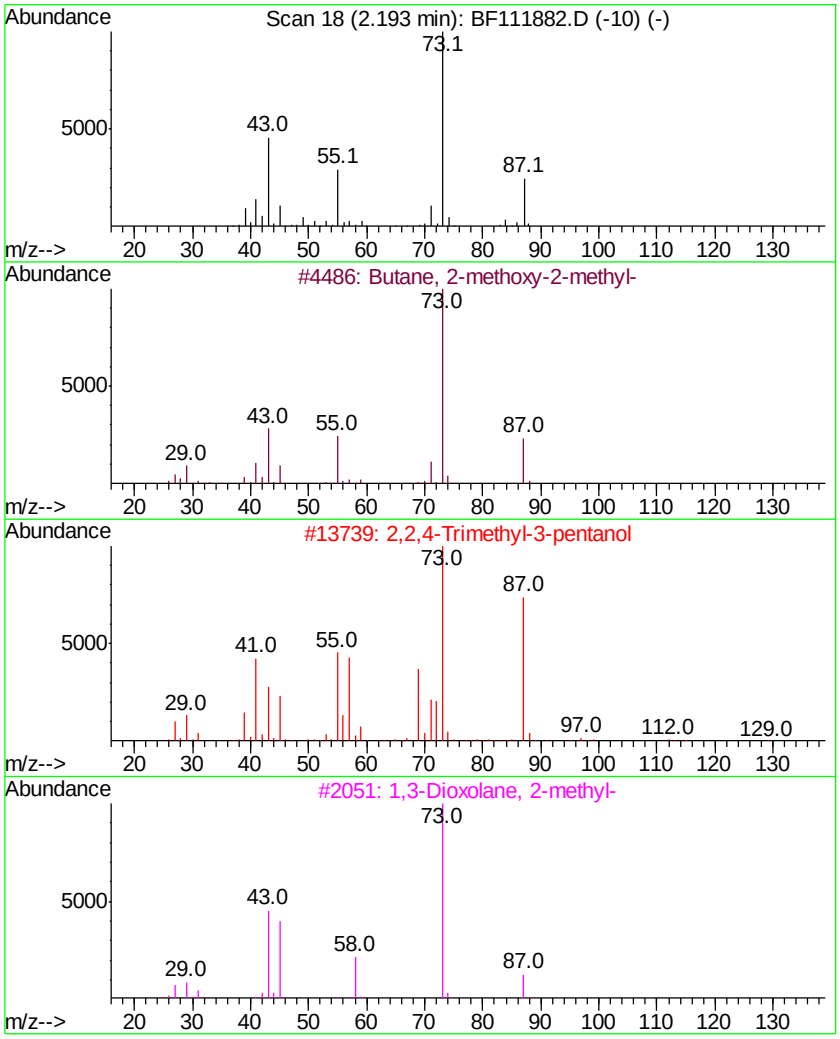
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

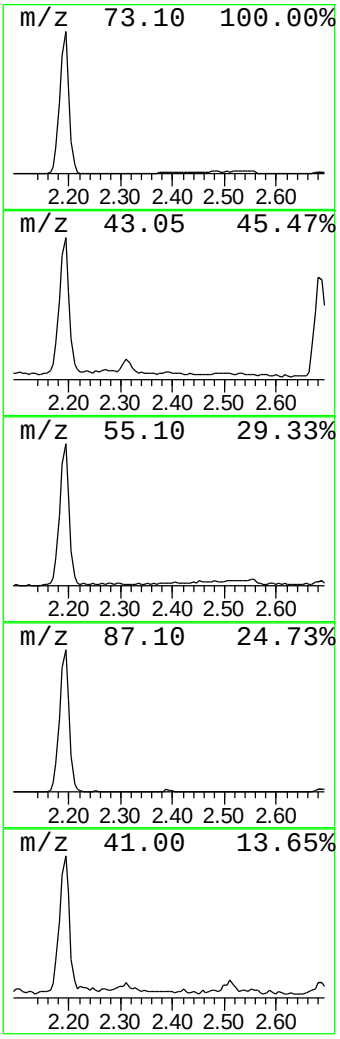
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	12.12 ng	570076	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	17
4	N,N'-Methylenebis(formamide)	102	C3H6N2O2	006921-98-8	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

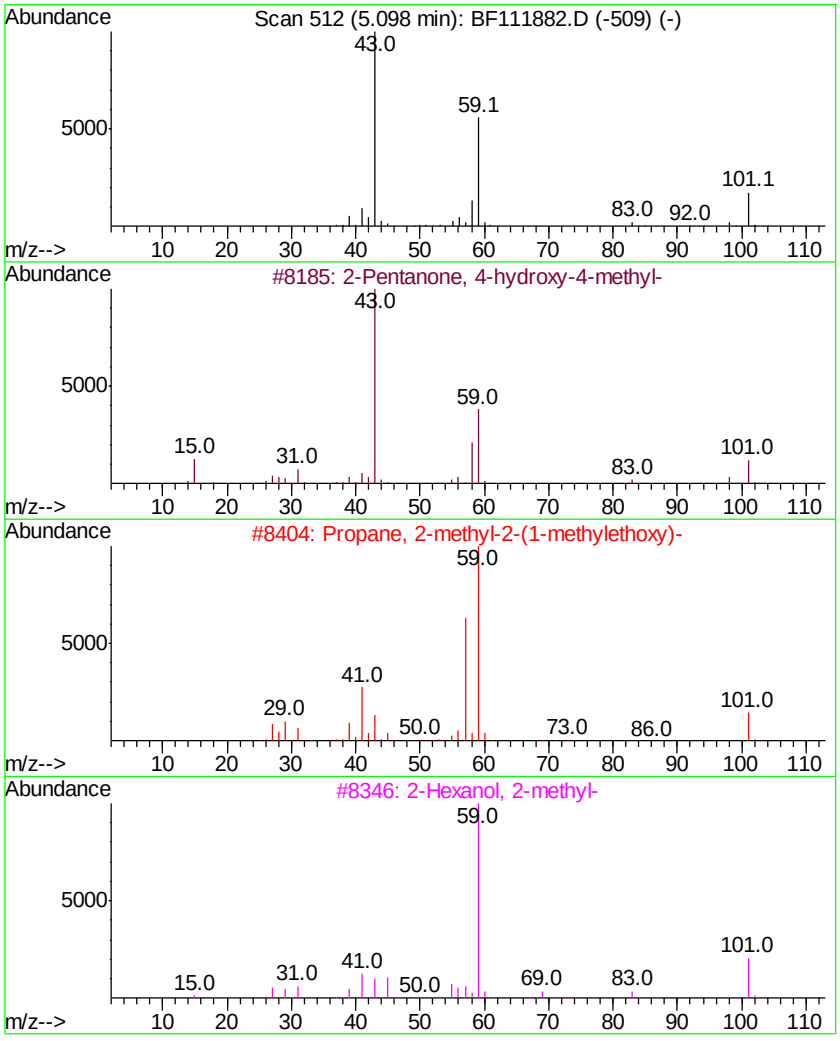
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

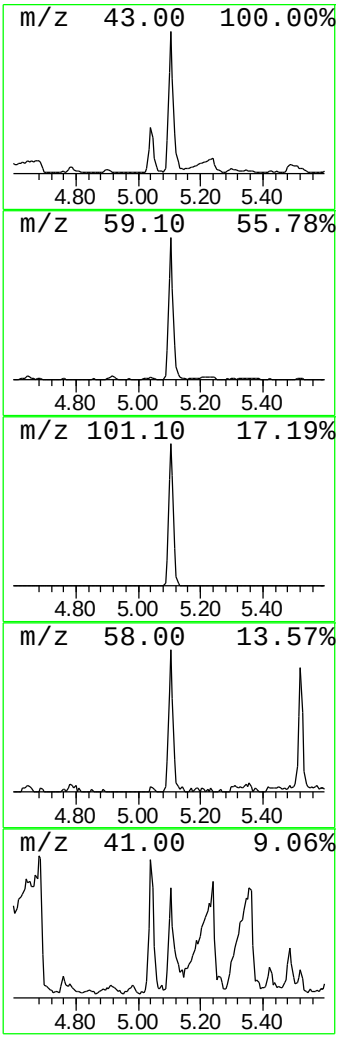
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	7.04 ng	331140	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

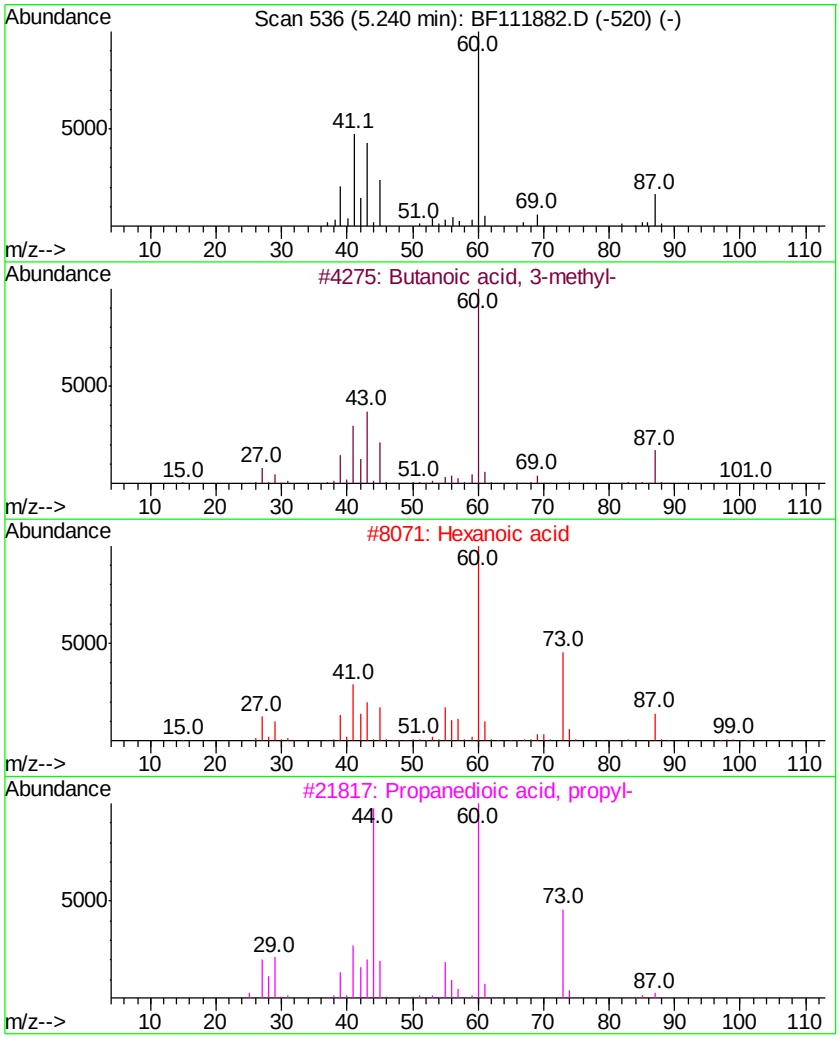
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

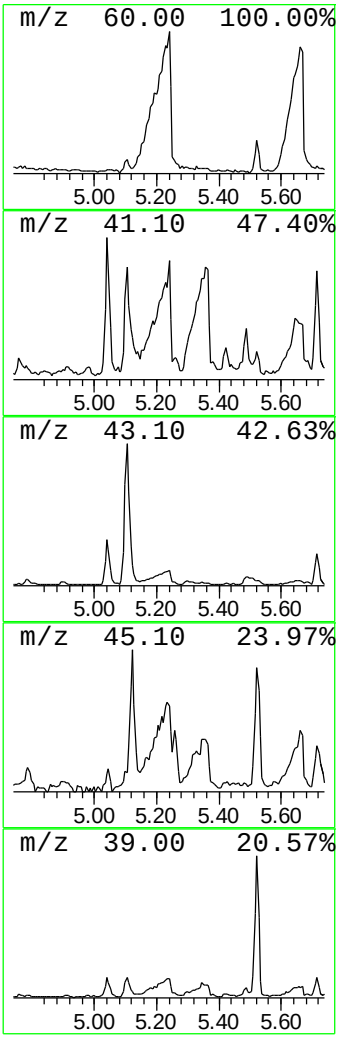
****

Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	4.47 ng	210139	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	83
2	Hexanoic acid	116	C6H12O2	000142-62-1	43
3	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	40
4	Pentanoic acid	102	C5H10O2	000109-52-4	38
5	1-Pentanamine	87	C5H13N	000110-58-7	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

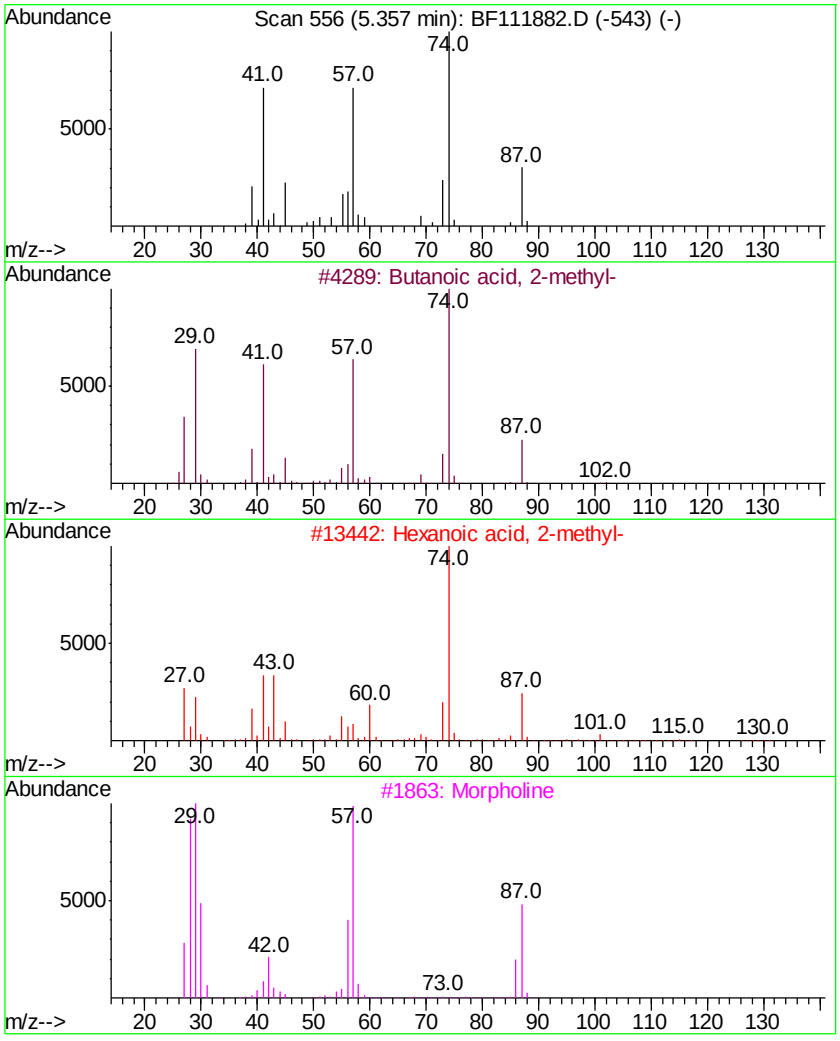
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

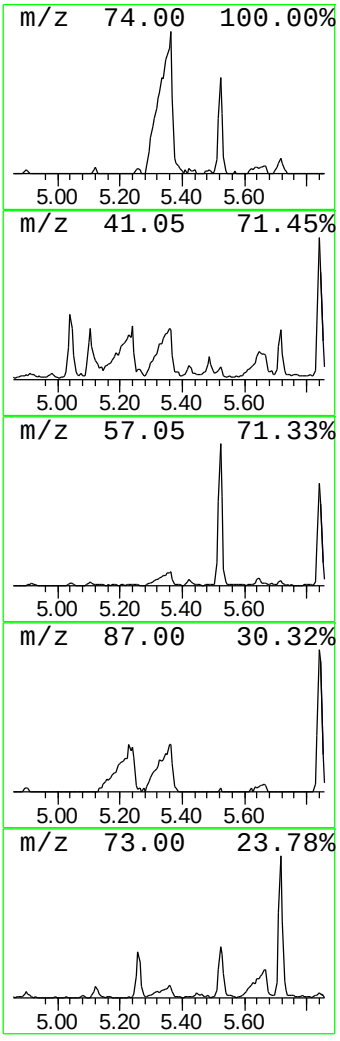
****

Peak Number 4 Butanoic acid, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.36	4.94 ng	232498	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
2	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	38
3	Morpholine	87	C4H9NO	000110-91-8	9
4	Propanoic acid	74	C3H6O2	000079-09-4	9
5	Oxirane, (butoxymethyl)-	130	C7H14O2	002426-08-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

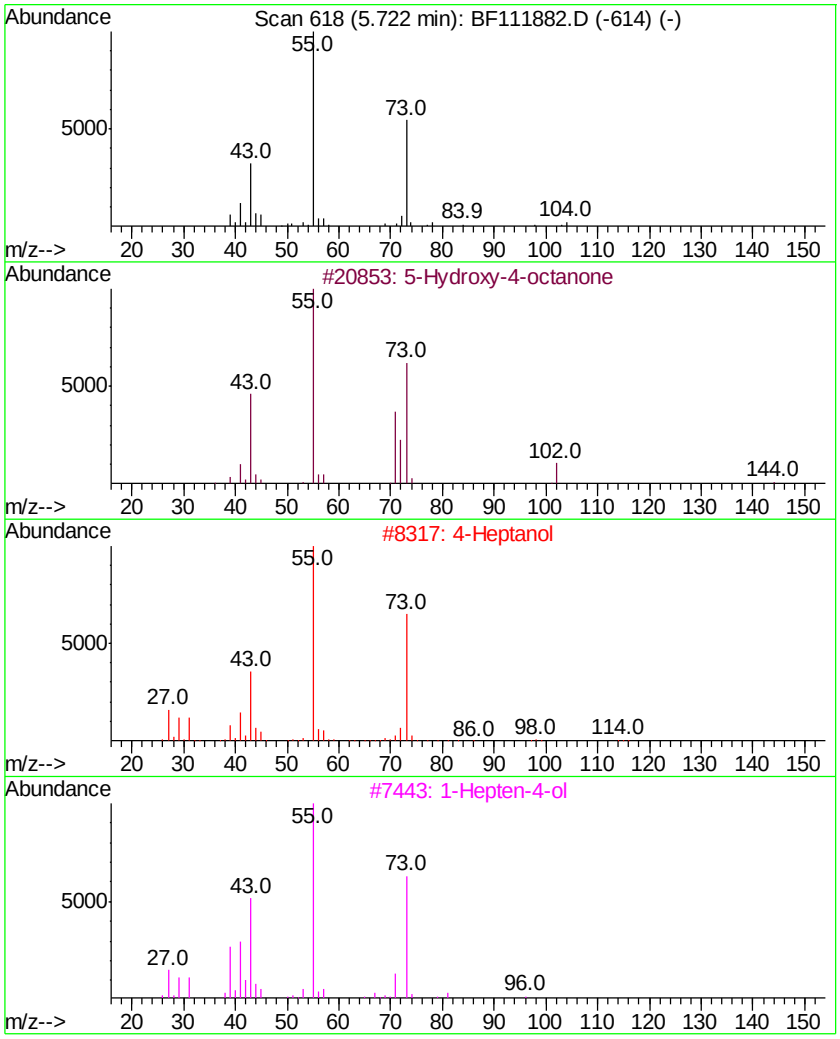
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

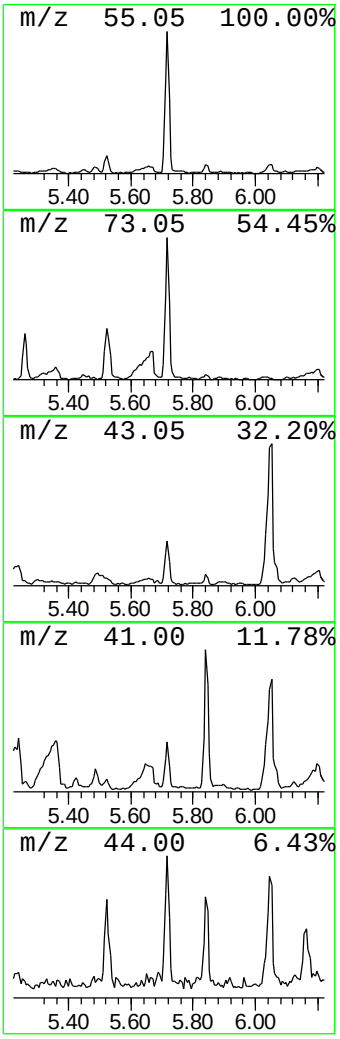
****

Peak Number 5 5-Hydroxy-4-octanone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	3.81 ng	179250	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	64
2	4-Heptanol	116	C7H16O	000589-55-9	50
3	1-Hepten-4-ol	114	C7H14O	003521-91-3	39
4	2-Propenoic acid, butyl ester	128	C7H12O2	000141-32-2	28
5	Isobutylamine	73	C4H11N	000078-81-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

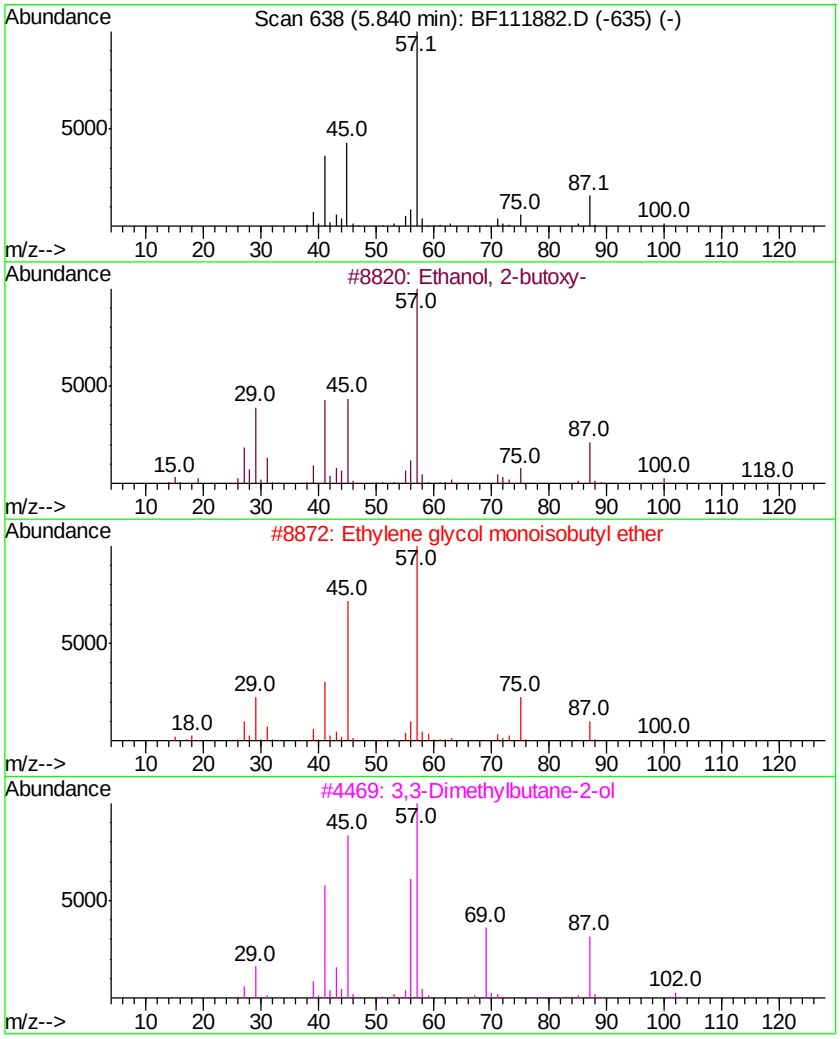
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

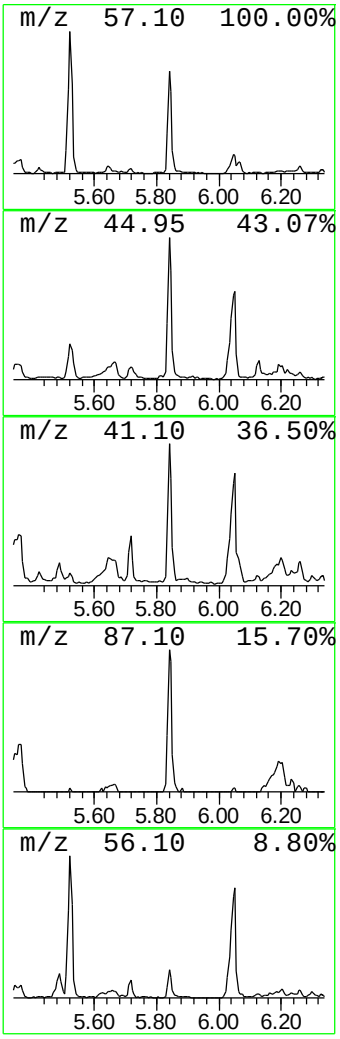
****

Peak Number 6 Ethanol, 2-butoxy- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.84	4.22 ng	198635	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	36
4	Isobutyl ether	130	C8H18O	000628-55-7	27
5	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	12





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Operator : JU/SJ
Sample : K1053-07
Misc :
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Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

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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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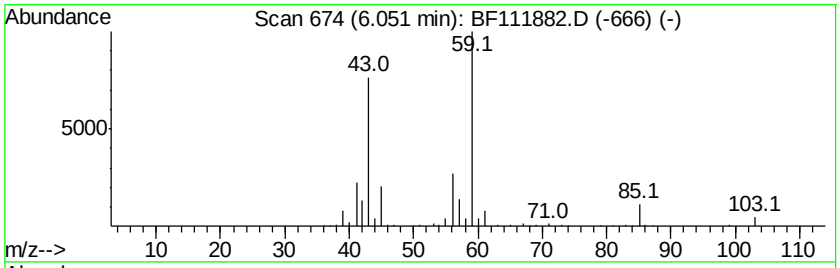
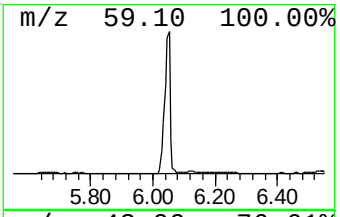
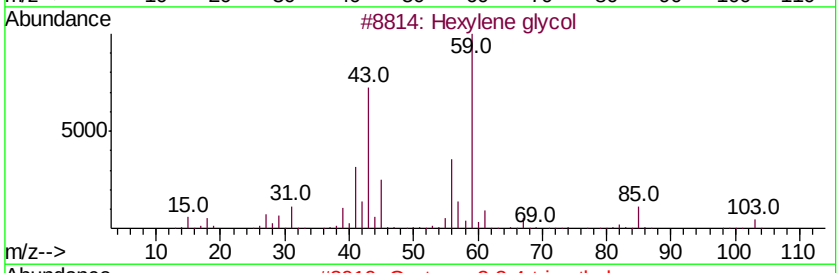
Peak Number 7 Hexylene glycol Concentration Rank 7

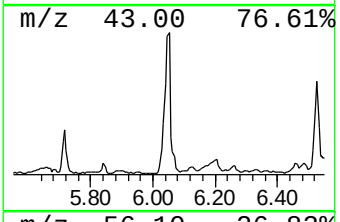
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.05	11.05 ng	519800	1,4-Dichlorobenzene-d4	6.89

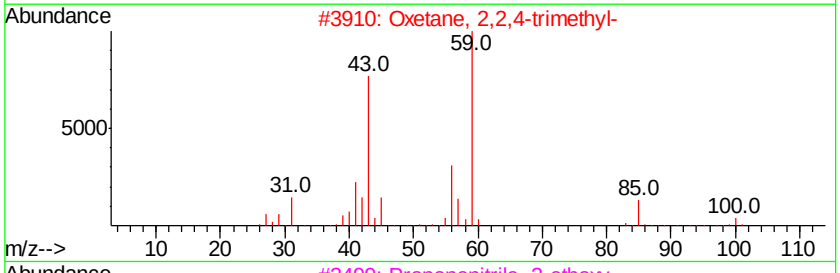
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	86
2	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	78
3	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	50
4	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	47
5	dl-Erythro-O-methylthreonine	133	C5H11NO3	1000214-70-7	42

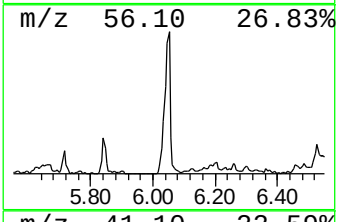


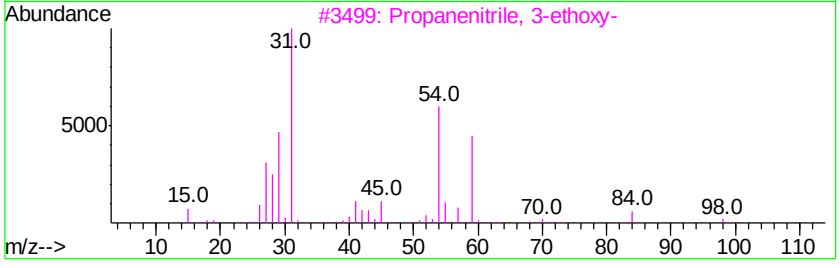


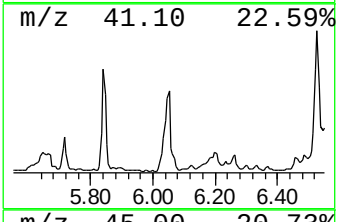


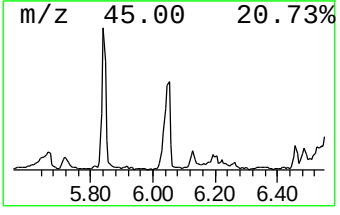












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Acq On : 7 Jan 2019 17:53
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Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

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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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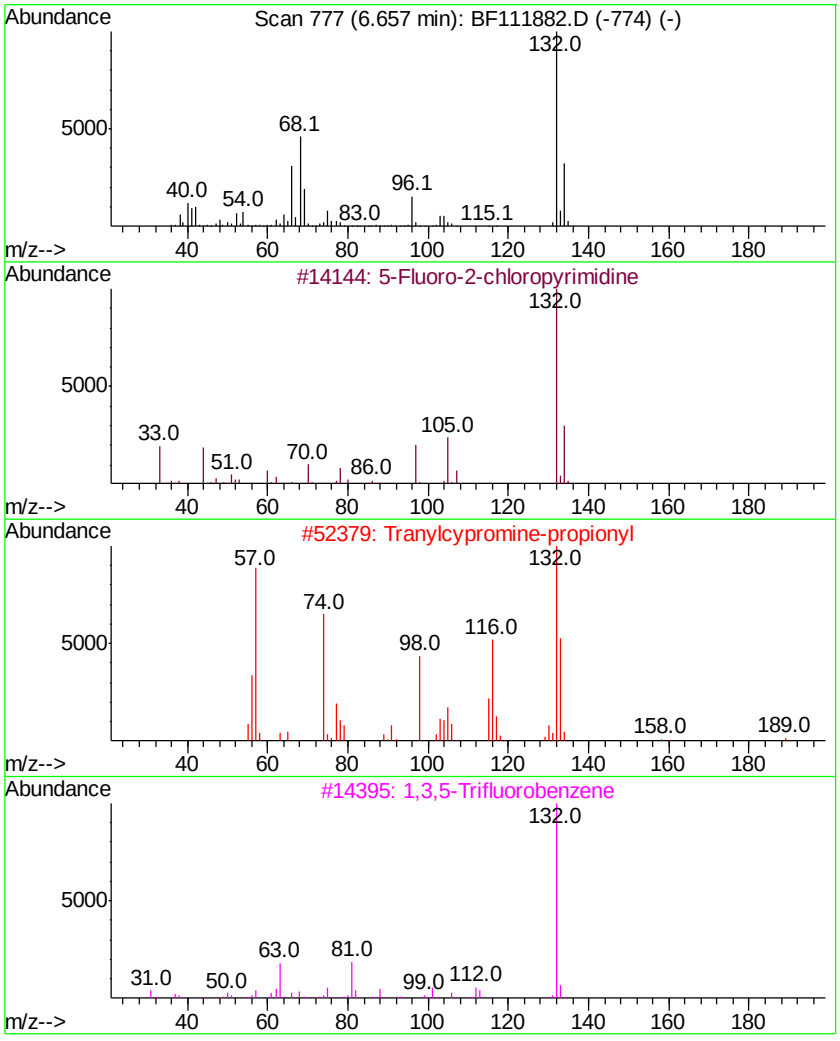
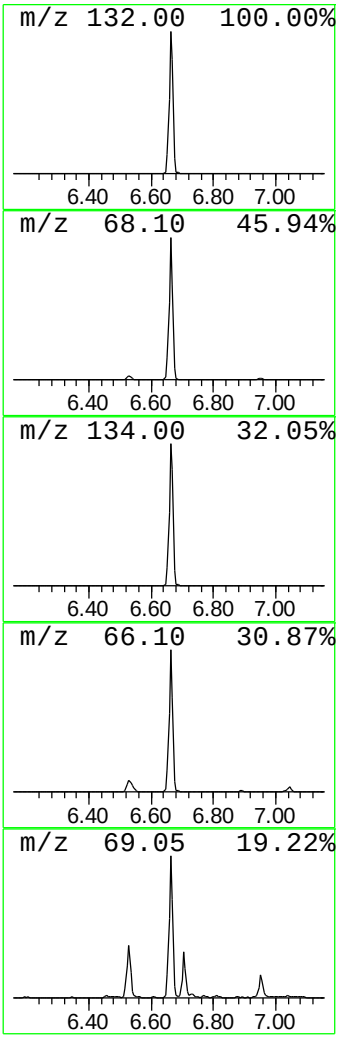
Peak Number 8 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	74.52 ng	3505370	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

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

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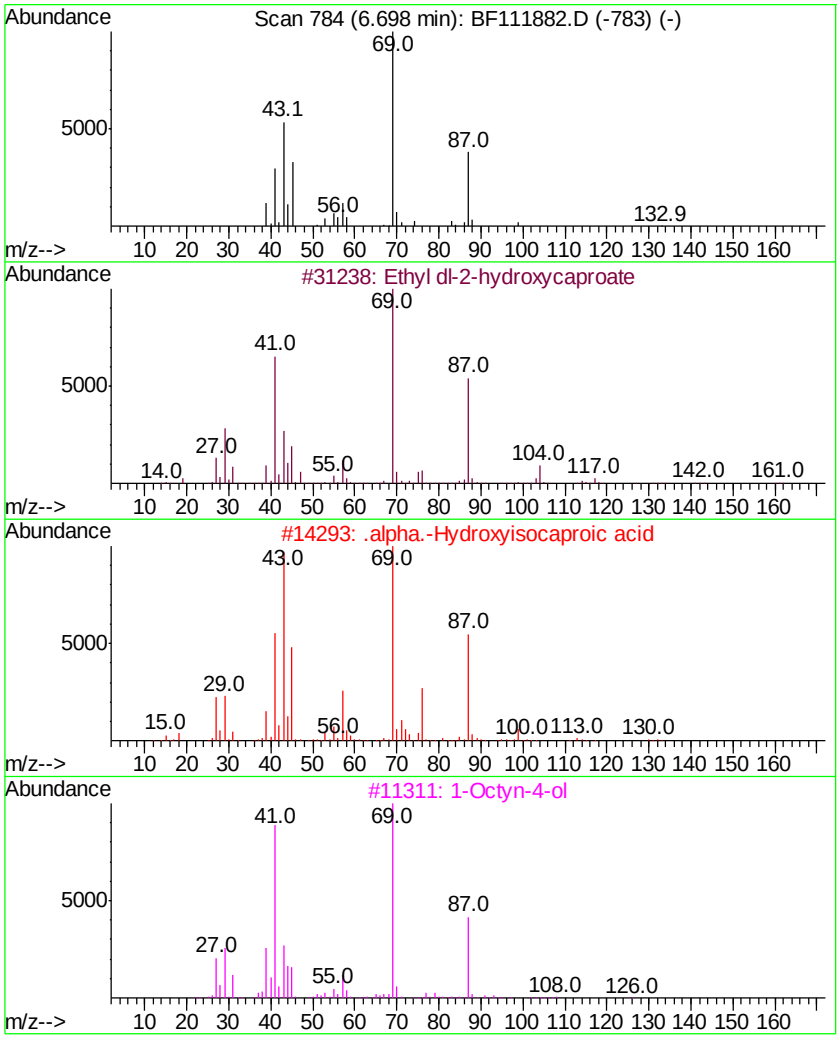
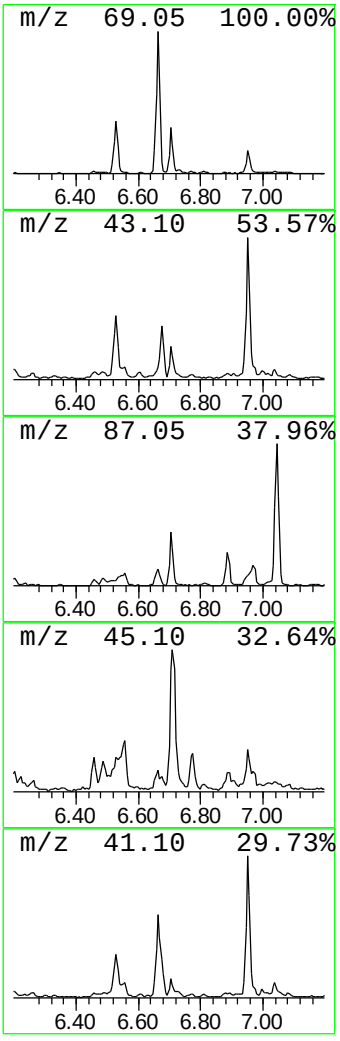
Peak Number 9 Ethyl dl-2-hydroxycaproate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	5.61 ng	264129	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl dl-2-hydroxycaproate	160	C8H16O3	006946-90-3	78
2	.alpha.-Hydroxyisocaproic acid	132	C6H12O3	000498-36-2	72
3	1-Octyn-4-ol	126	C8H14O	052517-92-7	64
4	5-Nonanol	144	C9H20O	000623-93-8	64
5	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	64





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Misc :
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Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

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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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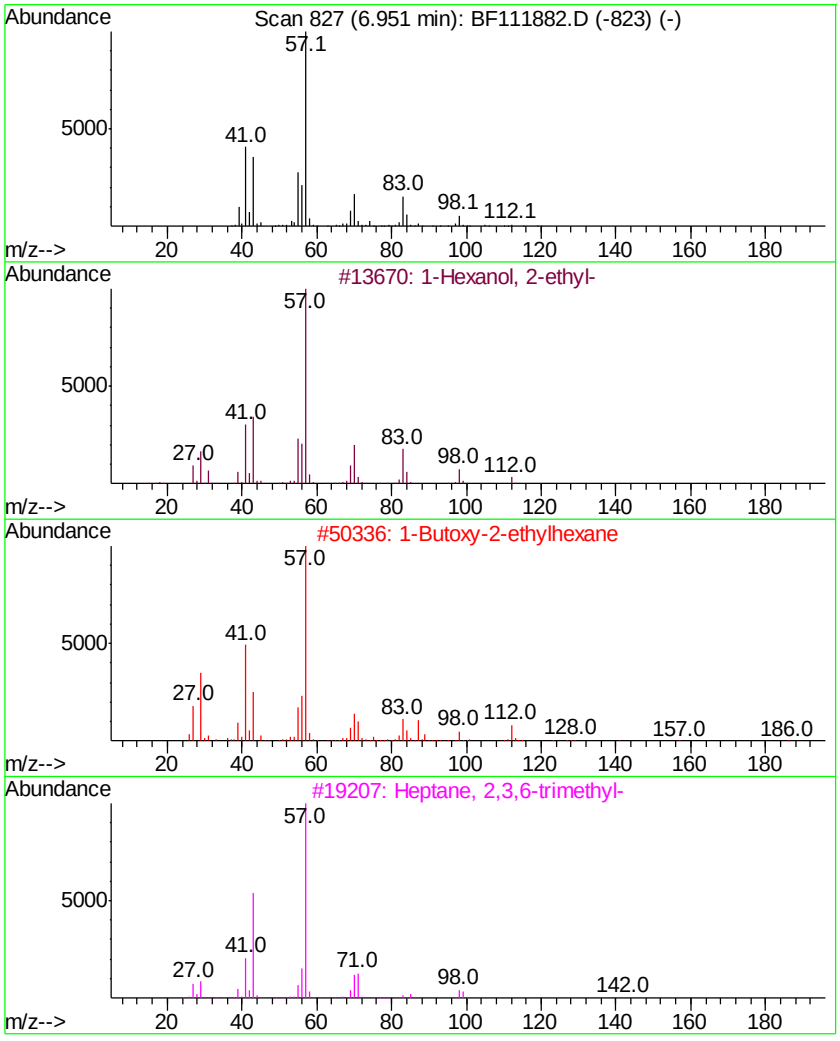
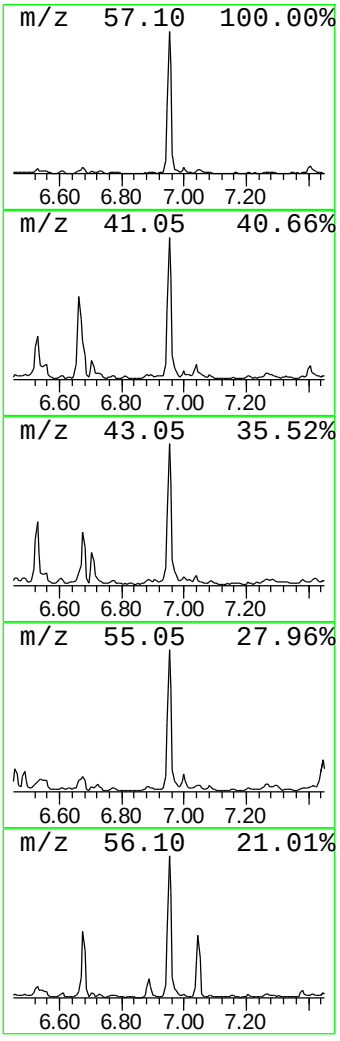
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	23.37 ng	1099440	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	74
3	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
4	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	59
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	53





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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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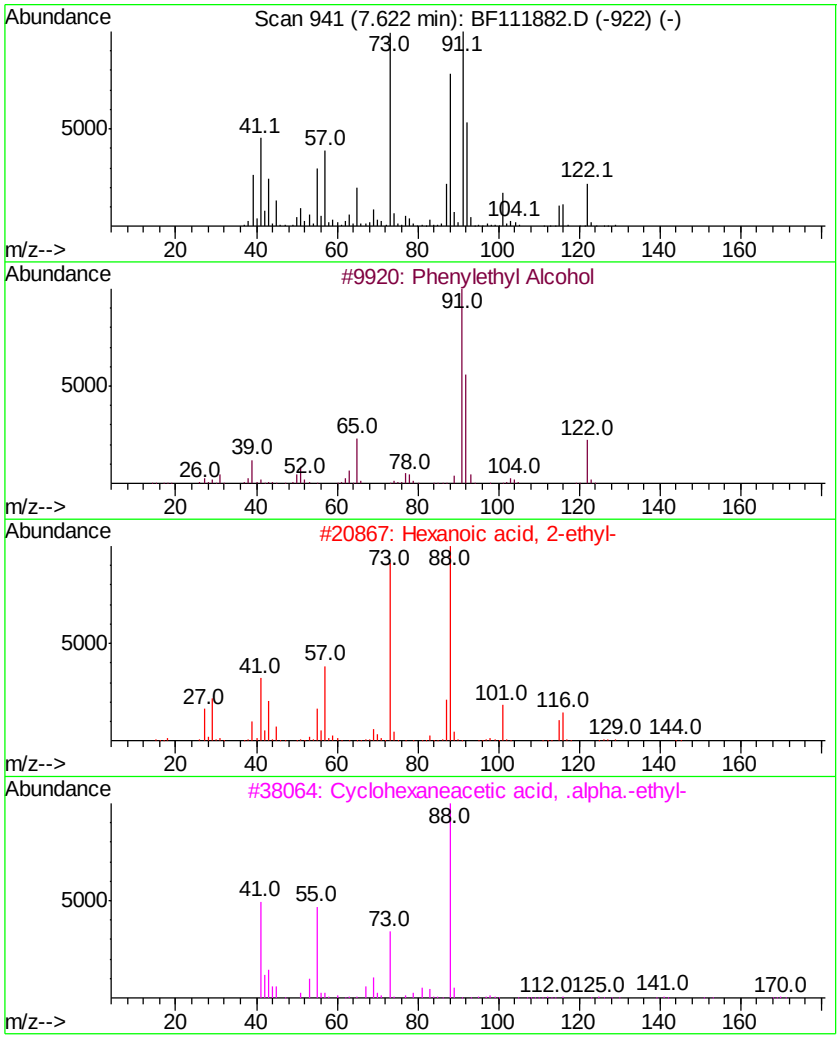
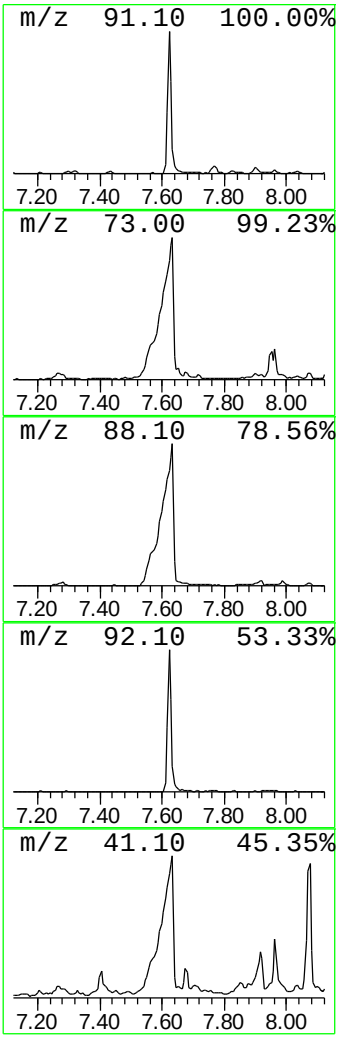
Peak Number 11 Phenylethyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	52.05 ng	2638030	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenylethyl Alcohol	122	C8H10O	000060-12-8	80
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	49
3	Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	27
4	Toluene	92	C7H8	000108-88-3	20
5	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	18





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Misc :
ALS Vial : 6 Sample Multiplier: 1

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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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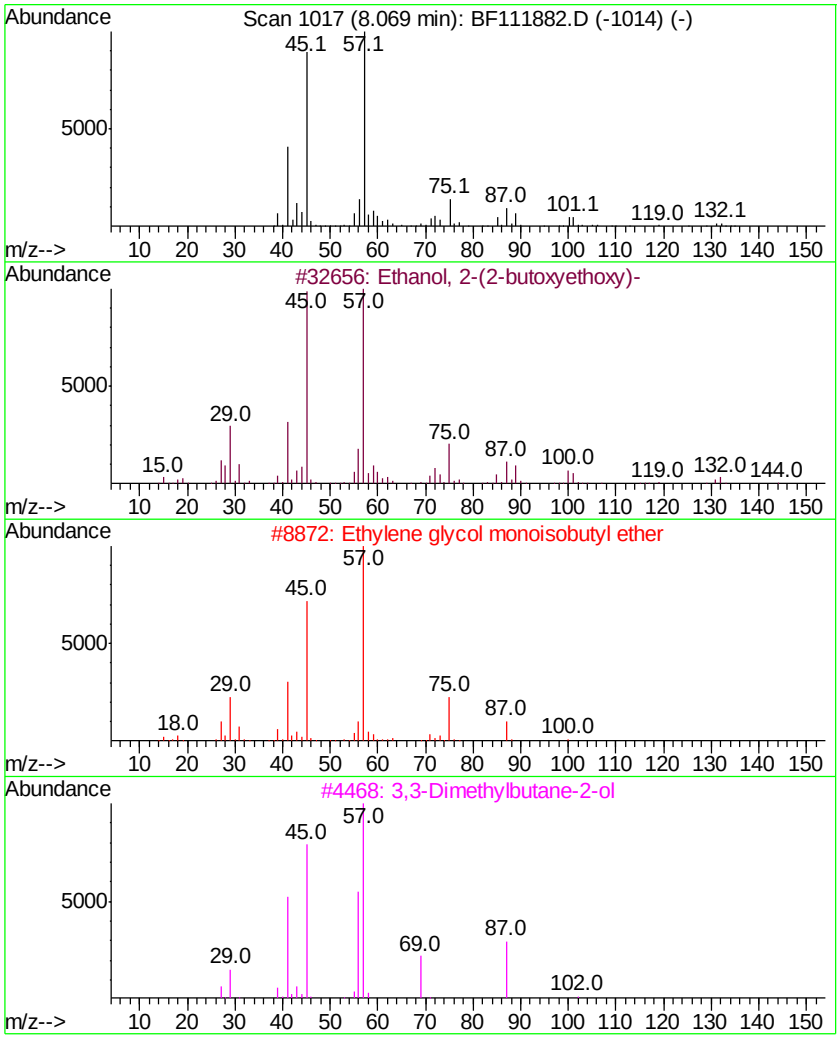
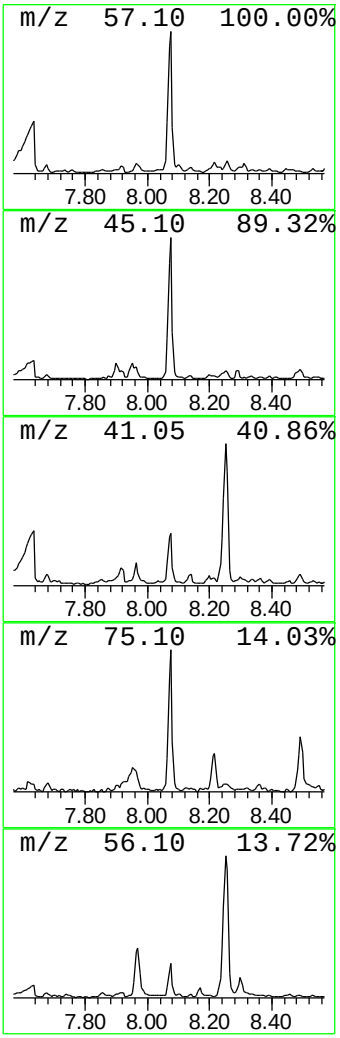
Peak Number 12 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.07	12.56 ng	636455	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	Propanoic acid, 2-hydroxy-, butyl...	146	C7H14O3	000138-22-7	50
5	2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	47





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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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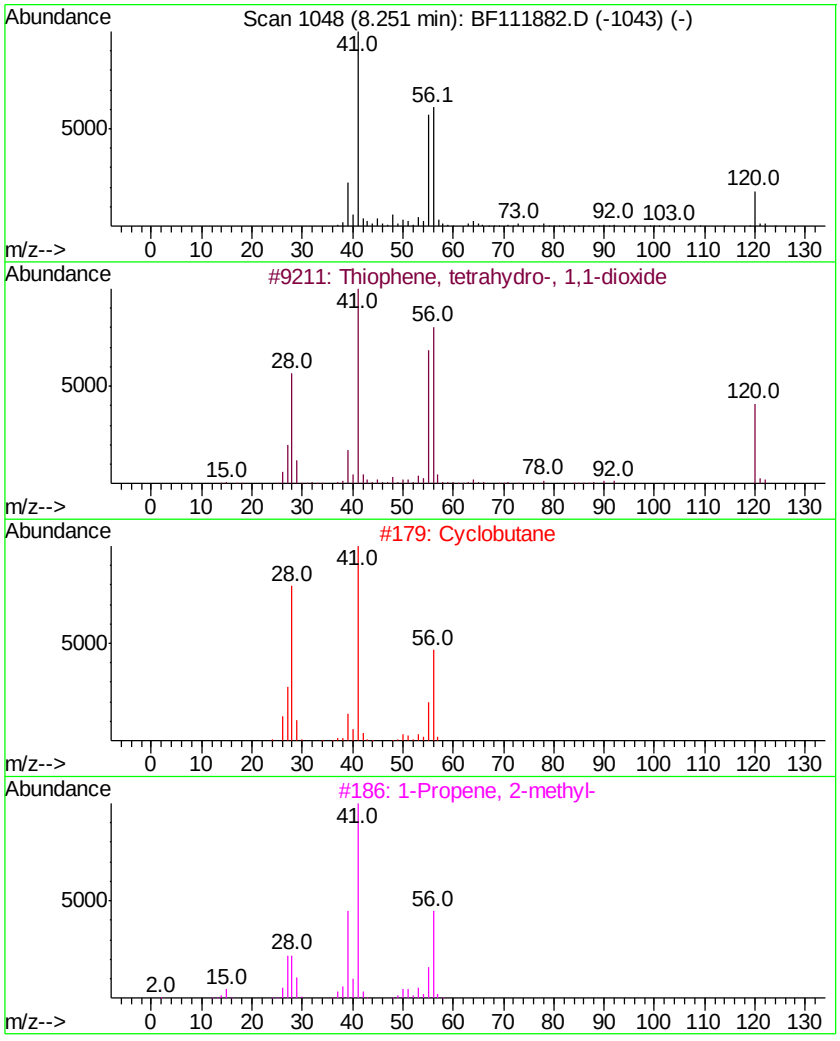
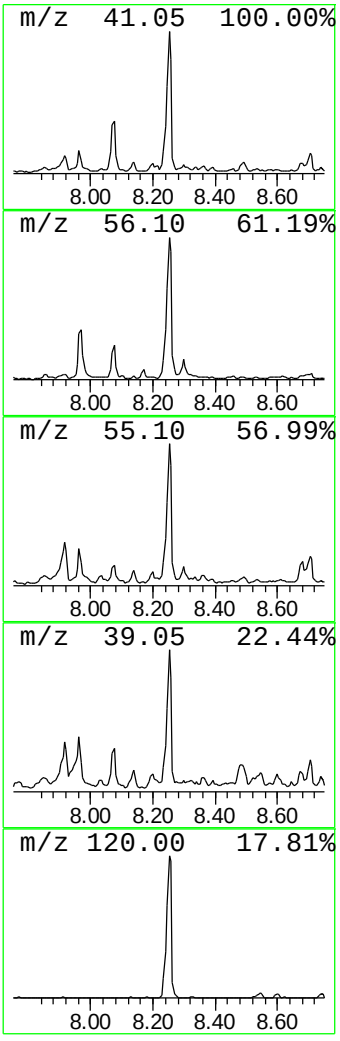
Peak Number 13 Thiophene, tetrahydro-, 1,1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	13.32 ng	674954	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-, 1,1-dioxide	120	C4H8O2S	000126-33-0	86
2	Cyclobutane	56	C4H8	000287-23-0	53
3	1-Propene, 2-methyl-	56	C4H8	000115-11-7	43
4	2-Butene, (E)-	56	C4H8	000624-64-6	43
5	2-Butene, (Z)-	56	C4H8	000590-18-1	37





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Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

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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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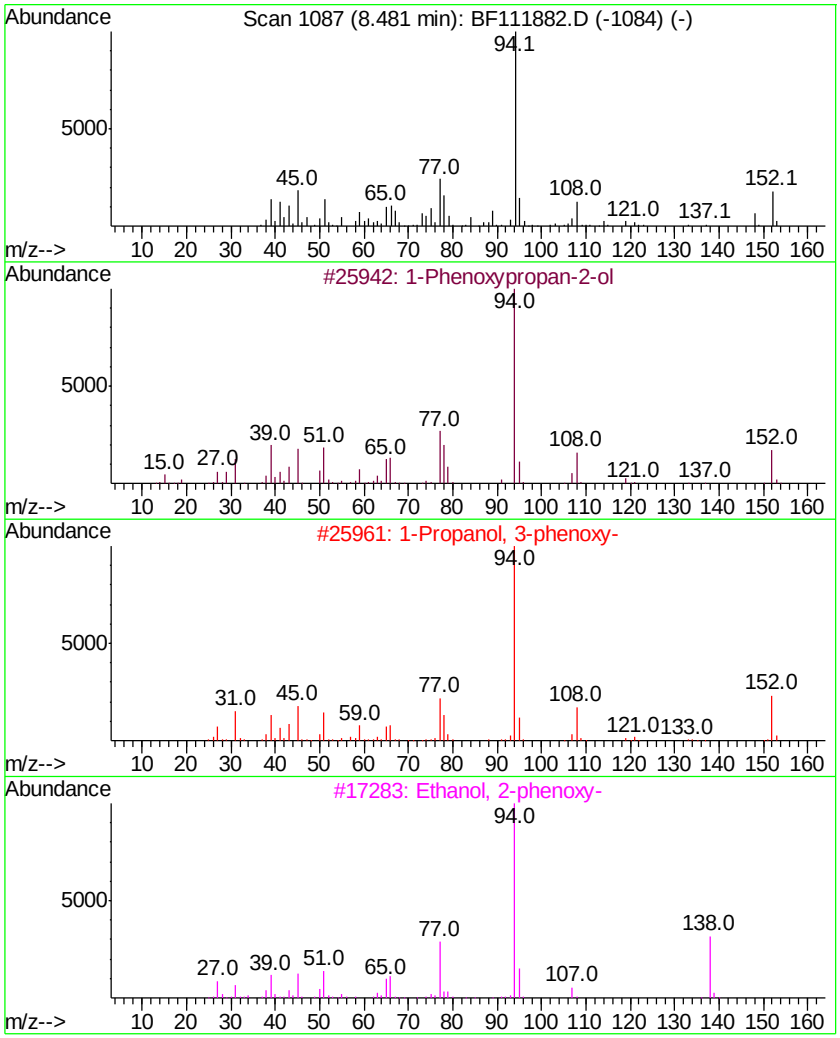
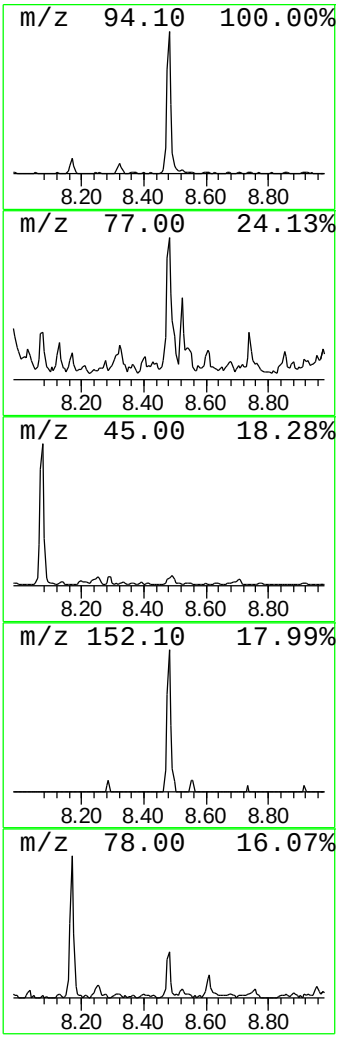
Peak Number 14 1-Phenoxypropan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.48	5.63 ng	285089	Naphthalene-d8	8.17

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	93
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53
5	Benzene, propoxy-	136	C9H12O	000622-85-5	53





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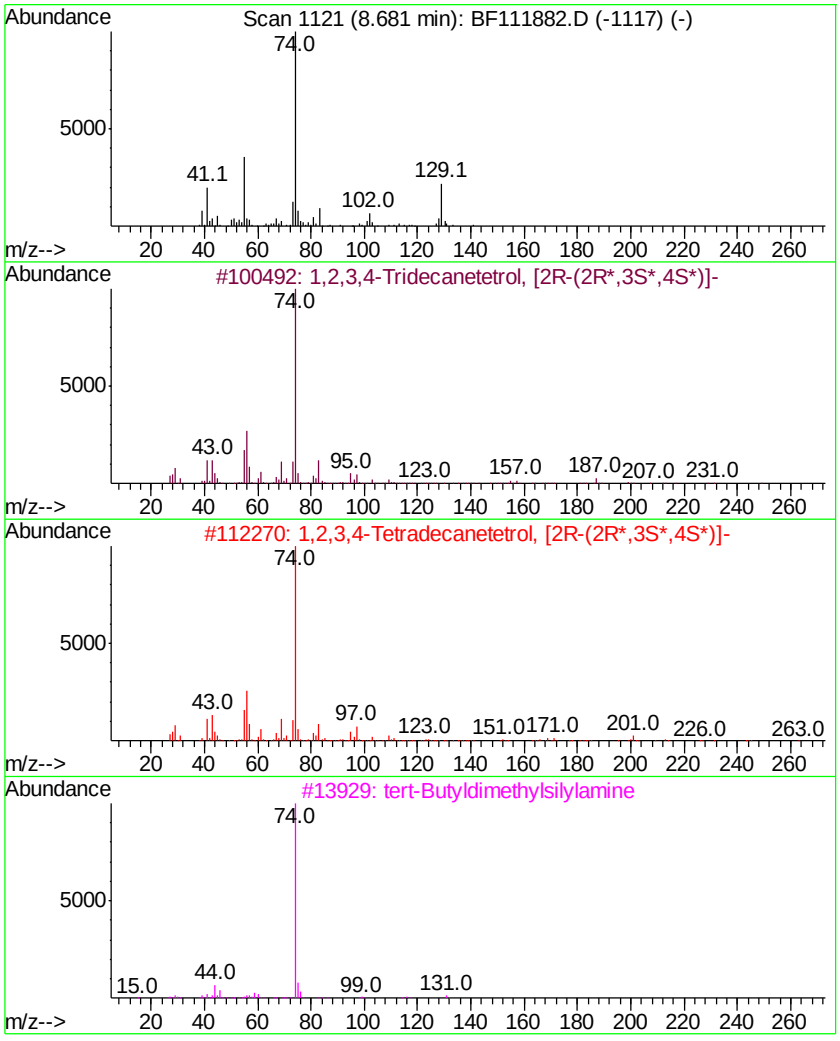
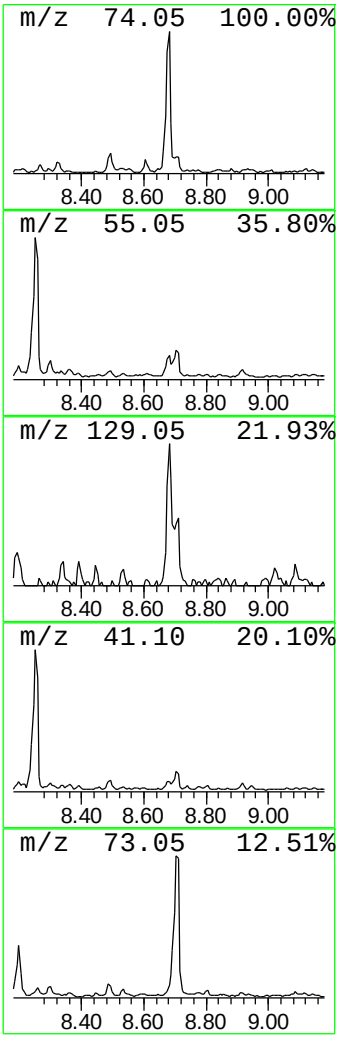
Peak Number 15 unknown8.68 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.68	3.14 ng	159297	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3,4-Tridecanetetrol, [2R-(2R...	248	C13H28O4	136953-03-2	36
2	1,2,3,4-Tetradecanetetrol, [2R-(...	262	C14H30O4	136953-04-3	36
3	tert-Butyldimethylsilylamine	131	C6H17NSi	1000366-62-1	9
4	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	9
5	Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	9





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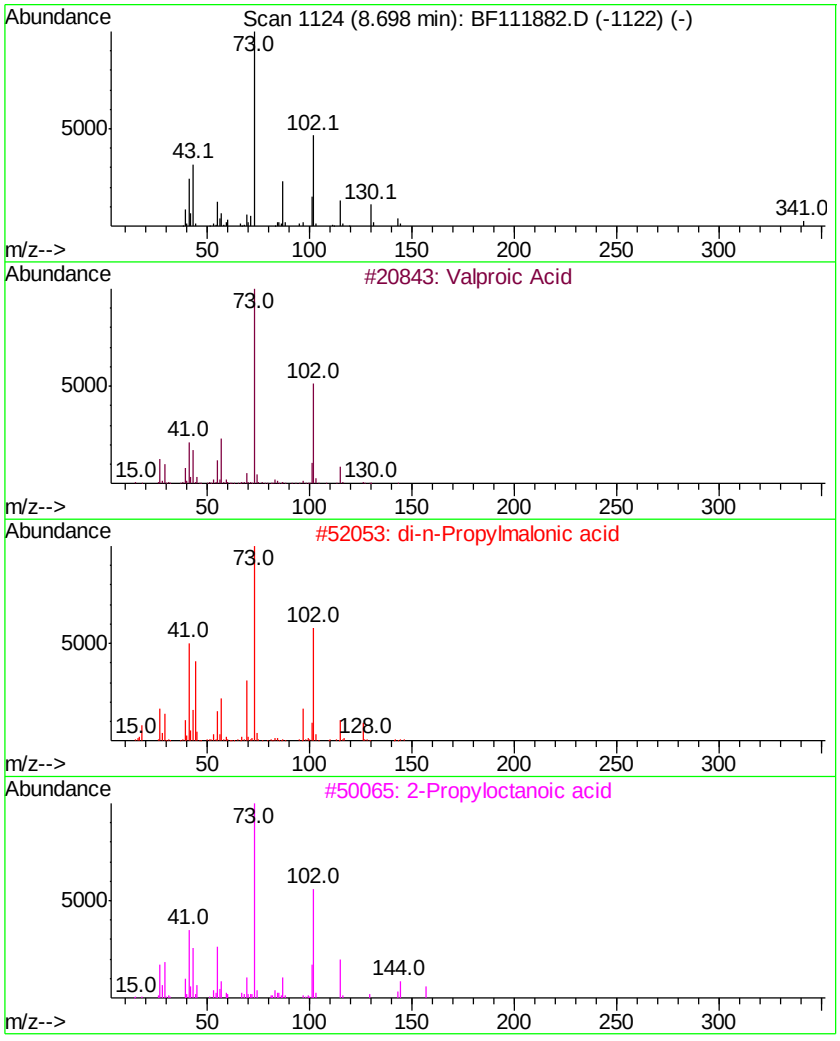
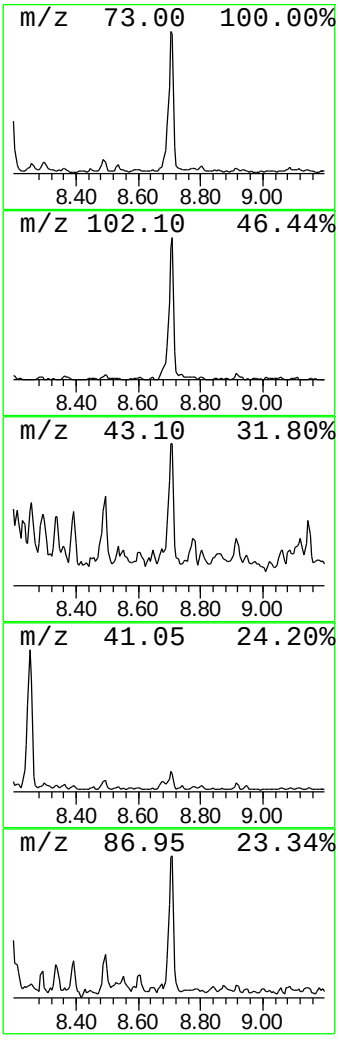
Peak Number 16 Valproic Acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	6.62 ng	335629	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Valproic Acid	144	C8H16O2	000099-66-1	50
2	di-n-Propylmalonic acid	188	C9H16O4	001636-27-7	40
3	2-Propyloctanoic acid	186	C11H22O2	031080-41-8	32
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	17
5	Scyllo-Inositol, 1-C-methyl-	194	C7H14O6	000564-92-1	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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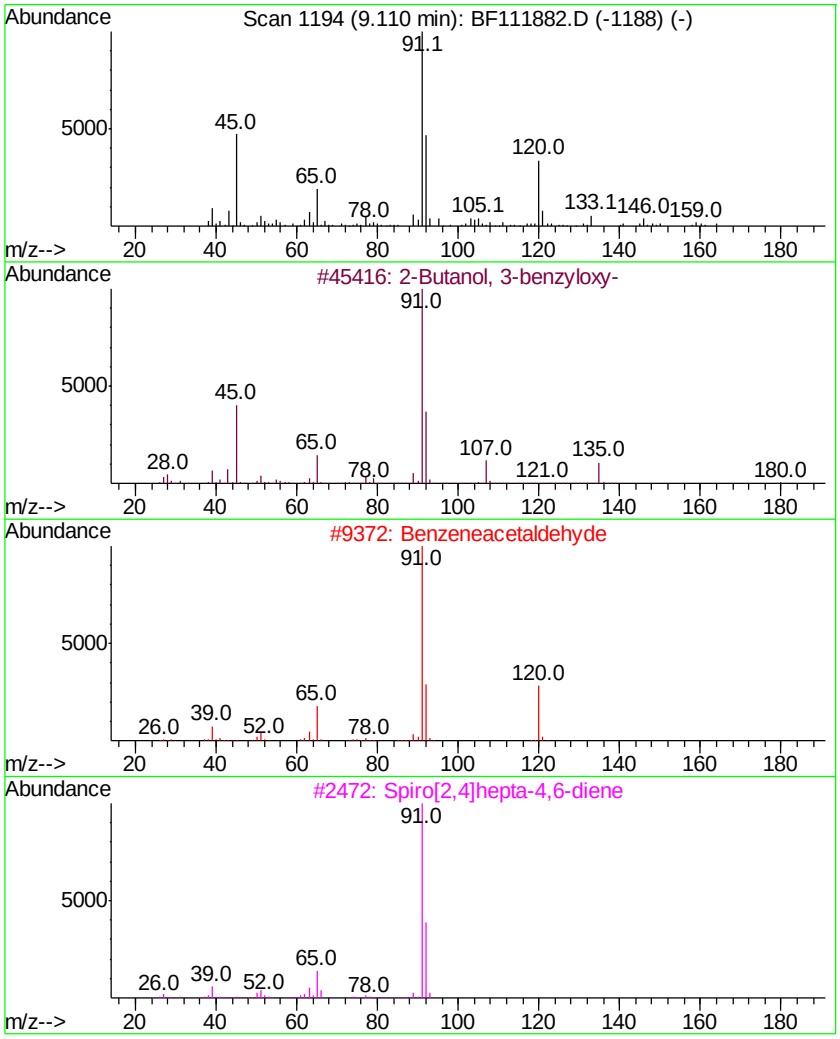
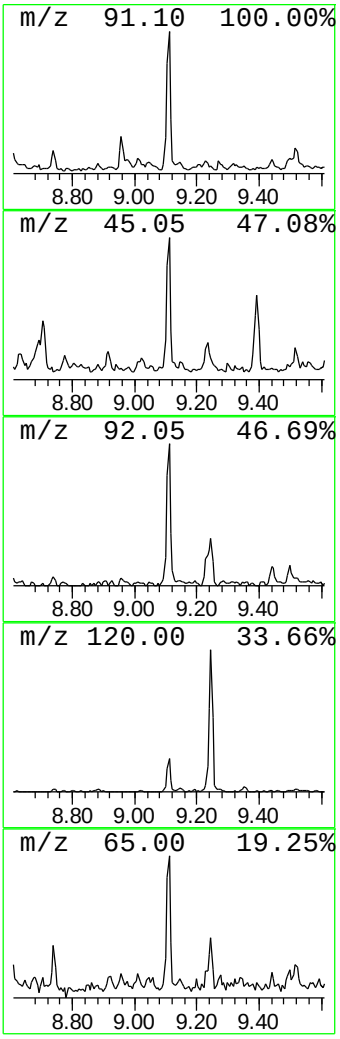
Peak Number 17 2-Butanol, 3-benzyloxy- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.11	3.40 ng	193609	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 3-benzyloxy-	180	C11H16O2	1000163-56-1	53
2	Benzeneacetaldehyde	120	C8H8O	000122-78-1	43
3	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	41
4	Phenylethyl Alcohol	122	C8H10O	000060-12-8	38
5	Benzene, propyl-	120	C9H12	000103-65-1	38





Library Search Compound Report

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Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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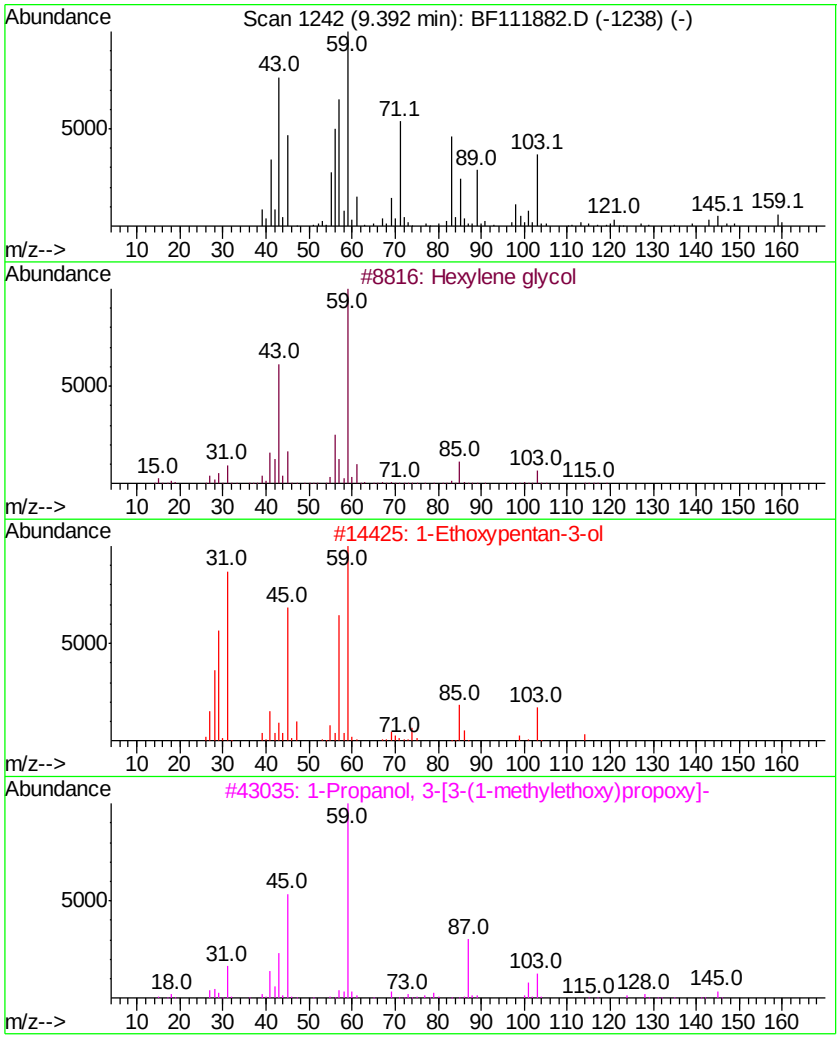
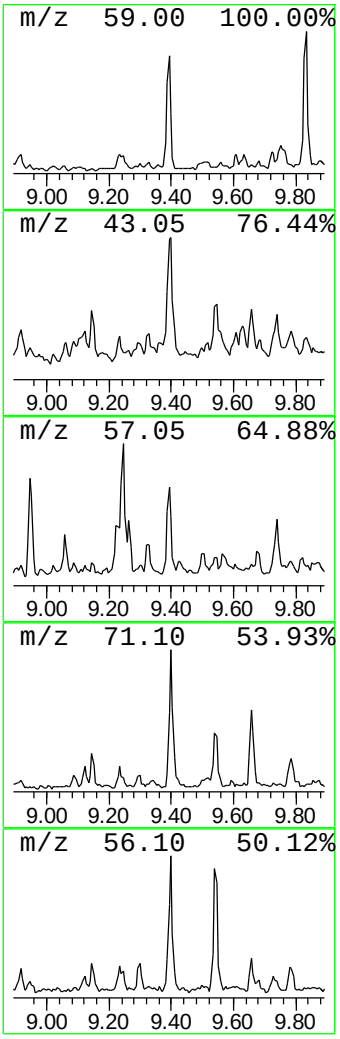
Peak Number 18 unknown9.39 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.39	3.45 ng	196459	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	38
2	1-Ethoxypentan-3-ol	132	C7H16O2	100910-92-7	35
3	1-Propanol, 3-[3-(1-methylethoxy...	176	C9H20O3	054518-03-5	27
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	25
5	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	22





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Data File : BF111882.D
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Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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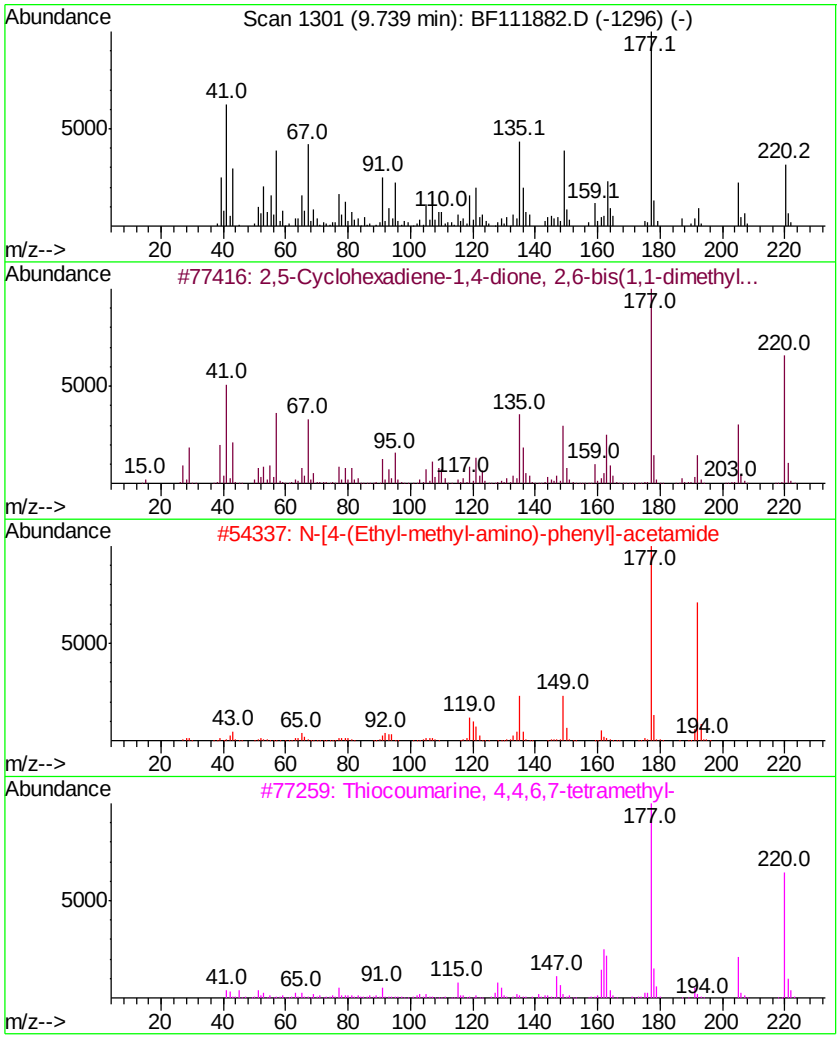
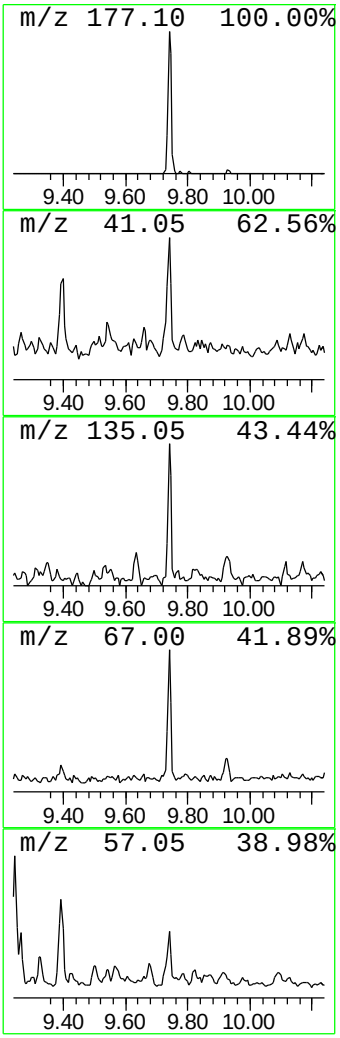
Peak Number 19 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	3.98 ng	226194	Acenaphthene-d10	9.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2	N-[4-(Ethyl-methyl-amino)-phenyl...	192	C11H16N2O	099981-45-0	43
3	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	41
4	trans-.beta.-Ionone	192	C13H20O	000079-77-6	38
5	Propanamine, 2-(1-adamantyl)-2-m...	207	C14H25N	079594-24-4	38





Library Search Compound Report

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Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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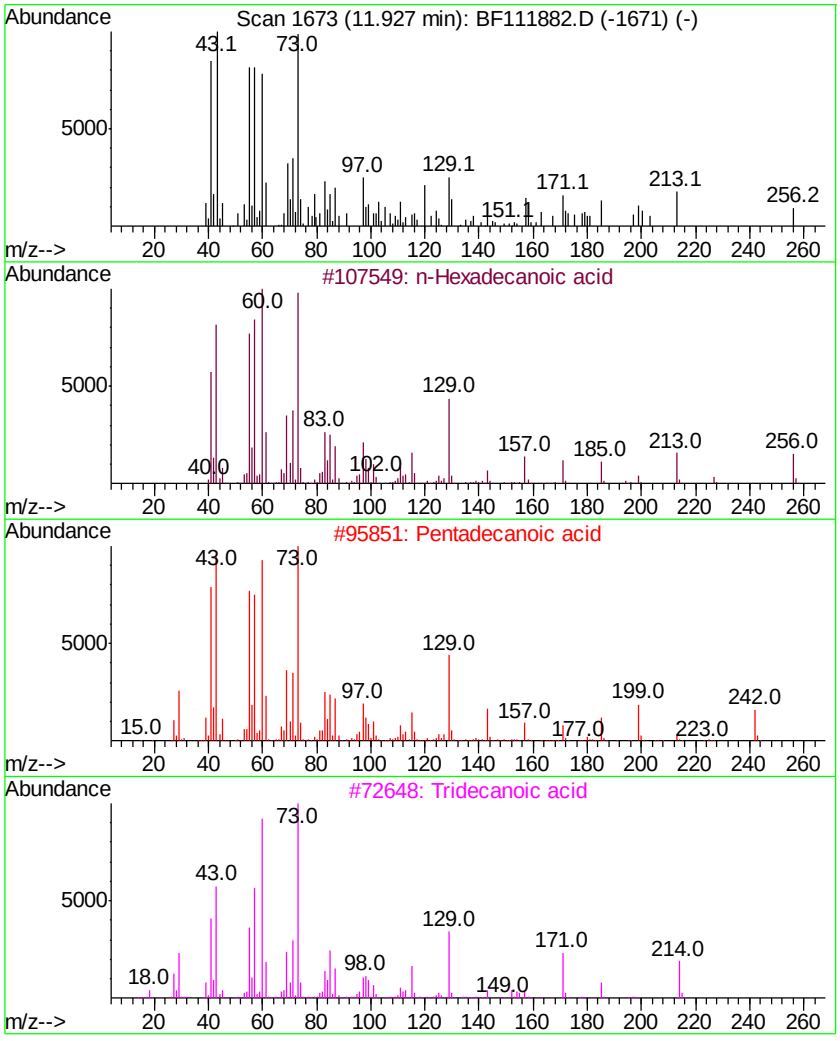
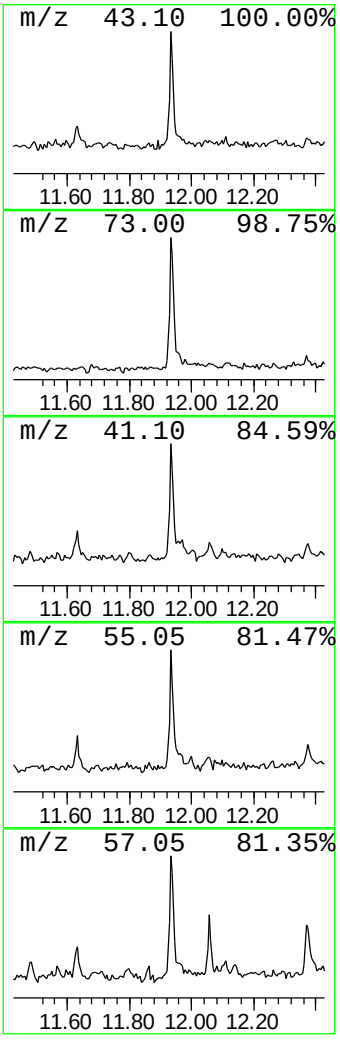
Peak Number 20 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	4.60 ng	224004	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010719\
Data File : BF111882.D
Acq On : 7 Jan 2019 17:53
Operator : JU/SJ
Sample : K1053-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-3-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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
Butane, 2-methoxy...	2.19	12.1	ng	570076	1	6.89	940841	20.0
2-Pentanone, 4-hy...	5.10	7.0	ng	331140	1	6.89	940841	20.0
Butanoic acid, 3-...	5.24	4.5	ng	210139	1	6.89	940841	20.0
Butanoic acid, 2-...	5.36	4.9	ng	232498	1	6.89	940841	20.0
5-Hydroxy-4-octanone	5.72	3.8	ng	179250	1	6.89	940841	20.0
Ethanol, 2-butoxy-	5.84	4.2	ng	198635	1	6.89	940841	20.0
Hexylene glycol	6.05	11.1	ng	519800	1	6.89	940841	20.0
unknown6.66	6.66	74.5	ng	3505370	1	6.89	940841	20.0
Ethyl dl-2-hydrox...	6.70	5.6	ng	264129	1	6.89	940841	20.0
1-Hexanol, 2-ethyl-	6.95	23.4	ng	1099440	1	6.89	940841	20.0
Phenylethyl Alcohol	7.62	52.0	ng	2638030	2	8.17	1013620	20.0
Ethanol, 2-(2-but...	8.07	12.6	ng	636455	2	8.17	1013620	20.0
Thiophene, tetrah...	8.25	13.3	ng	674954	2	8.17	1013620	20.0
1-Phenoxypropan-2-ol	8.48	5.6	ng	285089	2	8.17	1013620	20.0
unknown8.68	8.68	3.1	ng	159297	2	8.17	1013620	20.0
Valproic Acid	8.70	6.6	ng	335629	2	8.17	1013620	20.0
2-Butanol, 3-benz...	9.11	3.4	ng	193609	3	9.93	1137510	20.0
unknown9.39	9.39	3.5	ng	196459	3	9.93	1137510	20.0
2,5-Cyclohexadien...	9.74	4.0	ng	226194	3	9.93	1137510	20.0
n-Hexadecanoic acid	11.93	4.6	ng	224004	4	11.41	974716	20.0