LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108439.D
Acq On : 23 Aug 2018 23:43
Operator : JU/SJ
Sample : J4559-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

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-BF080818.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	2.366	3	5	21	rVB3	358997	524613	45.80%	3.114%
2	2.490	23	26	31	rVV	31426	40823	3.56%	0.242%
3	2.584	38	42	46	rVB3	20961	29725	2.60%	0.176%
4	2.725	59	66	75	rVB	781168	1083182	94.57%	6.429%
5	3.301	158	164	170	rVB2	25598	45427	3.97%	0.270%
6	5.231	489	492	499	rVB2	26614	34654	3.03%	0.206%
7	5.501	535	538	541	rBV	26590	23830	2.08%	0.141%
8	5.619	551	558	570	rVB2	807746	962471	84.03%	5.713%
9	5.778	582	585	590	rVB3	13183	21307	1.86%	0.126%
10	5.825	590	593	596	rVB	40517	32908	2.87%	0.195%
11	5.860	596	599	603	rBV3	44564	50723	4.43%	0.301%
12	6.031	620	628	631	rBV3	55784	72184	6.30%	0.428%
13	6.066	631	634	636	rBV	24439	22858	2.00%	0.136%
14	6.166	648	651	654	rBV2	53912	44316	3.87%	0.263%
15	6.237	659	663	664	rBV	85389	74799	6.53%	0.444%
16	6.254	664	666	670	rVV	101791	97578	8.52%	0.579%
17	6.295	670	673	676	rVB2	62852	53207	4.65%	0.316%
18	6.331	676	679	682	rBV2	22152	25770	2.25%	0.153%
19	6.425	691	695	699	rBV4	35160	61941	5.41%	0.368%
20	6.484	703	705	708	rVB	37042	30552	2.67%	0.181%
21	6.537	708	714	716	rBV2	75550	117944	10.30%	0.700%
22	6.607	722	726	730	rBV	746296	676984	59.11%	4.018%
23	6.642	730	732	734	rVV2	41584	39110	3.41%	0.232%
24	6.672	734	737	739	rVV2	39547	37636	3.29%	0.223%
25	6.695	739	741	743	rVV2	27458	23069	2.01%	0.137%
26	6.737	743	748	749	rVV2	59906	83895	7.32%	0.498%
27	6.760	749	752	759	rVB	779235	755033	65.92%	4.481%
28	6.819	759	762	766	rBV	134201	126567	11.05%	0.751%
29	6.848	766	767	770	rVB2	42217	34333	3.00%	0.204%
30	6.907	774	777	778	rBV2	23619	20322	1.77%	0.121%
31	6.948	781	784	785	rVV	43966	38798	3.39%	0.230%
32	6.995	789	792	796	rVV	1001571	845456	73.82%	5.018%
33	7.036	796	799	800	rVV2	32187	38767	3.38%	0.230%
34	7.054	800	802	804	rVV2	39712	34960	3.05%	0.208%

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Operator : JU/SJ
Sample : J4559-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	7.095	804	809	812	rVV4	59271	84478	7.38%	0.501%
36	7.154	812	819	827	rVB	638692	693963	60.59%	4.119%
37	7.213	827	829	831	rBV	44633	31973	2.79%	0.190%
38	7.242	831	834	835	rVV3	36885	35694	3.12%	0.212%
39	7.266	835	838	840	rVB	66338	62808	5.48%	0.373%
40	7.307	843	845	848	rBV	30590	28193	2.46%	0.167%
41	7.395	852	860	862	rBV3	70745	106812	9.33%	0.634%
42	7.413	862	863	868	rVB4	38040	44773	3.91%	0.266%
43	7.478	868	874	877	rBV5	28913	56633	4.94%	0.336%
44	7.525	877	882	884	rBV3	116747	139465	12.18%	0.828%
45	7.554	884	887	892	rVV	502641	498330	43.51%	2.958%
46	7.636	896	901	904	rVB4	67268	107304	9.37%	0.637%
47	7.684	904	909	912	rVB2	57209	78721	6.87%	0.467%
48	7.731	912	917	919	rBV3	33323	46606	4.07%	0.277%
49	7.760	919	922	924	rBV	94875	70545	6.16%	0.419%
50	7.784	924	926	928	rVV2	26938	24850	2.17%	0.147%
51	7.801	928	929	936	rVB3	56519	66344	5.79%	0.394%
52	7.860	936	939	941	rBV	32027	38495	3.36%	0.228%
53	7.889	941	944	946	rBV	46133	34378	3.00%	0.204%
54	7.919	946	949	951	rBV3	37820	25884	2.26%	0.154%
55	8.013	963	965	974	rVB3	65715	75884	6.63%	0.450%
56	8.089	974	978	982	rVV4	20637	30606	2.67%	0.182%
57	8.142	985	987	990	rVB2	28589	25344	2.21%	0.150%
58	8.283	1007	1011	1016	rBV	1119441	952616	83.17%	5.654%
59	8.325	1016	1018	1021	rVB	91499	70514	6.16%	0.419%
60	8.360	1021	1024	1030	rVB6	26844	38553	3.37%	0.229%
61	8.560	1055	1058	1063	rVB4	28500	33283	2.91%	0.198%
62	8.683	1077	1079	1082	rVB	58039	42321	3.70%	0.251%
63	8.954	1122	1125	1129	rVB2	19365	21257	1.86%	0.126%
64	9.095	1147	1149	1155	rBV2	23756	23204	2.03%	0.138%
65	9.283	1179	1181	1184	rVB	62580	46697	4.08%	0.277%
66	9.354	1189	1193	1202	rBV	922963	764859	66.78%	4.540%
67	9.425	1202	1205	1208	rVV2	23978	32137	2.81%	0.191%
68	9.695	1249	1251	1254	rVB2	25114	20382	1.78%	0.121%
69	9.742	1254	1259	1263	rBV	240828	227677	19.88%	1.351%
70	9.901	1280	1286	1289	rBV6	15501	21677	1.89%	0.129%
71	9.954	1292	1295	1299	rVV	25739	25270	2.21%	0.150%

LSC Area Percent Report

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Sample : J4559-04
Misc :
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Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	10.048	1305	1311	1314	rVV2	1107141	1145330	100.00%	6.798%
73	10.077	1314	1316	1322	rVB	29476	28909	2.52%	0.172%
74	10.277	1348	1350	1359	rVB4	18018	27550	2.41%	0.164%
75	10.430	1373	1376	1378	rBV	70654	60198	5.26%	0.357%
76	10.448	1378	1379	1382	rVB2	31380	24799	2.17%	0.147%
77	10.589	1400	1403	1411	rVB2	19388	30191	2.64%	0.179%
78	10.672	1411	1417	1421	rBV2	36643	49963	4.36%	0.297%
79	10.836	1441	1445	1451	rBV	369851	349133	30.48%	2.072%
80	10.942	1458	1463	1467	rBV	64110	78763	6.88%	0.467%
81	11.377	1534	1537	1539	rBV	38096	33524	2.93%	0.199%
82	11.407	1539	1542	1545	rVB2	49440	48413	4.23%	0.287%
83	11.542	1561	1565	1567	rBV	1096059	985943	86.08%	5.852%
84	11.566	1567	1569	1573	rVB	189713	157420	13.74%	0.934%
85	11.613	1575	1577	1580	rBV	33260	29998	2.62%	0.178%
86	11.760	1599	1602	1606	rBV2	36501	51766	4.52%	0.307%
87	11.807	1607	1610	1612	rVB	26390	26786	2.34%	0.159%
88	11.954	1632	1635	1638	rBV5	16123	25636	2.24%	0.152%
89	12.042	1647	1650	1652	rBV2	21118	21692	1.89%	0.129%
90	12.071	1652	1655	1659	rVV2	36046	48187	4.21%	0.286%
91	12.154	1667	1669	1672	rBV2	34376	33822	2.95%	0.201%
92	12.336	1698	1700	1703	rBV2	25993	25756	2.25%	0.153%
93	12.495	1724	1727	1730	rBV	36296	43143	3.77%	0.256%
94	12.707	1761	1763	1767	rBV3	34525	38540	3.36%	0.229%
95	12.760	1769	1772	1775	rVB	361994	293315	25.61%	1.741%
96	12.989	1805	1811	1817	rBV	272119	385103	33.62%	2.286%
97	13.089	1825	1828	1830	rBV	65430	77437	6.76%	0.460%
98	13.124	1830	1834	1837	rVV	451518	431940	37.71%	2.564%
99	14.195	2012	2016	2019	rBV	786740	802543	70.07%	4.763%
100	15.748	2277	2280	2284	rVB	422809	558082	48.73%	3.312%

Sum of corrected areas: 16848154

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
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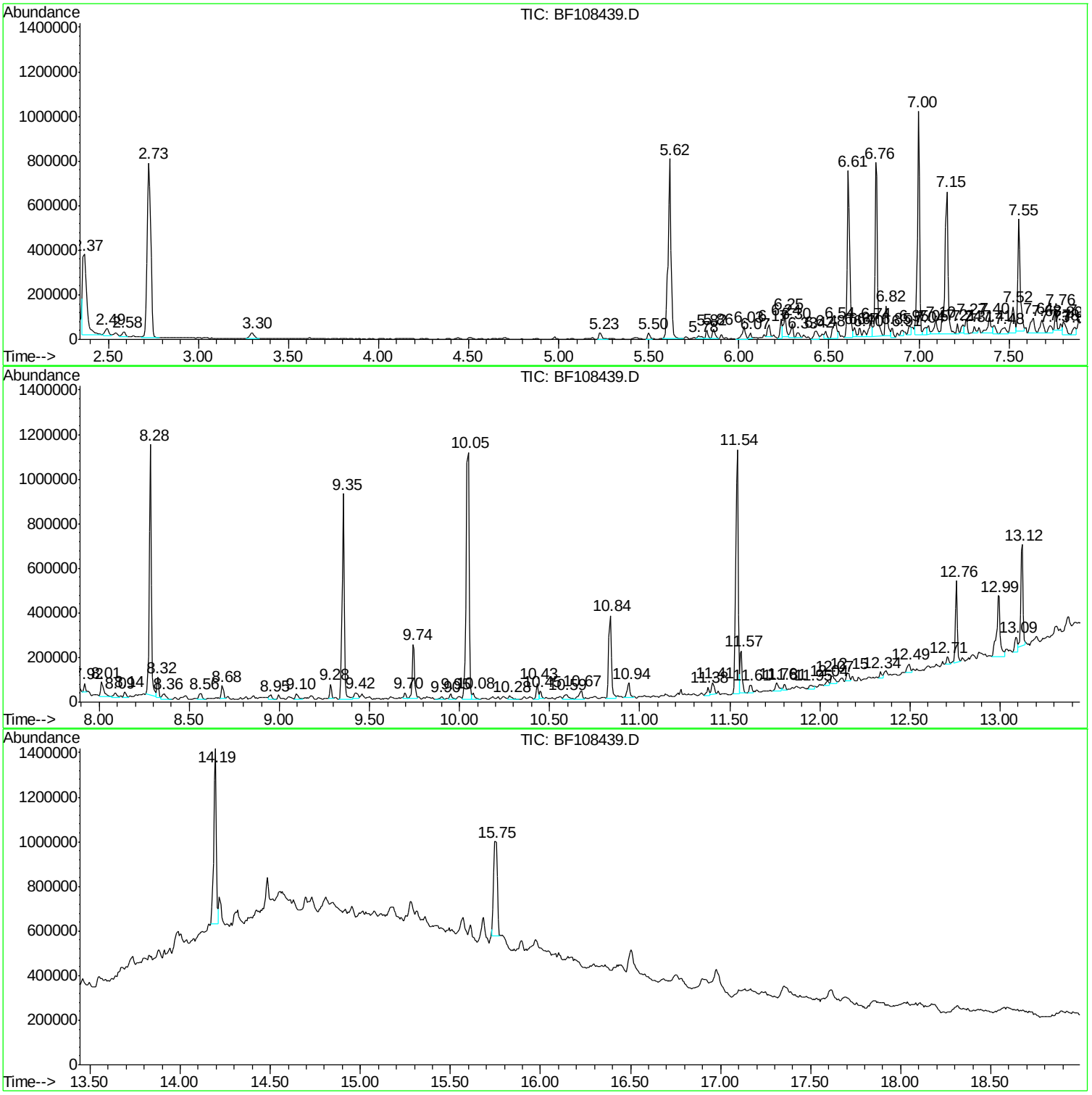
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

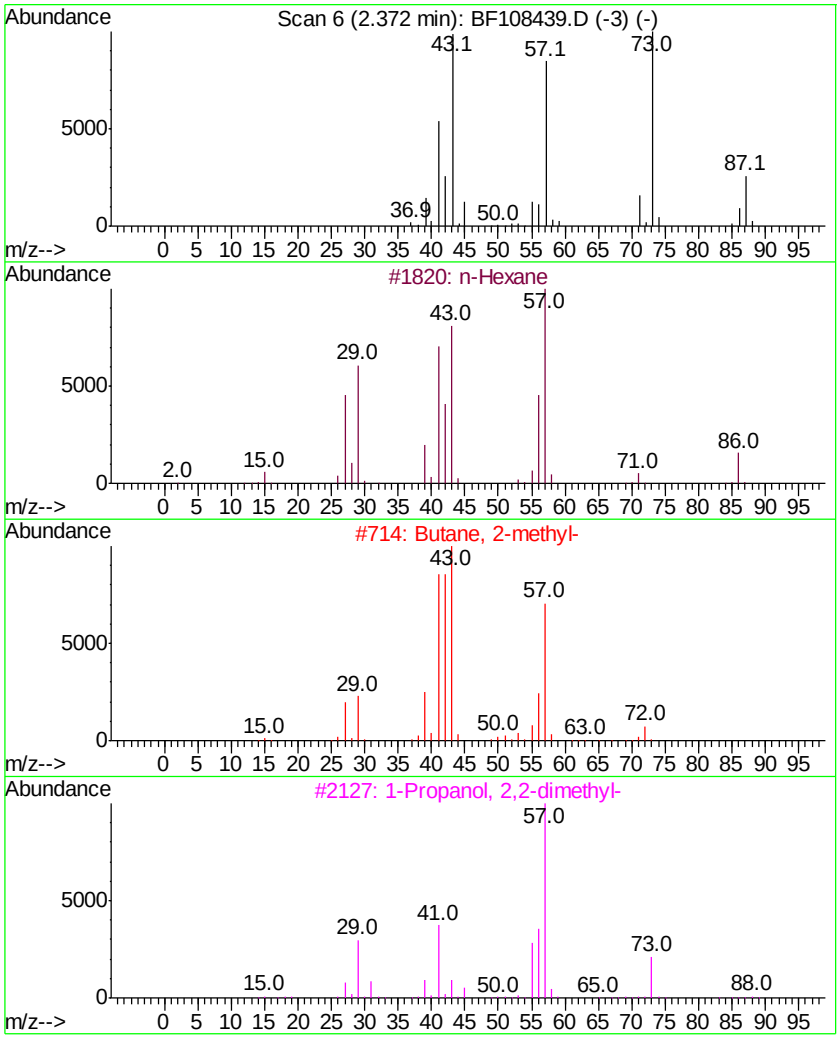
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

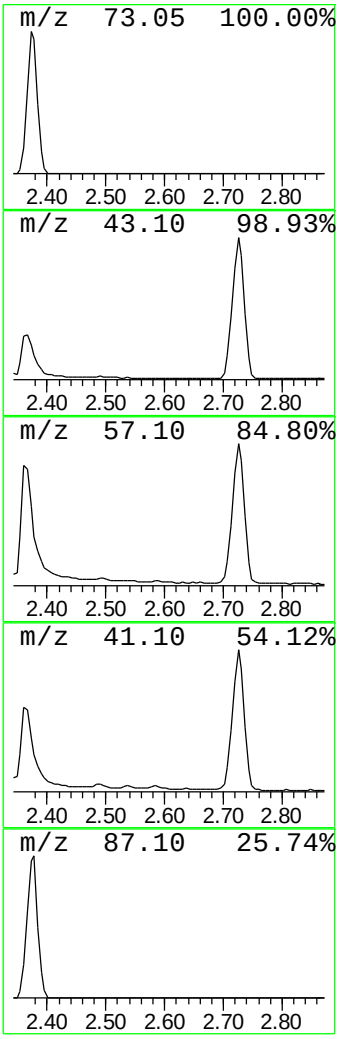
****

Peak Number 1 unknown2.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	12.41 ng	524613	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	43
2	Butane, 2-methyl-	72	C5H12	000078-78-4	38
3	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	38
4	Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	25
5	Oxetane, 2,2-dimethyl-	86	C5H10O	006245-99-4	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108439.D
Acq On : 23 Aug 2018 23:43
Operator : JU/SJ
Sample : J4559-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

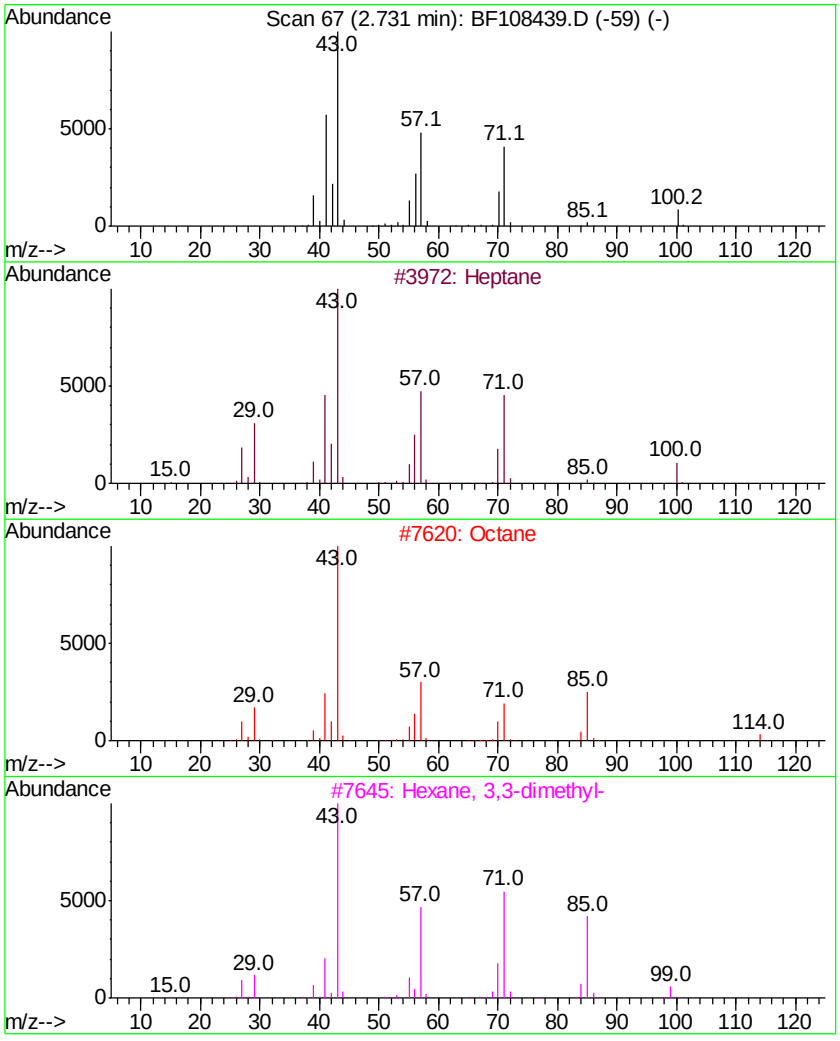
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

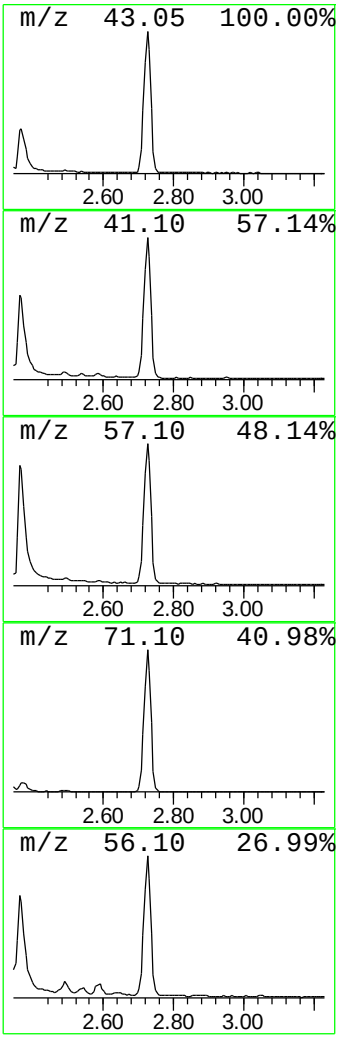
****

Peak Number 2 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.73	25.62 ng	1083180	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Octane	114	C8H18	000111-65-9	59
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	47
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	45





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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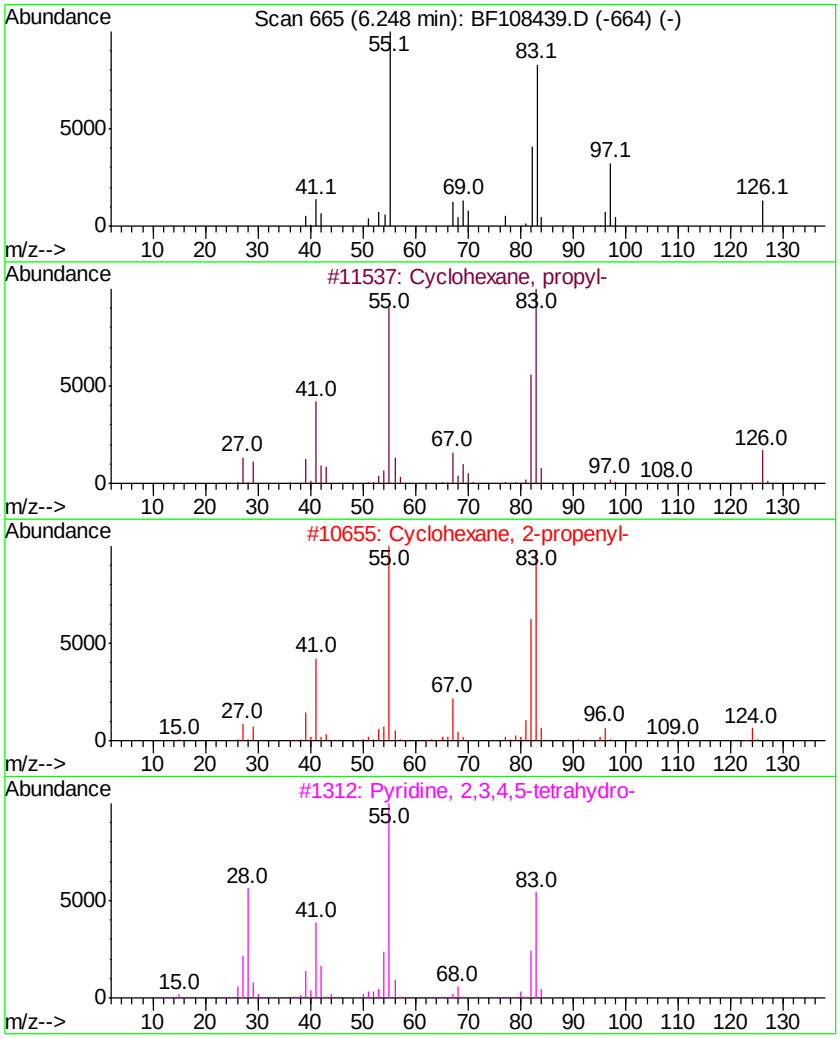
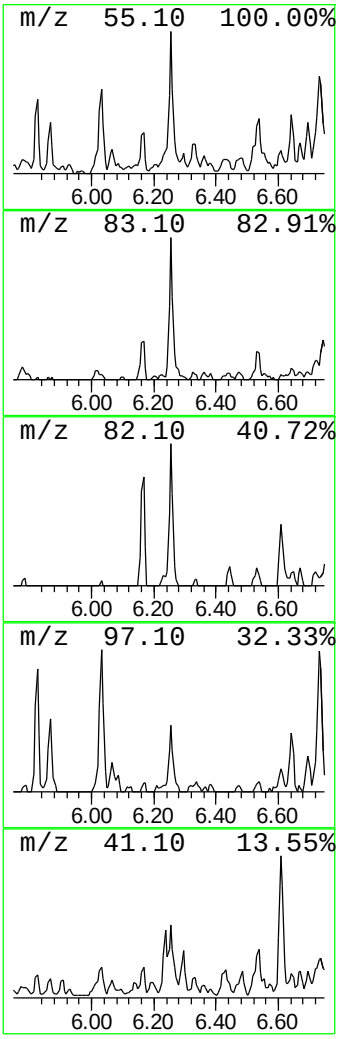
Peak Number 3 Cyclohexane, propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.25	2.31 ng	97578	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
2	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	64
3	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	53
4	Oxalic acid, cyclohexyl propyl e...	214	C11H18O4	1000309-30-3	47
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	47





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Misc :
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Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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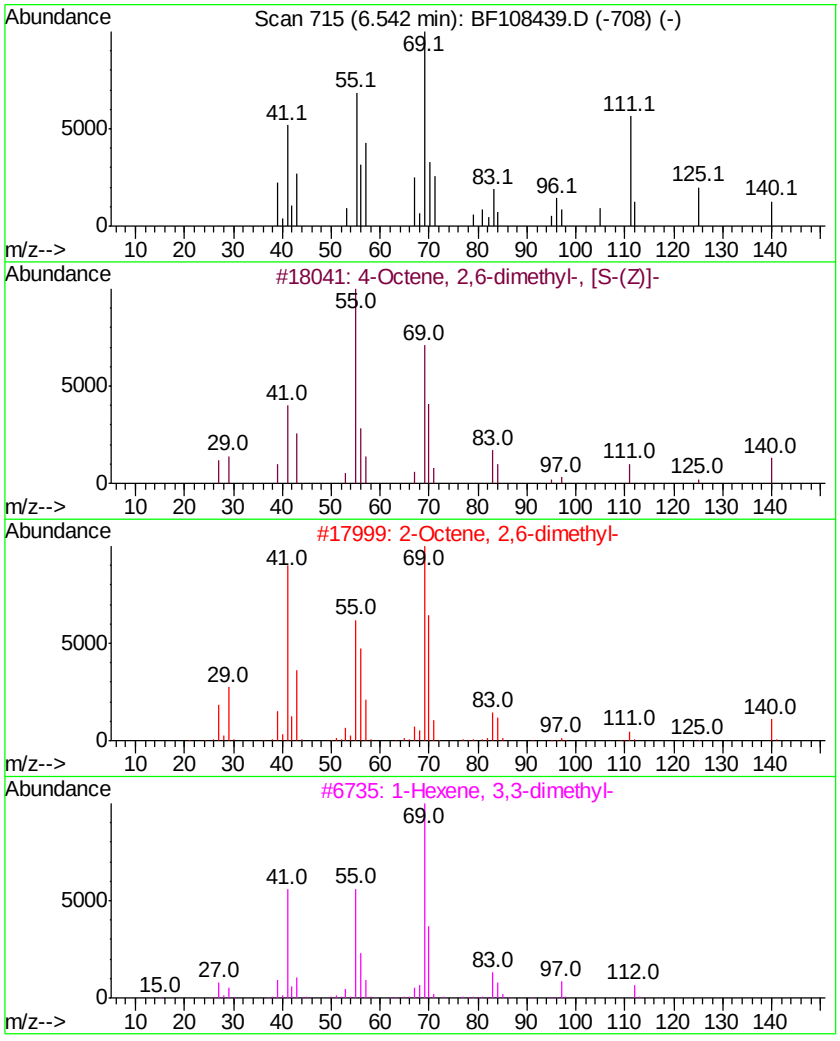
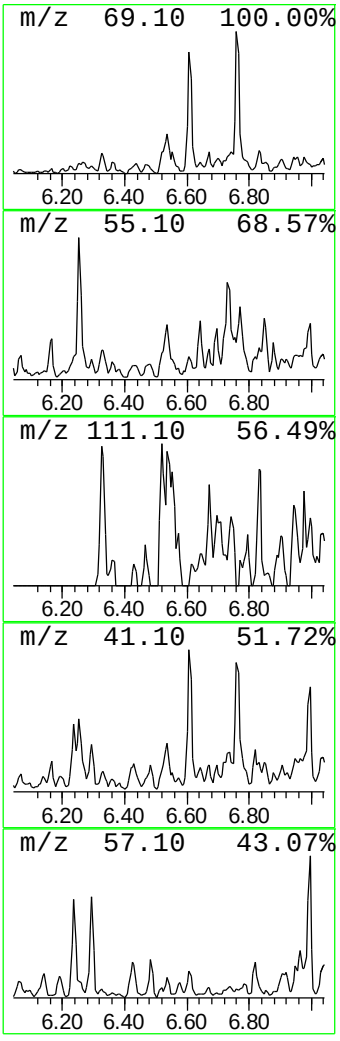
Peak Number 4 4-Octene, 2,6-dimethyl-, [S... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	2.79 ng	117944	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	64
2	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	58
3	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	52
4	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	46
5	3-Octene, 2,6-dimethyl-	140	C10H20	006874-28-8	45





Library Search Compound Report

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Sample : J4559-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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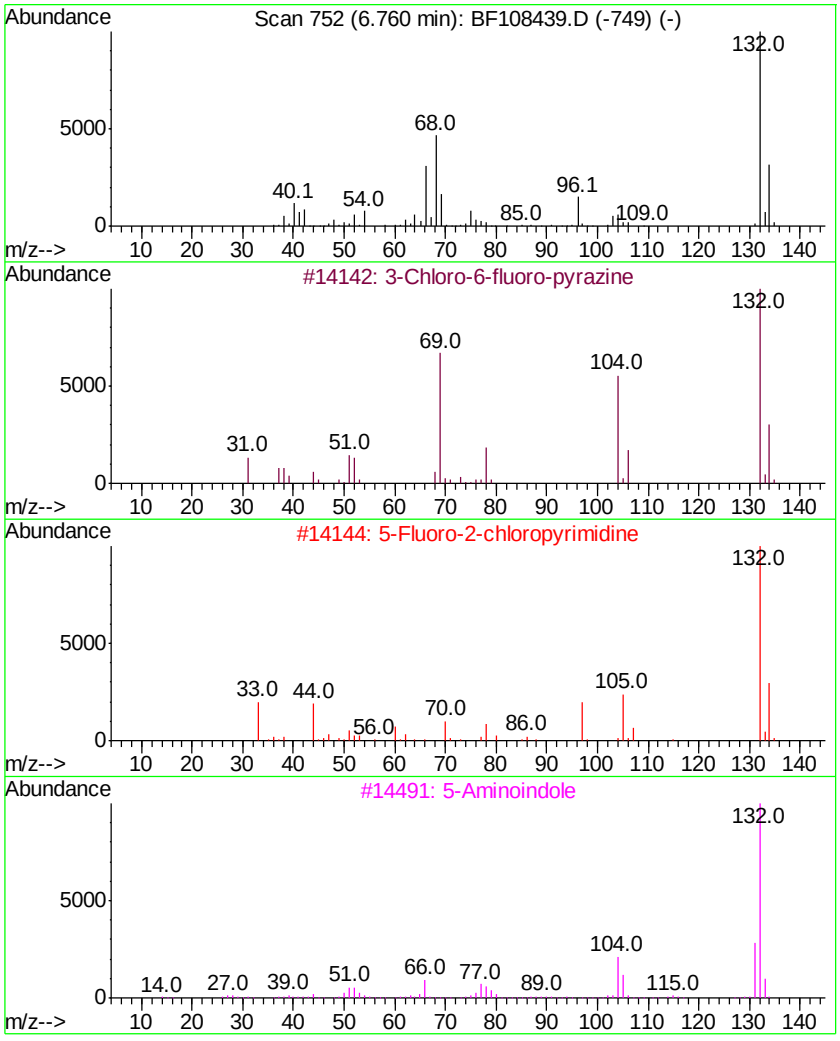
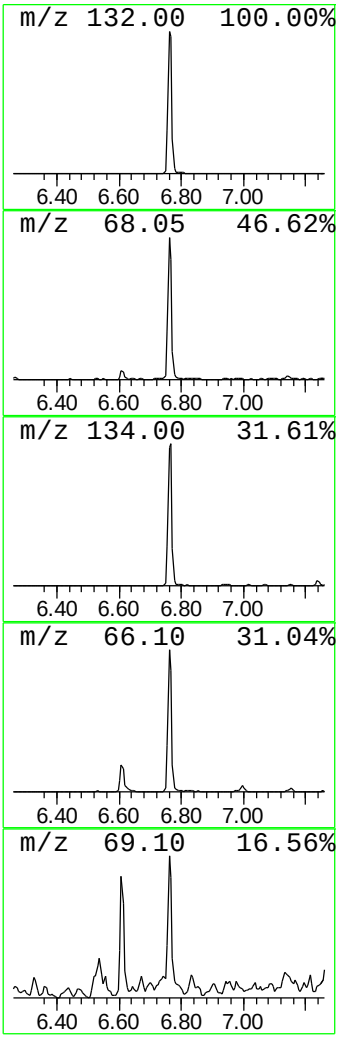
Peak Number 5 unknown6.76 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	17.86 ng	755033	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9





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Data File : BF108439.D
Acq On : 23 Aug 2018 23:43
Operator : JU/SJ
Sample : J4559-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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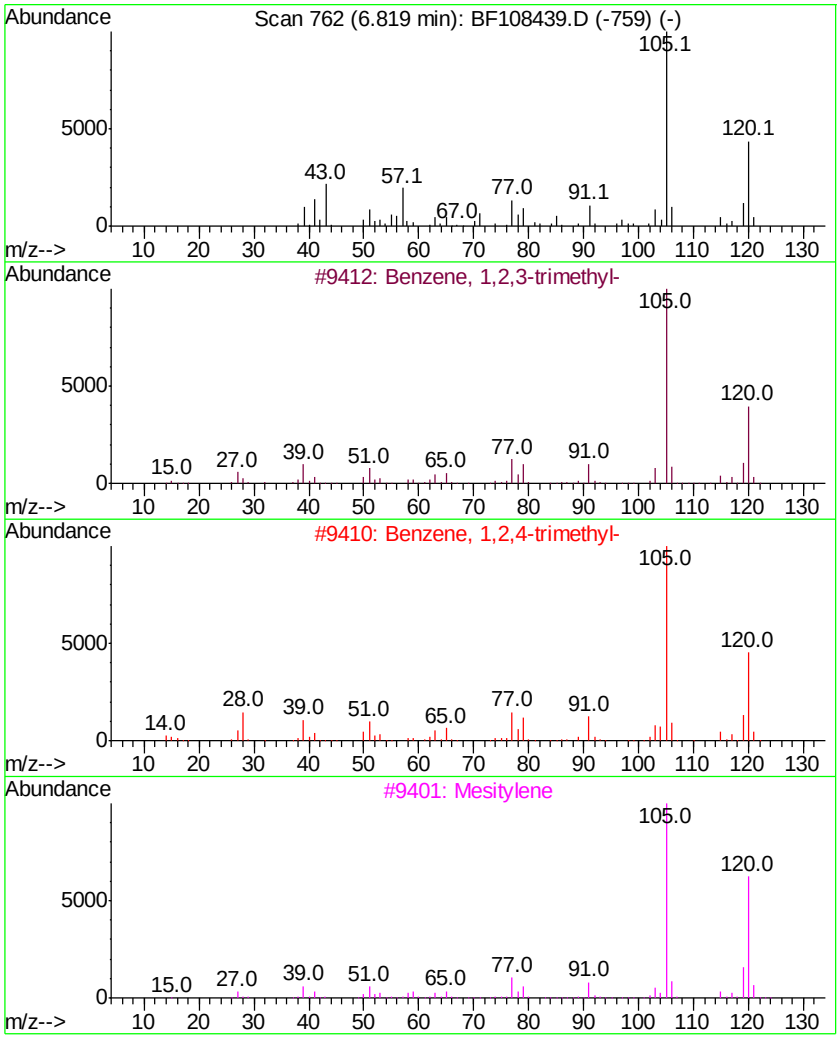
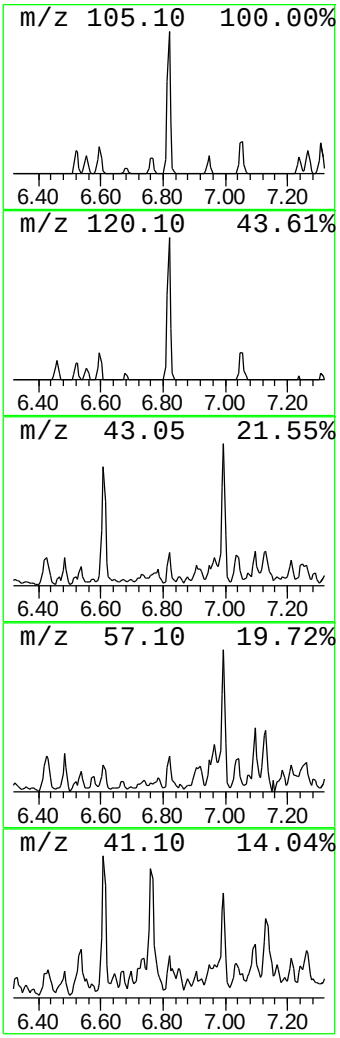
Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.82	2.99 ng	126567	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108439.D
Acq On : 23 Aug 2018 23:43
Operator : JU/SJ
Sample : J4559-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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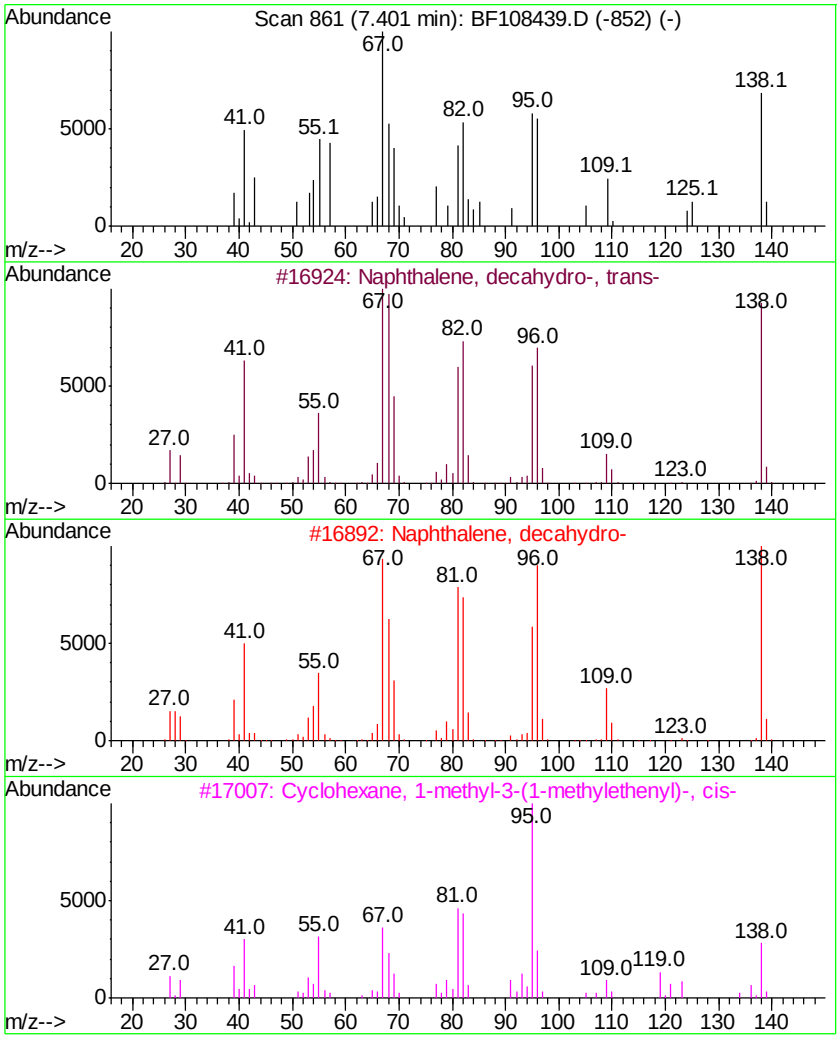
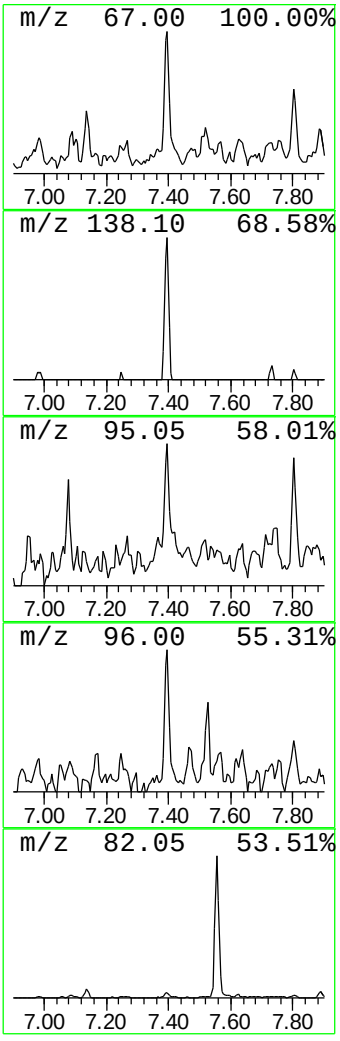
Peak Number 8 Naphthalene, decahydro-, tr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	2.53 ng	106812	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
2	Naphthalene, decahydro-	138	C10H18	000091-17-8	93
3	Cyclohexane, 1-methyl-3-(1-methy...	138	C10H18	024399-15-3	76
4	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	74
5	1,1'-Bicyclopentyl	138	C10H18	001636-39-1	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108439.D
Acq On : 23 Aug 2018 23:43
Operator : JU/SJ
Sample : J4559-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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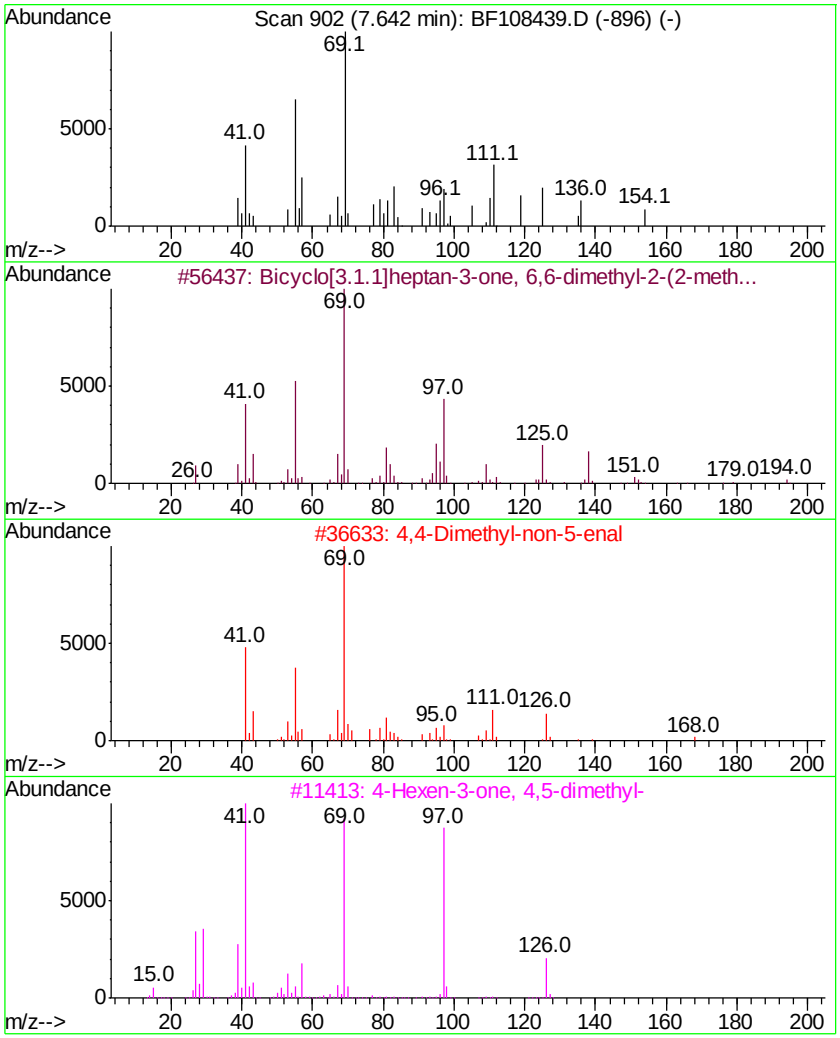
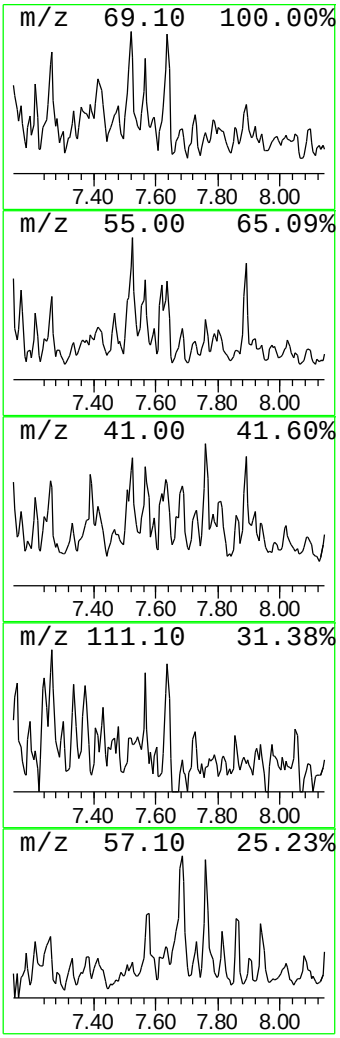
Peak Number 9 Bicyclo[3.1.1]heptan-3-one,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	2.54 ng	107304	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-3-one, 6,6-...	194	C13H22O	1000163-97-9	53
2	4,4-Dimethyl-non-5-enal	168	C11H20O	066821-98-5	47
3	4-Hexen-3-one, 4,5-dimethyl-	126	C8H14O	017325-90-5	43
4	Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	38
5	1,1'-Bicyclooctyl	222	C16H30	006708-17-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
Data File : BF108439.D
Acq On : 23 Aug 2018 23:43
Operator : JU/SJ
Sample : J4559-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081718-SSW-75-048

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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
unknown2.37	2.37	12.4	ng	524613	1	7.00	845456	20.0
Heptane	2.73	25.6	ng	1083180	1	7.00	845456	20.0
Cyclohexane, propyl-	6.25	2.3	ng	97578	1	7.00	845456	20.0
4-Octene, 2,6-dim...	6.54	2.8	ng	117944	1	7.00	845456	20.0
unknown6.76	6.76	17.9	ng	755033	1	7.00	845456	20.0
Benzene, 1,2,3-tr...	6.82	3.0	ng	126567	1	7.00	845456	20.0
Naphthalene, deca...	7.40	2.5	ng	106812	1	7.00	845456	20.0
Bicyclo[3.1.1]hep...	7.64	2.5	ng	107304	1	7.00	845456	20.0