LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016285.D
Acq On : 09 Aug 2018 17:17
Operator : SJ/JU
Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

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_M\METHODS\8270-BM072318.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	4.663	228	234	243	rBV2	26882	60207	2.12%	0.206%
2	5.187	317	323	333	rBV	48899	76800	2.70%	0.262%
3	5.663	399	404	421	rVB	437119	698761	24.56%	2.386%
4	7.310	677	684	703	rBV	237296	417636	14.68%	1.426%
5	7.663	737	744	755	rBV	965360	1548631	54.43%	5.287%
6	8.134	818	824	834	rBV	199866	327007	11.49%	1.116%
7	8.451	871	878	889	rBV	973573	1588541	55.84%	5.423%
8	9.186	996	1003	1007	rBV4	18339	36904	1.30%	0.126%
9	9.322	1019	1026	1041	rBV	711435	1193876	41.96%	4.076%
10	9.651	1076	1082	1087	rBV2	58322	88646	3.12%	0.303%
11	9.969	1130	1136	1143	rVB3	29776	55148	1.94%	0.188%
12	10.116	1153	1161	1167	rBV6	15520	38730	1.36%	0.132%
13	10.227	1172	1180	1187	rBV2	15270	31939	1.12%	0.109%
14	10.369	1196	1204	1211	rVB3	43410	102322	3.60%	0.349%
15	10.698	1246	1260	1265	rBV5	55758	170610	6.00%	0.582%
16	10.839	1274	1284	1289	rBV	142103	312477	10.98%	1.067%
17	10.898	1289	1294	1296	rVV3	26480	43258	1.52%	0.148%
18	10.945	1296	1302	1315	rVB	224659	448951	15.78%	1.533%
19	11.116	1321	1331	1337	rVB3	37670	71964	2.53%	0.246%
20	11.210	1337	1347	1353	rBV6	19200	51383	1.81%	0.175%
21	11.304	1353	1363	1367	rBV7	38110	123019	4.32%	0.420%
22	11.357	1367	1372	1380	rVV3	87544	234807	8.25%	0.802%
23	11.433	1380	1385	1392	rVB5	71366	152627	5.36%	0.521%
24	11.551	1398	1405	1410	rBV	118006	217673	7.65%	0.743%
25	11.733	1423	1436	1442	rBV	232876	662759	23.30%	2.263%
26	11.839	1449	1454	1459	rVV4	59030	111296	3.91%	0.380%
27	11.980	1472	1478	1484	rVB5	32046	70844	2.49%	0.242%
28	12.057	1484	1491	1500	rVB5	105446	319312	11.22%	1.090%
29	12.204	1502	1516	1521	rBV	190529	413152	14.52%	1.410%
30	12.263	1521	1526	1531	rBV3	63682	113740	4.00%	0.388%
31	12.327	1531	1537	1543	rVB2	139903	249203	8.76%	0.851%
32	12.427	1549	1554	1556	rBV3	48651	76929	2.70%	0.263%
33	12.533	1565	1572	1573	rBV6	50932	91083	3.20%	0.311%
34	12.574	1574	1579	1582	rVV2	102456	204165	7.18%	0.697%

LSC Area Percent Report

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Operator : SJ/JU
Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

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_M\METHODS\8270-BM072318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.627	1582	1588	1593	rVV2	181680	369559	12.99%	1.262%
36	12.692	1593	1599	1604	rVV4	84519	192728	6.77%	0.658%
37	12.780	1605	1614	1623	rVB5	178656	523215	18.39%	1.786%
38	12.874	1625	1630	1635	rBV3	118444	243766	8.57%	0.832%
39	12.945	1635	1642	1651	rVB6	134138	408201	14.35%	1.394%
40	13.027	1651	1656	1664	rBV4	148292	298473	10.49%	1.019%
41	13.104	1664	1669	1671	rBV4	59256	93056	3.27%	0.318%
42	13.210	1682	1687	1693	rBV6	58463	140462	4.94%	0.480%
43	13.274	1694	1698	1702	rVB3	77595	114442	4.02%	0.391%
44	13.327	1702	1707	1712	rBV4	65290	121824	4.28%	0.416%
45	13.386	1712	1717	1724	rVB	1672045	2388187	83.94%	8.153%
46	13.445	1724	1727	1731	rVB4	37440	46655	1.64%	0.159%
47	13.516	1731	1739	1743	rBV4	81917	164888	5.80%	0.563%
48	13.563	1744	1747	1751	rVB4	43076	58271	2.05%	0.199%
49	13.616	1751	1756	1760	rBV6	81764	176219	6.19%	0.602%
50	13.657	1760	1763	1767	rVV3	77233	117271	4.12%	0.400%
51	13.698	1767	1770	1773	rVV3	52822	67043	2.36%	0.229%
52	13.757	1776	1780	1784	rVV2	103604	179652	6.31%	0.613%
53	13.827	1788	1792	1795	rVV4	98741	150714	5.30%	0.515%
54	13.868	1796	1799	1803	rVB4	57619	84855	2.98%	0.290%
55	14.004	1817	1822	1825	rBV	159873	251013	8.82%	0.857%
56	14.039	1825	1828	1832	rVV3	188682	321857	11.31%	1.099%
57	14.092	1832	1837	1842	rVV	272674	473726	16.65%	1.617%
58	14.151	1842	1847	1850	rVV4	98153	193897	6.82%	0.662%
59	14.186	1851	1853	1857	rVV3	116890	178898	6.29%	0.611%
60	14.233	1857	1861	1866	rVV3	102534	176165	6.19%	0.601%
61	14.292	1868	1871	1874	rVB3	32287	36117	1.27%	0.123%
62	14.427	1886	1894	1898	rBV5	118933	216842	7.62%	0.740%
63	14.474	1899	1902	1906	rBV4	44445	71857	2.53%	0.245%
64	14.598	1919	1923	1924	rBV3	35612	48603	1.71%	0.166%
65	14.645	1927	1931	1936	rVB2	110444	188423	6.62%	0.643%
66	14.727	1942	1945	1948	rBV4	56391	69449	2.44%	0.237%
67	14.768	1948	1952	1955	rVV2	274925	392726	13.80%	1.341%
68	14.810	1955	1959	1965	rVB4	270131	471378	16.57%	1.609%
69	14.880	1969	1971	1976	rVB5	64607	82349	2.89%	0.281%
70	14.927	1976	1979	1982	rBV3	76658	106524	3.74%	0.364%
71	14.986	1986	1989	1992	rVB	99379	113697	4.00%	0.388%

LSC Area Percent Report

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Sample : J4369-03
Misc :
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Instrument : BNA_M
ClientSampleId : MW-27

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_M\METHODS\8270-BM072318.M
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72	15.104	2006	2009	2016	rVB2	108831	180128	6.33%	0.615%
73	15.174	2018	2021	2024	rBV3	86754	98443	3.46%	0.336%
74	15.268	2033	2037	2041	rBV2	156582	239455	8.42%	0.817%
75	15.521	2077	2080	2081	rBV	51688	54279	1.91%	0.185%
76	15.586	2088	2091	2098	rVB3	121178	199746	7.02%	0.682%
77	15.680	2104	2107	2111	rVB2	99059	129453	4.55%	0.442%
78	15.745	2111	2118	2122	rBV3	141616	265806	9.34%	0.907%
79	15.780	2122	2124	2127	rVV3	41582	50110	1.76%	0.171%
80	15.827	2127	2132	2137	rVB3	187317	302826	10.64%	1.034%
81	15.886	2138	2142	2148	rBV5	114833	207720	7.30%	0.709%
82	16.045	2165	2169	2174	rVB3	72893	107882	3.79%	0.368%
83	16.098	2174	2178	2181	rBV2	99432	147601	5.19%	0.504%
84	16.215	2195	2198	2200	rBV3	37009	36738	1.29%	0.125%
85	16.257	2200	2205	2211	rBV	1380500	1975862	69.45%	6.745%
86	16.309	2211	2214	2219	rVB	142568	206439	7.26%	0.705%
87	16.521	2245	2250	2252	rBV6	52390	83925	2.95%	0.287%
88	16.574	2257	2259	2265	rVB	75885	110933	3.90%	0.379%
89	16.698	2276	2280	2284	rVB2	63383	83552	2.94%	0.285%
90	16.898	2312	2314	2315	rBV2	35300	30990	1.09%	0.106%
91	17.080	2342	2345	2348	rVB2	37335	39587	1.39%	0.135%
92	17.121	2350	2352	2355	rVV2	32013	35660	1.25%	0.122%
93	17.433	2402	2405	2412	rBV5	48558	86445	3.04%	0.295%
94	17.503	2412	2417	2423	rVB2	338901	487610	17.14%	1.665%
95	18.362	2560	2563	2568	rBV6	44015	56824	2.00%	0.194%
96	18.580	2596	2600	2609	rVB	232351	330439	11.61%	1.128%
97	19.621	2774	2777	2786	rVB3	53249	79459	2.79%	0.271%
98	20.086	2850	2856	2861	rBV	2337299	2845011	100.00%	9.713%
99	21.633	3115	3119	3126	rVB	419882	525084	18.46%	1.793%
100	23.974	3511	3517	3524	rVB2	289298	556229	19.55%	1.899%

Sum of corrected areas: 29291638

LSC Report - Integrated Chromatogram

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Misc :
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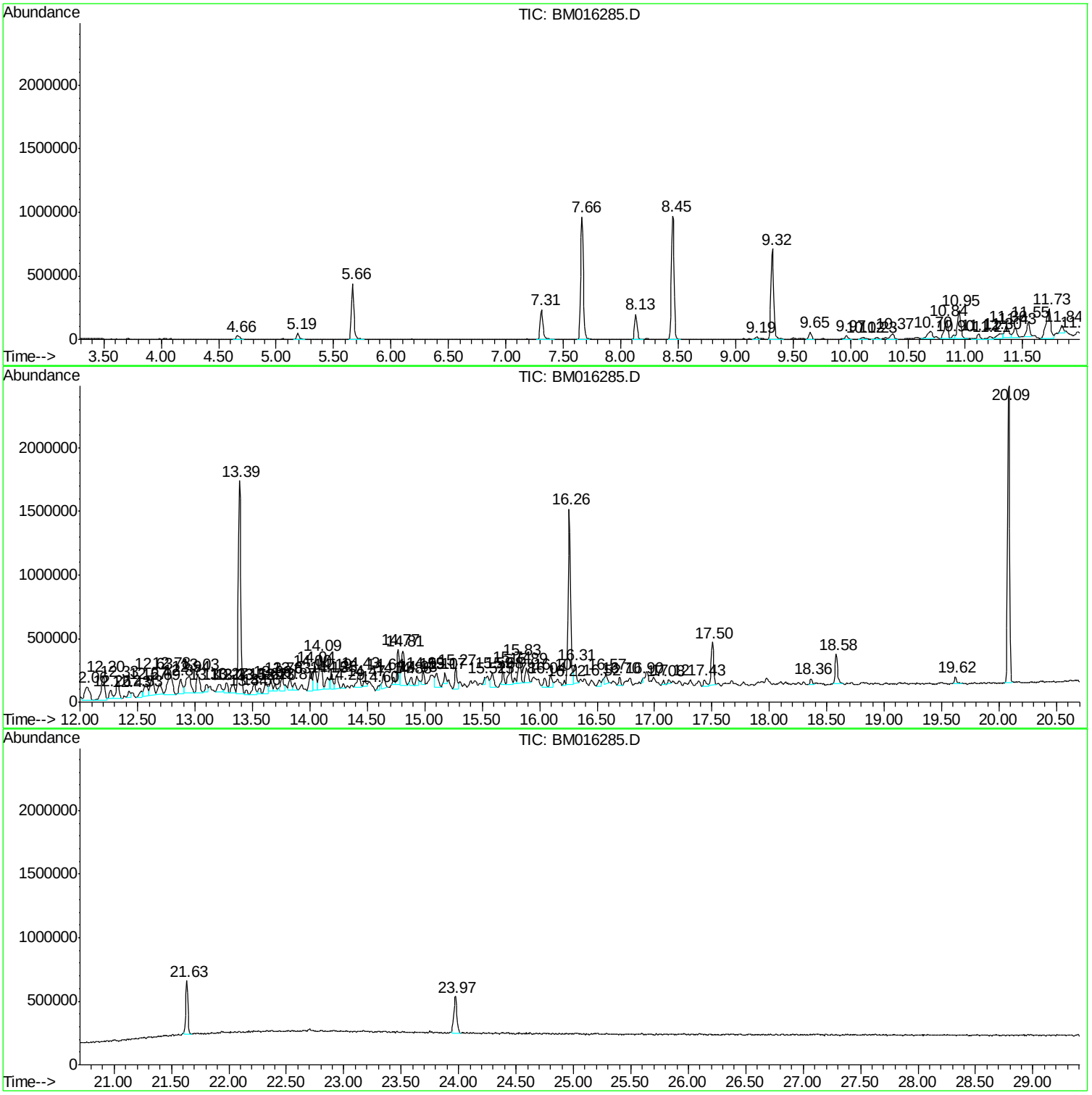
Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
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Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

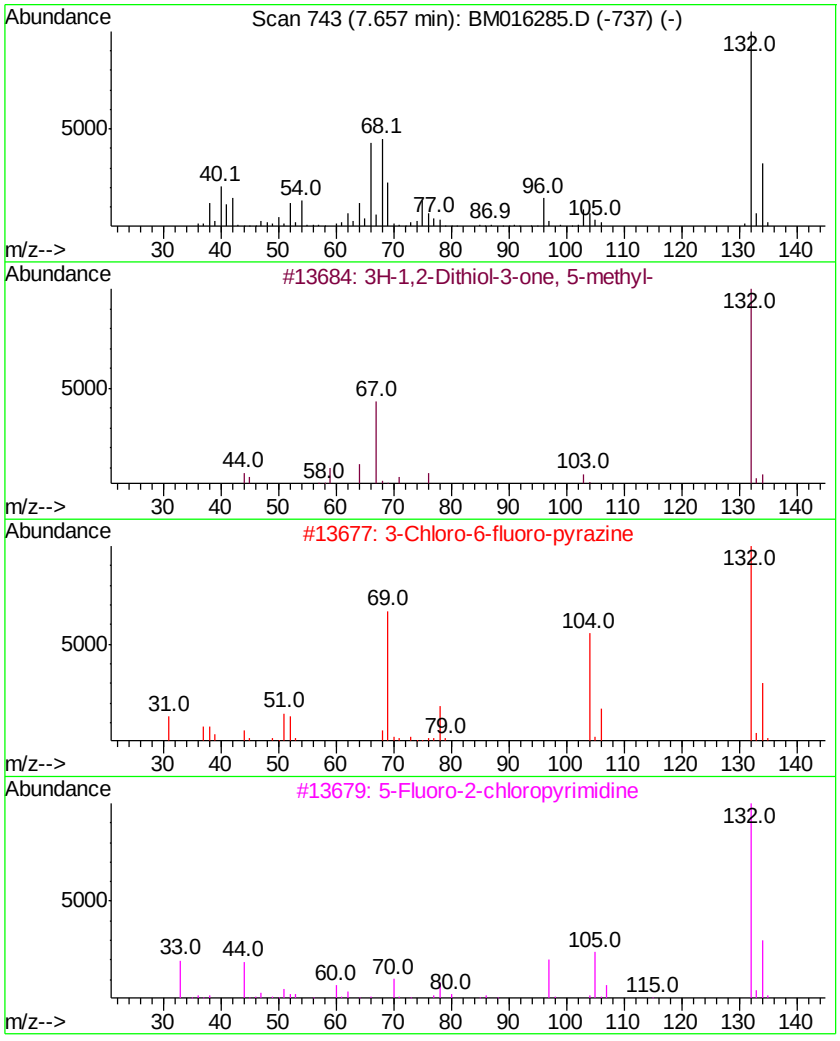
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

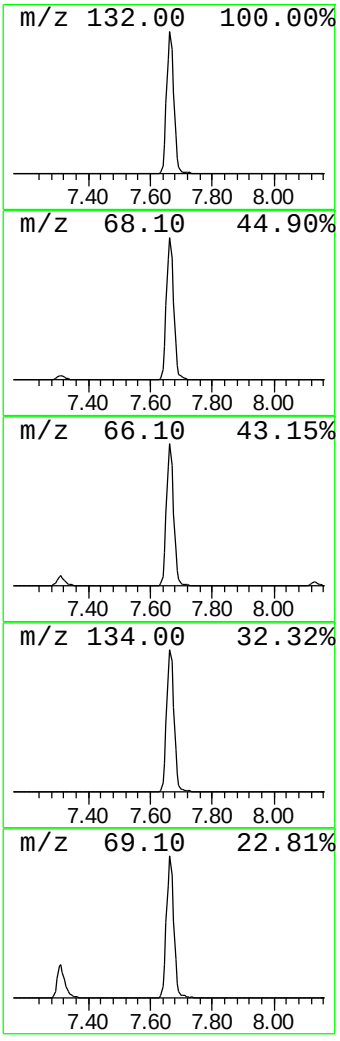
****

Peak Number 1 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	94.72 ng	1548630	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12





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Instrument : BNA_M
ClientSampleId : MW-27

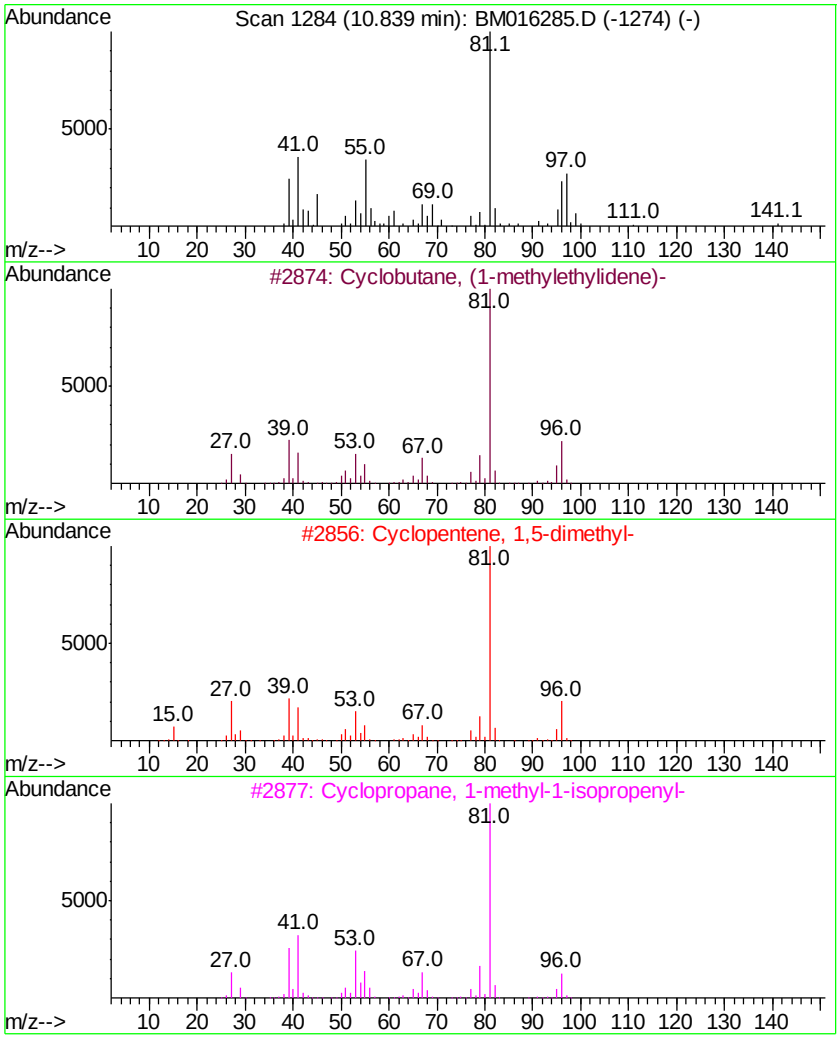
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

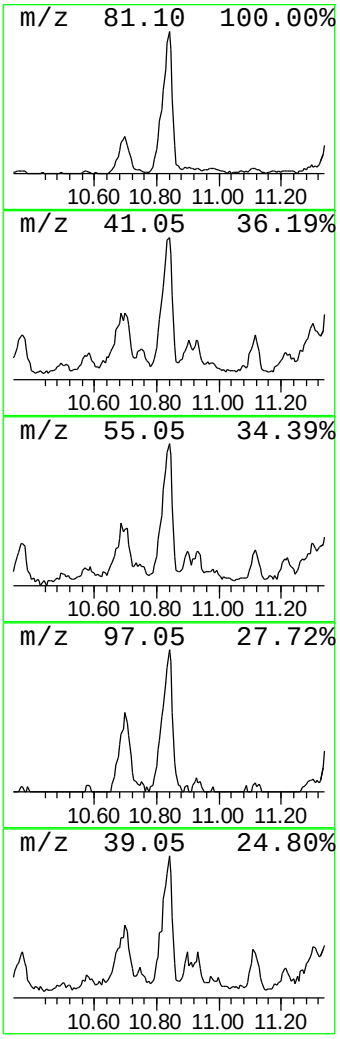
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclobutane, (1-methylethyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	13.92 ng	312477	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	76
2	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	64
3	Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	59
4	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	58
5	2,4-Hexadienal, (E,E)-	96	C6H8O	000142-83-6	50





Library Search Compound Report

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Misc :
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Instrument : BNA_M
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TIC Library : C:\DATABASE\NIST02.L
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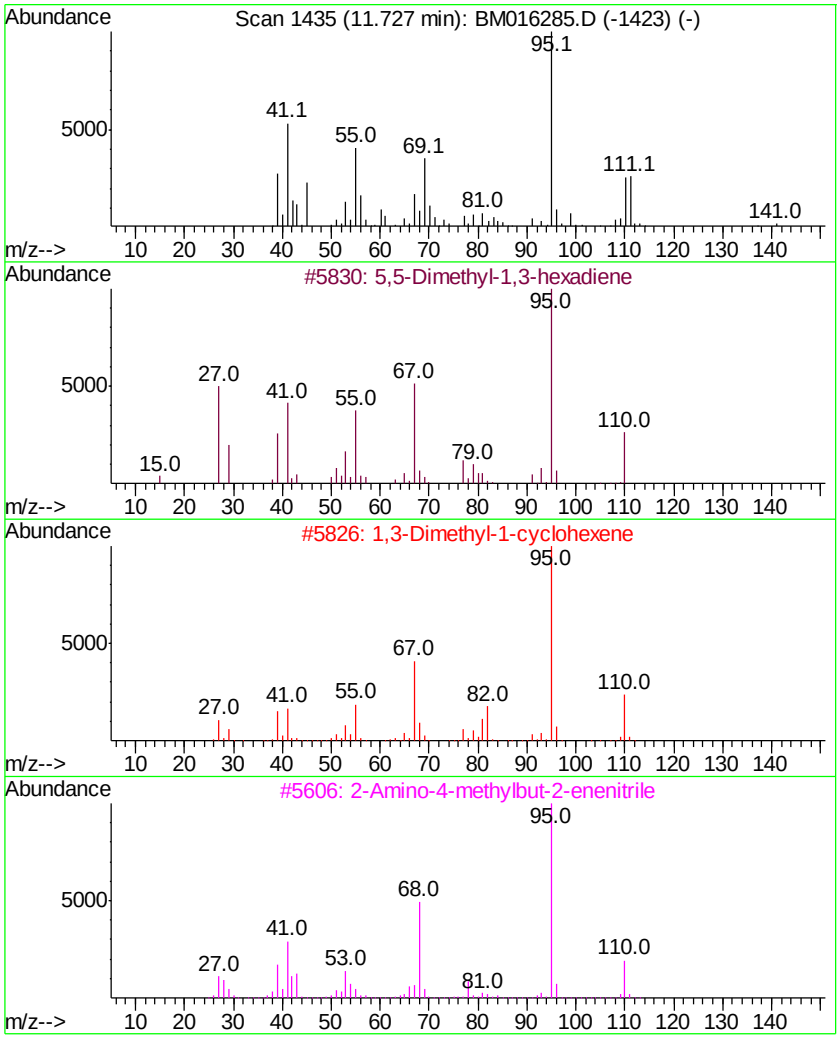
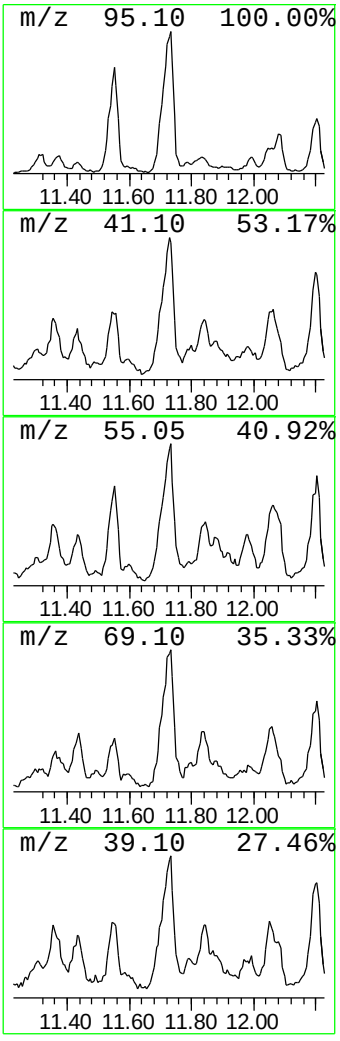
Peak Number 4 5,5-Dimethyl-1,3-hexadiene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	29.52 ng	662759	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	53
2	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	52
3	2-Amino-4-methylbut-2-enenitrile	110	C6H10N2	1000197-39-9	50
4	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	50
5	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	50





Library Search Compound Report

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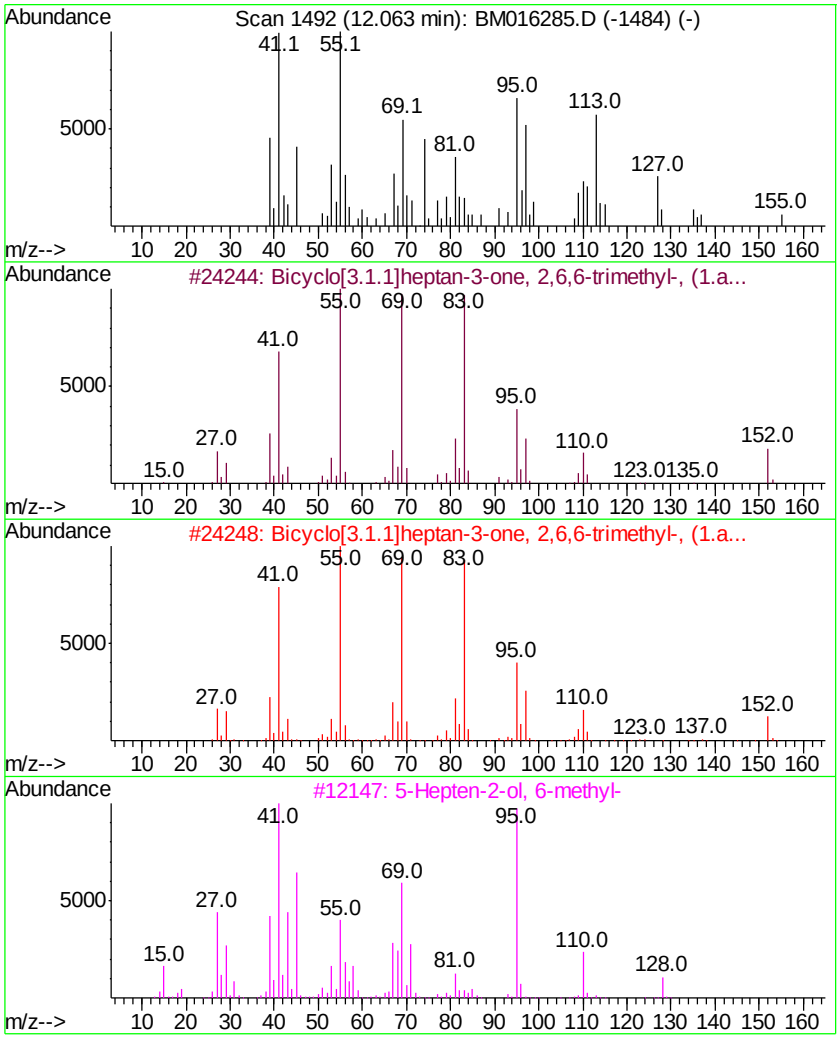
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

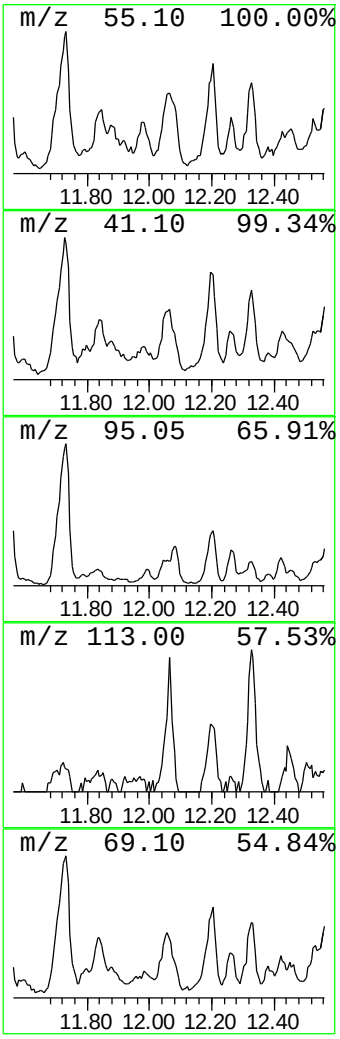
****

Peak Number 5 unknown12.06 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	14.22 ng	319312	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	38
2	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	38
3	5-Hepten-2-ol, 6-methyl-	128	C8H16O	001569-60-4	30
4	3-(But-3-enyl)-cyclohexanone	152	C10H16O	003636-03-1	27
5	dl-6-Methyl-5-hepten-2-ol	128	C8H16O	004630-06-2	18





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Data File : BM016285.D
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Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

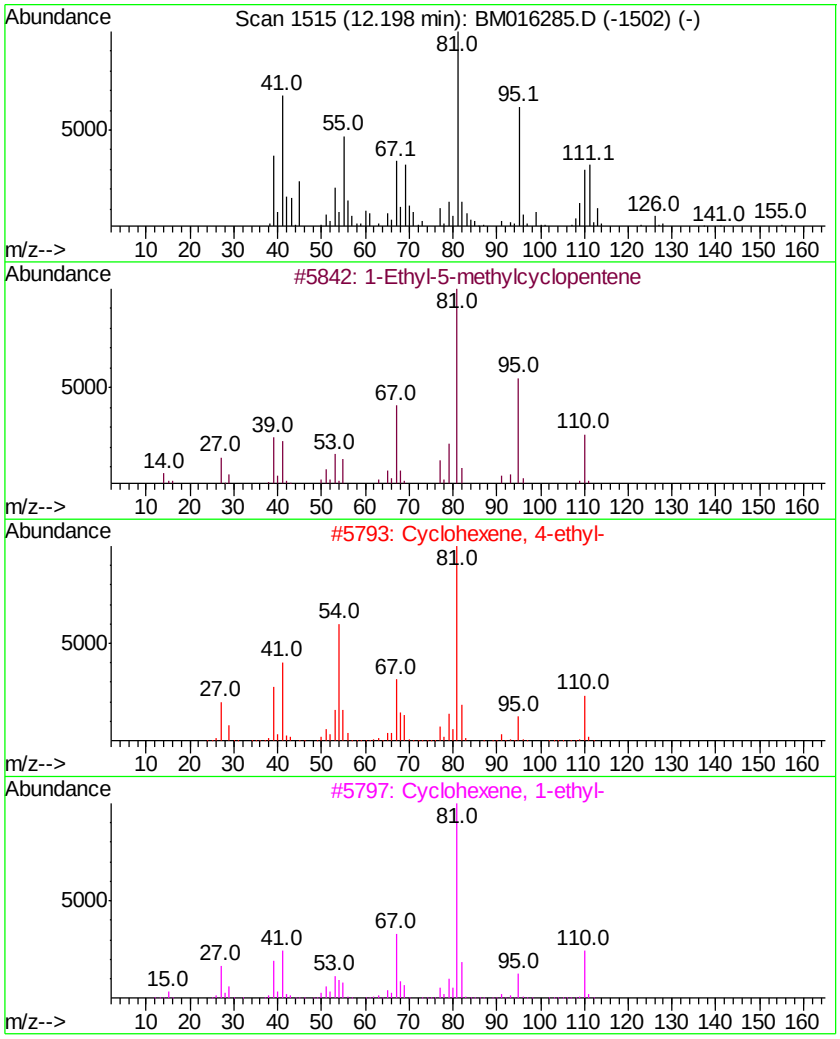
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

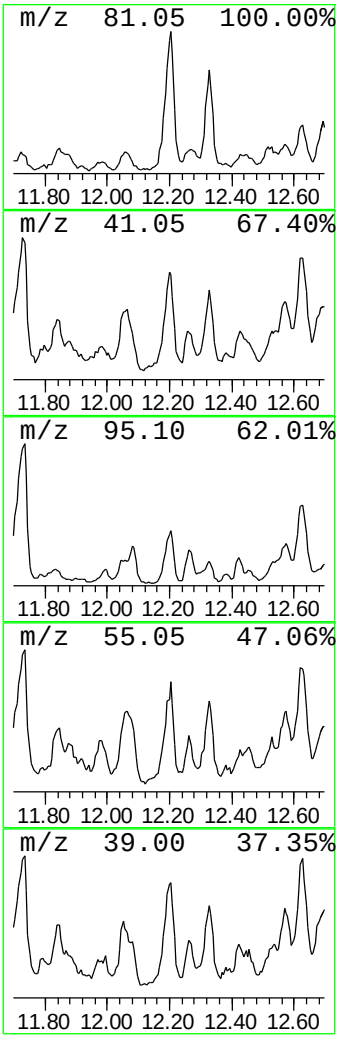
****

Peak Number 6 1-Ethyl-5-methylcyclopentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.20	18.41 ng	413152	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	52
2	Cyclohexene, 4-ethyl-	110	C8H14	003742-42-5	49
3	Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	46
4	2,4-Heptadienal, (E,E)-	110	C7H10O	004313-03-5	46
5	1,5-Hexadiene, 2-methyl-	96	C7H12	004049-81-4	43





Library Search Compound Report

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Data File : BM016285.D
Acq On : 09 Aug 2018 17:17
Operator : SJ/JU
Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

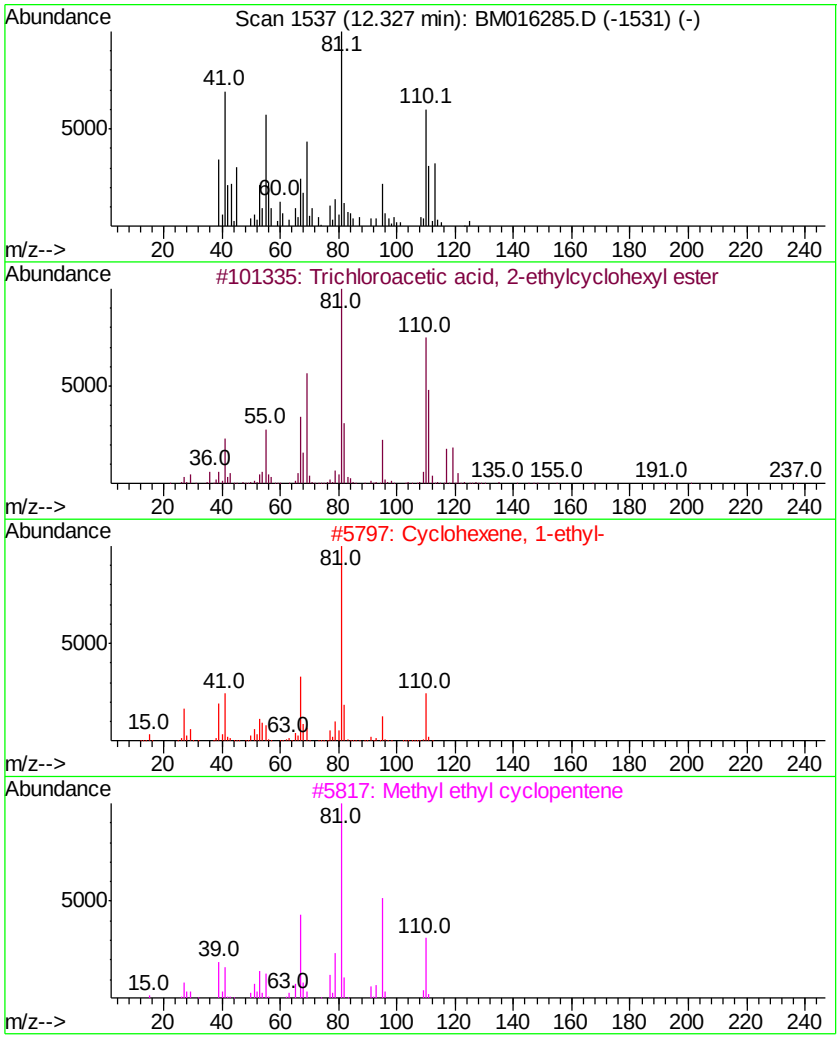
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

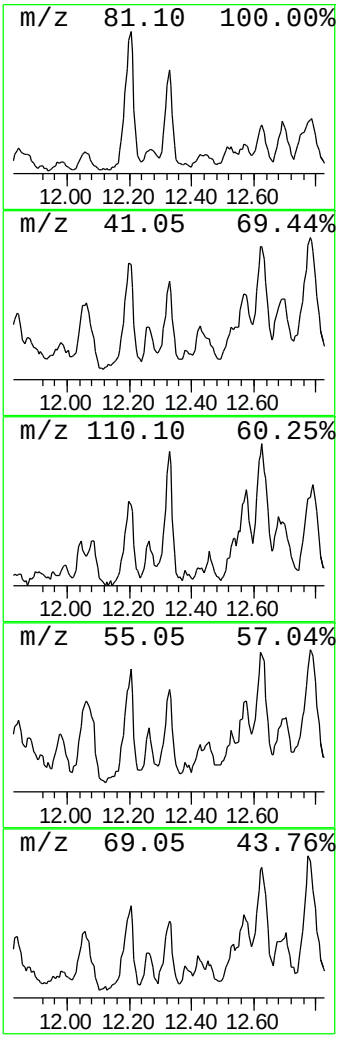
****

Peak Number 7 Trichloroacetic acid, 2-eth... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	11.10 ng	249203	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, 2-ethylcyc...	272	C10H15Cl3O2	1000282-57-3	53
2	Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	50
3	Methyl ethyl cyclopentene	110	C8H14	019780-56-4	43
4	2,4-Heptadienal, (E,E)-	110	C7H10O	004313-03-5	43
5	Cyclohexane, ethenyl-	110	C8H14	000695-12-5	43





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Operator : SJ/JU
Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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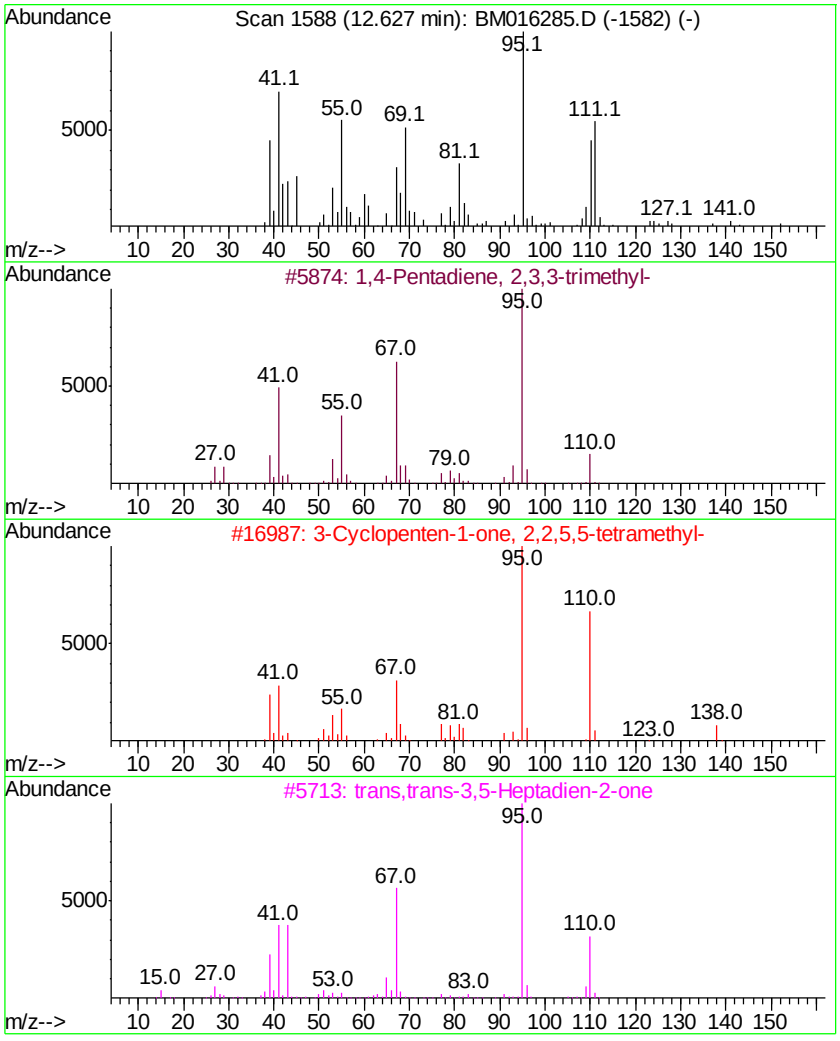
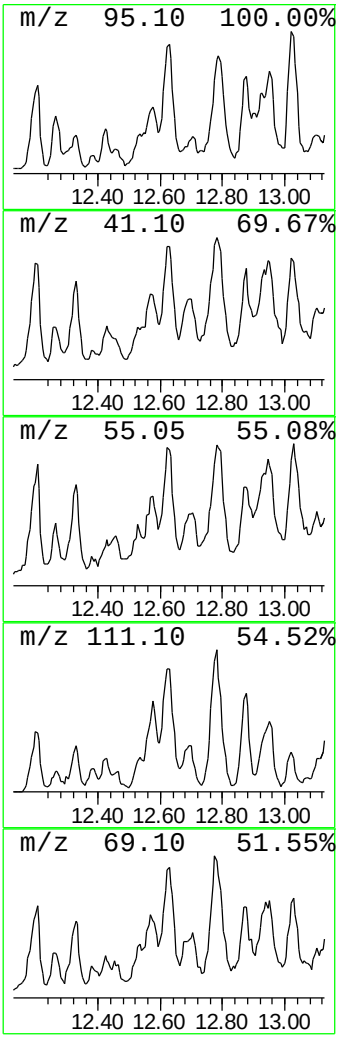
Peak Number 8 unknown12.63 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	16.46 ng	369559	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	47
2	3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	43
3	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	43
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	43
5	dl-6-Methyl-5-hepten-2-ol	128	C8H16O	004630-06-2	38





Library Search Compound Report

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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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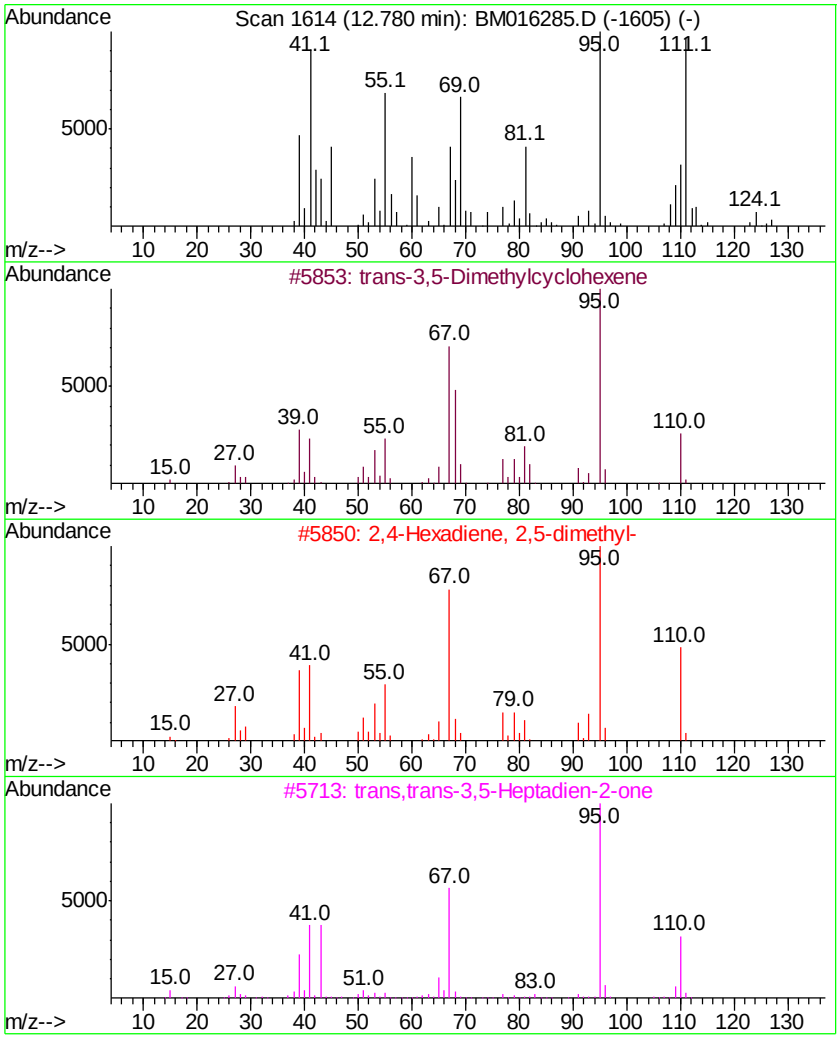
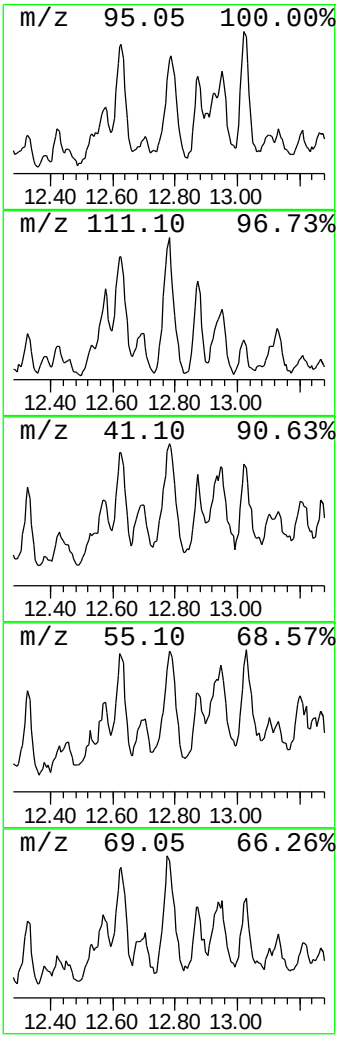
Peak Number 9 unknown12.78 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	23.31 ng	523215	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-3,5-Dimethylcyclohexene	110	C8H14	056021-63-7	38
2	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	35
3	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	35
4	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	30
5	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	091884-67-2	30





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Acq On : 09 Aug 2018 17:17
Operator : SJ/JU
Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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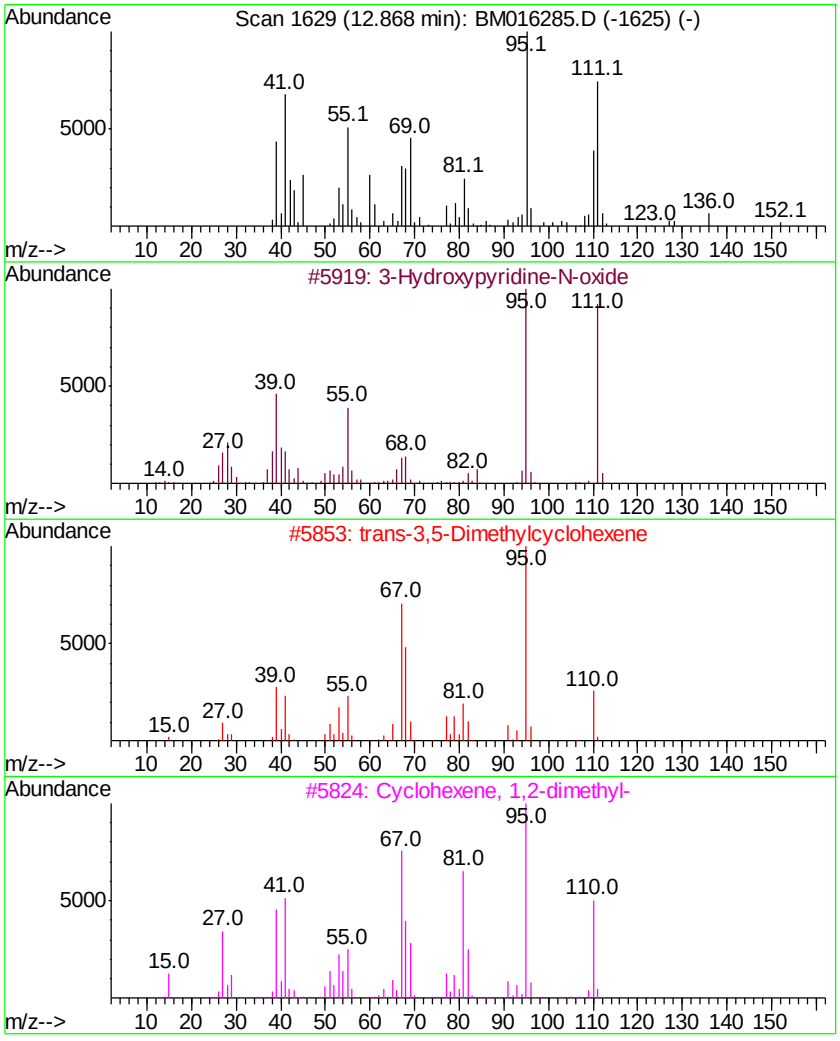
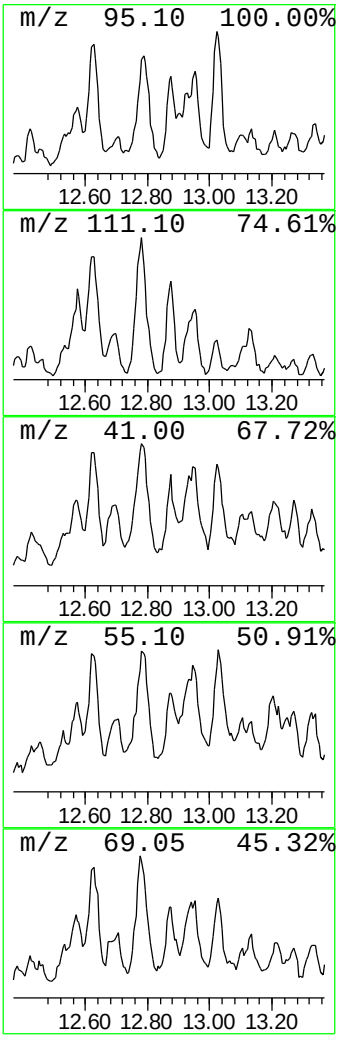
Peak Number 10 unknown12.87 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	12.41 ng	243766	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hydroxypyridine-N-oxide	111	C5H5NO2	006602-28-4	46
2	trans-3,5-Dimethylcyclohexene	110	C8H14	056021-63-7	43
3	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	42
4	4-Methyl-1,3-heptadiene (c,t)	110	C8H14	017603-57-5	38
5	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	38





Library Search Compound Report

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Acq On : 09 Aug 2018 17:17
Operator : SJ/JU
Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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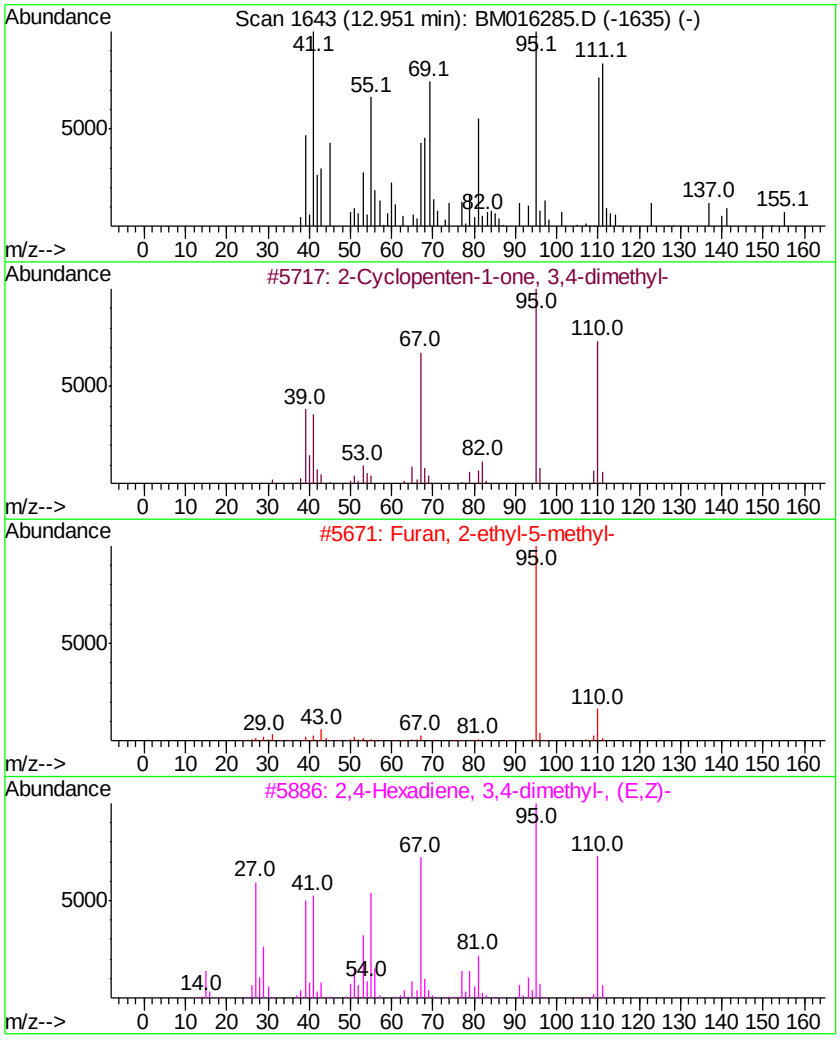
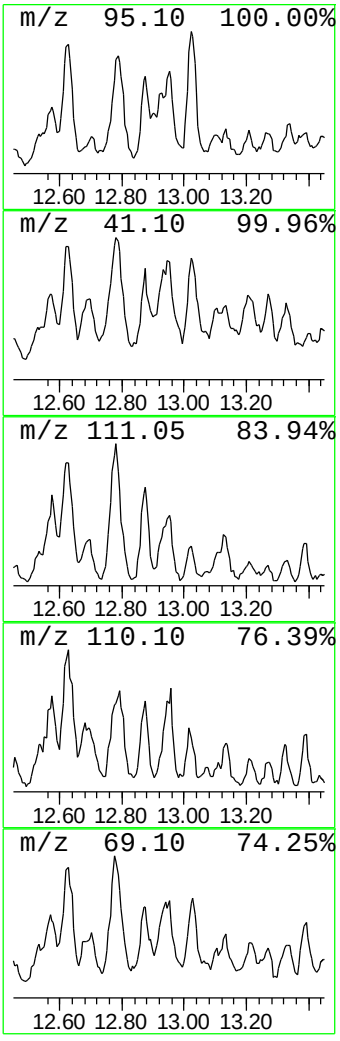
Peak Number 11 unknown12.95 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.95	20.79 ng	408201	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	43
2	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	43
3	2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	41
4	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	41
5	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	38





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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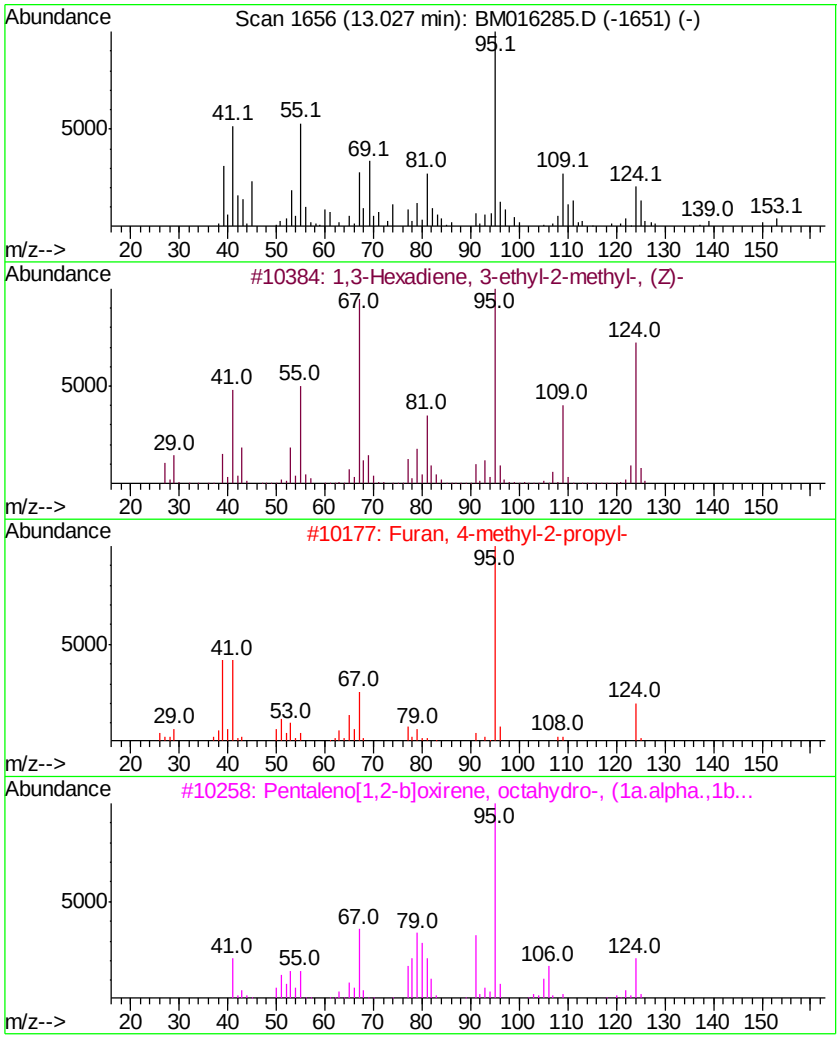
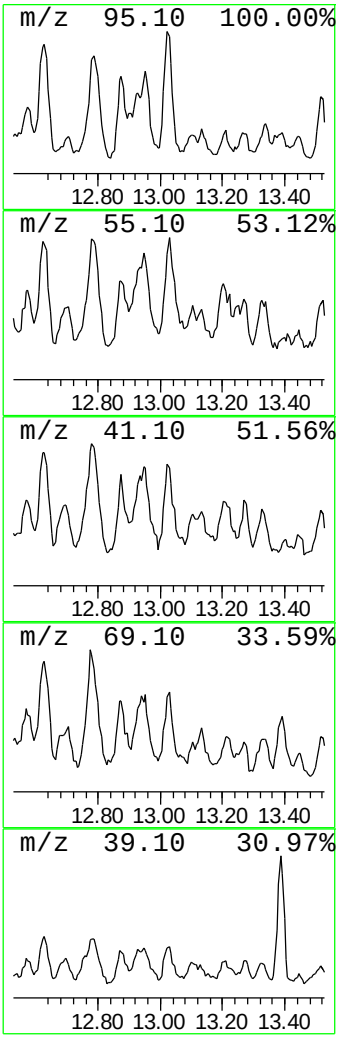
Peak Number 12 1,3-Hexadiene, 3-ethyl-2-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.03	15.20 ng	298473	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexadiene, 3-ethyl-2-methyl-...	124	C9H16	074752-97-9	62
2	Furan, 4-methyl-2-propyl-	124	C8H12O	006148-37-4	52
3	Pentaleno[1,2-b]oxirene, octahyd...	124	C8H12O	055449-71-3	49
4	Silane, diethyldifluoro-	124	C4H10F2Si	000358-06-5	47
5	Cyclohexanemethanol, 4-(1-methyl...	156	C10H20O	013828-37-0	47





Library Search Compound Report

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Operator : SJ/JU
Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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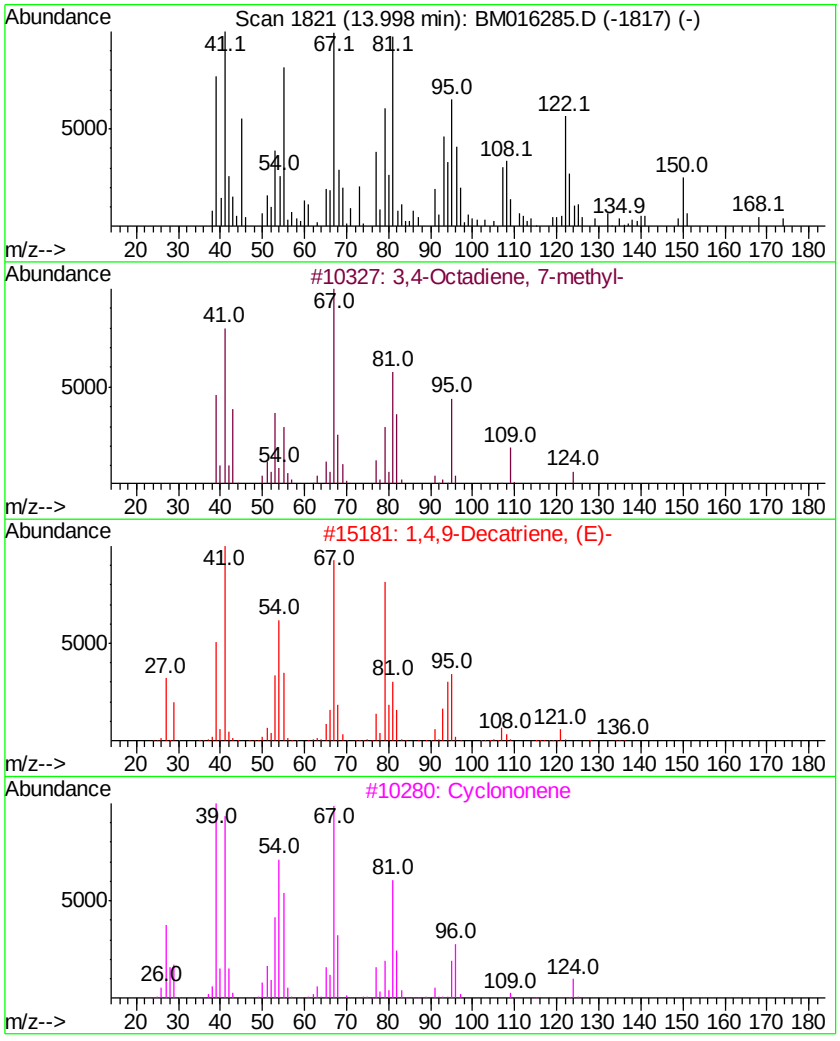
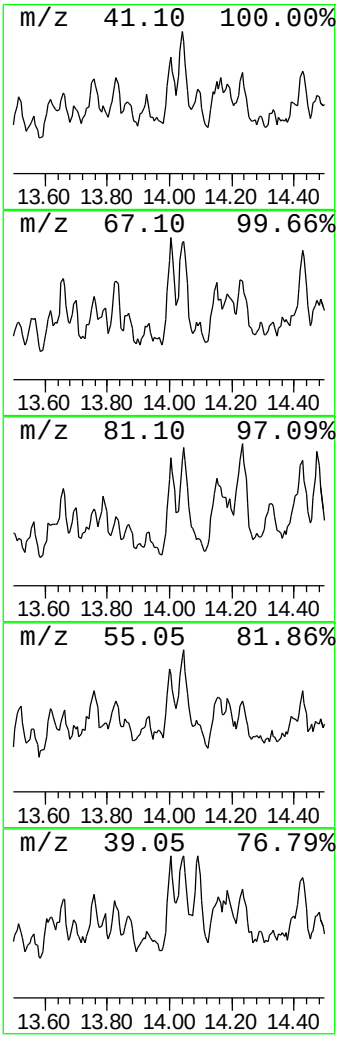
Peak Number 13 unknown14.00 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	12.78 ng	251013	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	49
2	1,4,9-Decatriene, (E)-	136	C10H16	013393-60-7	45
3	Cyclononene	124	C9H16	003618-11-9	43
4	Furan, 2-ethyl-	96	C6H8O	003208-16-0	43
5	1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	43





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Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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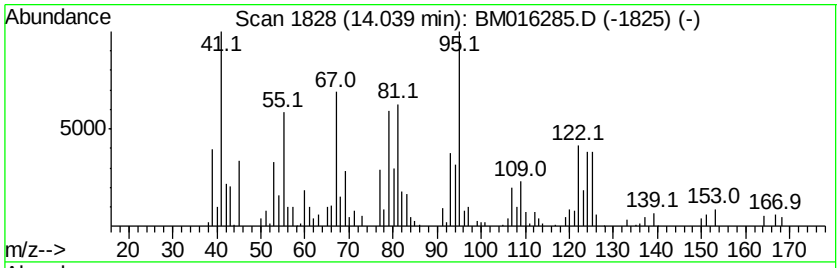
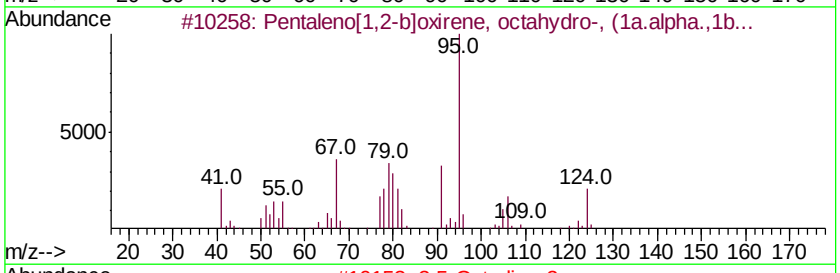
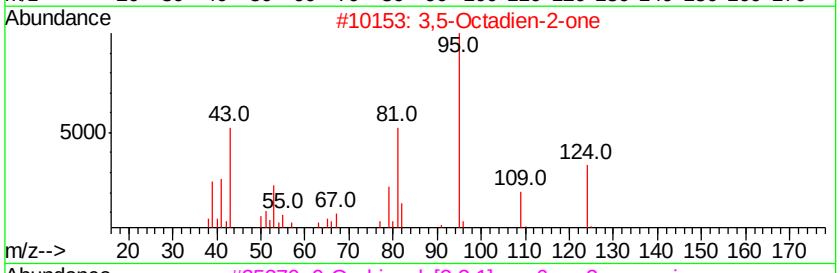
Peak Number 14 unknown14.04 Concentration Rank 9

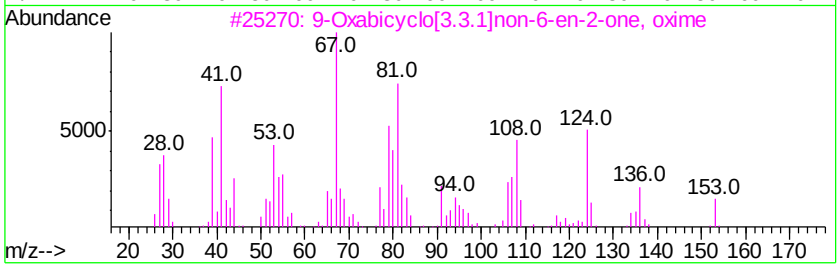
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	16.39 ng	321857	Acenaphthene-d10	14.77

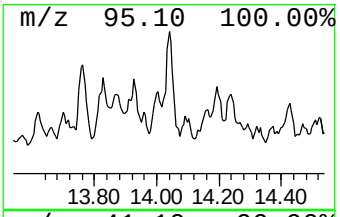
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaleno[1,2-b]oxirene, octahyd...	124	C8H12O	055449-71-3	49
2	3,5-Octadien-2-one	124	C8H12O	038284-27-4	45
3	9-Oxabicyclo[3.3.1]non-6-en-2-on...	153	C8H11NO2	063827-16-7	41
4	Pentaleno[1,2-b]oxirene, octahyd...	124	C8H12O	055449-70-2	41
5	trans-1-Butenylcyclopentane	124	C9H16	1000113-50-9	38

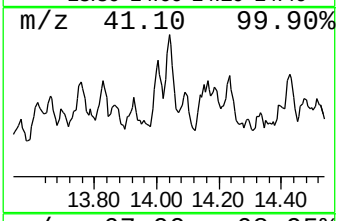


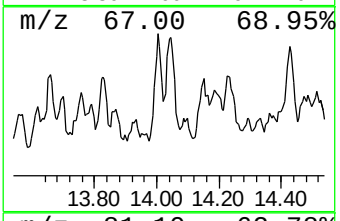


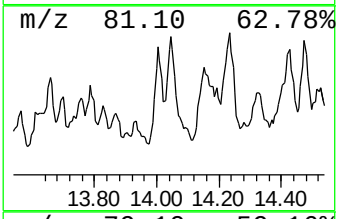


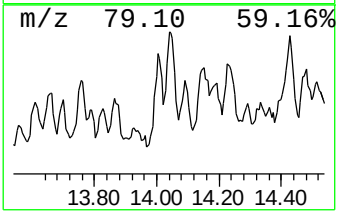












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Instrument : BNA_M
ClientSampleId : MW-27

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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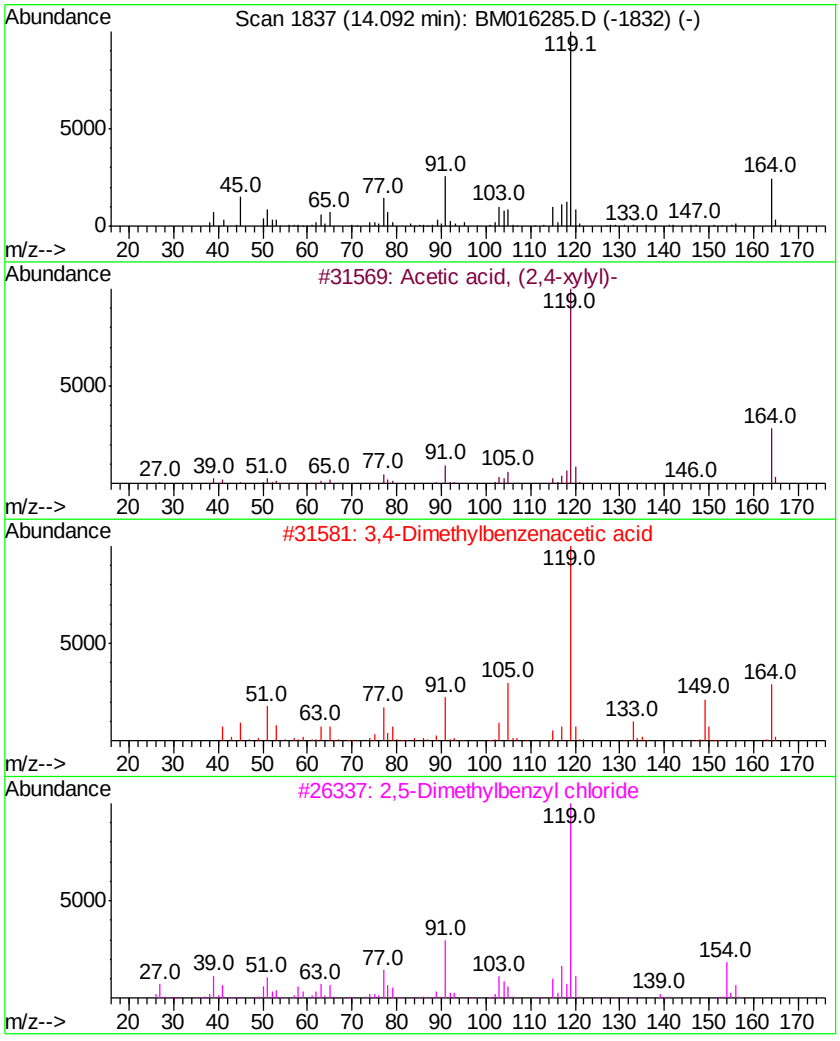
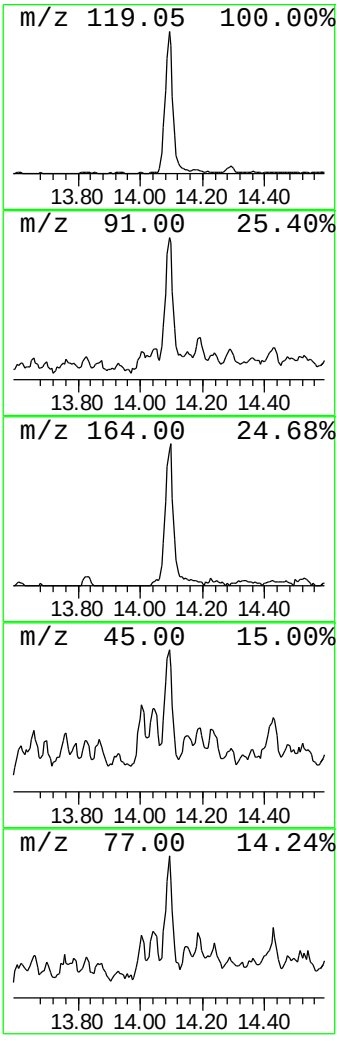
Peak Number 15 Acetic acid, (2,4-xylyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	24.13 ng	473726	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	72
2	3,4-Dimethylbenzenacetic acid	164	C10H12O2	017283-16-8	72
3	2,5-Dimethylbenzyl chloride	154	C9H11Cl	000824-45-3	64
4	1-(2-Methoxy-1-methylethyl)-2-me...	164	C11H16O	1000210-02-1	64
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	59





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Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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TIC Integration Parameters: LSCINT.P

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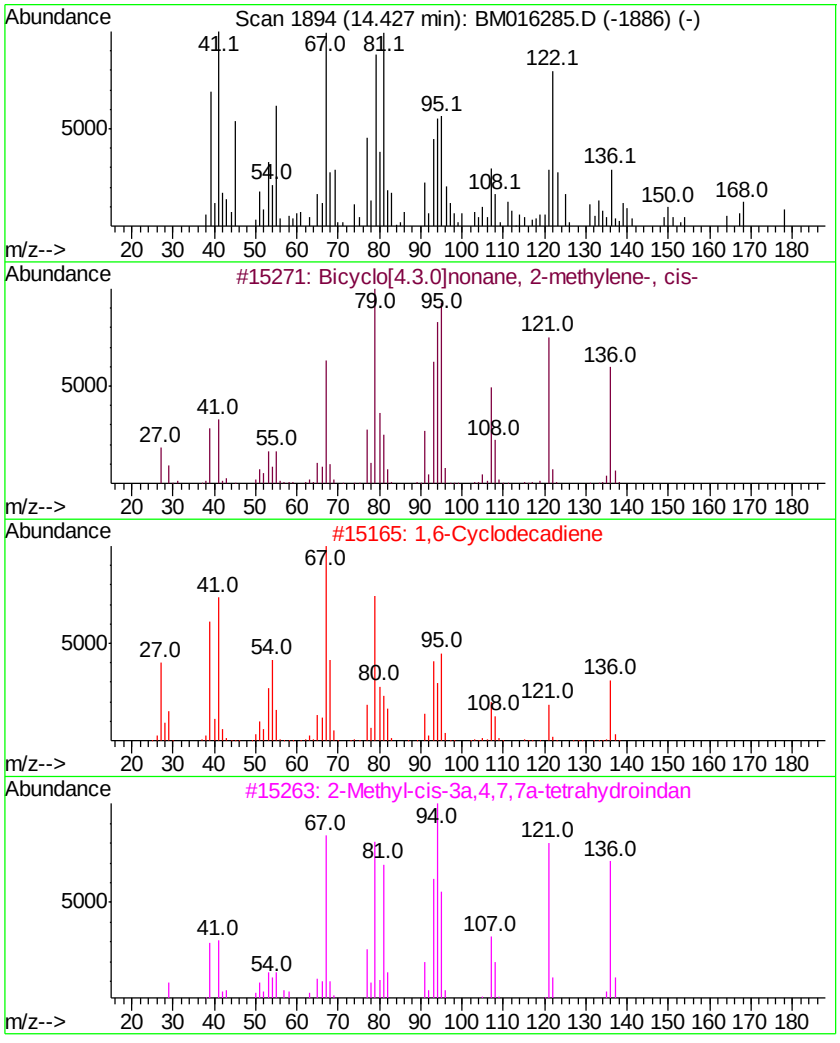
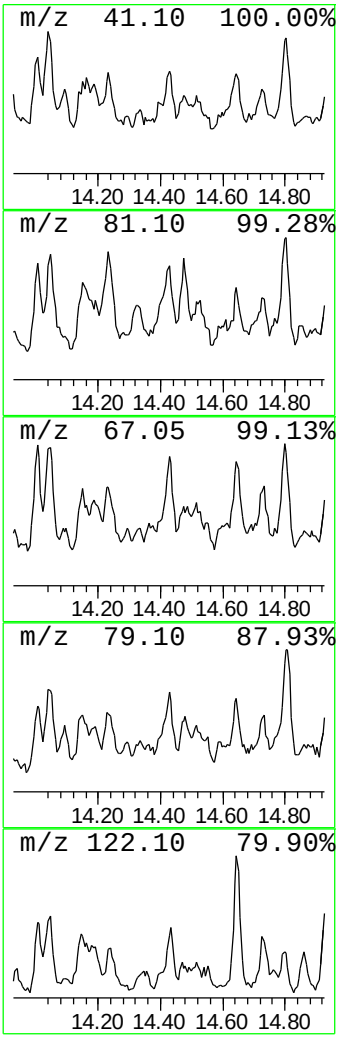
Peak Number 16 Bicyclo[4.3.0]nonane, 2-met... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	11.04 ng	216842	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.3.0]nonane, 2-methylen...	136	C10H16	040954-37-8	91
2	1,6-Cyclodecadiene	136	C10H16	007049-13-0	70
3	2-Methyl-cis-3a,4,7,7a-tetrahydr...	136	C10H16	1000145-00-7	50
4	1,4,9-Decatriene, (Z)-	136	C10H16	1000155-93-2	49
5	Allylidenecyclohexane	122	C9H14	005664-10-8	49





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Data File : BM016285.D
Acq On : 09 Aug 2018 17:17
Operator : SJ/JU
Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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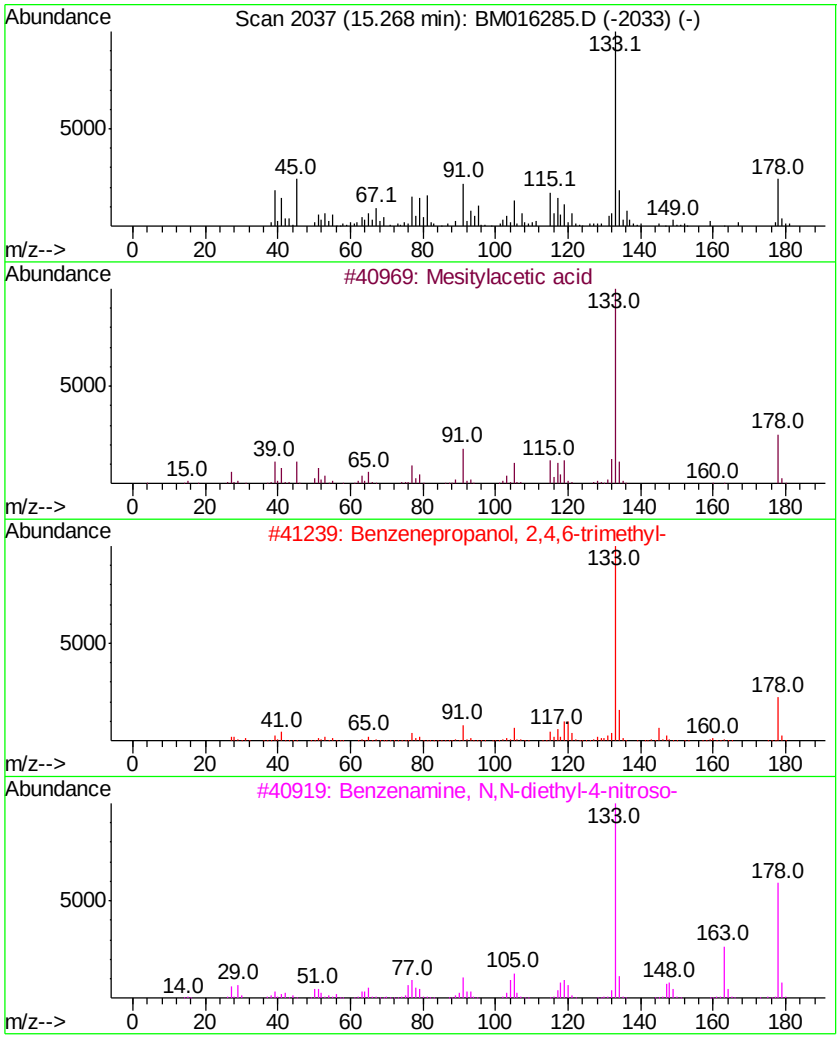
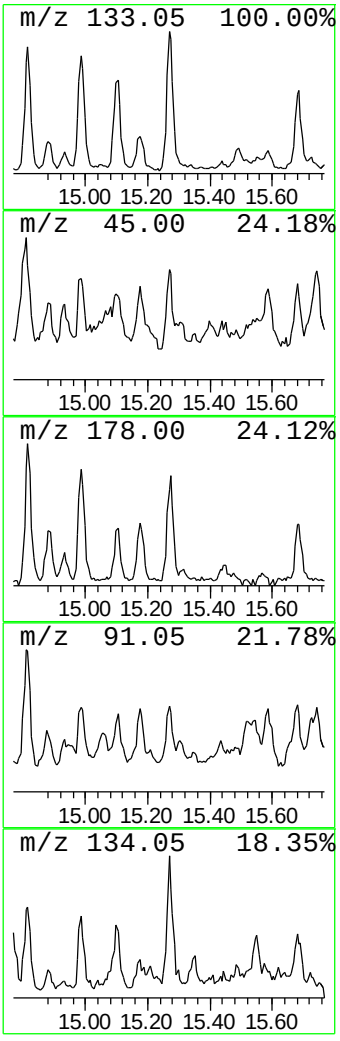
Peak Number 17 Mesitylacetic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	12.19 ng	239455	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylacetic acid	178	C11H14O2	004408-60-0	87
2	Benzenepropanol, 2,4,6-trimethyl-	178	C12H18O	027645-07-4	64
3	Benzenamine, N,N-diethyl-4-nitroso-	178	C10H14N2O	000120-22-9	59
4	Benzamide, 4-[5-(2,4,6-trimethyl...	353	C18H19N5OS	309735-33-9	47
5	5-Aminoindazole	133	C7H7N3	019335-11-6	45





Library Search Compound Report

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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

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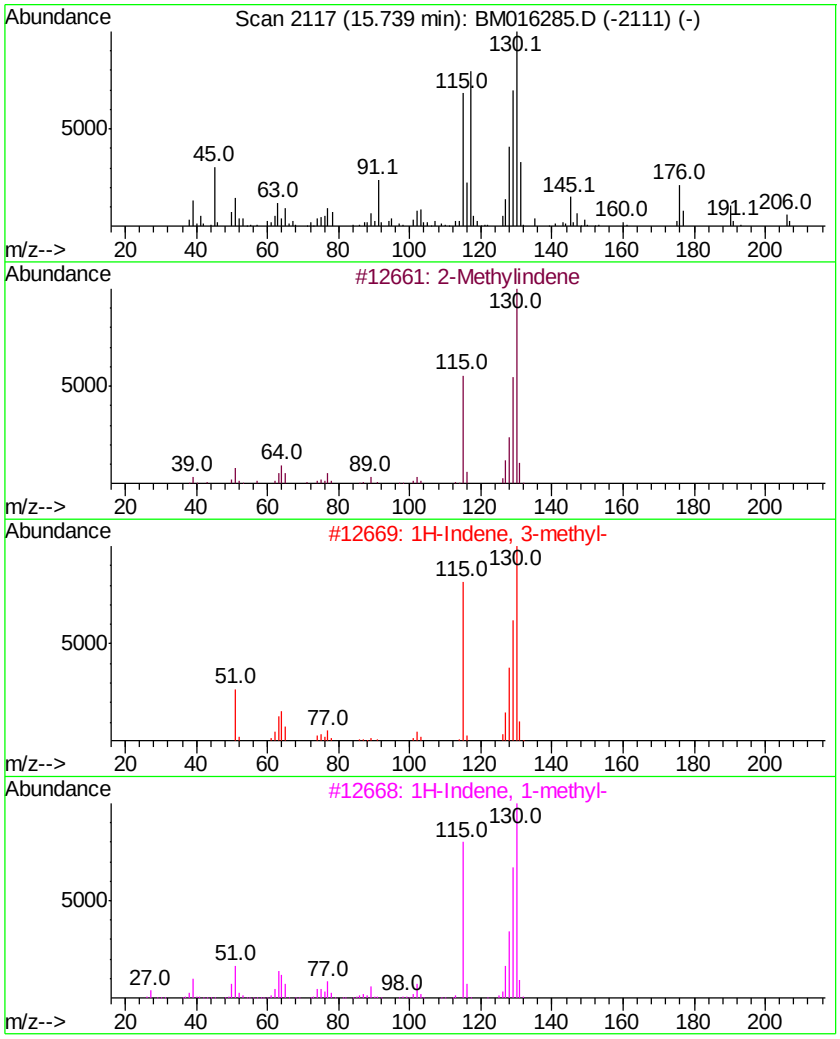
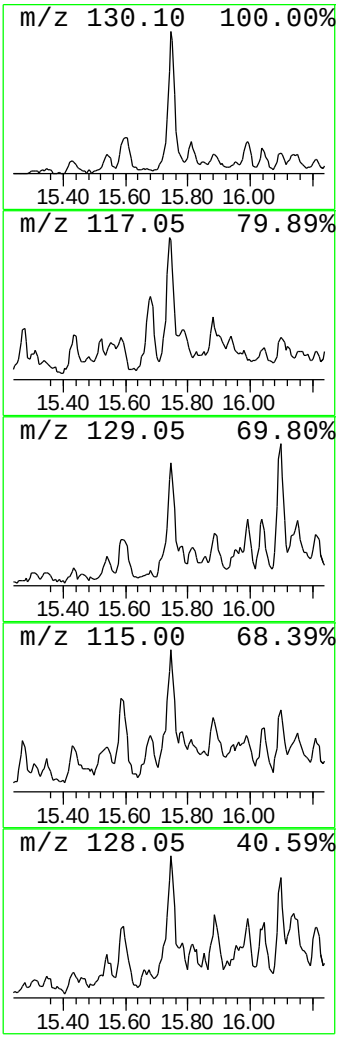
Peak Number 18 2-Methylindene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	13.54 ng	265806	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	64
2	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	60
3	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	53
4	Benzene, 1-butynyl-	130	C10H10	000622-76-4	53
5	1,2,3,4-Tetrahydro-2-naphthoic acid	176	C11H12O2	053440-12-3	47





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Data File : BM016285.D
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Operator : SJ/JU
Sample : J4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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TIC Integration Parameters: LSCINT.P

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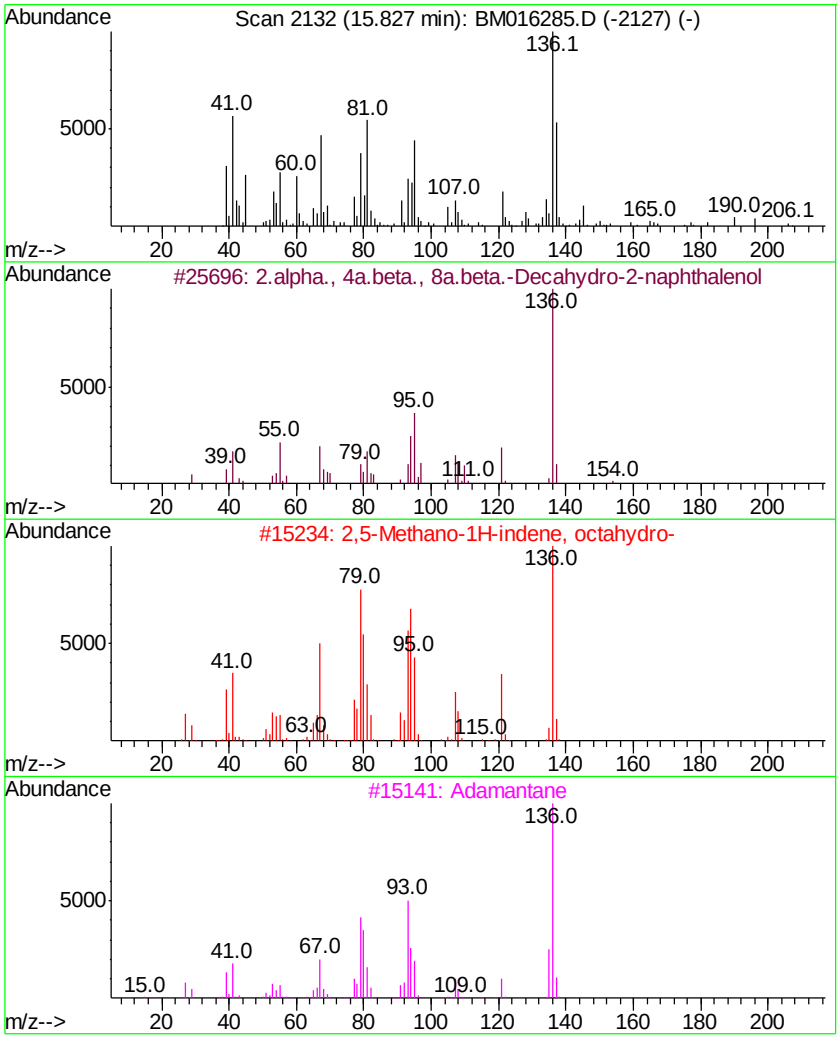
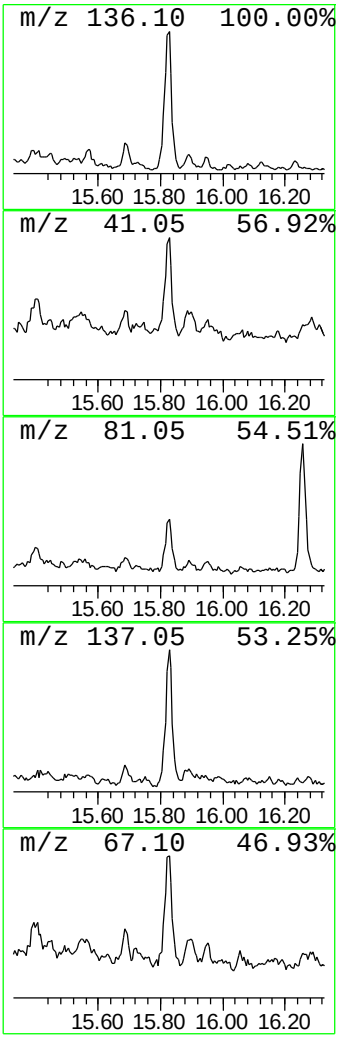
Peak Number 19 2.alpha., 4a.beta., 8a.beta... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	15.42 ng	302826	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2.alpha., 4a.beta., 8a.beta.-Dec...	154	C10H18O	001424-37-9	53
2	2,5-Methano-1H-indene, octahydro-	136	C10H16	019026-94-9	45
3	Adamantane	136	C10H16	000281-23-2	38
4	Bicyclo[3.2.2]non-6-en-3-one	136	C9H12O	1000072-31-7	38
5	Phenol, 3-(dimethylamino)-	137	C8H11NO	000099-07-0	38





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : MW-27

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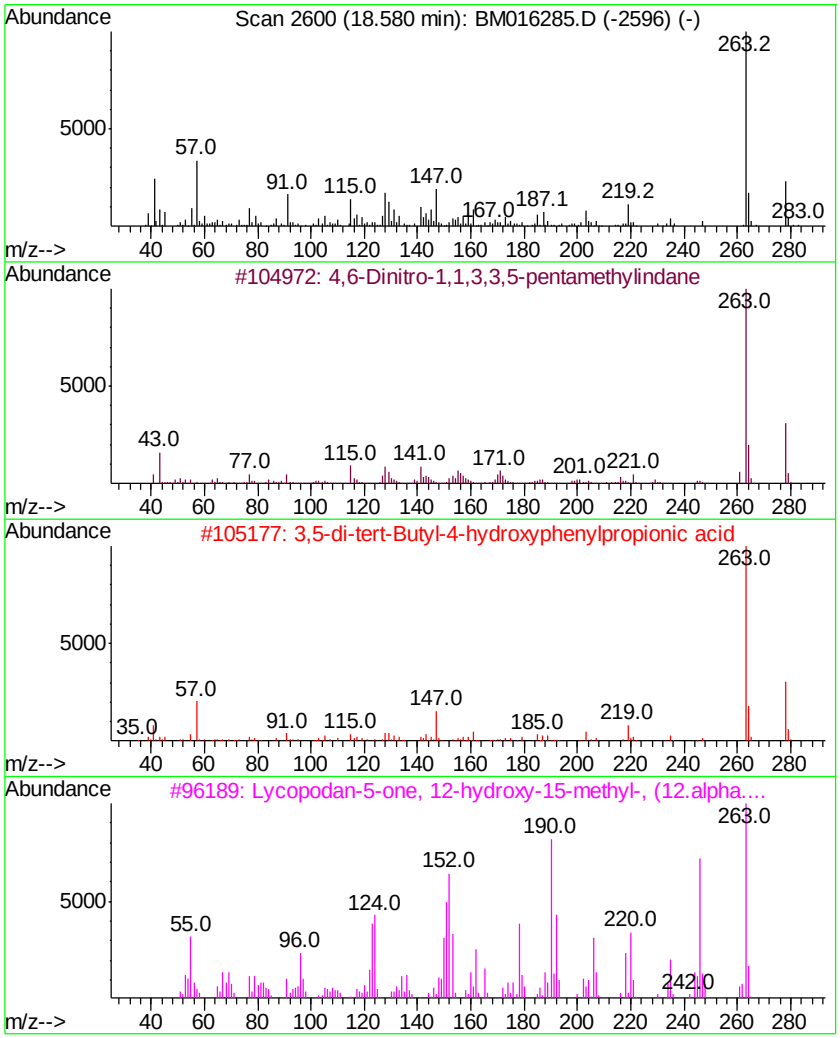
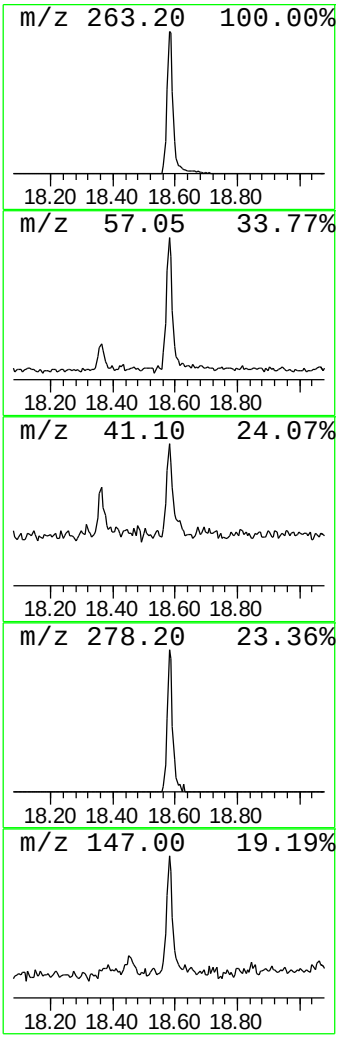
Peak Number 20 4,6-Dinitro-1,1,3,3,5-penta... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	13.55 ng	330439	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6-Dinitro-1,1,3,3,5-pentamethy...	278	C14H18N2O4	000116-66-5	86
2	3,5-di-tert-Butyl-4-hydroxyphenyl...	278	C17H26O3	020170-32-5	81
3	Lycopodan-5-one, 12-hydroxy-15-m...	263	C16H25NO2	021061-90-5	50
4	Trimethyl(2,6 ditert.-butylpheno...	278	C17H30OSi	010416-73-6	47
5	2-(4-Methoxy-phenyl)-1H-1,3a,8-t...	263	C16H13N3O	036289-23-3	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080918\
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Operator : SJ/JU
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Misc :
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Instrument : BNA_M
ClientSampleId : MW-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.66	7.66	94.7	ng	1548630	1	8.13	327007	20.0
Cyclobutane, (1-m...	10.84	13.9	ng	312477	2	10.95	448951	20.0
5,5-Dimethyl-1,3-...	11.73	29.5	ng	662759	2	10.95	448951	20.0
unknown12.06	12.06	14.2	ng	319312	2	10.95	448951	20.0
1-Ethyl-5-methylc...	12.20	18.4	ng	413152	2	10.95	448951	20.0
Trichloroacetic a...	12.33	11.1	ng	249203	2	10.95	448951	20.0
unknown12.63	12.63	16.5	ng	369559	2	10.95	448951	20.0
unknown12.78	12.78	23.3	ng	523215	2	10.95	448951	20.0
unknown12.87	12.87	12.4	ng	243766	3	14.77	392726	20.0
unknown12.95	12.95	20.8	ng	408201	3	14.77	392726	20.0
1,3-Hexadiene, 3-...	13.03	15.2	ng	298473	3	14.77	392726	20.0
unknown14.00	14.00	12.8	ng	251013	3	14.77	392726	20.0
unknown14.04	14.04	16.4	ng	321857	3	14.77	392726	20.0
Acetic acid, (2,4...	14.09	24.1	ng	473726	3	14.77	392726	20.0
Bicyclo[4.3.0]non...	14.43	11.0	ng	216842	3	14.77	392726	20.0
Mesitylacetic acid	15.27	12.2	ng	239455	3	14.77	392726	20.0
2-Methylindene	15.74	13.5	ng	265806	3	14.77	392726	20.0
2.alpha., 4a.beta...	15.83	15.4	ng	302826	3	14.77	392726	20.0
4,6-Dinitro-1,1,3...	18.58	13.6	ng	330439	4	17.50	487610	20.0