LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016278.D
Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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	5.187	318	323	333	rBV	51492	77238	2.45%	0.406%
2	5.663	395	404	418	rBV	471323	745114	23.63%	3.915%
3	6.181	486	492	499	rVB	57228	88652	2.81%	0.466%
4	7.304	678	683	695	rBV	256314	434707	13.79%	2.284%
5	7.663	737	744	755	rBV	1011210	1600625	50.76%	8.410%
6	8.128	818	823	836	rBV	183370	315564	10.01%	1.658%
7	8.451	871	878	893	rVB	970761	1599272	50.72%	8.403%
8	9.322	1019	1026	1042	rBV	694837	1198801	38.02%	6.299%
9	9.757	1094	1100	1105	rBV3	34815	58715	1.86%	0.309%
10	10.292	1184	1191	1194	rBV3	20606	36906	1.17%	0.194%
11	10.334	1194	1198	1206	rVB3	40499	71520	2.27%	0.376%
12	10.945	1296	1302	1307	rBV	207879	352177	11.17%	1.850%
13	10.998	1307	1311	1316	rVB	49566	79008	2.51%	0.415%
14	11.510	1393	1398	1411	rVB6	30076	74215	2.35%	0.390%
15	11.669	1420	1425	1431	rVB2	32302	58073	1.84%	0.305%
16	11.792	1441	1446	1447	rBV4	20836	32803	1.04%	0.172%
17	12.010	1477	1483	1490	rVB9	12801	40571	1.29%	0.213%
18	12.475	1558	1562	1567	rBV7	17181	34942	1.11%	0.184%
19	12.722	1600	1604	1615	rVB6	25735	58691	1.86%	0.308%
20	12.827	1616	1622	1627	rVV5	33288	69763	2.21%	0.367%
21	12.886	1627	1632	1643	rVB5	25960	67846	2.15%	0.356%
22	12.992	1643	1650	1655	rVB9	24857	59907	1.90%	0.315%
23	13.098	1664	1668	1675	rVB7	14782	35781	1.13%	0.188%
24	13.216	1678	1688	1698	rBV	417065	747585	23.71%	3.928%
25	13.292	1698	1701	1710	rVB6	39166	77009	2.44%	0.405%
26	13.386	1710	1717	1725	rVB	1674580	2399322	76.09%	12.607%
27	13.574	1744	1749	1752	rBV7	22545	40543	1.29%	0.213%
28	14.004	1818	1822	1827	rBV5	41222	62942	2.00%	0.331%
29	14.051	1827	1830	1834	rBV2	28908	37149	1.18%	0.195%
30	14.598	1919	1923	1931	rVB8	29232	58205	1.85%	0.306%
31	14.769	1946	1952	1963	rBV3	290937	484097	15.35%	2.544%
32	14.863	1963	1968	1972	rBV5	41823	75370	2.39%	0.396%
33	14.957	1981	1984	1989	rVB2	23746	32484	1.03%	0.171%
34	15.245	2029	2033	2036	rBV4	28283	45015	1.43%	0.237%

LSC Area Percent Report

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Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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	15.533	2075	2082	2085	rBV7	33585	77935	2.47%	0.409%
36	15.745	2115	2118	2123	rVB	70555	96117	3.05%	0.505%
37	15.798	2123	2127	2134	rVV4	53565	81566	2.59%	0.429%
38	16.257	2199	2205	2217	rBV	1403889	2067920	65.58%	10.865%
39	16.486	2240	2244	2255	rBV3	61812	162770	5.16%	0.855%
40	17.068	2340	2343	2347	rBV5	21774	34590	1.10%	0.182%
41	17.504	2412	2417	2423	rBV	307626	444403	14.09%	2.335%
42	18.357	2558	2562	2568	rBV2	90603	119907	3.80%	0.630%
43	18.574	2595	2599	2608	rBV	266884	376205	11.93%	1.977%
44	19.615	2772	2776	2782	rBV3	55989	81323	2.58%	0.427%
45	20.086	2850	2856	2861	rBV	2727679	3153068	100.00%	16.567%
46	21.303	3060	3063	3068	rVB6	39382	49327	1.56%	0.259%
47	21.633	3114	3119	3125	rVB	410450	513089	16.27%	2.696%
48	23.968	3511	3516	3525	rVB2	258776	523567	16.61%	2.751%

Sum of corrected areas: 19032399

LSC Report - Integrated Chromatogram

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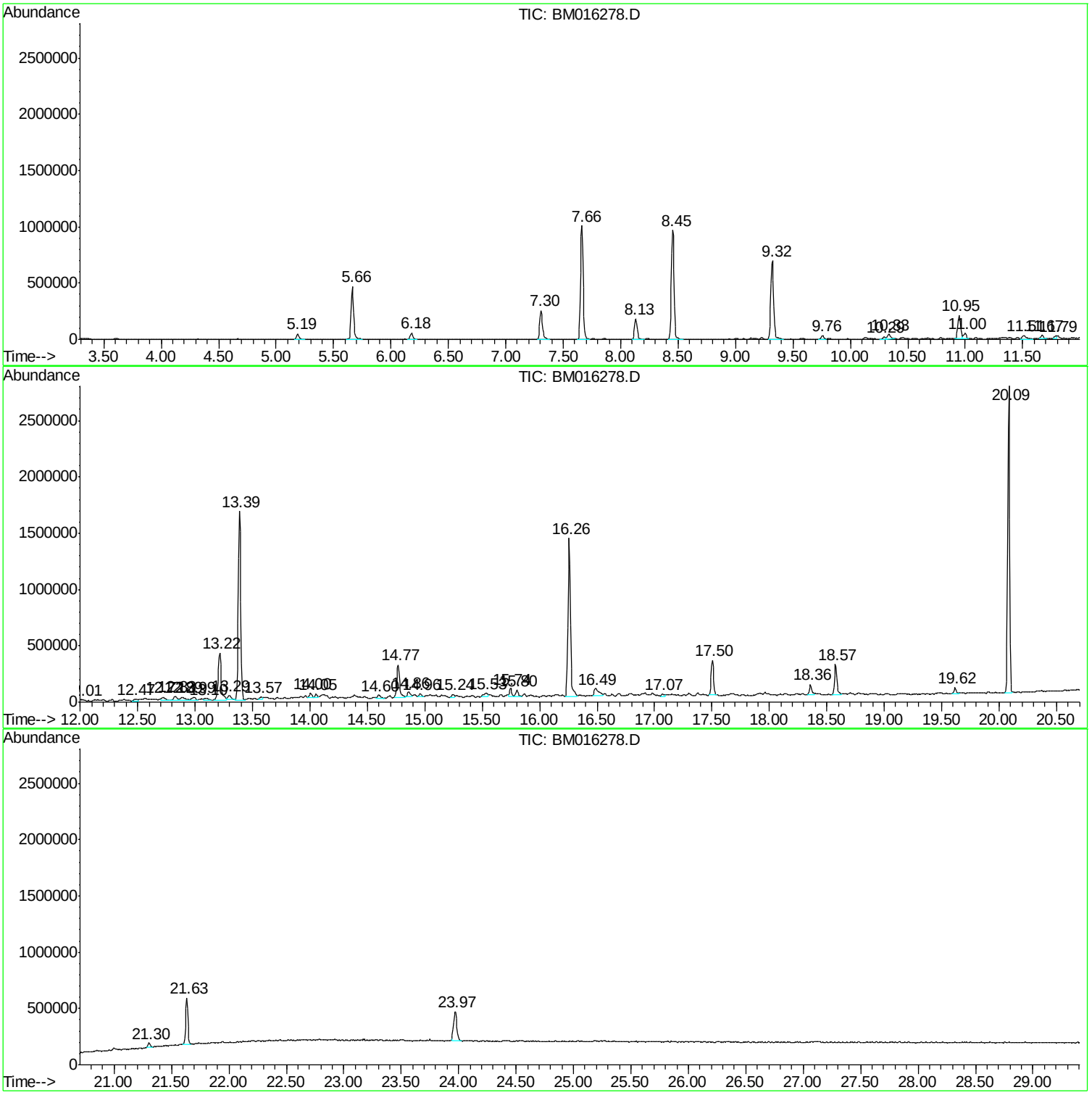
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-11

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\
Data File : BM016278.D
Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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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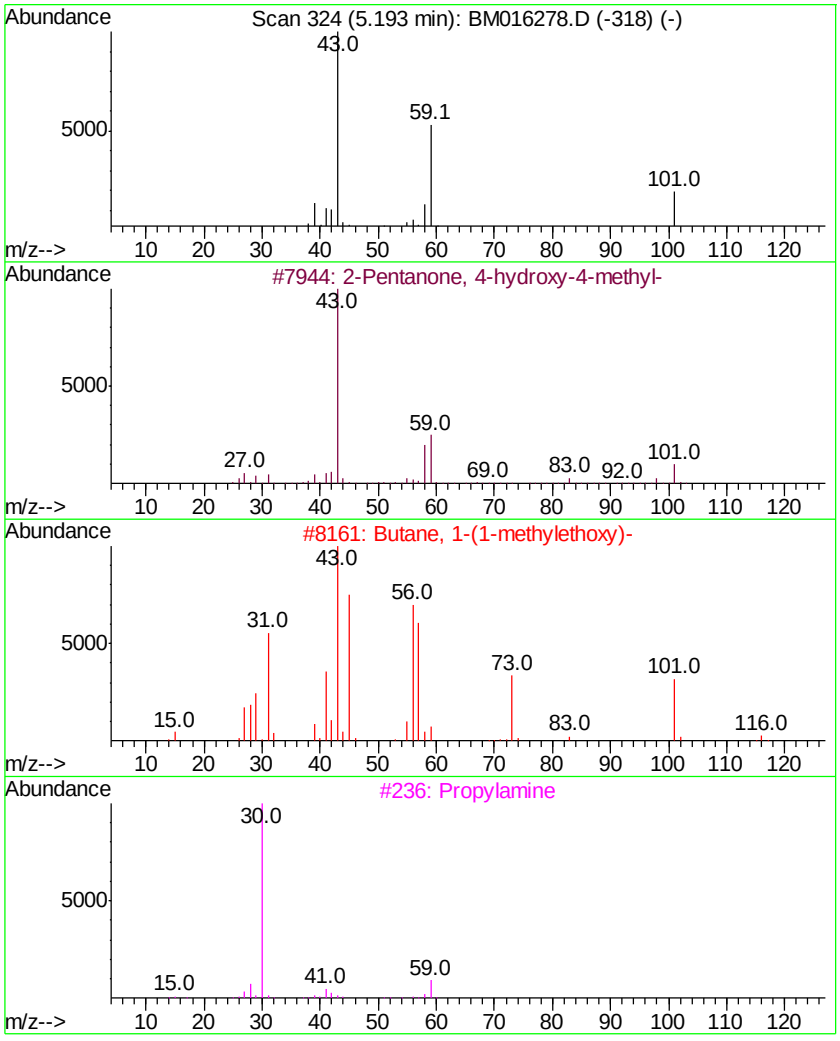
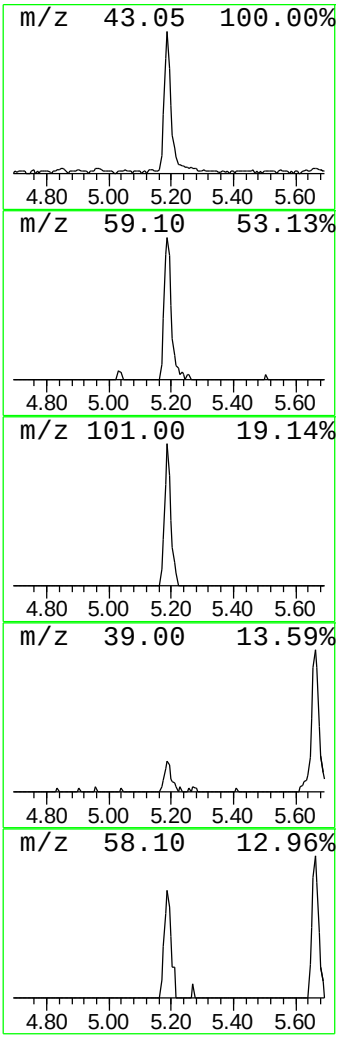
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	4.90 ng	77238	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	46
3	Propylamine	59	C3H9N	000107-10-8	42
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
5	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	38





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Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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

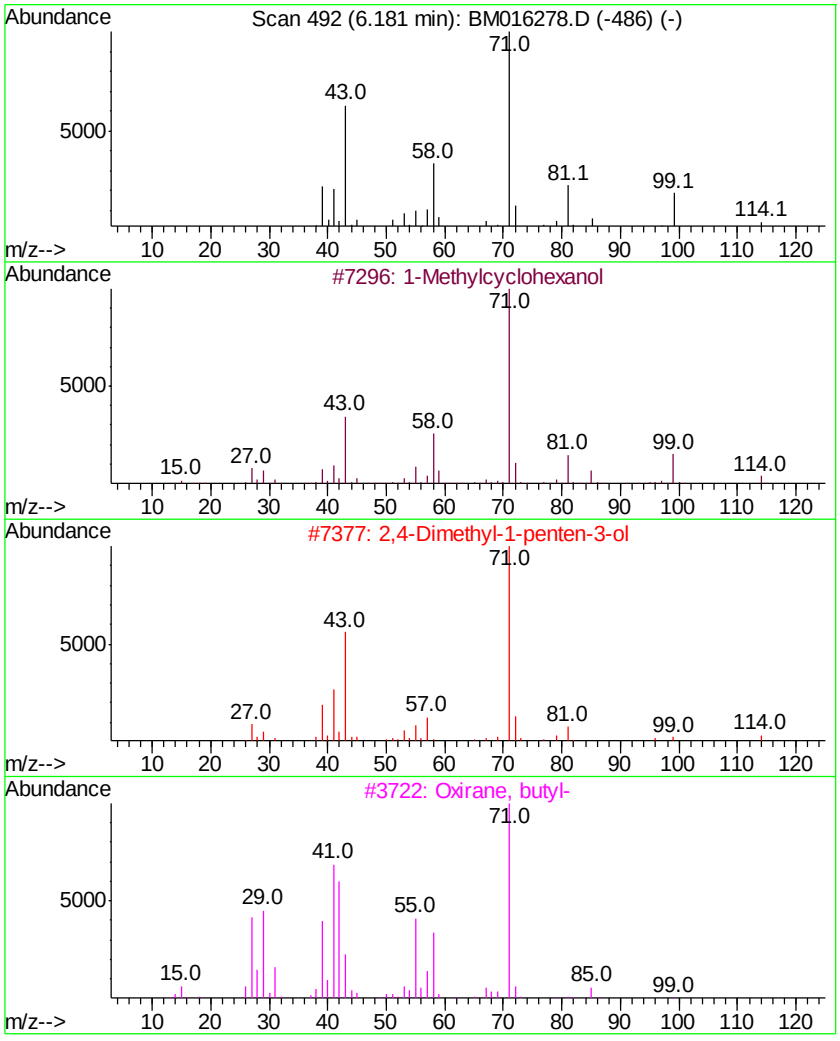
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

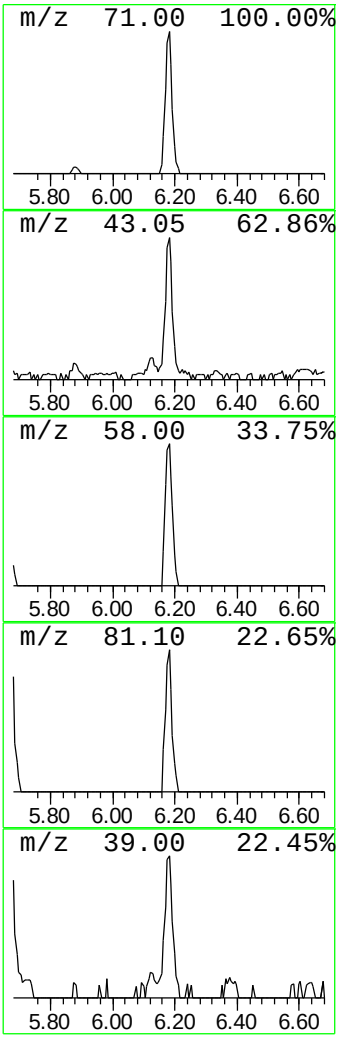
****

Peak Number 2 1-Methylcyclohexanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	5.62 ng	88652	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylcyclohexanol	114	C7H14O	000590-67-0	91
2	2,4-Dimethyl-1-penten-3-ol	114	C7H14O	019781-54-5	58
3	Oxirane, butyl-	100	C6H12O	001436-34-6	50
4	3-Methoxyhex-1-ene	114	C7H14O	108811-41-2	47
5	2(3H)-Furanone, dihydro-3-hydrox...	130	C6H10O3	052126-90-6	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016278.D
Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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

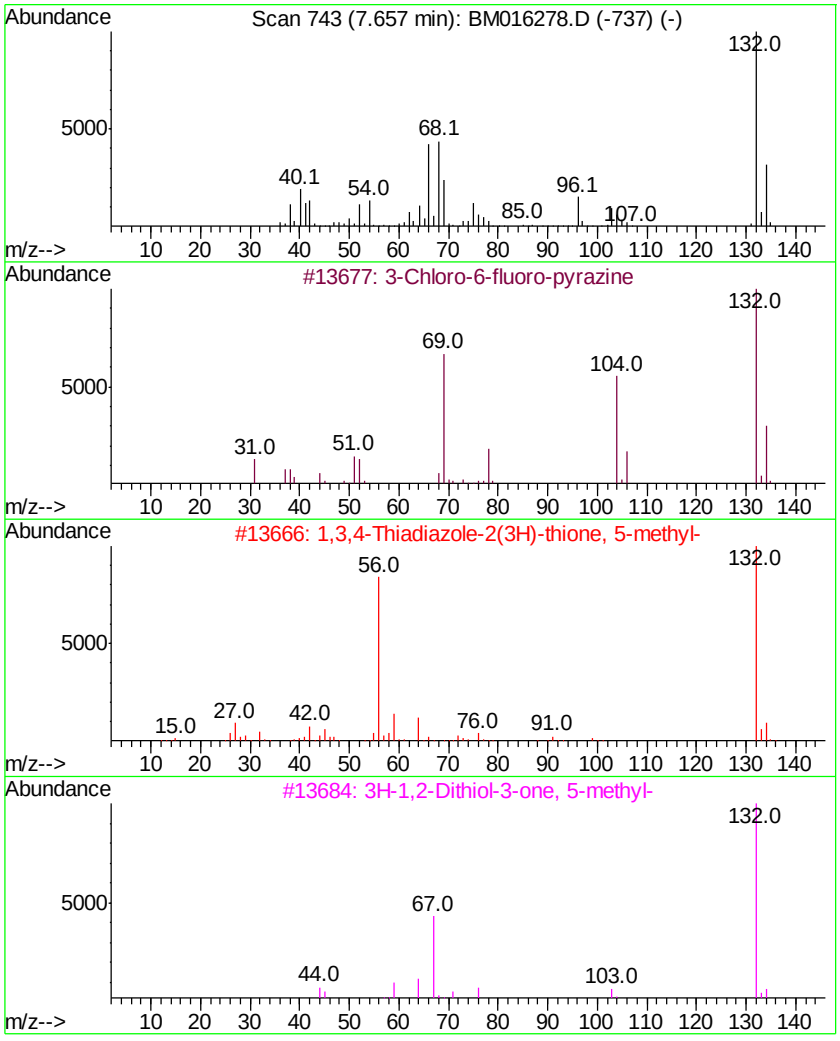
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

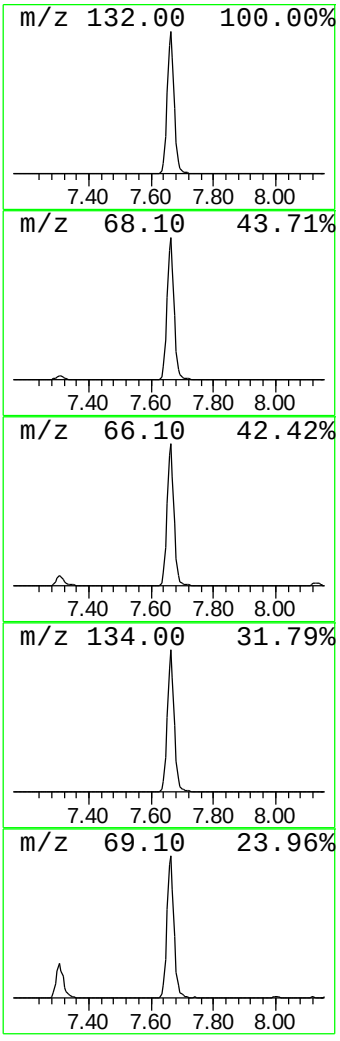
****

Peak Number 3 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	101.45 ng	1600630	1,4-Dichlorobenzene-d4	8.13

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





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Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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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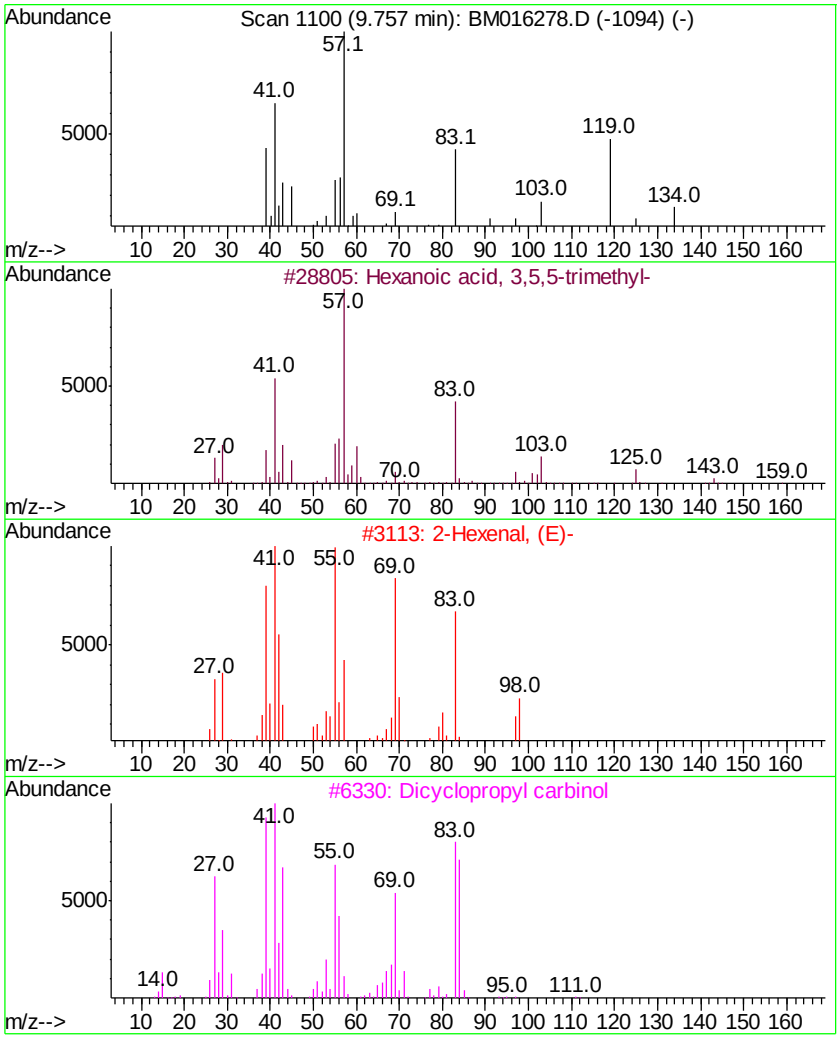
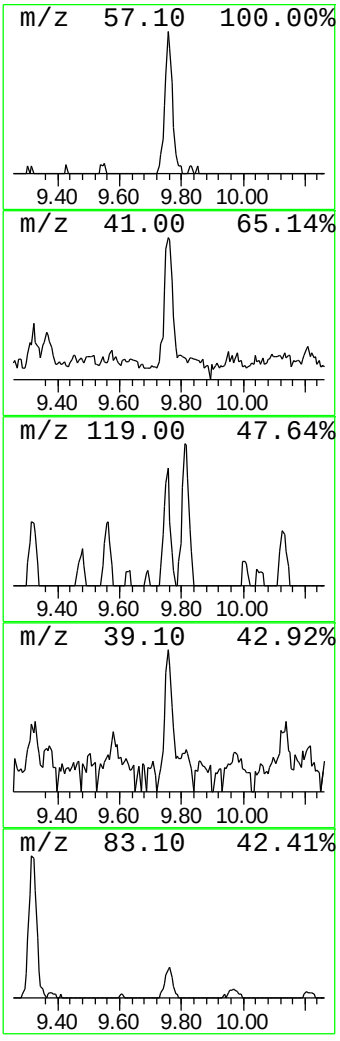
Peak Number 5 unknown9.76 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	3.33 ng	58715	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	32
2	2-Hexenal, (E)-	98	C6H10O	006728-26-3	12
3	Dicyclopropyl carbinol	112	C7H12O	014300-33-5	12
4	1,6;3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	10
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	10





Library Search Compound Report

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Data File : BM016278.D
Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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

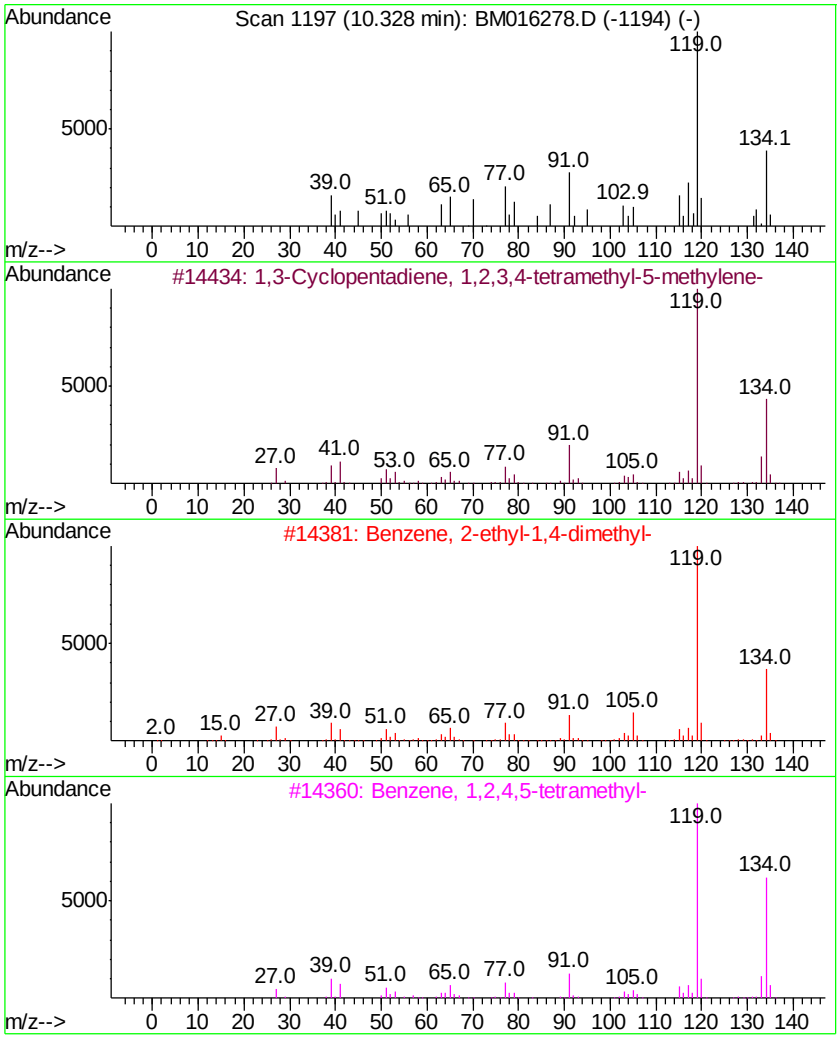
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

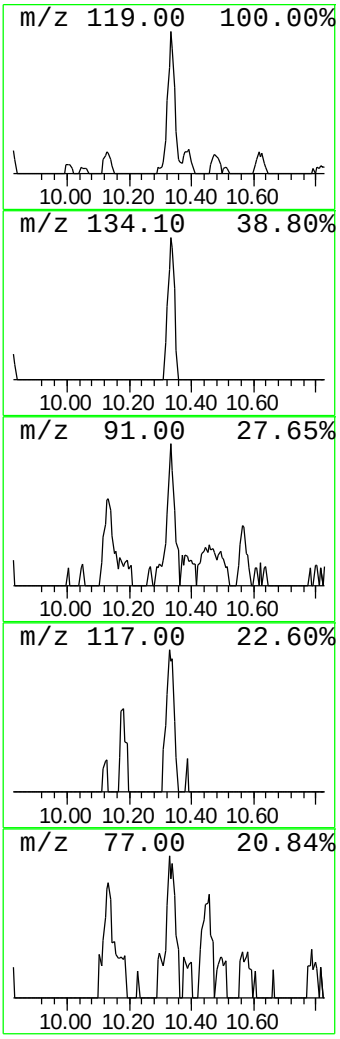
****

Peak Number 6 1,3-Cyclopentadiene, 1,2,3,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	4.06 ng	71520	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	87
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	83
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	83
4	Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	81
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	81





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Data File : BM016278.D
Acq On : 09 Aug 2018 13:00
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Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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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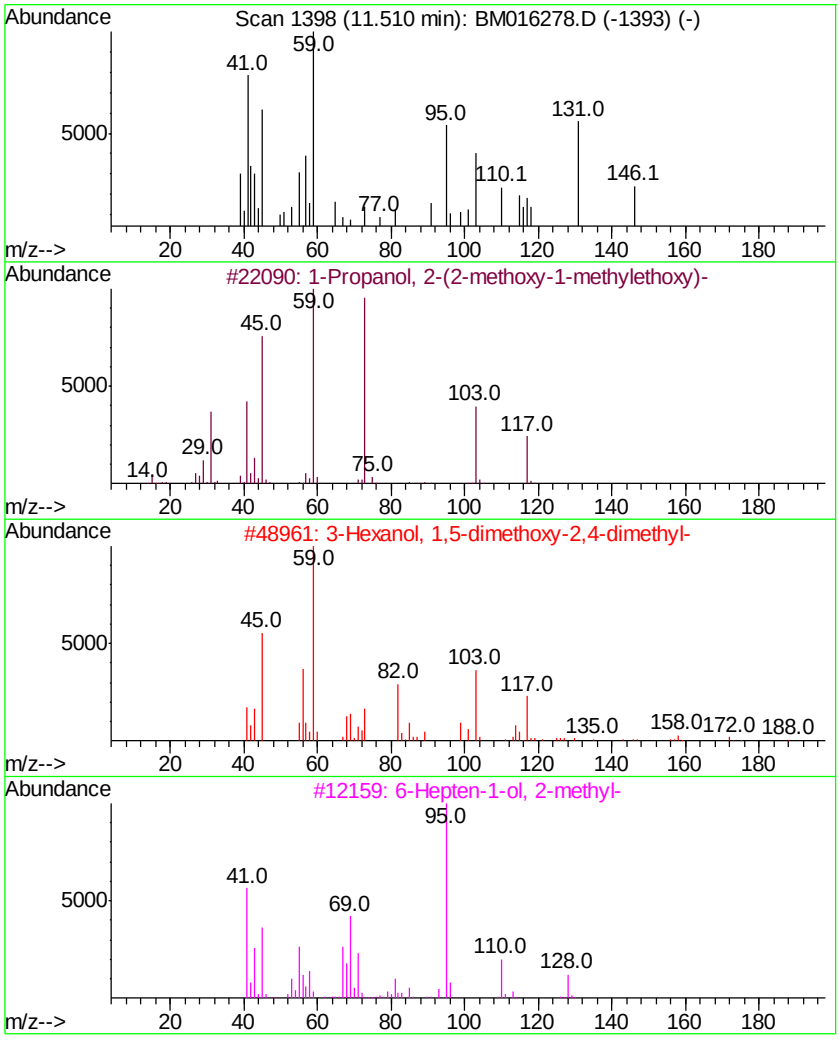
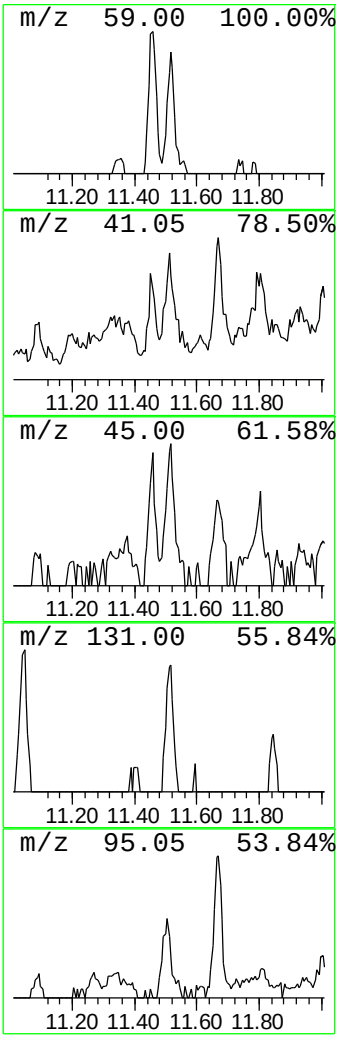
Peak Number 7 unknown11.51 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.51	4.21 ng	74215	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-methoxy-1-methy...	148	C7H16O3	055956-21-3	25
2	3-Hexanol, 1,5-dimethoxy-2,4-dim...	190	C10H22O3	013897-22-8	23
3	6-Hepten-1-ol, 2-methyl-	128	C8H16O	1000132-12-0	14
4	Hydrazine, 2-butyl-1,1-dimethyl-	116	C6H16N2	054007-23-7	10
5	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	10





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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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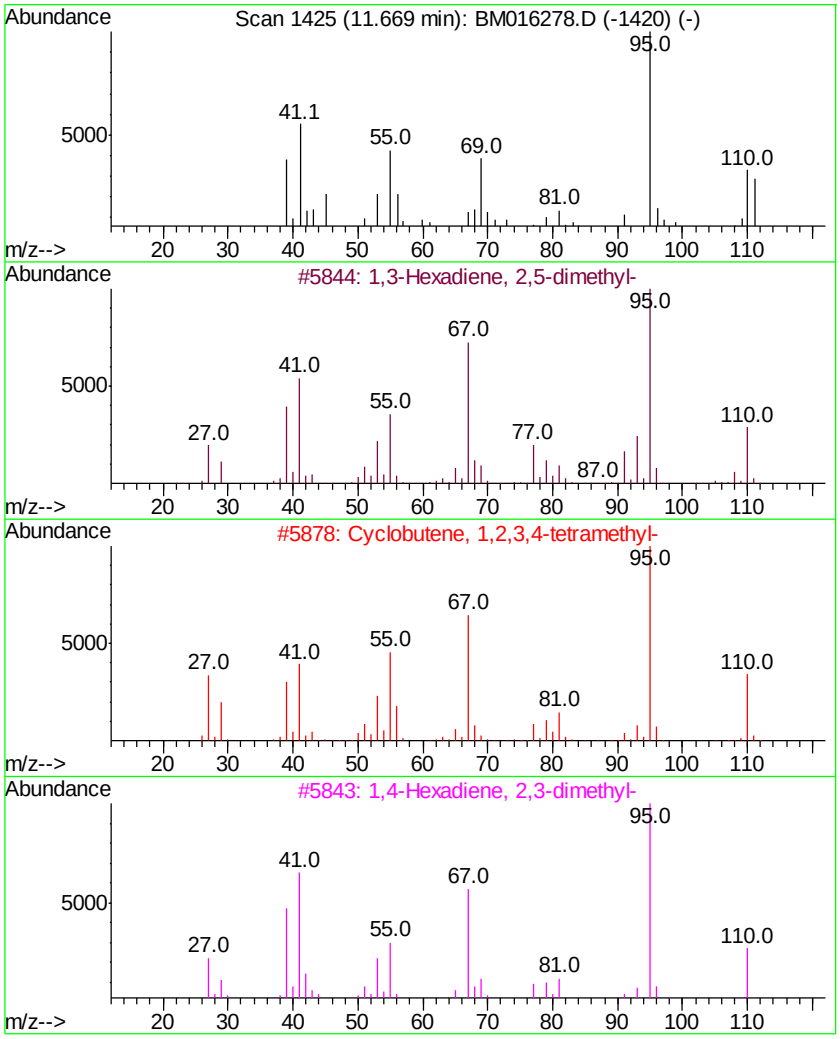
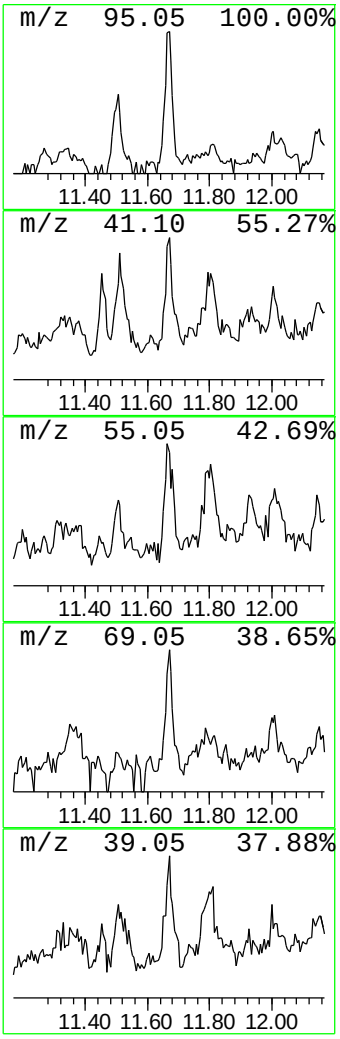
Peak Number 8 1,3-Hexadiene, 2,5-dimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	3.30 ng	58073	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexadiene, 2,5-dimethyl-	110	C8H14	029253-64-3	53
2	Cyclobutene, 1,2,3,4-tetramethyl-	110	C8H14	090346-45-5	52
3	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	49
4	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	47
5	4-Methyl-1,3-heptadiene (c,t)	110	C8H14	017603-57-5	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016278.D
Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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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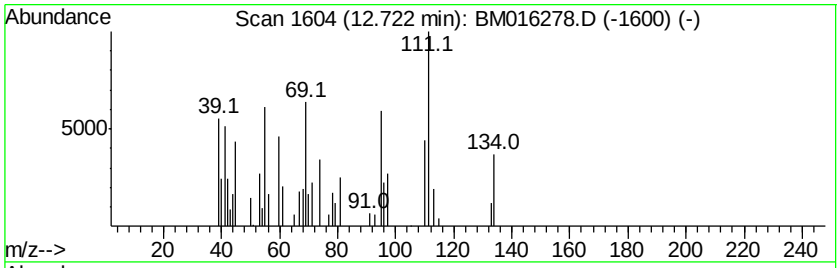
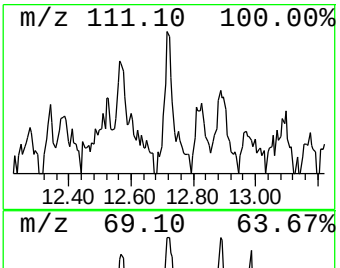
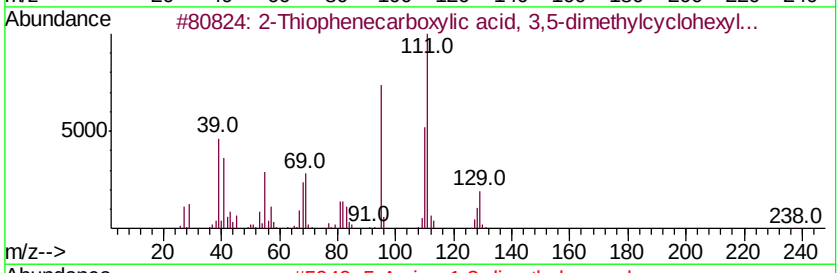
Peak Number 9 unknown12.72 Concentration Rank 15

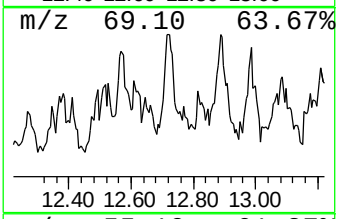
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	3.33 ng	58691	Naphthalene-d8	10.95

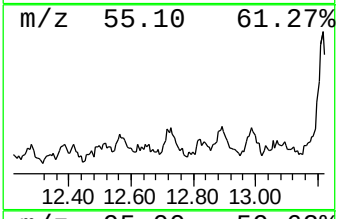
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenecarboxylic acid, 3,5-...	238	C13H18O2S	1000278-87-5	38
2	5-Amino-1,3-dimethylpyrazole	111	C5H9N3	003524-32-1	27
3	3-Propylglutaric acid	174	C8H14O4	004165-98-4	12
4	1,1'-Bicyclooctyl	222	C16H30	006708-17-4	12
5	Cyclohexane, 1-methyl-4-(2-hydro...	142	C9H18O	004916-87-4	10

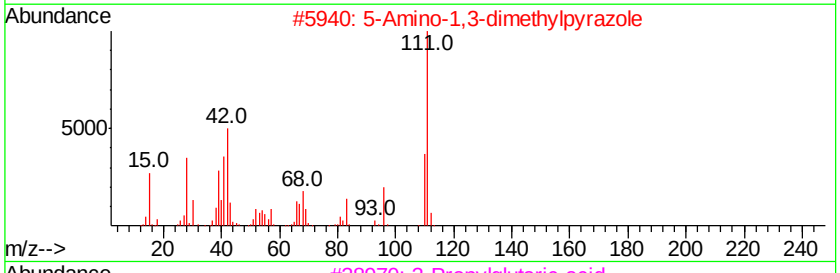


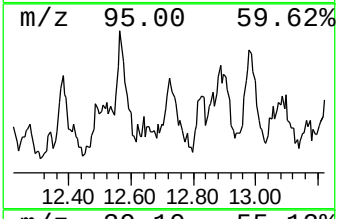


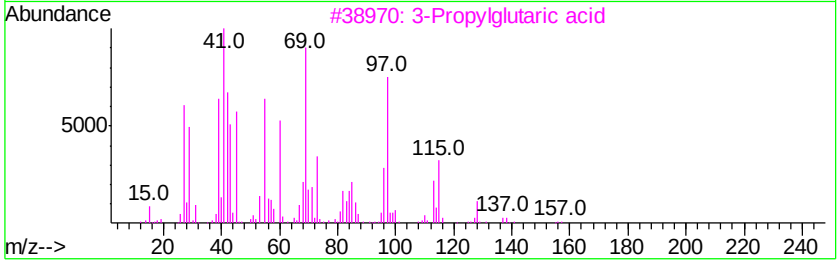


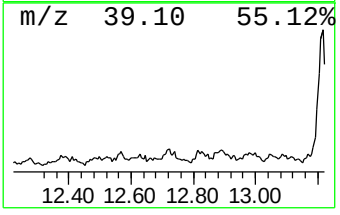












Library Search Compound Report

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Data File : BM016278.D
Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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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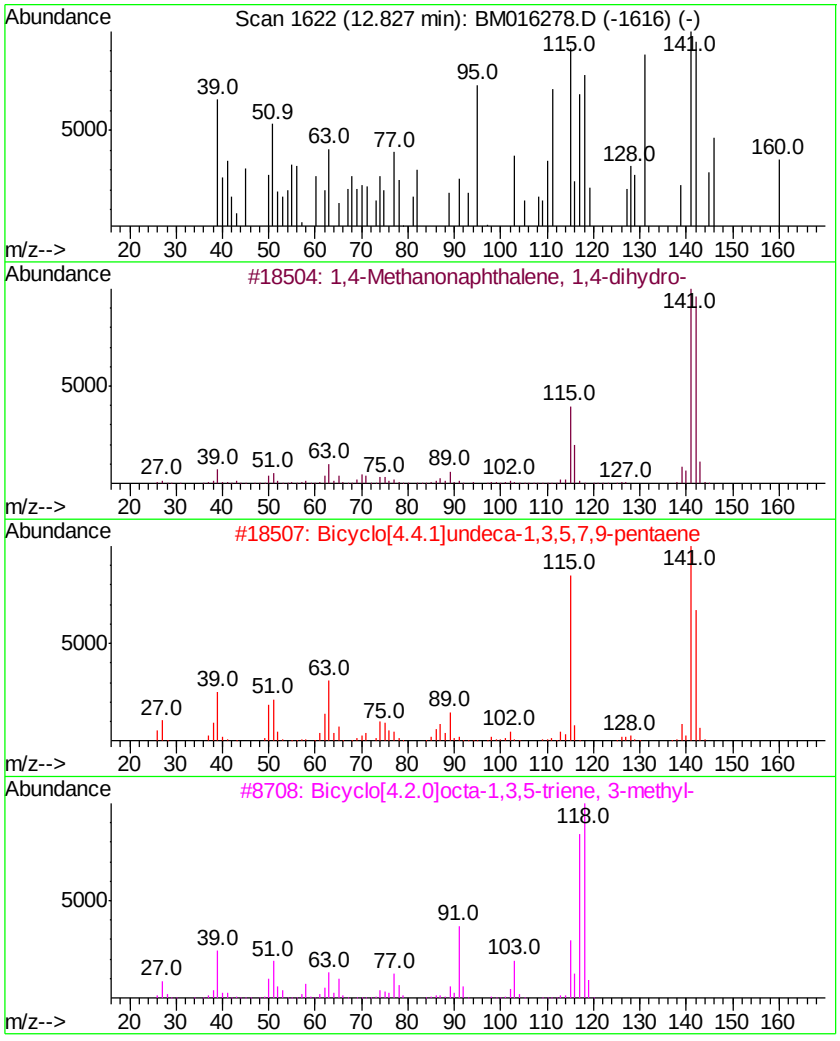
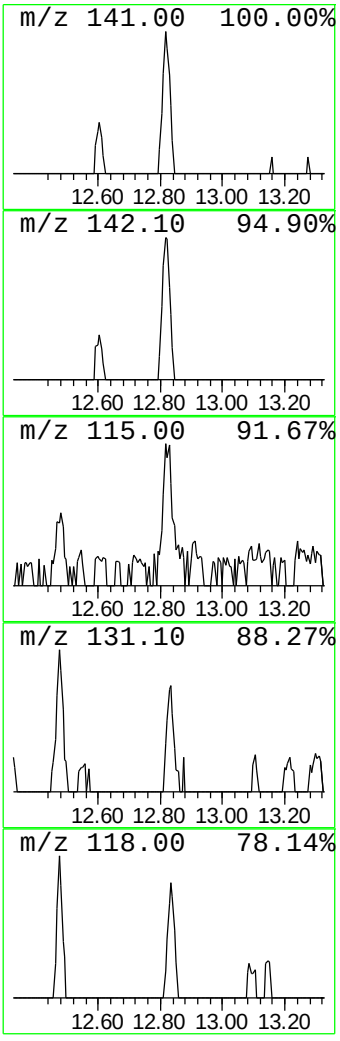
Peak Number 10 unknown12.83 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	3.96 ng	69763	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	49
2	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	49
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	022250-74-4	46
4	1H-Tetrazole, 5-phenyl-	146	C7H6N4	018039-42-4	41
5	Ethyl-2-benzofuran	146	C10H10O	003131-63-3	38





Library Search Compound Report

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Acq On : 09 Aug 2018 13:00
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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

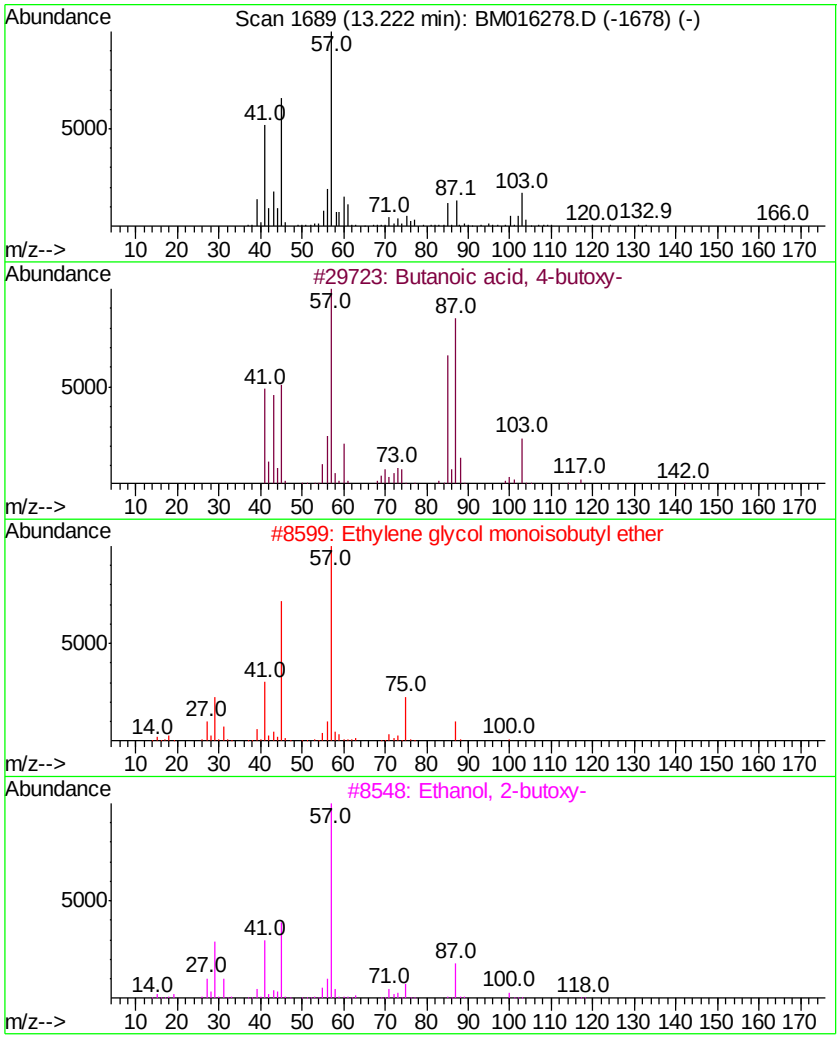
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

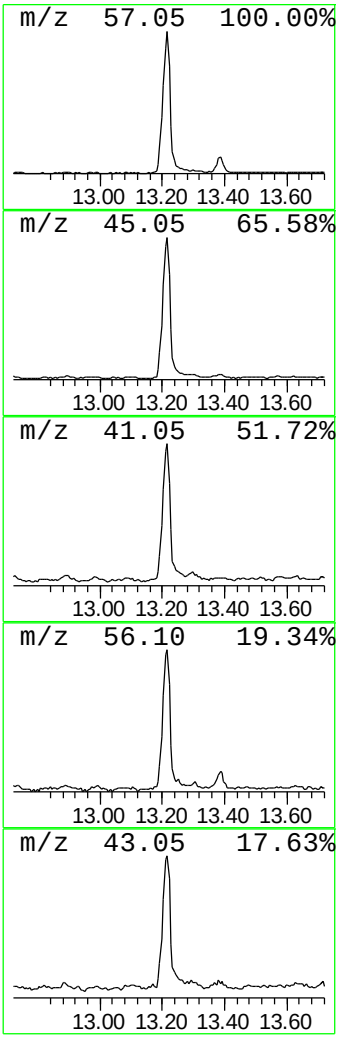
****

Peak Number 11 unknown13.22 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.22	30.89 ng	747585	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-butoxy-	160	C8H16O3	055724-73-7	40
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	37
4	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	37
5	Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	37





Library Search Compound Report

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Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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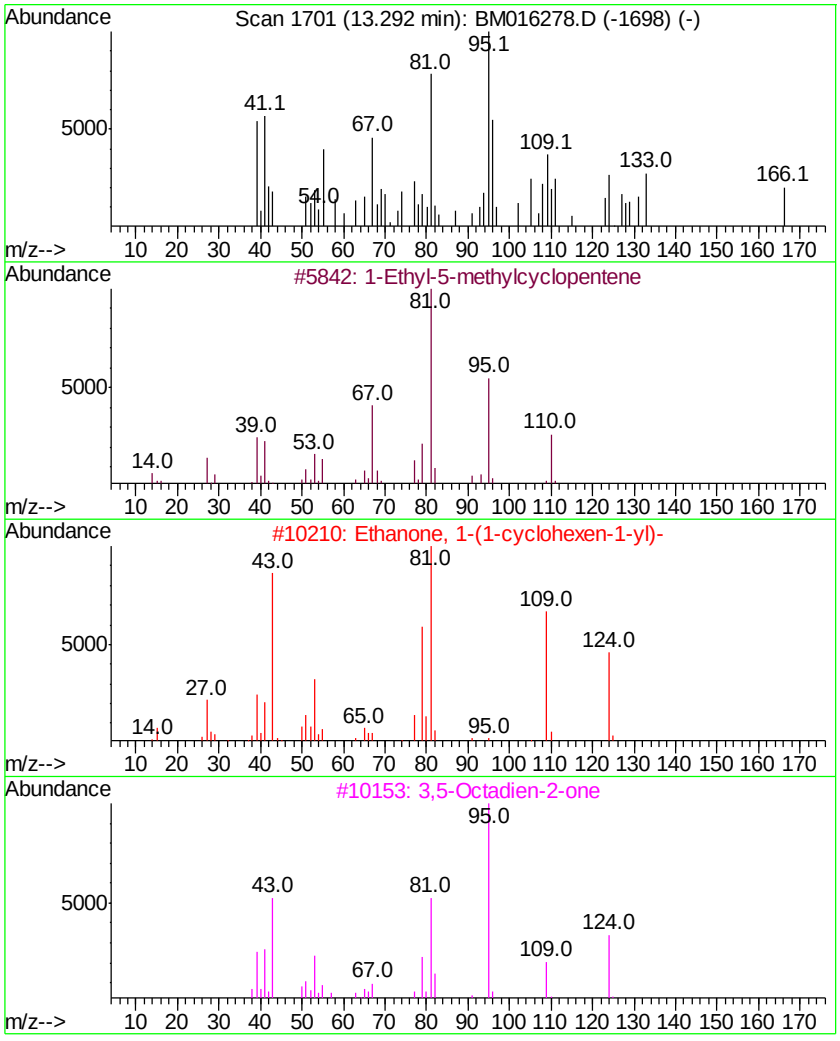
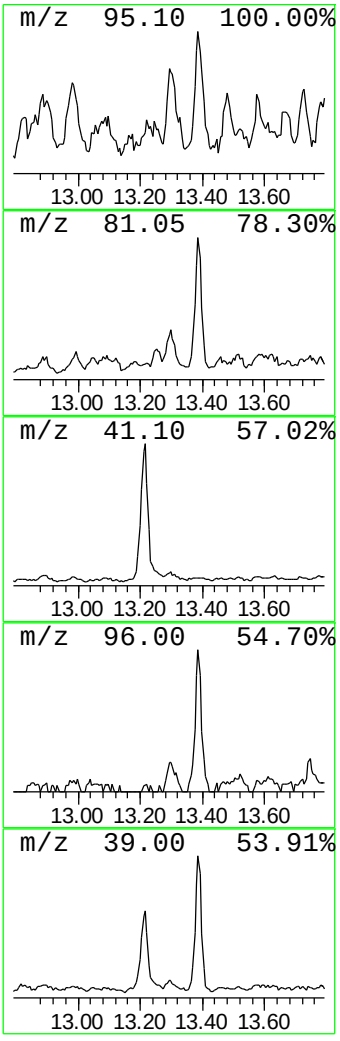
Peak Number 12 unknown13.29 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	3.18 ng	77009	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	27
2	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	25
3	3,5-Octadien-2-one	124	C8H12O	038284-27-4	25
4	1,3-Hexadiene, 3-ethyl-2-methyl-...	124	C9H16	074752-97-9	25
5	Cyclohexane, (1-methylethylidene)-	124	C9H16	005749-72-4	25





Library Search Compound Report

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Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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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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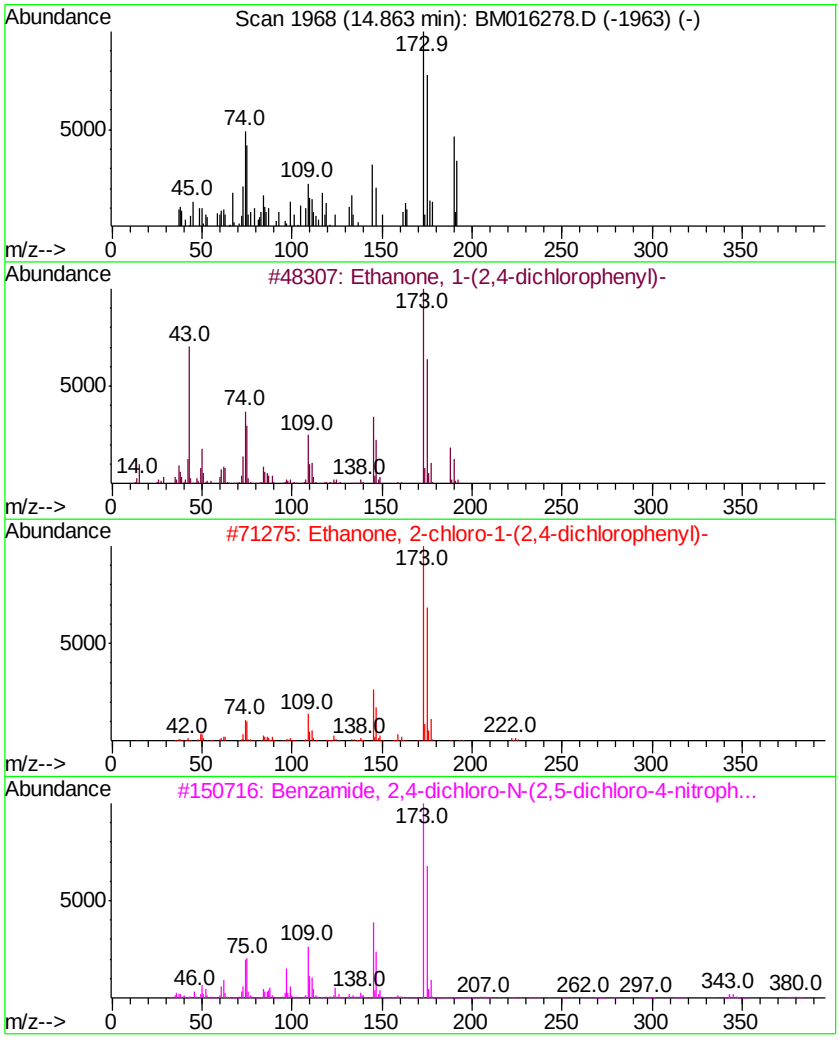
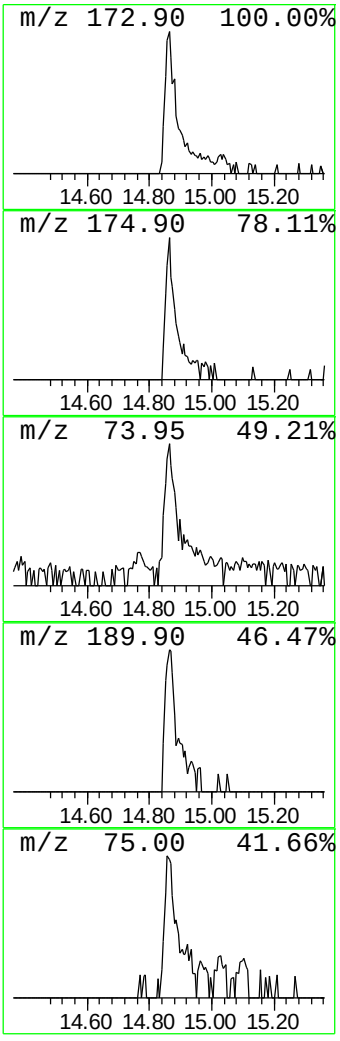
Peak Number 13 Ethanone, 1-(2,4-dichloroph... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	3.11 ng	75370	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(2,4-dichlorophenyl)-	188	C8H6Cl2O	002234-16-4	58
2	Ethanone, 2-chloro-1-(2,4-dichlo...	222	C8H5Cl3O	004252-78-2	53
3	Benzamide, 2,4-dichloro-N-(2,5-d...	378	C13H6Cl4N2O3	1000263-62-1	53
4	Ethanone, 1-(2,5-dichlorophenyl)-	188	C8H6Cl2O	002476-37-1	50
5	Benzoic acid, 2,4-dichloro-, 4-f...	284	C13H7Cl2FO2	283171-60-8	50





Library Search Compound Report

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Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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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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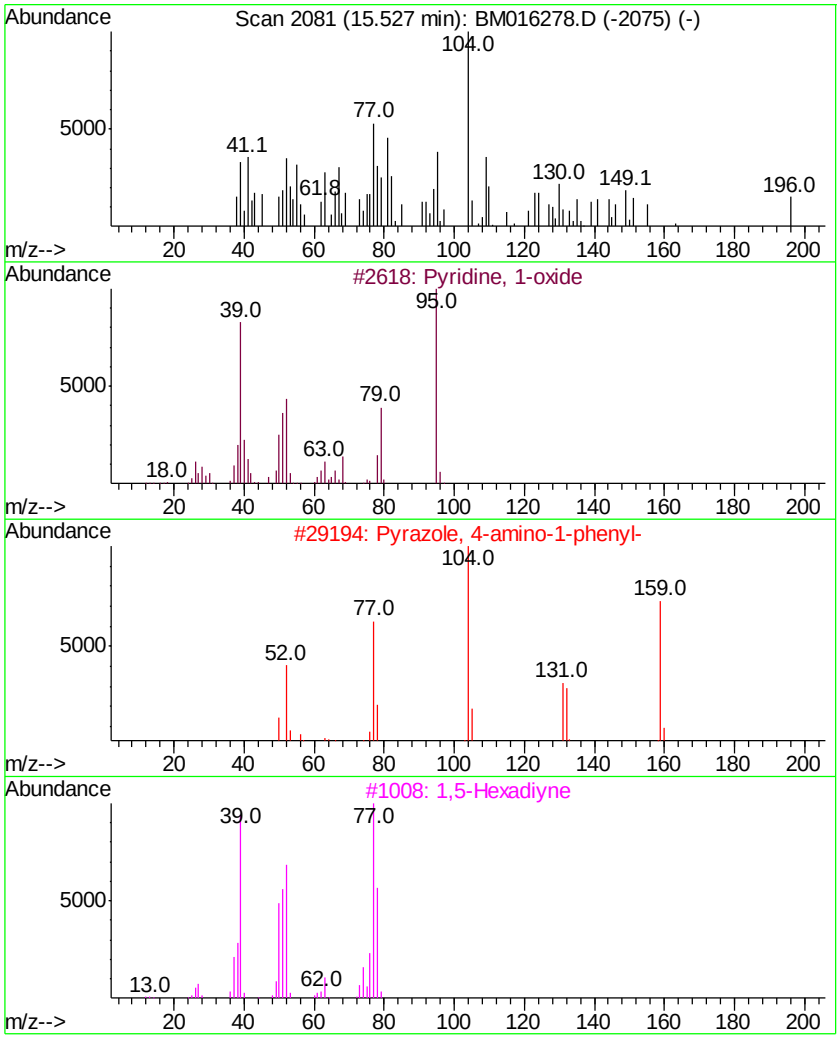
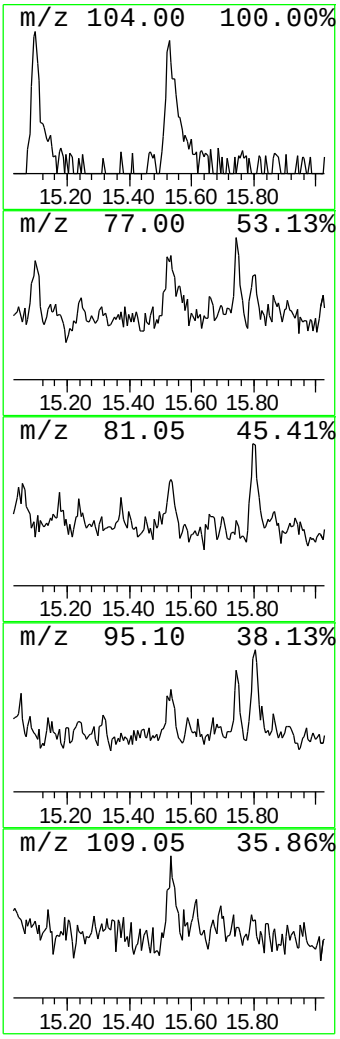
Peak Number 14 unknown15.53 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	3.22 ng	77935	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	38
2	Pyrazole, 4-amino-1-phenyl-	159	C9H9N3	001128-53-6	23
3	1,5-Hexadiyne	78	C6H6	000628-16-0	18
4	2-Oxabicyclo[2.2.0]hex-5-en-3-one	96	C5H4O2	022980-23-0	14
5	Butanoic acid, 4-[4-methylimidaz...	196	C10H16N2O2	1000116-74-5	10





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Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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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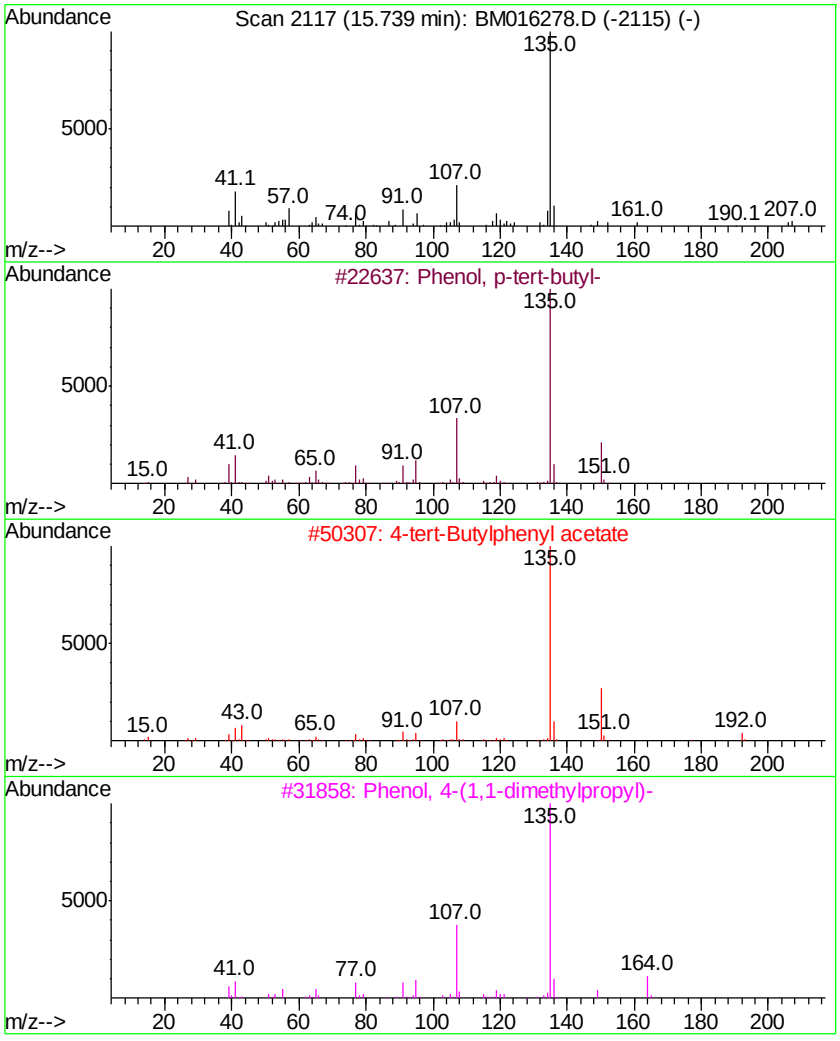
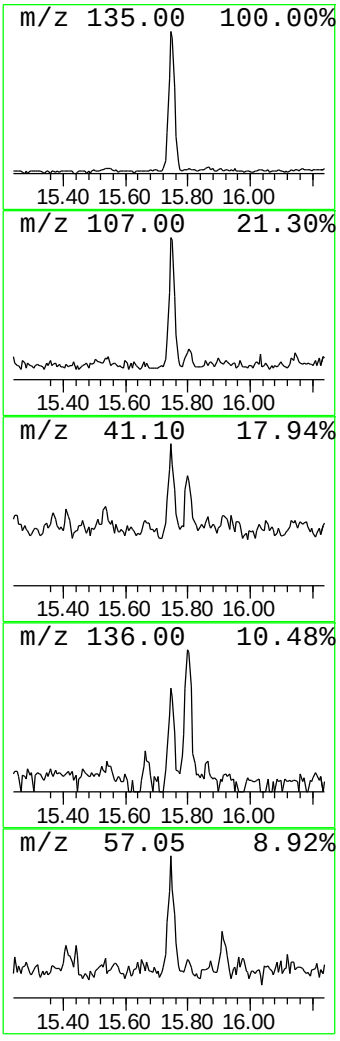
Peak Number 15 Phenol, p-tert-butyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	3.97 ng	96117	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
2	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	72
3	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	72
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
5	Benzeneacetonitrile, 4-fluoro-	135	C8H6FN	000459-22-3	64





Library Search Compound Report

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Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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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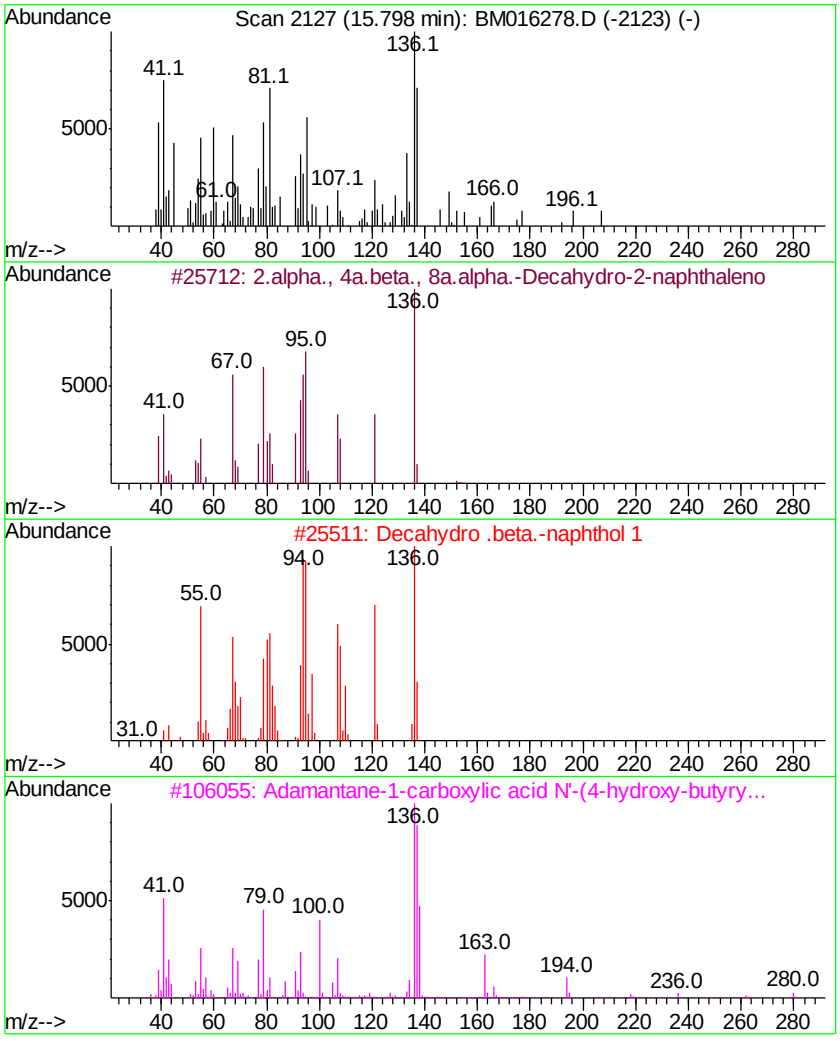
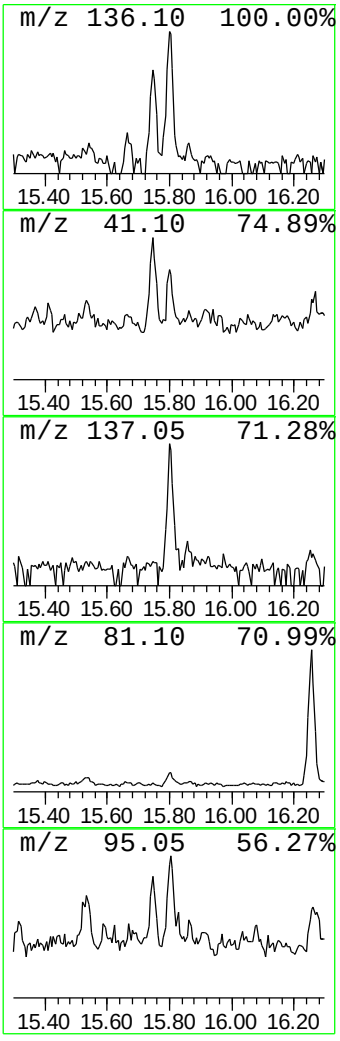
Peak Number 16 unknown15.80 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	3.37 ng	81566	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2.alpha., 4a.beta., 8a.alpha.-De...	154	C10H18O	005779-35-1	47
2	Decahydro .beta.-naphthol 1	154	C10H18O	1000285-14-4	43
3	Adamantane-1-carboxylic acid N'-...	280	C15H24N2O3	1000294-38-3	38
4	Adamantane	136	C10H16	000281-23-2	27
5	Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	005113-87-1	27





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Acq On : 09 Aug 2018 13:00
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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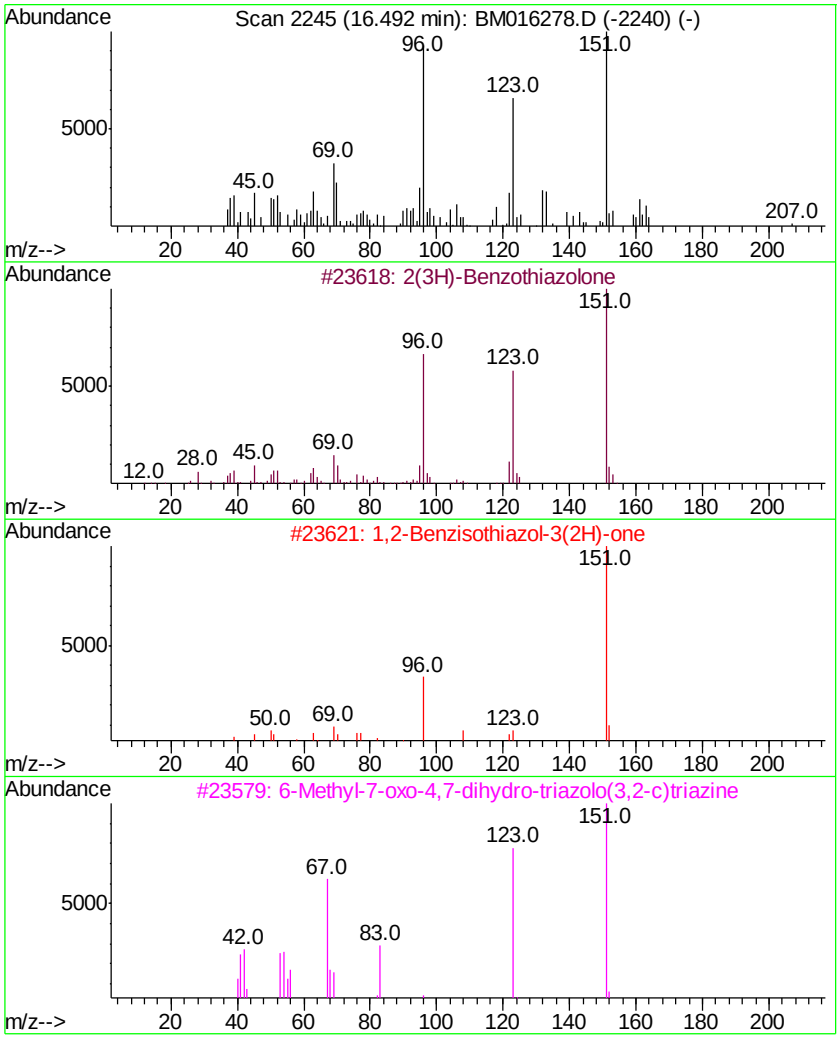
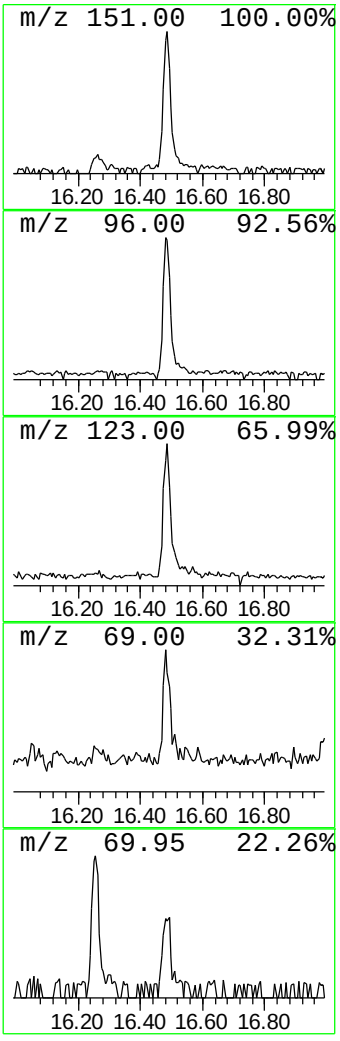
Peak Number 17 2(3H)-Benzothiazolone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	7.33 ng	162770	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	80
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	52
3	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	35
4	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	35
5	Thieno[3,2-c]pyridin-4(5H)-one	151	C7H5NOS	027685-92-3	25





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Instrument : BNA_M
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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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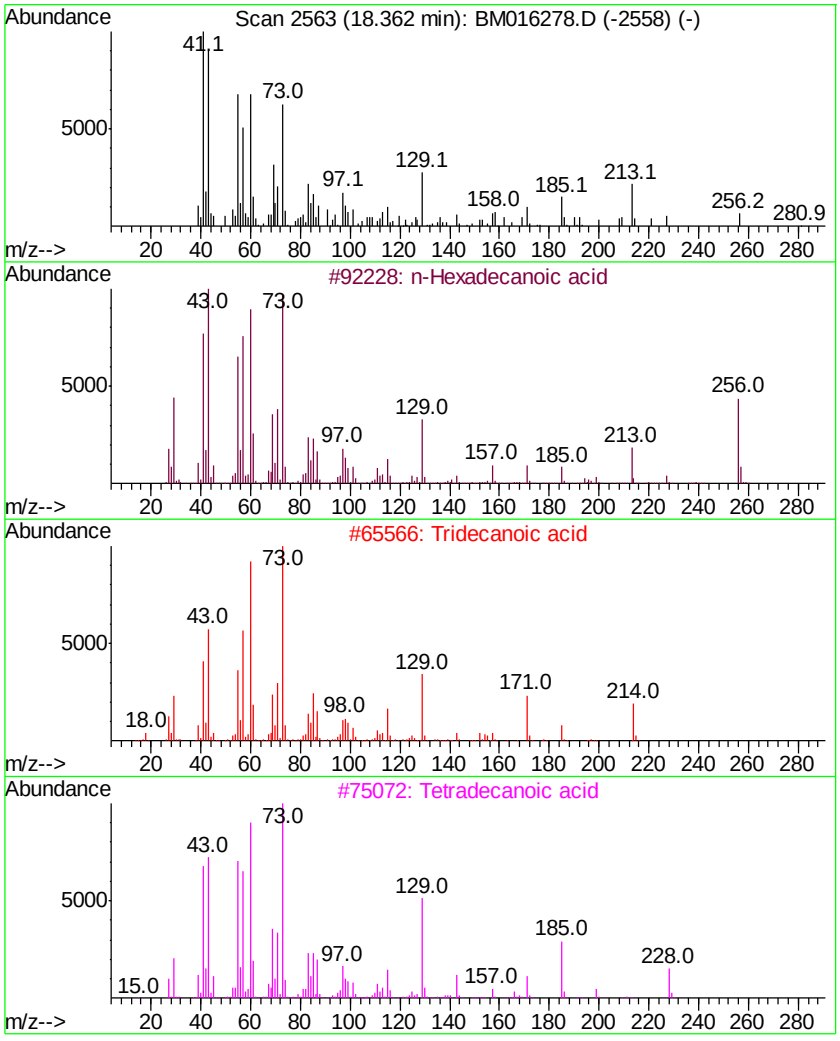
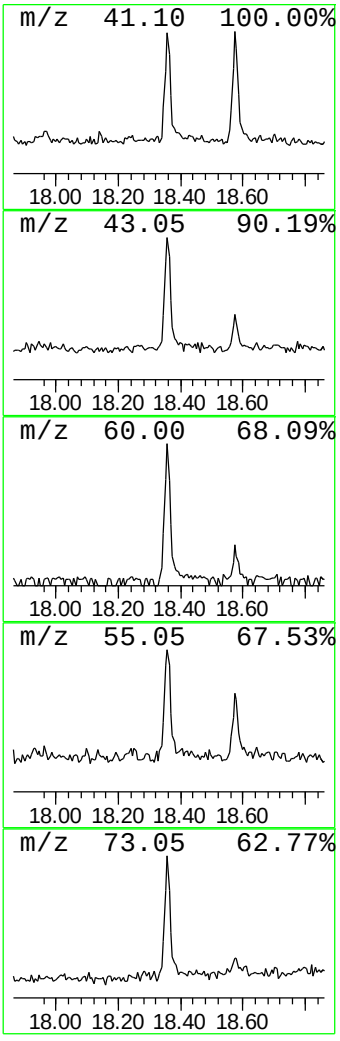
Peak Number 18 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	5.40 ng	119907	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Nonanoic acid	158	C9H18O2	000112-05-0	58





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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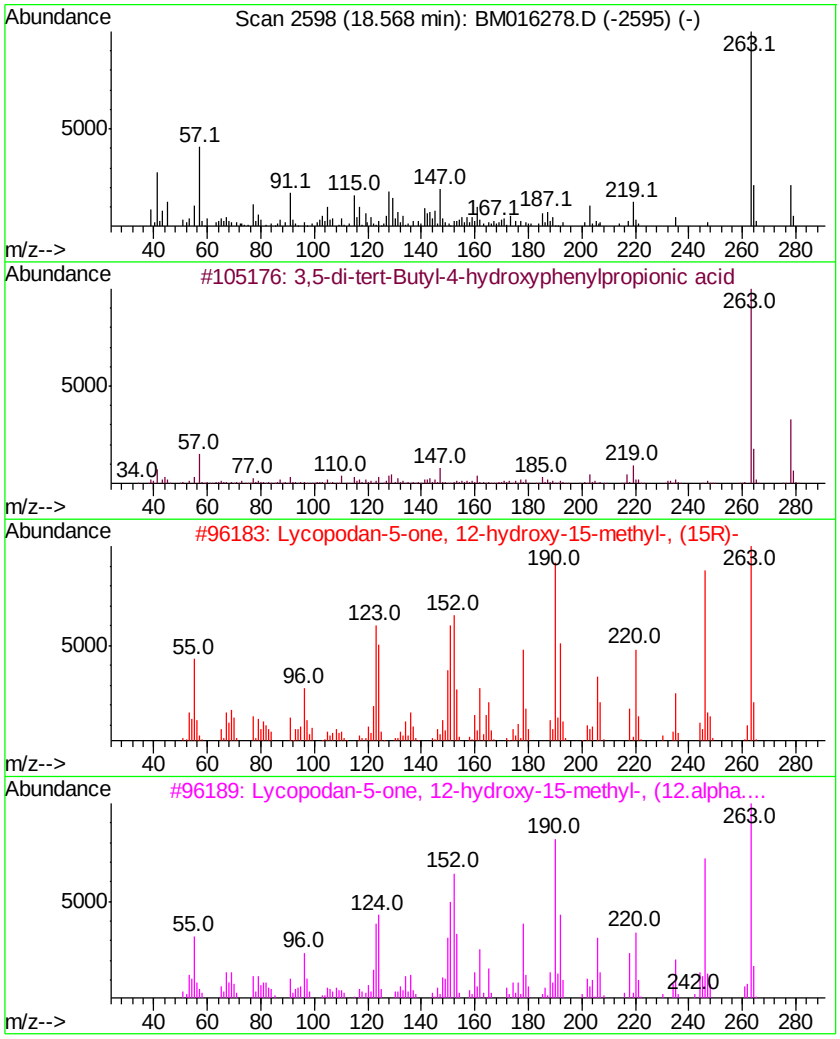
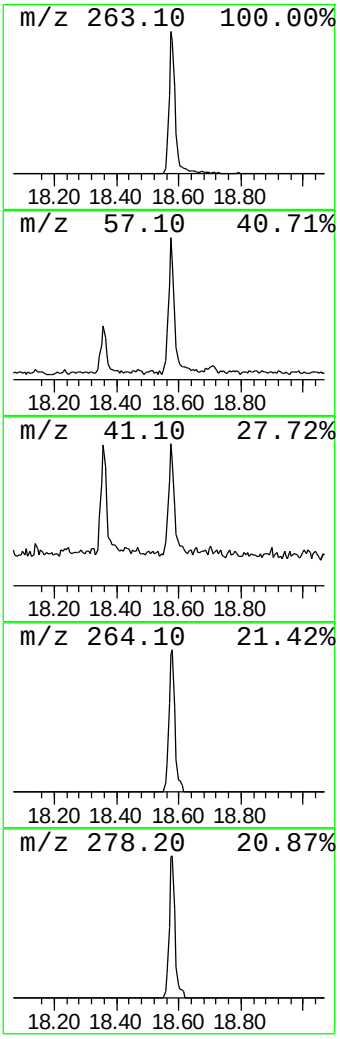
Peak Number 19 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	16.93 ng	376205	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxyphenyl...	278	C17H26O3	020170-32-5	91
2	Lycopodan-5-one, 12-hydroxy-15-m...	263	C16H25NO2	006900-92-1	90
3	Lycopodan-5-one, 12-hydroxy-15-m...	263	C16H25NO2	021061-90-5	89
4	4,6-Dinitro-1,1,3,3,5-pentamethy...	278	C14H18N2O4	000116-66-5	50
5	1H-Pyrazole-4-carbonitrile, 3-(4...	263	C12H10ClN3S	068364-67-0	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016278.D
Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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

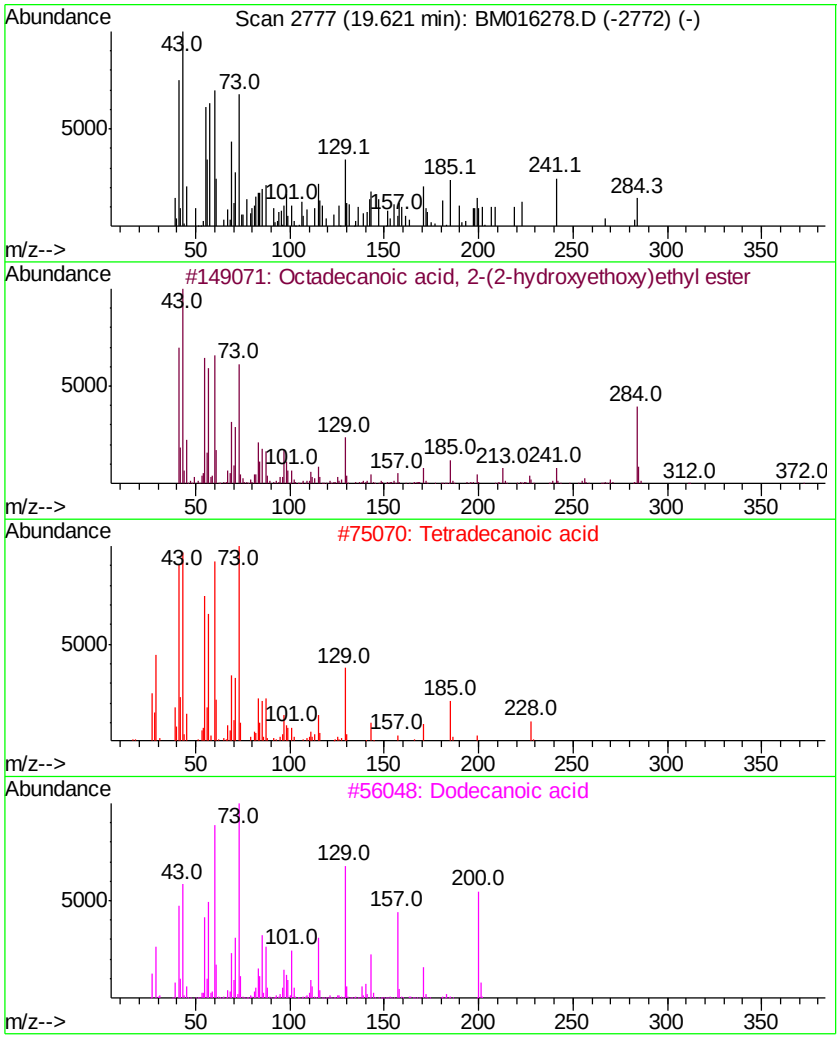
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

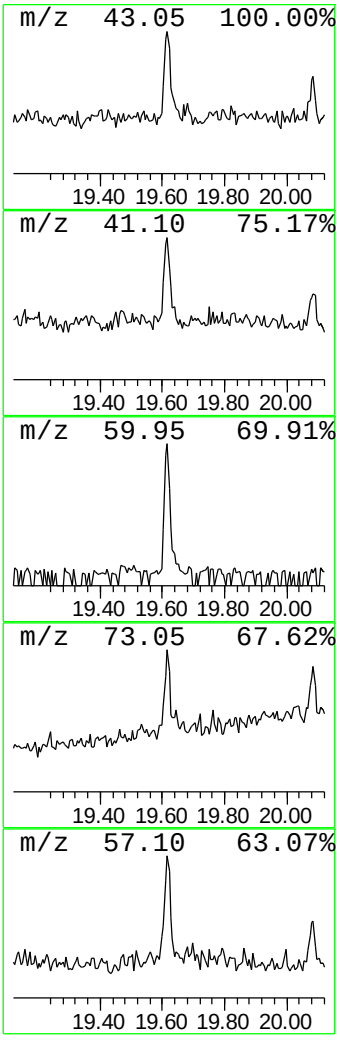
****

Peak Number 20 Octadecanoic acid, 2-(2-hyd... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	3.17 ng	81323	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	58
4	Octadecanoic acid	284	C18H36O2	000057-11-4	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080918\
Data File : BM016278.D
Acq On : 09 Aug 2018 13:00
Operator : SJ/JU
Sample : J4356-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-11

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
2-Pentanone, 4-hy...	5.19	4.9	ng	77238	1	8.13	315564	20.0
1-Methylcyclohexanol	6.18	5.6	ng	88652	1	8.13	315564	20.0
unknown7.66	7.66	101.5	ng	1600630	1	8.13	315564	20.0
unknown9.76	9.76	3.3	ng	58715	2	10.95	352177	20.0
1,3-Cyclopentadie...	10.33	4.1	ng	71520	2	10.95	352177	20.0
unknown11.51	11.51	4.2	ng	74215	2	10.95	352177	20.0
1,3-Hexadiene, 2,...	11.67	3.3	ng	58073	2	10.95	352177	20.0
unknown12.72	12.72	3.3	ng	58691	2	10.95	352177	20.0
unknown12.83	12.83	4.0	ng	69763	2	10.95	352177	20.0
unknown13.22	13.22	30.9	ng	747585	3	14.77	484097	20.0
unknown13.29	13.29	3.2	ng	77009	3	14.77	484097	20.0
Ethanone, 1-(2,4-...	14.86	3.1	ng	75370	3	14.77	484097	20.0
unknown15.53	15.53	3.2	ng	77935	3	14.77	484097	20.0
Phenol, p-tert-bu...	15.74	4.0	ng	96117	3	14.77	484097	20.0
unknown15.80	15.80	3.4	ng	81566	3	14.77	484097	20.0
2(3H)-Benzothiazo...	16.49	7.3	ng	162770	4	17.50	444403	20.0
n-Hexadecanoic acid	18.36	5.4	ng	119907	4	17.50	444403	20.0
3,5-di-tert-Butyl...	18.57	16.9	ng	376205	4	17.50	444403	20.0
Octadecanoic acid...	19.62	3.2	ng	81323	5	21.63	513089	20.0