LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016277.D
Acq On : 09 Aug 2018 12:24
Operator : SJ/JU
Sample : J4356-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-29

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	4.658	227	233	242	rBV	53540	77199	2.18%	0.417%
2	5.187	318	323	334	rVB	57887	89511	2.52%	0.484%
3	5.663	398	404	418	rBV	506260	796168	22.43%	4.305%
4	7.304	677	683	693	rBV	285987	483164	13.61%	2.613%
5	7.663	737	744	757	rBV	1077324	1715560	48.34%	9.277%
6	8.134	817	824	835	rBB	190047	316649	8.92%	1.712%
7	8.451	871	878	890	rBV	1028616	1645061	46.35%	8.896%
8	9.322	1019	1026	1039	rBV	739878	1244977	35.08%	6.733%
9	10.945	1296	1302	1309	rBV	212457	358613	10.10%	1.939%
10	13.204	1681	1686	1696	rVB	171915	271105	7.64%	1.466%
11	13.386	1709	1717	1723	rBV	1816894	2523621	71.11%	13.647%
12	14.110	1835	1840	1848	rBV	18319	50756	1.43%	0.274%
13	14.222	1855	1859	1863	rVB	40750	54314	1.53%	0.294%
14	14.604	1919	1924	1930	rBV10	22058	41516	1.17%	0.225%
15	14.769	1946	1952	1957	rBV2	295706	454453	12.80%	2.458%
16	14.828	1958	1962	1964	rVV2	42289	61794	1.74%	0.334%
17	14.857	1964	1967	1974	rVB2	52377	97856	2.76%	0.529%
18	15.245	2029	2033	2037	rBV5	29475	52967	1.49%	0.286%
19	15.804	2124	2128	2134	rBV3	53331	93153	2.62%	0.504%
20	15.869	2136	2139	2145	rVB7	40179	61823	1.74%	0.334%
21	16.257	2199	2205	2218	rBV	1589943	2266707	63.87%	12.258%
22	17.504	2412	2417	2422	rVB	336472	465645	13.12%	2.518%
23	18.363	2560	2563	2567	rBV2	112947	131430	3.70%	0.711%
24	18.586	2597	2601	2610	rVB	212027	299158	8.43%	1.618%
25	19.621	2774	2777	2781	rBV5	61714	80090	2.26%	0.433%
26	20.086	2850	2856	2862	rBV	3096496	3549099	100.00%	19.193%
27	20.998	3009	3011	3019	rVB	76911	96324	2.71%	0.521%
28	21.633	3115	3119	3125	rVB	431201	533521	15.03%	2.885%
29	23.968	3511	3516	3524	rVB2	300112	579667	16.33%	3.135%

Sum of corrected areas: 18491901

LSC Report - Integrated Chromatogram

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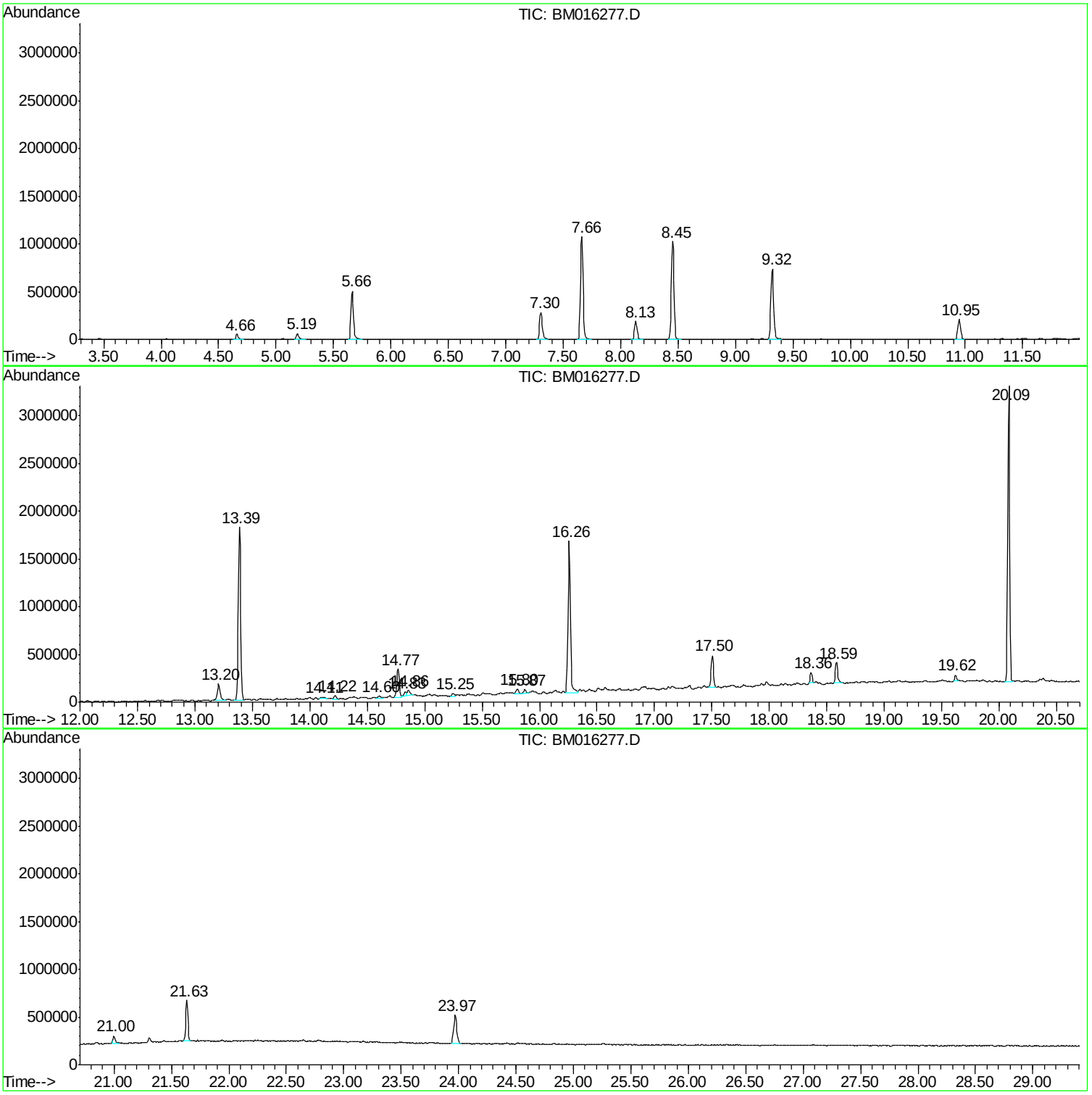
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-29

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

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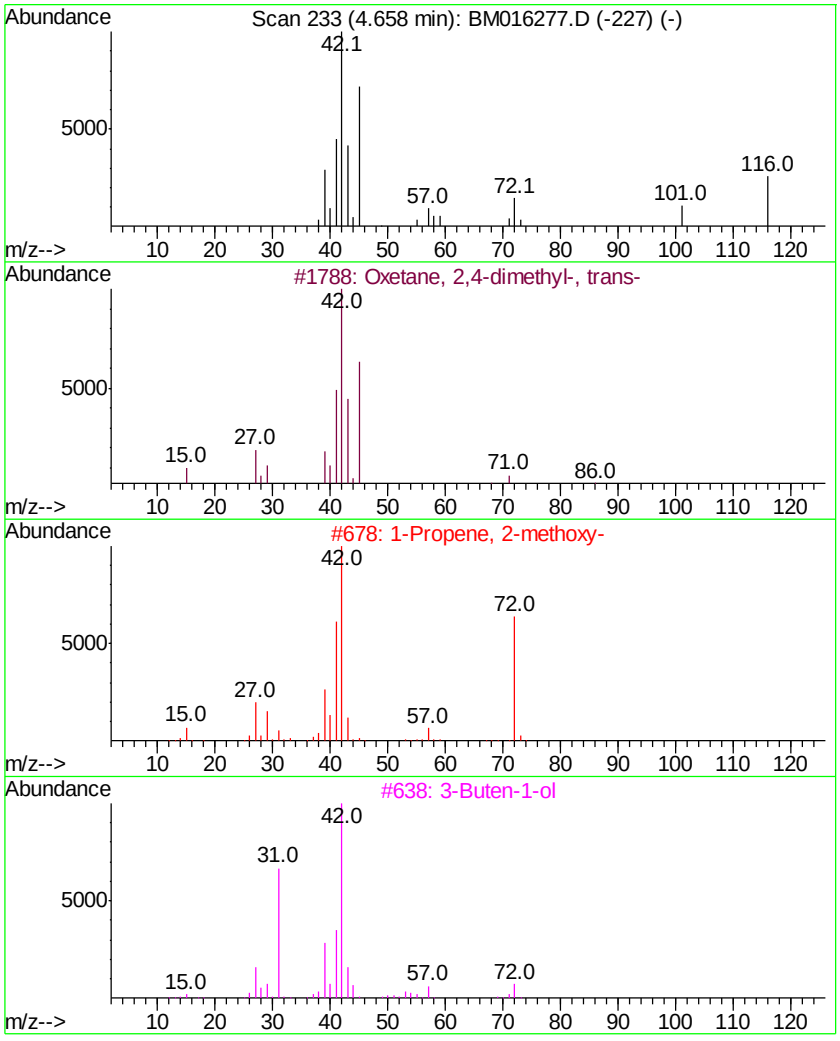
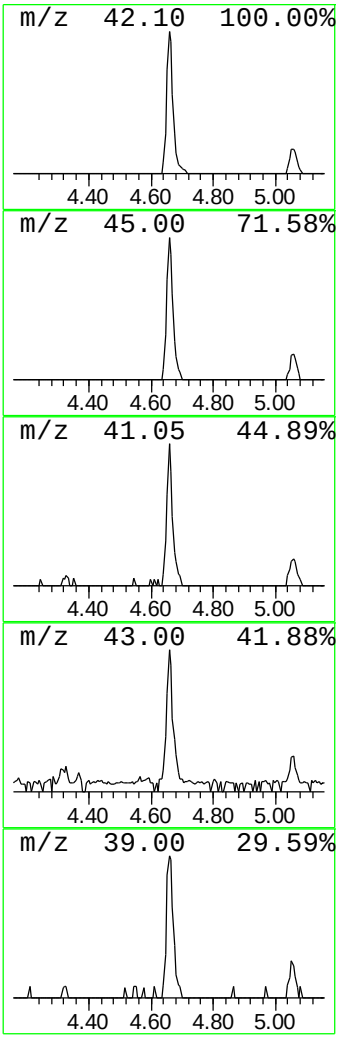
****

Peak Number 1 unknown4.66 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.66	4.88 ng	77199	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxetane, 2,4-dimethyl-, trans-	86	C5H10O	029424-94-0	40
2	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	38
3	3-Buten-1-ol	72	C4H8O	000627-27-0	38
4	2,3-Butanedione, dioxime	116	C4H8N2O2	000095-45-4	25
5	Ethylenimine	43	C2H5N	000151-56-4	9





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Operator : SJ/JU
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-29

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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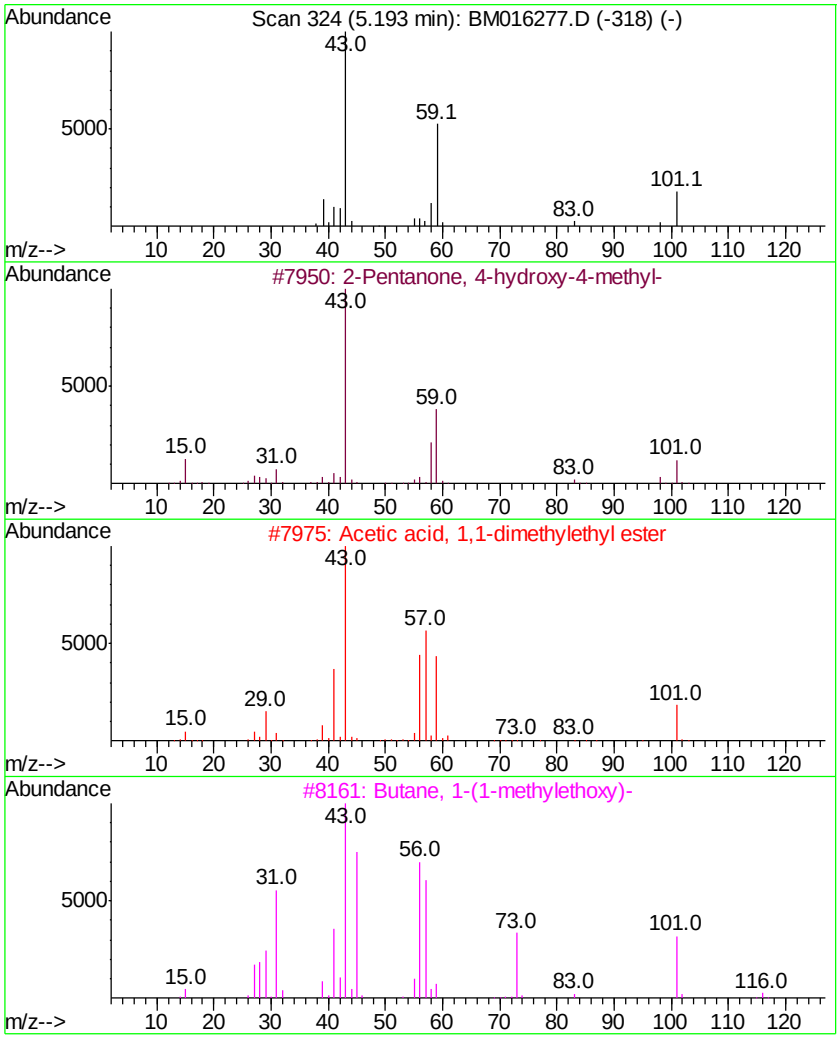
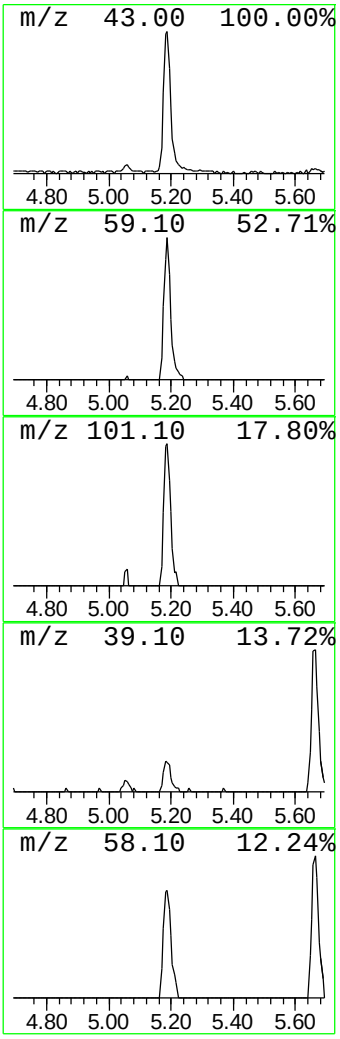
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	5.65 ng	89511	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	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
3	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	25
4	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	25
5	Butane	58	C4H10	000106-97-8	22





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Operator : SJ/JU
Sample : J4356-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-29

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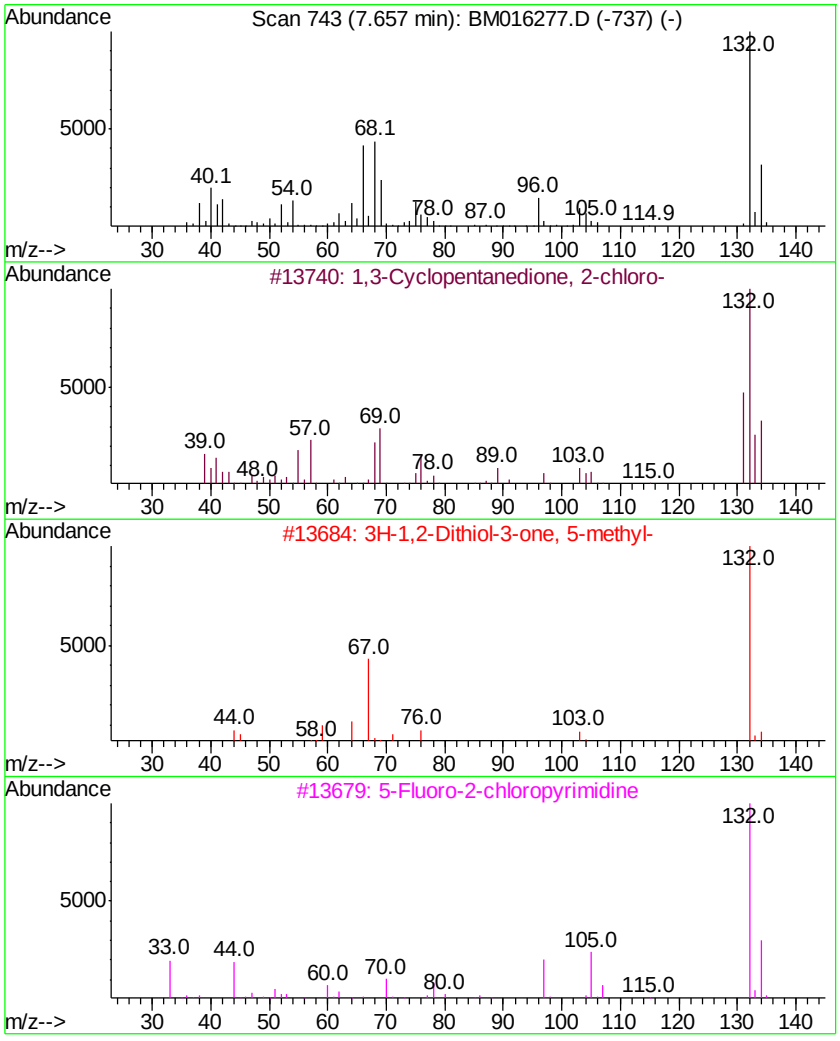
TIC Integration Parameters: LSCINT.P

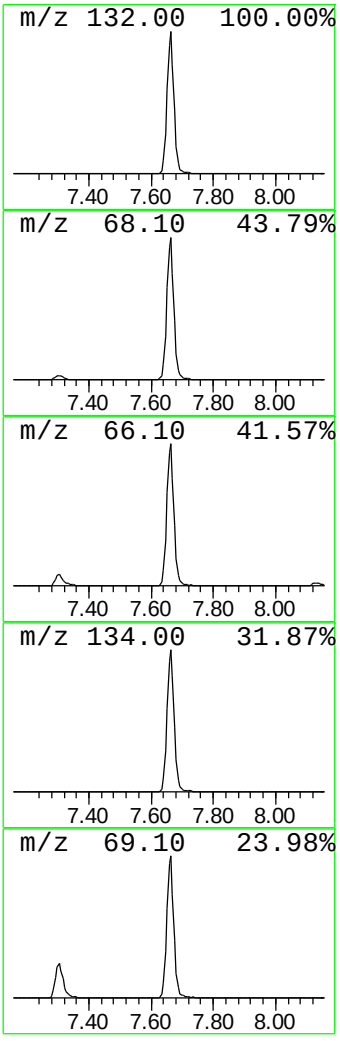
****

Peak Number 3 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	108.36 ng	1715560	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14





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Operator : SJ/JU
Sample : J4356-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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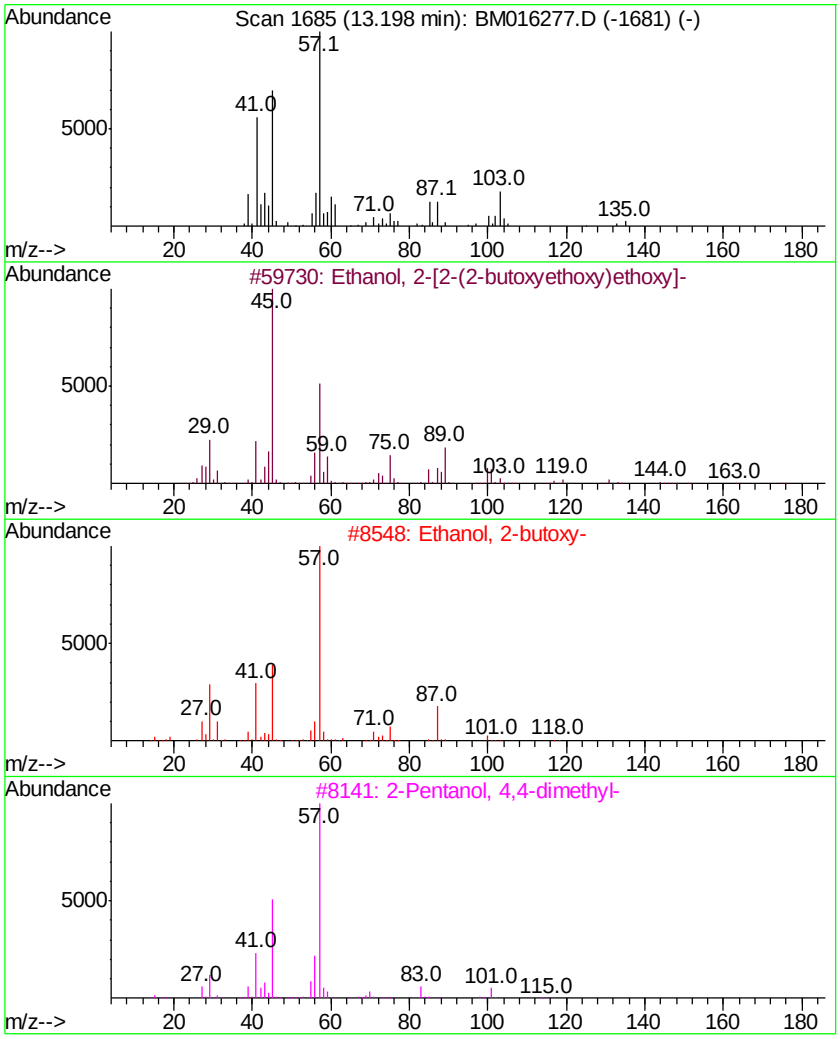
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

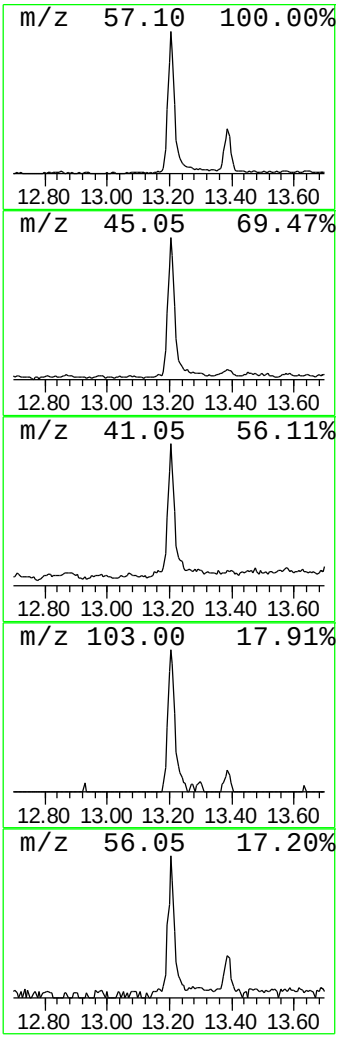
****

Peak Number 5 unknown13.20 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	11.93 ng	271105	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	42
2	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	37
3	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	37
4	Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	37
5	Propanoic acid, 2,2-dimethyl-, h...	186	C11H22O2	005434-57-1	35





Library Search Compound Report

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Sample : J4356-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-29

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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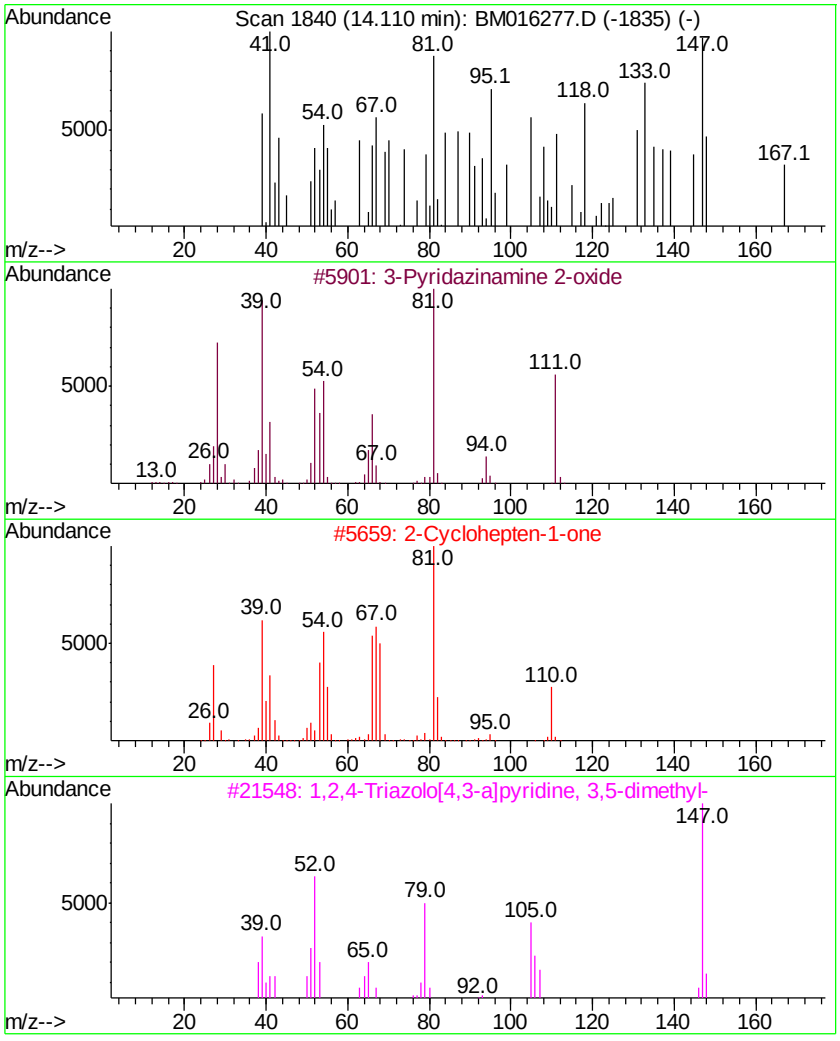
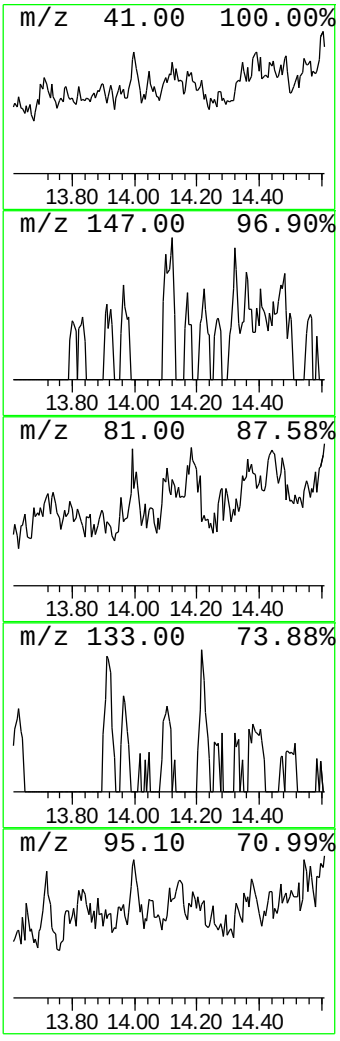
****

Peak Number 6 unknown14.11 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.11	2.23 ng	50756	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pyridazinamine 2-oxide	111	C4H5N3O	033471-48-6	25
2	2-Cyclohepten-1-one	110	C7H10O	001121-66-0	15
3	1,2,4-Triazolo[4,3-a]pyridine, 3...	147	C8H9N3	004919-12-4	14
4	3-Octen-1-yne, (E)-	108	C8H12	042104-42-7	12
5	Benzofurazan, 4,5,6,7-tetrahydro...	169	C6H7N3O3	1000262-66-9	12





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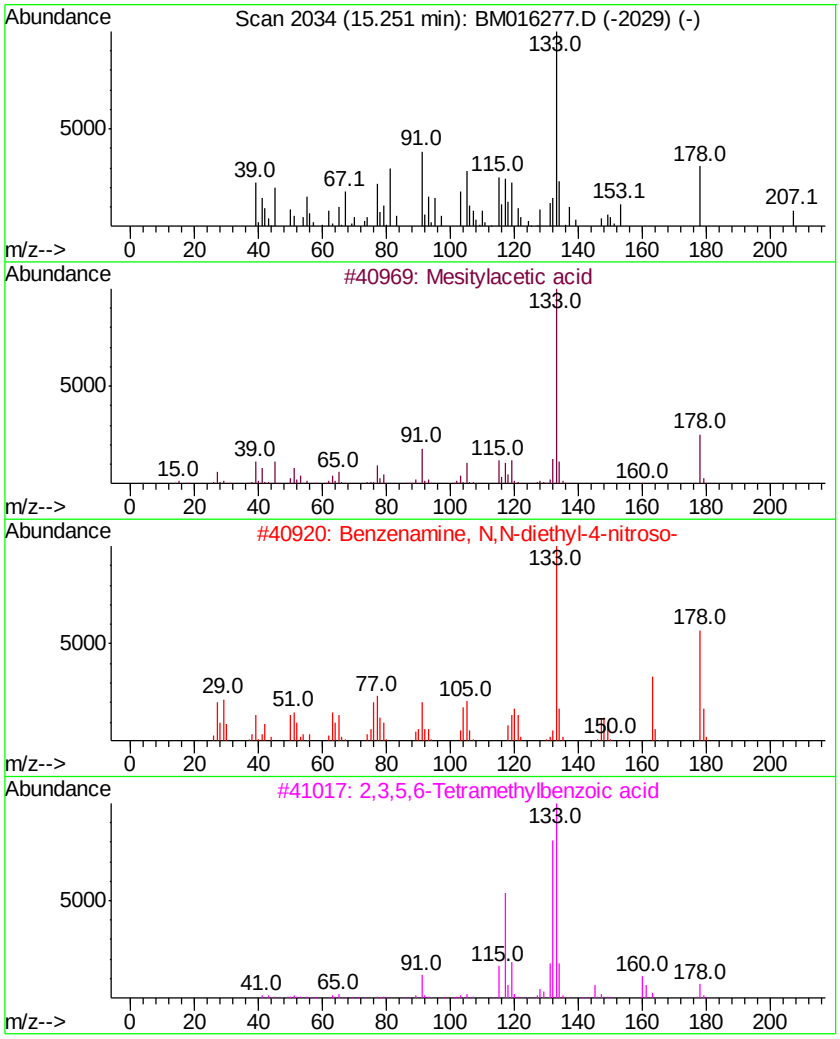
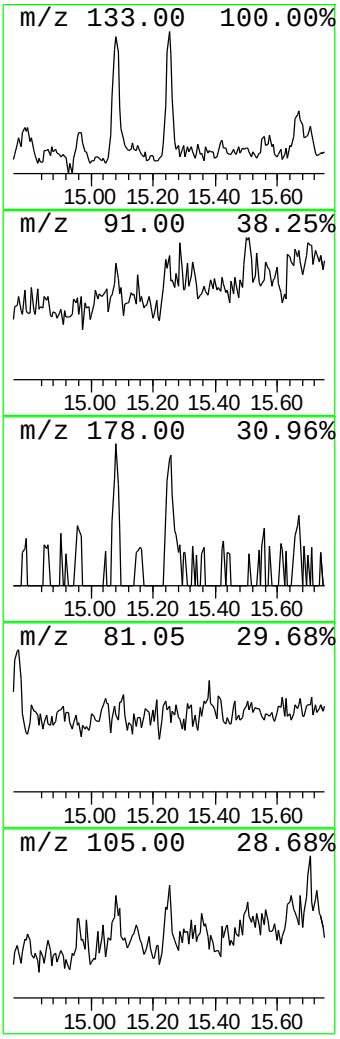
****

Peak Number 7 Mesitylacetic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	2.33 ng	52967	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylacetic acid	178	C11H14O2	004408-60-0	52
2	Benzenamine, N,N-diethyl-4-nitroso-	178	C10H14N2O	000120-22-9	43
3	2,3,5,6-Tetramethylbenzoic acid	178	C11H14O2	002604-45-7	37
4	Benzeneacetaldehyde, .alpha.,2,5...	162	C11H14O	052417-50-2	32
5	Benzoic acid, 4-ethyl-, methyl e...	164	C10H12O2	007364-20-7	27





Library Search Compound Report

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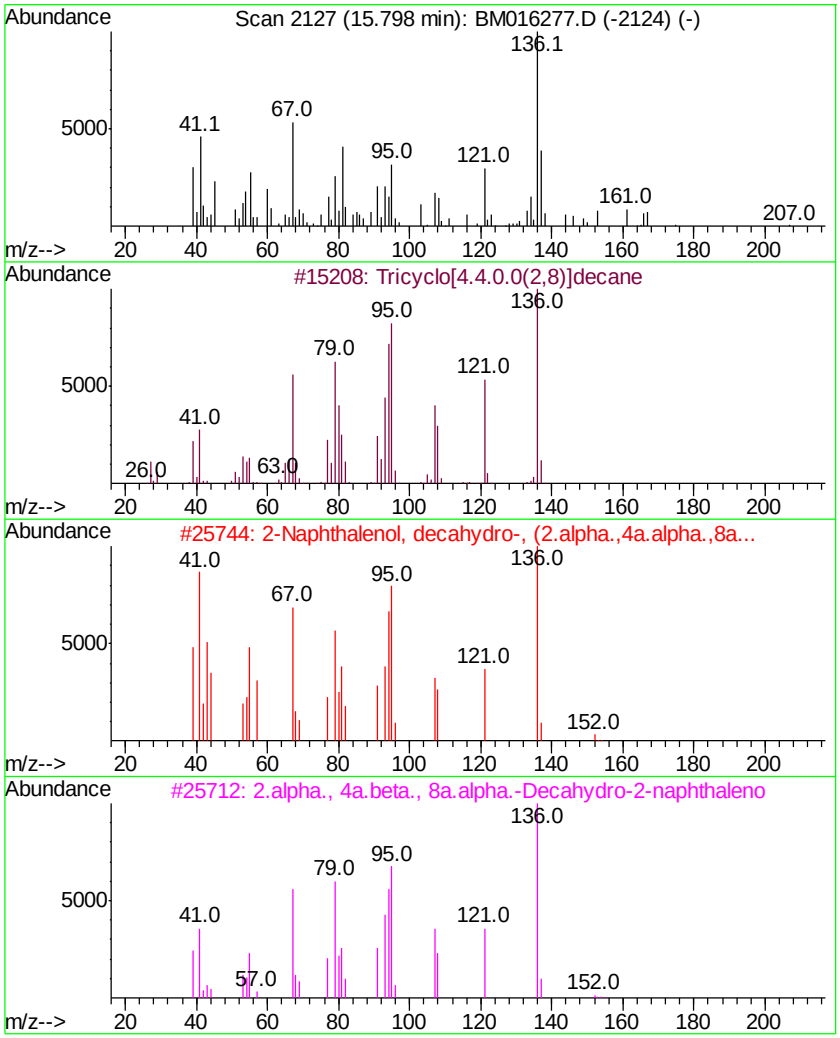
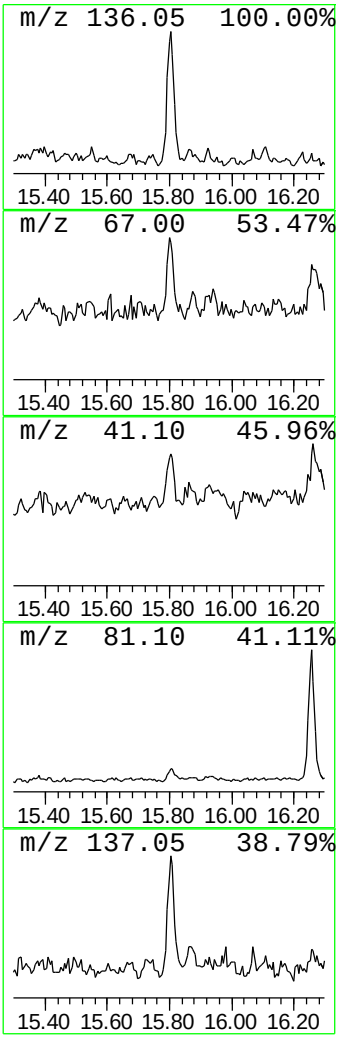
****

Peak Number 8 Tricyclo[4.4.0.0(2,8)]decane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	4.10 ng	93153	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[4.4.0.0(2,8)]decane	136	C10H16	049700-59-6	70
2	2-Naphthalenol, decahydro-, (2.a...	154	C10H18O	002529-06-8	58
3	2.alpha., 4a.beta., 8a.alpha.-De...	154	C10H18O	005779-35-1	53
4	2.alpha., 4a.alpha., 8a.alpha.-D...	154	C10H18O	001424-36-8	53
5	3-Methoxybenzylamine	137	C8H11NO	005071-96-5	47





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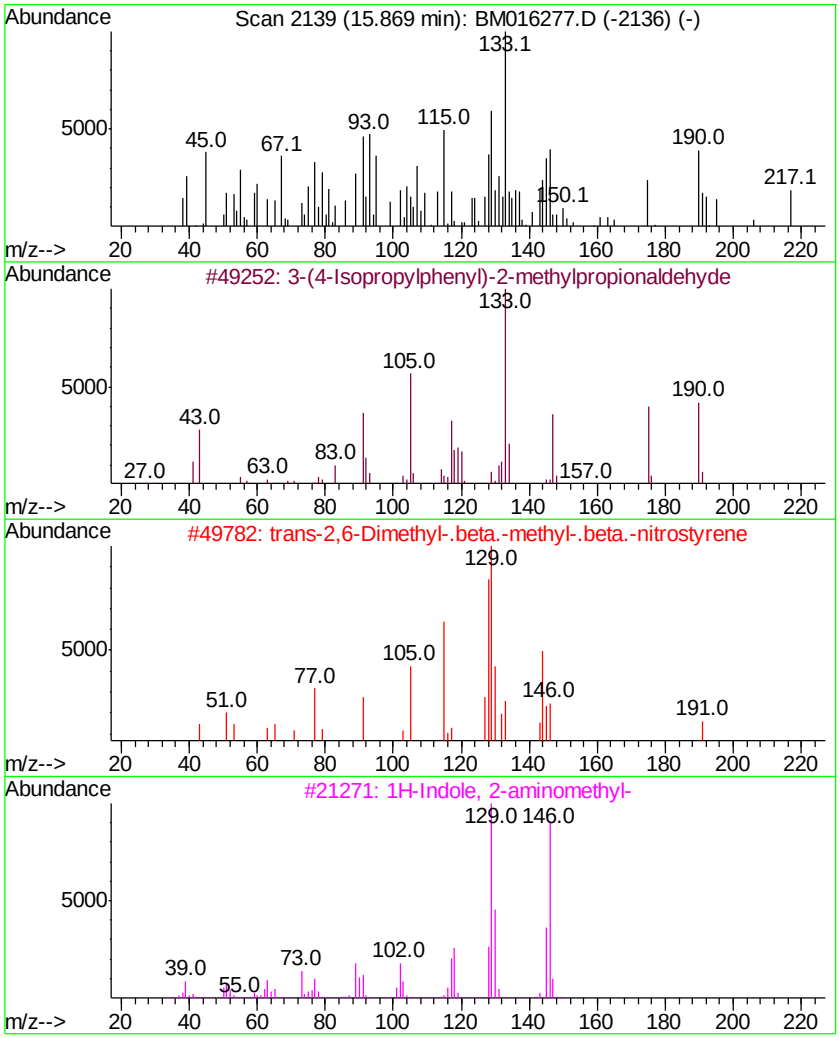
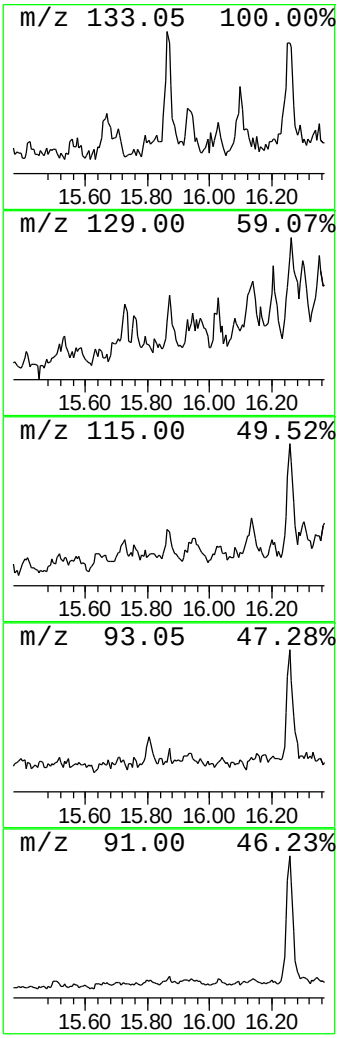
****

Peak Number 9 unknown15.87 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.72 ng	61823	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(4-Isopropylphenyl)-2-methylpr...	190	C13H18O	000103-95-7	27
2	trans-2,6-Dimethyl-.beta.-methyl...	191	C11H13NO2	147102-59-8	20
3	1H-Indole, 2-aminomethyl-	146	C9H10N2	021109-25-1	14
4	1,1,3,3-Tetramethyl-1,3-di-n-pro...	218	C10H26OSi2	018001-73-5	14
5	1H-Indol-3-ol, acetate	175	C10H9NO2	000608-08-2	14





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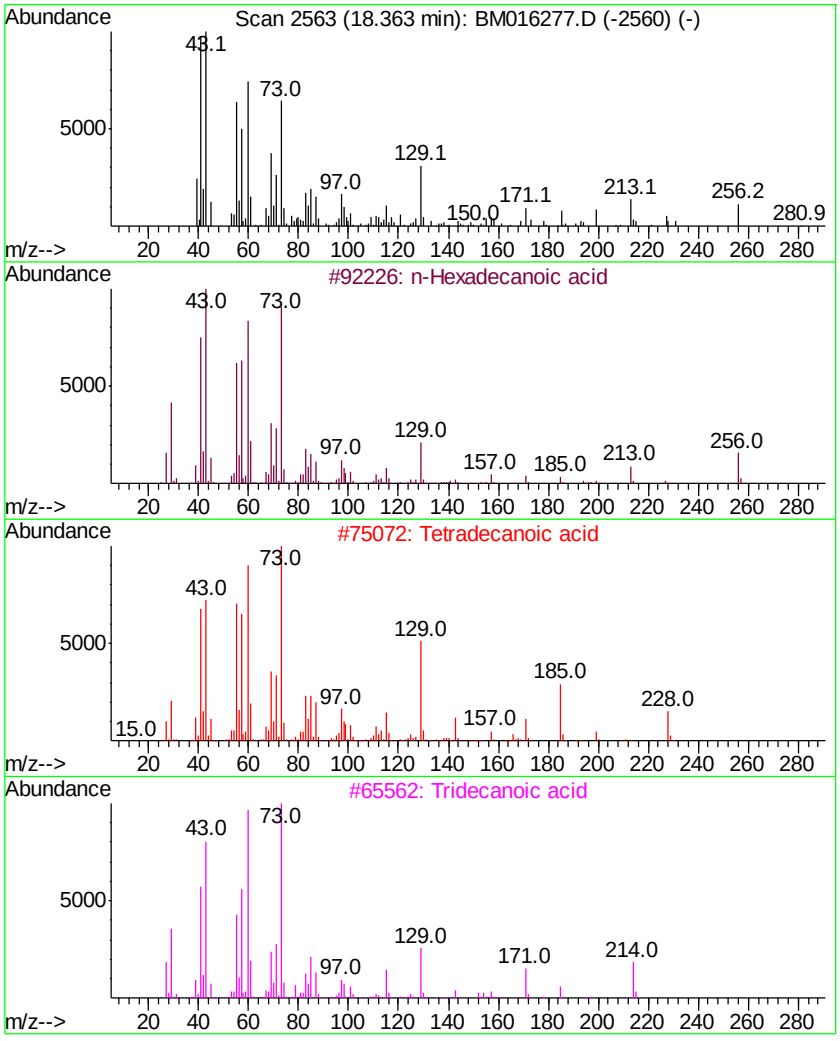
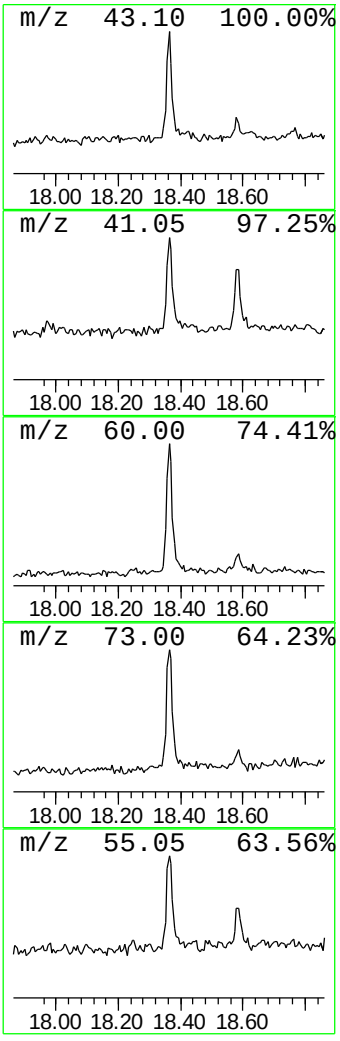
Peak Number 10 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	5.65 ng	131430	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	Nonanoic acid	158	C9H18O2	000112-05-0	55
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Data File : BM016277.D
Acq On : 09 Aug 2018 12:24
Operator : SJ/JU
Sample : J4356-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-29

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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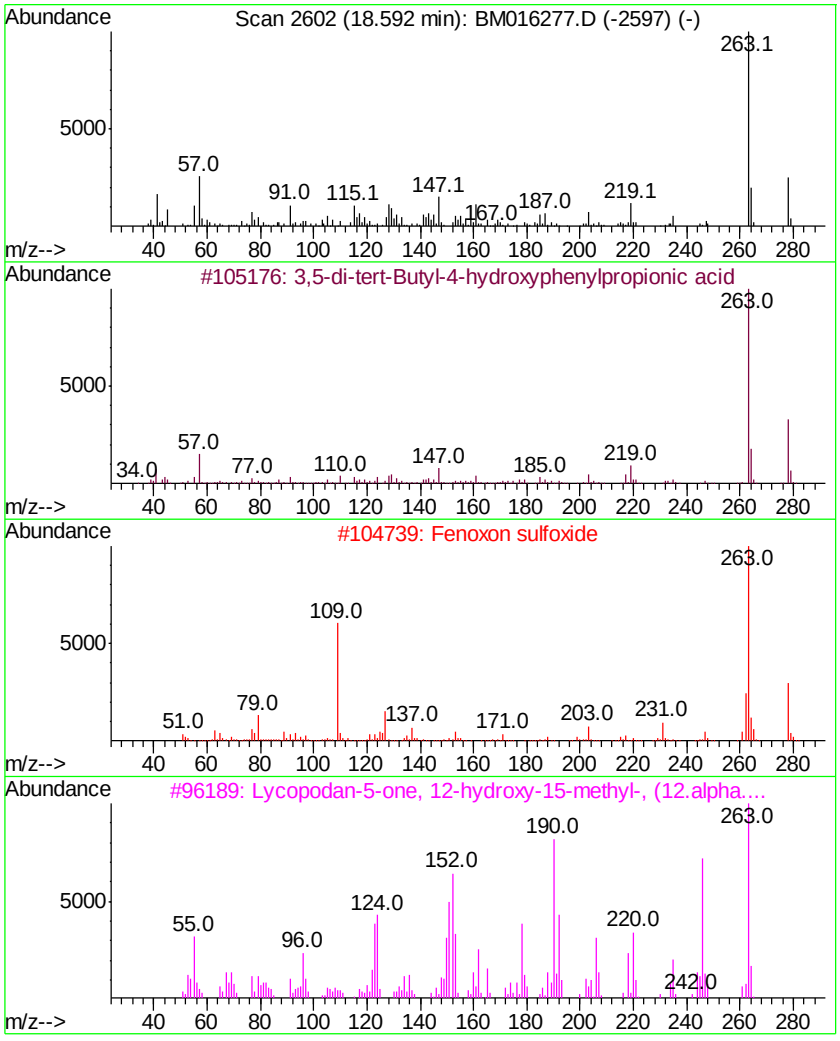
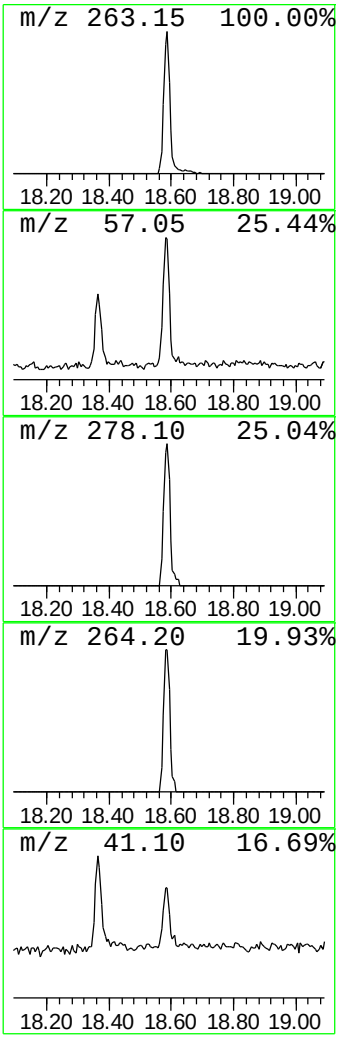
Peak Number 11 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.59	12.85 ng	299158	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxyphenv...	278	C17H26O3	020170-32-5	94
2	Fenoxon sulfoxide	278	C10H15O5PS	006552-13-2	58
3	Lycopodan-5-one, 12-hydroxy-15-m...	263	C16H25NO2	021061-90-5	50
4	Lycopodan-5-one, 12-hydroxy-15-m...	263	C16H25NO2	006900-92-1	50
5	4,6-Dinitro-1,1,3,3,5-pentamethy...	278	C14H18N2O4	000116-66-5	46





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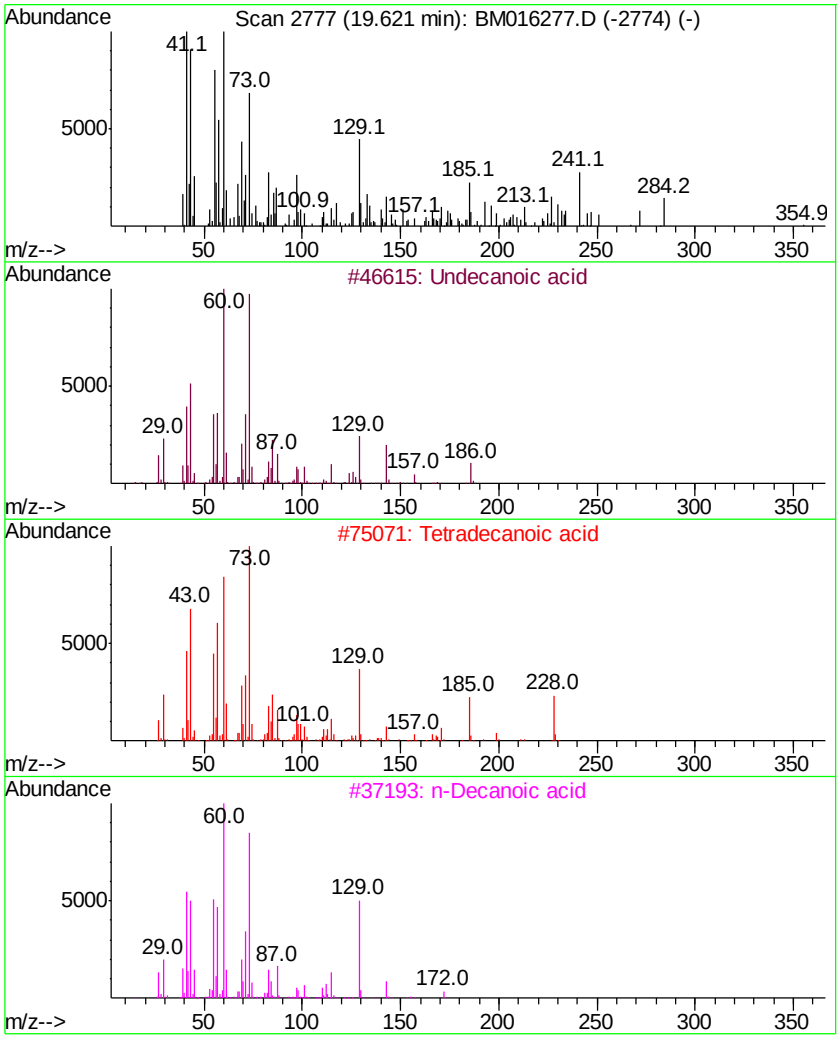
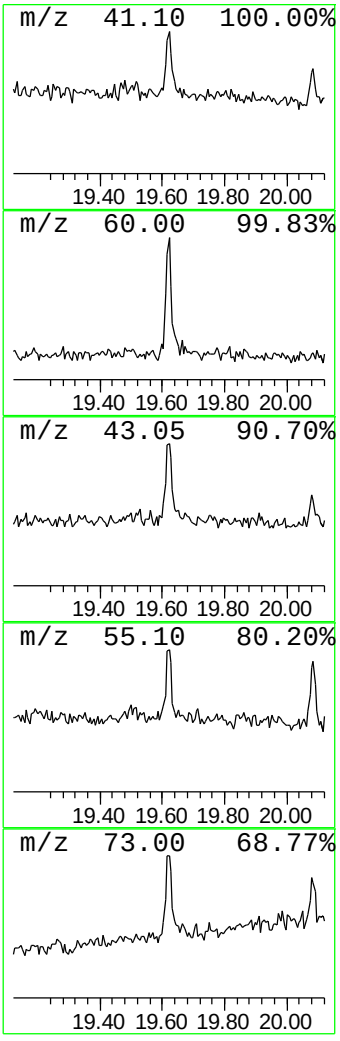
Peak Number 12 Undecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	3.00 ng	80090	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	62
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	43
4	Octadecanoic acid	284	C18H36O2	000057-11-4	41
5	1,3,4-Thiadiazol-2-amine, 5-ethyl-	129	C4H7N3S	014068-53-2	38





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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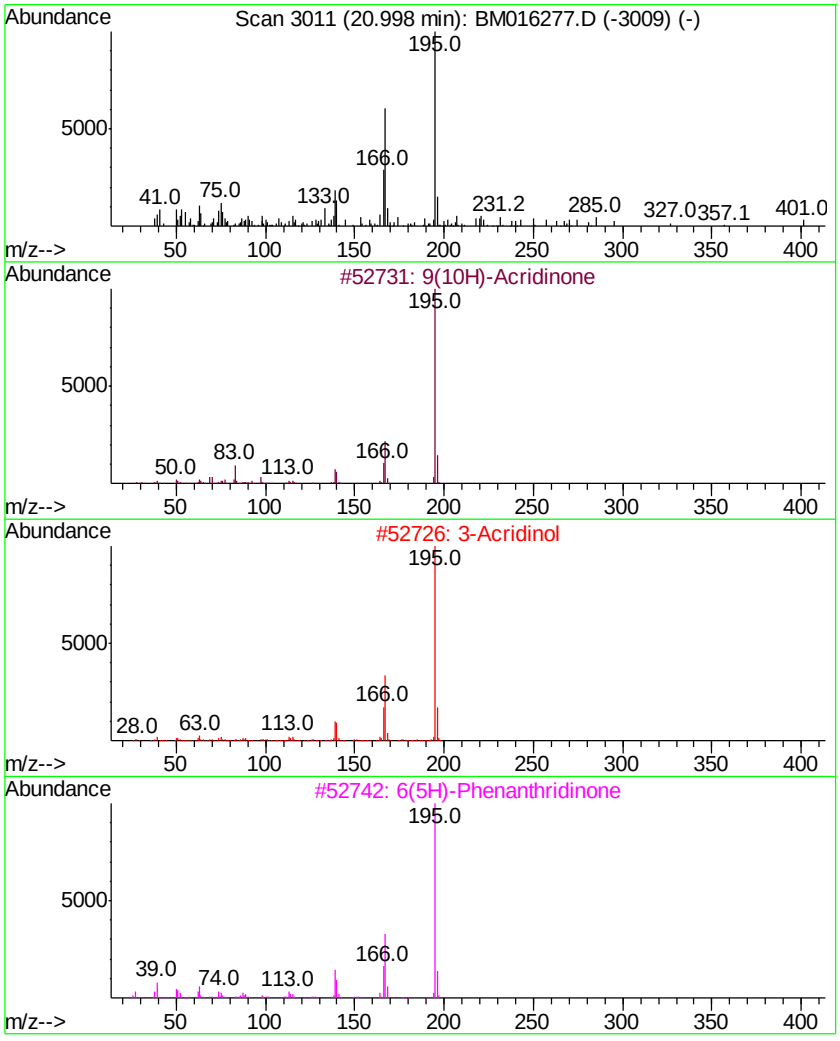
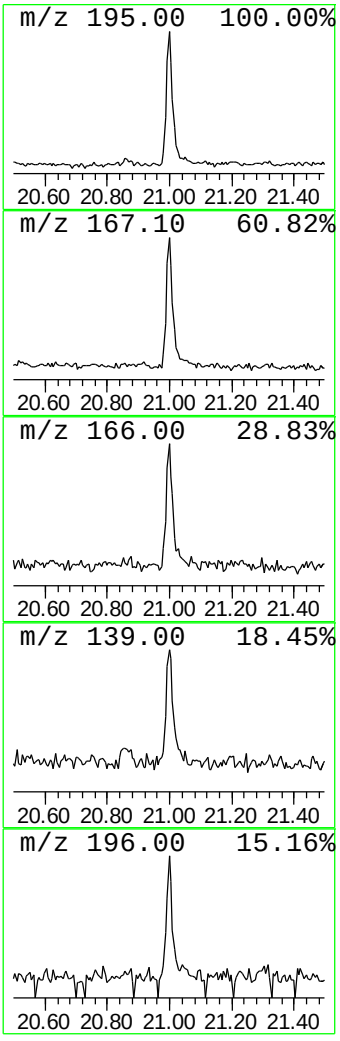
Peak Number 13 9(10H)-Acridinone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	3.61 ng	96324	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9(10H)-Acridinone	195	C13H9NO	000578-95-0	90
2	3-Acridinol	195	C13H9NO	007132-70-9	90
3	6(5H)-Phenanthridinone	195	C13H9NO	001015-89-0	90
4	8-Methyl-4-azafluorenone	195	C13H9NO	064292-03-1	90
5	Dibenz[b,f][1,4]oxazepine	195	C13H9NO	000257-07-8	90





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_M
ClientSampleId : MW-29

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
unknown4.66	4.66	4.9	ng	77199	1	8.13	316649	20.0
2-Pentanone, 4-hy...	5.19	5.7	ng	89511	1	8.13	316649	20.0
unknown7.66	7.66	108.4	ng	1715560	1	8.13	316649	20.0
unknown13.20	13.20	11.9	ng	271105	3	14.77	454453	20.0
unknown14.11	14.11	2.2	ng	50756	3	14.77	454453	20.0
Mesitylacetic acid	15.25	2.3	ng	52967	3	14.77	454453	20.0
Tricyclo[4.4.0.0(...	15.80	4.1	ng	93153	3	14.77	454453	20.0
unknown15.87	15.87	2.7	ng	61823	3	14.77	454453	20.0
n-Hexadecanoic acid	18.36	5.7	ng	131430	4	17.50	465645	20.0
3,5-di-tert-Butyl...	18.59	12.9	ng	299158	4	17.50	465645	20.0
Undecanoic acid	19.62	3.0	ng	80090	5	21.63	533521	20.0
9(10H)-Acridinone	21.00	3.6	ng	96324	5	21.63	533521	20.0