LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016287.D
Acq On : 09 Aug 2018 18:31
Operator : SJ/JU
Sample : J4369-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-36

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	317	323	333	rBV	47327	75824	2.79%	0.532%
2	5.669	399	405	416	rBV	394562	627231	23.10%	4.398%
3	7.310	679	684	702	rVB	215354	382036	14.07%	2.679%
4	7.663	737	744	756	rBV	856689	1345381	49.55%	9.433%
5	8.134	818	824	831	rBV	181210	298466	10.99%	2.093%
6	8.451	871	878	890	rVB	838808	1341512	49.41%	9.406%
7	9.322	1018	1026	1045	rBV	580742	997639	36.74%	6.995%
8	9.651	1075	1082	1087	rVB3	29232	44695	1.65%	0.313%
9	10.945	1296	1302	1310	rBV	194059	335634	12.36%	2.353%
10	11.663	1418	1424	1432	rBV2	17296	28942	1.07%	0.203%
11	13.386	1711	1717	1725	rVB	1379352	1945910	71.67%	13.643%
12	14.221	1854	1859	1864	rVB	64018	86326	3.18%	0.605%
13	14.768	1946	1952	1957	rBV2	252351	395026	14.55%	2.770%
14	14.963	1978	1985	1990	rBV	34186	55286	2.04%	0.388%
15	15.051	1995	2000	2006	rVB6	20273	40876	1.51%	0.287%
16	15.563	2083	2087	2096	rVB7	15399	28207	1.04%	0.198%
17	16.257	2199	2205	2215	rBV	1141762	1617878	59.59%	11.343%
18	16.786	2288	2295	2303	rBV2	33650	59709	2.20%	0.419%
19	17.504	2411	2417	2423	rBV	304358	453287	16.69%	3.178%
20	18.356	2558	2562	2567	rBV	103438	131895	4.86%	0.925%
21	18.574	2595	2599	2606	rBV	64104	96191	3.54%	0.674%
22	19.615	2773	2776	2782	rVB2	54280	69594	2.56%	0.488%
23	20.080	2850	2855	2861	rBV	2300021	2715149	100.00%	19.037%
24	21.633	3115	3119	3126	rVB	422842	536450	19.76%	3.761%
25	23.968	3511	3516	3526	rVB2	280989	553609	20.39%	3.882%

Sum of corrected areas: 14262753

LSC Report - Integrated Chromatogram

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Data File : BM016287.D
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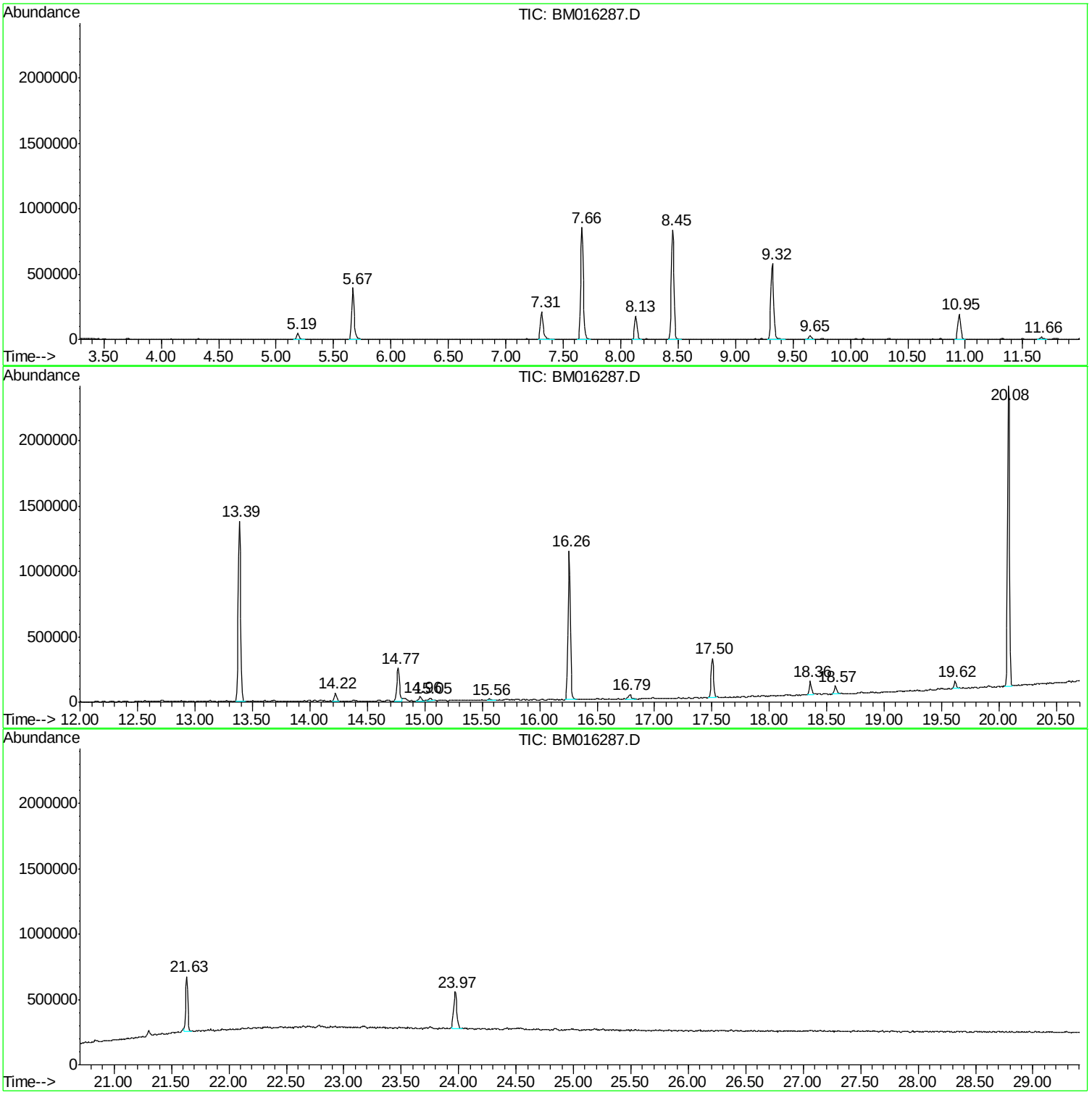
Sample : J4369-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-36

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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Operator : SJ/JU
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Instrument : BNA_M
ClientSampleId : MW-36

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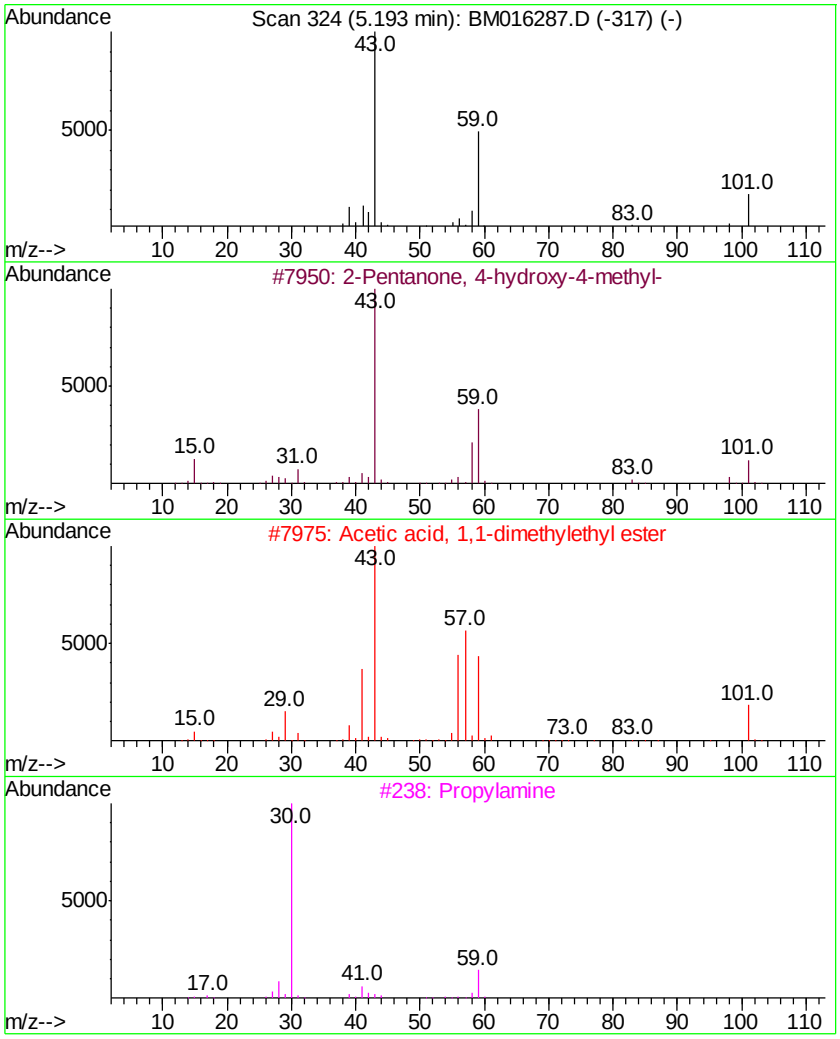
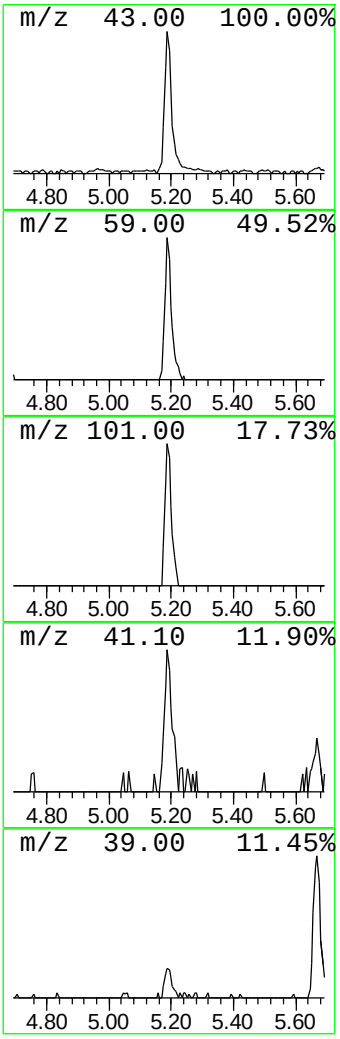
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	5.08 ng	75824	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	Propylamine	59	C3H9N	000107-10-8	40
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Butane	58	C4H10	000106-97-8	12





Library Search Compound Report

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Operator : SJ/JU
Sample : J4369-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-36

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

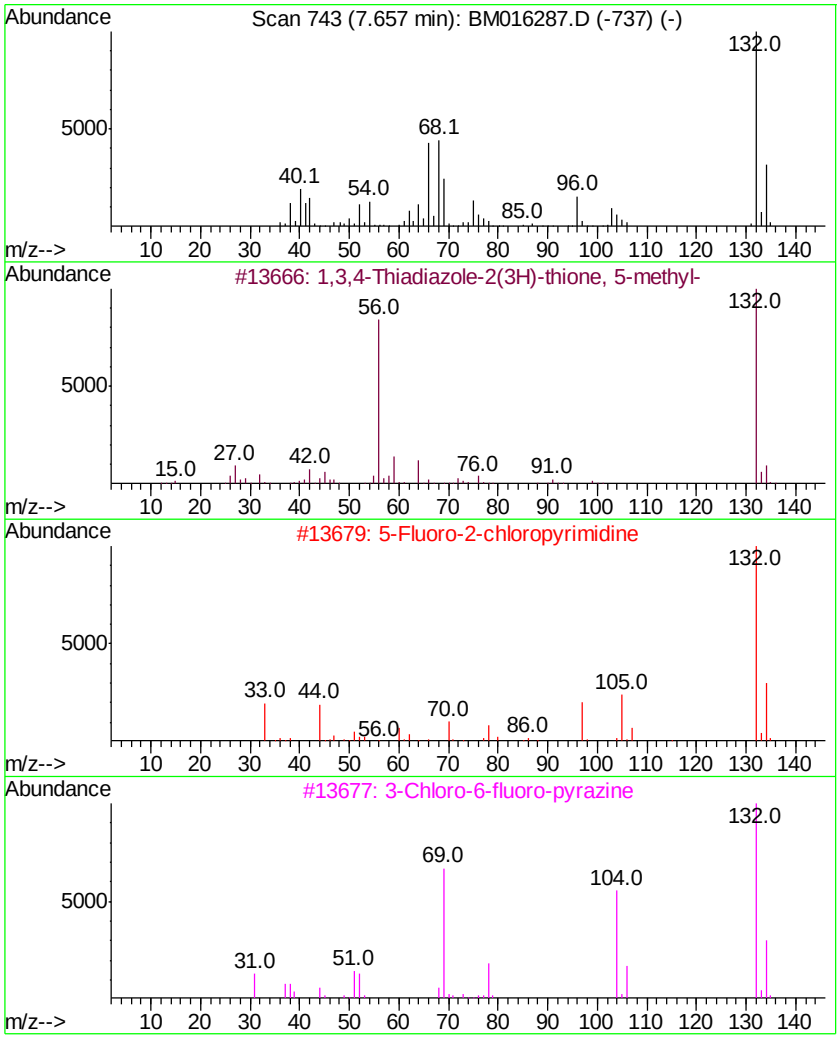
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

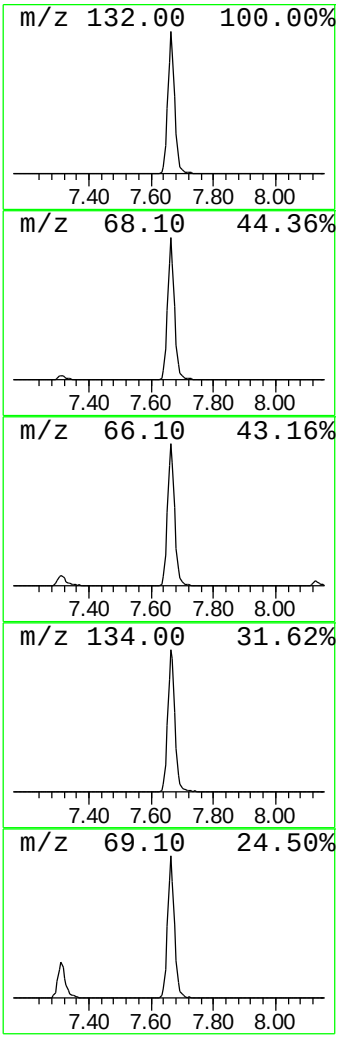
****

Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	90.15 ng	1345380	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14





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Operator : SJ/JU
Sample : J4369-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-36

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
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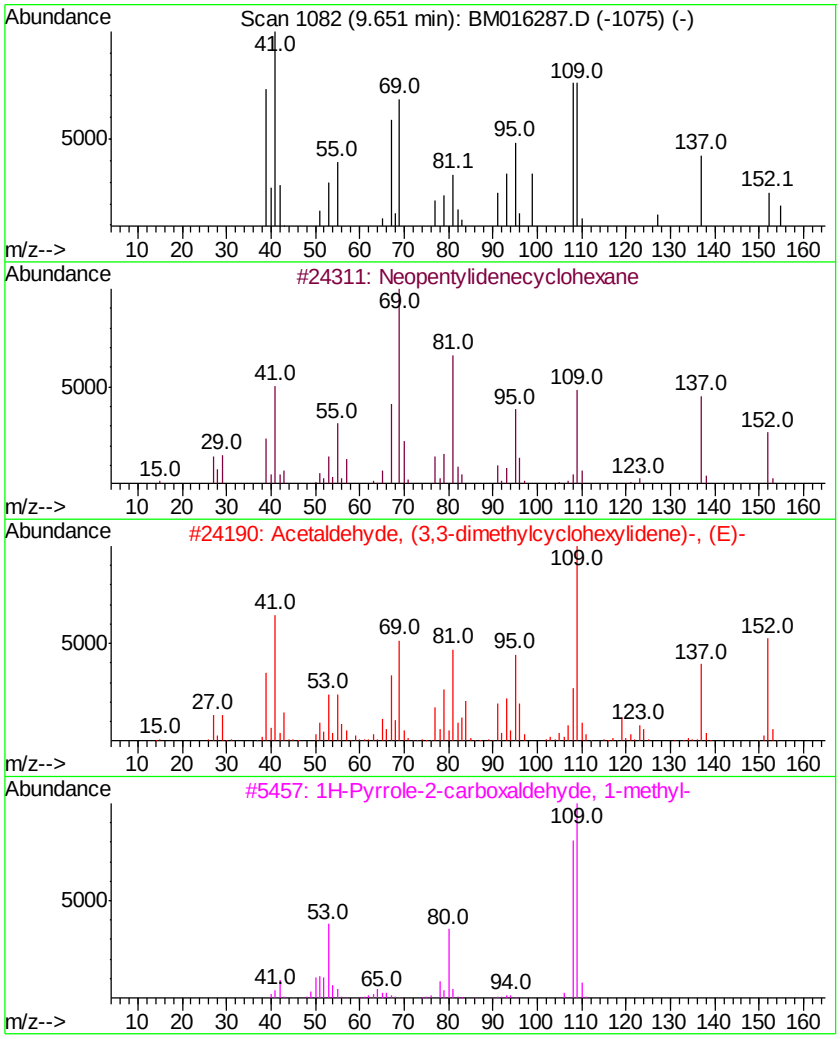
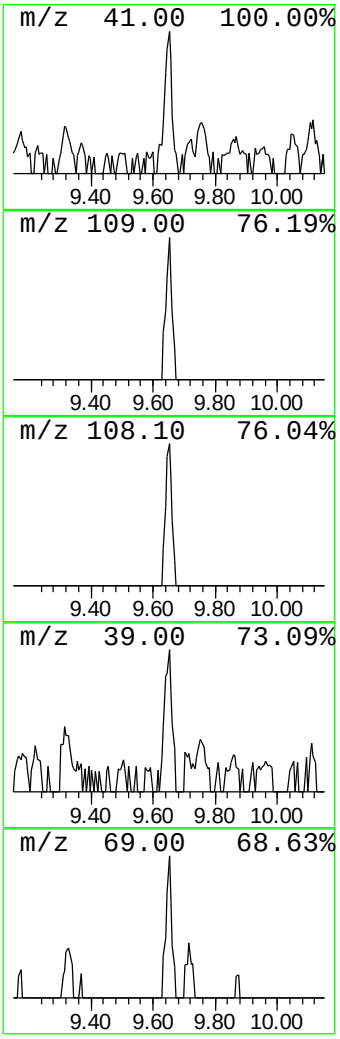
****

Peak Number 4 Neopentylidenecyclohexane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.65	2.66 ng	44695	Naphthalene-d8	10.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentylidenecyclohexane	152	C11H20	039546-80-0	53
2	Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-25-2	43
3	1H-Pyrrole-2-carboxaldehyde, 1-m...	109	C6H7NO	001192-58-1	35
4	1H-Pyrrole-2-carboxaldehyde, 5-m...	109	C6H7NO	001192-79-6	35
5	1H-1,3a-Ethanopentalen-4-ol, hex...	152	C10H16O	117221-75-7	35





Library Search Compound Report

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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-36

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

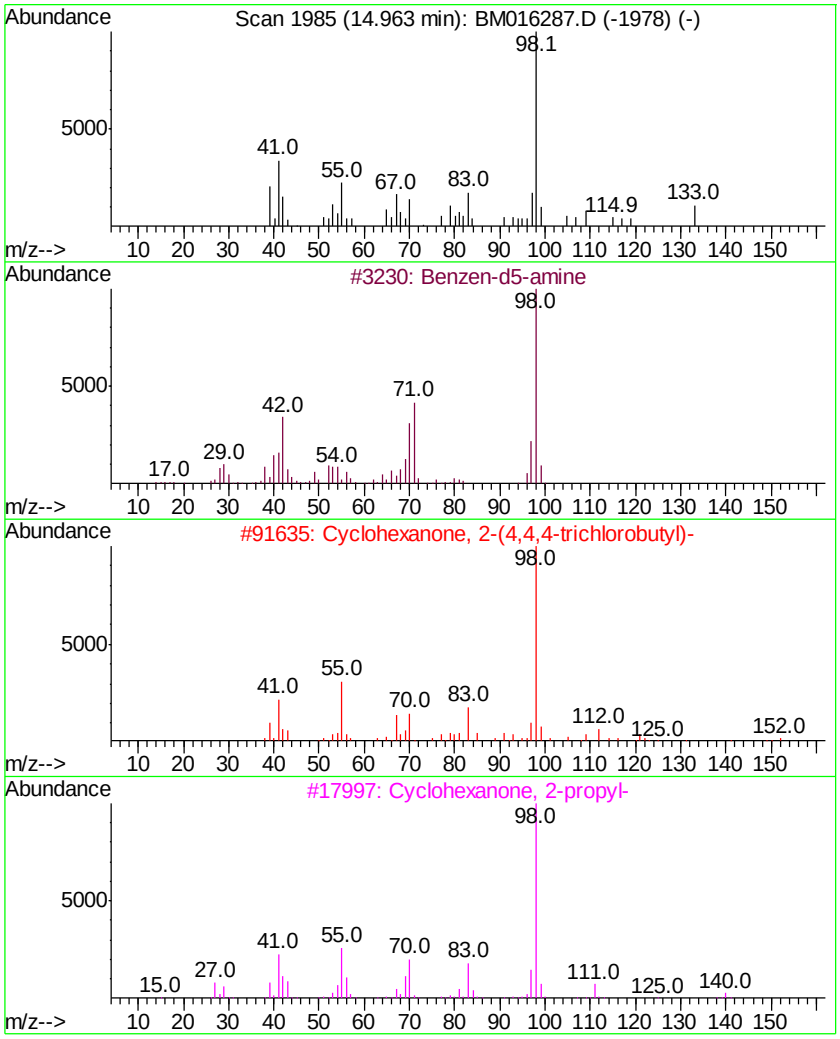
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

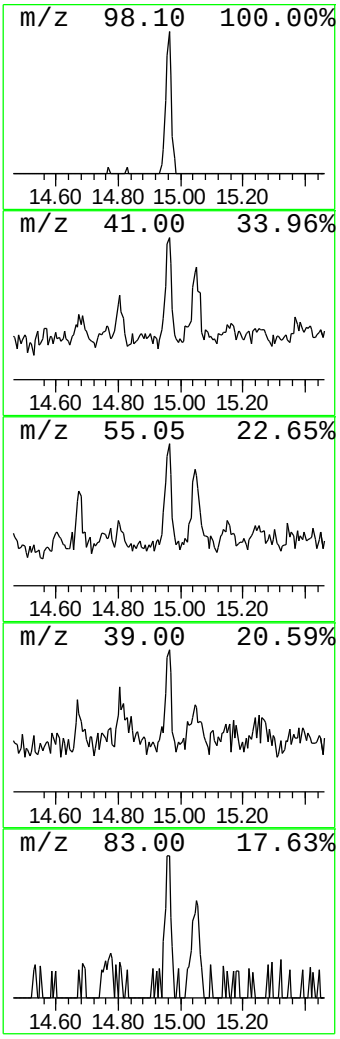
****

Peak Number 5 Benzen-d5-amine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.80 ng	55286	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzen-d5-amine	98	C6H2D5N	004165-61-1	64
2	Cyclohexanone, 2-(4,4,4-trichlor...	256	C10H15Cl3O	1000115-25-1	59
3	Cyclohexanone, 2-propyl-	140	C9H16O	000094-65-5	59
4	Allopregan-3-ol, 20-[3-methylpip...	401	C27H47NO	1000214-18-6	59
5	Cyclohexanone, 2-(2-bromo-4,4,4-...	334	C10H14BrCl3O	097250-47-0	59





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Operator : SJ/JU
Sample : J4369-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-36

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

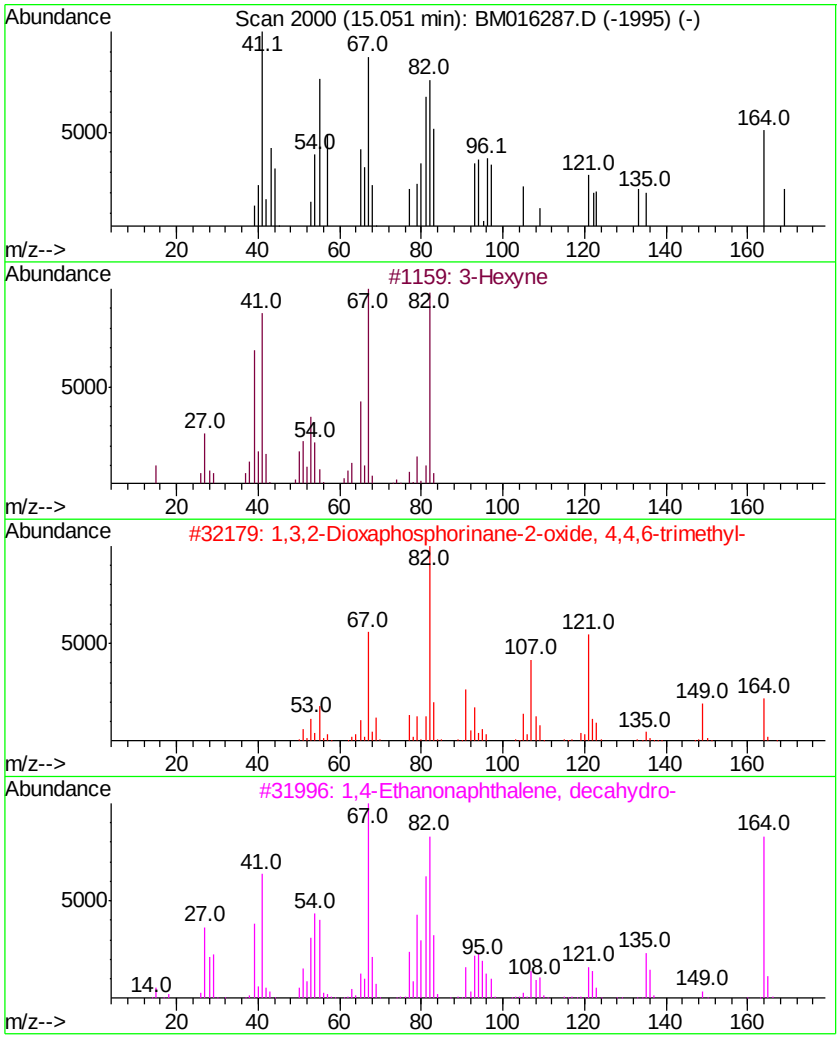
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

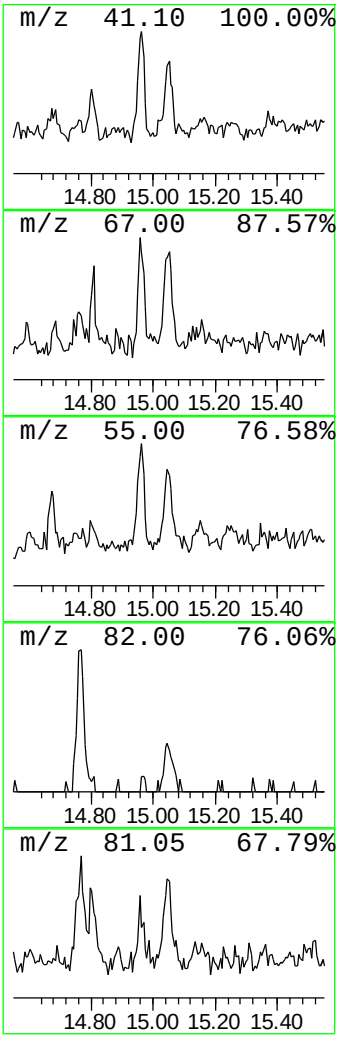
****

Peak Number 6 unknown15.05 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	2.07 ng	40876	Acenaphthene-d10	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexyne	82	C6H10	000928-49-4	47
2	1,3,2-Dioxaphosphorinane-2-oxide...	164	C6H13O3P	016832-97-6	30
3	1,4-Ethanonaphthalene, decahydro-	164	C12H20	000703-34-4	30
4	3-Cyclopentyl-1-propyne	108	C8H12	116279-08-4	22
5	2-Cyclohexylcyclohexanol	182	C12H22O	006531-86-8	22





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Instrument : BNA_M
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TIC Library : C:\DATABASE\NIST02.L
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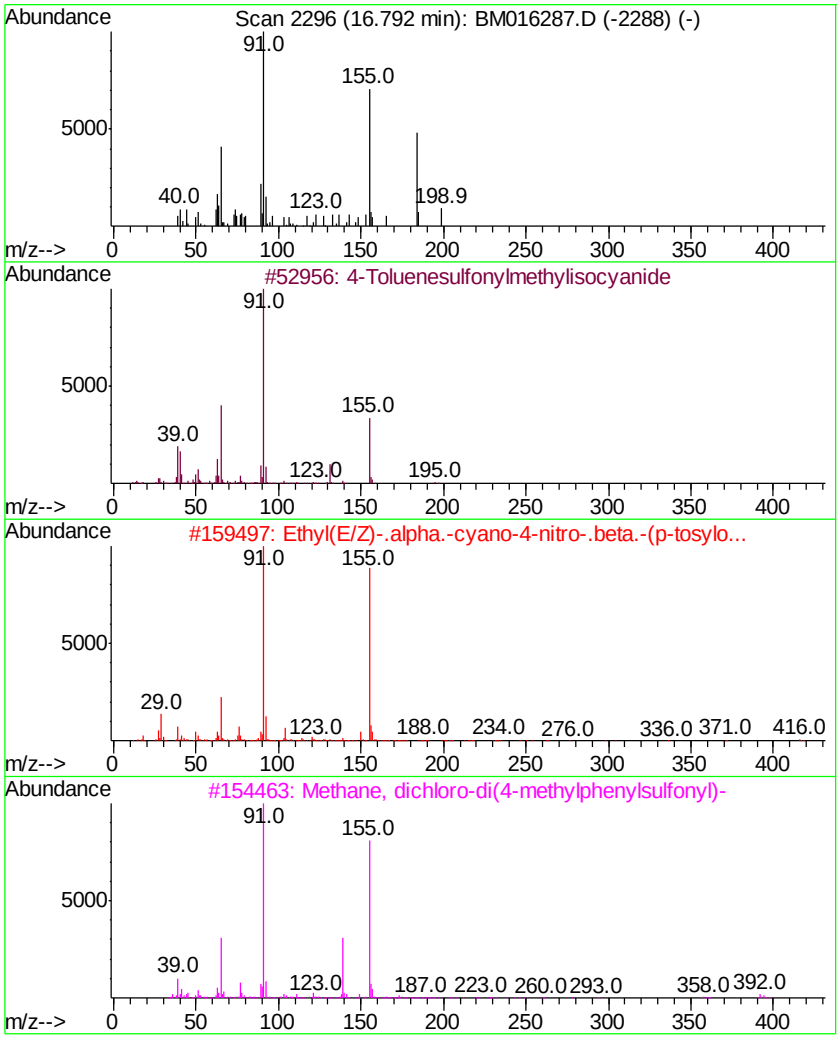
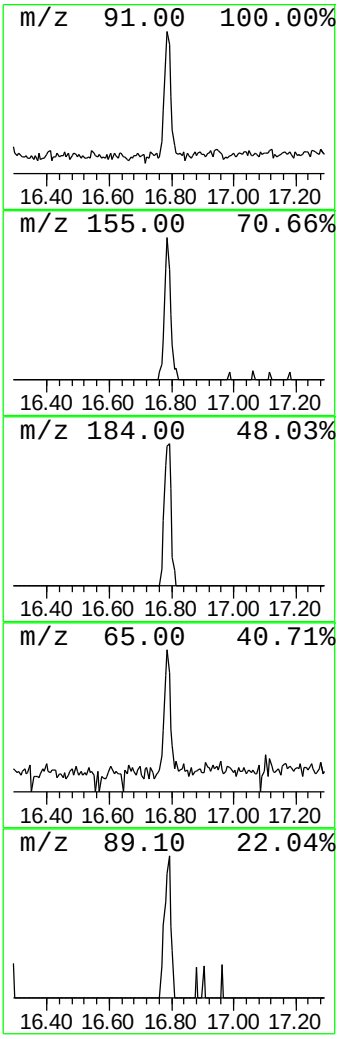
****

Peak Number 7 4-Toluenesulfonylmethylisoc... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.79	2.63 ng	59709	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	72
2	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	64
3	Methane, dichloro-di(4-methylphe...	392	C15H14Cl2O4S2	018087-01-9	64
4	p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	59
5	2-(Toluene-4-sulfonyloxy)propion...	244	C10H12O5S	1000210-27-2	59





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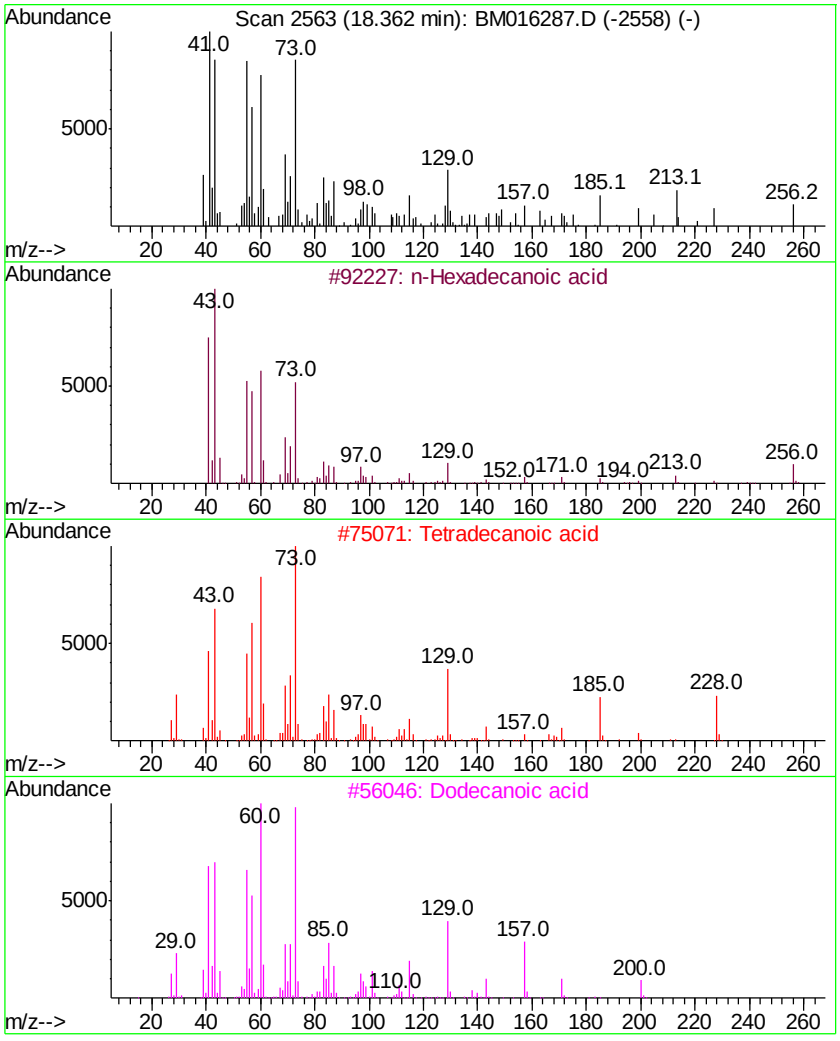
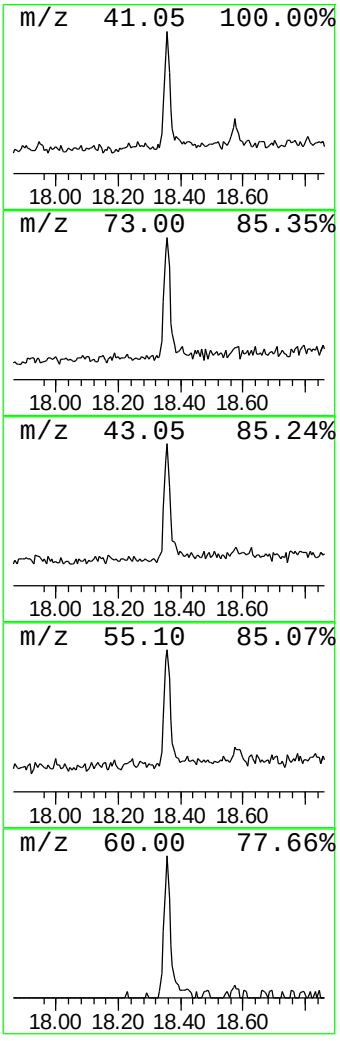
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	5.82 ng	131895	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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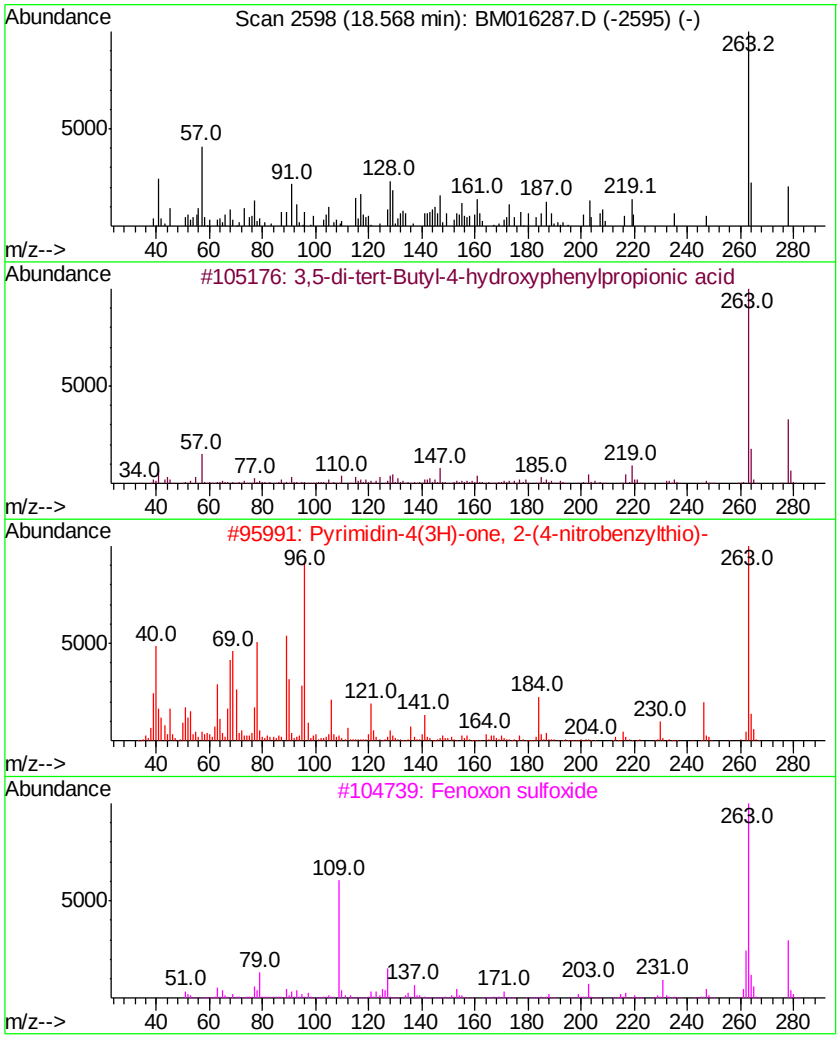
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

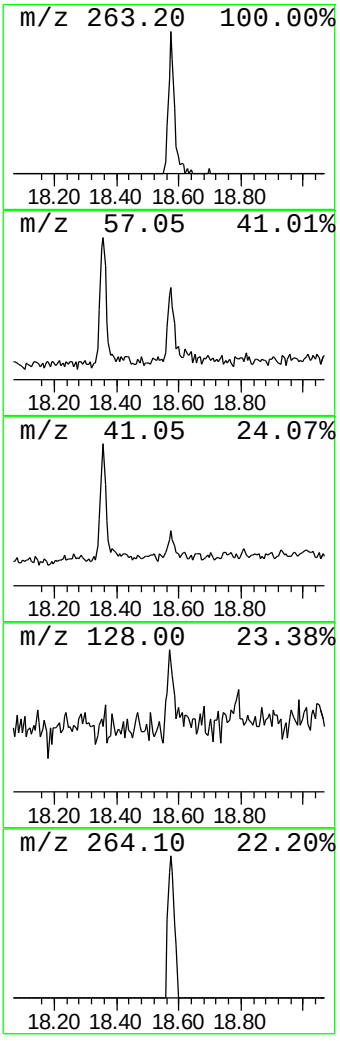
****

Peak Number 9 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	4.24 ng	96191	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	93
2	Pyrimidin-4(3H)-one, 2-(4-nitrob...	263	C11H9N3O3S	078932-23-7	87
3	Fenoxon sulfoxide	278	C10H15O5PS	006552-13-2	59
4	1-Piperidinophenazine	263	C17H17N3	021942-93-8	50
5	7-Methyl-2-phenylquinoline-4-car...	263	C17H13NO2	181048-54-4	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

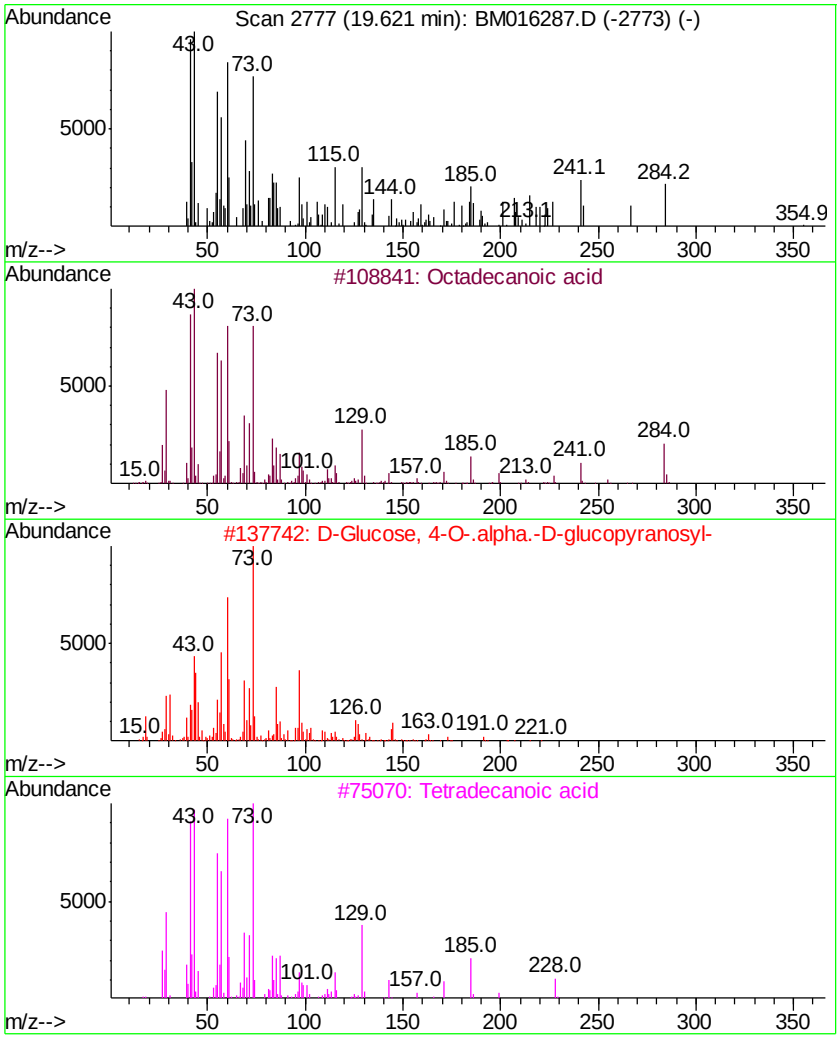
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

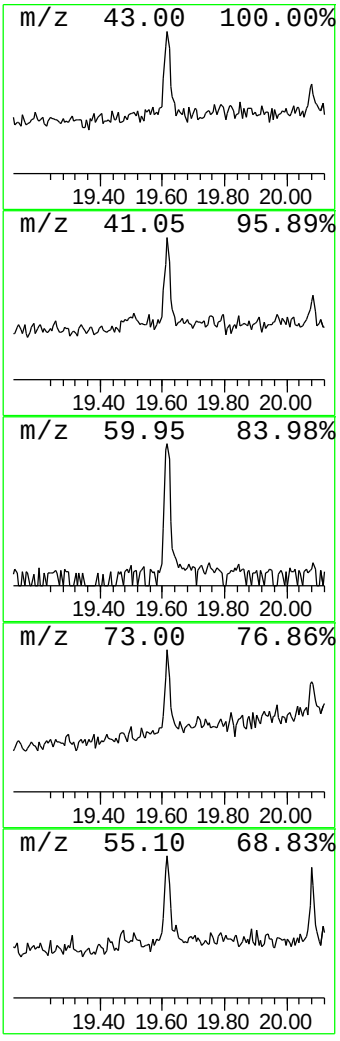
****

Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	2.59 ng	69594	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	52
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47





Tentatively Identified Compound (LSC) summary

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ClientSampleId : MW-36

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	5.1	ng	75824	1	8.13	298466	20.0
unknown7.66	7.66	90.2	ng	1345380	1	8.13	298466	20.0
Neopentylidenecyc...	9.65	2.7	ng	44695	2	10.95	335634	20.0
Benzen-d5-amine	14.96	2.8	ng	55286	3	14.77	395026	20.0
unknown15.05	15.05	2.1	ng	40876	3	14.77	395026	20.0
4-Toluenesulfonyl...	16.79	2.6	ng	59709	4	17.50	453287	20.0
n-Hexadecanoic acid	18.36	5.8	ng	131895	4	17.50	453287	20.0
3,5-di-tert-Butyl...	18.57	4.2	ng	96191	4	17.50	453287	20.0
Octadecanoic acid	19.62	2.6	ng	69594	5	21.63	536450	20.0