LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016282.D
Acq On : 09 Aug 2018 15:27
Operator : SJ/JU
Sample : J4356-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-39

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	316	323	331	rBV	44211	68650	1.95%	0.430%
2	5.669	399	405	421	rBV	428740	690489	19.61%	4.321%
3	7.310	679	684	699	rBV	249179	435898	12.38%	2.728%
4	7.663	738	744	760	rBV	928478	1464699	41.60%	9.166%
5	8.133	819	824	832	rBV	156882	252213	7.16%	1.578%
6	8.451	871	878	892	rBB	872475	1412585	40.12%	8.840%
7	9.322	1019	1026	1042	rBV	634509	1048406	29.77%	6.561%
8	10.951	1296	1303	1314	rBV	162940	280487	7.97%	1.755%
9	13.386	1711	1717	1727	rBV	1460873	2066593	58.69%	12.933%
10	14.221	1853	1859	1867	rVB	41148	57489	1.63%	0.360%
11	14.768	1946	1952	1959	rVB2	220655	326992	9.29%	2.046%
12	16.256	2199	2205	2217	rBV	1329900	1823439	51.78%	11.412%
13	17.503	2412	2417	2423	rBV2	281097	399352	11.34%	2.499%
14	18.356	2557	2562	2573	rBV	122186	188581	5.36%	1.180%
15	18.574	2594	2599	2609	rBV	350277	530977	15.08%	3.323%
16	19.474	2749	2752	2755	rBV4	34735	44488	1.26%	0.278%
17	19.615	2771	2776	2784	rBV3	70529	117260	3.33%	0.734%
18	19.868	2815	2819	2822	rBV	31474	36993	1.05%	0.232%
19	20.086	2850	2856	2861	rBV	3128108	3521184	100.00%	22.036%
20	20.850	2982	2986	2988	rBV3	24510	36284	1.03%	0.227%
21	21.303	3059	3063	3068	rBV	94383	135648	3.85%	0.849%
22	21.633	3115	3119	3126	rVB	412781	509068	14.46%	3.186%
23	23.968	3511	3516	3525	rVB	255737	531128	15.08%	3.324%

Sum of corrected areas: 15978903

LSC Report - Integrated Chromatogram

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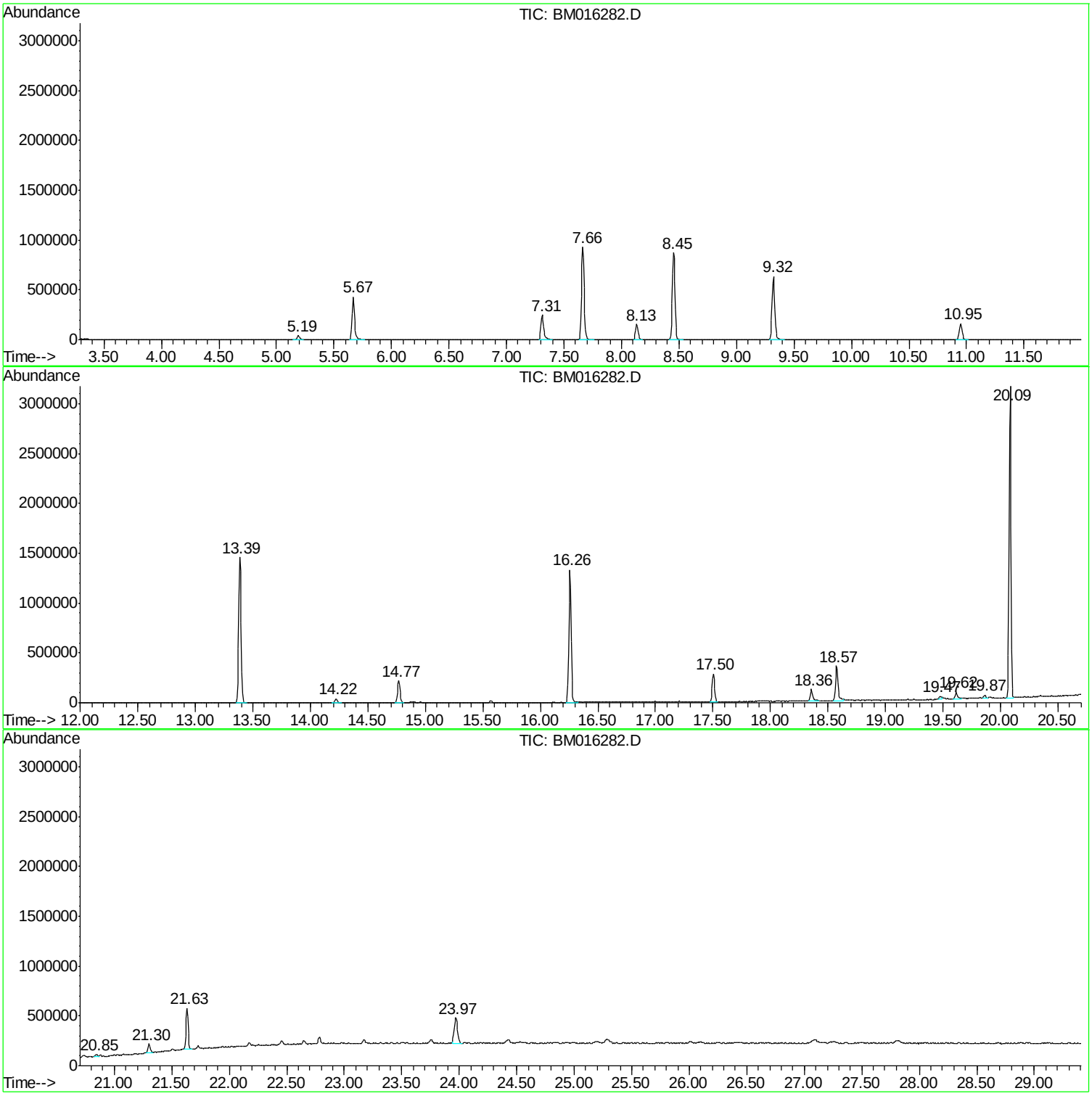
Sample : J4356-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-39

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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Data File : BM016282.D
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Operator : SJ/JU
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ALS Vial : 10 Sample Multiplier: 1

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

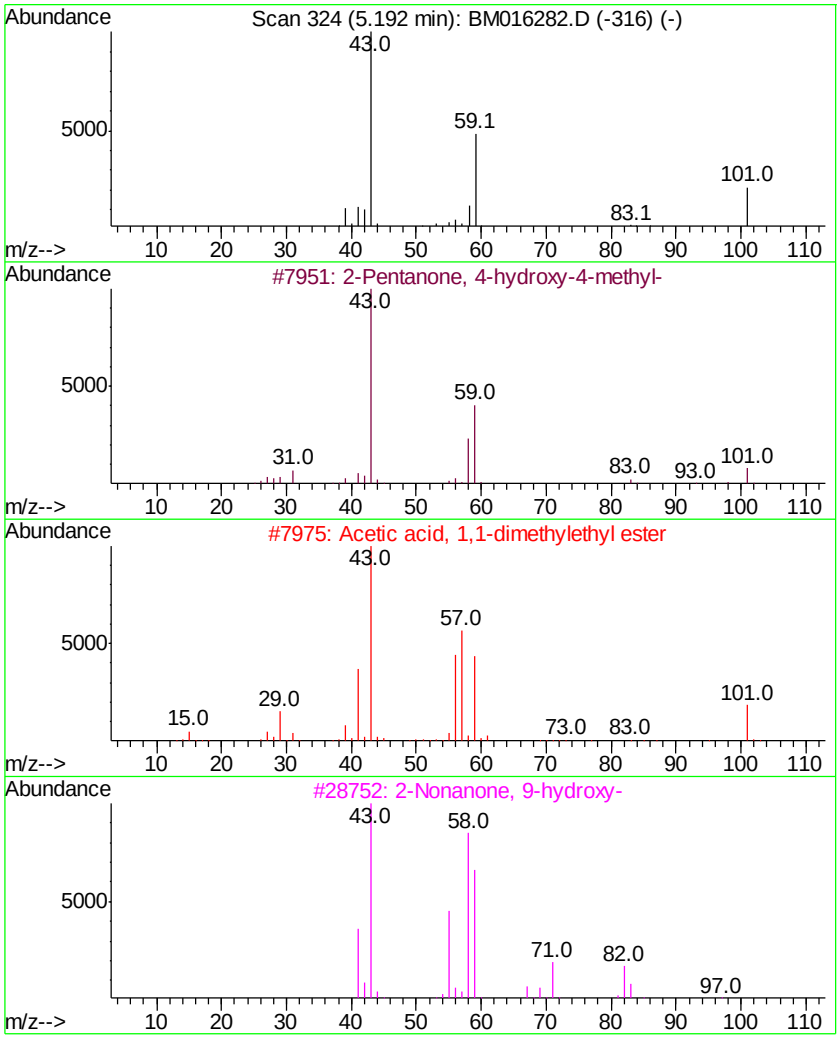
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

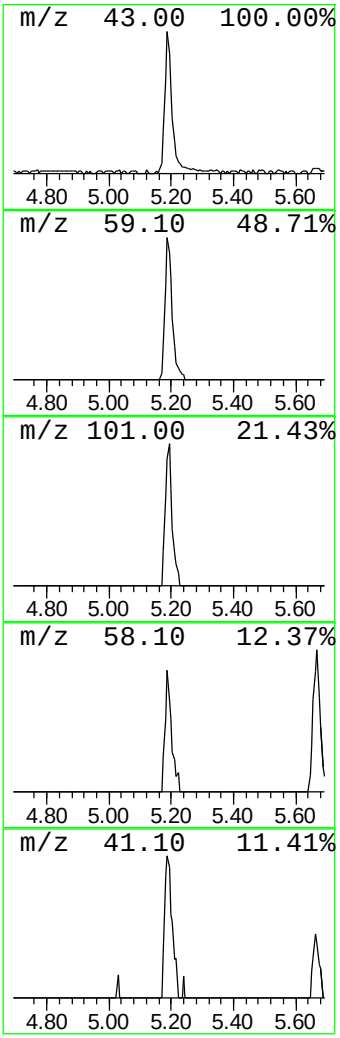
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	5.44 ng	68650	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	38
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
4	Butane	58	C4H10	000106-97-8	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





Library Search Compound Report

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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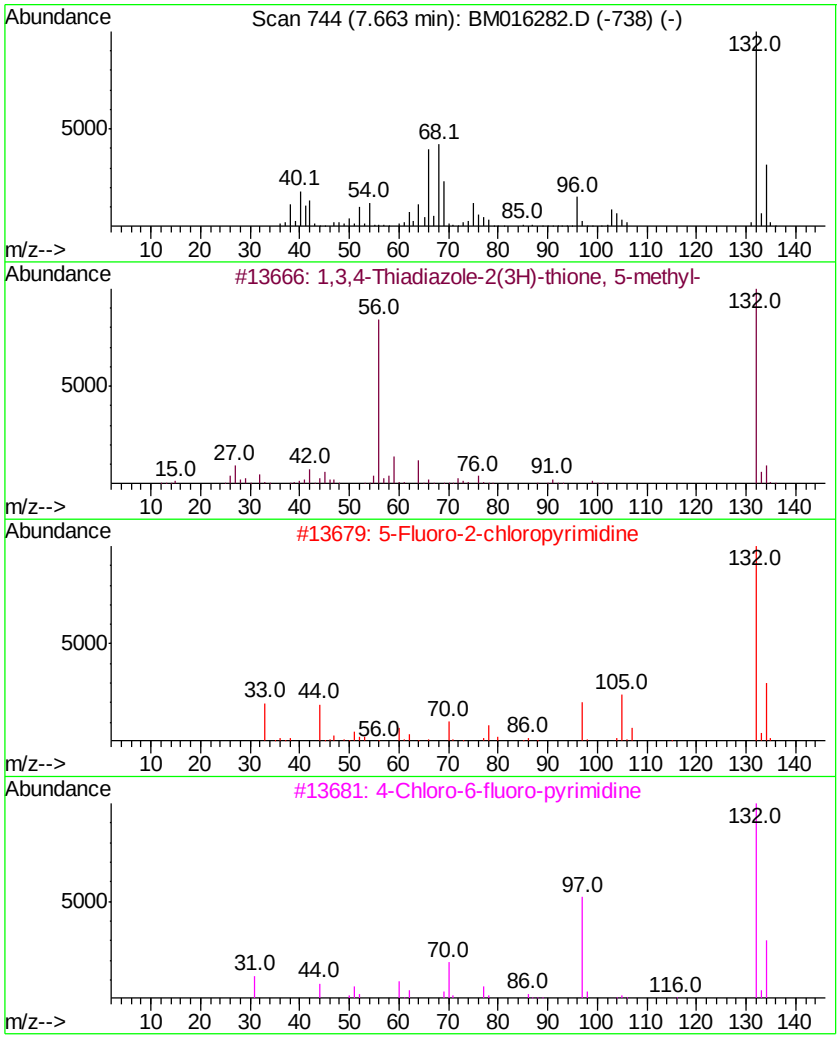
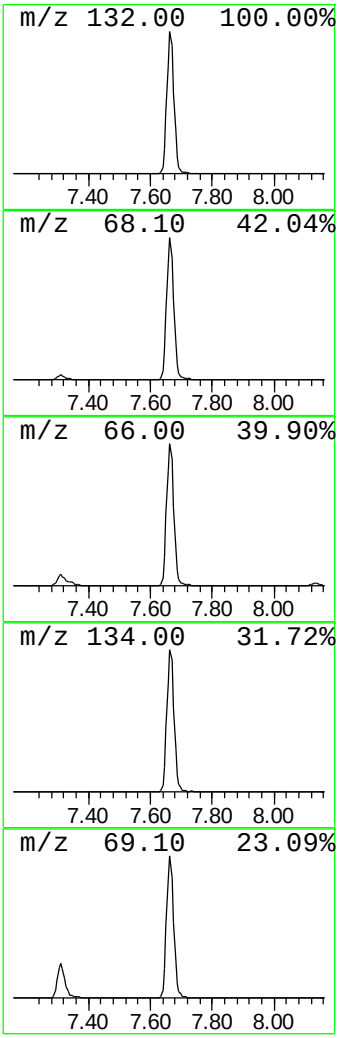
****

Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	116.15 ng	1464700	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	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14





Library Search Compound Report

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Data File : BM016282.D
Acq On : 09 Aug 2018 15:27
Operator : SJ/JU
Sample : J4356-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-39

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

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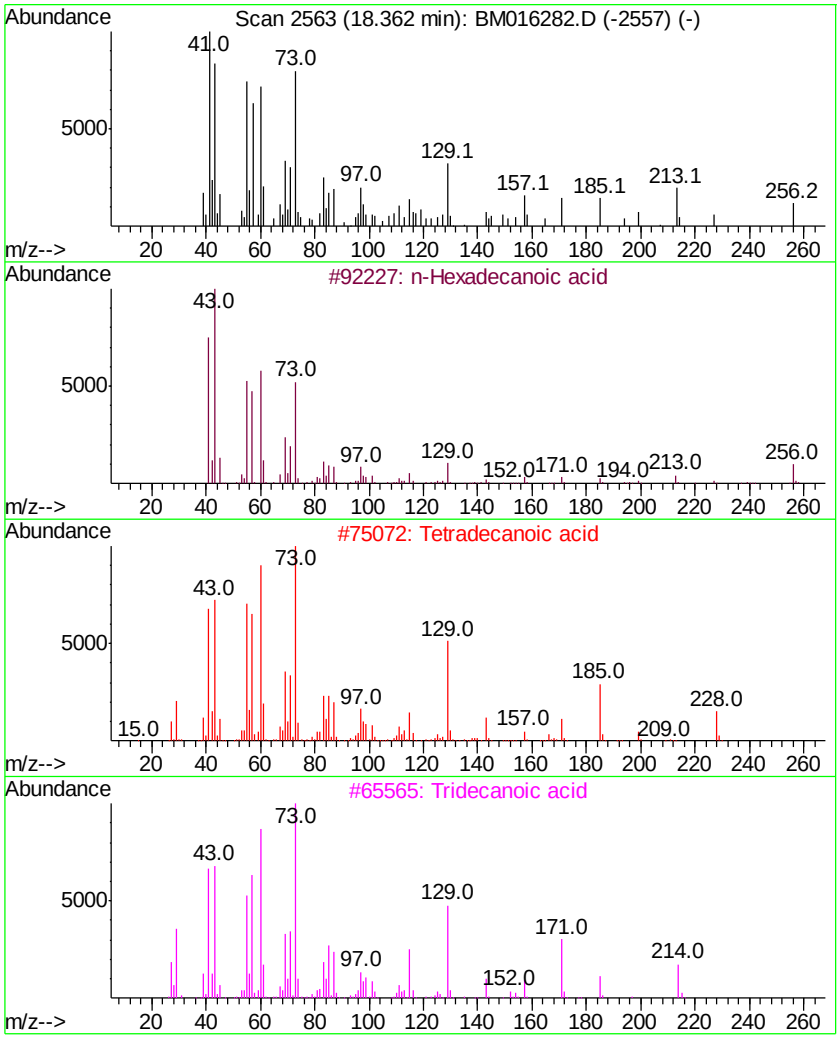
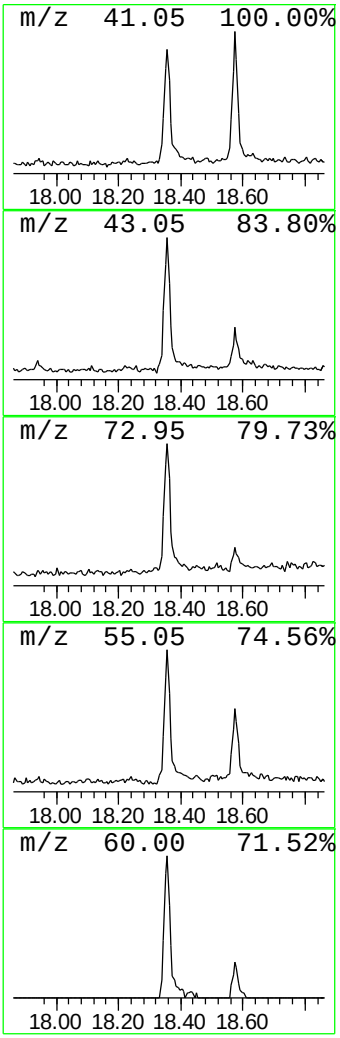
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	9.44 ng	188581	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Tridecanoic acid	214	C13H26O2	000638-53-9	58
4	Undecanoic acid	186	C11H22O2	000112-37-8	49
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





Library Search Compound Report

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Data File : BM016282.D
Acq On : 09 Aug 2018 15:27
Operator : SJ/JU
Sample : J4356-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-39

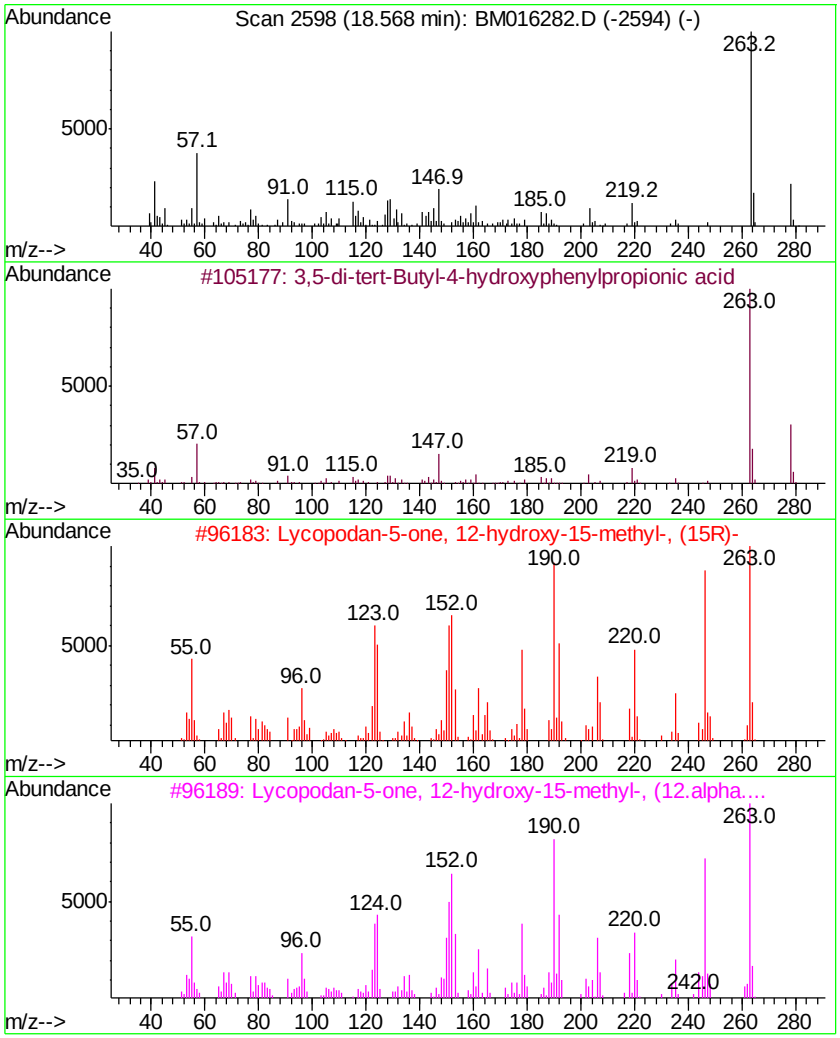
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

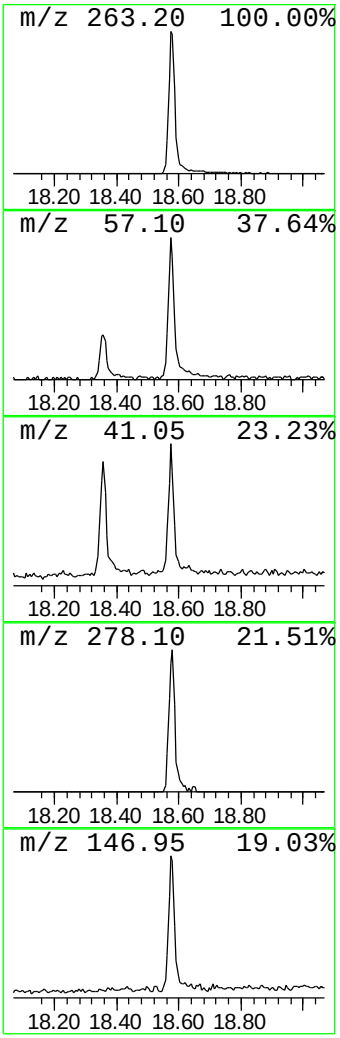
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	26.59 ng	530977	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	87
3	Lycopodan-5-one, 12-hydroxy-15-m...	263	C16H25NO2	021061-90-5	55
4	Trimethyl(2,6 ditert.-butylpheno...	278	C17H30OSi	010416-73-6	53
5	Pentan-2-one, 4-(2-fluorenylimino)-	263	C18H17NO	050651-58-6	49





Library Search Compound Report

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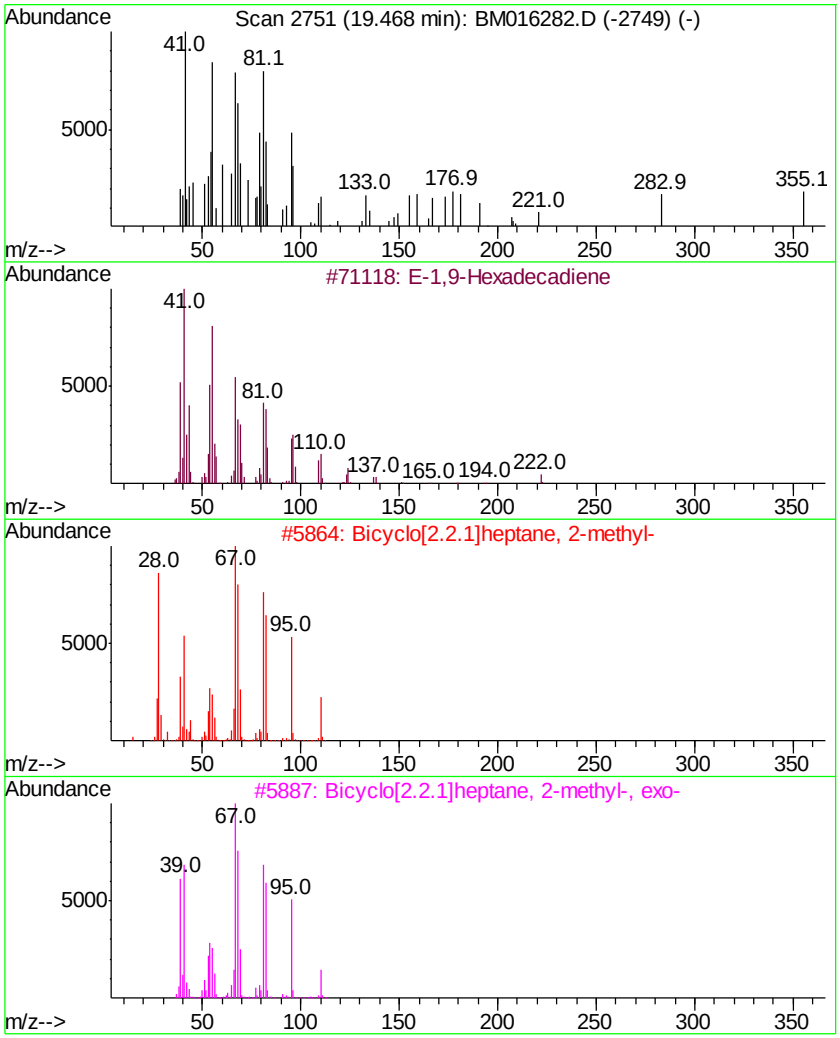
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

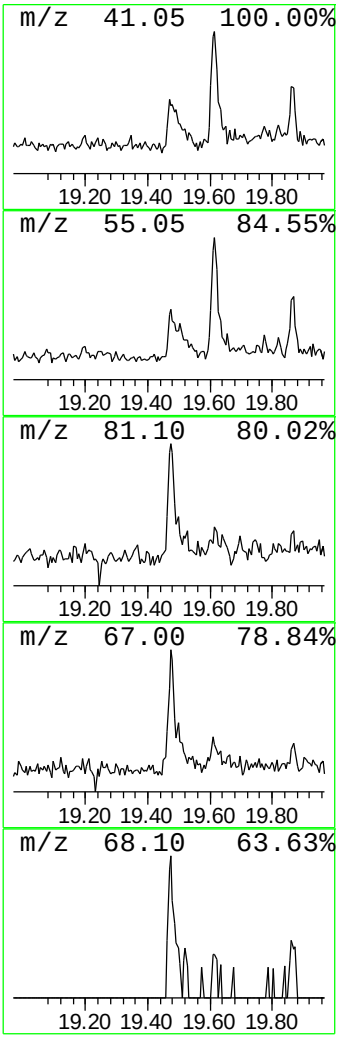
****

Peak Number 6 E-1,9-Hexadecadiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.47	2.23 ng	44488	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-1,9-Hexadecadiene	222	C16H30	1000245-71-4	58
2	Bicyclo[2.2.1]heptane, 2-methyl-	110	C8H14	015185-11-2	55
3	Bicyclo[2.2.1]heptane, 2-methyl-...	110	C8H14	000872-78-6	55
4	Phenanthrene, tetradecahydro-	192	C14H24	005743-97-5	49
5	1,E-8,Z-10-Tetradecatriene	192	C14H24	080625-31-6	49





Library Search Compound Report

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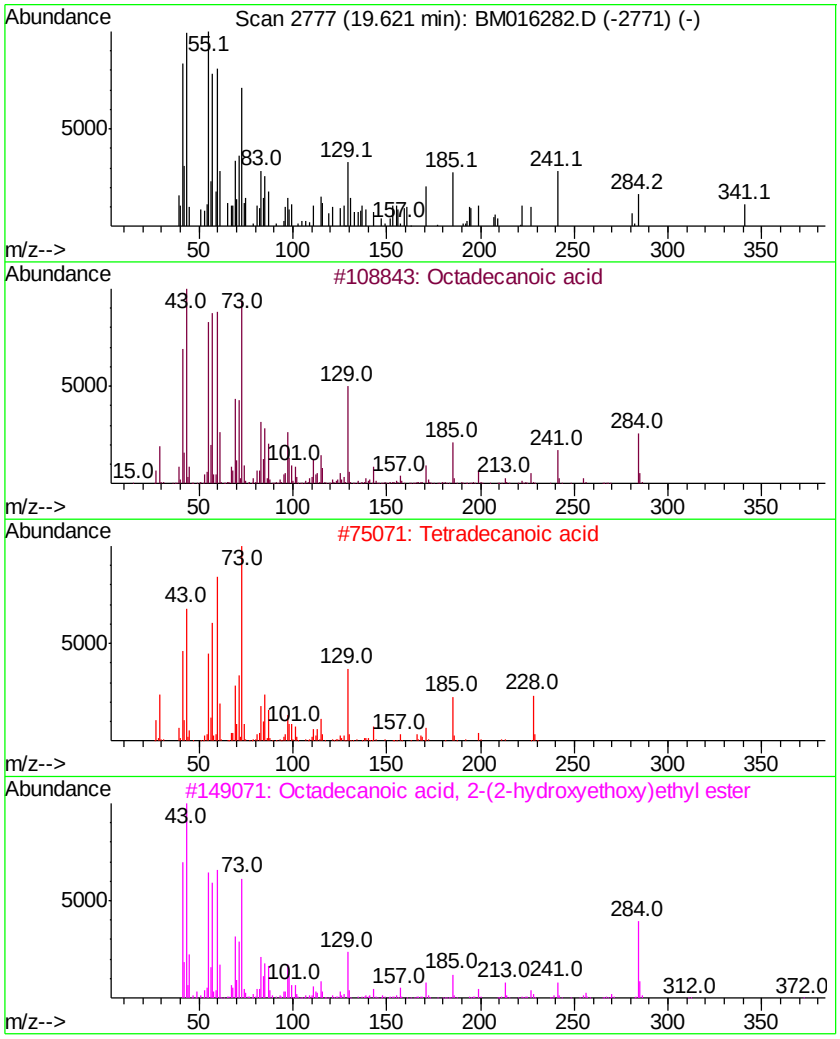
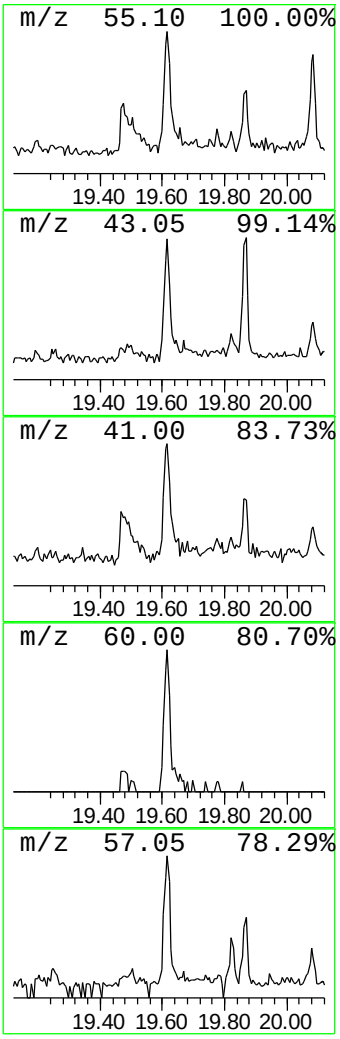
****

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	4.61 ng	117260	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	47
4	Undecanoic acid	186	C11H22O2	000112-37-8	45
5	Tridecanoic acid	214	C13H26O2	000638-53-9	43





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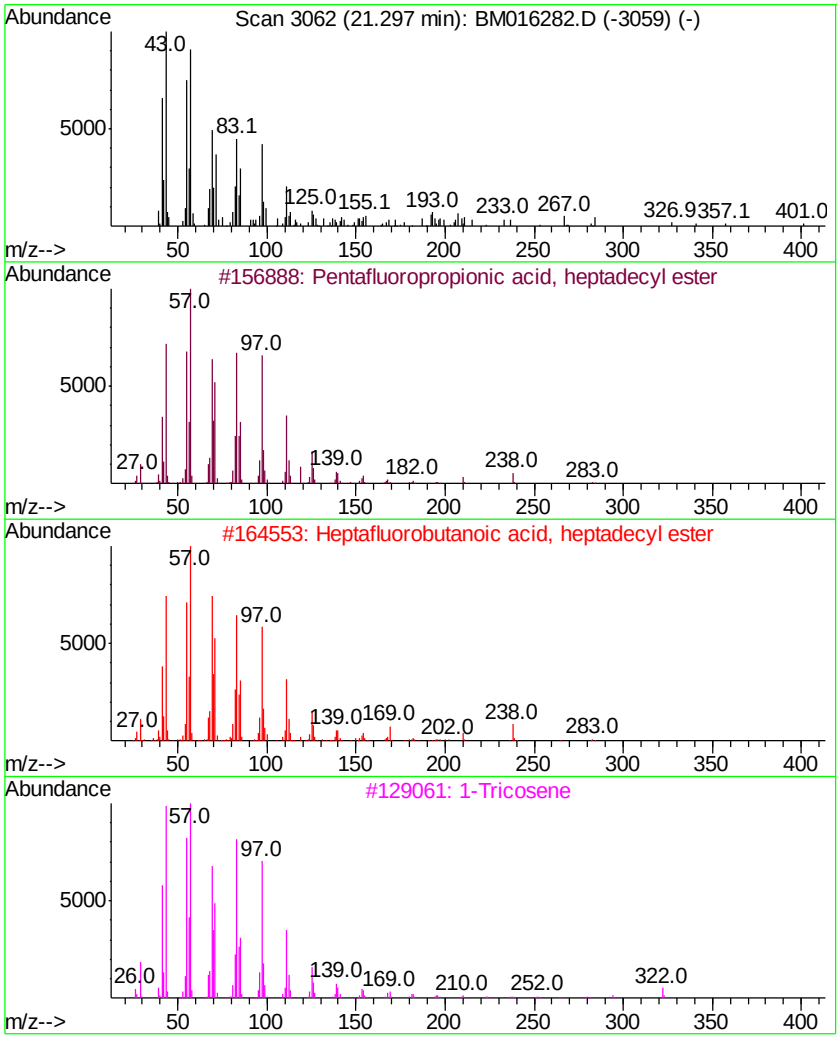
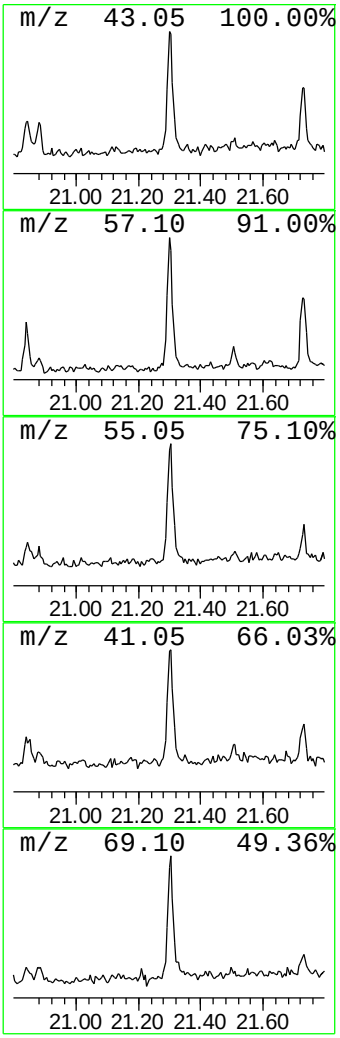
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	5.33 ng	135648	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	93
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
3	1-Tricosene	322	C23H46	018835-32-0	90
4	17-Pentatriacontene	491	C35H70	006971-40-0	90
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90





Tentatively Identified Compound (LSC) summary

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TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	5.4	ng	68650	1	8.13	252213	20.0
unknown7.66	7.66	116.2	ng	1464700	1	8.13	252213	20.0
n-Hexadecanoic acid	18.36	9.4	ng	188581	4	17.50	399352	20.0
3,5-di-tert-Butyl...	18.57	26.6	ng	530977	4	17.50	399352	20.0
E-1,9-Hexadecadiene	19.47	2.2	ng	44488	4	17.50	399352	20.0
Octadecanoic acid	19.62	4.6	ng	117260	5	21.63	509068	20.0
Pentafluoropropio...	21.30	5.3	ng	135648	5	21.63	509068	20.0