LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031319\
Data File : BM019158.D
Acq On : 13 Mar 2019 22:32
Operator : JU/SJ
Sample : K1869-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1

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-BM031119.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	5.257	380	386	401	rBV	3194559	4670699	37.70%	6.679%
2	6.840	647	655	676	rBV	3450823	5523522	44.58%	7.899%
3	7.192	708	715	738	rBV	3435686	5383904	43.45%	7.699%
4	7.657	787	794	804	rBV	683927	1074996	8.68%	1.537%
5	7.975	840	848	860	rBV	2274511	3652351	29.48%	5.223%
6	8.828	985	993	1014	rBV	1744831	3069566	24.77%	4.390%
7	10.445	1260	1268	1283	rBV	868987	1542772	12.45%	2.206%
8	12.927	1682	1690	1714	rBV	5054895	7767429	62.69%	11.108%
9	13.780	1829	1835	1851	rBV	319666	503155	4.06%	0.720%
10	14.251	1909	1915	1920	rBV	252605	357009	2.88%	0.511%
11	14.310	1920	1925	1938	rVB2	1569985	2440468	19.70%	3.490%
12	15.810	2171	2180	2202	rBV	4987901	7299792	58.91%	10.439%
13	17.068	2387	2394	2408	rBV	2061525	3133771	25.29%	4.482%
14	17.956	2540	2545	2565	rBV	421843	761156	6.14%	1.089%
15	19.245	2759	2764	2771	rBV2	106656	188952	1.52%	0.270%
16	19.703	2836	2842	2855	rBV	10041104	12390466	100.00%	17.719%
17	20.821	3028	3032	3039	rBV	607373	696249	5.62%	0.996%
18	20.962	3052	3056	3065	rBV	978378	1227749	9.91%	1.756%
19	21.262	3102	3107	3118	rBV	2657165	3603772	29.09%	5.154%
20	21.397	3127	3130	3137	rBV2	153595	200007	1.61%	0.286%
21	21.833	3200	3204	3207	rBV2	184784	266259	2.15%	0.381%
22	22.291	3278	3282	3289	rVB	210244	270166	2.18%	0.386%
23	22.415	3300	3303	3310	rVB	291102	365399	2.95%	0.523%
24	22.791	3363	3367	3372	rVB	216264	290651	2.35%	0.416%
25	23.350	3459	3462	3467	rVB	164357	247604	2.00%	0.354%
26	23.503	3481	3488	3501	rVB	1577364	2998840	24.20%	4.289%

Sum of corrected areas: 69926704

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031319\
Data File : BM019158.D
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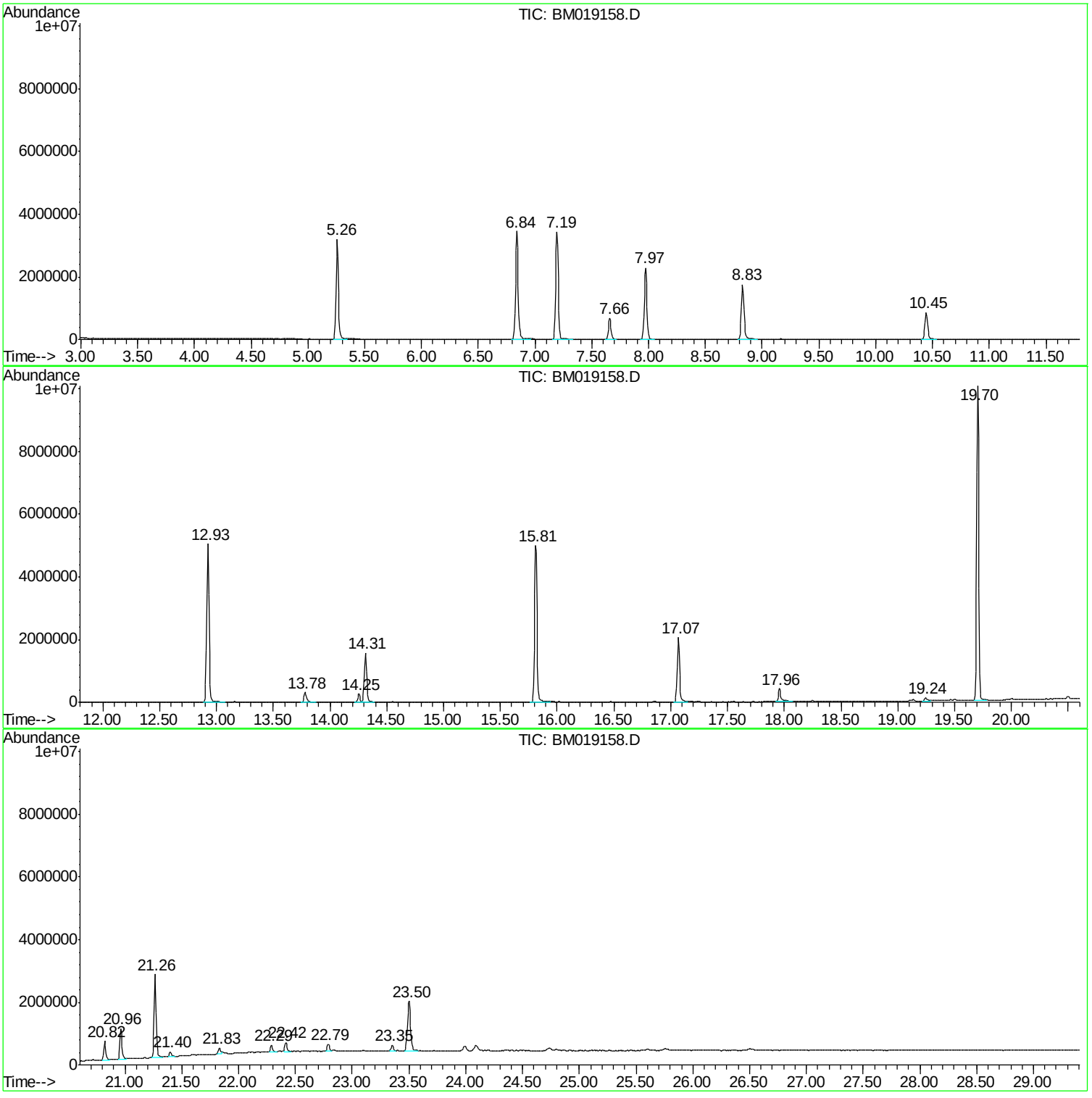
Operator : JU/SJ
Sample : K1869-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.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\BM031319\
Data File : BM019158.D
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Operator : JU/SJ
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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

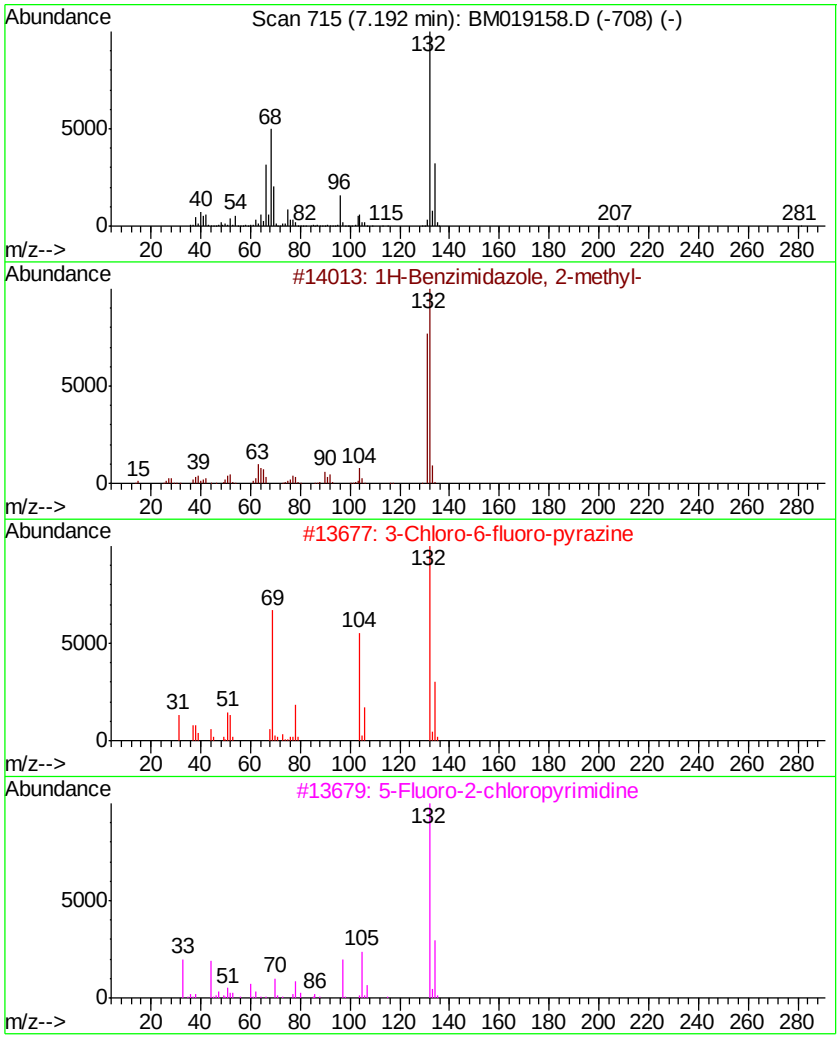
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

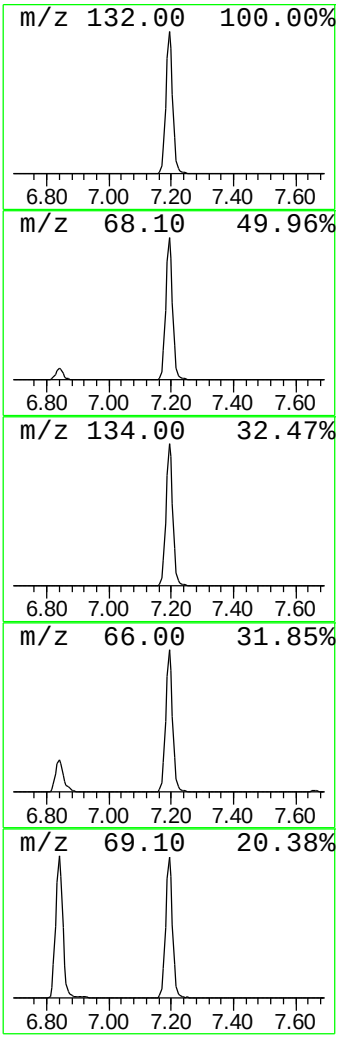
****

Peak Number 1 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	100.17 ng	5383900	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.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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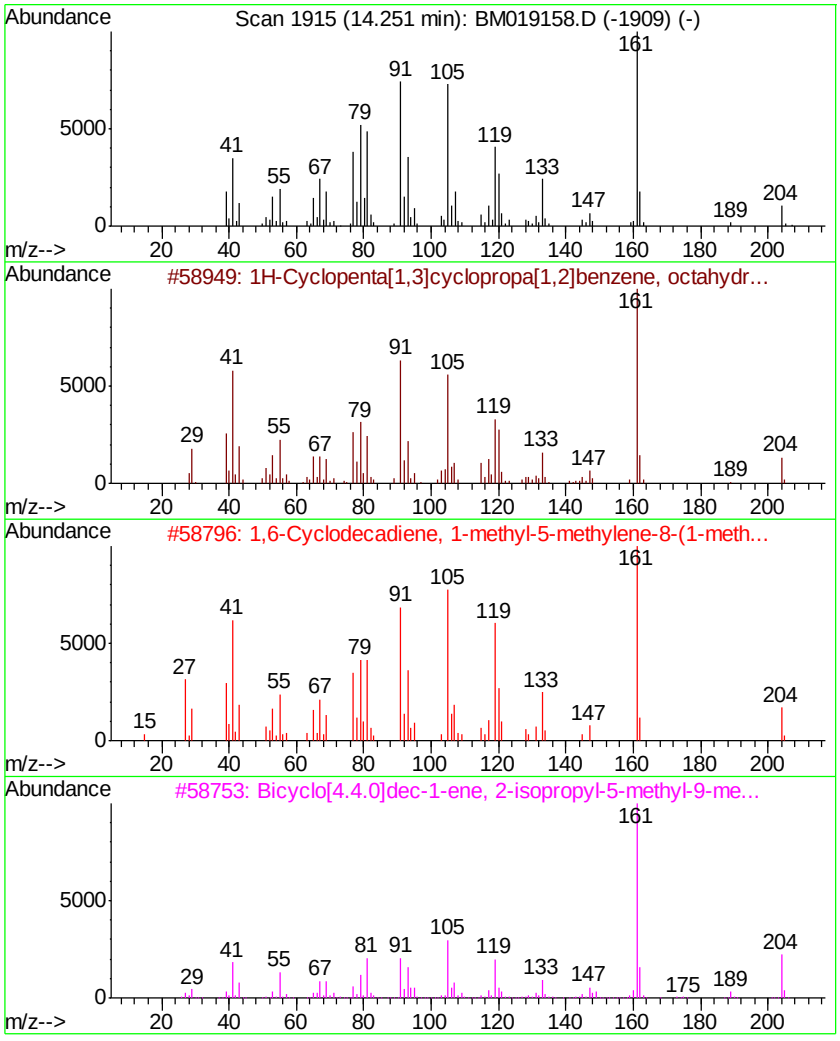
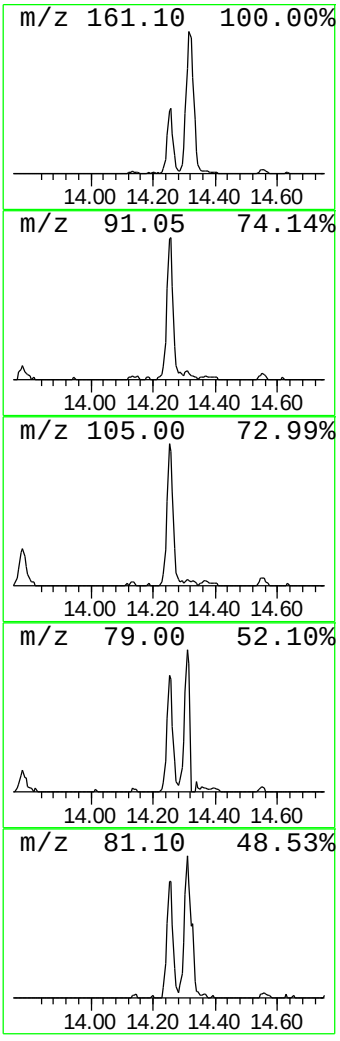
Peak Number 3 1H-Cyclopenta[1,3]cycloprop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	2.93 ng	357009	Acenaphthene-d10	14.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	83
2	1,6-Cyclodecadiene, 1-methyl-5-m...	204	C15H24	023986-74-5	83
3	Bicyclo[4.4.0]dec-1-ene, 2-isopr...	204	C15H24	150320-52-8	70
4	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	039029-41-9	64
5	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	53





Library Search Compound Report

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Acq On : 13 Mar 2019 22:32
Operator : JU/SJ
Sample : K1869-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1

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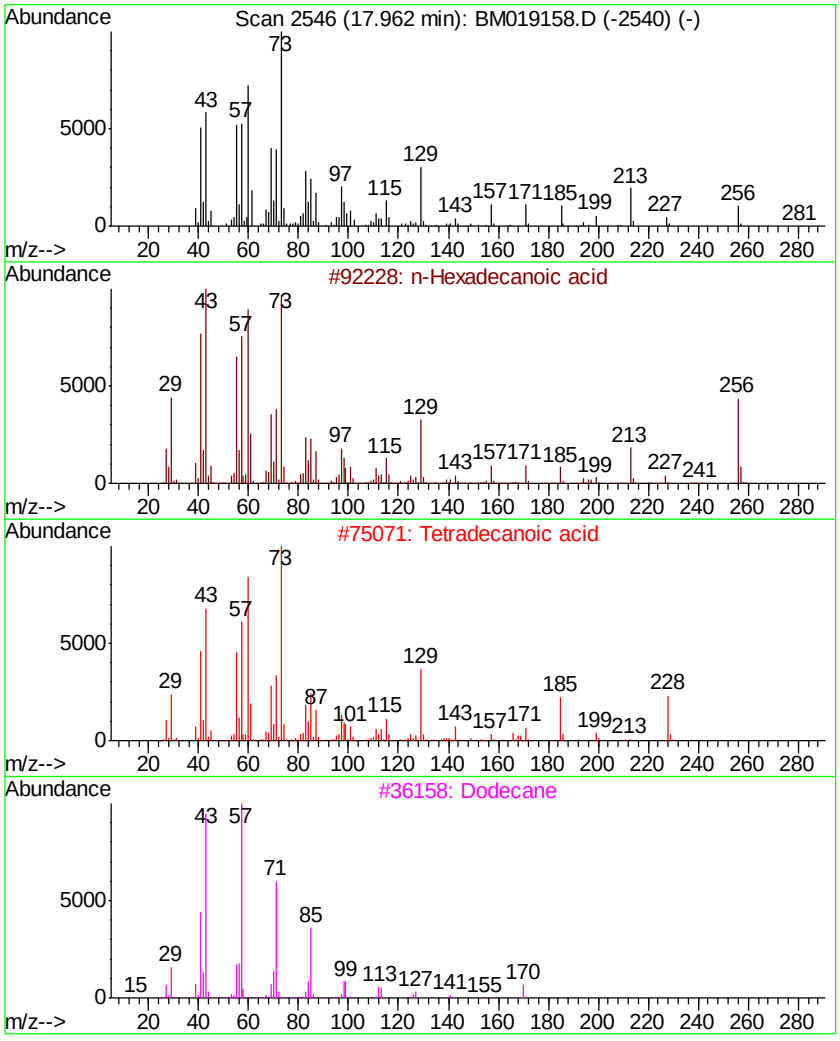
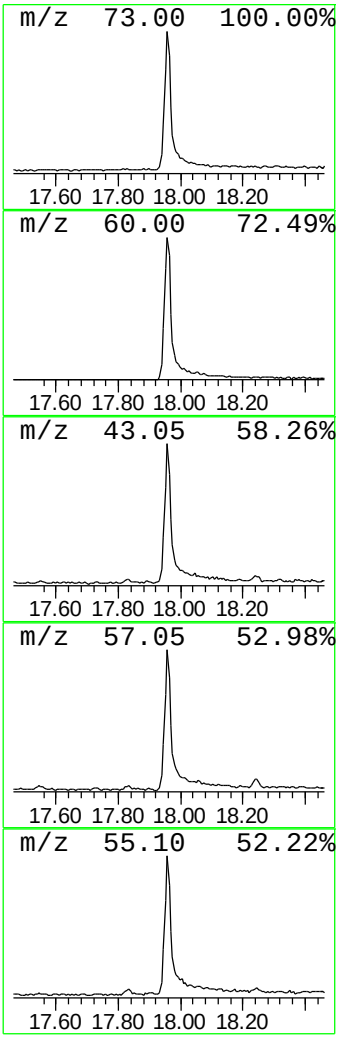
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	4.86 ng	761156	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Dodecane	170	C12H26	000112-40-3	25
4	Tridecane	184	C13H28	000629-50-5	25
5	Tritetracontane	605	C43H88	007098-21-7	18





Library Search Compound Report

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Operator : JU/SJ
Sample : K1869-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

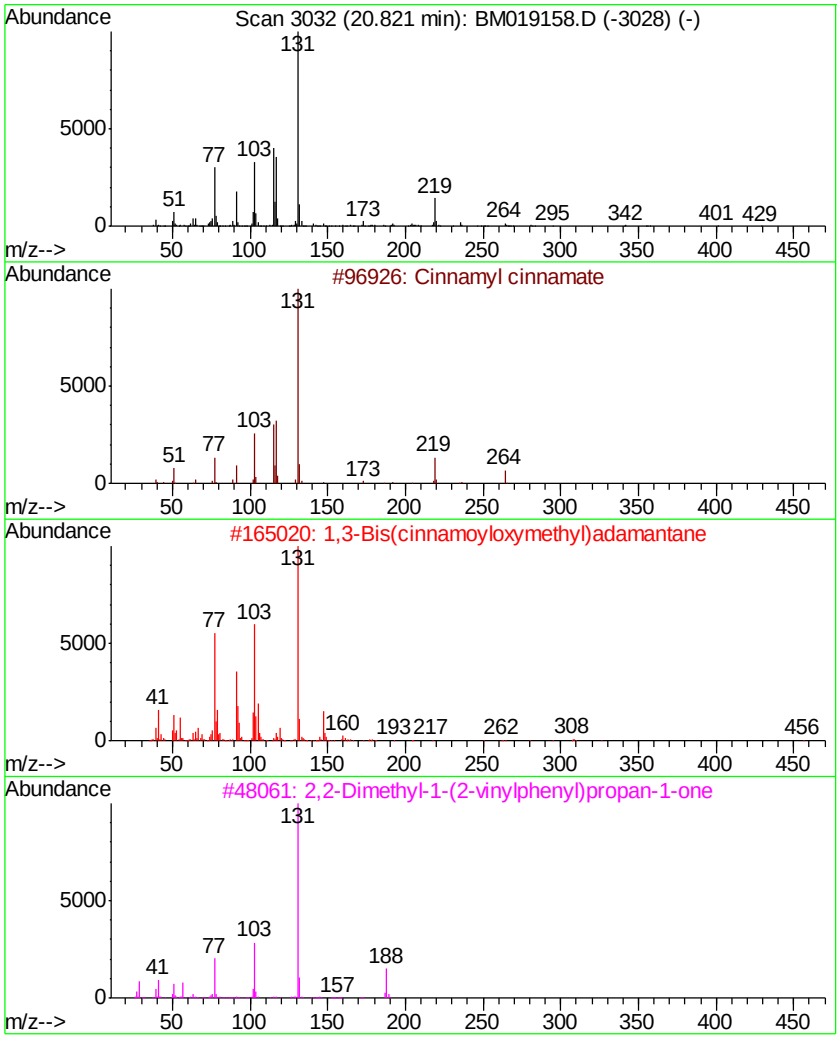
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

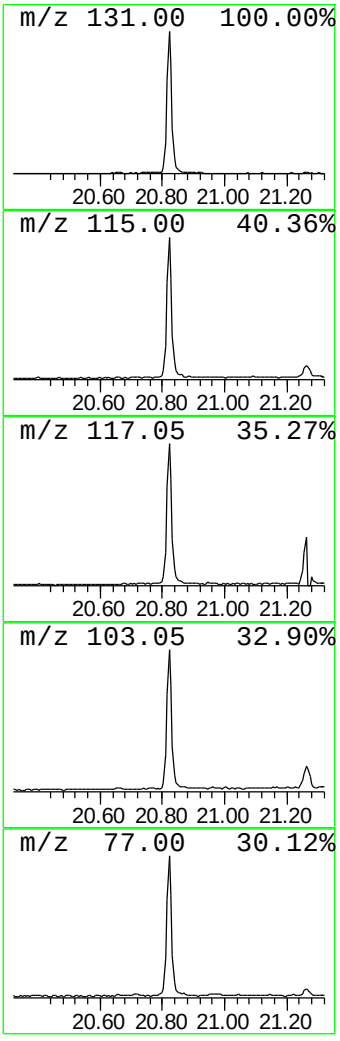
****

Peak Number 5 Cinnamyl cinnamate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.82	3.86 ng	696249	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
2	1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	47
3	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47
4	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	47
5	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	43





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : SP-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

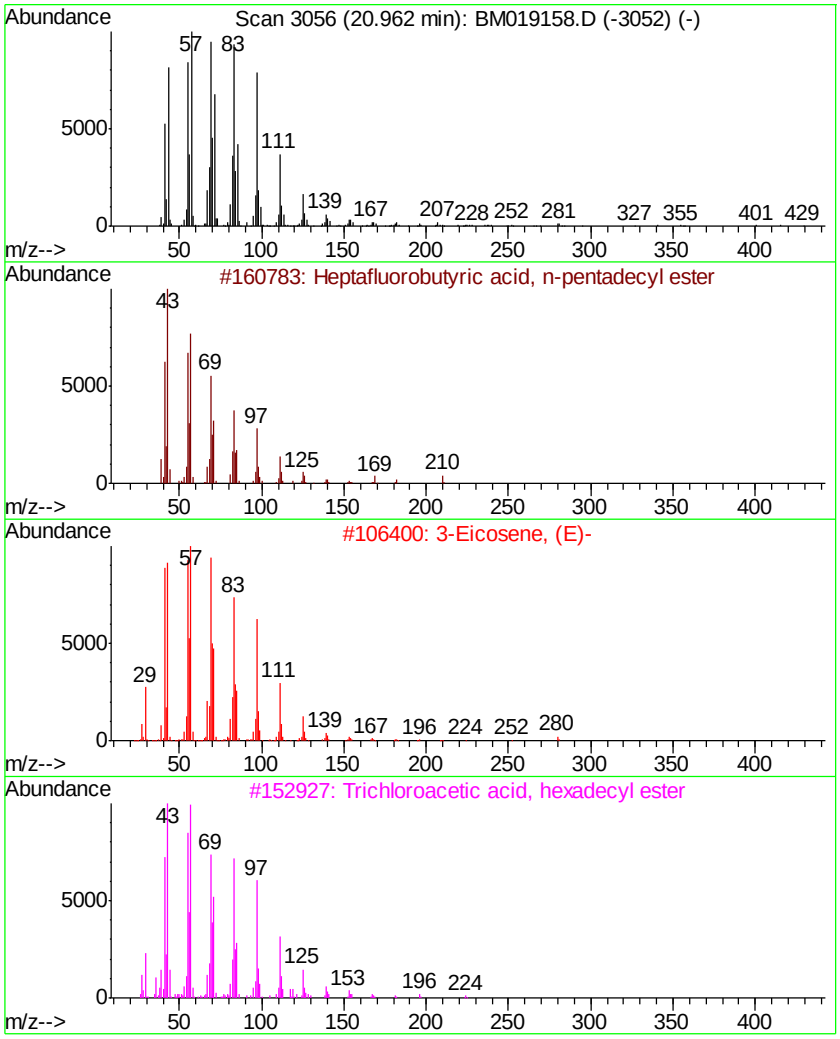
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

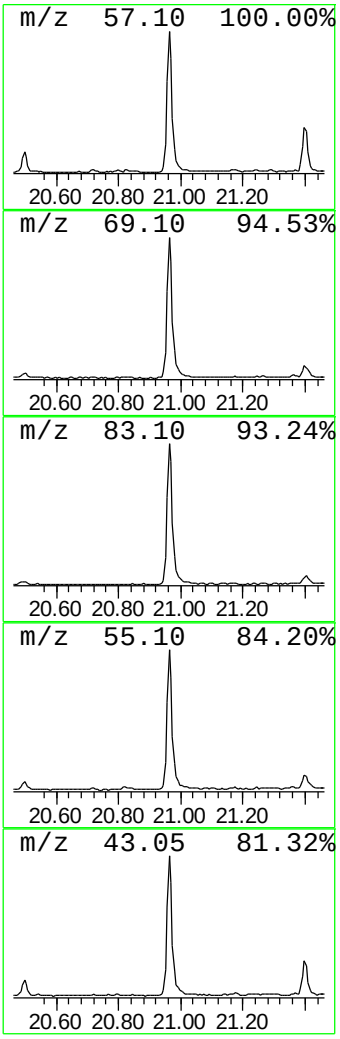
****

Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.96	6.81 ng	1227750	Chrysene-d12	21.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

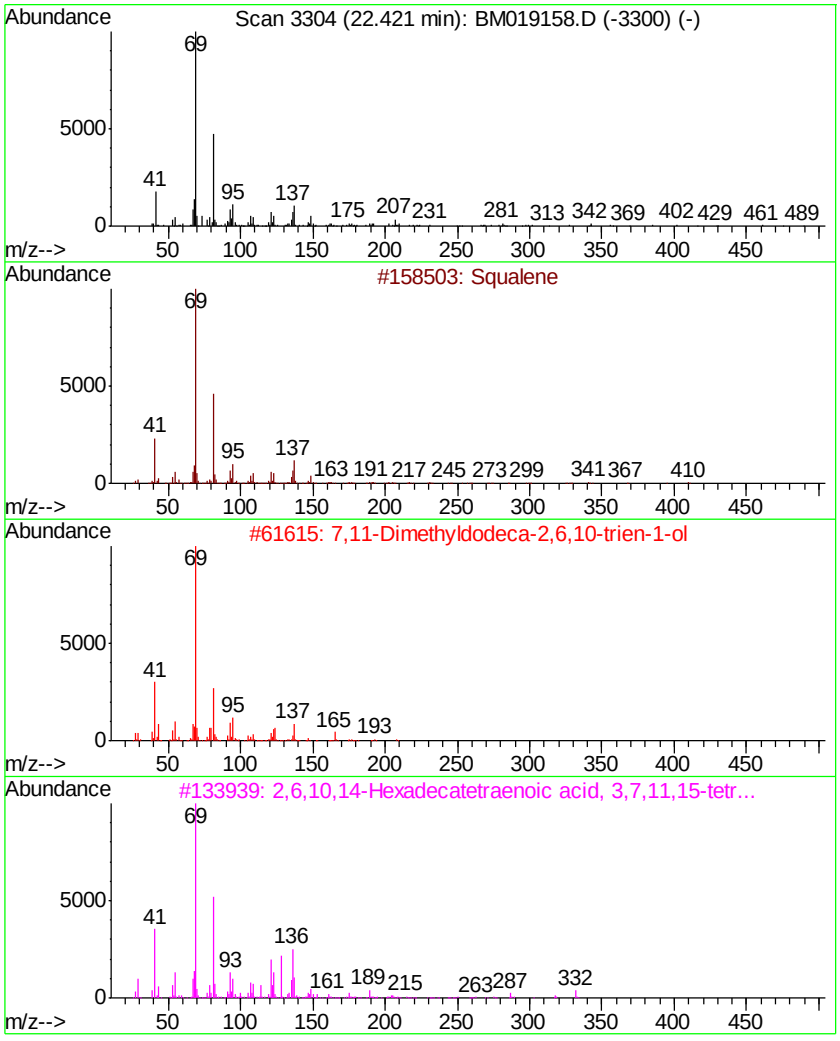
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

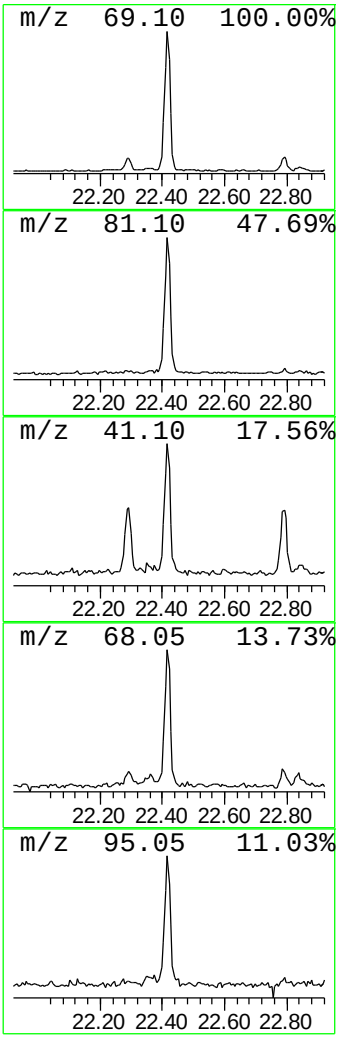
****

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.42	2.44 ng	365399	Perylene-d12	23.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	56





Tentatively Identified Compound (LSC) summary

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Acq On : 13 Mar 2019 22:32
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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
unknown7.19	7.19	100.2	ng	5383900	1	7.66	1075000	20.0
1H-Cyclopenta[1,3...	14.25	2.9	ng	357009	3	14.31	2440470	20.0
n-Hexadecanoic acid	17.96	4.9	ng	761156	4	17.07	3133770	20.0
Cinnamyl cinnamate	20.82	3.9	ng	696249	5	21.26	3603770	20.0
Heptafluorobutyri...	20.96	6.8	ng	1227750	5	21.26	3603770	20.0
Squalene	22.42	2.4	ng	365399	6	23.50	2998840	20.0