LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

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-BM010919.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	4.881	300	305	312	rVB	292476	422474	4.11%	0.390%
2	5.328	375	381	388	rBV	5116222	7400647	72.05%	6.830%
3	6.916	643	651	664	rVB	5229032	8290904	80.71%	7.652%
4	7.275	704	712	720	rBV	5624020	8751059	85.19%	8.076%
5	7.740	785	791	798	rBV	1491580	2325648	22.64%	2.146%
6	8.057	837	845	854	rVB	4228726	6647139	64.71%	6.135%
7	8.904	980	989	1003	rBV	3219464	5476564	53.31%	5.054%
8	10.528	1259	1265	1271	rBV	1940698	3142621	30.59%	2.900%
9	13.004	1674	1686	1694	rBV	7124750	10272230	100.00%	9.480%
10	13.192	1712	1718	1725	rBV2	55198	116551	1.13%	0.108%
11	13.269	1725	1731	1737	rBV	471105	706142	6.87%	0.652%
12	13.704	1800	1805	1810	rBV2	59859	114716	1.12%	0.106%
13	13.845	1823	1829	1836	rBV	1947320	2683022	26.12%	2.476%
14	14.269	1894	1901	1909	rVB2	112215	216359	2.11%	0.200%
15	14.386	1910	1921	1928	rBV2	2697090	4181040	40.70%	3.859%
16	14.786	1978	1989	1995	rBV6	73921	161663	1.57%	0.149%
17	15.169	2046	2054	2058	rBV7	63670	126512	1.23%	0.117%
18	15.222	2058	2063	2069	rVB4	93794	130393	1.27%	0.120%
19	15.498	2102	2110	2114	rBV2	194729	275373	2.68%	0.254%
20	15.880	2166	2175	2183	rBV	4736704	6677925	65.01%	6.163%
21	16.110	2206	2214	2220	rBV2	137413	322709	3.14%	0.298%
22	16.880	2337	2345	2349	rBV2	132460	192954	1.88%	0.178%
23	17.139	2382	2389	2394	rBV	3141565	4505344	43.86%	4.158%
24	17.180	2394	2396	2401	rVB	248077	285777	2.78%	0.264%
25	17.621	2467	2471	2474	rVB	121632	148258	1.44%	0.137%
26	18.027	2533	2540	2544	rBV2	1282843	1903508	18.53%	1.757%
27	18.198	2565	2569	2574	rBV3	121545	197280	1.92%	0.182%
28	18.245	2574	2577	2583	rVB	82803	115502	1.12%	0.107%
29	18.315	2585	2589	2594	rBV2	116857	175164	1.71%	0.162%
30	18.515	2619	2623	2628	rBV	94991	151258	1.47%	0.140%
31	18.563	2628	2631	2641	rVB5	80958	158246	1.54%	0.146%
32	18.933	2689	2694	2700	rBV2	194286	436284	4.25%	0.403%
33	19.074	2714	2718	2723	rBV3	68276	145723	1.42%	0.134%
34	19.198	2735	2739	2744	rVB	436090	635348	6.19%	0.586%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

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-BM010919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.310	2753	2758	2767	rBV2	495097	742865	7.23%	0.686%
36	19.533	2793	2796	2798	rBV2	135117	157504	1.53%	0.145%
37	19.562	2798	2801	2810	rVV	323327	527018	5.13%	0.486%
38	19.639	2810	2814	2820	rVB2	101117	154527	1.50%	0.143%
39	19.768	2831	2836	2846	rVB	7569962	9683161	94.27%	8.937%
40	19.880	2852	2855	2859	rBV2	76415	121919	1.19%	0.113%
41	20.068	2884	2887	2891	rVB3	146214	186780	1.82%	0.172%
42	20.568	2969	2972	2975	rVB	120599	137294	1.34%	0.127%
43	21.027	3046	3050	3059	rBV	851199	1085507	10.57%	1.002%
44	21.333	3096	3102	3106	rBV	2844820	4096142	39.88%	3.780%
45	21.468	3122	3125	3130	rVB	218417	237497	2.31%	0.219%
46	21.903	3196	3199	3209	rVB	420885	658729	6.41%	0.608%
47	22.374	3275	3279	3286	rVB	954757	1196672	11.65%	1.104%
48	22.886	3361	3366	3377	rBV2	1318654	2310883	22.50%	2.133%
49	23.462	3459	3464	3478	rVB2	1417141	2685650	26.14%	2.479%
50	23.603	3482	3488	3498	rVB	1890617	3474776	33.83%	3.207%
51	24.121	3570	3576	3586	rVB	1132227	2135108	20.79%	1.970%
52	24.880	3700	3705	3712	rVB	603979	1269289	12.36%	1.171%

Sum of corrected areas: 108353658

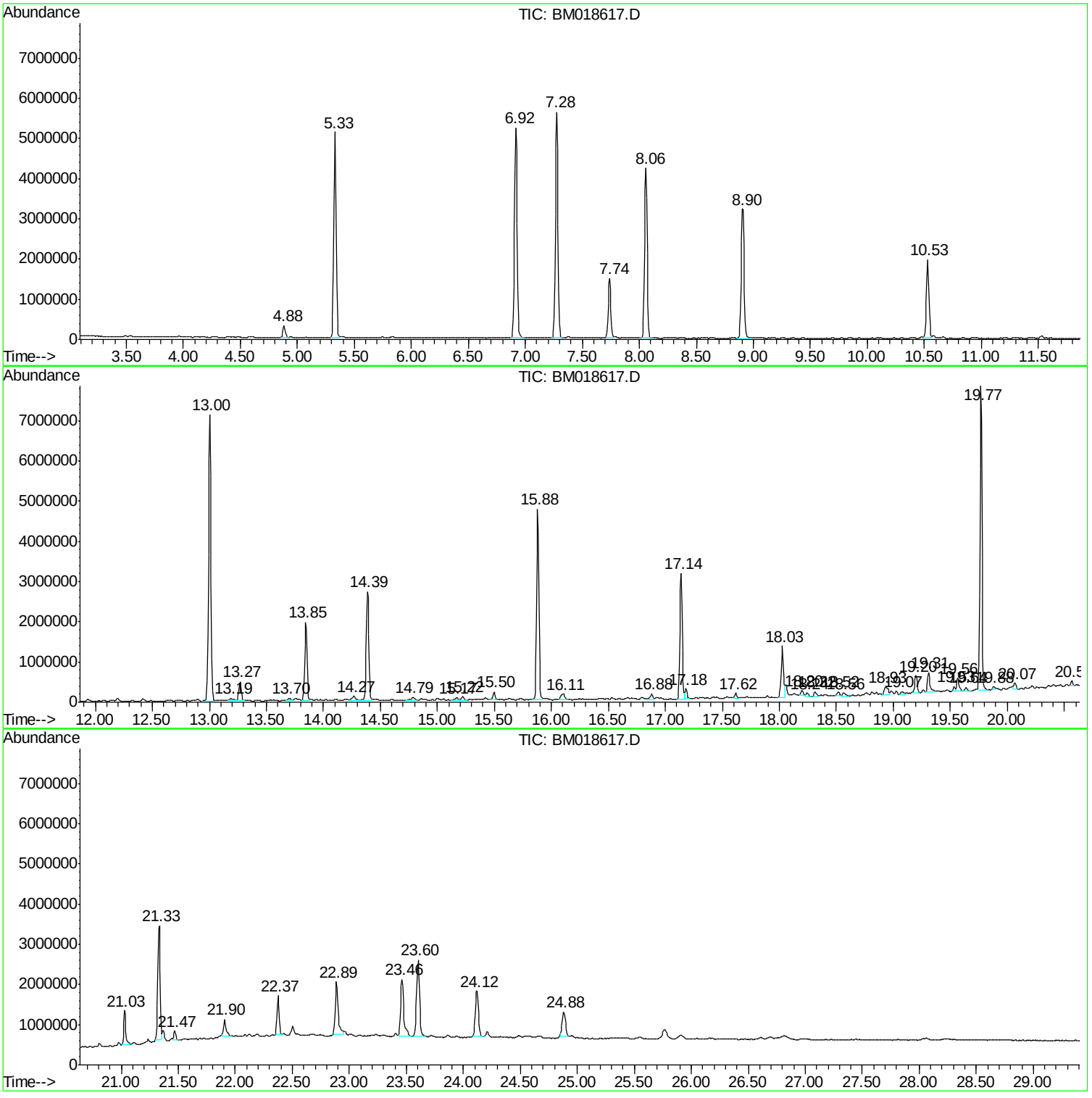
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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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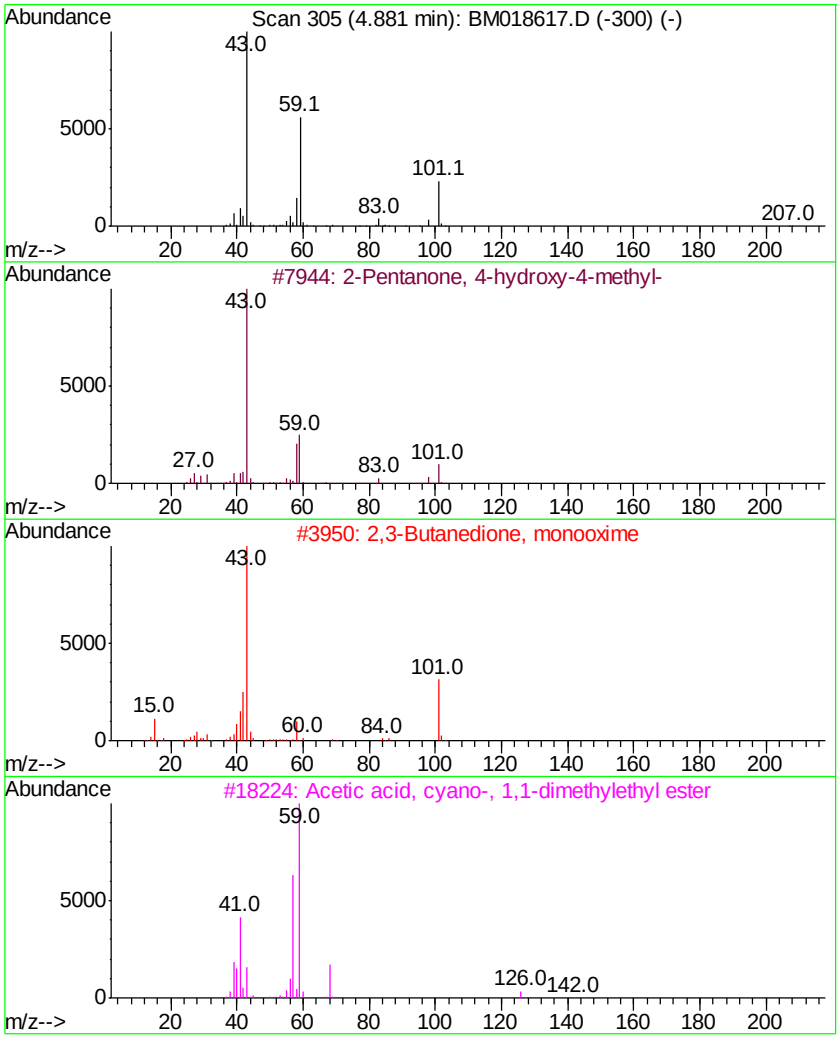
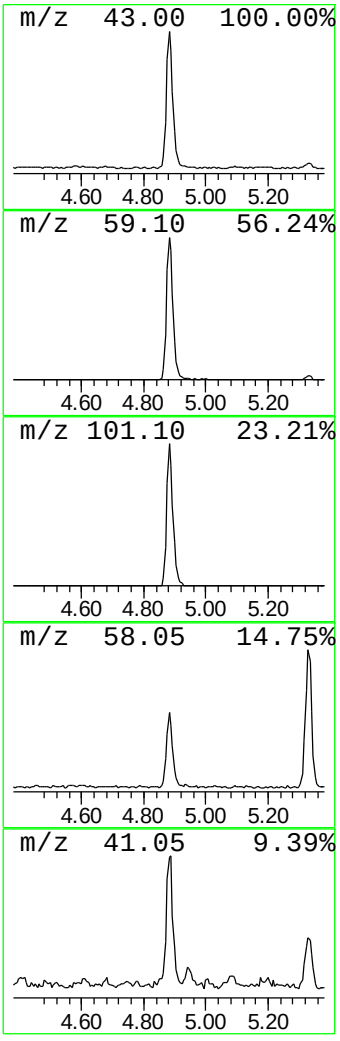
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	3.63 ng	422474	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

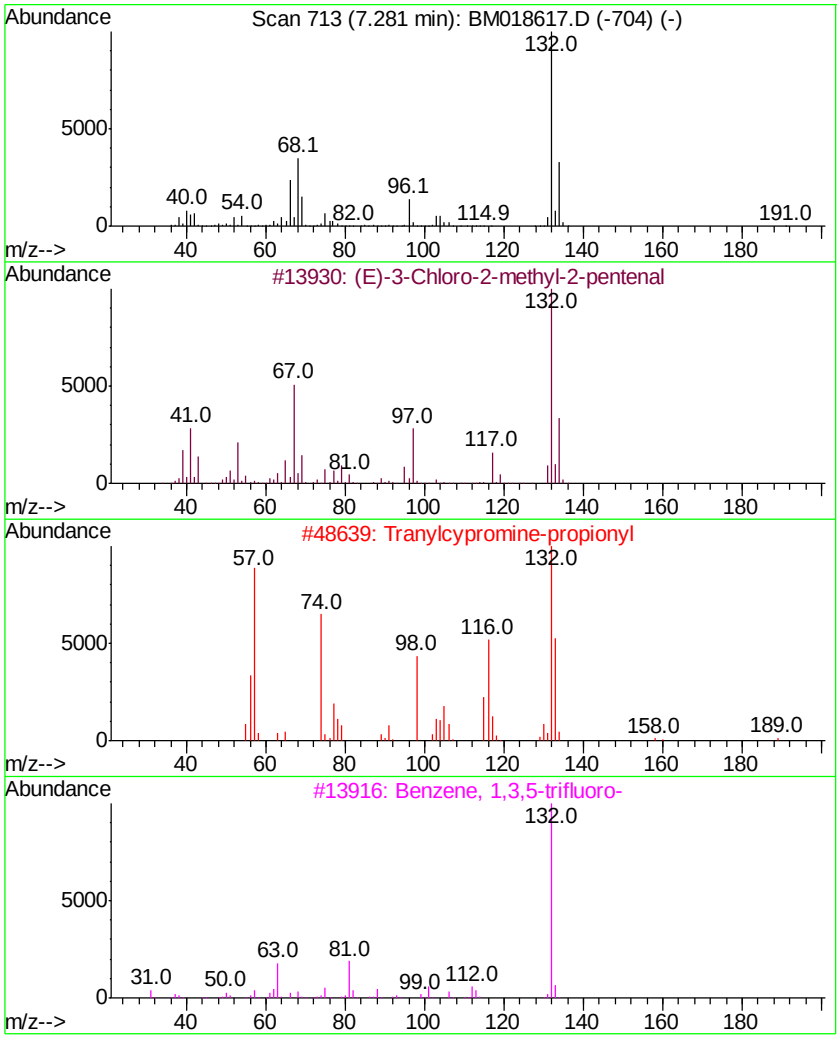
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

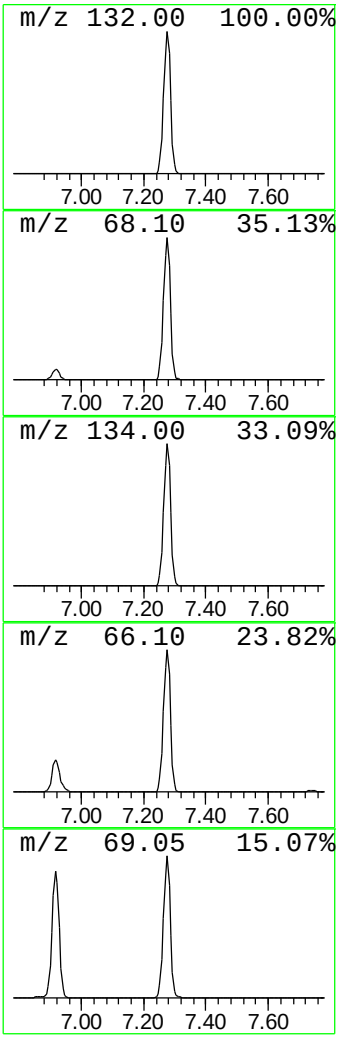
****

Peak Number 2 unknown7.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	75.26 ng	8751060	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

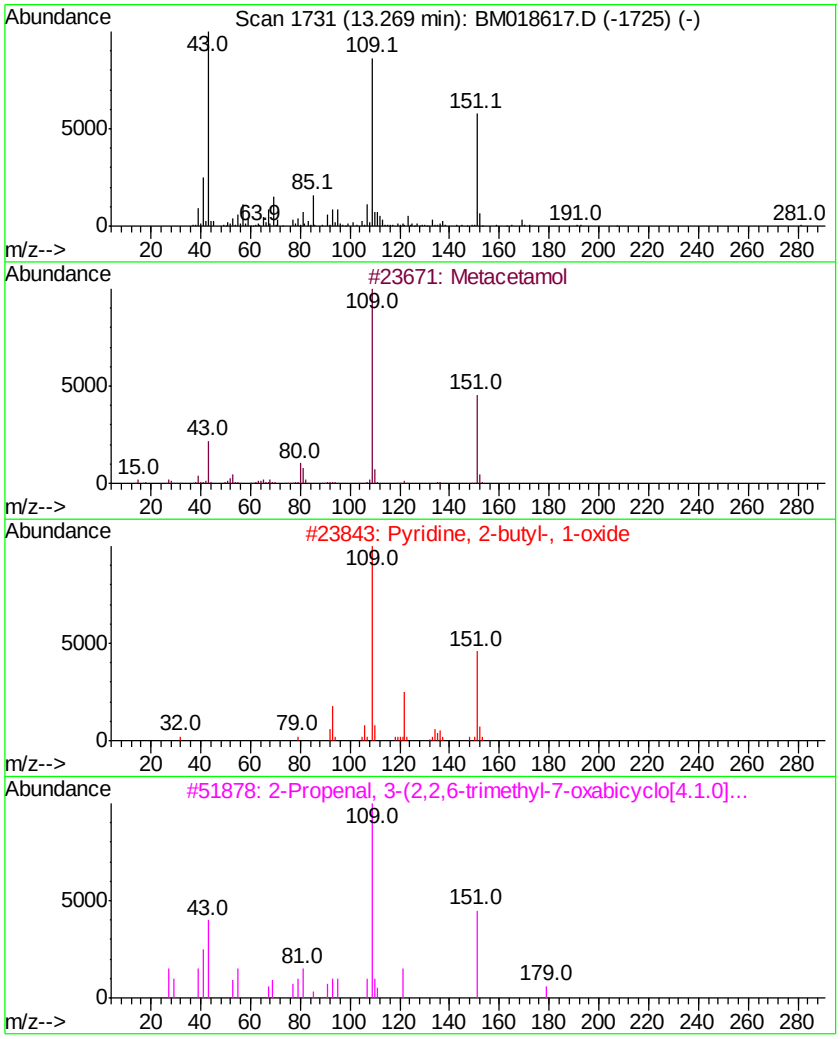
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

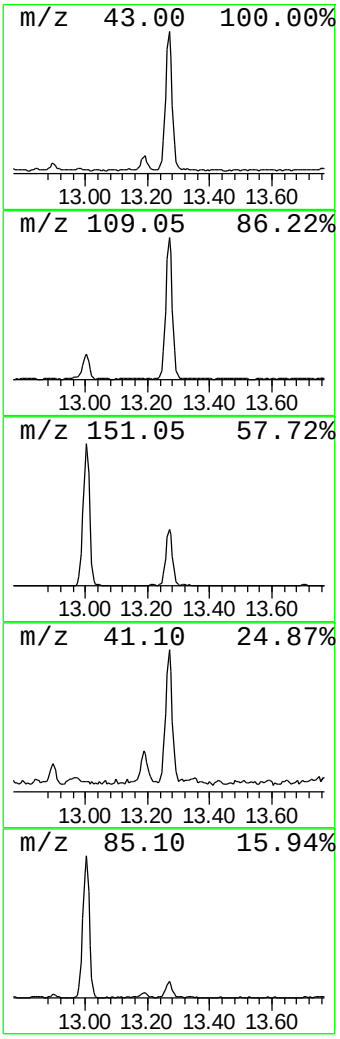
****

Peak Number 4 Metacetamol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	3.38 ng	706142	Acenaphthene-d10	14.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	64
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	53
4	Acetaminophen	151	C8H9NO2	000103-90-2	45
5	N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

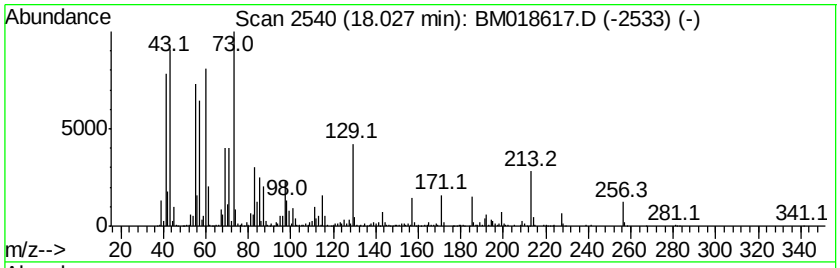
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

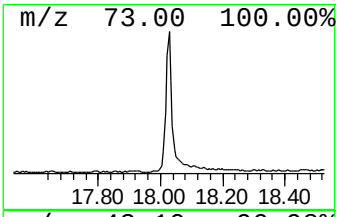
****

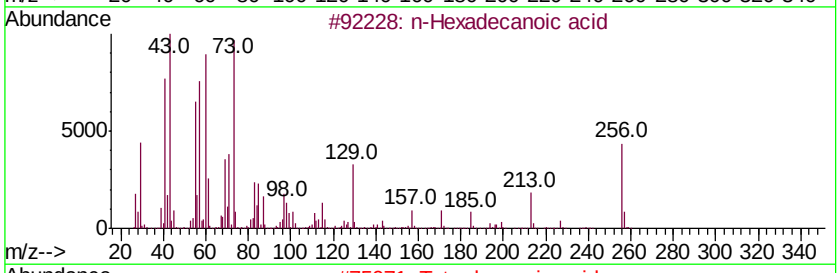
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

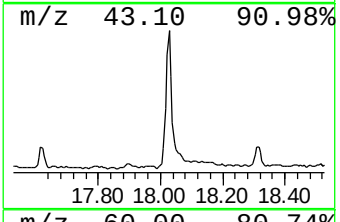
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	8.45 ng	1903510	Phenanthrene-d10	17.14

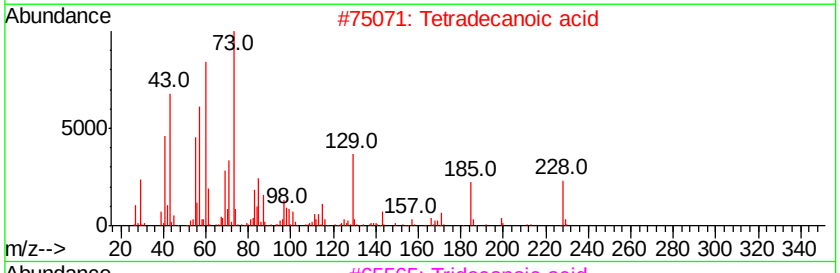
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Undecanoic acid	186	C11H22O2	000112-37-8	83
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	74

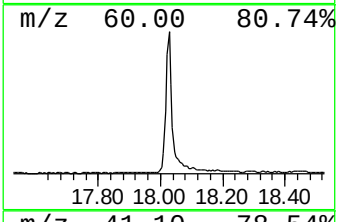


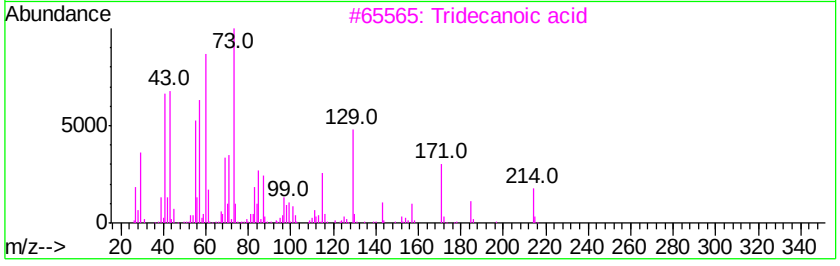


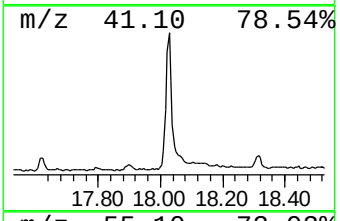


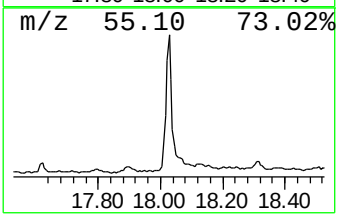












Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

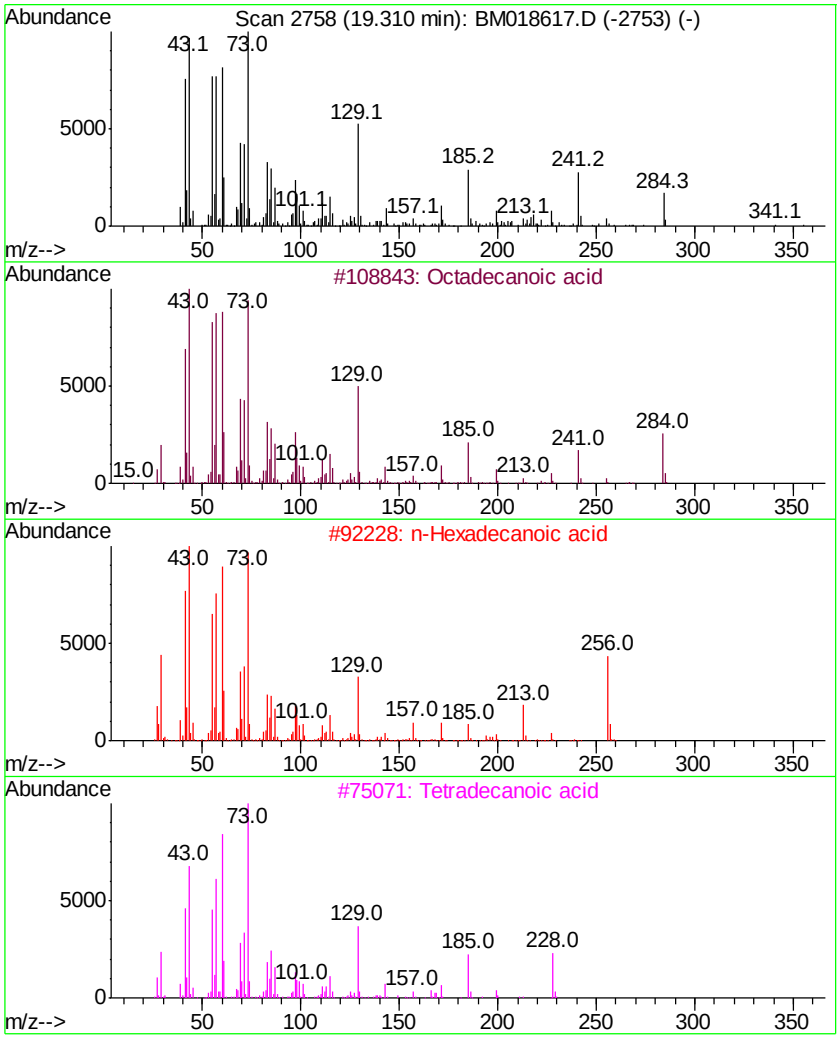
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

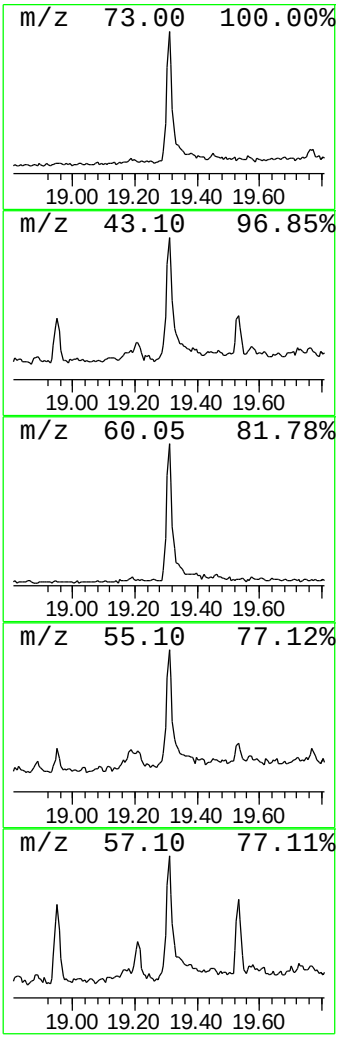
****

Peak Number 7 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	3.63 ng	742865	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
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Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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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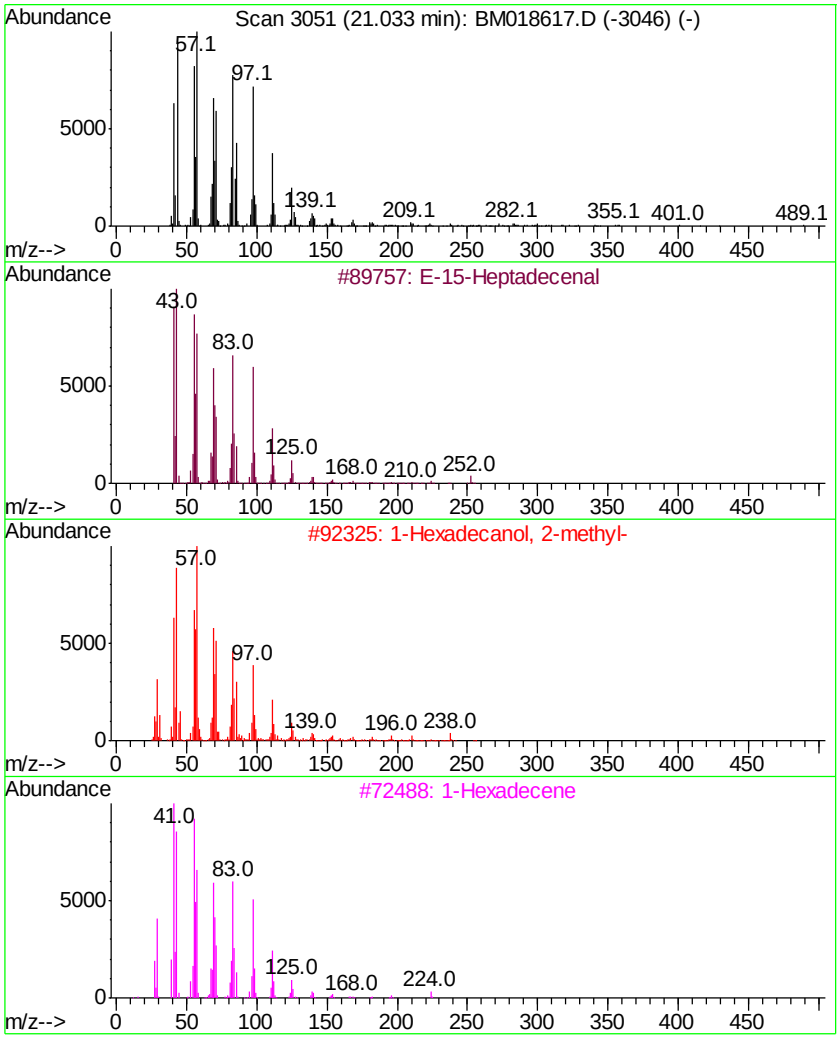
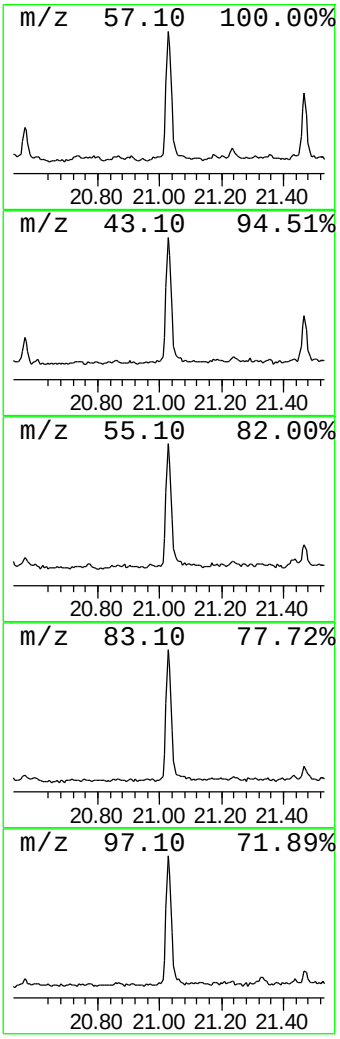
Peak Number 8 E-15-Heptadecenal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	5.30 ng	1085510	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	95
3	1-Hexadecene	224	C16H32	000629-73-2	94
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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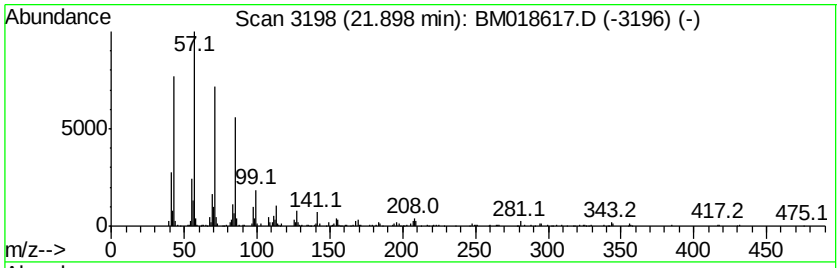
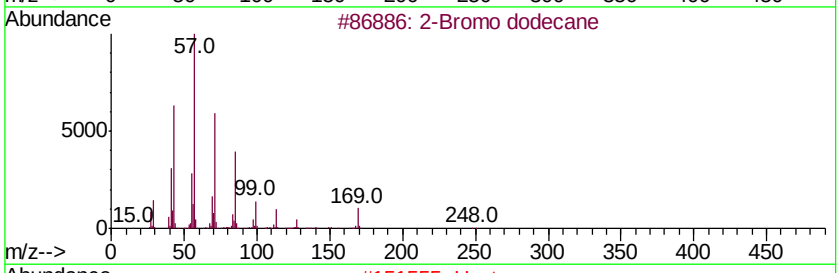
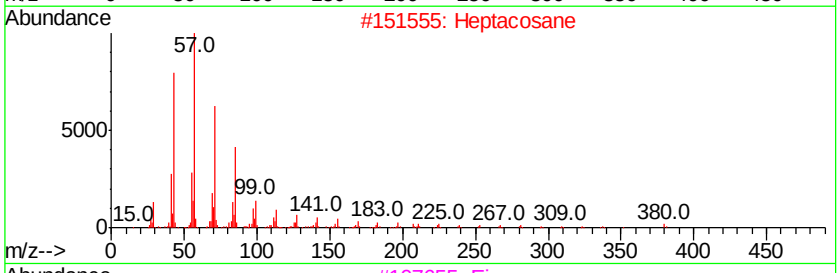
Peak Number 9 2-Bromo dodecane Concentration Rank 13

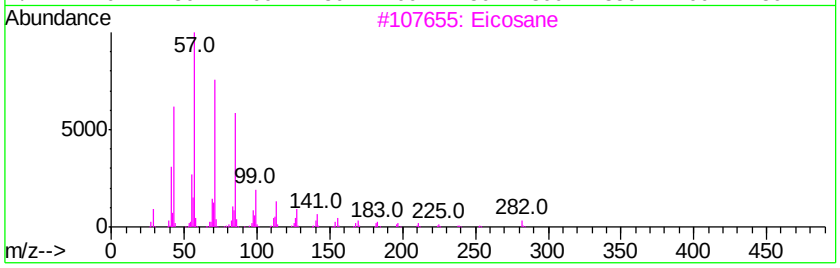
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.90	3.22 ng	658729	Chrysene-d12	21.33

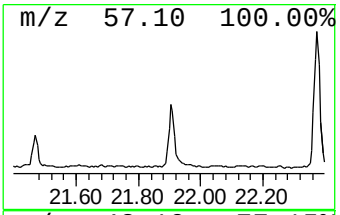
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90

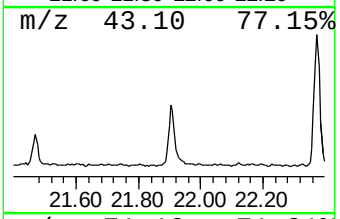


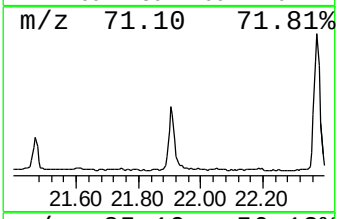


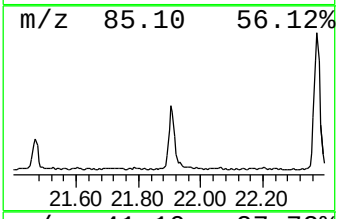


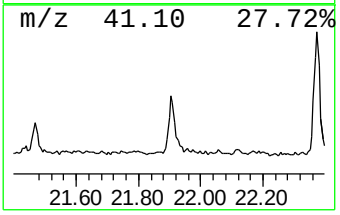












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Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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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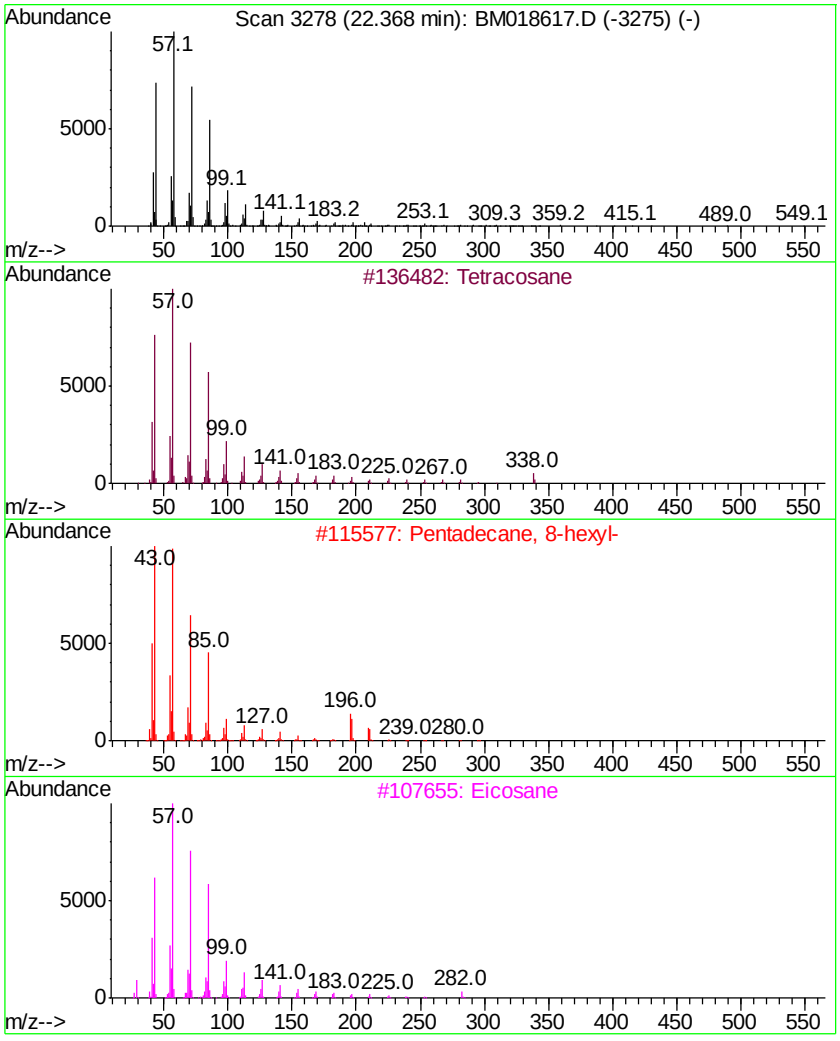
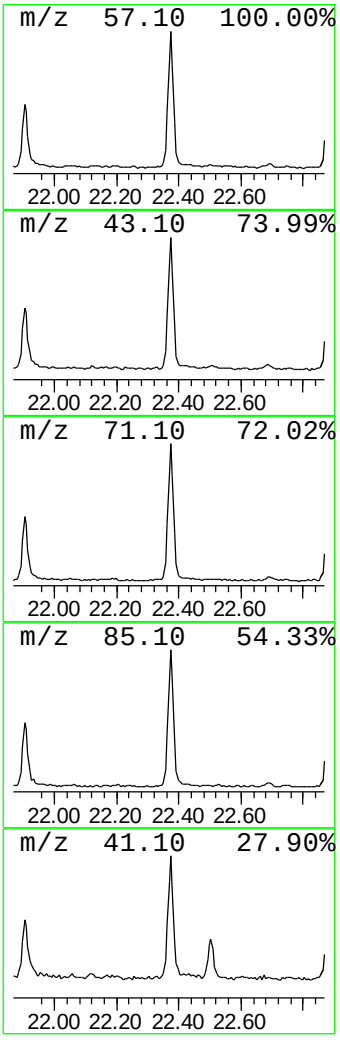
Peak Number 10 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	5.84 ng	1196670	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	98
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3	Eicosane	282	C20H42	000112-95-8	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Heneicosane	296	C21H44	000629-94-7	91





Library Search Compound Report

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Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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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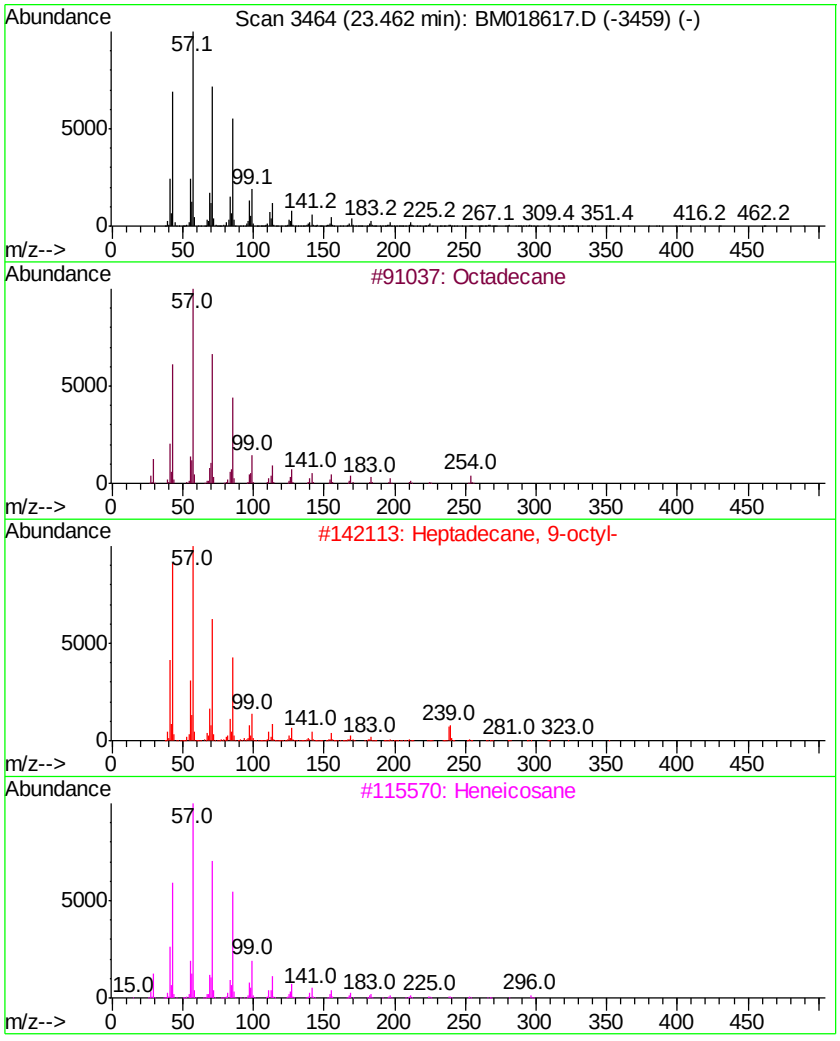
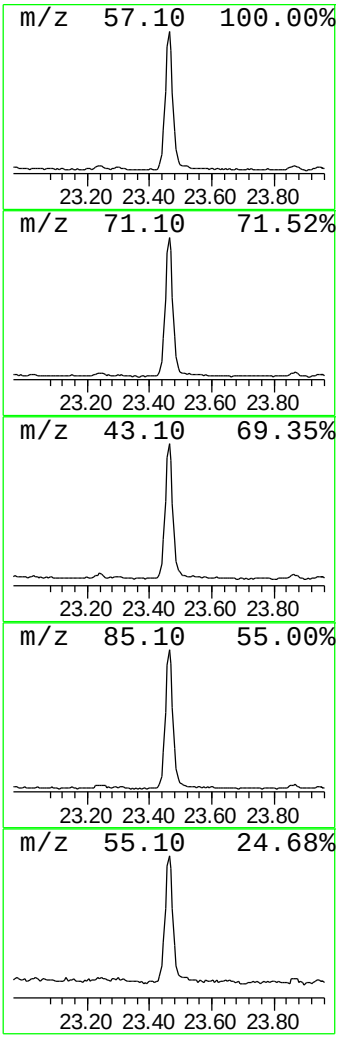
Peak Number 12 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.46	15.46 ng	2685650	Perylene-d12	23.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	97
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Docosane	310	C22H46	000629-97-0	91





Library Search Compound Report

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Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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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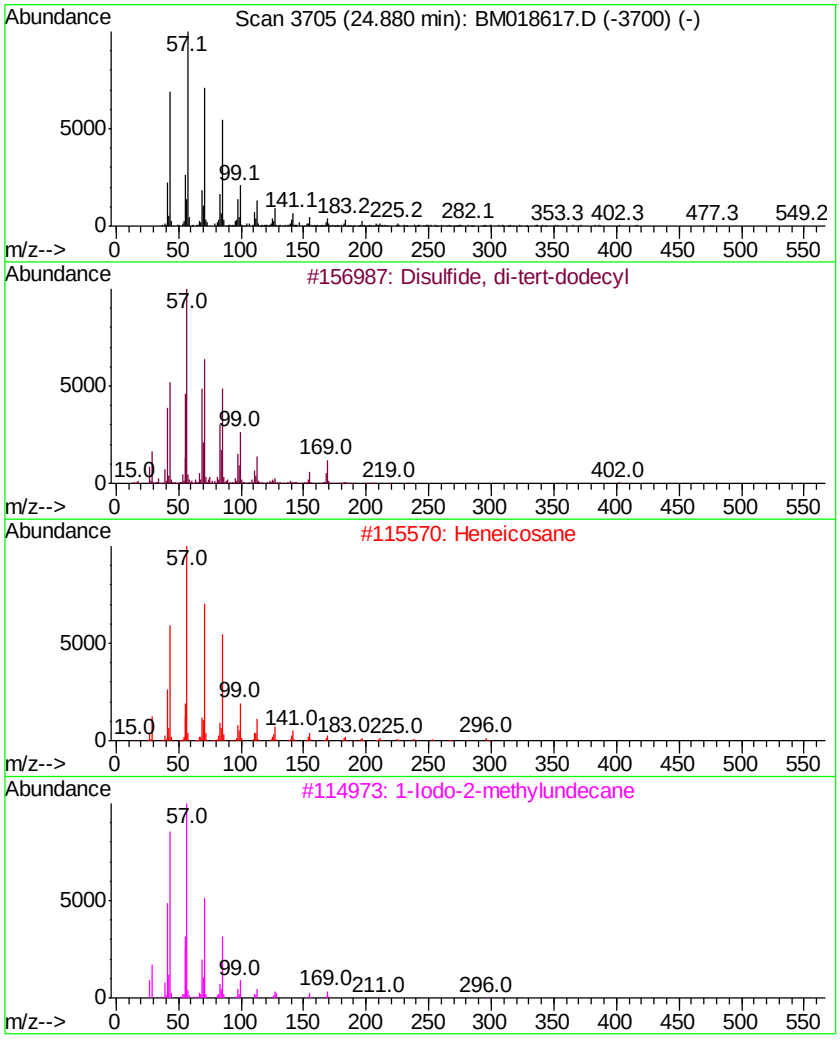
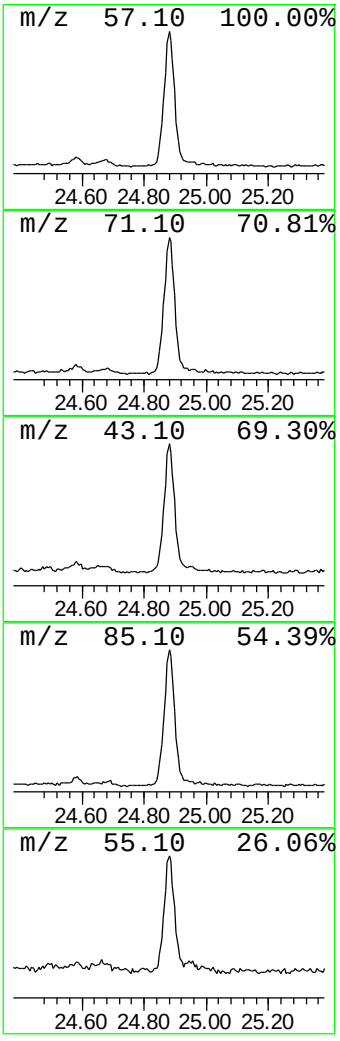
Peak Number 14 Disulfide, di-tert-dodecyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.88	7.31 ng	1269290	Perylene-d12	23.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	91
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
5	Docosane	310	C22H46	000629-97-0	90





Tentatively Identified Compound (LSC) summary

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Data File : BM018617.D
Acq On : 17 Jan 2019 16:59
Operator : JU/SJ
Sample : K1139-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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...	4.88	3.6	ng	422474	1	7.74	2325650	20.0
unknown7.28	7.28	75.3	ng	8751060	1	7.74	2325650	20.0
Metacetamol	13.27	3.4	ng	706142	3	14.39	4181040	20.0
n-Hexadecanoic acid	18.03	8.4	ng	1903510	4	17.14	4505340	20.0
Octadecanoic acid	19.31	3.6	ng	742865	5	21.33	4096140	20.0
E-15-Heptadecenal	21.03	5.3	ng	1085510	5	21.33	4096140	20.0
2-Bromo dodecane	21.90	3.2	ng	658729	5	21.33	4096140	20.0
Tetracosane	22.37	5.8	ng	1196670	5	21.33	4096140	20.0
Octadecane	23.46	15.5	ng	2685650	6	23.60	3474780	20.0
Disulfide, di-ter...	24.88	7.3	ng	1269290	6	23.60	3474780	20.0