LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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	4.887	301	306	314	rVB	66283	108103	2.53%	0.259%
2	5.334	376	382	394	rVB	1175109	1770421	41.48%	4.234%
3	6.916	645	651	663	rBV	1238041	1979778	46.38%	4.735%
4	7.281	706	713	722	rBV	1273165	2041136	47.82%	4.881%
5	7.745	785	792	798	rBV	545024	842391	19.74%	2.015%
6	8.063	839	846	854	rVB	932495	1478567	34.64%	3.536%
7	8.910	982	990	999	rBV	775423	1271637	29.79%	3.041%
8	10.533	1259	1266	1273	rBV	683735	1157365	27.12%	2.768%
9	13.010	1680	1687	1695	rVB	1563165	2375184	55.65%	5.680%
10	13.851	1823	1830	1836	rVB	511946	688475	16.13%	1.646%
11	14.116	1870	1875	1878	rBV2	30830	52142	1.22%	0.125%
12	14.151	1878	1881	1888	rVV2	30156	72177	1.69%	0.173%
13	14.263	1894	1900	1912	rVB3	102596	248363	5.82%	0.594%
14	14.392	1915	1922	1929	rBV2	1062295	1596946	37.41%	3.819%
15	14.804	1986	1992	1998	rBV7	26903	57796	1.35%	0.138%
16	15.174	2050	2055	2060	rBV6	20920	42937	1.01%	0.103%
17	15.886	2170	2176	2184	rVB	1425041	1957081	45.85%	4.680%
18	16.121	2208	2216	2219	rBV8	22346	62465	1.46%	0.149%
19	16.174	2219	2225	2229	rVB4	44868	82977	1.94%	0.198%
20	16.433	2259	2269	2274	rBV8	28189	74202	1.74%	0.177%
21	16.533	2282	2286	2291	rVB6	56518	87018	2.04%	0.208%
22	17.139	2383	2389	2395	rBV2	1333801	1989908	46.62%	4.759%
23	17.186	2395	2397	2400	rVB	46976	45891	1.08%	0.110%
24	17.804	2498	2502	2510	rVB3	59336	85174	2.00%	0.204%
25	18.033	2533	2541	2557	rBV	2030159	3282822	76.91%	7.851%
26	18.321	2587	2590	2594	rVV2	73564	94982	2.23%	0.227%
27	18.362	2595	2597	2612	rVB2	71982	141858	3.32%	0.339%
28	18.503	2617	2621	2629	rVB3	47130	96623	2.26%	0.231%
29	18.933	2691	2694	2700	rBV4	44585	89420	2.09%	0.214%
30	19.115	2722	2725	2730	rVB	140033	164037	3.84%	0.392%
31	19.198	2732	2739	2746	rBV2	237171	519409	12.17%	1.242%
32	19.321	2754	2760	2777	rVB	2812174	4268296	100.00%	10.208%
33	19.568	2799	2802	2811	rVB	117043	187251	4.39%	0.448%
34	19.774	2832	2837	2842	rBV	2891289	3504698	82.11%	8.381%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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	21.033	3047	3051	3057	rBV	407223	473987	11.10%	1.134%
36	21.333	3097	3102	3106	rBV	2177654	2719461	63.71%	6.504%
37	21.909	3197	3200	3203	rBV	191878	213873	5.01%	0.511%
38	22.380	3276	3280	3285	rBV	421701	547042	12.82%	1.308%
39	22.509	3299	3302	3306	rVB	212083	255641	5.99%	0.611%
40	22.891	3363	3367	3373	rBV	484289	797789	18.69%	1.908%
41	23.468	3461	3465	3470	rBV	488604	747808	17.52%	1.788%
42	23.609	3483	3489	3497	rVB2	1424074	2712438	63.55%	6.487%
43	24.127	3572	3577	3586	rVB	409864	829414	19.43%	1.984%

Sum of corrected areas: 41814983

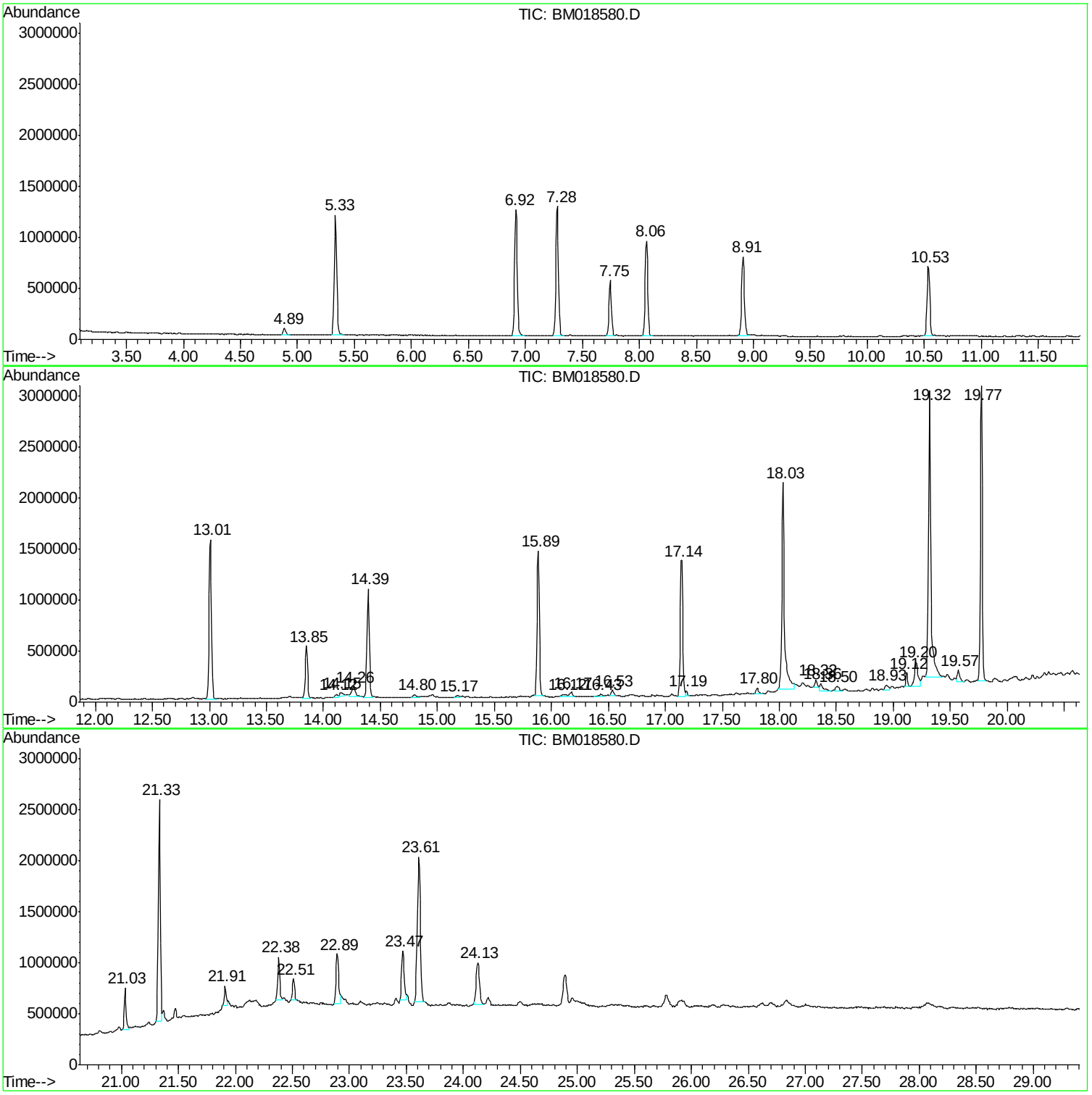
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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

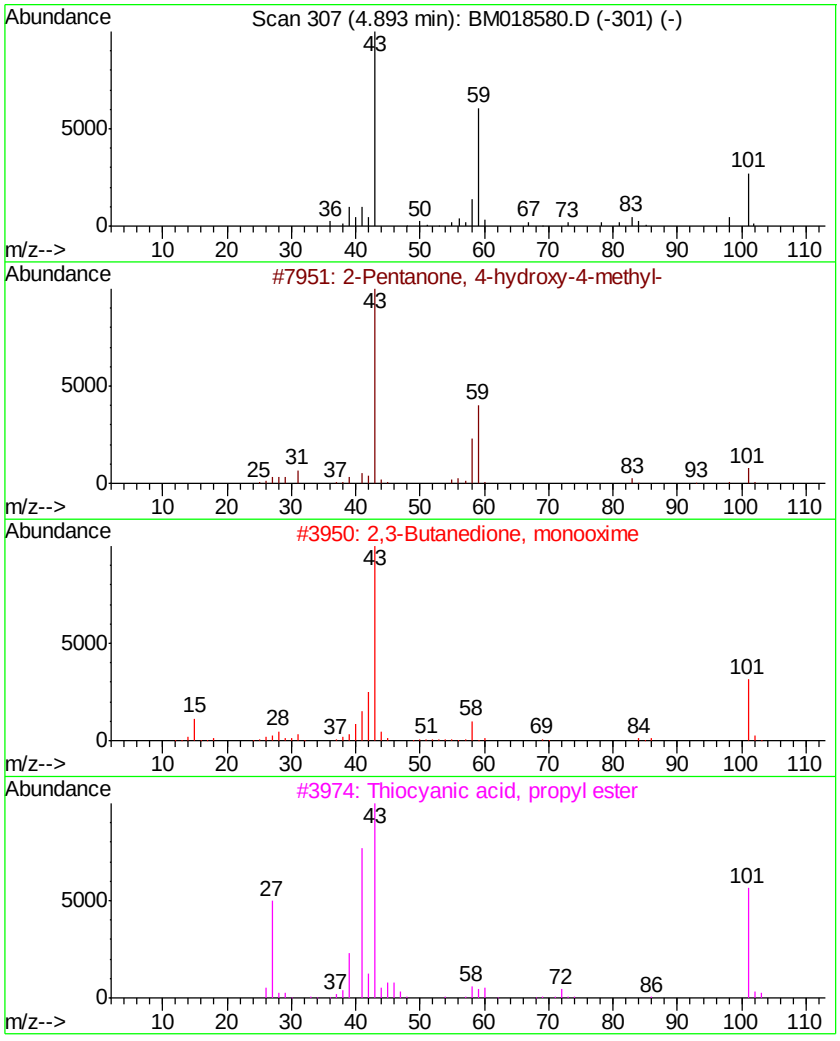
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

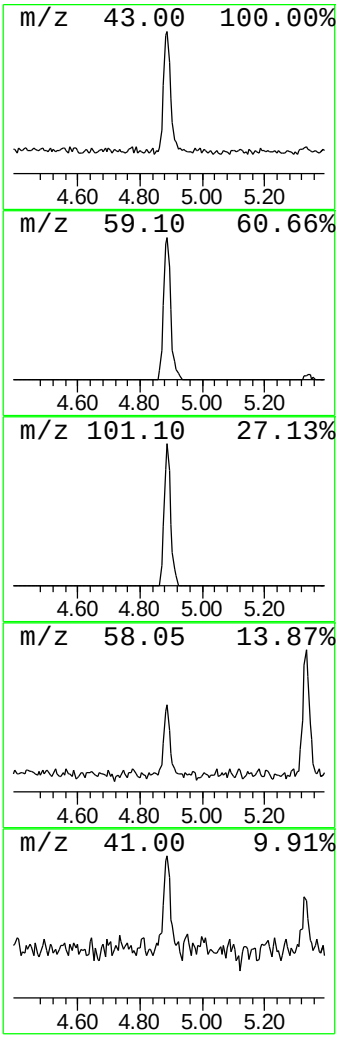
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.57 ng	108103	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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

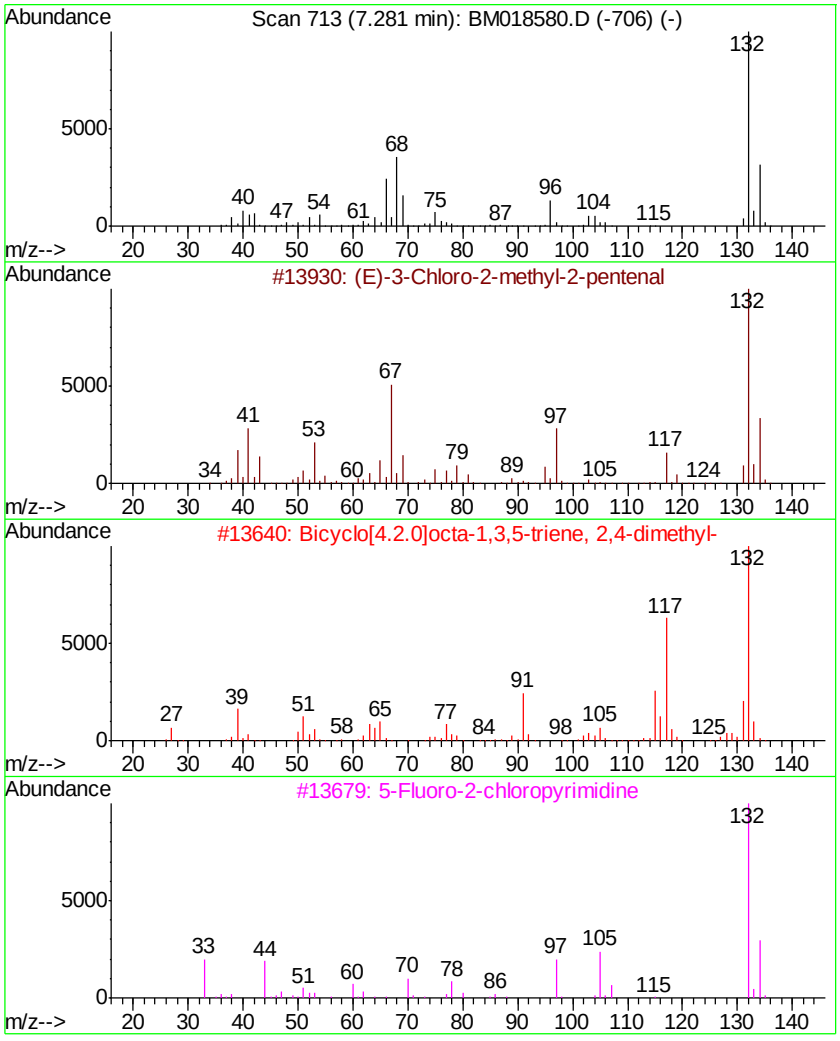
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

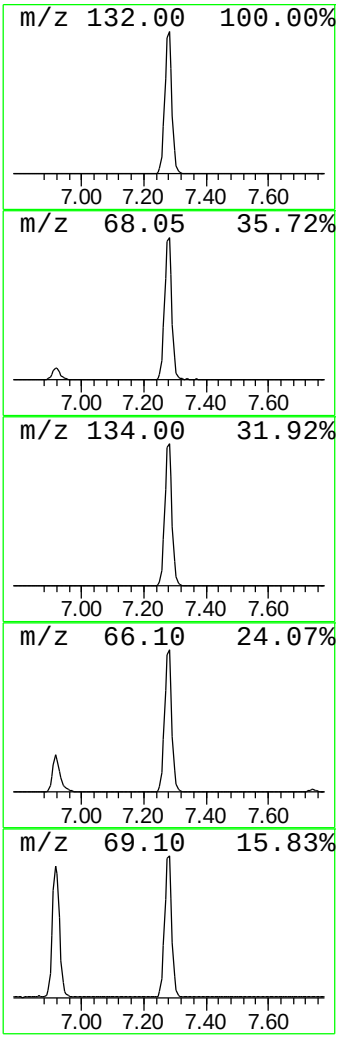
****

Peak Number 2 unknown7.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	48.46 ng	2041140	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	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\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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

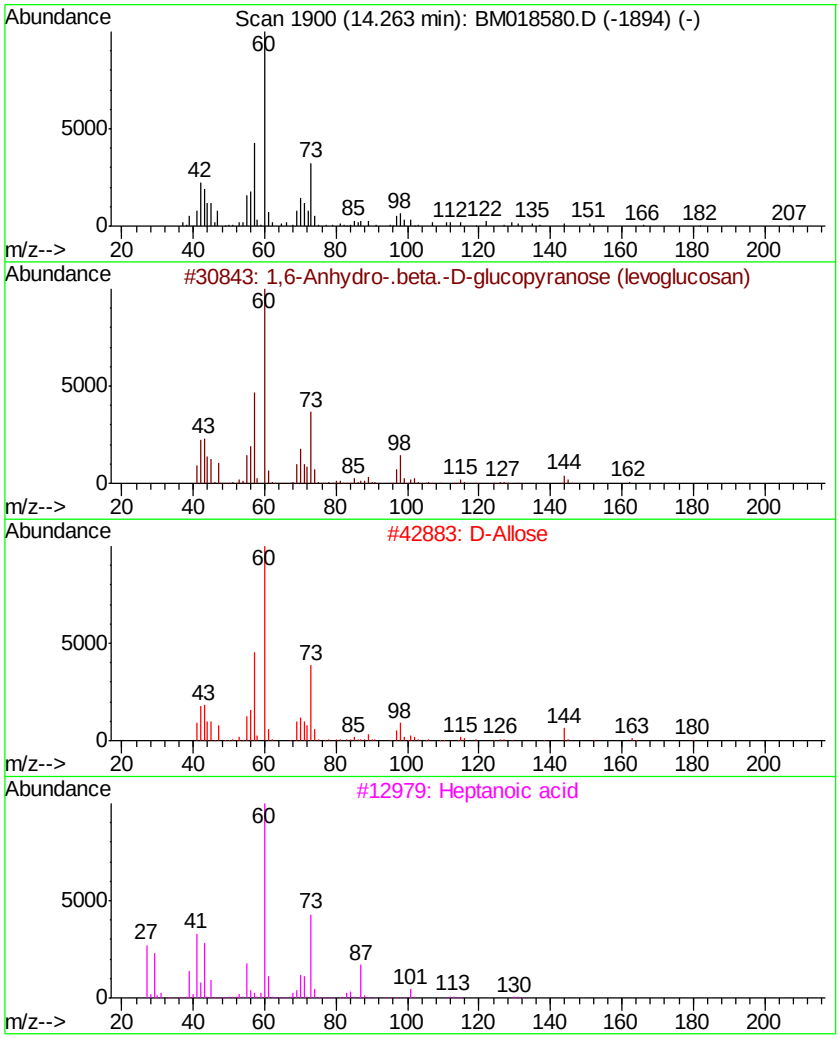
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

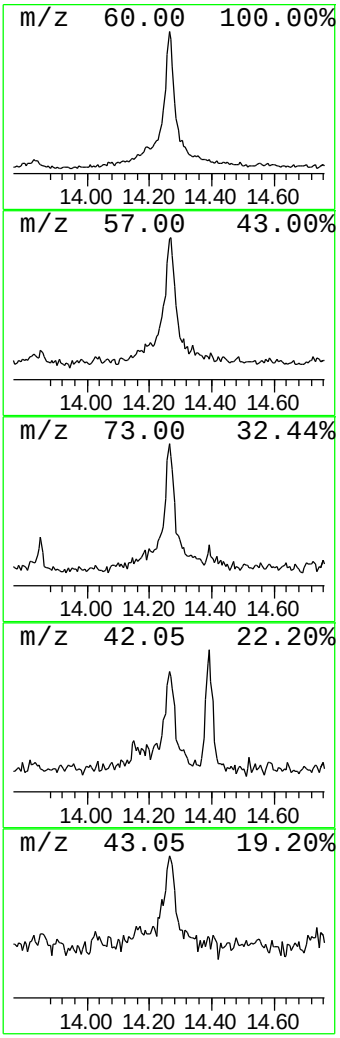
****

Peak Number 4 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	3.11 ng	248363	Acenaphthene-d10	14.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	90
2	D-Allose	180	C6H12O6	002595-97-3	80
3	Heptanoic acid	130	C7H14O2	000111-14-8	45
4	.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	45
5	D-Galactose, 6-deoxy-	164	C6H12O5	003615-37-0	45





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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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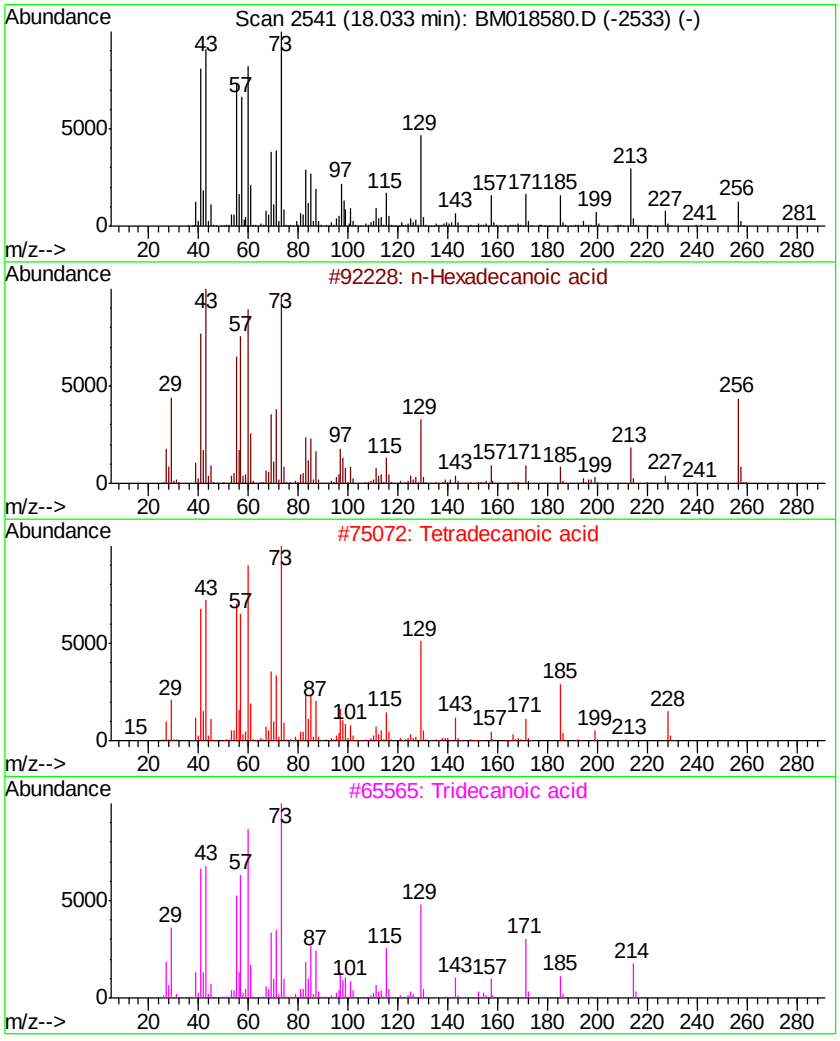
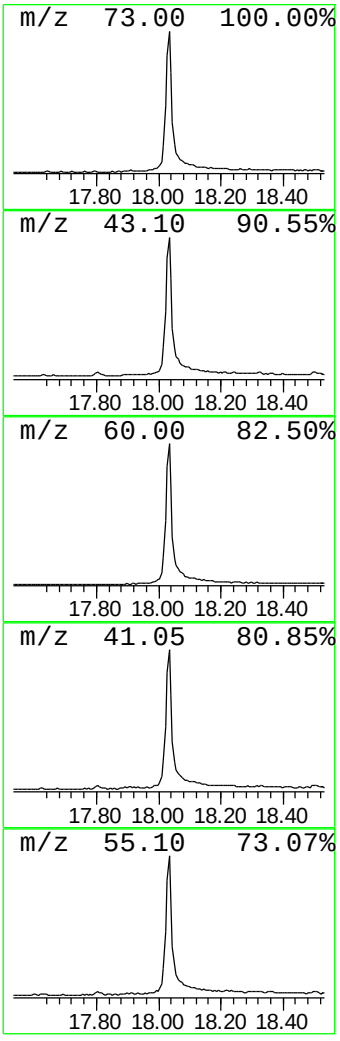
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	32.99 ng	3282820	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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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

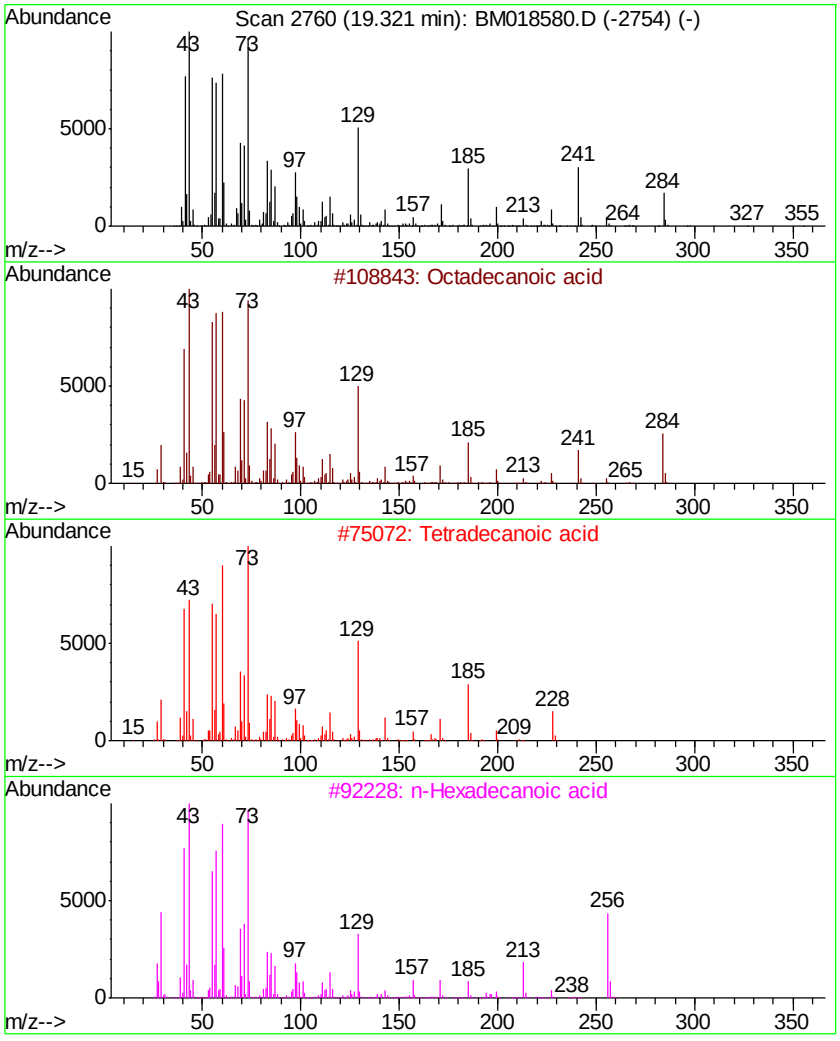
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

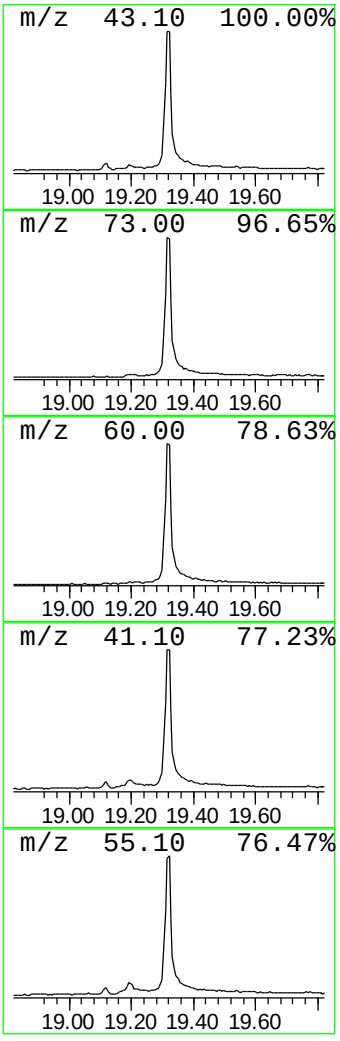
****

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	31.39 ng	4268300	Chrysene-d12	21.33

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	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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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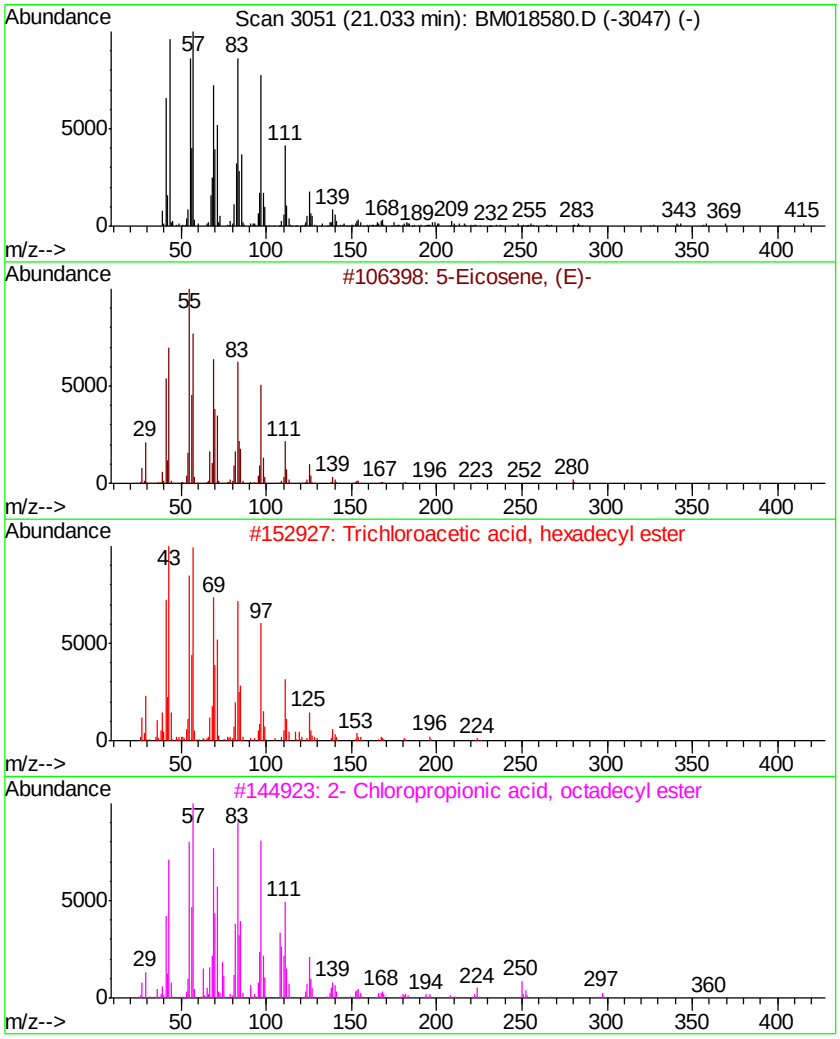
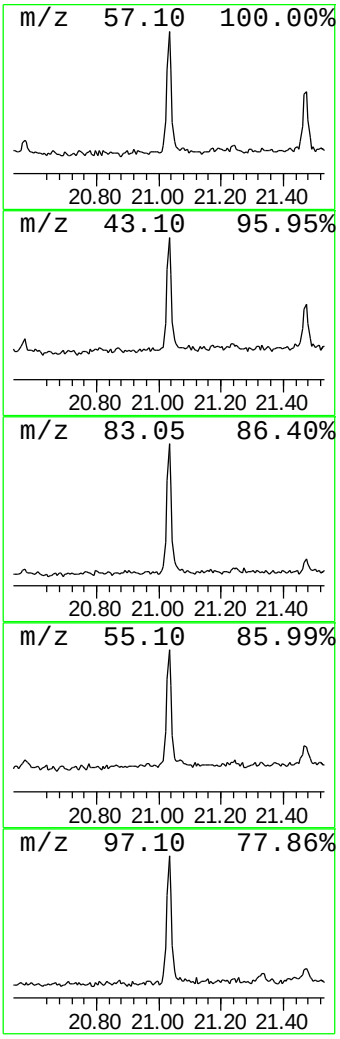
Peak Number 8 5-Eicosene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	3.49 ng	473987	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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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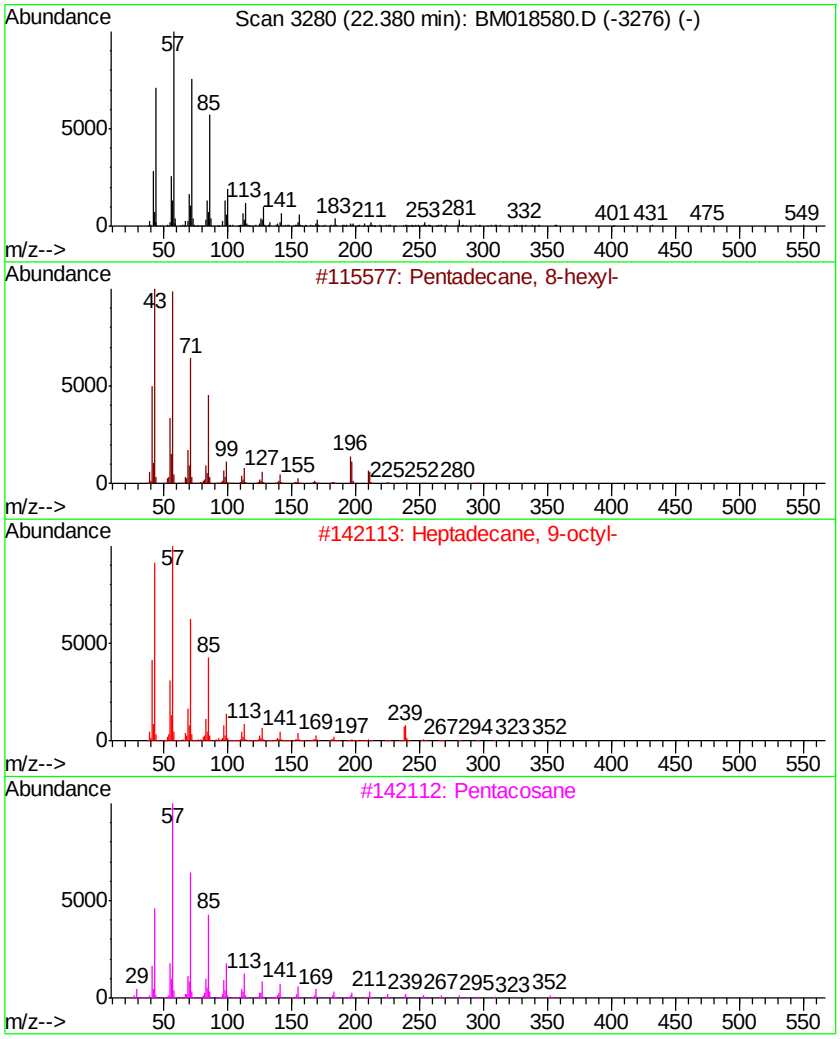
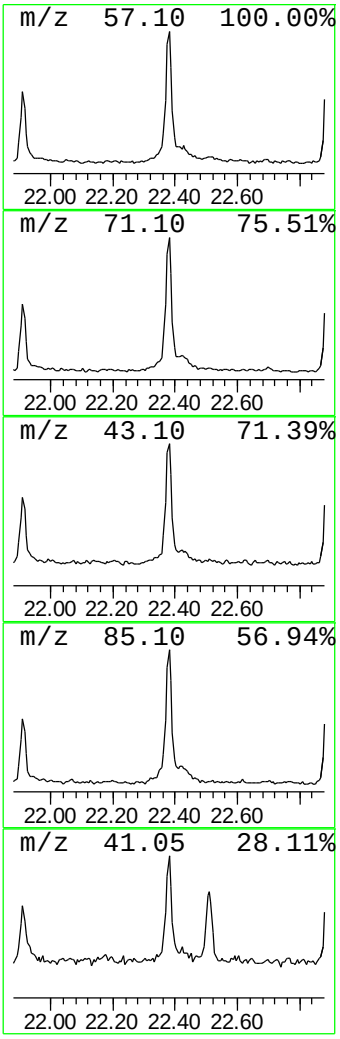
Peak Number 9 Pentadecane, 8-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.38	4.02 ng	547042	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	96
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane	240	C17H36	000629-78-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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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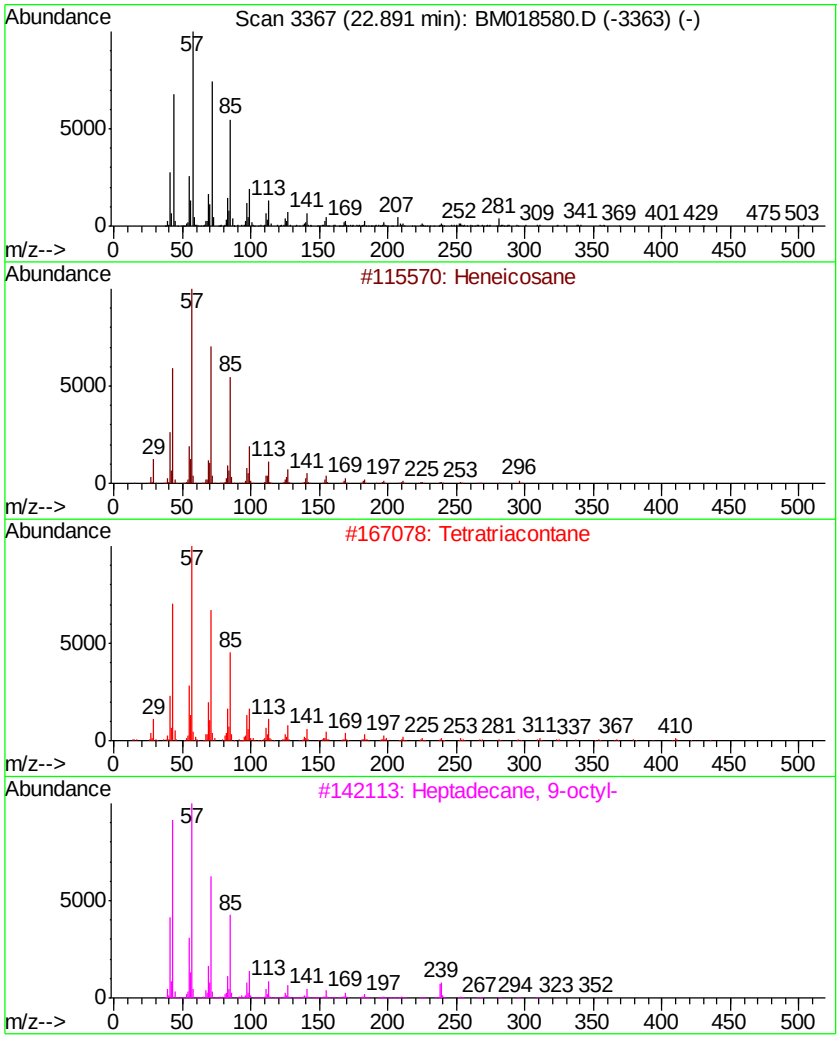
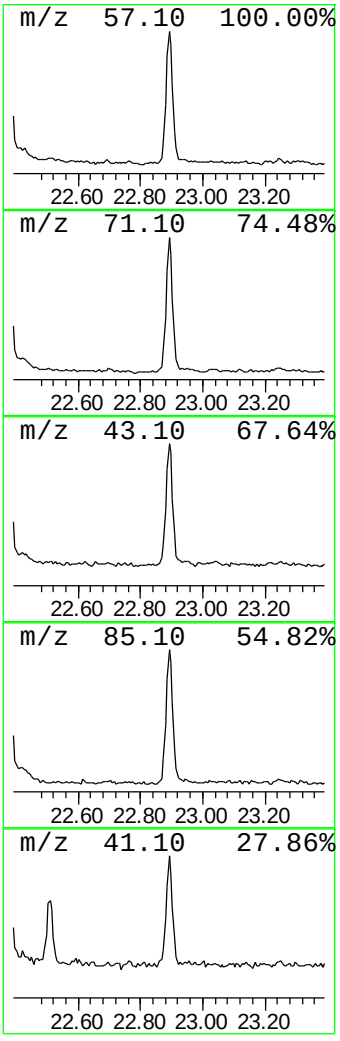
Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.89	5.88 ng	797789	Perylene-d12	23.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Tetratriacontane	479	C34H70	014167-59-0	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
5	Tetracosane	338	C24H50	000646-31-1	87





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Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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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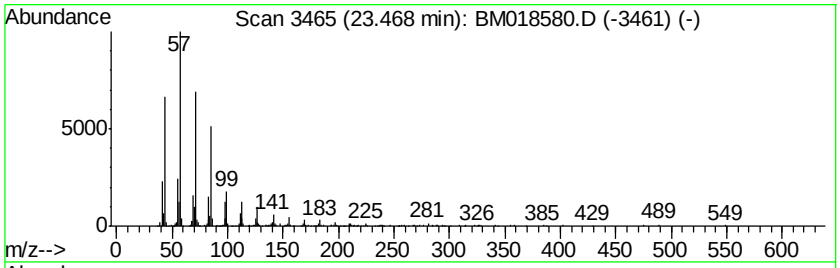
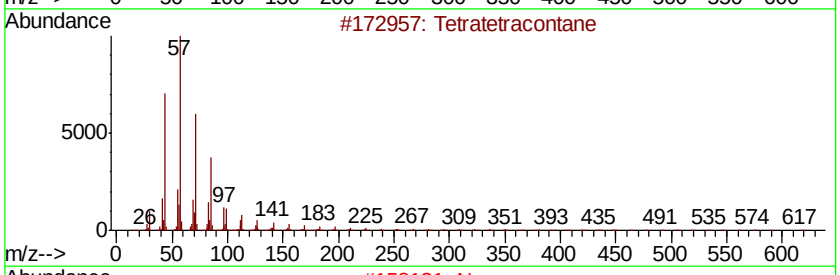
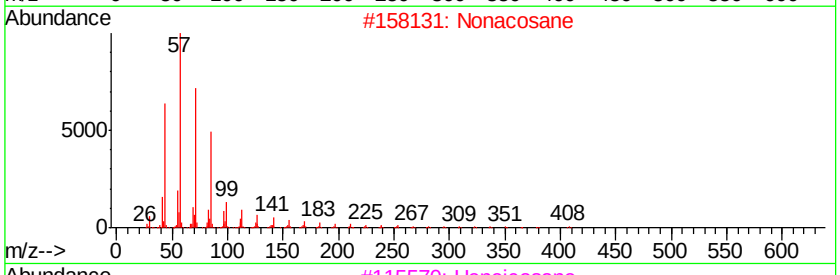
Peak Number 11 Tetratetracontane Concentration Rank 7

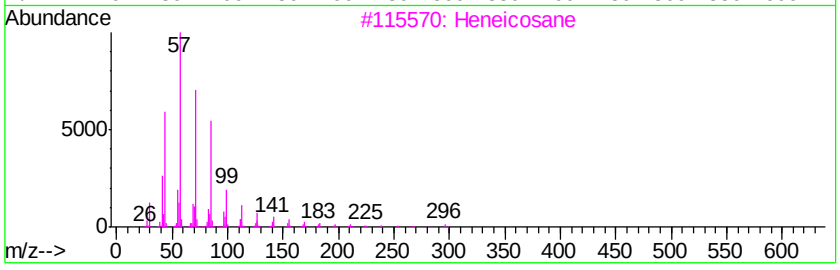
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.47	5.51 ng	747808	Perylene-d12	23.61

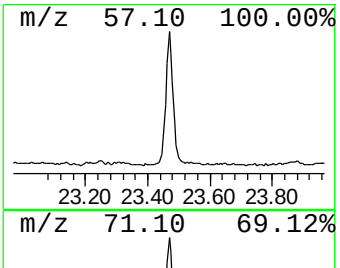
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Nonacosane	408	C29H60	000630-03-5	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91

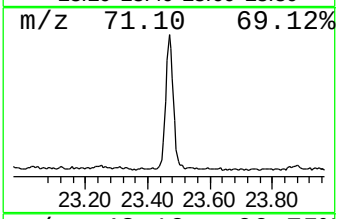


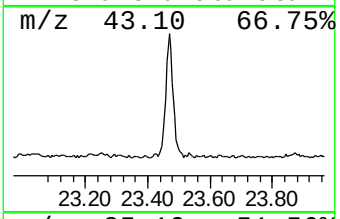


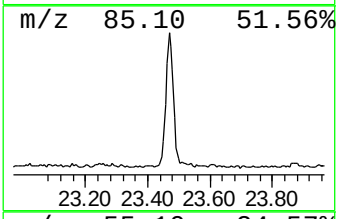


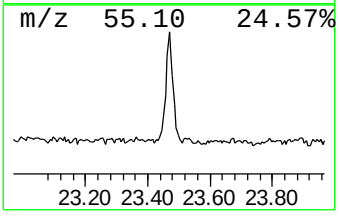












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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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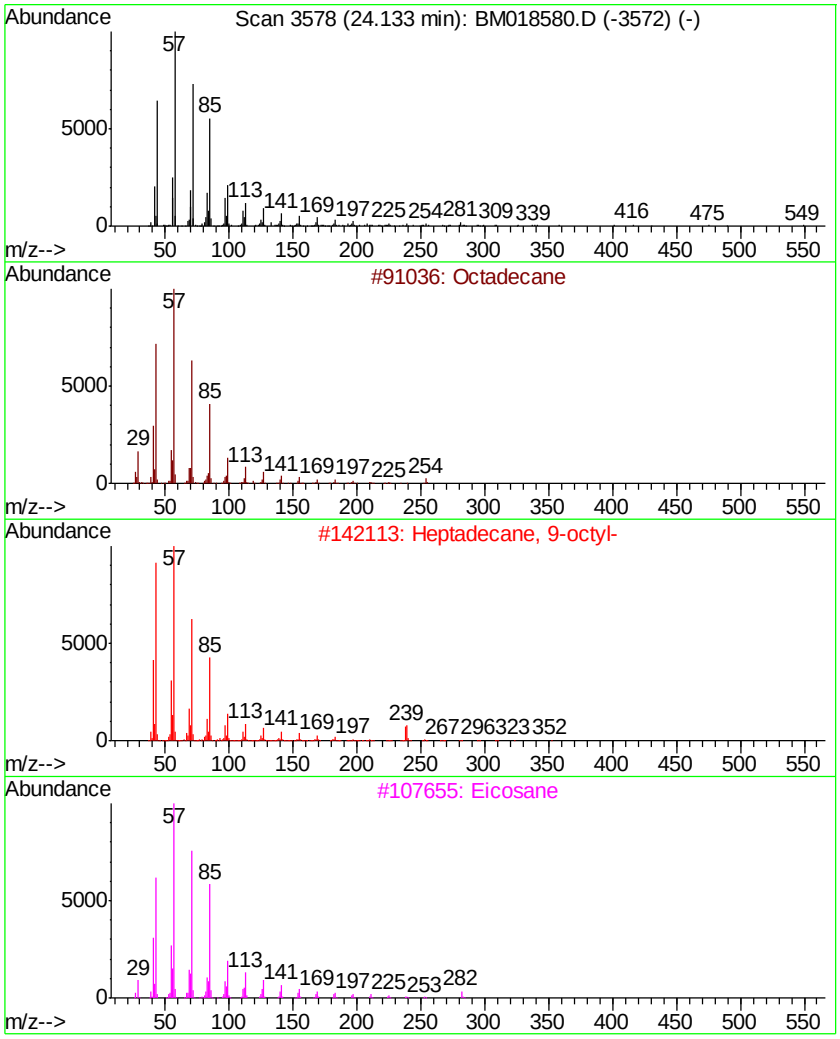
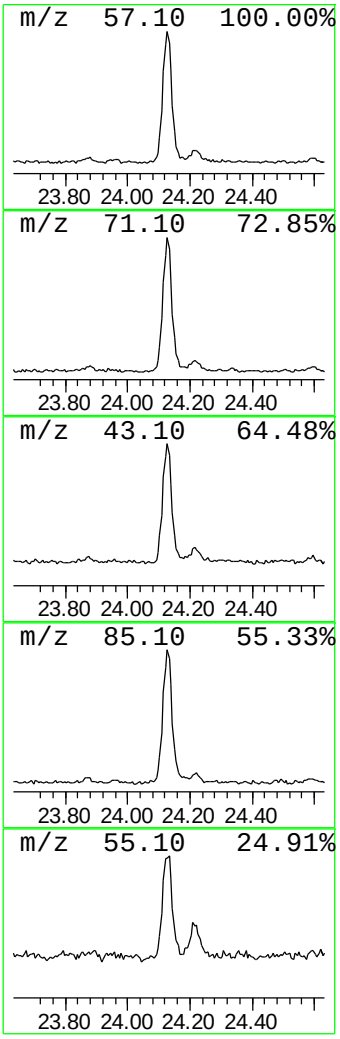
Peak Number 12 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.13	6.12 ng	829414	Perylene-d12	23.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM011619\
Data File : BM018580.D
Acq On : 16 Jan 2019 12:37
Operator : JU/SJ
Sample : K1139-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : S-2

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...	4.89	2.6	ng	108103	1	7.75	842391	20.0
unknown7.28	7.28	48.5	ng	2041140	1	7.75	842391	20.0
1,6-Anhydro-.beta...	14.26	3.1	ng	248363	3	14.39	1596950	20.0
n-Hexadecanoic acid	18.03	33.0	ng	3282820	4	17.14	1989910	20.0
Octadecanoic acid	19.32	31.4	ng	4268300	5	21.33	2719460	20.0
5-Eicosene, (E)-	21.03	3.5	ng	473987	5	21.33	2719460	20.0
Pentadecane, 8-he...	22.38	4.0	ng	547042	5	21.33	2719460	20.0
Heneicosane	22.89	5.9	ng	797789	6	23.61	2712440	20.0
Tetratetracontane	23.47	5.5	ng	747808	6	23.61	2712440	20.0
Octadecane	24.13	6.1	ng	829414	6	23.61	2712440	20.0