LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
Data File : BM018860.D
Acq On : 19 Feb 2019 17:11
Operator : JU/SJ
Sample : K1515-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TS-7

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-BM021119.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	4.857	296	301	315	rVB	308871	448762	2.31%	0.365%
2	5.299	369	376	393	rBV	7596687	10819326	55.76%	8.800%
3	6.881	637	645	661	rBV	7132480	11807642	60.86%	9.604%
4	7.240	698	706	722	rBV	7713112	11911511	61.39%	9.689%
5	7.704	778	785	792	rBV	1267837	1951357	10.06%	1.587%
6	8.022	831	839	850	rBV	5388443	8456478	43.58%	6.878%
7	8.875	975	984	1001	rBV	4205852	7009101	36.12%	5.701%
8	10.492	1252	1259	1274	rBV	1550585	2629490	13.55%	2.139%
9	12.969	1673	1680	1697	rBV	10292907	14816117	76.36%	12.051%
10	13.816	1817	1824	1842	rBV	408448	657044	3.39%	0.534%
11	14.351	1904	1915	1933	rBV2	2095209	3326903	17.15%	2.706%
12	15.851	2163	2170	2189	rBV	8043479	11520607	59.38%	9.371%
13	17.104	2377	2383	2397	rBV	2684909	3852838	19.86%	3.134%
14	17.992	2527	2534	2545	rBV	796383	1230977	6.34%	1.001%
15	19.280	2748	2753	2771	rBV	397460	706354	3.64%	0.575%
16	19.739	2825	2831	2846	rBV	16309980	19402478	100.00%	15.782%
17	21.003	3041	3046	3054	rBV	523938	759134	3.91%	0.617%
18	21.298	3091	3096	3106	rBV	3141152	3944504	20.33%	3.208%
19	21.439	3116	3120	3126	rBV	379907	434538	2.24%	0.353%
20	21.868	3190	3193	3201	rBV	573211	661867	3.41%	0.538%
21	22.333	3268	3272	3281	rVB	714863	889375	4.58%	0.723%
22	22.839	3354	3358	3364	rBV	608038	882561	4.55%	0.718%
23	23.409	3450	3455	3461	rBV	518785	819227	4.22%	0.666%
24	23.550	3473	3479	3489	rVB2	1773720	3269475	16.85%	2.659%
25	24.056	3561	3565	3575	rVB	389720	734681	3.79%	0.598%

Sum of corrected areas: 122942347

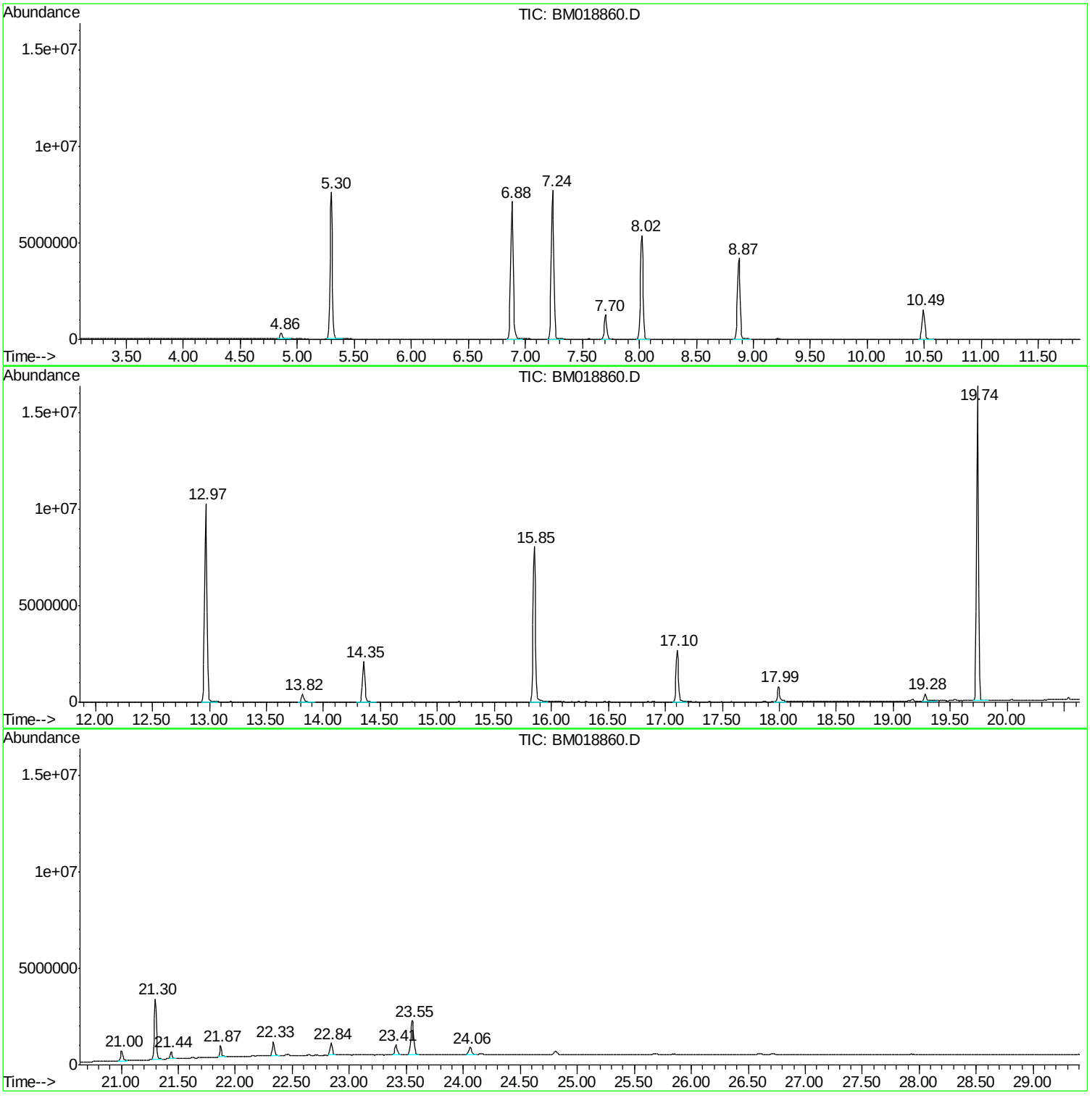
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
Data File : BM018860.D
Acq On : 19 Feb 2019 17:11
Operator : JU/SJ
Sample : K1515-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TS-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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\BM021919\
Data File : BM018860.D
Acq On : 19 Feb 2019 17:11
Operator : JU/SJ
Sample : K1515-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TS-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

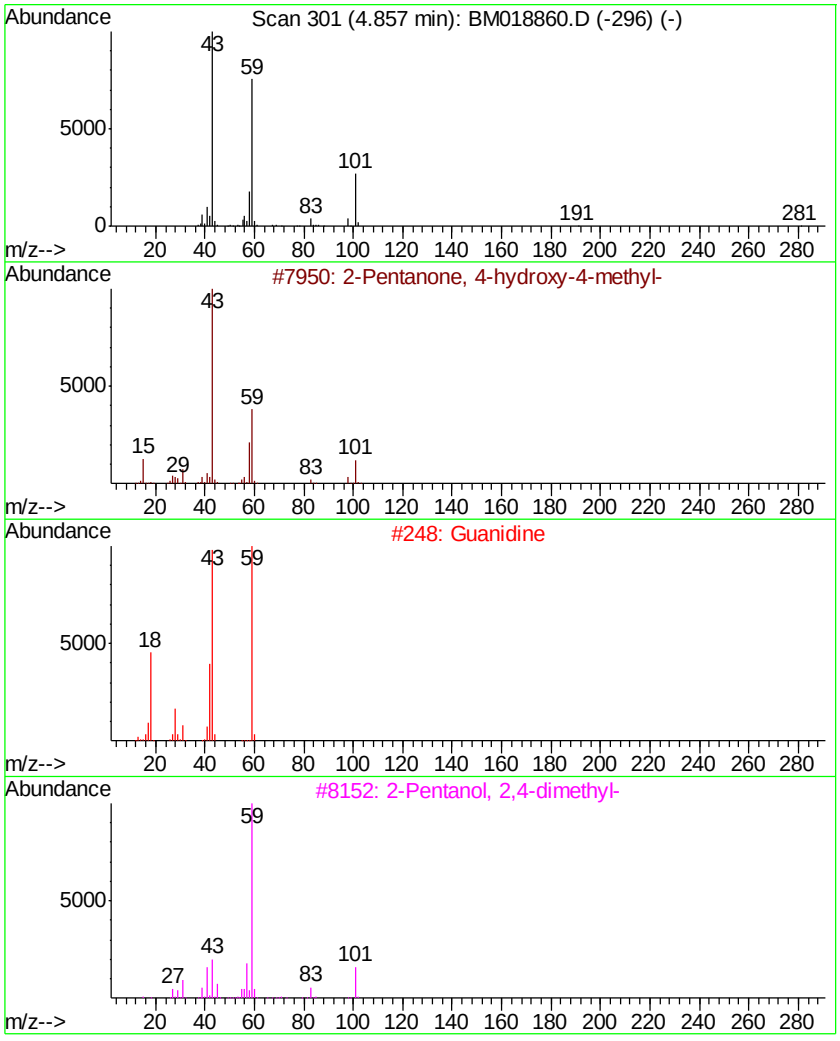
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

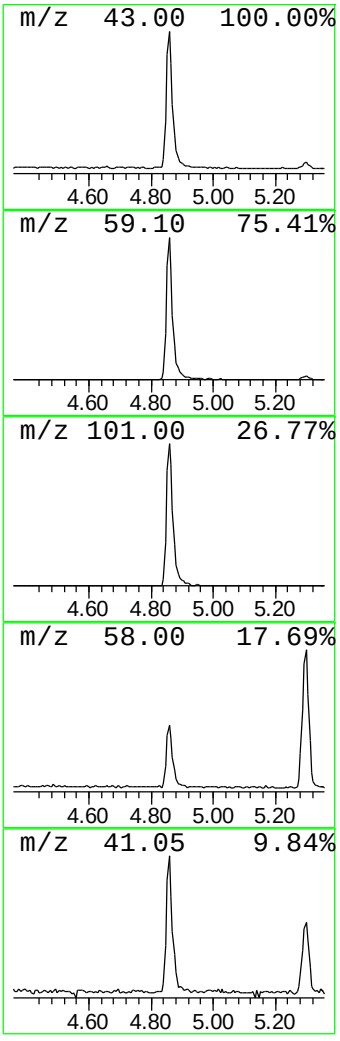
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	4.60 ng	448762	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	50
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	42
5	Dimethadione	129	C5H7NO3	000695-53-4	36





Library Search Compound Report

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Data File : BM018860.D
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Operator : JU/SJ
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Misc :
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Instrument : BNA_M
ClientSampleId : TS-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

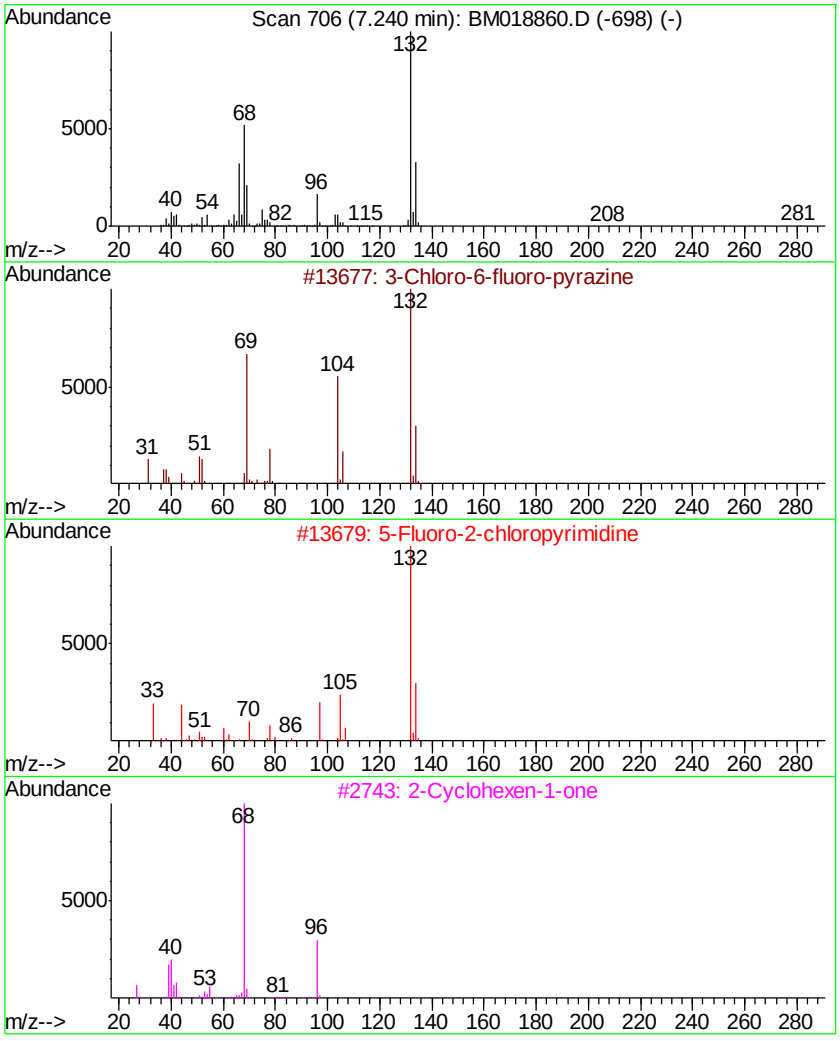
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

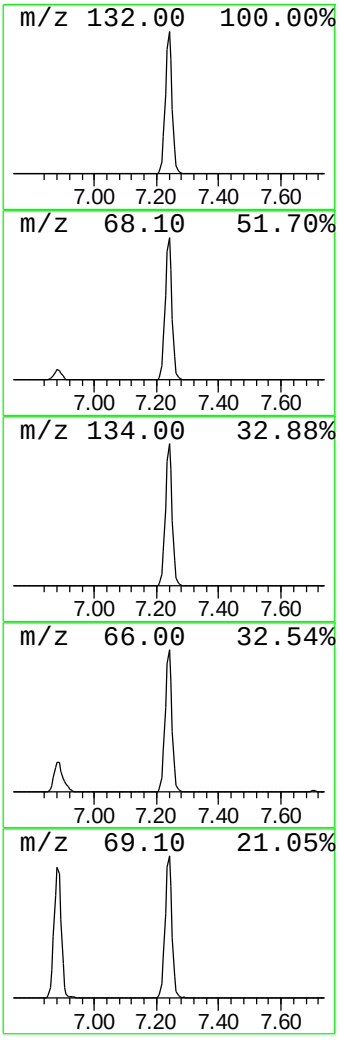
****

Peak Number 2 unknown7.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.24	122.08 ng	11911500	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

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Data File : BM018860.D
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Operator : JU/SJ
Sample : K1515-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TS-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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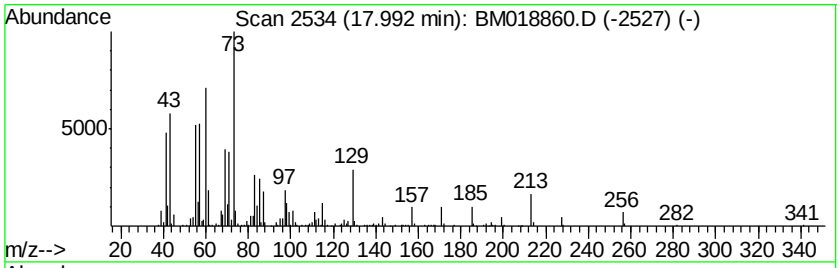
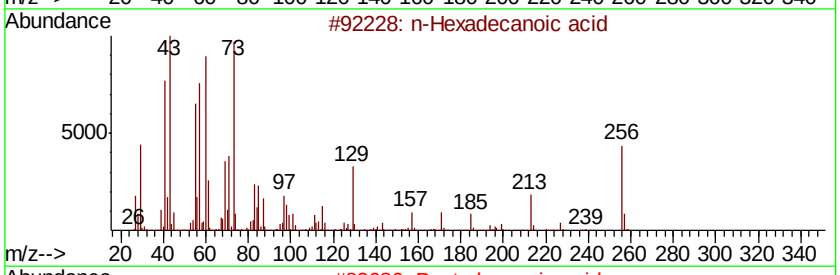
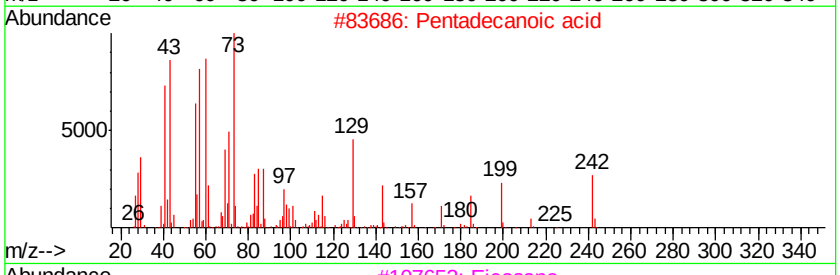
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

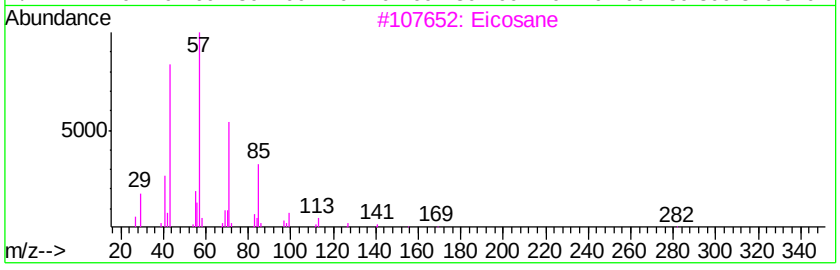
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	6.39 ng	1230980	Phenanthrene-d10	17.10

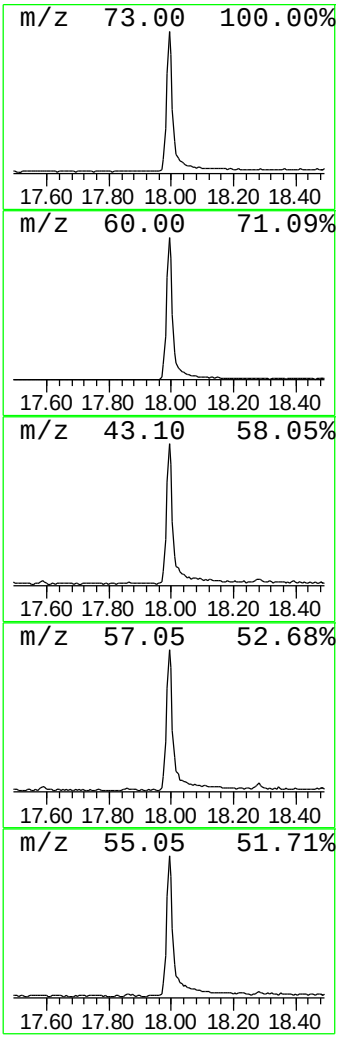
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Eicosane	282	C20H42	000112-95-8	60
4	Tridecanoic acid	214	C13H26O2	000638-53-9	55
5	d-Glucitol, 4-O-nonyl-	308	C15H32O6	132591-06-1	27











Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
Data File : BM018860.D
Acq On : 19 Feb 2019 17:11
Operator : JU/SJ
Sample : K1515-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TS-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

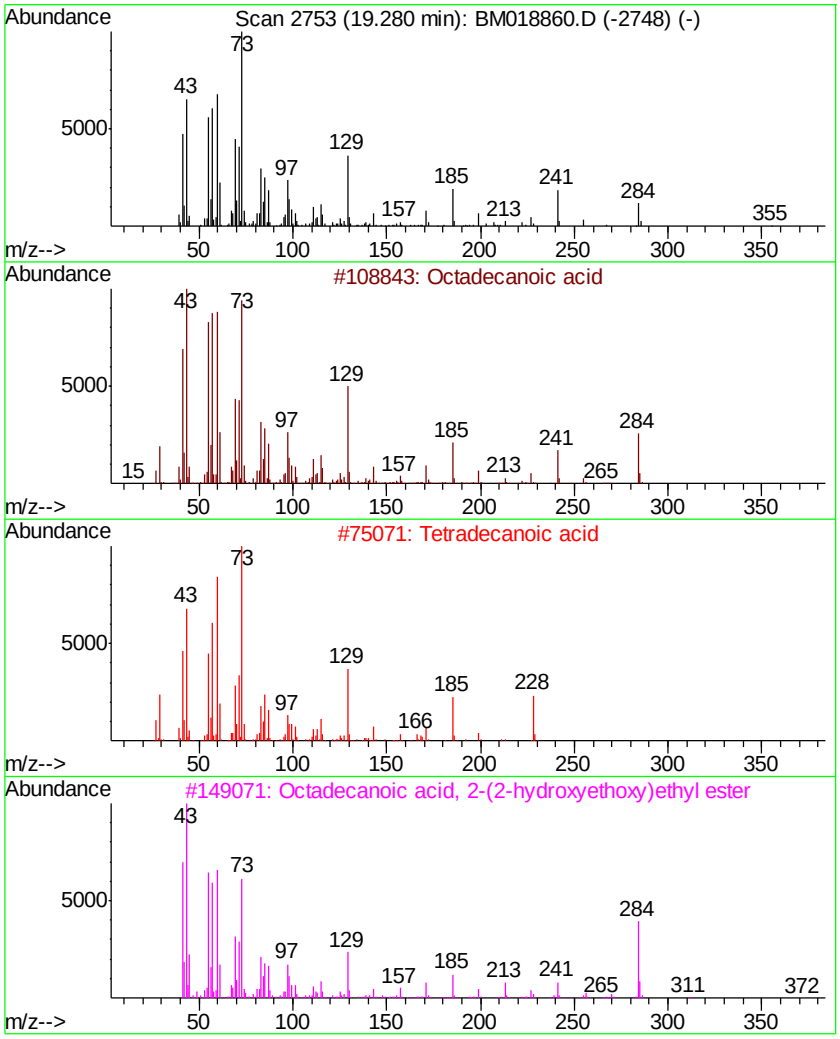
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

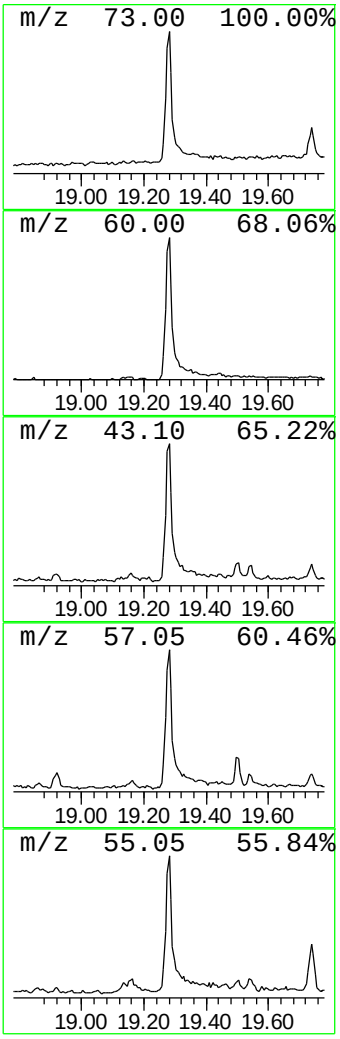
****

Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.28	3.58 ng	706354	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5	Dotriacontane	451	C32H66	000544-85-4	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021919\
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Instrument : BNA_M
ClientSampleId : TS-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
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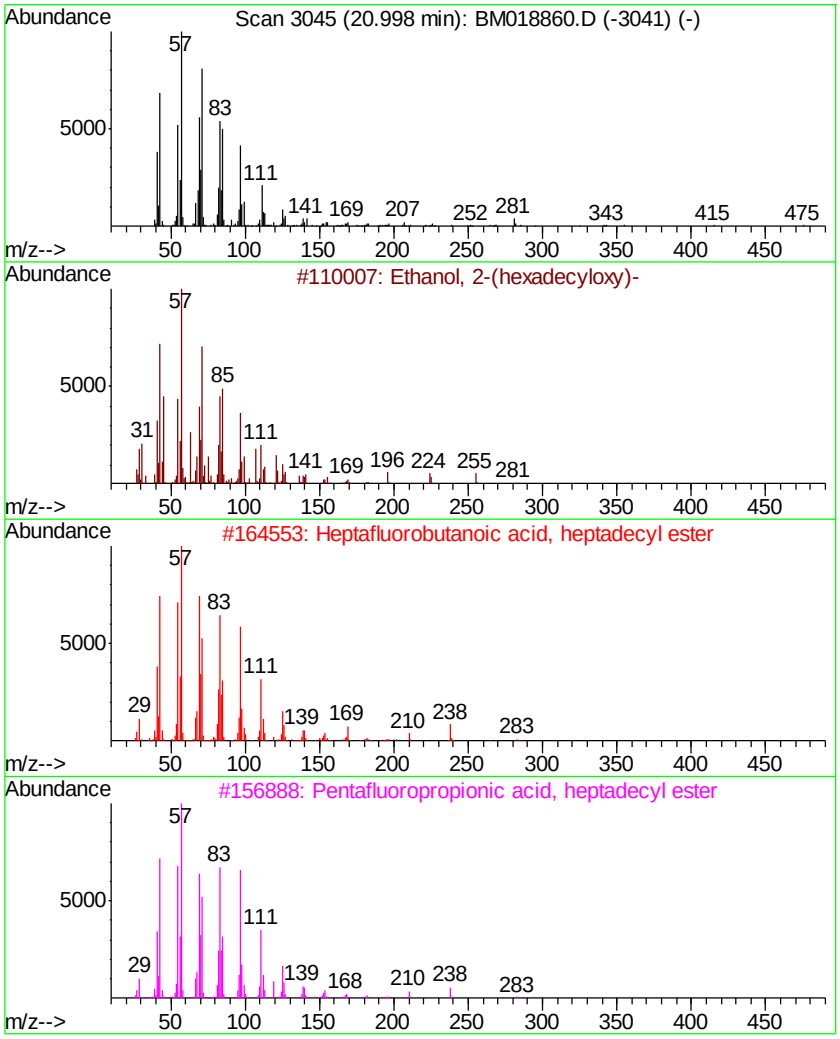
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

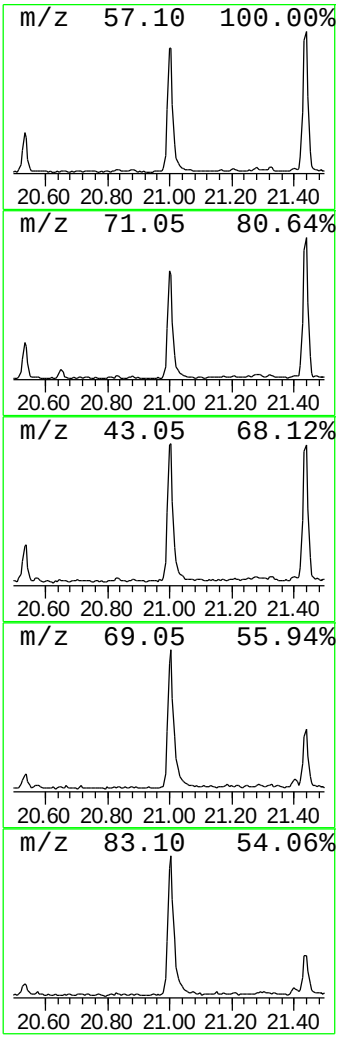
****

Peak Number 6 Ethanol, 2-(hexadecyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	3.85 ng	759134	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	86
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	76
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	68
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	68
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	68





Library Search Compound Report

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Sample : K1515-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TS-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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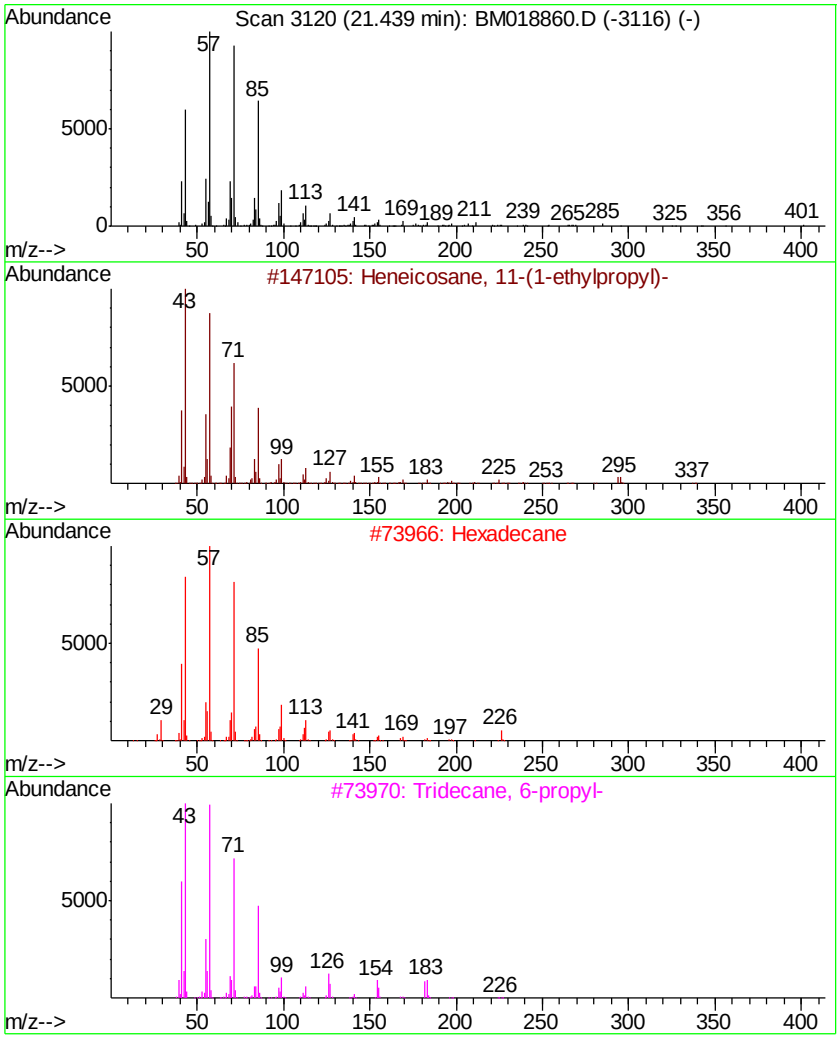
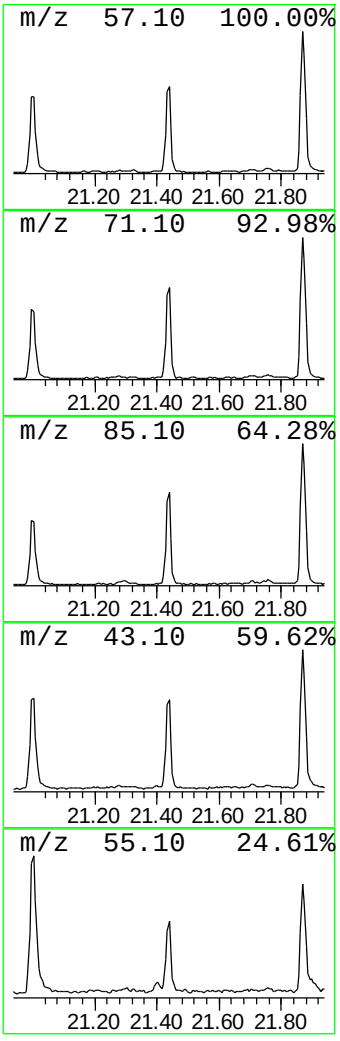
****

Peak Number 7 Heneicosane, 11-(1-ethylpro... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.44	2.20 ng	434538	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
4	Octadecane	254	C18H38	000593-45-3	87
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : TS-7

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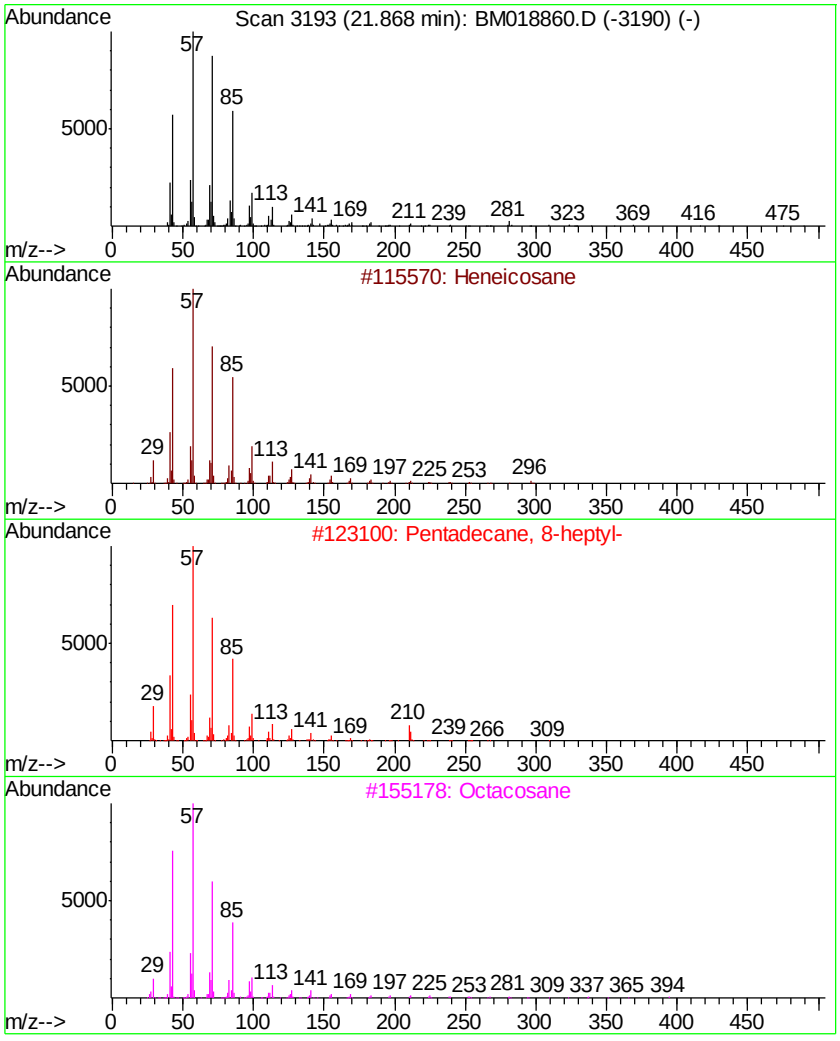
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

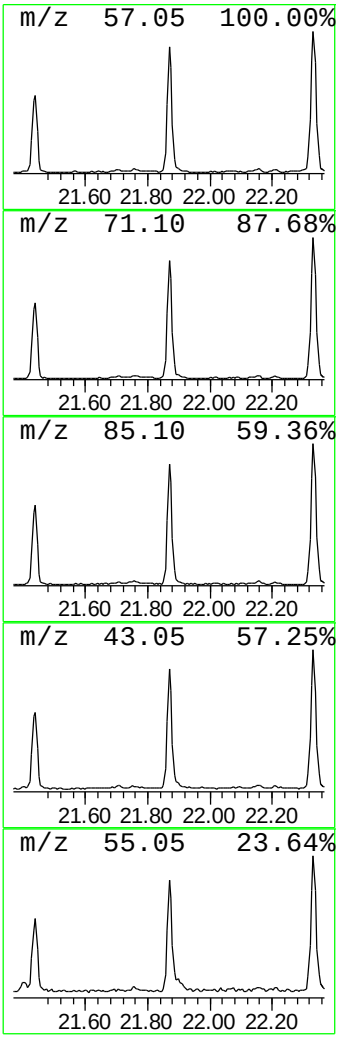
****

Peak Number 8 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.87	3.36 ng	661867	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	87





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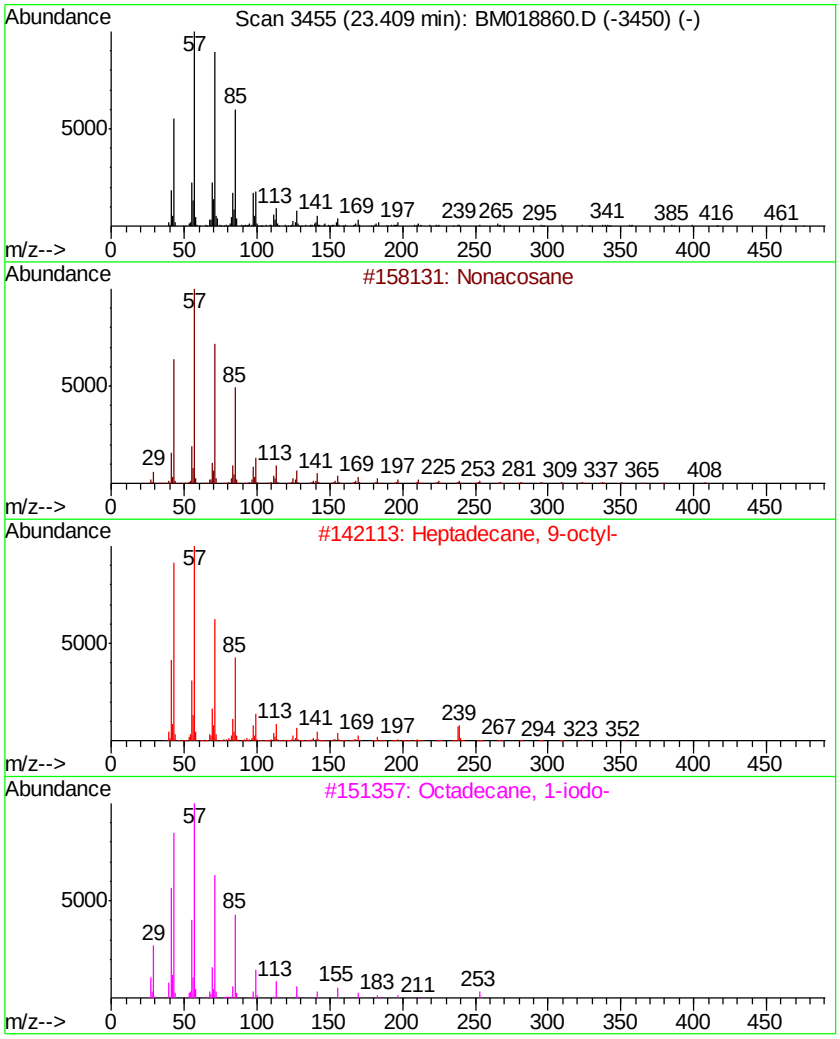
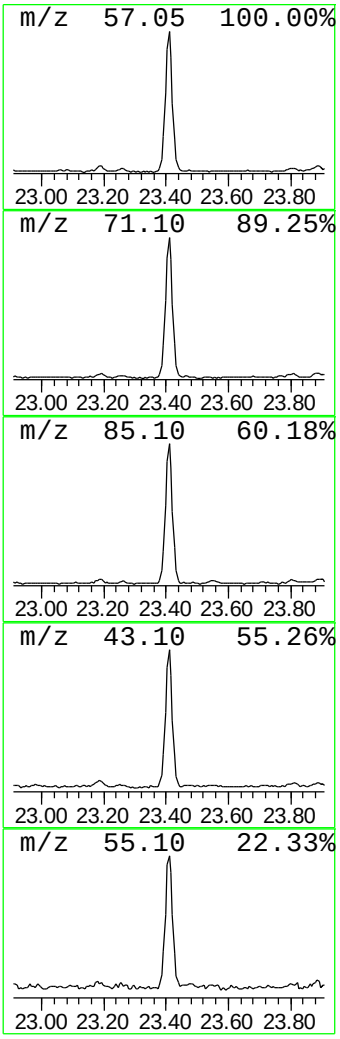
****

Peak Number 11 Nonacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.41	5.01 ng	819227	Perylene-d12	23.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosane	408	C29H60	000630-03-5	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
5	Octadecane	254	C18H38	000593-45-3	83





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Data File : BM018860.D
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Sample : K1515-07
Misc :
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Instrument : BNA_M
ClientSampleId : TS-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

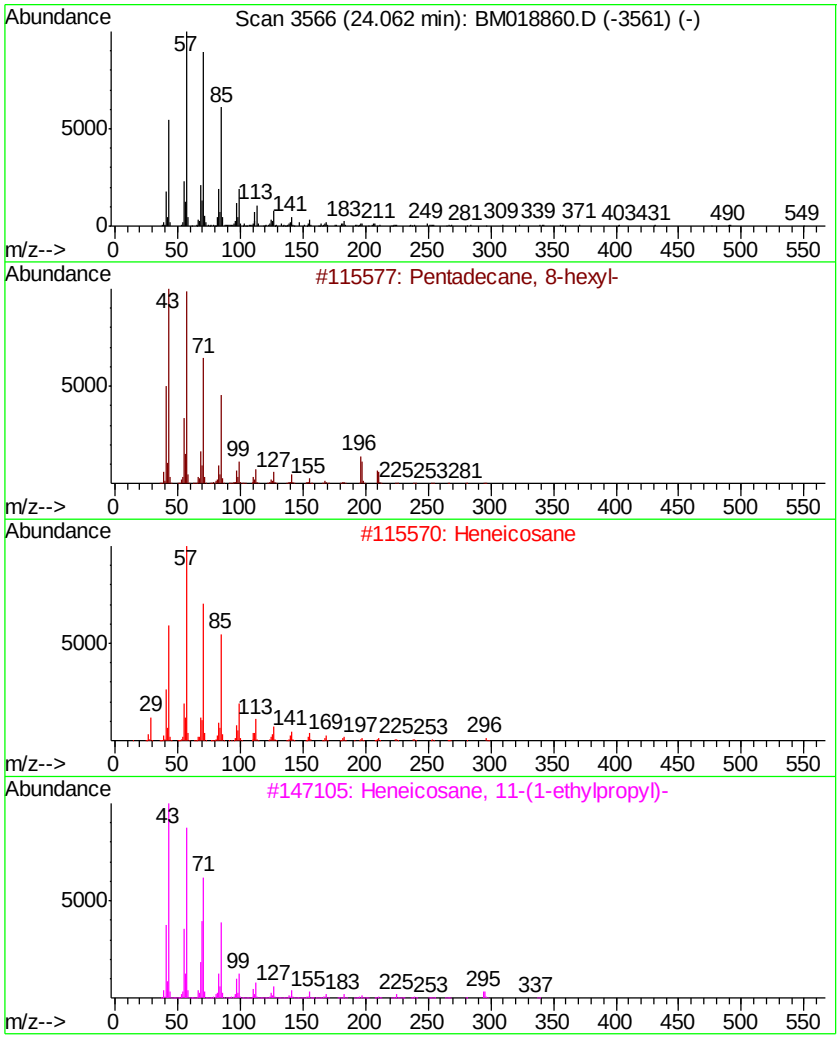
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

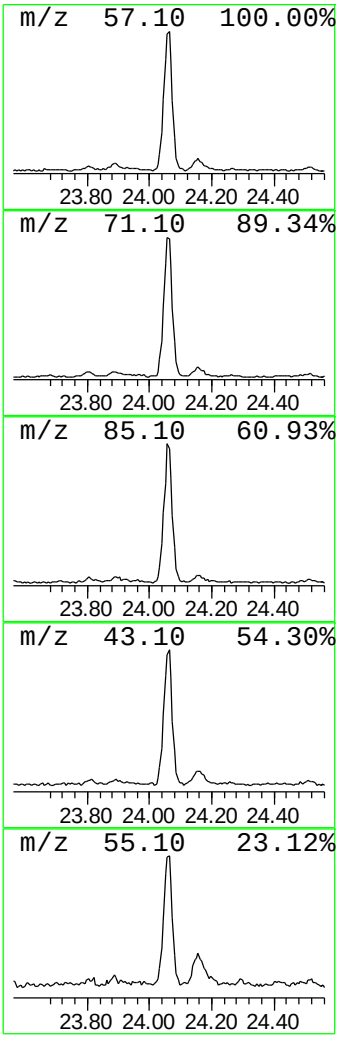
****

Peak Number 12 Pentadecane, 8-hexyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.06	4.49 ng	734681	Perylene-d12	23.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5	Docosane	310	C22H46	000629-97-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM021919\
Data File : BM018860.D
Acq On : 19 Feb 2019 17:11
Operator : JU/SJ
Sample : K1515-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TS-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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...	4.86	4.6	ng	448762	1	7.70	1951360	20.0
unknown7.24	7.24	122.1	ng	11911500	1	7.70	1951360	20.0
n-Hexadecanoic acid	17.99	6.4	ng	1230980	4	17.10	3852840	20.0
Octadecanoic acid	19.28	3.6	ng	706354	5	21.30	3944500	20.0
Ethanol, 2-(hexad...	21.00	3.9	ng	759134	5	21.30	3944500	20.0
Heneicosane, 11-(...	21.44	2.2	ng	434538	5	21.30	3944500	20.0
Heneicosane	21.87	3.4	ng	661867	5	21.30	3944500	20.0
Nonacosane	23.41	5.0	ng	819227	6	23.55	3269480	20.0
Pentadecane, 8-he...	24.06	4.5	ng	734681	6	23.55	3269480	20.0