LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
Data File : BM018840.D
Acq On : 18 Feb 2019 16:11
Operator : JU/SJ
Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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	297	301	313	rBV	280123	400384	2.72%	0.376%
2	5.298	369	376	391	rBV	6658178	9321353	63.34%	8.747%
3	6.881	638	645	660	rBV	6309736	10327707	70.17%	9.692%
4	7.239	699	706	722	rBV	6776277	10386596	70.57%	9.747%
5	7.704	778	785	793	rBV	1303201	2008191	13.65%	1.885%
6	8.022	832	839	850	rBV	4483107	7040021	47.84%	6.606%
7	8.875	976	984	999	rBV	3623002	6069713	41.24%	5.696%
8	10.492	1252	1259	1275	rBV	1646631	2753044	18.71%	2.584%
9	12.969	1673	1680	1696	rBV	7667873	11483029	78.02%	10.776%
10	13.816	1819	1824	1838	rBV	425254	695121	4.72%	0.652%
11	14.357	1908	1916	1929	rBV2	2271653	3531963	24.00%	3.314%
12	15.851	2163	2170	2194	rBV	6858387	10179523	69.17%	9.553%
13	17.104	2377	2383	2397	rBV2	2622692	4064426	27.62%	3.814%
14	17.992	2529	2534	2545	rBV	602109	956583	6.50%	0.898%
15	19.280	2748	2753	2762	rBV	292835	440031	2.99%	0.413%
16	19.739	2825	2831	2846	rBV	12186560	14717186	100.00%	13.811%
17	20.997	3042	3045	3054	rBV	427538	640161	4.35%	0.601%
18	21.297	3091	3096	3107	rBV	2828922	3689040	25.07%	3.462%
19	21.439	3116	3120	3126	rBV	391519	398446	2.71%	0.374%
20	21.868	3190	3193	3200	rBV	584613	712651	4.84%	0.669%
21	22.333	3268	3272	3281	rBV	788396	1069301	7.27%	1.003%
22	22.838	3354	3358	3363	rBV	703613	1005301	6.83%	0.943%
23	23.409	3451	3455	3461	rVB	587114	930818	6.32%	0.873%
24	23.556	3474	3480	3489	rVB2	1606579	3014585	20.48%	2.829%
25	24.062	3561	3566	3574	rVB	383528	727139	4.94%	0.682%

Sum of corrected areas: 106562313

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
Data File : BM018840.D
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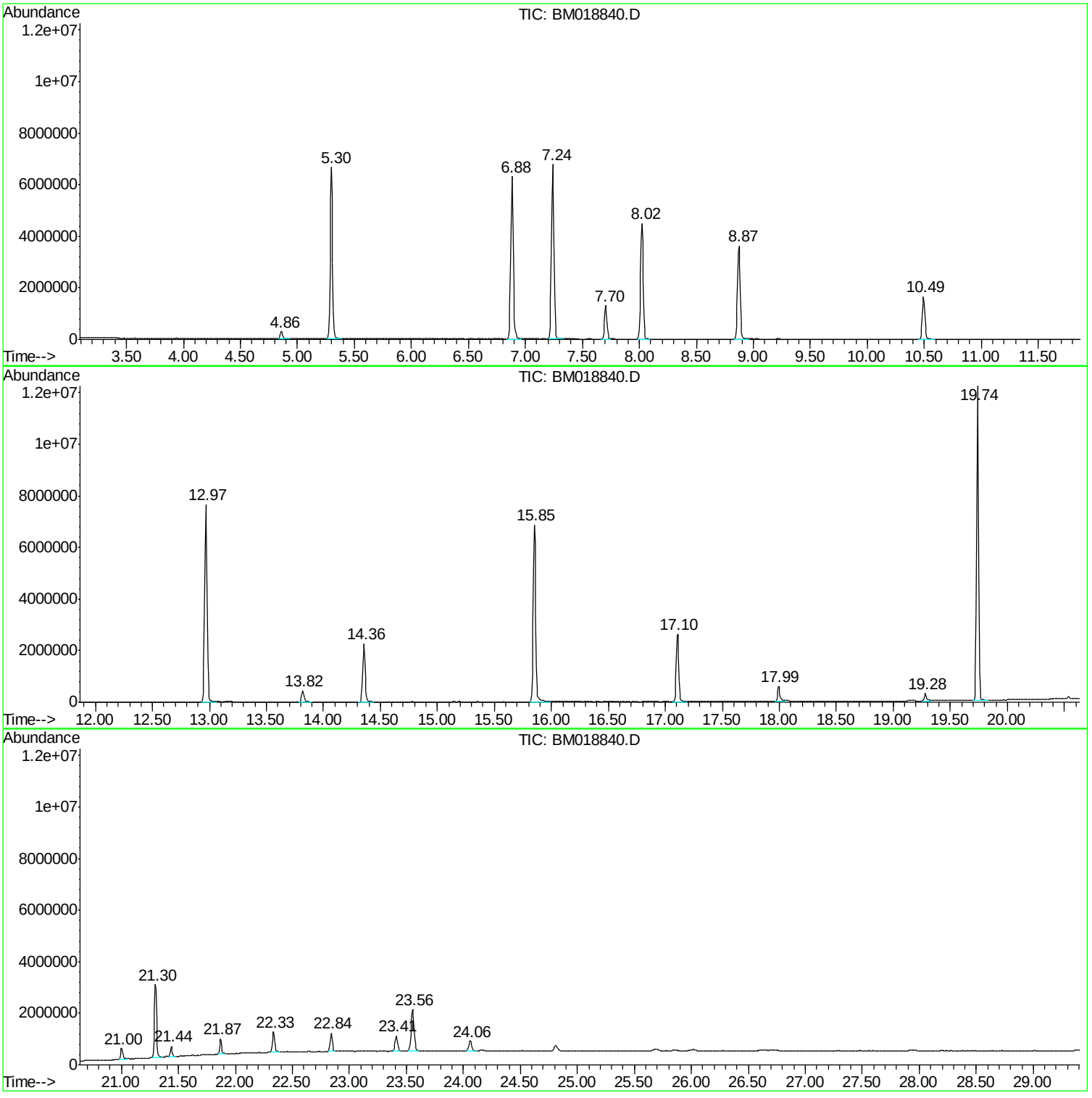
Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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

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Data File : BM018840.D
Acq On : 18 Feb 2019 16:11
Operator : JU/SJ
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Misc :
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Instrument : BNA_M
ClientSampleId : G-021519

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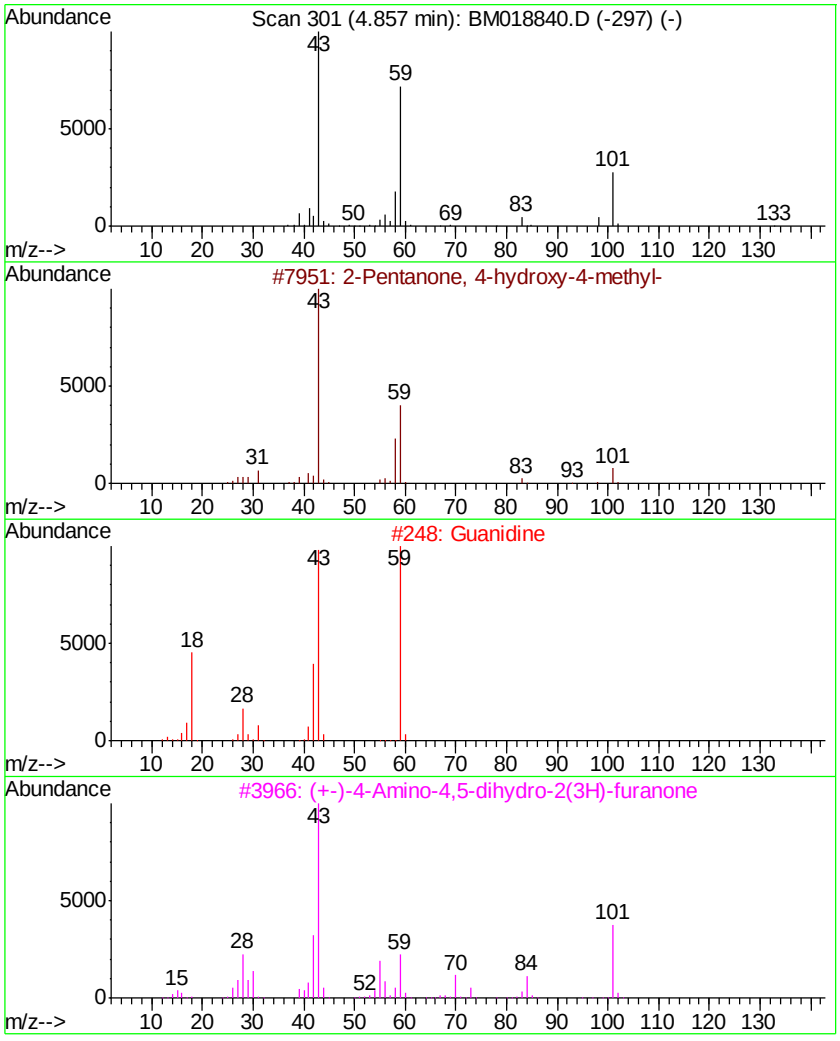
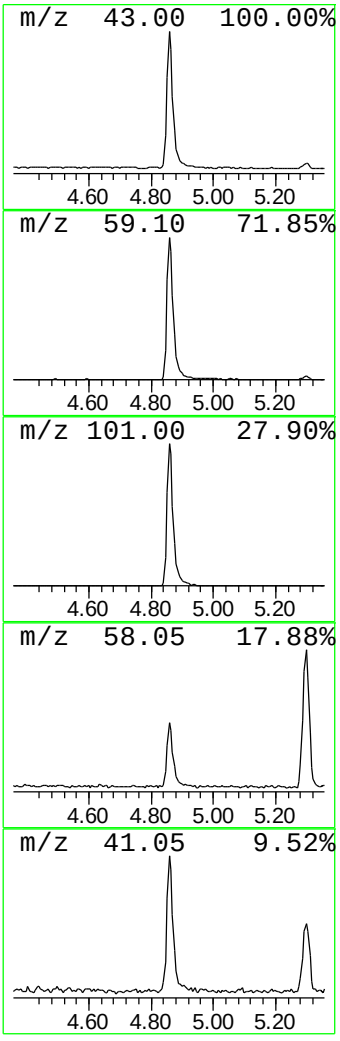
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	3.99 ng	400384	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	50
2	Guanidine	59	CH5N3	000113-00-8	43
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	10





Library Search Compound Report

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Data File : BM018840.D
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Operator : JU/SJ
Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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

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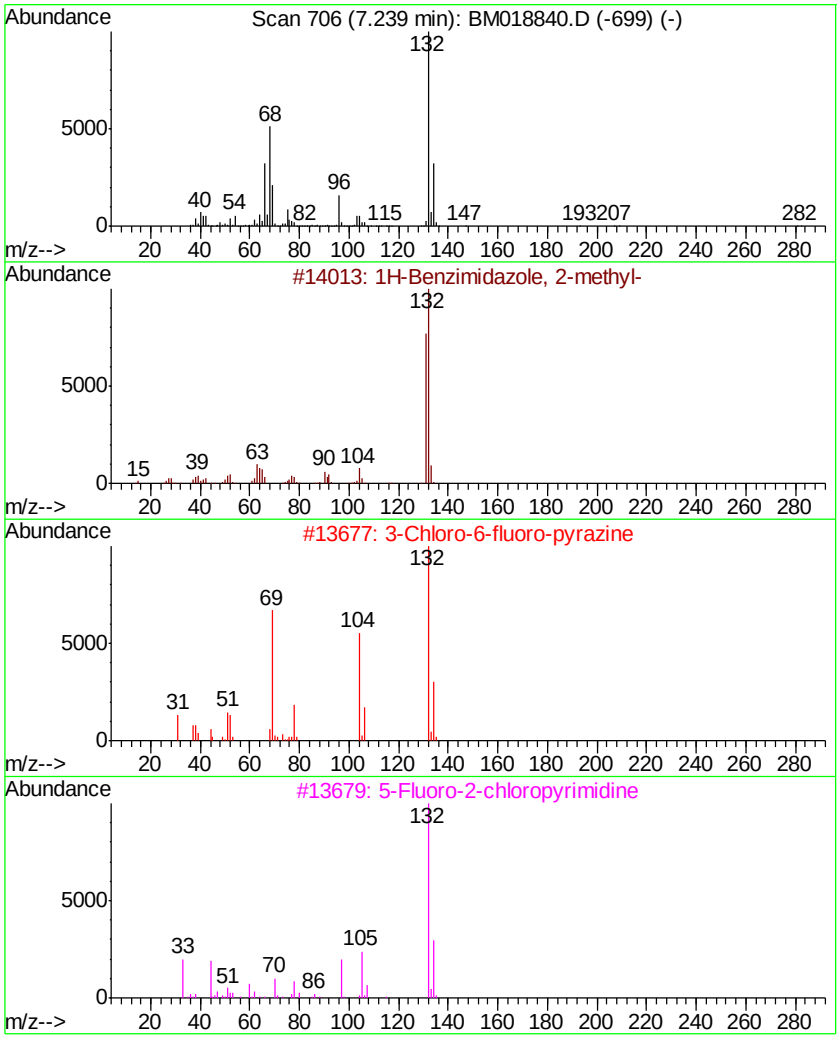
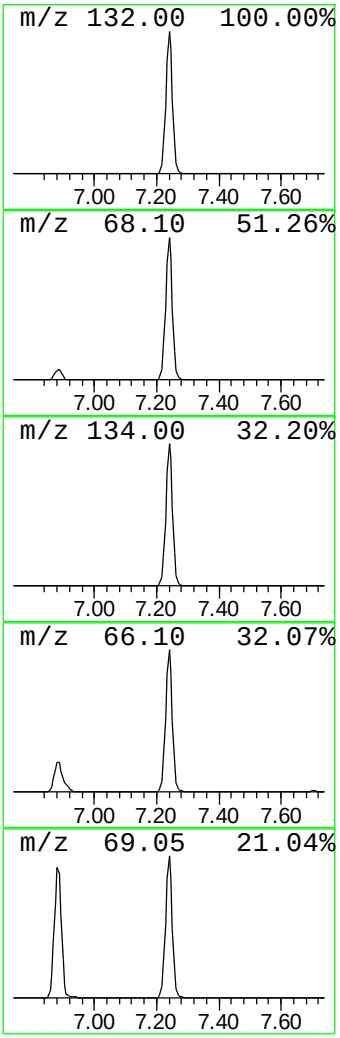
Peak Number 2 unknown7.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.24	103.44 ng	10386600	1,4-Dichlorobenzene-d4	7.70

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	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

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Data File : BM018840.D
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Operator : JU/SJ
Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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

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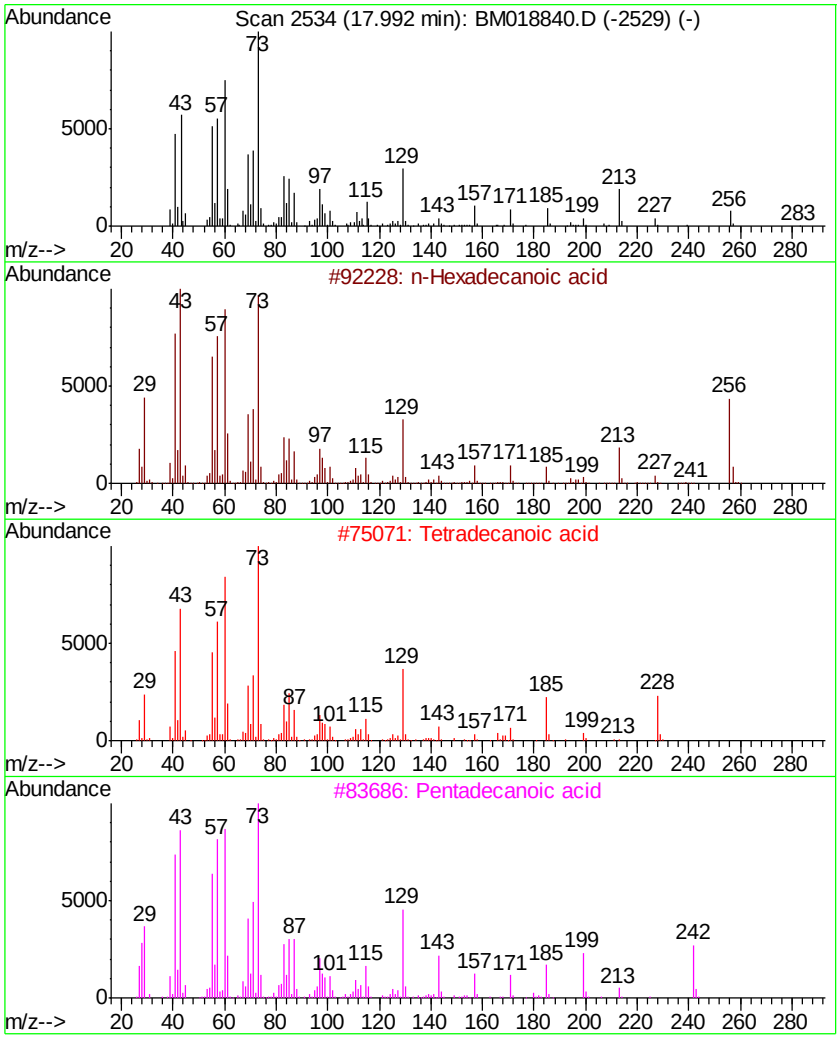
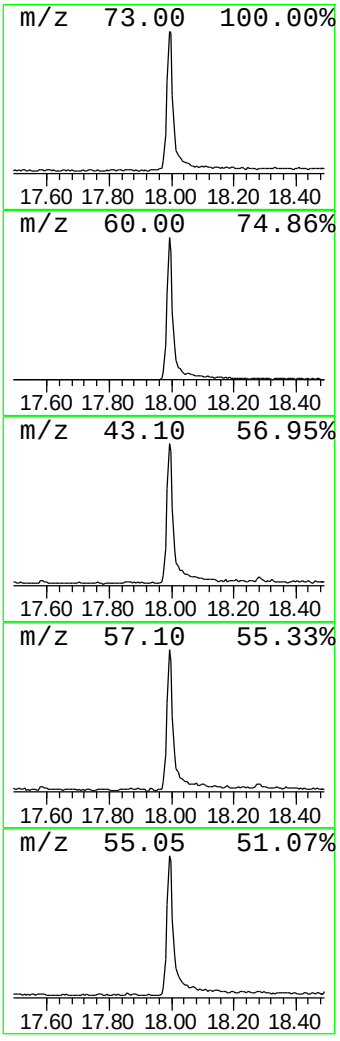
Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	4.71 ng	956583	Phenanthrene-d10	17.10

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	50
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
4	Tridecane	184	C13H28	000629-50-5	11
5	Hexadecane	226	C16H34	000544-76-3	11





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
Data File : BM018840.D
Acq On : 18 Feb 2019 16:11
Operator : JU/SJ
Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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

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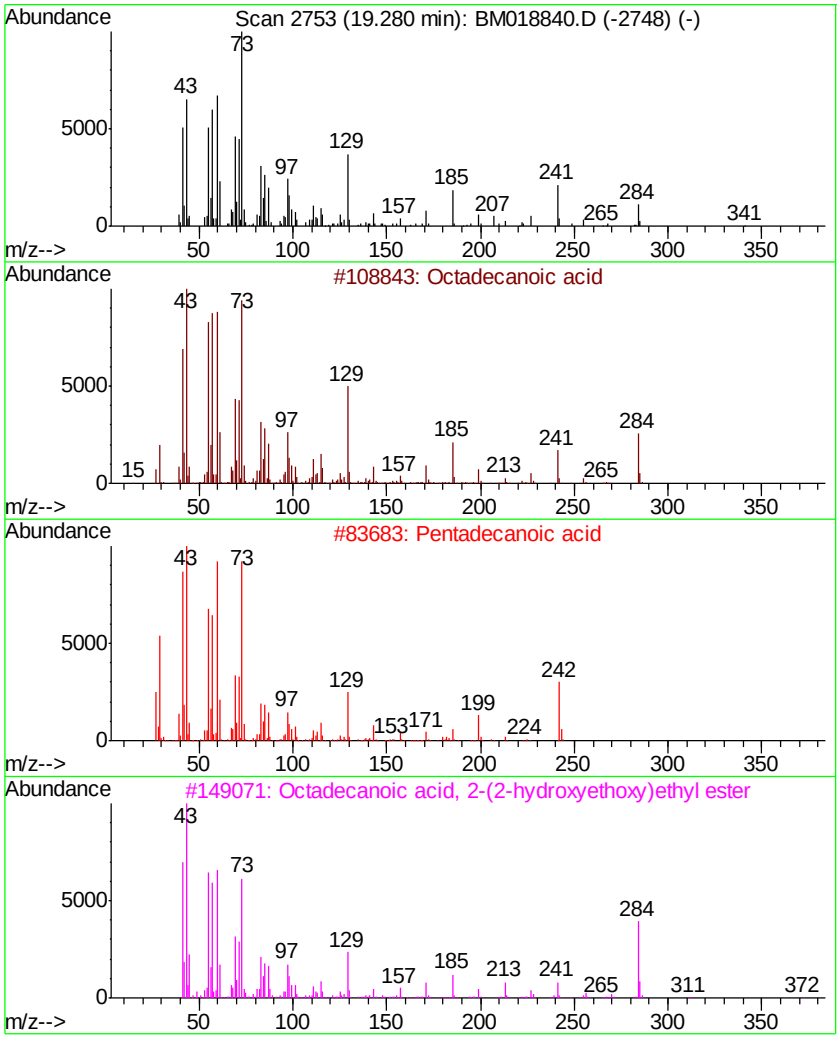
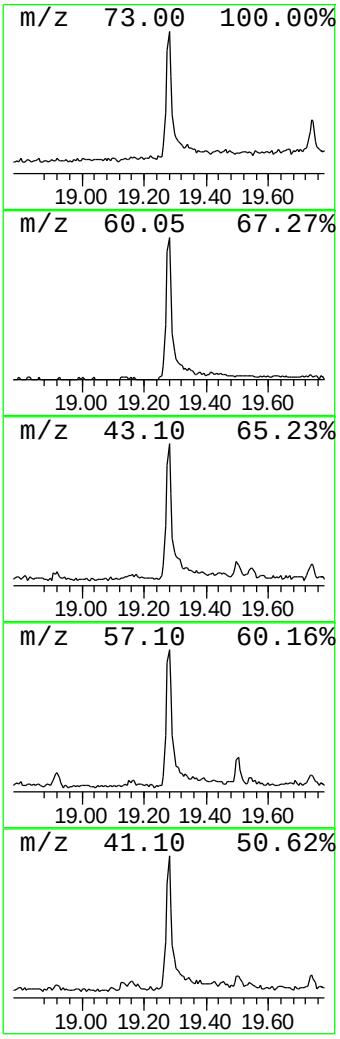
Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.28	2.39 ng	440031	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	58
4	Eicosane	282	C20H42	000112-95-8	56
5	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
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Acq On : 18 Feb 2019 16:11
Operator : JU/SJ
Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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

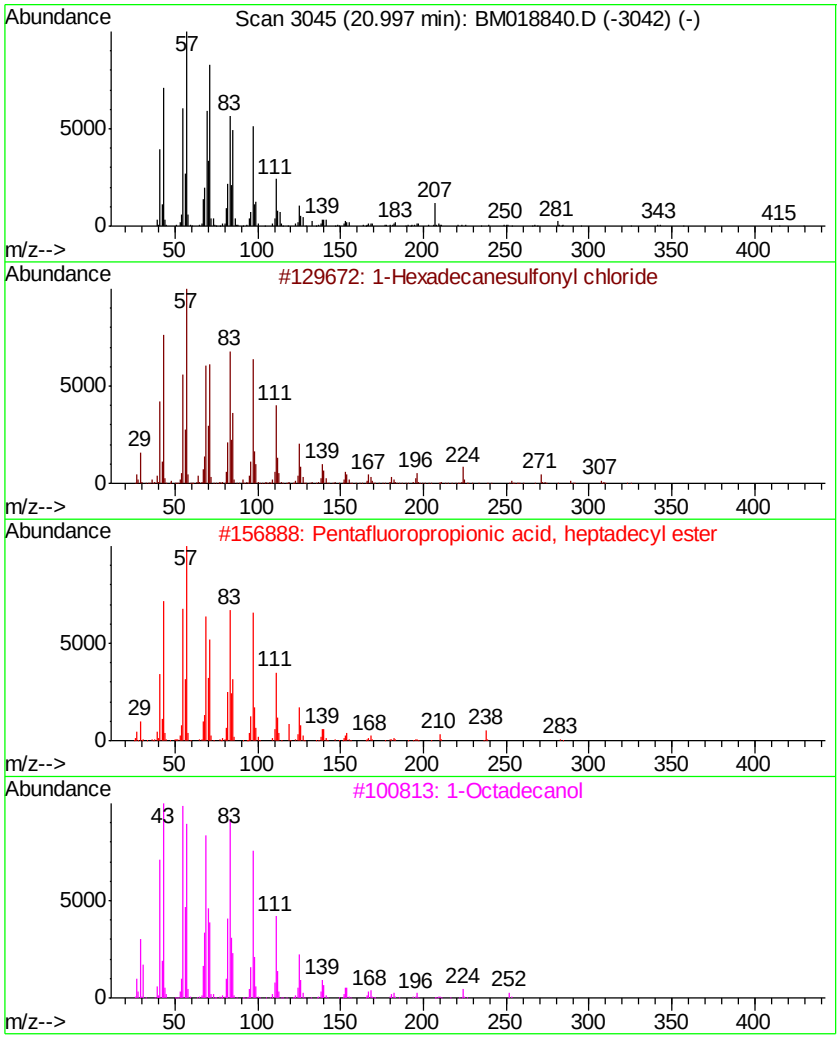
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

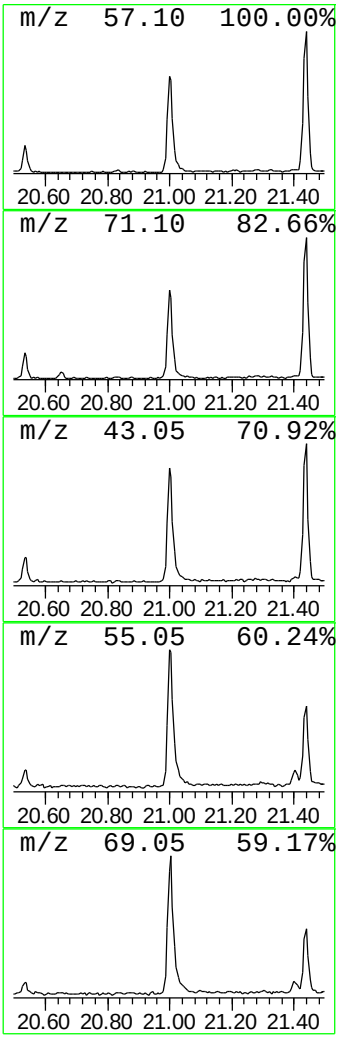
****

Peak Number 6 1-Hexadecanesulfonyl chloride Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	3.47 ng	640161	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	64
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	64
3	1-Octadecanol	270	C18H38O	000112-92-5	60
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	58
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
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Operator : JU/SJ
Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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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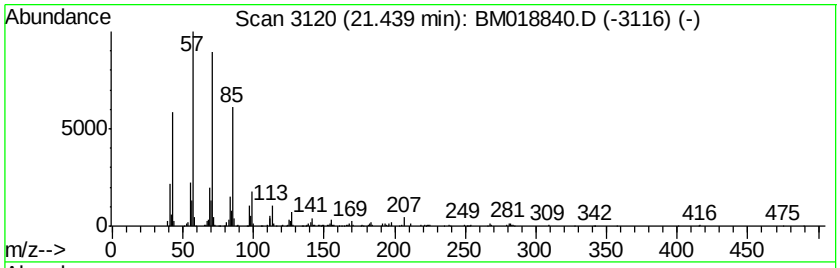
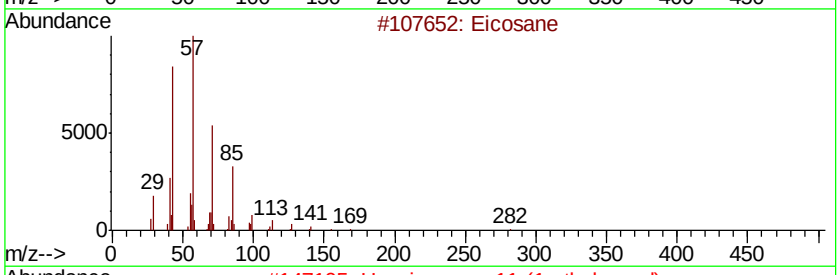
****

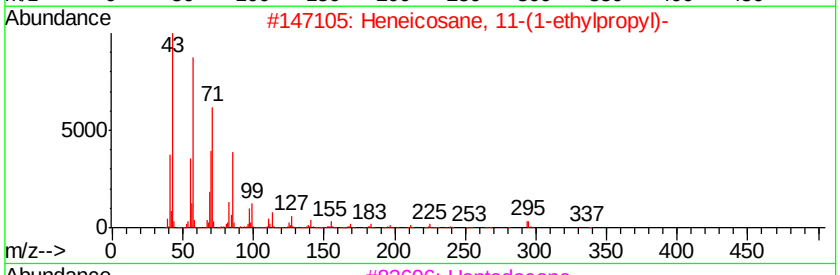
Peak Number 7 Eicosane Concentration Rank 12

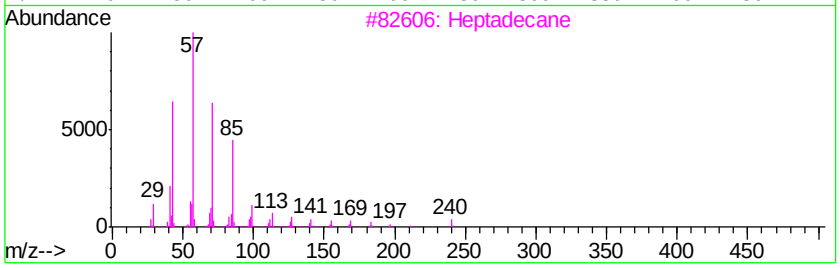
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.44	2.16 ng	398446	Chrysene-d12	21.30

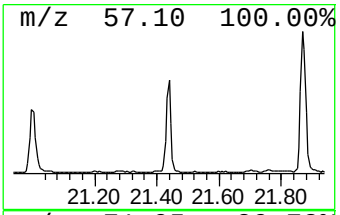
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
3	Heptadecane	240	C17H36	000629-78-7	86
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86

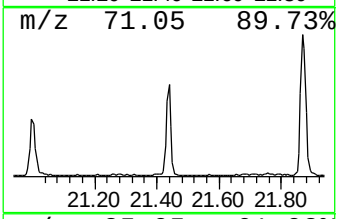


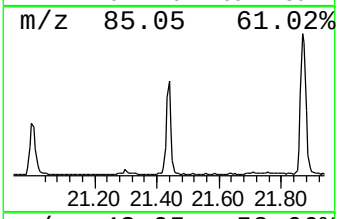


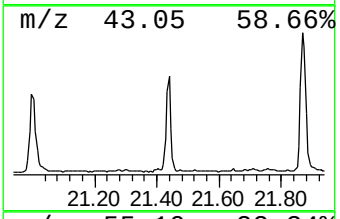


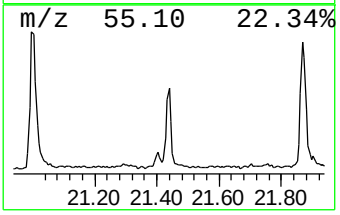












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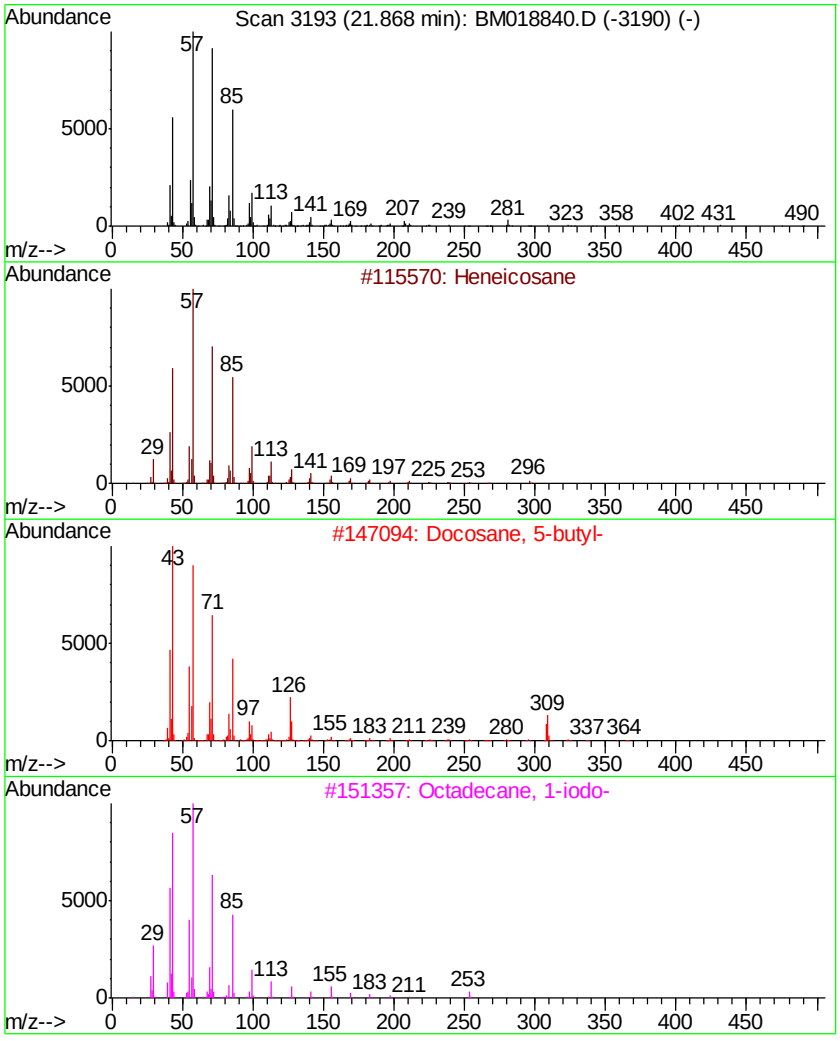
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

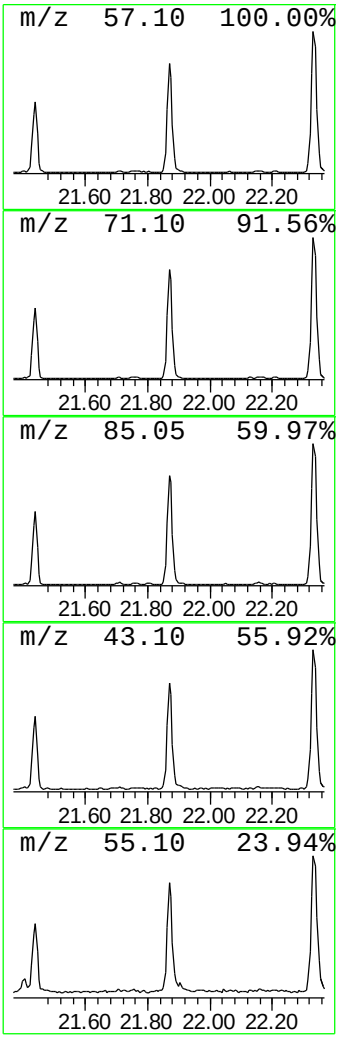
****

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.87	3.86 ng	712651	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Docosane, 5-butyl-	366	C26H54	055282-16-1	90
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	Dodecane	170	C12H26	000112-40-3	83
5	2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	80





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TIC Library : C:\DATABASE\NIST02.L
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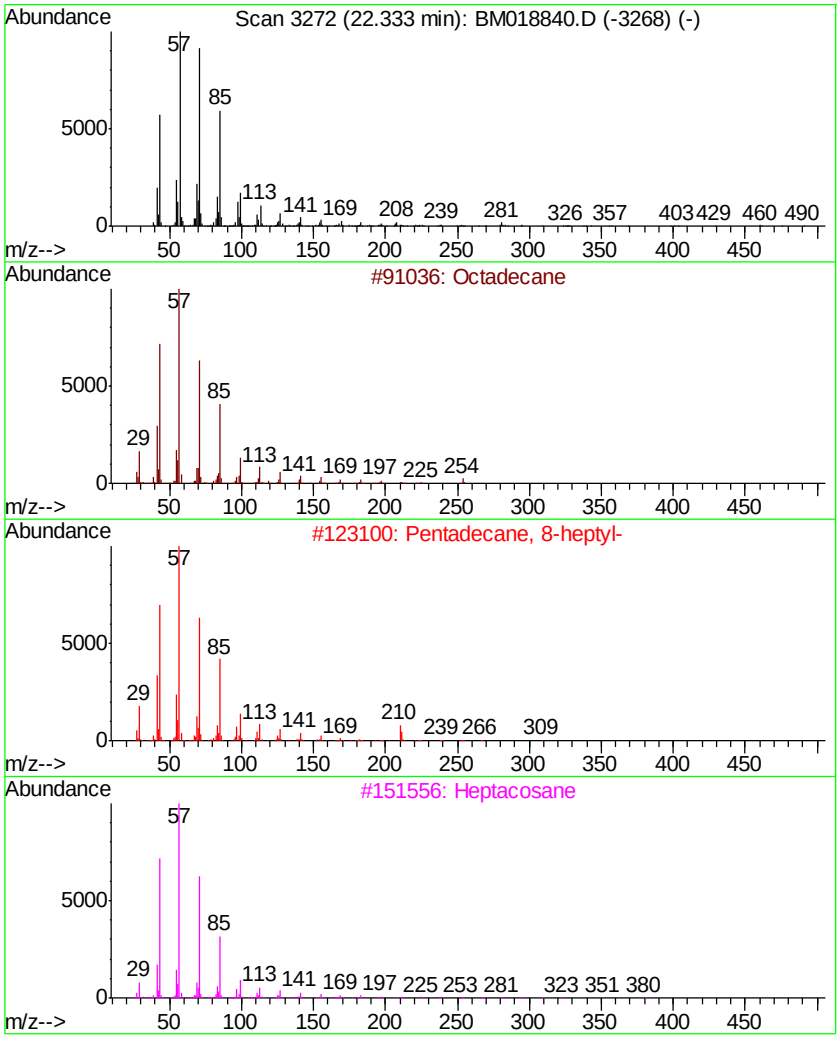
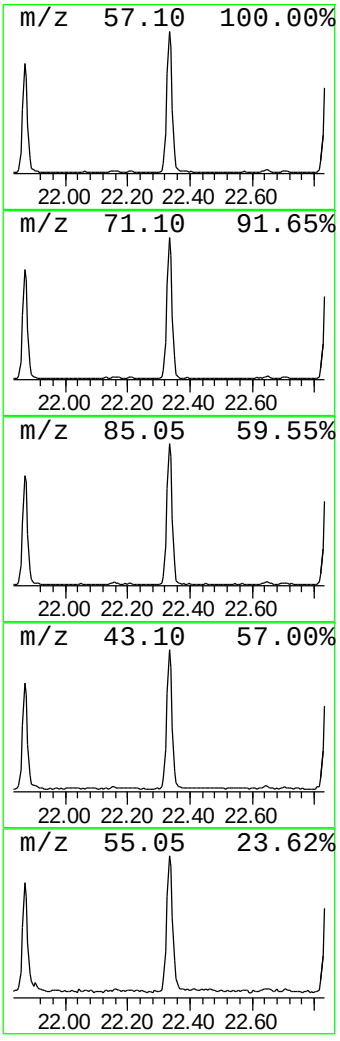
Peak Number 9 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.33	5.80 ng	1069300	Chrysene-d12	21.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Docosane	310	C22H46	000629-97-0	86





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Data File : BM018840.D
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Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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

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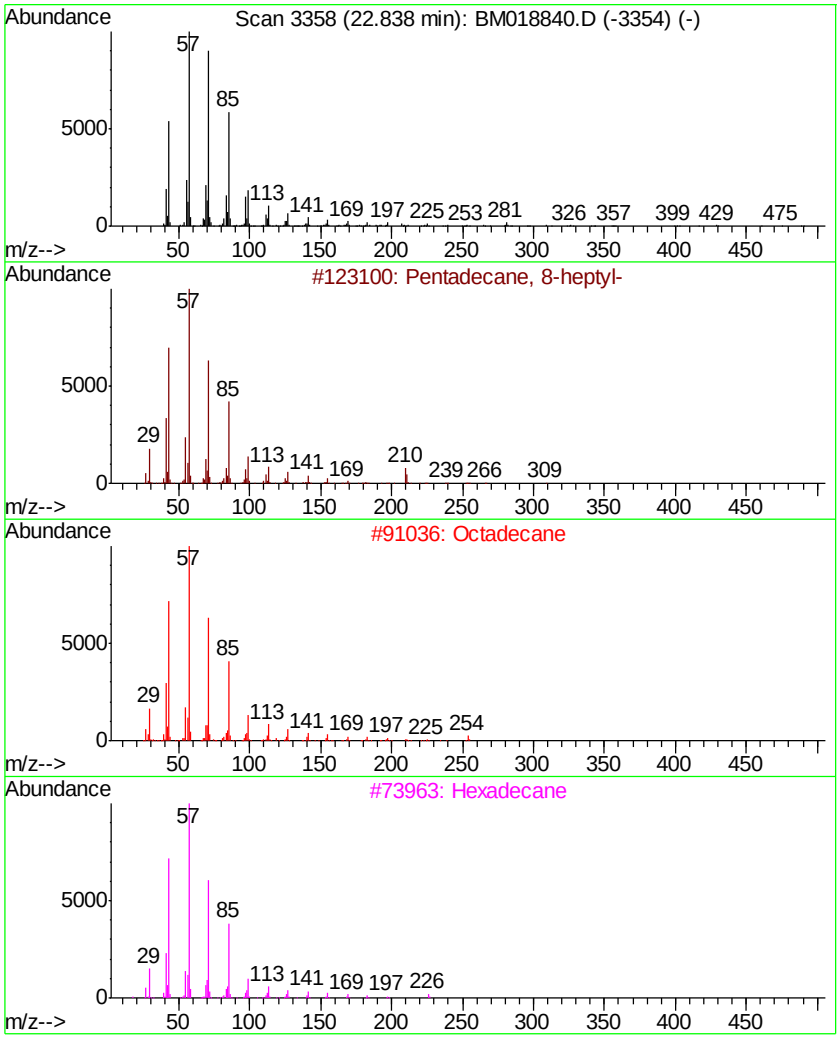
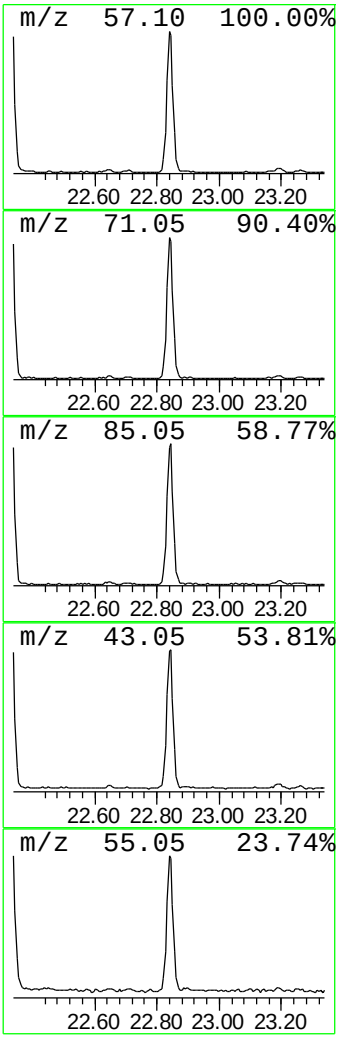
Peak Number 10 Pentadecane, 8-heptyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.84	6.67 ng	1005300	Perylene-d12	23.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2	Octadecane	254	C18H38	000593-45-3	87
3	Hexadecane	226	C16H34	000544-76-3	86
4	Octacosane	394	C28H58	000630-02-4	83
5	Heptacosane	380	C27H56	000593-49-7	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
Data File : BM018840.D
Acq On : 18 Feb 2019 16:11
Operator : JU/SJ
Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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

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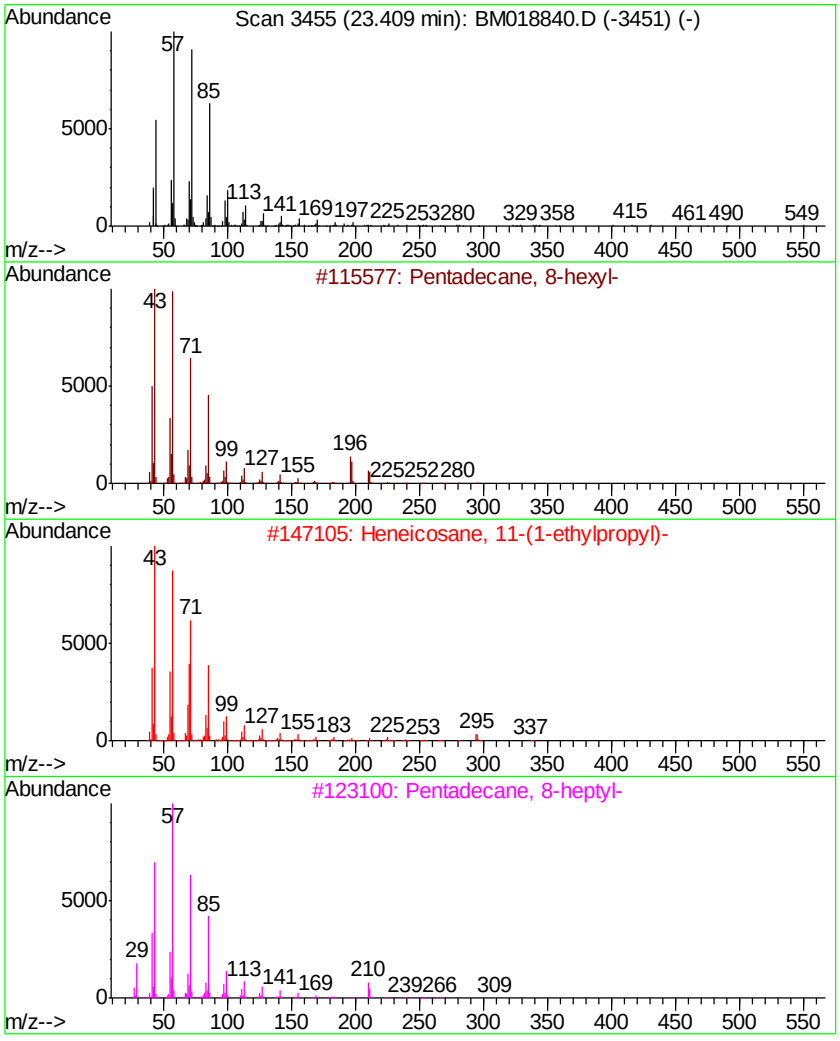
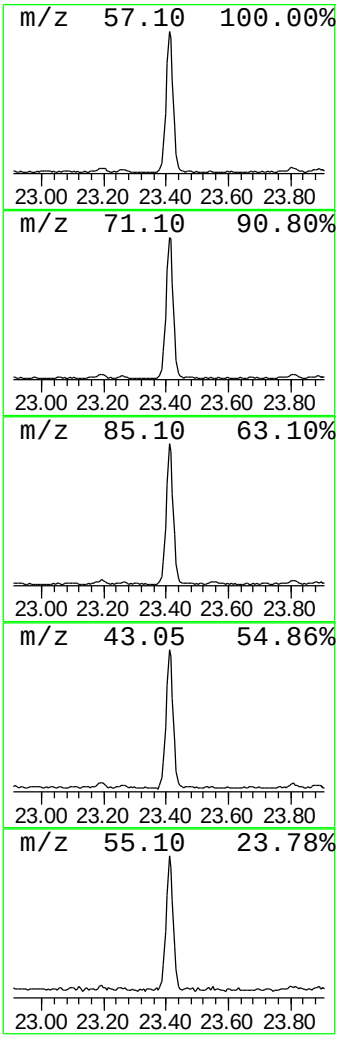
Peak Number 11 Pentadecane, 8-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.41	6.18 ng	930818	Perylene-d12	23.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5	10-Methylnonadecane	282	C20H42	056862-62-5	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM021819\
Data File : BM018840.D
Acq On : 18 Feb 2019 16:11
Operator : JU/SJ
Sample : K1517-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : G-021519

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	4.0	ng	400384	1	7.70	2008190	20.0
unknown7.24	7.24	103.4	ng	10386600	1	7.70	2008190	20.0
n-Hexadecanoic acid	17.99	4.7	ng	956583	4	17.10	4064430	20.0
Octadecanoic acid	19.28	2.4	ng	440031	5	21.30	3689040	20.0
1-Hexadecanesulfo...	21.00	3.5	ng	640161	5	21.30	3689040	20.0
Eicosane	21.44	2.2	ng	398446	5	21.30	3689040	20.0
Heneicosane	21.87	3.9	ng	712651	5	21.30	3689040	20.0
Octadecane	22.33	5.8	ng	1069300	5	21.30	3689040	20.0
Pentadecane, 8-he...	22.84	6.7	ng	1005300	6	23.56	3014590	20.0
Pentadecane, 8-he...	23.41	6.2	ng	930818	6	23.56	3014590	20.0