LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019950.D
Acq On : 17 Apr 2019 22:18
Operator : JU/SJ
Sample : K2423-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

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-BM041519.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	5.140	360	366	391	rBV	3478091	5128237	73.00%	9.353%
2	6.722	628	635	656	rBV	3545558	5647849	80.40%	10.301%
3	7.063	686	693	713	rBV	3811281	5876356	83.65%	10.718%
4	7.522	764	771	782	rBV	663297	1080367	15.38%	1.970%
5	7.840	817	825	838	rBV	2595336	4125949	58.73%	7.525%
6	8.698	964	971	997	rBV	1763050	3311525	47.14%	6.040%
7	10.304	1237	1244	1263	rBV	746910	1429443	20.35%	2.607%
8	12.798	1661	1668	1688	rBV	4798061	7024697	100.00%	12.812%
9	13.669	1810	1816	1829	rBV	397179	707126	10.07%	1.290%
10	14.192	1899	1905	1920	rBV2	1171112	1761285	25.07%	3.212%
11	15.704	2155	2162	2186	rBV	3050189	4711917	67.08%	8.594%
12	16.957	2369	2375	2391	rBV2	1137895	1792850	25.52%	3.270%
13	17.851	2521	2527	2538	rBV	147195	283077	4.03%	0.516%
14	19.039	2725	2729	2734	rVB	53010	75760	1.08%	0.138%
15	19.145	2743	2747	2754	rBV2	76882	130522	1.86%	0.238%
16	19.404	2787	2791	2797	rVB	71495	90099	1.28%	0.164%
17	19.604	2819	2825	2834	rBV	5335551	6550269	93.25%	11.947%
18	20.392	2956	2959	2964	rBV	74040	85497	1.22%	0.156%
19	20.868	3035	3040	3049	rBV3	194121	338881	4.82%	0.618%
20	21.174	3087	3092	3103	rVB	1226130	1673036	23.82%	3.051%
21	21.298	3110	3113	3117	rBV	152599	171214	2.44%	0.312%
22	21.721	3182	3185	3189	rBV	182028	194858	2.77%	0.355%
23	22.168	3258	3261	3267	rVB	186201	226620	3.23%	0.413%
24	22.656	3340	3344	3349	rVB	189301	243173	3.46%	0.444%
25	23.197	3432	3436	3442	rVB2	171131	273741	3.90%	0.499%
26	23.362	3459	3464	3481	rVB	984712	1892935	26.95%	3.453%

Sum of corrected areas: 54827283

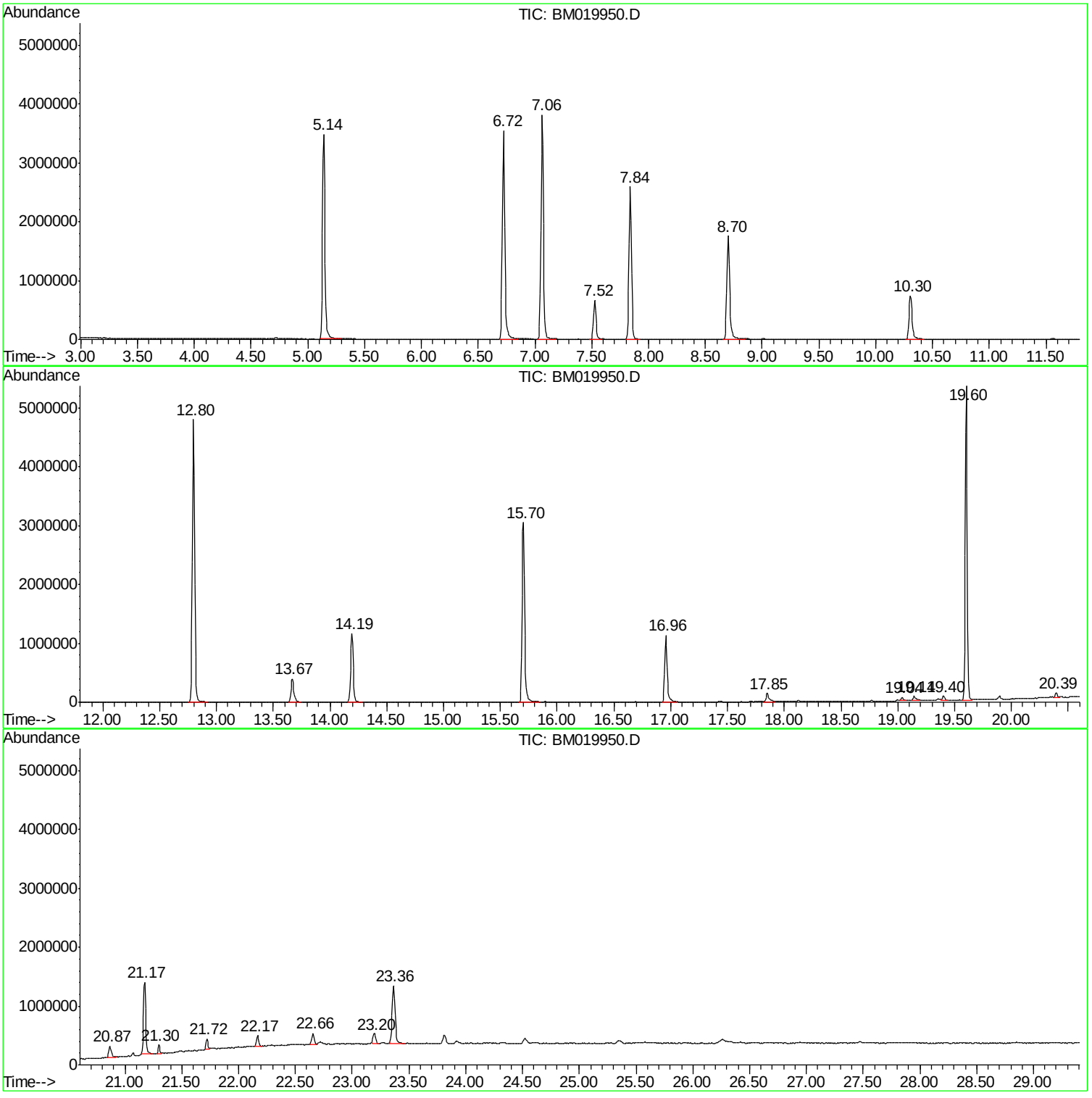
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019950.D
Acq On : 17 Apr 2019 22:18
Operator : JU/SJ
Sample : K2423-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.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\BM041719\
Data File : BM019950.D
Acq On : 17 Apr 2019 22:18
Operator : JU/SJ
Sample : K2423-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

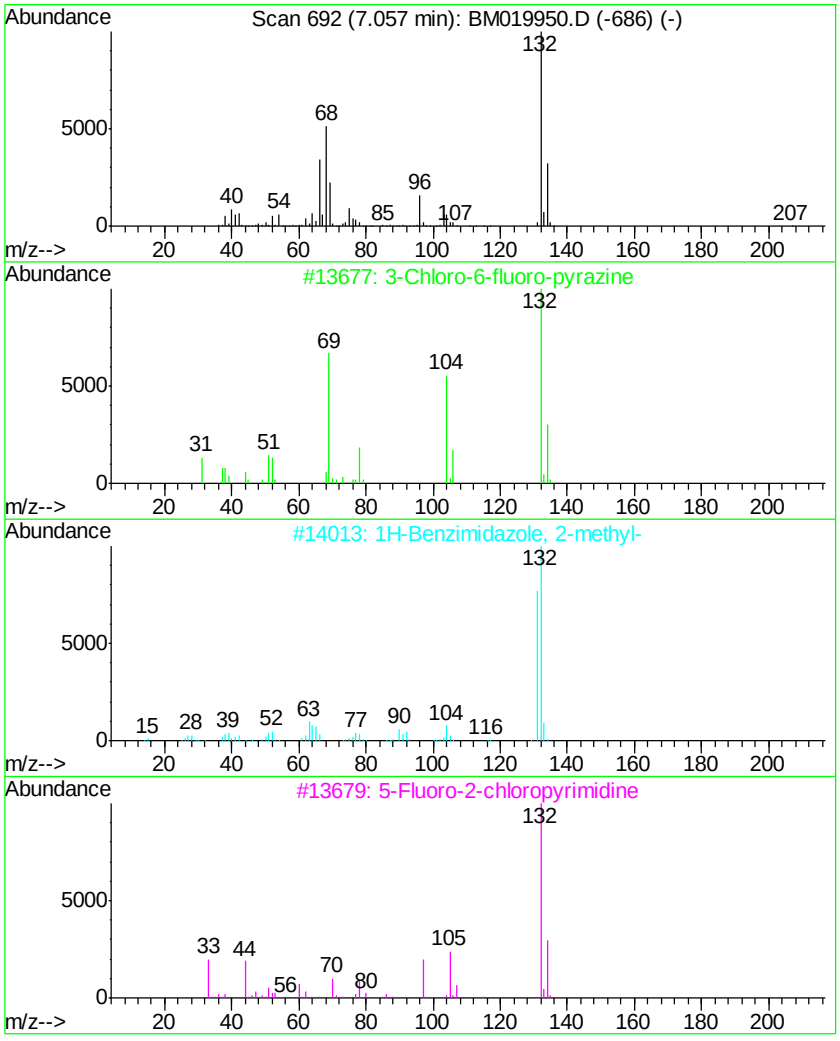
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

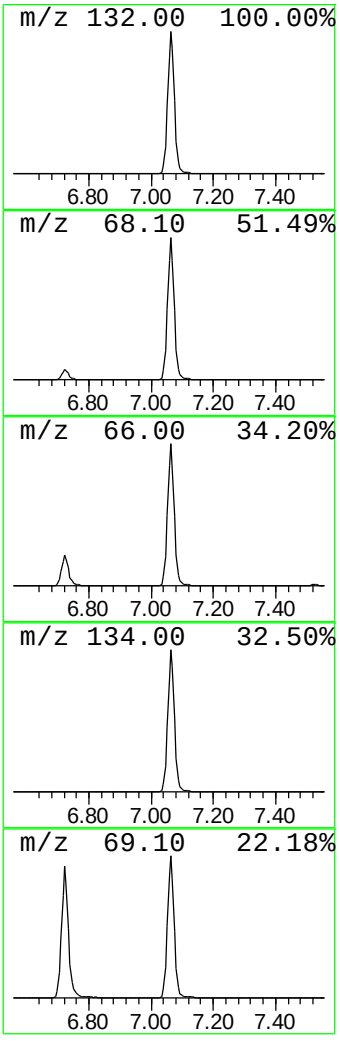
****

Peak Number 1 unknown7.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	108.78 ng	5876360	1,4-Dichlorobenzene-d4	7.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Amphetaminil	250	C17H18N2	017590-01-1	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019950.D
Acq On : 17 Apr 2019 22:18
Operator : JU/SJ
Sample : K2423-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

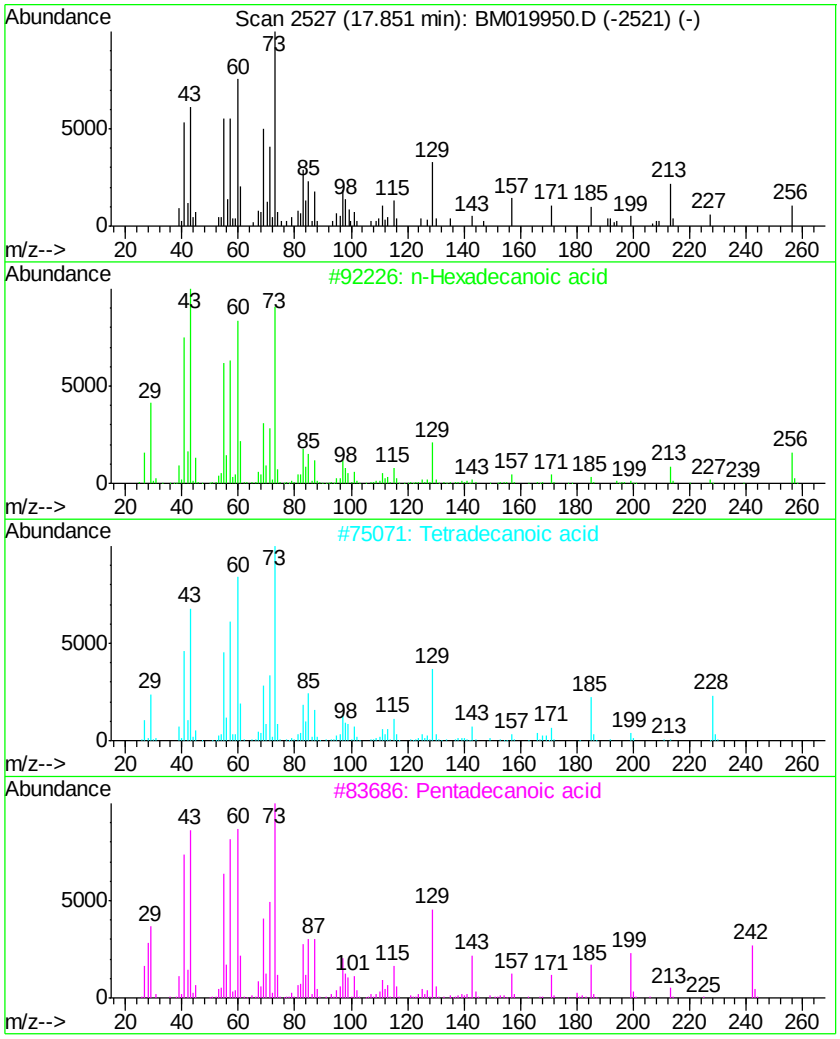
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

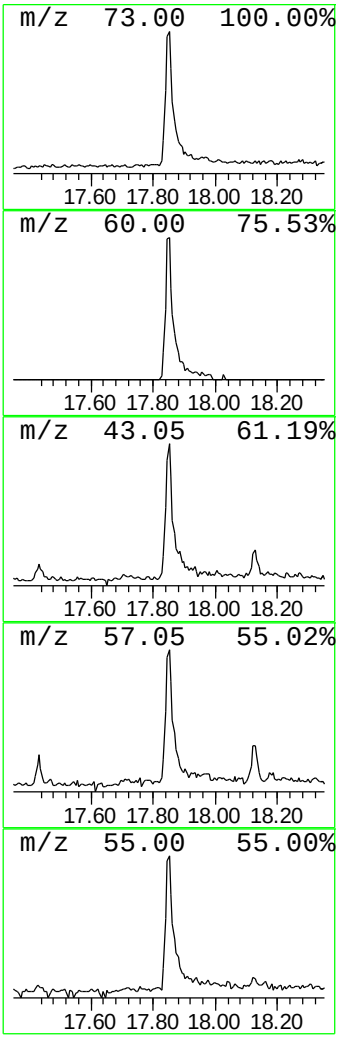
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	3.16 ng	283077	Phenanthrene-d10	16.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019950.D
Acq On : 17 Apr 2019 22:18
Operator : JU/SJ
Sample : K2423-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

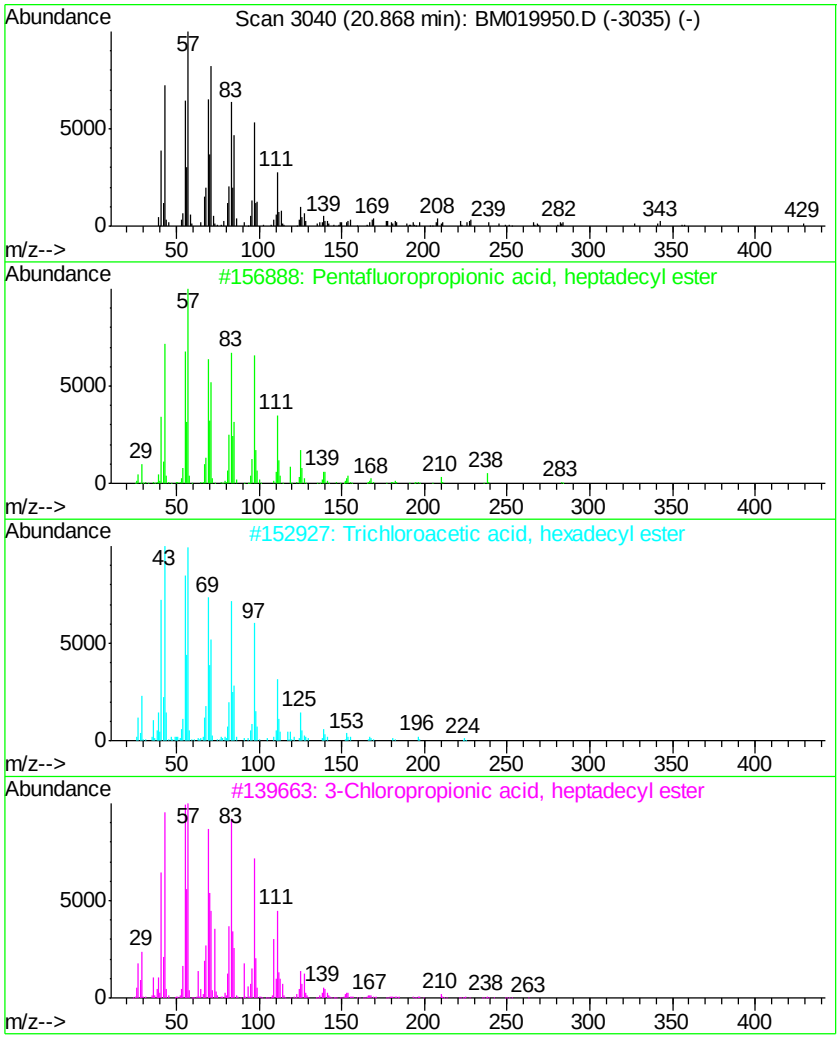
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

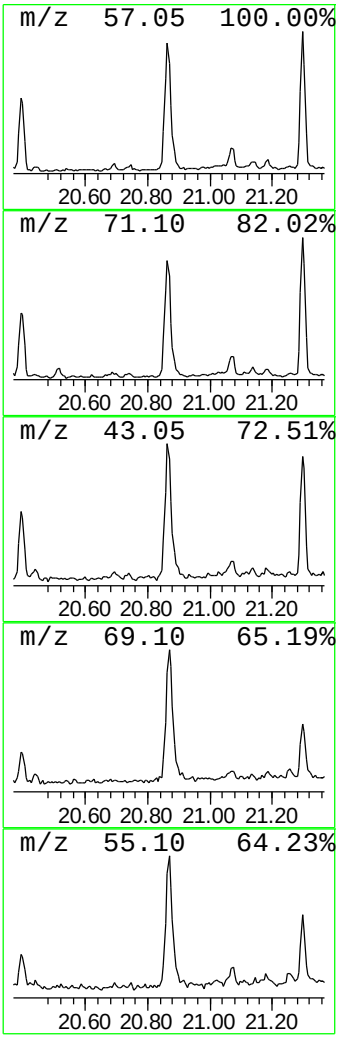
****

Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	4.05 ng	338881	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	70
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	62
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	60
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	60
5	1-Nonadecene	266	C19H38	018435-45-5	60





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019950.D
Acq On : 17 Apr 2019 22:18
Operator : JU/SJ
Sample : K2423-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

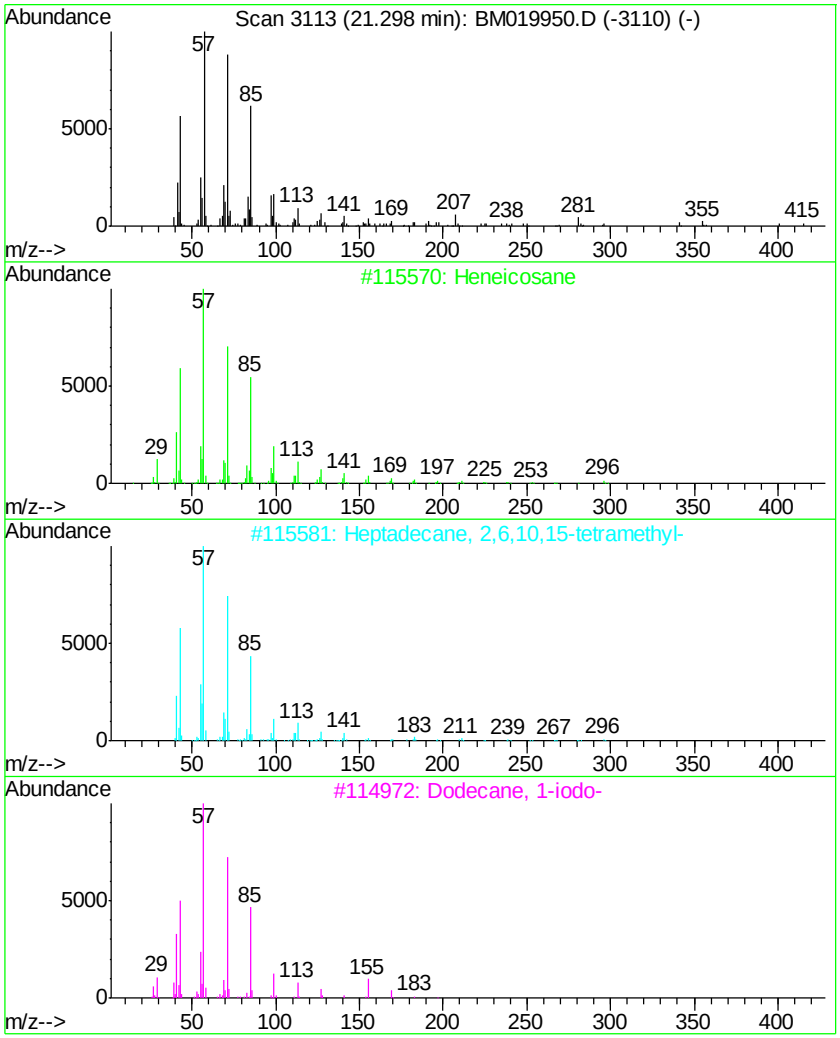
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

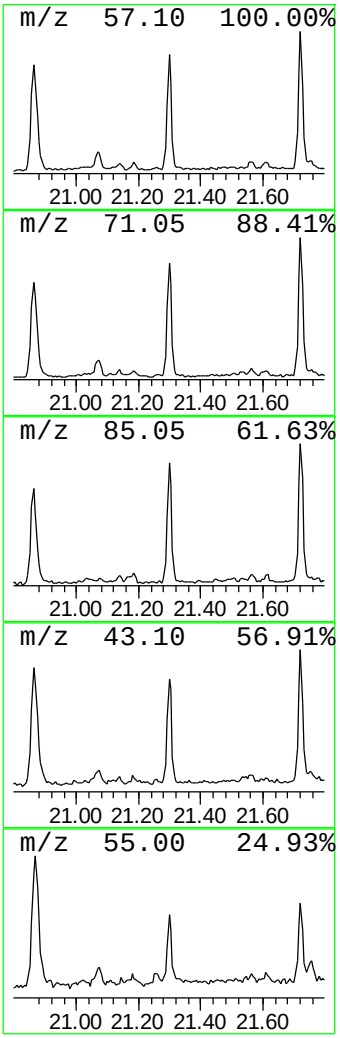
****

Peak Number 5 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	2.05 ng	171214	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
Data File : BM019950.D
Acq On : 17 Apr 2019 22:18
Operator : JU/SJ
Sample : K2423-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

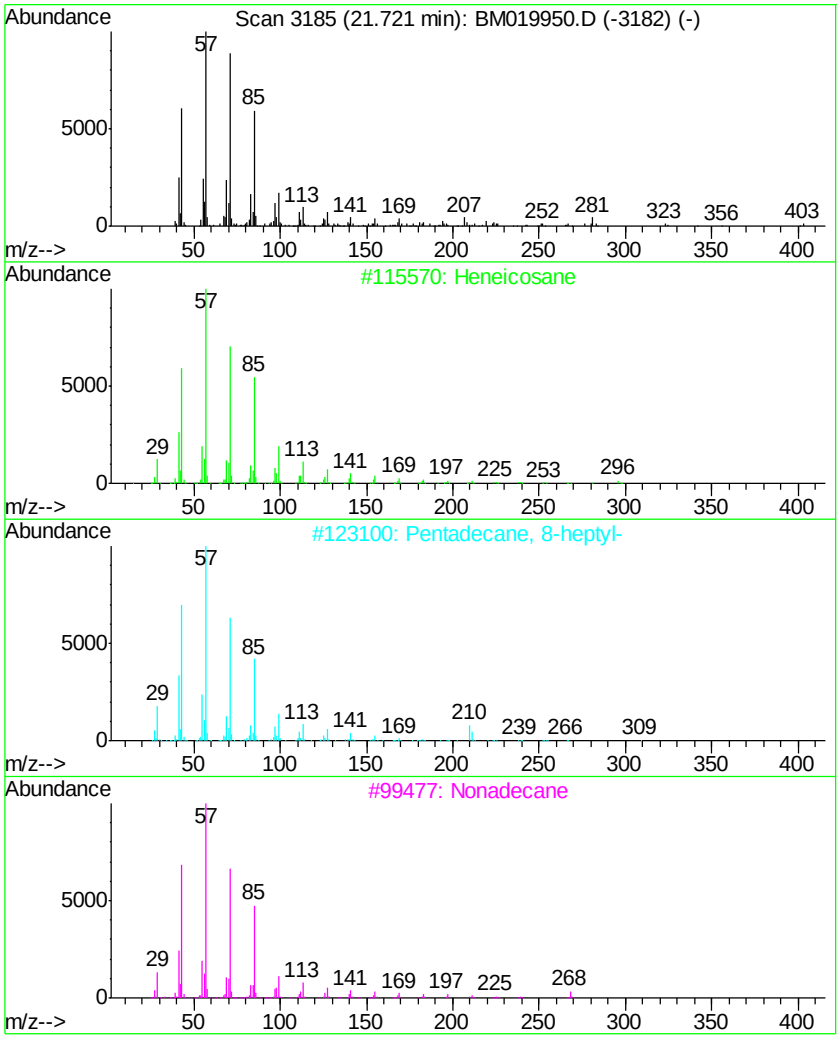
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

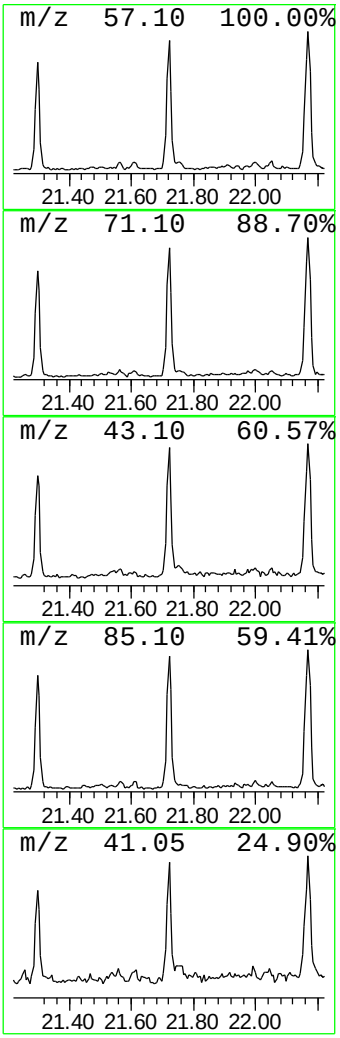
****

Peak Number 6 Pentadecane, 8-heptyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	2.33 ng	194858	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
3	Nonadecane	268	C19H40	000629-92-5	86
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





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Sample : K2423-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

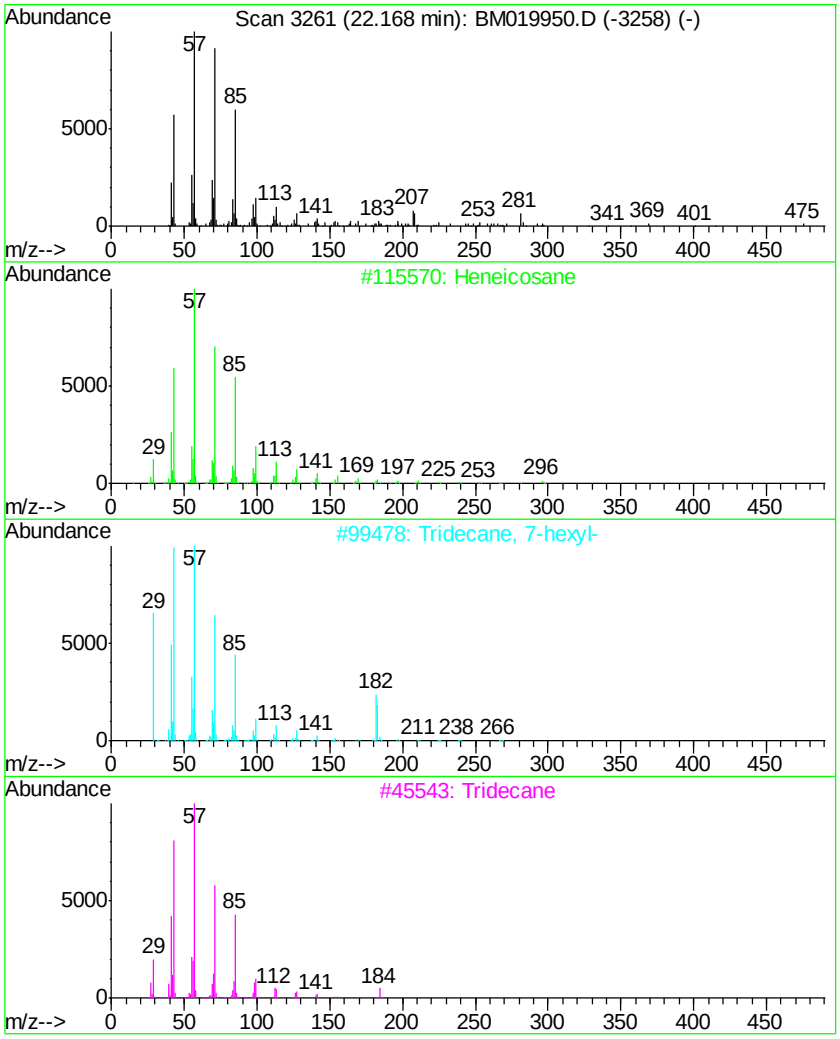
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

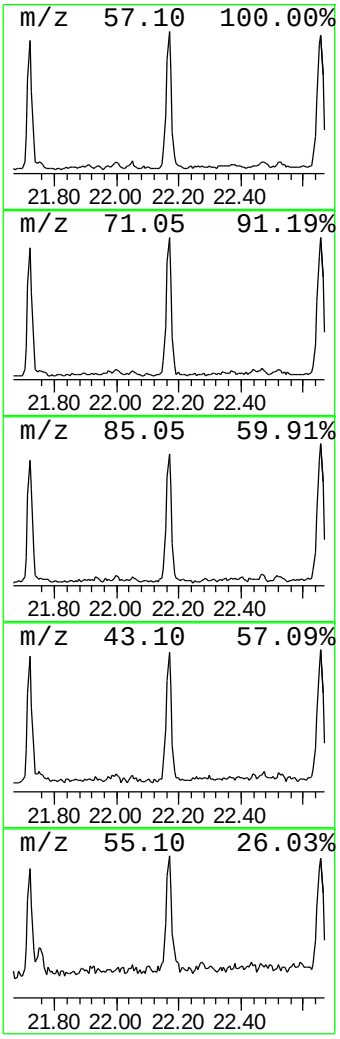
****

Peak Number 7 Tridecane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.17	2.71 ng	226620	Chrysene-d12	21.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	90
3	Tridecane	184	C13H28	000629-50-5	87
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Docosane	310	C22H46	000629-97-0	86





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Acq On : 17 Apr 2019 22:18
Operator : JU/SJ
Sample : K2423-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

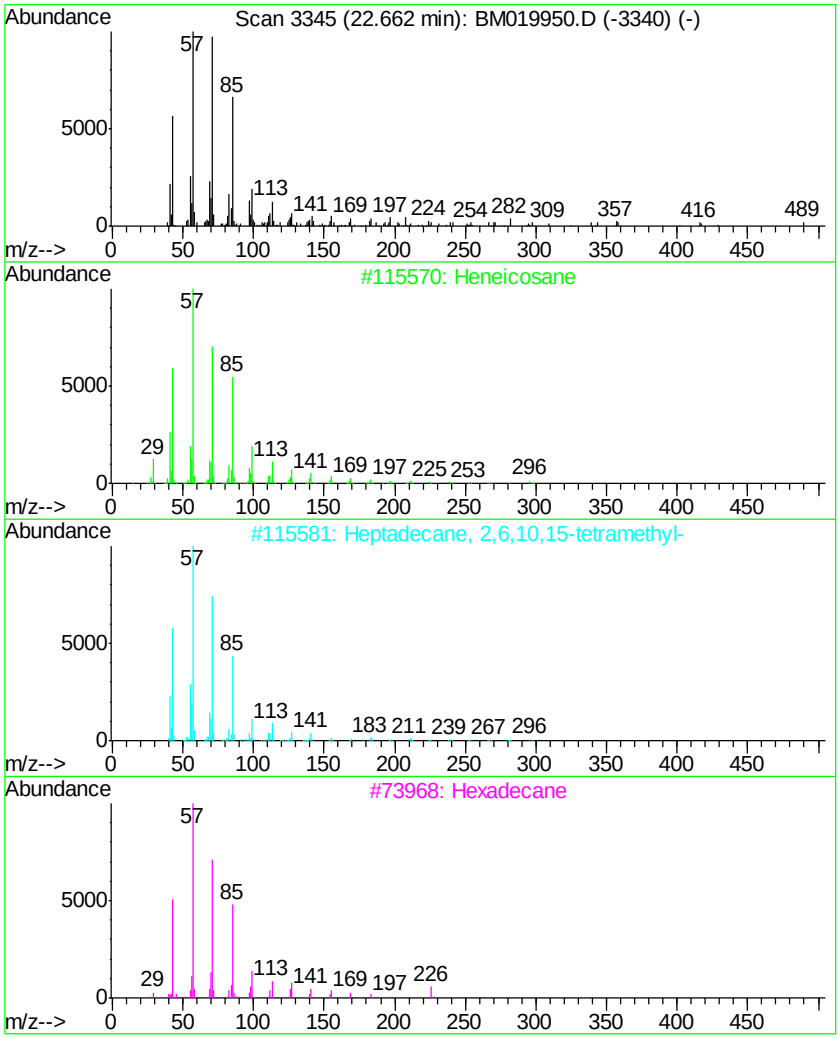
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

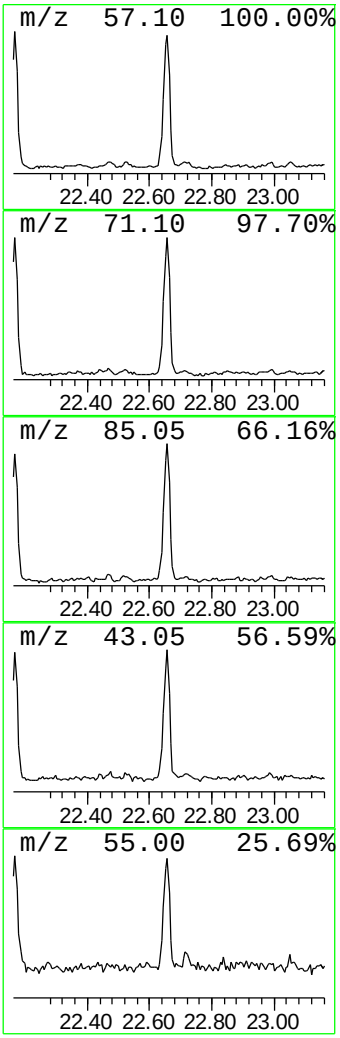
****

Peak Number 8 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.66	2.57 ng	243173	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3	Hexadecane	226	C16H34	000544-76-3	83
4	Octacosane	394	C28H58	000630-02-4	74
5	Heptacosane	380	C27H56	000593-49-7	74





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP5-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM041519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

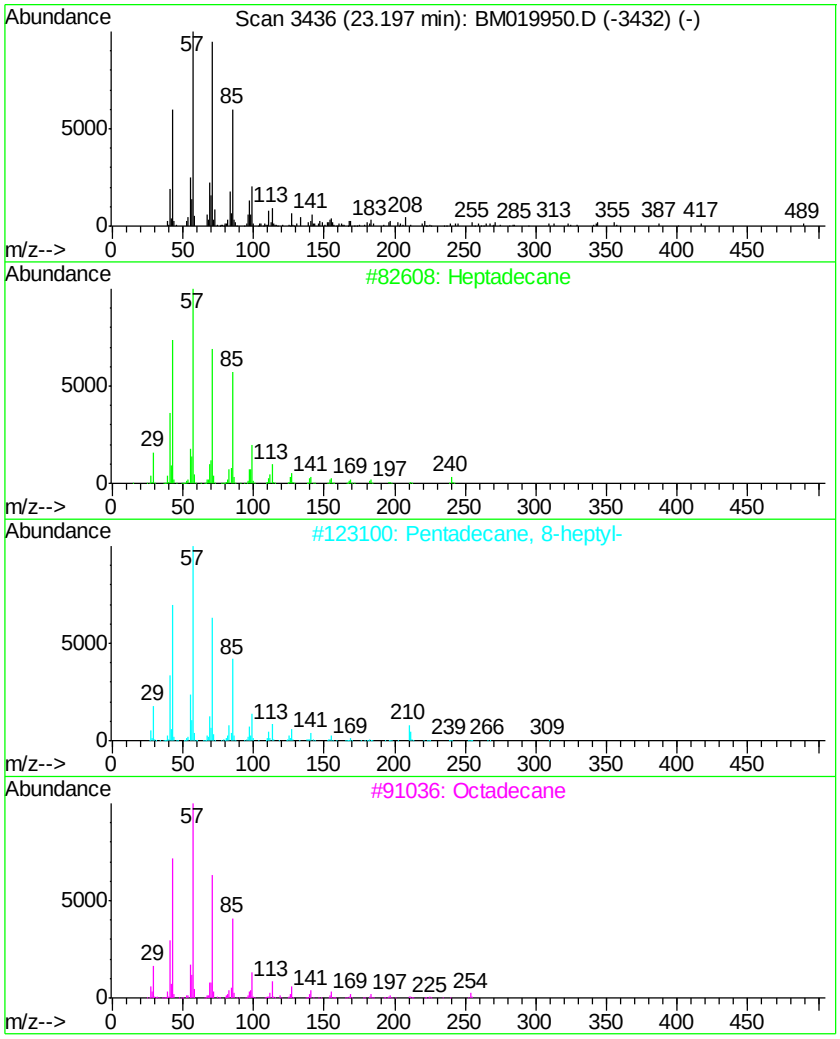
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

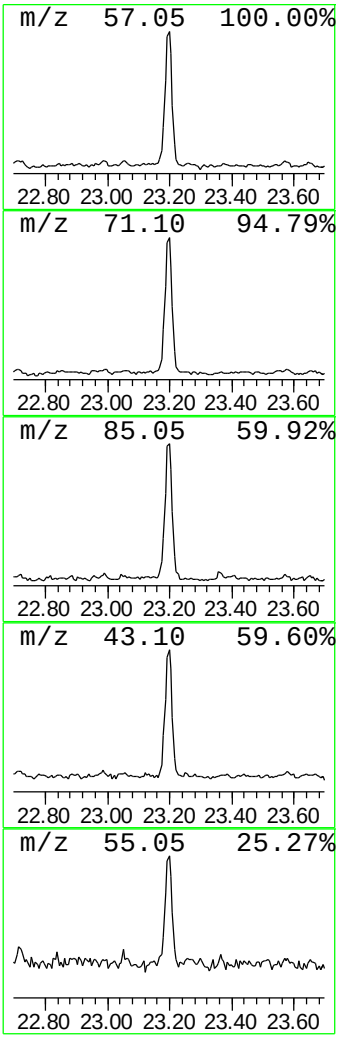
****

Peak Number 9 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.20	2.89 ng	273741	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
3	Octadecane	254	C18H38	000593-45-3	72
4	Hentriacontane	437	C31H64	000630-04-6	64
5	Eicosane	282	C20H42	000112-95-8	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM041719\
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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
unknown7.06	7.06	108.8	ng	5876360	1	7.52	1080370	20.0
n-Hexadecanoic acid	17.85	3.2	ng	283077	4	16.96	1792850	20.0
Pentafluoropropio...	20.87	4.0	ng	338881	5	21.17	1673040	20.0
Heneicosane	21.30	2.0	ng	171214	5	21.17	1673040	20.0
Pentadecane, 8-he...	21.72	2.3	ng	194858	5	21.17	1673040	20.0
Tridecane, 7-hexyl-	22.17	2.7	ng	226620	5	21.17	1673040	20.0
Heptadecane, 2,6,...	22.66	2.6	ng	243173	6	23.37	1892940	20.0
Heptadecane	23.20	2.9	ng	273741	6	23.37	1892940	20.0