LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117560.D
Acq On : 28 Oct 2019 14:43
Operator : JU
Sample : K5543-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R-1

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_F\METHODS\8270-BF101819.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	4.922	478	482	494	rBV	98391	145274	13.45%	1.602%
2	5.351	552	555	573	rBV	720721	836390	77.41%	9.223%
3	6.381	726	730	747	rBV	872145	945215	87.48%	10.423%
4	6.504	747	751	762	rVB	984112	976124	90.35%	10.764%
5	6.728	786	789	800	rBV	228839	234174	21.67%	2.582%
6	6.881	811	815	827	rBV	799868	710694	65.78%	7.837%
7	7.292	881	885	904	rBV	501380	563814	52.18%	6.217%
8	8.010	1003	1007	1022	rBV	286805	314159	29.08%	3.464%
9	9.080	1185	1189	1202	rBV	1219600	1080439	100.00%	11.914%
10	9.480	1253	1257	1270	rBB	124634	123787	11.46%	1.365%
11	9.757	1301	1304	1318	rBV	419493	371967	34.43%	4.102%
12	10.551	1436	1439	1451	rBV	562073	572005	52.94%	6.308%
13	11.245	1554	1557	1567	rBV	351194	348689	32.27%	3.845%
14	11.774	1644	1647	1654	rBV	21125	23608	2.19%	0.260%
15	12.827	1822	1826	1829	rBV	1147465	1017244	94.15%	11.217%
16	13.727	1975	1979	1992	rBV2	80929	141767	13.12%	1.563%
17	13.892	2003	2007	2015	rBV	243098	246144	22.78%	2.714%
18	14.345	2080	2084	2086	rBV	16649	16440	1.52%	0.181%
19	14.639	2131	2134	2139	rVB	28006	24878	2.30%	0.274%
20	14.709	2142	2146	2149	rVB	44991	44649	4.13%	0.492%
21	14.951	2184	2187	2192	rVB	29621	29941	2.77%	0.330%
22	15.321	2244	2250	2263	rBV	152710	239507	22.17%	2.641%
23	15.709	2312	2316	2320	rVB2	18734	24868	2.30%	0.274%
24	15.798	2325	2331	2335	rBV6	8664	20444	1.89%	0.225%
25	16.180	2391	2396	2400	rVB5	9541	16213	1.50%	0.179%

Sum of corrected areas: 9068434

LSC Report - Integrated Chromatogram

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Sample : K5543-01
Misc :
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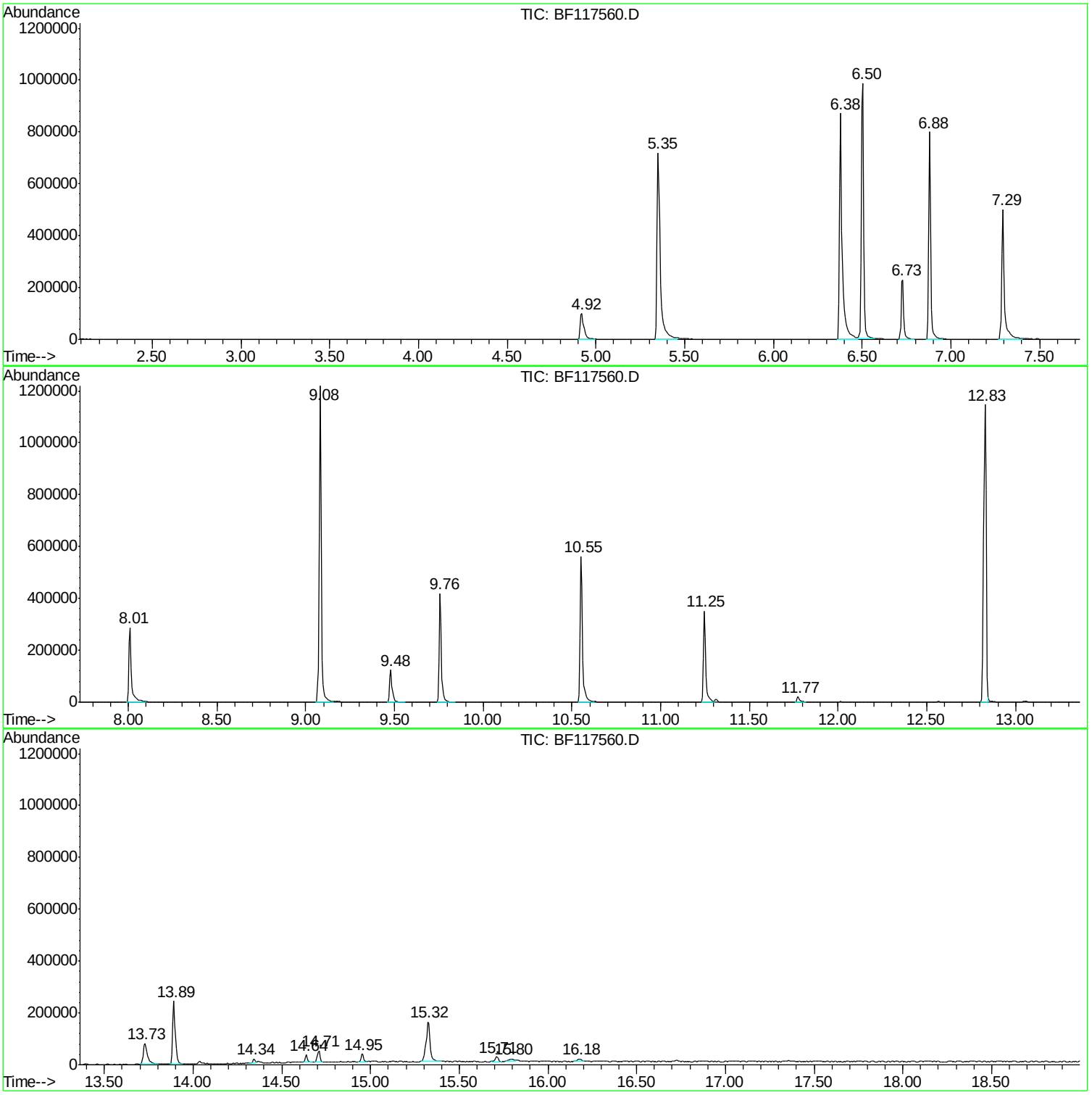
Instrument : BNA_F
ClientSampleId : R-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117560.D
Acq On : 28 Oct 2019 14:43
Operator : JU
Sample : K5543-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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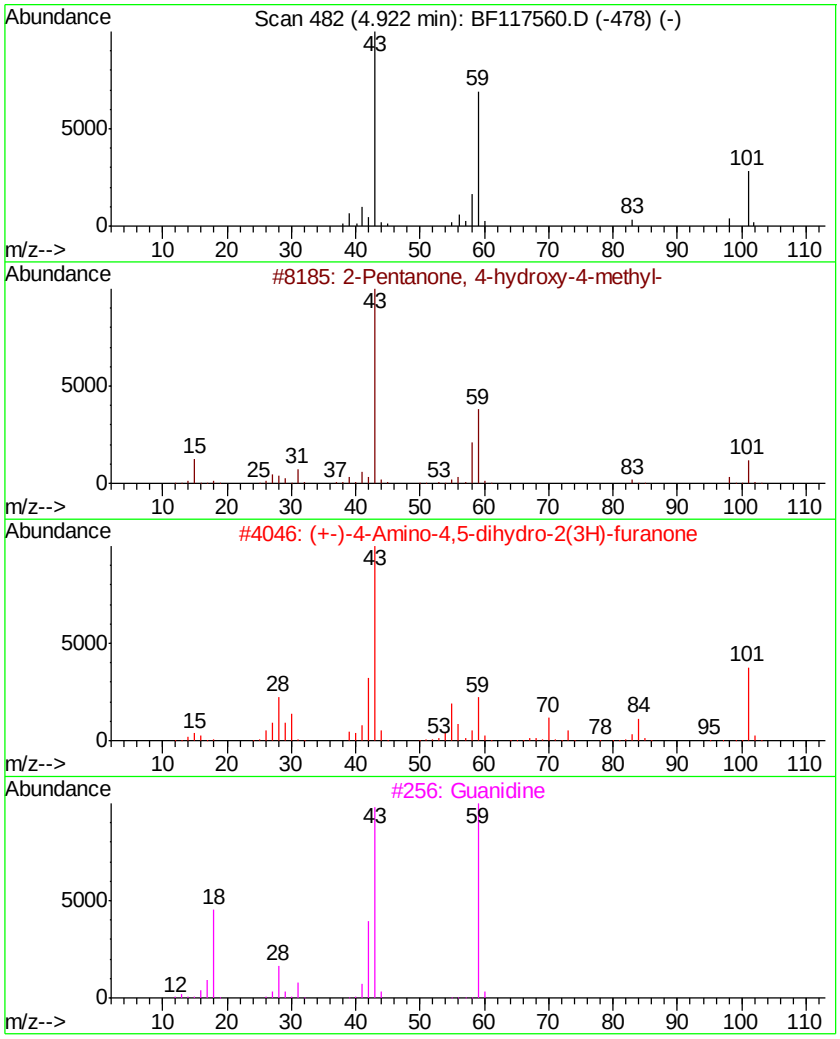
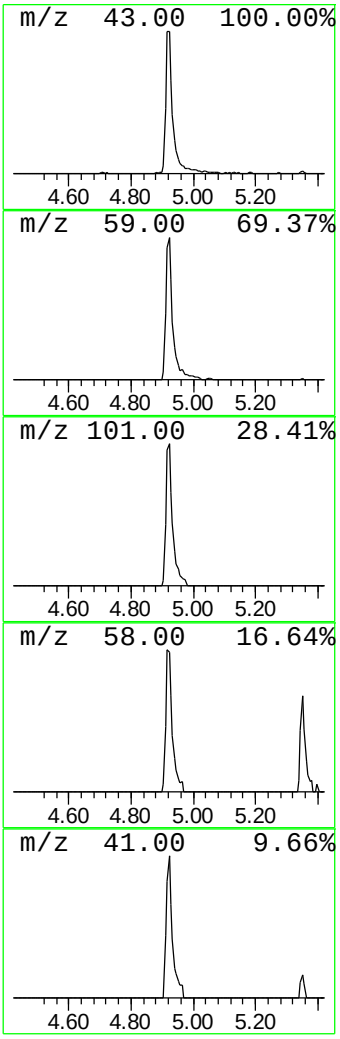
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	12.41 ng	145274	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Guanidine	59	CH5N3	000113-00-8	43
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17





Library Search Compound Report

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Data File : BF117560.D
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Operator : JU
Sample : K5543-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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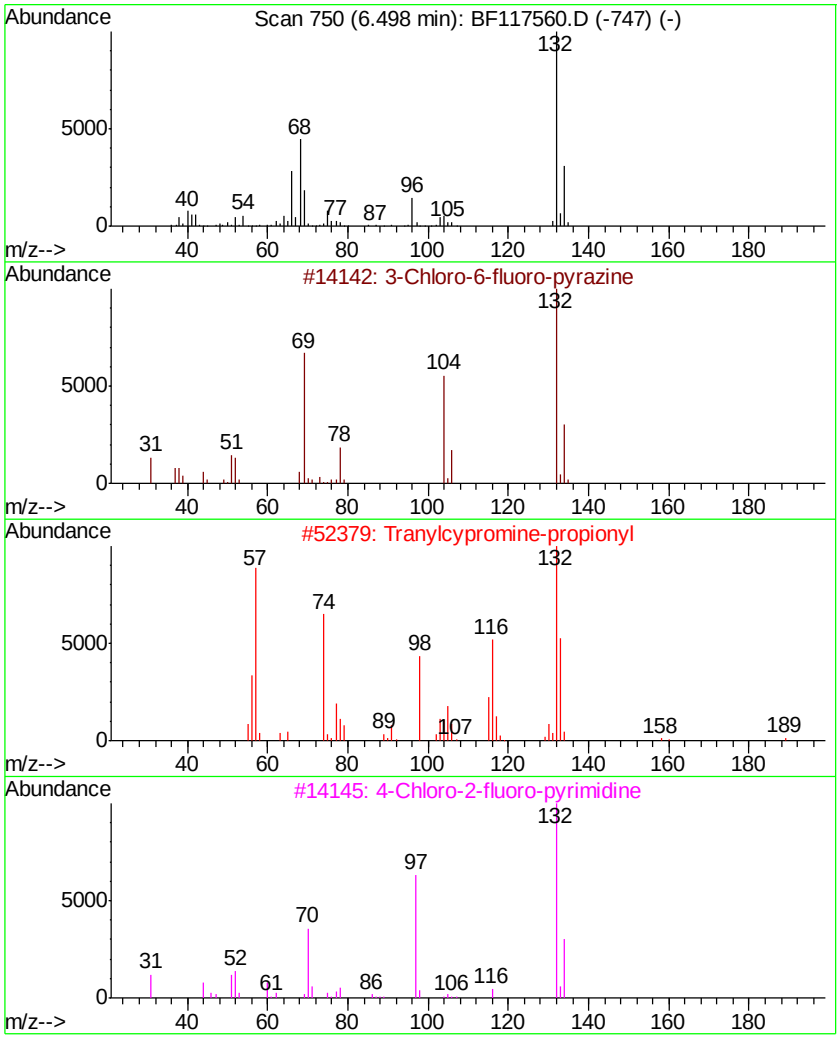
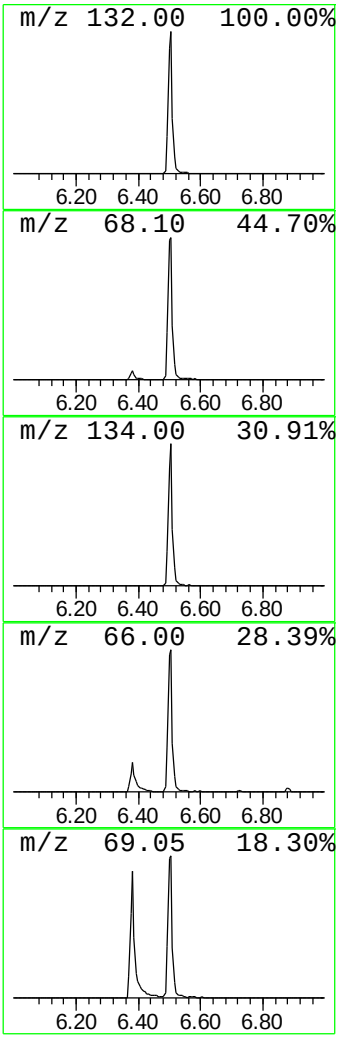
Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	83.37 ng	976124	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Xenon	132	Xe	007440-63-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117560.D
Acq On : 28 Oct 2019 14:43
Operator : JU
Sample : K5543-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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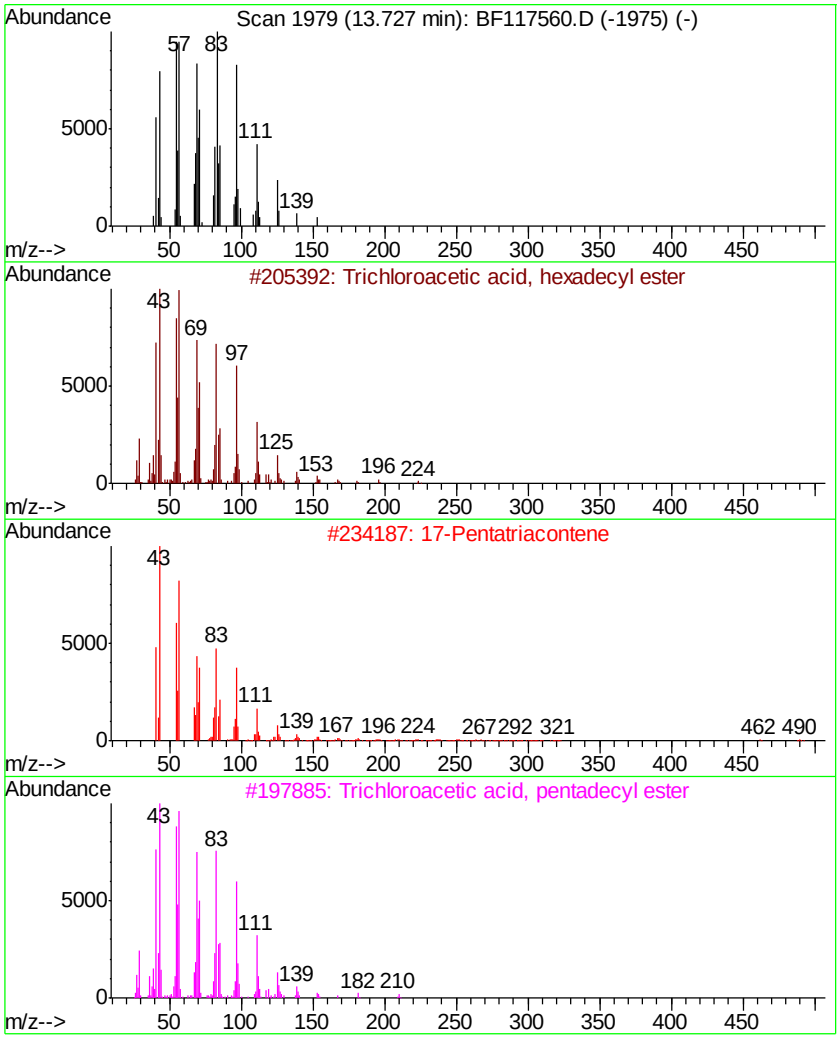
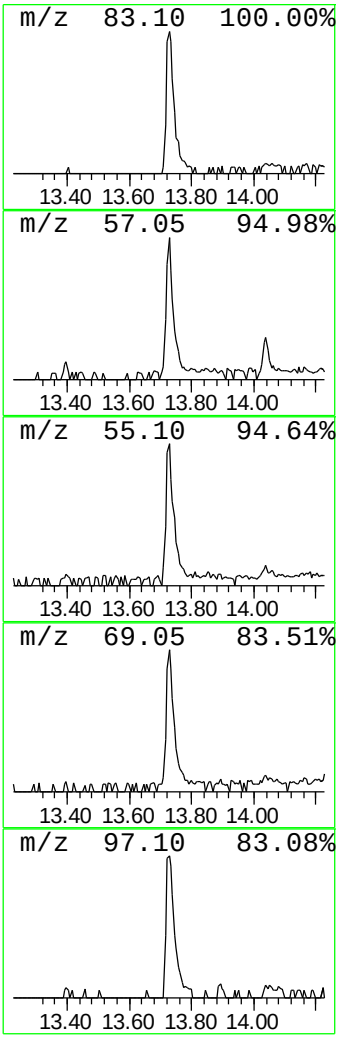
Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	11.52 ng	141767	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102819\
Data File : BF117560.D
Acq On : 28 Oct 2019 14:43
Operator : JU
Sample : K5543-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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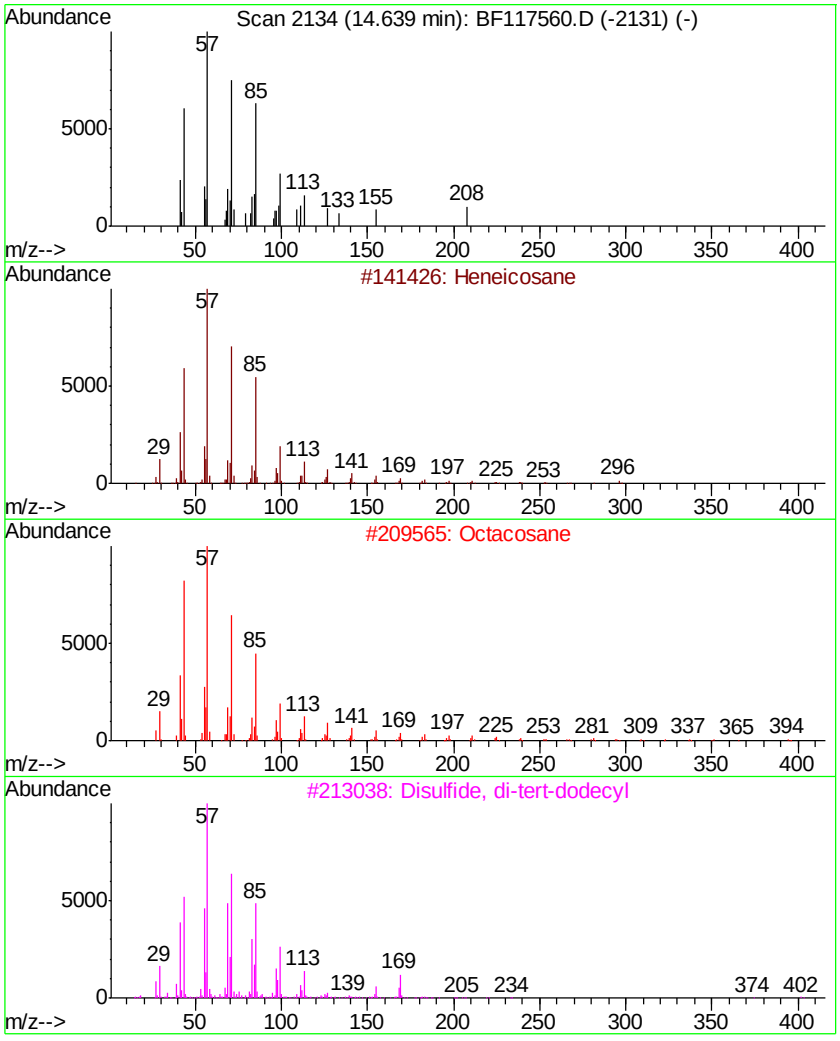
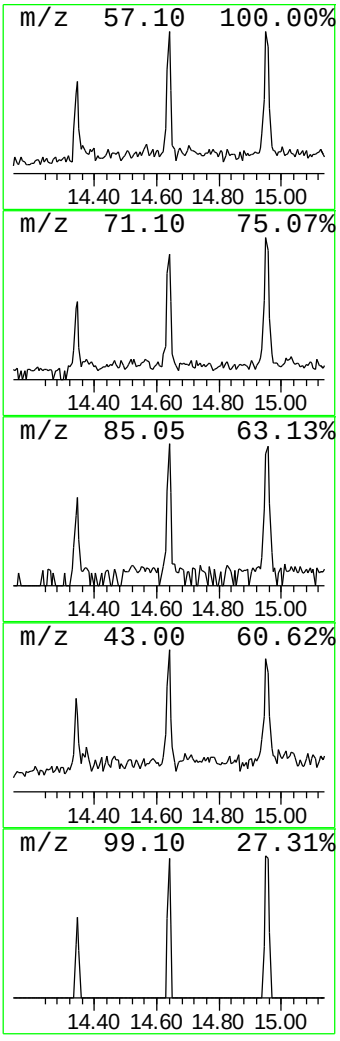
Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.08 ng	24878	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Octacosane	394	C28H58	000630-02-4	78
3	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	78
4	Heptadecane	240	C17H36	000629-78-7	78
5	Hentriacontane	437	C31H64	000630-04-6	72





Library Search Compound Report

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Data File : BF117560.D
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Operator : JU
Sample : K5543-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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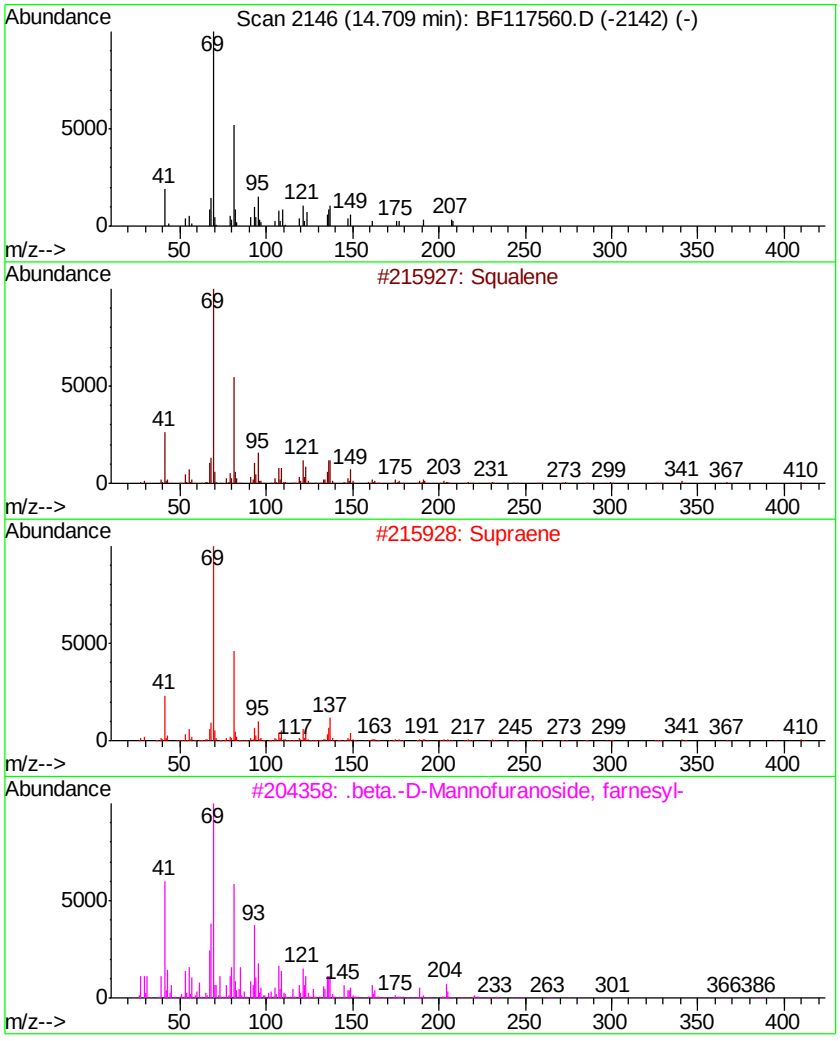
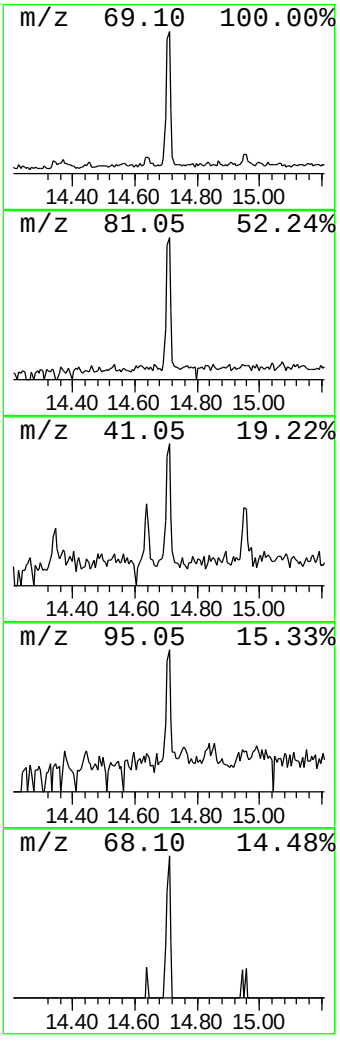
Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.73 ng	44649	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	87
3	.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	72
4	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	56
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	50





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

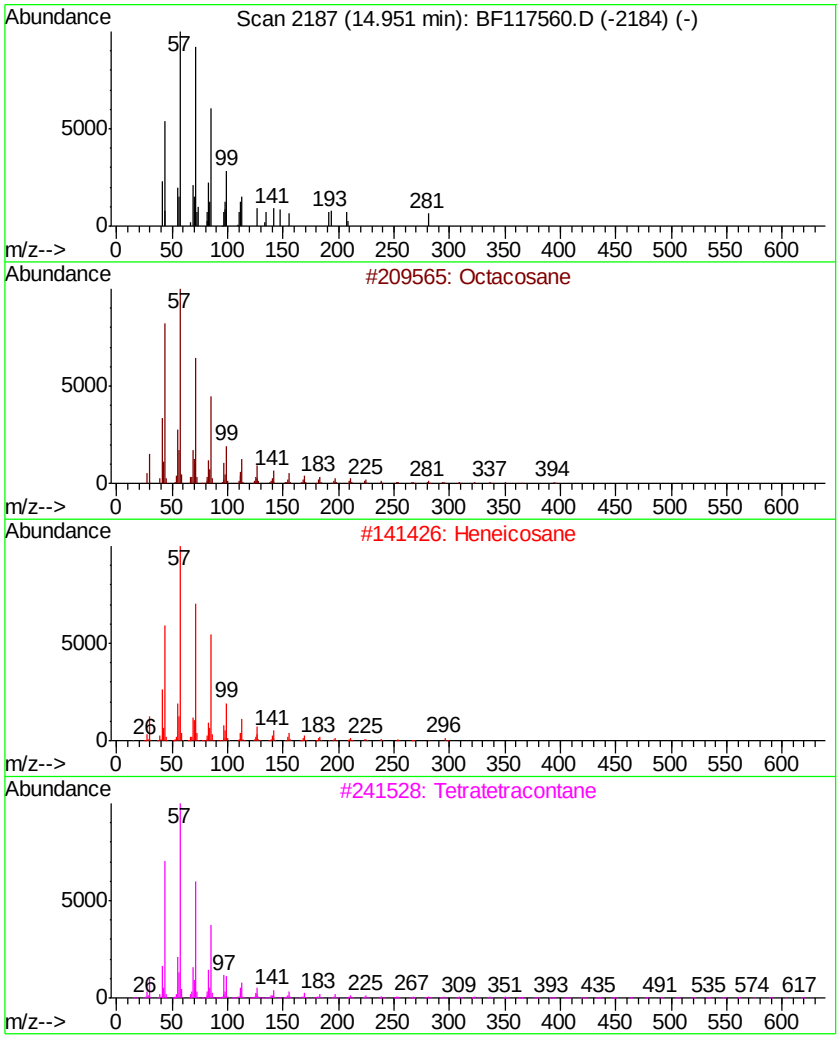
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

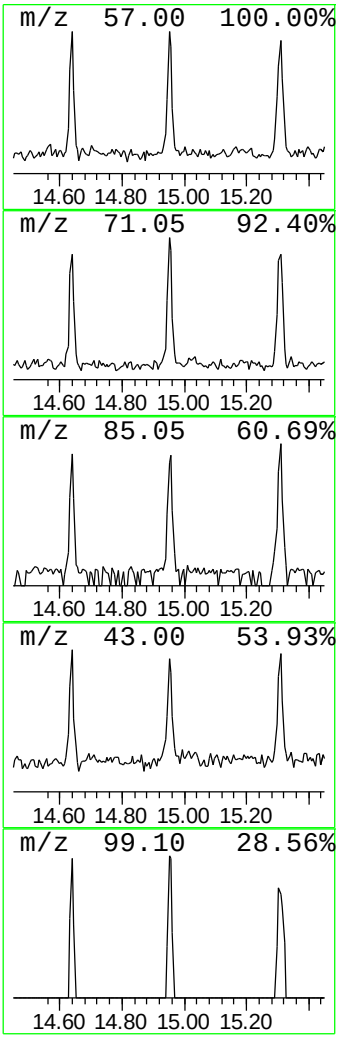
****

Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.50 ng	29941	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tetratetracontane	619	C44H90	007098-22-8	80
4	Hentriacontane	437	C31H64	000630-04-6	80
5	Heptacosane	380	C27H56	000593-49-7	80





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Instrument : BNA_F
ClientSampleId : R-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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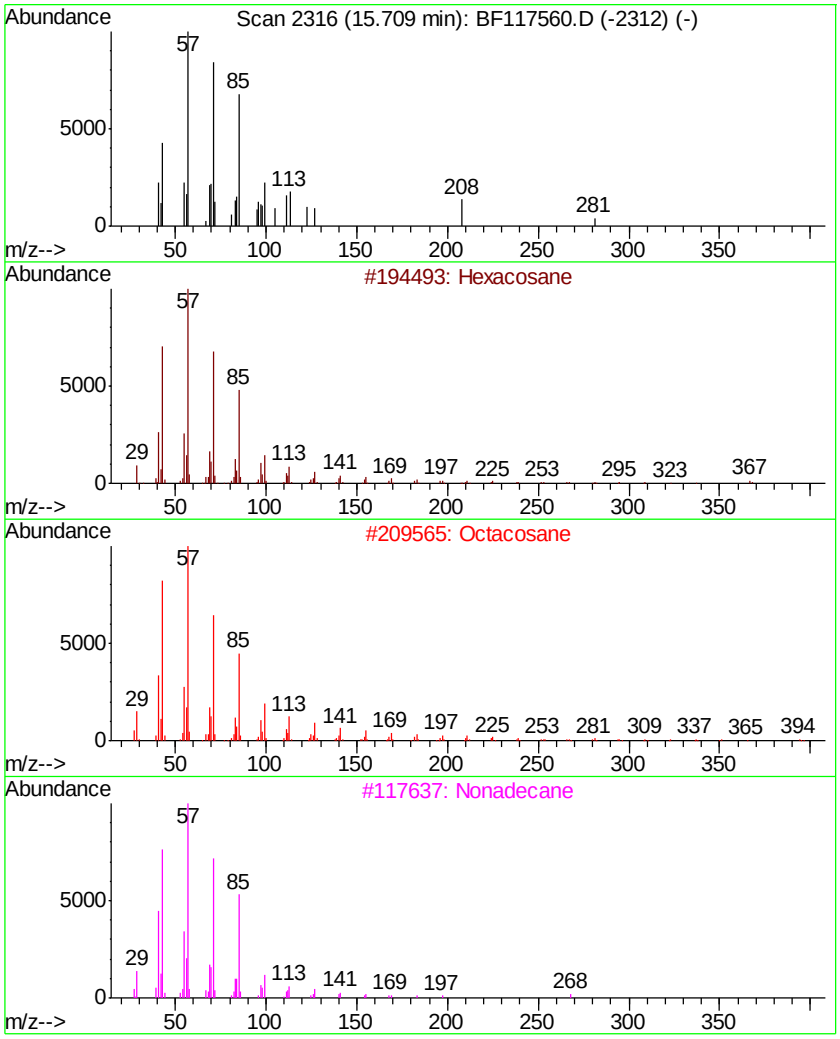
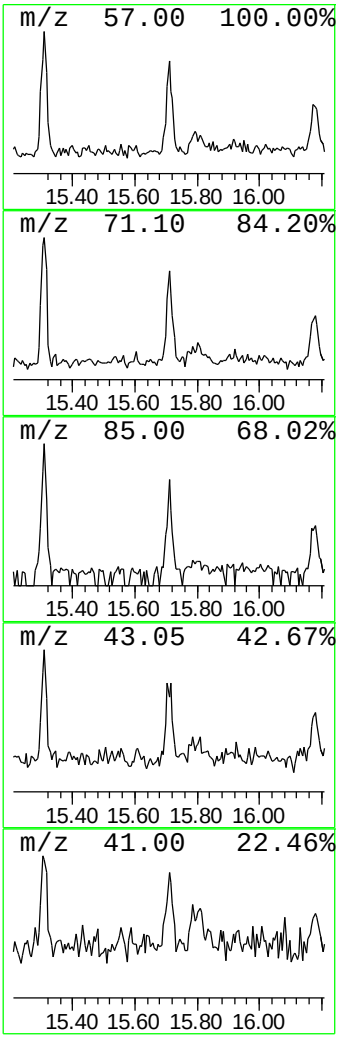
Peak Number 8 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.08 ng	24868	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	72
2	Octacosane	394	C28H58	000630-02-4	72
3	Nonadecane	268	C19H40	000629-92-5	72
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	72
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	64





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	12.4	ng	145274	1	6.73	234174	20.0
unknown6.50	6.50	83.4	ng	976124	1	6.73	234174	20.0
Trichloroacetic a...	13.73	11.5	ng	141767	5	13.89	246144	20.0
Heneicosane	14.64	2.1	ng	24878	6	15.33	239507	20.0
Squalene	14.71	3.7	ng	44649	6	15.33	239507	20.0
Octacosane	14.95	2.5	ng	29941	6	15.33	239507	20.0
Hexacosane	15.71	2.1	ng	24868	6	15.33	239507	20.0