LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108917.D
Acq On : 11 Sep 2018 2:37
Operator : JU/SJ
Sample : J4830-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-S

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-BF090518.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	4.925	436	440	448	rVB	122849	132846	3.16%	0.479%
2	5.348	507	512	515	rBV	1454827	1400166	33.33%	5.051%
3	6.366	681	685	693	rBV	1126790	934371	22.24%	3.371%
4	6.507	705	709	712	rBV	2909943	2439576	58.08%	8.801%
5	6.737	745	748	752	rBV	1093115	881798	20.99%	3.181%
6	6.895	771	775	778	rBV	3732718	3319629	79.03%	11.975%
7	7.301	838	844	847	rBV	2613721	2597106	61.83%	9.369%
8	8.019	962	966	969	rBV	1285790	998366	23.77%	3.602%
9	9.095	1145	1149	1152	rBV	4824543	4200436	100.00%	15.153%
10	9.484	1212	1215	1224	rVB	417660	325393	7.75%	1.174%
11	9.766	1260	1263	1272	rVB	1071970	958720	22.82%	3.458%
12	10.448	1376	1379	1382	rVB	101218	73437	1.75%	0.265%
13	10.554	1393	1397	1409	rBV	1558272	1519485	36.17%	5.481%
14	11.248	1511	1515	1518	rBV	989024	883829	21.04%	3.188%
15	12.830	1779	1784	1787	rBV	4295269	3941956	93.85%	14.220%
16	13.742	1934	1939	1949	rBV	142541	238846	5.69%	0.862%
17	13.871	1957	1961	1965	rBV	1230186	1062853	25.30%	3.834%
18	14.654	2091	2094	2099	rBV	61681	60781	1.45%	0.219%
19	14.724	2103	2106	2110	rVV	251964	238886	5.69%	0.862%
20	14.977	2146	2149	2153	rVB	102943	103505	2.46%	0.373%
21	15.277	2196	2200	2205	rBV	627509	731249	17.41%	2.638%
22	15.336	2206	2210	2215	rVB	122486	153771	3.66%	0.555%
23	15.742	2274	2279	2284	rBV	135189	191809	4.57%	0.692%
24	16.212	2354	2359	2366	rVB	123242	197651	4.71%	0.713%
25	16.765	2448	2453	2460	rVB2	72670	134327	3.20%	0.485%

Sum of corrected areas: 27720792

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
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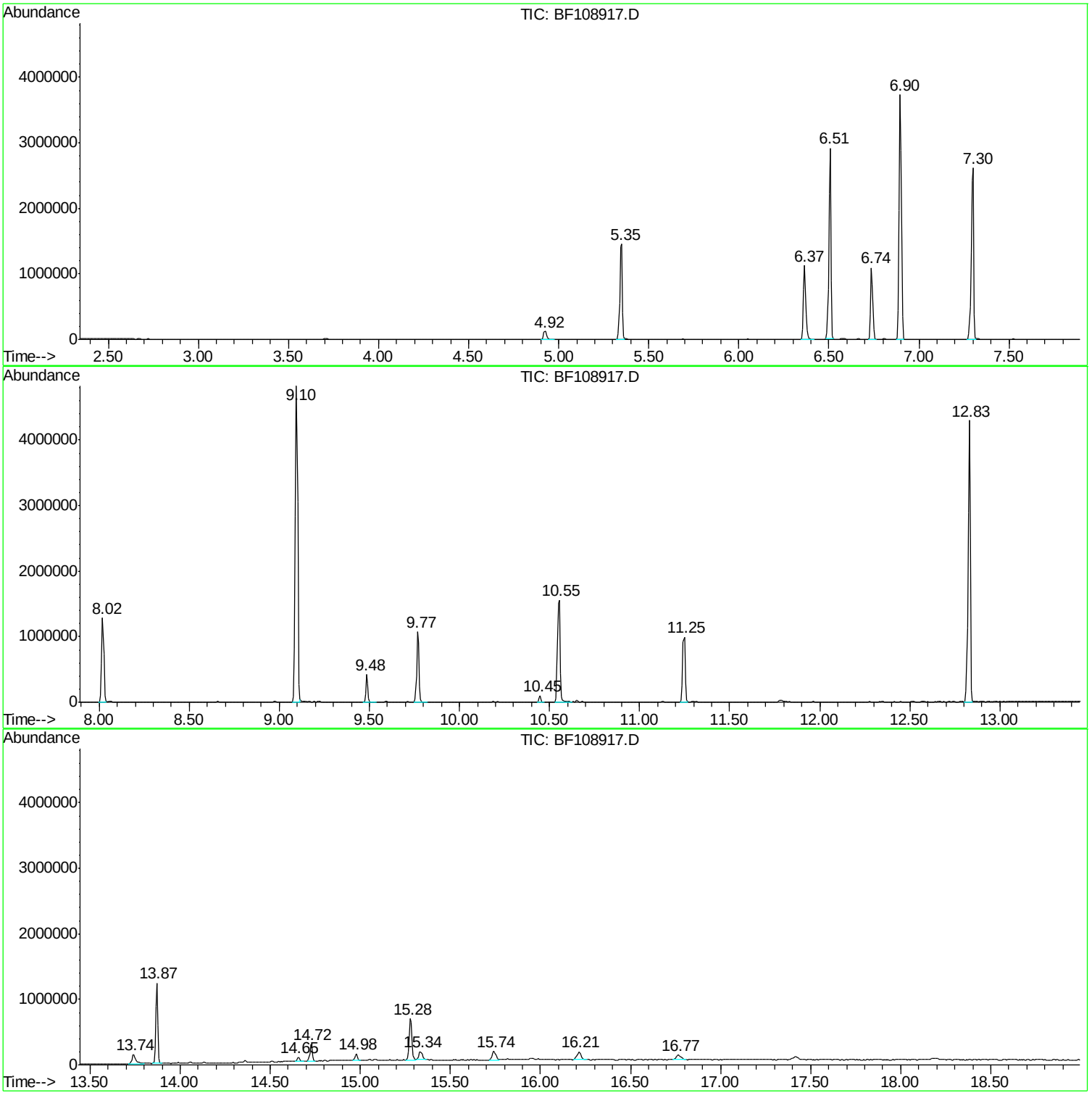
Operator : JU/SJ
Sample : J4830-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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\BF091018\
Data File : BF108917.D
Acq On : 11 Sep 2018 2:37
Operator : JU/SJ
Sample : J4830-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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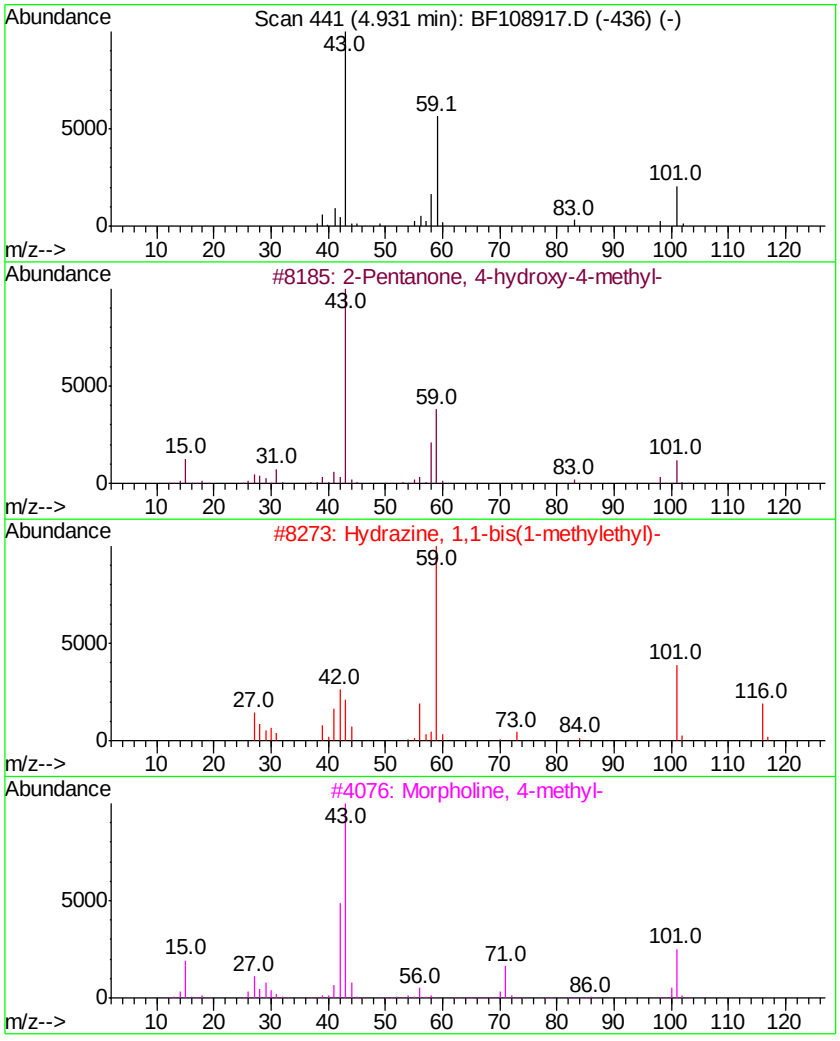
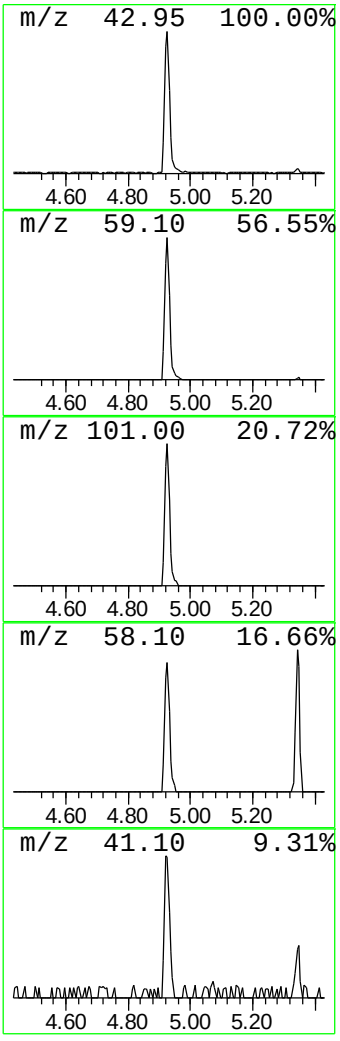
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	3.01 ng	132846	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108917.D
Acq On : 11 Sep 2018 2:37
Operator : JU/SJ
Sample : J4830-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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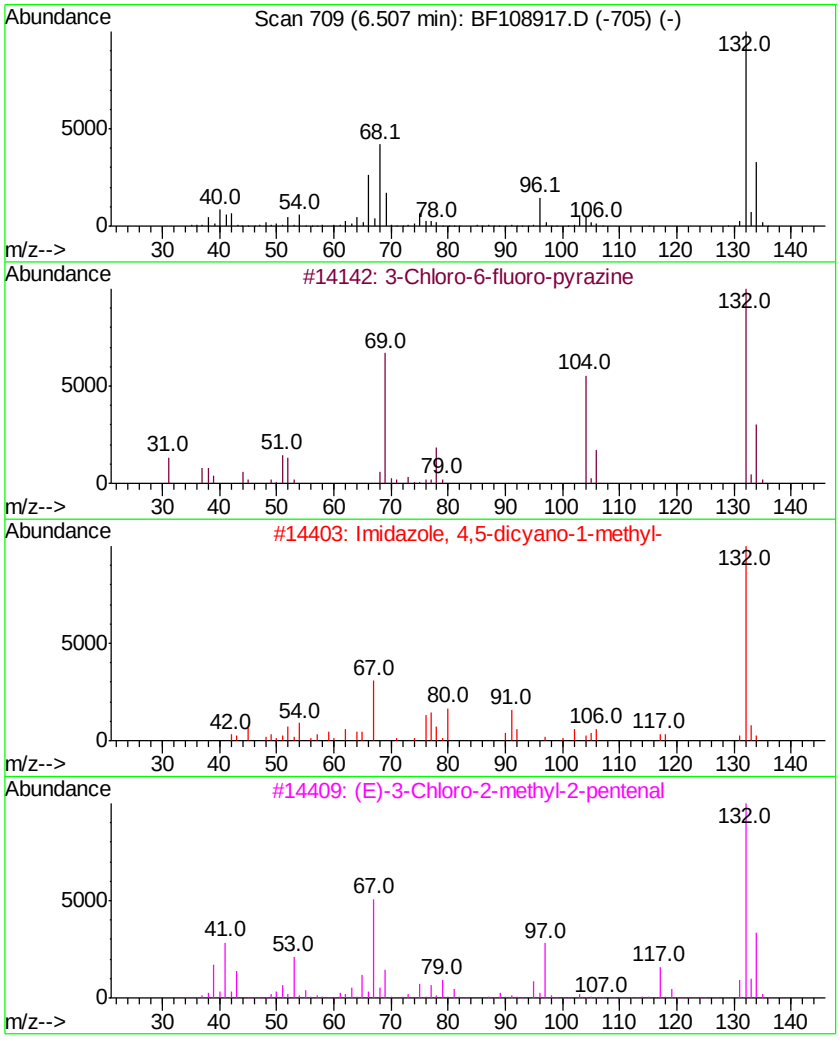
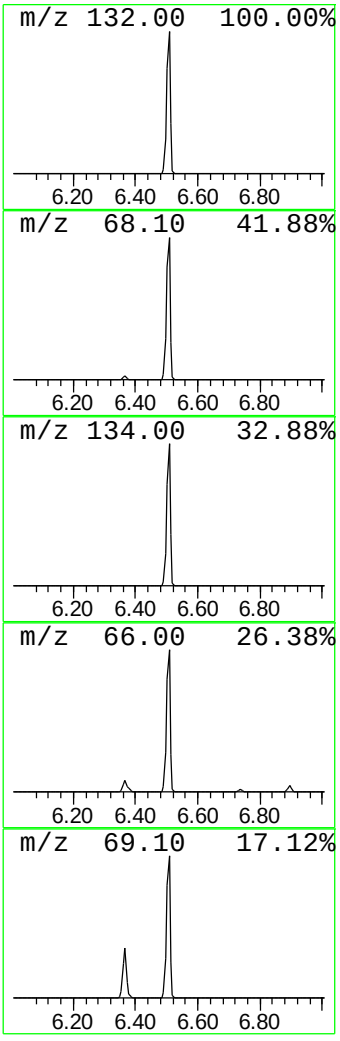
Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	55.33 ng	2439580	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108917.D
Acq On : 11 Sep 2018 2:37
Operator : JU/SJ
Sample : J4830-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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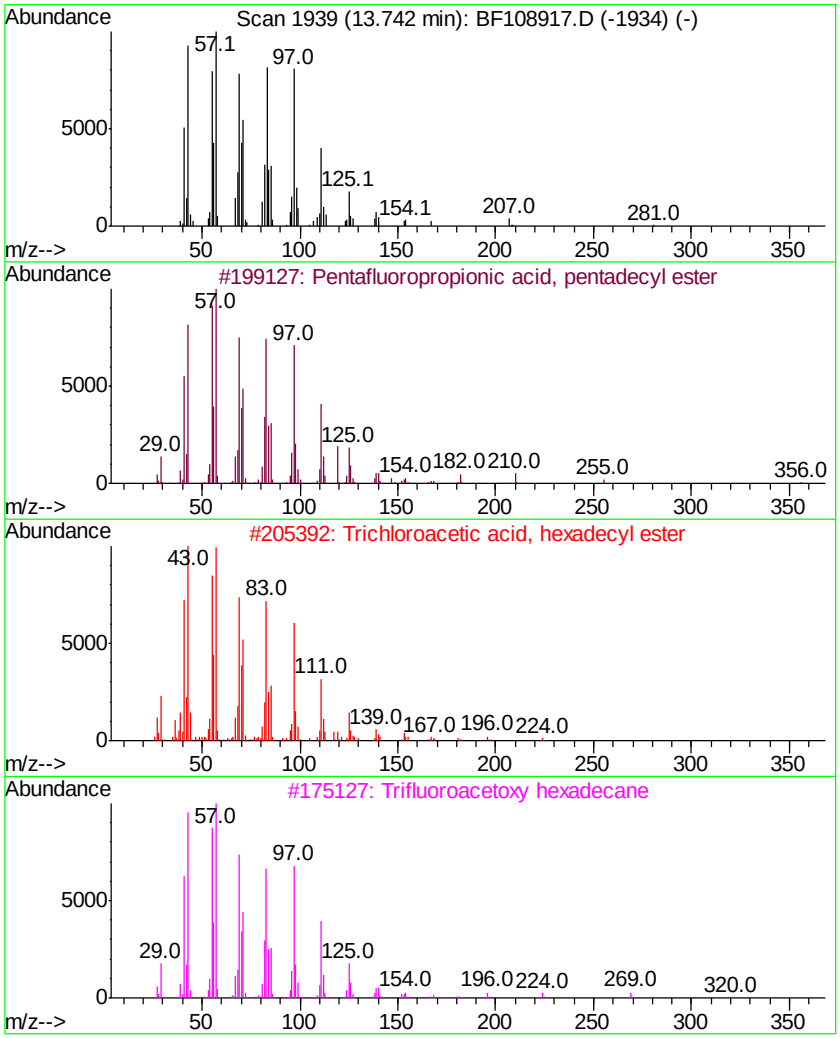
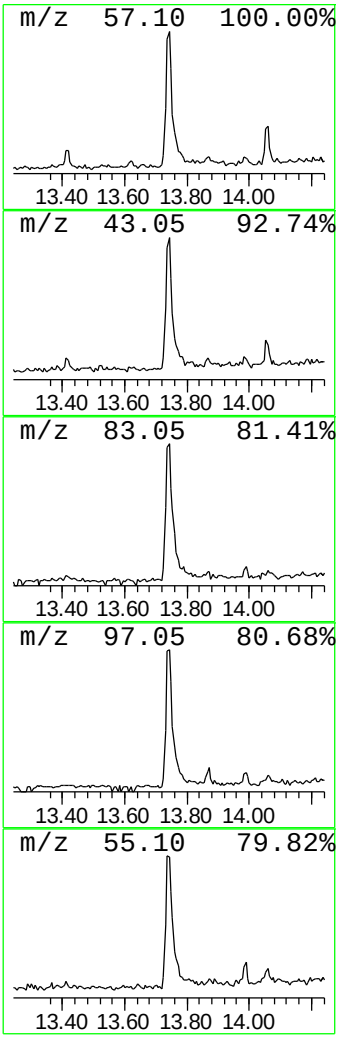
Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	4.49 ng	238846	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108917.D
Acq On : 11 Sep 2018 2:37
Operator : JU/SJ
Sample : J4830-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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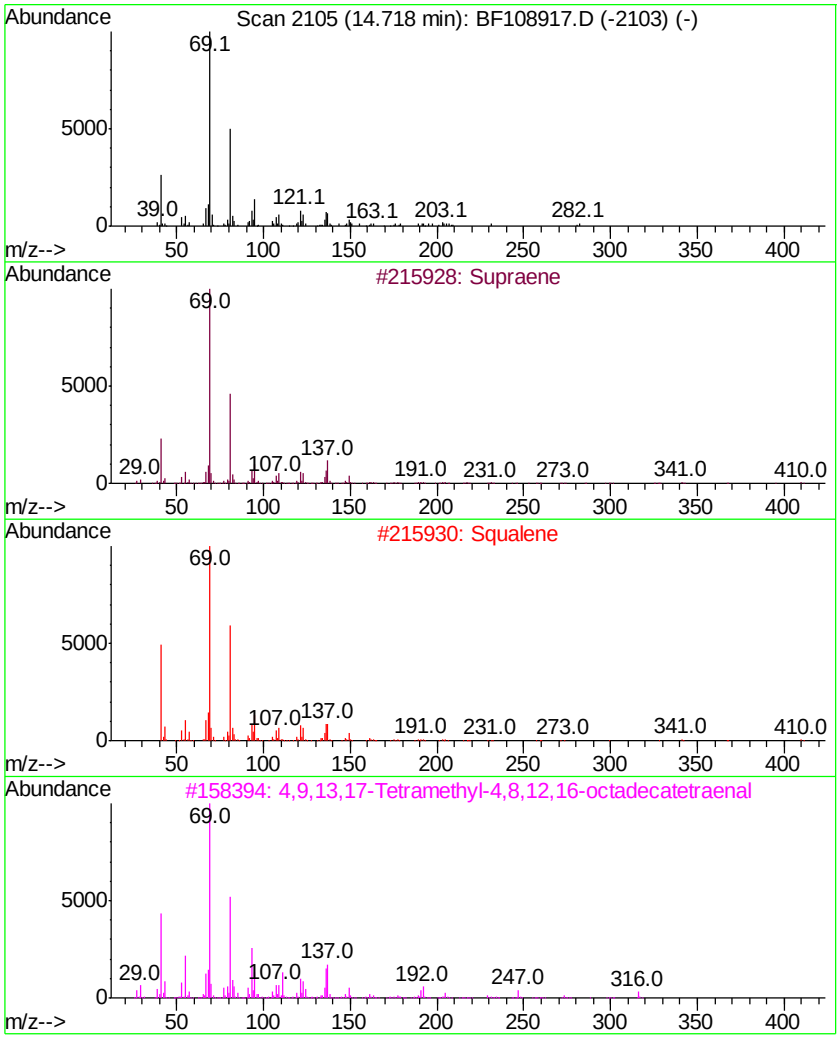
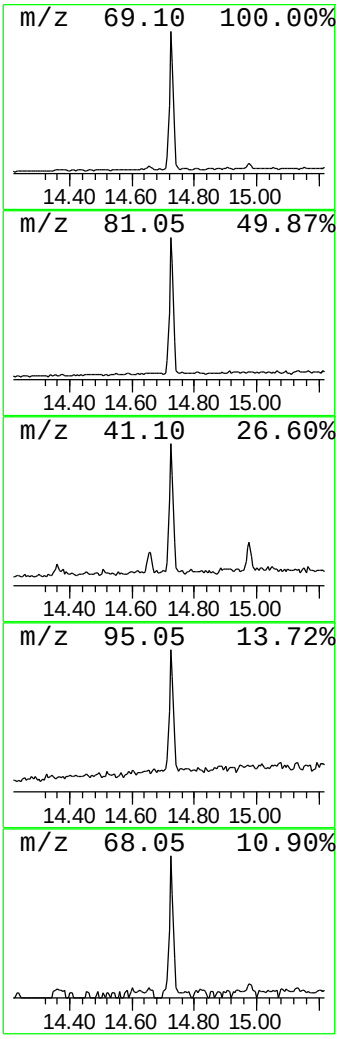
Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	6.53 ng	238886	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108917.D
Acq On : 11 Sep 2018 2:37
Operator : JU/SJ
Sample : J4830-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

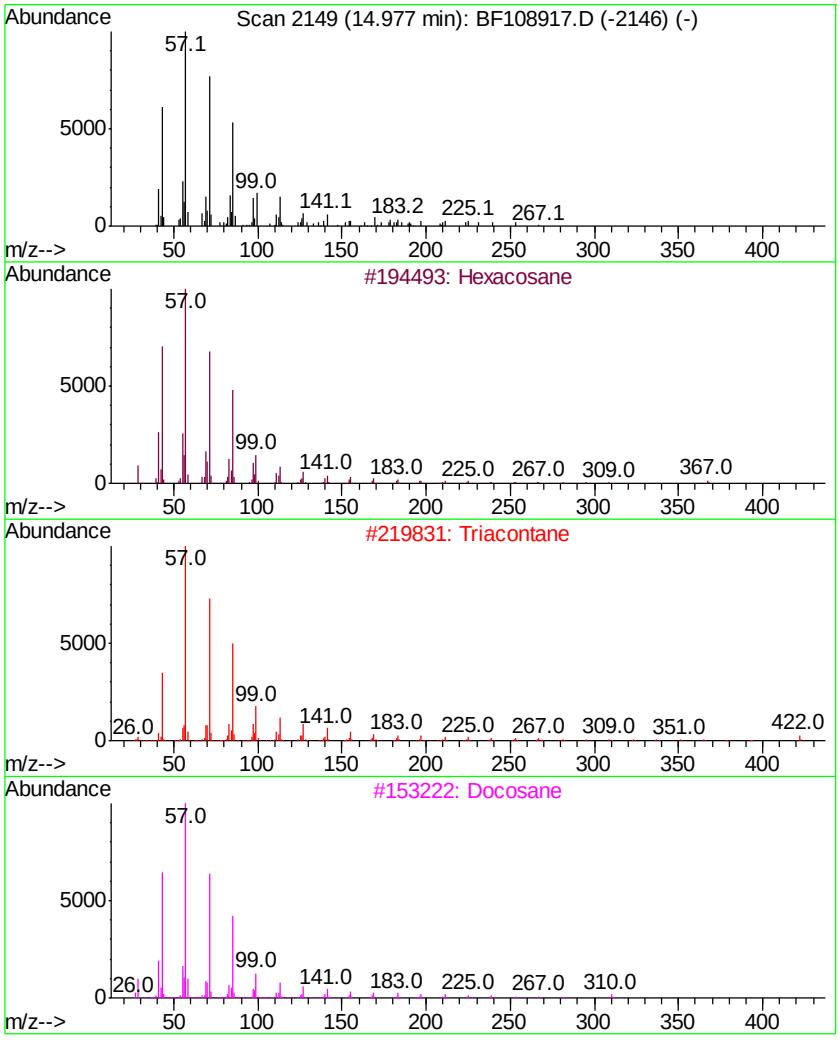
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

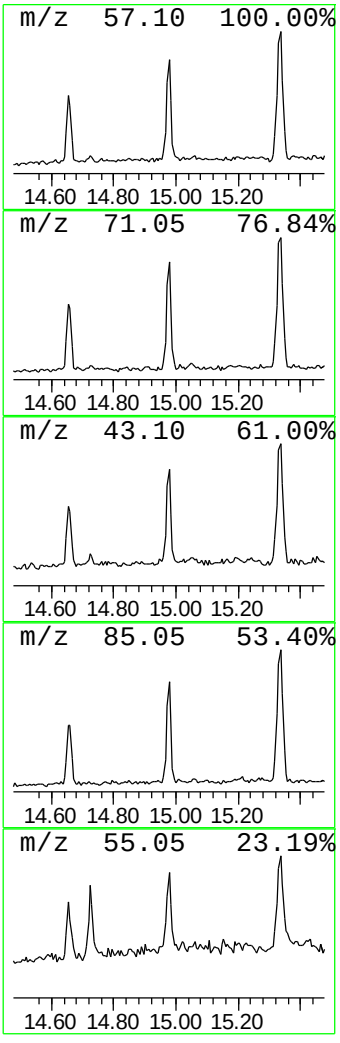
****

Peak Number 6 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.83 ng	103505	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Docosane	310	C22H46	000629-97-0	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Pentacosane	352	C25H52	000629-99-2	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108917.D
Acq On : 11 Sep 2018 2:37
Operator : JU/SJ
Sample : J4830-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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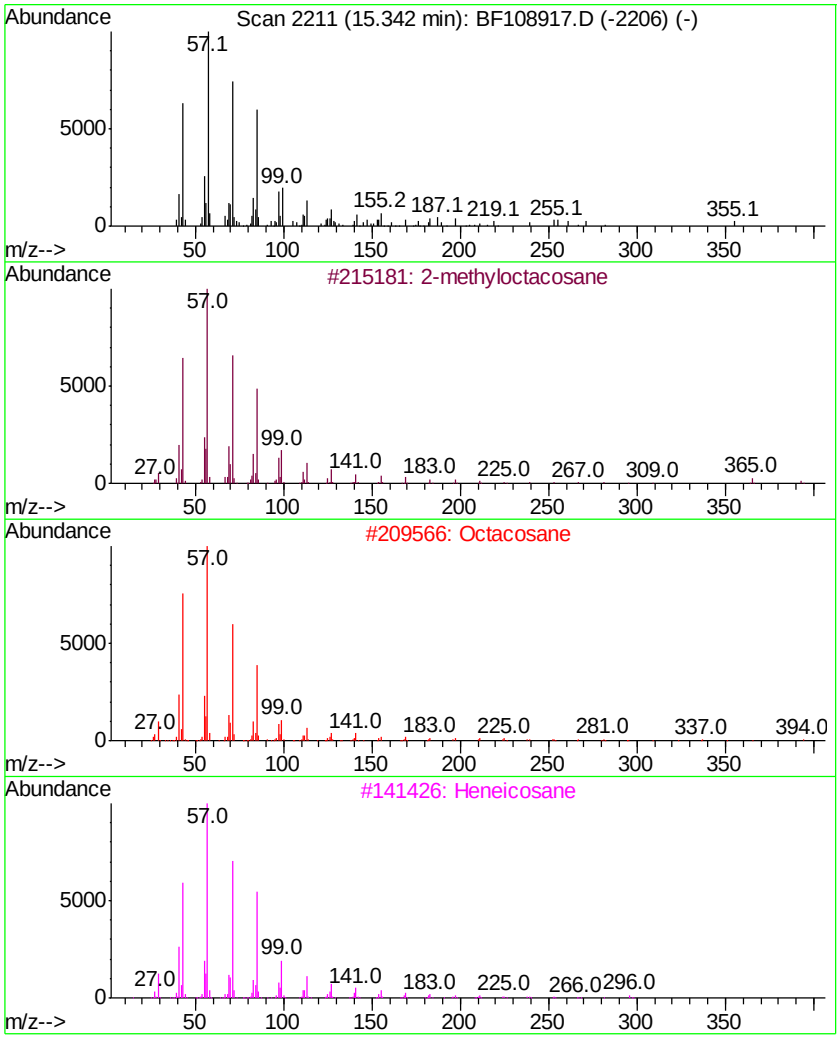
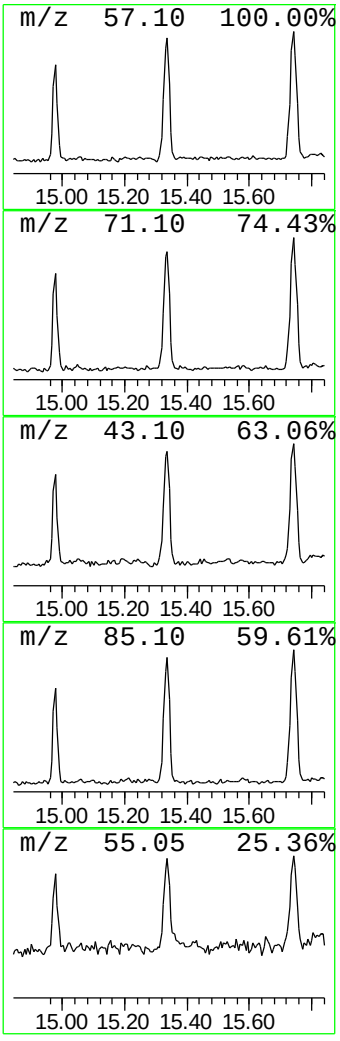
Peak Number 7 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	4.21 ng	153771	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Docosane	310	C22H46	000629-97-0	87





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Sample : J4830-03
Misc :
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Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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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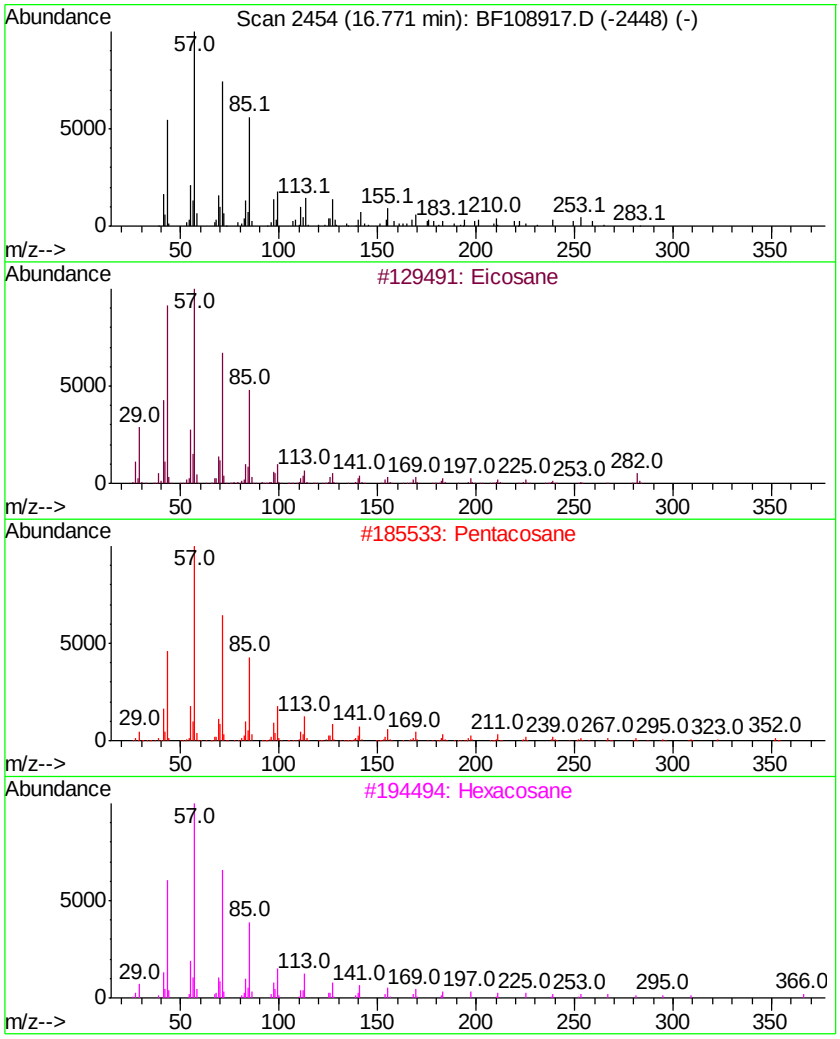
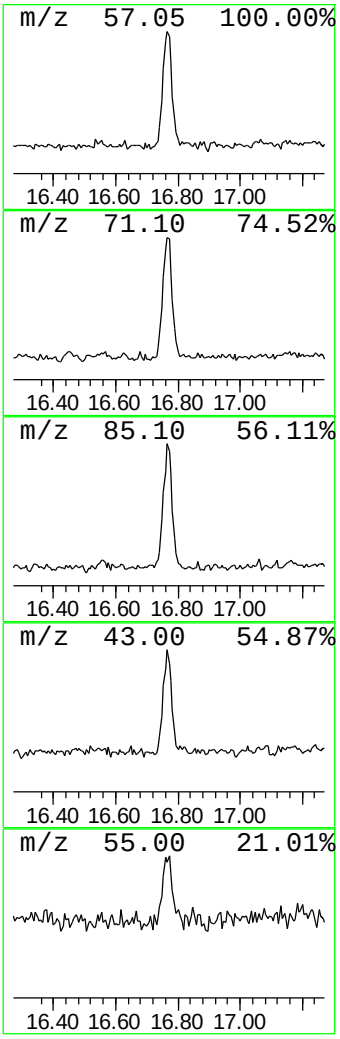
Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	3.67 ng	134327	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Pentacosane	352	C25H52	000629-99-2	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

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Data File : BF108917.D
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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...	4.93	3.0	ng	132846	1	6.74	881798	20.0
unknown6.51	6.51	55.3	ng	2439580	1	6.74	881798	20.0
Pentafluoropropio...	13.74	4.5	ng	238846	5	13.87	1062850	20.0
Supraene	14.72	6.5	ng	238886	6	15.28	731249	20.0
Hexacosane	14.98	2.8	ng	103505	6	15.28	731249	20.0
2-methyloctacosane	15.34	4.2	ng	153771	6	15.28	731249	20.0
Eicosane	16.77	3.7	ng	134327	6	15.28	731249	20.0