LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108920.D
Acq On : 11 Sep 2018 3:58
Operator : JU/SJ
Sample : J4830-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-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	4.919	436	439	446	rVB	108639	115768	3.00%	0.455%
2	5.342	507	511	515	rBV	1334947	1195245	31.00%	4.695%
3	6.366	681	685	694	rVB	900497	790107	20.49%	3.103%
4	6.507	705	709	712	rBV	2521211	2181942	56.58%	8.570%
5	6.736	745	748	752	rBV	1127272	919071	23.83%	3.610%
6	6.895	771	775	778	rBV	3483662	3020557	78.33%	11.864%
7	7.301	838	844	846	rBV	2409871	2388989	61.95%	9.384%
8	8.019	962	966	969	rBV	1356331	1038346	26.93%	4.079%
9	9.095	1145	1149	1152	rBV	4598751	3856191	100.00%	15.147%
10	9.483	1212	1215	1225	rVB	250176	210008	5.45%	0.825%
11	9.766	1260	1263	1267	rVB	1059246	977178	25.34%	3.838%
12	10.448	1375	1379	1383	rVB	75155	57811	1.50%	0.227%
13	10.548	1393	1396	1410	rBV	1370808	1340413	34.76%	5.265%
14	11.248	1511	1515	1518	rBV	966917	883319	22.91%	3.470%
15	12.666	1752	1756	1759	rVB	52714	44397	1.15%	0.174%
16	12.830	1779	1784	1787	rBV	3650248	3314944	85.96%	13.021%
17	13.736	1934	1938	1948	rBV	123743	188043	4.88%	0.739%
18	13.871	1957	1961	1964	rBV	1228992	1060469	27.50%	4.165%
19	14.360	2041	2044	2048	rBV	46291	49301	1.28%	0.194%
20	14.654	2091	2094	2097	rVB	73380	67405	1.75%	0.265%
21	14.724	2102	2106	2111	rBV	565766	546276	14.17%	2.146%
22	14.977	2145	2149	2153	rBV	83612	97781	2.54%	0.384%
23	15.277	2195	2200	2206	rBV	667405	790400	20.50%	3.105%
24	15.330	2206	2209	2216	rVB	97089	130916	3.39%	0.514%
25	15.742	2274	2279	2284	rBV	79587	113020	2.93%	0.444%
26	16.212	2355	2359	2368	rVB3	45779	81028	2.10%	0.318%

Sum of corrected areas: 25458925

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
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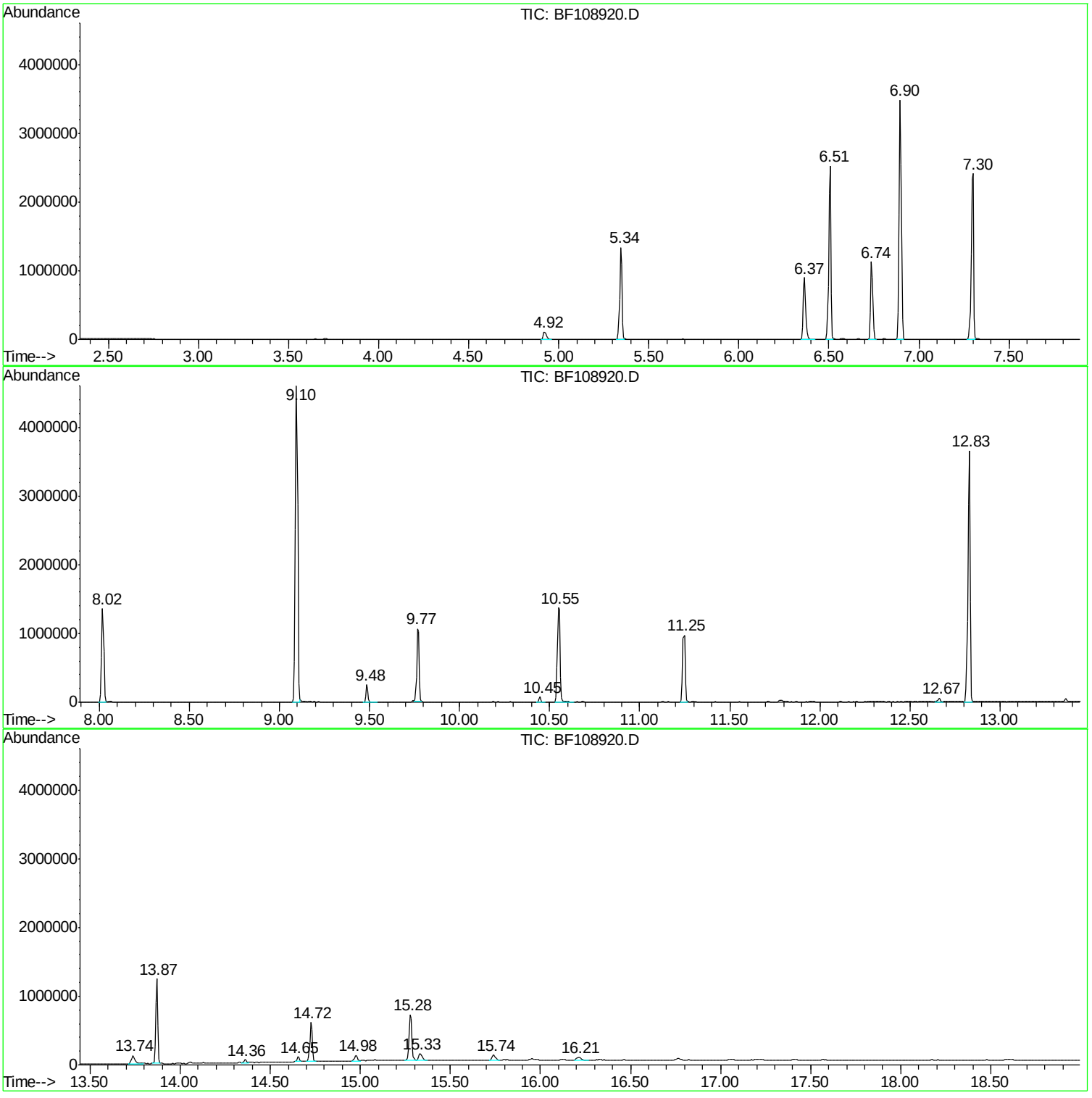
Acq On : 11 Sep 2018 3:58
Operator : JU/SJ
Sample : J4830-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-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 : BF108920.D
Acq On : 11 Sep 2018 3:58
Operator : JU/SJ
Sample : J4830-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-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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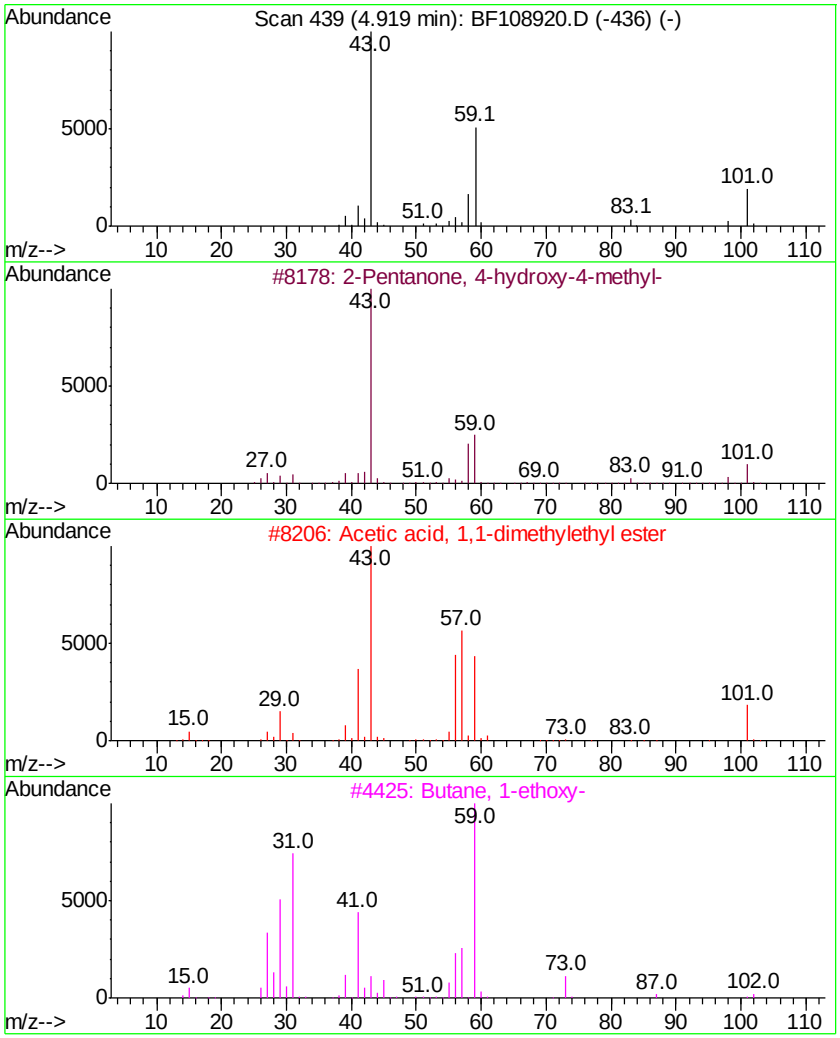
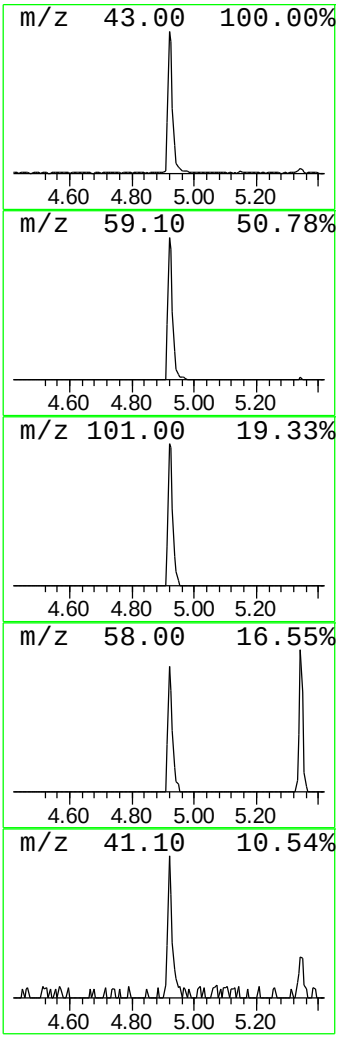
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.52 ng	115768	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	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108920.D
Acq On : 11 Sep 2018 3:58
Operator : JU/SJ
Sample : J4830-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-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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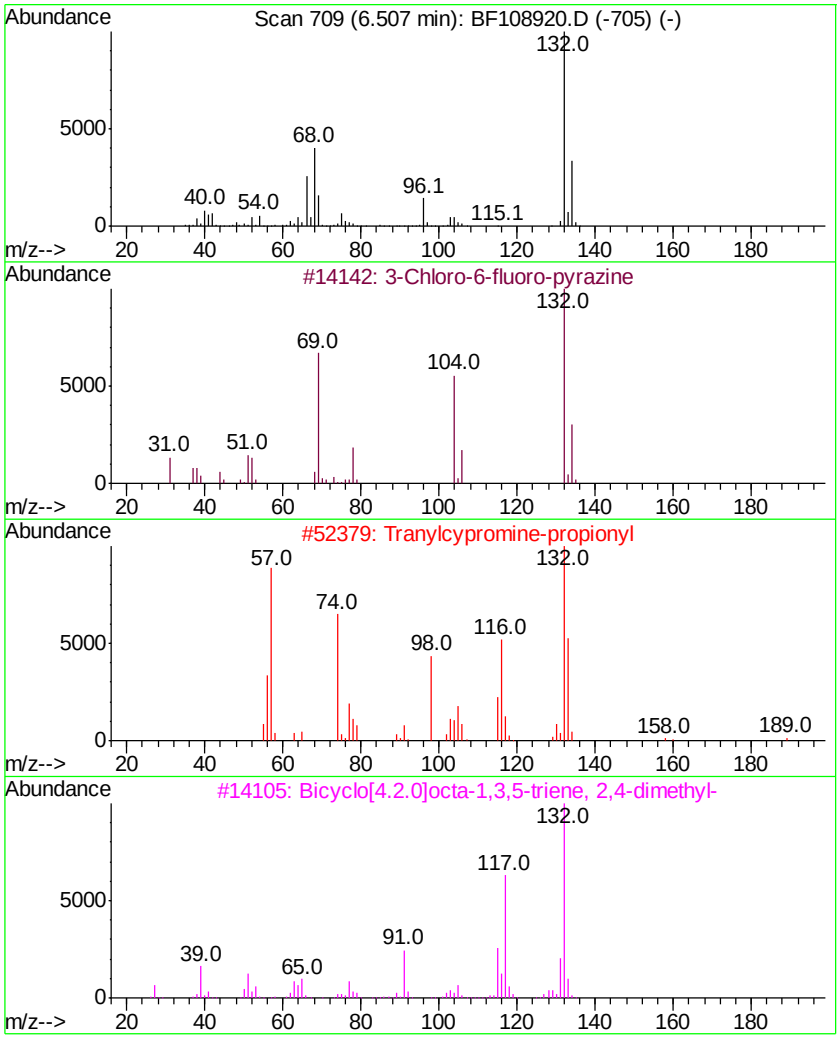
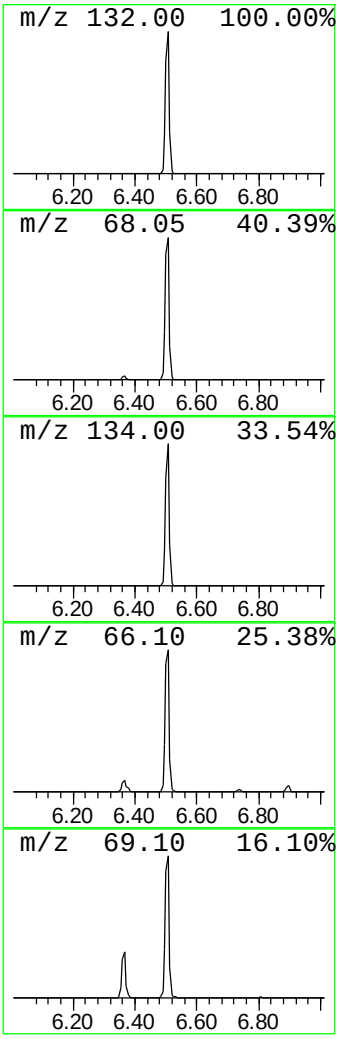
Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	47.48 ng	2181940	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108920.D
Acq On : 11 Sep 2018 3:58
Operator : JU/SJ
Sample : J4830-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-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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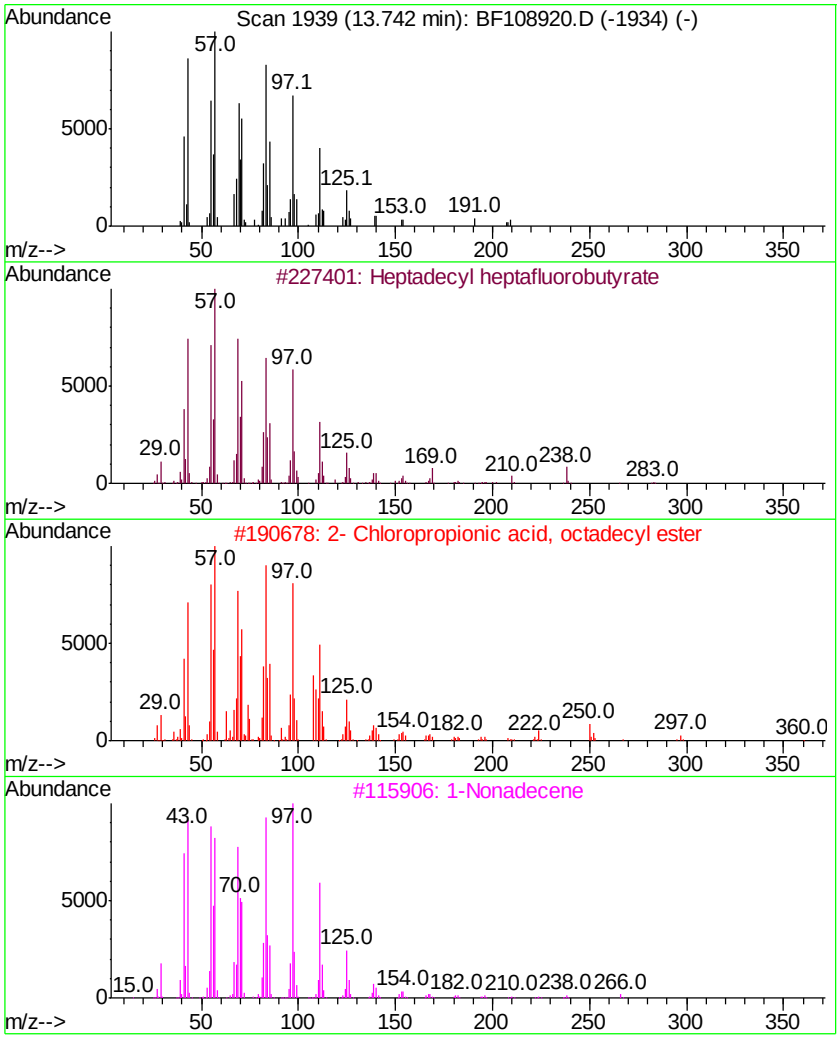
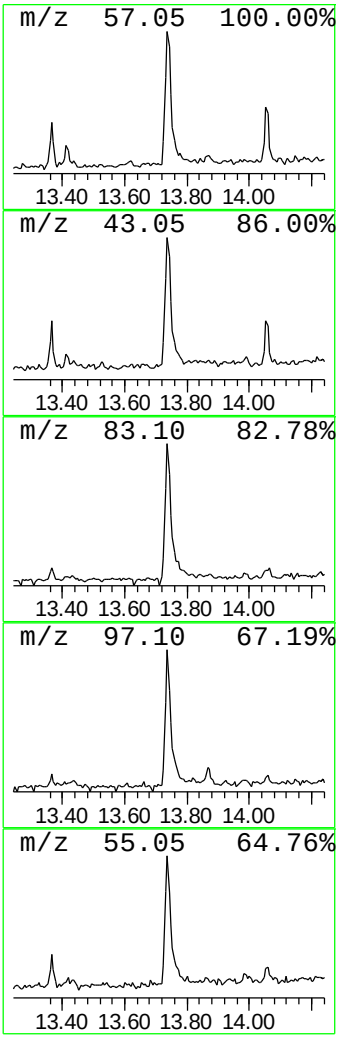
Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.55 ng	188043	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108920.D
Acq On : 11 Sep 2018 3:58
Operator : JU/SJ
Sample : J4830-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-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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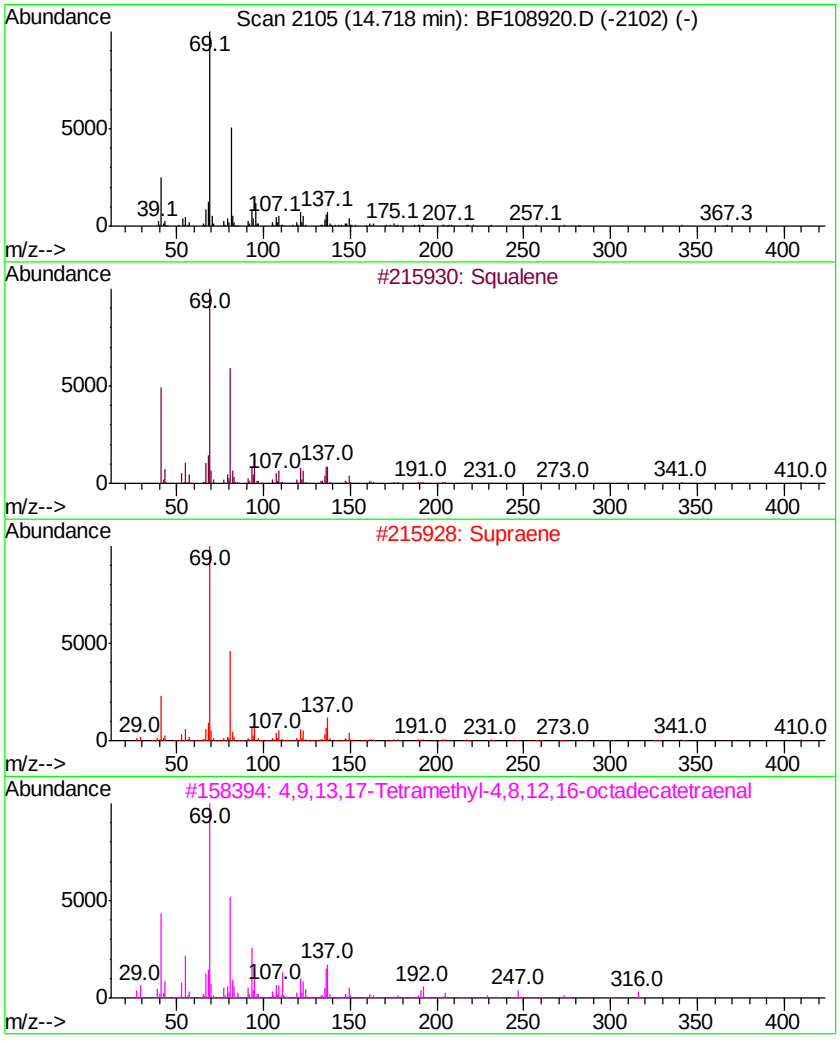
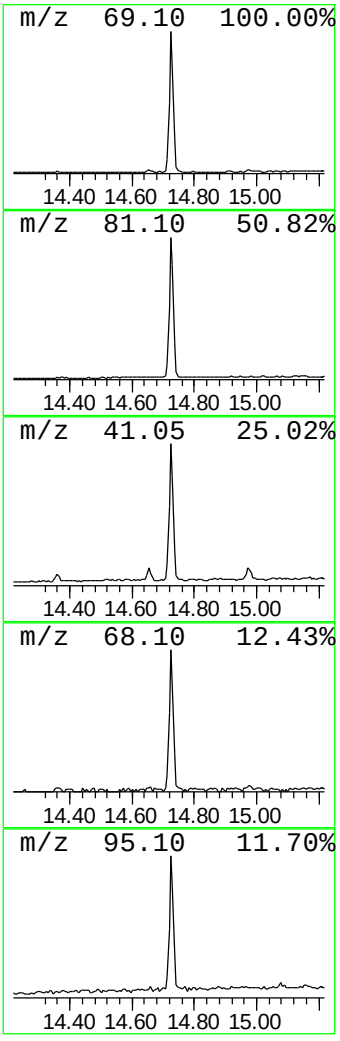
Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	13.82 ng	546276	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	78
5	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108920.D
Acq On : 11 Sep 2018 3:58
Operator : JU/SJ
Sample : J4830-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

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

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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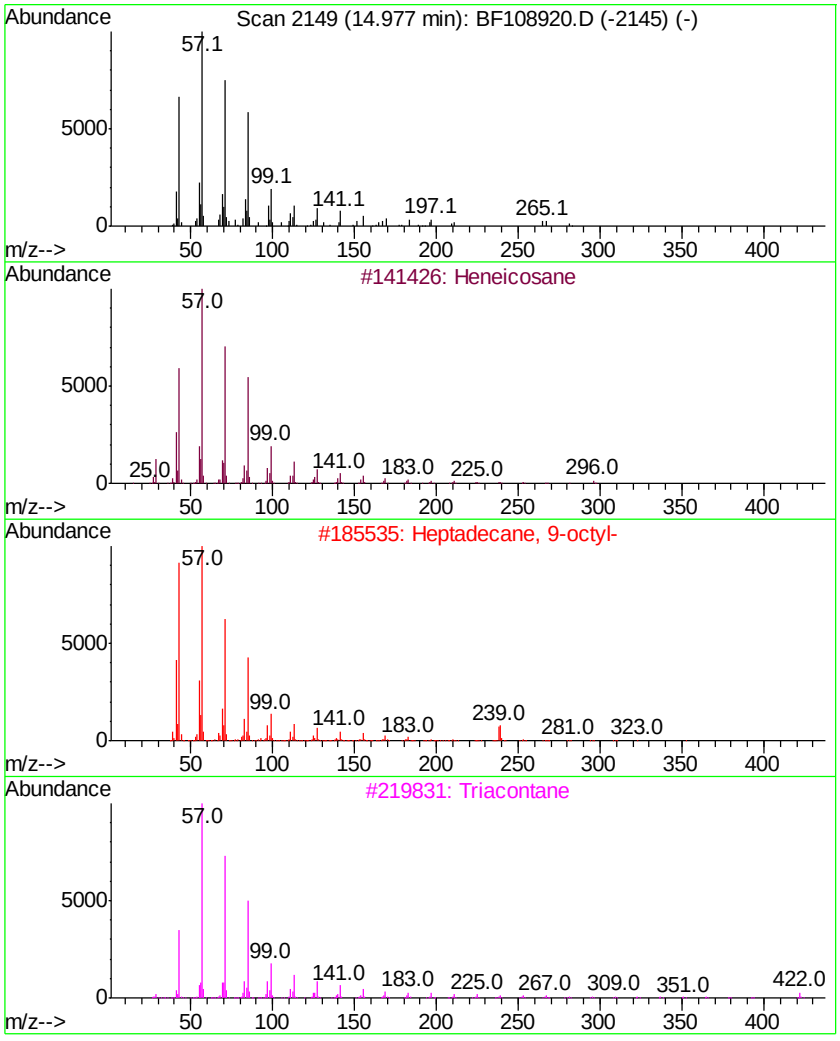
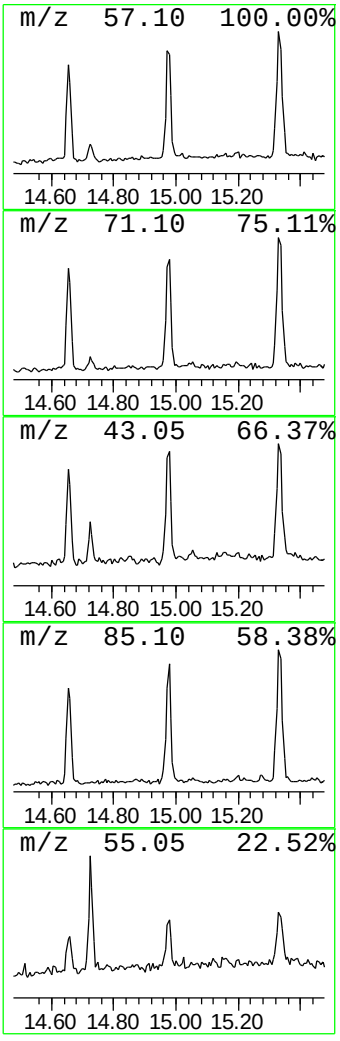
Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.47 ng	97781	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Octadecane	254	C18H38	000593-45-3	91





Library Search Compound Report

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Acq On : 11 Sep 2018 3:58
Operator : JU/SJ
Sample : J4830-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

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

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

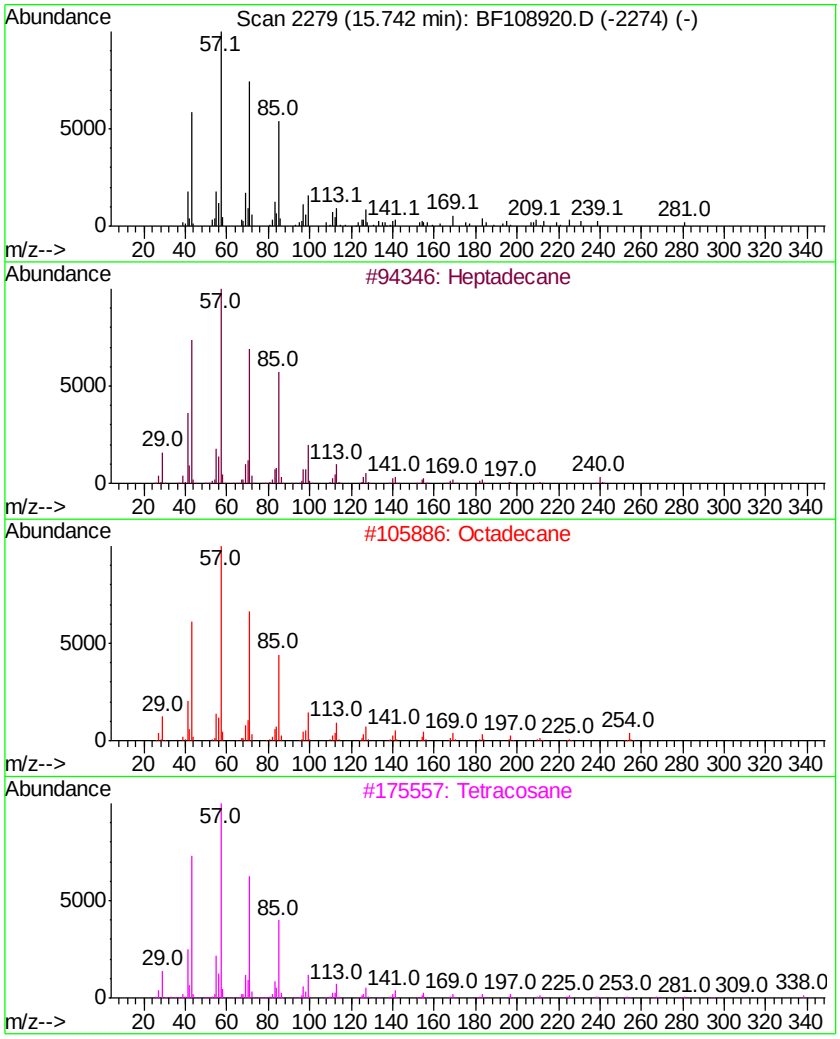
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

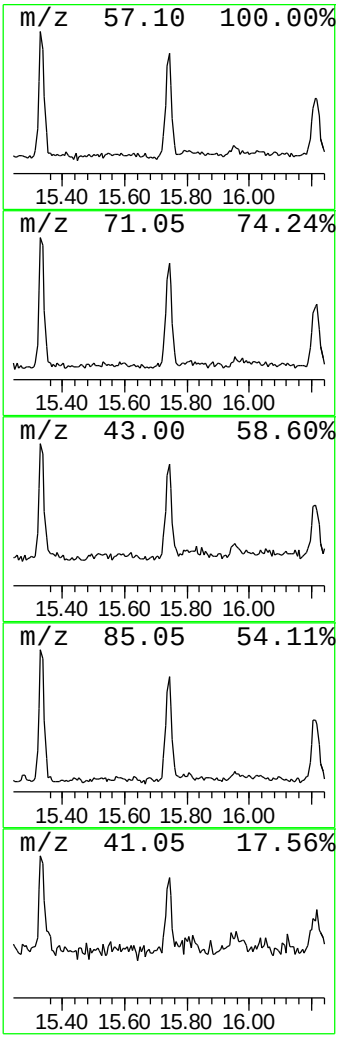
****

Peak Number 8 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.86 ng	113020	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Octadecane	254	C18H38	000593-45-3	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Hentriacontane	437	C31H64	000630-04-6	87





Library Search Compound Report

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Instrument :
BNA_F
ClientSampleId :
090618-SIDI-F-U-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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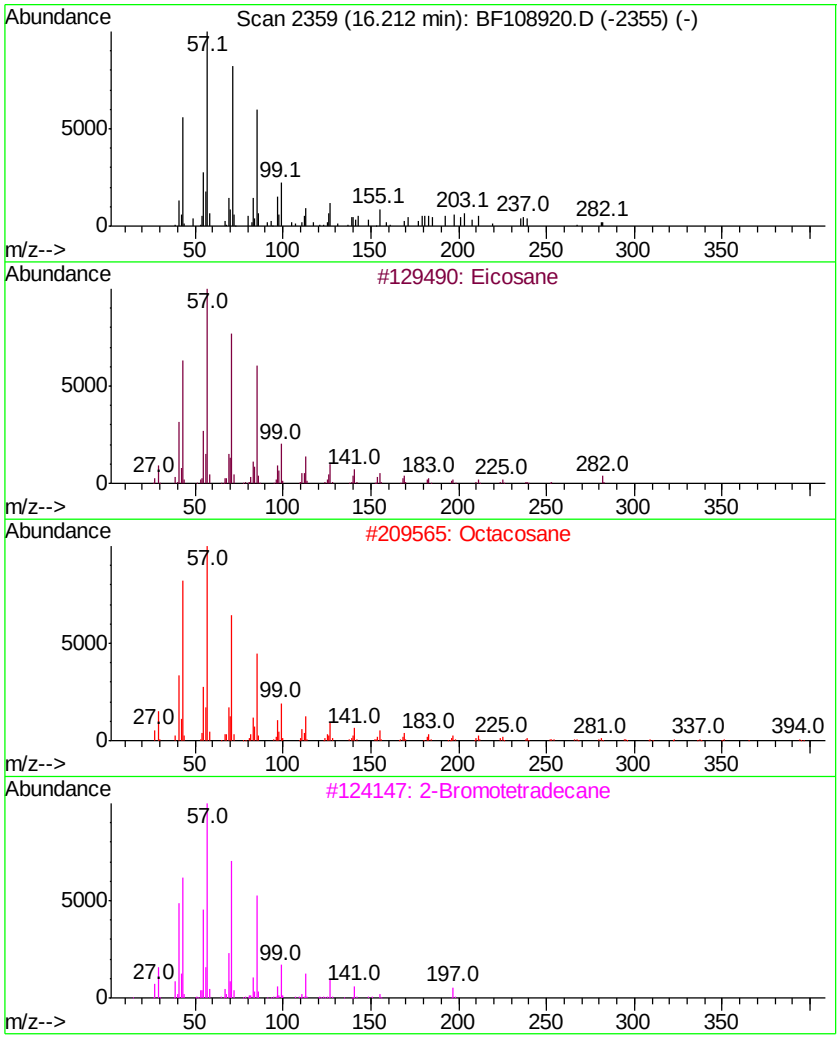
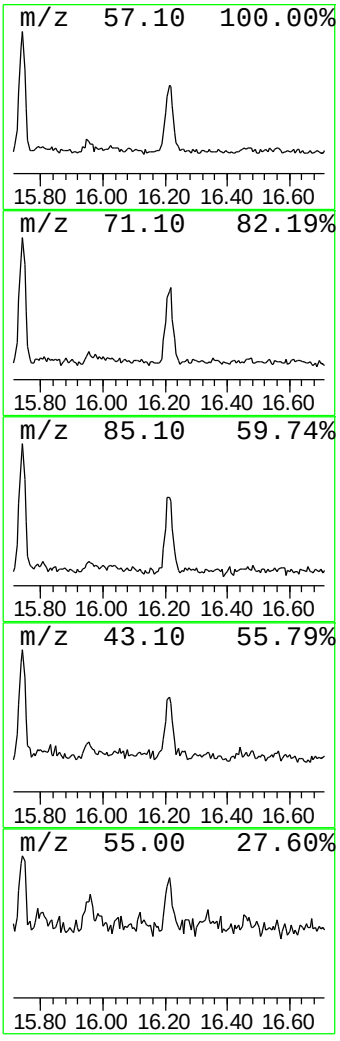
Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	2.05 ng	81028	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Octacosane	394	C28H58	000630-02-4	80
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	80
4	1-Decanol, 2,2-dimethyl-	186	C12H26O	002370-15-2	80
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80





Tentatively Identified Compound (LSC) summary

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Data File : BF108920.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...	4.92	2.5	ng	115768	1	6.74	919071	20.0
unknown6.51	6.51	47.5	ng	2181940	1	6.74	919071	20.0
Heptadecyl heptaf...	13.74	3.5	ng	188043	5	13.87	1060470	20.0
Squalene	14.72	13.8	ng	546276	6	15.28	790400	20.0
Heneicosane	14.98	2.5	ng	97781	6	15.28	790400	20.0
Heptadecane	15.74	2.9	ng	113020	6	15.28	790400	20.0
Eicosane	16.21	2.0	ng	81028	6	15.28	790400	20.0