LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108918.D
Acq On : 11 Sep 2018 3:04
Operator : JU/SJ
Sample : J4830-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

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

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	451	rVB	151168	164198	3.54%	0.569%
2	5.349	507	512	515	rBV	1721641	1526278	32.93%	5.292%
3	6.366	681	685	695	rBV	1406608	1139399	24.58%	3.951%
4	6.507	702	709	712	rBV	3127163	2693906	58.12%	9.340%
5	6.737	745	748	752	rBV	1180768	971302	20.95%	3.368%
6	6.895	771	775	778	rBV	3932568	3605632	77.79%	12.501%
7	7.301	838	844	847	rBV	3012889	2872420	61.97%	9.959%
8	8.019	962	966	969	rBV	1437147	1114694	24.05%	3.865%
9	9.095	1145	1149	1152	rBV	5038676	4635208	100.00%	16.071%
10	9.484	1212	1215	1224	rVB	275094	216779	4.68%	0.752%
11	9.766	1260	1263	1274	rVB	1209693	1072225	23.13%	3.718%
12	10.448	1375	1379	1382	rBV	169138	124526	2.69%	0.432%
13	10.554	1393	1397	1407	rBV	1544493	1503074	32.43%	5.211%
14	11.242	1511	1514	1518	rBV	998681	912437	19.68%	3.164%
15	12.830	1779	1784	1787	rBV	4111038	3781929	81.59%	13.113%
16	13.742	1935	1939	1949	rBV3	36871	68486	1.48%	0.237%
17	13.871	1957	1961	1965	rBV	1311055	1076913	23.23%	3.734%
18	14.654	2091	2094	2098	rVB	58445	56285	1.21%	0.195%
19	14.724	2102	2106	2110	rBV	230837	227786	4.91%	0.790%
20	14.977	2145	2149	2154	rBV	73203	85594	1.85%	0.297%
21	15.277	2196	2200	2205	rVB	618714	719942	15.53%	2.496%
22	15.330	2205	2209	2216	rBV	82204	104209	2.25%	0.361%
23	15.742	2274	2279	2286	rBV	67950	106959	2.31%	0.371%
24	16.213	2355	2359	2365	rVB2	37030	61436	1.33%	0.213%

Sum of corrected areas: 28841617

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
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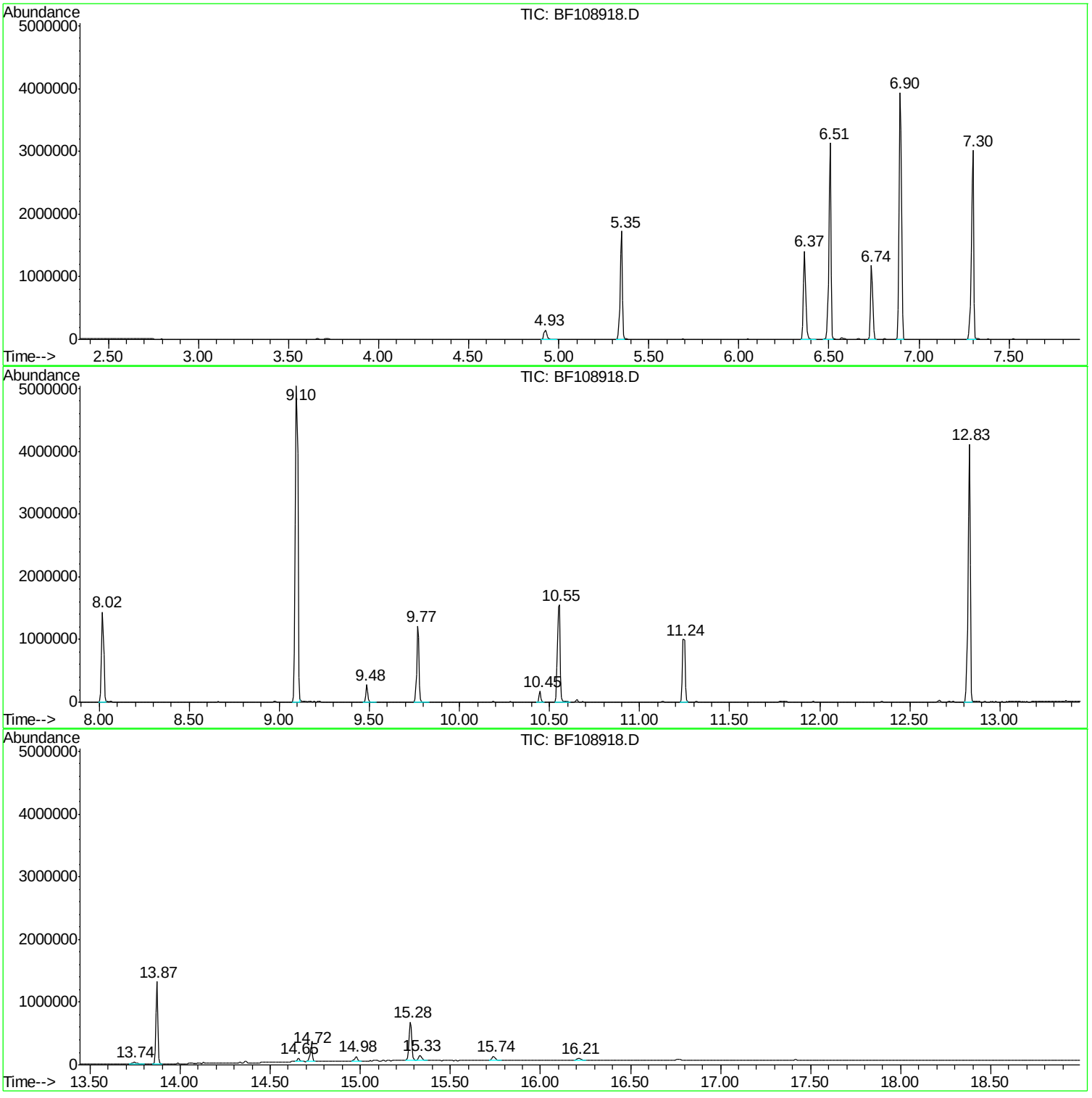
Operator : JU/SJ
Sample : J4830-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

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

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108918.D
Acq On : 11 Sep 2018 3:04
Operator : JU/SJ
Sample : J4830-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

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

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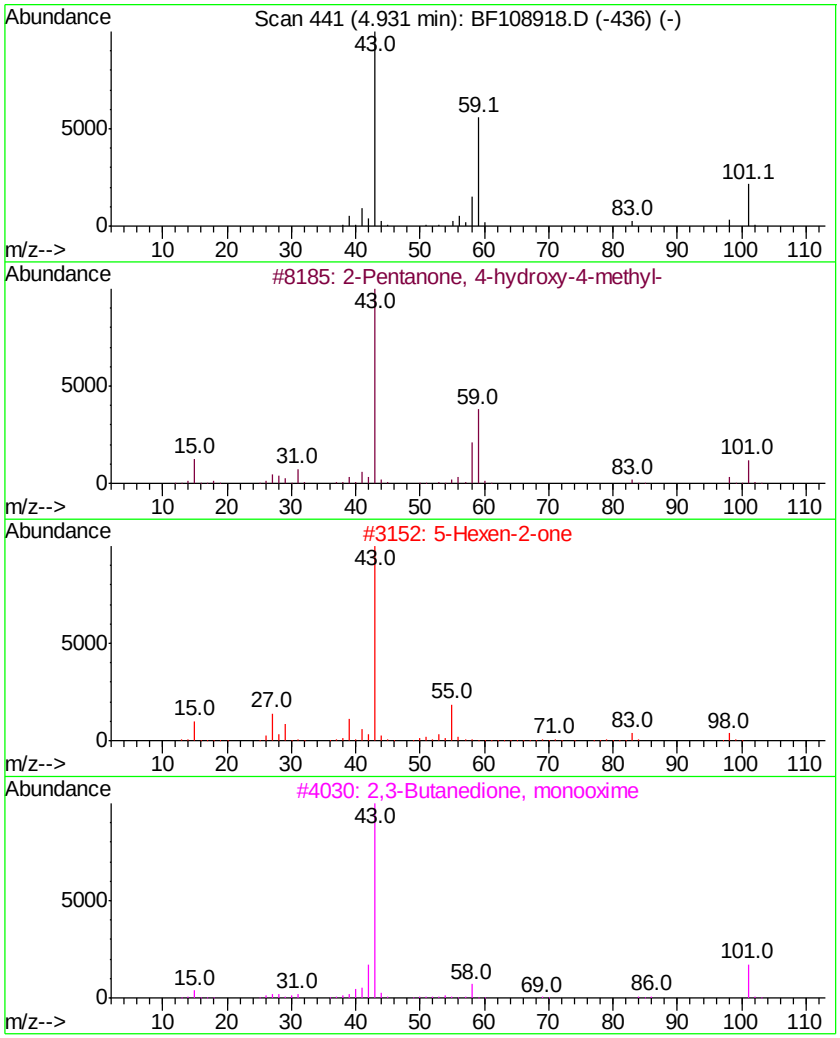
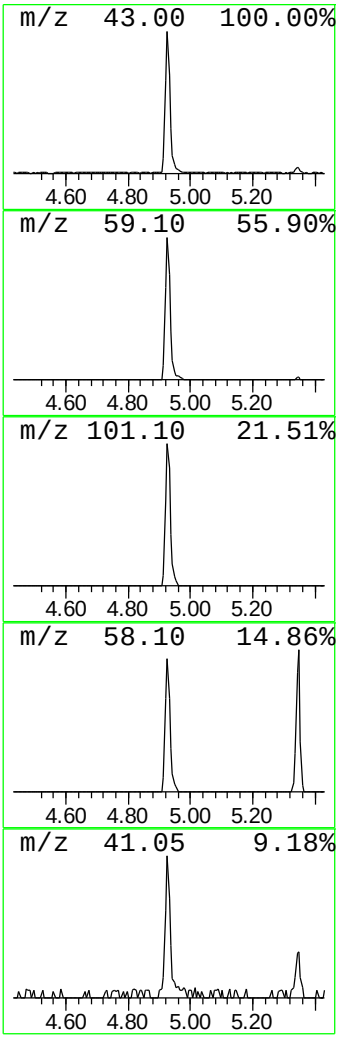
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	3.38 ng	164198	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	59
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108918.D
Acq On : 11 Sep 2018 3:04
Operator : JU/SJ
Sample : J4830-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

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

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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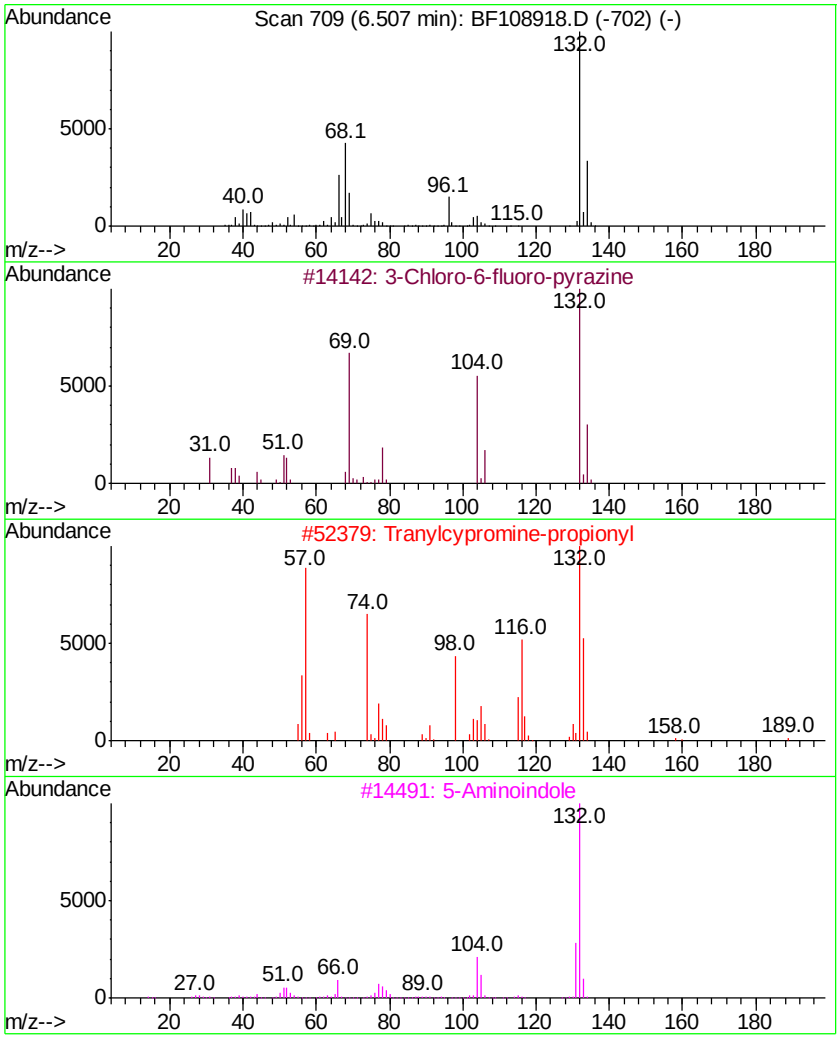
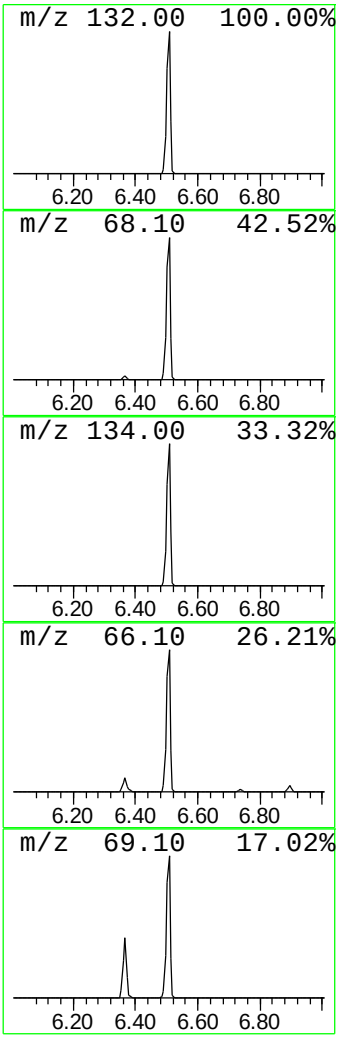
Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	55.47 ng	2693910	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	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Aminoindole	132	C8H8N2	005192-03-0	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108918.D
Acq On : 11 Sep 2018 3:04
Operator : JU/SJ
Sample : J4830-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

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

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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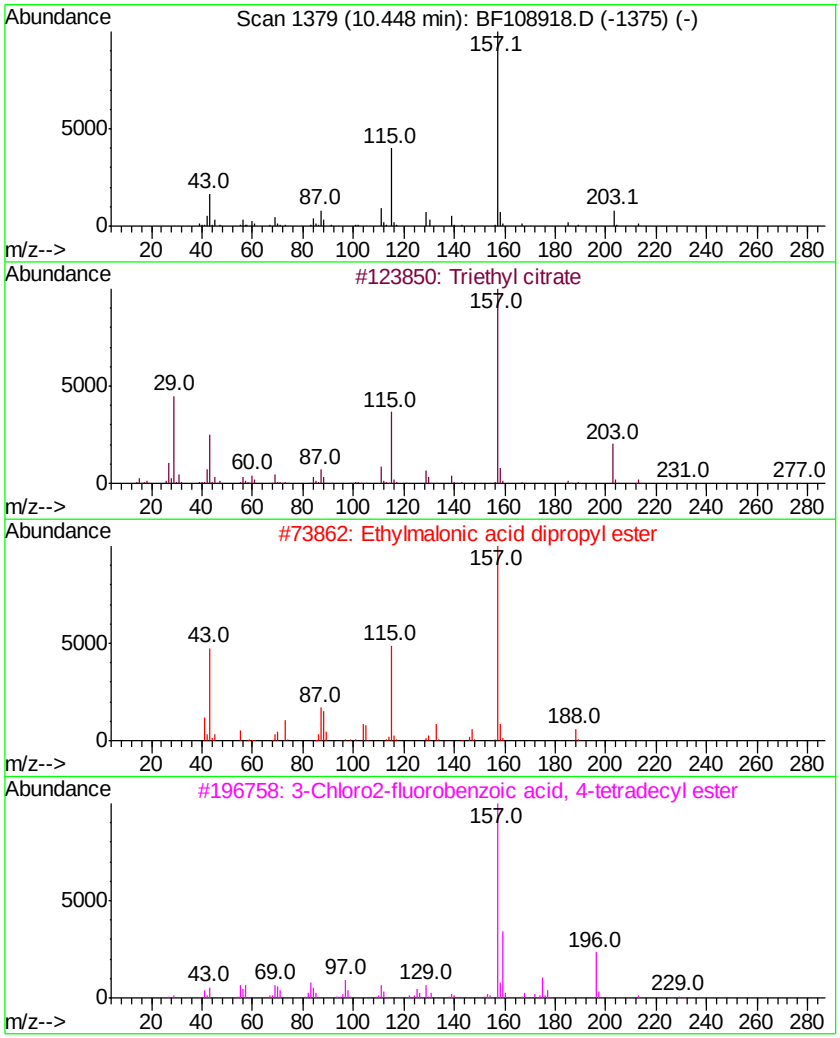
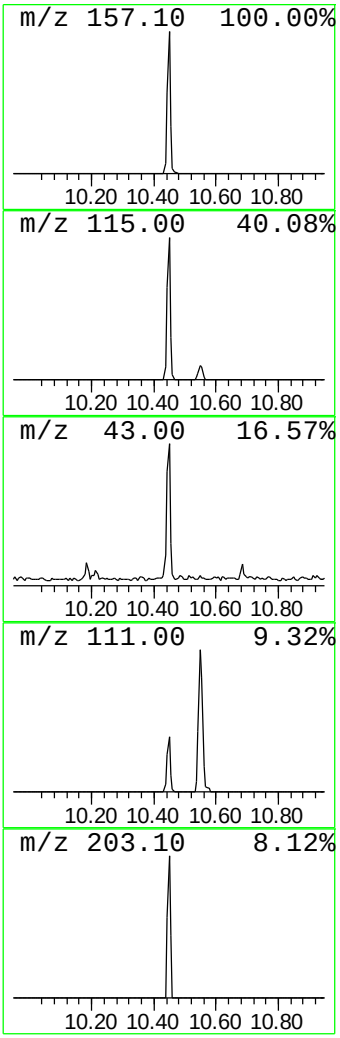
Peak Number 4 Triethyl citrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.32 ng	124526	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	90
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	45
3	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	40
4	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	37
5	3-Chloro2-fluorobenzoic acid, 6-...	342	C19H28ClFO2	1000338-64-1	33





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108918.D
Acq On : 11 Sep 2018 3:04
Operator : JU/SJ
Sample : J4830-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

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

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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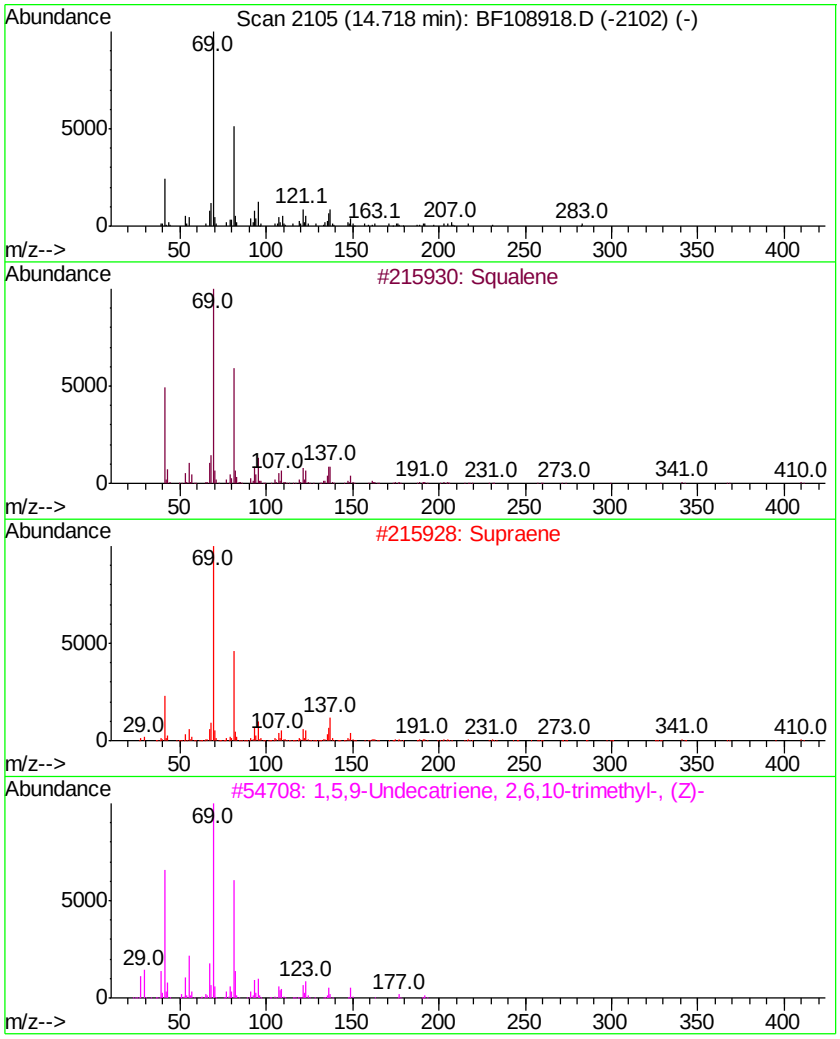
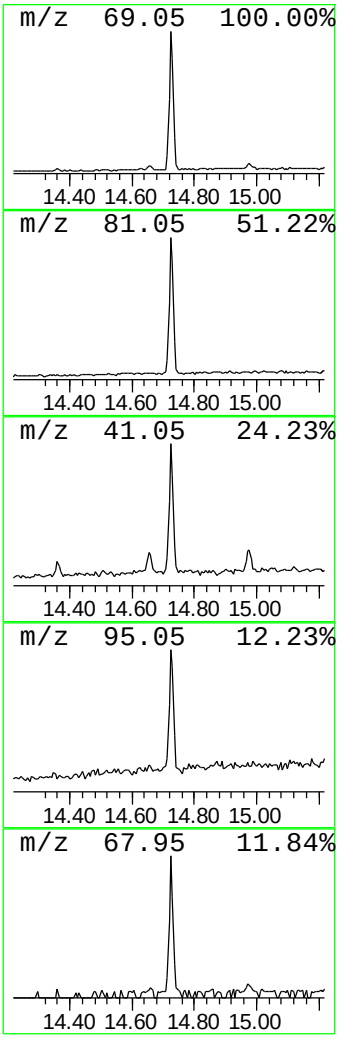
Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	6.33 ng	227786	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	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108918.D
Acq On : 11 Sep 2018 3:04
Operator : JU/SJ
Sample : J4830-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

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

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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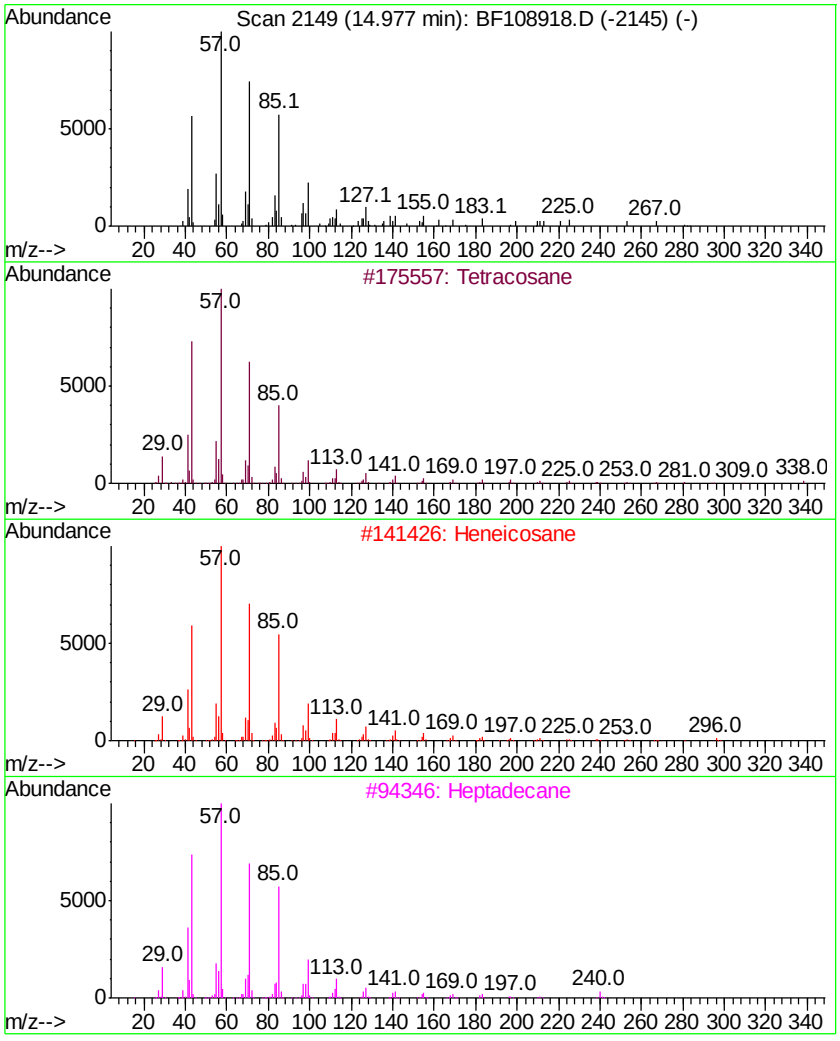
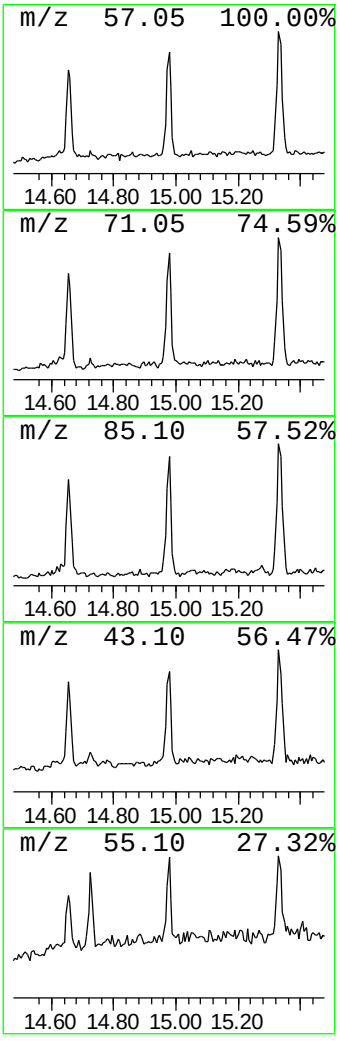
Peak Number 6 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.38 ng	85594	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Heneicosane	296	C21H44	000629-94-7	87
3	Heptadecane	240	C17H36	000629-78-7	87
4	Tridecane, 3-methyl-	198	C14H30	006418-41-3	86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108918.D
Acq On : 11 Sep 2018 3:04
Operator : JU/SJ
Sample : J4830-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

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

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

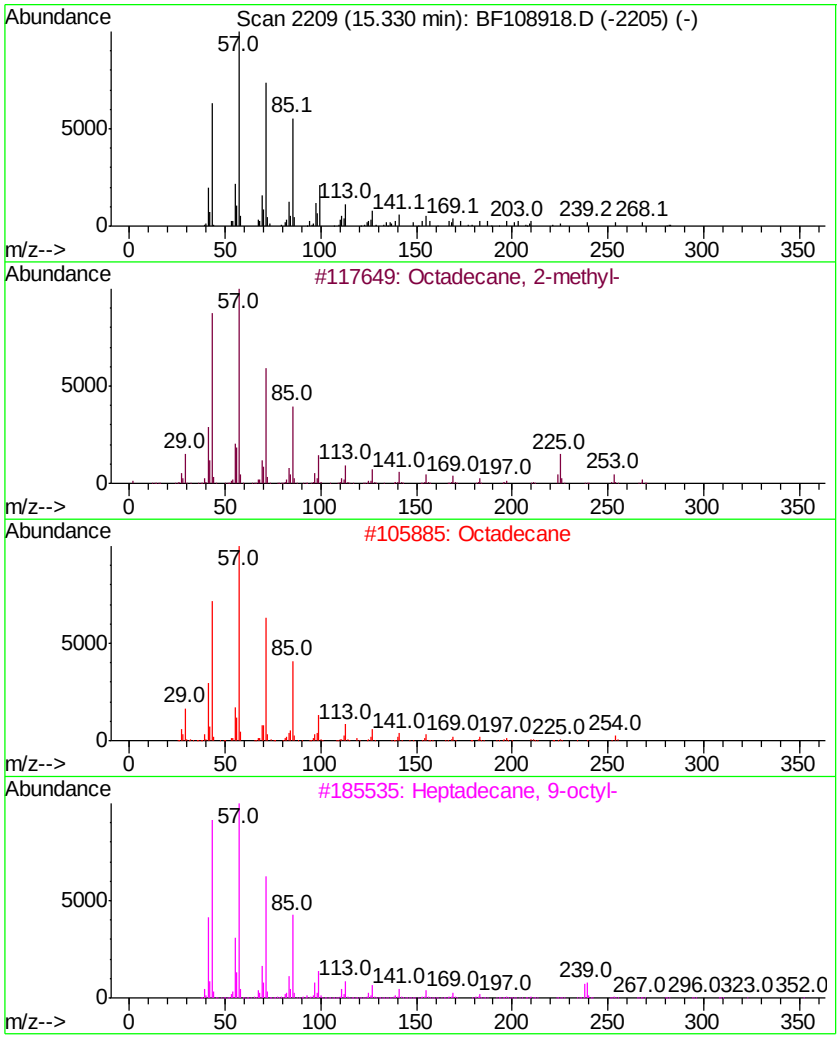
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

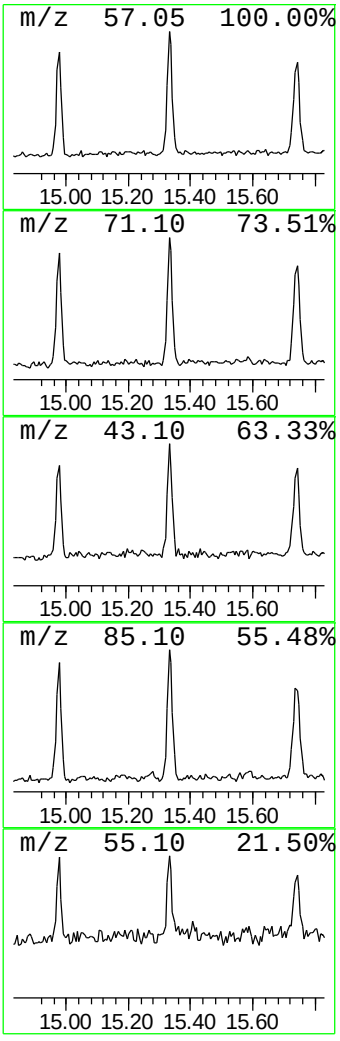
****

Peak Number 7 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	2.89 ng	104209	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
2	Octadecane	254	C18H38	000593-45-3	93
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
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Acq On : 11 Sep 2018 3:04
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Sample : J4830-04
Misc :
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Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-U-B

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

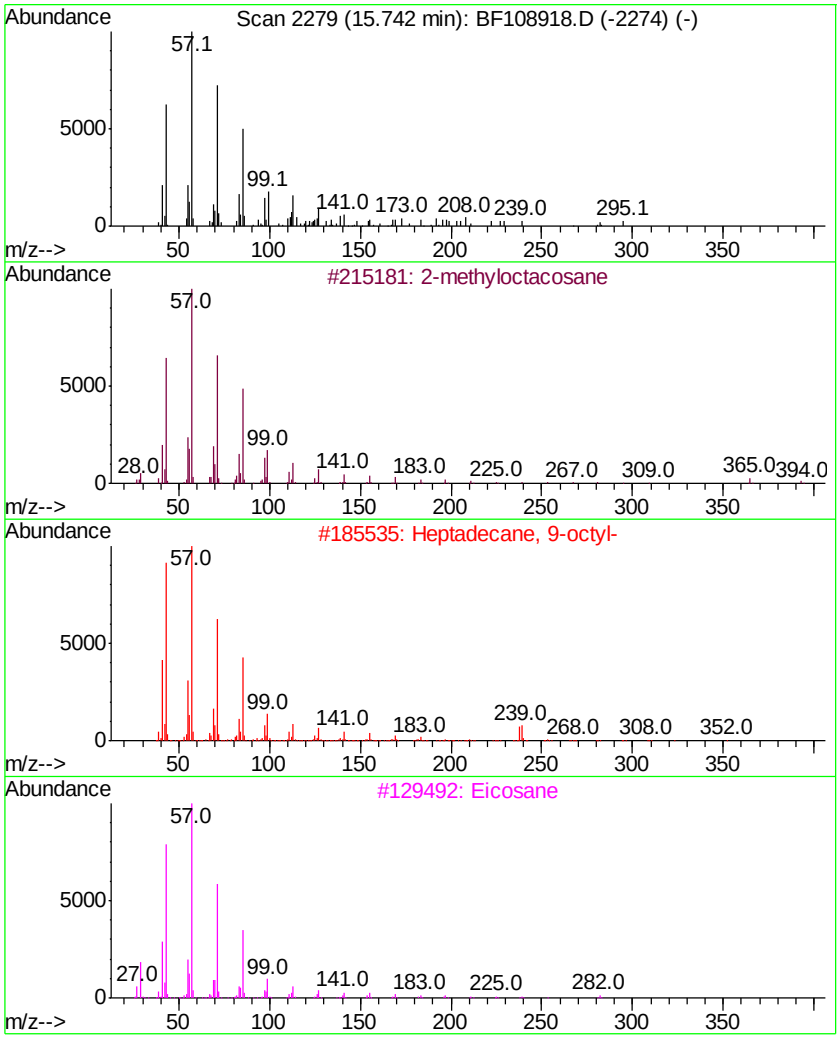
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

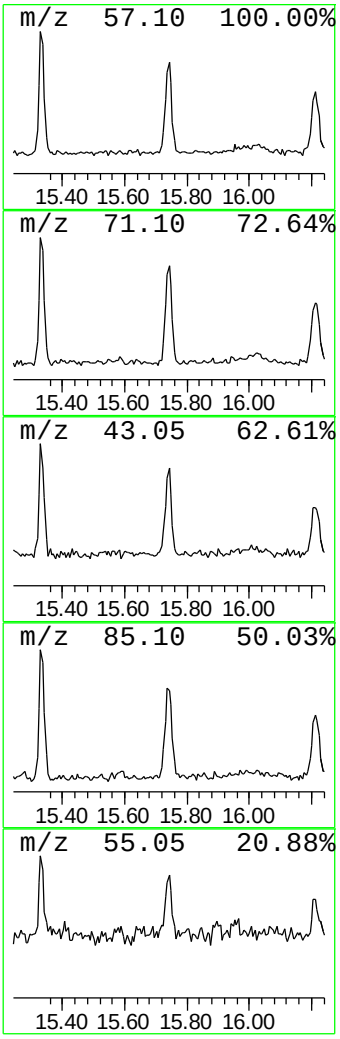
****

Peak Number 8 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.97 ng	106959	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	87
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3	Eicosane	282	C20H42	000112-95-8	81
4	Hexadecane	226	C16H34	000544-76-3	80
5	Heptadecane	240	C17H36	000629-78-7	80





Tentatively Identified Compound (LSC) summary

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Data File : BF108918.D
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Instrument : BNA_F
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	3.4	ng	164198	1	6.74	971302	20.0
unknown6.51	6.51	55.5	ng	2693910	1	6.74	971302	20.0
Triethyl citrate	10.45	2.3	ng	124526	3	9.77	1072230	20.0
Squalene	14.72	6.3	ng	227786	6	15.28	719942	20.0
Tetracosane	14.98	2.4	ng	85594	6	15.28	719942	20.0
Octadecane, 2-met...	15.33	2.9	ng	104209	6	15.28	719942	20.0
2-methyloctacosane	15.74	3.0	ng	106959	6	15.28	719942	20.0