LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108915.D
Acq On : 11 Sep 2018 1:44
Operator : JU/SJ
Sample : J4830-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-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	447	rBV	133132	141221	3.07%	0.495%
2	5.348	507	512	515	rBV	1624463	1506020	32.79%	5.283%
3	6.366	681	685	693	rBV	1383715	1110648	24.18%	3.896%
4	6.507	701	709	712	rBV	3039106	2637090	57.41%	9.250%
5	6.737	745	748	752	rBV	1163604	978056	21.29%	3.431%
6	6.895	771	775	779	rBV	3593968	3495753	76.10%	12.262%
7	7.301	838	844	847	rBV	2908299	2794762	60.84%	9.803%
8	8.019	962	966	970	rBV	1391485	1142950	24.88%	4.009%
9	9.095	1145	1149	1152	rBV	4774724	4593561	100.00%	16.113%
10	9.483	1212	1215	1224	rVB	242941	202773	4.41%	0.711%
11	9.772	1260	1264	1268	rVB	1178534	1103840	24.03%	3.872%
12	10.448	1376	1379	1382	rBV	228244	160026	3.48%	0.561%
13	10.554	1393	1397	1409	rBV	1555529	1484975	32.33%	5.209%
14	11.248	1511	1515	1518	rBV	1103336	928586	20.21%	3.257%
15	12.830	1780	1784	1787	rBV	3973269	3693485	80.41%	12.956%
16	13.742	1935	1939	1945	rBV	90044	129197	2.81%	0.453%
17	13.871	1957	1961	1965	rBV	1259692	1099804	23.94%	3.858%
18	14.660	2091	2095	2098	rBV	57517	54178	1.18%	0.190%
19	14.730	2103	2107	2113	rBV	160848	170593	3.71%	0.598%
20	14.977	2145	2149	2153	rBV	80420	87987	1.92%	0.309%
21	15.283	2196	2201	2205	rBV	681948	780070	16.98%	2.736%
22	15.336	2206	2210	2216	rVB	84137	112967	2.46%	0.396%
23	15.742	2275	2279	2284	rVB	67111	100399	2.19%	0.352%

Sum of corrected areas: 28508941

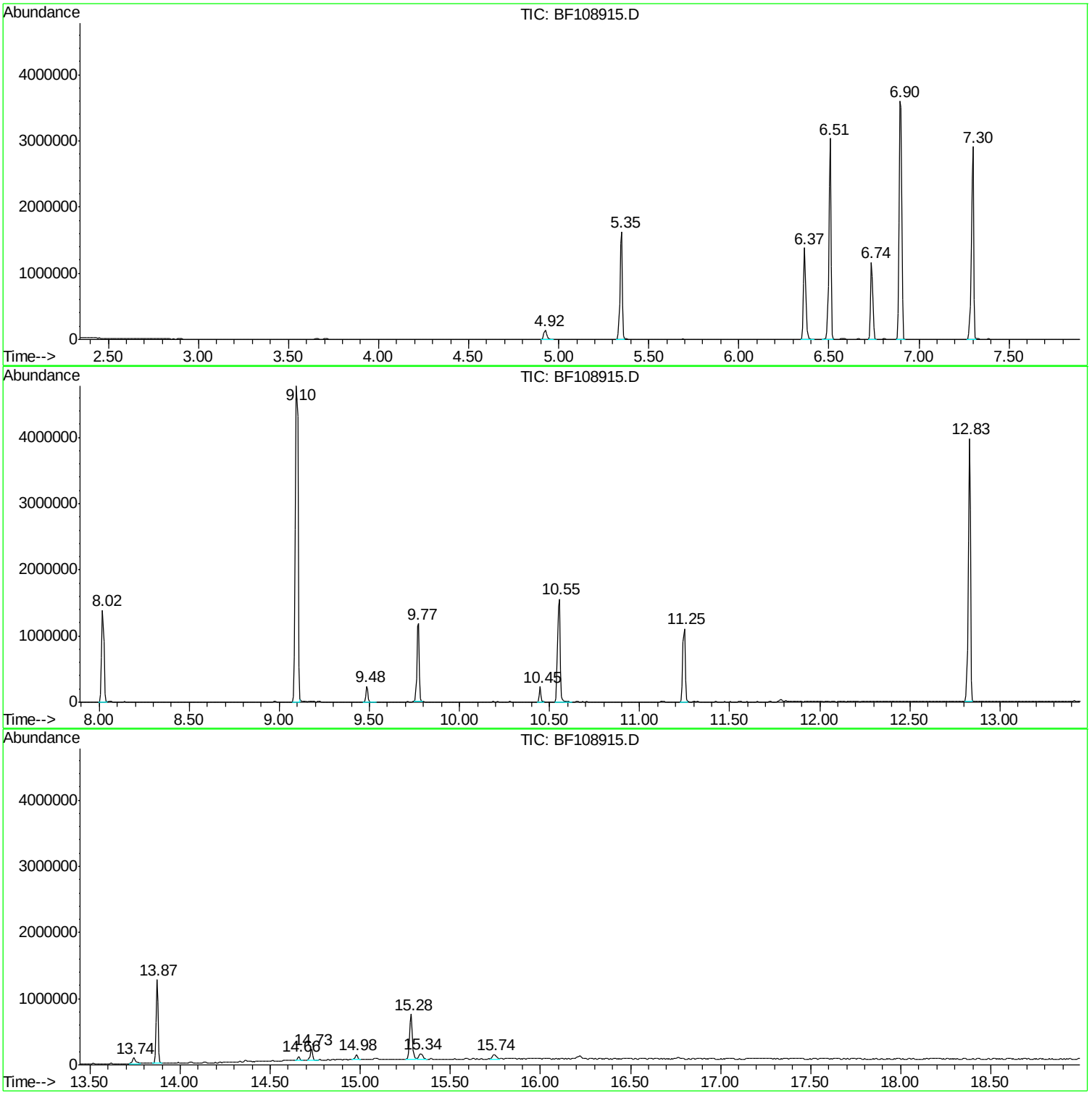
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108915.D
Acq On : 11 Sep 2018 1:44
Operator : JU/SJ
Sample : J4830-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-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 : BF108915.D
Acq On : 11 Sep 2018 1:44
Operator : JU/SJ
Sample : J4830-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

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

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

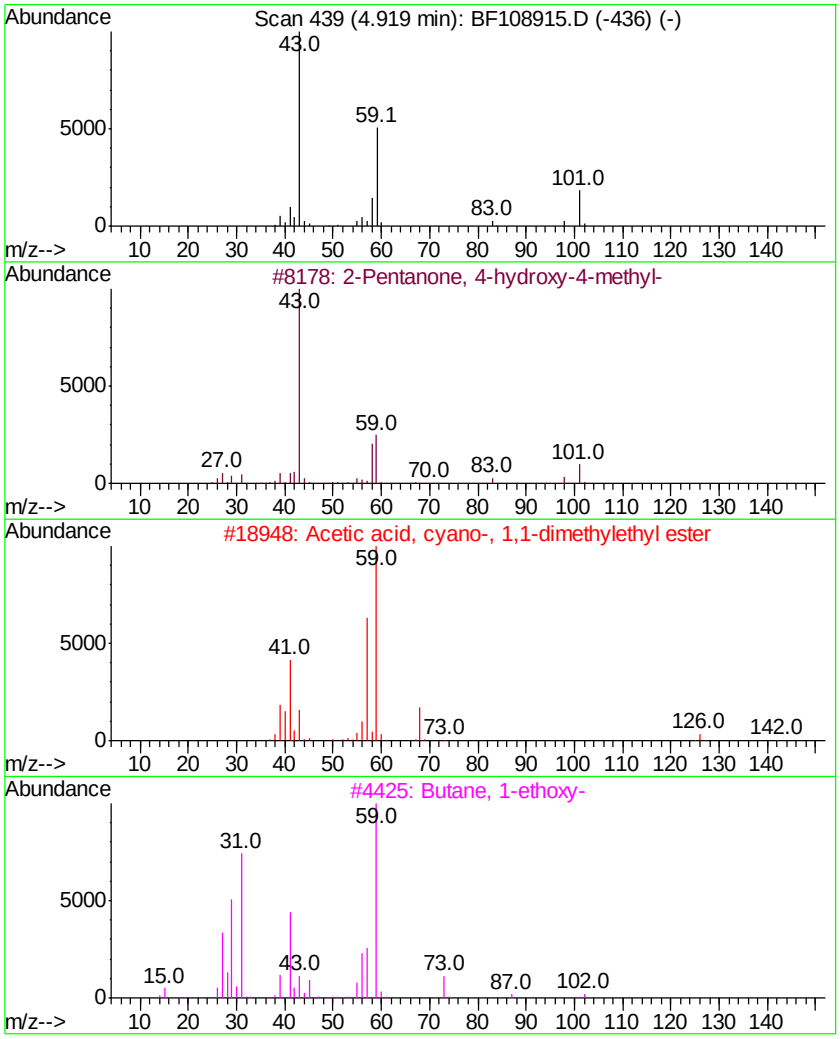
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

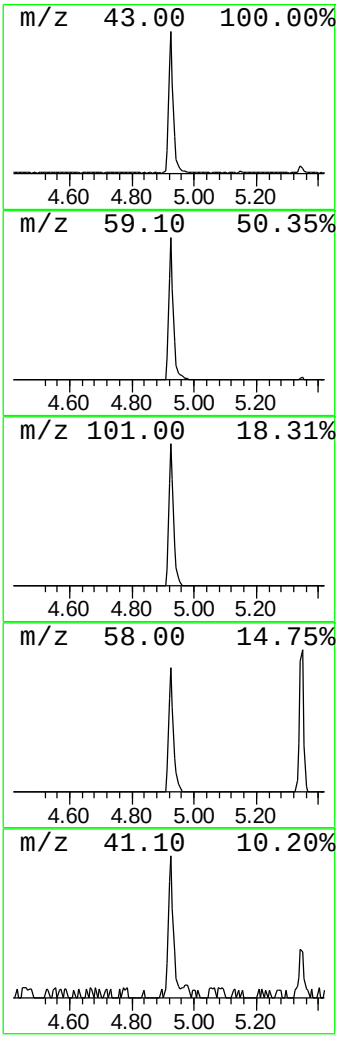
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.89 ng	141221	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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108915.D
Acq On : 11 Sep 2018 1:44
Operator : JU/SJ
Sample : J4830-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

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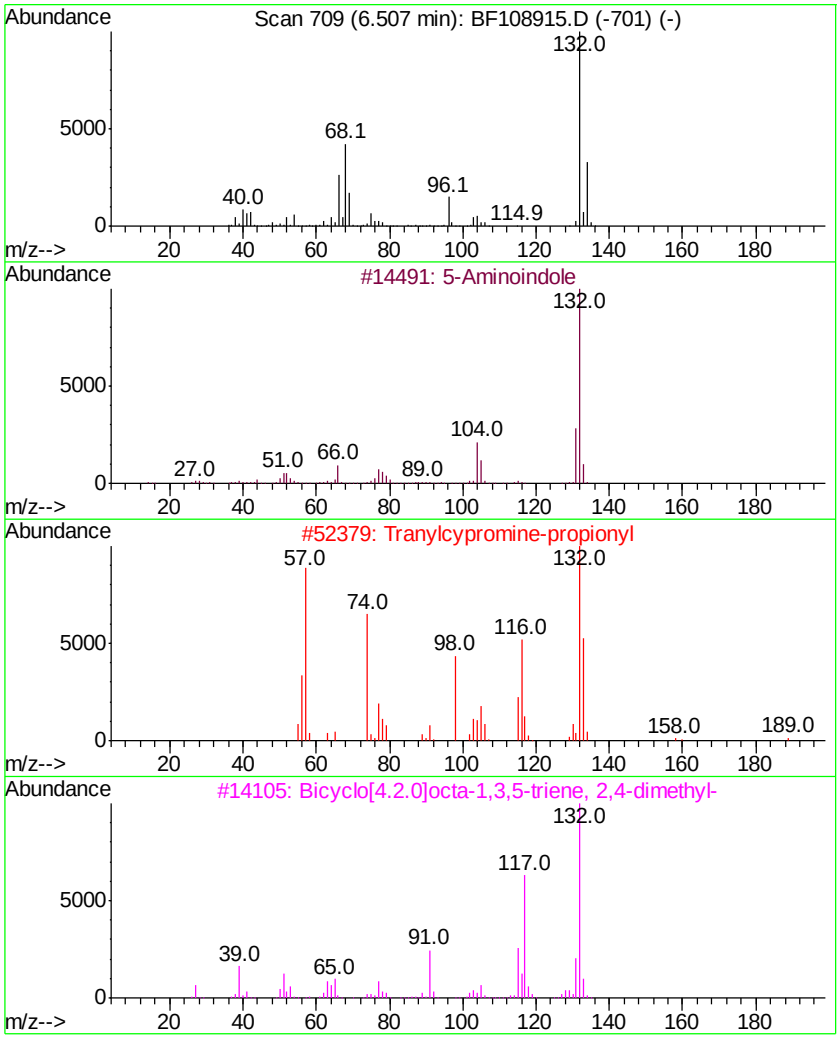
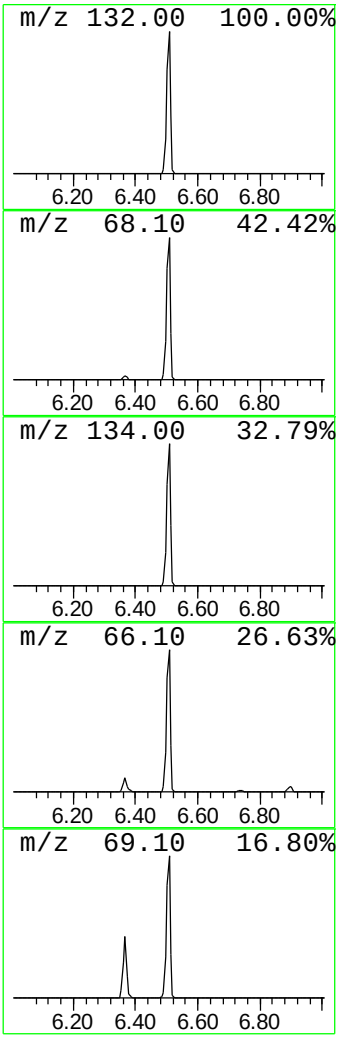
Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	53.93 ng	2637090	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	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 : BF108915.D
Acq On : 11 Sep 2018 1:44
Operator : JU/SJ
Sample : J4830-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-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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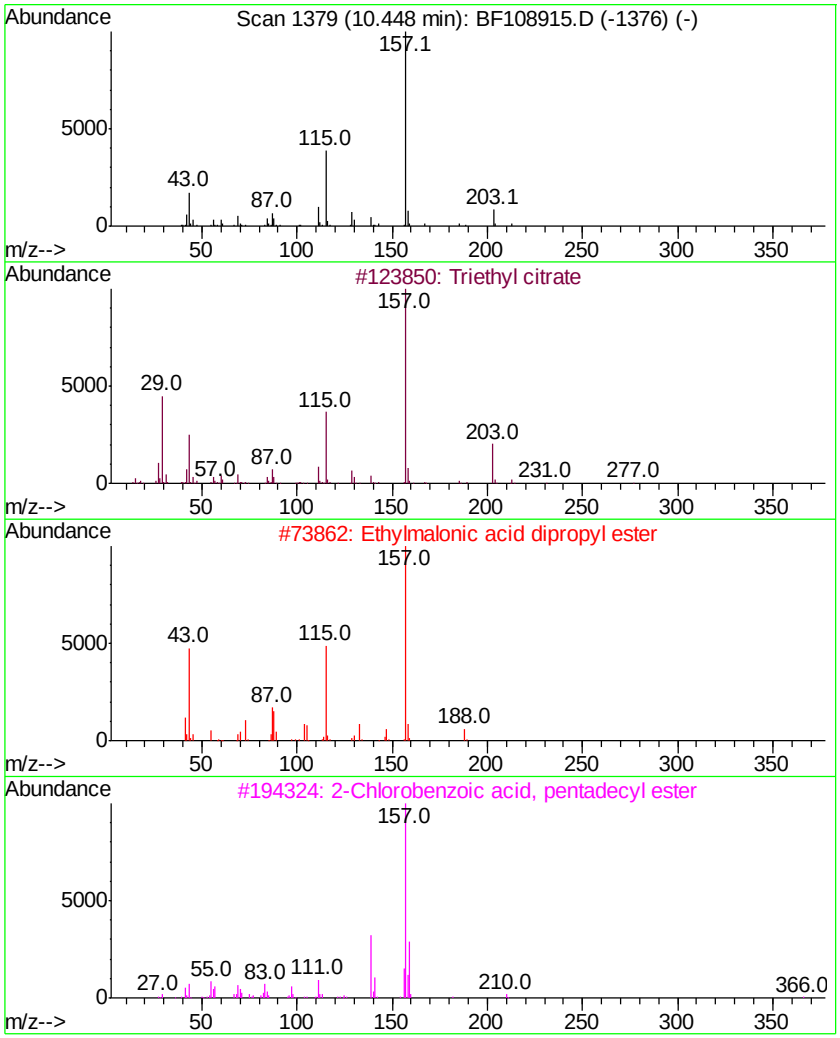
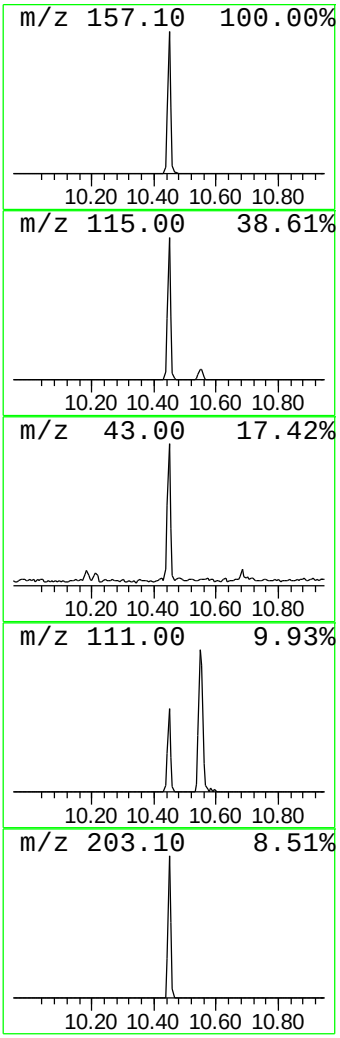
Peak Number 4 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.90 ng	160026	Acenaphthene-d10	9.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	2-Chlorobenzoic acid, pentadecyl...	366	C22H35ClO2	1000292-43-0	38
4	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	38
5	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	37





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108915.D
Acq On : 11 Sep 2018 1:44
Operator : JU/SJ
Sample : J4830-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-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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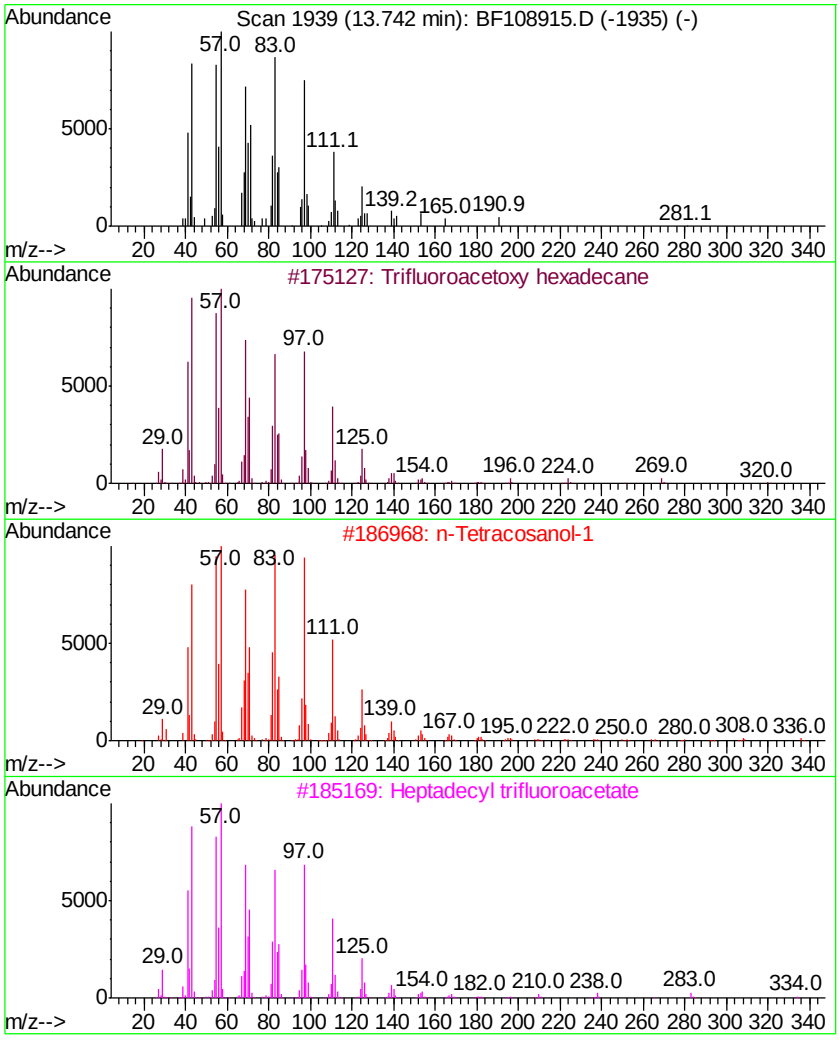
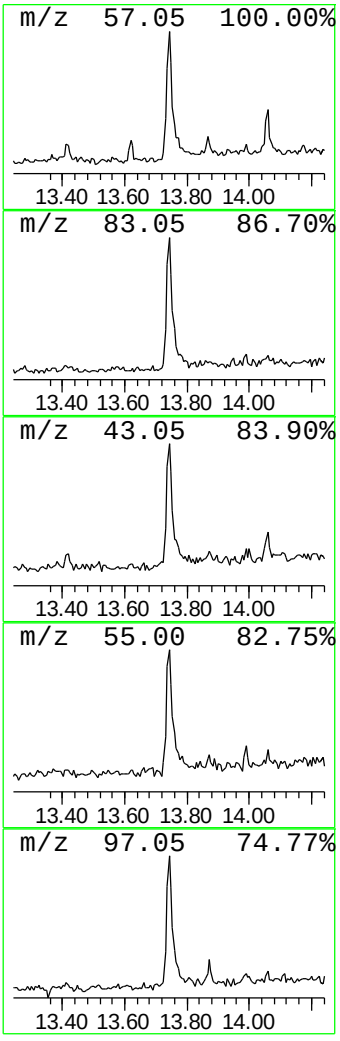
Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.35 ng	129197	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108915.D
Acq On : 11 Sep 2018 1:44
Operator : JU/SJ
Sample : J4830-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-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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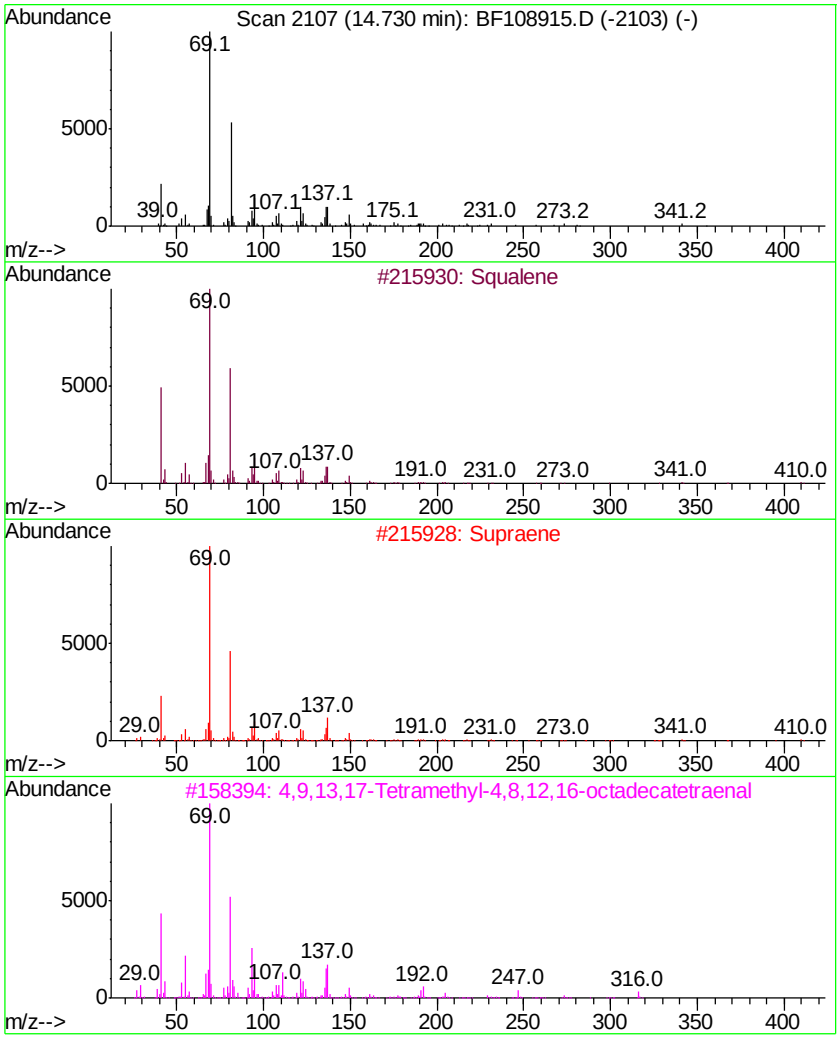
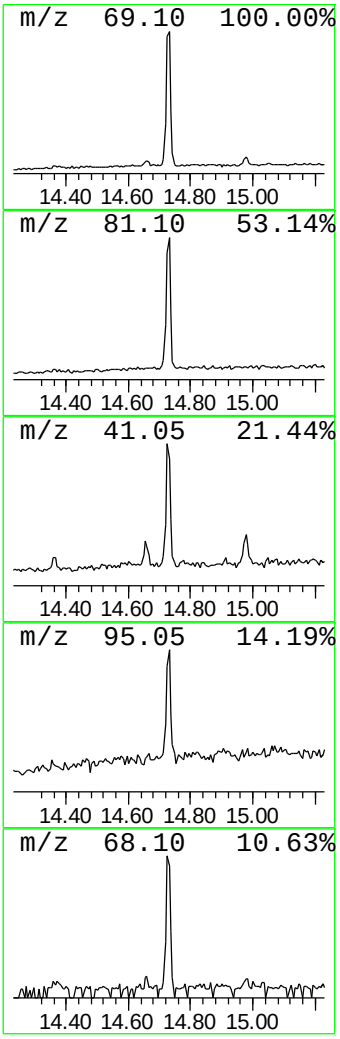
Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	4.37 ng	170593	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	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108915.D
Acq On : 11 Sep 2018 1:44
Operator : JU/SJ
Sample : J4830-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

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

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

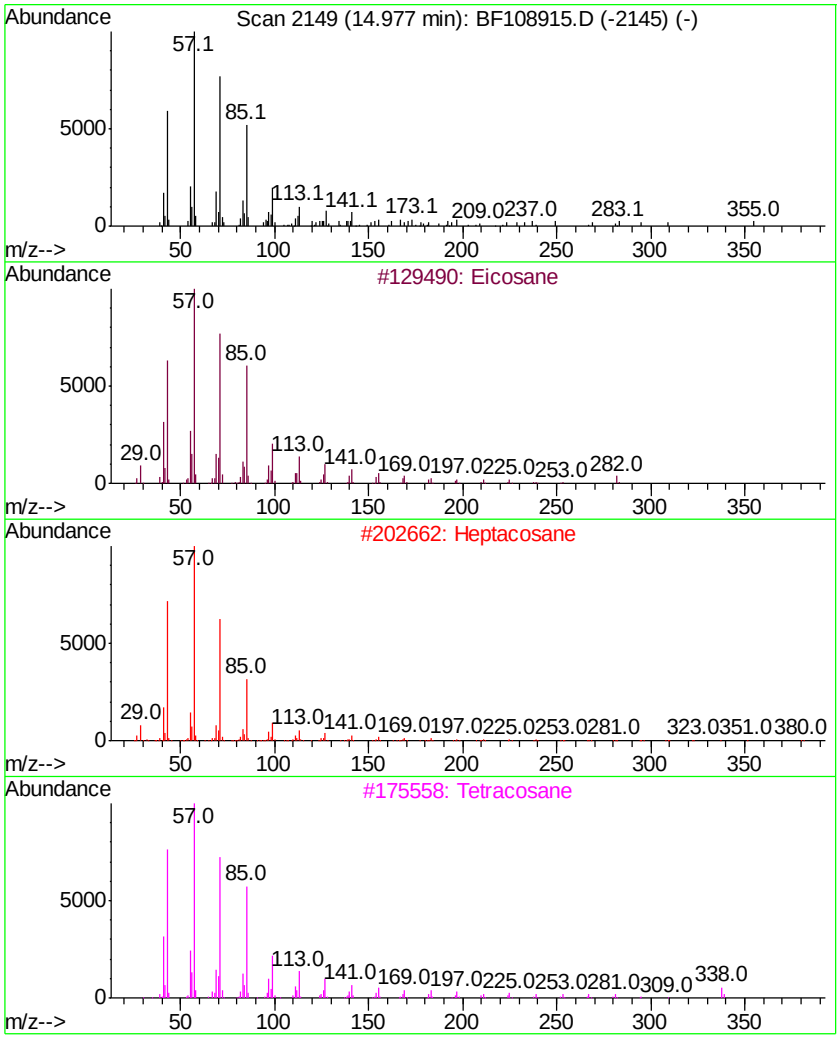
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

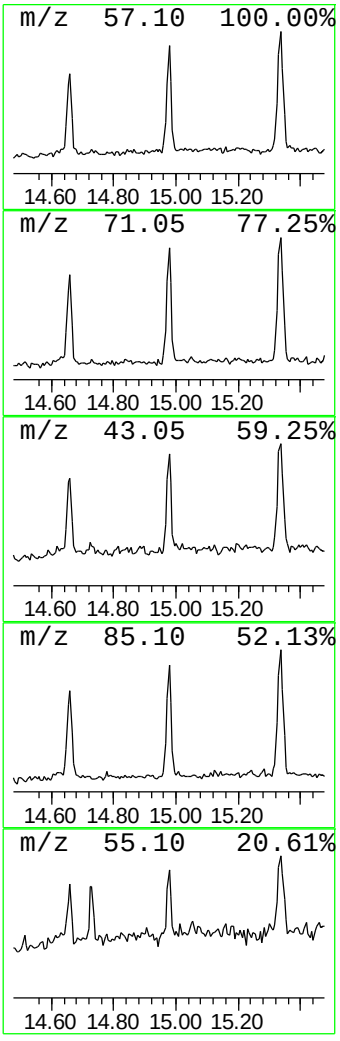
****

Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.26 ng	87987	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Heptacosane	380	C27H56	000593-49-7	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
5	Octadecane	254	C18H38	000593-45-3	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108915.D
Acq On : 11 Sep 2018 1:44
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Sample : J4830-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-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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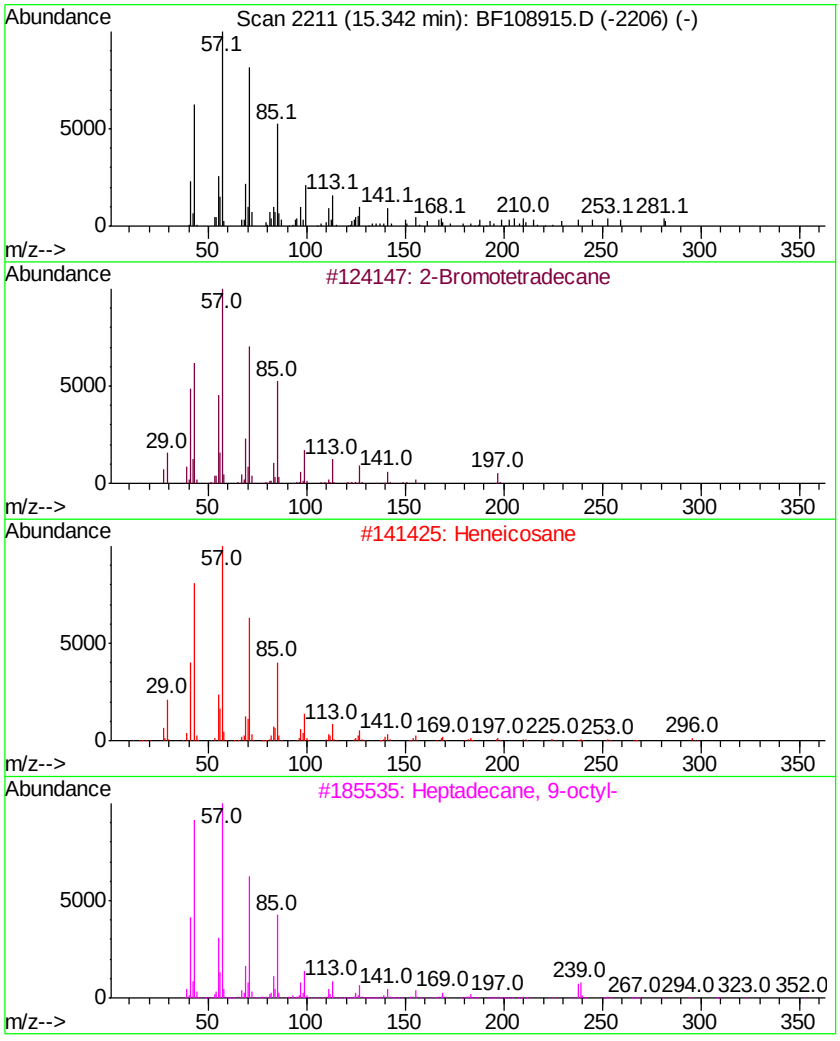
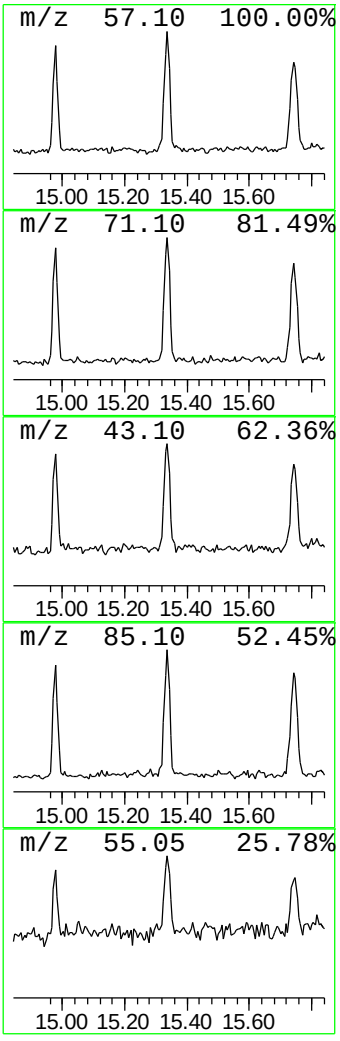
Peak Number 8 2-Bromotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	2.90 ng	112967	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromotetradecane	276	C14H29Br	074036-95-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane	394	C28H58	000630-02-4	91





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Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-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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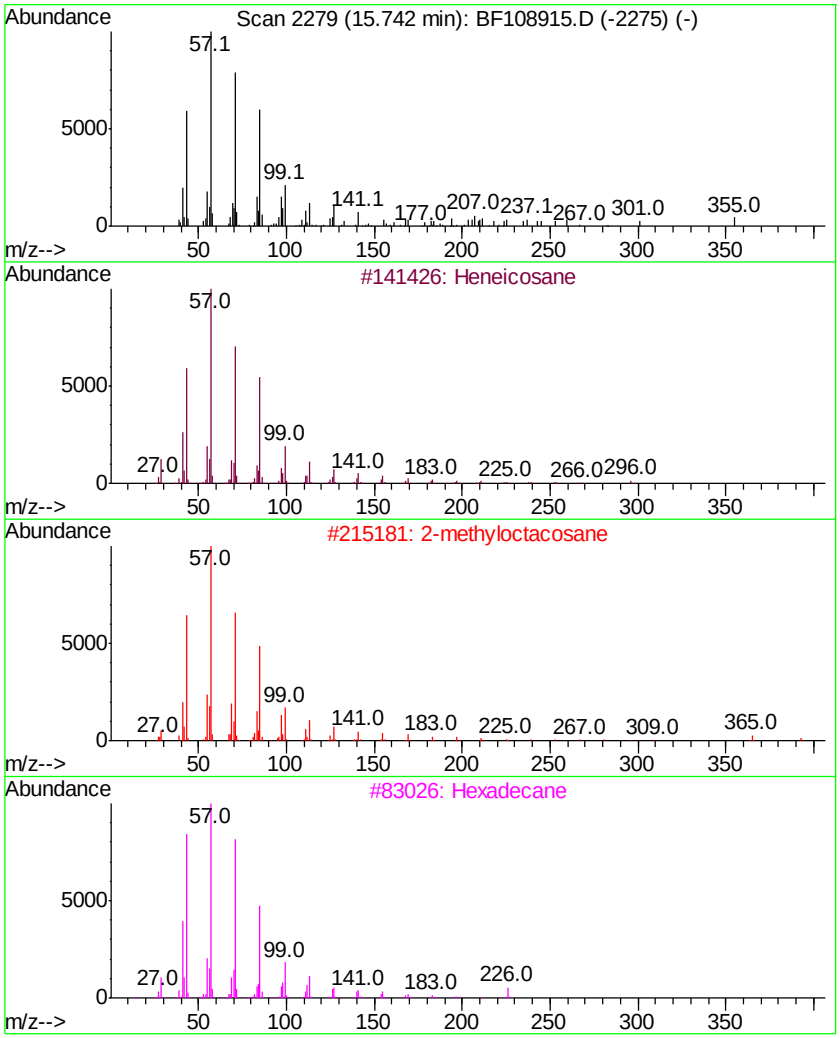
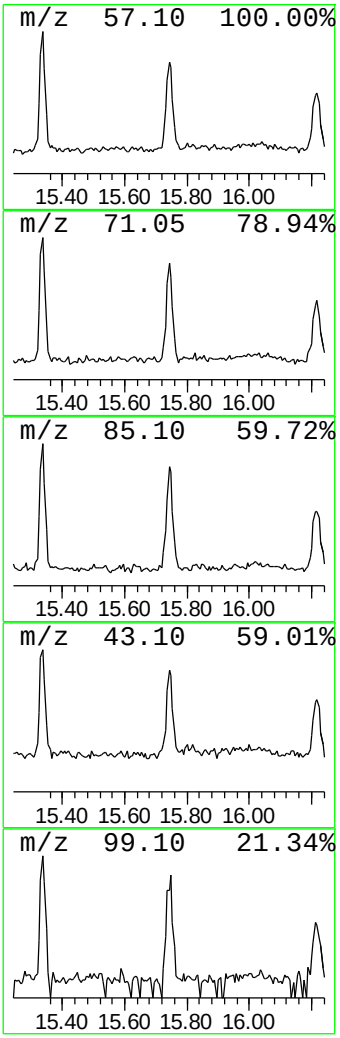
Peak Number 9 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.57 ng	100399	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	2-methyloctacosane	408	C29H60	1000376-72-8	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Pentacosane	352	C25H52	000629-99-2	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091018\
Data File : BF108915.D
Acq On : 11 Sep 2018 1:44
Operator : JU/SJ
Sample : J4830-01
Misc :
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Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	2.9	ng	141221	1	6.74	978056	20.0
unknown6.51	6.51	53.9	ng	2637090	1	6.74	978056	20.0
Triethyl citrate	10.45	2.9	ng	160026	3	9.77	1103840	20.0
Trifluoroacetoxy ...	13.74	2.4	ng	129197	5	13.87	1099800	20.0
Squalene	14.73	4.4	ng	170593	6	15.28	780070	20.0
Eicosane	14.98	2.3	ng	87987	6	15.28	780070	20.0
2-Bromotetradecane	15.34	2.9	ng	112967	6	15.28	780070	20.0
Heneicosane	15.74	2.6	ng	100399	6	15.28	780070	20.0