LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106842.D
Acq On : 27 Jun 2018 00:43
Operator : JU/SJ
Sample : J3639-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 062018-DBRI-E-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-BF061918.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	5.190	482	485	492	rBB	18615	20438	1.64%	0.261%
2	5.601	551	555	571	rBV	315667	295493	23.67%	3.769%
3	6.601	721	725	734	rBV2	235492	239114	19.15%	3.050%
4	6.736	744	748	751	rBV	630952	550303	44.07%	7.019%
5	6.960	782	786	789	rBV	296602	237916	19.05%	3.034%
6	7.119	808	813	816	rBV	905404	841778	67.42%	10.736%
7	7.525	877	882	885	rBV	672298	607102	48.62%	7.743%
8	8.242	1000	1004	1020	rBV	322327	278354	22.29%	3.550%
9	9.313	1182	1186	1198	rBV	1201756	1148470	91.98%	14.648%
10	10.001	1300	1303	1312	rVB	301722	283554	22.71%	3.617%
11	10.660	1412	1415	1417	rBV	44721	35809	2.87%	0.457%
12	10.795	1434	1438	1446	rBV	402697	377466	30.23%	4.814%
13	11.495	1553	1557	1564	rBV	313565	296327	23.73%	3.780%
14	13.077	1821	1826	1829	rBV	1294075	1248589	100.00%	15.925%
15	14.142	2003	2007	2011	rBV	364314	319269	25.57%	4.072%
16	14.436	2041	2057	2072	rBV2	256872	801302	64.18%	10.220%
17	14.654	2089	2094	2099	rBV8	7103	15843	1.27%	0.202%
18	14.983	2146	2150	2154	rBV	30117	30780	2.47%	0.393%
19	15.677	2262	2268	2274	rBV	148144	212466	17.02%	2.710%

Sum of corrected areas: 7840373

LSC Report - Integrated Chromatogram

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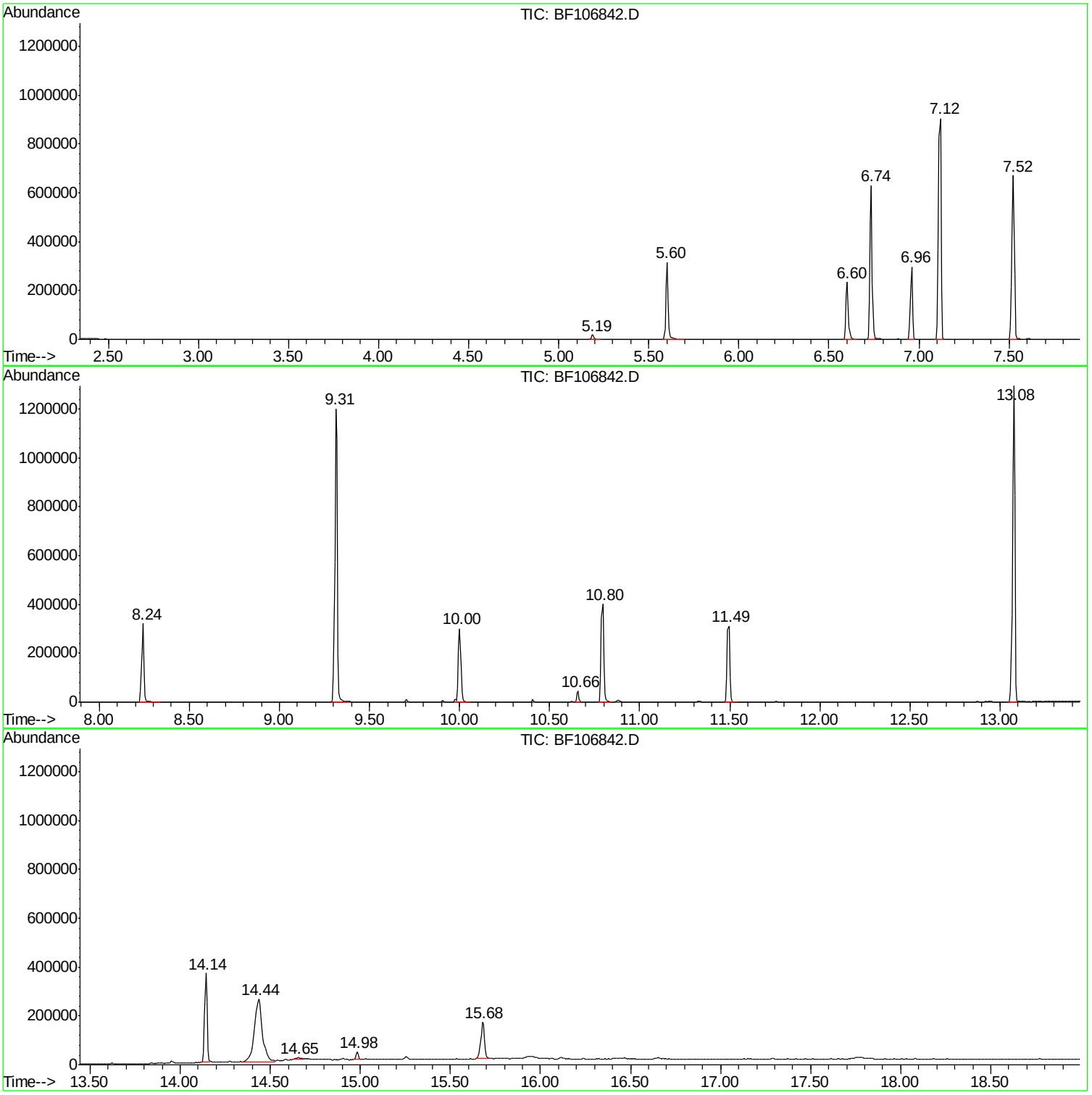
Sample : J3639-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
062018-DBRI-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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\BF062618\
Data File : BF106842.D
Acq On : 27 Jun 2018 00:43
Operator : JU/SJ
Sample : J3639-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 062018-DBRI-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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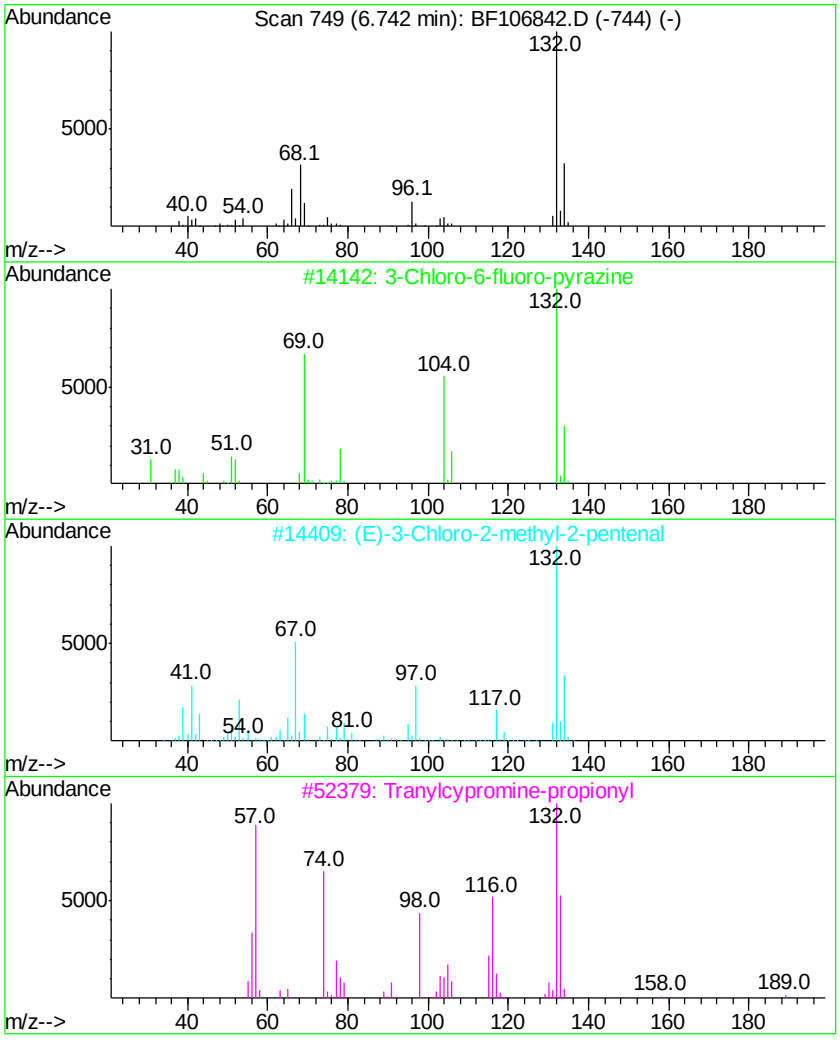
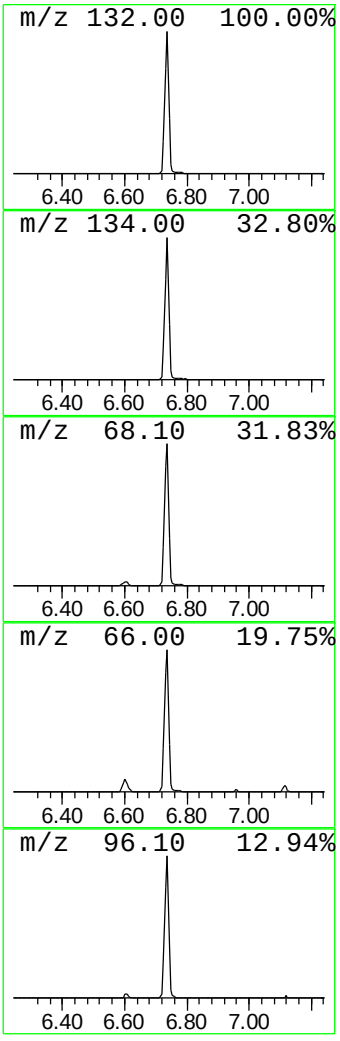
Peak Number 1 unknown6.74 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	46.26 ng	550303	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Acq On : 27 Jun 2018 00:43
Operator : JU/SJ
Sample : J3639-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 062018-DBRI-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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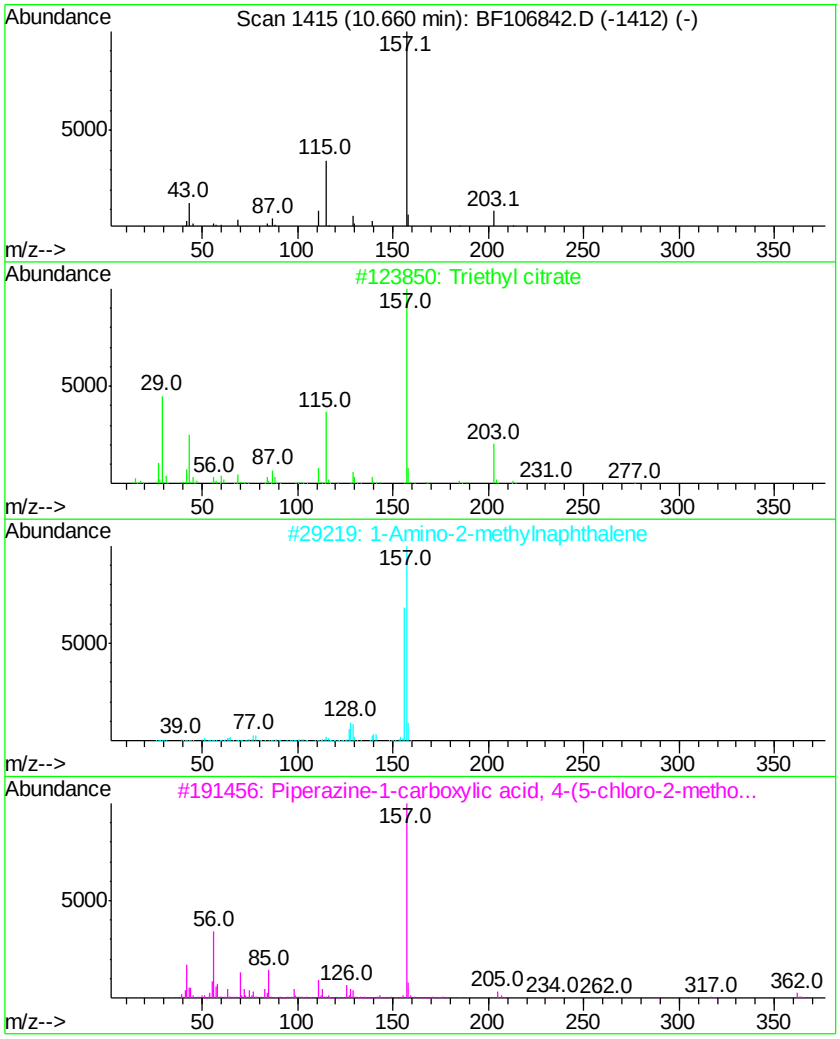
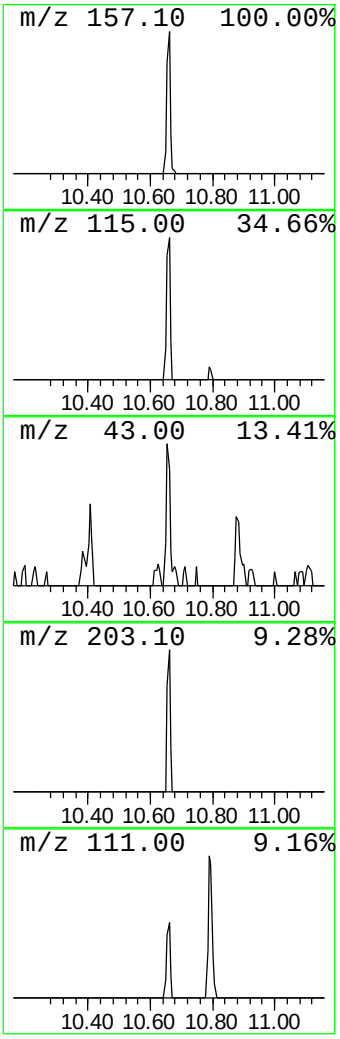
Peak Number 3 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.53 ng	35809	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	78
2	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	50
3	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	33
4	Adipic acid, ethyl pent-4-en-2-y...	242	C13H22O4	1000354-11-7	28
5	Adipic acid, ethyl 4-methylpent-...	258	C14H26O4	1000353-49-9	9





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Data File : BF106842.D
Acq On : 27 Jun 2018 00:43
Operator : JU/SJ
Sample : J3639-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 062018-DBRI-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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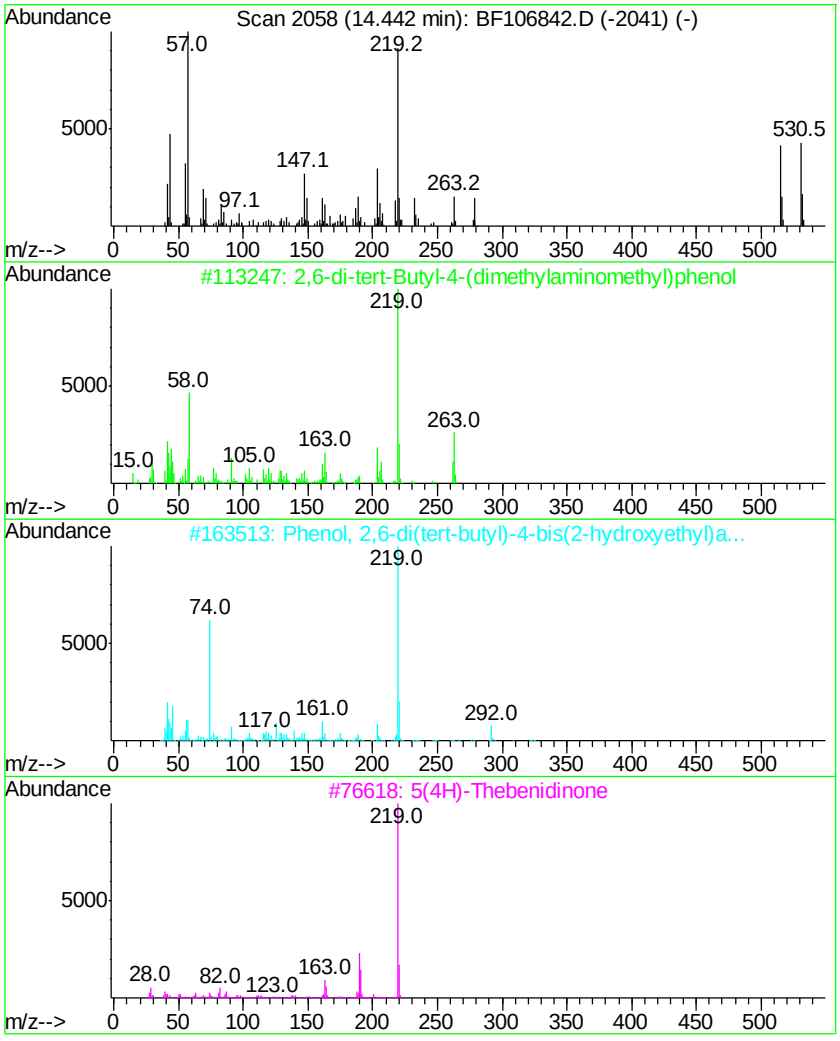
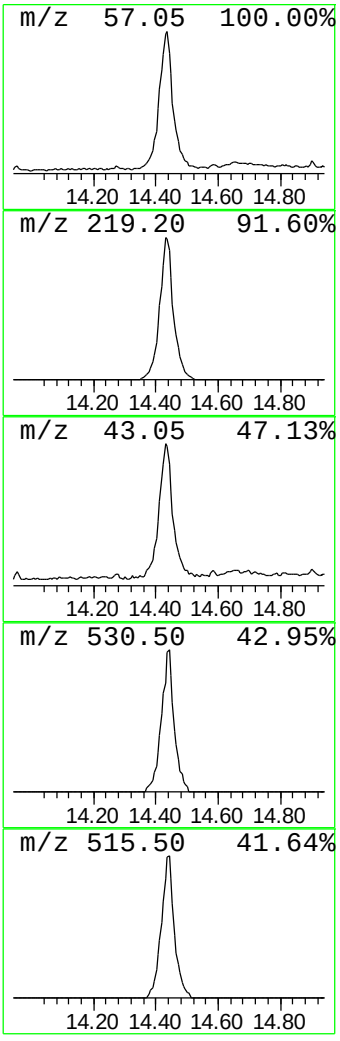
Peak Number 4 unknown14.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	50.20 ng	801302	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-di-tert-Butyl-4-(dimethylami...	263	C17H29NO	000088-27-7	45
2	Phenol, 2,6-di(tert-butyl)-4-bis...	323	C19H33NO3	1000294-01-7	35
3	5(4H)-Thebenidinone	219	C15H9NO	064884-40-8	35
4	2,4,5-Trifluorobenzyl alcohol, b...	312	C10H12BrF3OSi	1000376-06-6	35
5	Isophthalic acid, pentyl undec-2...	388	C24H36O4	1000343-90-6	35





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Data File : BF106842.D
Acq On : 27 Jun 2018 00:43
Operator : JU/SJ
Sample : J3639-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 062018-DBRI-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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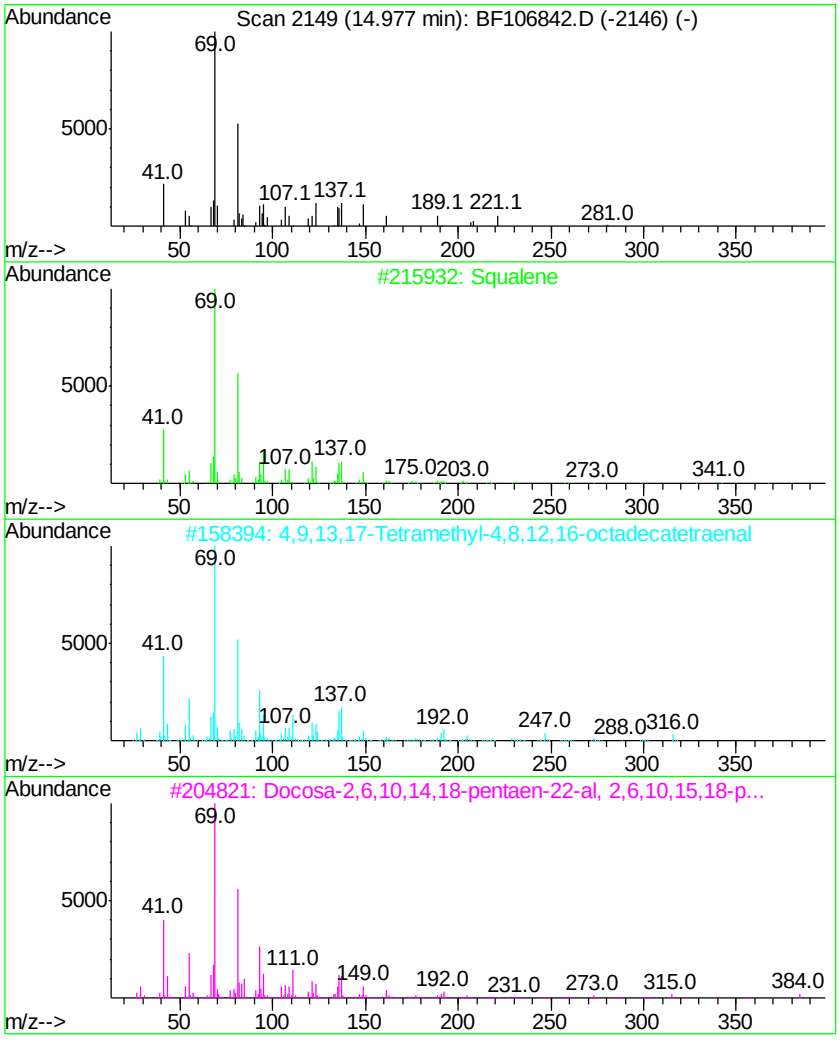
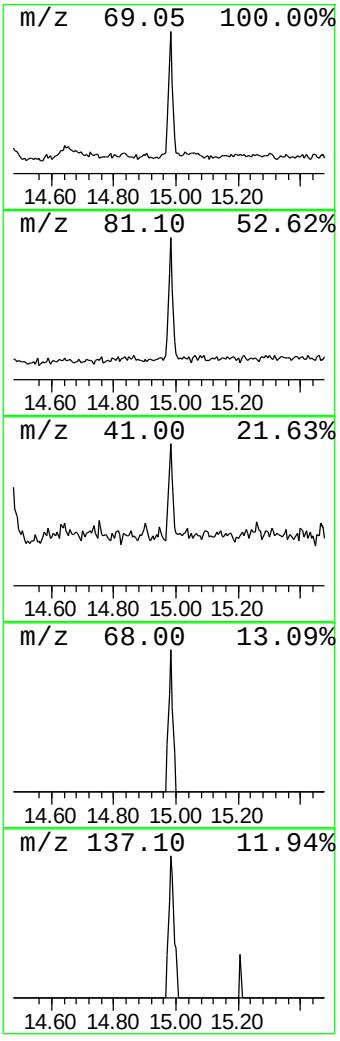
Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.90 ng	30780	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	72
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
4	Supraene	410	C30H50	007683-64-9	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062618\
Data File : BF106842.D
Acq On : 27 Jun 2018 00:43
Operator : JU/SJ
Sample : J3639-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 062018-DBRI-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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
unknown6.74	6.74	46.3	ng	550303	1	6.96	237916	20.0
Triethyl citrate	10.66	2.5	ng	35809	3	10.00	283554	20.0
unknown14.44	14.44	50.2	ng	801302	5	14.14	319269	20.0
Squalene	14.98	2.9	ng	30780	6	15.68	212466	20.0