LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108548.D
Acq On : 28 Aug 2018 9:06
Operator : JU/SJ
Sample : J4660-04
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-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-BF080818.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	5.231	489	492	503	rBV	80552	83867	2.47%	0.426%
2	5.625	555	559	571	rBV	1148665	1048847	30.86%	5.324%
3	6.613	724	727	741	rBV	859714	777249	22.87%	3.946%
4	6.766	749	753	757	rBV	2089338	1805567	53.13%	9.166%
5	6.995	789	792	796	rBV	690942	620665	18.26%	3.151%
6	7.154	815	819	823	rBV	2792376	2545684	74.91%	12.923%
7	7.560	883	888	892	rBV	1939028	2035641	59.90%	10.334%
8	8.284	1007	1011	1027	rBV	748277	700370	20.61%	3.555%
9	9.354	1189	1193	1196	rBV	3859073	3398284	100.00%	17.251%
10	9.742	1256	1259	1265	rBV	74980	70308	2.07%	0.357%
11	10.042	1307	1310	1321	rVB	741220	652803	19.21%	3.314%
12	10.701	1418	1422	1425	rBV	91478	81528	2.40%	0.414%
13	10.836	1441	1445	1458	rBV	1058886	1082919	31.87%	5.497%
14	11.536	1560	1564	1572	rBV	668817	586215	17.25%	2.976%
15	13.124	1829	1834	1837	rBV	3277558	2921351	85.97%	14.830%
16	14.189	2011	2015	2025	rVB	778941	713003	20.98%	3.619%
17	15.030	2154	2158	2165	rVB	60882	67045	1.97%	0.340%
18	15.742	2271	2279	2288	rBV	342395	507824	14.94%	2.578%

Sum of corrected areas: 19699170

LSC Report - Integrated Chromatogram

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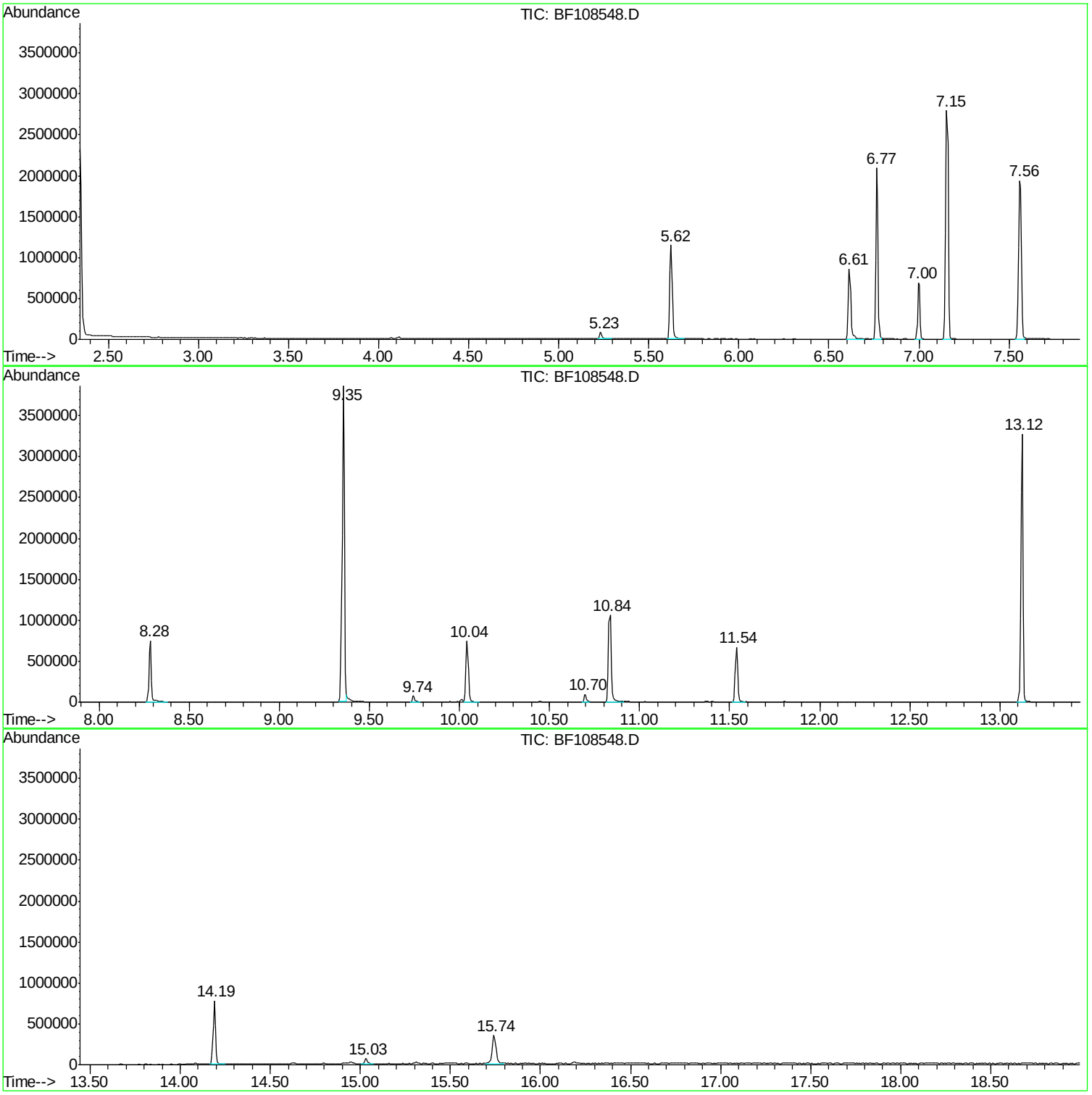
Sample : J4660-04
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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\BF082718\
Data File : BF108548.D
Acq On : 28 Aug 2018 9:06
Operator : JU/SJ
Sample : J4660-04
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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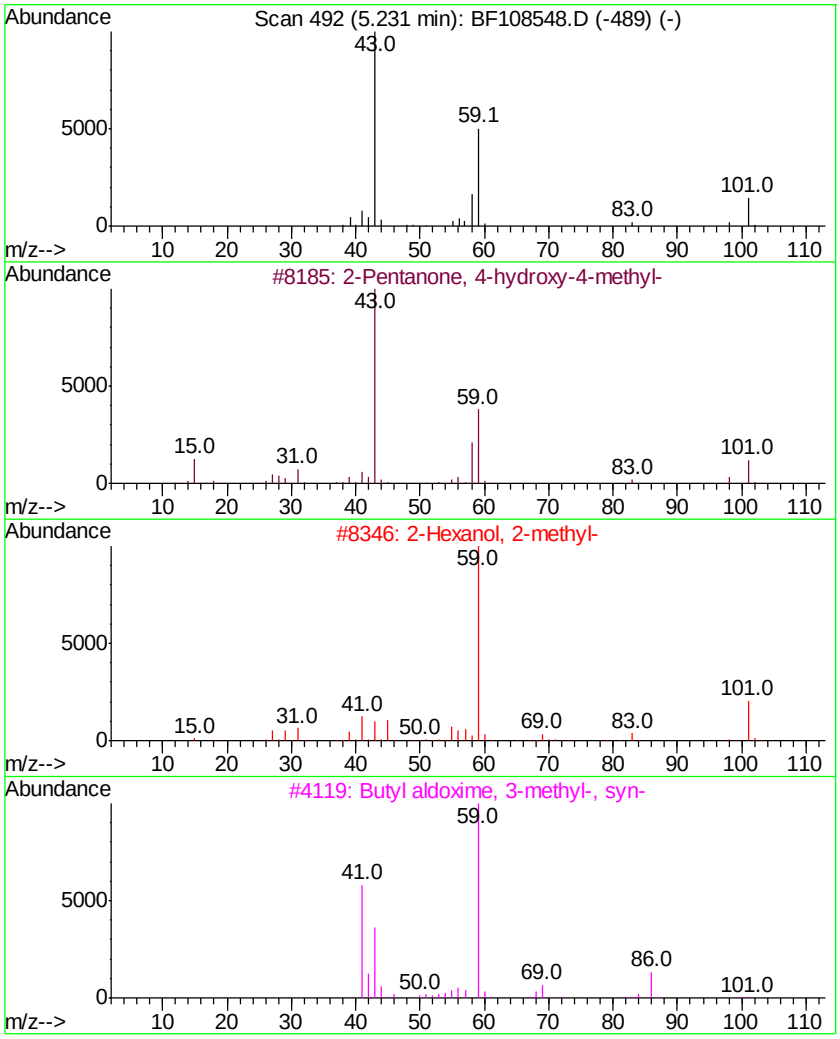
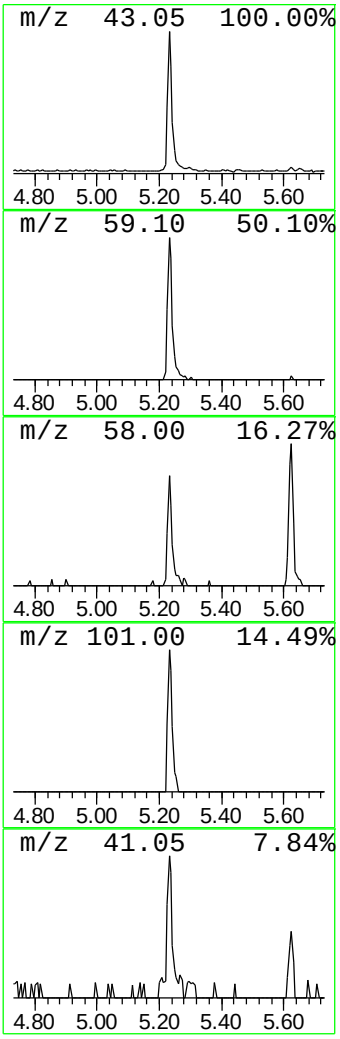
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	2.70 ng	83867	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	3-Octanol	130	C8H18O	000589-98-0	9





Library Search Compound Report

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Data File : BF108548.D
Acq On : 28 Aug 2018 9:06
Operator : JU/SJ
Sample : J4660-04
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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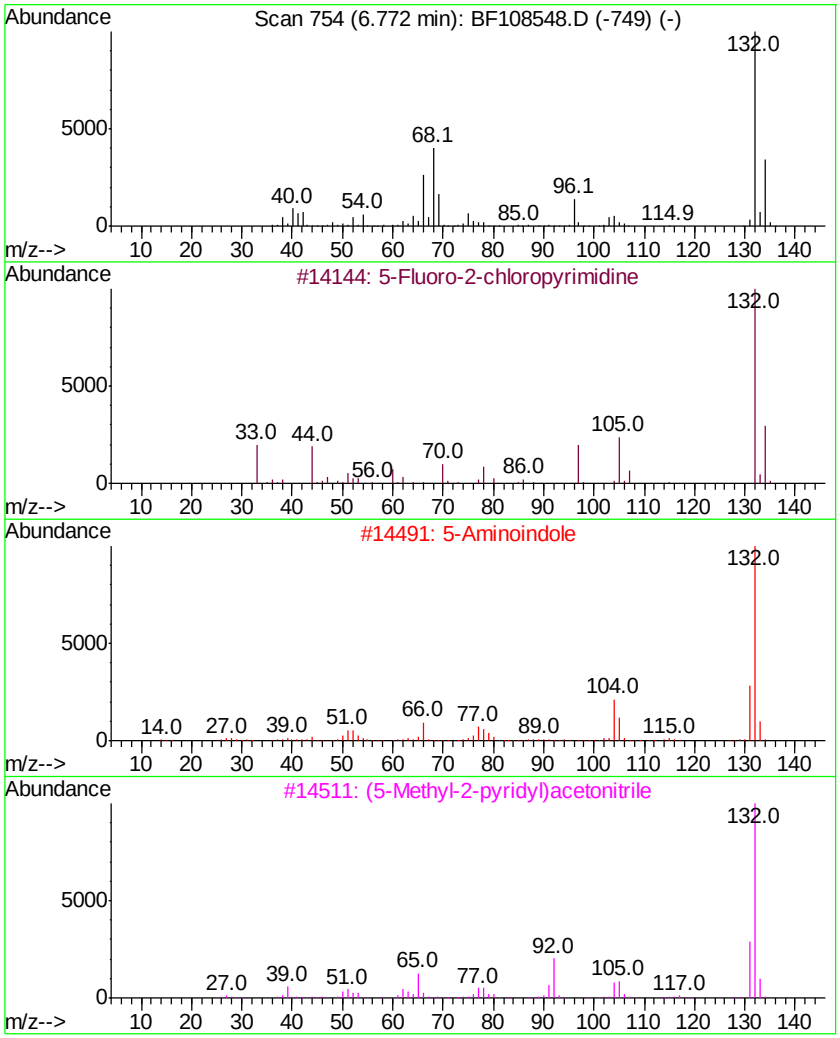
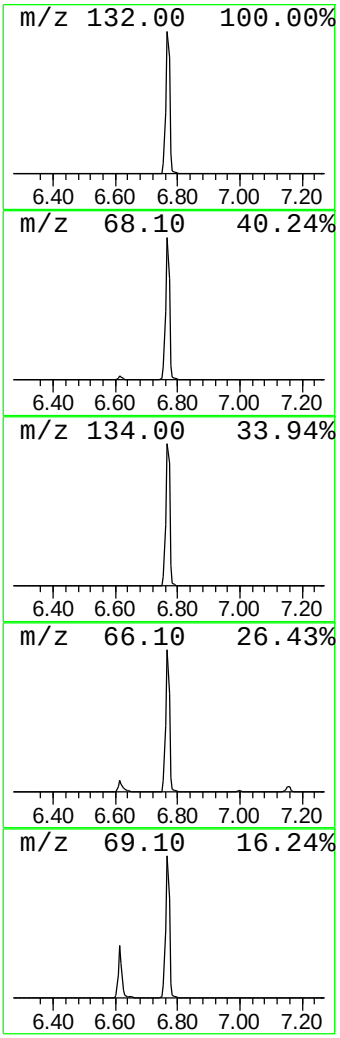
Peak Number 2 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	58.18 ng	1805570	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9





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Acq On : 28 Aug 2018 9:06
Operator : JU/SJ
Sample : J4660-04
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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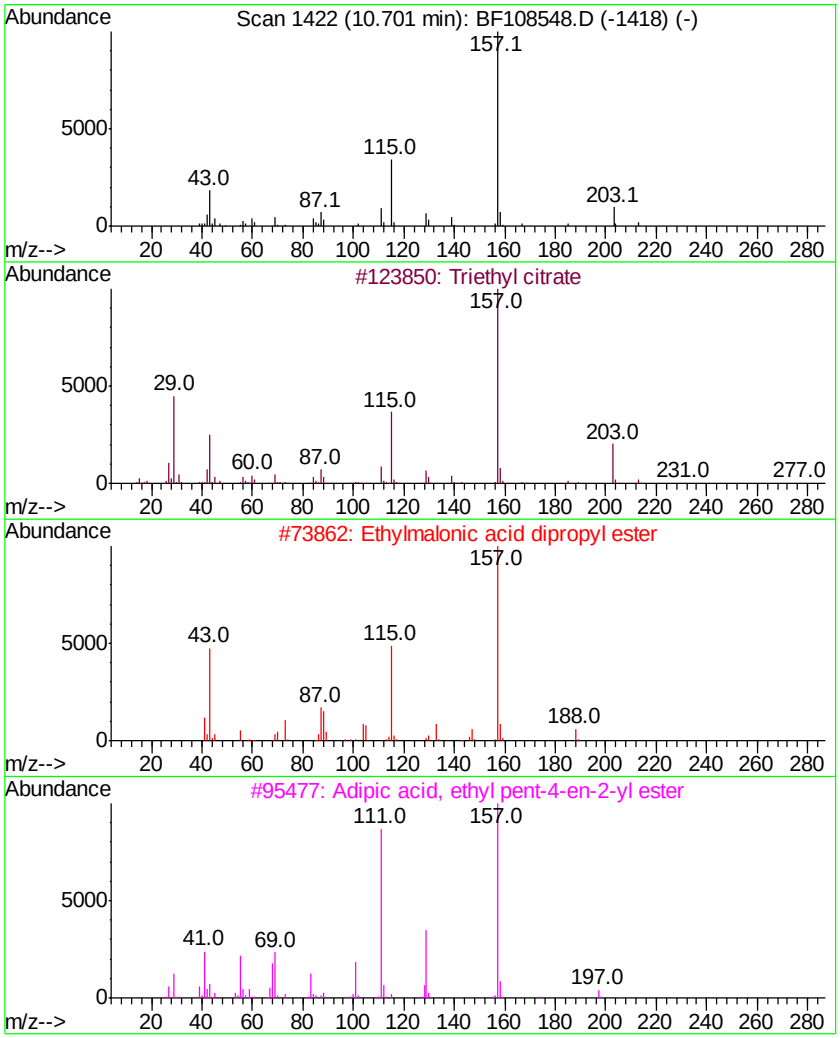
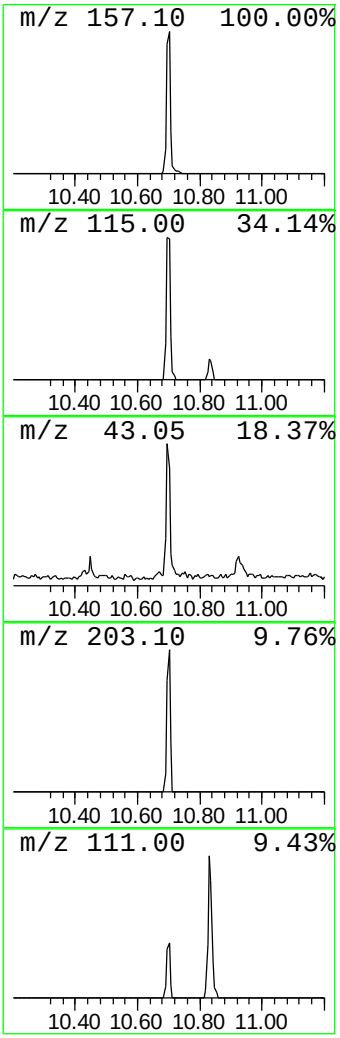
Peak Number 4 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.50 ng	81528	Acenaphthene-d10	10.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	87
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	Adipic acid, ethyl pent-4-en-2-y...	242	C13H22O4	1000354-11-7	40
4	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	36
5	3-Chloro2-fluorobenzoic acid, 4-...	356	C20H30ClFO2	1000338-64-4	33





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Operator : JU/SJ
Sample : J4660-04
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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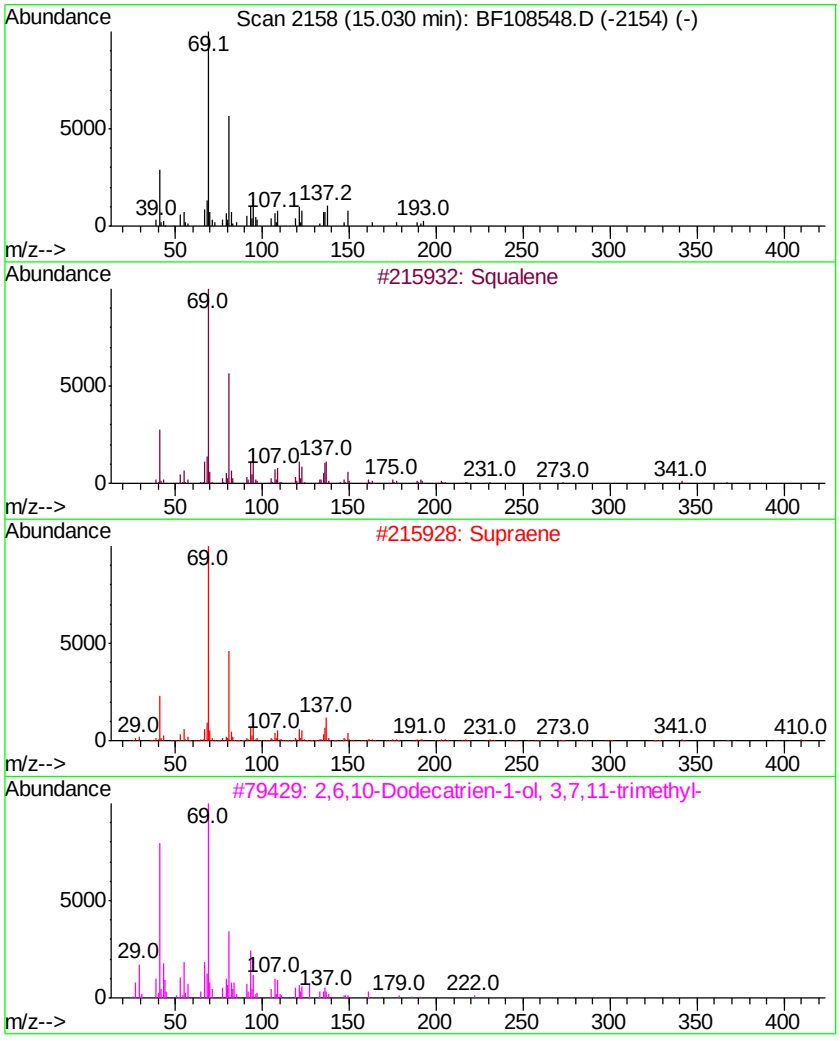
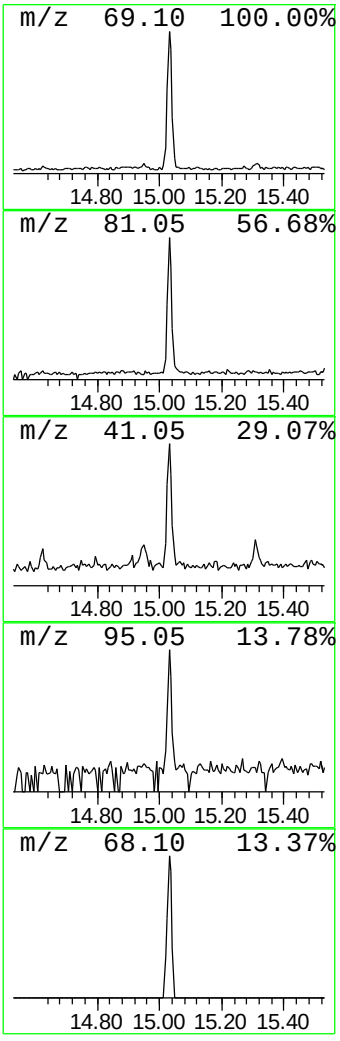
Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	2.64 ng	67045	Perylene-d12	15.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	56
4	Succinic acid, di(3-methylbut-3-...	254	C14H22O4	1000353-45-6	53
5	2H-1-Benzopyran-2-one, 7-[(3,7-d...	298	C19H22O3	000495-02-3	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082718\
Data File : BF108548.D
Acq On : 28 Aug 2018 9:06
Operator : JU/SJ
Sample : J4660-04
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	5.23	2.7	ng	83867	1	7.00	620665	20.0
unknown6.77	6.77	58.2	ng	1805570	1	7.00	620665	20.0
Triethyl citrate	10.70	2.5	ng	81528	3	10.04	652803	20.0
Squalene	15.03	2.6	ng	67045	6	15.74	507824	20.0