LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108550.D
Acq On : 28 Aug 2018 9:59
Operator : JU/SJ
Sample : J4660-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

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

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	500	rBV	63359	67208	1.98%	0.345%
2	5.625	555	559	570	rBV	1035919	1003882	29.64%	5.160%
3	6.613	724	727	741	rBV	732058	685378	20.24%	3.523%
4	6.766	749	753	757	rBV	2027029	1747815	51.61%	8.984%
5	6.995	789	792	796	rBV	686014	624648	18.44%	3.211%
6	7.154	815	819	823	rBV	2693662	2503920	73.94%	12.870%
7	7.560	883	888	892	rBV	1907536	1974794	58.31%	10.150%
8	8.284	1007	1011	1024	rBV	726671	692389	20.44%	3.559%
9	9.354	1189	1193	1203	rBV	3684215	3386594	100.00%	17.407%
10	9.742	1256	1259	1267	rBV	59270	57304	1.69%	0.295%
11	10.042	1307	1310	1321	rVB	736048	637545	18.83%	3.277%
12	10.701	1419	1422	1425	rBV	132216	105933	3.13%	0.544%
13	10.836	1441	1445	1457	rBV	1109605	1051532	31.05%	5.405%
14	11.536	1561	1564	1572	rVB	638708	563423	16.64%	2.896%
15	13.125	1829	1834	1837	rBV	3172730	2814081	83.09%	14.464%
16	14.189	2011	2015	2023	rBV	766753	712747	21.05%	3.663%
17	14.630	2086	2090	2094	rVB3	36556	49647	1.47%	0.255%
18	14.948	2142	2144	2149	rVB2	38634	40646	1.20%	0.209%
19	15.036	2155	2159	2162	rVB	122055	129329	3.82%	0.665%
20	15.313	2203	2206	2210	rVB	38466	44550	1.32%	0.229%
21	15.748	2272	2280	2286	rVB	338940	500859	14.79%	2.574%
22	16.195	2352	2356	2364	rVB2	32768	61597	1.82%	0.317%

Sum of corrected areas: 19455821

LSC Report - Integrated Chromatogram

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Misc :
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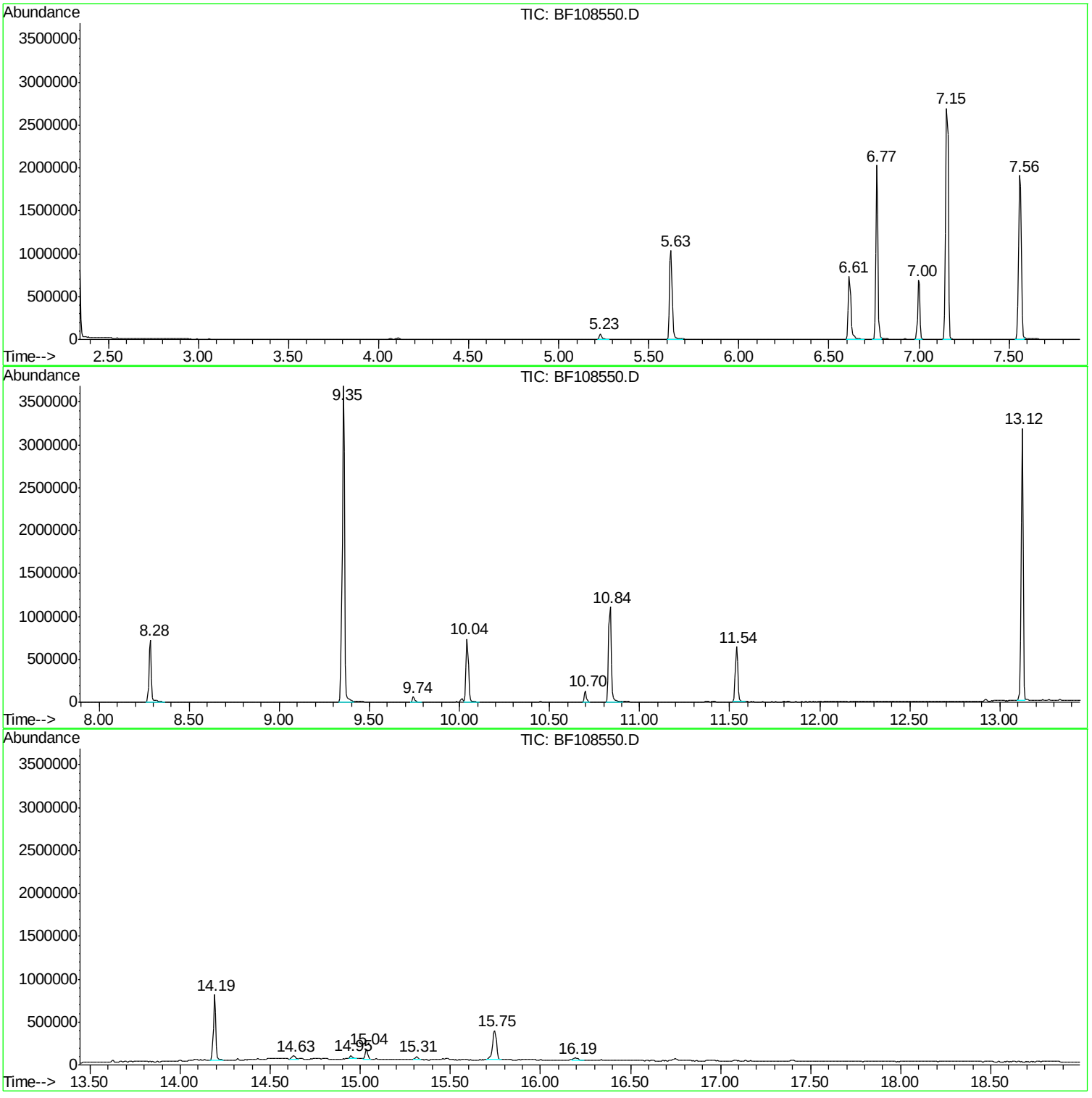
Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-U-M

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

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

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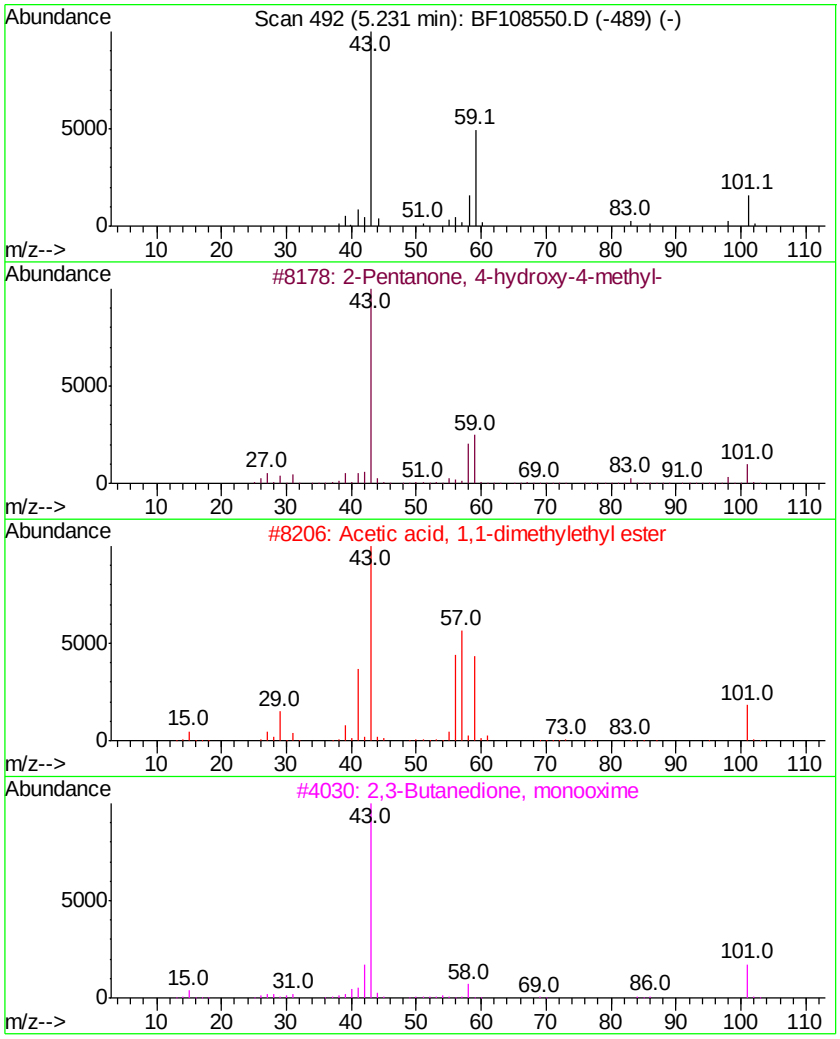
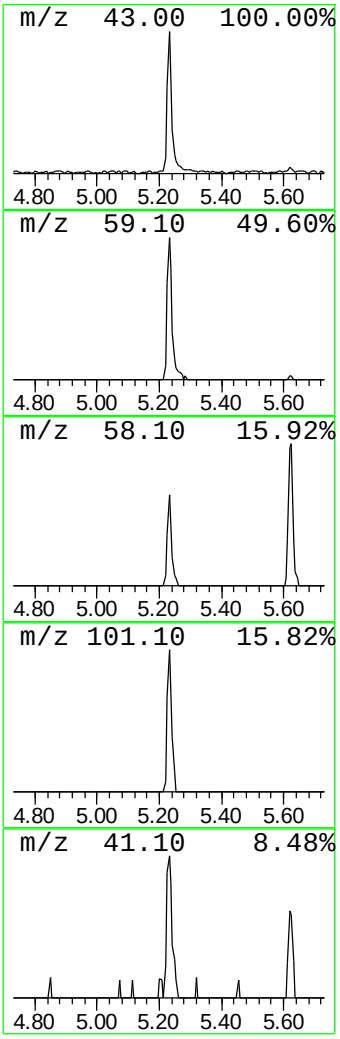
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	2.15 ng	67208	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	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





Library Search Compound Report

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Misc :
ALS Vial : 52 Sample Multiplier: 1

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

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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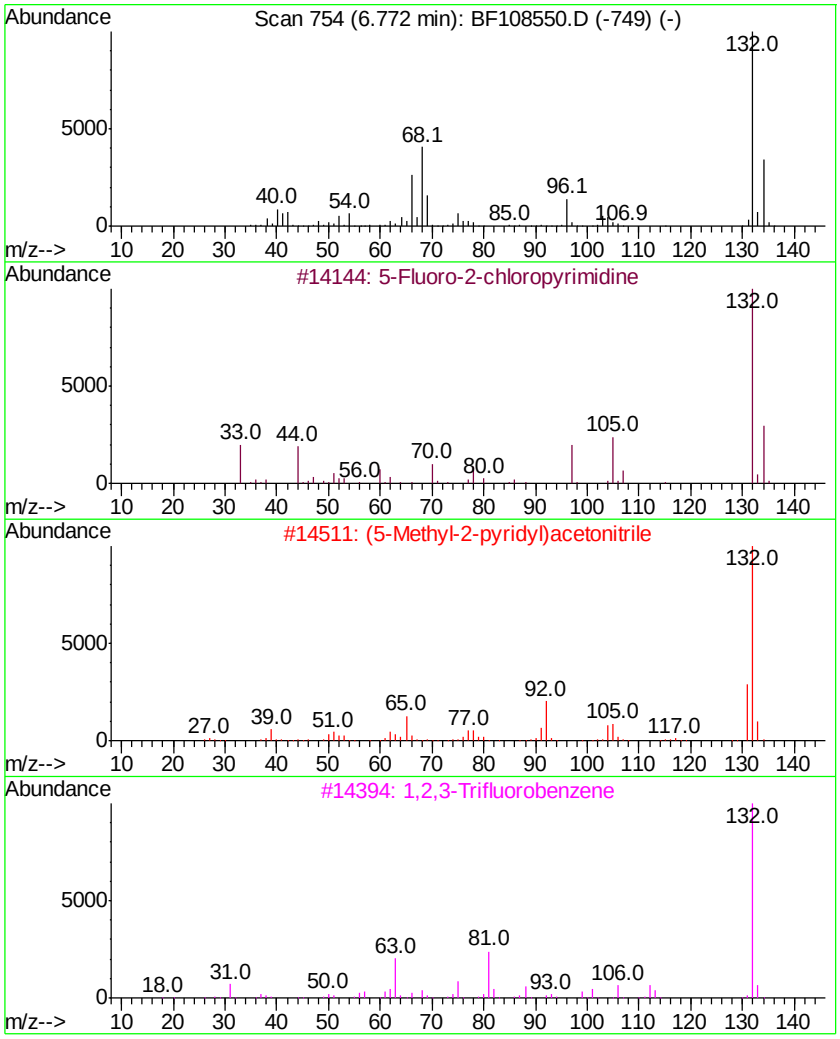
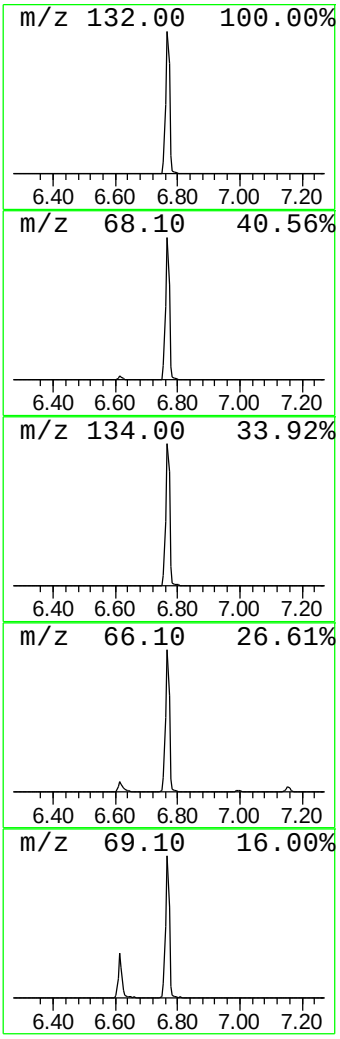
Peak Number 2 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	55.96 ng	1747820	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-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
3	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Acq On : 28 Aug 2018 9:59
Operator : JU/SJ
Sample : J4660-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

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

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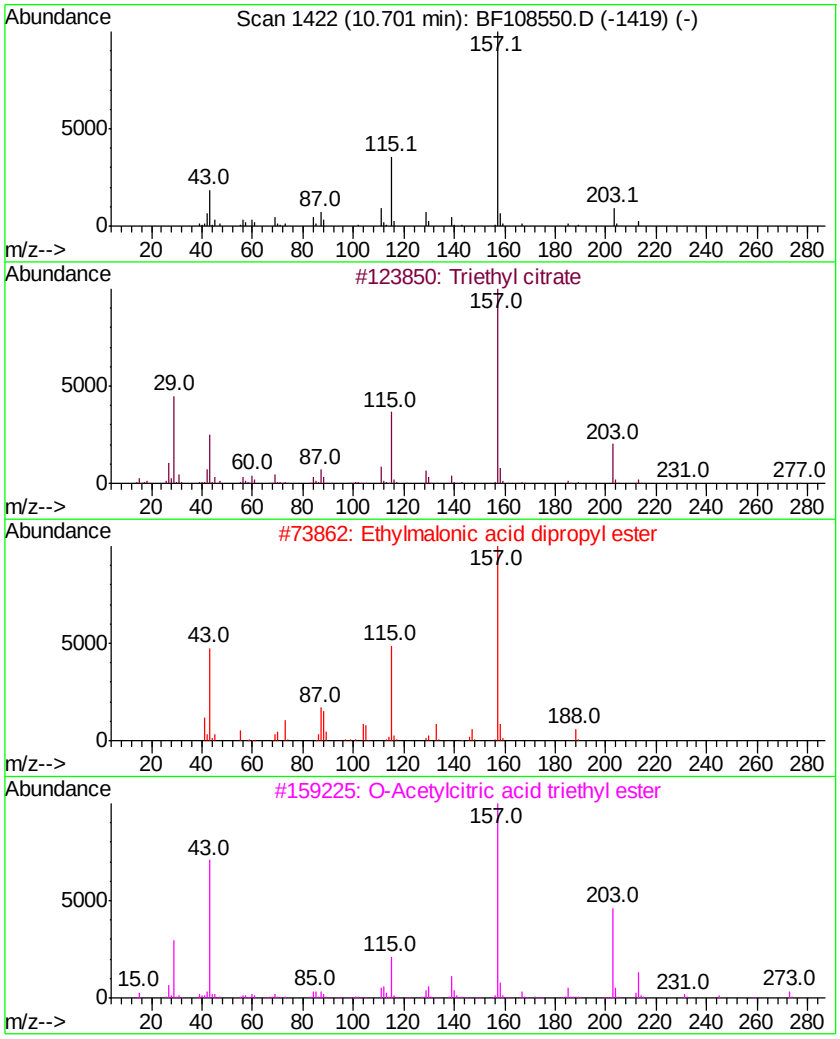
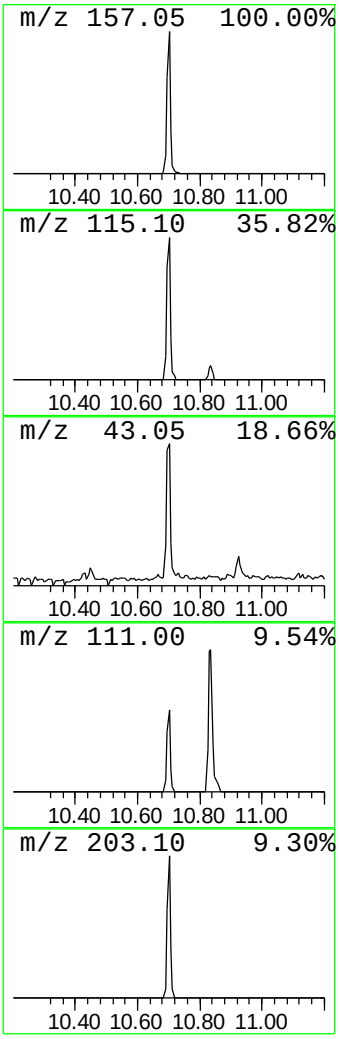
Peak Number 4 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	3.32 ng	105933	Acenaphthene-d10	10.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	86
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	59
3	O-Acetylcitric acid triethyl ester	318	C14H22O8	000077-89-4	56
4	3-Chloro2-fluorobenzoic acid, 4-...	384	C22H34ClFO2	1000338-65-1	36
5	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	36





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Sample : J4660-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

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

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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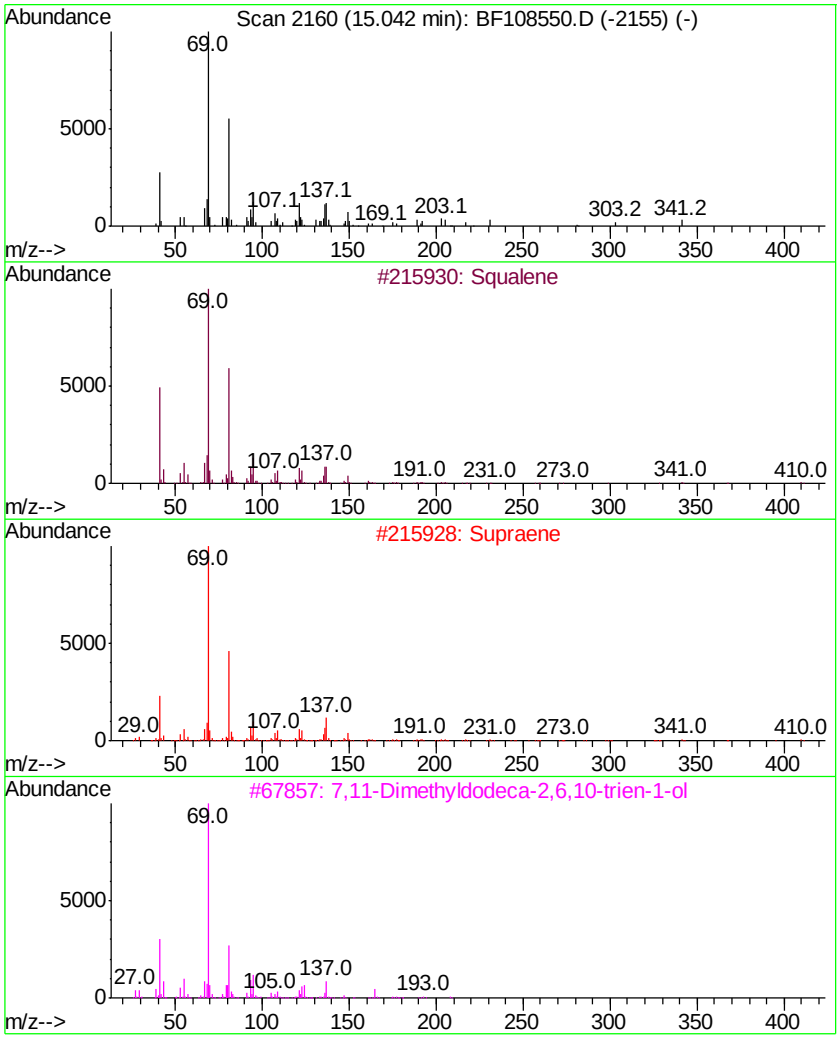
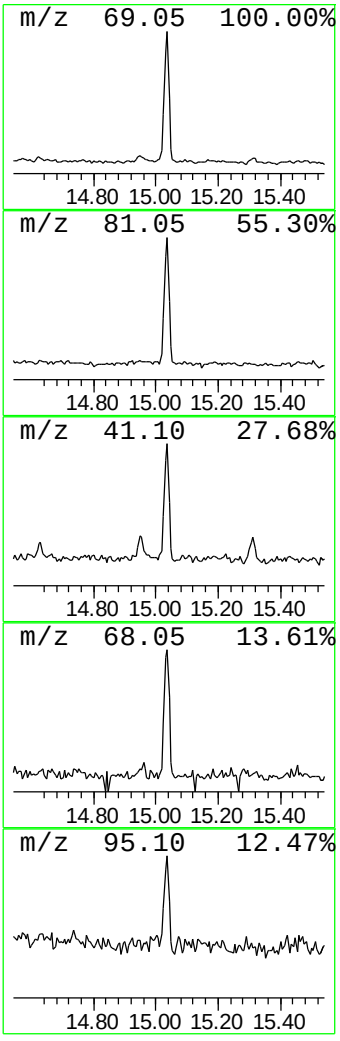
Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	5.16 ng	129329	Perylene-d12	15.75

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	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	Farnesol, acetate	264	C17H28O2	1000352-67-2	59
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58





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Misc :
ALS Vial : 52 Sample Multiplier: 1

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

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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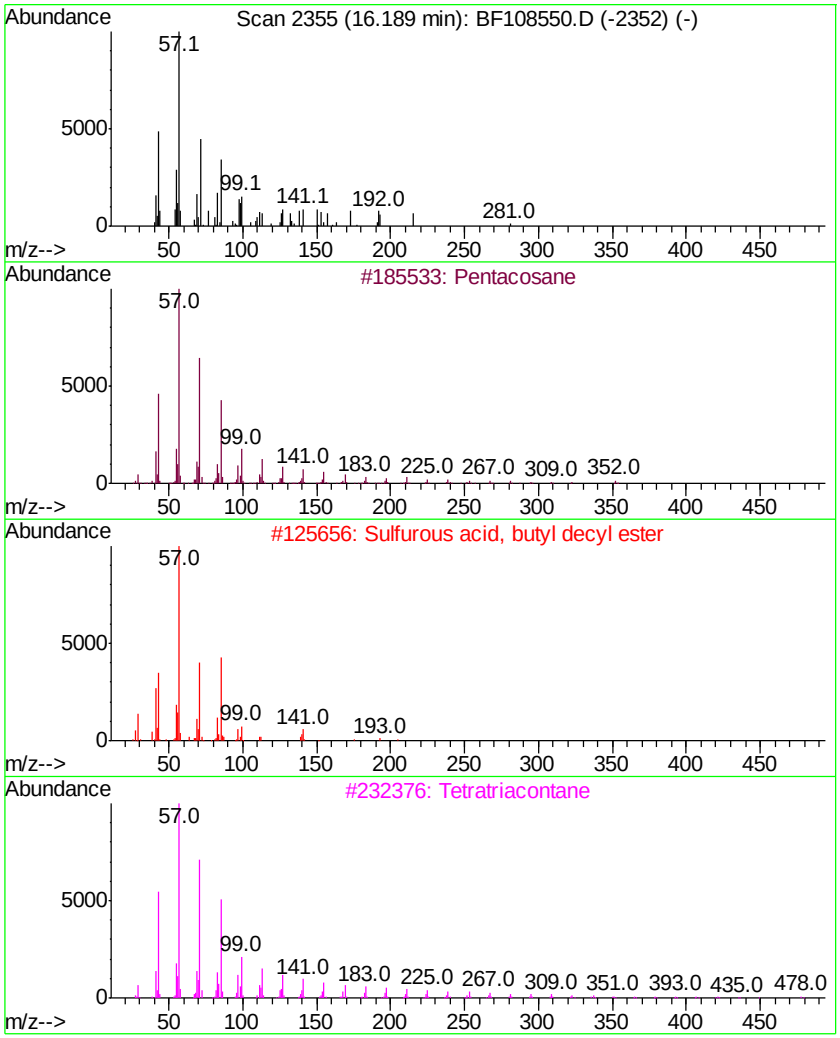
TIC Integration Parameters: LSCINT.P

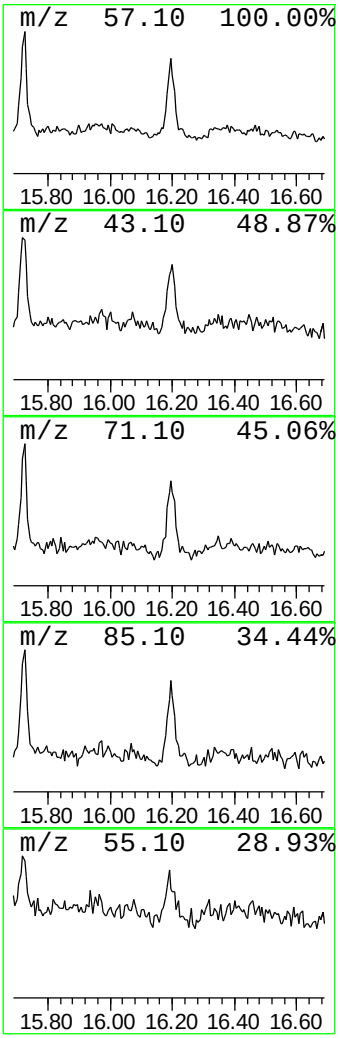
****

Peak Number 6 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.46 ng	61597	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	72
2	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	64
3	Tetratriacontane	479	C34H70	014167-59-0	59
4	Tetracontane	563	C40H82	004181-95-7	53
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	53





Tentatively Identified Compound (LSC) summary

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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...	5.23	2.1	ng	67208	1	7.00	624648	20.0
unknown6.77	6.77	56.0	ng	1747820	1	7.00	624648	20.0
Triethyl citrate	10.70	3.3	ng	105933	3	10.04	637545	20.0
Squalene	15.04	5.2	ng	129329	6	15.75	500859	20.0
Pentacosane	16.19	2.5	ng	61597	6	15.75	500859	20.0