LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108725.D
Acq On : 1 Sep 2018 8:16
Operator : JU/SJ
Sample : J4729-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-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-BF083018.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	5.684	560	569	570	rBV4	33276	78341	2.83%	0.553%
2	6.660	729	735	739	rBV	56563	112156	4.05%	0.791%
3	6.772	751	754	790	rVV	423335	1070644	38.68%	7.553%
4	7.007	790	794	815	rVB	138339	390223	14.10%	2.753%
5	7.154	815	819	849	rBV	1294627	1923946	69.50%	13.573%
6	7.566	886	889	922	rBV	529804	1446176	52.24%	10.202%
7	8.283	1007	1011	1025	rBV	172047	399004	14.41%	2.815%
8	9.354	1189	1193	1230	rBV	1785818	2768229	100.00%	19.529%
9	9.742	1256	1259	1273	rBV	41093	66137	2.39%	0.467%
10	10.036	1306	1309	1329	rBV	331388	489785	17.69%	3.455%
11	10.695	1418	1421	1430	rBV	63558	66321	2.40%	0.468%
12	10.836	1441	1445	1473	rBV	439340	927706	33.51%	6.545%
13	11.542	1561	1565	1585	rBV	293355	564739	20.40%	3.984%
14	13.118	1829	1833	1856	rBV	2274810	2745908	99.19%	19.371%
15	14.195	2012	2016	2026	rBV	424388	589727	21.30%	4.160%
16	14.936	2139	2142	2150	rVB	29151	31704	1.15%	0.224%
17	15.295	2199	2203	2207	rBV	28750	34200	1.24%	0.241%
18	15.701	2267	2272	2276	rBV	32499	49972	1.81%	0.353%
19	15.754	2276	2281	2298	rVB	187203	383752	13.86%	2.707%
20	16.171	2348	2352	2358	rVB2	24317	36485	1.32%	0.257%

Sum of corrected areas: 14175155

LSC Report - Integrated Chromatogram

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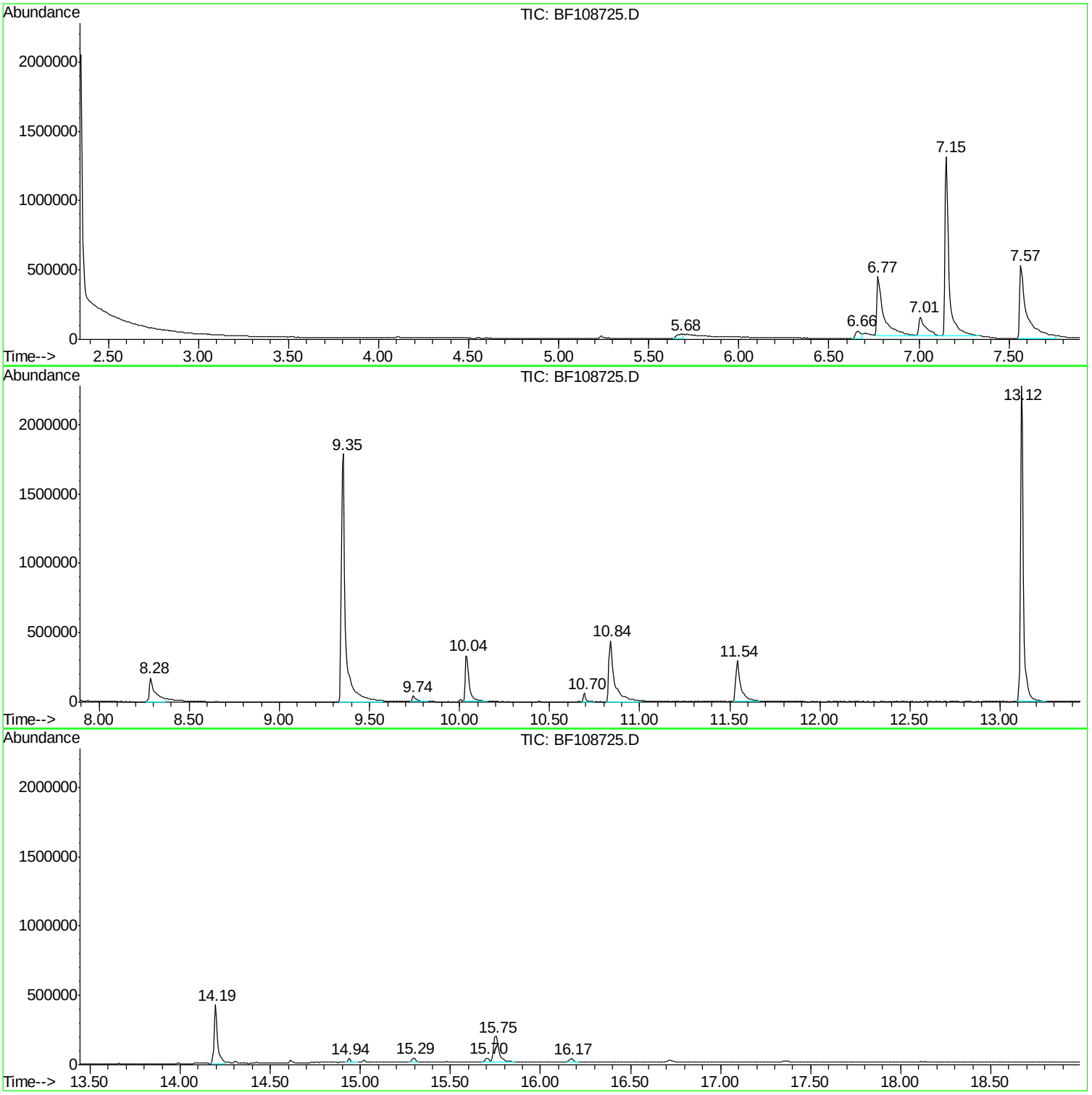
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-SIDI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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\BF083118\
Data File : BF108725.D
Acq On : 1 Sep 2018 8:16
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : 082918-SIDI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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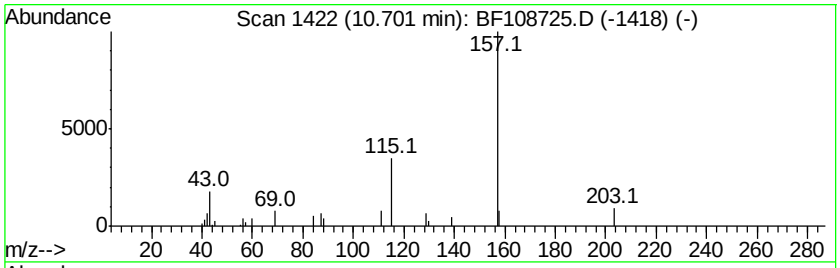
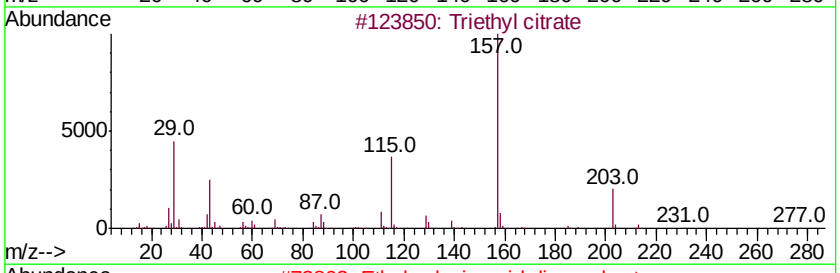
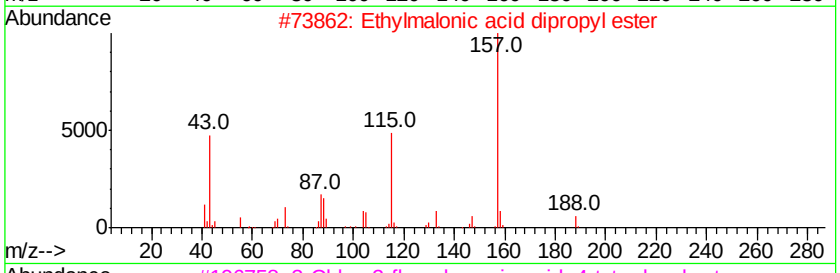
Peak Number 3 Triethyl citrate Concentration Rank 3

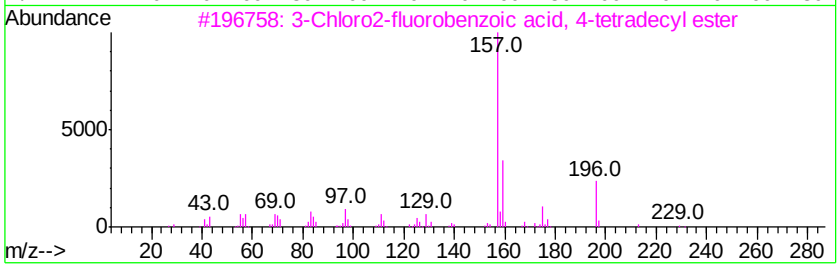
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.71 ng	66321	Acenaphthene-d10	10.04

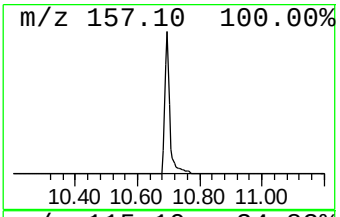
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	87
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	59
3	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	36
4	Piperazine-1-carboxylic acid, 4-...	396	C14H18Cl2N2O5S	1000303-80-3	36
5	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	36

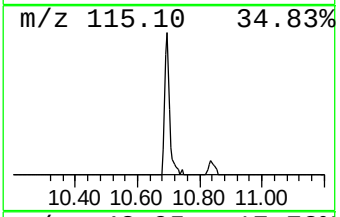


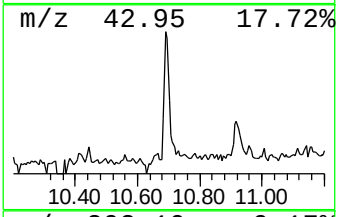


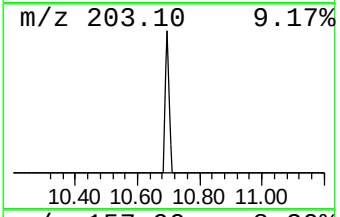


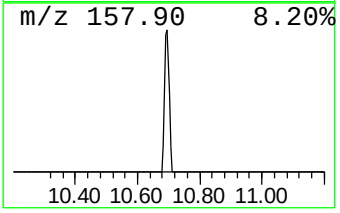












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108725.D
Acq On : 1 Sep 2018 8:16
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Misc :
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Instrument : BNA_F
ClientSampleId : 082918-SIDI-F-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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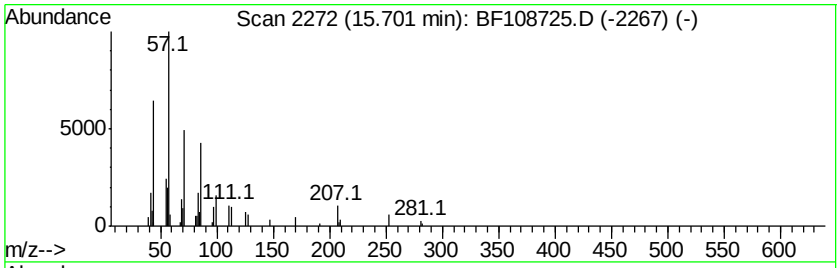
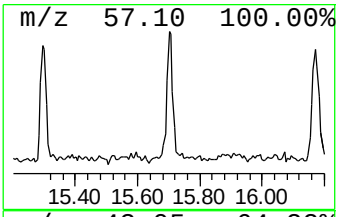
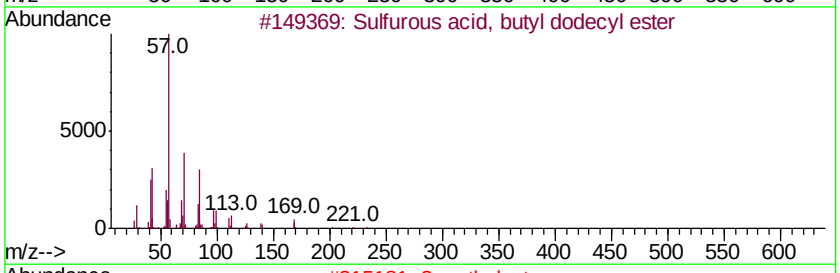
Peak Number 4 Sulfurous acid, butyl dodec... Concentration Rank 4

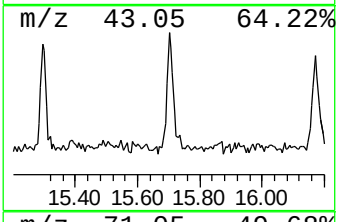
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	2.60 ng	49972	Perylene-d12	15.75

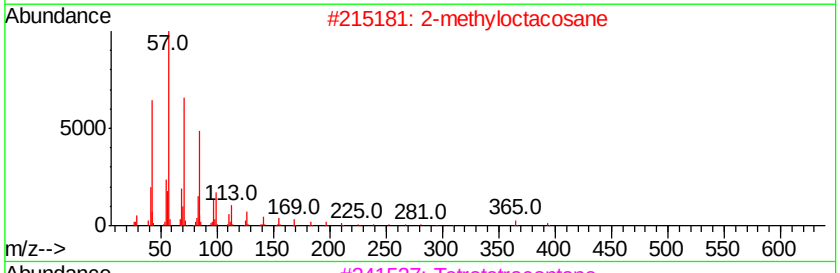
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
2	2-methyloctacosane	408	C29H60	1000376-72-8	80
3	Tetratetracontane	619	C44H90	007098-22-8	72
4	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	72
5	Octacosane	394	C28H58	000630-02-4	72

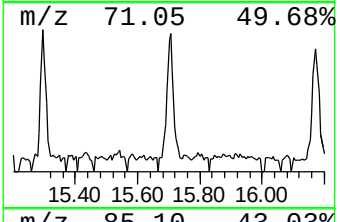


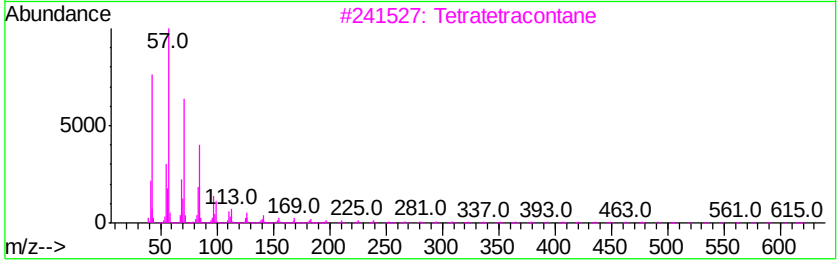


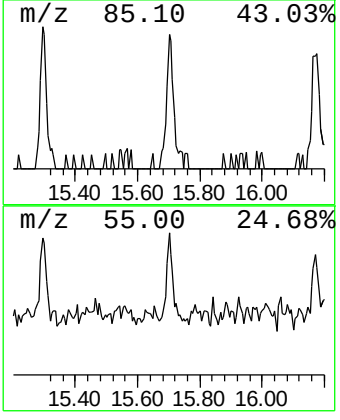












Tentatively Identified Compound (LSC) summary

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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
Triethyl citrate	10.70	2.7	ng	66321	3	10.04	489785	20.0
Sulfurous acid, b...	15.70	2.6	ng	49972	6	15.75	383752	20.0