LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108709.D
Acq On : 1 Sep 2018 00:18
Operator : JU/SJ
Sample : J4729-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-JETT-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-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	5.237	490	493	500	rBV	22412	29516	1.16%	0.215%
2	5.678	559	568	570	rBV3	35187	93181	3.65%	0.680%
3	6.660	730	735	739	rBV	50775	102547	4.01%	0.749%
4	6.778	751	755	782	rBV	375550	940920	36.82%	6.868%
5	7.007	790	794	815	rVB	145640	391698	15.33%	2.859%
6	7.154	815	819	851	rVB	1261266	1740653	68.11%	12.705%
7	7.566	886	889	934	rBV	502493	1359373	53.19%	9.922%
8	8.283	1007	1011	1030	rBV	203237	444656	17.40%	3.246%
9	9.354	1189	1193	1220	rBV	1894798	2460878	96.30%	17.962%
10	9.742	1256	1259	1272	rBV	62190	96235	3.77%	0.702%
11	10.042	1306	1310	1328	rBV	399067	505032	19.76%	3.686%
12	10.695	1418	1421	1429	rBV	141773	131026	5.13%	0.956%
13	10.836	1441	1445	1457	rBV	525356	883089	34.56%	6.446%
14	11.542	1561	1565	1580	rBV	375341	603937	23.63%	4.408%
15	13.124	1829	1834	1848	rBV	2241403	2555470	100.00%	18.653%
16	14.048	1985	1991	2000	rBV	16118	49895	1.95%	0.364%
17	14.195	2012	2016	2026	rBV	489745	626161	24.50%	4.570%
18	14.618	2085	2088	2095	rVB3	23061	27814	1.09%	0.203%
19	14.942	2139	2143	2147	rVB	31035	36181	1.42%	0.264%
20	15.024	2153	2157	2162	rVB	86270	92229	3.61%	0.673%
21	15.301	2200	2204	2210	rVB	37291	46631	1.82%	0.340%
22	15.706	2270	2273	2276	rBV2	32281	38038	1.49%	0.278%
23	15.754	2276	2281	2290	rVV	223280	397442	15.55%	2.901%
24	16.177	2350	2353	2361	rVB2	33123	47731	1.87%	0.348%

Sum of corrected areas: 13700333

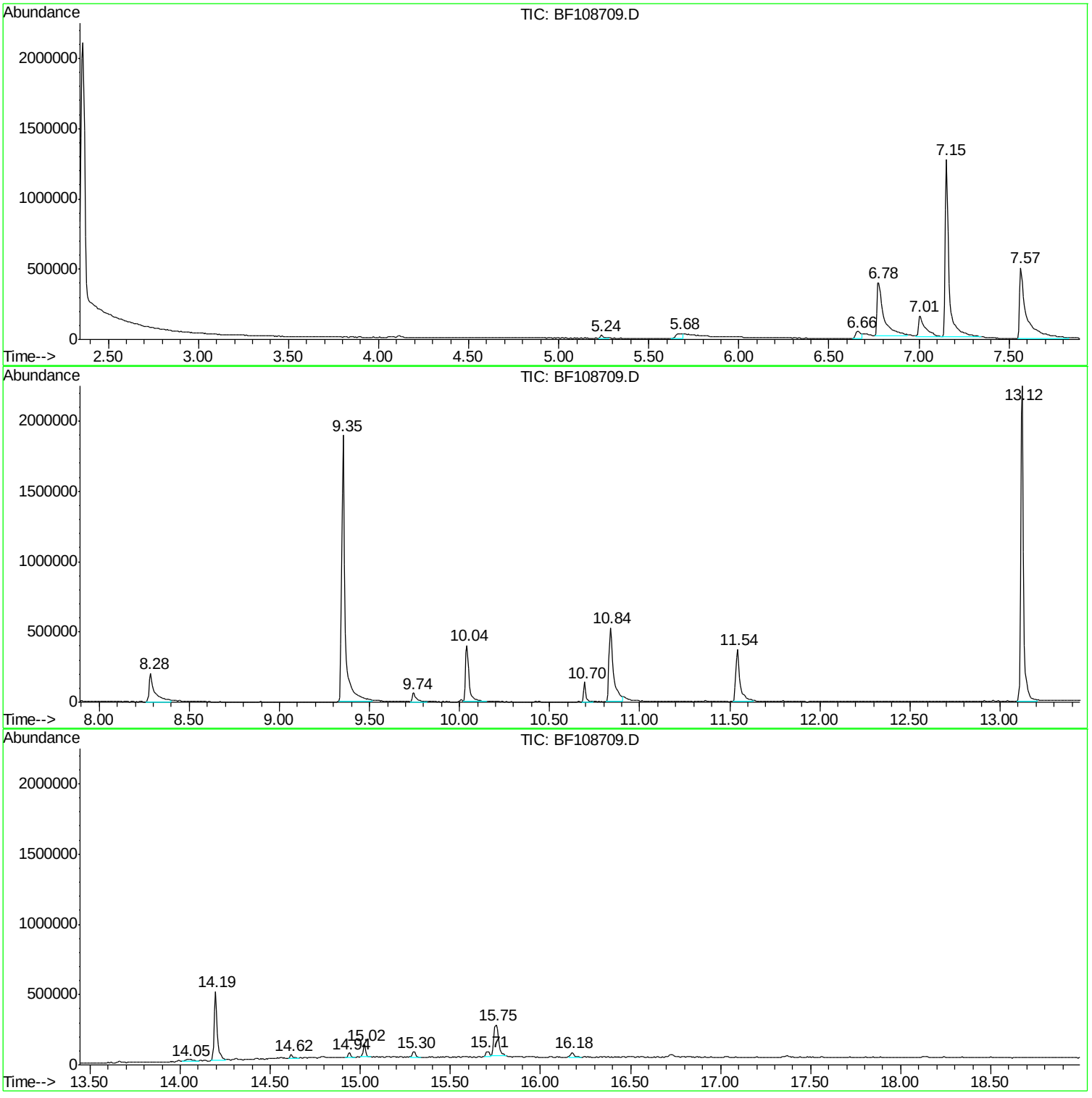
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108709.D
Acq On : 1 Sep 2018 00:18
Operator : JU/SJ
Sample : J4729-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-JETT-E-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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108709.D
Acq On : 1 Sep 2018 00:18
Operator : JU/SJ
Sample : J4729-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

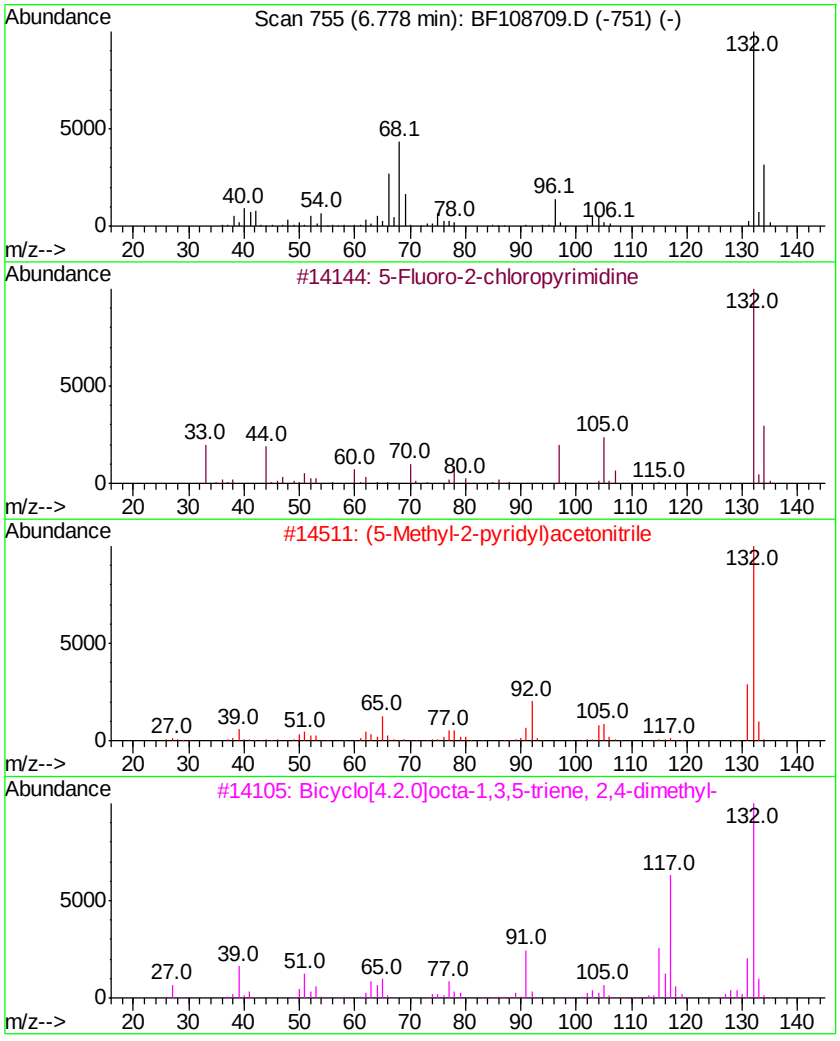
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

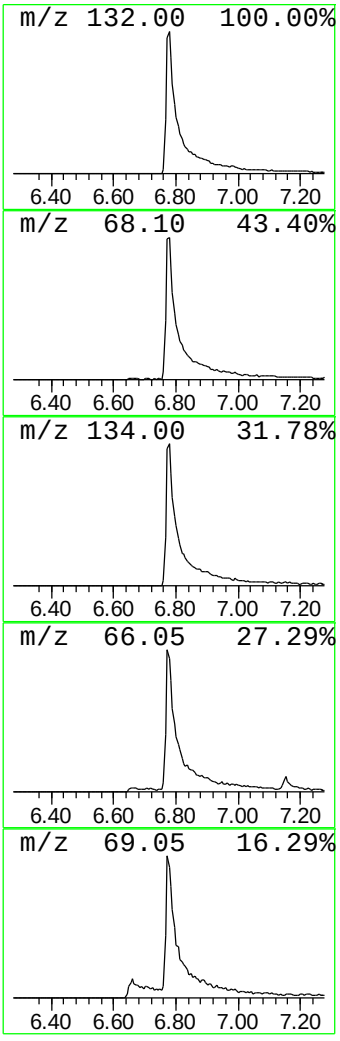
****

Peak Number 1 unknown6.78 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	48.04 ng	940920	1,4-Dichlorobenzene-d4	7.01

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	1-Aminoindan	133	C9H11N	034698-41-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108709.D
Acq On : 1 Sep 2018 00:18
Operator : JU/SJ
Sample : J4729-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

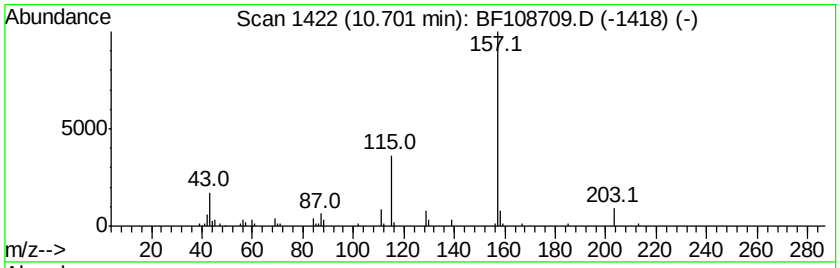
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

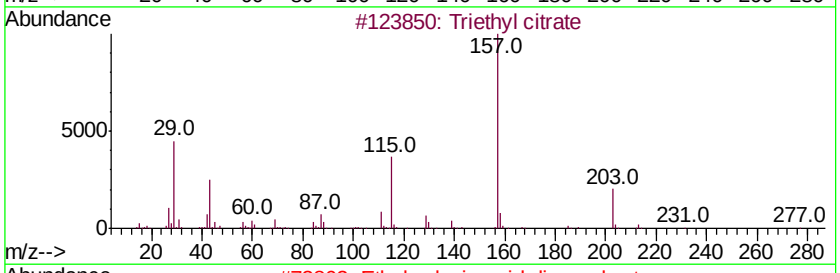
****

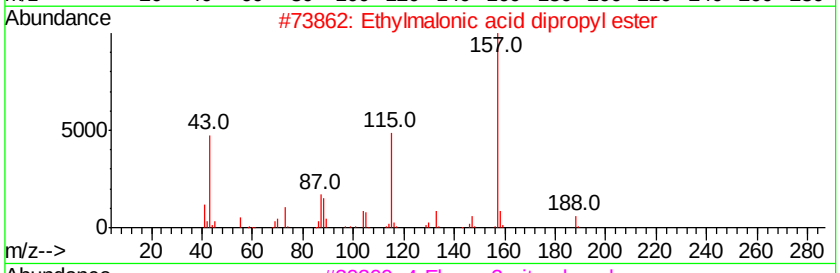
Peak Number 3 Triethyl citrate Concentration Rank 3

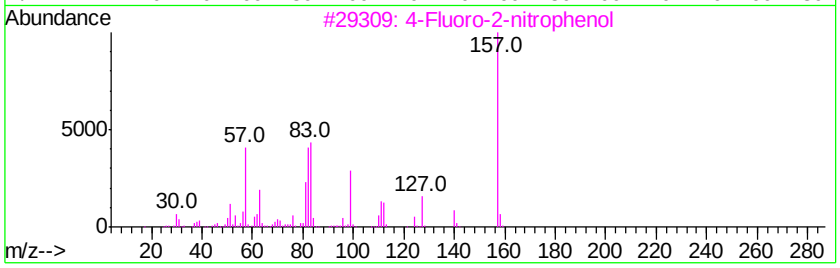
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	5.19 ng	131026	Acenaphthene-d10	10.04

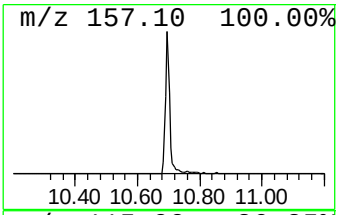
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	87
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	59
3	4-Fluoro-2-nitrophenol	157	C6H4FNO3	000394-33-2	40
4	Adipic acid, ethyl 2-methylpent-...	258	C14H26O4	1000353-55-5	40
5	Hexanedioic acid, 3-ethyl-, bis(...	286	C16H30O4	057983-54-7	39

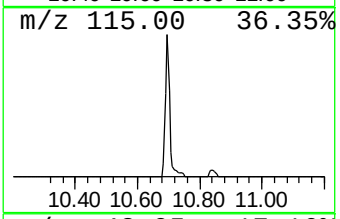


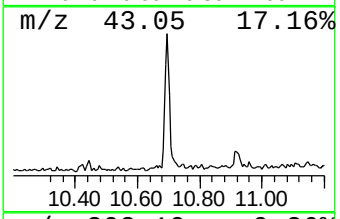


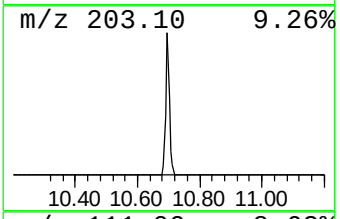


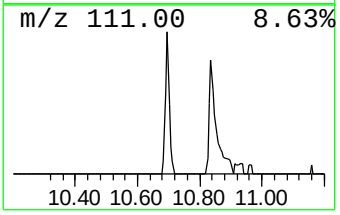












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108709.D
Acq On : 1 Sep 2018 00:18
Operator : JU/SJ
Sample : J4729-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

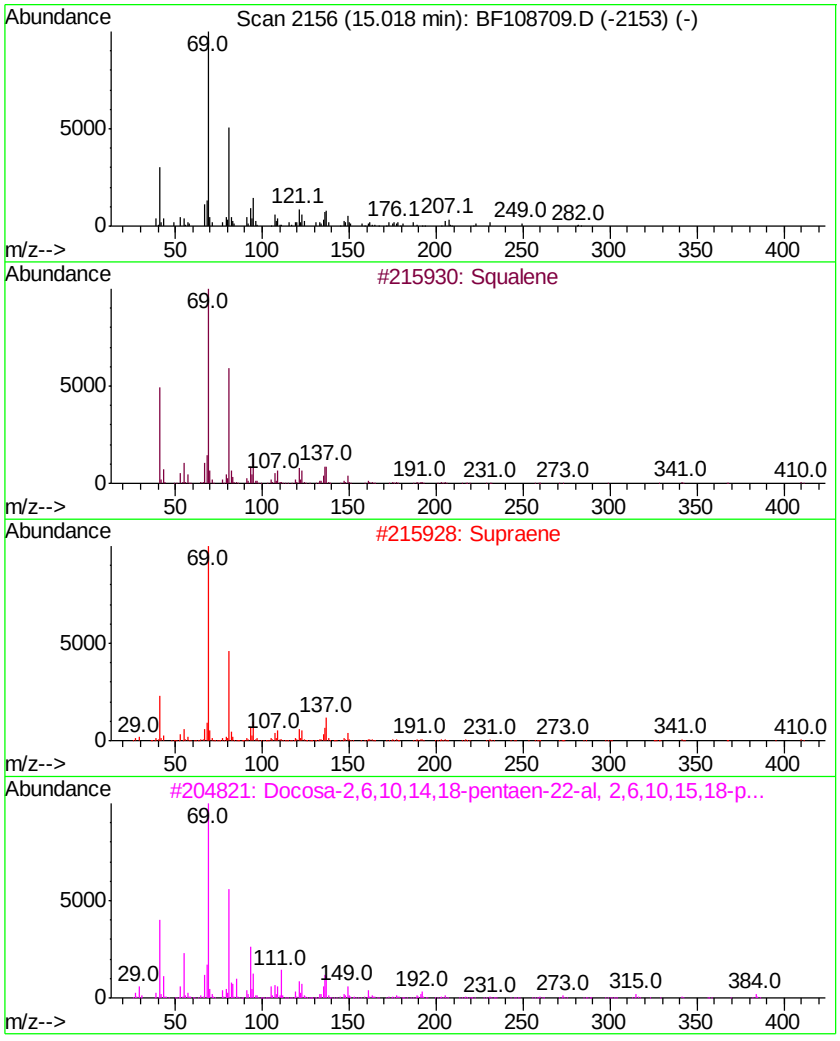
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

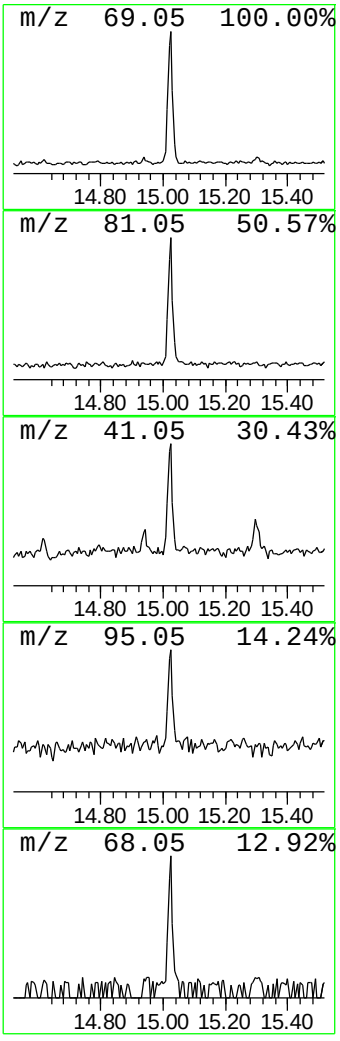
****

Peak Number 4 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	4.64 ng	92229	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	83
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5	Cyclopropanecarboxylic acid, 4-i...	204	C13H16O2	1000331-01-9	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108709.D
Acq On : 1 Sep 2018 00:18
Operator : JU/SJ
Sample : J4729-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

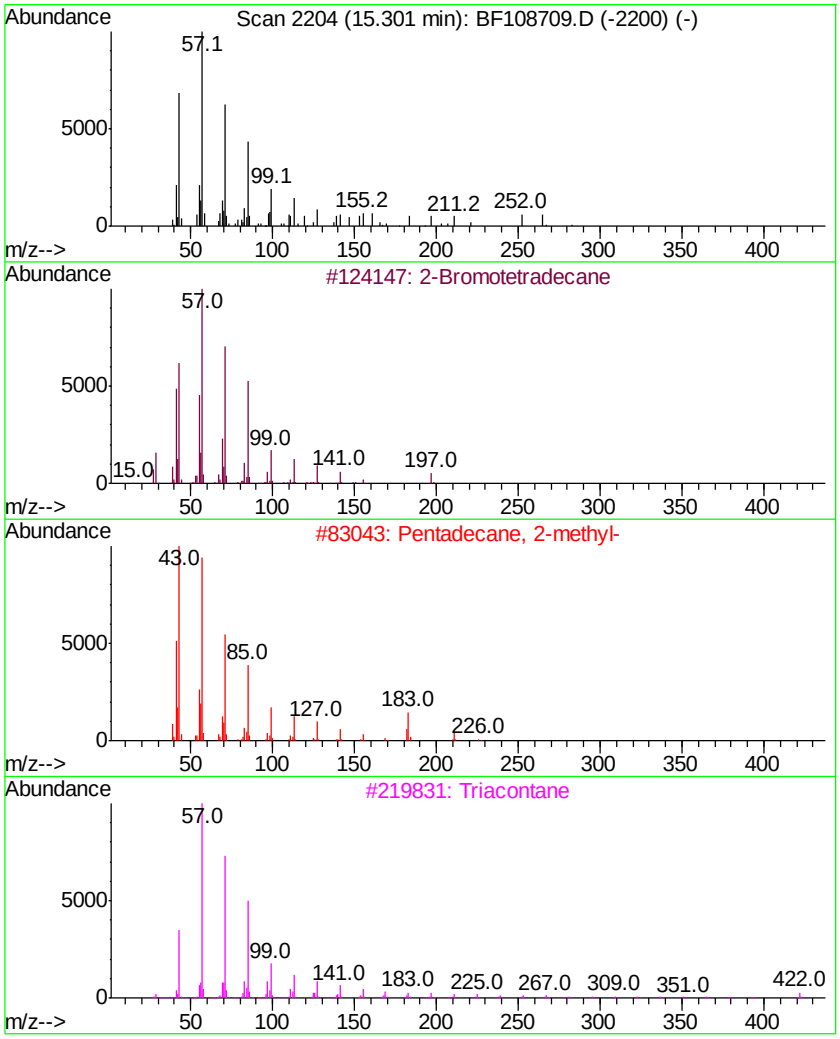
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

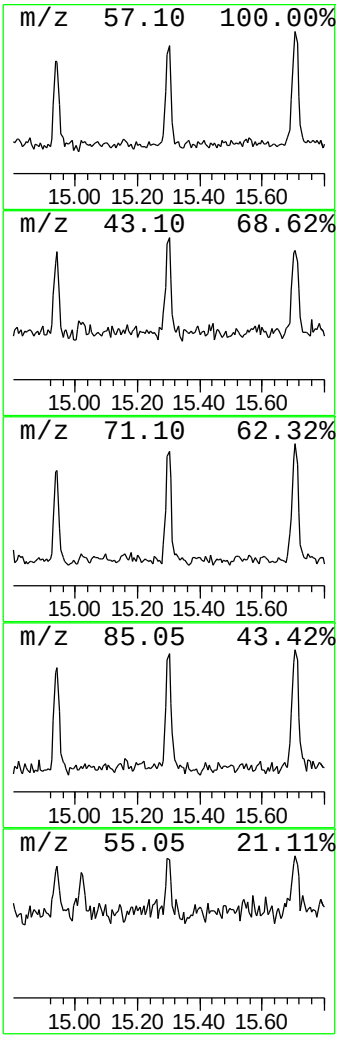
****

Peak Number 5 2-Bromotetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	2.35 ng	46631	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromotetradecane	276	C14H29Br	074036-95-6	83
2	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	80
3	Triacontane	422	C30H62	000638-68-6	80
4	Hexacosane	366	C26H54	000630-01-3	74
5	Heneicosane	296	C21H44	000629-94-7	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108709.D
Acq On : 1 Sep 2018 00:18
Operator : JU/SJ
Sample : J4729-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-JETT-E-D-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

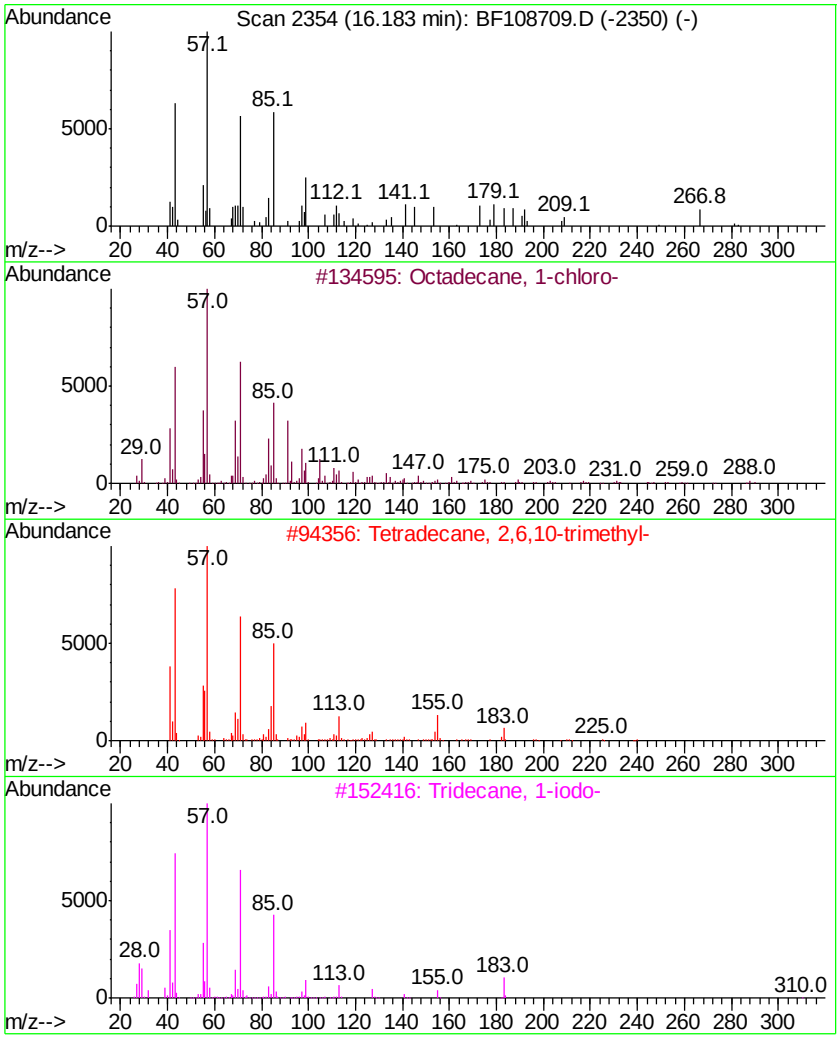
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

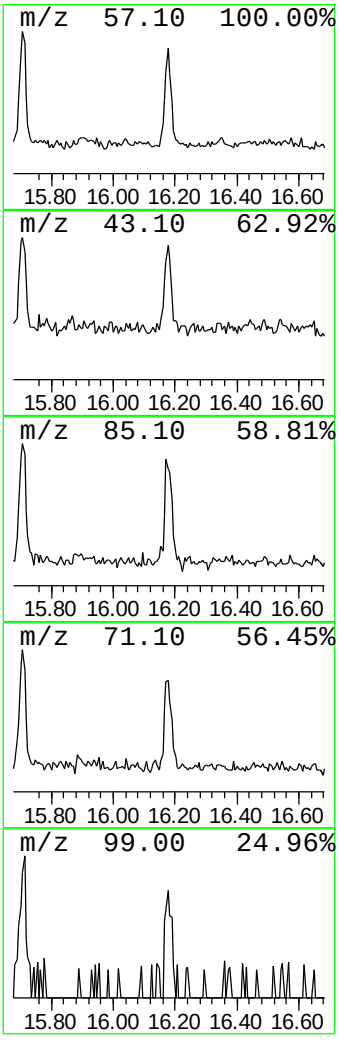
****

Peak Number 6 Octadecane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.40 ng	47731	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	53
2	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	53
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	52
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	47
5	Decane, 3-bromo-	220	C10H21Br	030571-71-2	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083118\
Data File : BF108709.D
Acq On : 1 Sep 2018 00:18
Operator : JU/SJ
Sample : J4729-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-JETT-E-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.78	6.78	48.0	ng	940920	1	7.01	391698	20.0
Triethyl citrate	10.70	5.2	ng	131026	3	10.04	505032	20.0
Squalene	15.02	4.6	ng	92229	6	15.75	397442	20.0
2-Bromotetradecane	15.30	2.4	ng	46631	6	15.75	397442	20.0
Octadecane, 1-chl...	16.18	2.4	ng	47731	6	15.75	397442	20.0