LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107573.D
Acq On : 21 Jul 2018 13:48
Operator : JU/SJ
Sample : J4094-06
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071818-DBRI-E-U-S

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-BF072018.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	5.201	484	487	494	rBV	121843	133122	1.53%	0.251%
2	5.601	551	555	570	rBV	1951736	2565765	29.49%	4.847%
3	6.595	721	724	745	rBV	1164599	1907869	21.93%	3.604%
4	6.742	745	749	767	rVV	4394871	4866586	55.94%	9.193%
5	6.972	785	788	810	rVB	1698304	1967708	22.62%	3.717%
6	7.131	810	815	841	rBV	6185478	6733412	77.40%	12.719%
7	7.536	879	884	894	rBV	4208464	5337256	61.35%	10.082%
8	8.254	1002	1006	1023	rBV	2175027	2410675	27.71%	4.554%
9	9.330	1184	1189	1200	rBV	7734844	8699210	100.00%	16.432%
10	9.725	1252	1256	1266	rVB	110082	121251	1.39%	0.229%
11	10.013	1302	1305	1317	rVB	2093159	2241437	25.77%	4.234%
12	10.677	1415	1418	1426	rBV	545492	435500	5.01%	0.823%
13	10.807	1436	1440	1454	rBV	3095193	3342867	38.43%	6.315%
14	11.507	1556	1559	1568	rBV	1871606	2031441	23.35%	3.837%
15	12.019	1642	1646	1657	rBV2	85665	124931	1.44%	0.236%
16	13.095	1825	1829	1842	rBV	5822406	5820985	66.91%	10.996%
17	13.977	1975	1979	1986	rBV	81814	114339	1.31%	0.216%
18	14.160	2006	2010	2017	rBV	2029188	1937396	22.27%	3.660%
19	15.012	2151	2155	2159	rVB	316541	343857	3.95%	0.650%
20	15.283	2198	2201	2208	rVB	75833	92632	1.06%	0.175%
21	15.695	2266	2271	2281	rBV	1066435	1612195	18.53%	3.045%
22	16.159	2346	2350	2355	rVB	65302	98826	1.14%	0.187%

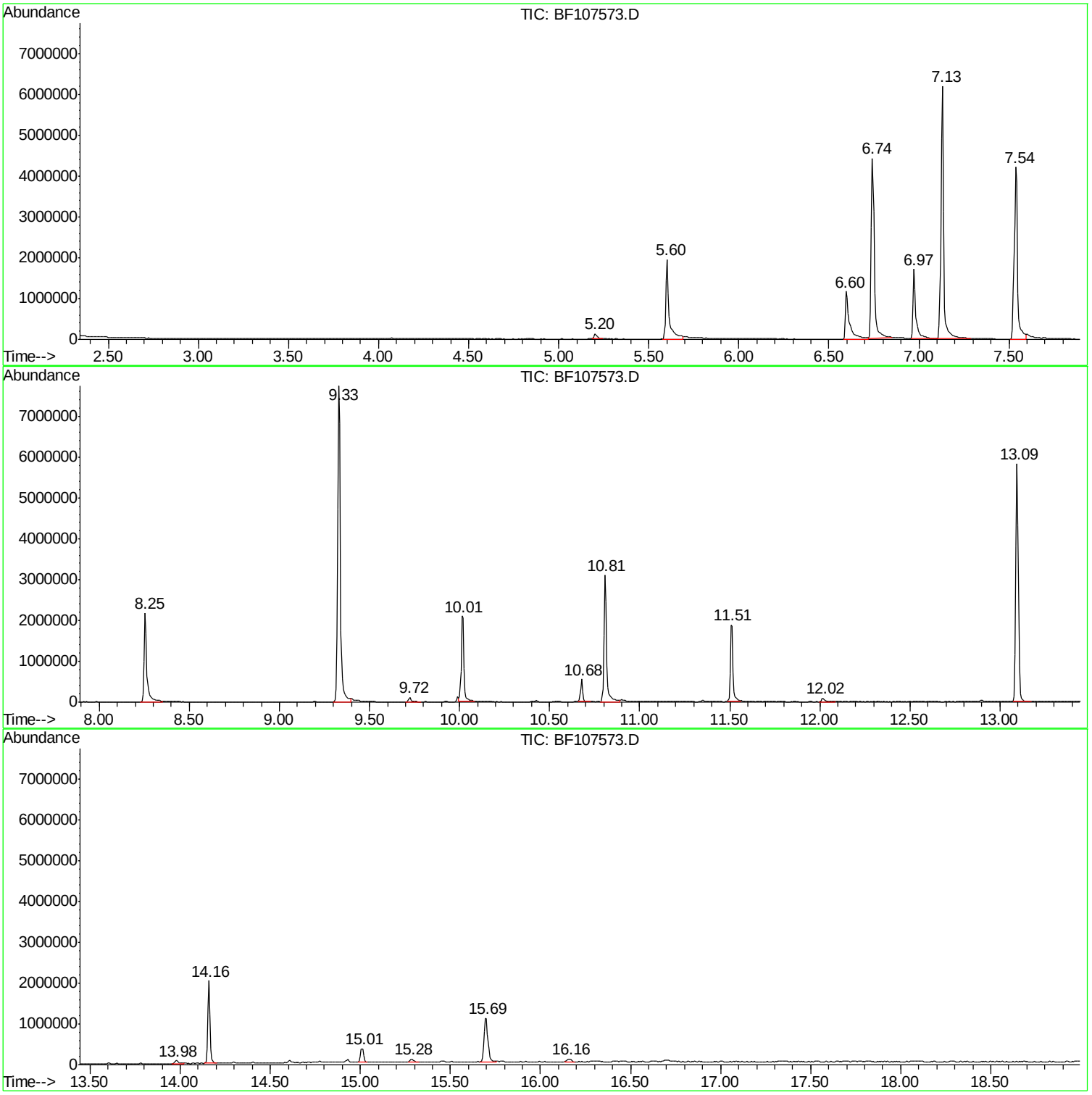
Sum of corrected areas: 52939260

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107573.D
Acq On : 21 Jul 2018 13:48
Operator : JU/SJ
Sample : J4094-06
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
071818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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\BF072018\
Data File : BF107573.D
Acq On : 21 Jul 2018 13:48
Operator : JU/SJ
Sample : J4094-06
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

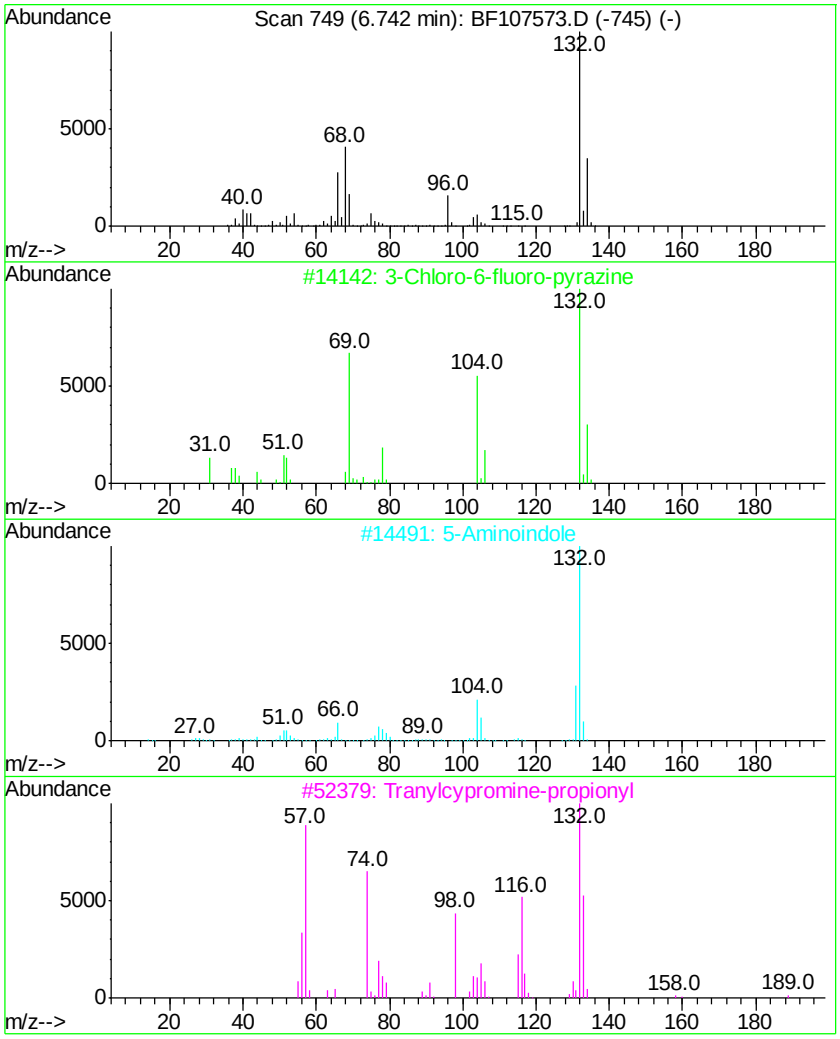
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

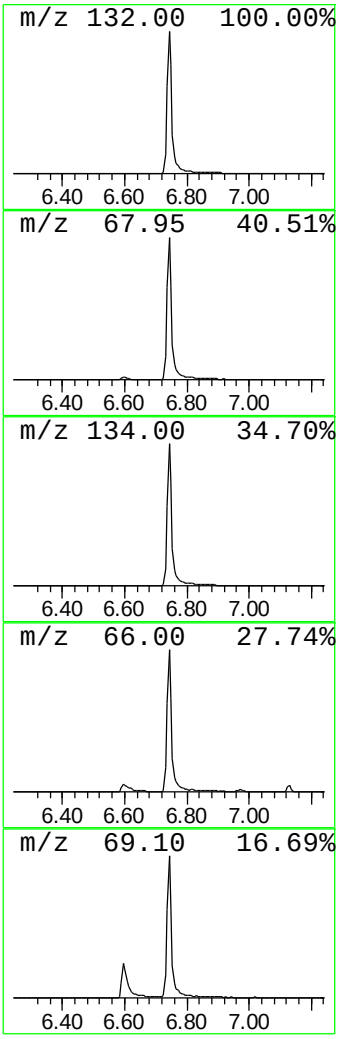
****

Peak Number 1 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	49.46 ng	4866590	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107573.D
Acq On : 21 Jul 2018 13:48
Operator : JU/SJ
Sample : J4094-06
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

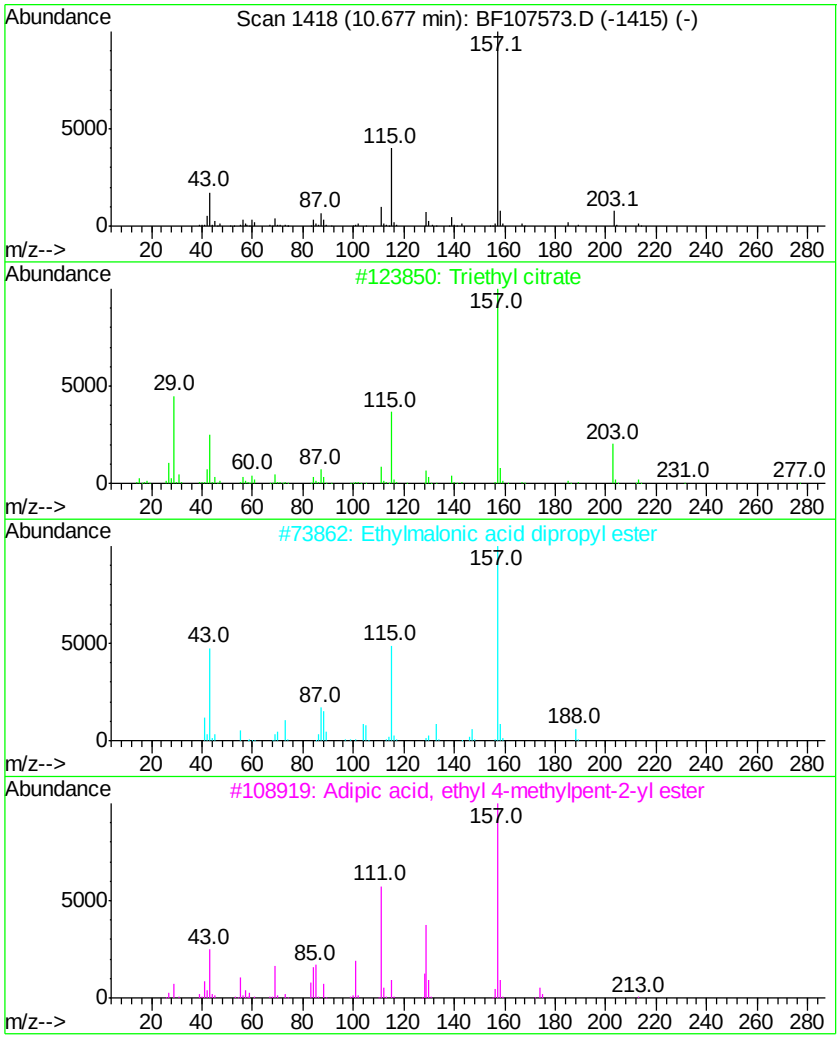
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

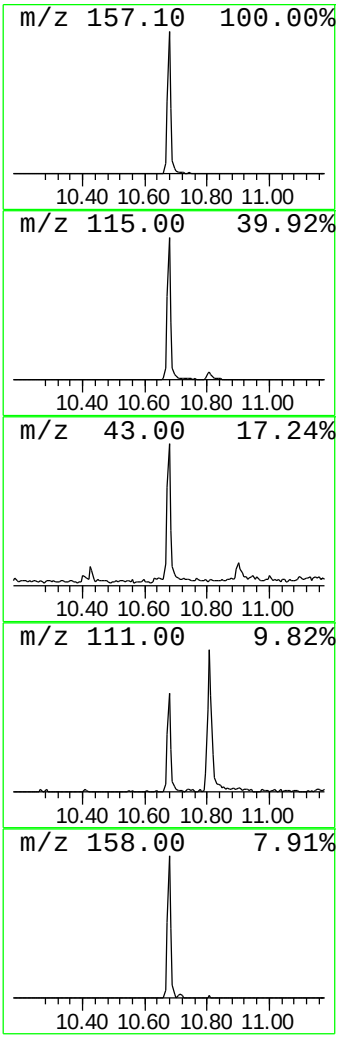
****

Peak Number 3 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	3.89 ng	435500	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	Adipic acid, ethyl 4-methylpent-...	258	C14H26O4	1000353-49-9	38
4	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	38
5	Adipic acid, ethyl pent-4-en-2-y...	242	C13H22O4	1000354-11-7	37





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107573.D
Acq On : 21 Jul 2018 13:48
Operator : JU/SJ
Sample : J4094-06
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

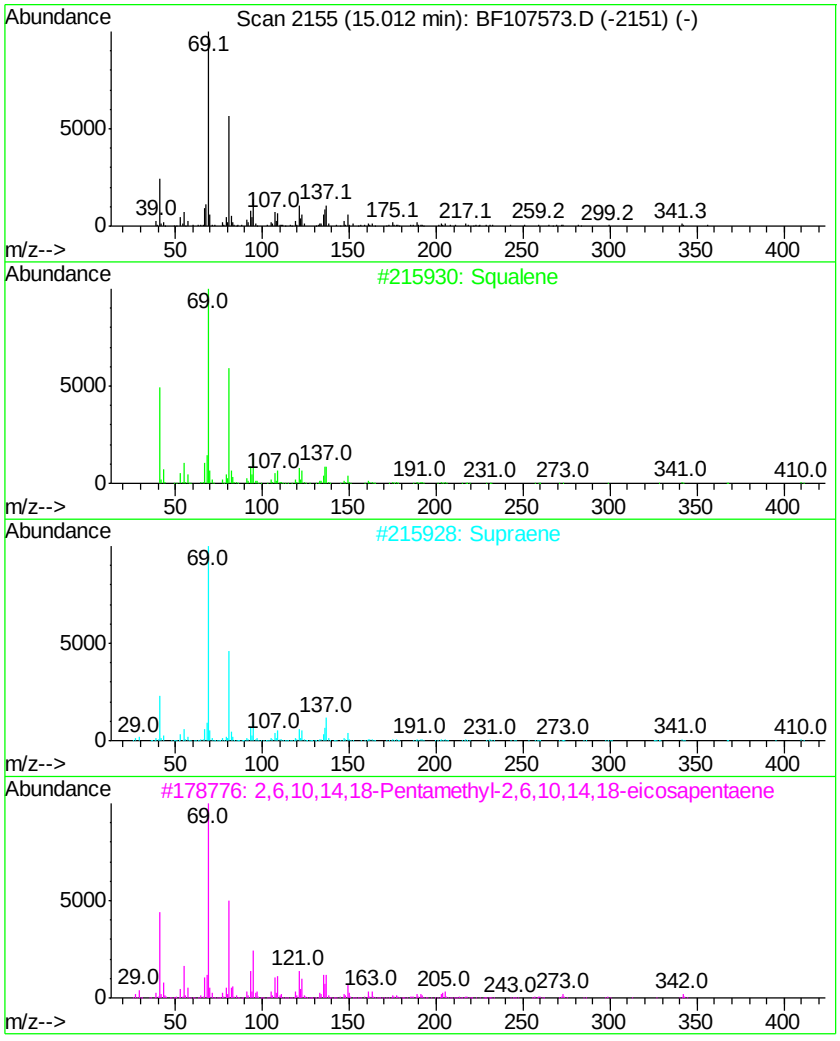
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

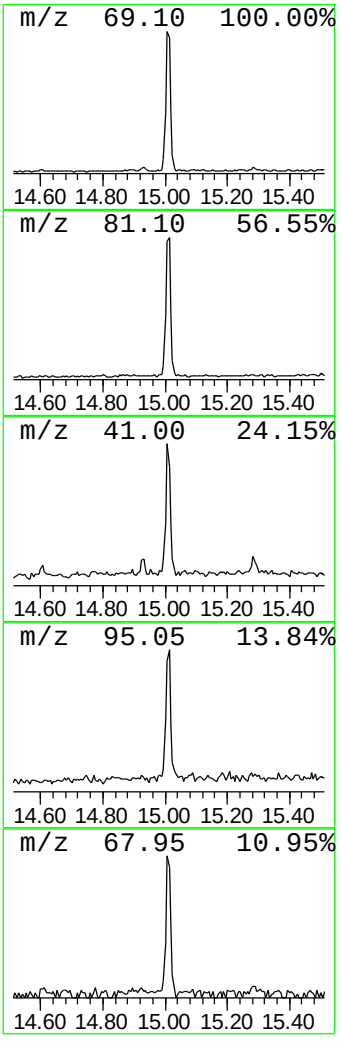
****

Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	4.27 ng	343857	Perylene-d12	15.70

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	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	84
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072018\
Data File : BF107573.D
Acq On : 21 Jul 2018 13:48
Operator : JU/SJ
Sample : J4094-06
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071818-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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	49.5	ng	4866590	1	6.97	1967710	20.0
Triethyl citrate	10.68	3.9	ng	435500	3	10.01	2241440	20.0
Squalene	15.01	4.3	ng	343857	6	15.70	1612200	20.0