LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082818\
Data File : BF108577.D
Acq On : 29 Aug 2018 1:34
Operator : JU/SJ
Sample : J4660-05
Misc :
ALS Vial : 24 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	5.237	489	493	501	rBV	29085	46586	1.20%	0.220%
2	5.637	557	561	586	rBV	391506	917596	23.57%	4.327%
3	6.631	726	730	750	rBV	322556	714796	18.36%	3.370%
4	6.772	750	754	778	rVB	1598067	1891314	48.59%	8.918%
5	7.001	789	793	808	rBV	516959	642676	16.51%	3.030%
6	7.154	815	819	846	rBV	2535842	2680020	68.85%	12.637%
7	7.566	884	889	912	rBV	1993897	2242589	57.61%	10.574%
8	8.284	1007	1011	1027	rBV	665136	785551	20.18%	3.704%
9	9.354	1189	1193	1204	rBV	4053629	3892469	100.00%	18.354%
10	9.748	1256	1260	1267	rBV	61105	68768	1.77%	0.324%
11	10.042	1307	1310	1322	rVB2	824695	798815	20.52%	3.767%
12	10.701	1418	1422	1427	rBV	145052	130206	3.35%	0.614%
13	10.836	1441	1445	1458	rBV	1265317	1263178	32.45%	5.956%
14	11.536	1561	1564	1576	rBV	679446	669138	17.19%	3.155%
15	12.919	1796	1799	1805	rBV	59933	45581	1.17%	0.215%
16	13.124	1829	1834	1837	rBV	3316259	2858286	73.43%	13.477%
17	14.195	2012	2016	2024	rBV	722344	715046	18.37%	3.372%
18	14.948	2141	2144	2147	rVB	46098	41880	1.08%	0.197%
19	15.030	2154	2158	2164	rVB	101929	107726	2.77%	0.508%
20	15.307	2201	2205	2211	rBV	47160	61688	1.58%	0.291%
21	15.718	2271	2275	2276	rBV2	44510	51196	1.32%	0.241%
22	15.748	2276	2280	2287	rVB	392682	528538	13.58%	2.492%
23	16.189	2351	2355	2362	rVB2	34851	54603	1.40%	0.257%

Sum of corrected areas: 21208246

LSC Report - Integrated Chromatogram

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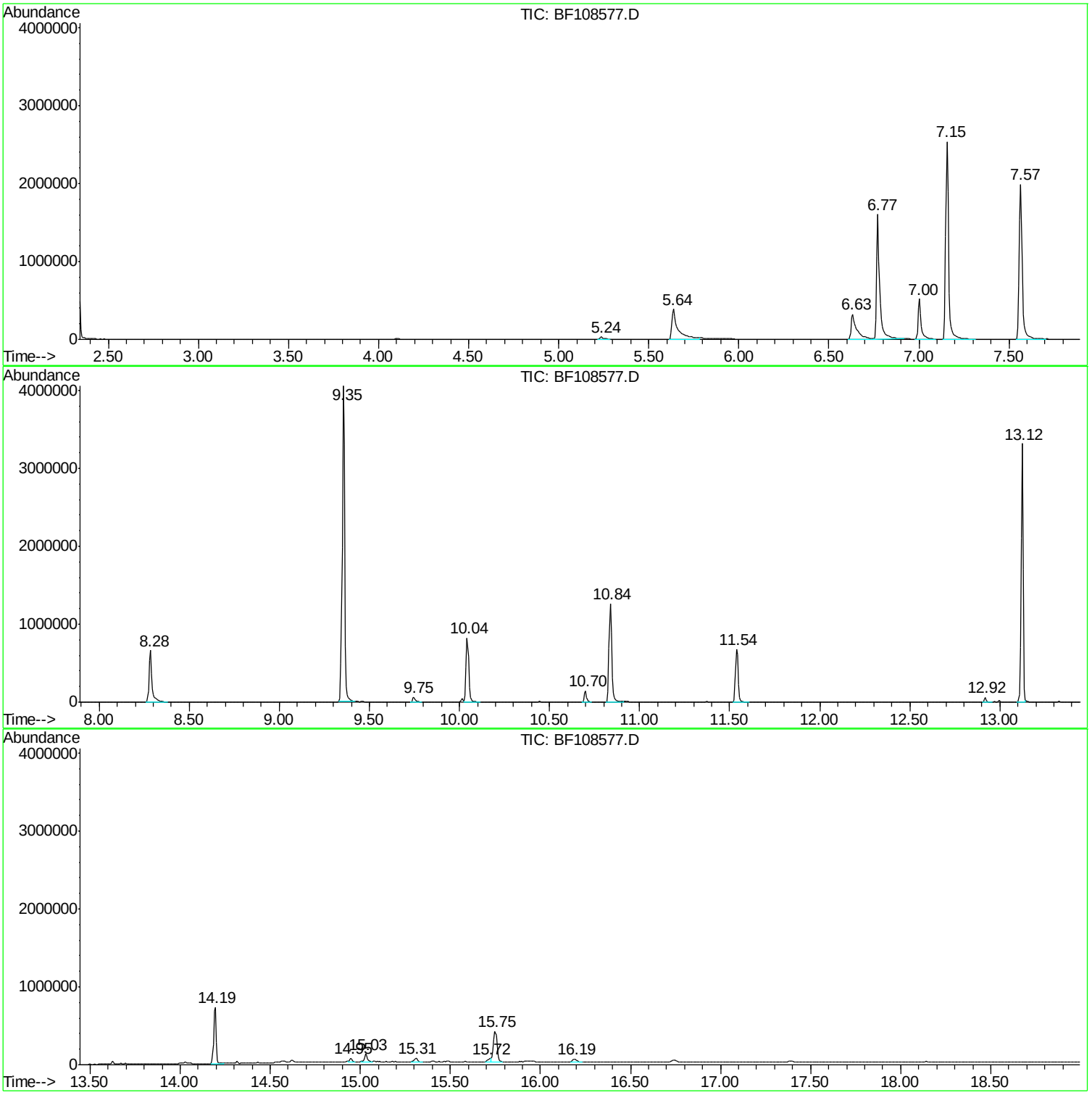
Instrument : BNA_F
ClientSampleId : 082318-SIDI-F-U-M

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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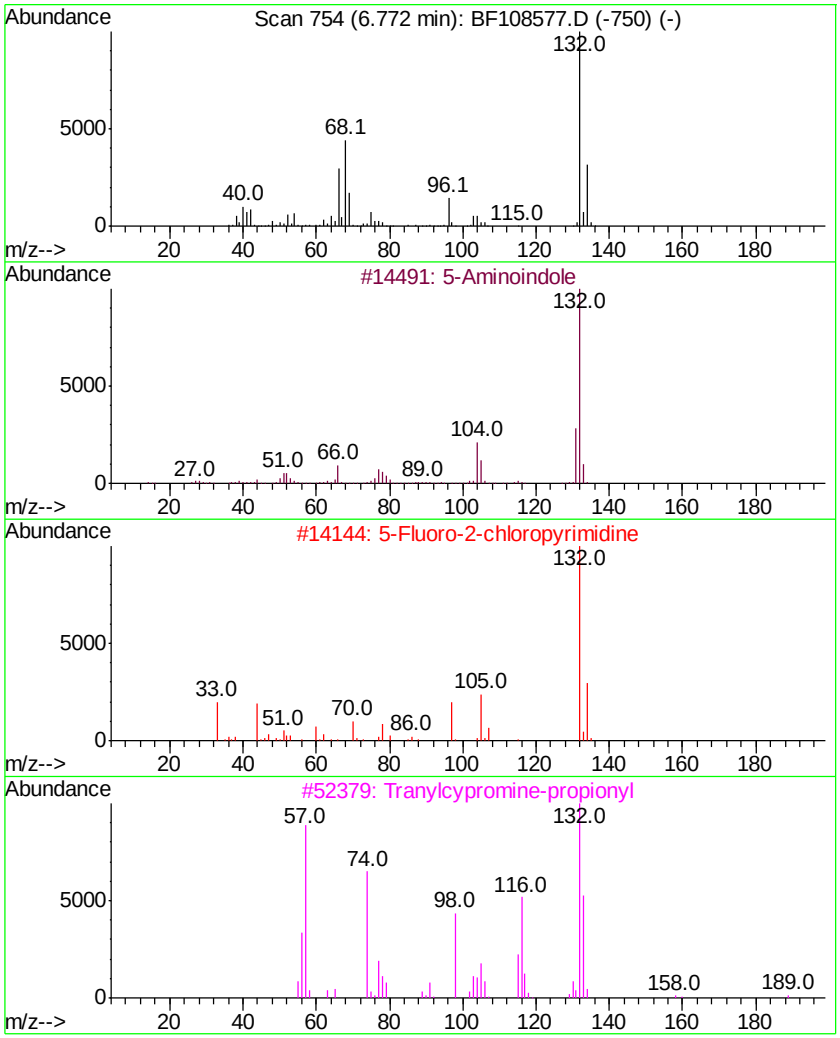
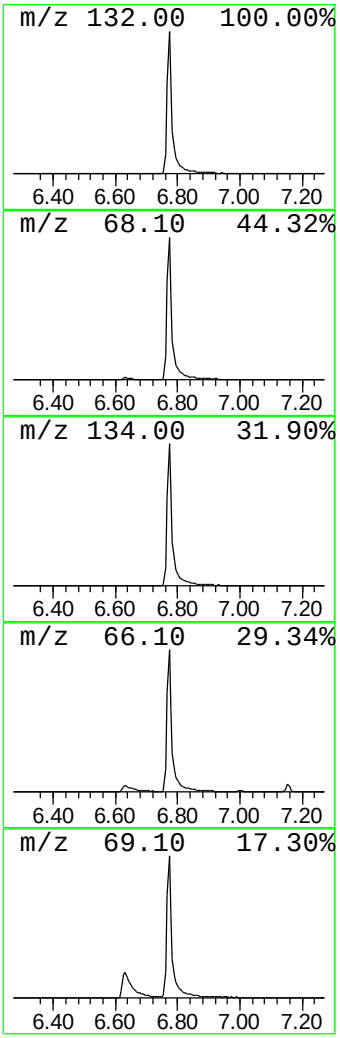
Peak Number 1 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	58.86 ng	1891310	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

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Sample : J4660-05
Misc :
ALS Vial : 24 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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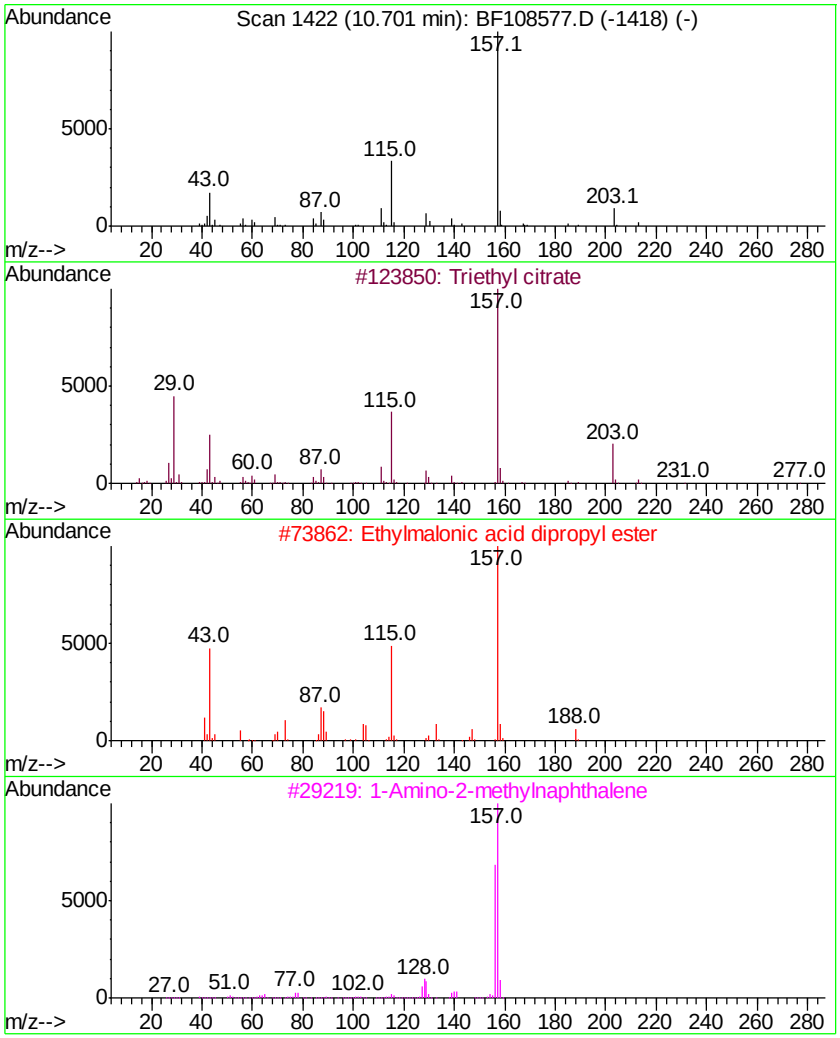
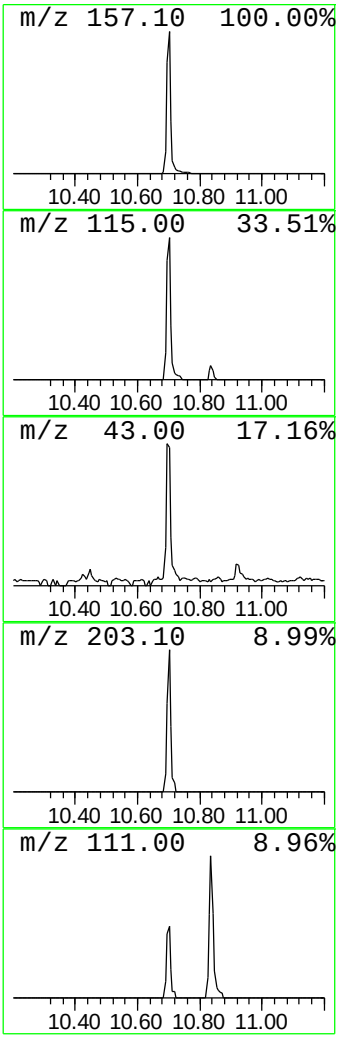
Peak Number 3 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	3.26 ng	130206	Acenaphthene-d10	10.04

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	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	42
4	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	42
5	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	38





Library Search Compound Report

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Data File : BF108577.D
Acq On : 29 Aug 2018 1:34
Operator : JU/SJ
Sample : J4660-05
Misc :
ALS Vial : 24 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 Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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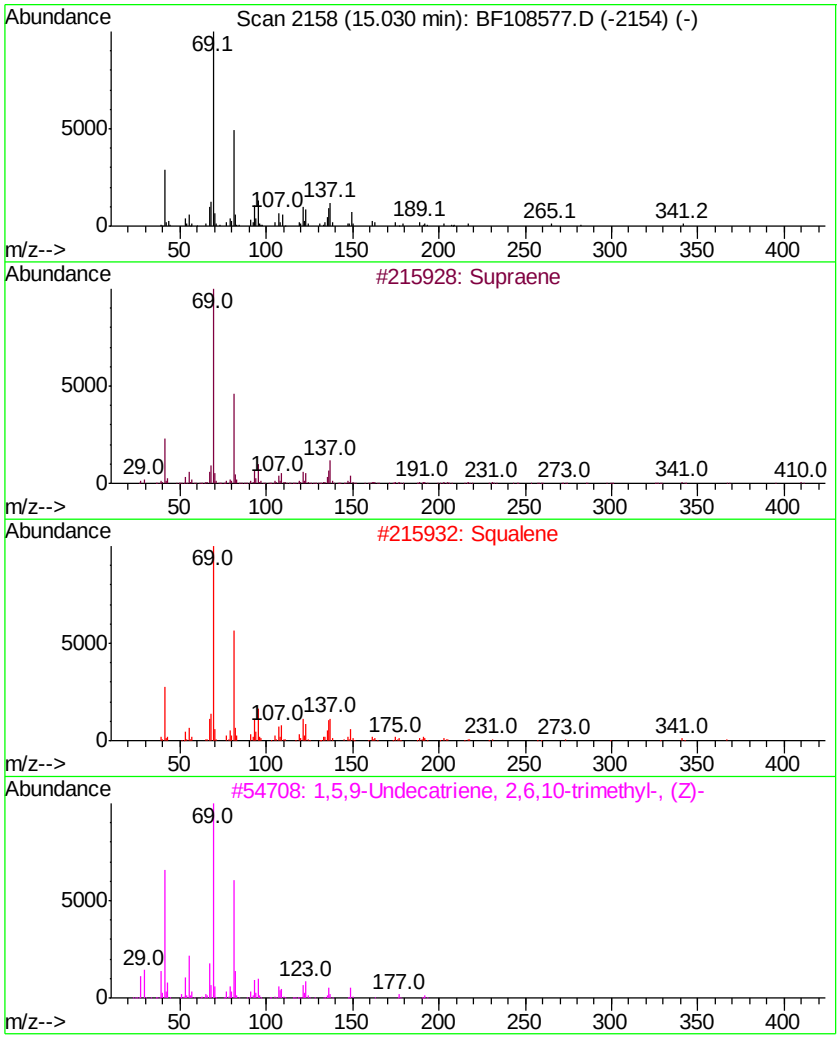
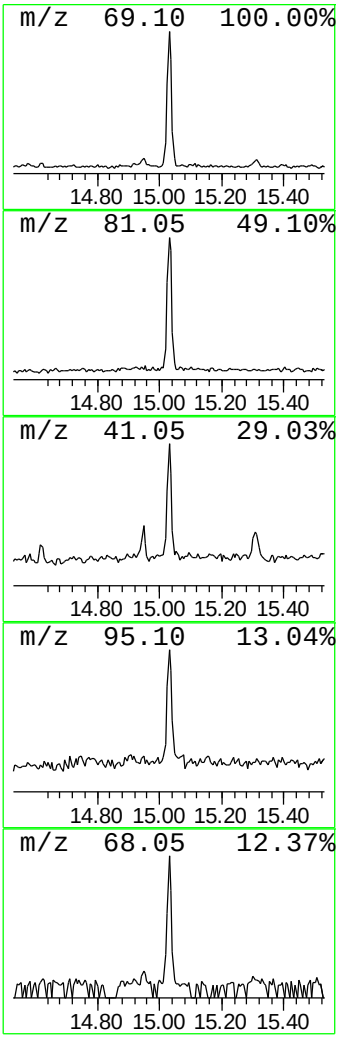
Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	4.08 ng	107726	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





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Sample : J4660-05
Misc :
ALS Vial : 24 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 Library : C:\DATABASE\NIST11.L
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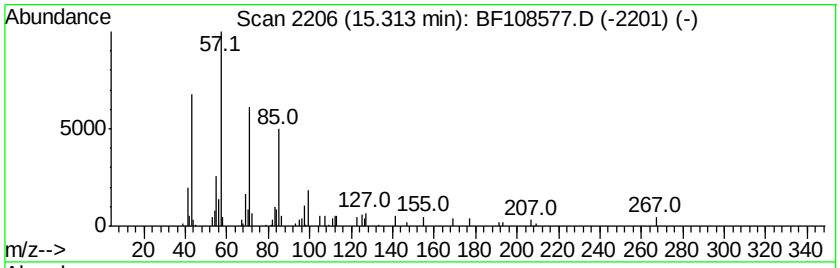
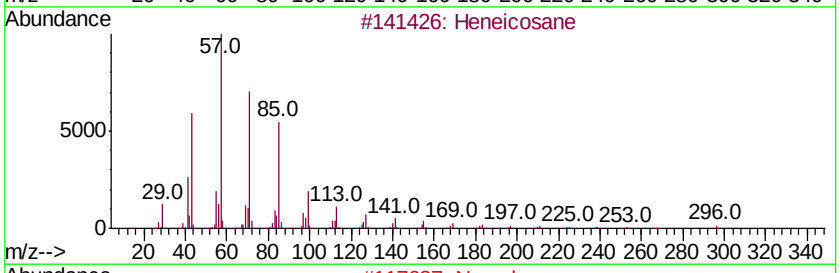
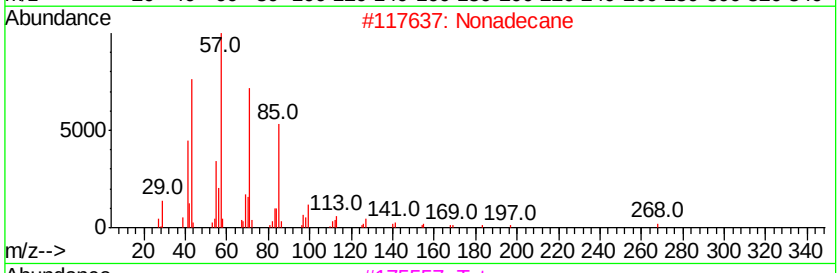
Peak Number 5 Heneicosane Concentration Rank 5

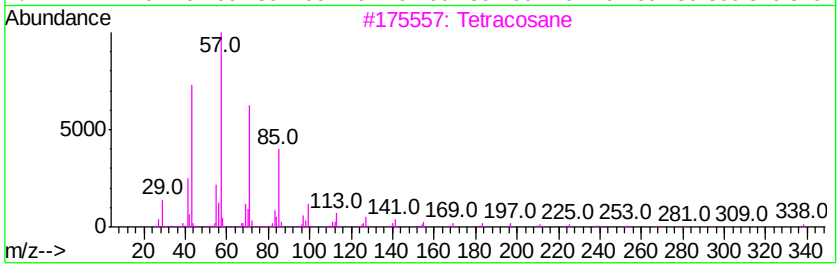
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.33 ng	61688	Perylene-d12	15.75

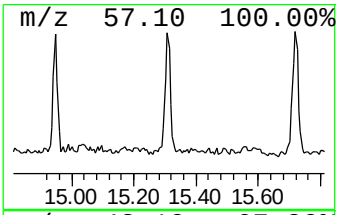
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Nonadecane	268	C19H40	000629-92-5	83
3	Tetracosane	338	C24H50	000646-31-1	80
4	Hentriacontane	437	C31H64	000630-04-6	72
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	72

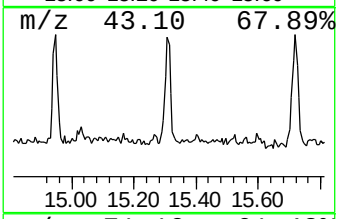


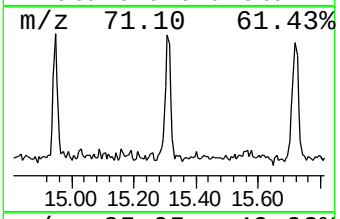


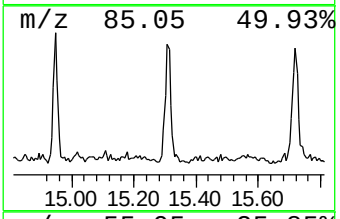


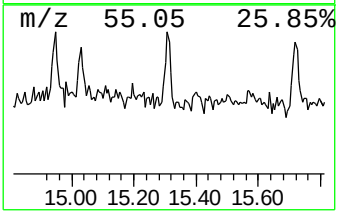












Library Search Compound Report

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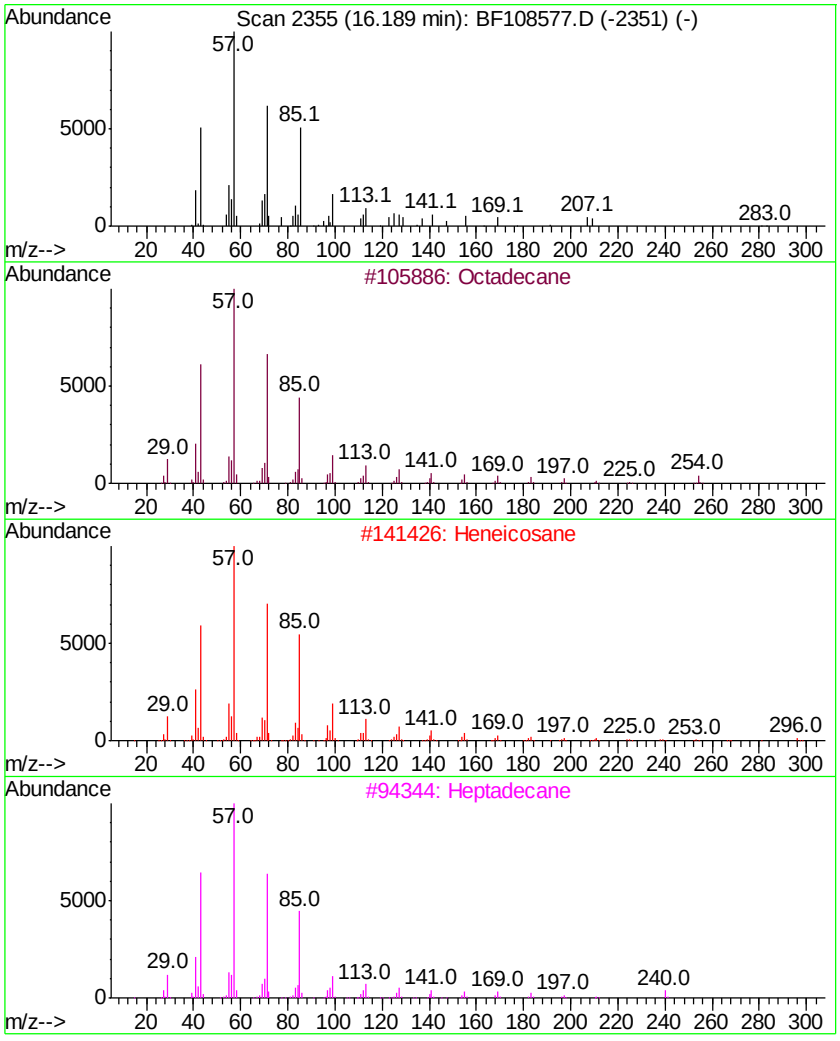
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

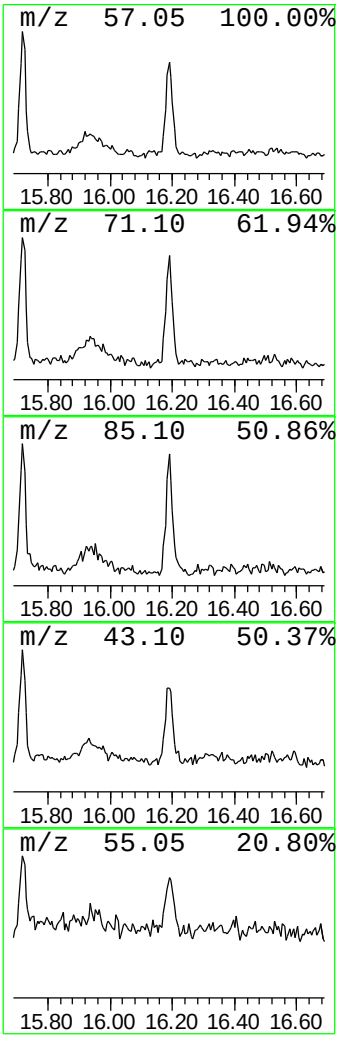
****

Peak Number 6 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.07 ng	54603	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Heptadecane	240	C17H36	000629-78-7	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.77	6.77	58.9	ng	1891310	1	7.00	642676	20.0
Triethyl citrate	10.70	3.3	ng	130206	3	10.04	798815	20.0
Supraene	15.03	4.1	ng	107726	6	15.75	528538	20.0
Heneicosane	15.31	2.3	ng	61688	6	15.75	528538	20.0
Octadecane	16.19	2.1	ng	54603	6	15.75	528538	20.0