LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061518\
Data File : BF106520.D
Acq On : 16 Jun 2018 4:44
Operator : JU/SJ
Sample : J3447-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-23

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-BF061118.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	5.189	482	485	493	rVB	74211	84945	3.18%	0.452%
2	5.607	553	556	564	rBV	1191270	1252998	46.85%	6.660%
3	6.607	722	726	736	rBV2	904365	867630	32.44%	4.612%
4	6.742	745	749	753	rBV	2279047	2058868	76.99%	10.943%
5	6.966	783	787	790	rBV	829796	642909	24.04%	3.417%
6	7.125	809	814	817	rBV	2127059	1973926	73.81%	10.492%
7	7.530	877	883	886	rBV	1622805	1624536	60.75%	8.635%
8	8.248	1001	1005	1008	rBV	900921	708945	26.51%	3.768%
9	9.319	1183	1187	1191	rBV	2566570	2535140	94.80%	13.475%
10	9.713	1250	1254	1261	rVB	117600	109789	4.11%	0.584%
11	9.919	1286	1289	1293	rVB	42277	32909	1.23%	0.175%
12	10.007	1300	1304	1310	rVB	757975	656039	24.53%	3.487%
13	10.419	1371	1374	1377	rVB2	60129	46490	1.74%	0.247%
14	10.801	1434	1439	1442	rBV	1487602	1395723	52.19%	7.419%
15	10.895	1452	1455	1460	rVB	40638	42513	1.59%	0.226%
16	11.495	1554	1557	1561	rBV	730280	645577	24.14%	3.431%
17	13.083	1823	1827	1830	rBV	2808774	2674322	100.00%	14.215%
18	13.965	1974	1977	1987	rBV	70955	92698	3.47%	0.493%
19	14.148	2004	2008	2014	rVB	716605	717716	26.84%	3.815%
20	15.001	2149	2153	2158	rVB	152860	153813	5.75%	0.818%
21	15.677	2263	2268	2276	rVB	395284	496219	18.55%	2.638%

Sum of corrected areas: 18813705

LSC Report - Integrated Chromatogram

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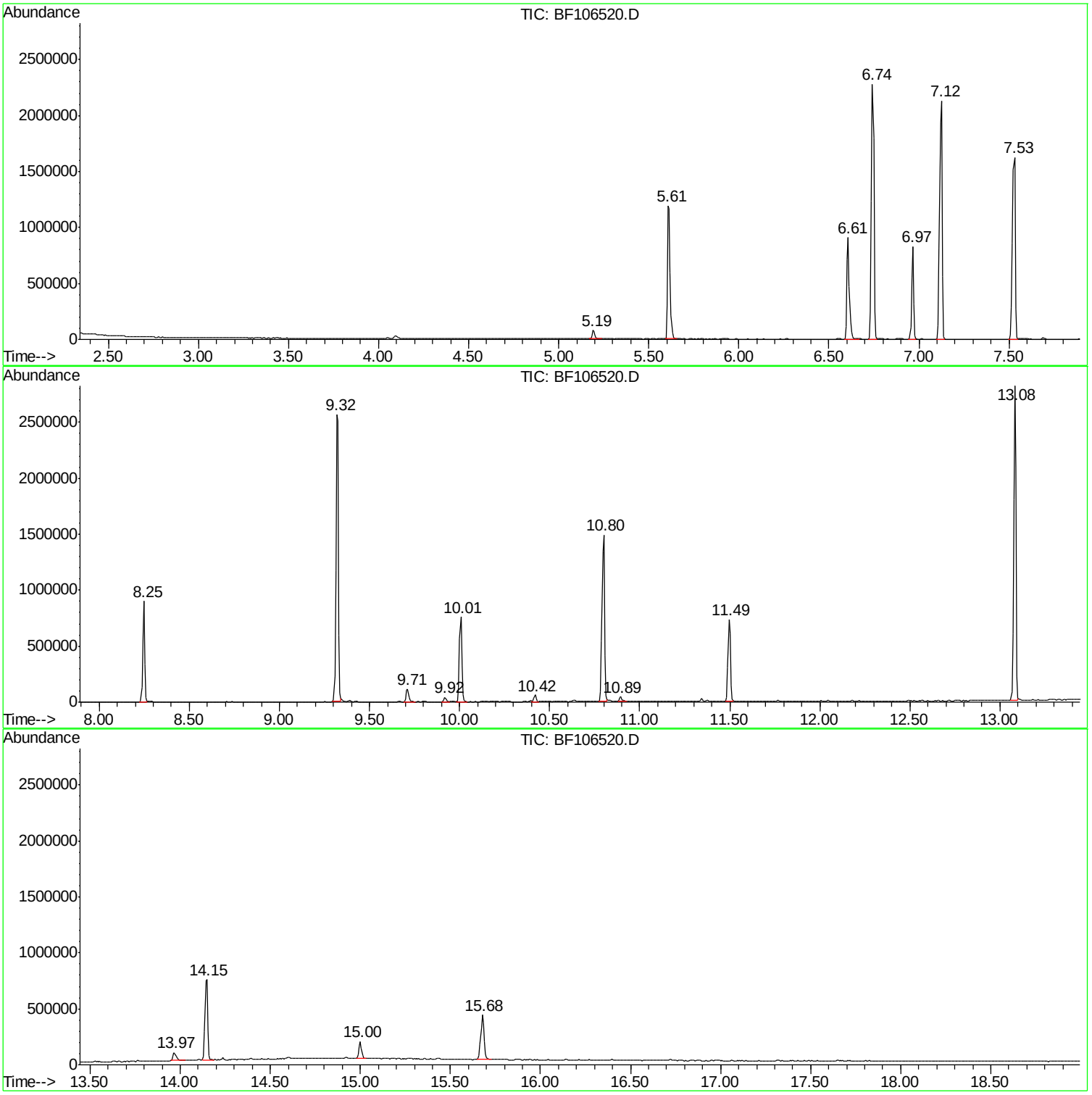
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-23

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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\BF061518\
Data File : BF106520.D
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Operator : JU/SJ
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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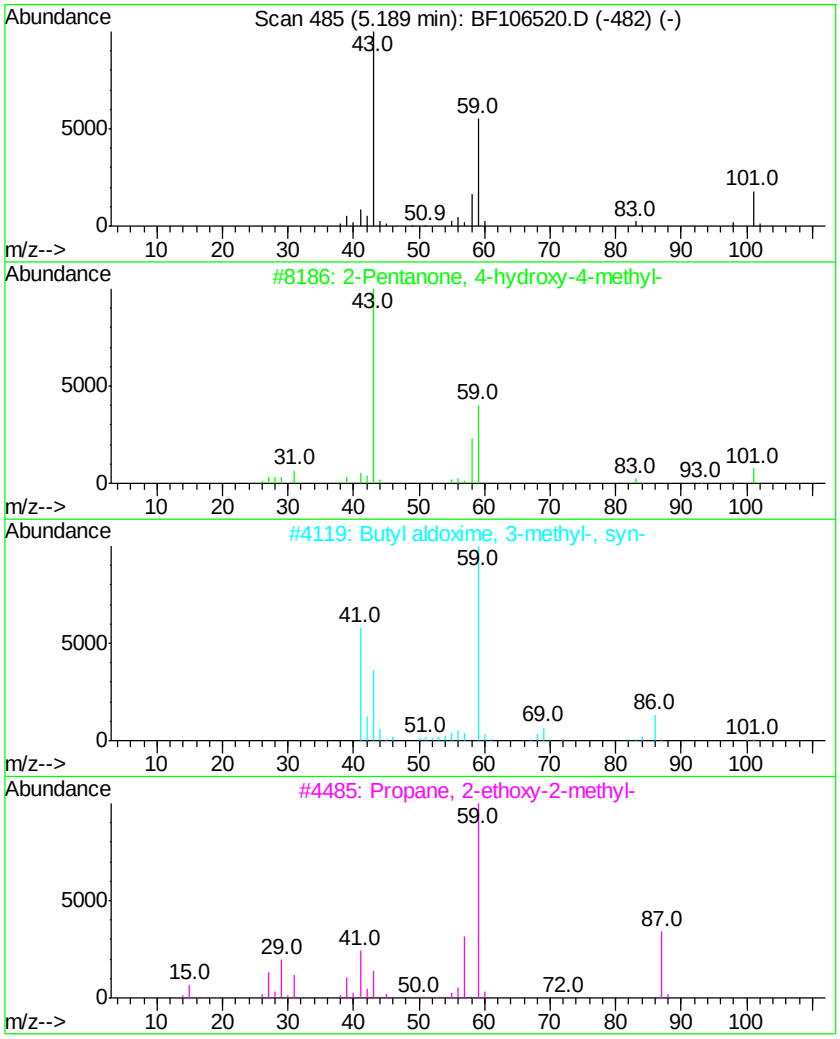
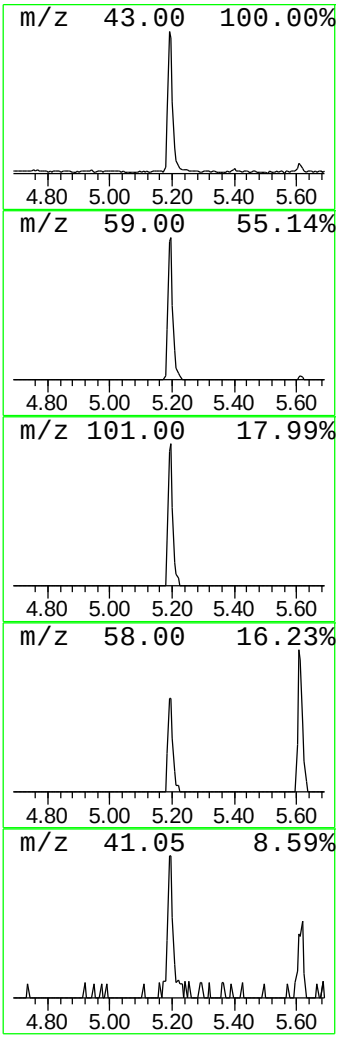
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.64 ng	84945	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument : BNA_F
ClientSampleId : W-23

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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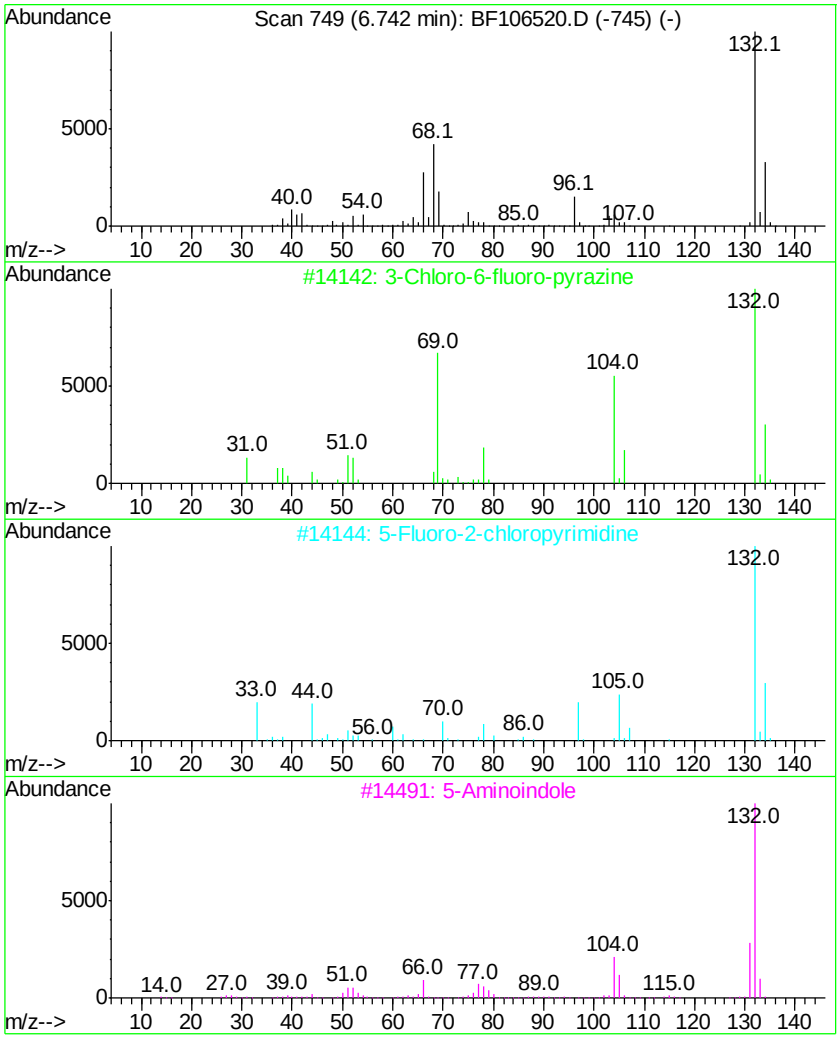
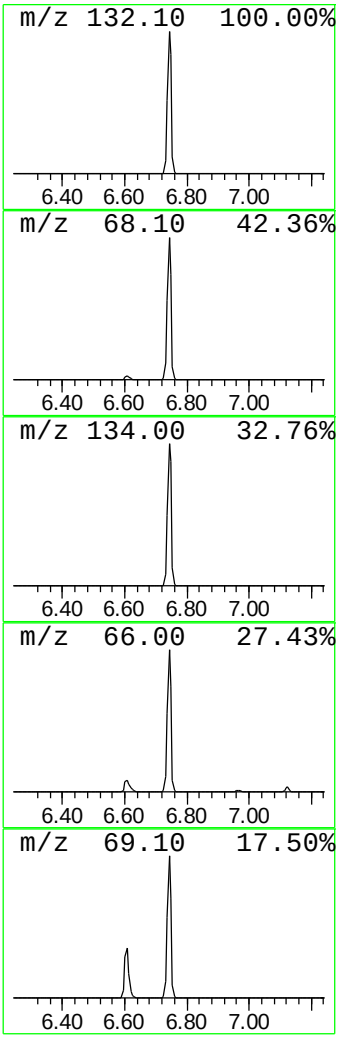
Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	64.05 ng	2058870	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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-23

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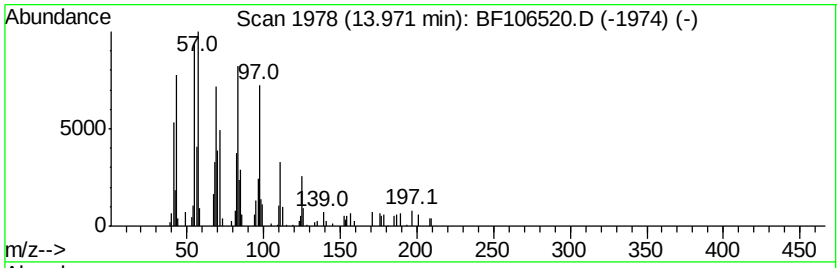
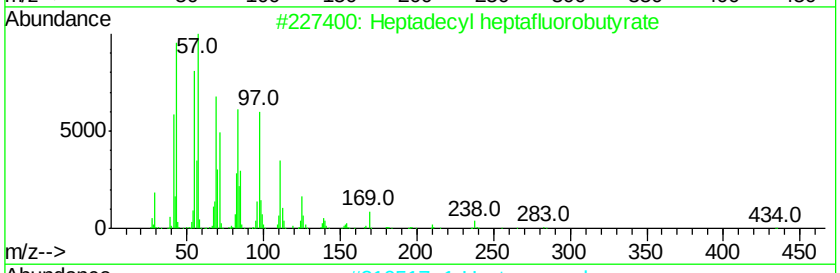
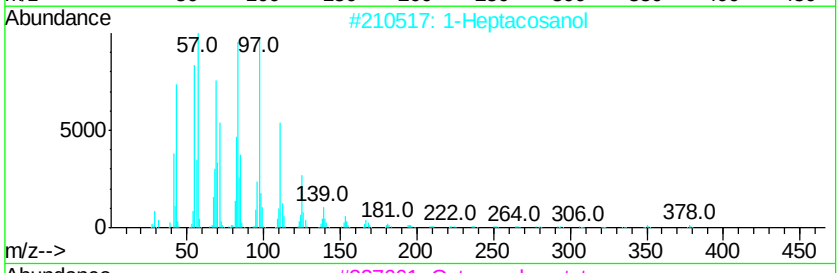
Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 5

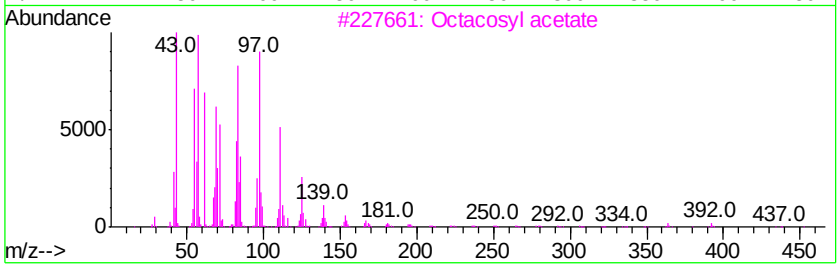
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.58 ng	92698	Chrysene-d12	14.15

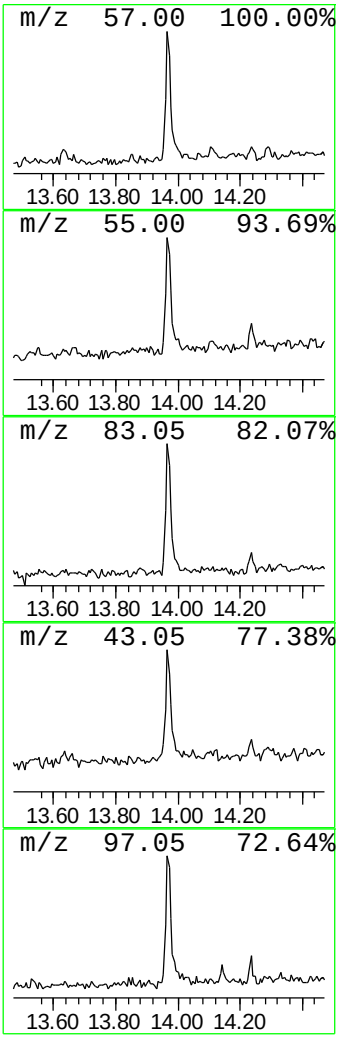
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	93
3	Octacosyl acetate	452	C30H60O2	018206-97-8	93
4	Octacosanol	410	C28H58O	000557-61-9	93
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90











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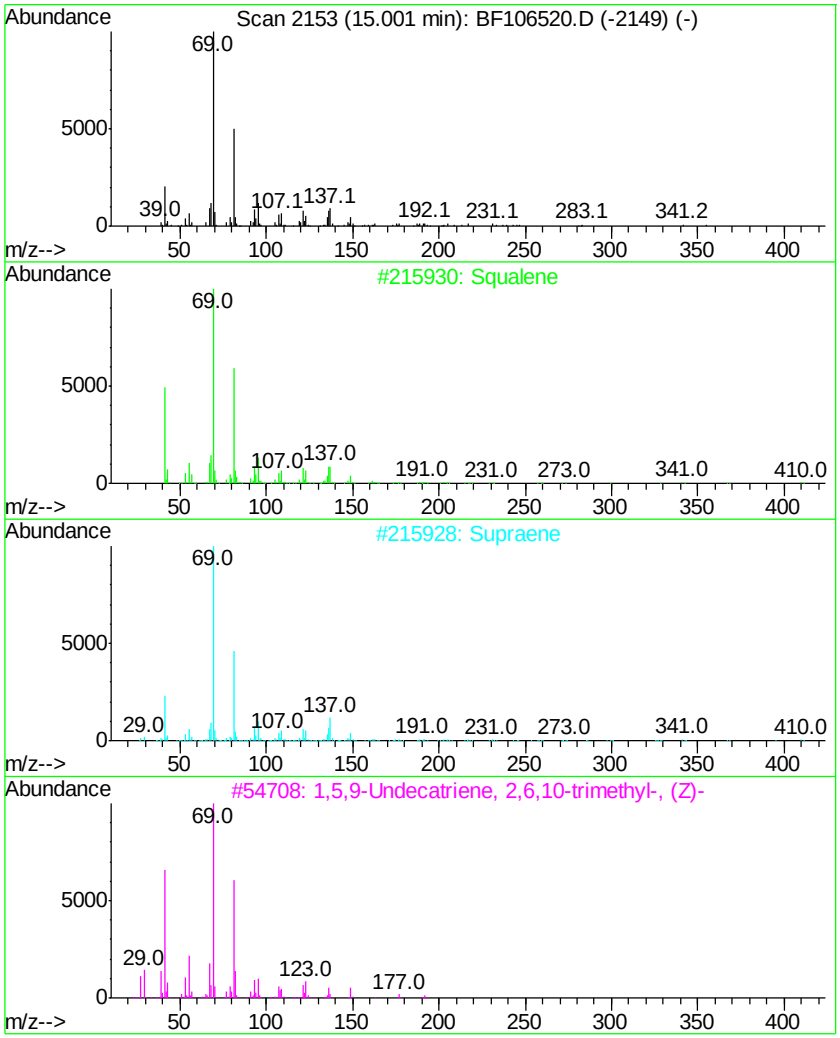
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

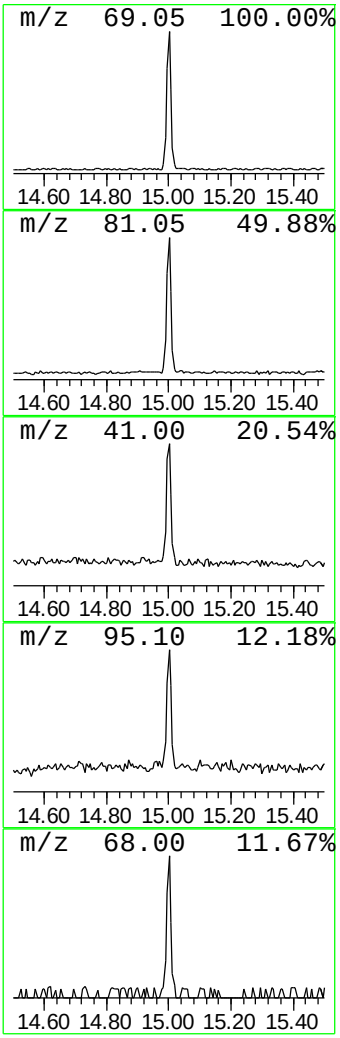
****

Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	6.20 ng	153813	Perylene-d12	15.68

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	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4	trans-Farnesol	222	C15H26O	000106-28-5	83
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78





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
2-Pentanone, 4-hy...	5.19	2.6	ng	84945	1	6.97	642909	20.0
unknown6.74	6.74	64.0	ng	2058870	1	6.97	642909	20.0
Heptadecyl heptaf...	13.97	2.6	ng	92698	5	14.15	717716	20.0
Squalene	15.00	6.2	ng	153813	6	15.68	496219	20.0