LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106389.D
Acq On : 13 Jun 2018 14:23
Operator : JU/SJ
Sample : J3396-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-29

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	5.190	482	485	492	rVB	133217	139495	2.95%	0.432%
2	5.613	553	557	563	rBV	1562099	1870914	39.59%	5.788%
3	6.613	724	727	736	rBV	1028079	1258354	26.63%	3.893%
4	6.748	746	750	753	rBV	3365653	2981752	63.09%	9.225%
5	6.966	783	787	790	rVB	1113620	883363	18.69%	2.733%
6	7.125	809	814	817	rVB	3085371	2933172	62.07%	9.075%
7	7.531	877	883	886	rBV	2576377	2613423	55.30%	8.085%
8	8.248	1001	1005	1008	rBV	1366781	1136378	24.05%	3.516%
9	9.325	1183	1188	1191	rBV	4374610	4294386	90.87%	13.286%
10	9.713	1250	1254	1256	rBV	297961	236391	5.00%	0.731%
11	9.919	1285	1289	1294	rBV2	113564	113757	2.41%	0.352%
12	10.007	1300	1304	1307	rVB	1505413	1291505	27.33%	3.996%
13	10.419	1372	1374	1377	rVB2	124990	99437	2.10%	0.308%
14	10.801	1434	1439	1442	rBV	2890181	2936259	62.13%	9.084%
15	10.895	1452	1455	1461	rBV	107274	112131	2.37%	0.347%
16	11.342	1528	1531	1534	rBV	62962	47761	1.01%	0.148%
17	11.495	1553	1557	1561	rBV	1697411	1406179	29.75%	4.350%
18	12.007	1641	1644	1649	rBV	84551	94780	2.01%	0.293%
19	13.083	1822	1827	1831	rBV	4154432	4725866	100.00%	14.621%
20	13.966	1973	1977	1980	rBV2	115057	151945	3.22%	0.470%
21	14.001	1980	1983	1999	rVB7	115927	302527	6.40%	0.936%
22	14.142	2003	2007	2011	rBV	1218657	1085548	22.97%	3.358%
23	14.260	2018	2027	2042	rBV4	176538	620802	13.14%	1.921%
24	14.607	2083	2086	2094	rVB7	37626	48100	1.02%	0.149%
25	15.683	2263	2269	2278	rBV	708003	938754	19.86%	2.904%

Sum of corrected areas: 32322979

LSC Report - Integrated Chromatogram

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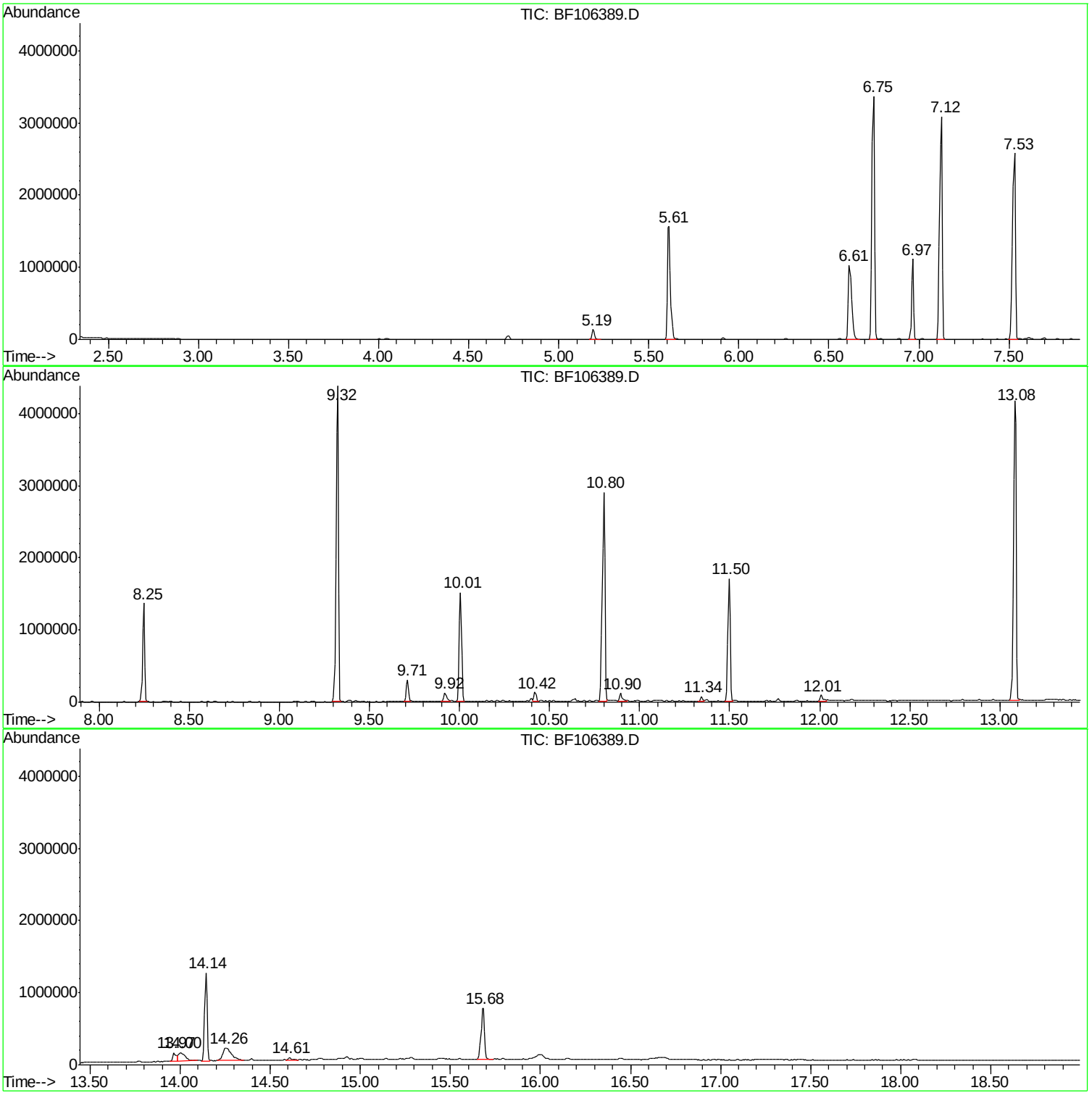
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-29

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

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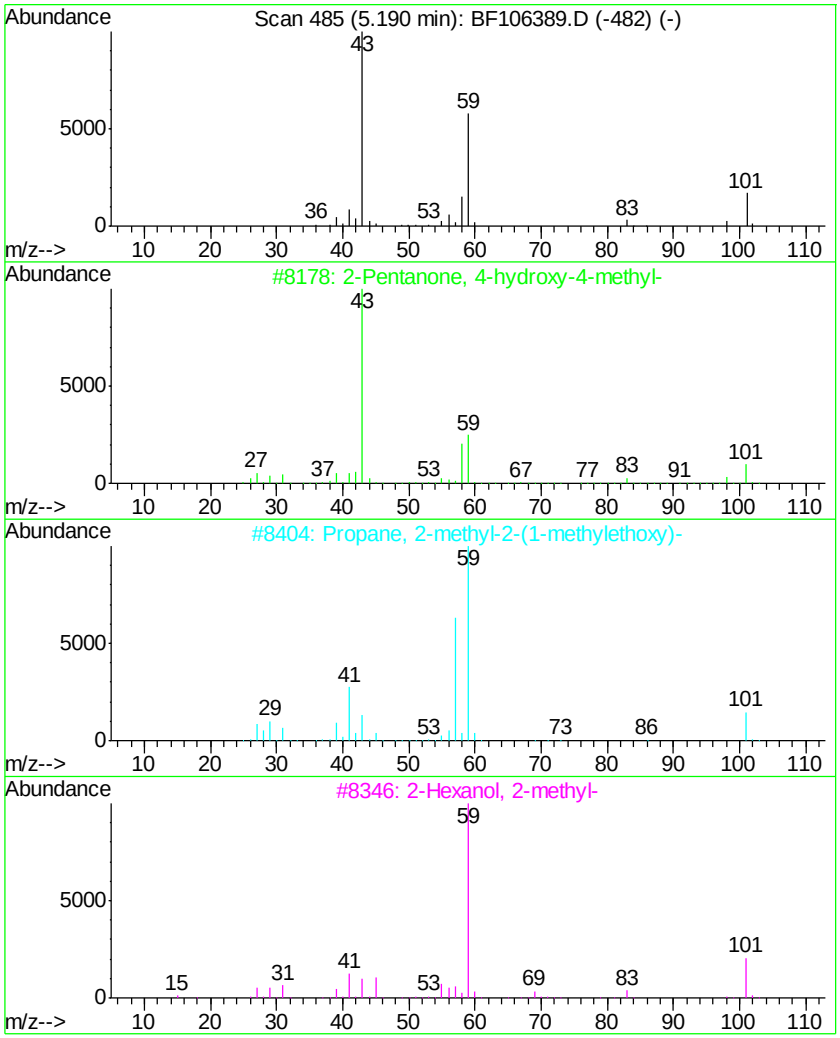
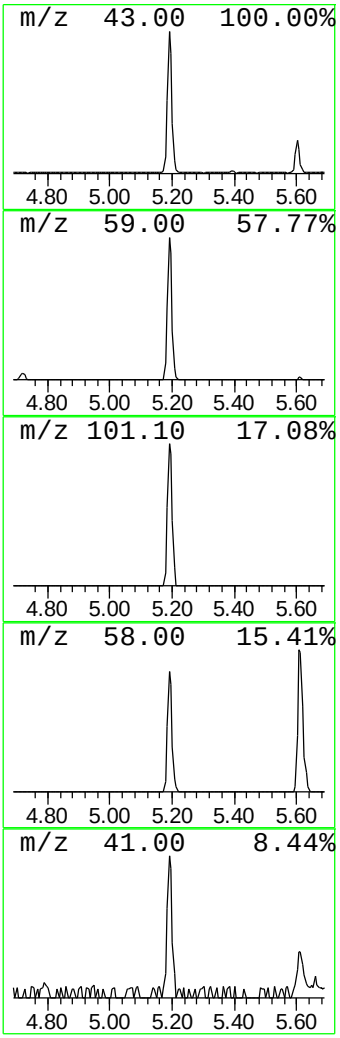
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.16 ng	139495	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	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





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ClientSampleId : W-29

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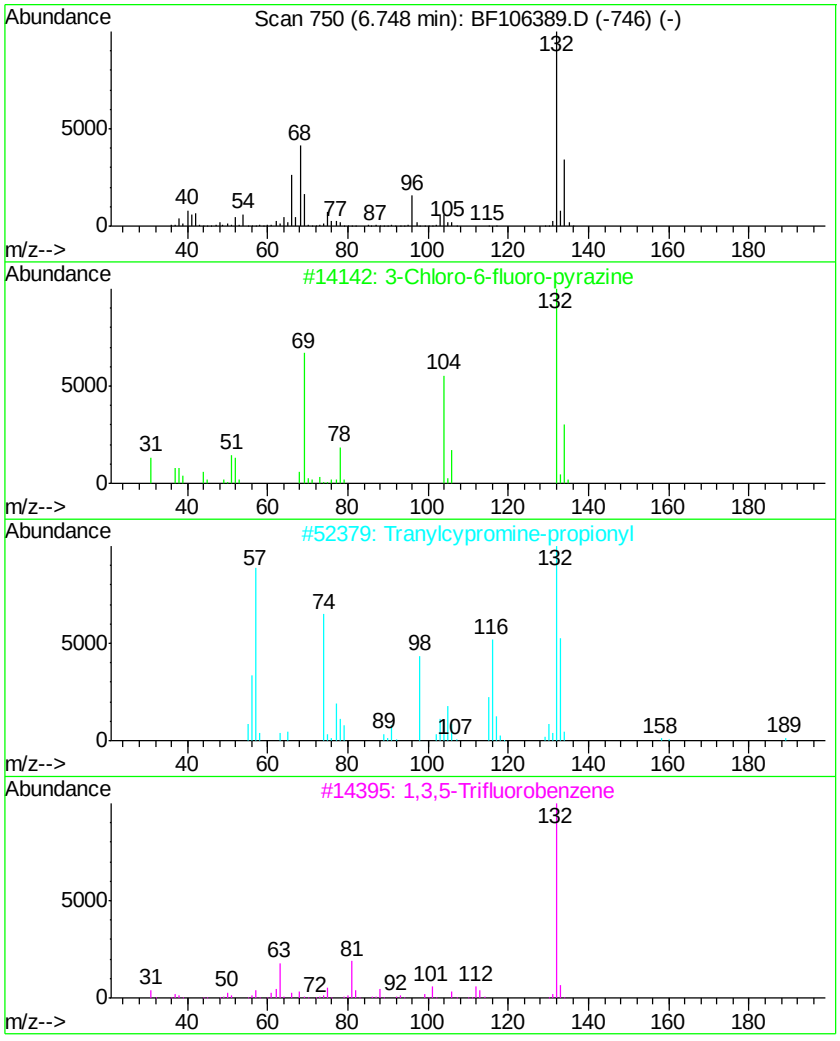
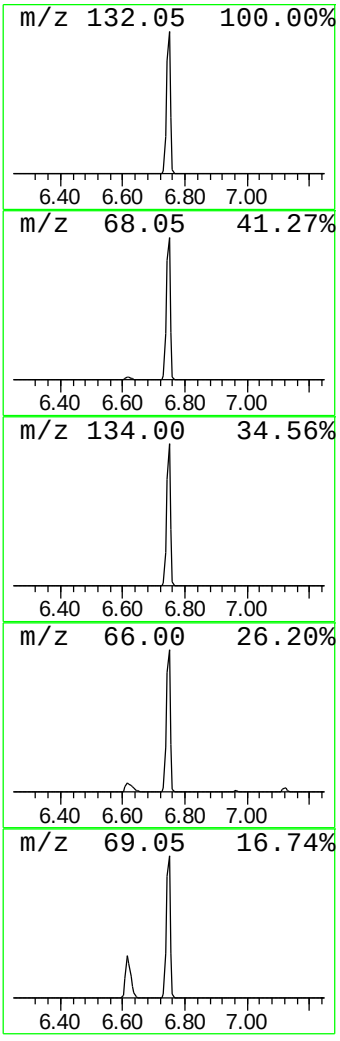
Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	67.51 ng	2981750	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Instrument : BNA_F
ClientSampleId : W-29

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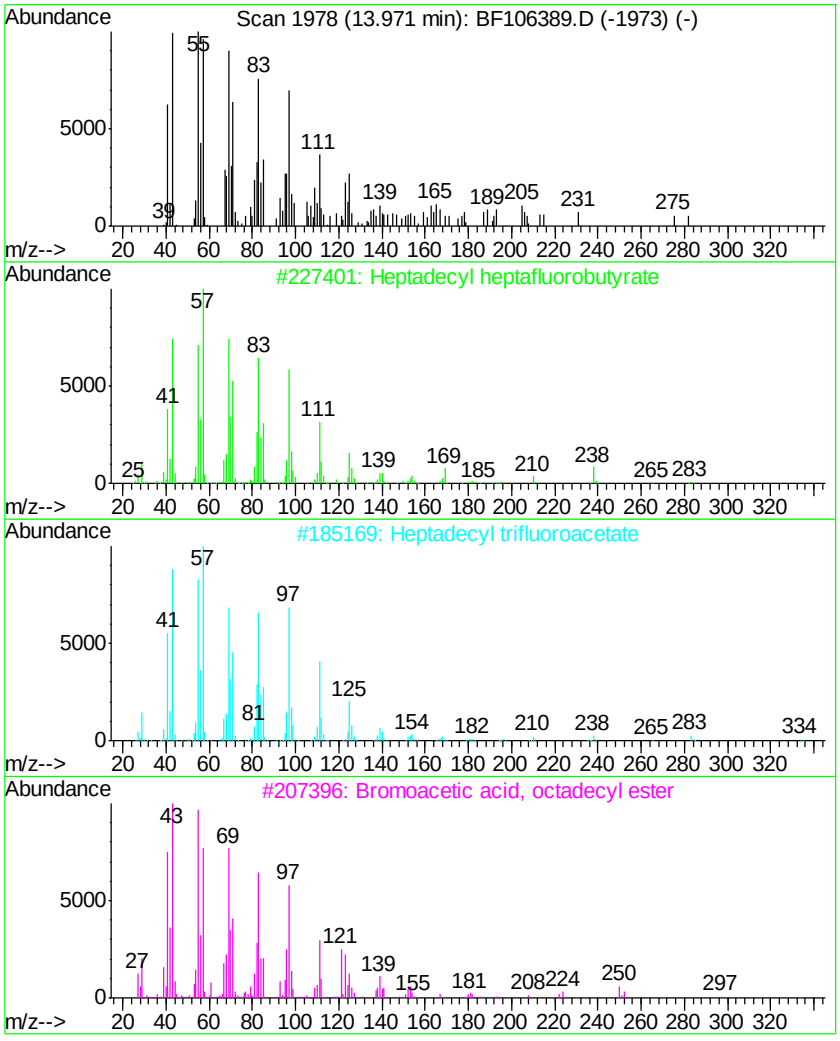
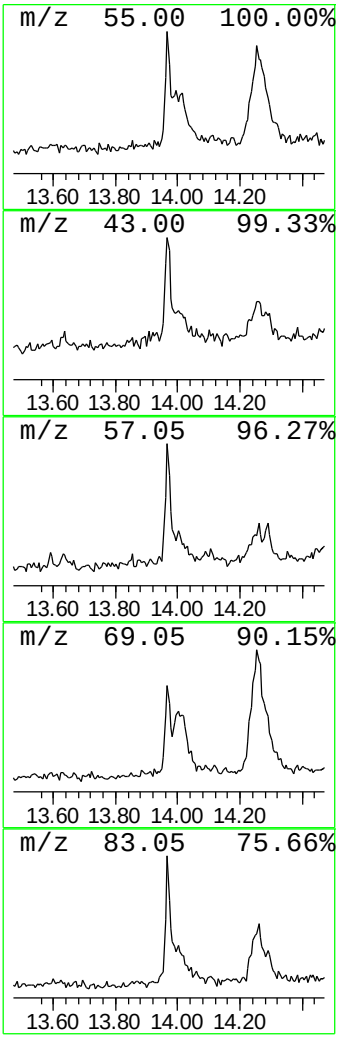
Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.80 ng	151945	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5	1-Heptacosanol	396	C27H56O	002004-39-9	90





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Instrument : BNA_F
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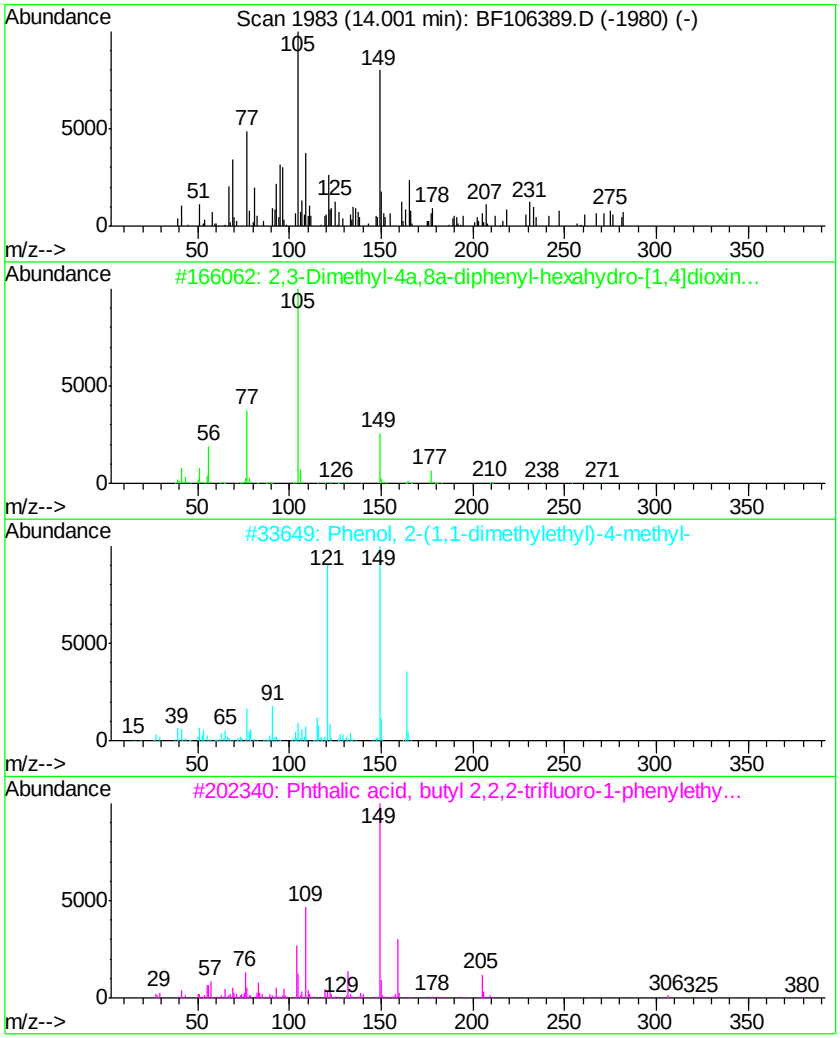
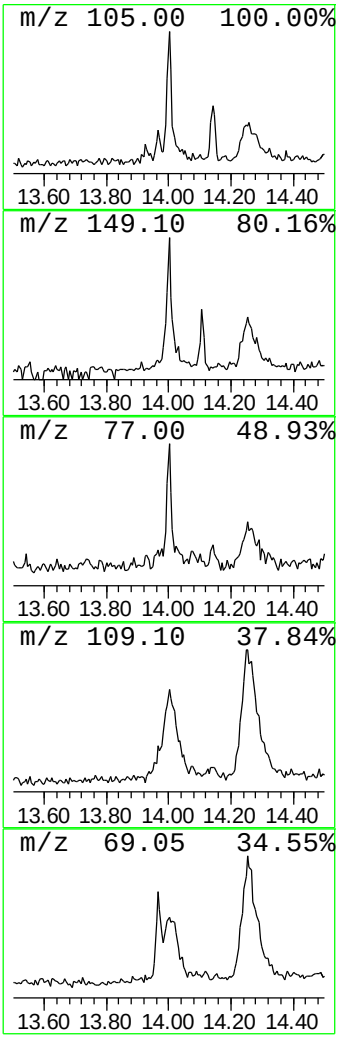
Peak Number 5 unknown14.00 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	5.57 ng	302527	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	43
2	Phenol, 2-(1,1-dimethylethyl)-4-...	164	C11H16O	002409-55-4	37
3	Phthalic acid, butyl 2,2,2-trifl...	380	C20H19F3O4	1000377-70-2	35
4	2-Propenamide, N-cyclopropyl-3-(...	205	C12H12FNO	1000351-61-1	27
5	2-Methyl-2-(4'-methoxyphenyl)pen...	206	C13H18O2	185700-49-6	27





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ALS Vial : 4 Sample Multiplier: 1

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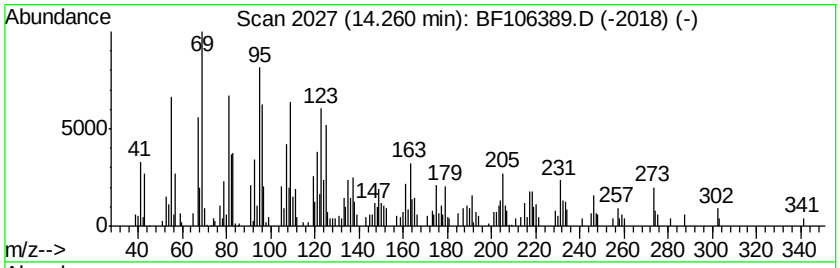
TIC Integration Parameters: LSCINT.P

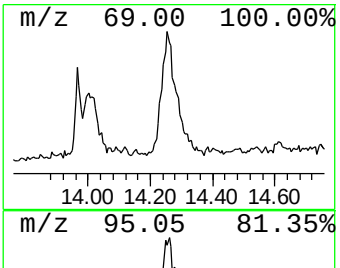
****

Peak Number 6 (2Z,4E)-3,7,11-Trimethyl-2,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	11.44 ng	620802	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	72
2	Caparratriene	206	C15H26	1000374-08-7	70
3	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
4	Sesquirosefuran	218	C15H22O	039007-93-7	50
5	1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	41





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	3.2	ng	139495	1	6.97	883363	20.0
unknown6.75	6.75	67.5	ng	2981750	1	6.97	883363	20.0
Heptadecyl heptaf...	13.97	2.8	ng	151945	5	14.14	1085550	20.0
unknown14.00	14.00	5.6	ng	302527	5	14.14	1085550	20.0
(2Z,4E)-3,7,11-Tr...	14.26	11.4	ng	620802	5	14.14	1085550	20.0