LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122217\
Data File : BF101680.D
Acq On : 23 Dec 2017 4:33
Operator : SJ/JU
Sample : I6971-16
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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	5.010	493	497	509	rBV	67307	128492	2.73%	0.411%
2	5.404	561	564	591	rBV	1267422	1895000	40.24%	6.054%
3	6.428	735	738	756	rBV	866683	1288185	27.36%	4.116%
4	6.557	756	760	767	rBV	2854016	2864139	60.82%	9.151%
5	6.786	796	799	809	rBV	1157444	1083276	23.01%	3.461%
6	6.939	821	825	841	rBV	3171679	3437569	73.00%	10.983%
7	7.363	892	897	921	rBV	2864695	3267123	69.38%	10.438%
8	8.069	1014	1017	1035	rVB	1462639	1400800	29.75%	4.476%
9	9.145	1195	1200	1203	rBV	4562776	4708866	100.00%	15.045%
10	9.822	1312	1315	1328	rVB2	1509439	1427084	30.31%	4.560%
11	10.616	1446	1450	1463	rBV	1758574	1990020	42.26%	6.358%
12	11.316	1565	1569	1578	rBV	1391488	1338135	28.42%	4.275%
13	12.698	1801	1804	1808	rBV	311826	261316	5.55%	0.835%
14	12.774	1815	1817	1821	rVB	67341	56074	1.19%	0.179%
15	12.898	1833	1838	1841	rBV	3633322	3692687	78.42%	11.798%
16	13.404	1921	1924	1928	rVB	247819	185697	3.94%	0.593%
17	13.780	1984	1988	1997	rBV2	112277	175827	3.73%	0.562%
18	13.962	2015	2019	2028	rBV	1015053	970541	20.61%	3.101%
19	14.698	2140	2144	2147	rBV	50125	48522	1.03%	0.155%
20	15.021	2195	2199	2206	rBV	43517	51718	1.10%	0.165%
21	15.427	2263	2268	2283	rVB	606025	857435	18.21%	2.739%
22	15.803	2327	2332	2337	rVB2	40523	59236	1.26%	0.189%
23	16.286	2408	2414	2420	rBV2	36745	63893	1.36%	0.204%
24	16.856	2506	2511	2518	rVB4	22541	47452	1.01%	0.152%

Sum of corrected areas: 31299087

LSC Report - Integrated Chromatogram

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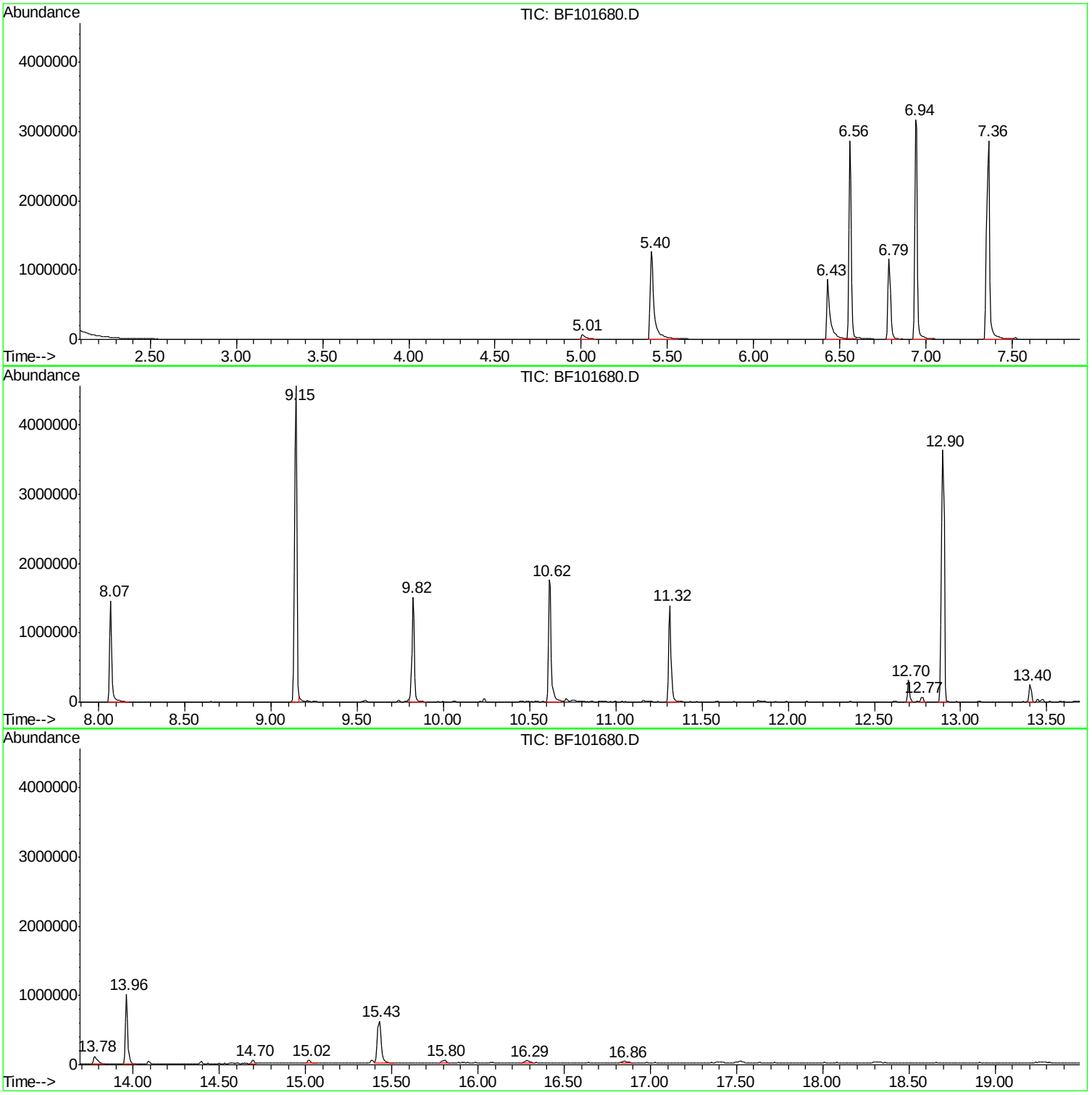
Instrument :
BNA_F
ClientSampleId :
121517-TIFR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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ClientSampleId : 121517-TIFR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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TIC Library : C:\DATABASE\NIST11.L
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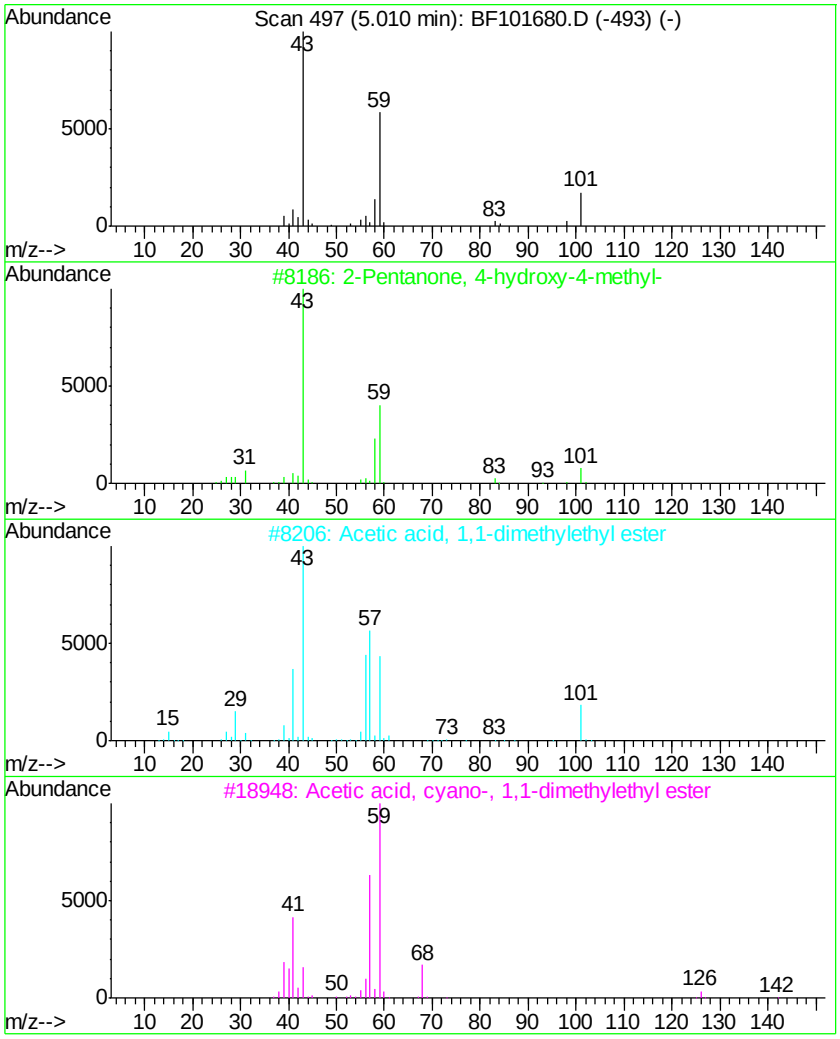
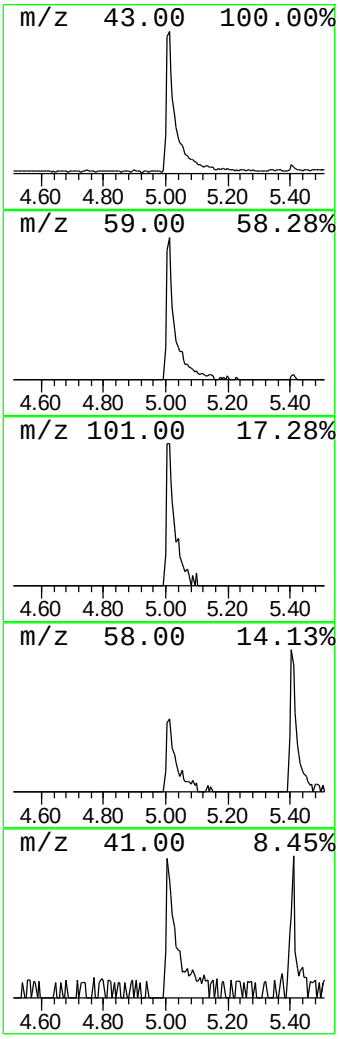
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	2.37 ng	128492	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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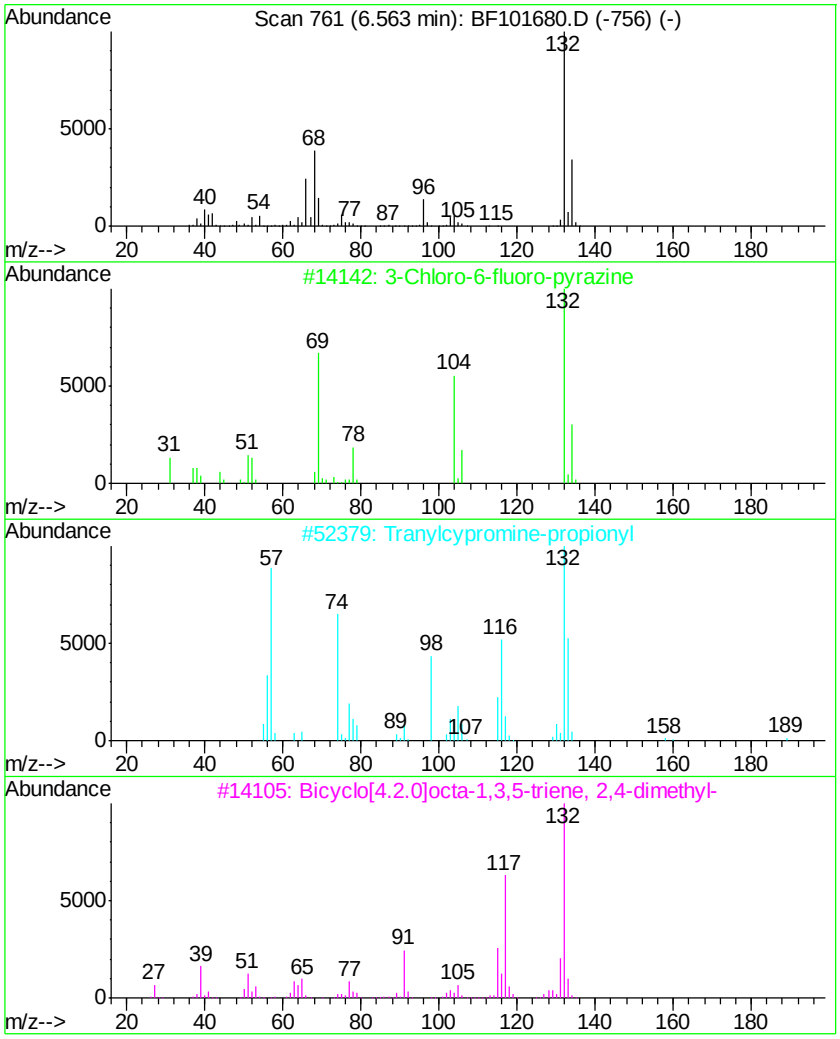
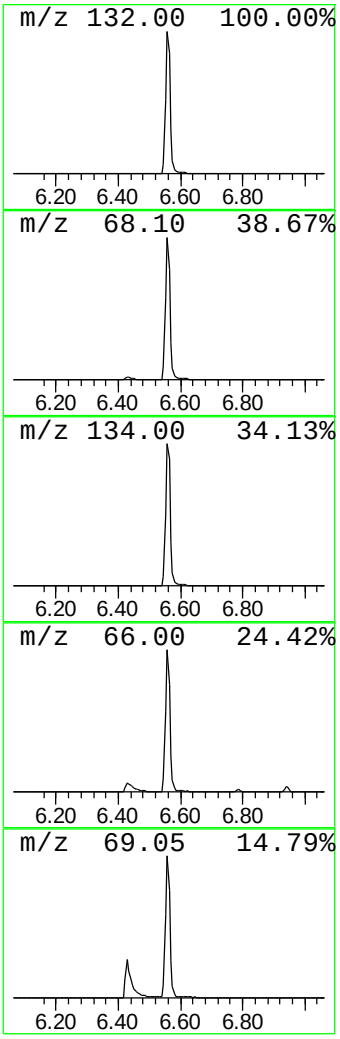
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	52.88 ng	2864140	1,4-Dichlorobenzene-d4	6.79

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	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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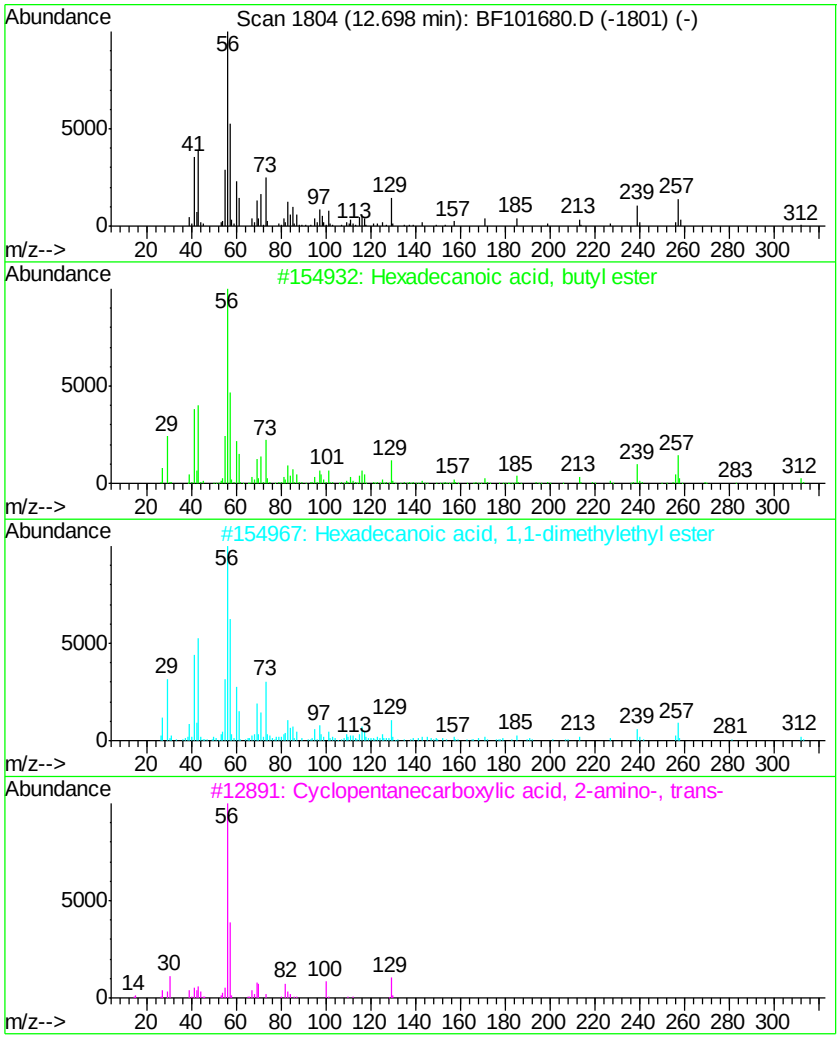
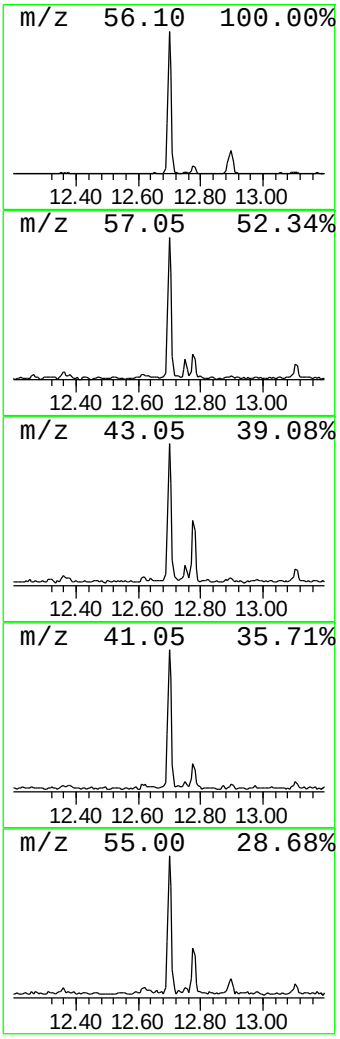
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	5.38 ng	261316	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38





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Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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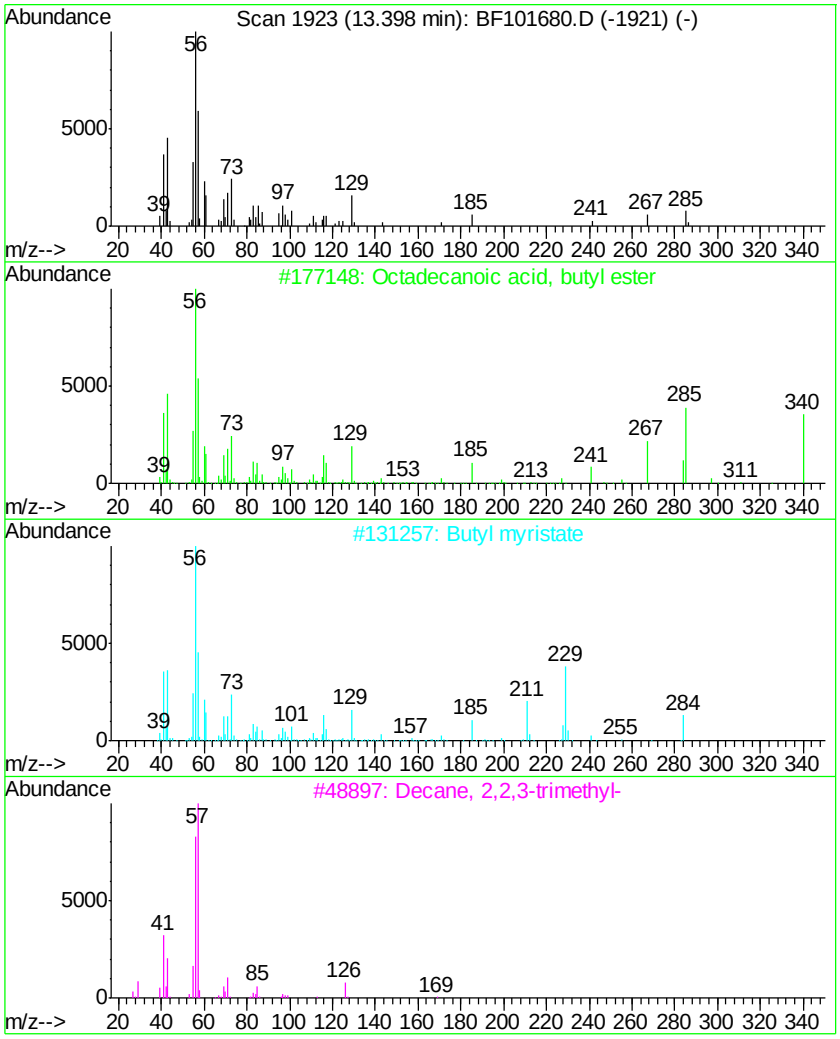
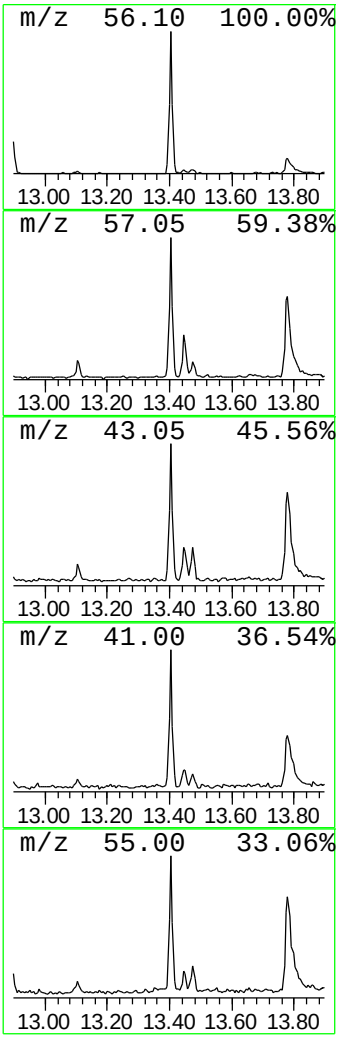
Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	3.83 ng	185697	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2	Butyl myristate	284	C18H36O2	000110-36-1	64
3	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	43
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35





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Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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TIC Integration Parameters: LSCINT.P

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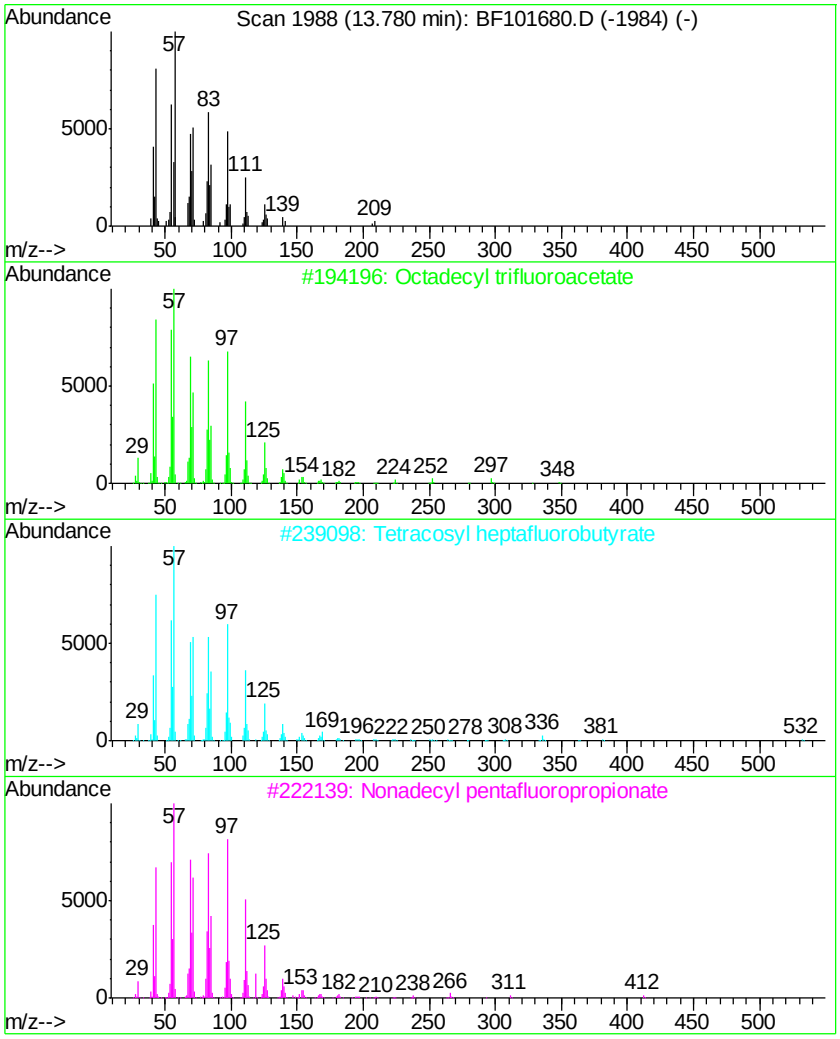
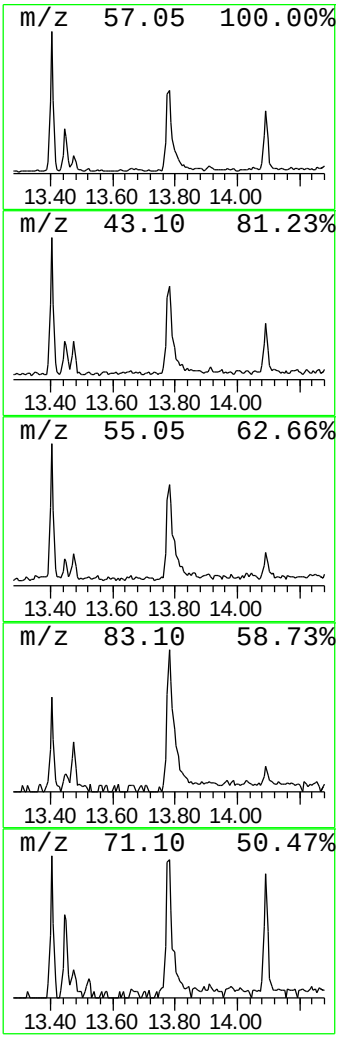
Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	3.62 ng	175827	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	90
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90





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...	5.01	2.4	ng	128492	1	6.79	1083280	20.0
unknown6.56	6.56	52.9	ng	2864140	1	6.79	1083280	20.0
Hexadecanoic acid...	12.70	5.4	ng	261316	5	13.96	970541	20.0
Octadecanoic acid...	13.40	3.8	ng	185697	5	13.96	970541	20.0
Octadecyl trifluo...	13.78	3.6	ng	175827	5	13.96	970541	20.0