LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101648.D
Acq On : 22 Dec 2017 11:10
Operator : SJ/JU
Sample : I7008-14
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121817-TIFR-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:\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	494	497	522	rBV	115563	196949	5.04%	0.792%
2	5.416	563	566	596	rBV	1159062	1674918	42.89%	6.738%
3	6.440	737	740	758	rBV2	709272	1190759	30.49%	4.790%
4	6.569	758	762	769	rBV	2477891	2389824	61.20%	9.614%
5	6.798	797	801	809	rBV	862369	883408	22.62%	3.554%
6	6.951	823	827	843	rBV	3129798	3037590	77.79%	12.220%
7	7.369	894	898	919	rBV	2411614	2565297	65.69%	10.320%
8	8.081	1015	1019	1037	rBV	1004433	1135419	29.08%	4.568%
9	9.151	1197	1201	1212	rBV	3959590	3904970	100.00%	15.709%
10	9.833	1314	1317	1330	rVB	1006957	997823	25.55%	4.014%
11	10.628	1448	1452	1465	rBV	1096252	1216979	31.16%	4.896%
12	11.322	1565	1570	1581	rBV	812548	832493	21.32%	3.349%
13	11.686	1629	1632	1636	rBV	73783	66828	1.71%	0.269%
14	12.710	1802	1806	1809	rBV	88929	75775	1.94%	0.305%
15	12.904	1835	1839	1842	rBV	2868085	2692238	68.94%	10.831%
16	13.410	1921	1925	1929	rBV	66041	61853	1.58%	0.249%
17	13.792	1986	1990	1998	rBV4	59986	111973	2.87%	0.450%
18	13.968	2017	2020	2027	rVB	848163	889754	22.79%	3.579%
19	14.104	2040	2043	2049	rVB3	42705	59665	1.53%	0.240%
20	14.333	2079	2082	2087	rBV7	22283	40515	1.04%	0.163%
21	14.404	2091	2094	2098	rBV2	51346	51886	1.33%	0.209%
22	14.627	2129	2132	2136	rBV3	32850	42126	1.08%	0.169%
23	14.704	2142	2145	2149	rVB	46951	47180	1.21%	0.190%
24	15.439	2265	2270	2280	rVB	449608	642829	16.46%	2.586%
25	15.815	2331	2334	2339	rVB3	38200	48818	1.25%	0.196%

Sum of corrected areas: 24857869

LSC Report - Integrated Chromatogram

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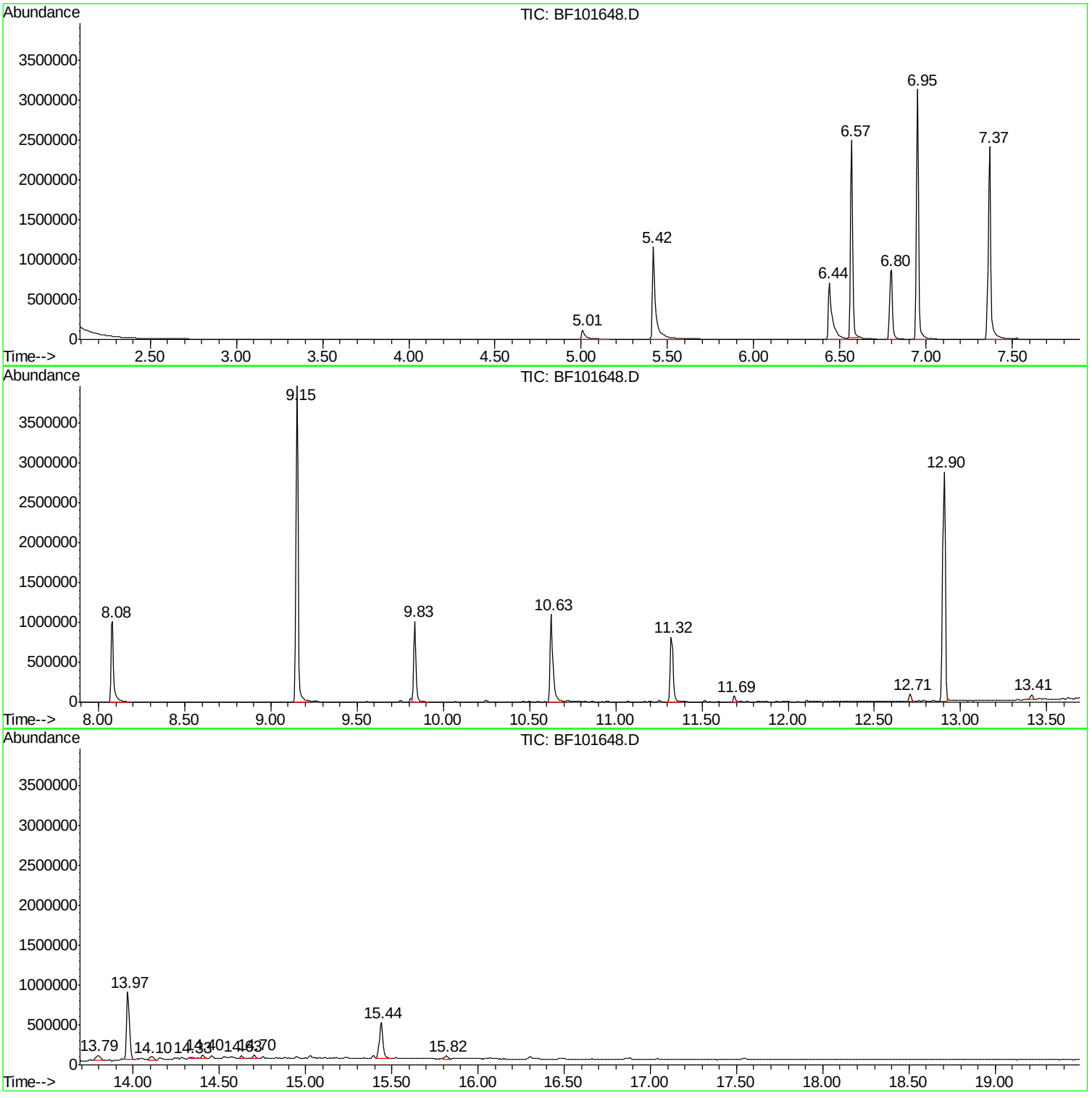
Instrument : BNA_F
ClientSampleId : 121817-TIFR-E-U-S

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101648.D
Acq On : 22 Dec 2017 11:10
Operator : SJ/JU
Sample : I7008-14
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121817-TIFR-E-U-S

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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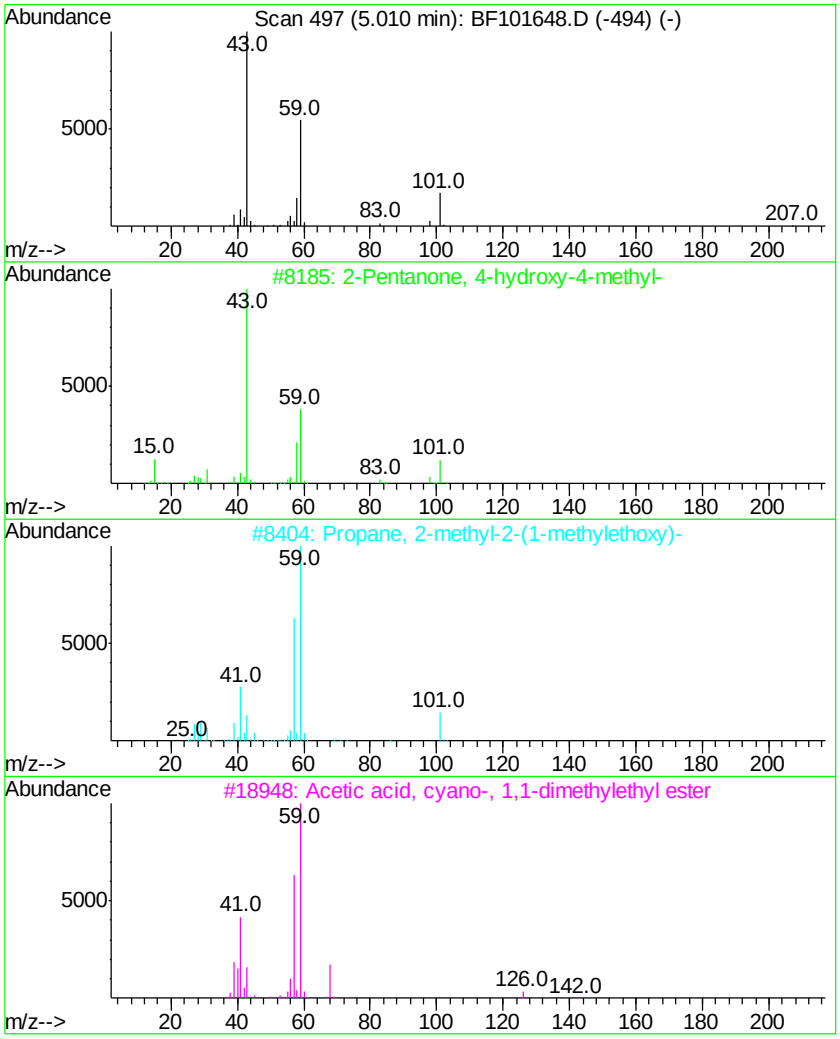
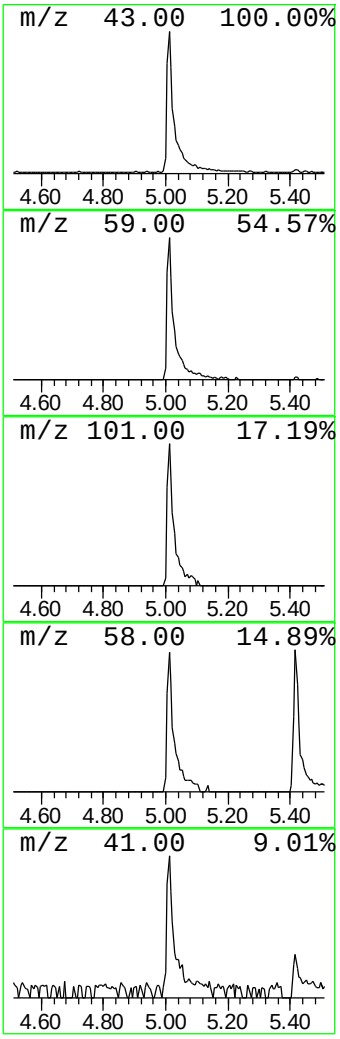
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	4.46 ng	196949	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : I7008-14
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121817-TIFR-E-U-S

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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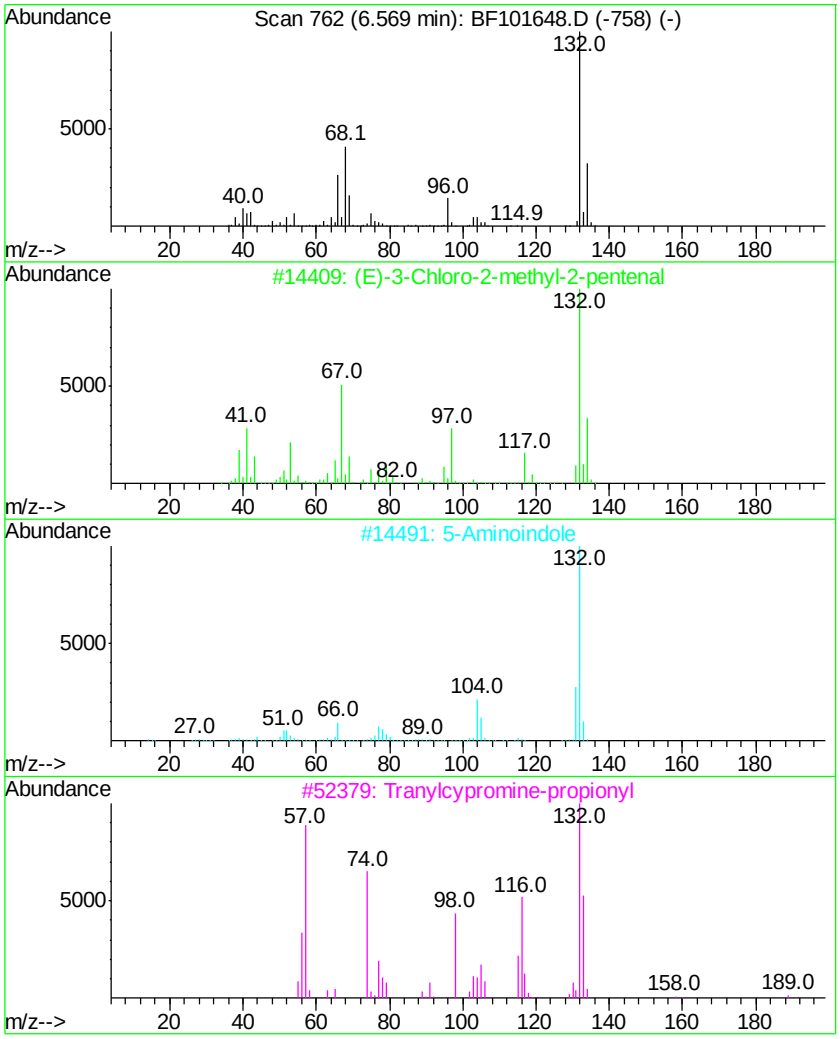
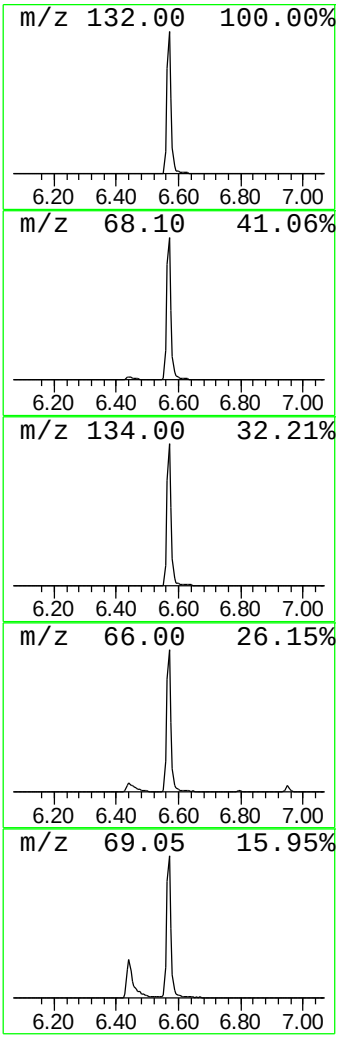
Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	54.10 ng	2389820	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : SJ/JU
Sample : I7008-14
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121817-TIFR-E-U-S

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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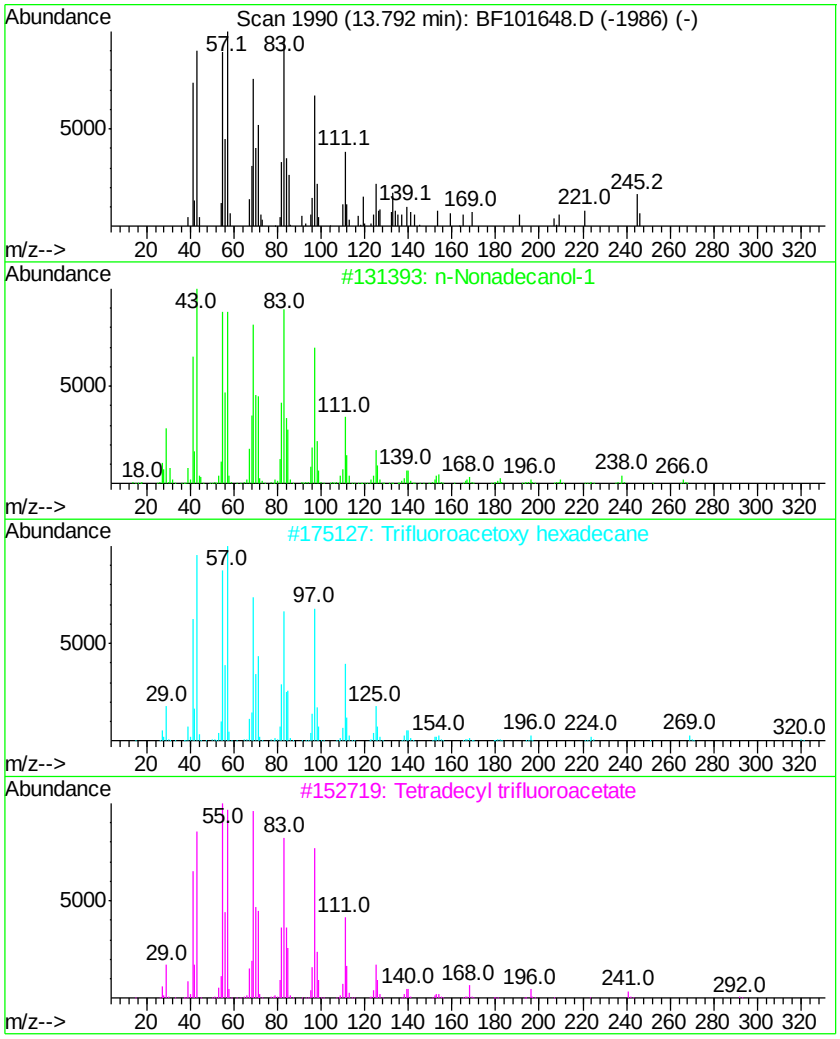
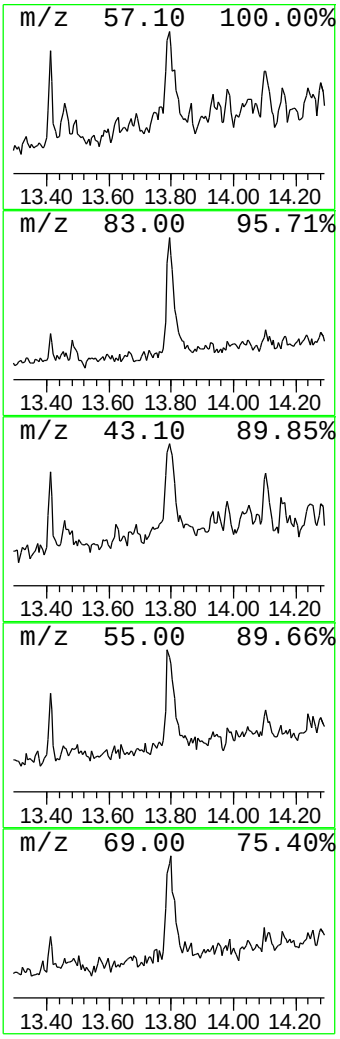
Peak Number 4 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.52 ng	111973	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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...	5.01	4.5	ng	196949	1	6.80	883408	20.0
unknown6.57	6.57	54.1	ng	2389820	1	6.80	883408	20.0
n-Nonadecanol-1	13.79	2.5	ng	111973	5	13.97	889754	20.0