LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095691.D
Acq On : 6 Jun 2017 00:50
Operator : SJ/MA
Sample : I3466-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-230-060217

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-BF060517.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	1.602	8	11	25	rBV	135662	240792	10.04%	1.181%
2	4.613	519	523	551	rBV	66856	189943	7.92%	0.932%
3	5.295	635	639	664	rBV	1354237	2397342	100.00%	11.762%
4	6.954	916	921	933	rBV	1394265	2072407	86.45%	10.167%
5	7.054	933	938	950	rVB	1715549	2334304	97.37%	11.452%
6	7.395	992	996	1009	rBV	419401	540649	22.55%	2.652%
7	7.636	1031	1037	1055	rBV	1392902	1875641	78.24%	9.202%
8	8.313	1146	1152	1173	rBV	1054433	1445018	60.28%	7.089%
9	9.425	1337	1341	1365	rBV	630919	817205	34.09%	4.009%
10	11.207	1638	1644	1657	rBV	1792134	2248987	93.81%	11.034%
11	11.895	1757	1761	1769	rBV	248339	296698	12.38%	1.456%
12	12.248	1816	1821	1827	rBV2	595608	721825	30.11%	3.541%
13	13.107	1963	1967	1972	rVB2	20617	24122	1.01%	0.118%
14	13.542	2036	2041	2057	rVB	906730	1168963	48.76%	5.735%
15	13.877	2094	2098	2108	rBV	23917	34906	1.46%	0.171%
16	14.642	2223	2228	2241	rVB	501205	657131	27.41%	3.224%
17	15.659	2395	2401	2411	rBV2	123354	177373	7.40%	0.870%
18	16.459	2530	2537	2542	rBV	18311	25617	1.07%	0.126%
19	16.759	2584	2588	2593	rBV2	59352	79179	3.30%	0.388%
20	17.012	2624	2631	2635	rBV	1460909	1692651	70.61%	8.304%
21	18.265	2841	2844	2852	rBV	104130	184336	7.69%	0.904%
22	18.348	2854	2858	2863	rBV	484290	600071	25.03%	2.944%
23	20.018	3138	3142	3147	rBV	465311	520025	21.69%	2.551%
24	23.941	3805	3809	3810	rBV4	25562	37675	1.57%	0.185%

Sum of corrected areas: 20382860

LSC Report - Integrated Chromatogram

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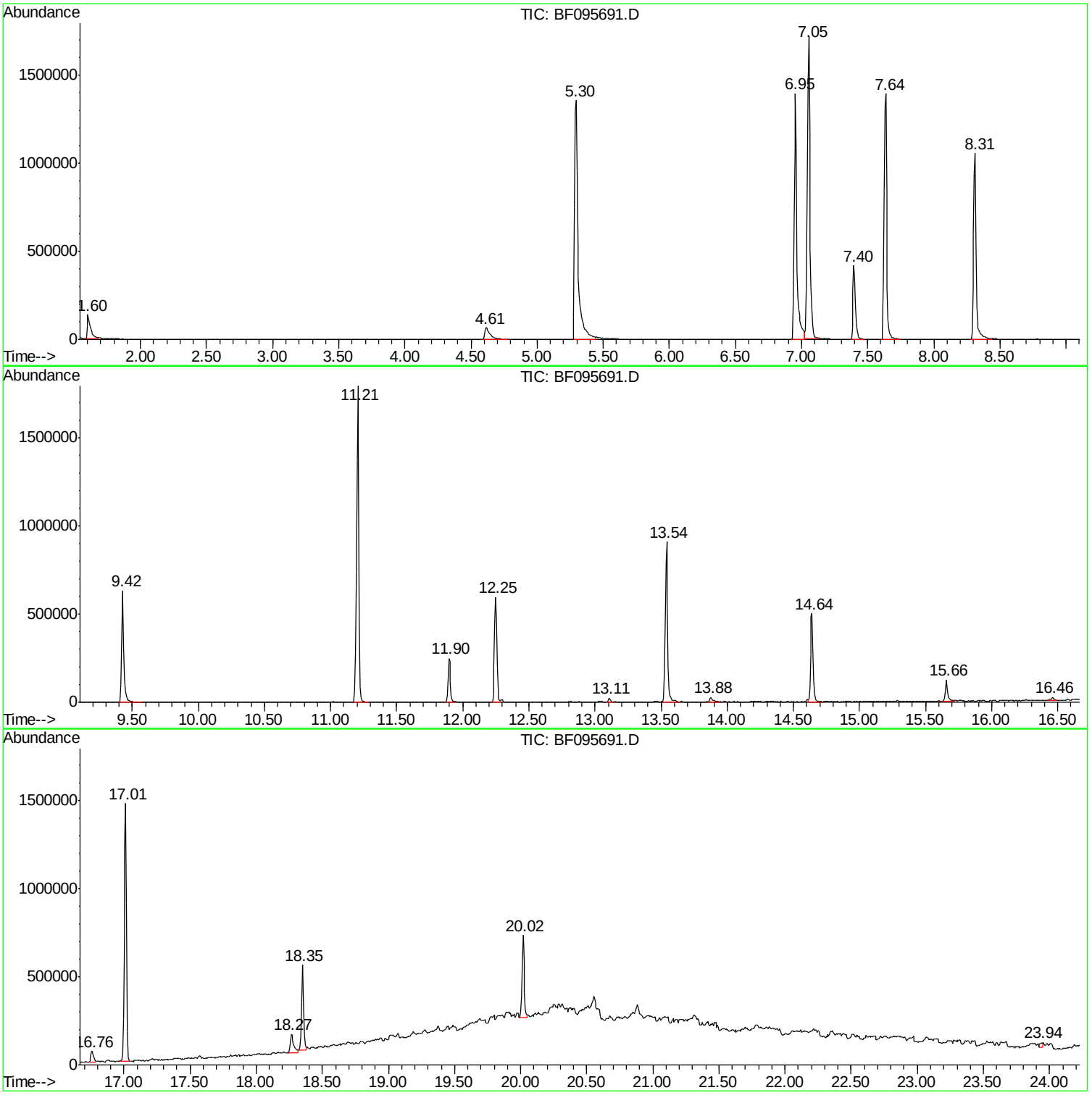
Instrument :
BNA_F
ClientSampleId :
SU-RO-230-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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Sample : I3466-01
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Instrument : BNA_F
ClientSampleId : SU-RO-230-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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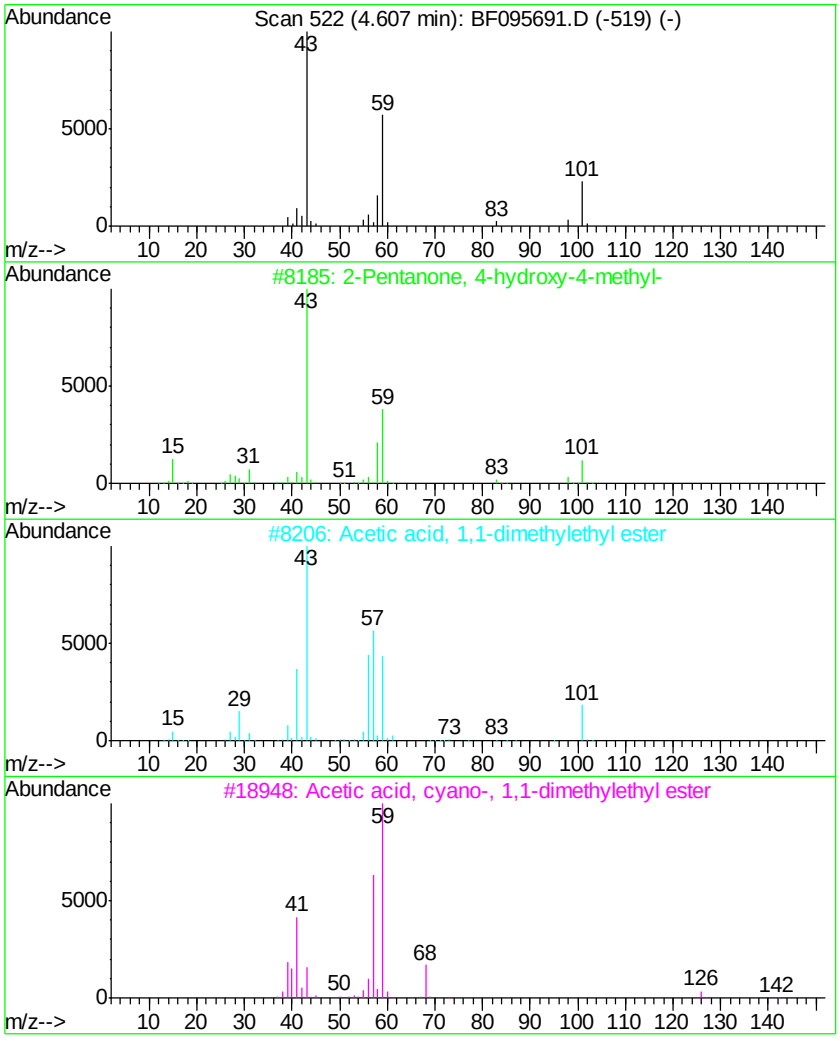
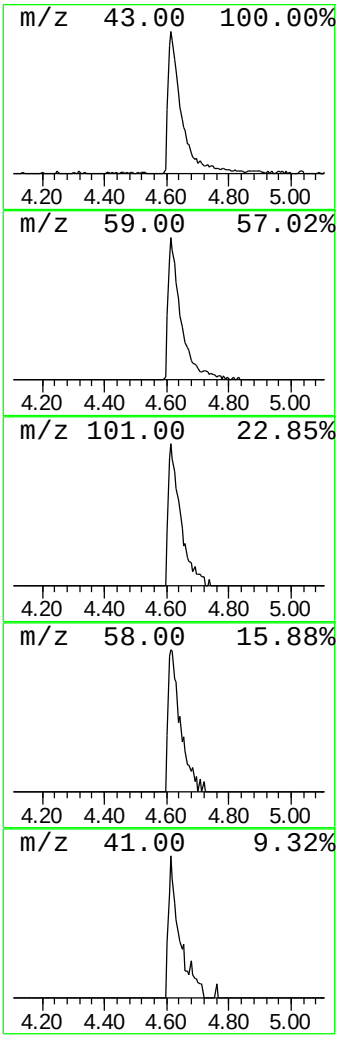
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	7.03 ng	189943	1,4-Dichlorobenzene-d4	7.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095691.D
Acq On : 6 Jun 2017 00:50
Operator : SJ/MA
Sample : I3466-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-230-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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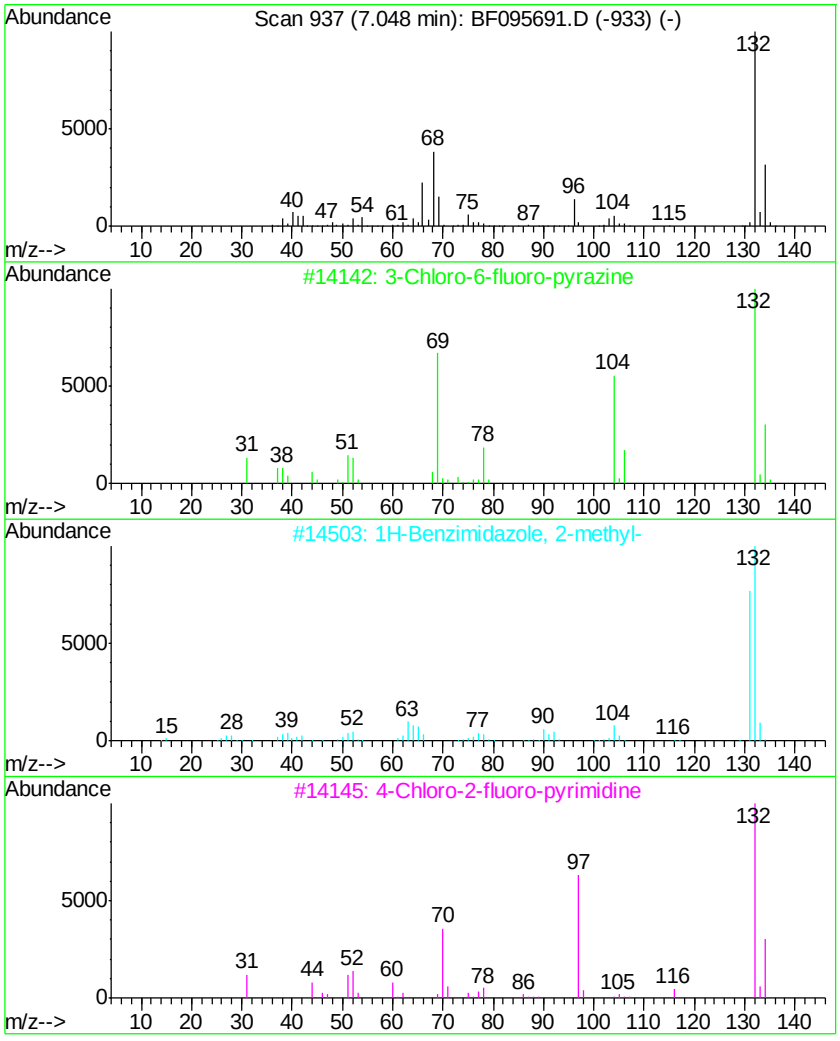
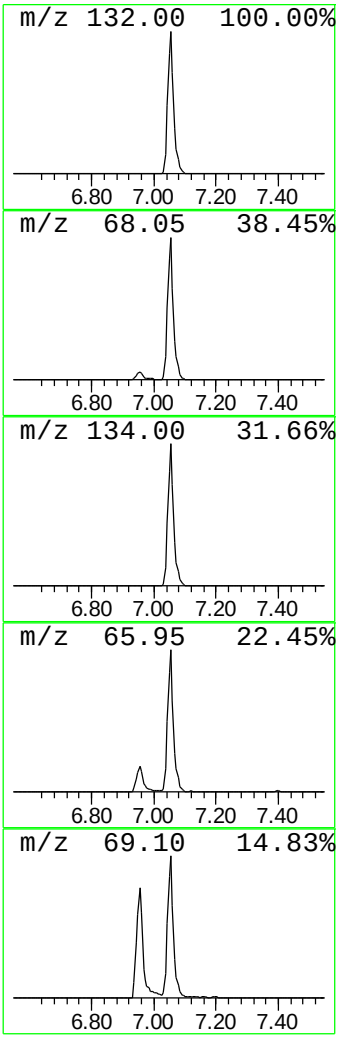
Peak Number 3 unknown7.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	86.35 ng	2334300	1,4-Dichlorobenzene-d4	7.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Operator : SJ/MA
Sample : I3466-01
Misc :
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Instrument : BNA_F
ClientSampleId : SU-RO-230-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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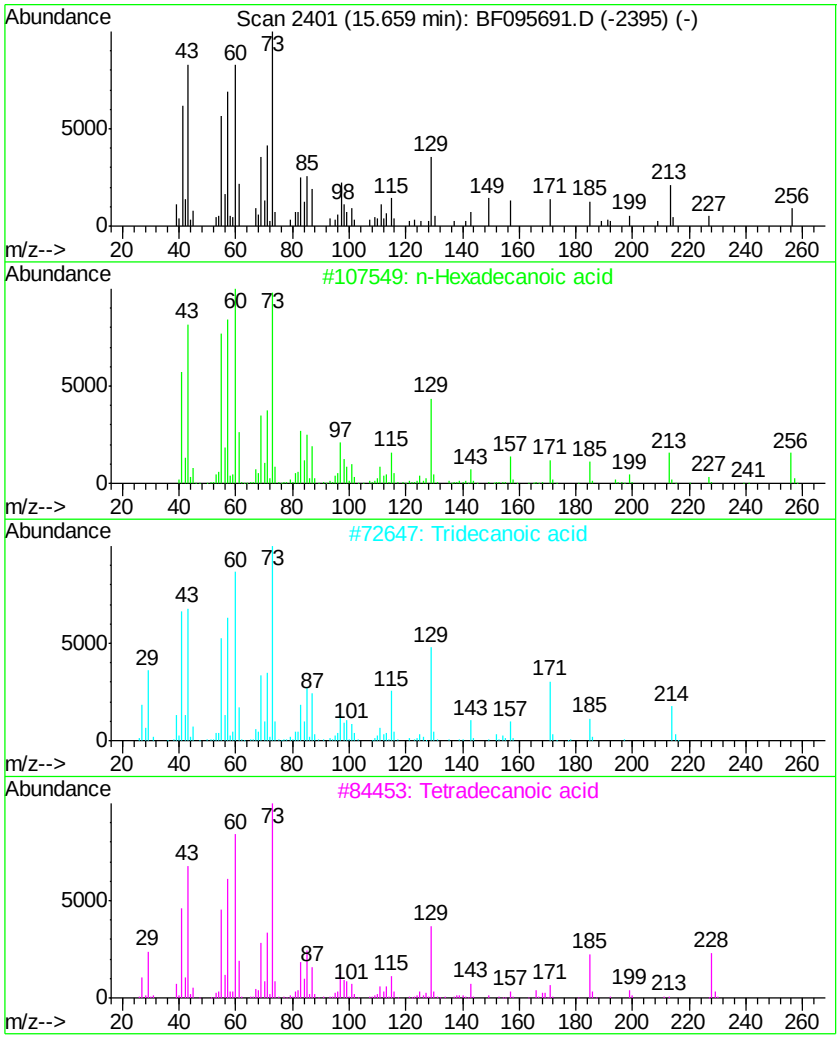
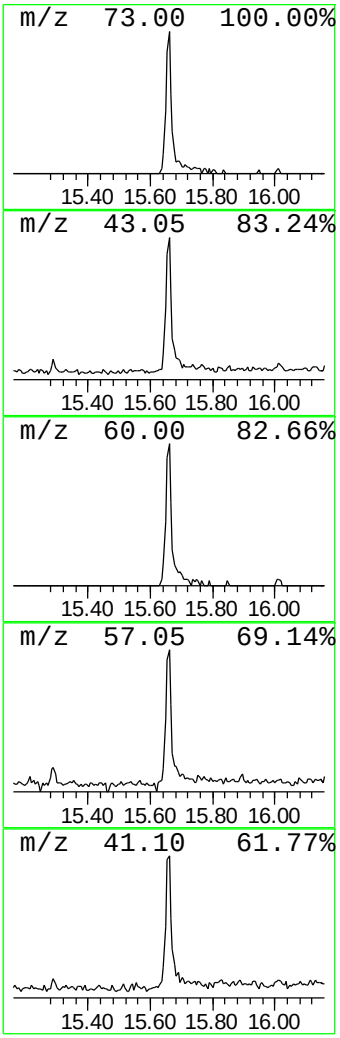
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	5.40 ng	177373	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30





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Sample : I3466-01
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Instrument : BNA_F
ClientSampleId : SU-RO-230-060217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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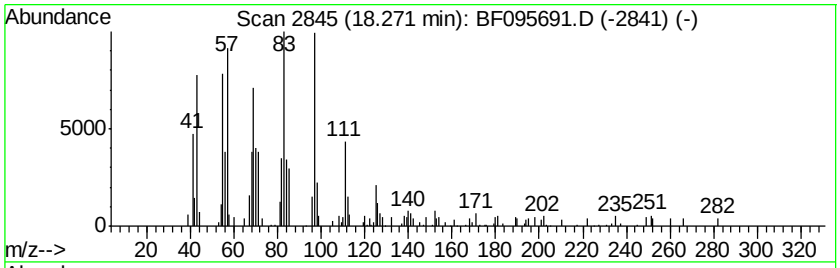
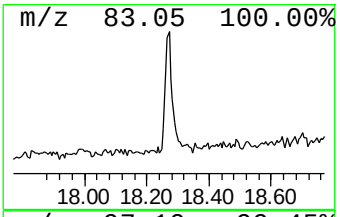
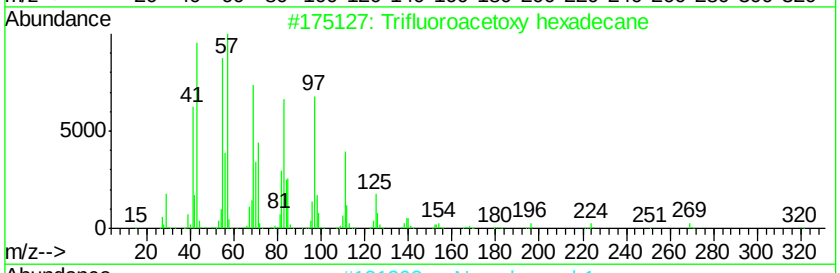
Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 5

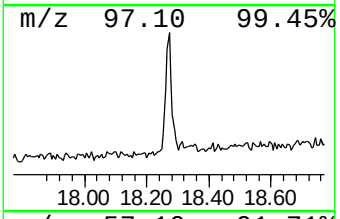
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	6.14 ng	184336	Chrysene-d12	18.35

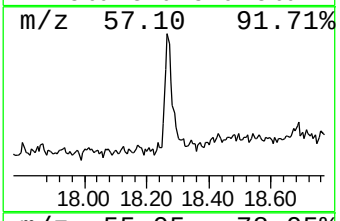
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	1-Octadecene	252	C18H36	000112-88-9	95
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94

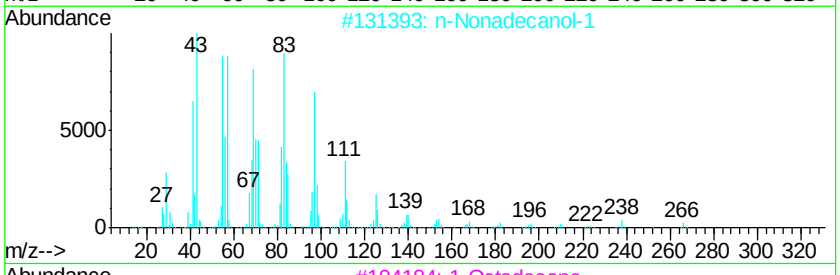


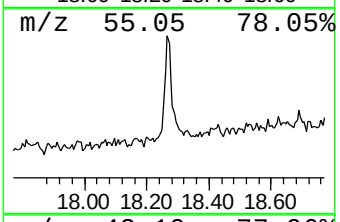


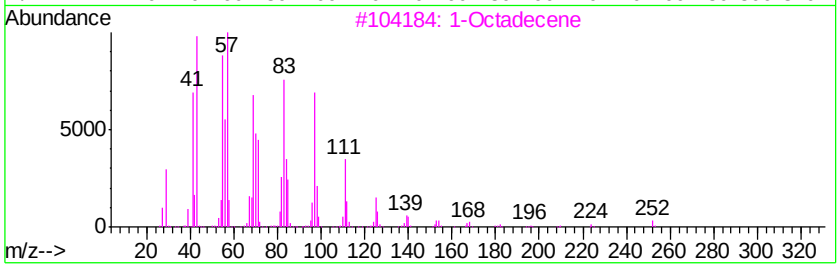


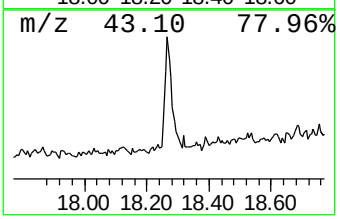












Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.61	7.0	ng	189943	1	7.40	540649	20.0
unknown7.05	7.05	86.3	ng	2334300	1	7.40	540649	20.0
n-Hexadecanoic acid	15.66	5.4	ng	177373	4	14.64	657131	20.0
Trifluoroacetoxy ...	18.27	6.1	ng	184336	5	18.35	600071	20.0