LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098784.D
Acq On : 25 Sep 2017 15:36
Operator : SJ/JU
Sample : I5364-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-125-17(5-10)

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-BF092317.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	2.216	19	22	48	rVB4	138340	470209	16.14%	1.885%
2	5.140	516	519	531	rVB	393839	459784	15.78%	1.843%
3	5.534	581	586	589	rBV	2788496	2624879	90.09%	10.522%
4	6.539	751	757	760	rBV	2657003	2673559	91.76%	10.717%
5	6.681	777	781	785	rBV	2687282	2709018	92.97%	10.859%
6	6.916	817	821	824	rBV	1158318	877500	30.12%	3.518%
7	7.075	843	848	851	rBV	2251241	2098094	72.01%	8.410%
8	7.475	911	916	919	rBV	1806891	1577234	54.13%	6.323%
9	8.198	1035	1039	1042	rBV	1422008	1154048	39.61%	4.626%
10	9.269	1216	1221	1225	rBV	3168557	2913741	100.00%	11.680%
11	9.657	1284	1287	1291	rBV	250739	219082	7.52%	0.878%
12	9.951	1333	1337	1341	rVB	1240064	1116260	38.31%	4.475%
13	10.374	1406	1409	1412	rVB	49378	36546	1.25%	0.146%
14	10.739	1467	1471	1474	rBV	1519195	1224929	42.04%	4.910%
15	10.845	1486	1489	1494	rBV	57596	56225	1.93%	0.225%
16	11.439	1586	1590	1593	rBV	1139641	912793	31.33%	3.659%
17	11.951	1674	1677	1682	rBV	36623	34311	1.18%	0.138%
18	13.021	1855	1859	1863	rBV	2262714	1995079	68.47%	7.998%
19	13.904	2006	2009	2016	rBV	118138	114427	3.93%	0.459%
20	14.080	2035	2039	2042	rBV	849448	784083	26.91%	3.143%
21	14.698	2141	2144	2148	rBV	54382	47920	1.64%	0.192%
22	14.927	2180	2183	2187	rVB	43131	42334	1.45%	0.170%
23	15.192	2226	2228	2231	rBV	32502	31582	1.08%	0.127%
24	15.568	2287	2292	2300	rVB	507905	692911	23.78%	2.778%
25	16.033	2367	2371	2376	rBV2	54642	79643	2.73%	0.319%

Sum of corrected areas: 24946191

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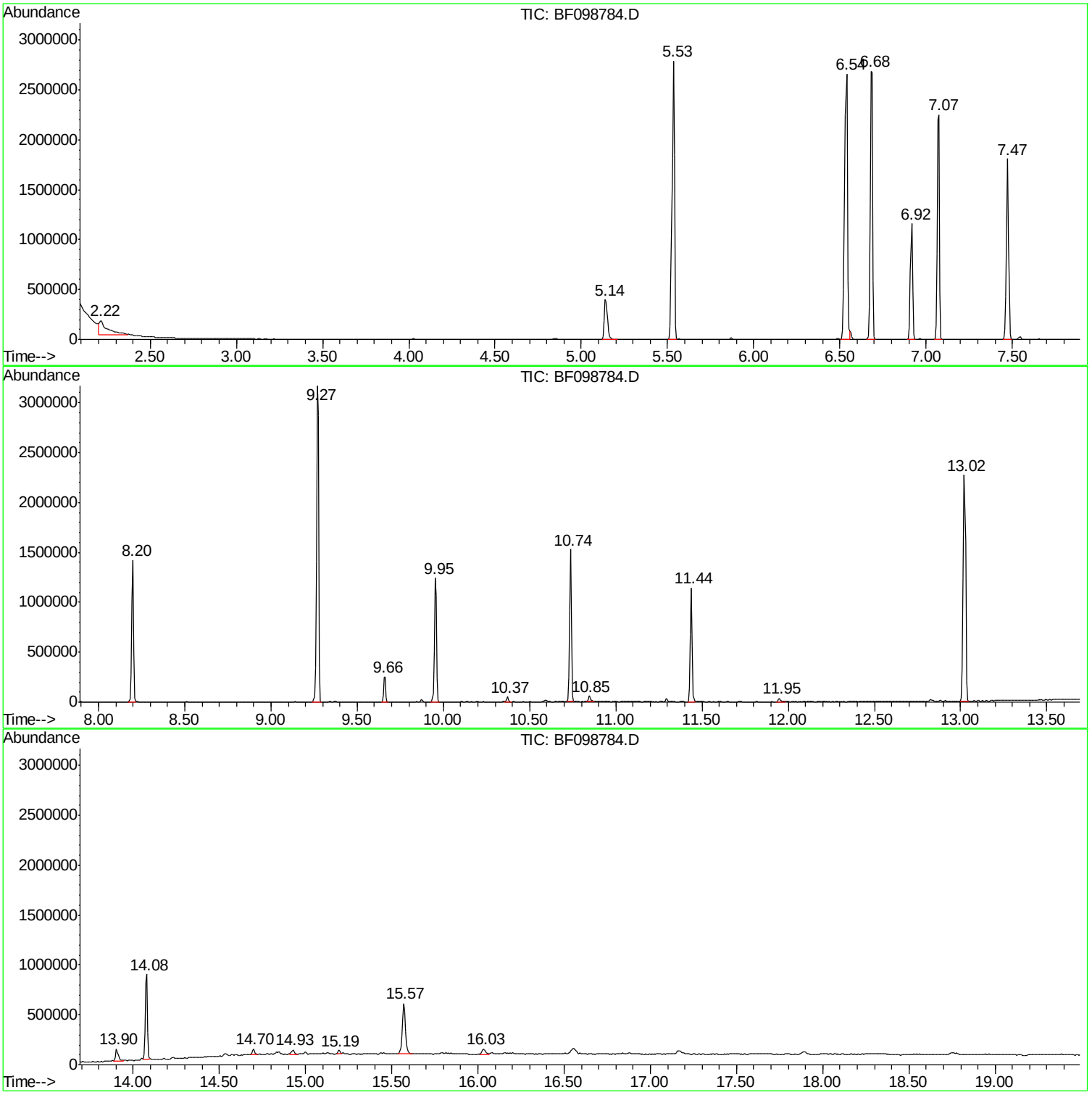
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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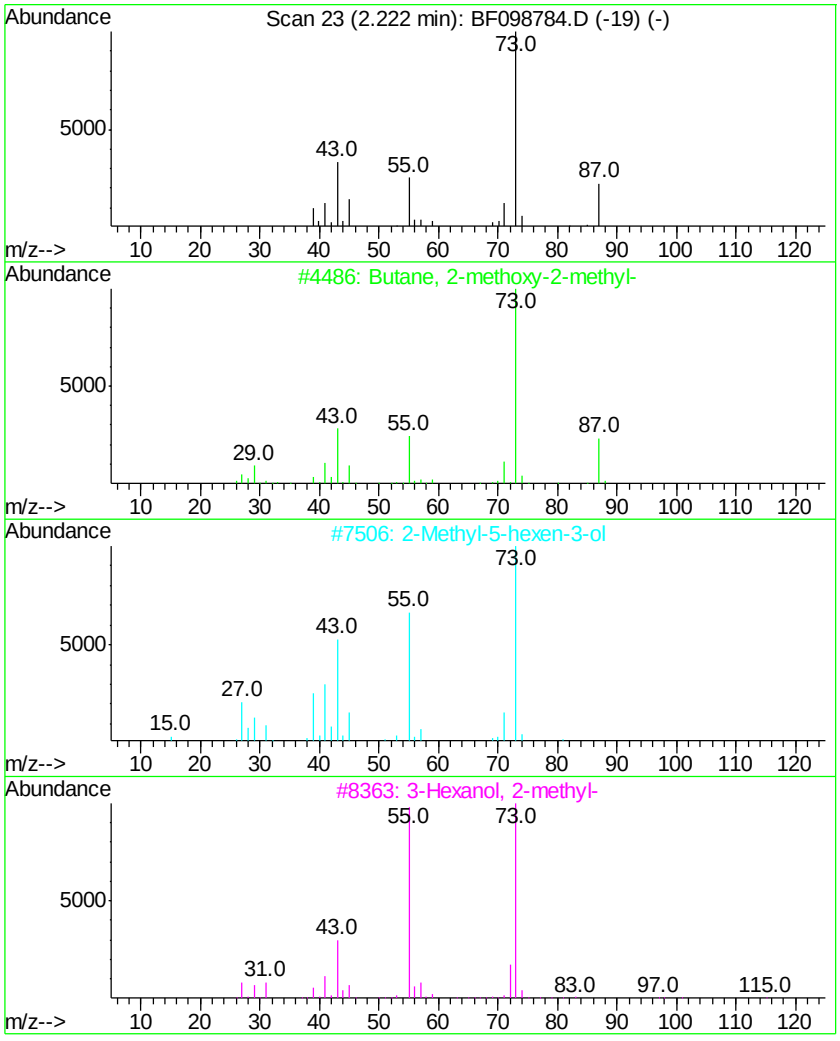
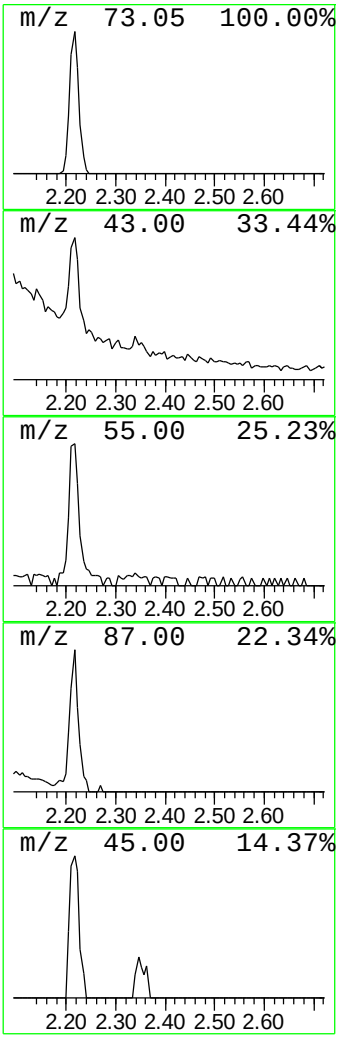
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	10.72 ng	470209	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	43
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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SASP2P-ENV-125-17(5-10)

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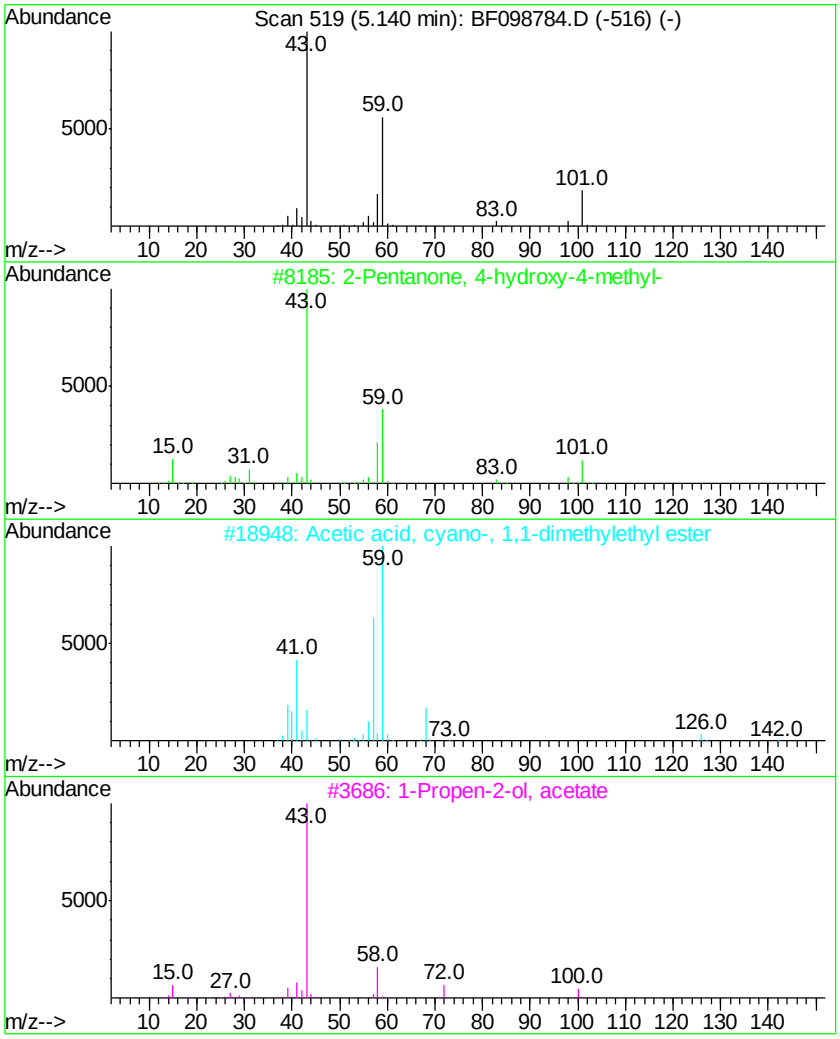
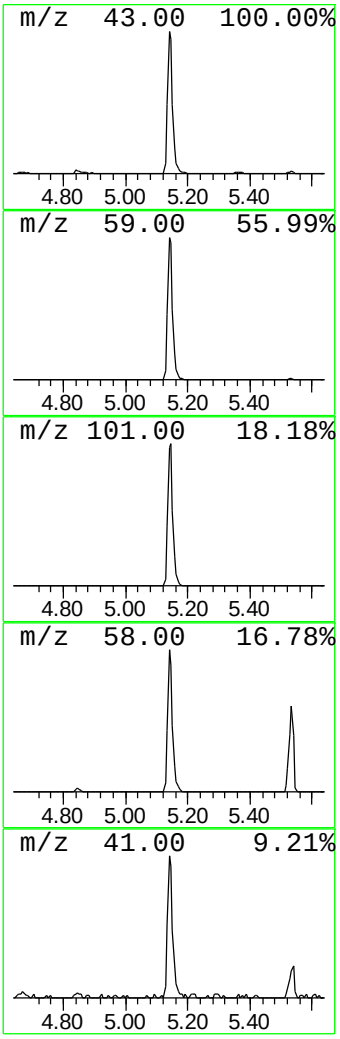
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	10.48 ng	459784	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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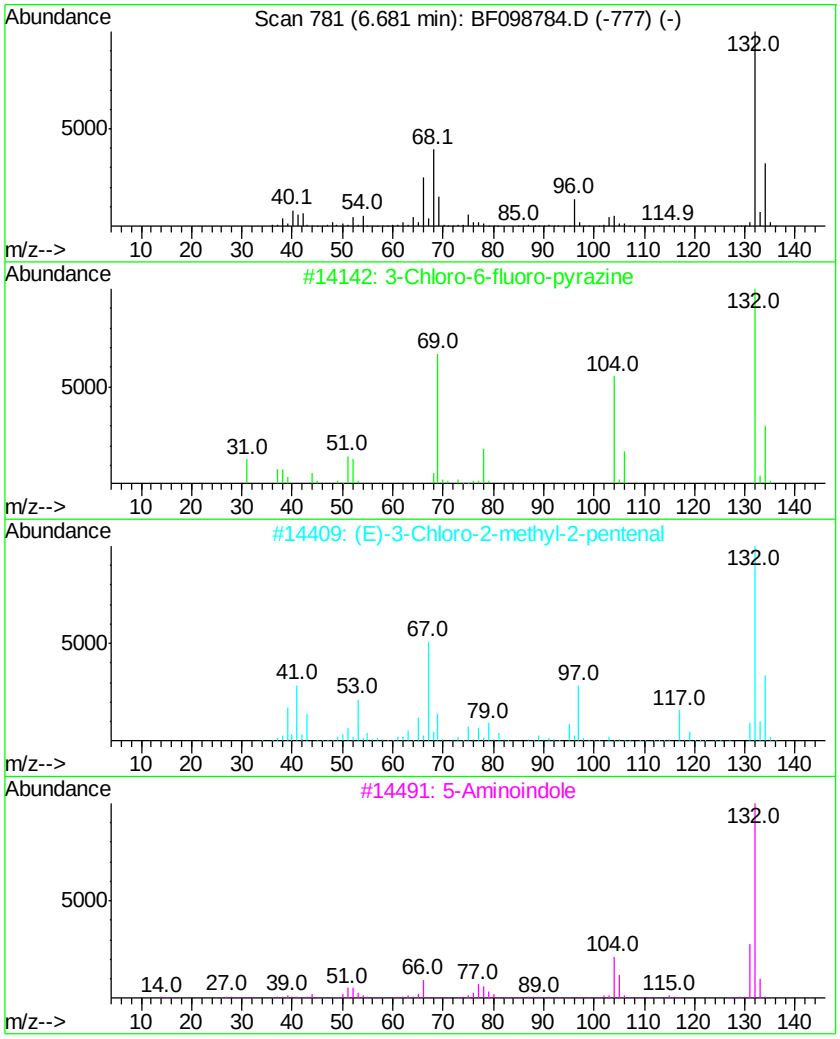
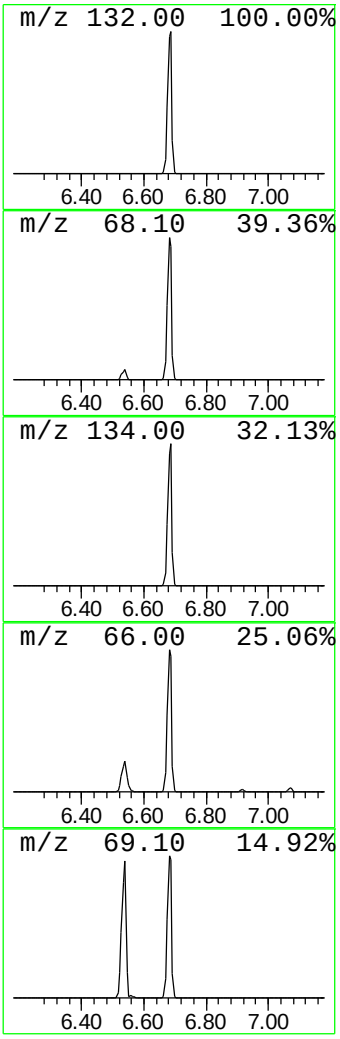
Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	61.74 ng	2709020	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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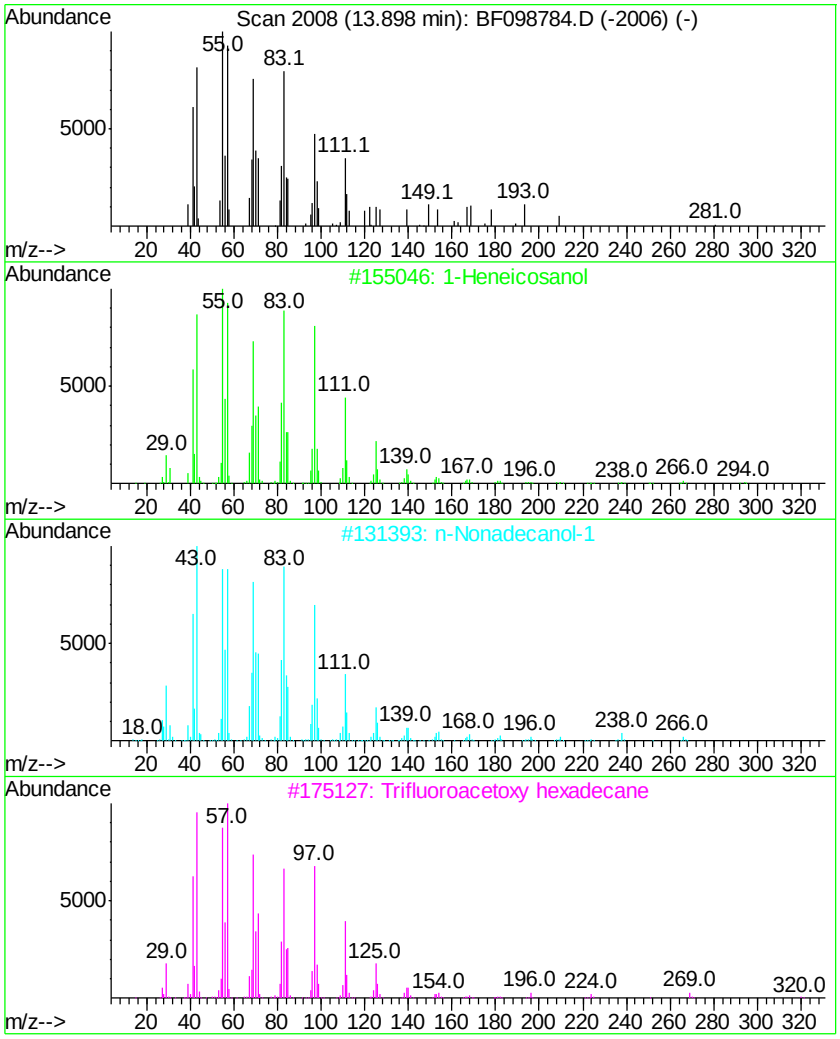
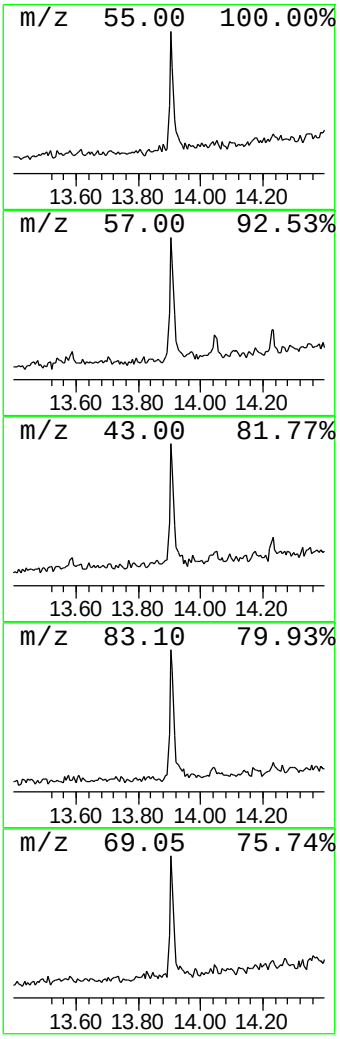
Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	2.92 ng	114427	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94





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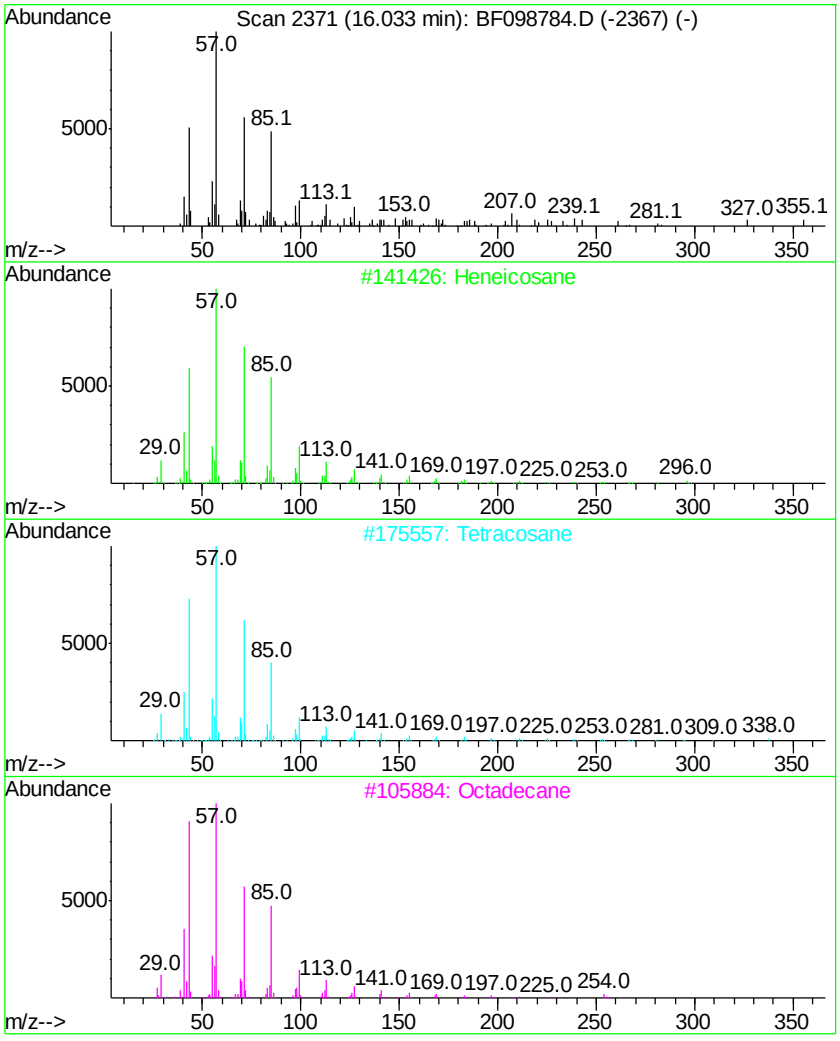
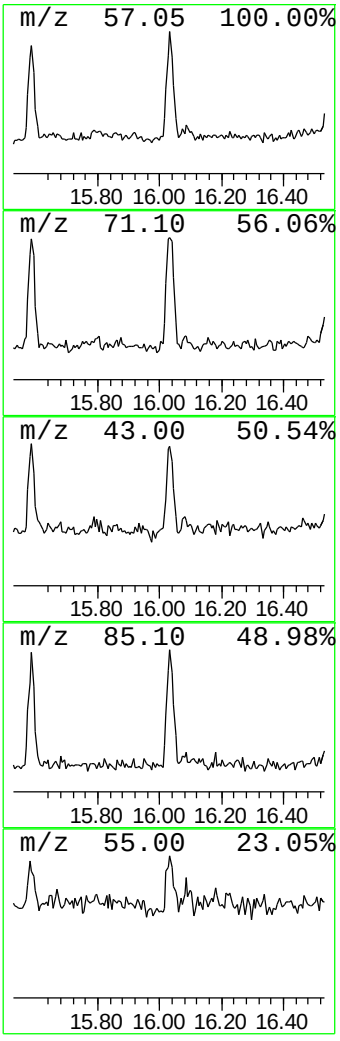
Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.30 ng	79643	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Tetracosane	338	C24H50	000646-31-1	86
3	Octadecane	254	C18H38	000593-45-3	86
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Heptadecane	240	C17H36	000629-78-7	80





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	10.7	ng	470209	1	6.92	877500	20.0
2-Pentanone, 4-hy...	5.14	10.5	ng	459784	1	6.92	877500	20.0
unknown6.68	6.68	61.7	ng	2709020	1	6.92	877500	20.0
1-Heneicosanol	13.90	2.9	ng	114427	5	14.08	784083	20.0
Heneicosane	16.03	2.3	ng	79643	6	15.57	692911	20.0