LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098695.D
Acq On : 22 Sep 2017 13:01
Operator : SJ/JU
Sample : I5309-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5-COMP

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-BF092117.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	2.246	25	27	43	rVB	114733	230321	6.30%	0.741%
2	5.163	518	523	536	rVB	497952	652632	17.84%	2.099%
3	5.546	583	588	592	rBV	3329424	3601223	98.43%	11.581%
4	6.545	752	758	761	rBV	3118937	3658679	100.00%	11.766%
5	6.698	779	784	787	rBV	3631360	3597099	98.32%	11.568%
6	6.928	819	823	826	rBV	1126432	866268	23.68%	2.786%
7	7.087	845	850	853	rBV	2587914	2415004	66.01%	7.767%
8	7.487	913	918	921	rBV	2222253	2159423	59.02%	6.945%
9	8.210	1036	1041	1044	rBV	1269465	1125552	30.76%	3.620%
10	9.281	1218	1223	1226	rBV	3802374	3486788	95.30%	11.213%
11	9.669	1286	1289	1292	rBV	522154	406131	11.10%	1.306%
12	9.963	1335	1339	1343	rBV	1319221	1082501	29.59%	3.481%
13	10.386	1408	1411	1414	rVB	56813	41081	1.12%	0.132%
14	10.751	1466	1473	1476	rBV	1975955	1831920	50.07%	5.891%
15	10.857	1488	1491	1499	rBV	67296	61745	1.69%	0.199%
16	11.451	1588	1592	1594	rBV	977659	898221	24.55%	2.889%
17	11.963	1675	1679	1684	rBV2	77070	82320	2.25%	0.265%
18	12.480	1764	1767	1772	rBV2	43963	40494	1.11%	0.130%
19	12.657	1794	1797	1800	rBV	69059	59009	1.61%	0.190%
20	12.745	1809	1812	1818	rBV3	31543	38708	1.06%	0.124%
21	12.886	1831	1836	1840	rBV	49571	51751	1.41%	0.166%
22	13.033	1856	1861	1864	rBV	2910274	2566047	70.14%	8.252%
23	13.916	2008	2011	2017	rBV	170619	160444	4.39%	0.516%
24	14.086	2036	2040	2043	rBV	1074943	889443	24.31%	2.860%
25	14.551	2115	2119	2125	rBV9	28295	59772	1.63%	0.192%
26	15.133	2215	2218	2227	rBV2	32156	76626	2.09%	0.246%
27	15.580	2288	2294	2302	rVB	722771	955797	26.12%	3.074%

Sum of corrected areas: 31094999

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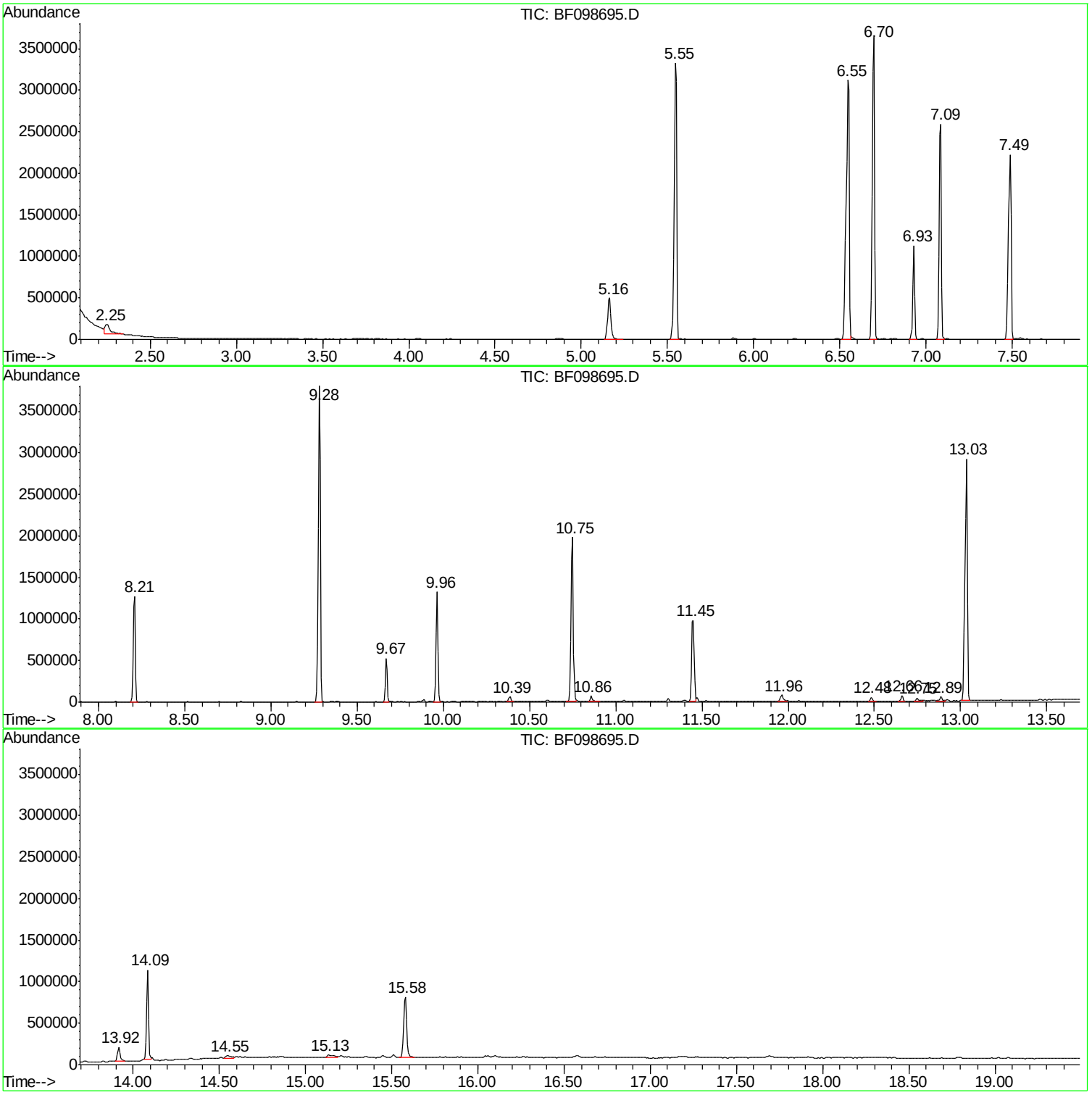
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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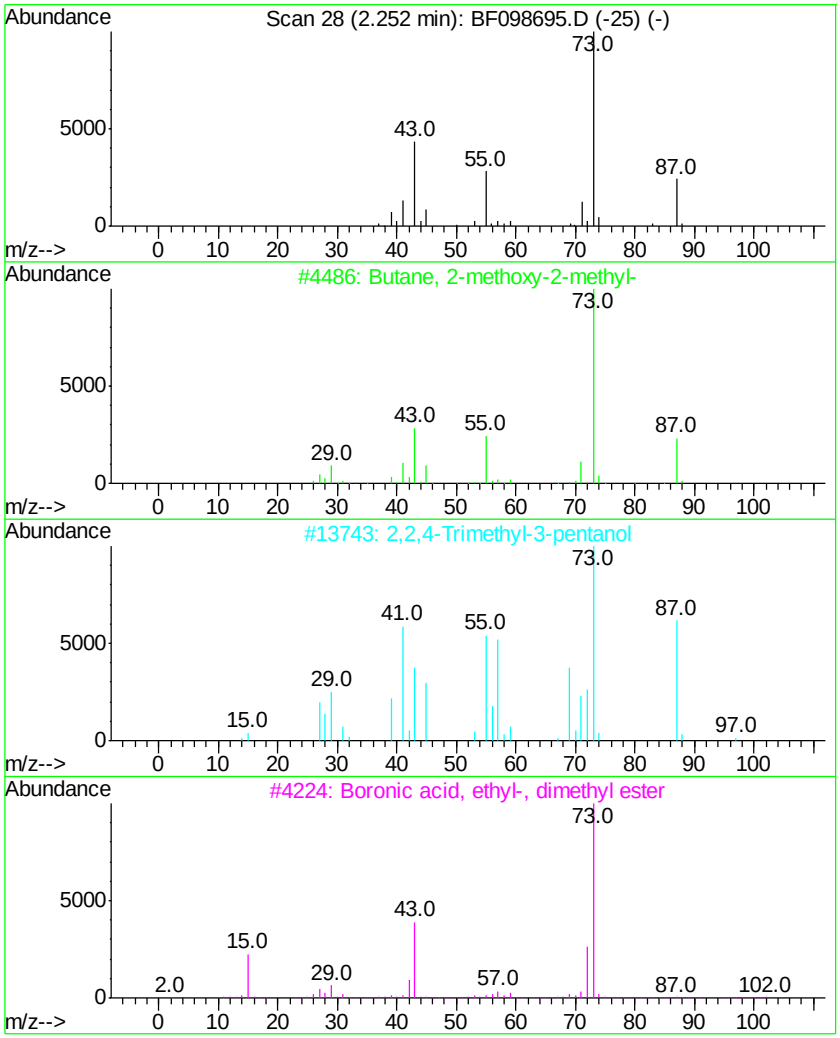
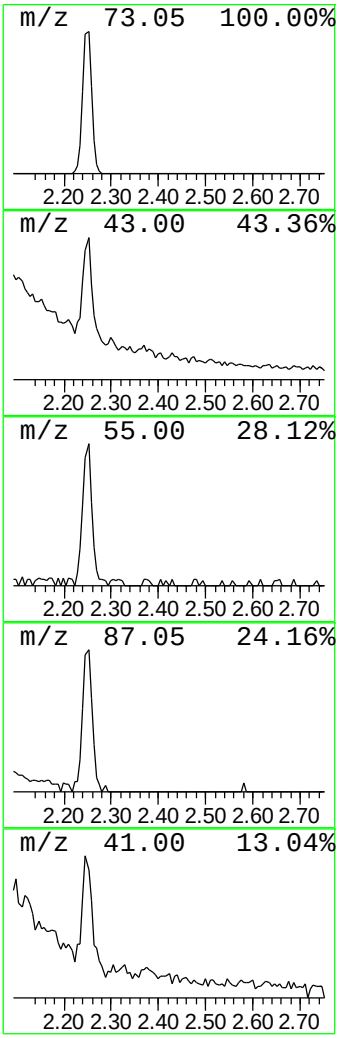
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	5.32 ng	230321	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





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Instrument : BNA_F
ClientSampleId : TP-5-COMP

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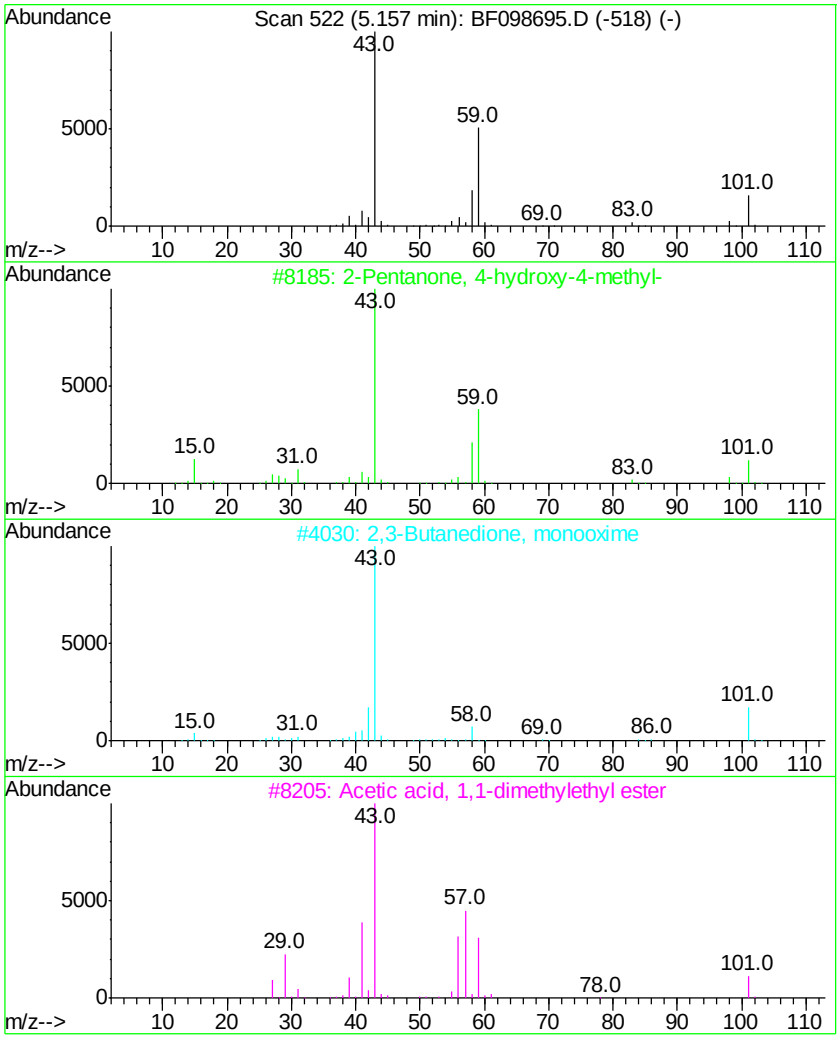
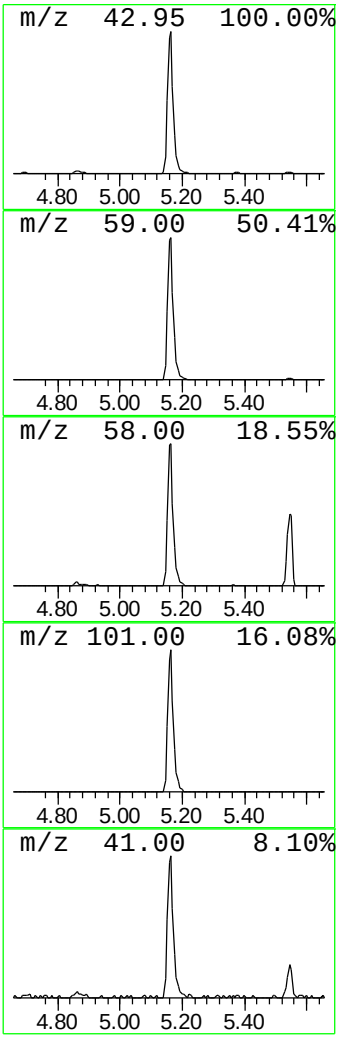
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	15.07 ng	652632	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Allyl acetate	100	C5H8O2	000591-87-7	9





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Sample : I5309-05
Misc :
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Instrument : BNA_F
ClientSampleId : TP-5-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
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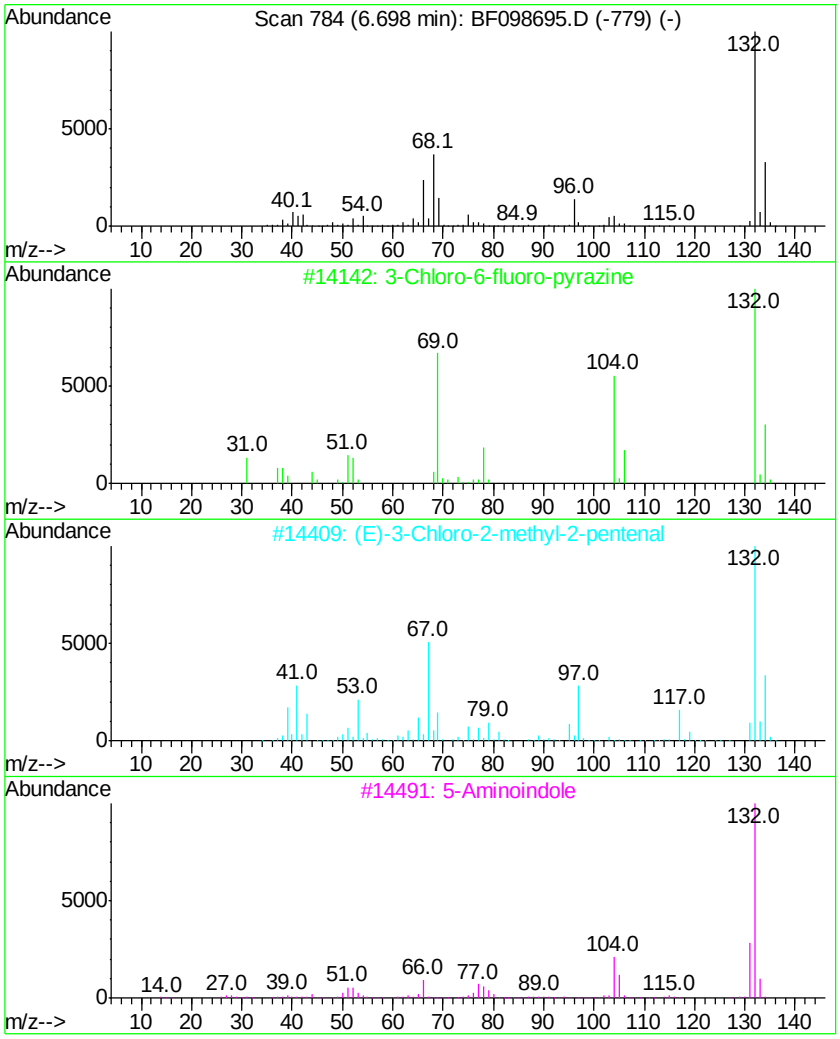
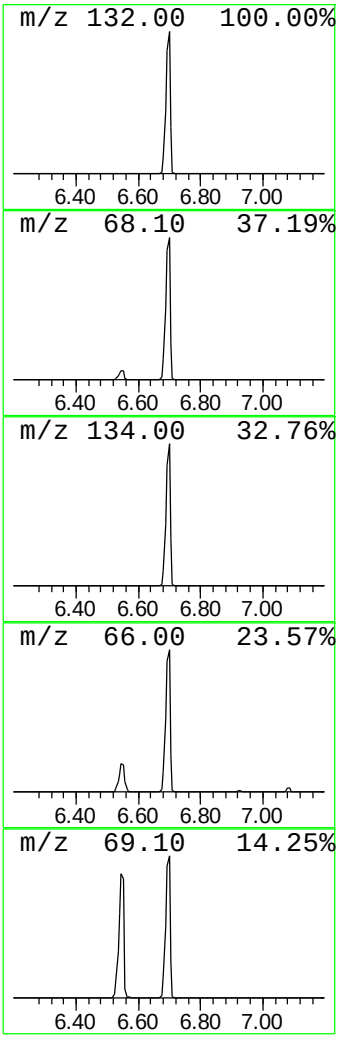
Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	83.05 ng	3597100	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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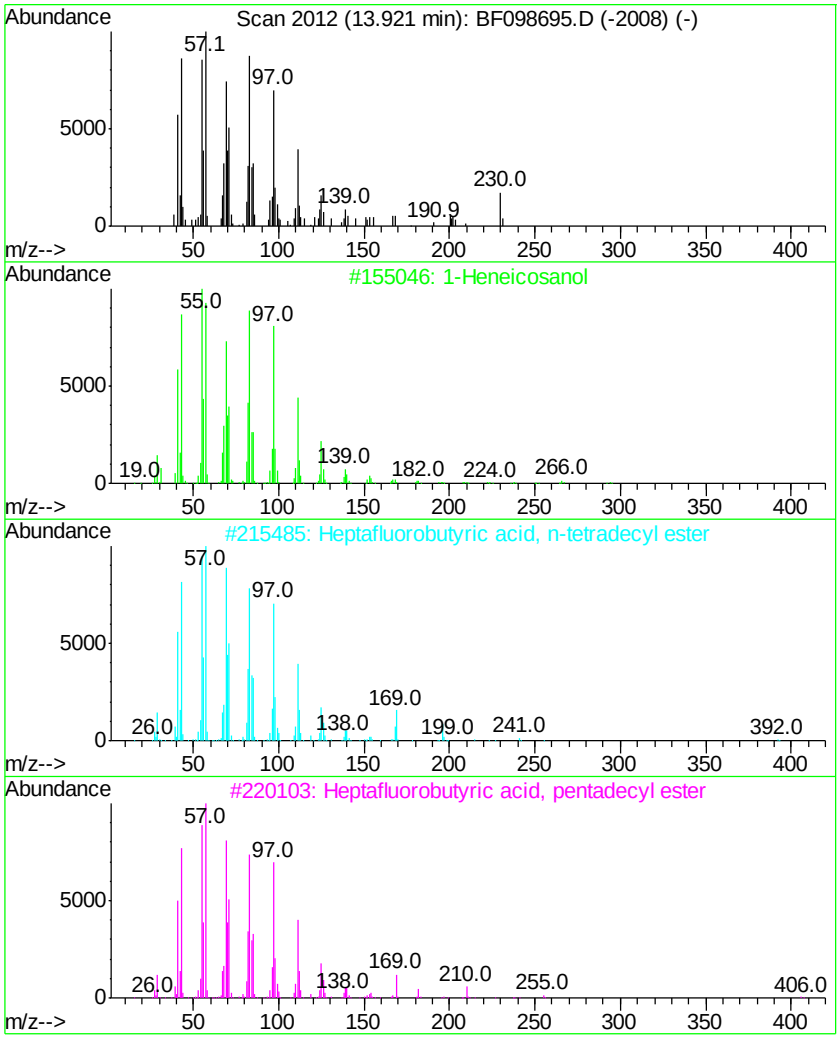
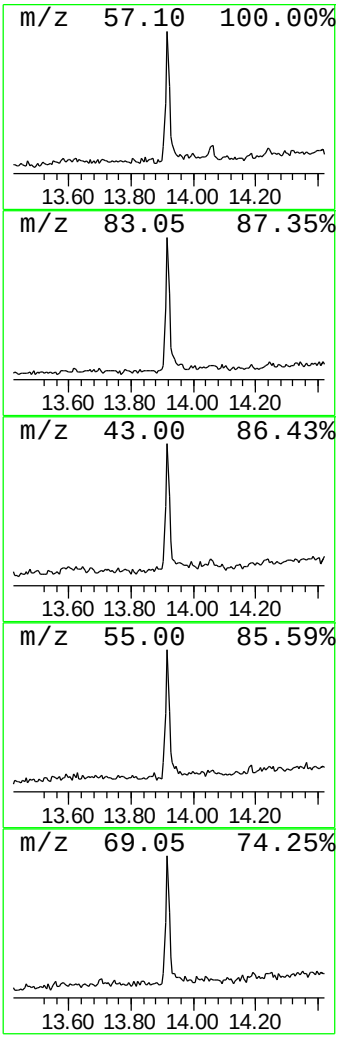
Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.61 ng	160444	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





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...	2.25	5.3	ng	230321	1	6.93	866268	20.0
2-Pentanone, 4-hy...	5.16	15.1	ng	652632	1	6.93	866268	20.0
unknown6.70	6.70	83.0	ng	3597100	1	6.93	866268	20.0
1-Heneicosanol	13.92	3.6	ng	160444	5	14.09	889443	20.0