LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
Data File : BF098053.D
Acq On : 26 Aug 2017 1:55
Operator : SJ/JU
Sample : I4945-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-4-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-BF081517.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	2.210	17	21	30	rVB	66855	96919	2.79%	0.395%
2	4.287	371	374	382	rBV	63624	80501	2.32%	0.328%
3	4.716	442	447	452	rVB	33301	36110	1.04%	0.147%
4	4.940	481	485	498	rVB	285754	402720	11.61%	1.641%
5	5.357	550	556	559	rBV	2919184	3107574	89.56%	12.659%
6	6.387	725	731	741	rBV	3030294	3469759	100.00%	14.135%
7	6.516	748	753	756	rBV	2994610	2974128	85.72%	12.116%
8	6.745	788	792	795	rBV	692658	626539	18.06%	2.552%
9	6.898	814	818	822	rBV	2395182	2158658	62.21%	8.794%
10	7.310	882	888	891	rBV	1729072	1668370	48.08%	6.796%
11	8.028	1006	1010	1013	rBV	828006	733231	21.13%	2.987%
12	9.104	1188	1193	1196	rBV	3049377	2643867	76.20%	10.770%
13	9.492	1256	1259	1263	rBV	379459	345303	9.95%	1.407%
14	9.775	1304	1307	1311	rBV	717582	662203	19.08%	2.698%
15	10.563	1437	1441	1445	rBV	1434105	1412842	40.72%	5.755%
16	10.686	1458	1462	1467	rBV	50031	47272	1.36%	0.193%
17	11.257	1555	1559	1563	rBV	703965	642604	18.52%	2.618%
18	12.845	1824	1829	1833	rBV	2458785	2389506	68.87%	9.734%
19	13.745	1979	1982	1989	rVB	83437	93074	2.68%	0.379%
20	13.892	2003	2007	2011	rBV	652121	580180	16.72%	2.363%
21	15.310	2244	2248	2252	rBV	303542	376487	10.85%	1.534%

Sum of corrected areas: 24547847

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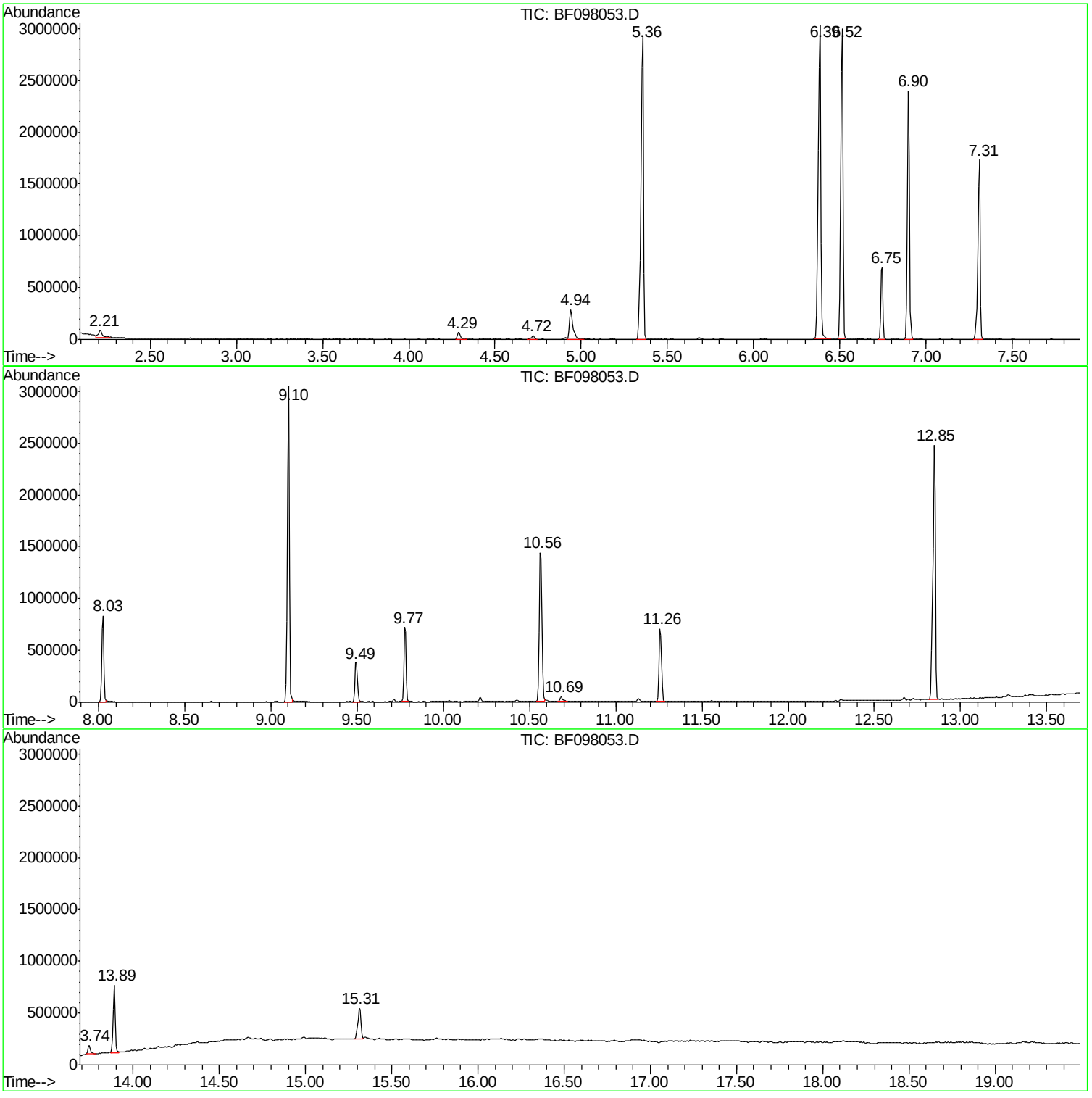
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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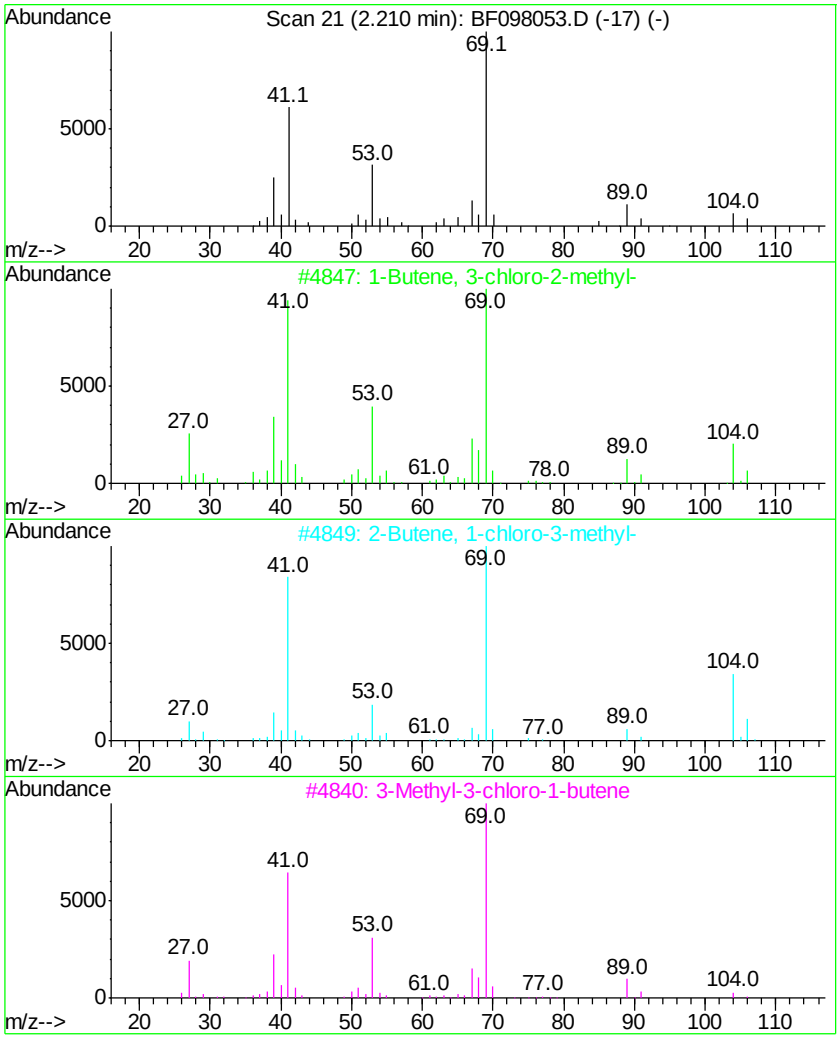
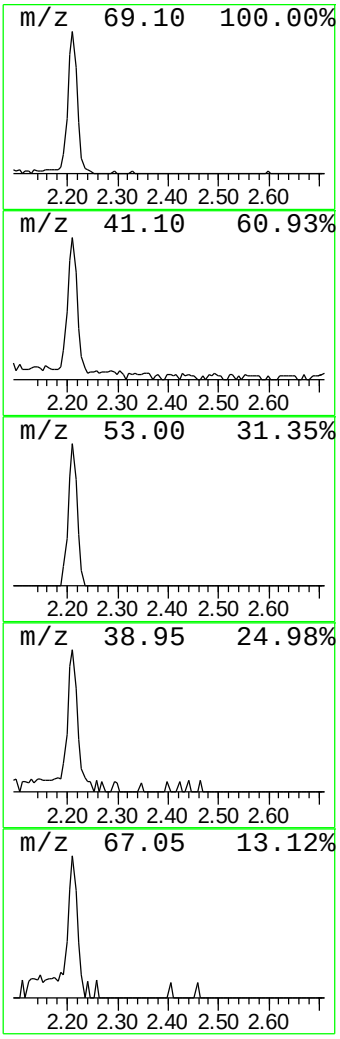
Peak Number 1 1-Butene, 3-chloro-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	3.09 ng	96919	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 3-chloro-2-methyl-	104	C5H9Cl	005166-35-8	72
2	2-Butene, 1-chloro-3-methyl-	104	C5H9Cl	000503-60-6	59
3	3-Methyl-3-chloro-1-butene	104	C5H9Cl	002190-48-9	50
4	Pentane, 2,4-dichloro-	140	C5H10Cl2	000625-67-2	36
5	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	36





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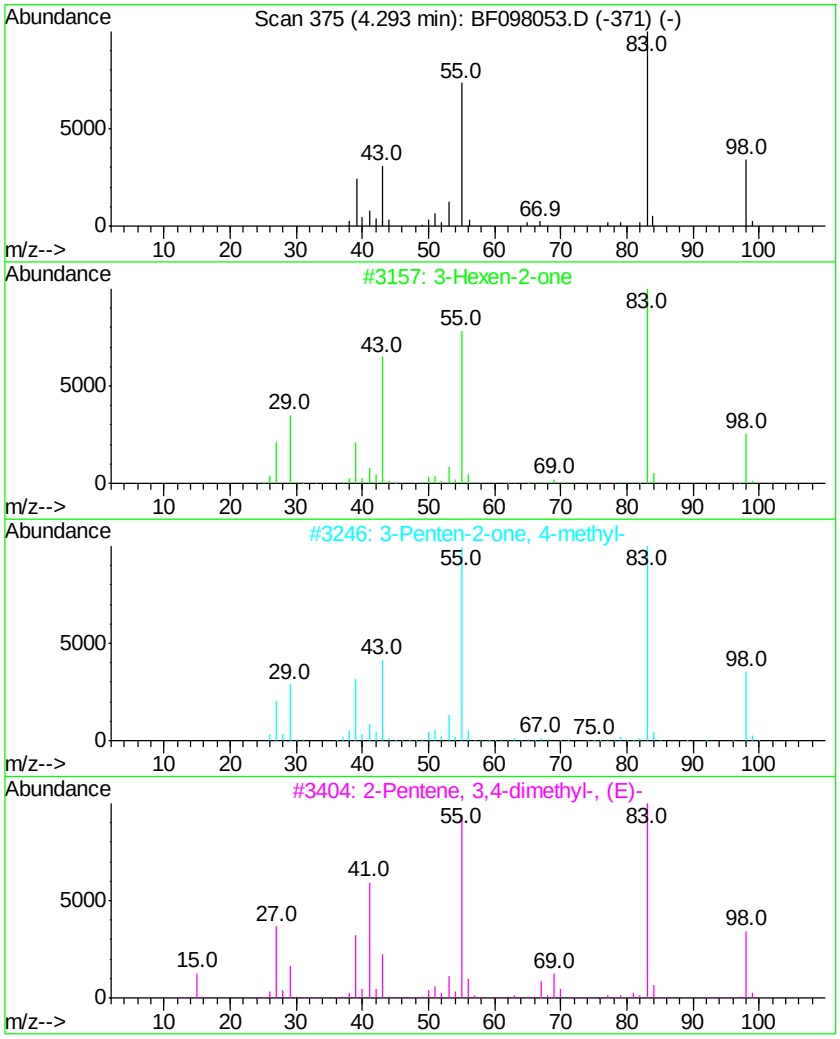
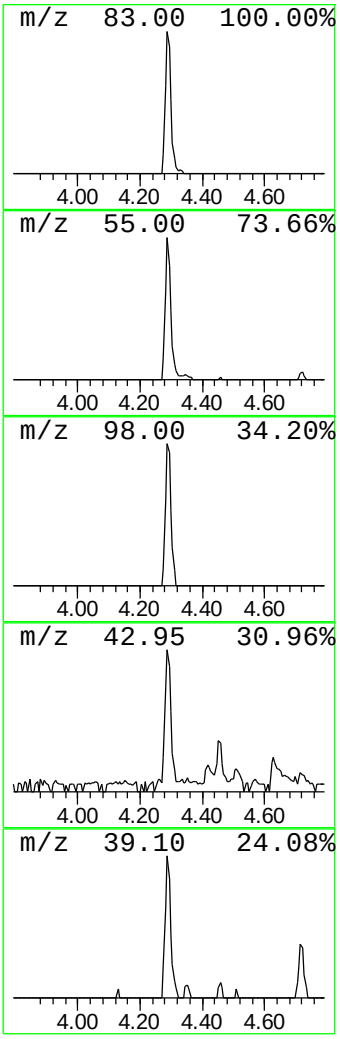
Peak Number 2 3-Hexen-2-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	2.57 ng	80501	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





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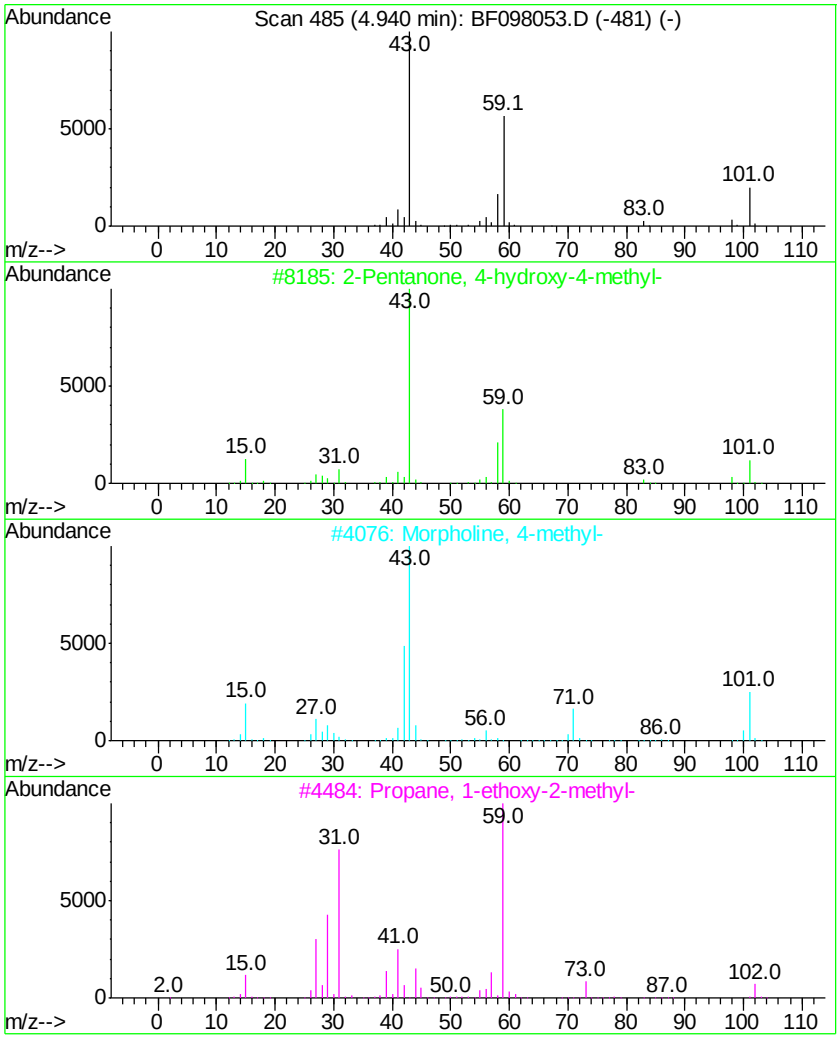
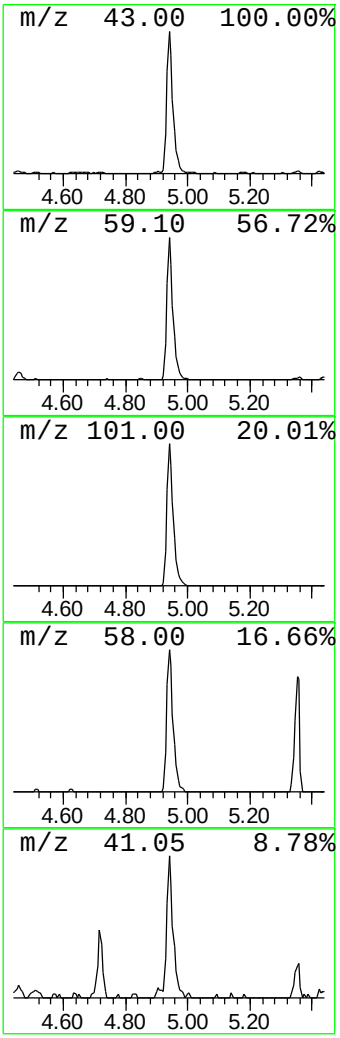
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	12.86 ng	402720	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





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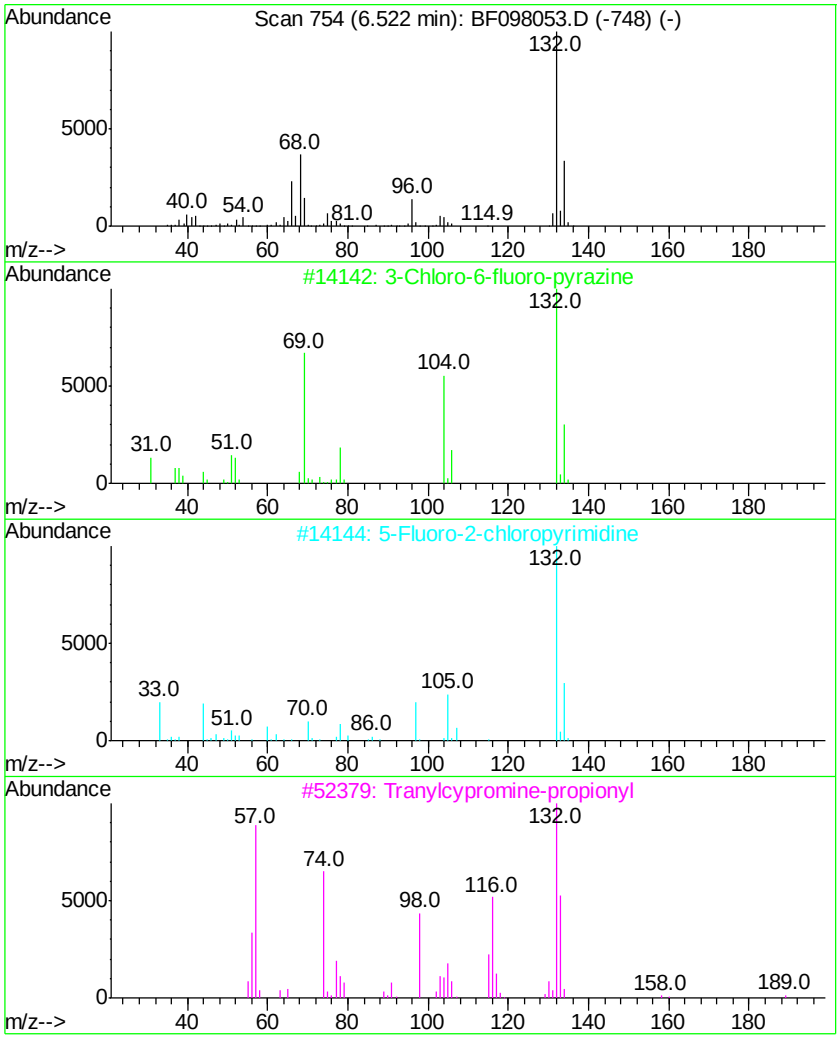
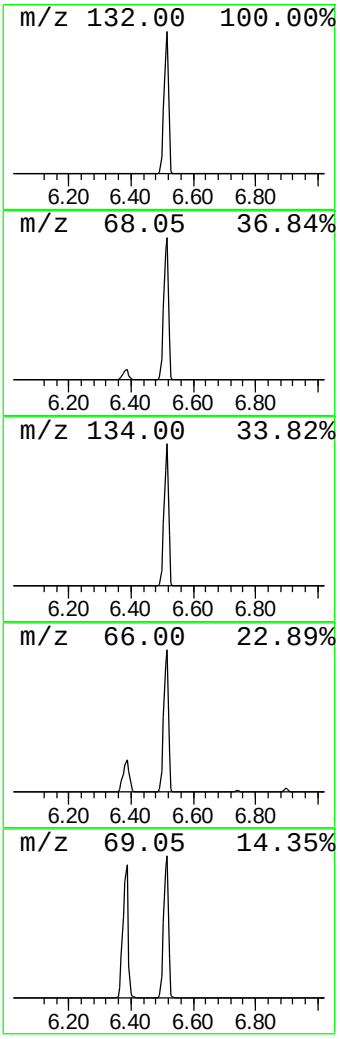
Peak Number 4 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	94.94 ng	2974130	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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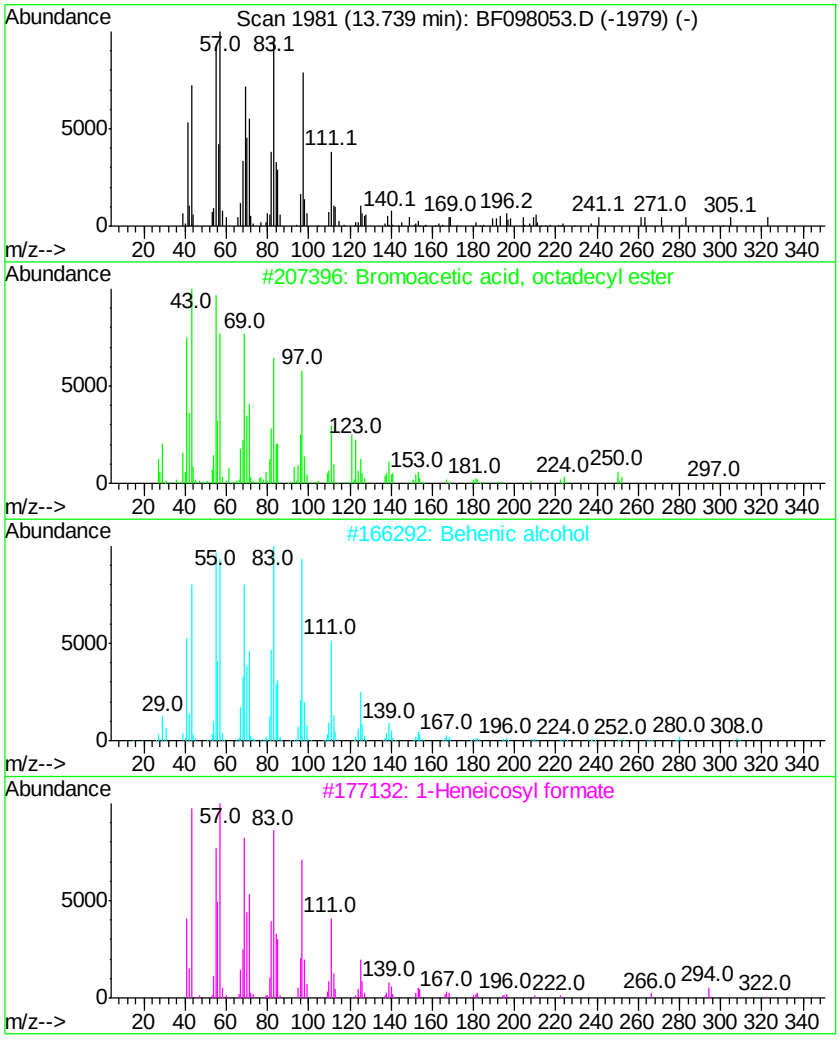
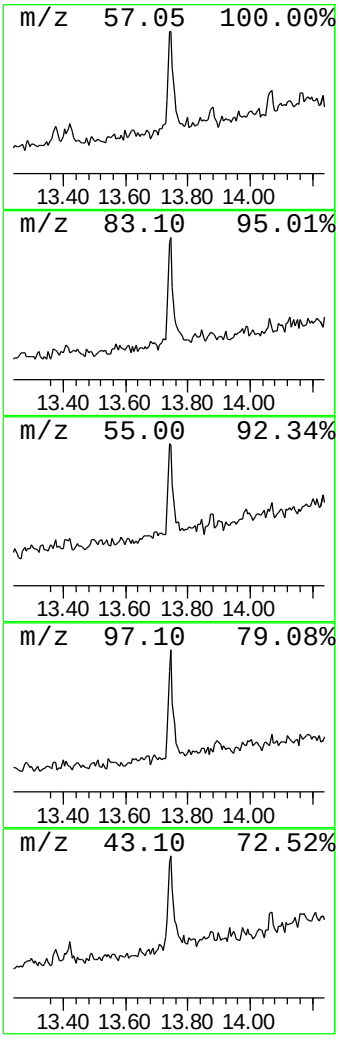
Peak Number 6 Bromoacetic acid, octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.21 ng	93074	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	Behenic alcohol	326	C22H46O	000661-19-8	90
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	81
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	74





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Butene, 3-chlor...	2.21	3.1	ng	96919	1	6.75	626539	20.0
3-Hexen-2-one	4.29	2.6	ng	80501	1	6.75	626539	20.0
2-Pentanone, 4-hy...	4.94	12.9	ng	402720	1	6.75	626539	20.0
unknown6.52	6.52	94.9	ng	2974130	1	6.75	626539	20.0
Bromoacetic acid,...	13.74	3.2	ng	93074	5	13.89	580180	20.0