LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032817\
Data File : BF094012.D
Acq On : 29 Mar 2017 00:16
Operator : SJ/MA
Sample : I2422-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HHD-S1

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-BF032217.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	2.481	97	101	106	rVB	91572	92421	1.72%	0.228%
2	3.551	279	283	289	rBV	200916	225327	4.19%	0.555%
3	3.710	306	310	313	rBV	58425	59768	1.11%	0.147%
4	4.093	368	375	385	rVB	574191	849274	15.78%	2.092%
5	4.475	434	440	443	rBV	3627399	4132892	76.77%	10.182%
6	5.534	614	620	623	rBV	3179239	4116658	76.47%	10.142%
7	5.681	639	645	648	rBV	3731012	4449186	82.65%	10.961%
8	5.928	683	687	691	rBV	1050636	905561	16.82%	2.231%
9	6.110	713	718	721	rBV	3460309	3586533	66.62%	8.836%
10	6.404	765	768	778	rVB	56520	61820	1.15%	0.152%
11	6.581	792	798	801	rVB	2416310	2949266	54.78%	7.266%
12	7.428	937	942	945	rBV	1258961	1249108	23.20%	3.077%
13	7.451	945	946	949	rVB	136952	95883	1.78%	0.236%
14	7.763	992	999	1009	rBV	89828	129567	2.41%	0.319%
15	8.410	1102	1109	1117	rBV2	64165	84216	1.56%	0.207%
16	8.757	1161	1168	1171	rBV	4360082	5383489	100.00%	13.263%
17	9.569	1297	1306	1310	rBV2	1302323	1351148	25.10%	3.329%
18	10.545	1465	1472	1475	rBV	2456841	3051328	56.68%	7.517%
19	11.392	1611	1616	1620	rBV	1335875	1324639	24.61%	3.263%
20	13.380	1947	1954	1957	rBV	3713960	4739251	88.03%	11.676%
21	14.645	2164	2169	2174	rBV	895324	992868	18.44%	2.446%
22	16.274	2441	2446	2457	rBV	622412	761098	14.14%	1.875%

Sum of corrected areas: 40591301

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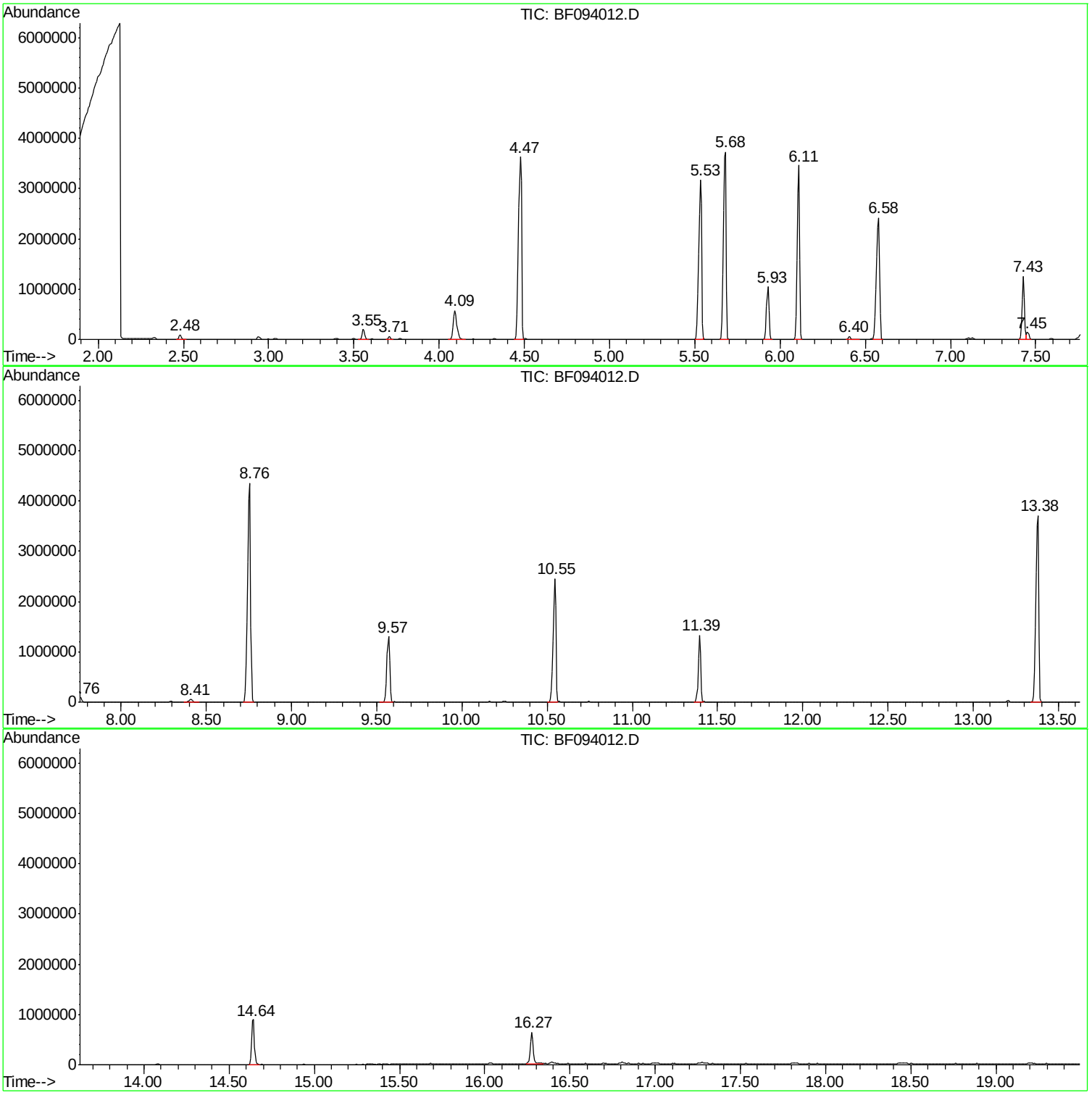
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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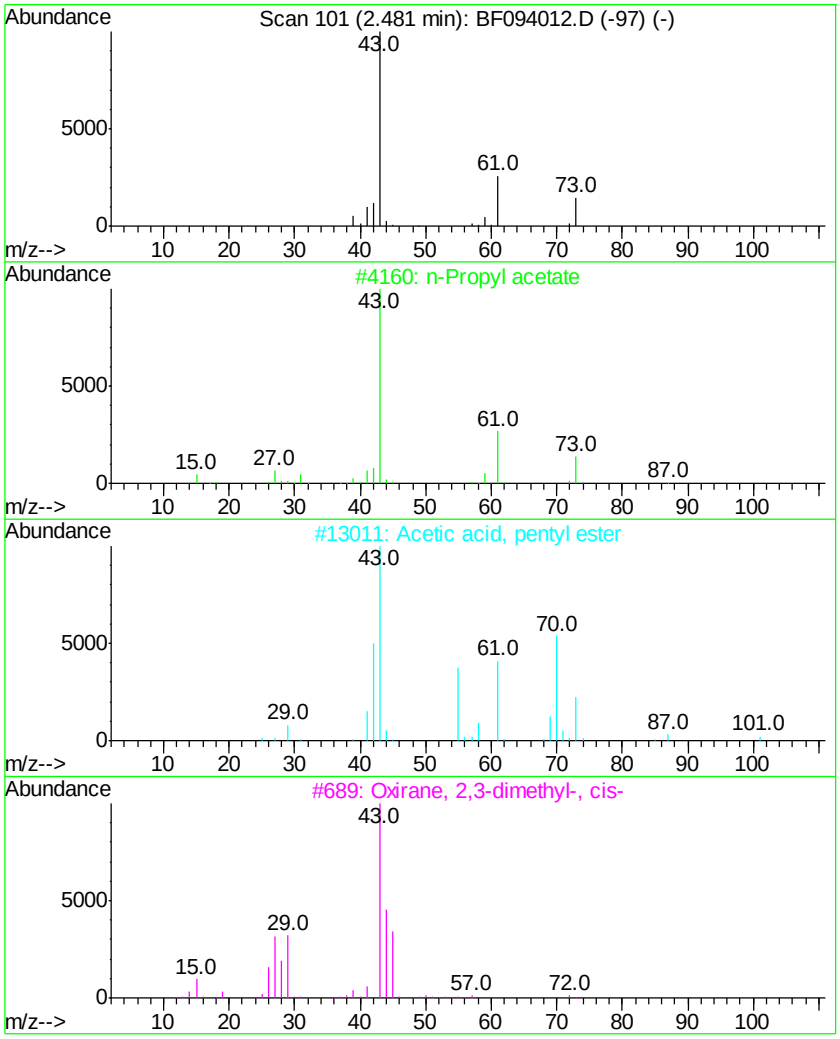
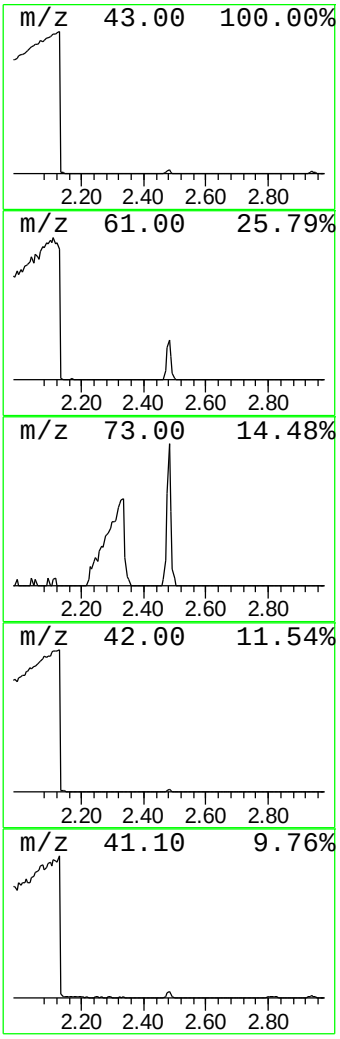
Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.48	2.04 ng	92421	1,4-Dichlorobenzene-d4	5.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
3	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	7





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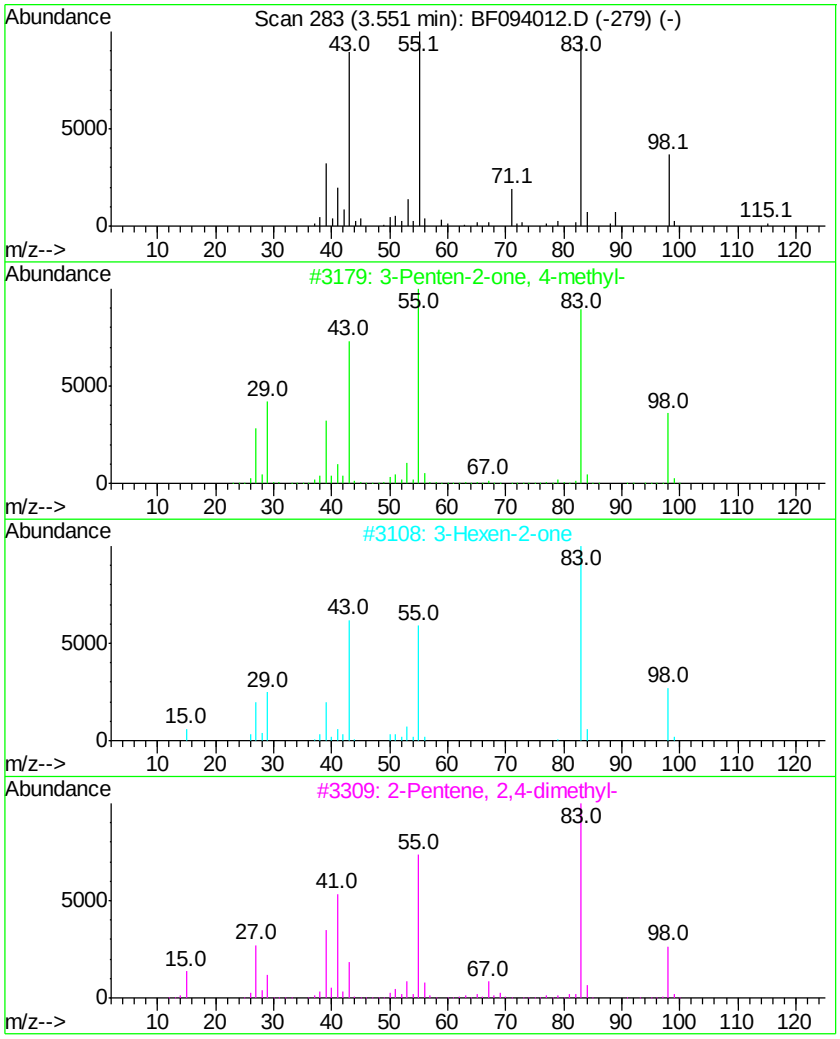
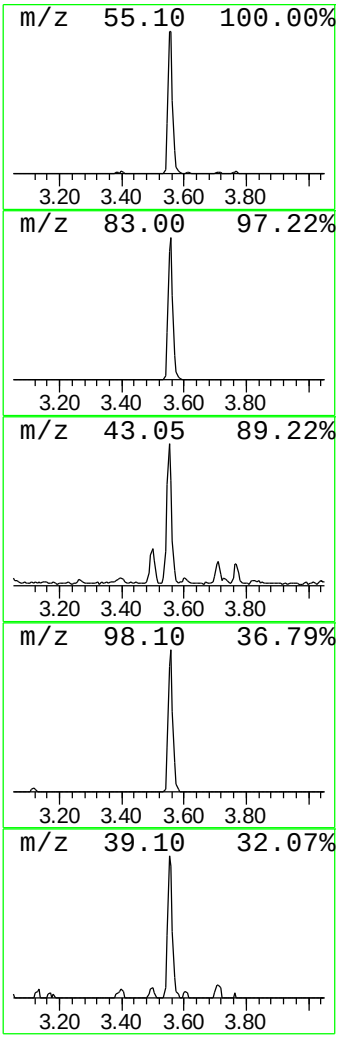
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.55	4.98 ng	225327	1,4-Dichlorobenzene-d4	5.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2	3-Hexen-2-one	98	C6H10O	000763-93-9	74
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	64
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	64
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64





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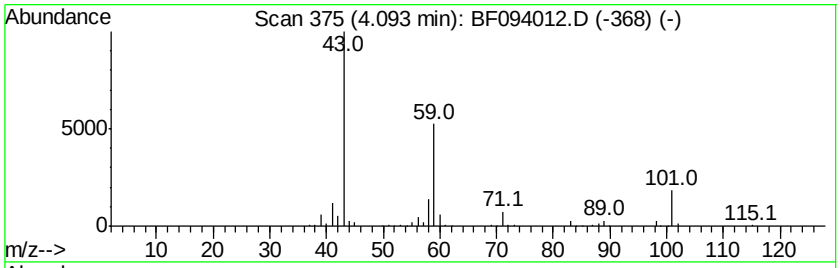
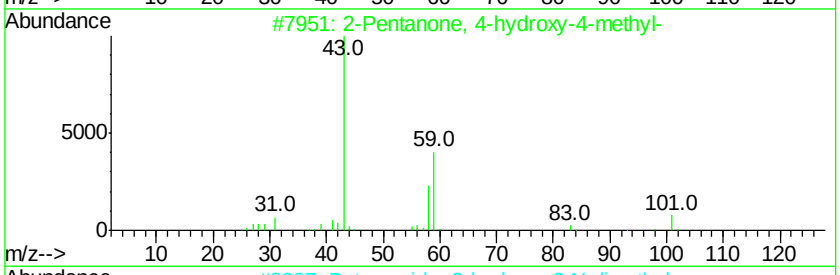
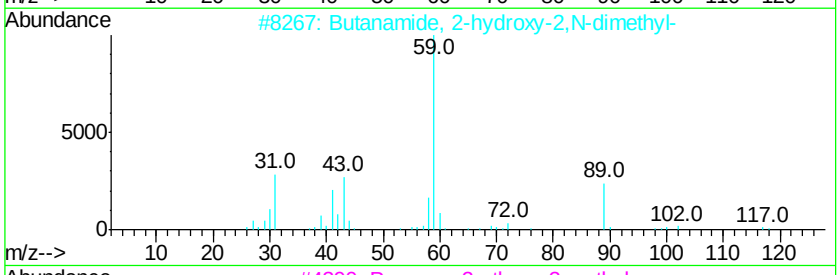
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

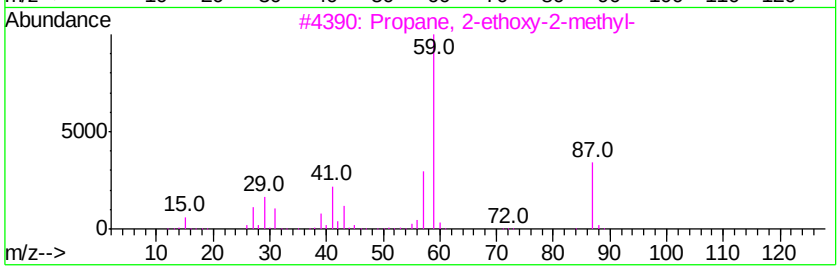
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	18.76 ng	849274	1,4-Dichlorobenzene-d4	5.93

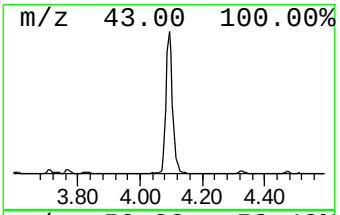
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	23
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
4	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

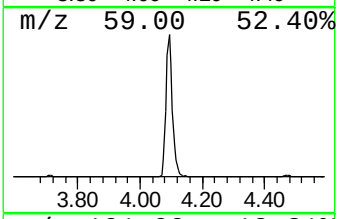


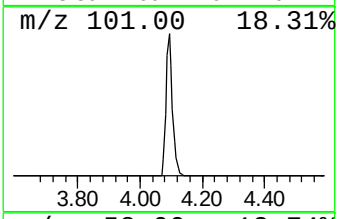


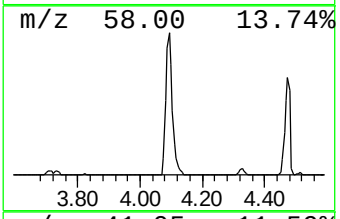


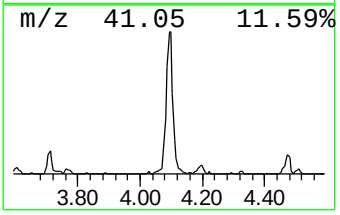












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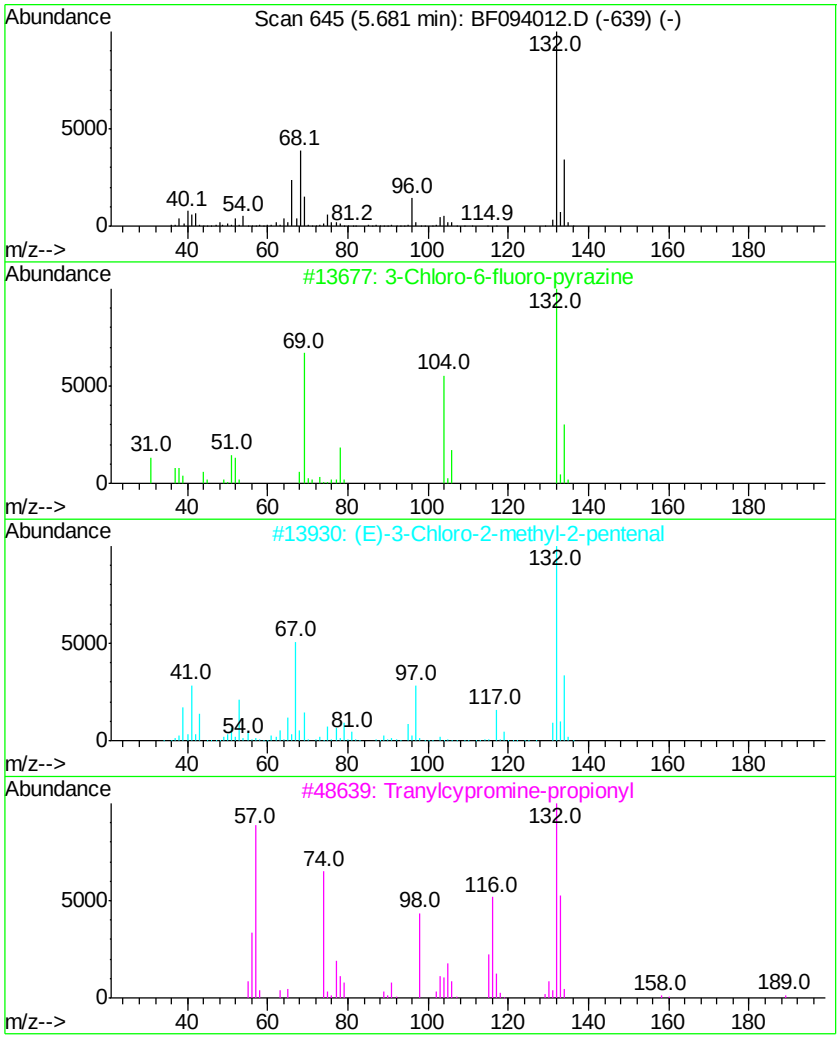
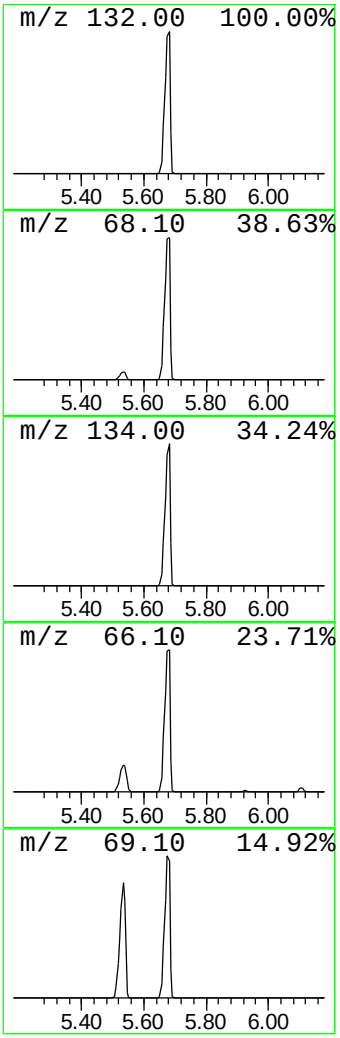
Peak Number 4 unknown5.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	98.26 ng	4449190	1,4-Dichlorobenzene-d4	5.93

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Xenon	132	Xe	007440-63-3	9





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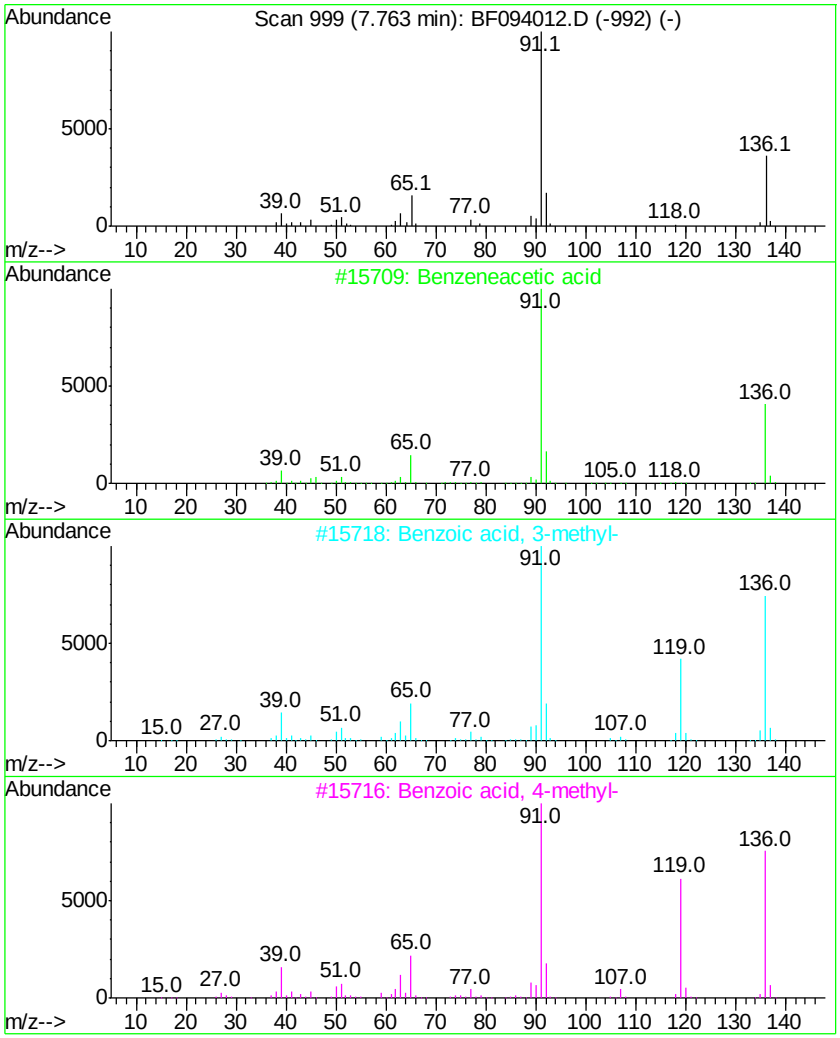
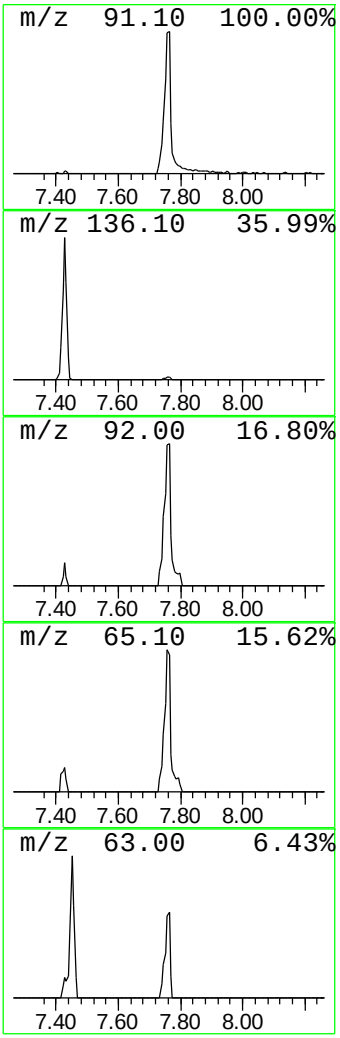
Peak Number 6 Benzeneacetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.76	2.07 ng	129567	Naphthalene-d8	7.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	83
2	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	64
3	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	53
4	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	53
5	3-Oxo-4-phenylbutyronitrile	159	C10H9NO	019212-27-2	50





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.48	2.0	ng	92421	1	5.93	905561	20.0
3-Penten-2-one, 4...	3.55	5.0	ng	225327	1	5.93	905561	20.0
2-Pentanone, 4-hy...	4.09	18.8	ng	849274	1	5.93	905561	20.0
unknown5.68	5.68	98.3	ng	4449190	1	5.93	905561	20.0
Benzeneacetic acid	7.76	2.1	ng	129567	2	7.43	1249110	20.0