

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093631.D
 Acq On : 14 Mar 2017 2:30
 Operator : SJ/MA
 Sample : I2199-23
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-93

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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	2.435	45	48	58	rBV	53745	157189	2.71%	0.326%
2	4.161	196	199	205	rBV	52730	91045	1.57%	0.189%
3	4.401	218	220	229	rVB	42006	103871	1.79%	0.215%
4	4.870	258	261	280	rBV	1125632	2283048	39.42%	4.735%
5	5.316	297	300	333	rBV	3596001	5469796	94.44%	11.345%
6	5.716	333	335	346	rVB	56994	111373	1.92%	0.231%
7	6.367	390	392	400	rBV	3381360	5043604	87.09%	10.461%
8	6.482	400	402	405	rVB	4767345	4853897	83.81%	10.068%
9	6.710	420	422	431	rVB	982052	1070193	18.48%	2.220%
10	6.859	433	435	438	rBV	3788718	3905630	67.44%	8.101%
11	7.282	470	472	487	rBV	2906190	3585145	61.90%	7.436%
12	8.002	532	535	546	rBV	1339990	1455386	25.13%	3.019%
13	9.088	627	630	632	rBV	4058331	5791545	100.00%	12.012%
14	9.762	686	689	691	rBV	1382590	1553094	26.82%	3.221%
15	10.551	756	758	761	rBV2	2098851	3096311	53.46%	6.422%
16	11.248	817	819	824	rBV	1698544	1626827	28.09%	3.374%
17	12.654	940	942	944	rBV	184350	160032	2.76%	0.332%
18	12.836	955	958	961	rBV	4393230	5334549	92.11%	11.065%
19	13.362	1001	1004	1006	rBV	101978	100473	1.73%	0.208%
20	13.899	1049	1051	1062	rBV	1025585	1384053	23.90%	2.871%
21	15.305	1171	1174	1187	rVB	656569	1035797	17.88%	2.148%

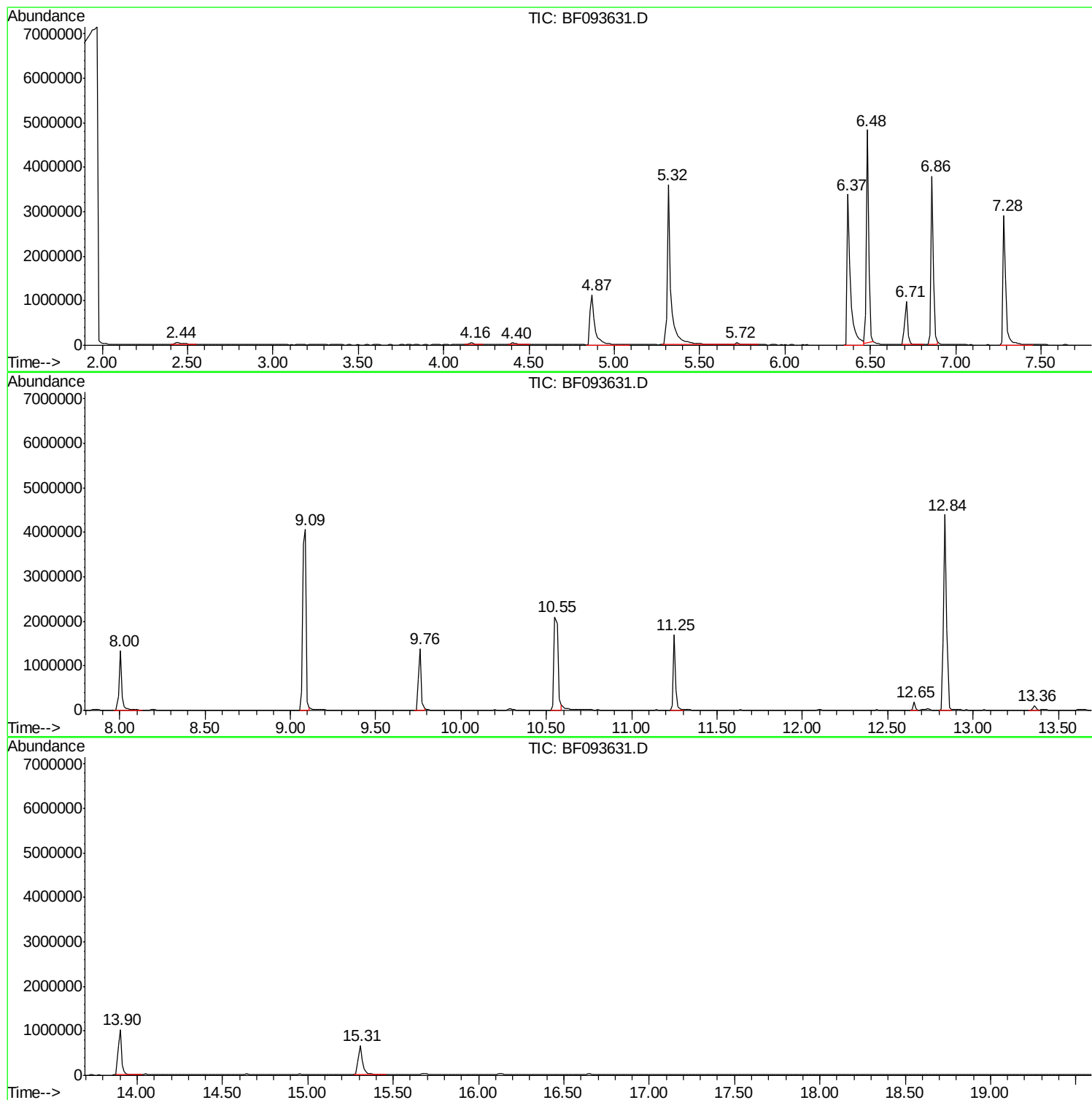
Sum of corrected areas: 48212858

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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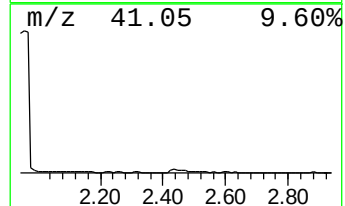
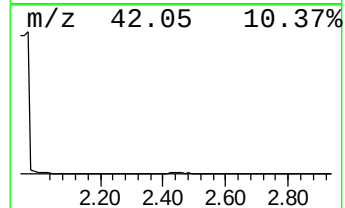
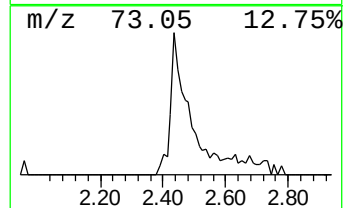
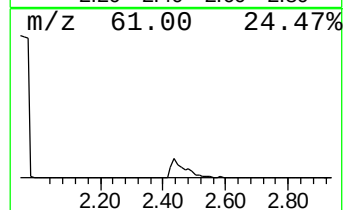
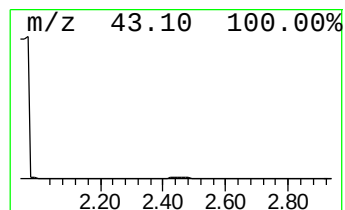
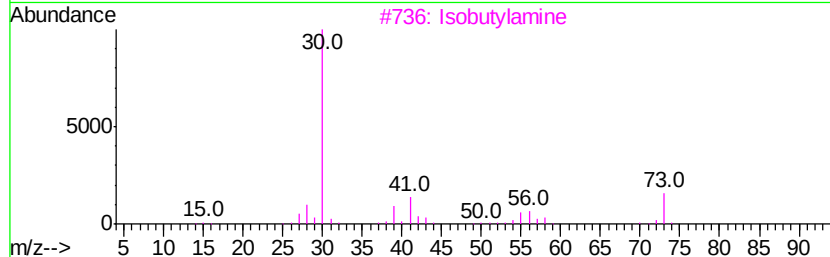
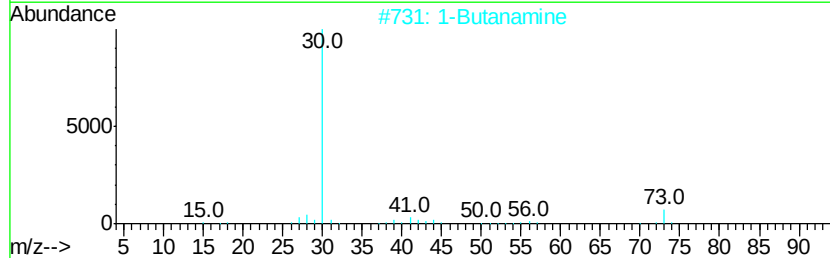
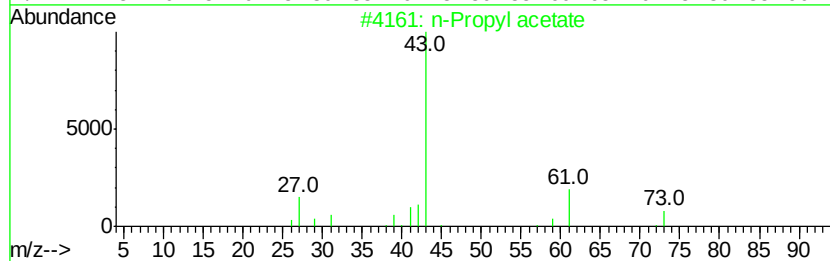
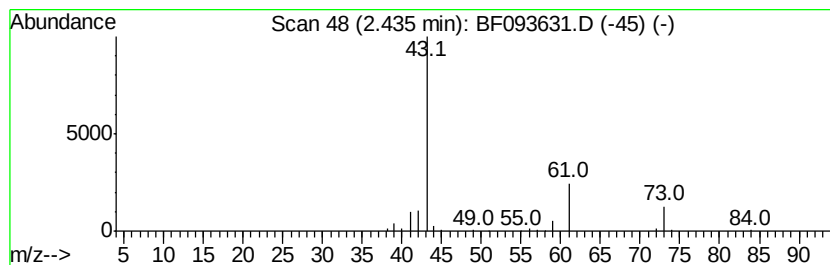
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	2.94 ng	157189	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	72
2		1-Butanamine	73	C4H11N	000109-73-9	9
3		Isobutylamine	73	C4H11N	000078-81-9	7
4		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5
5		Oxazolidine	73	C3H7NO	000504-76-7	4



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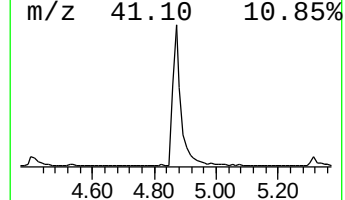
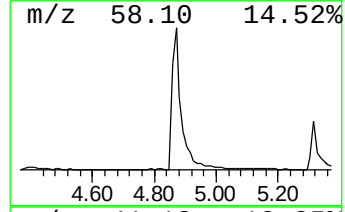
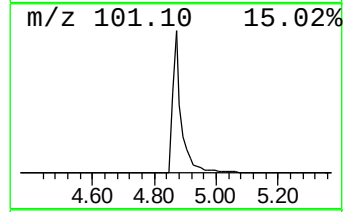
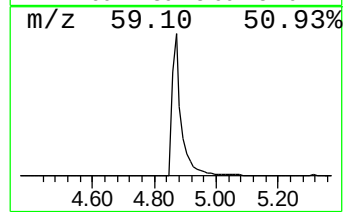
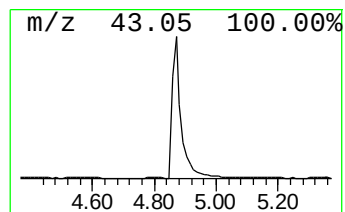
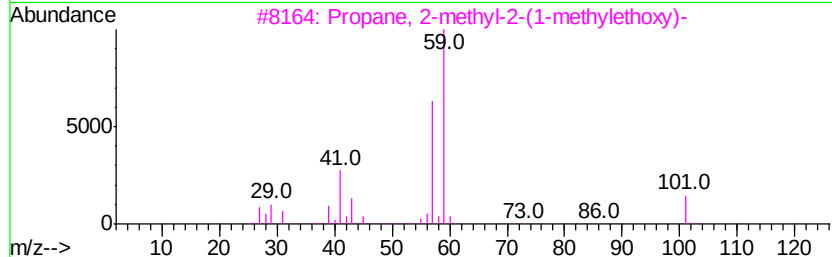
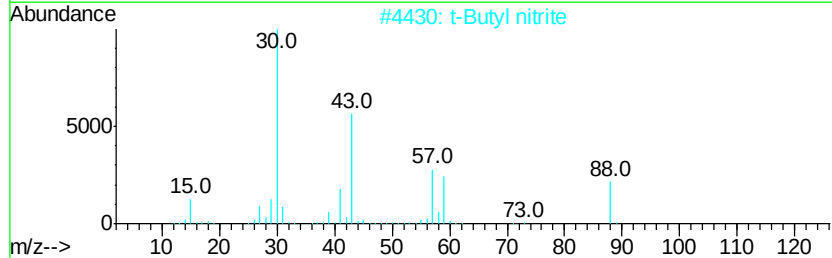
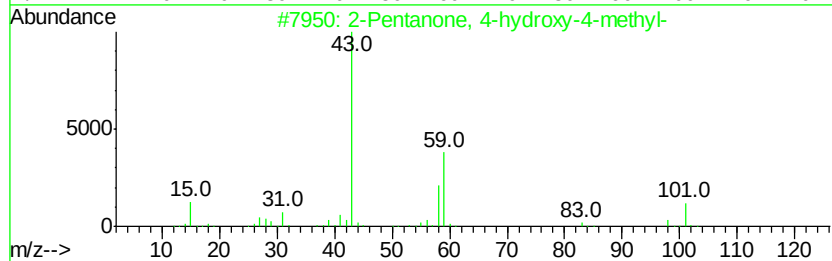
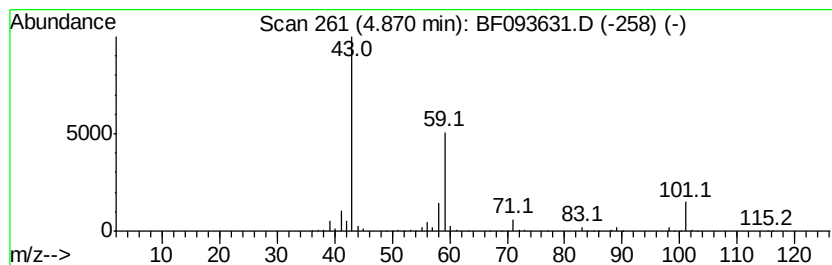
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	42.67 ng	2283050	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
3		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5		1,2-Butanediol, (+/-)-	90	C4H10O2	026171-83-5	25



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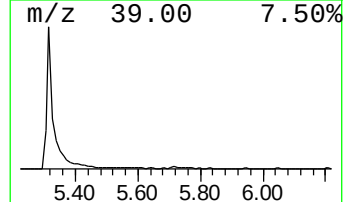
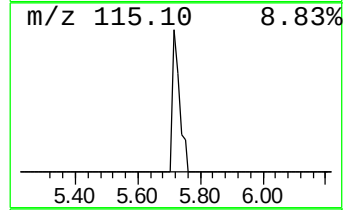
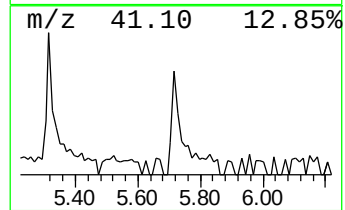
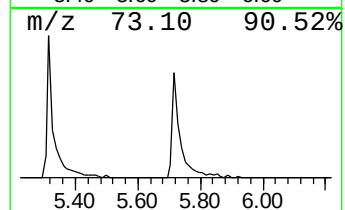
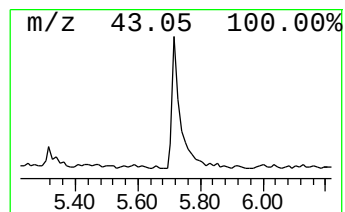
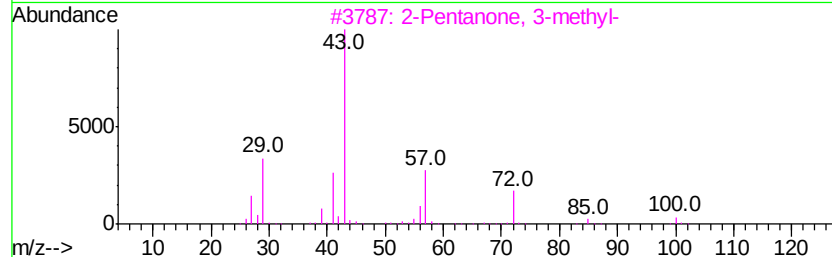
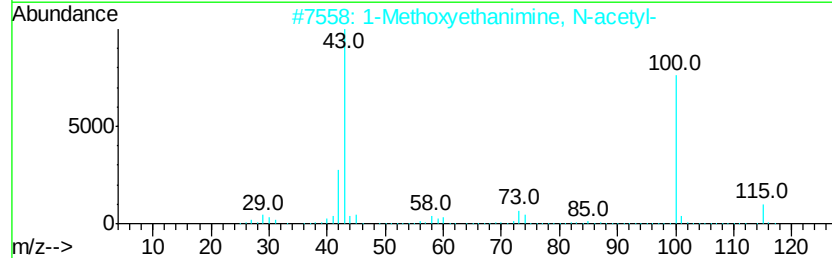
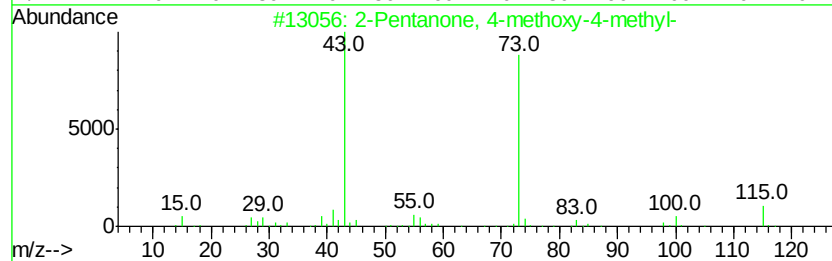
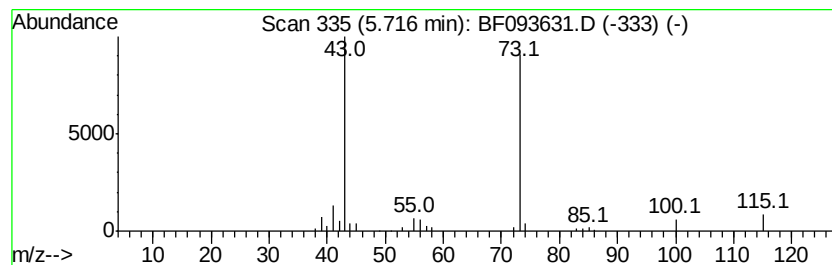
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.08 ng	111373	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	32
3			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	27
4			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
5			2-Heptanone	114	C7H14O	000110-43-0	12



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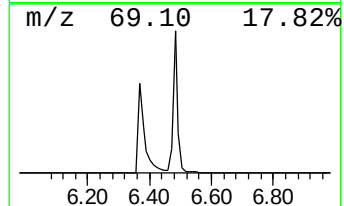
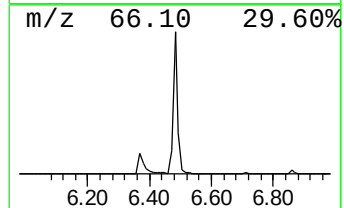
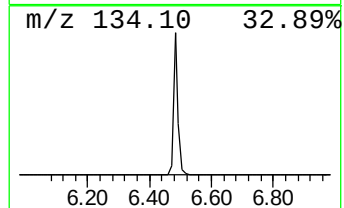
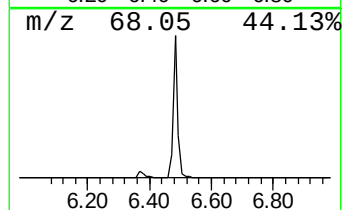
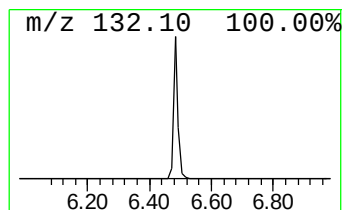
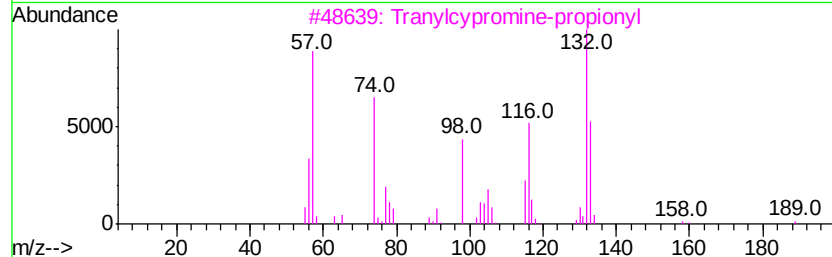
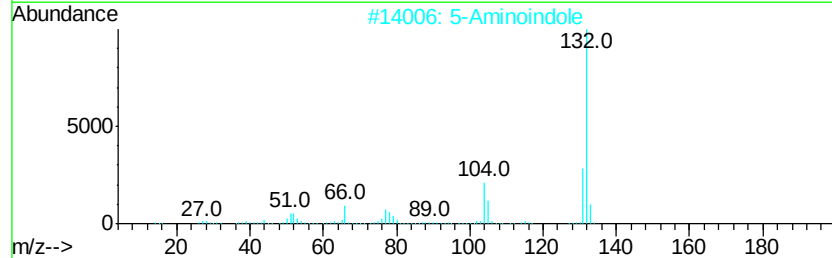
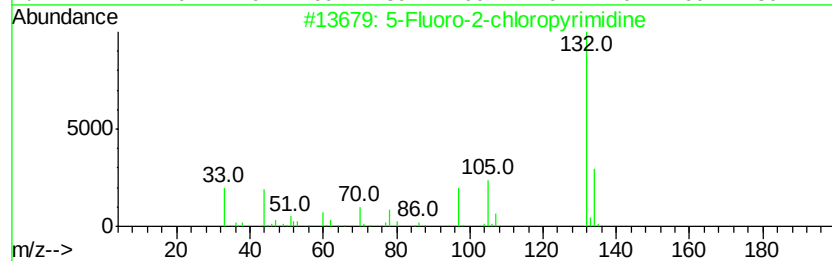
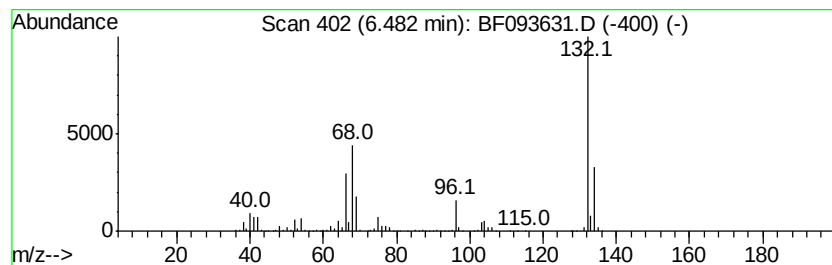
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Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	90.71 ng	4853900	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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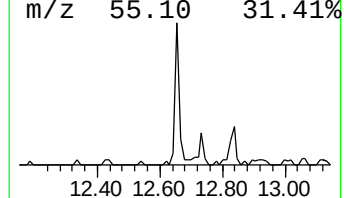
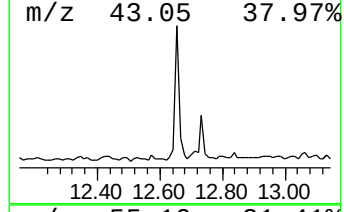
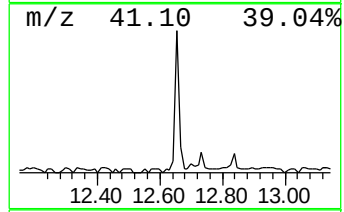
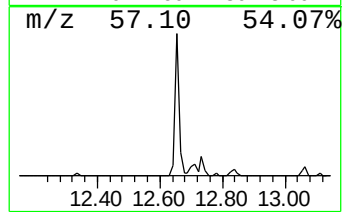
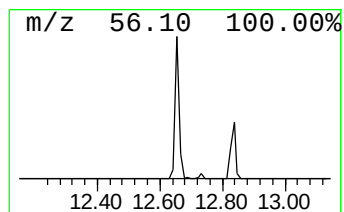
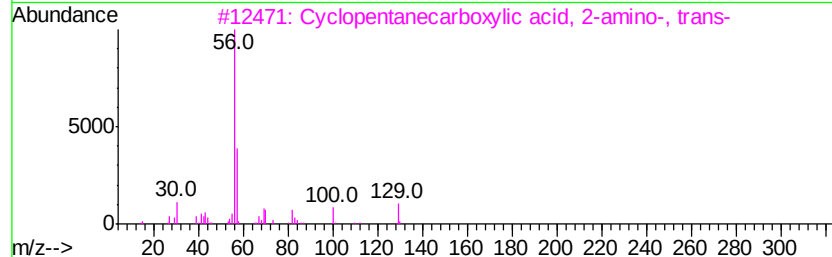
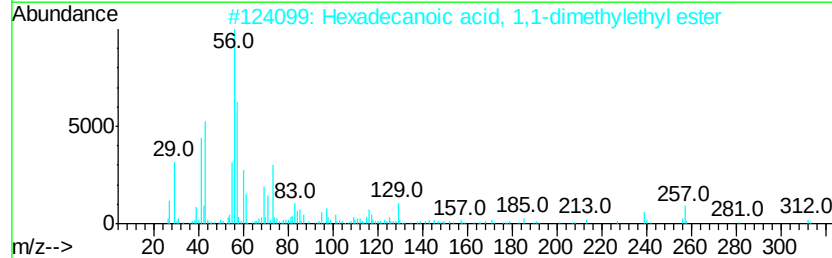
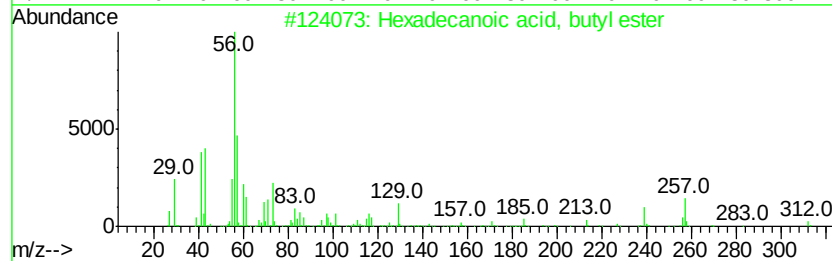
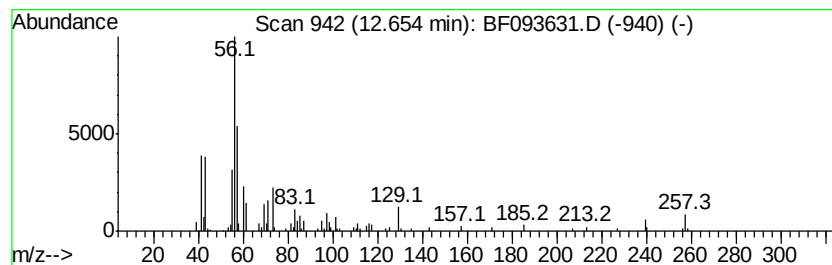
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.65	2.31 ng	160032	Chrysene-d12	13.90		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	43
5		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.44	2.9	ng	157189	1	6.71	1070190	20.0
2-Pentanone, 4-hy...	4.87	42.7	ng	2283050	1	6.71	1070190	20.0
2-Pentanone, 4-me...	5.72	2.1	ng	111373	1	6.71	1070190	20.0
unknown6.48	6.48	90.7	ng	4853900	1	6.71	1070190	20.0
Hexadecanoic acid...	12.65	2.3	ng	160032	5	13.90	1384050	20.0