

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
 Data File : BF093619.D
 Acq On : 13 Mar 2017 20:39
 Operator : SJ/MA
 Sample : I2230-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-1-CHAR

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-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	2.413	44	46	56	rVB	63992	161625	3.11%	0.379%
2	4.150	196	198	207	rVB	76218	122755	2.36%	0.288%
3	4.401	217	220	228	rBV	46510	94464	1.82%	0.222%
4	4.870	259	261	277	rBV	824105	1598045	30.74%	3.749%
5	5.316	297	300	322	rBV	3041776	5033561	96.83%	11.810%
6	5.716	333	335	342	rBV	54480	87182	1.68%	0.205%
7	6.367	390	392	400	rBV	3292397	4552107	87.57%	10.680%
8	6.482	400	402	405	rVB	4659155	4569470	87.90%	10.721%
9	6.710	419	422	431	rVB	968206	1000066	19.24%	2.346%
10	6.859	433	435	438	rBV	3503932	3687910	70.94%	8.653%
11	7.282	470	472	486	rBV	2978564	3417732	65.75%	8.019%
12	8.002	532	535	547	rBV	1233440	1314863	25.29%	3.085%
13	9.076	627	629	632	rBV	3795268	5198365	100.00%	12.197%
14	9.751	686	688	691	rBV	983934	1403020	26.99%	3.292%
15	10.551	756	758	761	rBV	2337829	2759468	53.08%	6.474%
16	11.248	817	819	825	rBV	1444358	1402822	26.99%	3.291%
17	12.837	955	958	960	rBV	4332634	4509837	86.75%	10.581%
18	13.900	1049	1051	1061	rBV	686527	962174	18.51%	2.257%
19	15.305	1171	1174	1187	rVB	488998	745923	14.35%	1.750%

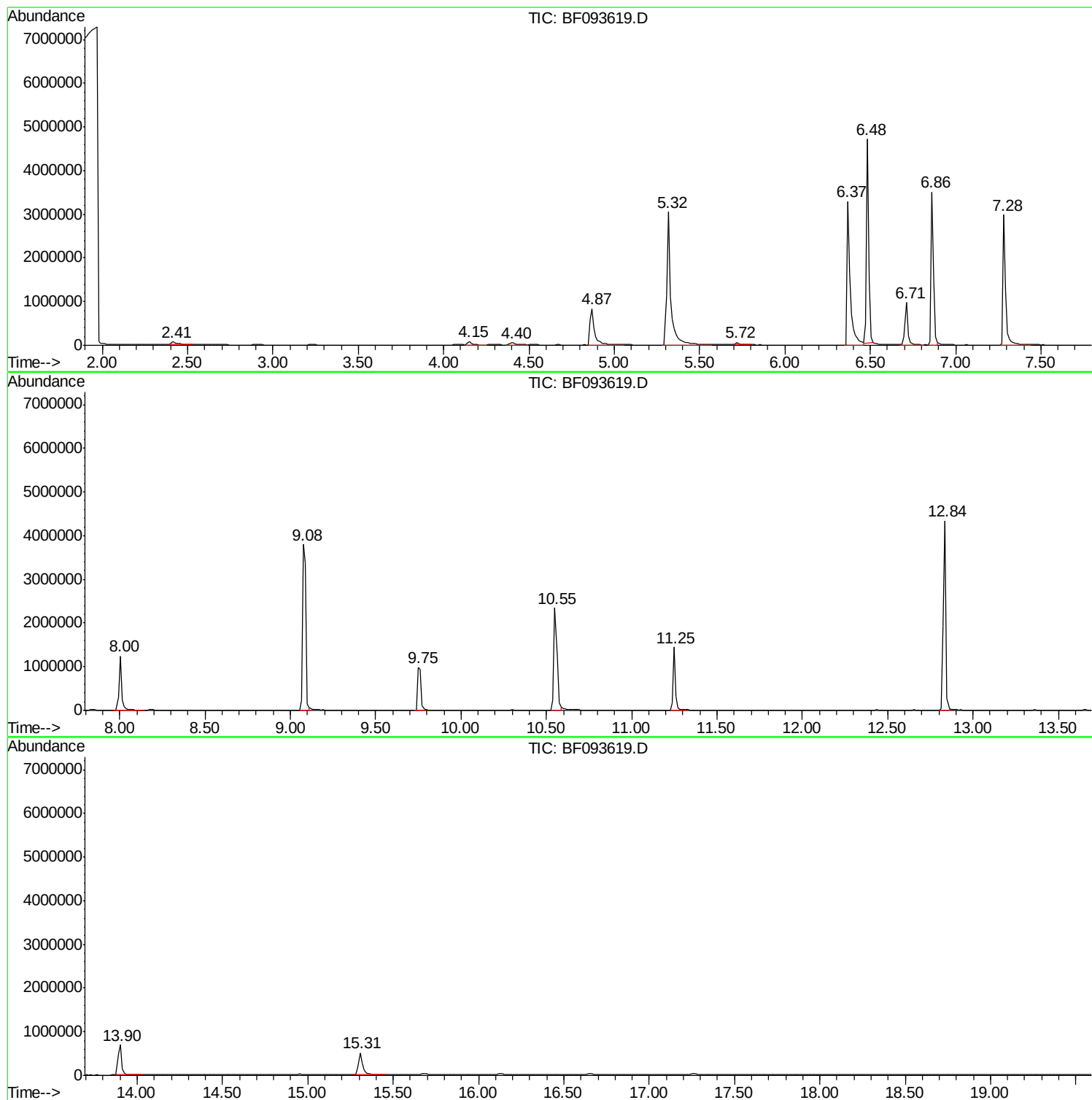
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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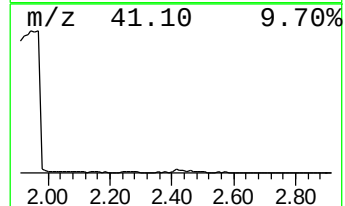
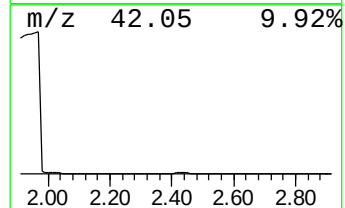
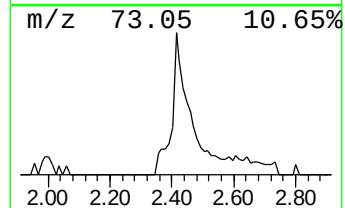
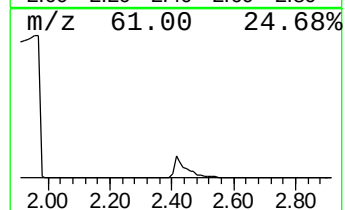
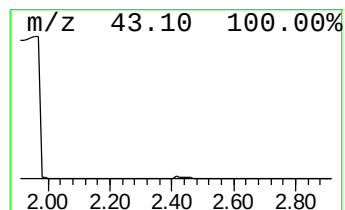
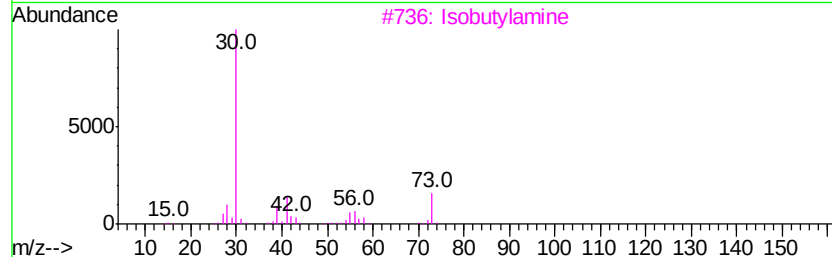
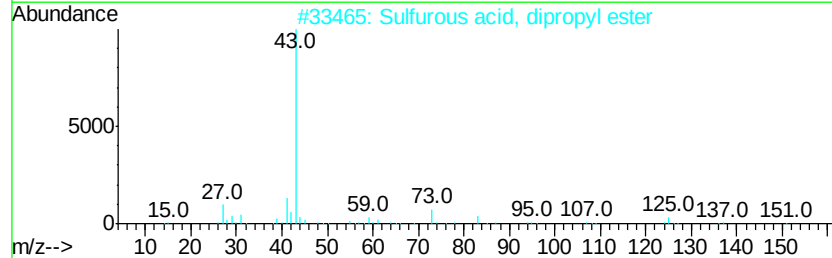
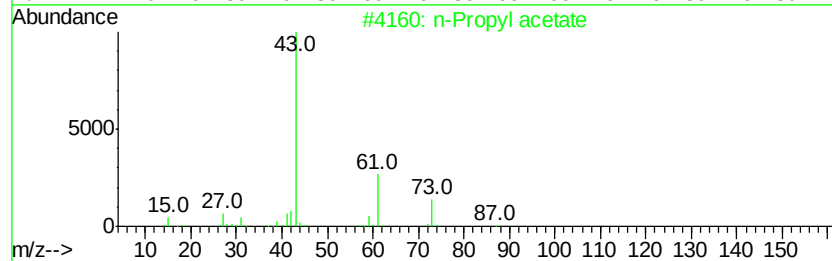
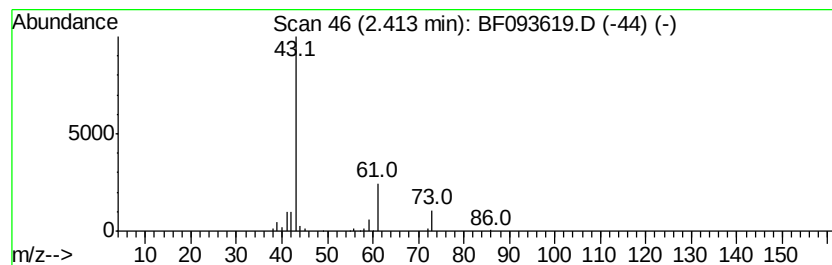
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.41	3.23 ng	161625	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		Sulfurous acid, dipropyl ester	166	C6H14O3S	000623-98-3	9
3		Isobutylamine	73	C4H11N	000078-81-9	7
4		1-Butanamine	73	C4H11N	000109-73-9	5
5		Isobutane	58	C4H10	000075-28-5	4



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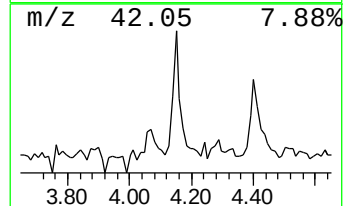
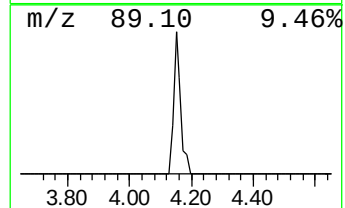
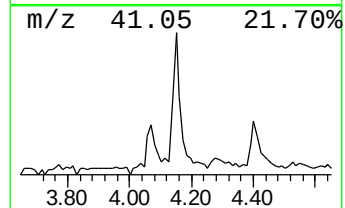
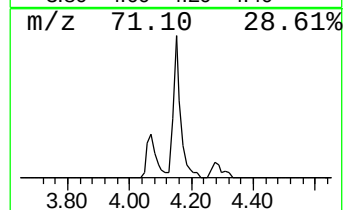
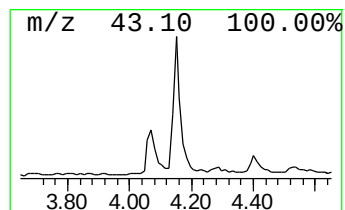
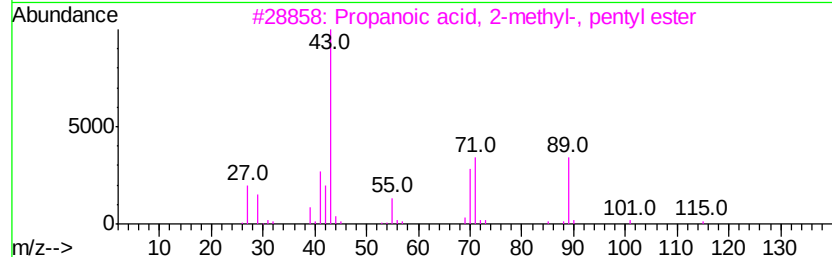
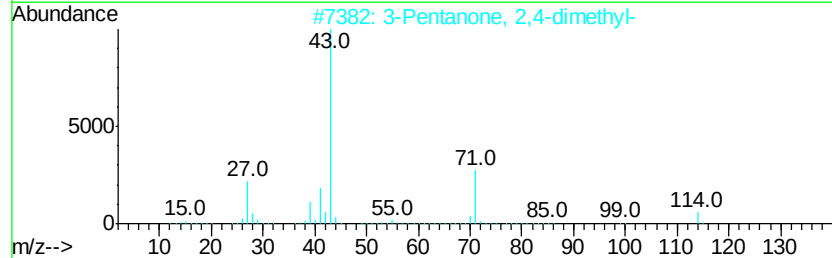
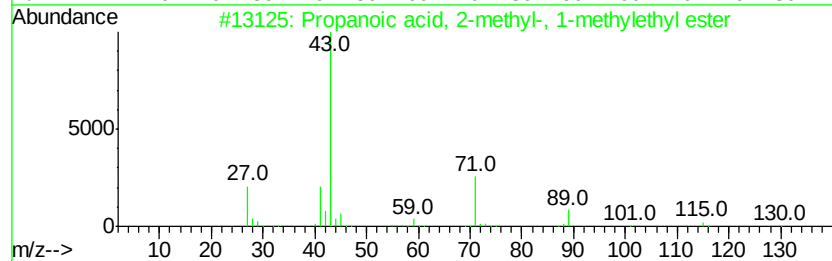
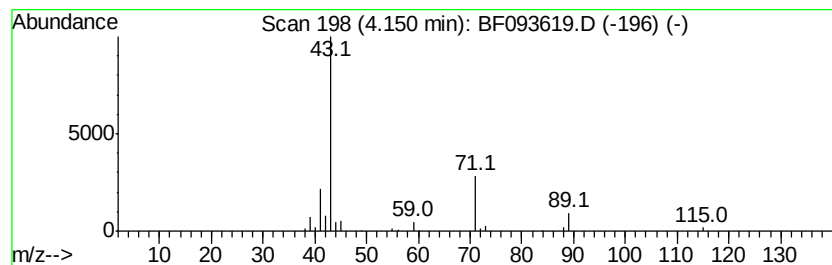
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Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.15	2.45 ng	122755	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2		3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	40
3		Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	38
4		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	33
5		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	33



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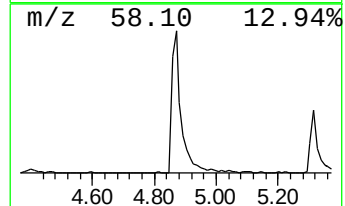
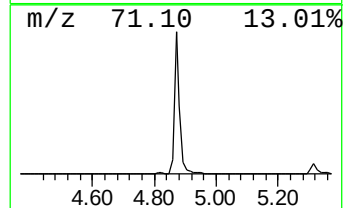
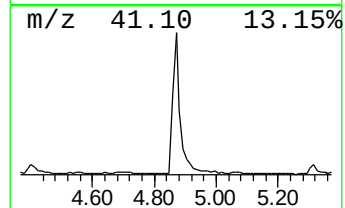
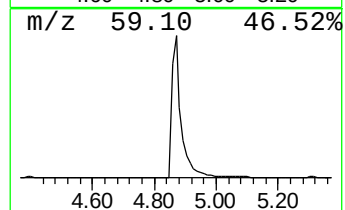
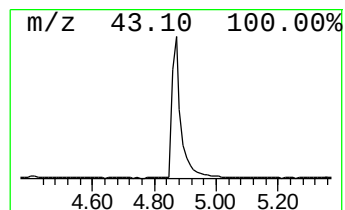
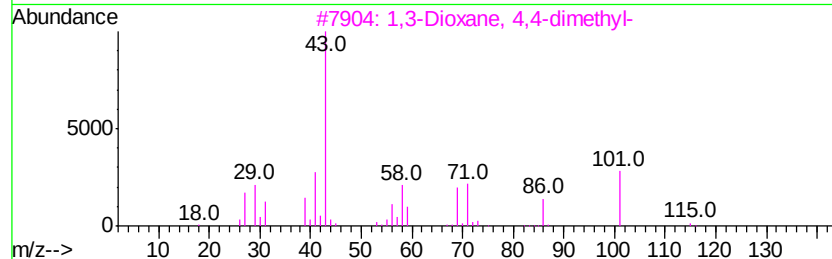
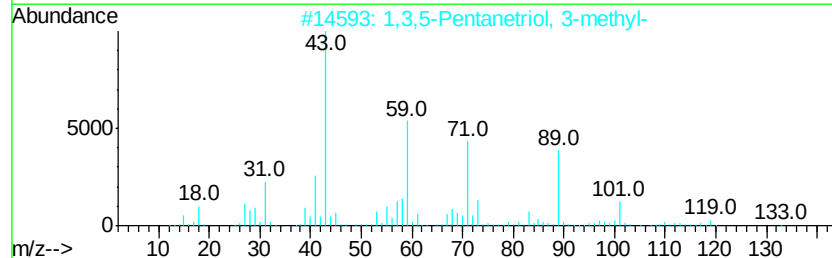
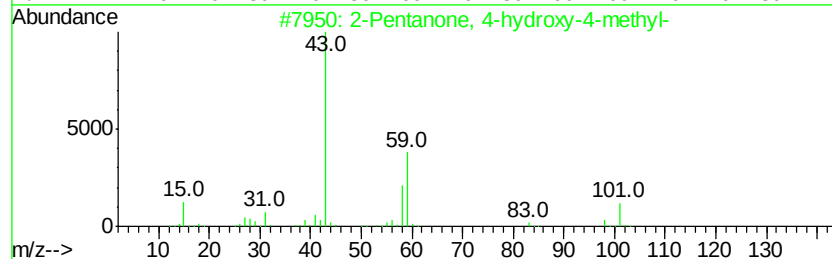
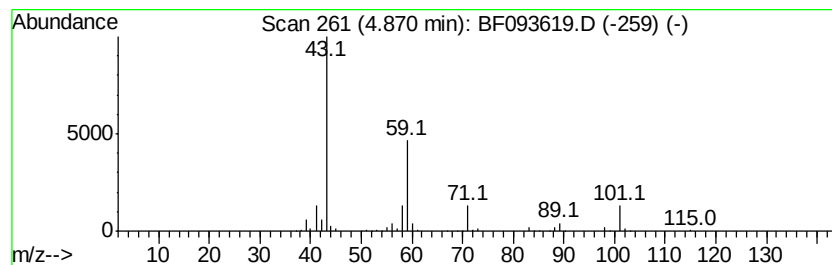
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	31.96 ng	1598050	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	40
2		1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	38
3		1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	10
4		2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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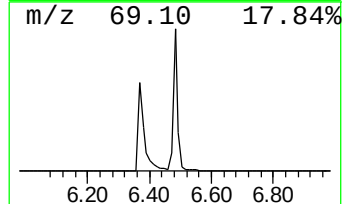
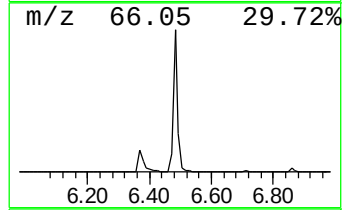
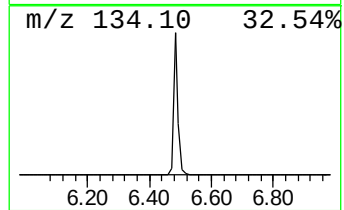
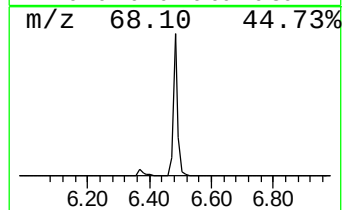
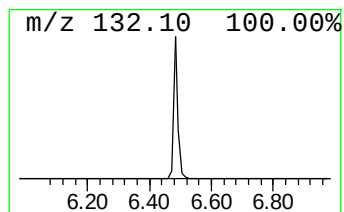
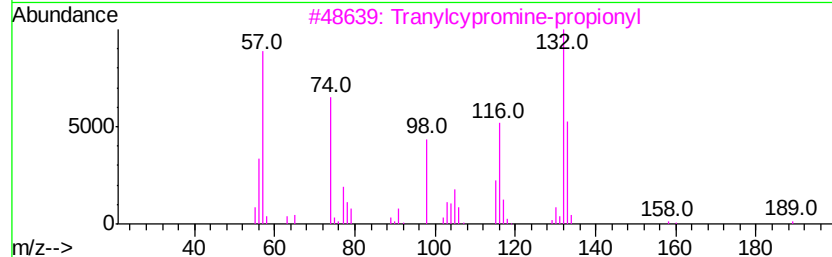
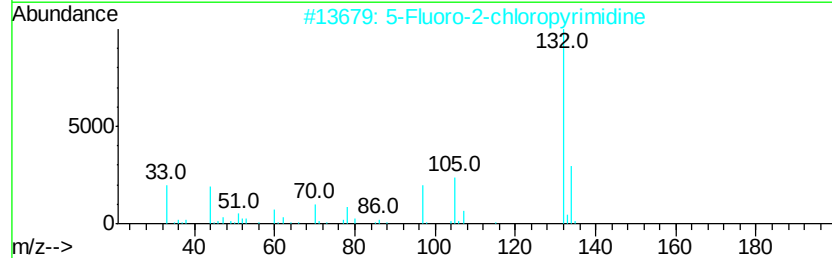
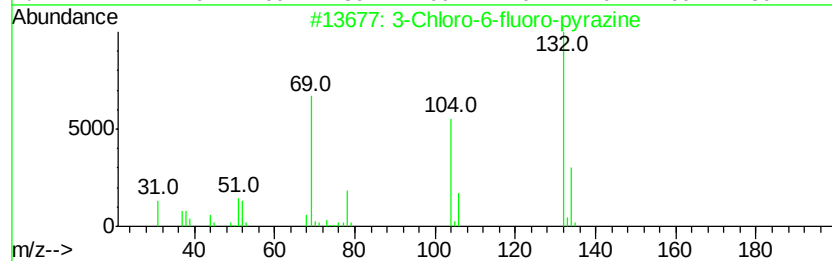
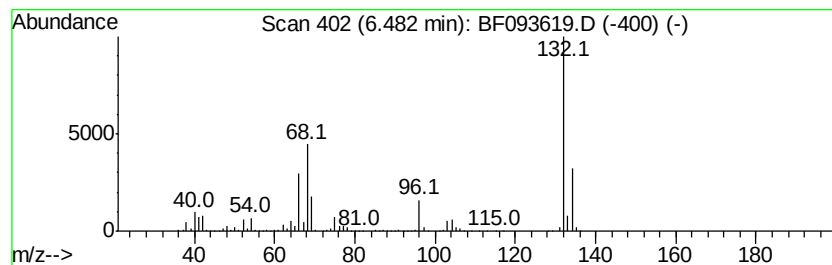
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Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	91.38 ng	4569470	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
3	Tranvlcypropine-propionyl			189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene, ...			132	C10H12	028749-81-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.41	3.2	ng	161625	1	6.71	1000070	20.0
Propanoic acid, 2...	4.15	2.5	ng	122755	1	6.71	1000070	20.0
2-Pentanone, 4-hy...	4.87	32.0	ng	1598050	1	6.71	1000070	20.0
unknown6.48	6.48	91.4	ng	4569470	1	6.71	1000070	20.0