

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093620.D
 Acq On : 13 Mar 2017 21:07
 Operator : SJ/MA
 Sample : I2230-04
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-2-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	2.447	47	49	60	rVB	55899	151371	2.61%	0.313%
2	4.161	196	199	200	rBV	81473	105839	1.83%	0.219%
3	4.184	200	201	217	rVB	247173	613490	10.58%	1.268%
4	4.402	218	220	224	rBV	39418	77819	1.34%	0.161%
5	4.882	260	262	276	rBV	684379	1516285	26.15%	3.134%
6	5.316	298	300	322	rBV	4220852	5795970	99.95%	11.979%
7	5.716	333	335	345	rVB	40495	90891	1.57%	0.188%
8	6.367	390	392	400	rBV	3422489	5322260	91.78%	11.000%
9	6.482	400	402	405	rVB	4928985	5067484	87.39%	10.473%
10	6.710	420	422	430	rVB	962705	1091686	18.83%	2.256%
11	6.859	433	435	438	rBV	3909719	3999950	68.98%	8.267%
12	7.282	470	472	487	rBV	3175371	3718600	64.13%	7.685%
13	8.002	532	535	547	rBV	1209871	1455989	25.11%	3.009%
14	9.076	627	629	632	rBV	4006921	5798933	100.00%	11.985%
15	9.762	686	689	691	rBV	1138584	1549232	26.72%	3.202%
16	10.551	756	758	761	rBV2	2356068	3175711	54.76%	6.563%
17	11.248	816	819	824	rBV	1660309	1584859	27.33%	3.276%
18	12.837	955	958	961	rBV	4553195	5059098	87.24%	10.456%
19	13.900	1049	1051	1060	rVB	957559	1304516	22.50%	2.696%
20	15.305	1171	1174	1187	rVB	608901	905113	15.61%	1.871%

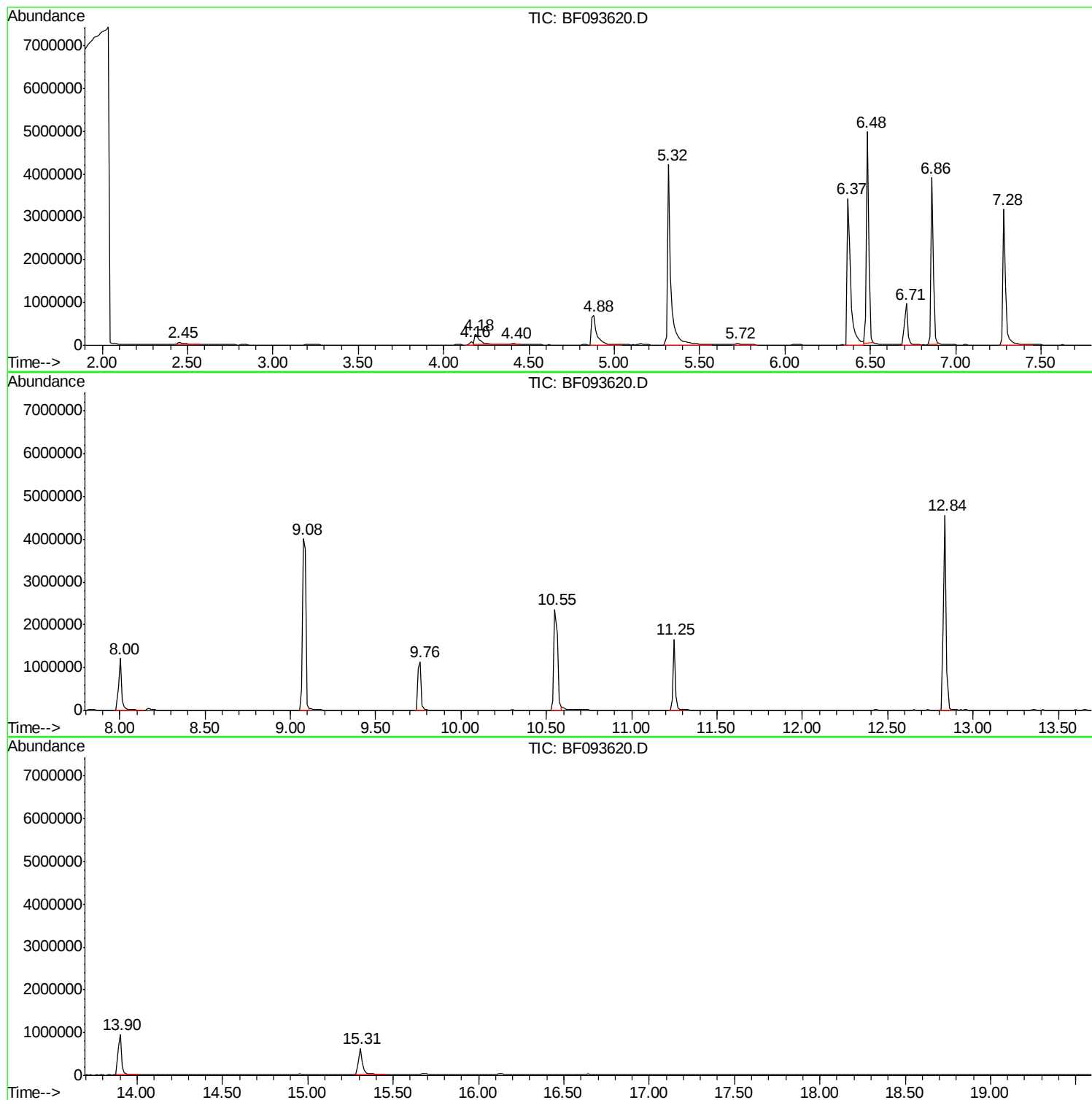
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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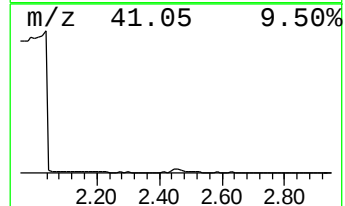
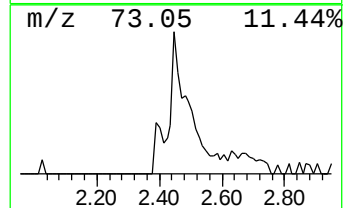
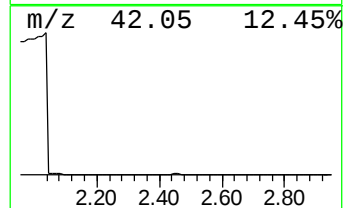
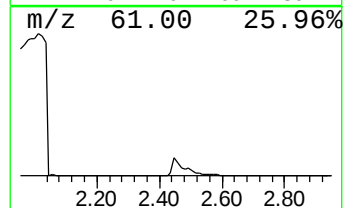
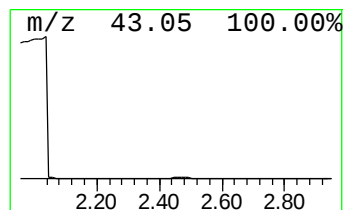
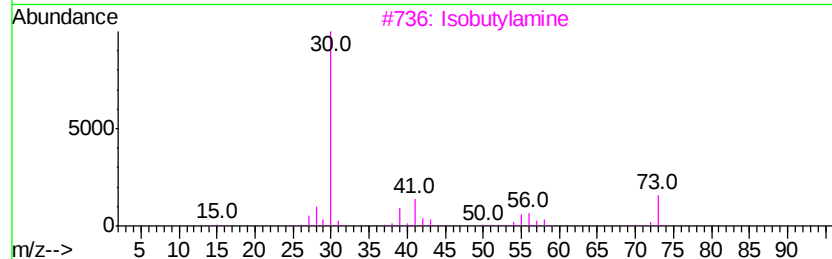
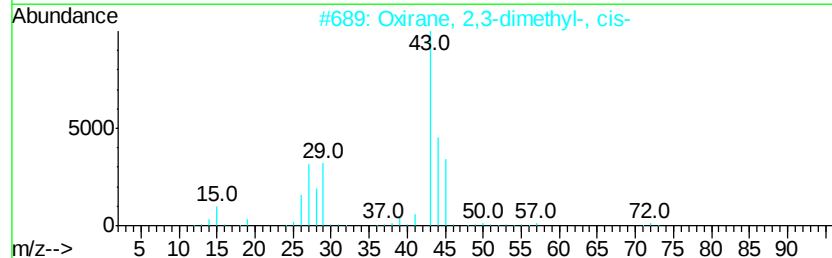
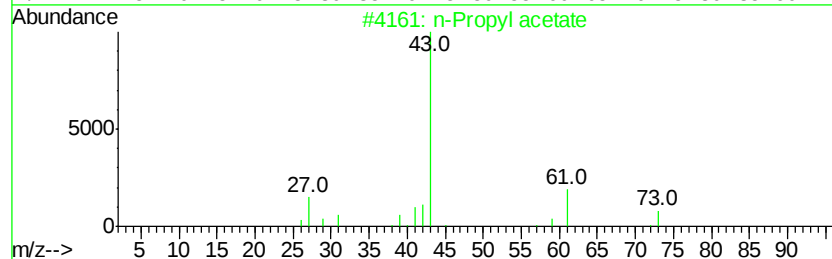
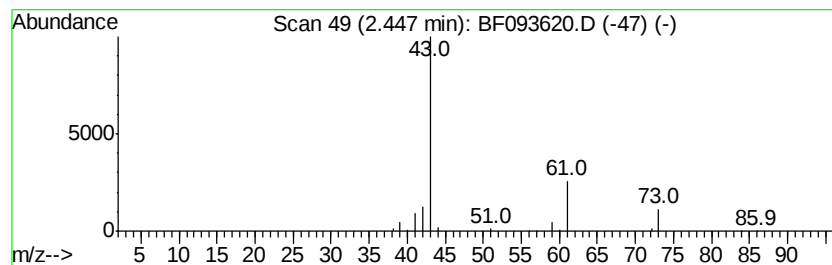
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	2.77 ng	151371	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
3		Isobutylamine	73	C4H11N	000078-81-9	7
4		Butane, 2-methyl-	72	C5H12	000078-78-4	4
5		1-Butanamine	73	C4H11N	000109-73-9	4



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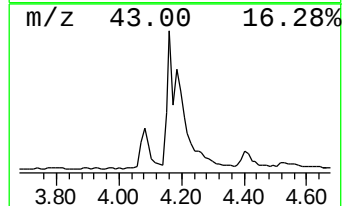
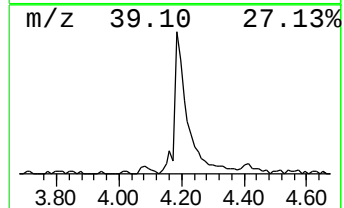
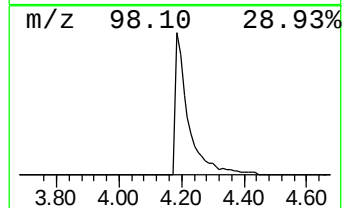
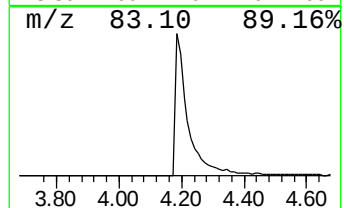
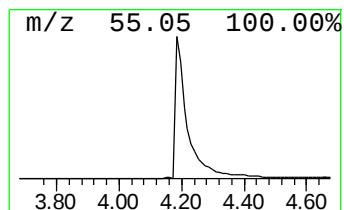
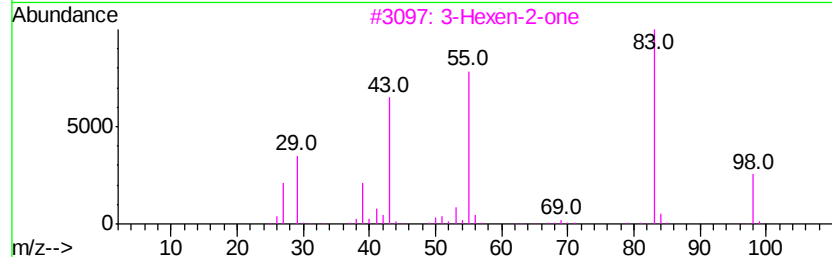
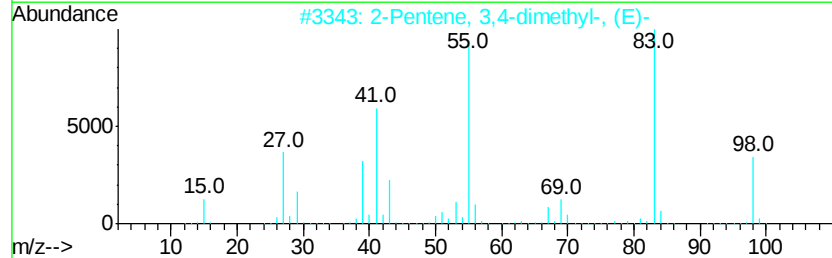
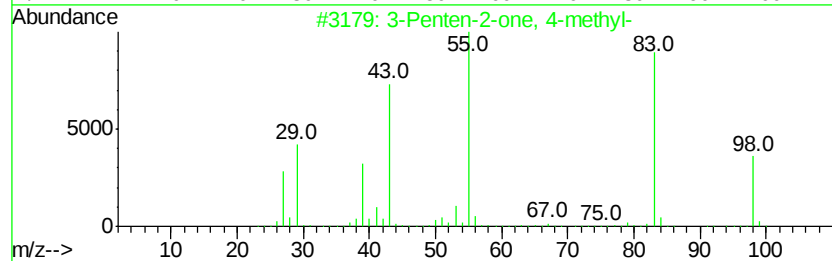
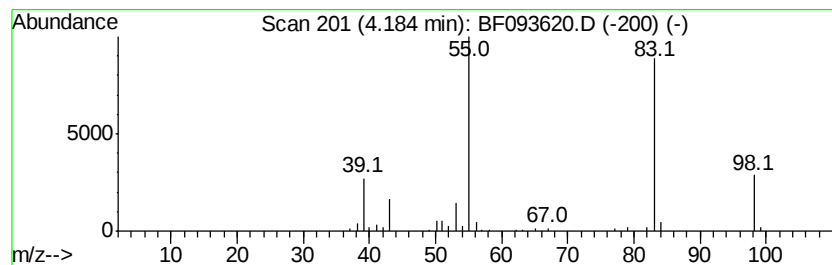
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	11.24 ng	613490	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3		3-Hexen-2-one	98	C6H10O	000763-93-9	90
4		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	78
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78



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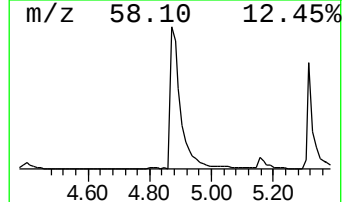
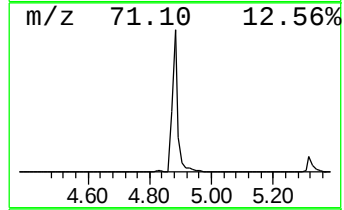
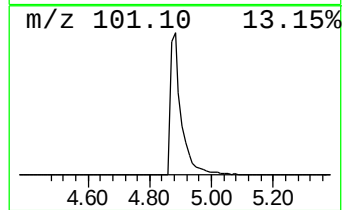
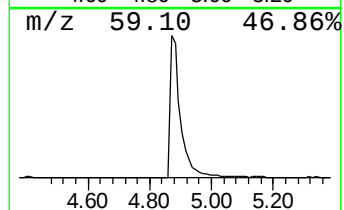
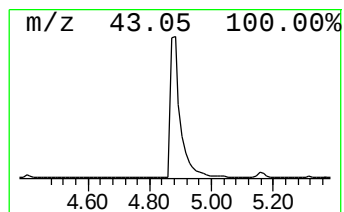
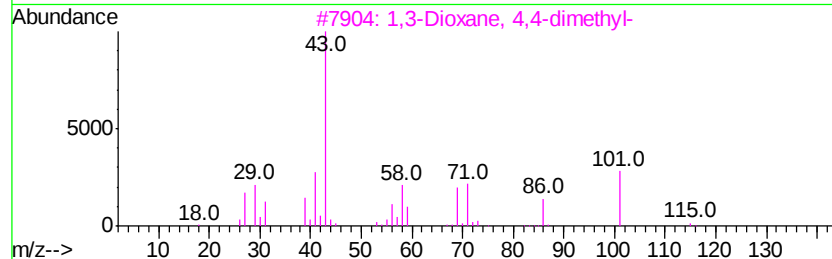
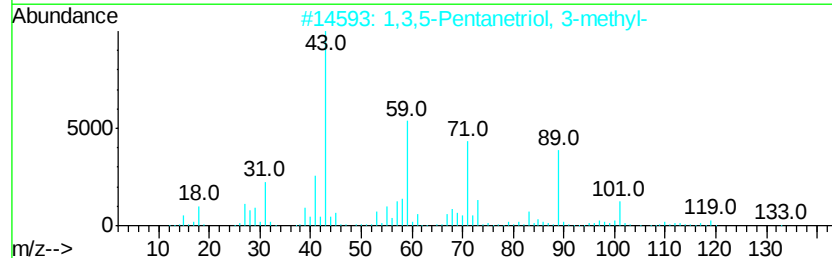
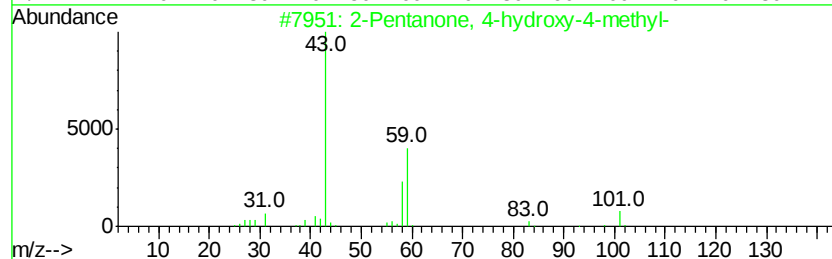
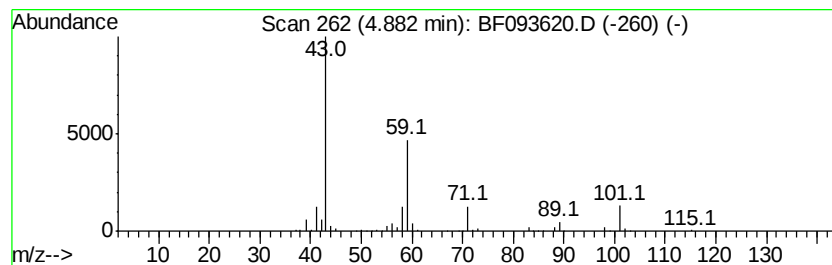
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	27.78 ng	1516290	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		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	9



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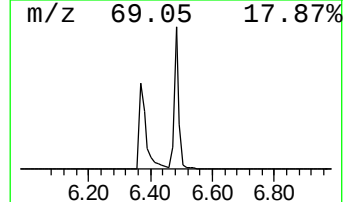
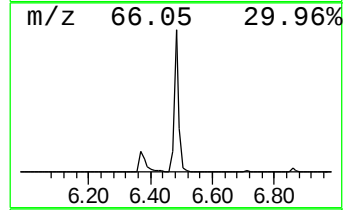
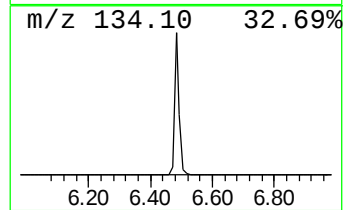
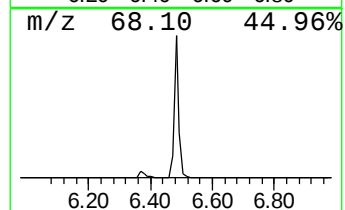
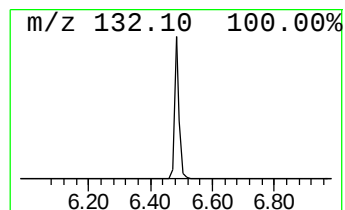
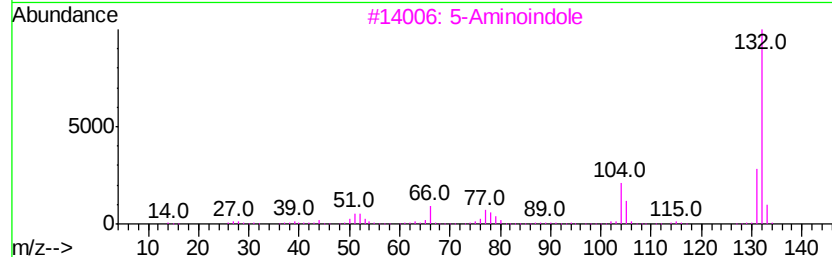
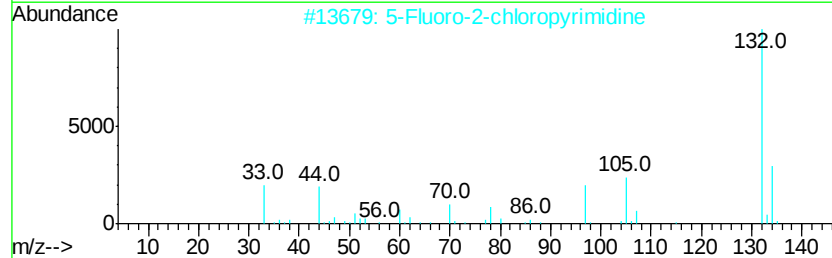
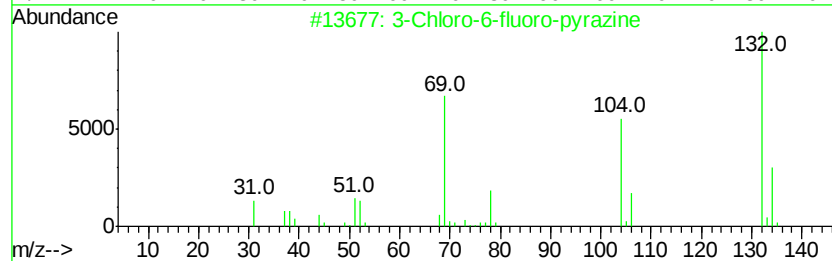
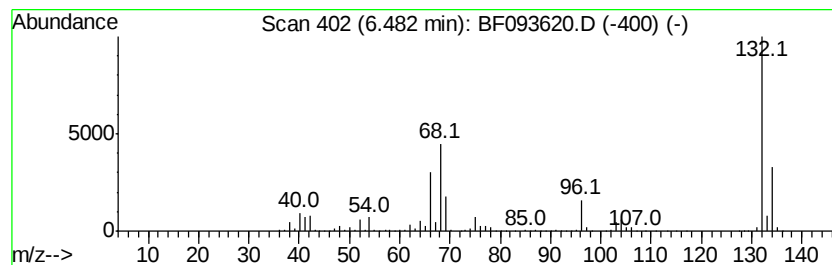
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Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	92.84 ng	5067480	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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	2.45	2.8	ng	151371	1	6.71	1091690	20.0
3-Penten-2-one, 4...	4.18	11.2	ng	613490	1	6.71	1091690	20.0
2-Pentanone, 4-hy...	4.88	27.8	ng	1516290	1	6.71	1091690	20.0
unknown6.48	6.48	92.8	ng	5067480	1	6.71	1091690	20.0