

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042016\
 Data File : BF086312.D
 Acq On : 20 Apr 2016 16:50
 Operator : UM/SJ
 Sample : PB89945BL
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB89945BL

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-BF042016.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	2.167	5	7	28	rVB3	90976	415895	6.41%	0.789%
2	5.059	257	260	269	rBV	1216914	2215124	34.14%	4.200%
3	5.470	292	296	298	rBV	3764343	5711542	88.04%	10.830%
4	5.870	329	331	333	rBV	216601	198294	3.06%	0.376%
5	5.950	335	338	349	rVB2	34947	108916	1.68%	0.207%
6	6.487	382	385	388	rBV	3739752	5415580	83.48%	10.269%
7	6.624	395	397	400	rBV	4285984	5597015	86.27%	10.613%
8	6.864	416	418	429	rVB	1111600	1521121	23.45%	2.884%
9	7.013	429	431	434	rBV	3576195	4553521	70.19%	8.635%
10	7.425	464	467	488	rBV	3250371	4121336	63.53%	7.815%
11	8.145	527	530	539	rBV	1785067	2021701	31.16%	3.834%
12	8.270	539	541	554	rVB	22493	75954	1.17%	0.144%
13	9.230	622	625	627	rBV	4876875	6487538	100.00%	12.302%
14	9.905	681	684	686	rBV	1460254	1971871	30.39%	3.739%
15	10.682	750	752	770	rBV2	2356937	3472027	53.52%	6.584%
16	11.379	811	813	826	rBV	1618154	1837031	28.32%	3.483%
17	12.968	949	952	961	rBV	4091287	4521486	69.69%	8.574%
18	14.008	1041	1043	1052	rBV	998957	1262942	19.47%	2.395%
19	15.437	1165	1168	1176	rVB	851993	1227181	18.92%	2.327%

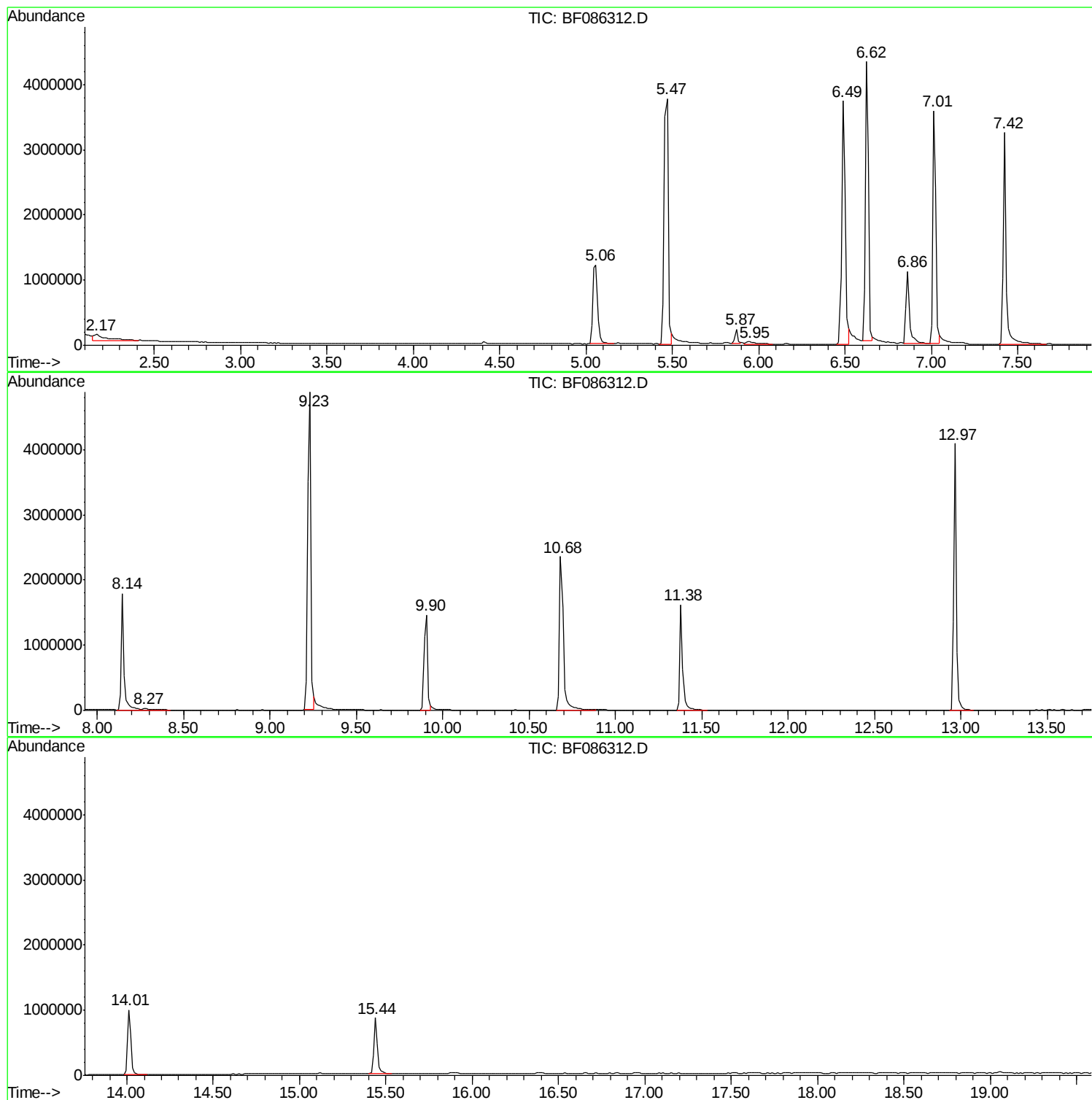
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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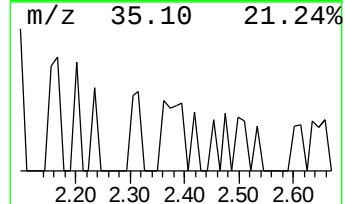
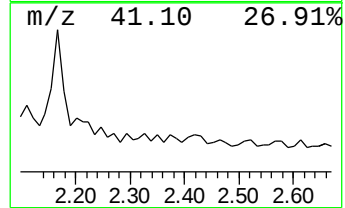
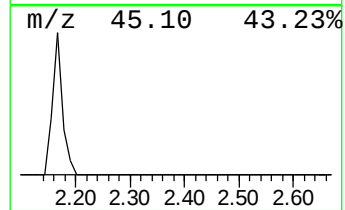
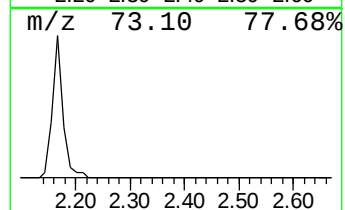
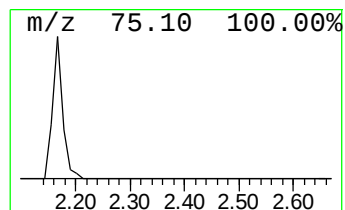
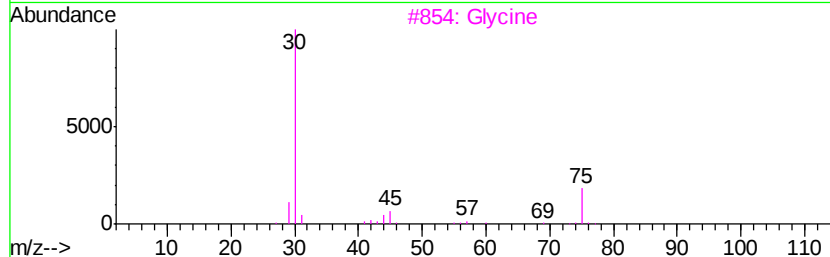
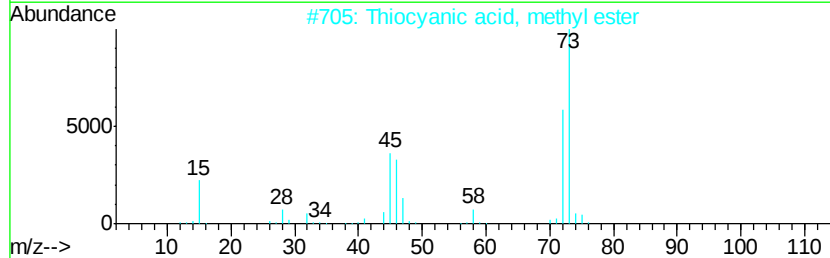
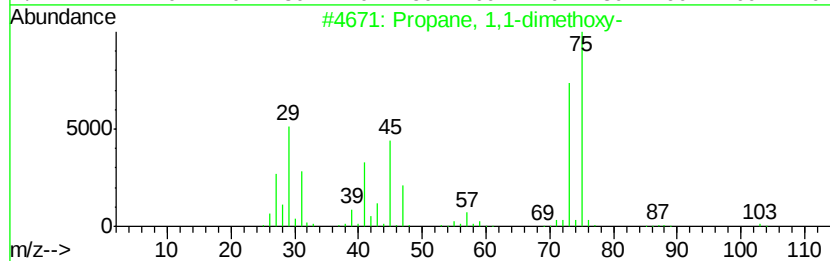
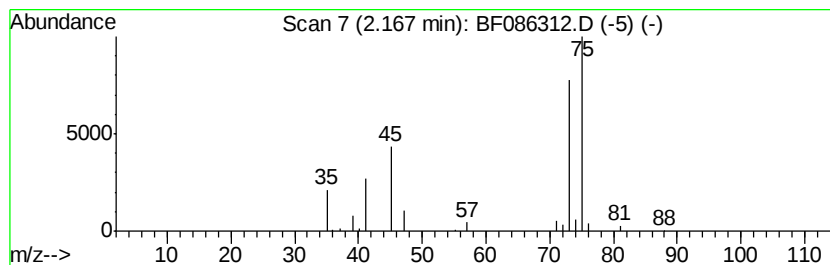
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.17 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	5.47 ng	415895	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	28
2		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	7
3		Glycine	75	C2H5NO2	000056-40-6	5
4		1-Propene-1-thiol	74	C3H6S	000925-89-3	4
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	4



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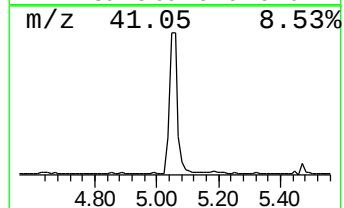
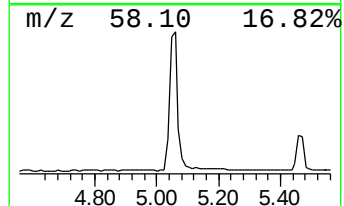
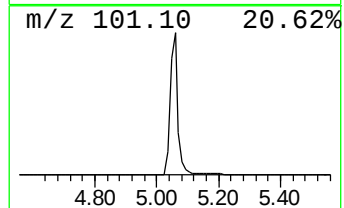
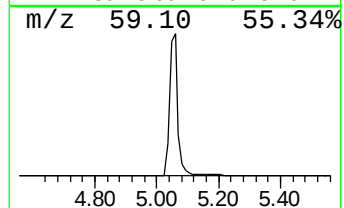
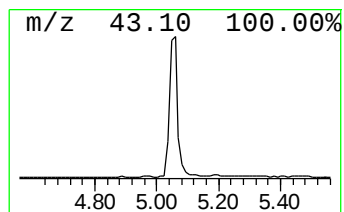
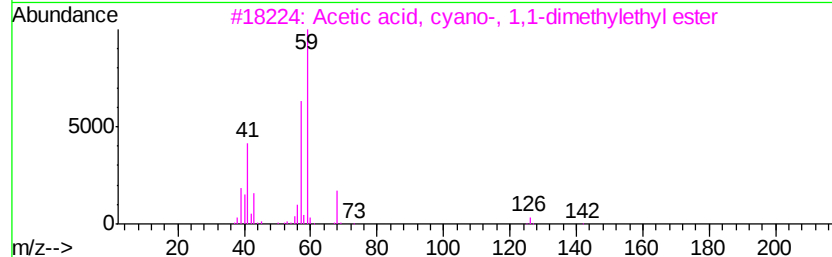
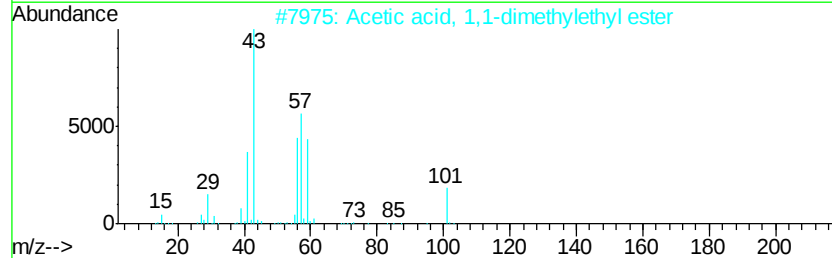
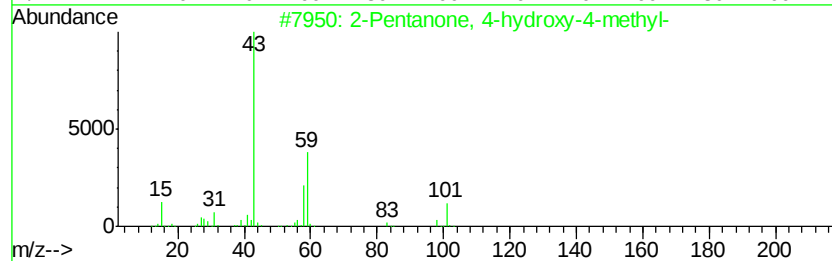
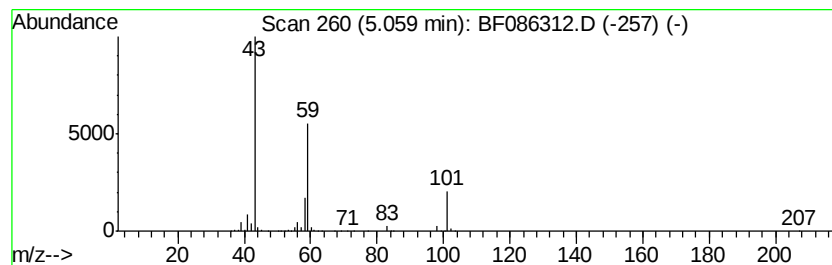
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	29.12 ng	2215120	1,4-Dichlorobenzene-d4	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2		000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethv...	141	C7H11NO2		001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O		000628-81-9	9
5	Acetone	58	C3H6O		000067-64-1	9



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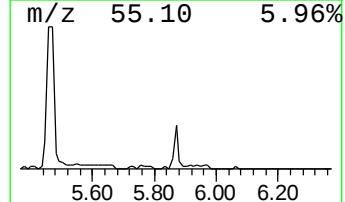
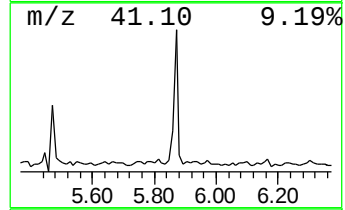
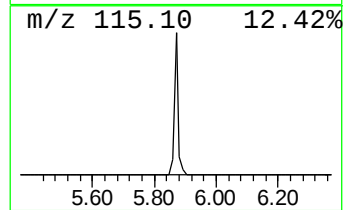
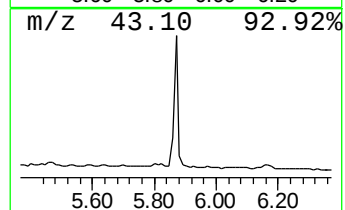
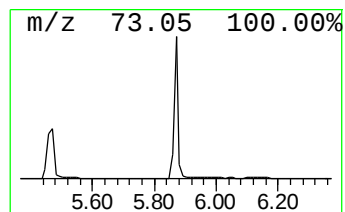
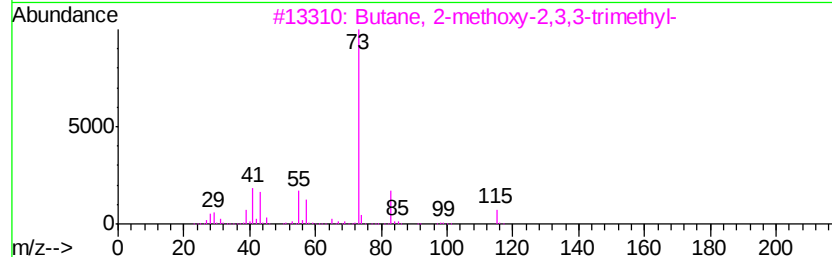
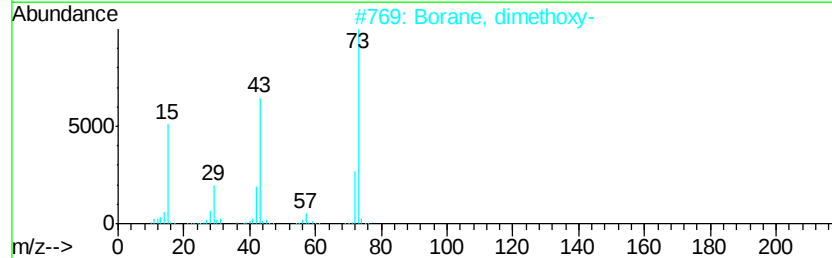
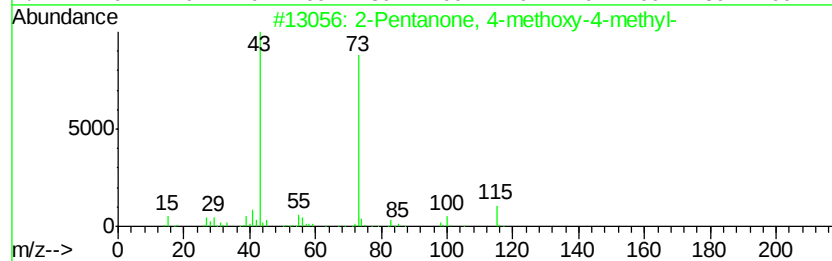
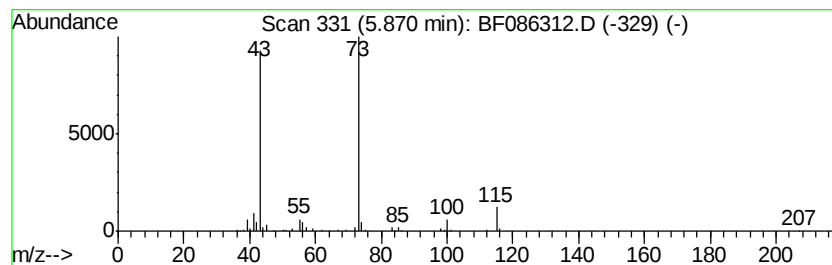
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.87	2.61 ng	198294	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	38
3		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10



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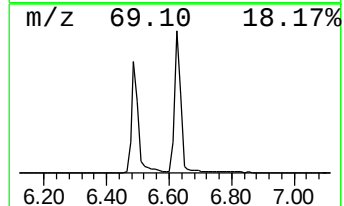
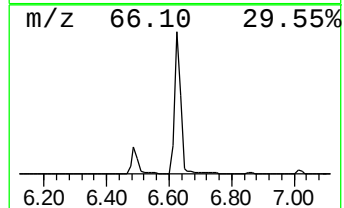
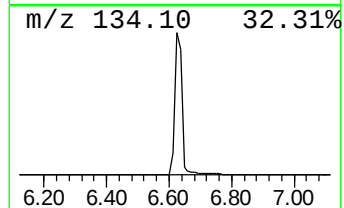
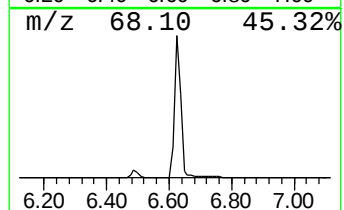
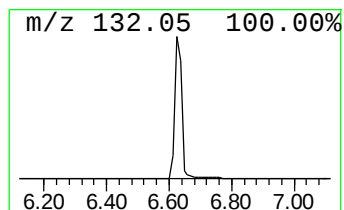
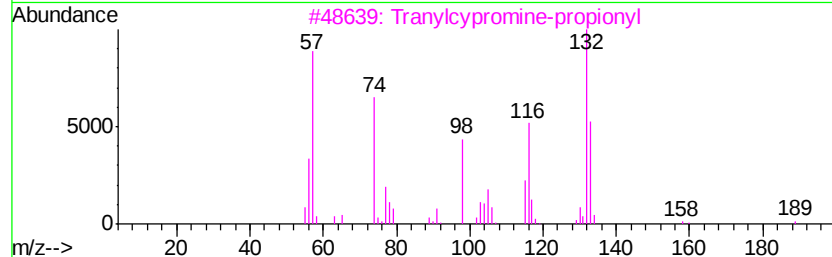
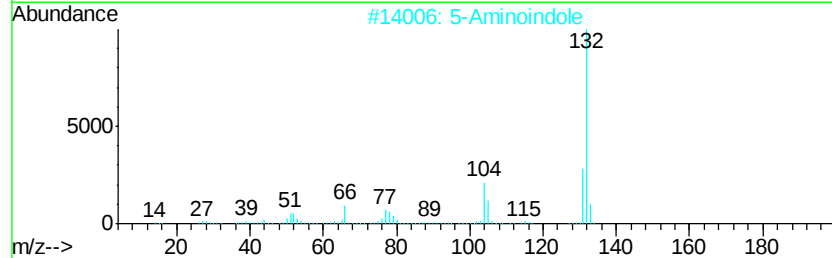
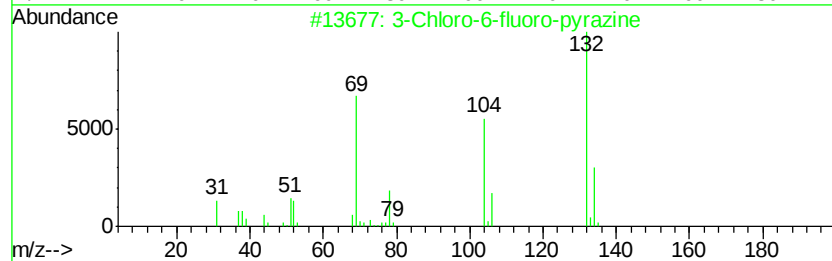
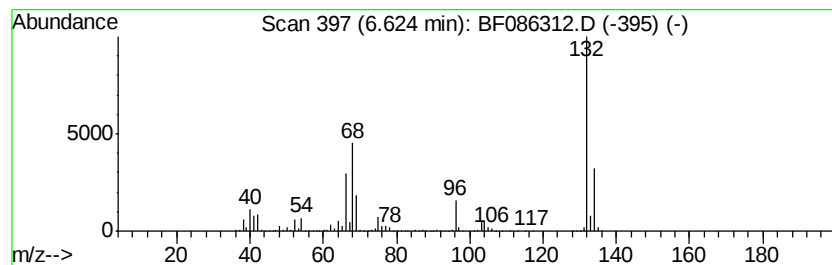
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Peak Number 4 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	73.59 ng	5597020	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypropine-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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.17	2.17	5.5	ng	415895	1	6.86	1521120	20.0
2-Pentanone, 4-hy...	5.06	29.1	ng	2215120	1	6.86	1521120	20.0
2-Pentanone, 4-me...	5.87	2.6	ng	198294	1	6.86	1521120	20.0
unknown6.62	6.62	73.6	ng	5597020	1	6.86	1521120	20.0