

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080432.D
Acq On : 13 Jul 2015 18:06
Operator : TP/UM
Sample : G2945-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-PMW-43

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-BF071015.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	2.155	4	6	15	rBV	331378	500930	47.12%	7.248%
2	2.281	15	17	28	rVB	461614	622056	58.51%	9.000%
3	5.356	284	286	296	rVB	89647	107058	10.07%	1.549%
4	5.767	320	322	330	rBV	268004	275302	25.90%	3.983%
5	6.156	354	356	360	rBB	21757	22474	2.11%	0.325%
6	6.773	408	410	416	rBV	129837	172376	16.21%	2.494%
7	6.910	420	422	425	rBV	643396	526452	49.52%	7.617%
8	7.139	440	442	444	rBB	87208	119235	11.22%	1.725%
9	7.287	453	455	458	rBV	368183	429782	40.43%	6.218%
10	7.699	489	491	493	rBV	486361	381441	35.88%	5.519%
11	8.419	552	554	557	rBV	203885	177144	16.66%	2.563%
12	9.368	635	637	639	rBV	12443	10737	1.01%	0.155%
13	9.493	646	648	650	rVB	1116724	846898	79.66%	12.253%
14	9.893	681	683	684	rBV	31648	30539	2.87%	0.442%
15	10.179	706	708	711	rVB	270696	224678	21.13%	3.251%
16	10.888	768	770	772	rBB	20475	15859	1.49%	0.229%
17	10.968	775	777	780	rBV	565764	518806	48.80%	7.506%
18	11.676	836	839	841	rBV	188149	245459	23.09%	3.551%
19	12.168	881	882	885	rBV	13074	14663	1.38%	0.212%
20	13.299	978	981	983	rBV	907929	1063101	100.00%	15.382%
21	14.271	1064	1066	1070	rBV2	14351	24171	2.27%	0.350%
22	14.500	1083	1086	1088	rBV	248015	301901	28.40%	4.368%
23	16.225	1234	1237	1240	rBV	188244	280427	26.38%	4.057%

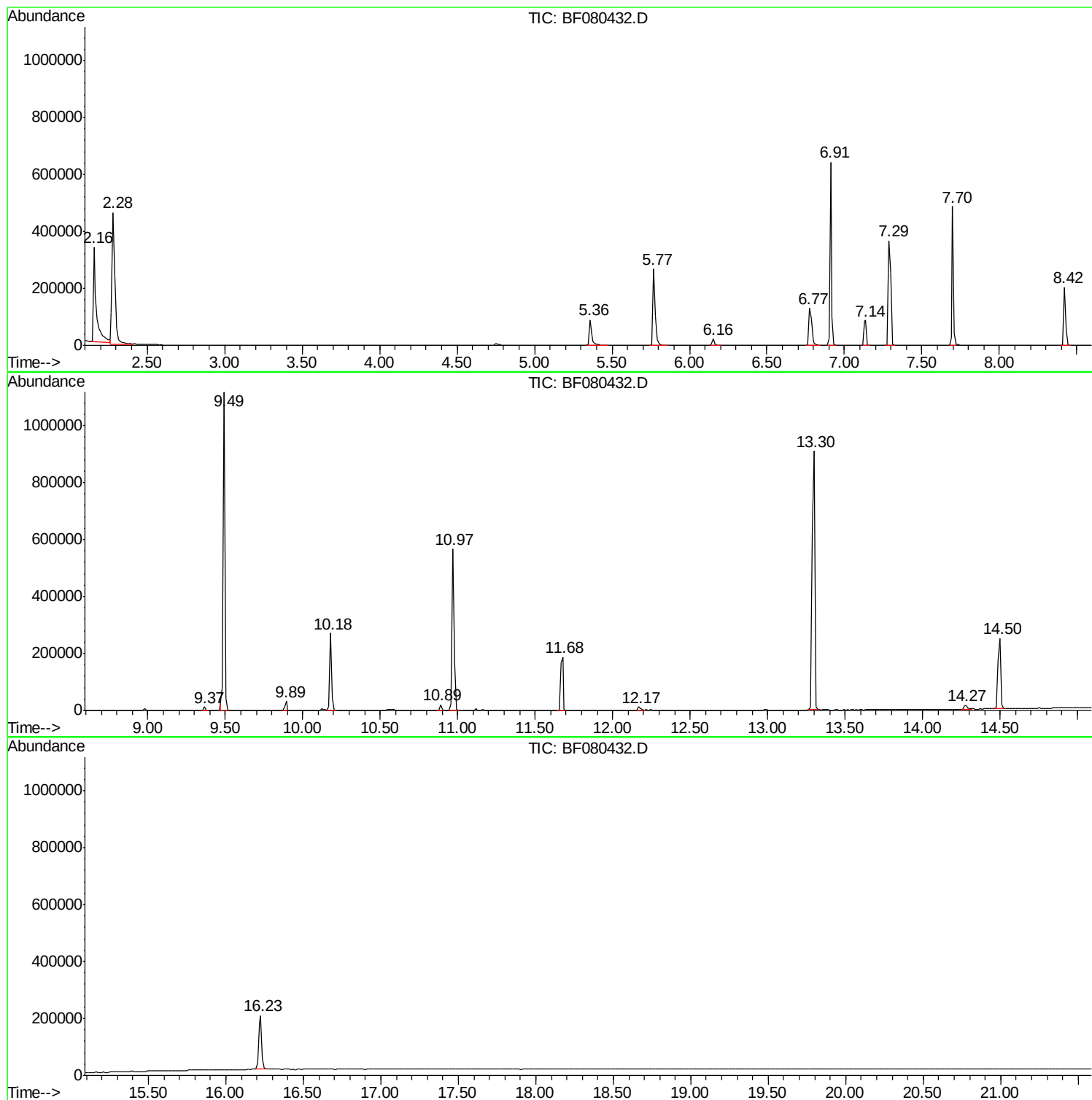
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 7 Sample Multiplier: 1

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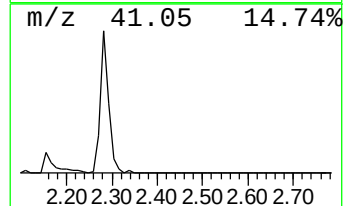
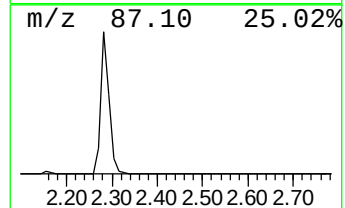
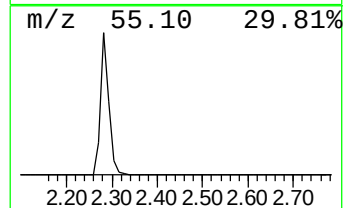
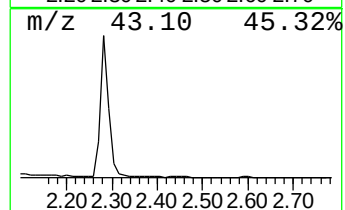
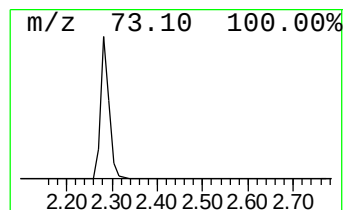
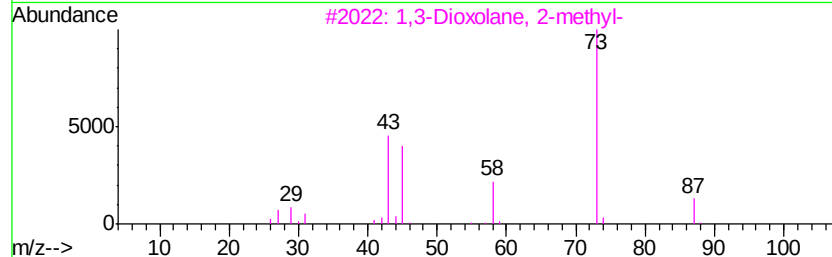
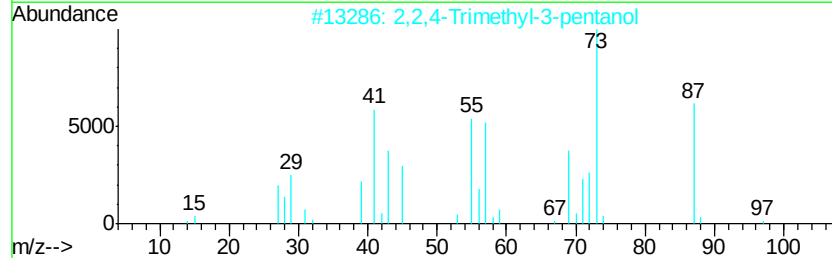
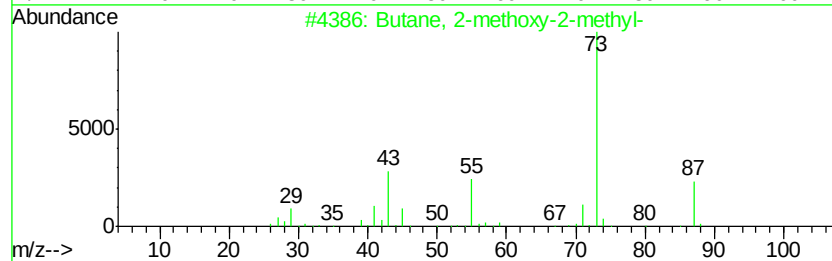
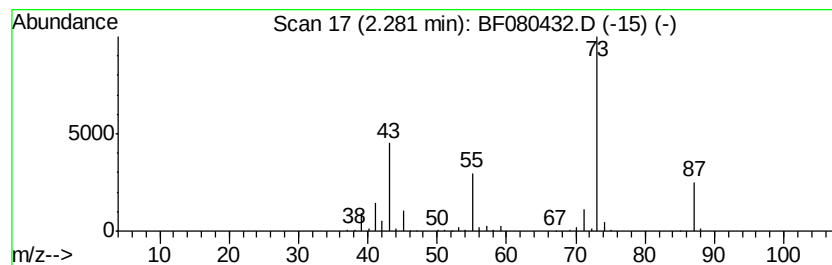
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.28	104.34 ng	622056	1,4-Dichlorobenzene-d4	7.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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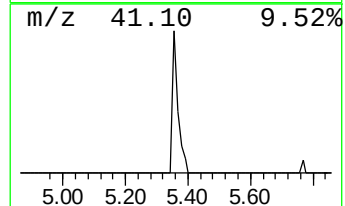
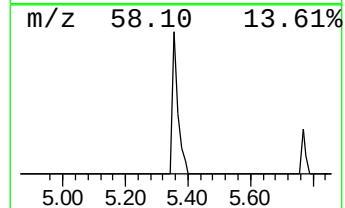
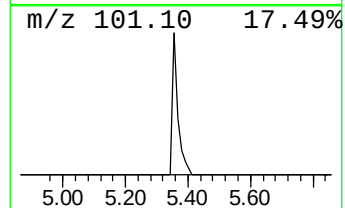
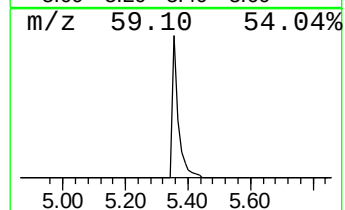
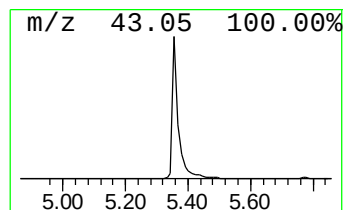
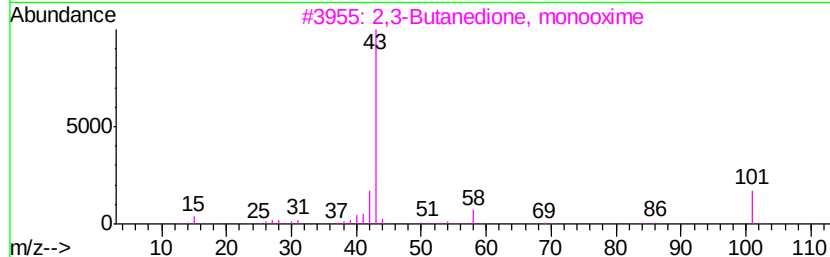
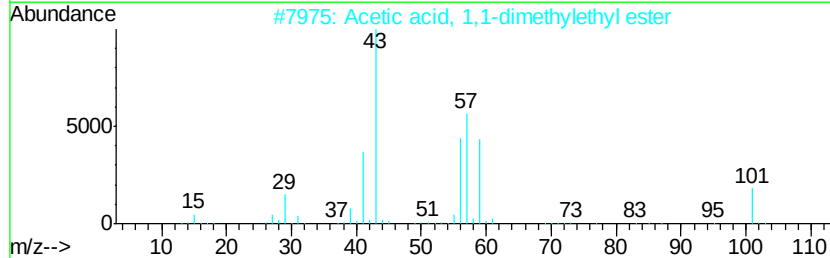
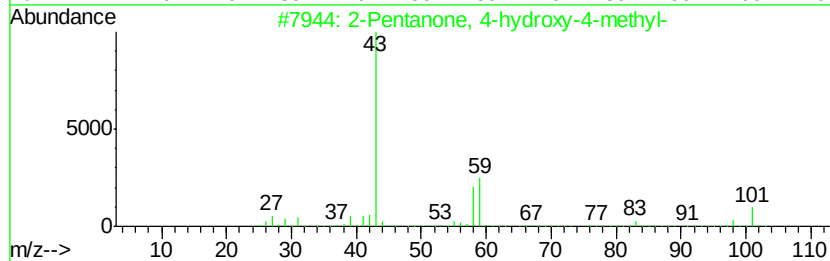
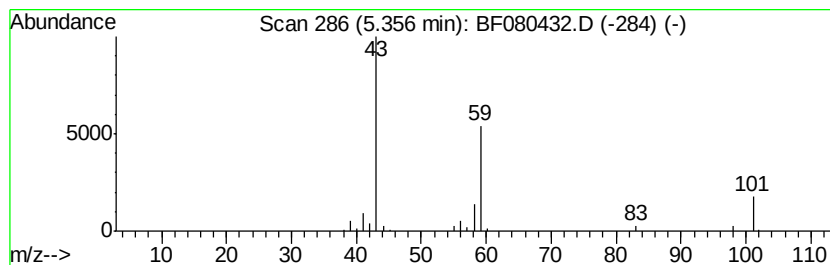
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.36	17.96 ng	107058	1,4-Dichlorobenzene-d4	7.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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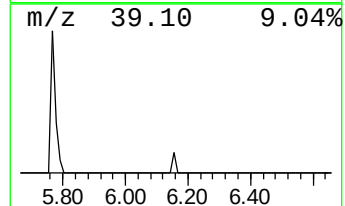
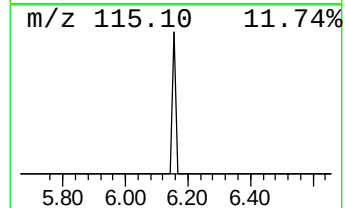
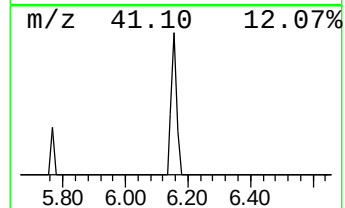
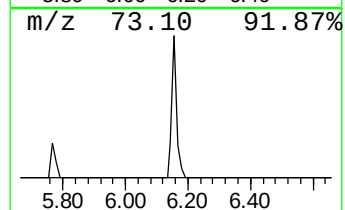
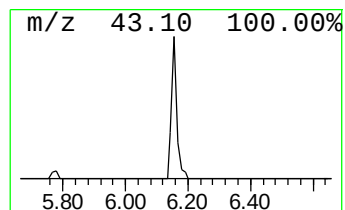
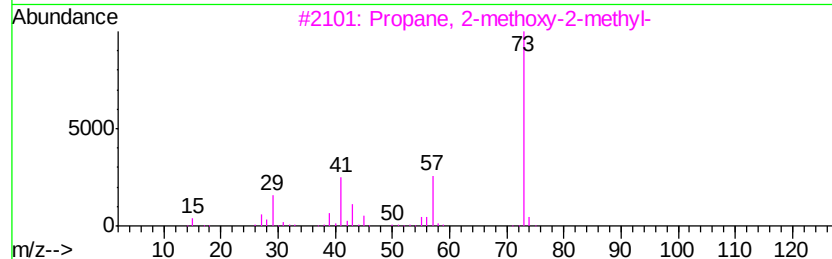
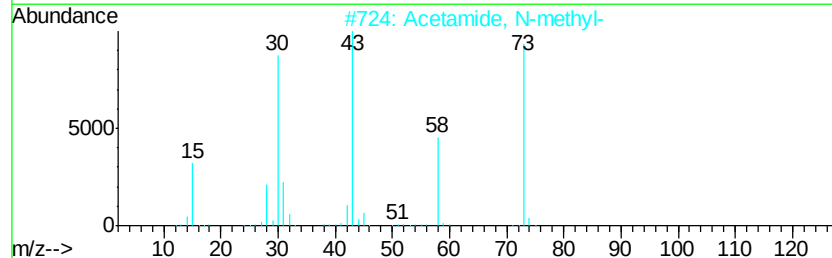
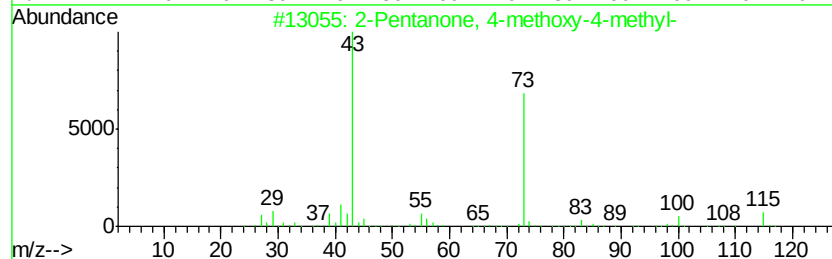
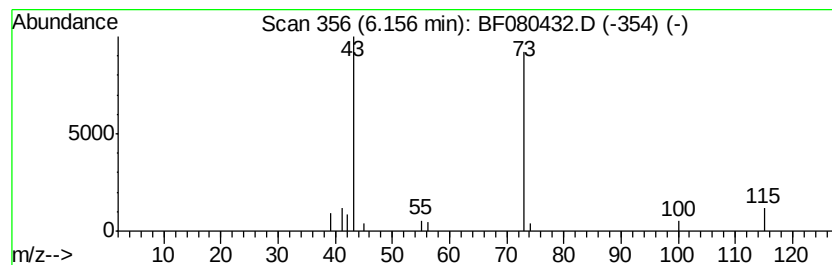
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	3.77 ng	22474	1,4-Dichlorobenzene-d4	7.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83	
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	40	
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9	
4	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	7	
5	N-Ethylformamide	73	C3H7NO	000627-45-2	7	



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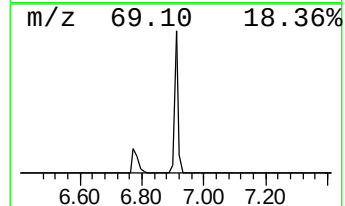
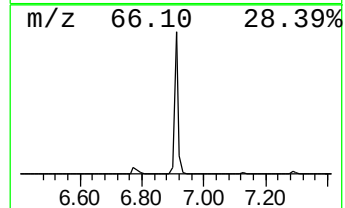
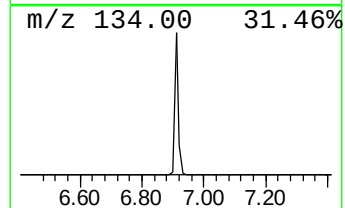
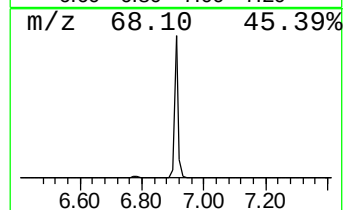
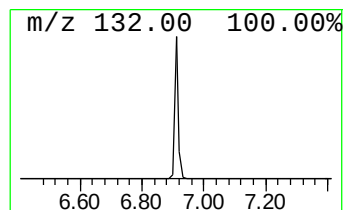
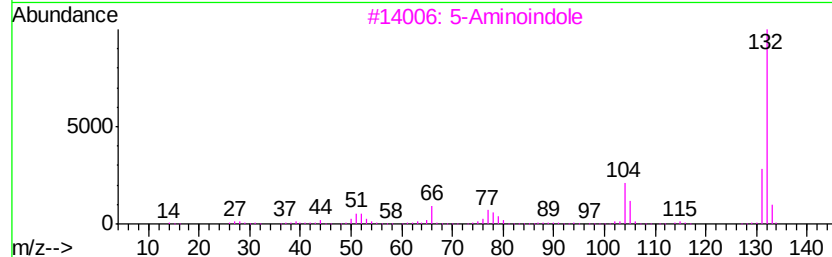
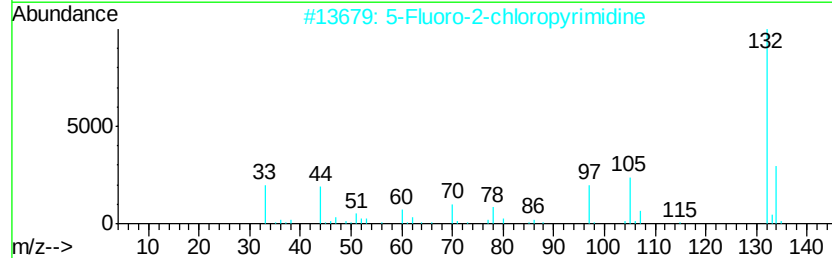
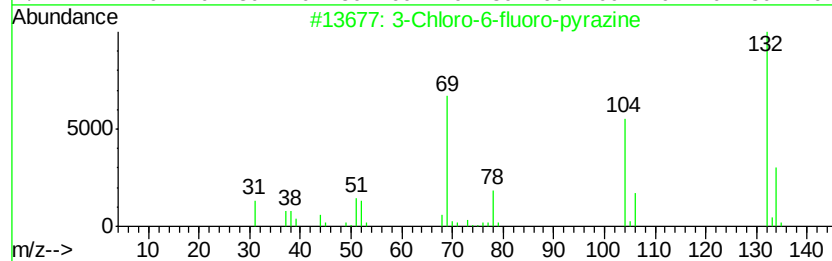
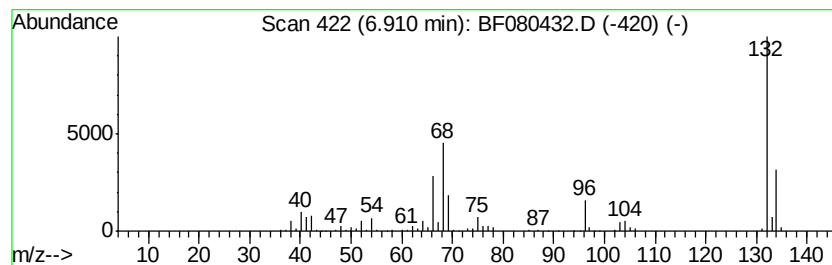
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Peak Number 5 unknown6.91 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.91	88.30 ng	526452	1,4-Dichlorobenzene-d4	7.14

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
Butane, 2-methoxy...	2.28	104.3	ng	622056	1	7.14	119235	20.0
2-Pentanone, 4-hy...	5.36	18.0	ng	107058	1	7.14	119235	20.0
2-Pentanone, 4-me...	6.16	3.8	ng	22474	1	7.14	119235	20.0
unknown6.91	6.91	88.3	ng	526452	1	7.14	119235	20.0