

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031819\
 Data File : BM019223.D
 Acq On : 18 Mar 2019 19:40
 Operator : JU/SJ
 Sample : K1930-08
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-4

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.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	3.222	36	40	51	rVB	492410	570499	3.37%	0.684%
2	4.322	222	227	234	rBV	334248	406732	2.41%	0.488%
3	4.757	297	301	307	rBV	230870	311325	1.84%	0.373%
4	4.816	307	311	323	rVB	162354	235838	1.39%	0.283%
5	5.251	379	385	401	rBV	4161210	5903912	34.92%	7.079%
6	6.834	647	654	669	rBV	3608366	5679136	33.59%	6.810%
7	7.187	706	714	728	rBV	5126178	7867010	46.53%	9.433%
8	7.651	786	793	802	rBV	784170	1256511	7.43%	1.507%
9	7.963	839	846	858	rBV	3446743	5331286	31.53%	6.393%
10	8.822	984	992	1010	rBV	2783691	4821979	28.52%	5.782%
11	10.433	1259	1266	1284	rBV	1016425	1801230	10.65%	2.160%
12	12.916	1681	1688	1706	rBV	8140495	11806037	69.83%	14.156%
13	14.304	1915	1924	1938	rBV2	1746261	2714311	16.05%	3.255%
14	15.804	2172	2179	2206	rBV	6860905	9954837	58.88%	11.937%
15	17.056	2386	2392	2408	rBV	1974990	3036925	17.96%	3.642%
16	19.697	2835	2841	2855	rBV	14428632	16906641	100.00%	20.272%
17	21.256	3101	3106	3117	rBV	1837984	2527841	14.95%	3.031%
18	23.491	3480	3486	3502	rVB	1105584	2265401	13.40%	2.716%

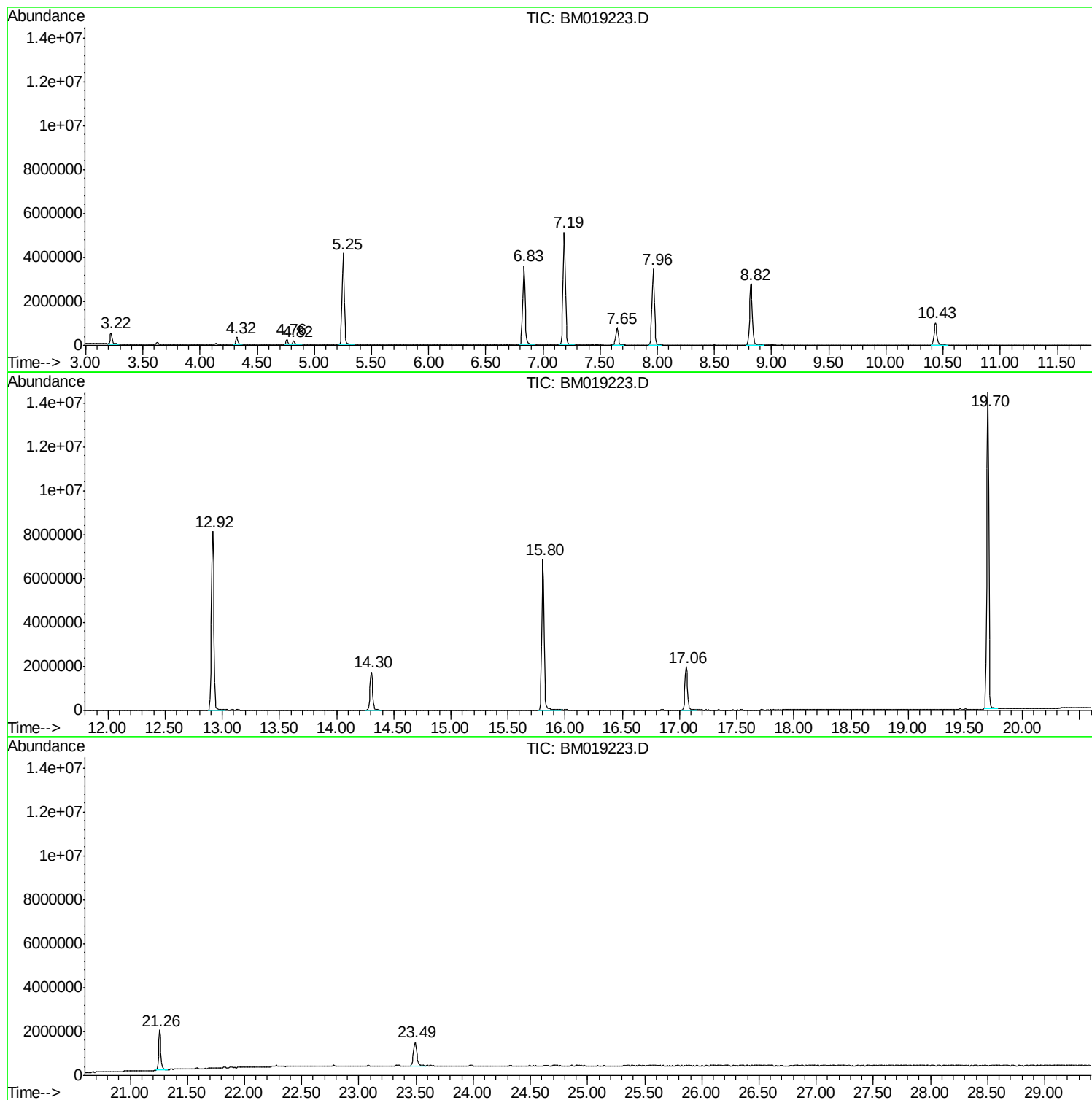
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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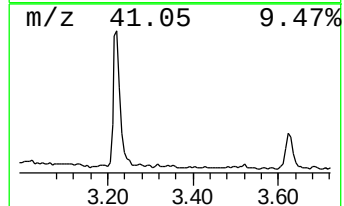
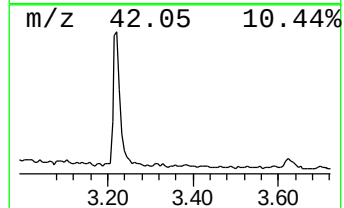
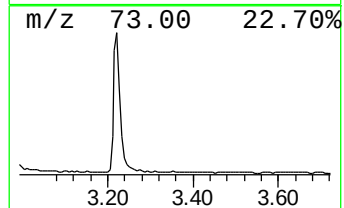
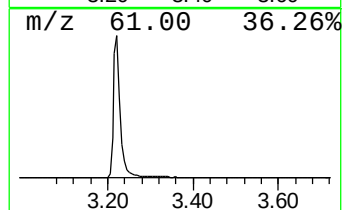
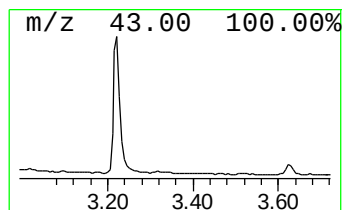
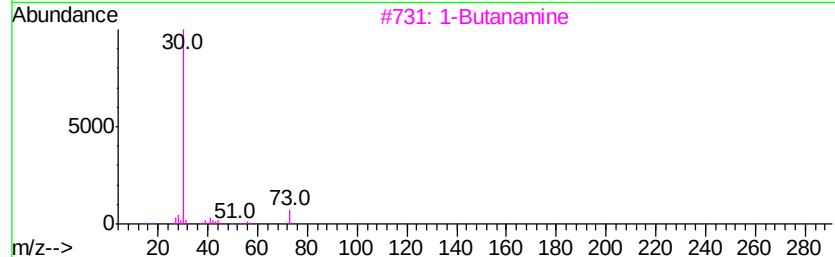
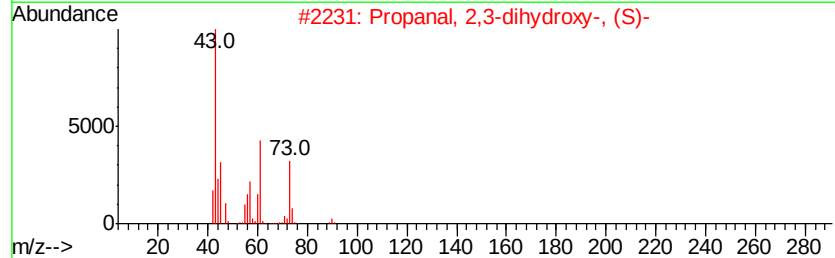
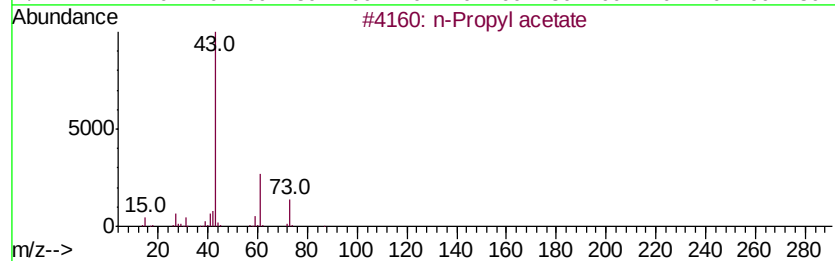
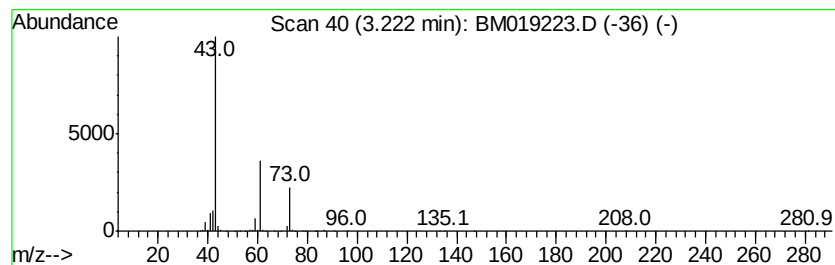
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.22	9.08 ng	570499	1,4-Dichlorobenzene-d4	7.65	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38
3	1-Butanamine	73	C4H11N	000109-73-9	5
4	Isobutylamine	73	C4H11N	000078-81-9	4
5	Butane, 1-propoxy-	116	C7H16O	003073-92-5	4



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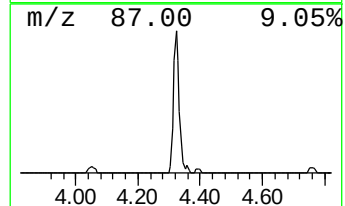
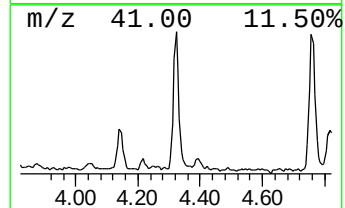
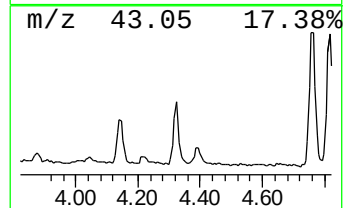
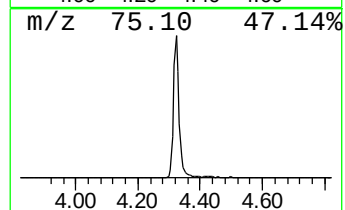
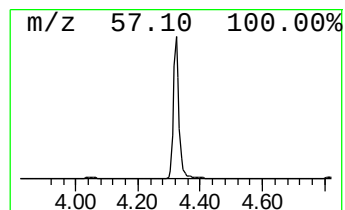
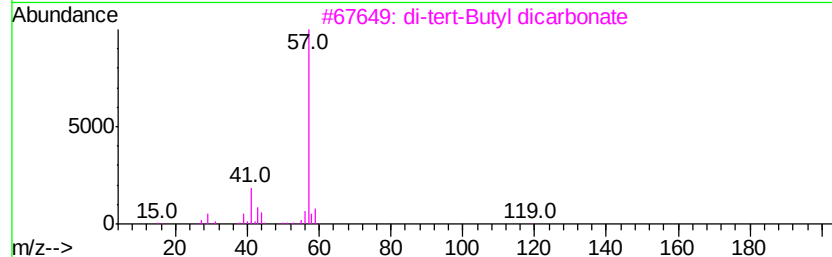
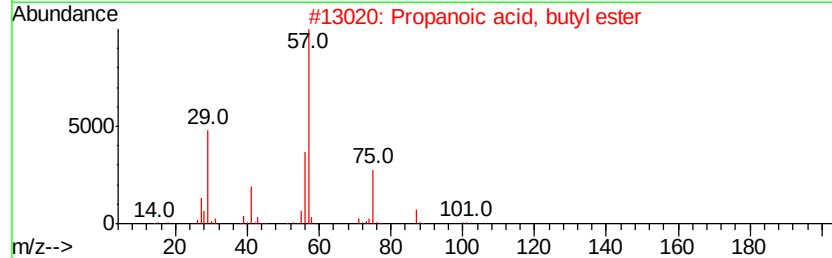
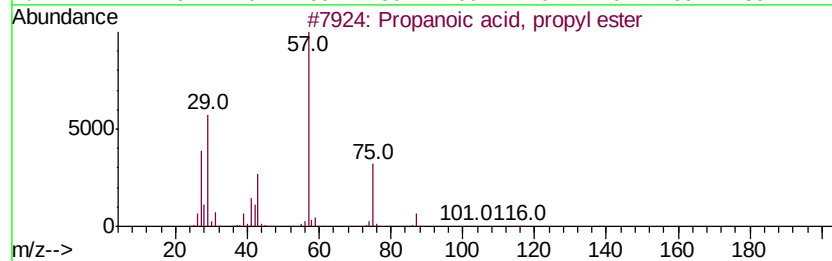
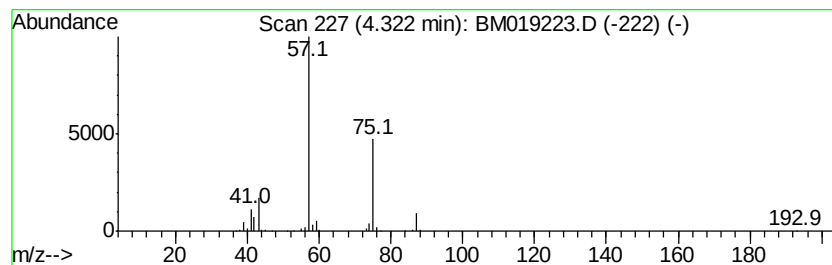
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Peak Number 2 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	6.47 ng	406732	1,4-Dichlorobenzene-d4	7.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	33
3		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5		S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	7



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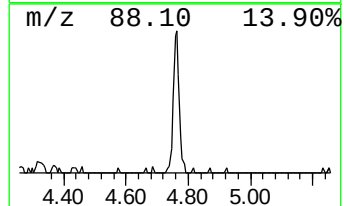
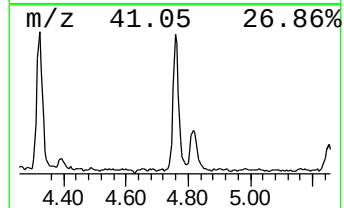
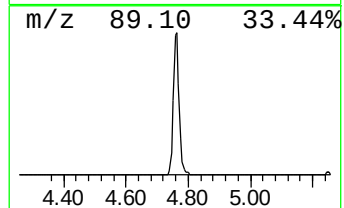
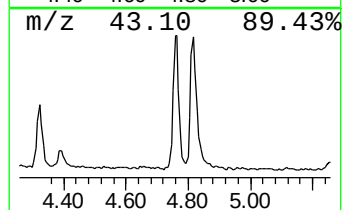
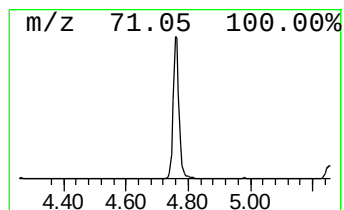
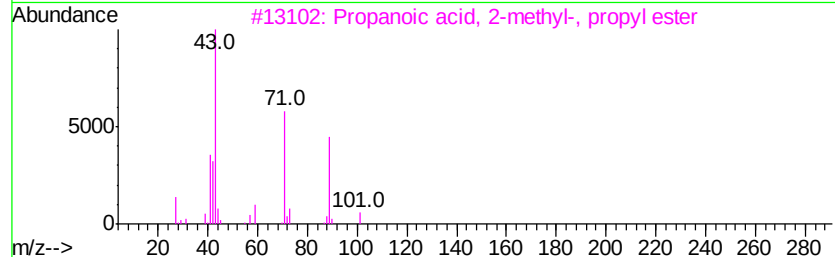
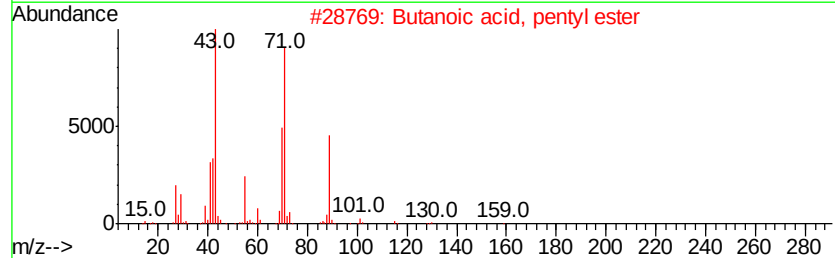
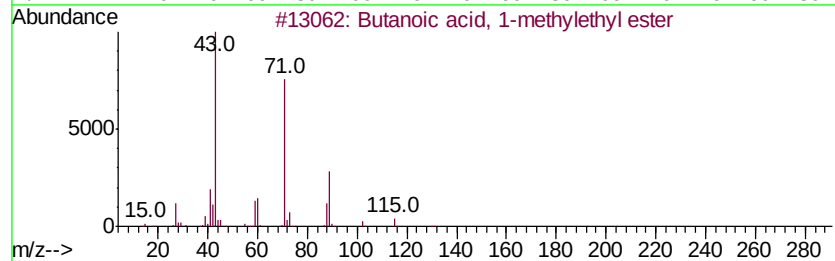
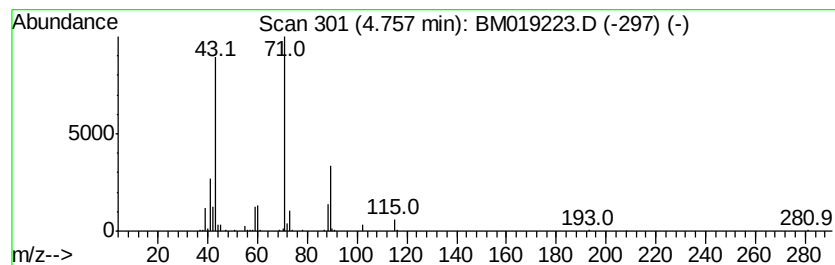
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Peak Number 3 Butanoic acid, 1-methylethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	4.96 ng	311325	1,4-Dichlorobenzene-d4	7.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2		Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
3		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	64
4		Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
5		Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	59



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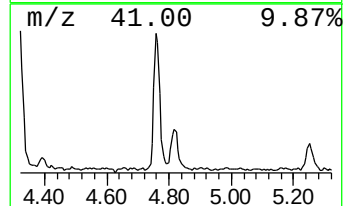
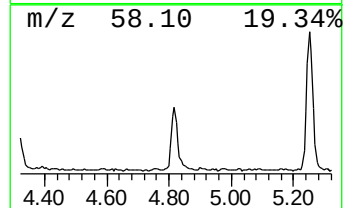
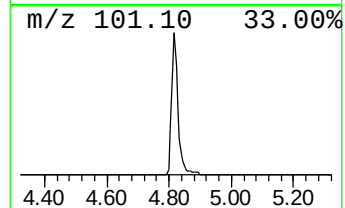
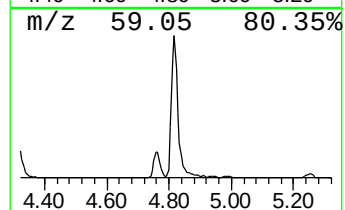
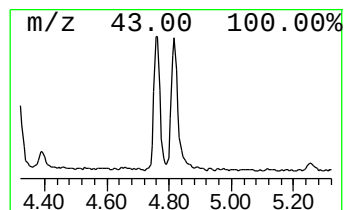
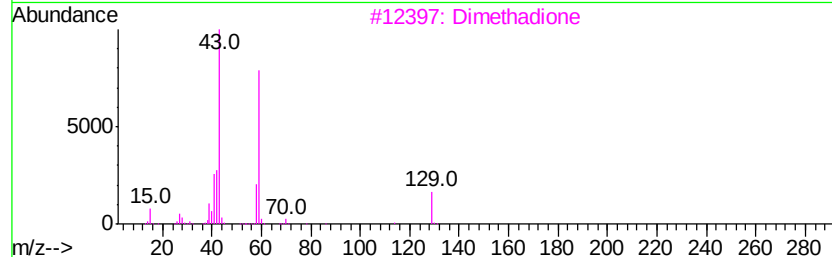
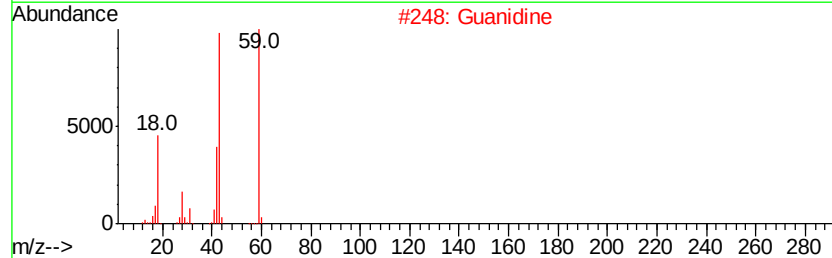
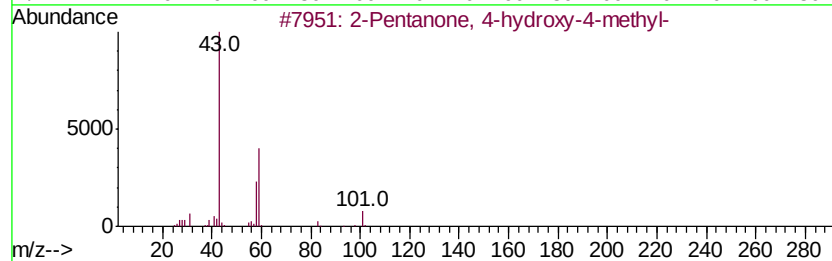
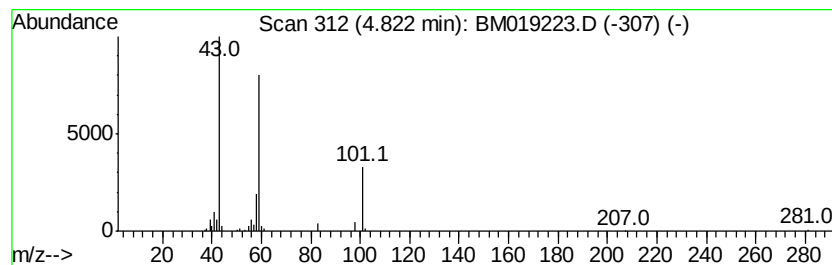
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	3.75 ng	235838	1,4-Dichlorobenzene-d4	7.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	47
3		Dimethadione	129	C5H7N03	000695-53-4	38
4		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28



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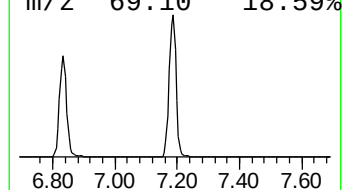
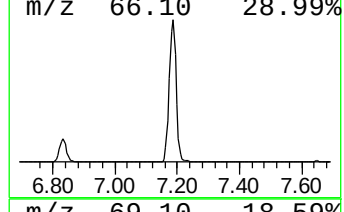
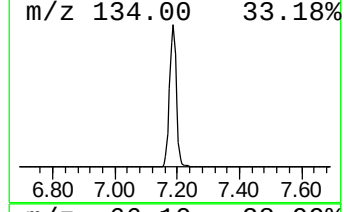
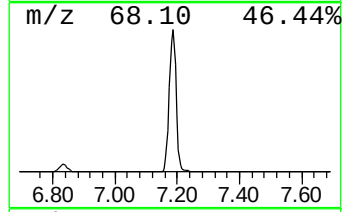
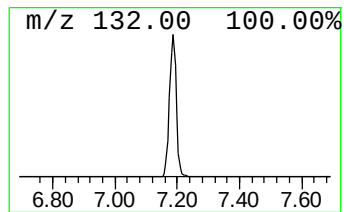
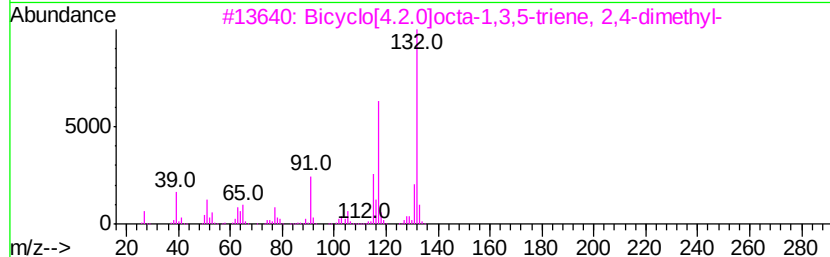
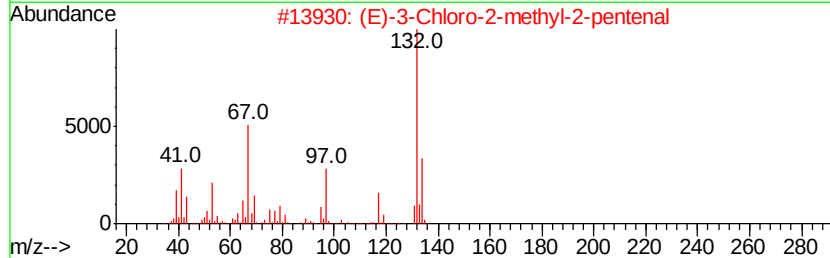
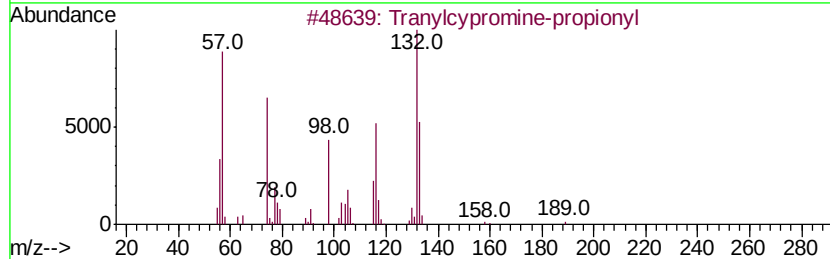
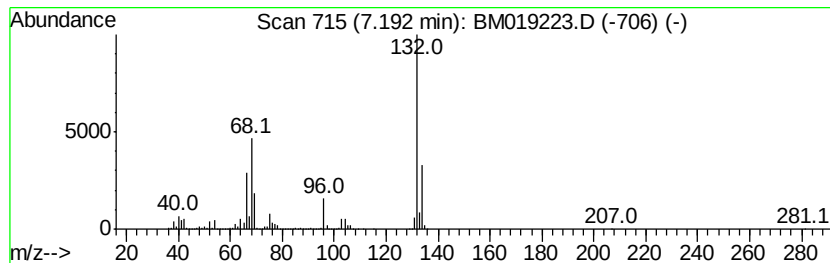
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Peak Number 5 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	125.22 ng	7867010	1,4-Dichlorobenzene-d4	7.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	3.22	9.1 ng		570499	1	7.65	1256510	20.0
Propanoic acid, p...	4.32	6.5 ng		406732	1	7.65	1256510	20.0
Butanoic acid, 1-...	4.76	5.0 ng		311325	1	7.65	1256510	20.0
2-Pentanone, 4-hy...	4.82	3.8 ng		235838	1	7.65	1256510	20.0
unknown7.19	7.19	125.2 ng		7867010	1	7.65	1256510	20.0