

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110818\
 Data File : BG037907.D
 Acq On : 9 Nov 2018 6:16
 Operator : JU/SJ
 Sample : J5838-10
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG101818.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

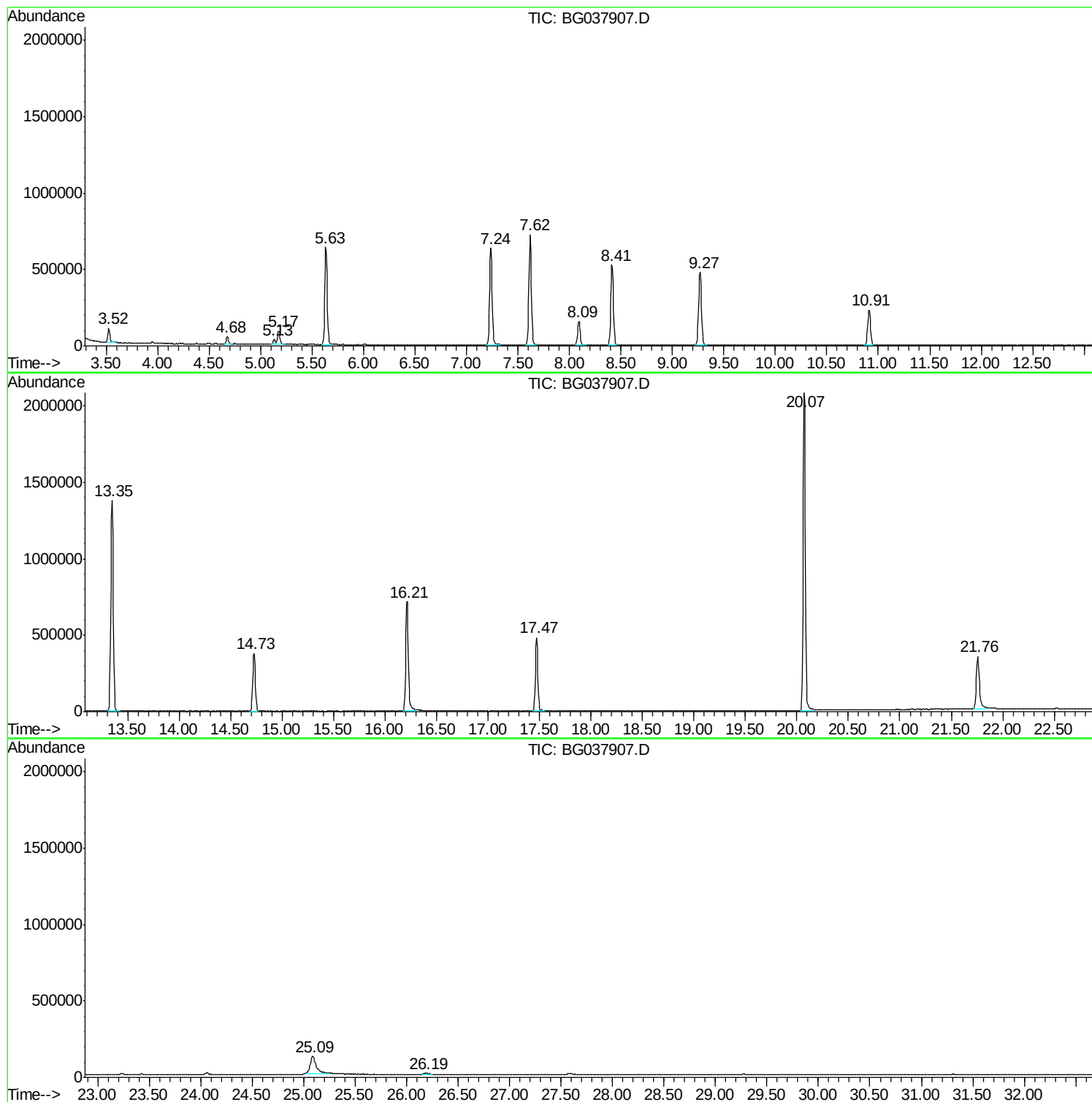
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.524	36	40	50	rVB	93533	125257	4.16%	0.805%
2	4.675	231	236	244	rVB	45836	69474	2.31%	0.447%
3	5.128	309	313	317	rBV	30791	47556	1.58%	0.306%
4	5.175	317	321	330	rVB	89140	141302	4.69%	0.909%
5	5.633	392	399	408	rBV	638288	1078676	35.79%	6.937%
6	7.237	664	672	687	rBV	634007	1119631	37.15%	7.200%
7	7.619	729	737	747	rBV	722440	1282877	42.57%	8.250%
8	8.089	811	817	829	rVB	156027	279695	9.28%	1.799%
9	8.412	865	872	881	rBV	525015	963881	31.99%	6.198%
10	9.270	1009	1018	1029	rBV	477975	902656	29.95%	5.805%
11	10.909	1288	1297	1304	rBV	230645	433253	14.38%	2.786%
12	13.347	1704	1712	1724	rBV	1379700	2227126	73.90%	14.322%
13	14.728	1939	1947	1954	rBV2	379065	648204	21.51%	4.168%
14	16.215	2193	2200	2214	rBV2	718298	1251978	41.55%	8.051%
15	17.472	2407	2414	2427	rBV	481249	762380	25.30%	4.903%
16	20.069	2850	2856	2872	rBV	2079367	3013505	100.00%	19.379%
17	21.755	3136	3143	3157	rBV	347268	729605	24.21%	4.692%
18	25.087	3698	3710	3735	rBV3	110815	440435	14.62%	2.832%
19	26.191	3892	3898	3907	rVB8	10989	32954	1.09%	0.212%

Sum of corrected areas: 15550445

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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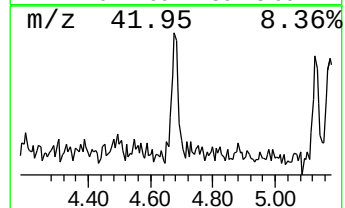
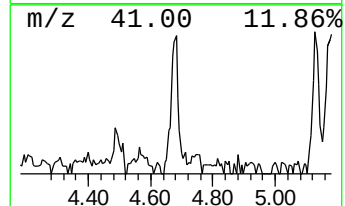
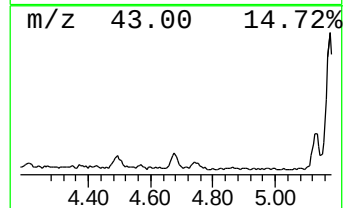
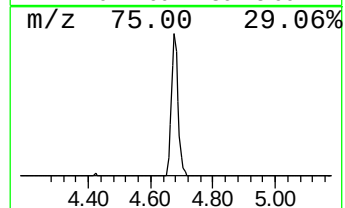
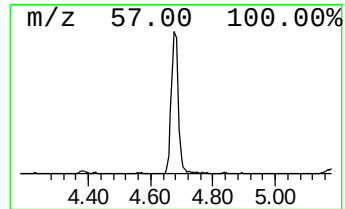
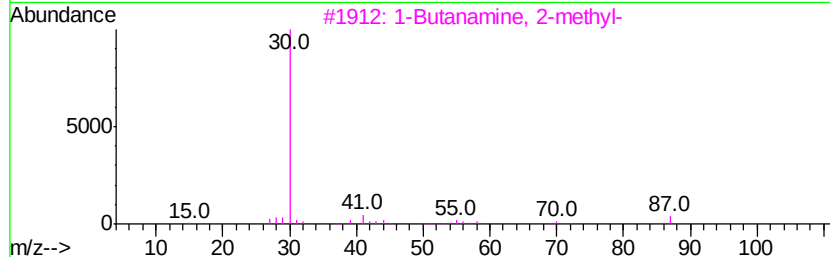
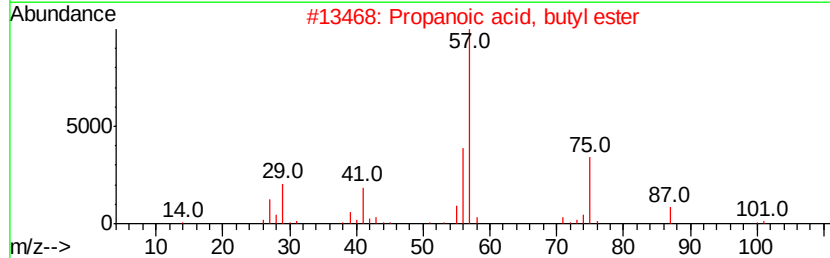
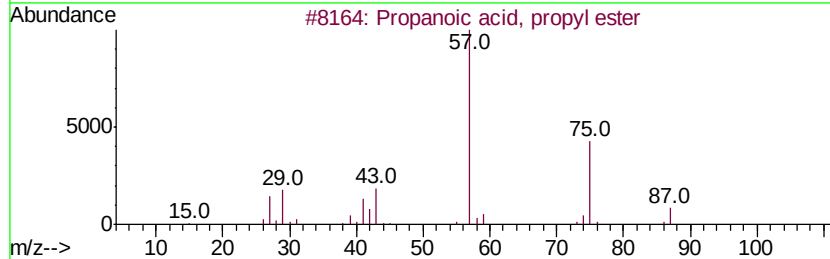
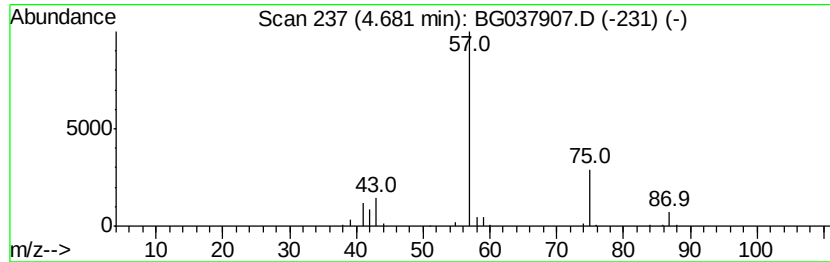
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	4.97 ng	69474	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38
3		1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	9
4		1-Penten-3-ol	86	C5H10O	000616-25-1	5
5		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5



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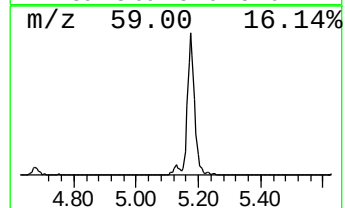
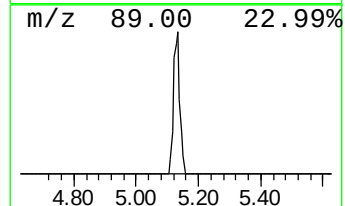
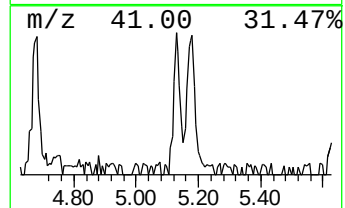
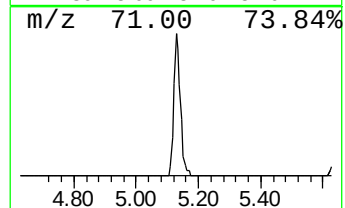
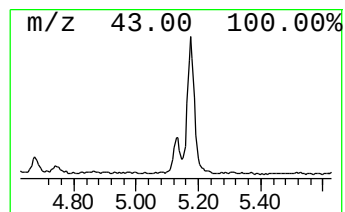
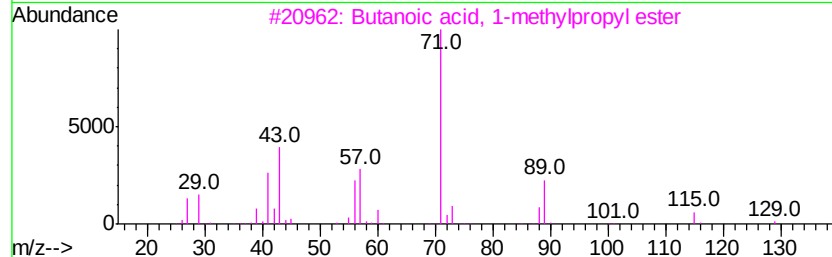
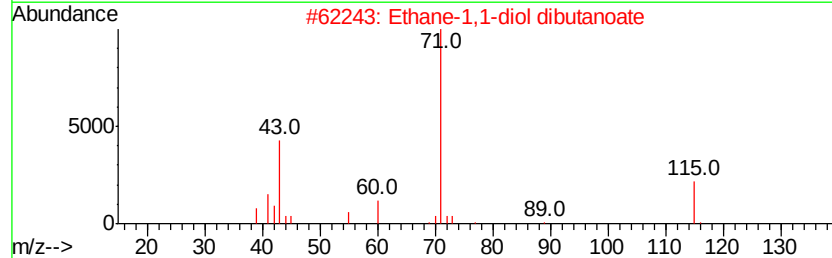
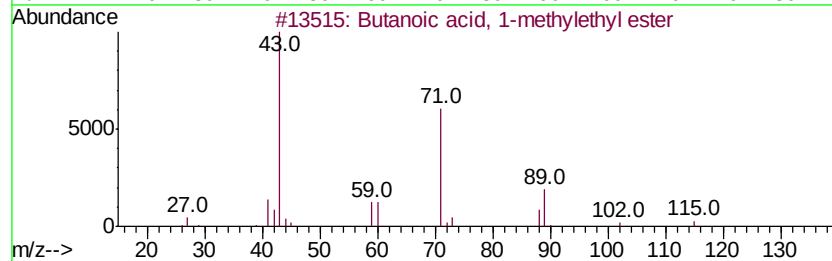
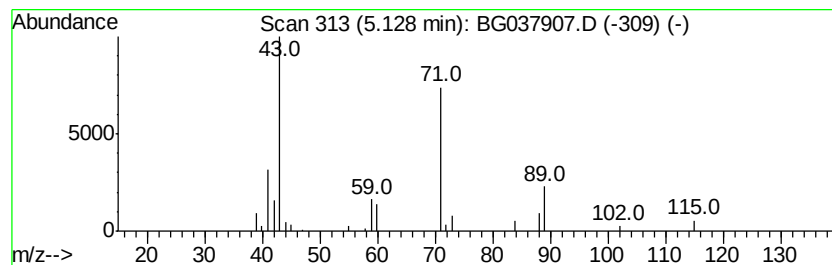
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Peak Number 3 Butanoic acid, 1-methylethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	3.40 ng	47556	1,4-Dichlorobenzene-d4	8.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2			Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	53
3			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	50
4			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	50
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	45



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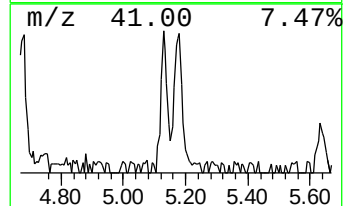
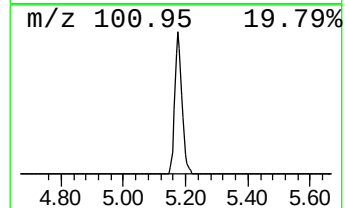
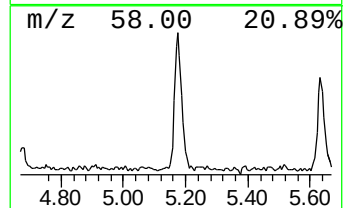
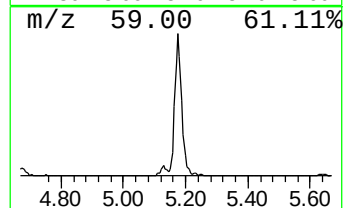
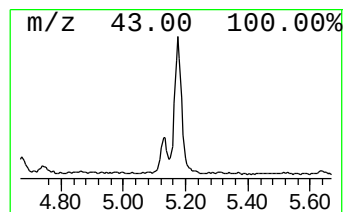
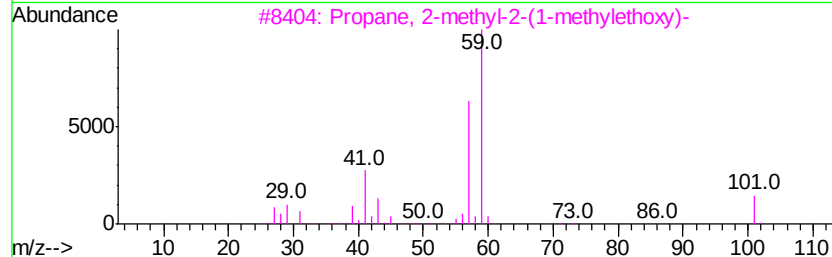
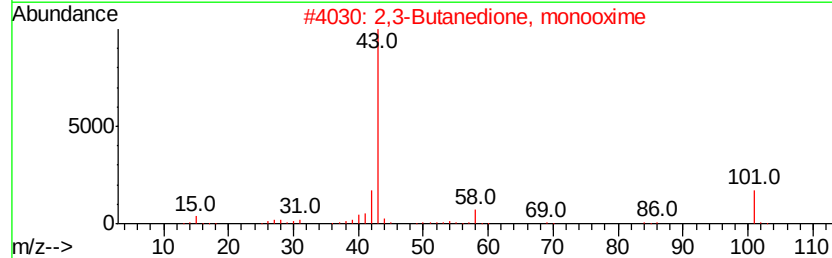
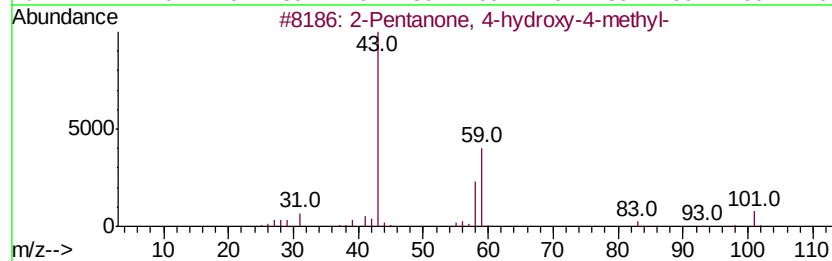
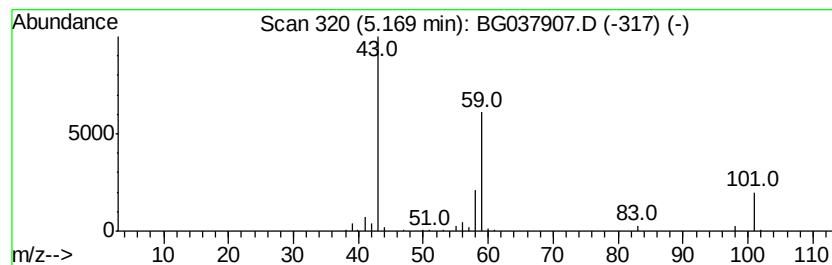
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	10.10 ng	141302	1,4-Dichlorobenzene-d4	8.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	7
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7



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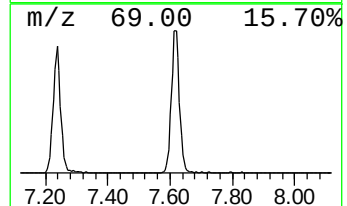
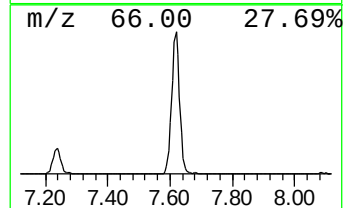
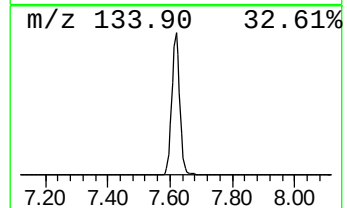
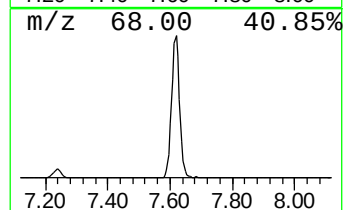
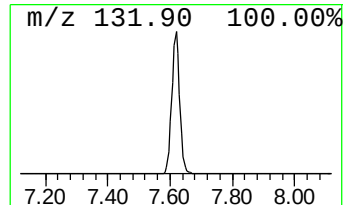
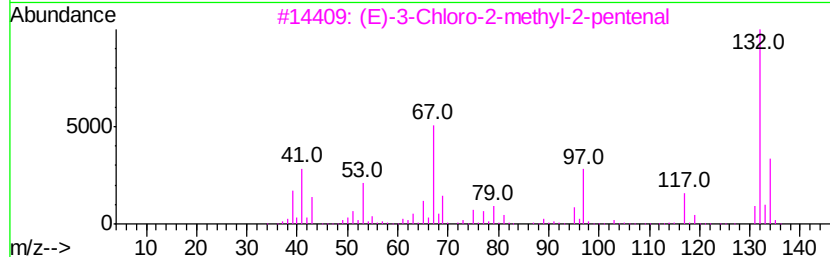
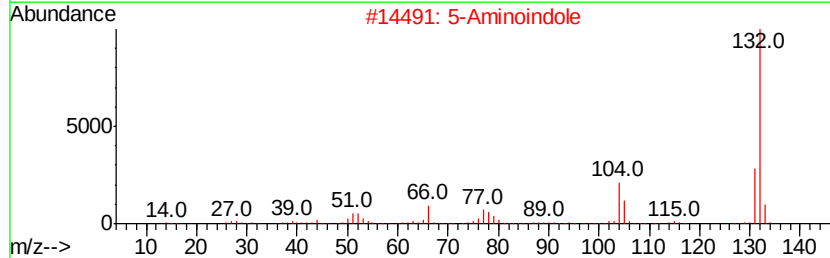
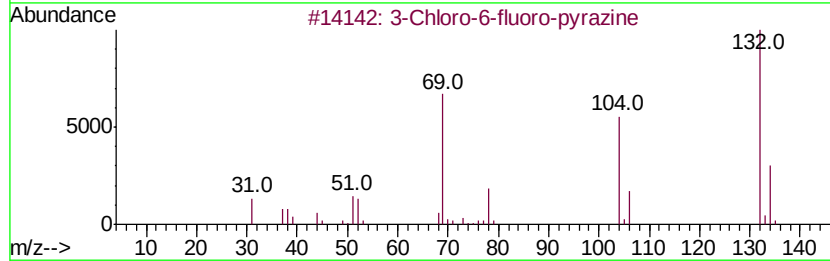
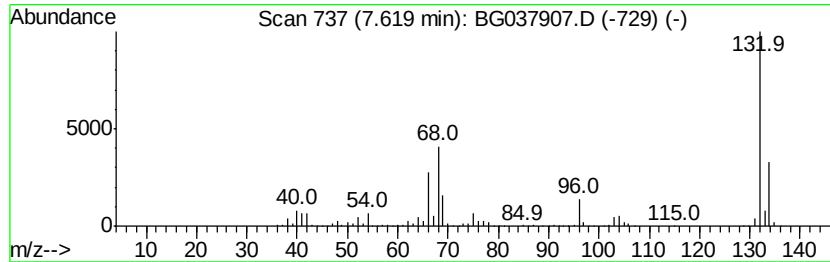
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Peak Number 5 unknown7.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	91.73 ng	1282880	1,4-Dichlorobenzene-d4	8.09

Hit#	of	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12	
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	
5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	9	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid, p...	4.68	5.0	ng	69474	1	8.09	279695	20.0
Butanoic acid, 1-...	5.13	3.4	ng	47556	1	8.09	279695	20.0
2-Pentanone, 4-hy...	5.17	10.1	ng	141302	1	8.09	279695	20.0
unknown7.62	7.62	91.7	ng	1282880	1	8.09	279695	20.0