

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012418\
 Data File : BG032267.D
 Acq On : 24 Jan 2018 19:03
 Operator : SJ/JU
 Sample : J1250-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 AB-10(0-2)

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_G\METHODS\8270-BG011218.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	3.382	9	16	24	rBV5	10785	22732	1.03%	0.183%
2	3.470	25	31	44	rVB	304267	499673	22.55%	4.022%
3	5.649	396	402	410	rBV3	21529	38584	1.74%	0.311%
4	6.155	479	488	499	rBV	419831	725949	32.76%	5.843%
5	7.835	766	774	786	rBV	427717	800560	36.12%	6.444%
6	8.235	834	842	853	rBV	437732	810668	36.58%	6.525%
7	8.722	918	925	936	rBV	118655	213410	9.63%	1.718%
8	9.057	975	982	992	rBV	339541	637469	28.77%	5.131%
9	9.921	1121	1129	1143	rVB	247465	470605	21.24%	3.788%
10	11.601	1407	1415	1429	rBB	145952	287994	13.00%	2.318%
11	13.987	1814	1821	1834	rVB	813688	1275832	57.57%	10.269%
12	14.780	1951	1956	1962	rBV	65059	96527	4.36%	0.777%
13	15.362	2047	2055	2064	rVB2	275464	457944	20.66%	3.686%
14	16.689	2275	2281	2287	rBV2	19173	28029	1.26%	0.226%
15	16.830	2298	2305	2315	rBV	716686	1127079	50.86%	9.072%
16	18.094	2512	2520	2529	rBV2	434043	681647	30.76%	5.487%
17	18.910	2655	2659	2664	rBV2	22755	33639	1.52%	0.271%
18	20.632	2945	2952	2958	rBV	1598294	2216101	100.00%	17.838%
19	21.960	3174	3178	3187	rBV3	48506	76515	3.45%	0.616%
20	22.424	3247	3257	3265	rBV2	519977	960958	43.36%	7.735%
21	26.108	3870	3884	3897	rBV2	302229	961673	43.39%	7.741%

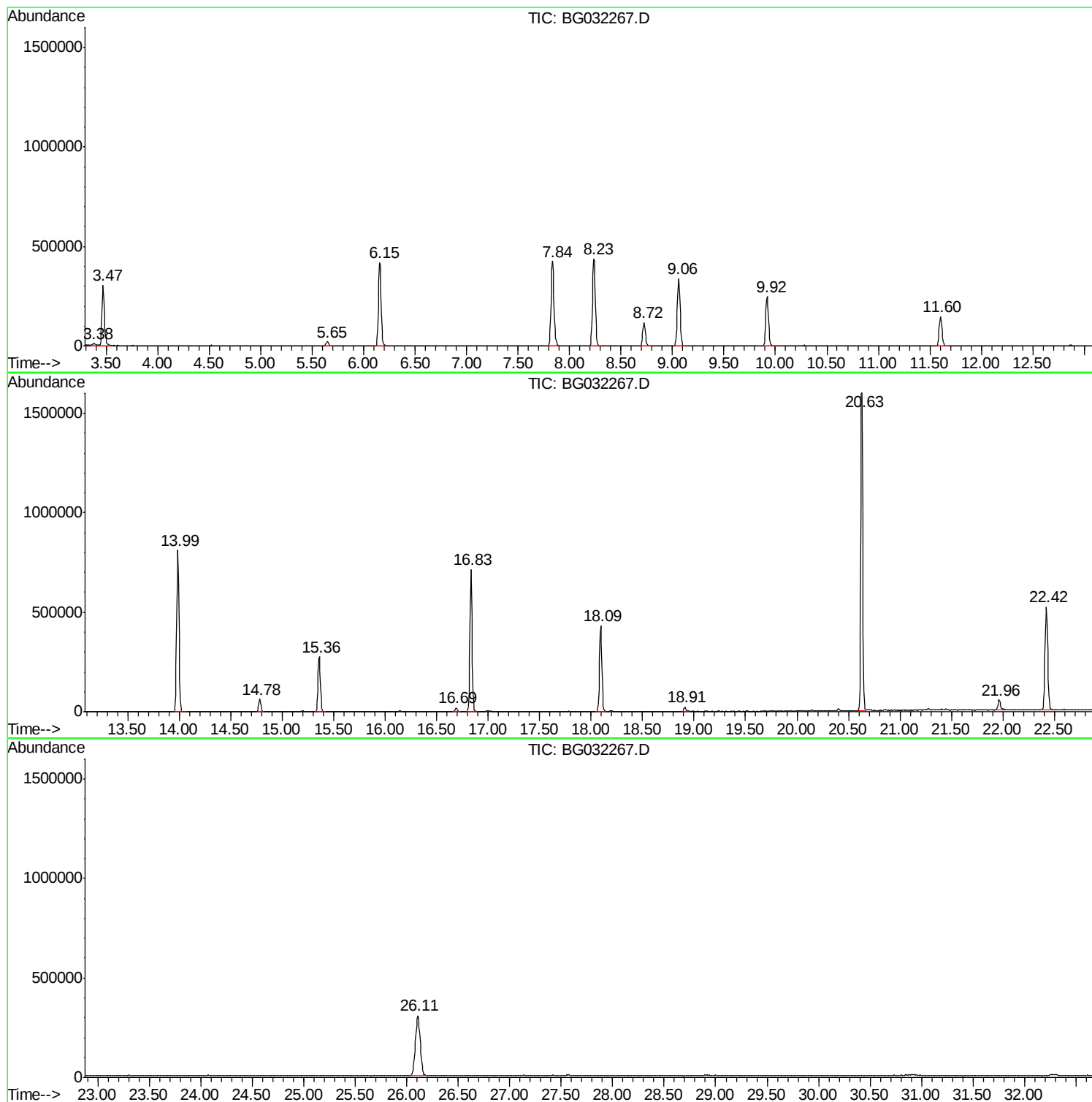
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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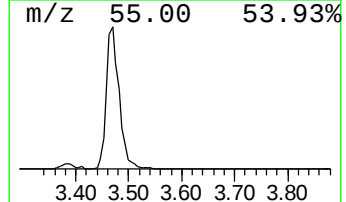
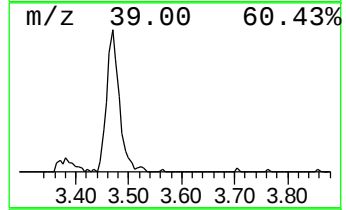
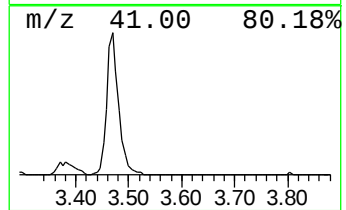
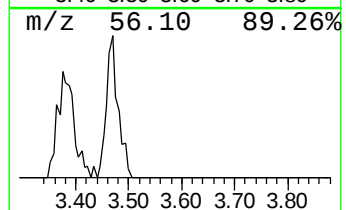
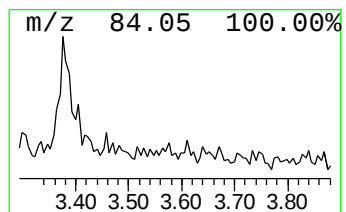
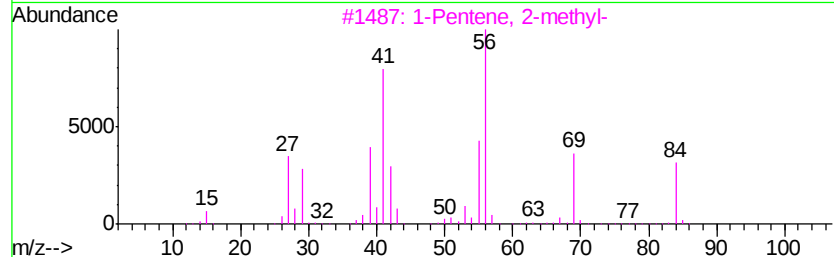
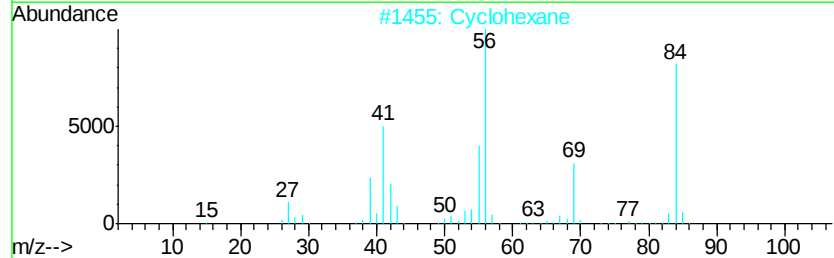
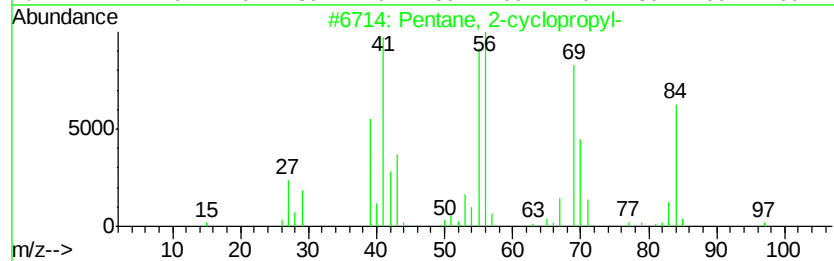
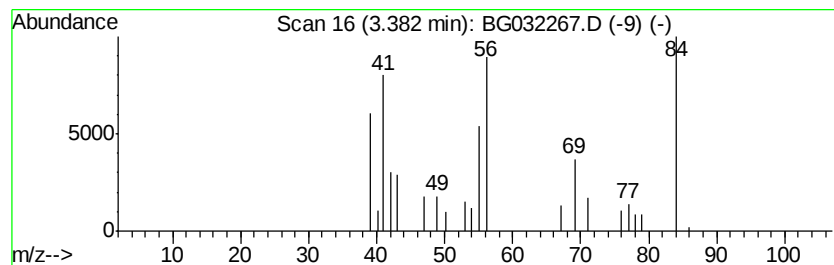
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentane, 2-cyclopropyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	2.13 ng	22732	1,4-Dichlorobenzene-d4	8.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	56
2			Cyclohexane	84	C6H12	000110-82-7	50
3			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
4			Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	43
5			2-Amino-oxazole	84	C3H4N2O	004570-45-0	40



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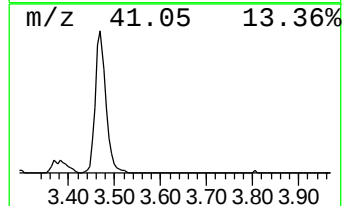
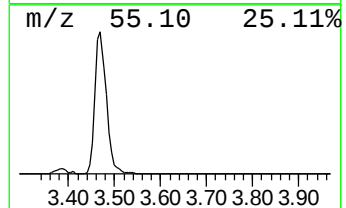
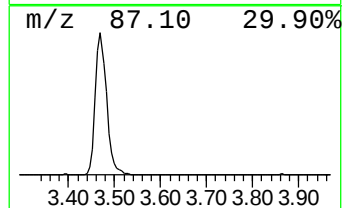
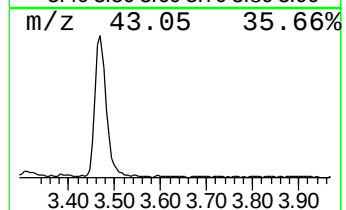
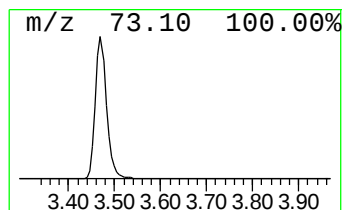
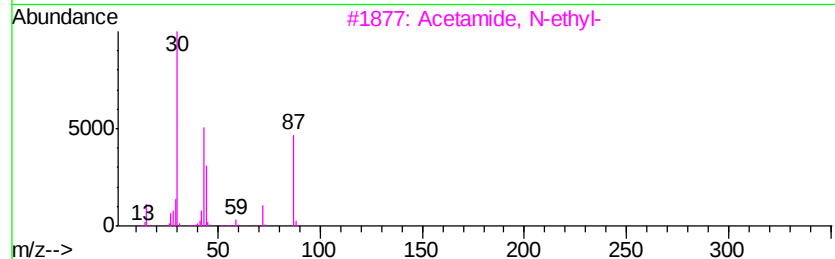
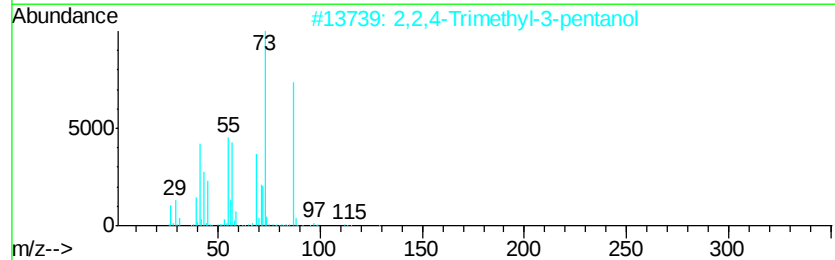
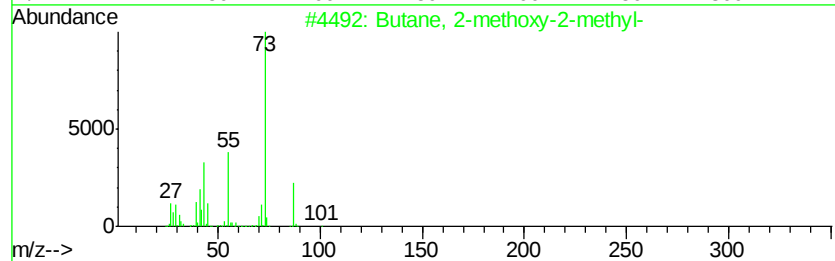
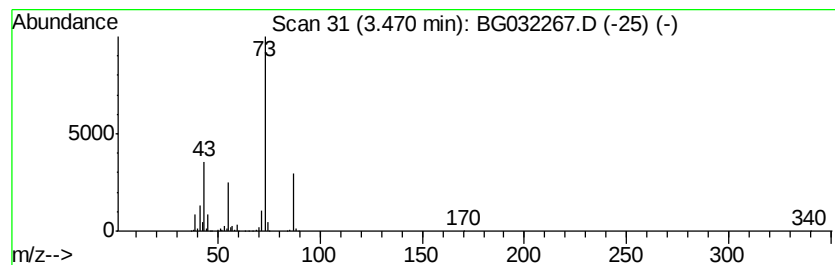
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.47	46.83 ng	499673	1,4-Dichlorobenzene-d4	8.72

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	40
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23



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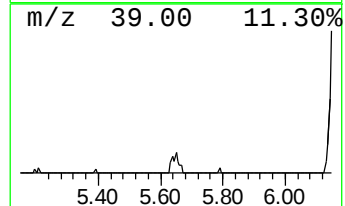
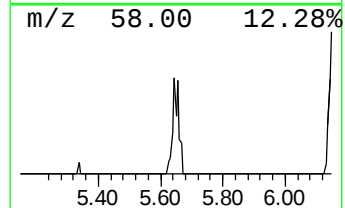
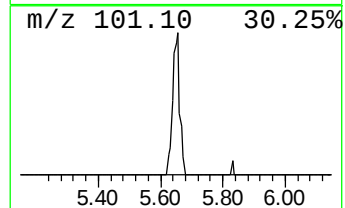
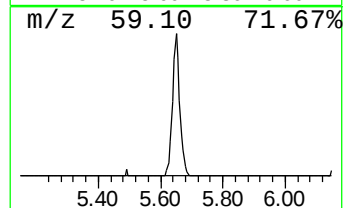
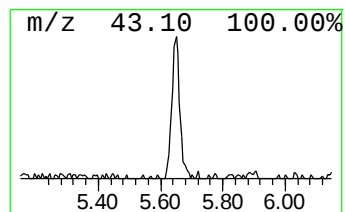
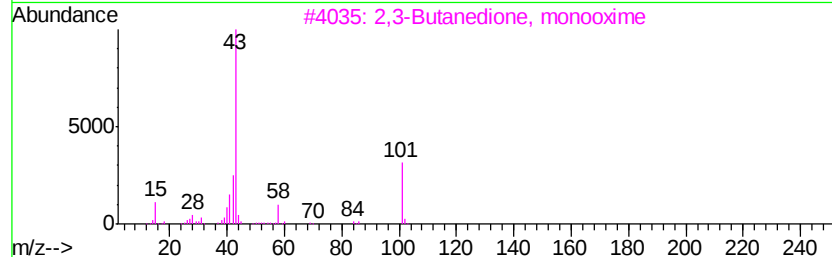
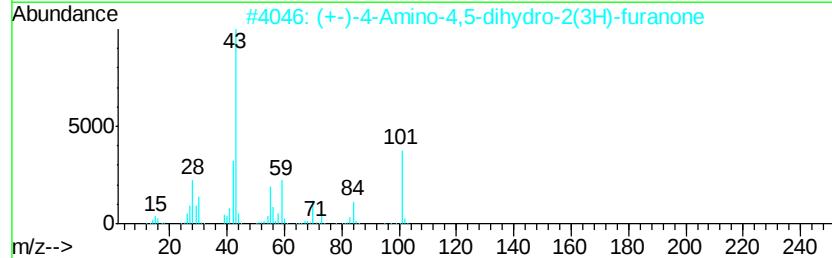
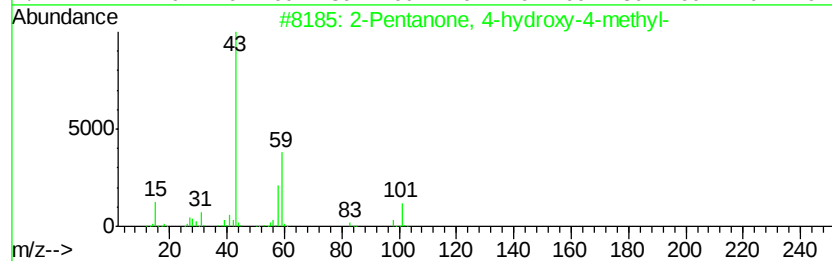
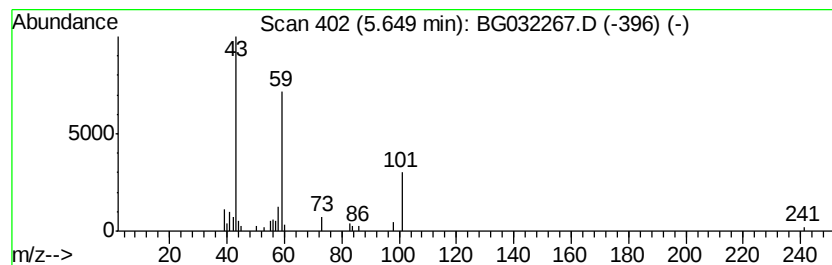
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.65	3.62 ng	38584	1,4-Dichlorobenzene-d4	8.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	43
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
5			Butanoic acid, 3-hydroxy-3-methy...	132	C6H12O3	006149-45-7	33



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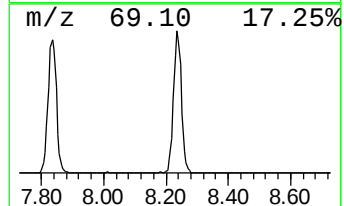
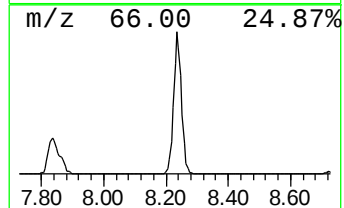
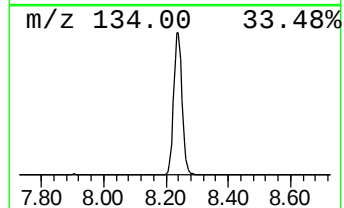
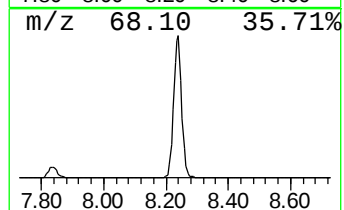
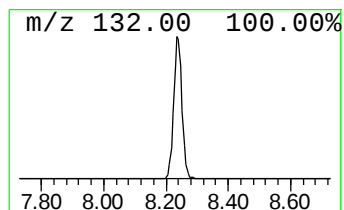
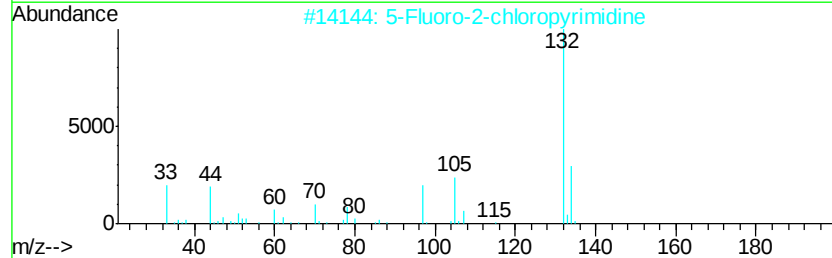
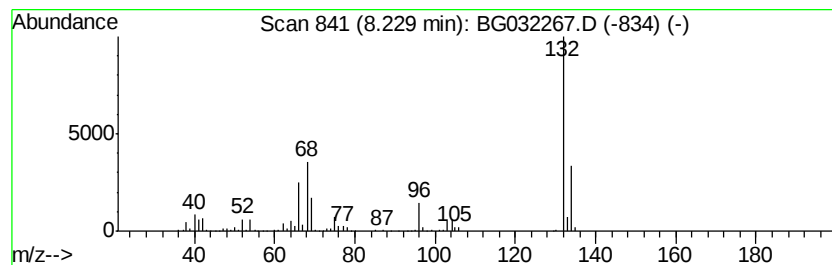
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Peak Number 4 unknown8.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.23	75.97 ng	810668	1,4-Dichlorobenzene-d4	8.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2-cyclop...	3.38	2.1	ng	22732	1	8.72	213410	20.0
Butane, 2-methoxy...	3.47	46.8	ng	499673	1	8.72	213410	20.0
2-Pentanone, 4-hy...	5.65	3.6	ng	38584	1	8.72	213410	20.0
unknown8.23	8.23	76.0	ng	810668	1	8.72	213410	20.0