

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040618\
 Data File : BG033671.D
 Acq On : 7 Apr 2018 19:57
 Operator : SJ/JU
 Sample : J2225-11
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 040218-SIDI-F-D-B

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-BG031918.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	3.476	26	32	42	rBV	144511	278503	7.29%	1.859%
2	3.565	42	47	55	rVB	109317	168789	4.42%	1.127%
3	5.768	416	422	432	rBV2	29163	55324	1.45%	0.369%
4	6.285	502	510	525	rBV	137539	314743	8.24%	2.101%
5	7.977	791	798	814	rBV	73421	226407	5.93%	1.511%
6	8.371	858	865	881	rBV2	328986	730778	19.13%	4.879%
7	8.858	942	948	961	rBV	88359	219614	5.75%	1.466%
8	9.193	995	1005	1018	rBV	465602	973408	25.48%	6.498%
9	10.057	1144	1152	1173	rBV	402863	949408	24.85%	6.338%
10	11.737	1430	1438	1455	rBV	157811	355141	9.30%	2.371%
11	14.105	1834	1841	1862	rBV	1362521	2414384	63.21%	16.118%
12	14.898	1967	1976	1981	rBV	48229	81653	2.14%	0.545%
13	15.474	2068	2074	2084	rBV2	332432	588786	15.41%	3.931%
14	16.238	2199	2204	2211	rVB	30390	40752	1.07%	0.272%
15	16.949	2318	2325	2339	rBV	721389	1249333	32.71%	8.340%
16	17.096	2345	2350	2361	rVB2	26879	51434	1.35%	0.343%
17	18.206	2530	2539	2551	rBV	435937	757617	19.83%	5.058%
18	20.727	2962	2968	2979	rBV	2664777	3819850	100.00%	25.501%
19	22.078	3193	3198	3207	rBV5	31447	81904	2.14%	0.547%
20	22.554	3271	3279	3293	rBV	411875	840097	21.99%	5.608%
21	24.417	3590	3596	3604	rBV5	18895	43564	1.14%	0.291%
22	26.320	3909	3920	3941	rBV2	206377	737966	19.32%	4.927%

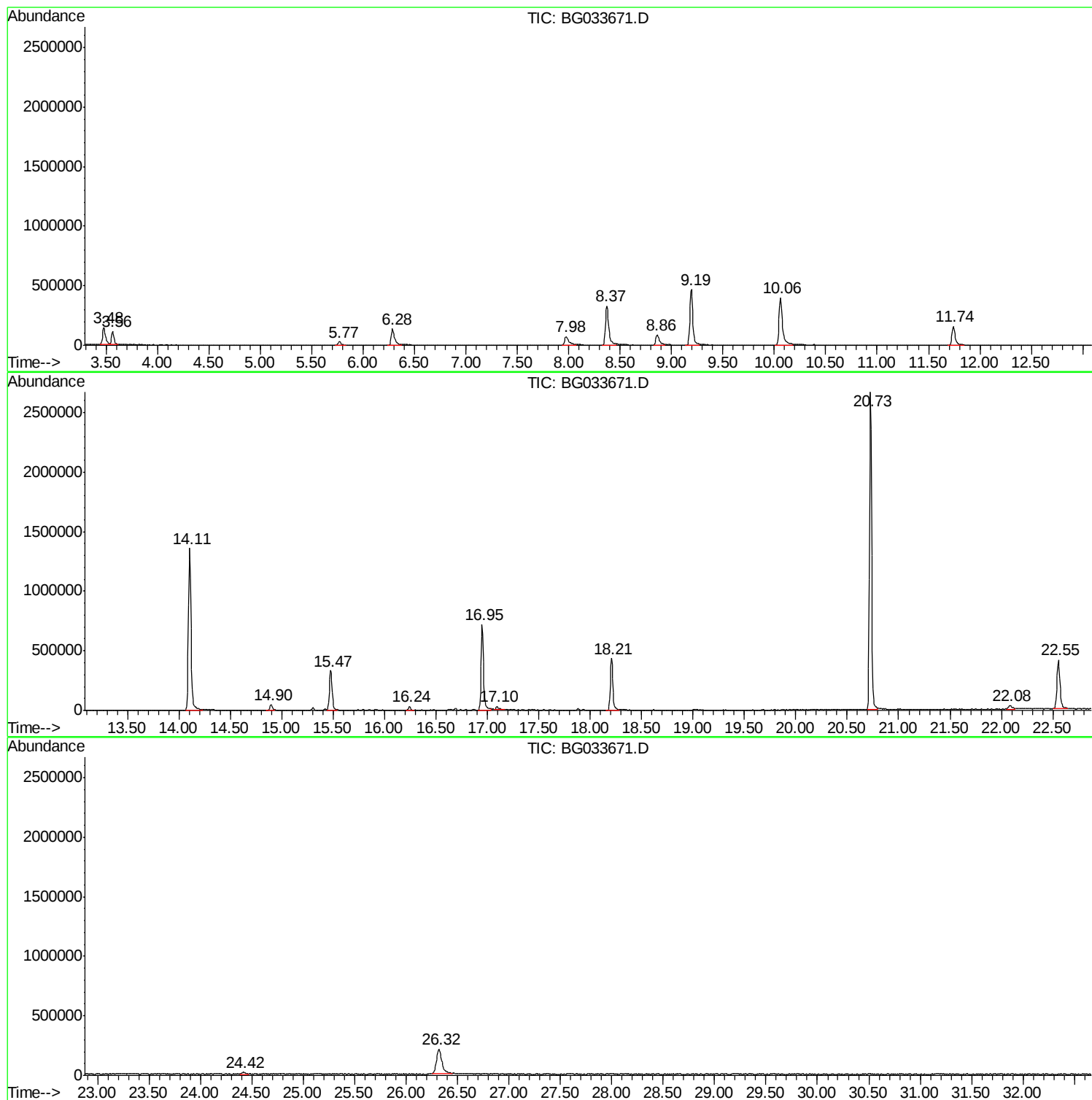
Sum of corrected areas: 14979455

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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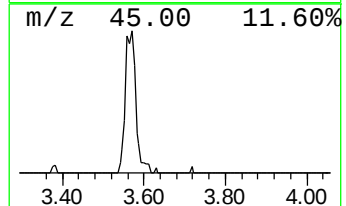
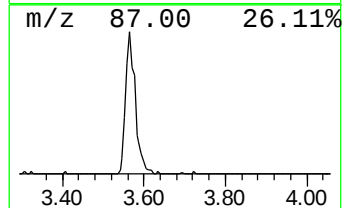
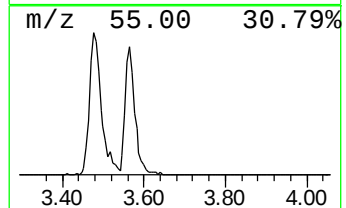
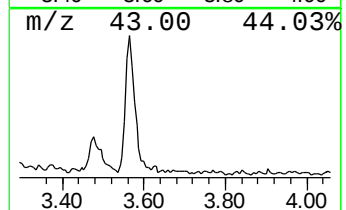
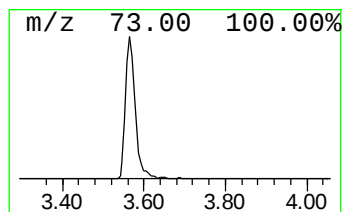
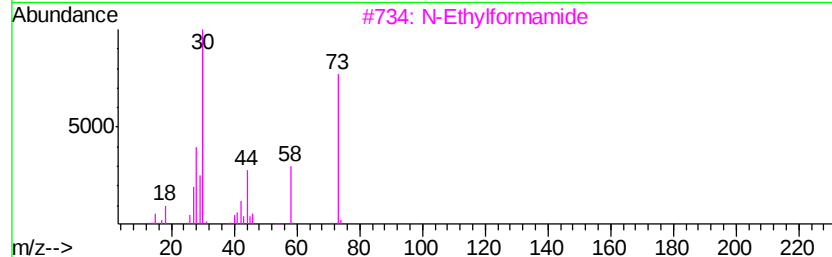
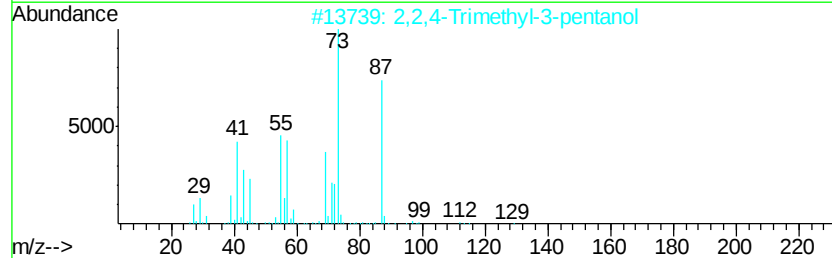
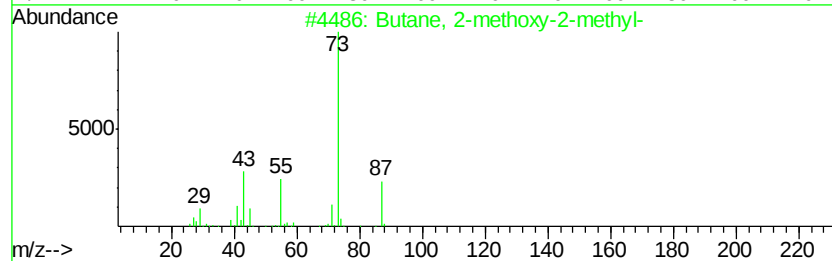
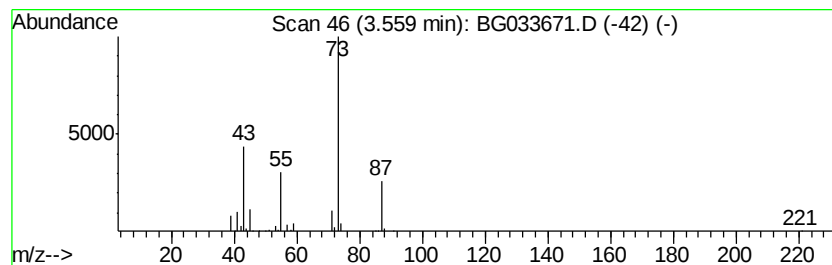
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.56	15.37 ng	168789	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	42
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9



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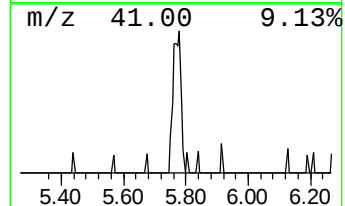
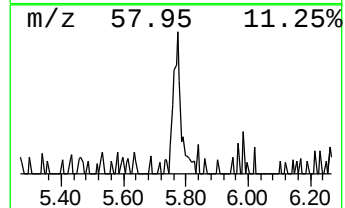
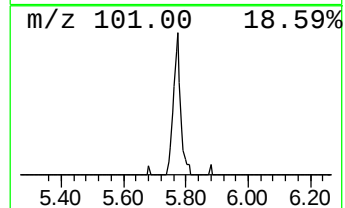
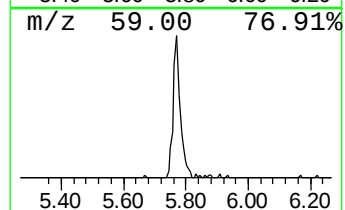
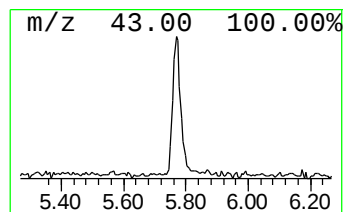
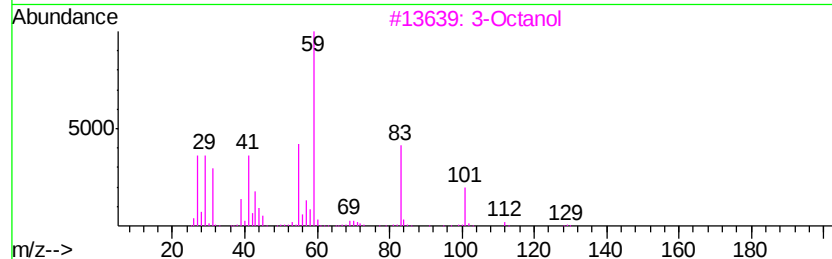
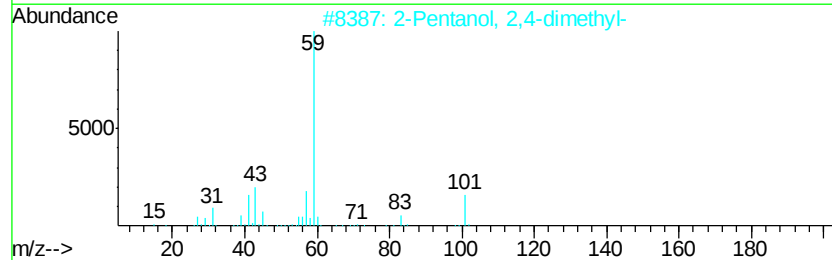
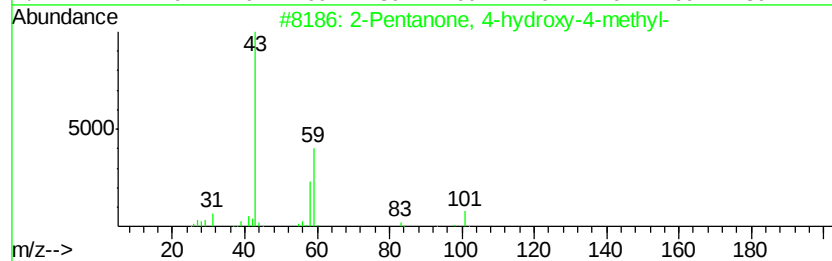
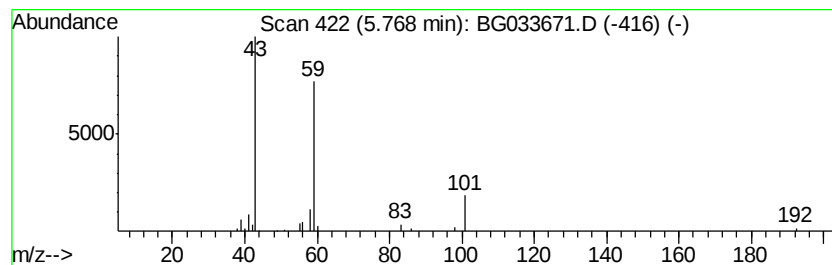
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	5.04 ng	55324	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	45
3		3-Octanol	130	C8H18O	000589-98-0	38
4		3-Heptanol	116	C7H16O	000589-82-2	36
5		Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	36



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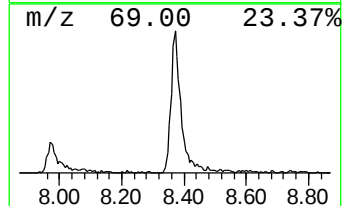
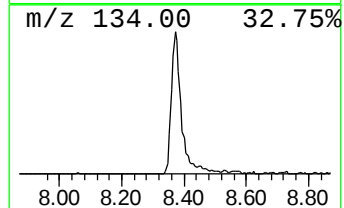
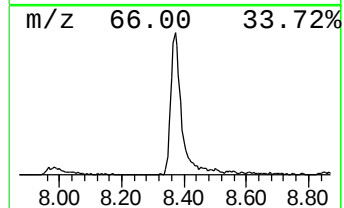
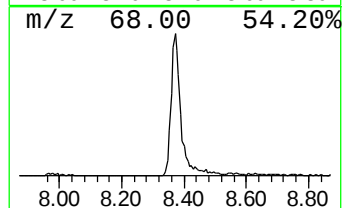
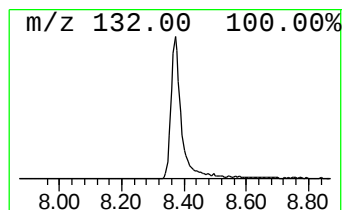
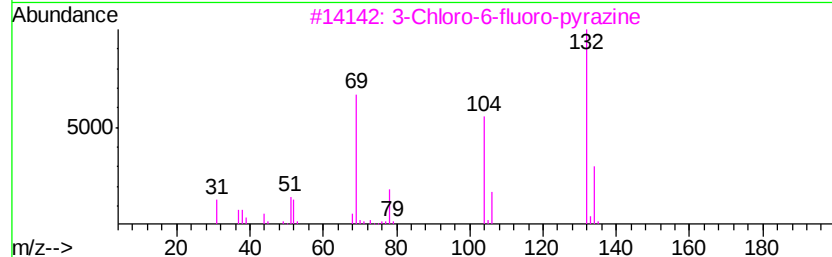
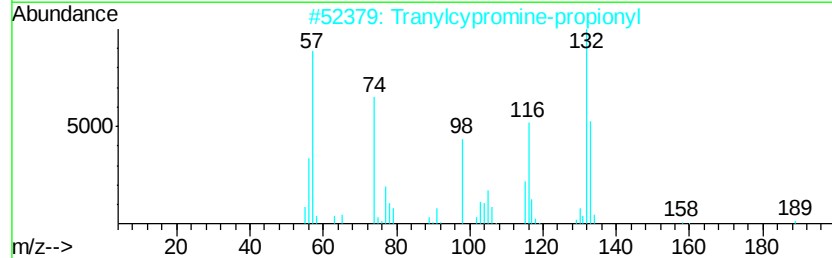
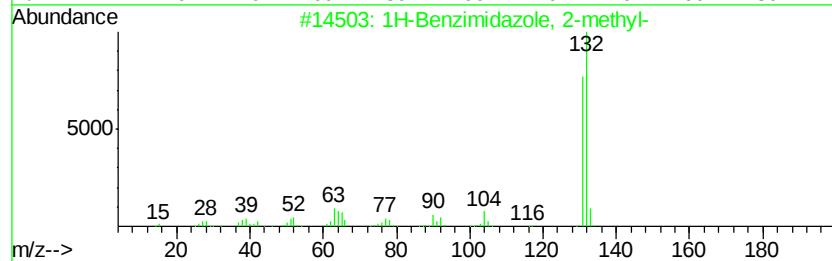
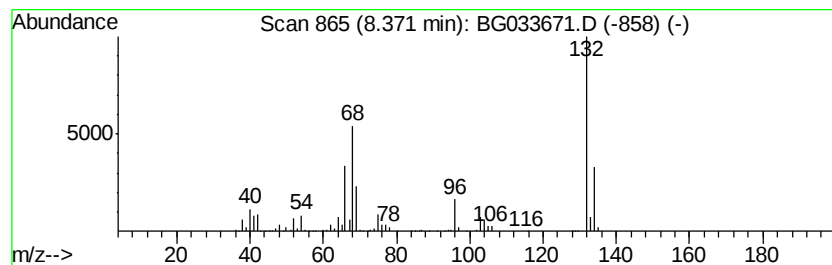
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Peak Number 4 unknown8.37 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	66.55 ng	730778	1,4-Dichlorobenzene-d4	8.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
3			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5			(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.56	15.4	ng	168789	1	8.86	219614	20.0
2-Pentanone, 4-hy...	5.77	5.0	ng	55324	1	8.86	219614	20.0
unknown8.37	8.37	66.5	ng	730778	1	8.86	219614	20.0