

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
 Data File : BG024587.D
 Acq On : 1 Nov 2016 11:29
 Operator : UM/SJ
 Sample : H5478-03
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SD-4

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:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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	3.132	44	50	70	rVB	9417261	20088309	100.00%	26.844%
2	5.335	417	425	435	rVB	524134	882258	4.39%	1.179%
3	5.799	497	504	515	rBV	2512085	4326343	21.54%	5.781%
4	7.403	769	777	787	rBV	2595698	4699405	23.39%	6.280%
5	7.797	836	844	853	rBV	2494496	4519335	22.50%	6.039%
6	8.267	917	924	932	rBV	453095	812332	4.04%	1.086%
7	8.596	969	980	988	rBV	1924792	3426523	17.06%	4.579%
8	9.442	1116	1124	1136	rBV	1562196	2951680	14.69%	3.944%
9	11.093	1398	1405	1414	rVB	566496	1089460	5.42%	1.456%
10	13.508	1805	1816	1827	rVB	3810259	6098857	30.36%	8.150%
11	14.318	1948	1954	1961	rBV	936851	1449903	7.22%	1.938%
12	14.882	2042	2050	2060	rVB	975148	1549078	7.71%	2.070%
13	16.363	2294	2302	2313	rBV	3542381	5639901	28.08%	7.537%
14	17.626	2510	2517	2527	rVB2	1239047	1981505	9.86%	2.648%
15	20.206	2949	2956	2962	rBV	7062130	9576852	47.67%	12.798%
16	21.498	3170	3176	3182	rBV4	110275	203309	1.01%	0.272%
17	21.915	3240	3247	3257	rVB	1559955	2740705	13.64%	3.662%
18	25.347	3819	3831	3843	rVB2	901144	2796928	13.92%	3.738%

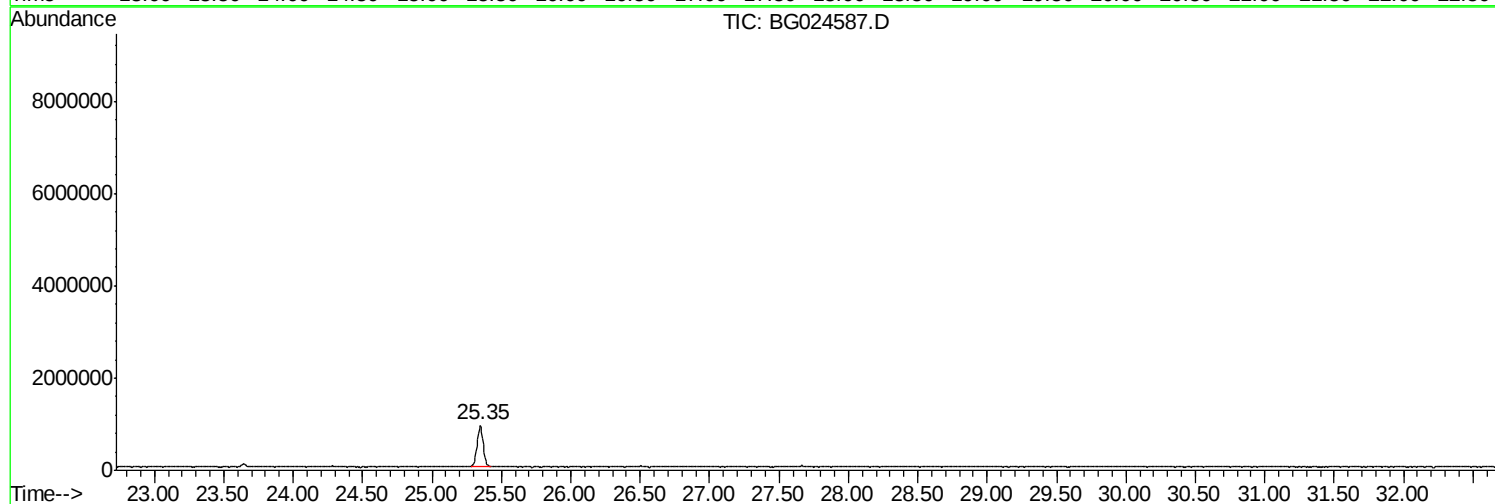
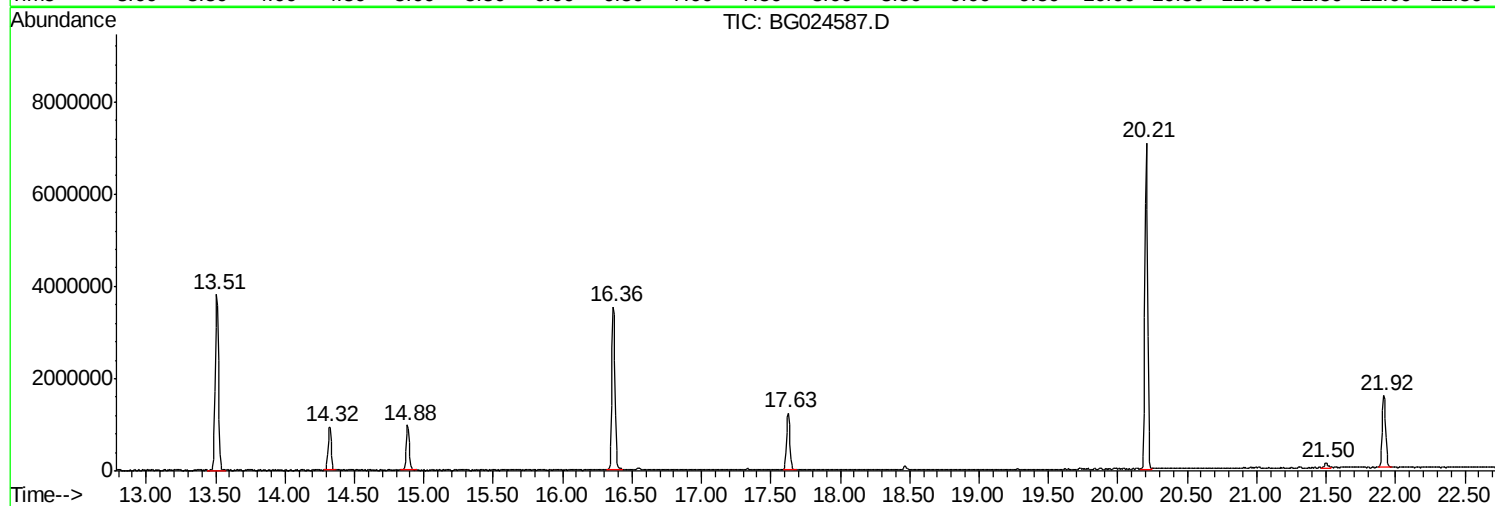
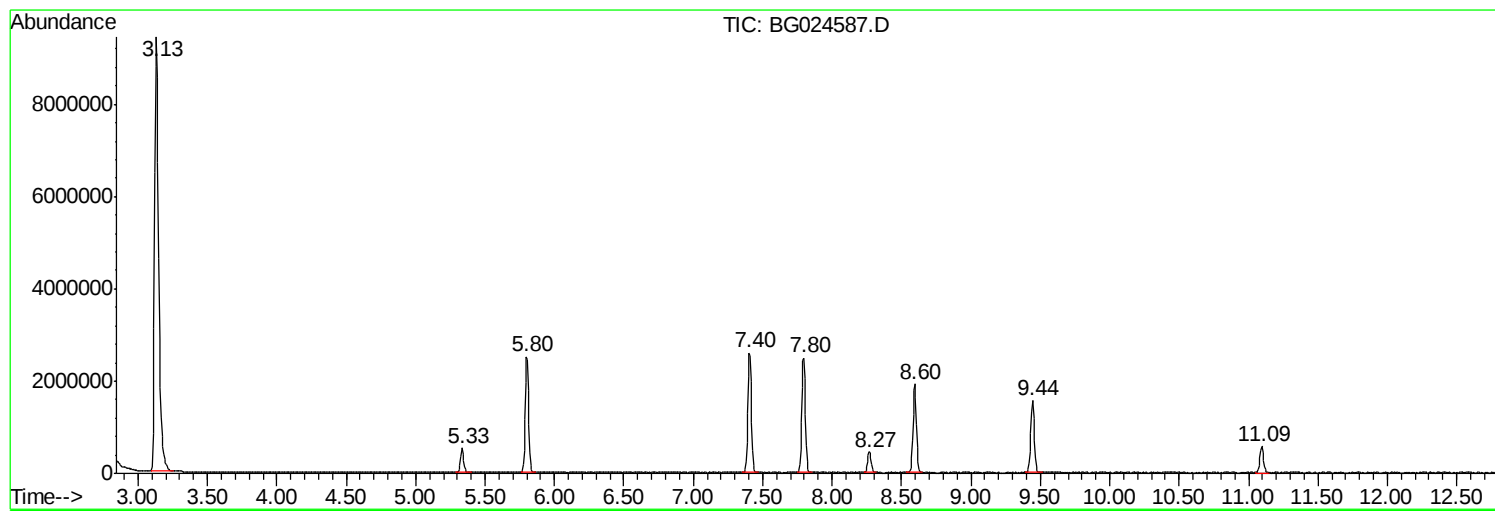
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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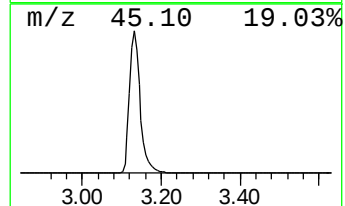
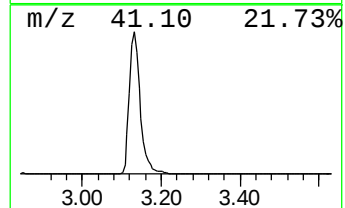
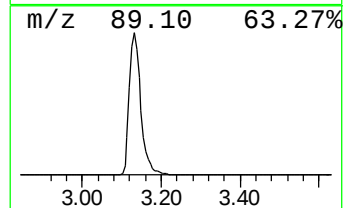
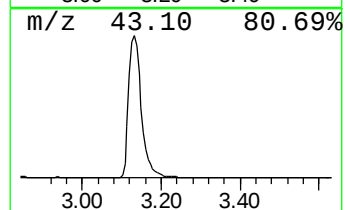
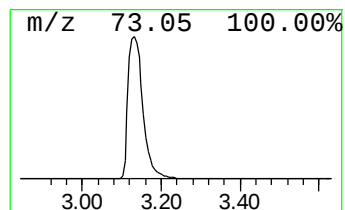
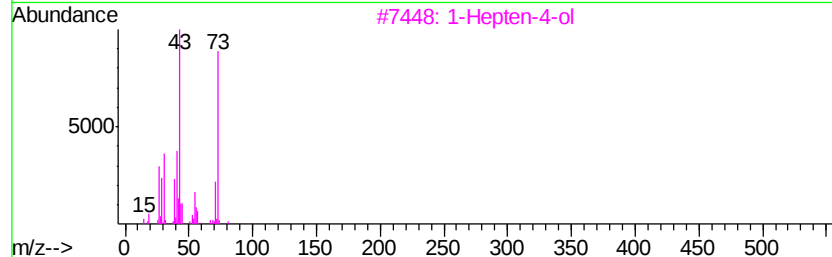
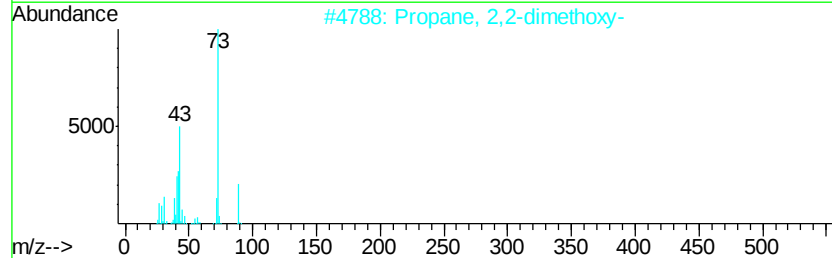
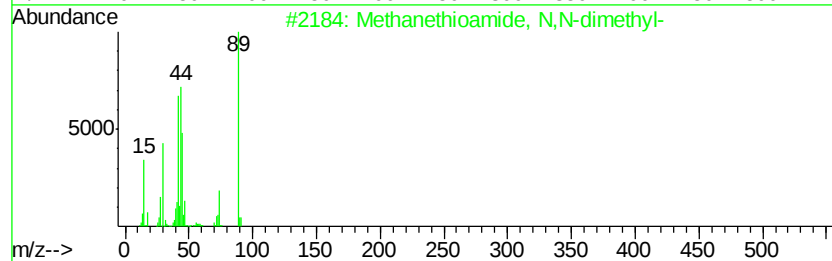
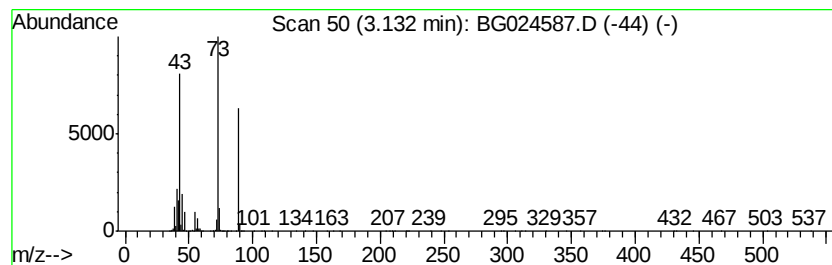
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	494.58 ng	20088300	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	38
2		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	25
3		1-Hepten-4-ol	114	C7H14O	003521-91-3	23
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	16
5		2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	12



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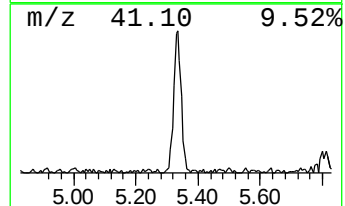
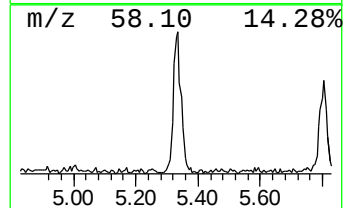
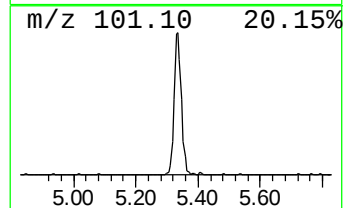
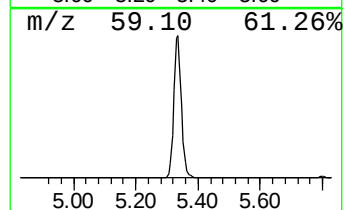
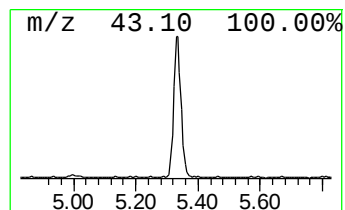
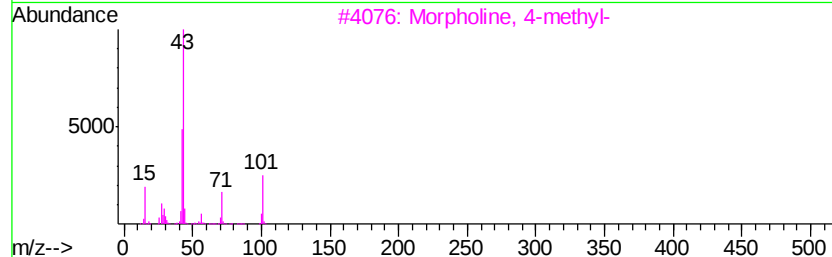
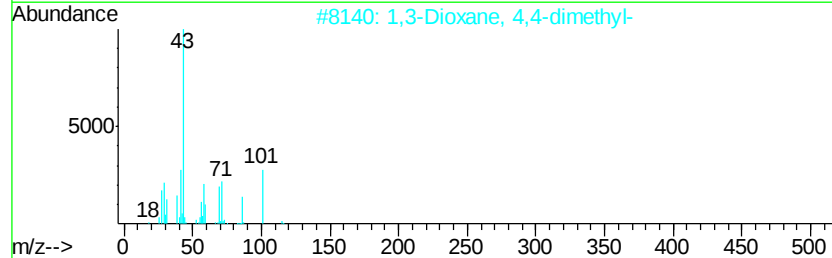
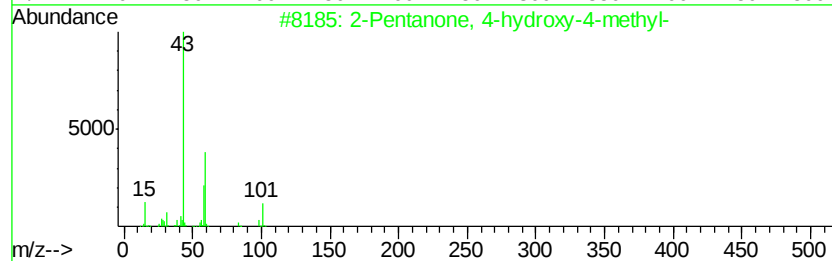
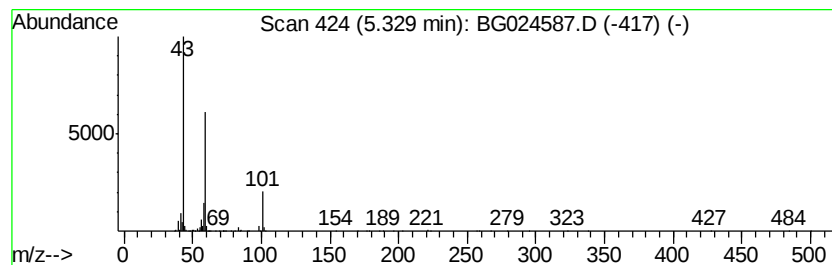
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	21.72 ng	882258	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9



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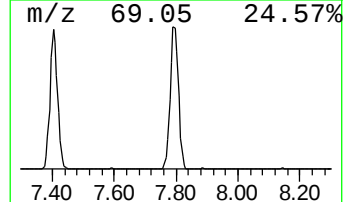
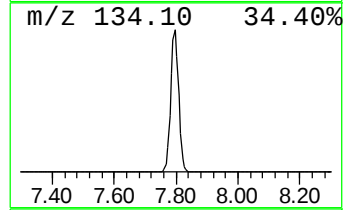
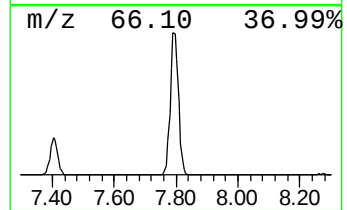
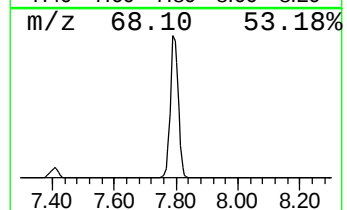
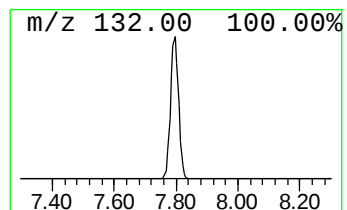
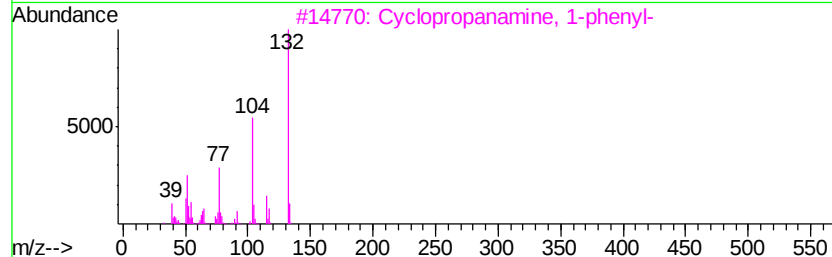
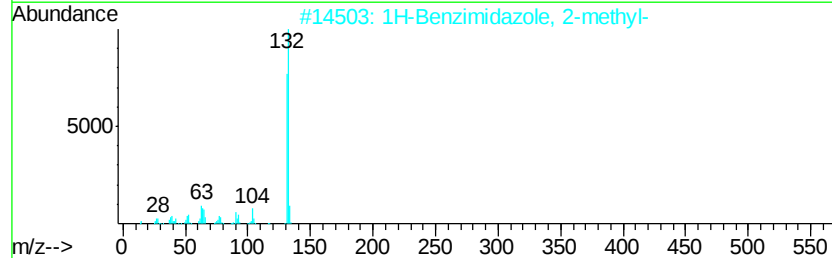
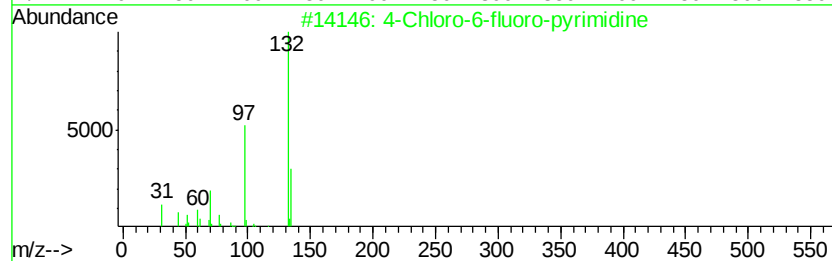
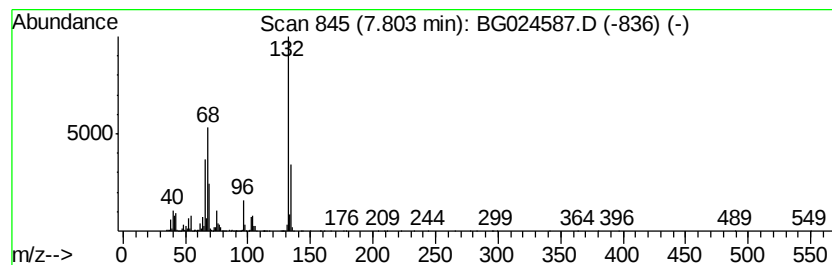
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Peak Number 3 unknown7.80 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	111.27 ng	4519340	1,4-Dichlorobenzene-d4	8.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.13	3.13	494.6	ng	20088300	1	8.27	812332	20.0
2-Pentanone, 4-hy...	5.33	21.7	ng	882258	1	8.27	812332	20.0
unknown7.80	7.80	111.3	ng	4519340	1	8.27	812332	20.0