

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
 Data File : BG024680.D
 Acq On : 4 Nov 2016 13:22
 Operator : UM/SJ
 Sample : H5502-20
 Misc :
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-88-19.5-20.0

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-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	3.126	43	49	71	rVB	7269764	12456452	100.00%	19.606%
2	5.330	417	424	431	rBV	504210	807844	6.49%	1.272%
3	5.800	494	504	514	rBV	2206572	3731850	29.96%	5.874%
4	7.404	769	777	787	rBV	2314243	4170372	33.48%	6.564%
5	7.791	833	843	853	rBV	2170704	3917947	31.45%	6.167%
6	8.267	916	924	934	rBV	424262	746420	5.99%	1.175%
7	8.590	969	979	991	rBV	1582156	2873960	23.07%	4.524%
8	9.442	1115	1124	1134	rBV	1414705	2615200	20.99%	4.116%
9	11.093	1398	1405	1414	rVB	523483	960154	7.71%	1.511%
10	13.508	1804	1816	1823	rBV	3331415	5312313	42.65%	8.362%
11	14.319	1947	1954	1962	rBV	841804	1265447	10.16%	1.992%
12	14.883	2042	2050	2057	rBV	886971	1384093	11.11%	2.179%
13	16.364	2295	2302	2310	rBV	3647321	5666522	45.49%	8.919%
14	17.621	2510	2516	2524	rBV	1215694	1953182	15.68%	3.074%
15	18.467	2654	2660	2666	rBV4	101462	174328	1.40%	0.274%
16	20.206	2949	2956	2966	rBV	6989464	9709682	77.95%	15.283%
17	21.499	3170	3176	3180	rBV5	130337	224324	1.80%	0.353%
18	21.922	3240	3248	3255	rVB	1587324	2764602	22.19%	4.351%
19	25.353	3819	3832	3847	rVB2	895446	2797797	22.46%	4.404%

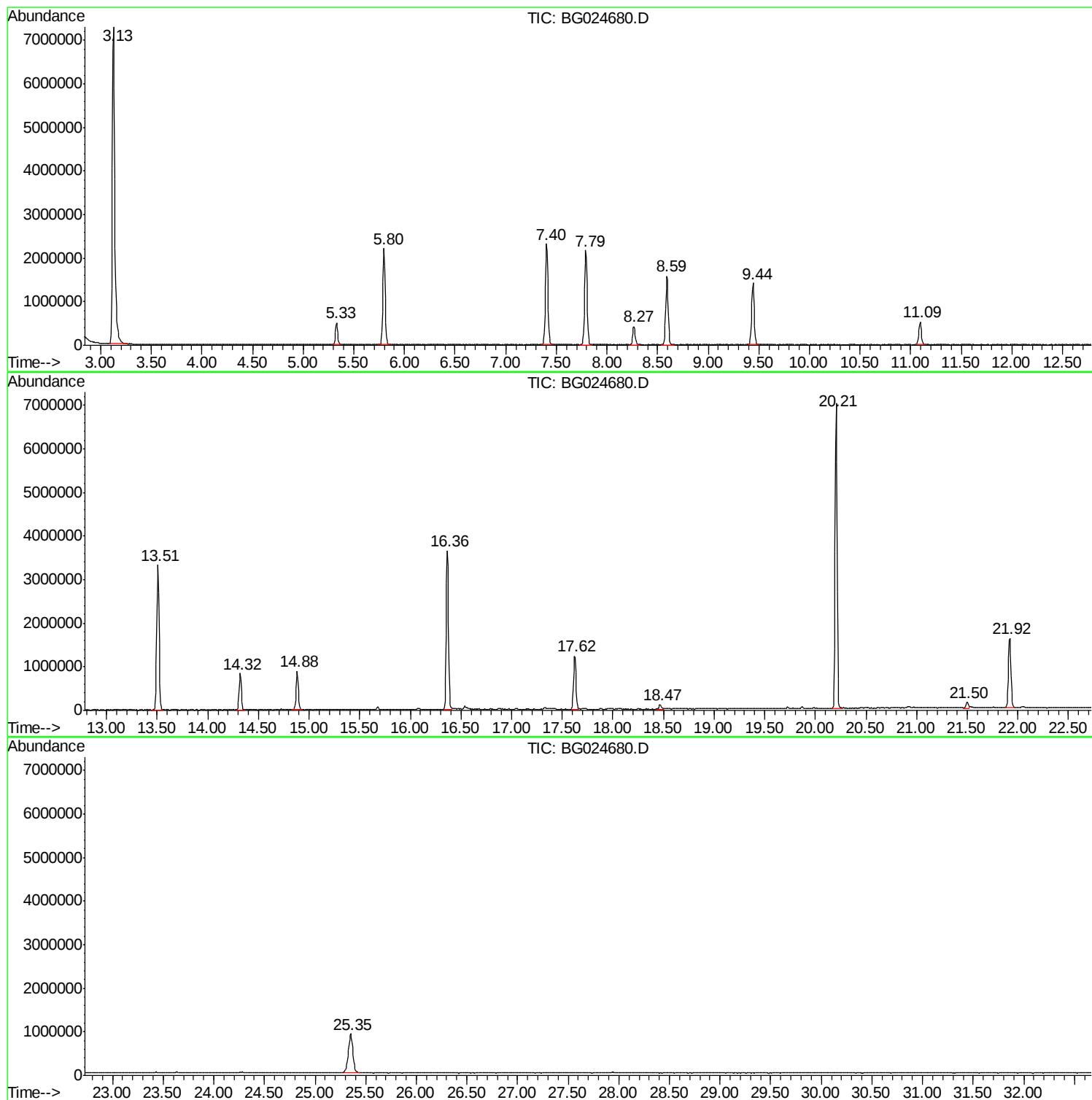
Sum of corrected areas: 63532489

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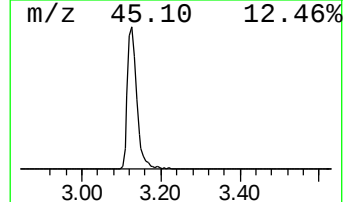
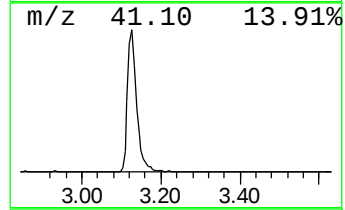
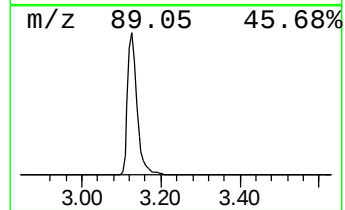
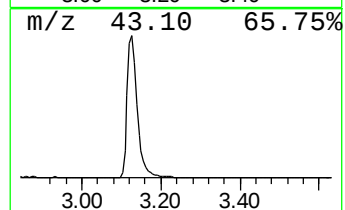
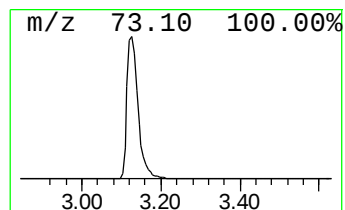
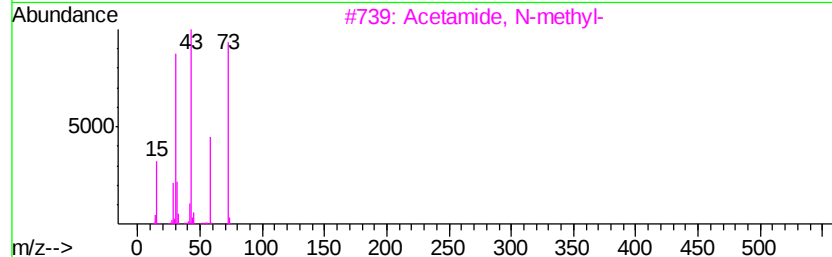
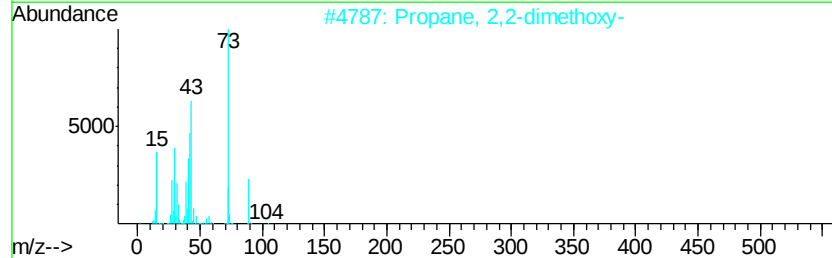
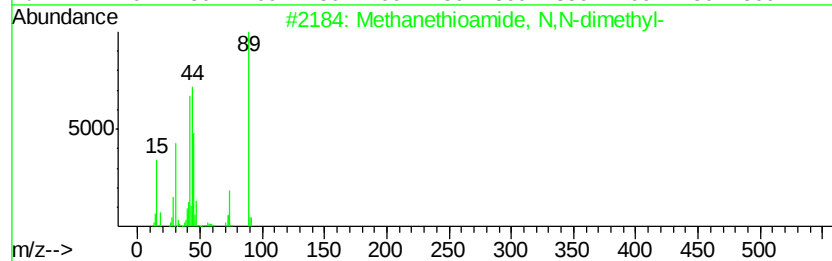
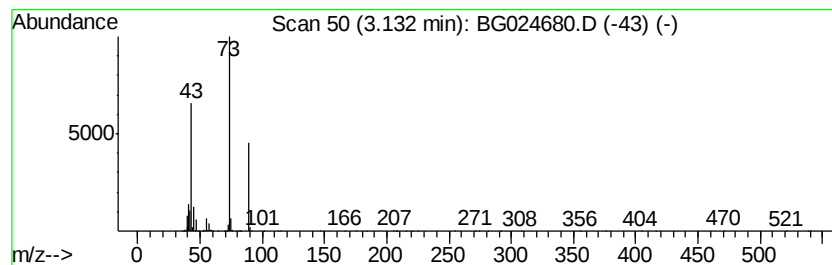
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	333.77 ng	12456500	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	42
2		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	25
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	12
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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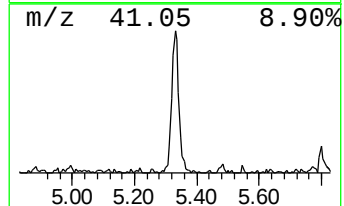
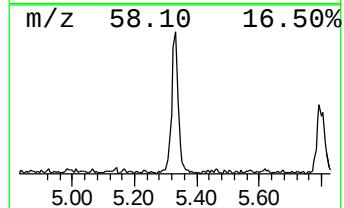
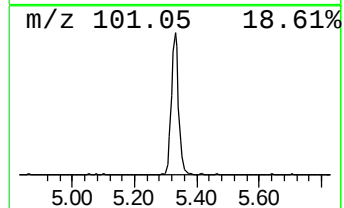
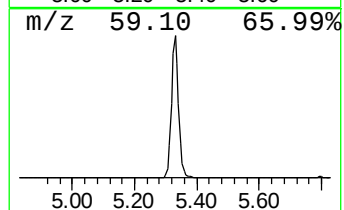
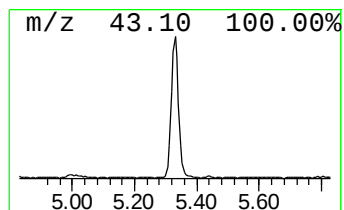
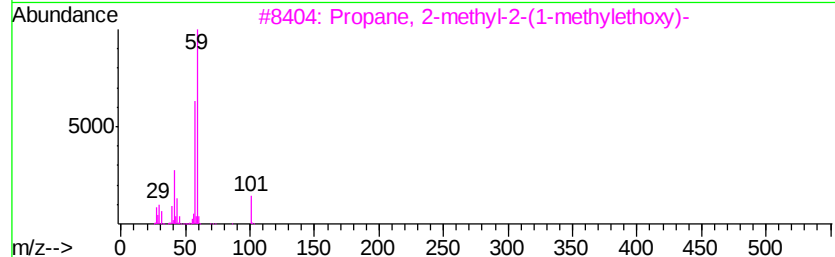
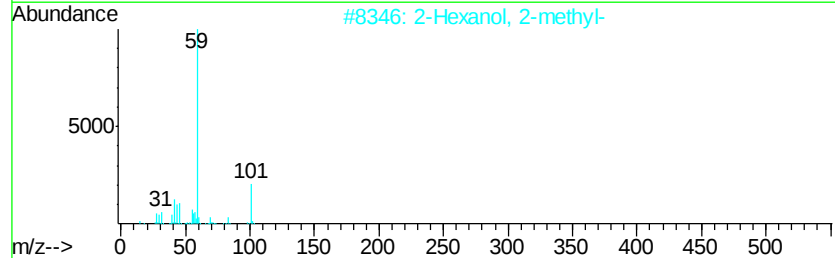
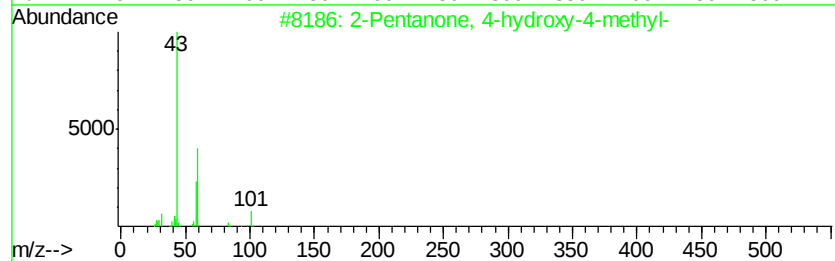
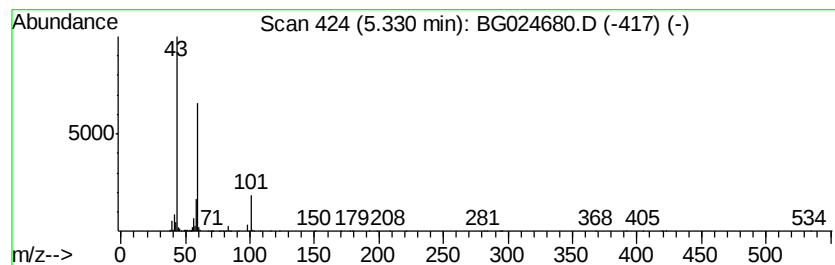
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	21.65 ng	807844	1,4-Dichlorobenzene-d4	8.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			3-Octanol	130	C8H18O	000589-98-0	28
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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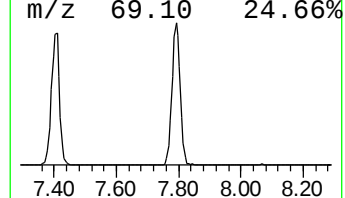
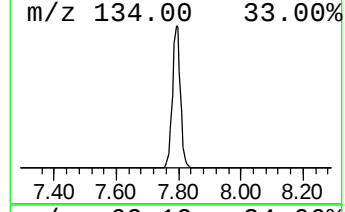
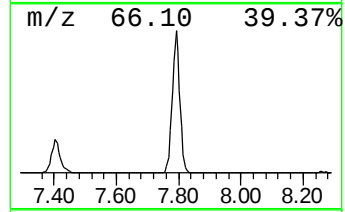
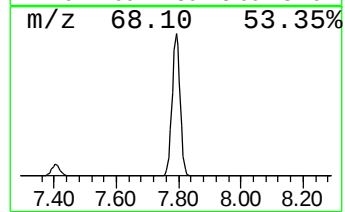
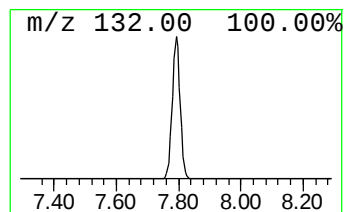
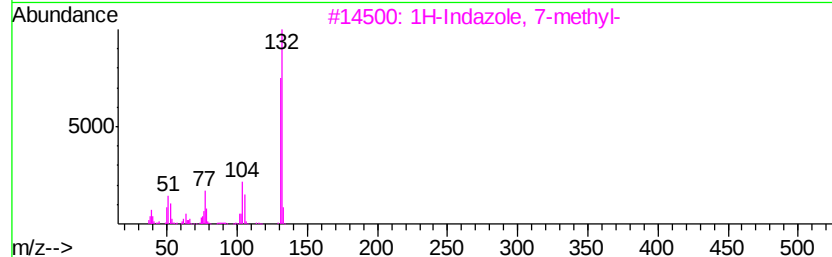
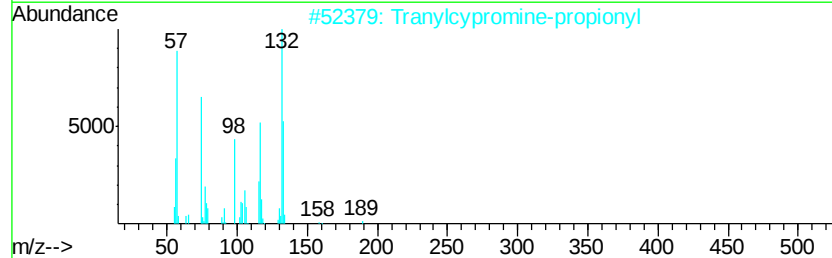
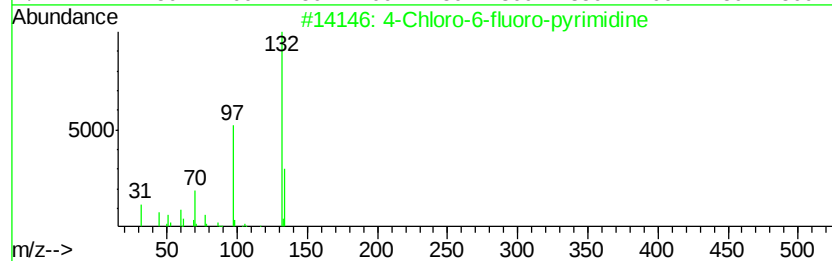
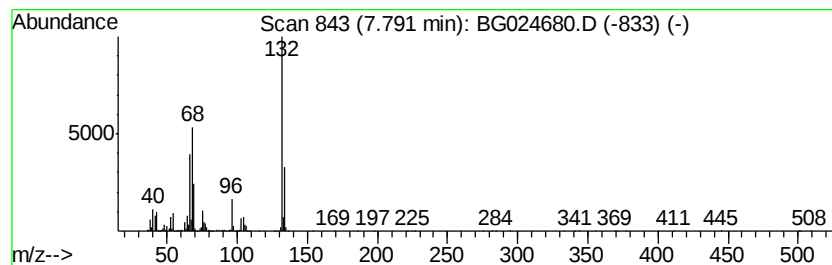
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Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	104.98 ng	3917950	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.13	3.13	333.8	ng	12456500	1	8.27	746420	20.0
2-Pentanone, 4-hy...	5.33	21.6	ng	807844	1	8.27	746420	20.0
unknown7.79	7.79	105.0	ng	3917950	1	8.27	746420	20.0