

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110216\
Data File : BG024633.D
Acq On : 2 Nov 2016 19:58
Operator : UM/SJ
Sample : PB94494BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB94494BL

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	68	rVB	9645202	18383434	100.00%	28.838%
2	5.329	417	424	432	rVB	433066	686500	3.73%	1.077%
3	5.799	497	504	513	rBV	2065107	3411722	18.56%	5.352%
4	7.403	768	777	786	rBV	2096105	3658479	19.90%	5.739%
5	7.791	836	843	852	rBV	1956060	3493359	19.00%	5.480%
6	8.267	917	924	931	rBV2	411807	726072	3.95%	1.139%
7	8.596	972	980	988	rBV	1495025	2684064	14.60%	4.210%
8	9.442	1113	1124	1134	rBV	1271400	2294674	12.48%	3.600%
9	11.093	1396	1405	1415	rBV	549525	985116	5.36%	1.545%
10	13.508	1809	1816	1823	rVB	3157888	4993606	27.16%	7.833%
11	14.883	2043	2050	2057	rVB	853205	1337330	7.27%	2.098%
12	16.363	2294	2302	2318	rBV	2778531	4391538	23.89%	6.889%
13	17.621	2510	2516	2525	rVB	1093842	1774083	9.65%	2.783%
14	20.206	2950	2956	2966	rVB	7060060	9544303	51.92%	14.972%
15	21.916	3240	3247	3255	rBV	1573202	2708281	14.73%	4.248%
16	25.347	3818	3831	3845	rBV	856991	2675630	14.55%	4.197%

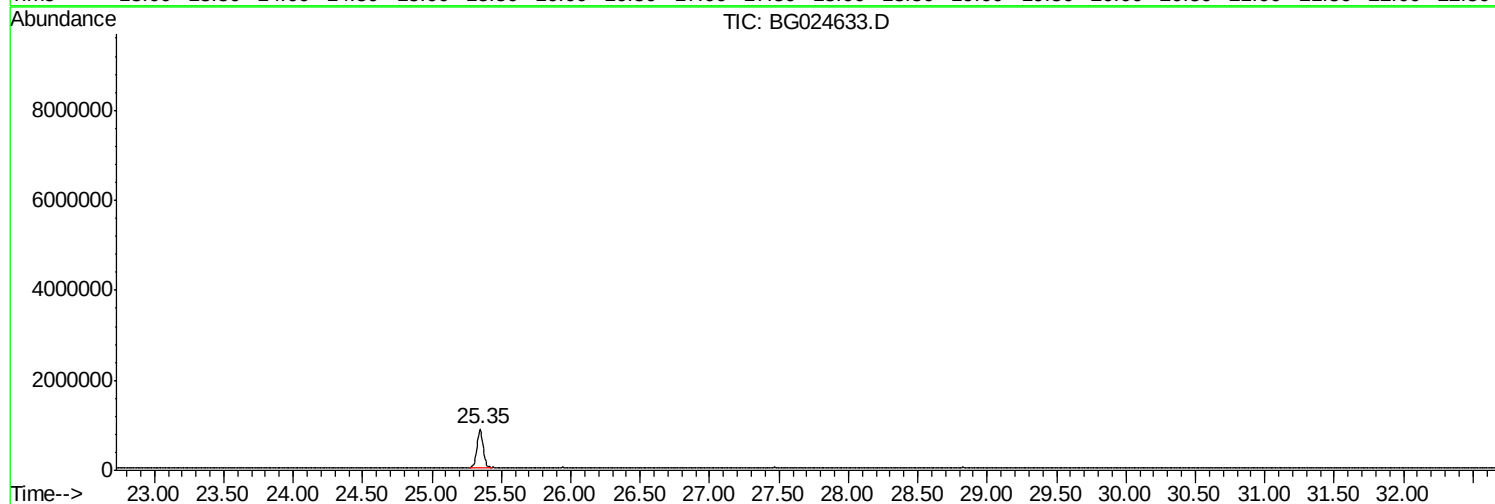
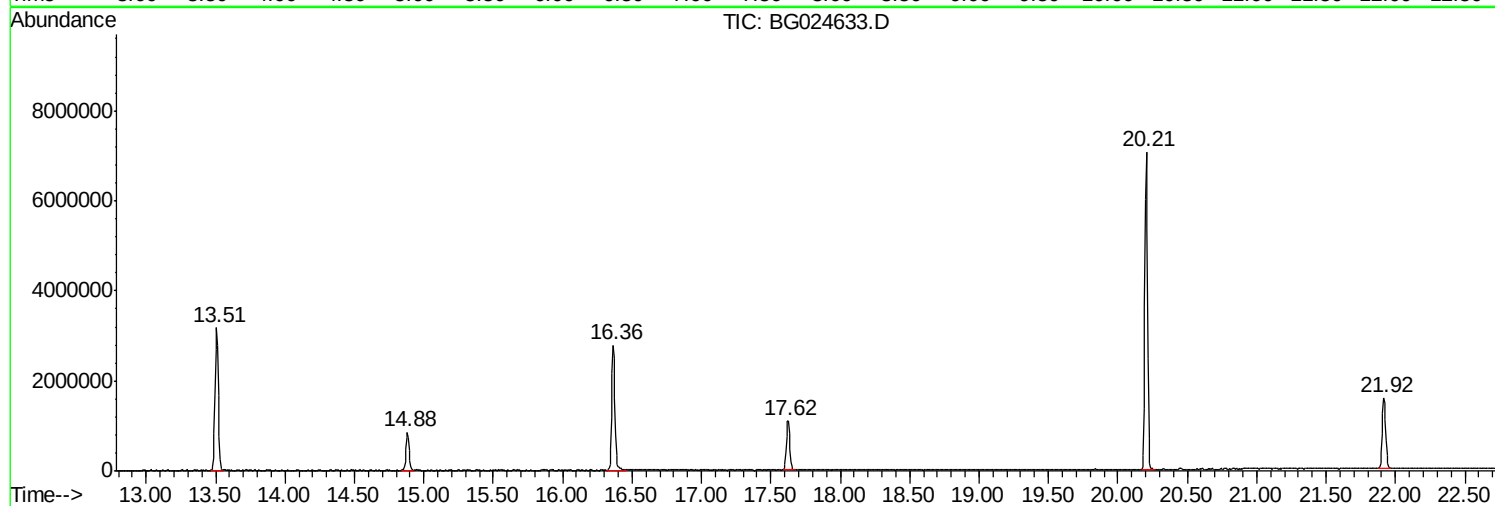
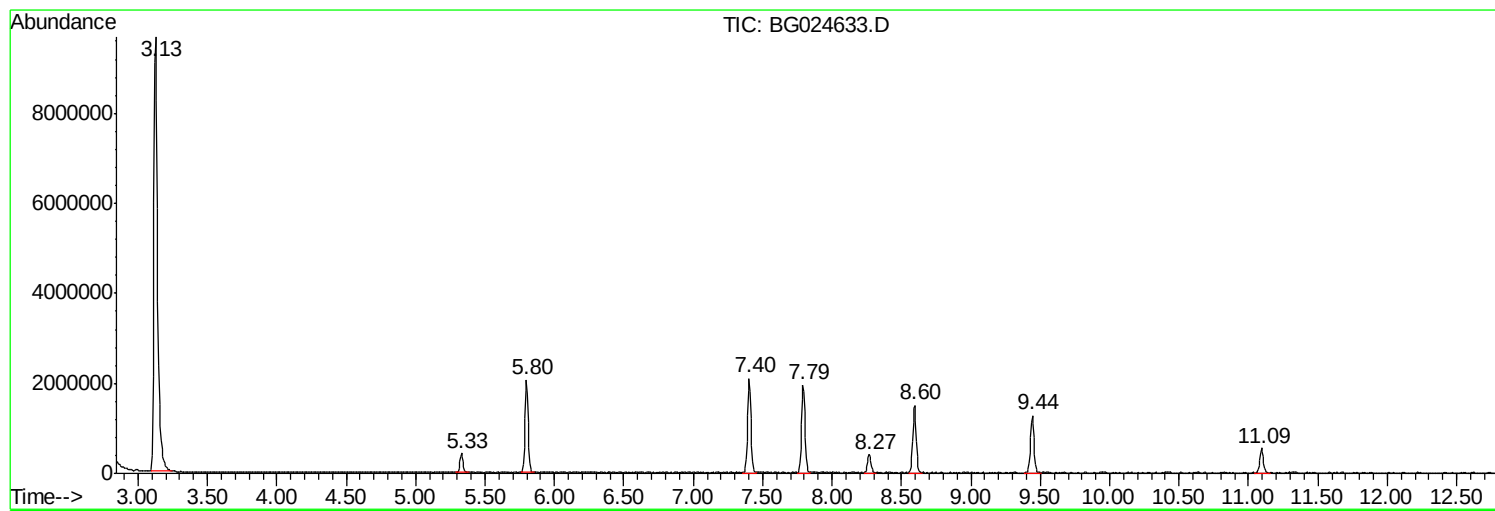
Sum of corrected areas: 63748191

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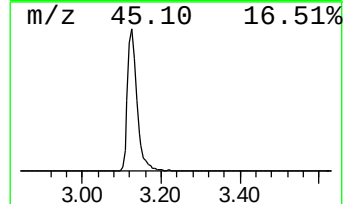
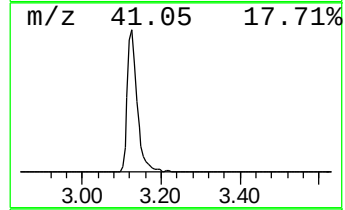
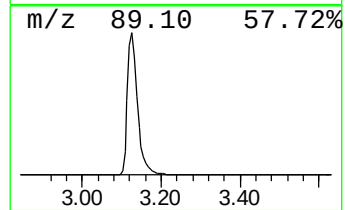
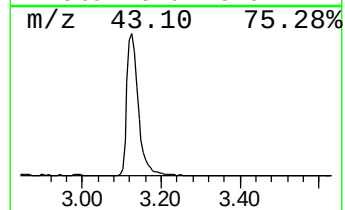
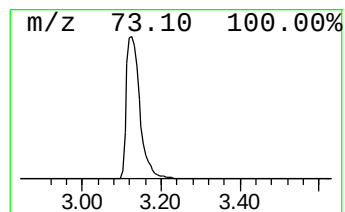
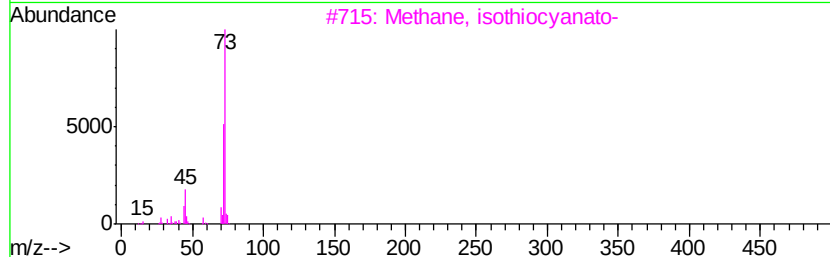
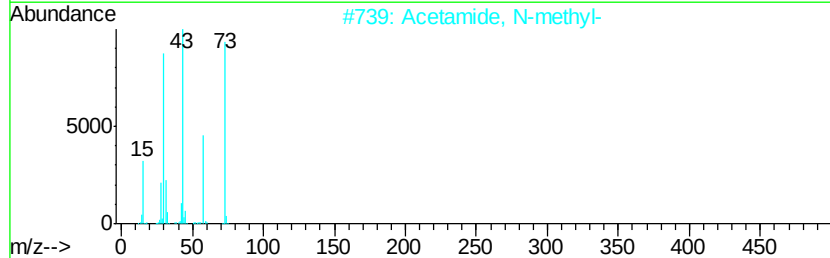
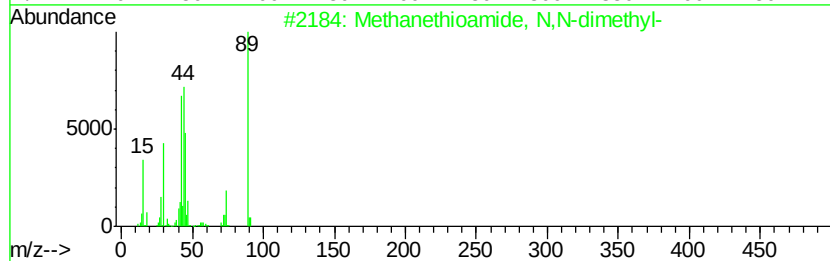
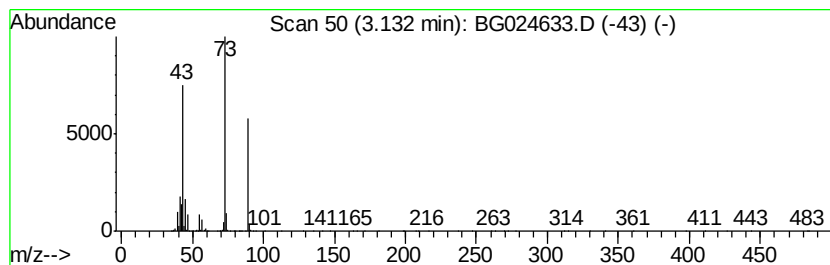
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	506.38 ng	18383400	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	32
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	16
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	10
5	Thiopropionamide	89	C3H7NS	000631-58-3	9



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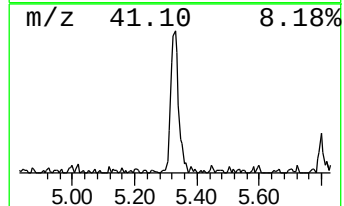
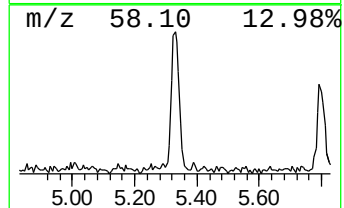
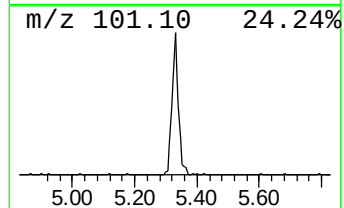
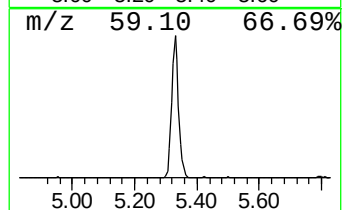
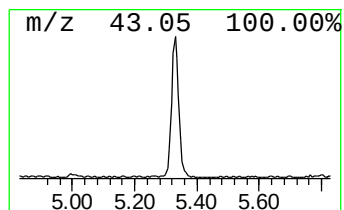
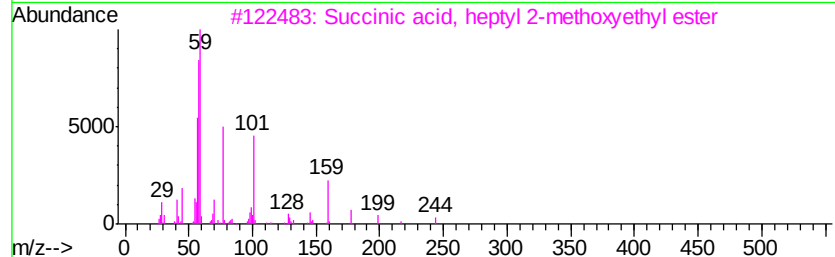
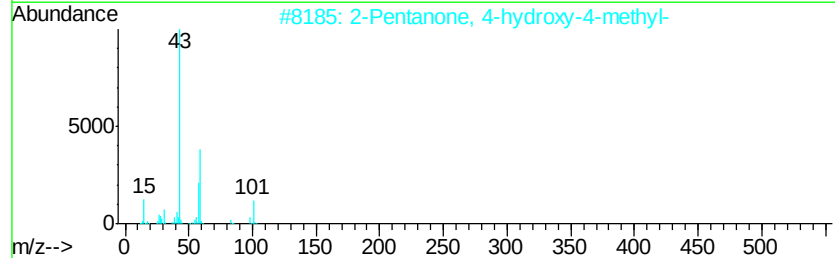
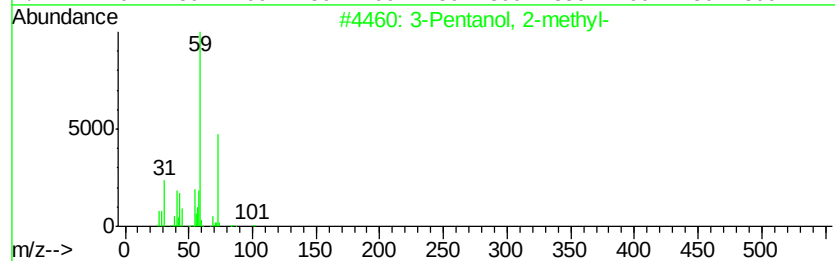
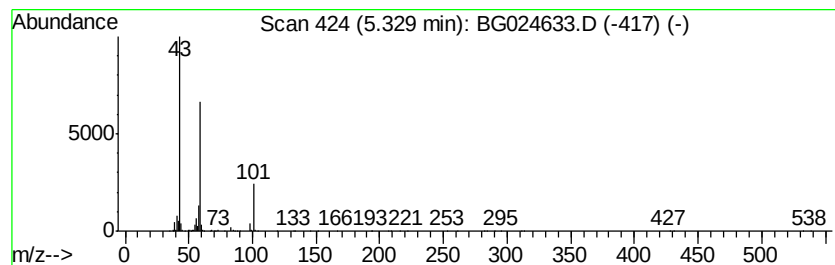
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Peak Number 2 unknown5.33 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	18.91 ng	686500	1,4-Dichlorobenzene-d4	8.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Pentanol, 2-methyl-	102	C6H14O	000565-67-3	43	
2	2	Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40	
3	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28		
4	3-Hexanol	102	C6H14O	000623-37-0	25		
5	3-Heptanol	116	C7H16O	000589-82-2	25		



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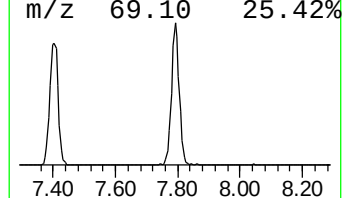
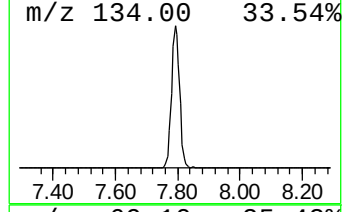
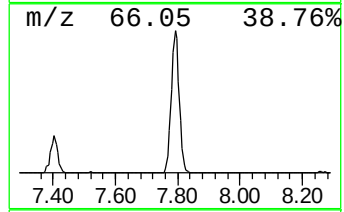
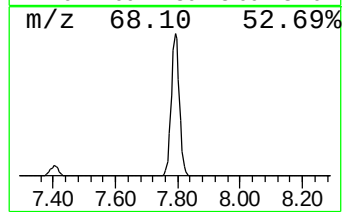
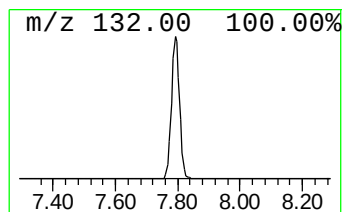
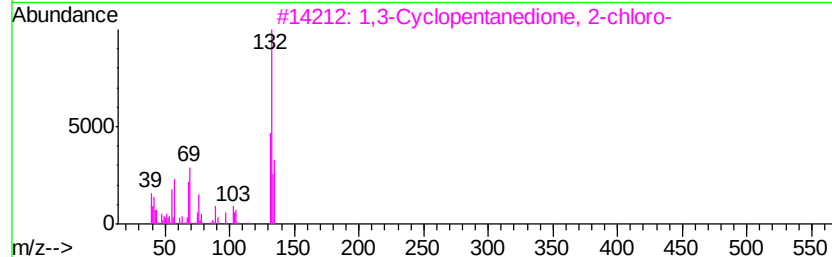
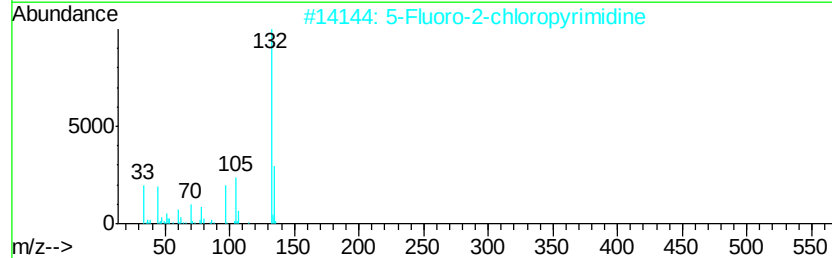
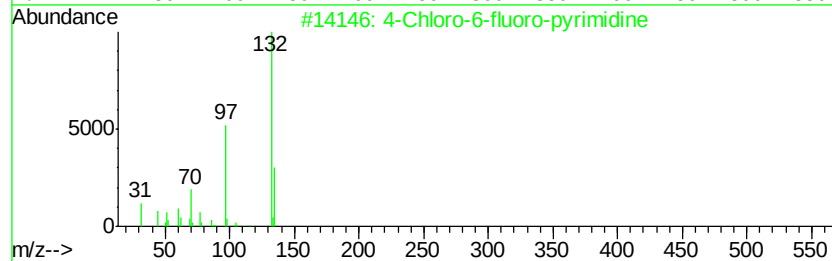
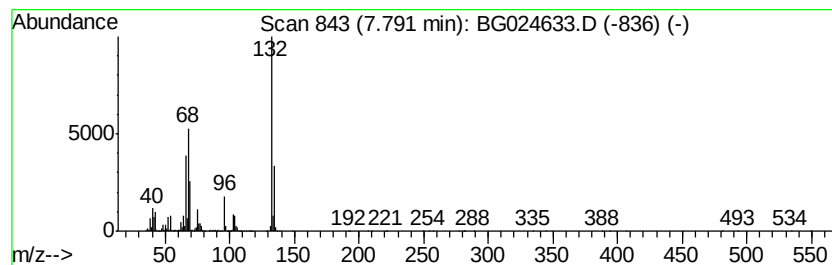
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Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	96.23 ng	3493360	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.13	3.13	506.4	ng	18383400	1	8.27	726072	20.0
unknown5.33	5.33	18.9	ng	686500	1	8.27	726072	20.0
unknown7.79	7.79	96.2	ng	3493360	1	8.27	726072	20.0