

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
 Data File : BG024558.D
 Acq On : 31 Oct 2016 16:14
 Operator : UM/SJ
 Sample : PB94433BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB94433BL

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	3.129	43	49	70	rVB	8283350	15745613	100.00%	25.637%
2	5.333	416	424	431	rBV2	410575	675265	4.29%	1.099%
3	5.797	495	503	514	rBV	2022101	3416183	21.70%	5.562%
4	7.401	768	776	787	rBV	2073712	3622536	23.01%	5.898%
5	7.794	834	843	852	rBV	1981216	3528787	22.41%	5.746%
6	8.270	917	924	932	rVB2	420702	762481	4.84%	1.241%
7	8.593	970	979	990	rBV	1476796	2700444	17.15%	4.397%
8	9.445	1116	1124	1132	rBV	1233063	2281005	14.49%	3.714%
9	11.096	1396	1405	1414	rBV	543015	1007992	6.40%	1.641%
10	13.511	1806	1816	1823	rBV	3177714	5048642	32.06%	8.220%
11	14.886	2042	2050	2058	rBV	855372	1374713	8.73%	2.238%
12	16.367	2292	2302	2315	rBV	2612940	4064198	25.81%	6.617%
13	17.624	2509	2516	2525	rBV	1144253	1855302	11.78%	3.021%
14	20.209	2949	2956	2964	rBV	6910834	9736077	61.83%	15.852%
15	21.919	3239	3247	3259	rBV	1574511	2814109	17.87%	4.582%
16	25.356	3818	3832	3843	rBV	880380	2784732	17.69%	4.534%

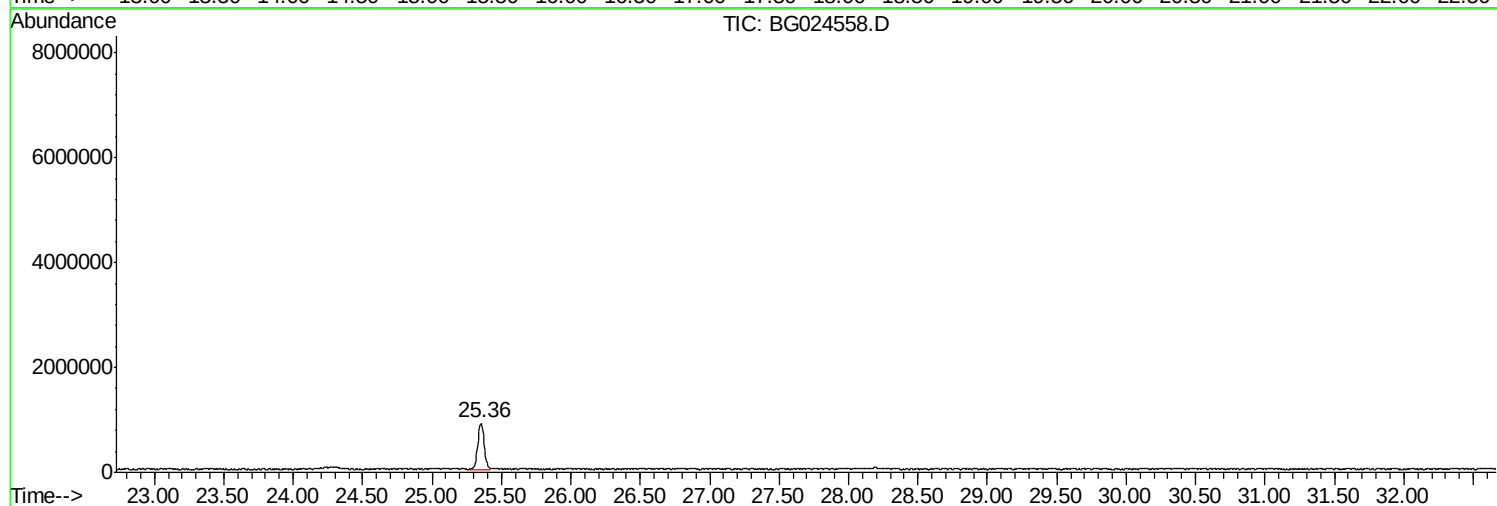
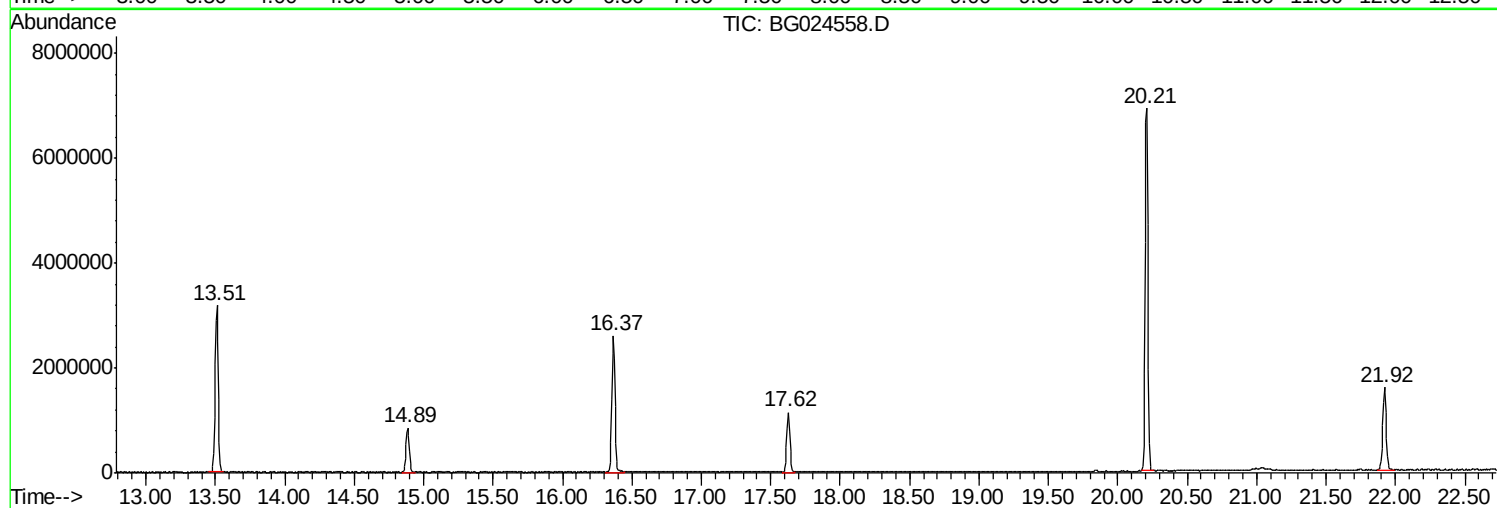
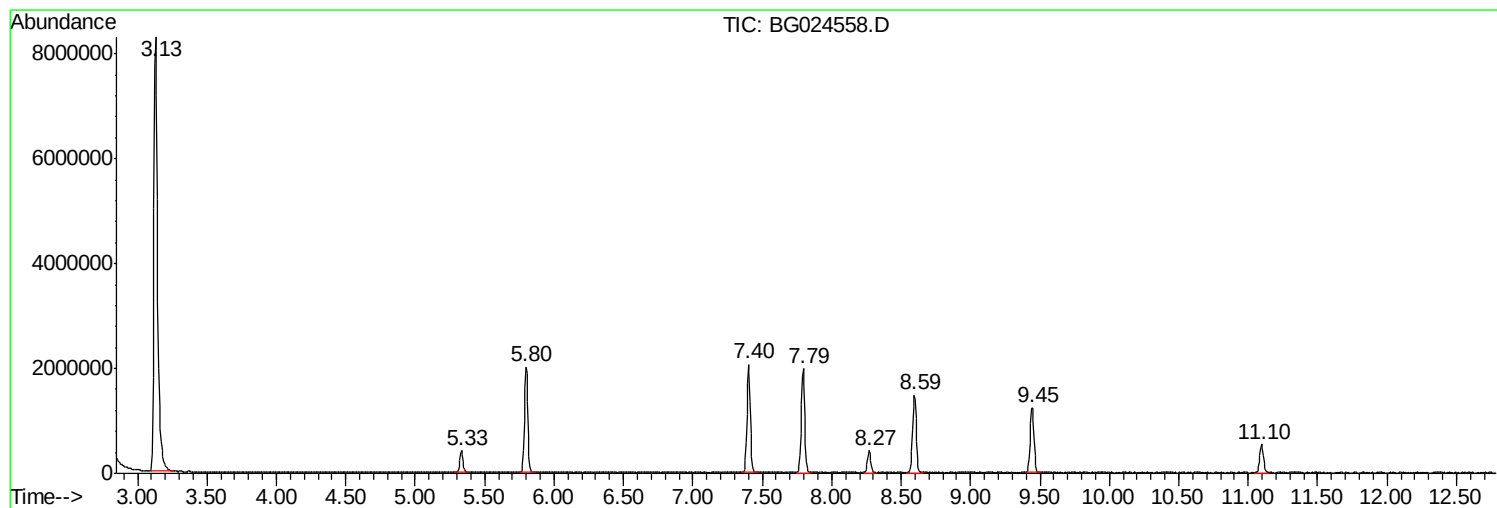
Sum of corrected areas: 61418079

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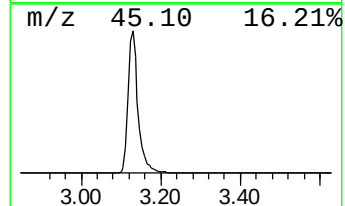
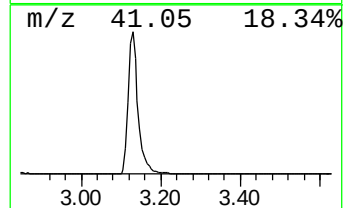
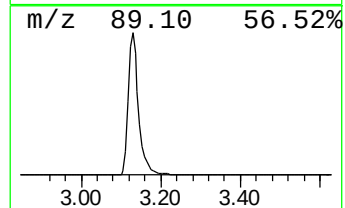
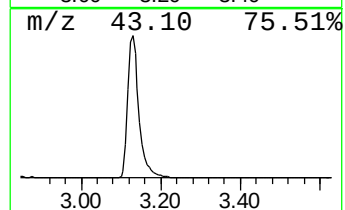
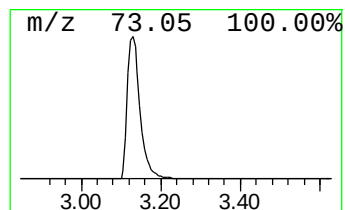
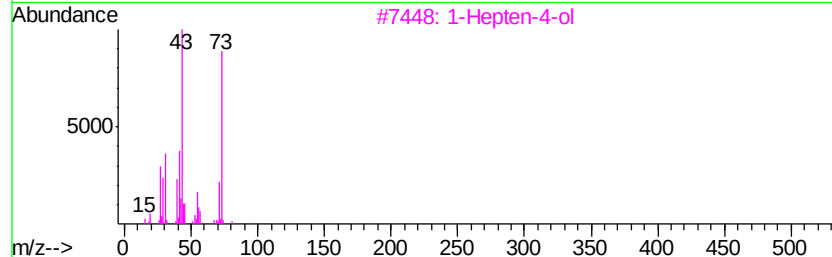
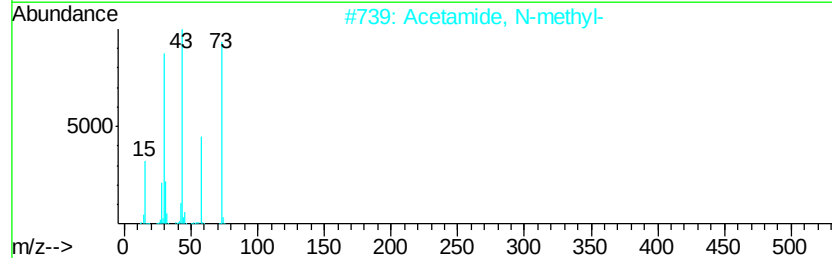
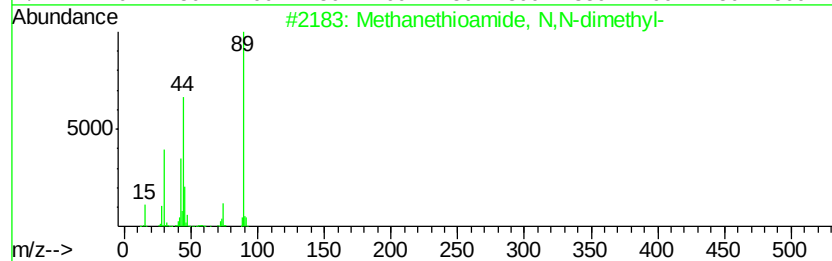
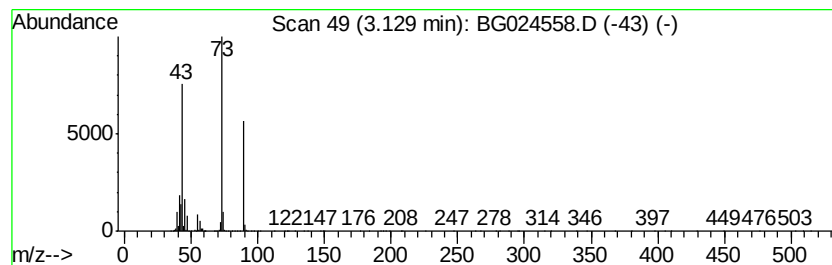
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	413.01 ng	15745600	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	37
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3		1-Hepten-4-ol	114	C7H14O	003521-91-3	23
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17
5		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9



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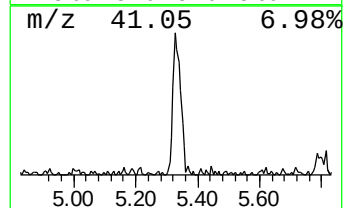
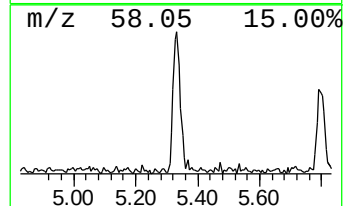
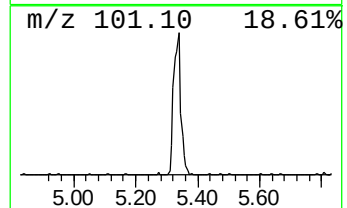
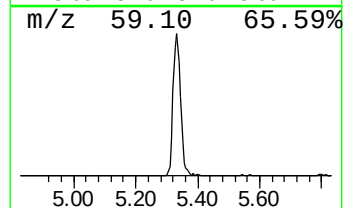
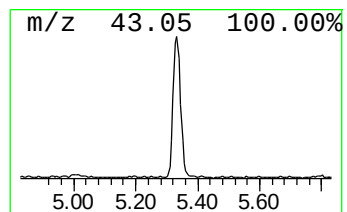
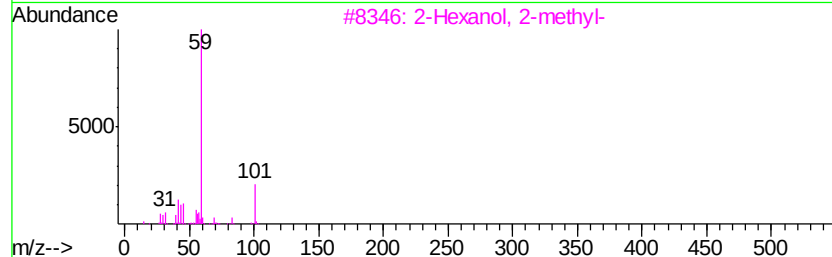
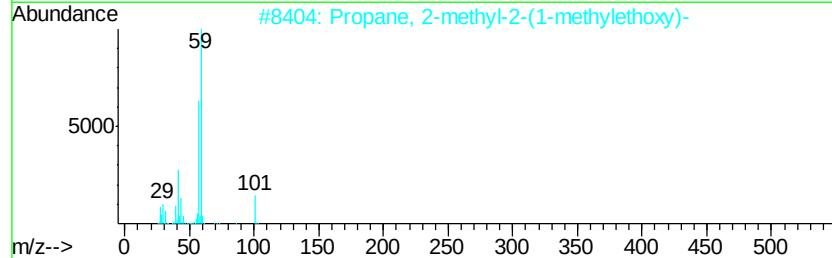
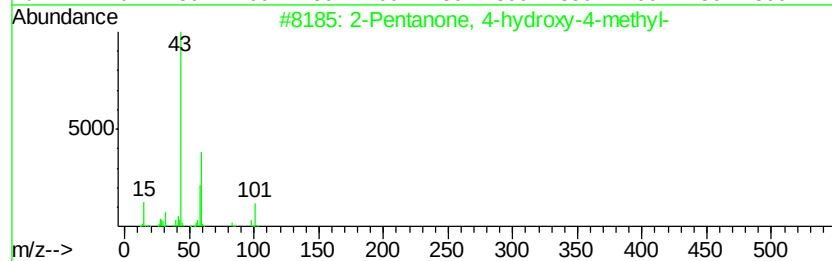
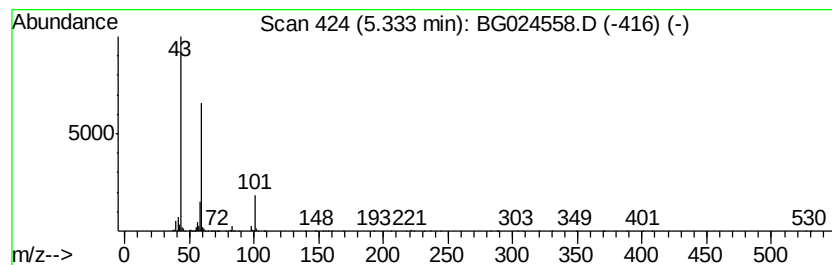
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	17.71 ng	675265	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	38
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5		1,2-Butanediol	90	C4H10O2	000584-03-2	25



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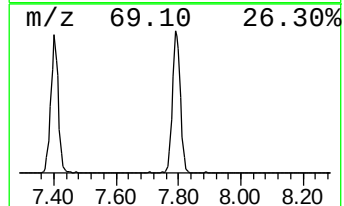
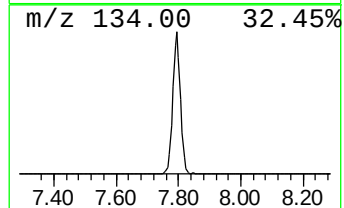
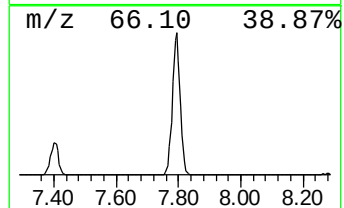
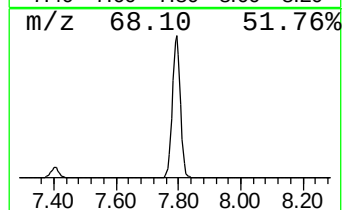
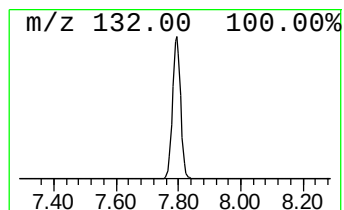
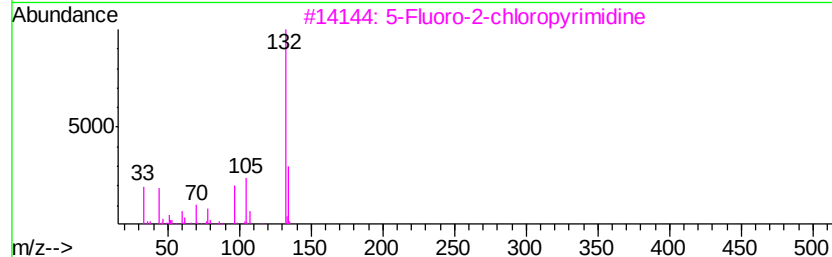
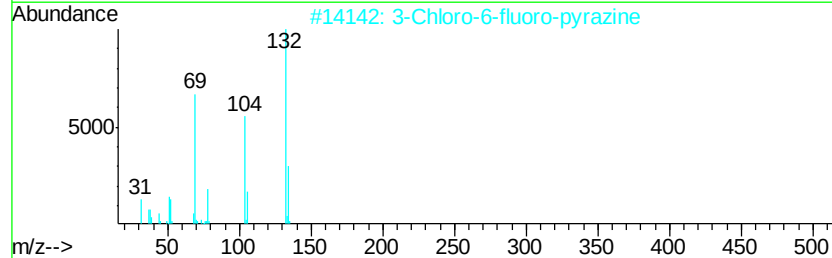
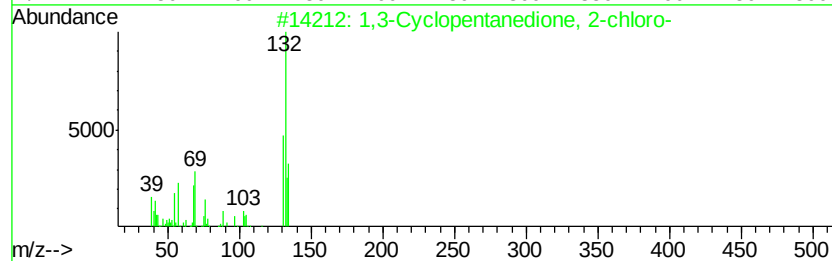
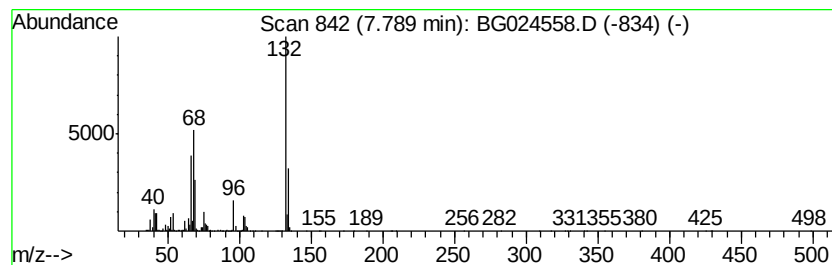
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Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	92.56 ng	3528790	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	18
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
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	413.0	ng	15745600	1	8.26	762481	20.0
2-Pentanone, 4-hy...	5.33	17.7	ng	675265	1	8.26	762481	20.0
unknown7.79	7.79	92.6	ng	3528790	1	8.26	762481	20.0