

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
 Data File : BG024726.D
 Acq On : 7 Nov 2016 12:42
 Operator : UM/SJ
 Sample : PB94545BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB94545BL

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	3.119	42	48	66	rBV	9811103	16995357	100.00%	28.613%
2	5.322	414	423	434	rBV	385819	632221	3.72%	1.064%
3	5.793	492	503	512	rBV	1874835	3105872	18.27%	5.229%
4	7.402	768	777	790	rBV	1856074	3263734	19.20%	5.495%
5	7.784	835	842	852	rVB	1787404	3140016	18.48%	5.286%
6	8.260	916	923	932	rBV2	382085	667790	3.93%	1.124%
7	8.589	970	979	990	rVB	1330657	2433506	14.32%	4.097%
8	9.435	1116	1123	1133	rVB	1082232	1998414	11.76%	3.364%
9	11.086	1396	1404	1412	rBV	474228	857186	5.04%	1.443%
10	13.501	1807	1815	1822	rBV	2894321	4601594	27.08%	7.747%
11	14.876	2042	2049	2056	rBV	814906	1254688	7.38%	2.112%
12	16.363	2294	2302	2310	rBV	2756530	4338933	25.53%	7.305%
13	17.620	2508	2516	2523	rBV	1071408	1673226	9.85%	2.817%
14	20.199	2949	2955	2961	rBV	6835720	9364509	55.10%	15.766%
15	21.915	3240	3247	3255	rBV	1491909	2580332	15.18%	4.344%
16	25.334	3820	3829	3840	rVB2	815566	2490346	14.65%	4.193%

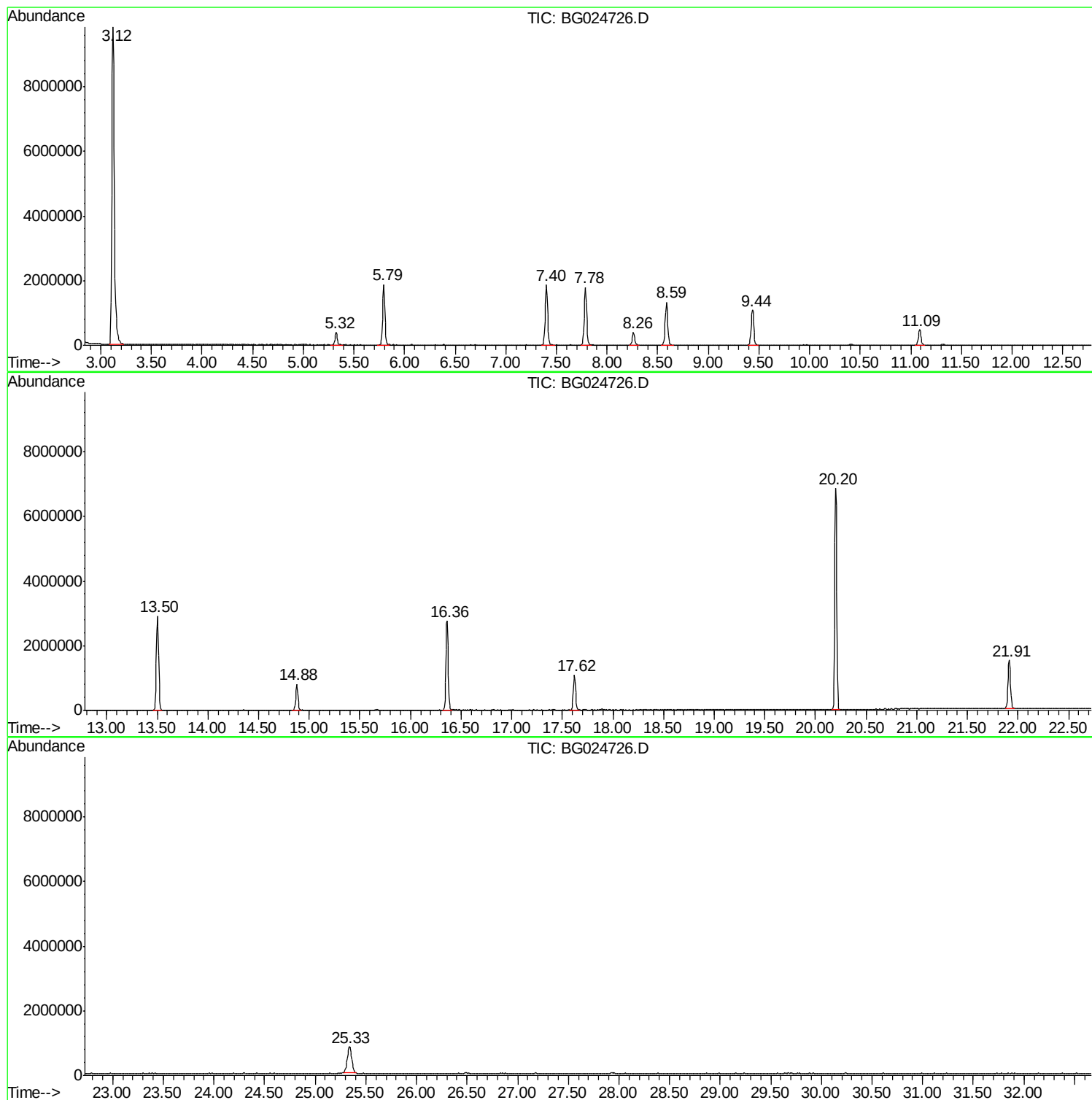
Sum of corrected areas: 59397724

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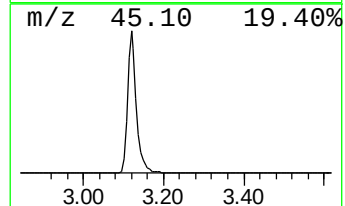
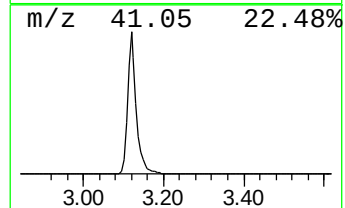
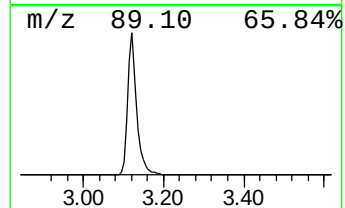
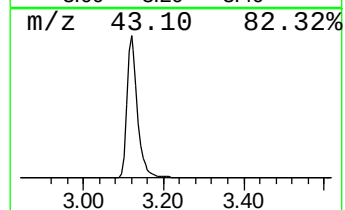
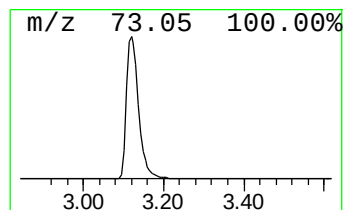
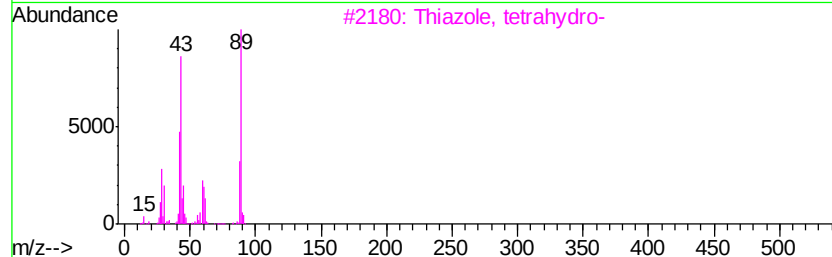
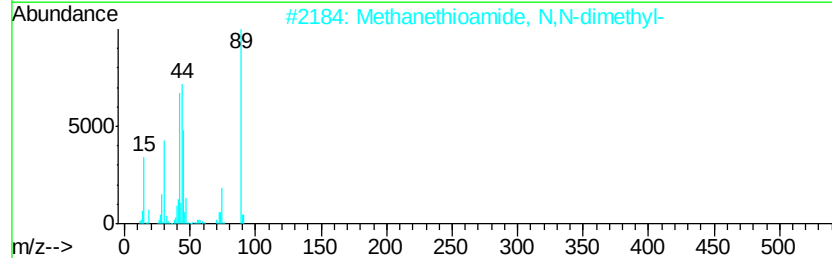
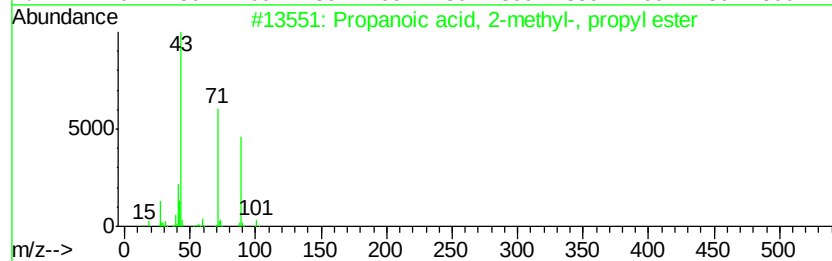
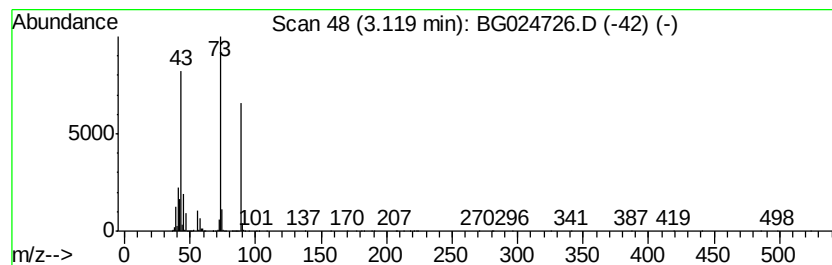
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	509.00 ng	16995400	1,4-Dichlorobenzene-d4	8.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	43
2		Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	32
3		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	28
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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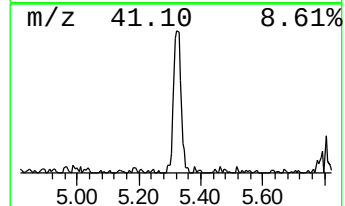
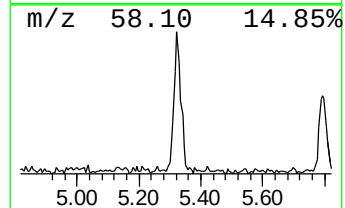
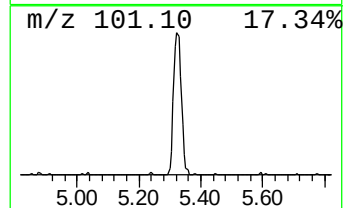
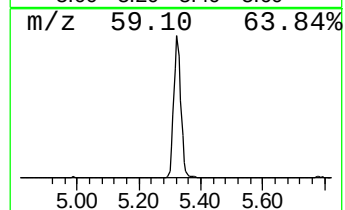
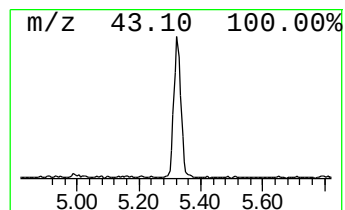
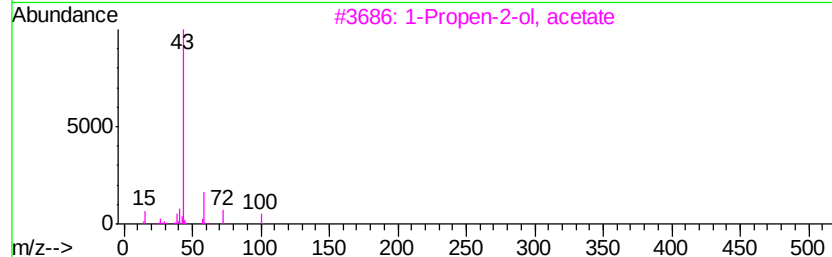
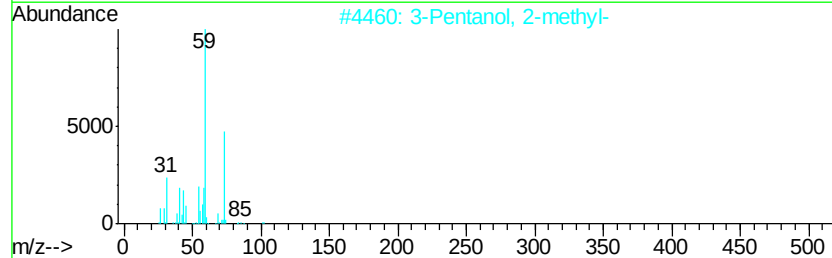
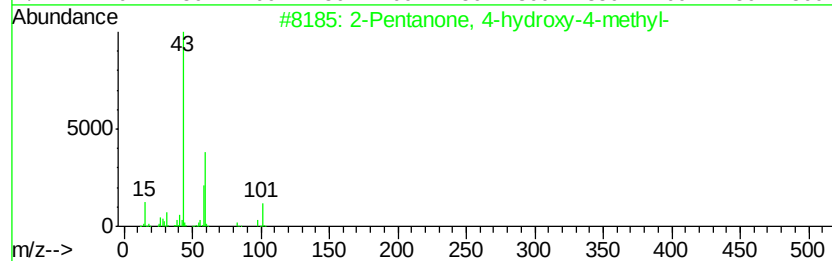
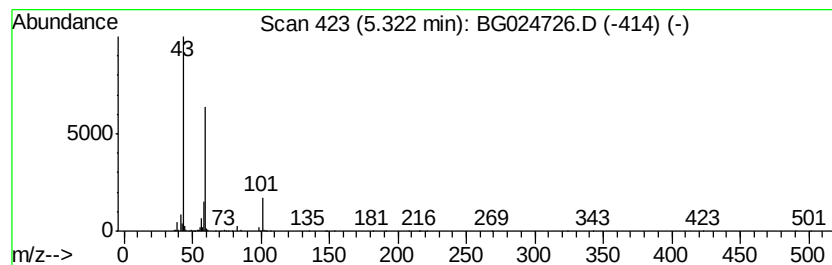
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	18.93 ng	632221	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	50
2		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	28
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Oxirane-2-carboxylic acid, methyl-	102	C4H6O3	004538-50-5	9
5		Guanidine	59	CH5N3	000113-00-8	9



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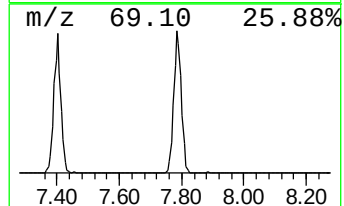
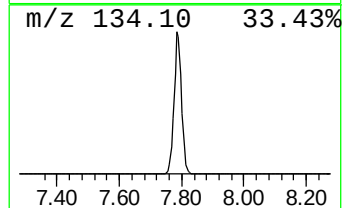
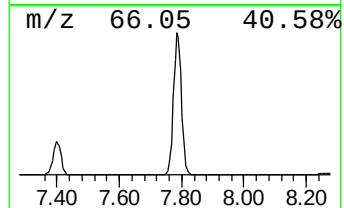
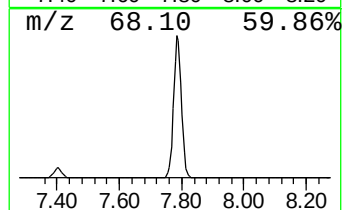
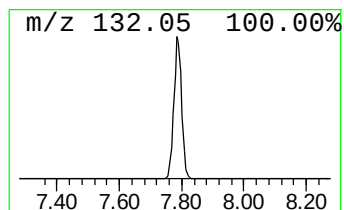
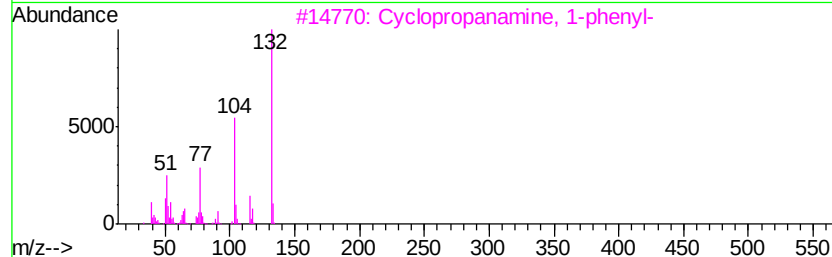
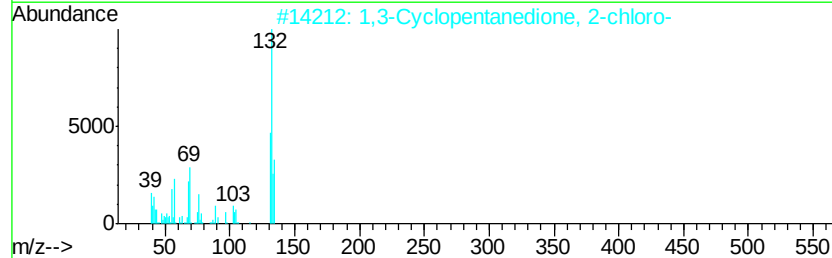
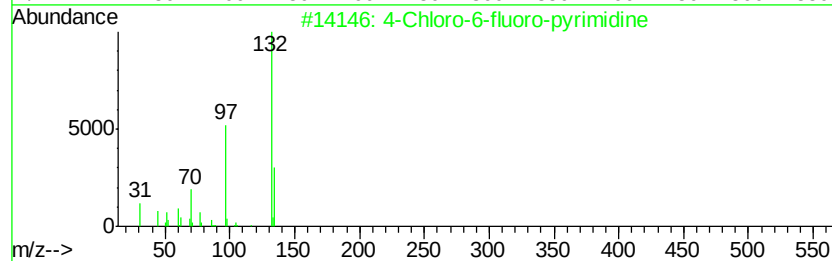
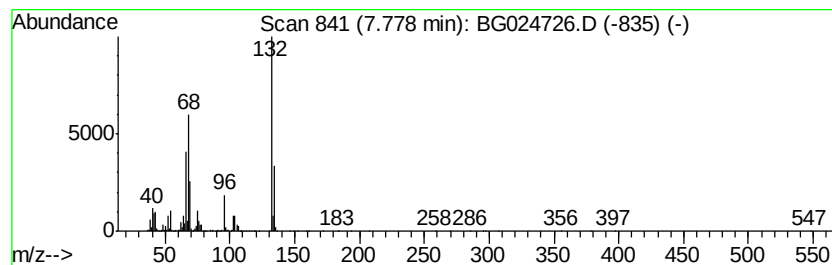
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Peak Number 3 unknown7.78 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	94.04 ng	3140020	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.12	3.12	509.0	ng	16995400	1	8.26	667790	20.0
2-Pentanone, 4-hy...	5.32	18.9	ng	632221	1	8.26	667790	20.0
unknown7.78	7.78	94.0	ng	3140020	1	8.26	667790	20.0