

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG102816\
 Data File : BG024540.D
 Acq On : 28 Oct 2016 15:48
 Operator : UM/SJ
 Sample : PB94361BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB94361BL

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	44	49	71	rVB	9357572	18726597	100.00%	30.823%
2	5.335	418	425	439	rVB	384321	662778	3.54%	1.091%
3	5.799	496	504	515	rBV	1827731	3129787	16.71%	5.152%
4	7.409	770	778	787	rBV	1883841	3334617	17.81%	5.489%
5	7.797	836	844	853	rBV	1825779	3243184	17.32%	5.338%
6	8.273	916	925	933	rBV	416370	718166	3.84%	1.182%
7	8.602	971	981	990	rVB	1361030	2491894	13.31%	4.102%
8	9.448	1117	1125	1134	rBV	1126996	2112926	11.28%	3.478%
9	11.099	1400	1406	1416	rVB	509115	922675	4.93%	1.519%
10	13.513	1810	1817	1825	rVB	2989329	4649653	24.83%	7.653%
11	14.888	2044	2051	2058	rBV	821499	1291423	6.90%	2.126%
12	16.369	2295	2303	2318	rBV	2572871	3911030	20.88%	6.437%
13	17.632	2510	2518	2524	rBV	1116260	1750513	9.35%	2.881%
14	20.212	2951	2957	2966	rVB	6525569	8756789	46.76%	14.413%
15	21.927	3242	3249	3259	rVB	1442888	2508992	13.40%	4.130%
16	25.364	3822	3834	3849	rVB	828246	2543794	13.58%	4.187%

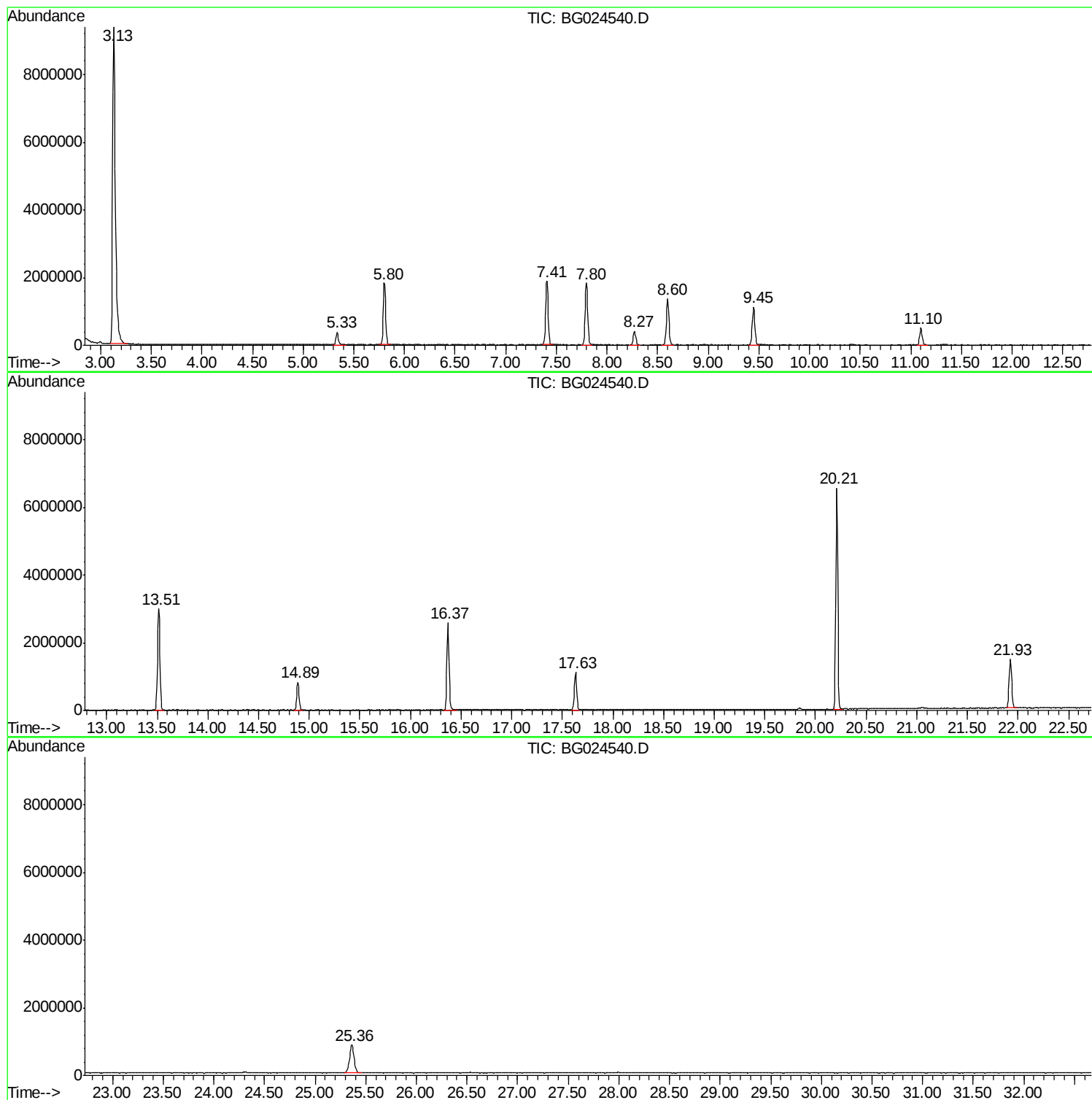
Sum of corrected areas: 60754818

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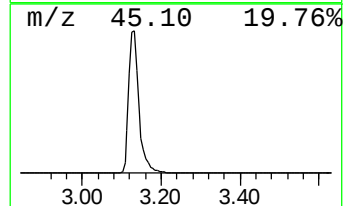
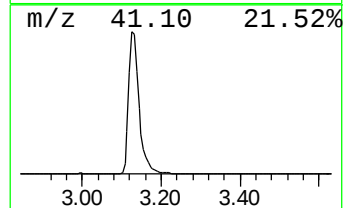
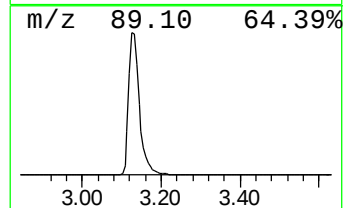
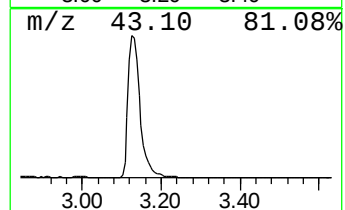
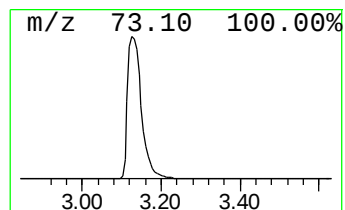
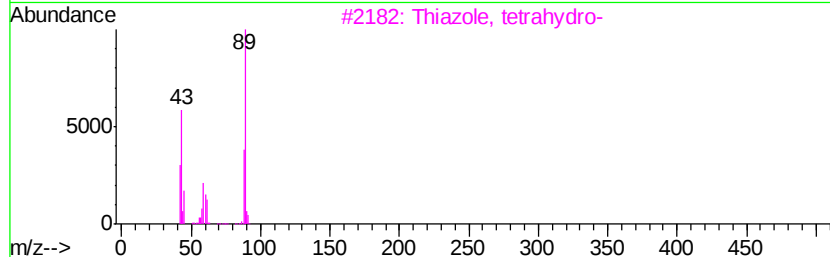
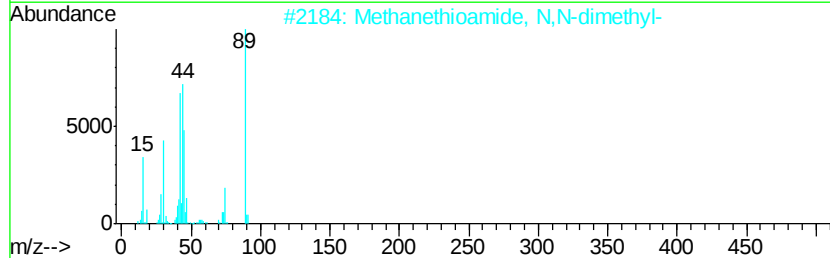
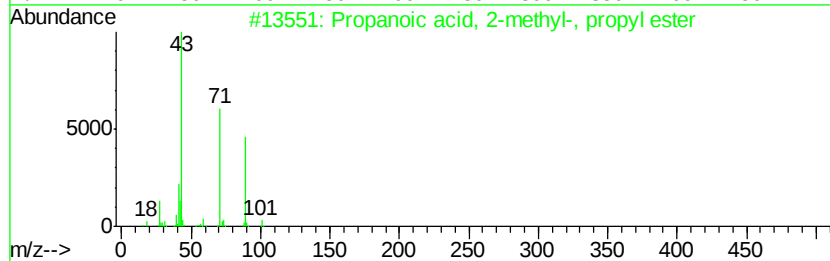
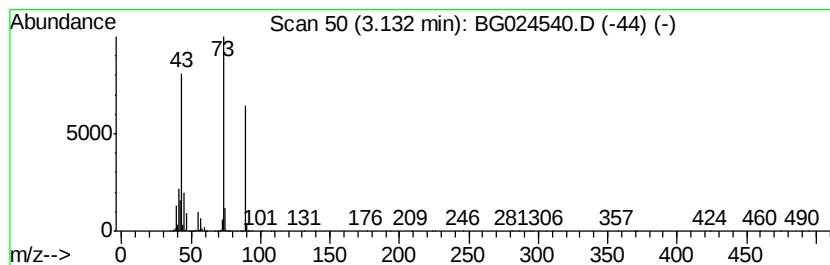
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	521.51 ng	18726600	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, propy...	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	32
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
5		N-Methoxydiacetamide	131	C5H9NO3	128459-09-6	23



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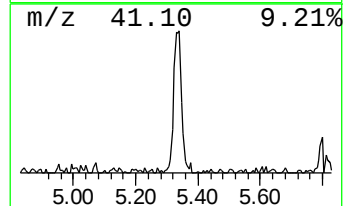
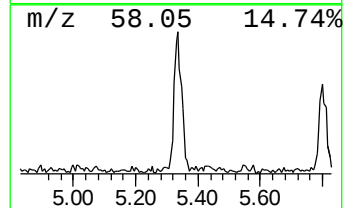
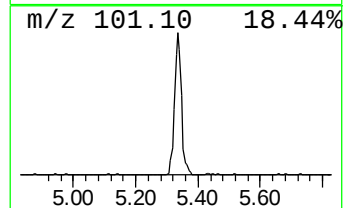
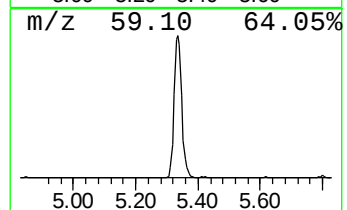
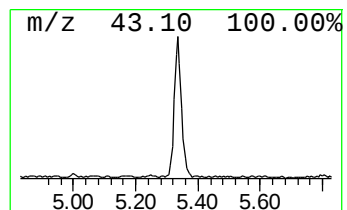
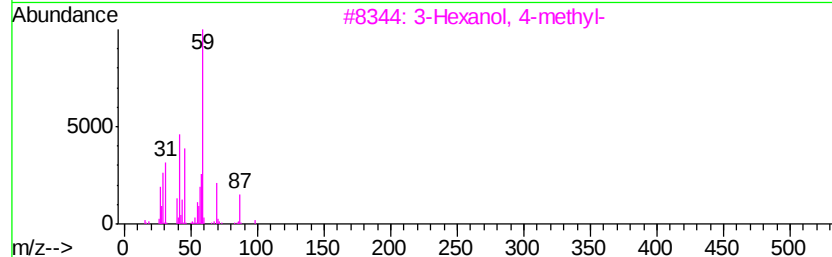
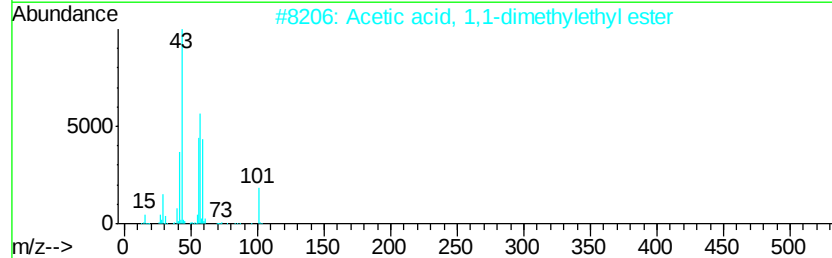
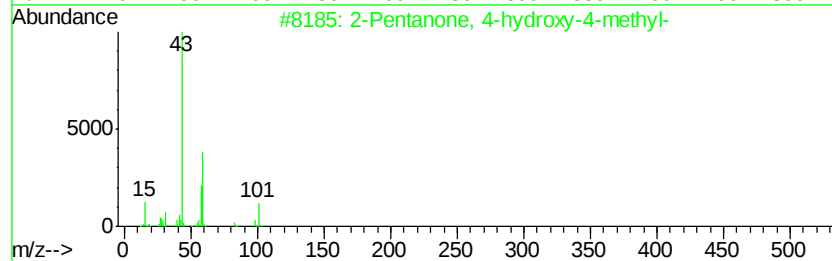
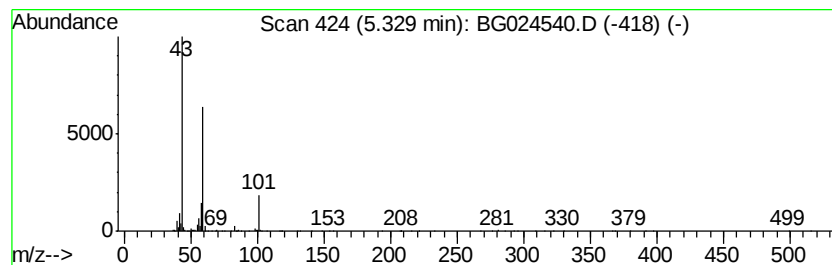
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	18.46 ng	662778	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	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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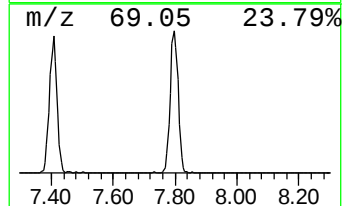
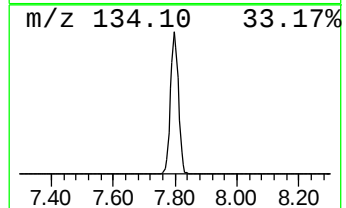
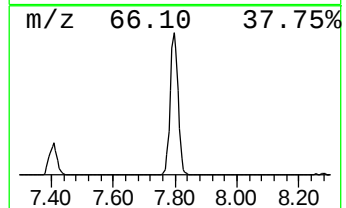
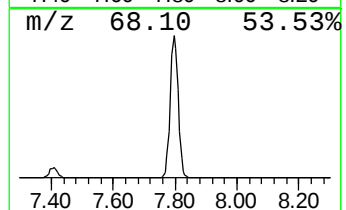
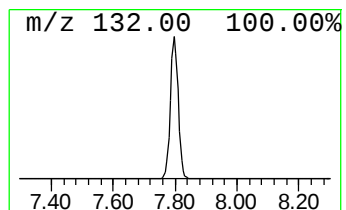
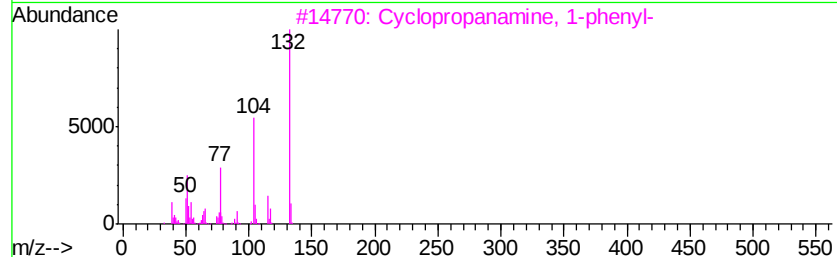
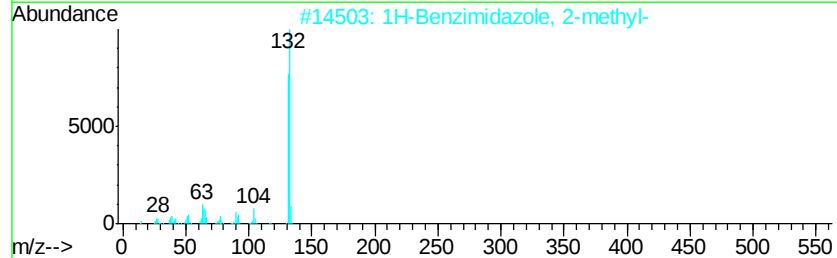
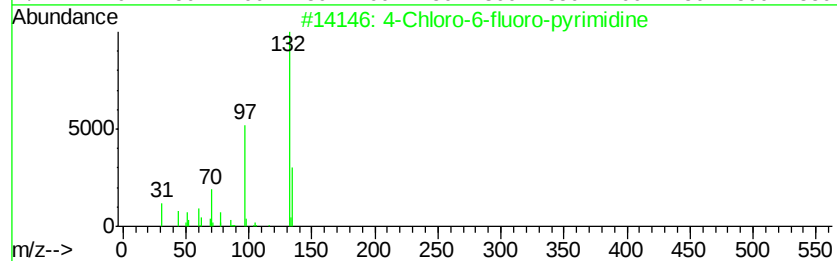
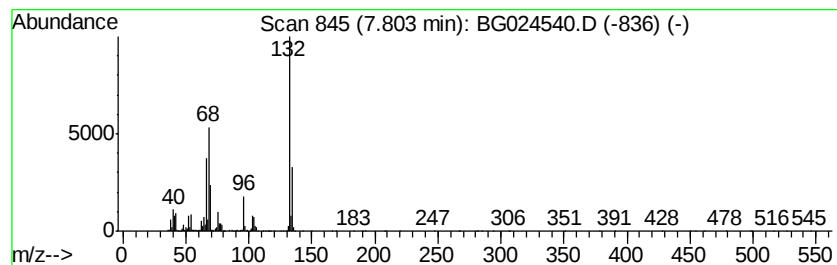
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Peak Number 3 unknown7.80 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	90.32 ng	3243180	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	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	16
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.13	3.13	521.5	ng	18726600	1	8.27	718166	20.0
2-Pentanone, 4-hy...	5.33	18.5	ng	662778	1	8.27	718166	20.0
unknown7.80	7.80	90.3	ng	3243180	1	8.27	718166	20.0