

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
 Data File : BG024686.D
 Acq On : 4 Nov 2016 21:56
 Operator : UM/SJ
 Sample : PB94526BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB94526BL

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	3.125	43	49	72	rVB	9176807	16475607	100.00%	26.596%
2	5.329	417	424	434	rBV	400746	650924	3.95%	1.051%
3	5.799	496	504	517	rBV	2020277	3400609	20.64%	5.489%
4	7.403	769	777	790	rBV	2076309	3638156	22.08%	5.873%
5	7.791	833	843	852	rBV	1982706	3494944	21.21%	5.642%
6	8.266	917	924	933	rVB	374531	672997	4.08%	1.086%
7	8.590	972	979	989	rVB	1440464	2584428	15.69%	4.172%
8	9.442	1115	1124	1132	rBV	1252467	2275787	13.81%	3.674%
9	11.093	1397	1405	1415	rVB	495046	927934	5.63%	1.498%
10	13.507	1808	1816	1823	rBV	3141286	5011903	30.42%	8.091%
11	14.882	2043	2050	2059	rVB2	815573	1297075	7.87%	2.094%
12	16.363	2296	2302	2315	rBV	2935636	4698183	28.52%	7.584%
13	17.626	2509	2517	2525	rBV2	1140595	1840483	11.17%	2.971%
14	20.205	2949	2956	2965	rBV	7090627	9928098	60.26%	16.027%
15	21.915	3240	3247	3257	rBV	1415786	2572970	15.62%	4.153%
16	25.346	3819	3831	3844	rBV2	783810	2477425	15.04%	3.999%

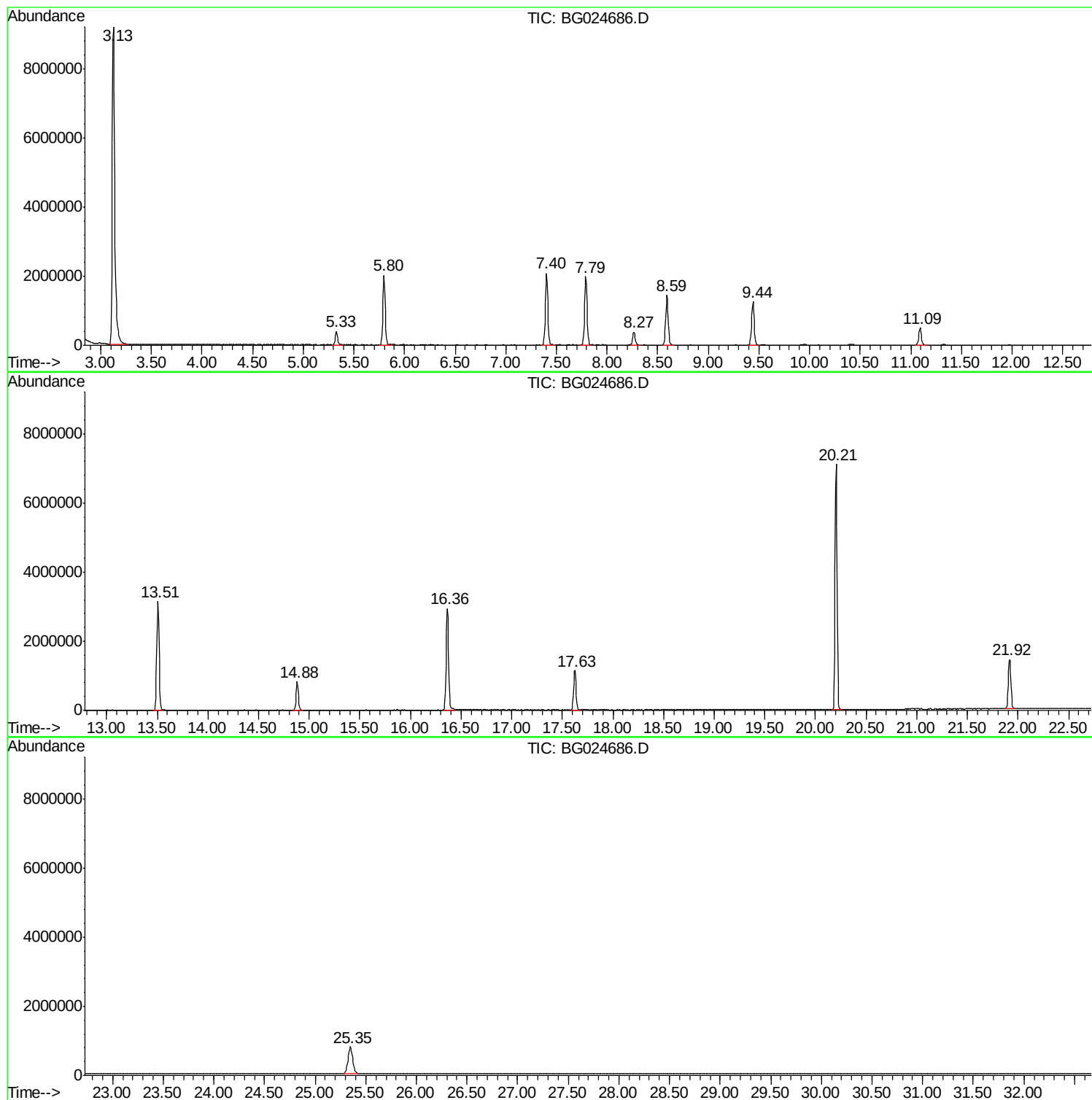
Sum of corrected areas: 61947523

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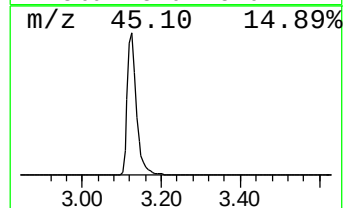
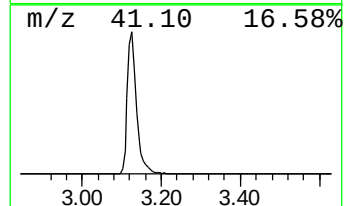
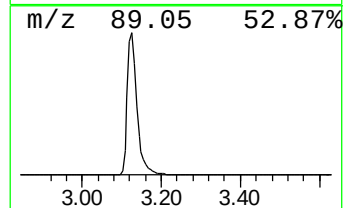
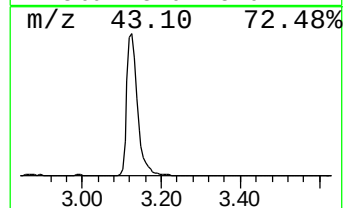
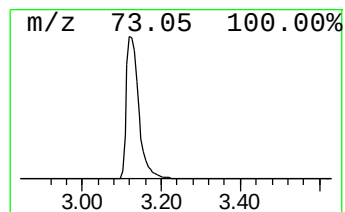
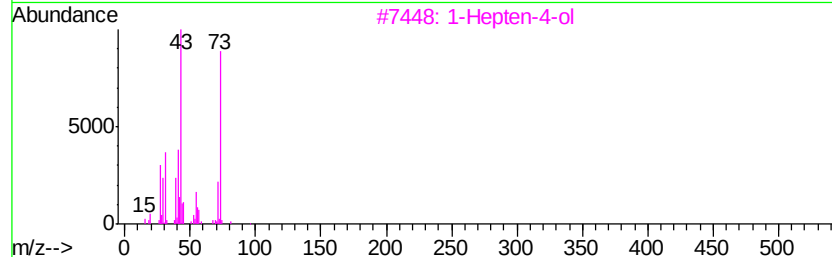
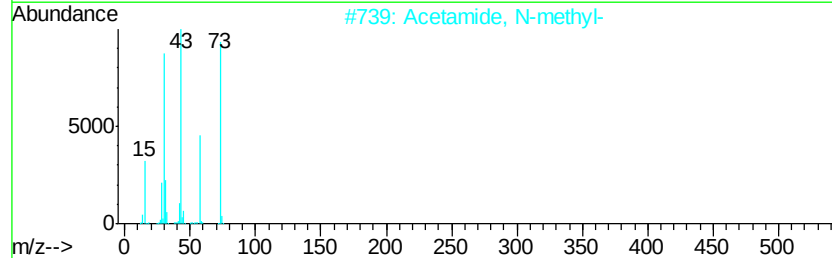
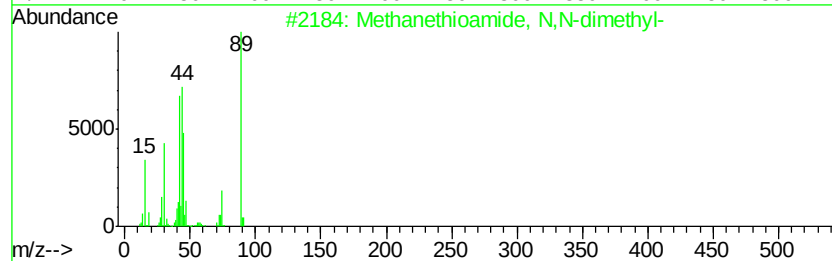
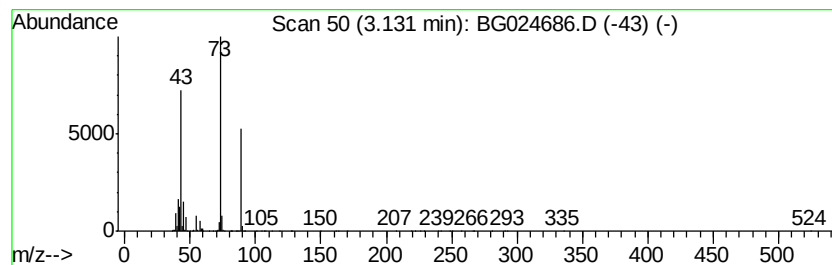
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	489.62 ng	16475600	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	37
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3		1-Hepten-4-ol	114	C7H14O	003521-91-3	23
4		Thiopropionamide	89	C3H7NS	000631-58-3	9
5		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9



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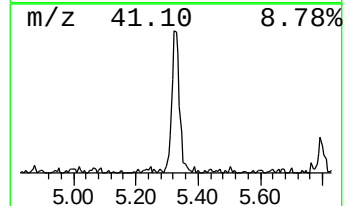
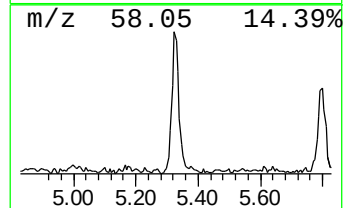
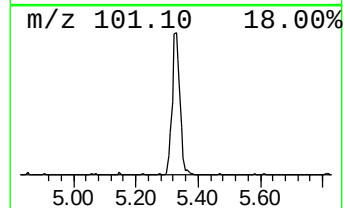
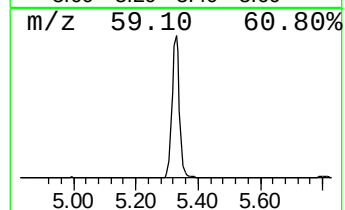
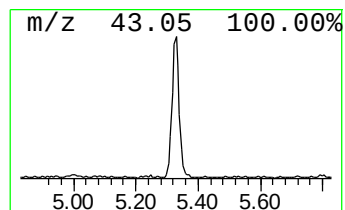
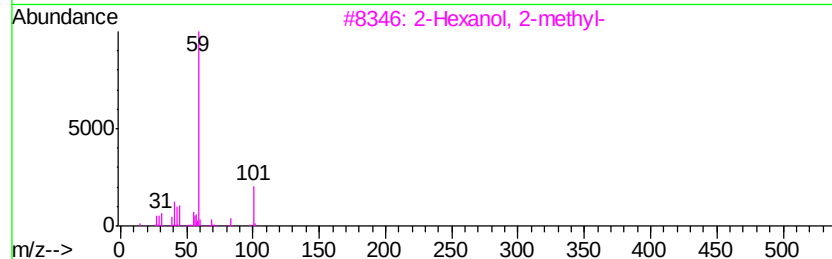
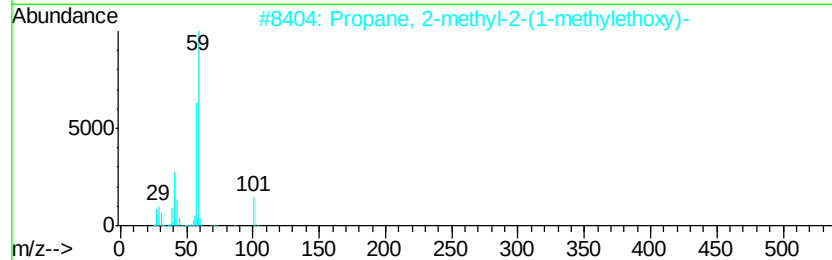
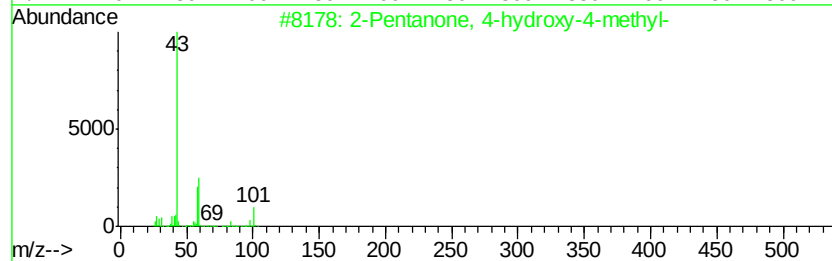
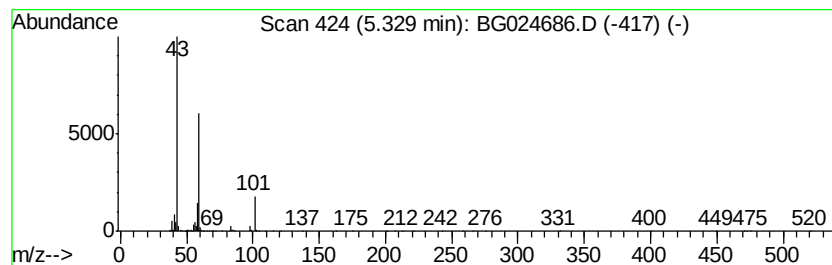
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	19.34 ng	650924	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	59
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		Acetic acid, chloro-, 1,1-dimethyl-	150	C6H11ClO2	000107-59-5	9



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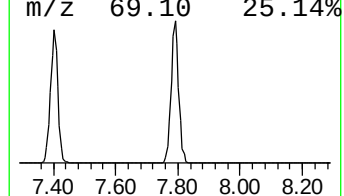
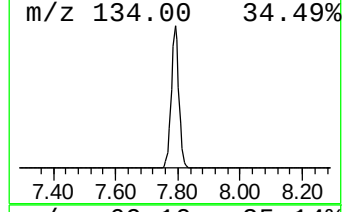
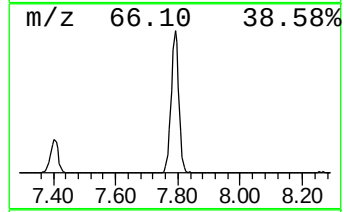
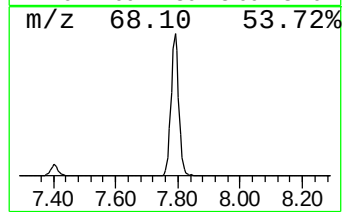
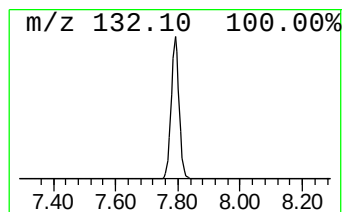
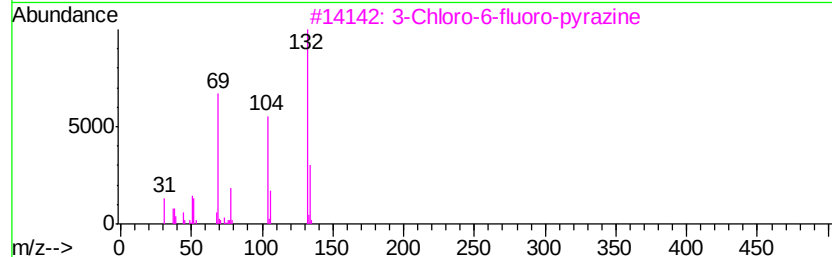
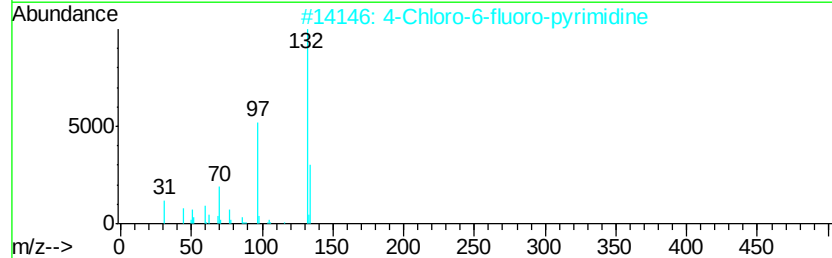
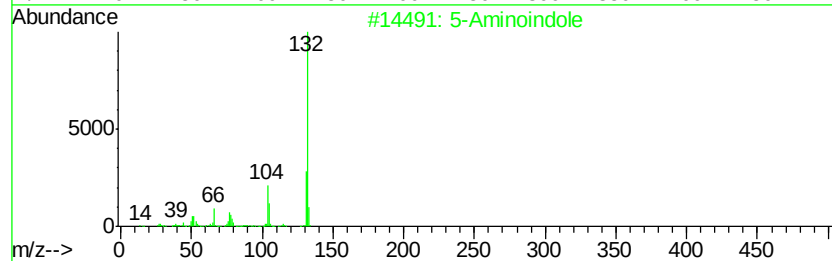
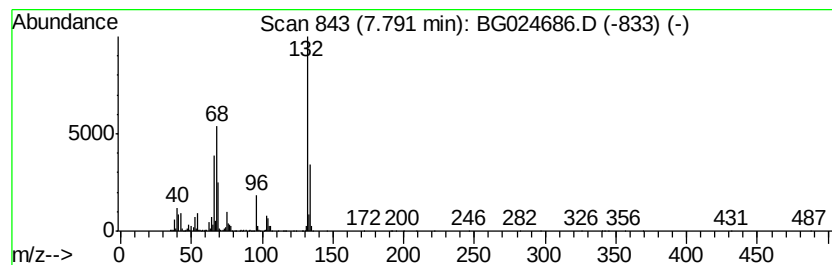
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Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	103.86 ng	3494940	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.13	3.13	489.6	ng	16475600	1	8.27	672997	20.0
2-Pentanone, 4-hy...	5.33	19.3	ng	650924	1	8.27	672997	20.0
unknown7.79	7.79	103.9	ng	3494940	1	8.27	672997	20.0