

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050915\
Data File : BG017026.D
Acq On : 10 May 2015 14:53
Operator : TP/IZ
Sample : PB83231BL
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB83231BL

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-BG050515.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	2.777	10	15	34	rBV	7155668	8703603	100.00%	28.853%
2	4.909	374	378	384	rBV	76559	102085	1.17%	0.338%
3	5.385	452	459	468	rBV	1137275	1676879	19.27%	5.559%
4	6.972	722	729	738	rBV	1199714	1899512	21.82%	6.297%
5	7.324	782	789	799	rBV	1119644	1805732	20.75%	5.986%
6	7.788	862	868	874	rBV	202560	324031	3.72%	1.074%
7	8.112	915	923	929	rBV	777310	1247019	14.33%	4.134%
8	8.946	1058	1065	1073	rBV	681729	1121435	12.88%	3.718%
9	10.579	1336	1343	1350	rBV	266524	455934	5.24%	1.511%
10	13.047	1757	1763	1770	rBV	1606170	2386950	27.42%	7.913%
11	14.428	1991	1998	2004	rBV2	422035	643803	7.40%	2.134%
12	15.914	2245	2251	2263	rBV	1617177	2371833	27.25%	7.863%
13	17.172	2455	2465	2470	rBV	657733	928363	10.67%	3.078%
14	19.798	2906	2912	2920	rBV	3702242	4526209	52.00%	15.004%
15	21.343	3170	3175	3180	rBV	788560	1017876	11.69%	3.374%
16	23.640	3559	3566	3575	rBV2	464935	954490	10.97%	3.164%

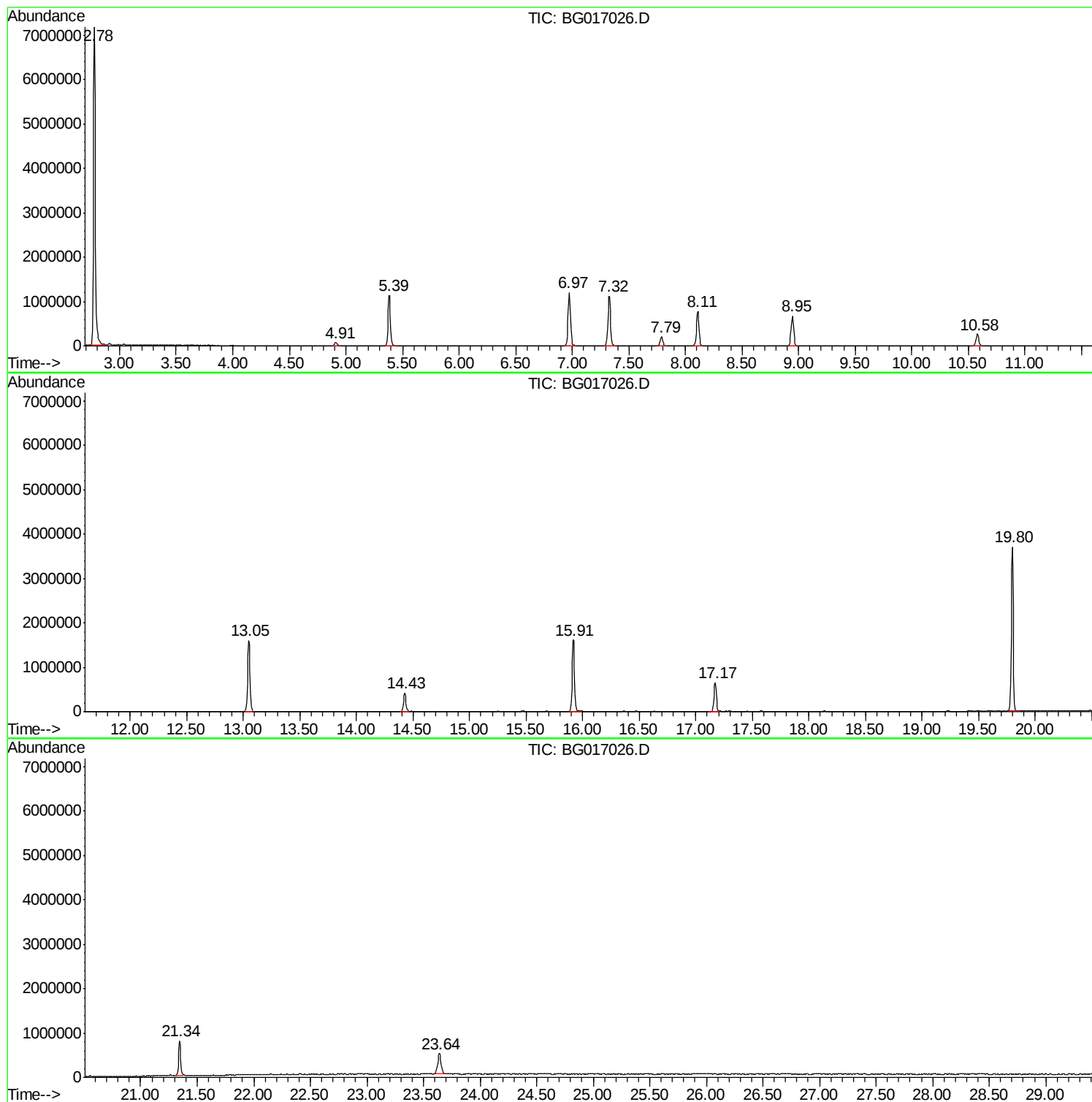
Sum of corrected areas: 30165754

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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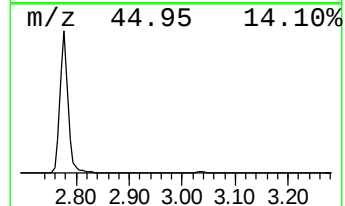
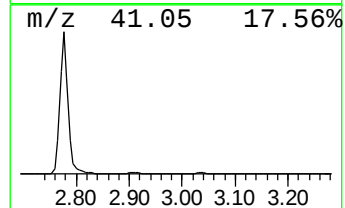
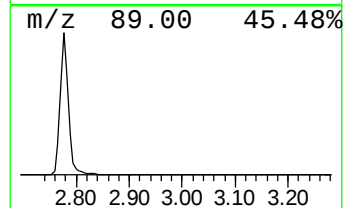
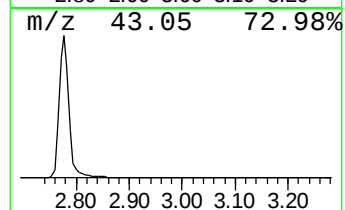
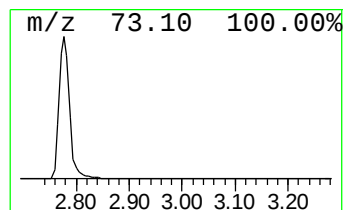
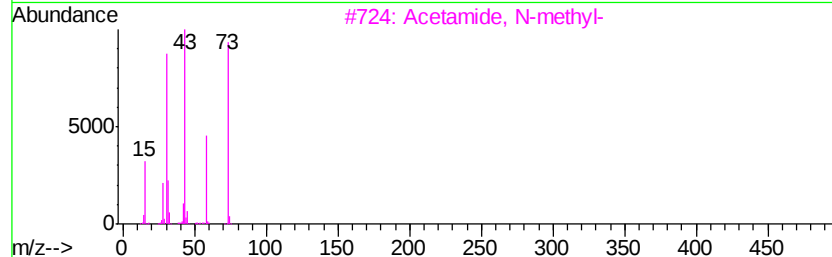
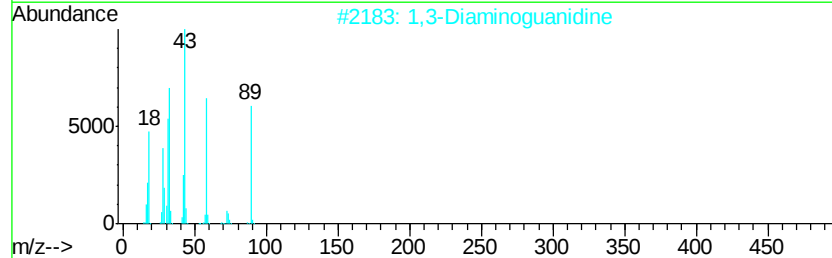
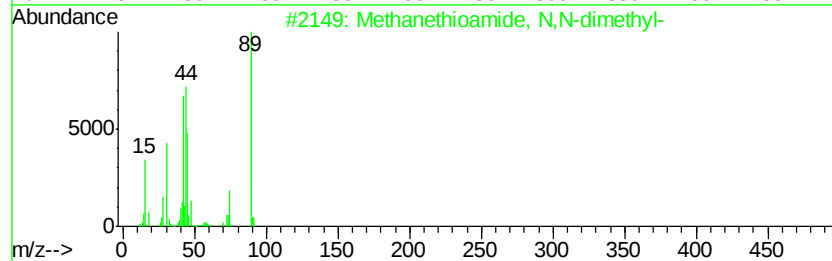
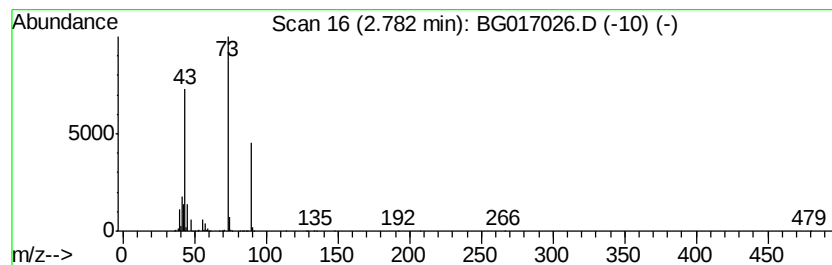
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.78	537.21 ng	8703600	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	47
2		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	33
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4		dl-Malic disodium salt	134	C4H6O5	000617-48-1	23
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23



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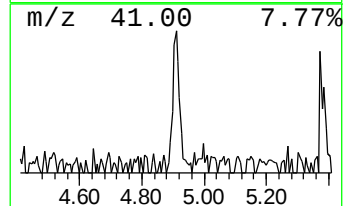
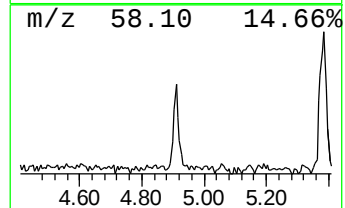
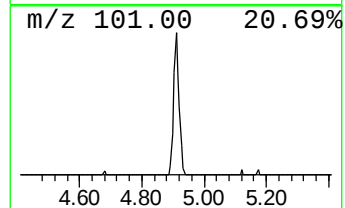
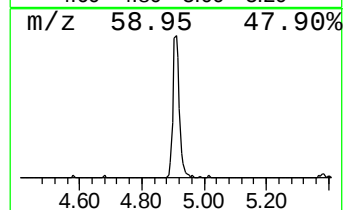
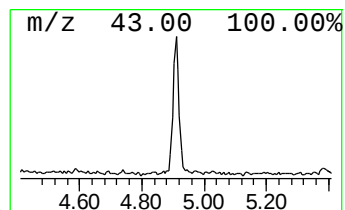
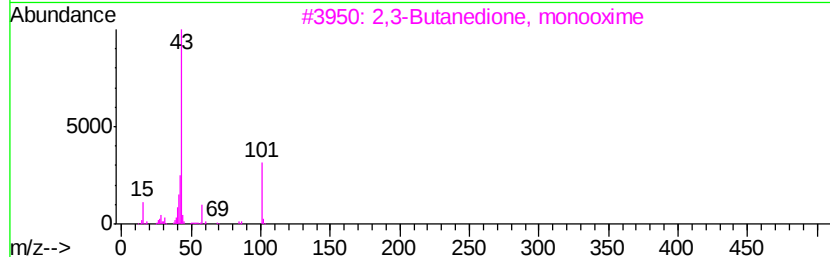
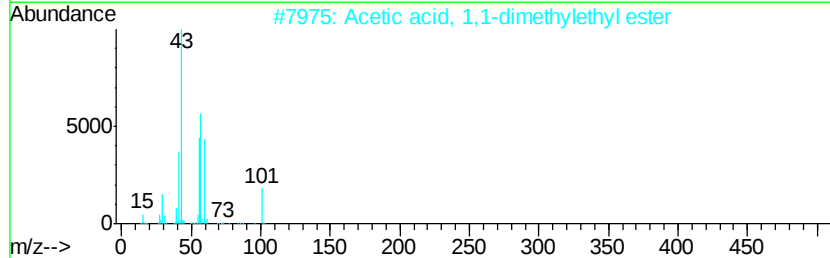
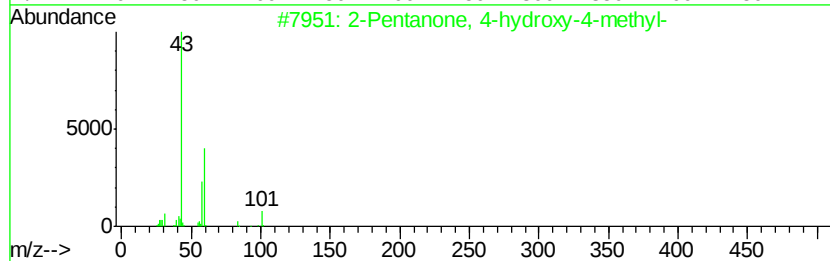
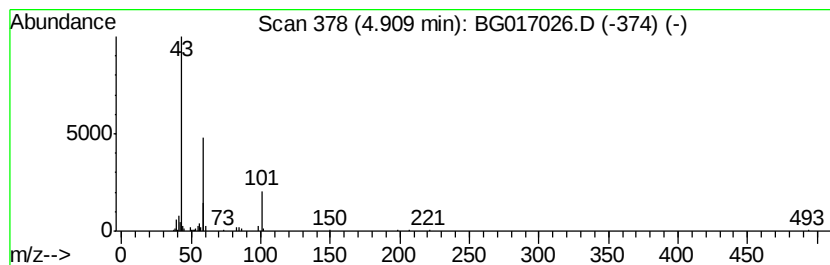
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	6.30 ng	102085	1,4-Dichlorobenzene-d4	7.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4			Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
5			Butane	58	C4H10	000106-97-8	9



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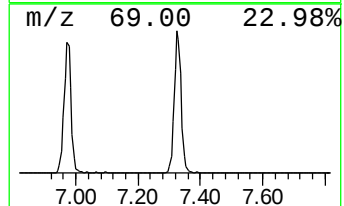
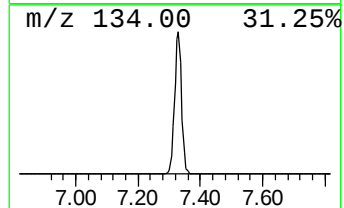
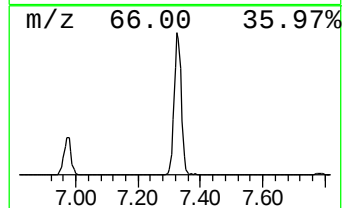
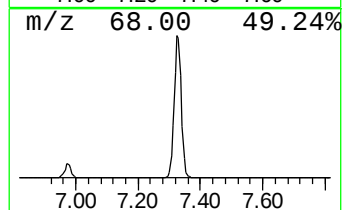
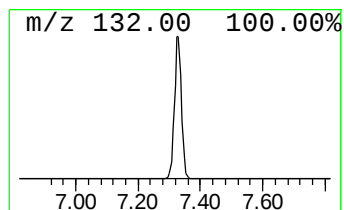
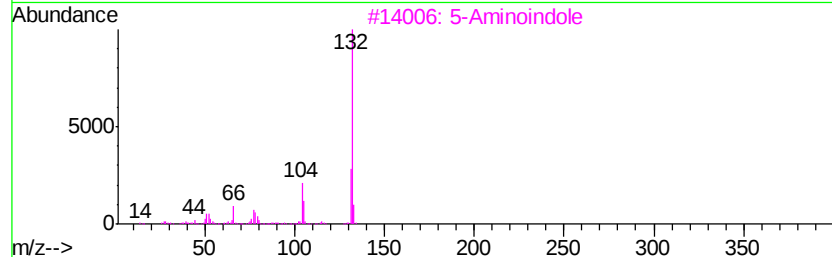
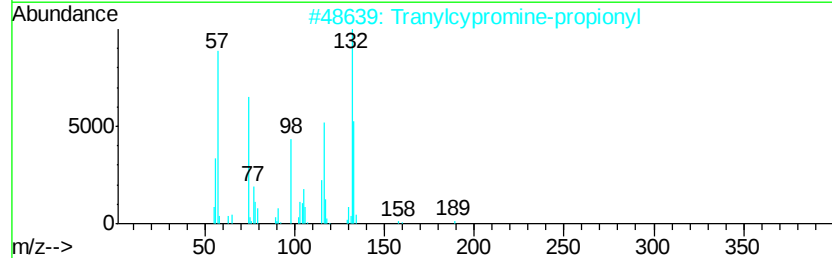
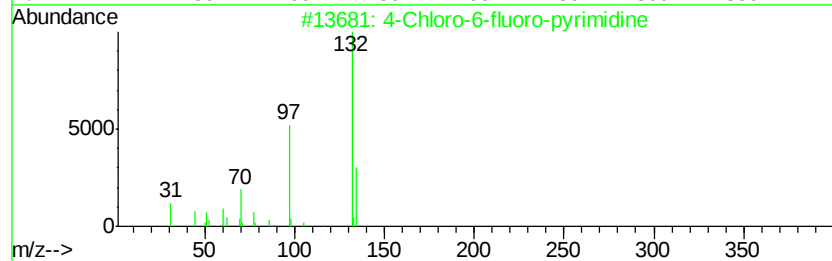
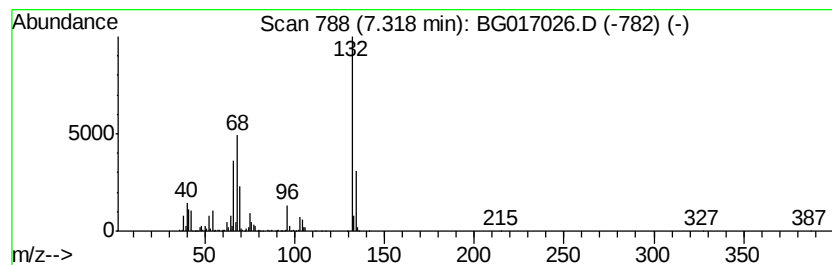
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Peak Number 3 unknown7.32 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	111.45 ng	1805730	1,4-Dichlorobenzene-d4	7.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	22
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.78	2.78	537.2	ng	8703600	1	7.79	324031	20.0
2-Pentanone, 4-hy...	4.91	6.3	ng	102085	1	7.79	324031	20.0
unknown7.32	7.32	111.5	ng	1805730	1	7.79	324031	20.0