

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061516\
 Data File : BF088044.D
 Acq On : 15 Jun 2016 20:08
 Operator : UM/SJ
 Sample : H3609-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 181-03-NE-06142016

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_F\METHODS\8270-BF060716.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	1.690	6	9	18	rVB2	323823	713517	26.92%	4.380%
2	1.815	18	20	31	rVB	1595302	2650592	100.00%	16.272%
3	2.158	48	50	71	rVB2	18637	78983	2.98%	0.485%
4	4.902	287	290	296	rBV	66921	88170	3.33%	0.541%
5	5.324	325	327	330	rBV	872985	1083626	40.88%	6.652%
6	6.376	417	419	422	rBV	1173679	1065217	40.19%	6.539%
7	6.502	428	430	433	rVB	1122230	1142154	43.09%	7.012%
8	6.742	449	451	453	rBV	674186	584064	22.04%	3.586%
9	6.890	462	464	467	rBV	750281	958990	36.18%	5.887%
10	7.302	498	500	503	rBV	651998	688247	25.97%	4.225%
11	8.022	561	563	566	rBV	573260	760715	28.70%	4.670%
12	9.108	655	658	660	rBV	1645807	1455405	54.91%	8.935%
13	9.508	690	693	695	rBV	154190	185695	7.01%	1.140%
14	9.782	714	717	719	rBB	928369	867737	32.74%	5.327%
15	10.559	783	785	788	rBV2	616372	722293	27.25%	4.434%
16	10.696	795	797	801	rBV	20063	35014	1.32%	0.215%
17	11.256	844	846	849	rBV	929374	813368	30.69%	4.993%
18	12.845	982	985	987	rBV	1218964	1173956	44.29%	7.207%
19	13.748	1061	1064	1074	rBV	19151	48096	1.81%	0.295%
20	13.885	1074	1076	1079	rBV2	557327	620423	23.41%	3.809%
21	15.291	1196	1199	1205	rVB	420704	553050	20.87%	3.395%

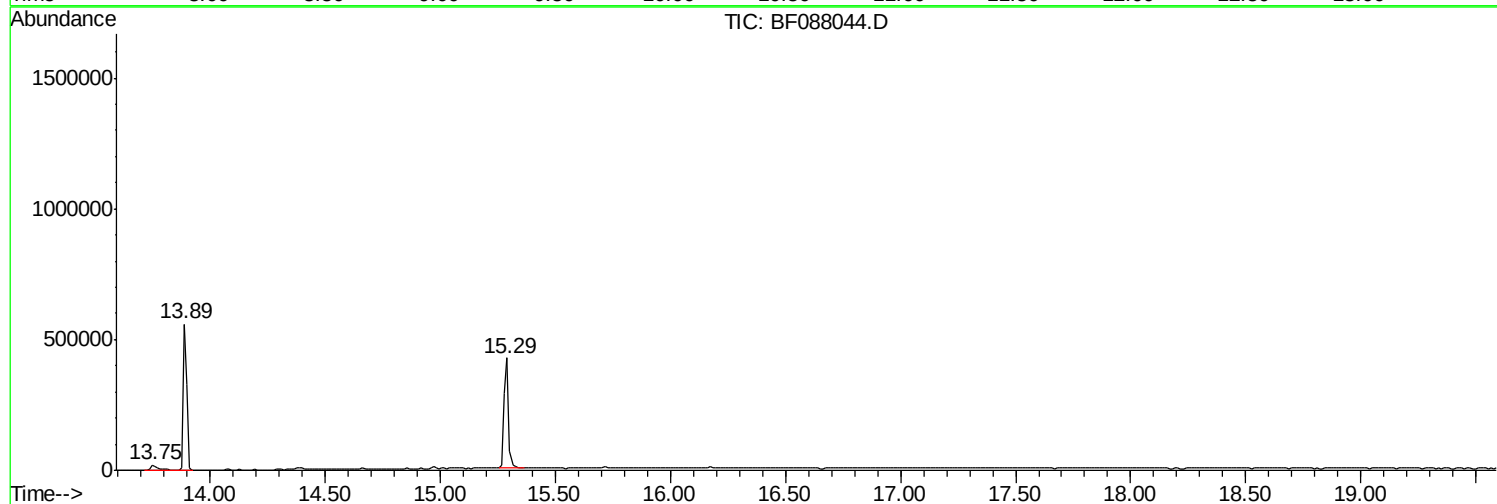
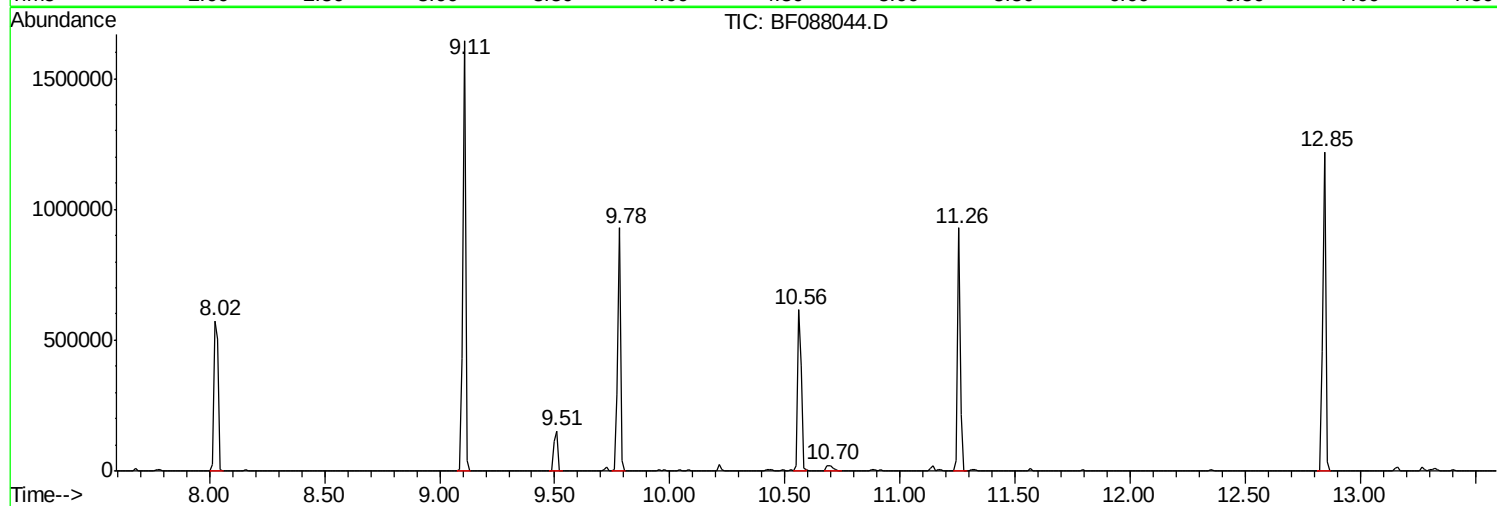
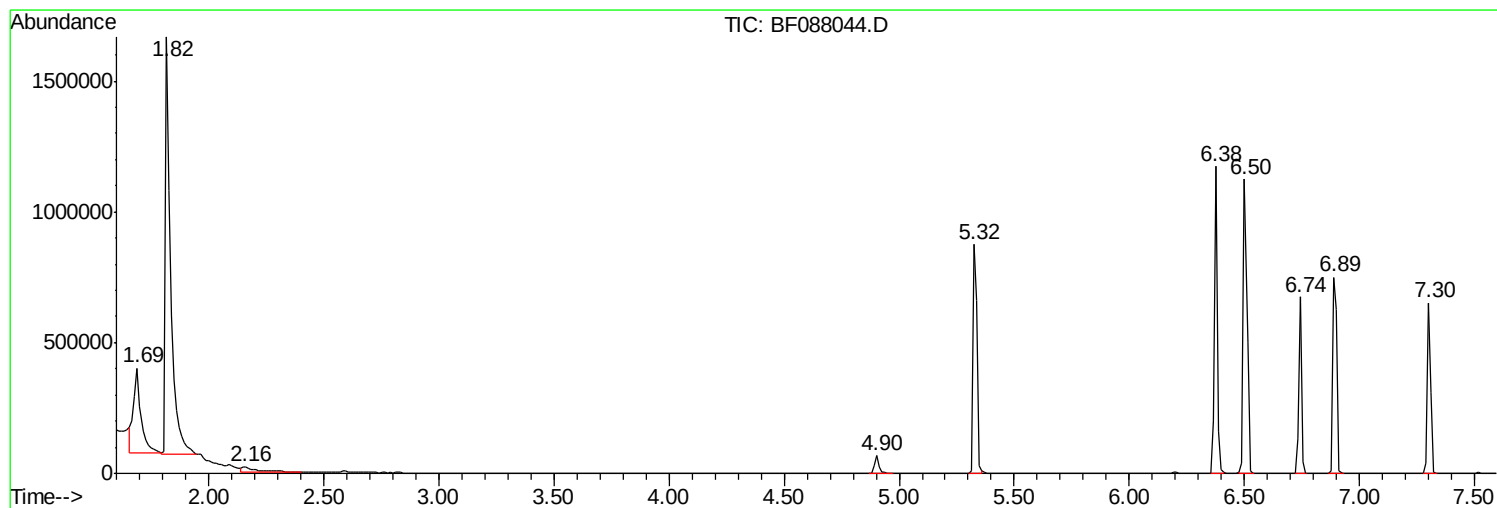
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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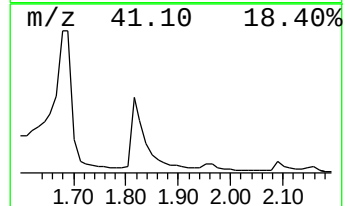
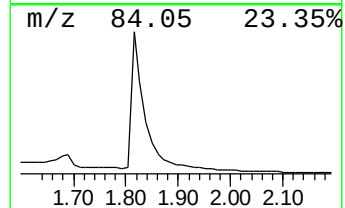
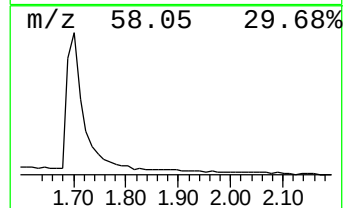
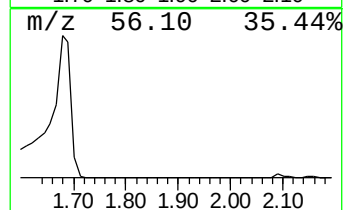
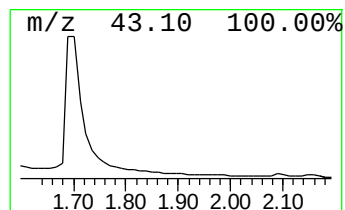
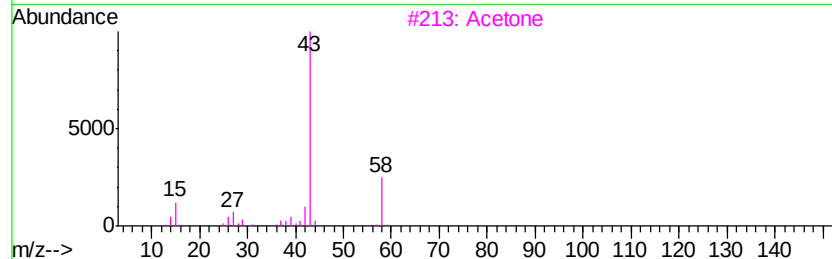
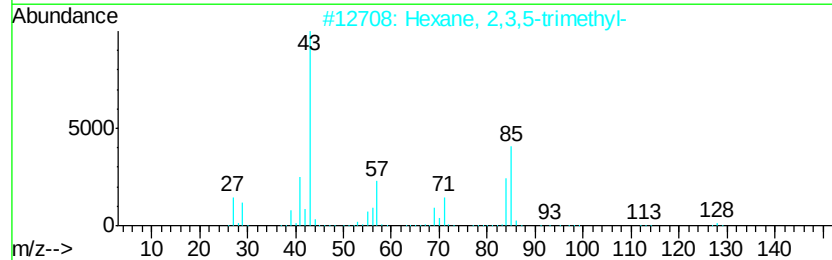
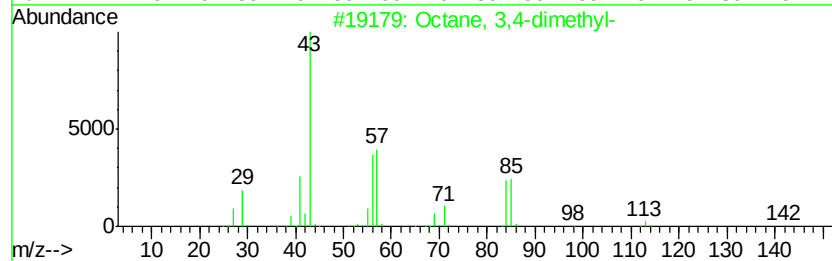
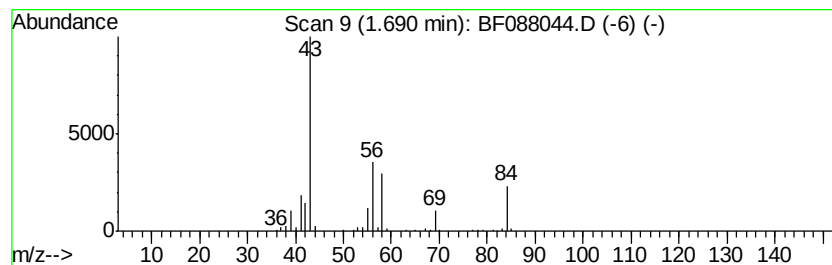
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.69 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.69	24.43 ng	713517	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 3,4-dimethyl-	142	C10H22	015869-92-8	36
2		Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	28
3		Acetone	58	C3H6O	000067-64-1	25
4		3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	25
5		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	23



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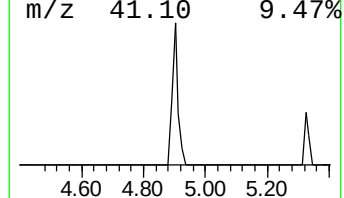
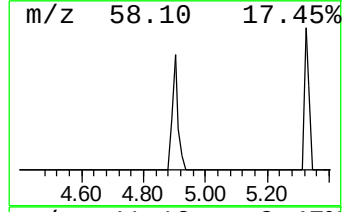
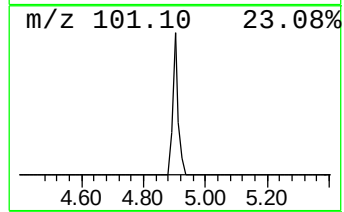
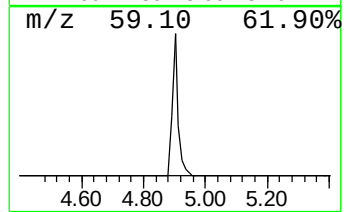
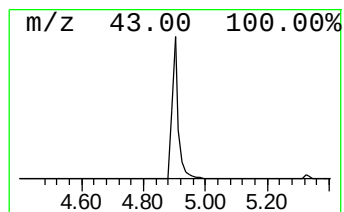
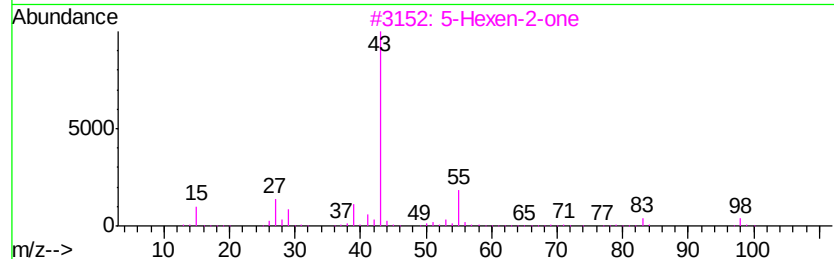
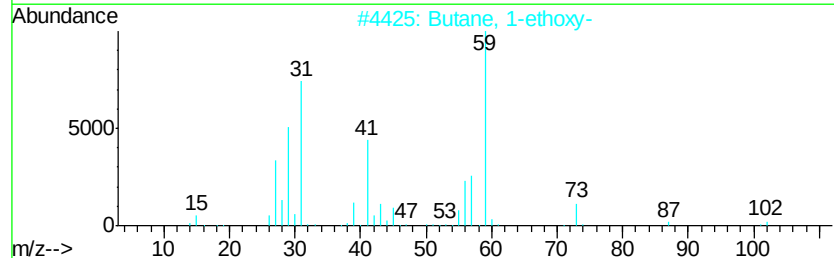
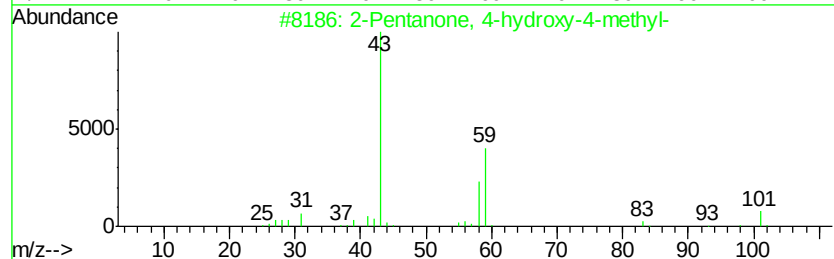
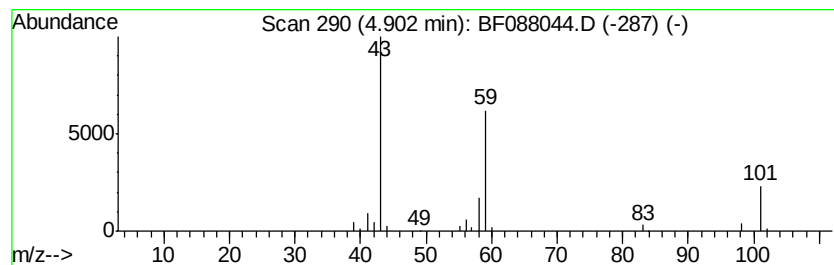
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.02 ng	88170	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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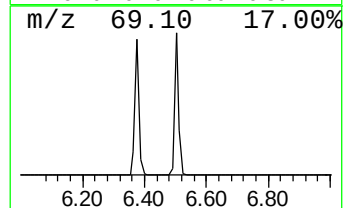
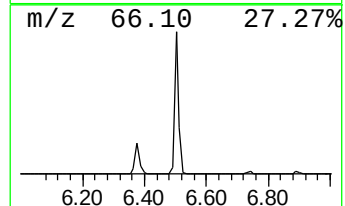
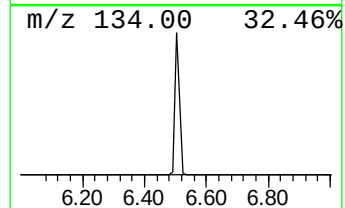
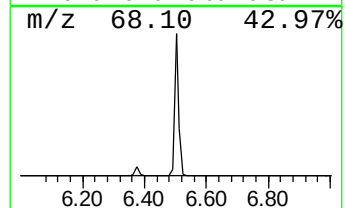
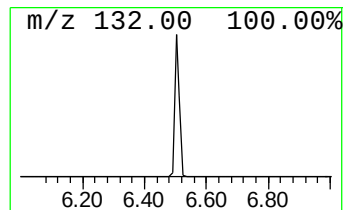
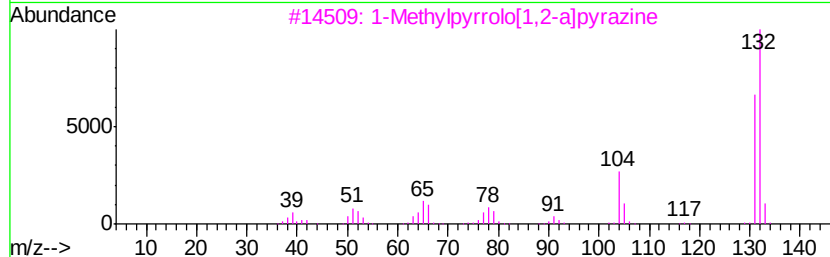
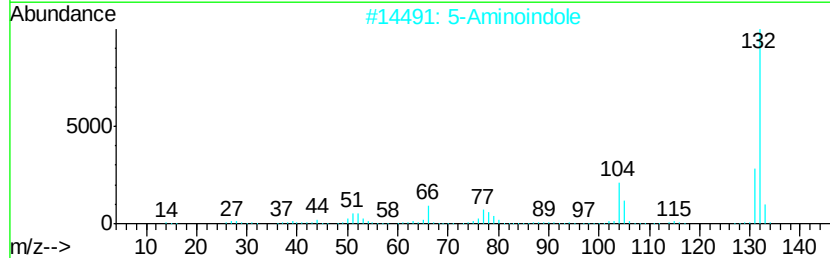
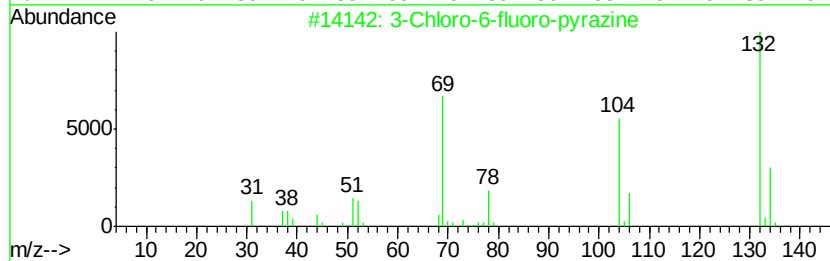
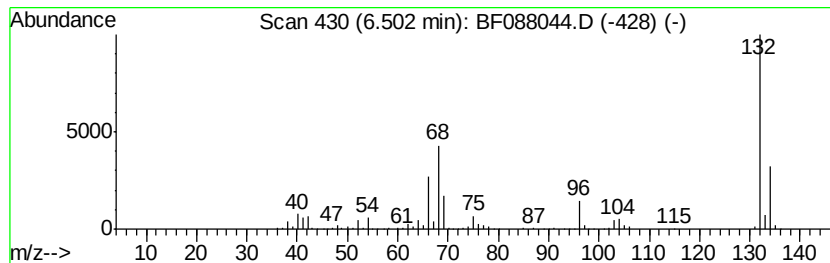
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Peak Number 5 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	39.11 ng	1142150	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	1-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-59-9	9
4	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...			132	C8H8N2	022291-85-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.69	1.69	24.4	ng	713517	1	6.74	584064	20.0
2-Pentanone, 4-hy...	4.90	3.0	ng	88170	1	6.74	584064	20.0
unknown6.50	6.50	39.1	ng	1142150	1	6.74	584064	20.0