

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
 Data File : BF088642.D
 Acq On : 3 Jul 2016 11:41
 Operator : UM/SJ
 Sample : PB91848BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91848BL

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-BF063016.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	1.655	3	6	8	rVB	781130	928967	26.27%	3.245%
2	1.724	10	12	19	rVV	122612	219915	6.22%	0.768%
3	1.850	21	23	39	rVB	478869	760033	21.50%	2.655%
4	4.970	293	296	304	rVB	112527	175942	4.98%	0.615%
5	5.381	329	332	335	rBV	2143331	2669221	75.49%	9.323%
6	6.422	420	423	425	rBV	2573743	2739092	77.47%	9.567%
7	6.547	432	434	437	rBV	2175310	2796049	79.08%	9.766%
8	6.787	453	455	457	rBV	565381	618407	17.49%	2.160%
9	6.936	466	468	471	rVB	1838838	2216294	62.68%	7.741%
10	7.347	501	504	506	rVB	1849684	1894586	53.59%	6.618%
11	8.067	564	567	569	rVB	962457	856352	24.22%	2.991%
12	9.142	658	661	664	rVB	2546279	3301881	93.39%	11.533%
13	9.816	717	720	722	rVB	1041715	952958	26.95%	3.329%
14	10.605	786	789	791	rBV	2035607	2100391	59.41%	7.336%
15	11.291	847	849	852	rVB	867991	974362	27.56%	3.403%
16	12.879	985	988	991	rBV	2604123	3535643	100.00%	12.349%
17	13.919	1077	1079	1082	rBV	1132547	985056	27.86%	3.441%
18	15.314	1198	1201	1204	rBV	785803	904709	25.59%	3.160%

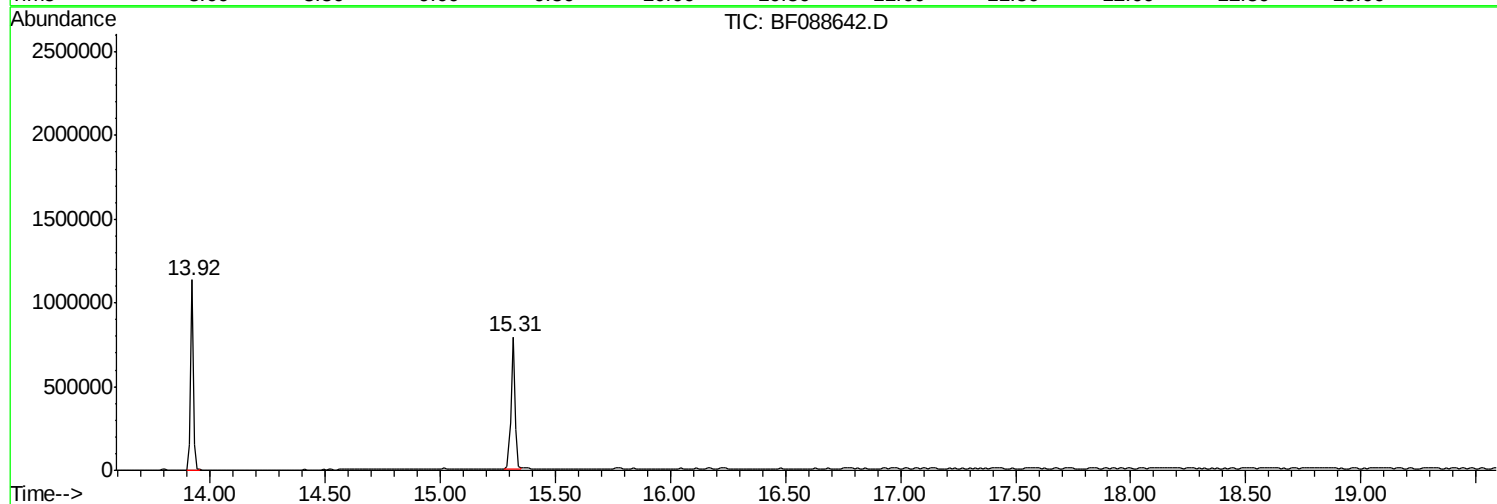
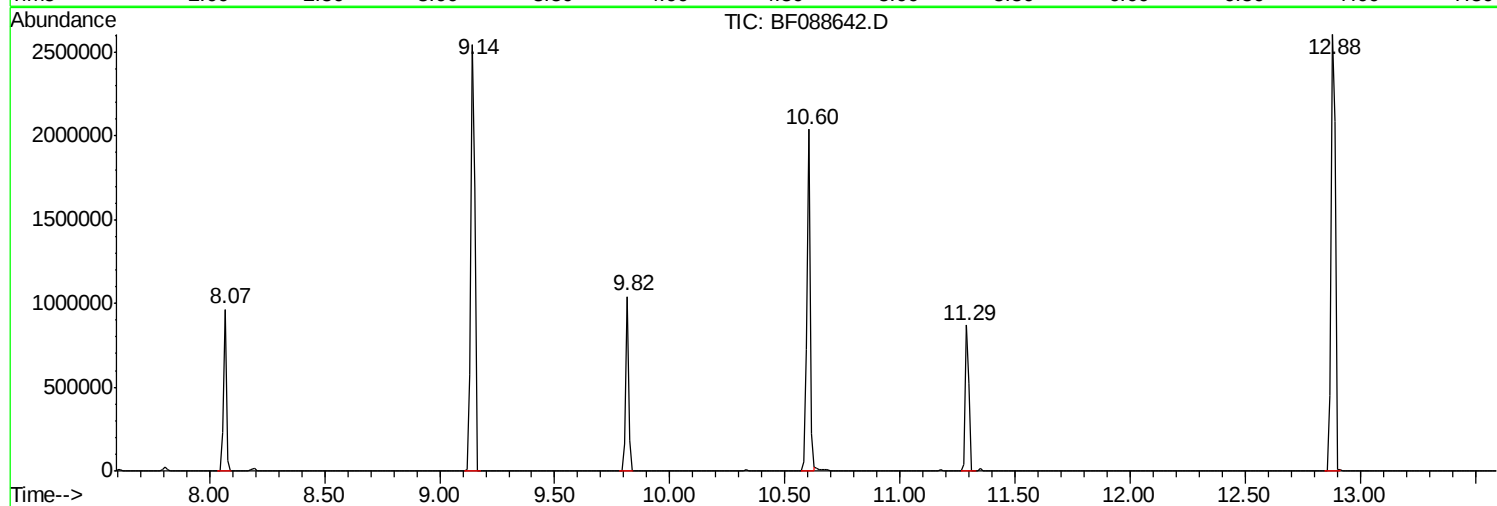
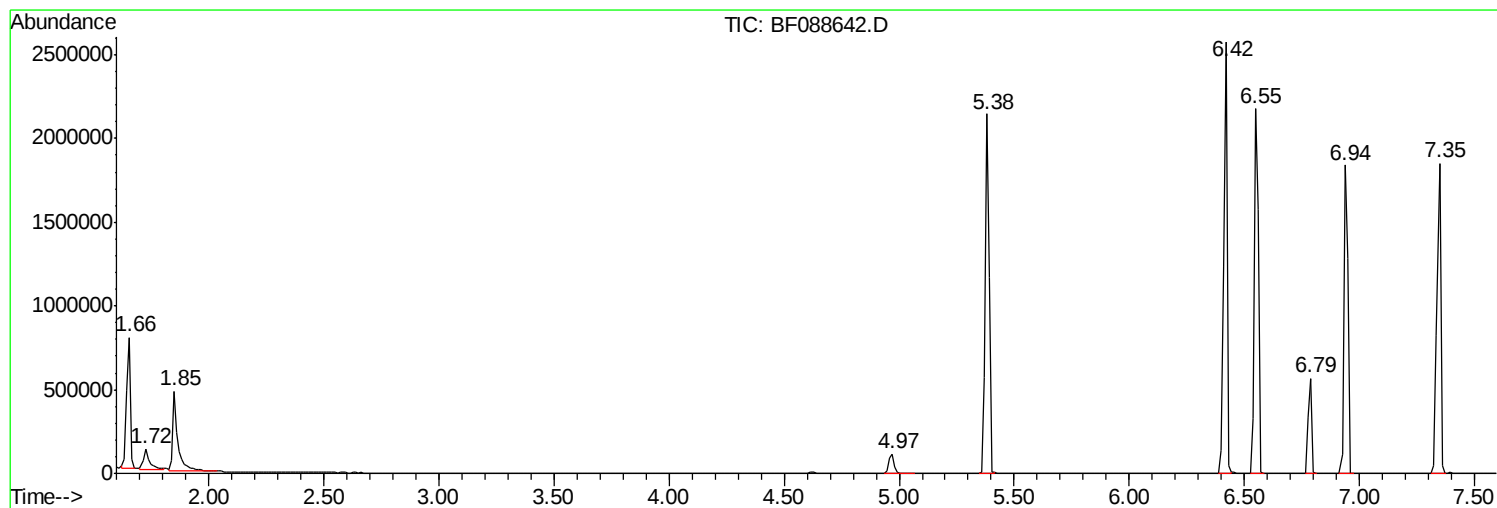
Sum of corrected areas: 28629858

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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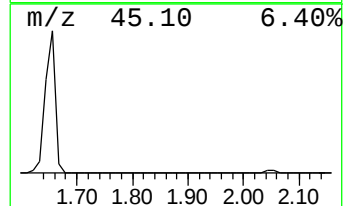
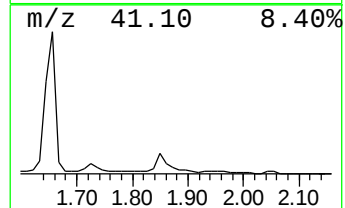
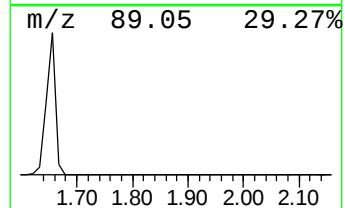
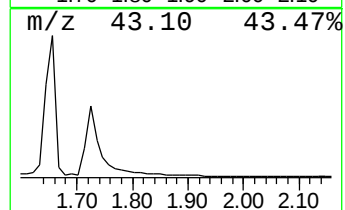
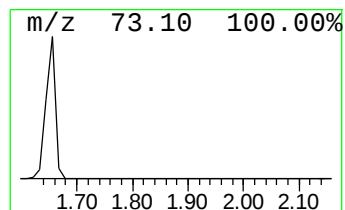
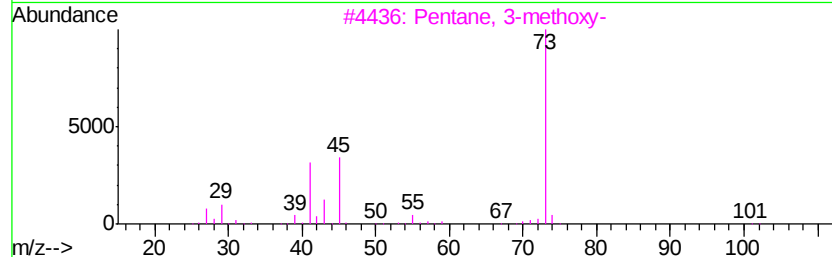
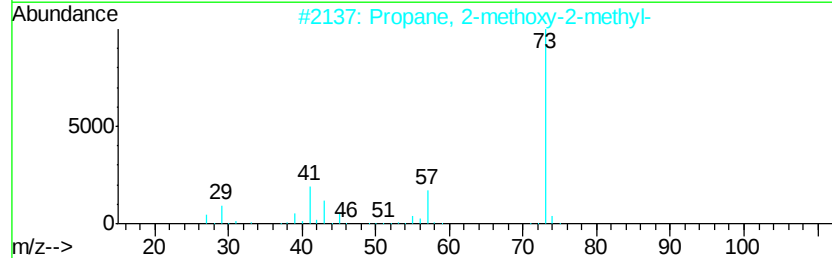
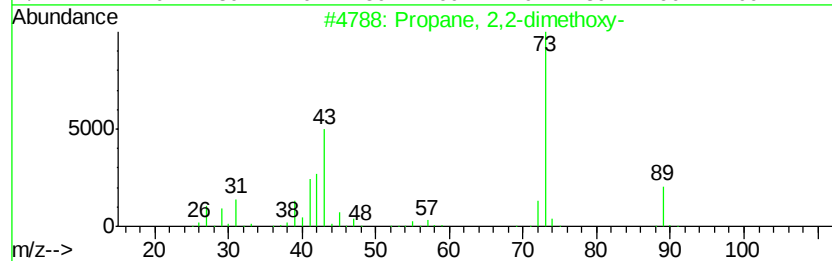
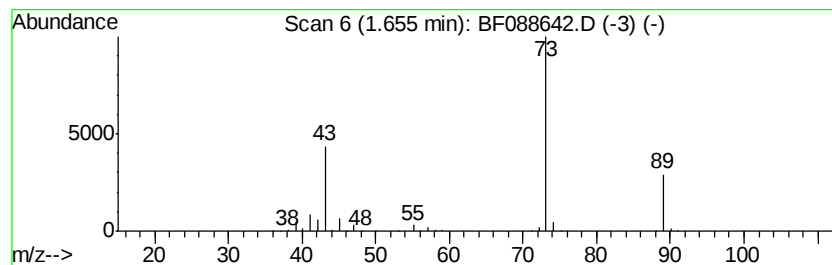
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.66 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.66	30.04 ng	928967	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	36
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7



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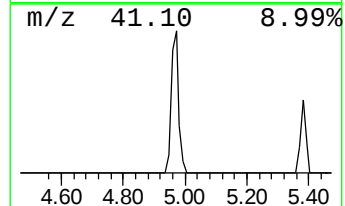
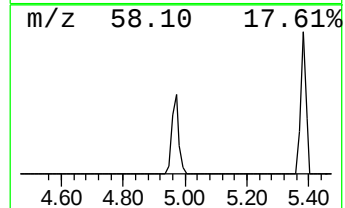
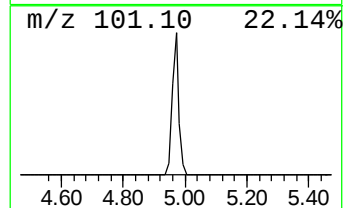
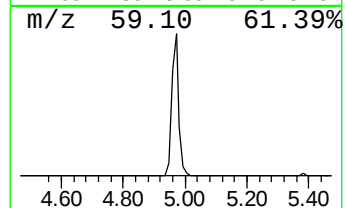
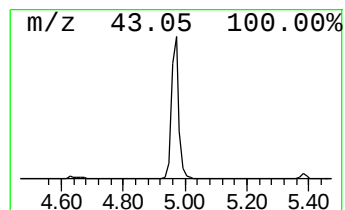
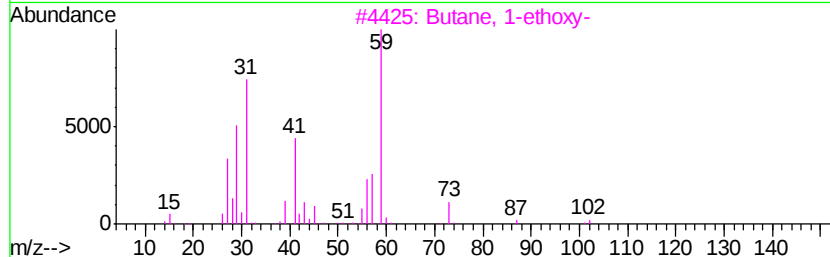
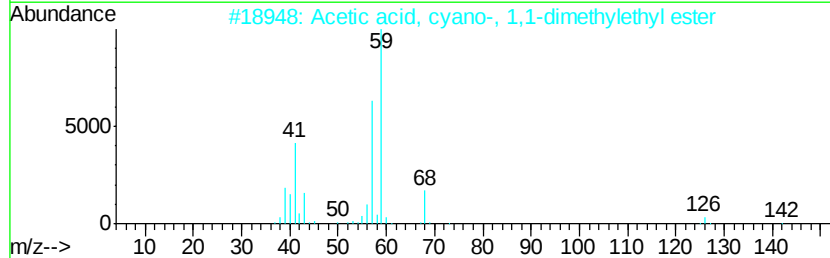
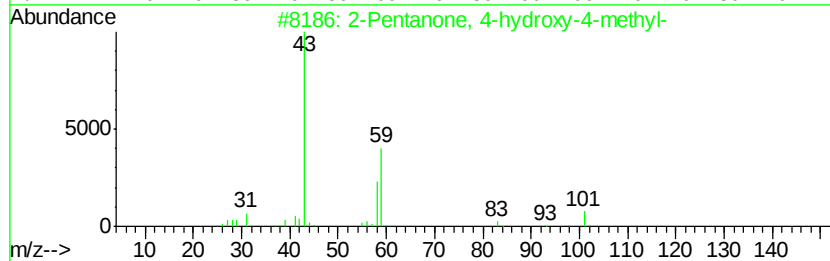
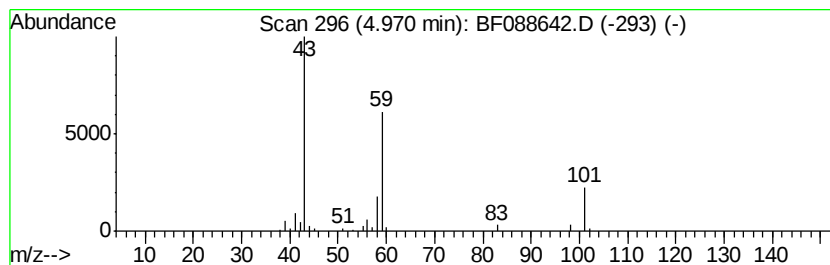
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	5.69 ng	175942	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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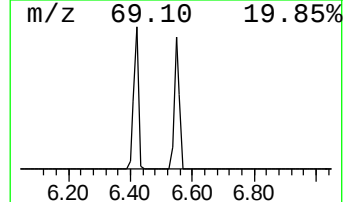
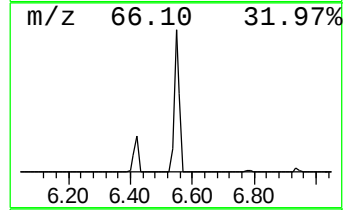
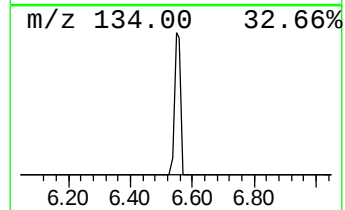
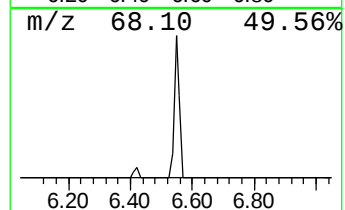
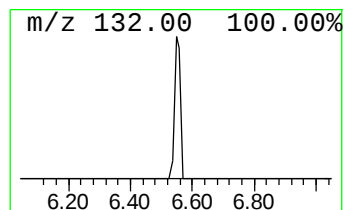
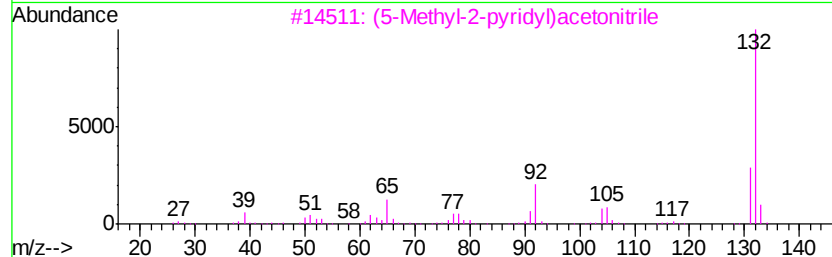
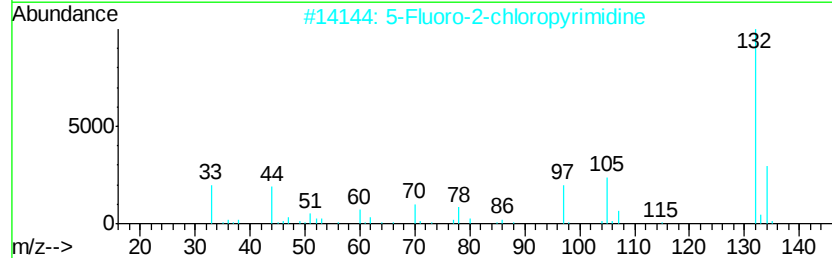
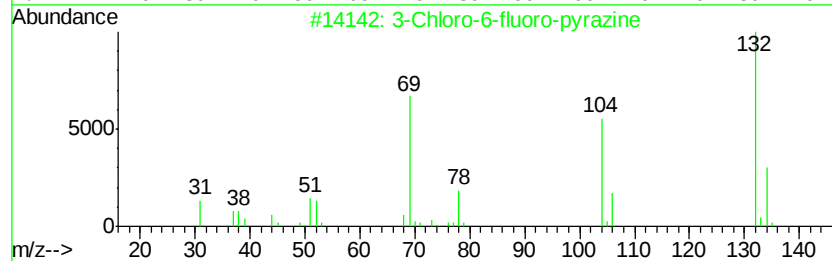
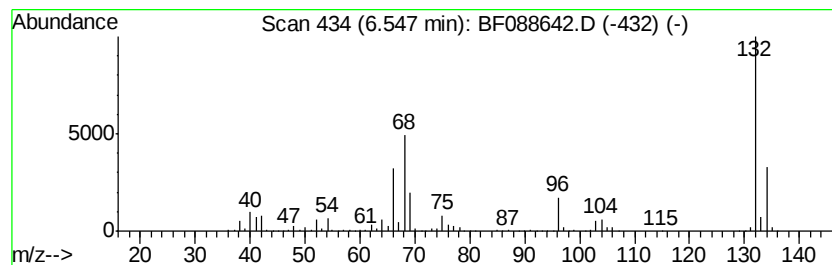
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Peak Number 5 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	90.43 ng	2796050	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.66	1.66	30.0	ng	928967	1	6.79	618407	20.0
2-Pentanone, 4-hy...	4.97	5.7	ng	175942	1	6.79	618407	20.0
unknown6.55	6.55	90.4	ng	2796050	1	6.79	618407	20.0