

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051616\
 Data File : BF087086.D
 Acq On : 16 May 2016 17:30
 Operator : UM/SJ
 Sample : PB90651BL
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90651BL

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_F\METHODS\8270-BF050916.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	1.735	11	13	66	rVB	1664049	4531663	100.00%	13.523%
2	4.741	273	276	290	rBV	1080841	1662665	36.69%	4.962%
3	5.210	314	317	319	rBV	2653942	3464722	76.46%	10.339%
4	5.599	349	351	354	rBV	142415	131589	2.90%	0.393%
5	6.273	408	410	413	rBV	2503439	3345892	73.83%	9.984%
6	6.376	417	419	422	rBV	2771810	3232145	71.32%	9.645%
7	6.604	437	439	450	rVB	995649	884917	19.53%	2.641%
8	6.764	450	453	455	rBV	2532919	2705509	59.70%	8.074%
9	7.176	487	489	492	rBV	1635712	1993999	44.00%	5.950%
10	7.896	549	552	554	rBV	1149367	1053871	23.26%	3.145%
11	8.970	644	646	649	rBV	2608539	3111935	68.67%	9.286%
12	9.645	702	705	707	rBV	996810	943170	20.81%	2.815%
13	10.433	771	774	776	rBV	1755941	1660748	36.65%	4.956%
14	11.119	832	834	837	rBV	925151	793025	17.50%	2.366%
15	12.708	970	973	975	rBV	2746440	2697640	59.53%	8.050%
16	13.748	1061	1064	1067	rBV	803998	766140	16.91%	2.286%
17	15.108	1181	1183	1186	rBV	470462	531277	11.72%	1.585%

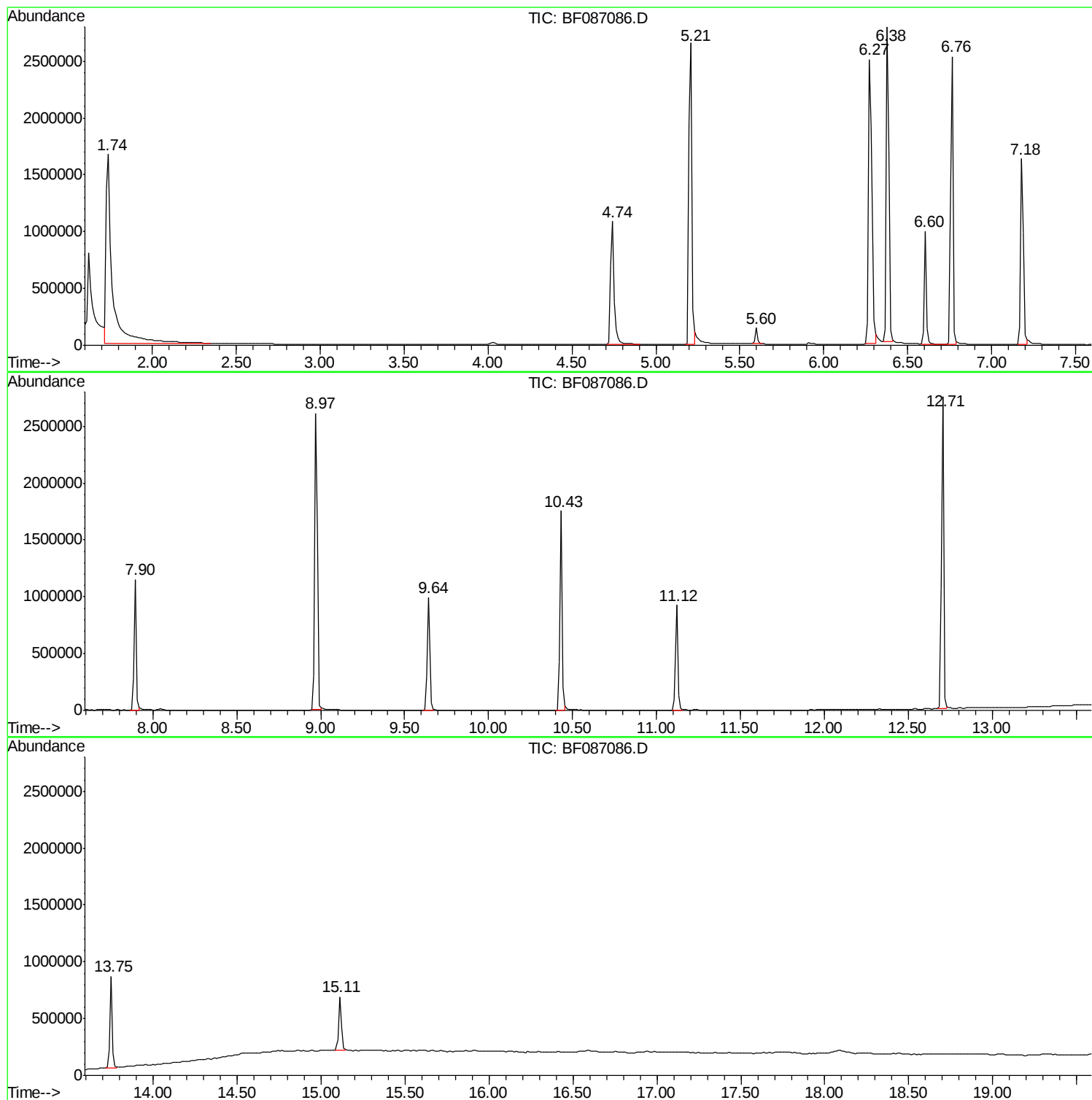
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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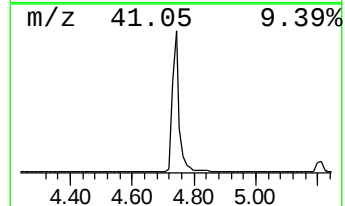
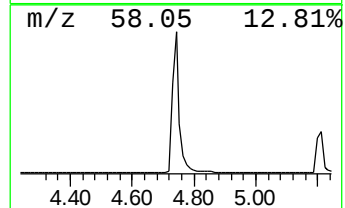
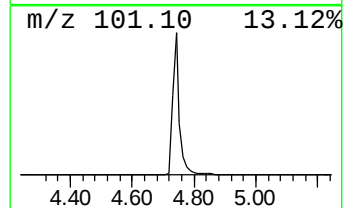
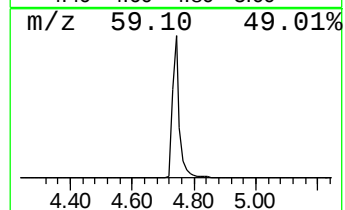
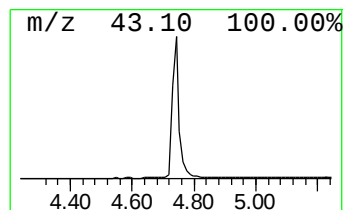
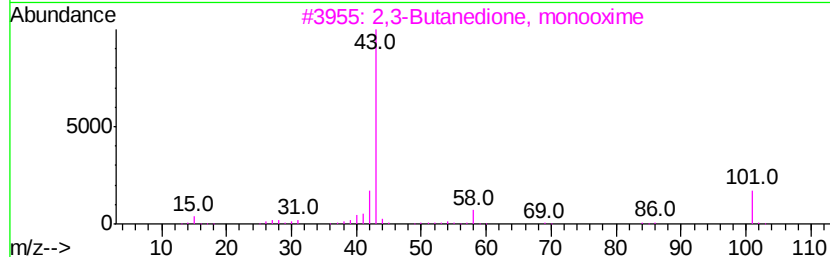
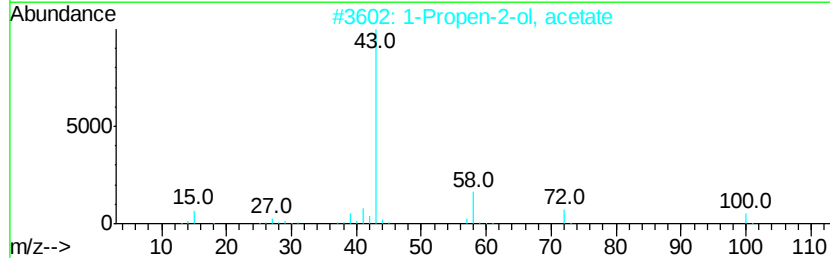
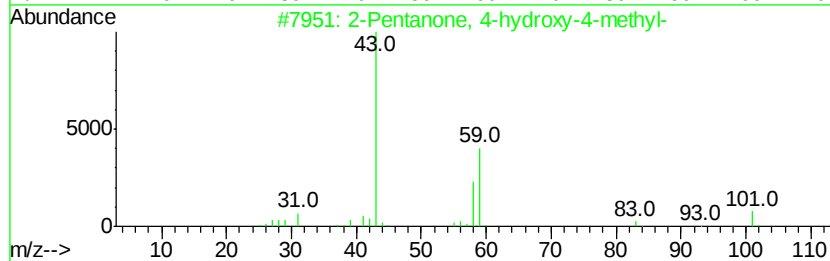
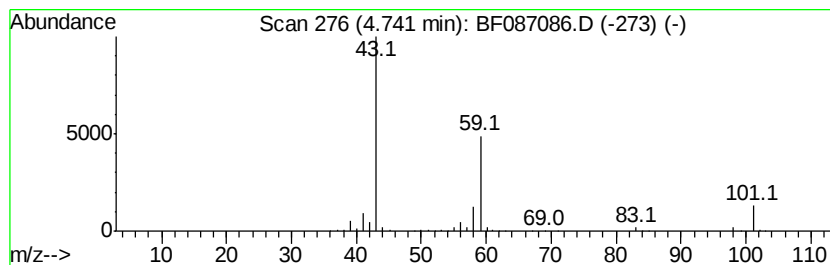
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	37.58 ng	1662670	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	7



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Instrument :
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ClientSampled :
PB90651BL

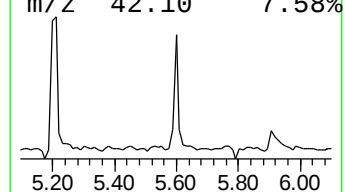
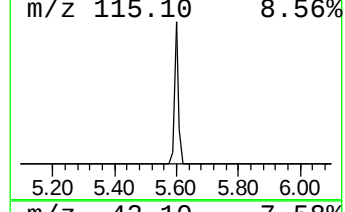
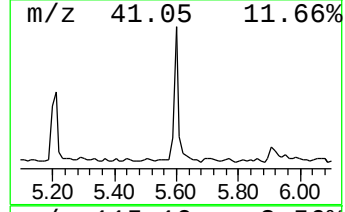
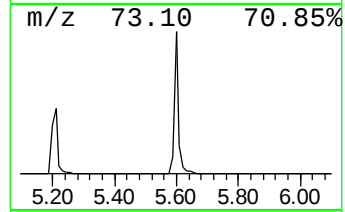
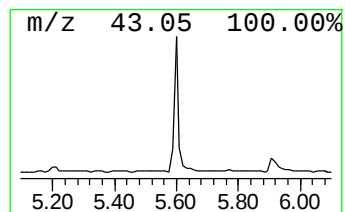
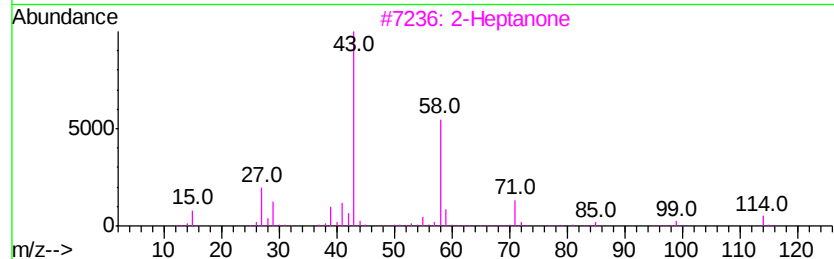
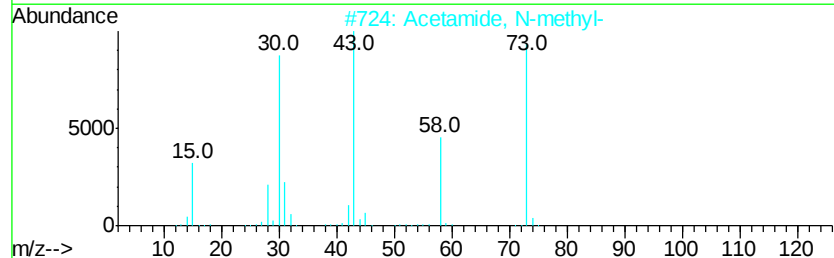
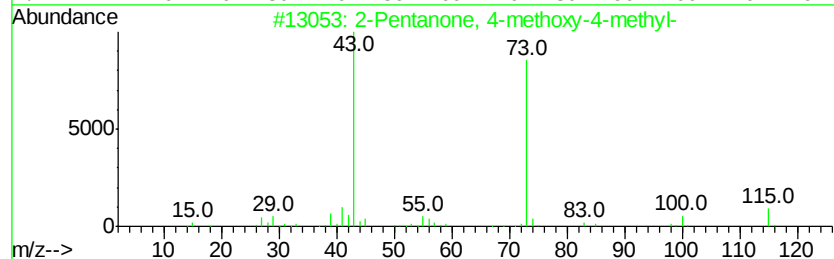
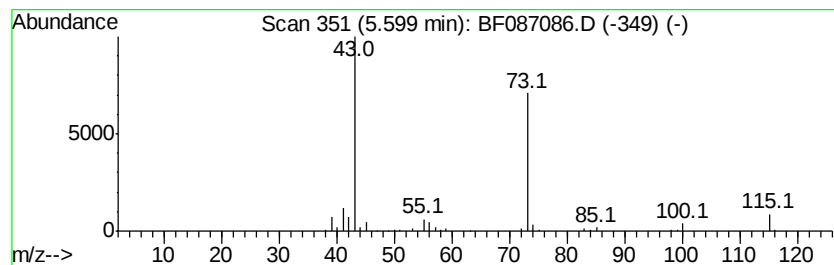
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	2.97 ng	131589	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	47
3		2-Heptanone	114	C7H14O	000110-43-0	17
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	12
5		N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



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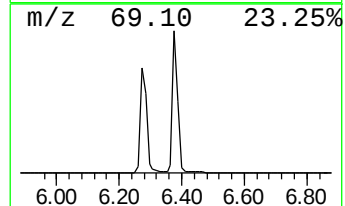
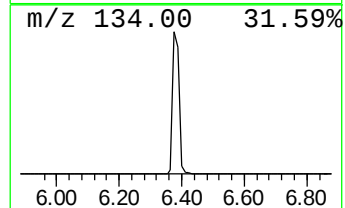
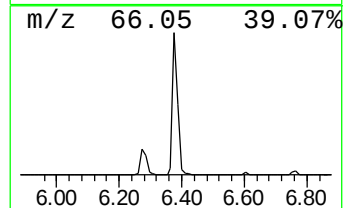
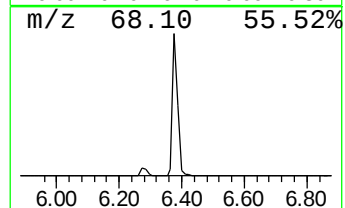
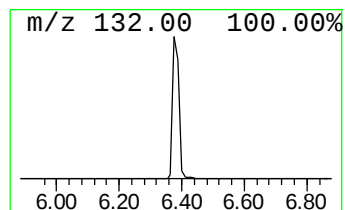
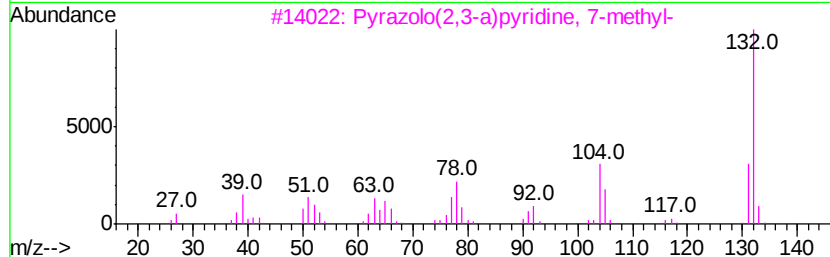
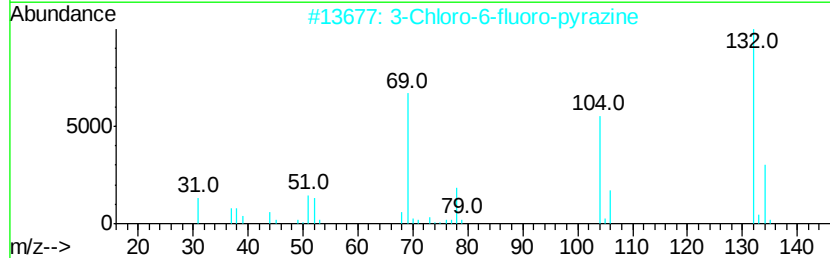
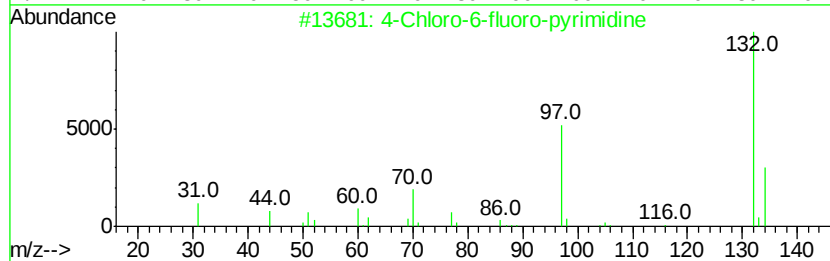
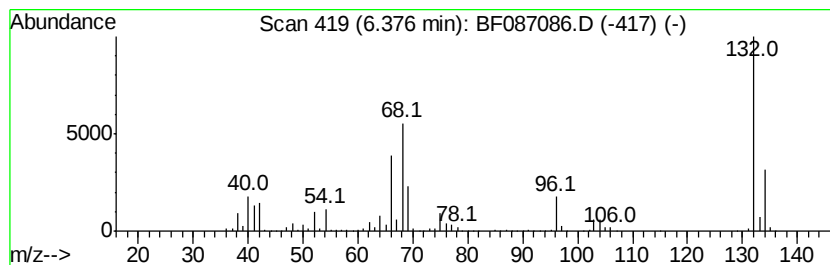
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Peak Number 4 unknown6.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	73.05 ng	3232150	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14		
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14		
3	Pvrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	14		
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10		
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10		



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.74	37.6	ng	1662670	1	6.60	884917	20.0
2-Pentanone, 4-me...	5.60	3.0	ng	131589	1	6.60	884917	20.0
unknown6.38	6.38	73.0	ng	3232150	1	6.60	884917	20.0