

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021517\
 Data File : BF092977.D
 Acq On : 16 Feb 2017 5:32
 Operator : SJ/MA
 Sample : I1836-04
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEST-PIT-A-COMP

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-BF013017.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	2.681	50	52	60	rVB	188578	254258	5.71%	0.674%
2	4.407	200	203	208	rBV	71972	115327	2.59%	0.306%
3	5.059	257	260	271	rBV	1330184	2012871	45.21%	5.335%
4	5.481	294	297	299	rBV	3901572	4066870	91.34%	10.779%
5	6.510	384	387	390	rBV	3233582	3564210	80.05%	9.447%
6	6.647	396	399	401	rBV	3541086	4452642	100.00%	11.802%
7	6.876	416	419	421	rBV	840378	935055	21.00%	2.478%
8	7.024	430	432	435	rBV	2426469	3212252	72.14%	8.514%
9	7.436	465	468	471	rBV	1993187	2966955	66.63%	7.864%
10	8.156	529	531	533	rBV	1490518	1366795	30.70%	3.623%
11	9.230	622	625	628	rBV	4035662	4281210	96.15%	11.347%
12	9.905	682	684	686	rBV	1440735	1286145	28.88%	3.409%
13	10.693	750	753	756	rBV	2181182	2255534	50.66%	5.978%
14	11.391	811	814	816	rBV	1336446	1206465	27.10%	3.198%
15	12.979	950	953	955	rBV	3306181	3899114	87.57%	10.335%
16	14.019	1042	1044	1047	rVB	853665	863723	19.40%	2.289%
17	15.460	1167	1170	1178	rVB	622485	845554	18.99%	2.241%
18	15.894	1205	1208	1212	rVB	45109	72485	1.63%	0.192%
19	16.374	1247	1250	1253	rBV	42316	70773	1.59%	0.188%

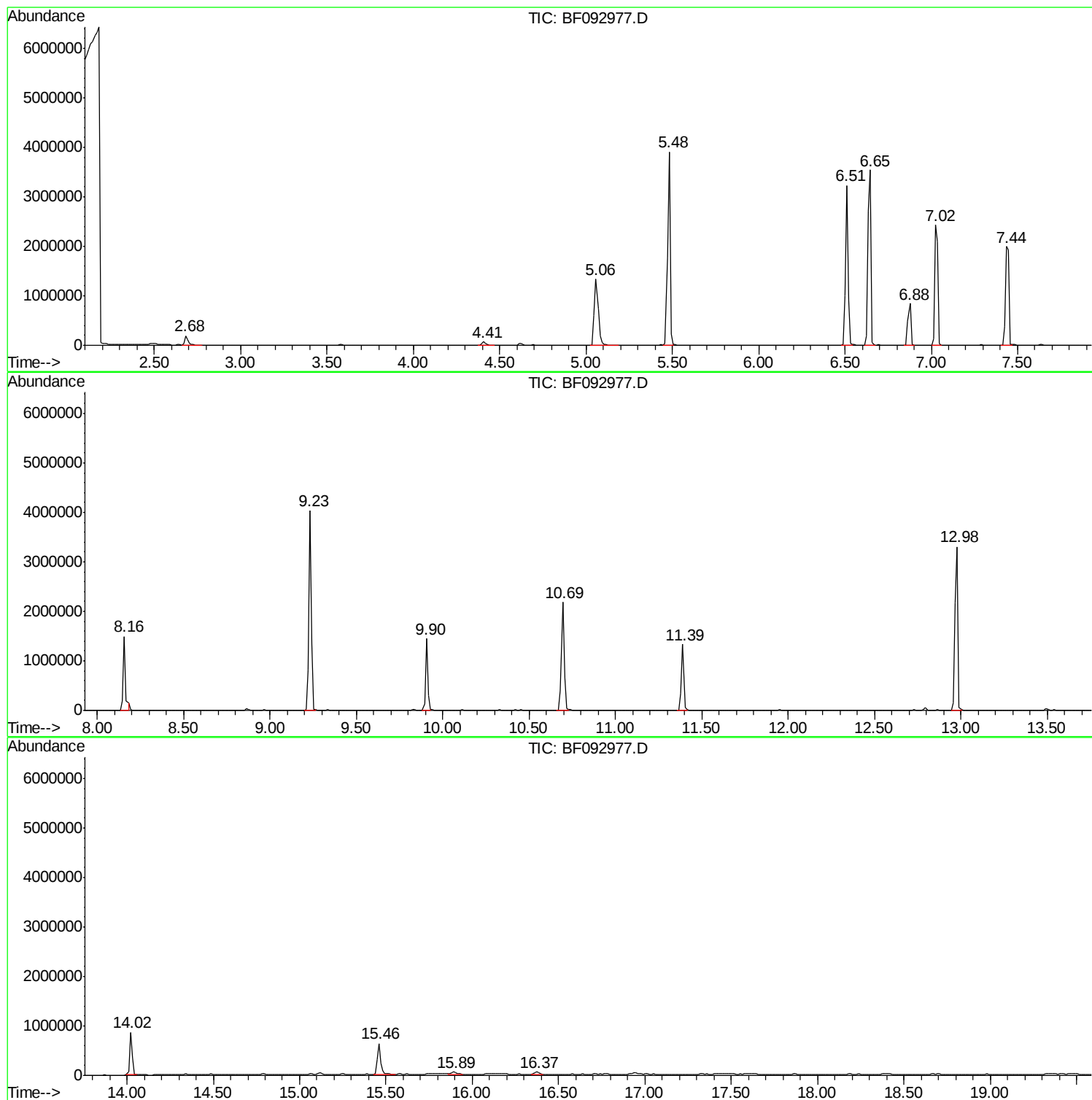
Sum of corrected areas: 37728238

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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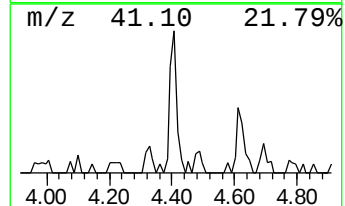
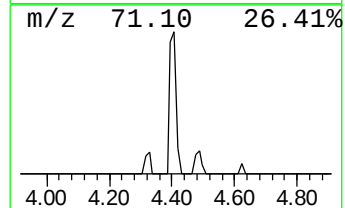
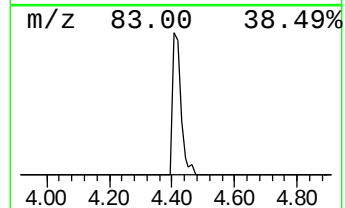
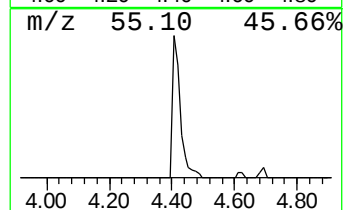
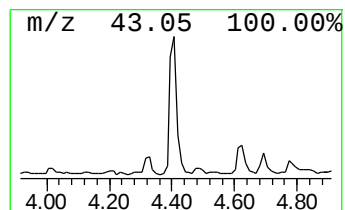
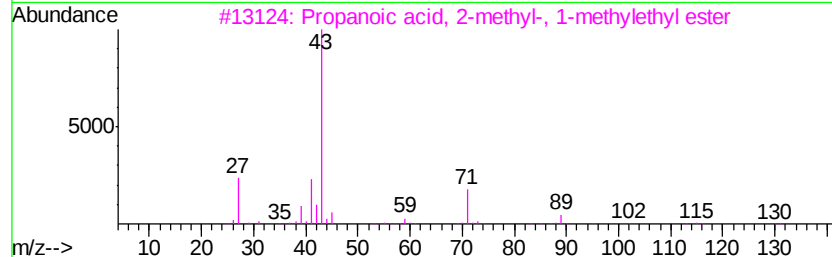
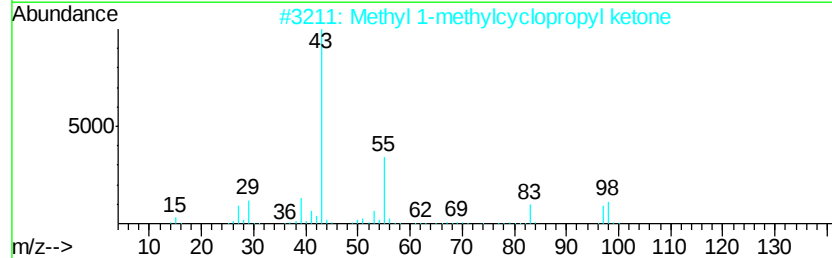
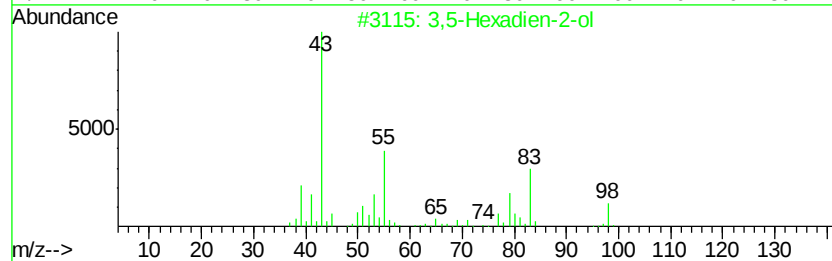
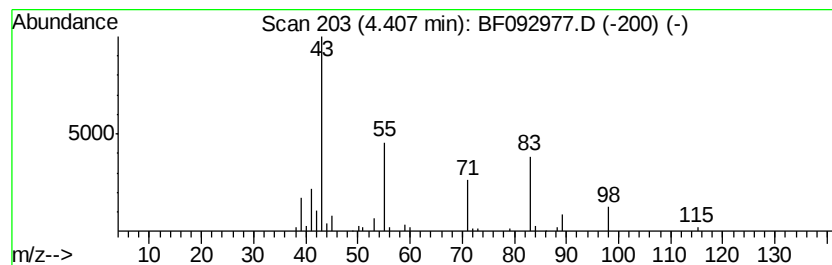
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown4.41 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	2.47 ng	115327	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-Hexadien-2-ol	98	C6H10O	003280-51-1	36
2		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	35
3		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	35
4		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	25
5		3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	12



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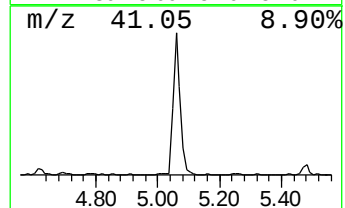
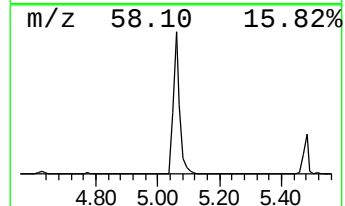
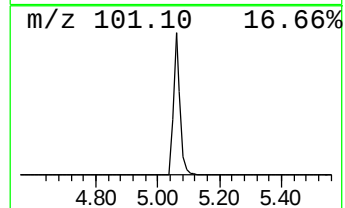
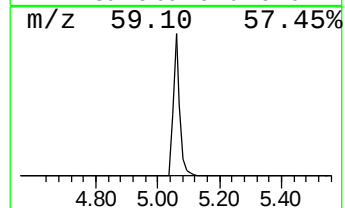
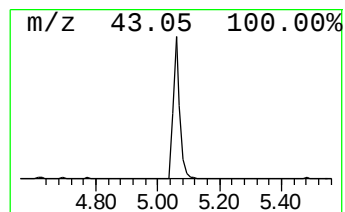
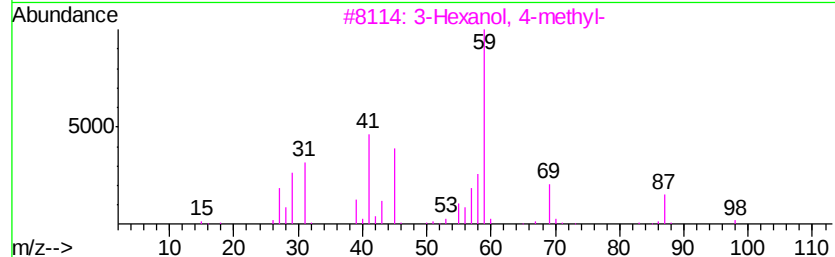
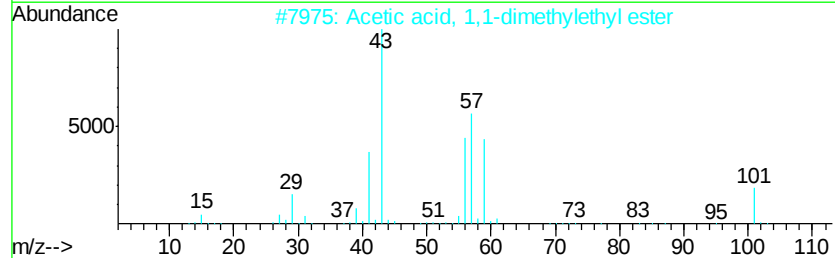
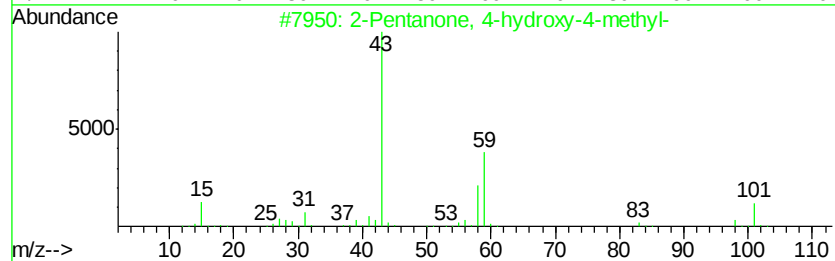
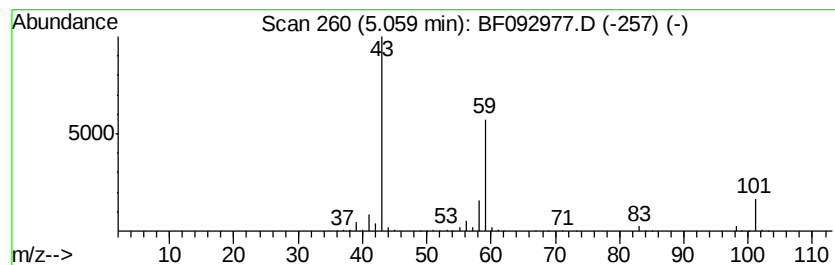
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	43.05 ng	2012870	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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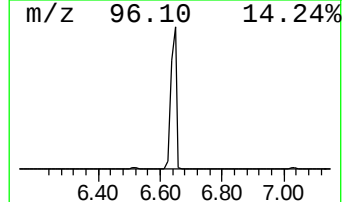
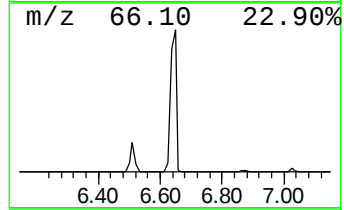
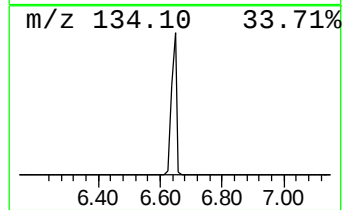
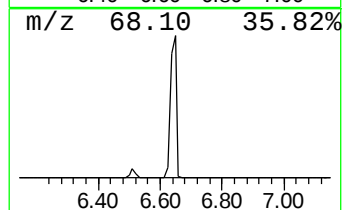
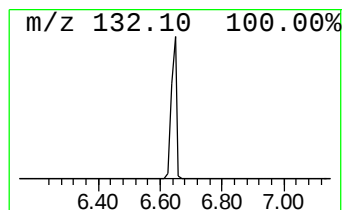
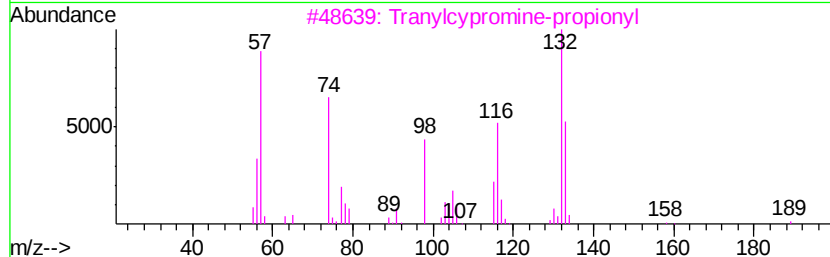
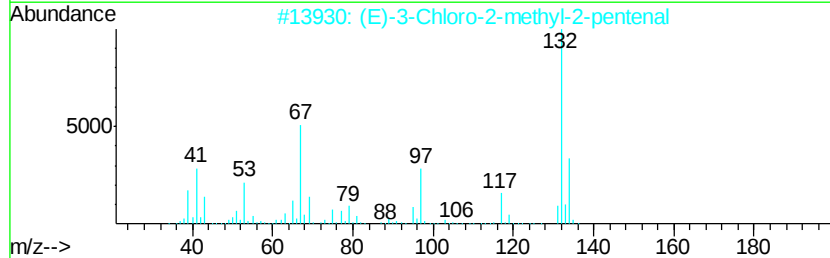
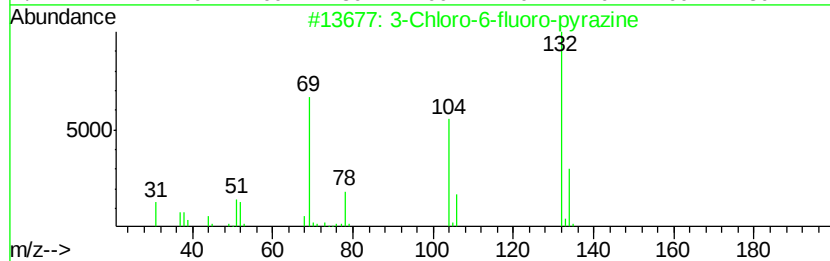
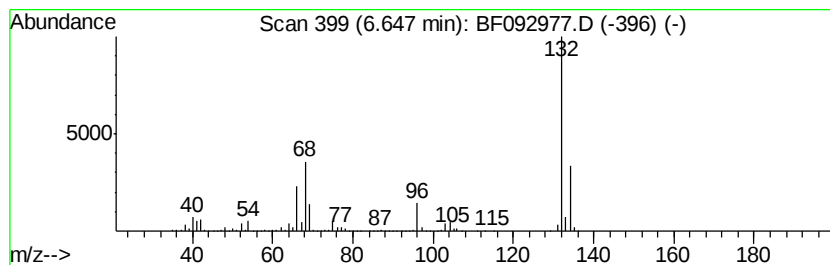
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Peak Number 4 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	95.24 ng	4452640	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	16
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown4.41	4.41	2.5	ng	115327	1	6.88	935055	20.0
2-Pentanone, 4-hy...	5.06	43.0	ng	2012870	1	6.88	935055	20.0
unknown6.65	6.65	95.2	ng	4452640	1	6.88	935055	20.0