

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080715\
 Data File : BF080942.D
 Acq On : 8 Aug 2015 1:07
 Operator : TP/UM
 Sample : PB84907BL
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84907BL

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-BF080715.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	4.293	191	193	197	rBB	100411	130607	7.35%	1.029%
2	4.967	249	252	255	rBV	629223	1015317	57.17%	8.001%
3	5.390	287	289	292	rBV	902748	853968	48.09%	6.730%
4	5.813	324	326	328	rBB	21909	28830	1.62%	0.227%
5	6.430	378	380	382	rBV	959375	844184	47.54%	6.652%
6	6.567	390	392	394	rBV	1029670	876389	49.35%	6.906%
7	6.807	411	413	415	rBB	505892	434635	24.48%	3.425%
8	6.967	424	427	429	rBB	750941	968468	54.54%	7.632%
9	7.367	459	462	465	rBV	819932	759832	42.79%	5.988%
10	8.087	523	525	528	rBV	541710	535320	30.15%	4.218%
11	9.173	617	620	622	rBV	1456187	1510173	85.04%	11.901%
12	9.848	676	679	681	rBV	506637	606748	34.17%	4.781%
13	10.625	745	747	750	rBV	679931	605217	34.08%	4.769%
14	11.322	806	808	810	rBV	841106	697136	39.26%	5.494%
15	12.911	944	947	949	rBV	1768802	1775816	100.00%	13.994%
16	13.951	1035	1038	1040	rBV	668619	631965	35.59%	4.980%
17	15.357	1158	1161	1164	rBV	350647	415281	23.39%	3.273%

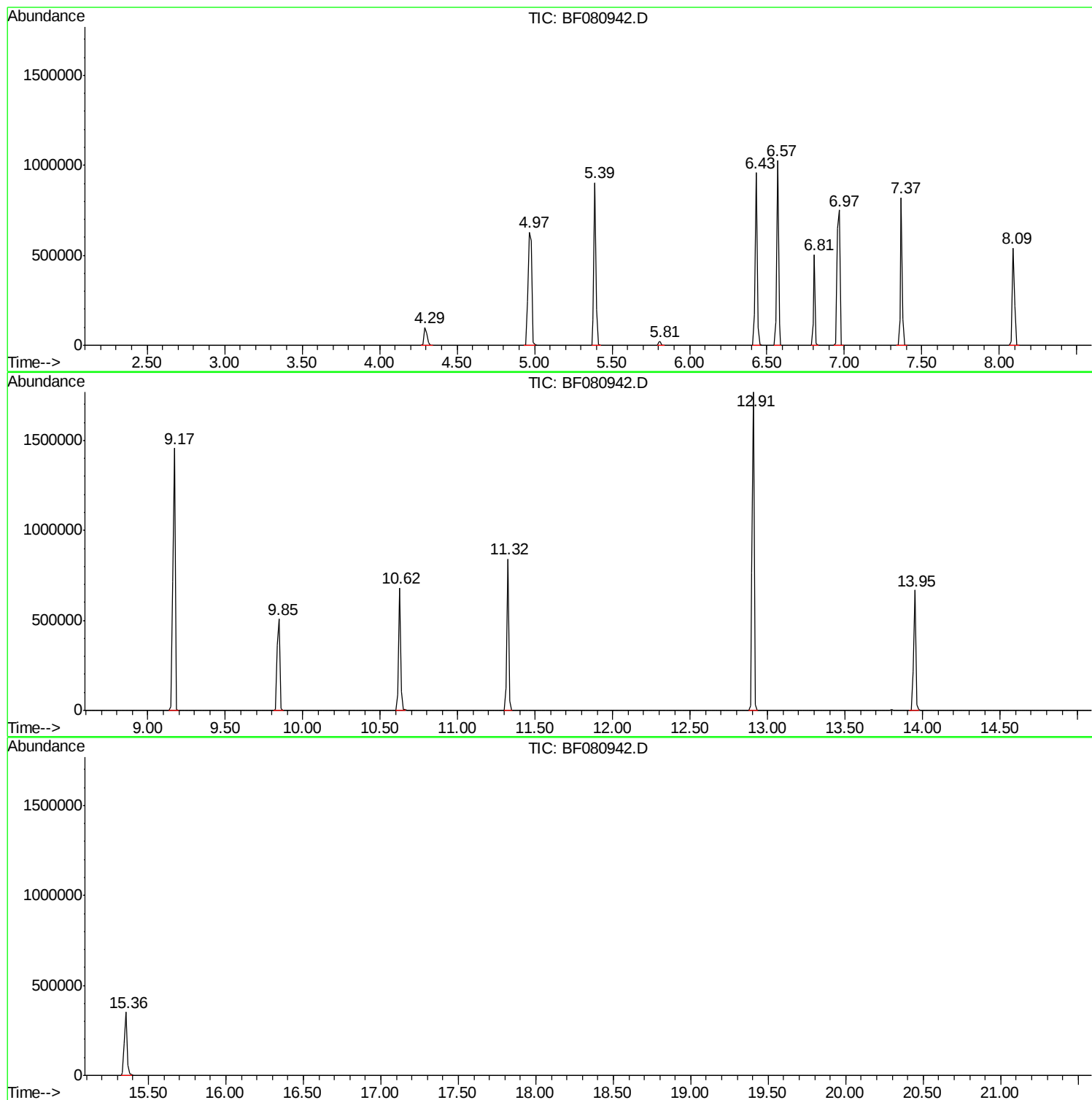
Sum of corrected areas: 12689886

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.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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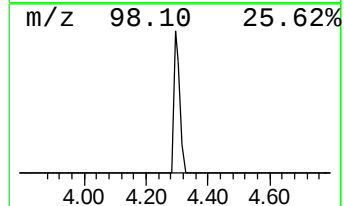
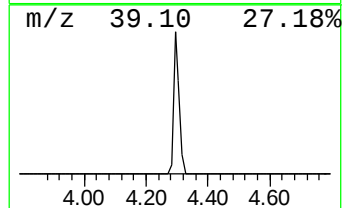
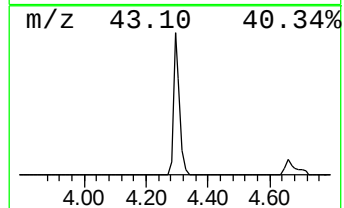
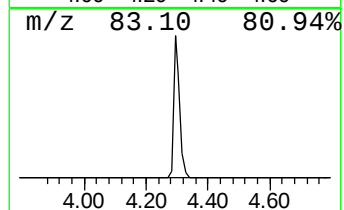
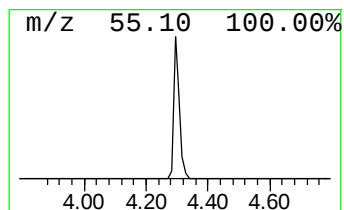
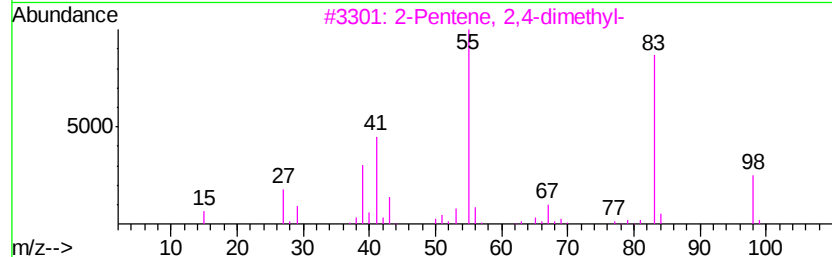
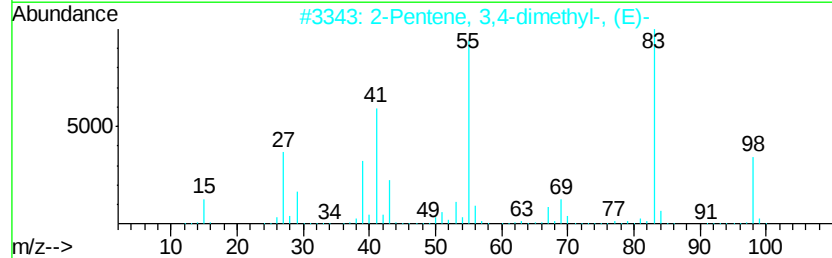
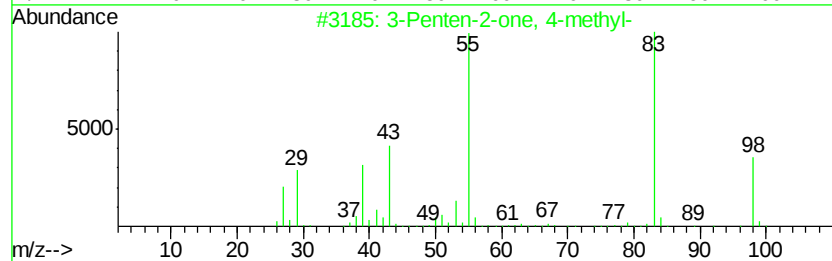
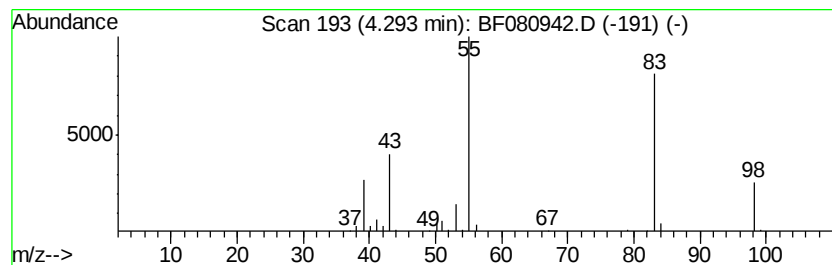
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	6.01 ng	130607	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
5			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	78



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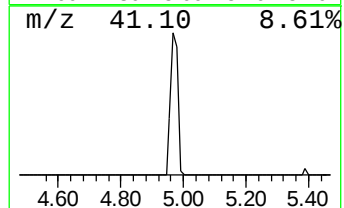
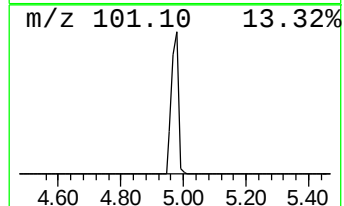
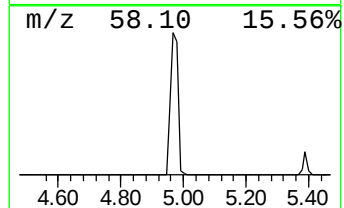
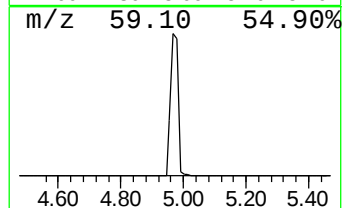
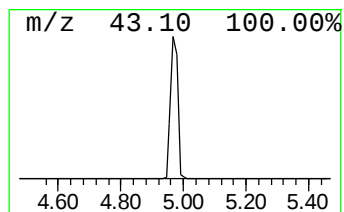
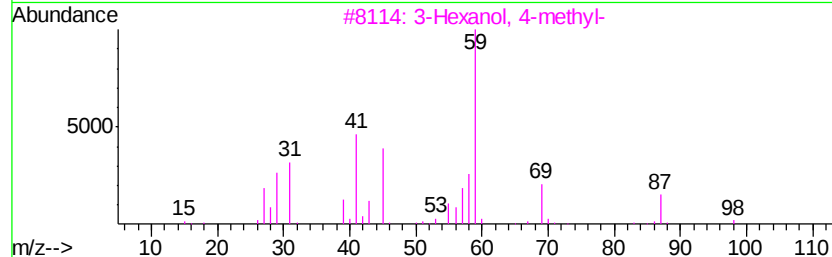
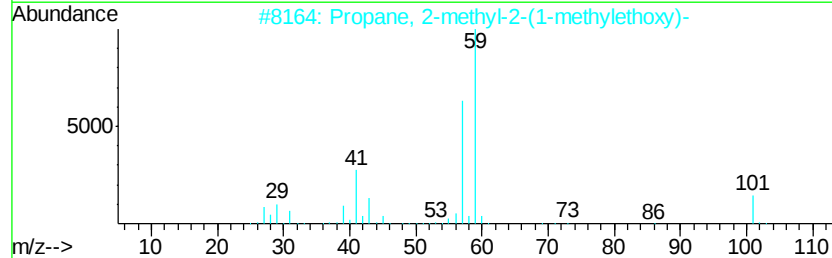
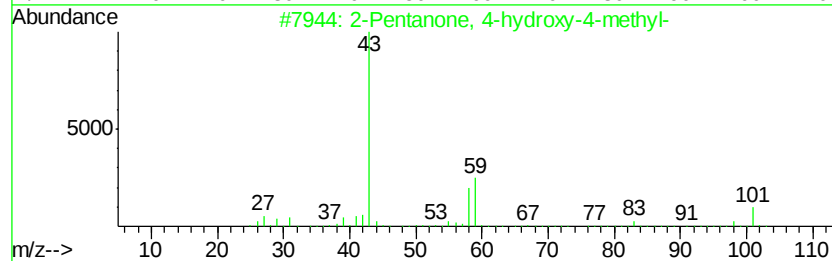
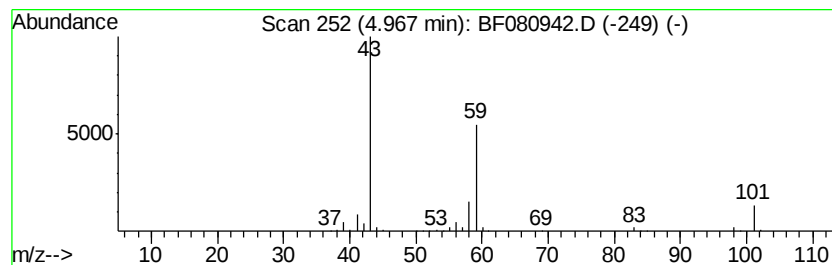
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	46.72 ng	1015320	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
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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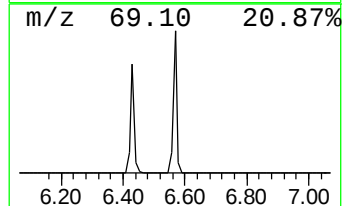
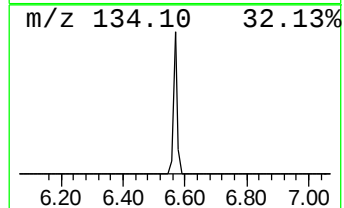
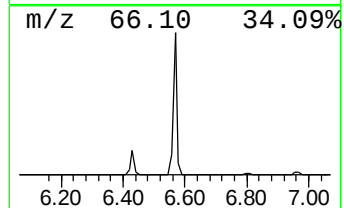
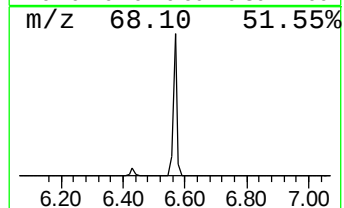
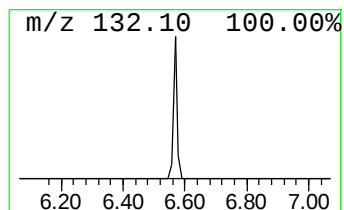
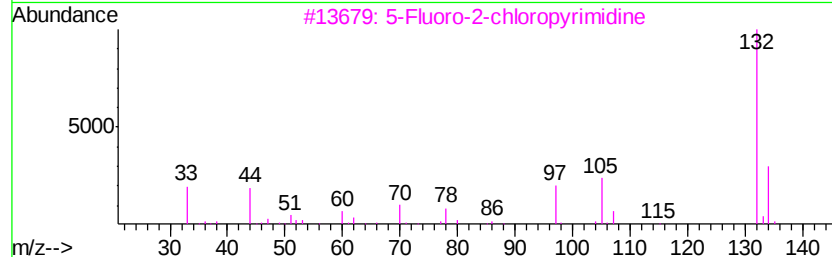
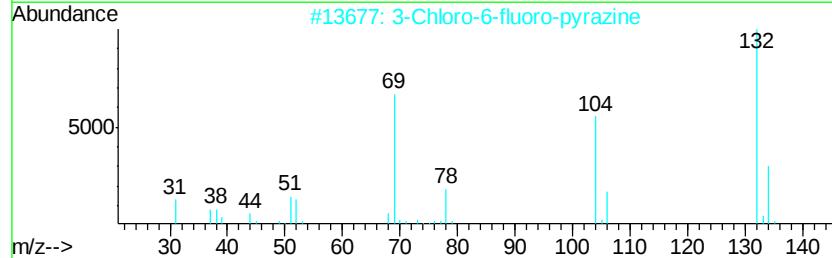
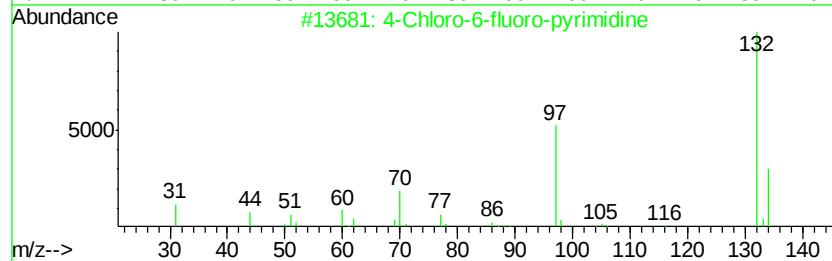
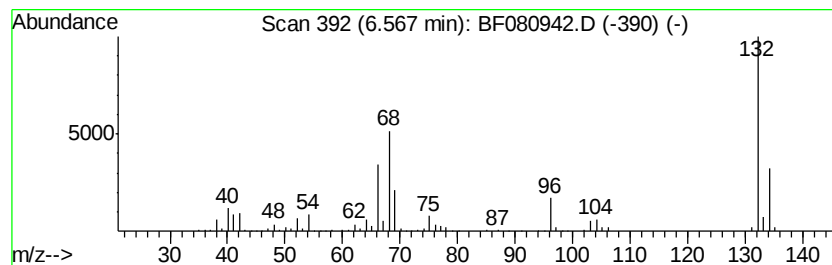
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Peak Number 3 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	40.33 ng	876389	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.29	6.0	ng	130607	1	6.81	434635	20.0
2-Pentanone, 4-hy...	4.97	46.7	ng	1015320	1	6.81	434635	20.0
unknown6.57	6.57	40.3	ng	876389	1	6.81	434635	20.0