

Data Path : U:\HPCHEM1\BNA_F\DATA\BF101915\
 Data File : BF082359.D
 Acq On : 19 Oct 2015 16:58
 Operator : UM/IZ
 Sample : PB86137BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB86137BL

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-BF101015.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	4.308	187	190	200	rBV	187499	249390	7.80%	0.995%
2	4.983	245	249	258	rBV	1055102	1631433	51.00%	6.510%
3	5.406	283	286	288	rBV	2213163	2287877	71.52%	9.129%
4	5.806	319	321	323	rBV	33180	46311	1.45%	0.185%
5	6.446	374	377	379	rBV	2077011	2332097	72.91%	9.306%
6	6.571	385	388	390	rBV	2451883	2478474	77.48%	9.890%
7	6.800	406	408	411	rBV	647561	566024	17.70%	2.259%
8	6.960	419	422	424	rBV	1686333	1969912	61.58%	7.860%
9	7.372	455	458	461	rBV	1304921	1390162	43.46%	5.547%
10	8.092	518	521	523	rBV	730017	732095	22.89%	2.921%
11	9.177	612	616	618	rBV	2258541	3064095	95.79%	12.226%
12	9.852	672	675	677	rBV	871795	900483	28.15%	3.593%
13	10.640	741	744	747	rBV	1569233	1695096	52.99%	6.764%
14	11.338	802	805	808	rBV	1026641	927631	29.00%	3.701%
15	12.949	943	946	949	rBV	3083688	3198737	100.00%	12.764%
16	14.081	1043	1045	1048	rBV	758240	876091	27.39%	3.496%
17	15.681	1182	1185	1196	rBV	489489	715328	22.36%	2.854%

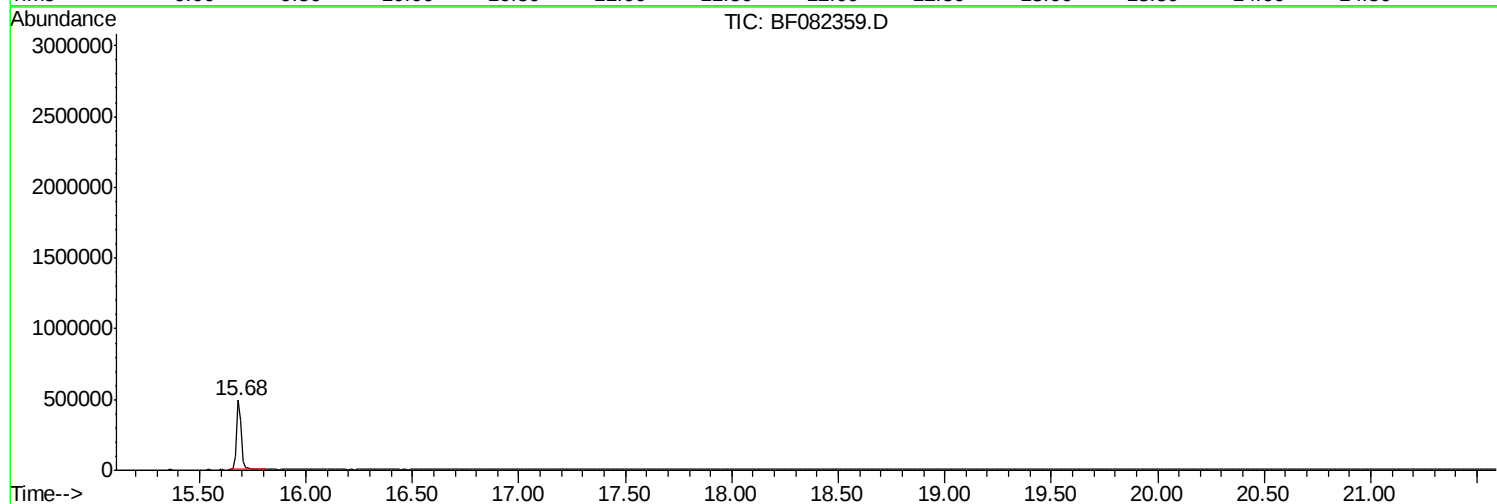
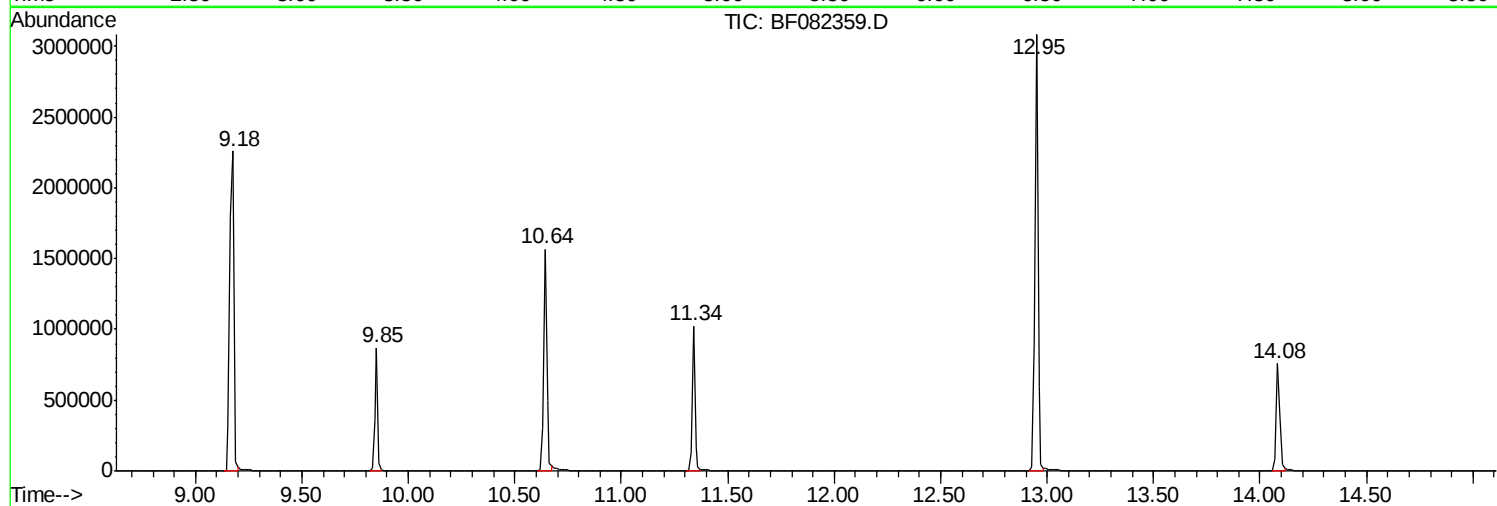
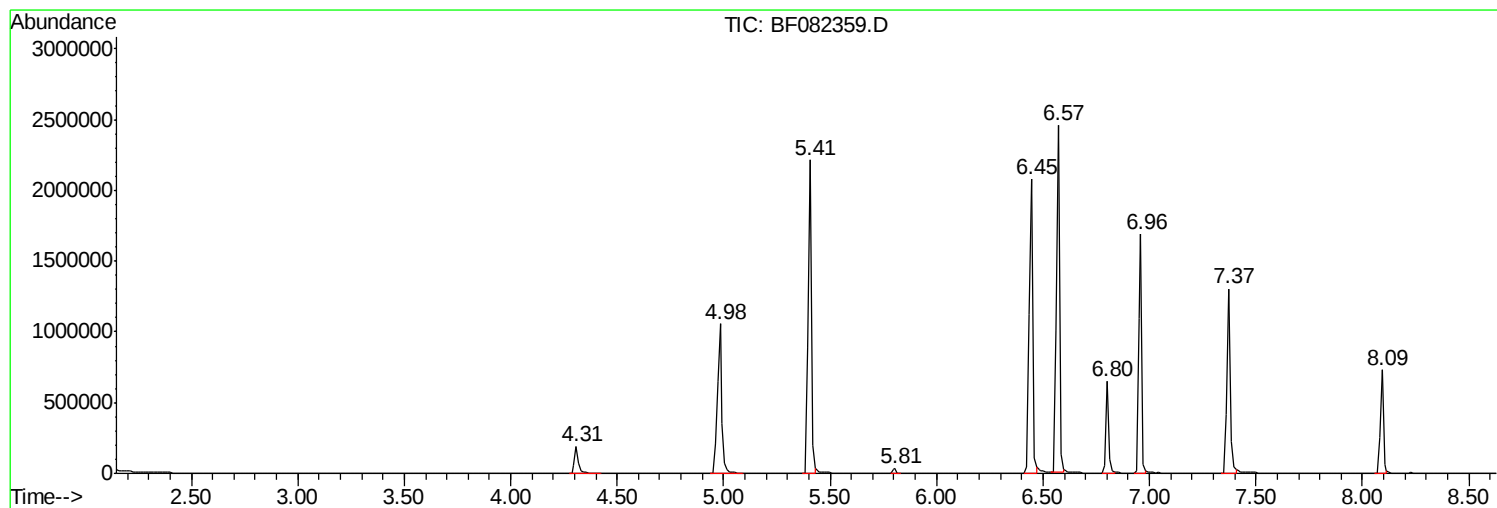
Sum of corrected areas: 25061236

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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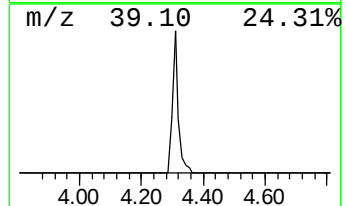
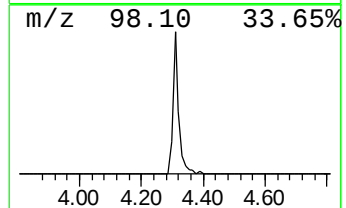
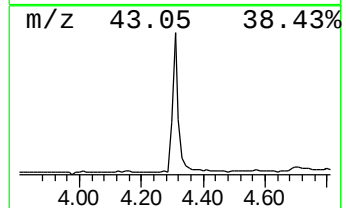
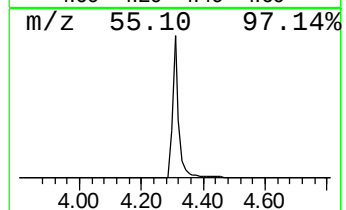
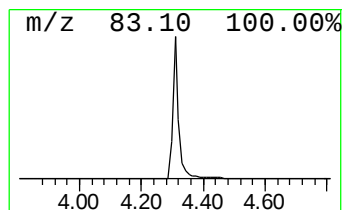
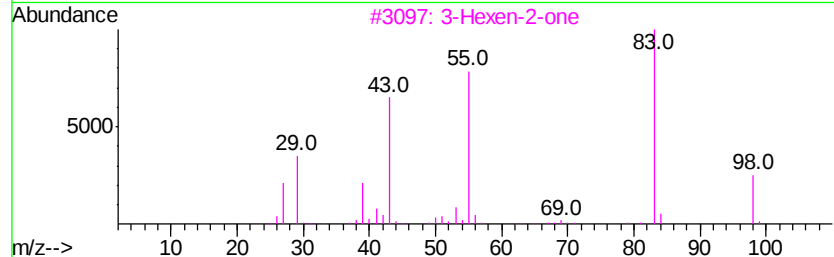
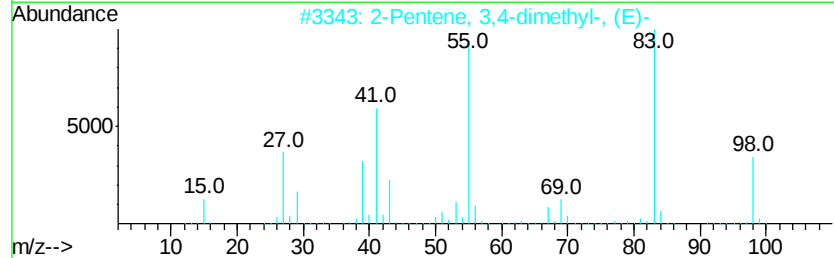
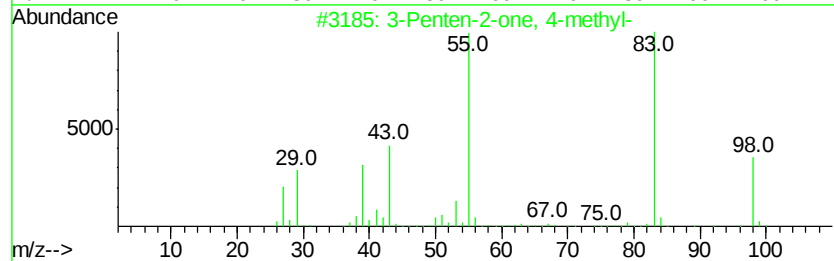
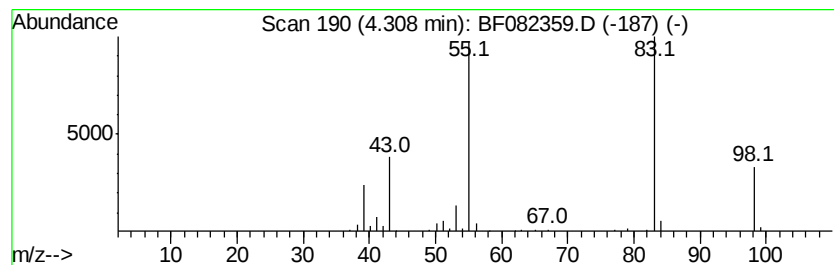
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.31	8.81 ng	249390	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3			3-Hexen-2-one	98	C6H10O	000763-93-9	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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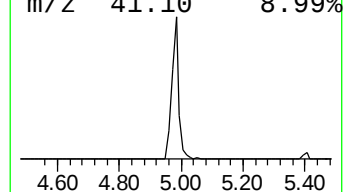
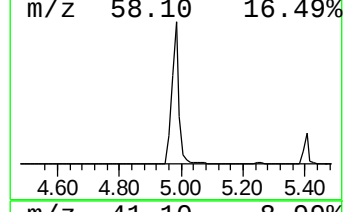
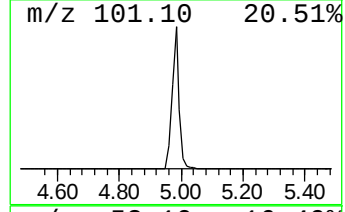
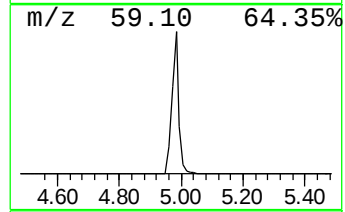
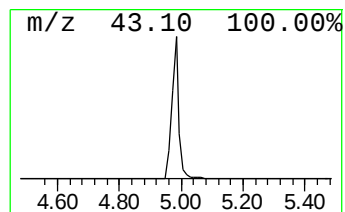
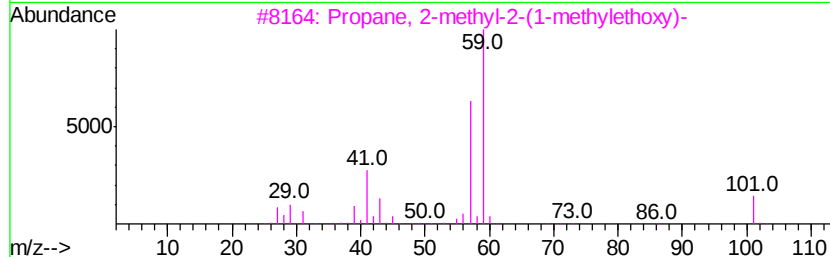
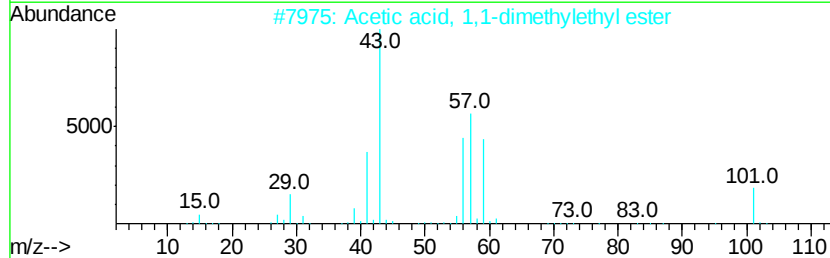
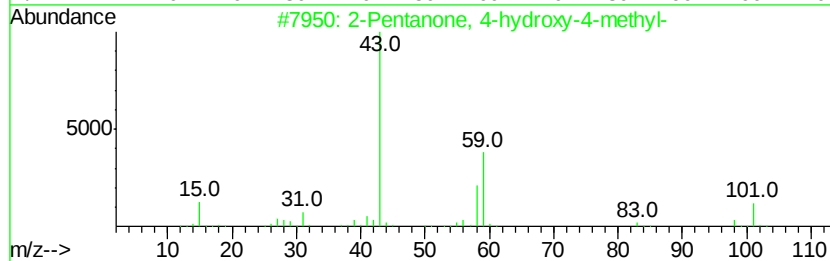
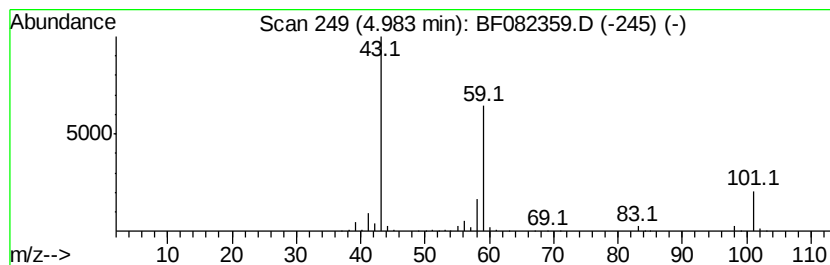
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	57.65 ng	1631430	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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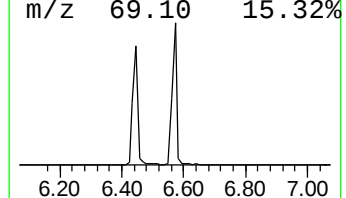
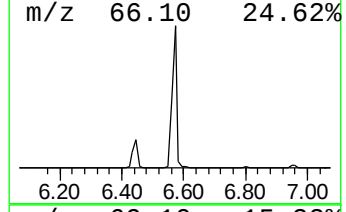
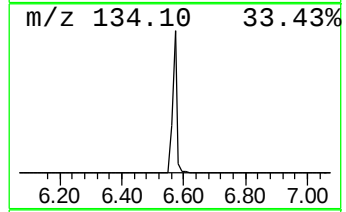
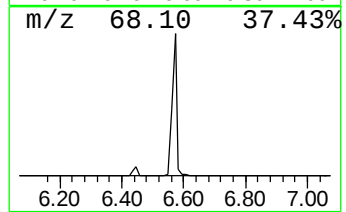
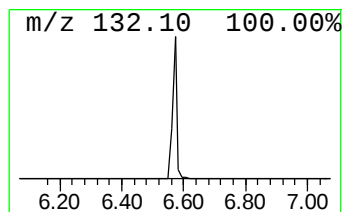
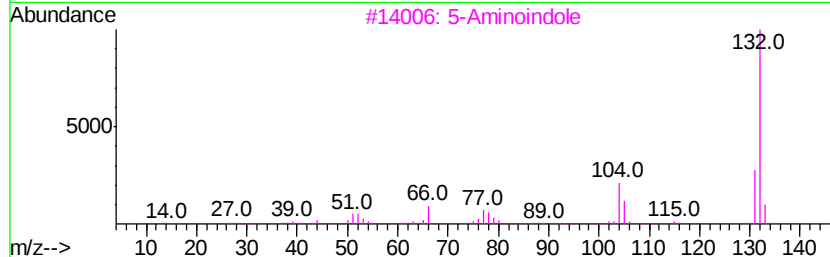
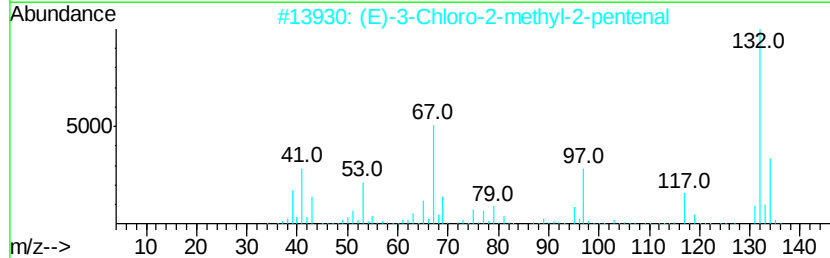
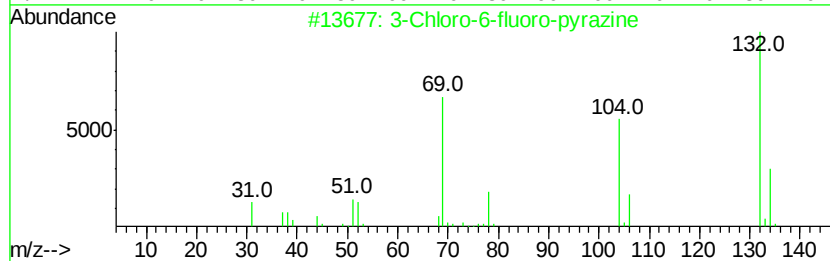
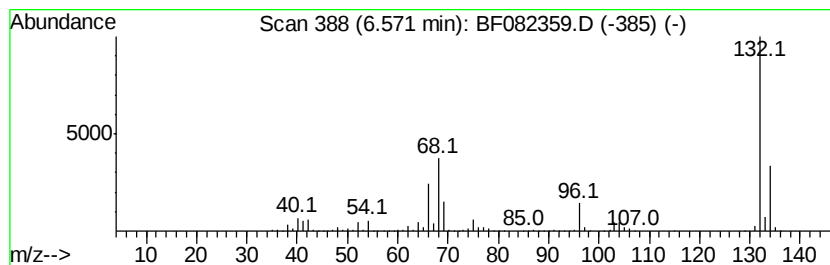
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Peak Number 3 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	87.57 ng	2478470	1,4-Dichlorobenzene-d4	6.80

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	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.31	8.8	ng	249390	1	6.80	566024	20.0
2-Pentanone, 4-hy...	4.98	57.6	ng	1631430	1	6.80	566024	20.0
unknown6.57	6.57	87.6	ng	2478470	1	6.80	566024	20.0