

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
 Data File : BF094219.D
 Acq On : 6 Apr 2017 11:02
 Operator : SJ/MA
 Sample : PB98067BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB98067BL

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-BF032217.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	3.463	264	268	277	rVB	757036	728195	14.19%	1.693%
2	4.004	354	360	370	rVB	1500057	2194113	42.75%	5.100%
3	4.398	421	427	430	rBV	4024526	4202972	81.89%	9.769%
4	4.781	488	492	497	rVB	103545	89628	1.75%	0.208%
5	5.463	601	608	611	rBV	3629881	4188943	81.62%	9.736%
6	5.598	626	631	635	rBV	3943481	4358958	84.93%	10.132%
7	5.851	670	674	678	rBV	1149135	1001126	19.51%	2.327%
8	6.034	699	705	708	rBV	3201926	3447025	67.16%	8.012%
9	6.498	778	784	788	rBV	2252112	2811754	54.78%	6.535%
10	7.351	923	929	933	rBV	1323345	1374040	26.77%	3.194%
11	8.681	1147	1155	1158	rBV	4136361	5132523	100.00%	11.930%
12	9.492	1286	1293	1297	rBV2	1462600	1507789	29.38%	3.505%
13	10.469	1451	1459	1462	rBV	2446532	2918481	56.86%	6.783%
14	11.316	1596	1603	1607	rVB	1452607	1521398	29.64%	3.536%
15	13.298	1930	1940	1943	rBV2	4015706	5023230	97.87%	11.676%
16	14.563	2150	2155	2159	rBV	1409493	1447012	28.19%	3.363%
17	16.192	2427	2432	2441	rVB	894458	1076079	20.97%	2.501%

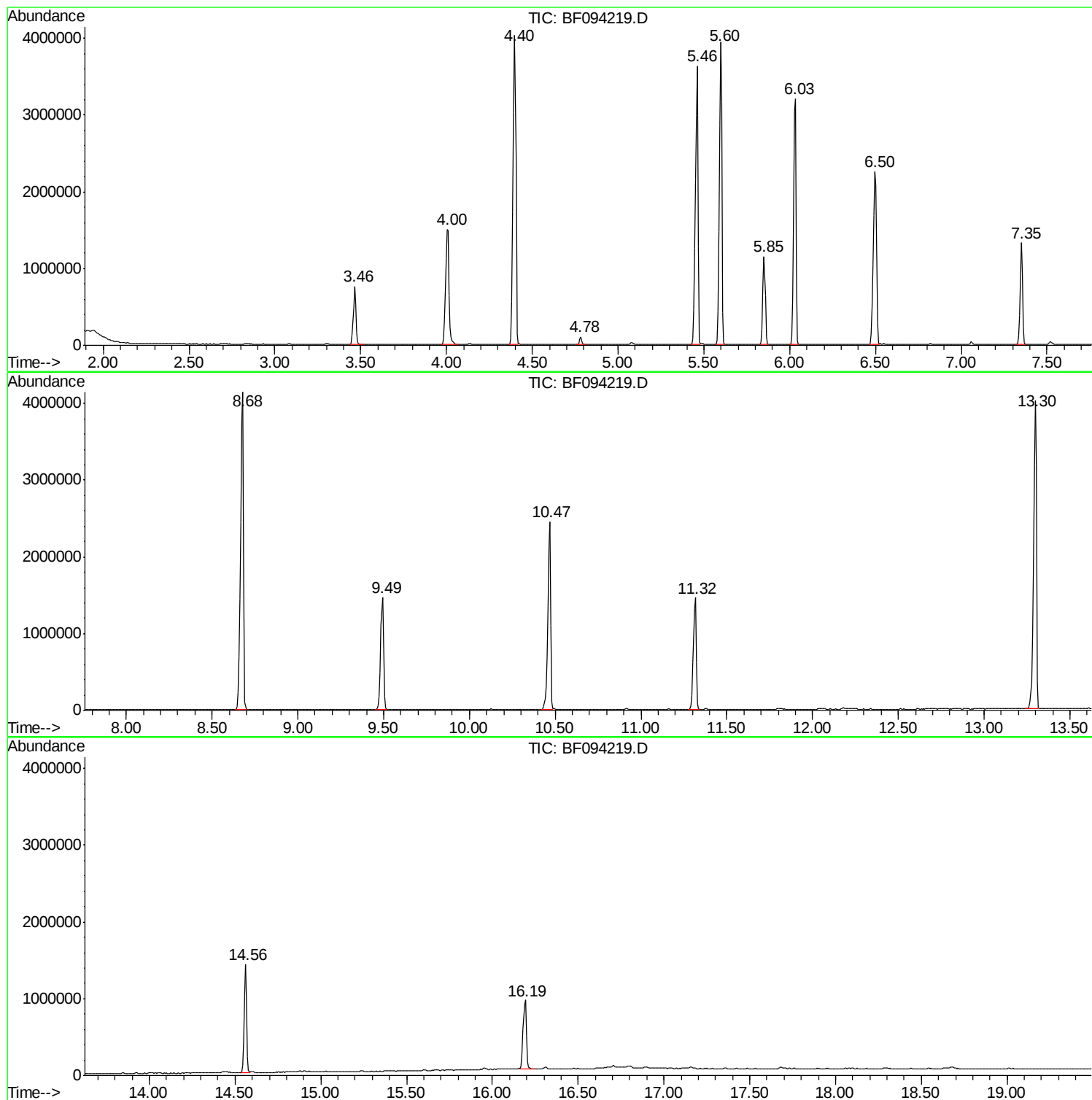
Sum of corrected areas: 43023266

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.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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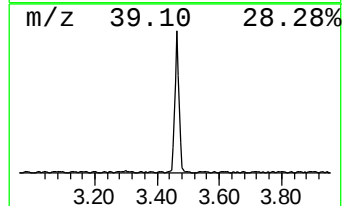
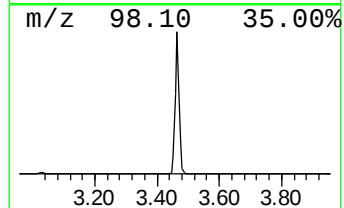
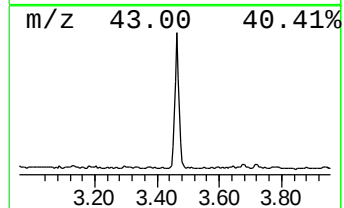
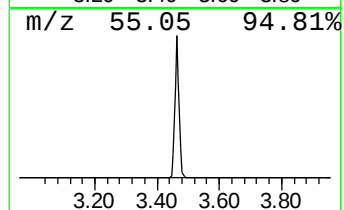
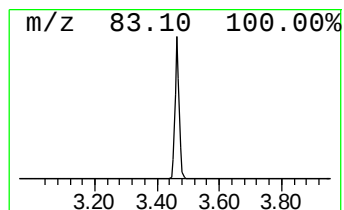
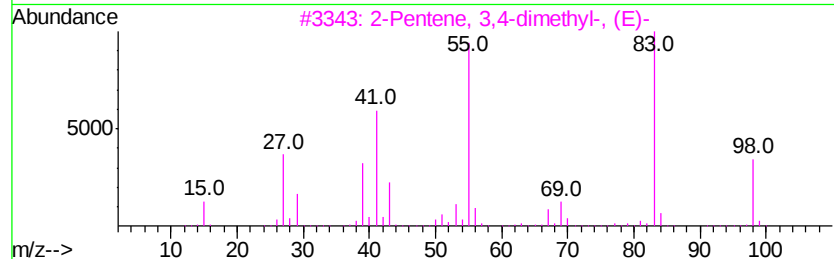
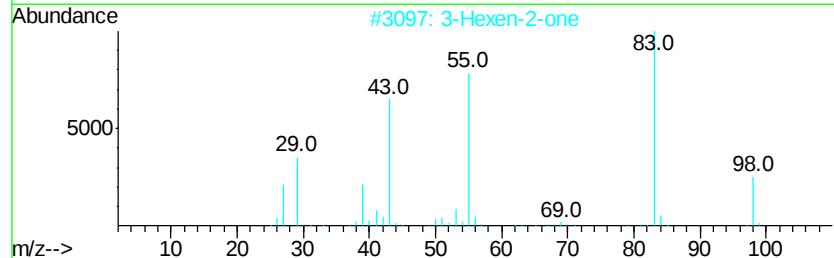
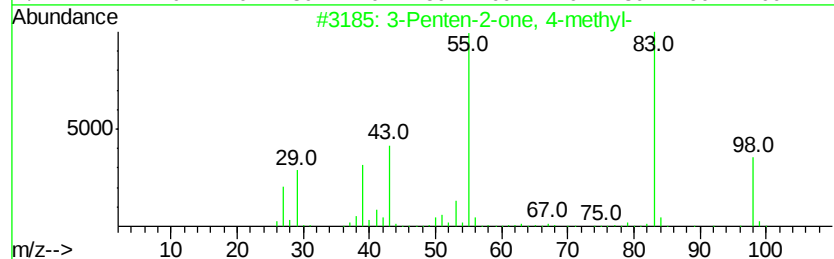
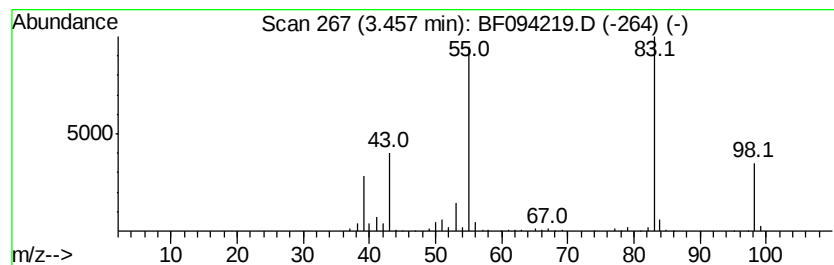
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.46	14.55 ng	728195	1,4-Dichlorobenzene-d4	5.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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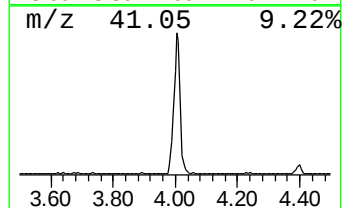
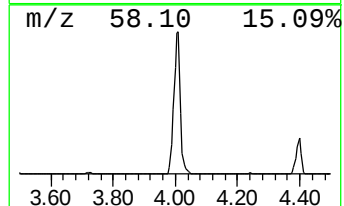
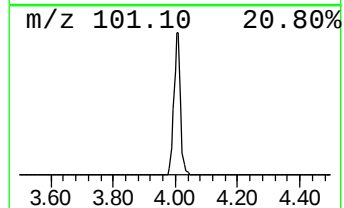
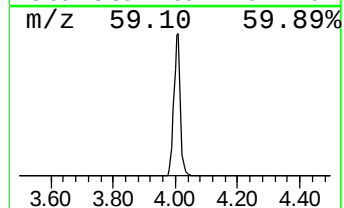
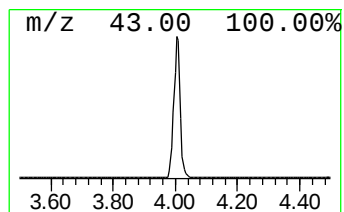
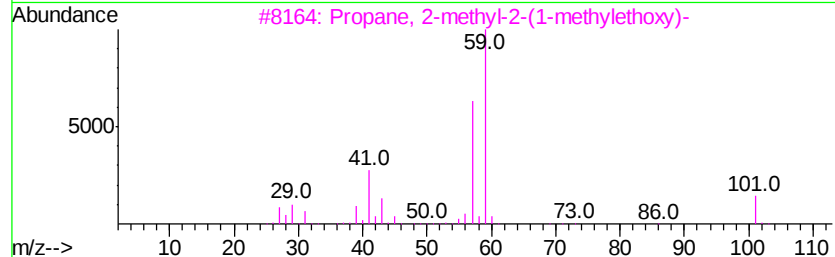
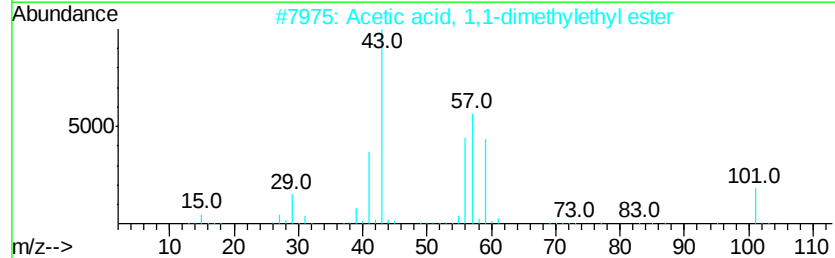
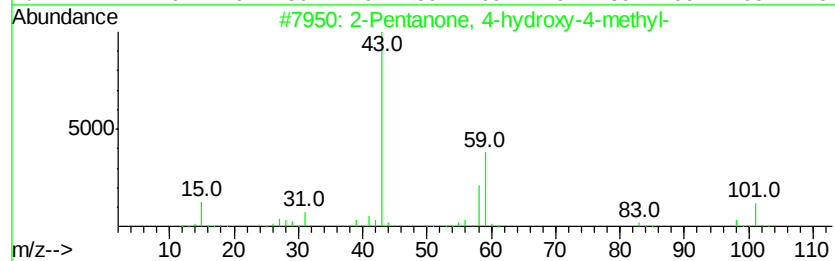
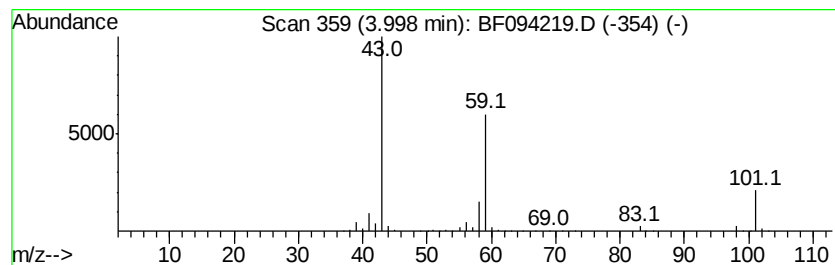
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	43.83 ng	2194110	1,4-Dichlorobenzene-d4	5.85

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	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9



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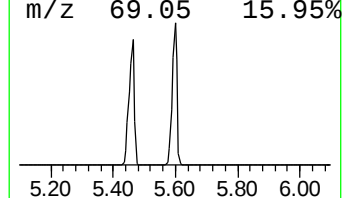
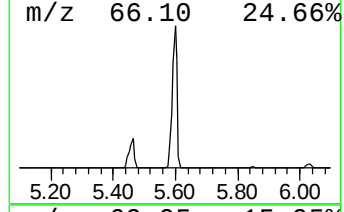
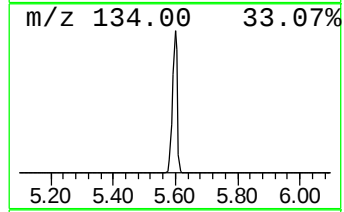
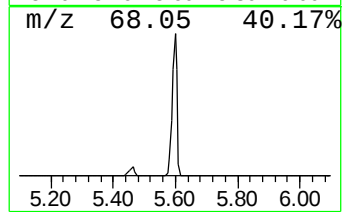
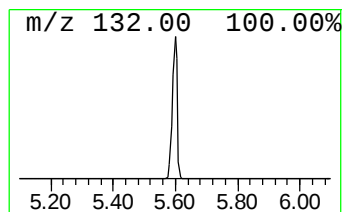
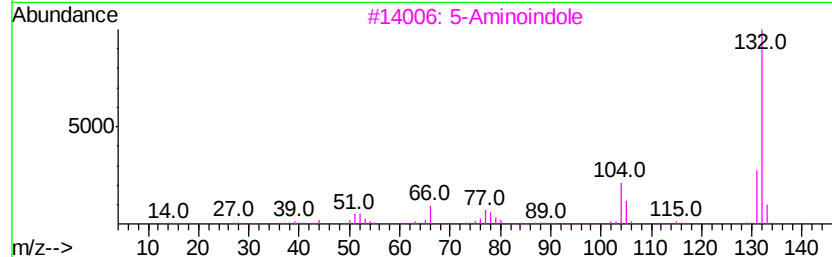
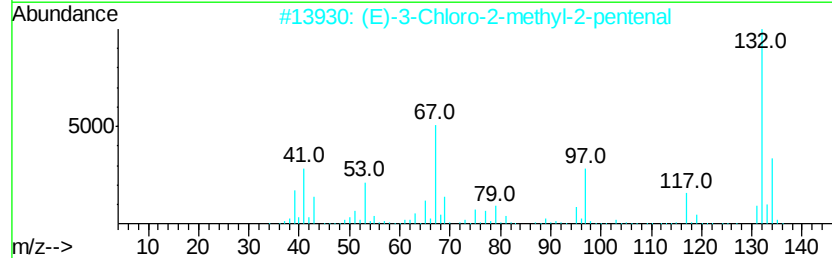
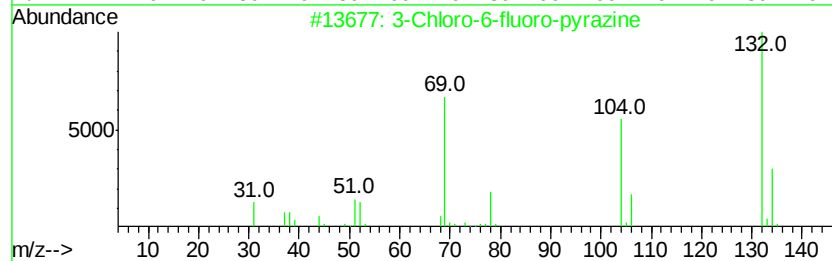
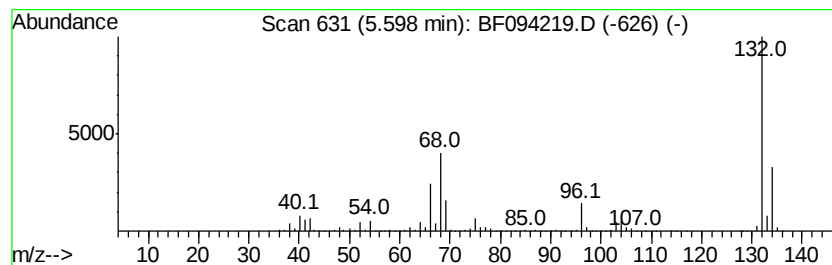
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Peak Number 3 unknown5.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	87.08 ng	4358960	1,4-Dichlorobenzene-d4	5.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.46	14.6	ng	728195	1	5.85	1001130	20.0
2-Pentanone, 4-hy...	4.00	43.8	ng	2194110	1	5.85	1001130	20.0
unknown5.60	5.60	87.1	ng	4358960	1	5.85	1001130	20.0