

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
 Data File : BF094879.D
 Acq On : 4 May 2017 17:58
 Operator : SJ/MA
 Sample : PB98591BL
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB98591BL

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-BF050217.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	4.107	365	369	384	rBV	88200	170603	5.56%	0.730%
2	5.043	522	528	545	rBV	341863	684824	22.32%	2.929%
3	5.678	631	636	666	rBV	1554272	2346077	76.47%	10.036%
4	7.266	901	906	921	rBV	1694471	2344098	76.41%	10.027%
5	7.384	921	926	938	rVB	2039595	2563424	83.56%	10.965%
6	7.725	979	984	994	rBV	428418	513435	16.74%	2.196%
7	7.960	1019	1024	1033	rBV	1719432	1980306	64.55%	8.471%
8	8.619	1130	1136	1155	rBV	1143923	1482306	48.32%	6.341%
9	9.742	1322	1327	1345	rBV	514000	689679	22.48%	2.950%
10	11.519	1623	1629	1645	rBV	2258710	2898847	94.49%	12.400%
11	12.572	1803	1808	1824	rBV2	546905	753577	24.56%	3.224%
12	13.866	2022	2028	2044	rBV	1150037	1616286	52.68%	6.914%
13	14.971	2211	2216	2228	rBV	537801	757597	24.69%	3.241%
14	17.301	2606	2612	2615	rBV	2571799	3067895	100.00%	13.123%
15	18.636	2834	2839	2853	rBV	639998	790677	25.77%	3.382%
16	20.300	3117	3122	3132	rBV	525592	717931	23.40%	3.071%

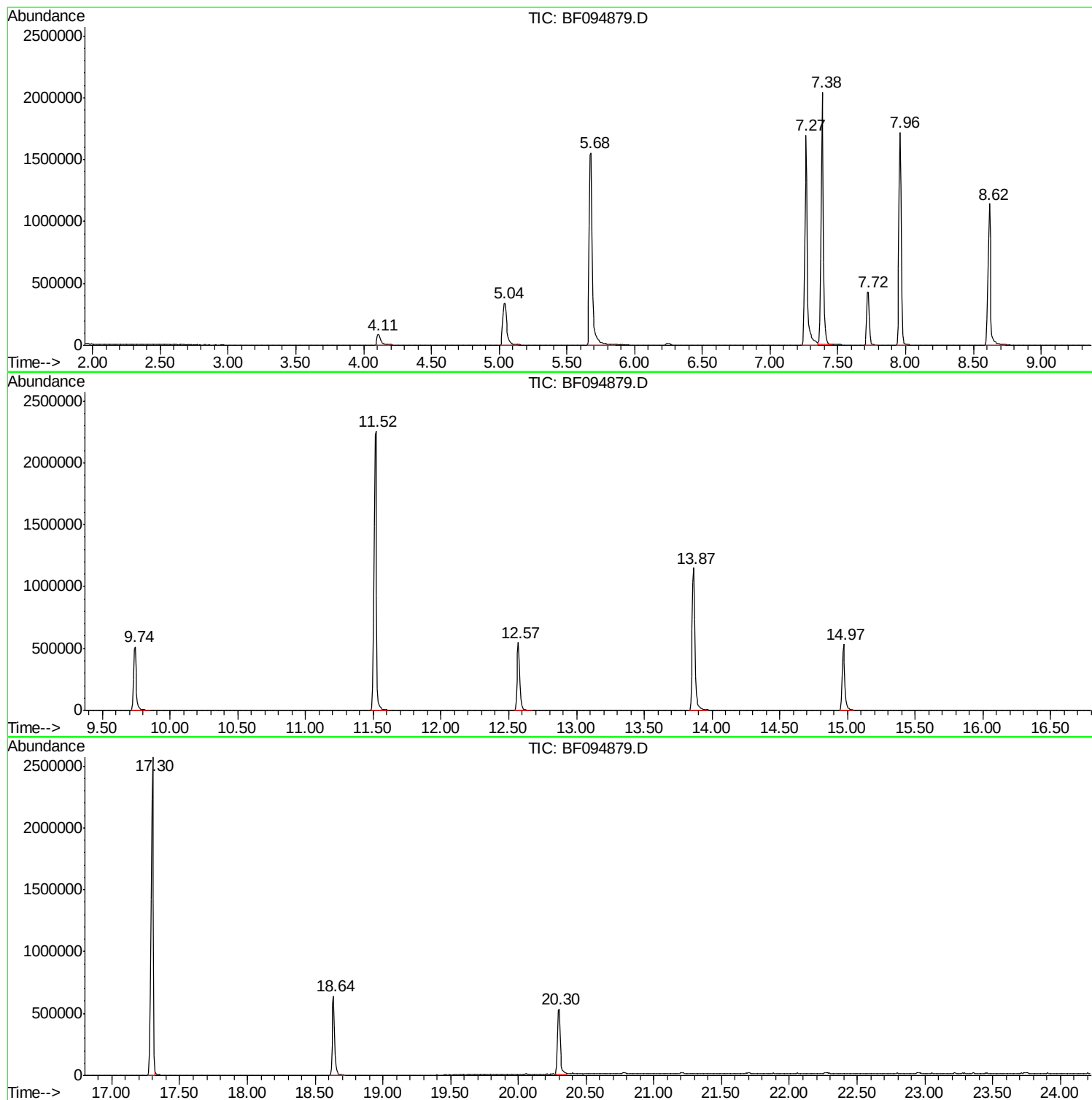
Sum of corrected areas: 23377562

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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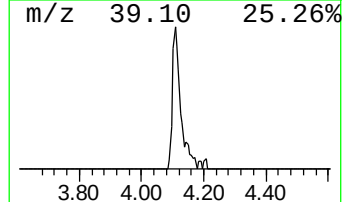
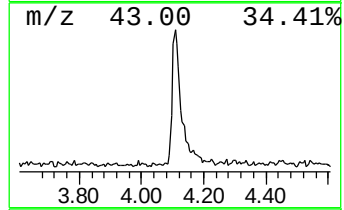
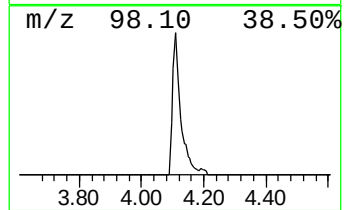
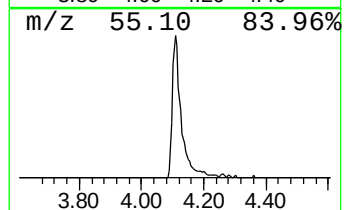
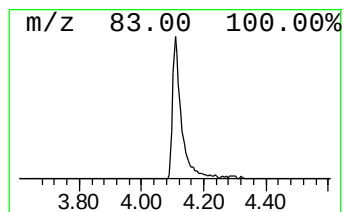
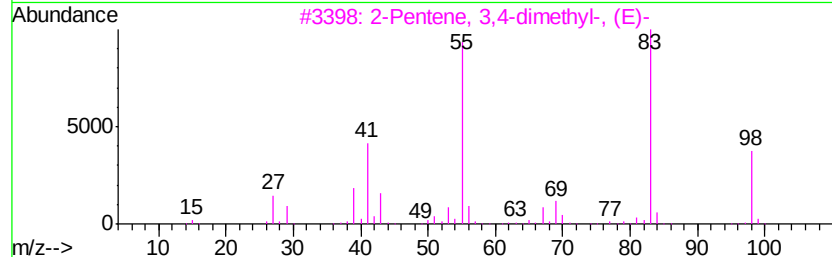
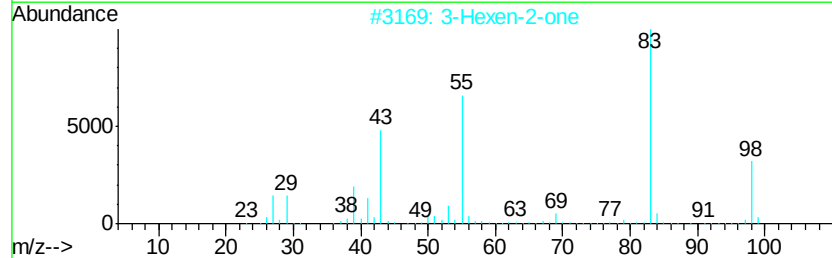
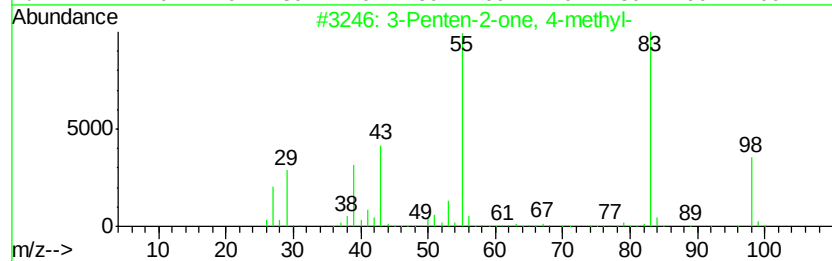
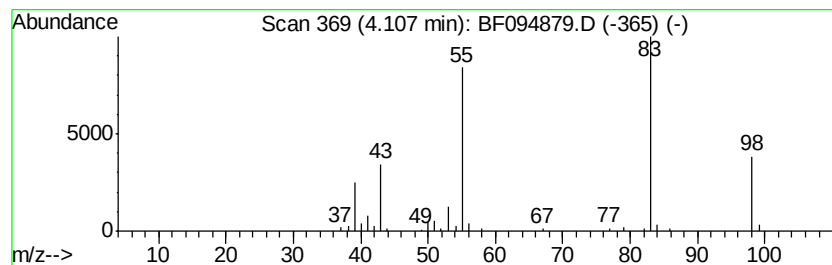
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
4.11	6.65 ng	170603	1,4-Dichlorobenzene-d4	7.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	78
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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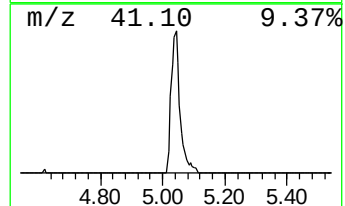
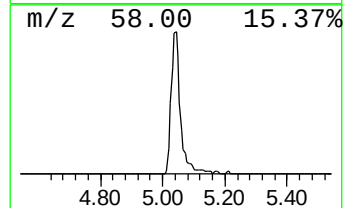
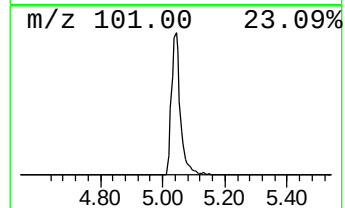
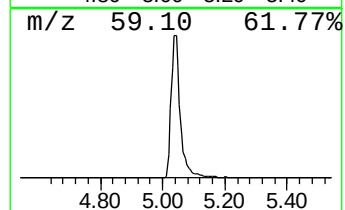
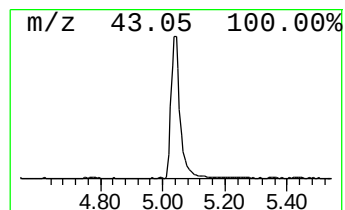
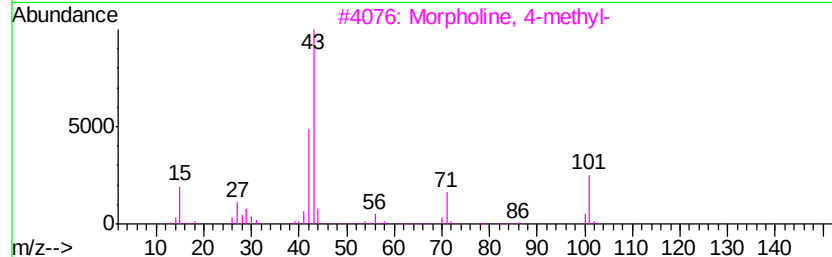
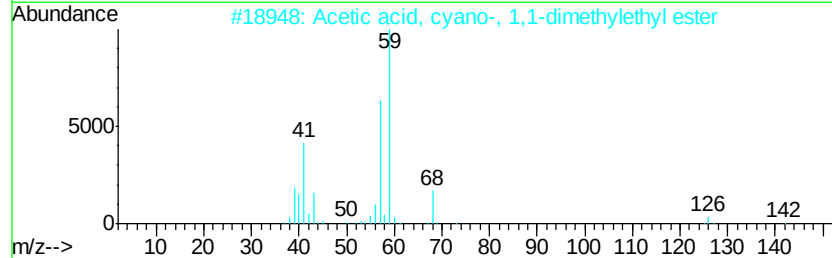
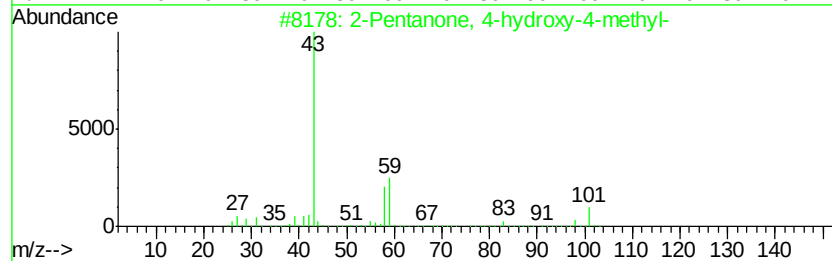
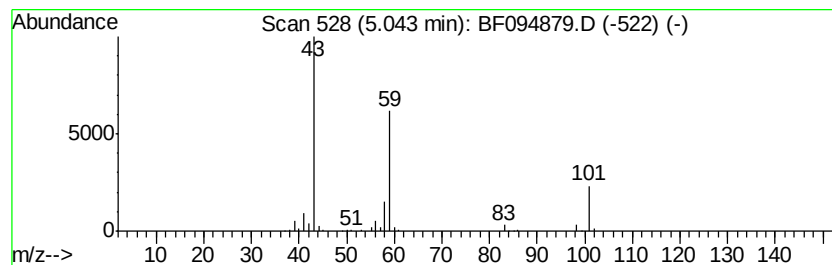
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	26.68 ng	684824	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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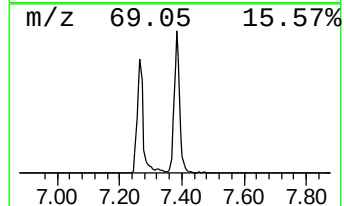
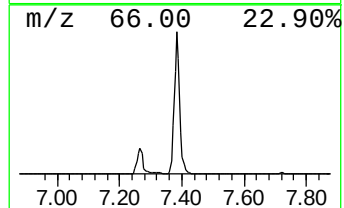
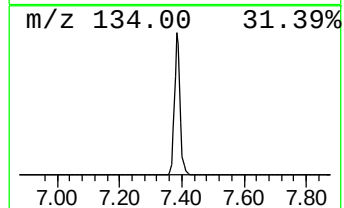
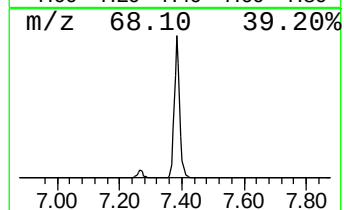
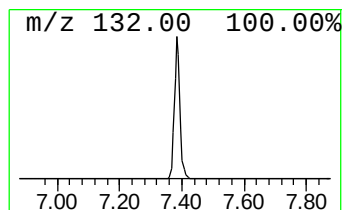
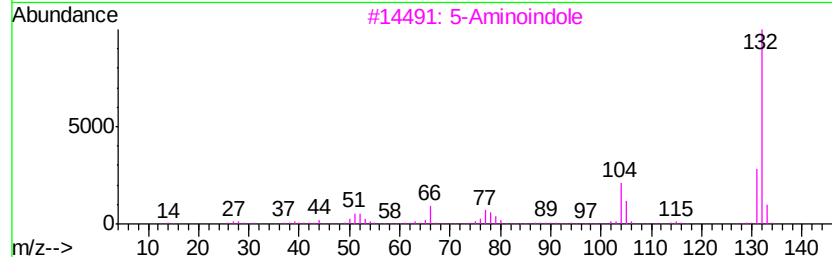
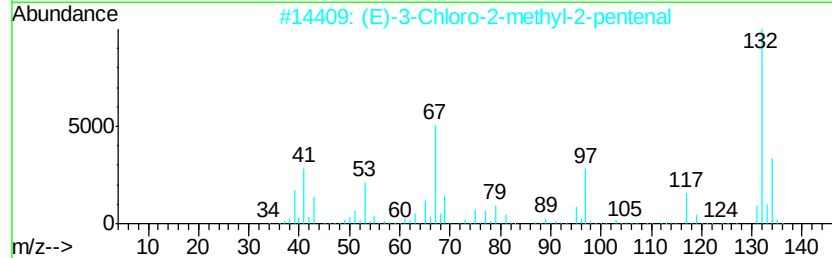
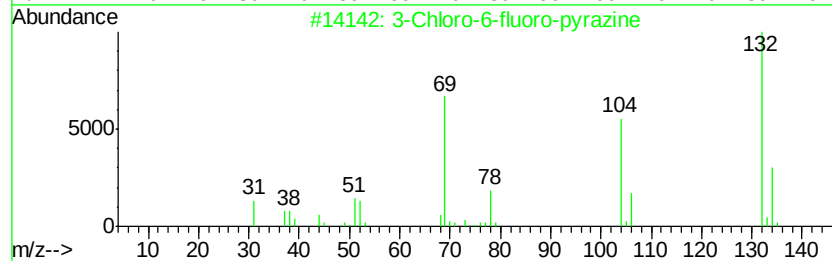
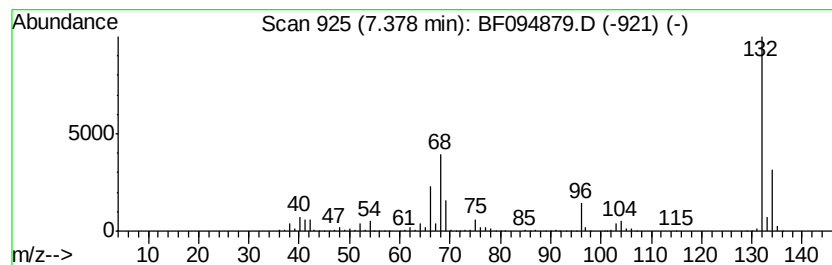
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Peak Number 3 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	99.85 ng	2563420	1,4-Dichlorobenzene-d4	7.72

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		Xenon	132	Xe	007440-63-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.11	6.7	ng	170603	1	7.72	513435	20.0
2-Pentanone, 4-hy...	5.04	26.7	ng	684824	1	7.72	513435	20.0
unknown7.38	7.38	99.8	ng	2563420	1	7.72	513435	20.0