AccuTOF™

Automated Exact Mass Measurements and Elemental Composition Determinations

Overview: The JEOL ***AccuTOF™*** LC/MS system offers easy exact-mass measurements and elemental composition determinations. A robust design and stable time-of-flight mass analyzer are combined with a detection system that provides high sensitivity and high dynamic range. Unlike other API/TOF mass spectrometer systems, the ***AccuTOF™*** provides excellent linearity and mass accuracy over a wide range of analyte concentrations.

To demonstrate the potential of the ***AccuTOF™*** for automated exact mass measurements, a variety of small-molecule drug samples were measured by using a macro that allows the user to submit samples for unattended elemental composition determinations. Samples were introduced by using the LC autosampler. The macro applied an automatic drift ("lock mass") correction to the reserpine reference standard and printed out elemental compositions for user-specified elemental limits. The results show high accuracy and stability regardless of sample concentration.

Mass Accuracy vs. Sample Concentration

Figure 1. shows the mass accuracy for measurements of flow injections of methanol solutions of chlorpromazine ($C_{17}H_{20}N_2ClS$) with concentrations ranging from 9 ppb to 900 ppm. Quinine (400 ppb) was added to the samples as a drift correction. All mass measurements are within 5 parts per million (ppm).

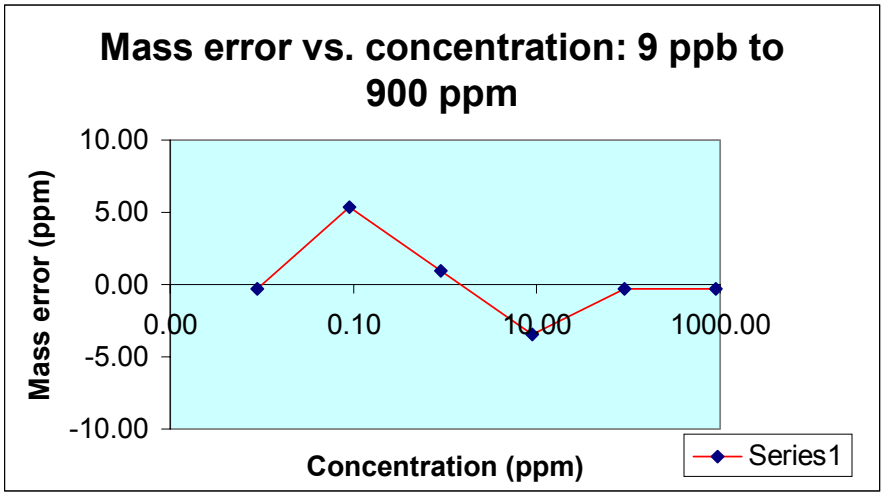

Figure 1. Mass measurement accuracy for chlorpromazine solutions at various concentrations.

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Mass Accuracy for Unattended Measurements Over 1 Week

A set of 10 samples was measured every day for 1 week without retuning or recalibrating the mass spectrometer. All samples gave mass measurements within 0.002 u or 5 ppm of the expected value. Figure 2 shows the mass accuracy for three representative compounds (thioridazine, erythromycin, and cinchonidine) over the course of one week. Table 1 shows the results for all 10 compounds compounds for the measurements on day 3.

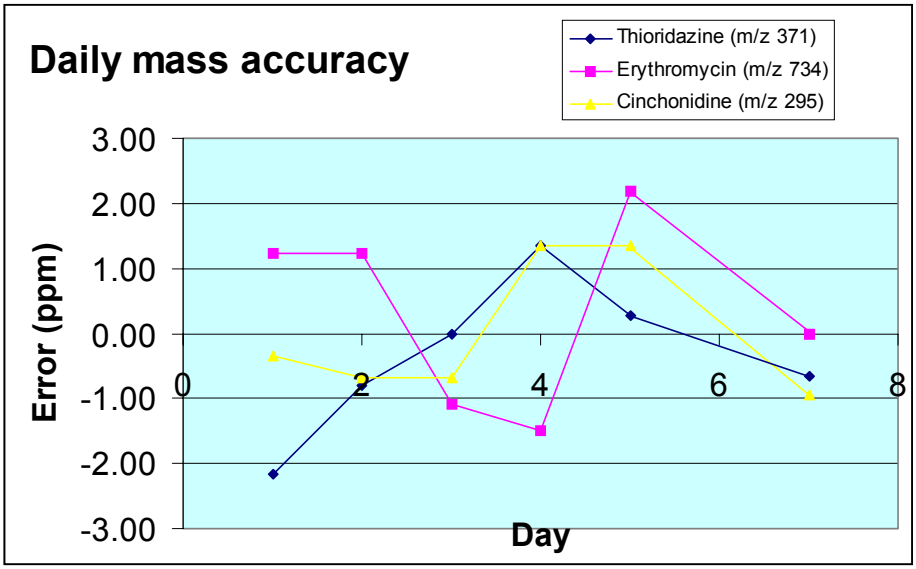

Figure 2. Mass accuracy for three samples measured daily for 1 week with no retuning or recalibration.

AccuTOF Automated Measurements 5/8/2002

Compound	Composition	Theor. m/z	Meas. m/z	Diff. (mmu)	Diff (ppm)	Notes
Chlorpromazine	C17 H20 Cl N2 S	319.1035	319.1035	0.00	0.00	
Hydrocortisone ([M+Na+MeOH]+)	C22 H34 O6 Na	417.2253	417.2275	2.20	5.27	1
Hydrocortisone (weak [M+Na]+)	C21 H30 O5 Na	385.1991	385.2029	3.80	9.87	1,2
Acriflavine [M+H]+	C14 H14 N3	224.1188	224.1173	-1.50	-6.69	
Nortriptylene [M+H]+	C19 H22 N	264.1752	264.1746	-0.60	-2.27	
Thioridazine [M+H]+	C21 H27 N2 S2	371.1616	371.1616	0.00	0.00	
Cinchonidine [M+H]+	C19 H23 N2 O	295.1810	295.1808	-0.20	-0.68	
Promazine [M+H]+	C17 H21 N2 S	285.1425	285.1417	-0.80	-2.81	
Raffinose [M+Na]+	C18 H32 O16 Na	527.1588	527.1576	-1.20	-2.28	
Erythromycin [M+H]+	C37 H68 N1 O13	734.4691	734.4683	-0.80	-1.09	
Rosaramycin [M+H]+	C31 H52 N1 O9	582.3642	582.3621	-2.10	-3.61	1,2
			Average	-0.11	-0.39	
			Std. Dev.	1.70	4.48	
			RMS	1.63	4.29	

Notes:
1. Weak sample, high chemical background level
2. Analyte peak was below reporting threshold, processed manually

Table 1. AccuTOF mass accuracy for unattended measurements of 10 compounds.

Summary: Unattended exact mass measurements with ***AccuTOF***^{TM} show high mass accuracy over a long time period and over a wide range of sample concentrations.