Crystallographic data for AY23

X-ray data for the compound were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoKα radiation (λ=0.71073Å) with ω-scan method.[1] Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Unit cell dimensions were determined using 5202 reflections. Integration and scaling of intensity data were accomplished using SAINT program.[1] The structures were solved by Direct Methods using SHELXS97[2] and refinement was carried out by full-matrix least-squares technique using SHELXL97.[2] Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms, with C-H distances of 0.93--0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}$ (C) or $1.5U_{eq}$ for methyl atoms. H bound to N was located from the difference Fourier map.

Crystal data for AY23: $C_{20}H_{25}N_2O_2S_1^+$. Br^-, M = 437.39, brown plate, 0.35 x 0.20 x 0.10 mm^3, monoclinic, space group $P2_1/c$ (No. 14), a = 11.7828(8), b = 11.0859(7), c = 16.1335(10) Å, β = 93.1990(10)°, V = 2104.1(2) $Å^3$, Z = 4, Dc = 1.381 g/cm^3, F_{000} = 904, CCD area detector, MoKα radiation, λ = 0.71073 Å, T = 293(2)K, $2\theta_{max}$ = 50.0º, 19639 reflections collected, 3696 unique (R_{int} = 0.0202), Final *GooF* = 1.040, R_1 = 0.0293, *wR2* = 0.0797, R indices based on 3291 reflections with $I > 2\sigma(I)$ (refinement on F^2), 241 parameters, μ = 2.069 mm^{-1}. CCDC 1410087 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk.

1. SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.
2. Sheldrick, G. M. SHELXS97 and SHELXL97, Programs for crystal structure solution and refinement; University of Gottingen: Germany, 1997.

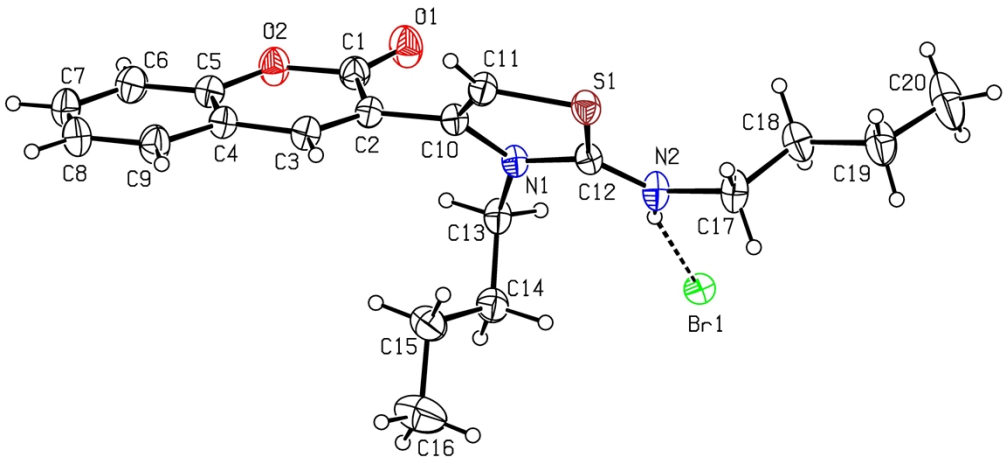

Figure caption: The molecular structure of AY23 with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius. The thiazoline derivative has crystallized in the form of a HBr salt. Dotted lines indicate hydrogen bonding between the protonated N2 atom and the bromide ion.