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NH \cdots O and OH \cdots O interactions of glycine derivatives with squaric acid

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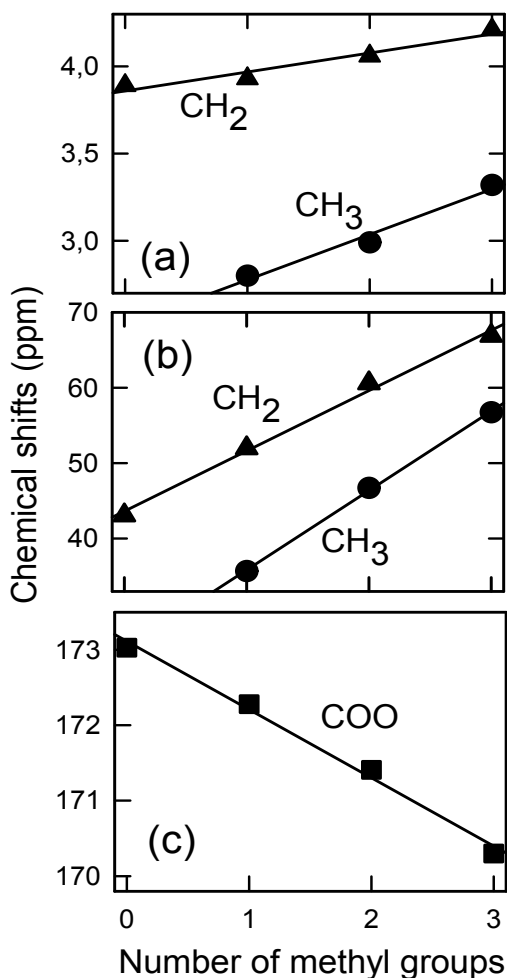


Figure S1. Relationships of the chemical shifts (ppm) versus the number of methyl groups in the glycine derivatives: (a) proton, (b) and (c) carbon-13;

● - methyl group, ▲ - methylene group, ■ - carboxylate group. Linear relationships are described by the equation $\delta = a + bx$, where x is the number of the methyl groups; $\delta^1\text{H}(\text{CH}_3) = 2.5240 + 0.2559x$, $r = 0.9874$; $\delta^1\text{H}(\text{CH}_2) = 3.8602 + 0.1079x$, $r = 0.9722$; $\delta^{13}\text{C}(\text{CH}_3) = 25.1628 + 10.6036x$, $r = 0.9996$; $\delta^{13}\text{C}(\text{CH}_2) = 43.4083 + 8.1407x$, $r = 0.9976$; $\delta^{13}\text{C}(\text{COO}) = 173.1150 - 0.9068x$, $r = 0.9960$.