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> New J. Chem. ART-02-2014-000212 NH…O and OH…O interactions of glycine derivatives with squaric acid Michalina Anioła, Zofia Dega-Szafran, Andrzej Katrusiak and Mirosław Szafran



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, \blacktriangle - methylene group, \blacksquare - carboxylate group. Linear relationships are described by the equation $\delta = a + bx$, where x is the number of the methyl groups; $\delta^{1}H(CH_{3}) = 2.5240 + 0.2559x$, r = 0.9874; $\delta^{1}H(CH_{2}) = 3.8602 + 0.1079x$, r = 0.9722; $\delta^{13}C(CH_{3}) = 25.1628 + 10.6036x$, r = 0.9996; $\delta^{13}C(CH_{2}) = 43.4083 + 8.1407x$, r = 0.9976; $\delta^{13}C(COO) = 173.1150 - 0.9068$, r = 0.9960.