HOMO- AND HETERONUCLEAR SCALAR COUPLING CONSTANTS $^{4,5}J_{H\text{-}H}$, $^{1}J_{C\text{-}C}$, $^{1\text{-}4}J_{C\text{-}H}$, $^{3}J_{N\text{-}H}$ IN PYRAZOLO[1,5-*a*]PYRIMIDINES

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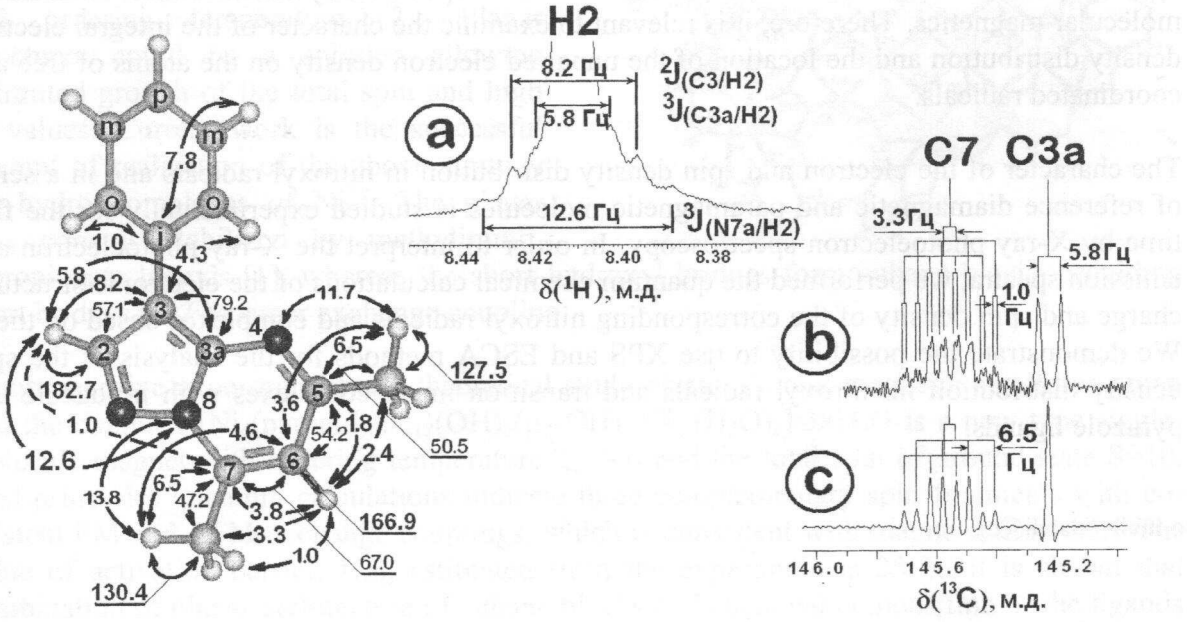
Scalar coupling constants between magnetic nuclei of molecules play an important role in their structural and conformational analysis on base NMR data. They are used as stable spectral characteristics to prove the structure of chemical compounds and also as parameters in different pulse sequences to rationalize their sensitivity and selectivity.

In this report the results of defining homo- and heteronuclear constants $^{4,5}J_{H\text{-}H}$, $^{1}J_{C\text{-}C}$, $^{1\text{-}4}J_{C\text{-}H}$ and $^{3}J_{N\text{-}H}$ in pyrazolo[1,5-*a*]pyrimidines are being discussed as well as the possibilities of their usage for confirming the regiostructure of these chemical compounds with high level of biological activity. The drawing presents the values (figures in Hz) of about 30 such scalar constants for one pyrazolo[1,5-*a*]pyrimidine and shows two simplest methods of their determination **a**) – from ^{13}C- and ^{15}N-satellite duplets at the bottom of proton H^2 signal in usual NMR ^{1}H spectrum and from heteronuclear selective decoupling experiment $^{13}C\{H^2\}$ which is shown on **c**) for carbon signals C^7 and C^{3a} against the same signals in NMR ^{13}C spectrum with broad band gate decoupling from protons during only relaxation delays – **b**).



It was found the values of scalar interactions H/H, C/C and C/H with C^6-C^7 participation of pyrimidine fragment profoundly overcome the similar values of couplings with C^5-C^6 participation. These differences in constant values can be used as the effective criteria of structural determination of pyrazolo[1,5-*a*]pyrimidine regioisomers.

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