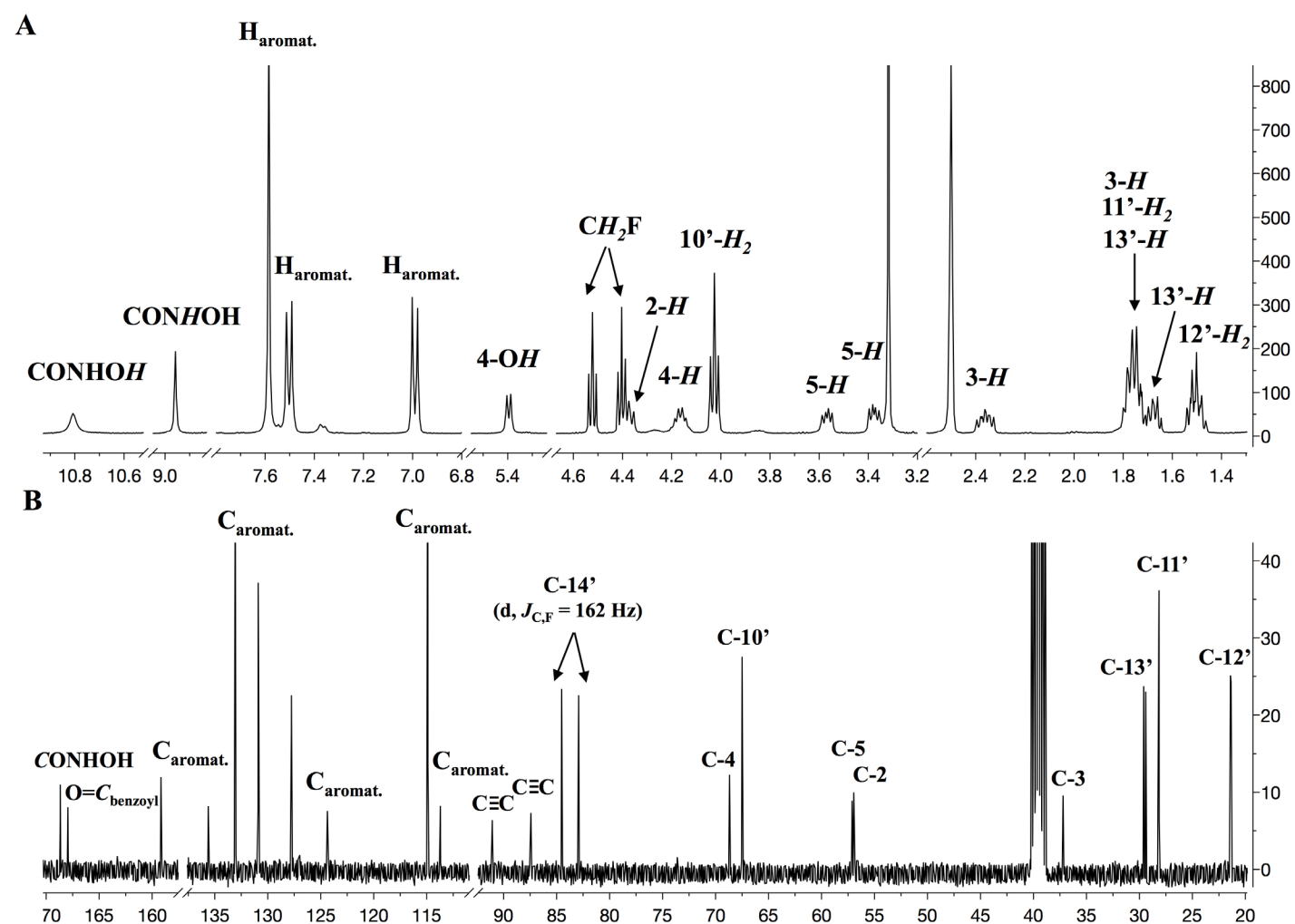




nmr is science



5-Fluoropentoxo-derived inhibitor of MMP-13 in DMSO-d₆

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Medicinal Chemistry Department | Institute of Pharmaceutical and Medicinal Chemistry

Field strength: 600 MHz

Why is this your favorite spectrum?

Newly synthesized compound KH240, which exhibits a picomolar inhibitory activity toward human matrix metalloproteinase 13 (MMP-13) and could be applied as a diagnostic tool for *in vivo* visualization (PET tracer) of pathologies, such as carcinomas, rheumatoid arthritis, and osteoarthritis. The compound comprises a 5-fluoropentoxo moiety, which gives beautiful patterns in NMR spectra. Whereas the signal for the two protons of the methylene group neighboring the oxygen atom appears as a triplet ($J = 6.4$ Hz) at 4.03 ppm, the signal for the protons of the methylene group adjacent to the terminal fluorine atom appears at 4.46 ppm as a doublet of triplets ($J = 47.5/6.1$ Hz) due to their additional coupling with the fluorine atom.