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Conformational Dependence on Long-range $^{13}C-^{19}F$ Scalar Couplings in 10-fluoreanthracyclinons

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$^{1}H-^{19}F$ and $^{13}C-^{19}F$ couplings are investigated with (7S,9R,10R)-, and (7S, 9S,10S)-6,9-dihydroxy-4,7-dimethoxy-10-fluoro-5,12-naphthacenedione (dHdMFNe). Although many cases of long-range $^{1}H-^{19}F$ and $^{13}C-^{19}F$ scalar couplings are known, it has not been reported that $^{13}C-^{19}F$ long range couplings are dependent upon the molecular conformation. Here, we show the correlation of the long-range $^{13}C-^{19}F$ coupling patterns and the molecular conformations. Eight-bond $^{8}J_{C\text{-}F}$ coupling (1.3 Hz) has been observed in the aromatic moietiy of (7S,9R,10R)-dHdMFNe, but for (7S,9S,10S)-dHdMFNe only five-bond $^{5}J_{C\ F}$ coupling (1.4Hz) has been observed. However, the long-range coupling pattern in the non-aromatic fluorocyclohexyl moiety was the opposite: the most distant coupling was two-bond coupling, $^{2}J_{C\ F}$ (27Hz), for (7S,9R,10R)-dHdMFNe, whereas four-bond coupling, $^{4}J_{C\ F}$ (1.1Hz), was observed for (7S,9S,10S)-dHdMFNe. Applying Karplus-type formula, torsion angles of the molecules were calculated from $^{3}J_{H\ H}$ and $^{3}J_{C\text{-}F}$. The results of the molecular dynamics simulation were in agreement with the measured coupling constants.