Supporting Information

The Intramolecular HB Interactions Evidenced in Dibenzoyl Oxalamide Derivatives: NMR, QTAIM, NCI Studies

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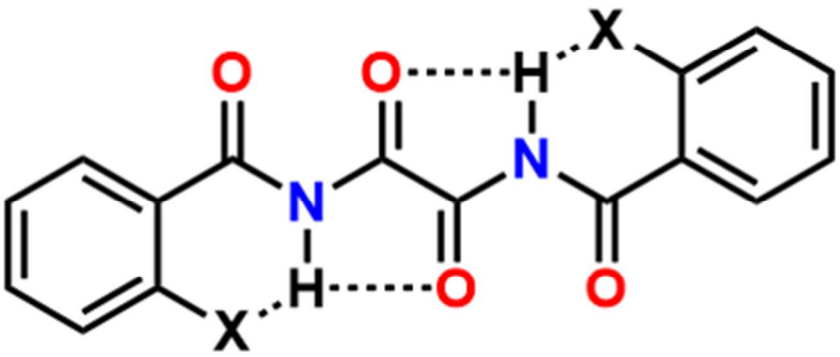
References



Molecule number	X
1	H
2	F
3	Cl
4	OMe
5	OH

Scheme S1: The chemical structures of N,N-dibenzoyloxalamide and its derivatives. The numbering of the molecules pertains to their substituents given in the table.

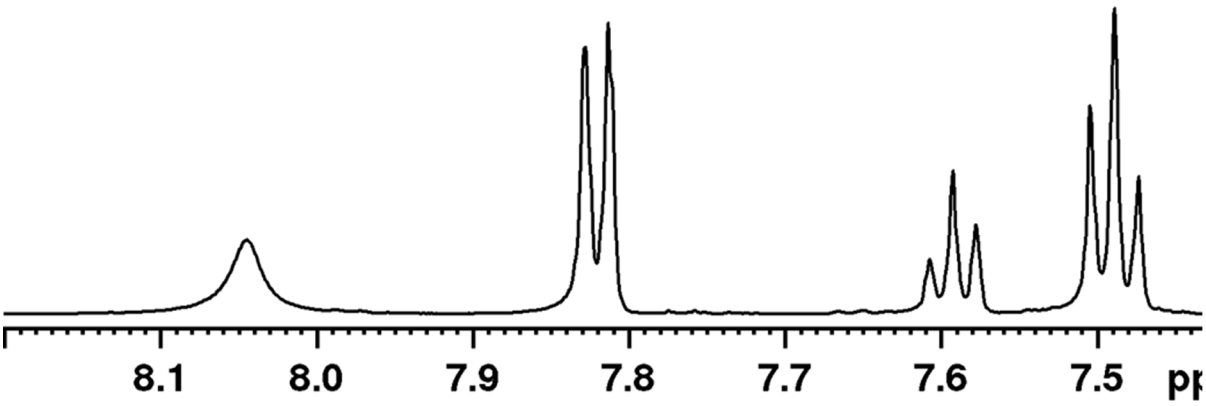


Figure S1: 400 MHz ^{1}H spectrum of molecule **1** in the solvent $CDCl_3$.

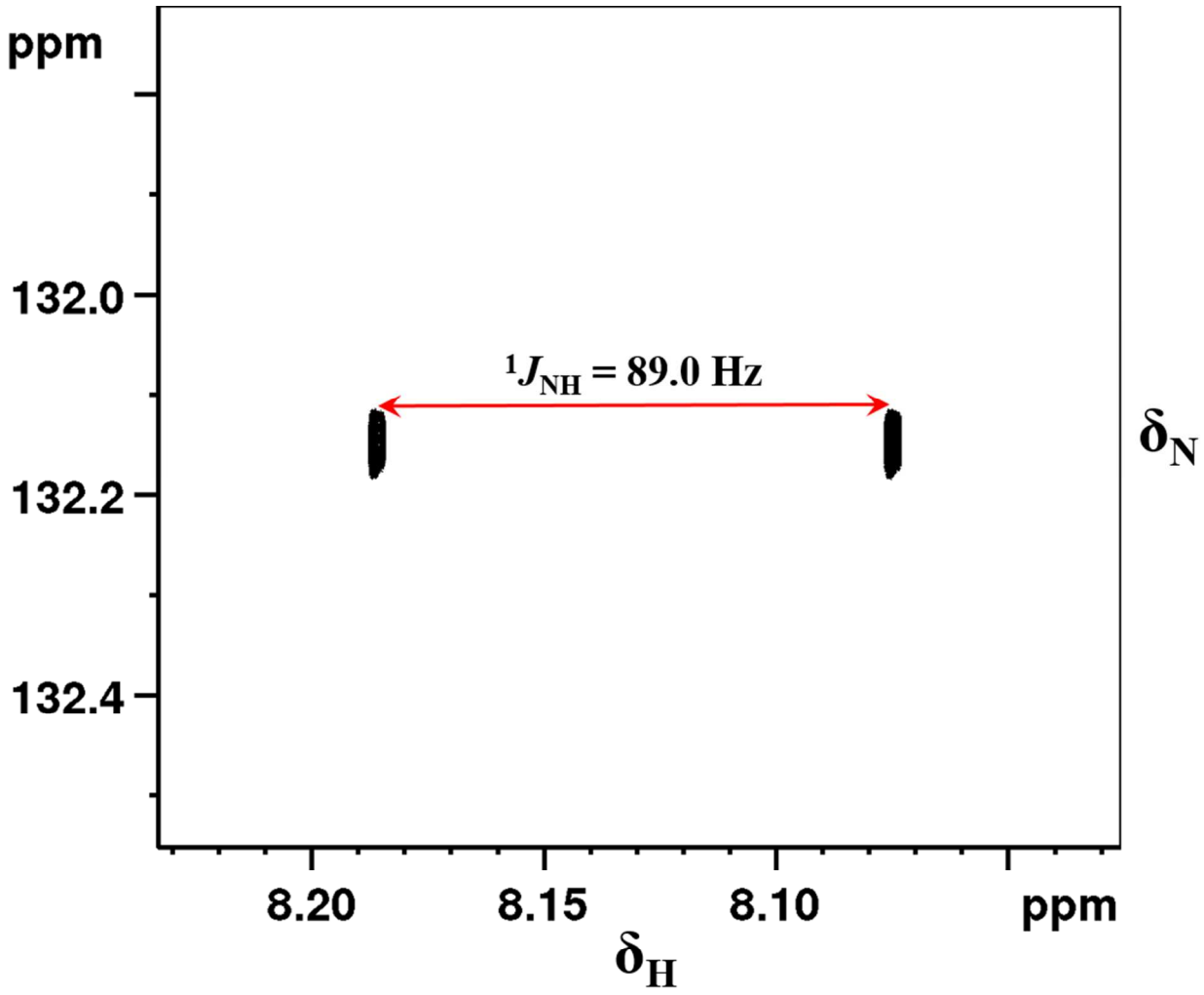


Figure S2: 800 MHz 2D ^{1}H-^{15}N coupled HSQC spectrum of molecule **1** in the solvent $CDCl_3$ showing scalar coupling $^1J_{NH}$.

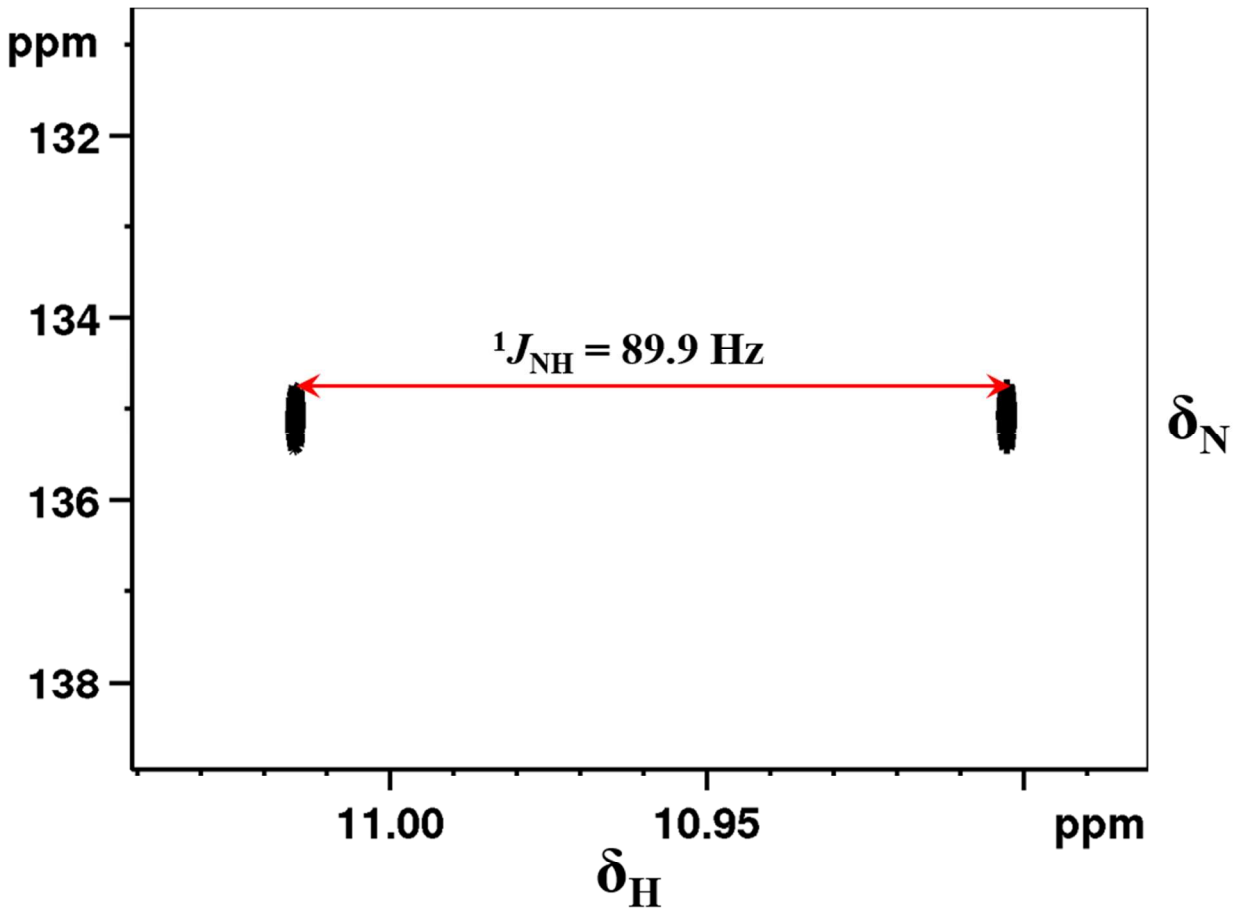


Figure S3: 800 MHz 2D ^{1}H-^{15}N coupled HSQC spectrum of molecule **1** in the solvent DMSO-d_6 showing scalar coupling $^1J_{NH.}$

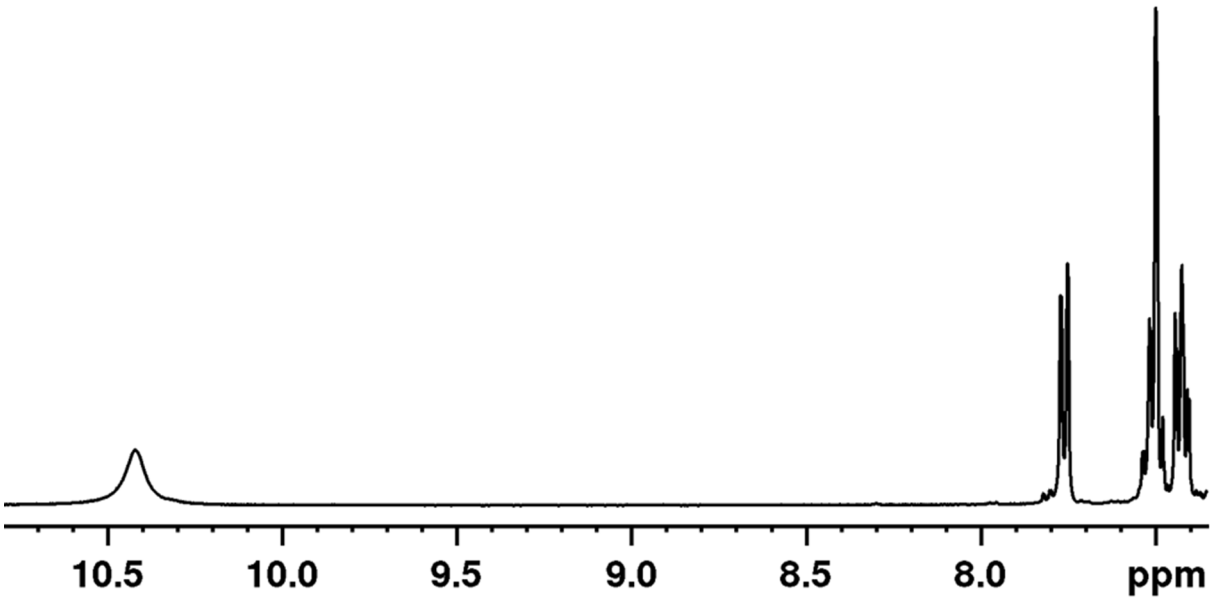


Figure S4: 400 MHz ^{1}H spectrum of molecule **3** in the solvent $CDCl_3$.

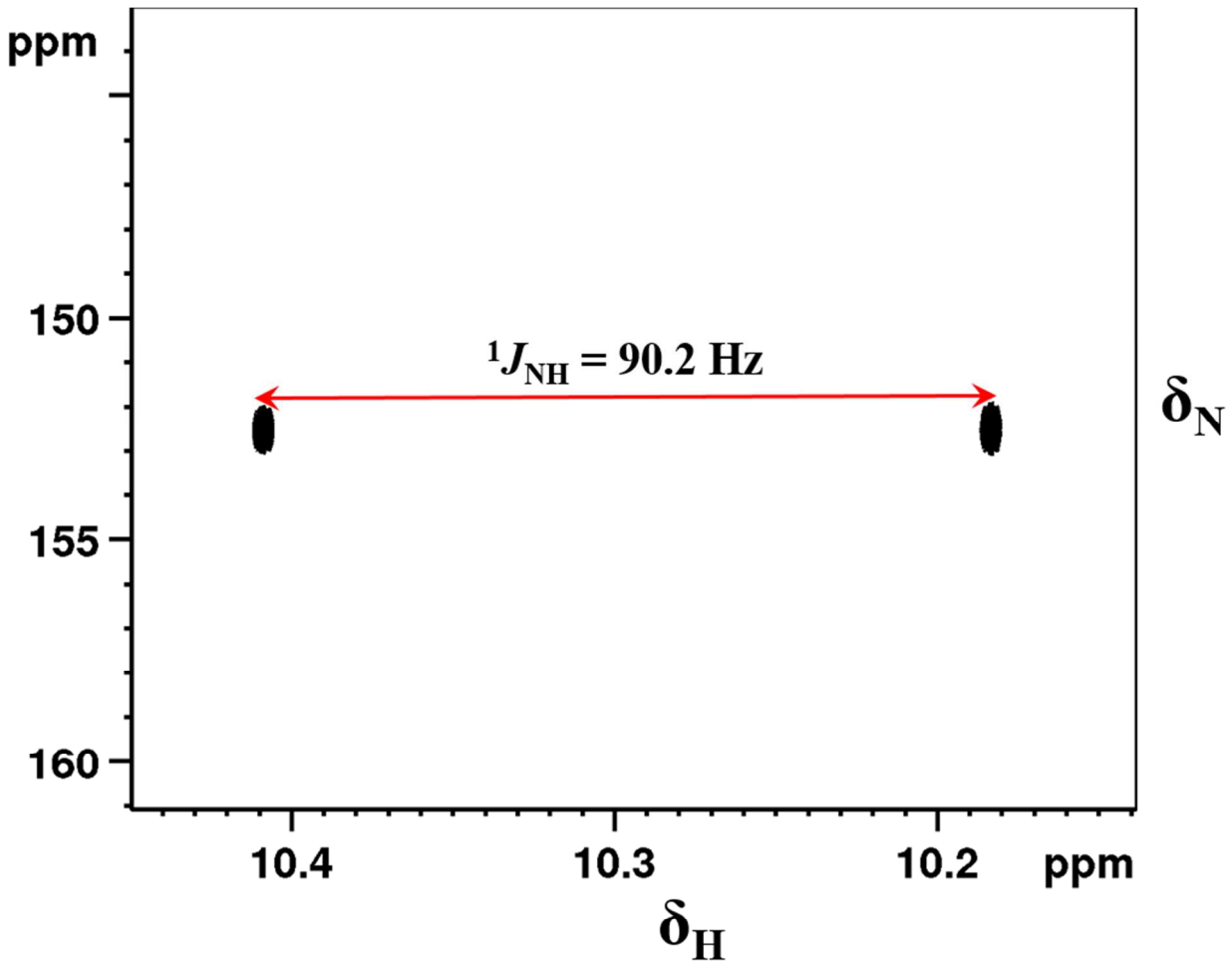


Figure S5: 800 MHz 2D ^{1}H-^{15}N Coupled HSQC spectrum of molecule **3** in the solvent $CDCl_3$ showing scalar coupling $^1J_{NH}$.

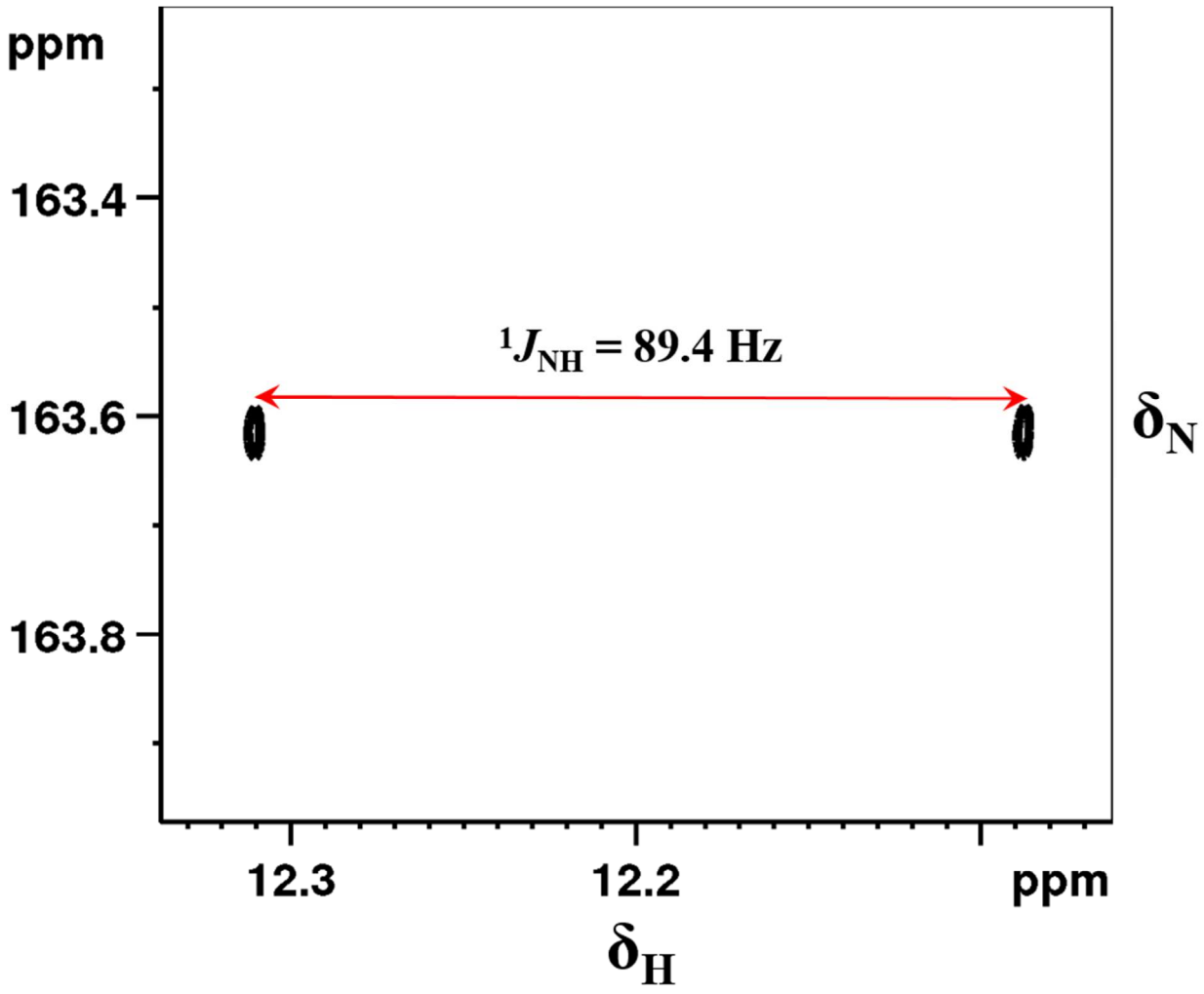
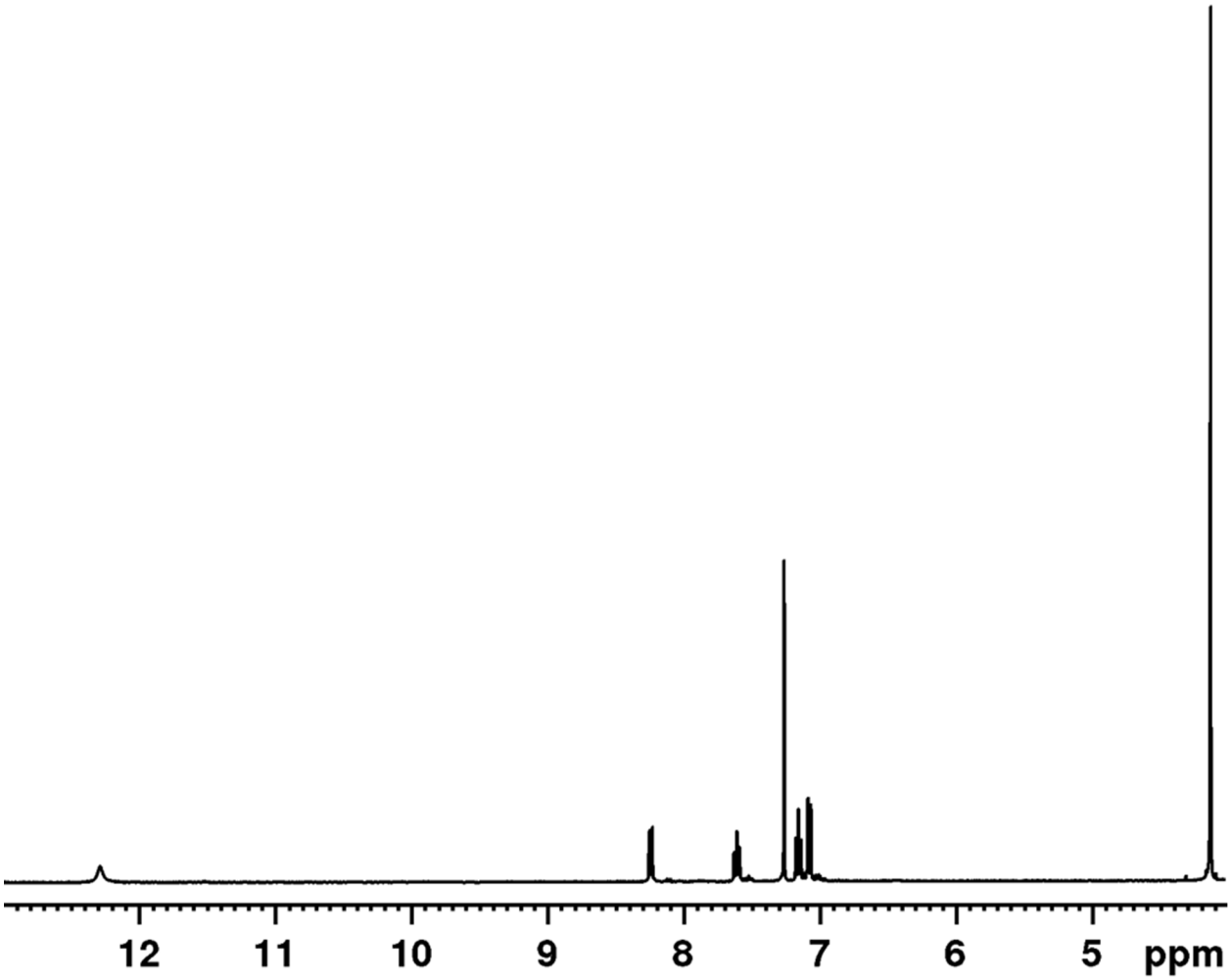


Figure S6: 800 MHz 2D ^{1}H-^{15}N coupled HSQC spectrum of molecule **3** in the solvent DMSO-d_6 showing scalar coupling $^1J_{NH}$.



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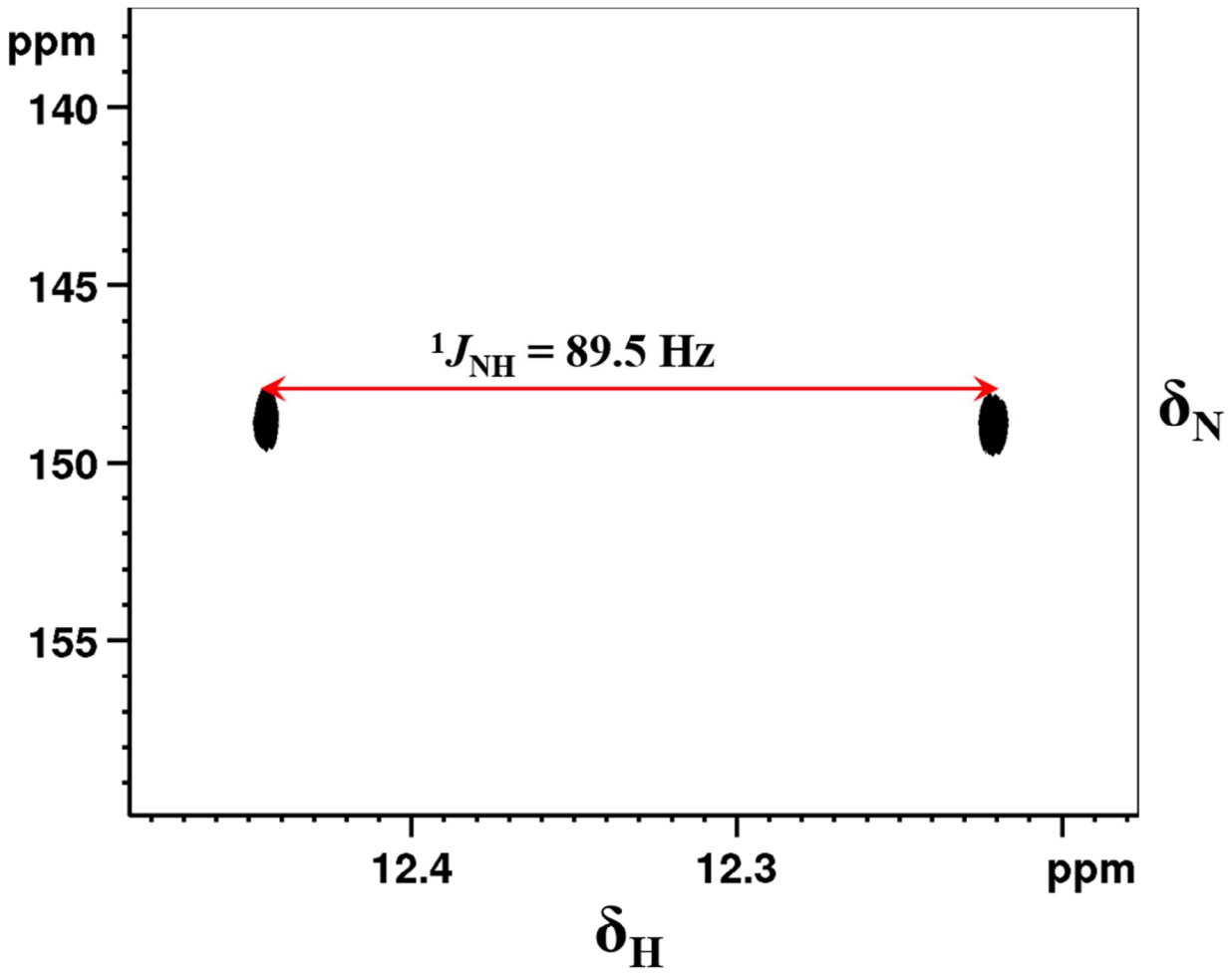


Figure S8: 800 MHz 2D ^{1}H-^{15}N coupled HSQC spectrum of molecule **4** in the solvent $CDCl_3$ showing scalar coupling $^1J_{NH}$.

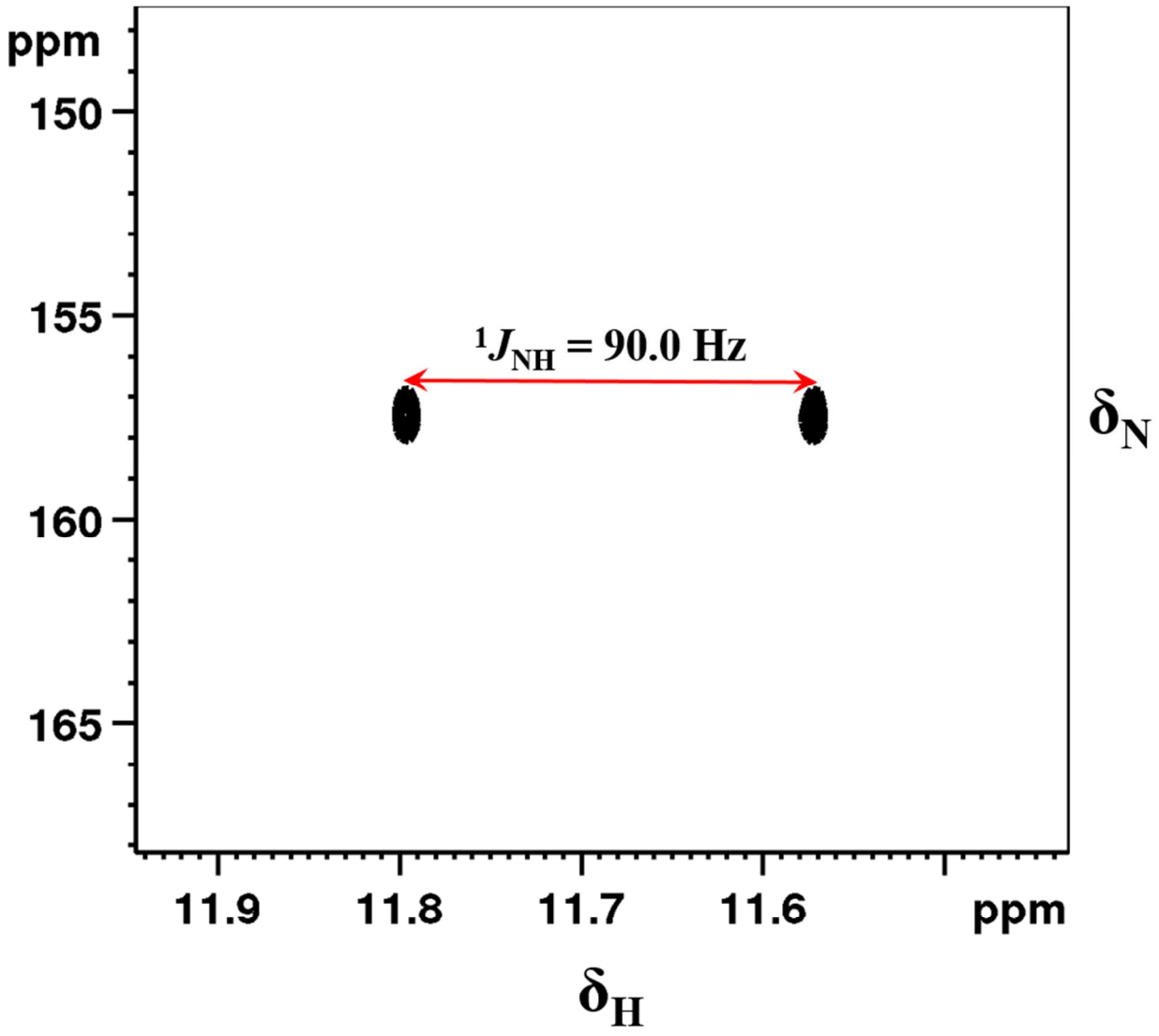


Figure S9: 800 MHz 2D ^{1}H-^{15}N coupled HSQC spectrum of molecule **4** in the solvent DMSO-d_6 showing scalar coupling $^1J_{NH}$.

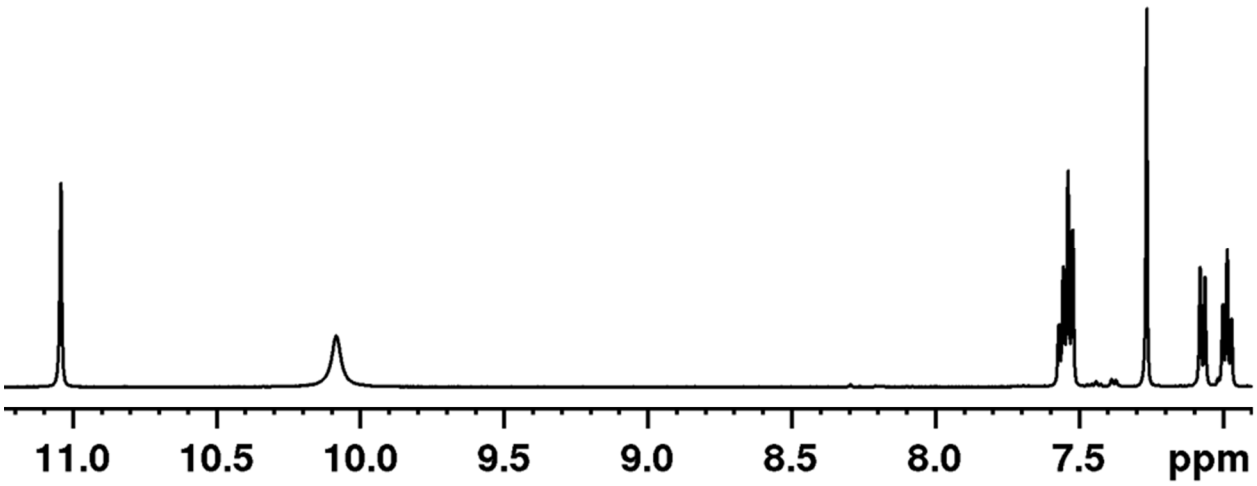


Figure S10: 400 MHz ^{1}H spectrum of molecule **5** in the solvent $CDCl_3$.

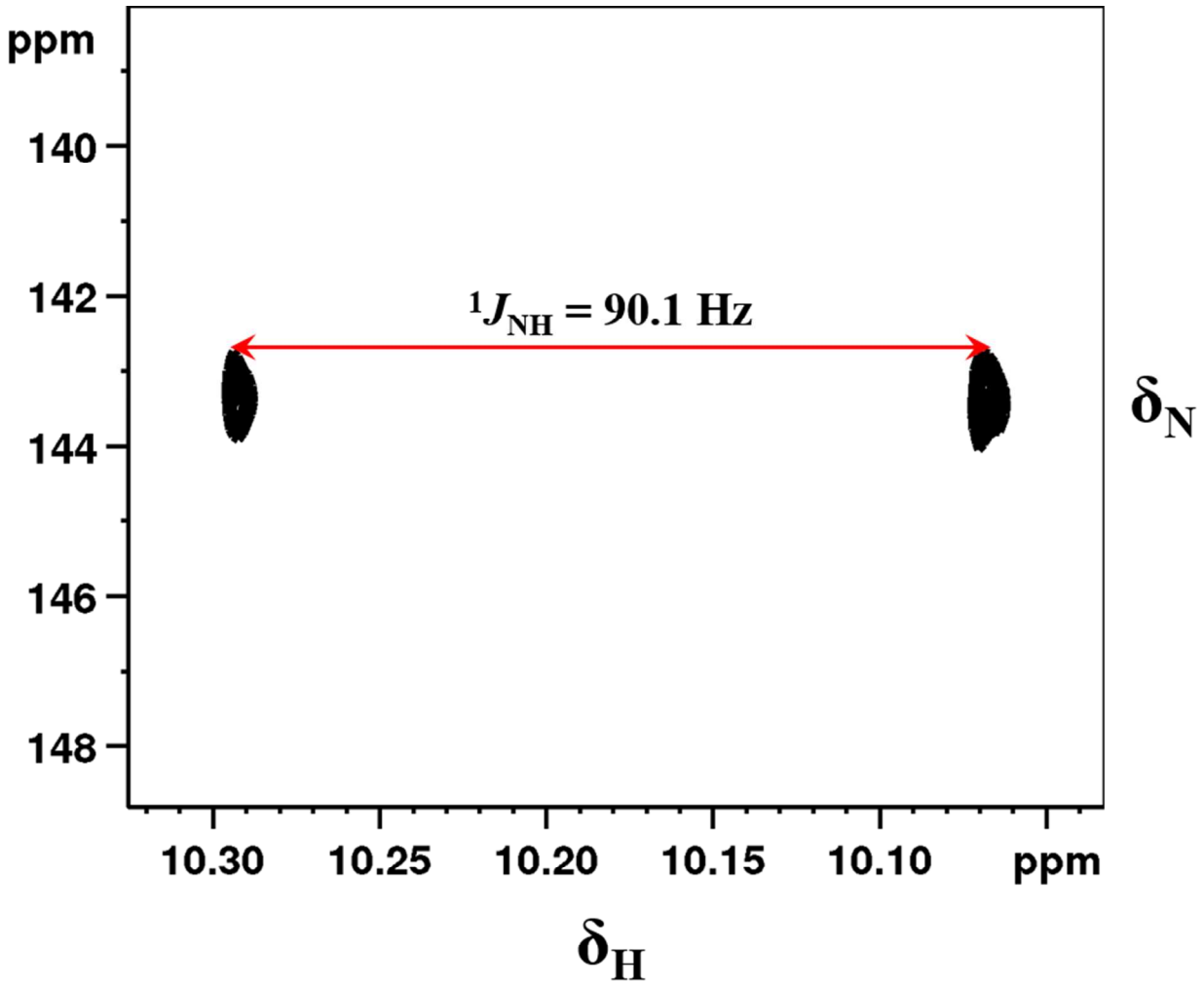


Figure S11: 800 MHz 2D ^{1}H-^{15}N coupled HSQC spectrum of molecule **5** in the solvent $CDCl_3$ showing scalar coupling $^{1}J_{NH}$.

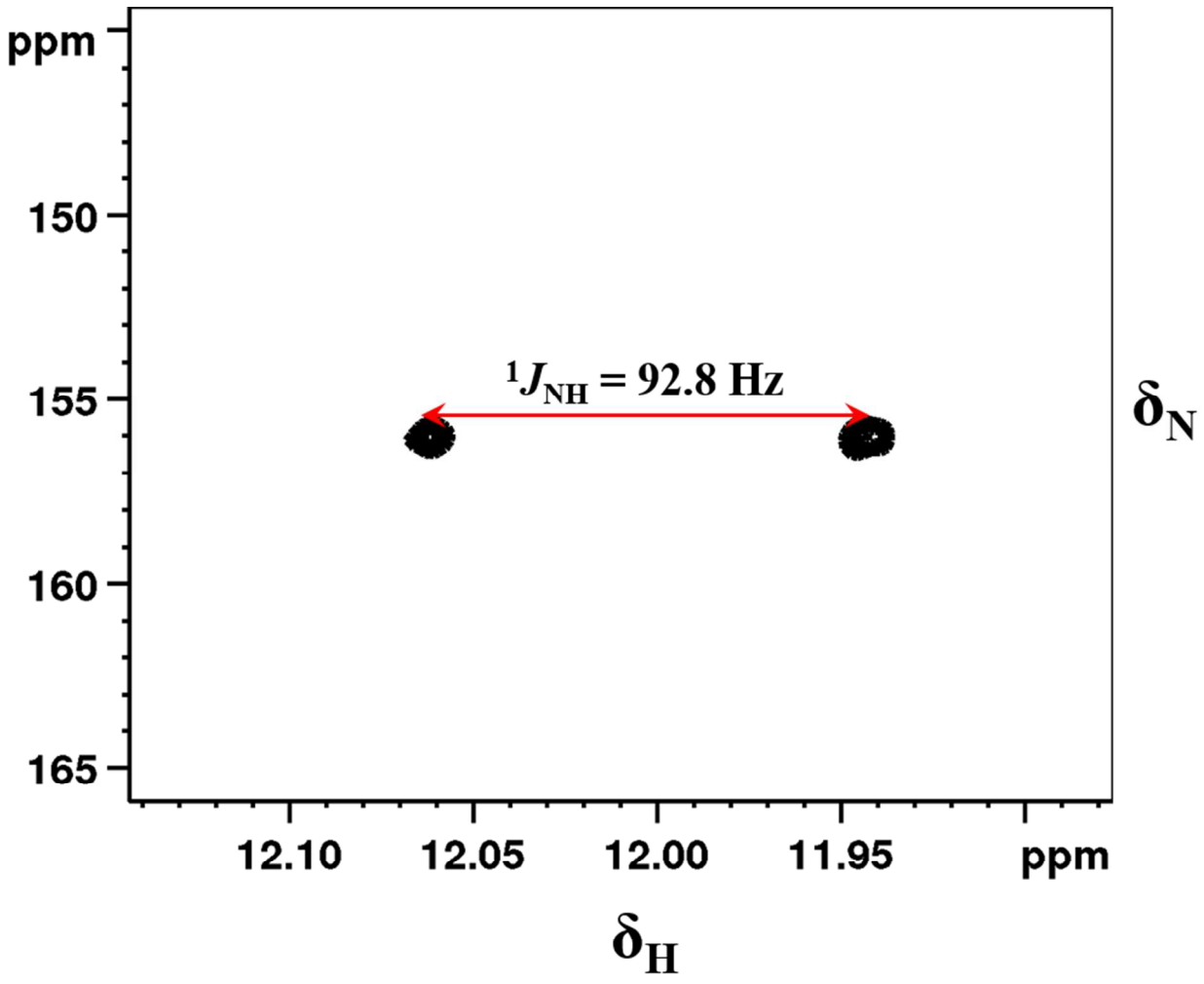


Figure S12: 800 MHz 2D ^{1}H-^{15}N coupled HSQC spectrum of molecule **5** in the solvent DMSO-d_6 showing scalar coupling $^1J_{NH}$.

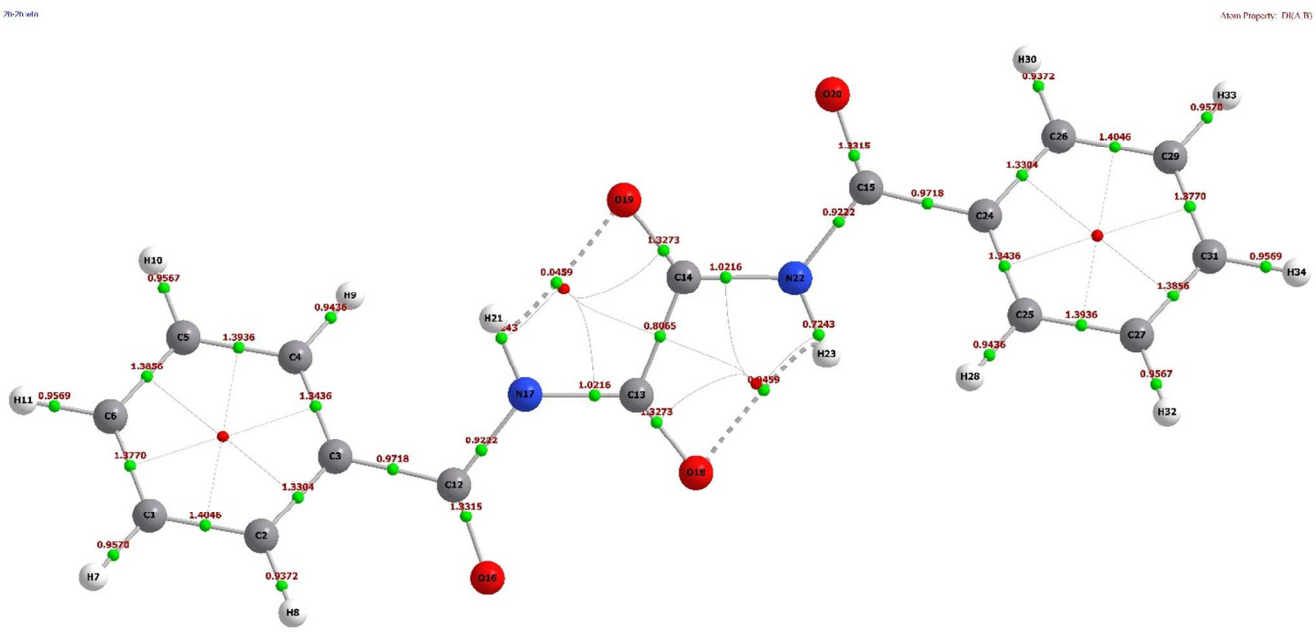
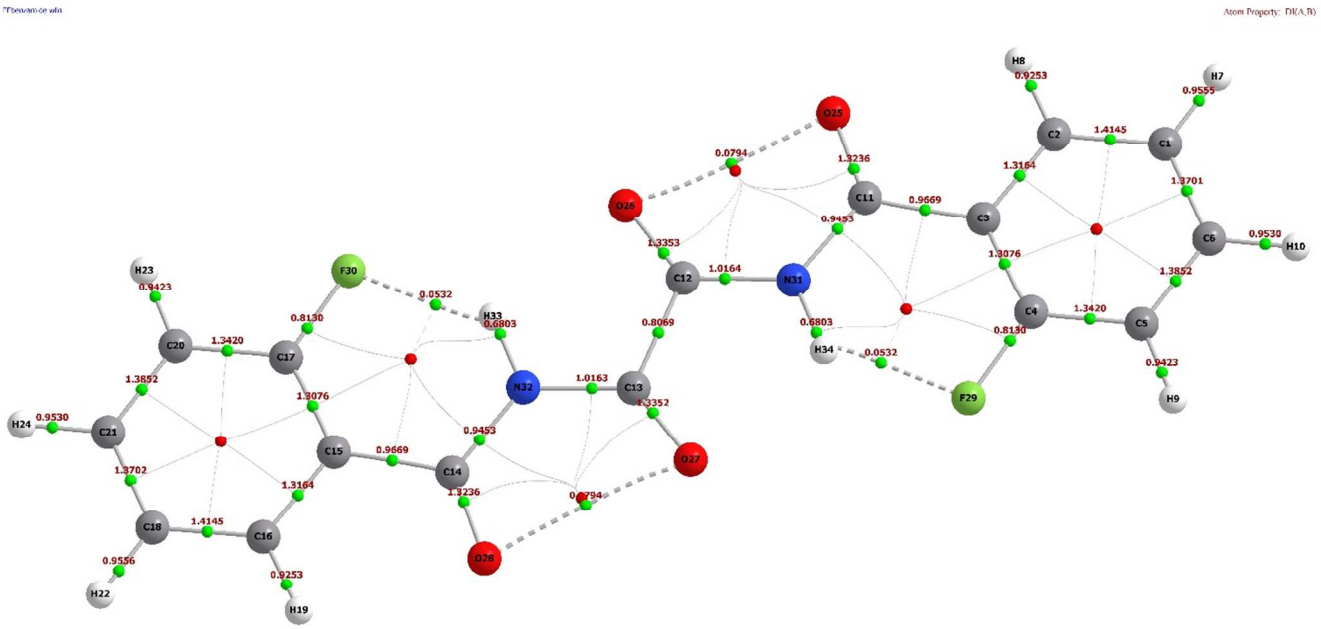


Figure S13: Delocalization indices of molecule 1 determined using QTAIM



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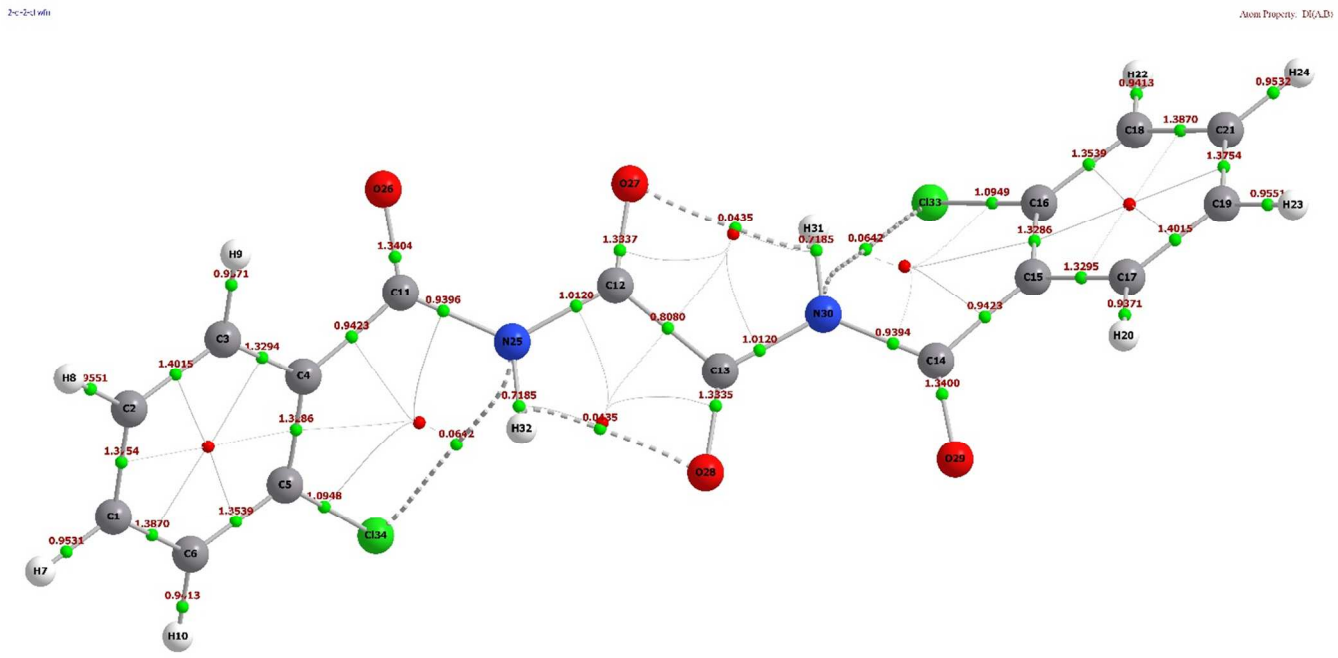

Figure S15: Delocalization indices of molecule 3 determined using QTAIM

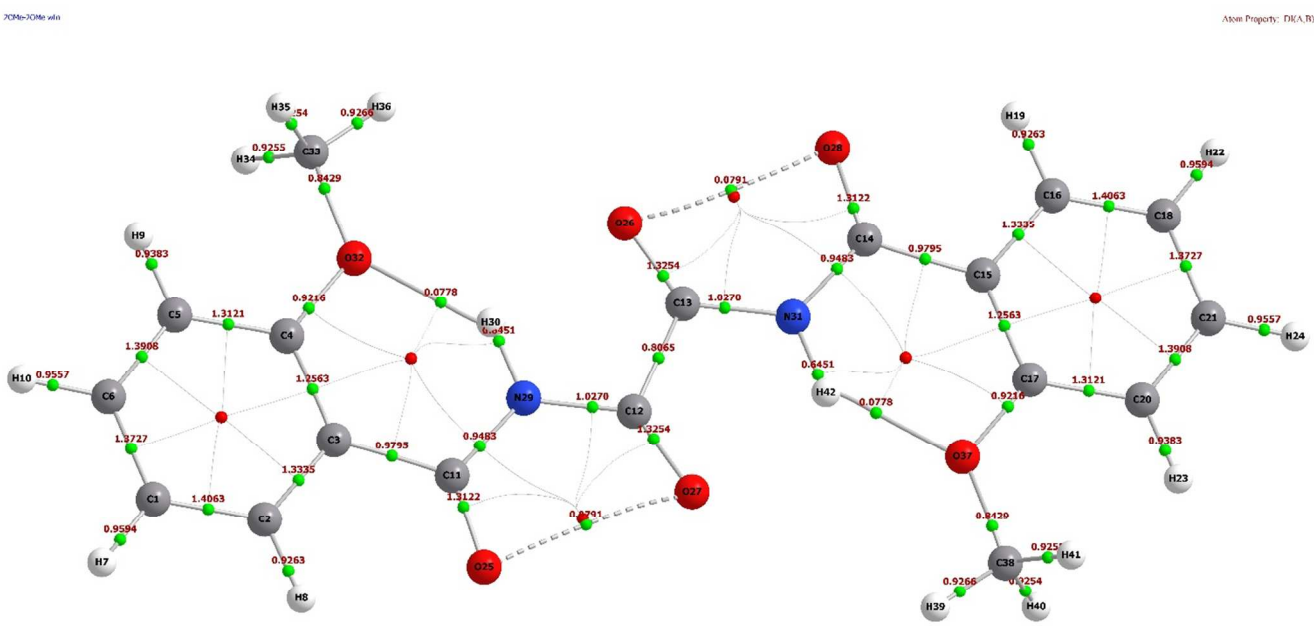

Figure S16: Delocalization indices of molecule 4 determined using QTAIM

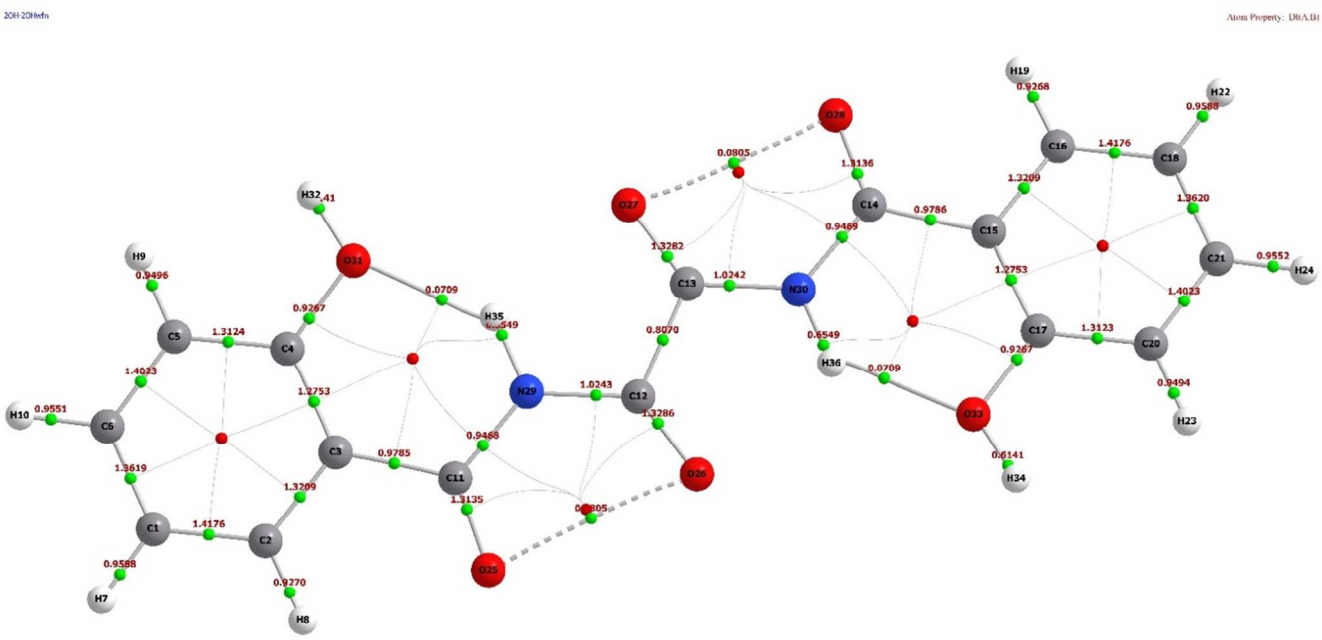

Figure S17: Delocalization indices of molecule 5a determined using QTAIM

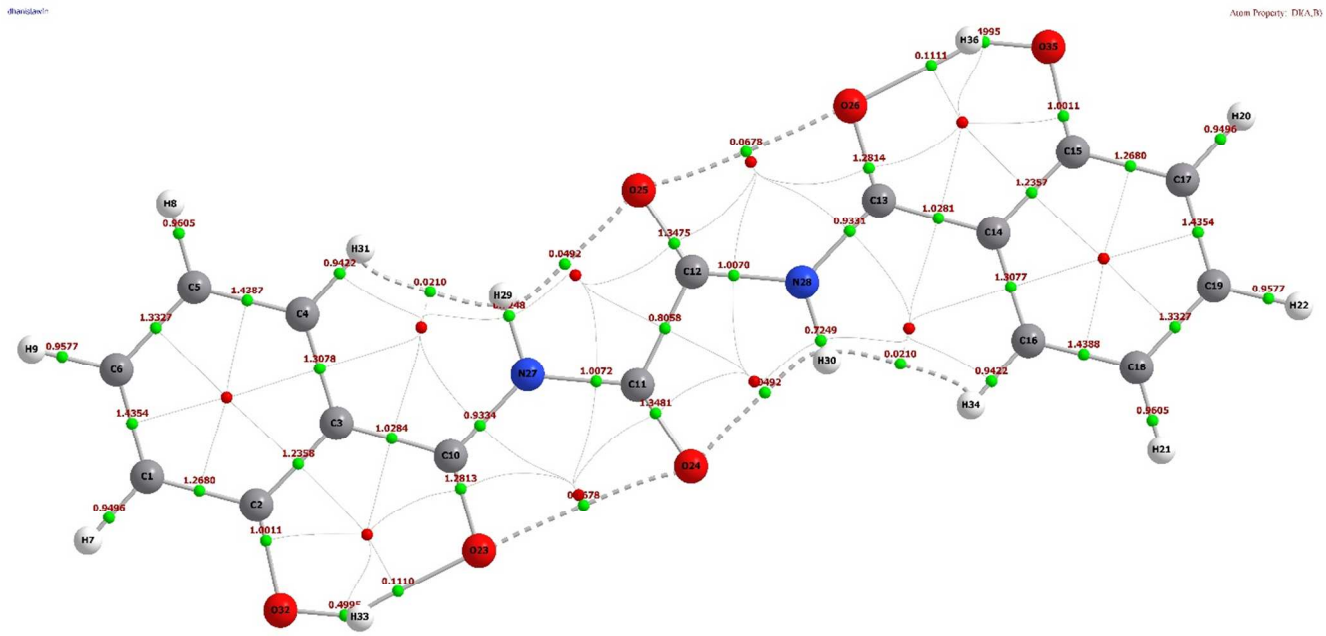

Figure S18: Delocalization indices of molecule 5b determined using QTAIM

Full Citation of References Containing More than 10 Authors

1. Arunan, E.; Desiraju, G. R.; Klein, R. A.; Sadlej, J.; Scheiner, S.; Alkorta, I.; Clary, D. C.; Crabtree, R. H.; Dannenberg, J. J.; Hobza, P.; Kjaergaard, H. G.; Legon, A. C.; Mennucci, B.; Nesbitt, D. J. Definition of the Hydrogen Bond (IUPAC Recommendations 2011). *Pure Appl. Chem.* **2011**, *83*, 1637–1641.

75. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M..; Heyd, J.J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J.M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford, CT, USA, 2009.