



Supporting Information

for

Synthesis of C₇₀-fragment buckybowls bearing alkoxy substituents

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**¹H and ¹³C NMR data of 3a, 3b, 4a, 4b and 5a–c, simulated
UV–vis spectra of 5a, 5b and 5c**

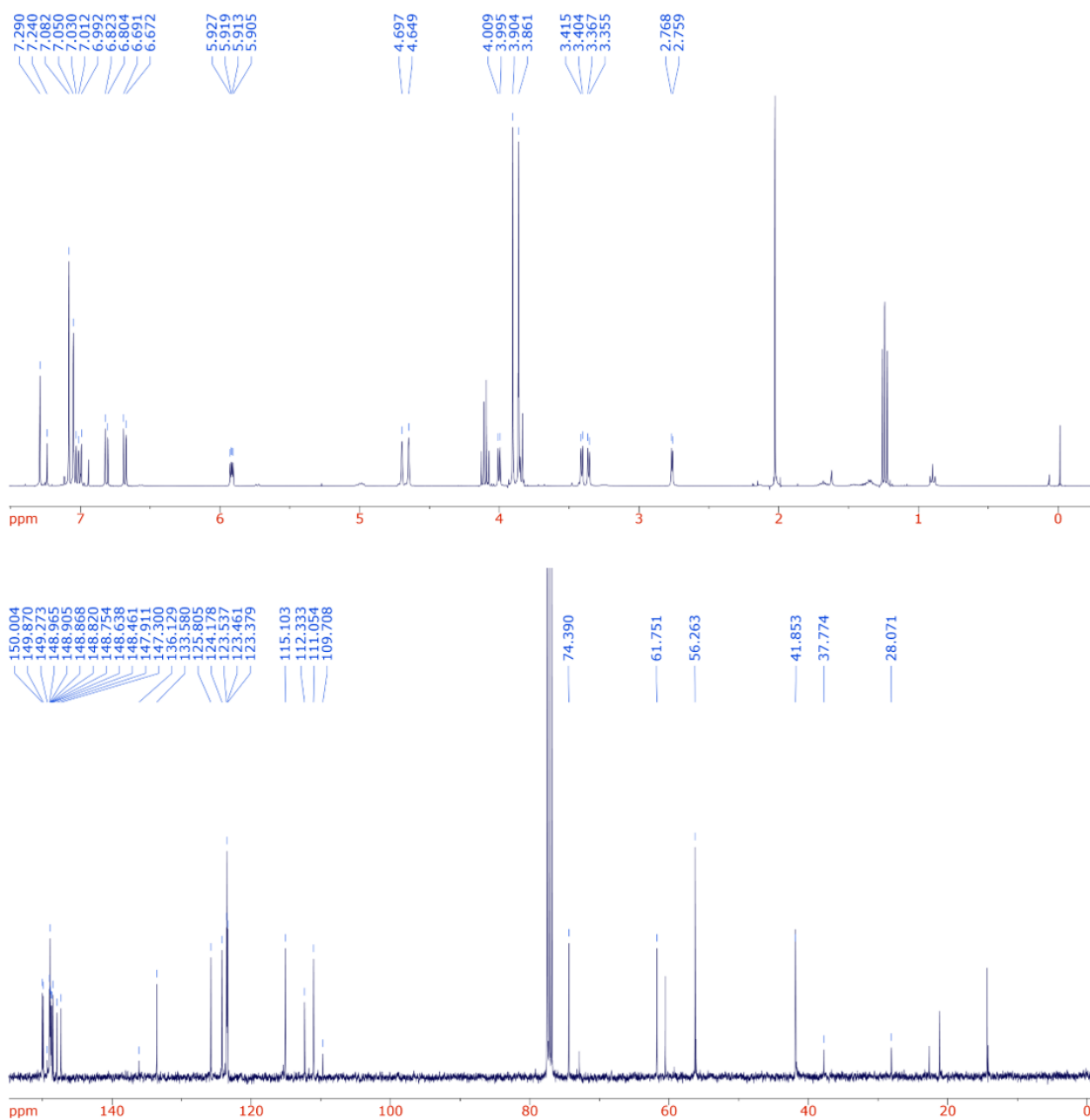


Figure S1. ¹H and ¹³C NMR spectra of **3a**.

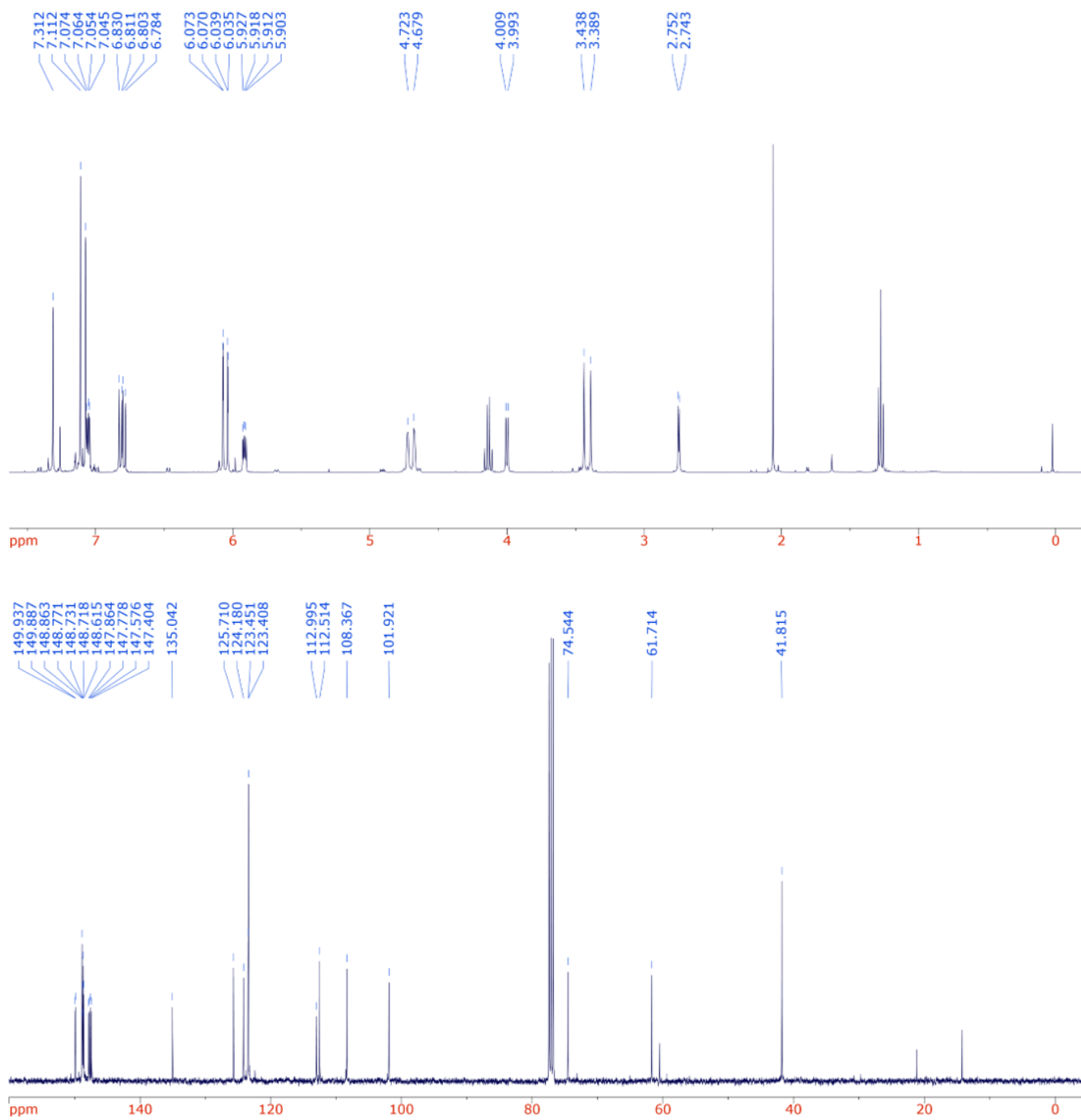


Figure S2. ¹H and ¹³C NMR spectra of **3b**.

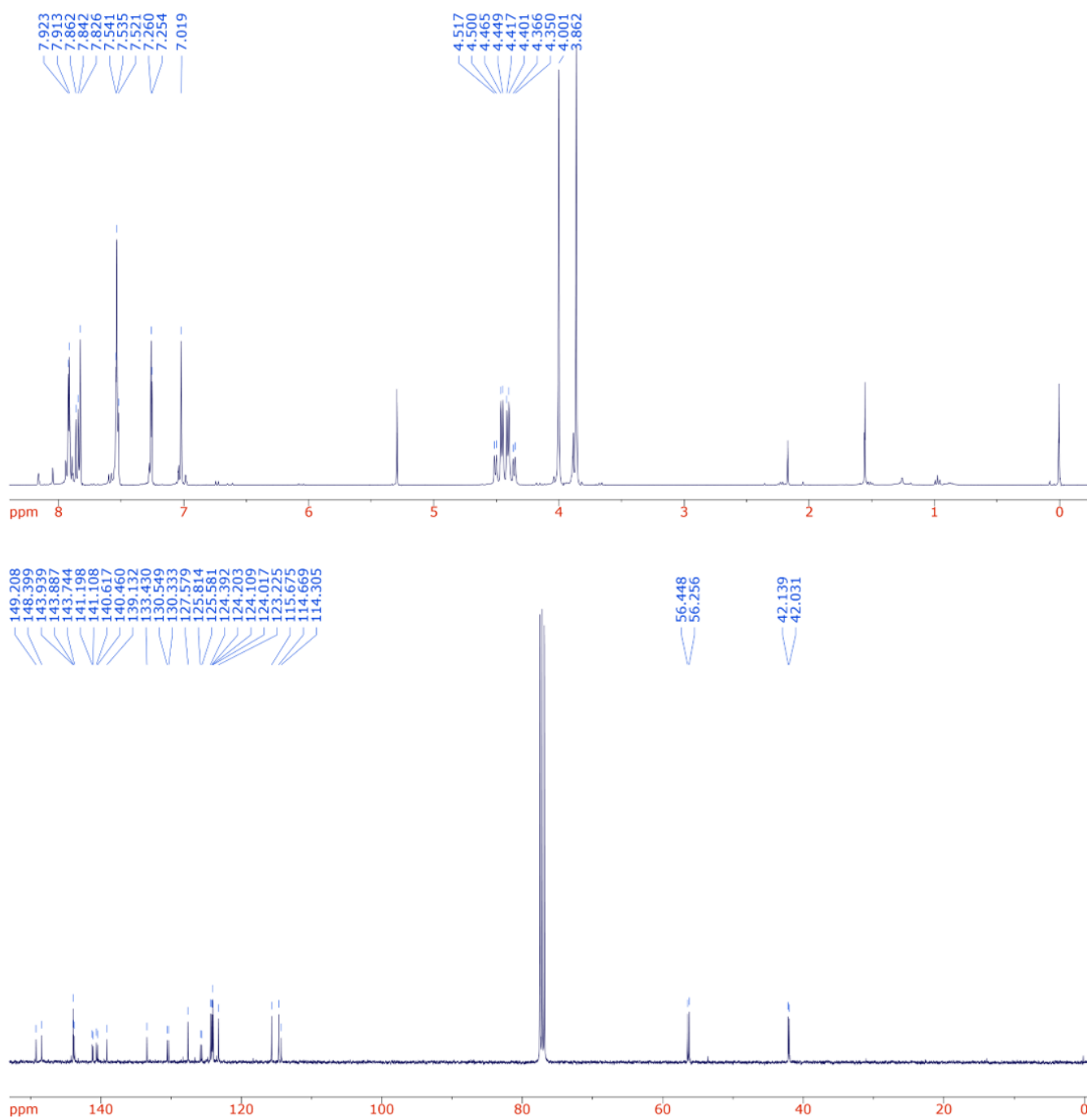


Figure S3. ^1H and ^{13}C NMR spectra of **4a**.

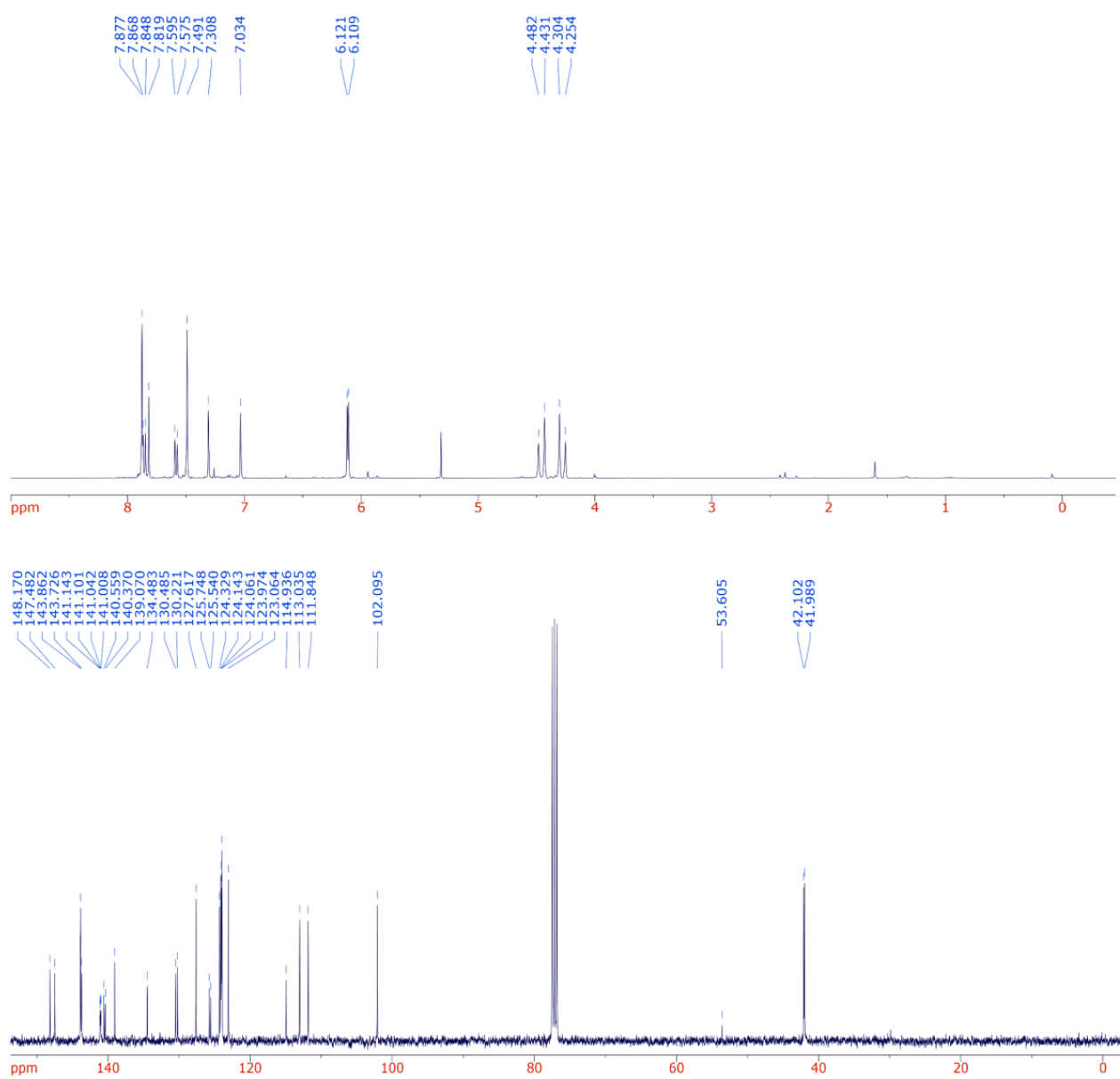


Figure S4. ¹H and ¹³C NMR spectra of **4b**.

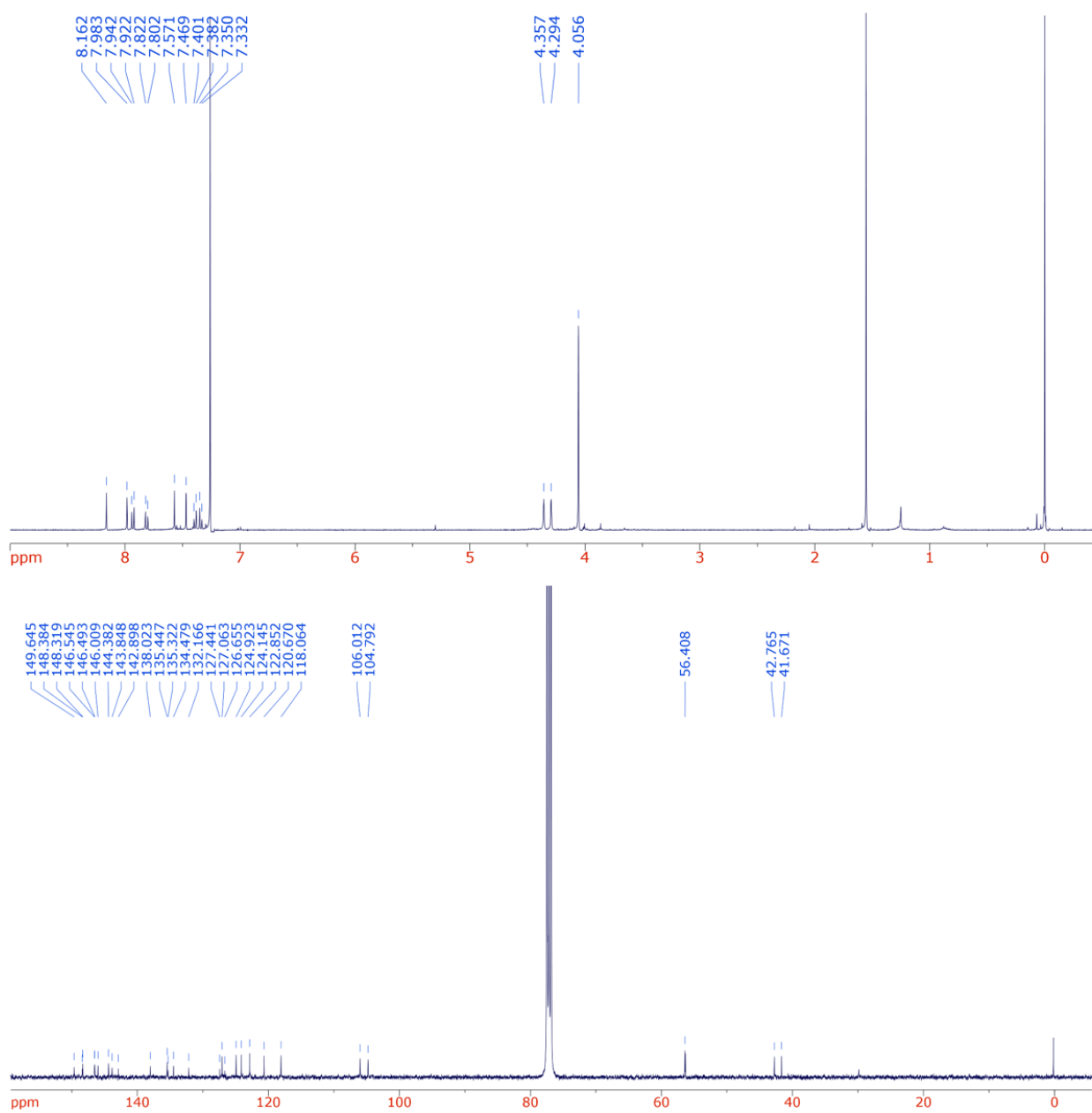


Figure S5. ¹H and ¹³C NMR spectra of **5a**.

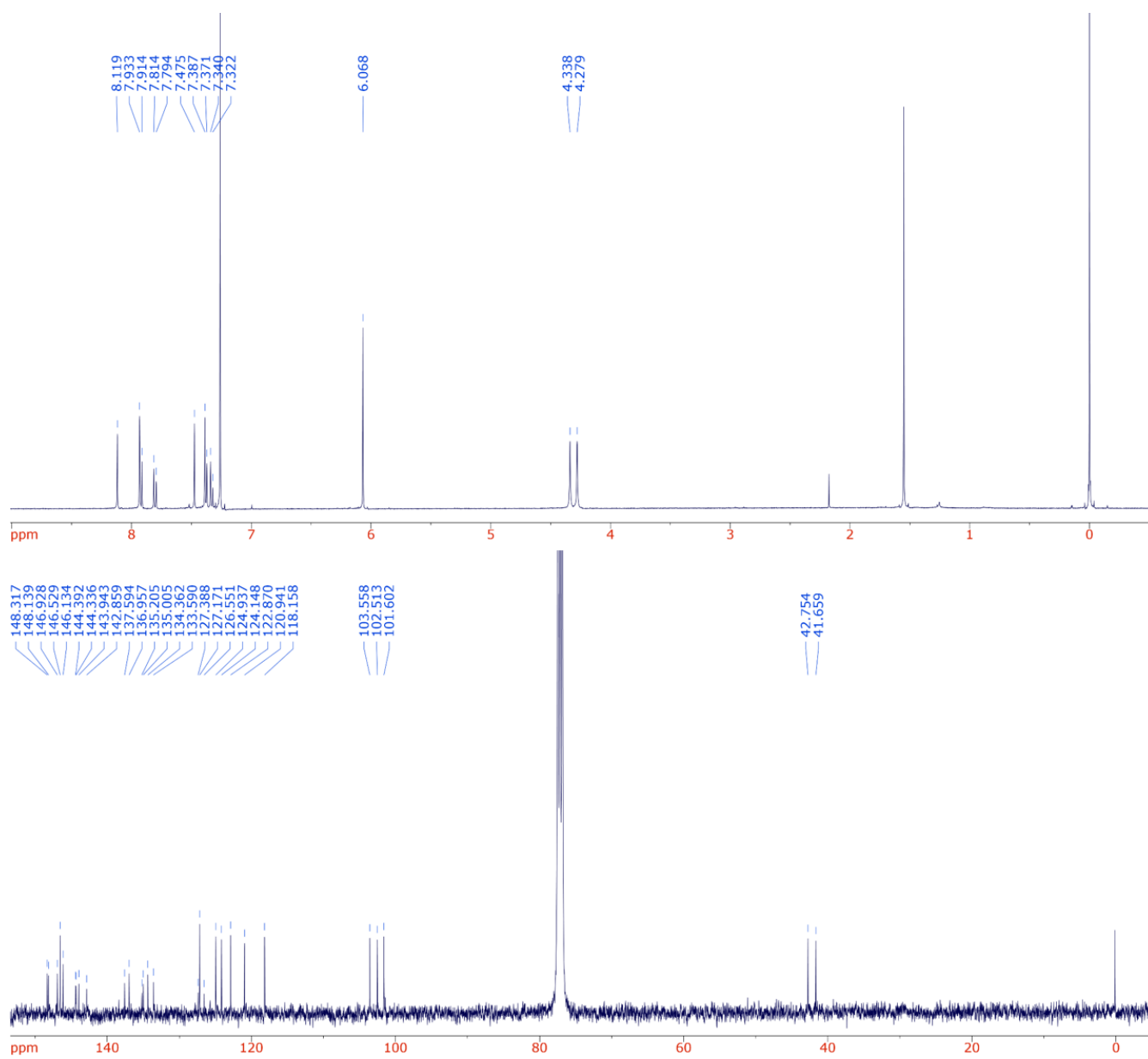


Figure S6. ^1H and ^{13}C NMR spectra of **5b**.

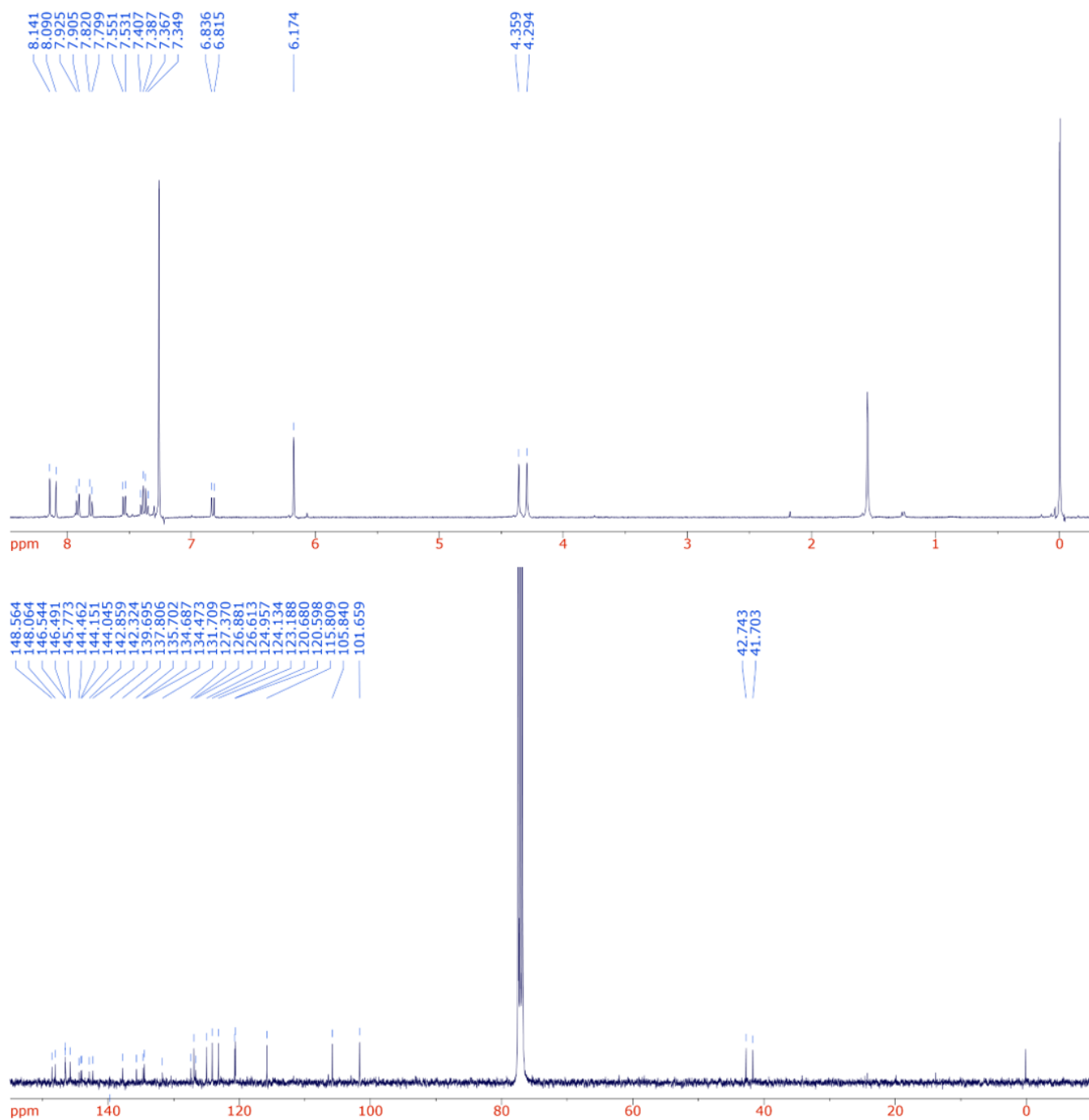


Figure S7. ^1H and ^{13}C NMR spectra of **5c**.

2. Computational data

All the theoretical calculations were conducted by Gaussian09.^{s1} Calculation of UV-vis spectra of **5a**, **5b** and **5c** was performed by TD-DFT (time dependent density functional theory) at the CAM-B3LYP/6-31G+(d,p) level of theory with using the optimized structures from single crystal X-ray analysis data.

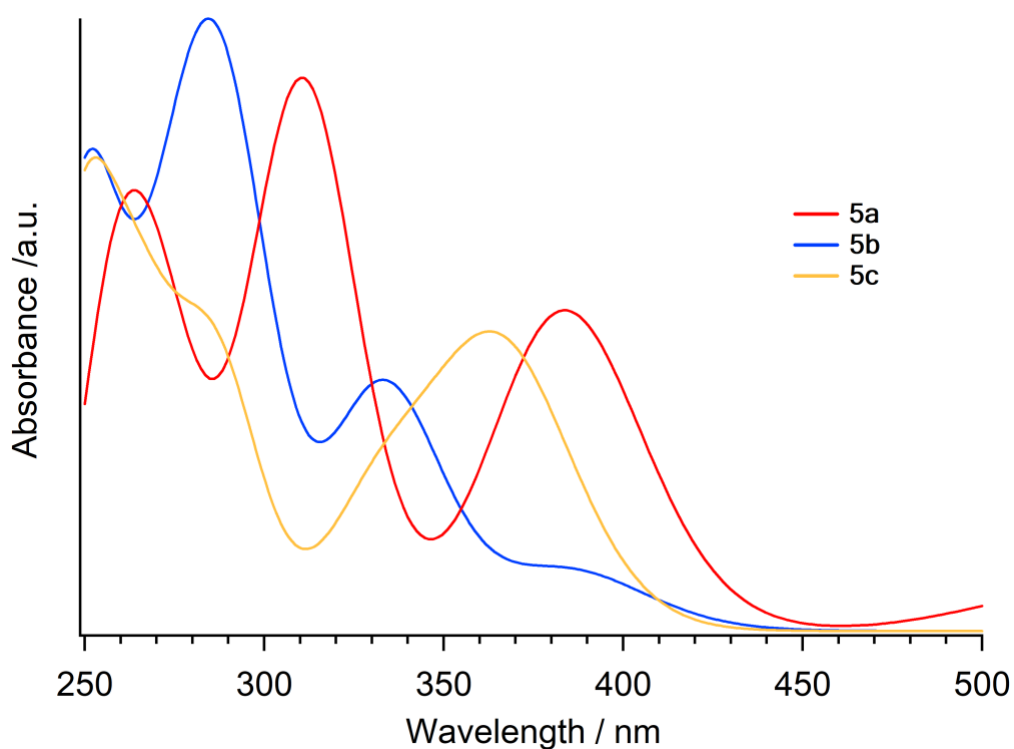


Figure S8. Simulated UV-vis spectra of **5a**, **5b** and **5c**.

Reference

S1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Maricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, I. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian09, Revision B.01; Gaussian Inc.: Wallingford, CT, 2010.