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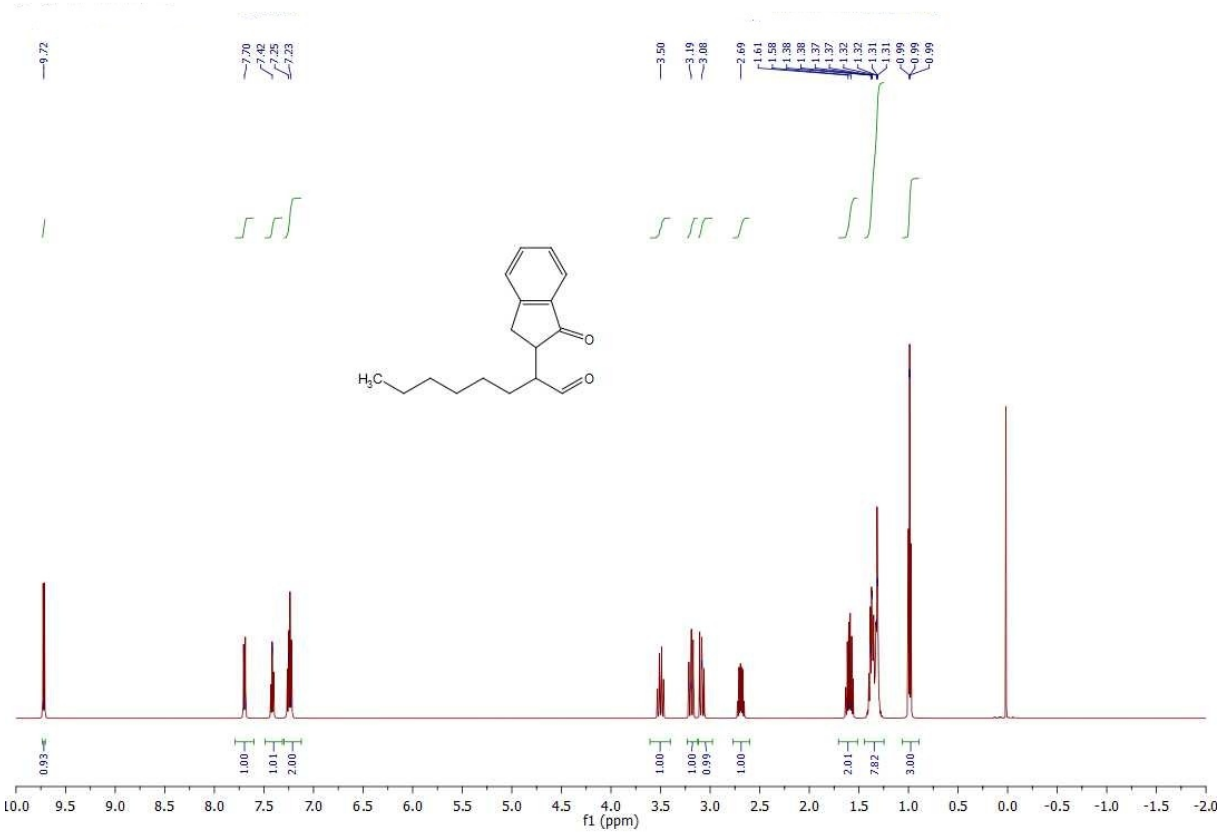
Supporting information for

Asymmetric organocatalytic SOMO reactions of enol silanes and silyl ketene (thio)acetals

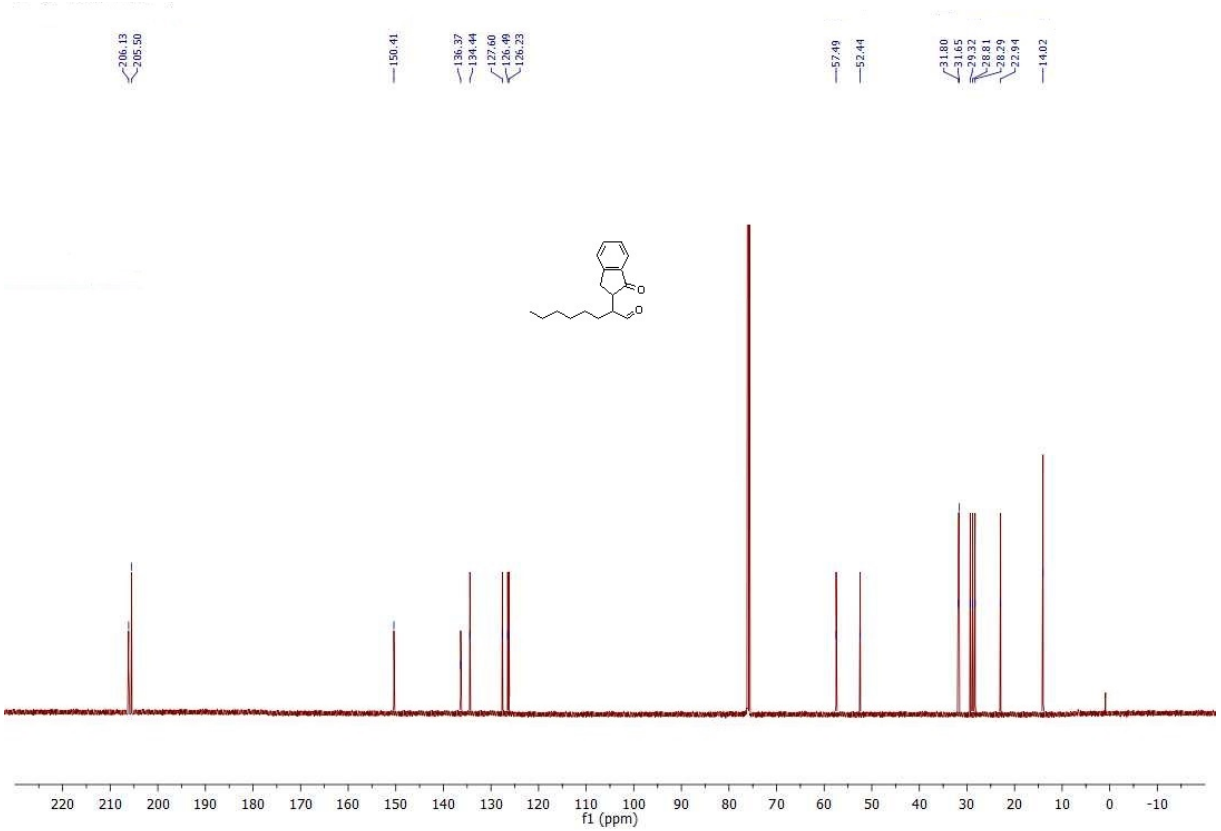
Pavol Tisovský, Mária Mečiarová, and Radovan Šebesta*

Contents

^{1}H NMR spectrum of **3a**



^{13}C spectrum of **3a**



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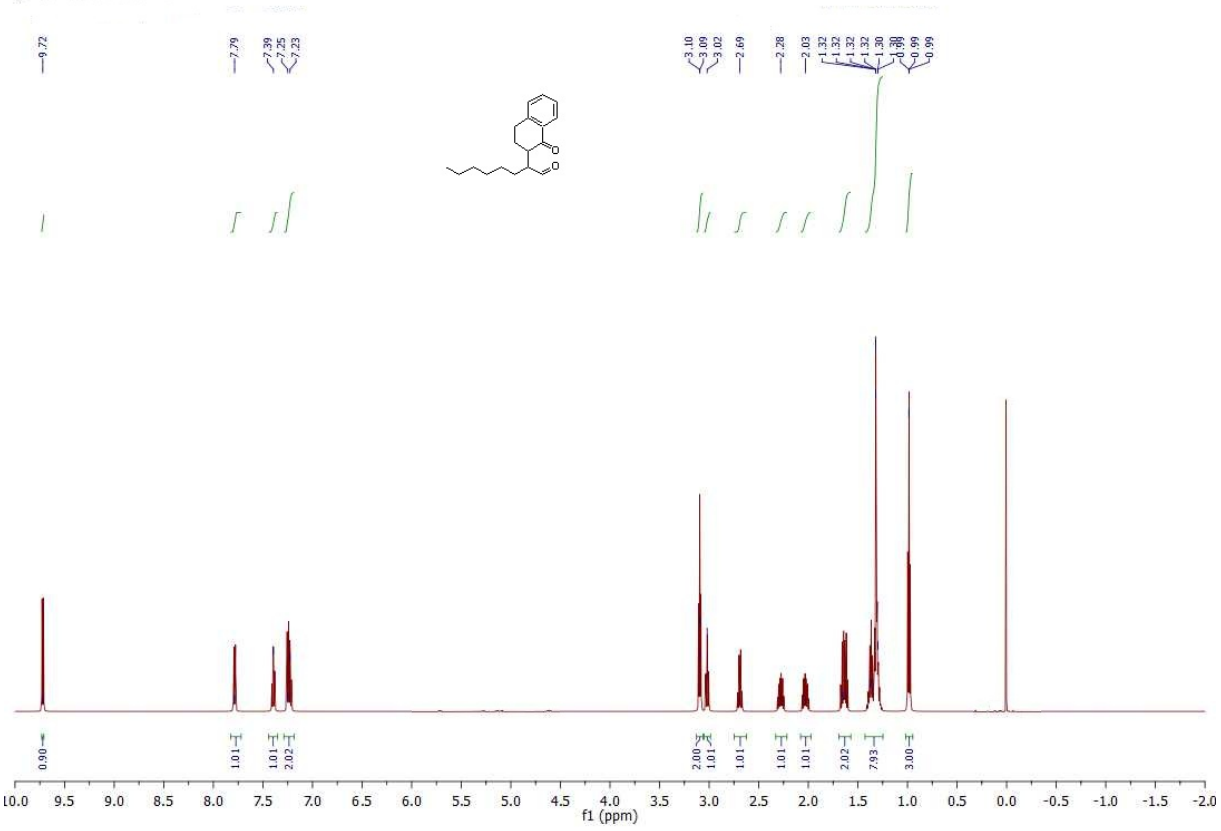
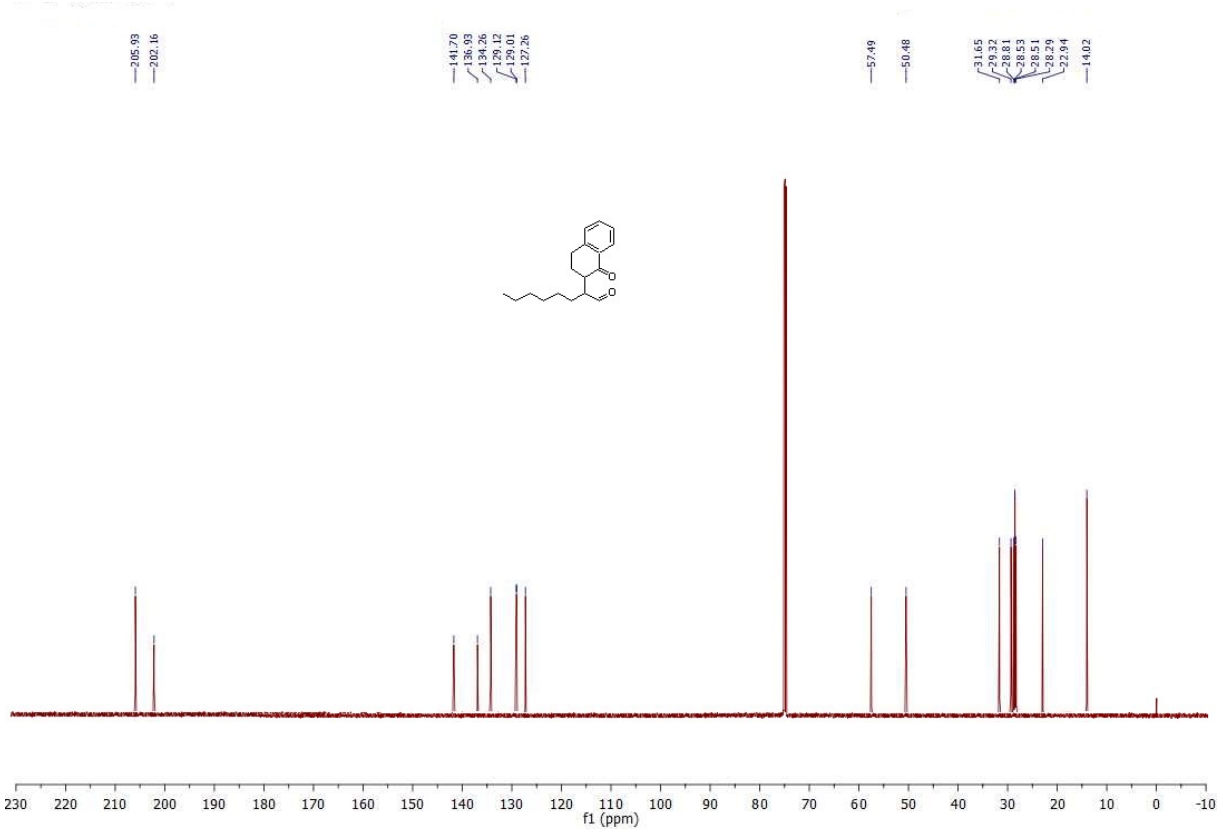
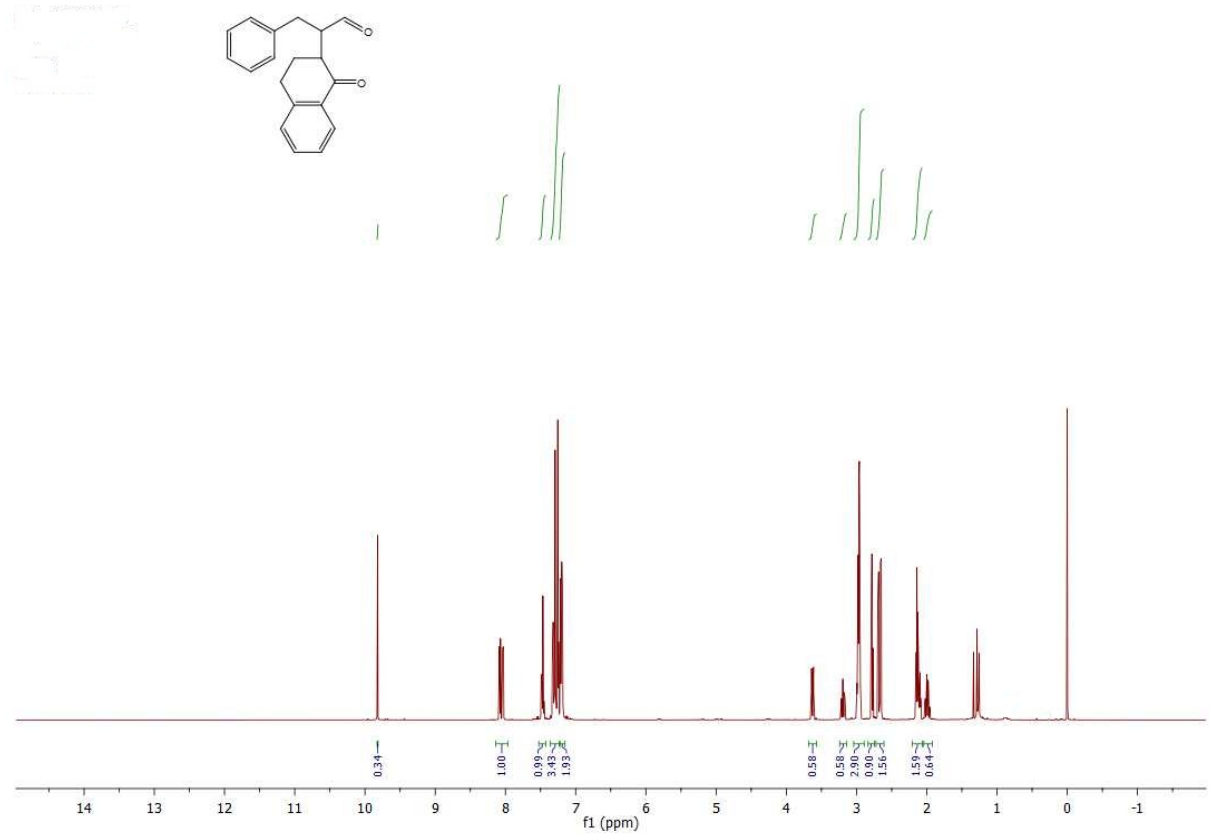


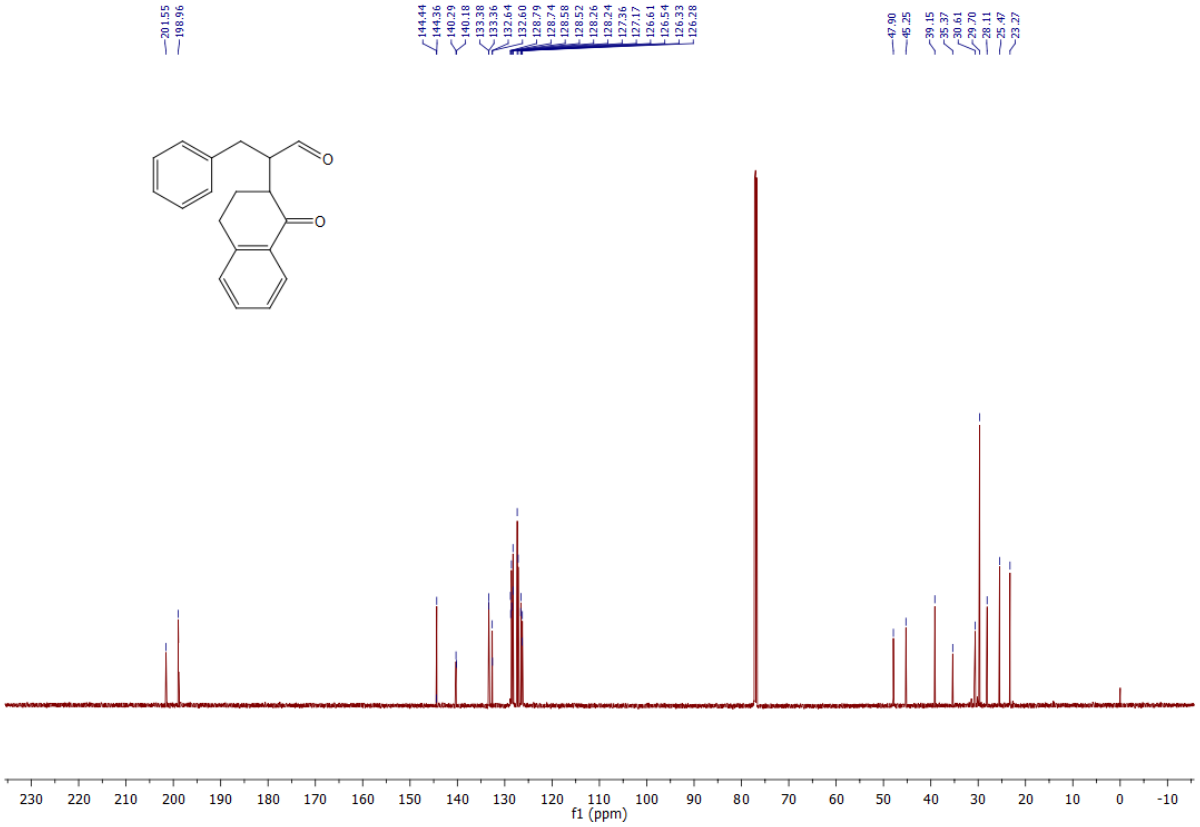
^{13}C spectrum of **3b**



^{1}H NMR spectrum of **3d**



^{13}C spectrum of **3d**

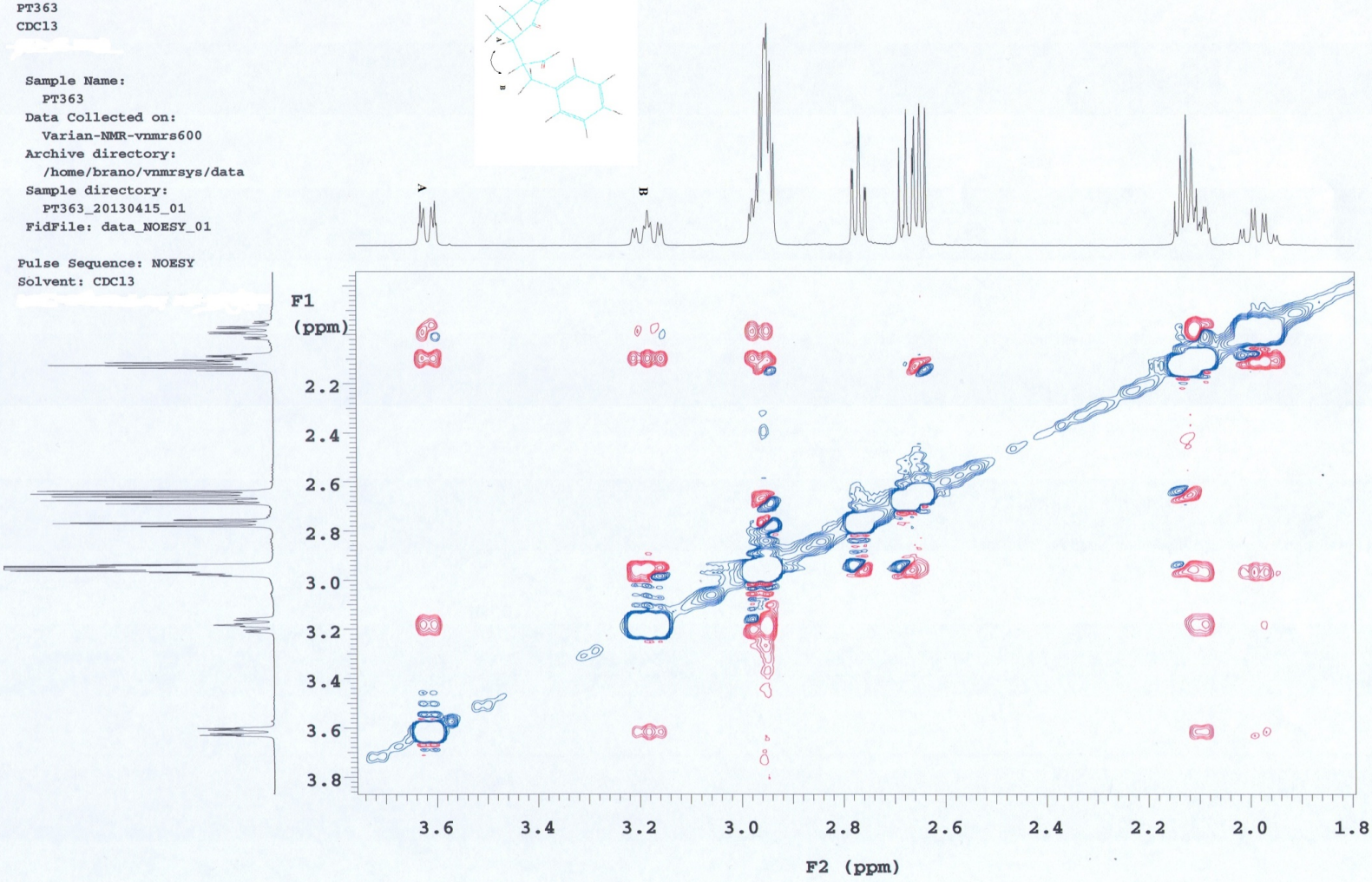


NOESY of **3d**

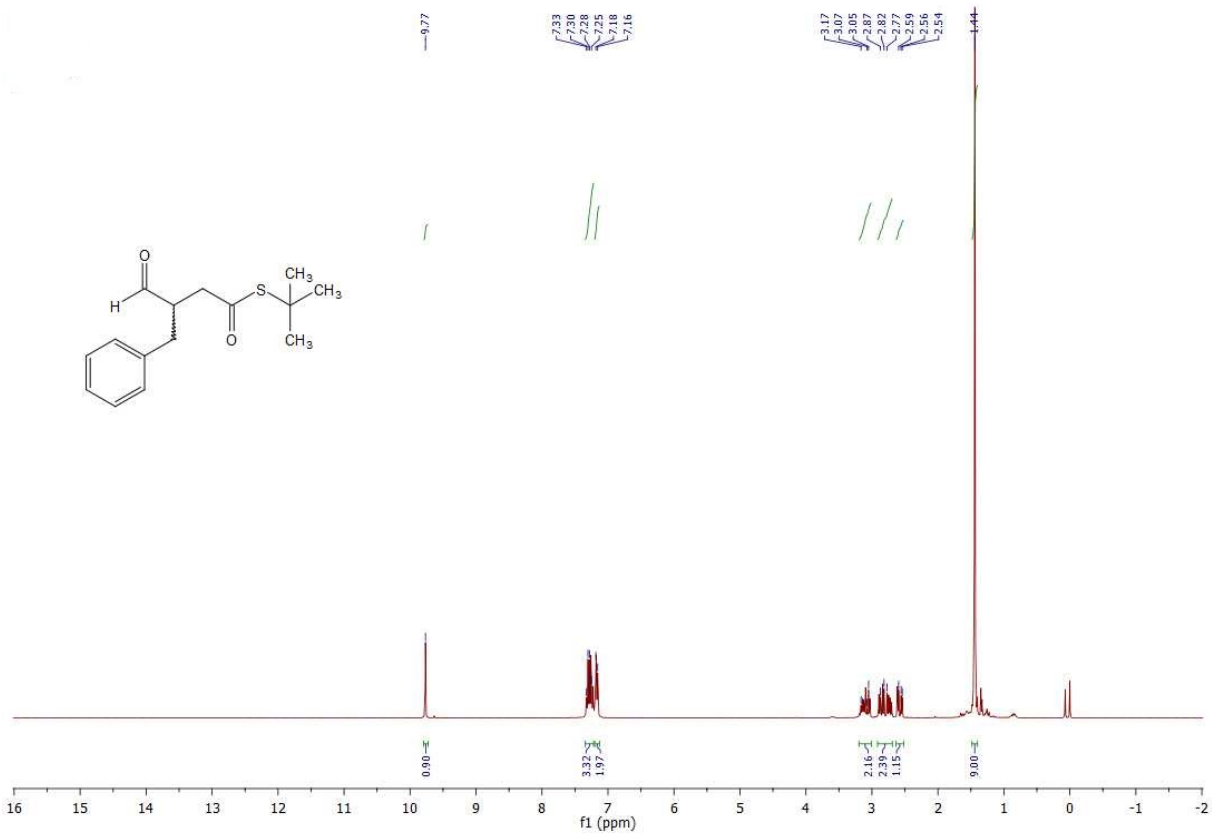
NOESY, 600 MHz
PT363
CDC13

Sample Name:
PT363
Data Collected on:
Varian-NMR-vnmrs600
Archive directory:
/home/brano/vnmrsys/data
Sample directory:
PT363_20130415_01
FidFile: data_NOESY_01

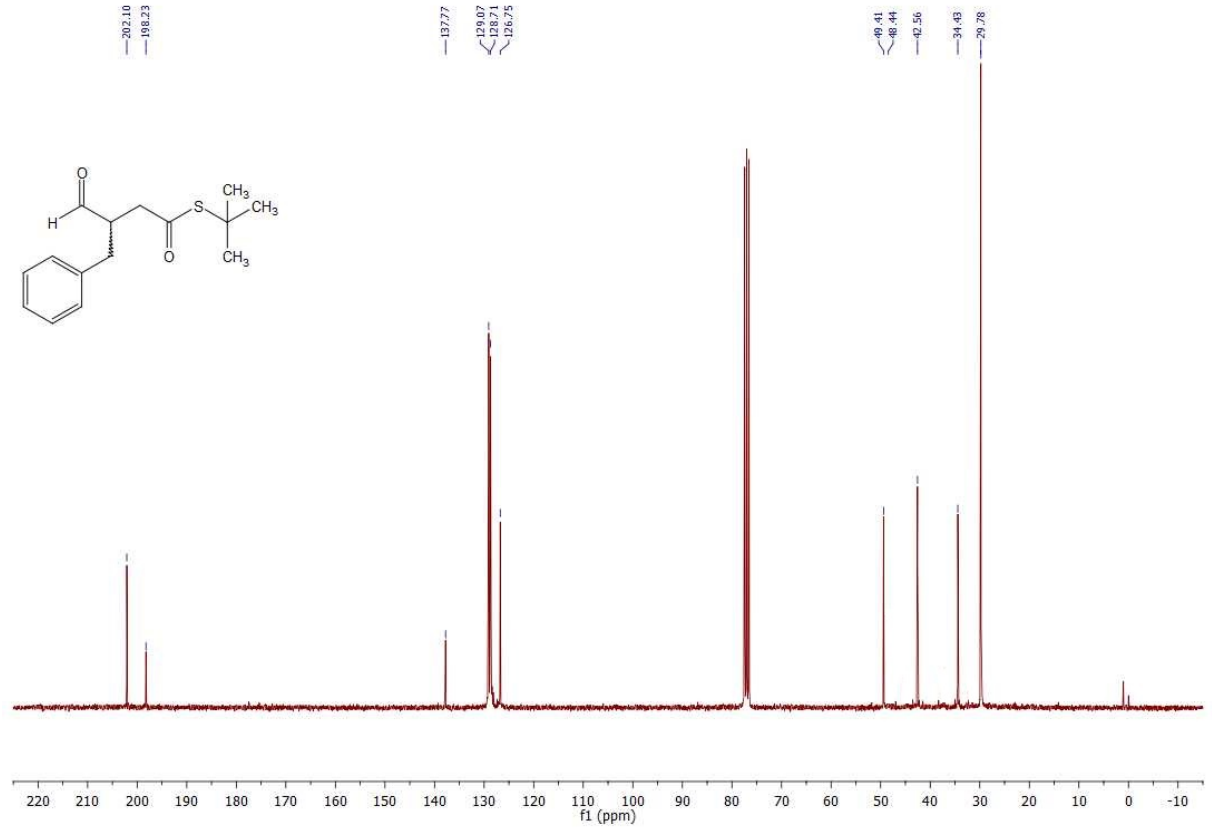
Pulse Sequence: NOESY
Solvent: CDC13



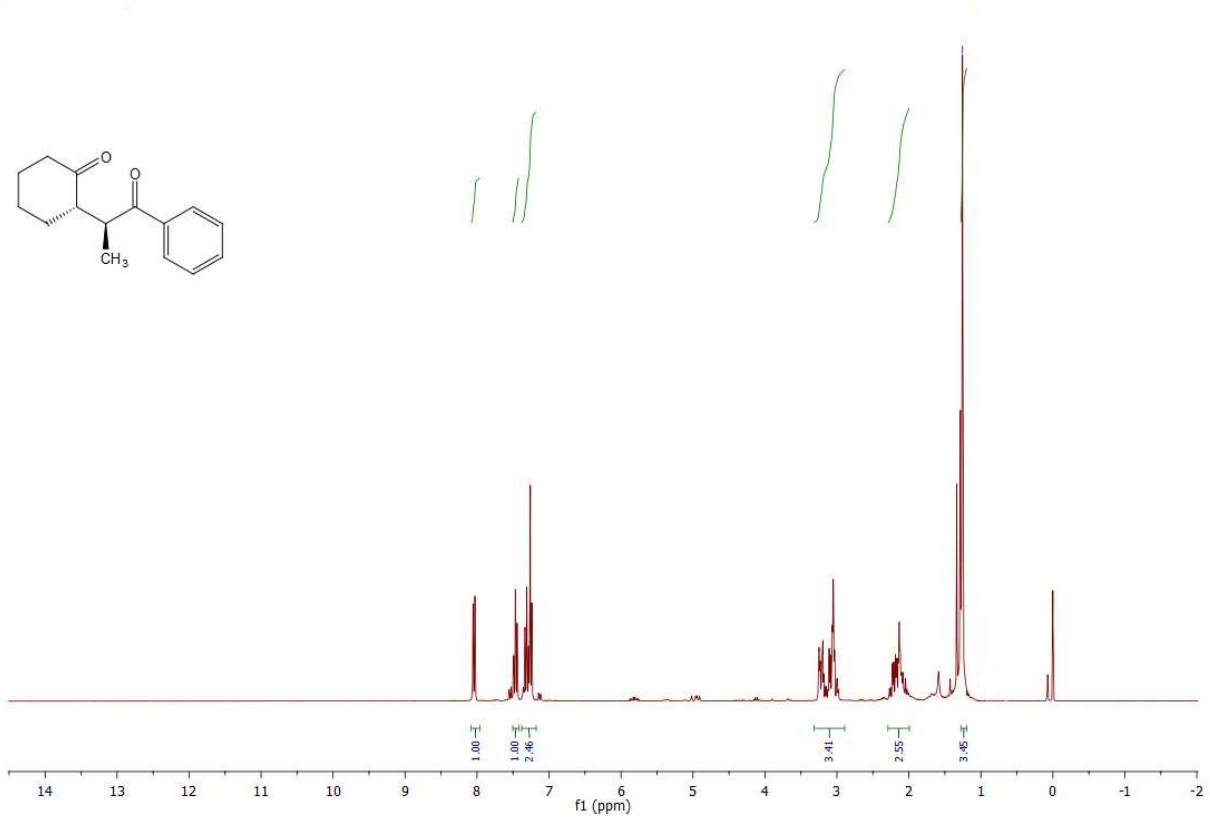
^{1}H NMR spectrum of **7a**



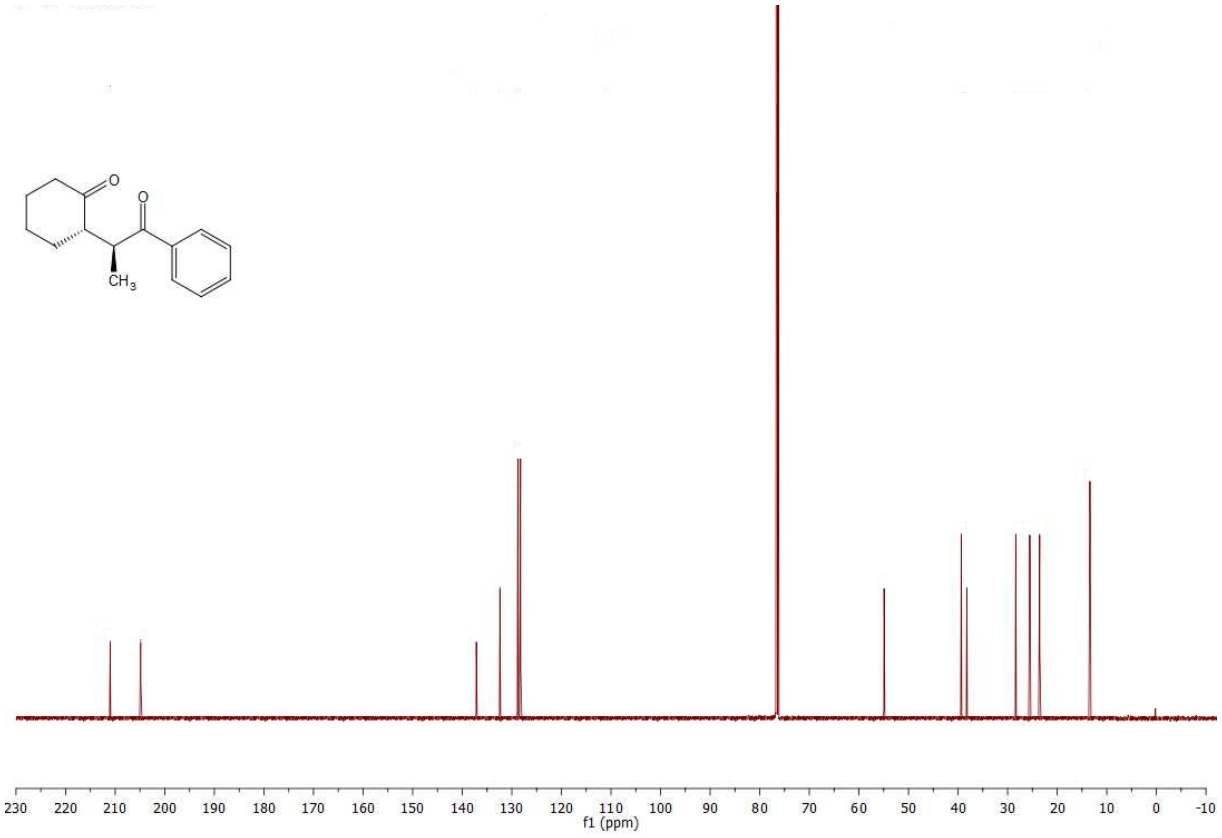
^{13}C spectrum of **7a**



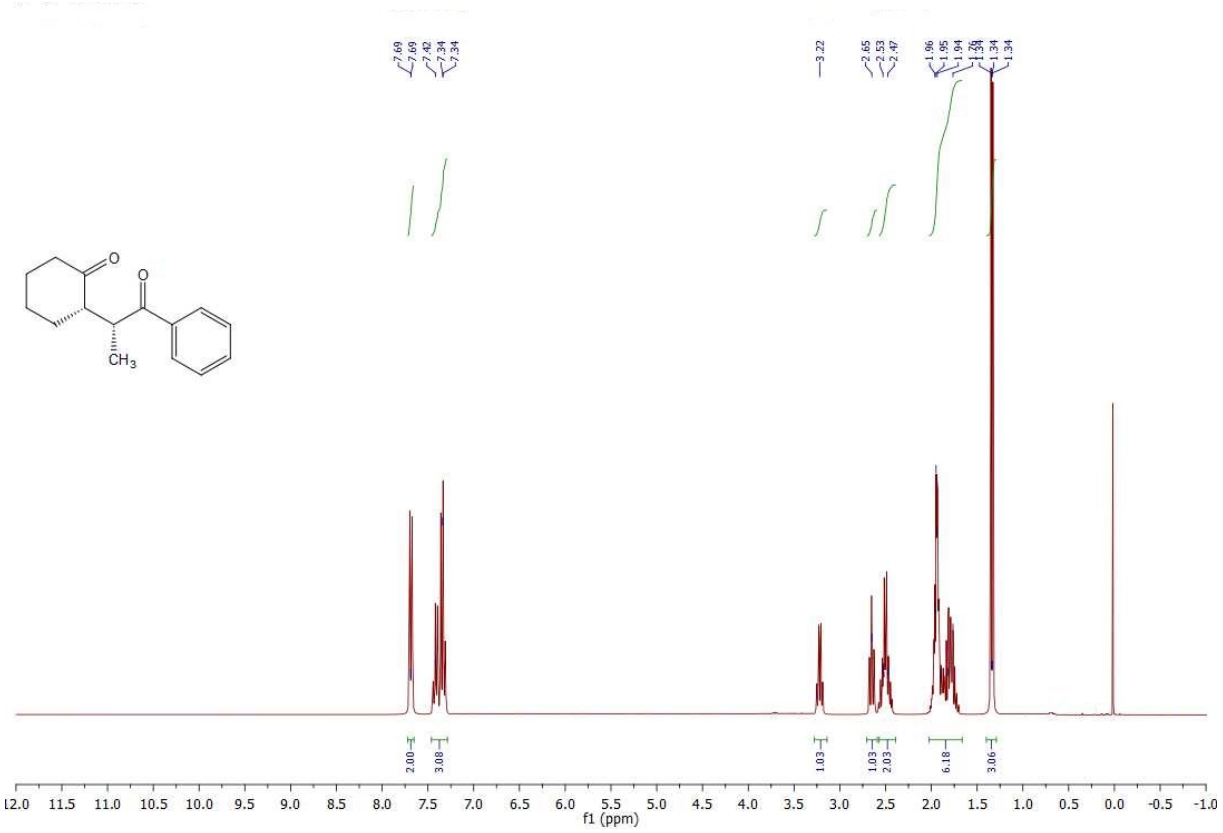
^{1}H NMR spectrum of (*S,S*)-**10b**



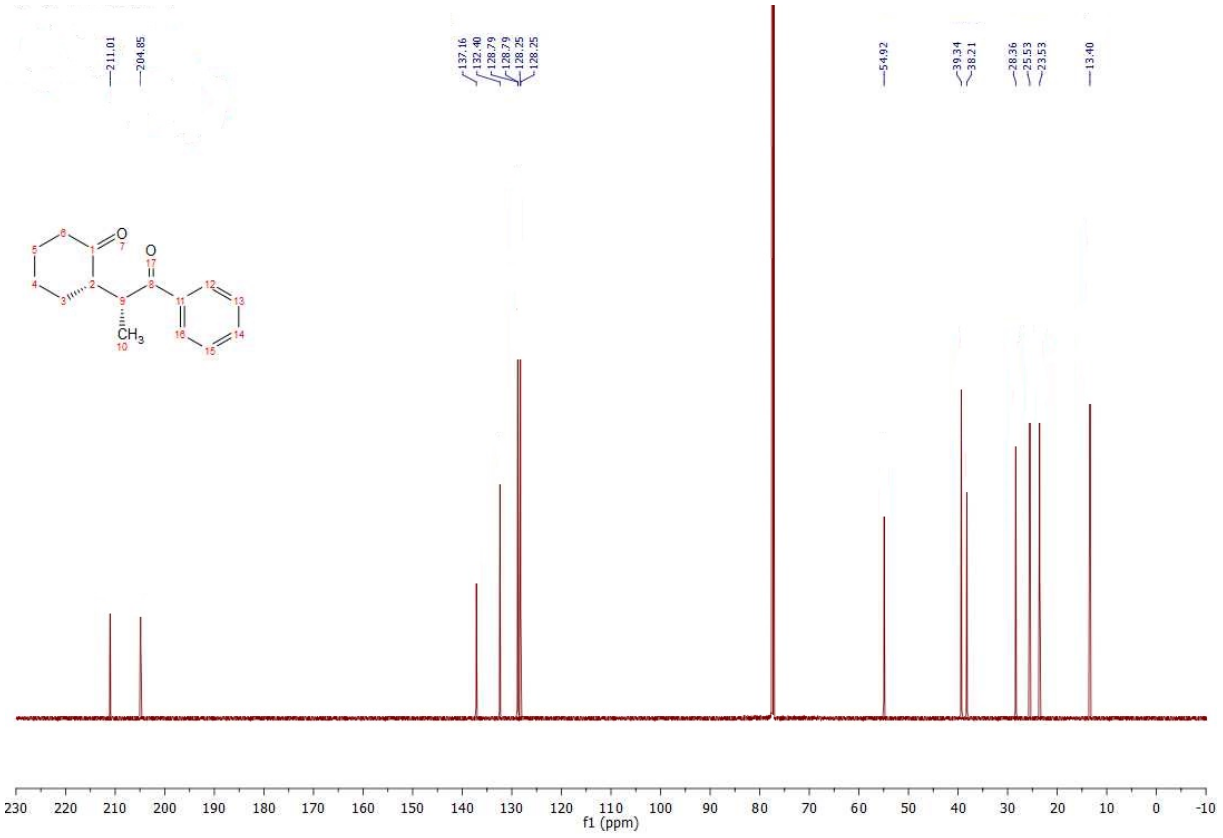
^{13}C spectrum of (*S,S*)-**10b**



^{1}H NMR spectrum of (*S,R*)-**10b**

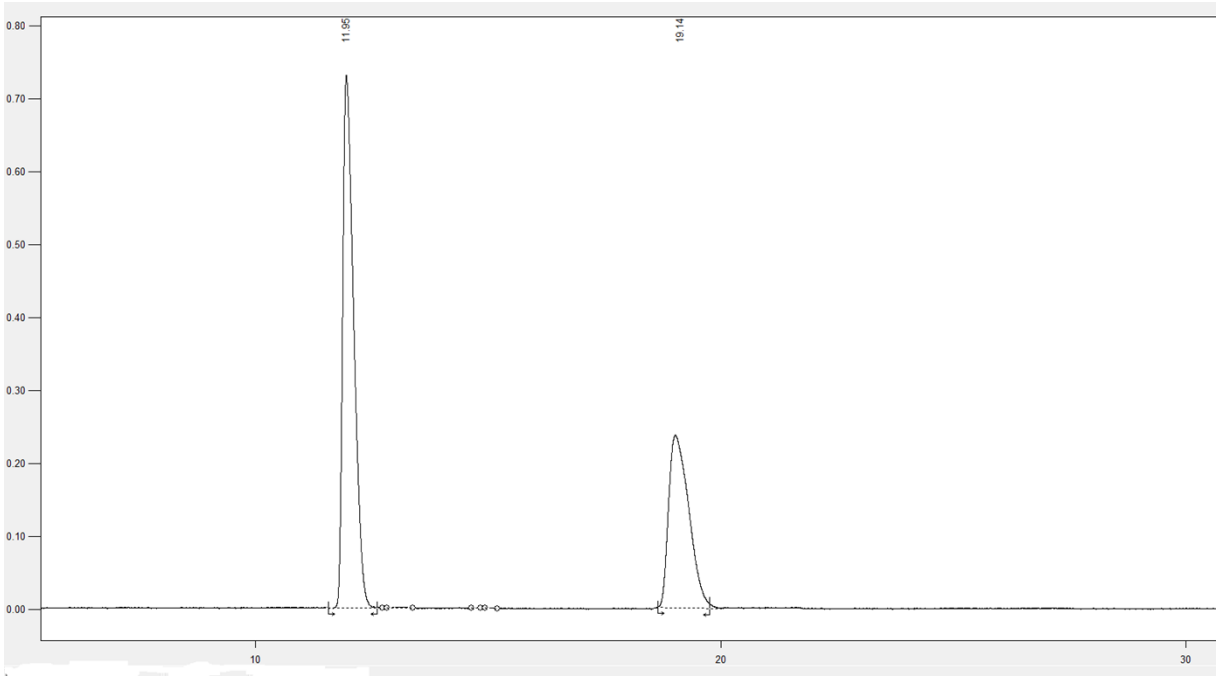


^{13}C spectrum of (*S,R*)-**10b**

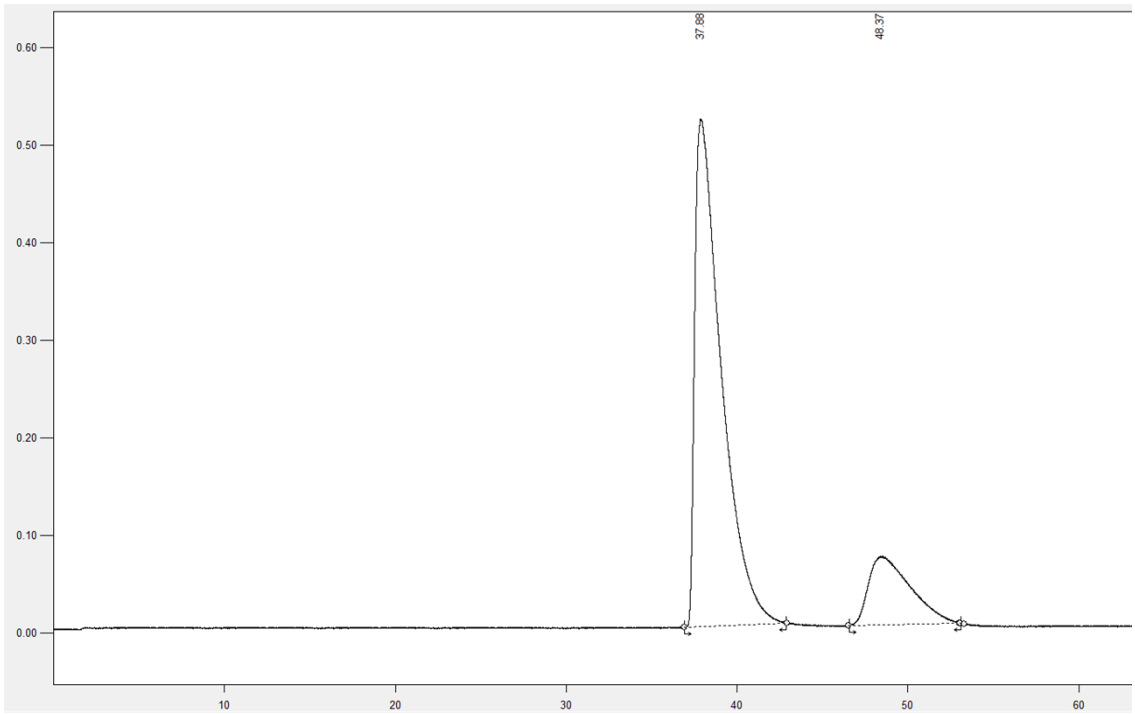


HPLC chromatograms

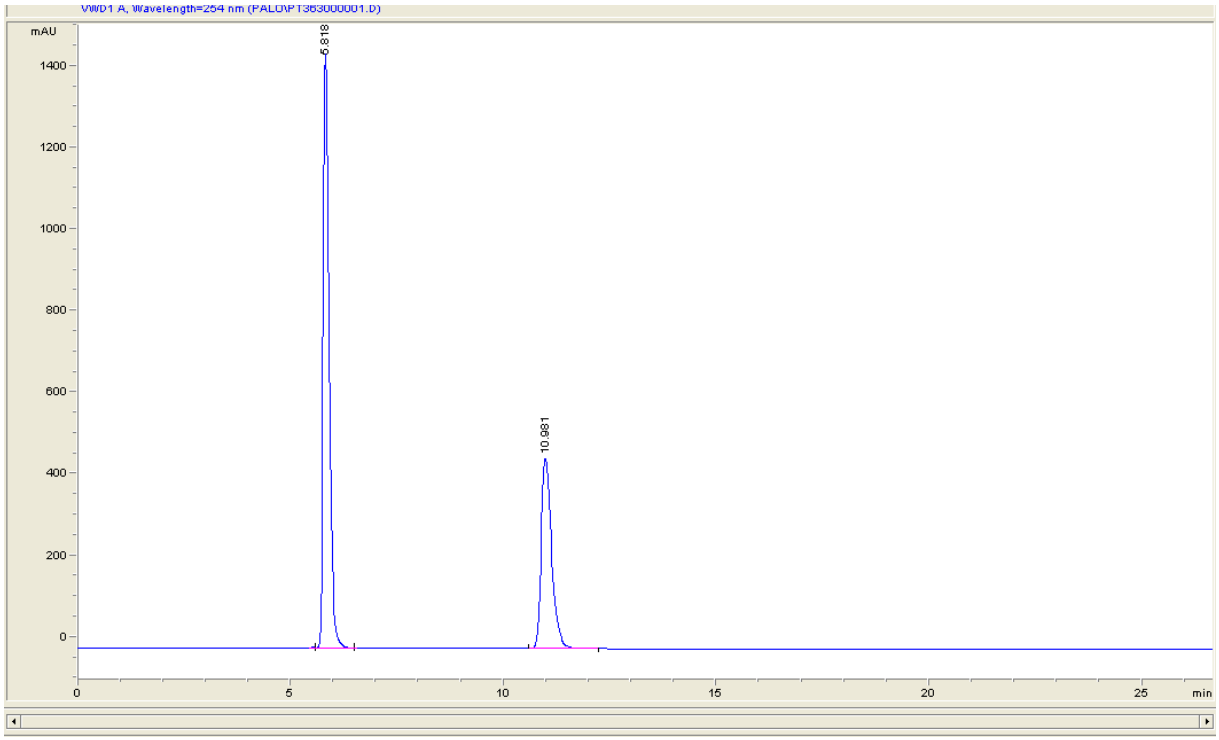
3a



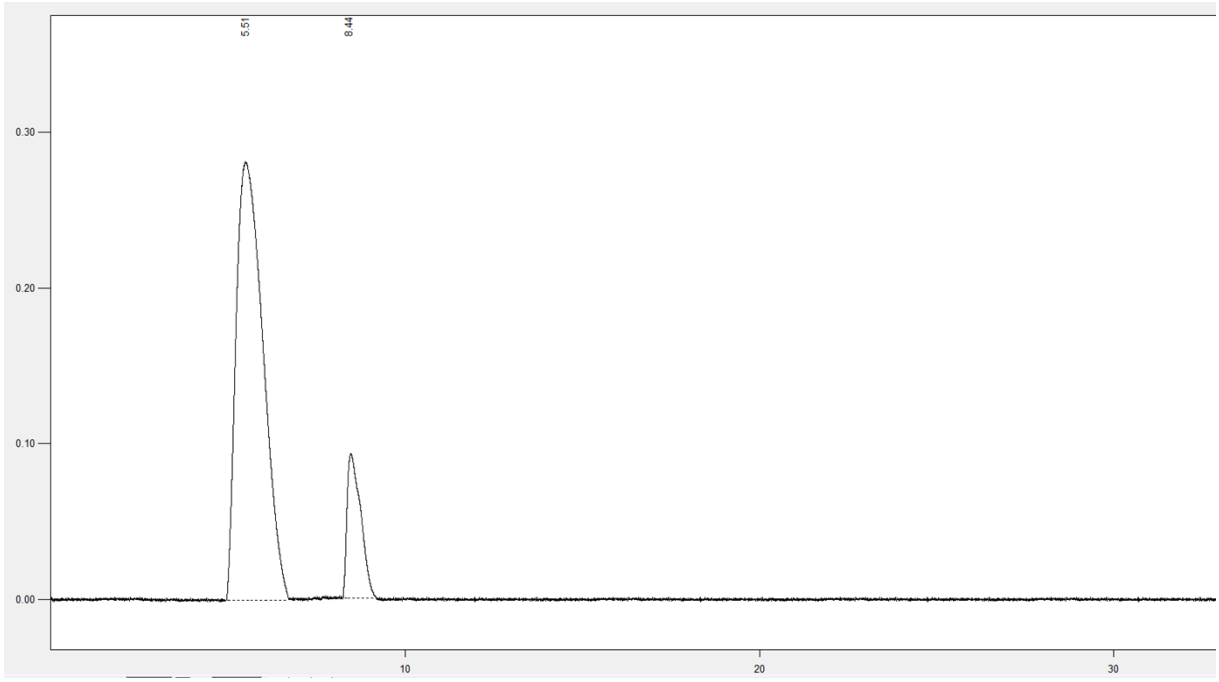
3b



3d


VWD1 A, Wavelength=254 nm (PALOVPT353000001.D)
mAU
1400
1200
1000
800
600
400
200
0
5.818
10.981
0
5
10
15
20
25
min

7a


5.51
8.44
0.30
0.20
0.10
0.00
10
20
30

Calculation of ECD spectra of 7a

The structures (*S*) and (*R*)-**7a** were drawn and optimized by AM1 method in Spartan program.[1] From the conformer distribution, ten most stable conformers were selected. From among these structures, four most stable conformers were pre-optimized in Spartan at HF/3-21G level.[2] The structures were then refined at RI-DFT[3] level using B3LYP/TZVP in Turbomole package.[4] ECD spectra of conformers 1-4 for each enantiomer were calculated by TD-DFT using M06/TZVP or B3LYP/TZVP (with Random phase approximation).[5]

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[1] Spartan ´08, Wavefunction, Inc., Irvine, CA

[2] Y. Shao, L. F. Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko, S. V. Levchenko, D. P. ONeill, R. A. D. Jr, R. C. Lochan, T. Wang, G. J. O. Beran, N. A. Besley, J. M. Herbert, C. Y. Lin, T. V. Voorhis, S. H. Chien, A. Sodt, R. P. Steele, V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson, B. Austin, J. Baker, E. F. C. Byrd, H. Dachsel, R. J. Doerksen, A. Dreuw, B. D. Dunietz, A. D. Dutoi, T. R. Furlani, S. R. Gwaltney, A. Heyden, S. Hirata, C.-P. Hsu, G. Kedziora, R. Z. Khalliulin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang, I. Lotan, N. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek, Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill, A. C. Simmonett, J. E. Subotnik, H. L. Woodcock III, W. Zhang, A. T. Bell and A. K. Chakraborty, *Phys. Chem. Chem. Phys*., 2006, **8**, 3172 - 3191.

[3] K. Eichkorn, O. Treutler, H. Öhm, M. Häser and R. Ahlrichs, *Chem. Phys. Lett*., 1995, **242**, 652-660; Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. *Theor. Chem. Acc*. 1997, **97**, 119-124.

[4] TURBOMOLE V6.6, TURBOMOLE GmbH, Karlsruhe, 2014.

[5] Furche, F.; Rappoport D. Ch. III of "Computational Photochemistry", Ed. by M. Olivucci, Vol. 16 of "Computational and Theoretical Chemistry", Elsevier, Amsterdam, 2005; Bauernschmitt, R.; Ahlrichs R. Chem. Phys. Letters 1996, 256, 454-464; Bauernschmitt, R.; Häser, M.; Treutler, O.; Ahlrichs; R. Chem. Phys. Letters 1997, 264, 573-701; Grimme, S.; Furche, F.; Ahlrichs, R. Chem. Phys. Letters 2002, 361, 321-328.
Kuehn, M.; Weigend, F. J. Chem. Theory Comput. 2013, 9, 5341-5348; van Setten, M.J.; Weigend, F.; Evers, F. J. Chem. Theory Comput. 2013, 9, 232-246; Bates, J. E.; Furche, F. J. Chem. Phys. 2012, 137, 164105.
Kuehn, M.; Weigend, F. Chem. Phys. Chem. 2011, 12, 3331-3336.