Supporting Information

Reactions of linear conjugated dienone structures with arenes under superelectrophilic activation. Experimental and theoretical study of intermediate multicentered electrophilic species

Matvey A. Kochurin,[a] Alina R. Ismagilova,[b] Dmitry N. Zakusilo,[b] Olesya V. Khoroshilova,[a] Irina A. Boyarskaya,[a] Aleksander V. Vasilyev[a,b] *

[a]*Department of Organic Chemistry, Institute of Chemistry, Saint Petersburg State University, Universitetskaya nab., 7/9, Saint Petersburg, 199034, Russia*

[b]*Department of Chemistry, Saint Petersburg State Forest Technical University, Institutsky per., 5, Saint Petersburg , 194021, Russia*

Corresponding Author

* E-mails: aleksvasil@mail.ru, a.vasilyev@spbu.ru (Aleksander V. Vasilyev)

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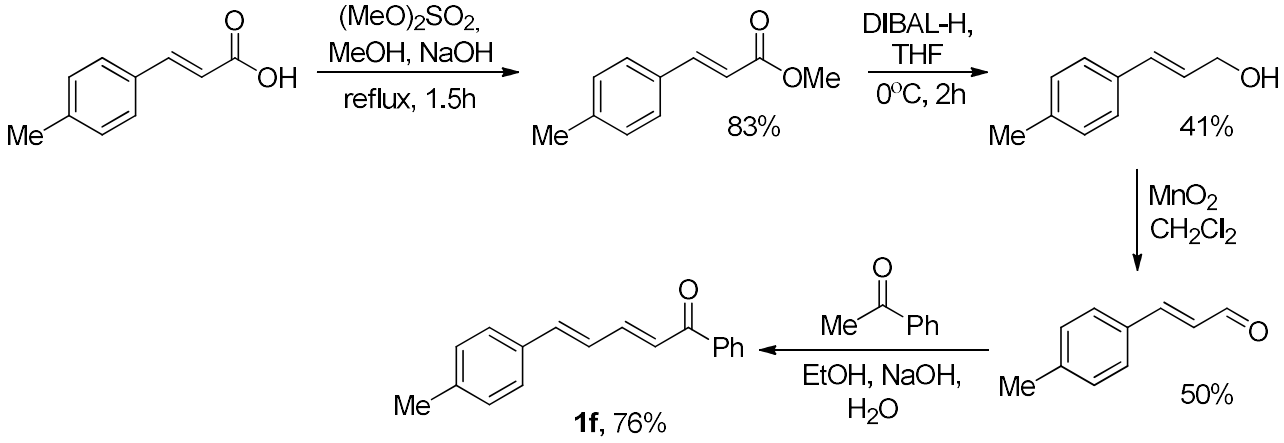
I. Synthesis and characterization of starting compounds 1a-h

Synthesis of 1,5-diarylpenta-2,4-dien-1-ones (1a-e)

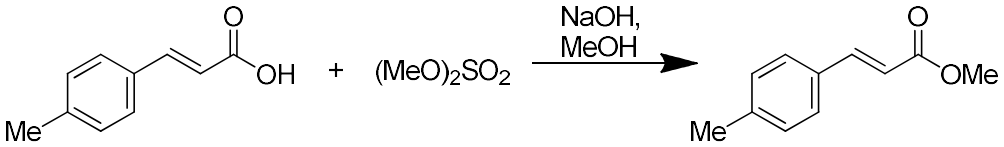
39.5 mg (0.98 mmol) of NaOH, 3 ml of water and 2 ml of EtOH were placed in a round bottom 20 ml flask with stirring on a magnetic stirrer. 180 mg (1.5 mmol, 1.1 eq) of the corresponding acetophenone (**1a**) were added to the reaction mixture. Then 180 mg (1.37 mmol) of cinnamic aldehyde (or 221 mg (1.37 mmol) of 3-(2-methoxyphenyl)prop-2-enal for synthesis of **1e**) were added in portions. The reaction mixture was stirred for 36 h at room temperature, the resulting precipitate was filtered on a Büchner funnel and recrystallized from EtOH. The reaction products yields were 76-95%.

Synthesis of 5-(4-methylphenyl)-1-phenylpent-2,4-dien-1-one (1f)

The synthesis of **1f** was carried out in several stages according to scheme below.

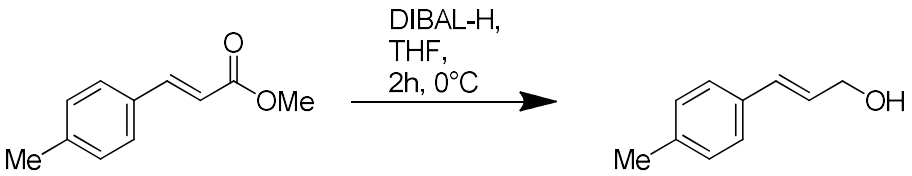


Synthesis of methyl (*E*)-3-(4-methylphenyl)prop-2-enoate.



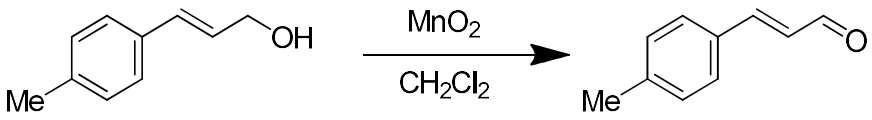
Solution of 1.65 g (10 mmol) (*E*)-3-(4-methylphenyl)prop-2-enoic acid in 15 ml of MeOH was prepared under refluxing in a round bottom 20 ml flask equipped with condenser and calcium chloride tube. The resulting solution was cooled to ~30ºC and of solution of 0.6 g (15 mmol) of NaOH and 15 ml of MeOH were added. The reaction mixture was refluxing till homogenization, then it was cooled down to ~ 40ºC and 2.25 ml (3 g, 24 mmol) of $(MeO)_2SO_2$ were added. The reaction mixture was reflixing for 1.5 h. Then the mixture was cooled to room temperature and poured into 100 ml of H_2O. The precipitated white solid was filtered off and washed with H_2O (2×10 ml). The yield of the target compound was1.5 g (83%).

Synthesis of (*E*)-3-(4-methylphenyl)prop-2-en-1-ol.



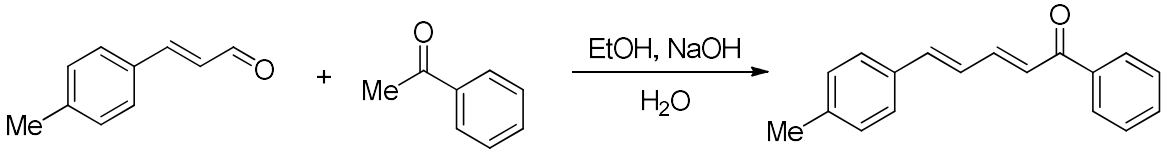
30 ml of THF and 1.5 g (8.52 mmol) of methyl (*E*)-3-(4-methylphenyl)prop-2-enoate were placed in a three-necked 100 ml round-bottomed flask equipped in 1-st throat with an argon inlet, in the 2-nd with an argon outlet with bubbler and in the 3r-d throat with a septum. The obtained solution was cooled in an ice bath to 0ºC under the argon atmosphere. Then 20.5 ml (2.9 g, 20.45 mmol) of a 1M solution of DIBAL-H in CH_2Cl_2 was added portion wise to the mixture. In the course of the synthesis after 1h, 1 ml (0.89 g, 1 mmol) of a 1M solution of DIBAL-H in CH_2Cl_2 was additionally added. The reaction mixture was stirred at 0ºC for 2 h. Then it was poured into 150 ml of H_2O, extracted with Et_2O (3×100 ml), combined extracts were dried with Na_2SO_4 and the solvent was evaporated under reduced pressure. The yield of the target compound was 0.62 g (41%).

Synthesis of (*E*)-3-(4-methylphenyl)prop-2-enal.



A mixture of (*E*)-3-(4-methylphenyl)prop-2-en-1-ol (620 mg, 4.18 mmol), manganese dioxide MnO_2 (2.92 g, 33.49 mmol) and dichloromethane (40 ml) was stirred at room temperature for 5 days. The reaction mass was filtered through 20 mm layer of silica gel in a glass filter, silica gel was washed with dichloromethane (3×20 ml). The solvent was evaporated under reduced pressure. The residue was dried in vacuum. The yield of the target compound was 350 mg (50%).

Synthesis of 5-(4-methylphenyl)-1-phenylpent-2,4-dien-1-one (1f)



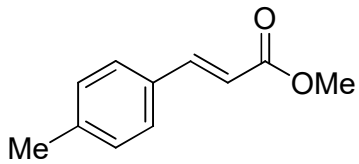
The compound **1f** was obtained according to the general procedure for the synthesis of dienones **1a-e** as described above.

Synthesis of 5-phenylpent-2,4-dienoic acid (1g)

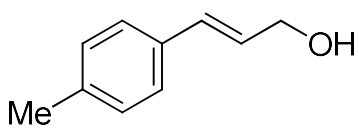
A solution of malonic acid 4.7 g (45 mmol), 5.25 ml (38 mmol) of cinnamic aldehyde in 10 ml of pyridine containing two drops of piperidine was stirred at 100°C for 4 h. Then it was poured into concentrated hydrochloric acid (30 ml), the formed precipitate was filtered off and recrystallized from ethanol. The yield of the target compound was 4 g (60%).

Synthesis of methyl 5-phenylpent-2,4-dienoate (1h)

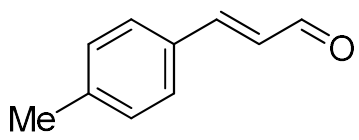
A mixture of 5-phenylpent-2,4-dienoic acid **1g** (1 g, 5.7 mmol) and $NaHCO_3$ (0.48 g, 5.7 mmol, 1 eq) in MeOH (20 ml) was boiled for 1 h in a round-bottom 50 ml flask equipped with a reflux condenser and a calcium chloride tube until the acid was completely dissolved. The solution was cooled to room temperature, and $(MeO)_2SO_2$ (1 ml, 6.1 mmol) was added. The reaction mixture was refluxing for 1 h, cooled and poured into 150 ml of Et_2O. The ether solution was consequently washed with water (2×50 ml), saturated aqueous solution of NaOH (3×50 ml), with water (2×50 ml), dried with Na_2SO_4. The solvent was distilled off under reduced pressure. The yield of the target compound was 0.96 g (90%).



Methyl (E)-3-(4-methylphenyl)propenoate.[1] Colorless solid. M.p. 55-57ºC, **^{1}H NMR** ($CDCl_3$, 400 MHz) δ, ppm: 2.37 (s, 3H, Me), 3.80 (s, 3H, MeO), 6.39 (d, 1H, *J* 16 Hz, =CH-), 7.19 (d, 2H, *J* 8 Hz), 7.42 (d, 2H, *J* 8 Hz), 7.67 (d, 1H, *J* 16 Hz, =CH-).

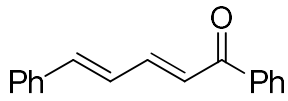


3-(4-Methylphenyl)prop-2-en-1-ol.[2] Oil. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ, ppm: 2.34 (s, 3H, Me), 4.31 (dd, 2H, *J* 6, 1 Hz, CH_2), 6.32 (dt, 1H, *J* 16, 6 Hz, =CH-), 6.59 (d, 1H, *J* 16 Hz, =CH), 7.13 (d, 2H, *J* 8 Hz), 7.29 (d, 2H, *J* 8 Hz). **^{13}C NMR** ($CDCl_3$, 100 MHz) δ, ppm: 21.2, 63.8, 126.4, 127.5, 129.3, 131.2, 133.9, 137.5.

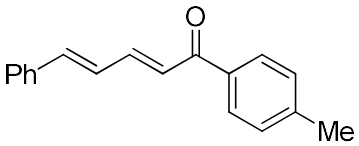


3-(4-Methylphenyl)propenal.[3] Yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ, ppm: 2.40 (s, 3H, Me), 6.68 (dd, 1H, -CH=, *J* 16, 8 Hz), 7.24 (d, 2H, *J* 8 Hz), 7.46 (m, 3H), 9.69 (d, 1H, *J* 8 Hz). **^{13}C NMR** ($CDCl_3$, 100 MHz) δ, ppm: 21.7, 127.9, 128.7, 130.0, 131.5, 142.1, 153.0, 193.9 (-CHO).

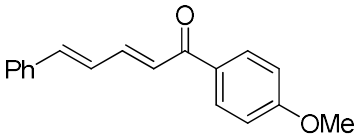
[1] Myrboh B., Ila H., Junjappa H. *J. Org. Chem.* **1983**. *48*, 26,5327–5332.
[2] Solladie-Cavallo A. *J. Org. Chem*. **1994**. *59*, 11, 3241.
[3] Attenburrow J., Cameron A.F.B., Chapman J.H., et al. *J. Chem. Soc.* **1952**. 1094.



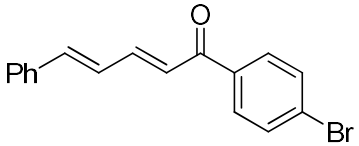
1,5-Diphenylpent-2,4-dien-1-one (**1a**).[4] Yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ, ppm: 7.02-7.04 (m, 2H), 7.10 (d, 1H, *J* 15 Hz), 7.33-7.40 (m, 3H), 7.47-7.52 (m, 4H), 7.55-7.64 (m, 2H), 7.97-8.00 (m, 2H). **^{13}C NMR** ($CDCl_3$, 100 MHz) δ, ppm: 125.5, 127.0, 127.3, 128.4, 128.6, 128.9, 129.2, 132.7, 136.2, 138.3, 141.9, 144.8, 190.5.



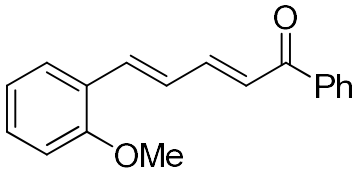
1-(4-Methylphenyl)-5-phenylpent-2,4-dien-1-one (**1b**).[5] Yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ, ppm: 2.43 (s, 3H, Me), 7.01-7.03 (m, 2H), 7.10 (d, 1H, *J* 15 Hz), 7.26-7.39 (m, 5H), 7.49-7.51 (m, 2H), 7.60 (ddd, 1H, *J* 15, 8, 3 Hz), 7.89-7.91 (m, 2H). **^{13}C NMR** ($CDCl_3$, 100 MHz) δ, ppm: 21.7, 125.5, 127.1, 127.3, 128.6, 128.9, 129.2, 129.3, 135.7, 136.2, 141.6, 143.5, 144.4, 190.0.



1-(4-Methoxyphenyl)-5-phenylpent-2,4-dien-1-one (**1c**).[6] Yellow solid. M. p. 88-90 ºC. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ, ppm: 3.88 (s, 3H, Me), 6.98 (m, 4H), 7.11 (d, 1H, *J* 15 Hz), 7.34 (m, 3H), 7.51 (m, 2H), 7.60 (m, 1H). **^{13}C NMR** ($CDCl_3$, 100 MHz) δ, ppm: 55.5, 113.8, 125.3, 127.1, 127.2, 128.9, 129.1, 130.7, 131.2, 136.3, 141.4, 144.0, 163.4, 188.7.



1-(4-Bromophenyl)-5-phenylpent-2,4-dien-1-one (**1d**).[7] Yellow solid substance. M. p. 140-142 ºC. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ, ppm: 7.08 (m, 3H), 7.35 (m, 3H), 7.50 (m, 2H), 7.60 (m, 3H), 7.84 (m, 2H). **^{13}C NMR** ($CDCl_3$, 100 MHz) δ, ppm: 124.8, 126.8, 127.4, 127.7, 128.9, 129.4, 129.9, 131.9, 136.0, 137.0, 142.4, 145.4, 189.3.



5-(2-Methoxyphenyl)-1-phenylpent-2,4-dien-1-one (**1e**).[8] Yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ, ppm: 3.88 (s, 3H), 6.90 (d, 1H, *J* 8 Hz), 6.96 (t, 1H, *J* 7 Hz), 7.04-7.12 (m, 2H), 7.27-7.32 (m, 1H), 7.35-7.39 (m, 1H), 7.48 (t, 2H, *J* 7 Hz), 7.52-7.57 (m, 2H), 7.63 (dd, 1H, *J* 15, 11 Hz), 7.96-7.98 (m, 2H). **^{13}C NMR** ($CDCl_3$, 100 MHz) δ, ppm: 55.5, 111.2, 120.8, 124.9, 125.1, 127.6, 128.4, 128.6, 130.4, 132.5, 137.3, 138.4, 146.1, 157.6, 190.8.

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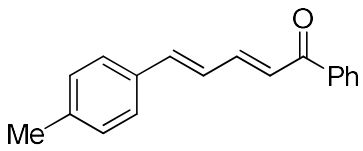
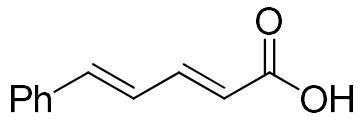
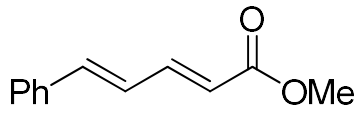
[4] Ratheesh Kumar V.K., Gopidas K.R. *Tetrahedron Lett.*. **2011**. *52*, 3102–3105.
[5] Santos C.M.M., Silva A.M.S., Cavaleiro J.A.S., et al. *Eur. J. Org. Chem.* **2007**. *17*, 2877–2887.
[6] Pal, R.; Mandal T., K.; Guha, C.; Mallik A.K. *Indian Chem. Soc*. **2012**. *88*, 11, 2012.
[7] Oliva C.G., Silva A.M.S., Resende D.I.S.P., et al. *Eur. J. Org. Chem*. **2010**. 3449–3458.
[8] Li Z., Song W. *J. Chem. Res*. **2018**. *42*, 7, 347–349.



5-(4-Methylphenyl)-1-phenylpent-2,4-dien-1-one (**1f**).[9] Light-yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ, ppm: 2.37 (s, 3H, Me), 6.69 (m, 2H), 7.07 (d, 1H, *J* 15 Hz), 7.18 (d, 2H, *J* 8 Hz), 7.40 (d, 2H, *J* 8 Hz), 7.49 (t, 2H, *J* 8 Hz), 7.6 (m, 2H), 7.97 (d, 2H, *J* 7 Hz). **^{13}C NMR** ($CDCl_3$, 100 MHz) δ, ppm: 21.5, 125.1, 126.2, 127.4, 128.5, 128.7, 129.7, 132.7, 133.6, 138.5, 139.7, 142.2, 145.3, 190.7.



5-Phenylpent-2,4-diene acid (**1g**).[10] Solid substance. M. p. 164-167 ºC. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ, ppm: 6.01 (d, 1H, *J* 15 Hz, CH), 6.88-6.98 (m, 2H), 7.31-7.58 (m, 4H), 7.49 (d, 1H, *J* 7 Hz, CH). **^{13}C NMR** ($CDCl_3$, 125 MHz) δ, ppm: 120.2, 126.0, 127.3, 128.9, 129.3, 135.8, 141.6, 146.9, 171.9. **MS**, *m/z* ($I_{rel.}$, %): 174 M^+ (25),129 (100),115 (8), 102 (8),77 (9), 51 (8).



Methyl 5-phenylpent-2,4-dienoate (**1h**).[11] Solid substance. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ, ppm: 3.77 (s, 3H, MeO), 6.0 (d, 1H, *J* 15 Hz, =CH), 6.87-6.92 (m, 2H, CH), 7.31-7.37 (m, 3H), 7.43-7.48 (m, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz) δ, ppm: 51.6, 120.9, 126.3, 127.2, 128.9, 129.1, 136.1, 140.6, 144.9, 167.9; **MS**, *m/z* (Irel., %): 188 M^+ (25), 157 (20), 129 (100), 115 (8), 102 (8), 77 (9), 51 (8).

[9] Santos C.M.M., Silva A.M.S., Cavaleiro J.A.S., et al. *Eur. J. Org. Chem.* **2007**. 2877–2887.
[10] Kokotos G., Hsu Y., Burke J.E., et al. *J. Med. Chem*. **2010**. *53*, 9, 3602–3610.
[11] El-batta A., Jiang C., Zhao W., et al. *J. Org. Chem*. **2007**. *72*, 5244–5259.

II. Copies of NMR spectra of compounds

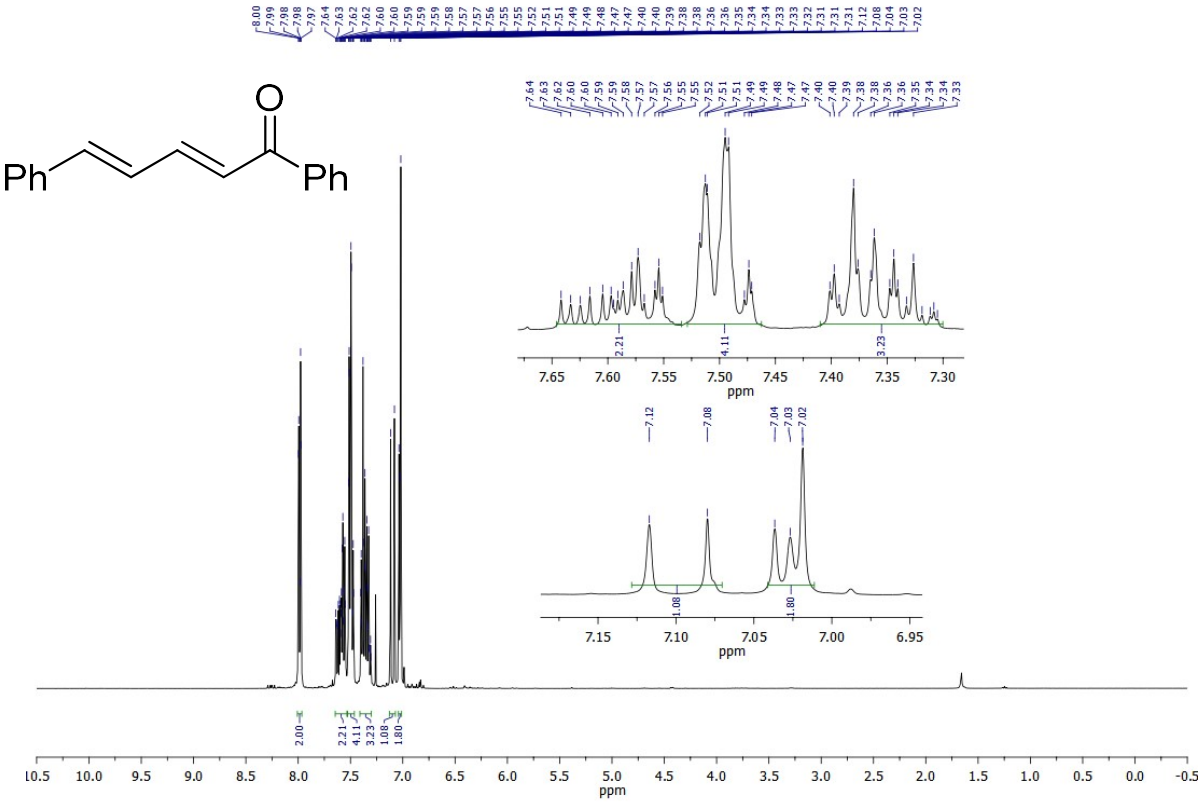


Fig. S1. ^{1}H NMR spectrum of the compound **1a** ($CDCl_3$, 400 MHz).

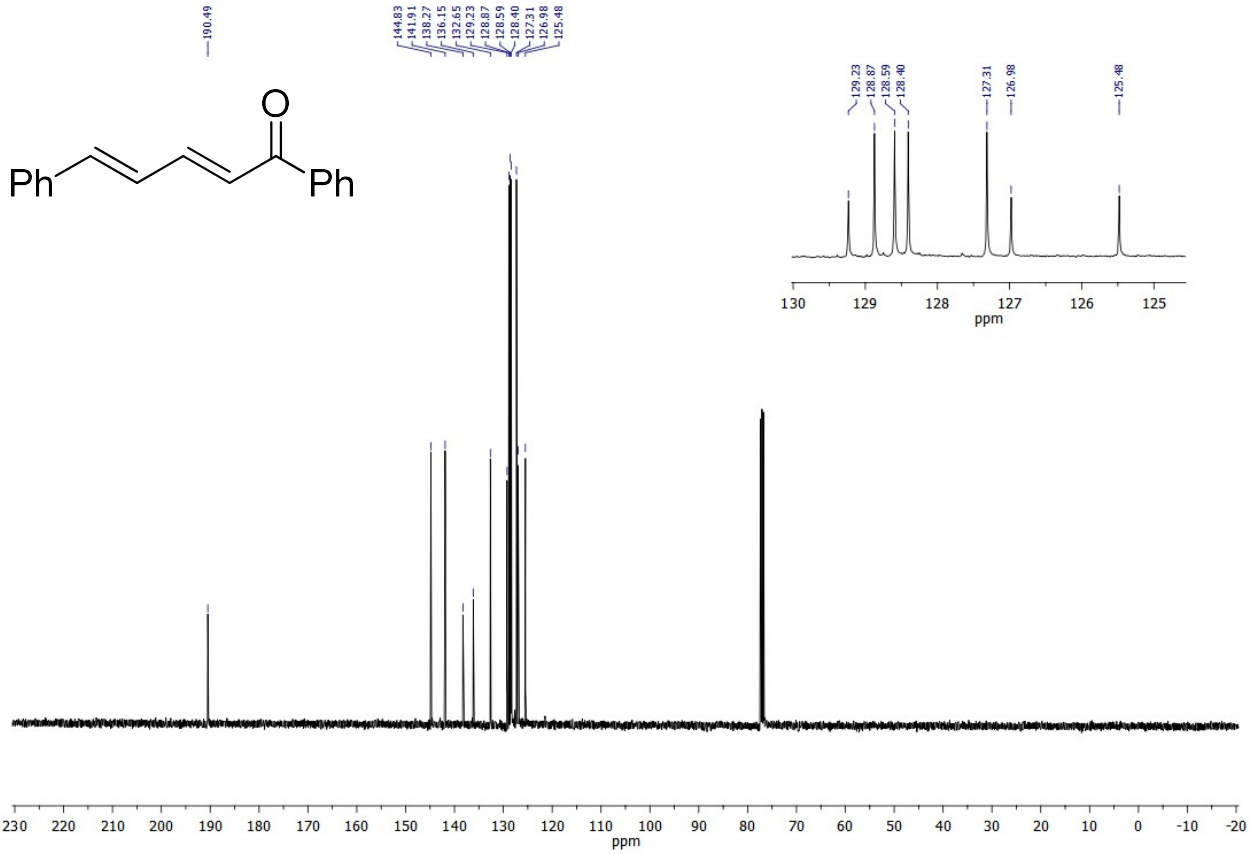


Fig. S2. ^{13}C NMR spectrum of the compound **1a** ($CDCl_3$, 101 MHz).

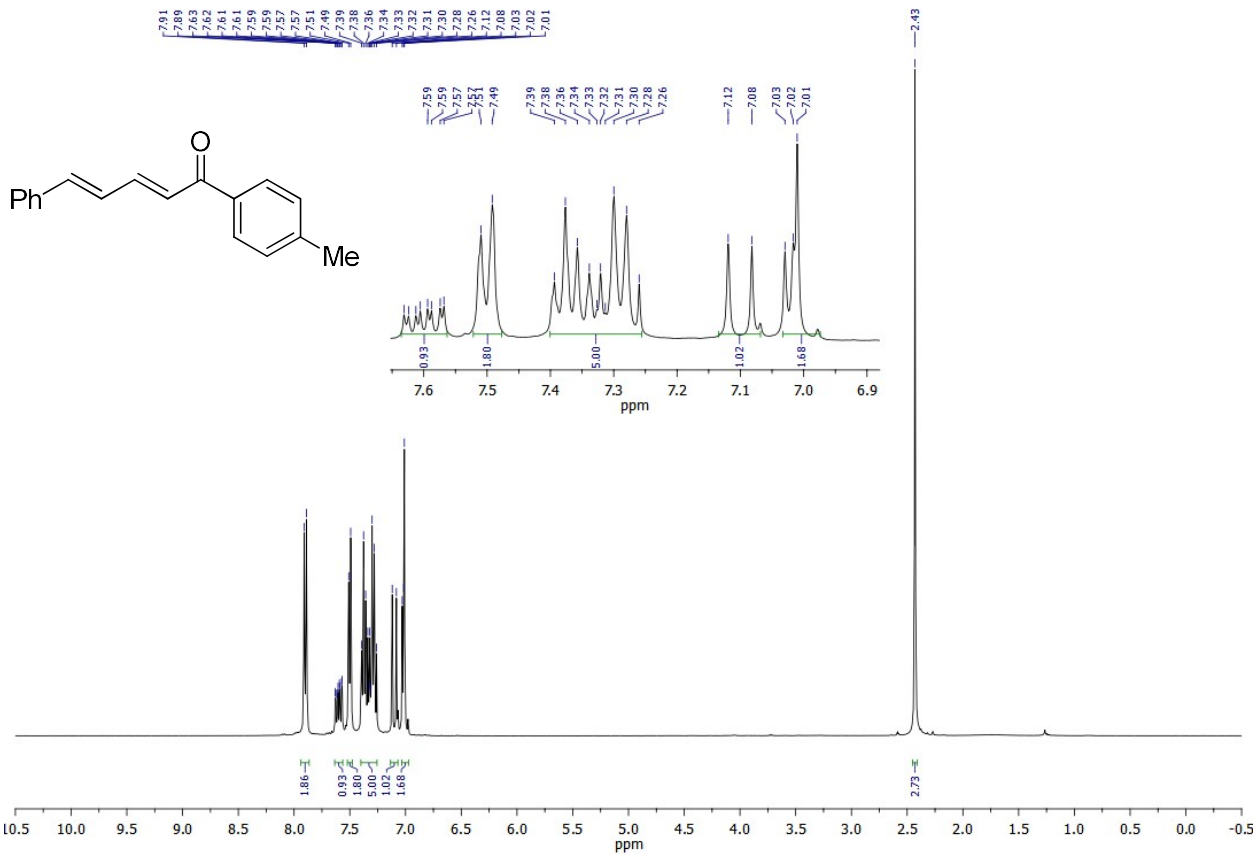


Fig. S3. ^{1}H NMR spectrum of the compound **1b** ($CDCl_3$, 400 MHz).

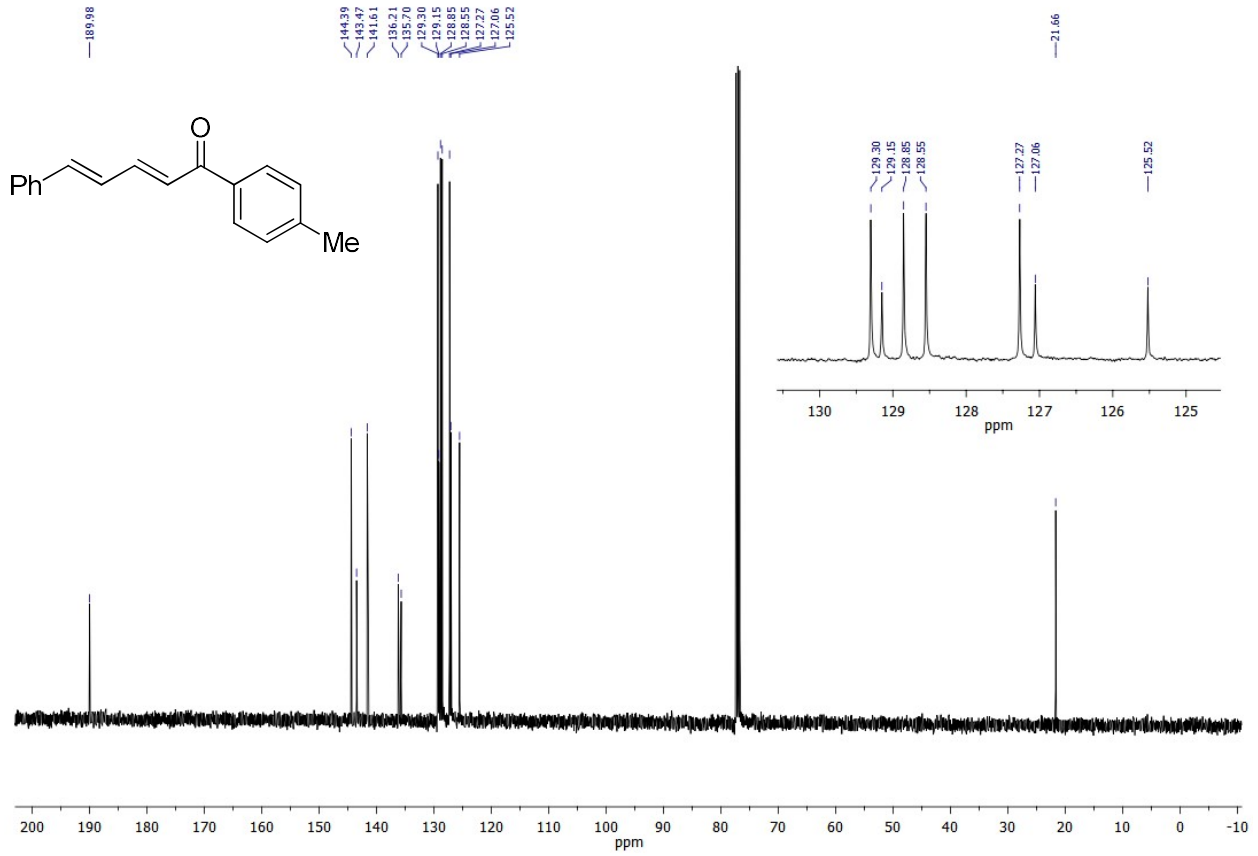


Fig. S4. ^{13}C NMR spectrum of the compound **1b** ($CDCl_3$, 101 MHz).

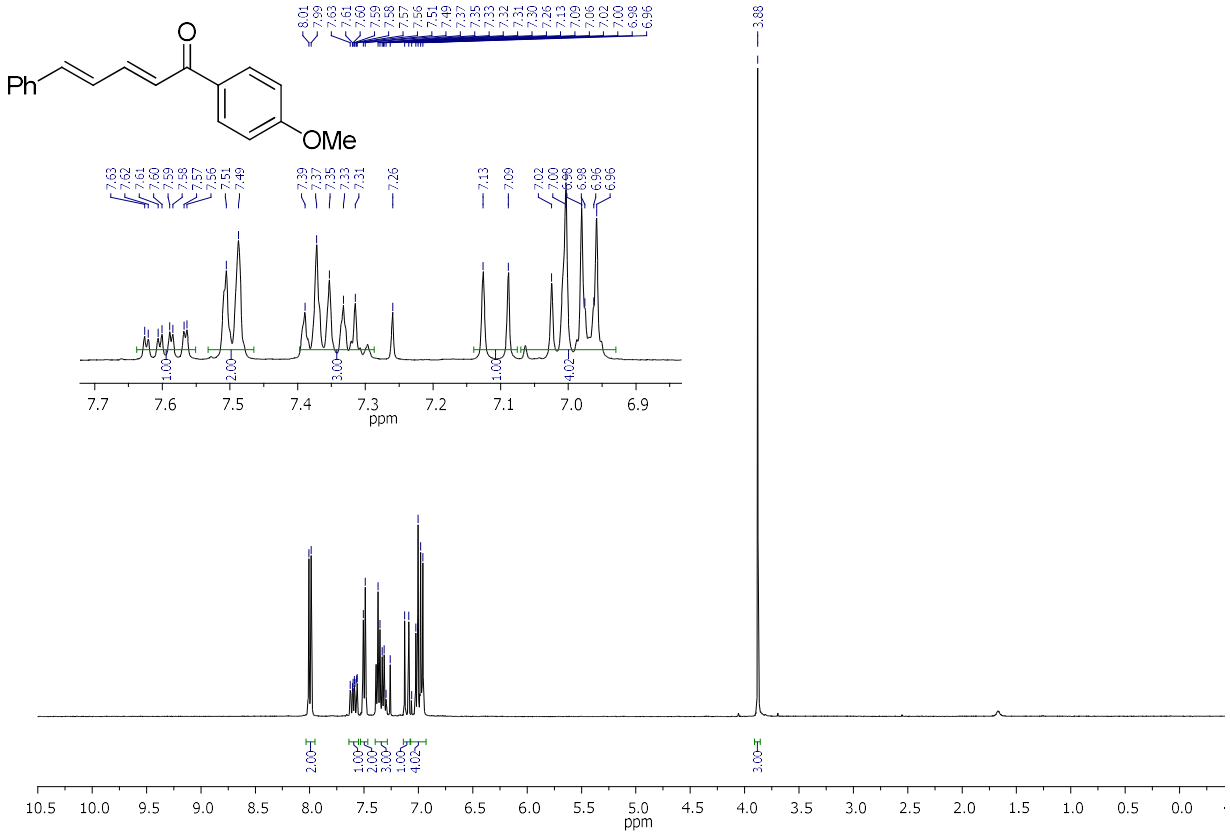


Fig. S5. ^{1}H NMR spectrum of the compound **1c** ($CDCl_3$, 400 MHz).

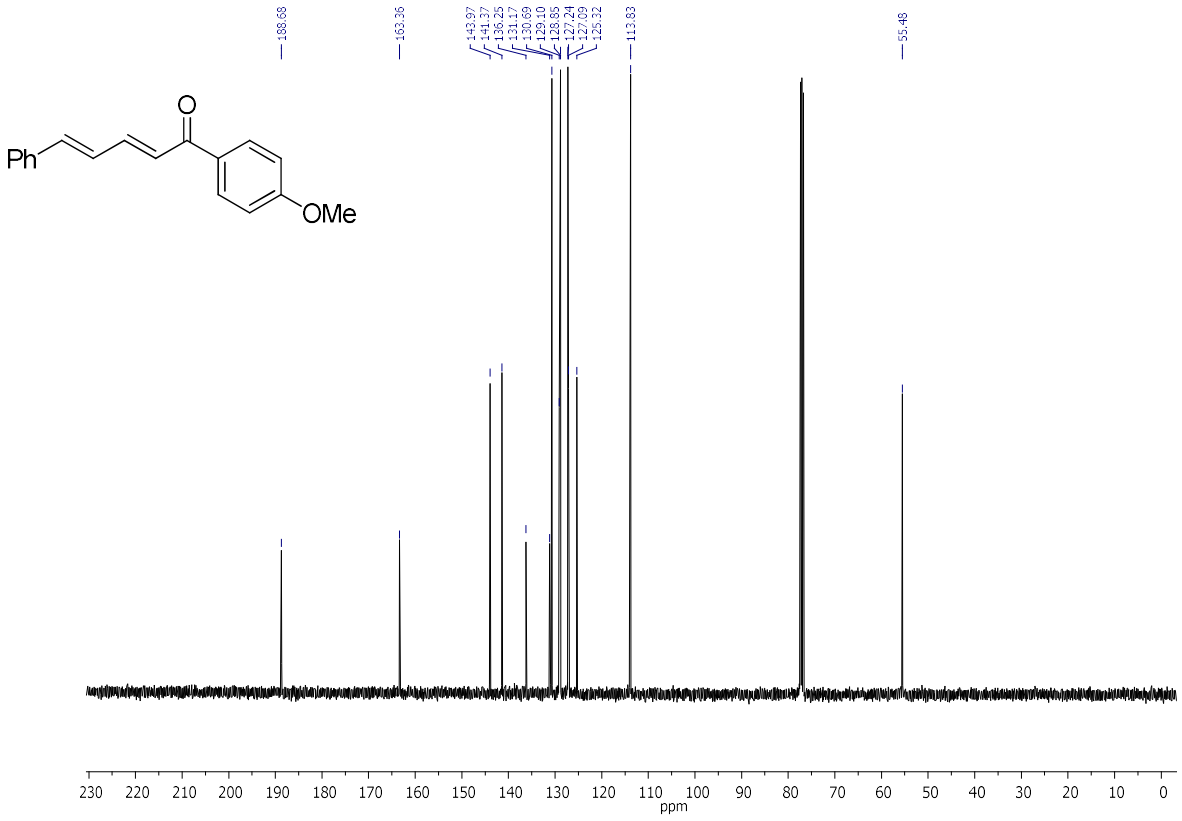


Fig. S6. ^{13}C NMR spectrum of the compound **1c** ($CDCl_3$, 101 MHz).

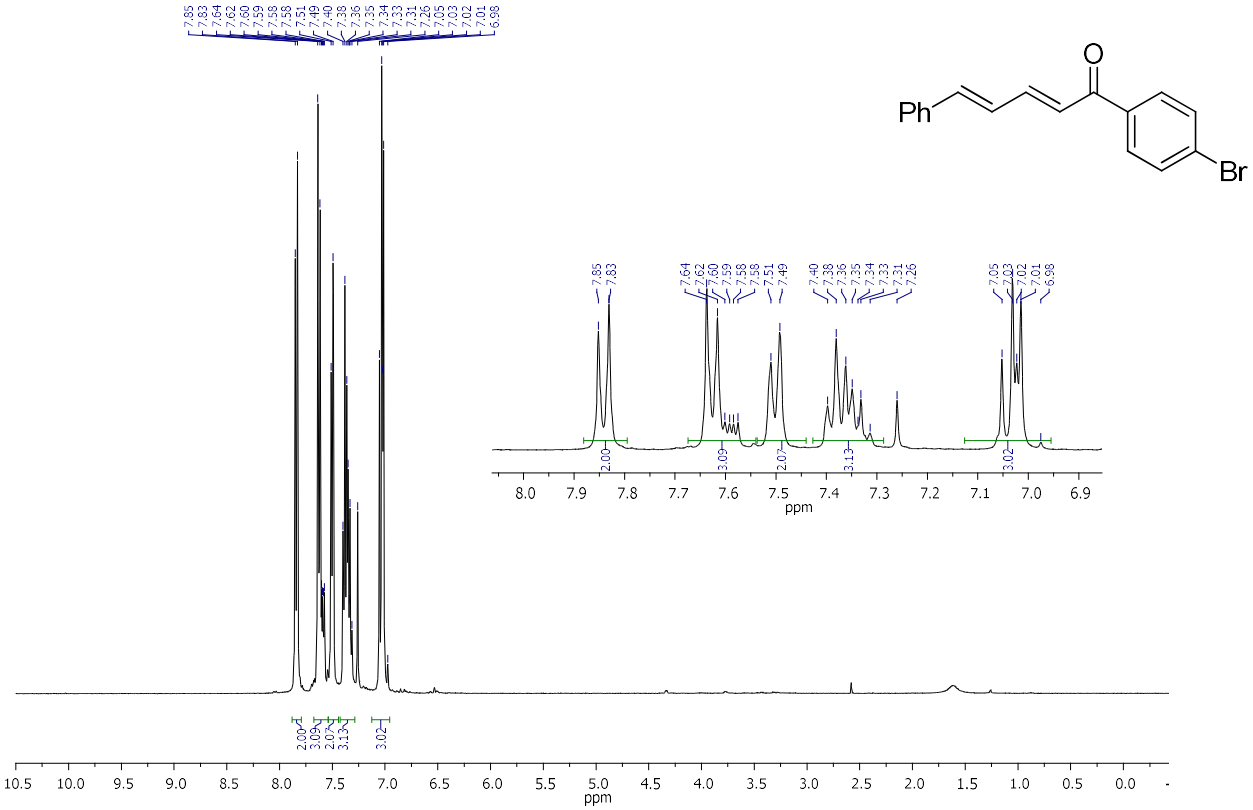


Fig. S7. ^{1}H NMR spectrum of the compound **1d** ($CDCl_3$, 400 MHz).

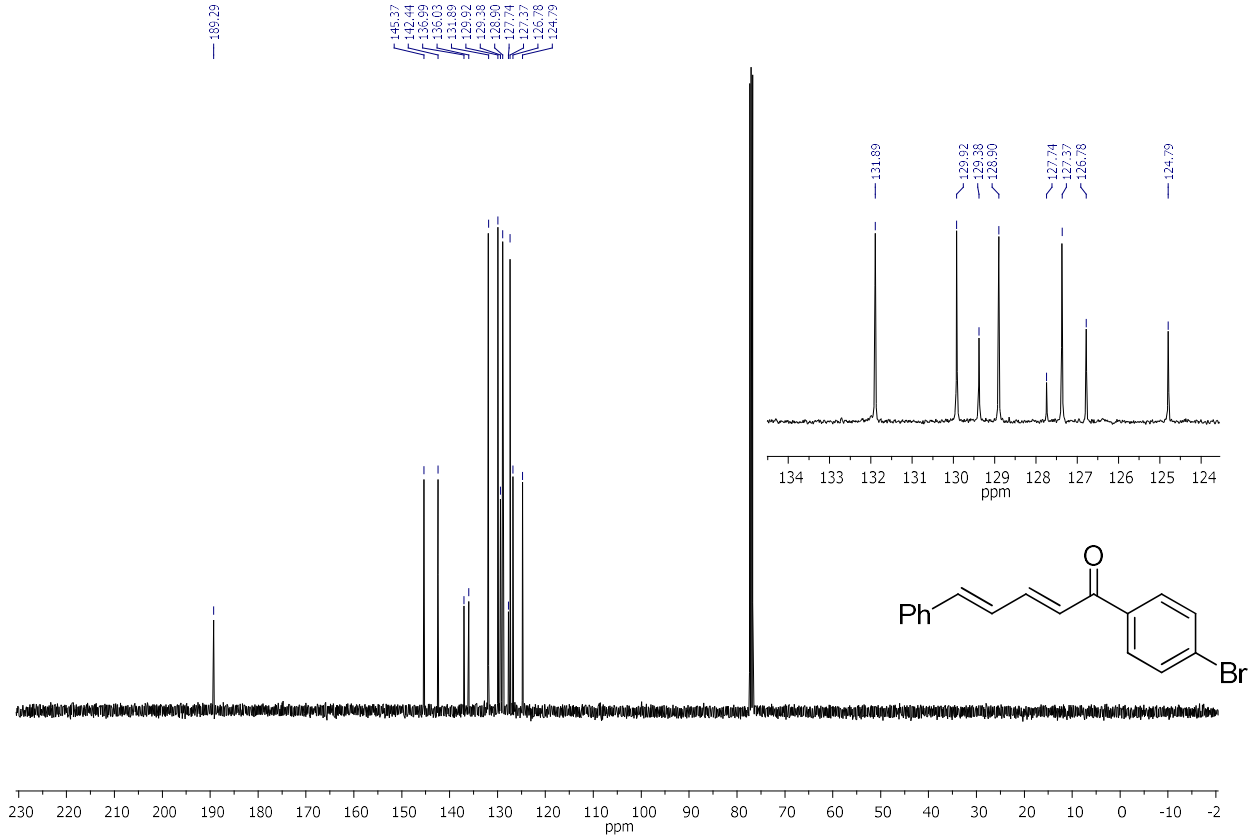


Fig. S8. ^{13}C NMR spectrum of the compound **1d** ($CDCl_3$, 101 MHz).

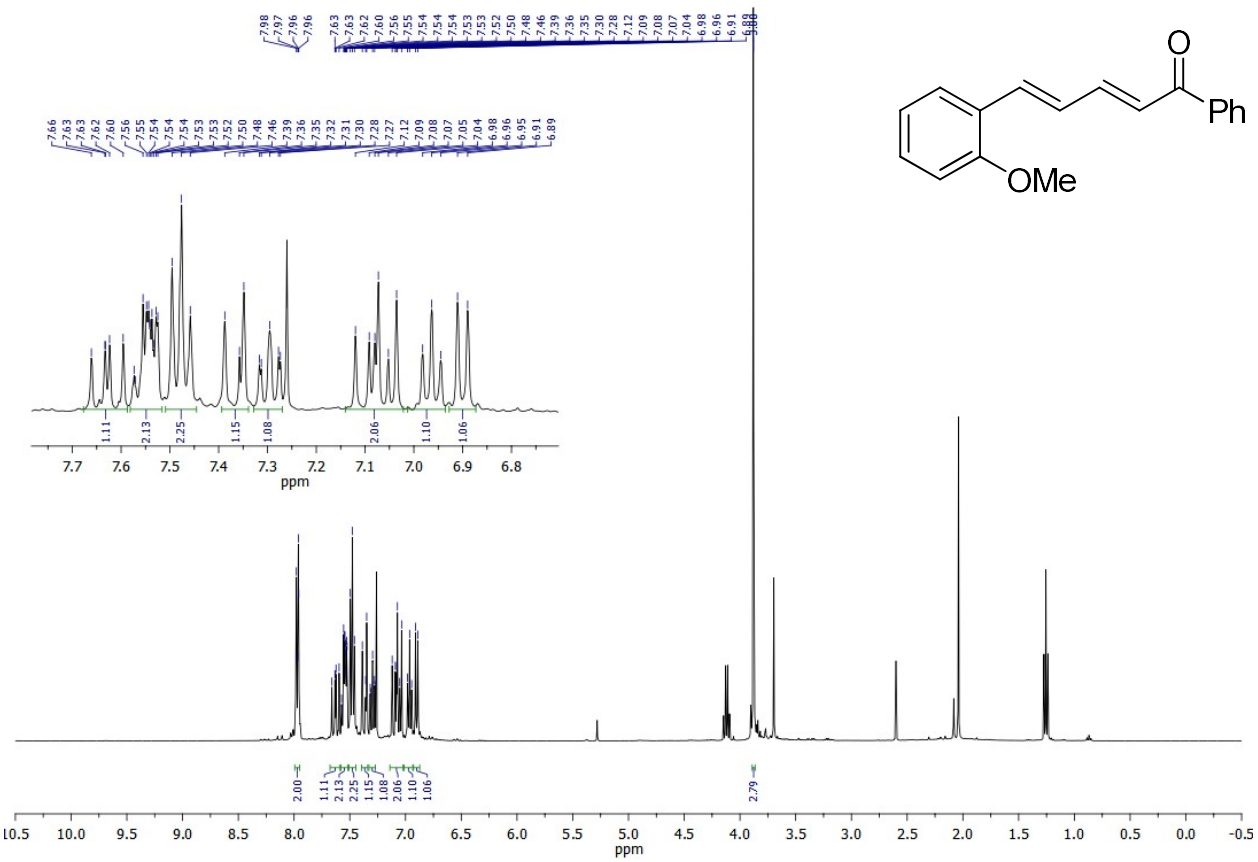


Fig. S9. ^{1}H NMR spectrum of the compound **1e** ($CDCl_3$, 400 MHz).

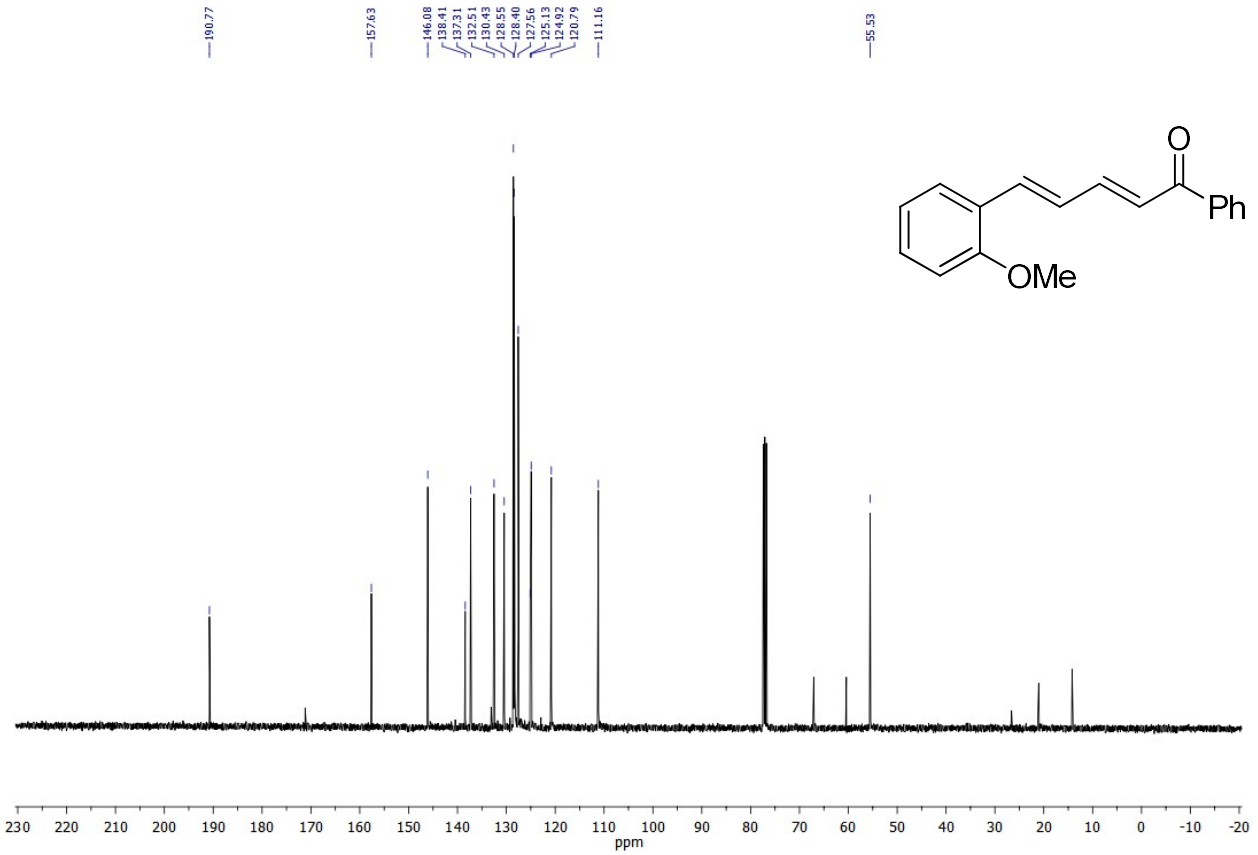


Fig. S10. ^{13}C NMR spectrum of the compound **1e** ($CDCl_3$, 101 MHz).

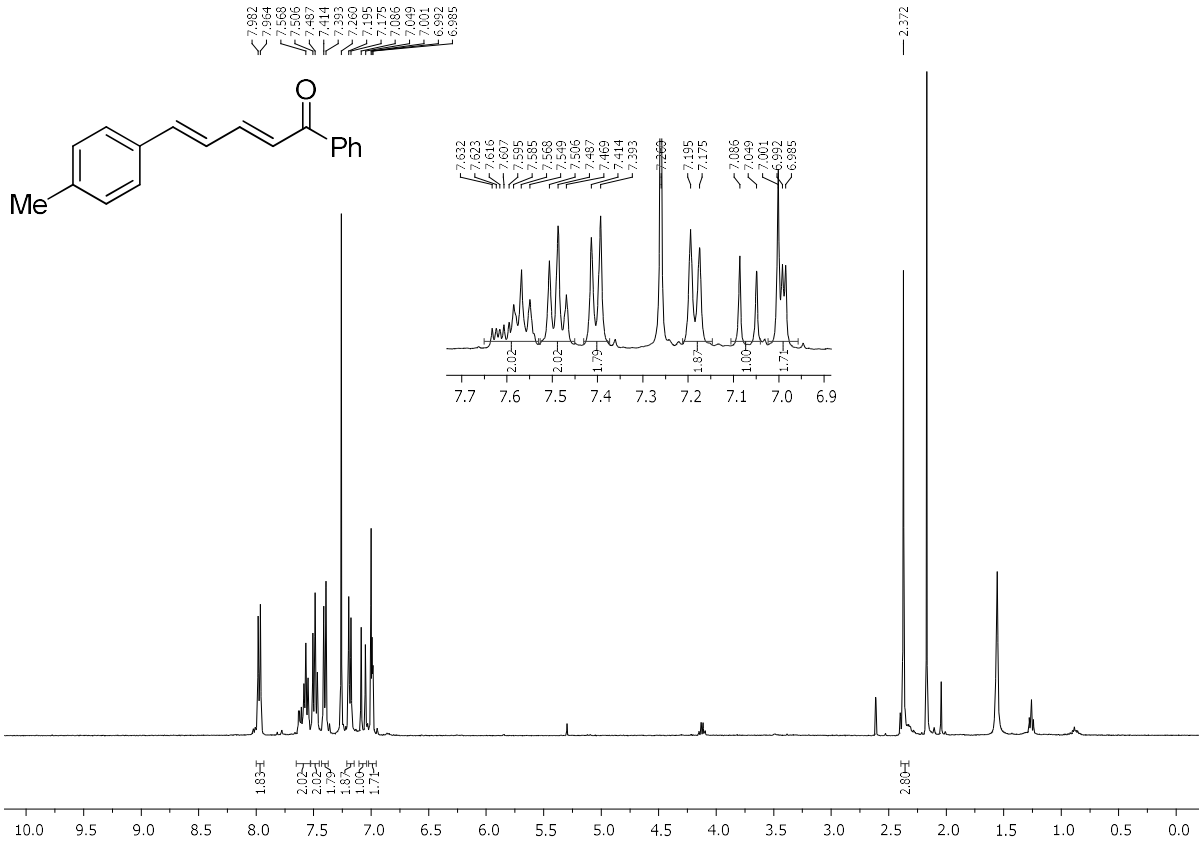


Fig. S11. ^{1}H NMR spectrum of the compound **1f** ($CDCl_3$, 400 MHz).

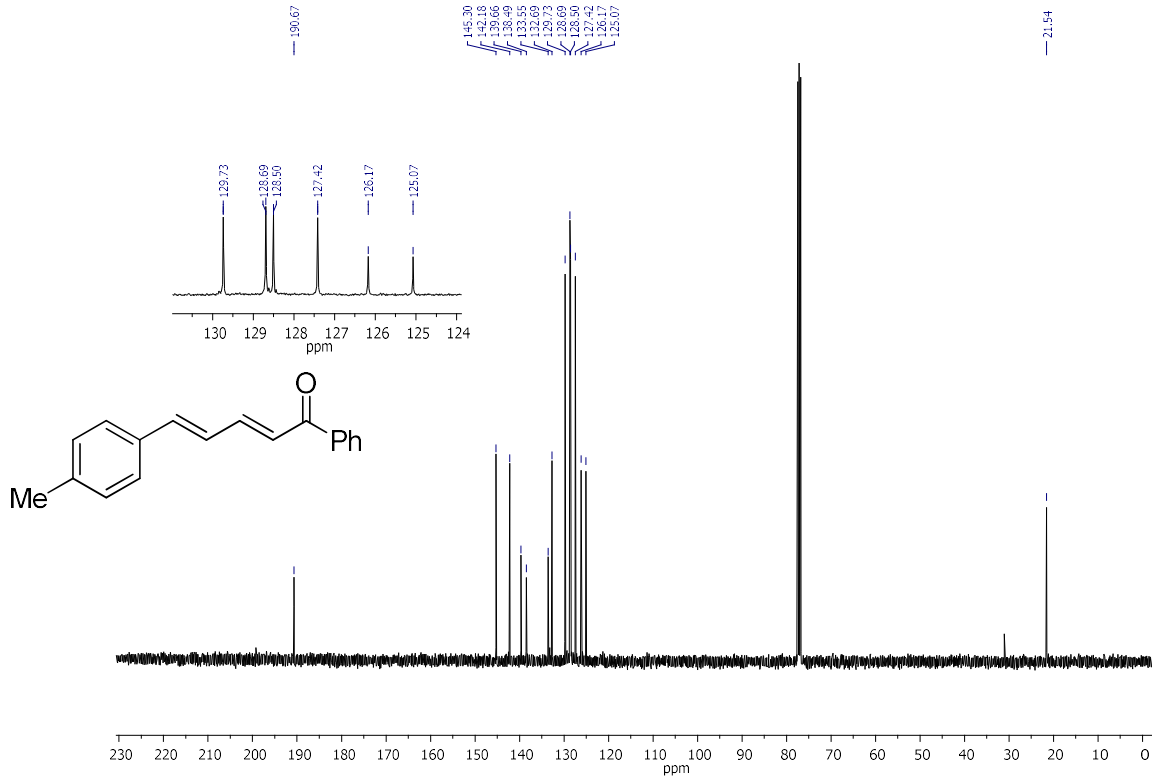


Fig. S12. ^{13}C NMR spectrum of the compound **1f** ($CDCl_3$, 101 MHz).

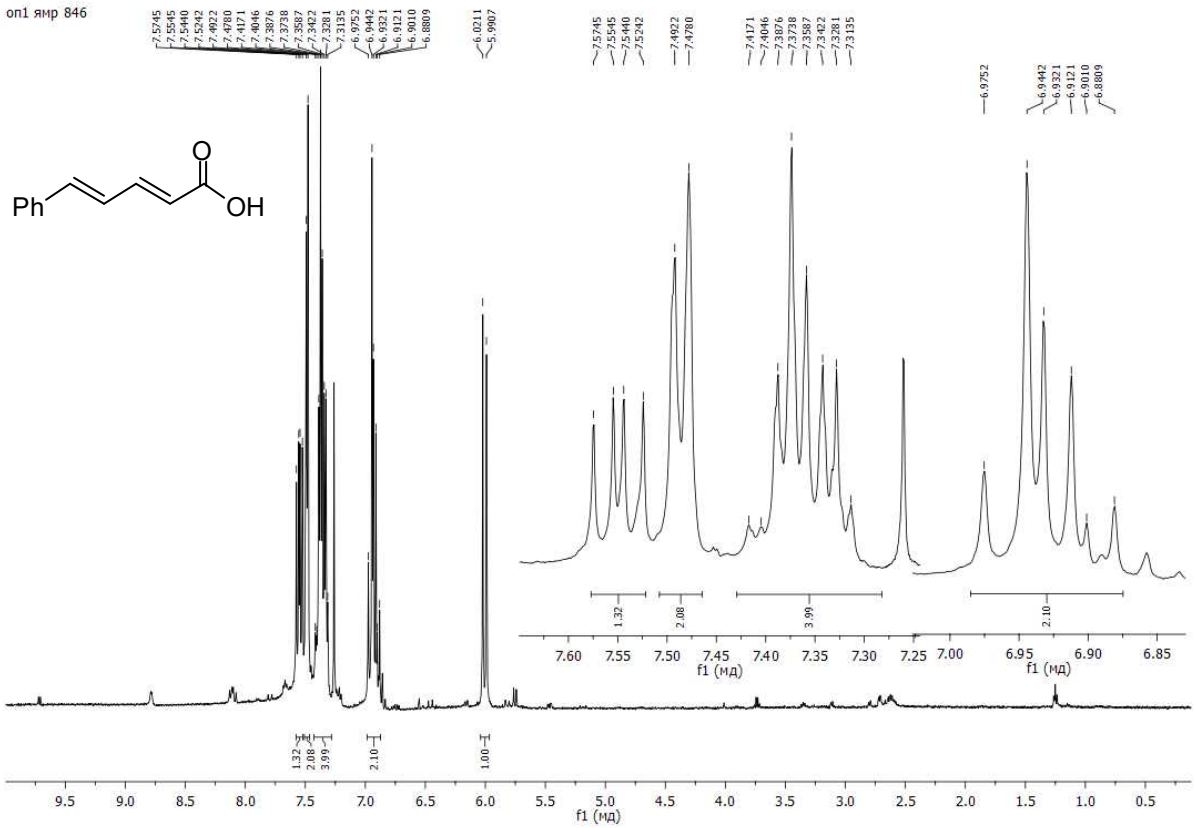


Fig. S13. ^{1}H NMR spectrum of the compound **1g** ($CDCl_3$, 400 MHz).

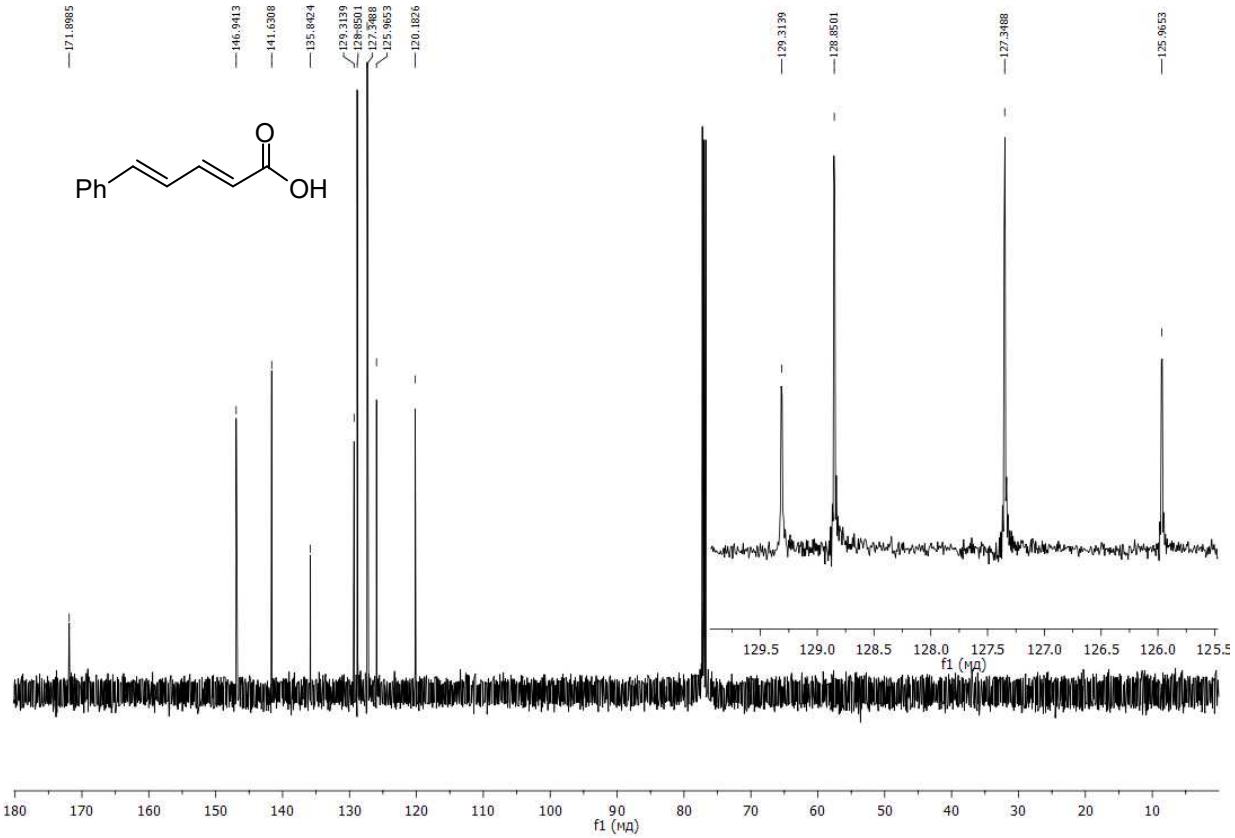


Fig. S14. ^{13}C NMR spectrum of the compound **1g** ($CDCl_3$, 101 MHz).

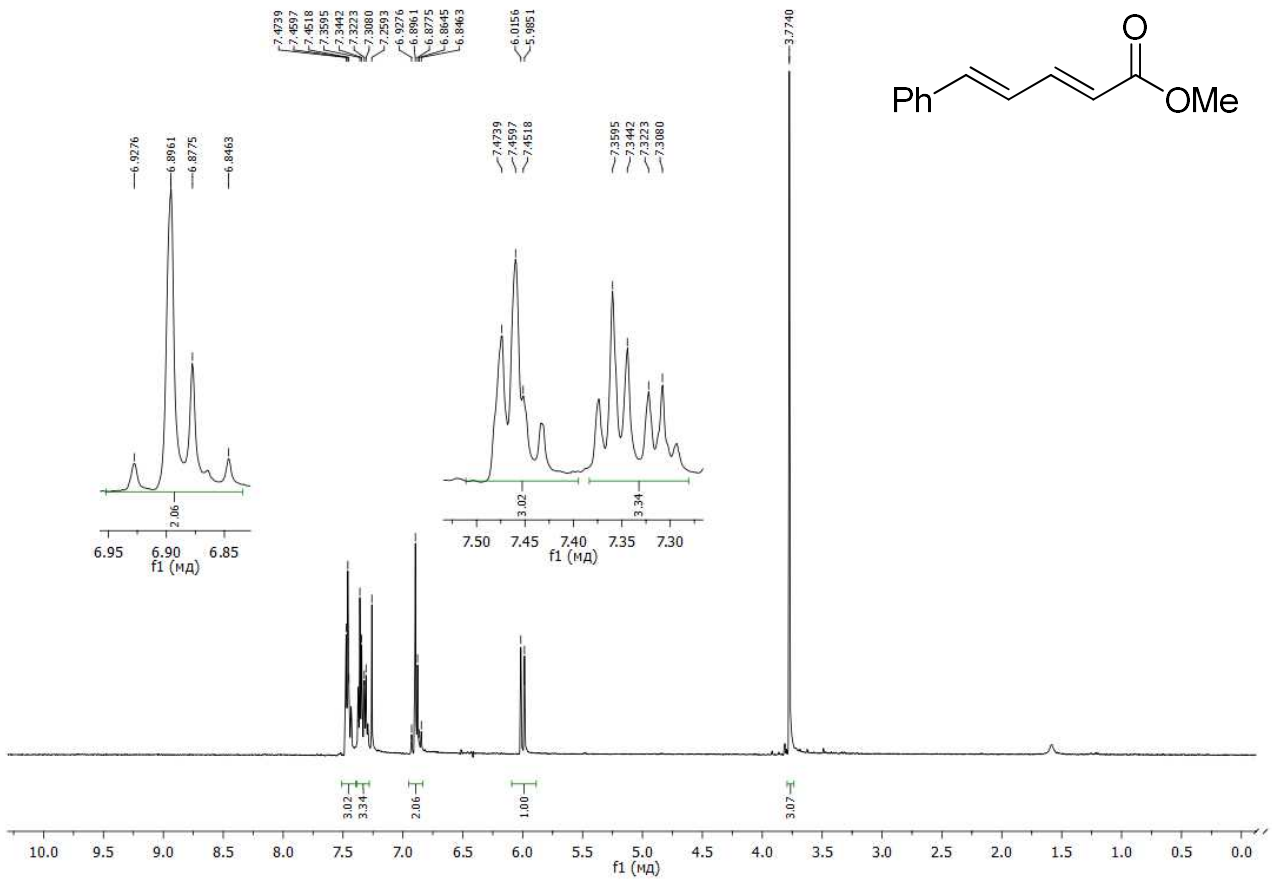


Fig. S15. ^{1}H NMR spectrum of the compound **1h** ($CDCl_3$, 500 MHz).

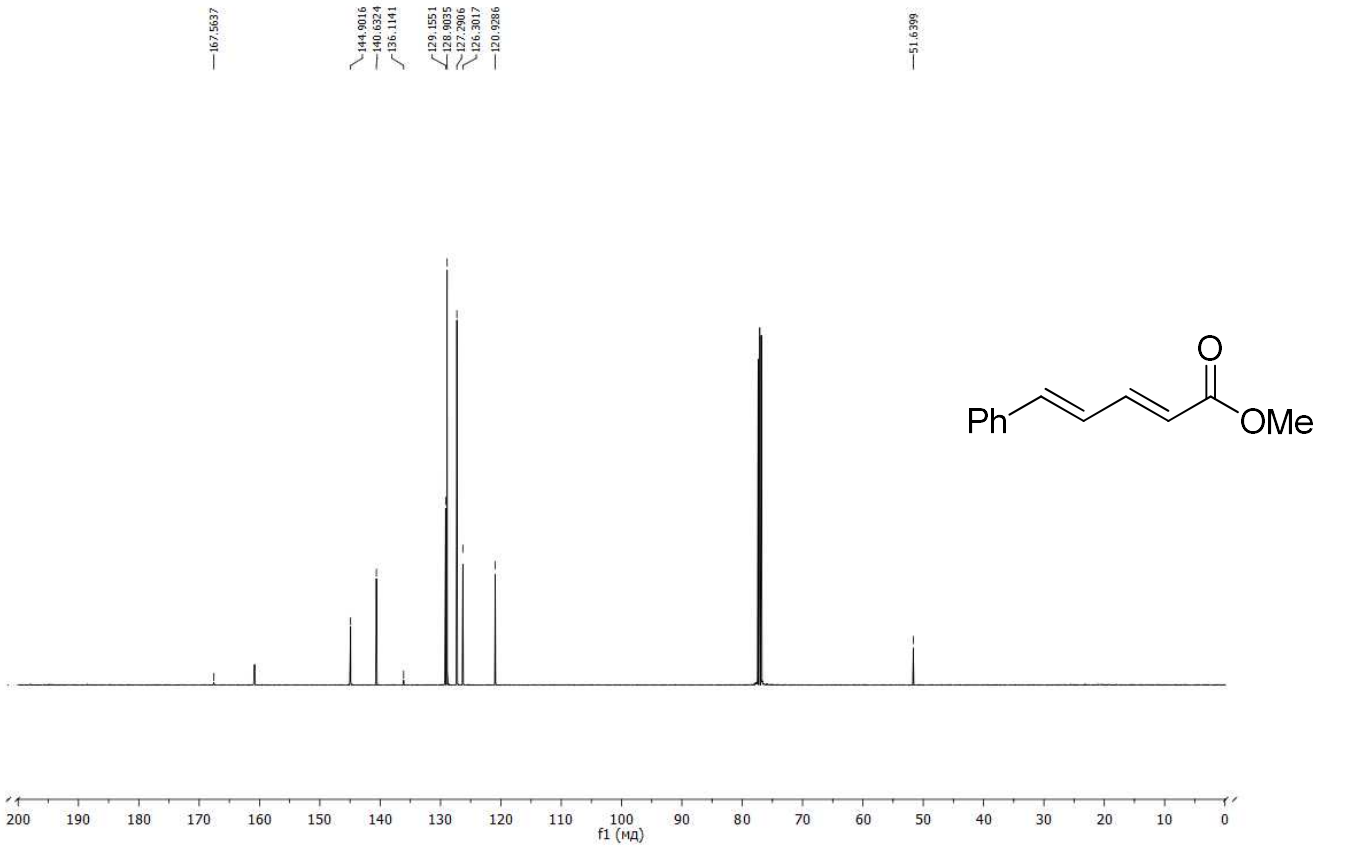


Fig. S16. ^{13}C NMR spectrum of the compound **1h** ($CDCl_3$, 125 MHz).

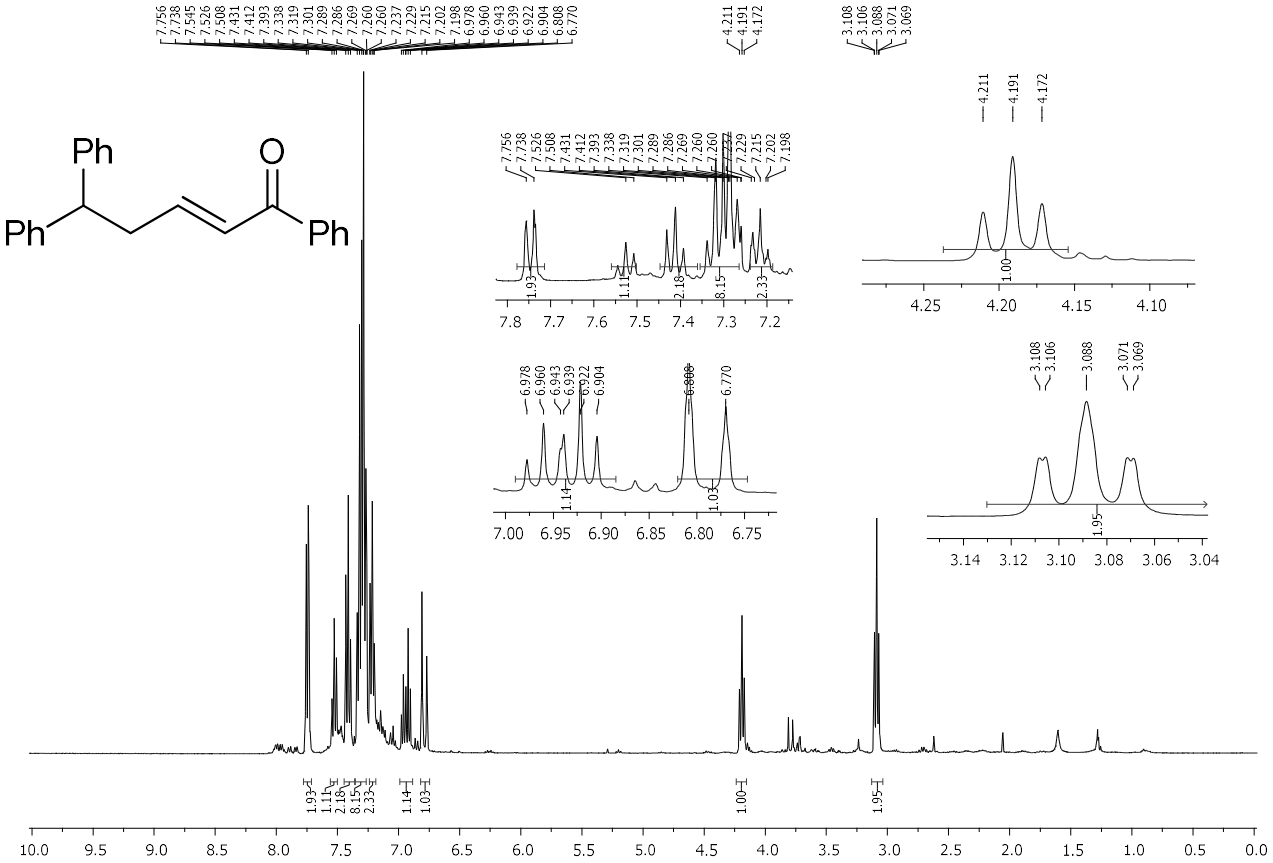


Fig. S17. ^{1}H NMR spectrum of the compound **2a** ($CDCl_3$, 400 MHz).

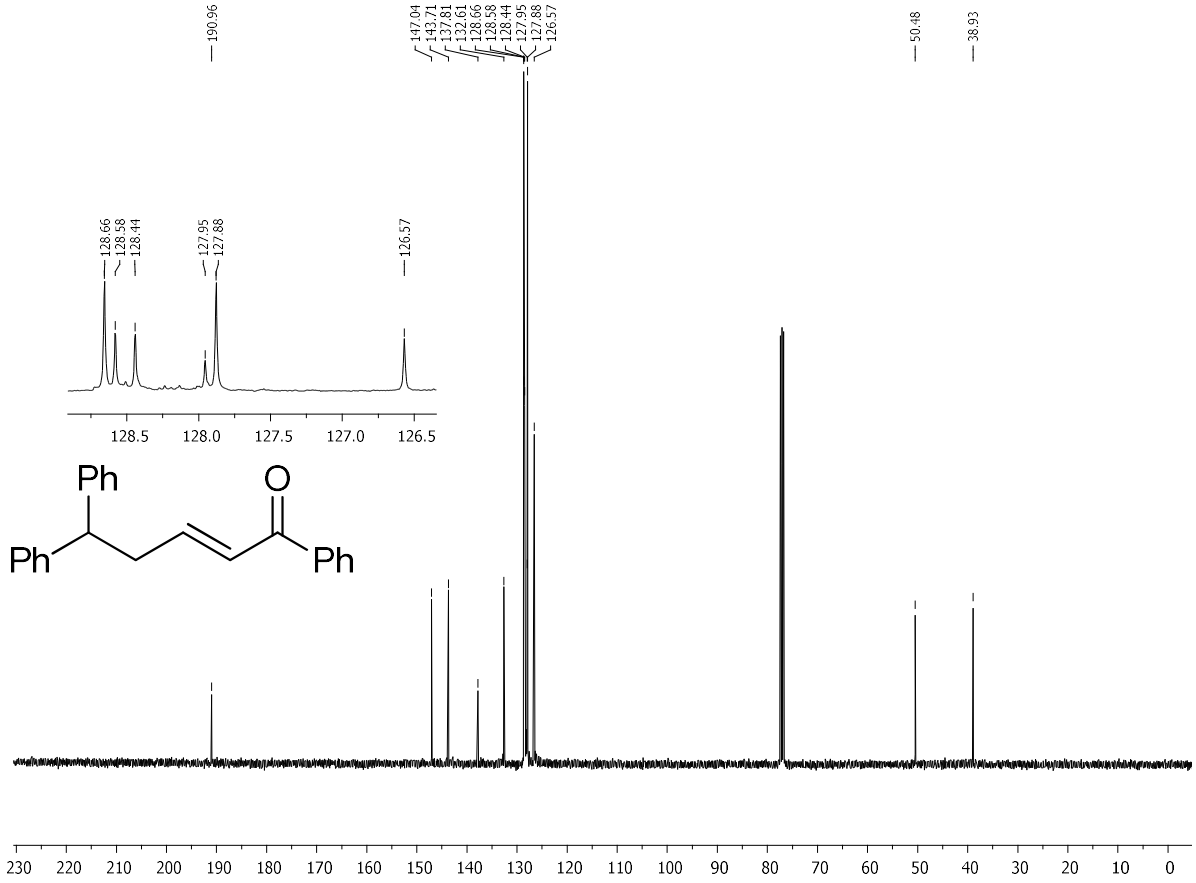


Fig. S18. ^{13}C NMR spectrum of the compound **2a** ($CDCl_3$, 101 MHz).

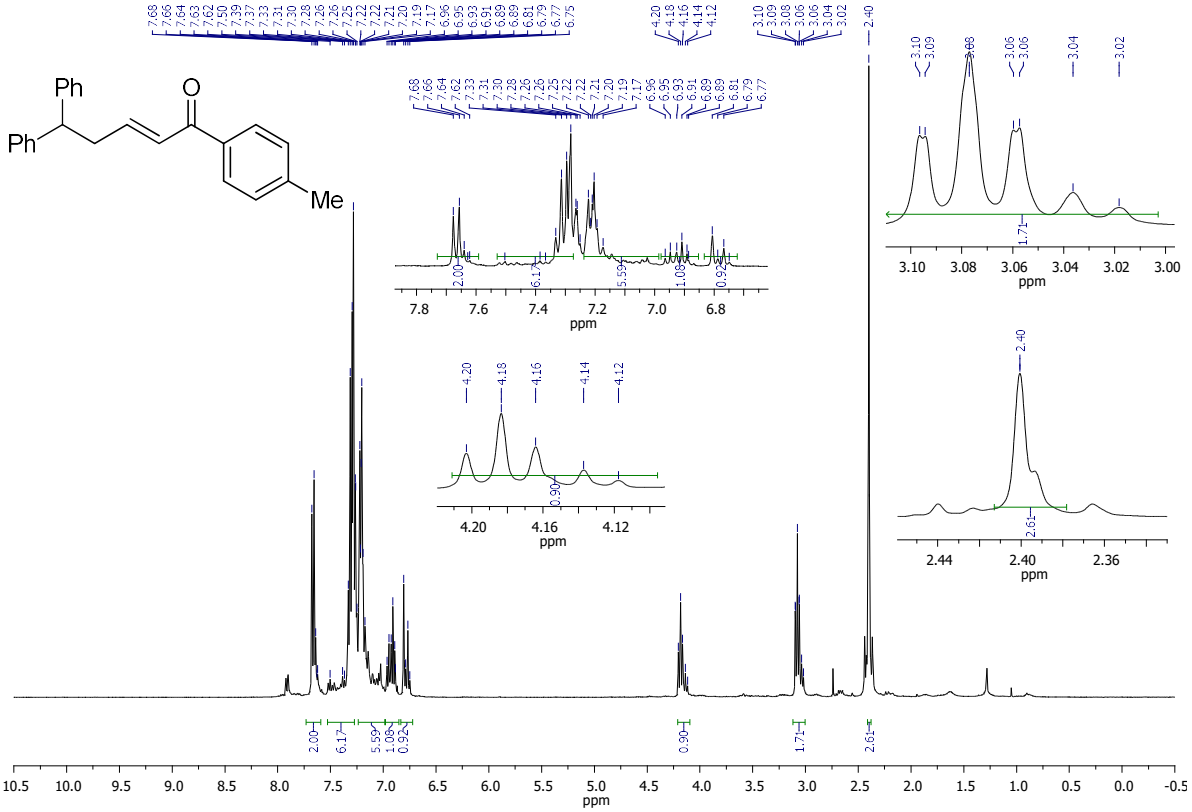


Fig. S19. ^{1}H NMR spectrum of the compound **2b** ($CDCl_3$, 400 MHz).

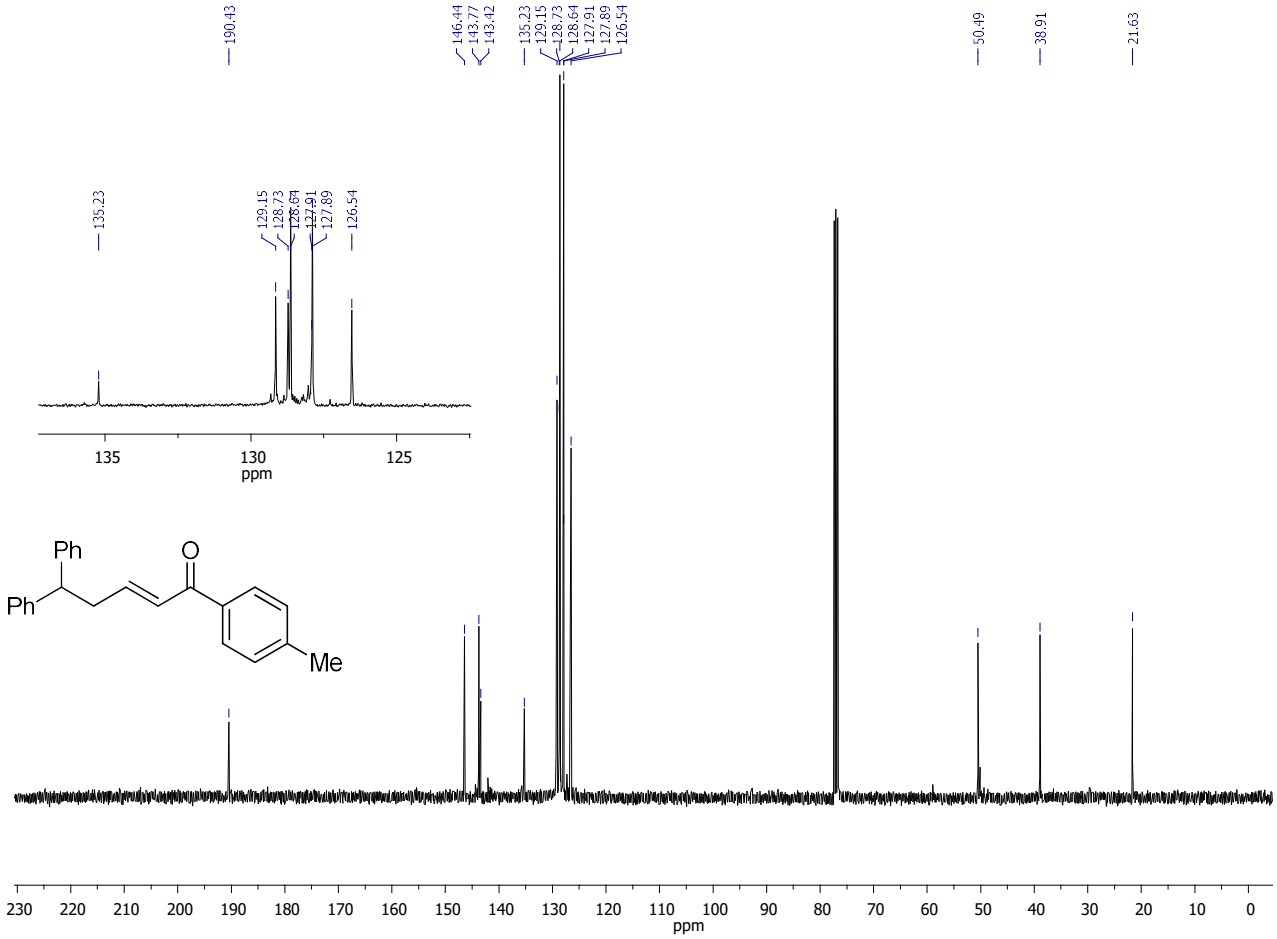


Fig. S20. ^{13}C NMR spectrum of the compound **2b** ($CDCl_3$, 101 MHz).

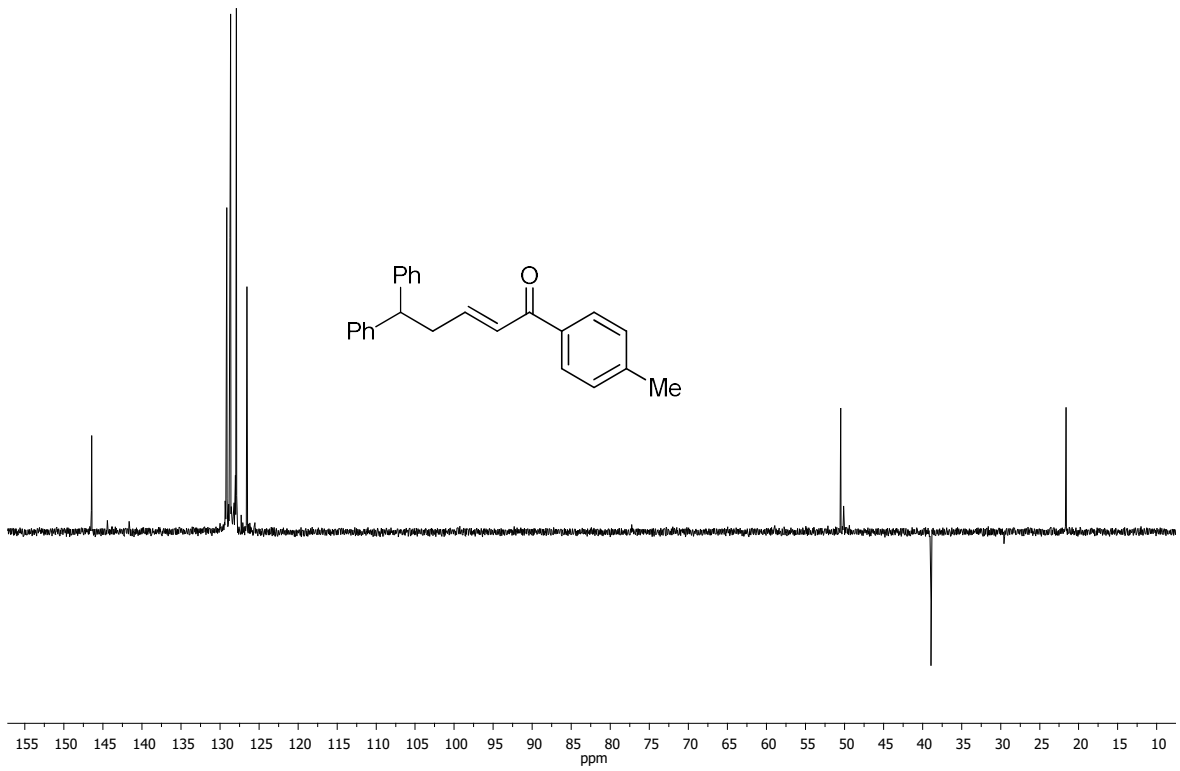


Fig. S21. DEPT spectrum of the compound **2b**.

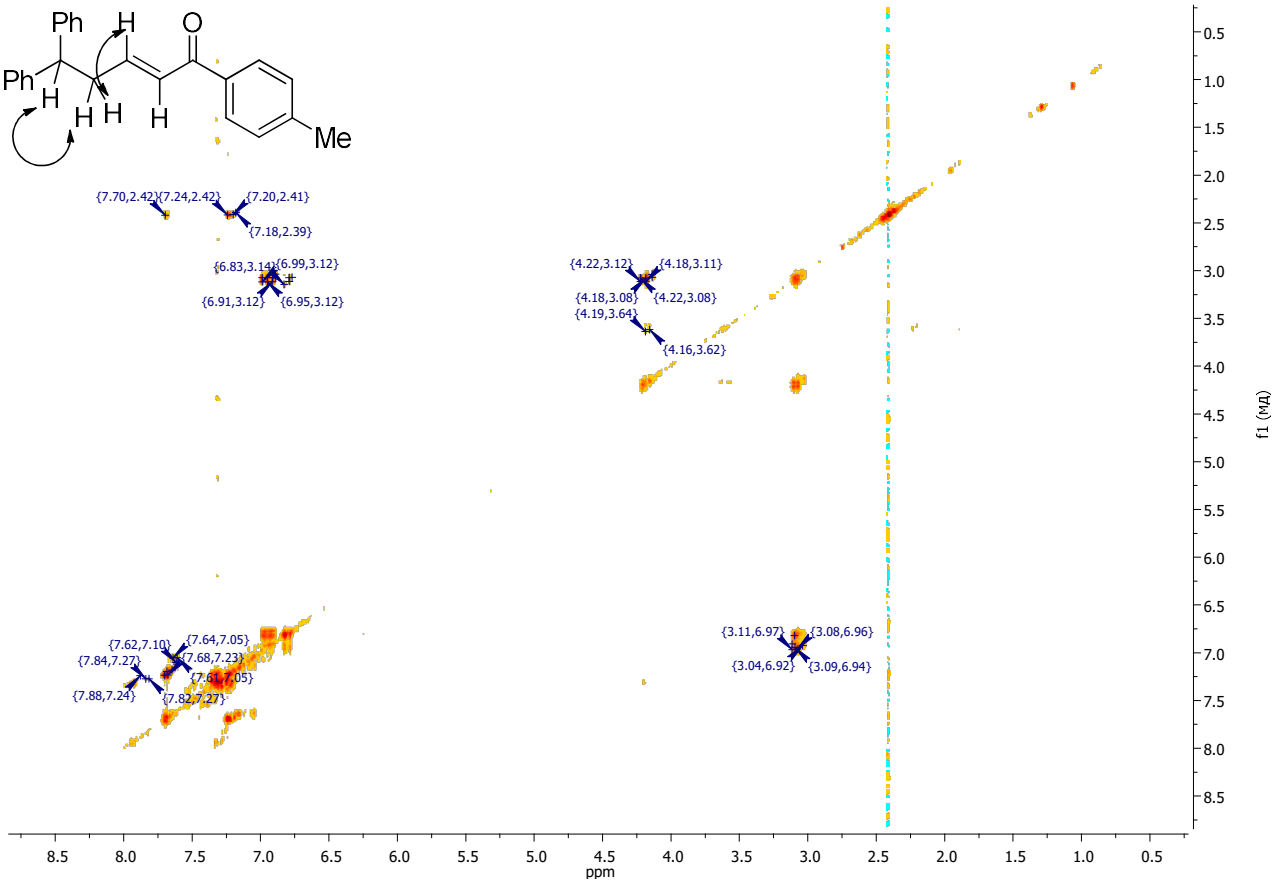


Fig. S22. H-H COSY spectrum of the compound **2b**.

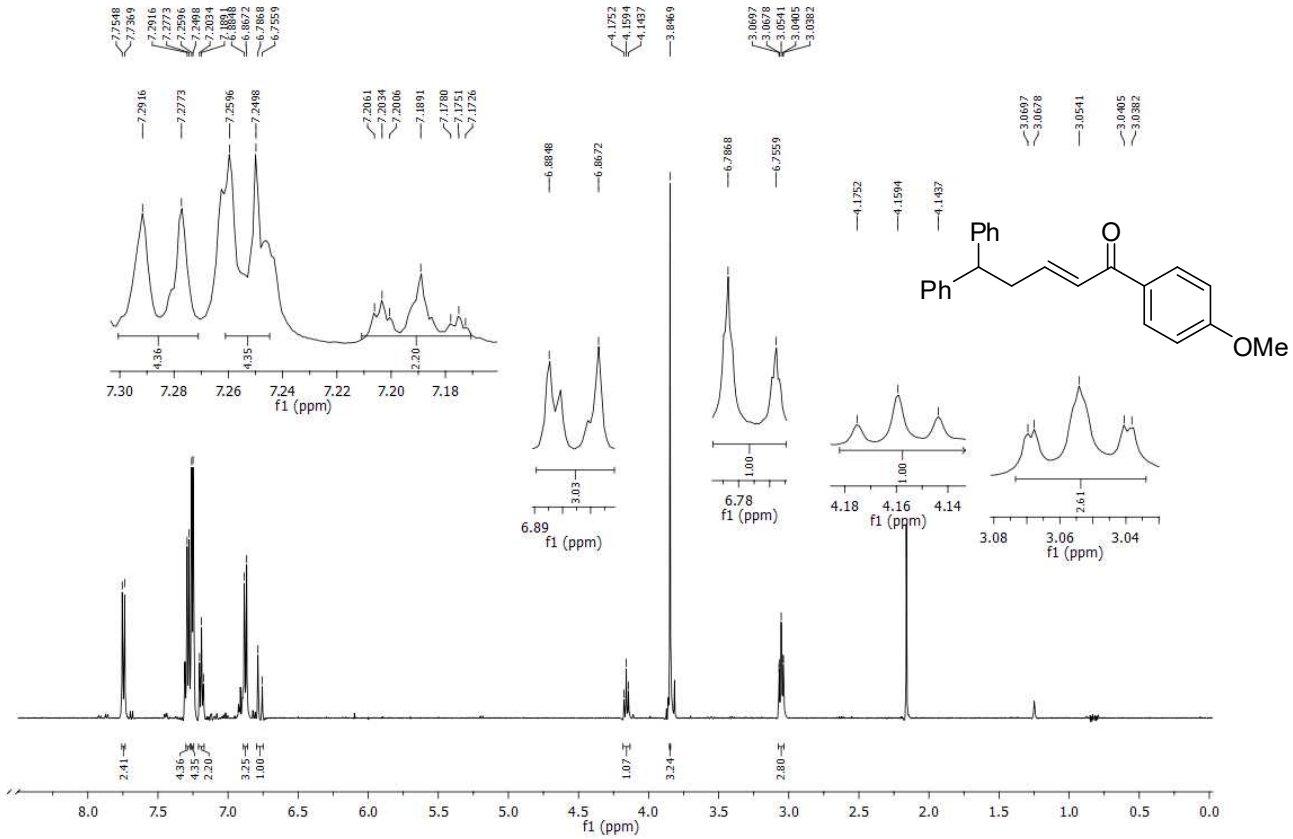


Fig. S23. ^{1}H NMR spectrum of the compound **2c** ($CDCl_3$, 500 MHz).

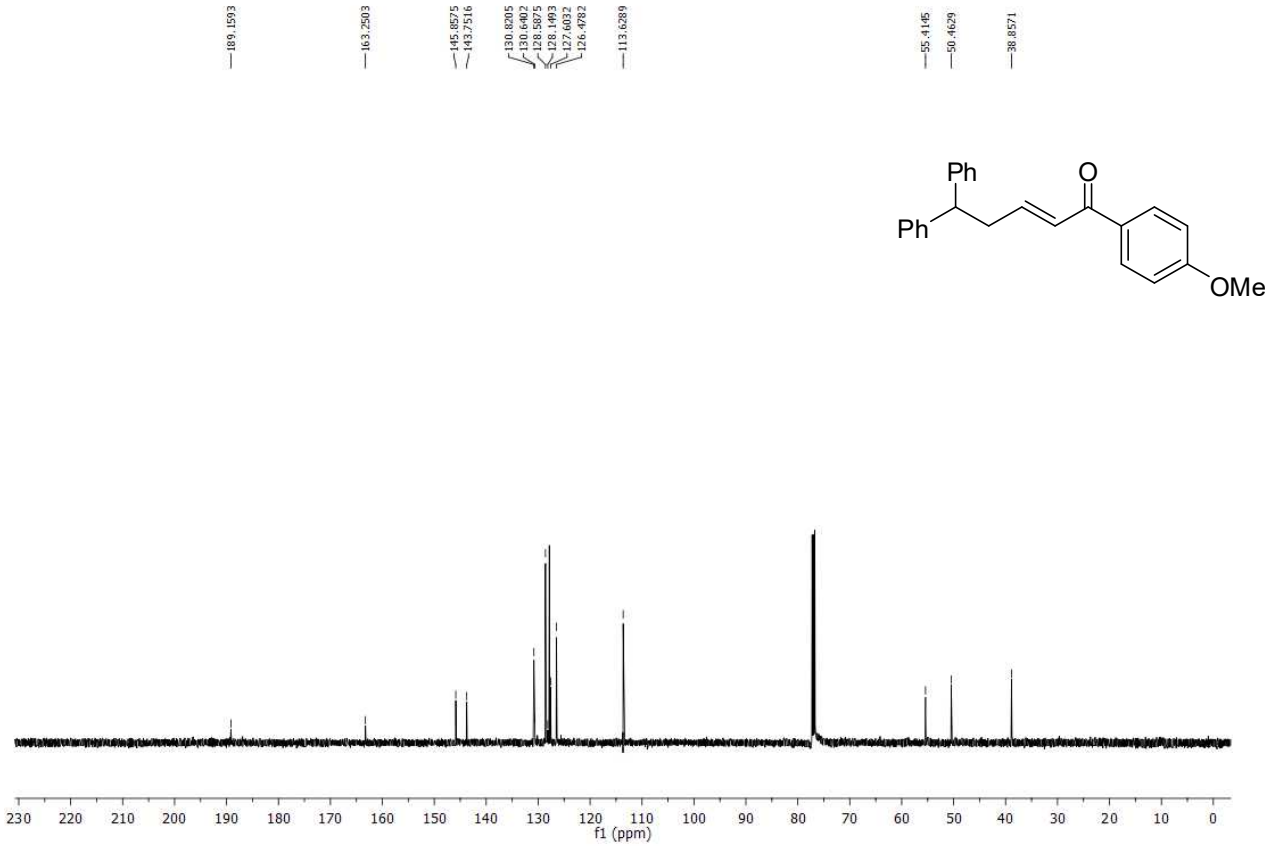


Fig. S24. ^{13}C NMR spectrum of the compound **2c** ($CDCl_3$, 125 MHz).

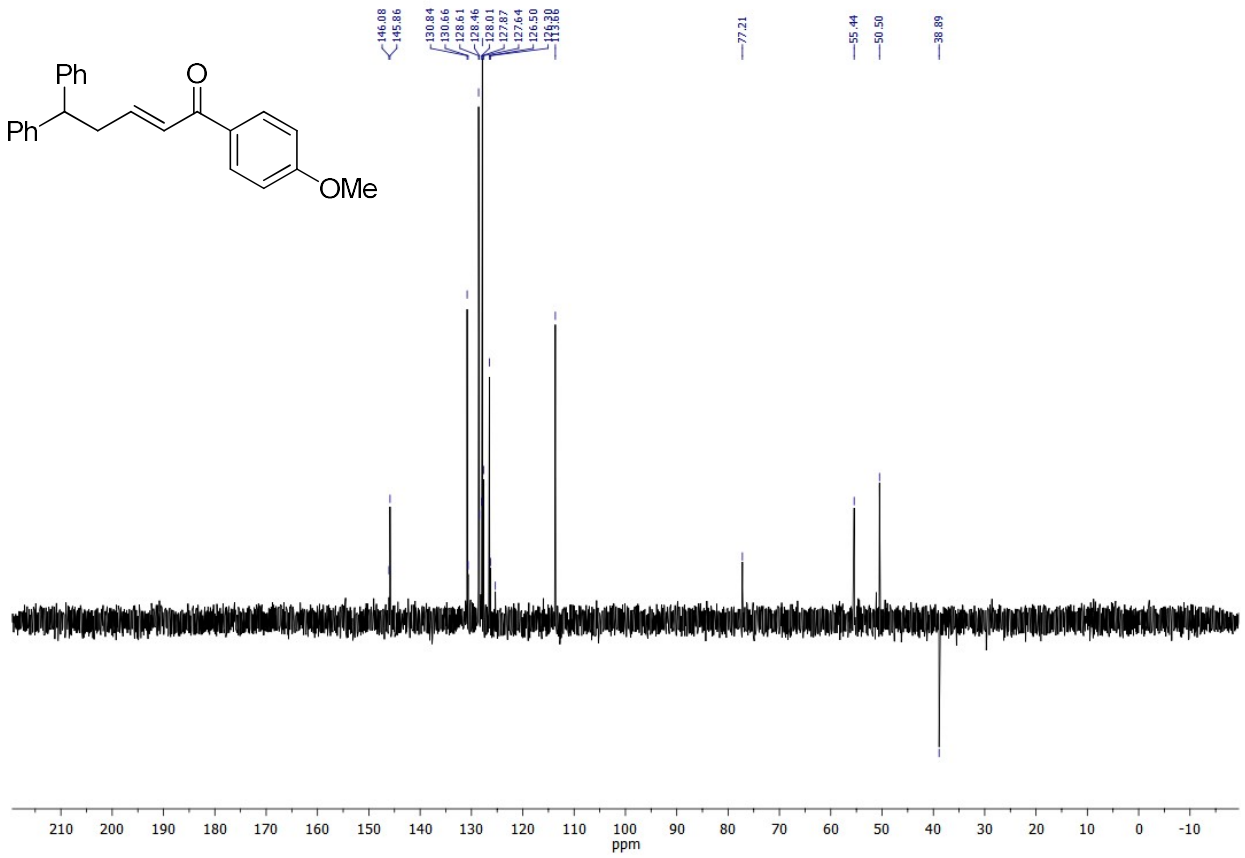


Fig. S25. DEPT spectrum of the compound **2c**.

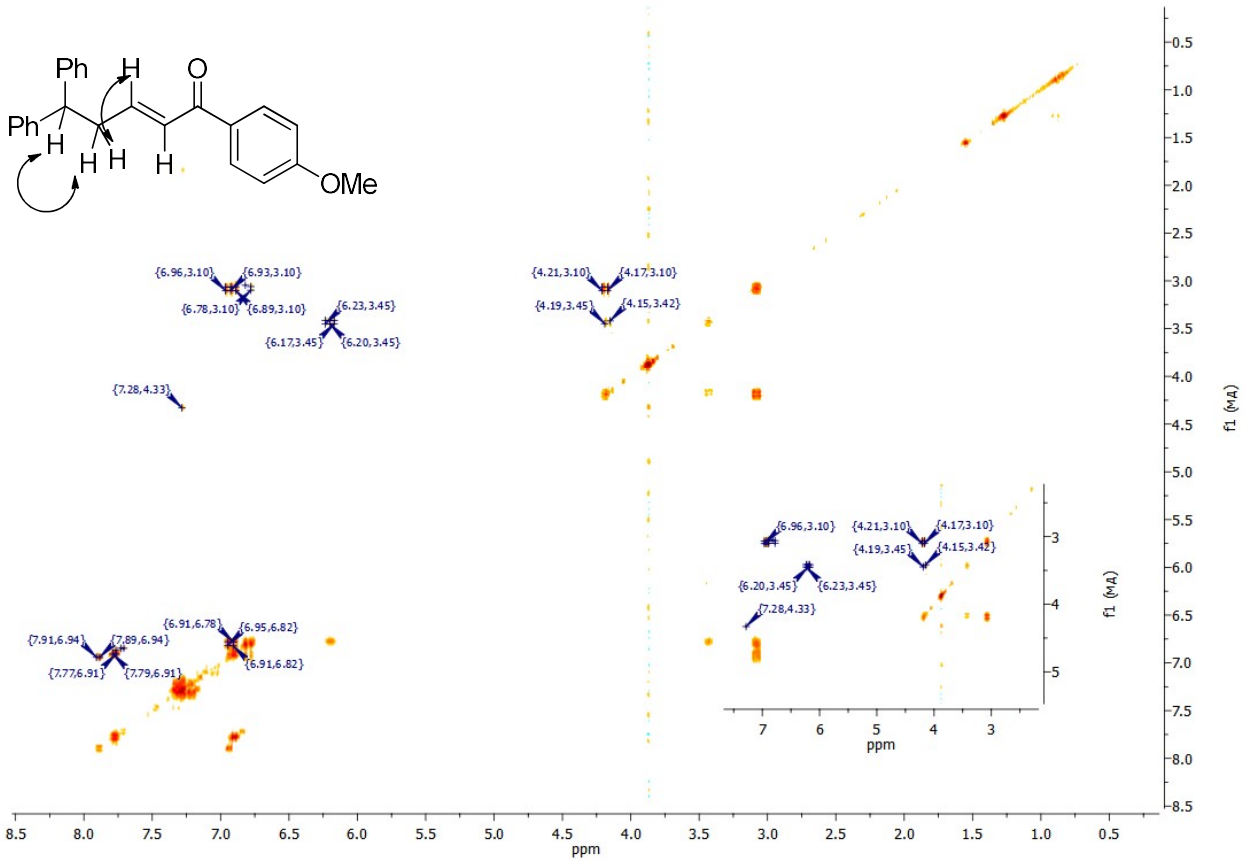


Fig. S26. H-H COSY spectrum of the compound **2c**.

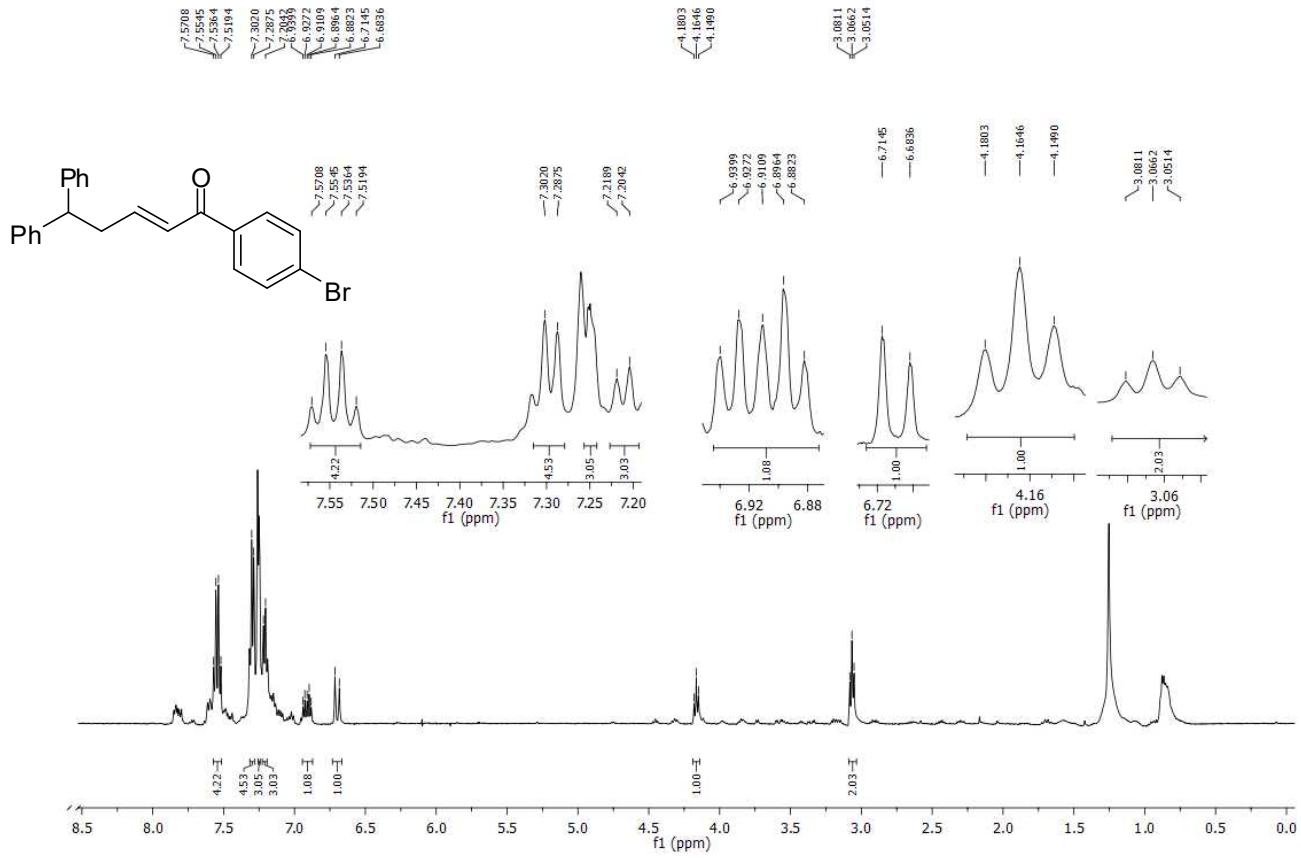


Fig. S27. ^{1}H NMR spectrum of the compound **2d** ($CDCl_3$, 500 MHz).

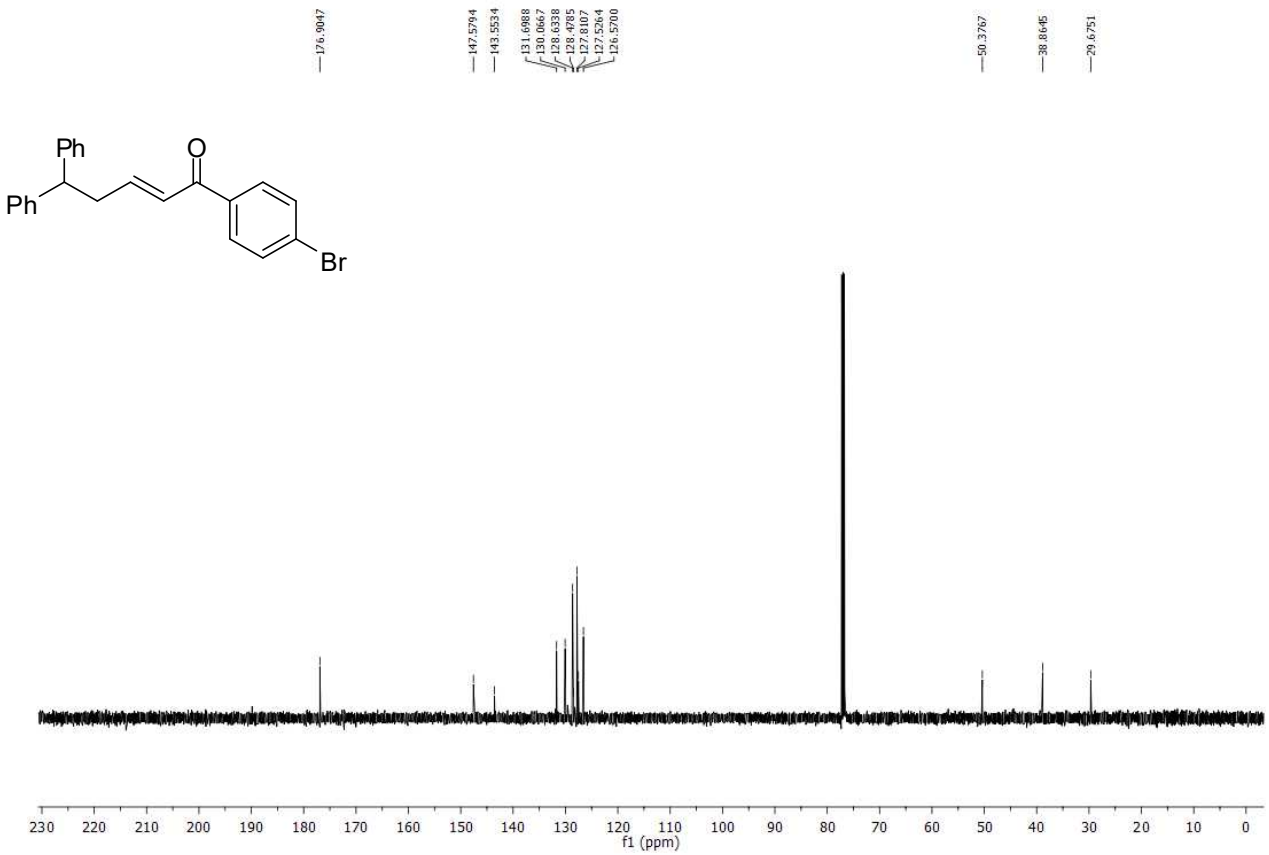


Fig. S28. ^{13}C NMR spectrum of the compound **2d** ($CDCl_3$, 125 MHz).

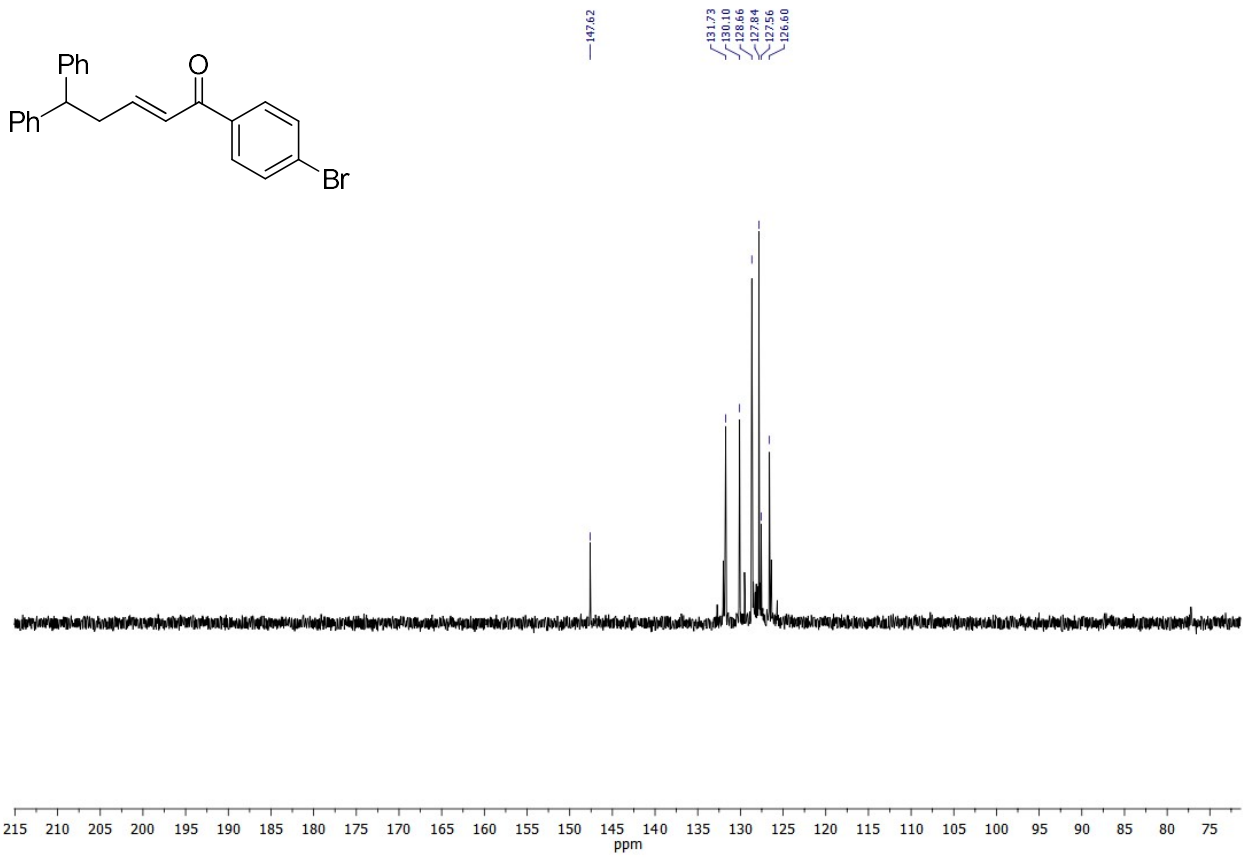


Fig. S29. DEPT spectrum of the compound **2d**.

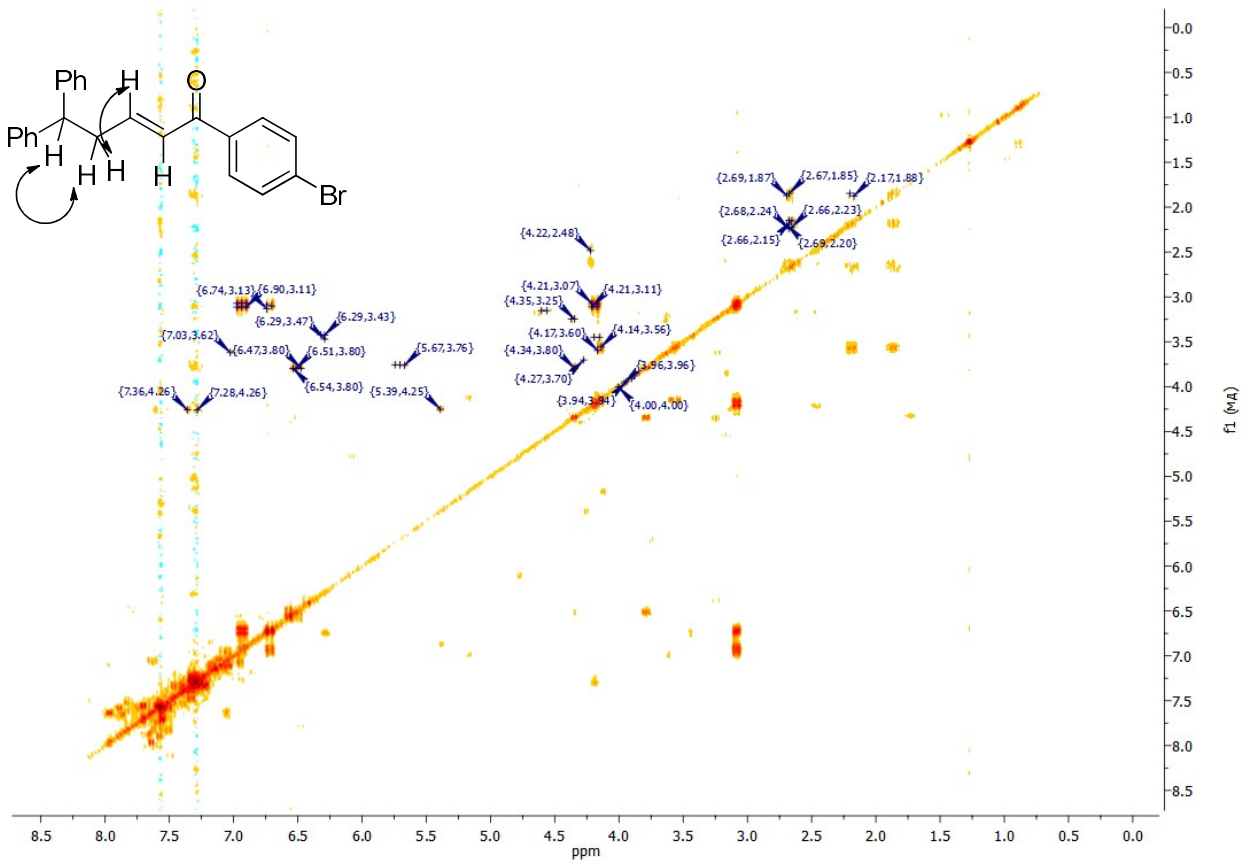


Fig. S30. H-H COSY spectrum of the compound **2d**.

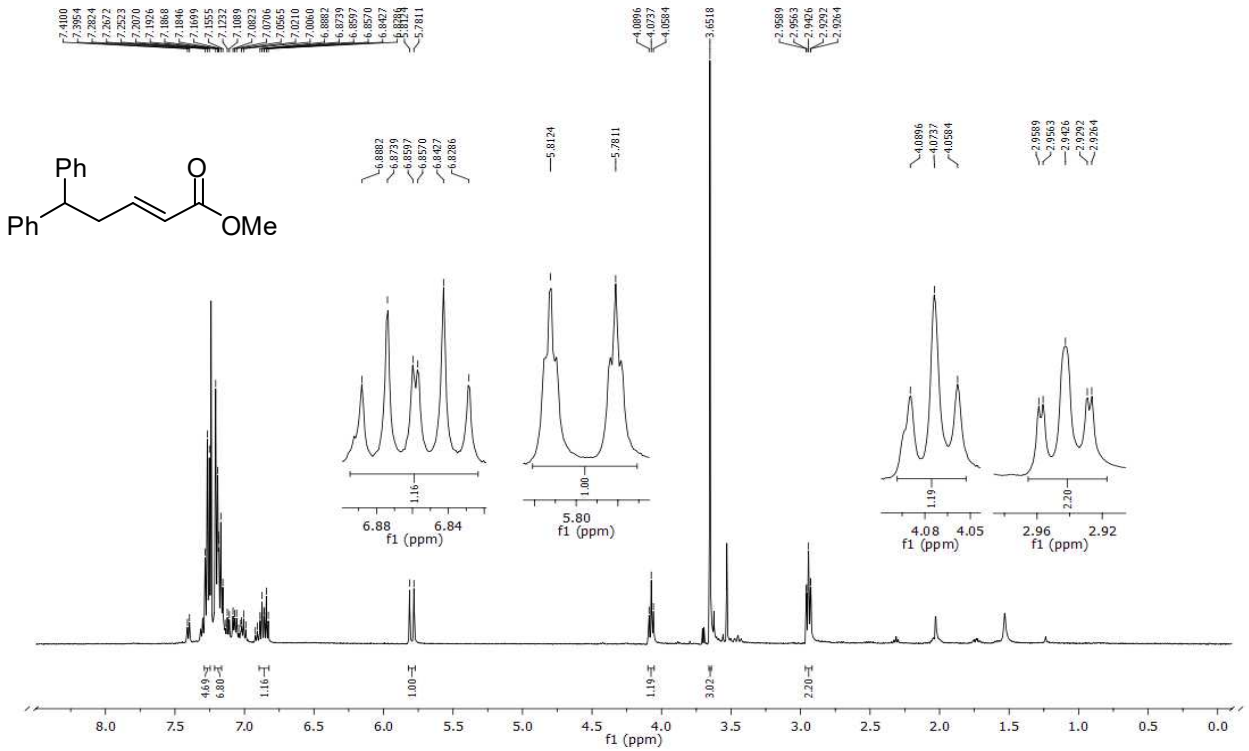


Fig. S31. ^{1}H NMR spectrum of the compound **2f** ($CDCl_3$, 500 MHz).

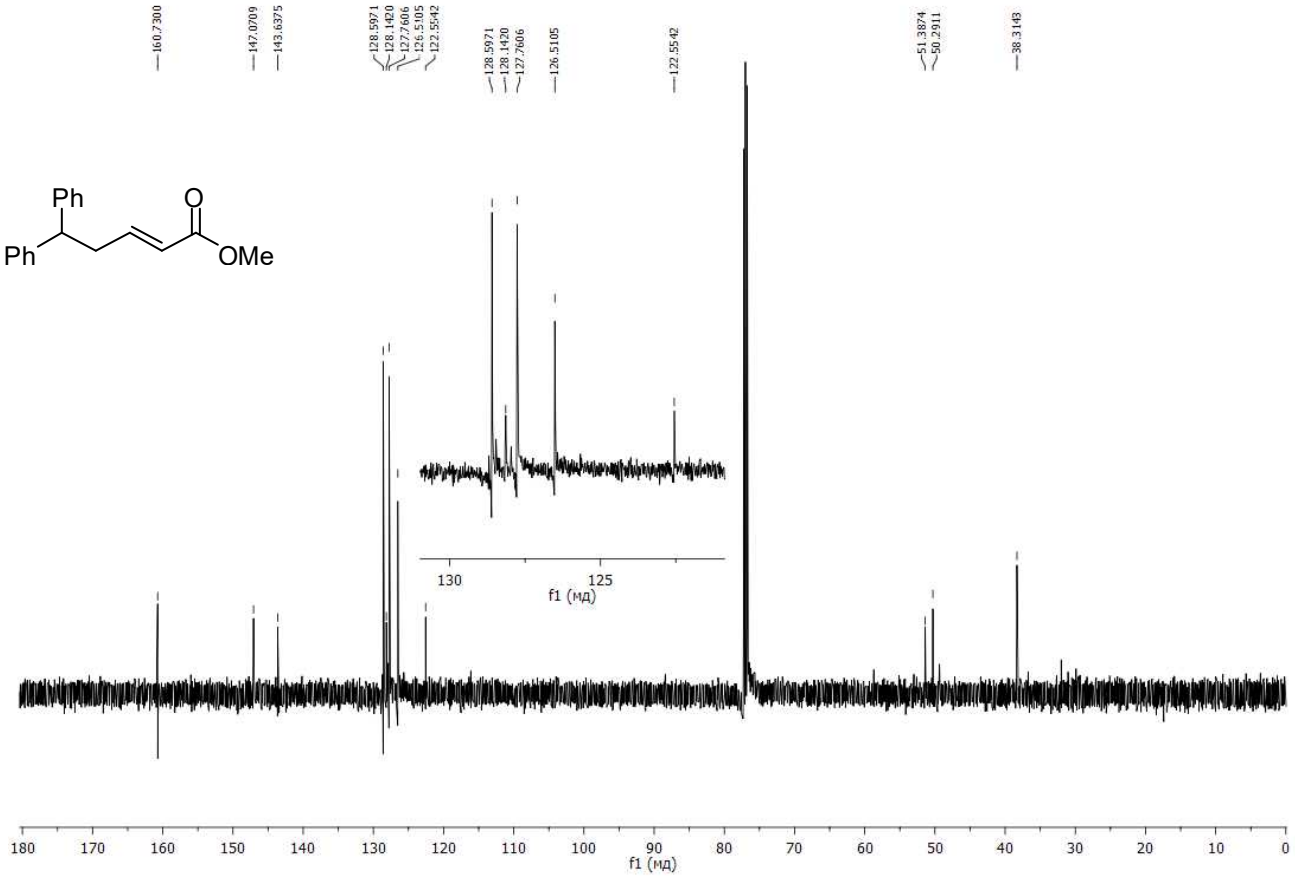


Fig. S32. ^{13}C NMR spectrum of the compound **2f** ($CDCl_3$, 125 MHz).

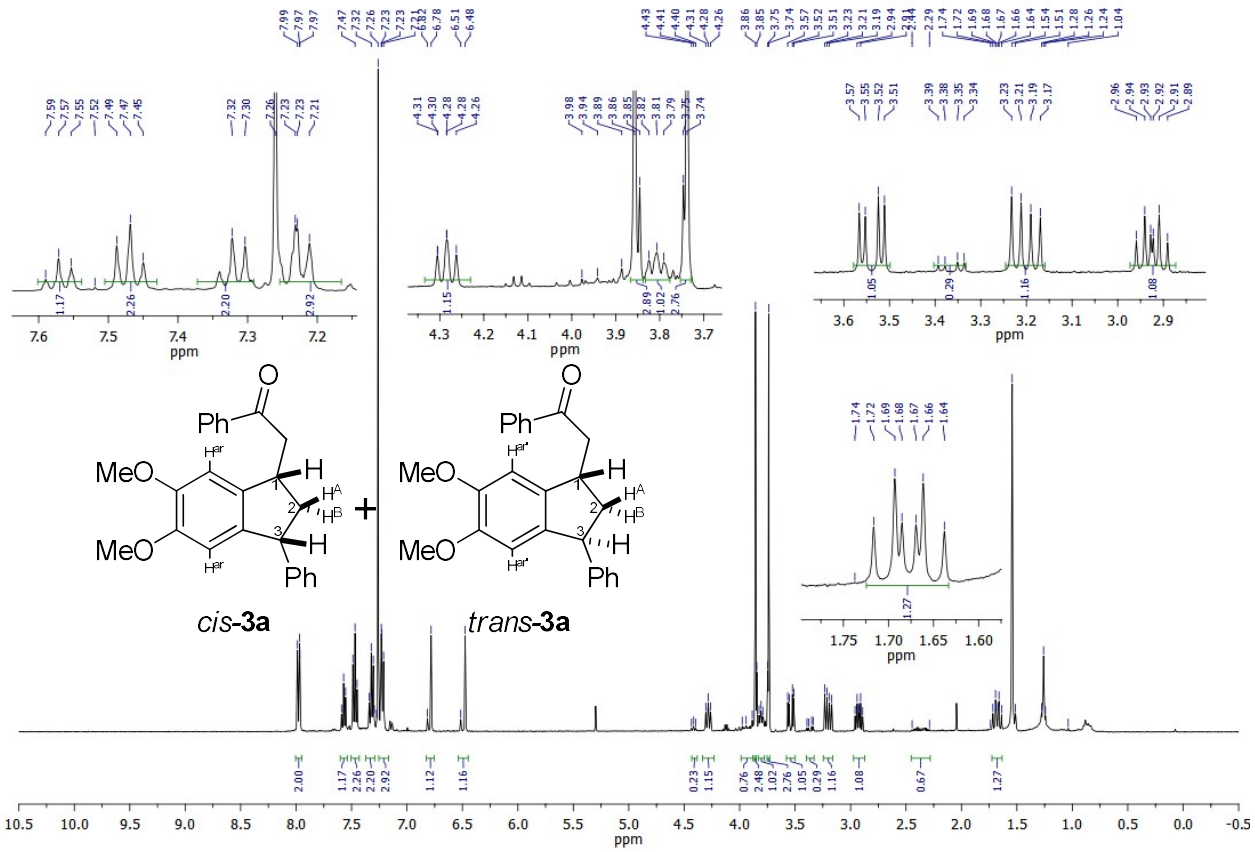


Fig. S33. ^{1}H NMR spectrum of mixture of compounds *cis*-**3a** and *trans*-**3a** ($CDCl_3$, 400 MHz).

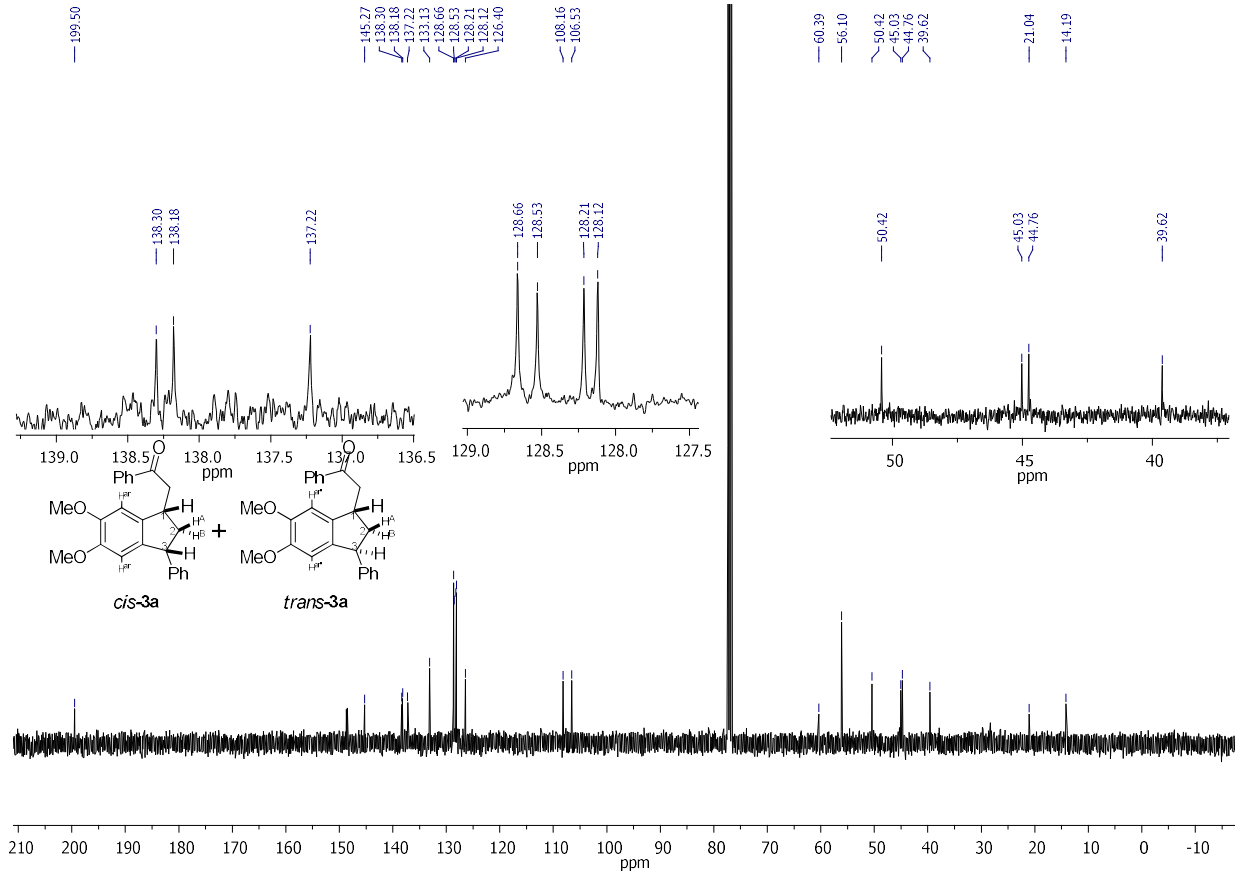


Fig. S34. ^{13}C NMR spectrum of mixture of compounds *cis*-**3a** and *trans*-**3a** ($CDCl_3$, 101 MHz).

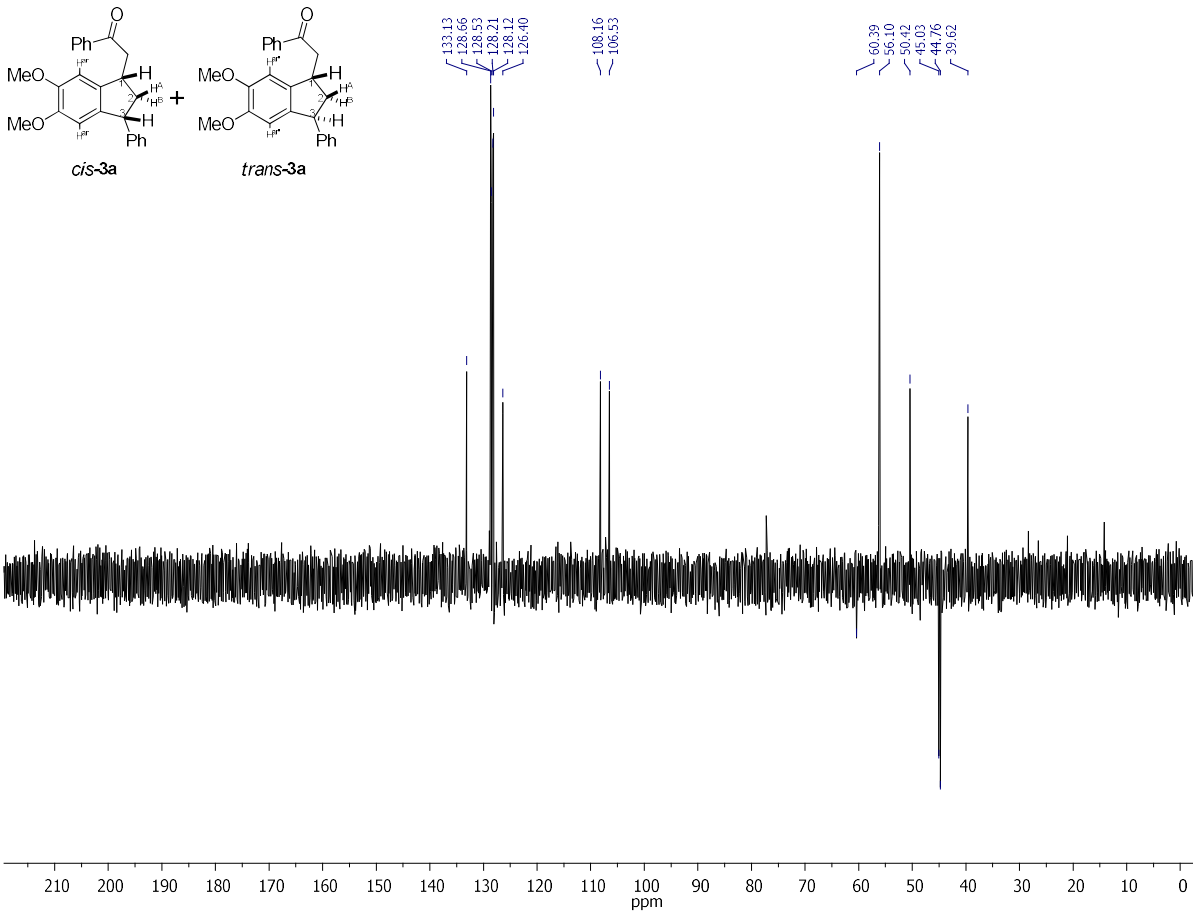


Fig. S35. DEPT of mixture of compounds *cis*-**3a** and *trans*-**3a**.

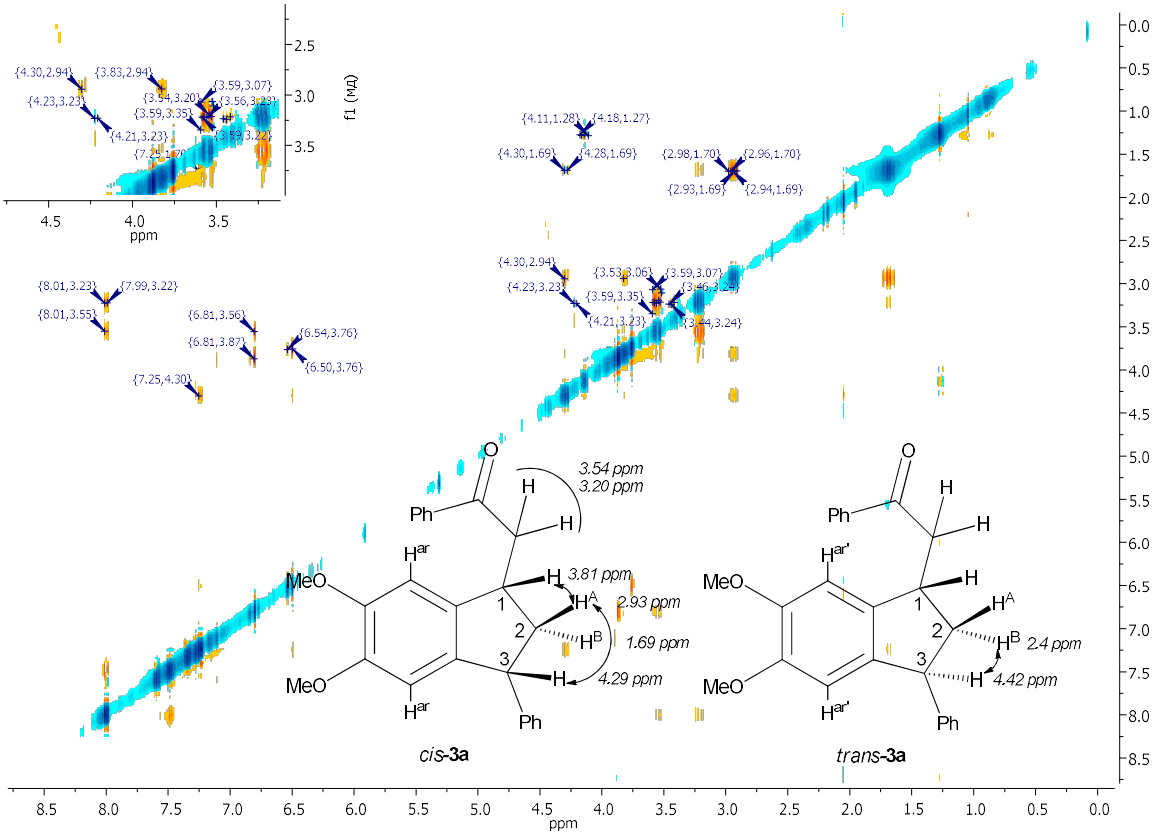


Fig. S36. NOESY spectrum of mixture of compounds *cis*-**3a** and *trans*-**3a**.

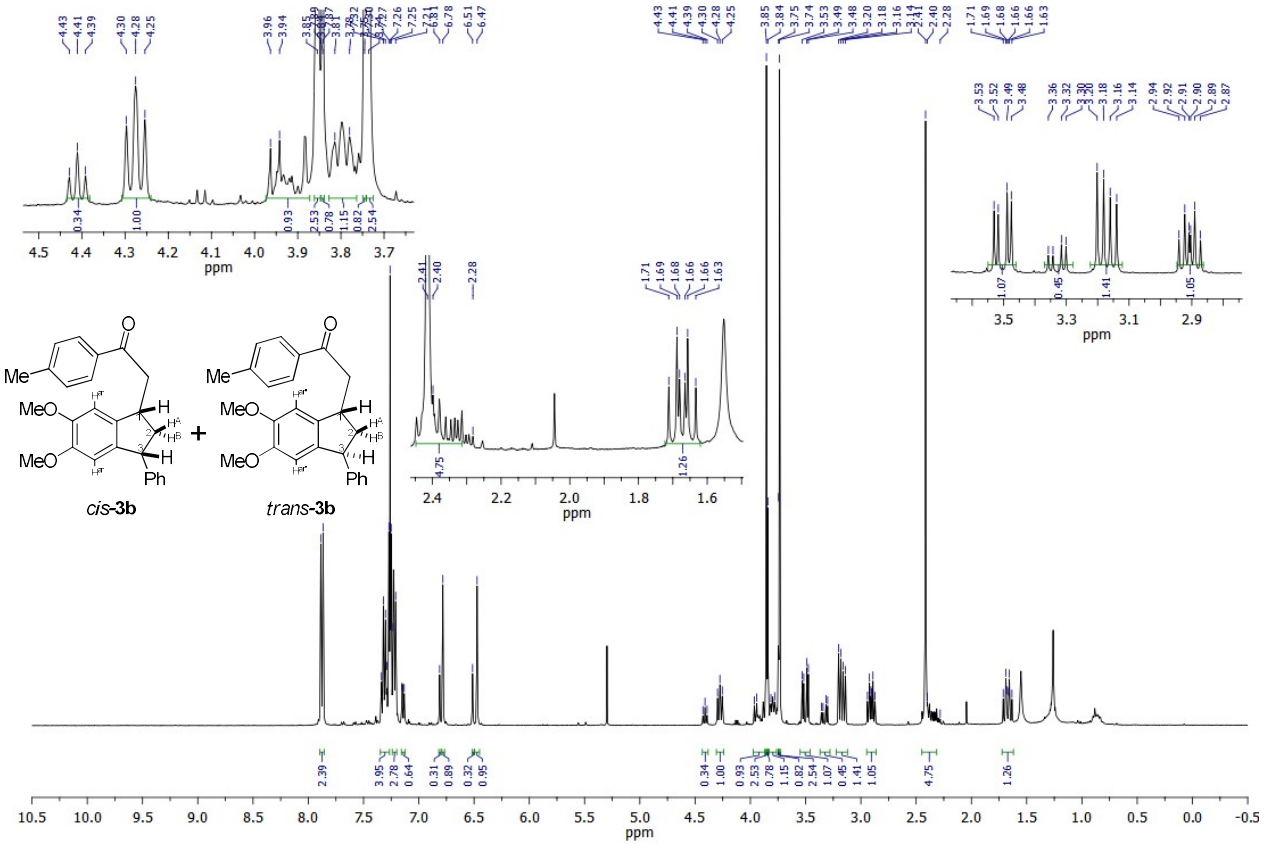


Fig. S37. ^{1}H NMR spectrum of mixture of compounds *cis*-**3b** and *trans*-**3b** ($CDCl_3$, 400 MHz).

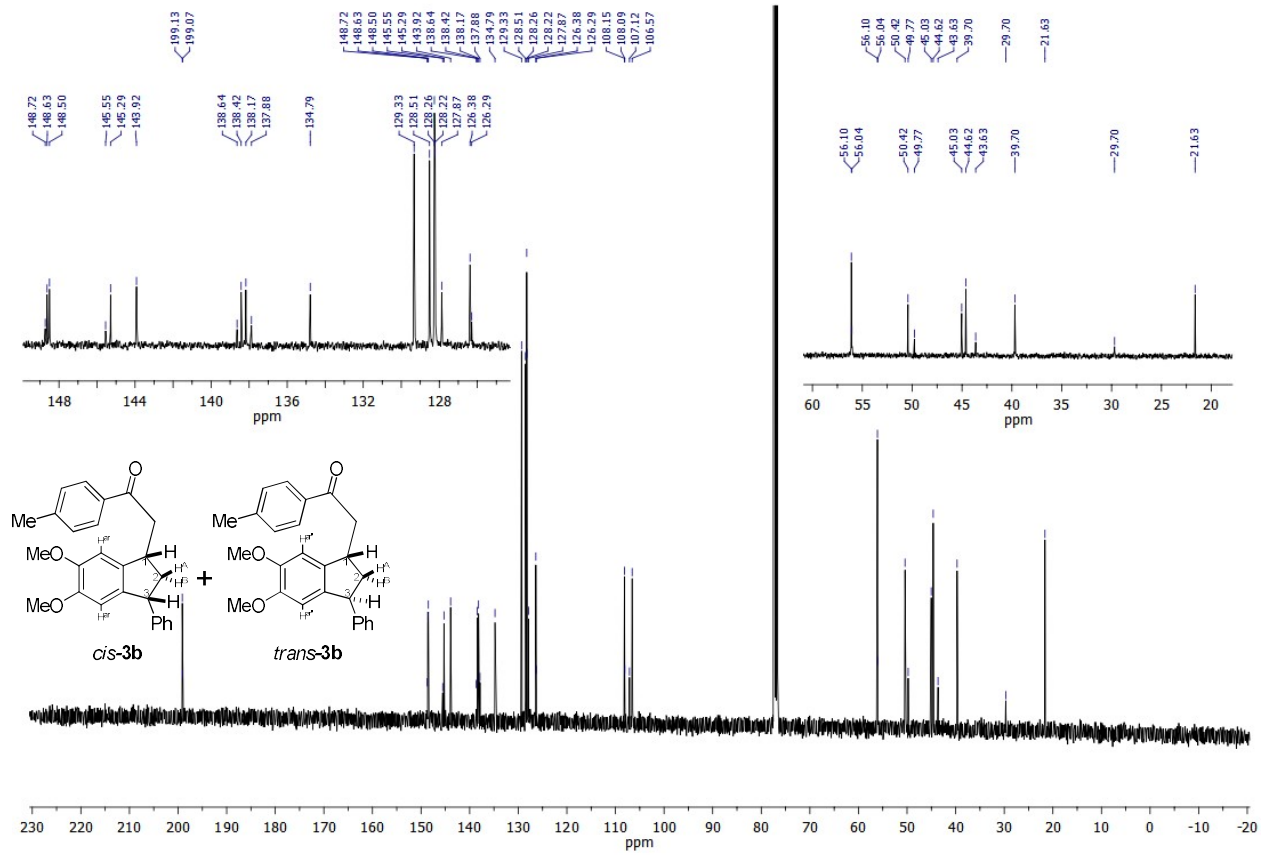


Fig. S38. ^{13}C NMR spectrum of mixture of compounds *cis*-**3b** and *trans*-**3b** ($CDCl_3$, 101 MHz).

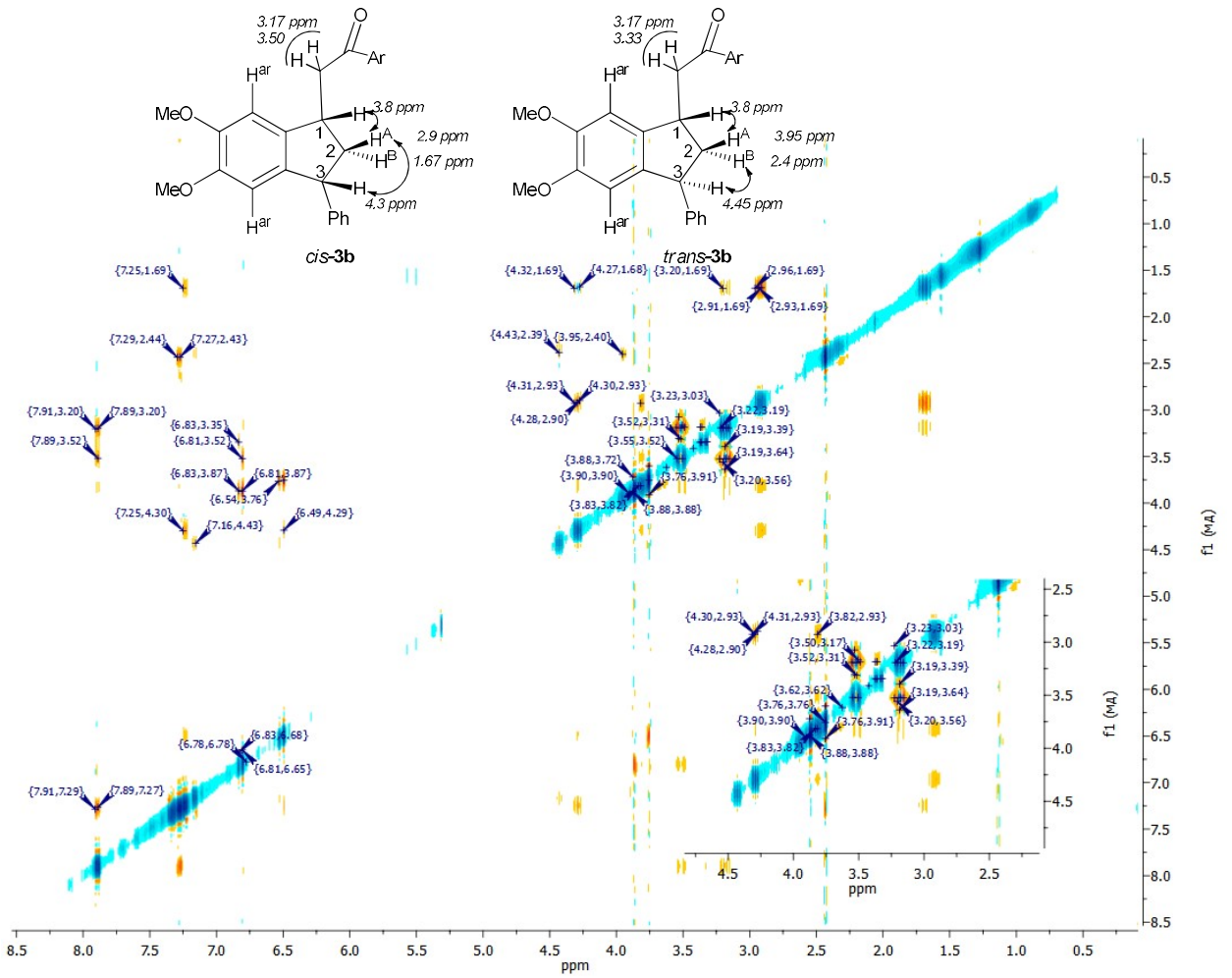


Fig. S39. NOESY spectrum of mixture of compounds *cis*-**3b** and *trans*-**3b**.

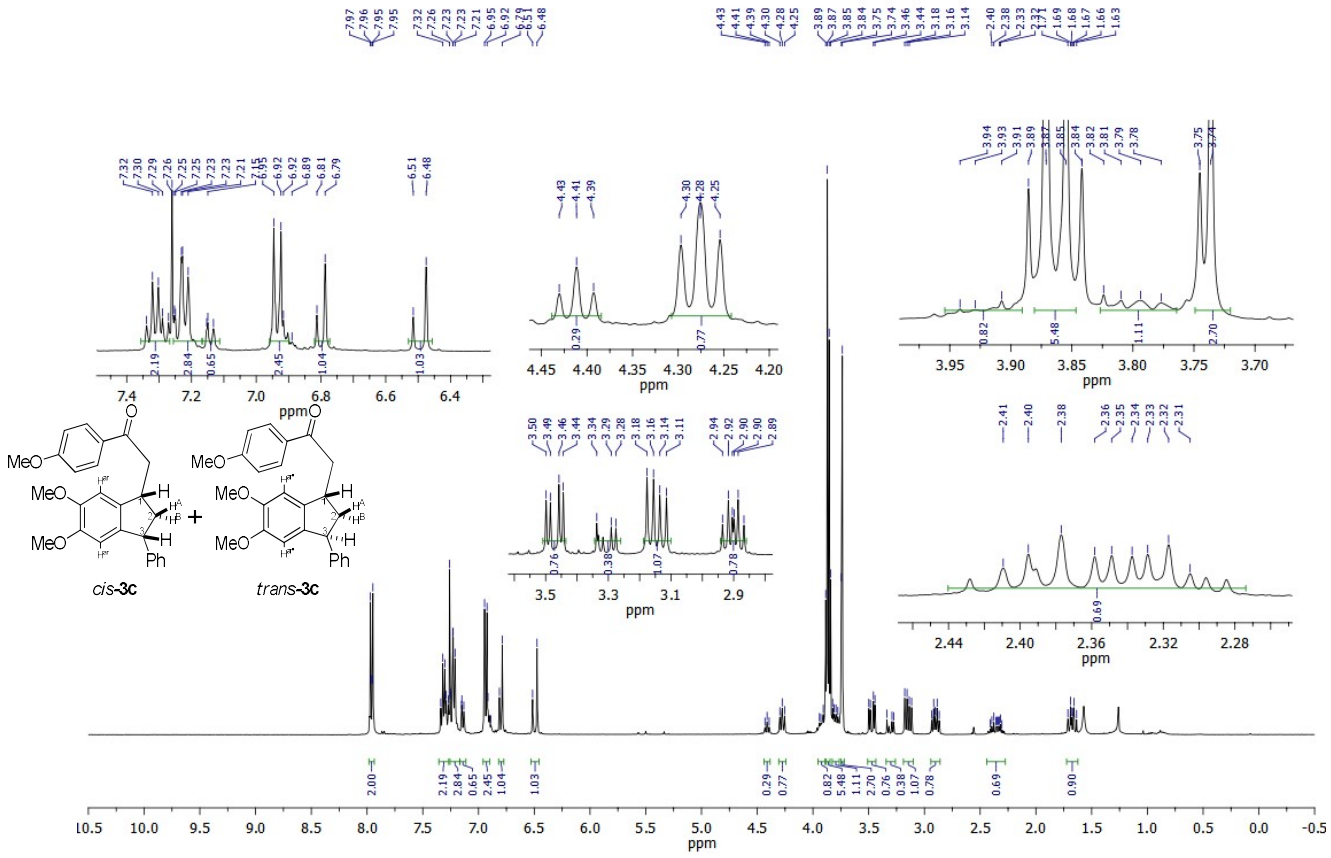


Fig. S40. ^{1}H NMR spectrum of mixture of compounds *cis*-**3c** and *trans*-**3c** ($CDCl_3$, 400 MHz).

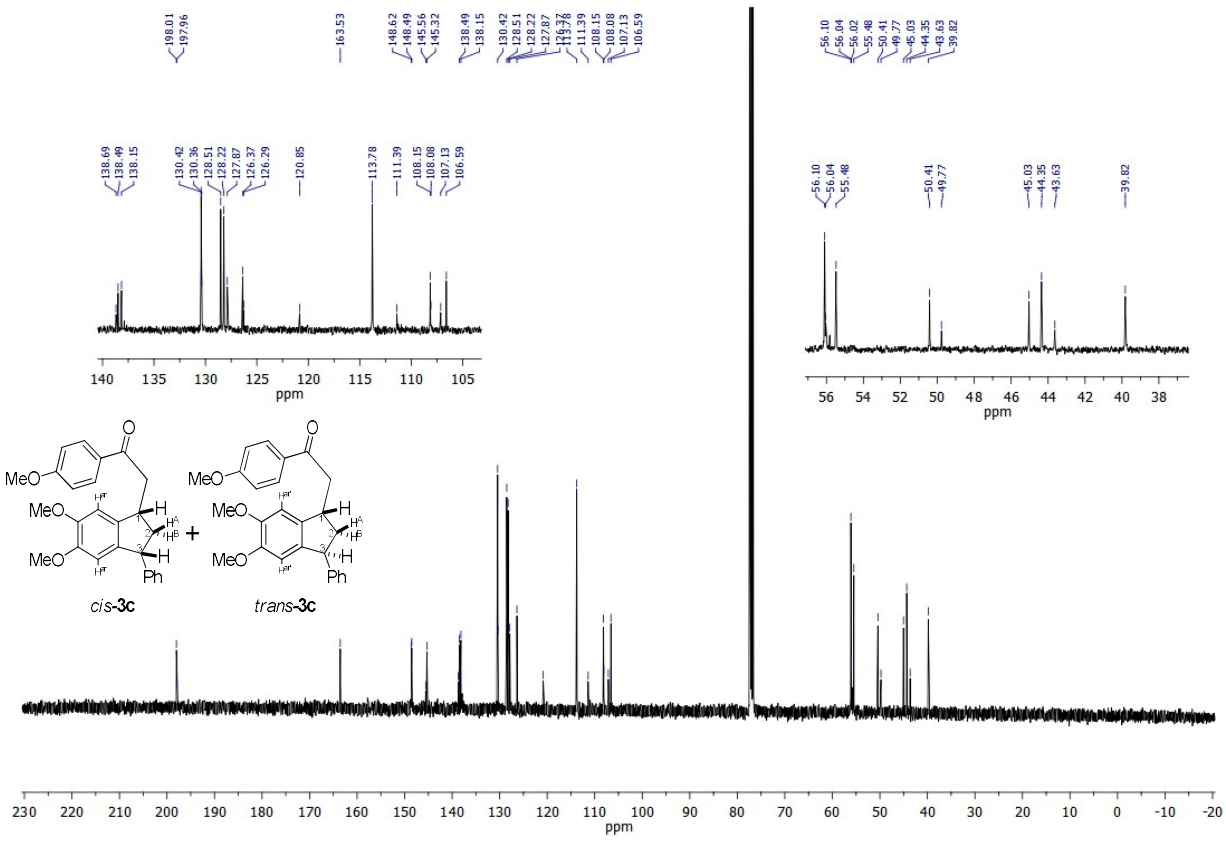


Fig. S41. ^{13}C NMR spectrum of mixture of compounds *cis*-**3c** and *trans*-**3c** ($CDCl_3$, 101 MHz).

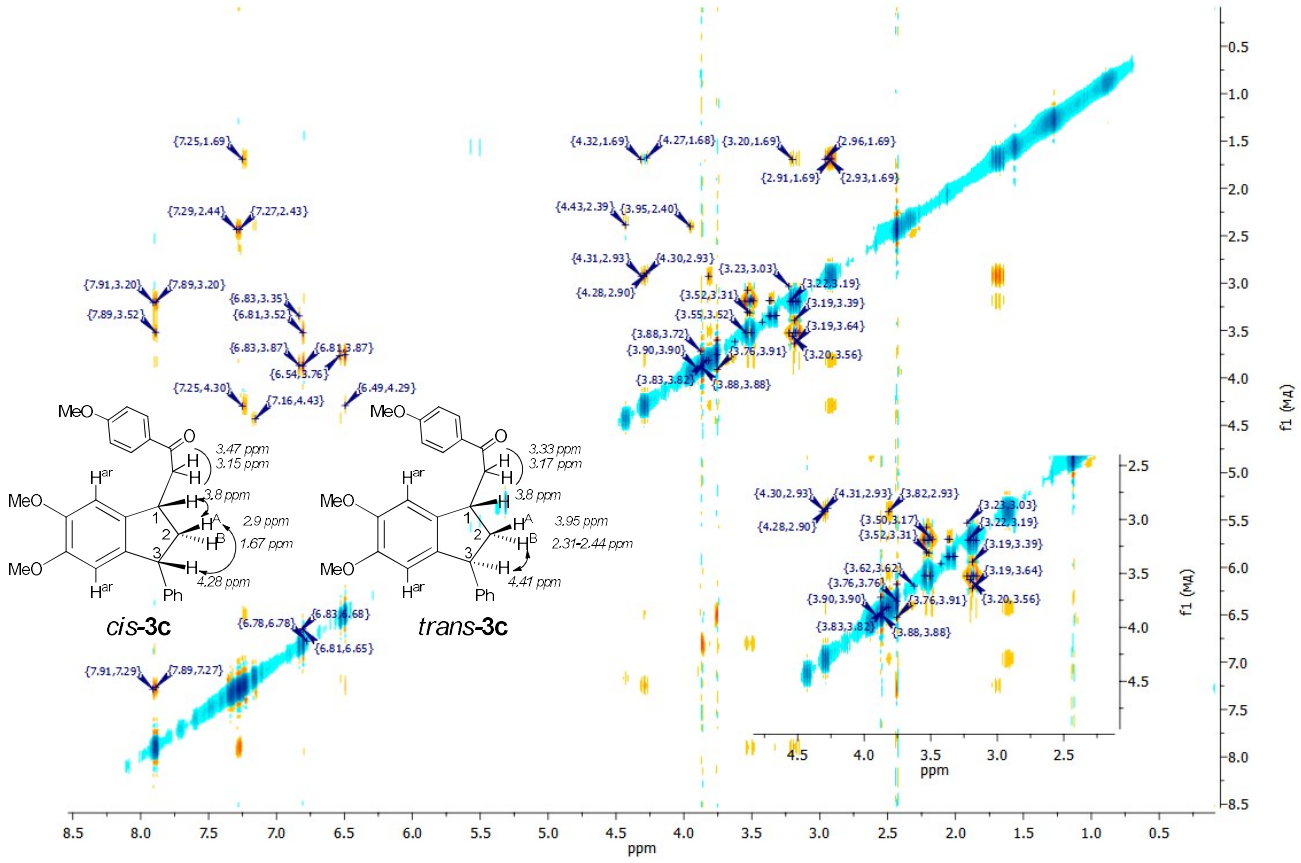


Fig. S42. NOESY spectrum of mixture of compounds *cis*-**3c** and *trans*-**3c**.

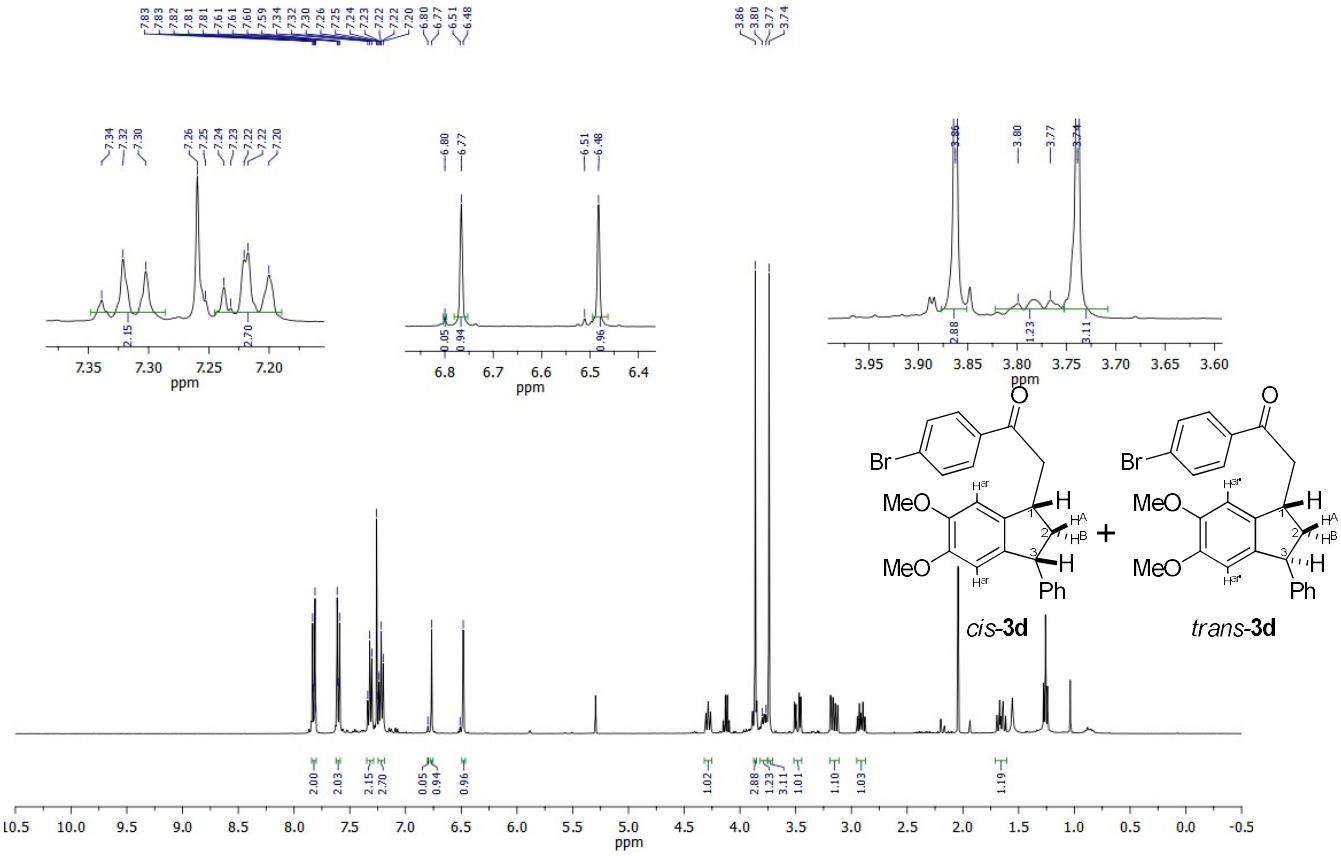


Fig. S43. ^{1}H NMR spectrum of mixture of compounds *cis*-**3d** and *trans*-**3d** ($CDCl_3$, 400 MHz).

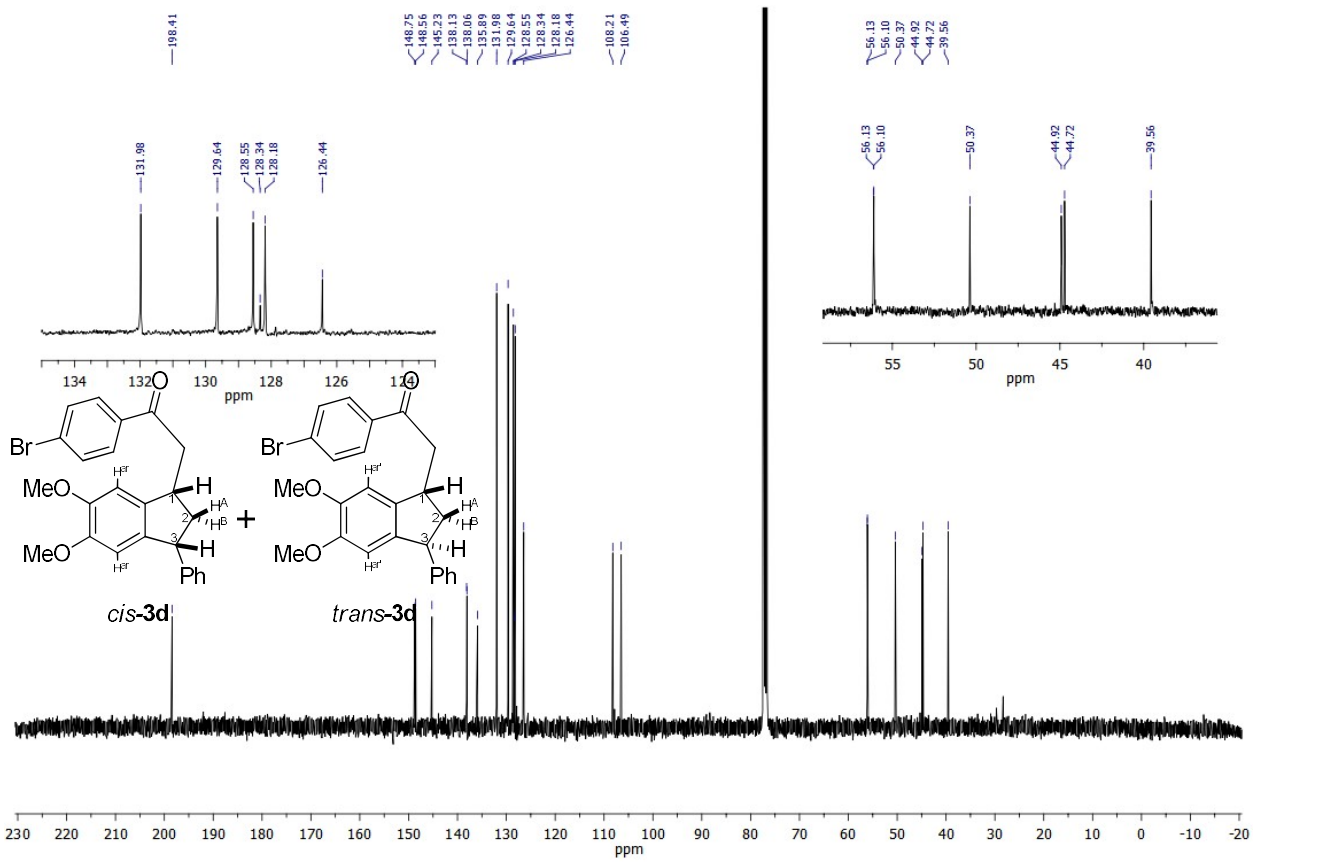


Fig. S44. ^{13}C NMR spectrum of mixture of compounds *cis*-**3d** and *trans*-**3d** ($CDCl_3$, 101 MHz).

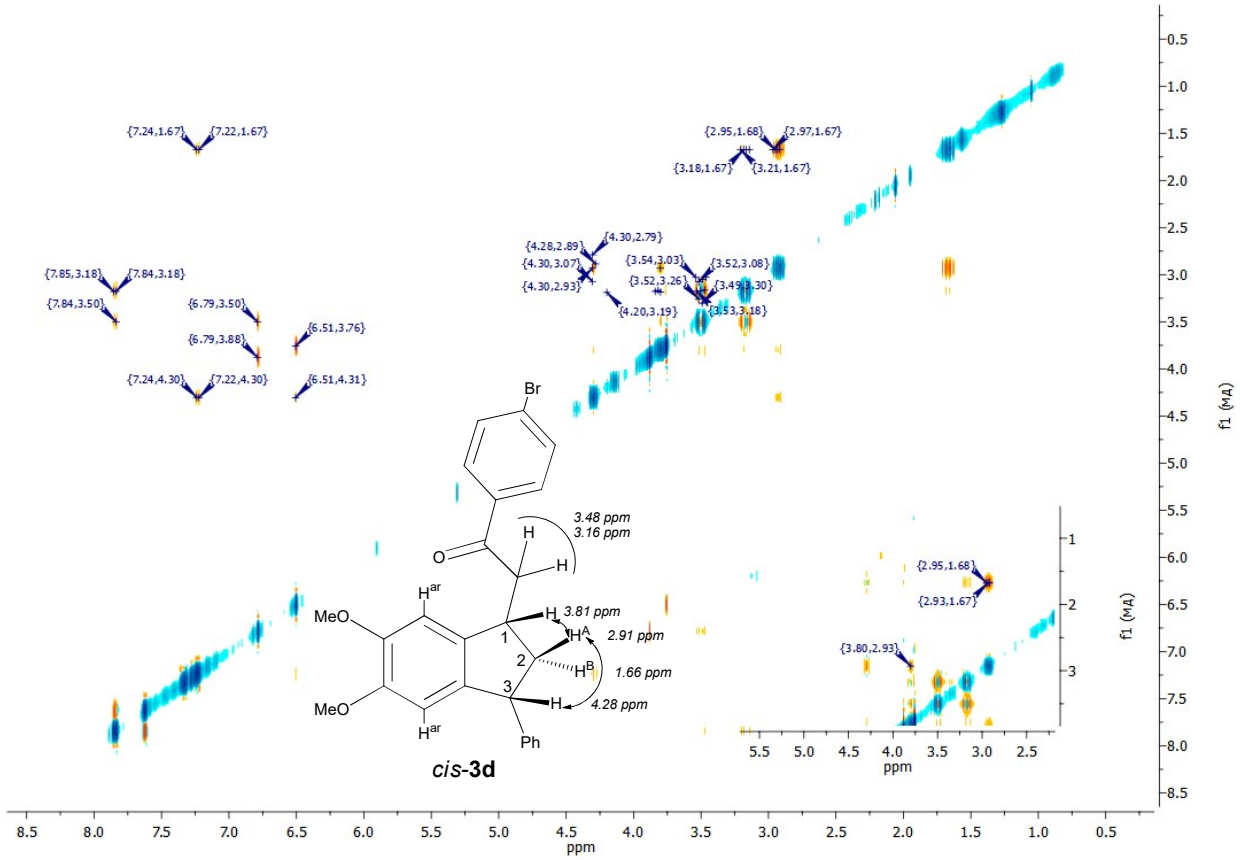


Fig. S45. NOESY spectrum of mixture of compounds *cis*-**3d** and *trans*-**3d**.

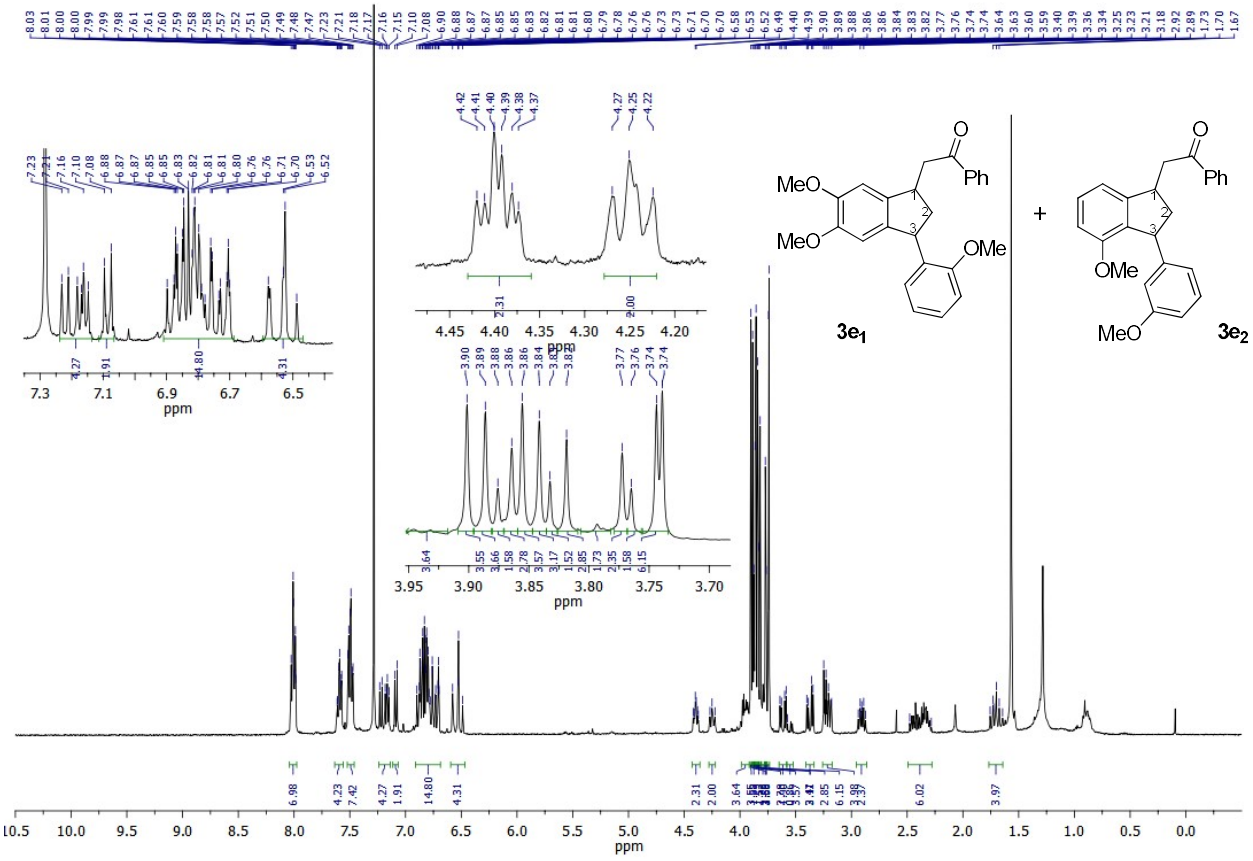


Fig. S46. ^{1}H NMR spectrum of mixture of compounds **3e$_1$** and **3e$_2$** ($CDCl_3$, 400 MHz).

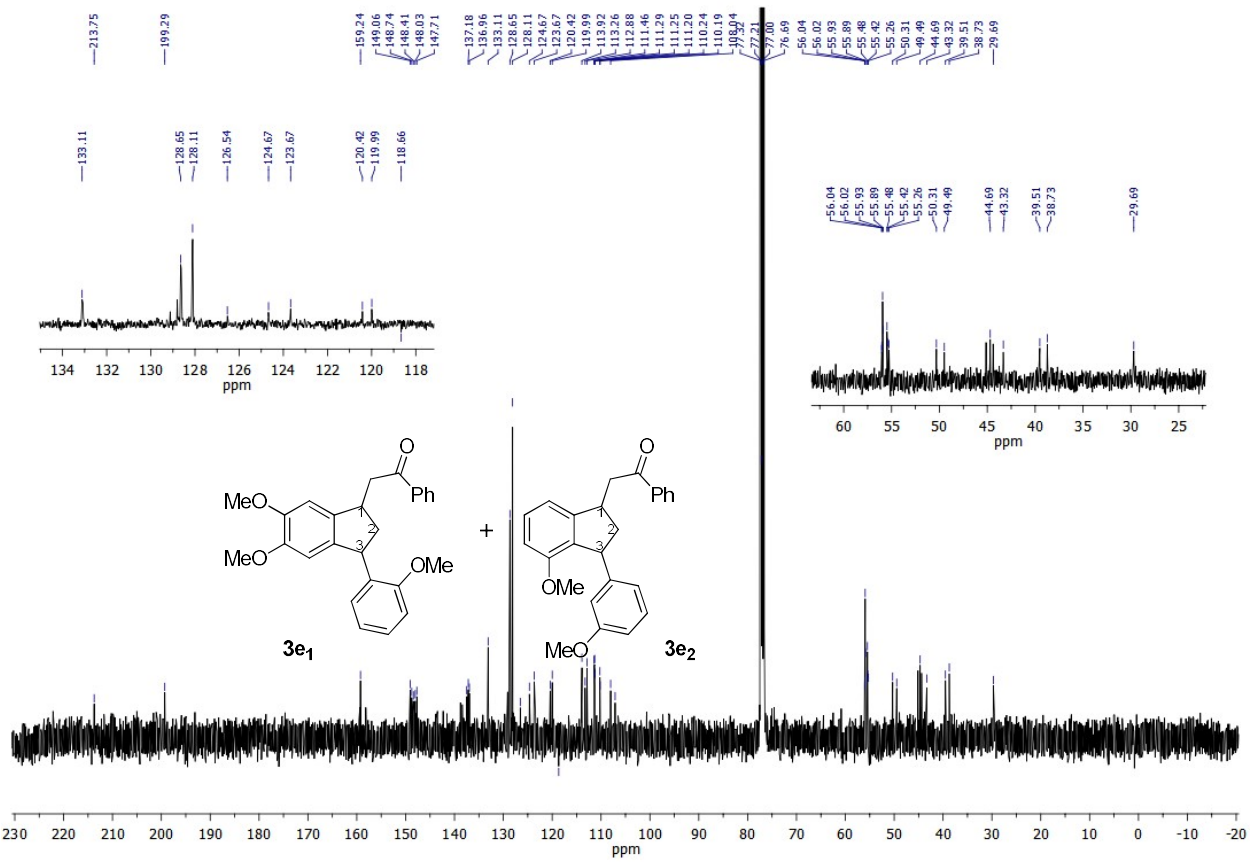


Fig. S47. ^{13}C NMR spectrum of mixture of compounds **3e$_1$** and **3e$_2$** ($CDCl_3$, 101 MHz).

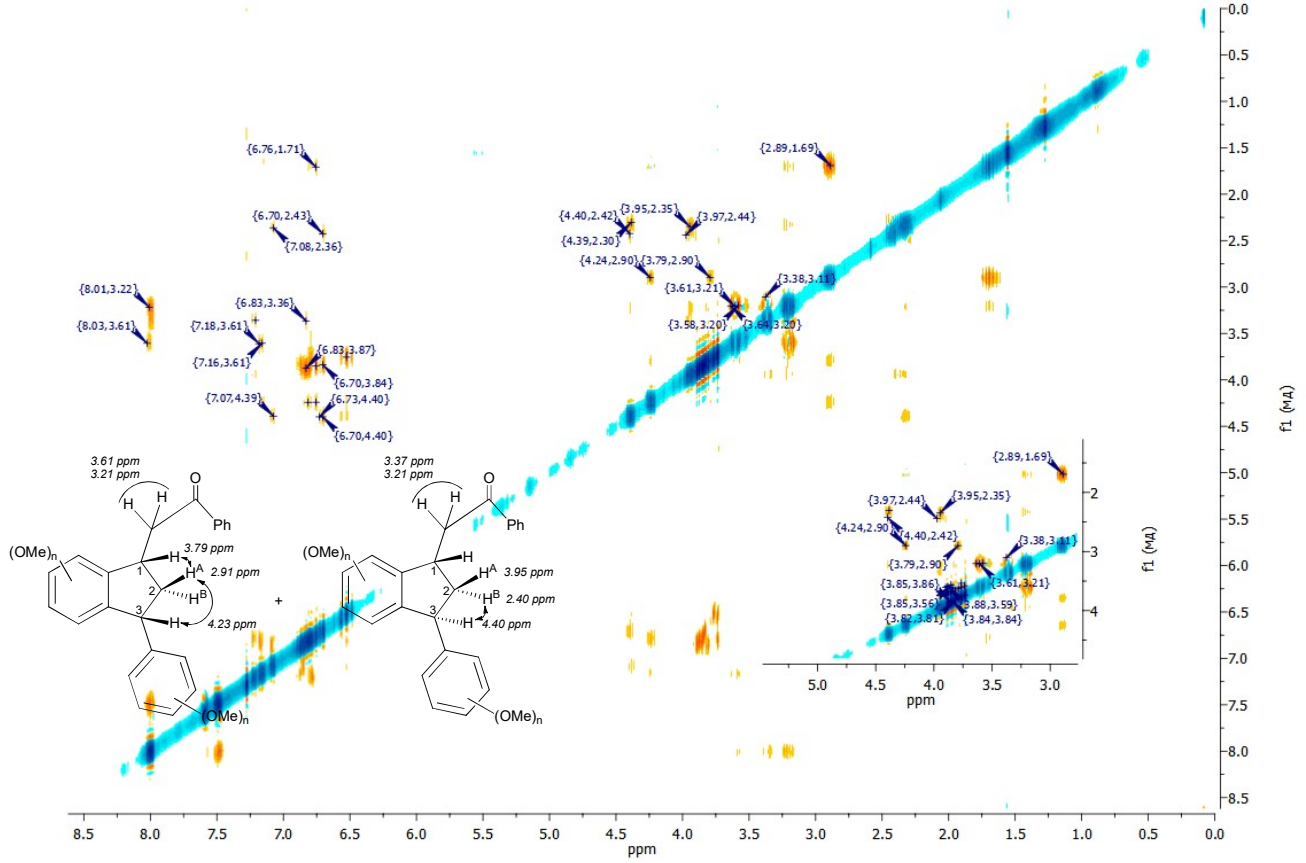


Fig. S48. NOESY spectrum of mixture of compounds **3e$_1$** and **3e$_2$**.

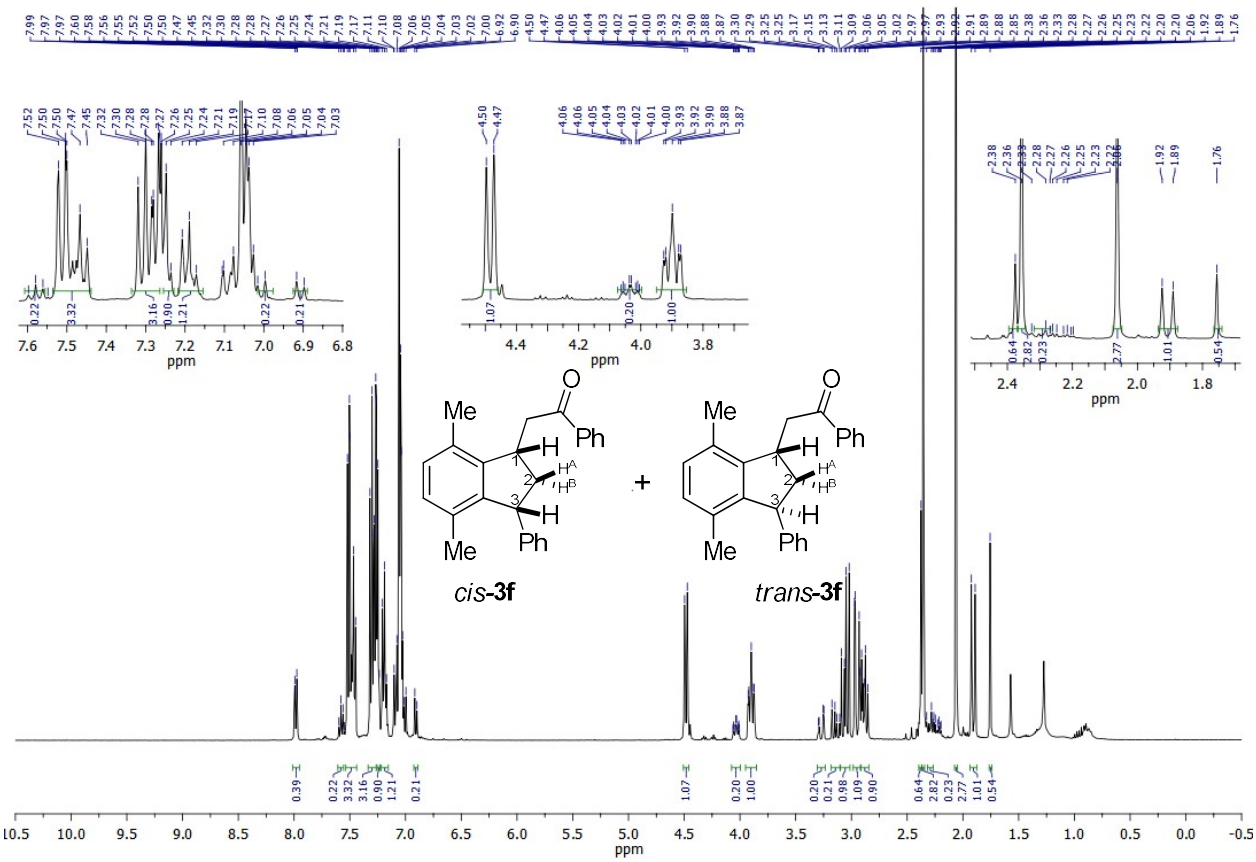


Fig. S49. ^{1}H NMR spectrum of mixture of compounds *cis*-**3f** and *trans*-**3f** ($CDCl_3$, 400 MHz).

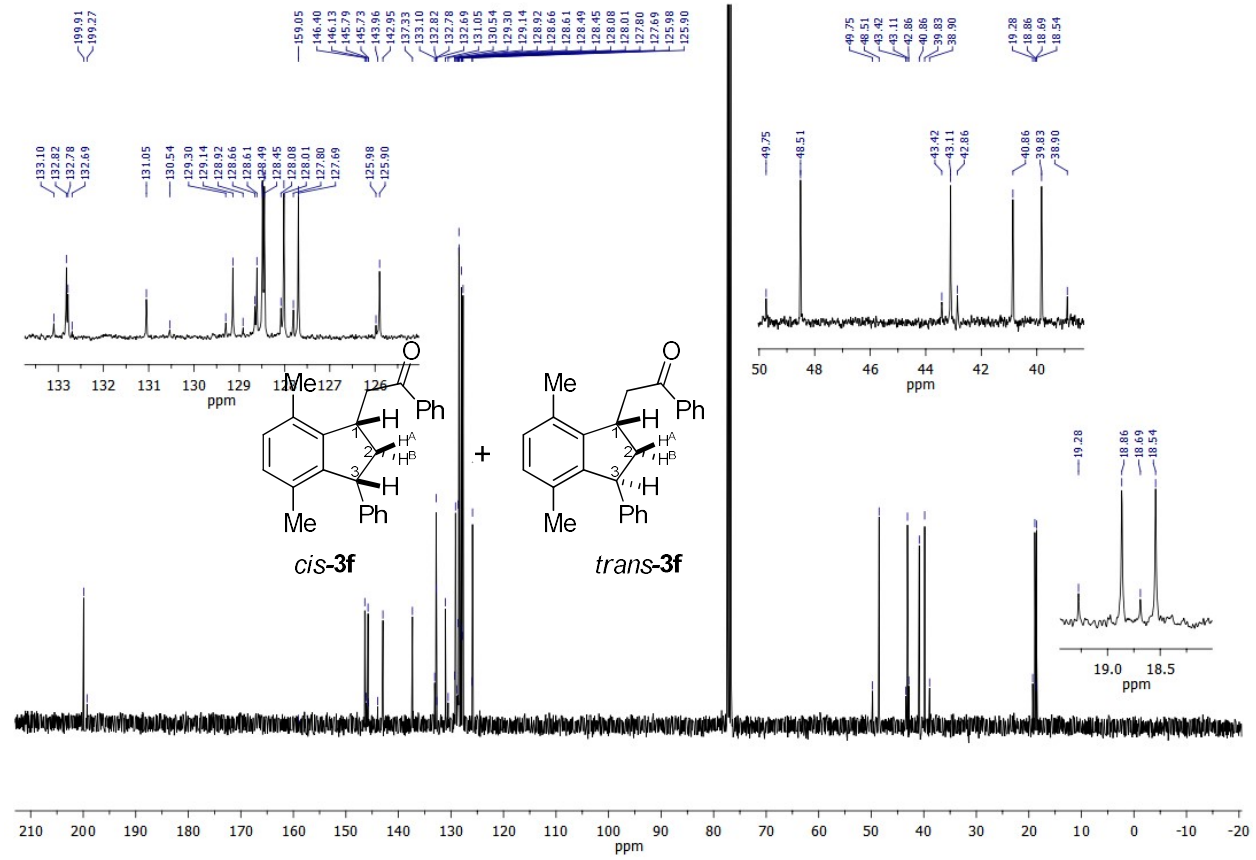


Fig. S50. ^{13}C NMR spectrum of mixture of compounds *cis*-**3f** and *trans*-**3f** ($CDCl_3$, 101 MHz).

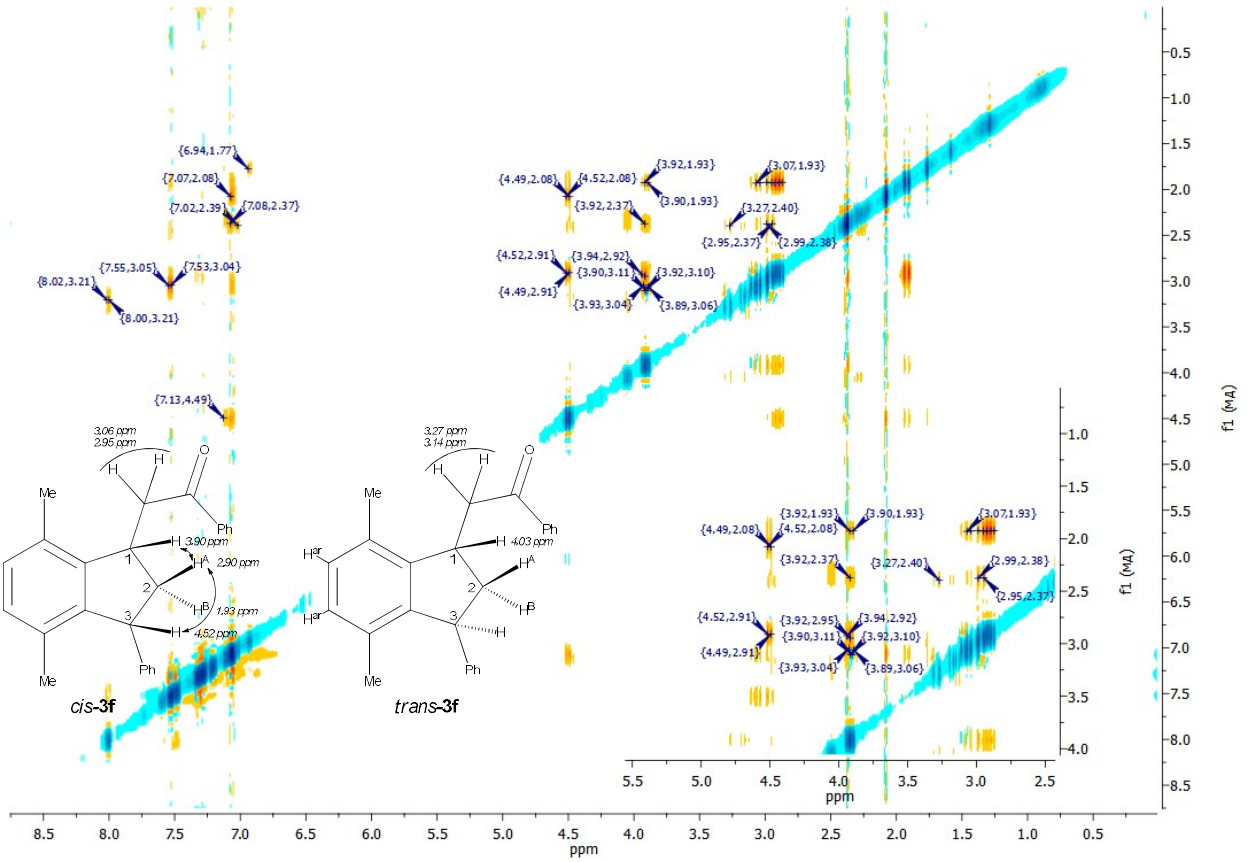


Fig. S51. NOESY spectrum of mixture of compounds *cis*-**3f** and *trans*-**3f**.

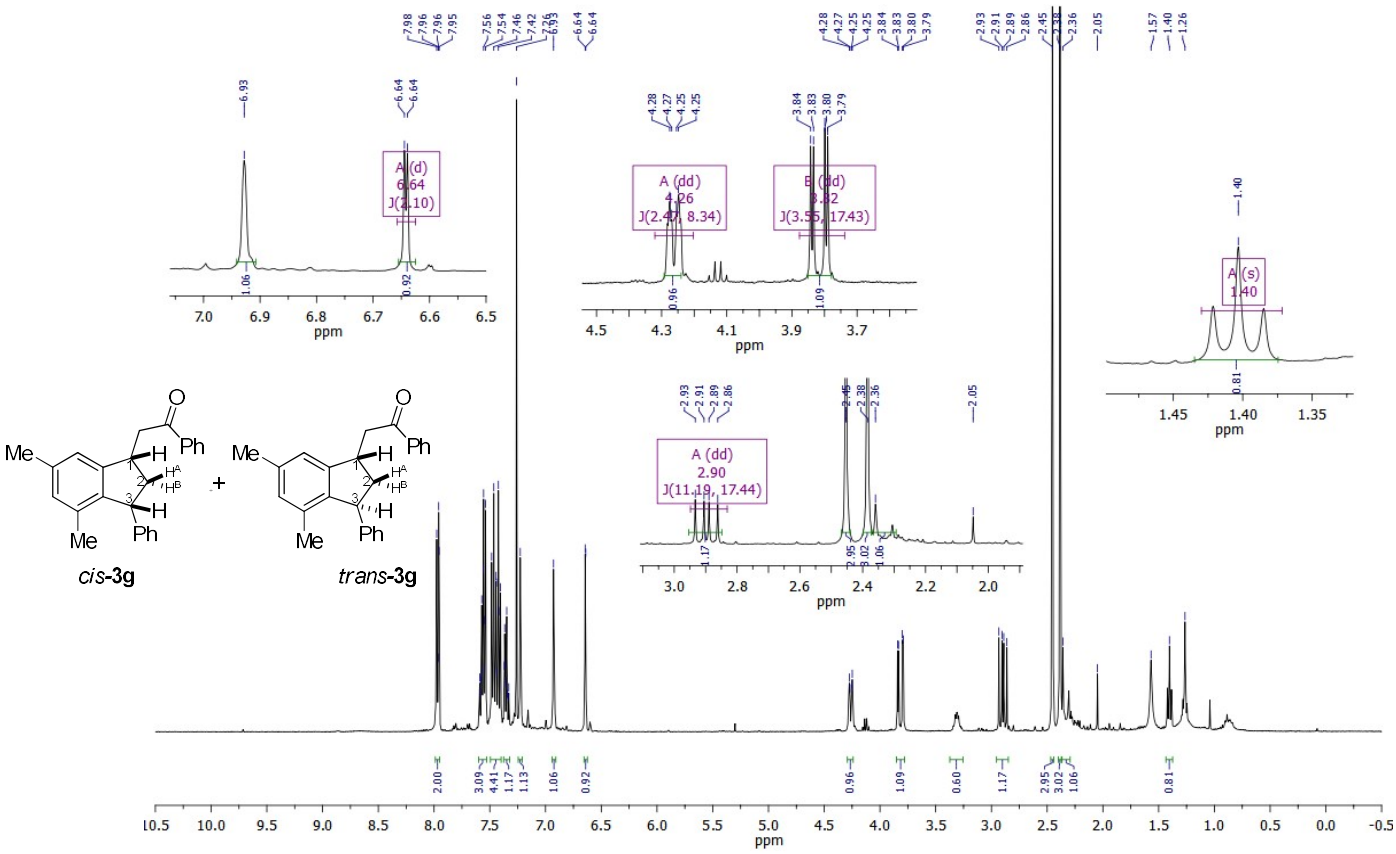


Fig. S52. ^{1}H NMR spectrum of mixture of compounds *cis*-**3g** and *trans*-**3g** ($CDCl_3$, 400 MHz).

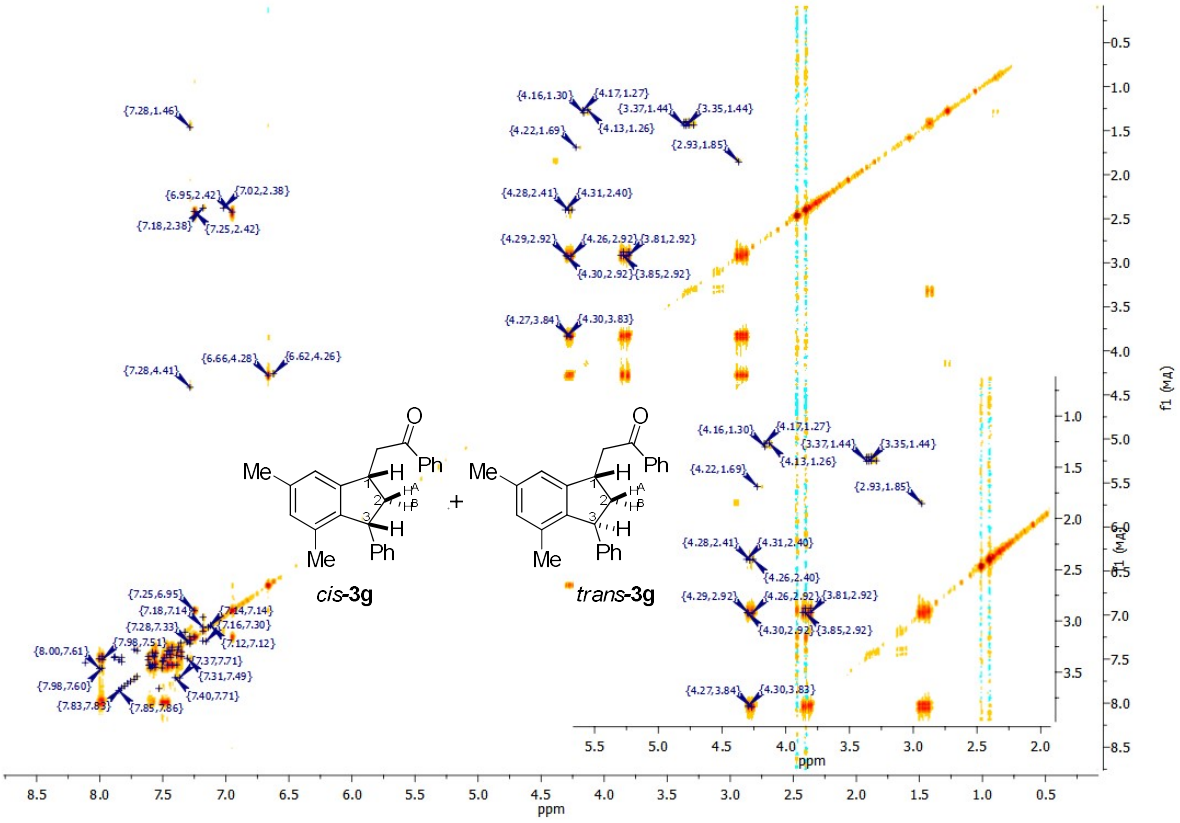


Fig. S53. COSY H-H spectrum of mixture of compounds *cis*-**3g** and *trans*-**3g**.

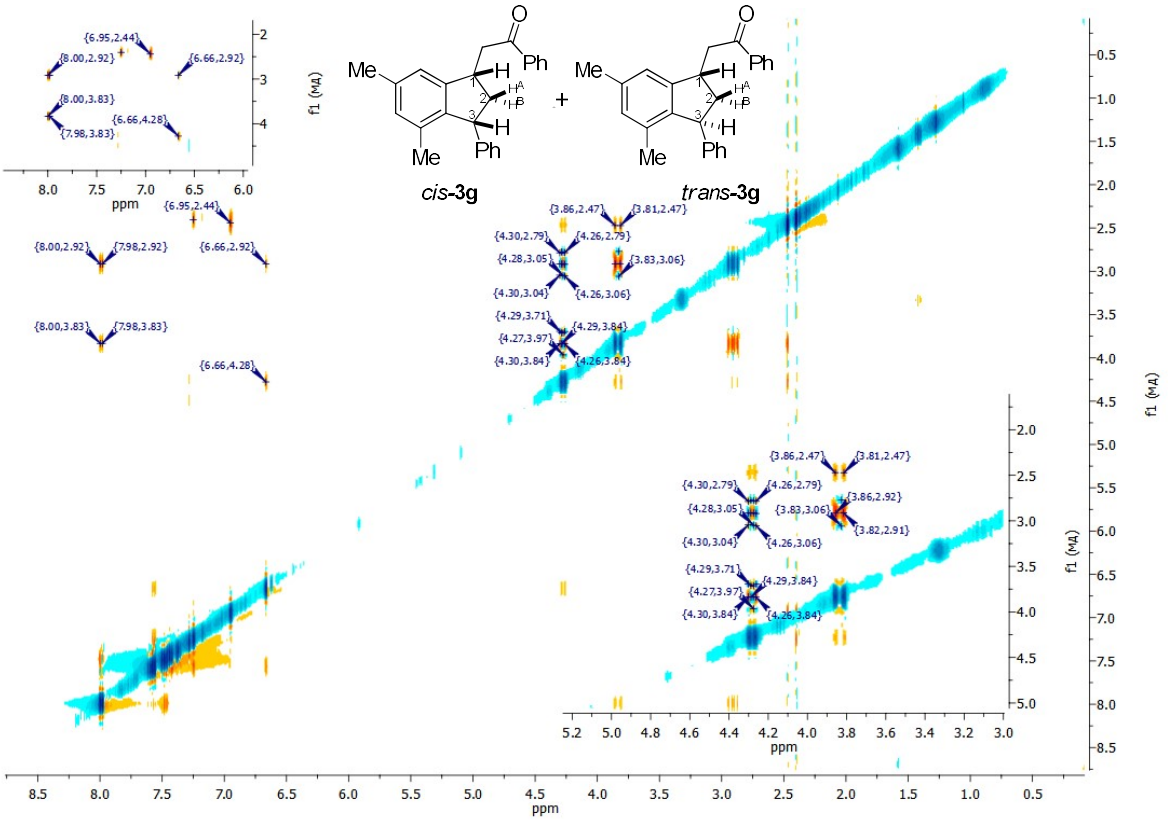


Fig. S54. NOESY spectrum of mixture of compounds *cis*-**3g** and *trans*-**3g**.

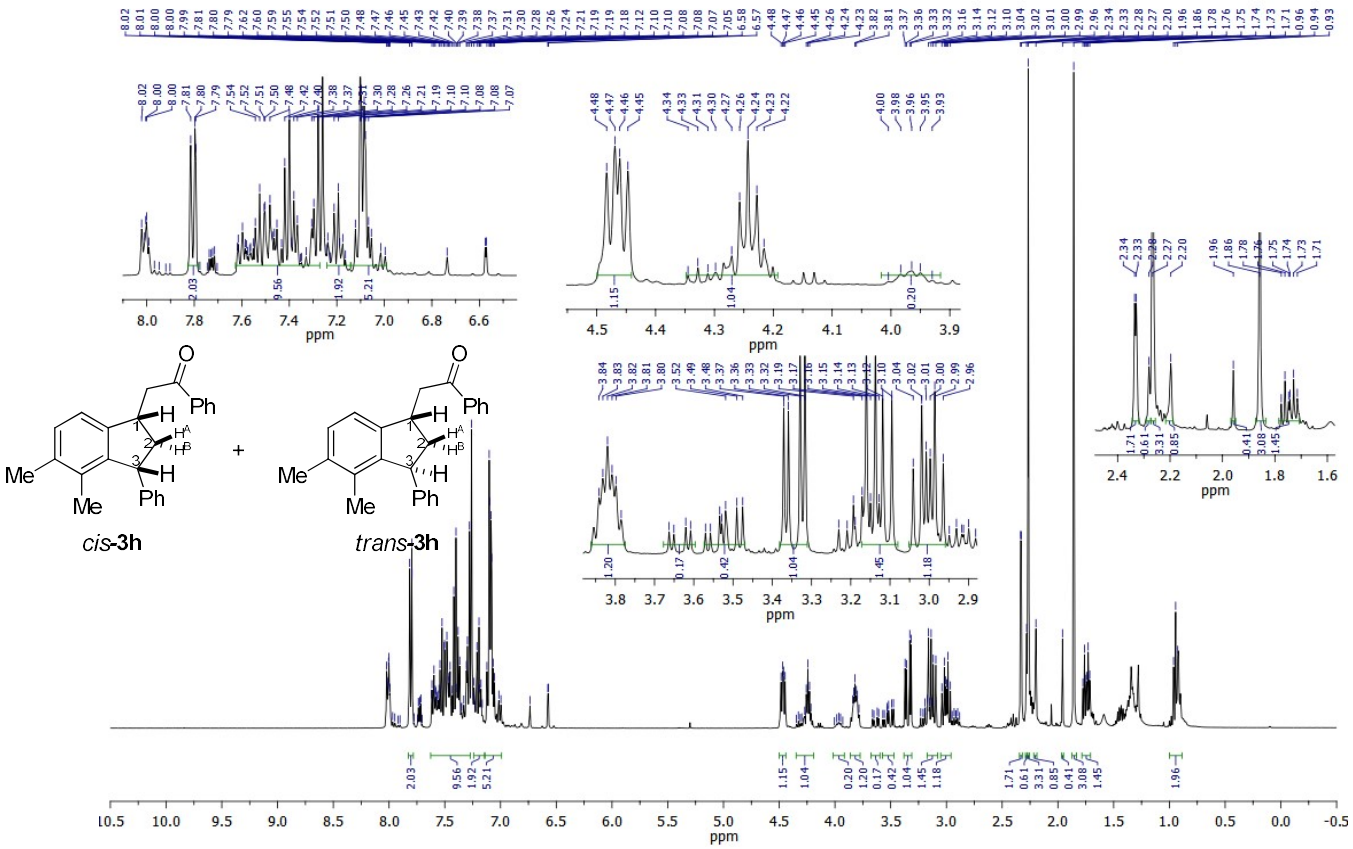


Fig. S55. ^{1}H NMR spectrum of mixture of compounds *cis*-**3h** and *trans*-**3h** ($CDCl_3$, 400 MHz).

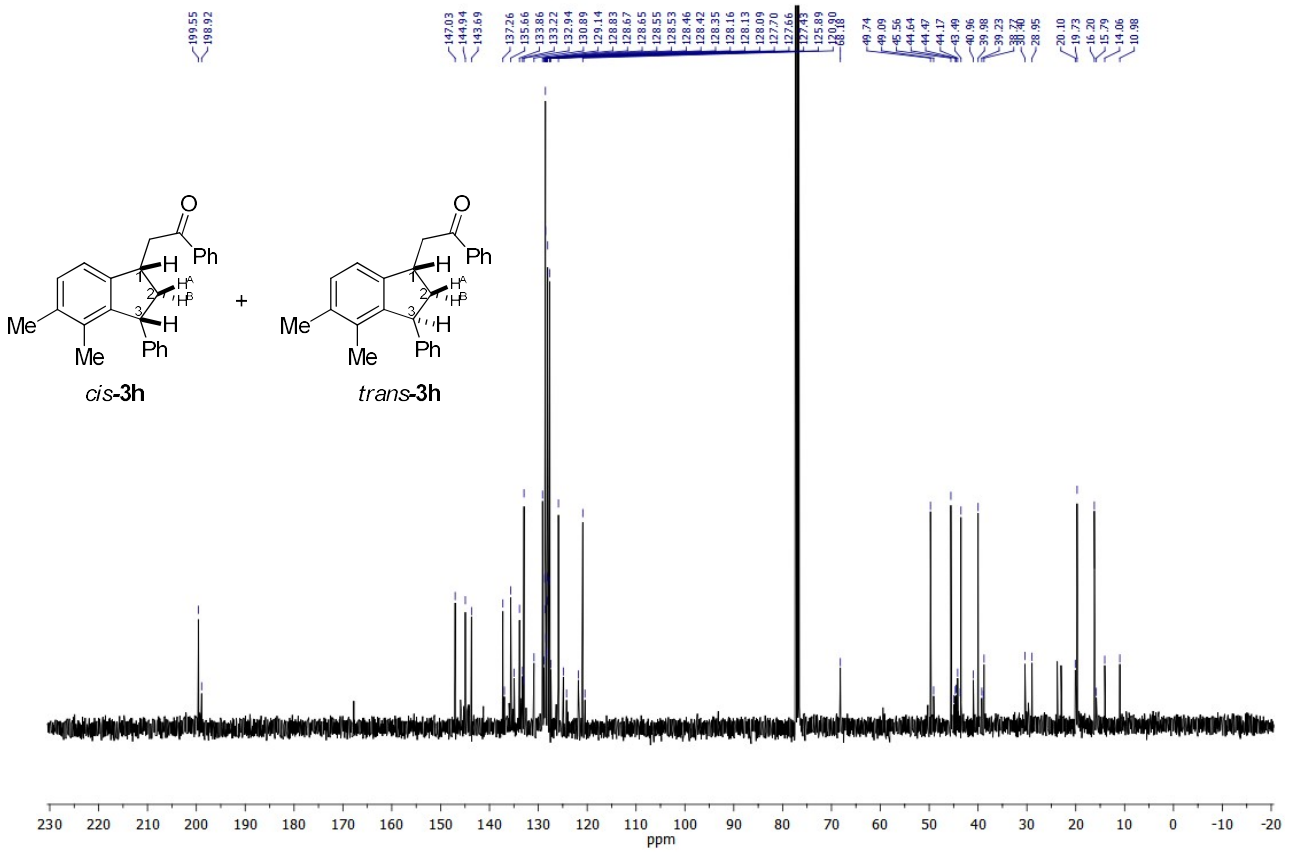


Fig. S56. ^{13}C NMR spectrum of mixture of compounds *cis*-**3h** and *trans*-**3h** ($CDCl_3$, 101 MHz).

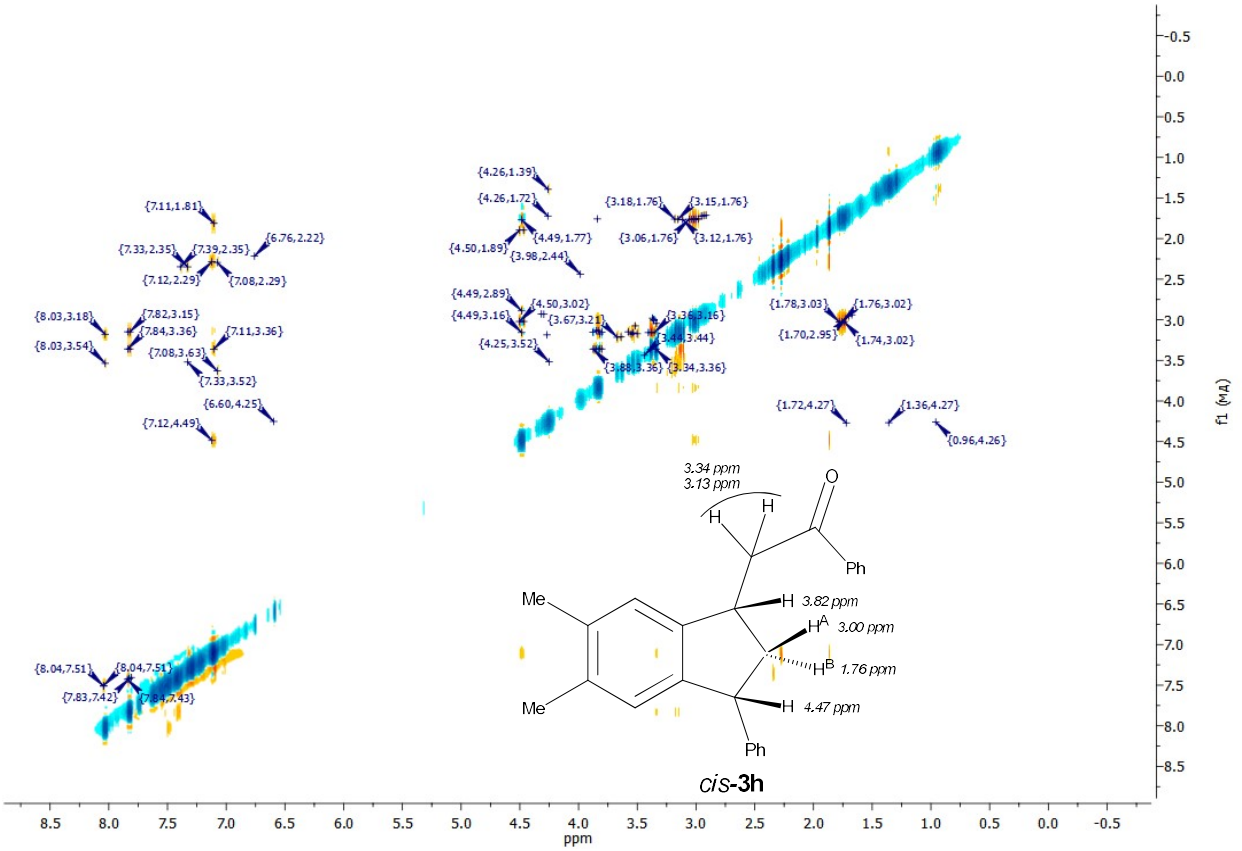


Fig. S57. NOESY spectrum of mixture of compounds *cis*-**3h** and *trans*-**3h**.

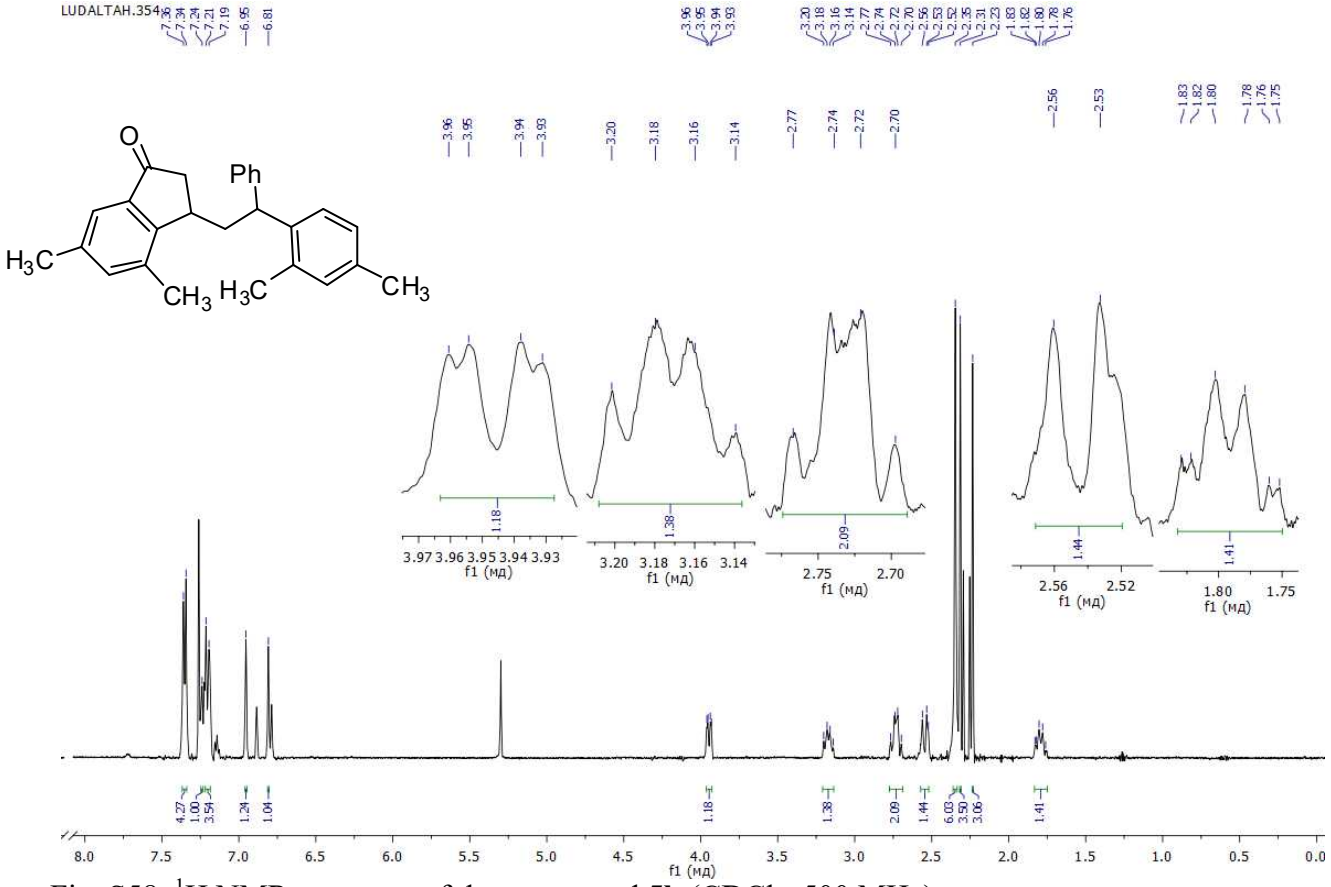


Fig. S58. ^{1}H NMR spectrum of the compound **5b** ($CDCl_3$, 500 MHz).

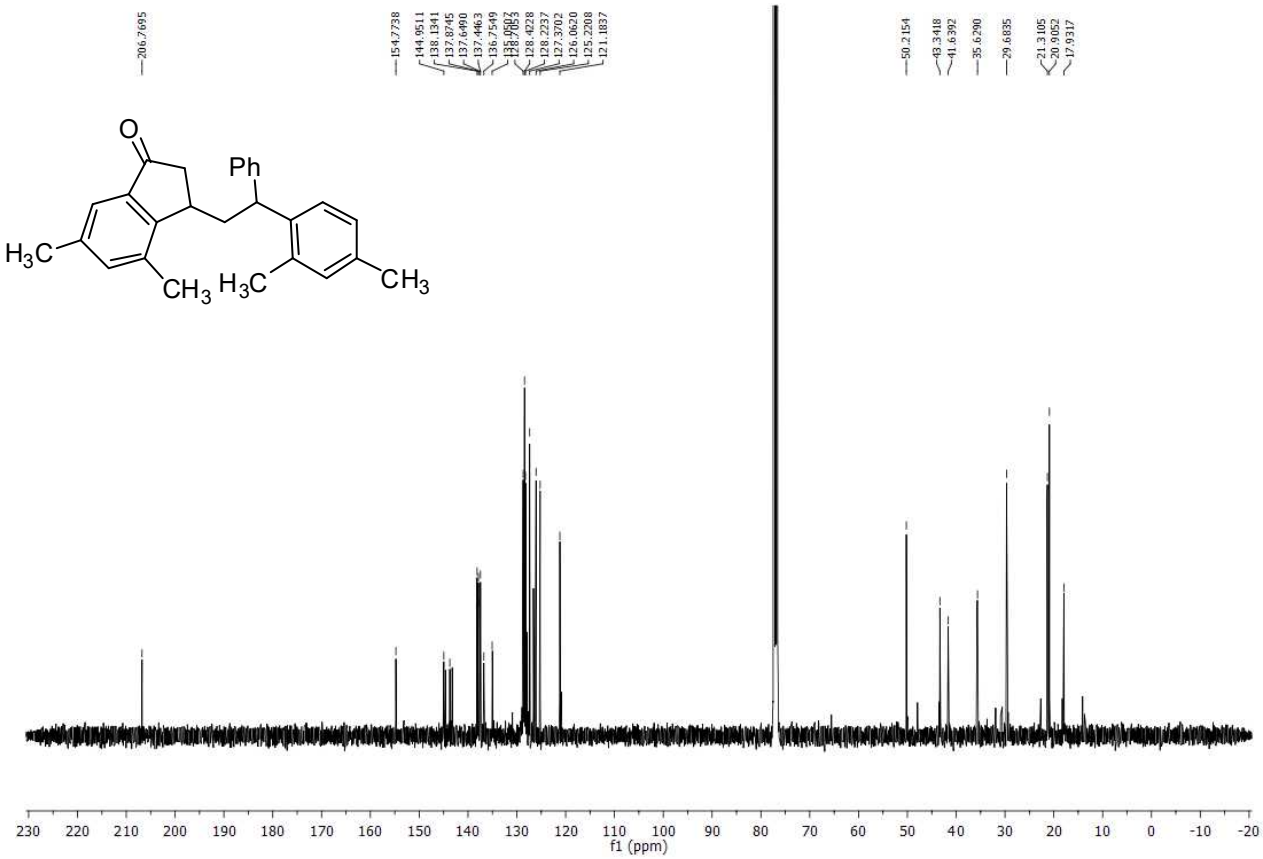


Fig. S59. ^{13}C NMR spectrum of the compound **5b** ($CDCl_3$, 125 MHz).

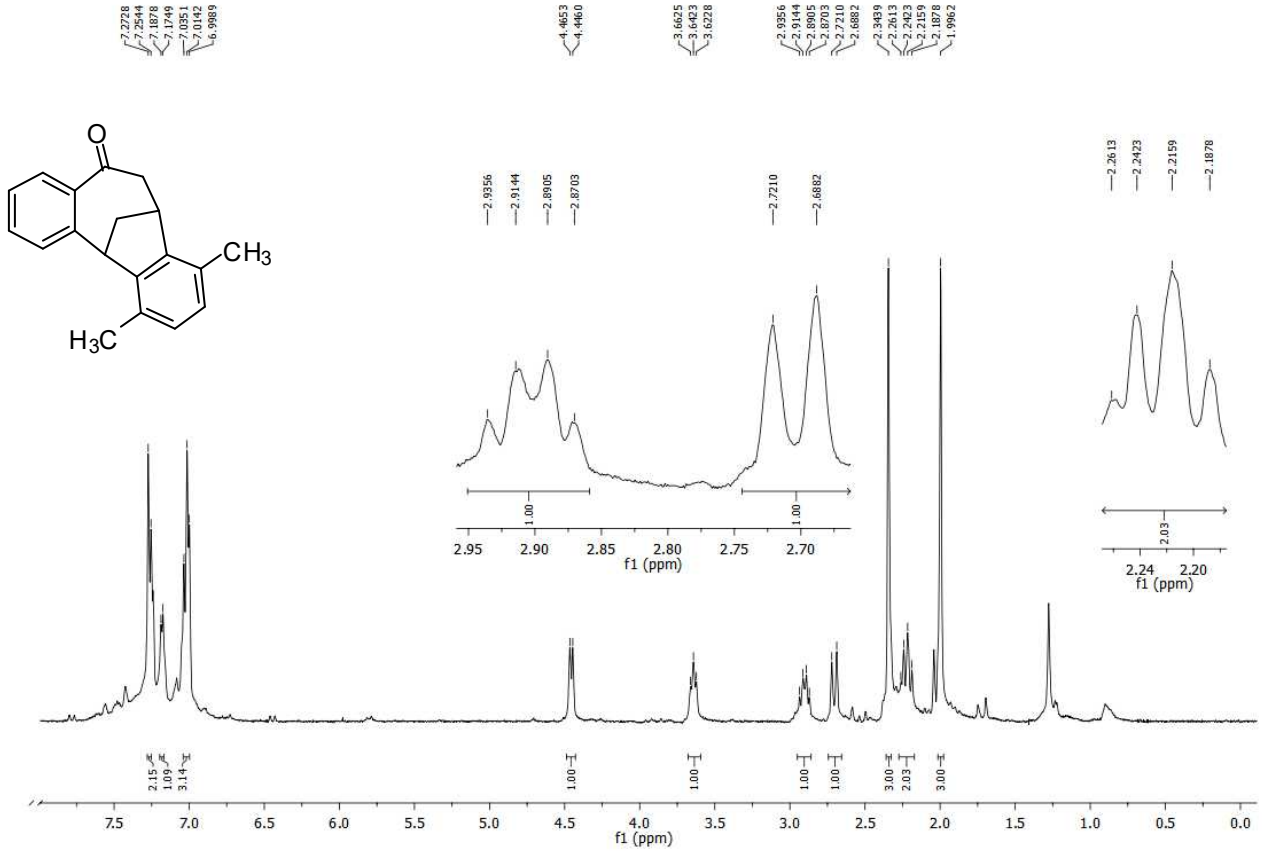


Fig. S60. ^{1}H NMR spectrum of the compound **6a** ($CDCl_3$, 500 MHz).

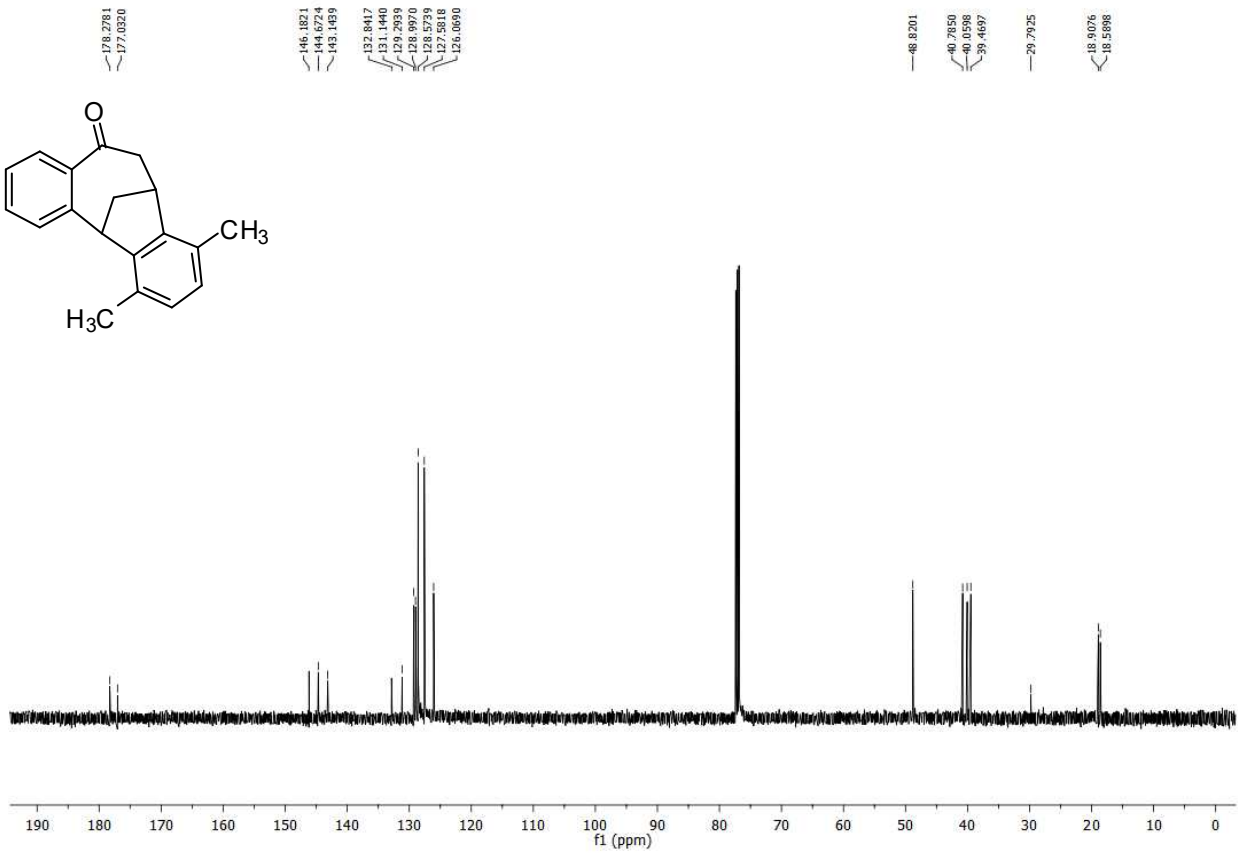


Fig. S61. ^{13}C NMR spectrum of the compound **6a** ($CDCl_3$, 125 MHz).

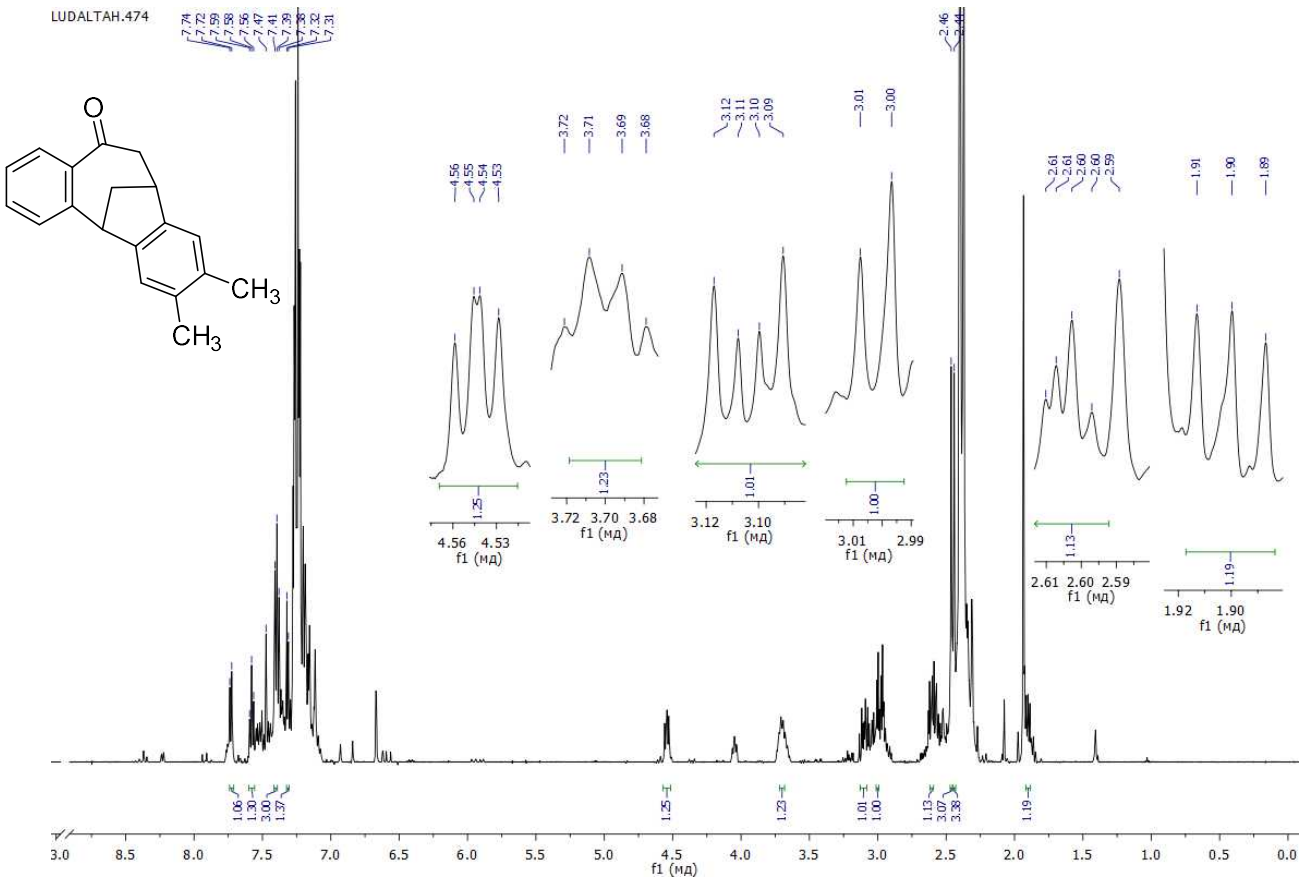


Fig. S62. ^{1}H NMR spectrum of the compound **6b** ($CDCl_3$, 500 MHz).

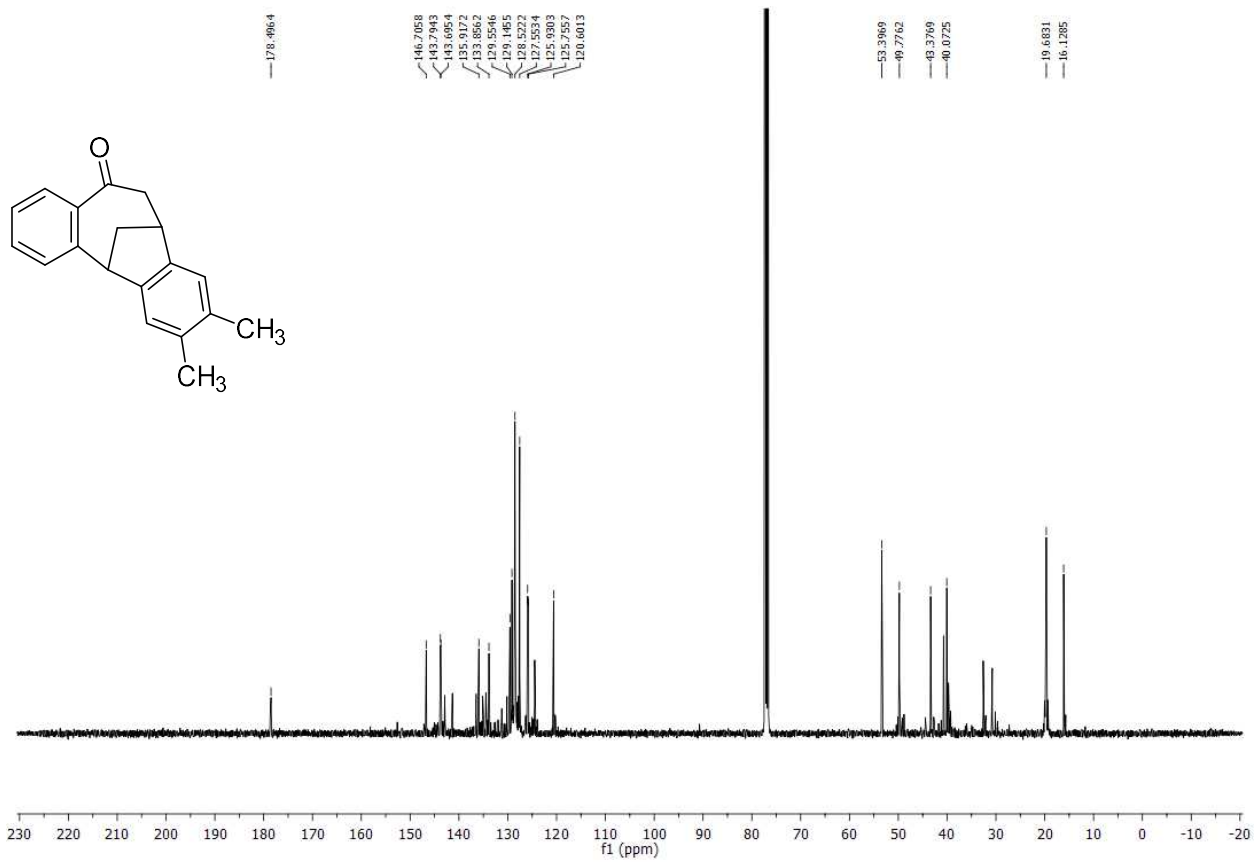


Fig. S63. ^{13}C NMR spectrum of the compound **6b** ($CDCl_3$, 125 MHz).

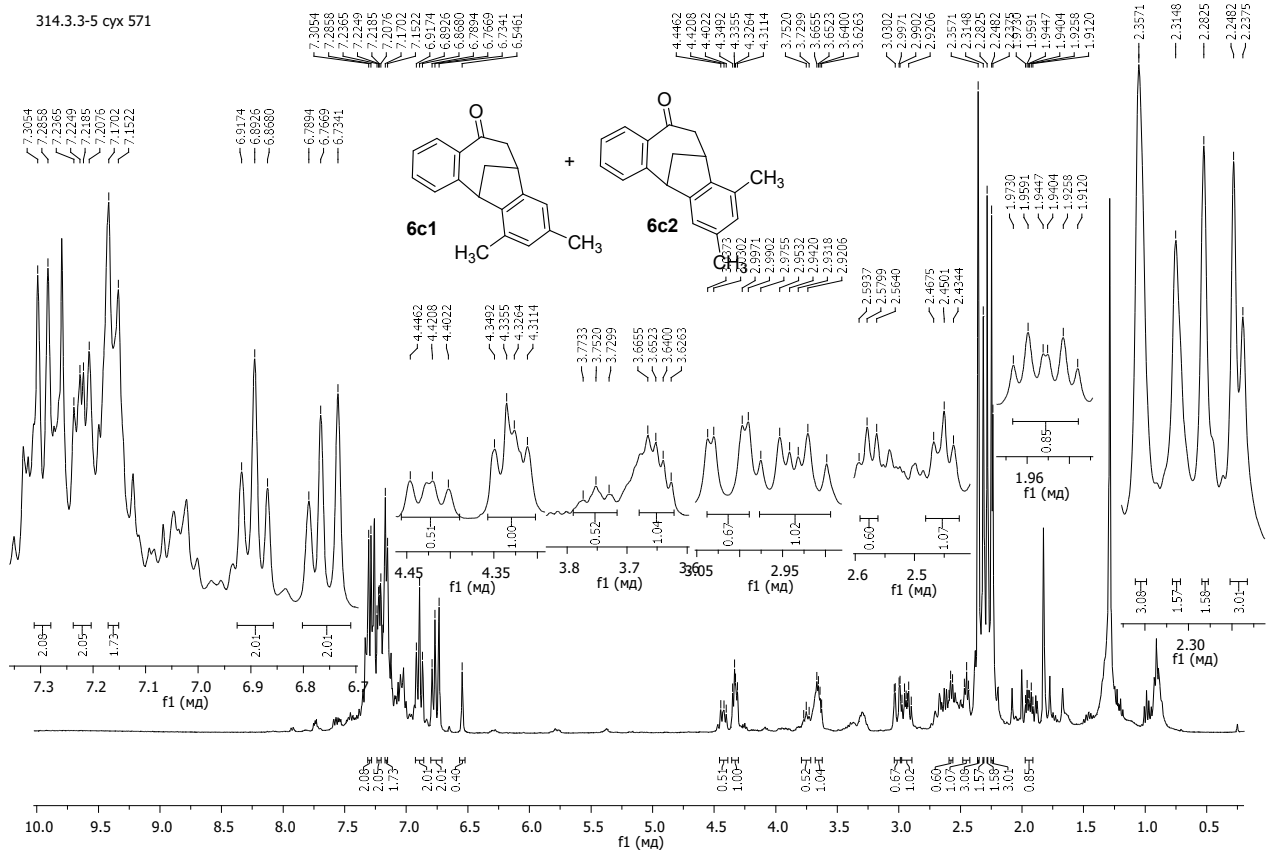


Fig. S64. ^{1}H NMR spectrum of the mixture of compounds **6c1** and **6c2** ($CDCl_3$, 400 MHz).

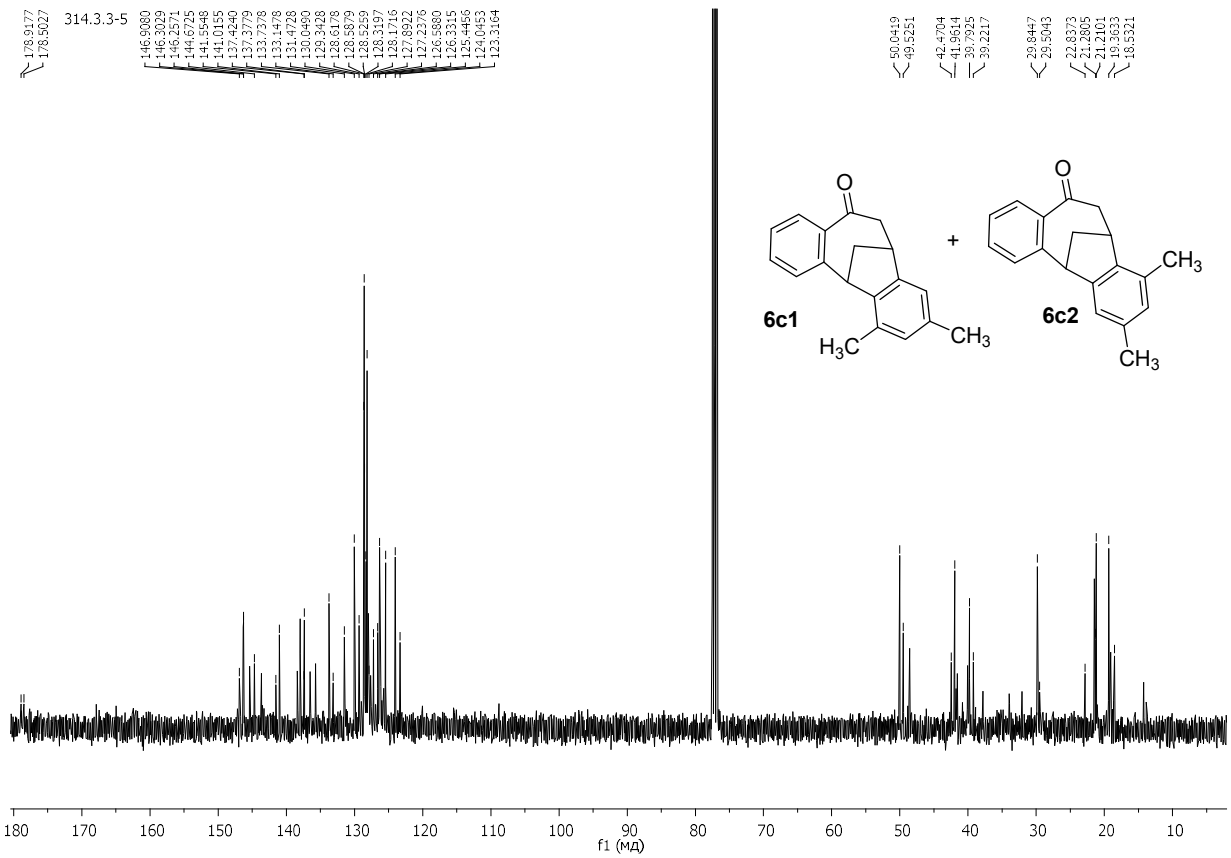


Fig. S65. ^{13}C NMR spectrum of the mixture of compounds **6c1** and **6c2** ($CDCl_3$, 100 MHz).

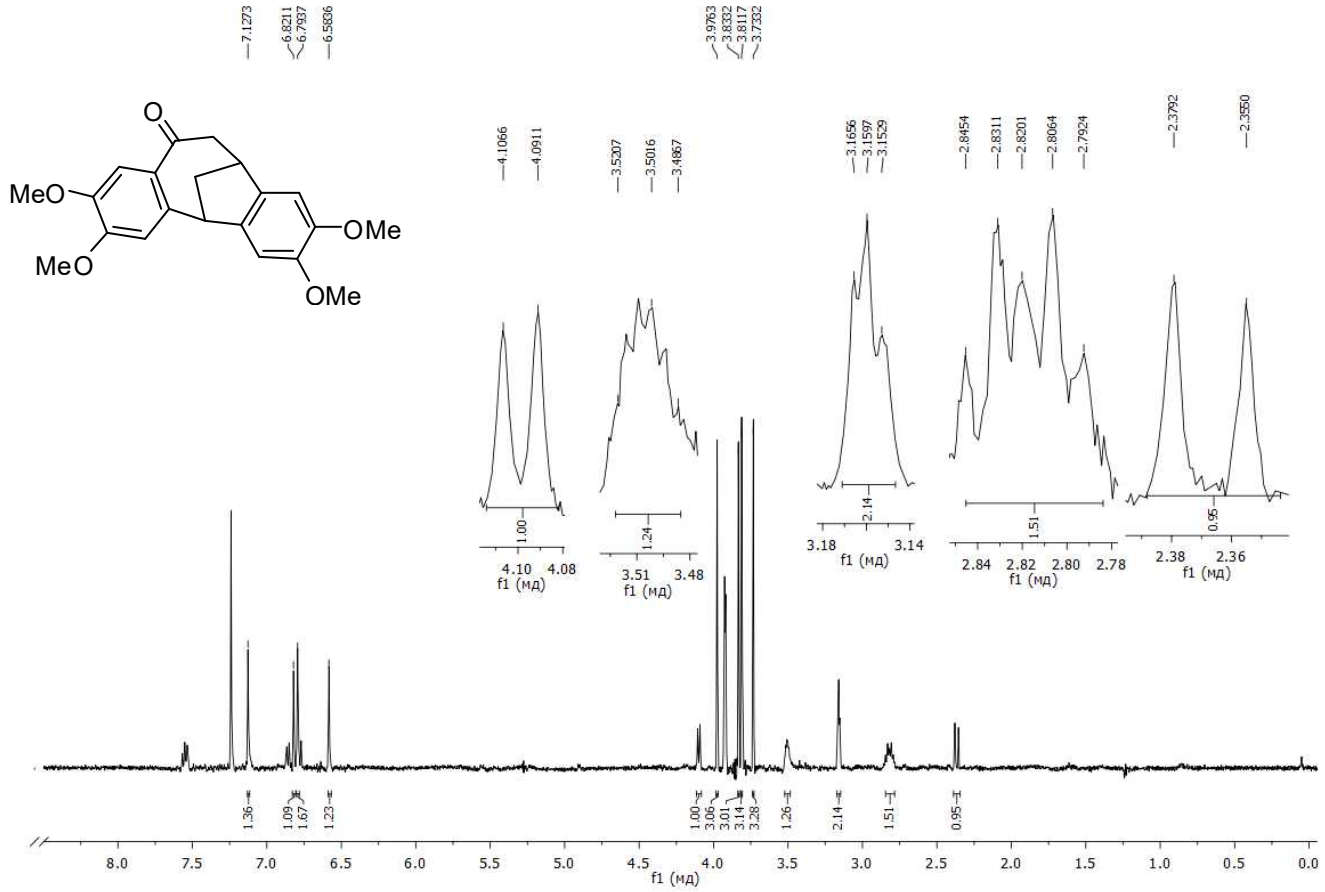


Fig. S66. ^{1}H NMR spectrum of the compound **6d** ($CDCl_3$, 500 MHz).

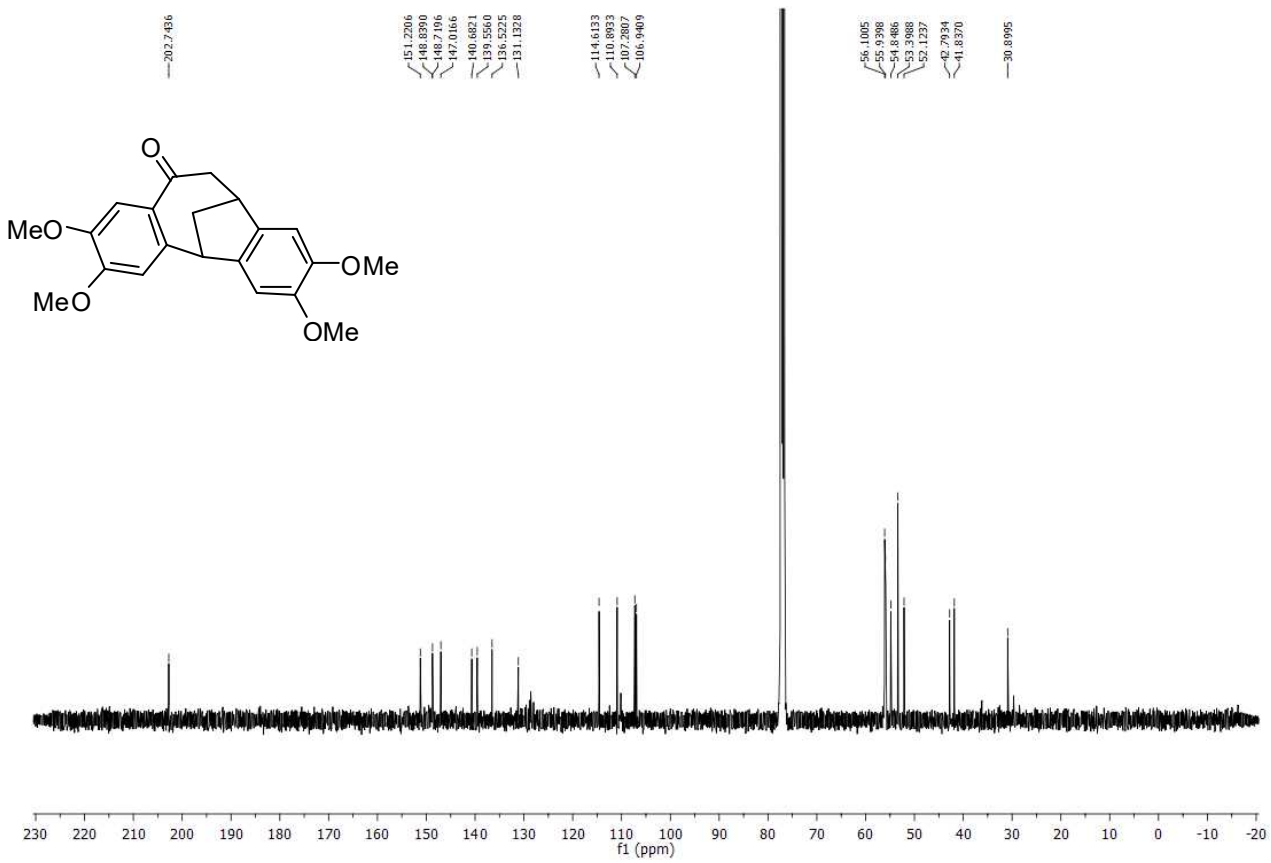


Fig. S67. ^{13}C NMR spectrum of the compound **6d** ($CDCl_3$, 125 MHz).

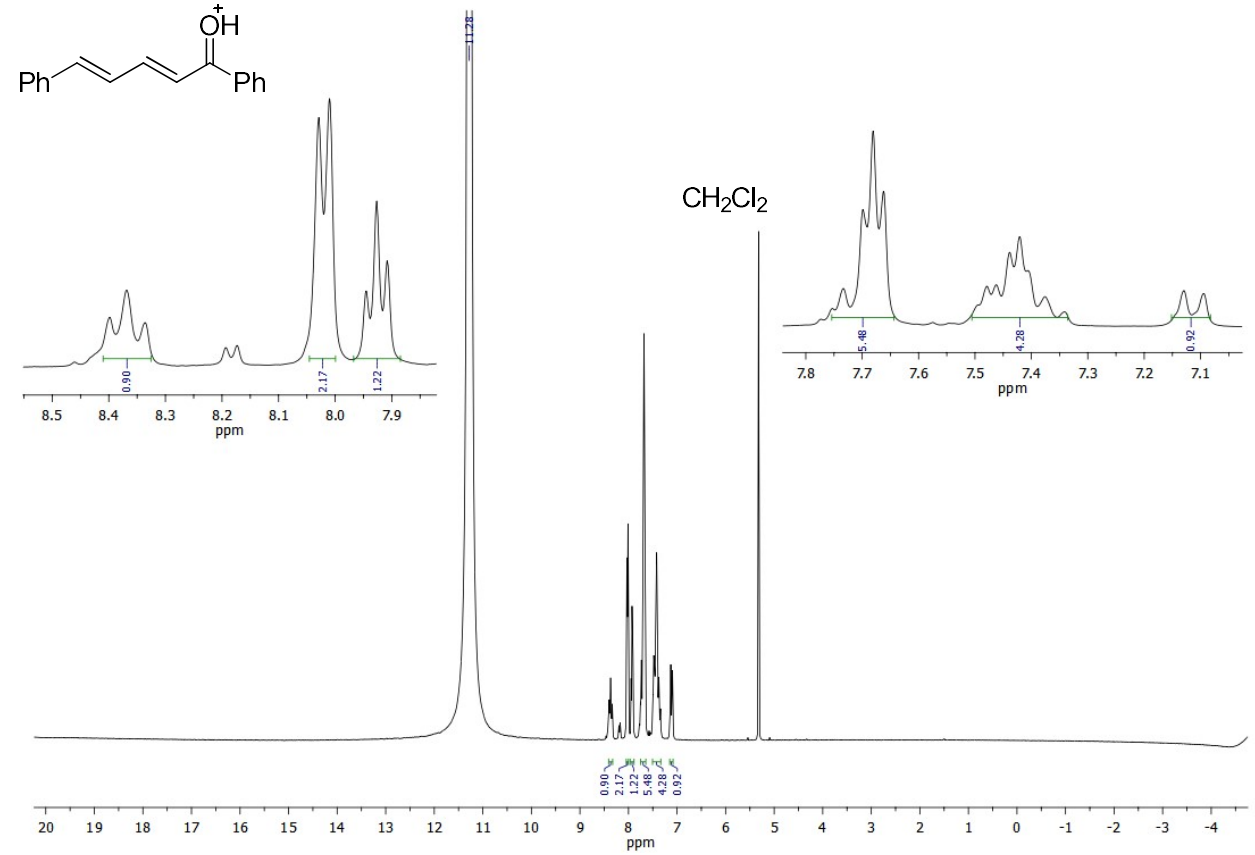


Fig. S68. ^{1}H NMR spectrum of cation **A1** generated at the protonation of **1a** in H_2SO_4 (H_2SO_4, room temperature, CH_2Cl_2, as internal standard, 400 MHz).

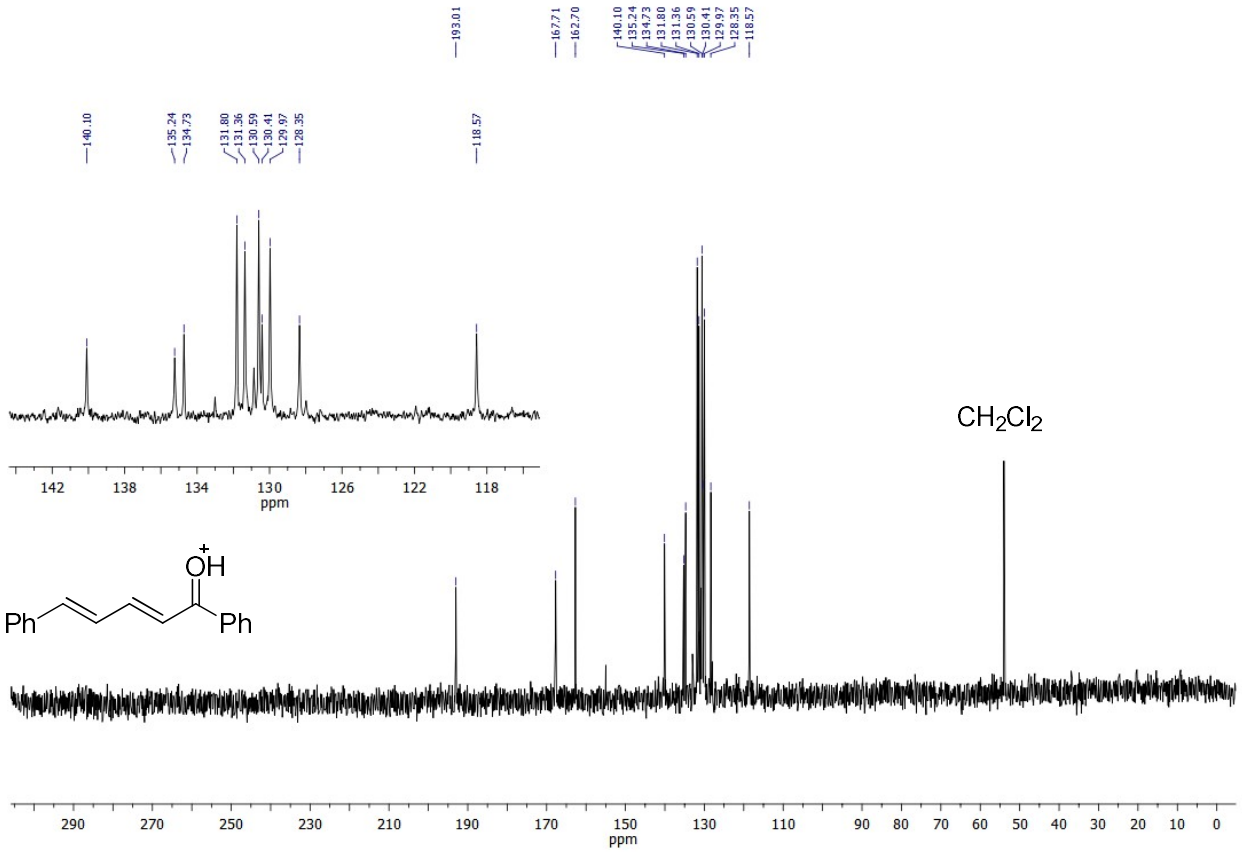


Fig. S69. ^{13}C NMR spectrum of cation **A1** generated at the protonation of **1a** in H_2SO_4 (H_2SO_4, room temperature, CH_2Cl_2, as internal standard, 100 MHz).

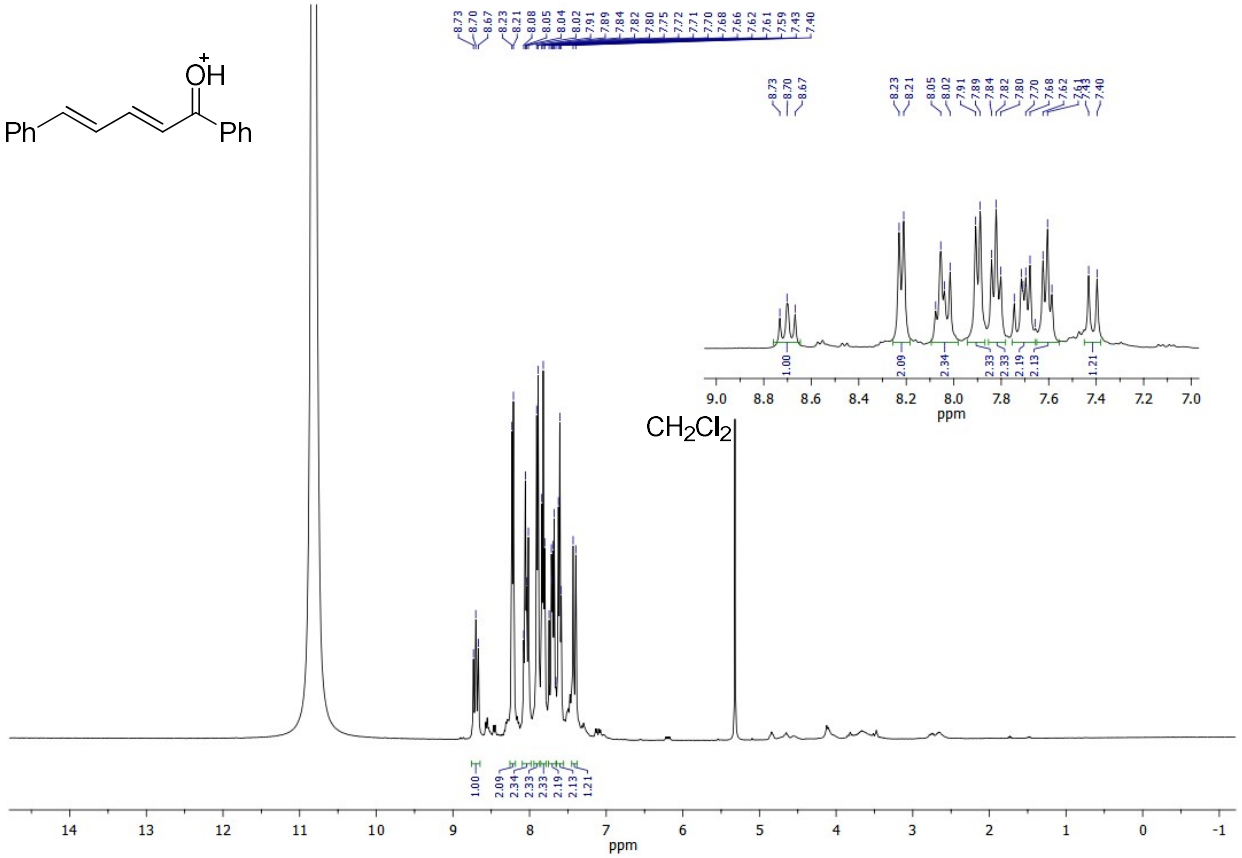


Fig. S70. ^{1}H NMR spectrum of cation **A1** generated at the protonation of **1a** in TfOH (TfOH, -40°C, CH_2Cl_2, as internal standard, 400 MHz).

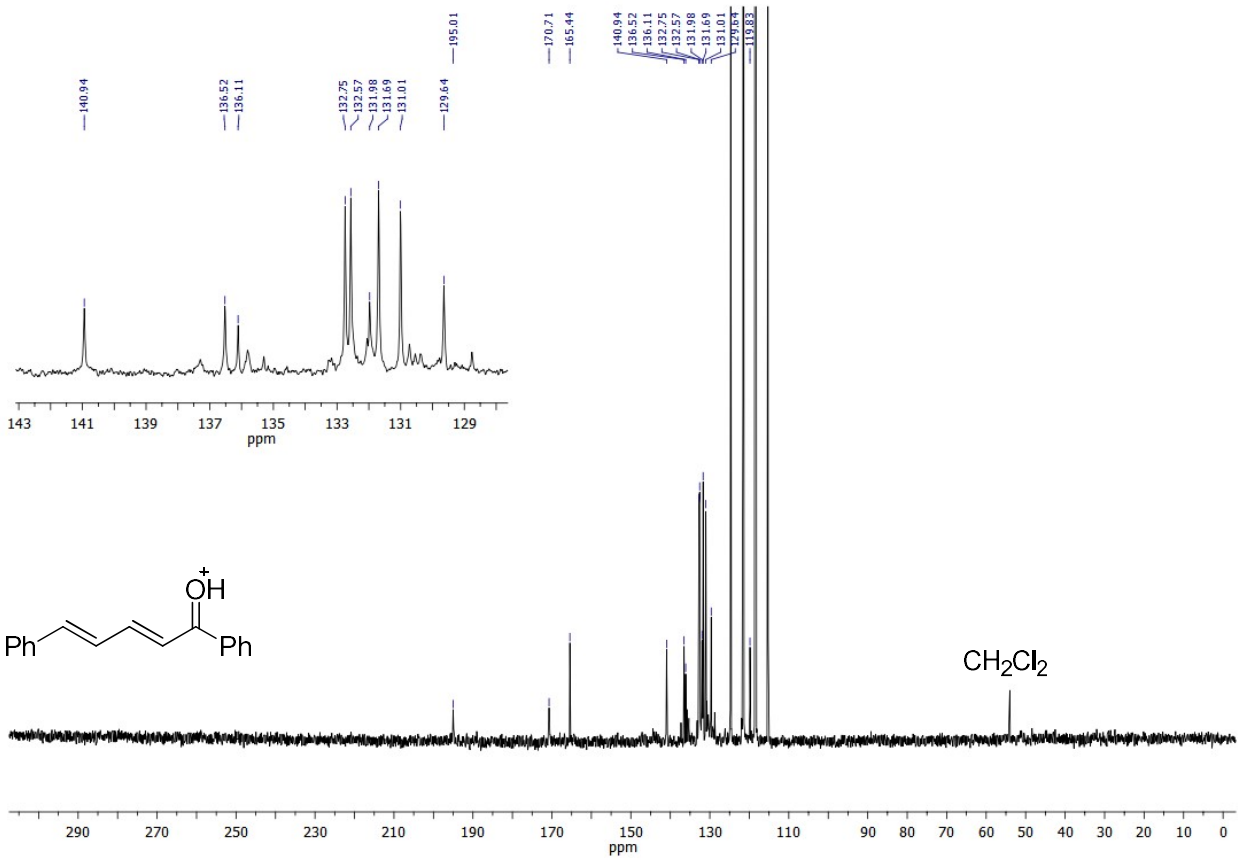


Fig. S71. ^{13}C NMR spectrum of cation **A1** generated at the protonation of **1a** in TfOH (TfOH, -40°C, CH_2Cl_2, as internal standard, 100 MHz).

III. X-Ray data of compounds 2a, 3h, 6a

2a

CCDC 1545936 – (**2a**)

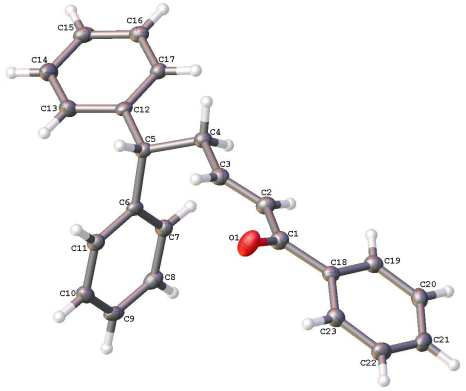


Table S1. Crystal data and structure refinement for 2a.

Identificationcode	2a
Empiricalformula	$C_{23}H_{20}O$
Formulaweight	312.39
Temperature/K	100(2)
Crystalsystem	triclinic
Spacegroup	P-1
a/Å	5.7804(3)
b/Å	8.8933(7)
c/Å	16.3510(11)
α/°	87.212(6)
β/°	84.983(5)
γ/°	89.862(6)
Volume/Å^3	836.34(10)
Z	2
ρ_{calc}g/cm^3	1.240
μ/mm^{-1}	0.074
F(000)	332.0
Crystalsize/mm^3	0.36 × 0.18 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.626 to 54.982
Indexranges	$-7 \le h \le 7$, $-10 \le k \le 11$, $-14 \le l \le 21$
Reflectionscollected	7027
Independentreflections	3839 [R_{int} = 0.0342, R_{sigma} = 0.0517]
Data/restraints/parameters	3839/0/217
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0533, wR_2 = 0.1356
Final R indexes [all data]	R_1 = 0.0637, wR_2 = 0.1470
Largest diff. peak/hole / e Å^{-3}	0.36/-0.25

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 2a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C5	1916(2)	9733.7(16)	2913.0(9)	18.3(3)
C17	5526(2)	8063.7(16)	2982.8(9)	20.1(3)
C18	-830(2)	12950.5(16)	-259.7(9)	18.7(3)
C6	2023(2)	11386.1(16)	3124.5(8)	17.5(3)
C23	-2595(3)	13917.9(18)	-482.7(9)	22.7(3)
O1	-3358.4(18)	11647.9(15)	747.4(8)	34.1(3)
C15	6832(3)	7187.4(17)	4280.5(10)	24.3(3)
C1	-1339(3)	11889.4(17)	476.0(9)	22.2(3)
C12	3668(2)	8816.7(16)	3377.0(9)	18.5(3)
C21	-66(3)	15046.2(18)	-1581.5(9)	25.5(3)
C8	4112(3)	13734.4(18)	3130.8(9)	23.2(3)
C11	170(2)	12037.4(17)	3580.3(9)	19.9(3)
C4	2179(3)	9525.6(17)	1978.0(9)	20.9(3)
C2	636(3)	11191.5(17)	873.9(9)	22.0(3)
C19	1333(3)	13028.6(17)	-716.0(9)	21.6(3)
C14	4982(3)	7932.4(18)	4683(1)	28.9(4)
C9	2263(3)	14371.4(17)	3593.5(9)	23.5(3)
C20	1694(3)	14073.1(18)	-1375.1(9)	24.4(3)
C7	3996(2)	12261.5(17)	2894.3(9)	20.7(3)
C3	289(3)	10293.1(17)	1544.2(9)	21.3(3)
C13	3416(3)	8732.4(18)	4236.0(9)	25.8(3)
C10	280(3)	13519.7(18)	3814.2(9)	23.1(3)
C16	7098(3)	7248.8(17)	3430.2(10)	22.1(3)
C22	-2216(3)	14964.4(18)	-1135.9(10)	25.9(3)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 2a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C5	19.9(7)	15.4(7)	19.5(7)	1.2(5)	-1.7(5)	0.1(5)
C17	24.8(7)	16.9(7)	18.4(7)	0.8(5)	-2.8(6)	1.1(6)
C18	22.2(7)	17.4(7)	17.3(7)	-2.5(5)	-5.7(5)	0.9(5)
C6	21.9(7)	14.9(7)	16.2(6)	1.3(5)	-6.3(5)	2.8(5)
C23	22.4(7)	24.9(8)	21.4(7)	-2.8(6)	-3.8(6)	2.9(6)
O1	20.9(6)	43.5(8)	36.1(7)	13.9(6)	-2.3(5)	-1.1(5)
C15	31.5(8)	16.8(7)	26.0(8)	0.4(6)	-11.1(6)	2.9(6)
C1	21.5(7)	22.6(8)	22.8(7)	-0.4(6)	-4.2(6)	0.2(6)
C12	24.3(7)	11.8(6)	19.5(7)	0.9(5)	-3.9(5)	-1.2(5)
C21	37.6(9)	23.0(8)	16.4(7)	0.6(6)	-5.8(6)	0.0(6)
C8	25.7(7)	21.1(8)	23.4(7)	4.7(6)	-7.7(6)	-2.9(6)
C11	19.8(7)	19.0(7)	20.8(7)	1.2(6)	-3.0(5)	1.6(5)

C4	25.9(7)	17.6(7)	19.5(7)	-0.4(6)	-4.4(6)	2.0(6)
C2	21.2(7)	21.0(8)	24.1(7)	0.5(6)	-5.1(6)	1.5(6)
C19	22.6(7)	20.8(7)	22.1(7)	-3.1(6)	-4.9(6)	2.8(6)
C14	46.2(10)	23.5(8)	17.8(7)	-1.6(6)	-7.0(7)	7.5(7)
C9	36.7(8)	13.7(7)	21.6(7)	-0.9(6)	-11.9(6)	3.8(6)
C20	27.9(8)	26.3(8)	18.8(7)	-3.5(6)	0.8(6)	-0.7(6)
C7	20.8(7)	20.4(7)	20.5(7)	0.7(6)	-1.4(5)	2.6(6)
C3	22.6(7)	19.7(7)	22.3(7)	-2.5(6)	-4.4(6)	0.1(6)
C13	34.1(8)	22.2(8)	21.0(7)	-2.0(6)	-1.5(6)	8.0(6)
C10	27.4(8)	23.0(8)	19.4(7)	-2.6(6)	-4.1(6)	8.9(6)
C16	22.7(7)	17.9(7)	25.7(8)	0.3(6)	-3.1(6)	2.1(6)
C22	31.2(8)	24.8(8)	22.7(7)	-0.7(6)	-8.7(6)	7.1(6)

Table S4. Bond Lengths for 2a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C5	C6	1.5285(19)	C15	C16	1.384(2)
C5	C12	1.5284(19)	C1	C2	1.483(2)
C5	C4	1.543(2)	C12	C13	1.398(2)
C17	C12	1.391(2)	C21	C20	1.387(2)
C17	C16	1.395(2)	C21	C22	1.385(2)
C18	C23	1.395(2)	C8	C9	1.390(2)
C18	C1	1.501(2)	C8	C7	1.387(2)
C18	C19	1.399(2)	C11	C10	1.393(2)
C6	C11	1.392(2)	C4	C3	1.499(2)
C6	C7	1.396(2)	C2	C3	1.325(2)
C23	C22	1.385(2)	C19	C20	1.390(2)
O1	C1	1.2274(18)	C14	C13	1.386(2)
C15	C14	1.389(2)	C9	C10	1.387(2)

Table S5. Bond Angles for 2a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	C5	C4	112.61(11)	C13	C12	C5	119.00(13)
C12	C5	C6	109.90(11)	C22	C21	C20	119.87(14)
C12	C5	C4	113.14(12)	C7	C8	C9	120.78(14)
C12	C17	C16	121.10(14)	C6	C11	C10	121.19(14)
C23	C18	C1	117.88(13)	C3	C4	C5	112.49(12)
C23	C18	C19	119.05(13)	C3	C2	C1	121.19(14)
C19	C18	C1	123.05(13)	C20	C19	C18	119.70(14)
C11	C6	C5	120.32(13)	C13	C14	C15	120.25(14)
C11	C6	C7	118.39(13)	C10	C9	C8	119.24(14)
C7	C6	C5	121.24(13)	C21	C20	C19	120.64(14)
C22	C23	C18	120.90(14)	C8	C7	C6	120.45(13)
C16	C15	C14	119.52(14)	C2	C3	C4	124.67(14)
O1	C1	C18	119.81(13)	C14	C13	C12	121.02(14)

O1	C1	C2	121.52(14)	C9	C10	C11	119.94(14)
C2	C1	C18	118.64(12)	C15	C16	C17	120.04(14)
C17	C12	C5	122.94(13)	C21	C22	C23	119.83(15)
C17	C12	C13	118.06(13)				

Table S6. Torsion Angles for 2a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C5	C6	C11	C10	176.77(13)	C12	C5	C6	C7	66.04(16)
C5	C6	C7	C8	-176.39(13)	C12	C5	C4	C3	173.62(12)
C5	C12	C13	C14	-179.03(14)	C12	C17	C16	C15	-0.4(2)
C5	C4	C3	C2	131.13(16)	C8	C9	C10	C11	0.8(2)
C17	C12	C13	C14	0.5(2)	C11	C6	C7	C8	1.3(2)
C18	C23	C22	C21	0.7(2)	C4	C5	C6	C11	121.29(14)
C18	C1	C2	C3	177.31(14)	C4	C5	C6	C7	-61.09(17)
C18	C19	C20	C21	0.4(2)	C4	C5	C12	C17	9.45(19)
C6	C5	C12	C17	-117.38(15)	C4	C5	C12	C13	-171.03(13)
C6	C5	C12	C13	62.15(17)	C19	C18	C23	C22	-1.2(2)
C6	C5	C4	C3	-61.00(16)	C19	C18	C1	O1	-165.07(15)
C6	C11	C10	C9	-0.1(2)	C19	C18	C1	C2	16.8(2)
C23	C18	C1	O1	16.2(2)	C14	C15	C16	C17	0.5(2)
C23	C18	C1	C2	-161.91(14)	C9	C8	C7	C6	-0.6(2)
C23	C18	C19	C20	0.7(2)	C20	C21	C22	C23	0.4(2)
O1	C1	C2	C3	-0.8(2)	C7	C6	C11	C10	-0.9(2)
C15	C14	C13	C12	-0.5(3)	C7	C8	C9	C10	-0.4(2)
C1	C18	C23	C22	177.55(14)	C16	C17	C12	C5	179.46(13)
C1	C18	C19	C20	-178.05(14)	C16	C17	C12	C13	-0.1(2)
C1	C2	C3	C4	179.11(14)	C16	C15	C14	C13	0.0(2)
C12	C5	C6	C11	-111.58(14)	C22	C21	C20	C19	-1.0(2)

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2a.

Atom	*x*	*y*	*z*	U(eq)
H5	368	9361	3118	22
H17	5725	8104	2412	24
H23	-4047	13859	-189	27
H15	7883	6651	4580	29
H21	198	15752	-2018	31
H8	5442	14302	2978	28
H11	-1165	11473	3732	24
H4A	3670	9927	1751	25
H4B	2160	8459	1880	25
H2	2145	11388	649	26
H19	2525	12385	-579	26
H14	4795	7894	5254	35

H9	2355	15357	3753	28
H20	3129	14120	-1681	29
H7	5241	11854	2580	25
H3	-1236	10127	1761	26
H13	2178	9220	4512	31
H10	-975	13937	4118	28
H16	8325	6747	3157	27
H22	-3403	15611	-1275	31

Experimental

Single crystals of $C_{23}H_{20}O$ **2a** were **growth from hexane-ethyl acetate sulution**. A suitable crystal was selected and **studied** on a **Xcalibur, Eos** diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. &Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). ActaCryst. A64, 112-122.
3. Sheldrick, G.M. (2015). ActaCryst. C71, 3-8.

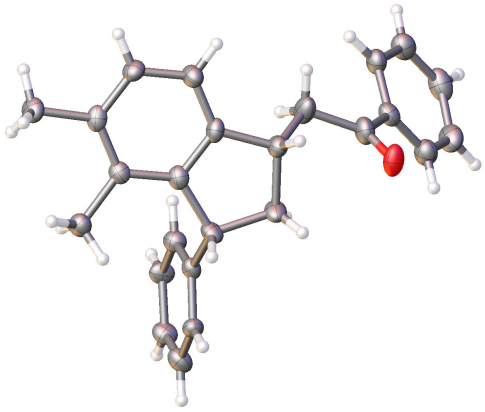
Crystal structure determination of 2a

Crystal Data for $C_{23}H_{20}O$ (M =312.39 g/mol): triclinic, space group P-1 (no. 2), a = 5.7804(3) Å, b = 8.8933(7) Å, c = 16.3510(11) Å, α = 87.212(6)°, β = 84.983(5)°, γ = 89.862(6)°, V = 836.34(10) Å^3, Z = 2, T = 100(2) K, μ(MoKα) = 0.074 mm^{-1}, *Dcalc* = 1.240 g/cm^3, 7027 reflections measured (6.626° ≤ 2Θ ≤ 54.982°), 3839 unique (R_{int} = 0.0342, R_{sigma} = 0.0517) which were used in all calculations. The final R_1 was 0.0533 (I >2σ(I)) and wR_2 was 0.1470 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:
1. Fixed Uiso
At 1.2 times of:
All C(H) groups, All C(H,H) groups
2.a Ternary CH refined with riding coordinates:
C5(H5)
2.b Secondary CH2 refined with riding coordinates:
C4(H4A,H4B)
2.c Aromatic/amide H refined with riding coordinates:
C17(H17), C23(H23), C15(H15), C21(H21), C8(H8), C11(H11), C2(H2), C19(H19), C14(H14), C9(H9), C20(H20), C7(H7), C3(H3), C13(H13), C10(H10), C16(H16), C22(H22)

Compound **3h**



CCDC 2153106 – (**3h**)

3h

Table S8. Crystal data and structure refinement for 3h.

Identification code	3h
Empirical formula	$C_{25}H_{24}O$
Formula weight	340.44
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.4843(7)
b/Å	5.6568(6)
c/Å	34.252(3)
α/°	90
β/°	96.212(8)
γ/°	90
Volume/Å^3	1826.9(3)
Z	4
ρ_{calc}g/cm^3	1.238
μ/mm^{-1}	0.562
F(000)	728.0
Crystal size/mm^3	0.05 × 0.01 × 0.01
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.19 to 140.748
Index ranges	$-11 \leq h \leq 11$, $-6 \leq k \leq 5$, $-35 \leq l \leq 41$
Reflections collected	9481
Independent reflections	3436 [R_{int} = 0.0520, R_{sigma} = 0.0505]
Data/restraints/parameters	3436/0/237
Goodness-of-fit on F^2	1.138
Final R indexes [I>=2σ (I)]	R_1 = 0.1357, wR_2 = 0.3570
Final R indexes [all data]	R_1 = 0.1501, wR_2 = 0.3648
Largest diff. peak/hole / e Å^{-3}	0.78/-0.55

Table S9. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3h. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O_{18}	3847(6)	-1082(10)	7257.3(15)	38.2(13)
C_{10}	5367(7)	1599(12)	5866.3(17)	22.7(14)
C_3	2444(7)	4581(13)	5626.7(18)	24.8(14)
C_7	2271(7)	3456(13)	6305.2(18)	25.5(14)
C_{11}	6077(7)	-62(13)	5666.8(18)	26.2(14)
C_5	942(7)	6738(13)	6024.8(19)	28.3(15)
C_{14}	7470(7)	4026(13)	5936(2)	28.5(15)
C_2	2836(7)	3163(13)	5951.0(18)	25.2(14)
C_{13}	8204(7)	2339(14)	5744(2)	29.4(16)
C_{21}	5178(7)	1902(13)	7614.0(19)	27.9(15)
C_8	2818(7)	1643(13)	6609.2(18)	26.8(15)
C_{20}	3045(7)	4197(14)	5239.3(19)	29.9(16)
C_9	3949(7)	250(14)	6412(2)	30.8(16)
C_6	1319(7)	5272(14)	6343.0(19)	28.5(15)
C_{15}	6052(7)	3651(14)	5993.8(19)	28.6(15)
C_1	3858(7)	1090(13)	5973.8(18)	25.6(15)
C_4	1480(7)	6404(12)	5664.2(18)	24.4(14)
C_{12}	7503(8)	311(15)	5608(2)	33.0(17)
C_{19}	1039(7)	8044(14)	5325(2)	30.6(16)
C_{17}	4120(8)	1033(14)	7286(2)	32.3(17)
C_{22}	5032(8)	4095(13)	7787.1(19)	30.2(16)
C_{16}	3419(9)	2805(15)	6996(2)	38.6(19)
C_{25}	7267(8)	1162(17)	8057(2)	41(2)
C_{26}	6302(8)	449(15)	7746(2)	35.7(17)
C_{23}	5971(8)	4753(15)	8110(2)	35.6(17)
C_{24}	7089(8)	3296(17)	8242(2)	41(2)

Table S10. Anisotropic Displacement Parameters (Å^2×10^3) for 3h. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O_{18}	50(3)	28(3)	34(3)	8(2)	-9(2)	-11(3)
C_{10}	26(3)	25(4)	17(3)	-3(3)	0(2)	-5(3)
C_3	20(3)	31(4)	23(3)	-2(3)	-2(2)	-5(3)
C_7	22(3)	28(4)	24(3)	3(3)	-6(2)	-2(3)
C_{11}	30(3)	24(3)	25(3)	-1(3)	3(3)	1(3)
C_5	21(3)	31(4)	32(3)	0(3)	0(3)	2(3)
C_{14}	26(3)	27(4)	32(3)	-9(3)	1(3)	-7(3)
C_2	23(3)	28(4)	23(3)	1(3)	-3(2)	-4(3)
C_{13}	20(3)	37(4)	31(4)	-5(3)	4(3)	-2(3)
C_{21}	28(3)	32(4)	24(3)	2(3)	3(3)	-2(3)
C_8	27(3)	29(4)	24(3)	3(3)	-1(3)	3(3)

C_{20}	29(3)	34(4)	25(3)	-1(3)	-1(3)	0(3)
C_9	21(3)	40(4)	32(4)	9(3)	7(3)	8(3)
C_6	25(3)	35(4)	24(3)	1(3)	-1(3)	1(3)
C_{15}	25(3)	33(4)	27(3)	-4(3)	0(3)	2(3)
C_1	22(3)	32(4)	23(3)	-1(3)	4(2)	-1(3)
C_4	21(3)	24(4)	26(3)	3(3)	-7(2)	-5(3)
C_{12}	32(4)	41(4)	27(3)	-4(3)	4(3)	-4(3)
C_{19}	24(3)	35(4)	30(3)	4(3)	-5(3)	2(3)
C_{17}	39(4)	32(4)	25(3)	6(3)	-3(3)	-3(3)
C_{22}	36(4)	29(4)	25(3)	1(3)	-2(3)	1(3)
C_{16}	49(5)	35(4)	29(4)	7(3)	-11(3)	1(4)
C_{25}	32(4)	54(5)	34(4)	7(4)	-6(3)	5(4)
C_{26}	43(4)	33(4)	30(4)	2(3)	-2(3)	0(4)
C_{23}	39(4)	35(4)	32(4)	-2(3)	-1(3)	-7(4)
C_{24}	35(4)	57(6)	29(4)	7(4)	-6(3)	-18(4)

Table S11. Bond Lengths for 3h.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O_{18}	C_{17}	1.226(9)	C_2	C_1	1.518(10)
C_{10}	C_{11}	1.379(9)	C_{13}	C_{12}	1.381(10)
C_{10}	C_{15}	1.377(10)	C_{21}	C_{17}	1.506(10)
C_{10}	C_1	1.544(9)	C_{21}	C_{22}	1.388(10)
C_3	C_2	1.388(9)	C_{21}	C_{26}	1.383(10)
C_3	C_{20}	1.515(9)	C_8	C_9	1.544(9)
C_3	C_4	1.393(10)	C_8	C_{16}	1.533(10)
C_7	C_2	1.388(9)	C_9	C_1	1.567(9)
C_7	C_8	1.513(9)	C_4	C_{19}	1.509(9)
C_7	C_6	1.383(10)	C_{17}	C_{16}	1.514(10)
C_{11}	C_{12}	1.405(10)	C_{22}	C_{23}	1.393(10)
C_5	C_6	1.385(10)	C_{25}	C_{26}	1.385(10)
C_5	C_4	1.400(9)	C_{25}	C_{24}	1.383(13)
C_{14}	C_{13}	1.389(10)	C_{23}	C_{24}	1.380(12)
C_{14}	C_{15}	1.397(9)			

Table S12. Bond Angles for 3h.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C_{11}	C_{10}	C_1	120.4(6)	C_{16}	C_8	C_9	112.7(6)
C_{15}	C_{10}	C_{11}	119.5(6)	C_8	C_9	C_1	107.2(5)
C_{15}	C_{10}	C_1	119.9(6)	C_7	C_6	C_5	119.1(6)
C_2	C_3	C_{20}	121.6(6)	C_{10}	C_{15}	C_{14}	120.8(7)
C_2	C_3	C_4	118.4(6)	C_{10}	C_1	C_9	109.2(5)
C_4	C_3	C_{20}	120.0(6)	C_2	C_1	C_{10}	116.6(6)
C_2	C_7	C_8	112.6(6)	C_2	C_1	C_9	104.6(5)
C_6	C_7	C_2	119.2(6)	C_3	C_4	C_5	119.1(6)
C_6	C_7	C_8	128.2(6)	C_3	C_4	C_{19}	121.0(6)
C_{10}	C_{11}	C_{12}	119.8(7)	C_5	C_4	C_{19}	119.9(6)
C_6	C_5	C_4	121.7(7)	C_{13}	C_{12}	C_{11}	120.8(7)

C_{13}	C_{14}	C_{15}	120.1(7)	O_{18}	C_{17}	C_{21}	119.8(7)
C_3	C_2	C_7	122.4(6)	O_{18}	C_{17}	C_{16}	121.3(7)
C_3	C_2	C_1	127.0(6)	C_{21}	C_{17}	C_{16}	118.9(7)
C_7	C_2	C_1	110.6(6)	C_{21}	C_{22}	C_{23}	119.5(7)
C_{12}	C_{13}	C_{14}	118.9(6)	C_{17}	C_{16}	C_8	112.3(7)
C_{22}	C_{21}	C_{17}	121.4(7)	C_{24}	C_{25}	C_{26}	120.2(8)
C_{26}	C_{21}	C_{17}	118.6(7)	C_{21}	C_{26}	C_{25}	120.0(8)
C_{26}	C_{21}	C_{22}	120.0(7)	C_{24}	C_{23}	C_{22}	120.3(8)
C_7	C_8	C_9	104.3(5)	C_{23}	C_{24}	C_{25}	119.8(7)
C_7	C_8	C_{16}	111.8(6)				

Table S13. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3h.

Atom	*x*	*y*	*z*	U(eq)
H_{11}	5602	-1456	5569	31
H_5	301	8003	6052	34
H_{14}	7935	5437	6029	34
H_{13}	9171	2577	5706	35
H_8	2028	552	6660	32
H_{20A}	3836	5290	5219	45
H_{20B}	2304	4486	5022	45
H_{20C}	3384	2565	5226	45
H_{9A}	3762	-1469	6424	37
H_{9B}	4905	568	6548	37
H_6	929	5511	6584	34
H_{15}	5553	4824	6122	34
H_1	3432	-206	5801	31
H_{12}	7992	-847	5473	40
H_{19A}	1879	8542	5204	46
H_{19B}	569	9437	5422	46
H_{19C}	383	7219	5131	46
H_{22}	4297	5139	7686	36
H_{16A}	4122	4020	6941	46
H_{16B}	2642	3607	7115	46
H_{25}	8053	182	8142	49
H_{26}	6411	-1039	7625	43
H_{23}	5843	6211	8239	43
H_{24}	7734	3756	8461	49

Experimental

Single crystals of $C_{25}H_{24}O$ **3h** were growth from methanol solution . A suitable crystal was selected and studied on a SuperNova diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.

3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

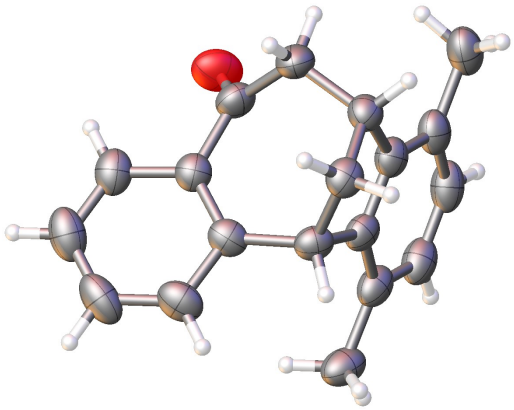
Crystal structure determination of 3h

Crystal Data for $C_{25}H_{24}O$ (M =340.44 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 9.4843(7) Å, b = 5.6568(6) Å, c = 34.252(3) Å, β = 96.212(8)°, V = 1826.9(3) Å^3, Z = 4, T = 100(2) K, μ(CuKα) = 0.562 mm^{-1}, *Dcalc* = 1.238 g/cm^3, 9481 reflections measured (5.19° ≤ 2Θ ≤ 140.748°), 3436 unique (R_{int} = 0.0520, R_{sigma} = 0.0505) which were used in all calculations. The final R_1 was 0.1357 (I > 2σ(I)) and wR_2 was 0.3648 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Ternary CH refined with riding coordinates:
 C8(H8), C1(H1)
2.b Secondary CH2 refined with riding coordinates:
 C9(H9A,H9B), C16(H16A,H16B)
2.c Aromatic/amide H refined with riding coordinates:
 C11(H11), C5(H5), C14(H14), C13(H13), C6(H6), C15(H15), C12(H12), C22(H22), C25(H25), C26(H26), C23(H23), C24(H24)
2.d Idealised Me refined as rotating group:
 C20(H20A,H20B,H20C), C19(H19A,H19B,H19C)

Compound **6a**



CCDC 2153107– (**6a**)

6a

Table S14. Crystal data and structure refinement for 6a.

Identification code	6a
Empirical formula	$C_{19}H_{18}O$
Formula weight	262.33
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.8475(4)
b/Å	16.8287(7)
c/Å	11.1852(5)
α/°	90
β/°	106.026(5)
γ/°	90
Volume/Å^3	1419.75(12)
Z	4
ρ_{calc}g/cm^3	1.227
μ/mm^{-1}	0.570
F(000)	560.0
Crystal size/mm^3	0.35 × 0.22 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.762 to 144.172
Index ranges	$-9 \le h \le 9$, $-20 \le k \le 20$, $-13 \le l \le 13$
Reflections collected	9098
Independent reflections	2769 [R_{int} = 0.0323, R_{sigma} = 0.0297]
Data/restraints/parameters	2769/0/183
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0684, wR_2 = 0.1852
Final R indexes [all data]	R_1 = 0.0815, wR_2 = 0.2033
Largest diff. peak/hole / e Å^{-3}	0.34/-0.28

Table S15. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 6a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O_1	3342(3)	3120.8(15)	5568(2)	69.2(6)
C_5	7028(3)	1508.7(14)	5812(2)	41.5(6)
C_6	5318(3)	1301.0(13)	5122(2)	42.8(6)
C_2	6216(3)	3315.2(15)	5385(2)	42.8(6)
C_4	7874(3)	2051.4(15)	5062(2)	42.6(6)
C_7	4917(3)	1685.1(15)	3847(2)	44.4(6)
C_{13}	6767(3)	1867.5(15)	3722(2)	46.0(6)
C_3	7805(3)	2915.6(15)	5436(2)	42.9(6)
C_{14}	7746(4)	1254.6(14)	7037(2)	47.8(6)
C_{17}	4237(4)	836.9(14)	5644(3)	49.5(6)
C_1	4397(3)	2953.7(15)	4975(2)	48.0(6)
C_{15}	6673(4)	780.0(15)	7539(2)	53.6(7)
C_8	3803(3)	2443.3(16)	3821(2)	50.2(6)
C_9	6260(4)	4111.7(16)	5763(2)	52.3(7)
C_{12}	9390(4)	3336.4(18)	5898(2)	54.6(7)
C_{16}	4970(4)	583.1(15)	6871(2)	54.2(7)
C_{18}	9594(4)	1484.0(18)	7759(2)	58.1(7)
C_{19}	2379(4)	620.8(17)	4922(3)	60.8(7)
C_{11}	9393(4)	4131.9(19)	6246(3)	63.6(8)
C_{10}	7834(5)	4519.3(17)	6173(3)	62.6(8)

Table S16. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 6a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O_1	48.8(11)	89.2(16)	74.2(14)	-15.2(12)	24.5(10)	4.5(10)
C_5	48.4(13)	39.3(12)	38.4(11)	-2.0(9)	14.8(10)	9.7(10)
C_6	53.1(14)	37.4(12)	41.6(12)	-4.2(9)	19.4(11)	3.3(10)
C_2	48.4(13)	44.6(13)	37.6(11)	0.3(9)	15.7(10)	0.4(10)
C_4	38.5(12)	51.2(14)	40.1(12)	0(1)	14.2(10)	5.7(10)
C_7	48.2(13)	42.4(12)	40.8(12)	-3.5(10)	9.1(10)	-0.4(10)
C_{13}	55.2(14)	48.0(13)	37.7(12)	-2.4(10)	17.5(11)	3.8(11)
C_3	43.4(12)	53.3(14)	35.8(11)	-1.7(10)	17.1(9)	-4.6(10)
C_{14}	63.1(16)	42.6(13)	38.6(12)	-2.4(10)	15.6(11)	12.6(11)
C_{17}	62.0(16)	37.7(12)	54.7(14)	-8.8(10)	26.0(12)	-2.8(11)
C_1	41.5(12)	50.2(14)	53.0(14)	0.4(11)	13.9(11)	9.3(11)
C_{15}	80(2)	41.2(13)	41.4(13)	-0.4(10)	20.5(13)	8.5(12)
C_8	44.0(13)	49.3(14)	51.2(14)	1.9(11)	3.2(11)	5.0(11)
C_9	71.0(18)	45.4(14)	45.5(13)	-0.7(11)	24.9(12)	0.0(12)
C_{12}	47.0(14)	70.5(18)	50.6(14)	-2.2(12)	20.5(12)	-12.8(12)
C_{16}	82.2(19)	37.3(12)	55.0(15)	-2.8(11)	39.0(14)	-2.7(13)
C_{18}	59.7(17)	65.1(17)	44.9(14)	-2.8(12)	6.7(12)	18.9(14)
C_{19}	66.8(18)	47.5(15)	74.5(19)	-13.9(13)	30.4(15)	-8.9(13)
C_{11}	75(2)	66.2(18)	54.1(16)	-11.9(13)	25.4(15)	-31.9(16)
C_{10}	89(2)	50.8(15)	58.0(16)	-9.3(13)	36.9(16)	-18.4(15)

Table S17. Bond Lengths for 6a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O_1	C_1	1.228(3)	C_7	C_8	1.542(3)
C_5	C_6	1.395(3)	C_3	C_{12}	1.400(4)
C_5	C_4	1.512(3)	C_{14}	C_{15}	1.386(4)
C_5	C_{14}	1.397(3)	C_{14}	C_{18}	1.503(4)
C_6	C_7	1.517(3)	C_{17}	C_{16}	1.400(4)
C_6	C_{17}	1.394(4)	C_{17}	C_{19}	1.503(4)
C_2	C_3	1.405(3)	C_1	C_8	1.513(4)
C_2	C_1	1.502(4)	C_{15}	C_{16}	1.380(4)
C_2	C_9	1.403(4)	C_9	C_{10}	1.376(4)
C_4	C_{13}	1.542(3)	C_{12}	C_{11}	1.394(4)
C_4	C_3	1.518(3)	C_{11}	C_{10}	1.369(5)
C_7	C_{13}	1.527(4)			

Table S18. Bond Angles for 6a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C_6	C_5	C_4	110.3(2)	C_{12}	C_3	C_4	119.4(2)
C_6	C_5	C_{14}	122.1(2)	C_5	C_{14}	C_{18}	121.1(2)
C_{14}	C_5	C_4	127.5(2)	C_{15}	C_{14}	C_5	116.6(3)
C_5	C_6	C_7	109.4(2)	C_{15}	C_{14}	C_{18}	122.3(2)
C_{17}	C_6	C_5	120.8(2)	C_6	C_{17}	C_{16}	116.6(3)
C_{17}	C_6	C_7	129.8(2)	C_6	C_{17}	C_{19}	121.5(3)
C_3	C_2	C_1	125.2(2)	C_{16}	C_{17}	C_{19}	121.9(3)
C_9	C_2	C_3	119.8(2)	O_1	C_1	C_2	117.9(2)
C_9	C_2	C_1	114.9(2)	O_1	C_1	C_8	119.8(2)
C_5	C_4	C_{13}	101.64(19)	C_2	C_1	C_8	122.2(2)
C_5	C_4	C_3	111.80(19)	C_{16}	C_{15}	C_{14}	121.7(2)
C_3	C_4	C_{13}	114.0(2)	C_1	C_8	C_7	114.4(2)
C_6	C_7	C_{13}	102.44(19)	C_{10}	C_9	C_2	121.5(3)
C_6	C_7	C_8	109.9(2)	C_{11}	C_{12}	C_3	121.5(3)
C_{13}	C_7	C_8	112.3(2)	C_{15}	C_{16}	C_{17}	122.1(3)
C_7	C_{13}	C_4	104.27(19)	C_{10}	C_{11}	C_{12}	120.5(3)
C_2	C_3	C_4	123.1(2)	C_{11}	C_{10}	C_9	119.2(3)
C_{12}	C_3	C_2	117.5(2)				

Table S19. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6a.

Atom	*x*	*y*	*z*	U(eq)
H_4	9134	1889	5172	51
H_7	4284	1304	3187	53
H_{13A}	6738	2330	3171	55
H_{13B}	7257	1405	3383	55
H_{15}	7123	585	8363	64
H_{8A}	3849	2766	3090	60
H_{8B}	2552	2287	3708	60
H_9	5179	4376	5735	63

H_{12}	10487	3074	5977	66
H_{16}	4272	265	7256	65
H_{18A}	10427	1335	7287	87
H_{18B}	9911	1207	8561	87
H_{18C}	9649	2059	7900	87
H_{19A}	1698	1106	4638	91
H_{19B}	1814	318	5456	91
H_{19C}	2414	297	4200	91
H_{11}	10486	4408	6535	76
H_{10}	7838	5063	6403	75

Experimental

Single crystals of $C_{19}H_{18}O$ **6a** were growth from methanol solution. A suitable crystal was selected and studied on a SuperNova diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of 6a

Crystal Data for $C_{19}H_{18}O$ (M =262.33 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 7.8475(4) Å, b = 16.8287(7) Å, c = 11.1852(5) Å, β = 106.026(5)°, V = 1419.75(12) Å^3, Z = 4, T = 100(2) K, μ(CuKα) = 0.570 mm^{-1}, *Dcalc* = 1.227 g/cm^3, 9098 reflections measured (9.762° ≤ 2Θ ≤ 144.172°), 2769 unique (R_{int} = 0.0323, R_{sigma} = 0.0297) which were used in all calculations. The final R_1 was 0.0684 (I > 2σ(I)) and wR_2 was 0.2033 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2.a Ternary CH refined with riding coordinates:
 C4(H4), C7(H7)
2.b Secondary CH2 refined with riding coordinates:
 C13(H13A,H13B), C8(H8A,H8B)
2.c Aromatic/amide H refined with riding coordinates:
 C15(H15), C9(H9), C12(H12), C16(H16), C11(H11), C10(H10)
2.d Idealised Me refined as rotating group:
 C18(H18A,H18B,H18C), C19(H19A,H19B,H19C)

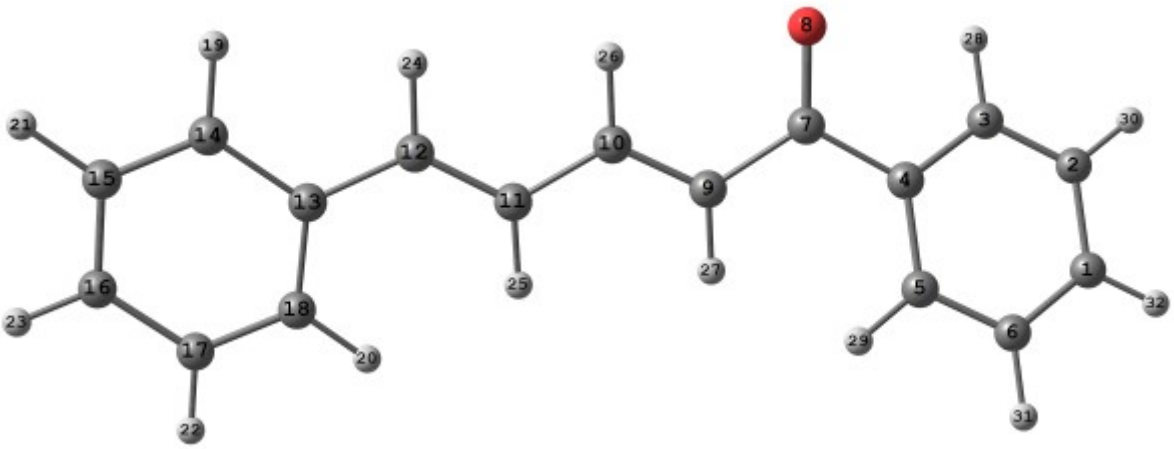
IV. Details of DFT calculations of cations A-D, intermediate π- and σ-complexes leading to indanes *cis-/trans*-3a, and indanes *cis-/trans*-3a

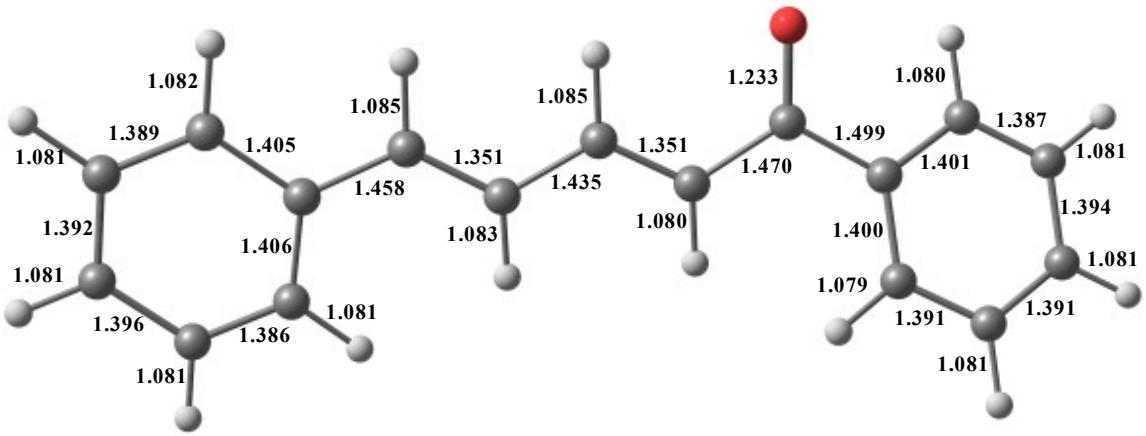
1a

Energy E(B3LYP) = -731.673194625 h, G^{298} = -731.461392 h, μ=5.16 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	6.139900	1.138180	0.034687
2	C	6.055274	-0.224661	0.317025
3	C	4.824950	-0.864627	0.285225
4	C	3.655380	-0.153740	-0.014284
5	C	3.751819	1.215403	-0.291600
6	C	4.987427	1.853992	-0.274164
7	C	2.357564	-0.903911	-0.047041
8	O	2.367385	-2.135172	-0.104991
9	C	1.099011	-0.145870	0.009518
10	C	-0.102438	-0.759961	-0.062573
11	C	-1.367284	-0.085902	0.005315
12	C	-2.542110	-0.749043	-0.072784
13	C	-3.886233	-0.186733	-0.014214
14	C	-4.983740	-1.055323	-0.131831
15	C	-6.286974	-0.576082	-0.083932
16	C	-6.522084	0.785201	0.084096
17	C	-5.443340	1.662409	0.204037
18	C	-4.142431	1.185518	0.155928
19	H	-4.805490	-2.114673	-0.262001
20	H	-3.322806	1.883085	0.252694
21	H	-7.116541	-1.263252	-0.177199
22	H	-5.620750	2.720904	0.335792
23	H	-7.534665	1.162233	0.122028
24	H	-2.500008	-1.826604	-0.193413
25	H	-1.347772	0.990824	0.123035
26	H	-0.117757	-1.838129	-0.178681
27	H	1.139661	0.926381	0.131086
28	H	4.750135	-1.921312	0.495679
29	H	2.873178	1.789865	-0.542923
30	H	6.948242	-0.783857	0.559994
31	H	5.048612	2.909114	-0.501608
32	H	7.098735	1.637691	0.055007





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.18537	1.99915	4.16581	0.02041	6.18537
C	2	-0.21341	1.99915	4.19410	0.02015	6.21341
C	3	-0.16951	1.99907	4.15007	0.02037	6.16951
C	4	-0.14171	1.99893	4.12230	0.02048	6.14171
C	5	-0.17863	1.99908	4.16154	0.01802	6.17863
C	6	-0.21477	1.99916	4.19519	0.02041	6.21477
C	7	0.52245	1.99917	3.44443	0.03396	5.47755

O	8	-0.65862	1.99977	6.63576	0.02309	8.65862
C	9	-0.31051	1.99900	4.29256	0.01895	6.31051
C	10	-0.10955	1.99908	4.09094	0.01953	6.10955
C	11	-0.22830	1.99905	4.21161	0.01763	6.22830
C	12	-0.12726	1.99906	4.10957	0.01862	6.12726
C	13	-0.11099	1.99903	4.09192	0.02004	6.11099
C	14	-0.16742	1.99891	4.14864	0.01987	6.16742
C	15	-0.22029	1.99917	4.19987	0.02125	6.22029
C	16	-0.19821	1.99916	4.17949	0.01956	6.19821
C	17	-0.21599	1.99918	4.19566	0.02115	6.21599
C	18	-0.17190	1.99892	4.15428	0.01871	6.17190
H	19	0.22113	0.00000	0.77719	0.00168	0.77887
H	20	0.21957	0.00000	0.77873	0.00170	0.78043
H	21	0.22344	0.00000	0.77491	0.00165	0.77656
H	22	0.22285	0.00000	0.77551	0.00164	0.77715
H	23	0.22218	0.00000	0.77624	0.00158	0.77782
H	24	0.21435	0.00000	0.78307	0.00258	0.78565
H	25	0.21429	0.00000	0.78286	0.00285	0.78571
H	26	0.21859	0.00000	0.77721	0.00420	0.78141
H	27	0.21671	0.00000	0.78053	0.00275	0.78329
H	28	0.23043	0.00000	0.76720	0.00237	0.76957
H	29	0.22447	0.00000	0.77385	0.00168	0.77553
H	30	0.22389	0.00000	0.77445	0.00166	0.77611
H	31	0.22457	0.00000	0.77378	0.00164	0.77543
H	32	0.22353	0.00000	0.77494	0.00153	0.77647
* Total *		0.00000	35.98404	87.61423	0.40172	124.00000

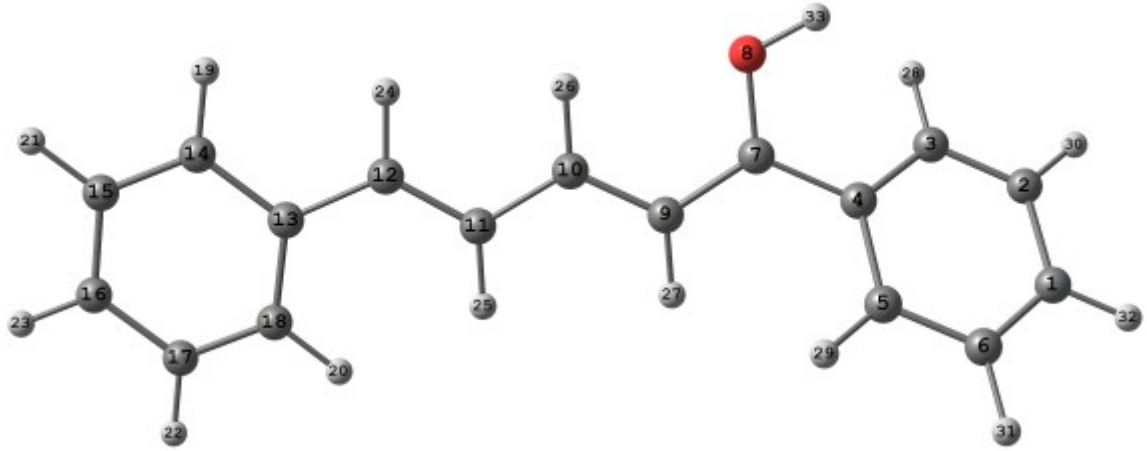
A1

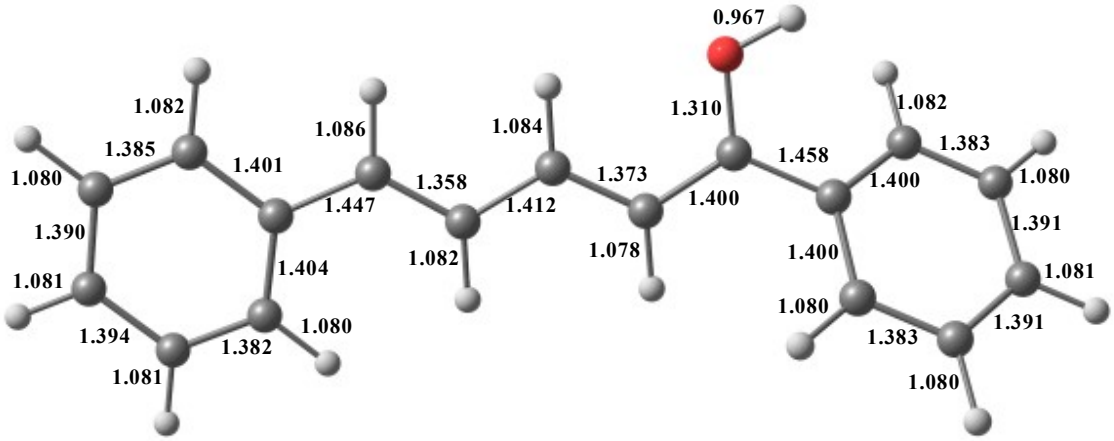
Energy E(B3LYP) = -732.099946379 h, G^{298} = -731.873839 h, μ=3.87 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	6.102301	1.077353	0.054365
2	C	5.950495	-0.229701	0.504896
3	C	4.706608	-0.833323	0.464575
4	C	3.599646	-0.122900	-0.016106
5	C	3.757443	1.196357	-0.456787
6	C	5.008011	1.786812	-0.428861
7	C	2.288030	-0.757360	-0.062868
8	O	2.207782	-2.060532	-0.164124
9	C	1.091716	-0.036390	0.024940
10	C	-0.127352	-0.657464	-0.092614
11	C	-1.365841	0.012673	0.017358
12	C	-2.523463	-0.685233	-0.117518
13	C	-3.871408	-0.166581	-0.027315
14	C	-4.937494	-1.060110	-0.197121
15	C	-6.248029	-0.618097	-0.118755
16	C	-6.508712	0.723898	0.130462
17	C	-5.457813	1.623660	0.301896
18	C	-4.149281	1.186046	0.224538
19	H	-4.726520	-2.103676	-0.390717

20	H	-3.344326	1.893840	0.360675
21	H	-7.062179	-1.315816	-0.251309
22	H	-5.665867	2.666103	0.496231
23	H	-7.529961	1.073125	0.192105
24	H	-2.442688	-1.750128	-0.312686
25	H	-1.361409	1.076905	0.210918
26	H	-0.150068	-1.724748	-0.282659
27	H	1.148591	1.024200	0.211666
28	H	4.596756	-1.837209	0.853637
29	H	2.913852	1.742925	-0.852360
30	H	6.798984	-0.773472	0.893258
31	H	5.131302	2.798320	-0.786833
32	H	7.076422	1.544870	0.082716
33	H	3.065722	-2.468829	-0.342161





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.15715	1.99916	4.13802	0.01997	6.15715
C	2	-0.20255	1.99915	4.18293	0.02047	6.20255
C	3	-0.16842	1.99906	4.14976	0.01960	6.16842
C	4	-0.15086	1.99892	4.13329	0.01864	6.15086
C	5	-0.14378	1.99907	4.12662	0.01809	6.14378
C	6	-0.20542	1.99915	4.18606	0.02021	6.20542
C	7	0.51856	1.99893	3.45434	0.02817	5.48144
O	8	-0.62546	1.99970	6.60124	0.02452	8.62546
C	9	-0.34880	1.99907	4.31850	0.03123	6.34880
C	10	0.05053	1.99914	3.93535	0.01497	5.94947
C	11	-0.27871	1.99913	4.25011	0.02948	6.27871
C	12	-0.05354	1.99908	4.03159	0.02287	6.05354
C	13	-0.12563	1.99900	4.10693	0.01970	6.12563
C	14	-0.15047	1.99908	4.13245	0.01893	6.15047
C	15	-0.21127	1.99915	4.19185	0.02028	6.21127
C	16	-0.15580	1.99916	4.13655	0.02009	6.15580
C	17	-0.20587	1.99916	4.18654	0.02017	6.20587
C	18	-0.15841	1.99906	4.14147	0.01787	6.15841
H	19	0.22866	0.00000	0.76958	0.00176	0.77134
H	20	0.22646	0.00000	0.77177	0.00177	0.77354
H	21	0.22819	0.00000	0.77015	0.00166	0.77181

H	22	0.22757	0.00000	0.77078	0.00165	0.77243
H	23	0.22507	0.00000	0.77345	0.00148	0.77493
H	24	0.22930	0.00000	0.76875	0.00195	0.77070
H	25	0.23149	0.00000	0.76567	0.00284	0.76851
H	26	0.22560	0.00000	0.76973	0.00466	0.77440
H	27	0.24607	0.00000	0.75136	0.00257	0.75393
H	28	0.23293	0.00000	0.76480	0.00227	0.76707
H	29	0.23487	0.00000	0.76333	0.00180	0.76513
H	30	0.23412	0.00000	0.76428	0.00160	0.76588
H	31	0.23343	0.00000	0.76498	0.00159	0.76657
H	32	0.23111	0.00000	0.76744	0.00145	0.76889
H	33	0.53860	0.00000	0.45869	0.00270	0.46140
* Total *		1.00044	35.98417	87.59838	0.41701	123.99956

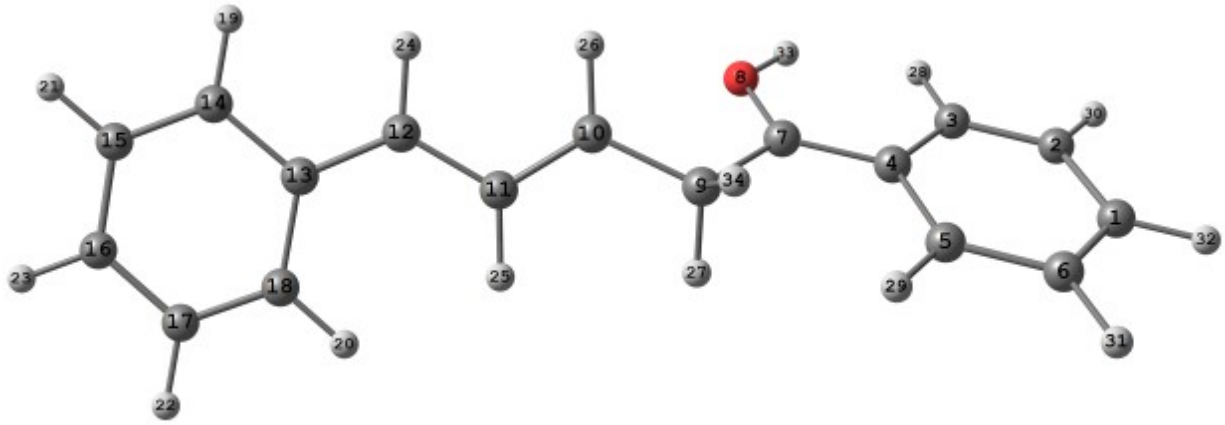
C1

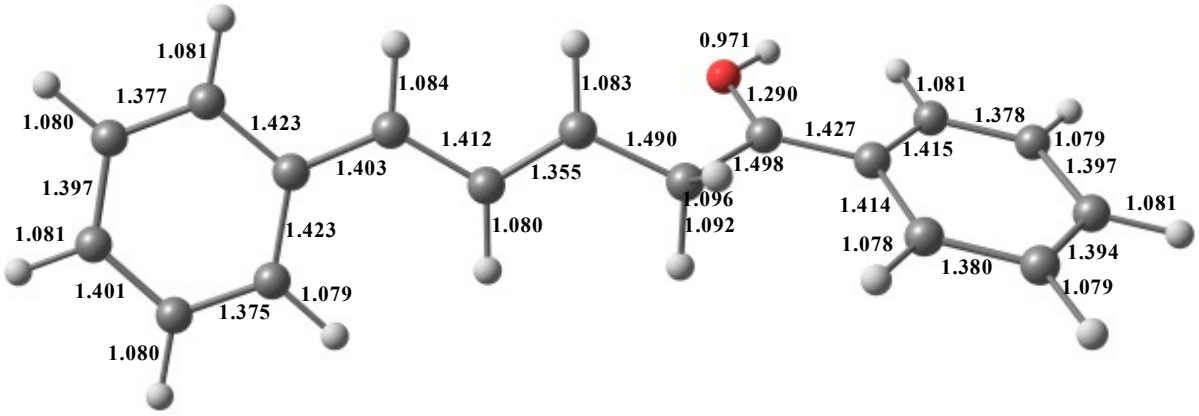
Energy E(B3LYP) = -732.482018588 h, G^{298} = -732.243737 h, μ=2.84 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	6.260175	0.727049	0.042168
2	C	5.945396	-0.544511	0.527831
3	C	4.635089	-0.971170	0.536243
4	C	3.608088	-0.126554	0.052211
5	C	3.946294	1.156602	-0.435433
6	C	5.261922	1.574498	-0.436300
7	C	2.244598	-0.547496	0.050775
8	O	1.857363	-1.702638	0.476245
9	C	1.114631	0.313704	-0.424454
10	C	-0.194292	-0.383890	-0.569618
11	C	-1.376504	0.156653	-0.188131
12	C	-2.571660	-0.548558	-0.446677
13	C	-3.881748	-0.149205	-0.143554
14	C	-4.943253	-1.026915	-0.499828
15	C	-6.250246	-0.685127	-0.231347
16	C	-6.526230	0.532900	0.395381
17	C	-5.498240	1.414053	0.757025
18	C	-4.189091	1.085120	0.494248
19	H	-4.708691	-1.964525	-0.983398
20	H	-3.400145	1.766687	0.771771
21	H	-7.056277	-1.350337	-0.501849
22	H	-5.737367	2.349454	1.240182
23	H	-7.551956	0.801965	0.605486
24	H	-2.463250	-1.508514	-0.938280
25	H	-1.399341	1.117910	0.304194
26	H	-0.189039	-1.351697	-1.055321
27	H	1.038055	1.176876	0.240001
28	H	4.428239	-1.959857	0.921994
29	H	3.185687	1.822409	-0.810908
30	H	6.725241	-1.193358	0.896394
31	H	5.514284	2.555405	-0.809550
32	H	7.289546	1.056084	0.037405

33	H	2.572781	-2.276557	0.796482
34	H	1.383759	0.716249	-1.407795





Summary of Natural Population Analysis:

Natural Population

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.09698	1.99917	4.07845	0.01936	6.09698
C	2	-0.20345	1.99916	4.18421	0.02009	6.20345
C	3	-0.11121	1.99907	4.09314	0.01901	6.11121
C	4	-0.19997	1.99891	4.18322	0.01784	6.19997
C	5	-0.09525	1.99910	4.07906	0.01709	6.09525
C	6	-0.20875	1.99915	4.18945	0.02015	6.20875

C	7	0.67164	1.99905	3.30475	0.02457	5.32836
O	8	-0.57472	1.99968	6.55070	0.02434	8.57472
C	9	-0.54024	1.99910	4.52228	0.01886	6.54024
C	10	0.04974	1.99914	3.93208	0.01905	5.95026
C	11	-0.26791	1.99901	4.24937	0.01953	6.26791
C	12	0.10267	1.99911	3.87964	0.01859	5.89733
C	13	-0.14309	1.99901	4.12449	0.01959	6.14309
C	14	-0.07792	1.99910	4.06051	0.01831	6.07792
C	15	-0.22022	1.99915	4.20109	0.01998	6.22022
C	16	-0.07551	1.99918	4.05729	0.01904	6.07551
C	17	-0.21364	1.99916	4.19460	0.01989	6.21364
C	18	-0.09155	1.99908	4.07521	0.01726	6.09155
H	19	0.24235	0.00000	0.75599	0.00166	0.75765
H	20	0.23871	0.00000	0.75959	0.00170	0.76129
H	21	0.24408	0.00000	0.75431	0.00161	0.75592
H	22	0.24337	0.00000	0.75503	0.00160	0.75663
H	23	0.23970	0.00000	0.75896	0.00134	0.76030
H	24	0.24229	0.00000	0.75580	0.00191	0.75771
H	25	0.24623	0.00000	0.75061	0.00316	0.75377
H	26	0.24363	0.00000	0.75406	0.00231	0.75637
H	27	0.29112	0.00000	0.70720	0.00168	0.70888
H	28	0.23514	0.00000	0.76253	0.00233	0.76486
H	29	0.23864	0.00000	0.75958	0.00178	0.76136
H	30	0.24454	0.00000	0.75390	0.00156	0.75546
H	31	0.24430	0.00000	0.75416	0.00154	0.75570
H	32	0.24034	0.00000	0.75830	0.00136	0.75966
H	33	0.55613	0.00000	0.44142	0.00245	0.44387
H	34	0.30582	0.00000	0.69253	0.00166	0.69418
* Total *		2.00000	35.98431	87.63350	0.38219	124.00000

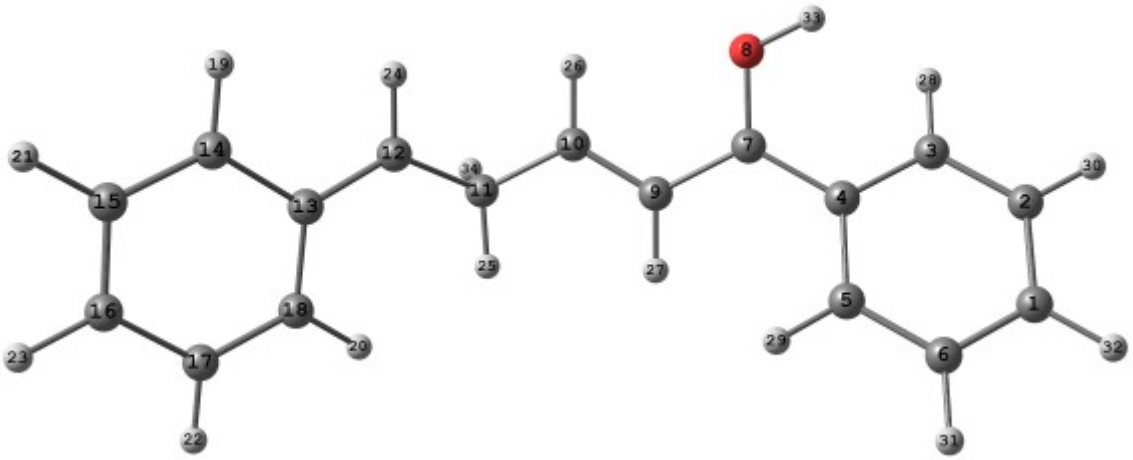
B1

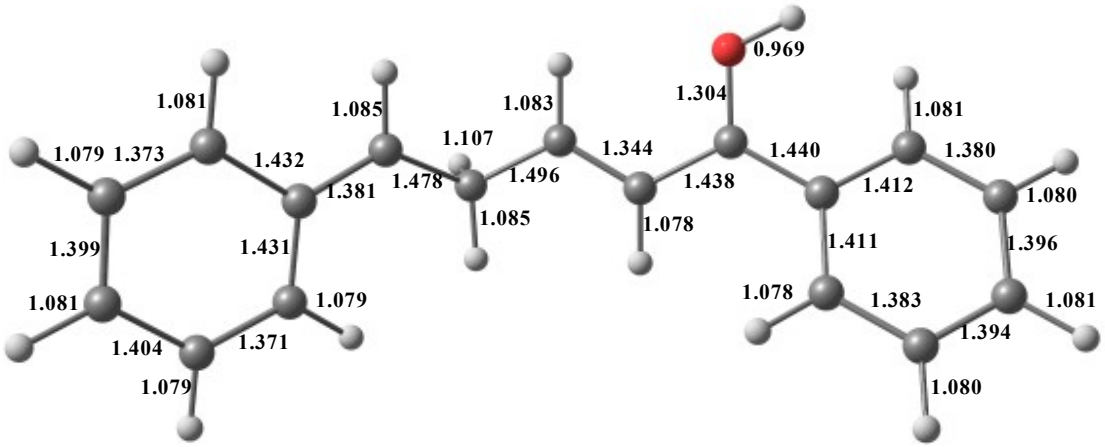
Energy E(B3LYP) = -732.472723433 h, G^{298} = -732.236072 h, μ=5.43 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	5.722648	1.493562	-0.343113
2	C	5.854281	0.106218	-0.261725
3	C	4.731460	-0.684277	-0.120829
4	C	3.451295	-0.094349	-0.045334
5	C	3.336265	1.310133	-0.110943
6	C	4.465785	2.091333	-0.270506
7	C	2.275500	-0.916423	0.077705
8	O	2.304169	-2.184461	-0.223173
9	C	1.013894	-0.417755	0.554002
10	C	-0.097070	-1.173513	0.550546
11	C	-1.407045	-0.698199	1.093792
12	C	-2.555043	-1.006888	0.215407
13	C	-3.699888	-0.258446	0.027674
14	C	-4.707146	-0.795828	-0.836999
15	C	-5.873688	-0.104907	-1.055629
16	C	-6.066388	1.128169	-0.422803

17	C	-5.097073	1.680822	0.429720
18	C	-3.924276	1.007569	0.655647
19	H	-4.532602	-1.750696	-1.311613
20	H	-3.175953	1.434609	1.304587
21	H	-6.635689	-0.504595	-1.706930
22	H	-5.278036	2.635498	0.899524
23	H	-6.984311	1.672542	-0.596426
24	H	-2.501956	-1.950896	-0.316319
25	H	-1.369123	0.337518	1.415608
26	H	-0.063573	-2.182014	0.158428
27	H	0.990187	0.589745	0.935332
28	H	4.862366	-1.752807	-0.020065
29	H	2.368706	1.784793	-0.075672
30	H	6.831997	-0.350066	-0.299693
31	H	4.370146	3.164590	-0.339094
32	H	6.603712	2.108716	-0.457846
33	H	3.140373	-2.463867	-0.626225
34	H	-1.600658	-1.300713	2.002108





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.11449	1.99917	4.09581	0.01951	6.11449
C	2	-0.20214	1.99916	4.18276	0.02022	6.20214
C	3	-0.13503	1.99907	4.11680	0.01916	6.13503
C	4	-0.16956	1.99893	4.15246	0.01818	6.16956
C	5	-0.11051	1.99909	4.09405	0.01737	6.11051
C	6	-0.20876	1.99915	4.18954	0.02007	6.20876
C	7	0.58125	1.99897	3.39453	0.02526	5.41875
O	8	-0.59408	1.99970	6.57034	0.02405	8.59408
C	9	-0.30259	1.99896	4.28461	0.01902	6.30259
C	10	0.02187	1.99909	3.96116	0.01788	5.97813
C	11	-0.52491	1.99916	4.50648	0.01928	6.52491
C	12	0.20752	1.99909	3.77722	0.01618	5.79248
C	13	-0.16849	1.99898	4.14984	0.01967	6.16849
C	14	-0.03885	1.99910	4.02134	0.01840	6.03885
C	15	-0.22802	1.99914	4.20881	0.02007	6.22802
C	16	-0.03558	1.99919	4.01761	0.01878	6.03558
C	17	-0.21821	1.99915	4.19908	0.01997	6.21821
C	18	-0.05862	1.99908	4.04234	0.01720	6.05862
H	19	0.24814	0.00000	0.75018	0.00168	0.75186
H	20	0.24198	0.00000	0.75629	0.00173	0.75802
H	21	0.25131	0.00000	0.74710	0.00159	0.74869

H	22	0.25041	0.00000	0.74800	0.00159	0.74959
H	23	0.24580	0.00000	0.75291	0.00129	0.75420
H	24	0.24559	0.00000	0.75250	0.00191	0.75441
H	25	0.25474	0.00000	0.74254	0.00273	0.74526
H	26	0.24478	0.00000	0.75276	0.00246	0.75522
H	27	0.25552	0.00000	0.74265	0.00183	0.74448
H	28	0.23544	0.00000	0.76228	0.00227	0.76456
H	29	0.23864	0.00000	0.75968	0.00168	0.76136
H	30	0.24073	0.00000	0.75770	0.00157	0.75927
H	31	0.24018	0.00000	0.75827	0.00155	0.75982
H	32	0.23654	0.00000	0.76207	0.00139	0.76346
H	33	0.54832	0.00000	0.44919	0.00249	0.45168
H	34	0.32108	0.00000	0.67718	0.00174	0.67892
* Total *		2.00000	35.98417	87.63606	0.37977	124.00000

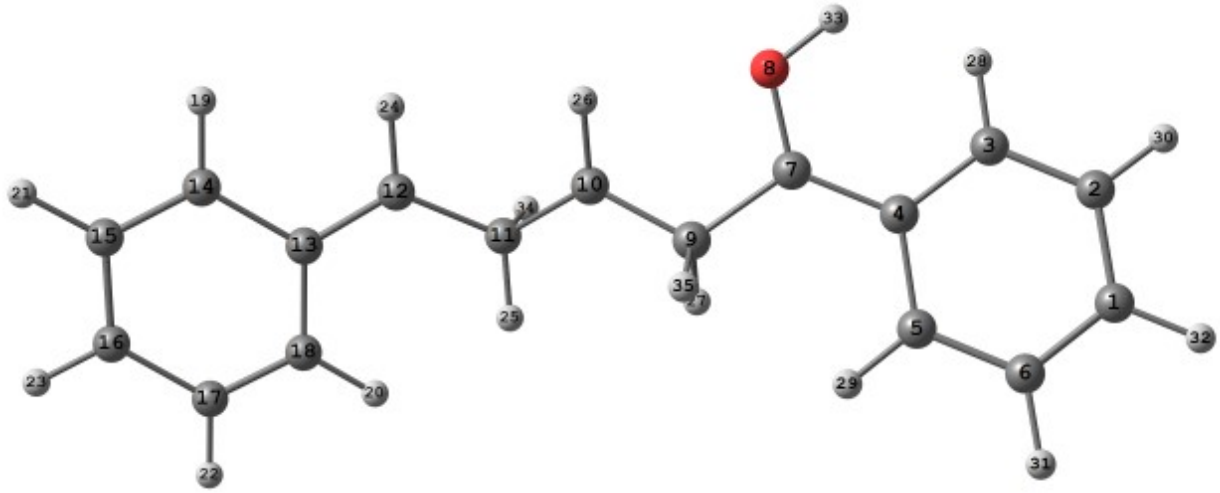
D1

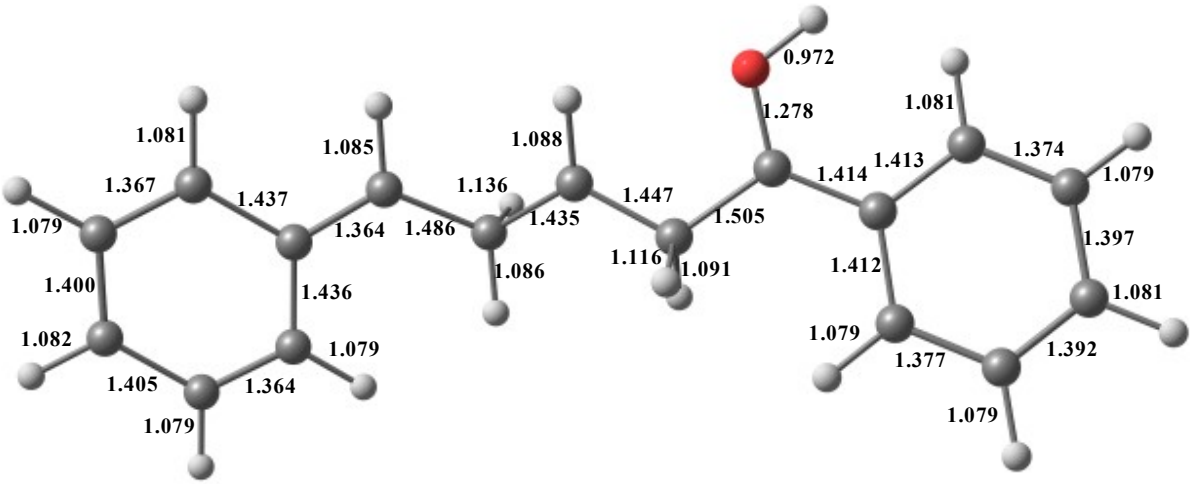
Energy E(B3LYP) = -732.802953022 h, G^{298} = -732.555979 h, μ=4.43 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	6.085545	1.113846	-0.119873
2	C	6.015484	-0.261925	0.109395
3	C	4.791811	-0.884739	0.148077
4	C	3.613586	-0.126428	-0.034819
5	C	3.699537	1.266684	-0.246831
6	C	4.933576	1.875158	-0.298714
7	C	2.346555	-0.754672	-0.019559
8	O	2.157446	-2.018530	-0.010475
9	C	1.061040	0.027641	-0.001367
10	C	-0.162920	-0.741161	0.059702
11	C	-1.387005	-0.175623	0.550625
12	C	-2.650657	-0.836410	0.133333
13	C	-3.868509	-0.229462	0.039768
14	C	-4.981593	-1.053385	-0.343792
15	C	-6.233499	-0.512101	-0.436836
16	C	-6.406117	0.848644	-0.158855
17	C	-5.338666	1.683098	0.214771
18	C	-4.081448	1.163628	0.313637
19	H	-4.807169	-2.099966	-0.551463
20	H	-3.257024	1.799759	0.597045
21	H	-7.079407	-1.118480	-0.720710
22	H	-5.519995	2.727223	0.416900
23	H	-7.396750	1.276444	-0.236499
24	H	-2.588012	-1.897384	-0.086015
25	H	-1.384234	0.908436	0.614928
26	H	-0.152980	-1.782247	-0.255192
27	H	1.077564	0.856865	0.707626
28	H	4.760025	-1.946603	0.349313
29	H	2.811710	1.863879	-0.389676
30	H	6.918213	-0.833568	0.260259
31	H	5.004268	2.937435	-0.474618

32	H	7.052405	1.596380	-0.154196
33	H	2.963307	-2.559131	-0.070935
34	H	-1.212233	-0.518801	1.619024
35	H	0.930428	0.521255	-0.993968





Summary of Natural Population Analysis:

Natural Population

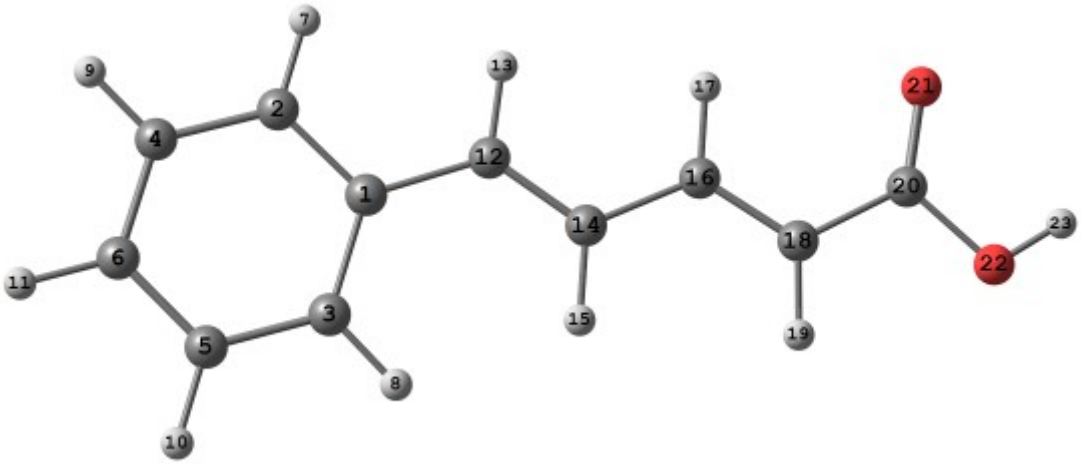
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.06921	1.99917	4.05078	0.01925	6.06921
C	2	-0.19607	1.99915	4.17685	0.02007	6.19607
C	3	-0.10125	1.99906	4.08328	0.01891	6.10125
C	4	-0.18893	1.99891	4.17214	0.01788	6.18893
C	5	-0.08783	1.99909	4.07186	0.01688	6.08783
C	6	-0.20450	1.99915	4.18510	0.02026	6.20450
C	7	0.64669	1.99903	3.32852	0.02575	5.35331
O	8	-0.56940	1.99967	6.54520	0.02454	8.56940
C	9	-0.60588	1.99904	4.58612	0.02073	6.60588
C	10	0.40456	1.99922	3.57979	0.01643	5.59544
C	11	-0.58135	1.99908	4.56001	0.02227	6.58135
C	12	0.15337	1.99904	3.82975	0.01784	5.84663
C	13	-0.14078	1.99897	4.12230	0.01951	6.14078
C	14	-0.02280	1.99910	4.00540	0.01831	6.02280
C	15	-0.22594	1.99913	4.20669	0.02012	6.22594
C	16	0.00604	1.99920	3.97613	0.01864	5.99396
C	17	-0.21400	1.99915	4.19466	0.02019	6.21400
C	18	-0.05328	1.99908	4.03718	0.01702	6.05328
H	19	0.25432	0.00000	0.74403	0.00165	0.74568
H	20	0.24514	0.00000	0.75302	0.00184	0.75486
H	21	0.25764	0.00000	0.74080	0.00156	0.74236
H	22	0.25688	0.00000	0.74157	0.00155	0.74312
H	23	0.24954	0.00000	0.74920	0.00126	0.75046
H	24	0.26659	0.00000	0.73153	0.00189	0.73341
H	25	0.30369	0.00000	0.69459	0.00172	0.69631
H	26	0.28596	0.00000	0.71106	0.00298	0.71404
H	27	0.33006	0.00000	0.66823	0.00170	0.66994
H	28	0.24154	0.00000	0.75625	0.00221	0.75846
H	29	0.24017	0.00000	0.75800	0.00183	0.75983
H	30	0.24786	0.00000	0.75060	0.00154	0.75214
H	31	0.24810	0.00000	0.75038	0.00152	0.75190
H	32	0.24234	0.00000	0.75634	0.00133	0.75766
H	33	0.57015	0.00000	0.42751	0.00234	0.42985
H	34	0.41774	0.00000	0.58034	0.00192	0.58226
H	35	0.39289	0.00000	0.60525	0.00186	0.60711
* Total *		3.00000	35.98424	87.63046	0.38531	124.00000

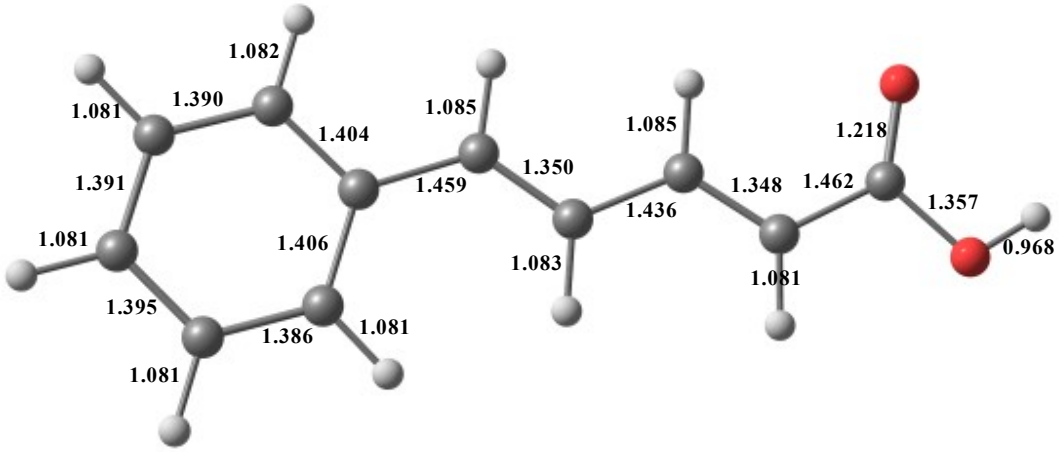
1g

Energy E(B3LYP) = -575.829970845 h, G^{298} = -575.687329 h, μ=4.31 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.015542	0.237505	0.000731
2	C	-2.972734	1.265104	-0.000859
3	C	-2.470834	-1.092716	0.001779
4	C	-4.332573	0.979473	-0.001712
5	C	-3.827897	-1.376468	0.000987
6	C	-4.765548	-0.342929	-0.000831
7	H	-2.639941	2.294830	-0.001497
8	H	-1.763378	-1.909516	0.003446
9	H	-5.051806	1.786789	-0.003011
10	H	-4.159369	-2.405735	0.001882
11	H	-5.822688	-0.569602	-0.001429
12	C	-0.602676	0.600180	0.001250
13	H	-0.403399	1.666820	0.002919
14	C	0.460741	-0.231980	-0.000383
15	H	0.323779	-1.306369	-0.002439
16	C	1.812030	0.254433	0.000356
17	H	1.954715	1.329529	0.002167
18	C	2.907195	-0.531456	-0.001033
19	H	2.828353	-1.609464	-0.002794
20	C	4.253263	0.039862	-0.000132
21	O	4.539958	1.223423	0.001672
22	O	5.208852	-0.923612	-0.001581
23	H	6.070709	-0.481818	-0.000895





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.10051	1.99901	4.08168	0.01982	6.10051
C	2	-0.17974	1.99908	4.16151	0.01914	6.17974
C	3	-0.18233	1.99907	4.16515	0.01811	6.18233
C	4	-0.21327	1.99915	4.19371	0.02040	6.21327
C	5	-0.20965	1.99916	4.19020	0.02029	6.20965
C	6	-0.20042	1.99916	4.18063	0.02063	6.20042
H	7	0.22192	0.00000	0.77623	0.00186	0.77808
H	8	0.22043	0.00000	0.77778	0.00179	0.77957
H	9	0.22321	0.00000	0.77512	0.00168	0.77679
H	10	0.22265	0.00000	0.77568	0.00167	0.77735
H	11	0.22223	0.00000	0.77622	0.00155	0.77777
C	12	-0.13101	1.99907	4.11269	0.01925	6.13101
H	13	0.21643	0.00000	0.78145	0.00211	0.78357
C	14	-0.23386	1.99905	4.21543	0.01937	6.23386
H	15	0.21523	0.00000	0.78115	0.00362	0.78477
C	16	-0.12004	1.99909	4.10100	0.01995	6.12004
H	17	0.22363	0.00000	0.77385	0.00252	0.77637
C	18	-0.33133	1.99897	4.31083	0.02152	6.33133
H	19	0.22786	0.00000	0.77003	0.00211	0.77214
C	20	0.78588	1.99937	3.17574	0.03901	5.21412
O	21	-0.68948	1.99974	6.66331	0.02643	8.68948

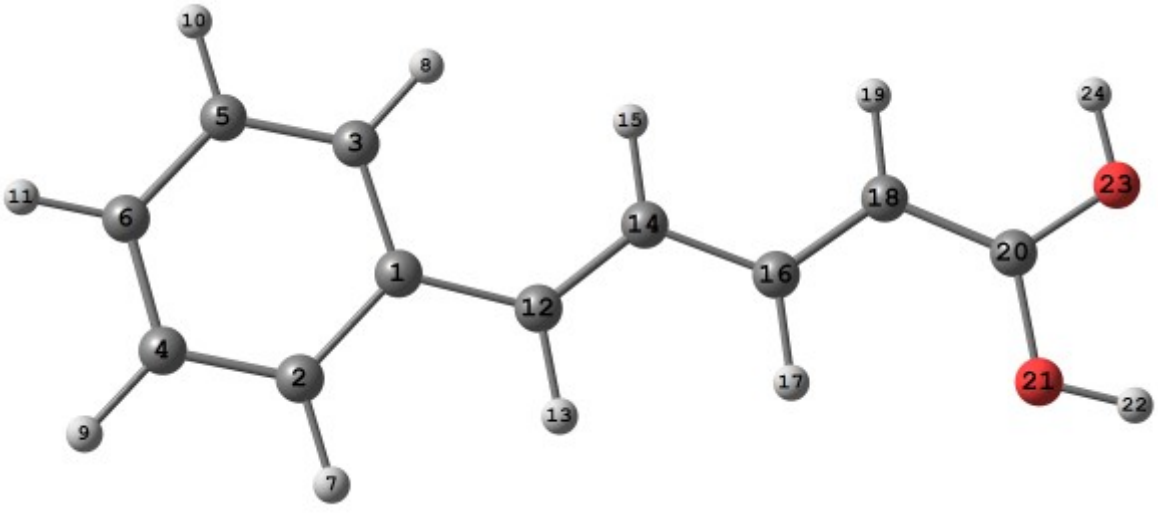
O	22	-0.71748	1.99975	6.69502	0.02270	8.71748
H	23	0.52965	0.00000	0.46728	0.00307	0.47035
* Total *		0.00000	25.98967	65.70170	0.30863	92.00000

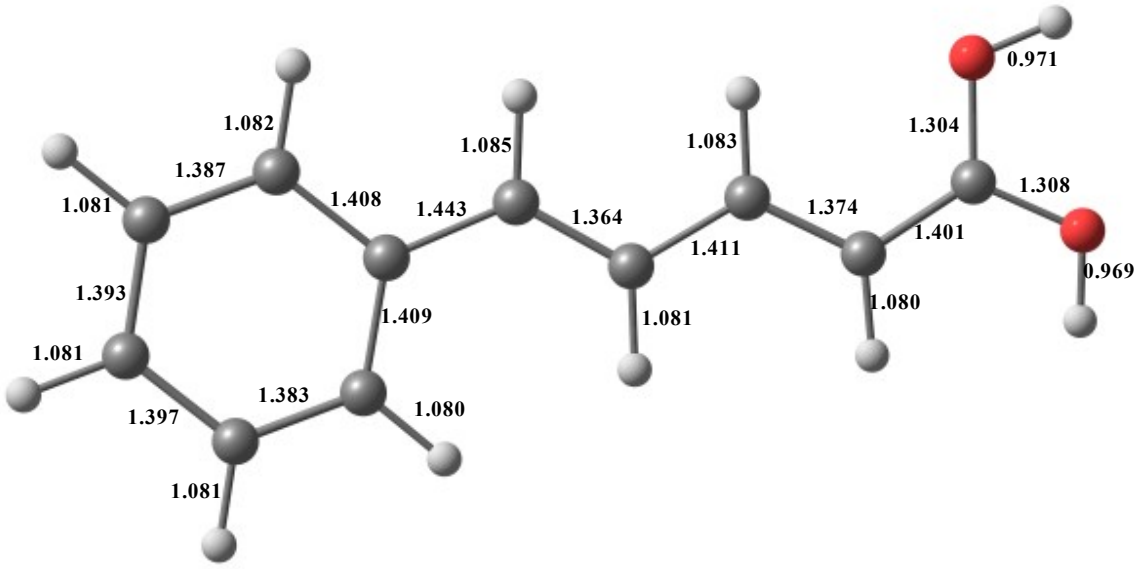
A2

Energy E(B3LYP) = -576.243337793 h, G^{298} = -576.088732 h, μ=10.0 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.043288	0.224478	0.000086
2	C	-2.978697	1.276685	-0.001143
3	C	-2.519973	-1.101612	0.001486
4	C	-4.340542	1.016264	-0.001224
5	C	-3.879716	-1.356809	0.001582
6	C	-4.793539	-0.300539	0.000167
7	H	-2.623230	2.298220	-0.002123
8	H	-1.827082	-1.930002	0.002754
9	H	-5.047039	1.833958	-0.002290
10	H	-4.235051	-2.377426	0.002828
11	H	-5.854719	-0.506858	0.000238
12	C	-0.639175	0.558270	0.000035
13	H	-0.415600	1.619587	0.000855
14	C	0.421837	-0.299557	-0.001034
15	H	0.276585	-1.371249	-0.002376
16	C	1.743445	0.193603	-0.000367
17	H	1.874784	1.268891	0.001218
18	C	2.864785	-0.599648	-0.001510
19	H	2.785940	-1.676722	-0.003384
20	C	4.154649	-0.053726	-0.000066
21	O	4.343694	1.236785	0.002845
22	H	5.289031	1.456586	0.004327
23	O	5.251493	-0.766774	-0.001252
24	H	5.076168	-1.719529	-0.002855





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.12614	1.99901	4.10746	0.01967	6.12614
C	2	-0.15149	1.99909	4.13352	0.01888	6.15149
C	3	-0.15938	1.99907	4.14248	0.01783	6.15938
C	4	-0.21248	1.99915	4.19309	0.02024	6.21248
C	5	-0.20740	1.99916	4.18812	0.02013	6.20740
C	6	-0.16059	1.99916	4.14134	0.02009	6.16059
H	7	0.22816	0.00000	0.77006	0.00178	0.77184
H	8	0.22619	0.00000	0.77206	0.00175	0.77381
H	9	0.22828	0.00000	0.77007	0.00166	0.77172
H	10	0.22771	0.00000	0.77064	0.00165	0.77229
H	11	0.22551	0.00000	0.77301	0.00148	0.77449
C	12	-0.05660	1.99909	4.03873	0.01877	6.05660
H	13	0.22839	0.00000	0.76963	0.00197	0.77161
C	14	-0.25629	1.99906	4.23756	0.01967	6.25629
H	15	0.22920	0.00000	0.76739	0.00341	0.77080
C	16	-0.03610	1.99914	4.01754	0.01942	6.03610
H	17	0.23534	0.00000	0.76245	0.00221	0.76466
C	18	-0.37376	1.99900	4.35511	0.01966	6.37376
H	19	0.25267	0.00000	0.74529	0.00204	0.74733
C	20	0.81891	1.99918	3.15268	0.02923	5.18109
O	21	-0.64193	1.99970	6.61693	0.02530	8.64193

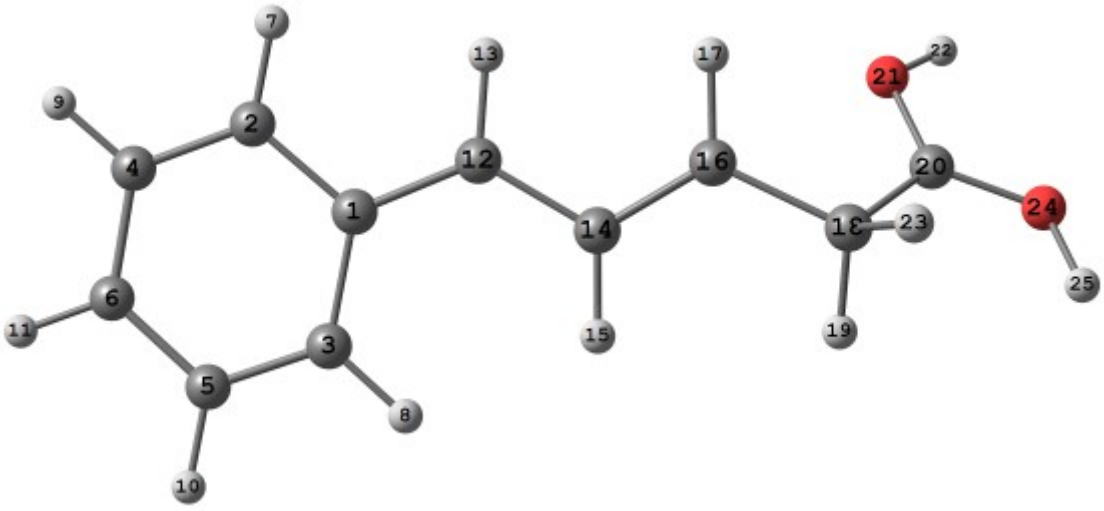
H	22	0.55940	0.00000	0.43791	0.00270	0.44060
O	23	-0.63944	1.99970	6.61493	0.02482	8.63944
H	24	0.56185	0.00000	0.43583	0.00232	0.43815
* Total *		1.00000	25.98950	65.71382	0.29669	92.00000

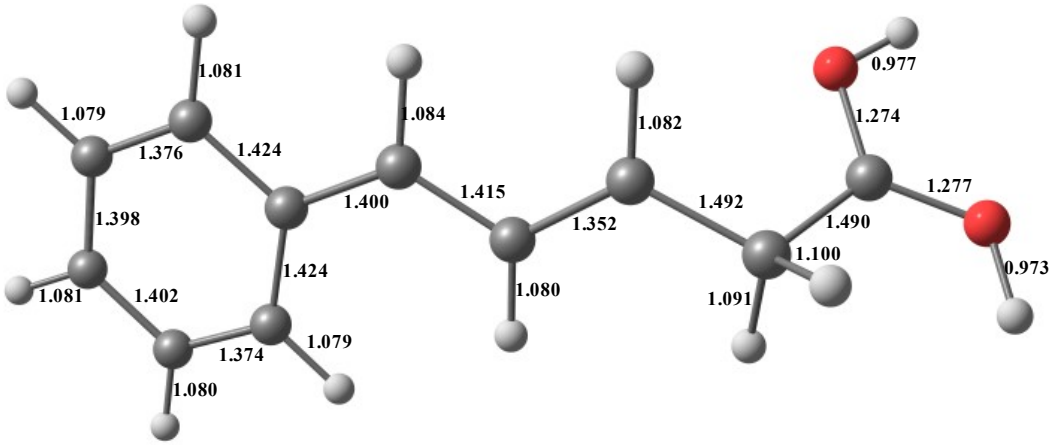
C2

Energy E(B3LYP) = -576.625554807 h, G^{298} = -576.457641 h, μ=13.6 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.028459	0.220377	0.110120
2	C	-2.990453	1.269711	0.152718
3	C	-2.467558	-1.112714	-0.132601
4	C	-4.325895	0.998427	-0.041393
5	C	-3.804493	-1.369494	-0.321747
6	C	-4.731052	-0.318406	-0.277537
7	H	-2.655562	2.280576	0.336516
8	H	-1.756542	-1.923479	-0.166884
9	H	-5.055944	1.793052	-0.011772
10	H	-4.144244	-2.377751	-0.504504
11	H	-5.779953	-0.532019	-0.428667
12	C	-0.685107	0.559088	0.309926
13	H	-0.474908	1.605836	0.497411
14	C	0.433983	-0.307032	0.286415
15	H	0.308673	-1.362904	0.096641
16	C	1.665799	0.208033	0.496934
17	H	1.774272	1.267706	0.687349
18	C	2.906371	-0.620671	0.534811
19	H	2.757764	-1.621661	0.126194
20	C	4.083312	-0.009031	-0.143495
21	O	3.958802	1.146270	-0.664752
22	H	4.779699	1.477101	-1.078017
23	H	3.202276	-0.766151	1.583780
24	O	5.220998	-0.582728	-0.231825
25	H	5.267370	-1.458380	0.189675





Summary of Natural Population Analysis:

Natural Population

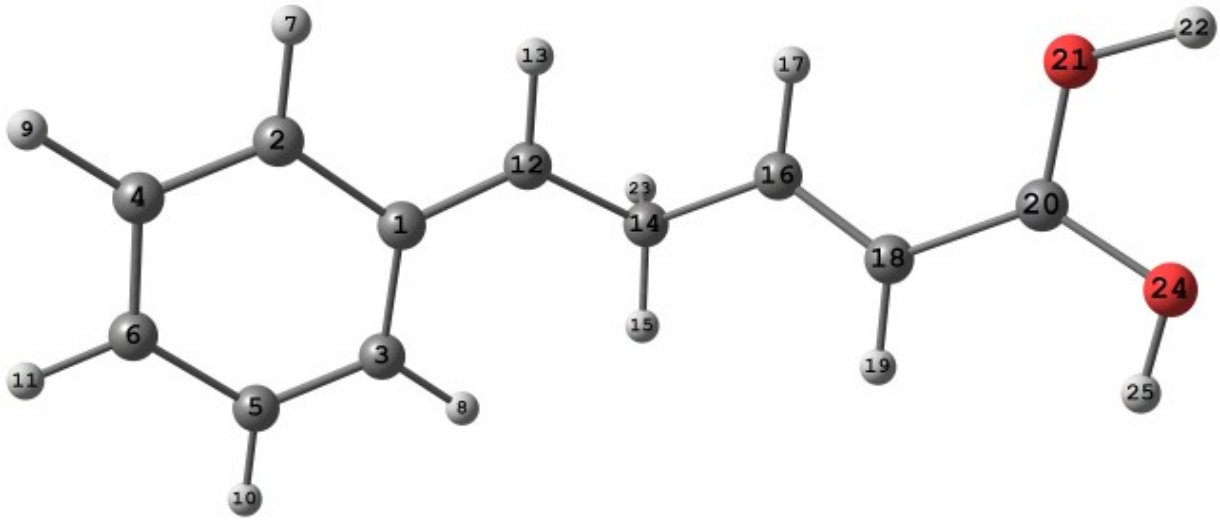
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.14364	1.99901	4.12504	0.01960	6.14364
C	2	-0.07428	1.99910	4.05688	0.01831	6.07428
C	3	-0.08879	1.99908	4.07244	0.01727	6.08879
C	4	-0.21955	1.99915	4.20038	0.02002	6.21955
C	5	-0.21318	1.99916	4.19410	0.01992	6.21318
C	6	-0.07471	1.99918	4.05651	0.01902	6.07471
H	7	0.24386	0.00000	0.75449	0.00165	0.75614
H	8	0.24032	0.00000	0.75800	0.00168	0.75968
H	9	0.24566	0.00000	0.75274	0.00160	0.75434
H	10	0.24498	0.00000	0.75343	0.00159	0.75502
H	11	0.24180	0.00000	0.75686	0.00134	0.75820
C	12	0.10062	1.99911	3.88176	0.01852	5.89938
H	13	0.24483	0.00000	0.75330	0.00187	0.75517
C	14	-0.26513	1.99901	4.24645	0.01967	6.26513
H	15	0.24901	0.00000	0.74790	0.00309	0.75099
C	16	0.04189	1.99913	3.94069	0.01829	5.95811
H	17	0.24588	0.00000	0.75205	0.00207	0.75412
C	18	-0.56059	1.99910	4.54295	0.01854	6.56059
H	19	0.29359	0.00000	0.70460	0.00180	0.70641
C	20	0.93804	1.99944	3.03185	0.03067	5.06196
O	21	-0.58285	1.99966	6.55720	0.02599	8.58285
H	22	0.58239	0.00000	0.41508	0.00253	0.41761
H	23	0.31778	0.00000	0.68053	0.00169	0.68222
O	24	-0.58938	1.99966	6.56289	0.02684	8.58938
H	25	0.58146	0.00000	0.41627	0.00227	0.41854
* Total *		2.00000	25.98978	65.71439	0.29583	92.00000

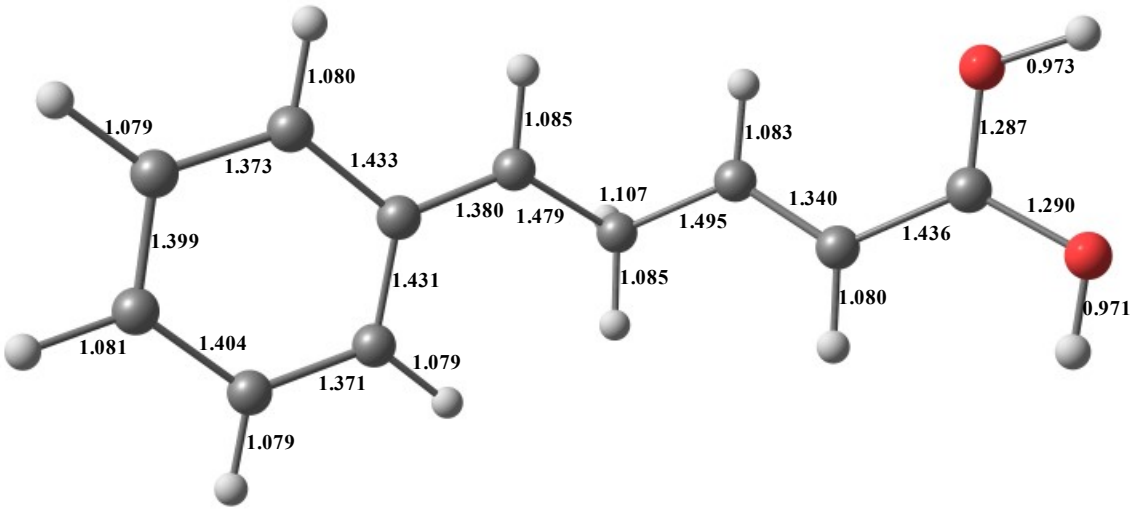
B2

Energy E(B3LYP) = -576.6167406 h, G^{298} = -576.449601 h, μ=6.64 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.973601	-0.269849	0.184733
2	C	-2.892528	-1.294944	-0.212294
3	C	-2.420129	1.089482	0.222770
4	C	-4.184485	-0.974172	-0.549148
5	C	-3.714870	1.390083	-0.112453
6	C	-4.592165	0.363593	-0.498385
7	H	-2.552182	-2.319977	-0.239805
8	H	-1.742774	1.877175	0.512697
9	H	-4.881066	-1.741636	-0.849685
10	H	-4.063123	2.411237	-0.086611
11	H	-5.609235	0.615526	-0.765155
12	C	-0.691703	-0.656358	0.517476
13	H	-0.470488	-1.716138	0.447528
14	C	0.411143	0.200508	1.005416
15	H	0.259179	1.258526	0.819346
16	C	1.762804	-0.262785	0.566768
17	H	1.973744	-1.321666	0.649284
18	C	2.708646	0.570113	0.111106
19	H	2.537502	1.631508	0.006343
20	C	4.004806	0.083264	-0.269271
21	O	4.287495	-1.166314	-0.151935
22	H	5.191088	-1.375148	-0.447791
23	H	0.384983	0.069225	2.104098
24	O	4.935640	0.841599	-0.740193
25	H	4.679782	1.775479	-0.813541





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.17016	1.99898	4.15154	0.01965	6.17016
C	2	-0.03886	1.99910	4.02136	0.01839	6.03886
C	3	-0.05878	1.99908	4.04249	0.01720	6.05878
C	4	-0.22849	1.99914	4.20926	0.02008	6.22849
C	5	-0.21858	1.99915	4.19944	0.01998	6.21858
C	6	-0.03491	1.99919	4.01693	0.01879	6.03491
H	7	0.24878	0.00000	0.74955	0.00167	0.75122
H	8	0.24256	0.00000	0.75572	0.00172	0.75744
H	9	0.25183	0.00000	0.74658	0.00159	0.74817
H	10	0.25099	0.00000	0.74742	0.00158	0.74901
H	11	0.24628	0.00000	0.75242	0.00129	0.75372
C	12	0.20987	1.99909	3.77492	0.01613	5.79013
H	13	0.24597	0.00000	0.75214	0.00189	0.75403
C	14	-0.52687	1.99916	4.50812	0.01959	6.52687
H	15	0.25611	0.00000	0.74112	0.00277	0.74389
C	16	0.03348	1.99910	3.94942	0.01800	5.96652
H	17	0.24702	0.00000	0.75086	0.00212	0.75298
C	18	-0.35520	1.99894	4.33726	0.01900	6.35520
H	19	0.26749	0.00000	0.73048	0.00203	0.73251
C	20	0.87064	1.99931	3.10034	0.02971	5.12936
O	21	-0.60673	1.99968	6.58162	0.02543	8.60673
H	22	0.57245	0.00000	0.42499	0.00256	0.42755
H	23	0.32251	0.00000	0.67579	0.00170	0.67749
O	24	-0.60129	1.99968	6.57609	0.02552	8.60129
H	25	0.57388	0.00000	0.42385	0.00227	0.42612

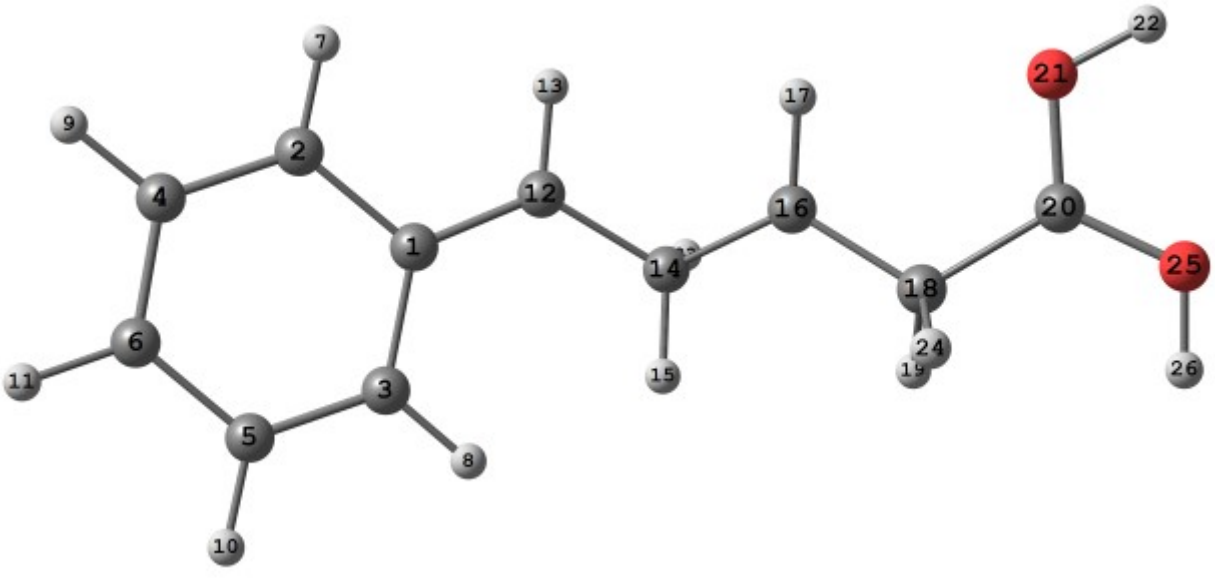
* Total *	2.00000	25.98960	65.71973	0.29067	92.00000	

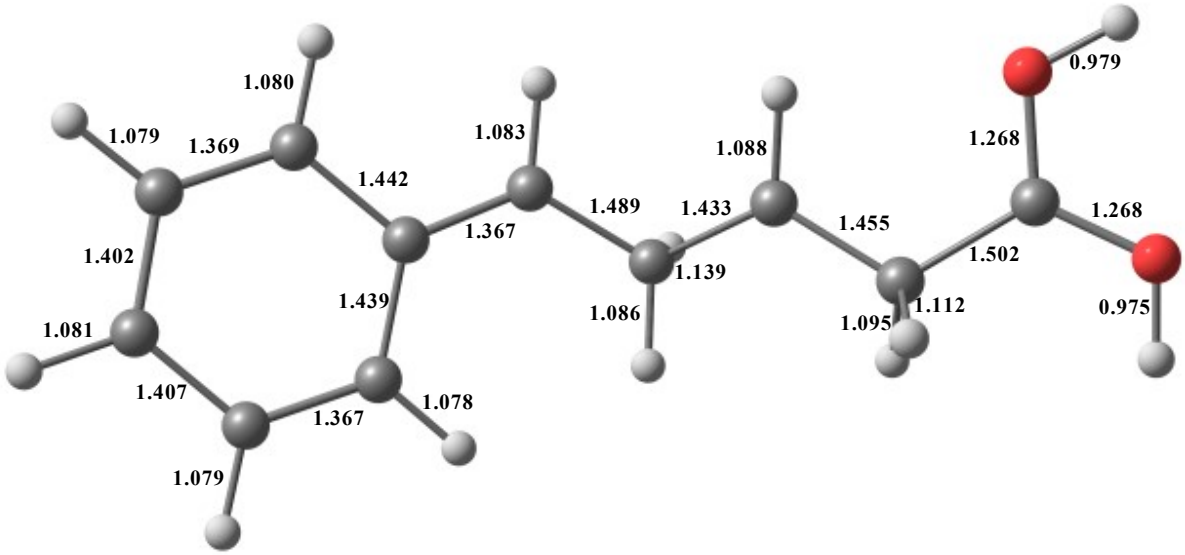
D2

Energy E(B3LYP) = -576.9395691 h, G^{298} = -576.762671 h, μ=15.2 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.068176	0.264287	0.142005
2	C	3.048947	1.305163	-0.040954
3	C	2.488406	-1.111015	0.089740
4	C	4.361652	0.983508	-0.256446
5	C	3.804911	-1.407527	-0.125663
6	C	4.736918	-0.367049	-0.298268
7	H	2.727981	2.335826	-0.002057
8	H	1.774305	-1.909061	0.216345
9	H	5.103122	1.755281	-0.392972
10	H	4.135241	-2.433796	-0.167492
11	H	5.774389	-0.618756	-0.469894
12	C	0.777378	0.661758	0.354799
13	H	0.572710	1.725258	0.378904
14	C	-0.391814	-0.229896	0.589164
15	H	-0.238121	-1.299569	0.481014
16	C	-1.670506	0.234557	0.139891
17	H	-1.819406	1.301267	-0.011831
18	C	-2.791440	-0.667320	-0.077786
19	H	-2.780009	-1.528326	0.598446
20	C	-4.151232	-0.034269	-0.151526
21	O	-4.210010	1.232242	-0.160149
22	H	-5.116936	1.594493	-0.221172
23	H	-0.642329	-0.110043	1.694126
24	H	-2.579669	-1.131175	-1.066208
25	O	-5.224291	-0.706996	-0.217421
26	H	-5.125240	-1.676553	-0.206394





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.13385	1.99898	4.11536	0.01951	6.13385
C	2	-0.01834	1.99910	4.00101	0.01823	6.01834
C	3	-0.04790	1.99908	4.03183	0.01699	6.04790
C	4	-0.22521	1.99914	4.20601	0.02006	6.22521
C	5	-0.21435	1.99915	4.19508	0.02011	6.21435
C	6	0.00827	1.99920	3.97397	0.01857	5.99173
H	7	0.25346	0.00000	0.74489	0.00165	0.74654
H	8	0.24518	0.00000	0.75300	0.00182	0.75482
H	9	0.25746	0.00000	0.74097	0.00156	0.74254
H	10	0.25681	0.00000	0.74164	0.00155	0.74319
H	11	0.25028	0.00000	0.74847	0.00126	0.74972
C	12	0.14507	1.99904	3.83814	0.01775	5.85493
H	13	0.26668	0.00000	0.73147	0.00185	0.73332
C	14	-0.58405	1.99907	4.56217	0.02280	6.58405
H	15	0.30921	0.00000	0.68910	0.00169	0.69079
C	16	0.41502	1.99922	3.57024	0.01552	5.58498
H	17	0.29005	0.00000	0.70744	0.00252	0.70995
C	18	-0.63303	1.99903	4.61416	0.01984	6.63303
H	19	0.34684	0.00000	0.65131	0.00185	0.65316
C	20	0.94179	1.99947	3.02783	0.03091	5.05821
O	21	-0.57720	1.99966	6.55186	0.02568	8.57720

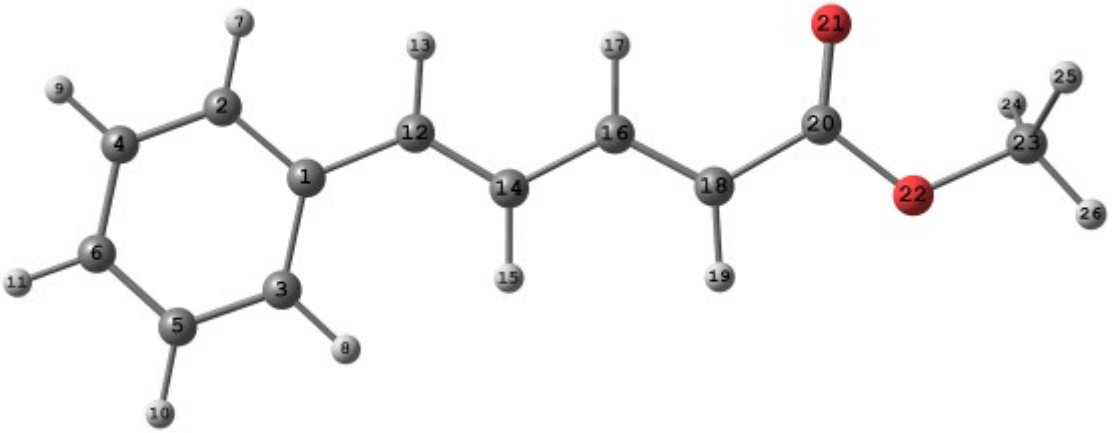
H	22	0.59651	0.00000	0.40111	0.00239	0.40349
H	23	0.42827	0.00000	0.56985	0.00188	0.57173
H	24	0.39366	0.00000	0.60465	0.00169	0.60634
O	25	-0.56242	1.99965	6.53602	0.02675	8.56242
H	26	0.59181	0.00000	0.40593	0.00225	0.40819
* Total *		3.00000	25.98980	65.71351	0.29669	92.00000

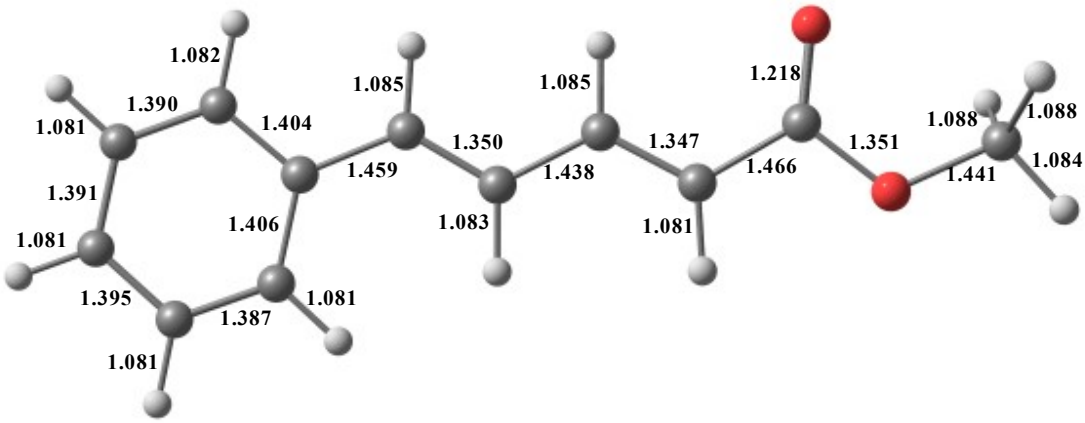
1h

Energy E(B3LYP) =-615.140510781 h, G^{298} = -614.972329 h, μ=3.44 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.560522	0.233857	0.000603
2	C	-3.538368	1.241685	-0.000705
3	C	-2.989582	-1.105003	0.001427
4	C	-4.892389	0.929119	-0.001429
5	C	-4.340840	-1.415844	0.000743
6	C	-5.299210	-0.401533	-0.000742
7	H	-3.226356	2.277919	-0.001205
8	H	-2.266155	-1.907746	0.002784
9	H	-5.627415	1.722128	-0.002488
10	H	-4.651488	-2.451639	0.001444
11	H	-6.351613	-0.649327	-0.001259
12	C	-1.154470	0.624845	0.001057
13	H	-0.976616	1.695305	0.002396
14	C	-0.075631	-0.186233	-0.000238
15	H	-0.193536	-1.263043	-0.001873
16	C	1.268955	0.322415	0.000357
17	H	1.394702	1.399664	0.001771
18	C	2.374687	-0.446616	-0.000709
19	H	2.310191	-1.525797	-0.002080
20	C	3.718053	0.141395	0.000014
21	O	3.982819	1.330413	0.001392
22	O	4.667297	-0.819652	-0.001073
23	C	6.034911	-0.366397	-0.000519
24	H	6.237574	0.228068	-0.888328
25	H	6.237669	0.225563	0.888944
26	H	6.638550	-1.267300	-0.001818





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.11035	1.99903	4.09125	0.02008	6.11035
C	2	-0.16911	1.99891	4.15029	0.01991	6.16911
C	3	-0.17350	1.99892	4.15585	0.01874	6.17350
C	4	-0.22034	1.99917	4.19988	0.02129	6.22034
C	5	-0.21587	1.99918	4.19551	0.02119	6.21587
C	6	-0.19979	1.99916	4.18104	0.01959	6.19979
H	7	0.22087	0.00000	0.77743	0.00169	0.77913
H	8	0.21948	0.00000	0.77880	0.00172	0.78052
H	9	0.22322	0.00000	0.77513	0.00165	0.77678
H	10	0.22259	0.00000	0.77577	0.00164	0.77741
H	11	0.22197	0.00000	0.77644	0.00159	0.77803
C	12	-0.13211	1.99906	4.11427	0.01879	6.13211
H	13	0.21357	0.00000	0.78342	0.00300	0.78643
C	14	-0.23027	1.99905	4.21274	0.01848	6.23027
H	15	0.21427	0.00000	0.78245	0.00328	0.78573
C	16	-0.12265	1.99909	4.10366	0.01990	6.12265
H	17	0.22275	0.00000	0.77489	0.00236	0.77725
C	18	-0.32389	1.99897	4.30289	0.02202	6.32389
H	19	0.22755	0.00000	0.77003	0.00241	0.77245
C	20	0.78887	1.99933	3.17104	0.04077	5.21113
O	21	-0.67881	1.99974	6.65313	0.02594	8.67881

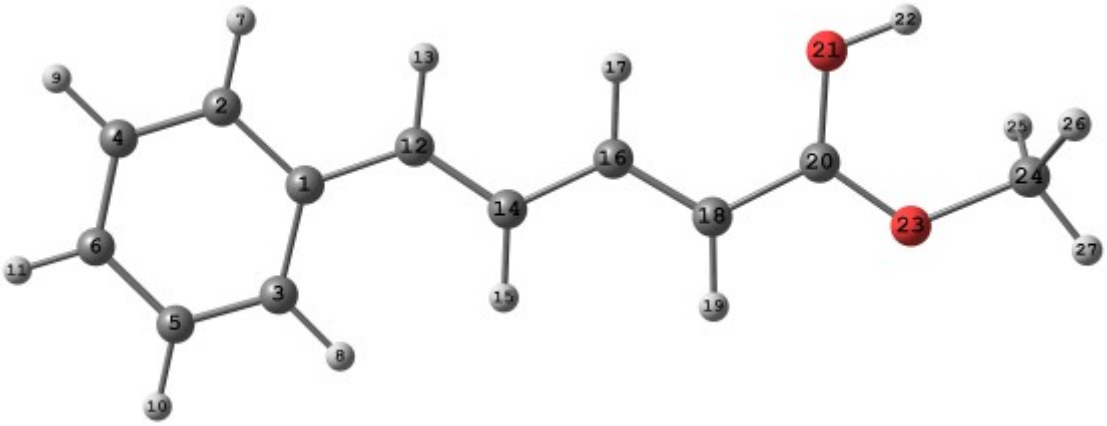
O	22	-0.55311	1.99973	6.53673	0.01665	8.55311
C	23	-0.21467	1.99923	4.20079	0.01465	6.21467
H	24	0.18830	0.00000	0.80982	0.00188	0.81170
H	25	0.18831	0.00000	0.80981	0.00188	0.81169
H	26	0.19271	0.00000	0.80597	0.00132	0.80729
* Total *		0.00000	27.98855	71.68902	0.32243	100.00000

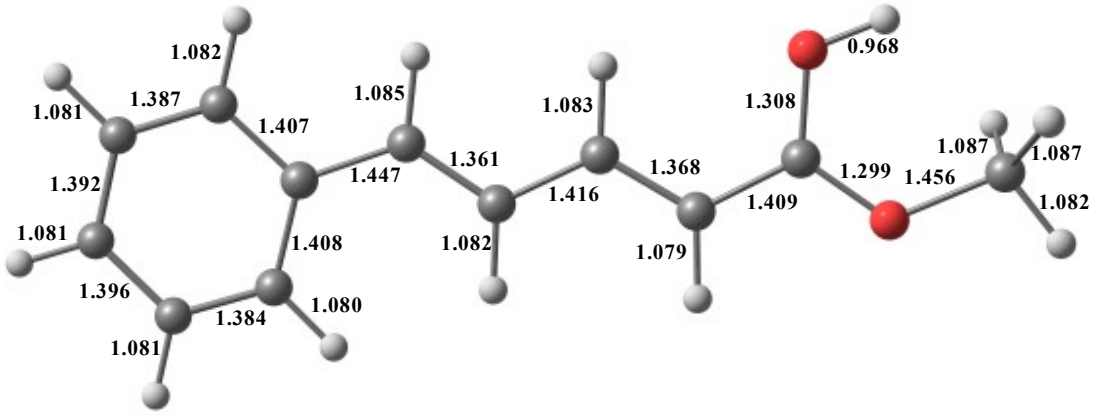
A3

Energy E(B3LYP) = -615.55173014 h, G^{298} = -615.37141 h, μ=12.4 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.583973	0.220839	0.000032
2	C	3.537288	1.255506	0.000005
3	C	3.038480	-1.112070	0.000057
4	C	4.895296	0.972094	-0.000018
5	C	4.394293	-1.391000	0.000039
6	C	5.326785	-0.351597	-0.000004
7	H	3.199756	2.283248	0.000000
8	H	2.331938	-1.929040	0.000106
9	H	5.615045	1.778306	-0.000042
10	H	4.731235	-2.417977	0.000061
11	H	6.384303	-0.576071	-0.000019
12	C	1.182124	0.579083	0.000030
13	H	0.977827	1.644315	0.000123
14	C	0.110156	-0.259369	-0.000084
15	H	0.239304	-1.333364	-0.000195
16	C	-1.211346	0.249811	-0.000055
17	H	-1.328694	1.326733	0.000015
18	C	-2.334105	-0.531268	-0.000094
19	H	-2.277970	-1.608938	-0.000141
20	C	-3.631511	0.018320	-0.000037
21	O	-3.793949	1.315699	0.000025
22	H	-4.718990	1.600696	-0.000096
23	O	-4.633957	-0.807375	-0.000035
24	C	-6.010201	-0.331841	0.000107
25	H	-6.203707	0.243106	0.902470
26	H	-6.203816	0.243443	-0.902022
27	H	-6.610369	-1.232109	-0.000047





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.12179	1.99901	4.10270	0.02008	6.12179
C	2	-0.14247	1.99891	4.12334	0.02021	6.14247
C	3	-0.15915	1.99907	4.14262	0.01745	6.15915
C	4	-0.22071	1.99917	4.20032	0.02122	6.22071
C	5	-0.20961	1.99916	4.19017	0.02028	6.20961
C	6	-0.17312	1.99916	4.15439	0.01956	6.17312
H	7	0.22591	0.00000	0.77240	0.00169	0.77409
H	8	0.22486	0.00000	0.77341	0.00173	0.77514

H	9	0.22817	0.00000	0.77021	0.00162	0.77183
H	10	0.22751	0.00000	0.77081	0.00168	0.77249
H	11	0.22669	0.00000	0.77180	0.00151	0.77331
C	12	-0.05243	1.99909	4.03472	0.01862	6.05243
H	13	0.22476	0.00000	0.77329	0.00195	0.77524
C	14	-0.25685	1.99906	4.23848	0.01931	6.25685
H	15	0.22785	0.00000	0.76875	0.00340	0.77215
C	16	-0.04789	1.99912	4.02977	0.01899	6.04789
H	17	0.23477	0.00000	0.76303	0.00220	0.76523
C	18	-0.34999	1.99901	4.32914	0.02184	6.34999
H	19	0.25483	0.00000	0.74307	0.00210	0.74517
C	20	0.82974	1.99914	3.14244	0.02868	5.17026
O	21	-0.63053	1.99969	6.60573	0.02510	8.63053
H	22	0.53935	0.00000	0.45786	0.00279	0.46065
O	23	-0.47754	1.99966	6.45383	0.02406	8.47754
C	24	-0.24246	1.99919	4.23012	0.01315	6.24246
H	25	0.20669	0.00000	0.79157	0.00175	0.79331
H	26	0.20673	0.00000	0.79152	0.00175	0.79327
H	27	0.22668	0.00000	0.77214	0.00117	0.77332
* Total *		1.00000	27.98845	71.69765	0.31390	100.00000

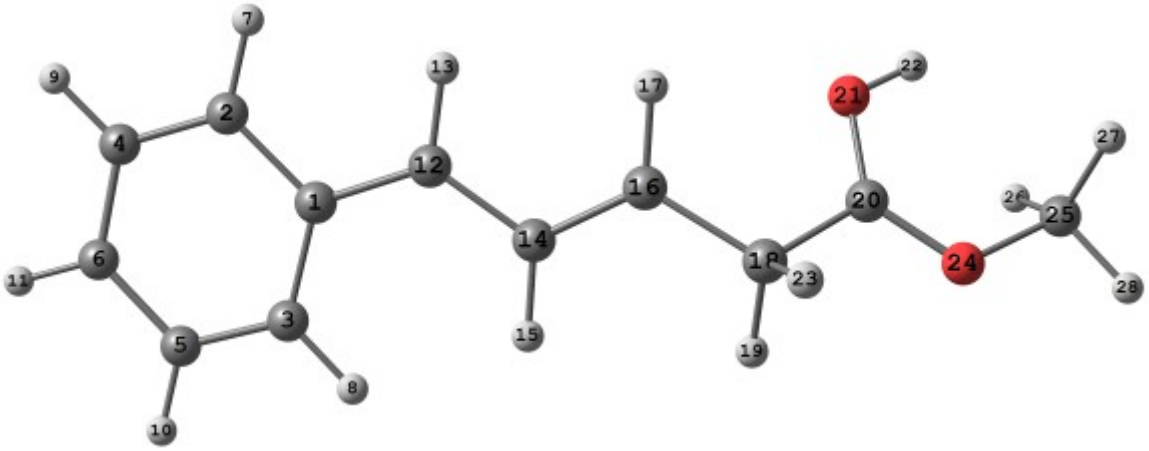
C3

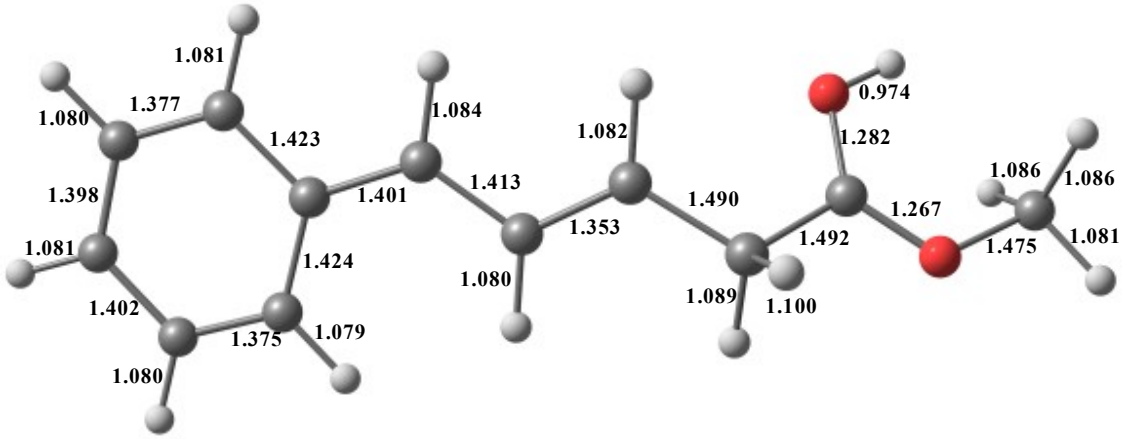
Energy E(B3LYP) =-615.938562877 h, G^{298} = -615.745345 h, μ=12.4 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.559939	0.223504	0.073139
2	C	-3.531153	1.263933	0.059921
3	C	-2.984592	-1.122427	-0.113282
4	C	-4.863012	0.971354	-0.130959
5	C	-4.317554	-1.400428	-0.303379
6	C	-5.254415	-0.357971	-0.312255
7	H	-3.207498	2.285213	0.201879
8	H	-2.265809	-1.927067	-0.106036
9	H	-5.600514	1.759618	-0.140879
10	H	-4.645658	-2.419073	-0.445649
11	H	-6.300053	-0.587996	-0.461854
12	C	-1.220172	0.583372	0.271642
13	H	-1.021124	1.640718	0.403376
14	C	-0.097123	-0.272865	0.318218
15	H	-0.212070	-1.339213	0.189886
16	C	1.128811	0.260370	0.529350
17	H	1.226439	1.331085	0.654362
18	C	2.364588	-0.561152	0.659024
19	H	2.246100	-1.573290	0.273732
20	C	3.591440	0.027248	0.046274
21	O	3.526796	1.221794	-0.414159
22	H	4.351465	1.573281	-0.793815
23	H	2.597165	-0.677653	1.727502
24	O	4.625850	-0.703687	0.032641
25	C	5.910843	-0.237269	-0.521527

26	H	5.782893	-0.036039	-1.580713
27	H	6.240604	0.631100	0.040673
28	H	6.580550	-1.071560	-0.367313





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.14227	1.99901	4.12367	0.01960	6.14227
C	2	-0.07530	1.99910	4.05788	0.01832	6.07530
C	3	-0.08930	1.99908	4.07294	0.01728	6.08930

C	4	-0.21955	1.99915	4.20039	0.02002	6.21955
C	5	-0.21331	1.99916	4.19424	0.01992	6.21331
C	6	-0.07584	1.99918	4.05762	0.01903	6.07584
H	7	0.24336	0.00000	0.75498	0.00165	0.75664
H	8	0.23988	0.00000	0.75844	0.00168	0.76012
H	9	0.24518	0.00000	0.75322	0.00160	0.75482
H	10	0.24455	0.00000	0.75386	0.00159	0.75545
H	11	0.24136	0.00000	0.75730	0.00134	0.75864
C	12	0.09931	1.99911	3.88305	0.01854	5.90069
H	13	0.24444	0.00000	0.75369	0.00187	0.75556
C	14	-0.26309	1.99902	4.24453	0.01954	6.26309
H	15	0.24868	0.00000	0.74817	0.00314	0.75132
C	16	0.03950	1.99913	3.94360	0.01778	5.96050
H	17	0.24585	0.00000	0.75210	0.00206	0.75415
C	18	-0.54557	1.99911	4.52608	0.02039	6.54557
H	19	0.29274	0.00000	0.70523	0.00203	0.70726
C	20	0.94316	1.99934	3.02757	0.02993	5.05684
O	21	-0.58452	1.99967	6.55911	0.02574	8.58452
H	22	0.56153	0.00000	0.43584	0.00263	0.43847
H	23	0.32031	0.00000	0.67781	0.00188	0.67969
O	24	-0.43438	1.99962	6.41106	0.02371	8.43438
C	25	-0.23907	1.99919	4.22532	0.01456	6.23907
H	26	0.21897	0.00000	0.77970	0.00133	0.78103
H	27	0.21812	0.00000	0.78053	0.00135	0.78188
H	28	0.23527	0.00000	0.76374	0.00098	0.76473
* Total *		2.00000	27.98884	71.70164	0.30951	100.00000

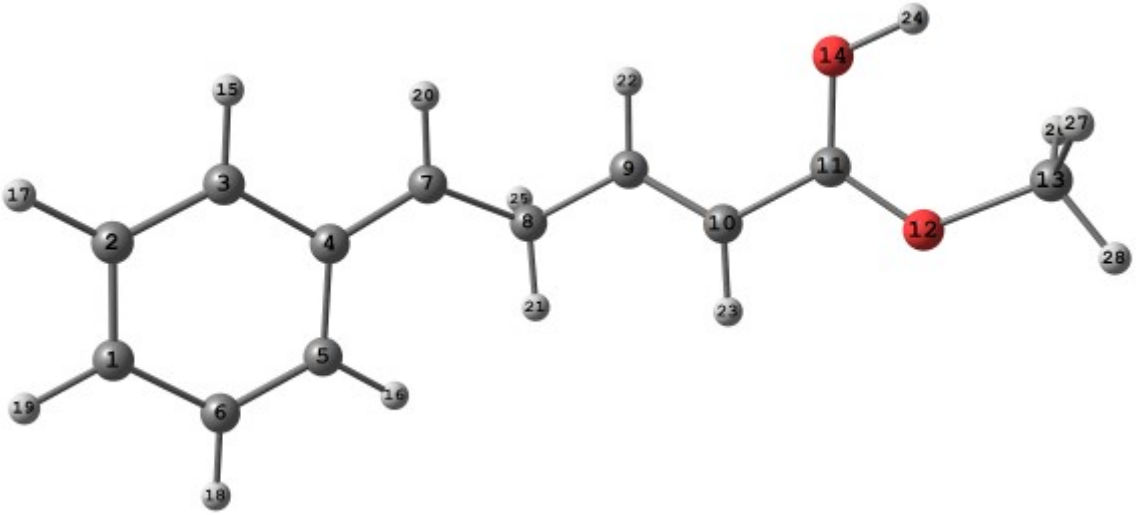
B3

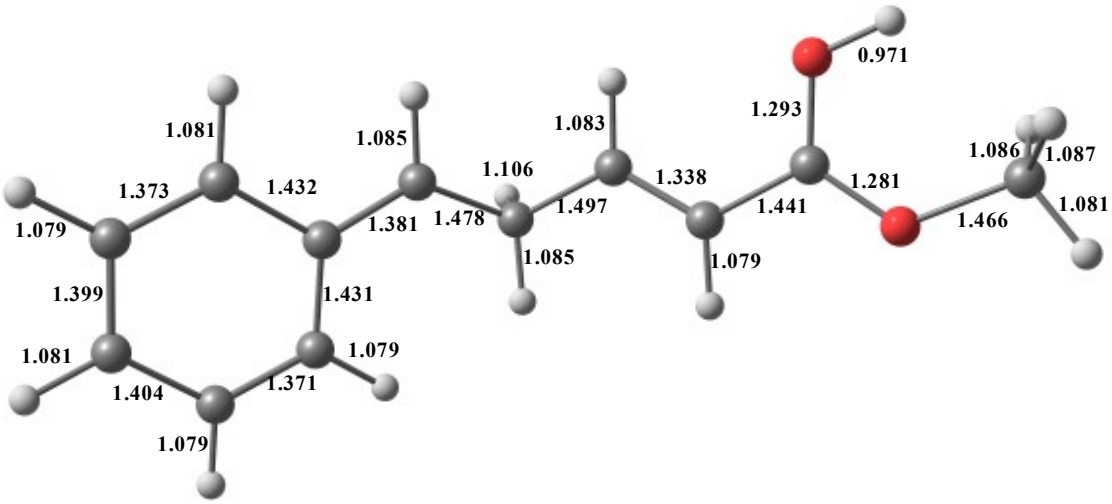
Energy E(B3LYP) = -615.928314647 h, G^{298} = -615.736402 h, μ=6.27 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	5.071858	-0.478818	-0.562919
2	C	4.693784	0.860199	-0.711958
3	C	3.419551	1.240101	-0.368034
4	C	2.490323	0.274765	0.137578
5	C	2.904984	-1.087885	0.272031
6	C	4.182128	-1.448213	-0.072769
7	C	1.231419	0.720395	0.487831
8	C	0.135777	-0.065267	1.093642
9	C	-1.228588	0.396674	0.687830
10	C	-2.201623	-0.444346	0.320271
11	C	-3.516981	0.027055	-0.030413
12	O	-4.369109	-0.861072	-0.383808
13	C	-5.740250	-0.513129	-0.767072
14	O	-3.774364	1.292532	0.024809
15	H	3.101975	2.267936	-0.469355
16	H	2.217340	-1.831742	0.642353
17	H	5.399244	1.582646	-1.092763
18	H	4.506228	-2.472984	0.025630
19	H	6.074901	-0.776984	-0.835072

20	H	1.032770	1.776702	0.339976
21	H	0.256800	-1.137744	0.980134
22	H	-1.418751	1.461951	0.722646
23	H	-2.063805	-1.513325	0.263086
24	H	-4.679799	1.540170	-0.222385
25	H	0.225510	0.145681	2.176078
26	H	-6.254402	-0.089380	0.090881
27	H	-5.717703	0.163253	-1.617238
28	H	-6.186815	-1.457041	-1.048081





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.03421	1.99919	4.01623	0.01879	6.03421
C	2	-0.22833	1.99914	4.20911	0.02008	6.22833
C	3	-0.03906	1.99910	4.02156	0.01840	6.03906
C	4	-0.16895	1.99898	4.15033	0.01965	6.16895
C	5	-0.05870	1.99908	4.04240	0.01721	6.05870
C	6	-0.21831	1.99915	4.19917	0.01999	6.21831
C	7	0.20592	1.99909	3.77889	0.01611	5.79408
C	8	-0.52499	1.99916	4.50632	0.01951	6.52499
C	9	0.01969	1.99909	3.96370	0.01751	5.98031
C	10	-0.33063	1.99894	4.31045	0.02124	6.33063
C	11	0.87402	1.99924	3.09755	0.02920	5.12598
O	12	-0.44039	1.99964	6.41657	0.02418	8.44039
C	13	-0.24184	1.99918	4.23011	0.01255	6.24184
O	14	-0.60230	1.99968	6.57724	0.02538	8.60230
H	15	0.24843	0.00000	0.74989	0.00167	0.75157
H	16	0.24211	0.00000	0.75617	0.00172	0.75789
H	17	0.25150	0.00000	0.74691	0.00159	0.74850
H	18	0.25069	0.00000	0.74773	0.00158	0.74931
H	19	0.24578	0.00000	0.75292	0.00129	0.75422
H	20	0.24647	0.00000	0.75163	0.00190	0.75353
H	21	0.25582	0.00000	0.74137	0.00281	0.74418
H	22	0.24563	0.00000	0.75229	0.00208	0.75437
H	23	0.26871	0.00000	0.72921	0.00208	0.73129
H	24	0.55210	0.00000	0.44522	0.00268	0.44790
H	25	0.32084	0.00000	0.67745	0.00172	0.67916
H	26	0.21519	0.00000	0.78322	0.00160	0.78481
H	27	0.21304	0.00000	0.78528	0.00168	0.78696
H	28	0.23174	0.00000	0.76712	0.00114	0.76826
* Total *		2.00000	27.98867	71.70600	0.30533	100

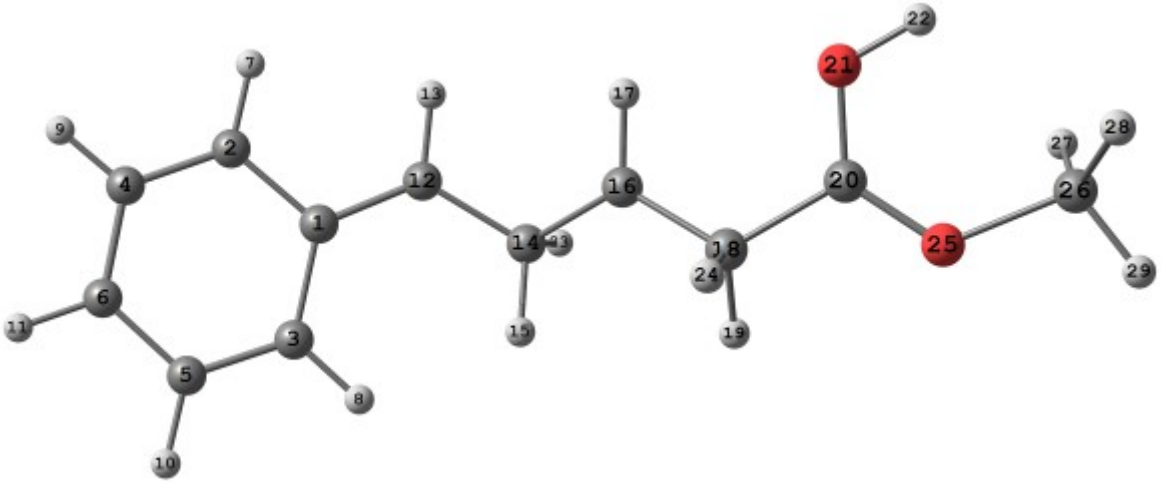
D3

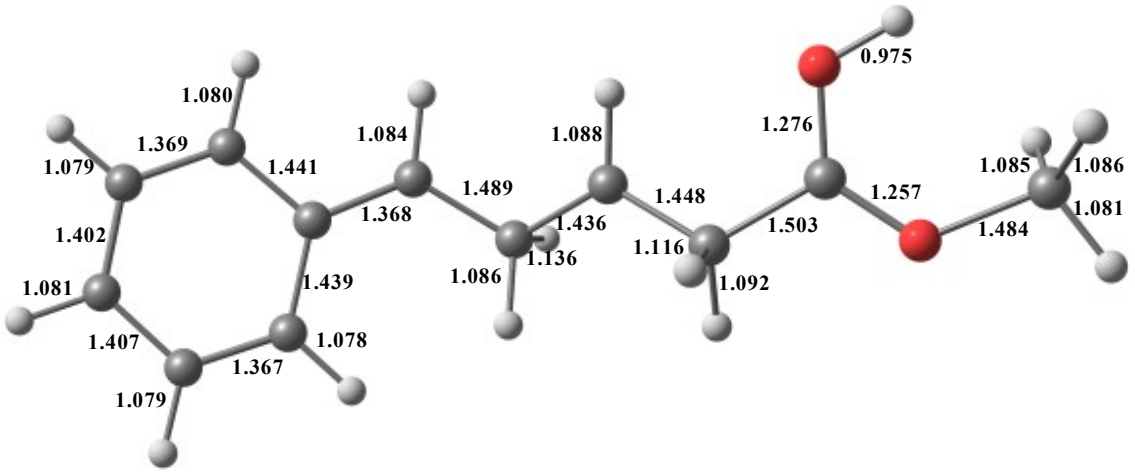
Energy E(B3LYP) = -616.256187541 h, G^{298} = -616.054029 h, μ=12.0 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.596594	0.256321	0.151587
2	C	3.593561	1.284892	-0.006628
3	C	2.994678	-1.123578	0.067731
4	C	4.900974	0.947079	-0.231350
5	C	4.307002	-1.436650	-0.151093
6	C	5.255296	-0.407807	-0.301534
7	H	3.289429	2.319559	0.055203
8	H	2.267440	-1.912440	0.176092
9	H	5.654325	1.709851	-0.352718
10	H	4.620936	-2.467058	-0.213258
11	H	6.288766	-0.672181	-0.478186

12	C	1.310858	0.666857	0.373812
13	H	1.122485	1.732379	0.430554
14	C	0.129136	-0.216263	0.572767
15	H	0.266370	-1.279610	0.398915
16	C	-1.145670	0.290025	0.148342
17	H	-1.280226	1.365508	0.056772
18	C	-2.267543	-0.578476	-0.141237
19	H	-2.255244	-1.523662	0.404925
20	C	-3.635709	0.043638	-0.137189
21	O	-3.700756	1.314449	-0.234901
22	H	-4.594173	1.703948	-0.256431
23	H	-0.109564	-0.159255	1.681502
24	H	-2.056253	-0.891072	-1.191271
25	O	-4.597747	-0.761322	-0.052058
26	C	-6.015786	-0.323704	-0.054812
27	H	-6.180213	0.301263	0.816795
28	H	-6.218532	0.183558	-0.992880
29	H	-6.567861	-1.249795	0.017289





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.13537	1.99898	4.11689	0.01950	6.13537
C	2	-0.01970	1.99910	4.00237	0.01823	6.01970
C	3	-0.04910	1.99908	4.03303	0.01699	6.04910
C	4	-0.22498	1.99914	4.20578	0.02006	6.22498
C	5	-0.21420	1.99915	4.19493	0.02012	6.21420
C	6	0.00766	1.99920	3.97456	0.01857	5.99234
H	7	0.25348	0.00000	0.74487	0.00165	0.74652
H	8	0.24512	0.00000	0.75306	0.00182	0.75488
H	9	0.25729	0.00000	0.74115	0.00156	0.74271
H	10	0.25671	0.00000	0.74175	0.00155	0.74329
H	11	0.25007	0.00000	0.74867	0.00126	0.74993
C	12	0.14740	1.99904	3.83587	0.01769	5.85260
H	13	0.26638	0.00000	0.73176	0.00186	0.73362
C	14	-0.58468	1.99908	4.56309	0.02252	6.58468
H	15	0.30795	0.00000	0.69033	0.00171	0.69205
C	16	0.41477	1.99922	3.57096	0.01505	5.58523
H	17	0.28805	0.00000	0.70948	0.00248	0.71195
C	18	-0.61495	1.99903	4.59332	0.02260	6.61495
H	19	0.34046	0.00000	0.65756	0.00199	0.65954
C	20	0.94653	1.99936	3.02394	0.03017	5.05347
O	21	-0.57701	1.99966	6.55201	0.02534	8.57701

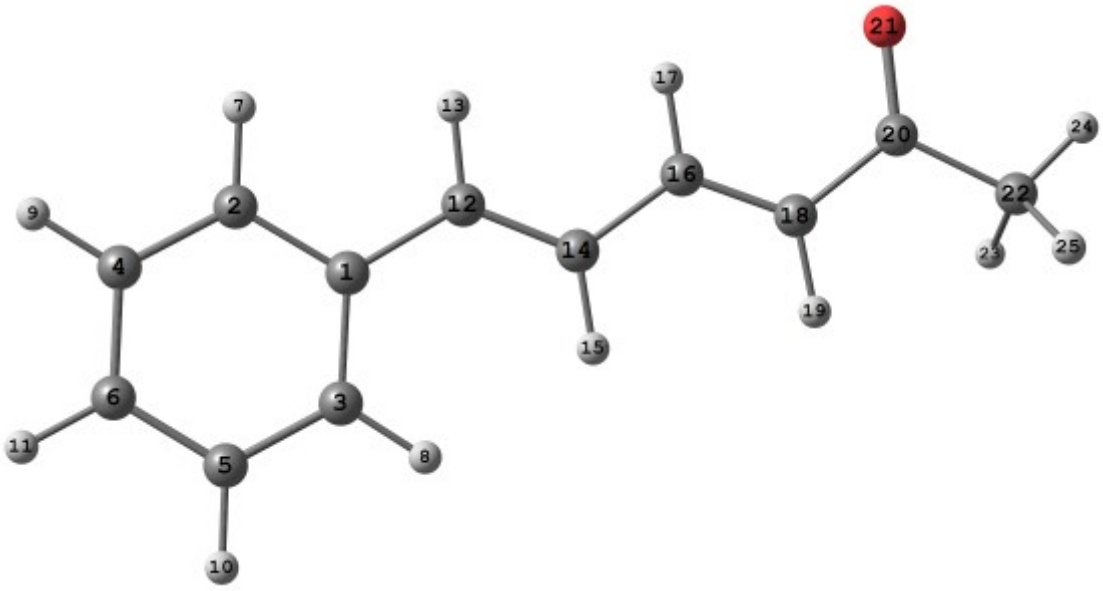
H	22	0.57550	0.00000	0.42198	0.00251	0.42450
H	23	0.42379	0.00000	0.57434	0.00186	0.57621
H	24	0.39925	0.00000	0.59891	0.00184	0.60075
O	25	-0.41573	1.99961	6.39278	0.02335	8.41573
C	26	-0.23146	1.99918	4.21826	0.01402	6.23146
H	27	0.22437	0.00000	0.77435	0.00128	0.77563
H	28	0.22380	0.00000	0.77490	0.00130	0.77620
H	29	0.23862	0.00000	0.76040	0.00098	0.76138
* Total *		3.00000	27.98884	71.70129	0.30987	100.00000

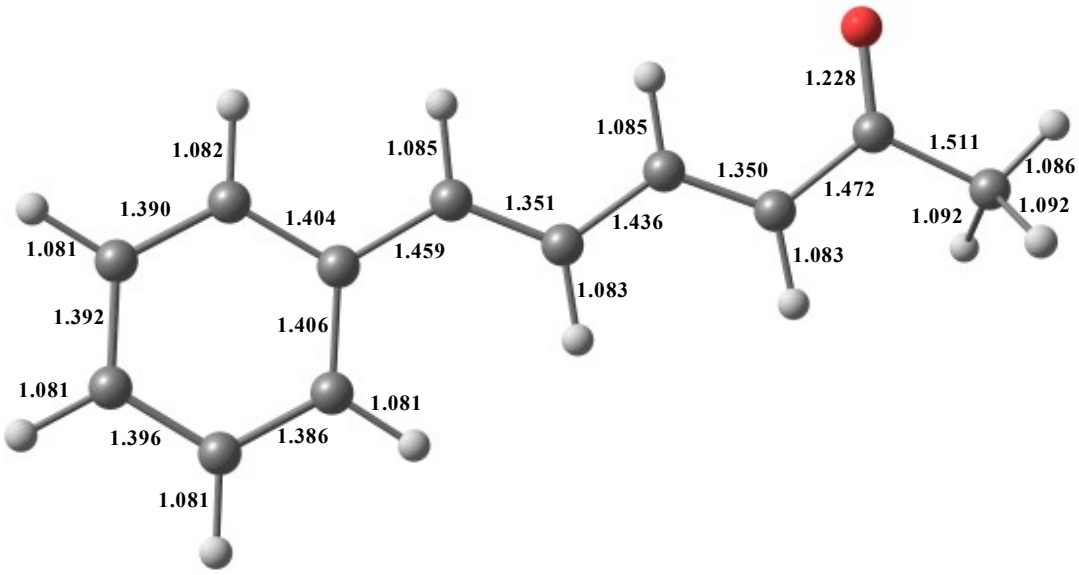
1i

Energy E(B3LYP) = -539.883472016 h, G^{298} = -539.719898 h, μ=5.42 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.035295	-0.237568	0.000180
2	C	-3.005871	-1.252680	-0.000228
3	C	-2.474164	1.098311	0.000446
4	C	-4.362031	-0.949907	-0.000436
5	C	-3.827583	1.399238	0.000245
6	C	-4.778464	0.377838	-0.000208
7	H	-2.686260	-2.286587	-0.000396
8	H	-1.756571	1.906234	0.000867
9	H	-5.091348	-1.748154	-0.000765
10	H	-4.145876	2.432695	0.000467
11	H	-5.832645	0.617929	-0.000357
12	C	-0.626985	-0.617961	0.000297
13	H	-0.440884	-1.687006	0.000693
14	C	0.446783	0.201445	-0.000074
15	H	0.320266	1.277369	-0.000546
16	C	1.793633	-0.296471	0.000109
17	H	1.927224	-1.373150	0.000537
18	C	2.899026	0.478040	-0.000235
19	H	2.807962	1.557172	-0.000665
20	C	4.259072	-0.085325	-0.000041
21	O	4.474132	-1.294665	0.000413
22	C	5.395404	0.910008	-0.000371
23	H	5.326152	1.557652	0.876026
24	H	6.352086	0.395612	-0.000625
25	H	5.325675	1.557754	-0.876643





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.10234	1.99901	4.08414	0.01920	6.10234
C	2	-0.18029	1.99908	4.16227	0.01893	6.18029
C	3	-0.18361	1.99907	4.16653	0.01800	6.18361
C	4	-0.21356	1.99915	4.19408	0.02033	6.21356
C	5	-0.20944	1.99916	4.19002	0.02026	6.20944
C	6	-0.19885	1.99916	4.17908	0.02062	6.19885
H	7	0.22229	0.00000	0.77598	0.00173	0.77771
H	8	0.22089	0.00000	0.77734	0.00177	0.77911
H	9	0.22341	0.00000	0.77491	0.00168	0.77659
H	10	0.22274	0.00000	0.77559	0.00167	0.77726
H	11	0.22213	0.00000	0.77632	0.00155	0.77787
C	12	-0.12982	1.99906	4.11176	0.01901	6.12982
H	13	0.21450	0.00000	0.78280	0.00270	0.78550
C	14	-0.22889	1.99905	4.21203	0.01781	6.22889
H	15	0.21393	0.00000	0.78271	0.00335	0.78607
C	16	-0.11358	1.99908	4.09430	0.02020	6.11358
H	17	0.21877	0.00000	0.77733	0.00390	0.78123
C	18	-0.31896	1.99899	4.30093	0.01904	6.31896
H	19	0.21719	0.00000	0.78094	0.00187	0.78281
C	20	0.54420	1.99932	3.42277	0.03371	5.45580
O	21	-0.65604	1.99976	6.63086	0.02542	8.65604

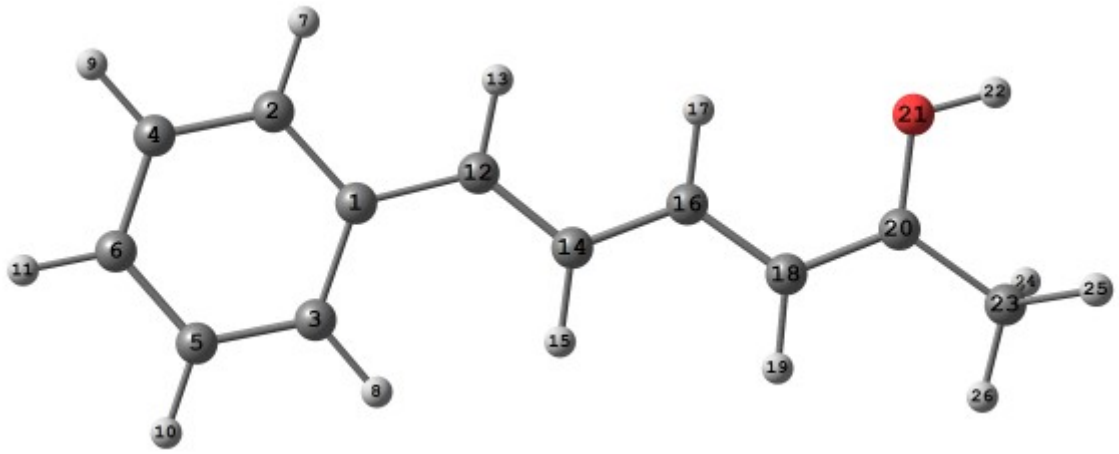
C	22	-0.66359	1.99926	4.65318	0.01114	6.66359
H	23	0.22978	0.00000	0.76871	0.00151	0.77022
H	24	0.21936	0.00000	0.77852	0.00212	0.78064
H	25	0.22976	0.00000	0.76873	0.00151	0.77024
* Total *		0.00000	25.98914	65.72183	0.28903	92.00000

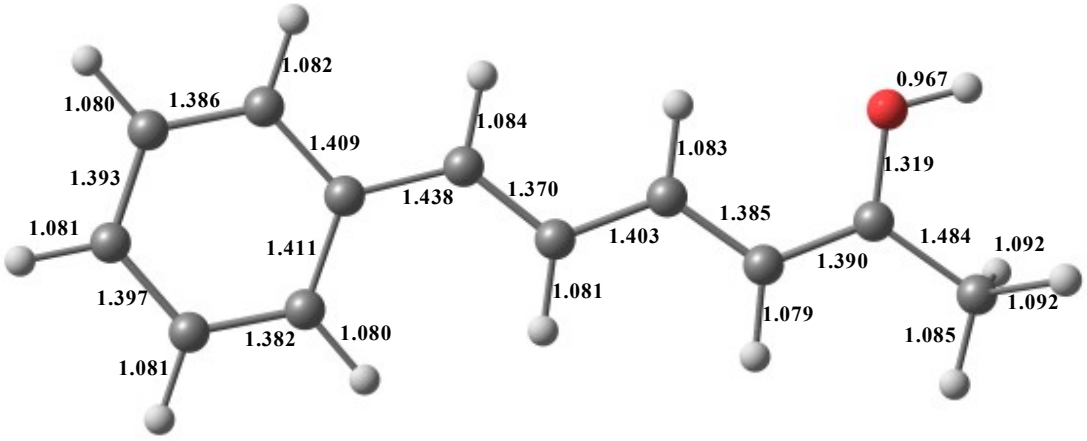
A4

Energy E(B3LYP) =-540.310370329 h, G^{298} = -540.132223 h, μ=9.41 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.066365	-0.227002	-0.000017
2	C	3.017515	-1.267179	-0.000015
3	C	2.523607	1.107564	-0.000016
4	C	4.374348	-0.986772	-0.000007
5	C	3.878653	1.381676	-0.000009
6	C	4.806889	0.337417	-0.000003
7	H	2.675946	-2.293336	-0.000020
8	H	1.818783	1.925612	-0.000024
9	H	5.093558	-1.793113	-0.000004
10	H	4.220295	2.406826	-0.000010
11	H	5.864929	0.559202	0.000003
12	C	0.671931	-0.579677	-0.000019
13	H	0.460654	-1.643383	-0.000046
14	C	-0.404257	0.267772	0.000013
15	H	-0.269684	1.340804	0.000045
16	C	-1.713310	-0.237861	0.000004
17	H	-1.836562	-1.314206	-0.000022
18	C	-2.849064	0.554640	0.000026
19	H	-2.755377	1.629944	0.000047
20	C	-4.138259	0.034688	0.000019
21	O	-4.290650	-1.275155	-0.000004
22	H	-5.222876	-1.533783	-0.000013
23	C	-5.352504	0.888341	0.000025
24	H	-5.959847	0.666445	-0.880462
25	H	-5.959870	0.666403	0.880485
26	H	-5.096238	1.942185	0.000052





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.13452	1.99902	4.11547	0.02003	6.13452
C	2	-0.12779	1.99892	4.10880	0.02008	6.12779
C	3	-0.14832	1.99908	4.13189	0.01735	6.14832
C	4	-0.21983	1.99917	4.19954	0.02112	6.21983
C	5	-0.20776	1.99916	4.18840	0.02020	6.20776
C	6	-0.14406	1.99917	4.12556	0.01933	6.14406
H	7	0.22911	0.00000	0.76924	0.00165	0.77089
H	8	0.22801	0.00000	0.77027	0.00172	0.77199
H	9	0.23035	0.00000	0.76804	0.00161	0.76965
H	10	0.22971	0.00000	0.76862	0.00167	0.77029
H	11	0.22709	0.00000	0.77145	0.00147	0.77291
C	12	-0.02798	1.99910	4.01042	0.01846	6.02798
H	13	0.23140	0.00000	0.76667	0.00193	0.76860
C	14	-0.25623	1.99907	4.23814	0.01902	6.25623
H	15	0.23204	0.00000	0.76459	0.00337	0.76796
C	16	-0.01488	1.99912	3.99586	0.01990	6.01488
H	17	0.23507	0.00000	0.76249	0.00244	0.76493
C	18	-0.33718	1.99898	4.31826	0.01993	6.33718
H	19	0.24619	0.00000	0.75207	0.00174	0.75381

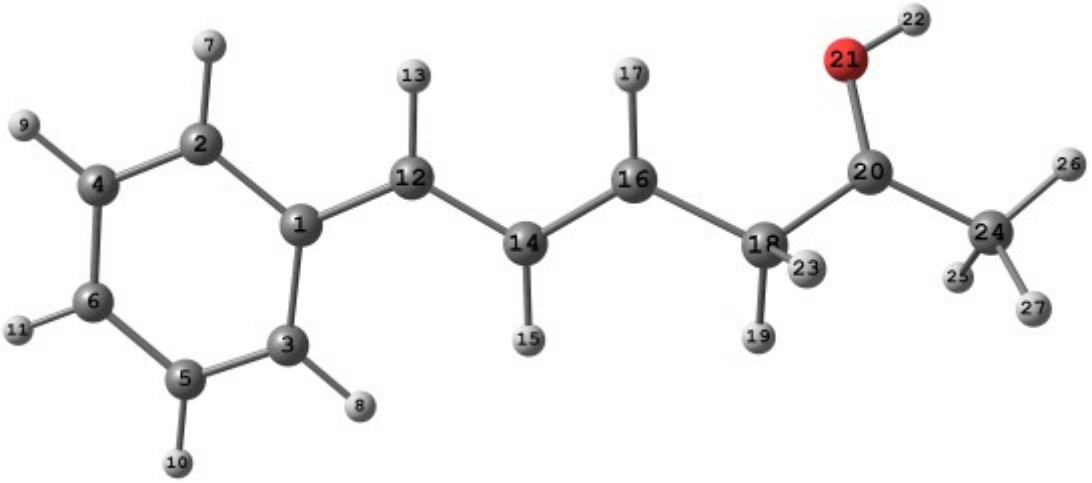
C	20	0.54138	1.99907	3.43720	0.02235	5.45862
O	21	-0.63184	1.99970	6.60704	0.02510	8.63184
H	22	0.54048	0.00000	0.45689	0.00263	0.45952
C	23	-0.66479	1.99923	4.65314	0.01242	6.66479
H	24	0.25123	0.00000	0.74700	0.00178	0.74877
H	25	0.25126	0.00000	0.74696	0.00178	0.74874
H	26	0.24186	0.00000	0.75681	0.00134	0.75814
* Total *		1.00000	25.98878	65.73080	0.28042	92.00000

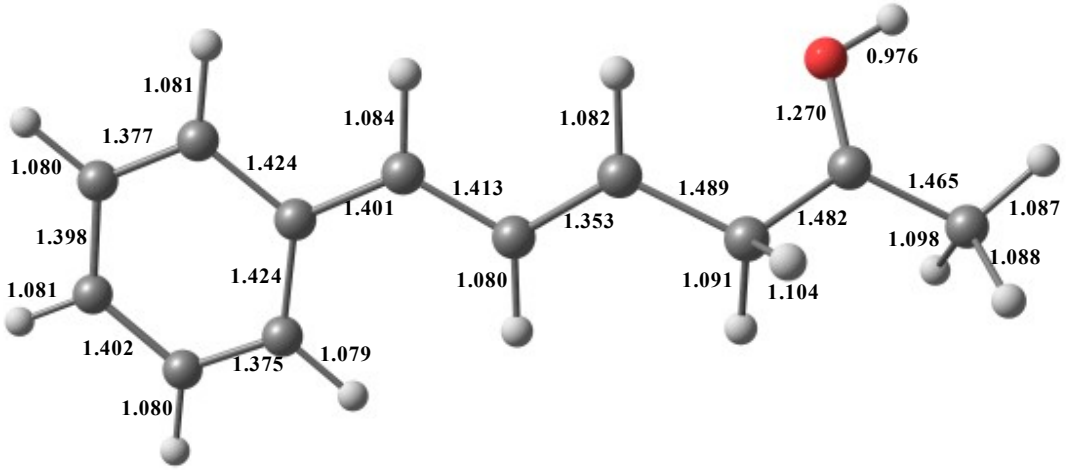
C4

Energy E(B3LYP) = -540.688305763 h, G^{298} = -540.499146 h, μ=14.9 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.065278	-0.233132	0.066303
2	C	3.043000	-1.267762	0.074411
3	C	2.487530	1.117161	-0.093679
4	C	4.378677	-0.964988	-0.067550
5	C	3.824276	1.405204	-0.235541
6	C	4.767536	0.368574	-0.221650
7	H	2.721381	-2.292395	0.195074
8	H	1.763978	1.917398	-0.104906
9	H	5.121257	-1.748473	-0.060089
10	H	4.150400	2.427141	-0.357239
11	H	5.816241	0.606471	-0.332558
12	C	0.722155	-0.601028	0.221802
13	H	0.522401	-1.660543	0.333242
14	C	-0.403690	0.252892	0.251738
15	H	-0.285624	1.321320	0.145537
16	C	-1.635356	-0.281985	0.420406
17	H	-1.739268	-1.354080	0.526321
18	C	-2.871540	0.542741	0.520489
19	H	-2.736698	1.565290	0.163714
20	C	-4.101185	-0.013320	-0.092252
21	O	-4.042917	-1.218017	-0.491324
22	H	-4.878160	-1.554399	-0.867465
23	H	-3.128006	0.661696	1.587657
24	C	-5.309994	0.801485	-0.240841
25	H	-5.164285	1.411337	-1.141933
26	H	-6.203119	0.195683	-0.370769
27	H	-5.417274	1.492631	0.592193





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.13934	1.99901	4.12070	0.01963	6.13934
C	2	-0.07401	1.99910	4.05661	0.01830	6.07401
C	3	-0.08788	1.99908	4.07153	0.01726	6.08788
C	4	-0.21886	1.99915	4.19972	0.02000	6.21886
C	5	-0.21247	1.99916	4.19341	0.01990	6.21247
C	6	-0.06899	1.99918	4.05079	0.01901	6.06899
H	7	0.24292	0.00000	0.75542	0.00165	0.75708

H	8	0.23922	0.00000	0.75910	0.00168	0.76078
H	9	0.24453	0.00000	0.75386	0.00160	0.75547
H	10	0.24387	0.00000	0.75454	0.00159	0.75613
H	11	0.24014	0.00000	0.75852	0.00134	0.75986
C	12	0.09313	1.99910	3.88922	0.01855	5.90687
H	13	0.24557	0.00000	0.75254	0.00189	0.75443
C	14	-0.25619	1.99902	4.23802	0.01915	6.25619
H	15	0.24849	0.00000	0.74841	0.00311	0.75151
C	16	0.03007	1.99912	3.95167	0.01914	5.96993
H	17	0.24766	0.00000	0.75006	0.00228	0.75234
C	18	-0.55666	1.99906	4.53802	0.01957	6.55666
H	19	0.29522	0.00000	0.70328	0.00150	0.70478
C	20	0.74274	1.99926	3.23454	0.02346	5.25726
O	21	-0.54617	1.99965	6.51930	0.02721	8.54617
H	22	0.57625	0.00000	0.42128	0.00247	0.42375
H	23	0.33221	0.00000	0.66630	0.00149	0.66779
C	24	-0.69391	1.99918	4.67928	0.01545	6.69391
H	25	0.29862	0.00000	0.70005	0.00132	0.70138
H	26	0.25966	0.00000	0.73822	0.00213	0.74034
H	27	0.27415	0.00000	0.72451	0.00134	0.72585
* Total *		2.00000	25.98908	65.72890	0.28202	92.00000

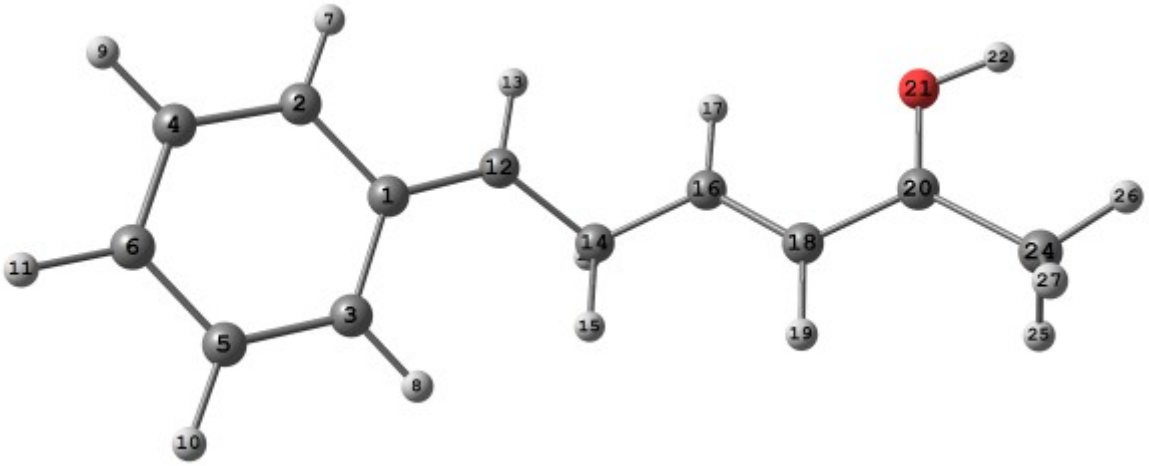
B4

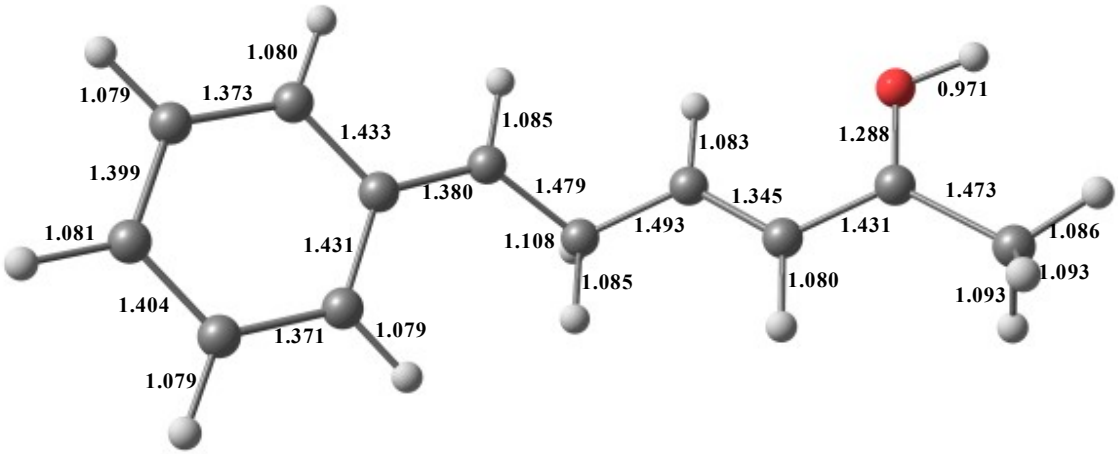
Energy E(B3LYP) = -540.680429986 h, G^{298} = -540.491958 h, μ=7.79 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.000317	-0.274486	0.170765
2	C	-2.936136	-1.276619	-0.244838
3	C	-2.425671	1.090314	0.238659
4	C	-4.224109	-0.928701	-0.569928
5	C	-3.716971	1.418031	-0.084141
6	C	-4.611256	0.413606	-0.488264
7	H	-2.612021	-2.306118	-0.295441
8	H	-1.734947	1.861315	0.541521
9	H	-4.933561	-1.678505	-0.884658
10	H	-4.049041	2.443738	-0.035175
11	H	-5.625414	0.686512	-0.745353
12	C	-0.723680	-0.686722	0.493573
13	H	-0.517835	-1.747918	0.402979
14	C	0.390895	0.145325	0.996296
15	H	0.251237	1.209419	0.836894
16	C	1.737877	-0.322211	0.552271
17	H	1.925152	-1.388675	0.580777
18	C	2.711853	0.515875	0.153727
19	H	2.553011	1.582694	0.102654
20	C	4.006847	0.049131	-0.236089
21	O	4.239134	-1.215706	-0.159739
22	H	5.136218	-1.455772	-0.444627
23	H	0.365520	-0.010336	2.092688
24	C	5.039150	0.985957	-0.712755

25	H	5.217050	1.737459	0.060197
26	H	5.970182	0.489941	-0.970114
27	H	4.650480	1.524889	-1.580092





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	-0.16763	1.99898	4.14902	0.01964	6.16763
C	2	-0.03830	1.99910	4.02082	0.01838	6.03830
C	3	-0.05726	1.99908	4.04100	0.01718	6.05726
C	4	-0.22713	1.99914	4.20791	0.02007	6.22713
C	5	-0.21749	1.99915	4.19836	0.01998	6.21749
C	6	-0.03514	1.99919	4.01717	0.01878	6.03514
H	7	0.24873	0.00000	0.74960	0.00167	0.75127
H	8	0.24210	0.00000	0.75618	0.00172	0.75790
H	9	0.25167	0.00000	0.74674	0.00159	0.74833
H	10	0.25086	0.00000	0.74755	0.00158	0.74914
H	11	0.24641	0.00000	0.75230	0.00129	0.75359
C	12	0.20452	1.99909	3.78021	0.01618	5.79548
H	13	0.24717	0.00000	0.75092	0.00191	0.75283
C	14	-0.53017	1.99915	4.51188	0.01914	6.53017
H	15	0.25784	0.00000	0.73941	0.00275	0.74216
C	16	0.07481	1.99909	3.90808	0.01802	5.92519
H	17	0.24517	0.00000	0.75243	0.00240	0.75483
C	18	-0.33506	1.99893	4.31647	0.01966	6.33506
H	19	0.26222	0.00000	0.73616	0.00162	0.73778
C	20	0.63558	1.99917	3.34220	0.02305	5.36442
O	21	-0.57115	1.99968	6.54540	0.02608	8.57115
H	22	0.56189	0.00000	0.43561	0.00250	0.43811
H	23	0.32742	0.00000	0.67088	0.00170	0.67258
C	24	-0.67850	1.99921	4.66564	0.01365	6.67850
H	25	0.27823	0.00000	0.72047	0.00130	0.72177
H	26	0.24484	0.00000	0.75311	0.00205	0.75516
H	27	0.27836	0.00000	0.72034	0.00130	0.72164
* Total *		2.00000	25.98898	65.73583	0.27519	92.00000

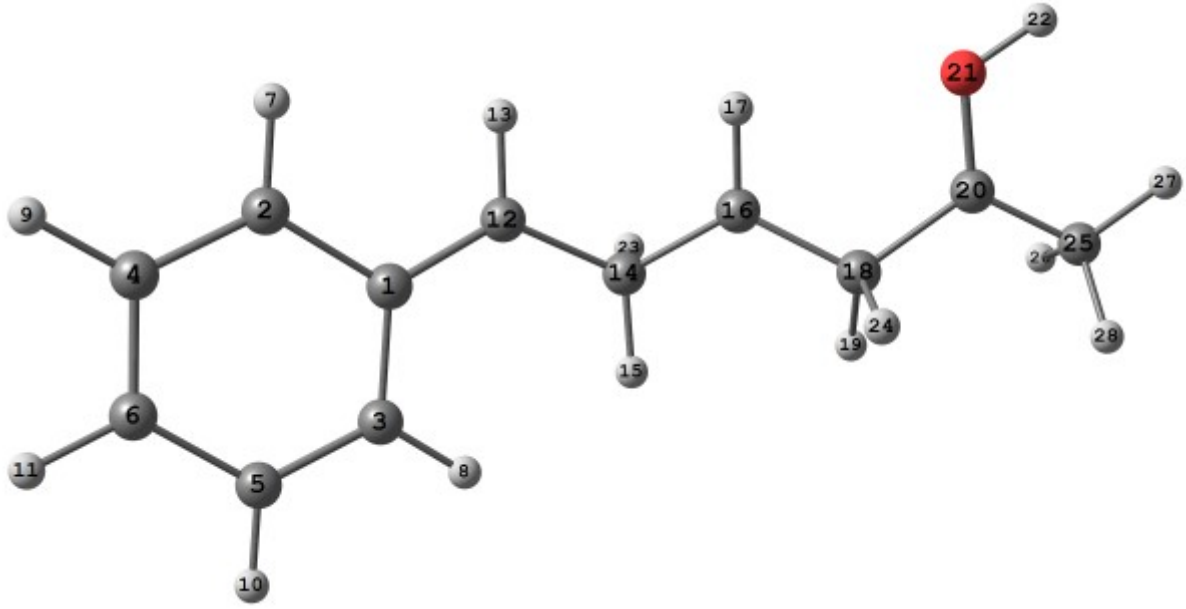
D4

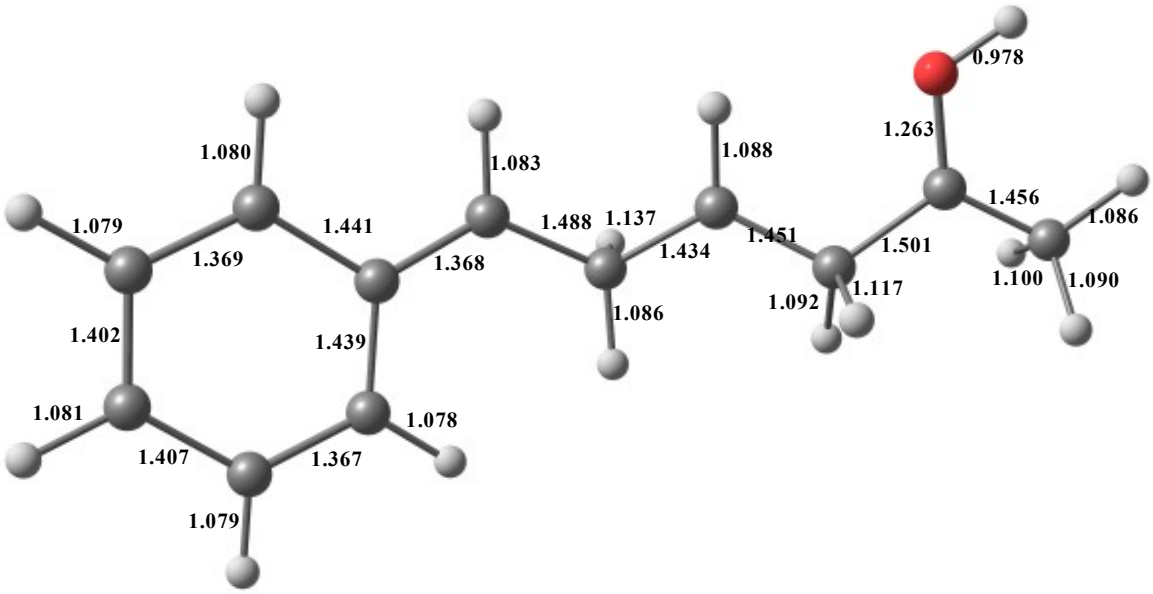
Energy E(B3LYP) = -541.004727105 h, G^{298} = -540.806397 h, μ=16.6 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.094145	-0.262987	0.141831
2	C	-3.088173	-1.294211	-0.018203
3	C	-2.498902	1.116064	0.077168
4	C	-4.399272	-0.959547	-0.225144
5	C	-3.814989	1.425862	-0.122388
6	C	-4.760415	0.394548	-0.274301
7	H	-2.778846	-2.328137	0.028153
8	H	-1.773653	1.906743	0.185518
9	H	-5.150496	-1.724162	-0.348036
10	H	-4.134103	2.455524	-0.168436
11	H	-5.797024	0.656316	-0.435731
12	C	-0.804773	-0.669589	0.349264

13	H	-0.610466	-1.734457	0.395923
14	C	0.373585	0.218887	0.543008
15	H	0.230305	1.282263	0.374013
16	C	1.649528	-0.280033	0.118288
17	H	1.789079	-1.354814	0.025706
18	C	2.772757	0.594885	-0.163817
19	H	2.735768	1.546229	0.371289
20	C	4.148260	-0.005250	-0.156957
21	O	4.189235	-1.266495	-0.202138
22	H	5.089294	-1.648259	-0.215906
23	H	0.620075	0.160417	1.651430
24	H	2.574163	0.908381	-1.217085
25	C	5.327463	0.846724	-0.090276
26	H	5.396288	1.199585	0.949376
27	H	6.238550	0.315069	-0.348372
28	H	5.191646	1.739129	-0.701573





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.13305	1.99898	4.11459	0.01948	6.13305
C	2	-0.01797	1.99910	4.00065	0.01822	6.01797
C	3	-0.04694	1.99908	4.03088	0.01698	6.04694
C	4	-0.22476	1.99914	4.20557	0.02005	6.22476
C	5	-0.21438	1.99915	4.19512	0.02011	6.21438
C	6	0.00710	1.99920	3.97514	0.01857	5.99290
H	7	0.25317	0.00000	0.74518	0.00165	0.74683
H	8	0.24458	0.00000	0.75359	0.00183	0.75542
H	9	0.25721	0.00000	0.74123	0.00156	0.74279
H	10	0.25665	0.00000	0.74180	0.00155	0.74335
H	11	0.25023	0.00000	0.74851	0.00126	0.74977
C	12	0.14470	1.99904	3.83854	0.01772	5.85530
H	13	0.26687	0.00000	0.73125	0.00188	0.73313
C	14	-0.58342	1.99908	4.56205	0.02230	6.58342
H	15	0.30891	0.00000	0.68938	0.00171	0.69109
C	16	0.41590	1.99922	3.56869	0.01620	5.58410
H	17	0.28825	0.00000	0.70890	0.00285	0.71175
C	18	-0.62546	1.99901	4.60520	0.02125	6.62546
H	19	0.33694	0.00000	0.66161	0.00145	0.66306

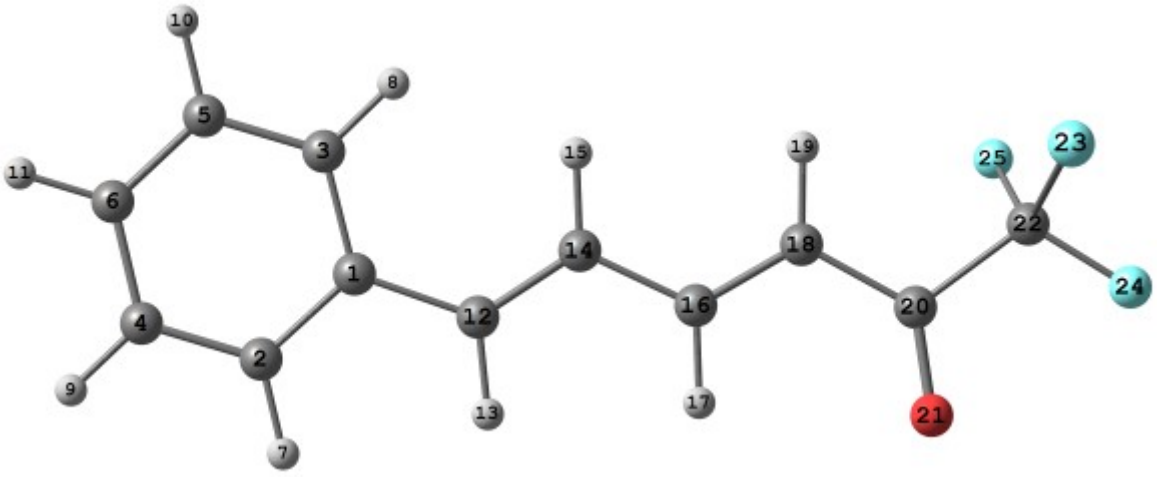
C	20	0.74807	1.99928	3.22842	0.02424	5.25193
O	21	-0.52718	1.99964	6.50051	0.02702	8.52718
H	22	0.59105	0.00000	0.40658	0.00237	0.40895
H	23	0.42692	0.00000	0.57116	0.00191	0.57308
H	24	0.40514	0.00000	0.59330	0.00156	0.59486
C	25	-0.69805	1.99918	4.68328	0.01560	6.69805
H	26	0.31179	0.00000	0.68692	0.00128	0.68821
H	27	0.26973	0.00000	0.72828	0.00199	0.73027
H	28	0.28801	0.00000	0.71072	0.00127	0.71199
* Total *		3.00000	25.98910	65.72704	0.28387	92.00000

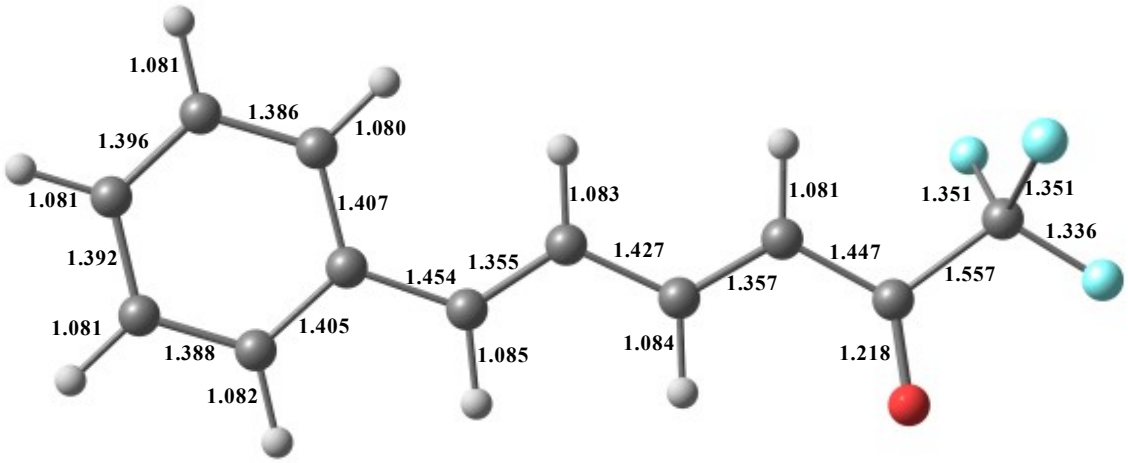
1j

Energy E(B3LYP) = -837.701349355 h, G^{298} =-837.565013 h, μ=8.90 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-3.252952	0.245603	-0.000156
2	C	-4.289092	1.194814	0.000193
3	C	-3.597895	-1.118339	-0.000495
4	C	-5.620494	0.800739	0.000223
5	C	-4.927114	-1.509423	-0.000486
6	C	-5.943842	-0.553006	-0.000121
7	H	-4.039544	2.247576	0.000457
8	H	-2.826154	-1.874425	-0.000795
9	H	-6.403094	1.546487	0.000509
10	H	-5.176094	-2.561507	-0.000773
11	H	-6.979230	-0.864204	-0.000116
12	C	-1.878788	0.720484	-0.000180
13	H	-1.765081	1.799416	-0.000135
14	C	-0.746409	-0.023057	-0.000234
15	H	-0.791067	-1.104792	-0.000205
16	C	0.545501	0.583720	-0.000337
17	H	0.586601	1.667412	-0.000508
18	C	1.719675	-0.097212	-0.000240
19	H	1.729635	-1.178453	0.000003
20	C	2.989329	0.595894	-0.000449
21	O	3.173601	1.800313	-0.001010
22	C	4.239319	-0.331657	0.000420
23	F	4.245969	-1.136007	-1.085386
24	F	5.379262	0.364503	-0.001500
25	F	4.247192	-1.131981	1.089198





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.11480	1.99902	4.09580	0.01999	6.11480
C	2	-0.15777	1.99891	4.13851	0.02035	6.15777
C	3	-0.17331	1.99907	4.15669	0.01755	6.17331
C	4	-0.22077	1.99917	4.20032	0.02128	6.22077
C	5	-0.20987	1.99916	4.19037	0.02034	6.20987
C	6	-0.18671	1.99916	4.16773	0.01982	6.18671
H	7	0.22329	0.00000	0.77499	0.00172	0.77671
H	8	0.22265	0.00000	0.77560	0.00174	0.77735
H	9	0.22541	0.00000	0.77296	0.00163	0.77459
H	10	0.22474	0.00000	0.77357	0.00169	0.77526
H	11	0.22381	0.00000	0.77465	0.00154	0.77619
C	12	-0.09226	1.99907	4.07454	0.01864	6.09226
H	13	0.21925	0.00000	0.77888	0.00186	0.78075
C	14	-0.24132	1.99905	4.22397	0.01829	6.24132
H	15	0.21997	0.00000	0.77671	0.00332	0.78003
C	16	-0.07512	1.99910	4.05530	0.02071	6.07512
H	17	0.22277	0.00000	0.77261	0.00462	0.77723
C	18	-0.34933	1.99901	4.33071	0.01961	6.34933
H	19	0.23466	0.00000	0.76296	0.00238	0.76534
C	20	0.45353	1.99919	3.50811	0.03916	5.54647
O	21	-0.59714	1.99976	6.57166	0.02572	8.59714

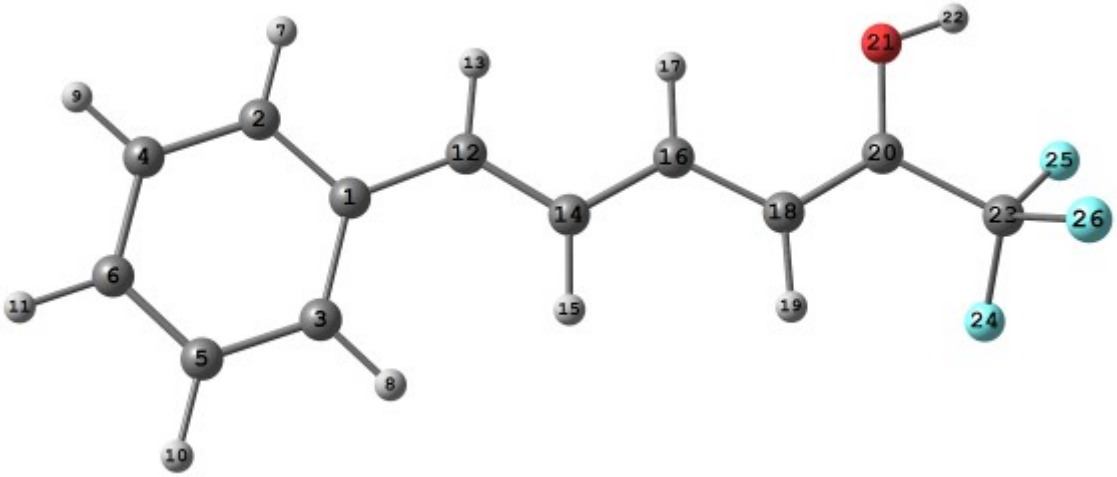
C	22	1.02239	1.99939	2.92650	0.05172	4.97761
F	23	-0.36081	1.99992	7.35147	0.00942	9.36081
F	24	-0.35248	1.99991	7.34101	0.01155	9.35248
F	25	-0.36080	1.99992	7.35146	0.00942	9.36080
* Total *		0.00000	31.98881	83.64709	0.36409	116.00000

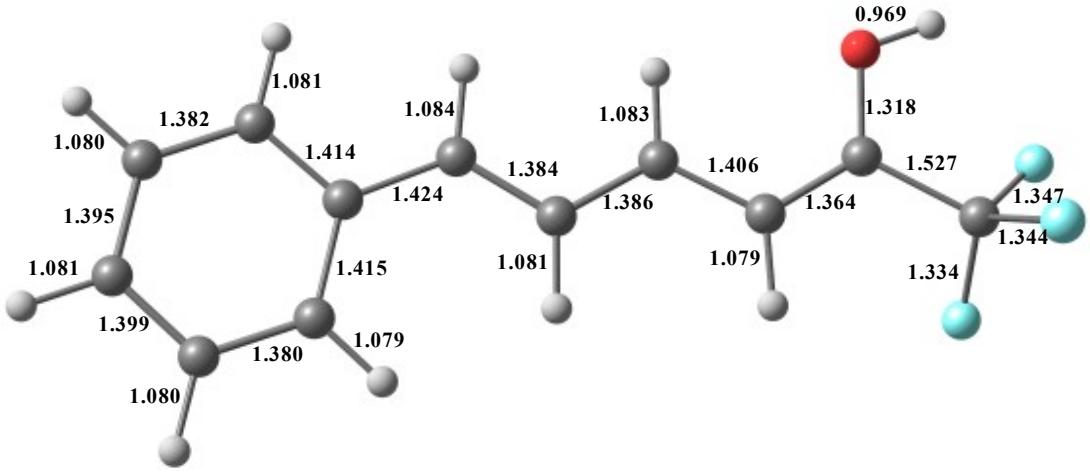
A5

Energy E(B3LYP) = -838.112129827 h, G^{298} = -837.961567 h, μ=5.05 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.265837	-0.237018	-0.000848
2	C	4.289516	-1.212694	0.015073
3	C	3.626160	1.131567	-0.012620
4	C	5.619698	-0.837248	0.020081
5	C	4.956274	1.497673	-0.008664
6	C	5.953584	0.516874	0.008046
7	H	4.018391	-2.259233	0.023835
8	H	2.864271	1.896078	-0.025840
9	H	6.396251	-1.587792	0.032907
10	H	5.228970	2.542812	-0.018532
11	H	6.993314	0.812750	0.011349
12	C	1.914229	-0.685217	-0.004942
13	H	1.774628	-1.760336	-0.000967
14	C	0.767544	0.090355	-0.012346
15	H	0.824883	1.169622	-0.013524
16	C	-0.478021	-0.516933	-0.017747
17	H	-0.519495	-1.599130	-0.017556
18	C	-1.691811	0.191781	-0.025763
19	H	-1.684486	1.270869	-0.031949
20	C	-2.901577	-0.437971	-0.028207
21	O	-3.020871	-1.750488	-0.011857
22	H	-3.940016	-2.044024	-0.099892
23	C	-4.198650	0.367581	0.004246
24	F	-4.082025	1.530164	-0.638432
25	F	-5.194231	-0.337553	-0.565759
26	F	-4.560014	0.624032	1.272766





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.13982	1.99902	4.12082	0.01998	6.13982
C	2	-0.10570	1.99893	4.08691	0.01987	6.10570
C	3	-0.12942	1.99908	4.11314	0.01720	6.12942
C	4	-0.22267	1.99917	4.20247	0.02103	6.22267
C	5	-0.20985	1.99915	4.19058	0.02011	6.20985
C	6	-0.11174	1.99917	4.09355	0.01901	6.11174
H	7	0.23424	0.00000	0.76416	0.00160	0.76576
H	8	0.23303	0.00000	0.76529	0.00169	0.76697
H	9	0.23567	0.00000	0.76274	0.00159	0.76433
H	10	0.23503	0.00000	0.76332	0.00165	0.76497
H	11	0.23100	0.00000	0.76759	0.00142	0.76900
C	12	0.01568	1.99911	3.96682	0.01840	5.98432
H	13	0.23748	0.00000	0.76064	0.00188	0.76252
C	14	-0.25302	1.99907	4.23494	0.01901	6.25302
H	15	0.23951	0.00000	0.75729	0.00320	0.76049
C	16	-0.00431	1.99914	3.98499	0.02018	6.00431
H	17	0.23950	0.00000	0.75798	0.00252	0.76050
C	18	-0.32080	1.99900	4.30151	0.02029	6.32080
H	19	0.26240	0.00000	0.73564	0.00196	0.73760
C	20	0.39081	1.99888	3.58051	0.02980	5.60919

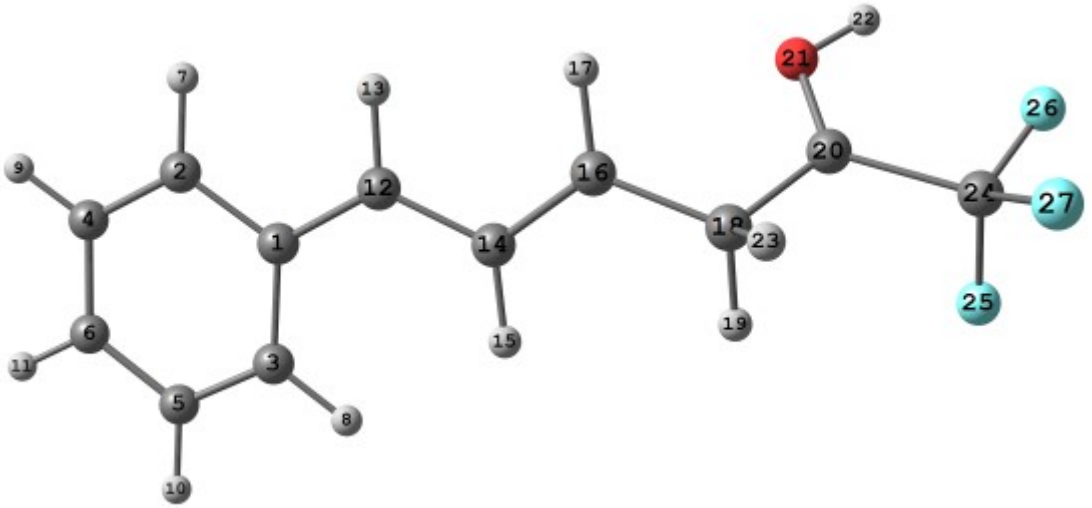
O	21	-0.61921	1.99971	6.59321	0.02629	8.61921
H	22	0.54698	0.00000	0.45013	0.00289	0.45302
C	23	1.04243	1.99930	2.90540	0.05287	4.95757
F	24	-0.33582	1.99991	7.32597	0.00994	9.33582
F	25	-0.35035	1.99992	7.34000	0.01043	9.35035
F	26	-0.34103	1.99991	7.33129	0.00983	9.34103
* Total *		1.00000	31.98846	83.65689	0.35465	116.00000

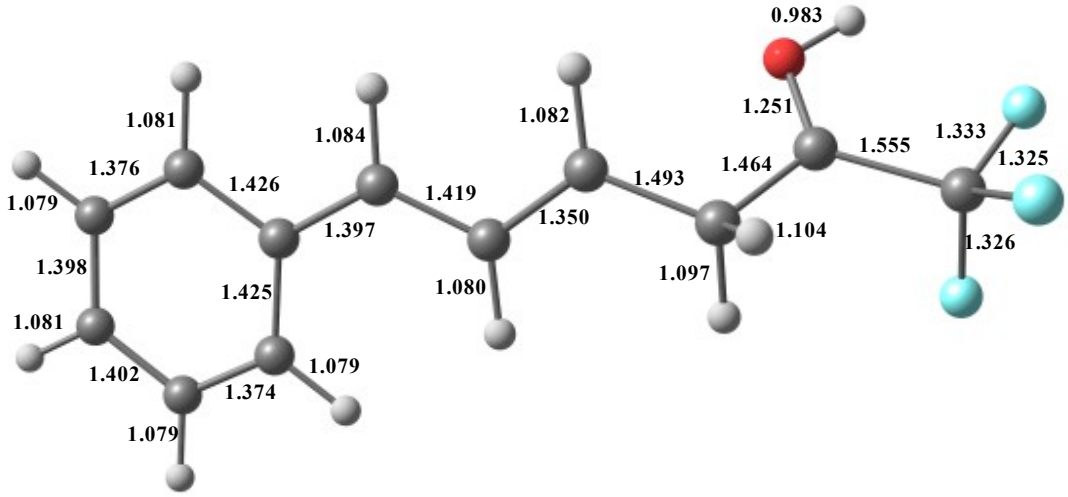
C5

Energy E(B3LYP) =-838.467932455 h, G^{298} =-838.305245 h, μ=3.27 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.269671	-0.237522	0.084354
2	C	4.307436	-1.213933	0.132304
3	C	3.611678	1.128388	-0.137589
4	C	5.621268	-0.840321	-0.031668
5	C	4.928025	1.486566	-0.299117
6	C	5.929843	0.506686	-0.245872
7	H	4.046106	-2.248928	0.300155
8	H	2.841855	1.882983	-0.178222
9	H	6.409065	-1.577346	0.004689
10	H	5.194933	2.519145	-0.465942
11	H	6.962521	0.800078	-0.373262
12	C	1.955265	-0.674700	0.264926
13	H	1.816706	-1.737004	0.428011
14	C	0.776697	0.114997	0.259714
15	H	0.831100	1.181530	0.098721
16	C	-0.415276	-0.485061	0.463396
17	H	-0.458389	-1.554305	0.626580
18	C	-1.702579	0.267319	0.533459
19	H	-1.634647	1.290671	0.143473
20	C	-2.853488	-0.370366	-0.107435
21	O	-2.725823	-1.453591	-0.719557
22	H	-3.554526	-1.810938	-1.110428
23	H	-1.993383	0.418240	1.587919
24	C	-4.260349	0.287542	-0.037519
25	F	-4.215792	1.463893	-0.647969
26	F	-5.141565	-0.504126	-0.648697
27	F	-4.605298	0.445460	1.232337





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.13426	1.99901	4.11562	0.01963	6.13426
C	2	-0.06971	1.99910	4.05235	0.01826	6.06971
C	3	-0.08472	1.99908	4.06842	0.01722	6.08472
C	4	-0.22329	1.99914	4.20417	0.01997	6.22329
C	5	-0.21314	1.99916	4.19411	0.01987	6.21314

C	6	-0.05550	1.99919	4.03739	0.01893	6.05550
H	7	0.24389	0.00000	0.75447	0.00165	0.75611
H	8	0.23986	0.00000	0.75846	0.00168	0.76014
H	9	0.24604	0.00000	0.75236	0.00160	0.75396
H	10	0.24477	0.00000	0.75364	0.00159	0.75523
H	11	0.24017	0.00000	0.75850	0.00133	0.75983
C	12	0.10535	1.99910	3.87699	0.01856	5.89465
H	13	0.24416	0.00000	0.75397	0.00188	0.75584
C	14	-0.23902	1.99902	4.22088	0.01912	6.23902
H	15	0.24999	0.00000	0.74706	0.00295	0.75001
C	16	-0.00221	1.99911	3.98394	0.01916	6.00221
H	17	0.25324	0.00000	0.74453	0.00223	0.74676
C	18	-0.57224	1.99908	4.55237	0.02079	6.57224
H	19	0.32454	0.00000	0.67359	0.00188	0.67546
C	20	0.66814	1.99923	3.30274	0.02989	5.33186
O	21	-0.48343	1.99964	6.45463	0.02917	8.48343
H	22	0.59037	0.00000	0.40682	0.00281	0.40963
H	23	0.34291	0.00000	0.65525	0.00184	0.65709
C	24	1.03290	1.99940	2.91175	0.05595	4.96710
F	25	-0.31115	1.99991	7.30303	0.00821	9.31115
F	26	-0.32632	1.99991	7.31767	0.00874	9.32632
F	27	-0.31132	1.99991	7.30318	0.00823	9.31132
* Total *		2.00000	31.98898	83.65790	0.35312	116.00000

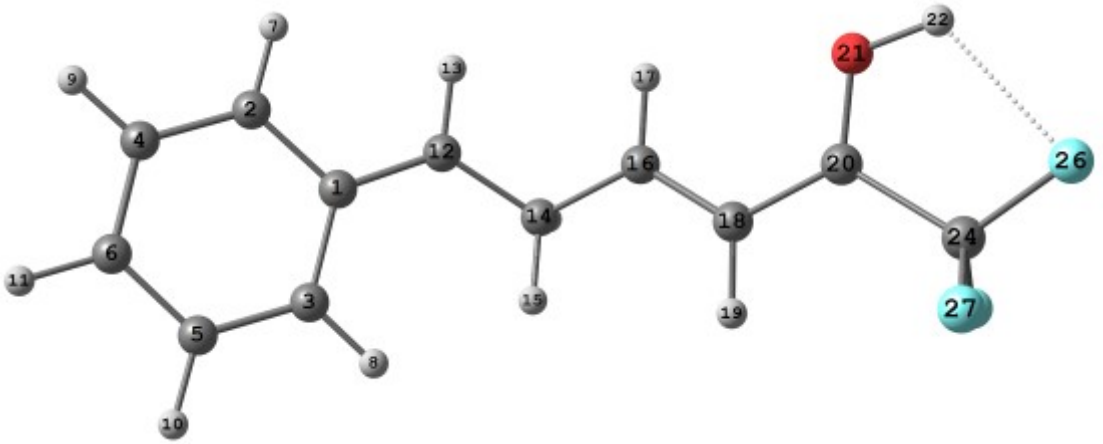
B5

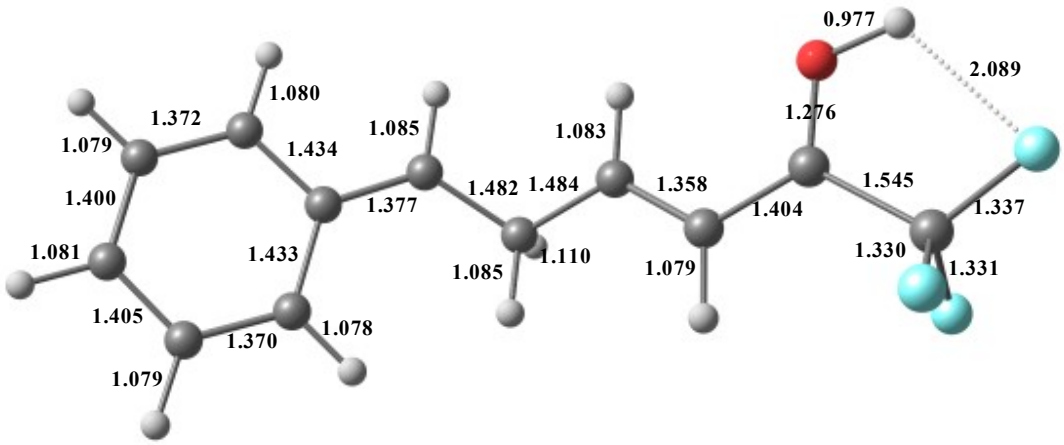
Energy E(B3LYP) = -838.468821051 h, G^{298} =-838.308007 h, μ=8.69 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.172576	0.291366	0.158960
2	C	4.198235	1.185584	-0.294758
3	C	3.459030	-1.109149	0.252859
4	C	5.439289	0.703283	-0.626300
5	C	4.704667	-1.571309	-0.081621
6	C	5.689533	-0.669956	-0.519258
7	H	3.976511	2.240569	-0.365471
8	H	2.698560	-1.800379	0.579758
9	H	6.215976	1.370517	-0.966804
10	H	4.932955	-2.624046	-0.016718
11	H	6.666704	-1.049748	-0.783832
12	C	1.953947	0.840648	0.488204
13	H	1.850280	1.913035	0.362780
14	C	0.772982	0.140109	1.044967
15	H	0.817657	-0.941905	0.978865
16	C	-0.526248	0.682692	0.575560
17	H	-0.590376	1.750385	0.403646
18	C	-1.629507	-0.087952	0.391489
19	H	-1.608329	-1.155707	0.548782
20	C	-2.845791	0.479851	-0.020948
21	O	-2.979578	1.728764	-0.248443
22	H	-3.877939	1.981977	-0.535744

23	H	0.799131	0.382130	2.128260
24	C	-4.080215	-0.428942	-0.213414
25	F	-4.390800	-1.009758	0.942687
26	F	-5.118222	0.303816	-0.631121
27	F	-3.812699	-1.364535	-1.120501





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.16171	1.99898	4.14312	0.01961	6.16171
C	2	-0.03301	1.99910	4.01555	0.01836	6.03301
C	3	-0.05551	1.99908	4.03930	0.01713	6.05551
C	4	-0.22929	1.99914	4.21008	0.02007	6.22929
C	5	-0.21889	1.99915	4.19975	0.01999	6.21889
C	6	-0.02387	1.99919	4.00593	0.01874	6.02387
H	7	0.24966	0.00000	0.74868	0.00167	0.75034
H	8	0.24305	0.00000	0.75525	0.00170	0.75695
H	9	0.25321	0.00000	0.74520	0.00158	0.74679
H	10	0.25240	0.00000	0.74603	0.00158	0.74760
H	11	0.24694	0.00000	0.75178	0.00128	0.75306
C	12	0.19200	1.99908	3.79255	0.01637	5.80800
H	13	0.25132	0.00000	0.74679	0.00189	0.74868
C	14	-0.54350	1.99915	4.52502	0.01934	6.54350
H	15	0.26714	0.00000	0.73019	0.00267	0.73286
C	16	0.12327	1.99913	3.85962	0.01799	5.87673
H	17	0.25519	0.00000	0.74228	0.00253	0.74481
C	18	-0.33983	1.99898	4.32015	0.02070	6.33983
H	19	0.28101	0.00000	0.71690	0.00208	0.71899
C	20	0.54574	1.99907	3.42324	0.03195	5.45426
O	21	-0.53415	1.99967	6.50697	0.02751	8.53415
H	22	0.57189	0.00000	0.42534	0.00278	0.42811
H	23	0.34312	0.00000	0.65521	0.00167	0.65688
C	24	1.03632	1.99938	2.91099	0.05332	4.96368
F	25	-0.31886	1.99991	7.30901	0.00995	9.31886
F	26	-0.33450	1.99991	7.32397	0.01062	9.33450
F	27	-0.31914	1.99991	7.30928	0.00994	9.31914
* Total *		2.00000	31.98884	83.65817	0.35300	116.00000

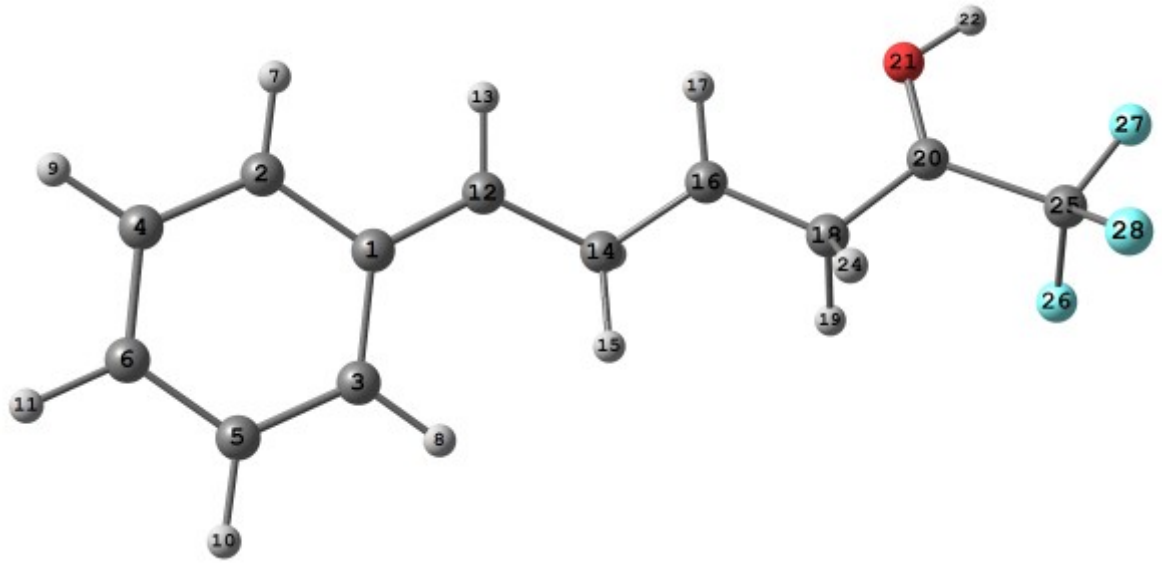
D5

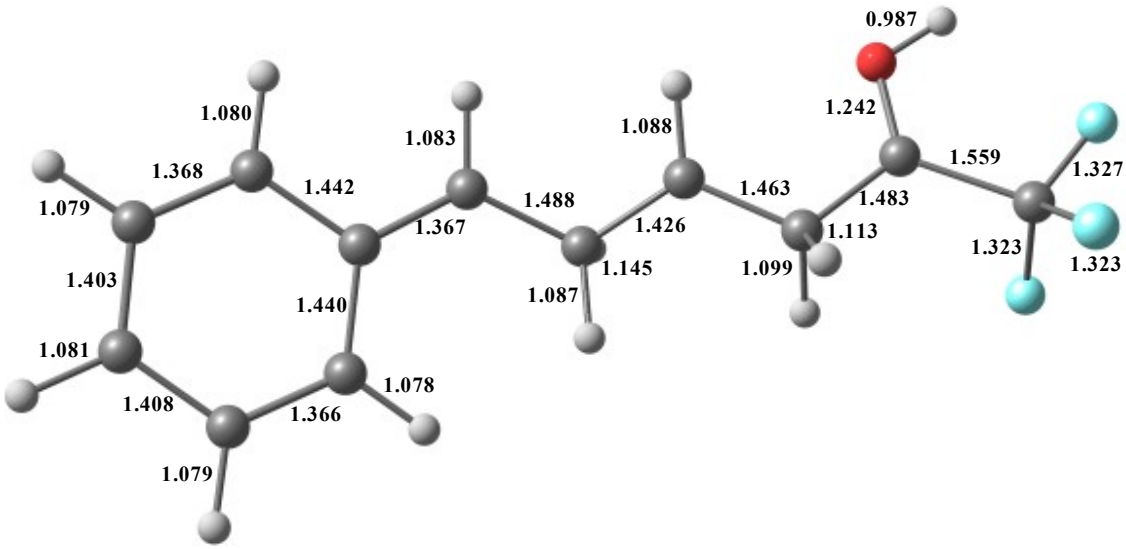
Energy E(B3LYP) =-838.776055407 h, G^{298} = -838,605353 h, μ=6.3 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-3.309279	0.274145	-0.039253
2	C	-4.363521	1.221882	0.226969
3	C	-3.639569	-1.120520	-0.182612
4	C	-5.659797	0.796727	0.329168
5	C	-4.941641	-1.520434	-0.078334
6	C	-5.946953	-0.568063	0.176032
7	H	-4.111138	2.266401	0.336576
8	H	-2.869150	-1.850436	-0.373324
9	H	-6.456313	1.497891	0.523523
10	H	-5.205619	-2.560890	-0.187242
11	H	-6.972443	-0.901109	0.257205
12	C	-2.040934	0.771639	-0.152313

13	H	-1.899712	1.839413	-0.040320
14	C	-0.820779	-0.026154	-0.451797
15	H	-0.891514	-1.106166	-0.352954
16	C	0.448473	0.534820	-0.121484
17	H	0.523563	1.611935	0.009980
18	C	1.659307	-0.278204	-0.002396
19	H	1.673878	-1.145300	-0.676779
20	C	2.960184	0.431555	-0.063698
21	O	2.991594	1.655384	-0.274246
22	H	3.889376	2.064690	-0.295145
23	H	-0.643064	0.121412	-1.572761
24	H	1.583518	-0.775386	0.990129
25	C	4.291635	-0.354975	0.130392
26	F	4.357313	-1.306261	-0.786354
27	F	5.307332	0.488339	-0.008699
28	F	4.293477	-0.879859	1.345168





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.12587	1.99899	4.10741	0.01947	6.12587
C	2	-0.02386	1.99910	4.00654	0.01821	6.02386
C	3	-0.05725	1.99908	4.04124	0.01692	6.05725
C	4	-0.21910	1.99914	4.19993	0.02003	6.21910
C	5	-0.20546	1.99915	4.18619	0.02011	6.20546
C	6	0.02813	1.99920	3.95416	0.01851	5.97187
H	7	0.25474	0.00000	0.74361	0.00164	0.74526
H	8	0.24603	0.00000	0.75216	0.00182	0.75397
H	9	0.25677	0.00000	0.74167	0.00155	0.74323
H	10	0.25596	0.00000	0.74250	0.00154	0.74404
H	11	0.24787	0.00000	0.75088	0.00125	0.75213
C	12	0.13079	1.99903	3.85243	0.01775	5.86921
H	13	0.27038	0.00000	0.72775	0.00187	0.72962
C	14	-0.57951	1.99907	4.55746	0.02299	6.57951
H	15	0.31639	0.00000	0.68197	0.00164	0.68361
C	16	0.40239	1.99922	3.58188	0.01650	5.59761
H	17	0.29382	0.00000	0.70337	0.00280	0.70618
C	18	-0.64559	1.99903	4.62509	0.02147	6.64559
H	19	0.36932	0.00000	0.62880	0.00188	0.63068
C	20	0.68101	1.99929	3.28564	0.03406	5.31899
O	21	-0.46631	1.99963	6.43764	0.02904	8.46631

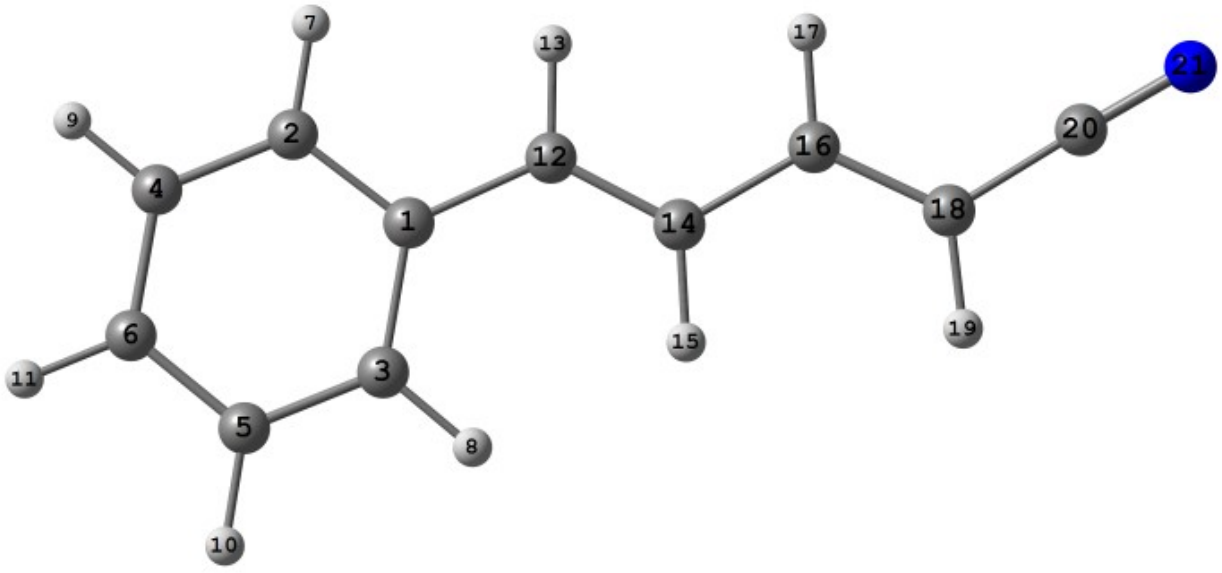
H	22	0.60701	0.00000	0.39030	0.00269	0.39299
H	23	0.44151	0.00000	0.55650	0.00199	0.55849
H	24	0.40419	0.00000	0.59394	0.00187	0.59581
C	25	1.03398	1.99943	2.91148	0.05511	4.96602
F	26	-0.30167	1.99991	7.29132	0.01045	9.30167
F	27	-0.31461	1.99991	7.30376	0.01094	9.31461
F	28	-0.30108	1.99991	7.29077	0.01040	9.30108
* Total *		3.00000	31.98909	83.64640	0.36452	116.00000

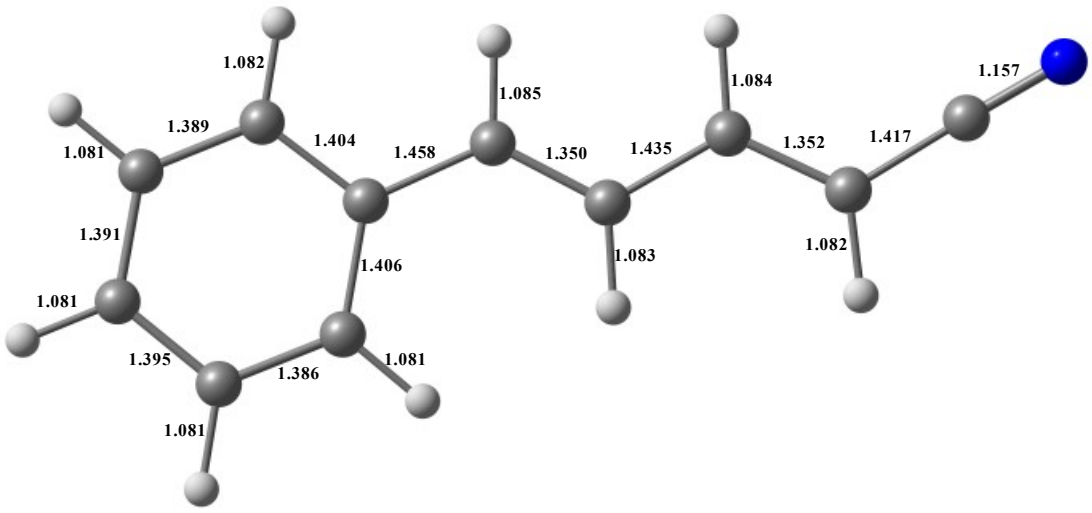
1k

Energy E(B3LYP) =-479.457133247 h, G^{298} = -479.328819 h, μ=8.03 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.437623	-0.250427	-0.000551
2	C	-2.383567	-1.288393	0.000065
3	C	-1.906682	1.074978	-0.000704
4	C	-3.746263	-1.017084	0.000720
5	C	-3.266610	1.344286	-0.000092
6	C	-4.193071	0.300702	0.000665
7	H	-2.039879	-2.314497	0.000073
8	H	-1.207957	1.899232	-0.001454
9	H	-4.456966	-1.831886	0.001239
10	H	-3.609068	2.369912	-0.000268
11	H	-5.252551	0.516112	0.001132
12	C	-0.021430	-0.598345	-0.001033
13	H	0.188886	-1.662810	-0.002540
14	C	1.032964	0.245085	0.000350
15	H	0.887454	1.318211	0.002114
16	C	2.387684	-0.229170	-0.000338
17	H	2.537059	-1.302598	-0.001993
18	C	3.469455	0.581427	0.000947
19	H	3.366420	1.658691	0.002579
20	C	4.794998	0.080567	0.000218
21	N	5.886783	-0.301732	-0.000338





Summary of Natural Population Analysis:

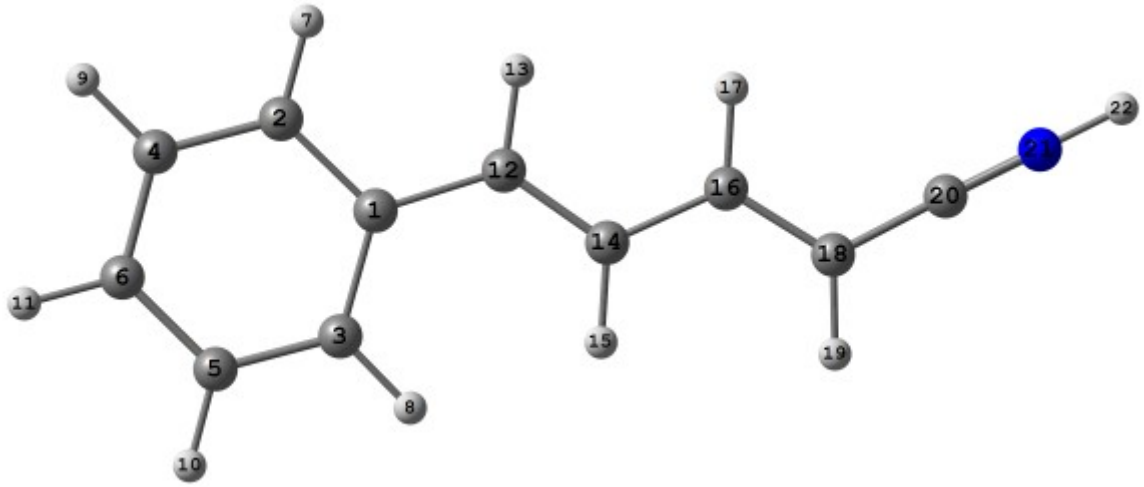
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.10389	1.99901	4.08508	0.01980	6.10389
C	2	-0.17890	1.99908	4.16068	0.01914	6.17890
C	3	-0.18192	1.99907	4.16476	0.01810	6.18192
C	4	-0.21349	1.99915	4.19394	0.02040	6.21349
C	5	-0.20927	1.99916	4.18983	0.02028	6.20927
C	6	-0.19733	1.99916	4.17757	0.02060	6.19733
H	7	0.22272	0.00000	0.77543	0.00185	0.77728
H	8	0.22114	0.00000	0.77707	0.00179	0.77886
H	9	0.22380	0.00000	0.77453	0.00168	0.77620
H	10	0.22318	0.00000	0.77515	0.00167	0.77682
H	11	0.22253	0.00000	0.77592	0.00155	0.77747
C	12	-0.12377	1.99907	4.10545	0.01925	6.12377
H	13	0.21740	0.00000	0.78051	0.00209	0.78260
C	14	-0.23748	1.99904	4.21905	0.01938	6.23748
H	15	0.21767	0.00000	0.77885	0.00348	0.78233
C	16	-0.10670	1.99909	4.08850	0.01911	6.10670
H	17	0.22661	0.00000	0.77152	0.00188	0.77339
C	18	-0.35818	1.99891	4.34359	0.01567	6.35818
H	19	0.25576	0.00000	0.74221	0.00203	0.74424
C	20	0.32224	1.99931	3.64458	0.03387	5.67776
N	21	-0.44211	1.99957	5.41448	0.02806	7.44211
* Total *		0.00000	23.98962	57.73871	0.27167	82.00000

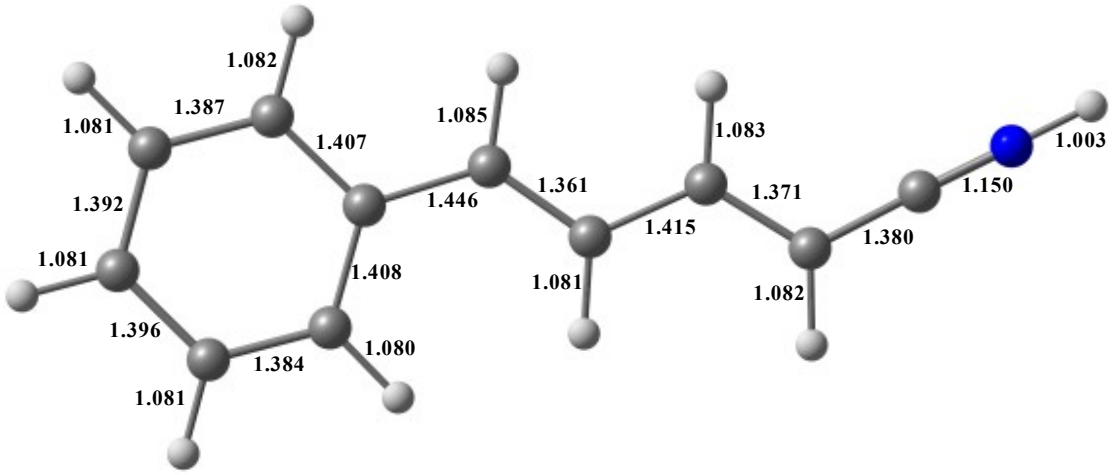
A6

Energy E(B3LYP) = -479.860288584 h, G^{298} = -479.722142 h, μ=14.1 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.501665	-0.240262	0.000118
2	C	-2.425951	-1.300995	0.000117
3	C	-1.991900	1.079943	0.000123
4	C	-3.791000	-1.054581	0.000134
5	C	-3.354653	1.321734	0.000131
6	C	-4.258132	0.256970	0.000137
7	H	-2.060691	-2.319119	0.000108
8	H	-1.307590	1.915554	0.000109
9	H	-4.488602	-1.879980	0.000137
10	H	-3.719684	2.338998	0.000127
11	H	-5.321374	0.452441	0.000141
12	C	-0.091309	-0.560336	0.000094
13	H	0.141918	-1.619645	-0.000007
14	C	0.957944	0.306544	0.000143
15	H	0.804933	1.377137	0.000251
16	C	2.288754	-0.174260	-0.000002
17	H	2.433019	-1.247683	-0.000128
18	C	3.394668	0.635488	0.000033
19	H	3.333167	1.715371	0.000142
20	C	4.667171	0.100272	-0.000146
21	N	5.736324	-0.322772	-0.001122
22	H	6.667070	-0.696777	0.001681





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.12129	1.99901	4.10258	0.01970	6.12129
C	2	-0.15588	1.99909	4.13786	0.01893	6.15588
C	3	-0.16073	1.99907	4.14380	0.01787	6.16073
C	4	-0.21501	1.99915	4.19560	0.02027	6.21501
C	5	-0.20977	1.99916	4.19046	0.02015	6.20977
C	6	-0.16624	1.99916	4.14691	0.02016	6.16624
H	7	0.22723	0.00000	0.77097	0.00179	0.77277
H	8	0.22494	0.00000	0.77329	0.00176	0.77506
H	9	0.22791	0.00000	0.77043	0.00166	0.77209
H	10	0.22721	0.00000	0.77114	0.00166	0.77279
H	11	0.22516	0.00000	0.77335	0.00149	0.77484
C	12	-0.05216	1.99909	4.03422	0.01885	6.05216
H	13	0.22524	0.00000	0.77277	0.00199	0.77476
C	14	-0.26250	1.99905	4.24382	0.01964	6.26250
H	15	0.22883	0.00000	0.76772	0.00344	0.77117
C	16	-0.02386	1.99911	4.00631	0.01845	6.02386
H	17	0.23716	0.00000	0.76104	0.00180	0.76284
C	18	-0.42808	1.99896	4.41272	0.01640	6.42808
H	19	0.28792	0.00000	0.71019	0.00188	0.71208
C	20	0.61839	1.99919	3.36366	0.01876	5.38161
N	21	-0.45297	1.99902	5.44419	0.00976	7.45297

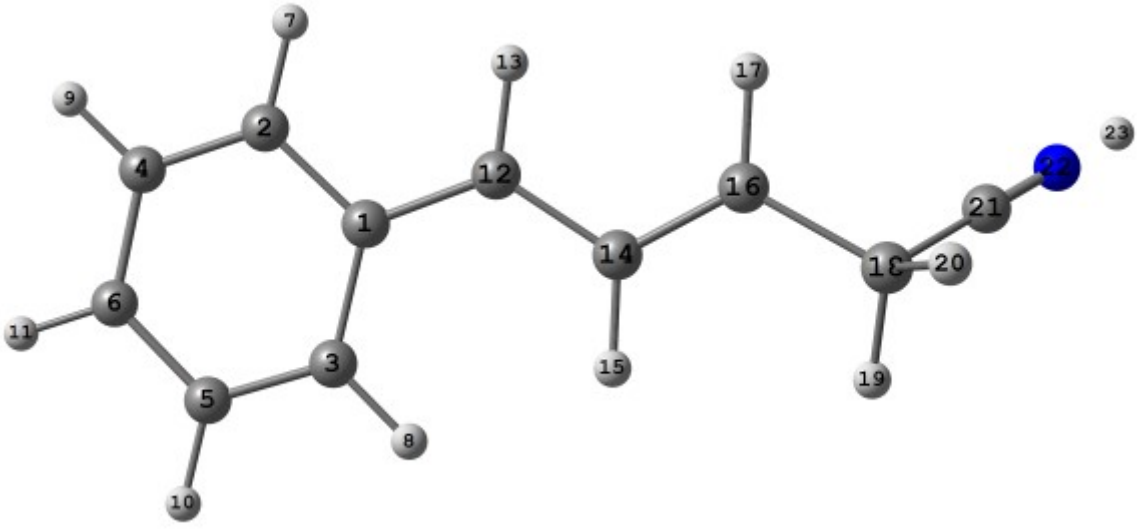
H	22	0.51851	0.00000	0.47889	0.00259	0.48149
* Total *		1.00000	23.98905	57.77194	0.23901	82.00000

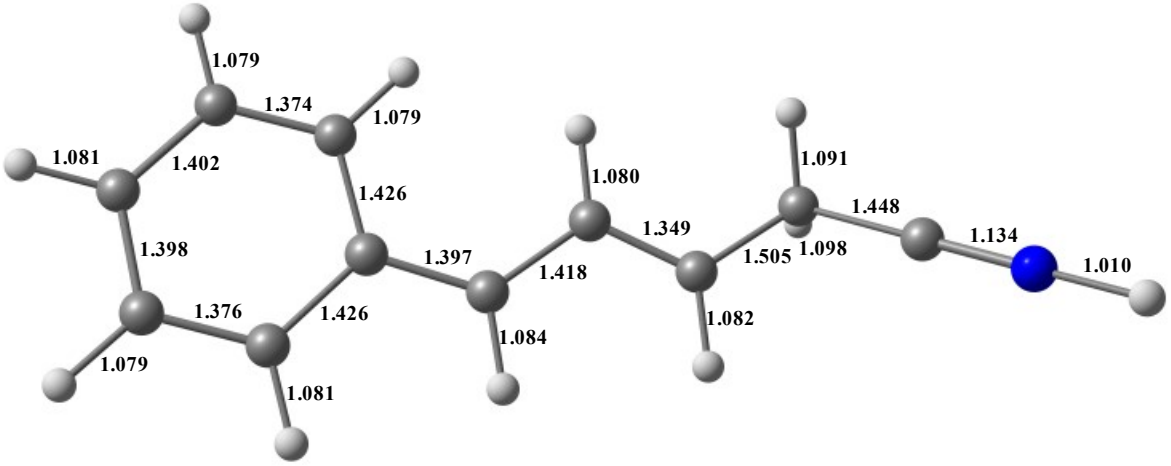
C6

Energy E(B3LYP) = -480.244662979 h, G^{298} = -480.093829 h, μ=17.3 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.509973	-0.256505	0.054384
2	C	2.467606	-1.312577	0.049509
3	C	1.960990	1.089239	-0.080235
4	C	3.808595	-1.034699	-0.082243
5	C	3.303340	1.351454	-0.208507
6	C	4.224510	0.294228	-0.209547
7	H	2.123980	-2.332075	0.150594
8	H	1.254491	1.904490	-0.079798
9	H	4.535668	-1.832508	-0.086634
10	H	3.652241	2.368130	-0.308105
11	H	5.278437	0.512620	-0.310616
12	C	0.163095	-0.599697	0.197735
13	H	-0.059203	-1.655356	0.301978
14	C	-0.948795	0.280695	0.219535
15	H	-0.808271	1.345557	0.107434
16	C	-2.186113	-0.229163	0.387839
17	H	-2.327958	-1.295154	0.503315
18	C	-3.406868	0.644991	0.489225
19	H	-3.248996	1.641745	0.074252
20	H	-3.681050	0.772071	1.545216
21	C	-4.569280	0.078457	-0.163153
22	N	-5.483204	-0.360304	-0.671567
23	H	-6.299233	-0.745921	-1.123927





Summary of Natural Population Analysis:

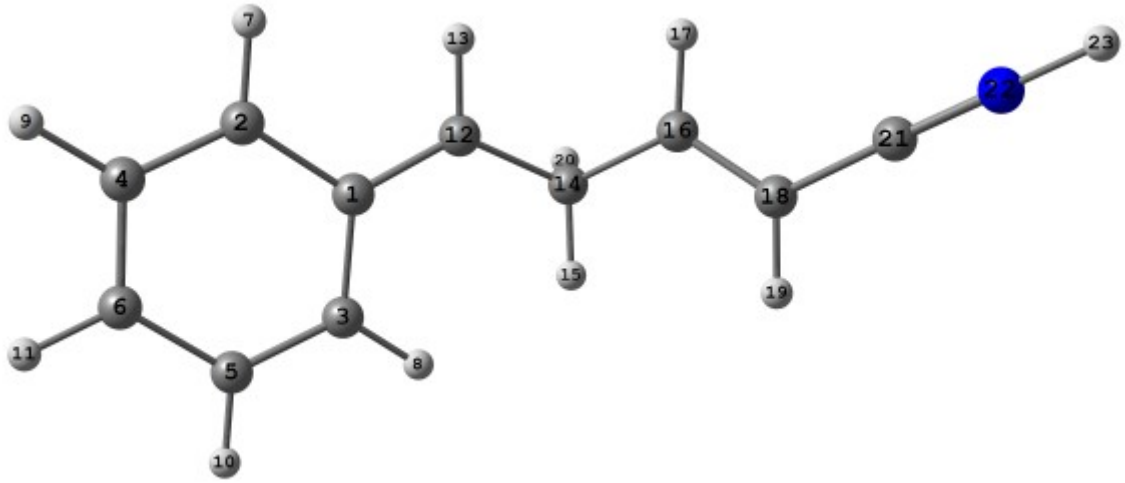
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.14116	1.99900	4.12250	0.01966	6.14116
C	2	-0.07176	1.99909	4.05429	0.01838	6.07176
C	3	-0.08792	1.99908	4.07148	0.01736	6.08792
C	4	-0.22236	1.99914	4.20313	0.02010	6.22236
C	5	-0.21500	1.99915	4.19584	0.02001	6.21500
C	6	-0.05901	1.99918	4.04075	0.01908	6.05901
H	7	0.24601	0.00000	0.75236	0.00164	0.75399
H	8	0.24244	0.00000	0.75589	0.00167	0.75756
H	9	0.24731	0.00000	0.75110	0.00158	0.75269
H	10	0.24656	0.00000	0.75187	0.00157	0.75344
H	11	0.24213	0.00000	0.75656	0.00132	0.75787
C	12	0.09932	1.99910	3.88287	0.01871	5.90068
H	13	0.24943	0.00000	0.74872	0.00185	0.75057
C	14	-0.25873	1.99900	4.23981	0.01992	6.25873
H	15	0.25404	0.00000	0.74288	0.00308	0.74596
C	16	0.02654	1.99908	3.95840	0.01599	5.97346
H	17	0.25574	0.00000	0.74243	0.00182	0.74426
C	18	-0.57114	1.99909	4.55617	0.01587	6.57114
H	19	0.31415	0.00000	0.68432	0.00154	0.68585
H	20	0.33295	0.00000	0.66554	0.00151	0.66705
C	21	0.67915	1.99918	3.30255	0.01913	5.32085
N	22	-0.36774	1.99891	5.35879	0.01004	7.36774
H	23	0.55907	0.00000	0.43849	0.00244	0.44093
* Total *		2.00000	23.98901	57.77673	0.23426	82.00000

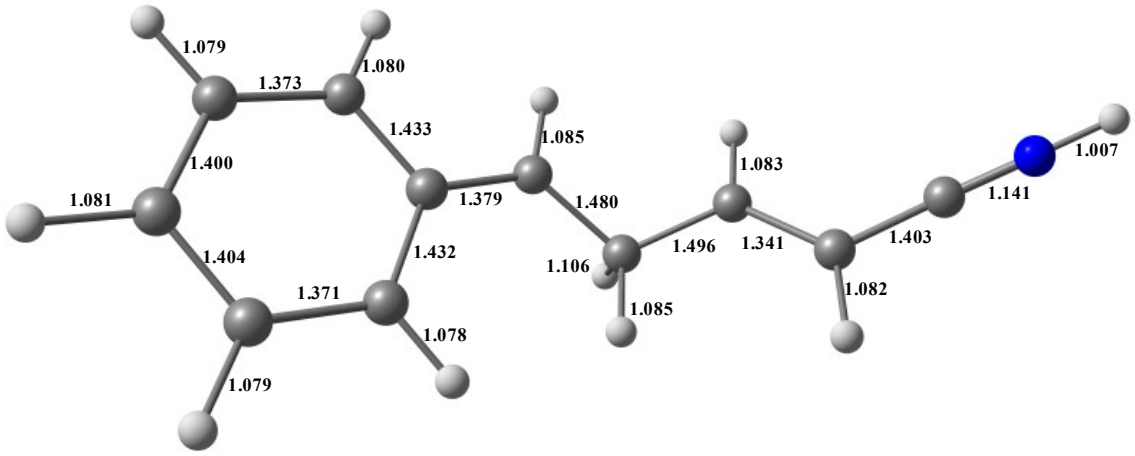
B6

Energy E(B3LYP) = -480.234982253 h, G^{298} = -480.085804 h, μ=11.9 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.448047	-0.272045	0.220502
2	C	-2.380699	-1.323114	-0.061223
3	C	-1.877154	1.089173	0.107917
4	C	-3.668576	-1.025161	-0.431296
5	C	-3.167734	1.367149	-0.260538
6	C	-4.058638	0.315406	-0.529996
7	H	-2.053257	-2.349087	0.023999
8	H	-1.189443	1.895454	0.308165
9	H	-4.375518	-1.811949	-0.645122
10	H	-3.502526	2.389246	-0.349642
11	H	-5.072399	0.549085	-0.824508
12	C	-0.171474	-0.635873	0.593328
13	H	0.039226	-1.699048	0.636020
14	C	0.941223	0.255204	0.991177
15	H	0.775483	1.299638	0.750254
16	C	2.276616	-0.223797	0.516575
17	H	2.510682	-1.271992	0.653432
18	C	3.177238	0.599583	-0.038603
19	H	3.008302	1.654474	-0.210191
20	H	0.964983	0.183564	2.094539
21	C	4.431893	0.112874	-0.436936
22	N	5.457985	-0.257568	-0.770957
23	H	6.360689	-0.592805	-1.065691





Summary of Natural Population Analysis:

Natural Population

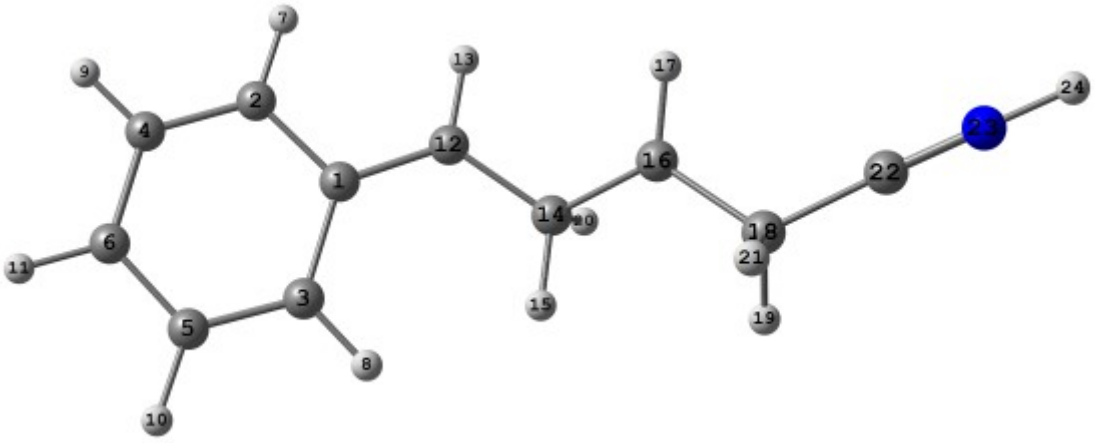
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.16899	1.99898	4.15031	0.01971	6.16899
C	2	-0.03837	1.99910	4.02088	0.01839	6.03837
C	3	-0.06110	1.99908	4.04481	0.01721	6.06110
C	4	-0.22659	1.99914	4.20740	0.02005	6.22659
C	5	-0.21599	1.99915	4.19687	0.01997	6.21599
C	6	-0.02624	1.99919	4.00830	0.01875	6.02624
H	7	0.24880	0.00000	0.74953	0.00167	0.75120
H	8	0.24290	0.00000	0.75538	0.00172	0.75710
H	9	0.25135	0.00000	0.74706	0.00159	0.74865
H	10	0.25056	0.00000	0.74786	0.00158	0.74944
H	11	0.24513	0.00000	0.75358	0.00129	0.75487
C	12	0.20271	1.99908	3.78197	0.01623	5.79729
H	13	0.24722	0.00000	0.75089	0.00188	0.75278
C	14	-0.52219	1.99915	4.50342	0.01962	6.52219
H	15	0.25522	0.00000	0.74204	0.00275	0.74478
C	16	0.02577	1.99908	3.95822	0.01694	5.97423
H	17	0.25431	0.00000	0.74398	0.00171	0.74569
C	18	-0.37299	1.99890	4.35841	0.01568	6.37299
H	19	0.29952	0.00000	0.69867	0.00181	0.70048
H	20	0.32067	0.00000	0.67766	0.00167	0.67933
C	21	0.63759	1.99918	3.34479	0.01844	5.36241
N	22	-0.37719	1.99899	5.36970	0.00850	7.37719
H	23	0.52793	0.00000	0.46964	0.00243	0.47207
* Total *		2.00000	23.98903	57.78137	0.22960	82.00000

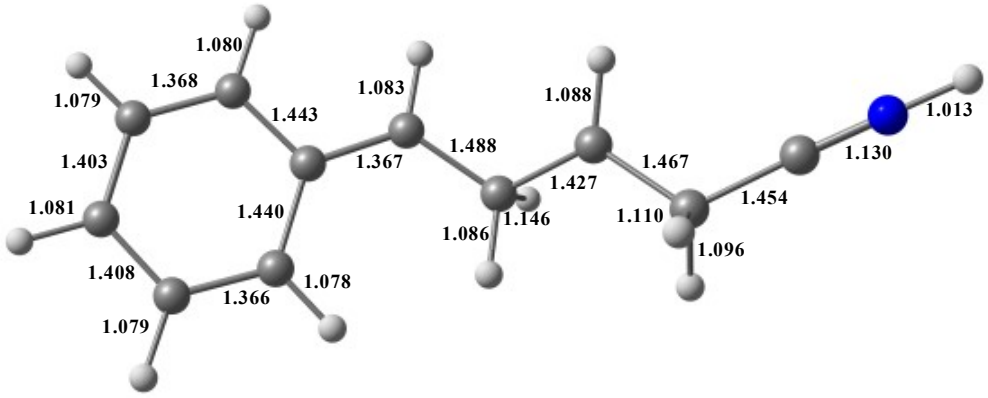
D6

Energy E(B3LYP) = -480.553283353 h, G^{298} = -480.393548 h, μ=21.9 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.553080	-0.296065	0.117643
2	C	-2.548615	-1.327611	-0.044464
3	C	-1.962512	1.084068	0.085114
4	C	-3.863834	-0.992661	-0.217297
5	C	-3.281484	1.393481	-0.090237
6	C	-4.227787	0.361924	-0.239894
7	H	-2.236082	-2.361345	-0.021383
8	H	-1.238519	1.875900	0.192850
9	H	-4.616467	-1.756639	-0.335064
10	H	-3.603311	2.422922	-0.117965
11	H	-5.267661	0.623961	-0.378434
12	C	-0.261476	-0.706179	0.294386
13	H	-0.060767	-1.770378	0.304747
14	C	0.913152	0.182074	0.510862
15	H	0.757228	1.253799	0.434622
16	C	2.189329	-0.271317	0.060501
17	H	2.353645	-1.335512	-0.094399
18	C	3.292497	0.671905	-0.155259
19	H	3.274472	1.524024	0.534283
20	H	1.197261	0.032639	1.610628
21	H	3.087418	1.127730	-1.146831
22	C	4.629477	0.101934	-0.193139
23	N	5.681788	-0.310044	-0.216405
24	H	6.626265	-0.676119	-0.237513





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.12922	1.99898	4.11074	0.01950	6.12922
C	2	-0.02157	1.99910	4.00425	0.01822	6.02157
C	3	-0.05185	1.99908	4.03581	0.01696	6.05185
C	4	-0.22438	1.99914	4.20518	0.02006	6.22438
C	5	-0.21246	1.99915	4.19318	0.02013	6.21246
C	6	0.02005	1.99920	3.96220	0.01855	5.97995
H	7	0.25523	0.00000	0.74313	0.00165	0.74477
H	8	0.24648	0.00000	0.75172	0.00180	0.75352
H	9	0.25844	0.00000	0.74000	0.00155	0.74156
H	10	0.25769	0.00000	0.74077	0.00154	0.74231
H	11	0.25004	0.00000	0.74871	0.00125	0.74996
C	12	0.13608	1.99903	3.84708	0.01781	5.86392
H	13	0.26989	0.00000	0.72828	0.00183	0.73011
C	14	-0.57888	1.99906	4.55657	0.02325	6.57888
H	15	0.31076	0.00000	0.68760	0.00164	0.68924
C	16	0.42280	1.99920	3.56439	0.01362	5.57720
H	17	0.29874	0.00000	0.69916	0.00210	0.70126
C	18	-0.64214	1.99901	4.62644	0.01669	6.64214
H	19	0.36722	0.00000	0.63125	0.00153	0.63278
H	20	0.43673	0.00000	0.56133	0.00195	0.56327
H	21	0.40257	0.00000	0.59588	0.00155	0.59743
C	22	0.68200	1.99917	3.30011	0.01873	5.31800
N	23	-0.30085	1.99895	5.29327	0.00863	7.30085

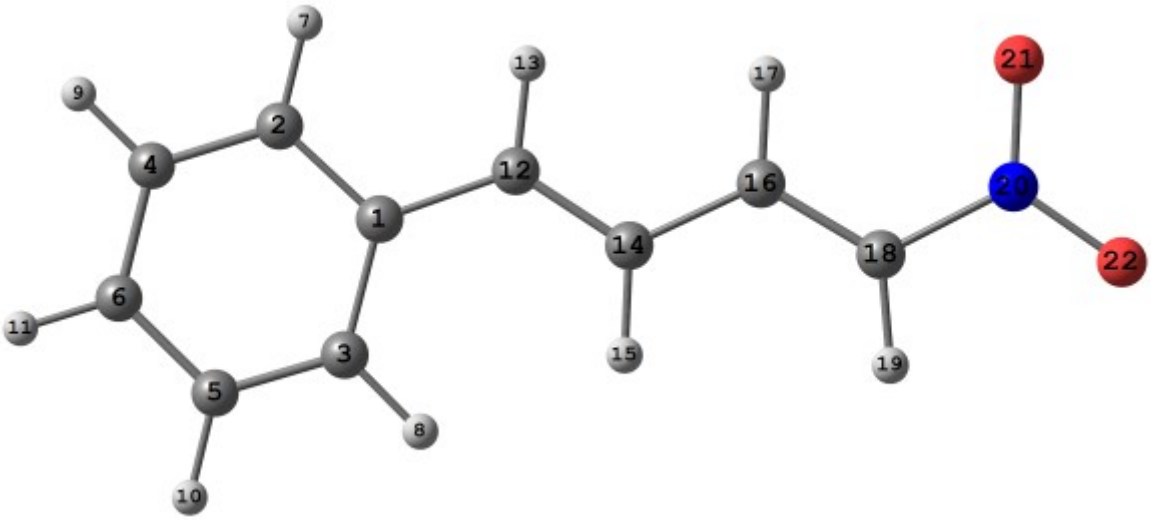
H	24	0.54666	0.00000	0.45099	0.00235	0.45334
* Total *		3.00000	23.98908	57.77803	0.23289	82.00000

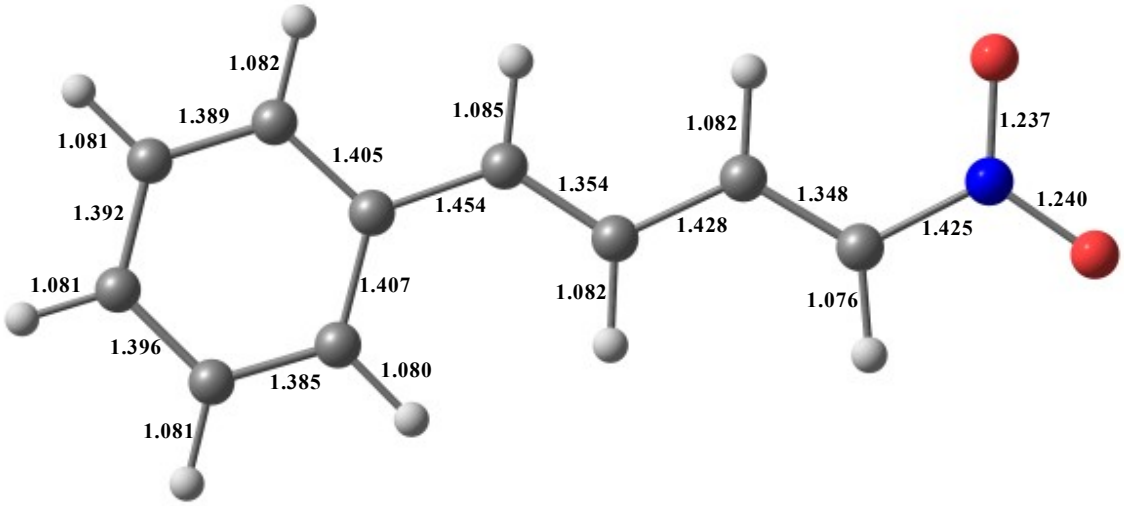
1l

Energy E(B3LYP) = -591.759791298 h, G^{298} =-591.629106 h, μ=10.1 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.967801	0.232983	0.000005
2	C	-2.915505	1.270563	0.000050
3	C	-2.432174	-1.094943	-0.000038
4	C	-4.276597	0.995693	0.000057
5	C	-3.790680	-1.366822	-0.000033
6	C	-4.718508	-0.324025	0.000016
7	H	-2.573254	2.296971	0.000080
8	H	-1.731199	-1.917047	-0.000082
9	H	-4.990147	1.807749	0.000093
10	H	-4.131845	-2.392680	-0.000069
11	H	-5.777413	-0.542060	0.000020
12	C	-0.556926	0.583890	0.000007
13	H	-0.347290	1.648207	-0.000008
14	C	0.502539	-0.259542	0.000029
15	H	0.360387	-1.332259	0.000051
16	C	1.844044	0.230497	0.000027
17	H	2.000158	1.301583	0.000009
18	C	2.928552	-0.569424	0.000048
19	H	2.914823	-1.645535	0.000065
20	N	4.247582	-0.030049	0.000046
21	O	4.422549	1.194222	-0.000109
22	O	5.182582	-0.845197	-0.000075





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.11303	1.99901	4.09425	0.01977	6.11303
C	2	-0.16771	1.99908	4.14960	0.01902	6.16771
C	3	-0.17292	1.99907	4.15585	0.01800	6.17292
C	4	-0.21198	1.99915	4.19250	0.02033	6.21198
C	5	-0.20746	1.99916	4.18809	0.02021	6.20746
C	6	-0.18281	1.99916	4.16327	0.02038	6.18281
H	7	0.22470	0.00000	0.77348	0.00182	0.77530
H	8	0.22294	0.00000	0.77528	0.00178	0.77706
H	9	0.22518	0.00000	0.77315	0.00167	0.77482
H	10	0.22462	0.00000	0.77372	0.00166	0.77538
H	11	0.22348	0.00000	0.77500	0.00152	0.77652
C	12	-0.09904	1.99908	4.08088	0.01909	6.09904
H	13	0.22268	0.00000	0.77530	0.00202	0.77732
C	14	-0.23833	1.99906	4.22012	0.01915	6.23833
H	15	0.22358	0.00000	0.77294	0.00348	0.77642
C	16	-0.12515	1.99909	4.10569	0.02036	6.12515
H	17	0.24366	0.00000	0.75358	0.00276	0.75634
C	18	-0.08977	1.99895	4.06802	0.02280	6.08977
H	19	0.23923	0.00000	0.75843	0.00234	0.76077
N	20	0.47549	1.99948	4.47517	0.04986	6.52451
O	21	-0.45558	1.99980	6.43334	0.02245	8.45558

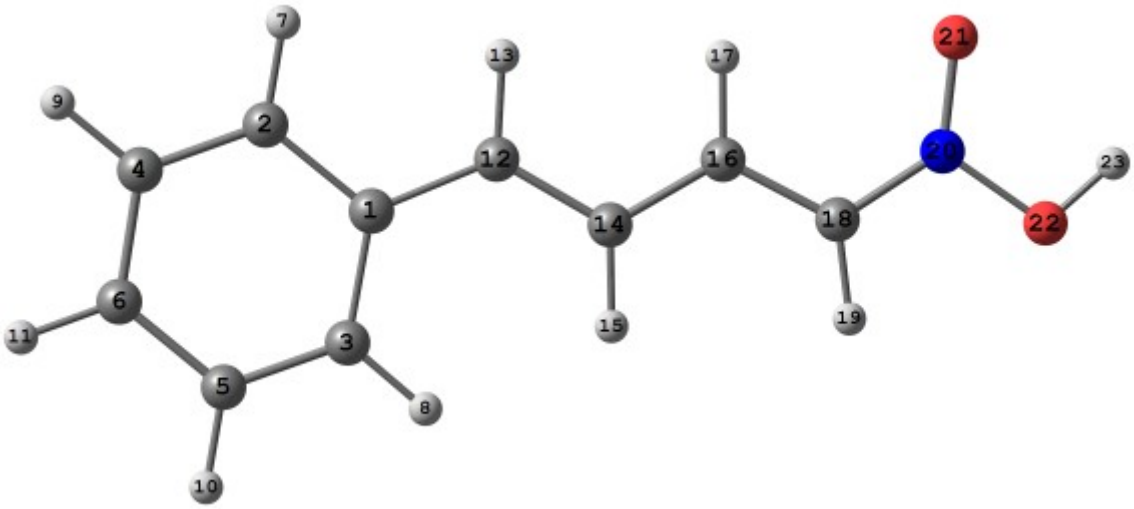
O	22	-0.46179	1.99980	6.44043	0.02155	8.46179
* Total *		0.00000	25.98988	65.69809	0.31204	92.00000

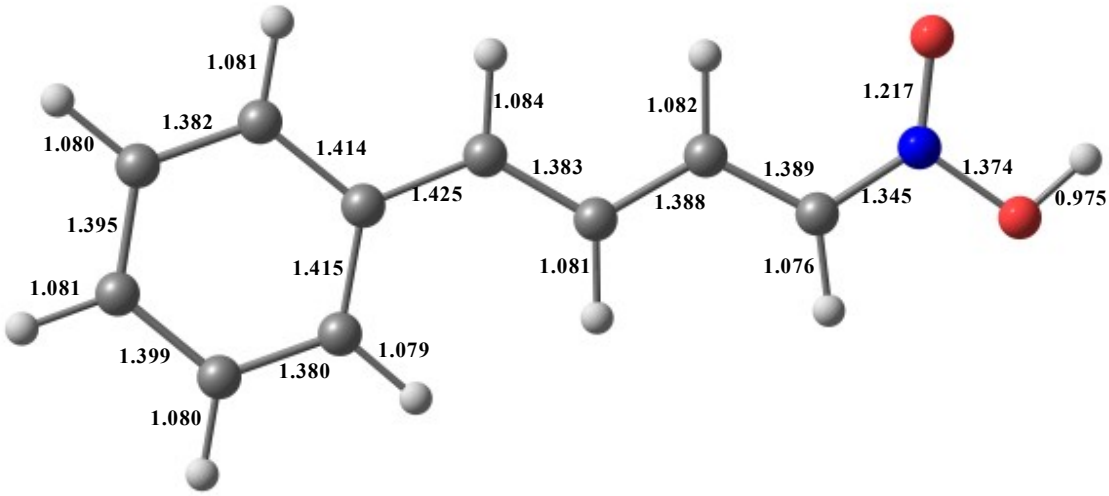
A7

Energy E(B3LYP) = -592.170371091 h, G^{298} = -592.027346 h, μ=2.16 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.019483	0.235074	-0.000001
2	C	2.977222	1.275870	0.000104
3	C	2.469748	-1.106629	-0.000112
4	C	4.329330	0.988464	0.000107
5	C	3.821008	-1.384643	-0.000112
6	C	4.751923	-0.340637	0.000000
7	H	2.638056	2.302461	0.000185
8	H	1.761049	-1.920793	-0.000201
9	H	5.054798	1.788642	0.000191
10	H	4.161415	-2.409774	-0.000199
11	H	5.808844	-0.567453	0.000000
12	C	0.640472	0.593821	0.000013
13	H	0.430106	1.657288	0.000074
14	C	-0.449529	-0.257264	-0.000033
15	H	-0.318454	-1.329791	-0.000085
16	C	-1.736910	0.262712	-0.000004
17	H	-1.874116	1.336323	0.000052
18	C	-2.872156	-0.538128	-0.000044
19	H	-2.864475	-1.613966	-0.000101
20	N	-4.091599	0.028277	-0.000007
21	O	-4.381330	1.210769	0.000086
22	O	-5.110751	-0.893116	-0.000014
23	H	-5.922914	-0.353947	0.000048





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.12907	1.99901	4.11038	0.01969	6.12907
C	2	-0.11904	1.99909	4.10135	0.01859	6.11904
C	3	-0.12904	1.99908	4.11239	0.01757	6.12904
C	4	-0.21681	1.99915	4.19756	0.02010	6.21681
C	5	-0.21093	1.99916	4.19177	0.02000	6.21093
C	6	-0.12213	1.99917	4.10338	0.01958	6.12213
H	7	0.23501	0.00000	0.76328	0.00171	0.76499
H	8	0.23209	0.00000	0.76619	0.00172	0.76791
H	9	0.23593	0.00000	0.76244	0.00163	0.76407
H	10	0.23525	0.00000	0.76313	0.00162	0.76475
H	11	0.23231	0.00000	0.76627	0.00142	0.76769
C	12	0.01751	1.99911	3.96471	0.01867	5.98249
H	13	0.23528	0.00000	0.76283	0.00189	0.76472
C	14	-0.24104	1.99908	4.22299	0.01897	6.24104
H	15	0.23983	0.00000	0.75695	0.00322	0.76017
C	16	-0.05881	1.99914	4.04102	0.01865	6.05881
H	17	0.25349	0.00000	0.74404	0.00247	0.74651
C	18	-0.06704	1.99907	4.04543	0.02254	6.06704
H	19	0.26507	0.00000	0.73311	0.00182	0.73493
N	20	0.43878	1.99931	4.52385	0.03806	6.56122
O	21	-0.37626	1.99978	6.35377	0.02271	8.37626

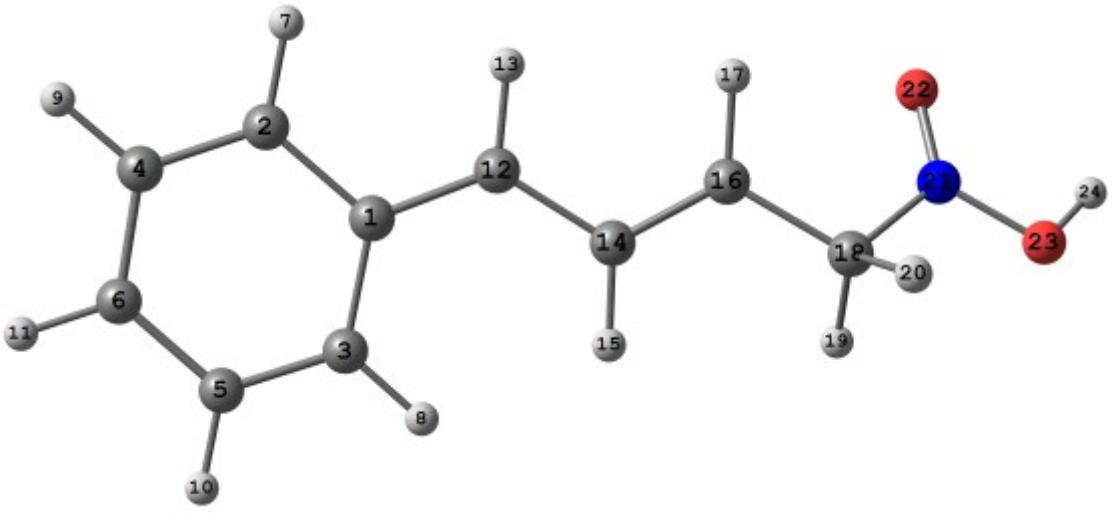
O	22	-0.49714	1.99978	6.47642	0.02094	8.49714
H	23	0.54676	0.00000	0.44984	0.00340	0.45324
* Total *		1.00000	25.98992	65.71311	0.29697	92.00000

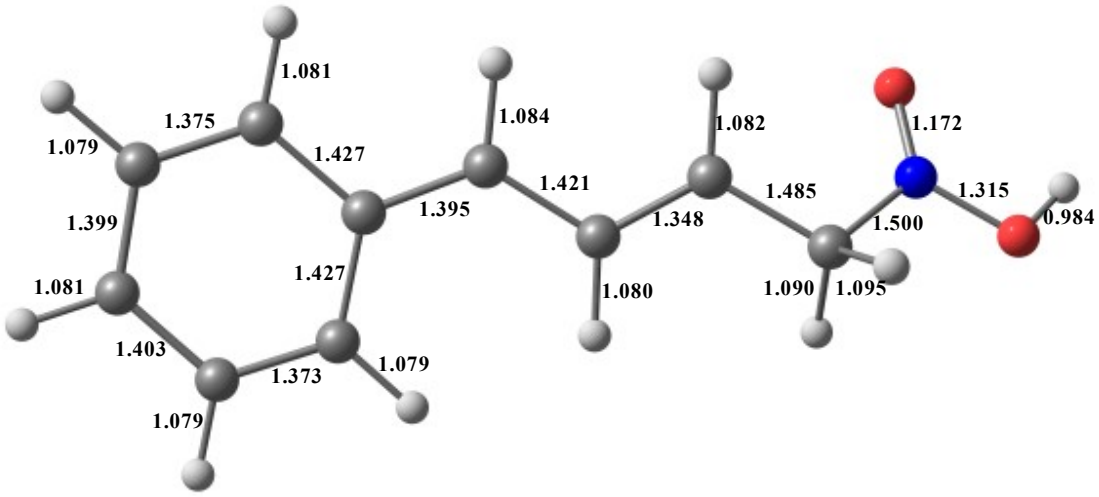
C7

Energy E(B3LYP) = -592.533804453 h, G^{298} =-592.378981 h, μ=11.2 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.035623	-0.244030	0.054180
2	C	3.014563	-1.281153	0.105044
3	C	2.464022	1.106784	-0.114533
4	C	4.351882	-0.980022	-0.002721
5	C	3.802989	1.391498	-0.220271
6	C	4.744242	0.353052	-0.163308
7	H	2.688246	-2.303483	0.231092
8	H	1.742322	1.907308	-0.158208
9	H	5.094922	-1.761901	0.036766
10	H	4.134756	2.410984	-0.345822
11	H	5.795918	0.589546	-0.245605
12	C	0.695149	-0.608042	0.182834
13	H	0.487132	-1.663782	0.312239
14	C	-0.431644	0.257701	0.164034
15	H	-0.300196	1.320868	0.028797
16	C	-1.666183	-0.258798	0.327740
17	H	-1.805421	-1.322759	0.465563
18	C	-2.865318	0.613486	0.413501
19	H	-2.788137	1.552576	-0.134194
20	H	-3.125408	0.849893	1.450768
21	N	-4.090409	-0.061607	-0.127105
22	O	-4.127916	-1.140178	-0.583408
23	O	-5.152102	0.707186	-0.022679
24	H	-5.923071	0.213076	-0.381967





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.13140	1.99901	4.11275	0.01963	6.13140
C	2	-0.06673	1.99910	4.04939	0.01824	6.06673
C	3	-0.08263	1.99908	4.06633	0.01723	6.08263
C	4	-0.22275	1.99914	4.20362	0.01998	6.22275
C	5	-0.21557	1.99916	4.19651	0.01990	6.21557
C	6	-0.04917	1.99919	4.03107	0.01891	6.04917
H	7	0.24554	0.00000	0.75282	0.00164	0.75446
H	8	0.24150	0.00000	0.75683	0.00167	0.75850
H	9	0.24757	0.00000	0.75084	0.00159	0.75243
H	10	0.24685	0.00000	0.75157	0.00158	0.75315
H	11	0.24168	0.00000	0.75700	0.00132	0.75832
C	12	0.09717	1.99910	3.88523	0.01850	5.90283
H	13	0.24817	0.00000	0.74999	0.00184	0.75183
C	14	-0.23047	1.99902	4.21212	0.01933	6.23047
H	15	0.25164	0.00000	0.74529	0.00307	0.74836
C	16	-0.04050	1.99909	4.02346	0.01795	6.04050
H	17	0.26336	0.00000	0.73436	0.00228	0.73664
C	18	-0.27961	1.99910	4.25897	0.02154	6.27961
H	19	0.30021	0.00000	0.69801	0.00179	0.69979
H	20	0.31257	0.00000	0.68567	0.00176	0.68743
N	21	0.56964	1.99956	4.39028	0.04052	6.43036

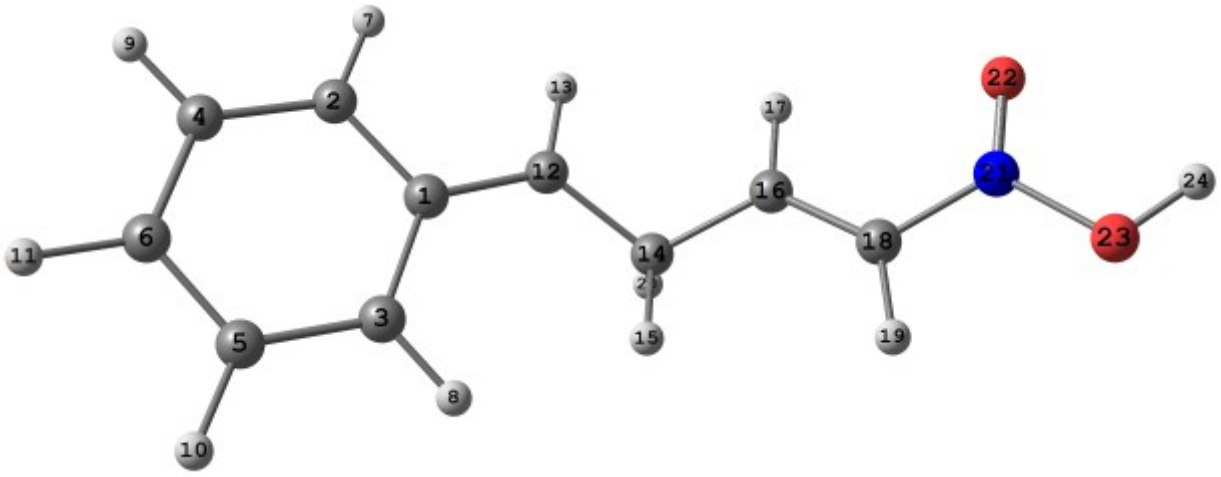
O	22	-0.13956	1.99974	6.11102	0.02881	8.13956
O	23	-0.39034	1.99975	6.36634	0.02426	8.39034
H	24	0.58286	0.00000	0.41447	0.00267	0.41714
* Total *		2.00000	25.99003	65.70393	0.30604	92.00000

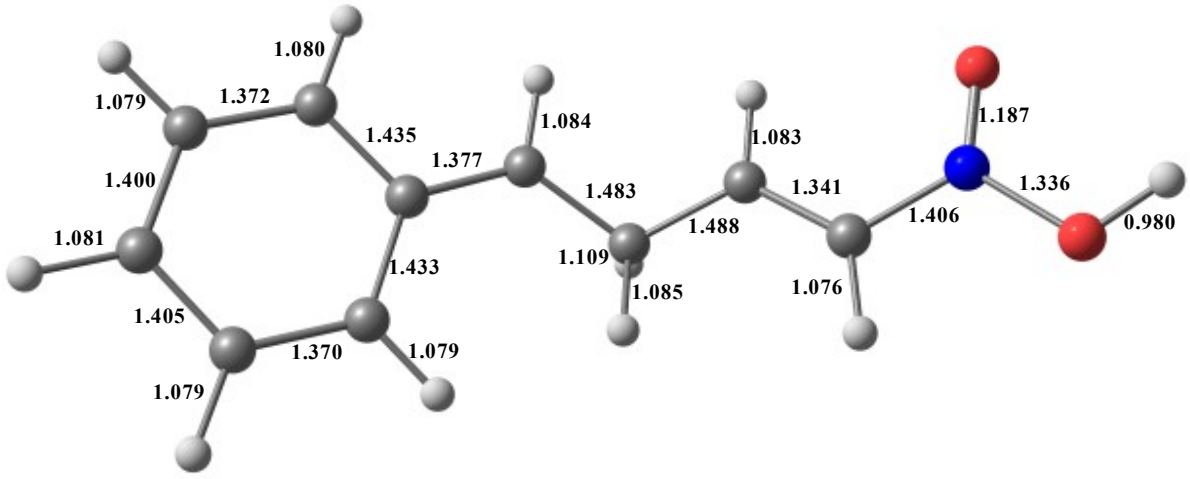
B7

Energy E(B3LYP) = -592.528451115 h, G^{298} = -592.374117 h, μ=4.60 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.969564	-0.269247	0.176957
2	C	-2.919038	-1.289561	-0.162530
3	C	-2.388283	1.100901	0.175903
4	C	-4.211696	-0.954108	-0.478088
5	C	-3.683791	1.415453	-0.139583
6	C	-4.590725	0.393405	-0.466061
7	H	-2.599931	-2.321754	-0.162414
8	H	-1.689292	1.885228	0.419799
9	H	-4.931167	-1.716748	-0.733354
10	H	-4.011110	2.443767	-0.143912
11	H	-5.608874	0.656713	-0.717276
12	C	-0.691839	-0.672920	0.493684
13	H	-0.491144	-1.737670	0.453104
14	C	0.435712	0.180149	0.940054
15	H	0.297388	1.237840	0.743325
16	C	1.768320	-0.310619	0.496192
17	H	1.952140	-1.378073	0.496062
18	C	2.750567	0.525546	0.128206
19	H	2.708252	1.599472	0.073617
20	H	0.437929	0.069340	2.043024
21	N	3.993543	-0.016461	-0.243326
22	O	4.300681	-1.163313	-0.265005
23	O	4.860292	0.936049	-0.599743
24	H	5.695238	0.481236	-0.839107





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.16151	1.99898	4.14287	0.01966	6.16151
C	2	-0.03716	1.99910	4.01971	0.01834	6.03716
C	3	-0.06294	1.99908	4.04671	0.01715	6.06294
C	4	-0.22722	1.99914	4.20802	0.02006	6.22722
C	5	-0.21490	1.99915	4.19576	0.01999	6.21490
C	6	-0.01642	1.99919	3.99850	0.01873	6.01642
H	7	0.25013	0.00000	0.74820	0.00166	0.74987
H	8	0.24394	0.00000	0.75436	0.00170	0.75606
H	9	0.25249	0.00000	0.74592	0.00159	0.74751
H	10	0.25158	0.00000	0.74684	0.00158	0.74842
H	11	0.24535	0.00000	0.75337	0.00128	0.75465
C	12	0.18864	1.99908	3.79602	0.01626	5.81136
H	13	0.25154	0.00000	0.74660	0.00187	0.74846
C	14	-0.52746	1.99915	4.50927	0.01904	6.52746
H	15	0.26577	0.00000	0.73173	0.00251	0.73423
C	16	0.04068	1.99912	3.94271	0.01749	5.95932
H	17	0.26862	0.00000	0.72897	0.00240	0.73138
C	18	-0.08443	1.99893	4.06419	0.02131	6.08443
H	19	0.28364	0.00000	0.71449	0.00187	0.71636
H	20	0.33556	0.00000	0.66283	0.00161	0.66444
N	21	0.52211	1.99944	4.43705	0.04140	6.47789

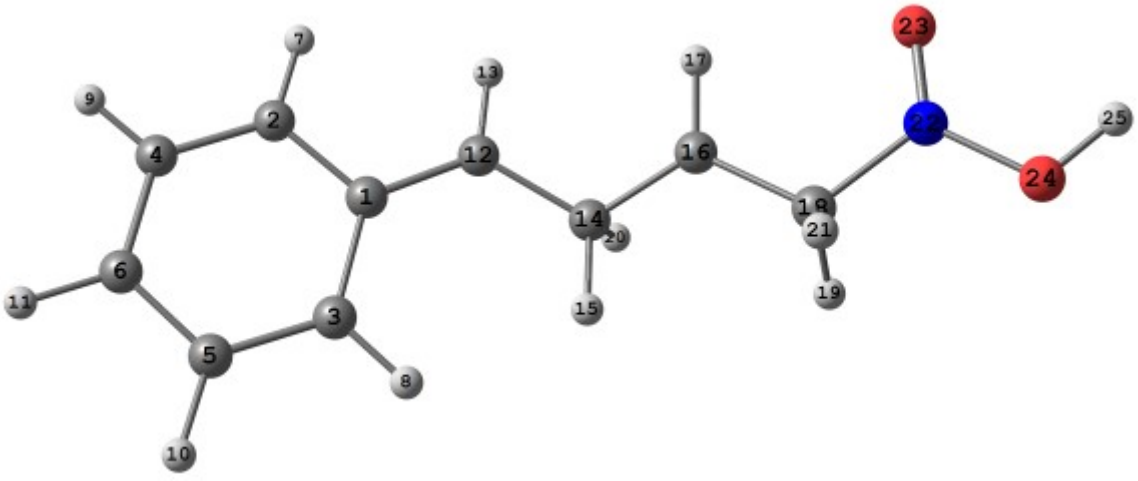
O	22	-0.21666	1.99976	6.19331	0.02360	8.21666
O	23	-0.42167	1.99976	6.40059	0.02131	8.42167
H	24	0.57032	0.00000	0.42670	0.00298	0.42968
* Total *		2.00000	25.98990	65.71474	0.29537	92.00000

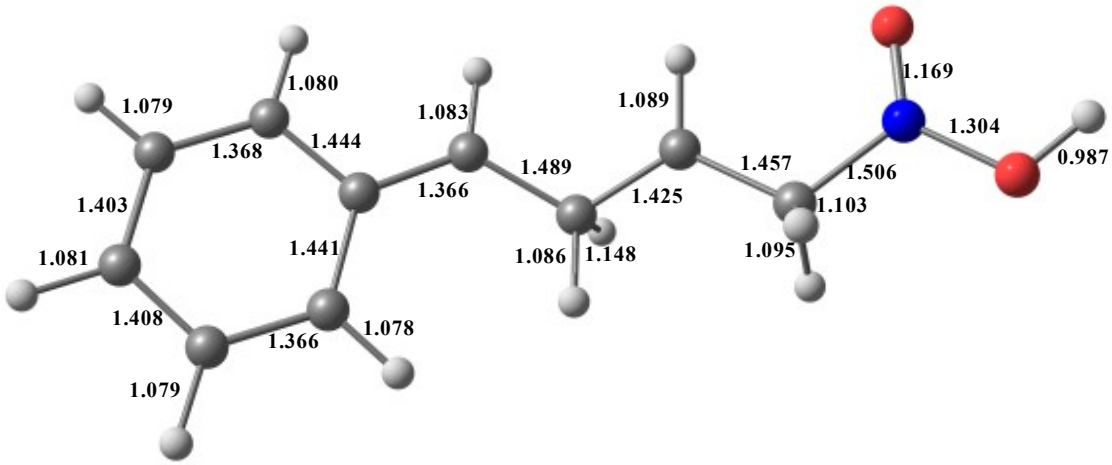
D7

Energy E(B3LYP) = -592.838017075 h, G^{298} = -592.675027 h, μ=13.5 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.058653	0.266002	0.127514
2	C	3.045859	1.303840	-0.051422
3	C	2.474152	-1.112573	0.081621
4	C	4.358140	0.976146	-0.254556
5	C	3.790430	-1.414145	-0.122518
6	C	4.728066	-0.376877	-0.289769
7	H	2.728538	2.335753	-0.017437
8	H	1.756713	-1.908150	0.204339
9	H	5.104355	1.744172	-0.385951
10	H	4.117553	-2.441585	-0.159353
11	H	5.765994	-0.633155	-0.451637
12	C	0.770262	0.671263	0.331498
13	H	0.567219	1.734908	0.357694
14	C	-0.399356	-0.221234	0.562384
15	H	-0.250029	-1.292834	0.473088
16	C	-1.684552	0.250761	0.168740
17	H	-1.849227	1.319615	0.041745
18	C	-2.810598	-0.656719	-0.005755
19	H	-2.927981	-1.395953	0.793516
20	H	-0.654984	-0.075411	1.672350
21	H	-2.664724	-1.237341	-0.932359
22	N	-4.124387	0.065908	-0.151182
23	O	-4.251377	1.228251	-0.163069
24	O	-5.106101	-0.784344	-0.269045
25	H	-5.949229	-0.281410	-0.367233





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.12752	1.99898	4.10903	0.01952	6.12752
C	2	-0.02029	1.99910	4.00299	0.01821	6.02029
C	3	-0.05155	1.99908	4.03549	0.01697	6.05155
C	4	-0.22427	1.99914	4.20506	0.02007	6.22427
C	5	-0.21245	1.99915	4.19317	0.02013	6.21245
C	6	0.01886	1.99920	3.96340	0.01854	5.98114
H	7	0.25602	0.00000	0.74234	0.00164	0.74398
H	8	0.24740	0.00000	0.75080	0.00180	0.75260
H	9	0.25949	0.00000	0.73896	0.00155	0.74051
H	10	0.25874	0.00000	0.73973	0.00154	0.74126
H	11	0.25147	0.00000	0.74728	0.00125	0.74853
C	12	0.13780	1.99903	3.84534	0.01783	5.86220
H	13	0.27040	0.00000	0.72776	0.00184	0.72960
C	14	-0.56775	1.99907	4.54549	0.02320	6.56775
H	15	0.31386	0.00000	0.68452	0.00162	0.68614
C	16	0.37558	1.99920	3.60934	0.01587	5.62442
H	17	0.30635	0.00000	0.69090	0.00275	0.69365
C	18	-0.36794	1.99899	4.34629	0.02266	6.36794
H	19	0.36031	0.00000	0.63789	0.00181	0.63969
H	20	0.44346	0.00000	0.55450	0.00204	0.55654
H	21	0.37702	0.00000	0.62115	0.00182	0.62298

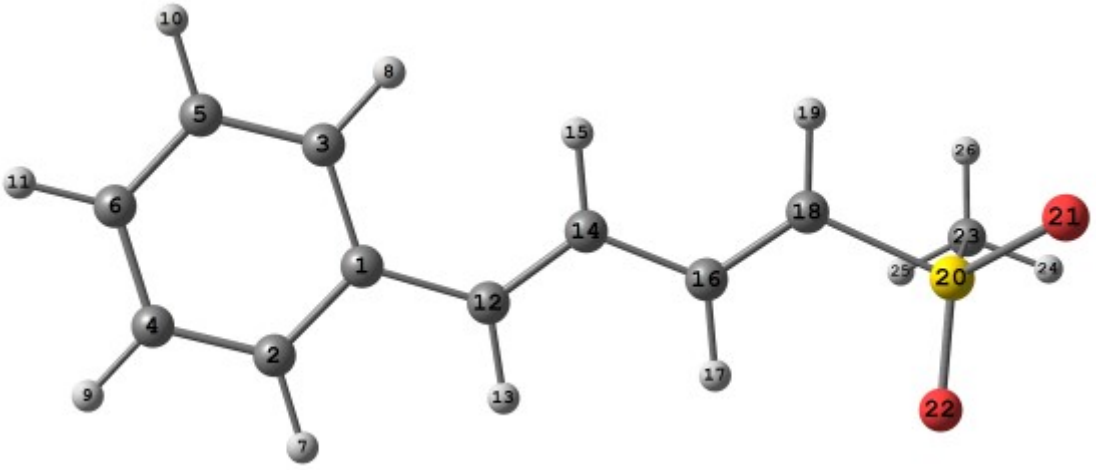
N	22	0.57588	1.99957	4.38376	0.04078	6.42412
O	23	-0.11453	1.99974	6.08599	0.02881	8.11453
O	24	-0.36400	1.99974	6.33995	0.02431	8.36400
H	25	0.59767	0.00000	0.39982	0.00250	0.40233
* Total *		3.00000	25.99000	65.70094	0.30906	92.00000

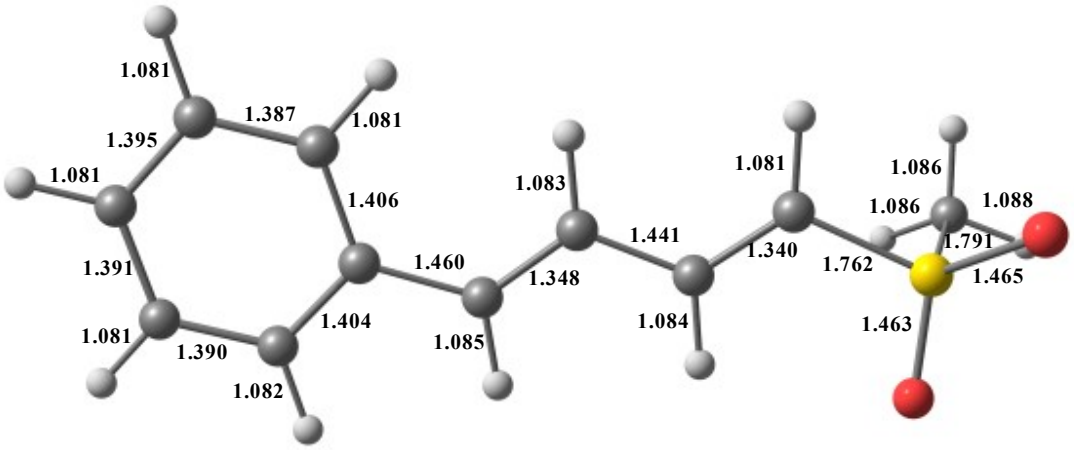
1m

Energy E(B3LYP) = -975.197099239 h, G^{298} = -975.034368 h, μ=7.97 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.814707	0.224527	0.006024
2	C	-3.754270	1.266976	0.044401
3	C	-3.290992	-1.097639	-0.019937
4	C	-5.118626	1.003036	0.055571
5	C	-4.652428	-1.359859	-0.008405
6	C	-5.572965	-0.311814	0.029282
7	H	-3.404914	2.290968	0.065204
8	H	-2.596876	-1.925311	-0.048416
9	H	-5.824566	1.821464	0.084968
10	H	-5.000449	-2.383433	-0.028508
11	H	-6.633567	-0.521505	0.038187
12	C	-1.395128	0.564616	-0.004005
13	H	-1.178557	1.627366	0.027387
14	C	-0.347957	-0.283773	-0.047207
15	H	-0.499573	-1.355099	-0.082682
16	C	1.013782	0.187222	-0.045598
17	H	1.171485	1.259102	-0.012988
18	C	2.087481	-0.614216	-0.087912
19	H	2.043376	-1.693293	-0.127396
20	S	3.722216	0.041231	-0.135217
21	O	4.463012	-0.669818	-1.180156
22	O	3.656720	1.501180	-0.207814
23	C	4.449299	-0.407263	1.439021
24	H	5.481332	-0.064988	1.406639
25	H	3.899003	0.090721	2.231321
26	H	4.409075	-1.487458	1.546100





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.10003	1.99901	4.08180	0.01922	6.10003
C	2	-0.17812	1.99908	4.16010	0.01894	6.17812
C	3	-0.18112	1.99907	4.16406	0.01800	6.18112
C	4	-0.21403	1.99915	4.19454	0.02034	6.21403
C	5	-0.21028	1.99916	4.19086	0.02026	6.21028
C	6	-0.19962	1.99916	4.17989	0.02057	6.19962
H	7	0.22227	0.00000	0.77599	0.00174	0.77773
H	8	0.22058	0.00000	0.77765	0.00177	0.77942
H	9	0.22369	0.00000	0.77464	0.00168	0.77631
H	10	0.22311	0.00000	0.77522	0.00167	0.77689
H	11	0.22268	0.00000	0.77577	0.00155	0.77732
C	12	-0.12219	1.99906	4.10424	0.01889	6.12219
H	13	0.21570	0.00000	0.78134	0.00297	0.78430
C	14	-0.23848	1.99903	4.21996	0.01949	6.23848
H	15	0.21812	0.00000	0.77839	0.00349	0.78188
C	16	-0.14542	1.99905	4.12404	0.02233	6.14542
H	17	0.23552	0.00000	0.76222	0.00226	0.76448
C	18	-0.49256	1.99887	4.46700	0.02669	6.49256
H	19	0.25052	0.00000	0.74687	0.00261	0.74948
S	20	2.11235	9.99851	3.69004	0.19910	13.88765
O	21	-1.00038	1.99980	6.96719	0.03338	9.00038

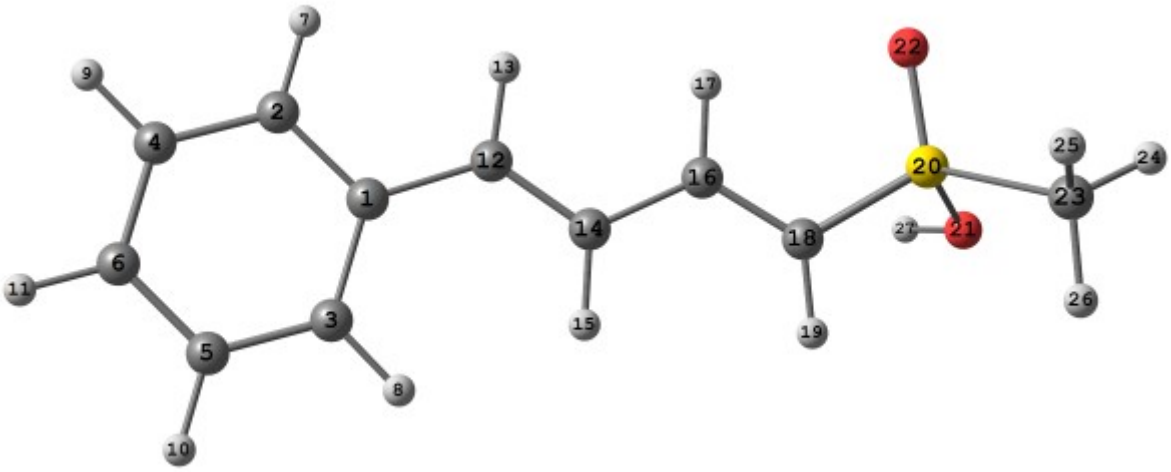
O	22	-0.99897	1.99980	6.96533	0.03384	8.99897
C	23	-0.79328	1.99923	4.77534	0.01871	6.79328
H	24	0.24634	0.00000	0.75162	0.00204	0.75366
H	25	0.24182	0.00000	0.75659	0.00159	0.75818
H	26	0.24179	0.00000	0.75676	0.00145	0.75821
* Total *		0.00000	35.98797	73.49745	0.51457	110.00000

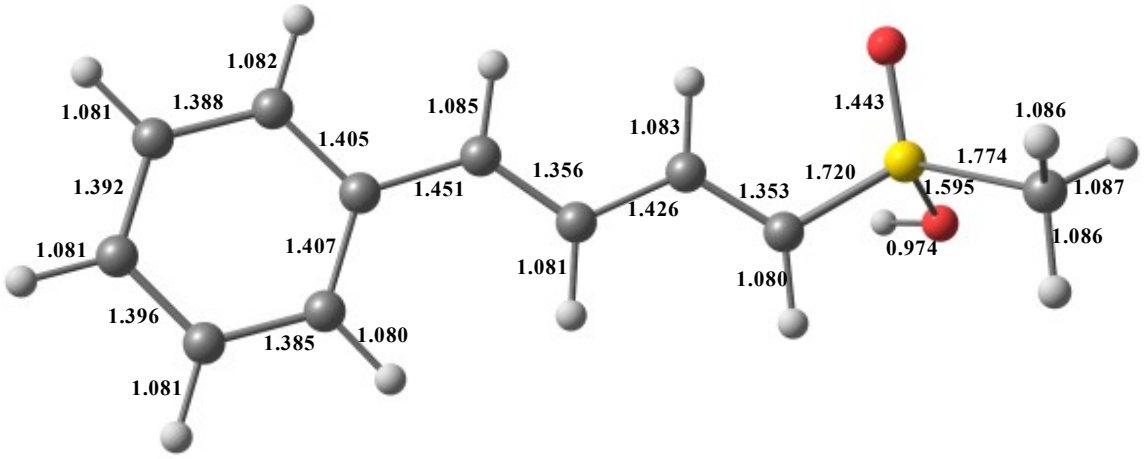
A8

Energy E(B3LYP) = -975.600053982 h, G^{298} = -975.425764 h, μ=9.21 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.849414	0.211574	0.015247
2	C	-3.777997	1.266500	0.028404
3	C	-3.334238	-1.109037	-0.002591
4	C	-5.143057	1.014479	0.023356
5	C	-4.696754	-1.357481	-0.007479
6	C	-5.605763	-0.298057	0.005285
7	H	-3.417907	2.286528	0.042168
8	H	-2.646581	-1.942054	-0.012917
9	H	-5.843402	1.837688	0.033295
10	H	-5.056214	-2.376793	-0.021522
11	H	-6.668179	-0.498104	0.001010
12	C	-1.435331	0.538788	0.018871
13	H	-1.209040	1.599543	0.032766
14	C	-0.386904	-0.320356	0.004767
15	H	-0.535016	-1.391435	-0.010654
16	C	0.952144	0.168793	0.004760
17	H	1.092129	1.242968	0.018261
18	C	2.049374	-0.623298	-0.016740
19	H	2.052327	-1.702958	-0.028975
20	S	3.608298	0.102467	-0.030479
21	O	4.426082	-0.598891	-1.207014
22	O	3.571810	1.542543	-0.111582
23	C	4.595742	-0.491575	1.318169
24	H	5.605303	-0.125058	1.150211
25	H	4.162471	-0.069174	2.220036
26	H	4.559047	-1.576650	1.325609
27	H	3.982346	-0.475183	-2.065153





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.11521	1.99901	4.09655	0.01966	6.11521
C	2	-0.16084	1.99908	4.14281	0.01895	6.16084
C	3	-0.16598	1.99907	4.14900	0.01791	6.16598
C	4	-0.21421	1.99915	4.19476	0.02029	6.21421
C	5	-0.20968	1.99916	4.19034	0.02018	6.20968
C	6	-0.17925	1.99916	4.15984	0.02024	6.17925

H	7	0.22606	0.00000	0.77214	0.00180	0.77394
H	8	0.22388	0.00000	0.77435	0.00177	0.77612
H	9	0.22711	0.00000	0.77123	0.00166	0.77289
H	10	0.22648	0.00000	0.77186	0.00166	0.77352
H	11	0.22549	0.00000	0.77301	0.00151	0.77451
C	12	-0.06608	1.99908	4.04837	0.01863	6.06608
H	13	0.22411	0.00000	0.77390	0.00199	0.77589
C	14	-0.26005	1.99904	4.24066	0.02035	6.26005
H	15	0.22860	0.00000	0.76792	0.00349	0.77140
C	16	-0.08557	1.99908	4.06435	0.02213	6.08557
H	17	0.24657	0.00000	0.75116	0.00226	0.75343
C	18	-0.54357	1.99891	4.51950	0.02516	6.54357
H	19	0.28034	0.00000	0.71721	0.00244	0.71966
S	20	2.06458	9.99833	3.76600	0.17110	13.93542
O	21	-0.87573	1.99979	6.84826	0.02768	8.87573
O	22	-0.90094	1.99978	6.86365	0.03751	8.90094
C	23	-0.77514	1.99922	4.75606	0.01987	6.77514
H	24	0.27033	0.00000	0.72787	0.00180	0.72967
H	25	0.26615	0.00000	0.73248	0.00137	0.73385
H	26	0.26743	0.00000	0.73120	0.00137	0.73257
H	27	0.57512	0.00000	0.42202	0.00286	0.42488
* Total *		1.00000	35.98786	73.52650	0.48564	110.00000

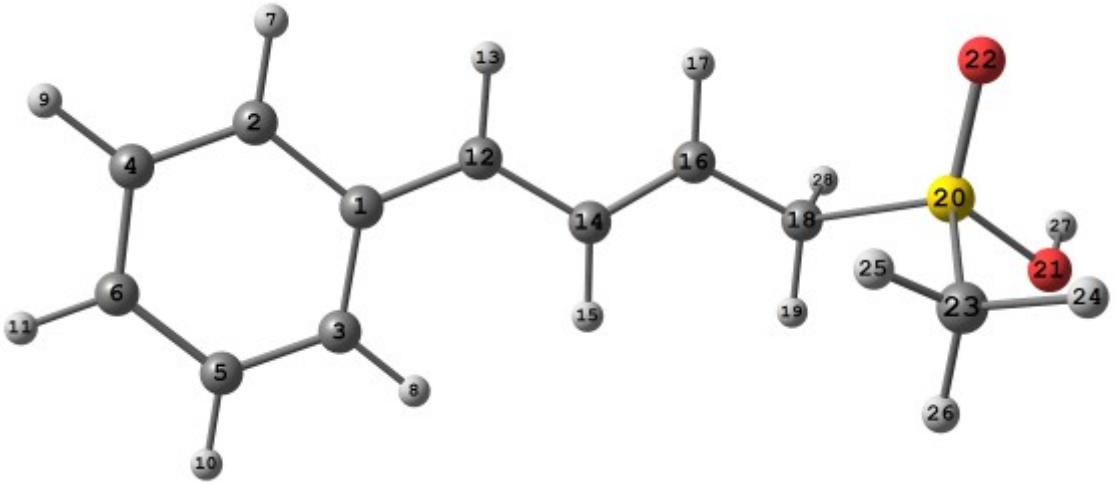
C8

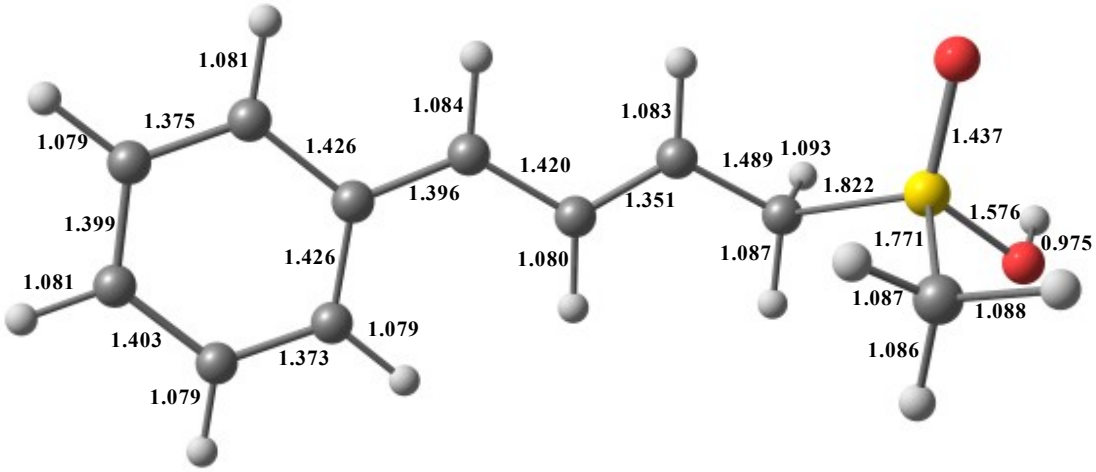
Energy E(B3LYP) = -975.995121247 h, G^{298} = -975.80785 h, μ=4.64 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.733316	0.288414	-0.074609
2	C	-3.742153	1.249970	0.228351
3	C	-3.101368	-1.082418	-0.216116
4	C	-5.052021	0.858791	0.379822
5	C	-4.413348	-1.457825	-0.061791
6	C	-5.385932	-0.491693	0.234586
7	H	-3.461974	2.288214	0.333730
8	H	-2.355035	-1.826970	-0.444067
9	H	-5.817948	1.584322	0.607740
10	H	-4.699714	-2.493177	-0.168235
11	H	-6.415779	-0.798710	0.352554
12	C	-1.422334	0.744204	-0.225343
13	H	-1.259327	1.807732	-0.096460
14	C	-0.275995	-0.035078	-0.531773
15	H	-0.361208	-1.103195	-0.666794
16	C	0.922856	0.570464	-0.675644
17	H	1.013843	1.641557	-0.547641
18	C	2.152518	-0.172143	-1.067531
19	H	2.012575	-1.243770	-1.181562
20	S	3.498497	0.050111	0.140607
21	O	4.689475	-0.811085	-0.427173
22	O	3.787503	1.439239	0.367011
23	C	3.147907	-0.877163	1.607568

24	H	4.019022	-0.747665	2.245653
25	H	2.263635	-0.434070	2.057750
26	H	2.992645	-1.917788	1.339492
27	H	5.118529	-0.403630	-1.202585
28	H	2.578067	0.246996	-1.983119





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.13409	1.99901	4.11548	0.01959	6.13409
C	2	-0.06775	1.99910	4.05039	0.01826	6.06775
C	3	-0.08524	1.99908	4.06893	0.01723	6.08524
C	4	-0.22018	1.99914	4.20106	0.01998	6.22018
C	5	-0.21243	1.99916	4.19337	0.01990	6.21243
C	6	-0.03915	1.99919	4.02105	0.01892	6.03915
H	7	0.24550	0.00000	0.75286	0.00164	0.75450
H	8	0.24146	0.00000	0.75687	0.00168	0.75854
H	9	0.24663	0.00000	0.75178	0.00159	0.75337
H	10	0.24585	0.00000	0.75257	0.00158	0.75415
H	11	0.23964	0.00000	0.75904	0.00132	0.76036
C	12	0.08630	1.99910	3.89591	0.01869	5.91370
H	13	0.25047	0.00000	0.74765	0.00188	0.74953
C	14	-0.24301	1.99901	4.22356	0.02044	6.24301
H	15	0.25291	0.00000	0.74387	0.00322	0.74709
C	16	-0.03488	1.99911	4.01691	0.01886	6.03488
H	17	0.25600	0.00000	0.74184	0.00216	0.74400
C	18	-0.61623	1.99910	4.58881	0.02833	6.61623
H	19	0.28467	0.00000	0.71328	0.00205	0.71533
S	20	2.07193	9.99855	3.76735	0.16216	13.92807
O	21	-0.84981	1.99977	6.82116	0.02887	8.84981
O	22	-0.86719	1.99978	6.82718	0.04023	8.86719
C	23	-0.78690	1.99922	4.76692	0.02076	6.78690
H	24	0.28531	0.00000	0.71219	0.00250	0.71469
H	25	0.27558	0.00000	0.72305	0.00137	0.72442
H	26	0.27955	0.00000	0.71903	0.00141	0.72045
H	27	0.58793	0.00000	0.40929	0.00278	0.41207
H	28	0.30712	0.00000	0.69019	0.00268	0.69288
* Total *		2.00000	35.98832	73.53161	0.48007	110.00000

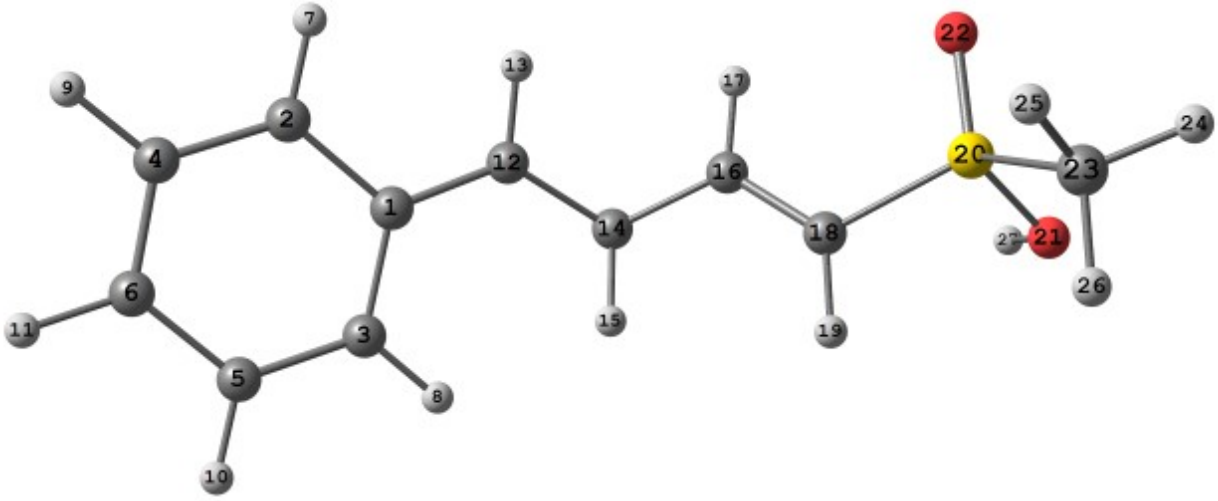
B8

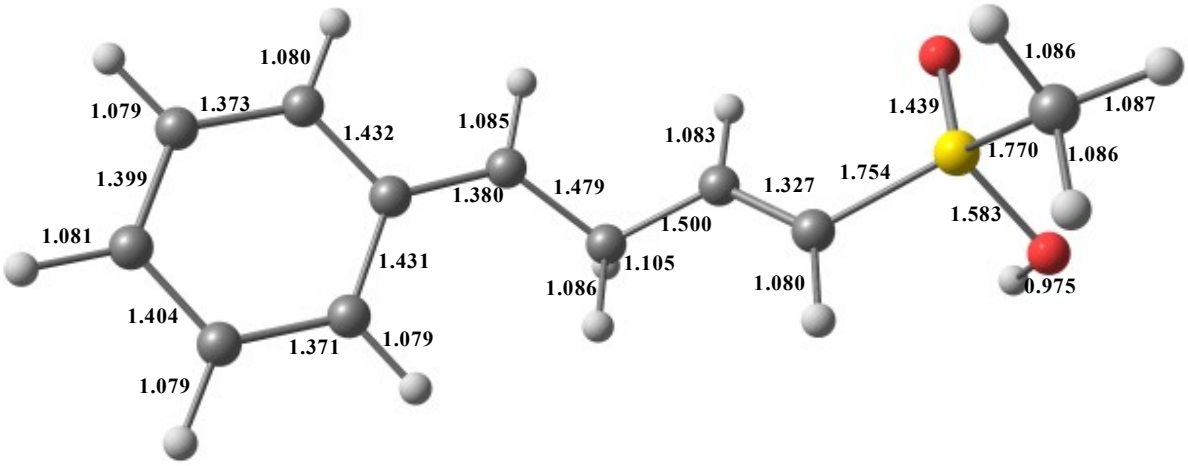
Energy E(B3LYP) = -975.97963567 h, G^{298} = -975.794459 h, μ=3.07 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.752120	0.228991	-0.202159
2	C	-3.660084	1.302884	0.069395
3	C	-3.214234	-1.120365	-0.086124
4	C	-4.958224	1.038170	0.430556
5	C	-4.514696	-1.365586	0.271356
6	C	-5.382090	-0.291648	0.529651
7	H	-3.306924	2.320110	-0.018117
8	H	-2.544907	-1.943873	-0.279322
9	H	-5.647137	1.843039	0.635840
10	H	-4.875226	-2.378976	0.359862
11	H	-6.403957	-0.499452	0.815304

12	C	-1.467978	0.560761	-0.583974
13	H	-1.237607	1.619460	-0.637788
14	C	-0.382552	-0.361030	-0.982329
15	H	-0.524126	-1.375622	-0.623111
16	C	0.989980	0.161523	-0.677626
17	H	1.215872	1.179581	-0.970979
18	C	1.926944	-0.583668	-0.104958
19	H	1.825291	-1.605324	0.230745
20	S	3.526524	0.099571	0.120460
21	O	4.525354	-0.977285	-0.471078
22	O	3.652883	1.420754	-0.434751
23	C	3.992570	-0.018918	1.824169
24	H	5.033491	0.291746	1.873944
25	H	3.346061	0.664930	2.366803
26	H	3.863183	-1.046323	2.151142
27	H	4.397855	-1.106213	-1.428978
28	H	-0.457245	-0.410648	-2.083807





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.16873	1.99898	4.15011	0.01963	6.16873
C	2	-0.04031	1.99910	4.02282	0.01839	6.04031
C	3	-0.06334	1.99908	4.04705	0.01721	6.06334
C	4	-0.22652	1.99914	4.20730	0.02007	6.22652
C	5	-0.21543	1.99915	4.19630	0.01998	6.21543
C	6	-0.02981	1.99919	4.01185	0.01877	6.02981
H	7	0.24894	0.00000	0.74939	0.00167	0.75106
H	8	0.24300	0.00000	0.75528	0.00172	0.75700
H	9	0.25140	0.00000	0.74701	0.00159	0.74860
H	10	0.25053	0.00000	0.74789	0.00158	0.74947
H	11	0.24536	0.00000	0.75335	0.00129	0.75464
C	12	0.20515	1.99909	3.77980	0.01597	5.79485
H	13	0.24718	0.00000	0.75094	0.00189	0.75282
C	14	-0.51820	1.99915	4.49878	0.02027	6.51820
H	15	0.25890	0.00000	0.73835	0.00276	0.74110
C	16	-0.04169	1.99903	4.02186	0.02080	6.04169
H	17	0.25958	0.00000	0.73827	0.00214	0.74042
C	18	-0.47216	1.99880	4.44928	0.02408	6.47216
H	19	0.28851	0.00000	0.70904	0.00245	0.71149
S	20	2.06906	9.99841	3.76405	0.16849	13.93094
O	21	-0.86408	1.99978	6.83617	0.02813	8.86408

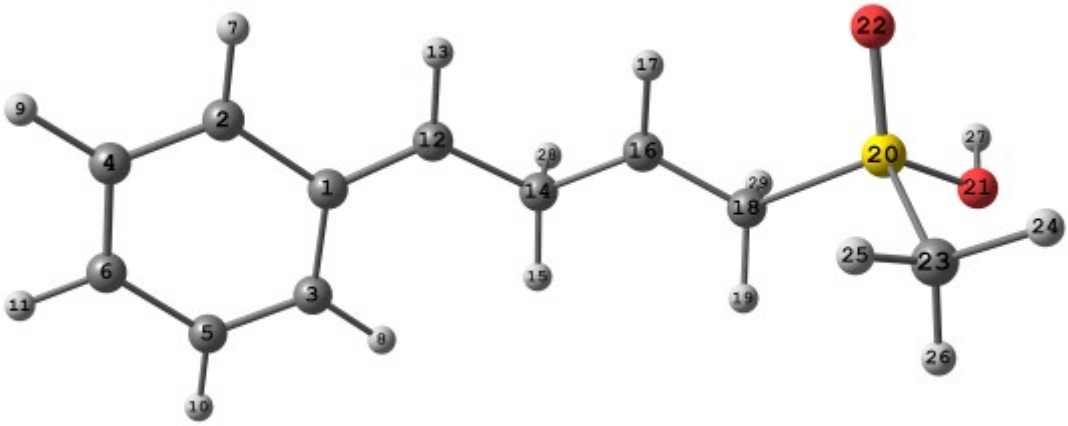
O	22	-0.88003	1.99978	6.84156	0.03870	8.88003
C	23	-0.77551	1.99922	4.75626	0.02003	6.77551
H	24	0.27746	0.00000	0.72024	0.00229	0.72254
H	25	0.27276	0.00000	0.72591	0.00133	0.72724
H	26	0.27404	0.00000	0.72462	0.00134	0.72596
H	27	0.58357	0.00000	0.41367	0.00276	0.41643
H	28	0.32038	0.00000	0.67792	0.00170	0.67962
* Total *		2.00000	35.98791	73.53506	0.47704	110.00000

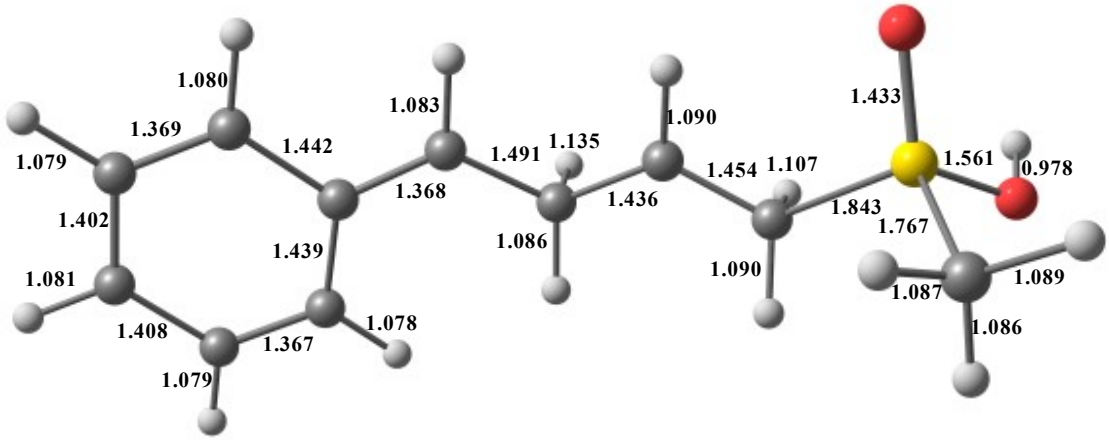
D8

Energy E(B3LYP) = -976.302976402 h, G^{298} = -976.109017 h, μ=6.09 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.810687	0.232763	-0.167173
2	C	-3.741206	1.309860	0.061707
3	C	-3.275250	-1.126056	-0.072099
4	C	-5.049426	1.038519	0.358397
5	C	-4.586153	-1.372060	0.225409
6	C	-5.468971	-0.296919	0.439723
7	H	-3.387305	2.327746	-0.009730
8	H	-2.599538	-1.950864	-0.234147
9	H	-5.753726	1.838135	0.527530
10	H	-4.949915	-2.385134	0.298853
11	H	-6.502628	-0.508909	0.675662
12	C	-1.525111	0.584305	-0.474136
13	H	-1.289995	1.640369	-0.529103
14	C	-0.405552	-0.350136	-0.783579
15	H	-0.543117	-1.396405	-0.525181
16	C	0.927493	0.142397	-0.579699
17	H	1.086780	1.220331	-0.548440
18	C	2.101771	-0.714513	-0.545830
19	H	1.961890	-1.688141	-0.076562
20	S	3.594792	0.127338	0.130489
21	O	4.793612	-0.684572	-0.453162
22	O	3.545182	1.526377	-0.175666
23	C	3.736651	-0.294293	1.840474
24	H	4.665891	0.167536	2.169867
25	H	2.876475	0.139782	2.344169
26	H	3.768920	-1.376718	1.928016
27	H	5.023749	-0.449564	-1.373707
28	H	-0.356428	-0.364919	-1.917006
29	H	2.350583	-0.908286	-1.606590





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.12966	1.99898	4.11117	0.01950	6.12966
C	2	-0.02018	1.99910	4.00286	0.01823	6.02018
C	3	-0.05316	1.99908	4.03710	0.01698	6.05316
C	4	-0.22448	1.99914	4.20529	0.02006	6.22448
C	5	-0.21155	1.99915	4.19229	0.02011	6.21155
C	6	0.01742	1.99920	3.96482	0.01856	5.98258
H	7	0.25405	0.00000	0.74430	0.00165	0.74595
H	8	0.24628	0.00000	0.75190	0.00182	0.75372

H	9	0.25763	0.00000	0.74081	0.00156	0.74237
H	10	0.25672	0.00000	0.74173	0.00155	0.74328
H	11	0.24929	0.00000	0.74946	0.00125	0.75071
C	12	0.13811	1.99904	3.84543	0.01742	5.86189
H	13	0.26877	0.00000	0.72933	0.00190	0.73123
C	14	-0.59410	1.99906	4.57166	0.02338	6.59410
H	15	0.31692	0.00000	0.68130	0.00178	0.68308
C	16	0.39511	1.99922	3.58925	0.01642	5.60489
H	17	0.29231	0.00000	0.70510	0.00259	0.70769
C	18	-0.71471	1.99896	4.68659	0.02916	6.71471
H	19	0.33571	0.00000	0.66226	0.00203	0.66429
S	20	2.08737	9.99858	3.74720	0.16685	13.91263
O	21	-0.84636	1.99977	6.81655	0.03004	8.84636
O	22	-0.83734	1.99978	6.79602	0.04155	8.83734
C	23	-0.77784	1.99922	4.75738	0.02124	6.77784
H	24	0.29476	0.00000	0.70288	0.00236	0.70524
H	25	0.28184	0.00000	0.71649	0.00167	0.71816
H	26	0.28716	0.00000	0.71147	0.00137	0.71284
H	27	0.60368	0.00000	0.39362	0.00271	0.39632
H	28	0.43343	0.00000	0.56468	0.00189	0.56657
H	29	0.39283	0.00000	0.60491	0.00226	0.60717
* Total *		3.00000	35.98828	73.52384	0.48789	110.00000

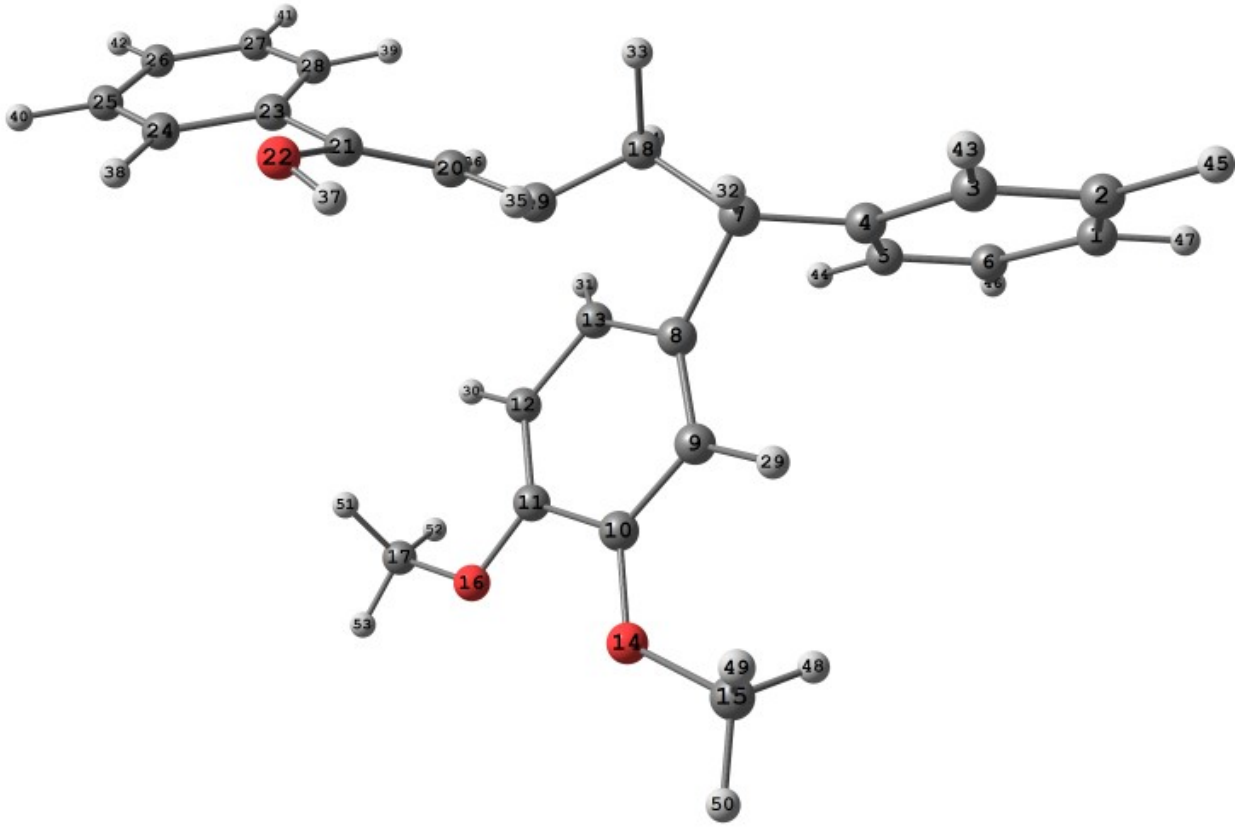
π -complex cis-3a

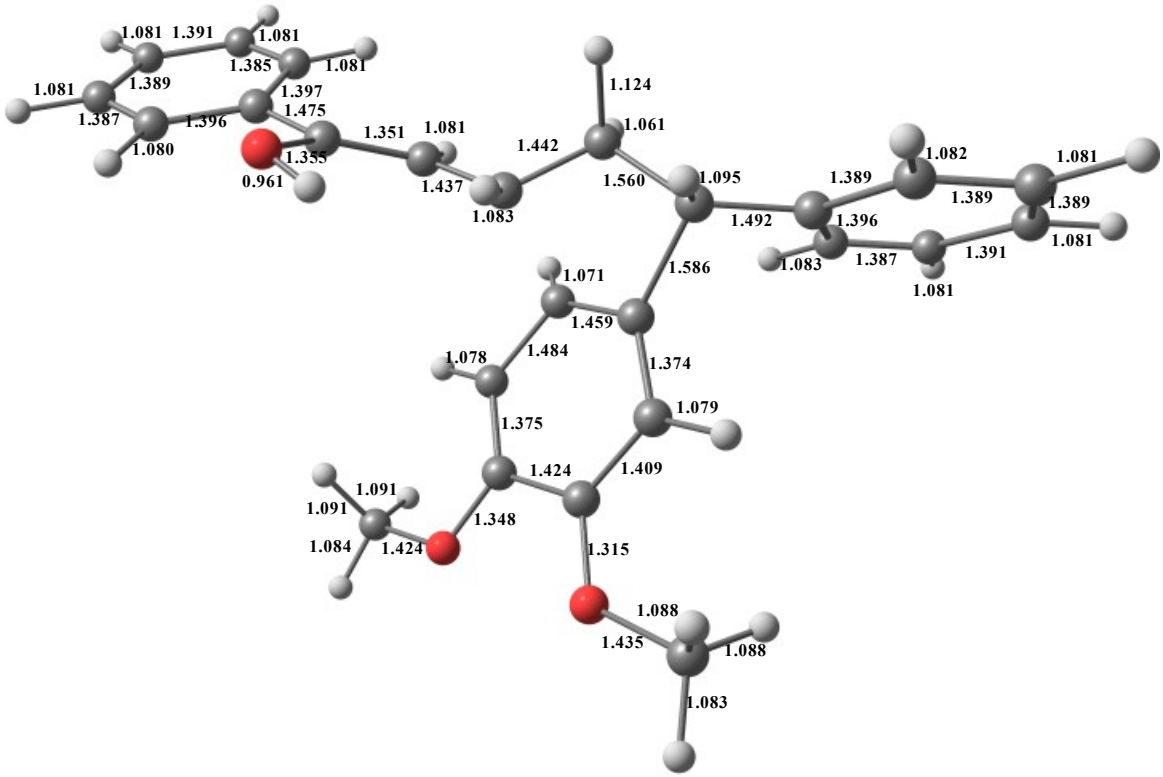
Energy E = -1192.96156761 h, G^{298} = -1192.575753 h, μ= 4.7 D

Cartesian coordinates, Å

1	C	-5.775216	-2.756283	-0.603500
2	C	-5.400384	-2.714883	0.733558
3	C	-4.132843	-2.274568	1.092101
4	C	-3.233284	-1.872889	0.112983
5	C	-3.611104	-1.913470	-1.230613
6	C	-4.877238	-2.352698	-1.586505
7	C	-1.879048	-1.401408	0.523548
8	C	-1.641755	0.087539	0.033062
9	C	-2.329209	1.220696	0.395016
10	C	-1.832215	2.506021	0.102467
11	C	-0.576328	2.655023	-0.551298
12	C	0.094171	1.529110	-0.968572
13	C	-0.435816	0.155716	-0.784790
14	O	-2.423694	3.628668	0.447607
15	C	-3.695300	3.583311	1.110778
16	O	-0.180456	3.935058	-0.695398
17	C	1.076621	4.142891	-1.330327
18	C	-0.442122	-1.886631	0.159649
19	C	0.450360	-0.808811	0.507077
20	C	1.812198	-0.955938	0.071861
21	C	2.902882	-0.638323	0.803528
22	O	2.883472	-0.069900	2.032992
23	C	4.281124	-0.861554	0.327508
24	C	5.317775	-0.081083	0.842292
25	C	6.616965	-0.257667	0.389172
26	C	6.897269	-1.217817	-0.575007
27	C	5.870568	-2.008086	-1.080912
28	C	4.571671	-1.835678	-0.630835
29	H	-3.220148	1.117671	0.995151
30	H	1.016398	1.619348	-1.519602
31	H	0.049176	-0.344064	-1.597997
32	H	-1.815156	-1.324120	1.614293
33	H	-0.145936	-2.743296	0.823912
34	H	-0.277637	-2.335548	-0.787966
35	H	0.324632	-0.539194	1.547977
36	H	1.970833	-1.338319	-0.926640
37	H	1.997081	0.195070	2.293871
38	H	5.101368	0.666118	1.591408
39	H	3.788140	-2.476456	-1.010295
40	H	7.410763	0.356206	0.790829
41	H	6.083687	-2.767678	-1.819663
42	H	7.910251	-1.356140	-0.925734
43	H	-3.843558	-2.241541	2.134344
44	H	-2.915456	-1.598219	-1.997921
45	H	-6.093442	-3.025447	1.502567
46	H	-5.163556	-2.379753	-2.628733
47	H	-6.762115	-3.100110	-0.879645

48	H	-4.415408	3.053578	0.490713
49	H	-3.588555	3.102726	2.080822
50	H	-3.988577	4.618291	1.233159
51	H	1.875153	3.657490	-0.767934
52	H	1.056675	3.762014	-2.352092
53	H	1.232362	5.215640	-1.339879



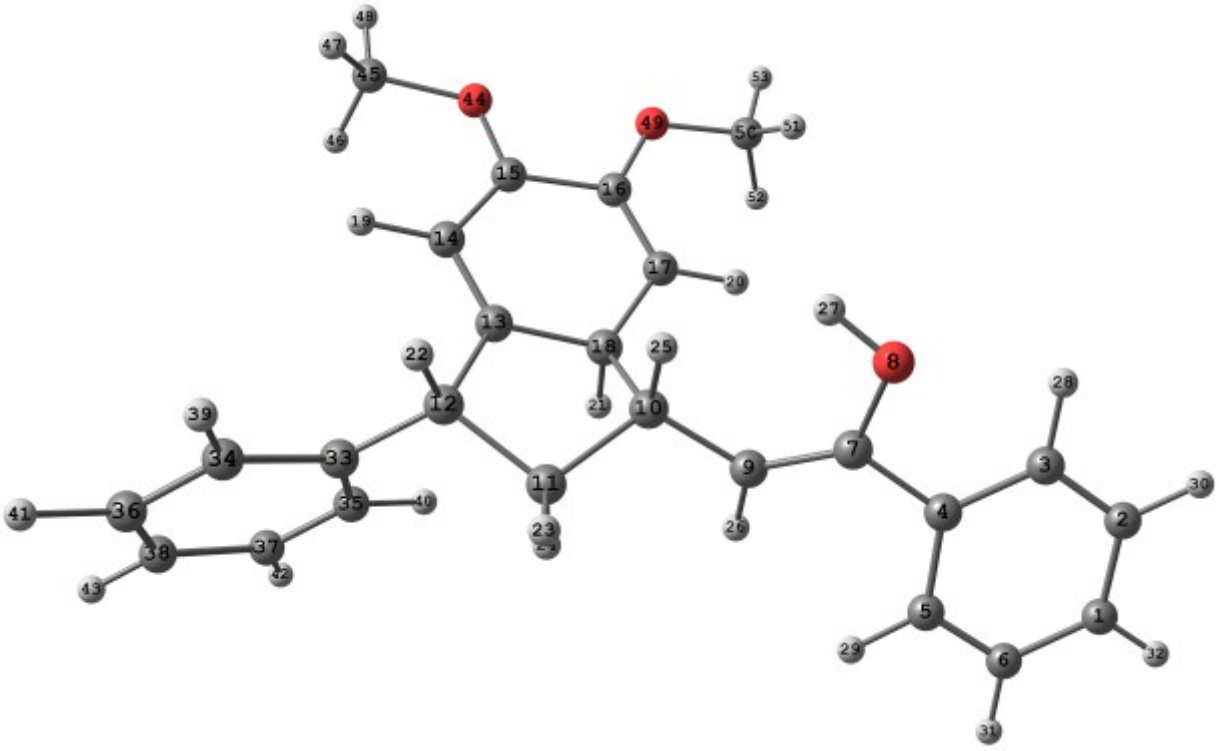


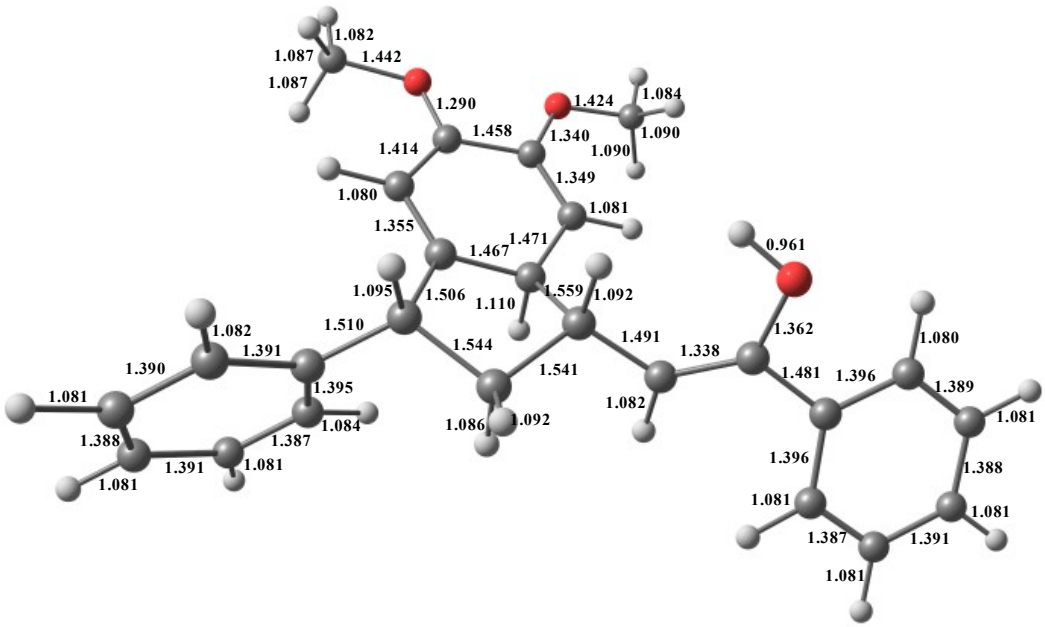
σ-complex cis-3a
Energy E = -1193.03112733 h, G^{298} = -1192.642382 h, μ=10.5 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	6.897434	-1.220144	-0.854482
2	C	6.699438	-0.137076	-0.008585
3	C	5.441161	0.114892	0.521821
4	C	4.361511	-0.712082	0.207081
5	C	4.572422	-1.808434	-0.631586
6	C	5.829411	-2.056637	-1.161566
7	C	3.021770	-0.410561	0.762602
8	O	3.106752	0.319850	1.909465
9	C	1.875068	-0.798541	0.192151
10	C	0.501411	-0.550830	0.716534
11	C	-0.427146	-1.780393	0.698137
12	C	-1.848211	-1.192822	0.839134
13	C	-1.714704	0.193299	0.266781
14	C	-2.655784	1.168069	0.247177
15	C	-2.243889	2.482488	-0.071311
16	C	-0.847510	2.813472	-0.329511
17	C	0.075183	1.830088	-0.347650
18	C	-0.332045	0.428878	-0.164193
19	H	-3.674453	0.968438	0.544053
20	H	1.113150	2.029941	-0.574007
21	H	-0.291123	-0.028918	-1.174400
22	H	-2.047178	-1.036843	1.904638
23	H	-0.198944	-2.490560	1.487793
24	H	-0.324970	-2.290924	-0.261637
25	H	0.515696	-0.151878	1.733365
26	H	1.937699	-1.327087	-0.749505
27	H	2.237121	0.613393	2.195254
28	H	5.289407	0.958415	1.178937
29	H	3.758429	-2.483830	-0.854565
30	H	7.525377	0.514769	0.240040
31	H	5.978441	-2.911227	-1.806710
32	H	7.877545	-1.417124	-1.266082
33	C	-2.978058	-2.013307	0.263144
34	C	-3.956805	-2.549850	1.093513
35	C	-3.049021	-2.248786	-1.109790
36	C	-4.988765	-3.316542	0.563710
37	C	-4.078872	-3.011899	-1.640301
38	C	-5.051600	-3.549062	-0.803335
39	H	-3.911153	-2.368787	2.159604
40	H	-2.297341	-1.834648	-1.771455
41	H	-5.741632	-3.729091	1.220841
42	H	-4.123506	-3.186981	-2.706142
43	H	-5.853562	-4.144286	-1.216970
44	O	-3.044098	3.493325	-0.111173
45	C	-4.456786	3.315434	0.119136
46	H	-4.858100	2.607917	-0.601311

47	H	-4.617177	2.973681	1.138228
48	H	-4.890566	4.296278	-0.025571
49	O	-0.639813	4.121644	-0.531219
50	C	0.706181	4.519916	-0.773331
51	H	1.339277	4.252117	0.072902
52	H	1.083533	4.054401	-1.683991
53	H	0.680554	5.596874	-0.891576





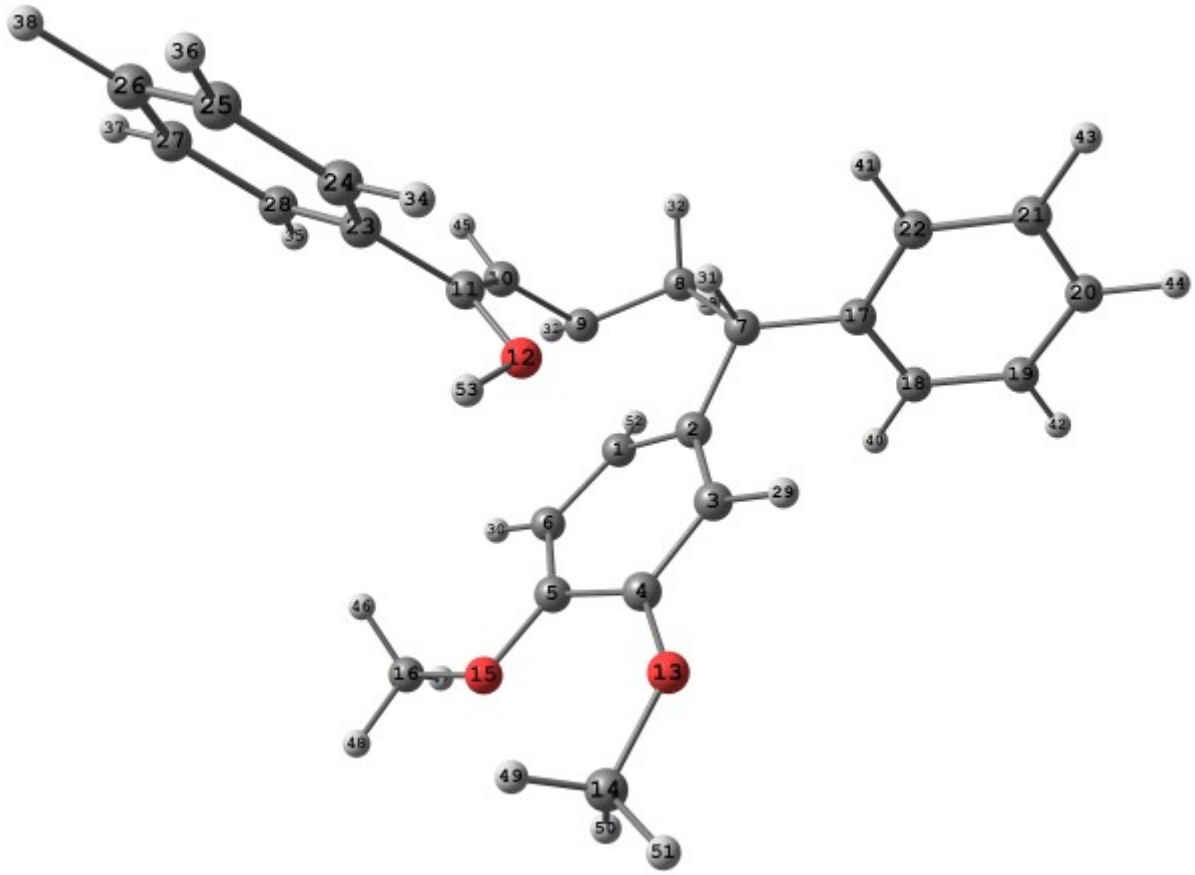
π -complex trans-3a

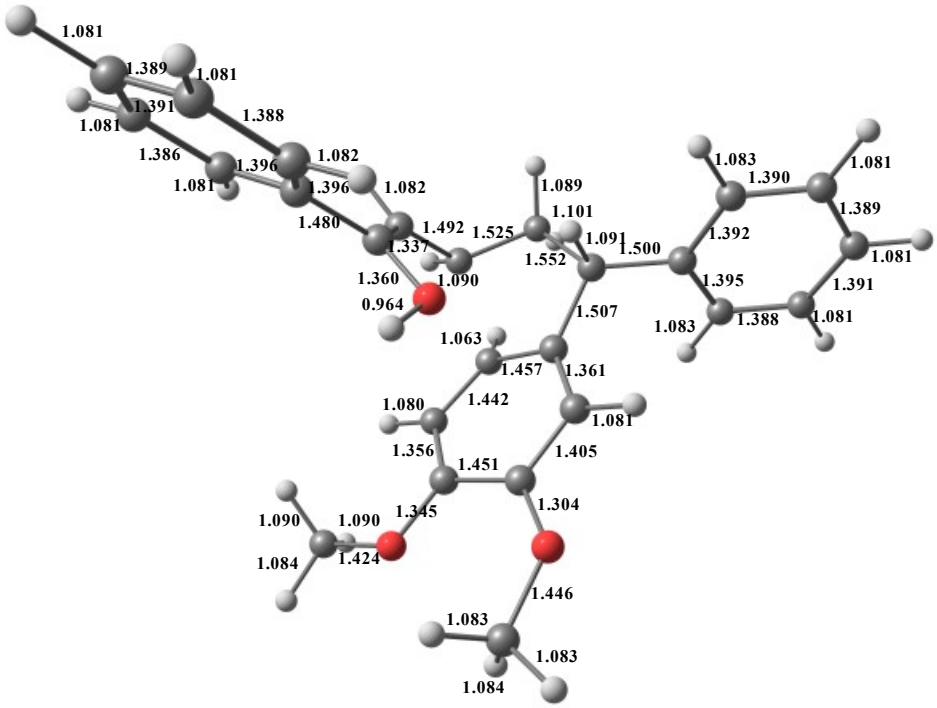
Energy E = -1192.9724723 h, G^{298} = -1192.584396 h, μ=7.2 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	0.677569	0.903619	1.703377
2	C	1.367390	0.404134	0.520837
3	C	1.433712	1.167967	-0.603224
4	C	0.695149	2.359999	-0.691730
5	C	-0.192734	2.754200	0.386711
6	C	-0.194921	2.039762	1.538773
7	C	1.836847	-1.024202	0.626124
8	C	1.256369	-1.541142	1.969858
9	C	-0.042613	-0.752988	2.096906
10	C	-1.321037	-1.187027	1.461892
11	C	-1.854570	-0.934522	0.262229
12	O	-1.167230	-0.229729	-0.675697
13	O	0.844340	3.003066	-1.815765
14	C	0.246925	4.266768	-2.184705
15	O	-0.960903	3.831327	0.142059
16	C	-1.861325	4.232110	1.169411
17	C	3.192863	-1.377992	0.090980
18	C	4.311265	-0.625241	0.448232
19	C	5.570471	-0.966125	-0.025583
20	C	5.725906	-2.067405	-0.860390
21	C	4.616705	-2.822622	-1.219387
22	C	3.356479	-2.478161	-0.746027
23	C	-3.179560	-1.447638	-0.153536
24	C	-3.408902	-1.775341	-1.491198
25	C	-4.643591	-2.268258	-1.891634
26	C	-5.662700	-2.435856	-0.963269
27	C	-5.443558	-2.104304	0.369648
28	C	-4.212920	-1.608575	0.771744
29	H	1.973994	0.853838	-1.485209
30	H	-0.785126	2.360107	2.384126
31	H	1.096400	-1.539204	-0.005609
32	H	1.020411	-2.603827	1.933718
33	H	-0.301004	-0.628586	3.148376
34	H	-2.614851	-1.668610	-2.218258
35	H	-4.056754	-1.324585	1.803263
36	H	-4.806150	-2.525530	-2.928829
37	H	-6.236724	-2.219816	1.094926
38	H	-6.624554	-2.816663	-1.276865
39	H	1.954282	-1.378044	2.791883
40	H	4.196363	0.233203	1.098815
41	H	2.493075	-3.066528	-1.029372
42	H	6.429606	-0.373003	0.255667
43	H	4.729748	-3.677742	-1.871158
44	H	6.706443	-2.333094	-1.230181
45	H	-1.893777	-1.846684	2.099662
46	H	-2.558524	3.426339	1.400736

47	H	-1.313358	4.521228	2.066307
48	H	-2.399930	5.085351	0.773250
49	H	-0.827598	4.160912	-2.271722
50	H	0.504404	5.025975	-1.455139
51	H	0.692692	4.489559	-3.146698
52	H	1.060171	0.542736	2.626953
53	H	-1.784205	0.198390	-1.279653





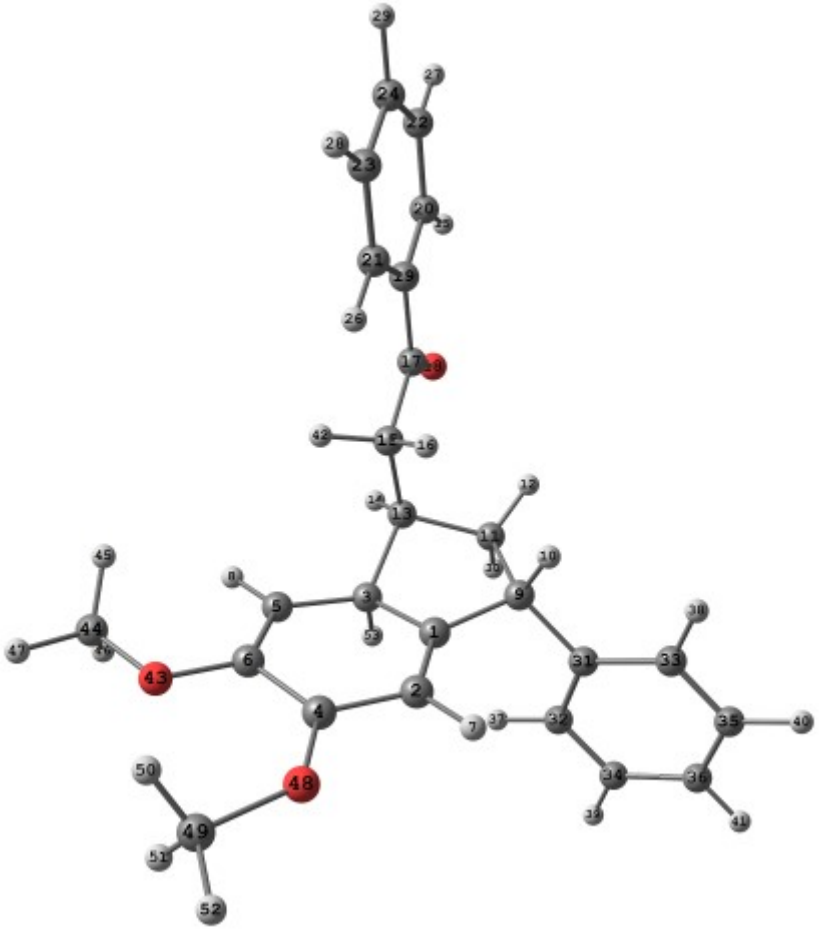
σ-complex trans-3a

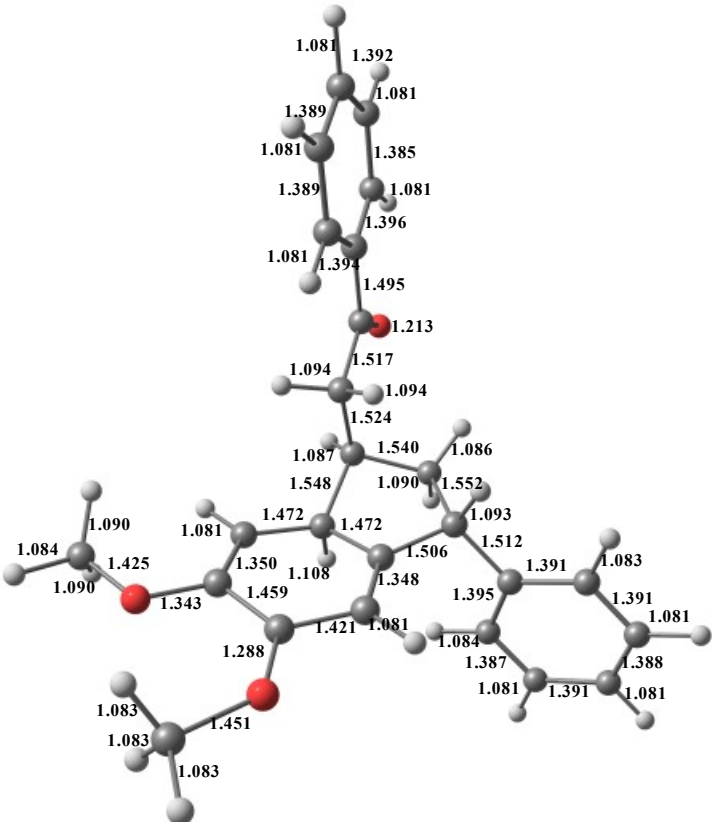
Energy E(B3LYP) = -1193.04042233 h, G^{298} = -1192.652419 h, μ=12.8 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.445527	0.060077	0.002147
2	C	-2.072143	0.892403	0.857589
3	C	-0.767853	0.557057	-1.205914
4	C	-1.993565	2.296896	0.653285
5	C	-0.570786	2.013360	-1.283818
6	C	-1.165773	2.854657	-0.411106
7	H	-2.606292	0.547529	1.732104
8	H	0.011670	2.399445	-2.108007
9	C	-1.219785	-1.422179	0.146816
10	H	-0.673172	-1.555178	1.084136
11	C	-0.284451	-1.760608	-1.044398
12	H	0.422078	-2.547066	-0.794074
13	C	0.404330	-0.433313	-1.413130
14	H	0.724793	-0.427635	-2.451836
15	C	1.590985	-0.100282	-0.517262
16	H	1.342829	-0.229803	0.540388
17	C	2.807970	-0.945445	-0.840944
18	O	2.782610	-1.745930	-1.751358
19	C	4.048011	-0.755003	-0.027394
20	C	5.169281	-1.525133	-0.340501
21	C	4.116693	0.165239	1.017999
22	C	6.342393	-1.377422	0.380199
23	C	5.293552	0.312806	1.740338
24	C	6.405272	-0.457124	1.422557

25	H	5.103377	-2.234114	-1.153502
26	H	3.260674	0.772383	1.276452
27	H	7.208138	-1.975362	0.132326
28	H	5.342458	1.027876	2.549213
29	H	7.321444	-0.340496	1.984753
30	H	-0.883141	-2.102280	-1.889264
31	C	-2.489721	-2.239442	0.227909
32	C	-3.480827	-2.093488	-0.743077
33	C	-2.681431	-3.157293	1.255536
34	C	-4.640089	-2.852853	-0.688118
35	C	-3.841747	-3.922505	1.310743
36	C	-4.822692	-3.772033	0.339922
37	H	-3.350127	-1.380034	-1.548329
38	H	-1.919699	-3.276604	2.015396
39	H	-5.401075	-2.727266	-1.445822
40	H	-3.976987	-4.634882	2.112685
41	H	-5.725339	-4.365406	0.382423
42	H	1.879760	0.948517	-0.630089
43	O	-1.067619	4.193855	-0.418301
44	C	-0.245944	4.774161	-1.427279
45	H	0.775937	4.404014	-1.342451
46	H	-0.644751	4.551055	-2.416890
47	H	-0.270867	5.842799	-1.249254
48	O	-2.671958	2.986999	1.503822
49	C	-2.822035	4.429135	1.556373
50	H	-1.869406	4.886372	1.793848
51	H	-3.205822	4.792976	0.611168
52	H	-3.539493	4.580591	2.353035
53	H	-1.475954	0.313174	-2.022542

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1.083
1.083

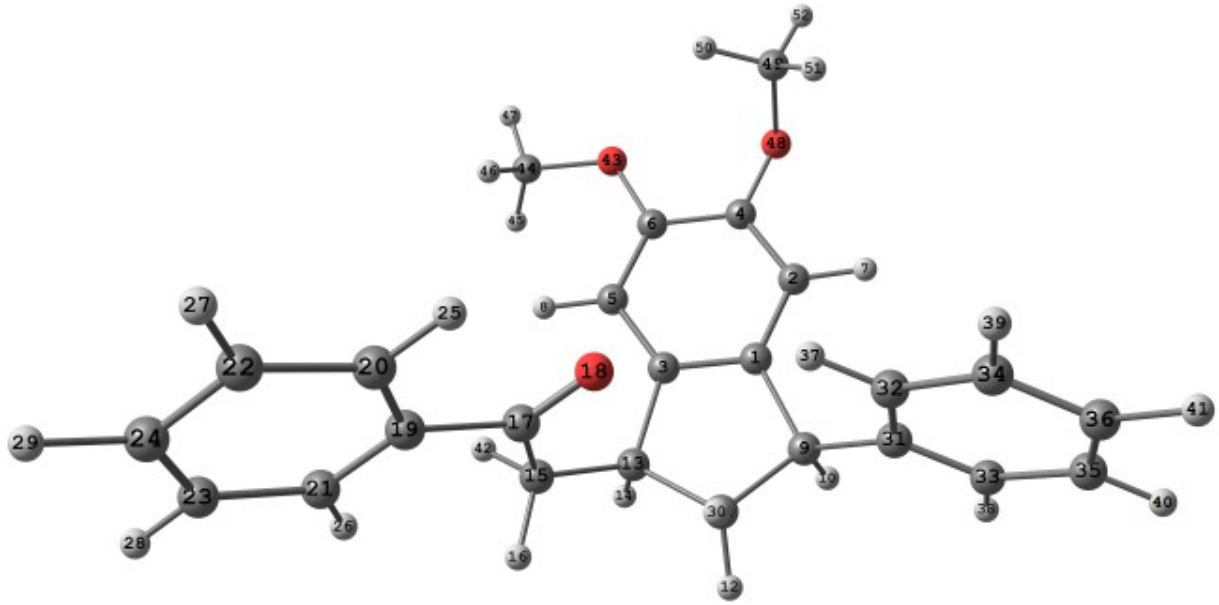
cis-3a

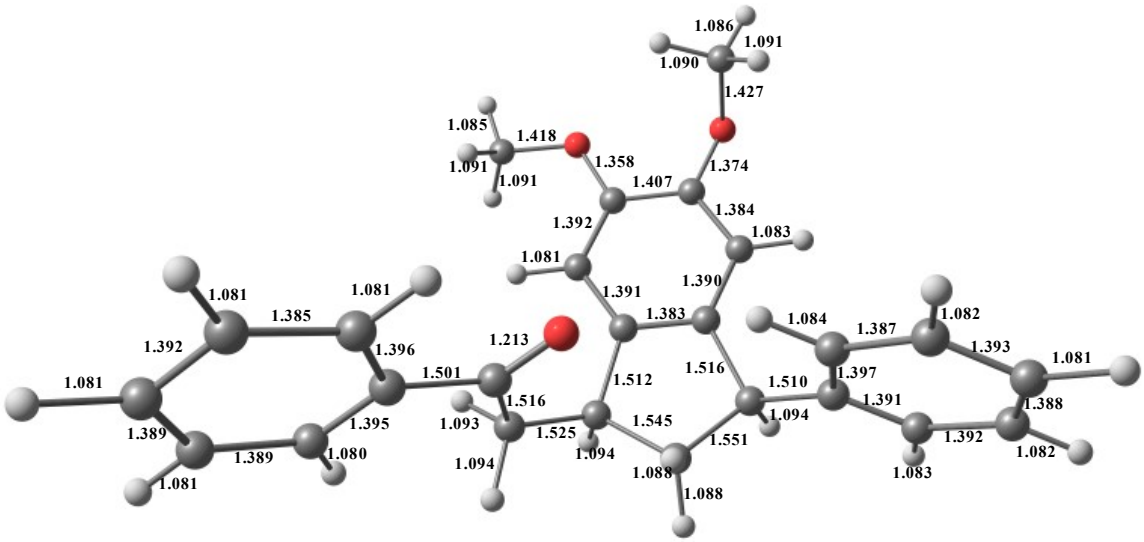
Energy E = -1192.65034289 h, G^{298} = -1192.274457 h, μ=7.1 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.667725	0.320606	-0.931433
2	C	2.532928	1.156105	-0.235153
3	C	0.399519	0.759419	-1.264792
4	C	2.118075	2.429205	0.113173
5	C	-0.031513	2.038111	-0.927591
6	C	0.831713	2.881230	-0.234426
7	H	3.526248	0.835961	0.054824
8	H	-1.024130	2.369414	-1.196778
9	C	1.917788	-1.088801	-1.431472
10	H	2.524508	-1.038560	-2.339996
11	C	0.489569	-1.574973	-1.793352
12	H	0.492751	-2.232363	-2.660811
13	C	-0.355537	-0.303641	-2.029835
14	H	-0.312369	-0.046163	-3.092440
15	C	-1.834485	-0.440959	-1.682089
16	H	-2.277478	-1.252282	-2.266617
17	C	-2.145025	-0.700344	-0.221010
18	O	-1.271760	-0.811254	0.613290
19	C	-3.586145	-0.819626	0.180304
20	C	-3.882519	-1.046884	1.525063
21	C	-4.628130	-0.711355	-0.740301
22	C	-5.197883	-1.163957	1.943623
23	C	-5.946990	-0.829201	-0.320650
24	C	-6.232968	-1.054890	1.019566
25	H	-3.068411	-1.130003	2.230900
26	H	-4.423481	-0.535414	-1.786449
27	H	-5.419255	-1.340125	2.986991
28	H	-6.748921	-0.743238	-1.040154
29	H	-7.259948	-1.145715	1.345340
30	H	0.081381	-2.129507	-0.950551
31	C	2.630204	-1.979347	-0.441387
32	C	2.111244	-2.146792	0.845008
33	C	3.801660	-2.648178	-0.780974
34	C	2.749344	-2.964938	1.765065
35	C	4.444398	-3.471975	0.139411
36	C	3.920513	-3.631969	1.414477
37	H	1.198606	-1.627731	1.115653
38	H	4.216167	-2.524656	-1.773888
39	H	2.335425	-3.084780	2.757285
40	H	5.353341	-3.986242	-0.141746
41	H	4.417987	-4.270259	2.131481
42	H	-2.379454	0.458916	-1.979776
43	O	0.528496	4.148996	0.146866
44	C	-0.768408	4.627302	-0.169704
45	H	-0.925620	4.644908	-1.249063
46	H	-1.537164	4.012492	0.300912

47	H	-0.820737	5.637794	0.221981
48	O	2.977824	3.271940	0.775212
49	C	2.701581	3.371939	2.171585
50	H	1.689990	3.741923	2.337986
51	H	2.823122	2.397992	2.649056
52	H	3.421023	4.073665	2.584303





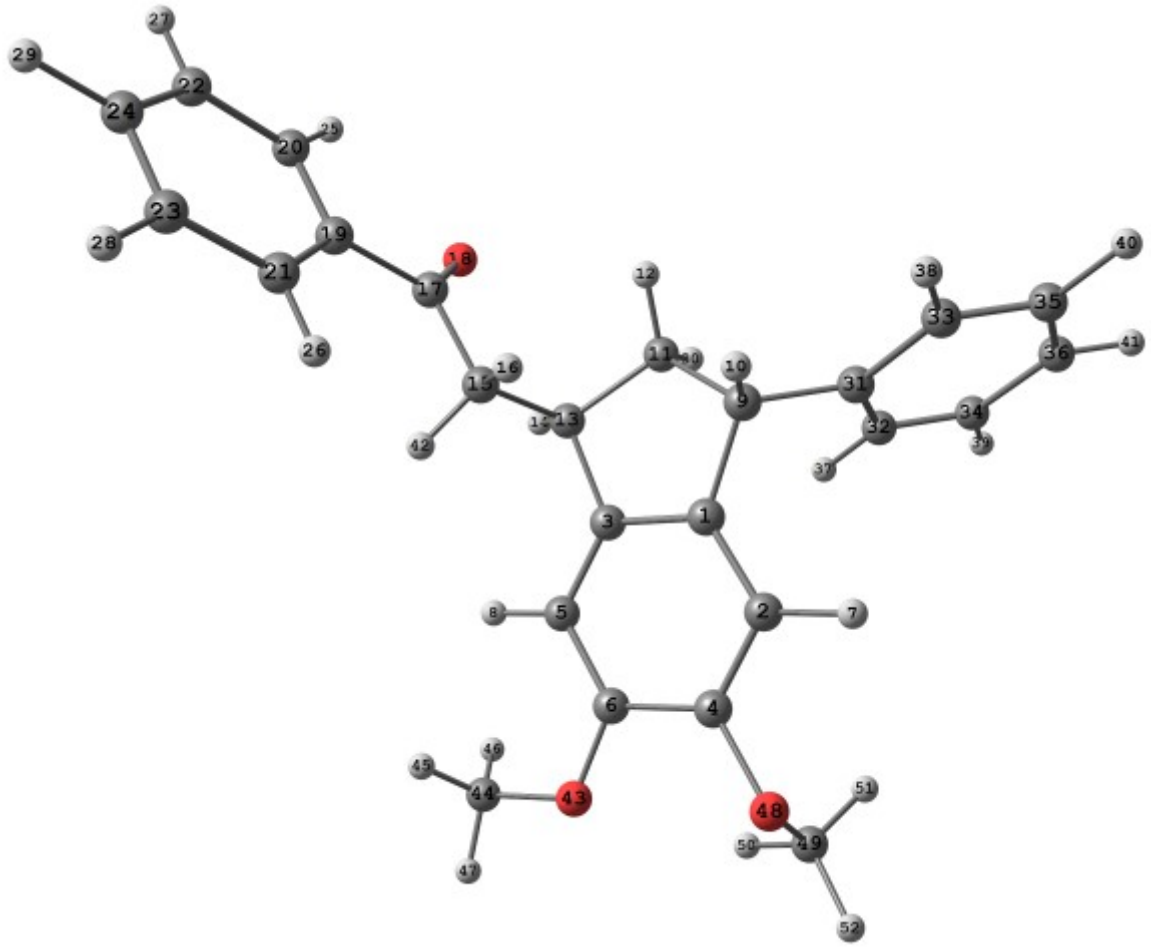
trans-3a

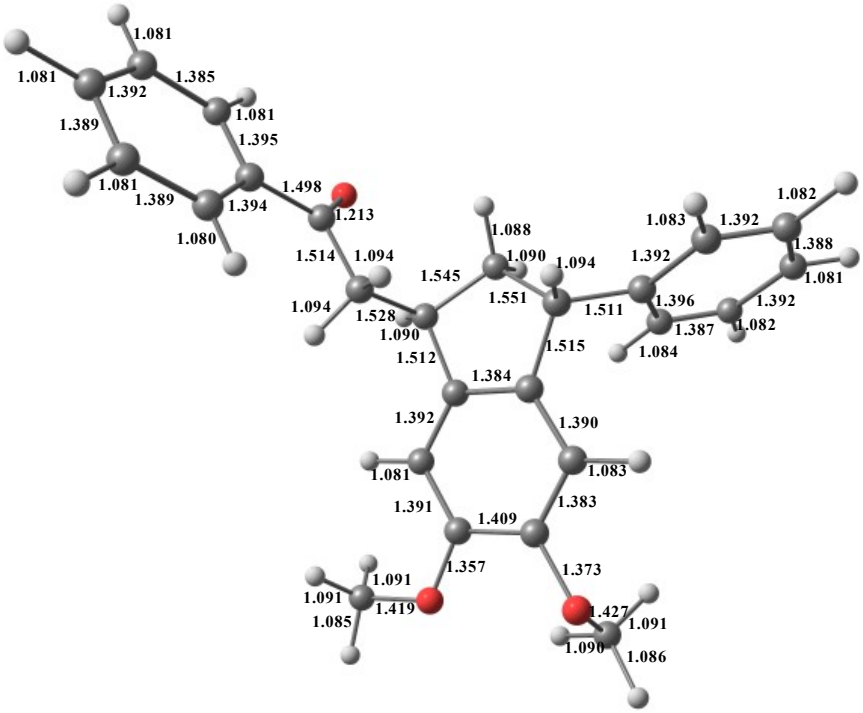
Energy E = -1192.65184283 h, G^{298} = -1192.275523 h, μ=3.4 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.382516	0.008389	0.254839
2	C	-2.498224	0.570182	0.865489
3	C	-0.538222	0.796910	-0.506776
4	C	-2.752325	1.919847	0.706178
5	C	-0.778190	2.158082	-0.674443
6	C	-1.893653	2.725603	-0.066989
7	H	-3.182495	-0.021569	1.461045
8	H	-0.107864	2.757953	-1.273350
9	C	-0.895342	-1.425660	0.306691
10	H	-0.370098	-1.588236	1.252179
11	C	0.122193	-1.460294	-0.863976
12	H	0.929797	-2.168830	-0.689440
13	C	0.624097	-0.009687	-1.039882
14	H	0.821629	0.212398	-2.088131
15	C	1.892573	0.281347	-0.239287
16	H	1.776055	-0.051817	0.796544
17	C	3.131175	-0.364523	-0.823356
18	O	3.081486	-1.005249	-1.852407
19	C	4.434587	-0.180970	-0.107366
20	C	5.575528	-0.790543	-0.630861
21	C	4.537985	0.582111	1.055067
22	C	6.800845	-0.639971	-0.002170
23	C	5.766879	0.734439	1.684188
24	C	6.897687	0.124334	1.156920
25	H	5.485771	-1.379122	-1.532807
26	H	3.667508	1.063419	1.477055
27	H	7.681034	-1.114351	-0.412821
28	H	5.839154	1.328755	2.584029
29	H	7.854340	0.243932	1.646555
30	H	-0.400431	-1.768162	-1.770151
31	C	-1.988126	-2.463137	0.199546
32	C	-2.923250	-2.392917	-0.834909
33	C	-2.087463	-3.505754	1.115891
34	C	-3.928053	-3.341481	-0.951626
35	C	-3.093992	-4.461055	1.002924
36	C	-4.016316	-4.381796	-0.030930
37	H	-2.864401	-1.581221	-1.550346
38	H	-1.372452	-3.571074	1.926596
39	H	-4.645184	-3.269727	-1.758022
40	H	-3.156638	-5.263695	1.725093
41	H	-4.799858	-5.121499	-0.120109
42	H	2.073819	1.358775	-0.187888
43	O	-2.237951	4.034929	-0.156787
44	C	-1.398120	4.873570	-0.933730
45	H	-0.385982	4.896425	-0.527457
46	H	-1.367618	4.540780	-1.972227

47	H	-1.833581	5.865957	-0.881450
48	O	-3.833808	2.491713	1.329373
49	C	-4.946267	2.684545	0.456619
50	H	-4.668339	3.315112	-0.387893
51	H	-5.310935	1.721874	0.094086
52	H	-5.721986	3.173362	1.039171

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