Supporting Information

Hydroarylation of Unsaturated Carbon-Carbon Bonds in Cross-Conjugated Enynones under the Action of Superacid CF_3SO_3H or Acidic Zeolite HUSY. Reaction Mechanism and DFT Study on Cationic Intermediate Species

Maiia I. Aleksandrova,[a] Stanislav V. Lozovskiy, [a] Steve Saulnier, [a] Alexander A. Golovanov,[b] Irina A. Boyarskaya,[a] and Aleksander V. Vasilyev*[a,c]

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

[b] Department of Chemistry, Chemical Processes and Technologies, Togliatti State University, Belorusskaya ul. 14, Togliatti, 445667, Russia

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

*E-mail : aleksvasil@mail.ru, a.vasilyev@spbu.ru

Contents

I. ^{1}H, ^{13}C, ^{19}F NMR spectra of compounds

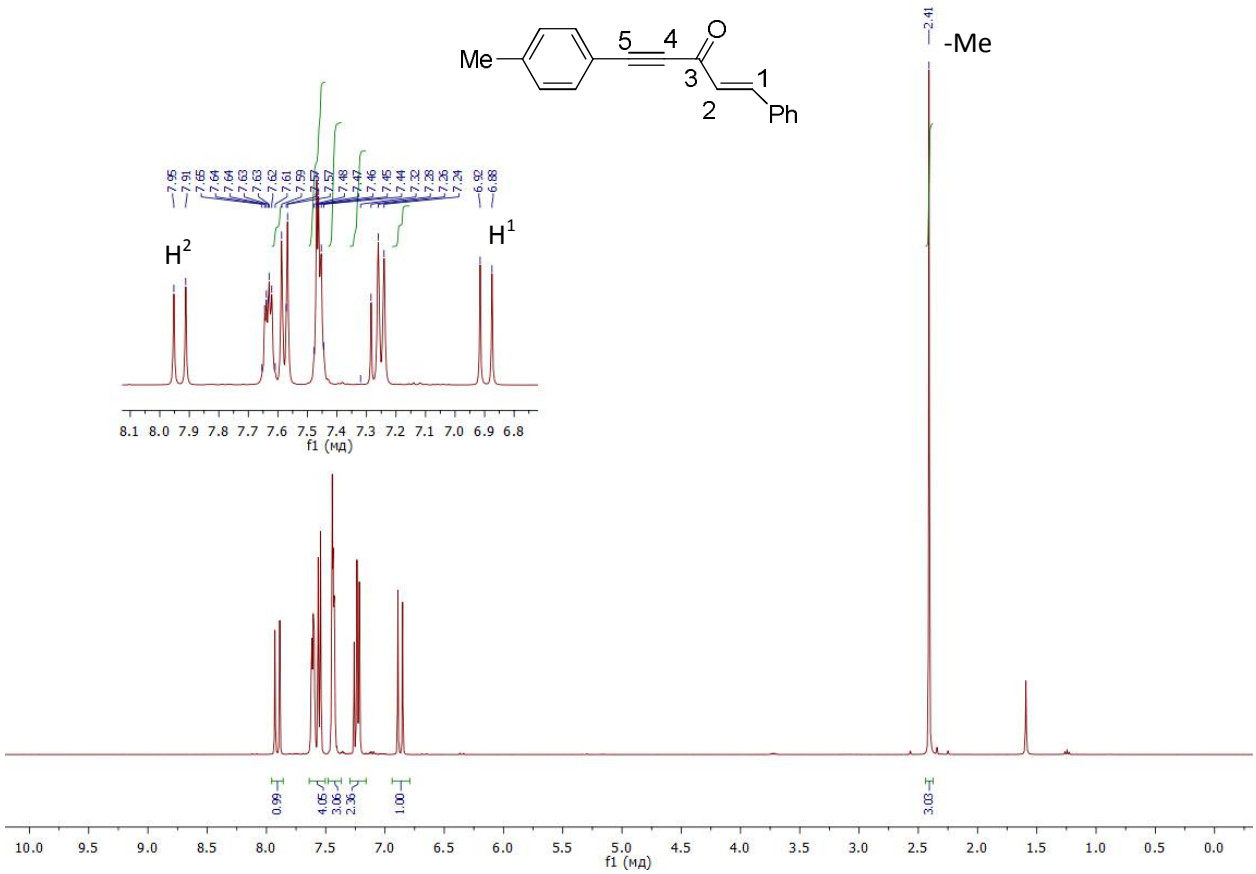


Fig.. S1. ^{1}H NMR Spectra of compound **1b** at 20 °C (400 МГц, $CDCl_3$).

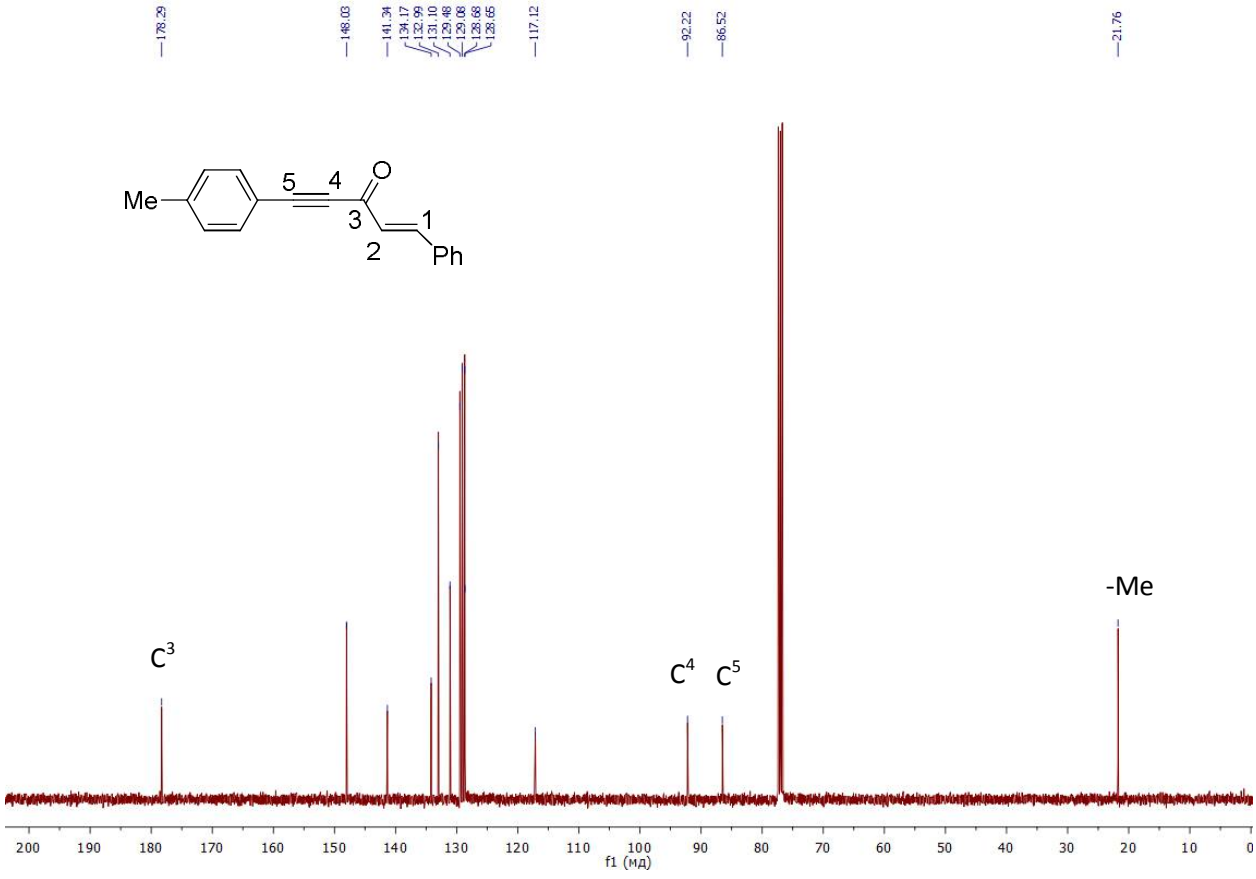


Fig. S2. ^{13}C NMR Spectra of compound **1b** at 20 °C (101МГц, $CDCl_3$).

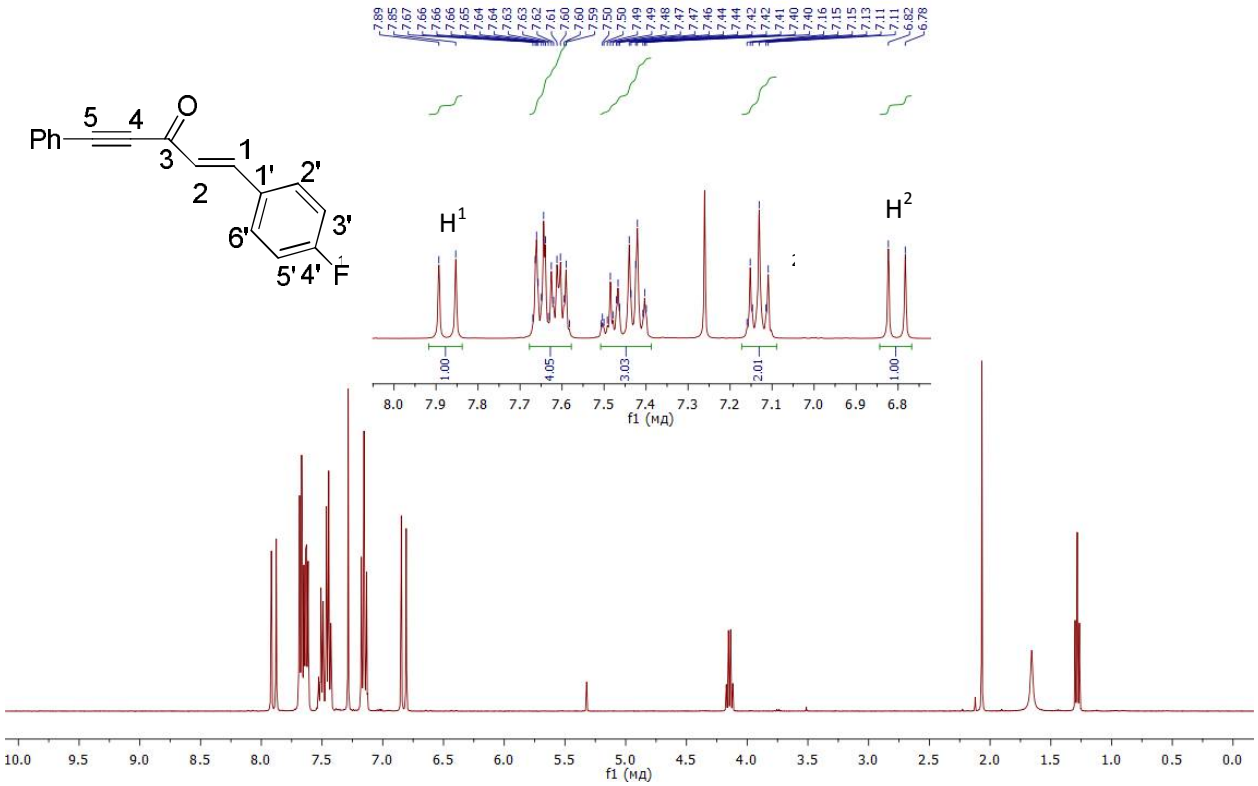


Fig. S3. ^{1}H NMR Spectra of compound **1g** at 20 °C (400 МГц, $CDCl_3$).

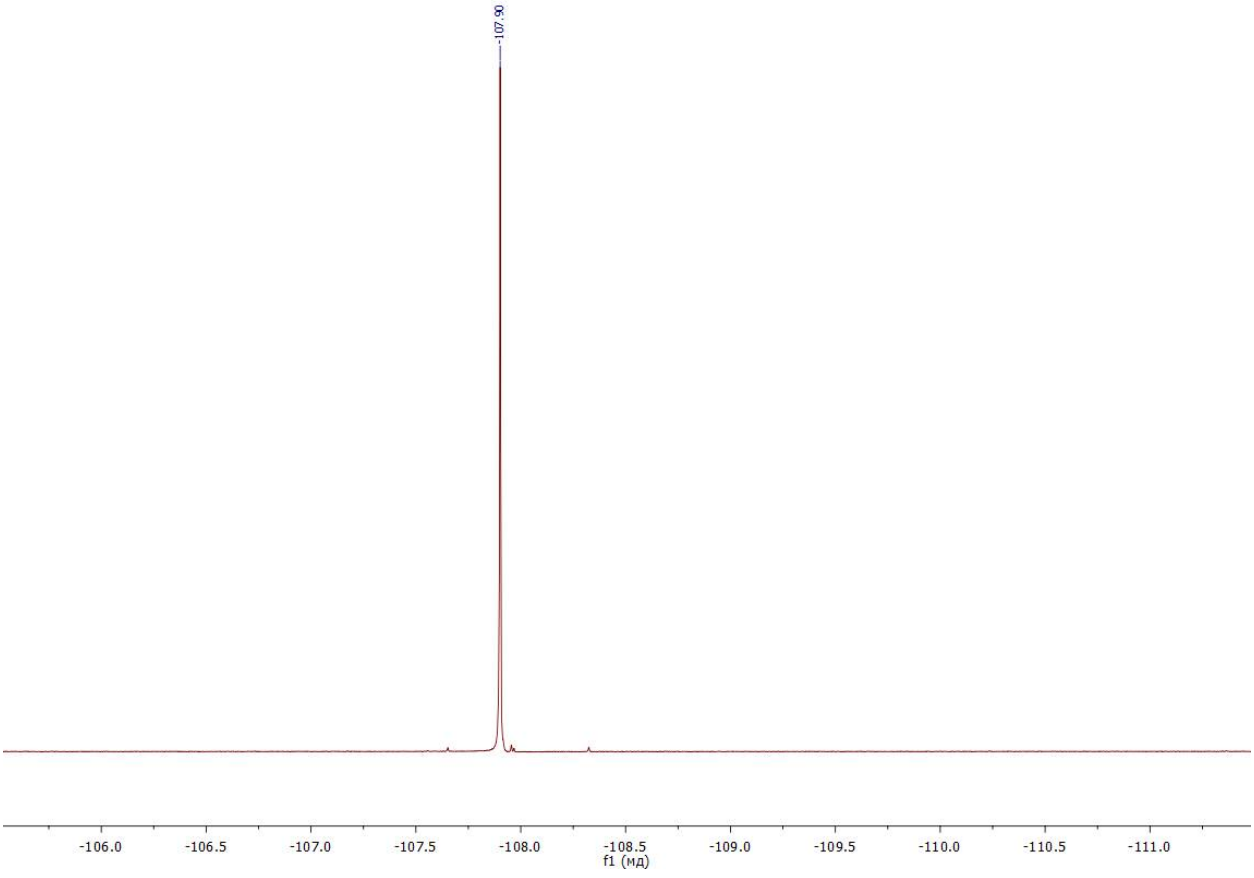


Fig. S4. $^{19}F\{^{1}H\}$ NMR Spectra of compound **1g** at 20 °C (400 МГц, $CDCl_3$).

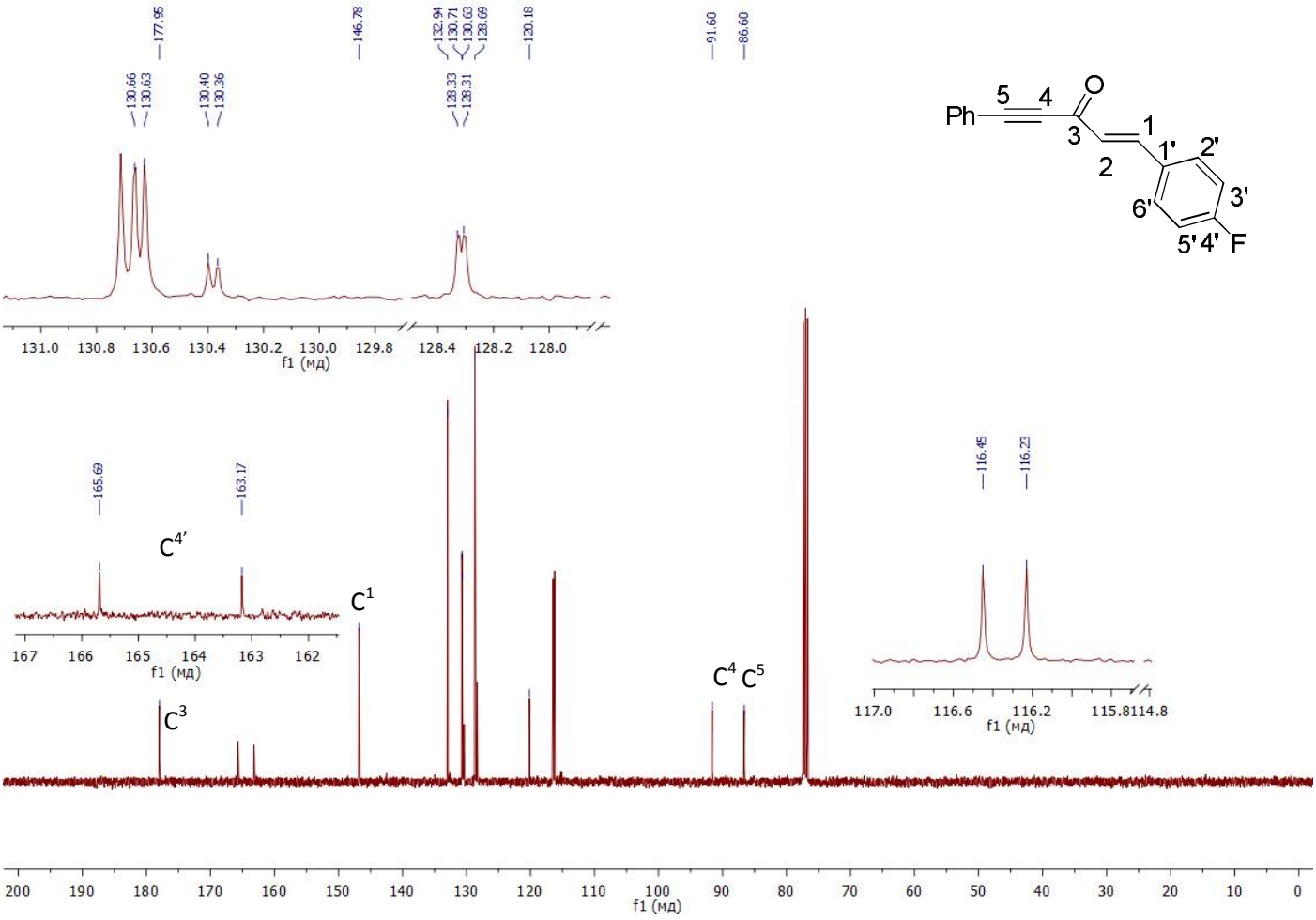


Fig. S5. ^{13}C NMR Spectra of compound **1g** at 20 °C (101МГц, $CDCl_3$).

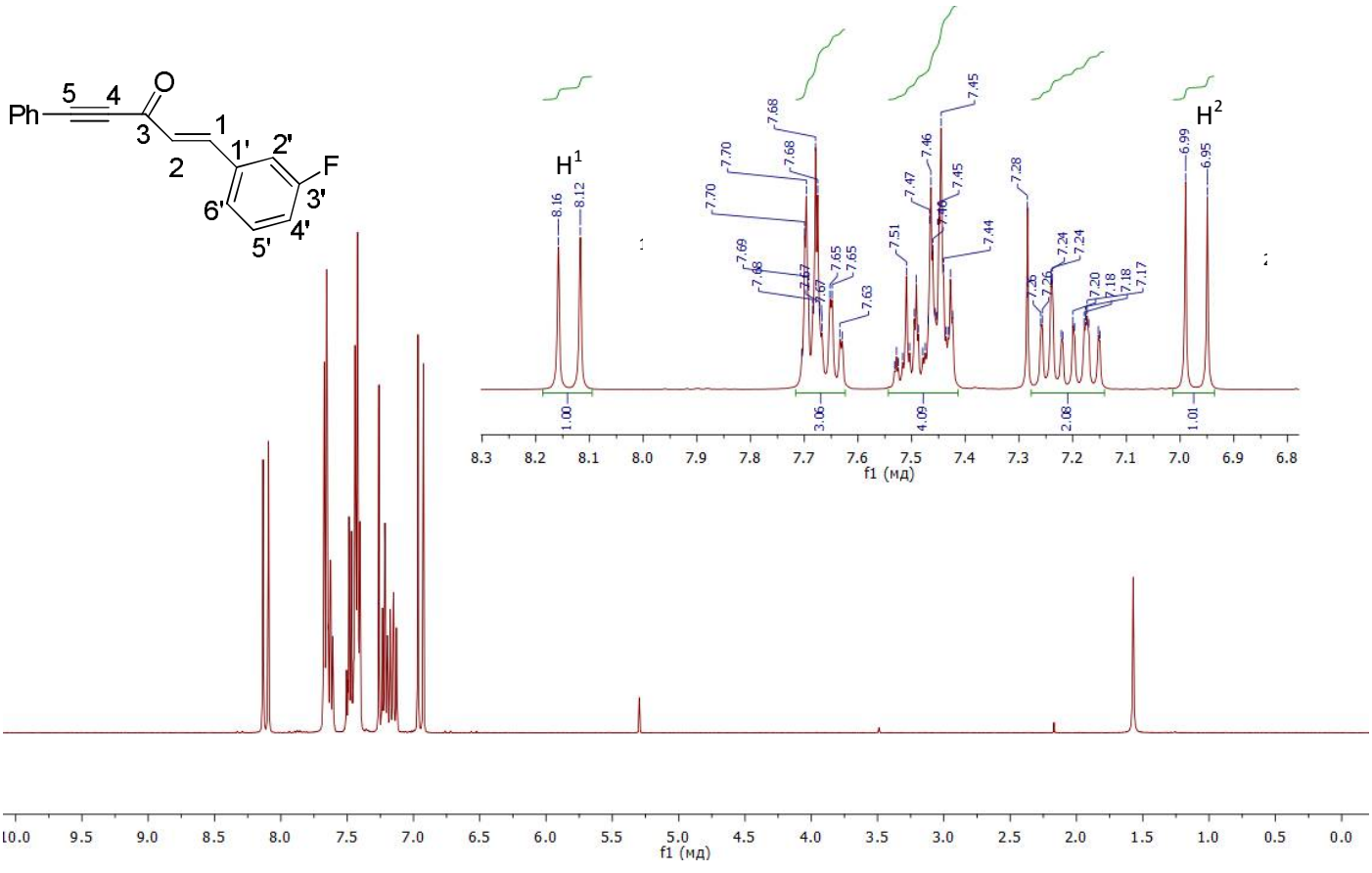


Fig. S6. ^{1}H NMR Spectra of compound **1h** at 20 °C (400 МГц, $CDCl_3$).

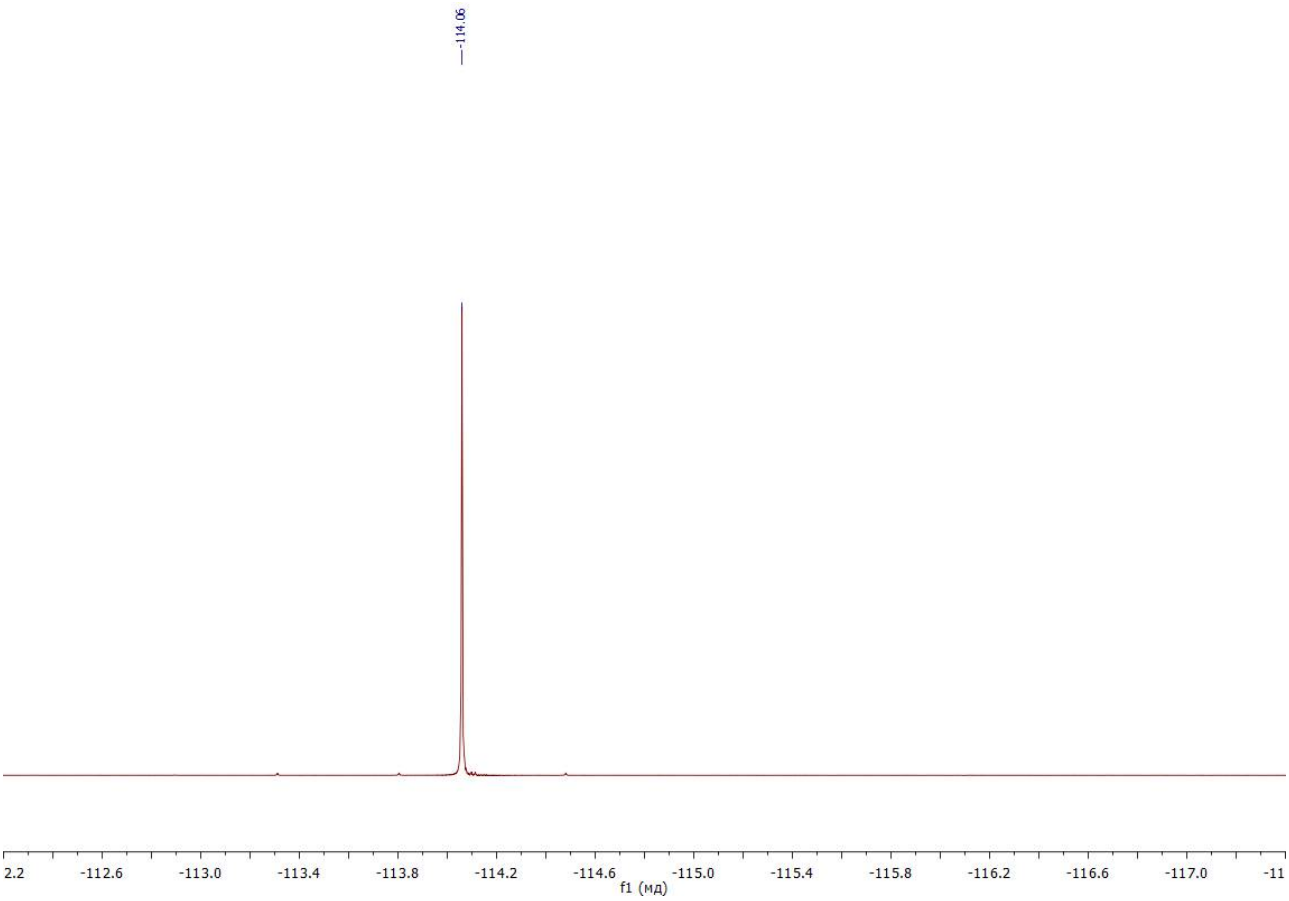


Fig. S7. $^{19}F\{^{1}H\}$ NMR Spectra of compound **1h** at 20 °C (400 МГц, $CDCl_3$).

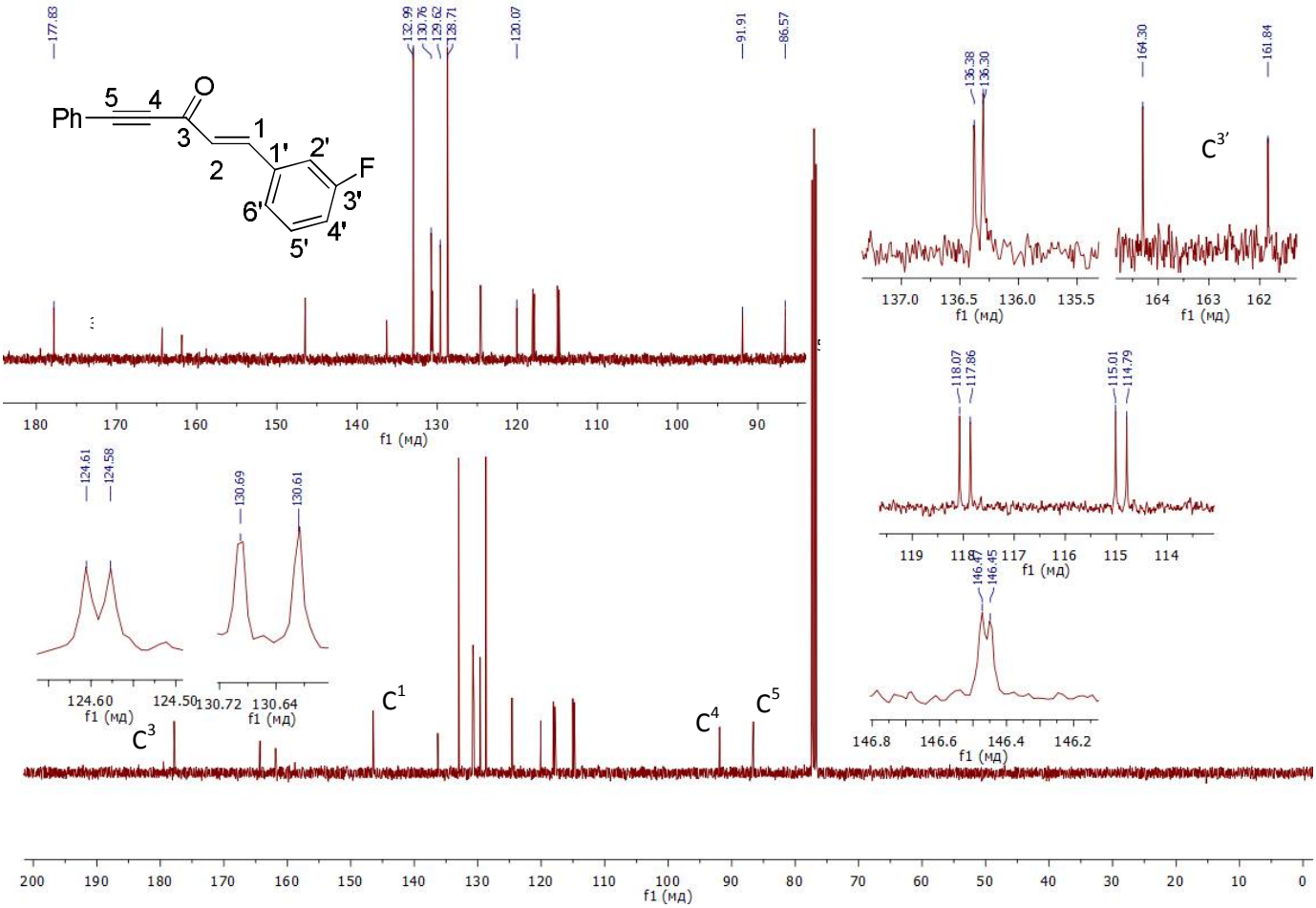


Fig. S8. ^{13}C NMR Spectra of compound **1h** at 20 °C (101МГц, $CDCl_3$).

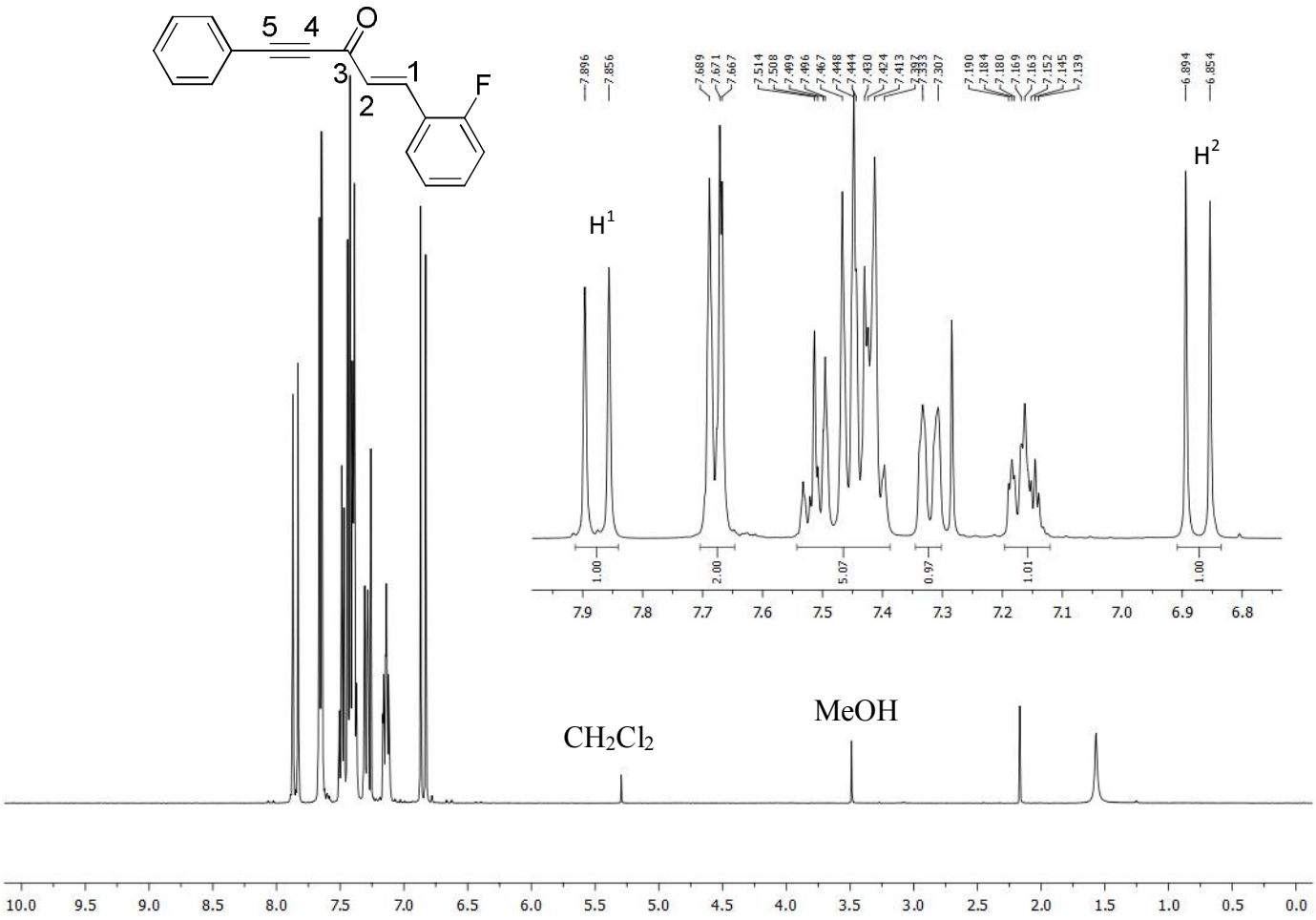


Fig. S9. ^{1}H NMR Spectra of compound **1i** at 20 °C (400 МГц, $CDCl_3$).

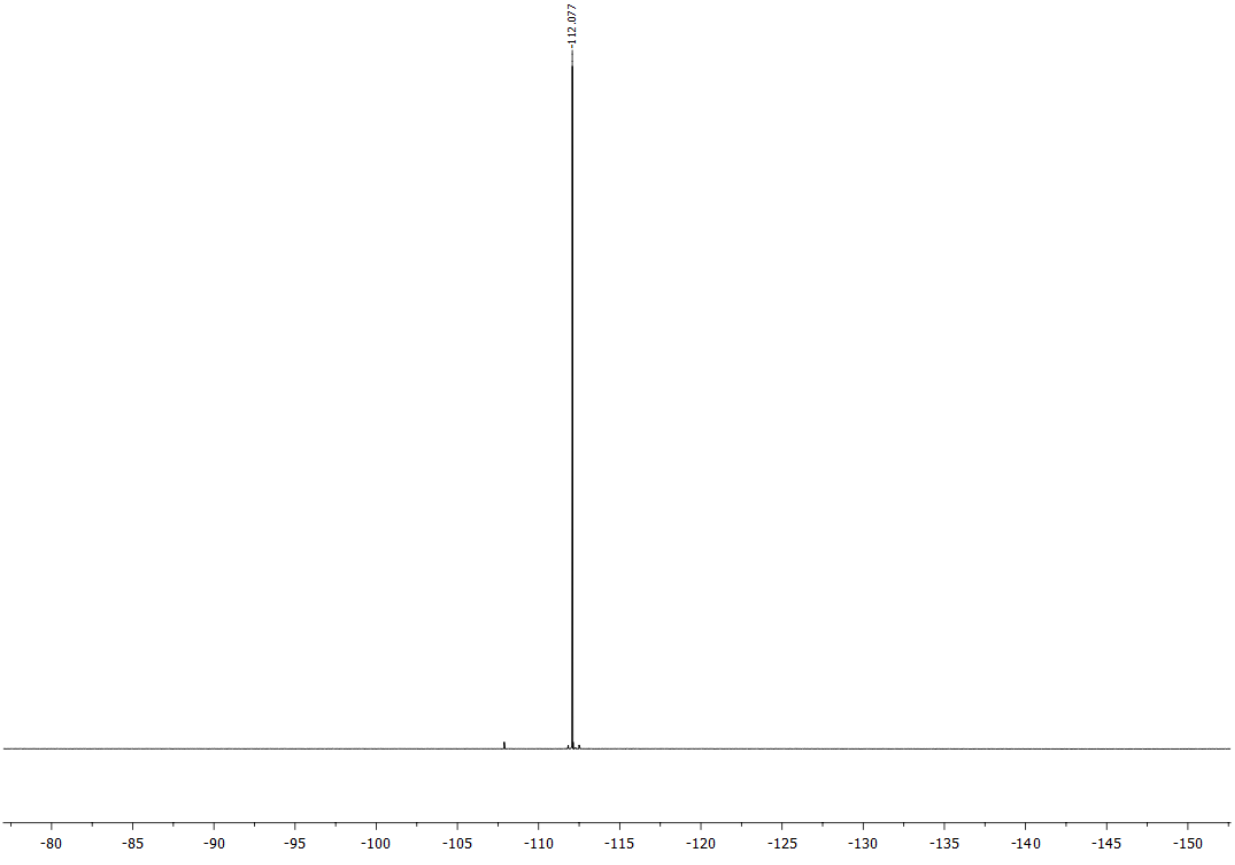


Fig. S10. $^{19}F\{^{1}H\}$ NMR Spectra of compound **1i** at 20 °C (400 МГц, $CDCl_3$).

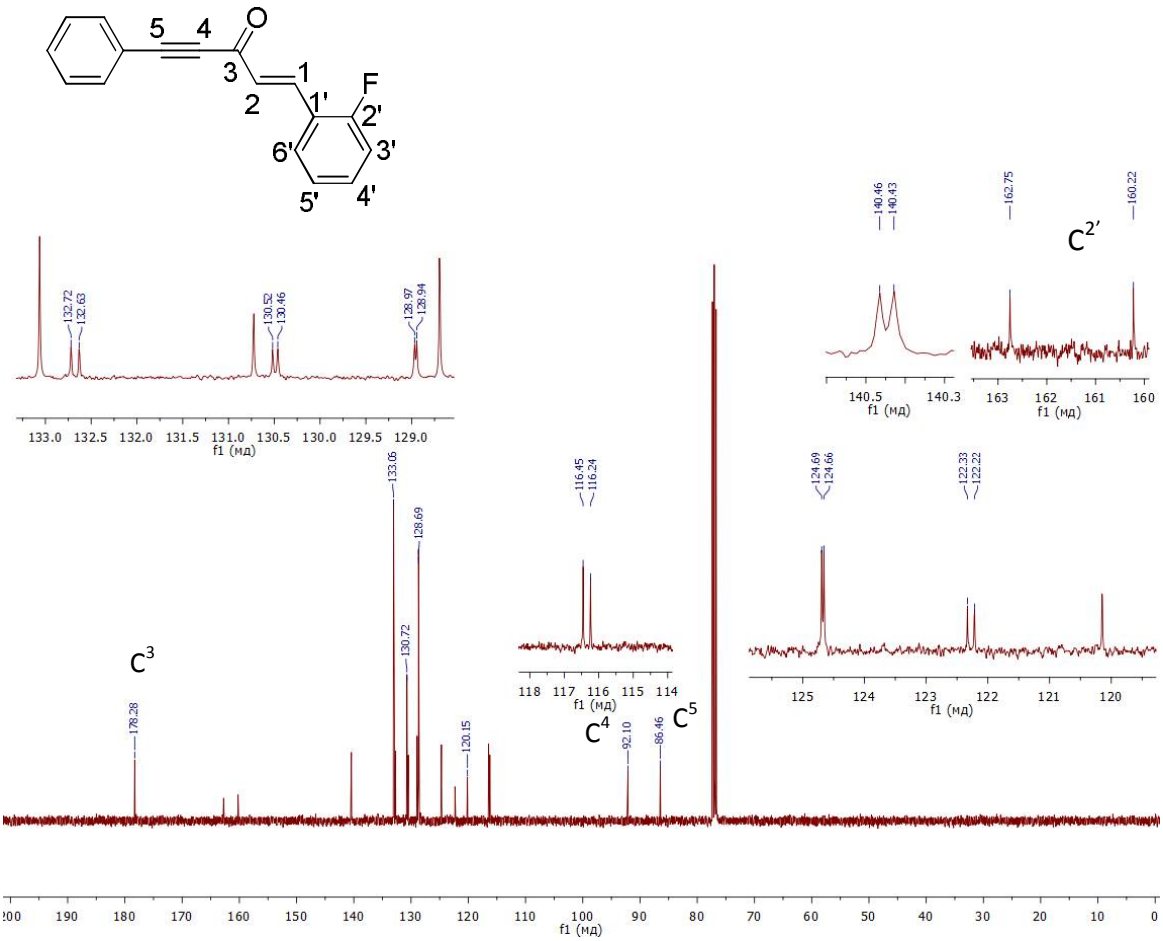


Fig. S11. ^{13}C NMR Spectra of compound **1i** at 20 °C (101МГц, $CDCl_3$).

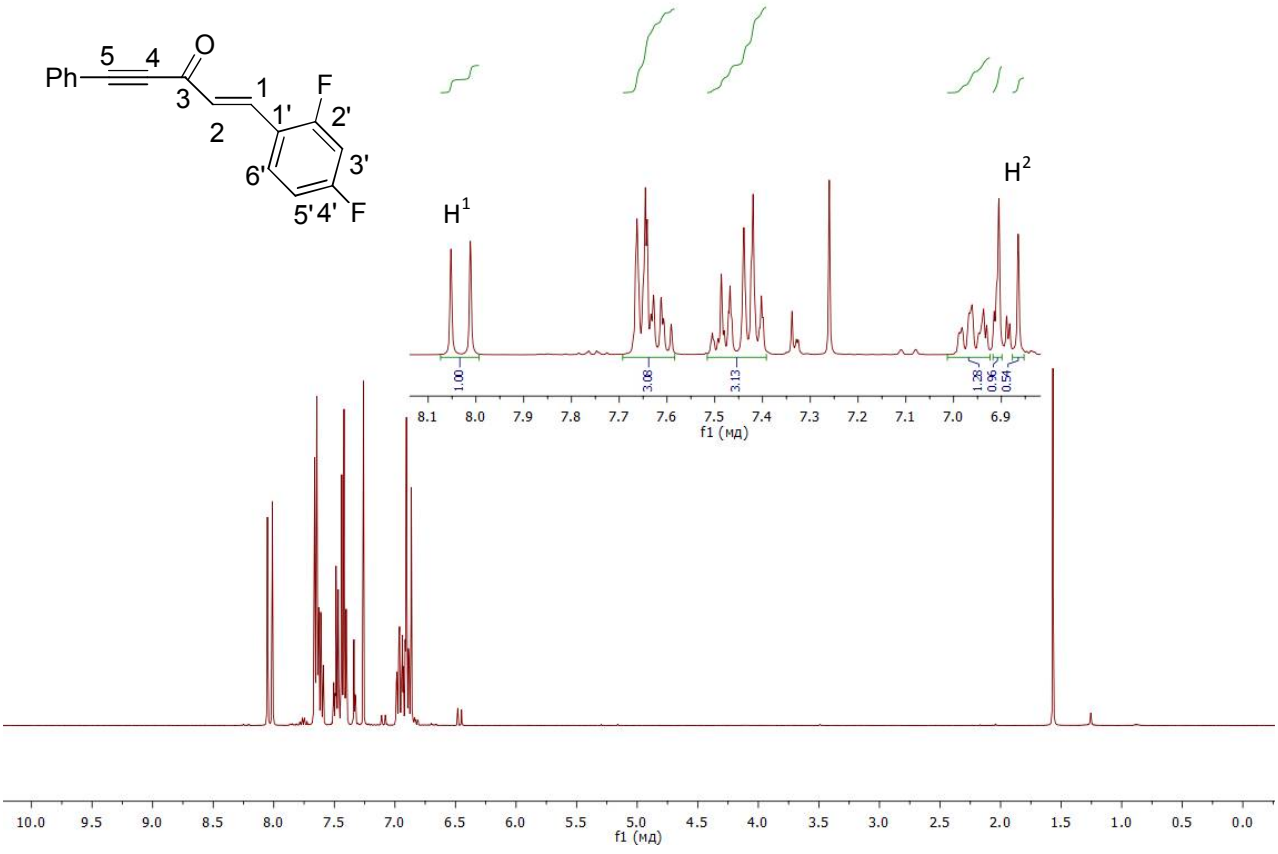


Fig. S12. ^{1}H NMR Spectra of compound **1j** at 20 °C (400 МГц, $CDCl_3$).

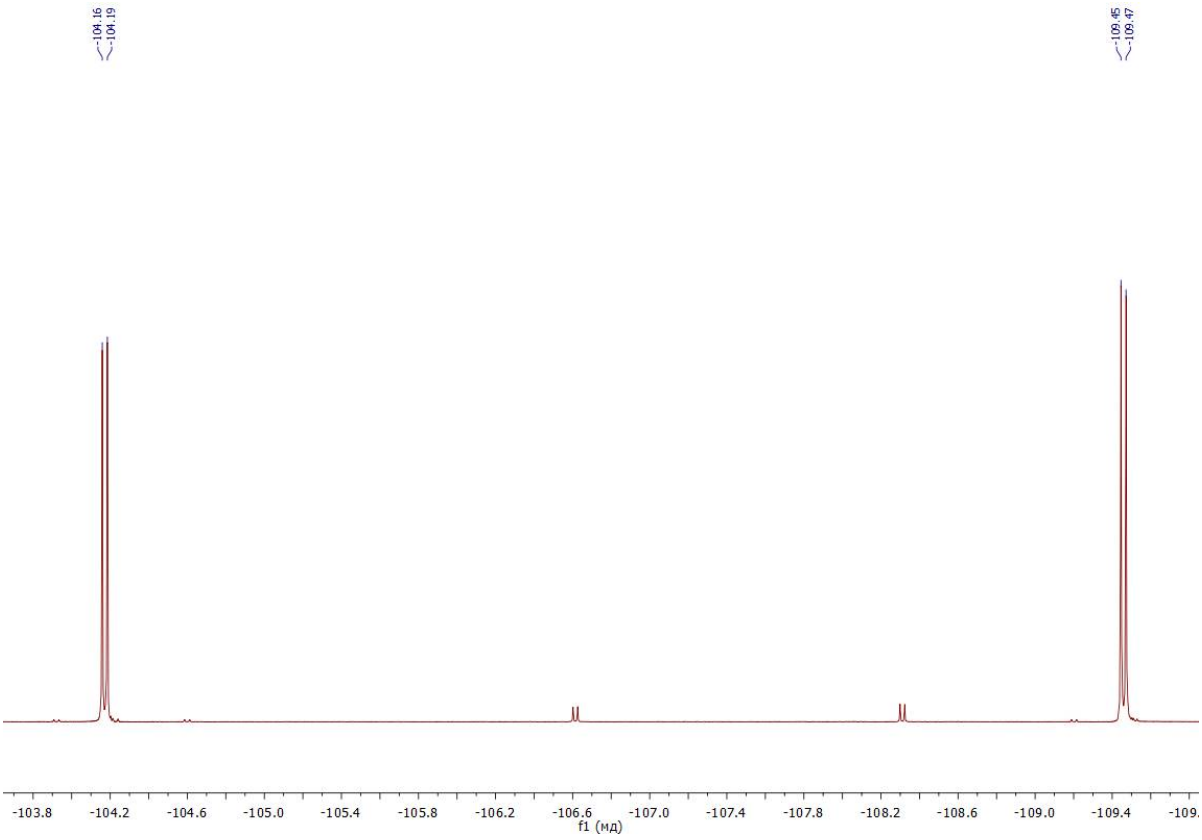


Fig. S13. $^{19}F\{^{1}H\}$ NMR Spectra of compound **1j** at 20 °C (400 МГц, $CDCl_3$).

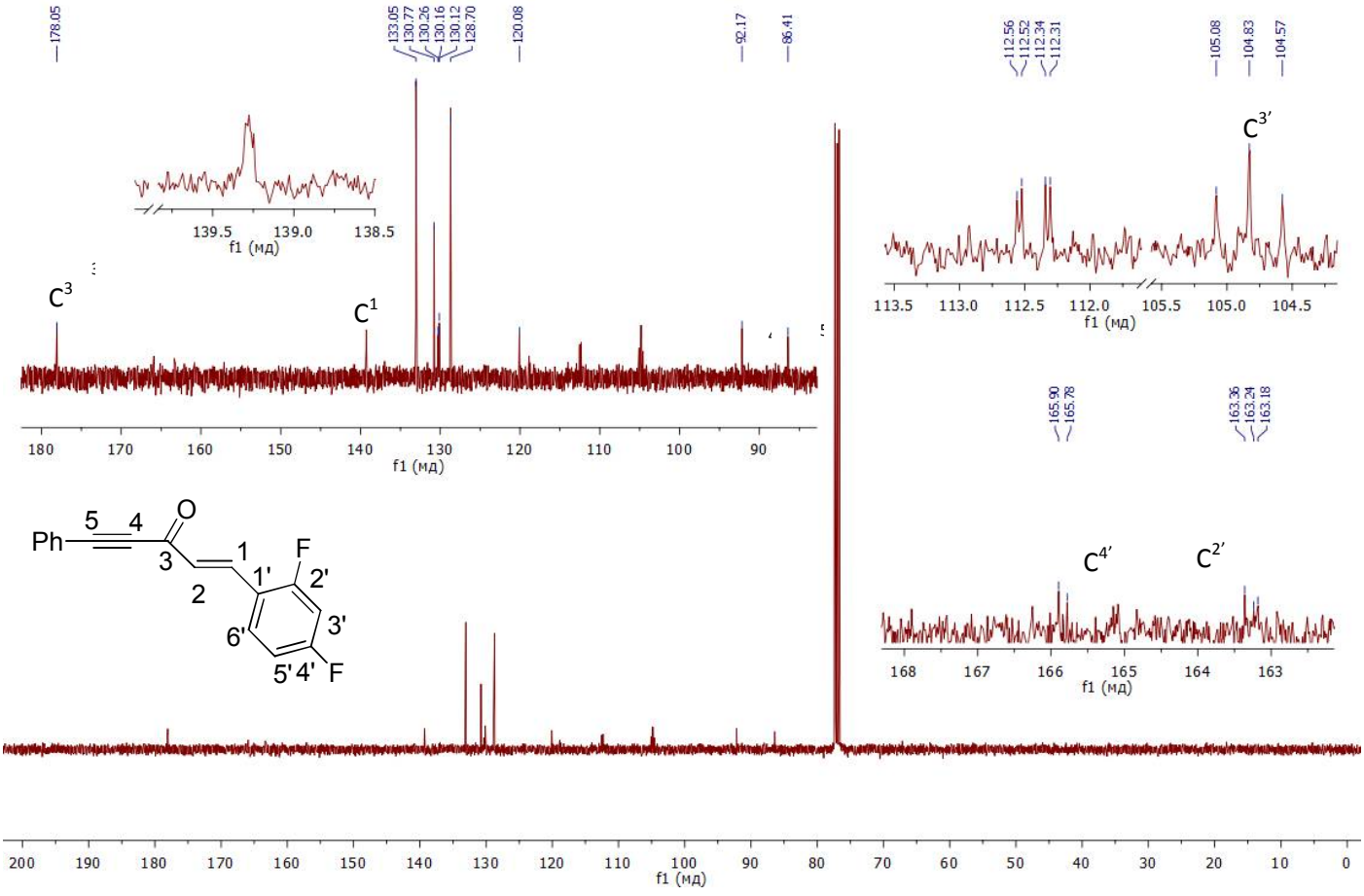


Fig. S14. ^{13}C NMR Spectra of compound **1j** at 20 °C (101МГц, $CDCl_3$).

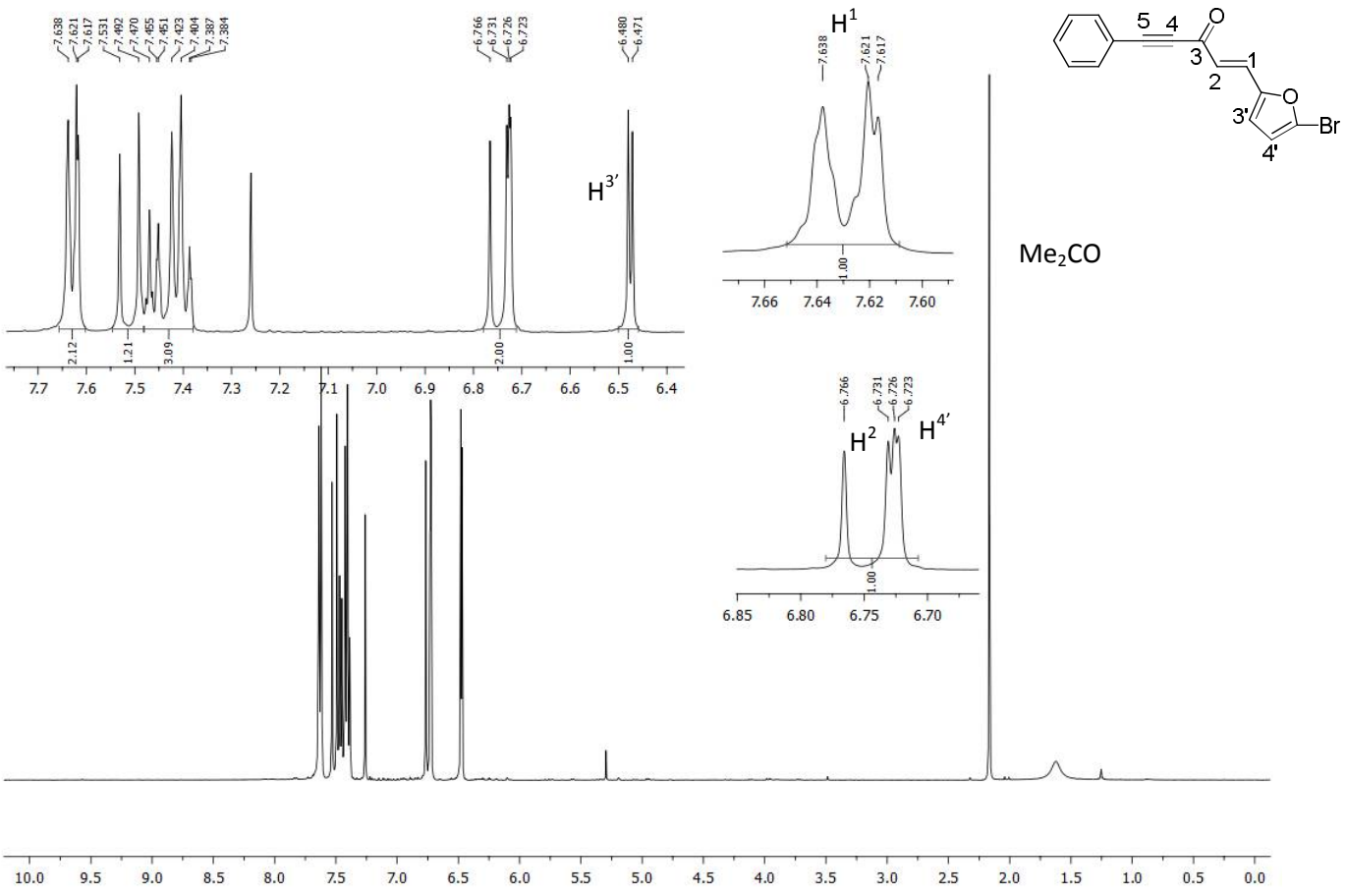


Fig. S15. ^{1}H NMR Spectra of compound **1k** at 20 °C (400 МГц, $CDCl_3$).

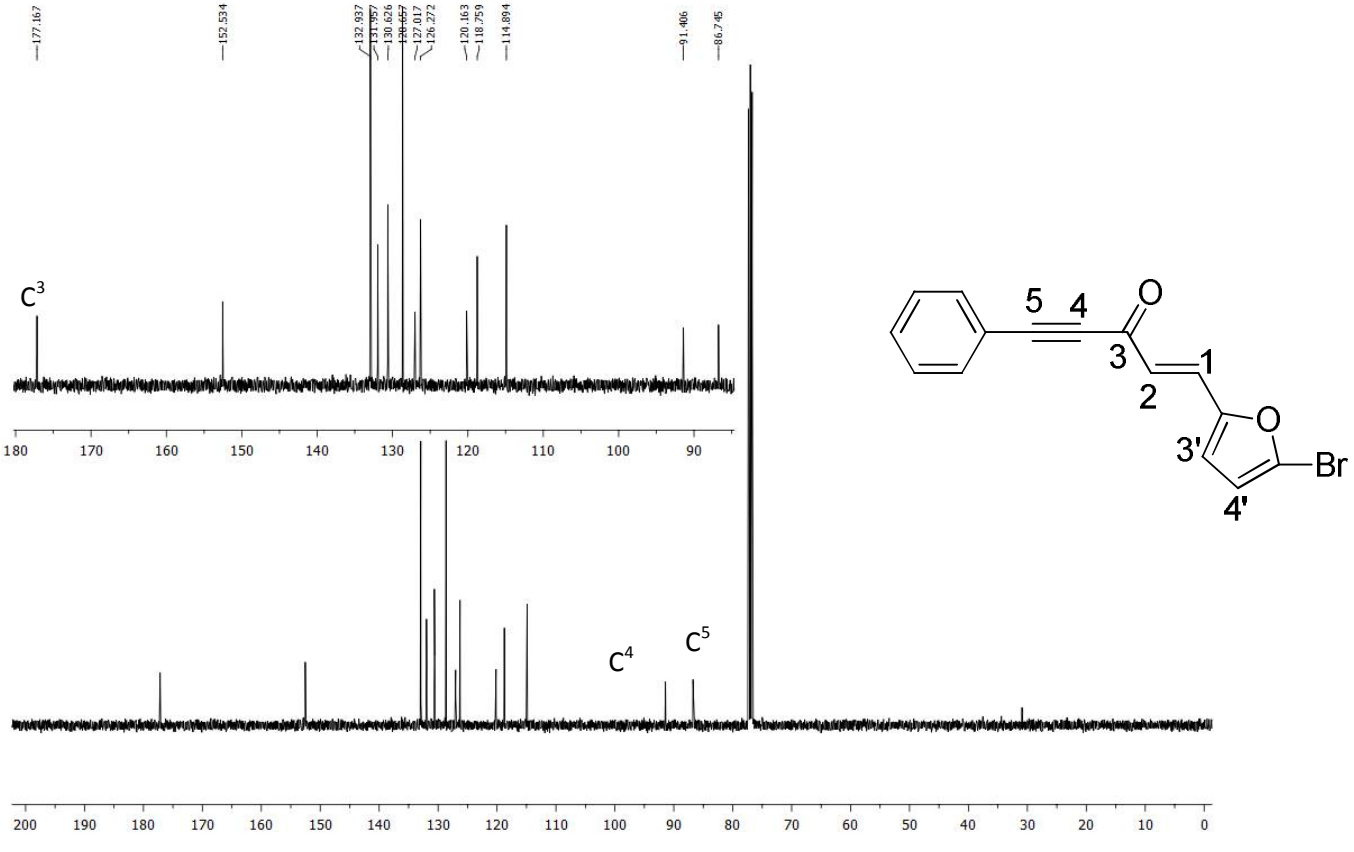


Fig. S16. ^{13}C NMR Spectra of compound **1k** at 20 °C (101МГц, $CDCl_3$).

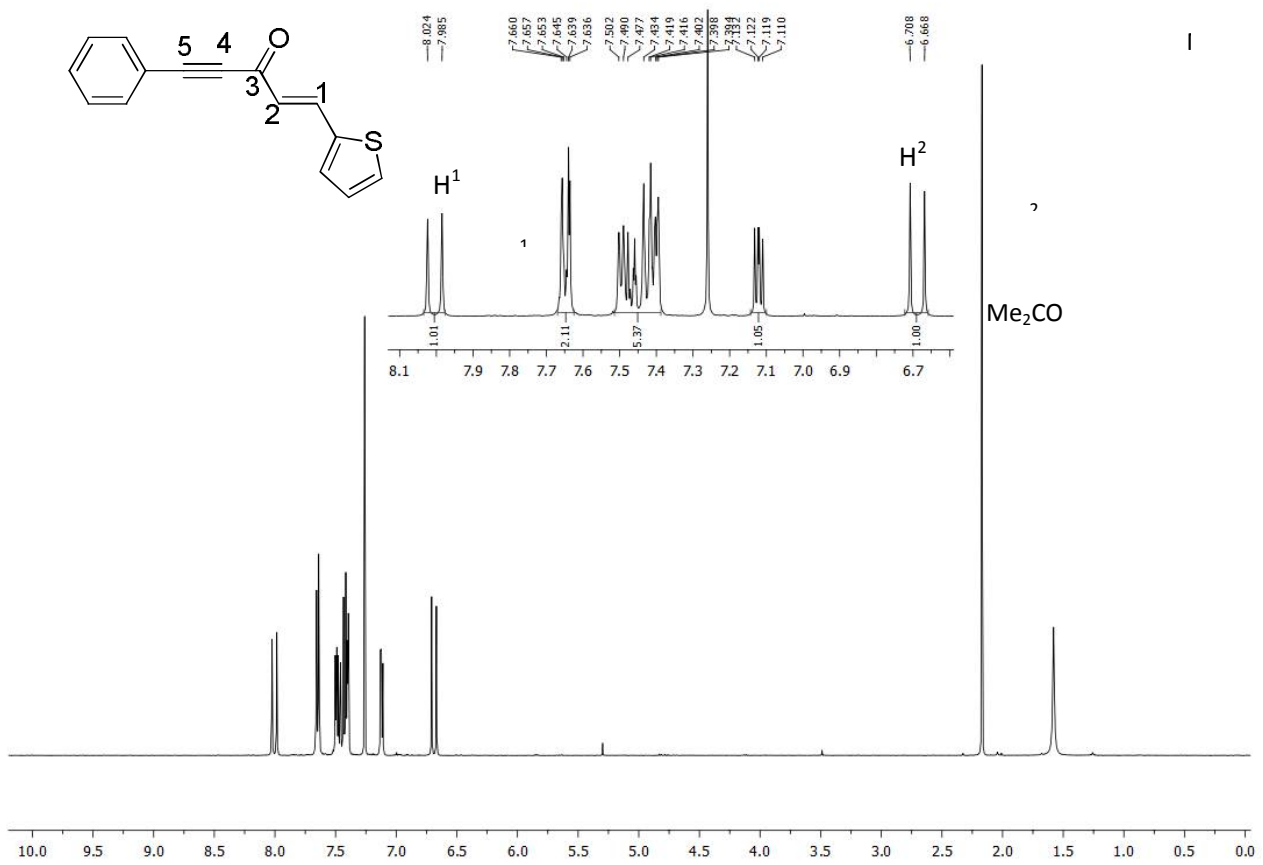


Fig. S17. ^{1}H NMR Spectra of compound **1l** at 20 °C (400 МГц, $CDCl_3$).

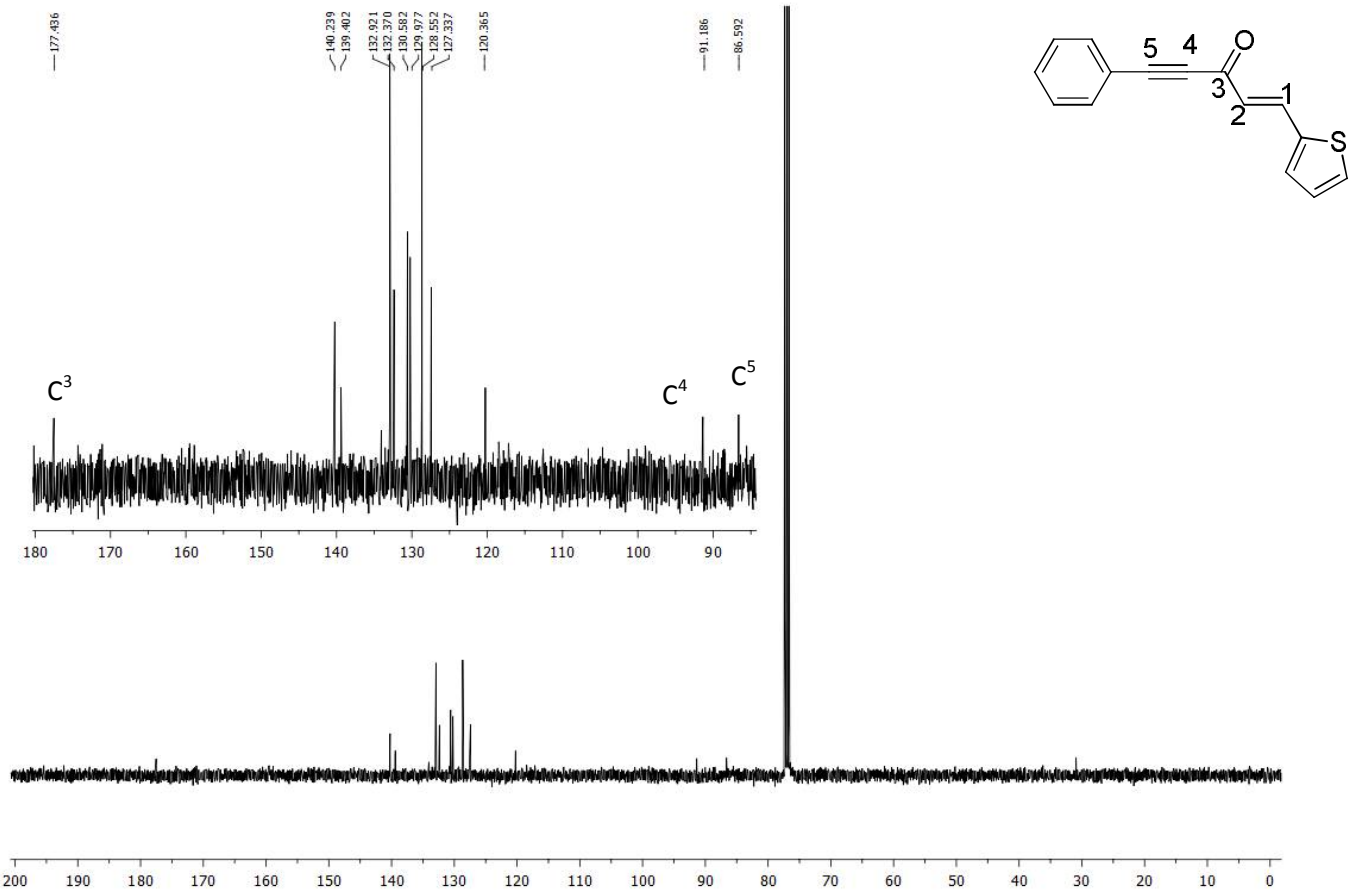


Fig. S18. ^{13}C NMR Spectra of compound **1l** at 20 °C (101МГц, $CDCl_3$).

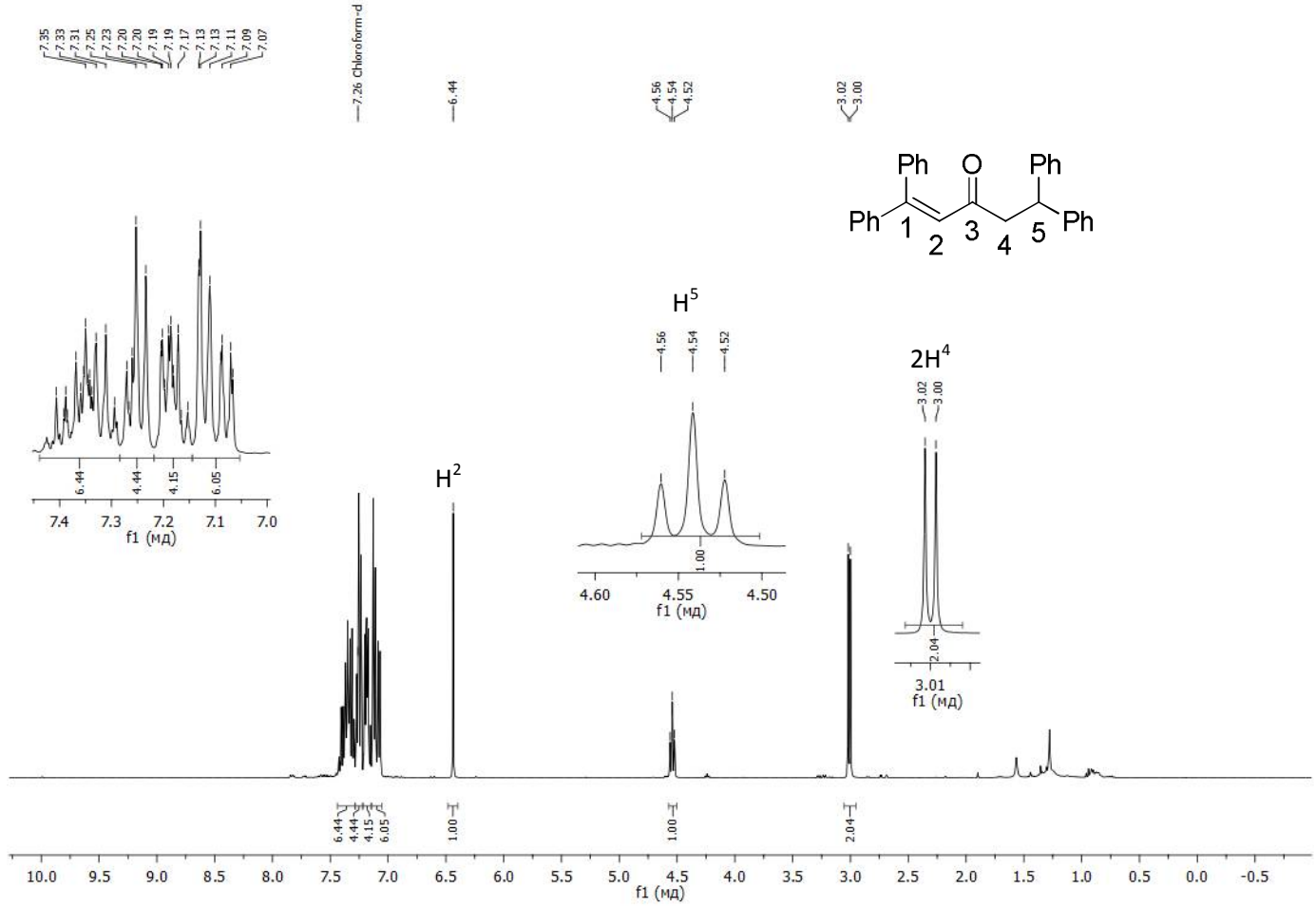


Fig. S19. ^{1}H NMR Spectra of compound **2a** at 20 °C (400 МГц, $CDCl_3$).

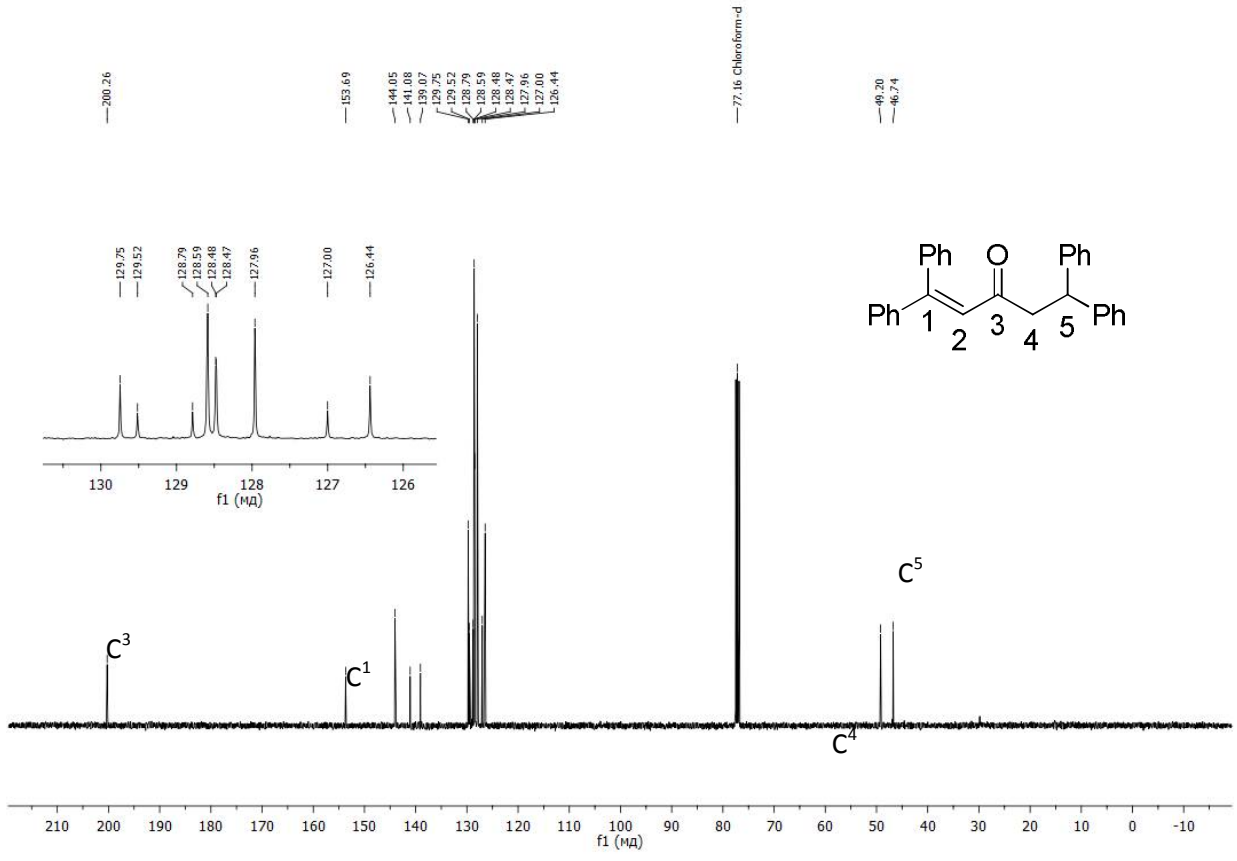


Fig. S20. ^{13}C NMR Spectra of compound **2a** at 20 °C (101МГц, $CDCl_3$).

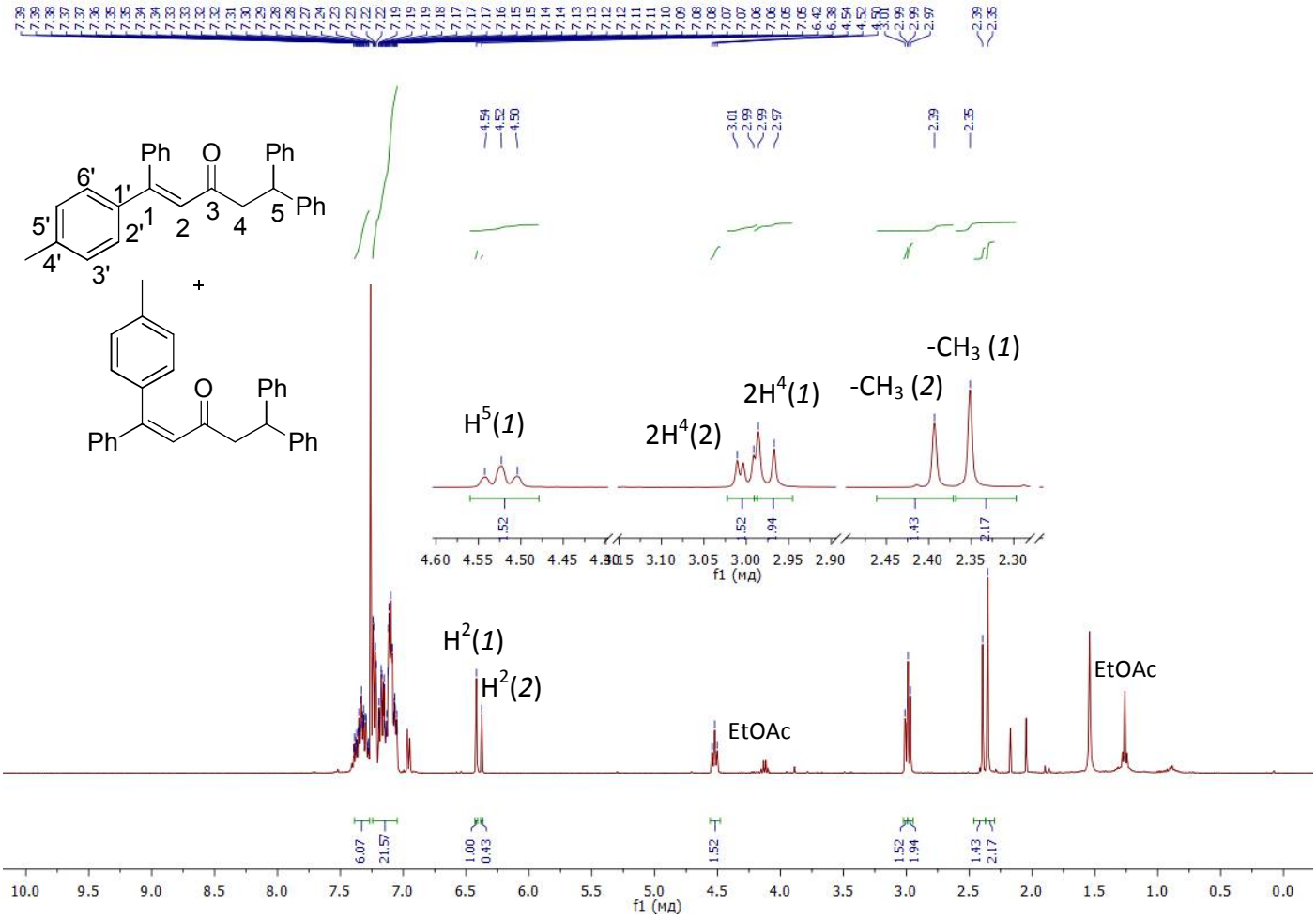


Fig. S21. ^{1}H NMR Spectra of compounds **2b** at 20 °C (400 МГц, $CDCl_3$).

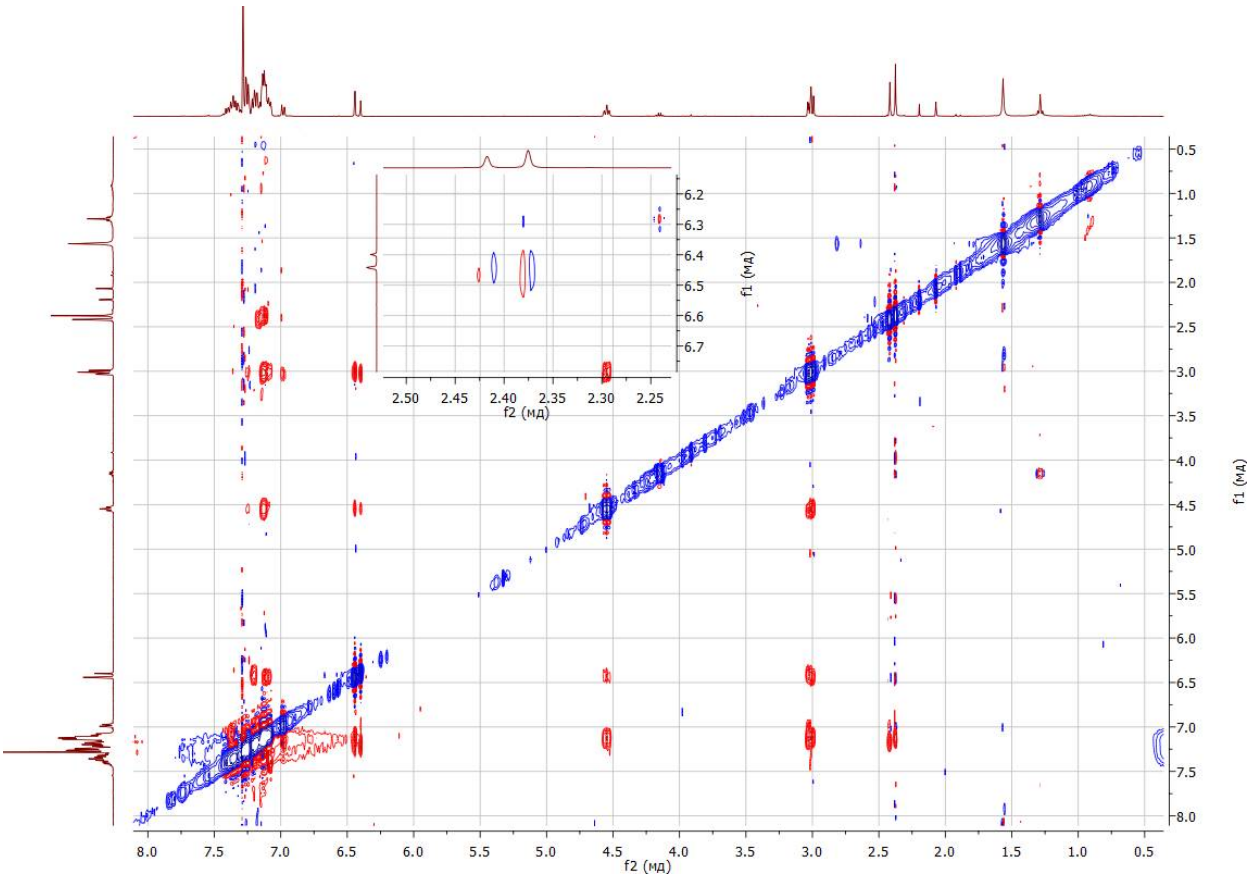


Fig. S22. ^{1}H-^{1}H NMR NOESY Spectra of compounds **2b** at 20 °C (400 МГц, $CDCl_3$).

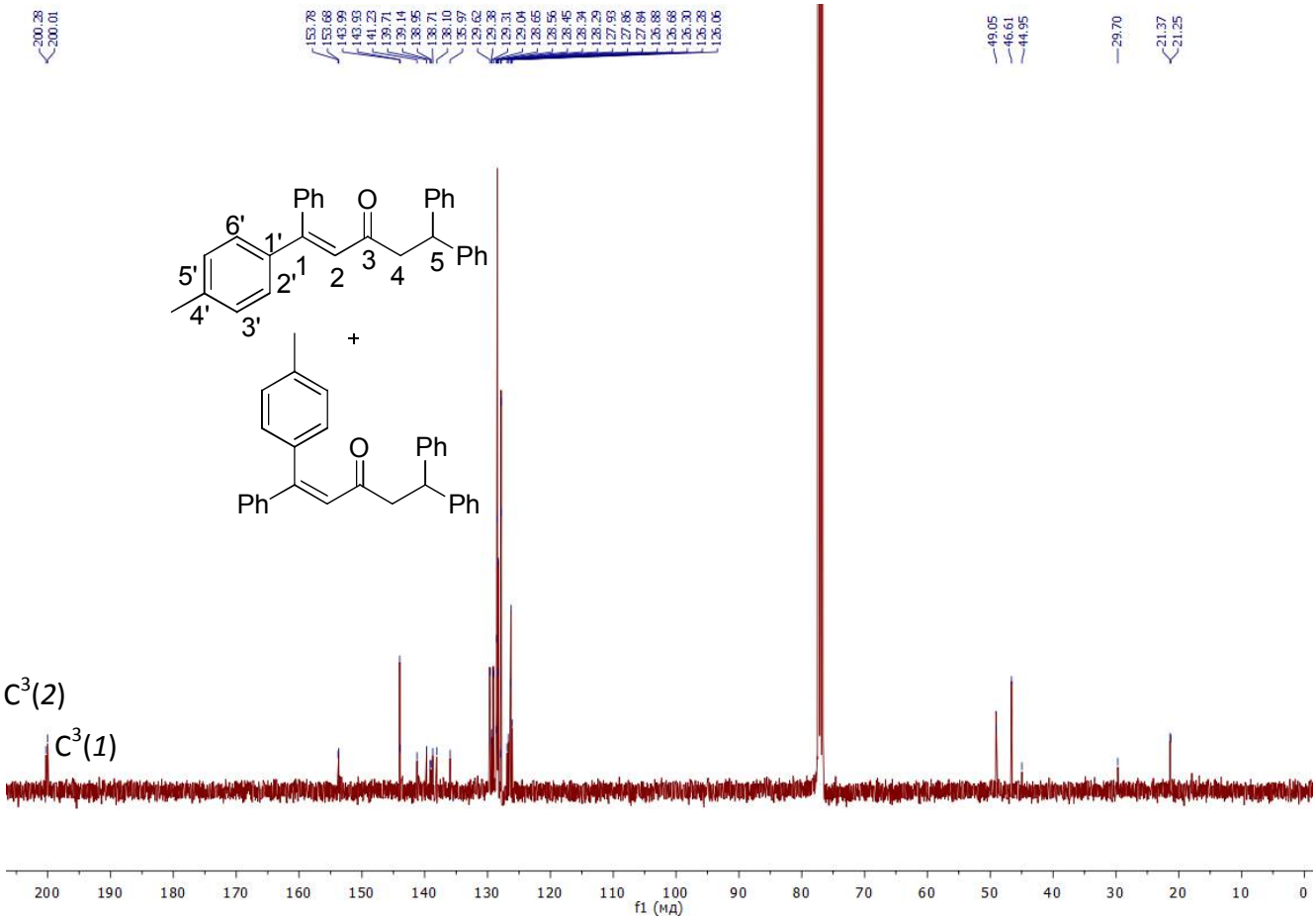


Fig. S23. ^{13}C NMR Spectra of compounds **2b** at 20 °C (101МГц, $CDCl_3$).

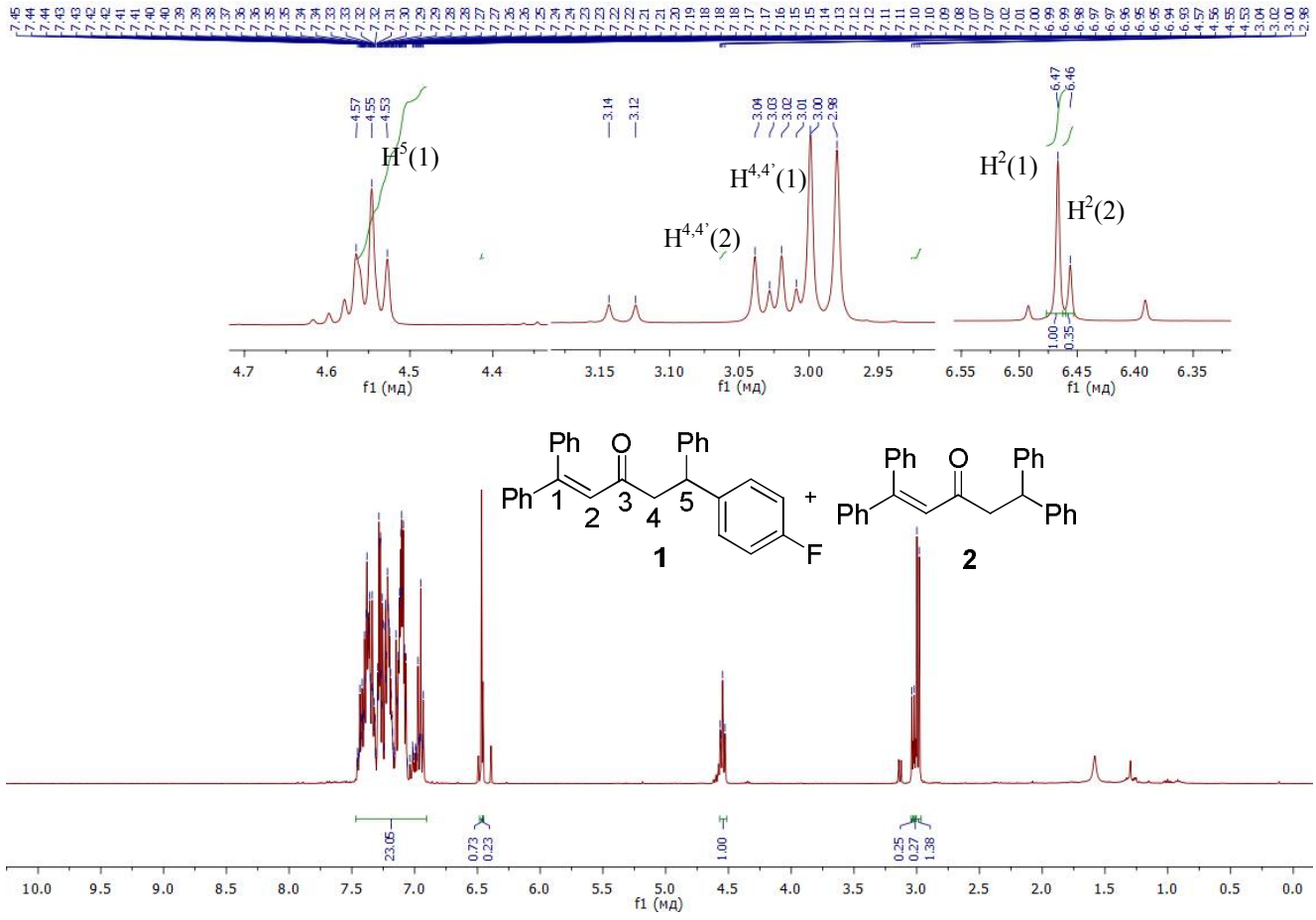


Fig. S24. ^{1}H NMR Spectra of compounds **2c** at 20 °C (400 МГц, $CDCl_3$).

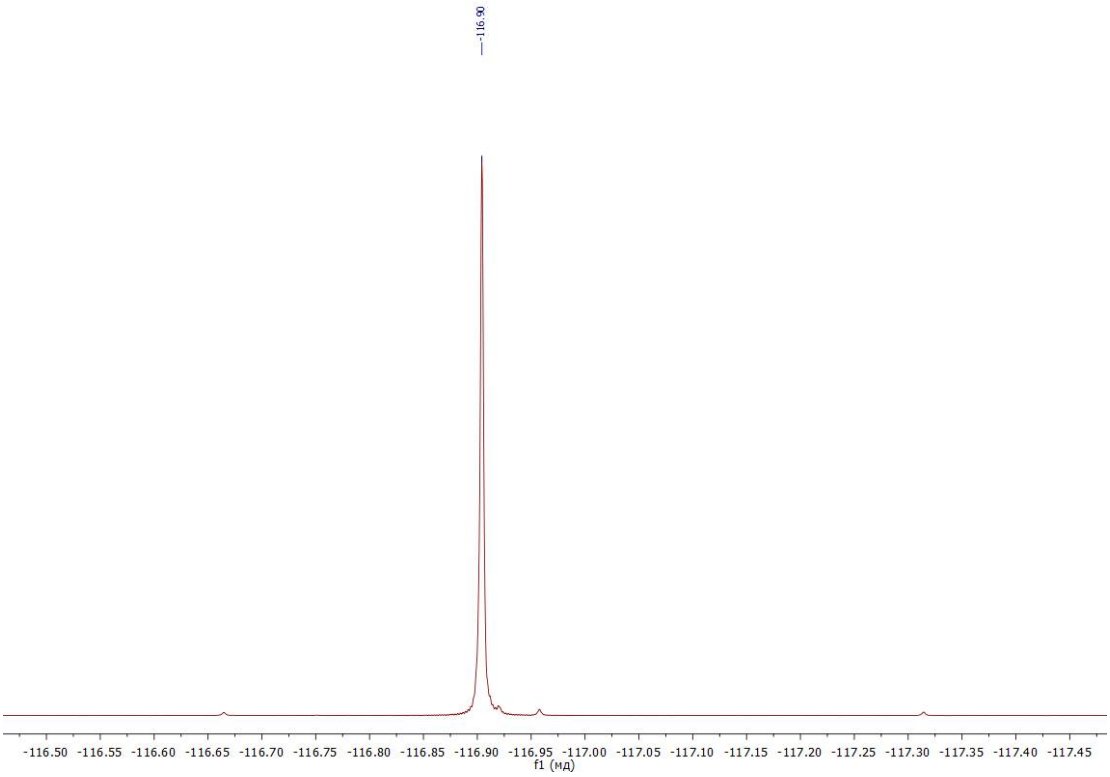


Fig. S25. $^{19}F\{^{1}H\}$ NMR Spectra of compound **2c** at 20 °C (400 МГц, $CDCl_3$).

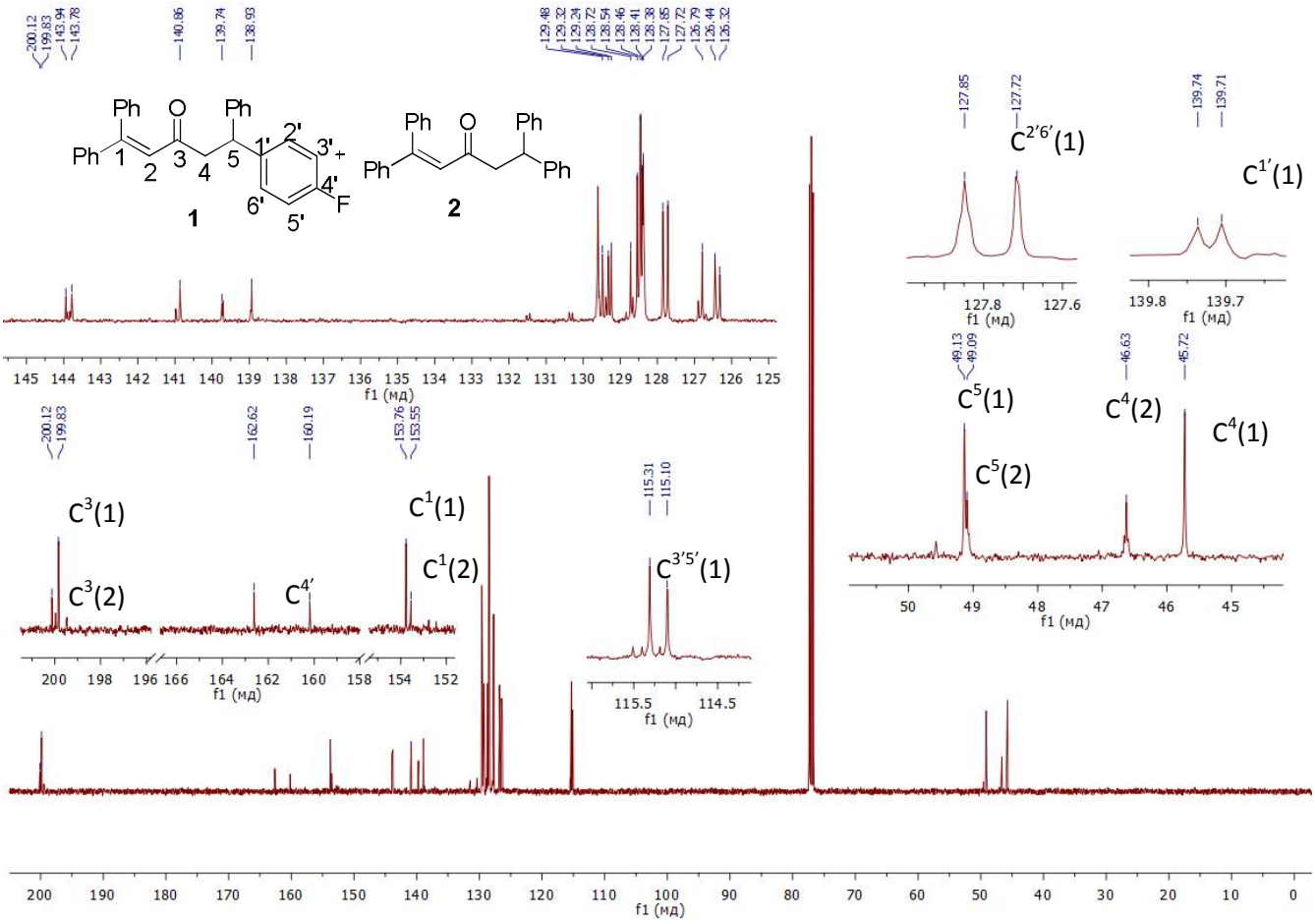


Fig. S26. ^{13}C NMR Spectra of compounds **2c** at 20 °C (101МГц, $CDCl_3$).

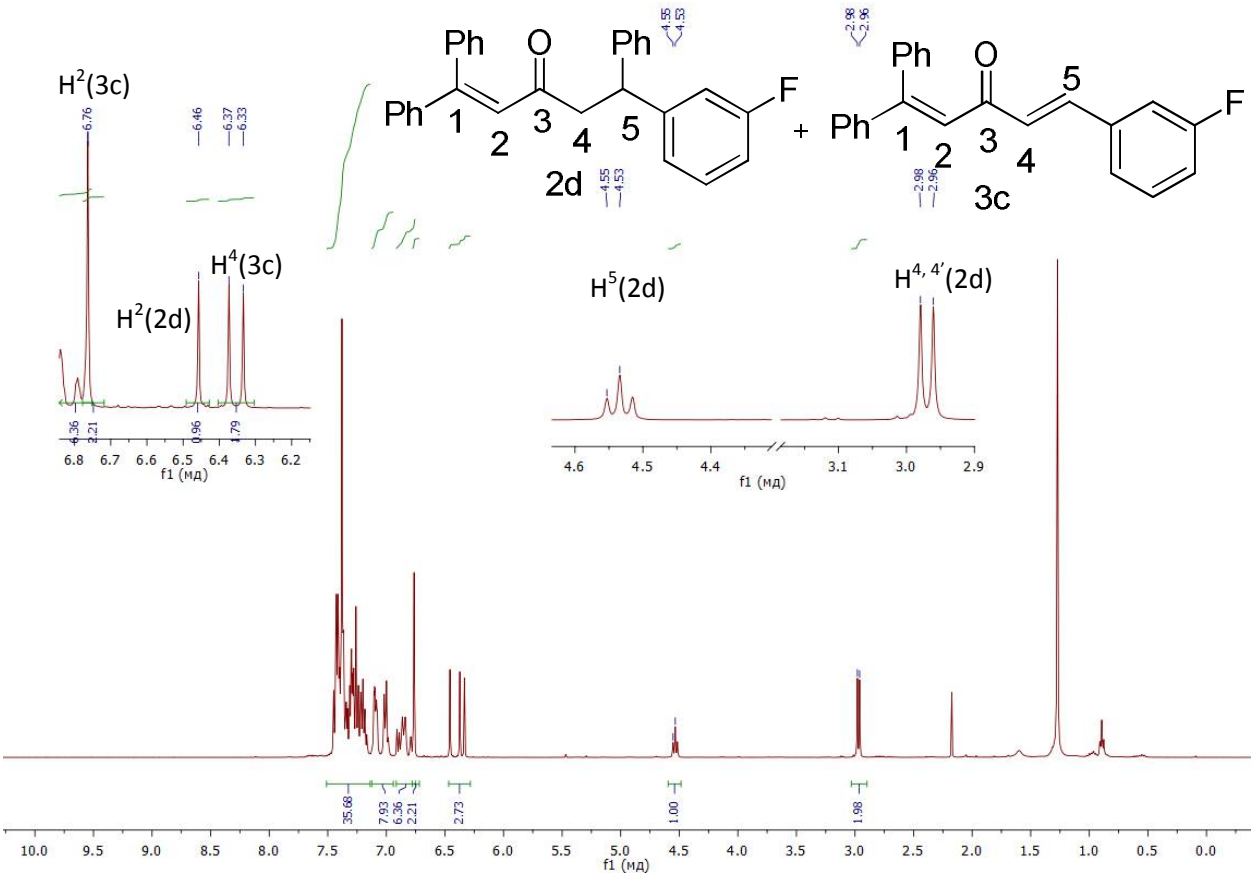


Fig. S27. ^{1}H NMR Spectra of compound **2d** at 20 °C (400МГц, $CDCl_3$).

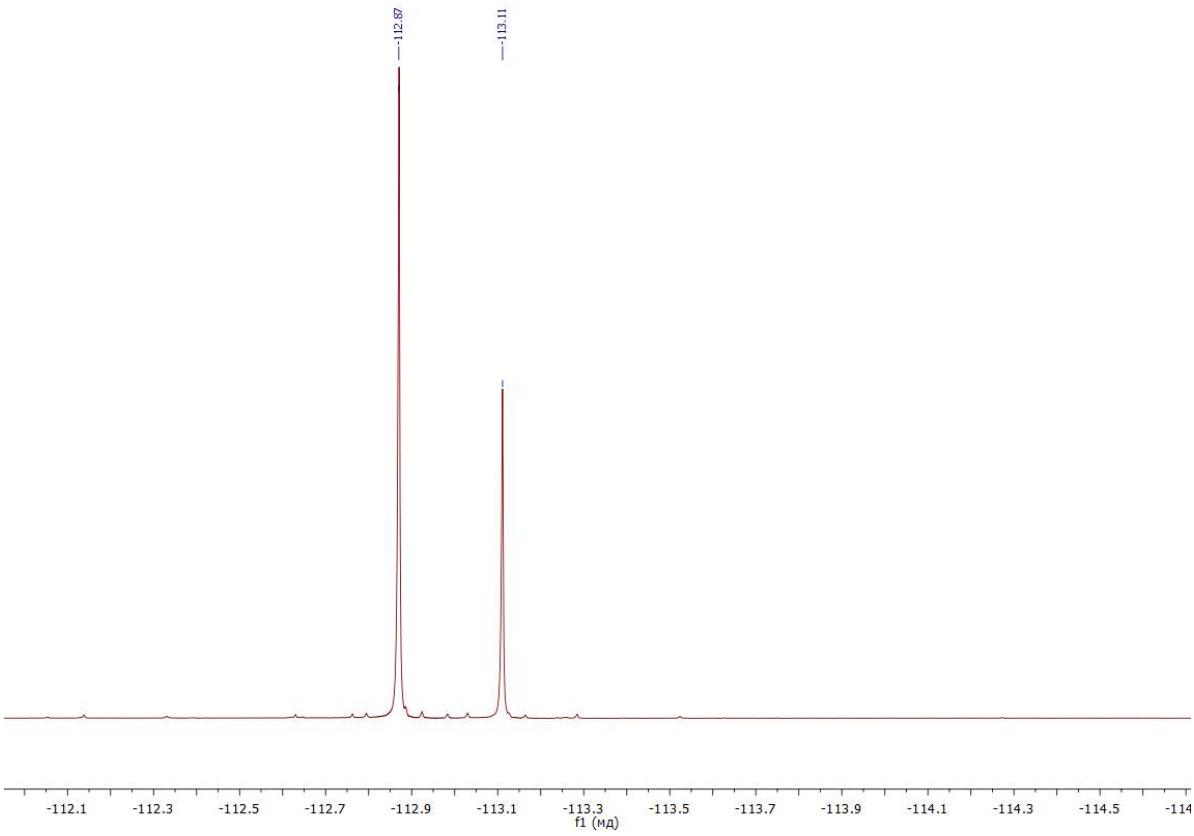


Fig. S28. $^{19}F\{^{1}H\}$ NMR Spectra of compound **2d** at 20 °C (400 МГц, $CDCl_3$).

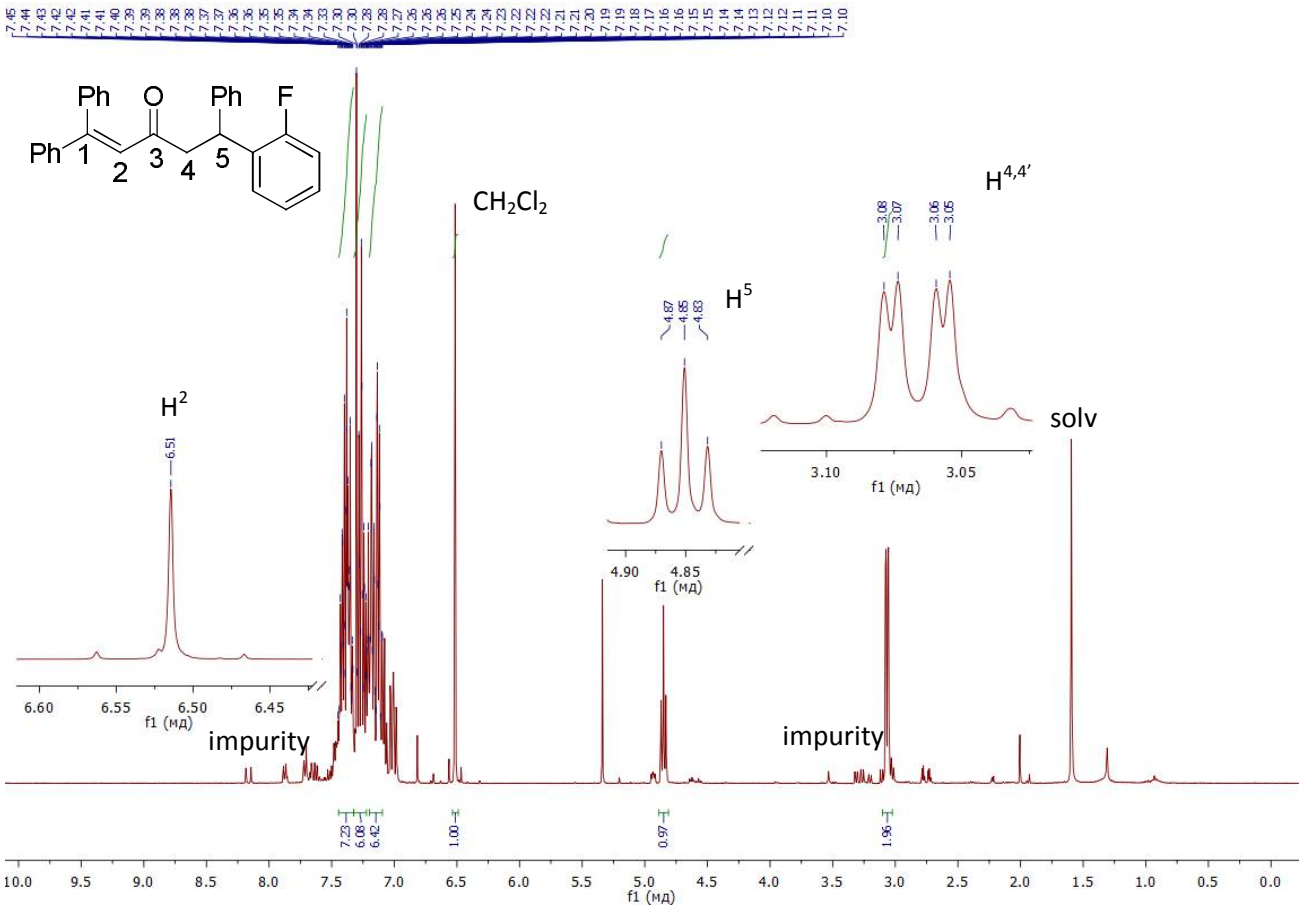


Fig. S29. ^{1}H NMR Spectra of compound **2e** at 20 °C (400МГц, $CDCl_3$).

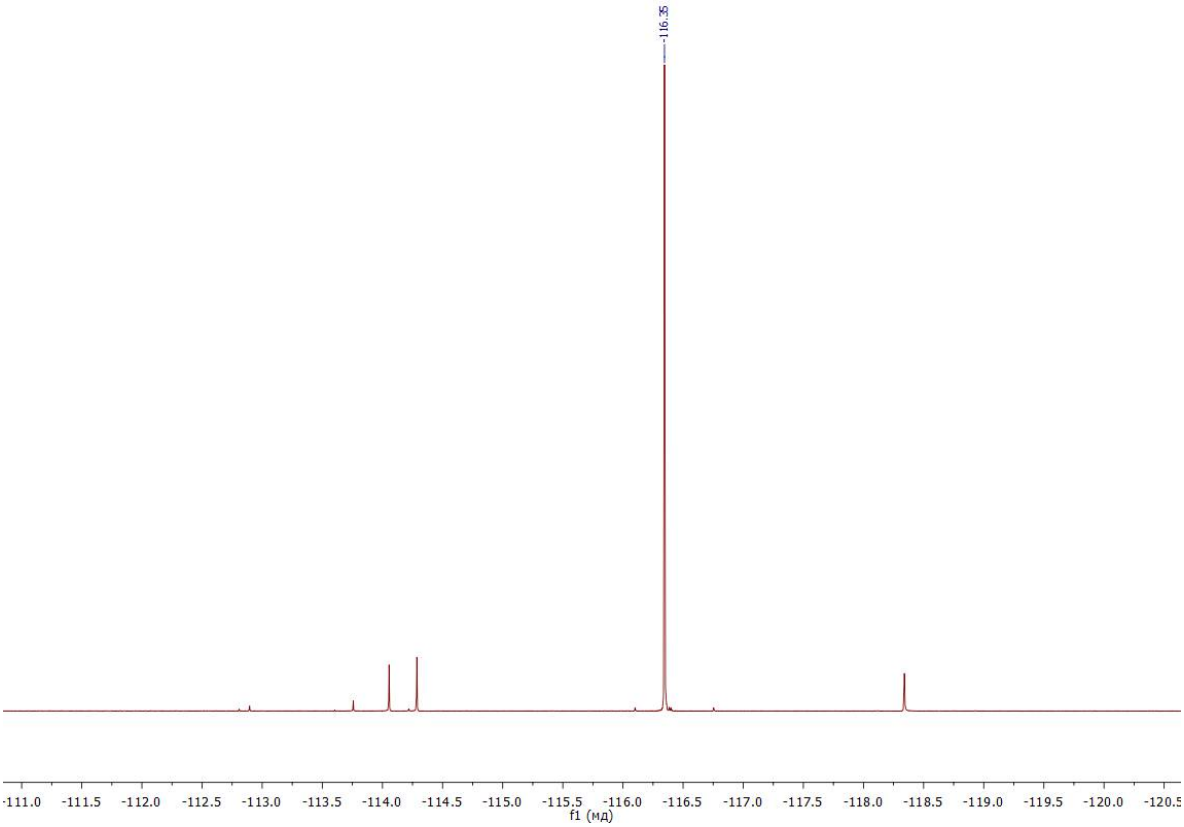


Fig. S30. $^{19}F\{^{1}H\}$ NMR Spectra of compound **2e** at 20 °C (400 МГц, $CDCl_3$).

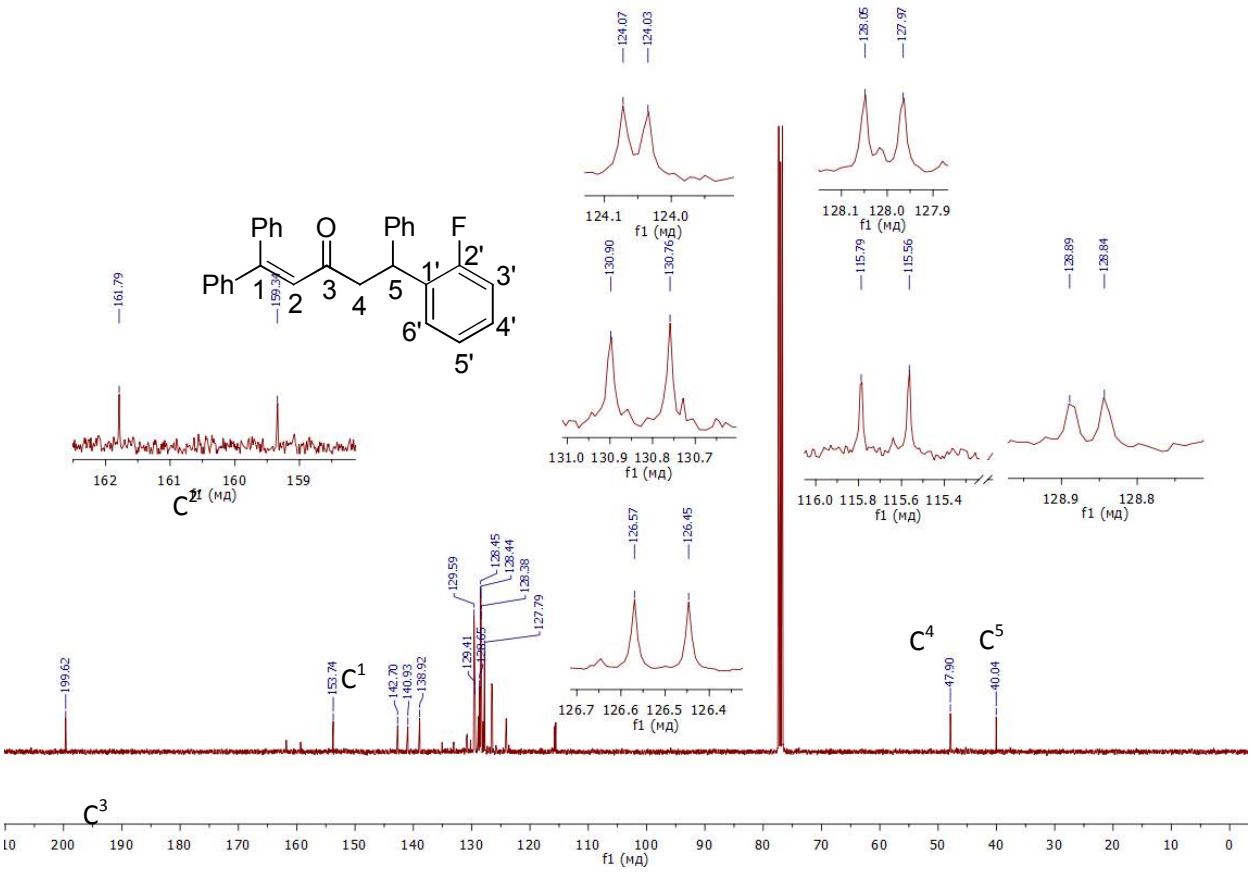


Fig. S31. ^{13}C NMR Spectra of compound **2e** at 20 °C (101МГц, $CDCl_3$).

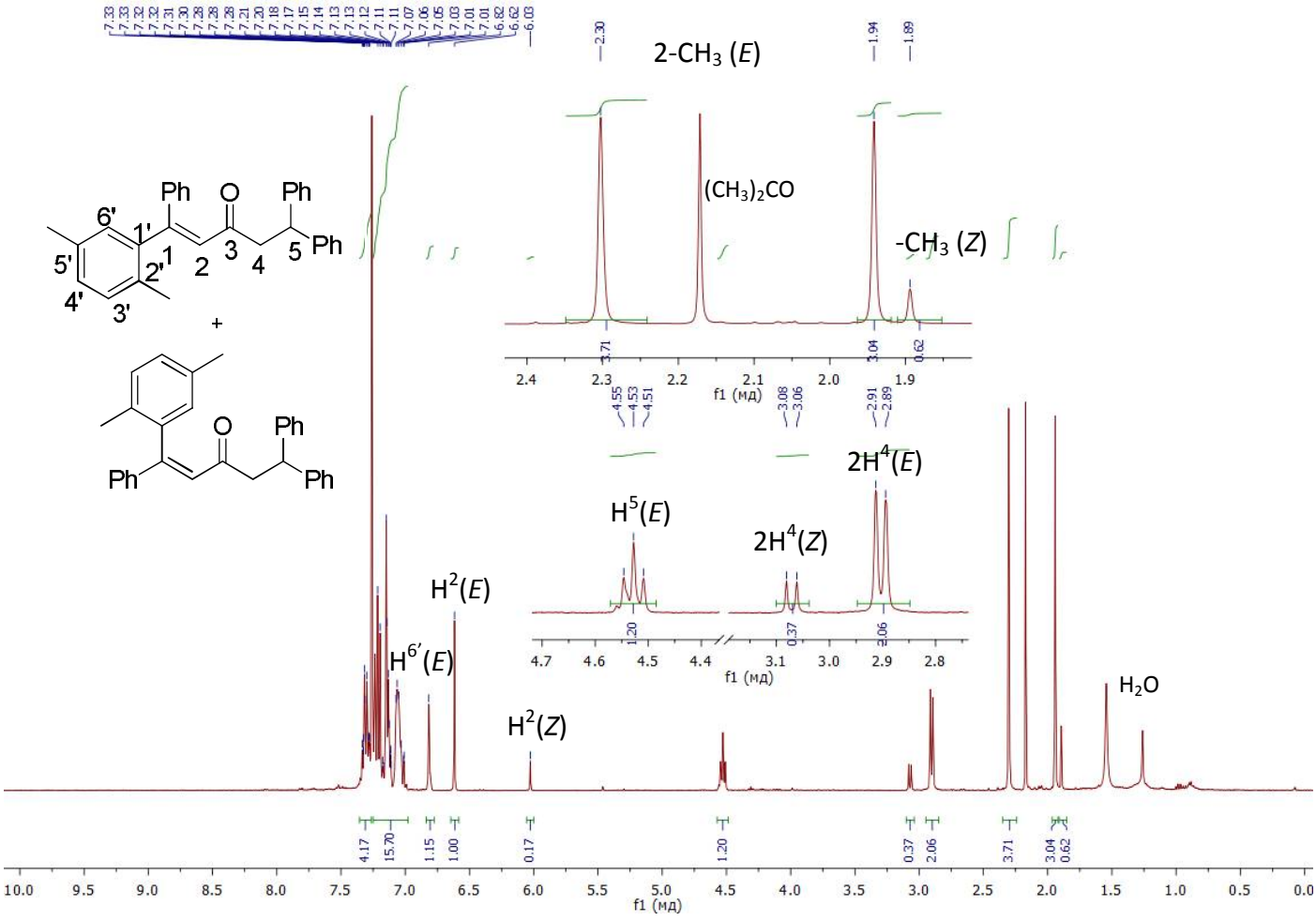


Fig. S32. ^{1}H NMR Spectra of compounds **2f** at 20 °C (400 МГц, $CDCl_3$).

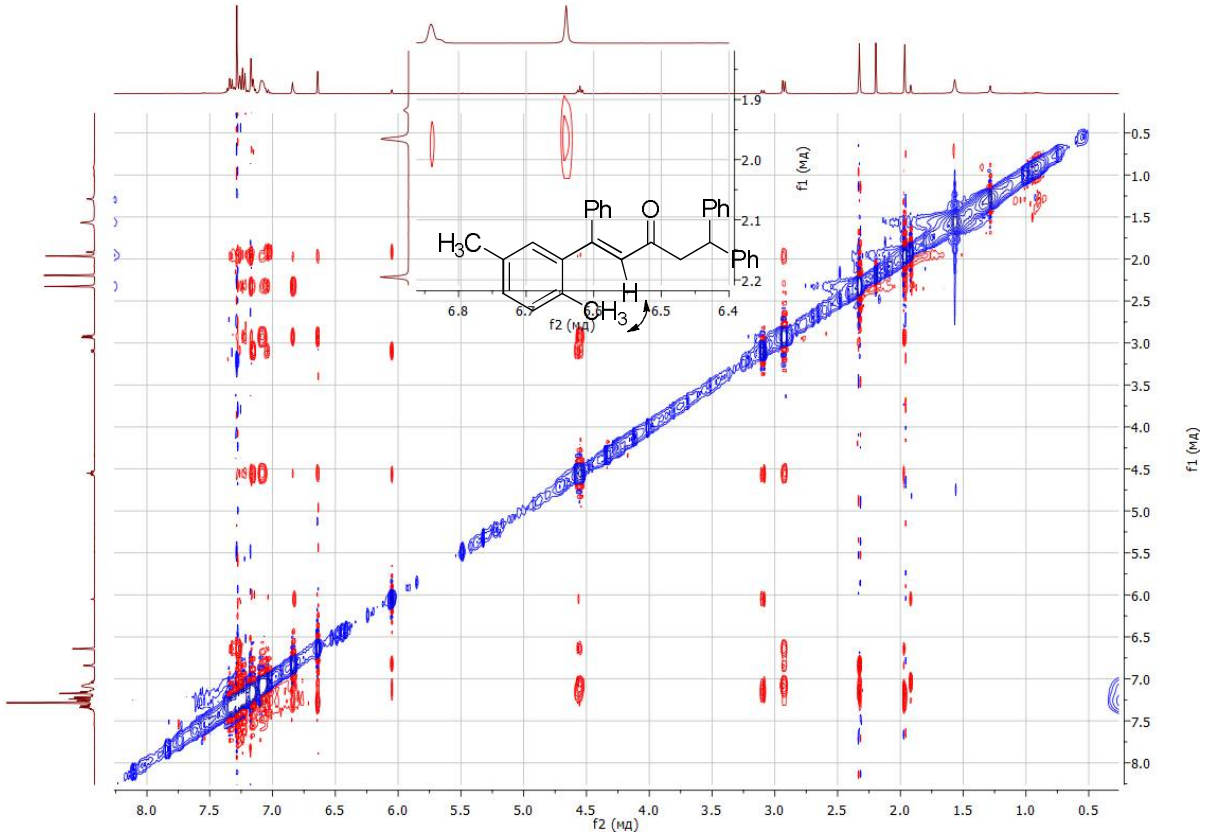


Fig. S33. ^{1}H-^{1}H NMR NOESY Spectra of compounds **2f** at 20 °C (400 МГц, $CDCl_3$).

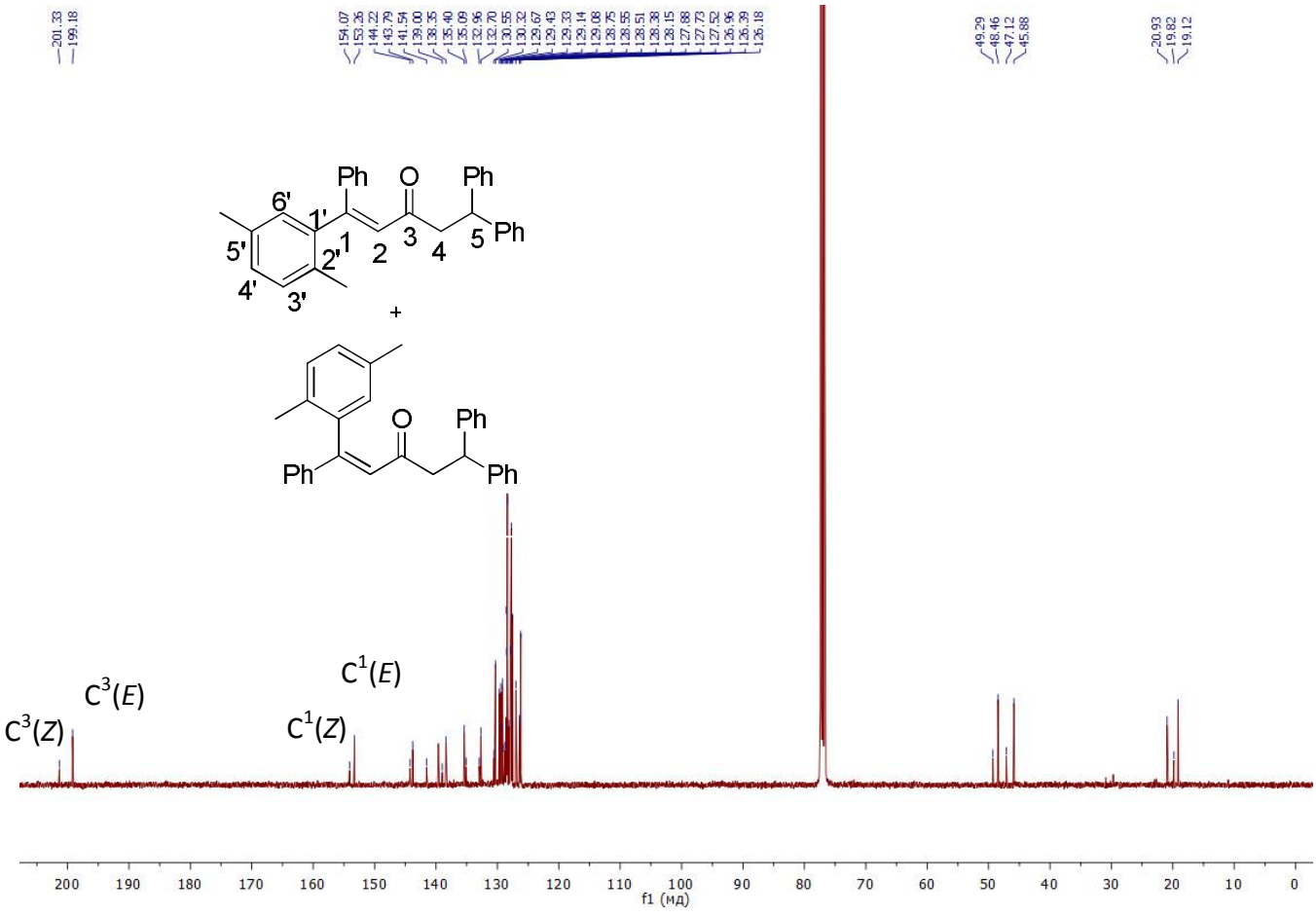


Fig. S34. ^{13}C NMR Spectra of compounds **2f** at 20 °C (101МГц, $CDCl_3$).

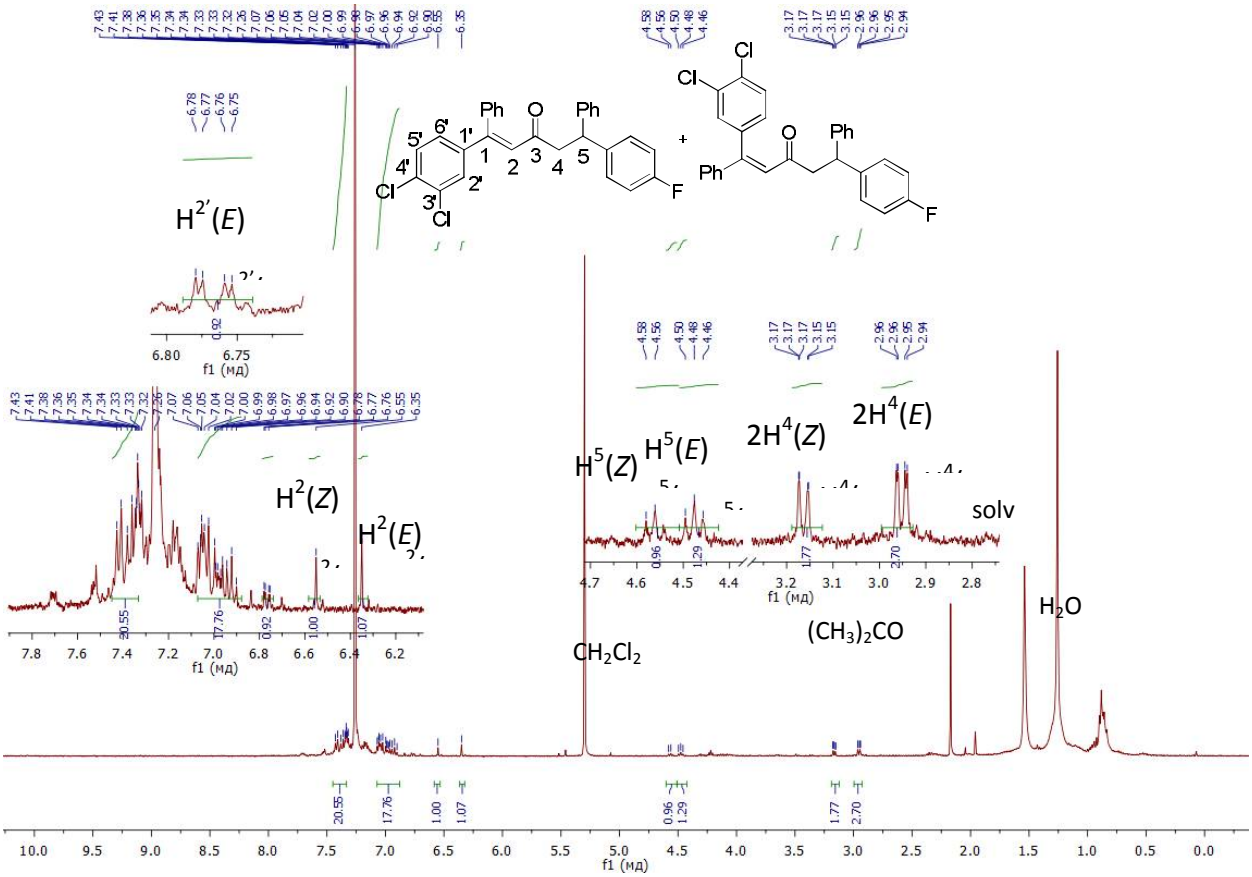


Fig. S35. ^{1}H NMR Spectra of compound **2g** at 20 °C (400 МГц, $CDCl_3$).

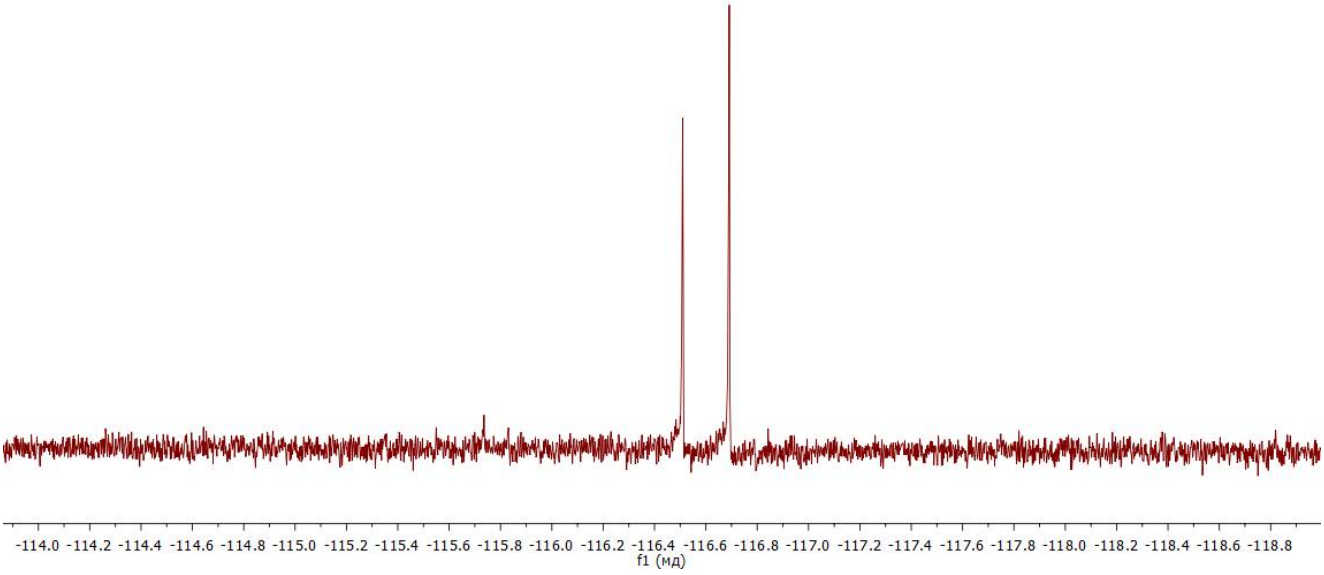


Fig. S36. $^{19}F\{^{1}H\}$ NMR Spectra of compound **2g** at 20 °C (400 МГц, $CDCl_3$).

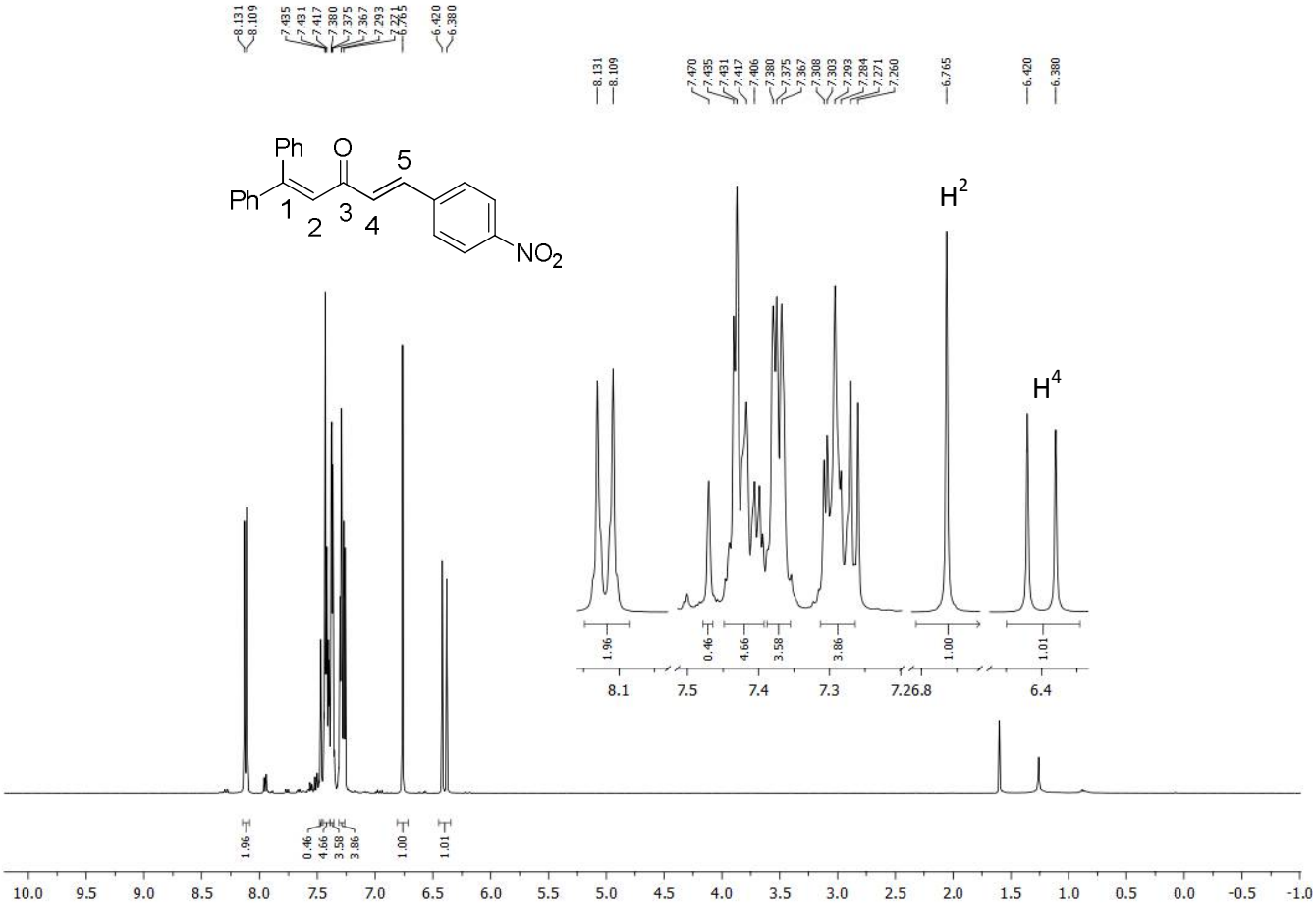


Fig. S37. ^{1}H NMR Spectra of compound **3a** at 20 °C (400 МГц, $CDCl_3$).

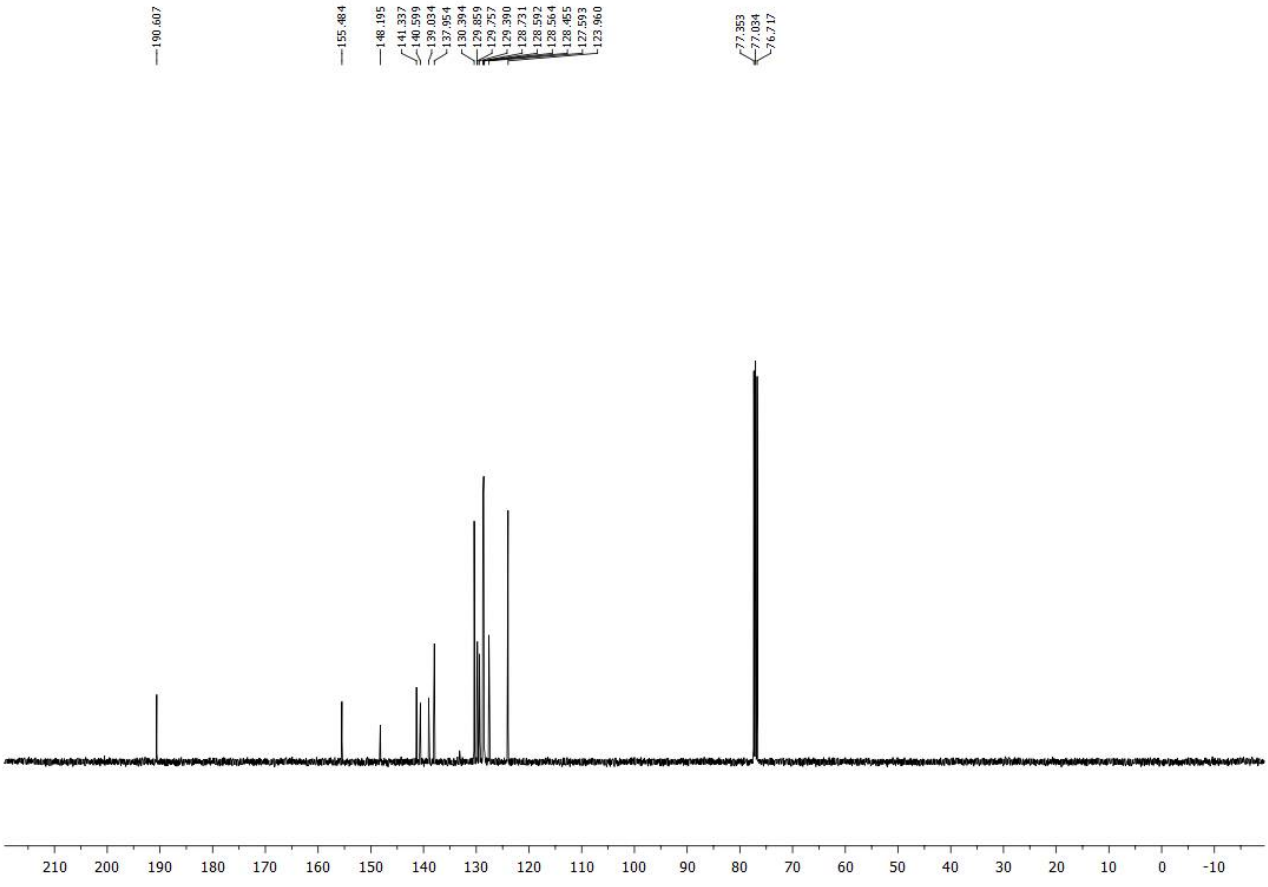


Fig. S38. ^{13}C NMR Spectra of compound **3a** at 20 °C (101МГц, $CDCl_3$).

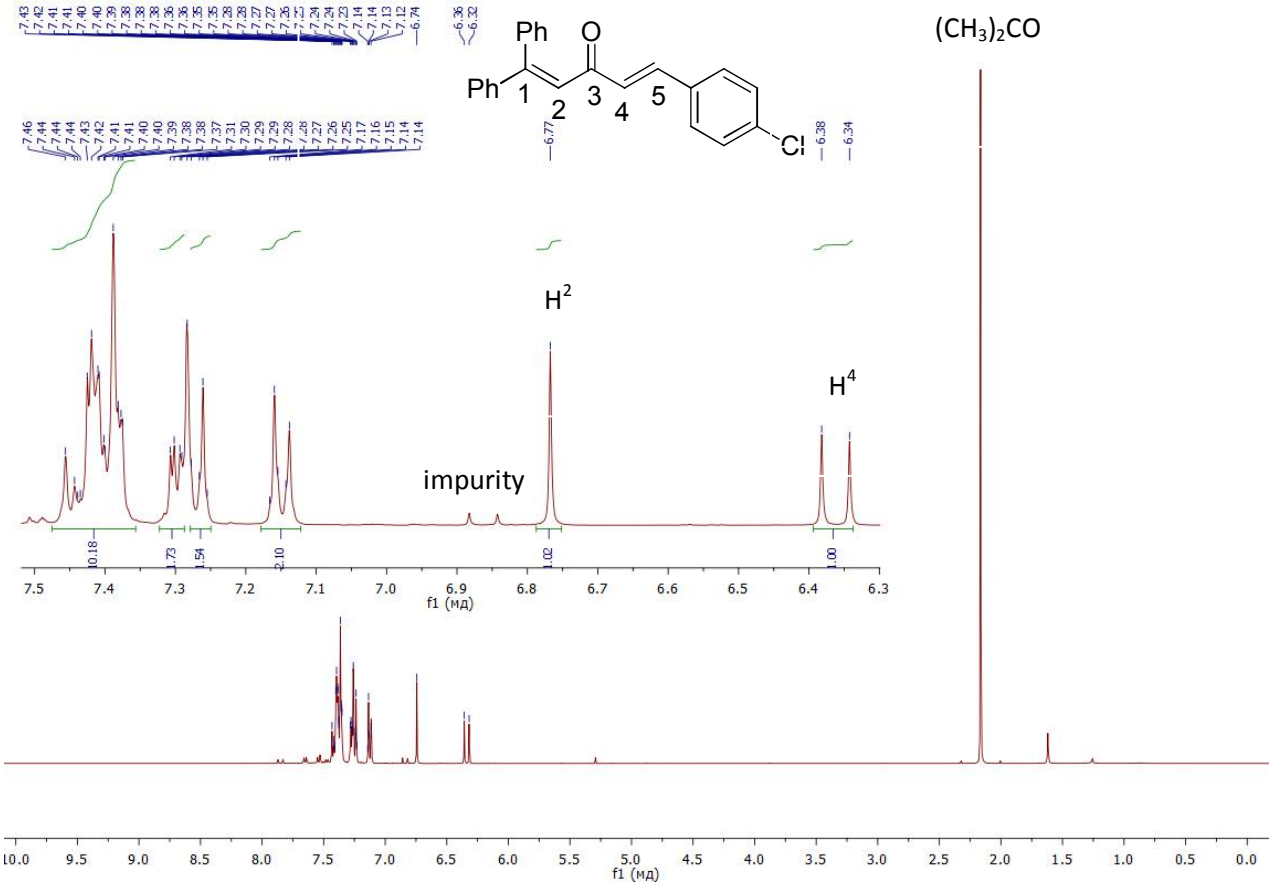


Fig. S39. ^{1}H NMR Spectra of compound **3b** at 20 °C (400 МГц, $CDCl_3$).

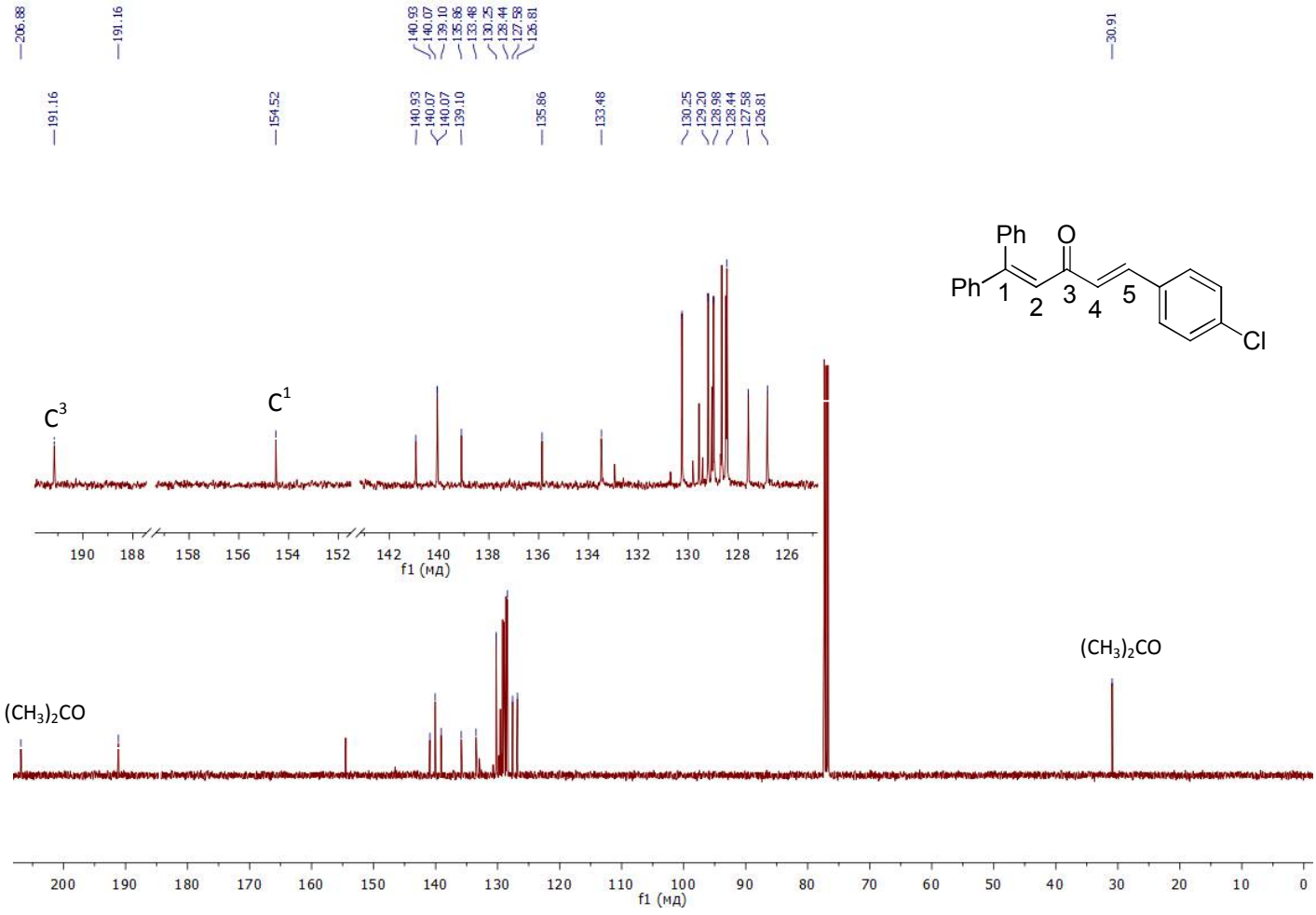


Fig. S40. ^{13}C NMR Spectra of compound **3b** at 20 °C (101МГц, $CDCl_3$).

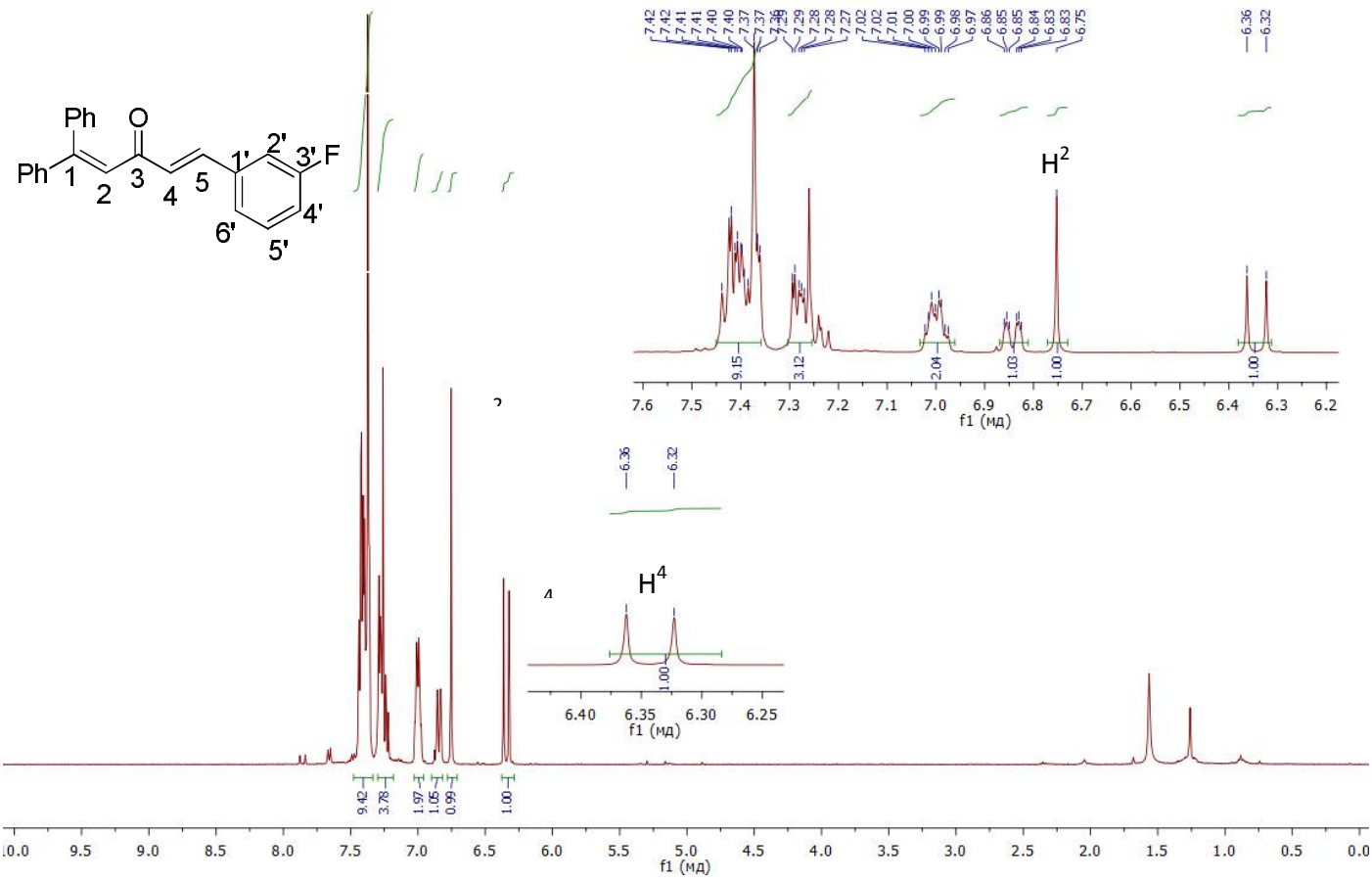


Fig. S41. ^{1}H NMR Spectra of compound **3c** at 20 °C (400 МГц, $CDCl_3$).

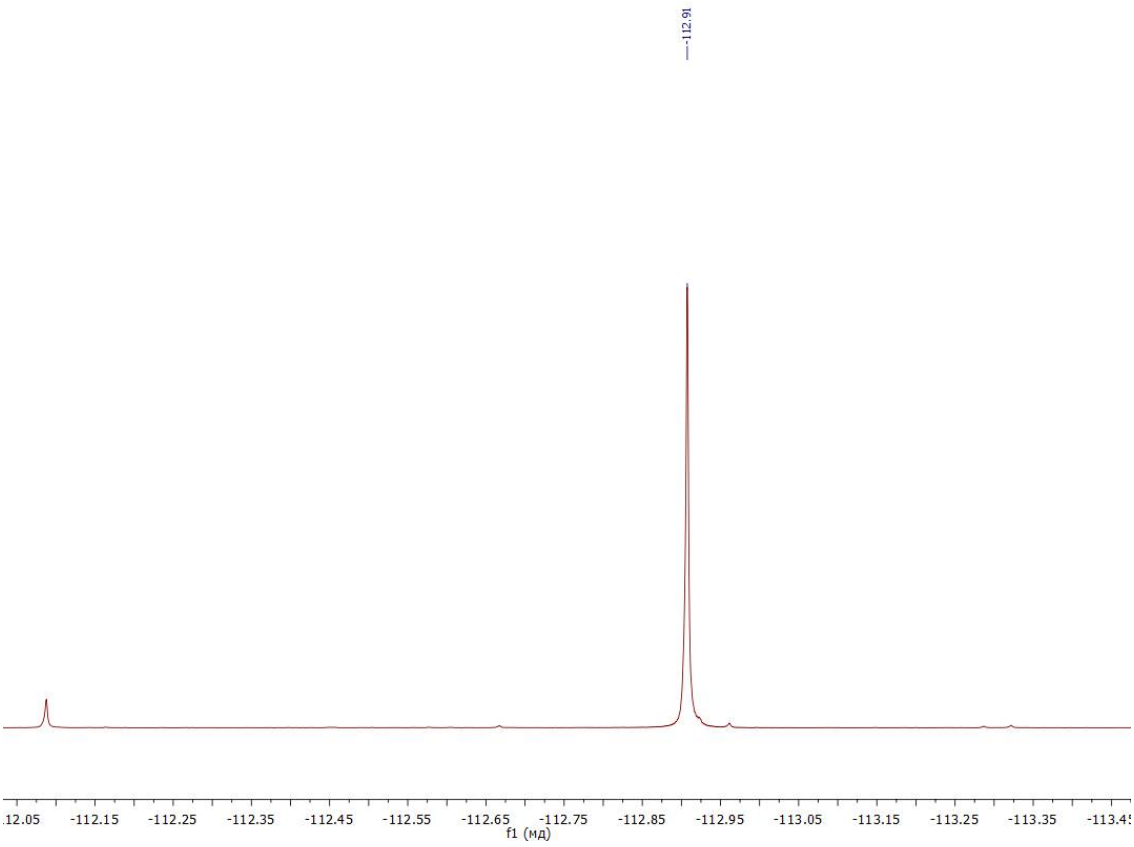


Fig. S42. $^{19}F\{^{1}H\}$ NMR Spectra of compound **3c** at 20 °C (376МГц, $CDCl_3$).

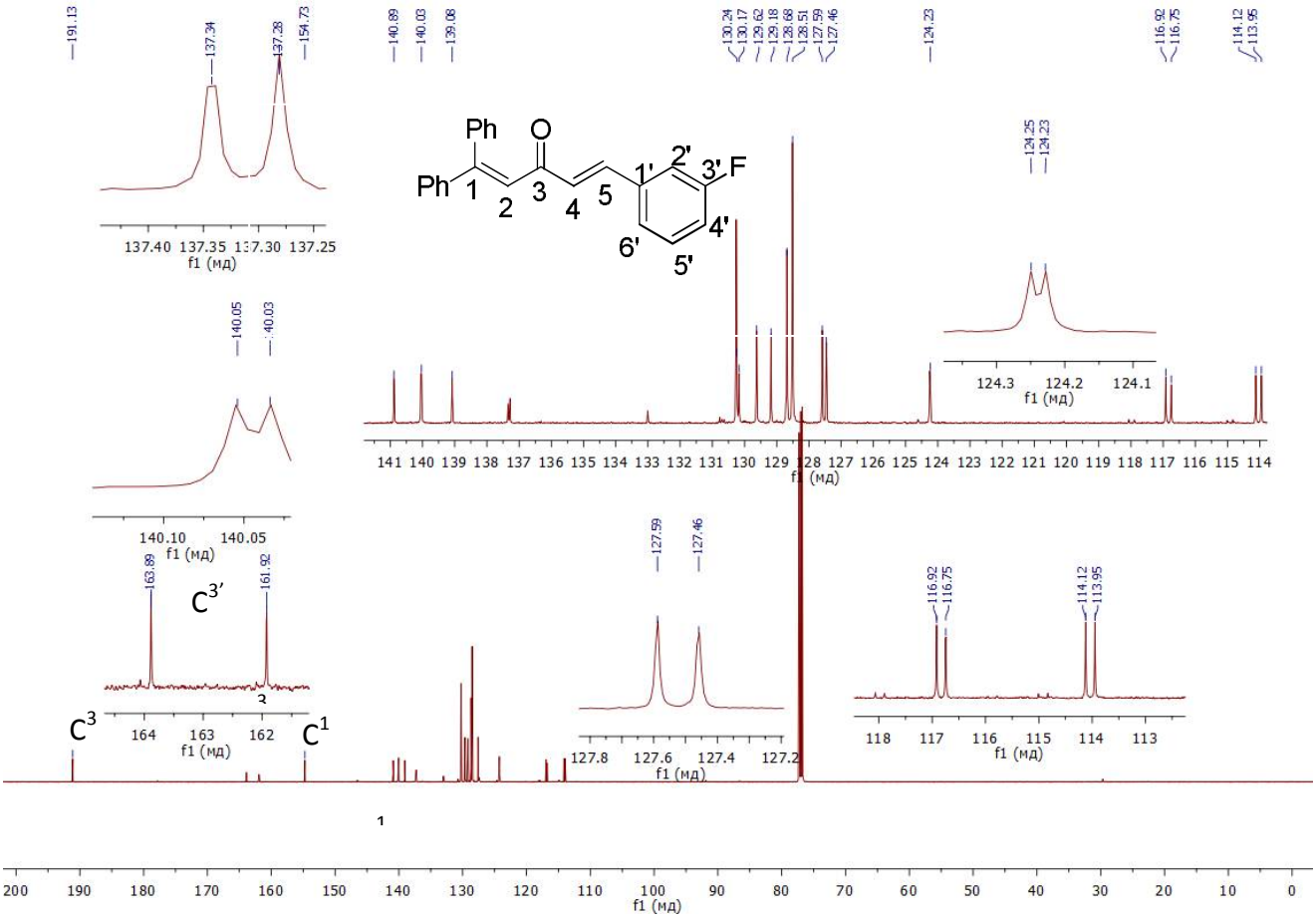


Fig. S43. ^{13}C NMR Spectra of compound **3c** at 20 °C (101МГц, $CDCl_3$).

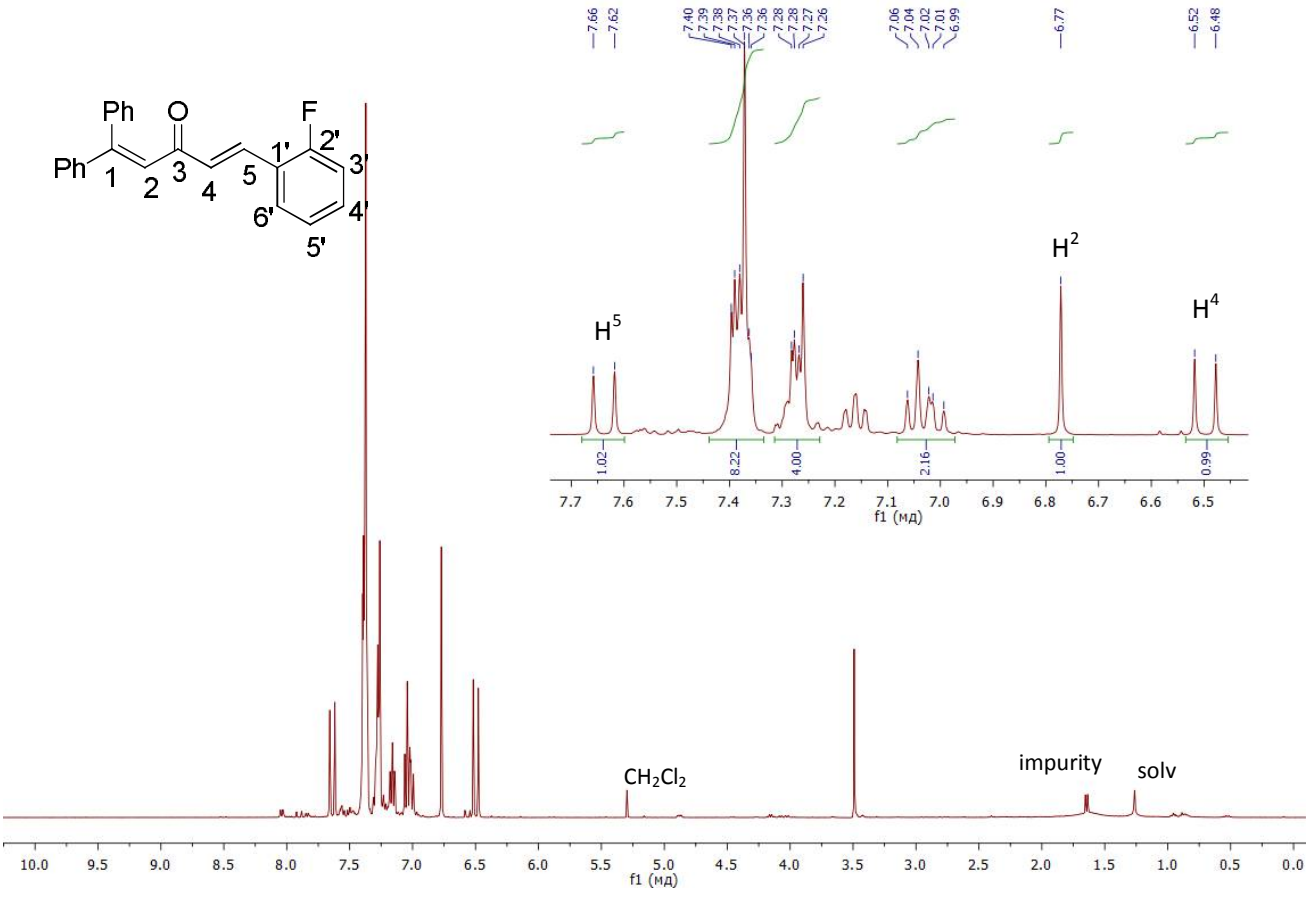


Fig. S44. ^{1}H NMR Spectra of compound **3d** at 20 °C (400 МГц, $CDCl_3$).

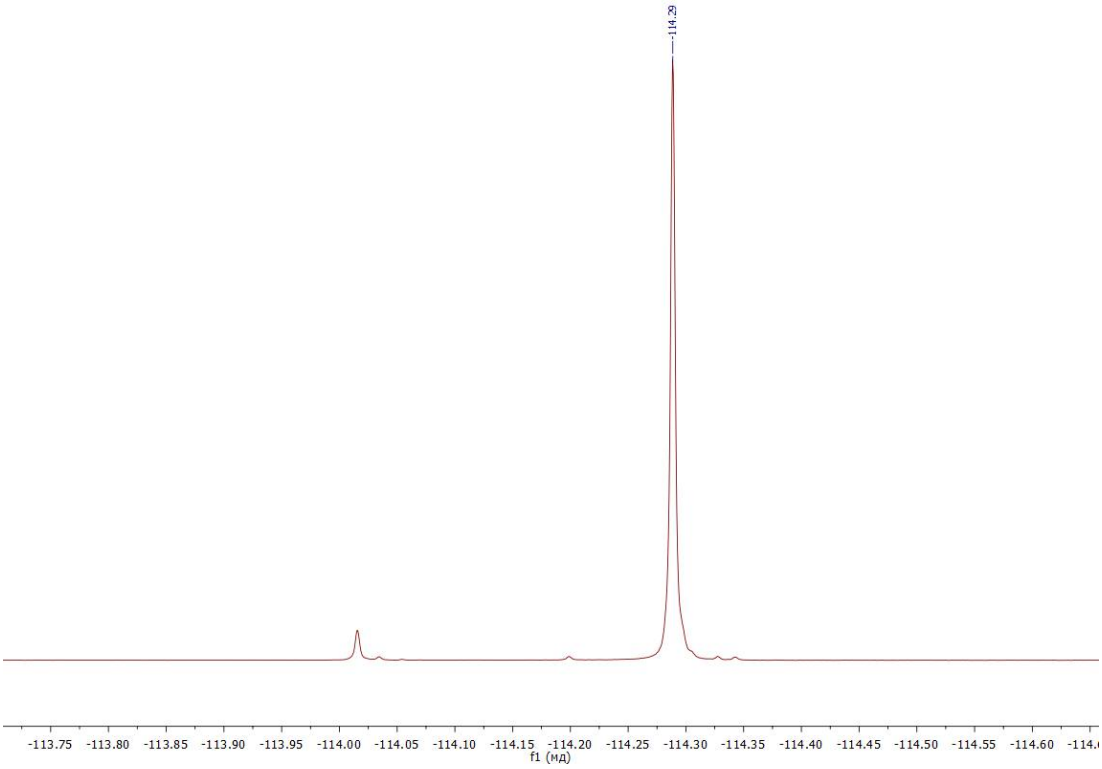


Fig. S45. $^{19}F\{^{1}H\}$ NMR Spectra of compound **3d** at 20 °C (376МГц, $CDCl_3$).

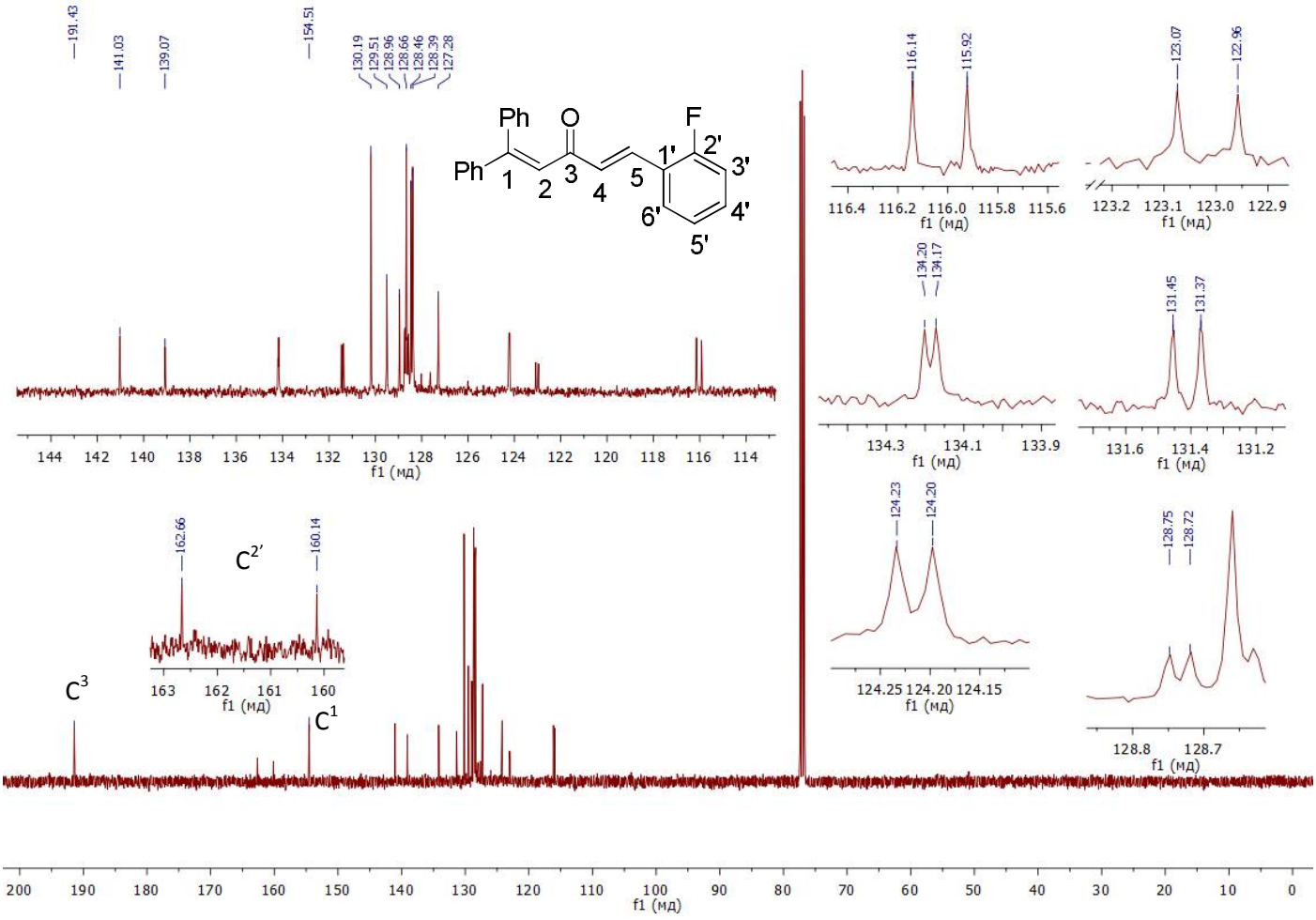


Fig. S46. ^{13}C NMR Spectra of compound **3d** at 20 °C (101МГц, $CDCl_3$).

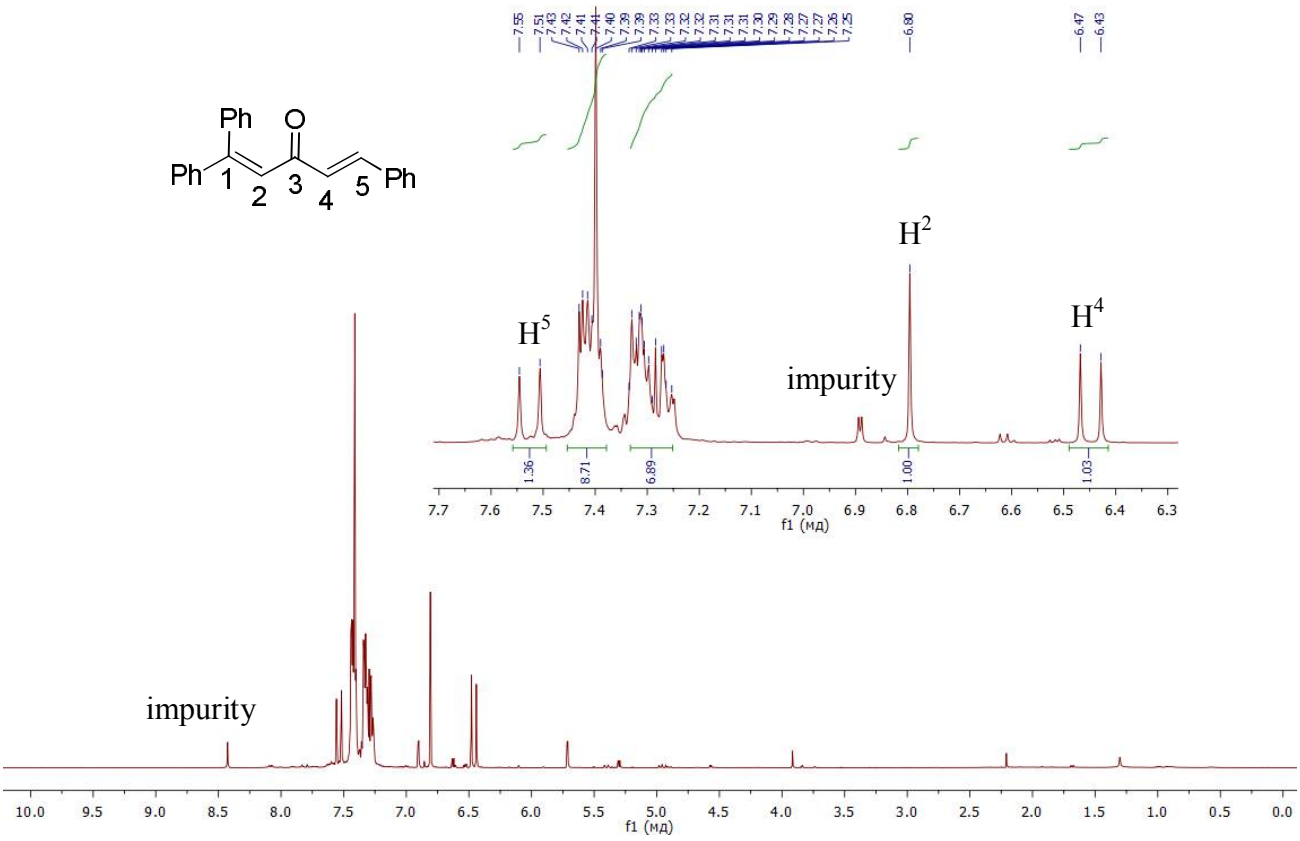


Fig. S47. ^{1}H NMR Spectra of compound **3e** at 20 °C (400 МГц, $CDCl_3$).

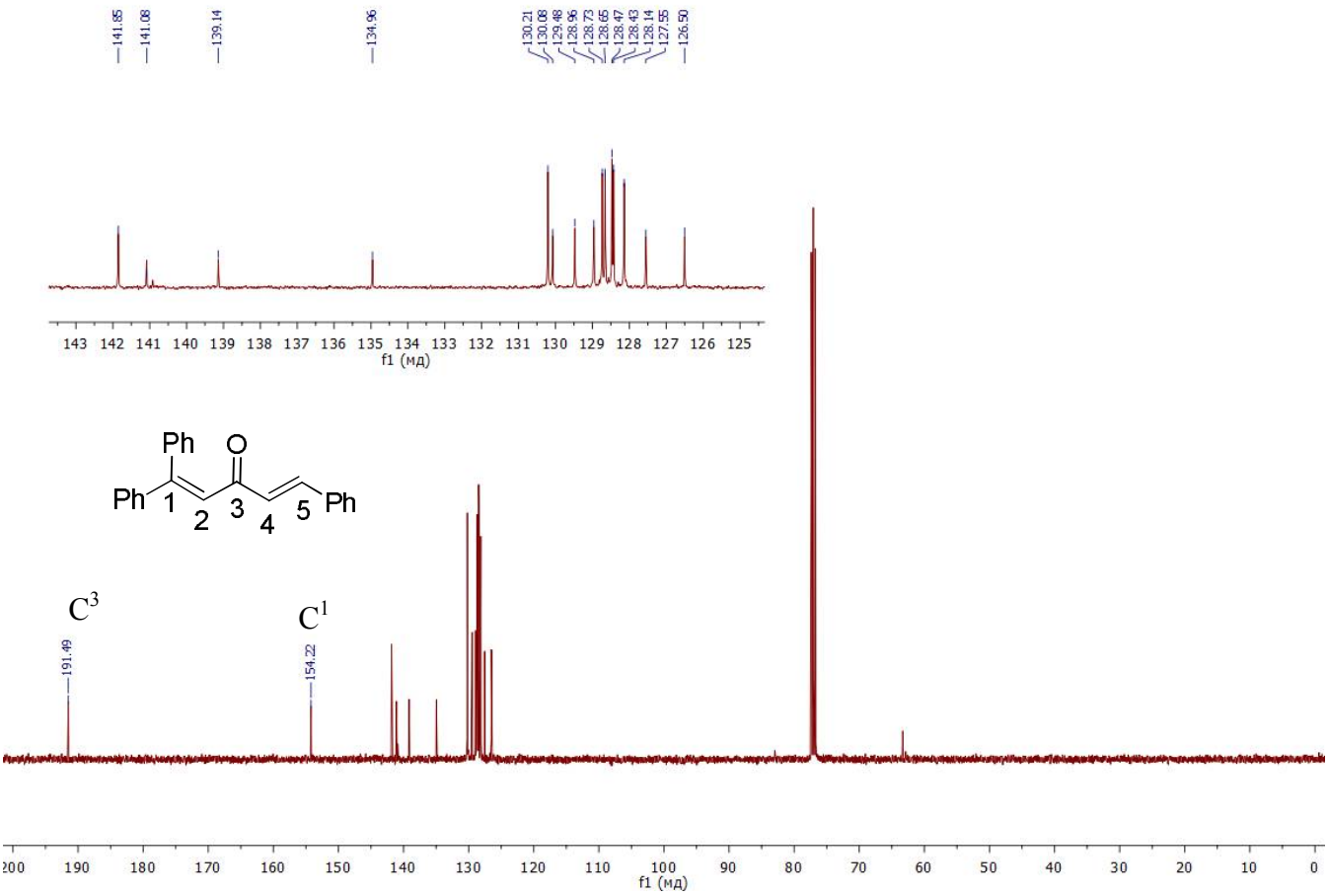


Fig. S48. ^{13}C NMR Spectra of compound **3e** at 20 °C (101МГц, $CDCl_3$).

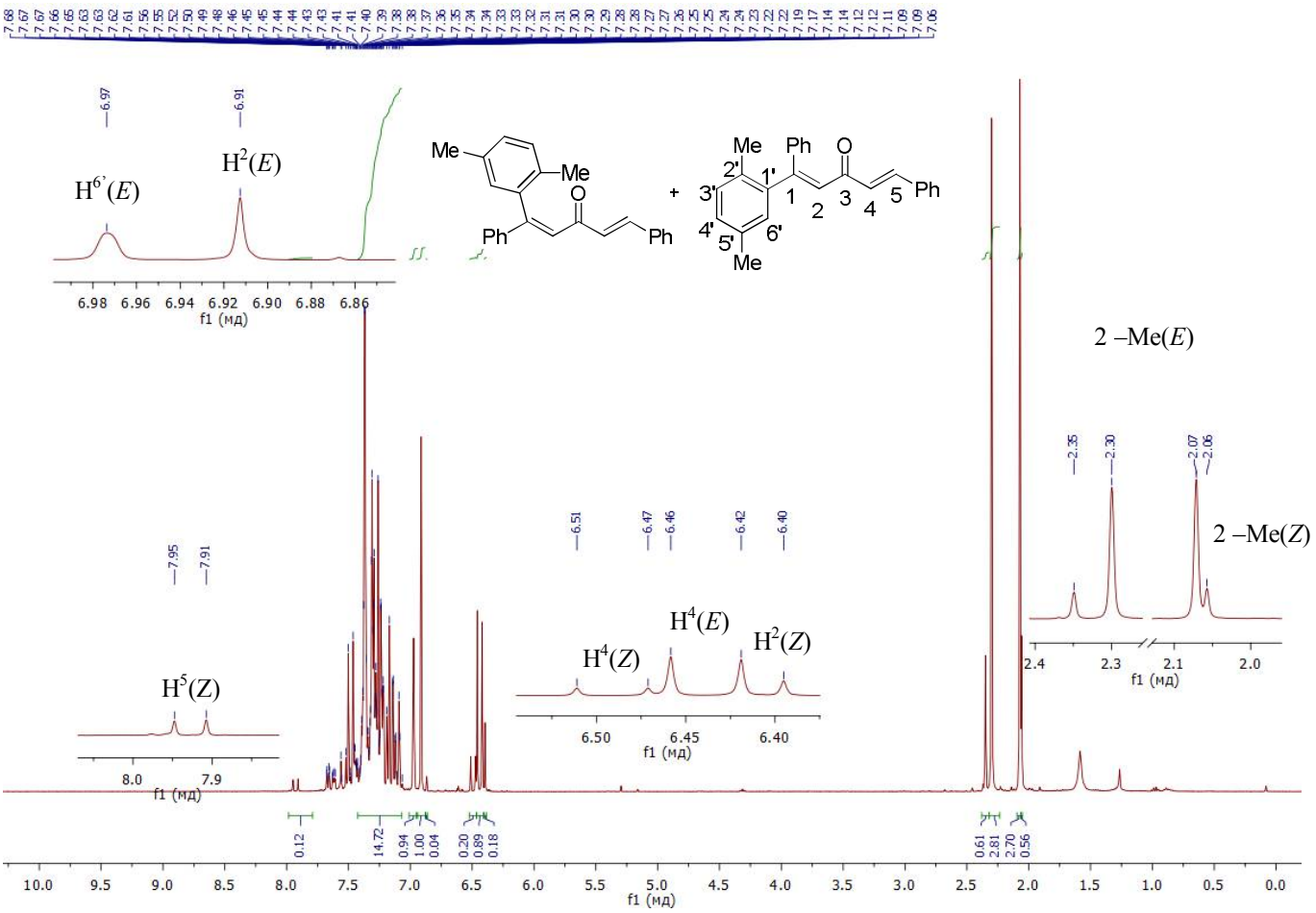


Fig. S49. ^{1}H NMR Spectra of compounds **3f** at 20 °C (400 МГц, $CDCl_3$).

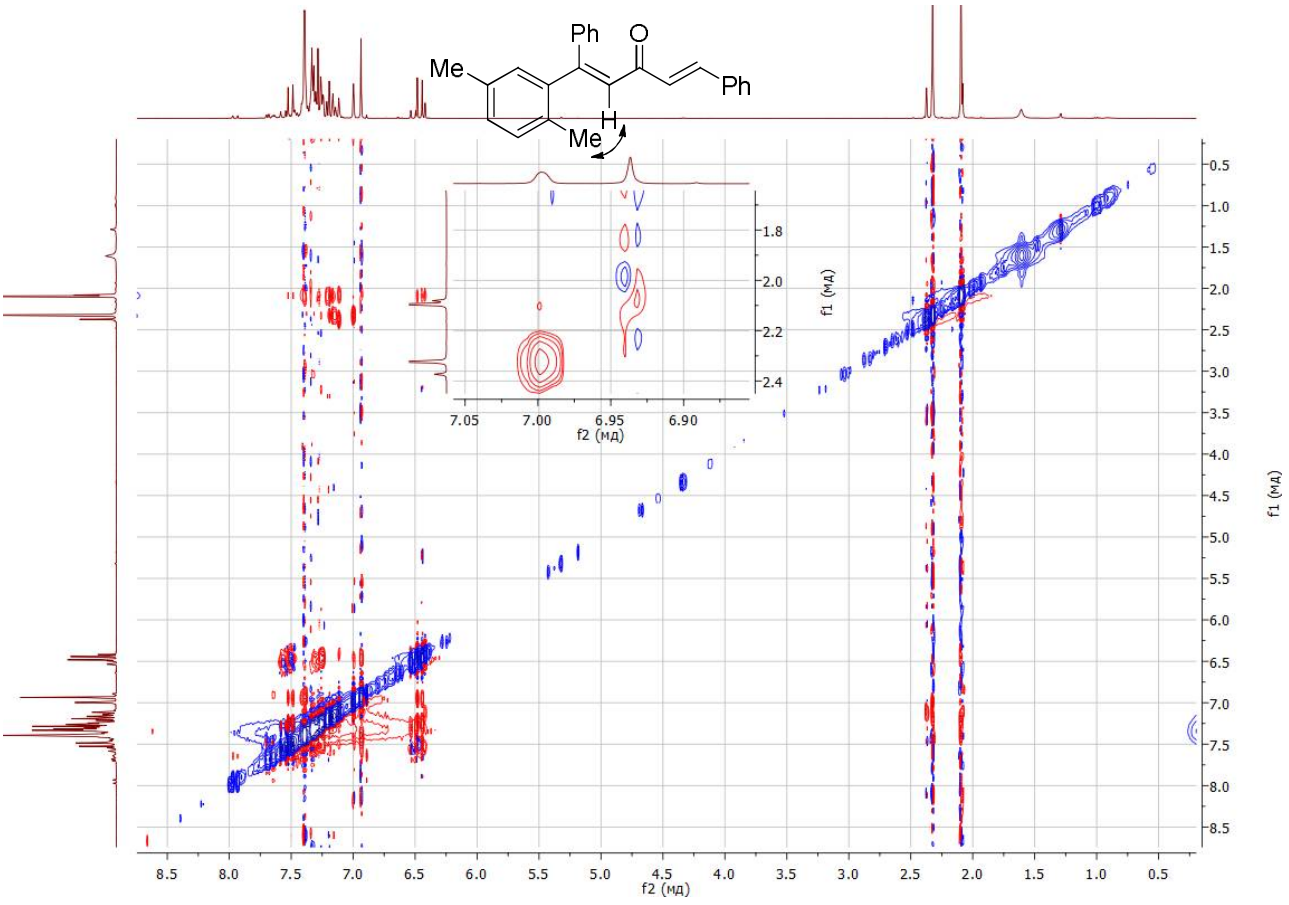


Fig. S50. ^{1}H-^{1}H NMR NOESY Spectra of compounds **3f** at 20 °C (400 МГц, $CDCl_3$).

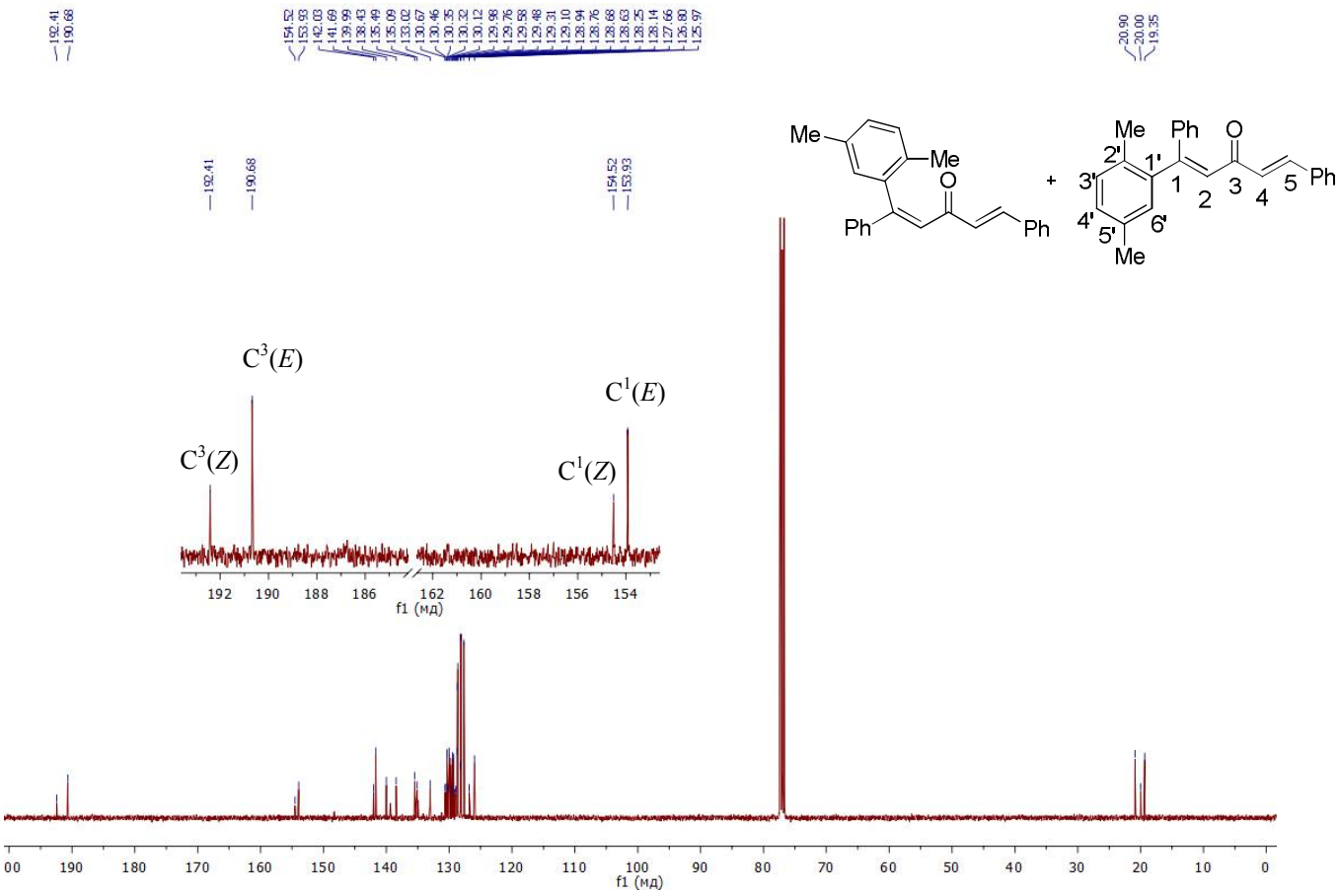


Fig. S51. ^{13}C NMR Spectra of compounds **3f** at 20 °C (101МГц, $CDCl_3$).

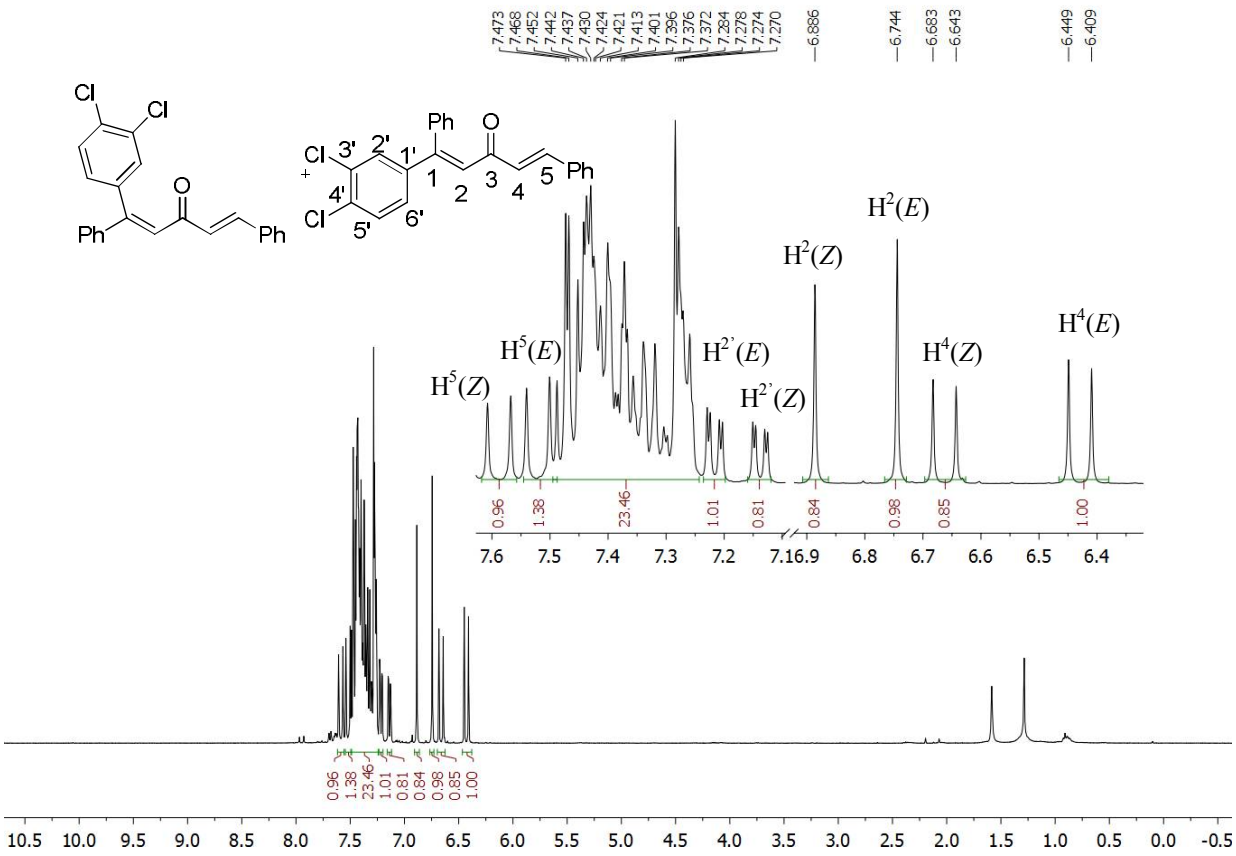


Fig. S52. ^{1}H NMR Spectra of compounds **3g** at 20 °C (400 МГц, $CDCl_3$).

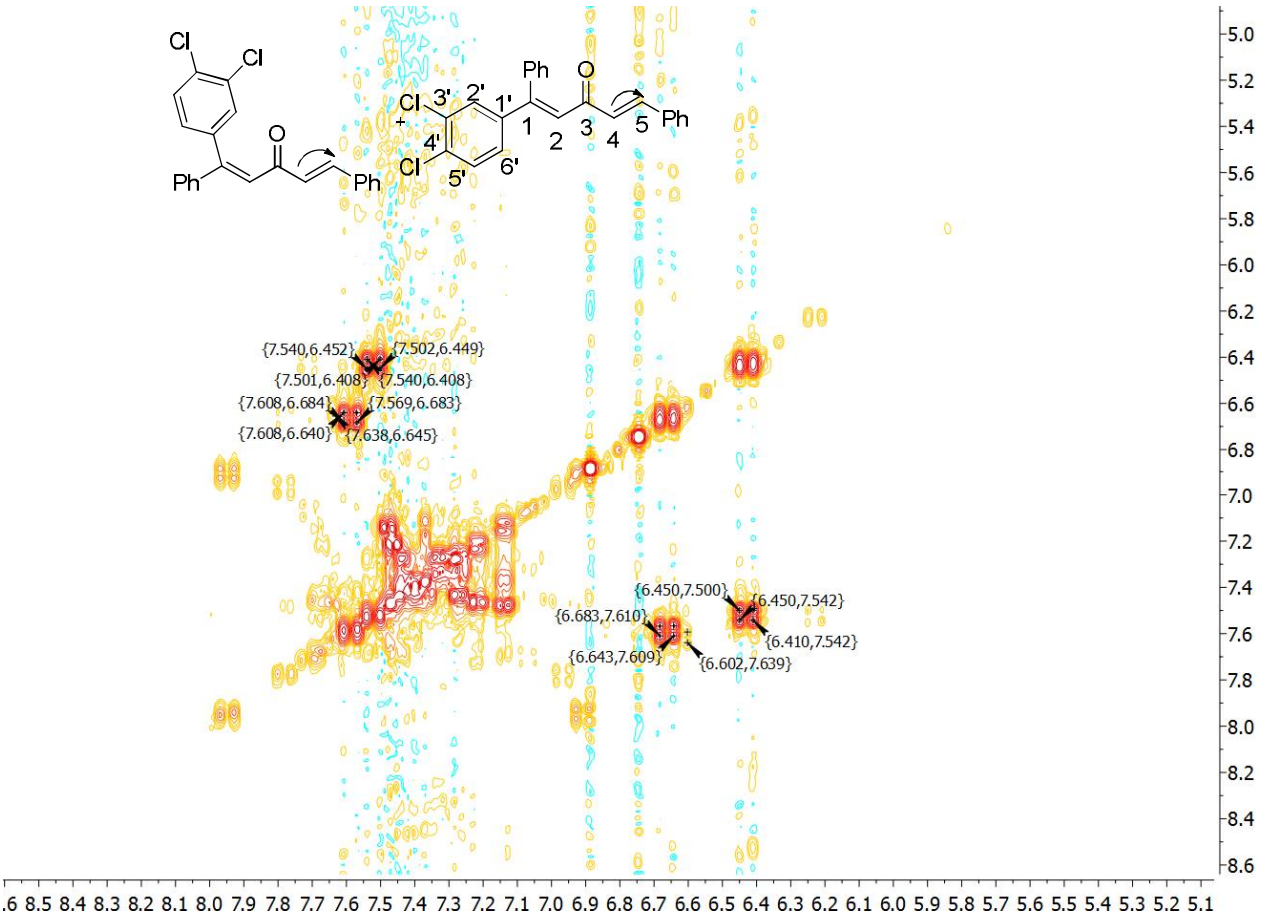


Fig. S53. ^{1}H-^{1}H COSY NMR Spectra of compounds **3g** at 20 °C (400 МГц, $CDCl_3$).

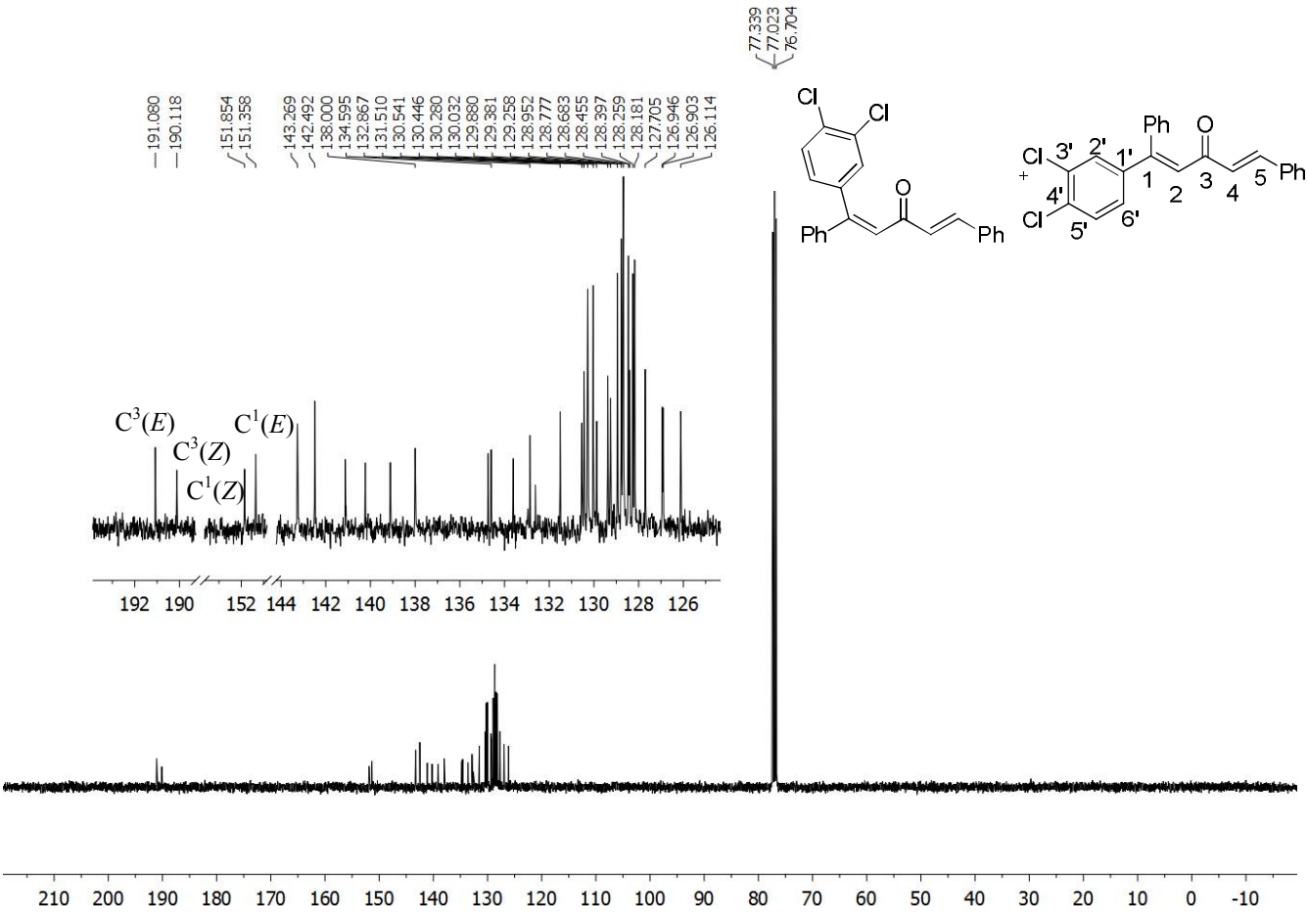


Fig. S54. ^{13}C NMR Spectra of compounds **3g** at 20 °C (101МГц, $CDCl_3$).

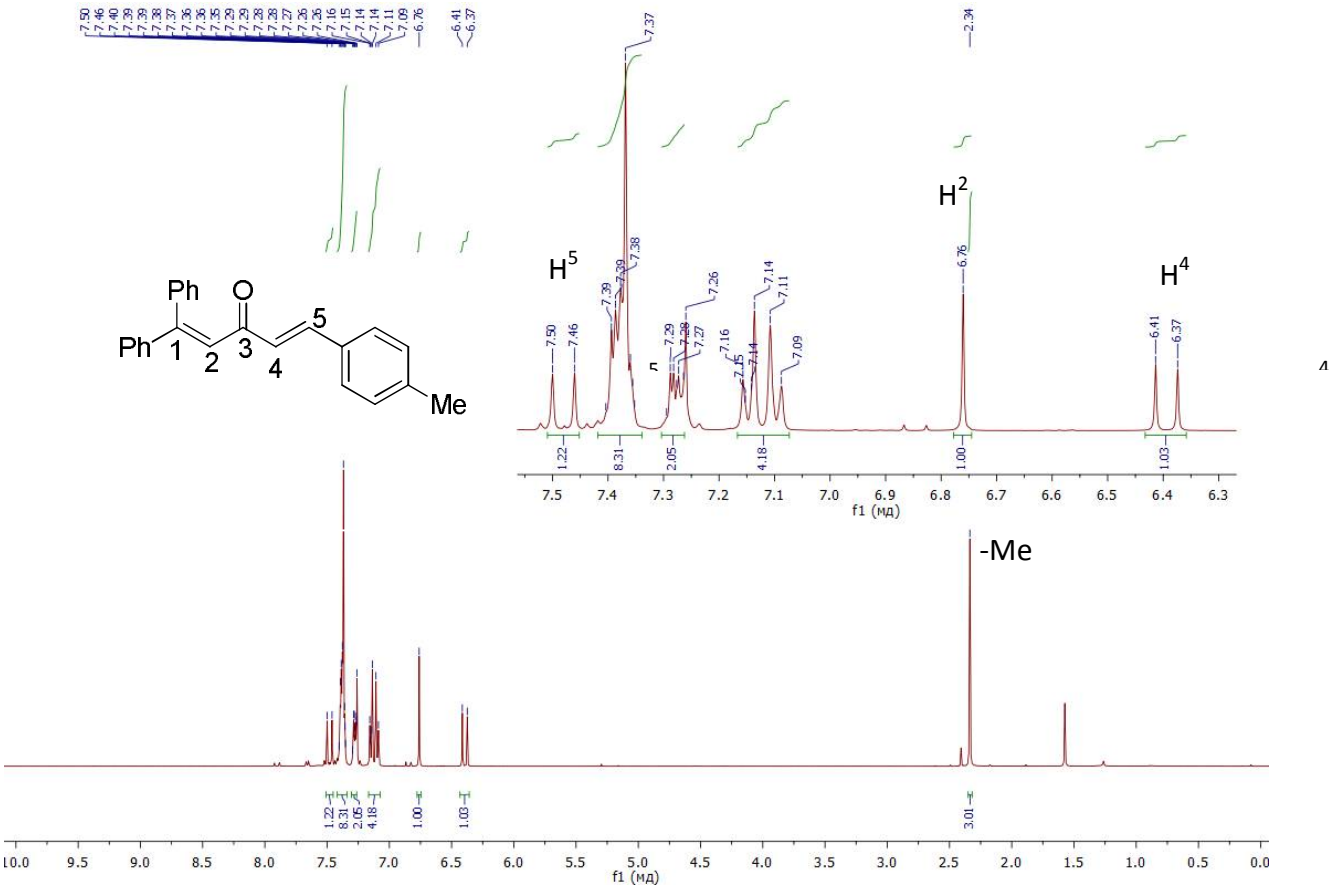


Fig. S55. ^{1}H NMR Spectra of compound **3h** at 20 °C (400 МГц, $CDCl_3$).

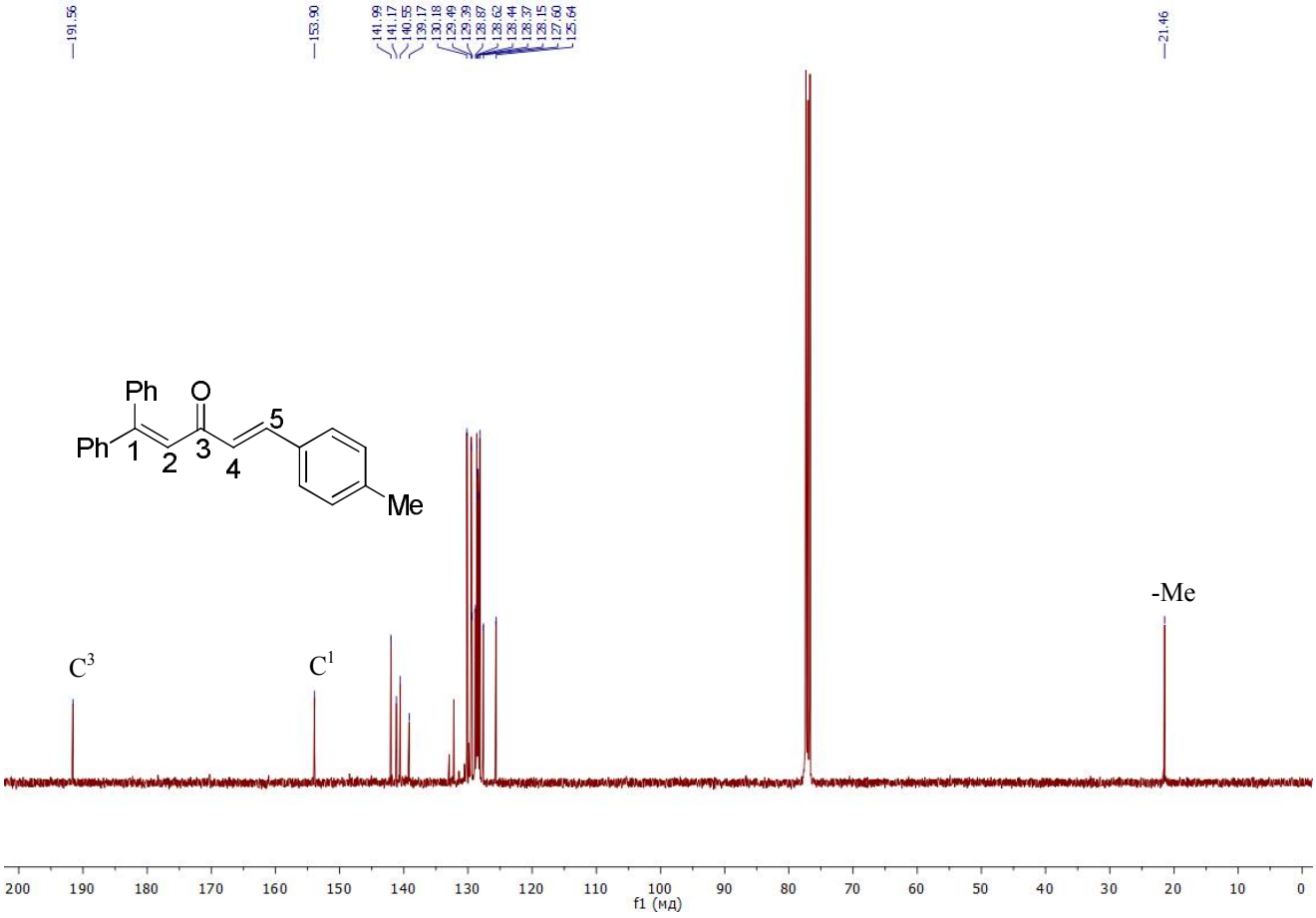


Fig. S56. ^{13}C NMR Spectra of compound **3h** at 20 °C (101МГц, $CDCl_3$).

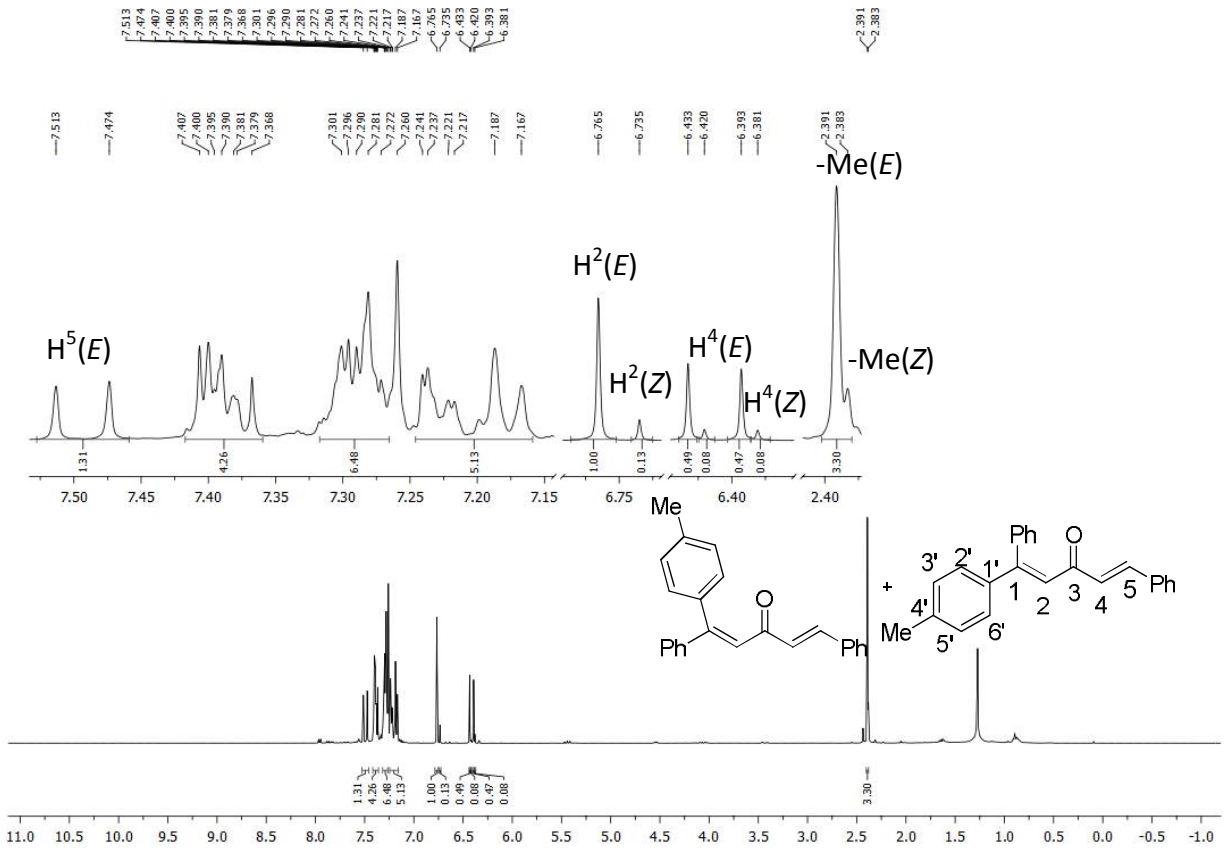


Fig. S57. ^{1}H NMR Spectra of compounds **3i** at 20 °C (400 МГц, $CDCl_3$).

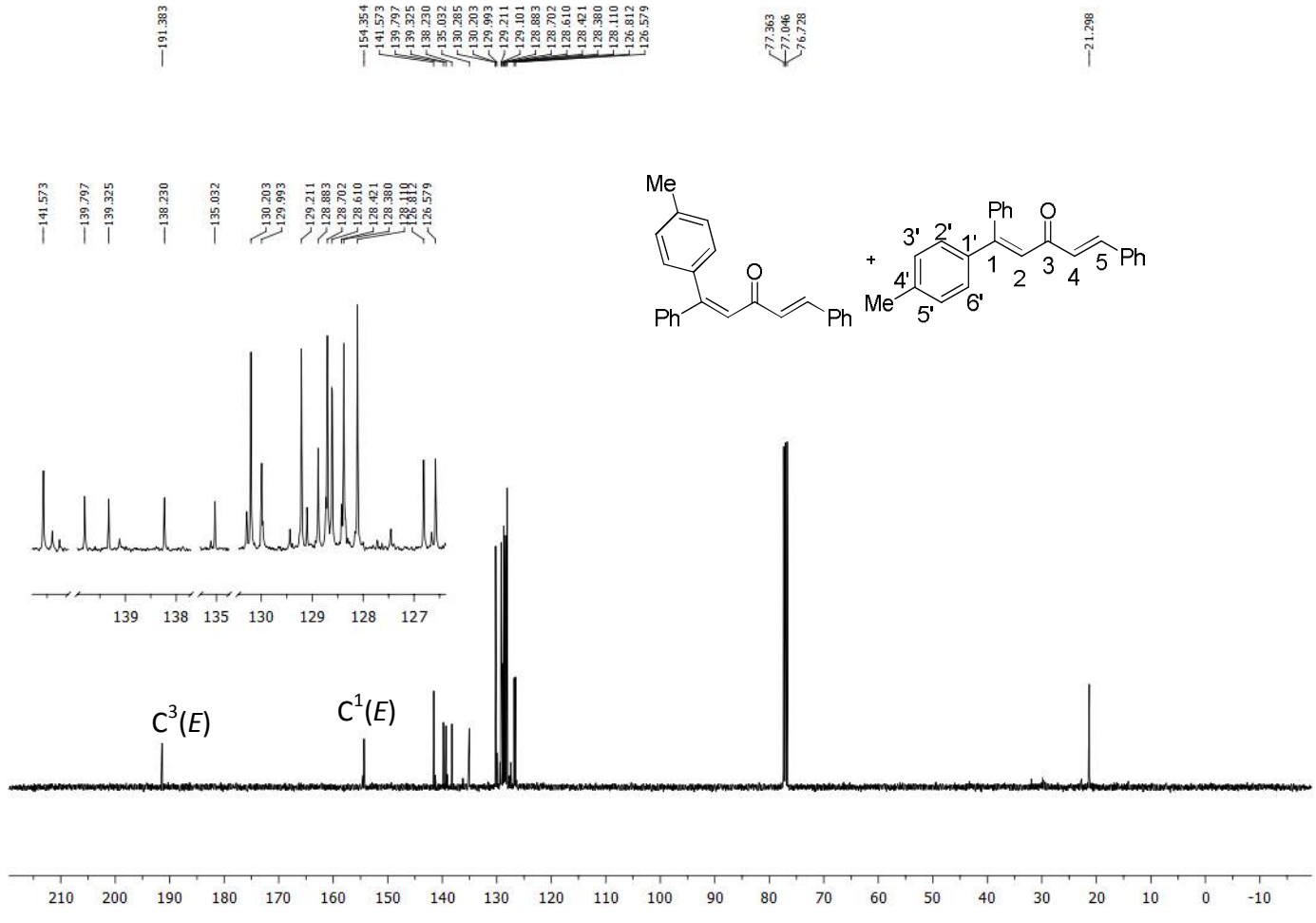


Fig. S58. ^{13}C NMR Spectra of compounds **3i** at 20 °C (101МГц, $CDCl_3$).

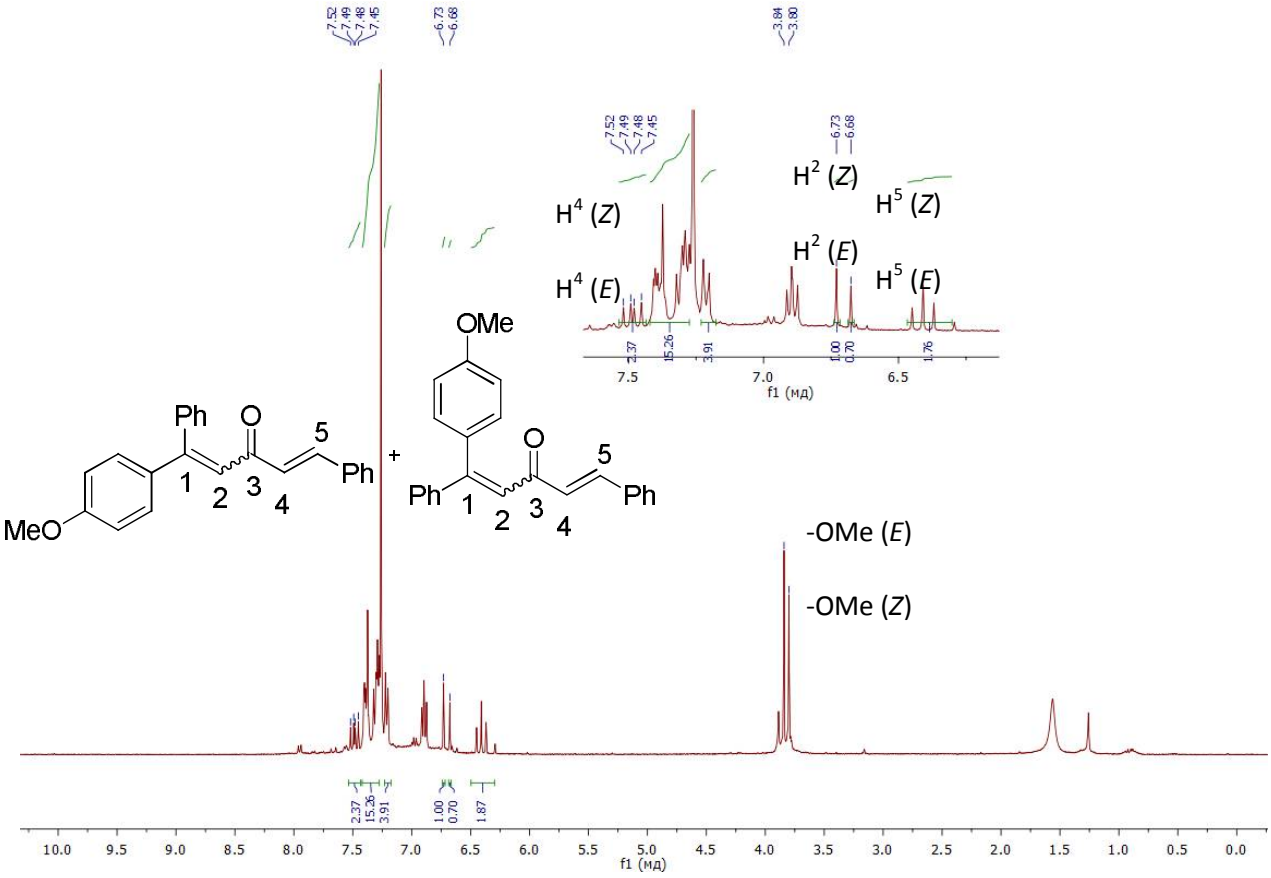


Fig. S59. ^{1}H NMR Spectra of compounds **3j** at 20 °C (400 МГц, $CDCl_3$).

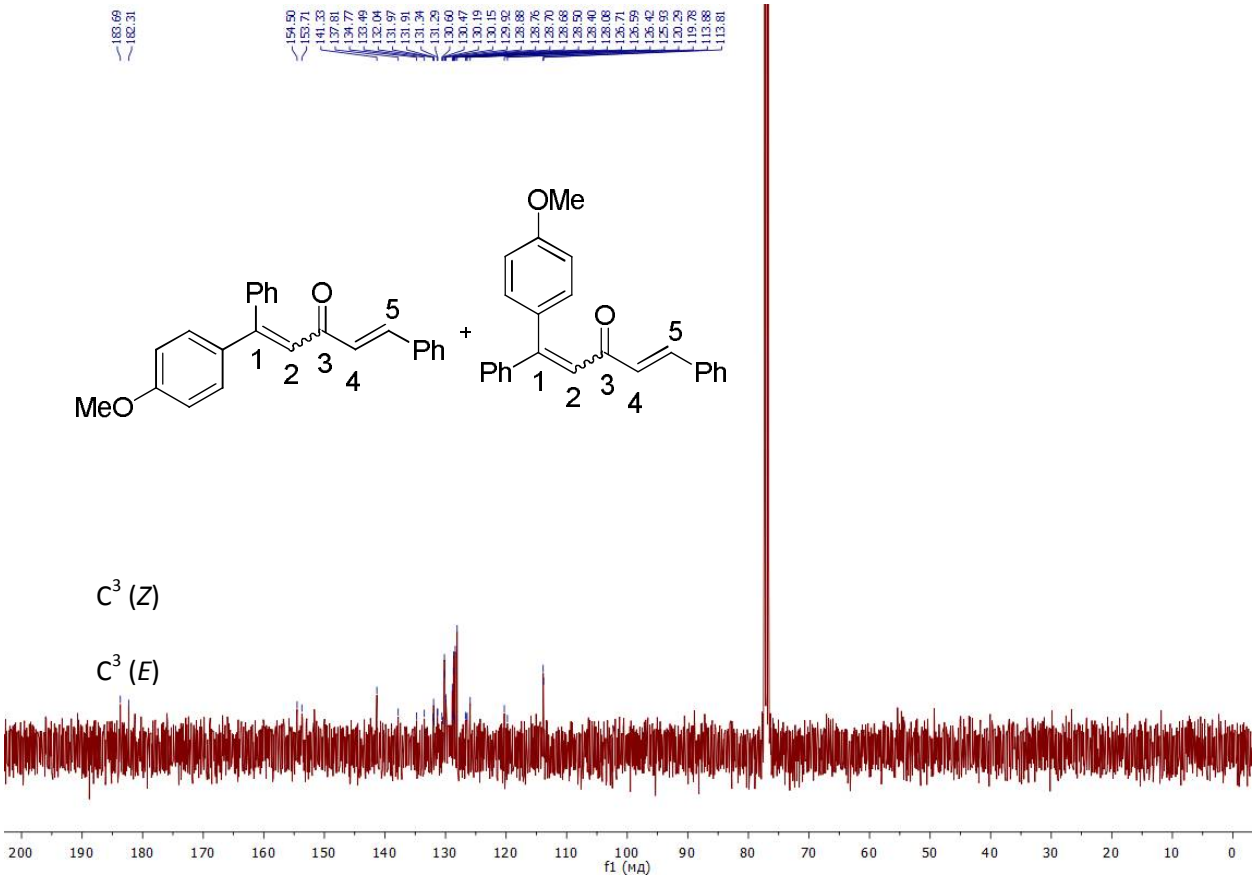


Fig. S60. ^{13}C NMR Spectra of compounds **3j** at 20 °C (101МГц, $CDCl_3$).

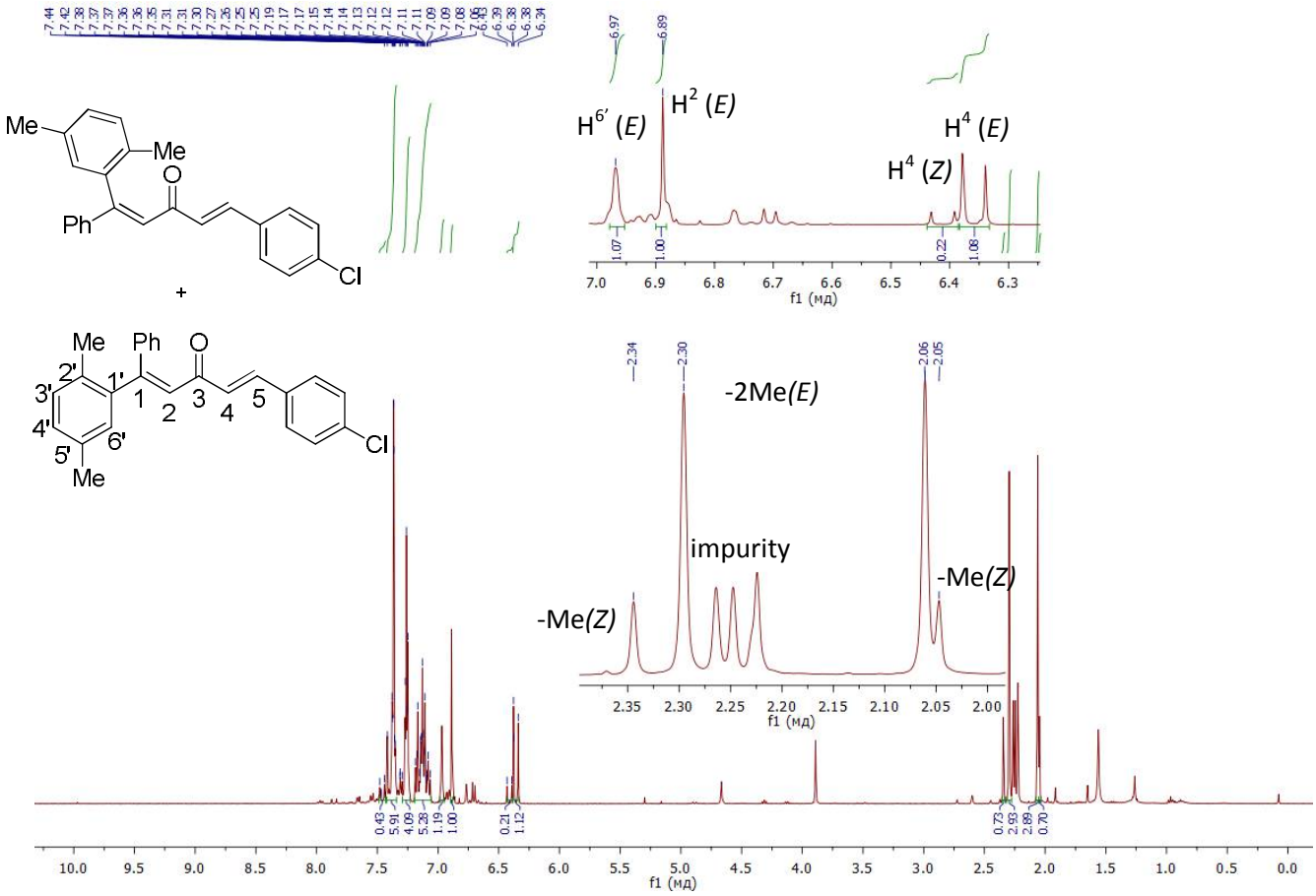


Fig. S61. ^{1}H NMR Spectra of compounds **3k** at 20 °C (400 МГц, $CDCl_3$).

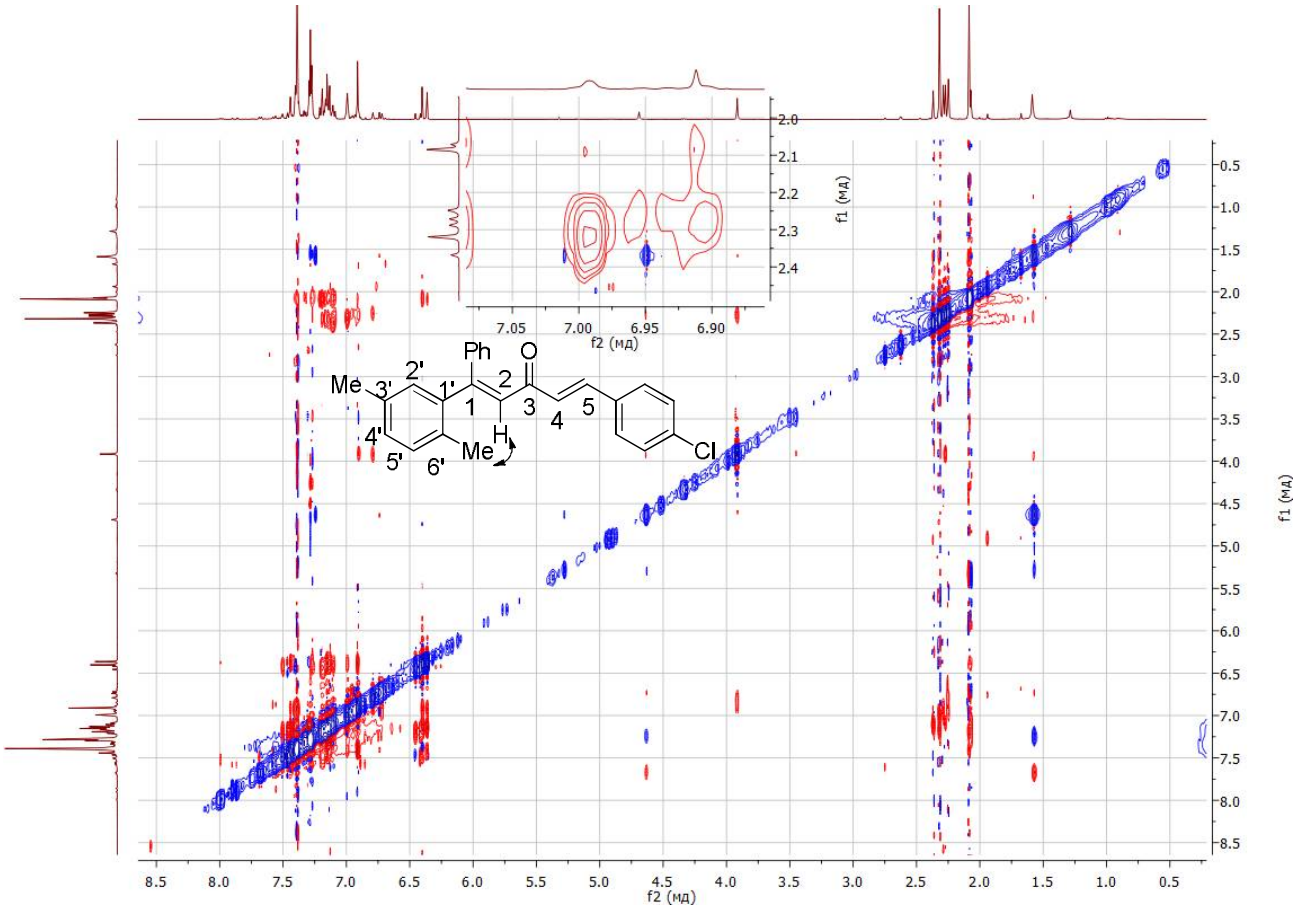


Fig. S62. ^{1}H-^{1}H NMR NOESY Spectra of compounds **3k** at 20 °C (400 МГц, $CDCl_3$).

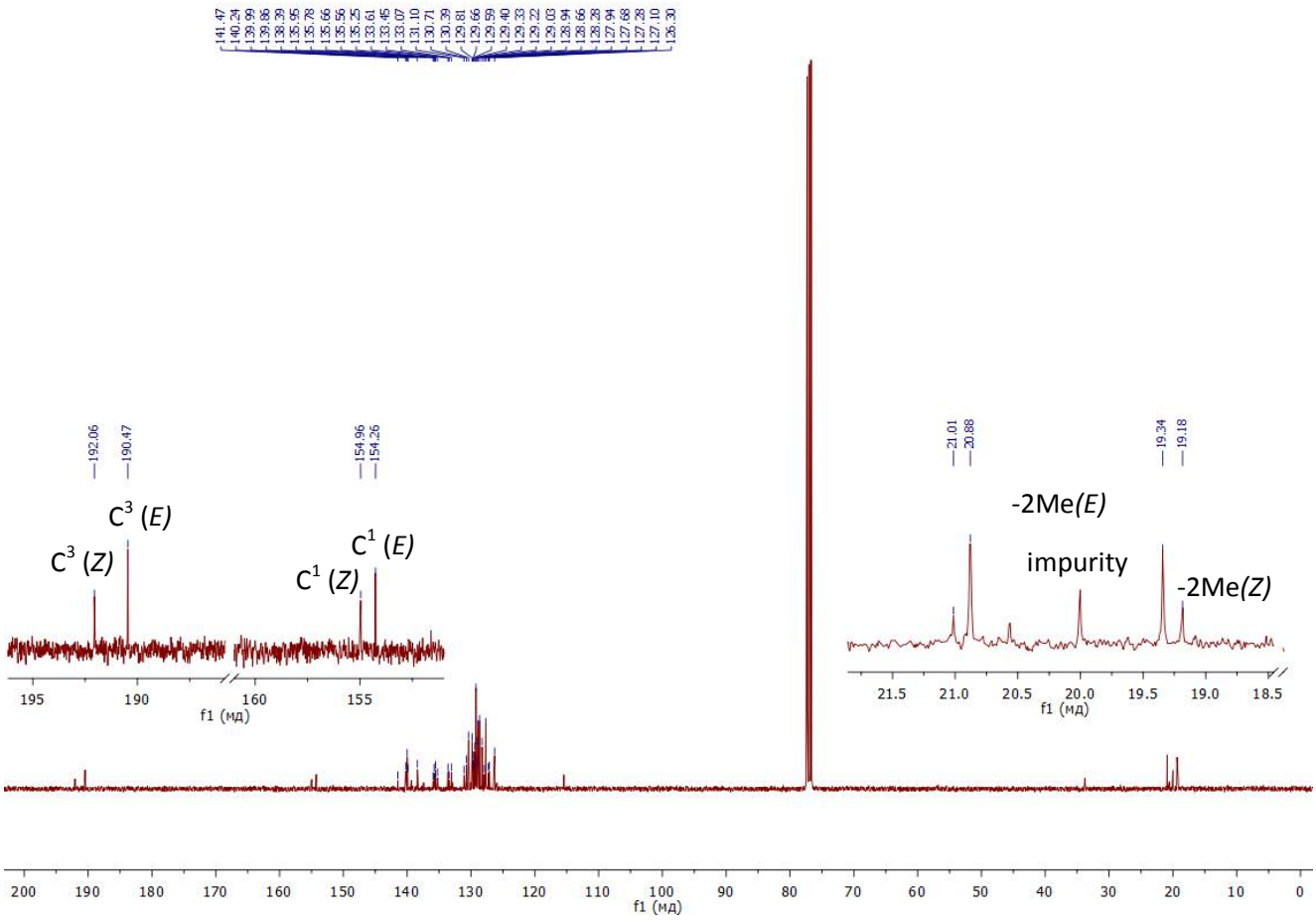


Fig. S63. ^{13}C NMR Spectra of compounds **3k** at 20 °C (101МГц, $CDCl_3$).

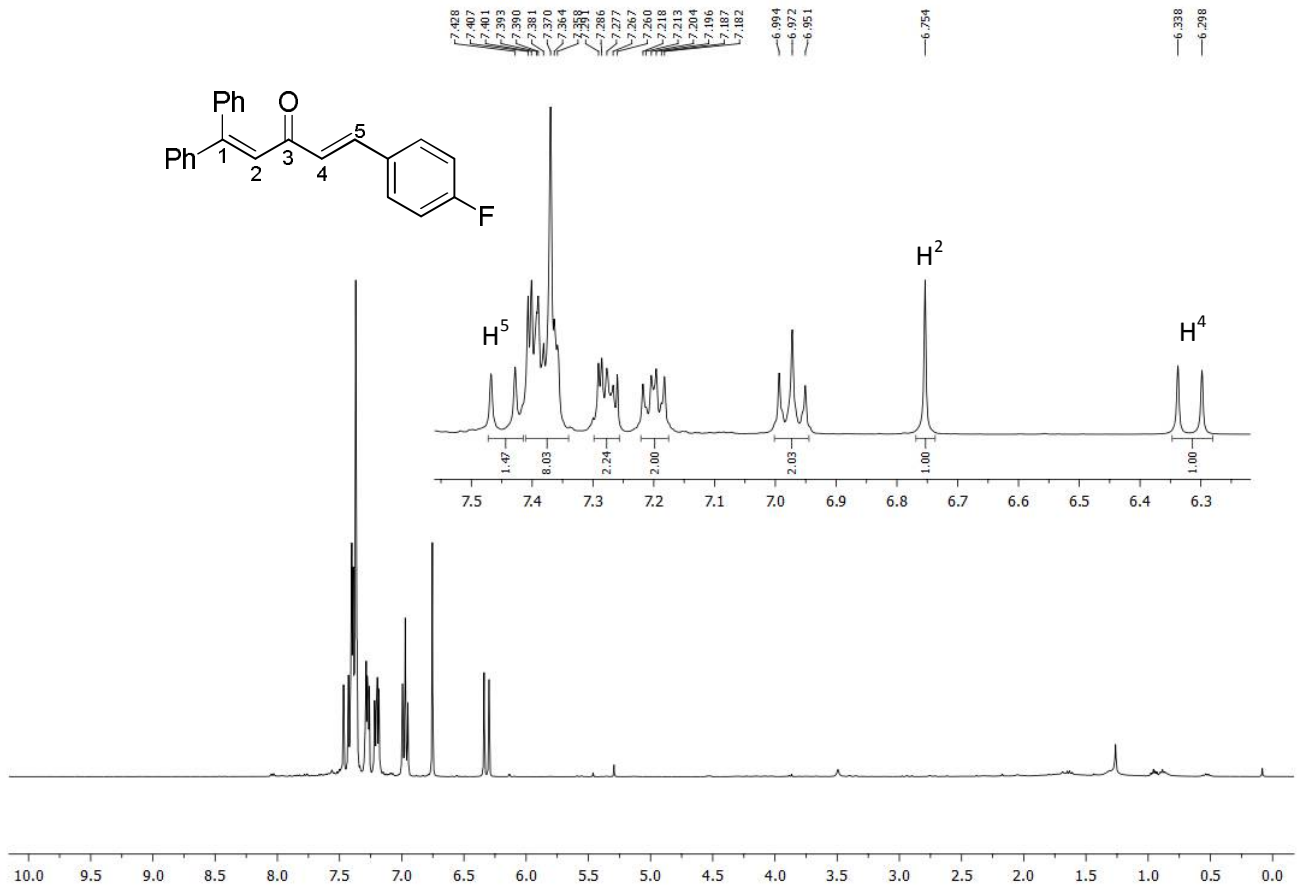


Fig. S64. ^{1}H NMR Spectra of compound **3l** at 20 °C (400 МГц, $CDCl_3$).

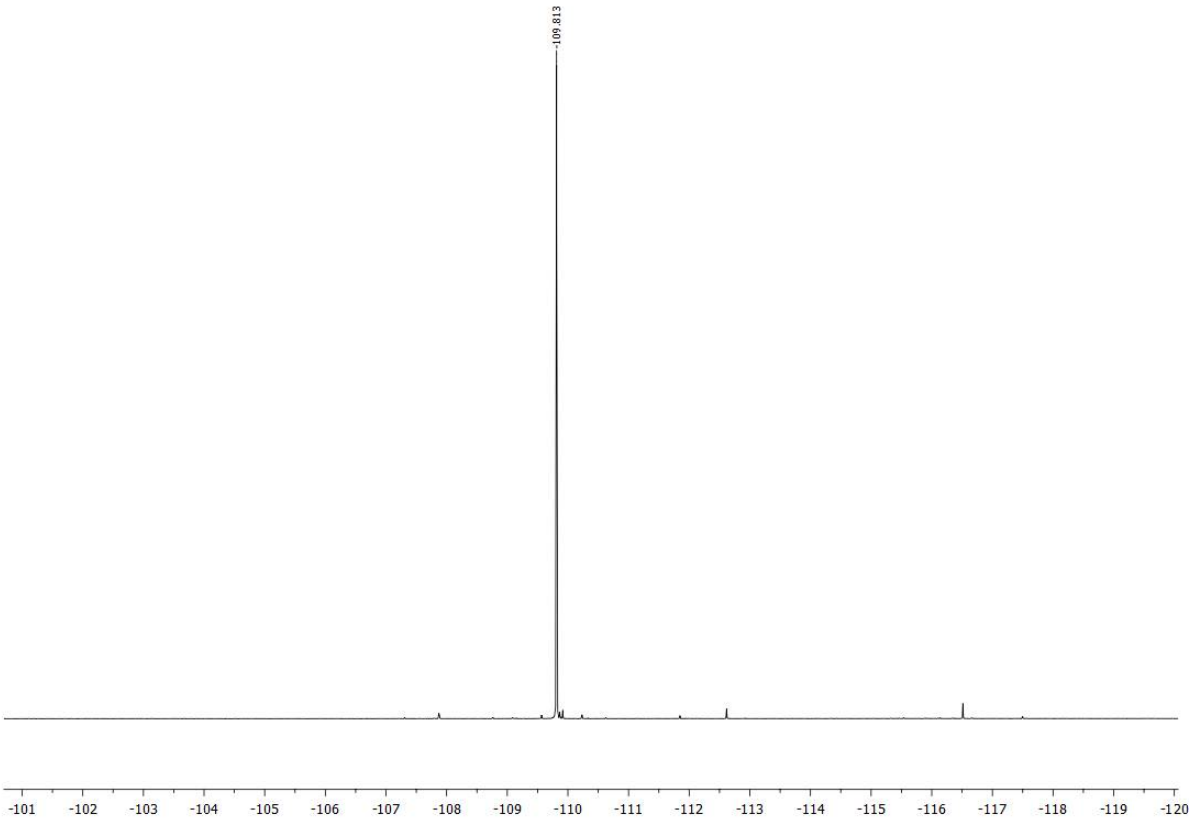


Fig. S65. $^{19}F\{^{1}H\}$ NMR Spectra of compound **3l** at 20 °C (376МГц, $CDCl_3$).

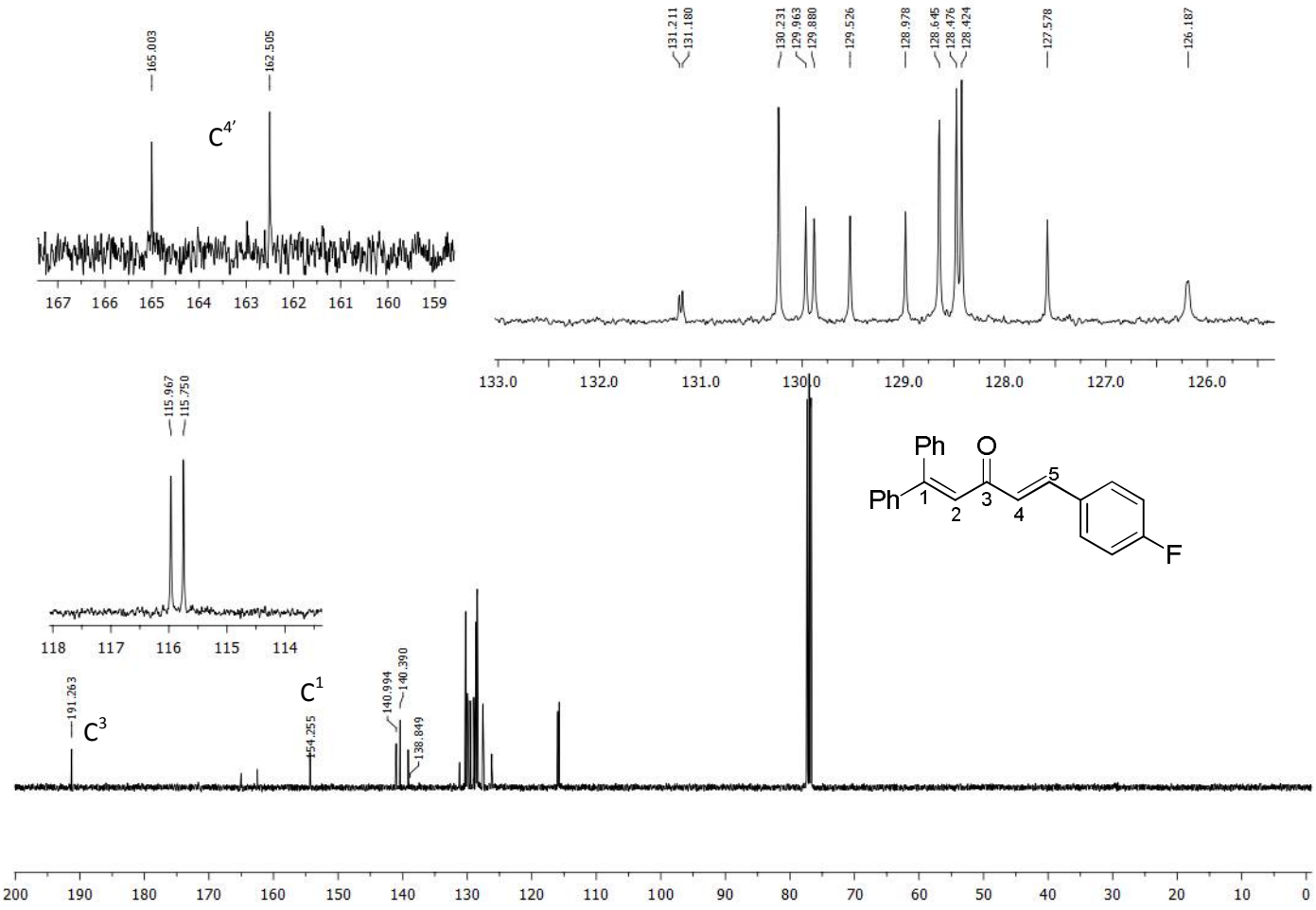


Fig. S66. ^{13}C NMR Spectra of compound **3l** at 20 °C (101МГц, $CDCl_3$).

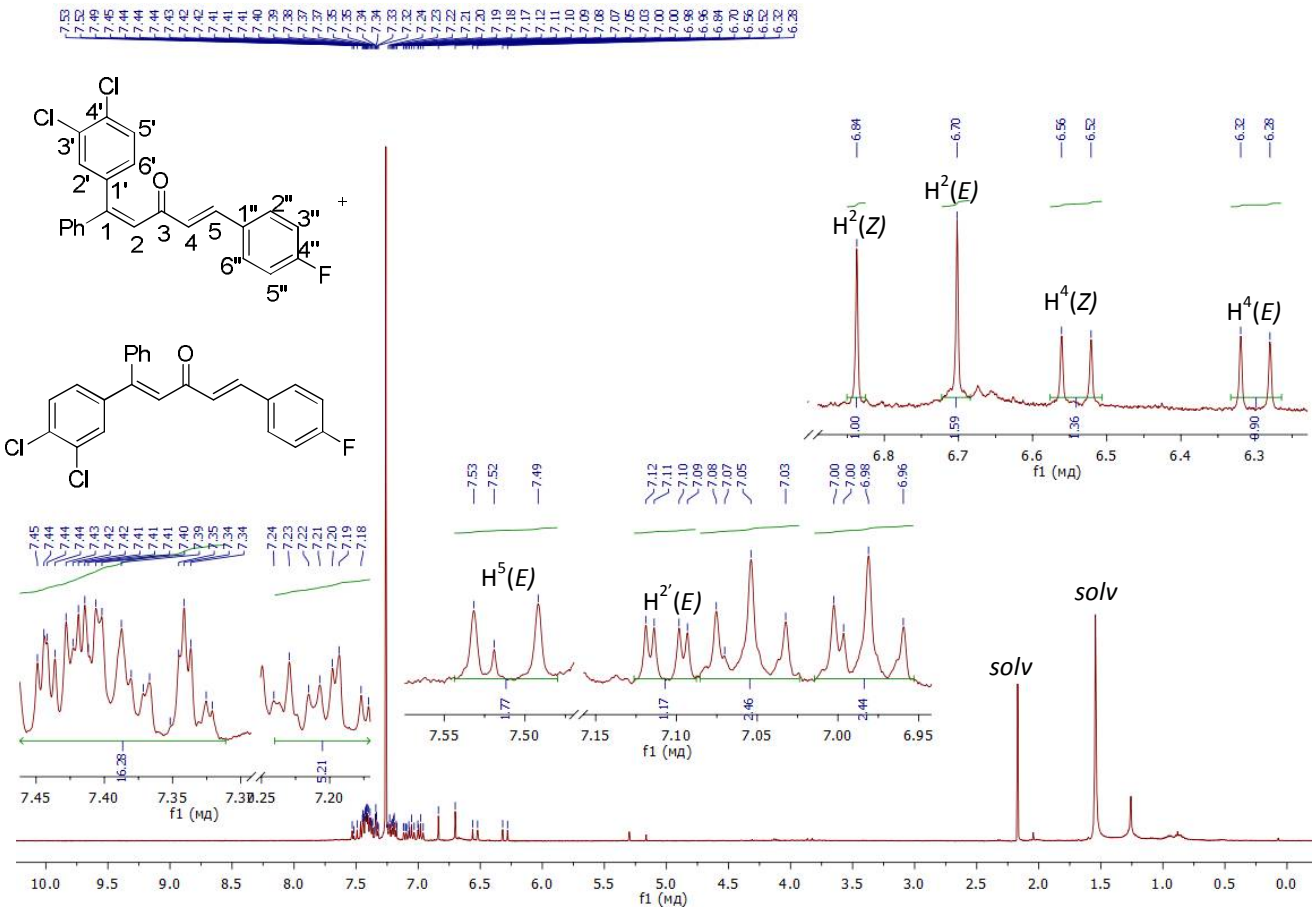


Fig. S67. ^{1}H NMR Spectra of compounds**3m** at 20 °C (400 МГц, $CDCl_3$).

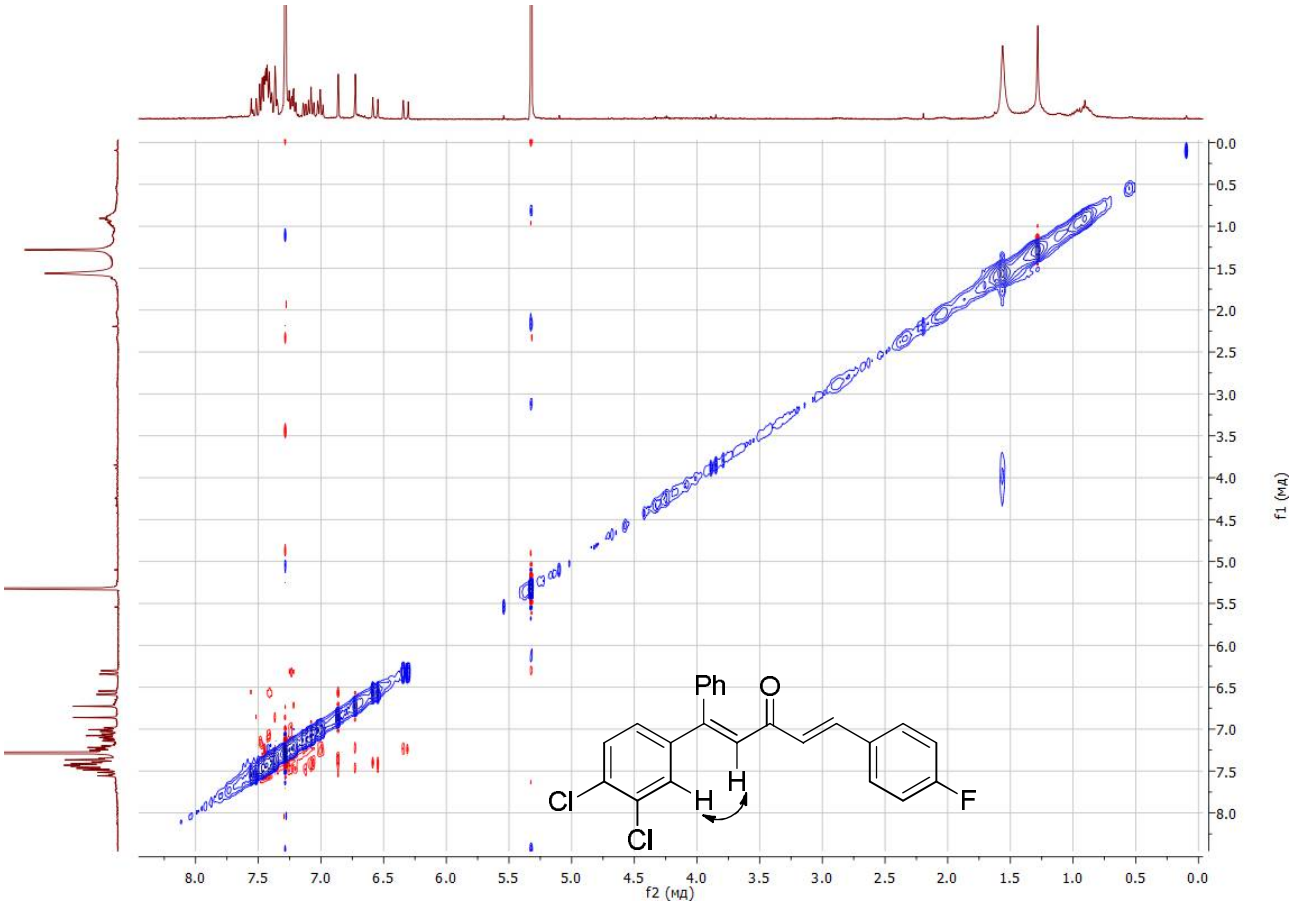


Fig. S68. ^{1}H-^{1}H NMR NOESY Spectra of compounds **3m** at 20 °C (400 МГц, $CDCl_3$).

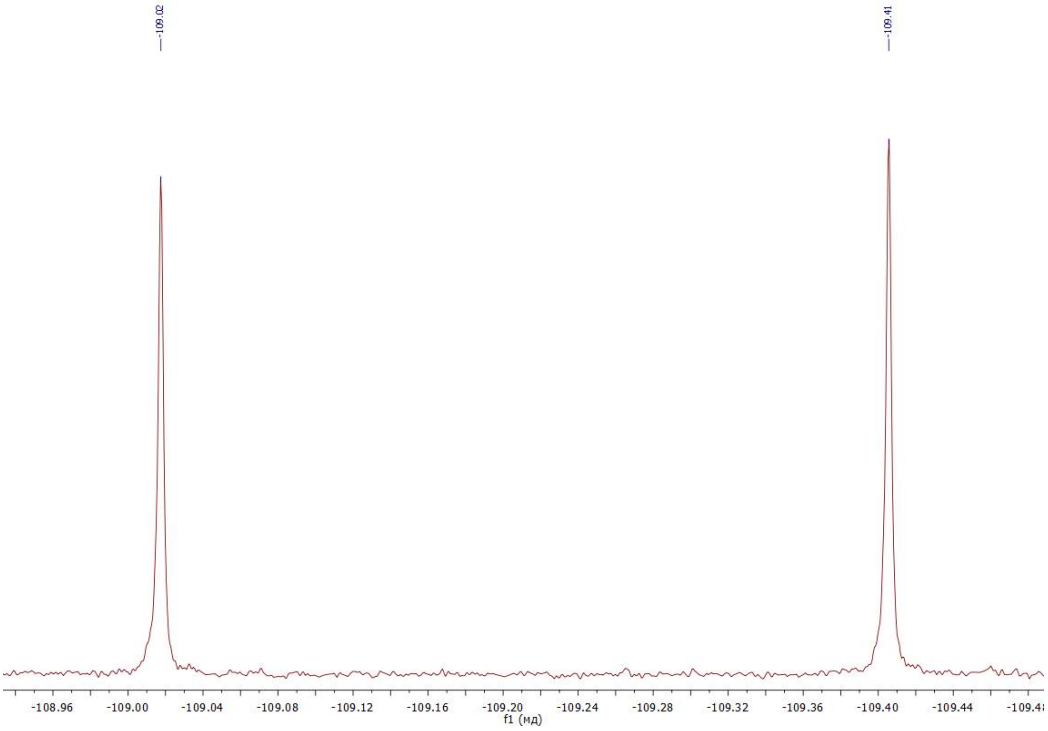


Fig. S69. $^{19}F\{^{1}H\}$ NMR Spectra of compounds **3m** at 20 °C (376МГц, $CDCl_3$).

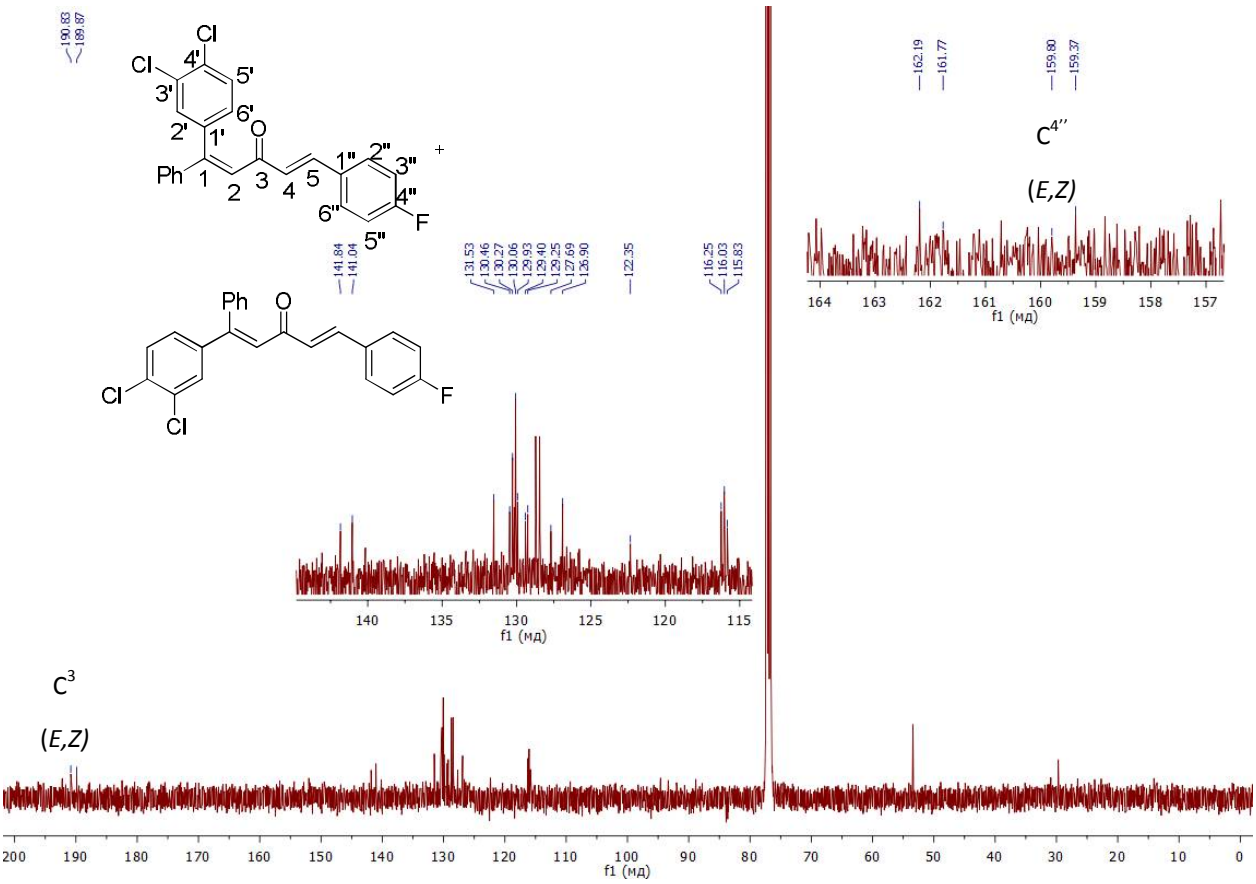


Fig. S70. ^{13}C NMR Spectra of compounds **3m** at 20 °C (101МГц, $CDCl_3$).

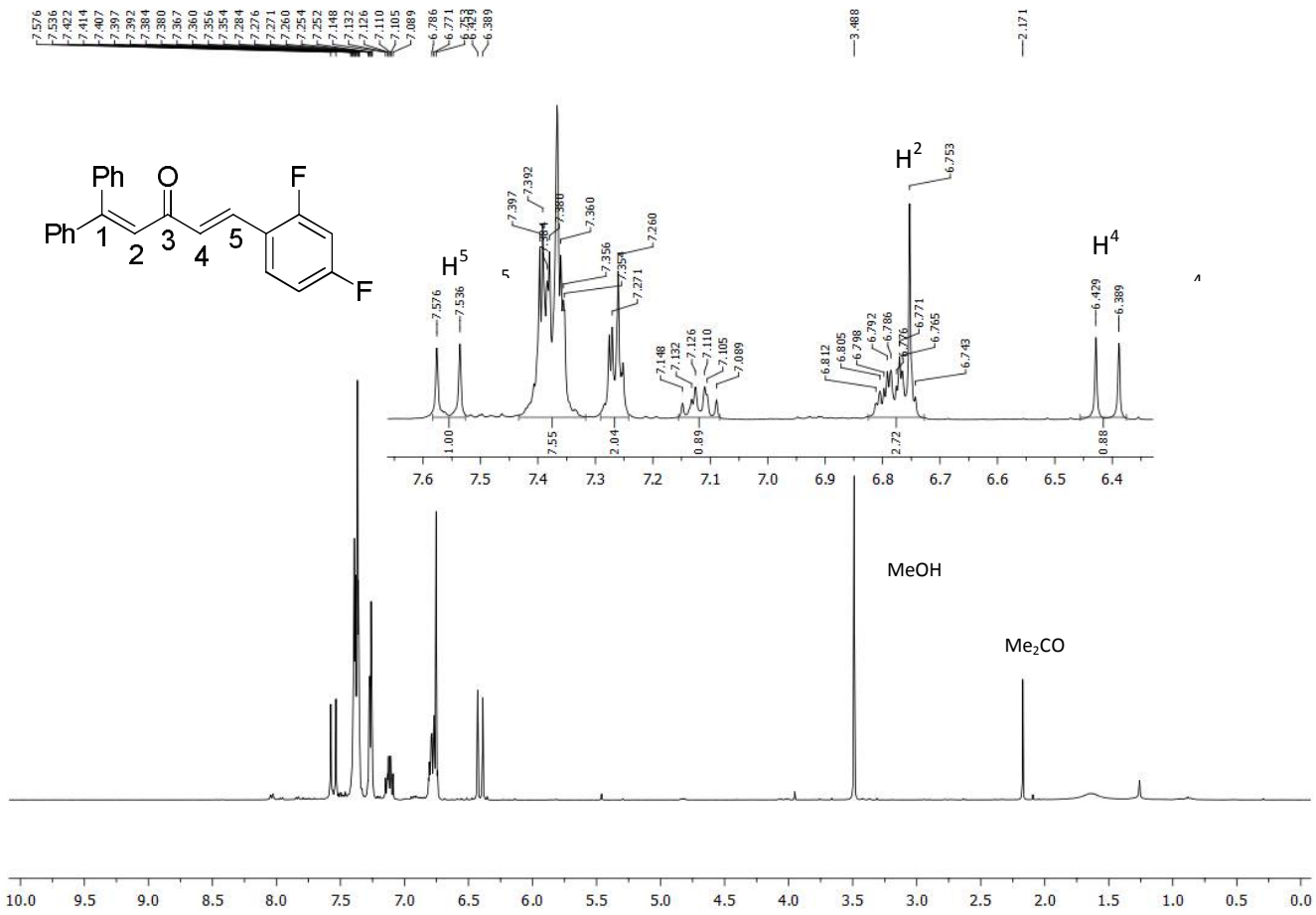


Fig. S71. ^{1}H NMR Spectra of compound **3n** at 20 °C (400 МГц, $CDCl_3$).

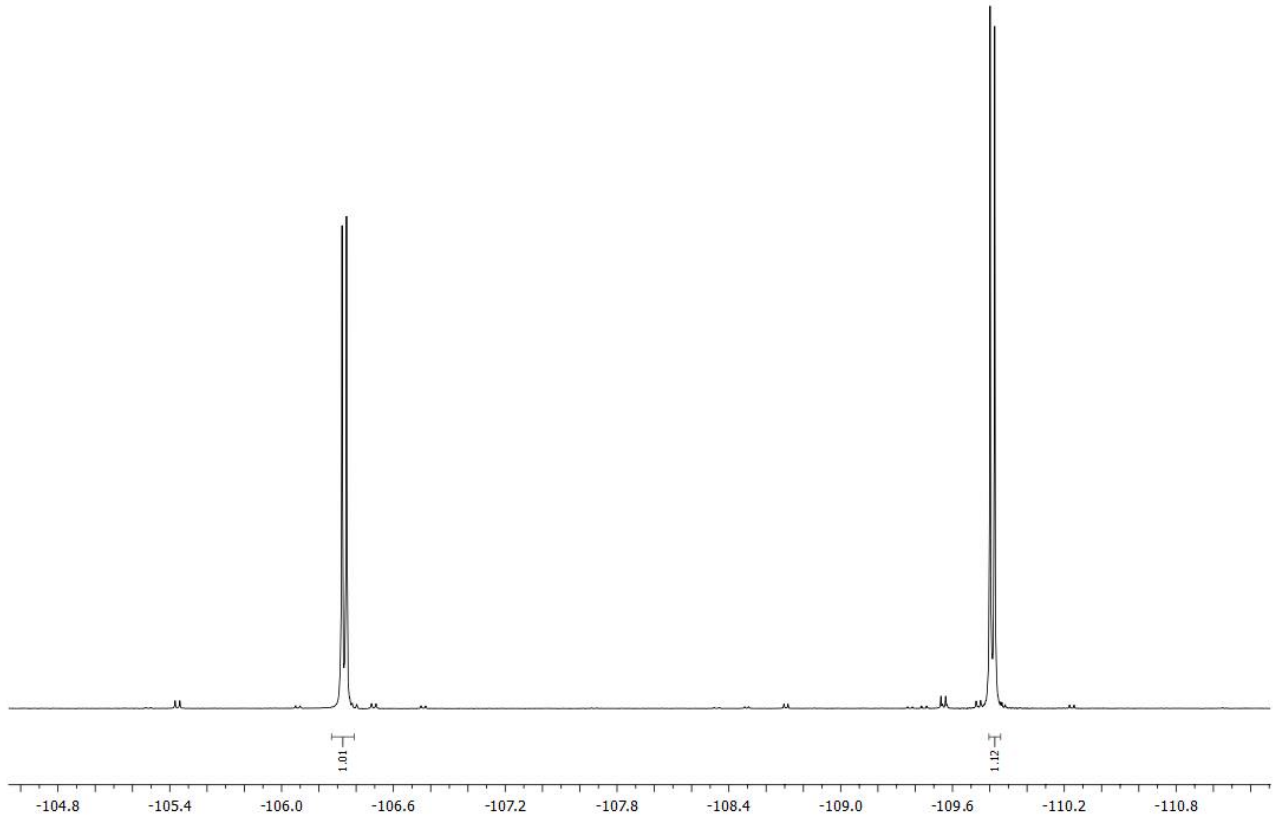


Fig. S72. $^{19}F\{^{1}H\}$ NMR Spectra of compound **3n** at 20 °C (376МГц, $CDCl_3$).

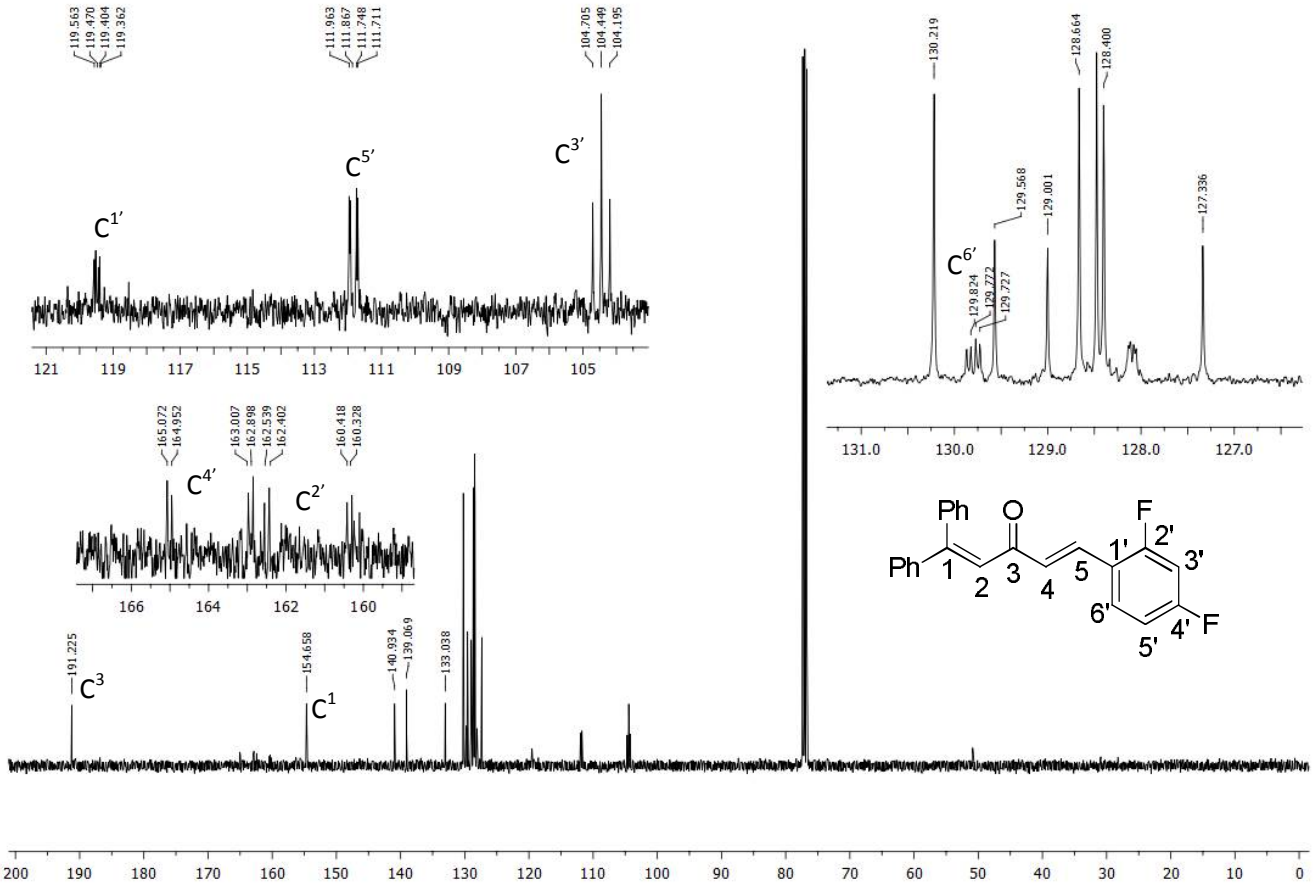


Fig. S73. ^{13}C NMR Spectra of compound **3n** at 20 °C (101МГц, $CDCl_3$).

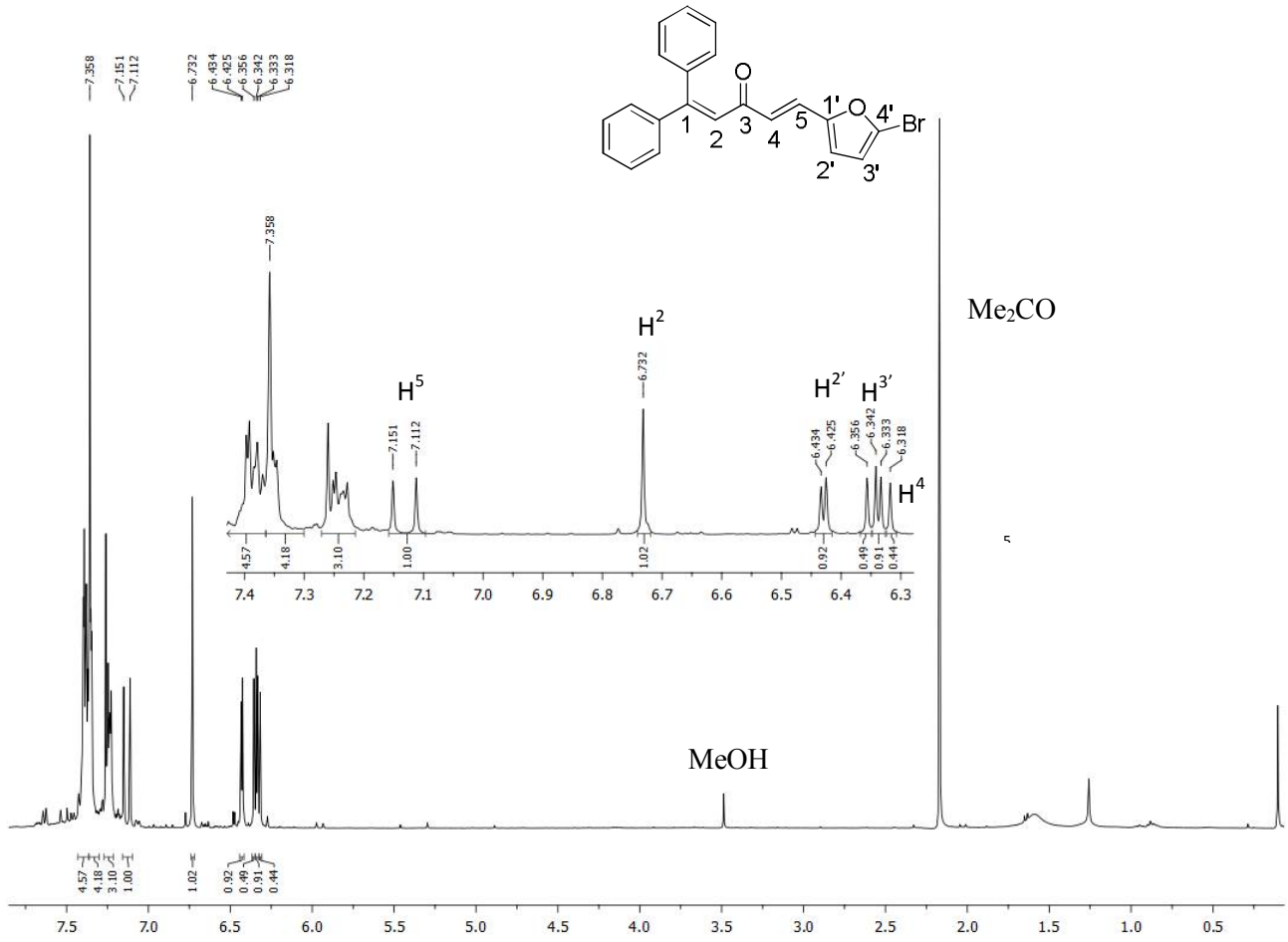


Fig. S74. ^{1}H NMR Spectra of compound **3o** at 20 °C (400 МГц, $CDCl_3$).

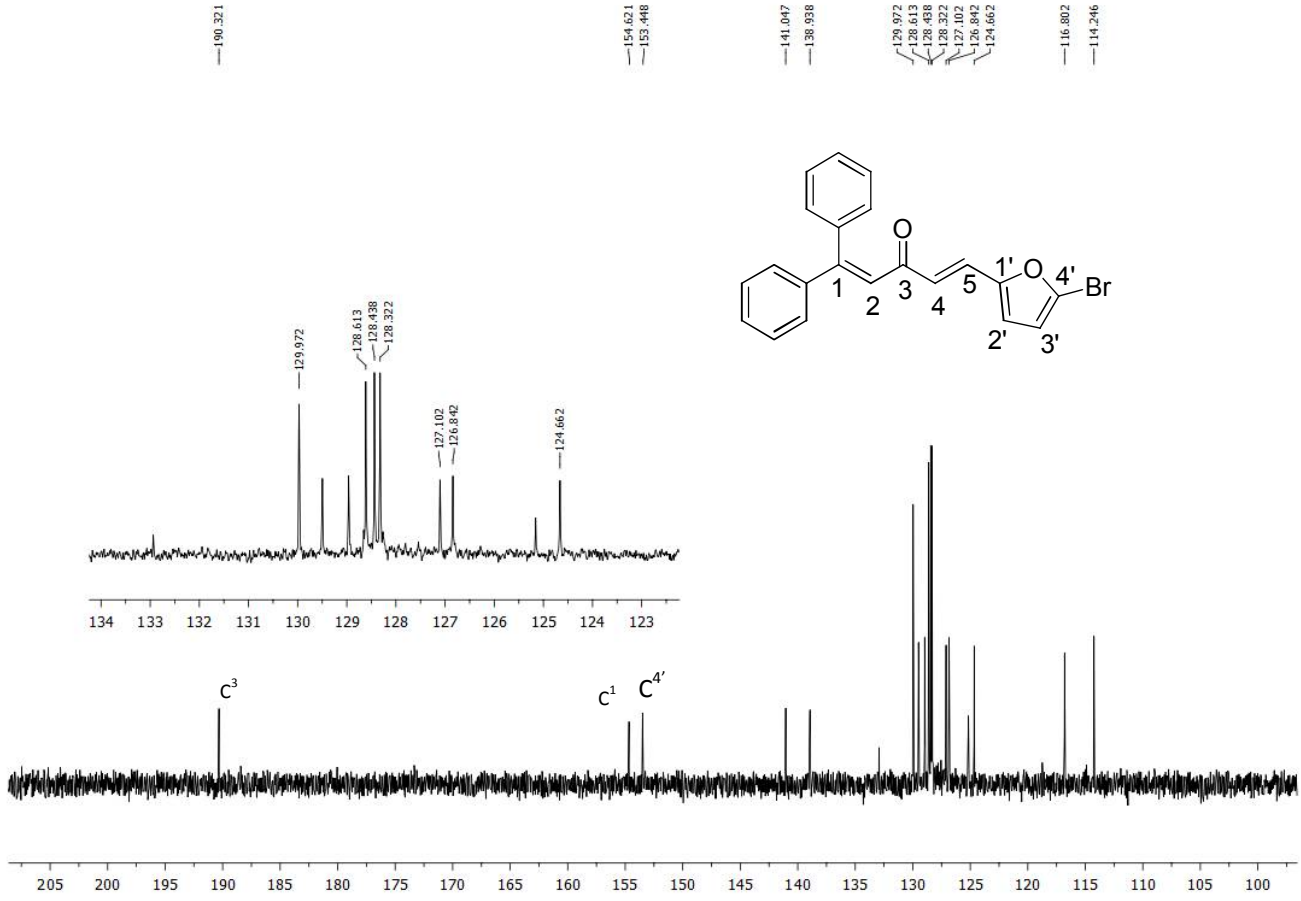


Fig. S75. ^{13}C NMR Spectra of compound **3o** at 20 °C (101МГц, $CDCl_3$).

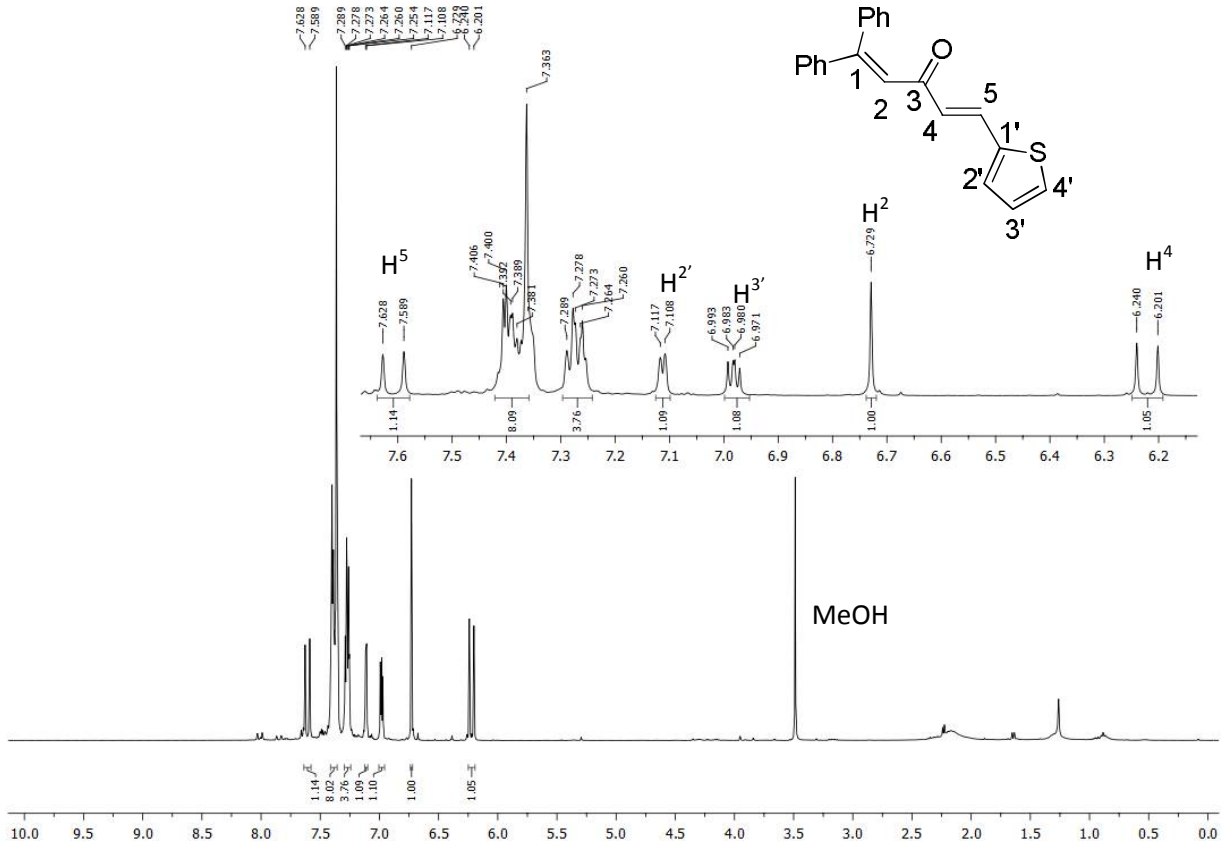


Fig. S76. ^{1}H NMR Spectra of compound **3p** at 20 °C (400 МГц, $CDCl_3$).

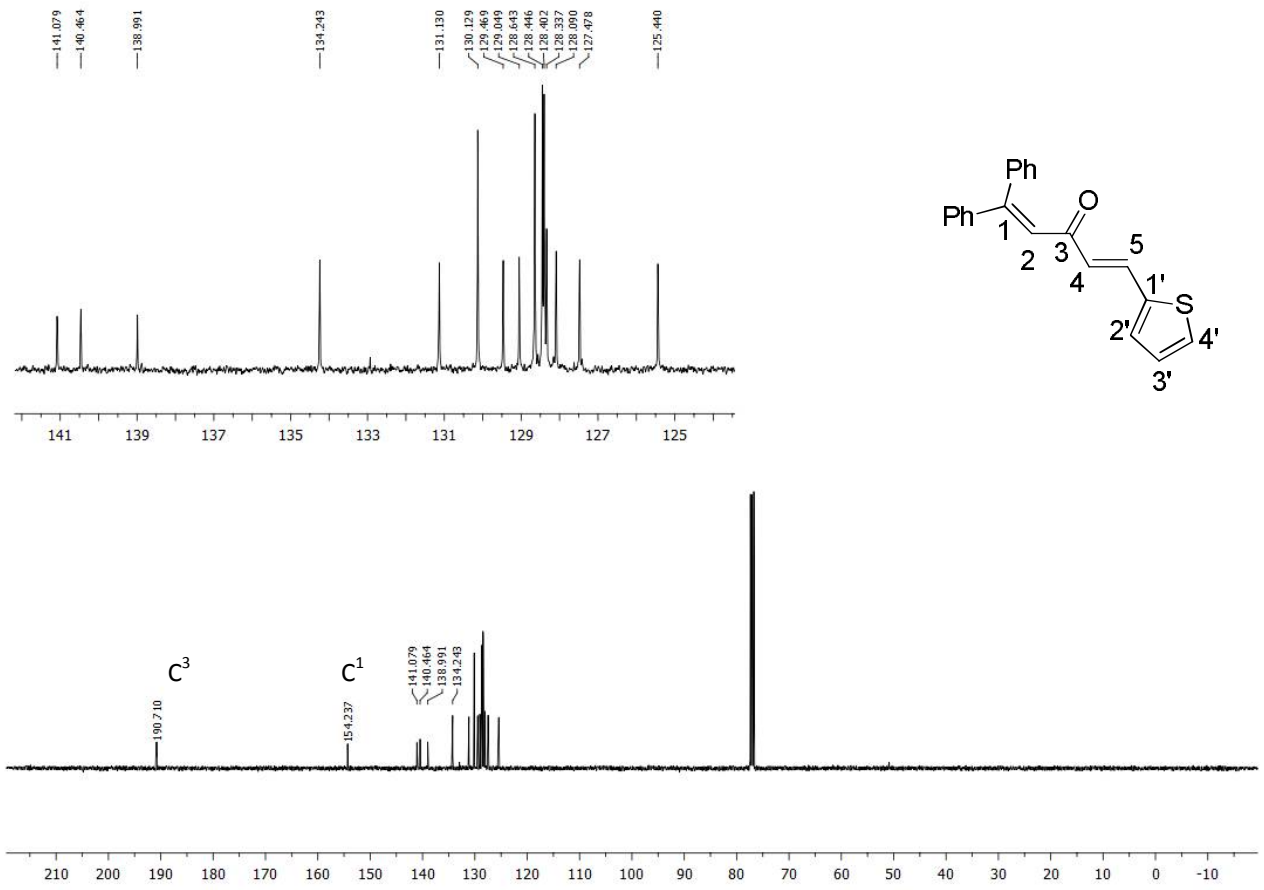


Fig. S77. ^{13}C NMR Spectra of compound **3p** at 20 °C (101МГц, $CDCl_3$).

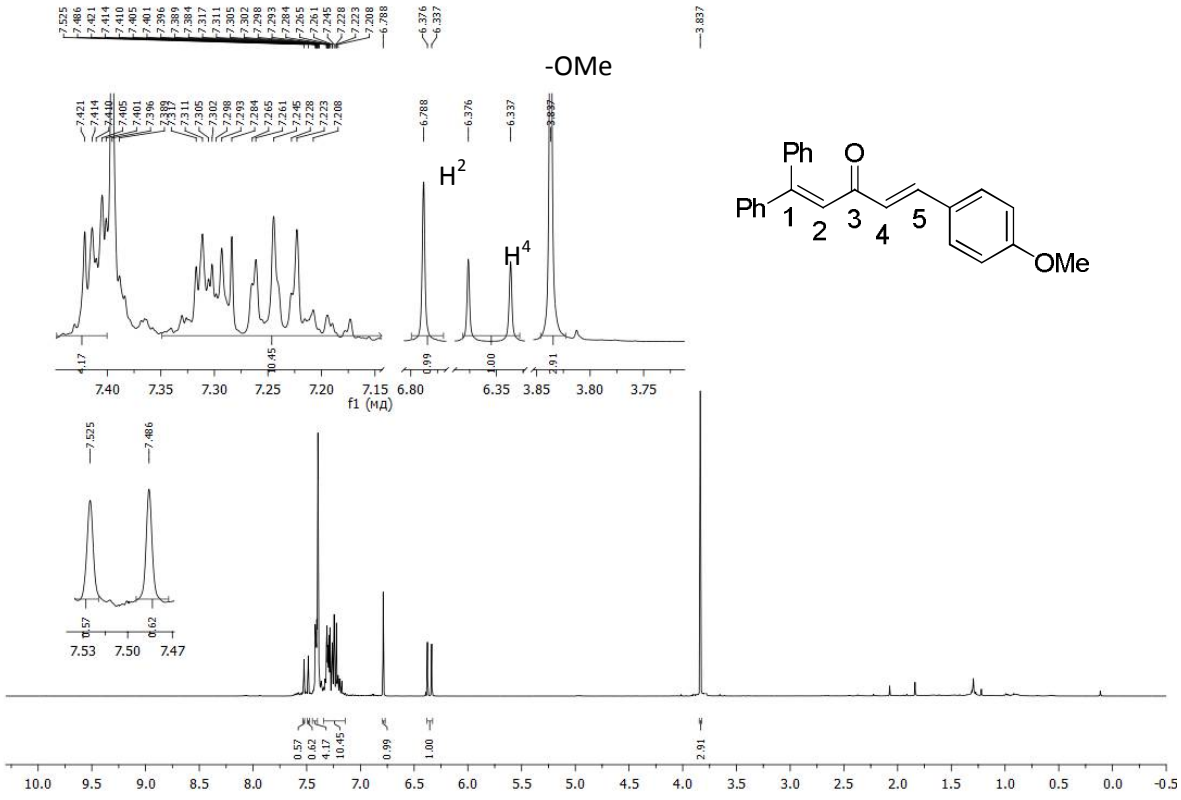


Fig. S78. ^{1}H NMR Spectra of compound **3q** at 20 °C (400 МГц, $CDCl_3$).

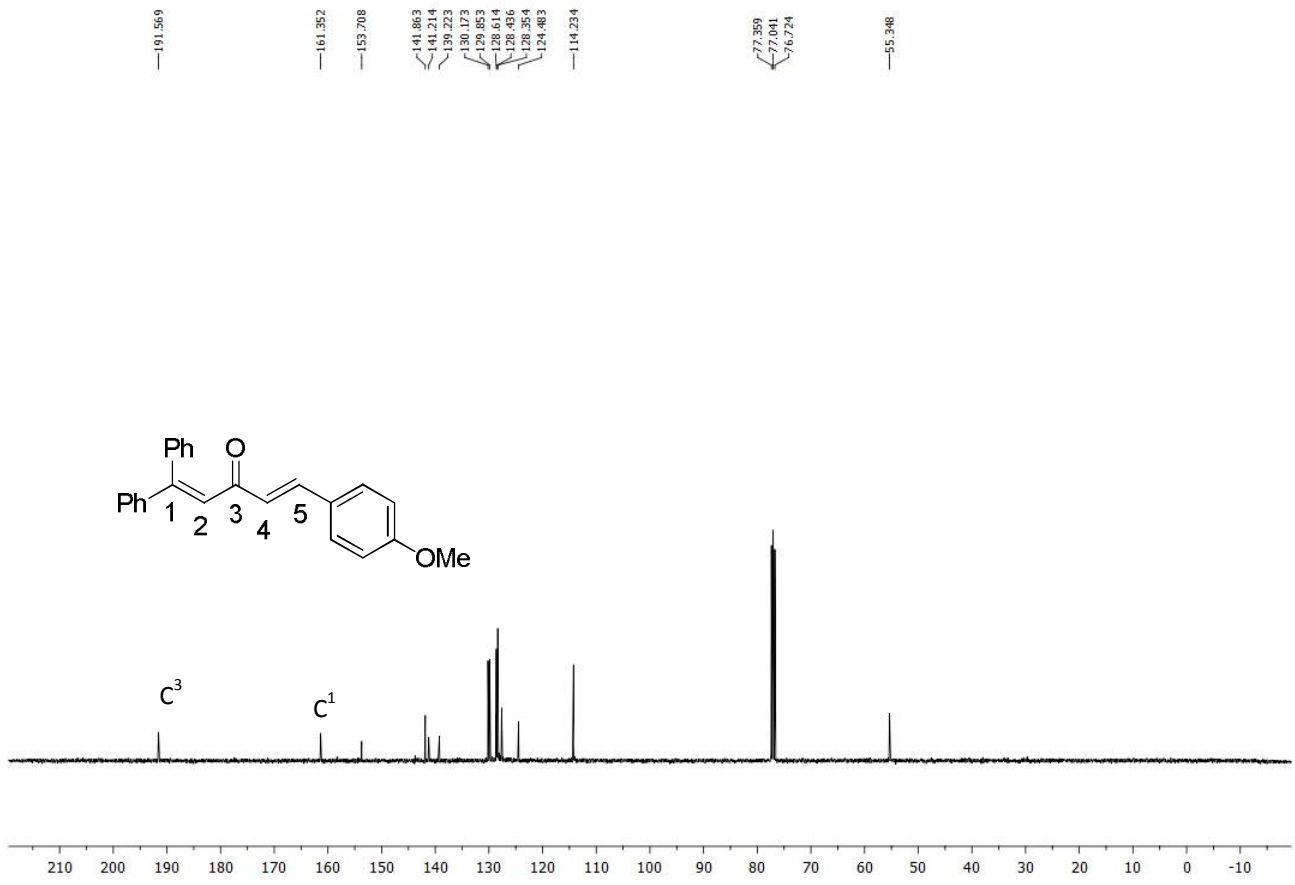


Fig. S79. ^{13}C NMR Spectra of compound **3q** at 20 °C (101МГц, $CDCl_3$).

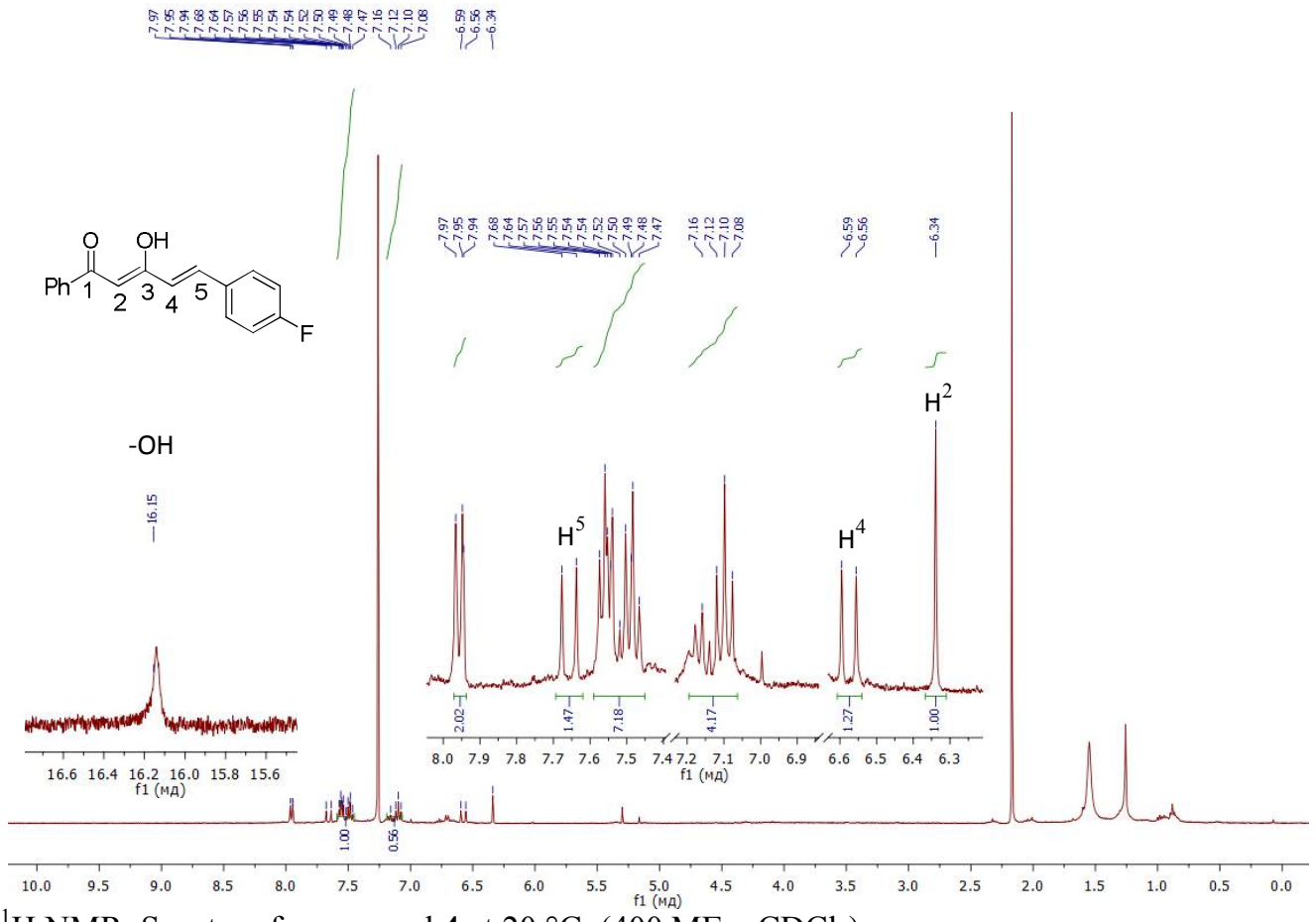


Fig. S80. ^{1}H NMR Spectra of compound **4** at 20 °C (400 МГц, $CDCl_3$).

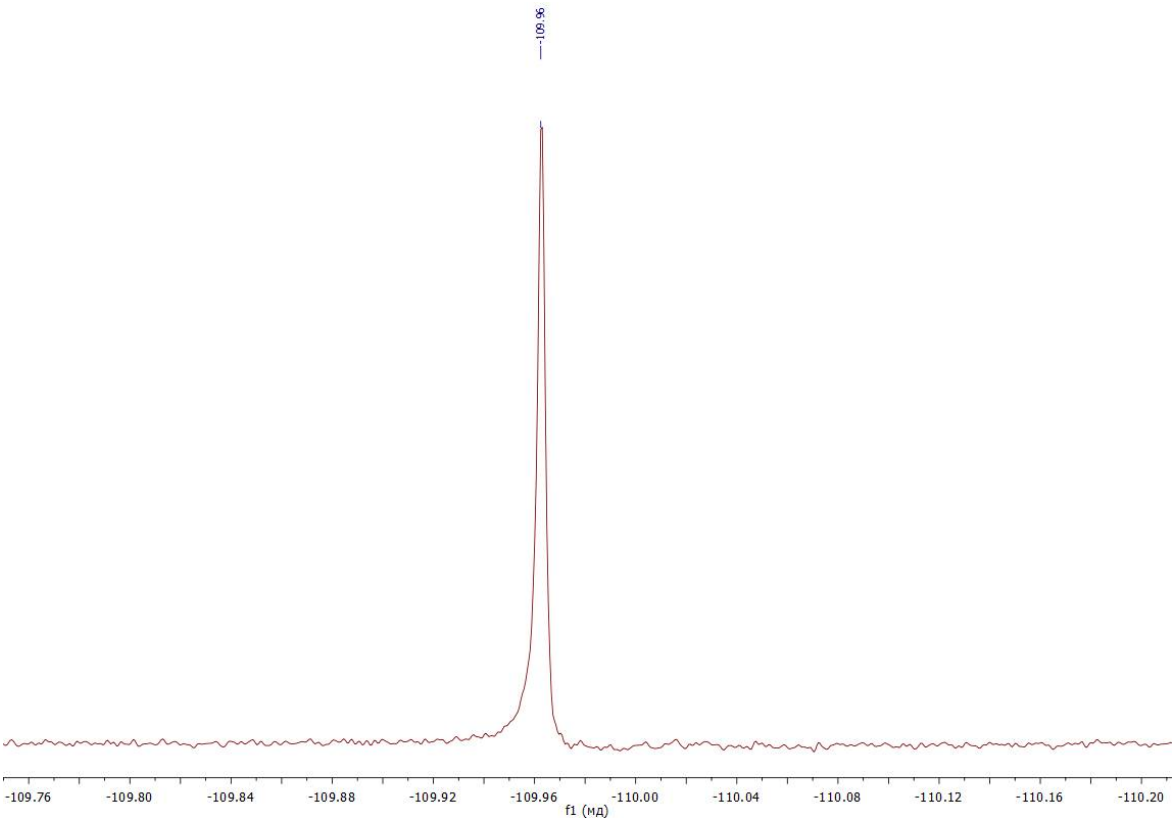


Fig. S81. $^{19}F\{^{1}H\}$ NMR Spectra of compound **4** at 20 °C (376МГц, $CDCl_3$).

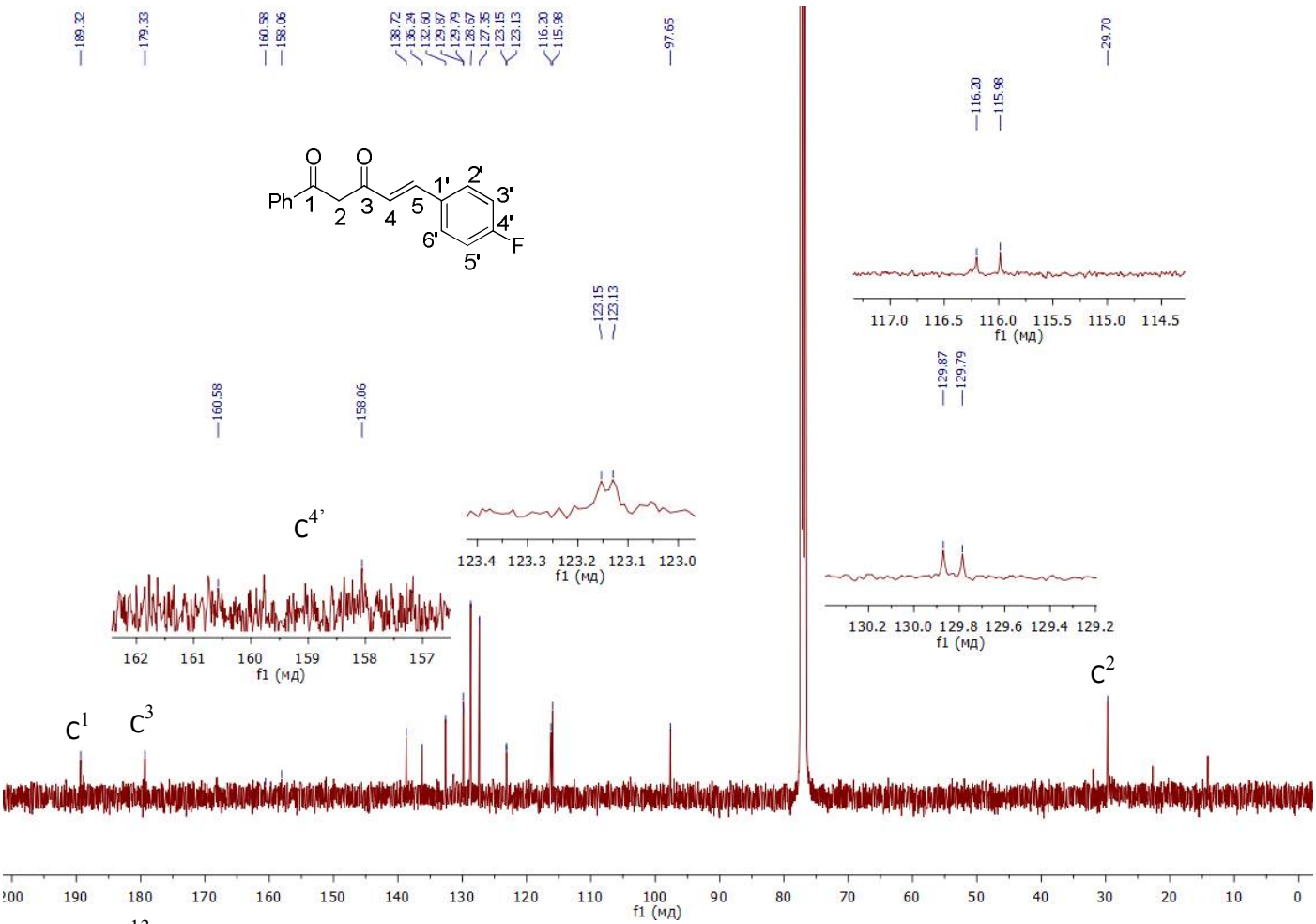


Fig. S82. ^{13}C NMR Spectra of compound **4** at 20 °C (101МГц, $CDCl_3$).

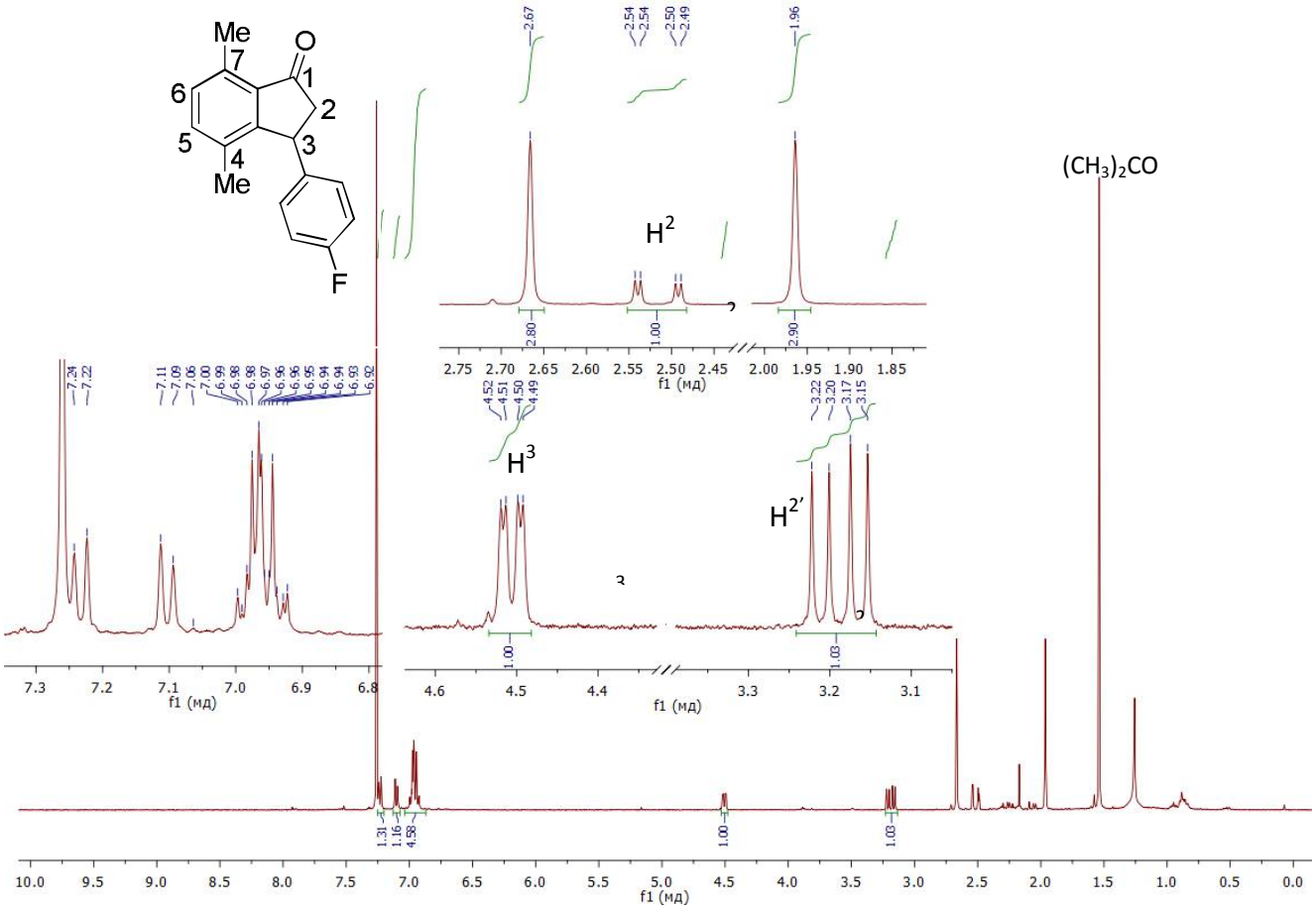


Fig. S83. ^{1}H NMR Spectra of compound **5** at 20 °C (400 МГц, $CDCl_3$).

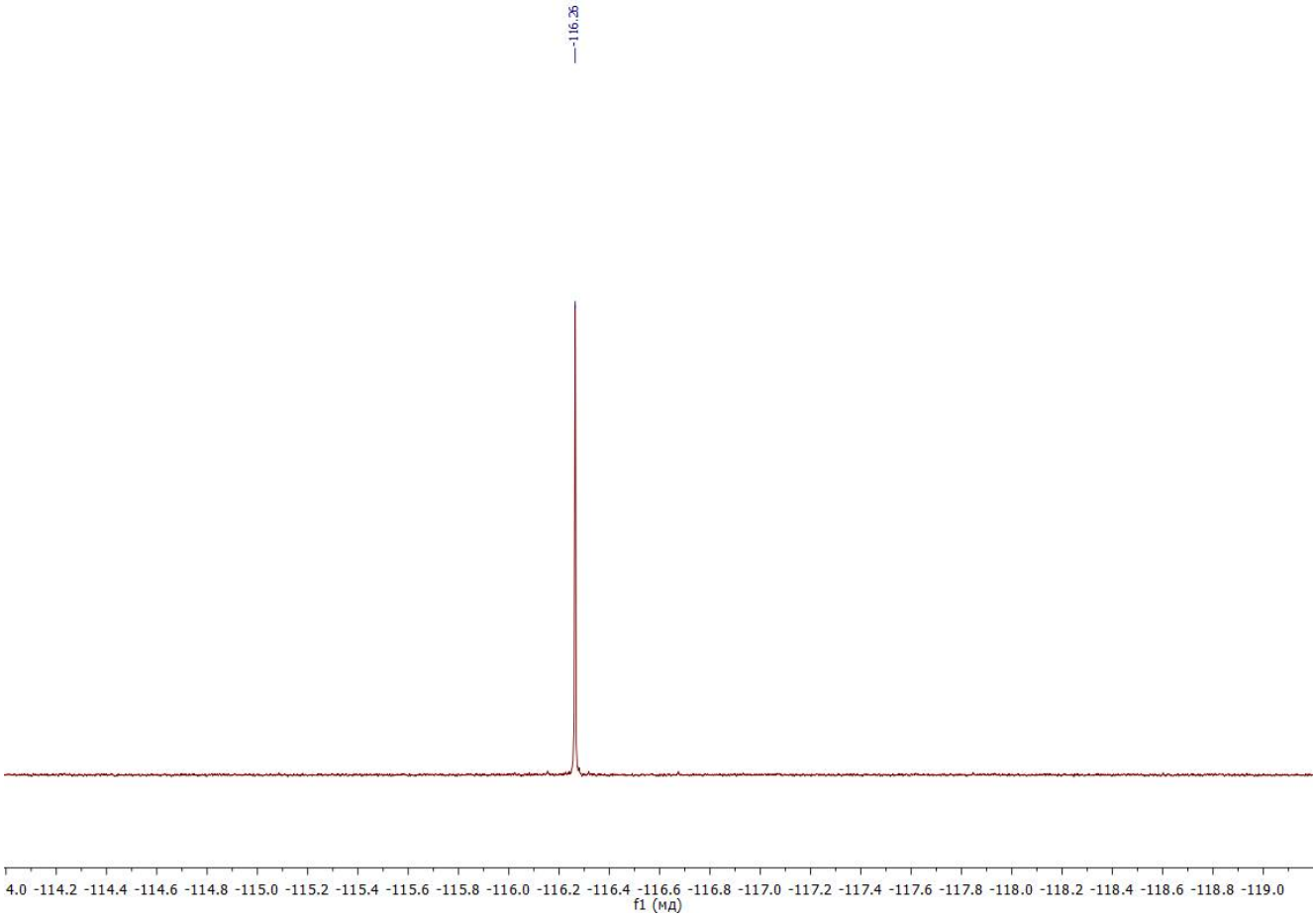


Fig. S84. $^{19}F\{^{1}H\}$ NMR Spectra of compound **5** at 20 °C (376МГц, $CDCl_3$).

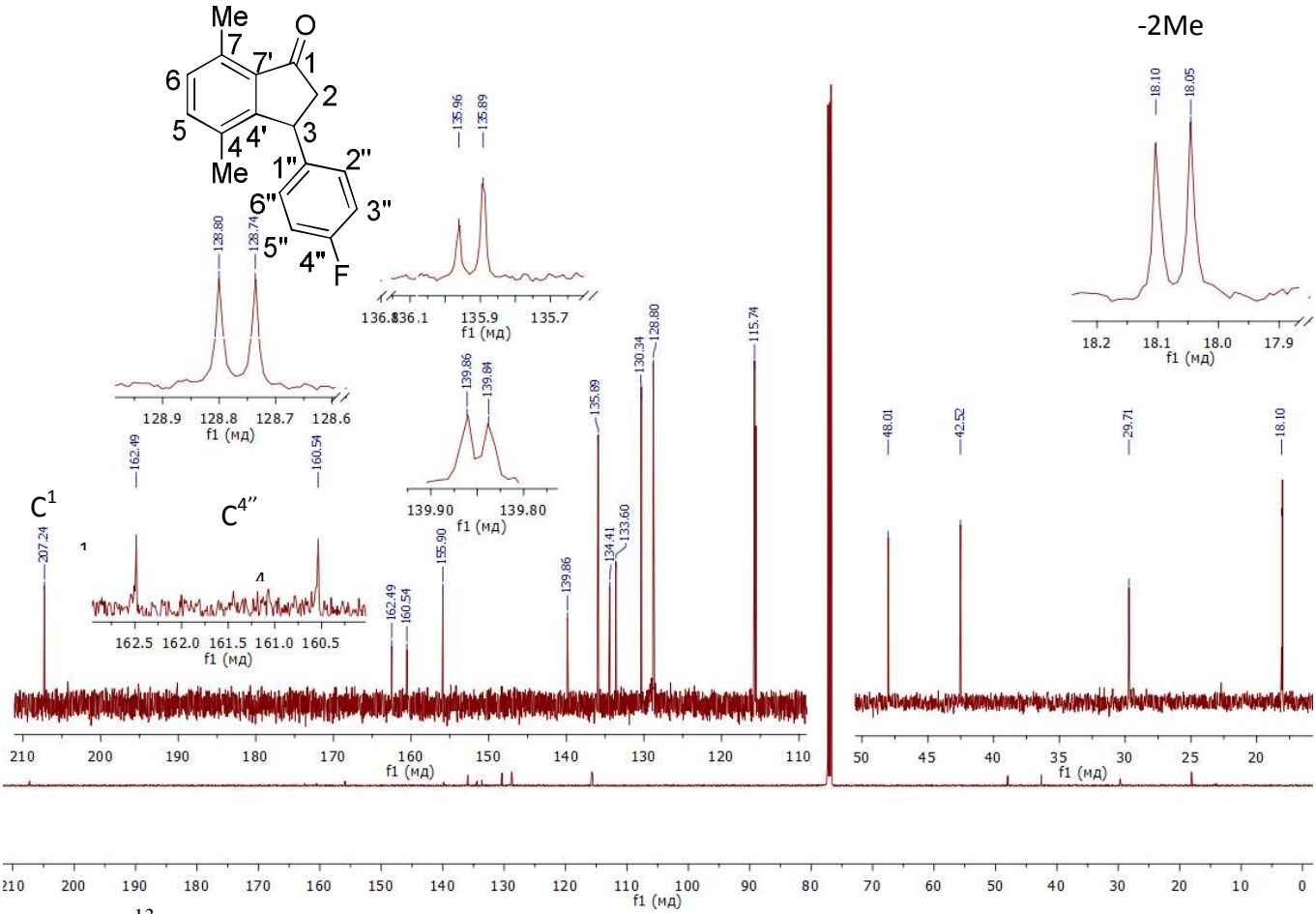
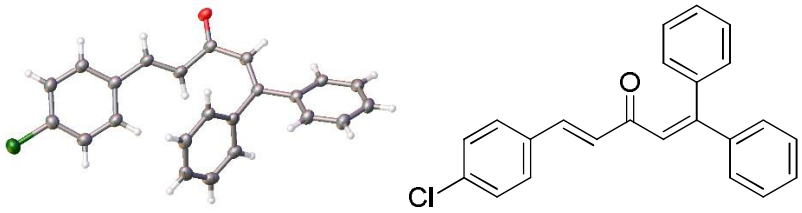


Fig. S85. ^{13}C NMR Spectra of compound **5** at 20 °C (101МГц, $CDCl_3$).

II. X-ray data

3b



CCDC 1847444

Table S1 Crystal data and structure refinement for 3b.

Identificationcode	7071-8899-IMA065_twin1_hklf4
Empiricalformula	$C_{23}H_{17}ClO$
Formulaweight	344.82
Temperature/K	100(2)
Crystalsystem	monoclinic
Spacegroup	$P2_1/c$
a/Å	6.23180(10)
b/Å	19.0611(3)
c/Å	30.5102(4)
α/°	90
β/°	95.1740(10)
γ/°	90
Volume/Å^3	3609.39(9)
Z	8
ρ_{calc}g/cm^3	1.269
μ/mm^{-1}	1.911
F(000)	1440.0
Crystalsize/mm^3	0.29 × 0.21 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.474 to 144.42
Indexranges	$-7 \le h \le 5$, $-23 \le k \le 23$, $-36 \le l \le 37$
Reflectionscollected	7095
Independentreflections	7095 [R_{int} = ?, R_{sigma} = 0.0115]
Data/restraints/parameters	7095/0/452
Goodness-of-fit on F^2	1.080
Final R indexes [I>=2σ (I)]	R_1 = 0.0525, wR_2 = 0.1530
Final R indexes [all data]	R_1 = 0.0570, wR_2 = 0.1576
Largest diff. peak/hole / e Å^{-3}	0.37/-0.53

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

Atom	*x*	*y*	*z*	U(eq)
Cl01	-5676.3(8)	5698.2(3)	1445.8(2)	47.33(16)
Cl02	12605.7(9)	502.1(3)	5178.4(2)	50.59(17)
O003	5648.8(18)	3284.7(7)	3252.7(4)	31.5(3)
O004	1134.6(17)	2492.3(7)	3105.9(4)	29.1(3)
C005	4441(2)	2102.2(8)	2233.6(5)	24.2(3)
C006	2373(2)	3876.0(8)	4084.1(5)	24.6(3)
C007	572(3)	4382.5(9)	4084.2(5)	25.3(3)

C008	3268(2)	3612.2(8)	4523.7(5)	24.8(3)
C009	4877(2)	3215.0(9)	3606.6(5)	27.9(3)
C00A	6248(2)	1607.2(9)	2181.8(5)	25.5(3)
C00B	7951(3)	1705.1(9)	4600.2(6)	32.4(4)
C00C	3685(2)	2182.6(9)	2631.1(5)	26.9(3)
C00D	3922(3)	3307.0(10)	1248.7(6)	34.8(4)
C00E	11101(3)	1021.9(10)	4797.4(7)	38.3(4)
C00F	8743(3)	1886.9(9)	4199.3(6)	30.5(4)
C00G	1958(3)	3198.0(9)	4766.5(5)	28.3(3)
C00H	5362(3)	3762.6(9)	4699.2(5)	29.4(3)
C00I	1162(3)	3249.4(9)	2496.1(5)	26.5(3)
C00J	9468(3)	1005.1(9)	2481.7(6)	31.6(4)
C00K	1788(3)	3199.6(10)	1084.5(5)	35.4(4)
C00L	7840(2)	1488.2(9)	2528.7(5)	26.7(3)
C00M	1930(2)	2637.5(9)	2762.4(5)	26.0(3)
C00N	-1858(2)	4086.7(9)	2280.5(5)	26.9(3)
C00O	3111(2)	3692.0(9)	3698.0(5)	27.4(3)
C00P	2746(3)	2919.9(10)	5169.1(6)	34.2(4)
C00Q	-2767(3)	5366.7(10)	4071.6(6)	33.6(4)
C00R	6130(3)	3494.8(10)	5107.6(6)	34.8(4)
C00S	-3807(3)	4349.8(9)	2404.1(5)	28.9(3)
C00T	-1080(3)	4350.7(9)	1893.1(6)	30.0(3)
C00U	-786(2)	3523.8(9)	2542.1(5)	26.9(3)
C00V	526(3)	4882.0(9)	4418.2(5)	30.0(3)
C00W	10736(3)	1610.4(10)	4104.9(6)	34.7(4)
C00X	3518(2)	2463.3(8)	1826.1(5)	24.9(3)
C00Y	-1096(2)	4383.0(9)	3743.5(5)	26.2(3)
C00Z	542(3)	2714.0(10)	1285.7(6)	33.9(4)
C010	-2749(3)	4871.4(9)	3737.8(5)	30.0(3)
C011	-2233(3)	4848.6(10)	1639.5(6)	33.5(4)
C012	5715(3)	2678.4(9)	3926.1(5)	28.8(3)
C013	6368(3)	1244.4(9)	1788.6(5)	30.1(3)
C014	11915(3)	1182.0(10)	4401.4(7)	38.3(4)
C015	9531(3)	633.3(9)	2091.5(6)	34.2(4)
C016	1387(2)	2349.2(9)	1656.4(5)	28.3(3)
C017	-4181(3)	5090.4(10)	1771.4(6)	33.3(4)
C018	4788(3)	2934.2(9)	1611.8(5)	28.6(3)
C019	4839(3)	3068.5(10)	5340.1(6)	36.7(4)
C01A	9108(3)	1273.1(10)	4897.7(6)	36.2(4)
C01B	-4969(3)	4853.7(10)	2155.6(6)	32.8(4)
C01C	-1120(3)	5371.1(9)	4409.2(5)	33.9(4)
C01D	7639(3)	2379.3(9)	3888.6(5)	30.1(4)
C01E	7985(3)	756.8(10)	1744.3(6)	34.5(4)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3b. 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}
Cl01	49.9(3)	50.4(3)	42.4(3)	13.1(2)	8.5(2)	17.2(2)
Cl02	50.0(3)	47.6(3)	52.4(3)	-2.3(2)	-4.7(2)	13.7(2)
O003	23.9(5)	48.7(7)	22.7(5)	-5.9(5)	5.5(4)	-5.4(5)
O004	23.0(5)	42.4(7)	22.3(5)	-2.6(5)	4.1(4)	-0.7(5)
C005	19.1(7)	29.2(8)	24.4(7)	-4.1(6)	1.8(5)	-3.0(6)
C006	23.3(7)	29.6(8)	21.3(7)	-2.5(6)	4.4(5)	-6.6(6)
C007	27.0(7)	30.4(8)	19.1(7)	1.5(6)	4.6(6)	-4.8(6)

C008	26.7(7)	28.1(8)	20.1(7)	-2.7(6)	4.6(6)	0.3(6)
C009	22.3(7)	38.0(9)	23.8(7)	-7.5(6)	3.4(6)	-8.5(6)
C00A	20.4(7)	30.2(8)	25.8(7)	-0.6(6)	2.3(6)	-3.7(6)
C00B	26.8(8)	36.1(9)	34.6(9)	-6.8(7)	5.0(7)	-1.4(7)
C00C	21.5(7)	35.1(8)	23.8(7)	-1.4(6)	0.4(6)	-0.6(6)
C00D	43.5(10)	36.0(9)	26.4(8)	-1.9(7)	11.8(7)	-2.7(7)
C00E	35.5(9)	36.4(9)	41.9(10)	-8.3(8)	-2.5(7)	2.0(7)
C00F	26.5(8)	34.2(8)	31.2(8)	-10.4(7)	4.4(6)	-3.8(7)
C00G	30.6(8)	30.7(8)	24.7(7)	-3.0(6)	7.9(6)	-1.9(6)
C00H	28.3(8)	35.3(9)	24.8(7)	-1.4(7)	3.2(6)	-3.3(7)
C00I	24.2(7)	33.8(8)	22.1(7)	-5.8(6)	5.7(6)	-2.8(6)
C00J	24.6(7)	37.5(9)	32.9(8)	7.0(7)	3.8(6)	0.5(7)
C00K	43.0(10)	41.5(10)	21.5(7)	-1.3(7)	1.7(7)	10.2(8)
C00L	21.5(7)	33.9(8)	25.0(7)	0.1(6)	3.6(6)	-3.3(6)
C00M	19.4(7)	36.0(8)	22.6(7)	-5.6(6)	1.2(5)	-3.6(6)
C00N	25.1(7)	31.8(8)	24.1(7)	-5.3(6)	3.4(6)	-2.5(6)
C00O	24.3(7)	36.4(8)	21.6(7)	-1.2(6)	3.2(6)	-5.3(6)
C00P	46.0(10)	31.9(9)	26.0(8)	2.5(6)	11.1(7)	0.1(7)
C00Q	38.1(9)	35.8(9)	27.3(8)	4.5(7)	5.1(7)	6.8(7)
C00R	31.8(8)	42.7(10)	29.0(8)	-3.0(7)	-2.9(6)	2.5(7)
C00S	25.3(8)	34.9(9)	26.6(8)	-4.8(6)	4.1(6)	-0.3(6)
C00T	26.0(8)	34.8(9)	29.9(8)	-2.6(7)	6.6(6)	-0.8(6)
C00U	23.8(7)	36.1(9)	21.2(7)	-6.0(6)	4.9(6)	-2.0(6)
C00V	35.9(8)	33.6(8)	20.2(7)	-1.0(6)	1.3(6)	-1.5(7)
C00W	27.8(8)	39.7(9)	37.1(9)	-12.2(7)	5.7(7)	-3.6(7)
C00X	23.6(7)	30.5(8)	20.7(7)	-5.2(6)	3.4(6)	1.7(6)
C00Y	26.2(7)	32.5(8)	20.2(7)	-1.4(6)	3.8(6)	-6.4(6)
C00Z	27.7(8)	48.1(10)	25.1(8)	-5.0(7)	-1.9(6)	6.3(7)
C010	28.3(7)	38.5(9)	23.6(7)	2.7(7)	3.2(6)	-2.2(7)
C011	35.7(9)	36.9(9)	28.9(8)	0.5(7)	8.3(7)	-0.1(7)
C012	26.2(7)	35.2(9)	25.9(7)	-6.3(6)	7.9(6)	-4.8(6)
C013	26.7(8)	34.3(9)	29.3(8)	-6.1(7)	2.3(6)	0.2(6)
C014	28.1(8)	40.7(10)	45.9(10)	-13.1(8)	2.9(7)	2.9(7)
C015	28.3(8)	33.0(9)	42.3(9)	1.2(7)	8.7(7)	5.7(7)
C016	23.0(7)	38.1(9)	24.0(7)	-2.6(6)	2.5(6)	-0.4(6)
C017	33.9(8)	33.8(9)	31.7(8)	0.6(7)	1.0(7)	2.9(7)
C018	25.7(7)	35.2(9)	25.6(7)	-6.8(6)	5.9(6)	-2.3(6)
C019	48.6(10)	38.2(9)	23.0(8)	0.8(7)	2.5(7)	9.3(8)
C01A	36.3(9)	38.6(9)	34.0(9)	-5.0(7)	4.4(7)	-0.2(7)
C01B	28.3(8)	36.5(9)	34.1(8)	-2.3(7)	5.3(6)	4.5(7)
C01C	45.5(10)	32.3(9)	24.1(8)	-3.9(6)	3.5(7)	3.5(7)
C01D	26.1(8)	37.4(9)	27.6(8)	-9.1(7)	6.4(6)	-4.2(6)
C01E	31.4(8)	36.4(9)	36.1(9)	-7.8(7)	5.7(7)	2.8(7)

Table S4 Bond Lengths for 3b.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl01	C017	1.7409(18)	C00G	C00P	1.386(2)
Cl02	C00E	1.737(2)	C00H	C00R	1.391(2)
O003	C009	1.228(2)	C00I	C00M	1.476(2)
O004	C00M	1.231(2)	C00I	C00U	1.341(2)
C005	C00A	1.488(2)	C00J	C00L	1.387(2)
C005	C00C	1.349(2)	C00J	C015	1.389(3)
C005	C00X	1.491(2)	C00K	C00Z	1.387(3)
C006	C007	1.481(2)	C00N	C00S	1.398(2)

C006	C008	1.493(2)	C00N	C00T	1.410(2)
C006	C00O	1.349(2)	C00N	C00U	1.463(2)
C007	C00V	1.397(2)	C00P	C019	1.389(3)
C007	C00Y	1.402(2)	C00Q	C010	1.390(3)
C008	C00G	1.396(2)	C00Q	C01C	1.387(2)
C008	C00H	1.395(2)	C00R	C019	1.383(3)
C009	C00O	1.474(2)	C00S	C01B	1.387(2)
C009	C012	1.475(2)	C00T	C011	1.384(3)
C00A	C00L	1.402(2)	C00V	C01C	1.385(2)
C00A	C013	1.393(2)	C00W	C014	1.380(3)
C00B	C00F	1.403(2)	C00X	C016	1.398(2)
C00B	C01A	1.380(3)	C00X	C018	1.397(2)
C00C	C00M	1.479(2)	C00Y	C010	1.387(2)
C00D	C00K	1.393(3)	C00Z	C016	1.390(2)
C00D	C018	1.384(3)	C011	C017	1.391(2)
C00E	C014	1.386(3)	C012	C01D	1.342(2)
C00E	C01A	1.391(3)	C013	C01E	1.386(2)
C00F	C00W	1.402(2)	C015	C01E	1.387(3)
C00F	C01D	1.461(3)	C017	C01B	1.387(3)

Table S5 Bond Angles for 3b.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C00A	C005	C00X	116.30(13)	C00I	C00M	C00C	121.67(14)
C00C	C005	C00A	119.76(14)	C00S	C00N	C00T	118.11(16)
C00C	C005	C00X	123.90(14)	C00S	C00N	C00U	118.78(15)
C007	C006	C008	116.18(13)	C00T	C00N	C00U	123.01(15)
C00O	C006	C007	119.20(14)	C006	C00O	C009	130.15(15)
C00O	C006	C008	124.61(15)	C00G	C00P	C019	120.03(16)
C00V	C007	C006	120.67(14)	C01C	C00Q	C010	119.61(16)
C00V	C007	C00Y	118.55(15)	C019	C00R	C00H	120.39(16)
C00Y	C007	C006	120.77(14)	C01B	C00S	C00N	121.65(16)
C00G	C008	C006	118.58(14)	C011	C00T	C00N	120.87(15)
C00H	C008	C006	122.46(14)	C00I	C00U	C00N	127.03(15)
C00H	C008	C00G	118.97(15)	C01C	C00V	C007	120.54(15)
O003	C009	C00O	117.26(16)	C014	C00W	C00F	121.10(17)
O003	C009	C012	120.83(15)	C016	C00X	C005	121.28(14)
C00O	C009	C012	121.91(14)	C018	C00X	C005	119.65(14)
C00L	C00A	C005	120.86(14)	C018	C00X	C016	119.06(15)
C013	C00A	C005	120.39(14)	C010	C00Y	C007	120.64(15)
C013	C00A	C00L	118.74(15)	C00K	C00Z	C016	120.51(16)
C01A	C00B	C00F	121.12(16)	C00Y	C010	C00Q	120.11(15)
C005	C00C	C00M	129.56(15)	C00T	C011	C017	119.20(16)
C018	C00D	C00K	120.20(17)	C01D	C012	C009	120.27(15)
C014	C00E	Cl02	119.44(15)	C01E	C013	C00A	120.83(16)
C014	C00E	C01A	121.35(18)	C00W	C014	C00E	119.13(17)
C01A	C00E	Cl02	119.21(16)	C01E	C015	C00J	119.77(16)
C00B	C00F	C01D	122.82(15)	C00Z	C016	C00X	120.06(16)
C00W	C00F	C00B	118.29(17)	C011	C017	Cl01	119.45(14)
C00W	C00F	C01D	118.80(16)	C01B	C017	Cl01	119.11(13)
C00P	C00G	C008	120.59(16)	C01B	C017	C011	121.44(16)
C00R	C00H	C008	120.19(16)	C00D	C018	C00X	120.53(15)
C00U	C00I	C00M	120.13(15)	C00R	C019	C00P	119.79(16)
C00L	C00J	C015	120.33(16)	C00B	C01A	C00E	118.99(18)
C00Z	C00K	C00D	119.57(16)	C00S	C01B	C017	118.70(16)

C00J	C00L	C00A	120.23(15)	C00V	C01C	C00Q	120.55(16)
O004	C00M	C00C	117.59(15)	C012	C01D	C00F	126.14(16)
O004	C00M	C00I	120.74(14)	C013	C01E	C015	120.06(16)

Table S6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3b.

Atom	*x*	*y*	*z*	U(eq)
H00B	6595	1882	4668	39
H00C	4383	1906	2861	32
H00D	4785	3637	1111	42
H00G	513	3106	4655	34
H00H	6266	4049	4539	35
H00I	2050	3449	2292	32
H00J	10545	928	2717	38
H00K	1191	3457	836	42
H00L	7803	1739	2797	32
H00O	2375	3903	3445	33
H00P	1855	2628	5328	41
H00Q	-3900	5700	4069	40
H00R	7549	3605	5228	42
H00S	-4351	4179	2665	35
H00T	253	4185	1805	36
H00U	-1552	3332	2769	32
H00V	1634	4886	4654	36
H00W	11283	1720	3832	42
H00Y	-1095	4046	3514	31
H00Z	-901	2630	1169	41
H010	-3871	4867	3505	36
H011	-1700	5023	1379	40
H012	4889	2544	4159	35
H013	5328	1332	1548	36
H014	13266	999	4335	46
H015	10631	295	2063	41
H016	515	2022	1795	34
H018	6257	2999	1716	34
H019	5381	2878	5616	44
H01A	8551	1149	5167	43
H01B	-6280	5033	2247	39
H01C	-1121	5712	4636	41
H01D	8351	2499	3636	36
H01E	8033	507	1476	41

Experimental

Single crystals of $C_{23}H_{17}ClO$ **[3b]** were **[obtained at slow evaporation of solution of 3d in hexanes - chloroform]**. A suitable crystal was selected and studied on a **Xcalibur, Eos** diffractometerThe crystal was kept at 100(2) K during data collection. Using Olex2 [1], the structure was solved with the Superflip [2] structure solution program using Charge Flipping and refined with the ShelXL [3] refinement package using Least Squares minimisation.

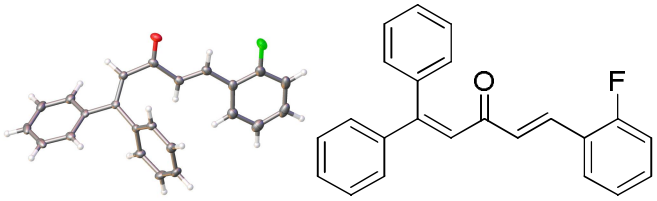
1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. &Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Palatinus, L. &Chapuis, G. (2007). J. Appl. Cryst., 40, 786-790; Palatinus, L. & van der Lee, A. (2008). J. Appl. Cryst. 41, 975-984; Palatinus, L., Prathapa, S. J. & van Smaalen, S. (2012). J. Appl. Cryst. 45, 575-580.
3. Sheldrick, G.M. (2015). ActaCryst. C71, 3-8.

Crystal structure determination of [3b]

Crystal Data for $C_{23}H_{17}ClO$ (*M* =344.82 g/mol): monoclinic, space group $P2_1/c$ (no. 14), *a* = 6.23180(10) Å, *b* = 19.0611(3) Å, *c* = 30.5102(4) Å, *β* = 95.1740(10)°, *V* = 3609.39(9) Å^3, *Z* = 8, *T* = 100(2) K, μ(CuKα) = 1.911 mm^{-1},*Dcalc* = 1.269 g/cm^3, 7095 reflections measured (5.474° ≤ 2Θ ≤ 144.42°), 7095 unique (R_{int} = ?, R_{sigma} = 0.0115) which were used in all calculations. The final R_1 was 0.0525 (I > 2σ(I)) and wR_2 was 0.1576 (all data).

Refinement model description
Number of restraints - 0, number of constraints - unknown.
Details:
1. Twinned data refinement
Scales: 0.37(5)
0.63(5)
2. Fixed Uiso
At 1.2 times of:
All C(H) groups
3.a Aromatic/amide H refined with riding coordinates:
C00B(H00B), C00C(H00C), C00D(H00D), C00G(H00G), C00H(H00H), C00I(H00I), C00J(H00J), C00K(H00K), C00L(H00L), C00O(H00O), C00P(H00P), C00Q(H00Q), C00R(H00R), C00S(H00S), C00T(H00T), C00U(H00U), C00V(H00V), C00W(H00W), C00Y(H00Y), C00Z(H00Z), C010(H010), C011(H011), C012(H012), C013(H013), C014(H014), C015(H015), C016(H016), C018(H018), C019(H019), C01A(H01A), C01B(H01B), C01C(H01C), C01D(H01D), C01E(H01E)

3d



CCDC 1847451

Table S7 Crystal data and structure refinement for 3d.

Identificationcode	7072-8496_vasilev073
Empiricalformula	$C_{23}H_{17}FO$
Formulaweight	328.36
Temperature/K	100(2)
Crystalsystem	monoclinic
Spacegroup	$P2_1/c$
a/Å	8.47709(19)
b/Å	19.3161(4)
c/Å	10.6412(2)
α/°	90
β/°	96.210(2)
γ/°	90
Volume/Å^3	1732.22(7)
Z	4
ρ_{calc}g/cm^3	1.259
μ/mm^{-1}	0.083
F(000)	688.0
Crystalsize/mm^3	0.2 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.274 to 54.986
Indexranges	-11 ≤ h ≤ 11, -25 ≤ k ≤ 25, -13 ≤ l ≤ 13
Reflectionscollected	30881
Independentreflections	3969 [R_{int} = 0.0422, R_{sigma} = 0.0219]
Data/restraints/parameters	3969/0/226
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0399, wR_2 = 0.0972
Final R indexes [all data]	R_1 = 0.0477, wR_2 = 0.1018
Largest diff. peak/hole / e Å^{-3}	0.39/-0.20

Table S8 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 3d. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	-1061.6(11)	5910.6(4)	5047.4(8)	41.2(2)
O2	1074.9(10)	4707.1(4)	1610.2(8)	25.3(2)
C1	4117.4(13)	6262.6(6)	541.9(10)	17.1(2)
C2	3753.5(13)	5738.6(5)	-1659(1)	18.0(2)
C3	3324.8(12)	5743.6(5)	-343.1(10)	16.6(2)
C4	1529.2(13)	5261.9(6)	1210.0(11)	19.5(2)
C5	4865.3(13)	6061.0(6)	1718.7(11)	20.5(2)
C6	2276.8(13)	5276.8(6)	15.5(11)	18.7(2)
C7	5313.2(14)	5869.6(6)	-1907.0(11)	20.7(2)
C8	1193.9(13)	5929.7(6)	1822.5(11)	20.4(2)
C9	95.8(13)	6588.2(6)	3542.0(11)	22.8(2)
C10	548.5(13)	5955.3(6)	2912.3(11)	21.8(2)
C11	5726.3(16)	5826.1(6)	-3131.4(12)	26.7(3)
C12	4095.6(14)	6963.5(6)	211.8(11)	22.4(2)
C13	2608.3(15)	5586.7(6)	-2667.8(11)	23.2(3)
C14	5562.2(15)	6553.7(7)	2558.1(12)	25.5(3)
C15	4581.9(18)	5676.4(6)	-4124.0(12)	30.2(3)
C16	4760.8(16)	7452.8(6)	1067.6(13)	29.6(3)
C17	-738.0(15)	6549.0(7)	4598.7(12)	29.1(3)
C18	5497.0(16)	7249.8(7)	2235.9(13)	28.8(3)
C19	413.1(15)	7259.7(7)	3128.6(12)	28.0(3)
C20	3025.8(17)	5558.4(6)	-3893.8(12)	29.3(3)
C21	-1287.2(16)	7117.0(8)	5200.2(13)	35.7(3)
C22	-988.4(16)	7768.8(8)	4744.8(14)	36.2(3)
C23	-127.7(17)	7841.8(7)	3716.3(13)	34.2(3)

Table S9 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3d. 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}
F1	51.0(5)	41.8(5)	35.2(5)	-5.0(4)	24.6(4)	-14.5(4)
O2	21.8(4)	21.9(4)	33.3(5)	5.5(3)	7.9(4)	-2.5(3)
C1	15.8(5)	15.3(5)	21.0(5)	-1.8(4)	5.5(4)	-1.1(4)
C2	22.7(6)	10.3(5)	21.8(5)	-0.4(4)	5.8(4)	1.8(4)
C3	15.7(5)	13.9(5)	20.4(5)	-0.4(4)	2.4(4)	2.2(4)
C4	13.6(5)	22.3(6)	22.5(6)	2.6(4)	1.2(4)	-0.9(4)
C5	20.4(5)	16.9(5)	24.3(6)	0.6(4)	3.5(4)	-1.1(4)
C6	17.7(5)	16.8(5)	21.5(5)	-2.4(4)	1.6(4)	-0.7(4)
C7	23.4(6)	12.3(5)	27.3(6)	2.4(4)	7.1(5)	1.8(4)
C8	17.0(5)	21.2(6)	23.1(6)	2.4(4)	2.9(4)	0.0(4)
C9	17.6(5)	30.2(6)	20.3(6)	-3.3(5)	0.4(4)	-1.6(5)
C10	18.1(5)	25.6(6)	21.4(6)	0.5(4)	1.0(4)	-3.2(4)
C11	34.1(7)	13.9(5)	35.5(7)	5.6(5)	18.9(6)	4.6(5)
C12	25.0(6)	17.1(5)	25.1(6)	1.7(4)	3.3(5)	-1.3(4)
C13	27.8(6)	17.6(5)	24.3(6)	-2.5(4)	3.4(5)	-1.0(4)
C14	25.7(6)	28.4(6)	22.1(6)	-2.1(5)	0.9(5)	-4.7(5)
C15	55.6(9)	13.6(5)	24.5(6)	0.7(5)	18.5(6)	3.7(5)
C16	35.9(7)	15.6(5)	37.8(7)	-2.9(5)	6.0(6)	-5.0(5)
C17	24.6(6)	36.7(7)	26.4(6)	-5.7(5)	5.1(5)	-7.8(5)
C18	31.7(7)	24.1(6)	31.0(7)	-10.7(5)	5.5(5)	-9.1(5)
C19	27.5(6)	30.8(7)	25.7(6)	-2.0(5)	2.1(5)	-1.4(5)
C20	46.7(8)	19.4(6)	21.5(6)	-3.2(5)	2.2(5)	-1.8(5)

C21	26.8(7)	50.2(9)	31.2(7)	-16.8(6)	8.0(5)	-6.3(6)
C22	28.5(7)	41.1(8)	37.9(8)	-20.4(6)	-1.6(6)	3.1(6)
C23	35.6(7)	30.2(7)	35.4(7)	-7.0(6)	-3.3(6)	0.1(6)

Table S10 Bond Lengths for 3d.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	C17	1.3609(16)	C9	C10	1.4650(17)
O2	C4	1.2304(14)	C9	C17	1.3934(17)
C1	C3	1.4854(15)	C9	C19	1.4051(18)
C1	C5	1.3965(16)	C11	C15	1.385(2)
C1	C12	1.3984(15)	C12	C16	1.3891(17)
C2	C3	1.4842(15)	C13	C20	1.3893(17)
C2	C7	1.3990(16)	C14	C18	1.3872(18)
C2	C13	1.3984(16)	C15	C20	1.386(2)
C3	C6	1.3496(15)	C16	C18	1.386(2)
C4	C6	1.4807(15)	C17	C21	1.3764(19)
C4	C8	1.4865(16)	C19	C23	1.3883(19)
C5	C14	1.3923(16)	C21	C22	1.382(2)
C7	C11	1.3878(17)	C22	C23	1.387(2)
C8	C10	1.3357(16)			

Table S11 Bond Angles for 3d.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C5	C1	C3	120.71(10)	C19	C9	C10	123.96(11)
C5	C1	C12	119.19(10)	C8	C10	C9	125.47(11)
C12	C1	C3	120.08(10)	C15	C11	C7	120.10(12)
C7	C2	C3	120.64(10)	C16	C12	C1	120.04(11)
C13	C2	C3	120.34(10)	C20	C13	C2	120.19(12)
C13	C2	C7	119.00(11)	C18	C14	C5	120.08(12)
C2	C3	C1	117.54(9)	C11	C15	C20	120.06(11)
C6	C3	C1	122.56(10)	C18	C16	C12	120.47(12)
C6	C3	C2	119.88(10)	F1	C17	C9	118.12(11)
O2	C4	C6	119.54(10)	F1	C17	C21	117.90(12)
O2	C4	C8	121.48(10)	C21	C17	C9	123.96(13)
C6	C4	C8	118.65(10)	C16	C18	C14	119.86(11)
C14	C5	C1	120.30(11)	C23	C19	C9	121.53(12)
C3	C6	C4	127.71(10)	C15	C20	C13	120.22(12)
C11	C7	C2	120.39(12)	C17	C21	C22	118.62(13)
C10	C8	C4	121.91(11)	C21	C22	C23	120.09(13)
C17	C9	C10	120.31(11)	C22	C23	C19	120.05(14)
C17	C9	C19	115.71(11)				

Table S12 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3d.

Atom	*x*	*y*	*z*	U(eq)
H5	4899	5585	1948	25
H6	1984	4915	-568	22
H7	6094	5989	-1233	25
H8	1446	6350	1427	24
H10	368	5527	3313	26
H11	6796	5899	-3289	32
H12	3625	7105	-598	27
H13	1542	5503	-2514	28
H14	6083	6413	3352	31

H15	4864	5655	-4963	36
H16	4711	7930	851	36
H18	5956	7587	2815	35
H19	1012	7317	2431	34
H20	2242	5458	-4577	35
H21	-1860	7062	5913	43
H22	-1373	8167	5137	43
H23	92	8290	3414	41

Experimental

Single crystals of $C_{23}H_{17}FO$ **[3d]** were **[obtained at slow evaporation of solution of 3d in hexanes - chloroform]**. 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 Superflip [2] structure solution program using Charge Flipping 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. Palatinus, L. &Chapuis, G. (2007). J. Appl. Cryst., 40, 786-790; Palatinus, L. & van der Lee, A. (2008). J. Appl. Cryst. 41, 975-984; Palatinus, L., Prathapa, S. J. & van Smaalen, S. (2012). J. Appl. Cryst. 45, 575-580.
3. Sheldrick, G.M. (2015). ActaCryst. C71, 3-8.

Crystal structure determination of [3d]

Crystal Data for $C_{23}H_{17}FO$ (M =328.36 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 8.47709(19) Å, b = 19.3161(4) Å, c = 10.6412(2) Å, β = 96.210(2)°, V = 1732.22(7) Å^3, Z = 4, T = 100(2) K, μ(MoKα) = 0.083 mm^{-1},*Dcalc* = 1.259 g/cm^3, 30881 reflections measured (5.274° ≤ 2Θ ≤ 54.986°), 3969 unique (R_{int} = 0.0422, R_{sigma} = 0.0219) which were used in all calculations. The final R_1 was 0.0399 (I > 2σ(I)) and wR_2 was 0.1018 (all data).

Refinement model description

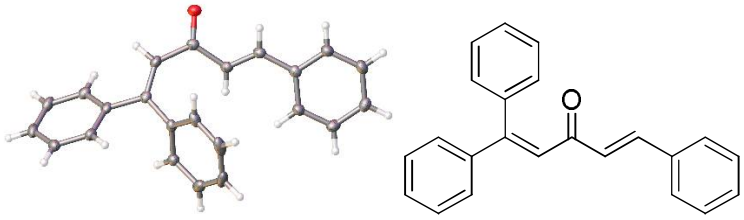
Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups

2.a Aromatic/amide H refined with riding coordinates:
 C5(H5), C6(H6), C7(H7), C8(H8), C10(H10), C11(H11), C12(H12), C13(H13),
 C14(H14), C15(H15), C16(H16), C18(H18), C19(H19), C20(H20), C21(H21), C22(H22),
  C23(H23)

3e



CCDC 1847452

Table S13 Crystal data and structure refinement for 3e.

Identificationcode	7071-8325_ima063
Empiricalformula	$C_{23}H_{18}O$
Formulaweight	310.37
Temperature/K	100.01(10)
Crystalsystem	orthorhombic
Spacegroup	$Pna2_1$
a/Å	7.75140(10)
b/Å	12.0257(2)
c/Å	17.7094(3)
α/°	90
β/°	90
γ/°	90

Volume/Å^3	1650.80(4)
Z	4
ρ_{calc}g/cm^3	1.249
μ/mm^{-1}	0.578
F(000)	656.0
Crystalsize/mm^3	0.2 × 0.2 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.888 to 139.92
Indexranges	$-9 \le h \le 6$, $-14 \le k \le 14$, $-21 \le l \le 21$
Reflectionscollected	14542
Independentreflections	3045 [R_{int} = 0.0369, R_{sigma} = 0.0235]
Data/restraints/parameters	3045/1/218
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0305, wR_2 = 0.0747
Final R indexes [all data]	R_1 = 0.0313, wR_2 = 0.0756
Largest diff. peak/hole / e Å^{-3}	0.15/-0.21
Flackparameter	0.2(3)

Table S14 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3e. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O12	3773.8(18)	8844.3(12)	4911.6(9)	27.4(3)
C7	2730(2)	6468.6(16)	6064.7(11)	19.0(4)
C10	2863(2)	7169.0(16)	4345.4(12)	19.8(4)
C19	2935(2)	5437.8(16)	5612.6(11)	19.2(4)
C11	3555(2)	7384.8(16)	3672.8(11)	20.1(4)
C8	2950(2)	7502.8(17)	5787.3(11)	21.6(4)
C9	3260(2)	7885.1(16)	5003.2(11)	19.7(4)
C6	2861(2)	5391.7(16)	7279.6(12)	21.5(4)
C1	2269(2)	6320.5(17)	6878.1(11)	19.5(4)
C13	3288(2)	6753.3(16)	2972.5(11)	19.5(4)
C24	1606(2)	4654.5(17)	5599.4(11)	22.6(4)
C14	3931(2)	7180.5(17)	2296.3(12)	24.0(4)
C4	1363(2)	6006.6(19)	8394.9(11)	26.1(4)
C5	2426(2)	5245.6(17)	8033.8(12)	24.2(4)
C18	2399(2)	5737.7(16)	2953.8(11)	22.1(4)
C2	1227(2)	7091.4(17)	7253.6(12)	22.1(4)
C20	4409(2)	5242.0(18)	5177.2(11)	25.5(4)
C3	768(2)	6932.0(18)	8002.5(12)	26.5(4)
C17	2119(2)	5194.5(18)	2273.7(13)	24.9(4)
C16	2748(2)	5640.4(17)	1602.8(11)	24.3(4)
C15	3665(3)	6631.6(18)	1617.0(12)	26.8(4)
C23	1713(3)	3731.3(18)	5139.1(13)	30.2(5)
C21	4519(3)	4301(2)	4732.4(12)	35.7(5)
C22	3171(3)	3552.3(19)	4702.0(13)	36.1(5)

Table S15 Anisotropic Displacement Parameters (Å^2×10^3) for 3e. 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}
O12	33.9(7)	20.5(7)	27.7(7)	0.8(6)	-0.8(6)	-4.6(6)
C7	15.1(7)	22.6(10)	19.3(9)	-2.2(8)	-2.6(7)	-0.3(6)
C10	19.0(8)	18.0(9)	22.4(9)	1.2(7)	-1.9(7)	0.0(7)
C19	21.3(8)	20.3(9)	15.9(8)	1.1(7)	-0.6(7)	3.0(7)
C11	18.0(8)	18.6(9)	23.7(9)	2.5(8)	-2.7(7)	-1.1(7)

C8	22.9(8)	22.0(9)	20.0(9)	-4.9(8)	-2.1(7)	-1.9(7)
C9	16.7(8)	19.0(9)	23.3(10)	1.3(8)	-1.7(7)	0.9(6)
C6	22.0(8)	21(1)	21.6(9)	-4.0(8)	1.7(7)	0.0(7)
C1	17.6(8)	22.6(10)	18.3(9)	-4.5(7)	-2.1(7)	-3.4(7)
C13	16.3(8)	20.6(9)	21.7(9)	2.3(8)	-1.3(7)	2.5(7)
C24	25.5(8)	22.1(10)	20.1(9)	1.2(8)	-1.2(7)	-1.0(7)
C14	25.5(9)	22.3(10)	24.2(10)	2.9(8)	0.8(8)	-3.0(7)
C4	26.3(9)	35.7(12)	16.3(9)	-4.9(8)	1.6(7)	-7.6(8)
C5	27.9(9)	24.6(10)	20.2(9)	1.6(8)	-2.1(8)	-5.7(7)
C18	22.0(9)	22.4(9)	21.9(10)	2.3(8)	2.8(7)	-2.0(7)
C2	20.0(9)	22.3(9)	23.9(10)	-4.1(8)	-3.8(7)	-0.8(7)
C20	24.9(9)	30.1(11)	21.3(10)	6.9(8)	3.5(8)	7.9(8)
C3	22.2(8)	32.9(11)	24.5(10)	-12.1(9)	0.3(8)	0.0(7)
C17	22.0(8)	23.5(10)	29.3(10)	-3.5(9)	1.2(8)	-3.0(7)
C16	22.3(9)	28.5(11)	22.2(10)	-5.0(8)	-2.7(8)	2.6(7)
C15	30.6(9)	28.5(11)	21.2(10)	5.1(8)	2.9(8)	0.6(8)
C23	46.4(12)	20.6(11)	23.5(10)	2.1(8)	-9.0(9)	-2.1(9)
C21	46.8(12)	38.7(13)	21.7(10)	5.8(9)	11.0(9)	21.1(10)
C22	67.3(15)	22.7(11)	18.3(10)	-3.9(8)	-2.9(10)	13.1(11)

Table S16 Bond Lengths for 3e.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O12	C9	1.231(2)	C13	C14	1.395(3)
C7	C19	1.484(3)	C13	C18	1.403(3)
C7	C8	1.348(3)	C24	C23	1.380(3)
C7	C1	1.495(3)	C14	C15	1.387(3)
C10	C11	1.332(3)	C4	C5	1.387(3)
C10	C9	1.481(3)	C4	C3	1.391(3)
C19	C24	1.396(3)	C18	C17	1.387(3)
C19	C20	1.398(3)	C2	C3	1.387(3)
C11	C13	1.469(3)	C20	C21	1.381(3)
C8	C9	1.482(3)	C17	C16	1.392(3)
C6	C1	1.401(3)	C16	C15	1.388(3)
C6	C5	1.389(3)	C23	C22	1.386(4)
C1	C2	1.398(3)	C21	C22	1.381(4)

Table S17 Bond Angles for 3e.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C19	C7	C1	116.48(17)	C14	C13	C18	118.41(18)
C8	C7	C19	124.09(18)	C18	C13	C11	122.62(17)
C8	C7	C1	119.43(18)	C23	C24	C19	120.54(19)
C11	C10	C9	120.45(17)	C15	C14	C13	121.07(18)
C24	C19	C7	119.57(16)	C5	C4	C3	119.64(19)
C24	C19	C20	118.68(18)	C4	C5	C6	120.3(2)
C20	C19	C7	121.72(17)	C17	C18	C13	120.49(18)
C10	C11	C13	126.72(17)	C3	C2	C1	120.78(19)
C7	C8	C9	130.39(18)	C21	C20	C19	120.2(2)
O12	C9	C10	120.56(18)	C2	C3	C4	120.22(18)
O12	C9	C8	117.80(18)	C18	C17	C16	120.33(19)
C10	C9	C8	121.54(16)	C15	C16	C17	119.65(19)
C5	C6	C1	120.62(18)	C14	C15	C16	120.02(19)
C6	C1	C7	120.37(18)	C24	C23	C22	120.3(2)
C2	C1	C7	121.17(18)	C22	C21	C20	120.6(2)
C2	C1	C6	118.45(19)	C21	C22	C23	119.6(2)

C14 C13 C11 118.96(17)

Table S18 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3e.

Atom	*x*	*y*	*z*	U(eq)
H10	2127	6564	4402	24
H11	4281	7999	3643	24
H8	2900	8067	6146	26
H6	3552	4868	7039	26
H24	640	4756	5903	27
H14	4547	7844	2301	29
H4	1051	5899	8897	31
H5	2848	4635	8298	29
H18	1995	5426	3401	27
H2	838	7719	6998	26
H20	5318	5747	5187	31
H3	60	7446	8243	32
H17	1508	4529	2266	30
H16	2554	5276	1147	29
H15	4102	6928	1171	32
H23	805	3227	5122	36
H21	5511	4171	4451	43
H22	3240	2932	4390	43

Experimental

Single crystals of $C_{23}H_{18}O$ **[3e]** were **[obtained at slow evaporation of solution of 3e in hexanes - chloroform]**. A suitable crystal was selected and **o**n a **Xcalibur, Eos** diffractometer. The crystal was kept at 100.01(10) 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). ActaCryst. A71, 3-8.
3. Sheldrick, G.M. (2015). ActaCryst. C71, 3-8.

Crystal structure determination of 3e

Crystal Data for $C_{23}H_{18}O$ (M =310.37 g/mol): orthorhombic, space group $Pna2_1$ (no. 33), a = 7.75140(10) Å, b = 12.0257(2) Å, c = 17.7094(3) Å, V = 1650.80(4) Å^3, Z = 4, T = 100.01(10) K, μ(CuKα) = 0.578 mm^{-1}, *Dcalc* = 1.249 g/cm^3, 14542 reflections measured (8.888° ≤ 2Θ ≤ 139.92°), 3045 unique (R_{int} = 0.0369, R_{sigma} = 0.0235) which were used in all calculations. The final R_1 was 0.0305 (I > 2σ(I)) and wR_2 was 0.0756 (all data).

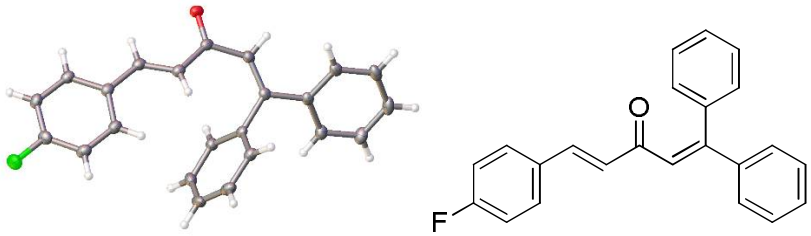
Refinement model description

Number of restraints - 1, number of constraints - unknown.

Details:

1. Twinned data refinement
 Scales: 0.8(4)
 0.2(4)
2. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
3.a Aromatic/amide H refined with riding coordinates:
 C10(H10), C11(H11), C8(H8), C6(H6), C24(H24), C14(H14), C4(H4), C5(H5),
 C18(H18), C2(H2), C20(H20), C3(H3), C17(H17), C16(H16), C15(H15), C23(H23),
 C21(H21), C22(H22)

3l



CCDC 1847453

Table S19 Crystal data and structure refinement for 3l.

Identificationcode	9137_AVV363
Empiricalformula	$C_{23}H_{17}FO$
Formulaweight	328.36
Temperature/K	293(2)
Crystalsystem	monoclinic
Spacegroup	$P2_1/c$
a/Å	6.20717(15)
b/Å	38.6061(11)
c/Å	14.5881(3)
α/°	90
β/°	99.406(2)
γ/°	90
Volume/Å^3	3448.81(15)
Z	8
ρ_{calc}g/cm^3	1.265
μ/mm^{-1}	0.668
F(000)	1376.0
Crystalsize/mm^3	0.4 × 0.2 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	4.578 to 143.934
Indexranges	-6 ≤ h ≤ 7, -47 ≤ k ≤ 45, -17 ≤ l ≤ 17
Reflectionscollected	27840
Independentreflections	6752 [R_{int} = 0.0428, R_{sigma} = 0.0353]
Data/restraints/parameters	6752/0/451
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	R_1 = 0.0418, wR_2 = 0.1103
Final R indexes [all data]	R_1 = 0.0472, wR_2 = 0.1144
Largest diff. peak/hole / e Å^{-3}	0.22/-0.27

Table S20 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3l. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F25	1051.8(14)	1730.8(2)	3517.3(6)	34.1(2)
F50	13617.9(14)	3181.2(2)	5909.5(6)	32.9(2)
O37	7400.4(14)	5120.7(2)	5473.2(6)	23.9(2)
O12	7223.2(15)	3675.6(3)	4015.2(6)	26.2(2)
C12	2901.1(19)	5058.1(3)	7797.5(9)	18.3(3)
C18	5489(2)	4553.0(3)	7753.4(8)	17.3(2)
C12A	11853.4(19)	3620.6(3)	1723.3(9)	18.3(3)
C18A	9322(2)	3110.6(3)	1752.7(8)	17.4(2)
C19A	10738(2)	2831.8(3)	1700.6(8)	19.4(3)
C2A	9589(2)	3582.4(3)	2958.4(9)	19.7(3)
C1A	10219.8(18)	3440.2(3)	2195.9(8)	17.6(2)

C1	4521.1(19)	4880.1(3)	7316.7(8)	17.2(2)
C4	7398(2)	4536.9(3)	5965.9(8)	19.3(3)
C6	10268(2)	4111.0(3)	5686.7(8)	19.5(3)
C5	9235(2)	4452.7(3)	5647.9(8)	20.3(3)
C13A	11715(2)	3595.8(3)	757.5(9)	21.5(3)
C3A	7967(2)	3461.2(3)	3525.6(8)	20.4(3)
C4A	7228(2)	3095.3(3)	3504.6(8)	20.5(3)
C19	7691(2)	4530.8(3)	8149.2(8)	20.6(3)
C3	6678.8(19)	4902.2(3)	5962.1(8)	18.9(3)
C17	1190.0(19)	5253.7(3)	7298.3(9)	20.4(3)
C17A	13530(2)	3823.6(3)	2219.5(9)	20.9(3)
C2	5080(2)	5022.5(3)	6543.3(9)	19.8(3)
C6A	4314(2)	2667.0(3)	3737.0(8)	20.3(3)
C5A	5348(2)	3009.6(3)	3783.5(8)	20.7(3)
C11	12144(2)	4067.0(3)	5275.4(8)	20.8(3)
C7	9536(2)	3829.2(3)	6162.3(9)	22.2(3)
C23	4155(2)	4261.6(3)	7762.0(9)	21.6(3)
C10	13275(2)	3754.8(3)	5337.4(9)	22.7(3)
C23A	7112(2)	3073.6(3)	1374.8(9)	21.1(3)
C11A	2417(2)	2620.6(4)	4128.7(9)	22.1(3)
C10A	1318(2)	2305.9(4)	4068.1(9)	24.0(3)
C20A	9949(2)	2517.0(3)	1320.1(9)	22.7(3)
C21A	7742(2)	2481.0(4)	958.1(9)	24.9(3)
C9	12496(2)	3488.2(3)	5820.3(9)	23.9(3)
C13	3077(2)	5042.5(3)	8767.3(9)	22.1(3)
C16A	14989(2)	3999.8(3)	1758.6(10)	25.6(3)
C7A	5096(2)	2385.1(4)	3277.8(9)	23.0(3)
C22	5031(2)	3950.4(4)	8128.2(9)	27.3(3)
C16	-249(2)	5433.7(3)	7757(1)	25.2(3)
C15	-16(2)	5424.9(4)	8721.1(10)	27.4(3)
C22A	6338(2)	2761.3(4)	976.0(9)	25.0(3)
C8	10645(2)	3516.6(4)	6230.4(9)	24.9(3)
C14	1647(2)	5227.6(4)	9226.5(10)	26.9(3)
C9A	2140(2)	2038.3(4)	3602.8(9)	25.1(3)
C20	8547(2)	4220.9(4)	8542.5(9)	27.0(3)
C15A	14811(2)	3976.7(3)	797.5(11)	27.4(3)
C8A	4011(2)	2069.9(4)	3206.7(10)	26.8(3)
C14A	13174(2)	3774.1(4)	300.2(10)	25.7(3)
C21	7223(3)	3929.9(4)	8527.1(10)	30.5(3)

Table S21 Anisotropic Displacement Parameters ($Å^2×10^3$) for 3l. 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}
F25	40.7(5)	25.8(4)	36.0(5)	-0.1(4)	7.0(4)	-11.5(4)
F50	41.4(5)	21.9(4)	37.7(5)	1.8(3)	12.8(4)	7.6(3)
O37	20.4(4)	26.6(5)	25.2(5)	8.2(4)	5.0(4)	-0.8(4)
O12	25.9(5)	29.8(5)	23.8(5)	-8.1(4)	6.6(4)	-2.3(4)
C12	15.5(6)	15.0(6)	24.4(6)	-1.7(5)	3.5(5)	-2.9(4)
C18	20.7(6)	17.1(6)	15.1(5)	-0.9(5)	6.0(4)	1.0(5)
C12A	15.2(5)	14.1(6)	25.5(6)	0.7(5)	3.1(5)	2.6(4)
C18A	19.3(6)	17.5(6)	15.8(5)	1.3(5)	3.4(4)	-0.5(5)
C19A	18.3(6)	21.3(6)	18.7(6)	1.0(5)	2.9(4)	1.5(5)
C2A	17.8(6)	19.0(6)	21.7(6)	-1.0(5)	1.5(5)	-2.0(5)
C1A	14.4(5)	17.0(6)	20.3(6)	1.9(5)	-0.4(4)	1.8(4)

C1	14.9(5)	16.8(6)	19.3(6)	-1.6(5)	0.8(4)	-1.8(4)
C4	19.5(6)	21.4(6)	17.1(6)	-0.2(5)	2.8(4)	-3.3(5)
C6	18.8(6)	22.7(7)	16.8(5)	-1.8(5)	2.4(4)	-2.8(5)
C5	20.1(6)	23.6(7)	16.7(5)	1.4(5)	2.0(5)	-3.8(5)
C13A	20.5(6)	19.2(6)	24.8(6)	0.6(5)	3.7(5)	-0.3(5)
C3A	17.6(6)	25.0(7)	17.6(6)	-0.7(5)	0.0(4)	1.5(5)
C4A	19.9(6)	23.0(7)	18.4(6)	1.3(5)	2.7(5)	2.4(5)
C19	19.7(6)	22.8(7)	19.6(6)	1.0(5)	4.2(5)	1.4(5)
C3	15.4(6)	23.6(7)	17.2(6)	2.8(5)	0.8(4)	-2.3(5)
C17	17.0(6)	17.1(6)	26.8(6)	0.5(5)	2.7(5)	-2.4(5)
C17A	17.1(6)	17.3(6)	27.9(6)	-2.3(5)	2.3(5)	2.7(5)
C2	17.6(6)	18.7(6)	22.6(6)	2.1(5)	2.0(5)	1.6(5)
C6A	18.7(6)	23.4(7)	17.9(6)	3.5(5)	0.1(5)	2.2(5)
C5A	20.7(6)	22.8(7)	18.2(6)	-0.1(5)	1.8(5)	3.0(5)
C11	22.0(6)	22.8(6)	18.0(6)	-1.2(5)	4.0(5)	-4.5(5)
C7	22.9(6)	24.3(7)	20.1(6)	-0.9(5)	5.6(5)	-3.3(5)
C23	23.3(6)	22.4(7)	20.1(6)	-1.9(5)	6.9(5)	-3.3(5)
C10	22.2(6)	25.1(7)	21.7(6)	-4.6(5)	6.7(5)	-1.3(5)
C23A	17.5(6)	22.9(7)	22.5(6)	-1.8(5)	2.3(5)	1.2(5)
C11A	20.3(6)	25.9(7)	19.4(6)	0.9(5)	0.9(5)	2.1(5)
C10A	19.8(6)	31.1(7)	20.4(6)	3.6(5)	1.5(5)	-1.4(5)
C20A	28.9(7)	18.6(6)	21.7(6)	-0.6(5)	6.9(5)	2.5(5)
C21A	31.4(7)	20.6(7)	23.5(6)	-4.3(5)	6.8(5)	-6.7(5)
C9	30.3(7)	18.0(6)	23.1(6)	-3.2(5)	3.8(5)	2.4(5)
C13	18.2(6)	23.9(7)	24.2(6)	-3.4(5)	3.1(5)	-0.3(5)
C16A	17.3(6)	16.1(6)	43.3(8)	-3.7(6)	5.1(5)	-1.1(5)
C7A	22.1(6)	24.3(7)	23.0(6)	3.1(5)	4.9(5)	3.0(5)
C22	40.7(8)	18.6(7)	25.7(7)	0.9(5)	14.3(6)	-2.7(6)
C16	19.2(6)	16.1(6)	39.9(8)	-0.8(6)	4.0(5)	0.7(5)
C15	21.6(6)	21.3(7)	41.2(8)	-10.4(6)	11.0(6)	-1.1(5)
C22A	20.2(6)	30.6(7)	23.5(6)	-4.2(5)	1.3(5)	-5.2(5)
C8	31.0(7)	21.8(7)	22.7(6)	-0.1(5)	6.8(5)	-4.2(5)
C14	25.0(7)	30.3(7)	26.0(7)	-9.3(6)	6.6(5)	-3.1(5)
C9A	29.0(7)	21.6(7)	23.1(6)	3.3(5)	-0.1(5)	-4.3(5)
C20	25.9(7)	31.9(8)	23.8(6)	5.2(6)	6.0(5)	10.6(6)
C15A	22.8(6)	19.2(7)	42.9(8)	4.8(6)	13.4(6)	0.1(5)
C8A	31.9(7)	22.4(7)	26.3(7)	0.7(5)	5.4(5)	3.6(6)
C14A	27.7(7)	23.1(7)	27.9(7)	5.0(5)	9.3(5)	2.6(5)
C21	43.5(8)	23.1(7)	27.7(7)	8.8(6)	14.4(6)	12.6(6)

Table S22 Bond Lengths for 3l.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F25	C9A	1.3616(15)	C4A	C5A	1.3386(18)
F50	C9	1.3701(15)	C19	C20	1.3940(18)
O37	C3	1.2348(15)	C3	C2	1.4814(17)
O12	C3A	1.2314(16)	C17	C16	1.3872(18)
C12	C1	1.4853(17)	C17A	C16A	1.3906(19)
C12	C17	1.4057(17)	C6A	C5A	1.4669(18)
C12	C13	1.4022(18)	C6A	C11A	1.4018(18)
C18	C1	1.4954(17)	C6A	C7A	1.4054(18)
C18	C19	1.3966(17)	C11	C10	1.3905(18)
C18	C23	1.3983(17)	C7	C8	1.3850(19)
C12A	C1A	1.4891(17)	C23	C22	1.3893(19)
C12A	C13A	1.4008(18)	C10	C9	1.3786(19)

C12A	C17A	1.4051(17)	C23A	C22A	1.3898(19)
C18A	C19A	1.3993(17)	C11A	C10A	1.3889(19)
C18A	C1A	1.4932(17)	C10A	C9A	1.379(2)
C18A	C23A	1.3999(17)	C20A	C21A	1.3921(19)
C19A	C20A	1.3916(18)	C21A	C22A	1.393(2)
C2A	C1A	1.3544(17)	C9	C8	1.3836(19)
C2A	C3A	1.4799(17)	C13	C14	1.3934(18)
C1	C2	1.3504(17)	C16A	C15A	1.391(2)
C4	C5	1.3395(18)	C7A	C8A	1.3867(19)
C4	C3	1.4790(18)	C22	C21	1.392(2)
C6	C5	1.4640(18)	C16	C15	1.390(2)
C6	C11	1.4047(17)	C15	C14	1.393(2)
C6	C7	1.4052(18)	C9A	C8A	1.3845(19)
C13A	C14A	1.3915(18)	C20	C21	1.390(2)
C3A	C4A	1.4839(18)	C15A	C14A	1.389(2)

Table S23 Bond Angles for 3l.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C17	C12	C1	121.09(11)	C16A	C17A	C12A	120.63(12)
C13	C12	C1	120.62(11)	C1	C2	C3	129.65(12)
C13	C12	C17	118.26(11)	C11A	C6A	C5A	119.13(12)
C19	C18	C1	121.72(11)	C11A	C6A	C7A	118.30(12)
C19	C18	C23	119.21(12)	C7A	C6A	C5A	122.51(11)
C23	C18	C1	119.06(11)	C4A	C5A	C6A	127.27(12)
C13A	C12A	C1A	119.95(11)	C10	C11	C6	121.47(12)
C13A	C12A	C17A	118.35(12)	C8	C7	C6	120.86(12)
C17A	C12A	C1A	121.69(11)	C22	C23	C18	120.26(12)
C19A	C18A	C1A	119.05(11)	C9	C10	C11	117.69(12)
C19A	C18A	C23A	118.95(11)	C22A	C23A	C18A	120.19(12)
C23A	C18A	C1A	122.00(11)	C10A	C11A	C6A	121.48(12)
C20A	C19A	C18A	120.68(11)	C9A	C10A	C11A	118.00(12)
C1A	C2A	C3A	130.19(12)	C19A	C20A	C21A	119.93(12)
C12A	C1A	C18A	115.62(10)	C20A	C21A	C22A	119.70(12)
C2A	C1A	C12A	120.04(11)	F50	C9	C10	118.63(12)
C2A	C1A	C18A	124.31(11)	F50	C9	C8	118.18(12)
C12	C1	C18	116.45(10)	C10	C9	C8	123.19(12)
C2	C1	C12	119.49(11)	C14	C13	C12	120.82(12)
C2	C1	C18	124.02(11)	C17A	C16A	C15A	120.35(12)
C5	C4	C3	120.23(11)	C8A	C7A	C6A	120.92(12)
C11	C6	C5	118.74(11)	C23	C22	C21	120.28(13)
C11	C6	C7	118.36(12)	C17	C16	C15	120.45(12)
C7	C6	C5	122.81(11)	C16	C15	C14	119.63(12)
C4	C5	C6	126.70(12)	C23A	C22A	C21A	120.48(12)
C14A	C13A	C12A	120.71(12)	C9	C8	C7	118.43(12)
O12	C3A	C2A	117.75(12)	C15	C14	C13	120.08(13)
O12	C3A	C4A	120.51(11)	F25	C9A	C10A	118.71(12)
C2A	C3A	C4A	121.74(11)	F25	C9A	C8A	118.42(12)
C5A	C4A	C3A	120.74(12)	C10A	C9A	C8A	122.86(13)
C20	C19	C18	120.29(12)	C21	C20	C19	120.14(13)
O37	C3	C4	121.05(11)	C14A	C15A	C16A	119.55(12)
O37	C3	C2	117.17(11)	C9A	C8A	C7A	118.44(13)
C4	C3	C2	121.79(11)	C15A	C14A	C13A	120.39(13)
C16	C17	C12	120.72(12)	C20	C21	C22	119.74(13)

Table S24 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3l.

Atom	*x*	*y*	*z*	U(eq)
H19A	12221	2857	1923	23
H2A	10286	3789	3157	24
H4	6571	4365	6190	23
H5	9925	4630	5374	24
H13A	10637	3459	418	26
H4A	8080	2924	3295	25
H19	8590	4724	8150	25
H17	1021	5263	6653	24
H17A	13665	3840	2862	25
H2	4353	5227	6346	24
H5A	4615	3187	4035	25
H11	12641	4251	4954	25
H7	8290	3853	6435	27
H23	2675	4276	7522	26
H10	14515	3727	5063	27
H23A	6158	3259	1391	25
H11A	1881	2805	4436	27
H10A	66	2277	4333	29
H20A	10895	2331	1308	27
H21A	7208	2271	705	30
H13	4162	4907	9108	27
H16A	16089	4134	2095	31
H7A	6359	2410	3018	28
H22	4149	3755	8107	33
H16	-1378	5561	7417	30
H15	-965	5550	9027	33
H22A	4871	2739	719	30
H8	10158	3330	6544	30
H14	1803	5219	9871	32
H20	10008	4209	8816	32
H15A	15781	4096	490	33
H8A	4528	1884	2900	32
H14A	13052	3758	-342	31
H21	7800	3722	8782	37

Experimental

Single crystals of $C_{23}H_{17}FO$ **[3l]** were **[obtained at slow evaporation of solution of 3e in hexanes - chloroform]**. A suitable crystal was selected and on a **Xcalibur, Eos** diffractometer. The crystal was kept at 293(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). ActaCryst. A71, 3-8.
3. Sheldrick, G.M. (2015). ActaCryst. C71, 3-8.

Crystal structure determination of 3l

Crystal Data for $C_{23}H_{17}FO$ (*M* =328.36 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 6.20717(15) Å, b = 38.6061(11) Å, c = 14.5881(3) Å, β = 99.406(2)°, V = 3448.81(15) Å^3, Z = 8, T = 293(2) K, μ(CuKα) = 0.668 mm^{-1},*Dcalc* = 1.265 g/cm^3, 27840 reflections measured (4.578° ≤ 2Θ ≤ 143.934°), 6752 unique (R_{int} = 0.0428, R_{sigma} = 0.0353) which were used in all calculations. The final R_1 was 0.0418 (I > 2σ(I)) and wR_2 was 0.1144 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

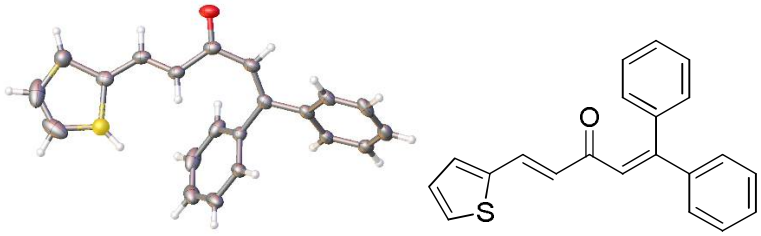
1. Fixed Uiso

At 1.2 times of:

All C(H) groups

2.a Aromatic/amide H refined with riding coordinates:
C19A(H19A), C2A(H2A), C4(H4), C5(H5), C13A(H13A), C4A(H4A), C19(H19), C17(H17), C17A(H17A), C2(H2), C5A(H5A), C11(H11), C7(H7), C23(H23), C10(H10), C23A(H23A), C11A(H11A), C10A(H10A), C20A(H20A), C21A(H21A), C13(H13), C16A(H16A), C7A(H7A), C22(H22), C16(H16), C15(H15), C22A(H22A), C8(H8), C14(H14), C20(H20), C15A(H15A), C8A(H8A), C14A(H14A), C21(H21)

3p



CCDC 1847454

Table S25 Crystal data and structure refinement for 3p.

Identificationcode	9176_Z-6
Empiricalformula	$C_{21}H_{16}OS$
Formulaweight	316.40
Temperature/K	100(2)
Crystalsystem	orthorhombic
Spacegroup	$Pna2_1$
a/Å	7.6982(5)
b/Å	12.0382(7)
c/Å	17.5134(12)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1623.01(18)
Z	4
ρ_{calc}g/cm^3	1.295
μ/mm^{-1}	1.768
F(000)	664.0
Crystalsize/mm^3	0.21 × 0.19 × 0.15
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.914 to 143.88
Indexranges	$-9 \le h \le 9$, $-14 \le k \le 14$, $-21 \le l \le 21$
Reflectionscollected	11405
Independentreflections	2925 [R_{int} = 0.0464, R_{sigma} = 0.0476]
Data/restraints/parameters	2925/2/201
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0508, wR_2 = 0.1173
Final R indexes [all data]	R_1 = 0.0566, wR_2 = 0.1205
Largest diff. peak/hole / e Å^{-3}	0.49/-0.49
Flackparameter	0.30(2)

Table S26 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3p. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1A	7697.8(16)	5565.2(7)	7125.3(11)	37.7(18)
S1	6299(3)	7254.0(17)	7907.5(17)	35(2)
O1	6259(4)	8806(2)	5092(2)	40.6(8)

C3	6793(5)	7841(3)	5014(3)	30.3(9)
C5	6496(5)	7416(4)	6377(3)	29.8(9)
C4	7147(5)	7144(3)	5691(3)	28.0(9)
C16	7072(5)	5359(4)	2719(3)	28.3(9)
C17	7102(5)	5370(3)	4414(3)	25.8(8)
C1	7324(5)	6406(3)	3950(3)	26.7(9)
C13	9359(5)	6791(4)	1992(3)	36.5(11)
C15	7478(5)	5208(4)	1951(3)	31.4(10)
C6	6775(2)	6800.5(8)	7078.0(19)	32.1(9)
C14	8638(6)	5910(4)	1592(3)	35.5(10)
C2	7137(6)	7442(4)	4238(3)	31.2(9)
C11	7786(5)	6245(3)	3127(3)	27.7(9)
C18	8425(6)	4580(3)	4408(3)	29.2(9)
C12	8925(6)	6961(4)	2753(3)	34.0(11)
C22	5630(6)	5163(4)	4849(3)	35.6(10)
C19	8320(7)	3630(4)	4855(3)	38.6(11)
C21	5538(8)	4194(4)	5291(3)	48.5(14)
C20	6884(8)	3451(4)	5297(3)	44.7(13)
C8	6904(8)	6321(5)	8390(4)	60.2(17)
C9	7644(7)	5456(5)	8015(4)	58.3(18)
C10	7697.8(16)	5565.2(7)	7125.3(11)	35(10)
C7	6299(3)	7254.0(17)	7907.5(17)	41(7)

Table S27 Anisotropic Displacement Parameters ($Å^2×10^3$) for3p. 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}
O1	43.5(18)	25.3(15)	53(2)	-2.6(15)	-7.3(16)	8.6(14)
C3	27(2)	24(2)	40(3)	-3.3(19)	-5.6(19)	-0.4(16)
C5	22(2)	24.1(19)	44(3)	-4.5(19)	-4.3(17)	0.3(15)
C4	25(2)	22.7(19)	36(2)	-4.3(18)	-3.6(17)	0.4(16)
C16	27.7(19)	27(2)	31(2)	6.6(18)	-1.2(17)	2.7(16)
C17	26.3(18)	25(2)	27(2)	-2.1(17)	-0.4(16)	-5.0(17)
C1	20.2(18)	27(2)	32(2)	3.1(18)	-5.3(16)	-1.9(15)
C13	27.2(19)	45(3)	37(3)	21(2)	-4.7(19)	-2.6(18)
C15	32(2)	28(2)	34(3)	0.5(18)	-2.9(18)	5.2(17)
C6	27.0(19)	27(2)	42(2)	-2(2)	-6(2)	-6.1(15)
C14	33(2)	41(3)	32(2)	7(2)	-2.5(18)	8.3(19)
C2	32(2)	23(2)	39(2)	4.2(18)	-7.1(19)	0.2(17)
C11	24.5(19)	26(2)	32(2)	7.1(17)	-2.6(16)	0.8(15)
C18	33(2)	24(2)	30(2)	2.8(18)	-3.9(17)	-1.8(17)
C12	28(2)	33(2)	41(3)	13(2)	-8.3(19)	-2.5(17)
C22	34(2)	37(2)	36(3)	-12(2)	7.8(19)	-9.8(18)
C19	53(3)	24(2)	39(3)	3(2)	-13(2)	-4.5(19)
C21	60(3)	52(3)	34(3)	-8(2)	15(2)	-36(3)
C20	65(3)	33(3)	35(3)	5(2)	-5(2)	-17(3)
C8	71(4)	75(4)	35(3)	-3(3)	4(3)	-48(3)
C9	49(3)	40(3)	86(5)	22(3)	-30(3)	-18(2)

Table S28 Bond Lengths for3p.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1A	C6	1.65000(8)	C1	C11	1.497(6)
S1A	C9	1.565(7)	C13	C14	1.387(7)
S1	C6	1.595(5)	C13	C12	1.389(7)
S1	C8	1.481(7)	C15	C14	1.381(6)

O1	C3	1.240(5)	C6	C10	1.65000(8)
C3	C4	1.477(6)	C6	C7	1.595(5)
C3	C2	1.465(7)	C11	C12	1.394(6)
C5	C4	1.343(6)	C18	C19	1.388(6)
C5	C6	1.450(6)	C22	C21	1.402(7)
C16	C15	1.393(7)	C19	C20	1.366(8)
C16	C11	1.397(6)	C21	C20	1.369(8)
C17	C1	1.498(6)	C8	C9	1.355(9)
C17	C18	1.393(6)	C8	C7	1.481(7)
C17	C22	1.388(6)	C9	C10	1.565(7)
C1	C2	1.353(6)			

Table S29 Bond Angles for3p.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	S1A	C6	96.6(3)	C5	C6	C7	124.22(19)
C8	S1	C6	100.8(3)	C15	C14	C13	119.9(5)
O1	C3	C4	120.3(4)	C1	C2	C3	131.8(4)
O1	C3	C2	118.0(4)	C16	C11	C1	119.9(4)
C2	C3	C4	121.7(4)	C12	C11	C16	118.6(4)
C4	C5	C6	125.3(4)	C12	C11	C1	121.5(4)
C5	C4	C3	120.8(4)	C19	C18	C17	121.0(4)
C15	C16	C11	120.4(4)	C13	C12	C11	120.8(4)
C18	C17	C1	118.8(4)	C17	C22	C21	119.6(5)
C22	C17	C1	122.7(4)	C20	C19	C18	119.8(5)
C22	C17	C18	118.5(4)	C20	C21	C22	120.6(5)
C2	C1	C17	123.6(4)	C19	C20	C21	120.3(5)
C2	C1	C11	120.2(4)	C9	C8	S1	116.0(5)
C11	C1	C17	116.2(4)	C9	C8	C7	116.0(5)
C14	C13	C12	120.0(4)	C8	C9	S1A	115.4(5)
C14	C15	C16	120.3(4)	C8	C9	C10	115.4(5)
C5	C6	S1A	124.5(3)	C9	C10	C6	96.6(3)
C5	C6	S1	124.22(19)	C8	C7	C6	100.8(3)
C5	C6	C10	124.5(3)				

Table S30 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for3p.

Atom	*x*	*y*	*z*	U(eq)
H5	5796	8064	6406	36
H4	7842	6497	5640	34
H16	6304	4857	2966	34
H13	10150	7279	1745	44
H15	6954	4619	1672	38
H14	8941	5790	1073	43
H2	7249	8017	3870	37
H18	9414	4693	4093	35
H12	9410	7573	3021	41
H22	4690	5674	4846	43
H19	9243	3106	4853	46
H21	4532	4052	5590	58
H20	6820	2808	5610	54
H8A	6780	6327	8929	72
H8B	6780	6327	8929	72
H9A	8100	4828	8275	70
H9B	8100	4828	8275	70
H10	8121	5081	6740	42

H7	5773	7936	8052	49

Table S31 Atomic Occupancy for3p.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
S1A	0.596(5)	S1	0.404(5)	H8A	0.404(5)
H8B	0.404(5)	H9A	0.596(5)	H9B	0.596(5)
C10	0.404(5)	H10	0.596(5)	C7	0.596(5)
H7	0.404(5)				

Experimental

Single crystals of $C_{21}H_{16}OS$ **[3p]** were **[obtained at slow evaporation of solution of 3e in hexanes - chloroform]**. A suitable crystal was selected andon a **SuperNova, Single source at offset/far, HyPix3000** 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). ActaCryst. A71, 3-8.
3. Sheldrick, G.M. (2015). ActaCryst. C71, 3-8.

Crystal structure determination of [3p]

Crystal Data for $C_{21}H_{16}OS$ (M =316.40 g/mol): orthorhombic, space group $Pna2_1$ (no. 33), a = 7.6982(5) Å, b = 12.0382(7) Å, c = 17.5134(12) Å, V = 1623.01(18) Å^3, Z = 4, T = 100(2) K, μ(CuKα) = 1.768 mm^{-1}, *Dcalc* = 1.295 g/cm^3, 11405 reflections measured (8.914° ≤ 2Θ ≤ 143.88°), 2925 unique (R_{int} = 0.0464, R_{sigma} = 0.0476) which were used in all calculations. The final R_1 was 0.0508 (I > 2σ(I)) and wR_2 was 0.1205 (all data).

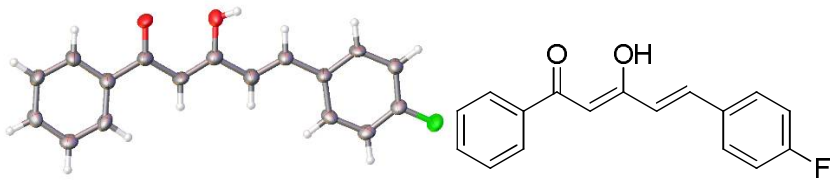
Refinement model description

Number of restraints - 2, number of constraints - unknown.

Details:

1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
2. Shared sites
{S1A, C10}
{S1, C7}
3. Restrained distances
 C6-S1A
 1.65 with sigma of 0.00002
4. Others
Sof(S1)=Sof(H8A)=Sof(H8B)=Sof(C10)=Sof(H7)=1-FVAR(1)
Sof(S1A)=Sof(H9A)=Sof(H9B)=Sof(H10)=Sof(C7)=FVAR(1)
5.a Aromatic/amide H refined with riding coordinates:
 C5(H5), C4(H4), C16(H16), C13(H13), C15(H15), C14(H14), C2(H2), C18(H18), C12(H12), C22(H22), C19(H19), C21(H21), C20(H20), C8(H8A), C8(H8B), C9(H9A), C9(H9B), C10(H10), C7(H7)

4



CCDC 1847456

Table S32 Crystal data and structure refinement for 4.

Identificationcode	4
Empiricalformula	$C_{17}H_{13}FO_2$
Formulaweight	268.27
Temperature/K	100(3)

Crystalsystem	monoclinic
Spacegroup	Cc
a/Å	30.335(6)
b/Å	5.7303(10)
c/Å	7.3960(18)
α/°	90
β/°	92.47(2)
γ/°	90
Volume/Å^3	1284.4(5)
Z	4
ρ_{calc}g/cm^3	1.387
μ/mm^{-1}	0.823
F(000)	560.0
Crystalsize/mm^3	0.2 × 0.08 × 0.07
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.832 to 139.692
Indexranges	-36 ≤ h ≤ 36, -5 ≤ k ≤ 6, -8 ≤ l ≤ 9
Reflectionscollected	3924
Independentreflections	1996 [R_{int} = 0.1108, R_{sigma} = 0.0985]
Data/restraints/parameters	1996/2/182
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0982, wR_2 = 0.2545
Final R indexes [all data]	R_1 = 0.1187, wR_2 = 0.2959
Largest diff. peak/hole / e Å^{-3}	0.48/-0.45
Flackparameter	-0.2(6)

Table S33 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	-5221.7(17)	591(8)	-2104(8)	41.9(13)
O1	-2397(2)	-10233(10)	-2769(11)	46.9(17)
O2	-3158.1(19)	-8803(10)	-3414(9)	43.2(16)
C1	-2293(3)	-8273(14)	-2076(12)	36.0(18)
C6	-1824(3)	-7899(14)	-1381(13)	37(2)
C15	-4874(3)	-870(13)	-2312(11)	32.0(17)
C3	-3038(3)	-6818(14)	-2624(12)	36.1(18)
C14	-4950(3)	-2985(14)	-3146(12)	33.5(17)
C12	-4161(3)	-3784(13)	-2778(12)	31.3(17)
C7	-1683(3)	-5924(14)	-447(13)	37.2(19)
C2	-2614(3)	-6454(14)	-1968(12)	36.3(19)
C5	-3796(2)	-5397(13)	-2994(11)	32.4(18)
C11	-1520(3)	-9669(14)	-1734(13)	36.3(19)
C9	-944(3)	-7449(14)	-214(12)	33.7(18)
C4	-3375(3)	-5068(15)	-2450(13)	37.7(19)
C13	-4589(3)	-4443(12)	-3375(11)	30.8(17)
C10	-1082(3)	-9409(13)	-1137(12)	35.1(19)
C16	-4461(3)	-154(14)	-1722(11)	34.0(18)
C8	-1245(3)	-5669(14)	169(12)	36.4(19)
C17	-4104(3)	-1583(13)	-1955(11)	32.5(17)

Table S34 Anisotropic Displacement Parameters (Å^2×10^3) for 4. 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}

F1	37(3)	24(3)	64(3)	3(2)	-2(2)	9.2(19)
O1	34(3)	25(3)	81(5)	-19(3)	-3(3)	5(2)
O2	28(3)	28(3)	73(5)	-3(3)	-1(3)	3(2)
C1	34(4)	24(4)	51(5)	-4(4)	5(3)	-3(3)
C6	33(4)	22(4)	56(5)	3(3)	2(4)	-2(3)
C15	36(4)	18(4)	42(5)	6(3)	2(3)	1(3)
C3	38(4)	24(4)	47(5)	0(3)	3(3)	-1(3)
C14	30(4)	23(4)	48(4)	3(3)	3(3)	-2(3)
C12	31(4)	18(4)	46(5)	0(3)	2(3)	-1(3)
C7	36(4)	23(4)	52(5)	6(4)	9(4)	8(3)
C2	37(4)	17(4)	55(5)	-6(3)	-3(4)	2(3)
C5	32(4)	20(4)	46(5)	3(3)	2(4)	-1(3)
C11	30(4)	24(4)	55(5)	2(4)	2(4)	-3(3)
C9	29(4)	25(4)	46(4)	13(3)	-4(3)	0(3)
C4	32(4)	25(4)	56(5)	1(4)	0(4)	0(3)
C13	36(4)	13(3)	43(4)	0(3)	-4(3)	-2(3)
C10	32(4)	24(4)	50(5)	0(3)	3(3)	6(3)
C16	43(5)	17(4)	42(5)	4(3)	3(4)	0(3)
C8	43(5)	18(4)	48(5)	4(3)	4(4)	-3(3)
C17	32(4)	20(4)	45(4)	7(3)	-6(3)	-5(3)

Table S35 Bond Lengths for 4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	C15	1.361(9)	C14	C13	1.394(11)
O1	C1	1.269(10)	C12	C5	1.456(10)
O2	C3	1.323(10)	C12	C13	1.404(11)
C1	C6	1.505(11)	C12	C17	1.408(11)
C1	C2	1.432(11)	C7	C8	1.393(12)
C6	C7	1.384(12)	C5	C4	1.335(11)
C6	C11	1.404(11)	C11	C10	1.390(12)
C15	C14	1.375(11)	C9	C10	1.370(12)
C15	C16	1.371(12)	C9	C8	1.406(11)
C3	C2	1.368(12)	C16	C17	1.374(11)
C3	C4	1.444(11)			

Table S36 Bond Angles for 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	C1	C6	118.6(7)	C13	C12	C17	118.1(7)
O1	C1	C2	120.6(8)	C17	C12	C5	122.4(7)
C2	C1	C6	120.9(7)	C6	C7	C8	121.3(7)
C7	C6	C1	123.7(7)	C3	C2	C1	120.0(7)
C7	C6	C11	119.4(7)	C4	C5	C12	126.8(7)
C11	C6	C1	116.9(7)	C10	C11	C6	119.4(8)
F1	C15	C14	118.5(7)	C10	C9	C8	120.6(7)
F1	C15	C16	118.8(7)	C5	C4	C3	123.2(8)
C16	C15	C14	122.7(8)	C14	C13	C12	121.4(7)
O2	C3	C2	121.6(7)	C9	C10	C11	120.8(7)
O2	C3	C4	116.9(7)	C15	C16	C17	119.7(7)
C2	C3	C4	121.4(7)	C7	C8	C9	118.4(8)
C15	C14	C13	117.8(7)	C16	C17	C12	120.4(7)
C13	C12	C5	119.4(7)				

Table S37 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4.

Atom	*x*	*y*	*z*	U(eq)
H2	-3410	-9180	-3090	65
H14	-5239	-3437	-3551	40
H7	-1889	-4719	-221	45
H2A	-2534	-4995	-1442	44
H5	-3865	-6834	-3583	39
H11	-1613	-11033	-2374	44
H9	-643	-7292	172	40
H4	-3294	-3609	-1922	45
H13	-4633	-5914	-3947	37
H10	-875	-10605	-1373	42
H16	-4422	1323	-1154	41
H8	-1152	-4323	832	44
H17	-3818	-1083	-1559	39

Experimental

Single crystals of $C_{17}H_{13}FO_2$ **[4]** were **[obtained at slow evaporation of solution of 3e in hexanes - chloroform]**. A suitable crystal was selected andon a **SuperNova, Single source at offset/far, HyPix3000** 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.

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

Crystal structure determination of [4]

Crystal Data for $C_{17}H_{13}FO_2$ (M =268.27 g/mol): monoclinic, space group Cc (no. 9), a = 30.335(6) Å, b = 5.7303(10) Å, c = 7.3960(18) Å, β = 92.47(2)°, V = 1284.4(5) Å^3, Z = 4, T = 100(3) K, μ(CuKα) = 0.823 mm^{-1}, *Dcalc* = 1.387 g/cm^3, 3924 reflections measured (5.832° ≤ 2Θ ≤ 139.692°), 1996 unique (R_{int} = 0.1108, R_{sigma} = 0.0985) which were used in all calculations. The final R_1 was 0.0982 (I > 2σ(I)) and wR_2 was 0.2959 (all data).

Refinement model description

Number of restraints - 2, number of constraints - unknown.
Details:
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
 At 1.5 times of:
  All O(H) groups
2.a Aromatic/amide H refined with riding coordinates:
 C14(H14), C7(H7), C2(H2A), C5(H5), C11(H11), C9(H9), C4(H4), C13(H13),
 C10(H10), C16(H16), C8(H8), C17(H17)
2.b Idealised tetrahedral OH refined as rotating group:
 O2(H2)

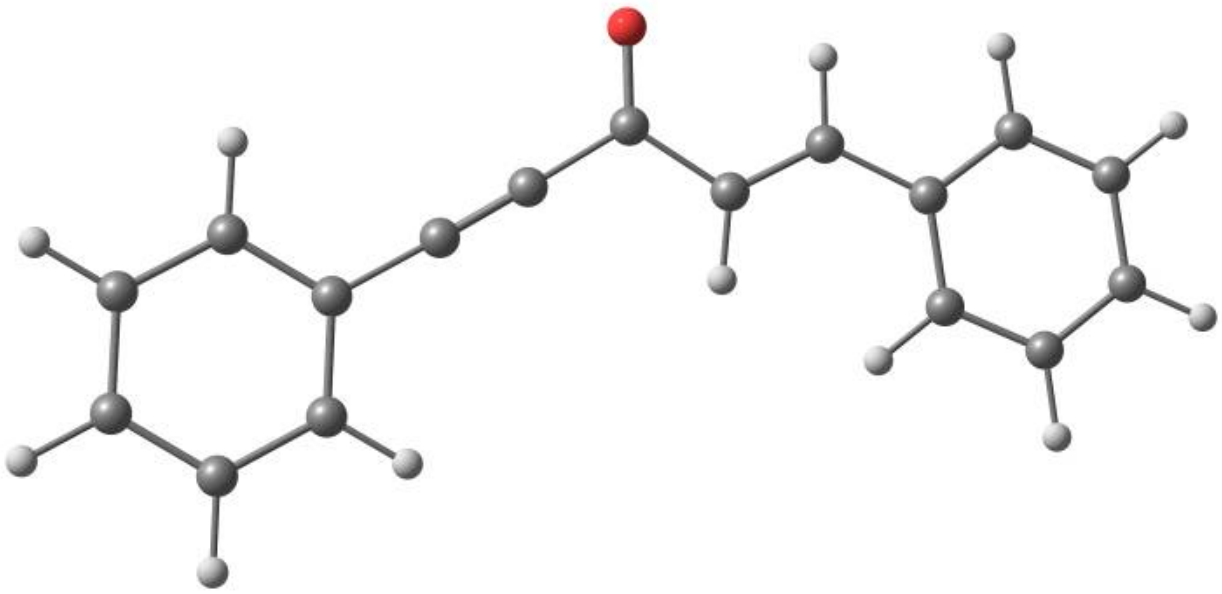
III. Data of DFT calculations

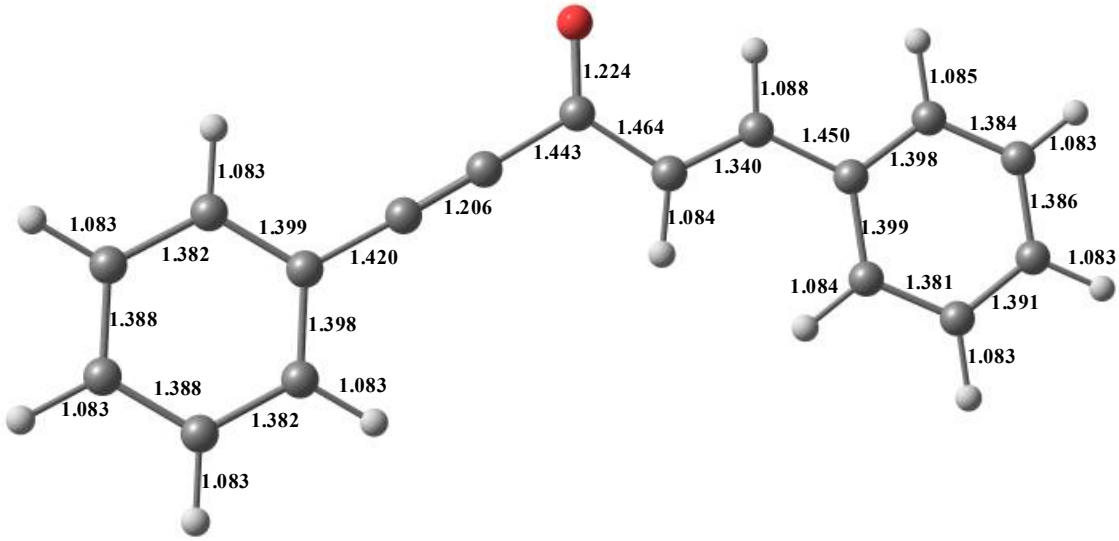
1a

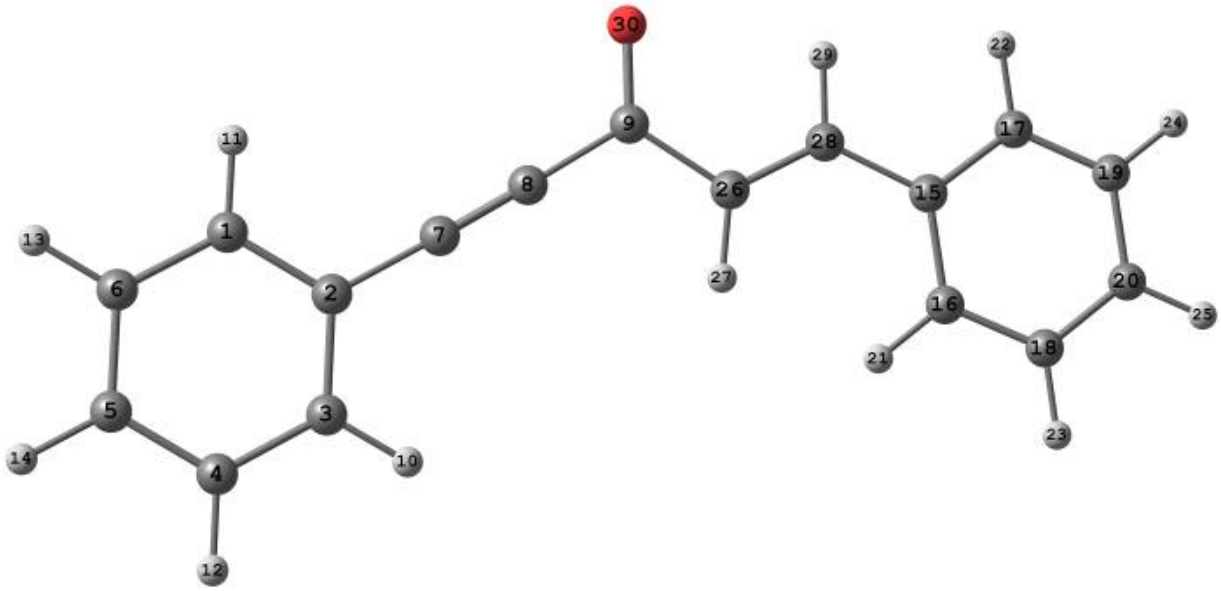
Energy **E(RM06) = -729.843502613h, G^{298} =-729.653887h, μ=5.49 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.767011	-0.843217	0.000223
2	C	-3.688162	0.046727	-0.000001
3	C	-3.931206	1.423448	-0.000253
4	C	-5.230048	1.896458	-0.000285
5	C	-6.295578	1.006596	-0.000057
6	C	-6.062244	-0.361809	0.000197
7	C	-2.359476	-0.455318	0.000018
8	C	-1.242651	-0.910696	0.000036
9	C	0.082426	-1.481175	0.000018
10	H	-3.093340	2.109875	-0.000424
11	H	-4.573825	-1.909025	0.000414
12	H	-5.413927	2.963603	-0.000486
13	H	-6.894181	-1.054951	0.000372
14	H	-7.311823	1.381243	-0.000079
15	C	3.657711	-0.125252	0.000041
16	C	3.632423	1.273663	0.000315
17	C	4.896738	-0.771753	-0.000247
18	C	4.809026	1.995762	0.000289
19	C	6.075786	-0.047522	-0.000284
20	C	6.034424	1.337782	-0.000015
21	H	2.683792	1.797704	0.000559
22	H	4.924461	-1.855907	-0.000455
23	H	4.776321	3.078268	0.000513
24	H	7.028041	-0.563574	-0.000509
25	H	6.954871	1.908870	-0.000023
26	C	1.183692	-0.516537	0.000043
27	H	0.916453	0.534412	0.000014
28	C	2.456112	-0.936274	0.000046
29	H	2.611475	-2.013310	0.000027
30	O	0.234990	-2.695315	-0.000054







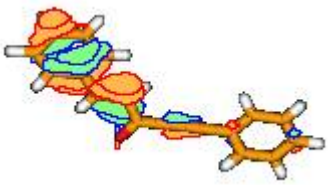
Summary of Natural Population Analysis:

Natural Population

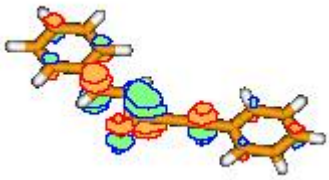
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.13642	1.99886	4.11812	0.01944	6.13642
C	2	-0.16632	1.99893	4.15082	0.01657	6.16632
C	3	-0.15056	1.99905	4.13384	0.01767	6.15056
C	4	-0.20473	1.99911	4.18583	0.01978	6.20473
C	5	-0.17399	1.99913	4.15579	0.01907	6.17399
C	6	-0.21199	1.99914	4.19221	0.02064	6.21199
C	7	0.07599	1.99842	3.91201	0.01358	5.92401
C	8	-0.09089	1.99829	4.07915	0.01344	6.09089
C	9	0.48712	1.99911	3.48336	0.03041	5.51288
H	10	0.21983	0.00000	0.77862	0.00155	0.78017

H	11	0.21887	0.00000	0.77964	0.00149	0.78113
H	12	0.21819	0.00000	0.78018	0.00163	0.78181
H	13	0.21835	0.00000	0.78009	0.00157	0.78165
H	14	0.21595	0.00000	0.78254	0.00151	0.78405
C	15	-0.11295	1.99897	4.09469	0.01929	6.11295
C	16	-0.16586	1.99904	4.14926	0.01756	6.16586
C	17	-0.16117	1.99905	4.14375	0.01837	6.16117
C	18	-0.20185	1.99913	4.18305	0.01967	6.20185
C	19	-0.20654	1.99912	4.18763	0.01980	6.20654
C	20	-0.17821	1.99913	4.15941	0.01968	6.17821
H	21	0.21216	0.00000	0.78587	0.00197	0.78784
H	22	0.21396	0.00000	0.78431	0.00174	0.78604
H	23	0.21571	0.00000	0.78266	0.00162	0.78429
H	24	0.21617	0.00000	0.78220	0.00164	0.78383
H	25	0.21454	0.00000	0.78398	0.00148	0.78546
C	26	-0.30574	1.99899	4.28849	0.01827	6.30574
H	27	0.21356	0.00000	0.78463	0.00181	0.78644
C	28	-0.06206	1.99885	4.04251	0.02069	6.06206
H	29	0.21573	0.00000	0.78179	0.00248	0.78427
O	30	-0.62657	1.99977	6.60187	0.02494	8.62657
* Total *		0.00027	35.98209	85.64831	0.36933	121.99973

homo



lumo

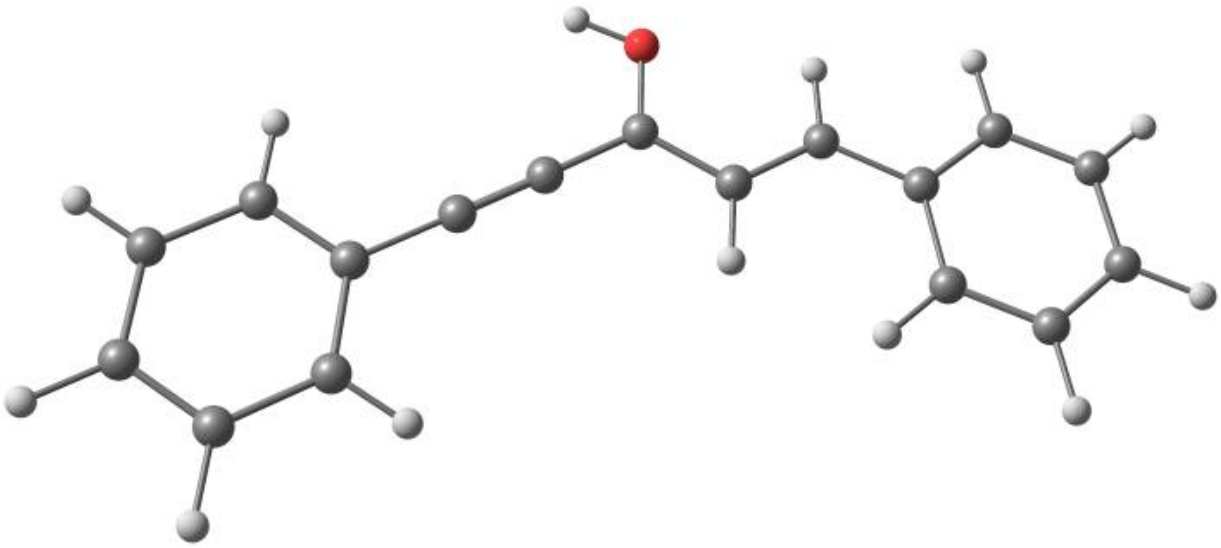


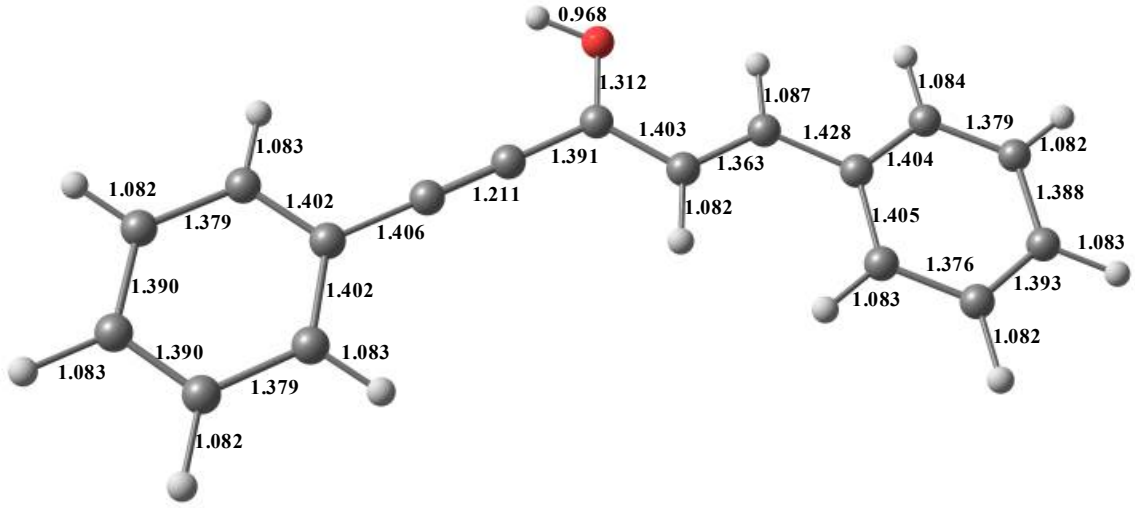
A1

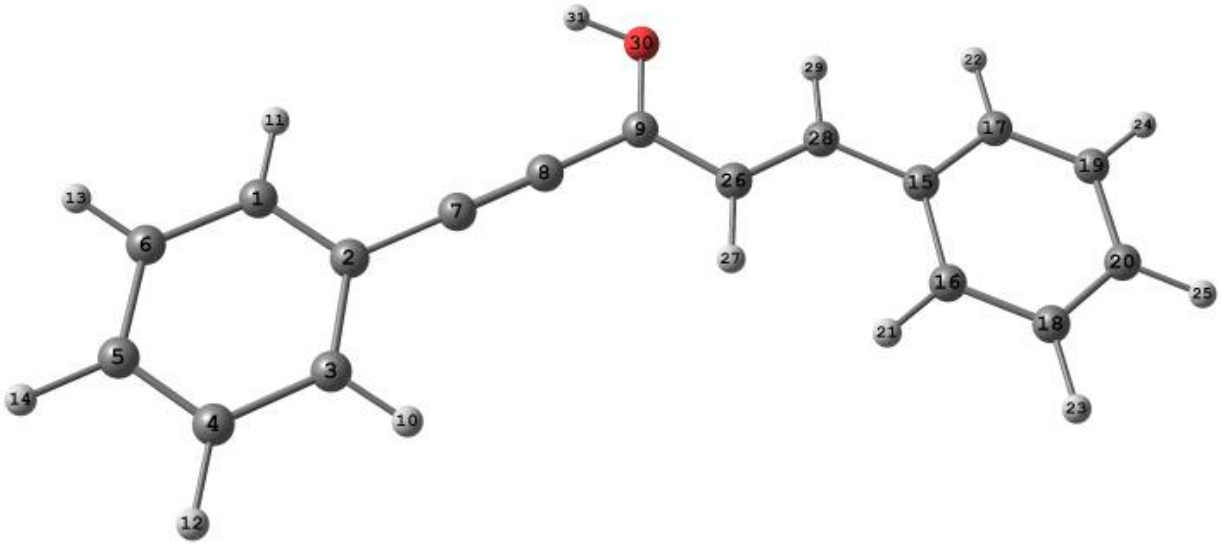
E(RM06) = -730.264096303h, G=^{298} -730.063735h, μ=2.03 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	4.750242	0.852463	0.000021
2	C	3.691169	-0.066211	0.000056
3	C	3.955338	-1.442778	0.000072
4	C	5.261062	-1.886909	0.000052
5	C	6.306124	-0.971119	0.000028
6	C	6.051021	0.394769	0.000018
7	C	2.364156	0.397536	0.000060
8	C	1.224199	0.805180	0.000006
9	C	-0.079167	1.291592	-0.000077
10	H	3.129190	-2.142489	0.000102
11	H	4.533182	1.913167	0.000008
12	H	5.470003	-2.948840	0.000058
13	H	6.871430	1.100666	0.000000
14	H	7.329512	-1.325281	0.000015
15	C	-3.655799	0.112948	-0.000012
16	C	-3.649556	-1.291779	-0.000252
17	C	-4.885768	0.789120	0.000230
18	C	-4.836200	-1.988644	-0.000220
19	C	-6.072435	0.086008	0.000281
20	C	-6.047671	-1.301565	0.000056
21	H	-2.711004	-1.831864	-0.000514
22	H	-4.890206	1.872891	0.000386
23	H	-4.828622	-3.070779	-0.000422
24	H	-7.017521	0.613364	0.000489
25	H	-6.977954	-1.856276	0.000086
26	C	-1.180067	0.421636	0.000040
27	H	-0.952321	-0.635616	0.000224
28	C	-2.458920	0.891755	-0.000047
29	H	-2.593887	1.970110	-0.000126
30	O	-0.290797	2.586416	-0.000211
31	H	0.538206	3.085599	-0.000479







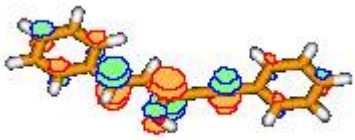
Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.12634	1.99906	4.10754	0.01974	6.12634
C	2	-0.21524	1.99894	4.17616	0.04014	6.21524
C	3	-0.12566	1.99906	4.10589	0.02071	6.12566
C	4	-0.20457	1.99912	4.18592	0.01953	6.20457
C	5	-0.14055	1.99913	4.12210	0.01931	6.14055
C	6	-0.20475	1.99912	4.18599	0.01964	6.20475
C	7	-0.33374	1.99839	4.21422	0.12113	6.33374
C	8	0.77317	1.99843	2.54466	0.68373	5.22683
C	9	0.22893	1.99872	3.61327	0.15908	5.77107
H	10	0.22350	0.00000	0.77289	0.00360	0.77650
H	11	0.22438	0.00000	0.77308	0.00255	0.77562
H	12	0.22397	0.00000	0.77438	0.00165	0.77603

H	13	0.22393	0.00000	0.77441	0.00166	0.77607
H	14	0.22048	0.00000	0.77806	0.00146	0.77952
C	15	-0.13763	1.99898	4.11695	0.02170	6.13763
C	16	-0.13019	1.99904	4.11289	0.01826	6.13019
C	17	-0.12041	1.99906	4.10228	0.01907	6.12041
C	18	-0.20362	1.99913	4.18468	0.01982	6.20362
C	19	-0.21014	1.99911	4.19125	0.01978	6.21014
C	20	-0.12671	1.99914	4.10829	0.01928	6.12671
H	21	0.21804	0.00000	0.78013	0.00183	0.78196
H	22	0.22144	0.00000	0.77684	0.00173	0.77856
H	23	0.22360	0.00000	0.77480	0.00160	0.77640
H	24	0.22406	0.00000	0.77430	0.00164	0.77594
H	25	0.22066	0.00000	0.77794	0.00140	0.77934
C	26	-0.33891	1.99905	4.29919	0.04066	6.33891
H	27	0.23735	0.00000	0.75950	0.00315	0.76265
C	28	0.03684	1.99890	3.94487	0.01939	5.96316
H	29	0.22605	0.00000	0.77132	0.00263	0.77395
O	30	-0.63346	1.99970	6.60612	0.02764	8.63346
H	31	0.53533	0.00000	0.46202	0.00265	0.46467
* Total *		1.00982	35.98208	84.67194	1.33617	121.99018

homo 

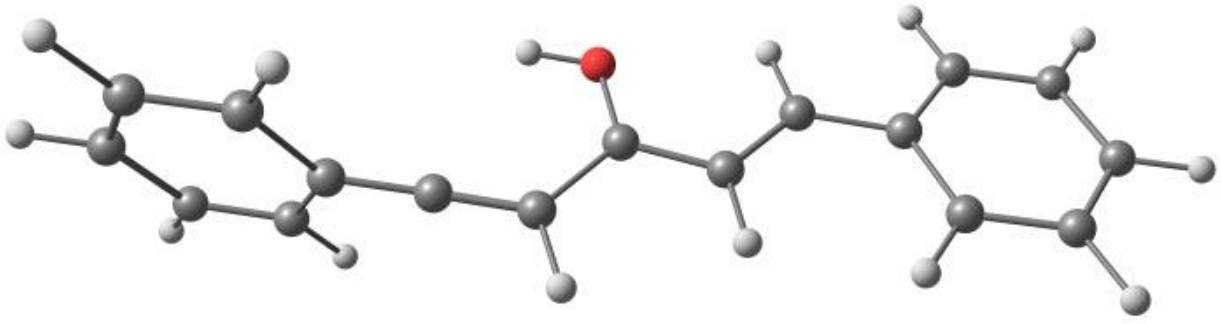
lumo 

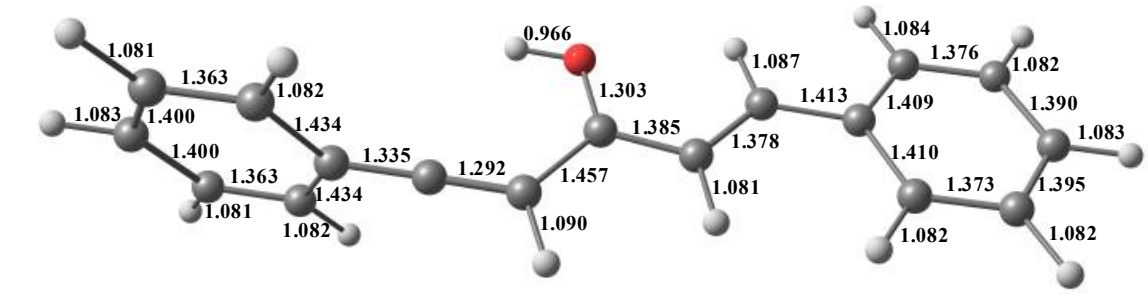
B1

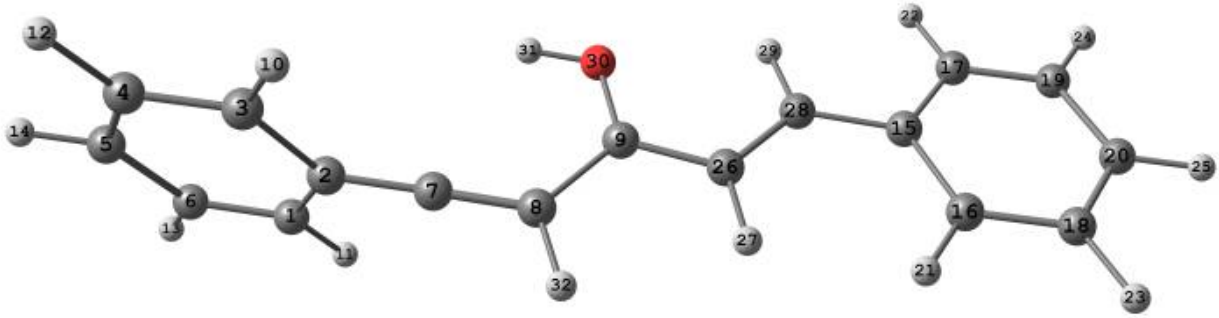
Energy **E(RM06) = -730. 640375158h, G^{298} = -730.428986h, μ=12.02 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.409639	-0.010106	1.250245
2	C	-3.699151	0.304603	0.045079
3	C	-4.384183	0.356651	-1.213826
4	C	-5.722890	0.104904	-1.246909
5	C	-6.395997	-0.199283	-0.058210
6	C	-5.747667	-0.257742	1.180903
7	C	-2.389144	0.556694	0.094673
8	C	-1.126688	0.825677	0.138412
9	C	-0.040651	-0.136393	0.008839
10	H	-3.822498	0.597079	-2.106459
11	H	-3.867419	-0.042315	2.185631
12	H	-6.265423	0.138783	-2.181023
13	H	-6.309606	-0.497072	2.072497
14	H	-7.460246	-0.397519	-0.098721
15	C	3.703294	-0.202220	-0.015577
16	C	4.160359	1.128957	0.071412
17	C	4.644410	-1.248446	-0.091533
18	C	5.507505	1.392953	0.081771
19	C	5.992973	-0.975654	-0.076856
20	C	6.422503	0.343082	0.008862
21	H	3.453111	1.946525	0.124874
22	H	4.289289	-2.269906	-0.160034
23	H	5.860860	2.413422	0.145291
24	H	6.714271	-1.779779	-0.133607
25	H	7.483462	0.560489	0.018014
26	C	1.264295	0.323587	0.058242
27	H	1.403130	1.388384	0.179406
28	C	2.332147	-0.542905	-0.036198
29	H	2.103367	-1.600971	-0.133638
30	O	-0.273472	-1.407563	-0.153847
31	H	-1.207851	-1.653592	-0.164866
32	H	-0.855520	1.870827	0.287428







Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.01028	1.99907	3.99338	0.01784	6.01028
C	2	-0.20410	1.99855	4.18451	0.02104	6.20410
C	3	-0.00973	1.99907	3.99283	0.01782	6.00973
C	4	-0.22032	1.99910	4.20202	0.01920	6.22032
C	5	0.02957	1.99917	3.95321	0.01805	5.97043
C	6	-0.22020	1.99910	4.20190	0.01919	6.22020
C	7	0.43197	1.99897	3.55109	0.01797	5.56803
C	8	-0.33069	1.99864	4.31632	0.01574	6.33069
C	9	0.53676	1.99890	3.43975	0.02459	5.46324
H	10	0.24799	0.00000	0.75063	0.00138	0.75201
H	11	0.24803	0.00000	0.75058	0.00138	0.75197
H	12	0.24823	0.00000	0.75026	0.00151	0.75177
H	13	0.24824	0.00000	0.75025	0.00151	0.75176
H	14	0.23862	0.00000	0.76011	0.00127	0.76138
C	15	-0.14168	1.99899	4.12382	0.01887	6.14168
C	16	-0.10538	1.99905	4.08940	0.01693	6.10538
C	17	-0.09121	1.99906	4.07434	0.01780	6.09121
C	18	-0.20557	1.99912	4.18689	0.01955	6.20557
C	19	-0.21332	1.99911	4.19455	0.01966	6.21332

C	20	-0.08850	1.99915	4.07066	0.01870	6.08850
H	21	0.22235	0.00000	0.77581	0.00185	0.77765
H	22	0.22632	0.00000	0.77208	0.00160	0.77368
H	23	0.22893	0.00000	0.76949	0.00158	0.77107
H	24	0.22963	0.00000	0.76877	0.00159	0.77037
H	25	0.22496	0.00000	0.77369	0.00134	0.77504
C	26	-0.31782	1.99899	4.30030	0.01853	6.31782
H	27	0.24285	0.00000	0.75539	0.00176	0.75715
C	28	0.08627	1.99891	3.89537	0.01945	5.91373
H	29	0.23257	0.00000	0.76553	0.00189	0.76743
O	30	-0.62116	1.99969	6.59702	0.02445	8.62116
H	31	0.53543	0.00000	0.46221	0.00237	0.46457
H	32	0.32123	0.00000	0.67688	0.00189	0.67877

==========

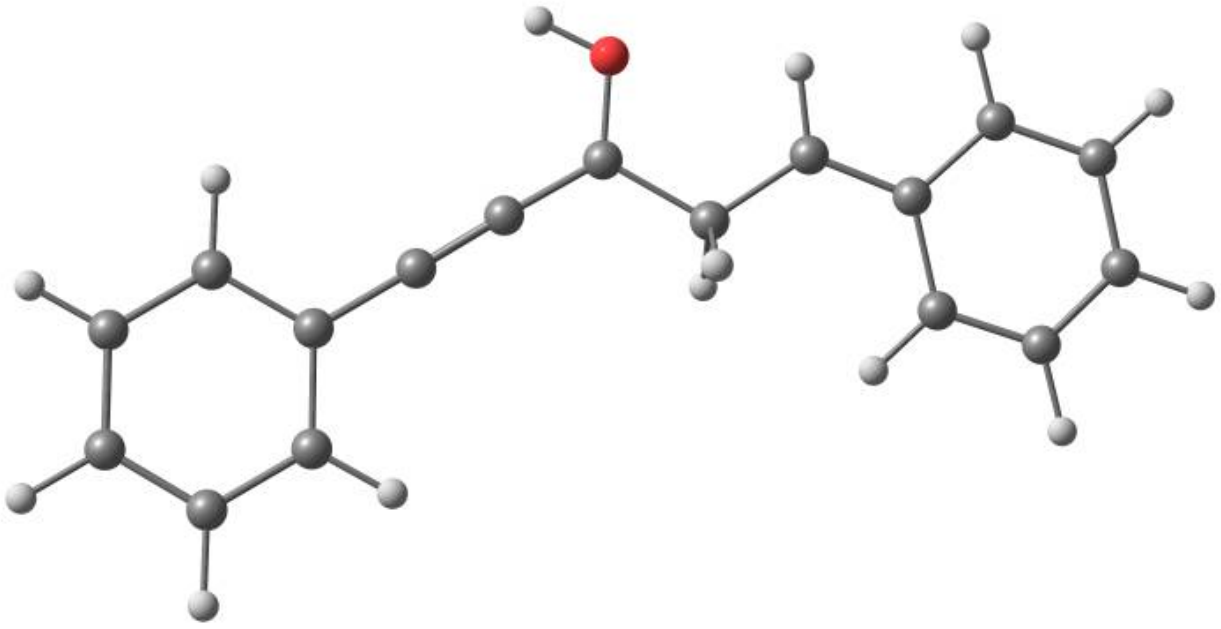
* Total *	2.00000	35.98265	85.64905	0.36829	122.00000

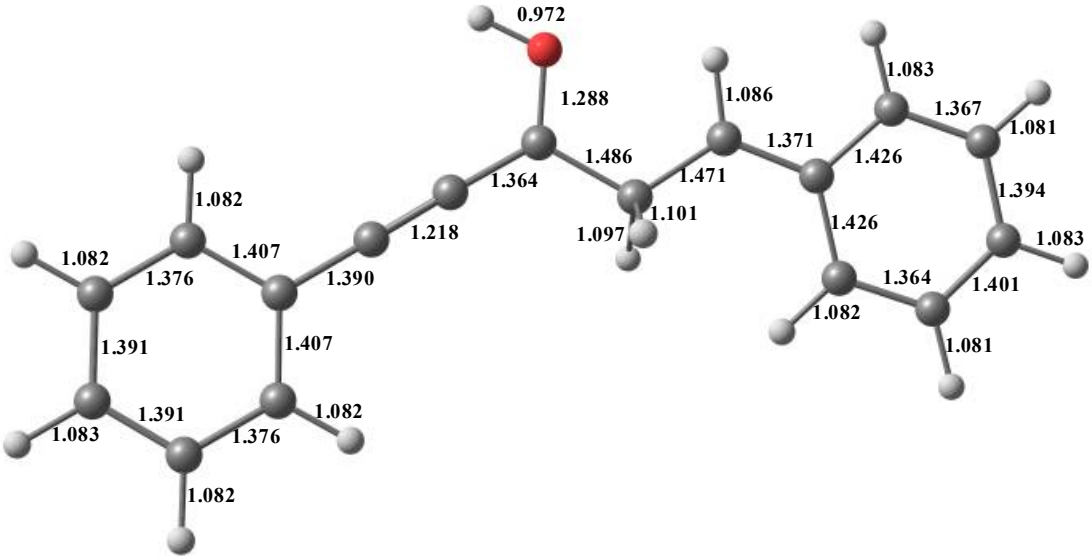
C1

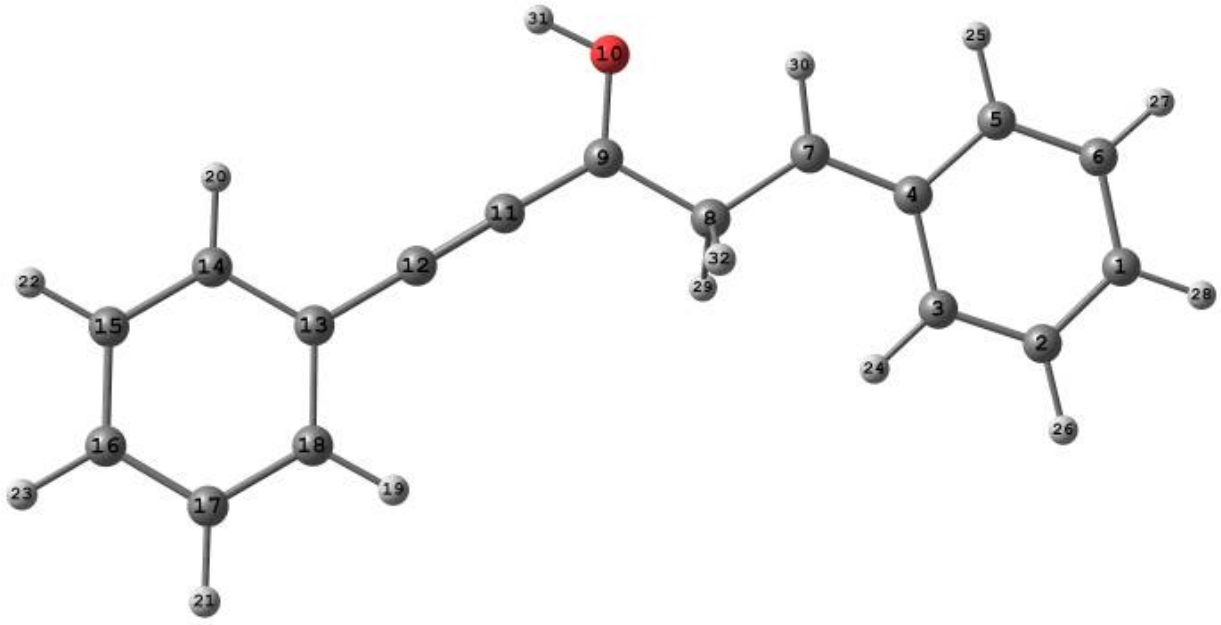
Energy **E(RM06) = -730.632176537h, G^{298} = -730.41923h, μ=8.46 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-6.056551	1.252843	-0.056061
2	C	-4.858619	1.979172	-0.038565
3	C	-3.668256	1.314635	-0.006104
4	C	-3.655975	-0.111052	0.014134
5	C	-4.892234	-0.822482	-0.005757
6	C	-6.077159	-0.140848	-0.040452
7	C	-2.499587	-0.846721	0.059492
8	C	-1.138279	-0.291564	0.102348
9	C	-0.022396	-1.269787	0.028384
10	O	-0.351748	-2.514765	-0.009358
11	C	1.270620	-0.836934	0.010643
12	C	2.414572	-0.418355	0.003072
13	C	3.725339	0.044266	-0.005464
14	C	4.788627	-0.875691	-0.059799
15	C	6.083454	-0.411420	-0.066911
16	C	6.327885	0.957463	-0.020675
17	C	5.282090	1.873558	0.033200
18	C	3.980897	1.427038	0.041107
19	H	3.150211	2.119550	0.082342
20	H	4.572300	-1.935584	-0.094967
21	H	5.491471	2.934321	0.068388
22	H	6.909176	-1.109057	-0.108210
23	H	7.349666	1.316100	-0.026594
24	H	-2.738278	1.867839	0.007702
25	H	-4.870100	-1.905020	0.007317
26	H	-4.885496	3.059493	-0.052429
27	H	-7.019395	-0.670160	-0.055633
28	H	-6.995444	1.792746	-0.083438
29	H	-0.984375	0.459528	-0.682105
30	H	-2.601809	-1.928174	0.077089
31	H	0.413527	-3.113289	-0.050438
32	H	-1.004038	0.285110	1.030298







Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.00464	1.99917	3.97810	0.01809	5.99536
C	2	-0.21049	1.99912	4.19160	0.01977	6.21049
C	3	-0.05134	1.99905	4.03495	0.01734	6.05134
C	4	-0.16503	1.99895	4.14649	0.01959	6.16503
C	5	-0.01779	1.99908	4.00052	0.01819	6.01779
C	6	-0.22641	1.99911	4.20756	0.01974	6.22641
C	7	0.19742	1.99904	3.78411	0.01944	5.80258
C	8	-0.58851	1.99908	4.55523	0.03419	6.58851
C	9	0.33531	1.99887	3.50347	0.16235	5.66469

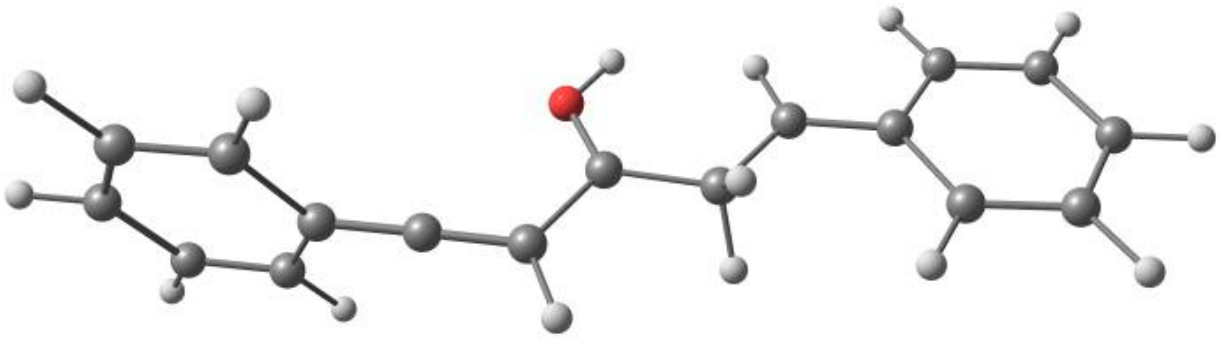
O	10	-0.60127	1.99969	6.56451	0.03707	8.60127
C	11	0.73646	1.99850	2.53076	0.73427	5.26354
C	12	-0.23692	1.99842	4.12081	0.11769	6.23692
C	13	-0.23319	1.99894	4.19340	0.04085	6.23319
C	14	-0.09718	1.99906	4.07799	0.02013	6.09718
C	15	-0.20764	1.99911	4.18880	0.01972	6.20764
C	16	-0.10158	1.99914	4.08336	0.01908	6.10158
C	17	-0.20758	1.99911	4.18881	0.01966	6.20758
C	18	-0.09625	1.99906	4.07631	0.02088	6.09625
H	19	0.22880	0.00000	0.76734	0.00387	0.77120
H	20	0.23011	0.00000	0.76731	0.00258	0.76989
H	21	0.22979	0.00000	0.76857	0.00164	0.77021
H	22	0.22981	0.00000	0.76858	0.00161	0.77019
H	23	0.22499	0.00000	0.77360	0.00141	0.77501
H	24	0.23349	0.00000	0.76478	0.00173	0.76651
H	25	0.23726	0.00000	0.76114	0.00160	0.76274
H	26	0.24166	0.00000	0.75680	0.00154	0.75834
H	27	0.24244	0.00000	0.75598	0.00158	0.75756
H	28	0.23457	0.00000	0.76418	0.00125	0.76543
H	29	0.31689	0.00000	0.68092	0.00219	0.68311
H	30	0.24437	0.00000	0.75315	0.00248	0.75563
H	31	0.55195	0.00000	0.44475	0.00330	0.44805
H	32	0.32949	0.00000	0.66808	0.00242	0.67051
* Total *		2.00831	35.98251	84.62196	1.38723	121.99169

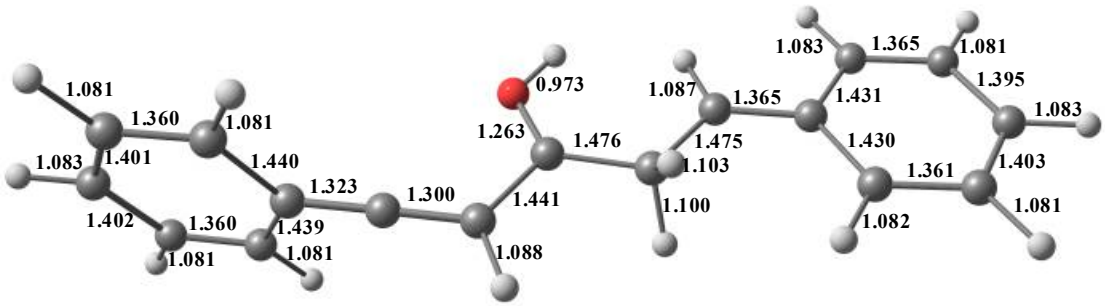
D1

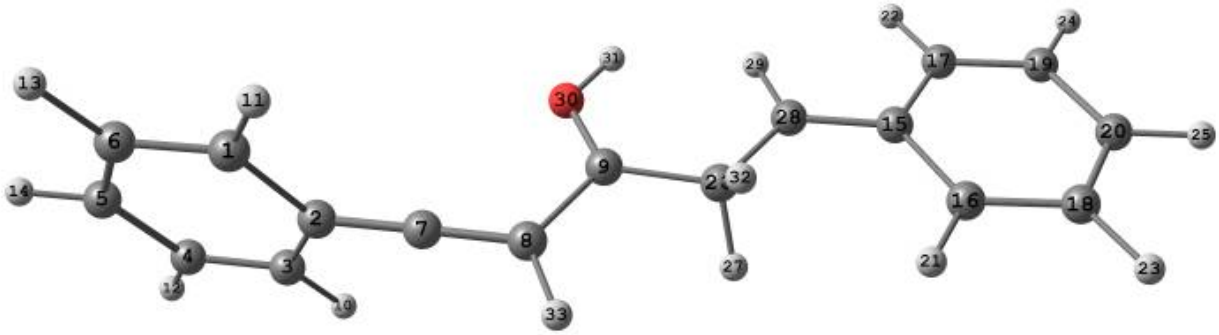
Energy **E(RM06) = -730.990786186h, G^{298} = -730.765989h, μ=1.33 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	4.387734	0.315807	1.226630
2	C	3.714185	0.311084	-0.045701
3	C	4.423159	-0.008281	-1.256818
4	C	5.747722	-0.305268	-1.176068
5	C	6.385116	-0.293064	0.072087
6	C	5.713269	0.014059	1.262734
7	C	2.426930	0.613525	-0.100386
8	C	1.168164	0.937166	-0.144069
9	C	0.130617	-0.054847	-0.022385
10	H	3.889203	-0.003558	-2.197051
11	H	3.826858	0.560444	2.118217
12	H	6.310443	-0.549184	-2.065783
13	H	6.249079	0.010425	2.201210
14	H	7.440826	-0.531656	0.118064
15	C	-3.699633	-0.234827	0.018239
16	C	-4.173587	1.112261	-0.060880
17	C	-4.644037	-1.308096	0.087512
18	C	-5.512989	1.354976	-0.069186
19	C	-5.983380	-1.044757	0.077693
20	C	-6.412620	0.280736	-0.000476
21	H	-3.474474	1.936116	-0.114475
22	H	-4.274849	-2.324479	0.146992
23	H	-5.888717	2.366474	-0.128569
24	H	-6.705829	-1.846632	0.129715
25	H	-7.475633	0.489367	-0.008541
26	C	-1.267932	0.415809	-0.037574
27	H	-1.368605	1.055594	-0.927268
28	C	-2.373108	-0.558270	0.029861
29	H	-2.150548	-1.620717	0.087350
30	O	0.509367	-1.253598	0.096264
31	H	-0.184970	-1.929434	0.185553
32	H	-1.342490	1.144277	0.786988
33	H	0.897093	1.983661	-0.269801







Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.00061	1.99906	3.98280	0.01753	5.99939
C	2	-0.20277	1.99854	4.18352	0.02071	6.20277
C	3	-0.00005	1.99906	3.98341	0.01758	6.00005
C	4	-0.21700	1.99910	4.19873	0.01917	6.21700
C	5	0.05360	1.99917	3.92933	0.01789	5.94640
C	6	-0.21735	1.99910	4.19905	0.01920	6.21735
C	7	0.54023	1.99896	3.44274	0.01807	5.45977
C	8	-0.38905	1.99875	4.37284	0.01746	6.38905
C	9	0.73544	1.99913	3.24050	0.02493	5.26456
H	10	0.25324	0.00000	0.74532	0.00144	0.74676
H	11	0.25311	0.00000	0.74546	0.00144	0.74689
H	12	0.25335	0.00000	0.74516	0.00149	0.74665
H	13	0.25342	0.00000	0.74509	0.00149	0.74658
H	14	0.24234	0.00000	0.75641	0.00126	0.75766
C	15	-0.14876	1.99897	4.13069	0.01911	6.14876
C	16	-0.04599	1.99906	4.03048	0.01646	6.04599
C	17	-0.00878	1.99907	3.99216	0.01755	6.00878
C	18	-0.20810	1.99912	4.18927	0.01971	6.20810
C	19	-0.22563	1.99911	4.20674	0.01978	6.22563

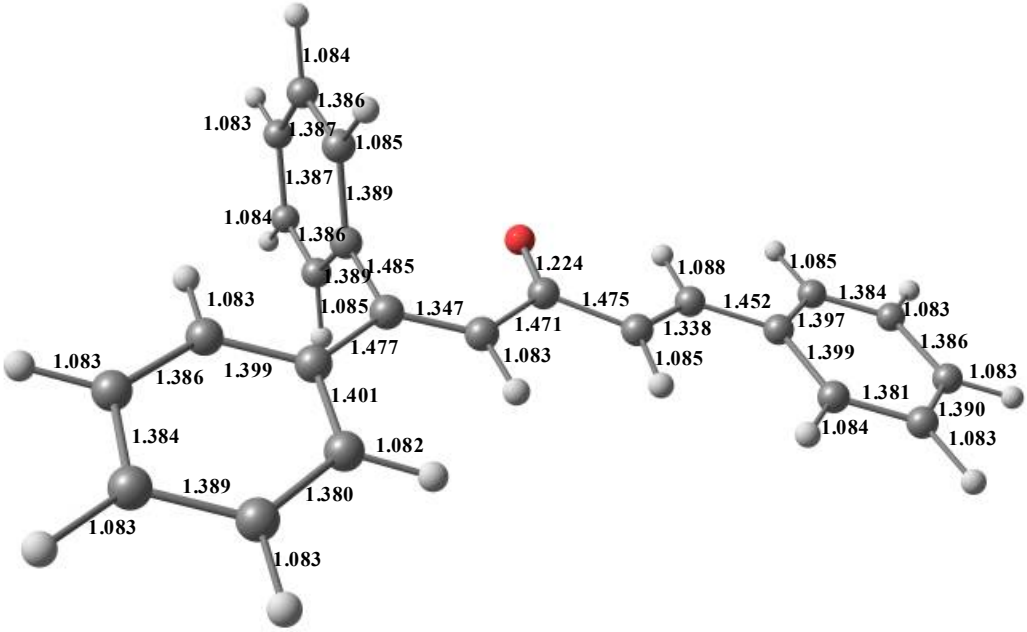
C	20	0.02880	1.99917	3.95408	0.01794	5.97120
H	21	0.23595	0.00000	0.76228	0.00177	0.76405
H	22	0.24018	0.00000	0.75829	0.00153	0.75982
H	23	0.24561	0.00000	0.75286	0.00153	0.75439
H	24	0.24654	0.00000	0.75190	0.00156	0.75346
H	25	0.23780	0.00000	0.76096	0.00123	0.76220
C	26	-0.59615	1.99904	4.57956	0.01755	6.59615
H	27	0.34085	0.00000	0.65753	0.00162	0.65915
C	28	0.17890	1.99889	3.80410	0.01811	5.82110
H	29	0.22696	0.00000	0.77088	0.00216	0.77304
O	30	-0.53950	1.99964	6.51363	0.02623	8.53950
H	31	0.55877	0.00000	0.43890	0.00233	0.44123
H	32	0.34587	0.00000	0.65254	0.00159	0.65413
H	33	0.32758	0.00000	0.67072	0.00170	0.67242
* Total *		3.00001	35.98295	85.64791	0.36913	121.99999

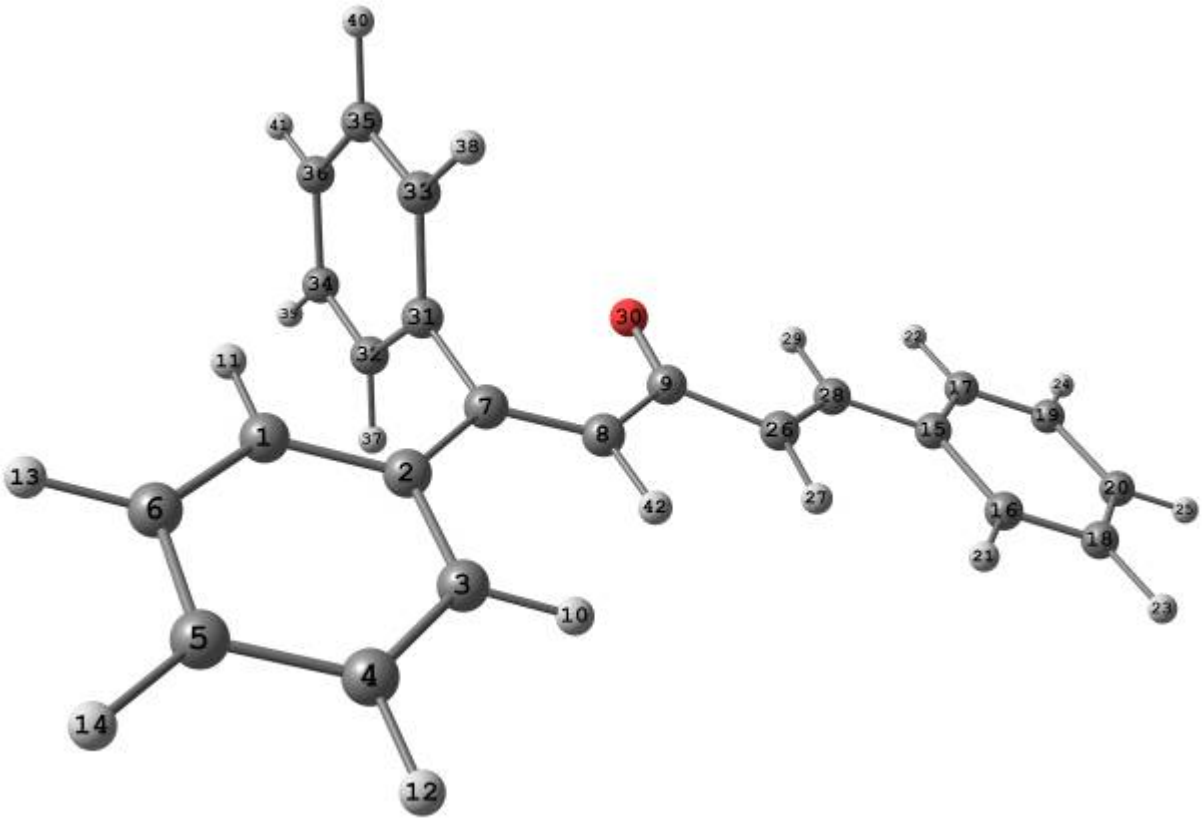
3e

Energy **E(RM06) = -962.020121211h, G^{298} = -961.735215h, μ=4.42 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.159333	-0.978788	-0.000032
2	C	-2.804057	-1.324357	-0.000028
3	C	-2.483411	-2.688543	-0.000081
4	C	-3.469448	-3.654387	-0.000118
5	C	-4.810229	-3.290351	-0.000125
6	C	-5.149054	-1.948533	-0.000087
7	C	-1.769360	-0.270295	0.000016
8	C	-0.453241	-0.557704	0.000157
9	C	0.662847	0.400456	-0.000001
10	H	-1.450385	-3.010817	-0.000121
11	H	-4.448066	0.064632	0.000022
12	H	-3.191496	-4.701279	-0.000156
13	H	-6.190121	-1.649657	-0.000097
14	H	-5.581884	-4.050494	-0.000163
15	C	4.485854	0.032154	0.000293
16	C	4.819405	-1.326668	0.000739
17	C	5.520613	0.971074	-0.000388
18	C	6.141226	-1.725806	0.000401
19	C	6.846009	0.571071	-0.000765
20	C	7.159570	-0.779016	-0.000396
21	H	4.037873	-2.077157	0.001437
22	H	5.271795	2.026862	-0.000646
23	H	6.384643	-2.781317	0.000774
24	H	7.634556	1.313634	-0.001342
25	H	8.195102	-1.096639	-0.000665
26	C	1.996648	-0.230348	-0.000218
27	H	2.038179	-1.314344	-0.000918
28	C	3.113248	0.507116	0.000447
29	H	2.985120	1.587947	0.001078
30	O	0.526391	1.616903	0.000018
31	C	-2.256189	1.132637	-0.000048
32	C	-2.511480	1.784661	-1.199666
33	C	-2.510999	1.784743	1.199672
34	C	-2.994392	3.083619	-1.199709
35	C	-2.993928	3.083671	1.199852
36	C	-3.234646	3.737237	0.000092
37	H	-2.321877	1.270811	-2.136546
38	H	-2.320959	1.270917	2.136475
39	H	-3.185212	3.586750	-2.140397
40	H	-3.184384	3.586851	2.140588
41	H	-3.612042	4.752673	0.000134
42	H	-0.145899	-1.596423	0.000362





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.17516	1.99904	4.15875	0.01738	6.17516
C	2	-0.10317	1.99891	4.07819	0.02607	6.10317
C	3	-0.17115	1.99903	4.14905	0.02308	6.17115
C	4	-0.20078	1.99912	4.18193	0.01973	6.20078
C	5	-0.18249	1.99912	4.16362	0.01975	6.18249

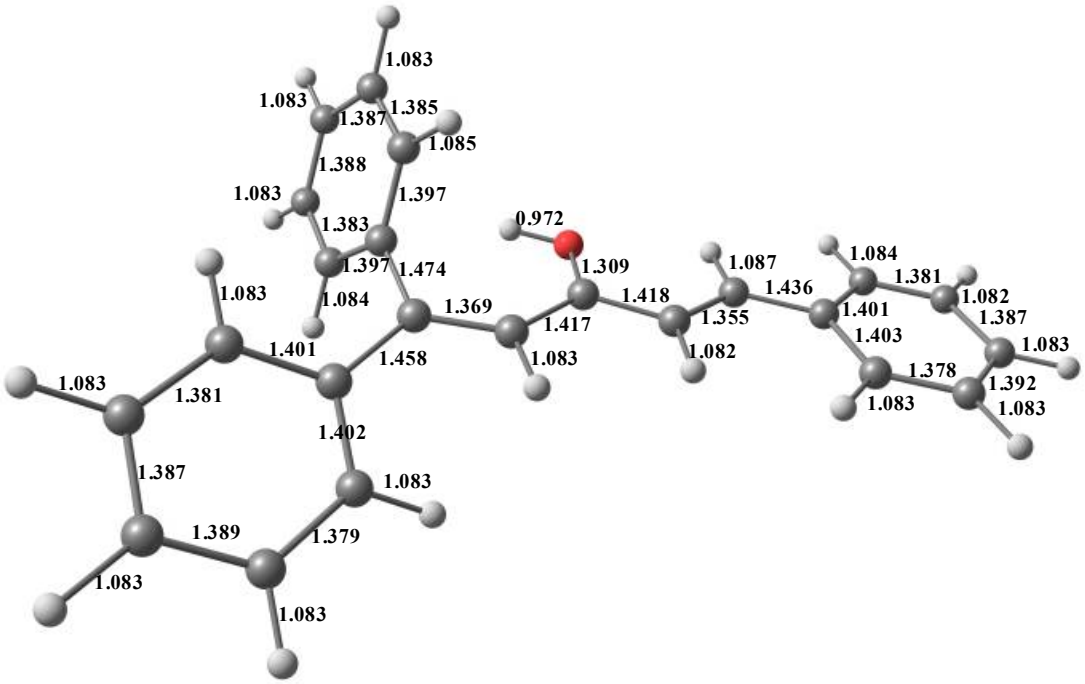
C	6	-0.20287	1.99912	4.18371	0.02005	6.20287
C	7	-0.03855	1.99879	3.95480	0.08496	6.03855
C	8	0.50456	1.99898	2.31156	1.18490	5.49544
C	9	-0.14576	1.99914	3.29292	0.85369	6.14576
H	10	0.20727	0.00000	0.78939	0.00334	0.79273
H	11	0.21946	0.00000	0.77801	0.00252	0.78054
H	12	0.21470	0.00000	0.78371	0.00159	0.78530
H	13	0.21452	0.00000	0.78384	0.00163	0.78548
H	14	0.21393	0.00000	0.78454	0.00153	0.78607
C	15	-0.39472	1.99898	4.19335	0.20239	6.39472
C	16	-0.19581	1.99902	4.15428	0.04252	6.19581
C	17	-0.19132	1.99902	4.15124	0.04106	6.19132
C	18	-0.21100	1.99912	4.18272	0.02916	6.21100
C	19	-0.23942	1.99911	4.18724	0.05307	6.23942
C	20	-0.19521	1.99912	4.16548	0.03060	6.19521
H	21	0.20965	0.00000	0.78771	0.00264	0.79035
H	22	0.19296	0.00000	0.78607	0.02097	0.80704
H	23	0.21036	0.00000	0.78399	0.00565	0.78964
H	24	0.20584	0.00000	0.78339	0.01076	0.79416
H	25	0.21342	0.00000	0.78494	0.00164	0.78658
C	26	-1.46263	1.99907	4.17957	1.28399	7.46263
H	27	0.19178	0.00000	0.80047	0.00775	0.80822
C	28	0.08715	1.99906	2.77635	1.13744	5.91285
H	29	0.05943	0.00000	0.82499	0.11558	0.94057
O	30	-0.70000	1.99980	6.63334	0.06686	8.70000
C	31	-0.06884	1.99885	4.03122	0.03877	6.06884
C	32	-0.20038	1.99895	4.18171	0.01972	6.20038
C	33	-0.20035	1.99895	4.18168	0.01972	6.20035
C	34	-0.19629	1.99911	4.17745	0.01973	6.19629
C	35	-0.19630	1.99911	4.17745	0.01973	6.19630
C	36	-0.21481	1.99912	4.19523	0.02046	6.21481
H	37	0.21111	0.00000	0.78621	0.00269	0.78889
H	38	0.21110	0.00000	0.78621	0.00269	0.78890
H	39	0.21205	0.00000	0.78622	0.00174	0.78795
H	40	0.21205	0.00000	0.78621	0.00174	0.78795
H	41	0.21110	0.00000	0.78729	0.00161	0.78890
H	42	-0.43013	0.00000	1.29622	0.13391	1.43013
* Total *		-2.31468	47.97763	112.74225	5.59480	166.31468

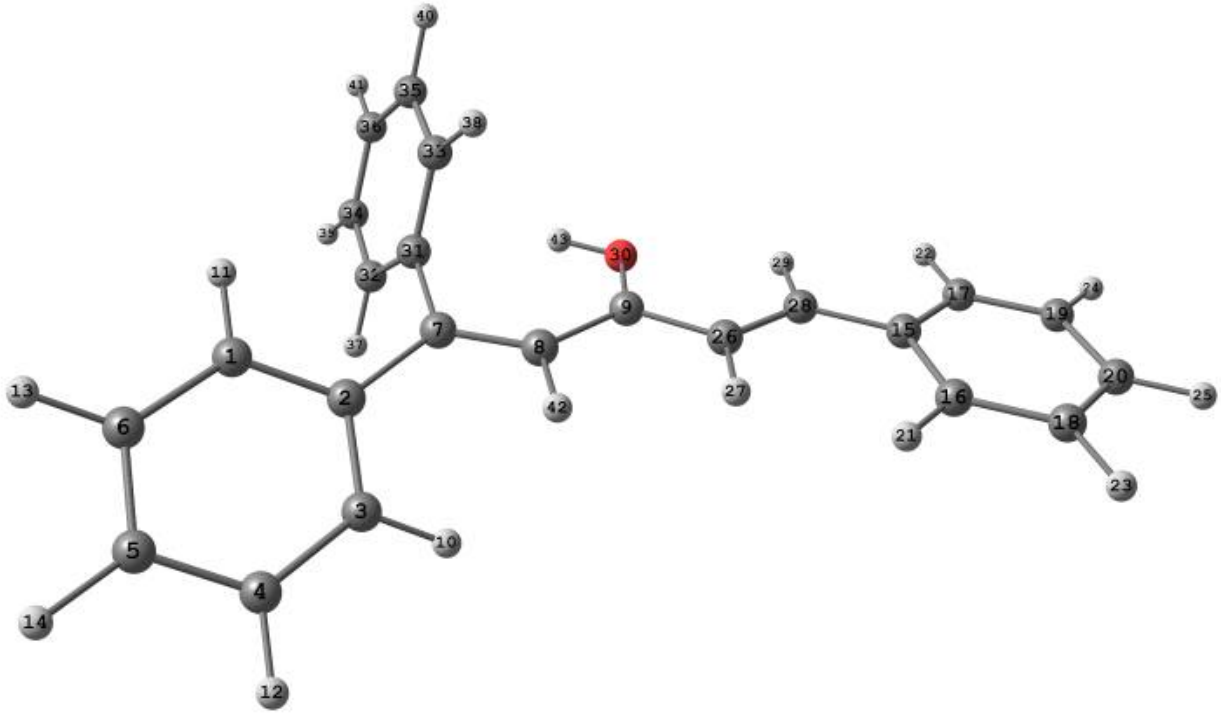
E1

Energy **E(RM06) = -962,45235954h, G^{298} = -962.153634h, μ=0.46 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	4.053322	-1.103569	-0.528655
2	C	2.763316	-1.319615	-0.026932
3	C	2.444016	-2.584454	0.485429
4	C	3.381409	-3.596437	0.487973
5	C	4.649884	-3.372368	-0.032257
6	C	4.982487	-2.125802	-0.541624
7	C	1.779760	-0.244060	-0.054099
8	C	0.444940	-0.540257	-0.126508
9	C	-0.668608	0.313938	0.072103
10	H	1.467929	-2.760678	0.920002
11	H	4.314593	-0.135066	-0.937465
12	H	3.128143	-4.563348	0.904035
13	H	5.969772	-1.950905	-0.949867
14	H	5.382189	-4.170321	-0.033328
15	C	-4.447948	0.034454	0.052382
16	C	-4.772727	-1.285400	-0.294584
17	C	-5.485485	0.939972	0.311406
18	C	-6.090185	-1.679796	-0.373794
19	C	-6.805458	0.540808	0.232058
20	C	-7.108657	-0.768875	-0.109877
21	H	-3.989586	-2.003578	-0.502935
22	H	-5.238725	1.961860	0.576933
23	H	-6.333234	-2.700214	-0.641453
24	H	-7.598911	1.248530	0.435341
25	H	-8.142741	-1.084760	-0.172076
26	C	-1.970978	-0.233769	-0.043892
27	H	-2.020799	-1.282304	-0.305725
28	C	-3.092903	0.499507	0.155360
29	H	-2.971471	1.546118	0.421771
30	O	-0.590936	1.578384	0.403553
31	C	2.292236	1.137616	-0.034122
32	C	3.118220	1.563033	1.009607
33	C	1.996607	2.018895	-1.077513
34	C	3.605551	2.856698	1.025858
35	C	2.510027	3.305159	-1.067333
36	C	3.306134	3.726348	-0.013170
37	H	3.358686	0.876818	1.813311
38	H	1.380852	1.681396	-1.904092
39	H	4.227774	3.185909	1.848342
40	H	2.289614	3.977350	-1.886728
41	H	3.699556	4.735117	-0.003619
42	H	0.165350	-1.571572	-0.299950
43	H	0.328754	1.890415	0.442177





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.16641	1.99902	4.13058	0.03681	6.16641
C	2	-0.14576	1.99891	4.09241	0.05444	6.14576
C	3	-0.16637	1.99903	4.13427	0.03307	6.16637
C	4	-0.21149	1.99912	4.18080	0.03158	6.21149
C	5	-0.15798	1.99913	4.13155	0.02730	6.15798
C	6	-0.20782	1.99911	4.18290	0.02581	6.20782
C	7	-0.04819	1.99894	3.88723	0.16201	6.04819

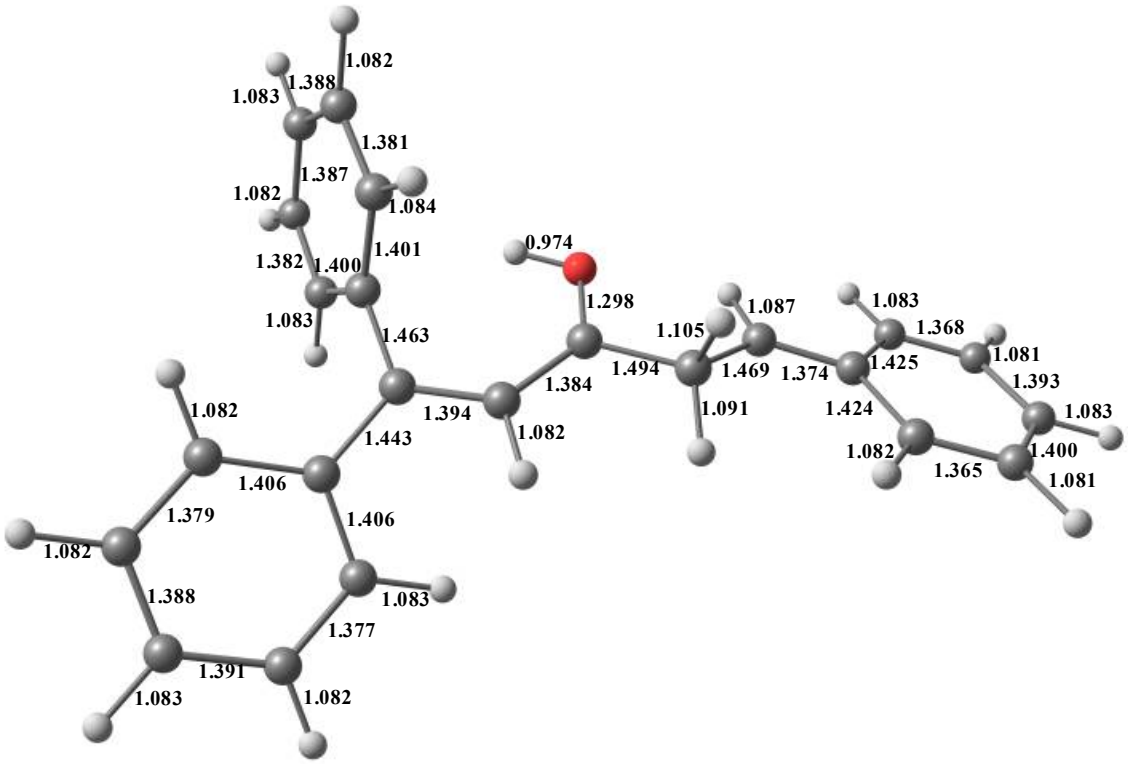
C	8	-0.34860	1.99884	4.29905	0.05071	6.34860
C	9	0.49850	1.99889	3.45343	0.04918	5.50150
H	10	0.21941	0.00000	0.77863	0.00196	0.78059
H	11	0.20744	0.00000	0.77515	0.01741	0.79256
H	12	0.22028	0.00000	0.77735	0.00237	0.77972
H	13	0.22086	0.00000	0.77724	0.00190	0.77914
H	14	0.21834	0.00000	0.77988	0.00179	0.78166
C	15	-0.13103	1.99898	4.10954	0.02251	6.13103
C	16	-0.14409	1.99904	4.12571	0.01934	6.14409
C	17	-0.12242	1.99889	4.10374	0.01978	6.12242
C	18	-0.20238	1.99912	4.18352	0.01974	6.20238
C	19	-0.21472	1.99914	4.19504	0.02055	6.21472
C	20	-0.14431	1.99913	4.12642	0.01876	6.14431
H	21	0.21529	0.00000	0.78284	0.00187	0.78471
H	22	0.21785	0.00000	0.78057	0.00158	0.78215
H	23	0.22076	0.00000	0.77762	0.00162	0.77924
H	24	0.22144	0.00000	0.77700	0.00156	0.77856
H	25	0.21867	0.00000	0.77989	0.00144	0.78133
C	26	-0.29265	1.99884	4.27149	0.02232	6.29265
H	27	0.22348	0.00000	0.77142	0.00510	0.77652
C	28	-0.01636	1.99905	3.98977	0.02753	6.01636
H	29	0.22428	0.00000	0.77336	0.00237	0.77572
O	30	-0.68054	1.99970	6.62483	0.05601	8.68054
C	31	0.08919	1.99896	2.74418	1.16767	5.91081
C	32	-0.67767	1.99869	4.48118	0.19779	6.67767
C	33	-0.70537	1.99872	4.51170	0.19496	6.70537
C	34	-0.20511	1.99897	4.16526	0.04088	6.20511
C	35	-0.20654	1.99897	4.16544	0.04214	6.20654
C	36	-0.18559	1.99916	4.15564	0.03079	6.18559
H	37	0.21178	0.00000	0.77801	0.01021	0.78822
H	38	0.21377	0.00000	0.77570	0.01053	0.78623
H	39	0.21706	0.00000	0.77696	0.00598	0.78294
H	40	0.21861	0.00000	0.77579	0.00560	0.78139
H	41	0.21907	0.00000	0.77817	0.00276	0.78093
H	42	0.23526	0.00000	0.76191	0.00282	0.76474
H	43	0.52285	0.00000	0.46645	0.01071	0.47715
* Total *		-0.32719	47.97634	114.88961	2.46124	165.32719

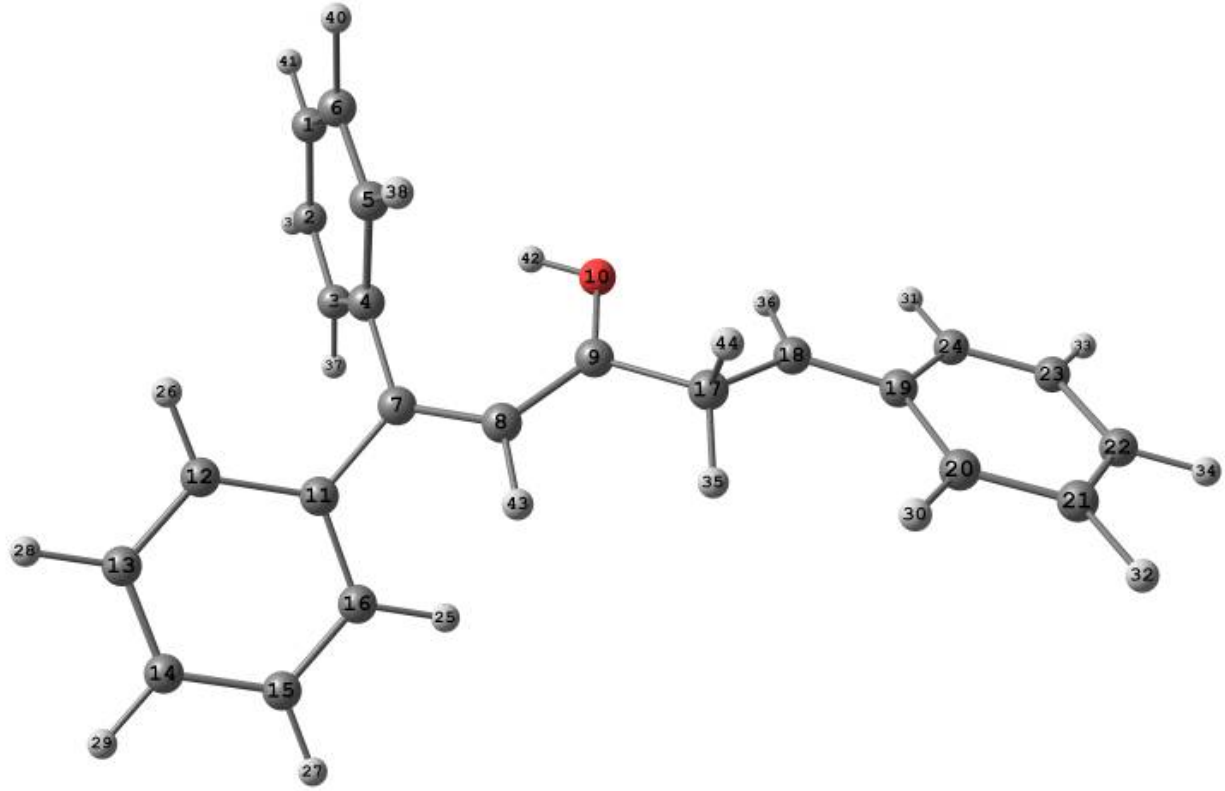
F1

Energy **E(RM06) = -962.827557261 h, G^{298} = -962.516801 h, μ=12.9 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.327877	3.715420	0.095891
2	C	3.589659	2.801946	1.106300
3	C	3.112033	1.508907	1.011486
4	C	2.328060	1.129532	-0.084972
5	C	2.063224	2.062078	-1.096755
6	C	2.573675	3.342735	-1.008620
7	C	1.821068	-0.238340	-0.193954
8	C	0.481204	-0.508514	-0.468427
9	C	-0.604040	0.333115	-0.296909
10	O	-0.602234	1.545999	0.166499
11	C	2.751318	-1.329599	-0.036401
12	C	4.118912	-1.135283	-0.296987
13	C	5.010315	-2.178934	-0.166303
14	C	4.560951	-3.425034	0.247551
15	C	3.213135	-3.633412	0.519706
16	C	2.313608	-2.602263	0.369680
17	C	-1.970801	-0.154524	-0.651547
18	C	-3.080664	0.462828	0.086266
19	C	-4.387141	0.037143	0.085382
20	C	-4.833639	-1.098038	-0.649994
21	C	-6.151089	-1.452266	-0.612765
22	C	-7.048906	-0.700606	0.155075
23	C	-6.641529	0.412395	0.887570
24	C	-5.324896	0.784096	0.855099
25	H	1.271330	-2.762634	0.614311
26	H	4.468459	-0.170684	-0.642161
27	H	2.870848	-4.602912	0.857346
28	H	6.057955	-2.024763	-0.389218
29	H	5.264624	-4.240440	0.360495
30	H	-4.133576	-1.674983	-1.239766
31	H	-4.974744	1.645957	1.409708
32	H	-6.505155	-2.309073	-1.168659
33	H	-7.359318	0.972271	1.470235
34	H	-8.091115	-0.994767	0.179026
35	H	-2.010360	-1.244692	-0.623828
36	H	-2.851591	1.351909	0.668812
37	H	3.314092	0.792202	1.798269
38	H	1.486216	1.762216	-1.964322
39	H	4.174668	3.096089	1.967961
40	H	2.387205	4.051551	-1.804823
41	H	3.716865	4.723396	0.166473
42	H	0.293808	1.874091	0.360798
43	H	0.220886	-1.513159	-0.773986
44	H	-2.117231	0.100141	-1.716890





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.12984	1.99893	4.11031	0.02061	6.12984
C	2	-0.19573	1.99913	4.17638	0.02021	6.19573
C	3	-0.14754	1.99901	4.13095	0.01758	6.14754
C	4	-0.16378	1.99890	4.14160	0.02327	6.16378
C	5	-0.18682	1.99902	4.16953	0.01827	6.18682

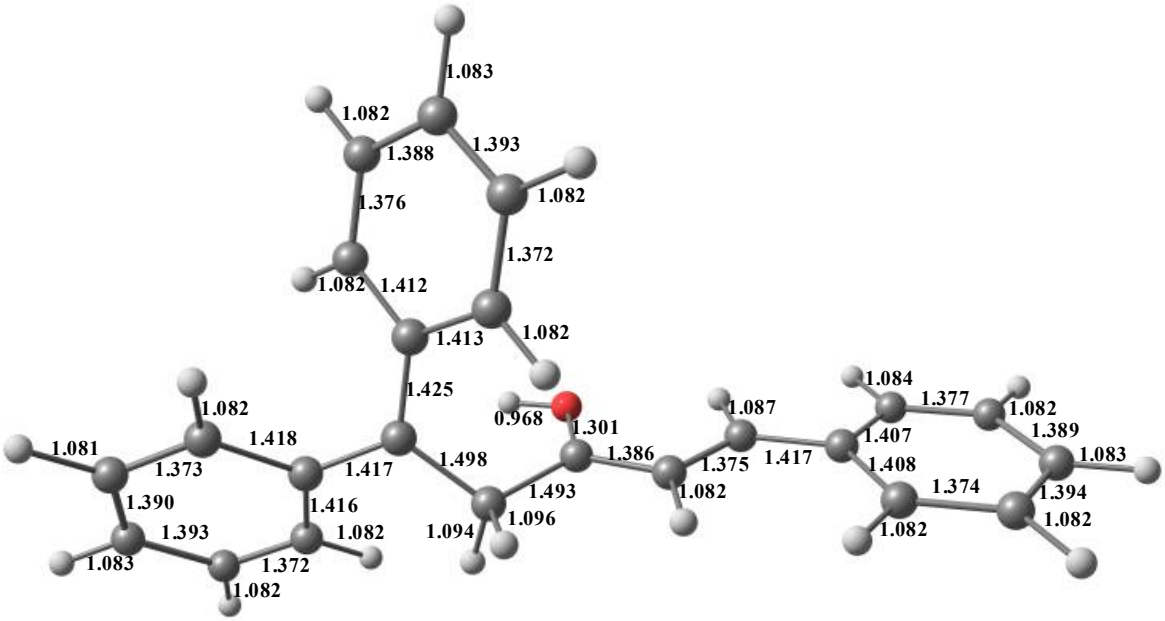
C	6	-0.19268	1.99913	4.17326	0.02029	6.19268
C	7	0.23397	1.99891	3.74496	0.02215	5.76603
C	8	-0.36476	1.99886	4.34782	0.01808	6.36476
C	9	0.59195	1.99896	3.38458	0.02452	5.40805
O	10	-0.63083	1.99969	6.60698	0.02417	8.63083
C	11	-0.11636	1.99872	4.09544	0.02220	6.11636
C	12	-0.12460	1.99905	4.10791	0.01764	6.12460
C	13	-0.20443	1.99911	4.18611	0.01921	6.20443
C	14	-0.11640	1.99913	4.09861	0.01865	6.11640
C	15	-0.20007	1.99912	4.18194	0.01900	6.20007
C	16	-0.12851	1.99905	4.11197	0.01749	6.12851
C	17	-0.55444	1.99906	4.53725	0.01813	6.55444
C	18	0.21391	1.99905	3.76979	0.01725	5.78609
C	19	-0.17582	1.99896	4.15784	0.01903	6.17582
C	20	-0.05192	1.99906	4.03637	0.01650	6.05192
C	21	-0.21144	1.99912	4.19253	0.01980	6.21144
C	22	-0.00395	1.99917	3.98718	0.01761	6.00395
C	23	-0.23228	1.99913	4.21270	0.02045	6.23228
C	24	-0.01041	1.99892	3.99256	0.01893	6.01041
H	25	0.22405	0.00000	0.77425	0.00170	0.77595
H	26	0.22746	0.00000	0.77038	0.00216	0.77254
H	27	0.22599	0.00000	0.77246	0.00155	0.77401
H	28	0.22619	0.00000	0.77226	0.00156	0.77381
H	29	0.22264	0.00000	0.77594	0.00141	0.77736
H	30	0.23283	0.00000	0.76544	0.00173	0.76717
H	31	0.23479	0.00000	0.76374	0.00146	0.76521
H	32	0.24006	0.00000	0.75837	0.00157	0.75994
H	33	0.24107	0.00000	0.75742	0.00151	0.75893
H	34	0.23355	0.00000	0.76518	0.00127	0.76645
H	35	0.28815	0.00000	0.71033	0.00152	0.71185
H	36	0.24194	0.00000	0.75598	0.00208	0.75806
H	37	0.23102	0.00000	0.76740	0.00158	0.76898
H	38	0.23145	0.00000	0.76626	0.00229	0.76855
H	39	0.22701	0.00000	0.77145	0.00154	0.77299
H	40	0.22799	0.00000	0.77045	0.00155	0.77201
H	41	0.22263	0.00000	0.77600	0.00137	0.77737
H	42	0.54011	0.00000	0.45640	0.00349	0.45989
H	43	0.25137	0.00000	0.74701	0.00162	0.74863
H	44	0.33258	0.00000	0.66577	0.00166	0.66742
* Total *		2.00008	47.97718	115.51708	0.50565	163.99992

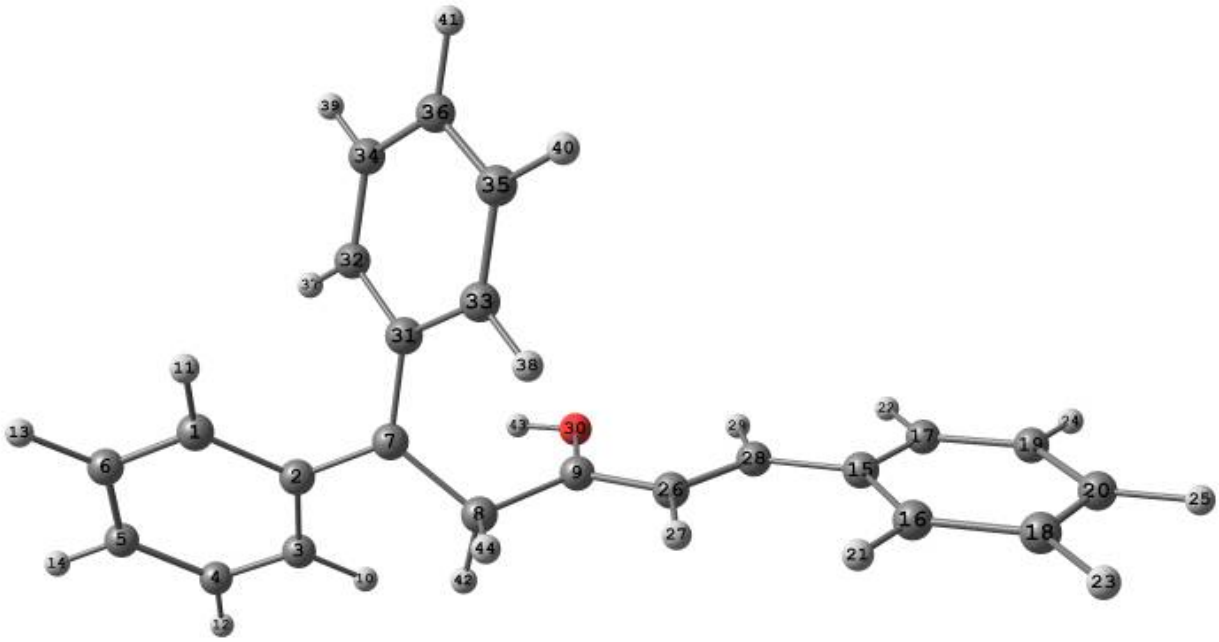
G1

Energy **E(RM06) = -962.837028254h, G^{298} = -962.526181h, μ=4.14 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	4.332300	-0.071611	-0.667609
2	C	3.222658	-0.823683	-0.206414
3	C	3.444987	-2.149564	0.237343
4	C	4.714784	-2.668058	0.264870
5	C	5.788360	-1.905257	-0.187913
6	C	5.593697	-0.614126	-0.664378
7	C	1.928043	-0.247978	-0.233296
8	C	0.731429	-1.126763	-0.432204
9	C	-0.466862	-0.828200	0.407587
10	H	2.629112	-2.746677	0.622506
11	H	4.169382	0.907821	-1.096652
12	H	4.880664	-3.668882	0.639704
13	H	6.429006	-0.043397	-1.046669
14	H	6.784696	-2.329438	-0.181270
15	C	-4.197173	-0.506793	0.200403
16	C	-4.562374	-0.565974	-1.158619
17	C	-5.201207	-0.356707	1.174924
18	C	-5.885383	-0.481047	-1.518817
19	C	-6.525638	-0.275792	0.806601
20	C	-6.865644	-0.337565	-0.538639
21	H	-3.805099	-0.674984	-1.924148
22	H	-4.917172	-0.309492	2.219654
23	H	-6.167647	-0.523892	-2.562348
24	H	-7.295332	-0.163156	1.558394
25	H	-7.906434	-0.272948	-0.831150
26	C	-1.737125	-0.774345	-0.143968
27	H	-1.811109	-0.890491	-1.216728
28	C	-2.852579	-0.591711	0.639015
29	H	-2.698276	-0.506064	1.711372
30	O	-0.324324	-0.663374	1.690079
31	C	1.725488	1.158790	-0.127853
32	C	2.594661	1.950911	0.654314
33	C	0.625407	1.779649	-0.759973
34	C	2.374222	3.303208	0.785387
35	C	0.435642	3.134382	-0.648747
36	C	1.304748	3.896567	0.128592
37	H	3.391899	1.477566	1.212147
38	H	-0.030951	1.204611	-1.400043
39	H	3.026851	3.897706	1.410291
40	H	-0.385086	3.609726	-1.168744
41	H	1.138997	4.961974	0.227846
42	H	0.984681	-2.179879	-0.276941
43	H	0.583302	-0.761002	2.010984
44	H	0.458457	-1.072104	-1.492467





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.08894	1.99904	4.07250	0.01739	6.08894
C	2	-0.14572	1.99885	4.12494	0.02194	6.14572
C	3	-0.09623	1.99904	4.08030	0.01689	6.09623
C	4	-0.20080	1.99912	4.18242	0.01926	6.20080
C	5	-0.06590	1.99914	4.04867	0.01808	6.06590
C	6	-0.20657	1.99910	4.18818	0.01929	6.20657
C	7	0.30836	1.99891	3.66913	0.02360	5.69164
C	8	-0.54194	1.99893	4.52032	0.02268	6.54194
C	9	0.59941	1.99897	3.37636	0.02526	5.40059
H	10	0.22597	0.00000	0.77219	0.00184	0.77403

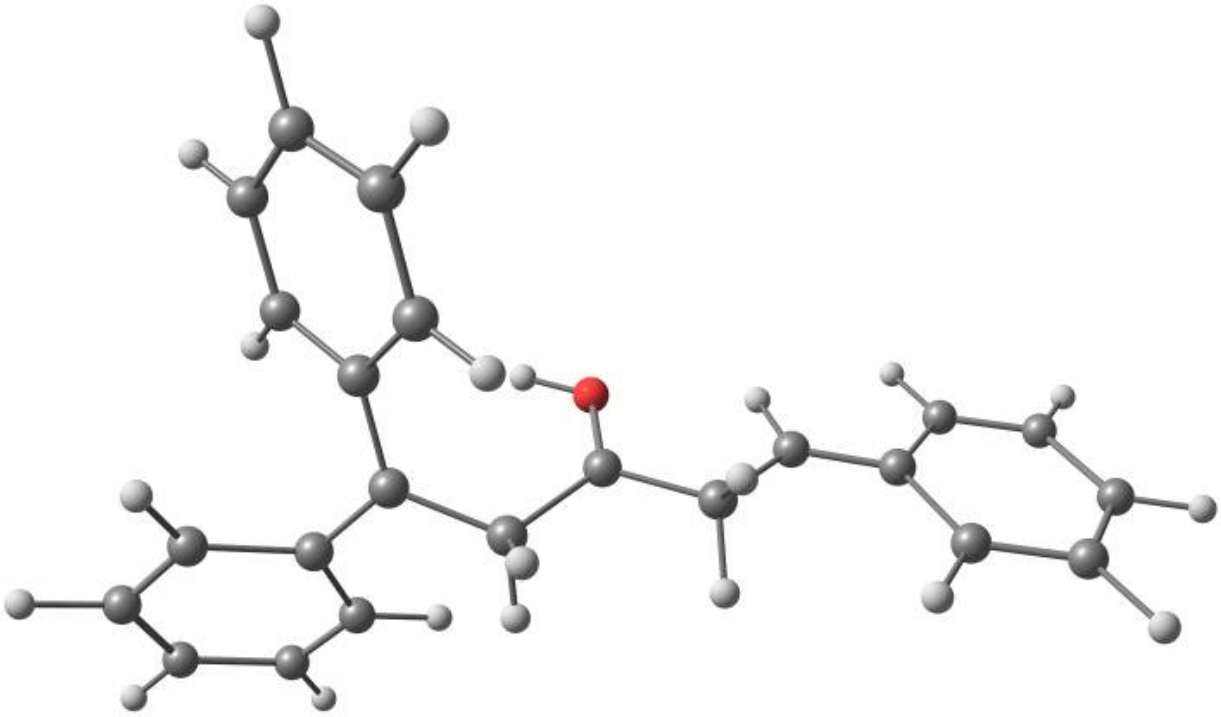
H	11	0.23431	0.00000	0.76342	0.00227	0.76569
H	12	0.23438	0.00000	0.76412	0.00150	0.76562
H	13	0.23505	0.00000	0.76344	0.00151	0.76495
H	14	0.22907	0.00000	0.76957	0.00135	0.77093
C	15	-0.14622	1.99898	4.12820	0.01904	6.14622
C	16	-0.10940	1.99905	4.09370	0.01665	6.10940
C	17	-0.08542	1.99890	4.06725	0.01927	6.08542
C	18	-0.20540	1.99912	4.18659	0.01969	6.20540
C	19	-0.21897	1.99913	4.19935	0.02049	6.21897
C	20	-0.09895	1.99914	4.08154	0.01826	6.09895
H	21	0.22129	0.00000	0.77695	0.00176	0.77871
H	22	0.22390	0.00000	0.77456	0.00154	0.77610
H	23	0.22741	0.00000	0.77099	0.00160	0.77259
H	24	0.22819	0.00000	0.77027	0.00154	0.77181
H	25	0.22383	0.00000	0.77479	0.00137	0.77617
C	26	-0.35108	1.99891	4.33383	0.01834	6.35108
H	27	0.24183	0.00000	0.75648	0.00170	0.75817
C	28	0.08219	1.99906	3.89946	0.01929	5.91781
H	29	0.23145	0.00000	0.76637	0.00218	0.76855
O	30	-0.62129	1.99967	6.59632	0.02530	8.62129
C	31	-0.15501	1.99886	4.13392	0.02222	6.15501
C	32	-0.09898	1.99904	4.08253	0.01742	6.09898
C	33	-0.12435	1.99903	4.10723	0.01809	6.12435
C	34	-0.20249	1.99911	4.18396	0.01943	6.20249
C	35	-0.19023	1.99911	4.17189	0.01923	6.19023
C	36	-0.08177	1.99914	4.06448	0.01815	6.08177
H	37	0.23537	0.00000	0.76304	0.00159	0.76463
H	38	0.22531	0.00000	0.77194	0.00275	0.77469
H	39	0.23407	0.00000	0.76443	0.00150	0.76593
H	40	0.23369	0.00000	0.76479	0.00153	0.76631
H	41	0.22839	0.00000	0.77023	0.00138	0.77161
H	42	0.29337	0.00000	0.70474	0.00189	0.70663
H	43	0.53551	0.00000	0.46237	0.00212	0.46449
H	44	0.30333	0.00000	0.69501	0.00166	0.69667
* Total *		2.00003	47.97737	115.51278	0.50983	163.99997

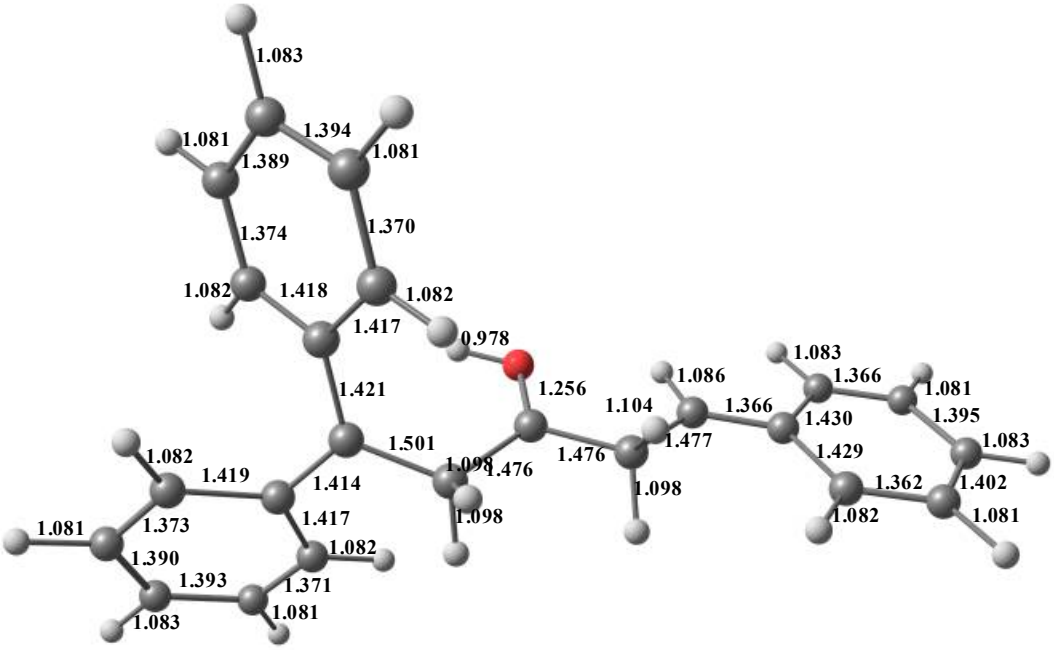
H1

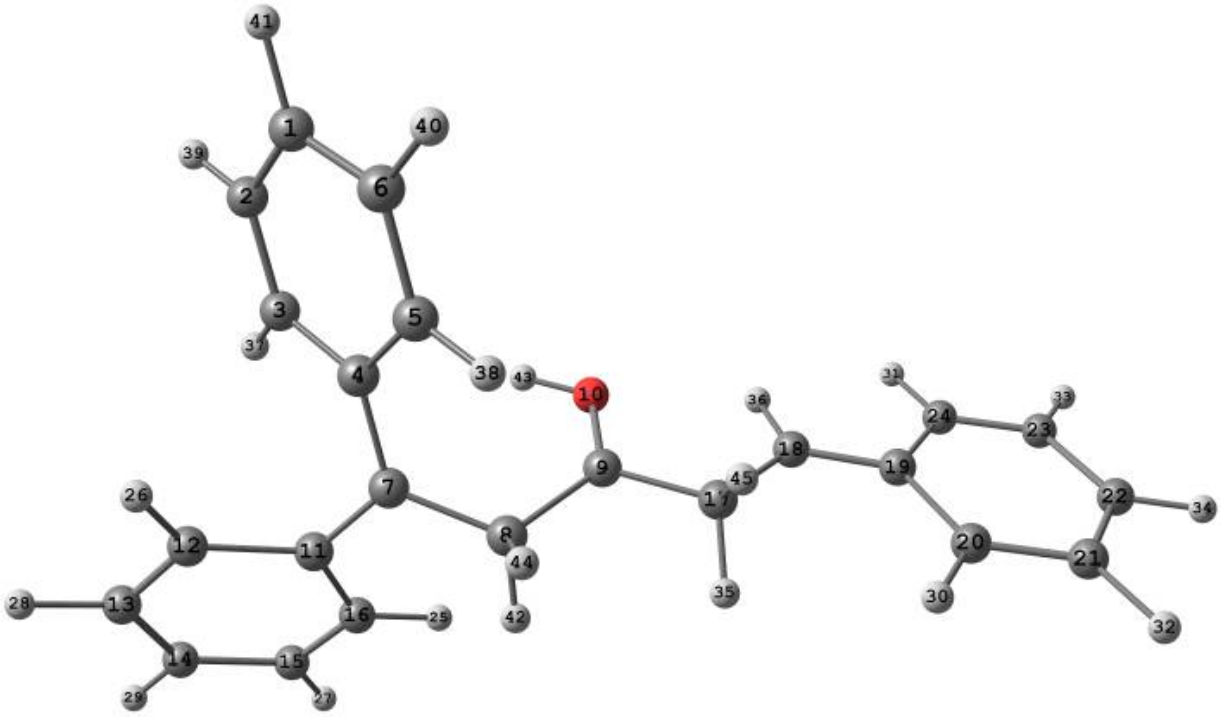
Energy **E(RM06) = -963.192797138 h, G^{298} =-962,869389 h, μ=8.88 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.816049	3.944489	0.129452
2	C	3.555400	2.996373	0.825113
3	C	3.279849	1.660048	0.663169
4	C	2.240131	1.241110	-0.204771
5	C	1.478681	2.231268	-0.872941
6	C	1.778476	3.559400	-0.718402
7	C	1.950882	-0.140622	-0.365076
8	C	0.560273	-0.535714	-0.768916
9	C	-0.574611	-0.146767	0.090335
10	O	-0.461904	0.254222	1.275455
11	C	2.925474	-1.151571	-0.199877
12	C	4.291493	-0.872871	-0.462564
13	C	5.245087	-1.845291	-0.291992
14	C	4.872041	-3.107385	0.156560
15	C	3.535670	-3.410763	0.409226
16	C	2.568638	-2.460154	0.208927
17	C	-1.944974	-0.261964	-0.445733
18	C	-3.048349	-0.133630	0.528483
19	C	-4.378243	-0.219788	0.226873
20	C	-4.867103	-0.447650	-1.096332
21	C	-6.209471	-0.521121	-1.315307
22	C	-7.096163	-0.371966	-0.239361
23	C	-6.651458	-0.147415	1.063812
24	C	-5.308896	-0.071434	1.302151
25	H	1.540070	-2.706982	0.436717
26	H	4.569073	0.087010	-0.876941
27	H	3.260408	-4.395418	0.761550
28	H	6.279911	-1.634877	-0.525033
29	H	5.627404	-3.870909	0.294281
30	H	-4.176804	-0.562537	-1.921591
31	H	-4.926998	0.101403	2.300605
32	H	-6.596778	-0.693397	-2.309465
33	H	-7.364221	-0.035585	1.868293
34	H	-8.161212	-0.432731	-0.427948
35	H	-2.013291	-1.195089	-1.019926
36	H	-2.785638	0.042680	1.567732
37	H	3.805997	0.925050	1.257698
38	H	0.701594	1.949899	-1.571346
39	H	4.333847	3.307894	1.508009
40	H	1.216498	4.306431	-1.262007
41	H	3.038248	4.996582	0.256159
42	H	0.460187	-1.621244	-0.898420
43	H	0.446511	0.330624	1.629610
44	H	0.357566	-0.166086	-1.782663
45	H	-2.030398	0.514020	-1.225930




1.083
1.081
1.394
1.389
1.081
1.374
1.370
1.082
1.418
1.082
1.417
0.978
1.421
1.256
1.086
1.104
1.366
1.083
1.366
1.081
1.430
1.395
1.083
1.501
1.477
1.429
1.082
1.419
1.098
1.476
1.476
1.414
1.098
1.362
1.402
1.417
1.098
1.082
1.081
1.373
1.082
1.081
1.390
1.393
1.371
1.083
1.081



Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.06063	1.99915	4.04338	0.01810	6.06063
C	2	-0.20137	1.99910	4.18261	0.01965	6.20137
C	3	-0.09113	1.99905	4.07465	0.01744	6.09113
C	4	-0.15490	1.99887	4.13397	0.02206	6.15490
C	5	-0.11834	1.99904	4.10149	0.01780	6.11834
C	6	-0.18797	1.99911	4.16942	0.01943	6.18797
C	7	0.26367	1.99890	3.71237	0.02506	5.73633
C	8	-0.57795	1.99896	4.55915	0.01983	6.57795
C	9	0.79931	1.99917	3.17548	0.02604	5.20069
O	10	-0.54142	1.99962	6.51452	0.02727	8.54142
C	11	-0.13296	1.99886	4.11245	0.02165	6.13296
C	12	-0.08812	1.99904	4.07138	0.01769	6.08812
C	13	-0.20435	1.99910	4.18593	0.01931	6.20435
C	14	-0.05615	1.99915	4.03896	0.01805	6.05615
C	15	-0.19695	1.99912	4.17851	0.01933	6.19695
C	16	-0.09984	1.99904	4.08397	0.01684	6.09984
C	17	-0.59315	1.99901	4.57618	0.01796	6.59315
C	18	0.18262	1.99903	3.80009	0.01826	5.81738
C	19	-0.15795	1.99896	4.13999	0.01901	6.15795
C	20	-0.04624	1.99906	4.03086	0.01632	6.04624
C	21	-0.20999	1.99912	4.19101	0.01986	6.20999
C	22	0.02081	1.99917	3.96251	0.01751	5.97919
C	23	-0.23236	1.99913	4.21273	0.02050	6.23236
C	24	0.00055	1.99892	3.98156	0.01897	5.99945
H	25	0.22707	0.00000	0.77115	0.00179	0.77293
H	26	0.23636	0.00000	0.76123	0.00241	0.76364
H	27	0.23666	0.00000	0.76185	0.00150	0.76334
H	28	0.23727	0.00000	0.76122	0.00151	0.76273
H	29	0.23096	0.00000	0.76770	0.00134	0.76904

	30	0.23480	0.00000	0.76348	0.00173	0.76520
	31	0.23786	0.00000	0.76068	0.00146	0.76214
H	32	0.24396	0.00000	0.75449	0.00155	0.75604
H	33	0.24490	0.00000	0.75361	0.00149	0.75510
H	34	0.23647	0.00000	0.76228	0.00125	0.76353
H	35	0.32967	0.00000	0.66879	0.00154	0.67033
H	36	0.24773	0.00000	0.74993	0.00234	0.75227
H	37	0.23901	0.00000	0.75934	0.00165	0.76099
H	38	0.22579	0.00000	0.77230	0.00191	0.77421
H	39	0.23802	0.00000	0.76046	0.00152	0.76198
H	40	0.23754	0.00000	0.76094	0.00152	0.76246
H	41	0.23162	0.00000	0.76704	0.00134	0.76838
H	42	0.32786	0.00000	0.67044	0.00170	0.67214
H	43	0.56258	0.00000	0.43420	0.00323	0.43742
H	44	0.33233	0.00000	0.66606	0.00161	0.66767
H	45	0.34636	0.00000	0.65200	0.00164	0.65364
* Total *		3.00001	47.97767	115.51235	0.50997	163.99999