SUPPORTING INFORMATION

EXPERIMENTAL SECTION

The reagents employed were of analar grade and the solvents used were purified and dried according to the standard procedure.[S1] Melting points were measured in a RAAGA melting point apparatus. Infrared spectra were measured as KBr pellets on a Jasco FT-IR 400-4000 cm^{-1} range. Electronic spectra of the compounds were recorded using JASCO 600 spectrophotometer. ^{1}H and ^{13}C NMR spectra were recorded at room temperature with a Bruker 400 MHz instrument, chemical shifts were relative to tetramethylsilane (TMS) and expressed in parts per million (ppm). The metal precursor $[Ru(acac)_2(CH_3CN)_2]$ and the ligands **HL¹** and **HL²** were prepared according to the reported procedure.[S2,S3] Mass spectra were recorded with a Bruker Q-TOF high-resolution mass spectrometer.

Spectral data of the products

A1: ^{1}H NMR ($CDCl_3$, δ ppm): 9.10 (d, *J* = 6.4 Hz, 1H), 8.21 (s, 1H), 8.07 (s, 1H), 7.81 (d, *J* = 5.6 Hz, 2H), 7.71-7.75 (t, *J* = 7.2 Hz, 2H), 7.57-7.63 (m, 5H), 4.88 (s, 1H), 4.70 (d, *J* = 10.4 Hz, 3H), 4.42 (s, 2H), 4.12 (s, 4H), 4.01 (s, 2H), 3.25 (d, *J* = 6.8 Hz, 1H), 3.10-3.14 (t, *J* = 6.8 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 190.5, 136.0, 127.8, 127.7, 127.5, 126.2, 125.0, 124.8, 124.6, 124.3, 124.0, 122.0, 85.0, 72.3, 69.8, 69.6, 62.0, 61.4, 29.7. ESI: m/z calcd. for $C_{34}H_{27}NO_2Fe$: 537.4287; Found: 537.1760 $[M]^+$.

A2: ^{1}H NMR ($CDCl_3$, δ ppm): 9.10 (s, 1H), 8.14 (d, *J* = 48 Hz, 1H), 7.62-7.81 (m, 8H), 4.87 (s, 1H), 4.69-4.76 (t, *J* = 16 Hz, 2H), 4.42 (s, 1H), 4.15 (d, *J* = 20 Hz, 2H), 4.02 (s, 2H), 3.20 (d, *J* = 56 Hz, 1H), 1.47-1.51 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 202.2, 137.3, 128.7, 126.9, 126.8, 125.5, 124.0, 79.2, 72.3, 69.8, 69.6, 53.5, 27.4.

A3: ^{1}H NMR ($CDCl_3$, δ ppm): 8.11 (s, 1H), 7.97 (s, 1H), 7.96-7.83 (t, *J* = 7.2 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.34-7.50 (m, 6H), 4.83 (s, 1H), 4.69 (s, 2H), 4.49 (d, *J* = 6.8 Hz, 1H), 4.42 (s, 1H), 4.13 (s, 2H), 4.01 (s, 2H), 3.08-3.21 (dd, *J* = 8 Hz, 1H), 2.42 (d, *J* = 16 Hz, 3H), 1.17 (s, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 200.7, 158.0, 142.7, 133.6, 132.1, 129.6, 125.09, 125.03, 123.5, 123.1, 77.7, 70.8, 68.3, 68.1, 60.2, 60.0, 25.9, 19.7.

A4: ^{1}H NMR ($CDCl_3$, δ ppm): 7.83 (s, 1H), 7.52-7.58 (m, 4H), 7.13 (d, *J* = 8 Hz, 3H), 4.69 (s, 3H), 4.48-4.53 (q, 2H), 4.43 (s, 1H), 4.13 (s, 1H), 4.01-4.05 (t, *J* = 12 Hz, 1H), 2.44 (s, 3H), 2.33 (s, 1H), 1.37-1.41 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 191.3, 160.1, 146.1, 139.4, 135.4, 127.0, 126.3, 126.1, 123.8, 123.0, 72.3, 69.8, 69.6, 61.8, 61.5, 29.7, 21.7.

A5: ^{1}H NMR ($CDCl_3$, δ ppm): 8.31 (s, 1H), 8.13 (d, *J* = 8 Hz, 1H), 7.64 (d, *J* = 8 Hz, 1H), 7.51-7.56 (m, 2H), 7.34-7.45 (m, 4H), 7.11 (d, *J* = 16 Hz, 1H), 4.85 (d, *J* = 8 Hz, 3H), 4.54 (d, *J* = 16 Hz, 3H), 4.15 (d, *J* = 12 Hz, 6H), 2.68 (d, *J* = 8 Hz, 3H), 1.17 (s, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 202.1, 139.4, 135.6, 130.4, 127.8, 126.99, 126.91, 126.5, 124.4, 120.4, 79.2, 72.8, 72.3, 70.1, 69.8, 69.6, 62.3, 27.4, 14.8.

A6: ^{1}H NMR ($CDCl_3$, δ ppm): 8.08 (s, 1H), 7.89 (d, *J* = 8 Hz, 3H), 7.72-7.77 (t, *J* = 12 Hz, 1H), 7.67-7.70 (t, *J* = 8 Hz, 1H), 7.56-7.62 (m, 2H), 7.42-7.48 (m, 3H), 7.34-7.37 (t, *J* = 8 Hz, 3H), 4.47-4.54 (q, 2H), 4.02 (d, *J* = 12 Hz, 1H), 1.35-1.39 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 198.8, 198.0, 136.9, 136.7, 136.6, 135.6, 135.0, 133.4, 133.1, 130.1, 128.7, 128.6, 128.1, 127.3, 127.1, 126.9, 126.6, 124.2, 124.1, 53.5, 29.72.

A7: ^{1}H NMR ($CDCl_3$, δ ppm): 8.08 (s, 1H), 7.97 (d, *J* = 8 Hz, 4H), 7.86 (d, *J* = 8 Hz, 1H), 7.53-7.57 (m, 3H), 7.49-7.51 (dd, *J* = 8 Hz, 1H), 7.43-7.47 (t, *J* = 8 Hz, 4H), 4.45-4.51 (q, 2H), 3.66 (s, 1H), 2.50 (s, 3H), 1.35-1.38 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 197.8, 197.5, 149.2, 144.1, 136.8, 136.0, 135.9, 135.6, 132.2, 132.0, 131.6, 131.1, 129.8, 127.6, 127.5, 127.1, 127.0, 126.7, 126.5, 125.39, 125.32, 124.9, 124.1, 60.6, 36.9, 20.5. ESI: m/z calcd. for $C_{27}H_{23}NO_2$: 393.4770; Found: 392.2936 $[M-H]^+$.

A8: ^{1}H NMR ($CDCl_3$, δ ppm): 8.12 (s, 1H), 7.97 (d, *J* = 8 Hz, 3H), 7.68 (d, *J* = 8 Hz, 1H), 7.60 (d, *J* = 8 Hz, 1H), 7.54-7.58 (t, *J* = 8 Hz, 3H), 7.51 (d, *J* = 8 Hz, 1H), 7.43-7.47 (t, *J* = 8 Hz, 4H), 7.41 (d, *J* = 8 Hz, 1H), 4.93 (s, 1H), 4.59-4.65 (p, 2H), 2.75 (d, *J* = 8 Hz, 3H), 1.47-1.50 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 197.0, 148.6, 146.9, 145.1, 144.6, 135.5, 135.3, 135.2, 133.5, 132.3, 131.0, 129.2, 129.0, 127.6, 127.1, 126.2, 125.8, 124.4, 124.2, 68.8, 28.6, 16.8, 16.7. ESI: m/z calcd. for $C_{27}H_{23}NO_2$: 393.4770; Found: 392.1630 $[M-H]^+$.

A9: ^{1}H NMR ($CDCl_3$, δ ppm): 9.04-9.13 (dd, *J* = 8 Hz, 1H), 7.94 (s, 1H), 7.80-7.82 (t, *J* = 4 Hz, 1H), 7.74 (s, 1H), 7.55-7.62 (m, 5H), 4.76 (s, 1H), 4.65-4.71 (q, 1H), 1.45-1.49 (t, *J* = 8 Hz, 2H). ^{13}C NMR ($CDCl_3$, δ ppm): 197.5, 149.0, 143.9, 137.5, 135.5, 132.5, 132.2, 129.3, 127.6, 127.3,

127.1, 127.0, 126.7, 126.2, 124.5, 123.5, 123.4, 123.3, 61.5, 28.6. ESI: m/z calcd. for $C_{30}H_{23}NO_2$: 429.5091; Found: 430.1357 $[M+H]^+$.

A10: ^{1}H NMR ($CDCl_3$, δ ppm): 8.04 (s, 1H), 7.90 (d, *J* = 8 Hz, 1H), 7.77 (d, *J* = 12 Hz, 1H), 7.73 (d, *J* = 8 Hz, 1H), 7.63-7.67 (m, 3H), 7.52-7.57 (dd, *J* = 8 Hz, 3H), 7.45-7.50 (m, 3H), 7.03-7.05 (t, *J* = 4 Hz, 1H), 4.71 (s, 1H), 4.50-4.55 (q, 2H), 1.38-1.41 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 196.6, 158.5, 142.6, 135.1, 134.9, 132.7, 132.6, 129.6, 129.3, 127.5, 127.3, 126.7, 126.6, 126.5, 126.2, 125.2, 124.0, 123.8, 123.5, 123.3, 122.9, 120.9, 61.0, 60.4, 28.6.

A11: ^{1}H NMR ($CDCl_3$, δ ppm): 8.50 (d, *J* = 8 Hz, 1H), 7.91 (d, *J* = 8 Hz, 1H), 7.79-7.82 (t, *J* = 8 Hz, 2H), 7.72 (s, 1H), 7.52 (d, *J* = 4 Hz, 1H), 7.43-7.50 (m, 4H), 7.40 (d, *J* = 8 Hz, 1H), 4.46-4.51 (q, 2H), 3.37 (s, 1H), 2.43 (s, 3H), 1.36-1.40 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 184.9, 147.1, 144.5, 136.2, 134.6, 131.4, 131.1, 126.8, 126.3, 125.4, 61.1, 28.6, 20.5.

A12: ^{1}H NMR ($CDCl_3$, δ ppm): 8.64 (s, 1H), 8.13 (s, 1H), 7.93 (s, 1H), 7.80 (d, *J* = 4 Hz, 2H), 7.76-7.79 (t, *J* = 12 Hz, 1H), 7.61-7.63 (dd, *J* = 4 Hz, 1H), 7.58 (d, *J* = 8 Hz, 2H), 7.40-7.42 (dd, *J* = 8 Hz, 2H), 7.12-7.17 (m, 2H), 4.55-4.60 (q, 2H), 2.53 (s, 1H), 2.46 (s, 3H), 1.49-1.52 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 181.4, 159.1, 146.0, 144.7, 140.5, 138.7, 138.0, 132.7, 130.7, 128.3, 127.2, 126.6, 125.6, 125.3, 123.3, 121.8, 117.9, 61.2, 20.9, 13.6. ESI: m/z calcd. for $C_{25}H_{21}NO_2S$: 399.5047; Found: 397.8281 $[M-2H]^+$.

A13: ^{1}H NMR ($CDCl_3$, δ ppm): 9.05-9.07 (t, *J* = 4 Hz, 1H), 7.96 (s, 1H), 7.82-7.83 (t, *J* = 4 Hz, 1H), 7.80 (d, *J* = 4 Hz, 1H), 7.75-7.78 (m, 1H), 7.65-7.67 (m, 1H), 7.63-7.64 (m, 1H), 7.61 (d, *J* = 4 Hz, 1H), 7.59 (d, *J* = 4 Hz, 2H), 7.57 (d, *J* = 4 Hz, 1H), 7.55-7.56 (m, 1H), 4.77 (s, 1H), 4.66-4.72 (q, 2H), 1.46-1.49 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 183.4, 146.8, 144.3, 134.9, 132.66, 132.62, 131.8, 129.2, 127.4, 127.2, 126.7, 126.2, 124.4, 123.5, 60.9, 28.6.

A14: ^{1}H NMR ($CDCl_3$, δ ppm): 8.66 (d, *J* = 8 Hz, 1H), 7.91 (d, *J* = 8 Hz, 2H), 7.85 (d, *J* = 8 Hz, 2H), 7.79 (d, *J* = 8 Hz, 2H), 7.50-7.54 (dt, *J* = 8 Hz, 2H), 7.39-7.47 (m, 4H), 4.76 (s, 1H), 4.55-4.61 (q, 2H), 1.43-1.47 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 200.8, 134.4, 132.9, 132.0, 129.1, 127.6, 127.3, 127.0, 125.4, 124.9, 123.2, 60.0, 28.9, 28.6. ESI: m/z calcd. for $C_{30}H_{23}NO_2$: 429.5091; Found: 428.4094 $[M-H]^+$.

A15: ^{1}H NMR ($CDCl_3$, δ ppm): 8.02 (s, 1H), 7.97 (d, *J* = 4 Hz, 3H), 7.88 (d, *J* = 8 Hz, 1H), 7.82 (s, 1H), 7.66 (d, *J* = 8 Hz, 1H), 7.52-7.58 (m, 4H), 7.42-7.48 (m, 4H), 7.37 (d, *J* = 8 Hz, 1H), 4.53-4.58 (q, 2H), 2.51 (s, 3H), 2.44 (s, 1H), 1.42-1.46 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 161.0, 153.8, 145.8, 143.1, 133.2, 131.3, 131.2, 130.0, 127.3, 125.5, 124.0, 116.9, 115.6, 59.6, 27.3, 19.2. ESI: m/z calcd. for $C_{31}H_{25}NO_2$: 443.5357; Found: 445.1693 $[M+2H]^+$.

A16: ^{1}H NMR ($CDCl_3$, δ ppm): 8.19 (s, 1H), 7.98 (d, *J* = 8 Hz, 3H), 7.87 (d, *J* = 8 Hz, 1H), 7.79 (d, *J* = 8 Hz, 2H), 7.67-7.71 (t, *J* = 8 Hz, 3H), 7.63 (d, *J* = 8 Hz, 2H), 7.53-7.57 (t, *J* = 8 Hz, 3H), 7.43-7.47 (t, *J* = 8 Hz, 4H), 4.76 (s, 1H), 4.55-4.60 (q, 2H), 1.44-1.48 (t, *J* = 8 Hz, 3H). ^{13}C NMR ($CDCl_3$, δ ppm): 202.3, 147.9, 145.4, 136.1, 135.9, 135.4, 133.9, 133.7, 132.9, 132.8, 130.3, 128.5, 128.4, 128.3, 127.8, 127.2, 126.5, 125.5, 124.6, 124.3, 62.0, 29.7. ESI: m/z calcd. for $C_{34}H_{25}NO_2$: 479.5678; Found: 476.1671 $[M-3H]^+$.

A17: ^{1}H NMR ($CDCl_3$, δ ppm): 8.06 (s, 1H), 7.97-7.99 (dd, *J* = 8 Hz, 2H), 7.93 (s, 1H), 7.85 (d, *J* = 20 Hz, 1H), 7.53-7.57 (t, *J* = 8 Hz, 3H), 7.41-7.48 (m, 5H), 4.78 (s, 1H), 4.58-4.64 (p, 2H), 2.76 (d, *J* = 8 Hz, 3H), 2.68 (s, 3H), 1.46-1.50 (q, 3H).

A18: ^{1}H NMR ($CDCl_3$, δ ppm): 8.30 (d, *J* = 8 Hz, 1H), 7.94 (d, *J* = 8 Hz, 1H), 7.86 (s, 2H), 7.71 (d, *J* = 8 Hz, 2H), 7.47 (s, 2H), 7.41-7.43 (dd, *J* = 8 Hz, 2H), 4.76 (s, 1H), 4.55-4.60 (q, 2H), 2.48 (s, 3H), 1.44-1.47 (t, *J* = 8 Hz, 3H).

A19: ^{1}H NMR ($CDCl_3$, δ ppm): 7.96-8.01 (m, 1H), 7.85-7.88 (t, *J* = 8 Hz, 2H), 7.71 (d, *J* = 8 Hz, 1H), 7.59-7.63 (m, 2H), 7.41-7.50 (m, 6H), 7.36 (d, *J* = 8 Hz, 1H), 4.76 (s, 1H), 4.55-4.60 (q, 2H), 2.48 (s, 3H), 1.53-1.56 (t, *J* = 8 Hz, 3H).

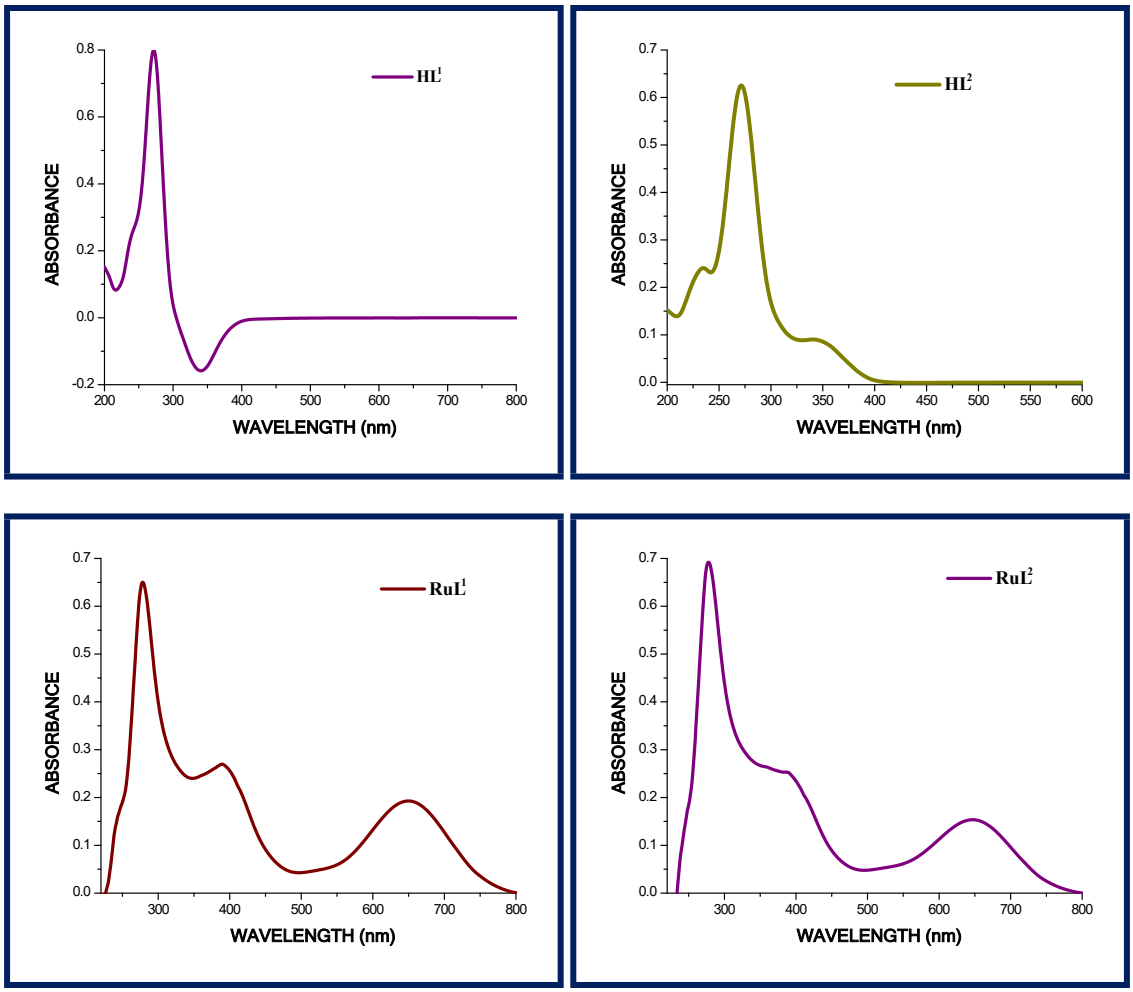

Fig. S1. Electronic spectra of the ligands **HL**^{1}, **HL**^{2} and complexes **RuL**^{1} and **RuL**^{2}

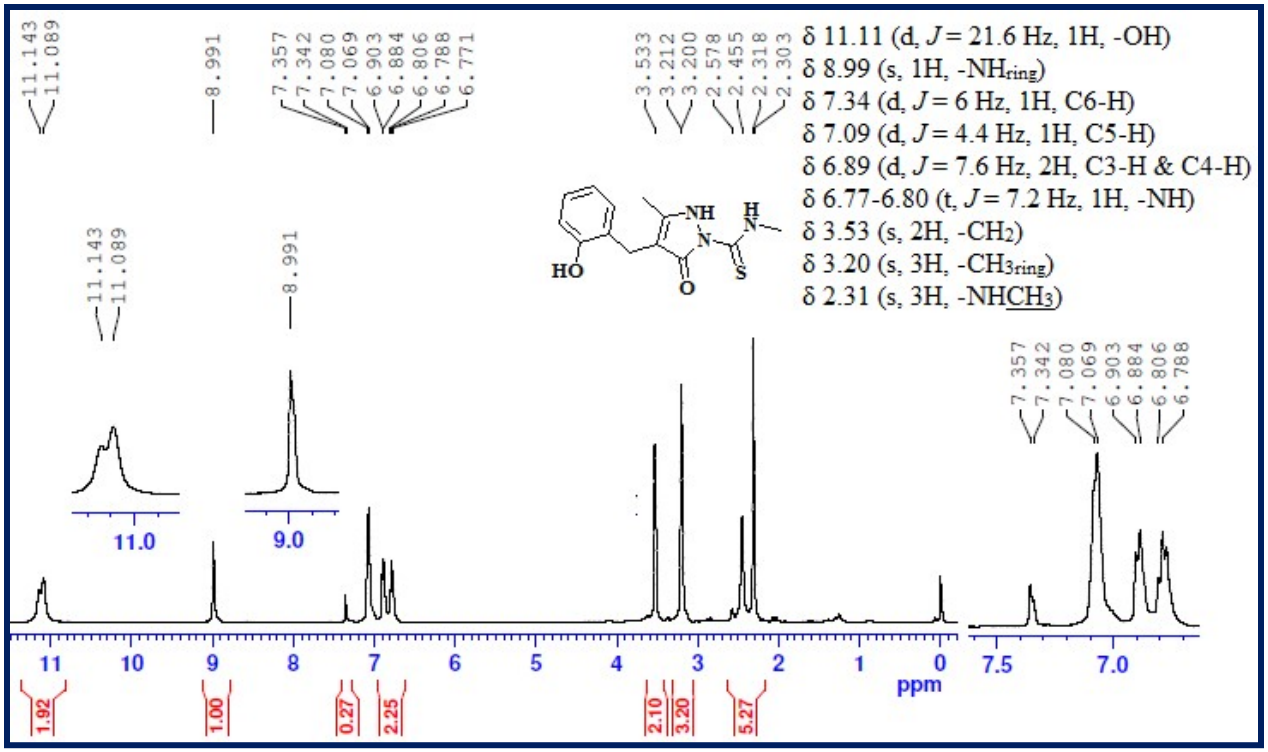

Fig. S2. [1]H NMR spectrum of the ligand **HL[1]**

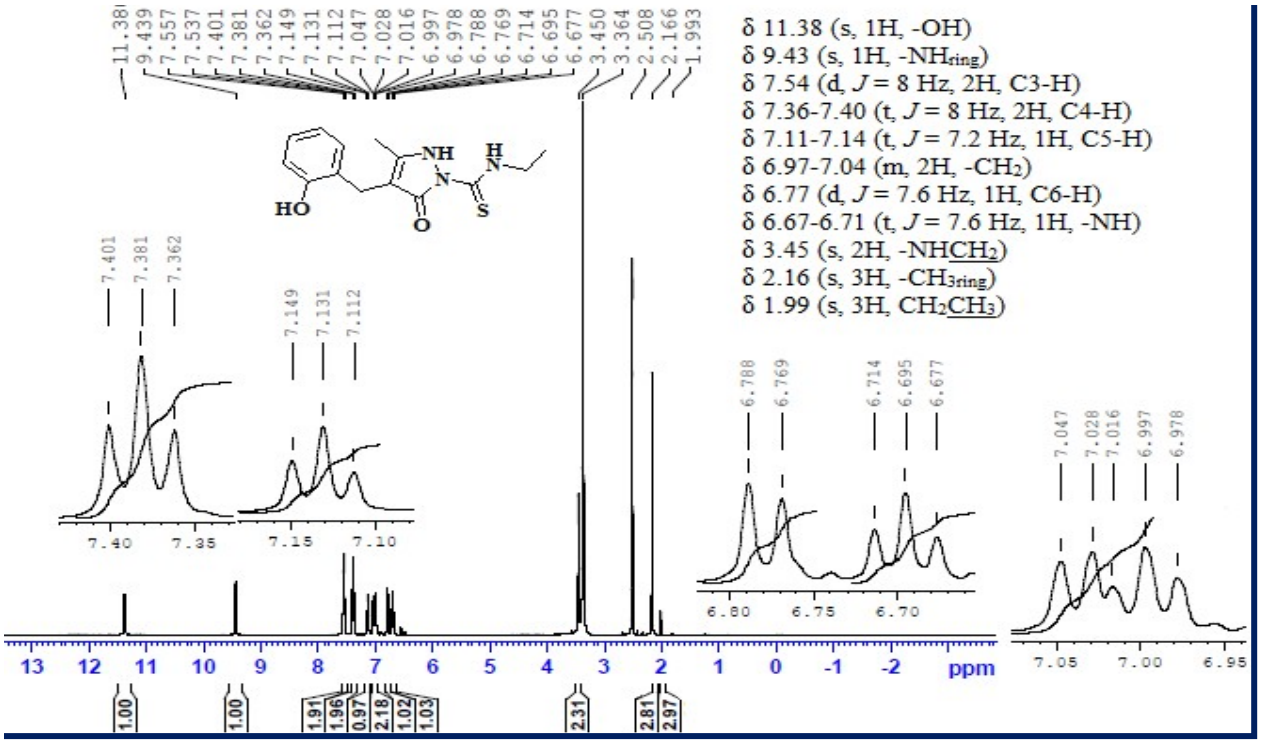

Fig. S3. [1]H NMR spectrum of the ligand **HL[2]**

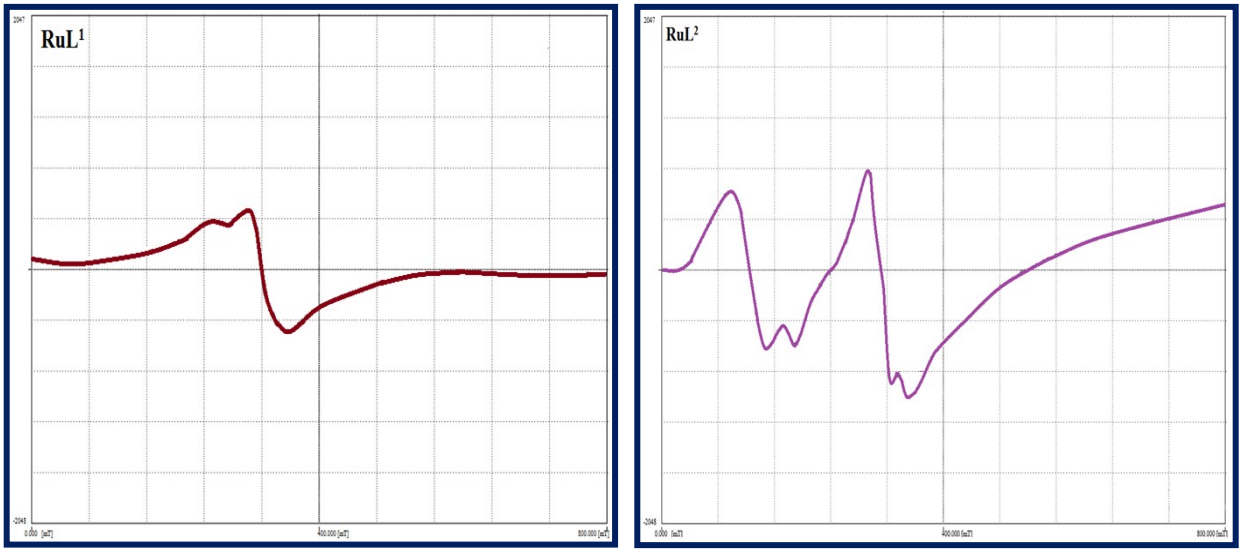

Fig. S4. EPR spectra of the Ru(III) complexes **RuL¹** and **RuL²**

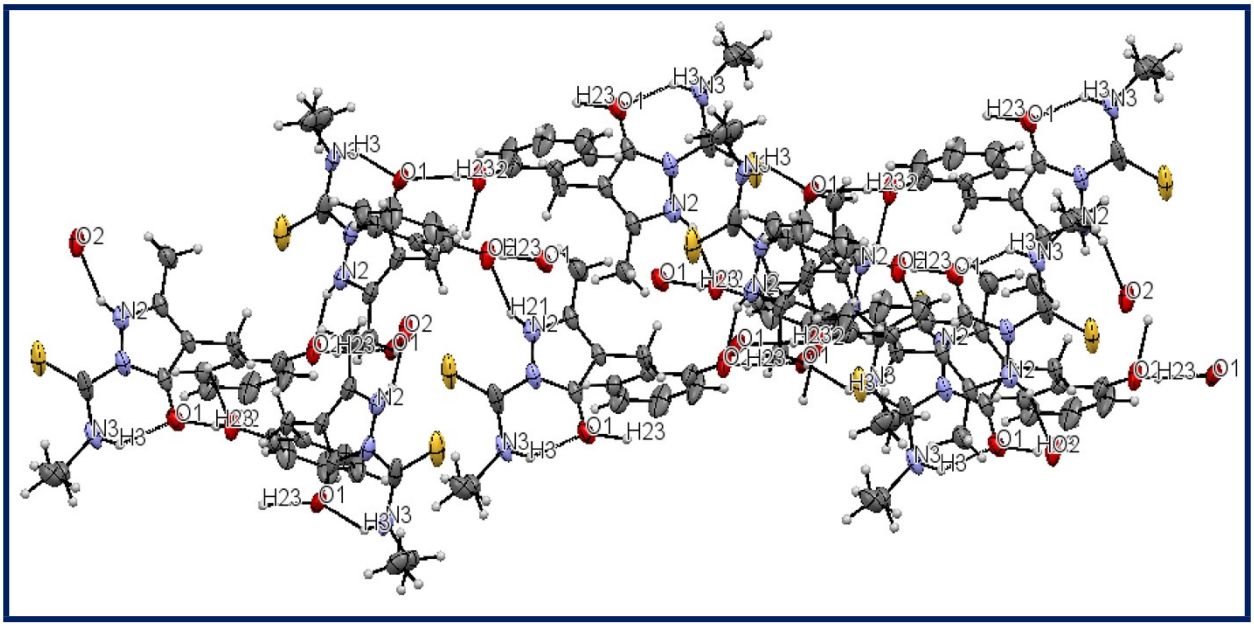

Fig. S5. Hydrogen bonding interactions in the ligand **HL²**

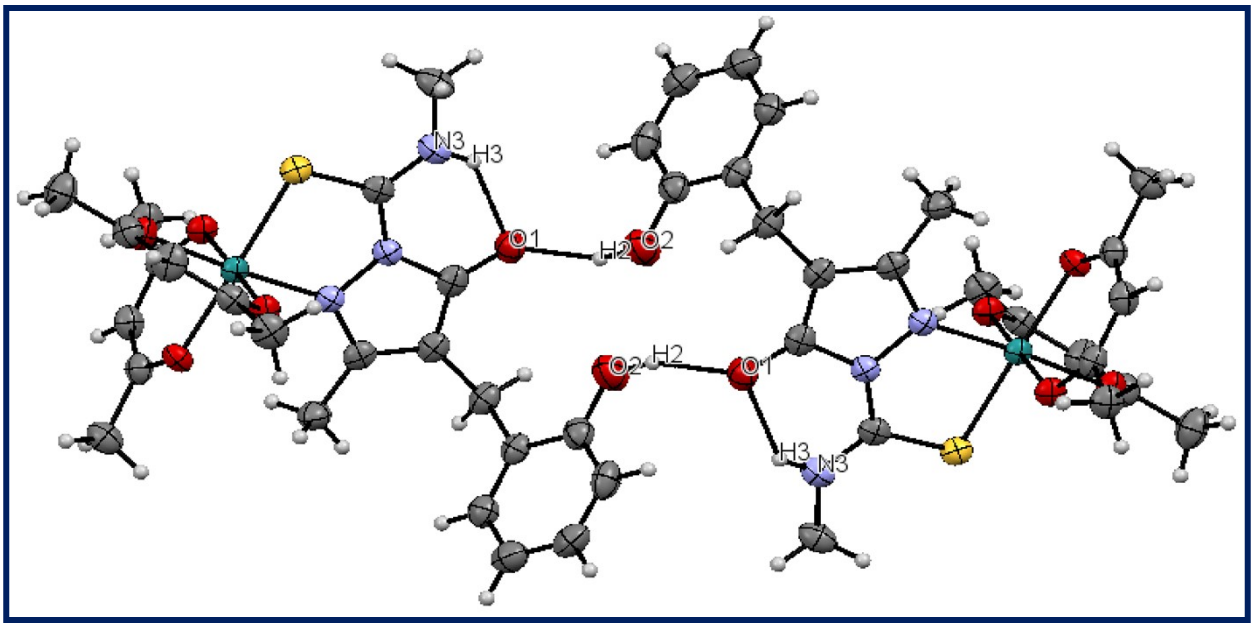

Fig. S6. Hydrogen bonding interaction in the complex **RuL[1]**

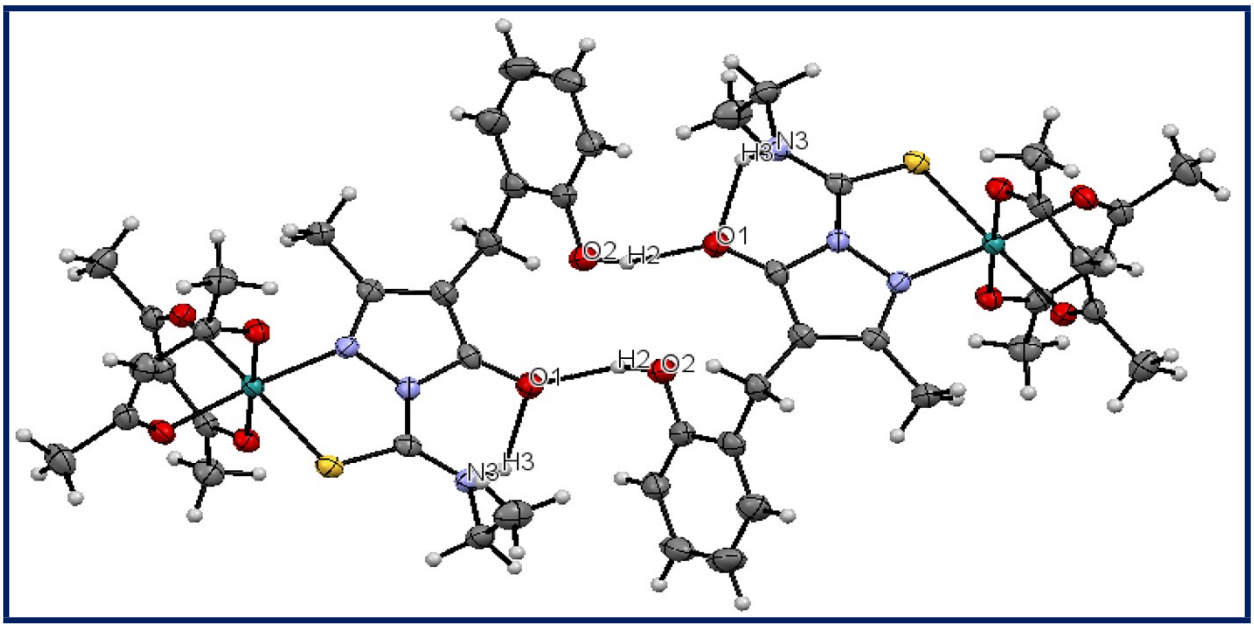

Fig. S7. Hydrogen bonding interaction in the complex **RuL[2]**

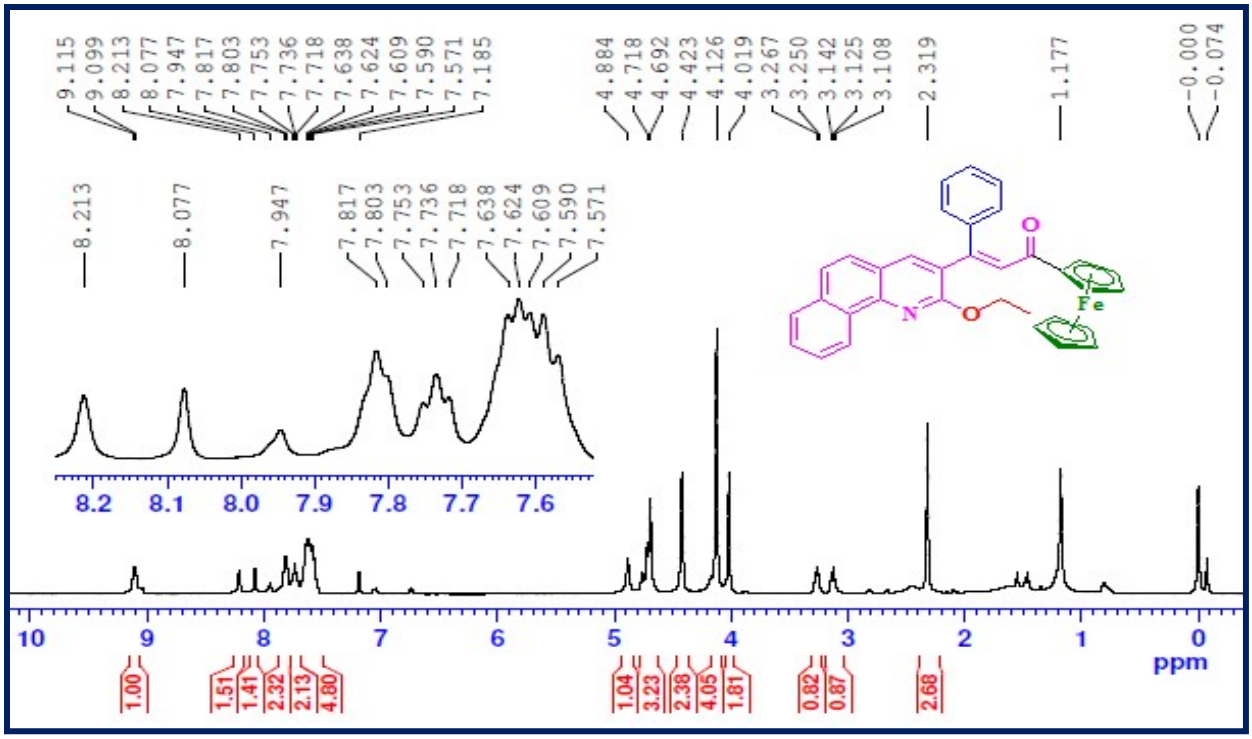

Fig. S8. [1]H NMR spectrum of **A1**

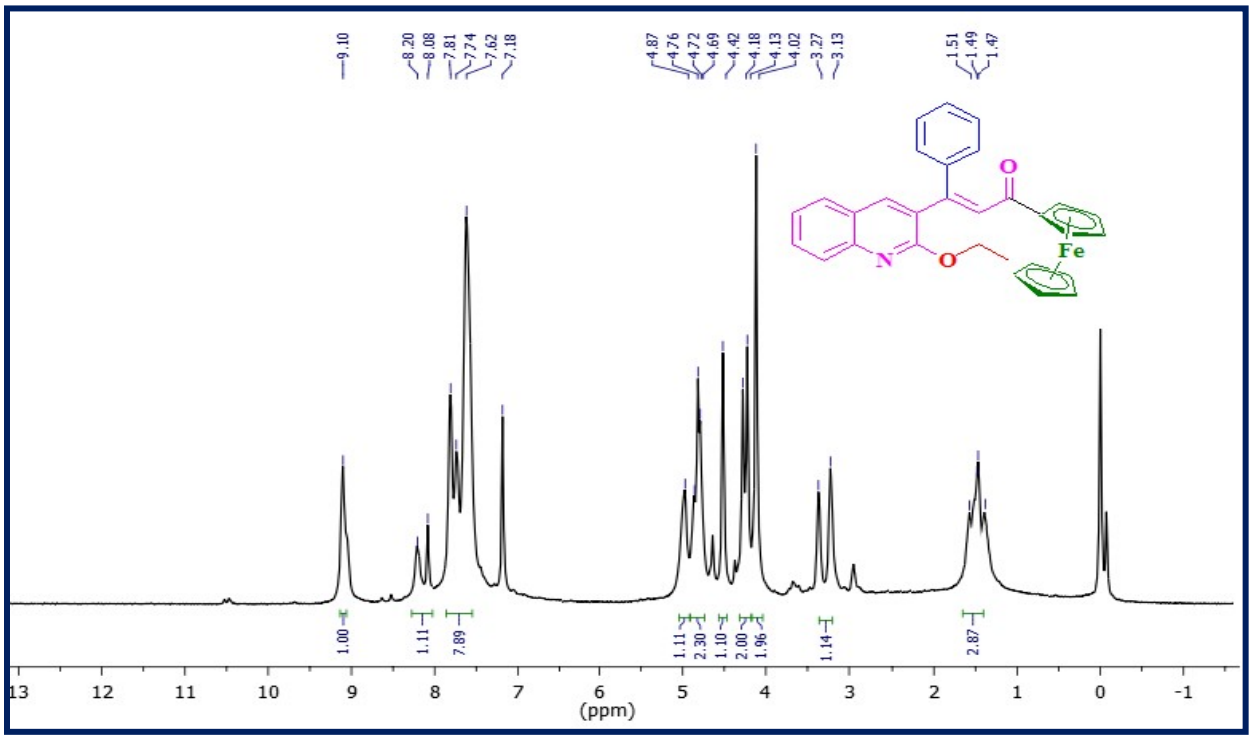

Fig. S9. [1]H NMR spectrum of **A2**

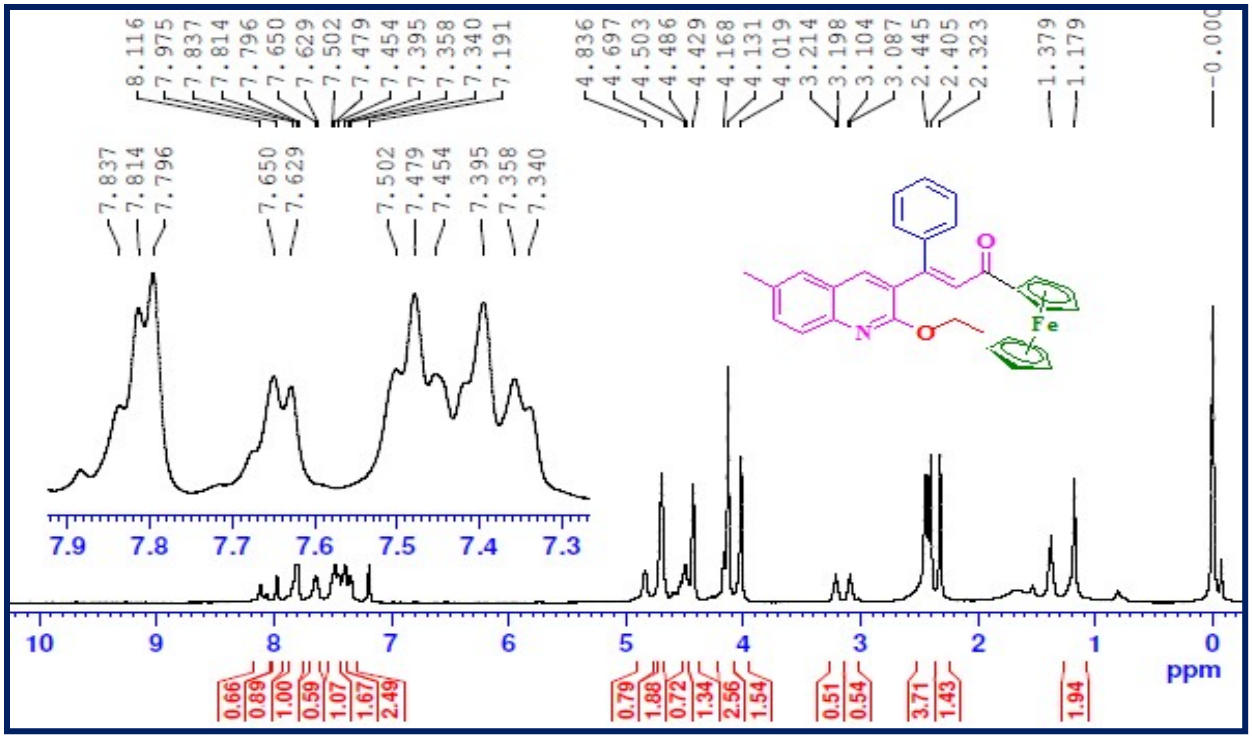

Fig. S10. [1]H NMR spectrum of **A3**

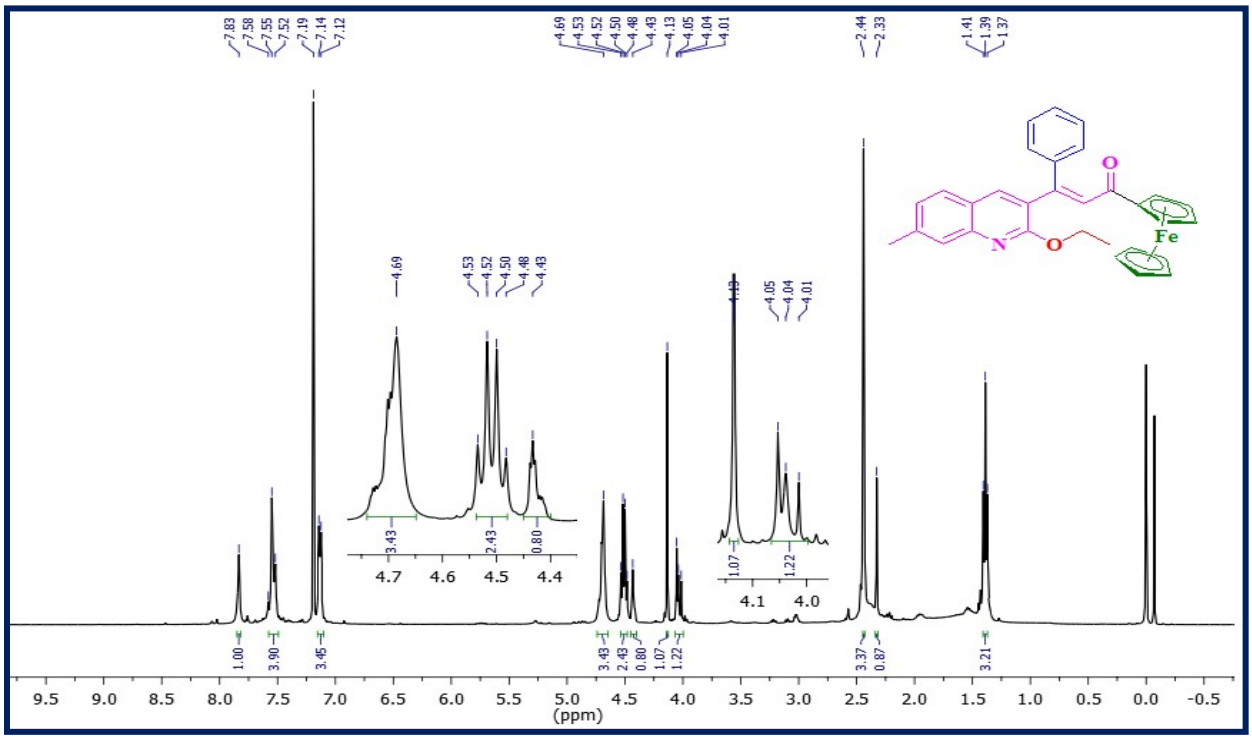

Fig. S11. [1]H NMR spectrum of **A4**

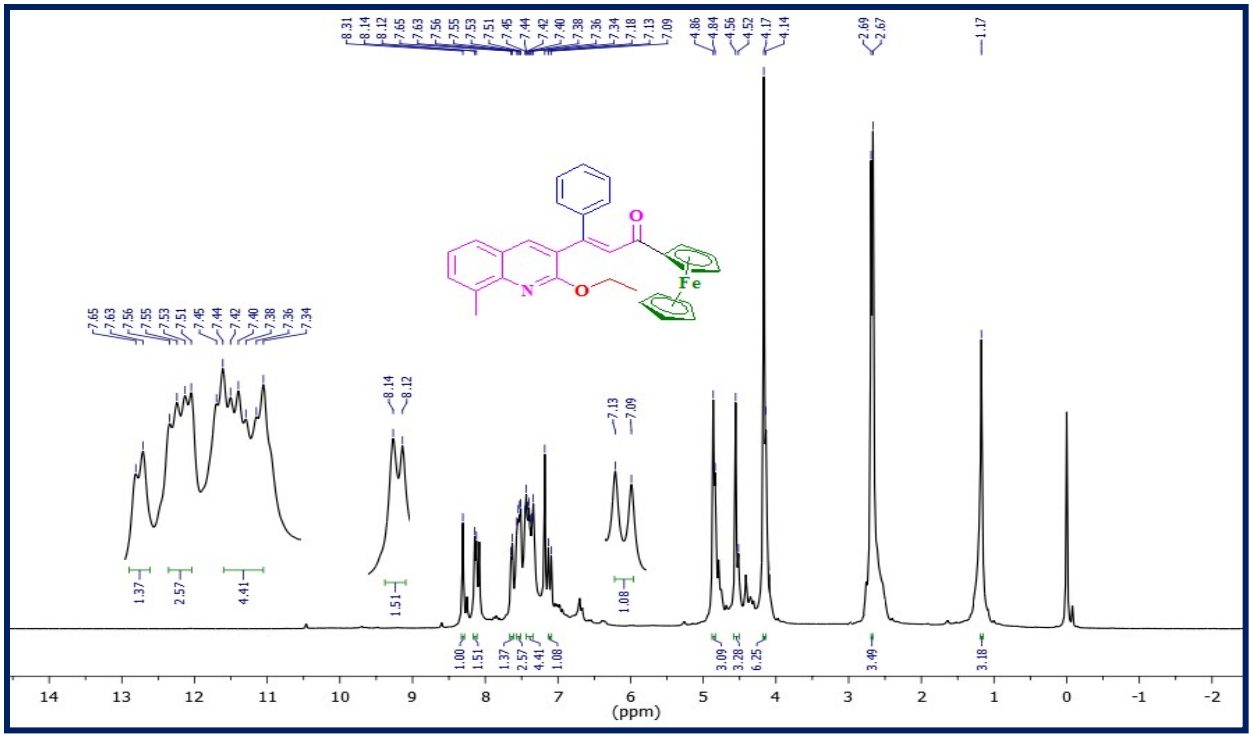

Fig. S12. ^{1}H NMR spectrum of **A5**

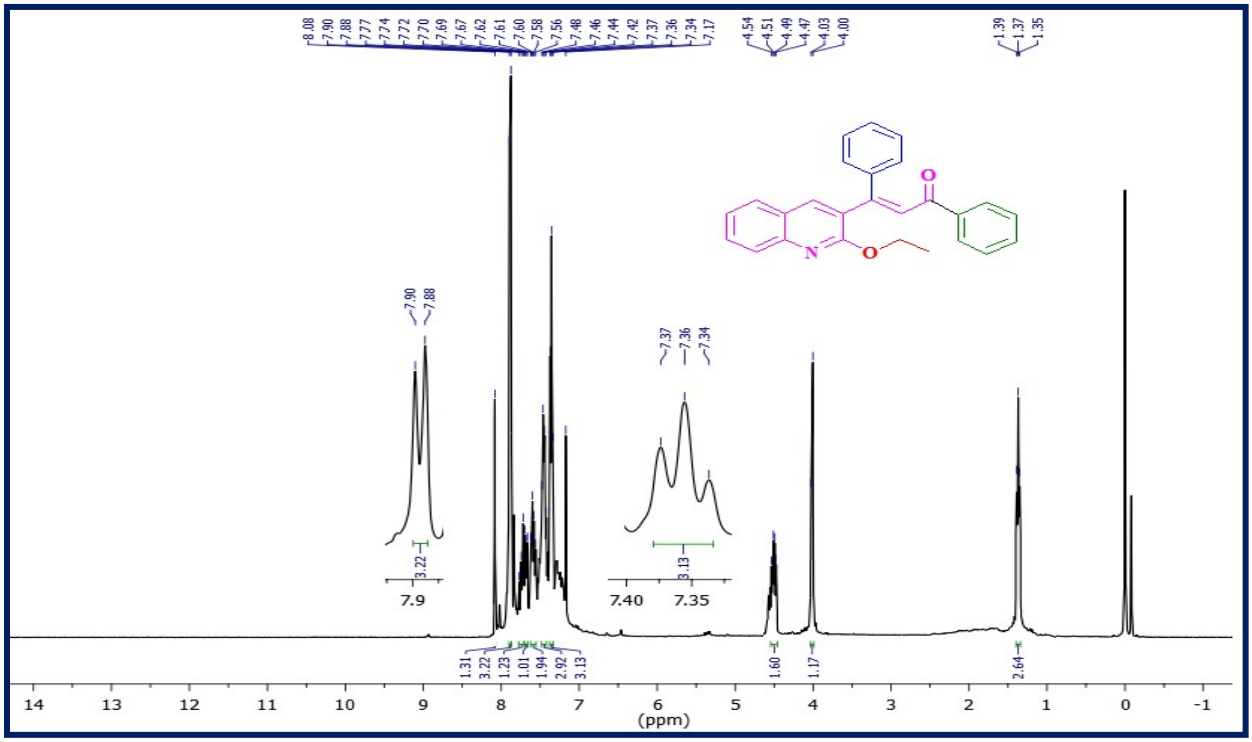

Fig. S13. ^{1}H NMR spectrum of **A6**

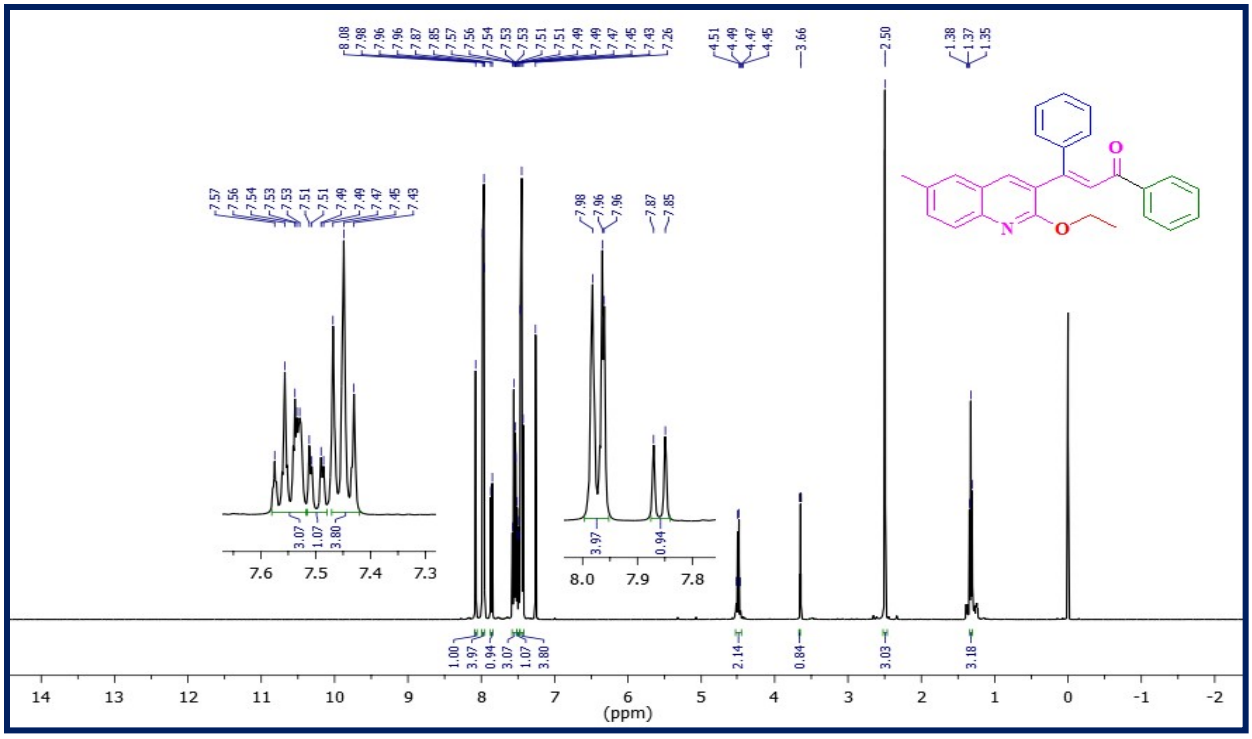

Fig. S14. ^{1}H NMR spectrum of **A7**

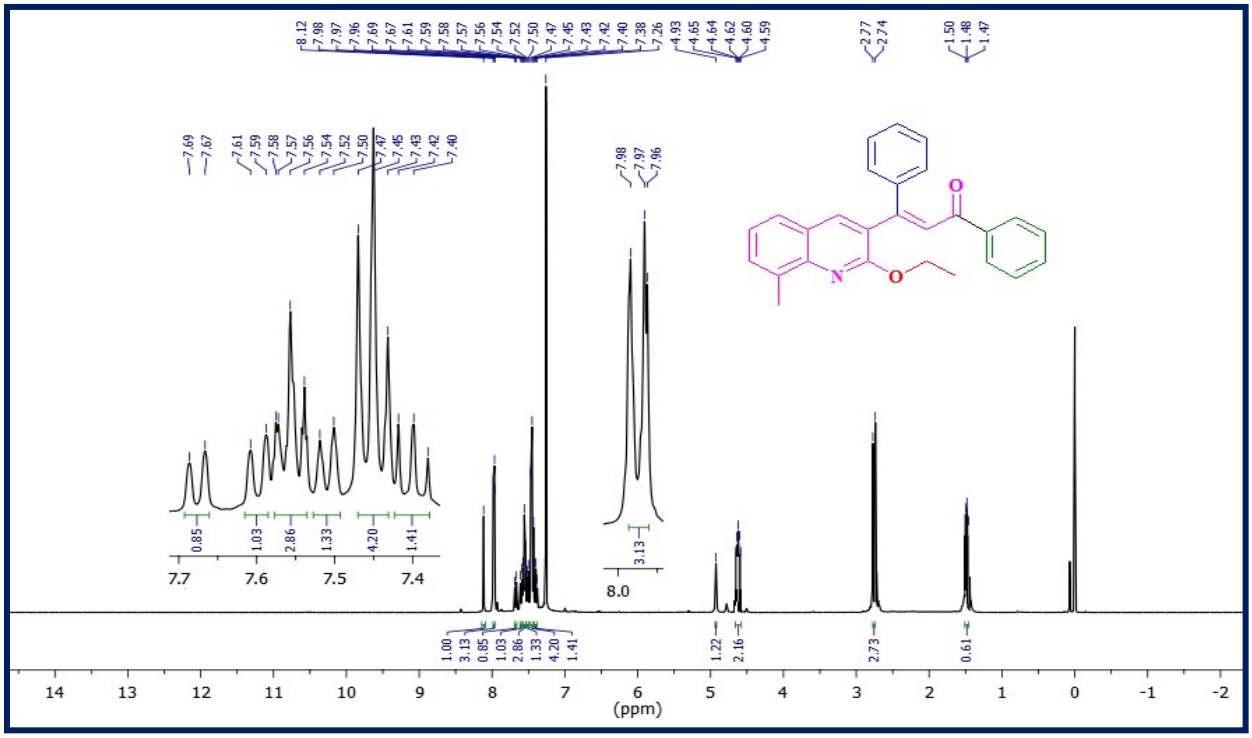

Fig. S15. ^{1}H NMR spectrum of **A8**

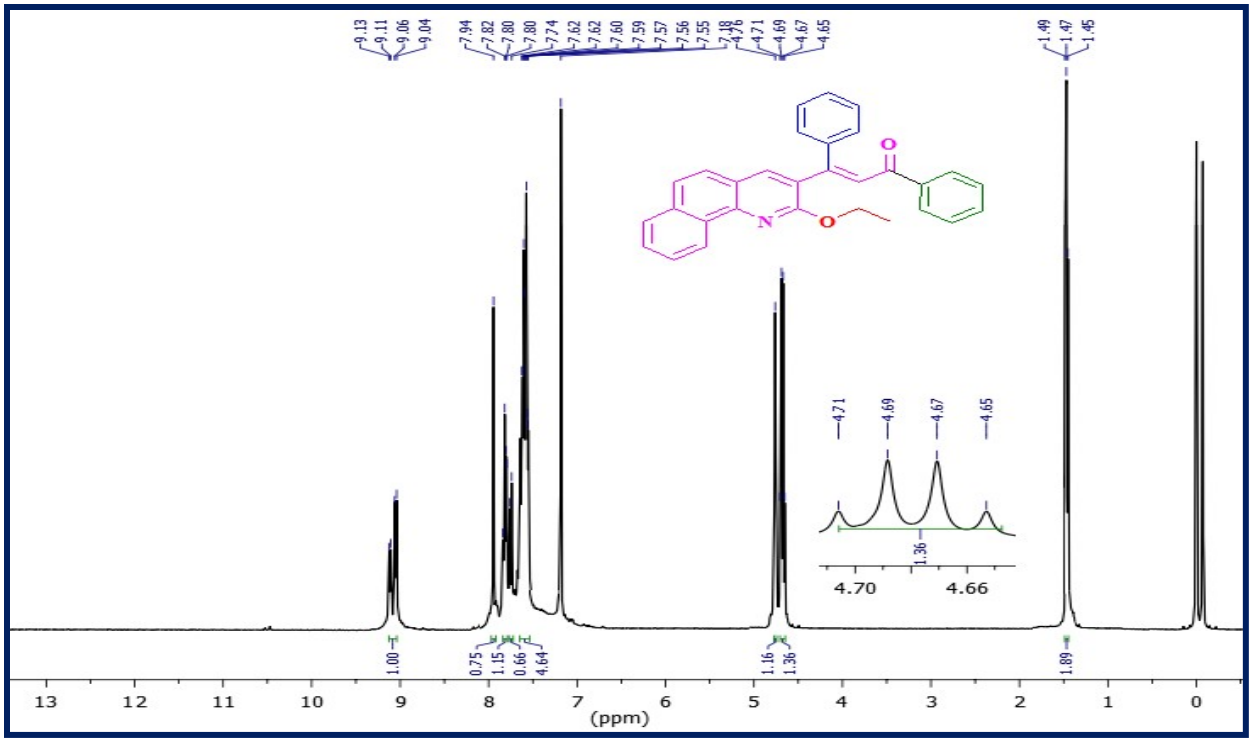

Fig. S16. [1]H NMR spectrum of **A9**

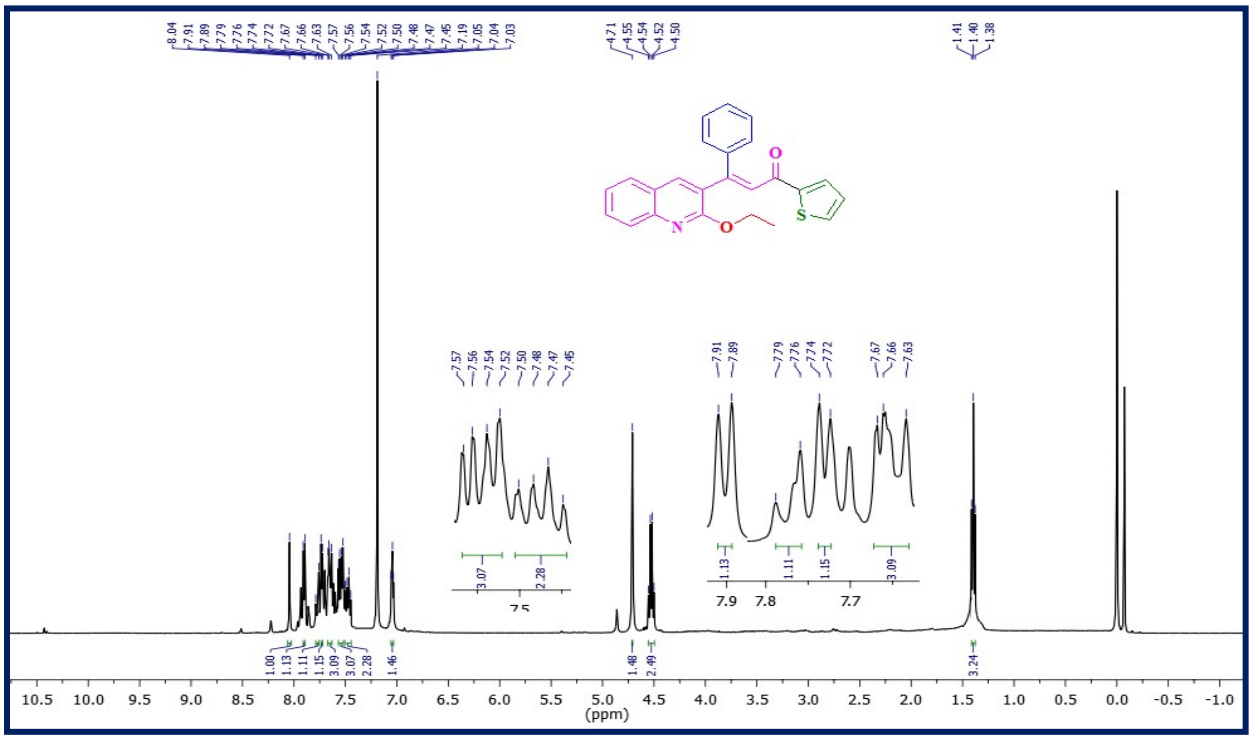

Fig. S17. [1]H NMR spectrum of **A10**

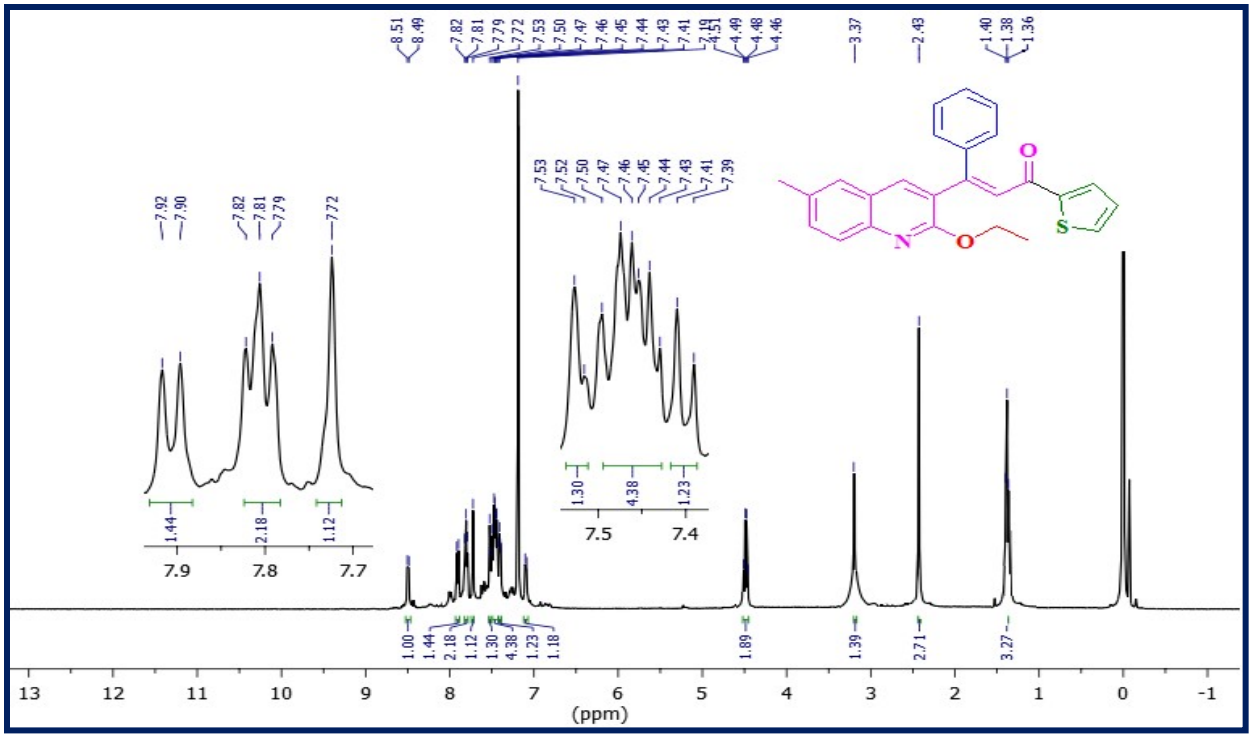

Fig. S18. ^{1}H NMR spectrum of **A11**

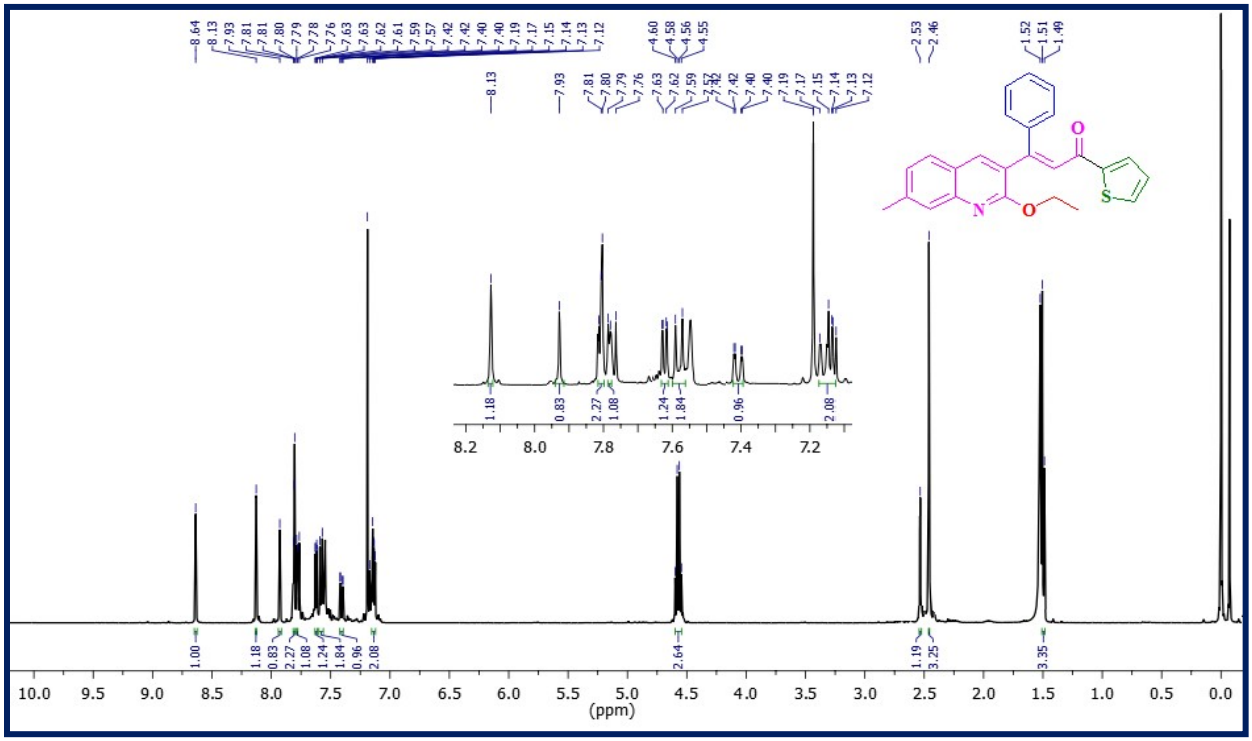

Fig. S19. ^{1}H NMR spectrum of **A12**

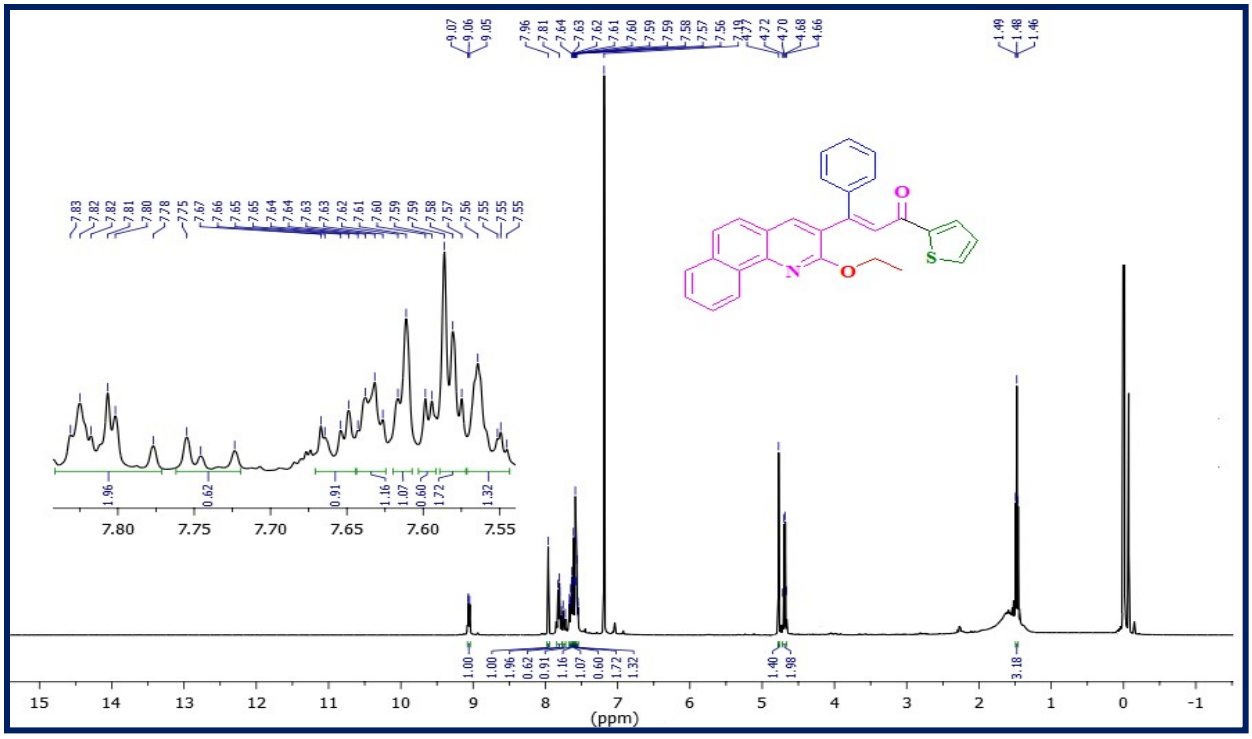

Fig. S20. ^{1}H NMR spectrum of **A13**

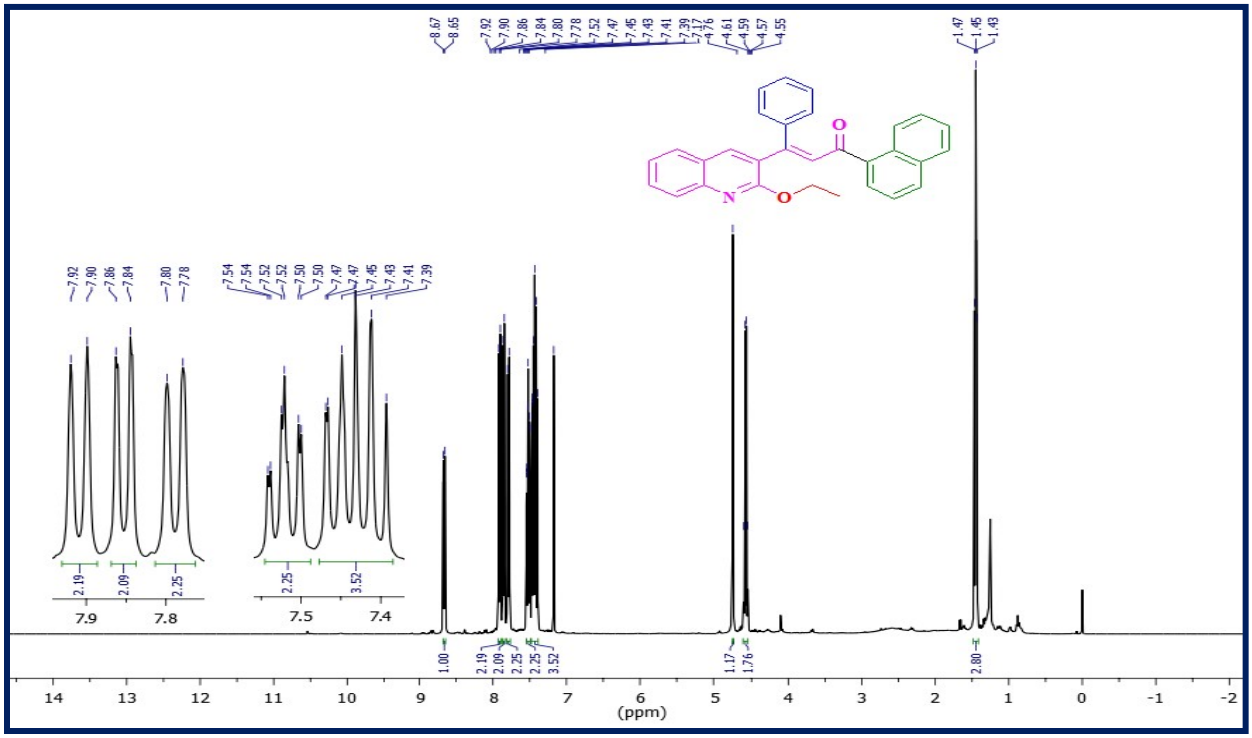

Fig. S21. ^{1}H NMR spectrum of **A14**

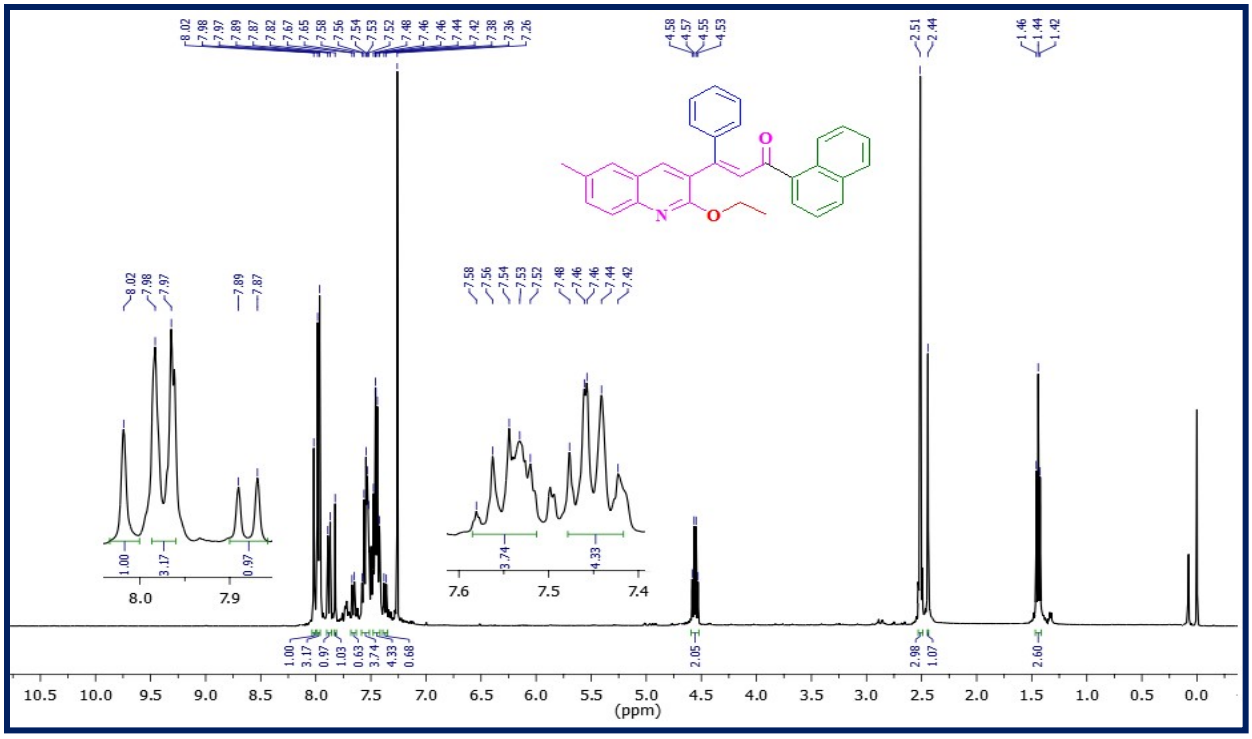

Fig. S22. ^{1}H NMR spectrum of **A15**

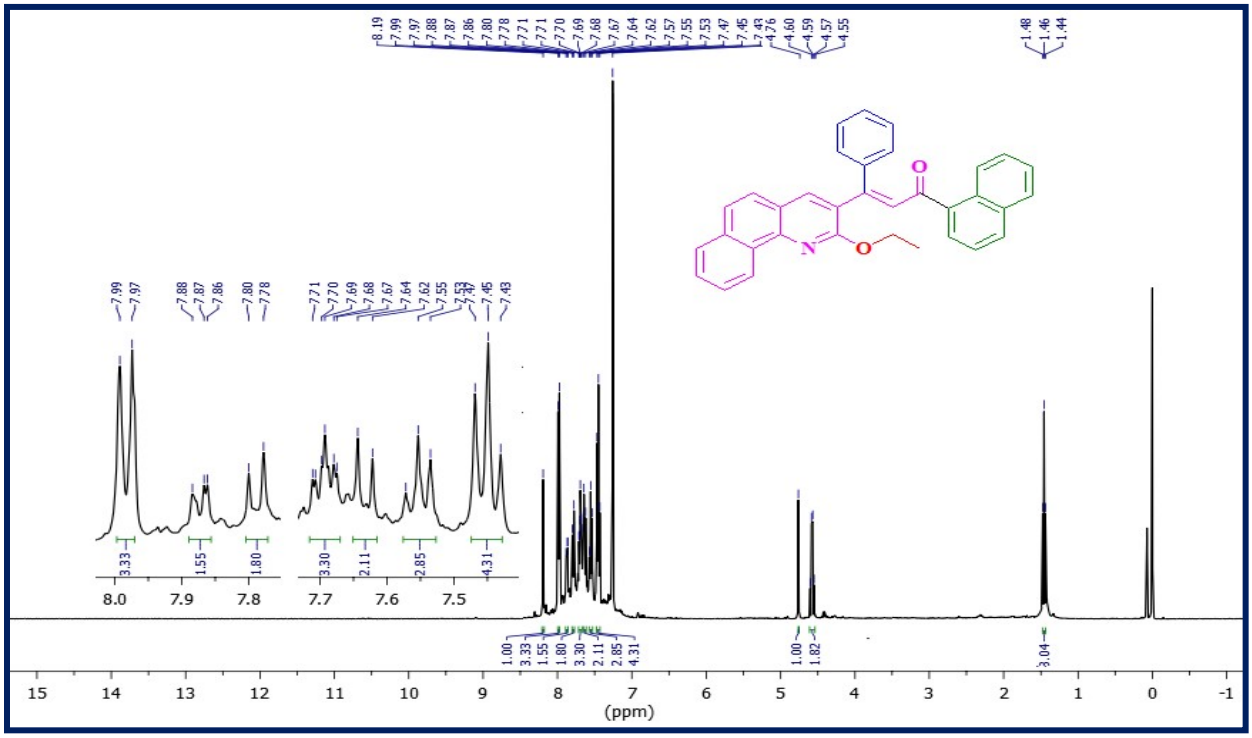

Fig. S23. ^{1}H NMR spectrum of **A16**

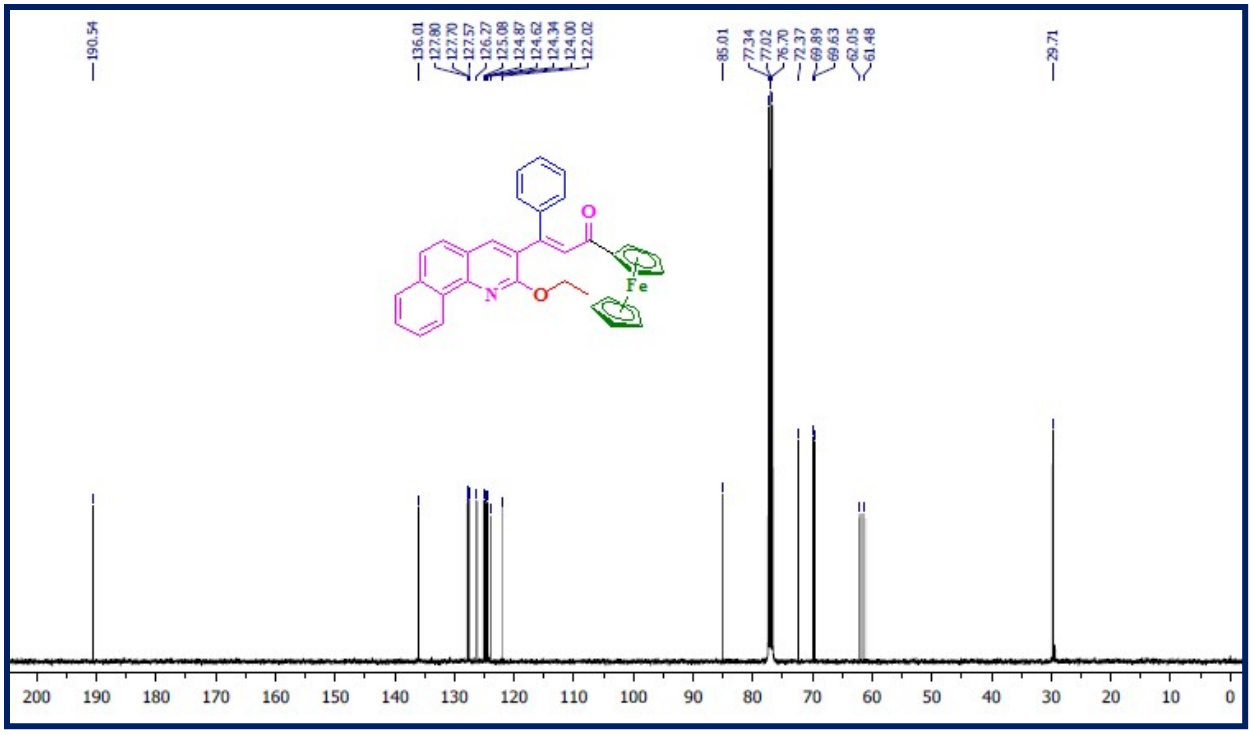

Fig. S24. ^{13}C NMR spectrum of **A1**

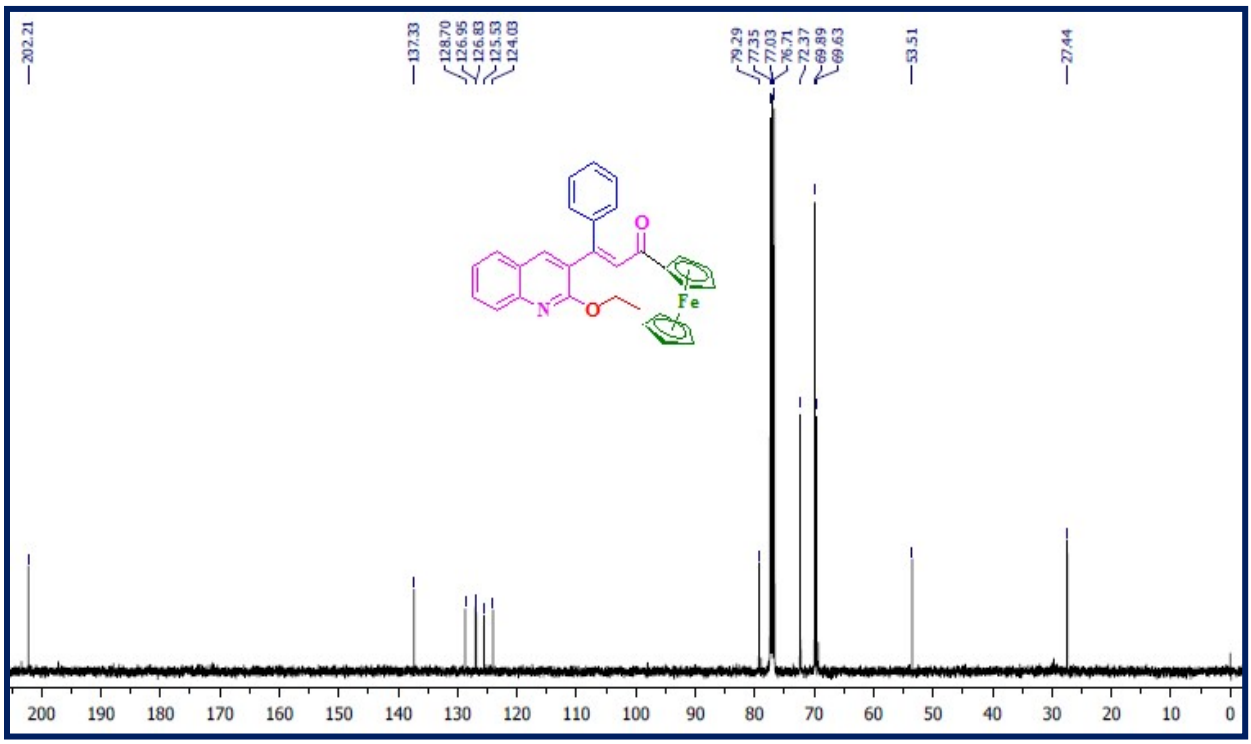

Fig. S25. ^{13}C NMR spectrum of **A2**

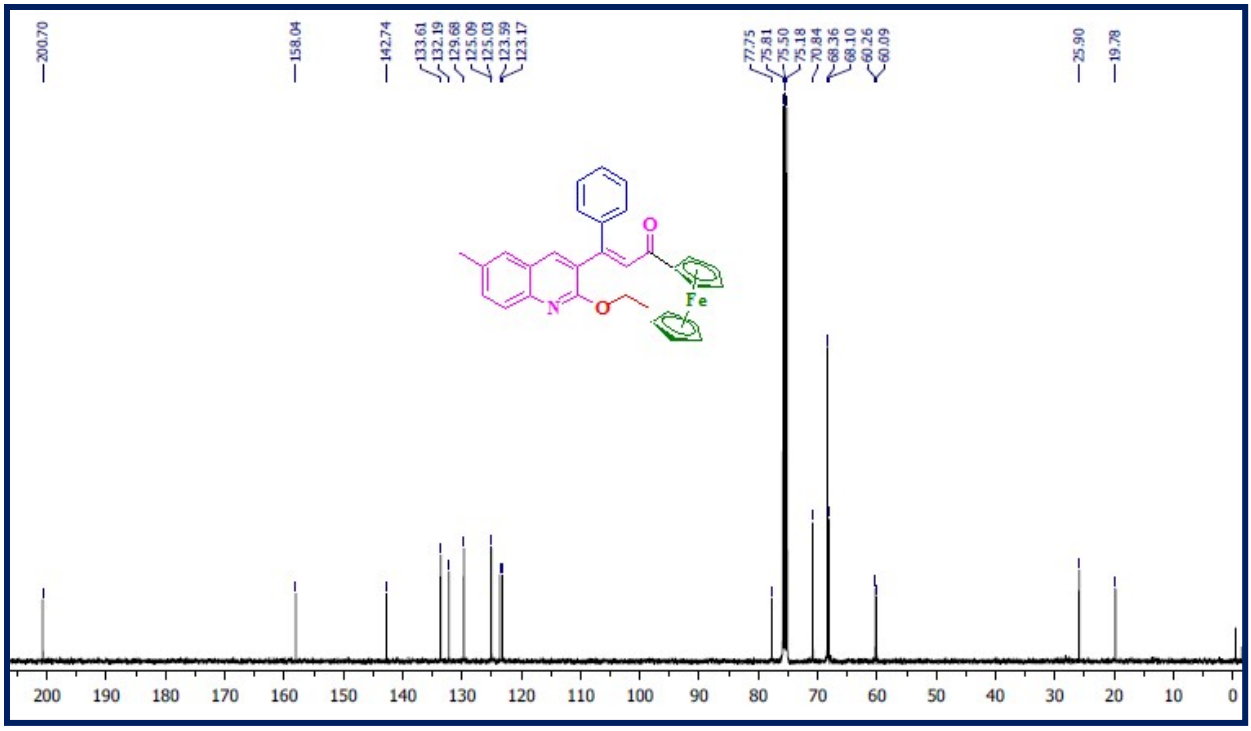

Fig. S26. ^{13}C NMR spectrum of **A3**

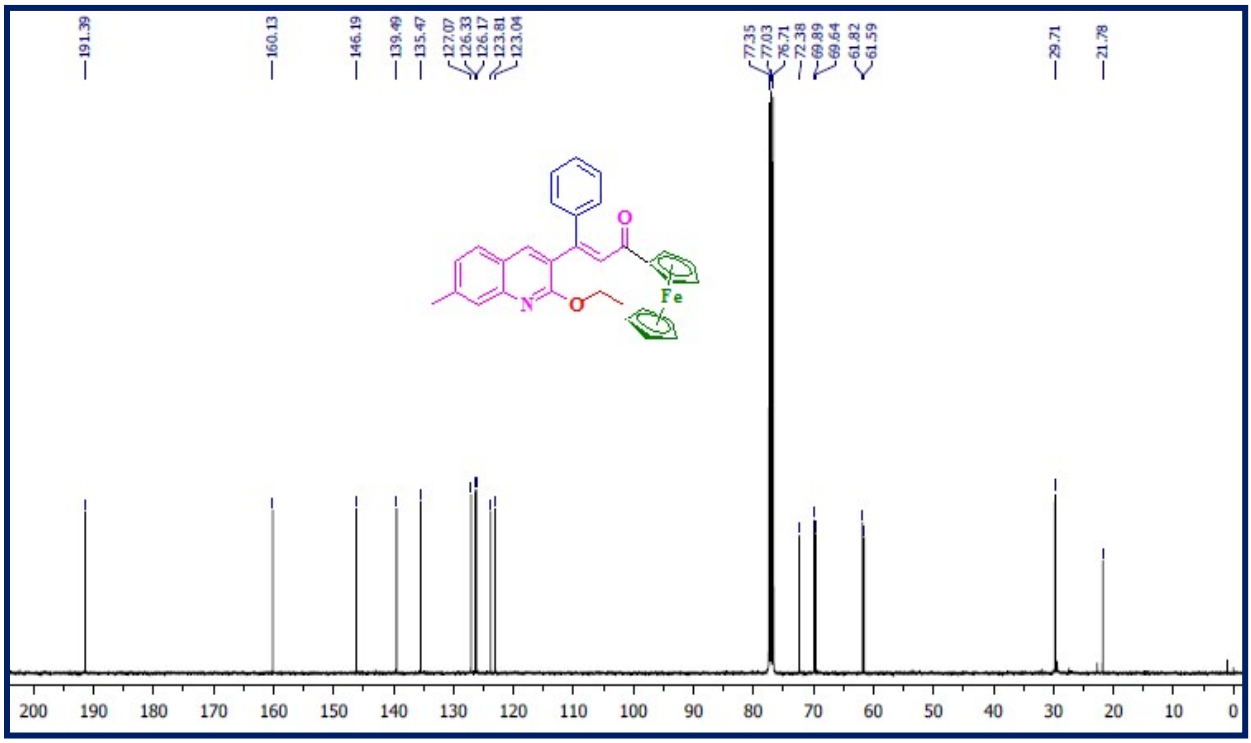

Fig. S27. ^{13}C NMR spectrum of **A4**

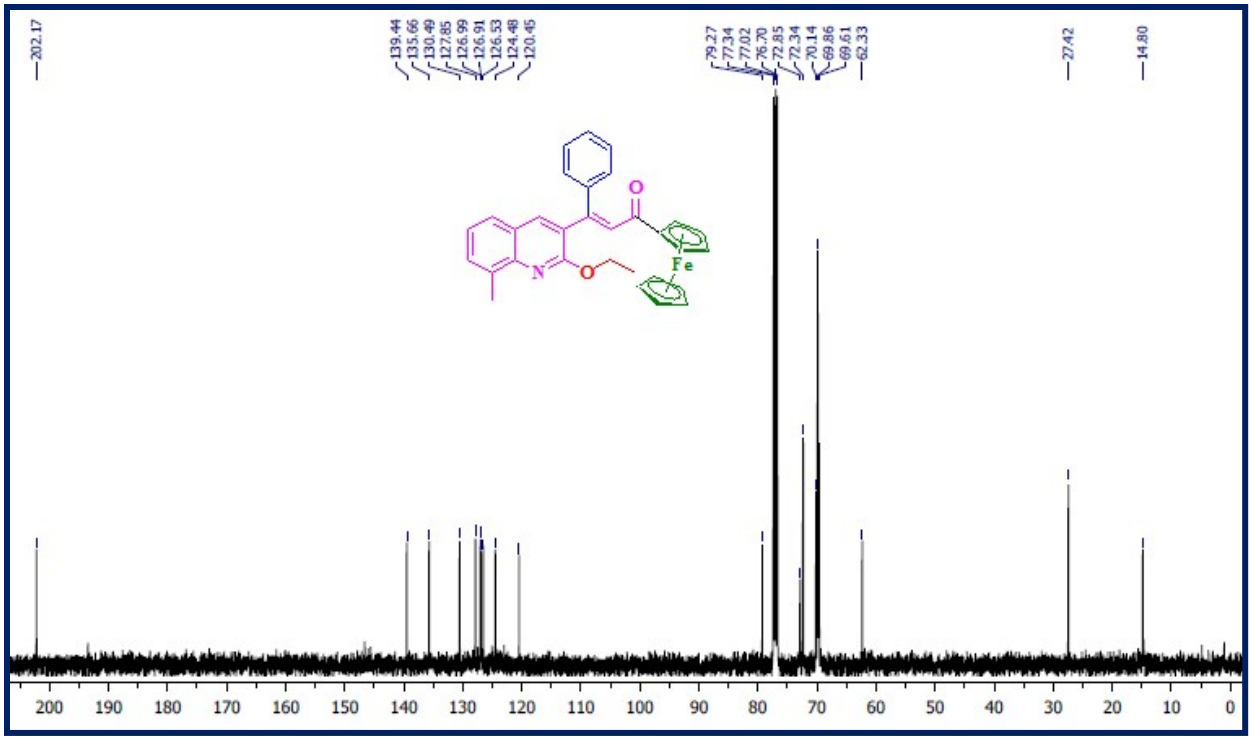

Fig. S28. ^{13}C NMR spectrum of **A5**

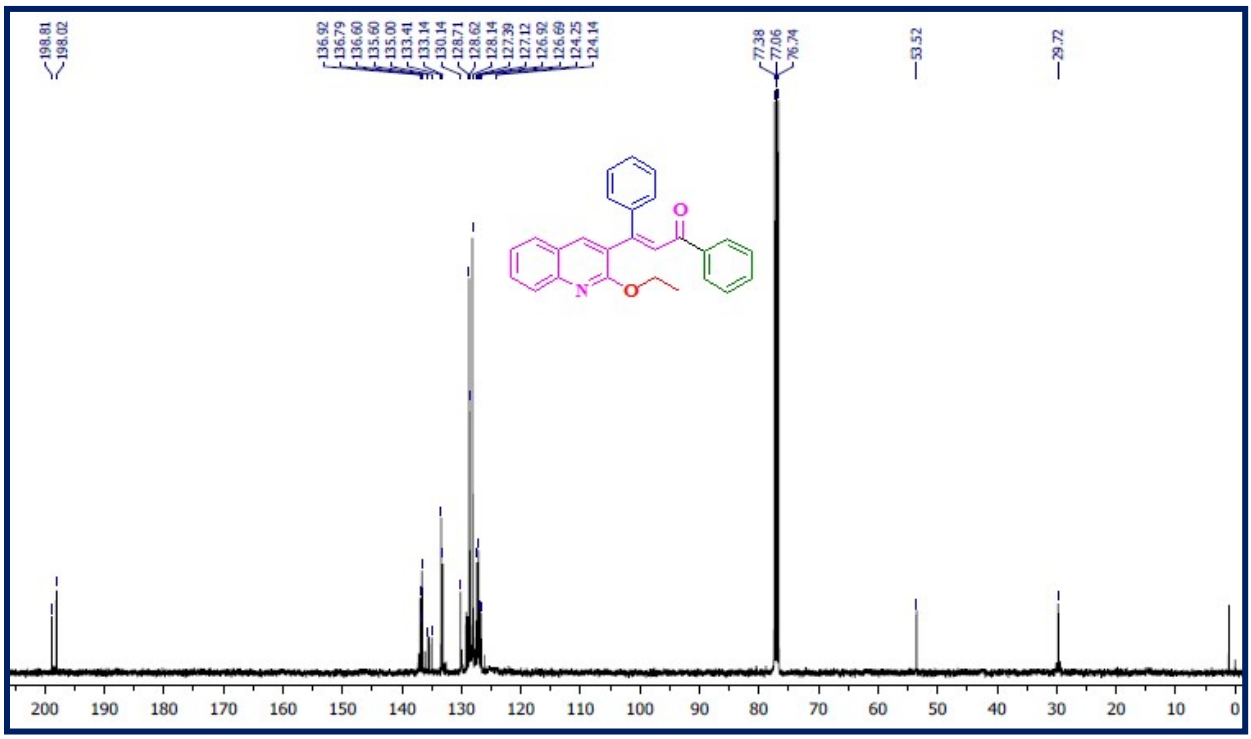

Fig. S29. ^{13}C NMR spectrum of **A6**

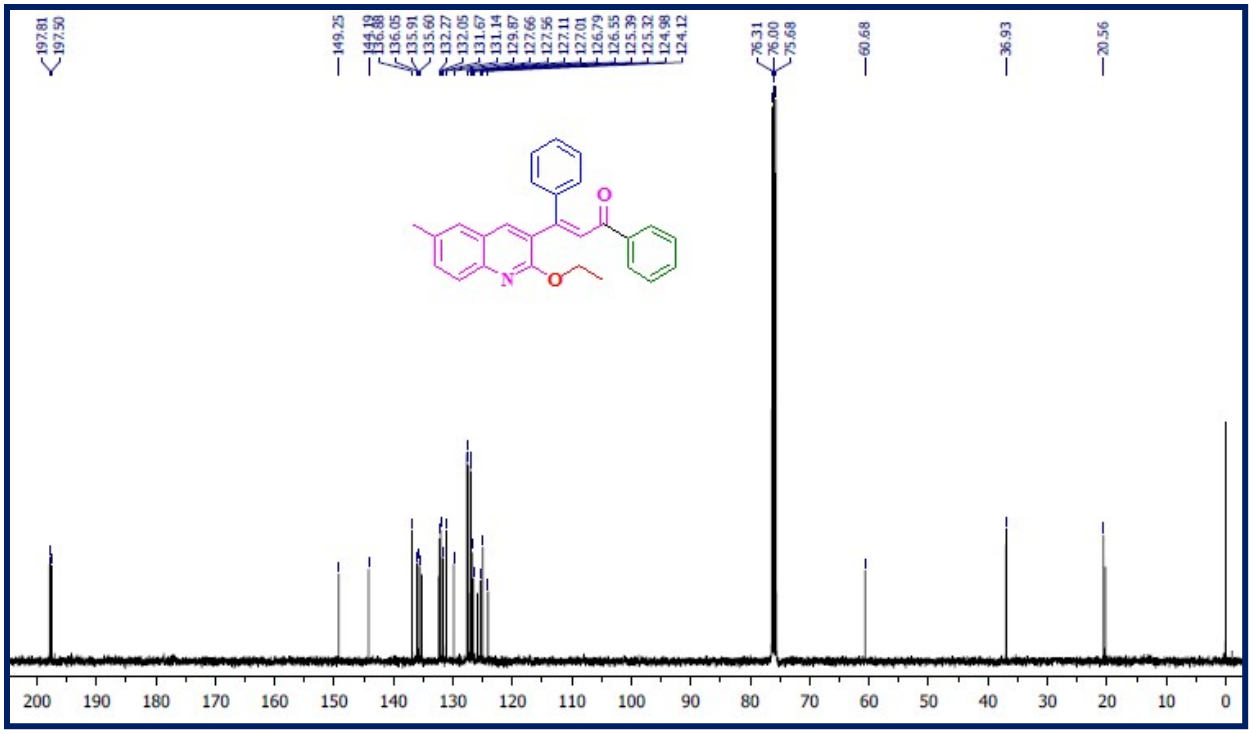

Fig. S30. ^{13}C NMR spectrum of **A7**

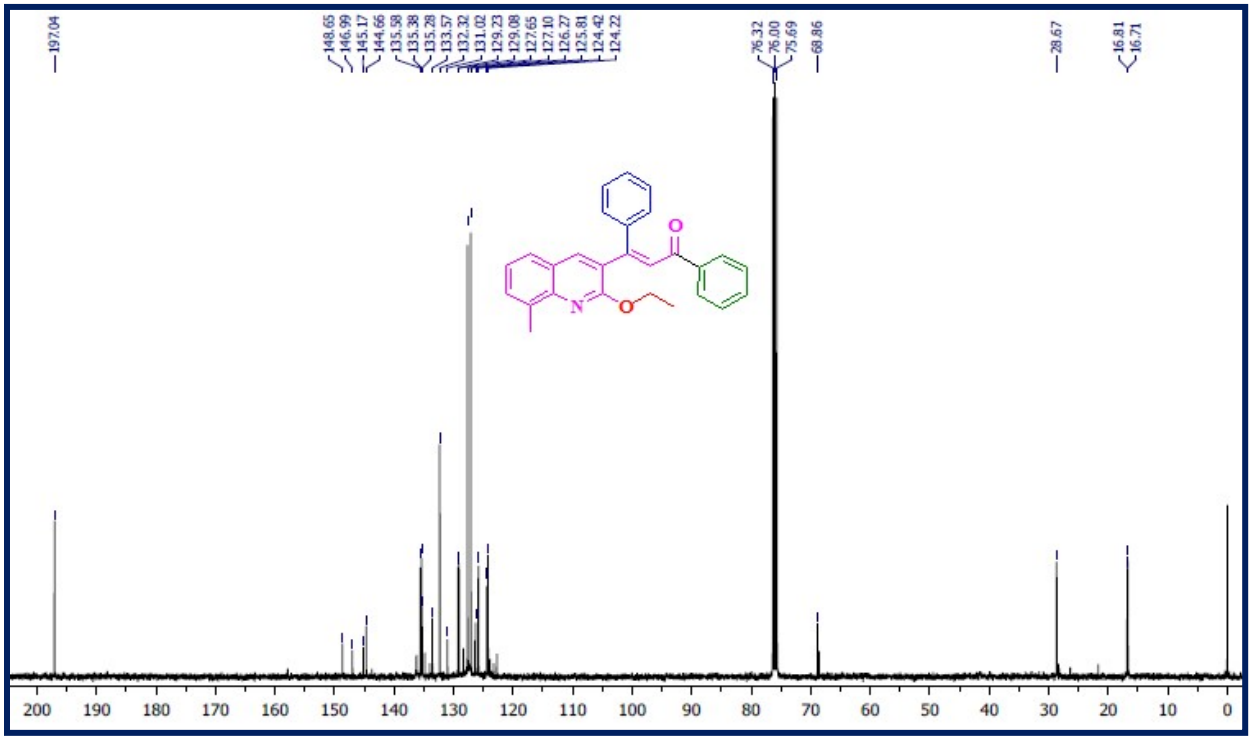

Fig. S31. ^{13}C NMR spectrum of **A8**

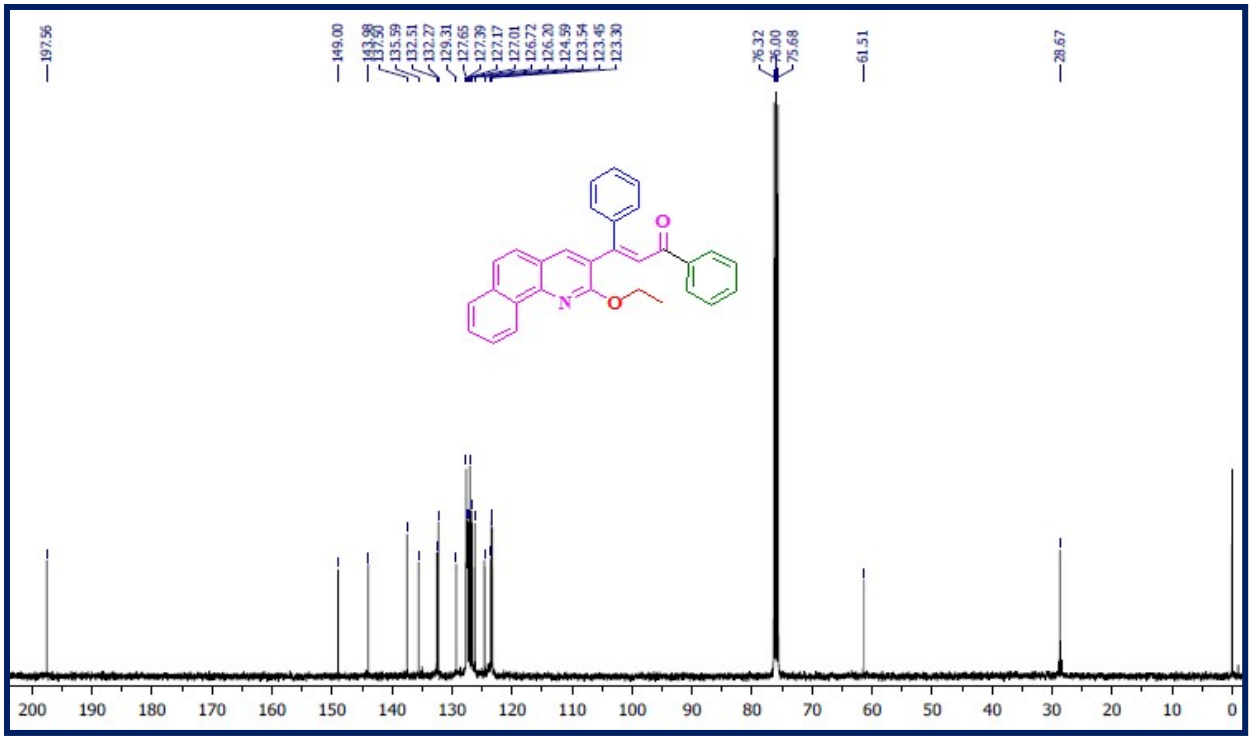

Fig. S32. ^{13}C NMR spectrum of **A9**

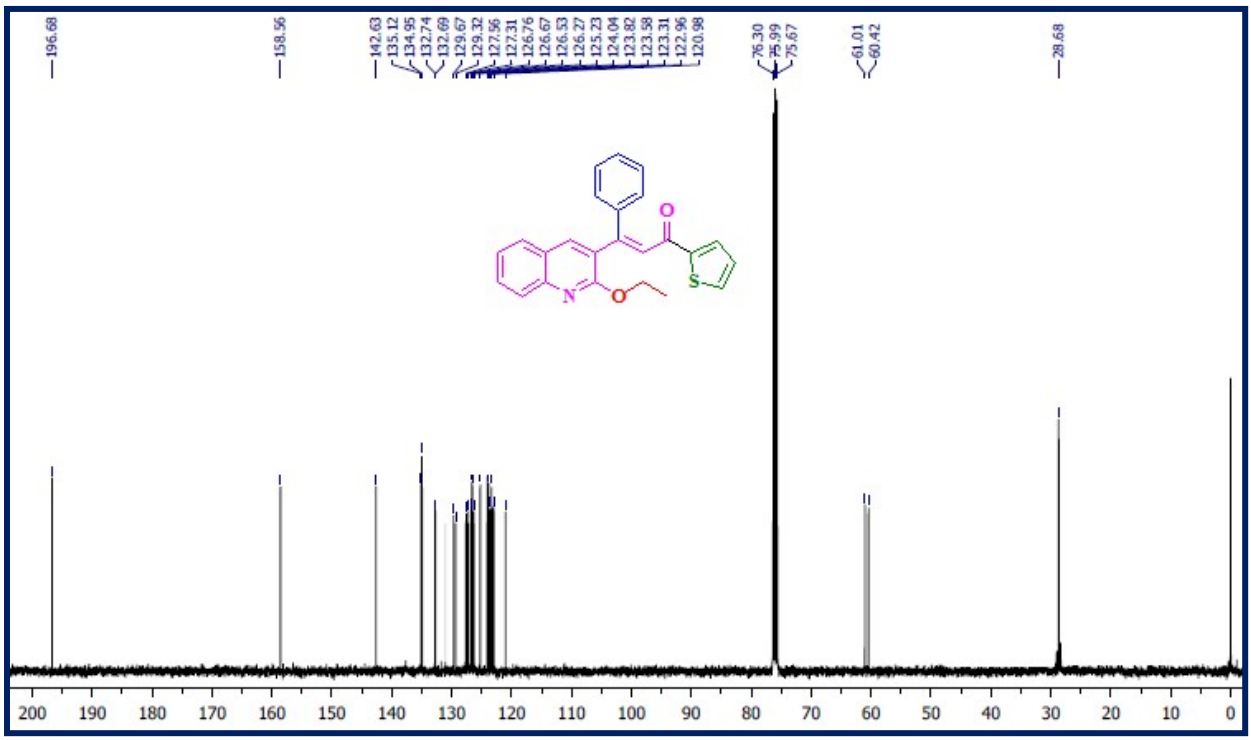

Fig. S33. ^{13}C NMR spectrum of **A10**

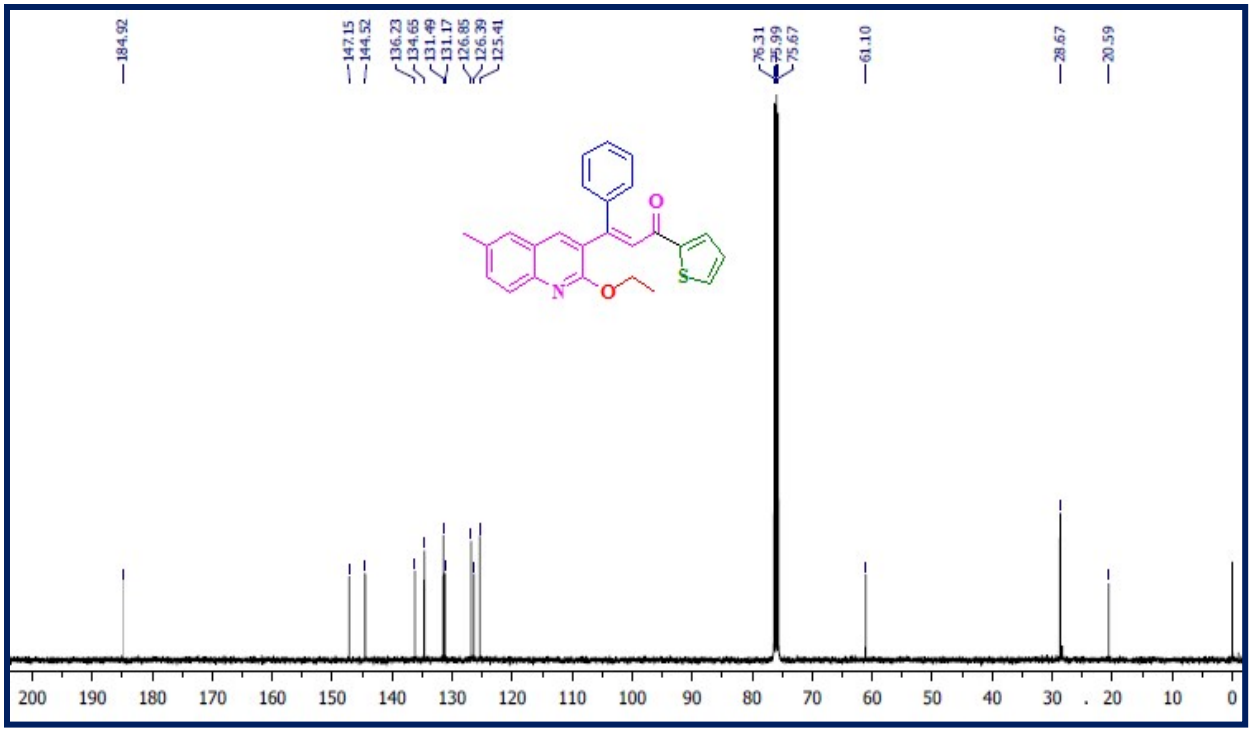

Fig. S34. ^{13}C NMR spectrum of **A11**

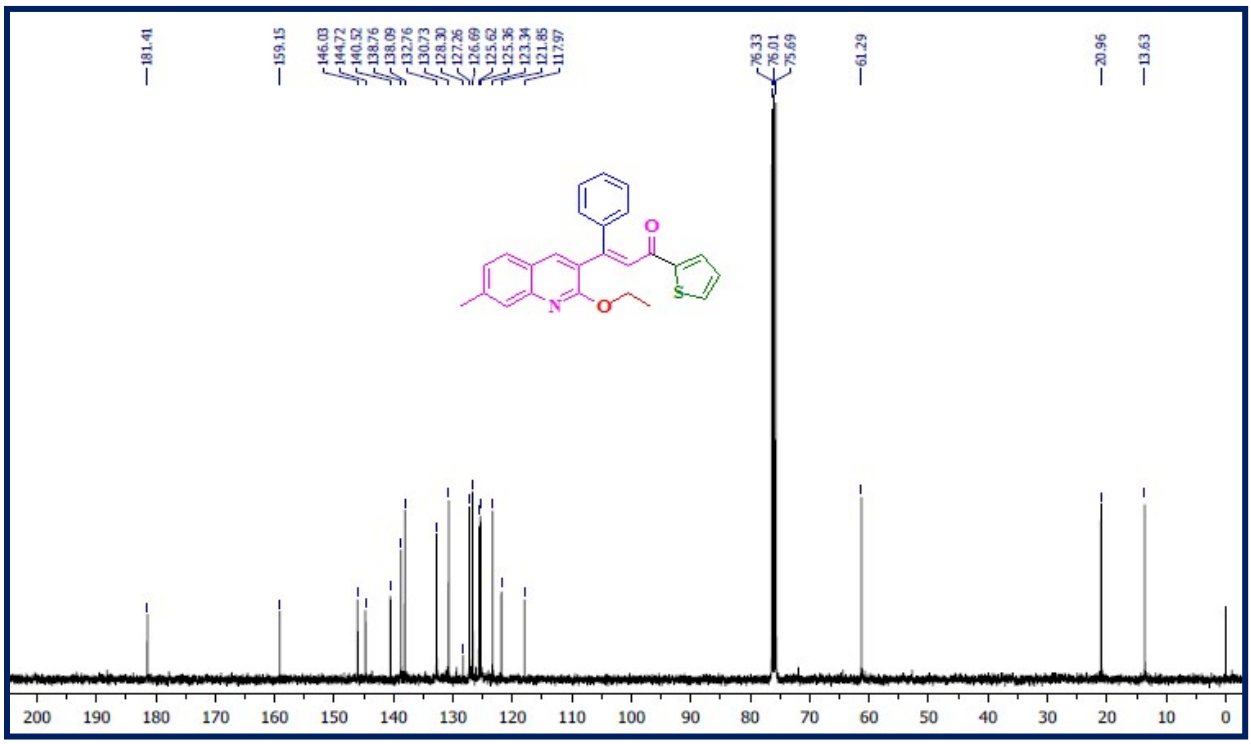

Fig. S35. ^{13}C NMR spectrum of **A12**

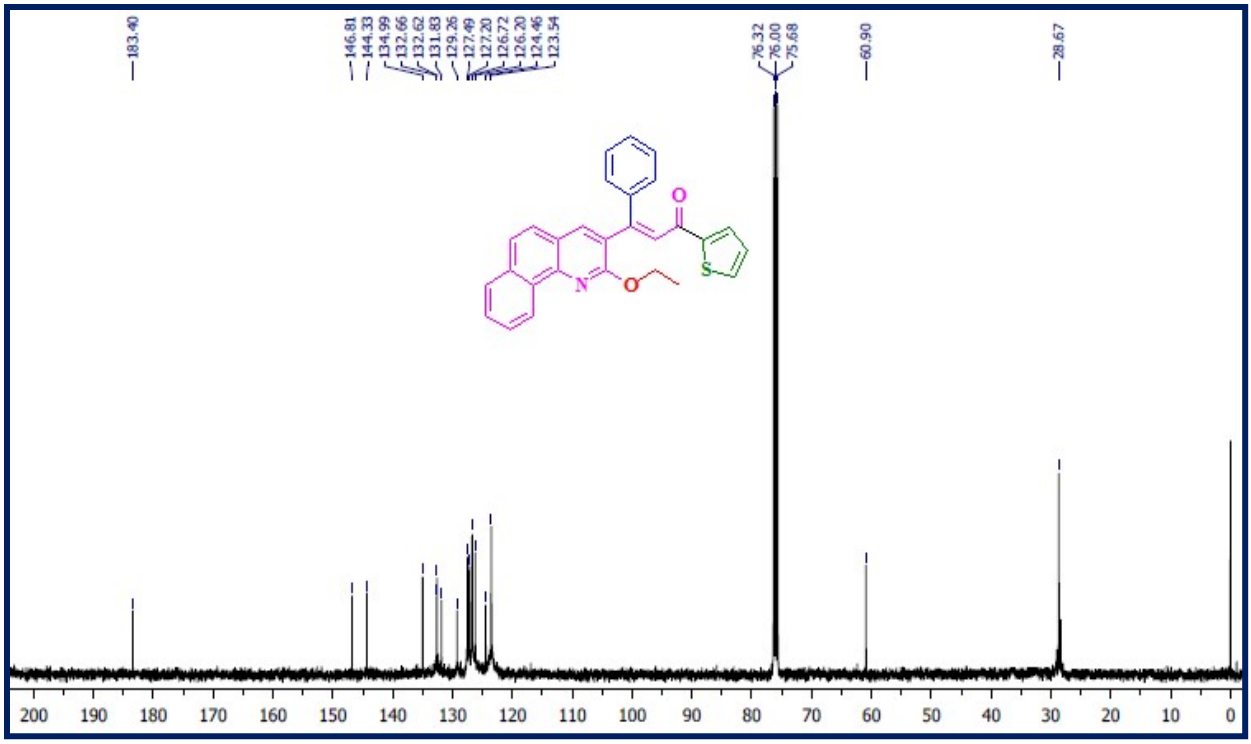

Fig. S36. ^{13}C NMR spectrum of **A13**

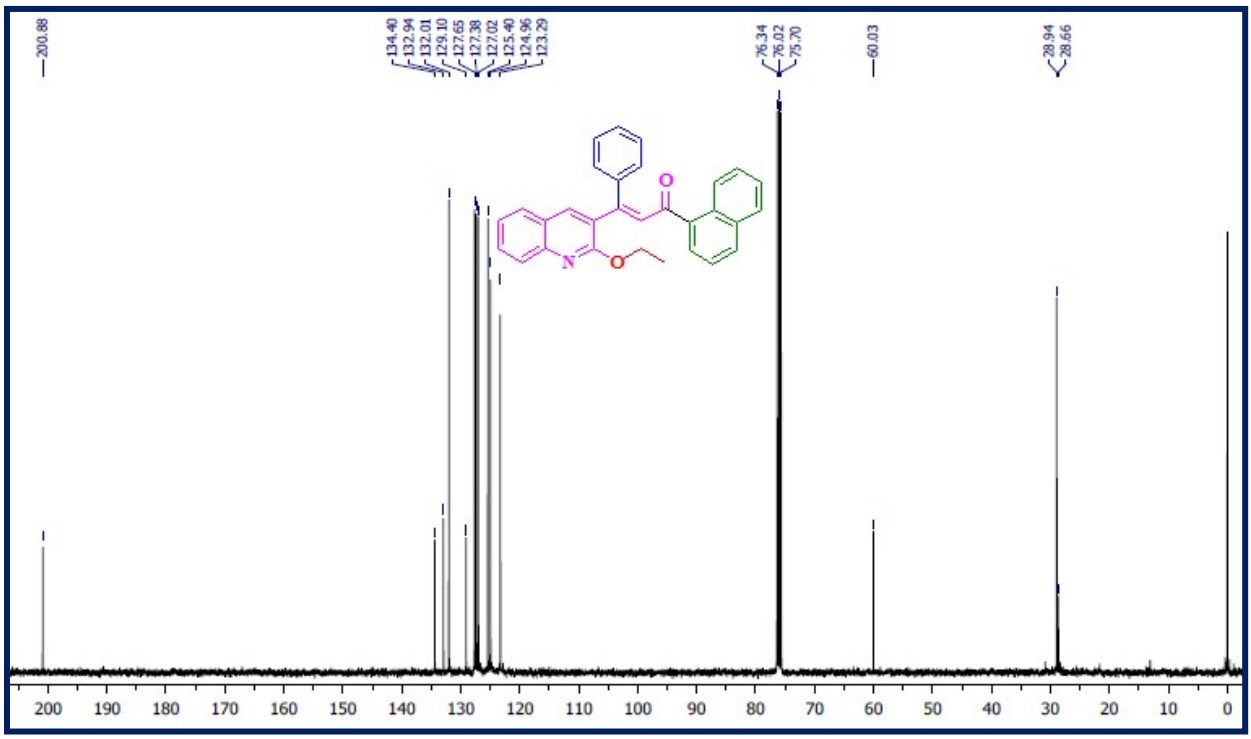

Fig. S37. ^{13}C NMR spectrum of **A14**

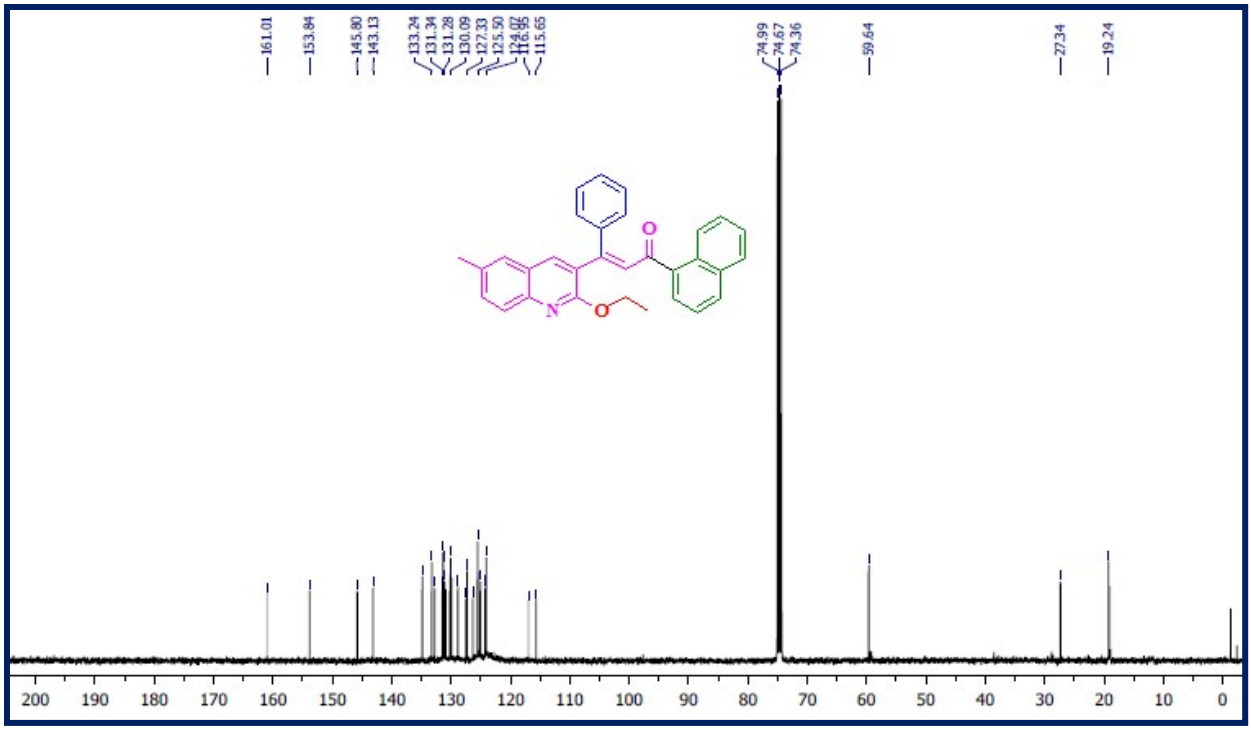

Fig. S38. ^{13}C NMR spectrum of **A15**

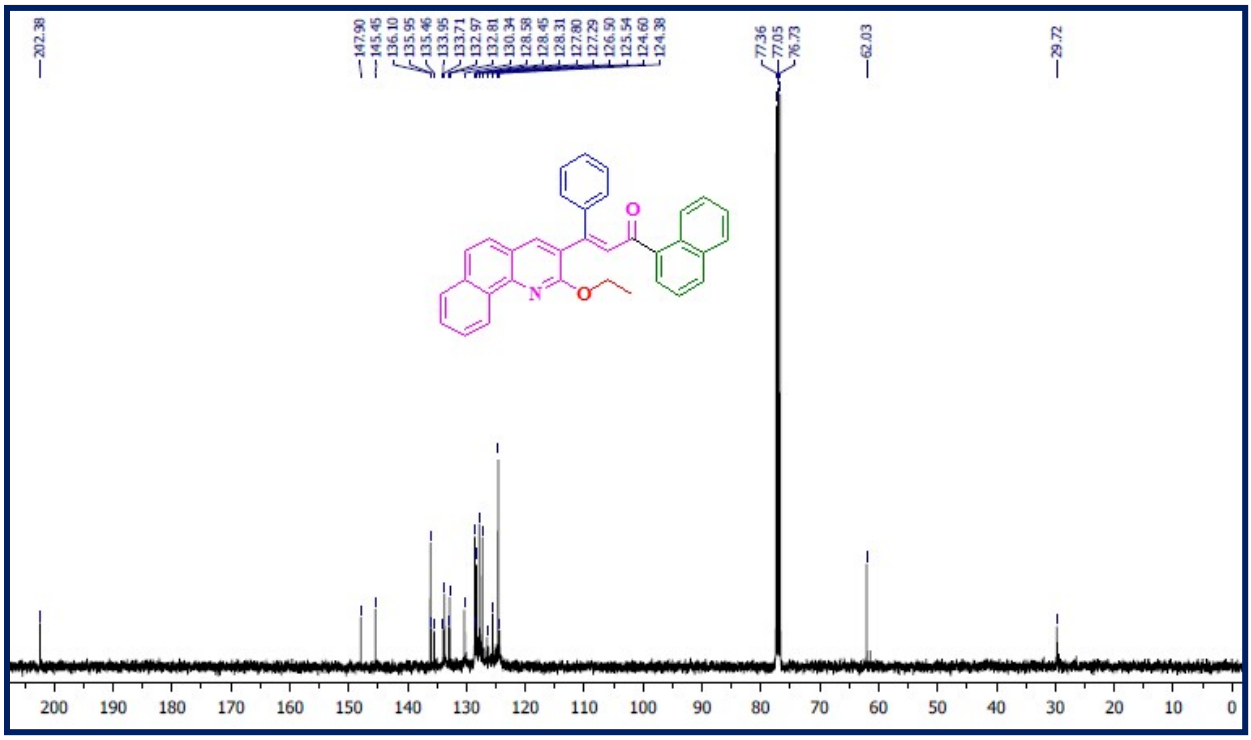

Fig. S39. ^{13}C NMR spectrum of **A16**

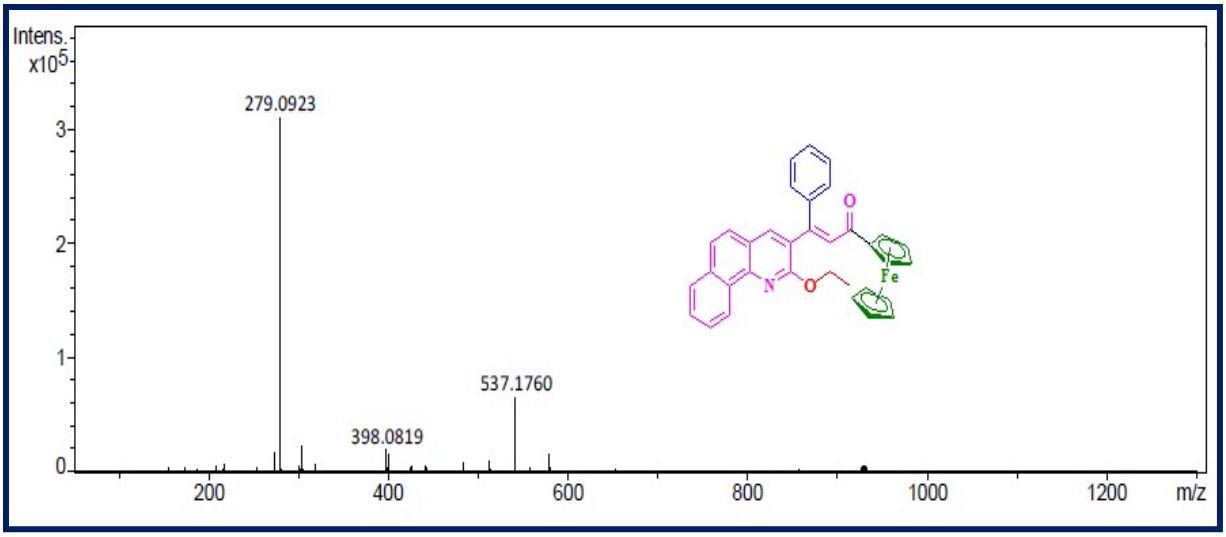

Fig. S40. Mass spectrum of **A1**

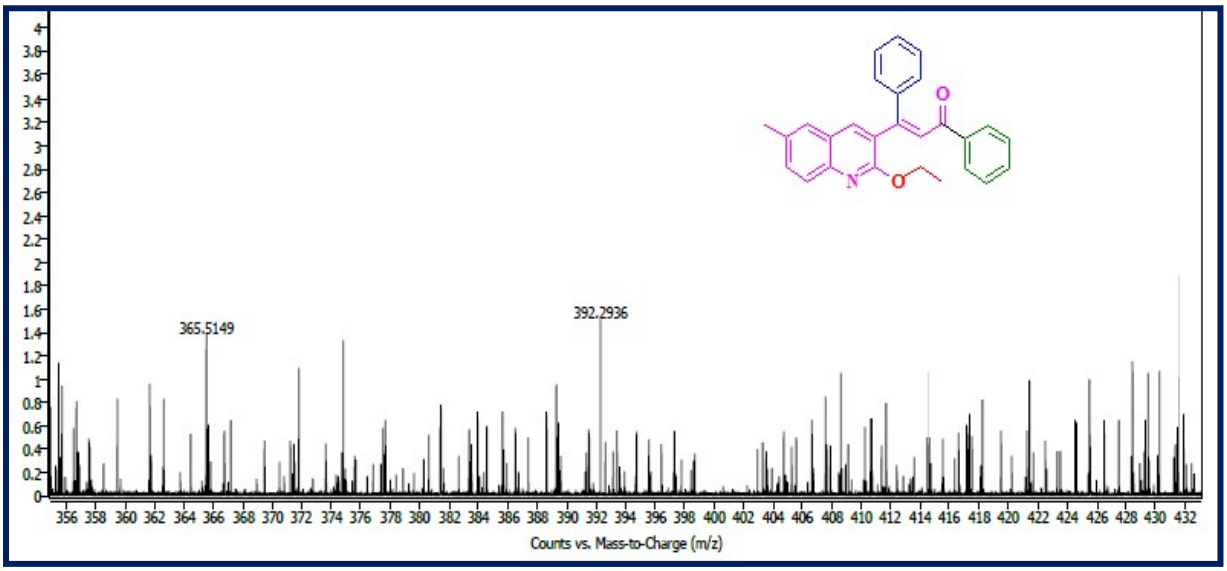

Fig. S41. Mass spectrum of **A7**

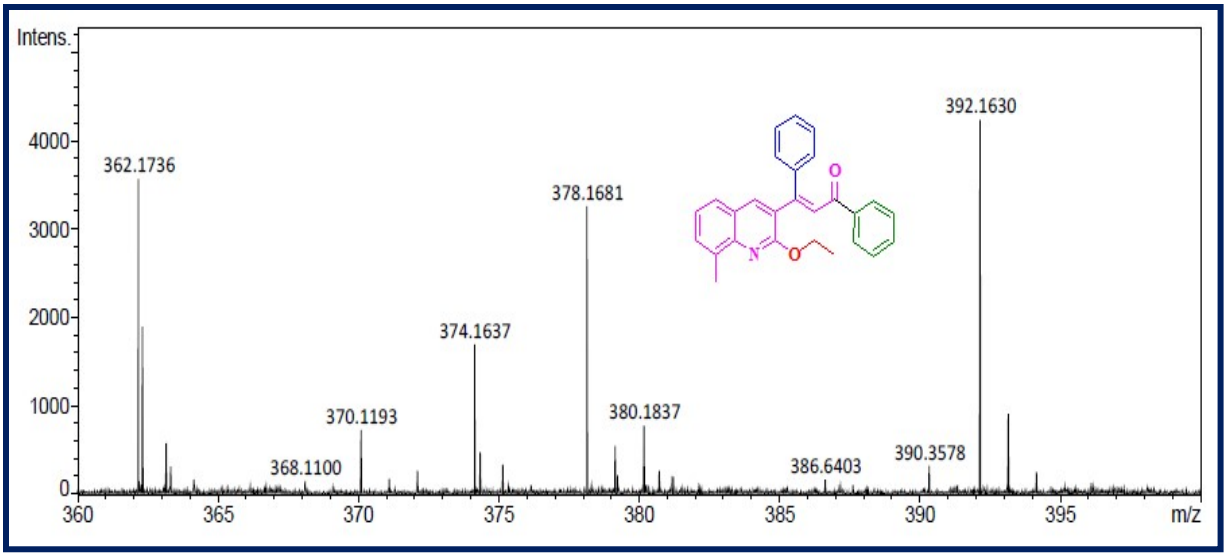

Fig. S42. Mass spectrum of **A8**

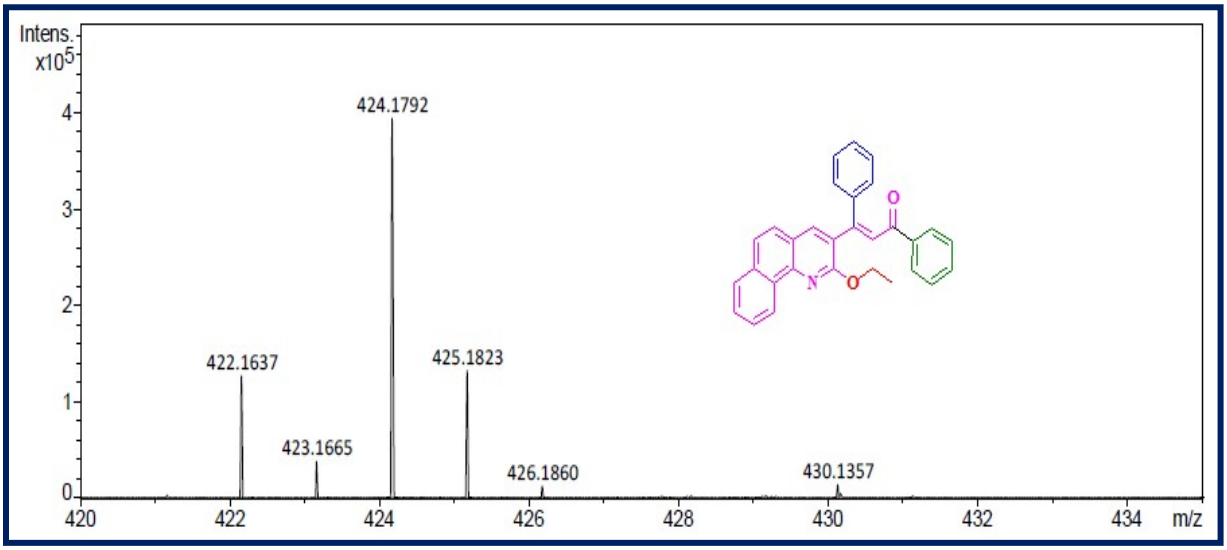

Fig. S43. Mass spectrum of **A9**

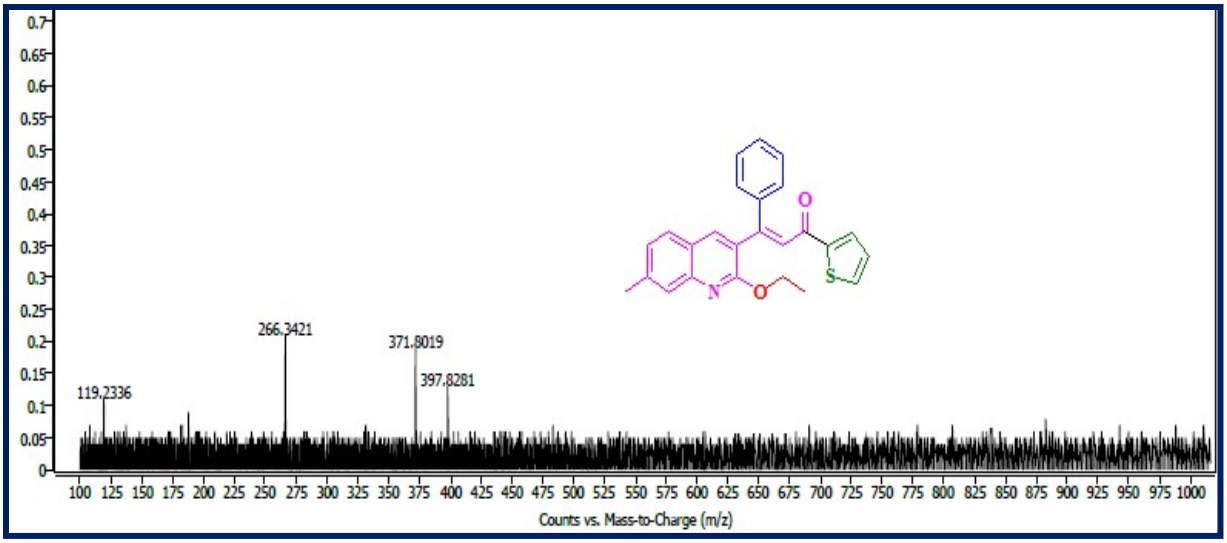

Fig. S44. Mass spectrum of **A12**

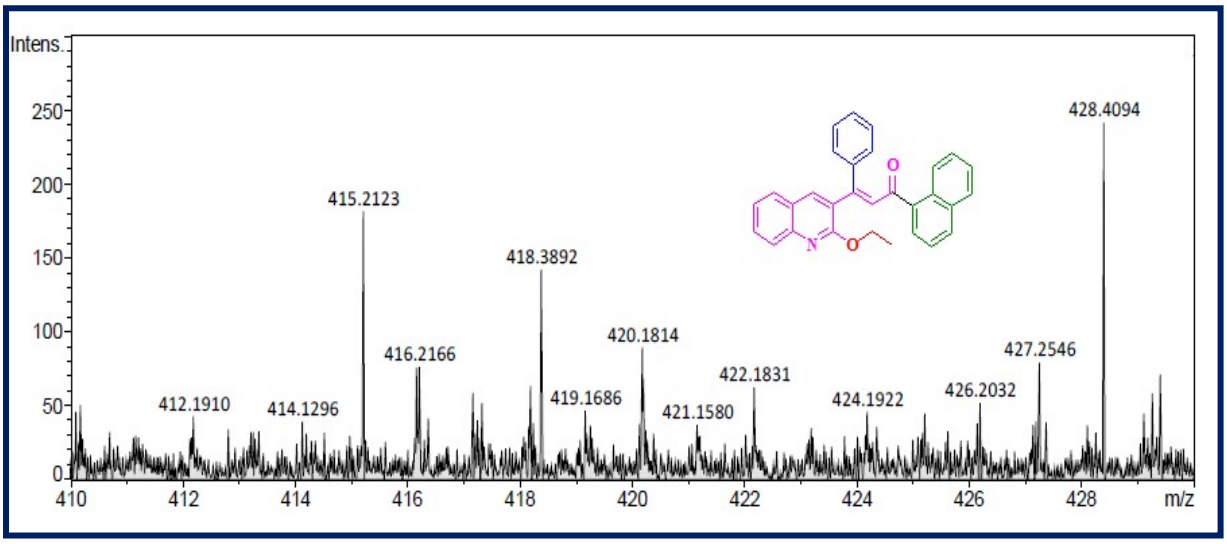

Fig. S45. Mass spectrum of **A14**

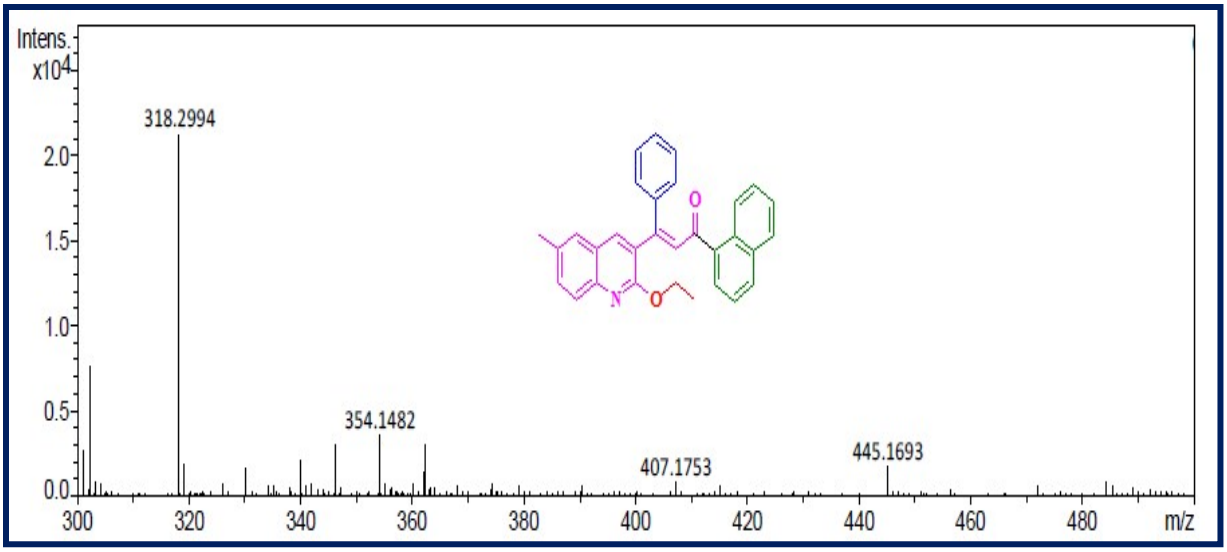

Fig. S46. Mass spectrum of **A15**

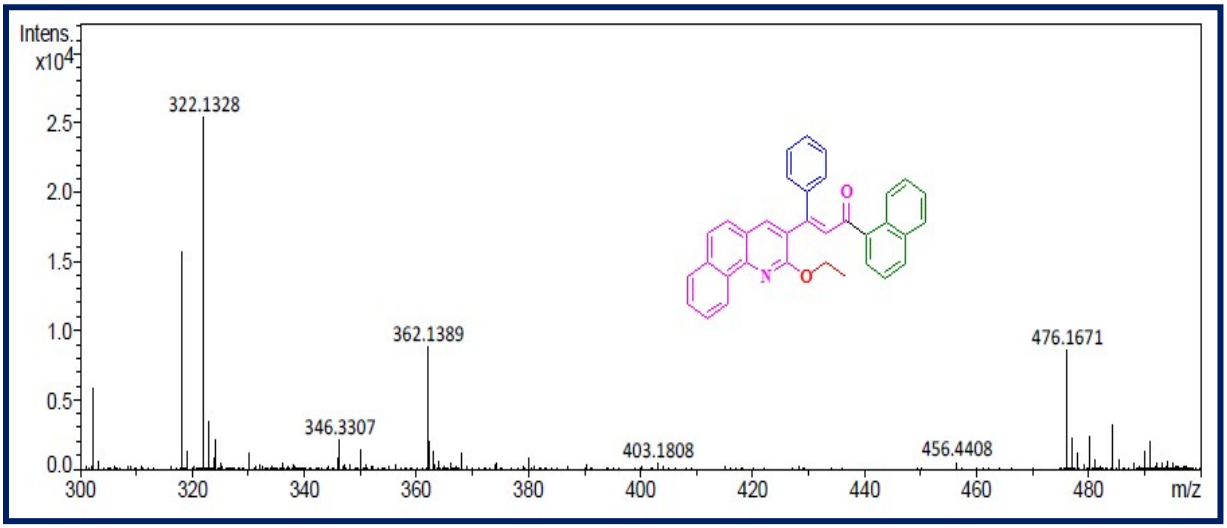

Fig. S47. Mass spectrum of **A16**

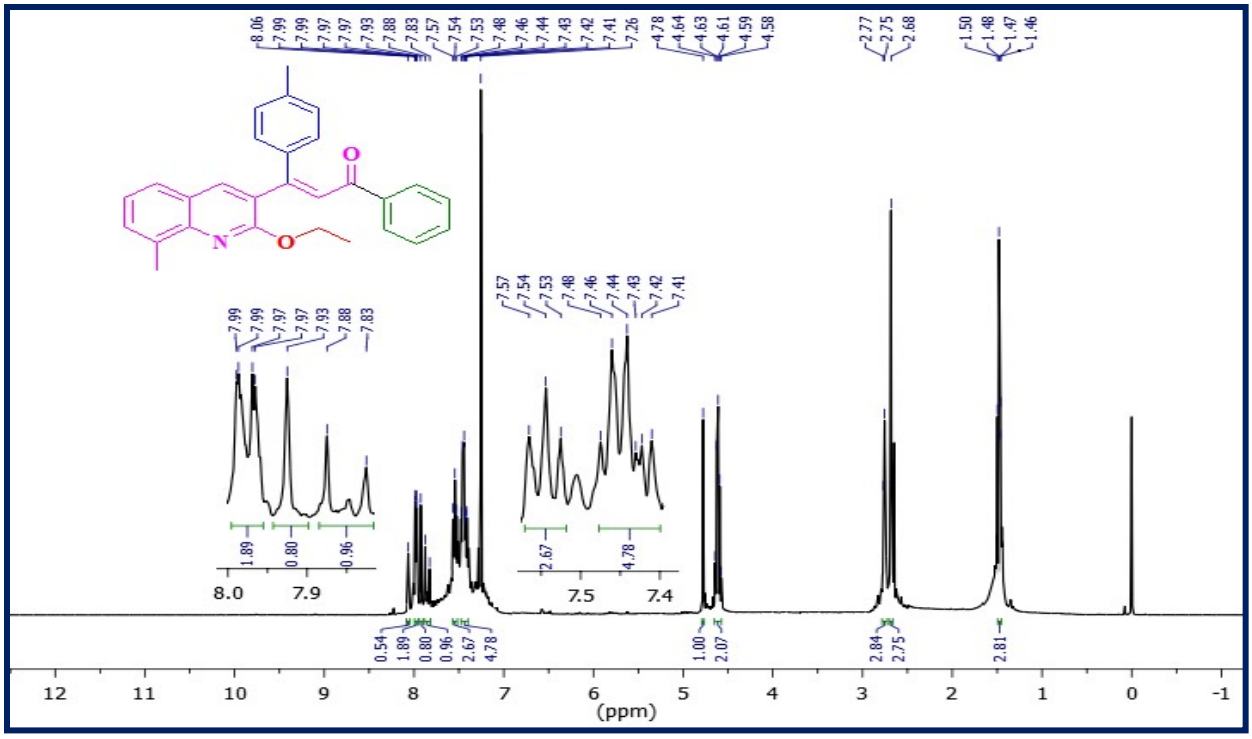

Fig. S48. [1]H NMR spectrum of **A17**

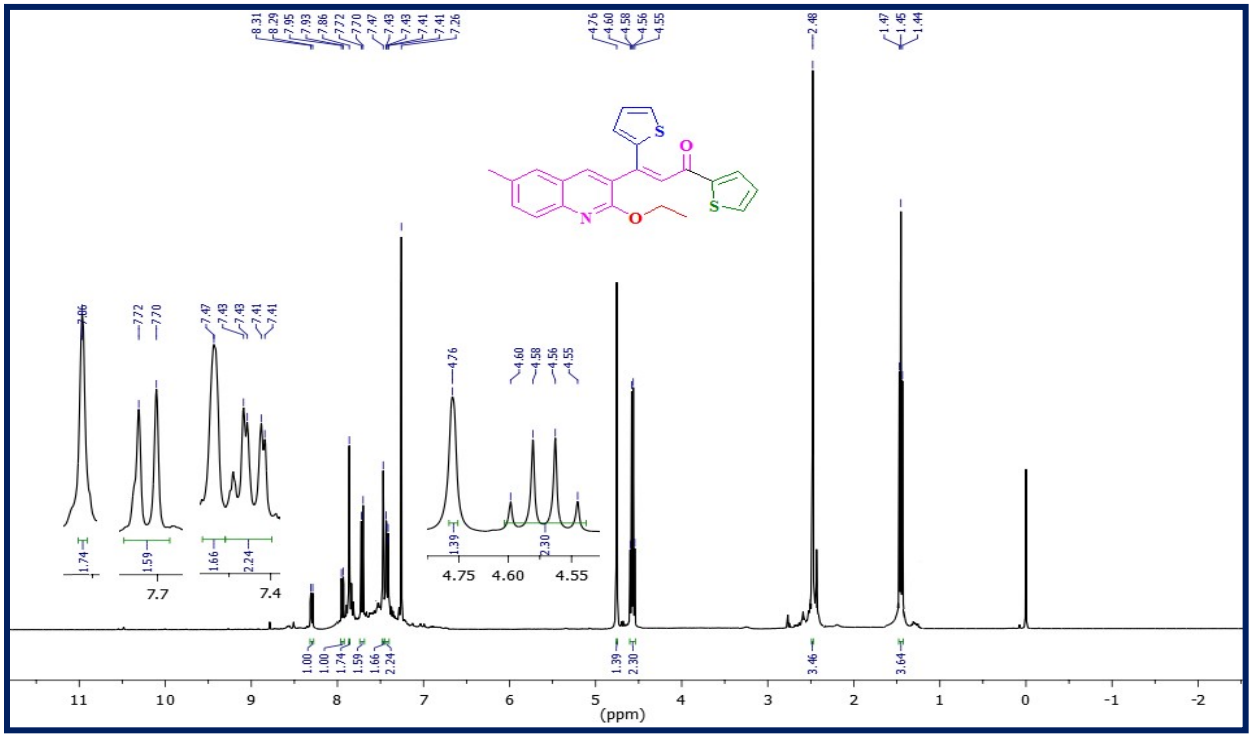

Fig. S49. [1]H NMR spectrum of **A18**

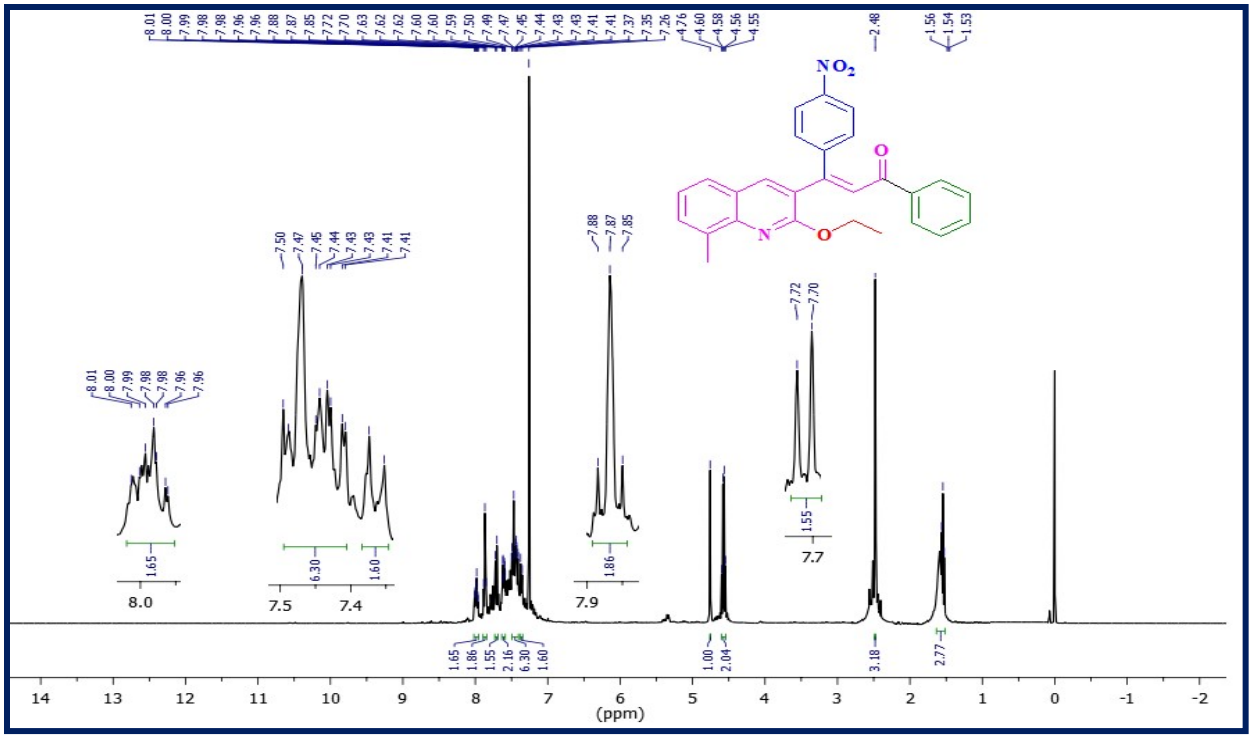

Fig. S50. ^{1}H NMR spectrum of **A19**

Table S1. EPR spectral data of the complexes

Complex	$g_{\parallel}$	$g_{\perp}$	g_{av}
6A	2.644	2.131	2.302
6B	2.181	1.996	2.057

$g_{av} = (g_{\parallel}+2xg_{\perp})/3$

Table S2. Hydrogen bonds for the ligand **HL²** and the Ru(III) complexes **RuL¹** and **RuL²** [Å and °]

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
HL²				
N(3)-H(3)...O(1)	0.879	1.888	2.623	139.90
O(2)-H(23)...O(1)	0.805	1.857	2.657	172.11
N(2)- H(21)...O(2)	0.858	2.017	2.817	154.71
Symmetry operation: **(x, y, z); (1/2-x,-y,1/2+z); (-x,1/2+y,1/2-z); (1/2+x,1/2-y,-z); (-x,-y,-z); (1/2+x,y,1/2-z); (x,1/2-y,1/2+z); (1/2-x,1/2+y,z)**				
RuL¹				
N(3)-H(3)...O(1)	0.860	1.963	2.652	136.29
O(2)-H(2)...O(1)	1.002	1.853	2.805	157.51
Symmetry operation**: (x, y, z); (-x,-y,-z)**				
RuL²				
N(3)-H(3)...O(1)	0.880	2.001	2.680	132.98
O(2)-H(2)...O(1)	0.921	1.818	2.708	161.79
Symmetry operation**: (x, y, z); (-x,-y,-z)**				

Table S3. Crystallographic data of the isolated ethoxy intermediate of **A12**

	A12 ethoxy intermediate
Empirical formula	$C_{19}H_{14}NO_2S$
Formula weight	320.37
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	
a	8.757(3) Å
b	12.951(4) Å
c	15.309(5) Å
α	107.153(7) °
β	94.363(7) °
γ	94.516(7) °
Volume	1644.8(9)
Z	4
Density	1.294 Mg/m^3
Absorption coefficient	0.205 mm^{-1}
F(000)	668
θ range for data collection	2.47 to 27.21 °
Limiting indices	$-11 \leq h \leq 11$, $-16 \leq k \leq 16$, $-19 \leq l \leq 19$
Reflections collected	72175
Independent reflections	7318 [R(int) = 0.4964]
Absorption correction	Multi-scan
Refinement method	Full-matrix least-squares on F^2
Data/restraints/ parameters	7318/0/419
Goodness-of-fit on F^2	0.957
Final *R* indices [$I>2\sigma(I)$]	R1 = 0.1009, wR2 = 0.1901
R indices (all data)	R1 = 0.3167, wR2 = 0.2581

REFERENCES

S1. A. I. Vogel, Textbook of Practical Organic Chemistry, 5th ed., Longman, London, 1989, 268.

S2. T. Kobayashi, Y. Nishina, K. Shimizu and G. P. Sato, *Chem. Lett*., 1988, 1137.

S3. R. Prabhakaran and S. Dharani, Indian Patent No. 202241023805 Filed.