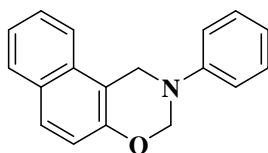


Supporting Information for

Fe_3O_4 @nano-coconut shell/Cu(II): A unique and reusable catalyst for green synthesis of naphtho[1,3]oxazine derivatives

Farhad Hajati, Bi Bi Fatemeh Mirjalili*

2-Phenyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine



White solid, FT-IR (ATR), \square (cm^{-1}) = 3050, 1600, 1494, 1230, 1057.

^1H NMR (Acetone- d_6 , 400 MHz), δ ppm = 7.89 (d, 1H, $^3J = 8.4$ Hz, Ar-H), 7.85 (d, 1H, $^3J = 8$ Hz, Ar-H), 7.73 (d, 1H, $^3J = 9.2$ Hz, Ar-H), 7.53-7.57 (m, 1H, Ar-H), 7.38-7.42 (m, 1H, Ar-H), 7.23-7.28 (m, 4H, Ar-H), 7.04 (d, 1H, $^3J = 8.8$ Hz, Ar-H), 6.87-6.91 (m, 1H, Ar-H), 5.54 (s, 2H, O- CH_2 -N), 5.06 (s, 2H, -Ar- CH_2 -N).

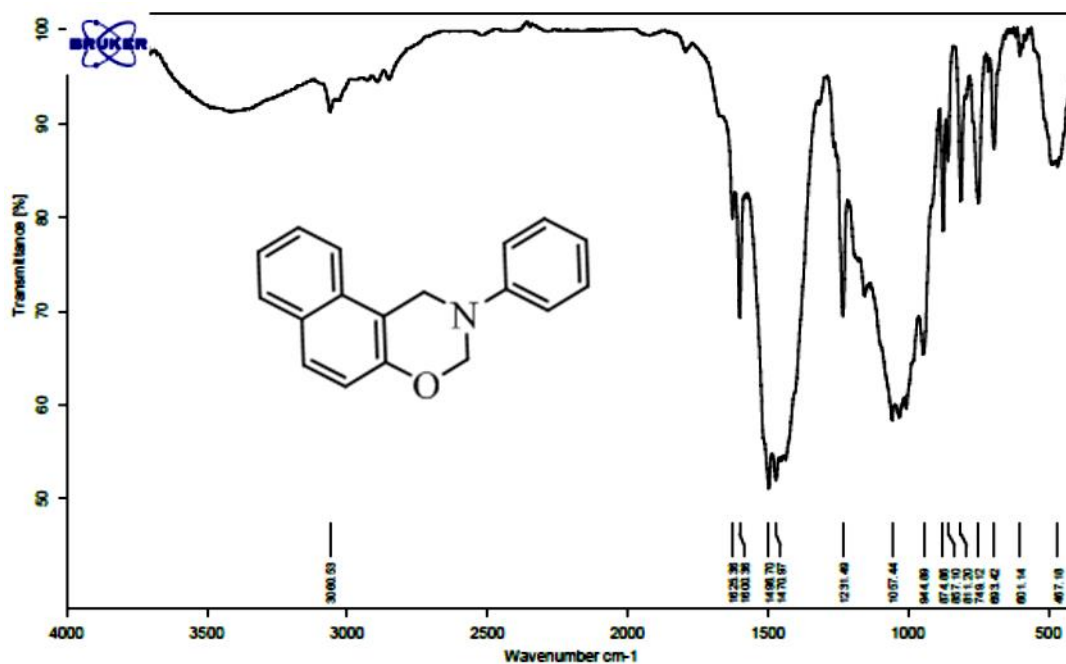


Fig.1: FTIR spectrum of 2-Phenyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

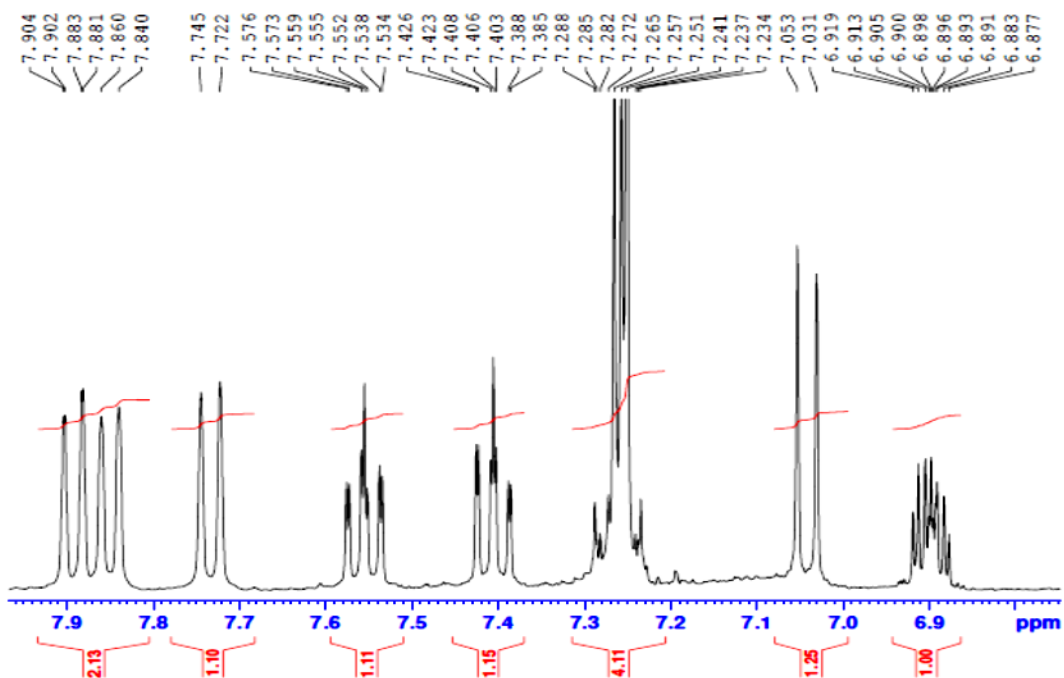


Fig 2. ^1H NMR (400 MHz, acetone- d_6) of 2-Phenyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

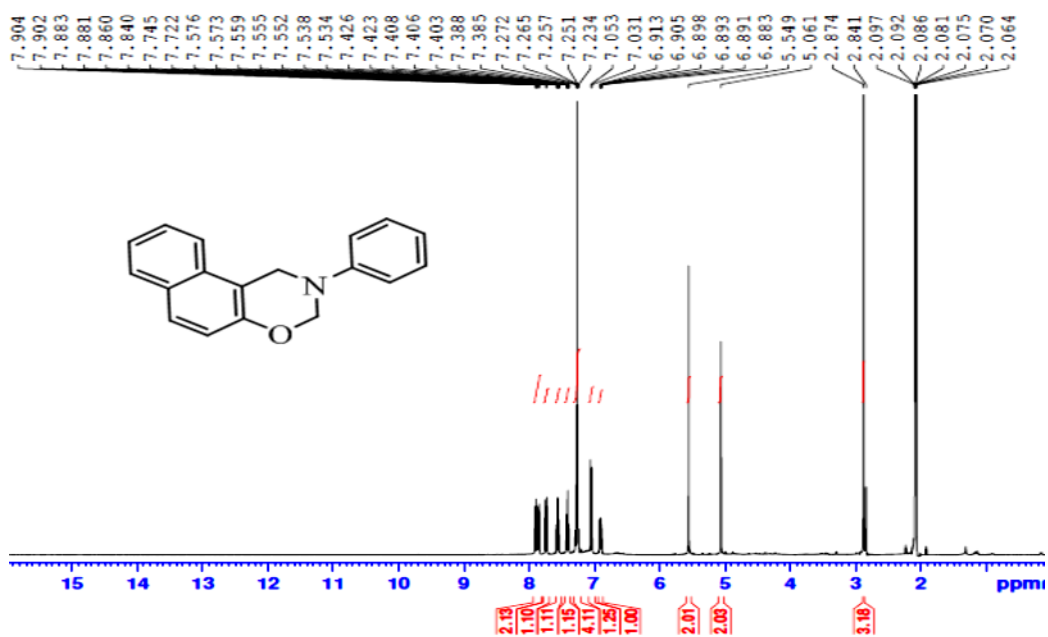
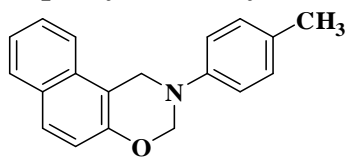


Fig 3. ^1H NMR (400 MHz, acetone- d_6) of 2-Phenyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

2-(p-tolyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine



Yellow solid, FT-IR (ATR), \square (cm^{-1}) = 1597, 1470, 1226, 1096.

^1H NMR (Acetone- d_6 , 400 MHz), δ ppm = 7.82 (t, 2H, $^3J = 8.8$ Hz, Ar-H), 7.69 (d, 1H, $^3J = 9.2$ Hz, Ar-H), 7.51 (t, 1H, $^3J = 8$ Hz, Ar-H), 7.36 (t, 1H, $^3J = 8$ Hz, Ar-H), 6.99-7.04 (m, 3H, Ar-H), 7.09-7.11 (m, 2H, Ar-H), 5.52 (s, 2H, O-CH $_2$ -N), 5.02 (s, 2H, -Ar-CH $_2$ -N), 2.24 (s, 3H, CH $_3$ -Ar).

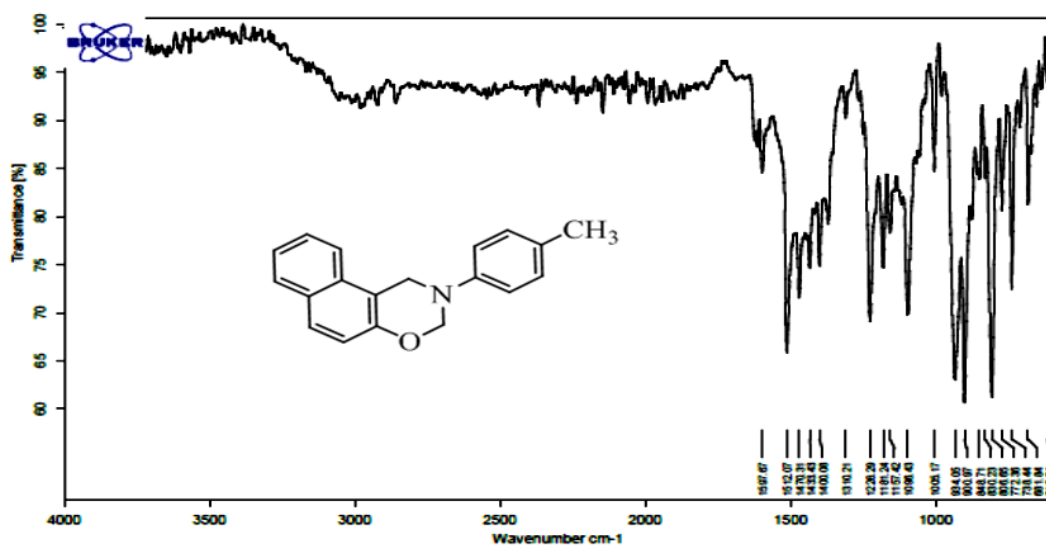


Fig.4: FTIR spectrum of 2-(p-Tolyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

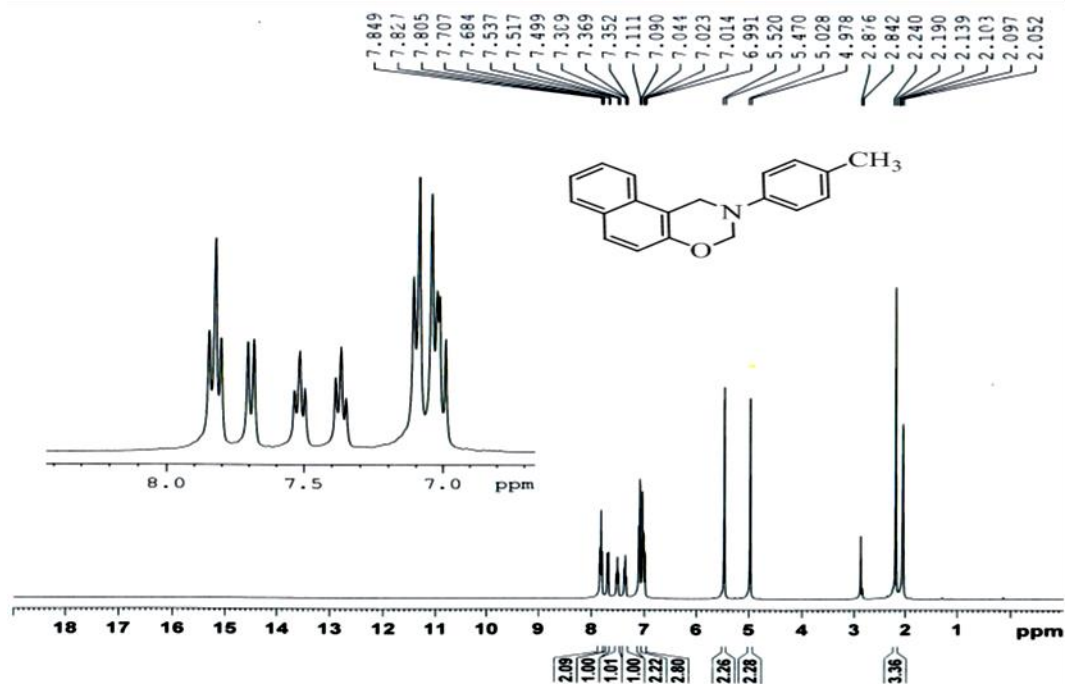
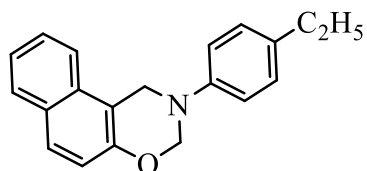


Fig 5. ¹H NMR (400 MHz, acetone-d₆) of 2-(p-tolyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

2-(4-ethylphenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine



Off-white solid, FT-IR (ATR), $\tilde{\nu}$ (cm⁻¹) = 1597, 1467, 1226, 1056.

¹H NMR (Acetone-d₆, 400 MHz), δ ppm = 7.80-7.85 (m, 2H, Ar-H), 7.69-7.71 (m, 1H, Ar-H), 7.50-7.55 (m, 1H, Ar-H), 7.35-7.40 (m, 1H, Ar-H), 6.99-7.14 (m, 5H, Ar-H), 5.49 (s, 2H, O-CH₂-N), 5.00 (s, 2H, -Ar-CH₂-N), 2.49-2.54 (m, 2H, -CH₂-CH₃), 1.15 (t, 3H, ³J = 7 Hz, -CH₂-CH₃).

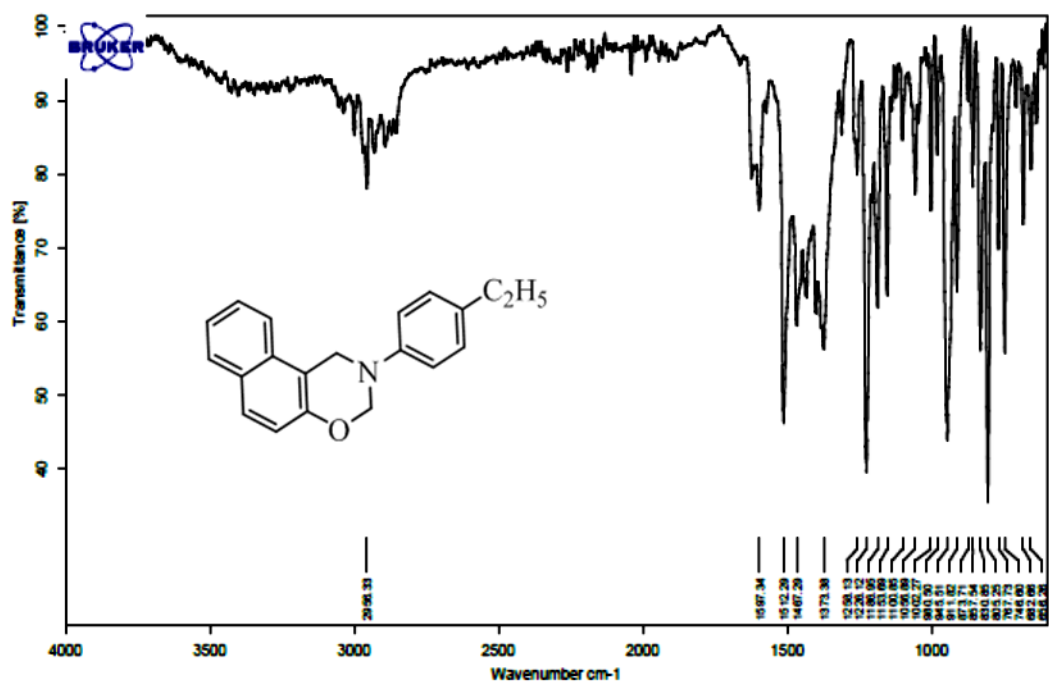


Fig.6: FTIR spectrum of 2-(4-ethylphenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

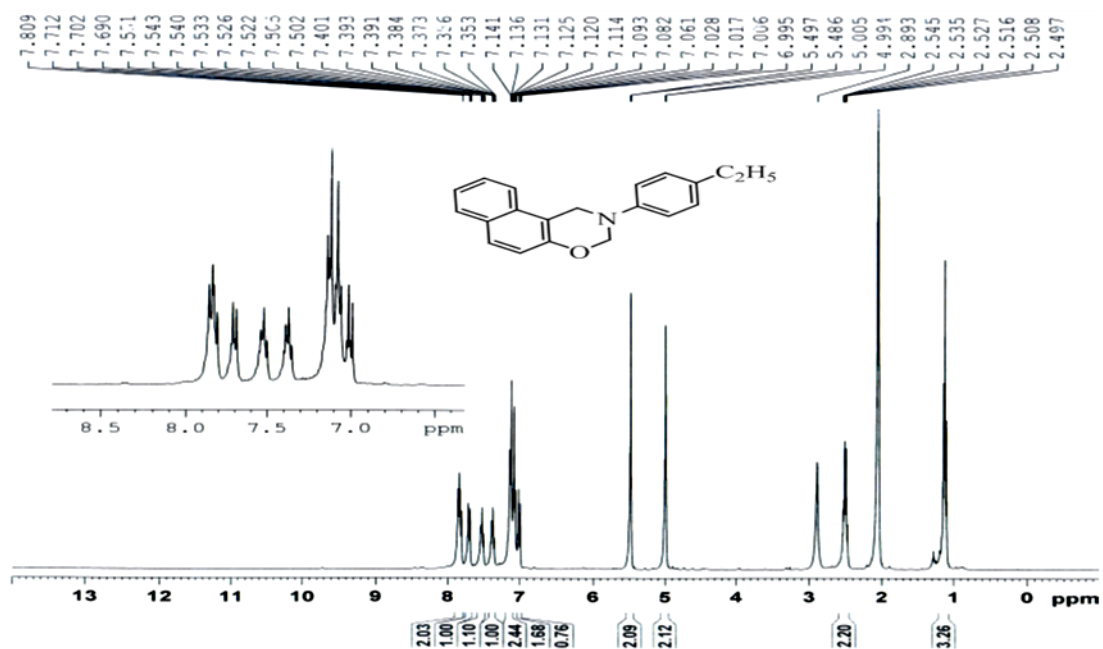
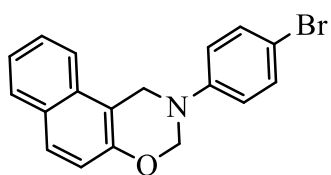


Fig 7. ¹H NMR (400 MHz, acetone-d₆) of 2-(4-ethylphenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

2-(4-bromophenyl)-2,3-dihydro-1H-naphtho[1,2-*e*][1,3]oxazine



White solid, FT-IR (ATR), \square (cm^{-1}) = 1588, 1489, 1223, 1092.

^1H NMR (Acetone- d_6 , 400 MHz), δ ppm = 7.84 (t, 2H, $^3J = 9.2$ Hz, Ar-H), 7.71 (d, 1H, $^3J = 9.2$ Hz, Ar-H), 7.52 (t, 1H, $^3J = 8.4$ Hz, Ar-H), 7.37-7.40 (m, 3H, Ar-H), 7.20 (d, 2H, $^3J = 9.2$ Hz, Ar-H), 7.01 (d, 1H, $^3J = 9.2$ Hz, Ar-H), 5.51 (s, 2H, O- CH_2 -N), 5.03 (s, 2H, -Ar- CH_2 -N).

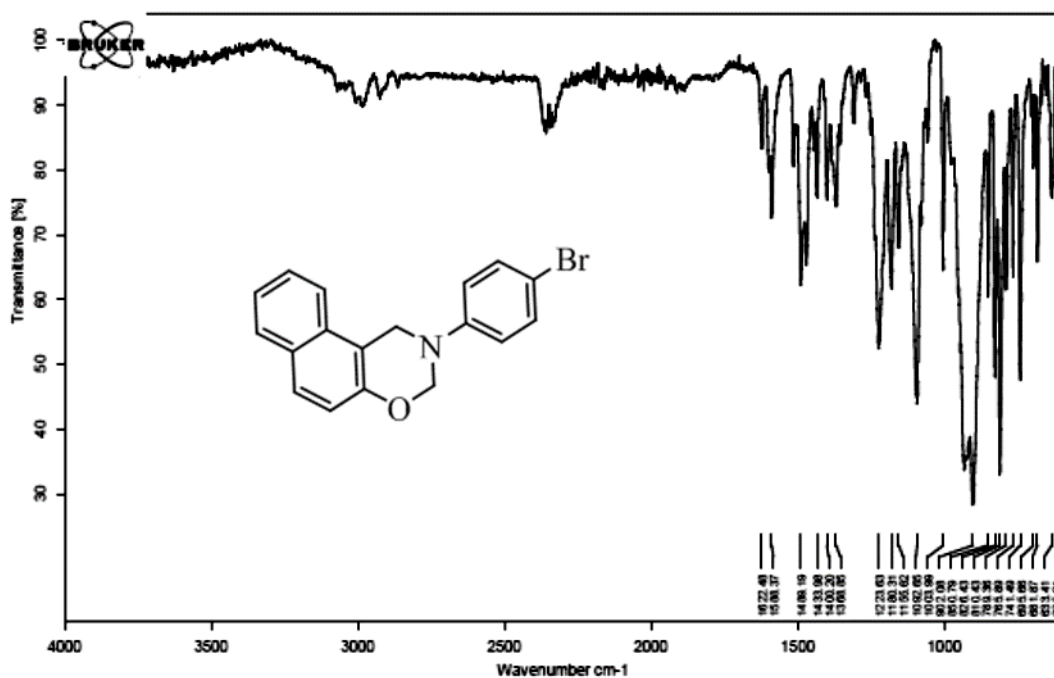


Fig. 8: FTIR spectrum of 2-(4-bromophenyl)-2,3-dihydro-1H-naphtho[1,2-*e*][1,3]oxazine

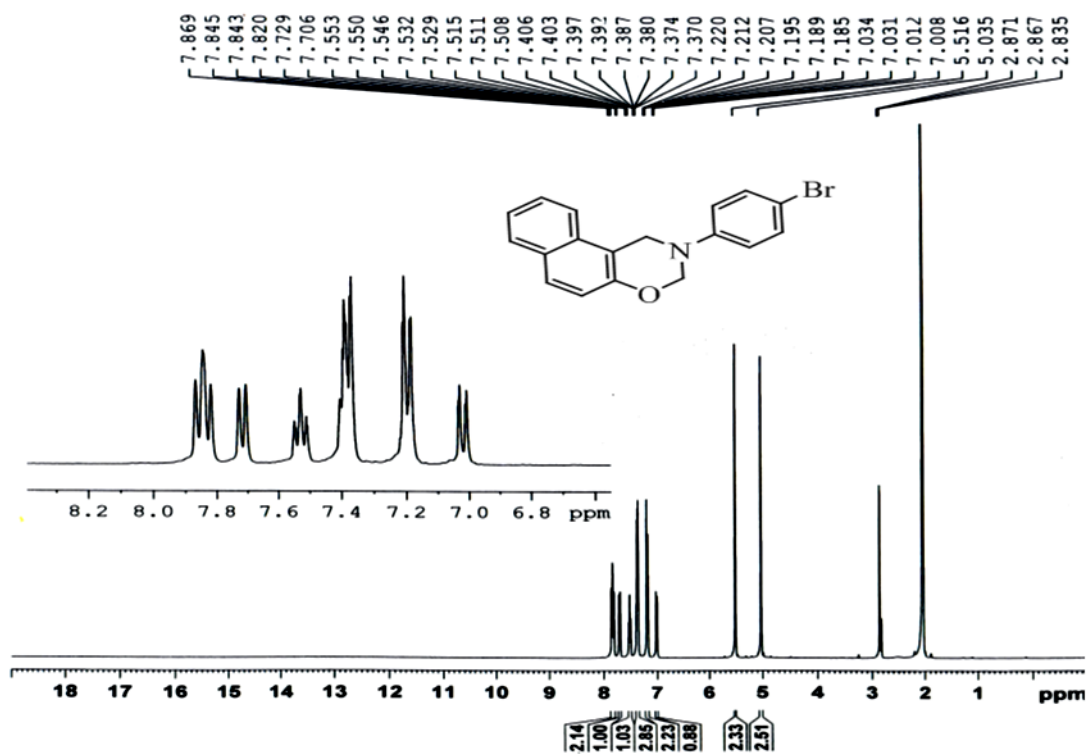
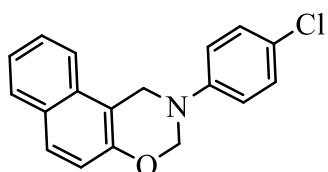


Fig 9. ^1H NMR (400 MHz, acetone- d_6) of 2-(4-bromophenyl)-2,3-dihydro-1H-naphtho[1,2-*e*][1,3]oxazine

2-(4-chlorophenyl)-2,3-dihydro-1H-naphtho[1,2-*e*][1,3]oxazine



White solid, FT-IR (ATR), \square (cm^{-1}) = 1593, 1492, 1225, 1092.

^1H NMR (Acetone- d_6 , 400 MHz), δ ppm = 7.84 (t, 2H, $^3J = 9.2$ Hz, Ar-H), 7.71 (d, 1H, $^3J = 8.8$ Hz, Ar-H), 7.53 (t, 1H, $^3J = 7.2$ Hz, Ar-H), 7.38 (t, 1H, $^3J = 7.6$ Hz, Ar-H), 7.24-7.29 (m, 4H, Ar-H), 7.02 (d, 1H, $^3J = 8.8$ Hz, Ar-H), 5.51 (s, 2H, O- CH_2 -N), 5.03 (s, 2H, -Ar- CH_2 -N).

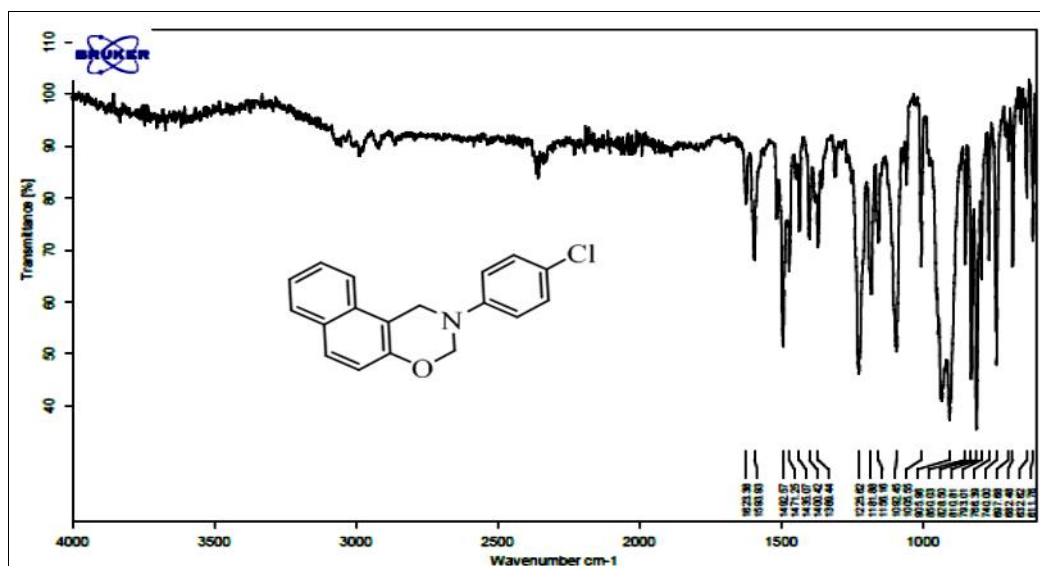


Fig.10: FTIR spectrum of 2-(4-chlorophenyl)-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

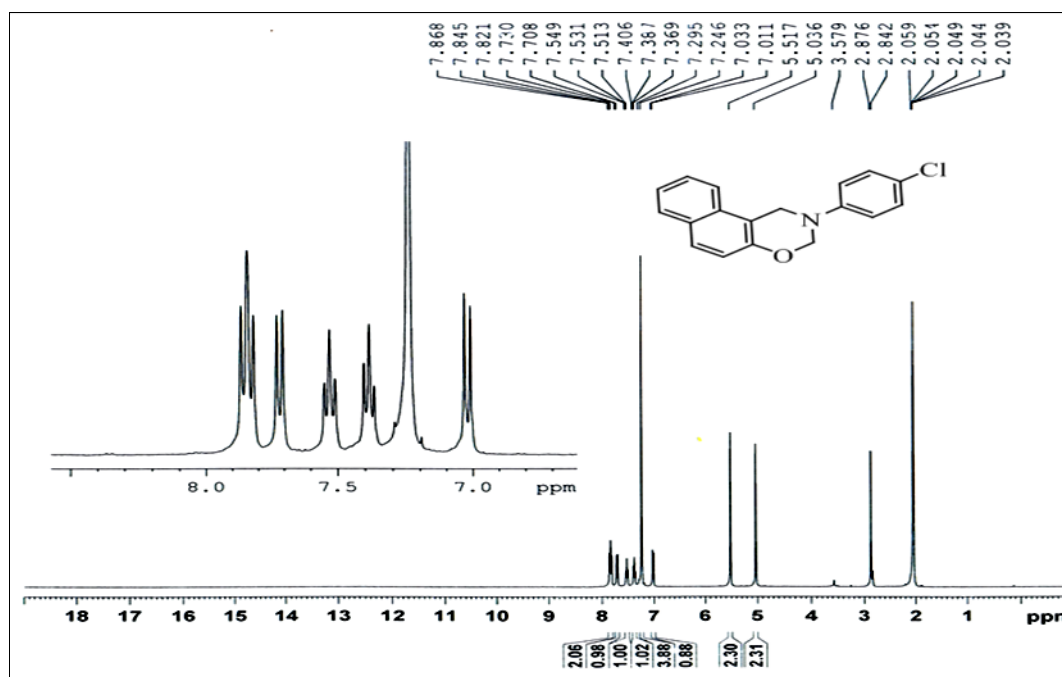
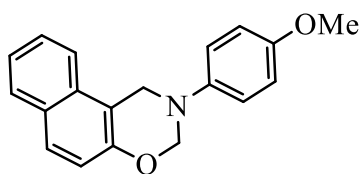


Fig 11. ^1H NMR (400 MHz, acetone- d_6) of 2-(4-chlorophenyl)-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

2-(4-methoxyphenyl)-2,3-dihydro-1H-naphtho[1,2-*e*][1,3]oxazine



Off-white solid, FT-IR (ATR), ν (cm^{-1}) = 1596, 1467, 1246, 1230, 1031.

^1H NMR (Acetone- d_6 , 400 MHz), δ ppm = 7.80-7.82 (m, 2H, Ar-H), 7.70 (d, 1H, $^3J = 8.8$ Hz, Ar-H), 7.51 (m, 1H, Ar-H), 7.36 (m, 1H, Ar-H), 7.13 (d, 2H, $^3J = 7.2$ Hz, Ar-H), 7.00 (d, 1H, $^3J = 8.8$ Hz, Ar-H), 6.80 (d, 2H, $^3J = 7.2$ Hz, Ar-H), 5.42 (s, 2H, O- CH_2 -N), 4.93 (s, 2H, -Ar- CH_2 -N), 3.68 (s, 3H, O- CH_3).

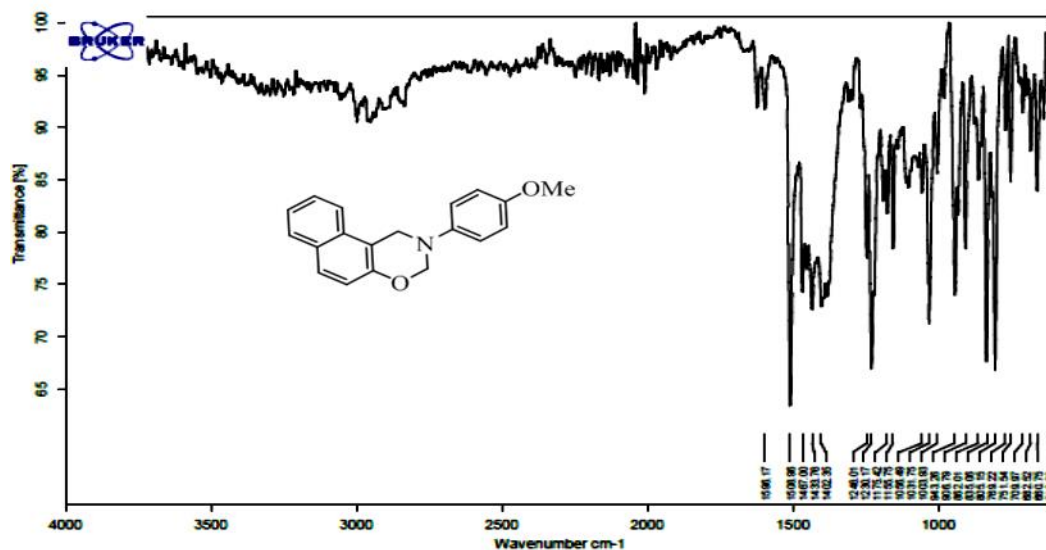


Fig.12: FTIR spectrum of 2-(4-methoxyphenyl)-2,3-dihydro-1H-naphtho[1,2-*e*][1,3]oxazine

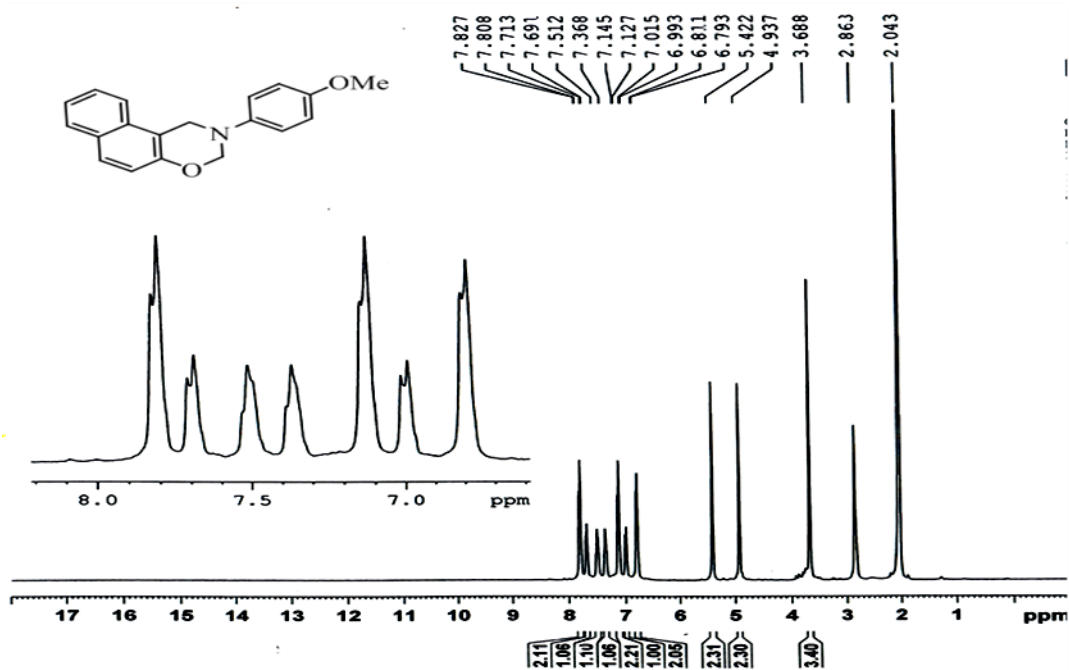
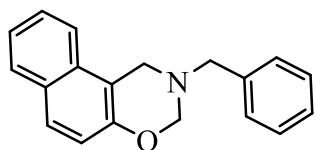


Fig 13. ¹H NMR (400 MHz, acetone-d₆) of 2-(4-methoxyphenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

2-benzyl-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine



Off-white, FT-IR (ATR), $\bar{\nu}$ (cm⁻¹) = 1597, 1461, 1223, 1058.

¹H NMR (DMSO-d₆, 500 MHz), δ ppm = 7.05-7.71 (m, 11H, Ar-H), 4.89 (s, 2H, O-CH₂-N), 4.22 (s, 2H, -Ar-CH₂-N), 3.89 (s, 2H, -Ar-CH₂-N).

¹³C NMR (DMSO-d₆, 100 MHz), δ ppm = 46.55, 55.17, 81.55, 111.67, 118.32, 121.15, 123.37, 126.57, 127.19, 127.76, 128.34, 128.39, 128.49, 128.59, 131.53, 138.33, 151.41.

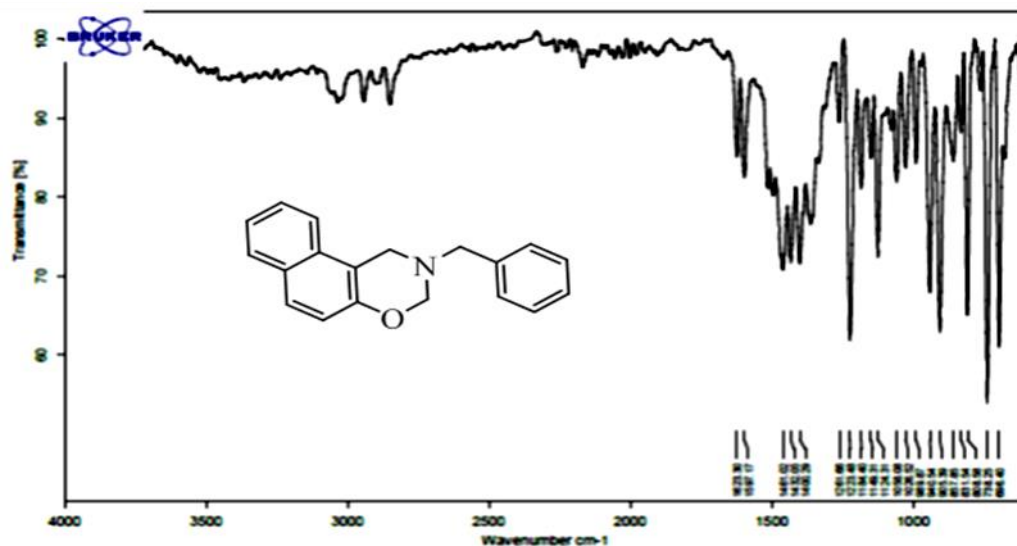


Fig.14: FTIR spectrum of 2-benzyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

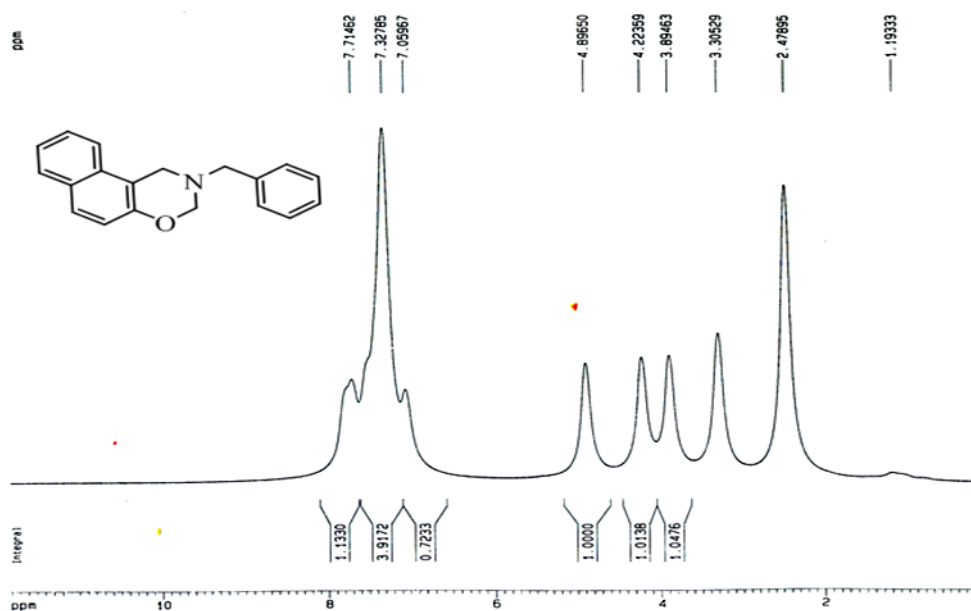


Fig 15. ¹H NMR (400 MHz, acetone-d₆) of 2-benzyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

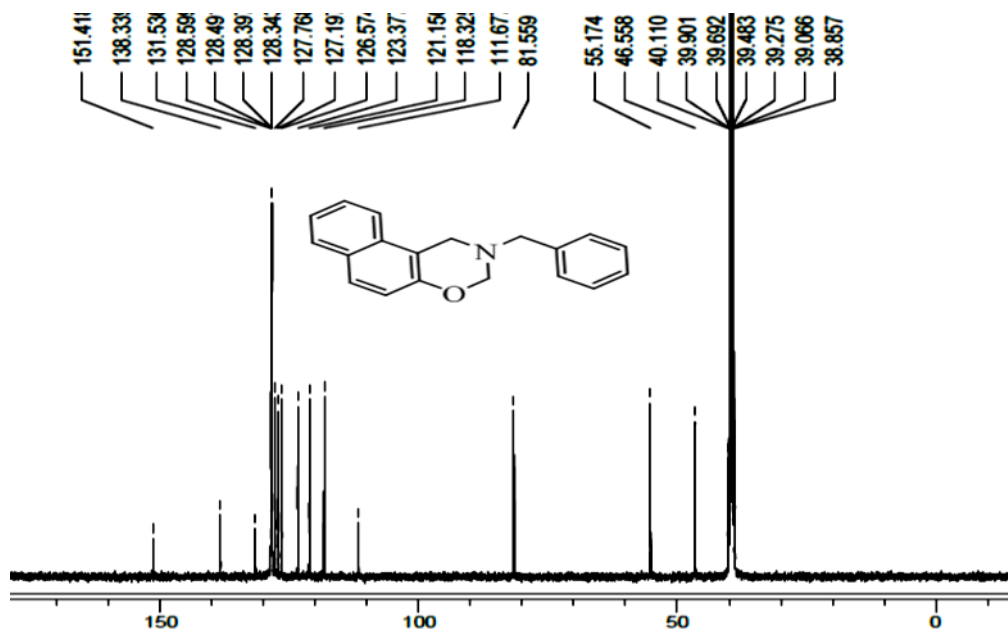


Fig 16. ^{13}C NMR (100 MHz, acetone- d_6) of 2-benzyl-2,3-dihydro-1H-naphtho[1,2-*e*][1,3]oxazine

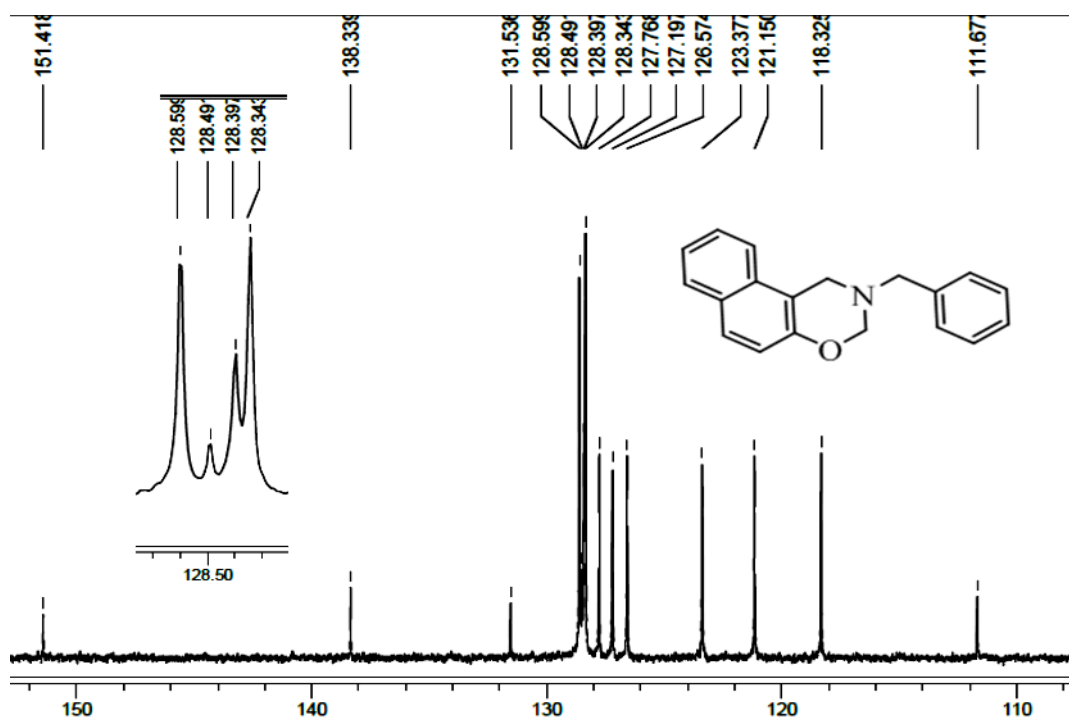
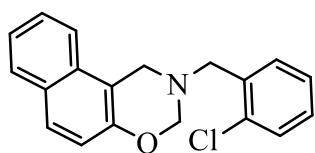


Fig 17. ^{13}C NMR (100 MHz, acetone- d_6) of 2-benzyl-2,3-dihydro-1H-naphtho[1,2-*e*][1,3]oxazine

2-(2-chlorobenzyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine



Yellow solid, FT-IR (ATR), ν (cm⁻¹): =1594, 1468, 1226, 1057.

¹H NMR (DMSO-d₆, 500 MHz), δ ppm = 7.07-7.82 (m, 10H, Ar-H), 4.95 (s, 2H, O-CH₂-N), 4.27 (s, 2H, -Ar-CH₂-N), 4.00 (s, 2H, -Ar-CH₂-N).

¹³C NMR (DMSO-d₆, 100 MHz), δ ppm = 46.82, 52.56, 81.94, 111.73, 118.33, 121.26, 123.42, 126.46, 127.23, 127.85, 128.39, 128.50, 128.90, 129.35, 130.61, 131.54, 133.23, 135.81, 151.41.

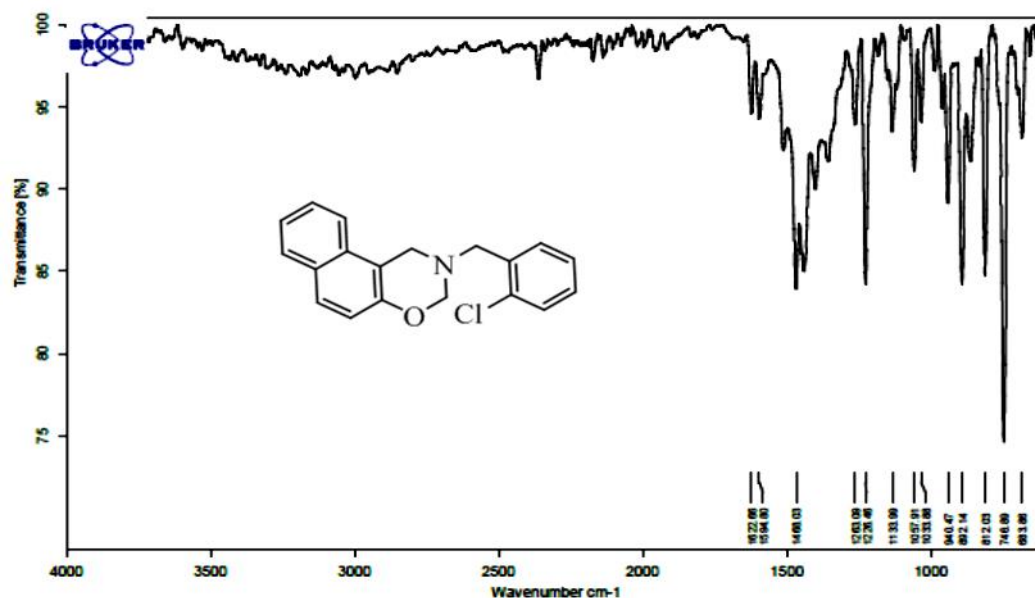


Fig.18: FTIR spectrum of 2-(2-chlorobenzyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

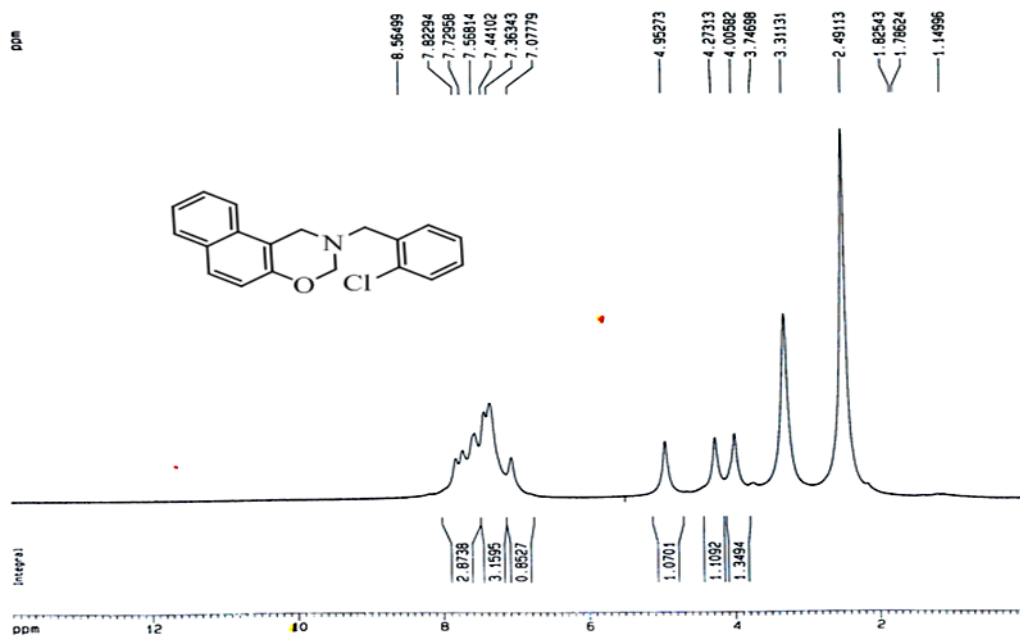


Fig 19. ¹H NMR (400 MHz, acetone-d₆) of 2-(2-chlorobenzyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

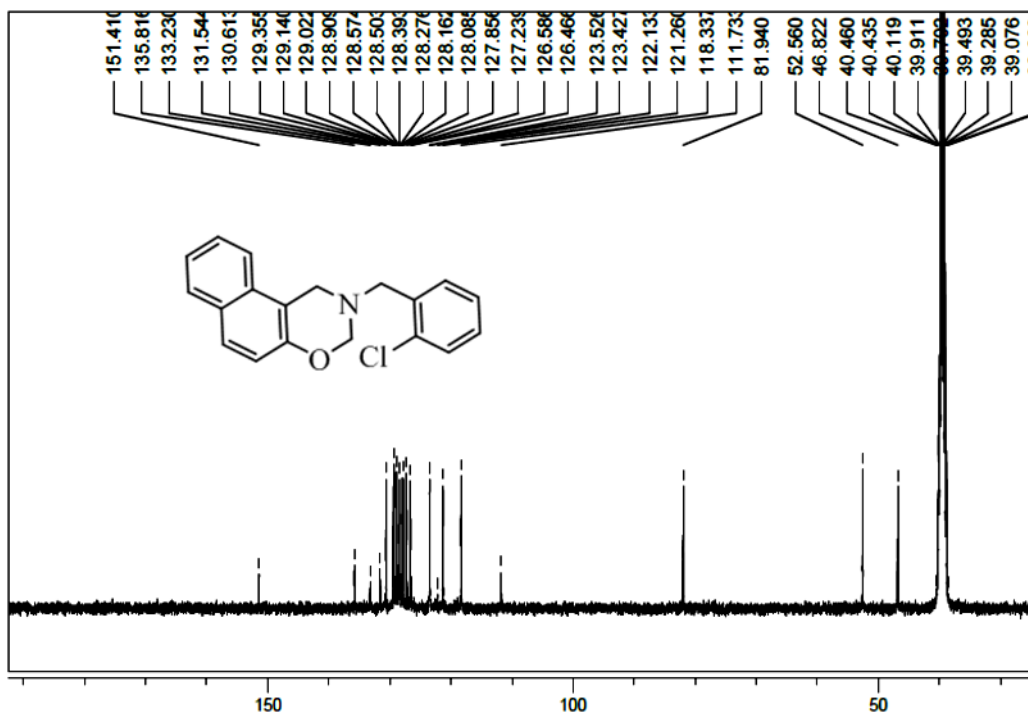


Fig 20. ¹³C NMR (100 MHz, acetone-d₆) of 2-(2-chlorobenzyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

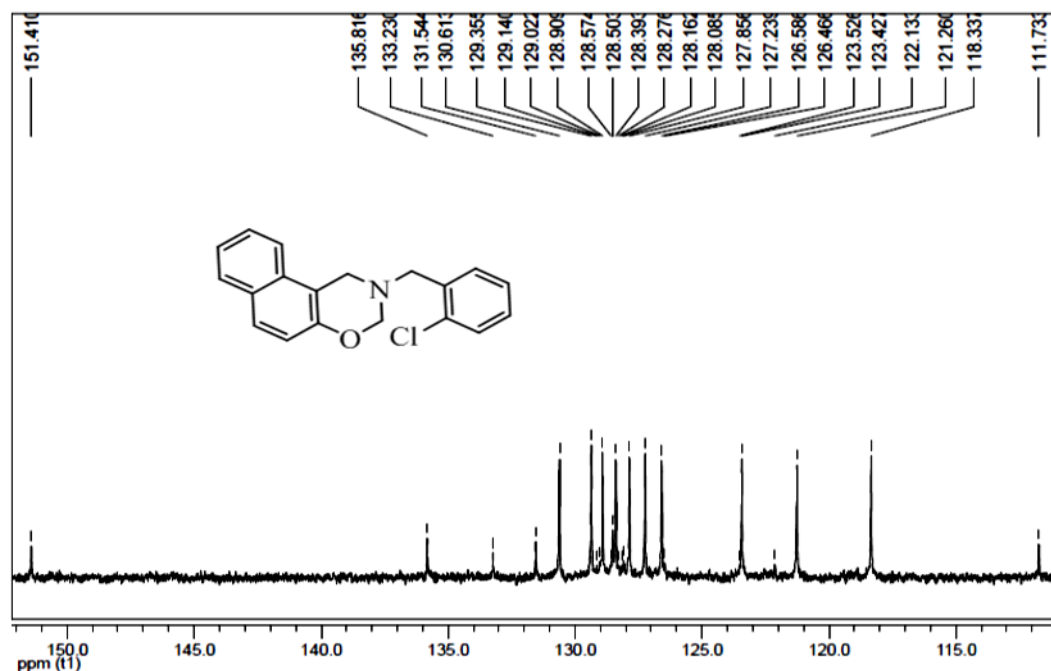
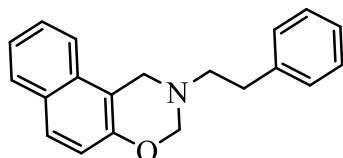


Fig 21. ¹³C NMR (100 MHz, acetone-d₆) of 2-(2-chlorobenzyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

2-phenethyl-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine



White solid, FT-IR (ATR), $\tilde{\nu}$ (cm⁻¹) = 1597, 1469, 1225, 1060.

¹H NMR (DMSO-d₆, 500 MHz), δ ppm = 7.81 (m, 1H, Ar-H), 7.69 (m, 2H, Ar-H), 7.49 (m, 1H, Ar-H), 7.35 (m, 1H, Ar-H), 7.24 (m, 5H, Ar-H), 7.02 (m, 1H, Ar-H), 4.92 (s, 2H, O-CH₂-N), 4.32 (s, 2H, -Ar-CH₂-N), 2.96 (m, 2H, Ar-CH₂-CH₂-N), 2.88 (m, 2H, Ar-CH₂-CH₂-N).

¹³C NMR (DMSO-d₆, 125 MHz), δ ppm = 34.86, 47.95, 53.92, 82.69, 113.08, 119.18, 122.26, 124.19, 126.74, 127.33, 128.51, 129.05, 129.22, 129.31, 129.54, 132.43, 140.88, 152.43.

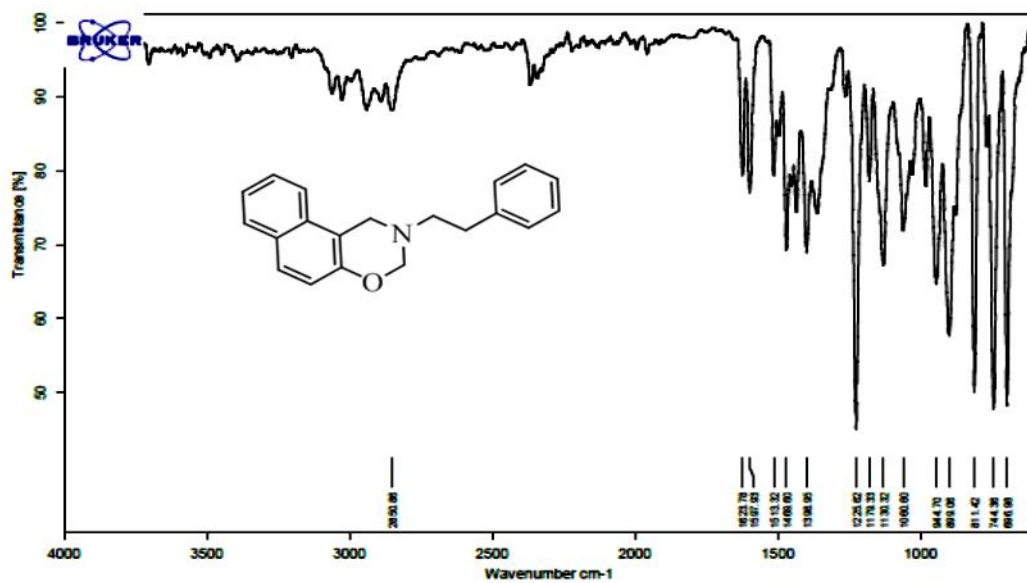


Fig.22: FTIR spectrum of 2-phenethyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

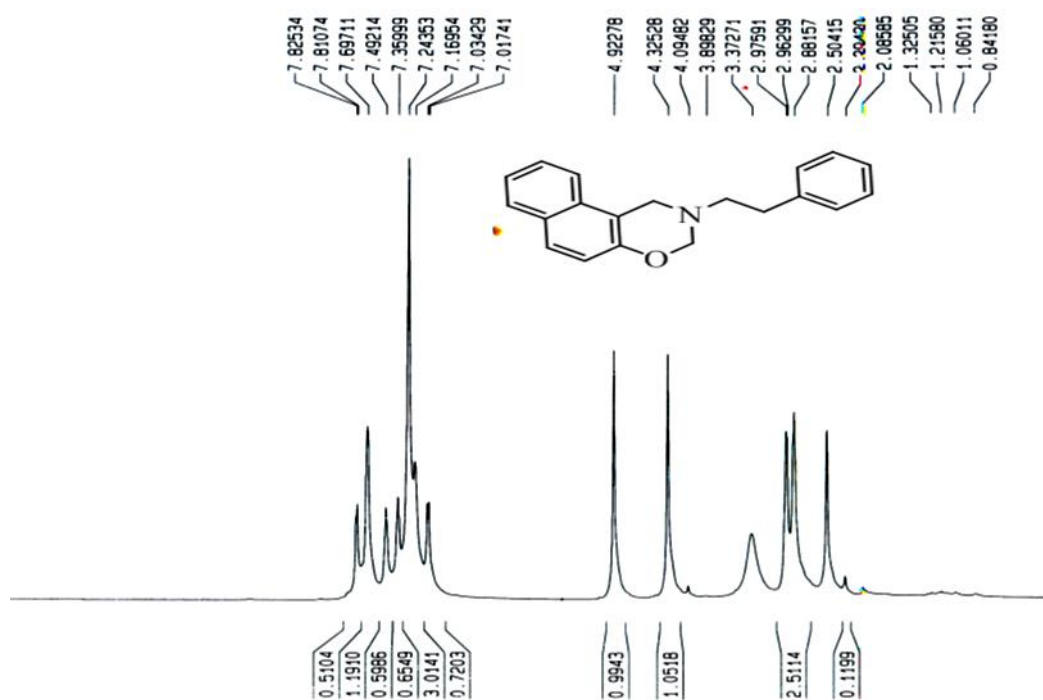


Fig 23. ¹H NMR (400 MHz, acetone-d₆) of 2-phenethyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

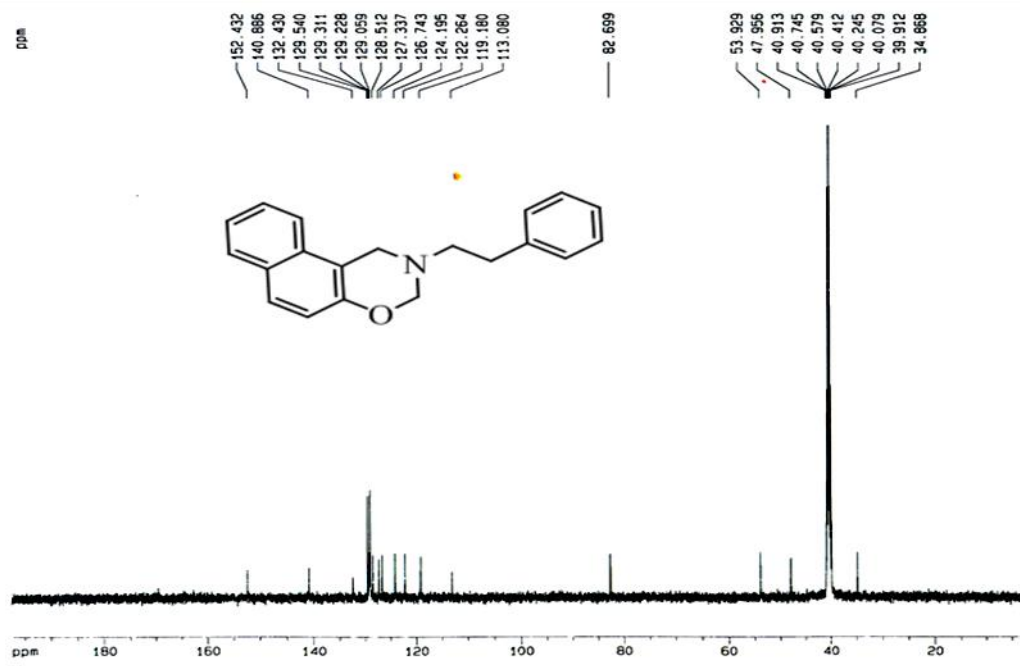
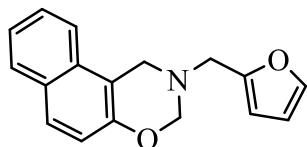


Fig 24. ¹³C NMR (100 MHz, acetone-d₆) of 2-phenethyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

2-(furan-2-yl methyl)-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine



Pale-pink, FT-IR (ATR), $\tilde{\nu}$ (cm⁻¹) = 1597, 1467, 1226, 1060.

¹H NMR (DMSO-d₆, 500 MHz), δ ppm = 7.71-8.02 (m, 4H, Ar-H), 7.36-7.61 (m, 2H, Ar-H), 7.04 (s, 1H, Ar-H), 6.32-6.52 (m, 2H, Ar-H), 4.89 (s, 2H, O-CH₂-N), 4.26 (s, 2H, -Ar-CH₂-N), 3.90 (s, 2H, furan-CH₂-N).

¹³C NMR (DMSO-d₆, 125 MHz), δ ppm = 46.37, 47.86, 81.22, 108.76, 110.42, 111.52, 118.27, 121.19, 123.43, 126.60, 127.80, 128.39, 128.50, 131.48, 142.70, 151.29, 151.79.

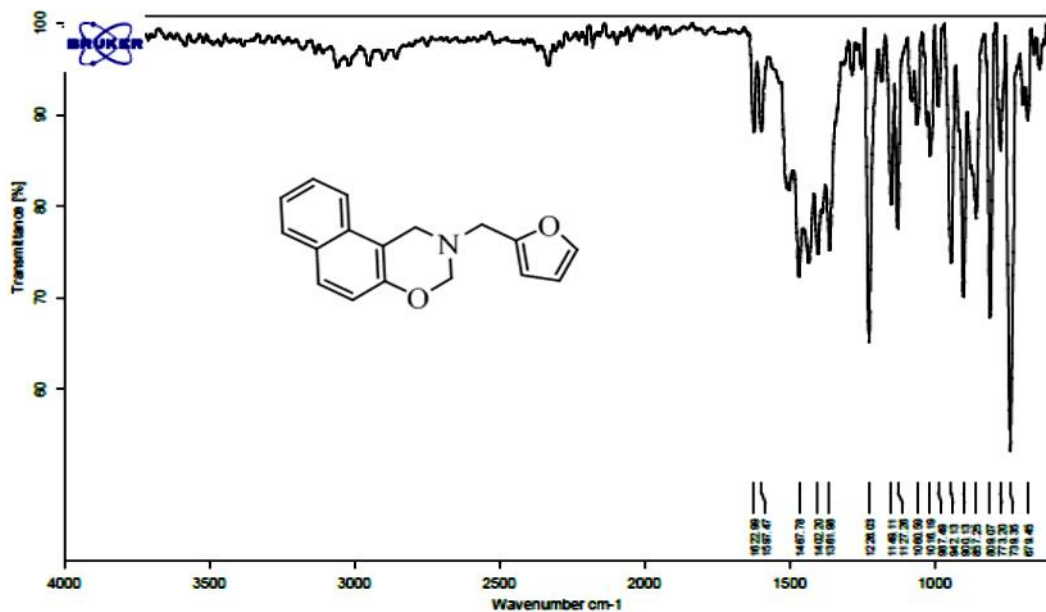


Fig.25: FTIR spectrum of 2-(furan-2-yl methyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

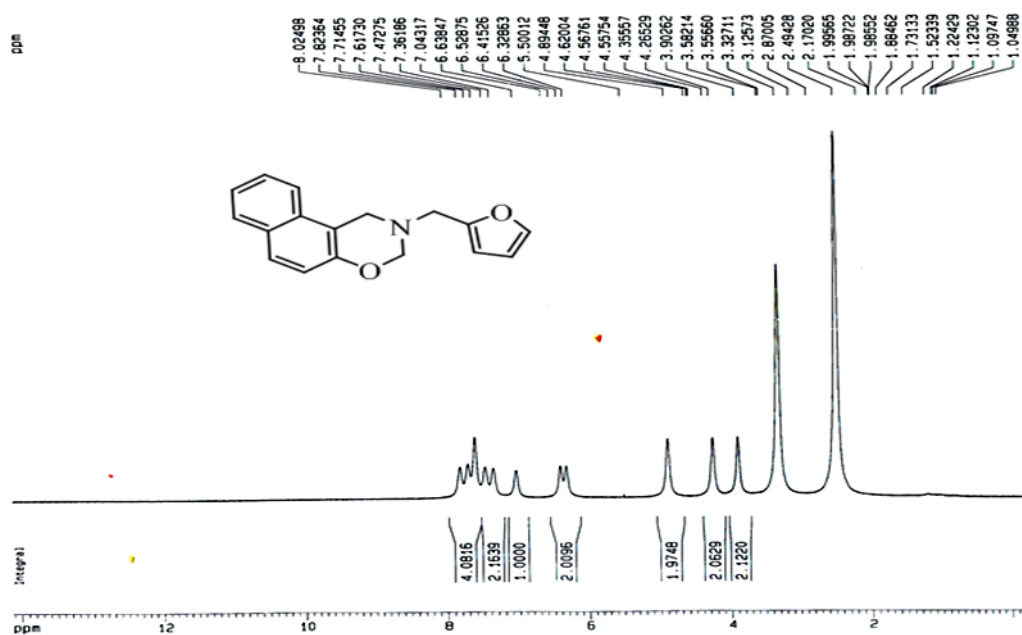
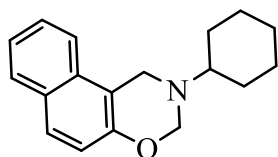


Fig 26. ¹H NMR (400 MHz, acetone-d₆) of 2-(furan-2-yl methyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine



Fig 27. ¹³C NMR (100 MHz, acetone-d₆) of 2-(furan-2-yl methyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine

2-cyclohexyl-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine



Off-white solid, FT-IR (ATR), $\tilde{\nu}$ (cm⁻¹) = 2926, 2852, 1597, 1467, 1227, 1058.

¹H NMR (DMSO-d₆, 500 MHz), δ ppm = 7.66-7.81 (m, 3H, Ar-H), 7.48 (m, 1H, Ar-H), 7.35 (m, 1H, Ar-H), 6.98 (m, 1H, Ar-H), 4.99 (s, 2H, O-CH₂-N), 4.33 (s, 2H, - Ar-CH₂-N), 2.70 (m, 1H, CH-N), 1.08-1.86 (m, 10H, 5CH₂).

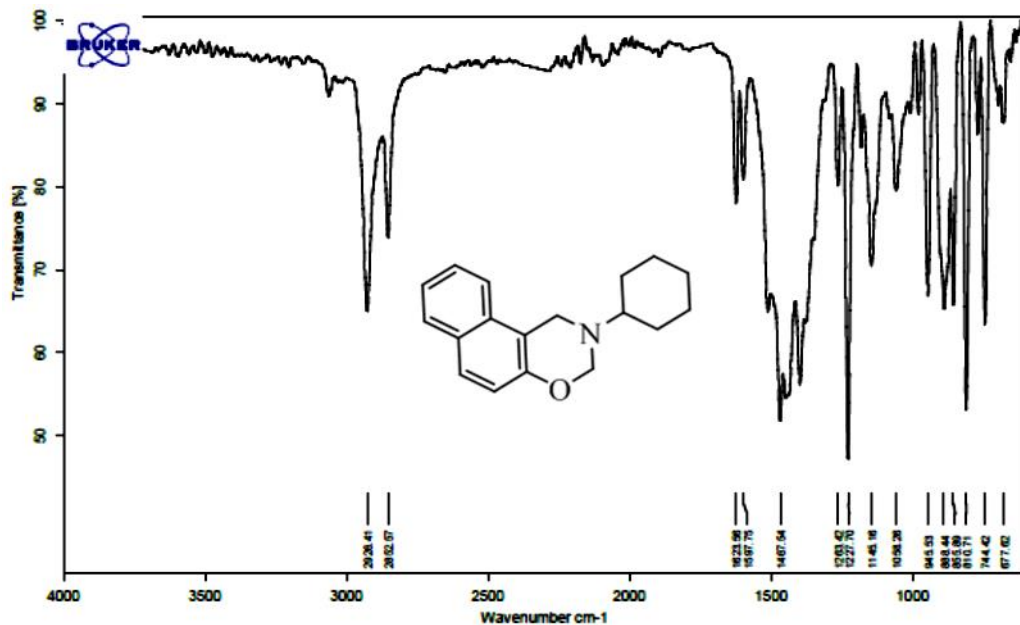


Fig.28: FTIR spectrum of 2-cyclohexyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

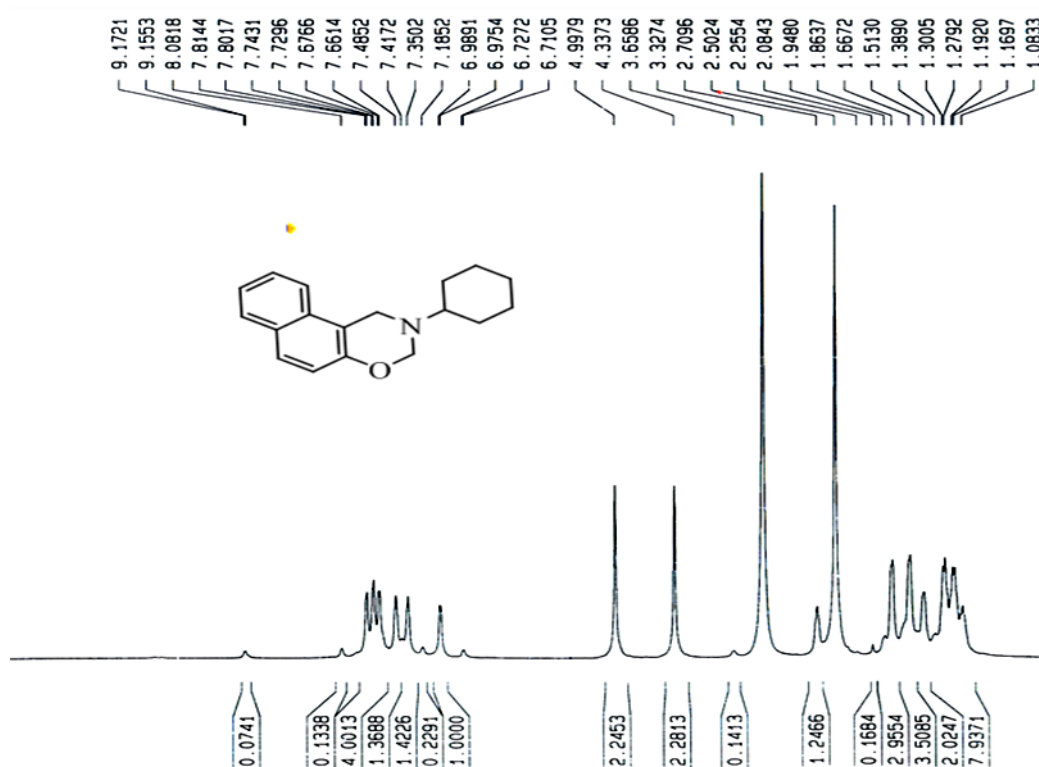
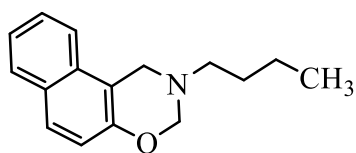


Fig 29. ^1H NMR (400 MHz, acetone- d_6) of 2-cyclohexyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

2-butyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine



White solid, FT-IR (ATR), $\bar{\nu}$ (cm⁻¹) = 2954, 2864, 1597, 1433, 1225, 1056.

¹H NMR (DMSO-d₆, 500 MHz), δ ppm = 7.81 (m, 1H, Ar-H), 7.69 (m, 2H, Ar-H), 7.47 (m, 1H, Ar-H), 7.35 (m, 1H, Ar-H), 7.00 (m, 1H, Ar-H), 4.88 (s, 2H, O-CH₂-N), 4.25 (s, 2H, -Ar-CH₂-N), 2.69 (m, 2H, -CH₂-N), 1.53 (m, 2H, CH₂), 1.31 (m, 2H, CH₂), 0.87 (m, 3H, CH₃).

¹³C NMR (DMSO-d₆, 100 MHz), δ ppm = 13.80, 19.80, 29.64, 46.94, 50.84, 81.81, 112.08, 118.25, 121.31, 123.26, 126.45, 127.57, 128.32, 128.37, 131.54, 151.51.

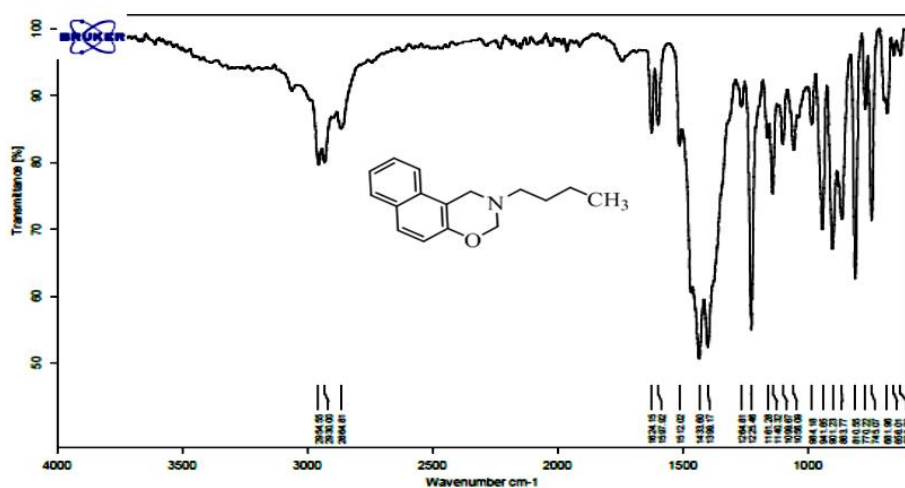


Fig.30: FTIR spectrum of 2-butyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

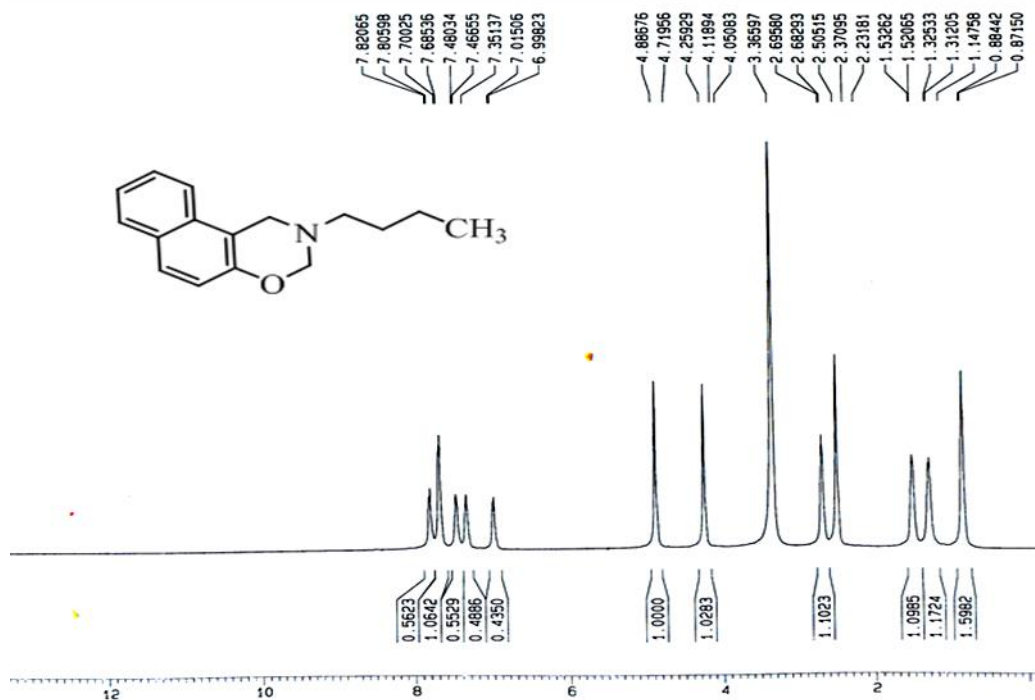


Fig 31. ¹H NMR (400 MHz, acetone-d₆) of 2-butyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

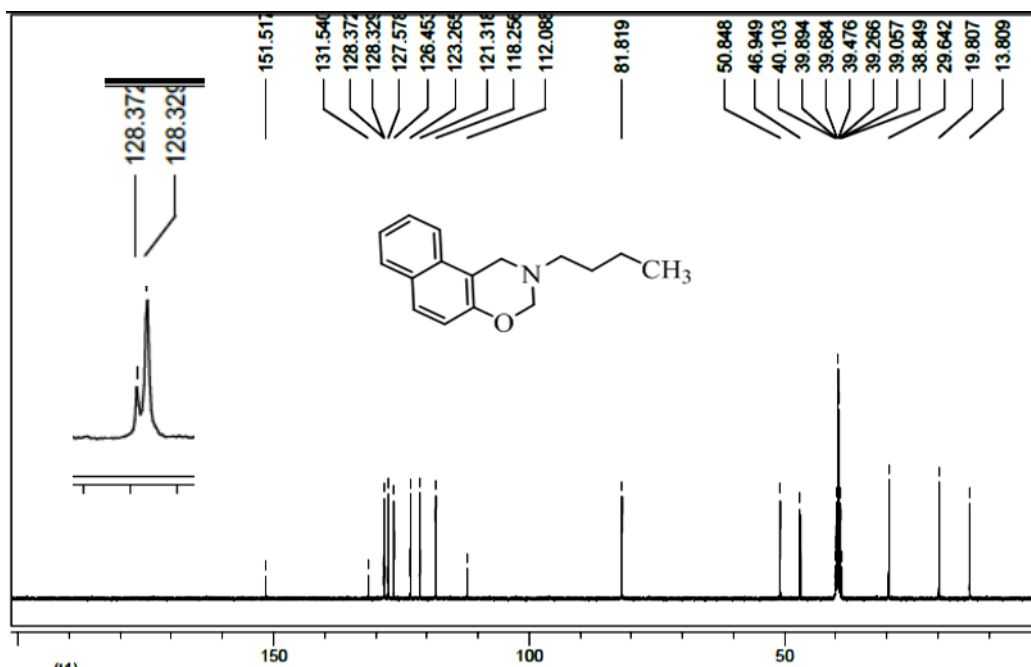
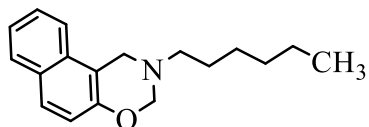


Fig 32. ¹³C NMR (100 MHz, acetone-d₆) of 2-butyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

2-hexyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine



Brown solid, FT-IR (ATR), $\tilde{\nu}$ (cm⁻¹) = 2927, 2854, 1597, 1467, 1225, 1057.

¹H NMR (DMSO-d₆, 500 MHz), δ ppm = 7.80 (m, 1H, Ar-H), 7.68 (m, 2H, Ar-H), 7.47 (m, 1H, Ar-H), 7.34 (m, 1H, Ar-H), 7.00 (m, 1H, Ar-H), 4.87 (s, 2H, O-CH₂-N), 4.25 (s, 2H, -Ar-CH₂-N), 2.68 (m, 2H, -CH₂-N), 1.53 (m, 2H, CH₂), 1.25 (m, 6H, 3CH₂), 0.84 (m, 3H, CH₃).

¹³C NMR (DMSO-d₆, 125 MHz), δ ppm = 14.77, 22.98, 27.23, 28.38, 32.02, 47.87, 52.09, 82.71, 112.97, 119.14, 122.18, 124.13, 127.32, 128.46, 129.21, 129.28, 132.44, 152.42.

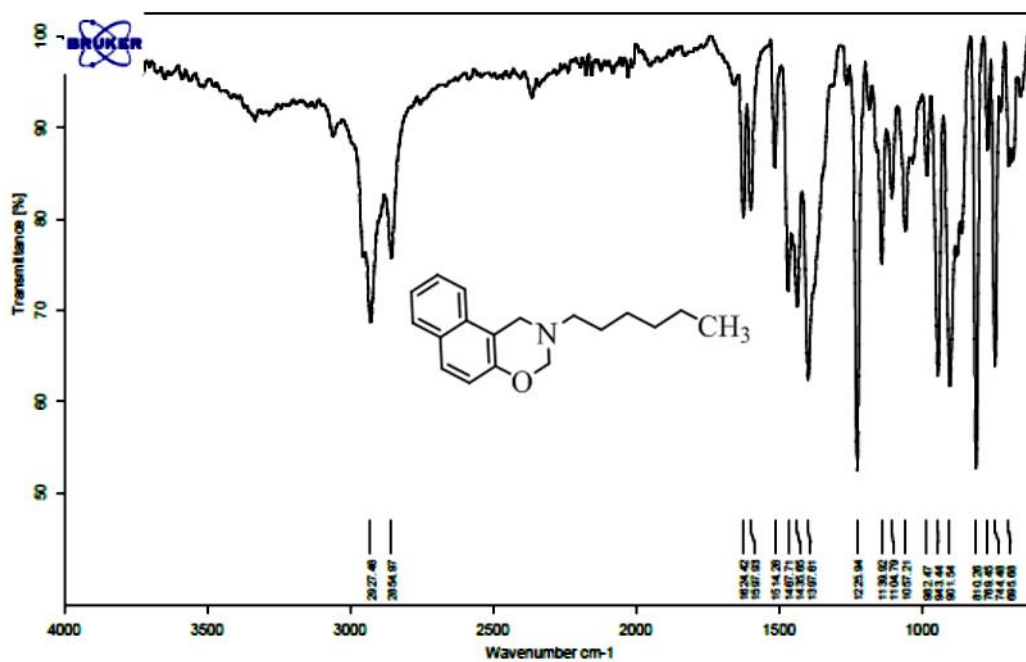


Fig.33: FTIR spectrum of 2-hexyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

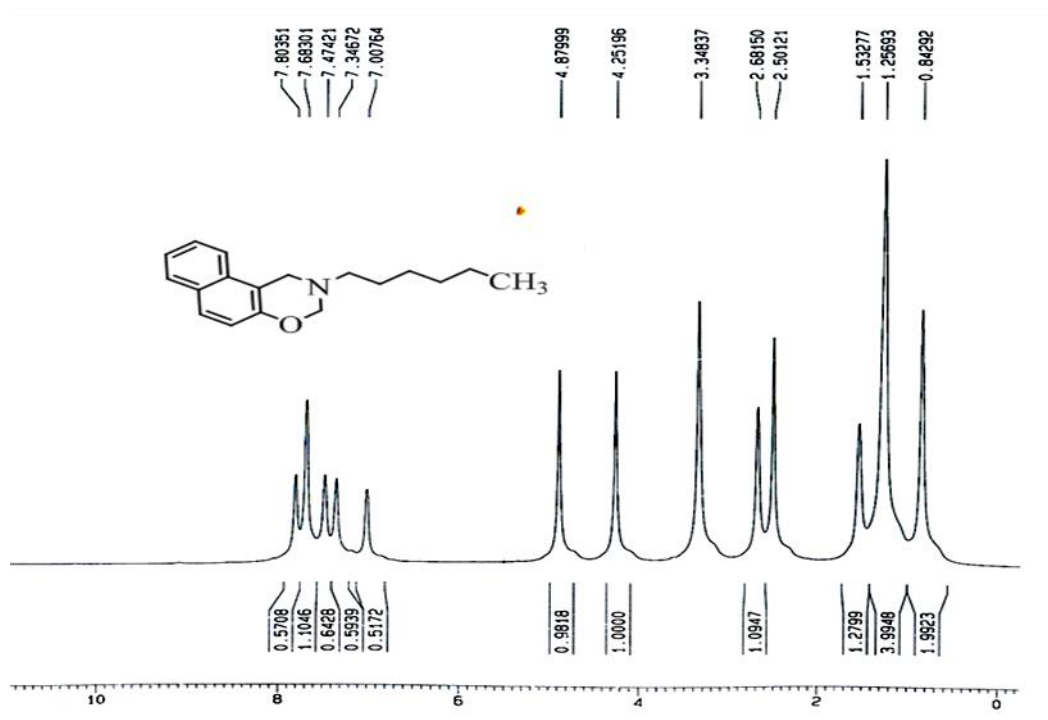


Fig 34. ^1H NMR (400 MHz, acetone- d_6) of 2-hexyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine

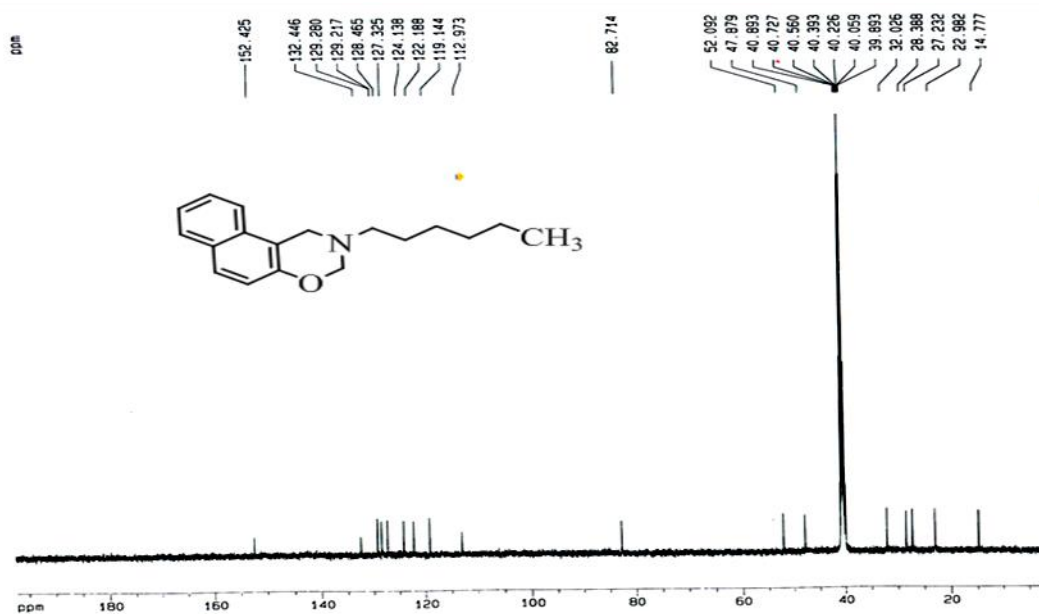


Fig 35. ^{13}C NMR (100 MHz, acetone- d_6) of 2-hexyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine