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Supplementary Information

A Facile Regioselective Synthesis of Novel Spiroacenaphthene Pyrroloisoquinolines Through 1,3-Dipolar Cycloaddition Reactions

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Characterization data for representative compounds

2'-Benzoyl-1'-phenyl-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**4a**)

Yellow solid (0.366 g, 82%); m.p. 183-185 °C; IR (KBr) ν_{max}/cm^{-1} 1713, 1681; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-6.72 (m, 20H, Ar-H), 5.37 (d, 1H, *J* 9.6 Hz, H_c), 4.62 (d, 1H, *J* 9.2 Hz, H_a), 4.48 (t, 1H, *J* 9.6 Hz, H_b), 2.98-2.89 (m, 2H), 2.66-2.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.3, 197.3, 142.5, 140.3, 138.2, 137.2, 136.9, 134.7, 132.0, 131.9, 131.7, 129.8, 129.1, 129.1, 128.8, 128.7, 127.8, 127.4, 127.2, 126.9, 126.3, 125.5, 125.1, 124.7, 123.5, 120.7, 74.7 (C-Spiro), 64.3, 63.8, 50.9, 42.5, 30.4; anal. calcd. for $C_{36}H_{27}NO_2$: C, 85.52; H, 5.38; N, 2.77; found: C, 85.1; H, 5.05; N, 2.35; MS (*m/z*): 505.

2'-Benzoyl-1'-(4-fluorophenyl)-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**4b**)

Orange solid (0.408 g, 78%); m.p. 230-232 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1708, 1681; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.132-6.61 (m, 19H, Ar-H), 5.43 (d, 1H, *J* 9.6 Hz, H_c), 4.62 (d, 1H, *J* 9.6 Hz, H_a), 4.55 (t, 1H, *J* 10.8 Hz, H_b), 2.96-2.89 (m, 2H), 2.67-2.62 (m, 1H), 2.56-2.48 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.3, 196.7, 150.4, 147.1, 142.6, 137.4, 136.6, 136.5, 134.8, 132.3, 132.2, 131.4, 130.0, 129.8, 129.1, 128.7, 127.9, 127.5, 127.1, 126.7, 125.6, 125.0, 124.7, 124.4, 123.4, 121.1, 74.7 (C-Spiro), 64.4, 63.6, 50.8, 42.5, 30.4; anal. calcd. for $C_{36}H_{26}FNO_2$: C, 82.58; H, 5.01; N, 2.68; found: C, 82.15; H, 4.85; N, 2.35; MS (*m/z*): 523.

2'-Benzoyl-1'-(4-chlorophenyl)-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**4c**)

Yellow solid (0.463 g, 86%); m.p. 199-201°C; FT-IR (KBr) ν_{max}/cm^{-1} 1708, 1682; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-6.76 (m, 19H, Ar-H), 5.98 (d, 1H, *J* 8.8 Hz, H_c), 5.33 (dd, 1H, *J* 7.2, 8.4 Hz, H_b), 4.42 (d, 1H, *J* 7.2 Hz, H_a), 3.20-3.12 (m, 1H), 2.81-2.72 (m, 2H), 2.64-2.60 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.2, 202.3, 142.7, 138.8, 138.4, 136.0, 135.0, 134.9, 133.0, 132.9, 132.3, 131.5, 130.3, 130.2, 129.2, 129.0, 128.6, 128.4, 128.3, 128.2, 127.4, 127.1, 125.9, 125.2, 121.1, 120.4, 80.0 (C-Spiro), 64.5, 59.9, 52.9, 43.1, 30.3; anal. calcd. for $C_{36}H_{26}ClNO_2$: C, 80.06; H, 4.85; N, 2.59; found: C, 80.56; H, 5.24; N, 2.14; MS (*m/z*): 540.

2'-Benzoyl-1'-(4-bromophenyl)-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**4d**)

Yellow solid (0.443 g, 76%); m.p. 194-196 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1705, 1684. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06-6.74 (m, 19H, Ar-H), 5.96 (d, 1H, *J* 8.4 Hz, H_c), 5.32 (dd, 1H, *J* 7.2, 7.2 Hz, H_b), 4.38 (d, 1H, *J* 7.2 Hz, H_a), 3.19-3.11 (m, 1H), 2.78-2.71 (m, 2H), 2.64-2.60 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.2, 202.3, 142.7, 138.8, 138.4, 136.0, 135.6, 135.4, 135.0, 132.9, 132.3, 131.5, 131.3, 130.5, 130.2, 129.2, 129.0, 128.6, 128.3, 128.2, 127.8, 125.9, 125.2, 121.2, 121.1, 120.5, 79.9 (C-Spiro), 64.5, 59.9, 52.8, 43.0, 30.3. anal. calcd. for $C_{36}H_{26}BrNO_2$: C, 73.98; H, 4.48; N, 2.40; found: C, 73.62; H, 4.73; N, 2.05; MS (*m/z*): 583.

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2'-Benzoyl-1'-(4-methylphenyl)-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene -1,3'-pyrrolo[2,1-a] isoquinolin]-2-one (**4e**)

Yellow solid (0.410 g, 79%); m.p. 191-193 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1700, 1682; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.12-6.65 (m, 19H, Ar-H), 5.16 (d, 1H, *J* 8.0 Hz, H_c), 4.51 (d, 1H, *J* 8.0 H_a), 4.21 (t, 1H, *J* 10 Hz, H_b), 2.75-2.69 (m, 2H), 2.61-2.58 (m, 1H), 2.35-2.33 (m, 1H), 2.31 (s, 3H, Me); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.8, 197.3, 142.4, 139.3, 138.2, 136.7, 136.6, 136.6, 135.9, 133.1, 132.9, 131.2, 130.3, 129.9, 129.4, 129.1, 128.8, 128.3, 127.24, 126.9, 125.8, 125.6, 124.8, 123.4, 121.6, 74.4 (C-Spiro), 64.3, 63.2, 50.9, 42.7, 30.2, 21.2; anal. calcd. for $C_{37}H_{29}NO_2$: C, 85.52; H, 5.63; N, 2.70; found: C, 85.24; H, 5.23; N, 2.35; MS (*m/z*): 519.

2'-Benzoyl-1'-(4-methoxyphenyl)-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a] isoquinolin]-2-one (**4f**)

Yellow solid (0.439 g, 82%); m.p. 192-194 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1708, 1686; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-6.52 (m, 19H, Ar-H), 5.97 (d, 1H, *J* 8.4 Hz, H_c), 5.32 (dd, 1H, *J* 7.2, 8.4 Hz, H_b), 4.38 (d, 1H, *J* 6.8 Hz, H_a), 3.63 (s, 3H, OMe), 3.21-3.13 (m, 1H), 2.82-2.71 (m, 2H), 2.64-2.60 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.7, 202.6, 158.5, 142.7, 139.0, 136.4, 135.0, 132.7, 132.5, 131.2, 130.2, 129.9, 129.2, 129.0, 128.5, 128.4, 128.2, 128.1, 125.9, 125.8, 125.2, 125.0, 121.0, 120.2, 113.5, 80.1(C-Spiro), 64.4, 60.2, 55.0, 53.2, 43.1, 30.3; anal. calcd. for $C_{37}H_{29}NO_3$: C, 82.97; H, 5.46; N, 2.61; found: C, 82.63; H, 4.67; N, 2.85; MS (*m/z*): 536.

2'-Benzoyl-1'-(4-nitrophenyl)-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a] isoquinolin]-2-one (**4g**)

Yellow solid (0.440 g, 80%); m.p. 201-202 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1707, 1681, 1510 and 1374; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-6.73 (m, 19H, Ar-H), 5.32 (d, 1H, *J* 10 Hz, H_c), 4.55 (d, 1H, *J* 9.6 Hz, H_a), 4.46 (t, 1H, *J* 9.6 Hz, H_b), 2.97-2.88 (m, 2H), 2.66-2.61 (m, 1H), 2.52-2.48 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.2, 197.2, 163.2, 160.7, 142.5, 136.8, 134.7, 132.1, 132.0, 131.6, 130.6, 130.5, 129.8, 128.9, 128.7, 127.8, 127.4, 127.1, 126.4, 125.5, 124.9, 124.8, 123.5, 120.8, 116.1, 115.8, 74.7 (C-Spiro), 64.4, 63.8, 50.2, 42.5, 30.4; anal. calcd. for $C_{36}H_{26}N_2O_4$: C, 78.53; H, 4.76; N, 5.09; found: C, 78.77; H, 4.35; N, 4.86; MS (*m/z*): 550.

2'-(4-Methoxybenzoyl)-1'-phenyl-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**4h**)

Yellow solid (0.439 g, 82%); m.p. 197-199 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1713, 1670; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-6.22 (m, 19H, Ar-H), 5.36 (d, 1H, *J* 10 Hz, H_c), 4.57 (d, 1H, *J* 9.2 Hz, H_a), 4.48 (t, 1H, *J* 9.6 Hz, H_b), 3.56 (s, 3H, OMe), 2.98-2.88 (m, 2H), 2.65-2.52 (m, 1H), 2.50-2.47 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.7, 195.6, 162.5, 142.6, 142.5, 138.3, 137.3, 134.8, 131.9, 131.7, 130.2, 129.8, 129.5, 129.1, 129.0, 128.8, 128.7, 128.7, 126.9, 126.3, 125.5, 125.1, 124.7, 123.6, 120.7, 112.6, 75.0 (C-Spiro), 64.3, 63.4, 55.2, 51.1, 42.6, 30.9; anal. calcd. for $C_{37}H_{29}NO_3$: C, 82.97; H, 5.46; N, 2.61; found: C, 82.66; H, 5.01; N, 2.43; MS (*m/z*): 535.

2'-(4-Chlorobenzoyl)-1'-phenyl-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**4i**)

Cream solid (0.447 g, 83%); m.p. 214-216 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1713, 1670; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-6.70 (m, 19H, Ar-H), 5.37 (d, 1H, *J* 9.6 Hz, H_c), 4.55 (d, 1H, *J* 9.6 Hz, H_a), 4.45 (t, 1H, *J* 9.8 Hz, H_b), 2.97-2.90 (m, 2H), 2.69-2.62 (m, 1H), 2.53-2.50 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.4, 196.2 (C=O, chalcone), 142.5, 142.1, 138.3, 138.1, 137.0, 135.3, 134.7, 132.1, 131.5, 129.9, 129.1, 129.1, 128.8, 128.7, 128.5, 128.0, 127.6, 127.0, 126.3, 125.5, 125.1, 124.9, 123.5, 120.9, 74.8 (C-Spiro), 64.3, 64.0, 51.0, 42.5, 30.4; anal. calcd. for $C_{36}H_{26}ClNO_2$: C, 80.06; H, 4.85; N, 2.59; found: C, 79.65; H, 4.56; N, 2.74; MS (*m/z*): 540.

2'-(3-Chlorobenzoyl)-1'-phenyl-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a] isoquinolin]-2-one (**4j**)

Orange solid (0.420 g, 78%); m.p. 212-214 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1704, 1687; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-6.63 (m, 19H, Ar-H), 5.39 (d, 1H, *J* 10 Hz, H_c), 4.52 (d, 1H, *J* 9.2 Hz, H_a), 4.45 (t, 1H, *J* 9.6 Hz, H_b), 2.99-2.91 (m, 2H), 2.68-2.58 (m, 1H), 2.55-2.50 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.4, 196.2, 142.4, 142.1, 138.4, 138.1, 137.0, 134.7, 133.8, 132.0, 131.8, 131.6, 129.8, 129.1, 129.1, 128.9, 128.7, 128.6, 128.0, 127.3, 127.1, 126.4, 125.5, 125.2, 125.1, 125.0, 123.4, 121.1, 74.7 (C-Spiro), 64.4, 63.6, 50.8, 42.5, 30.5; anal. calcd. for $C_{36}H_{26}ClNO_2$: C, 80.06; H, 4.85; N, 2.59; found: C, 79.76; H, 4.50; N, 2.33; MS (*m/z*): 540

2'-(4-Methoxybenzoyl)-1'-(4-methoxyphenyl)-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**4k**)

Orange solid (0.486 g, 86%); m.p. 163-165 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1713, 1676; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-6.23(m, 18H, Ar-H), 5.30 (d, 1H, *J* 10 Hz, H_c), 4.53 (d, 1H, *J* 9.6 Hz, H_a), 4,432 (t, 1H, *J* 9.6 Hz, H_b), 3.84 (s, 3H, OMe), 3.56 (s, 3H, OMe), 2.97-2.88 (m, 2H), 2.65-2.60 (m, 1H), 2.53-2.47 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.8, 195.8, 162.5, 158.5, 142.6, 138.4, 137.3, 134.8, 134.4, 131.9, 131.7, 130.3, 130.0, 129.8, 129.5, 128.8, 128.7, 127.7, 126.2, 125.5, 125.1, 124.7, 123.6, 120.7, 114.5, 112.6, 74.9 (C-Spiro), 64.2, 63.3, 55.3, 55.2, 50.4, 42.6, 30.5; anal. calcd. for $C_{38}H_{31}NO_4$: C, 80.69; H, 5.52; N, 2.48; found: C, 80.84; H, 5.74; N, 2.83; MS (*m/z*): 565.

2'-(3-Chlorobenzoyl)-1'-(4-chlorophenyl)-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**4l**)

Yellow solid (0.435 g, 76%); m.p. 205-207 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1708, 1686; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.12-6.58 (m, 18H, Ar-H), 5.18 (d, 1H, *J* 10 Hz, H_c), 4.54 (d, 1H, *J* 9.2 Hz, H_a), 4.92 (t, 1H, *J* 9.6 Hz, H_b), 2.78-2.71 (m, 2H), 2.61-2.58 (m, 1H), 2.39-2.35 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.3, 196.0, 142.5, 140.7, 138.2, 137.8, 136.8, 134.7, 133.9, 132.9, 132.1, 131.9, 131.5, 130.4, 129.8, 129.3, 129.0, 128.7, 128.6, 128.1, 127.2, 126.5, 125.6, 125.1, 125.1, 124.9, 123.4, 121.1, 74.6 (C-Spiro), 64.3, 64.2, 50.2, 42.5, 30.4; anal. calcd. for $C_{36}H_{25}Cl_2NO_2$: C, 75.26; H, 4.39; N, 2.44; found: C, 75.65; H, 4.69; N, 2.80; MS (*m/z*): 573.

1'-Nitro-2'-phenyl-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7a**)

Yellow solid (0.370 g, 83%); m.p. 196-198 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1708, 1553, 1366; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-7.13 (m, 15H, Ar-H), 6.27 (dd, 1H, *J* 4.8, 7 Hz, H_b), 5.99 (d, 1H, *J* 7 Hz, H_c), 4.78 (d, 1H, *J* 4.8 Hz, H_a), 3.15-3.06 (m, 1H), 2.80-2.67 (m, 2H), 2.64-2.60 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.3, 142.8, 137.7, 135.3, 134.1, 132.7, 132.0, 131.7, 130.3, 129.3, 129.2, 128.5, 128.4, 128.3, 127.8, 127.1, 126.1, 125.6, 124.7, 121.1, 120.7, 92.6 (CH-NO_2), 79.0 (C-Spiro), 64.3, 60.4, 42.5, 30.0; anal. calcd. for $C_{29}H_{22}N_2O_3$: C, 78.01; H, 4.97; N, 6.27; found: C, 77.74; H, 4.69; N, 6.67; MS (*m/z*): 447.

2'-(4-Fluorophenyl)-1'-nitro-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7b**)

Brown solid (0.376 g, 81%); m.p. 183-185 °C, FT-IR (KBr) ν_{max}/cm^{-1} 1704, 1551, 1305; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-6.73 (m, 14H, Ar-H), 6.20 (dd, 1H, *J* 4.8, 7.2 Hz, H_b), 5.96 (d, 1H, *J* 7.2 Hz, H_c), 4.73 (d, 1H, *J* 4.8 Hz, H_a), 3.14-3.06 (m, 1H), 2.79-2.67 (m, 2H), 2.64-2.60 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.5, 162.2, 160.9, 142.8, 137.4, 135.2, 132.6, 131.8, 130.3, 130.2, 129.3, 129.2, 128.4, 127.1, 126.1, 125.7, 124.6, 121.1, 120.8, 115.3, 92.8 (CH-NO_2), 79.0 (C-Spiro), 64.2, 59.74, 42.5, 30.0; anal. calcd. for $C_{29}H_{21}FN_2O_3$: C, 74.99; H, 4.56; N, 6.03; found: C, 74.54; H, 4.14; N, 6.43; MS (*m/z*): 464.

2'-(4-Cholorophenyl)-1'-nitro-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7c**)

Cream solid (0.365 g, 76%); m.p. 190-192 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1711, 1547, 1362; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-6.88 (m, 14H, Ar-H), 6.2 (dd, 1H, *J* 4.8, 7.2 Hz, H_b), 5.95 (d, 1H, *J* 7.2 Hz, H_c), 4.73 (d, 1H, *J* 4.8 Hz, H_a), 3.10-3.05 (m, 1H), 2.78-2.65 (m, 2H), 2.64-2.60 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.2, 142.8, 137.2, 135.2, 133.8, 132.6, 132.5, 131.9, 131.8, 130.3, 129.9, 129.3, 129.2, 128.7, 128.4, 127.2, 126.1, 125.8, 124.6, 121.1, 120.9, 92.5, 78.9 (C-Spiro), 64.2, 59.7, 42.5, 30.0; anal. calcd. for $C_{29}H_{21}ClN_2O_3$: C, 72.42; H, 4.40; N, 5.82; found: C, 72.76; H, 4.03; N, 5.53; MS (*m/z*): 480.

2'-(4-Boromophenyl)-1'-nitro-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-O3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7d**)

Cream solid (0.409 g, 78%); m.p. 186-188 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1711, 1557, 1362; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-6.82 (m, 14H, Ar-H), 6.19 (dd, 1H, *J* 4.8, 7.2 Hz, H_b), 5.94 (d, 1H, *J* 7.2 Hz, H_c), 4.72 (d, 1H, *J* 4.8 Hz, H_a), 3.12-3.05 (m, 1H), 2.76-2.64 (m, 2H), 2.63-2.59 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.2, 142.8, 137.2, 135.2, 133.1, 132.5, 131.9, 131.8, 131.6, 130.3, 129.3, 129.2, 128.4, 127.2, 126.1, 125.8, 125.7, 124.6, 122.0, 121.1, 121.0, 92.5 (CH-NO_2), 78.8 (C-Spiro), 64.2, 59.7, 42.5, 30.0; anal. calcd. for $C_{29}H_{21}BrN_2O_3$: C, 66.30; H, 4.03; N, 5.33; found: C, 66.53; H, 3.81; N, 5.64; MS (*m/z*): 524.

2›-(4-Methylophenyl)-1›-nitro-2›,5›,6›,10b›-tetrahydro-1›H,2H-spiro[acenaphthylene-1,3›-pyrrolo[2,1-a]isoquinolin]-2-one (**7e**)

Yellow solid (0.359 g, 78%); m.p. 195-197 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1712, 1549, 1360; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09-6.82 (m, 14H, Ar-H), 6.25 (dd, 1H, *J* 5.2, 7.2 Hz, H_b), 5.96 (d, 1H, *J* 7.2 Hz, H_c), 4.75 (d, 1H, *J* 4.8 Hz, H_a), 3.13-3.05 (m, 1H), 2.78-2.59 (m, 3H), 2.16 (s, 3H, Me); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.4 (C=O),

142.8, 137.8, 137.5, 135.3, 132.8, 132.0, 131.6, 131.0, 130.3, 129.3, 129.1, 128.4, 128.2, 127.1, 126.1, 125.5, 124.7, 121.1, 120.7, 92.8 (CH-NO_2), 78.9 (C-Spiro), 64.3, 60.1, 42.5, 30.0, 20.9; anal. calcd. for $C_{30}H_{24}N_2O_3$: C, 78.24; H, 5.25; N, 6.06; found: C, 77.91; H, 5.62; N, 5.73; MS (*m/z*): 460.

2'-(4-Methoxyphenyl)-1'-nitro-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7f**)

Yellow solid (0.385 g, 81%); m.p. 194-196 °C, FT-IR (KBr) ν_{max}/cm^{-1} 1705, 1569, 1367; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-6.57 (m, 14H, Ar-H), 6.22 (dd, 1H, *J* 5.2, 7.2 Hz, H_b), 5.97(d, 1H, *J* 7.2 Hz, H_c), 4.72 (d, 1H, *J* 4.8 Hz, H_a), 3.65 (s, 3H, OMe), 3.12-3.06 (m, 1H), 2.79-2.67 (m, 2H), 2.66-2.63 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.6 (C=O), 159.0, 142.8, 137.8, 135.3, 132.8, 132.0, 131.7, 130.3, 129.7, 129.3, 129.1, 128.3, 127.1, 126.1, 126.0, 125.5, 124.6, 121.1, 120.7, 113.8, 93.0 (CH-NO_2), 79.0 (C-Spiro), 64.2, 59.9, 55.1, 42.5, 30.0; anal. calcd. for $C_{30}H_{24}N_2O_4$: C, 75.61; H, 5.08; N, 5.88; found: C, 75.11; H, 4.73; N, 5.42; MS (*m/z*): 476.

2'-(3-Methoxyphenyl)-1'-nitro-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7g**)

Brown solid (0.371 g, 78%); m.p. 180-182 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1711, 1558, 1366; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-6.39 (m, 14H, Ar-H), 6.25 (dd, 1H, *J* 4.8, 7.2 Hz, H_b), 5.95 (d, 1H, *J* 6.8 Hz, H_c), 4.73 (d, 1H, *J* 4.8 Hz, H_a), 3.51 (s, 3H, OMe), 3.14-3.05 (m, 1H), 2.75-2.68 (m, 2H), 2.63-2.59 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.2 (C=O), 159.2, 142.8, 137.8, 135.5, 135.2, 132.7, 132.0, 131.6, 130.3, 129.5, 129.3, 129.2, 128.3, 127.1, 126.1, 125.6, 124.7, 121.1, 120.7, 120.7, 114.1, 113.4, 92.4 (CH-NO_2), 78.9 (C-Spiro), 64.2, 60.3, 55.0, 42.4, 30.0; anal. calcd. for $C_{30}H_{24}N_2O_4$: C, 75.61; H, 5.08; N, 5.88; found: C, 75.92; H, 5.43; N, 5.51; MS (*m/z*): 476.

2'-(4-(Dimethylamino)phenyl)-1'-nitro-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7h**)

Yellow solid (0.396 g, 81%); m.p. 114-116°C; FT-IR (KBr) ν_{max}/cm^{-1} 1708, 1547, 1360; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07-6.38 (m, 14H, Ar-H), 6.19 (dd, 1H, *J* 4.8, 6.8 Hz, H_b), 5.95 (d, 1H, *J* 7.2 Hz, H_c), 4.67 (d, 1H, *J* 4.8 Hz, H_a), 3.13-3.05 (m, 1H), 2.8 (s, 6H, NMe_2), 2.78-2.72 (m, 1H), 2.69-2.66 (m, 1H), 2.62-2.58 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.8 (C=O), 149.7, 142.8, 138.1, 135.3, 133.0, 132.2, 131.5, 130.2, 129.4, 129.3, 129.1, 128.2, 127.0, 126.0, 125.3, 124.6, 121.3, 121.0, 120.6, 112.2, 93.2 (CH-NO_2), 79.0 (C-Spiro), 64.2, 60.0, 42.5, 40.3, 30.0; anal. calcd. for $C_{31}H_{27}N_3O_3$: C, 76.05; H, 5.56; N, 8.58; found: C, 75.74; H, 5.87; N 8.84; MS (*m/z*): 489.

2'-(4-Nitrophenyl)-1'-nitro-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7i**)

Yellow solid (0.383 g, 78%); m.p. 185-187 °C; FT-IR (KBr) ν_{max}/cm^{-1} 1705, 1552, 1515, 1346, 1330; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-7.13 (m, 14H, Ar-H), 6.26 (dd, 1H, *J* 4.8, 7.2 Hz, H_b), 5.98 (d, 1H, *J* 7.2 Hz, H_c), 4.88 (d, 1H, *J* 4.8 Hz, H_a), 3.12-3.05 (m, 1H), 2.78-2.67 (m, 2H), 2.65-2.61 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.7, 147.3, 142.7, 141.5, 136.6, 135.1, 132.2, 132.1, 131.4, 130.3, 129.5, 129.4, 129.2, 128.6, 127.3, 126.2, 126.1, 124.7, 123.6, 121.3, 121.2, 92.0 (CH-NO_2), 79.0 (C-Spiro), 64.2, 59.6, 42.4, 29.9; anal. calcd. for $C_{29}H_{21}N_3O_5$: C, 70.87; H, 4.31; N, 8.55; found: C, 71.11; H, 4.73; N, 8.93; MS (*m/z*): 492.

2'-(4-Cyanophenyl)-1'-nitro-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7j**)

Yellow solid (0.386 g, 82%); m.p. 114-116 °C; FT-IR (KBr) ν_{max}/cm^{-1} 2228 (C≡N, str.), 1708 (C=O, str.), 1552 and 1343 (NO_2, str.); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-7.06 (m, 14H, Ar-H), 6.24 (dd, 1H, *J* 4.8, 7.2 Hz, H_b), 5.61 (d, 1H, *J* 6.8 Hz, H_c), 4.81 (d, 1H, *J* 5.2 Hz, H_a), 3.13-3.05 (m, 1H), 2.78-2.66 (m, 2H), 2.64-2.60 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.9, 142.7, 139.5, 136.8, 135.2, 132.2, 132.2, 131.5, 130.3, 129.4, 129.3, 129.2, 128.6, 127.3, 126.2, 126.1, 124.7, 121.3, 121.1, 118.2, 111.9, 91.9 (CH-NO_2), 79.0 (C-Spiro), 64.2, 59.9, 42.4, 30.0; anal. calcd. for $C_{30}H_{21}N_3O_3$: C, 76.42; H, 4.49; N, 8.91; found: C, 76.81; H, 4.79; N, 9.22; MS (*m/z*): 471.

2'-(2-Chloro-5-nitrophenyl)-1'-nitro-2',5',6',10b'-tetrahydro-1'H,2H-spiro[acenaphthylene-1,3'-pyrrolo[2,1-a]isoquinolin]-2-one (**7k**)

Brown solid (0.420 g, 80%); m.p. 186-188 °C, FT-IR (KBr) ν_{max}/cm^{-1} 1704, 1555, 1528, 1370, 1353; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.57-7.14 (m, 13H, Ar-H), 6.35 (dd, 1H, *J* 4, 8 Hz, H_b), 5.91 (d, 1H, *J* 4 Hz, H_c), 5.37 (d, 1H, *J* 4 Hz, H_a), 2.88-2.85 (m, 1H), 2.62-2.54 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 206.0, 146.7, 142.5, 140.7, 137.8, 135.7, 135.5, 133.0, 132.4, 131.2, 130.7, 130.3, 130.0, 129.4, 129.1, 127.5, 127.2, 126.9, 126.2, 126.0, 124.5, 122.0, 121.3, 92.5 (CH-NO_2), 78.1 (C-Spiro), 65.3, 55.0, 42.3, 30.0; anal. calcd. for $C_{29}H_{20}ClN_3O_5$: C, 66.23; H, 3.83; N, 7.99; found: C, 66.84; H, 4.11; N, 7.53; MS (*m/z*): 525.

1›-Methyl-1›-nitro-2›-phenyl-2›,5›,6›,10b›-tetrahydro-1›H,2H-spiro[acenaphthylene-1,3›-pyrrolo[2,1-a]isoquinolin]-2-one (**7l**)

Brown solid (0.368 g, 80%); m.p. 190-192 °C, FT-IR (KBr) ν_{max}/cm^{-1} 1708, 1537, 1340; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60-7.00 (m, 15H, Ar-H), 5.52 (s, 1H, H_b), 5.15 (s, 1H, H_a), 3.12-3.05 (m, 1H), 2.72-2.56 (m, 3H), 2.06 (s, 3H, Me); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.1, 142.9, 137.5, 134.9, 134.3, 132.7, 132.4, 132.0, 130.4, 129.5, 129.1, 128.7, 128.4, 128.3, 128.0, 126.6, 126.0, 125.5, 122.5, 120.9, 120.8, 98.0 (CH-NO_2), 77.3 (C-Spiro), 70.0, 65.9, 42.1, 30.1, 24.2; anal. calcd. for $C_{30}H_{24}N_2O_3$: C, 78.24; H, 5.25; N, 6.08; found: C, 78.63; H, 5.76; N, 6.51; MS (*m/z*): 460.

Table S1. Bond lengths (Å) for compound **4i**

C(1)-C(2)	1.390(8)	C(18)-H(18)	0.9300
C(1)-H(1)	0.9300	C(19)-C(20)	1.365(9)
C(2)-C(3)	1.370(9)	C(19)-H(19)	0.9300
C(2)-H(2)	0.9300	C(20)-C(21)	1.383(8)
C(3)-C(4)	1.375(8)	C(20)-H(20)	0.9300
C(3)-Cl1	1.749(6)	C(21)-C(22)	1.382(7)
C(4)-C(5)	1.389(7)	C(21)-H(21)	0.9300
C(4)-H(4)	0.9300	C(22)-C(23)	1.532(8)
C(5)-C(6)	1.371(8)	C(23)-C(24)	1.505(8)
C(5)-H(5)	0.9300	C(23)-H(23A)	0.9700
C(6)-C(7)	1.502(7)	C(23)-H(23B)	0.9700
C(7)-O(1)	1.209(7)	C(24)-N(1)	1.473(7)
C(7)-C(8)	1.531(7)	C(24)-H(24A)	0.9700
C(8)-C(25)	1.553(7)	C(24)-H(24B)	0.9700
C(8)-C(9)	1.563(6)	C(25)-N(1)	1.483(7)
C(8)-H(8)	0.9800	C(25)-C(35)	1.512(7)
C(9)-C(10)	1.510(7)	C(25)-C(26)	1.580(8)
C(9)-C(16)	1.534(7)	C(26)-O(2)	1.205(7)
C(9)-H(9)	0.9800	C(26)-C(27)	1.463(8)
C(10)-C(11)	1.369(8)	C(27)-C(28)	1.367(10)
C(10)-C(15)	1.401(8)	C(27)-C(36)	1.4(15)-(10)
C(11)-C(12)	1.392(9)	C(28)-C(29)	1.412(13)
C(11)-H(11)	0.9300	C(28)-H(28)	0.9300
C(12)-C(13)	1.349(9)	C(29)-C(30)	1.355((15)-)
C(12)-H(12)	0.9300	C(29)-H(29)	0.9300
C(13)-C(14)	1.345(10)	C(30)-C(31)	1.426((15)-)
C(13)-H(13)	0.9300	C(30)-H(30)	0.9300
C(14)-C(15)	1.396(8)	C(31)-C(32)	1.423(12)
C(14)-H(14)	0.9300	C(31)-C(36)	1.434(9)
C(15)-H(15)	0.9300	C(32)-C(33)	1.354(12)
C(16)-N(1)	1.463(6)	C(32)-H(32)	0.9300
C(16)-C(17)	1.524(7)	C(33)-C(34)	1.416(8)
C(16)-H(16)	0.9800	C(33)-H(33)	0.9300
C(17)-C(22)	1.384(7)	C(34)-C(35)	1.368(8)
C(17)-C(18)	1.398(7)	C(34)-H(34)	0.9300
C(18)-C(19)	1.376(8)	C(35)-C(36)	1.400(9)

Table S2. Bond angles (degree) for **4i**

C(2)-C(1)-C(6)	120.0(6)	C(16)-N(1)-C(24)	110.6(4)
C(2)-C(1)-H(1)	120.0	C(16)-N(1)-C(25)	109.2(4)
C(6)-C(1)-H(1)	120.0	C(24)-N(1)-C(25)	116.6(4)
C(3)-C(2)-C(1)	119.1(6)	C(18)-C(19)-H(19	119.8
C(3)-C(2)-H(2)	120.4	C(19)-C(20)-C(21)	119.1(5)
C(1)-C(2)-H(2)	120.4	C(19)-C(20)-H(20)	120.4
C(2)-C(3)-C(4)	122.4(5)	C(21)-C(20)-H(20)	120.4
C(2)-C(3)-C(11)	118.3(5)	C(22)-C(21)-C(20)	121.6(6)
C(4)-C(3)-C(11)	119.3(5)	C(22)-C(21)-H(21)	119.2
C(3)-C(4)-C(5)	117.8(6)	C(20)-C(21)-H(21)	119.2
C(3)-C(4)-H(4)	121.1	C(21)-C(22)-C(17)	119.1(5)
C(5)-C(4)-H(4)	121.1	C(21)-C(22)-C(23)	119.7(5)
C(6)-C(5)-C(4)	122.1(5)	C(17)-C(22)-C(23)	121.1(5)
C(6)-C(5)-H(5)	119.0	C(24)-C(23)-C(22)	113.8(5)
C(4)-C(5)-H(5)	119.0	C(24)-C(23)-H(23A)	108.8
C(5)-C(6)-C(1)	118.7(5)	C(22)-C(23)-H(23A)	108.8
C(5)-C(6)-C(7)	125.3(5)	C(24)-C(23)-H(23B)	108.8
C(1)-C(6)-C(7)	116.0(5)	C(22)-C(23)-H(23B)	108.8
O(1)-C(7)-C(6)	120.2(5)	H(23A)-C(23)-(23B)	107.7
O(1)-C(7)-C(8)	121.7(5)	N(1)-C(24)-C(23)	107.7(5)
C(6)-C(7)-C(8)	118.1(5)	N(1)-C(24)-H(24A)	110.2
C(7)-C(8)-C(25)	114.3(4)	C(23)-C(24)-H(24A)	110.2
C(7)-C(8)-C(9)	111.8(4)	N(1)-C(24)-H(24B)	110.2
C(25)-C(8)-C(9)	106.4(4)	C(23)-C(24)-H(24B)	110.2
C(7)-C(8)-H(8)	108.0	H(24A)-C24-H(24B)	108.5
C(25)-C(8)-H(8)	108.0	N(1)-C(25)-C(35)	110.5(4)
C(9)-C(8)-H(8)	108.0	N(1)-C(25)-C(8)	101.9(4)
C(10)-C(9)-C(16)	117.3(4)	C(35)-C(25)-C(8)	118.4(4)
C(10)-C(9)-C(8)	110.0(4)	N(1)-C(25)-C(26)	114.7(4)
C(16)-C(9)-C(8)	103.6(4)	C(35)-C(25)-C(26)	103.2(4)
C(10)-C(9)-H(9)	108.6	C(8)-C(25)-C(26)	108.7(5)
C(16)-C(9)-H(9)	108.6	O(2)-C(26)-C(27)	128.5(7)
C(8)-C(9)-H(9)	108.6	O(2)-C(26)-C(25)	124.2(5)
C(11)-C(10)-C(15)	117.0(5)	C(27)-C(26)-C(25)	107.3(5)
C(11)-C(10)-C(9)	120.2(5)	C(28)-C(27)-C(36)	119.9(7)
C(15)-C(10)-C(9)	122.6(5)	C(28)-C(27)-C(26)	133.0(8)
C(10)-C(11)-C(12)	121.6(6)	C(36)-C(27)-C(26)	107.2(6)
C(10)-C(11)-H(11)	119.2	C(27)-C(28)-C(29)	117.8(9)
C(12)-C(11)-H(11)	119.2	C(27)-C(28)-H(28)	121.1
C(13)-C(12)-C(11)	120.7(7)	C(29)-C(28)-H(28)	121.1
C(13)-C(12)-H(12)	119.7	C(30)-C(29)-C(28)	122.3(10)
C(11)-C(12)-H(12)	119.7	C(30)-C(29)-H(29)	118.8
C(14)-C(13)-C(12)	119.2(6)	C(28)-C(29)-H(29)	118.8
C(14)-C(13)-H(13)	120.4	C(29)-C(30)-C(31)	123.5(10)
C(12)-C(13)-H(13)	120.4	C(29)-C(30)-H(30)	118.2
C(13)-C(14)-C(15)	121.7(7)	C(31)-C(30)-H(30)	118.2
C(13)-C(14)-H(14)	119.2	C(32)-C(31)-C(30)	131.7(9)
C(15)-C(14)-H(14)	119.2	C(32)-C(31)-C(36)	1(15)-.9(8)
C(14)-C(15)-C(10)	119.7(6)	C(30)-C(31)-C(36)	112.4(10)
C(14)-C(15)-H(15)	120.1	C(33)-C(32)-C(31)	121.4(7)
C(10)-C(15)-H(15)	120.1	C(33)-C(32)-H(32)	119.3
N(1)-C(16)-C(17)	109.0(4)	C(31)-C(32)-H(32)	119.3
N(1)-C(16)-C(9)	101.0(4)	C(32)-C(33)-C(34)	121.7(8)
C(17)-C(16)-C(9)	117.1(4)	C(32)-C(33)-H(33)	119.2
N(1)-C(16)-H(16)	109.8	C(34)-C(33)-H(33)	119.2
C(17)-C(16)-H(16)	109.8	C(35)-C(34)-C(33)	119.2(7)
C(9)-C(16)-H(16)	109.8	C(35)-C(34)-H(34)	120.4
C(22)-C(17)-C(18)	118.9(5)	C(33)-C(34)-H(34)	120.4
C(22)-C(17)-C(16)	119.2(4)	C(34)-C(35)-C(36)	120.0(6)
C(18)-C(17)-C(16)	121.8(5)	C(34)-C(35)-C(25)	132.0(6)
C(19)-C(18)-C(17)	120.9(6)	C(36)-C(35)-C(25)	108.0(6)
C(19)-C(18)-H(18)	119.6	C(35)-C(36)-C(27)	114.2(5)
C(17)-C(18)-H(18)	119.6	C(35)-C(36)-C(31)	121.8(8)
C(20)-C(19)-C(18)	120.3(6)	C(27)-C(36)-C(31)	124.0(8)
C(20)-C(19)-H(19)	119.8		

Table S3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compound **4i**

	x	y	z	U(eq)
C(1)	0.3108(6)	0.1219(4)	–0.0957(4)	0.0666(17)
H(1)	0.3471	0.1068	–0.1408	0.080
C(2)	0.3857(6)	0.1038(4)	–0.0201(4)	0.074(2)
H(2)	0.4722	0.0766	–0.0143	0.089
C(3)	0.3306(6)	0.1265(4)	0.0457(4)	0.0642(17)
C(4)	0.2023(6)	0.1661(4)	0.0398(4)	0.0640(17)
H(4)	0.1657	0.1802	0.0852	0.077
C(5)	0.1294(6)	0.1842(3)	–0.0361(3)	0.0530(14)
H(5)	0.0433	0.2117	–0.0412	0.064
C(6)	0.1802(5)	0.1629(3)	–0.1038(3)	0.0467(13)
C(7)	0.1068(5)	0.1792(3)	–0.1878(3)	0.0480(13)
C(8)	–0.0216(5)	0.2342(3)	–0.2002(3)	0.0433(12)
H(8)	–0.0867	0.2206	–0.1626	0.052
C(9)	–0.1109(5)	0.2296(3)	–0.2866(3)	0.0420(12)
H(9)	–0.0460	0.2122	–0.3226	0.050
C(10)	–0.2341(6)	0.1736(3)	–0.2887(3)	0.0459(13)
C(11)	–0.2099(6)	0.0984(4)	–0.2982(4)	0.0683(18)
H(11)	–0.1193	0.0830	–0.3083	0.082
C(12)	–0.3175(8)	0.0447(4)	–0.2932(4)	0.078(2)
H(12)	–0.2975	–0.0060	–0.2995	0.093
C(13)	–0.4504(8)	0.0653(4)	–0.2793(4)	0.074(2)
H(13)	–0.5211	0.0290	–0.2746	0.089
C(14)	–0.4794(7)	0.1388(4)	–0.2723(4)	0.075(2)
H(14)	–0.5723	0.1531	–0.2650	0.090
C(15)	–0.3735(6)	0.1942(4)	–0.2756(4)	0.0674(17)
H(15)	–0.3953	0.2447	–0.2692	0.081
C(16)	–0.(15)-22(5)	0.3118(3)	–0.3075(3)	0.0420(12)
H(16)	–0.2367	0.3259	–0.2832	0.050
C(17)	–0.1787(5)	0.3336(3)	–0.3956(3)	0.0425(12)
C(18)	–0.2530(6)	0.2861(3)	–0.4541(3)	0.0521(14)
H(18)	–0.2814	0.2383	–0.4397	0.063
C(19)	–0.2847(6)	0.3090(4)	–0.5326(4)	0.0641(17)
H(19)	–0.3338	0.2767	–0.5708	0.077
C(20)	–0.2443(6)	0.3790(4)	–0.5547(3)	0.0645(17)
H(20)	–0.2655	0.3946	–0.6077	0.077
C(21)	–0.1714(6)	0.4265(4)	–0.4971(4)	0.0621(16)
H(21)	–0.1454	0.4746	–0.5119	0.075
C(22)	–0.1361(6)	0.4043(3)	–0.4181(3)	0.0522(14)
C(23)	–0.0475(7)	0.4572(3)	–0.3574(3)	0.0673(18)
H(23A)	0.0517	0.4599	–0.3681	0.081
H(23B)	–0.0887	0.5073	–0.3648	0.081
C(24)	–0.0436(7)	0.4332(3)	–0.2719(4)	0.0650(18)
H(24A)	0.0357	0.4585	–0.2376	0.078
H(24B)	–0.1345	0.4463	–0.2545	0.078
C(25)	0.0228(5)	0.3181(3)	–0.1865(3)	0.0464(13)
C(26)	–0.0598(7)	0.3511(3)	–0.1204(4)	0.0606(16)
C(27)	0.0512(9)	0.3788(4)	–0.0557(3)	0.0734(19)
C(28)	0.0438(11)	0.4093(5)	0.0172(4)	0.112(3)
H(28)	–0.0452	0.4155	0.0344	0.134
C(29)	0.1760(16)	0.4310(8)	0.0655(6)	0.148(5)
H(29)	0.1731	0.4508	0.1157	0.178
C(30)	0.3068(16)	0.4239(8)	0.0413(7)	0.154(5)
H(30)	0.3896	0.4410	0.0749	0.185

Table S3. continuation

	x	y	z	U(eq)
C(31)	0.3246(11)	0.3916(5)	–0.0331(5)	0.097(3)
C(32)	0.4511(9)	0.3779(5)	–0.0677(6)	0.106(3)
H(32)	0.5424	0.3902	–0.0392	0.127
H(32)	0.5424	0.3902	–0.0392	0.127
C(33)	0.4414(7)	0.3473(4)	–0.1412(6)	0.089(3)
H(33)	0.5259	0.3411	–0.1629	0.107
C(34)	0.3058(6)	0.3247(4)	–0.1857(4)	0.0675(18)
H(34)	0.3017	0.3022	–0.2353	0.081
C(35)	0.1809(6)	0.3364(3)	–0.1550(3)	0.0531(14)
C(36)	0.1883(8)	0.3690(4)	–0.0797(4)	0.074(2)
N(1)	–0.0219(5)	0.3510(2)	–0.2673(3)	0.0504(11)
O(1)	0.1498(4)	0.1498(3)	–0.2434(3)	0.0731(13)
O(2)	–0.1907(5)	0.3535(3)	–0.1261(3)	0.0834(14)
Cl(1)	0.4243(2)	0.10107(15)	0.14009(11)	0.1071(8)

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **4i**.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	0.063(4)	0.070(4)	0.067(4)	0.026(3)	0.015(3)	0.015(3)
C(2)	0.082(5)	0.049(3)	0.090(5)	0.032(4)	0.009(3)	0.014(3)
C(3)	0.053(3)	0.076(5)	0.059(4)	0.029(3)	–0.001(3)	0.002(3)
C(4)	0.062(4)	0.067(4)	0.061(4)	0.010(3)	0.005(3)	0.002(3)
C(5)	0.045(3)	0.054(4)	0.056(3)	0.010(3)	–0.001(3)	0.001(3)
C(6)	0.042(3)	0.037(3)	0.059(3)	0.011(3)	0.003(2)	–0.002(2)
C(7)	0.048(3)	0.039(3)	0.056(3)	0.005(3)	0.004(3)	–0.001(2)
C(8)	0.042(3)	0.038(3)	0.049(3)	0.008(2)	0.004(2)	–0.002(2)
C(9)	0.044(3)	0.040(3)	0.042(3)	0.003(2)	0.006(2)	0.006(2)
C(10)	0.054(3)	0.042(3)	0.038(3)	–0.002(2)	0.003(2)	–0.003(2)
C(11)	0.053(3)	0.054(4)	0.093(5)	–0.002(4)	–0.001(3)	–0.001(3)
C(12)	0.082(5)	0.046(4)	0.097(5)	0.001(4)	–0.010(4)	–0.010(3)
C(13)	0.072(5)	0.059(4)	0.082(5)	0.021(4)	–0.013(4)	–0.021(3)
C(14)	0.046(3)	0.094(6)	0.084(5)	0.010(4)	0.009(3)	–0.021(4)
C(15)	0.062(4)	0.059(4)	0.082(4)	–0.001(3)	0.014(3)	–0.003(3)
C(16)	0.033(2)	0.045(3)	0.045(3)	–0.001(2)	–0.001(2)	–0.006(2)
C(17)	0.040(3)	0.038(3)	0.048(3)	0.001(2)	0.005(2)	0.003(2)
C(18)	0.057(3)	0.049(3)	0.049(3)	–0.001(3)	0.003(3)	–0.007(3)
C(19)	0.063(4)	0.071(5)	0.054(4)	–0.006(3)	–0.004(3)	–0.002(3)
C(20)	0.062(4)	0.089(5)	0.041(3)	0.011(3)	0.003(3)	0.013(3)
C(21)	0.063(4)	0.056(4)	0.066(4)	0.018(3)	0.008(3)	0.001(3)
C(22)	0.050(3)	0.050(4)	0.055(3)	0.005(3)	0.004(2)	0.007(3)
C(23)	0.093(5)	0.039(3)	0.066(4)	0.007(3)	0.003(3)	–0.006(3)
C(24)	0.071(4)	0.039(3)	0.077(4)	–0.004(3)	–0.010(3)	–0.005(3)
C(25)	0.043(3)	0.044(3)	0.051(3)	–0.003(2)	0.003(2)	0.001(2)
C(26)	0.062(4)	0.049(4)	0.069(4)	–0.001(3)	0.004(3)	0.002(3)
C(27)	0.114(6)	0.060(4)	0.042(3)	0.001(3)	–0.002(3)	0.008(4)
C(28)	0.153(8)	0.116(8)	0.062(5)	–0.014(5)	0.007(5)	–0.004(6)
C(29)	0.229(14)	0.149(10)	0.055(5)	–0.038(6)	–0.010(8)	–0.011(11)
C(30)	0.194(13)	0.143(11)	0.096(9)	–0.009(8)	–0.059(9)	–0.030(11)
C(31)	0.121(7)	0.074(5)	0.076(5)	0.007(4)	–0.039(5)	–0.006(5)
C(32)	0.071(5)	0.095(6)	0.129(8)	0.026(6)	–0.048(5)	–0.014(5)

Table S4. continuation

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(33)	0.052(4)	0.068(5)	0.135(7)	0.030(5)	–0.019(4)	–0.007(3)
C(34)	0.057(4)	0.048(4)	0.093(5)	0.013(3)	0.001(3)	–0.002(3)
C(35)	0.057(3)	0.040(3)	0.057(3)	0.007(3)	–0.003(3)	–0.003(3)
C(36)	0.079(5)	0.058(4)	0.073(4)	0.012(3)	–0.024(4)	–0.003(3)
N(1)	0.059(3)	0.038(3)	0.050(3)	–0.001(2)	–0.002(2)	–0.002(2)
O(1)	0.073(3)	0.085(3)	0.060(3)	–0.010(2)	0.006(2)	0.027(2)
O(2)	0.067(3)	0.087(4)	0.099(4)	–0.014(3)	0.024(3)	0.003(3)
C(l1)	0.0880(13)	0.152(2)	0.0724(12)	0.0388(13)	–0.0110(10)	0.0253(13)

Table S5. Torsion angles (degree) for compound **4i**

C(9)-C(8)-C(25)-N(1)	–8.6(5)	C(26)-C(25)-C(35)-C(34)	–177.8(6)
C(7)-C(8)-C(25)-C(35)	–6.0(7)	N(1)-C(25)-C(35)-C(36)	127.2(5)
C(9)-C(8)-C(25)-C(35)	–130.0(5)	C(8)-C(25)-C(35)-C(36)	–116.0(6)
C(7)-C(8)-C(25)-C(26)	–123.2(5)	C(26)-C(25)-C(35)-C(36)	4.1(6)
C(9)-C(8)-C(25)-C(26)	112.8(5)	C(34)-C(35)-C(36)-C(27)	179.2(6)
N(1)-C(25)-C(26)-O(2)	53.5(8)	C(25)-C(35)-C(36)-C(27)	–2.5(7)
C(35)-C(25)-C(26)-O(2)	173.8(6)	C(34)-C(35)-C(36)-C(31)	0.5(9)
C(8)-C(25)-C(26)-O(2)	–59.7(7)	C(25)-C(35)-C(36)-C(31)	178.9(6)
N(1)-C(25)-C(26)-C(27)	–124.7(5)	C(28)-C(27)-C(36)-C(35)	179.1(7)
C(35)-C(25)-C(26)-C(27)	–4.5(6)	C(26)-C(27)-C(36)-C(35)	–0.5(8)
C(8)-C(25)-C(26)-C(27)	122.0(5)	C(28)-C(27)-C(36)-C(31)	–2.3(11)
O(2)-C(26)-C(27)-C(28)	5.5(13)	C(26)-C(27)-C(36)-C(31)	178.1(6)
C(25)-C(26)-C(27)-C(28)	–176.4(8)	C(32)-C(31)-C(36)-C(35)	–0.8(10)
O(2)-C(26)-C(27)-C(36)	–174.9(7)	C(30)-C(31)-C(36)-C(35)	179.7(8)
C(25)-C(26)-C(27)-C(36)	3.2(7)	C(32)-C(31)-C(36)-C(27)	–179.3(7)
C(36)-C(27)-C(28)-C(29)	1.0(13)	C(30)-C(31)-C(36)-C(27)	1.2(11)
C(26)-C(27)-C(28)-C(29)	–179.5(9)	C(17)-C(16)-N(1)-C(24)	62.4(6)
C(27)-C(28)-C(29)-C(30)	1.3(19)	C(9)-C(16)-N(1)-C(24)	–173.7(5)
C(28)-C(29)-C(30)-C(31)	–2(2)	C(17)-C(16)-N(1)-C(25)	–168.0(4)
C(29)-C(30)-C(31)-C(32)	–178.3(12)	C(9)-C(16)-N(1)-C(25)	–44.1(5)
C(29)-C(30)-C(31)-C(36)	1.1(17)	C(23)-C(24)-N(1)-C(16)	–69.6(6)
C(30)-C(31)-C(32)-C(33)	–178.7(10)	C(23)-C(24)-N(1)-C(25)	164.8(5)
C(36)-C(31)-C(32)-C(33)	1.9(12)	C(35)-C(25)-N(1)-C(16)	159.9(4)
C(31)-C(32)-C(33)-C(34)	–2.7(12)	C(8)-C(25)-N(1)-C(16)	33.2(5)
C(32)-C(33)-C(34)-C(35)	2.3(10)	C(26)-C(25)-N(1)-C(16)	–84.1(5)
C(33)-C(34)-C(35)-C(36)	–1.2(9)	C(35)-C(25)-N(1)-C(24)	–73.9(6)
C(33)-C(34)-C(35)-C(25)	–179.1(6)	C(8)-C(25)-N(1)-C(24)	159.5(5)
N(1)-C(25)-C(35)-C(34)	–54.8(8)	C(26)-C(25)-N(1)-C(24)	42.2(7)
C(8)-C(25)-C(35)-C(34)	62.1(8)		

Table S6. Bond lengths (Å) for compound **7f**

C(1)-O(1)	1.210(3)	C(17)-C(19)	1.381(4)
C(1)-C(2)	1.478(4)	C(18)-O(2)	1.410(3)
C(1)-C(12)	1.579(3)	C(18)-H(18A)	0.9600
C(2)-C(3)	1.372(4)	C(18)-H(18B)	0.9600
C(2)-C(11)	1.405(4)	C(18)-H(18C)	0.9600
C(3)-C(4)	1.416(5)	C(19)-C(20)	1.370(4)
C(3)-H(3)	0.9300	C(19)-H(19)	0.9300
C(4)-C(5)	1.370(6)	C(20)-H(20)	0.9300
C(4)-H(4)	0.9300	C(21)-N(2)	1.513(3)
C(5)-C(6)	1.409(6)	C(21)-C(22)	1.533(3)
C(5)-H(5)	0.9300	C(21)-H(21)	0.9800
C(6)-C(11)	1.410(4)	C(22)-N(1)	1.457(3)
C(6)-C(7)	1.416(5)	C(22)-C(23)	1.509(3)
C(7)-C(8)	1.361(5)	C(22)-H(22)	0.9800
C(7)-H(7)	0.9300	C(23)-C(28)	1.389(4)
C(8)-C(9)	1.408(4)	C(23)-C(24)	1.395(4)
C(8)-H(8)	0.9300	C(24)-C(25)	1.382(4)
C(9)-C(10)	1.362(4)	C(24)-H(24)	0.9300
C(9)-H(9)	0.9300	C(25)-C(26)	1.374(5)
C(10)-C(11)	1.401(4)	C(25)-H(25)	0.9300
C(10)-C(12)	1.513(3)	C(26)-C(27)	1.368(5)
C(12)-N(1)	1.466(3)	C(26)-H(26)	0.9300
C(12)-C(13)	1.566(3)	C(27)-C(28)	1.396(4)
C(13)-C(14)	1.509(3)	C(27)-H(27)	0.9300
C(13)-C(21)	1.548(3)	C(28)-C(29)	1.508(4)
C(13)-H(13)	0.9800	C(29)-C(30)	1.511(4)
C(14)-C(15)	1.386(3)	C(29)-H(29A)	0.9700
C(14)-C(20)	1.389(3)	C(29)-H(29B)	0.9700
C(15)-C(16)	1.390(4)	C(30)-(N1)	1.457(3)
C(15)-H(15)	0.9300	C(30)-H(30A)	0.9700
C(16)-C(17)	1.378(3)	C(30)-H(30B)	0.9700
C(16)-H(16)	0.9300	N(2)-O(4)	1.213(3)
C(17)-O(2)	1.363(3)	N(2)-O(3)	1.223(3)

Table S7. Bond angles (degree) for compound **7f**

O(1)-C(1)-C(2)	127.7(3)	H(18A)-C(18)-H(18B)	109.5
O(1)-C(1)-C(12)	124.8(2)	O(2)-C(18)-H(18C)	109.5
C(2)-C(1)-C(12)	107.3(2)	H(18A)-C(18)-H(18C)	109.5
C(3)-C(2)-C(11)	119.5(3)	H(18B)-C(18)-H(18C)	109.5
C(3)-C(2)-C(1)	132.9(3)	C(20)-C(19)-C(17)	120.8(2)
C(11)-C(2)-C(1)	107.6(2)	C(20)-C(19)-H(19)	119.6
C(2)-C(3)-C(4)	117.6(4)	C(17)-C(19)-H(19)	119.6
C(2)-C(3)-H(3)	121.2	C(19)-C(20)-C(14)	121.3(2)
C(4)-C(3)-H(3)	121.2	C(19)-C(20)-H(20)	119.4
C(5)-C(4)-C(3)	122.5(4)	C(14)-C(20)-H(20)	119.4
C(5)-C(4)-H(4)	118.7	N(2)-C(21)-C(22)	110.5(2)
C(3)-C(4)-H(4)	118.7	N(2)-C(21)-C(13)	110.6(2)
C(4)-C(5)-C(6)	121.5(4)	C(22)-C(21)-C(13)	104.7(2)
C(4)-C(5)-H(5)	119.2	N(2)-C(21)-H(21)	110.3
C(6)-C(5)-H(5)	119.2	C(22)-C(21)-H(21)	110.3
C(5)-C(6)-C(11)	114.8(4)	C(13)-C(21)-H(21)	110.3
C(5)-C(6)-C(7)	128.7(4)	N(1)-C(22)-C(23)	110.9(2)
C(11)-C(6)-C(7)	116.5(3)	N(1)-C(22)-C(21)	102.31(19)
C(8)-C(7)-C(6)	120.1(3)	C(23)-C(22)-C(21)	119.3(2)
C(8)-C(7)-H(7)	119.9	N(1)-C(22)-H(22)	107.9
C(6)-C(7)-H(7)	119.9	C(23)-C(22)-H(22)	107.9
C(7)-C(8)-C(9)	122.4(4)	C(21)-C(22)-H(22)	107.9
C(7)-C(8)-H(8)	118.8	C(28)-C(23)-C(24)	119.8(2)
C(9)-C(8)-H(8)	118.8	C(28)-C(23)-C(22)	119.3(2)
C(10)-C(9)-C(8)	119.0(3)	C(24)-C(23)-C(22)	120.9(2)
C(10)-C(9)-H(9)	120.5	C(25)-C(24)-C(23)	120.5(3)
C(8)-C(9)-H(9)	120.5	C(25)-C(24)-H(24)	119.8
C(9)-C(10)-C(11)	119.3(3)	C(23)-C(24)-H(24)	119.8
C(9)-C(10)-C(12)	131.4(3)	C(26)-C(25)-C(24)	119.7(3)
C(11)-C(10)-C(12)	109.4(2)	C(26)-C(25)-H(25)	120.1
C(10)-C(11)-C(2)	113.3(2)	C(24)-C(25)-H(25)	120.1
C(10)-C(11)-C(6)	122.7(3)	C(27)-C(26)-C(25)	120.1(3)
C(2)-C(11)-C(6)	124.0(3)	C(27)-C(26)-H(26)	119.9
N(1)-C(12)-C(10)	112.48(19)	C(25)-C(26)-H(26)	119.9
N(1)-C(12)-C(13)	102.57(19)	C(26)-C(27)-C(28)	121.5(3)
C(10)-C(12)-C(13)	113.3(2)	C(26)-C(27)-H(27)	119.3
N(1)-C(12)-C(1)	112.6(2)	C(28)-C(27)-H(27)	119.3
C(10)-C(12)-C(1)	102.4(2)	C(23)-C(28)-C(27)	118.4(3)
C(13)-C(12)-C(1)	113.91(19)	C(23)-C(28)-C(29)	121.7(2)
C(14)-C(13)-C(21)	115.7(2)	C(27)-C(28)-C(29)	119.8(3)
C(14)-C(13)-C(12)	115.14(19)	C(28)-C(29)-C(30)	113.7(2)
C(21)-C(13)-C(12)	105.21(19)	C(28)-C(29)-H(29A)	108.8
C(14)-C(13)-H(13)	106.7	C(30)-C(29)-H(29A)	108.8
C(21)-C(13)-H(13)	106.7	C(28)-C(29)-H(29B)	108.8
C(12)-C(13)-H(13)	106.7	C(30)-C(29)-H(29B)	108.8
C(15)-C(14)-C(20)	117.3(2)	H(29A)-C(29)-H(29B)	107.7
C(15)-C(14)-C(13)	119.3(2)	N(1)-C(30)-C(29)	108.1(2)
C(20)-C(14)-C(13)	123.3(2)	N(1)-C(30)-H(30A)	110.1
C(14)-C(15)-C(16)	121.9(2)	C(29)-C(30)-H(30A)	110.1
C(14)-C(15)-H(15)	119.1	N(1)-C(30)-H(30B)	110.1
C(16)-C(15)-H(15)	119.1	C(29)-C(30)-H(30B)	110.1
C(17)-C(16)-C(15)	119.4(2)	H(30A)-C(30)-H(30B)	108.4
C(17)-C(16)-H(16)	120.3	C(30)-N(1)-C(22)	112.3(2)
C(15)-C(16)-H(16)	120.3	C(30)-N(1)-C(12)	118.0(2)
O(2)-C(17)-C(16)	124.9(2)	C(22)-N(1)-C(12)	107.51(19)
O(2)-C(17)-C(19)	115.7(2)	O(4)-N(2)-O(3)	124.3(3)
C(16)-C(17)-C(19)	119.3(2)	O(4)-N(2)-C(21)	118.7(3)
O(2)-C(18)-H(18A)	109.5	O(3)-N(2)-C(21)	116.9(3)
O(2)-C(18)-H(18B)	109.5	C(17)-O(2)-C(18)	118.1(2)

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compound **7f**

	x	y	z	U(eq)
C(1)	0.82986(18)	0.47015(19)	0.9203(2)	0.0488(6)
C(2)	0.8255(2)	0.37850(19)	0.9789(3)	0.0560(7)
C(3)	0.8623(2)	0.2922(2)	0.9717(3)	0.0759(10)
H(3)	0.8977	0.2826	0.9215	0.091
C(4)	0.8445(3)	0.2184(2)	1.0436(4)	0.0985(15)
H(4)	0.8684	0.1592	1.0392	0.118
C(5)	0.7932(3)	0.2307(3)	1.1192(4)	0.0963(14)
H(5)	0.7846	0.1803	1.1660	0.116
C(6)	0.7533(2)	0.3179(2)	1.1278(3)	0.0731(10)
C(7)	0.6991(3)	0.3423(3)	1.2008(3)	0.0891(13)
H(7)	0.6858	0.2975	1.2516	0.107
C(8)	0.6664(3)	0.4312(3)	1.1968(3)	0.0834(11)
H(8)	0.6302	0.4456	1.2445	0.100
C(9)	0.6854(2)	0.5022(2)	1.1231(3)	0.0641(8)
H(9)	0.6623	0.5624	1.1224	0.077
C(10)	0.73825(19)	0.48147(19)	1.0528(2)	0.0493(6)
C(11)	0.7718(2)	0.39013(19)	1.0551(3)	0.0547(7)
C(12)	0.76971(17)	0.54115(17)	0.9651(2)	0.0426(6)
C(13)	0.68977(16)	0.58509(17)	0.8560(2)	0.0411(6)
H(13)	0.6377	0.5889	0.8853	0.049
C(14)	0.65943(16)	0.52870(16)	0.7367(2)	0.0391(5)
C(15)	0.59195(18)	0.46183(19)	0.7190(2)	0.0485(6)
H(15)	0.5643	0.4551	0.7792	0.058
C(16)	0.56451(18)	0.40457(19)	0.6139(3)	0.0495(6)
H(16)	0.5190	0.3603	0.6040	0.059
C(17)	0.60534(17)	0.41409(18)	0.5244(2)	0.0450(6)
C(18)	0.5253(2)	0.2852(2)	0.4043(3)	0.0751(9)
H(18A)	0.4680	0.3081	0.4055	0.090
H(18B)	0.5497	0.2414	0.4714	0.090
H(18C)	0.5171	0.2545	0.3261	0.090
C(19)	0.67109(18)	0.48204(18)	0.5394(2)	0.0485(6)
H(19)	0.6975	0.4900	0.4780	0.058
C(20)	0.69786(17)	0.53789(18)	0.6436(2)	0.0457(6)
H(20)	0.7426	0.5828	0.6521	0.055
C(21)	0.71952(17)	0.68721(17)	0.8439(2)	0.0436(6)
H(21)	0.7150	0.7004	0.7574	0.052
C(22)	0.81870(16)	0.69174(17)	0.9300(2)	0.0408(6)
H(22)	0.8565	0.6671	0.8837	0.049
C(23)	0.85818(16)	0.78463(17)	0.9864(2)	0.0431(6)
C(24)	0.83907(18)	0.86683(18)	0.9156(3)	0.0509(7)
H(24)	0.8007	0.8648	0.8329	0.061
C(25)	0.8768(2)	0.9513(2)	0.9674(3)	0.0635(8)
H(25)	0.8638	1.0059	0.9198	0.076
C(26)	0.9334(2)	0.9543(2)	1.0896(4)	0.0718(9)
H(26)	0.9581	1.0113	1.1252	0.086
C(27)	0.9537(2)	0.8738(2)	1.1590(3)	0.0663(8)
H(27)	0.9928	0.8766	1.2412	0.080
C(28)	0.91694(18)	0.7874(2)	1.1091(3)	0.0513(7)
C(29)	0.9412(2)	0.7001(2)	1.1886(3)	0.0654(8)
H(29A)	0.9132	0.7036	1.2527	0.079
H(29B)	1.0064	0.6984	1.2300	0.079
C(30)	0.91163(19)	0.6102(2)	1.1158(3)	0.0584(7)
H(30A)	0.9531	0.5945	1.0718	0.070

Table S8. continuation

	x	y	z	U(eq)
H(30B)	0.9117	0.5591	1.1722	0.070
N(1)	0.82057(14)	0.62414(14)	1.02699(19)	0.0429(5)
N(2)	0.66230(16)	0.75600(17)	0.8864(3)	0.0593(6)
O(1)	0.87438(15)	0.49068(15)	0.8554(2)	0.0671(6)
O(2)	0.58586(14)	0.36100(15)	0.41888(19)	0.0657(6)
O(3)	0.63236(15)	0.82365(15)	0.8189(3)	0.0842(7)
O(4)	0.64971(17)	0.74155(18)	0.9845(3)	0.0889(8)

Table S9. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **7f**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	0.0507(15)	0.0498(16)	0.0432(15)	–0.0010(12)	0.0124(13)	0.0095(12)
C(2)	0.0614(18)	0.0434(16)	0.0479(16)	–0.0014(13)	–0.0015(14)	0.0050(13)
C(3)	0.086(2)	0.0497(18)	0.068(2)	–0.0051(16)	–0.0059(18)	0.0119(16)
C(4)	0.115(4)	0.0370(19)	0.096(3)	–0.001(2)	–0.027(3)	0.0048(19)
C(5)	0.110(3)	0.058(2)	0.080(3)	0.019(2)	–0.022(2)	–0.031(2)
C(6)	0.086(2)	0.052(2)	0.0552(19)	0.0114(15)	–0.0102(18)	–0.0279(17)
C(7)	0.097(3)	0.104(3)	0.052(2)	0.022(2)	0.006(2)	–0.047(2)
C(8)	0.088(3)	0.113(3)	0.053(2)	0.005(2)	0.0278(19)	–0.037(2)
C(9)	0.074(2)	0.078(2)	0.0452(17)	–0.0052(15)	0.0265(16)	–0.0208(17)
C(10)	0.0599(17)	0.0483(16)	0.0381(14)	–0.0024(12)	0.0144(12)	–0.0133(13)
C(11)	0.0630(18)	0.0470(17)	0.0420(15)	0.0015(12)	0.0017(13)	–0.0136(13)
C(12)	0.0478(14)	0.0410(14)	0.0399(14)	–0.0006(11)	0.0159(12)	–0.0002(11)
C(13)	0.0383(13)	0.0427(14)	0.0453(14)	–0.0013(11)	0.0181(12)	0.0013(10)
C(14)	0.0399(13)	0.0355(13)	0.0422(13)	0.0022(11)	0.0141(11)	0.0031(10)
C(15)	0.0492(15)	0.0528(16)	0.0500(15)	–0.0006(13)	0.0252(13)	–0.0059(12)
C(16)	0.0434(14)	0.0504(16)	0.0554(16)	–0.0032(13)	0.0176(13)	–0.0141(12)
C(17)	0.0421(14)	0.0451(14)	0.0457(15)	–0.0044(12)	0.0119(12)	–0.0005(11)
C(18)	0.066(2)	0.077(2)	0.073(2)	–0.0281(18)	0.0126(17)	–0.0207(17)
C(19)	0.0525(16)	0.0554(17)	0.0444(15)	–0.0017(13)	0.0251(13)	–0.0062(12)
C(20)	0.0467(14)	0.0424(14)	0.0517(15)	–0.0008(12)	0.0212(13)	–0.0079(11)
C(21)	0.0459(14)	0.0379(14)	0.0457(14)	–0.0050(11)	0.0135(12)	0.0047(11)
C(22)	0.0404(13)	0.0402(14)	0.0456(14)	0.0010(11)	0.0194(11)	0.0022(10)
C(23)	0.0380(13)	0.0453(14)	0.0518(16)	–0.0045(12)	0.0226(12)	–0.0029(11)
C(24)	0.0451(15)	0.0453(15)	0.0640(18)	–0.0026(13)	0.0205(13)	–0.0005(12)
C(25)	0.0572(19)	0.0452(17)	0.090(2)	–0.0028(16)	0.0271(18)	–0.0033(14)
C(26)	0.062(2)	0.055(2)	0.100(3)	–0.0221(19)	0.028(2)	–0.0154(16)
C(27)	0.0598(19)	0.071(2)	0.067(2)	–0.0182(17)	0.0194(16)	–0.0172(16)
C(28)	0.0471(15)	0.0596(17)	0.0521(17)	–0.0084(14)	0.0233(13)	–0.0112(13)
C(29)	0.0584(18)	0.079(2)	0.0514(17)	0.0010(16)	0.0084(14)	–0.0163(16)
C(30)	0.0495(16)	0.0656(19)	0.0545(17)	0.0089(14)	0.0100(14)	–0.0010(14)
C(31)	0.0402(11)	0.0439(12)	0.0432(12)	0.0015(10)	0.0121(9)	–0.0016(9)
C(32)	0.0416(13)	0.0472(14)	0.0818(19)	–0.0175(13)	0.0109(13)	0.0011(11)
C(33)	0.0694(14)	0.0739(14)	0.0694(14)	0.0114(11)	0.0383(12)	0.0246(11)
C(34)	0.0662(13)	0.0744(14)	0.0585(12)	–0.0248(11)	0.0236(11)	–0.0211(11)
C(35)	0.0609(14)	0.0505(13)	0.123(2)	–0.0066(14)	0.0074(14)	0.0184(11)
C(36)	0.0887(18)	0.0922(18)	0.104(2)	–0.0220(15)	0.0563(17)	0.0118(14)

Table S10. Torsion angles (degree) for compound **7f**

O(1)-C(1)-C(2)-C(3)	–5.2(5)	C(14)-C(15)-C(16)-C(17)	0.1(4)
C(12)-C(1)-C(2)-C(3)	178.5(3)	C(15)-C(16)-C(17)-O(2)	178.5(3)
O(1)-C(1)-C(2)-C(11)	174.5(3)	C(15)-C(16)-C(17)-C(19)	–1.7(4)
C(12)-C(1)-C(2)-C(11)	–1.8(3)	O(2)-C(17)-C(19)-C(20)	–178.3(2)
C(11)-C(2)-C(3)-C(4)	–0.4(4)	C(16)-C(17)-C(19)-C(20)	1.9(4)
C(1)-C(2)-C(3)-C(4)	179.2(3)	C(17)-C(19)-C(20)-C(14)	–0.6(4)
C(2)-C(3)-C(4)-C(5)	–0.6(5)	C(15)-C(14)-C(20)-C(19)	–1.0(4)
C(3)-C(4)-C(5)-C(6)	1.4(6)	C(13)-C(14)-C(20)-C(19)	176.8(2)
C(4)-C(5)-C(6)-C(11)	–1.2(5)	C(14)-C(13)-C(21)-N(2)	121.3(2)
C(4)-C(5)-C(6)-C(7)	–179.9(4)	C(12)-C(13)-C(21)-N(2)	–110.4(2)
C(5)-C(6)-C(7)-C(8)	179.9(4)	C(14)-C(13)-C(21)-C(22)	–119.6(2)
C(11)-C(6)-C(7)-C(8)	1.2(5)	C(12)-C(13)-C(21)-C(22)	8.6(2)
C(6)-C(7)-C(8)-C(9)	–1.0(5)	N(2)-C(21)-C(22)-N(1)	88.4(2)
C(7)-C(8)-C(9)-C(10)	0.2(5)	C(13)-C(21)-C(22)-N(1)	–30.7(2)
C(8)-C(9)-C(10)-C(11)	0.3(4)	N(2)-C(21)-C(22)-C(23)	–34.4(3)
C(8)-C(9)-C(10)-C(12)	179.6(3)	C(13)-C(21)-C(22)-C(23)	–153.5(2)
C(9)-C(10)-C(11)-C(2)	–179.8(3)	N(1)-C(22)-C(23)-C(28)	22.3(3)
C(12)-C(10)-C(11)-C(2)	0.8(3)	C(21)-C(22)-C(23)-C(28)	140.7(2)
C(9)-C(10)-C(11)-C(6)	0.0(4)	N(1)-C(22)-C(23)-C(24)	–160.1(2)
C(12)-C(10)-C(11)-C(6)	–179.5(2)	C(21)-C(22)-C(23)-C(24)	–41.7(3)
C(3)-C(2)-C(11)-C(10)	–179.6(3)	C(28)-C(23)-C(24)-C(25)	–1.3(4)
C(1)-C(2)-C(11)-C(10)	0.7(3)	C(22)-C(23)-C(24)-C(25)	–178.9(2)
C(3)-C(2)-C(11)-C(6)	0.7(4)	C(23)-C(24)-C(25)-C(26)	0.0(4)
C(1)-C(2)-C(11)-C(6)	–179.1(3)	C(24)-C(25)-C(26)-C(27)	1.1(5)
C(5)-C(6)-C(11)-C(10)	–179.6(3)	C(25)-C(26)-C(27)-C(28)	–0.9(5)
C(7)-C(6)-C(11)-C(10)	–0.7(4)	C(24)-C(23)-C(28)-C(27)	1.5(4)
C(5)-C(6)-C(11)-C(2)	0.1(4)	C(22)-C(23)-C(28)-C(27)	179.1(2)
C(7)-C(6)-C(11)-C(2)	179.0(3)	C(24)-C(23)-C(28)-C(29)	–178.8(2)
C(9)-C(10)-C(12)-N(1)	57.7(4)	C(22)-C(23)-C(28)-C(29)	–1.1(4)
C(11)-C(10)-C(12)-N(1)	–122.9(2)	C(26)-C(27)-C(28)-C(23)	–0.4(4)
C(9)-C(10)-C(12)-C(13)	–58.0(4)	C(26)-C(27)-C(28)-C(29)	179.8(3)
C(11)-C(10)-C(12)-C(13)	121.3(2)	C(23)-C(28)-C(29)-C(30)	11.6(4)
C(9)-C(10)-C(12)-C(1)	178.9(3)	C(27)-C(28)-C(29)-C(30)	–168.6(3)
C(11)-C(10)-C(12)-C(1)	–1.8(3)	C(28)-C(29)-C(30)-N(1)	–42.4(3)
O(1)-C(1)-C(12)-N(1)	–53.2(3)	C(29)-C(30)-N(1)-C(22)	67.2(3)
C(2)-C(1)-C(12)-N(1)	123.2(2)	C(29)-C(30)-N(1)-C(12)	–166.8(2)
O(1)-C(1)-C(12)-C(10)	–174.3(3)	C(23)-C(22)-N(1)-C(30)	–56.6(3)
C(2)-C(1)-C(12)-C(10)	2.2(3)	C(21)-C(22)-N(1)-C(30)	175.1(2)
O(1)-C(1)-C(12)-C(13)	63.1(3)	C(23)-C(22)-N(1)-C(12)	172.00(19)
C(2)-C(1)-C(12)-C(13)	–120.5(2)	C(21)-C(22)-N(1)-C(12)	43.7(2)
N(1)-C(12)-C(13)-C(14)	145.0(2)	C(10)-C(12)-N(1)-C(30)	72.0(3)
C(10)-C(12)-C(13)-C(14)	–93.5(2)	C(13)-C(12)-N(1)-C(30)	–166.0(2)
C(1)-C(12)-C(13)-C(14)	23.0(3)	C(1)-C(12)-N(1)-C(30)	–43.1(3)
N(1)-C(12)-C(13)-C(21)	16.4(2)	C(10)-C(12)-N(1)-C(22)	–159.8(2)
C(10)-C(12)-C(13)-C(21)	137.9(2)	C(13)-C(12)-N(1)-C(22)	–37.7(2)
C(1)-C(12)-C(13)-C(21)	–105.6(2)	C(1)-C(12)-N(1)-C(22)	85.2(2)
C(21)-C(13)-C(14)-C(15)	–146.9(2)	C(22)-C(21)-N(2)-O(4)	–68.2(3)
C(12)-C(13)-C(14)-C(15)	89.9(3)	C(13)-C(21)-N(2)-O(4)	47.2(3)
C(21)-C(13)-C(14)-C(20)	35.3(3)	C(22)-C(21)-N(2)-O(3)	111.1(3)
C(12)-C(13)-C(14)-C(20)	–87.9(3)	C(13)-C(21)-N(2)-O(3)	–133.5(2)
C(20)-C(14)-C(15)-C(16)	1.2(4)	C(16)-C(17)-O(2)-C(18)	–5.8(4)
C(13)-C(14)-C(15)-C(16)	–176.7(2)	C(19)-C(17)-O(2)-C(18)	174.4(3)

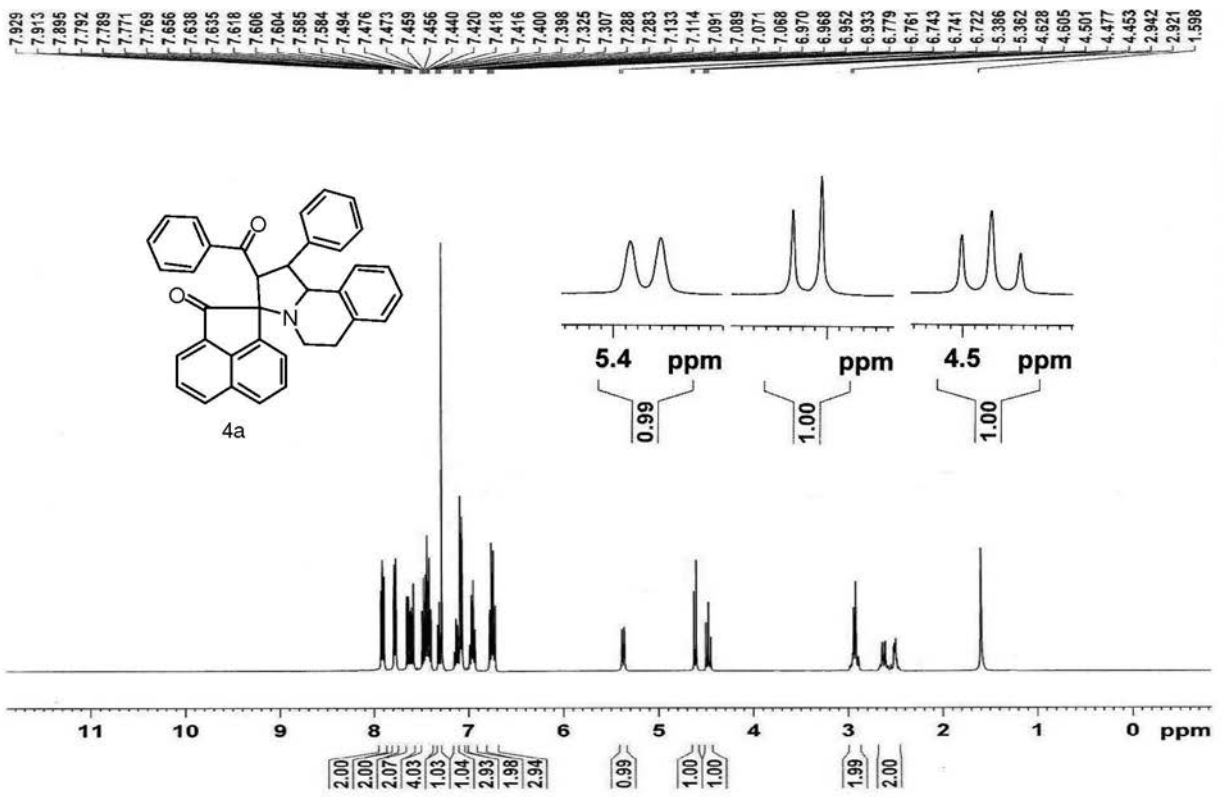

Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4a**).

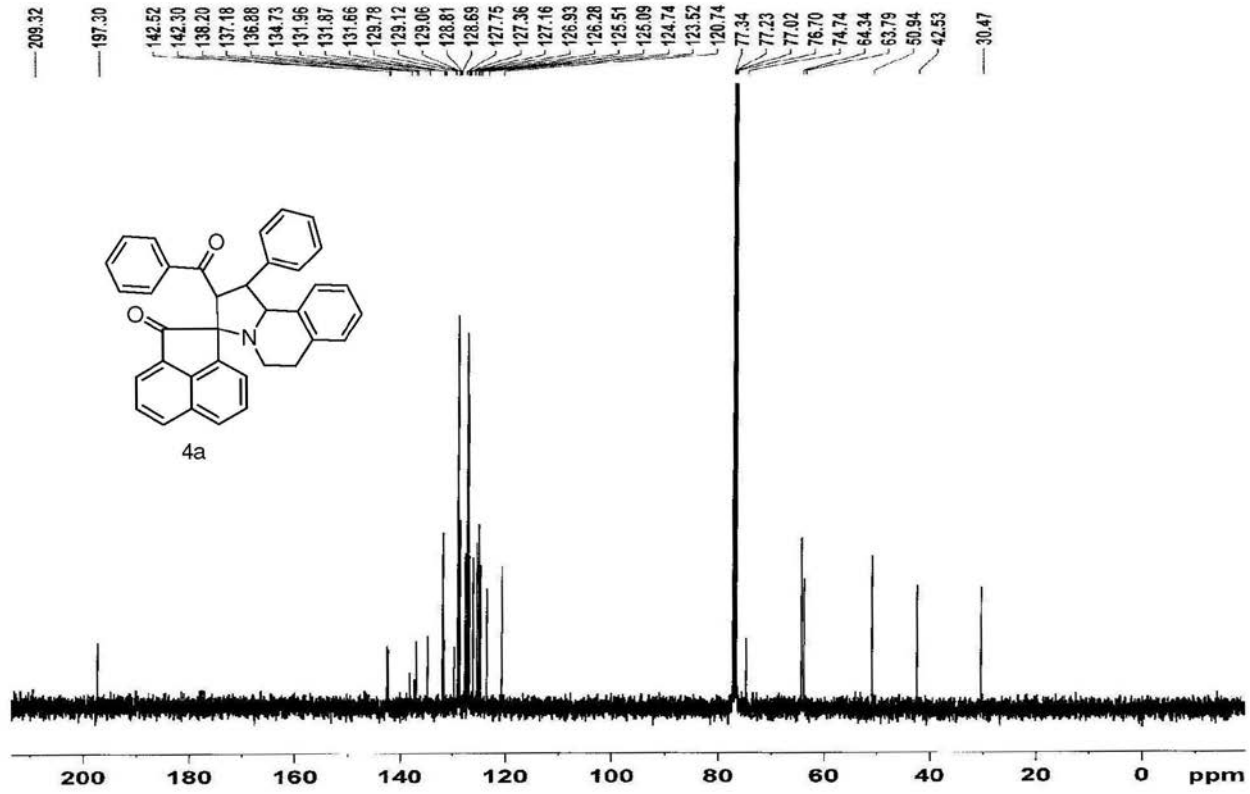

Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4a**).

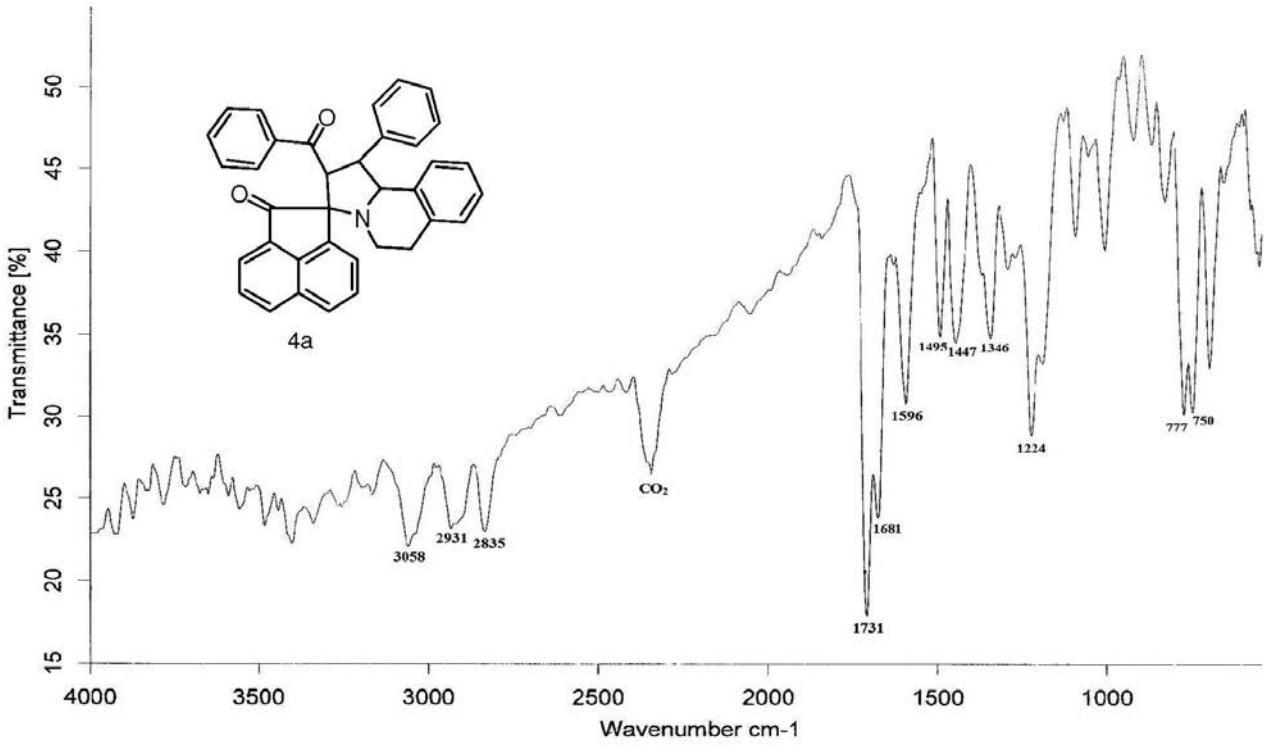

Figure S3. IR (KBr) of (**4a**).

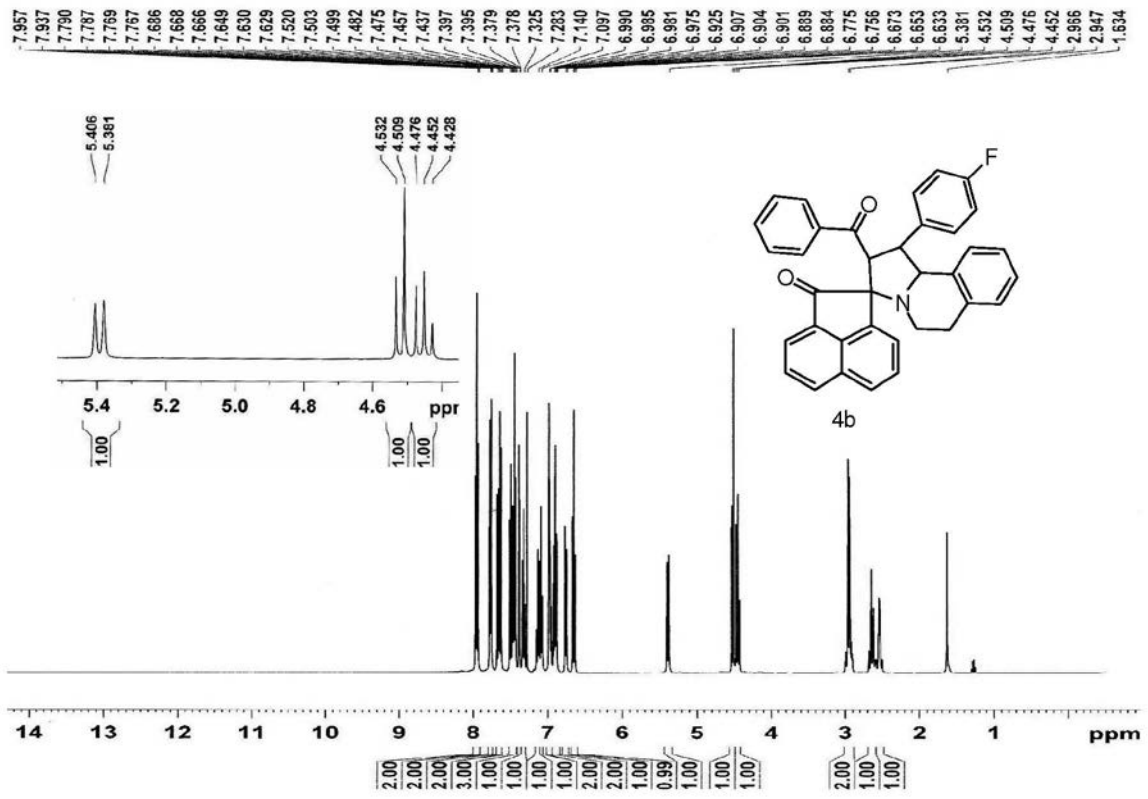

Figure S4. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4b**).

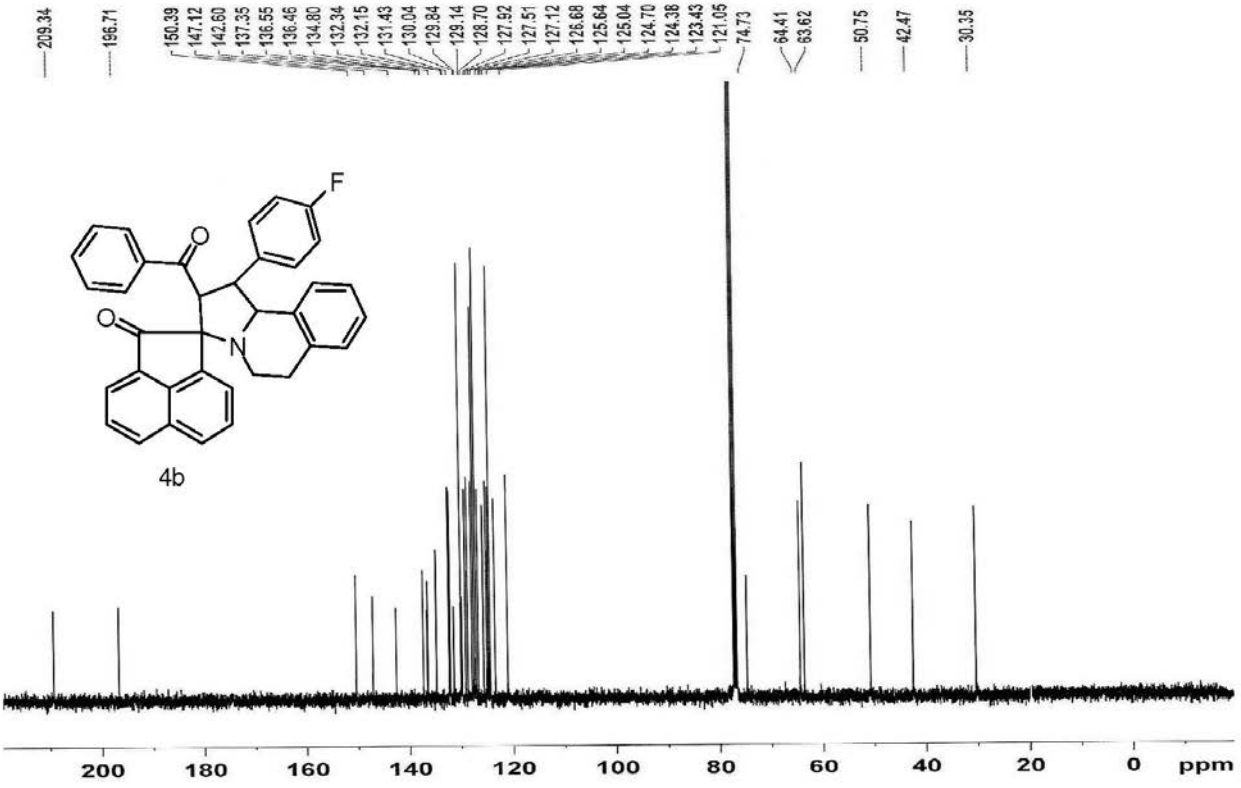

Figure S5. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4b**).

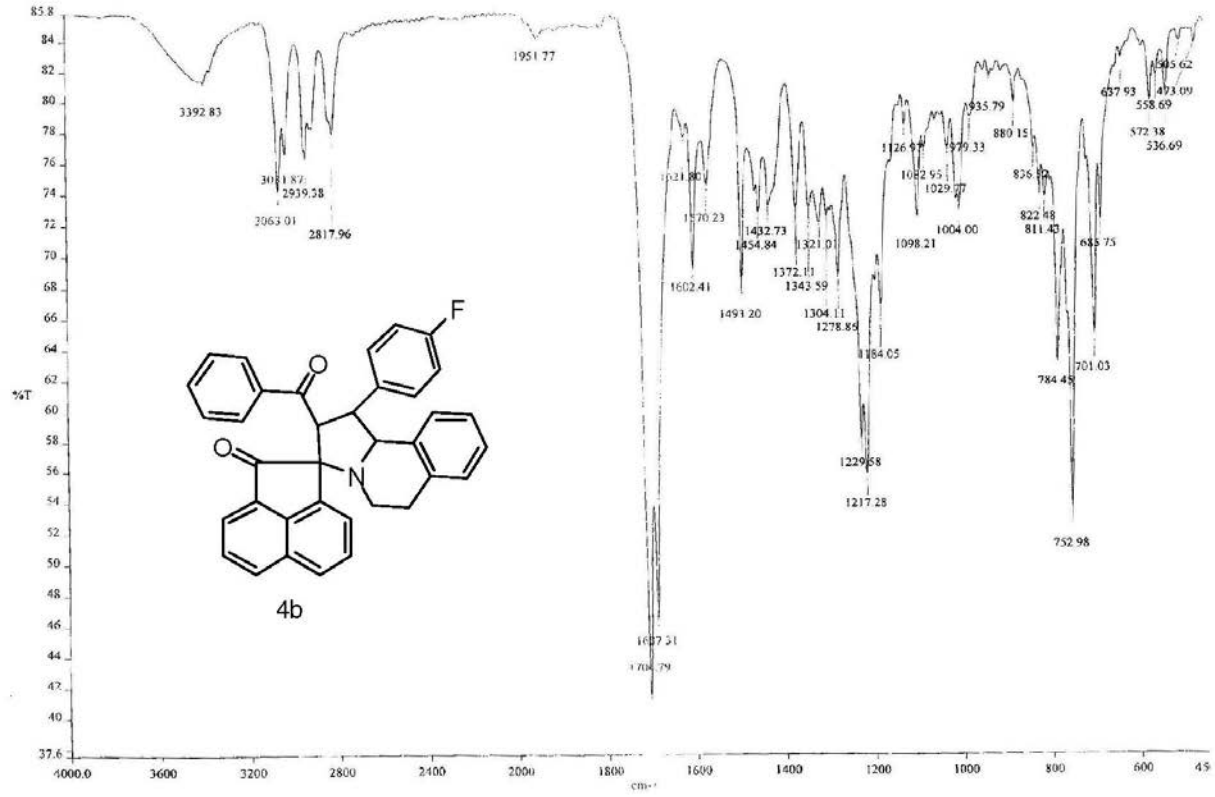

Figure S6. IR (film) of (**4b**).

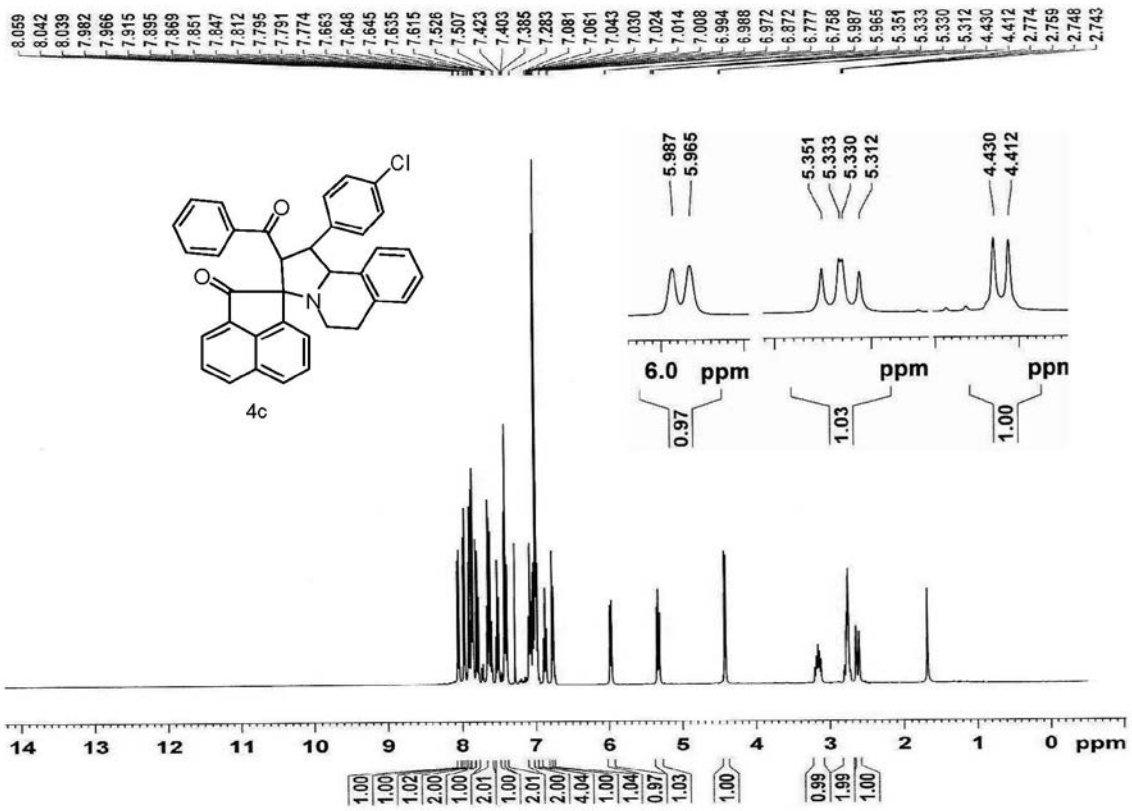

Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4c**).

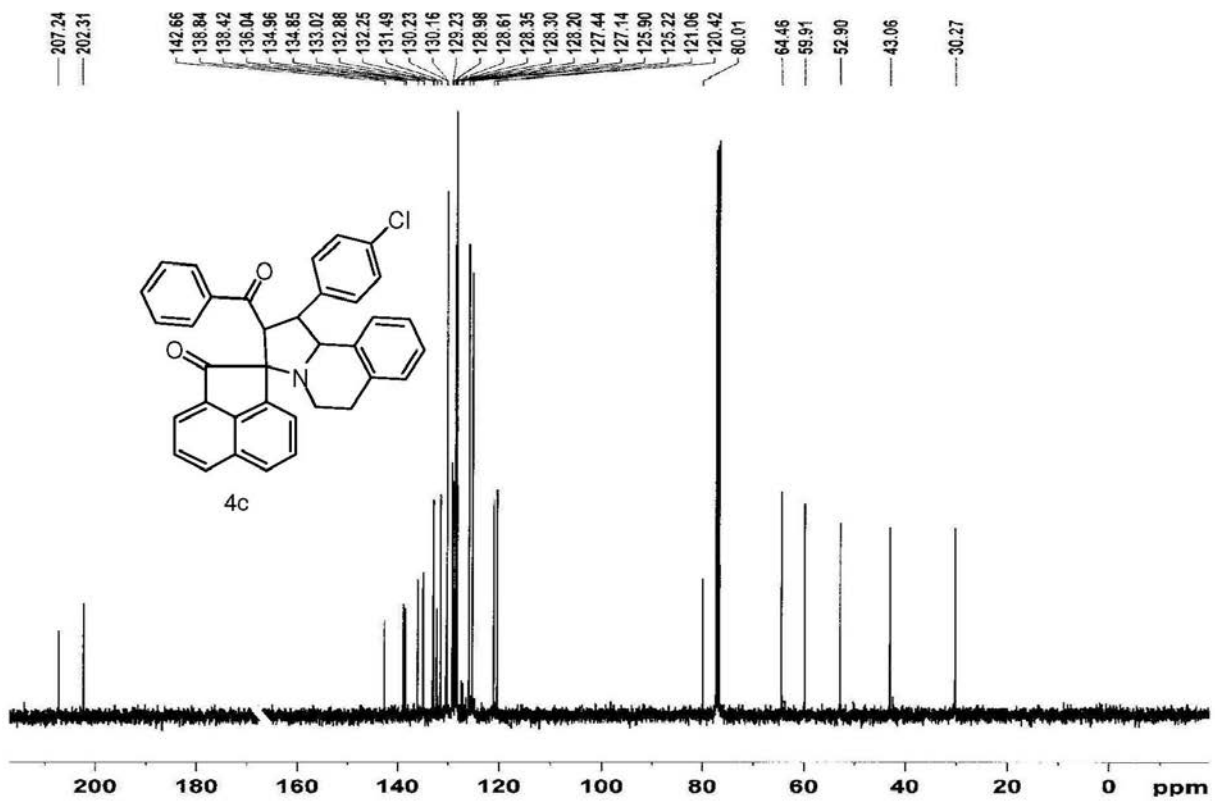

Figure S8. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4c**).

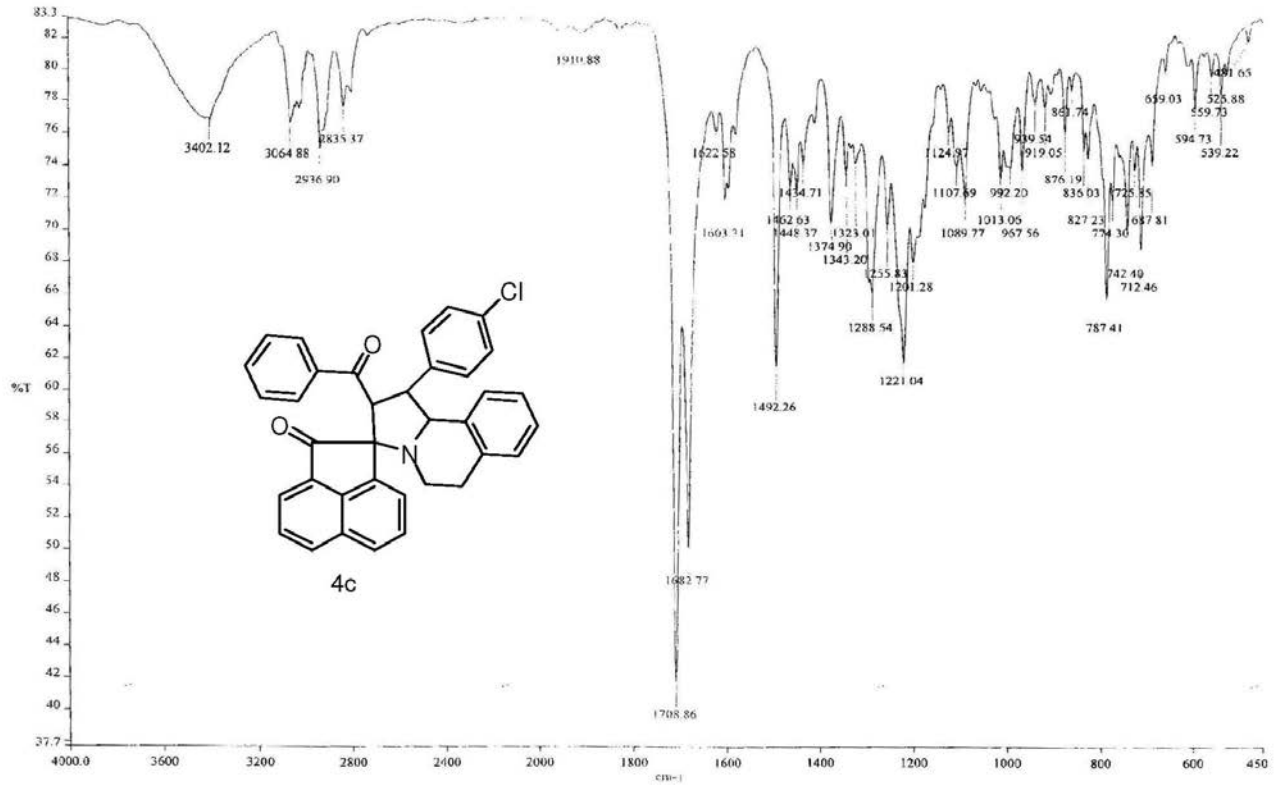

Figure S9. IR (KBr) of (**4c**).

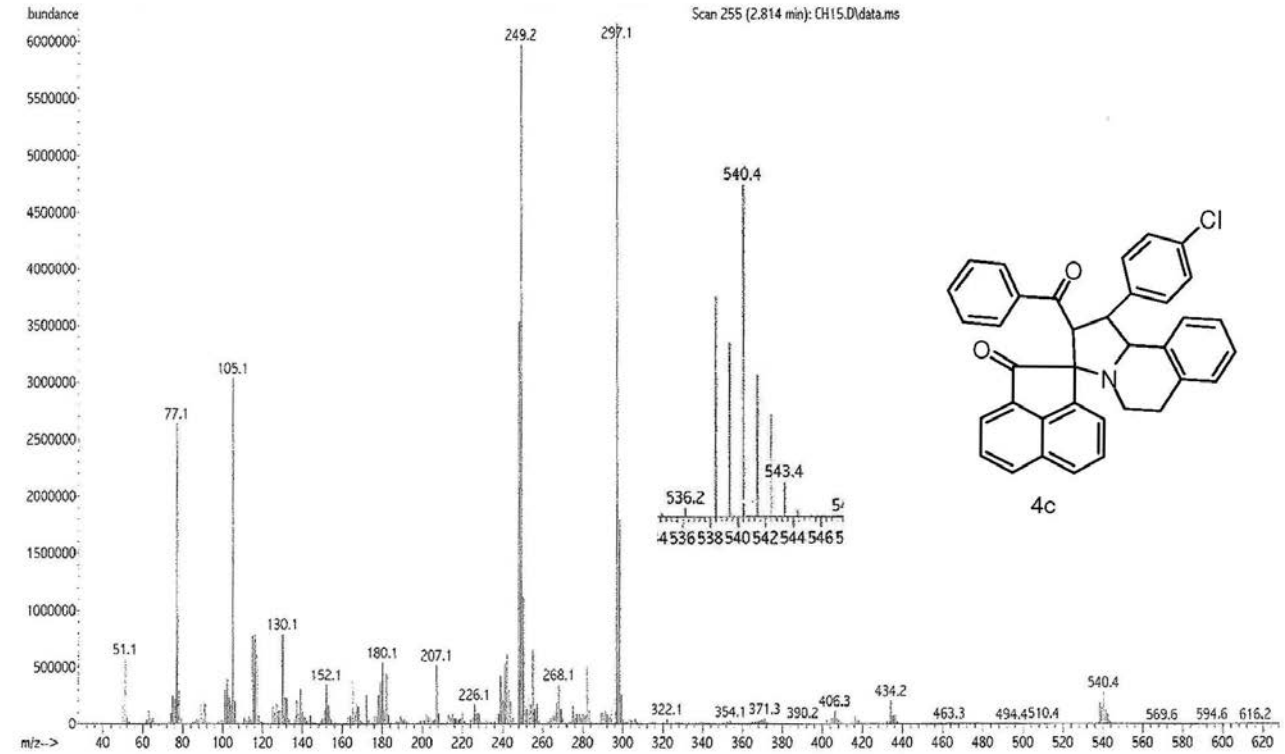

Figure S10. MS (70 eV) of (**4c**).

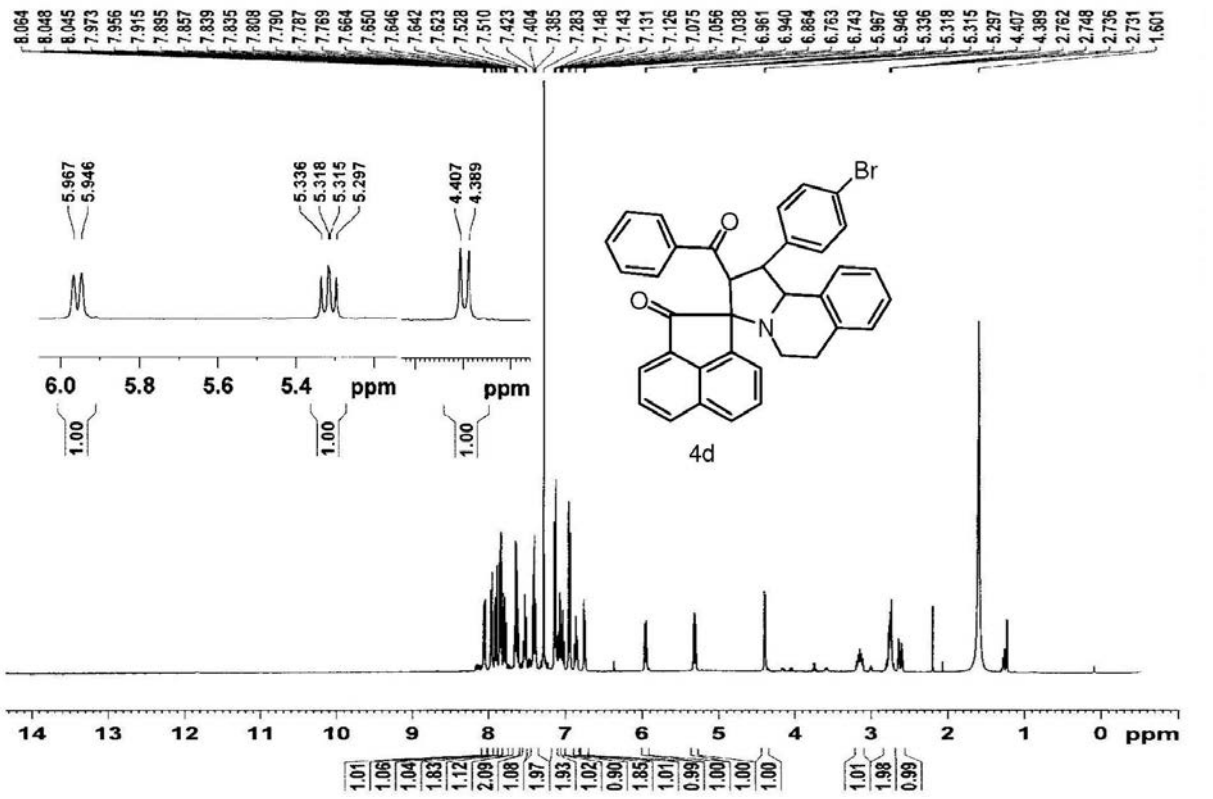

Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4d**).

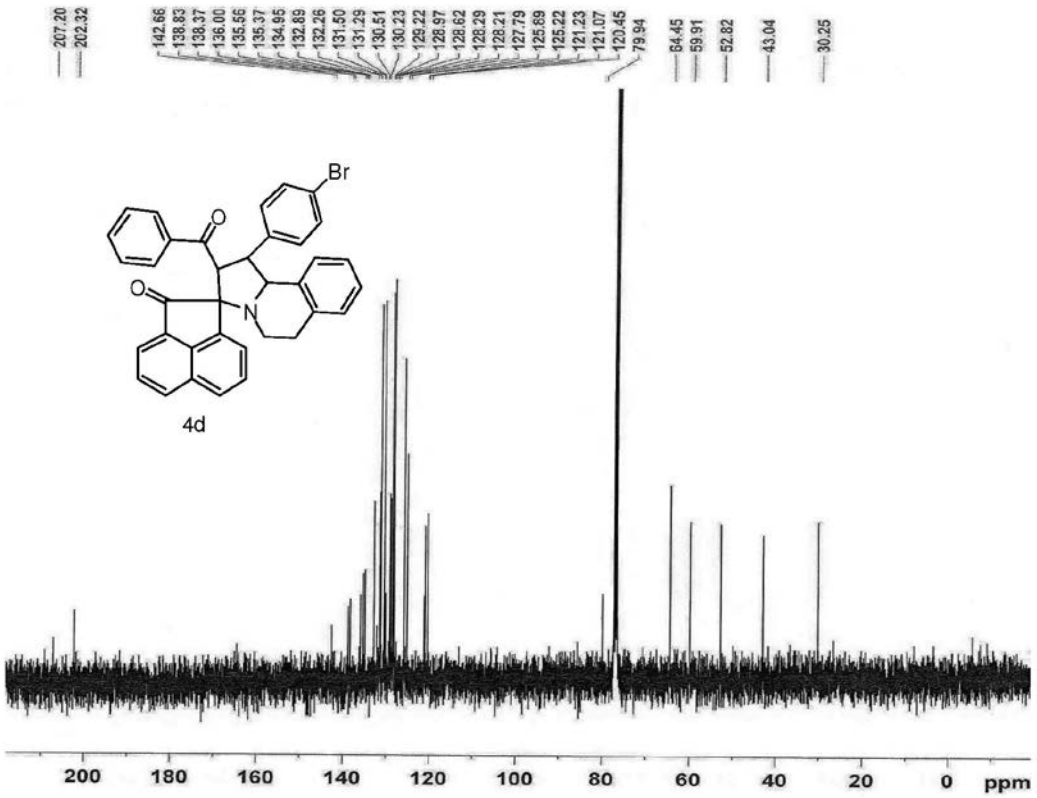

Figure S12. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4d**).

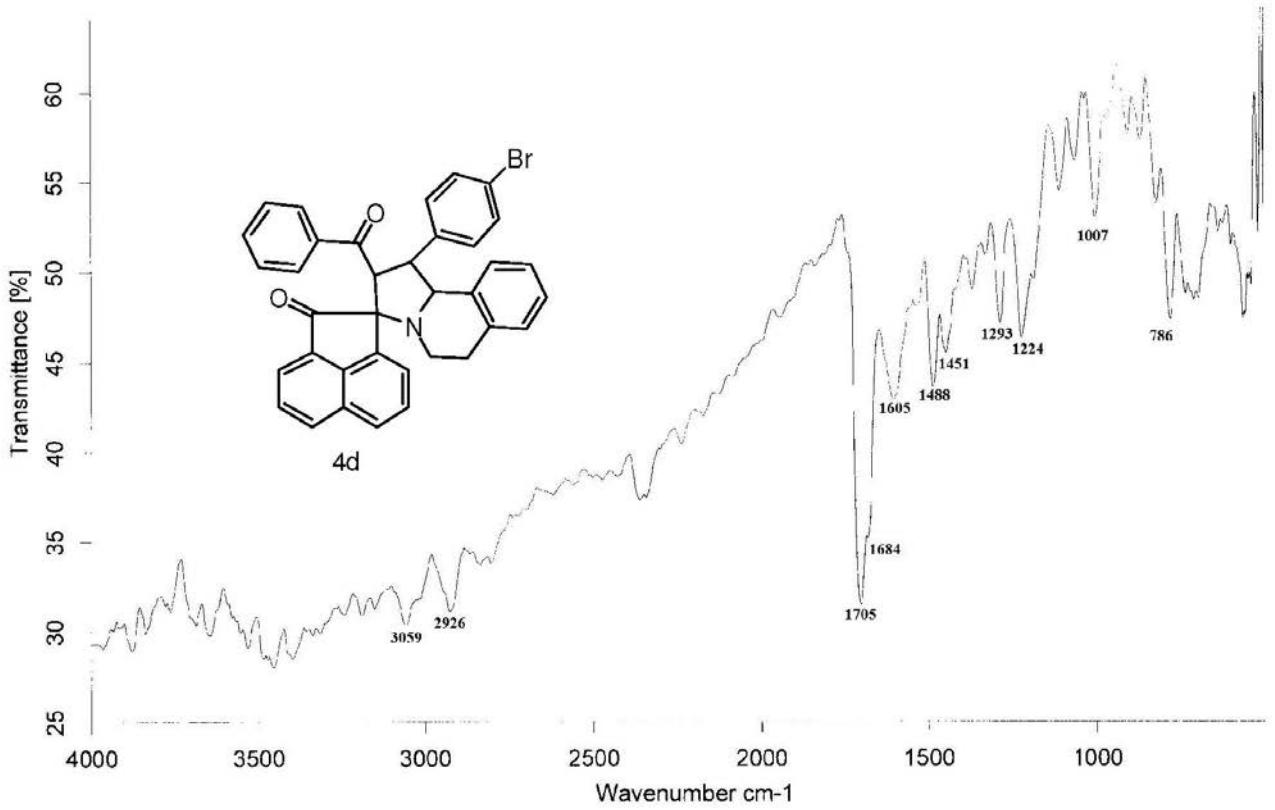

Figure S13. IR (KBr) of (**4d**).

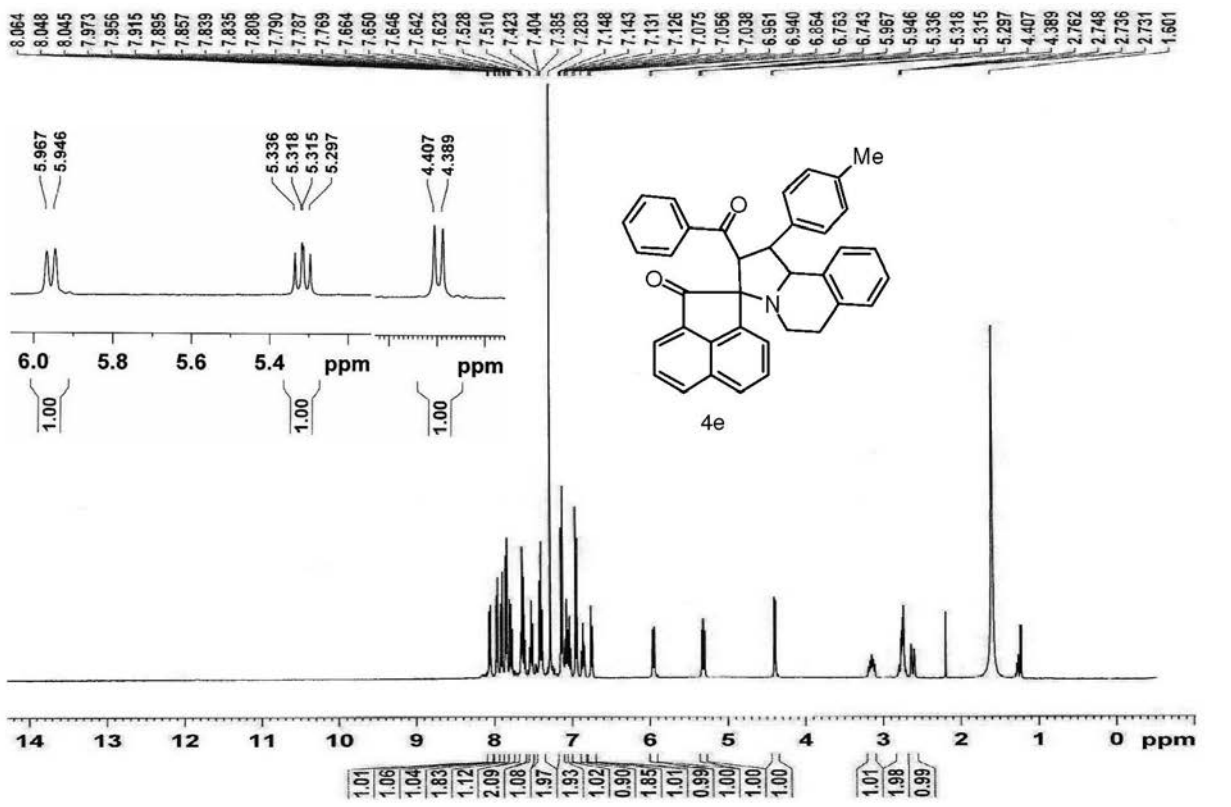

Figure S14. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4e**).

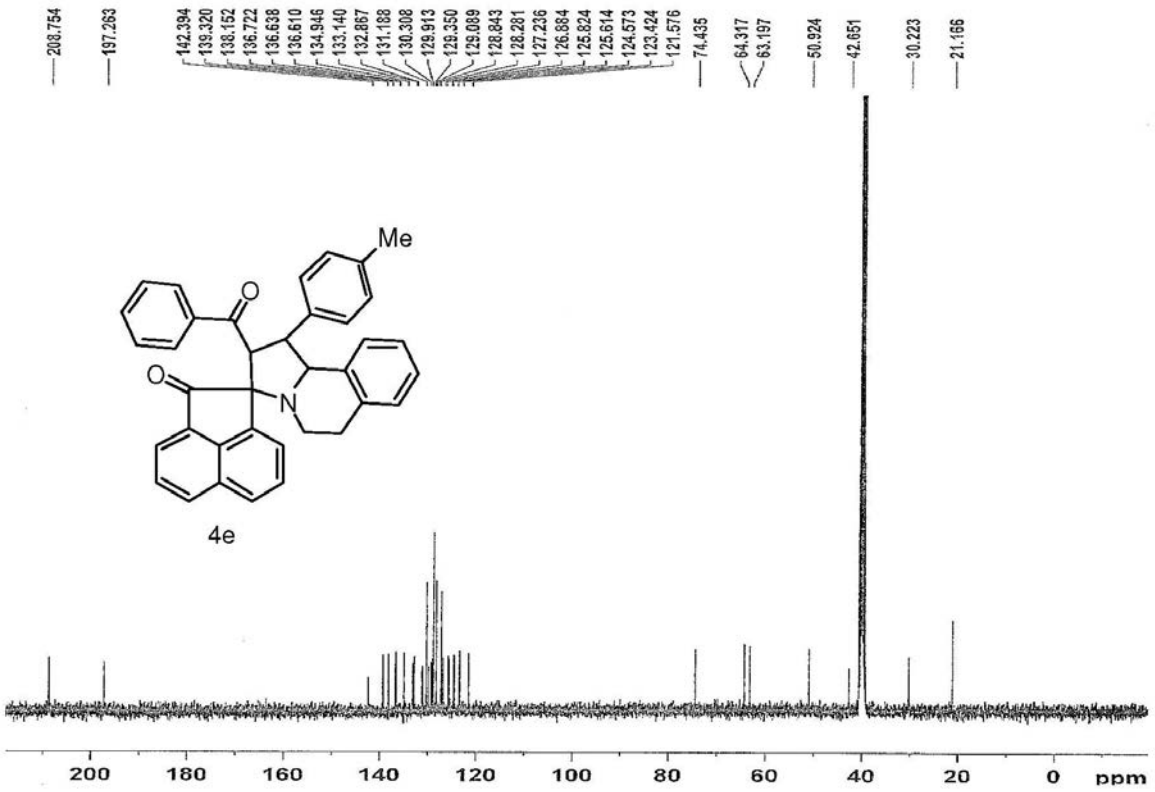

Figure S15. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4e**).

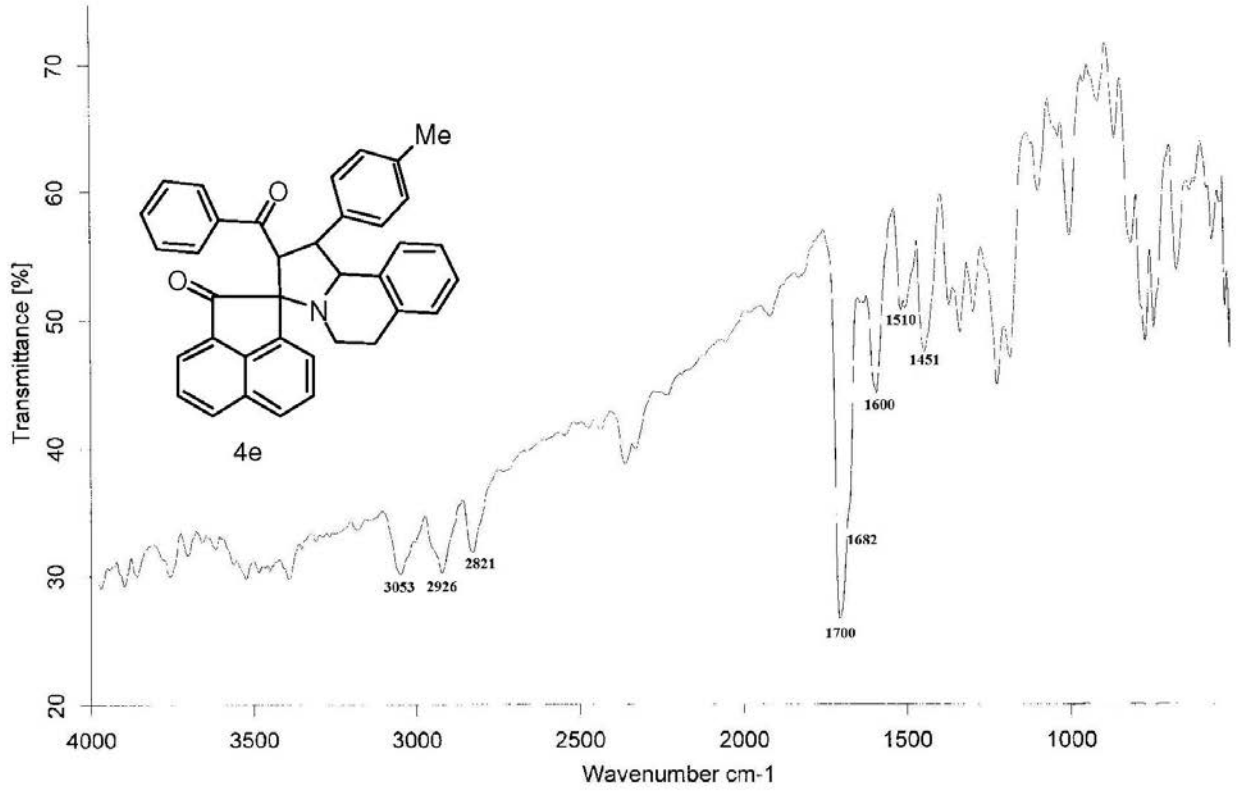

Figure S16. IR (KBr) of (**4e**).

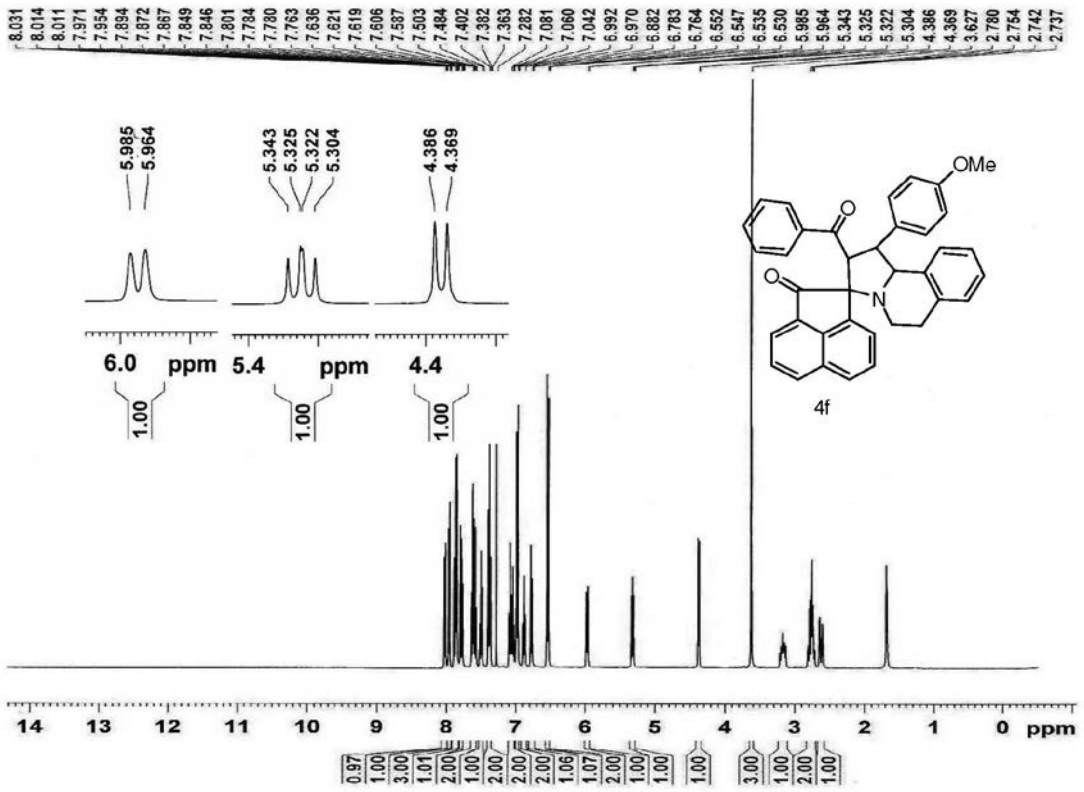

Figure S17. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4f**).

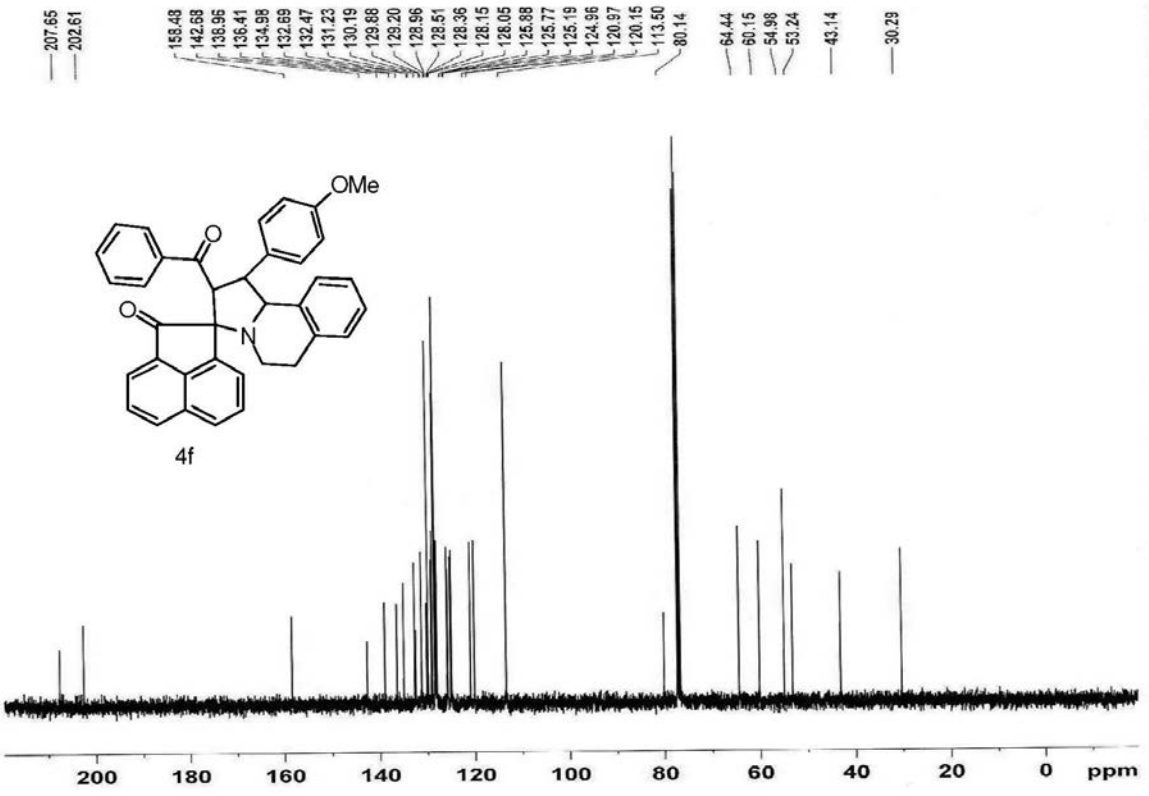

Figure S18. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4f**).

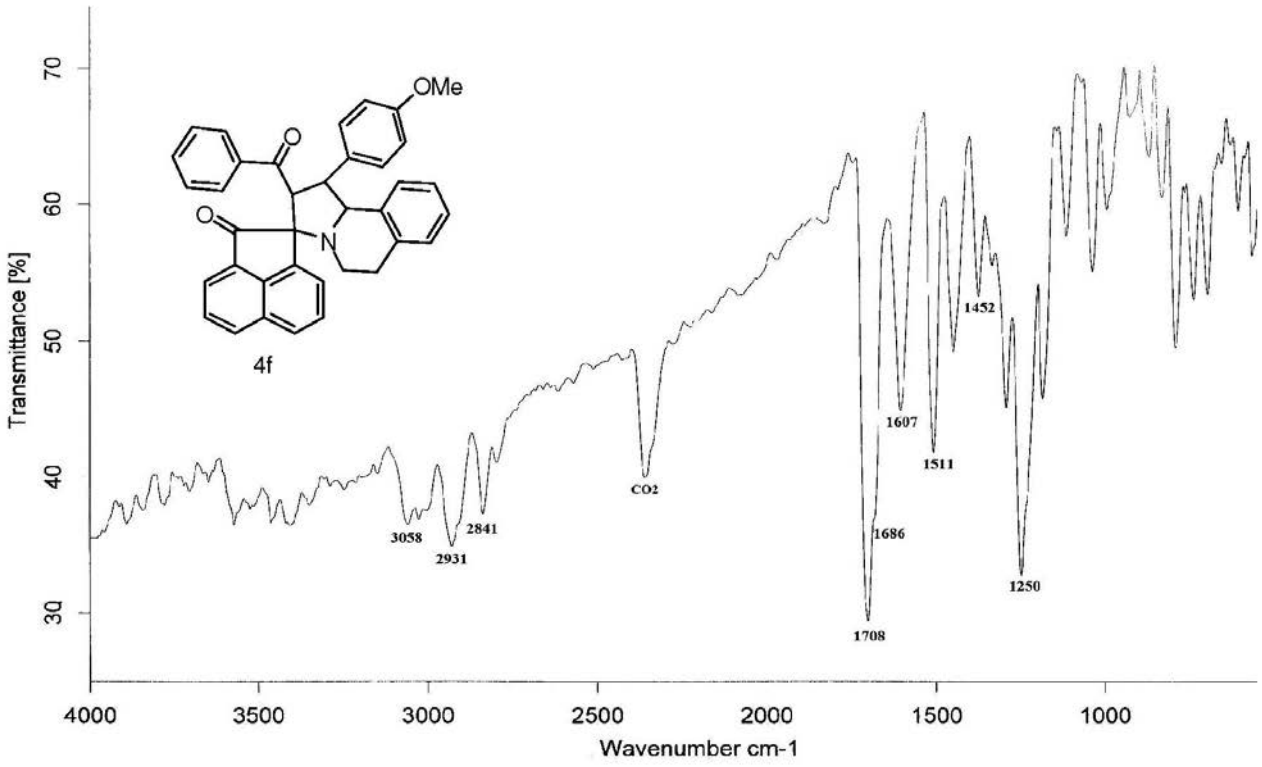

Figure S19. IR (KBr) of (**4f**).

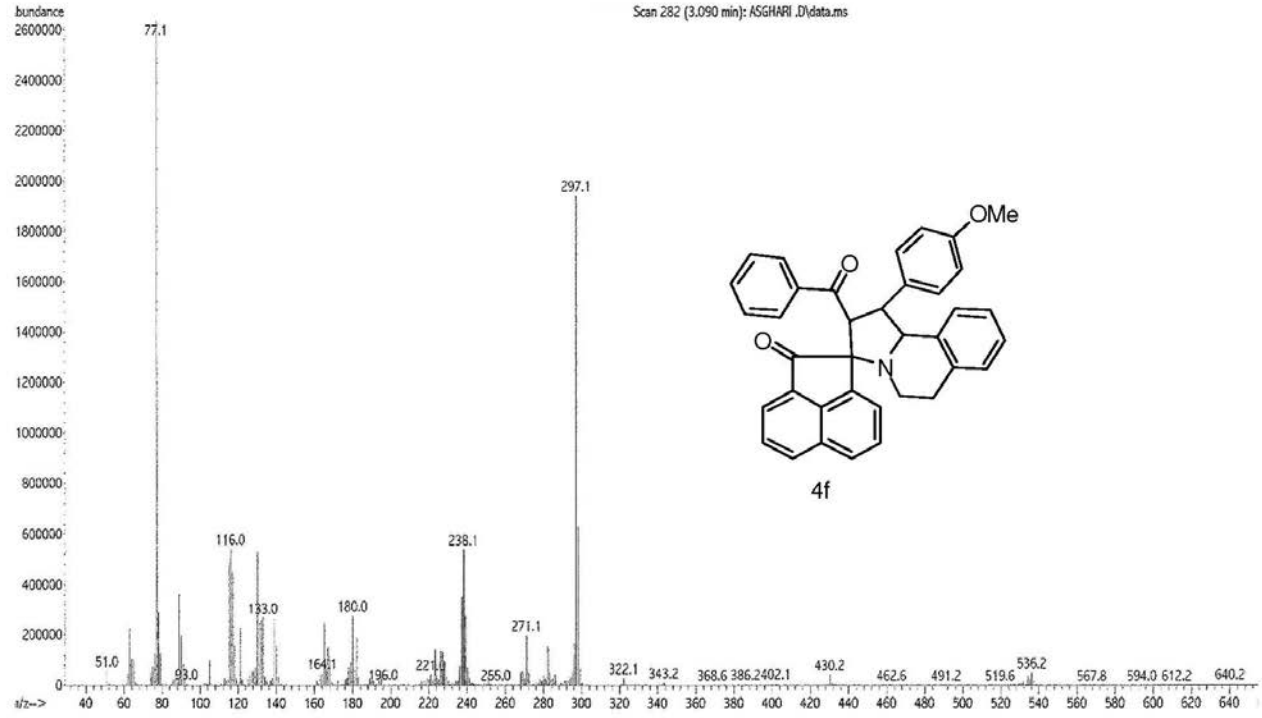

Figure S20. MS (70 eV) of (**4f**).

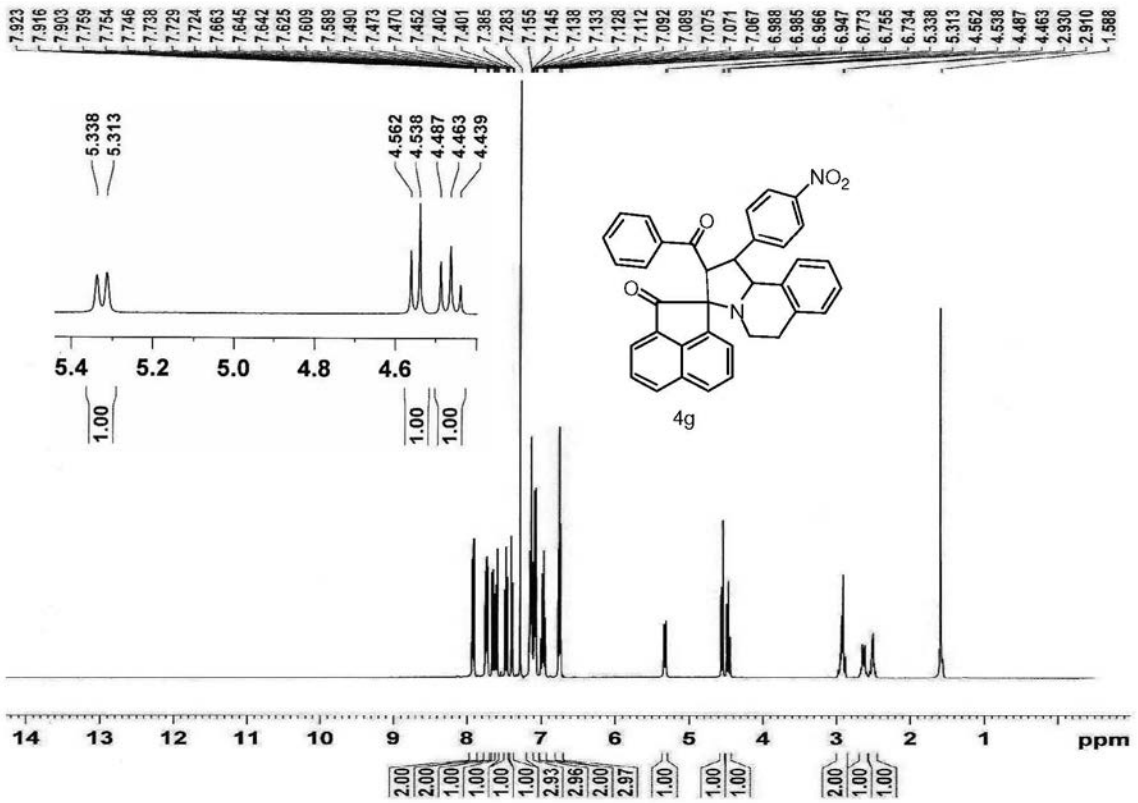

Figure S21. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4g**).

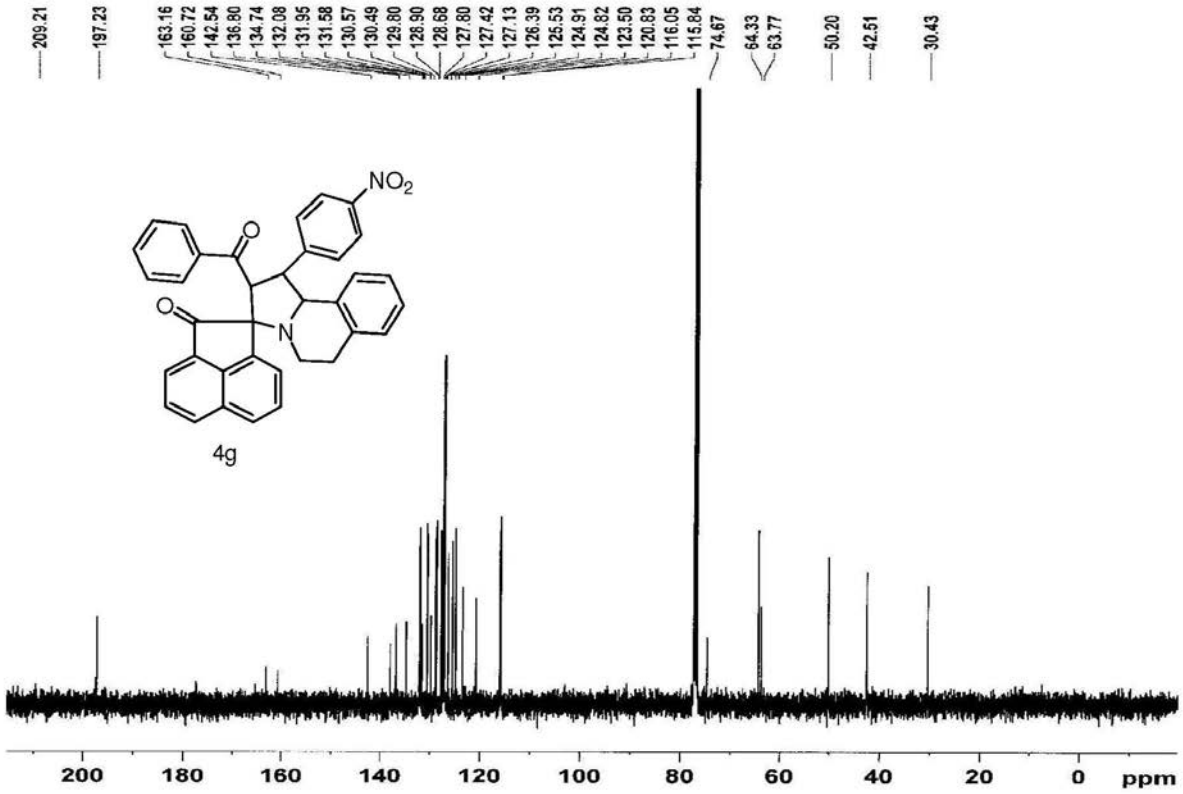

Figure S22. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4g**).

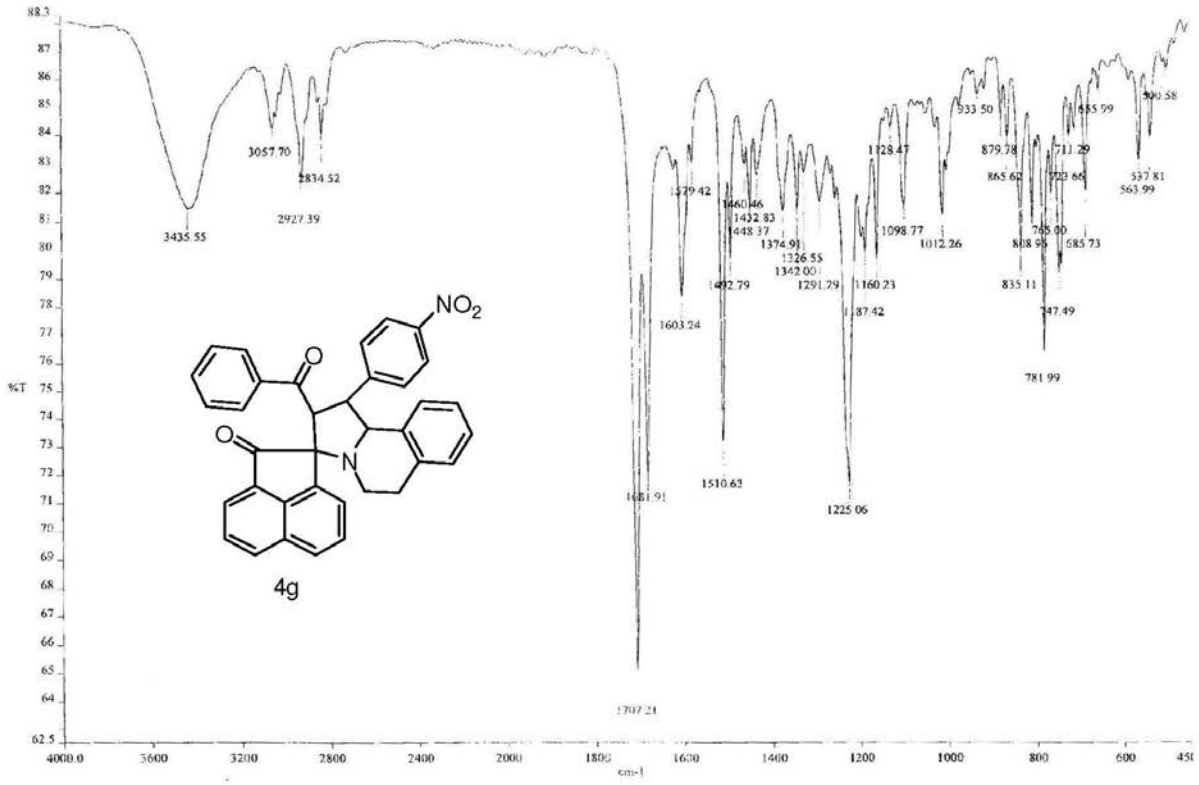

Figure S23. IR (KBr) of (**4g**).

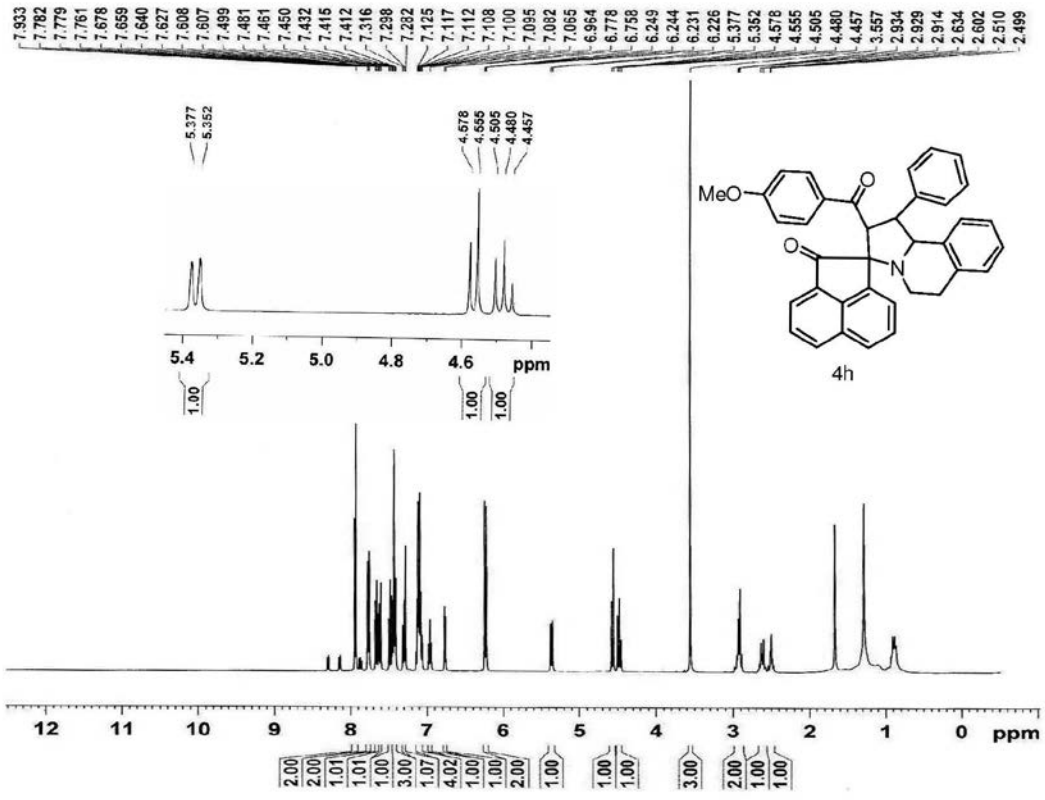

Figure S24. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4h**).

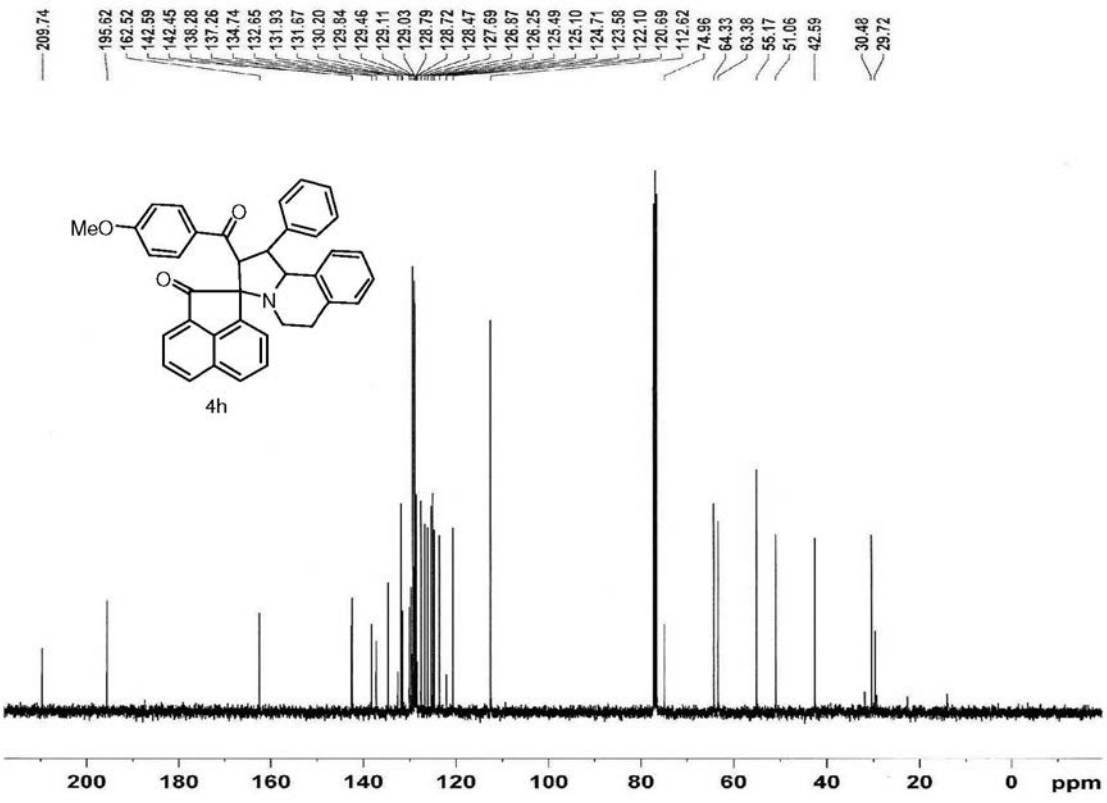

Figure S25. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4h**).

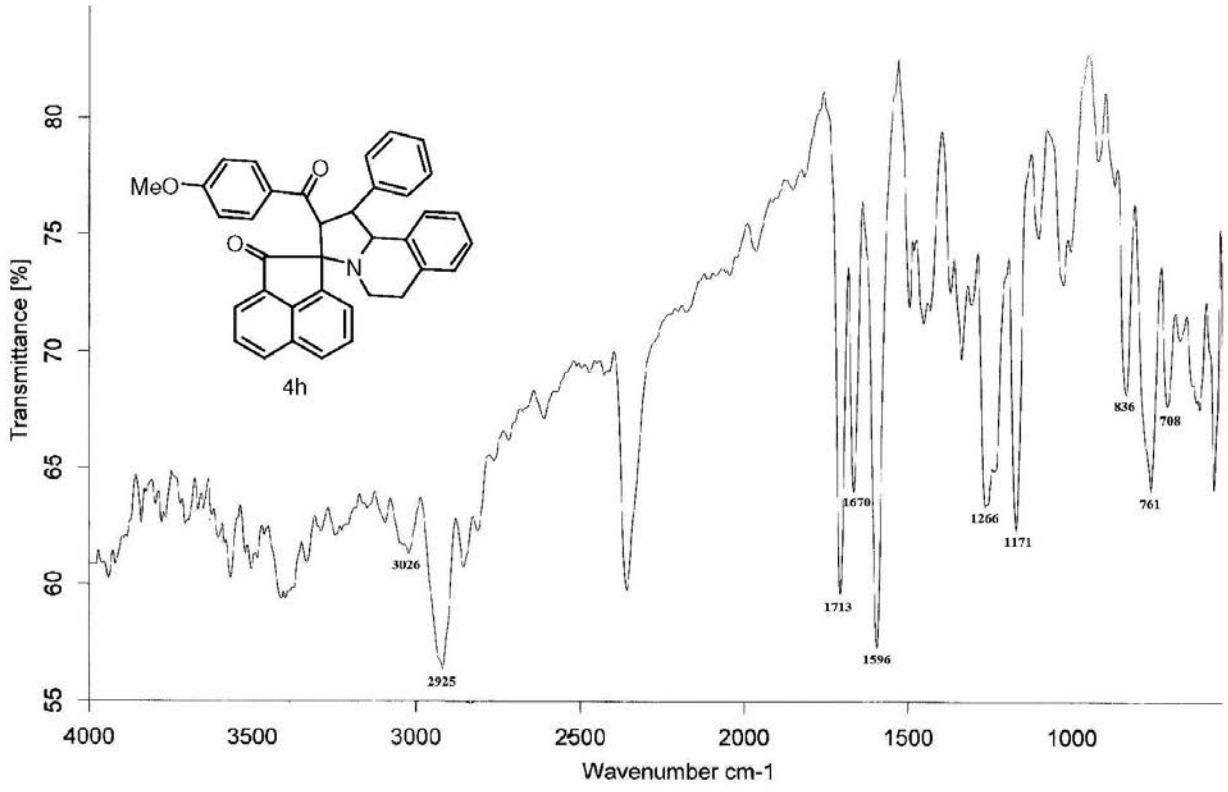

Figure S26. IR (KBr) of (**4h**).

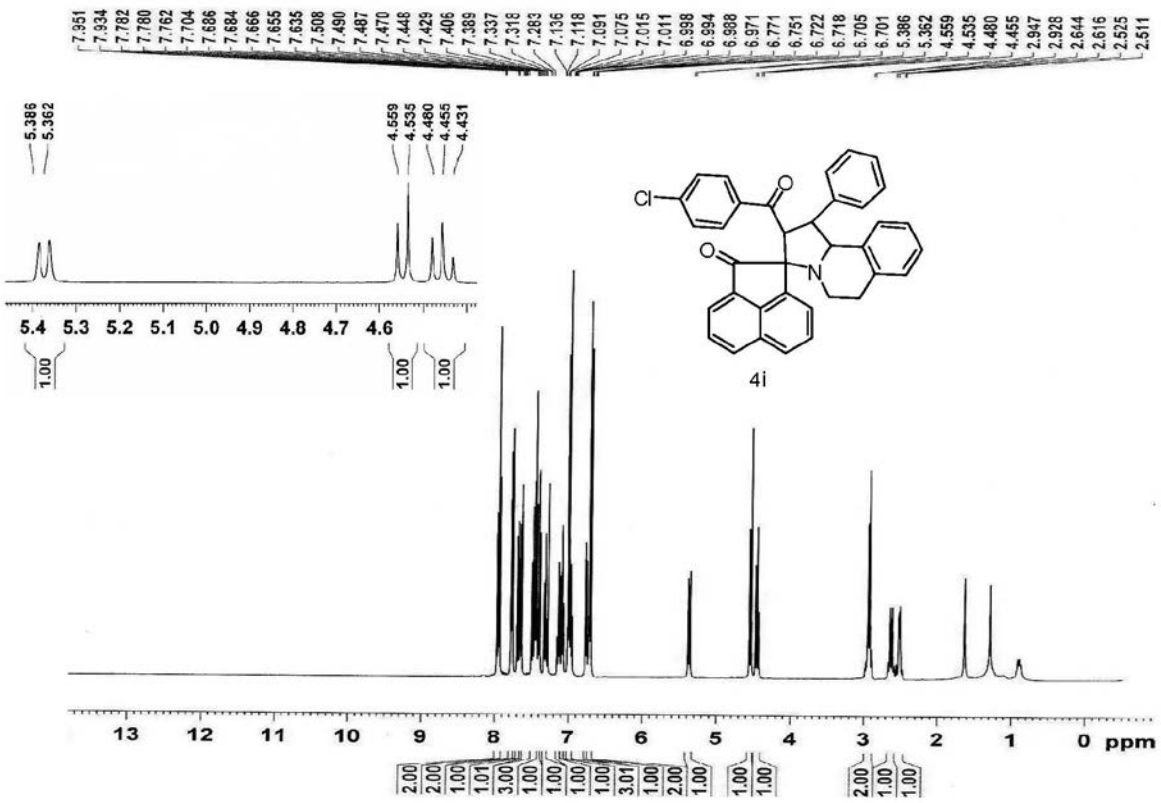

Figure S27. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4i**).

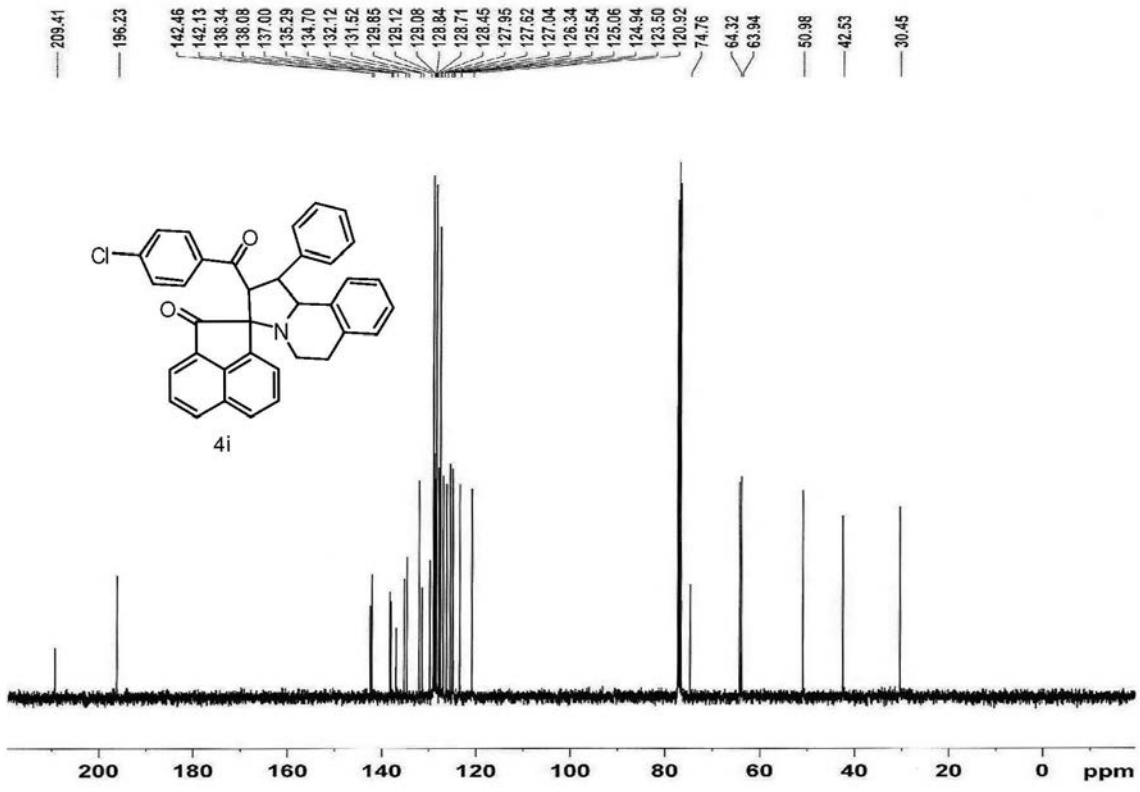

Figure S28. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4i**).

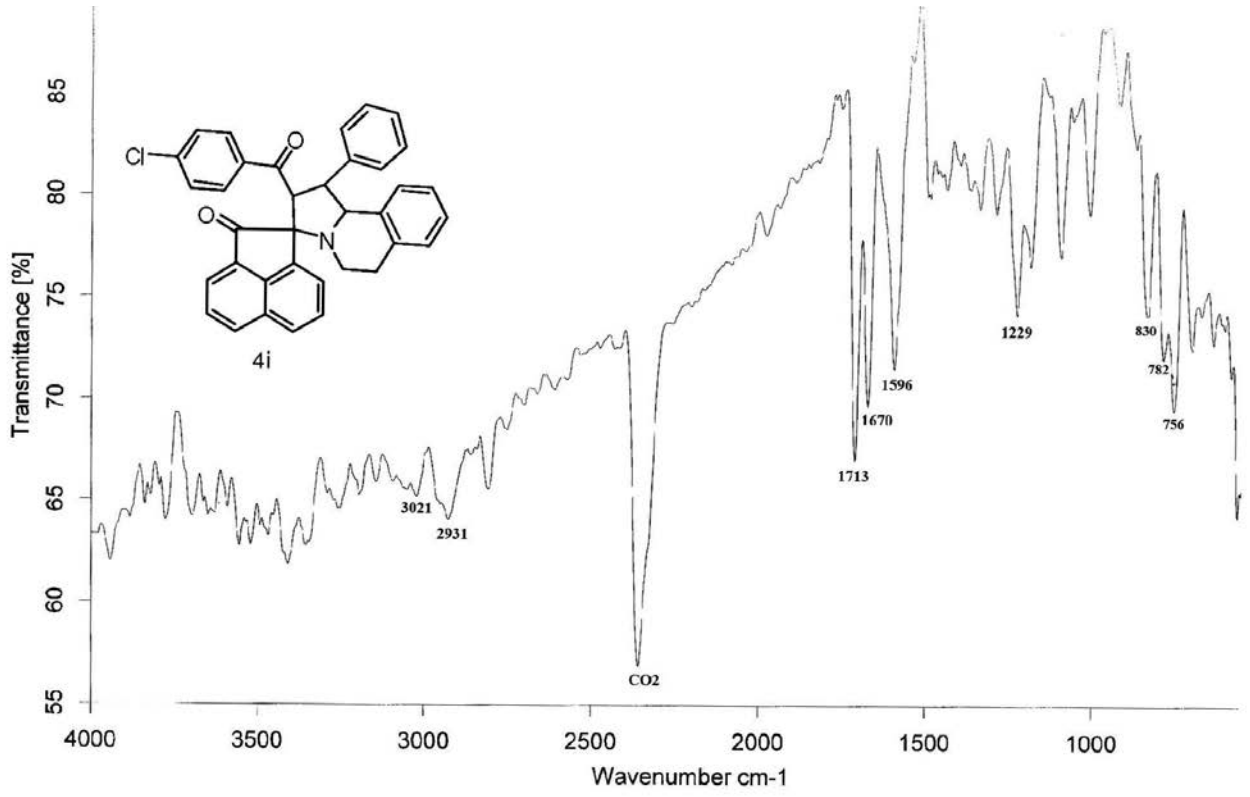

Figure S29. IR (KBr) of (**4i**).

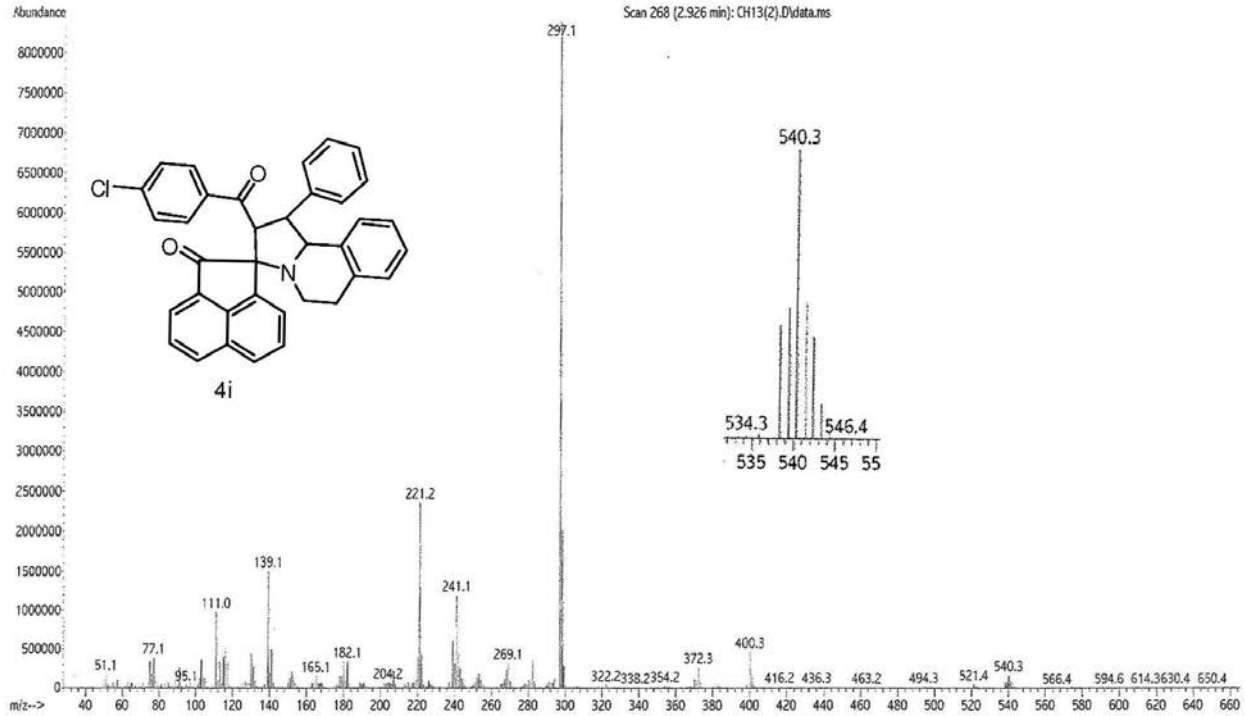

Figure S30. MS (70 eV) of (**4i**).

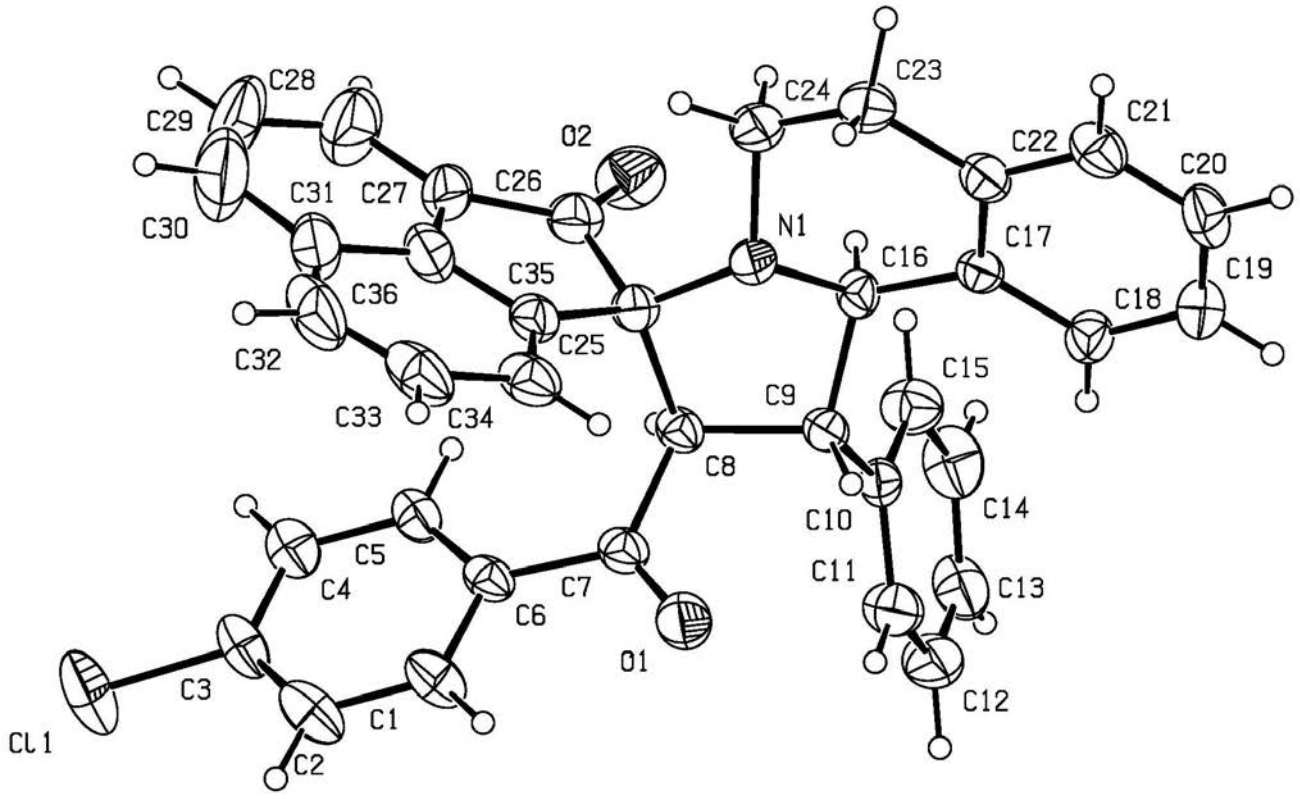

Figure S31. ORTEP diagram of (**4i**).

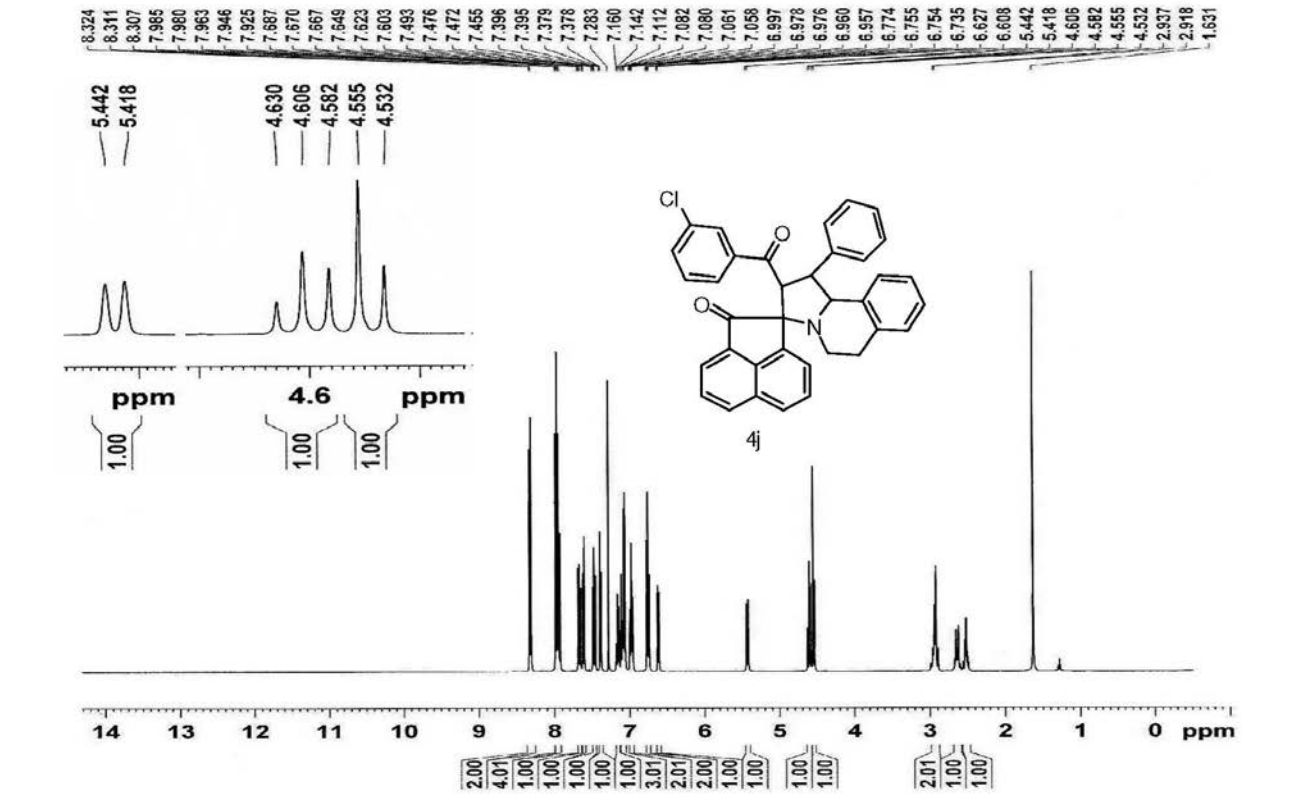

Figure S32. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4j**).

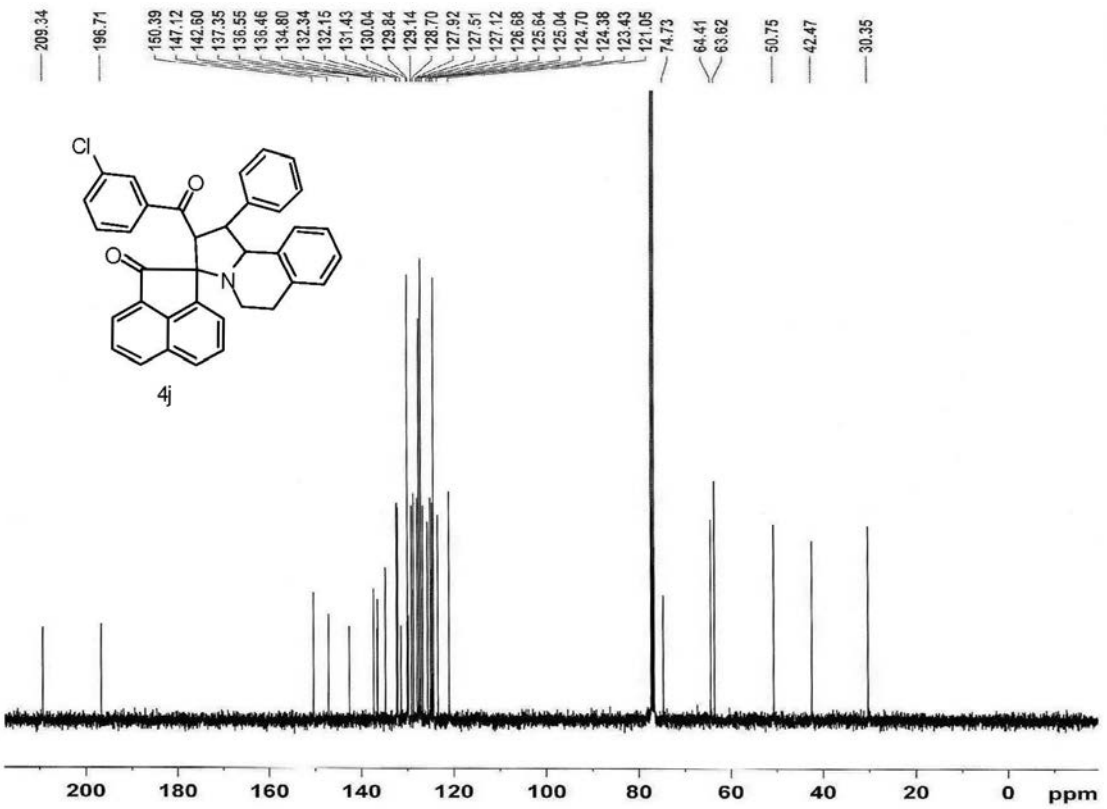

Figure S33. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4j**).

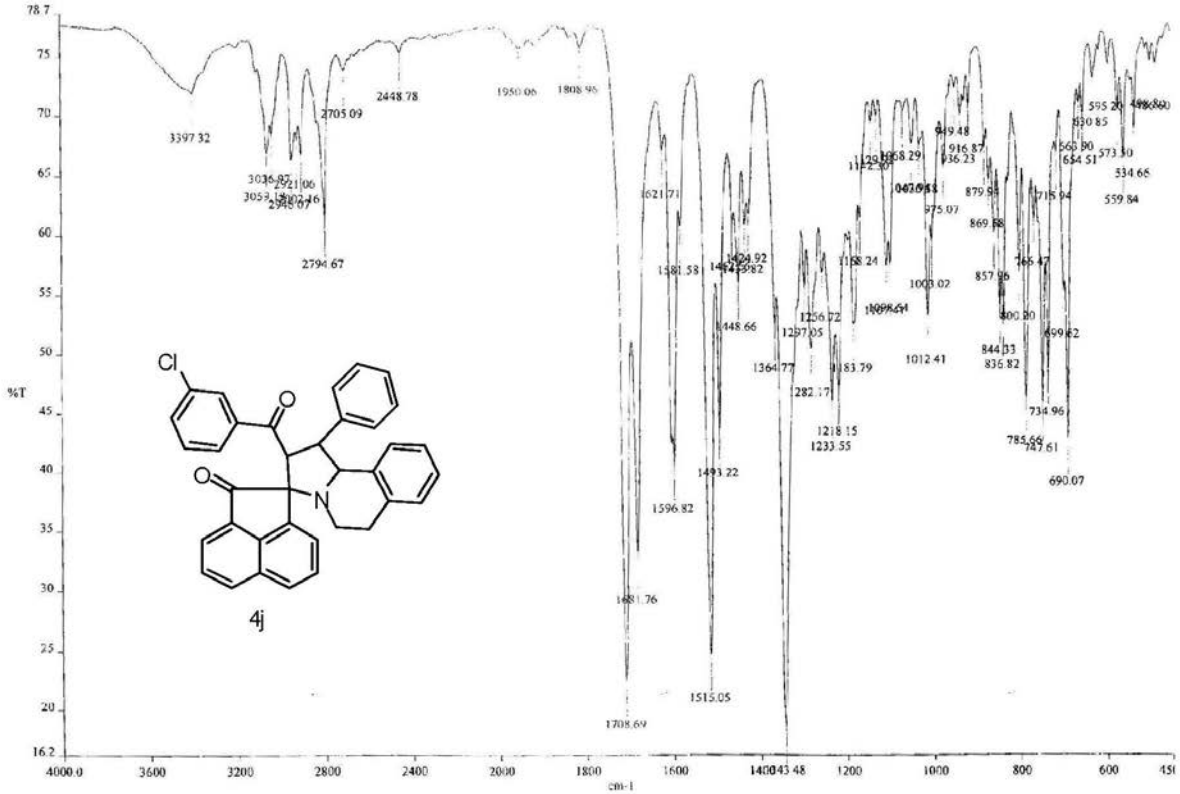

Figure S34. IR (KBr) of (**4j**).

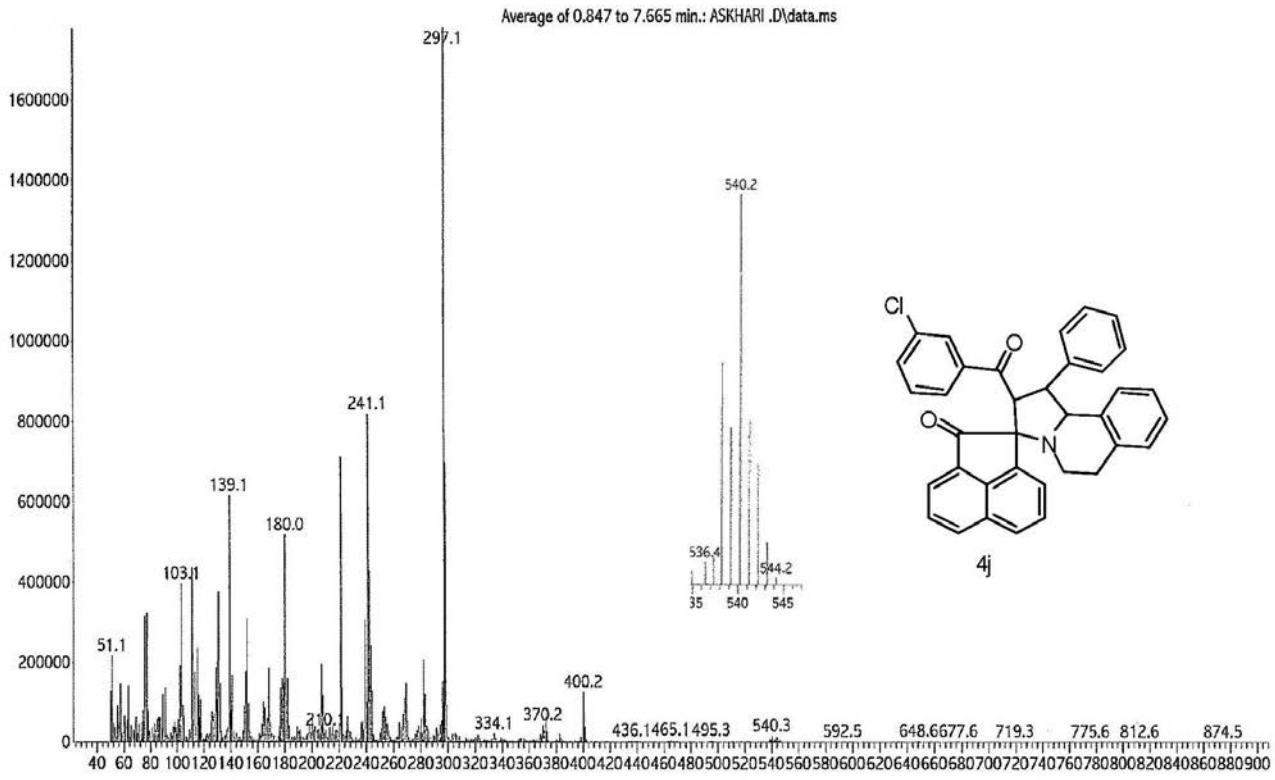

Figure S35. MS (70 eV) of (**4j**).

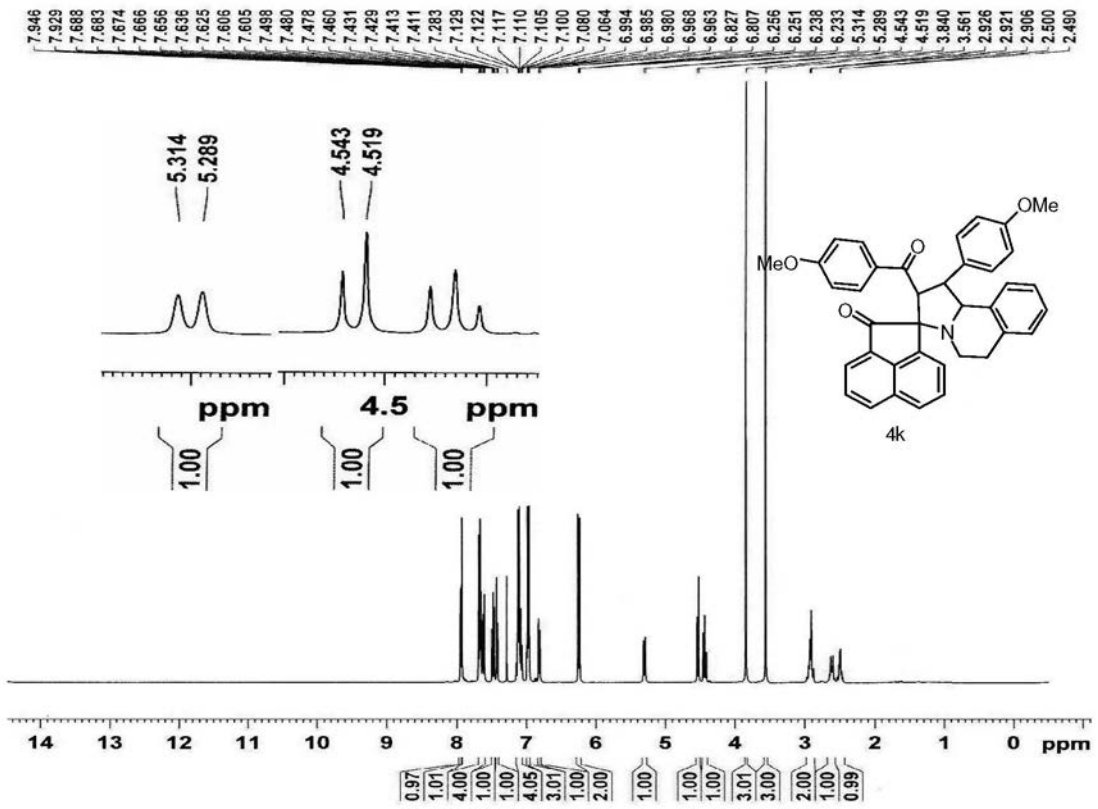

Figure S36. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4k**).

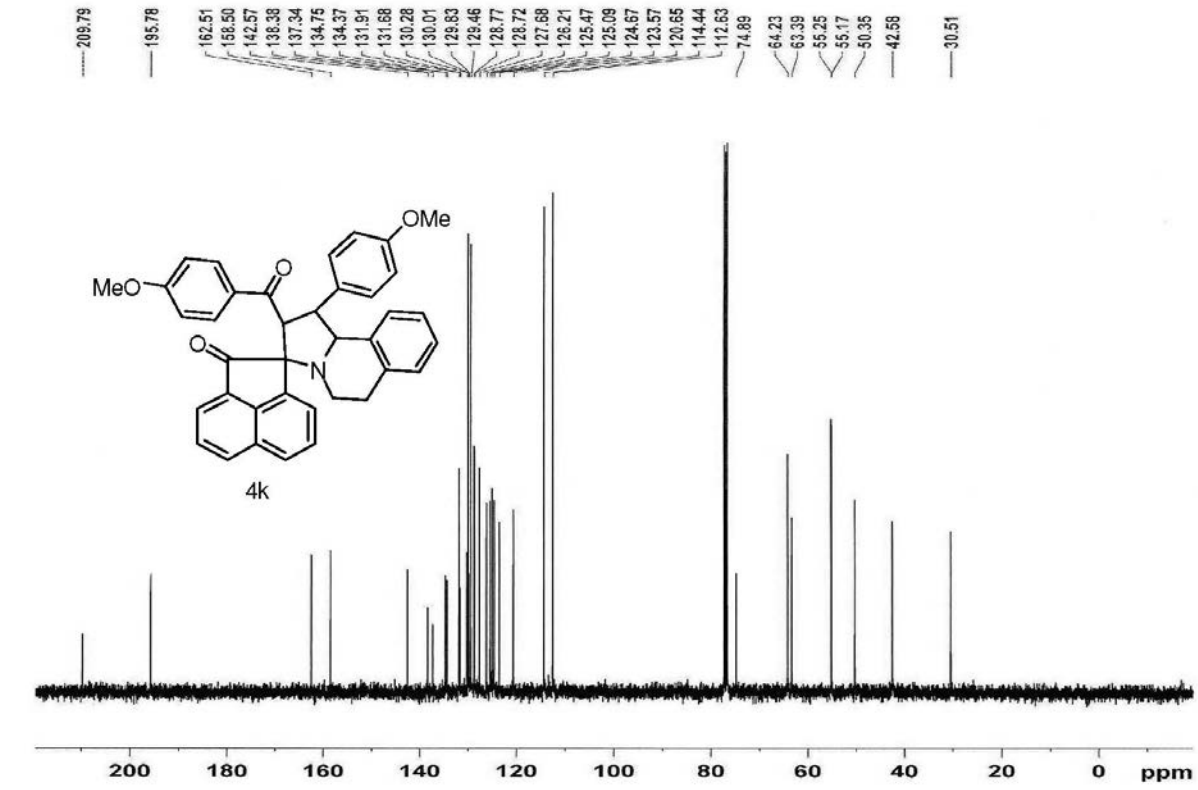

Figure S37. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4k**).

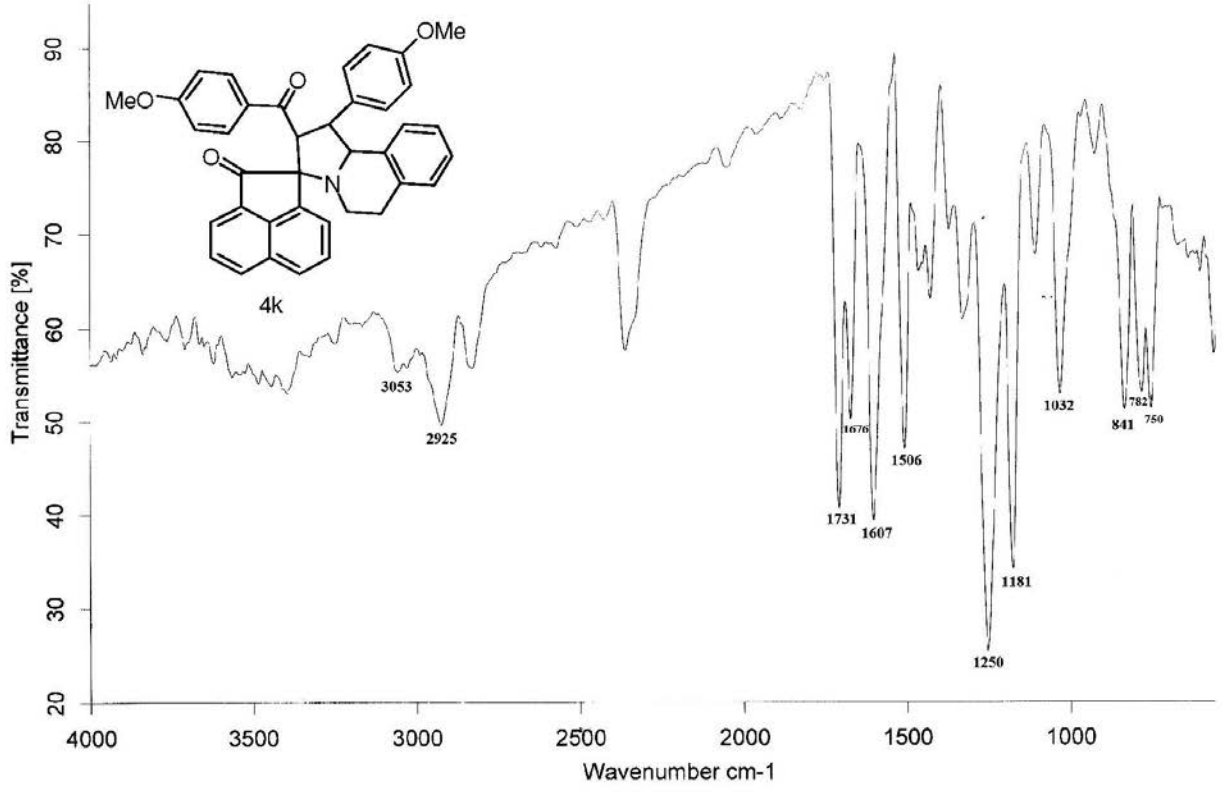

Figure S38. IR (KBr) of (**4k**).

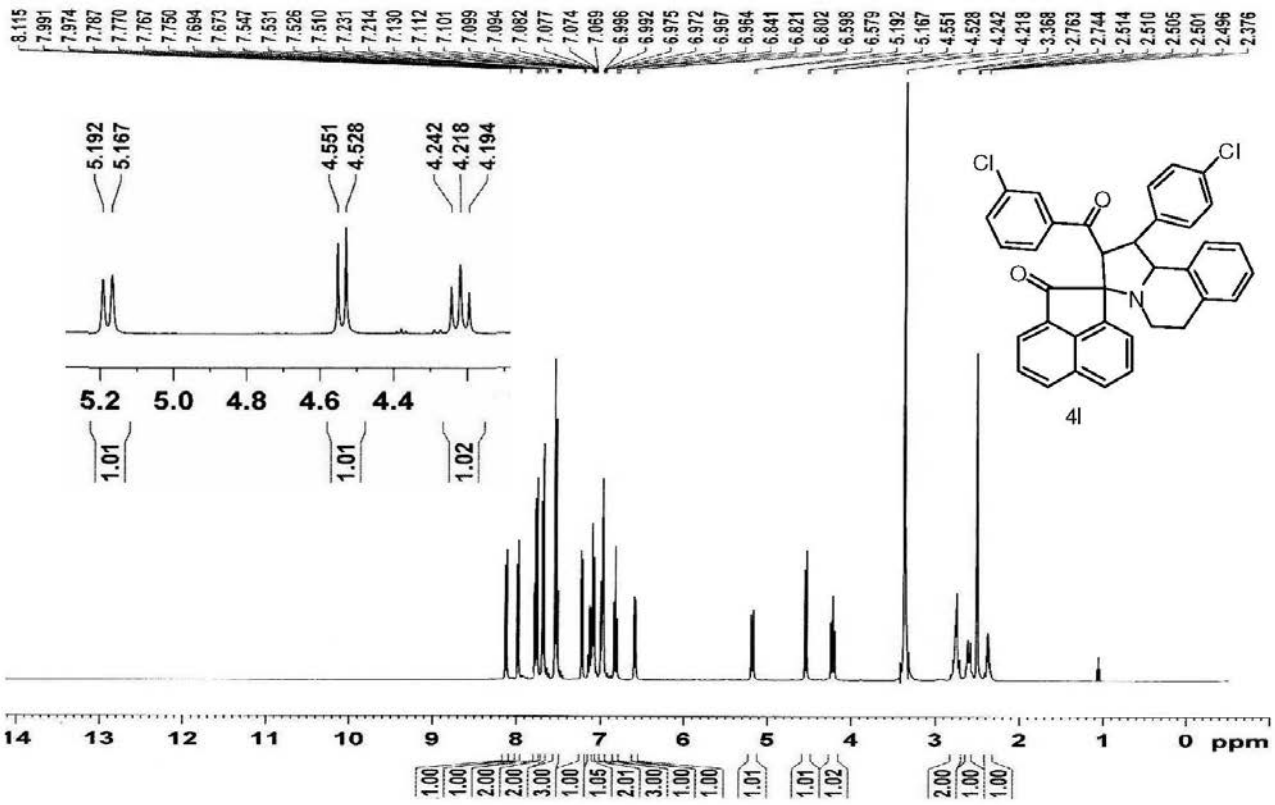

Figure S39. ^{1}H NMR (400 MHz, $CDCl_3$) of (**4l**).

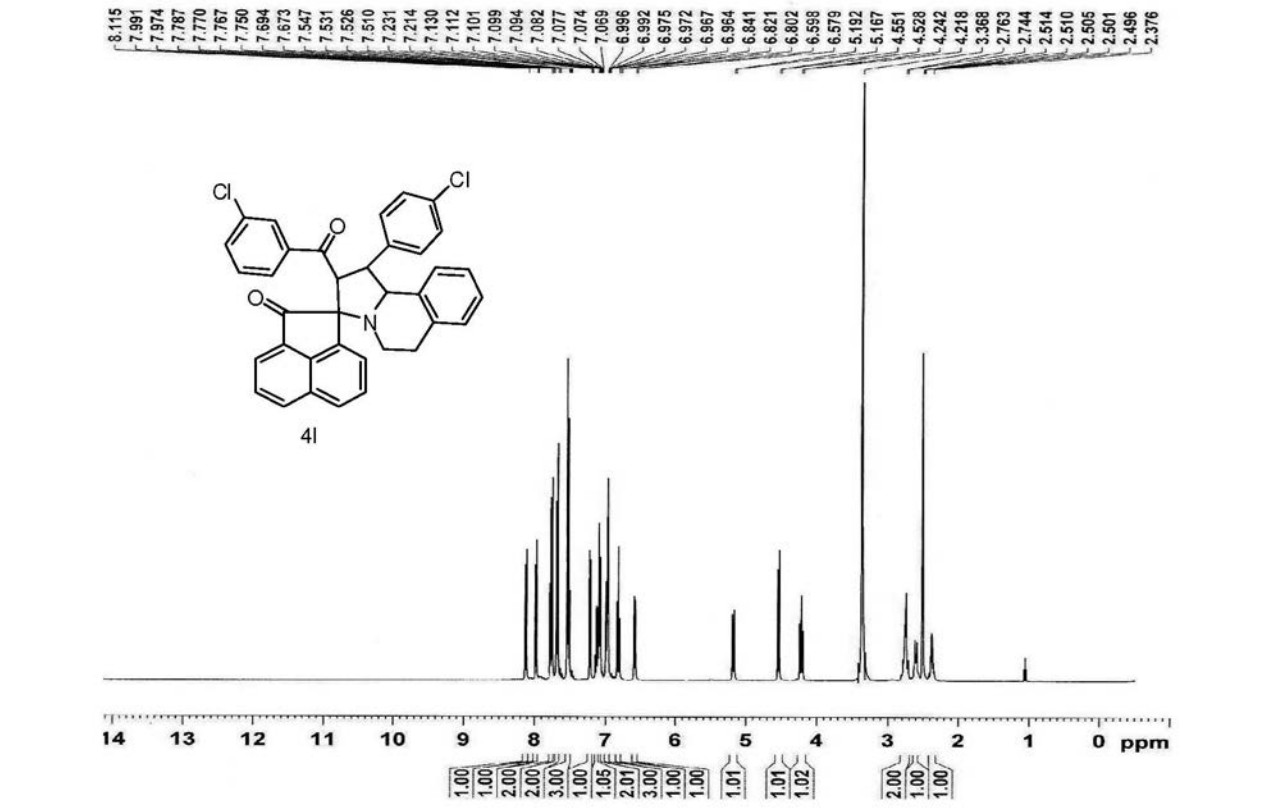

Figure S40. ^{13}C NMR (100 MHz, $CDCl_3$) of (**4l**).

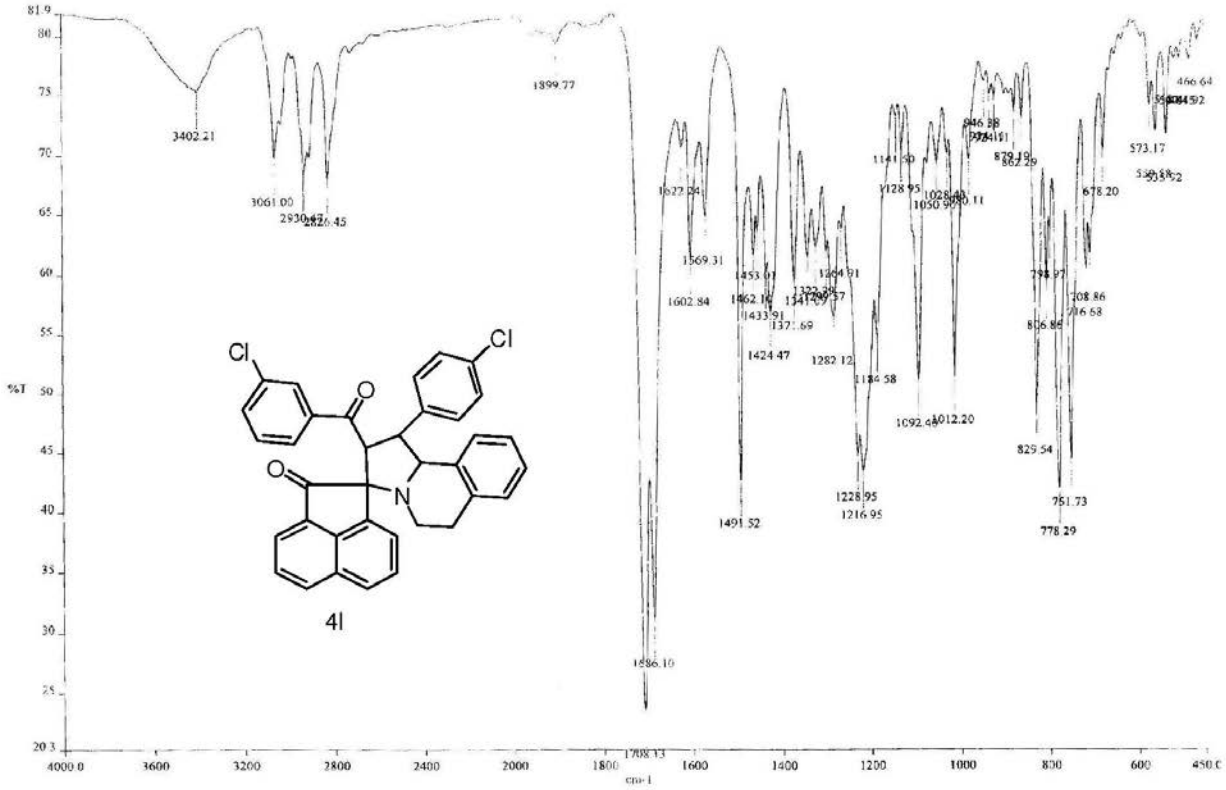

Figure S41. IR (KBr) of (**4l**).

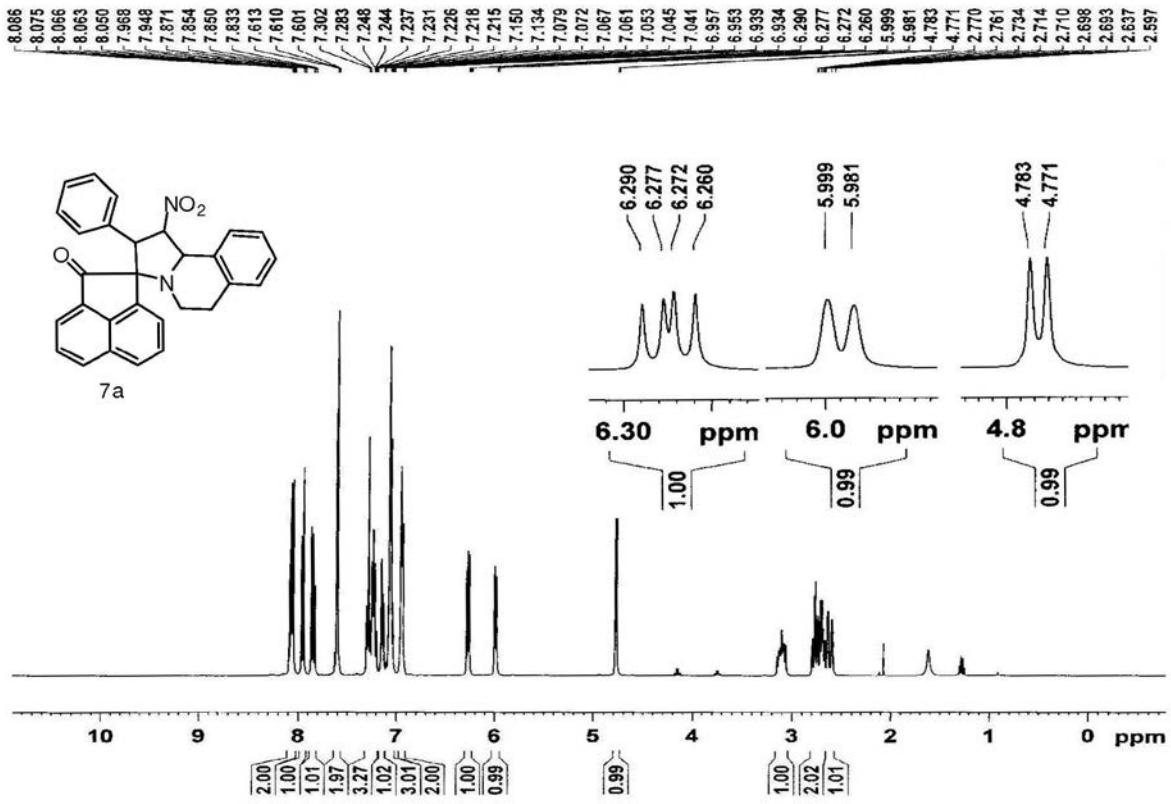

Figure S42. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7a**).

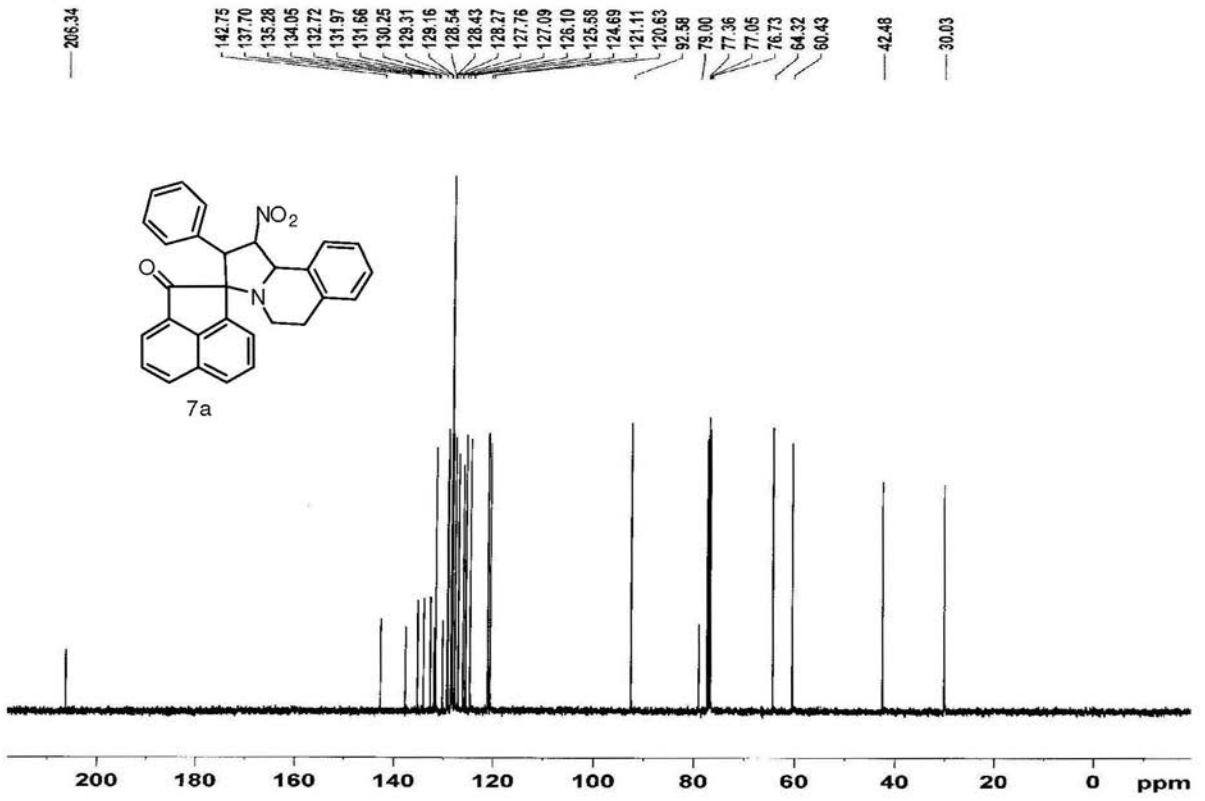

Figure S43. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7a**).

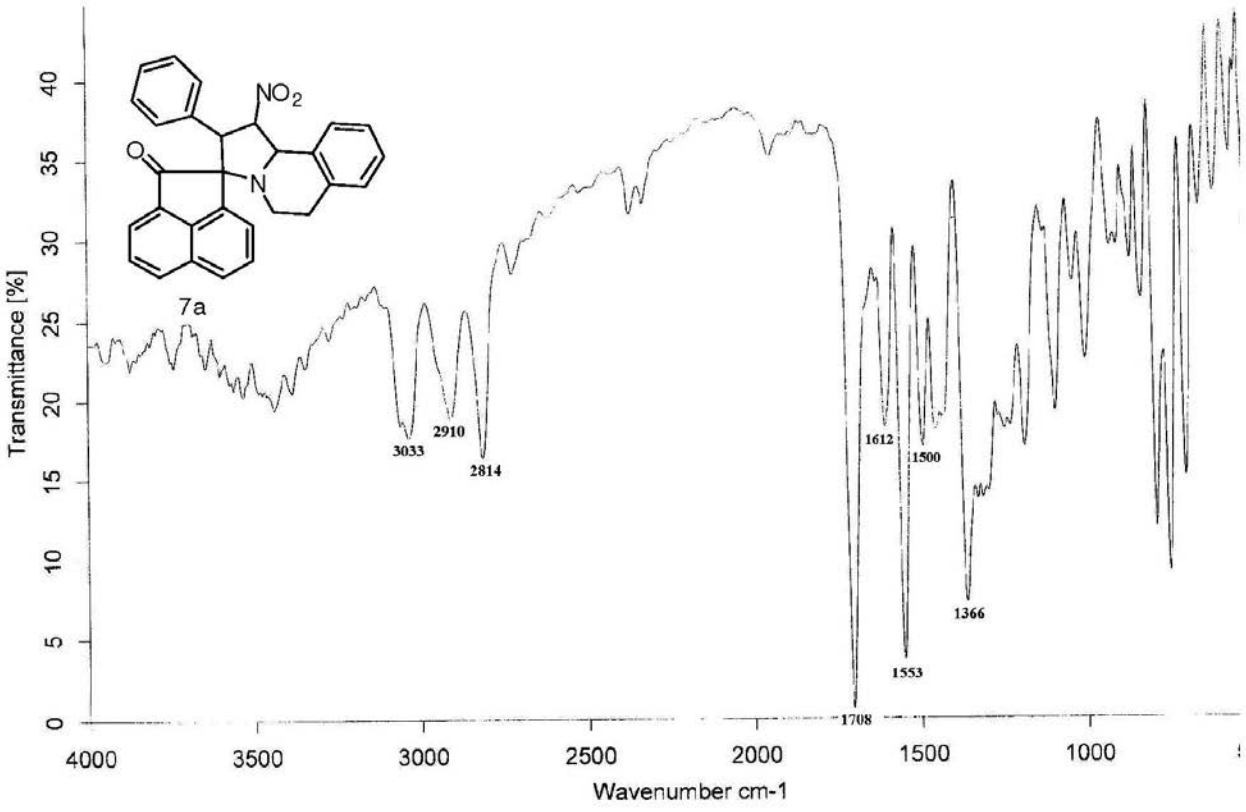

Figure S44. IR (KBr) of (**7a**).

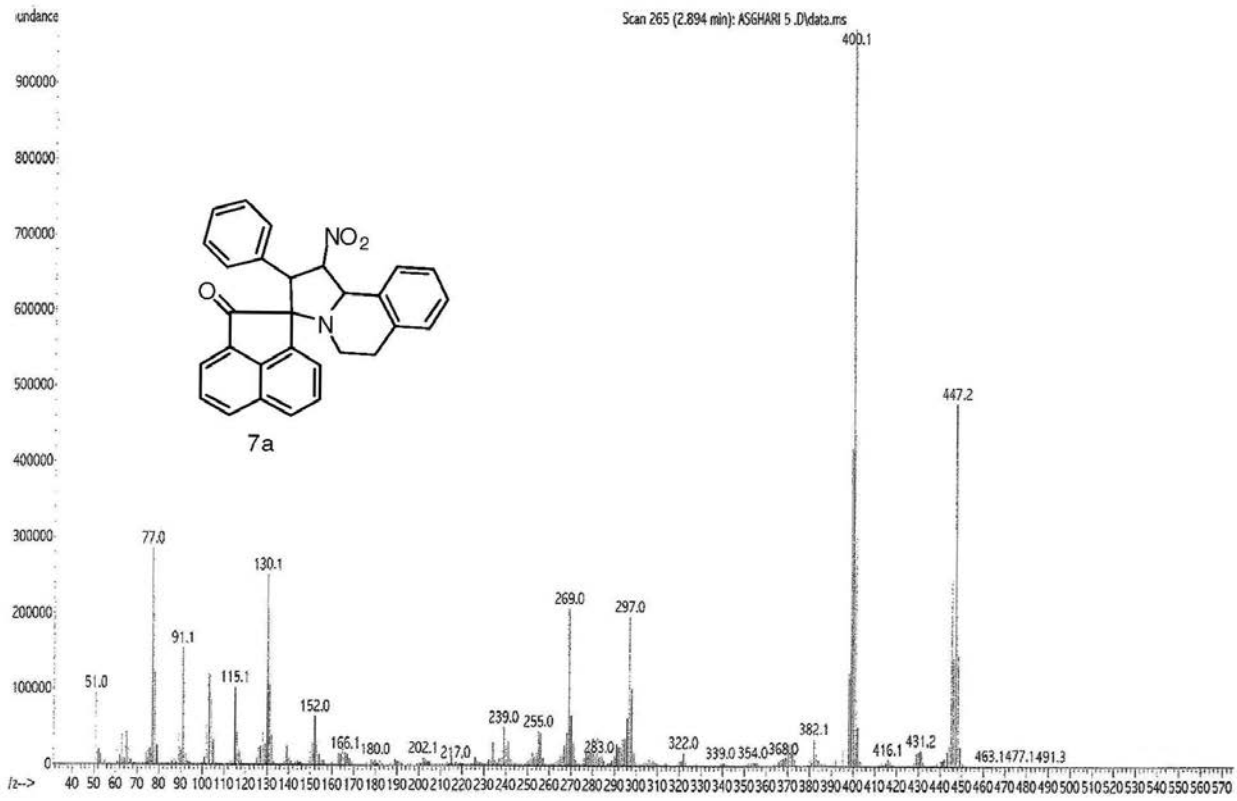

Figure S45. MS (70 eV) of (**7a**).

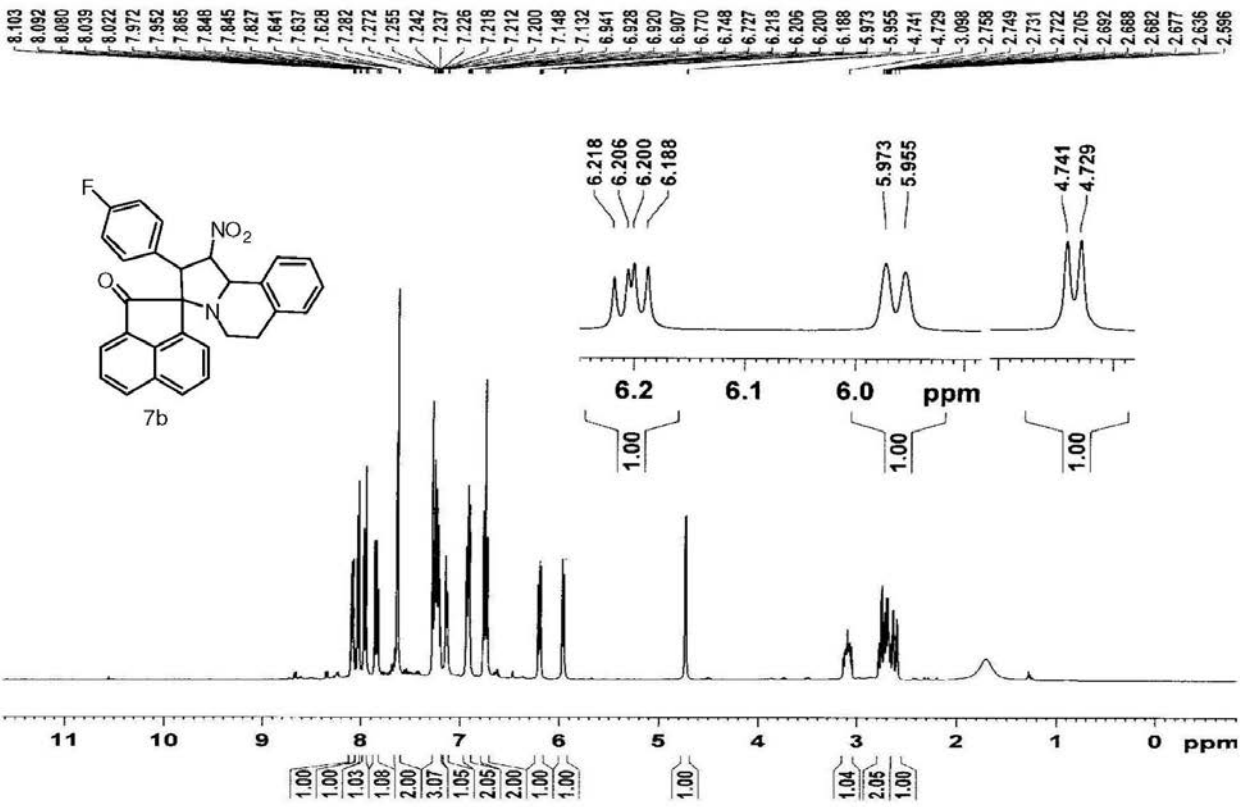

Figure S46. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7b**).

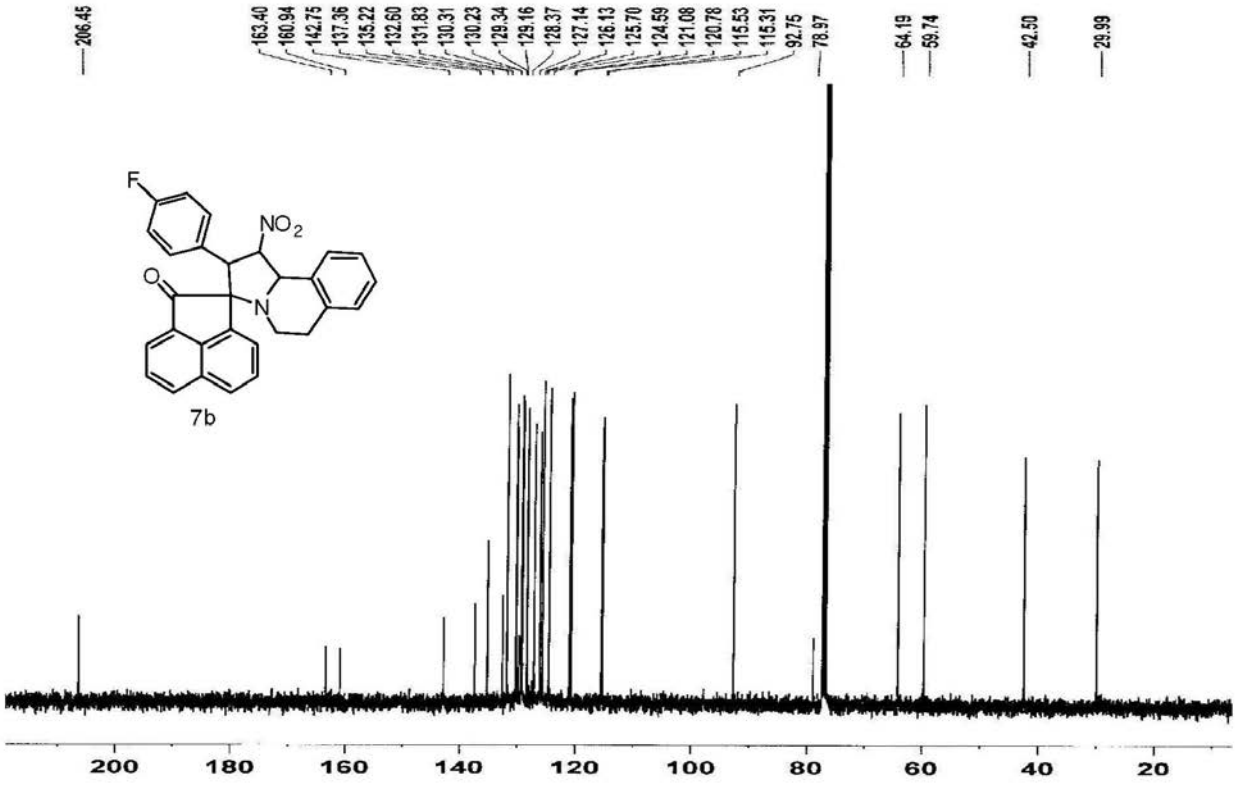

Figure S47. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7b**).

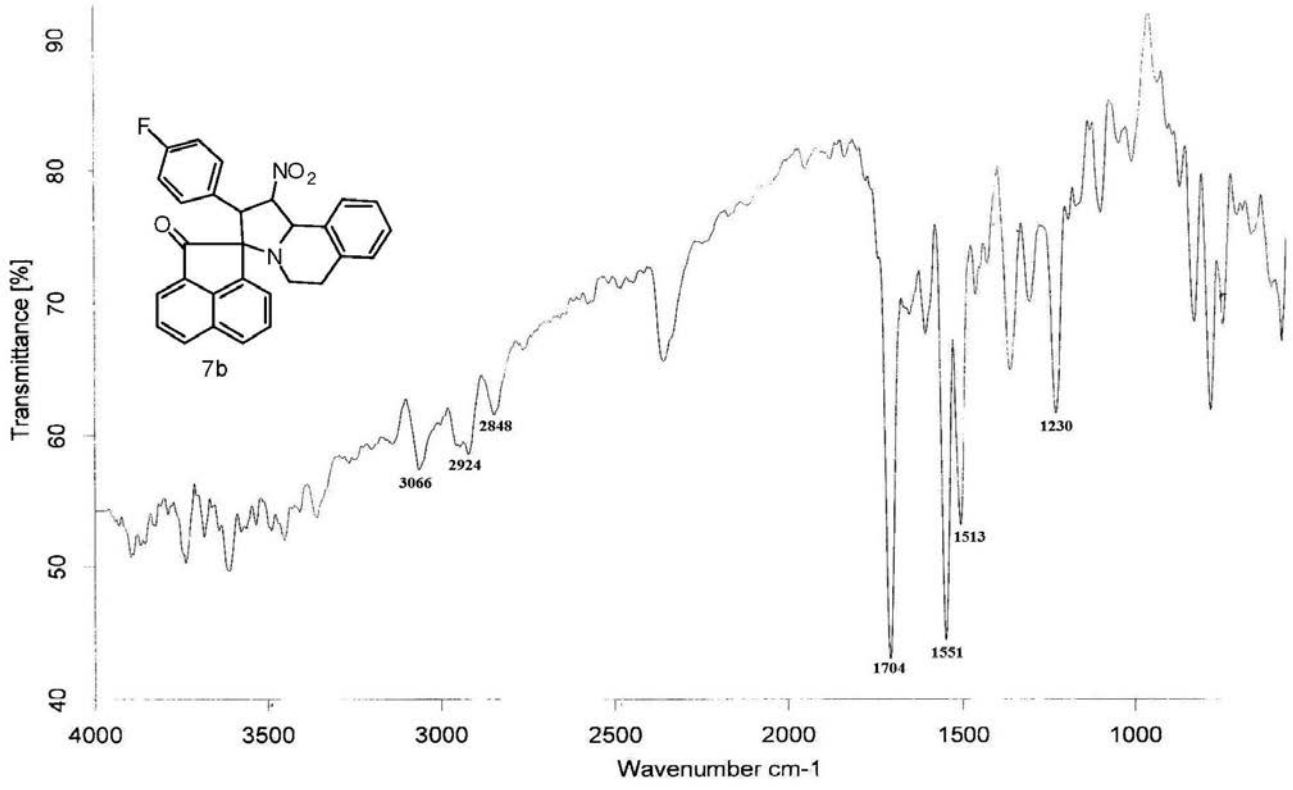

Figure S48. IR (KBr) of (**7b**).

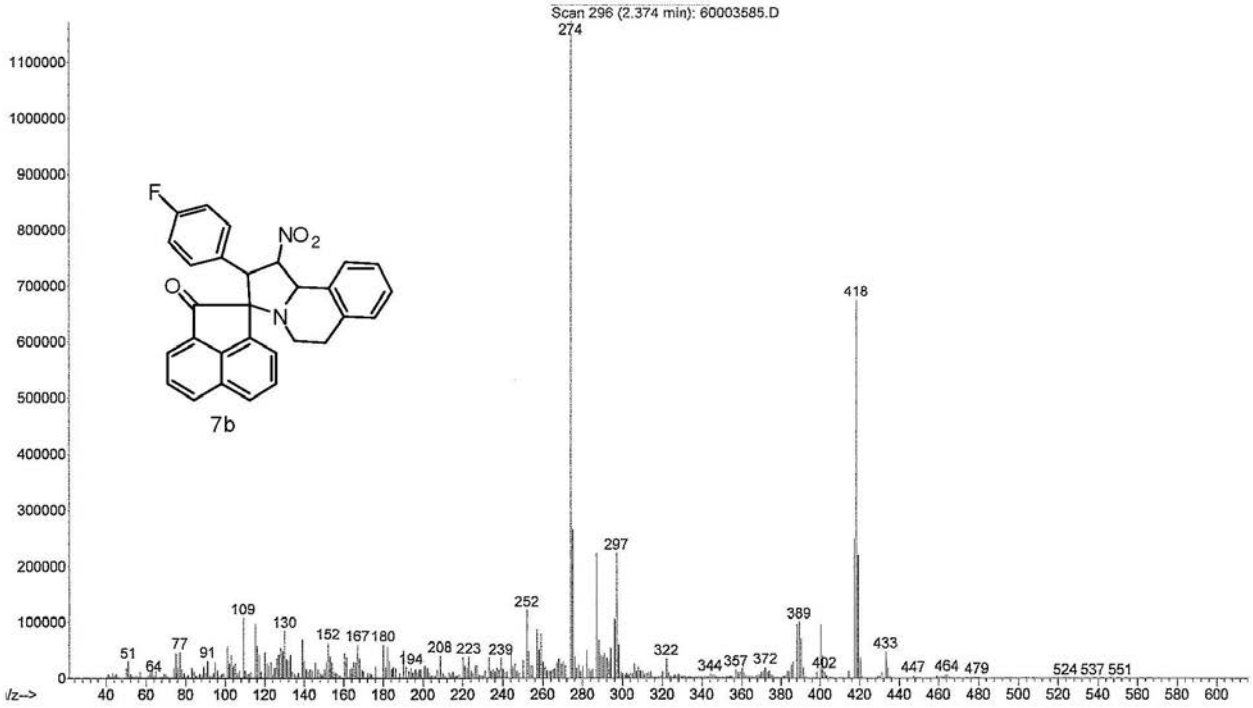

Figure S49. MS (70 eV) of (**7b**).

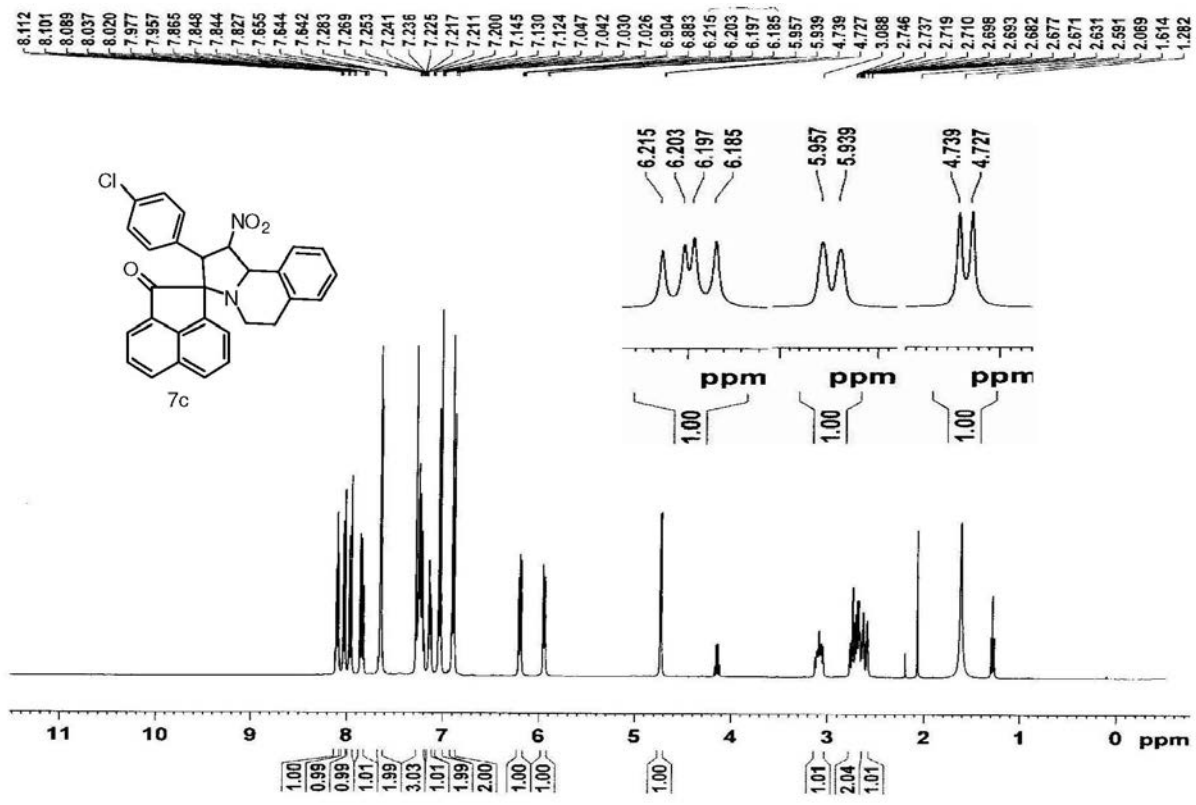

Figure S50. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7c**).

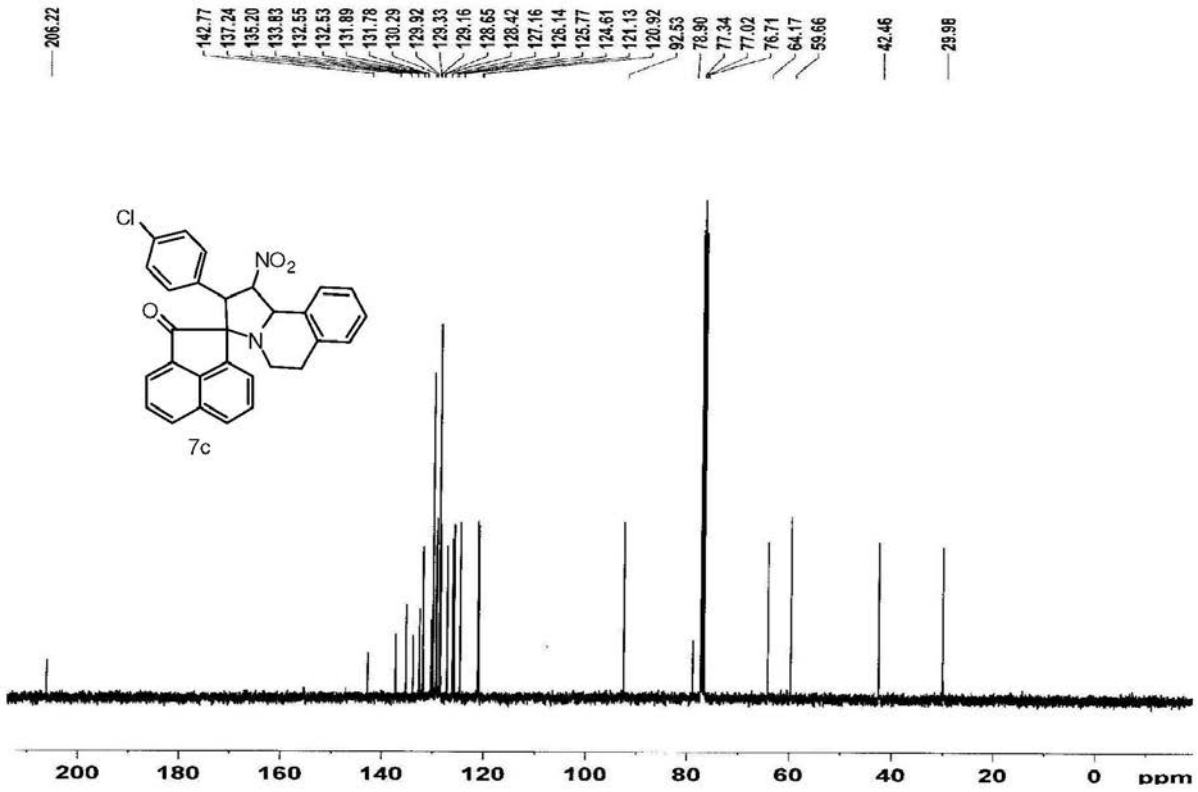

Figure S51. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7c**).

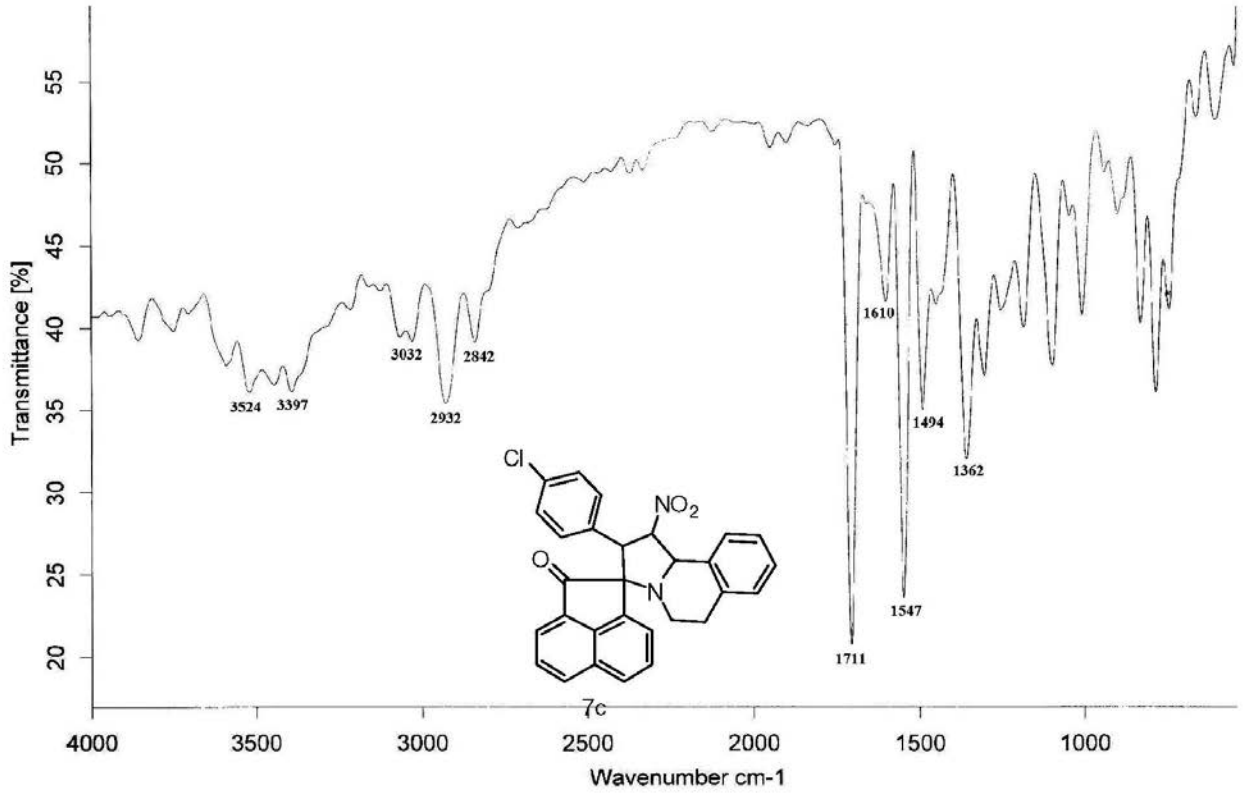

Figure S52. IR (KBr) of (**7c**).

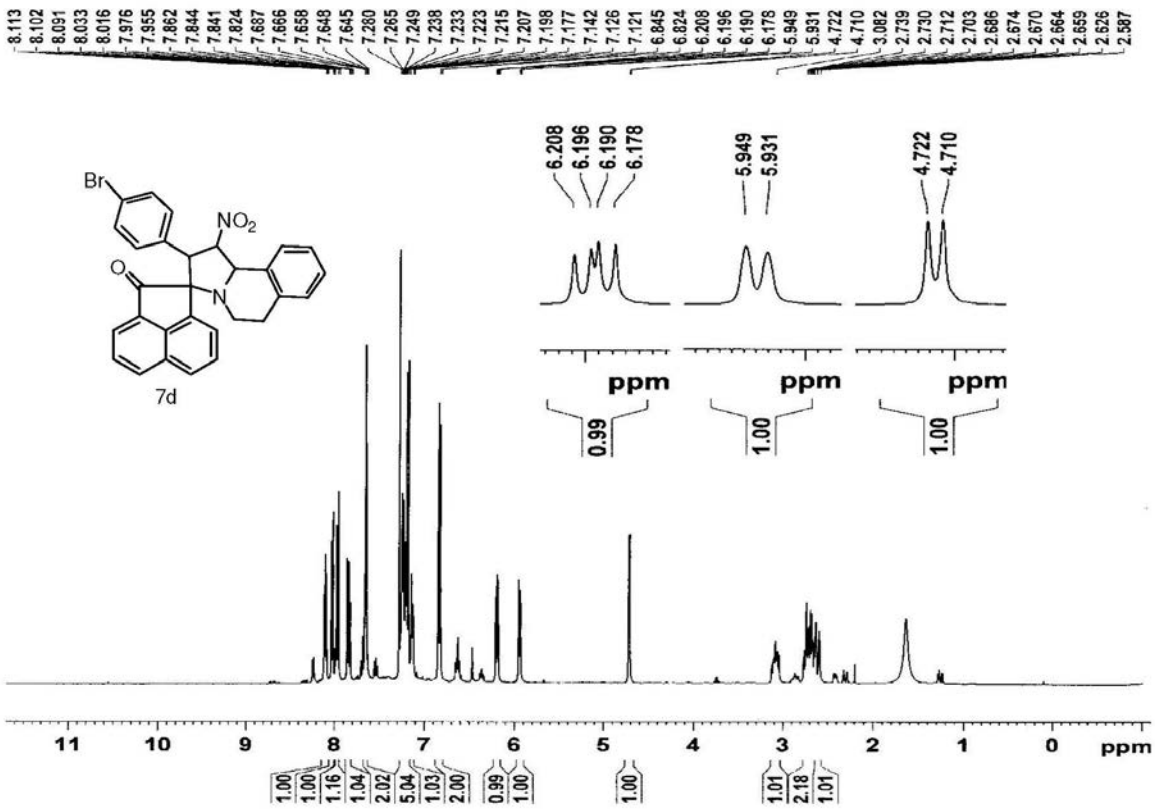

Figure S53. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7d**).

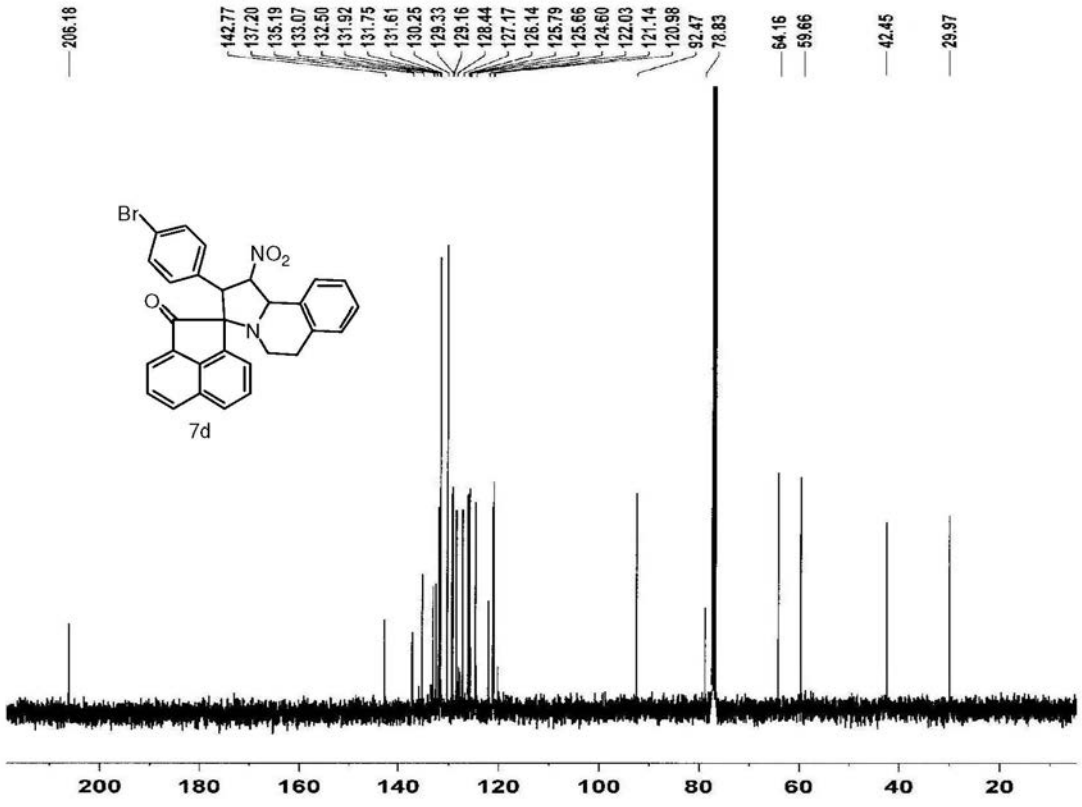

Figure S54. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7d**).

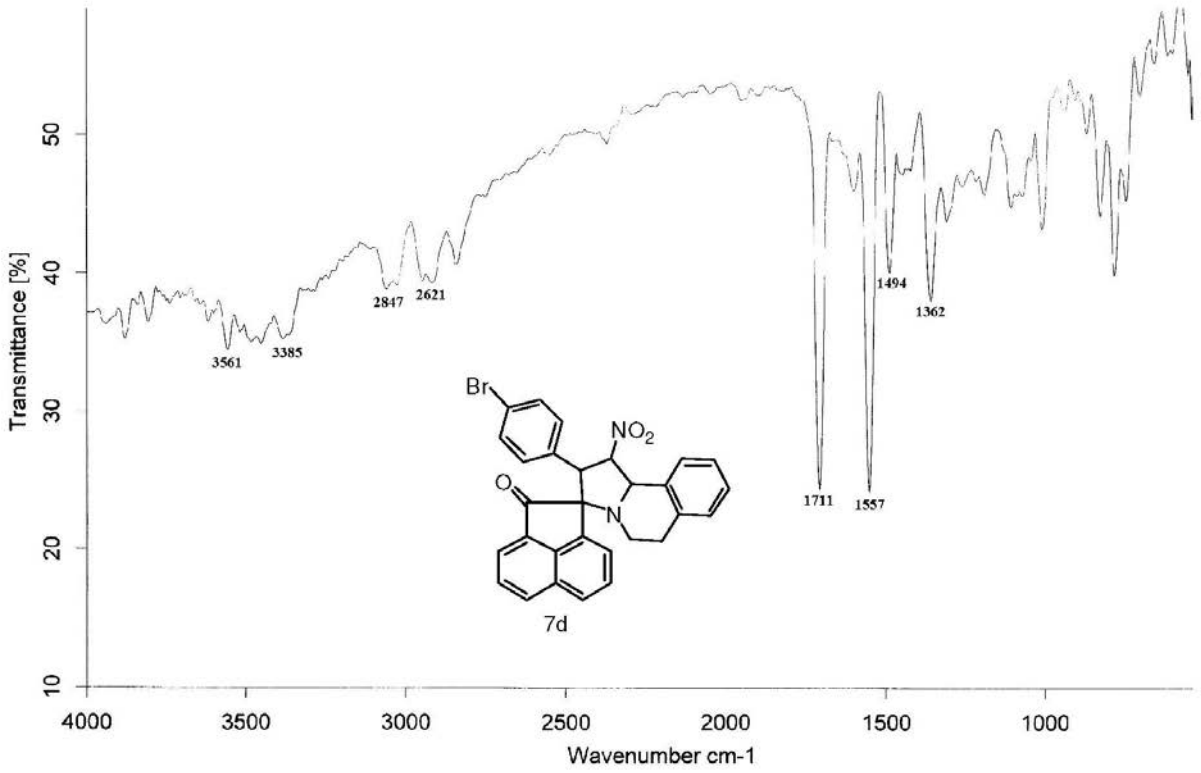

Figure S55. IR (KBr) of (**7d**).

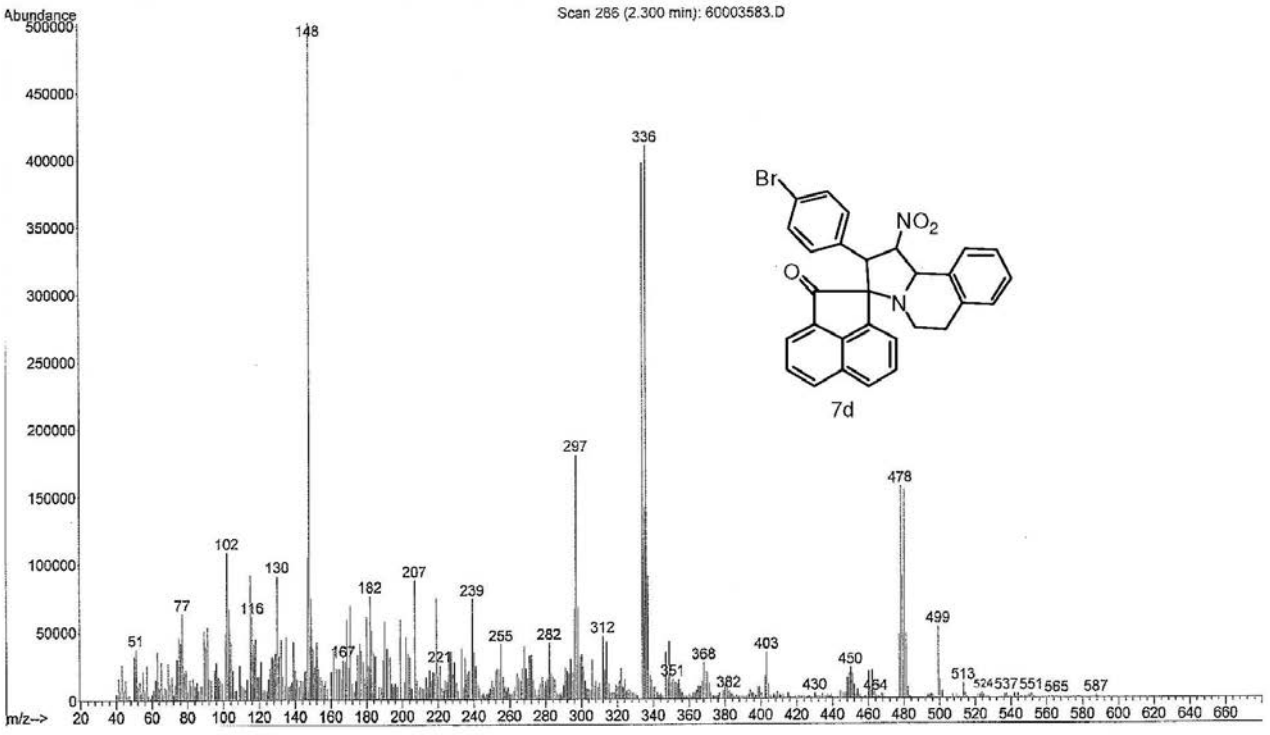

Figure S56. MS (70 eV) of (**7d**).

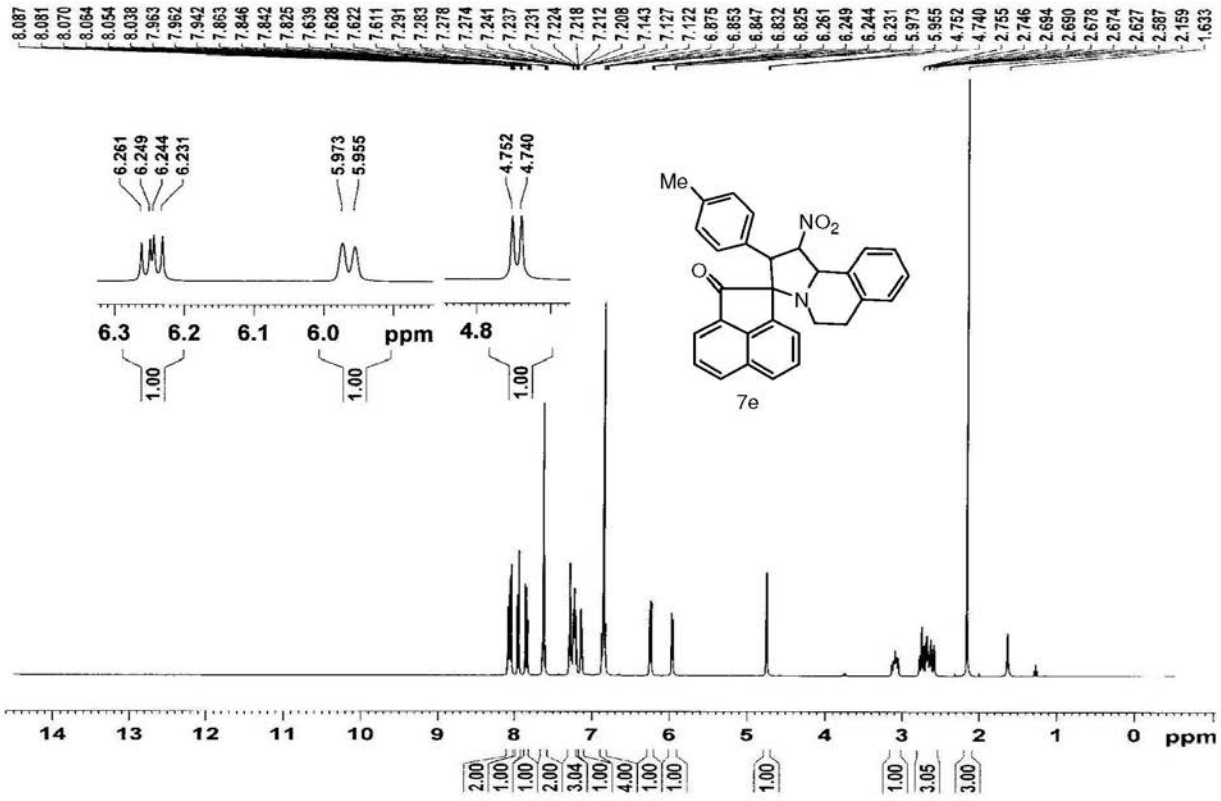

Figure S57. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7e**).

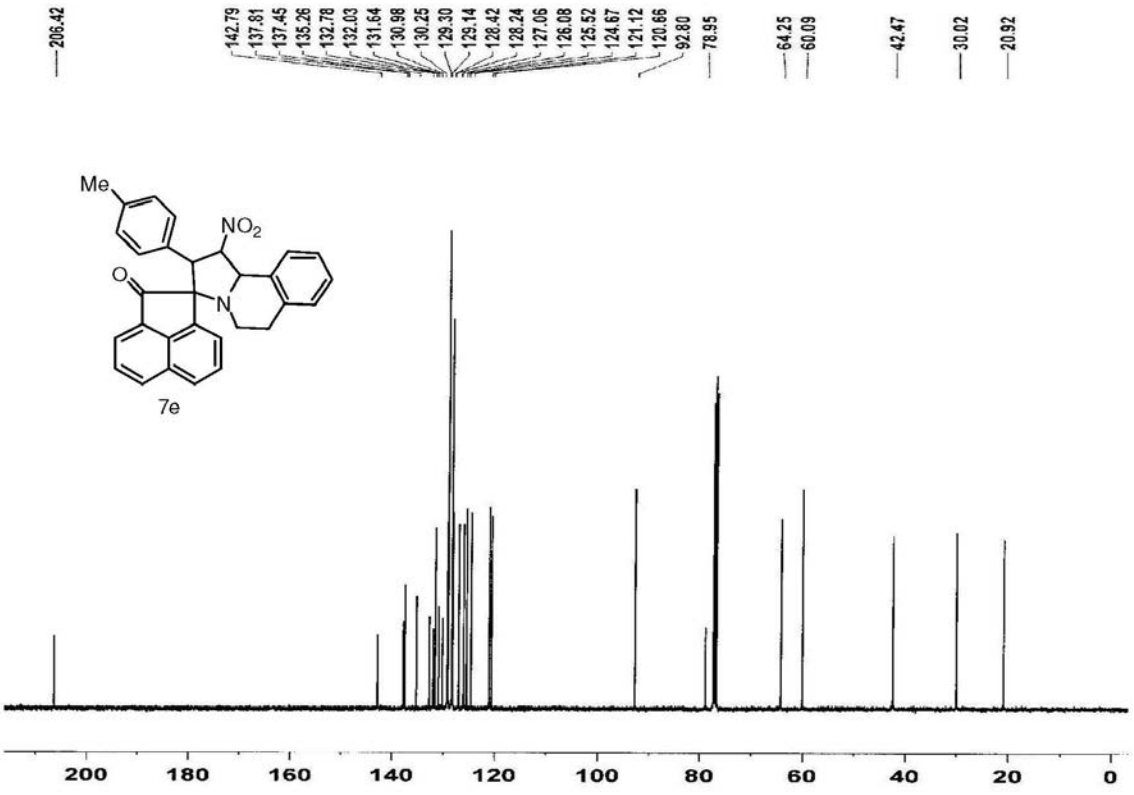

Figure S58. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7e**).

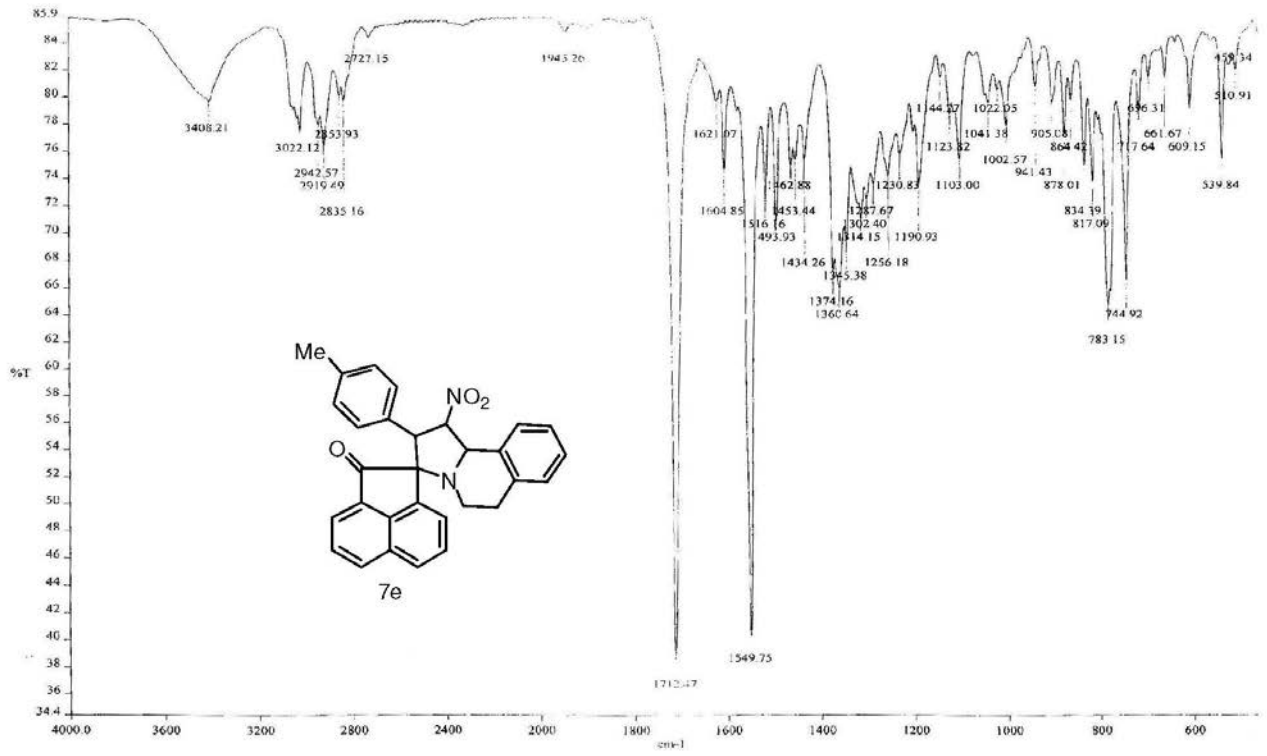

Figure S59. IR (KBr) of (**7e**).

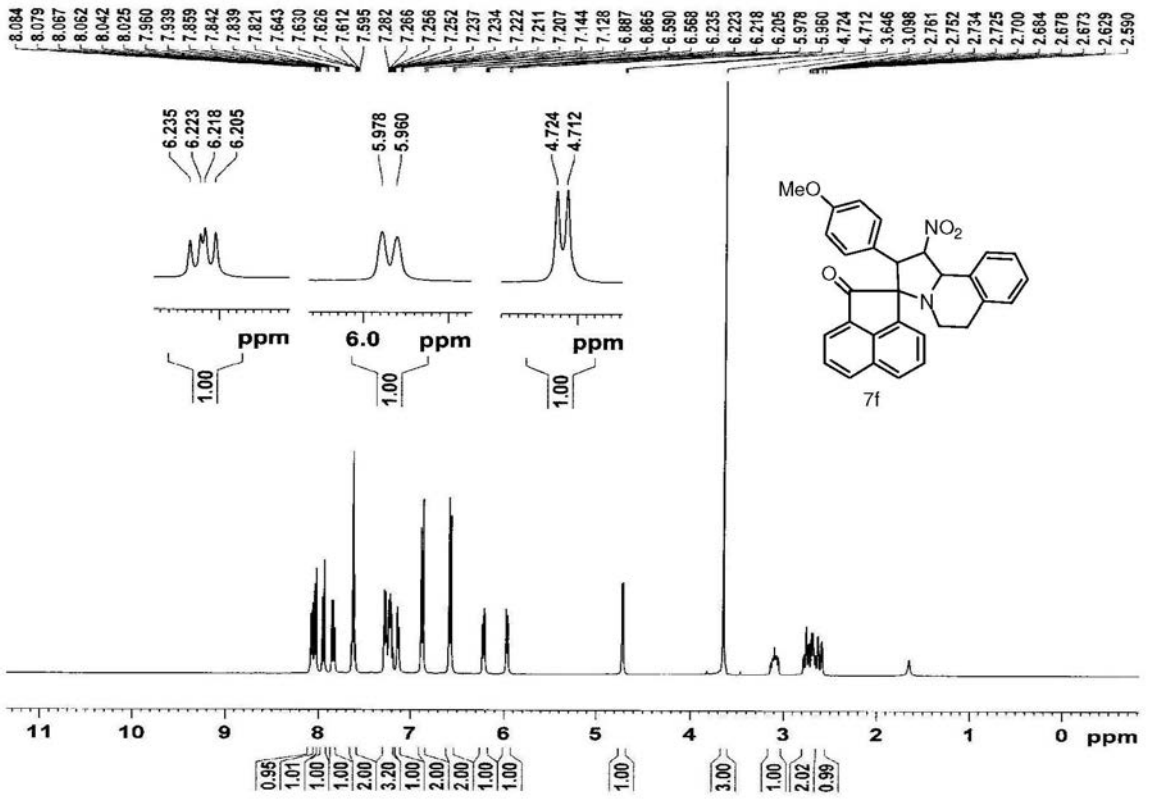

Figure S60. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7f**).

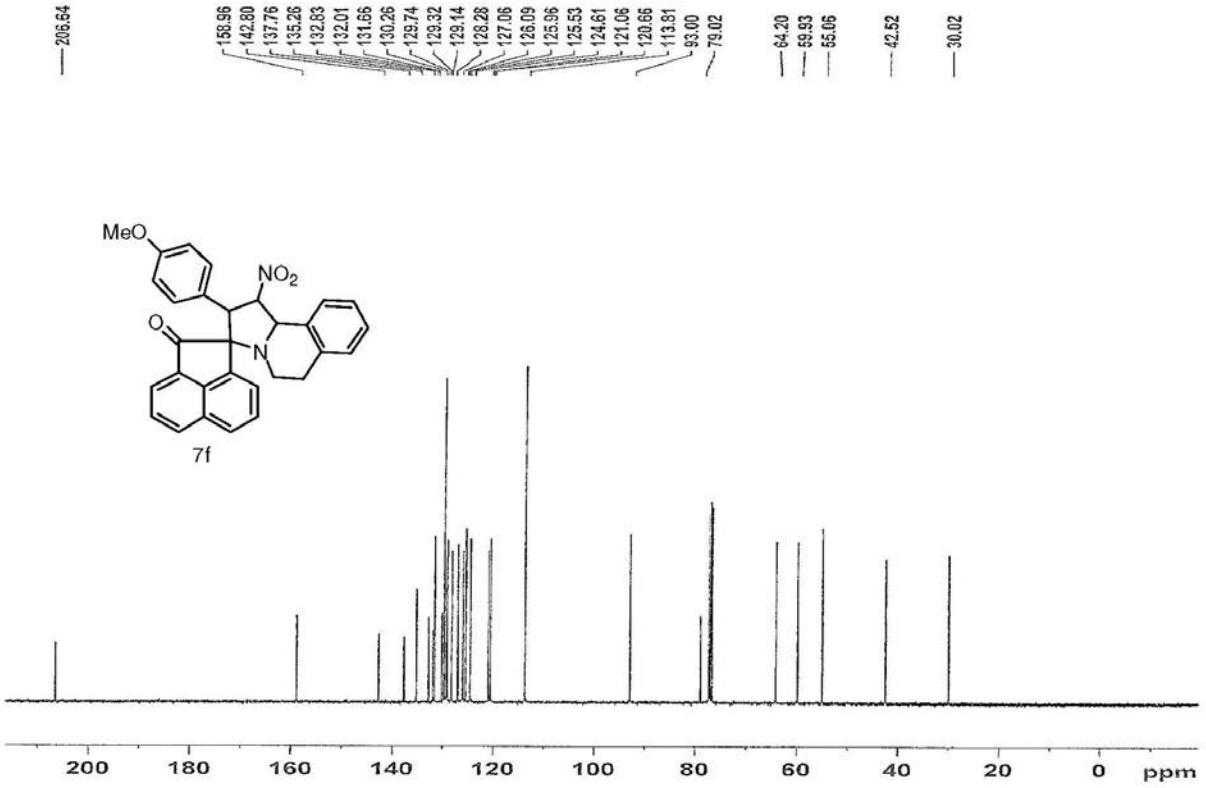

Figure S61. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7f**).

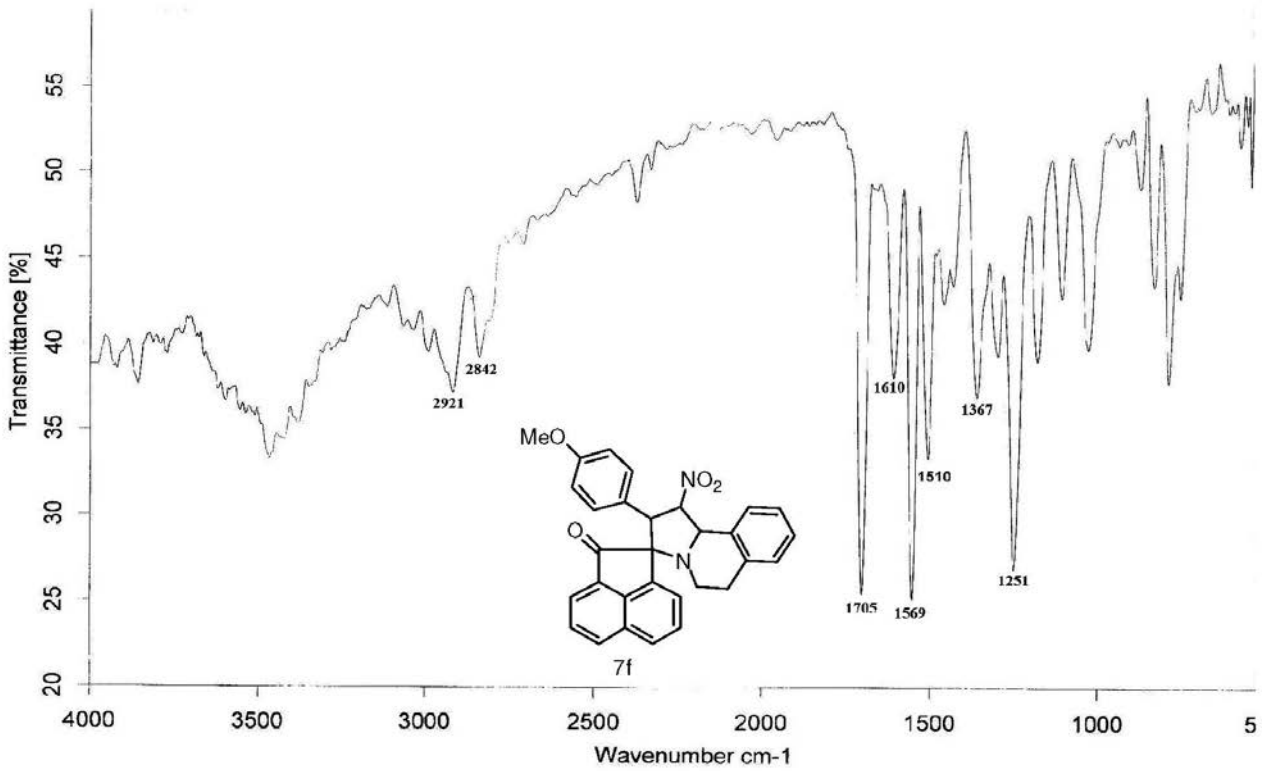

Figure S62. IR (KBr) of (**7f**).

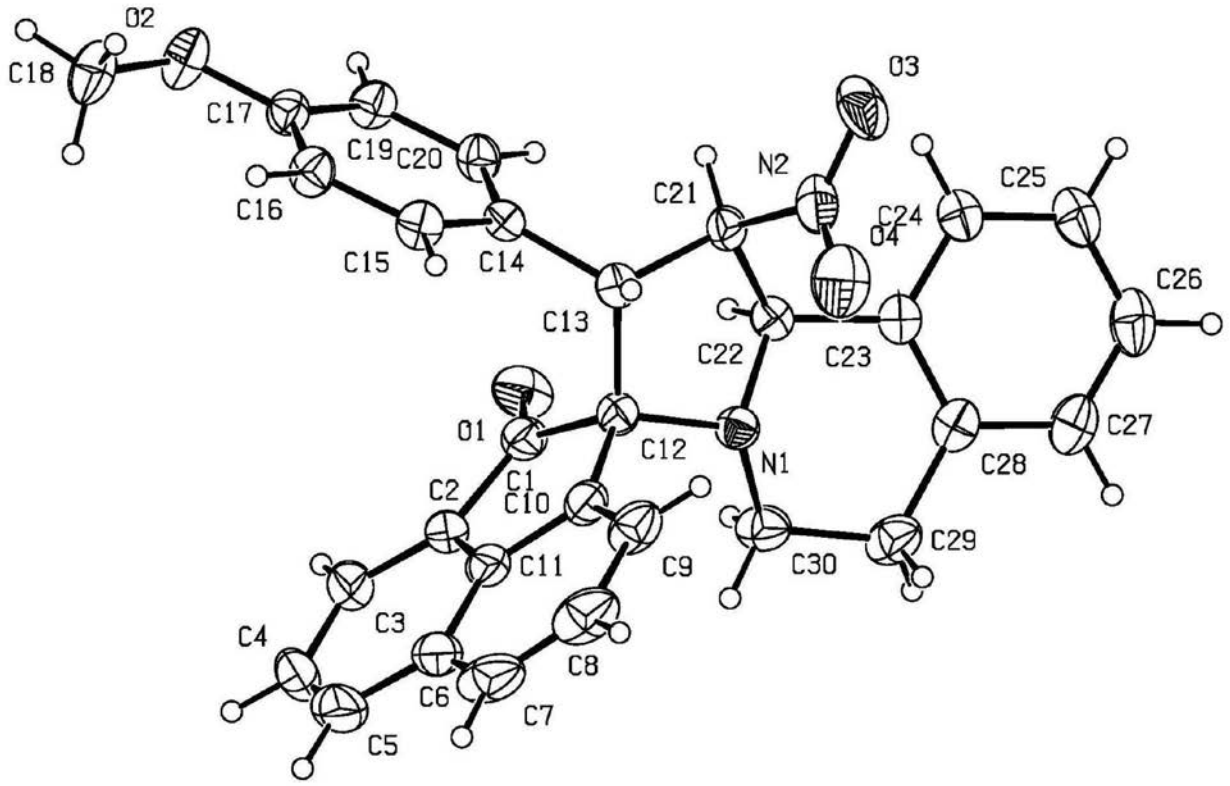

Figure S63. ORTEP diagram of (**7f**).

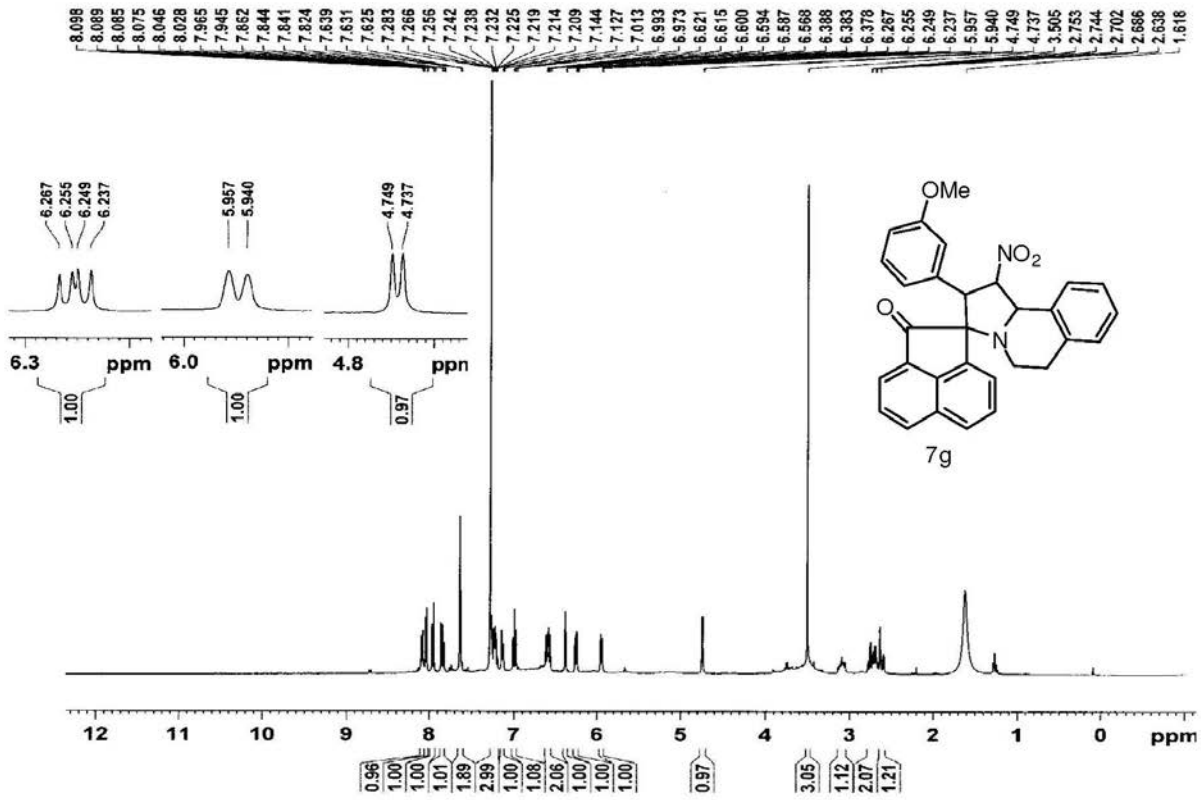

Figure S64. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7g**).

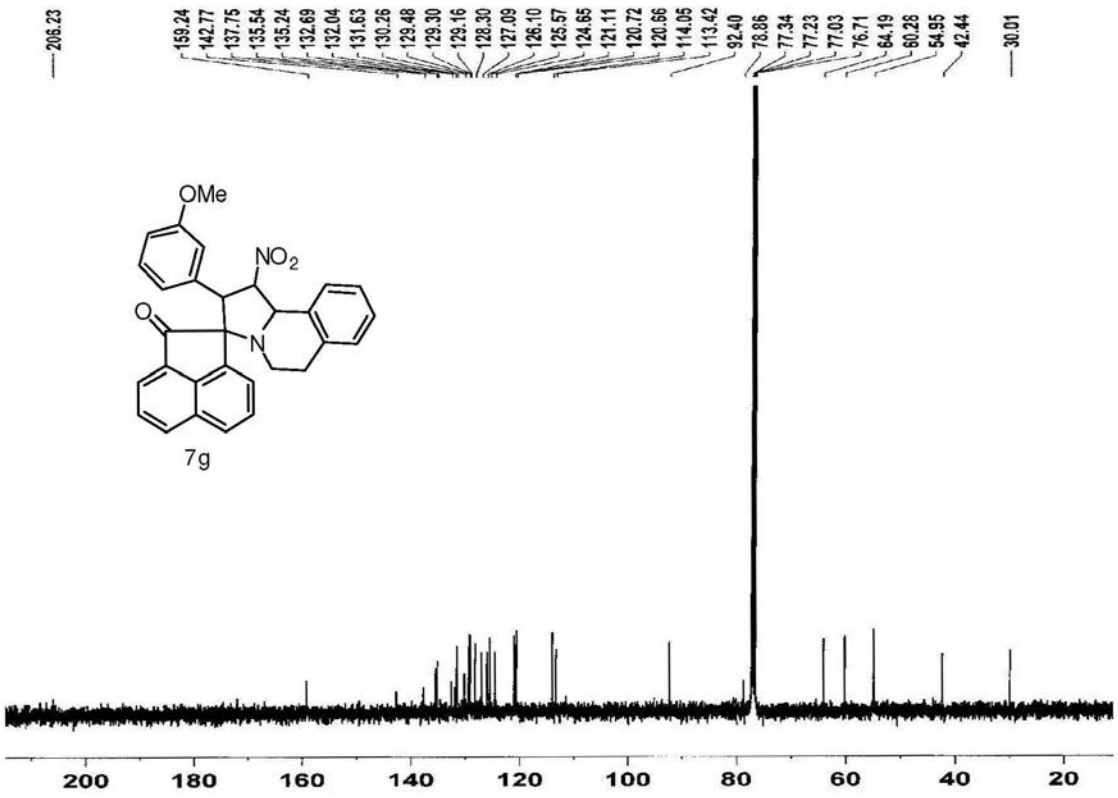

Figure S65. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7g**).

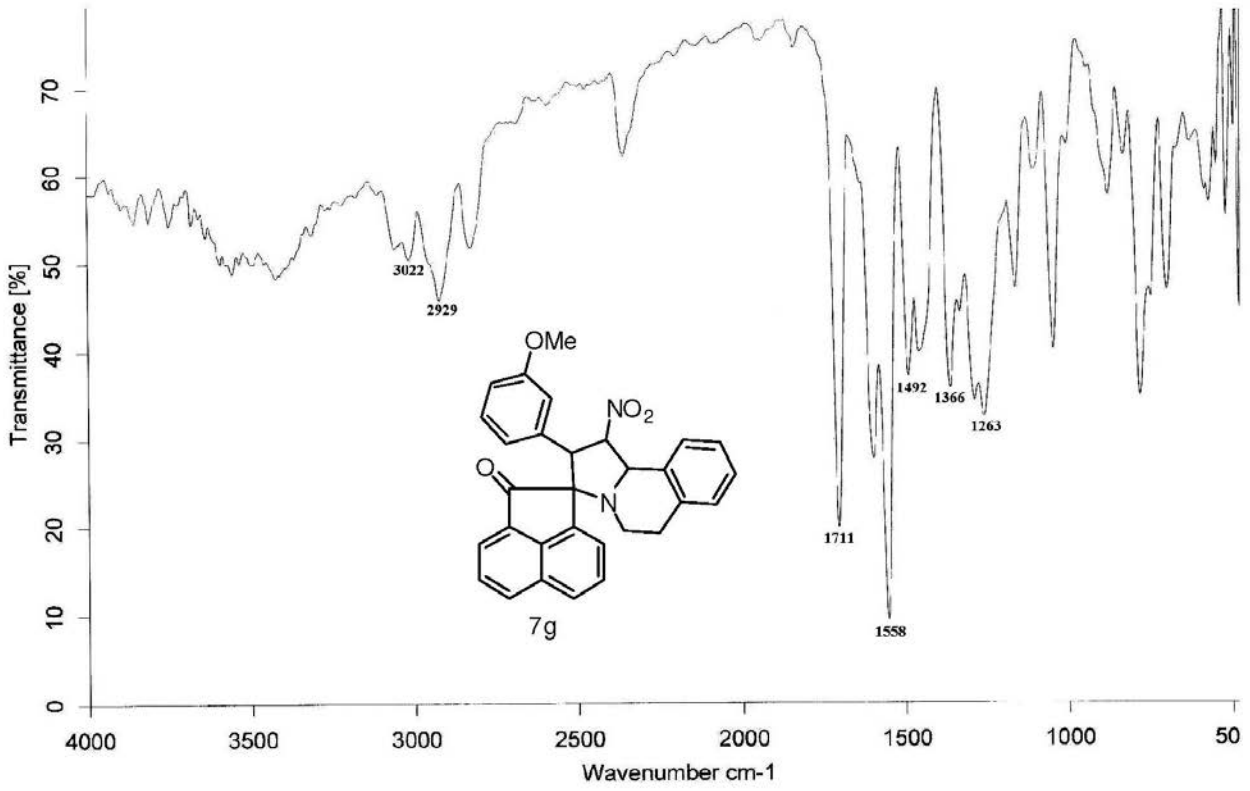

Figure S66. IR (KBr) of (**7g**).

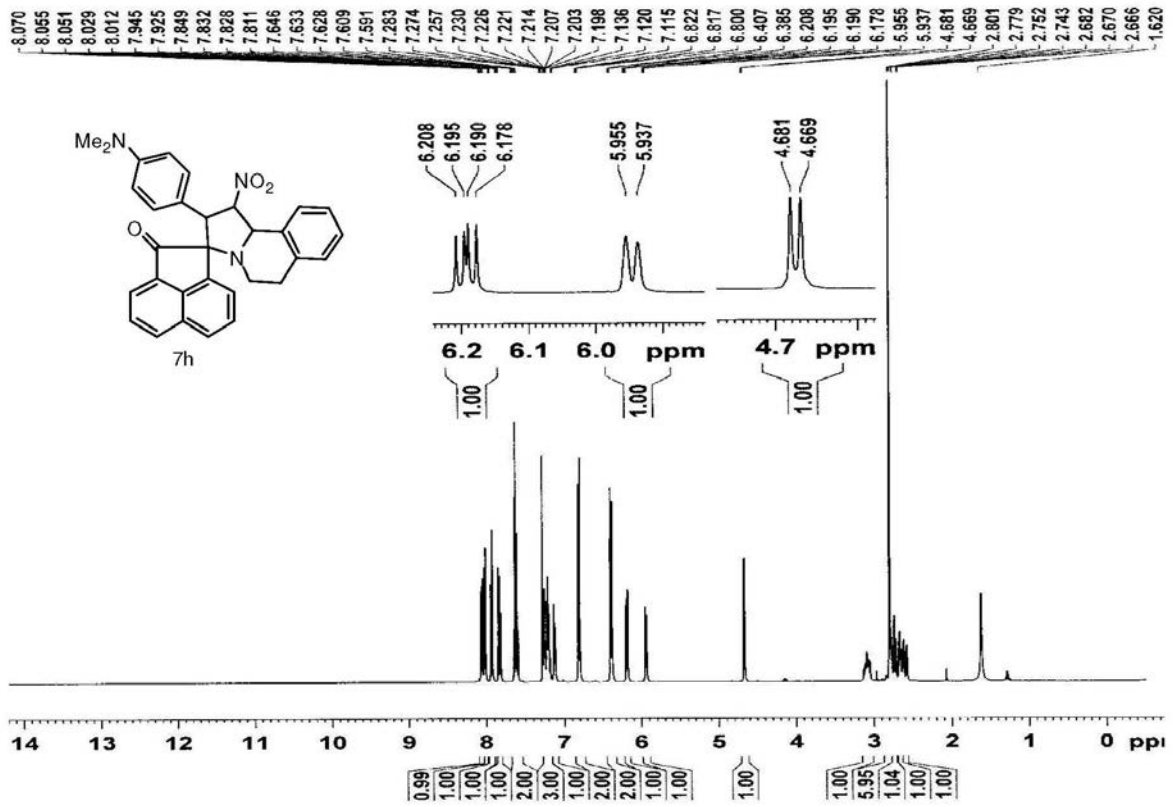

Figure S67. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7h**).

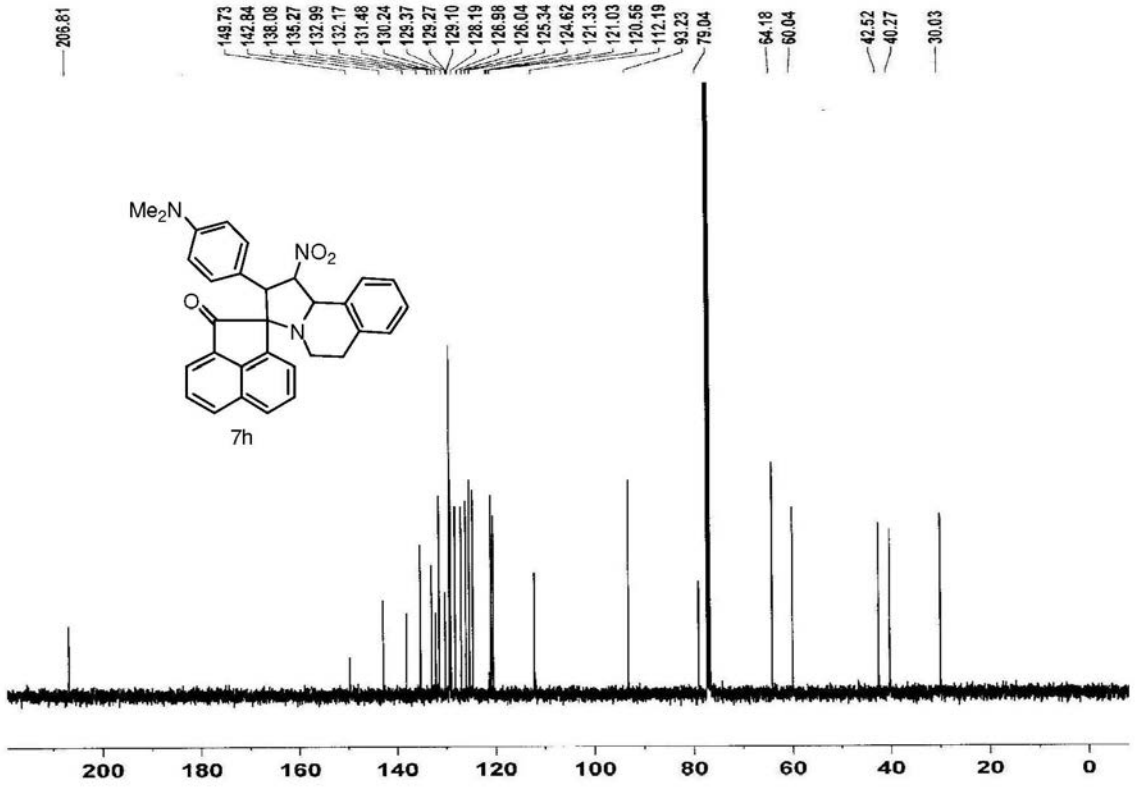

Figure S68. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7h**).

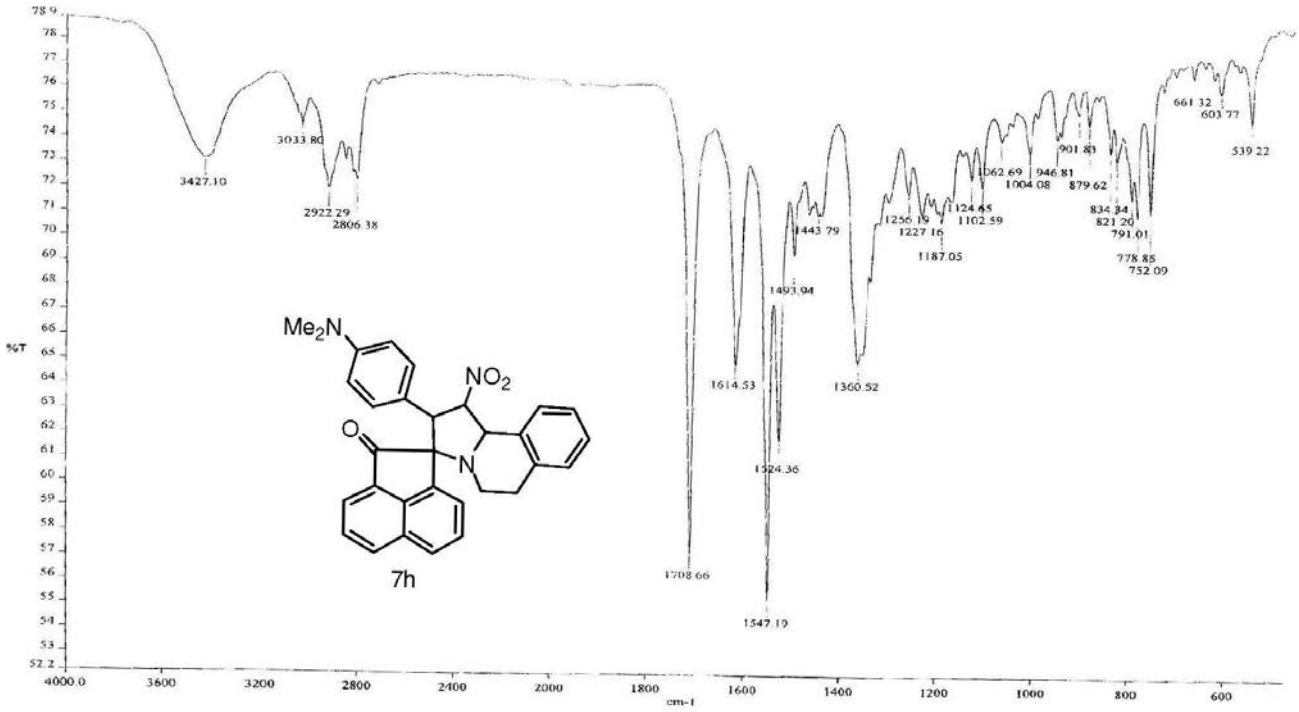

Figure S69. IR (KBr) of (**7h**).

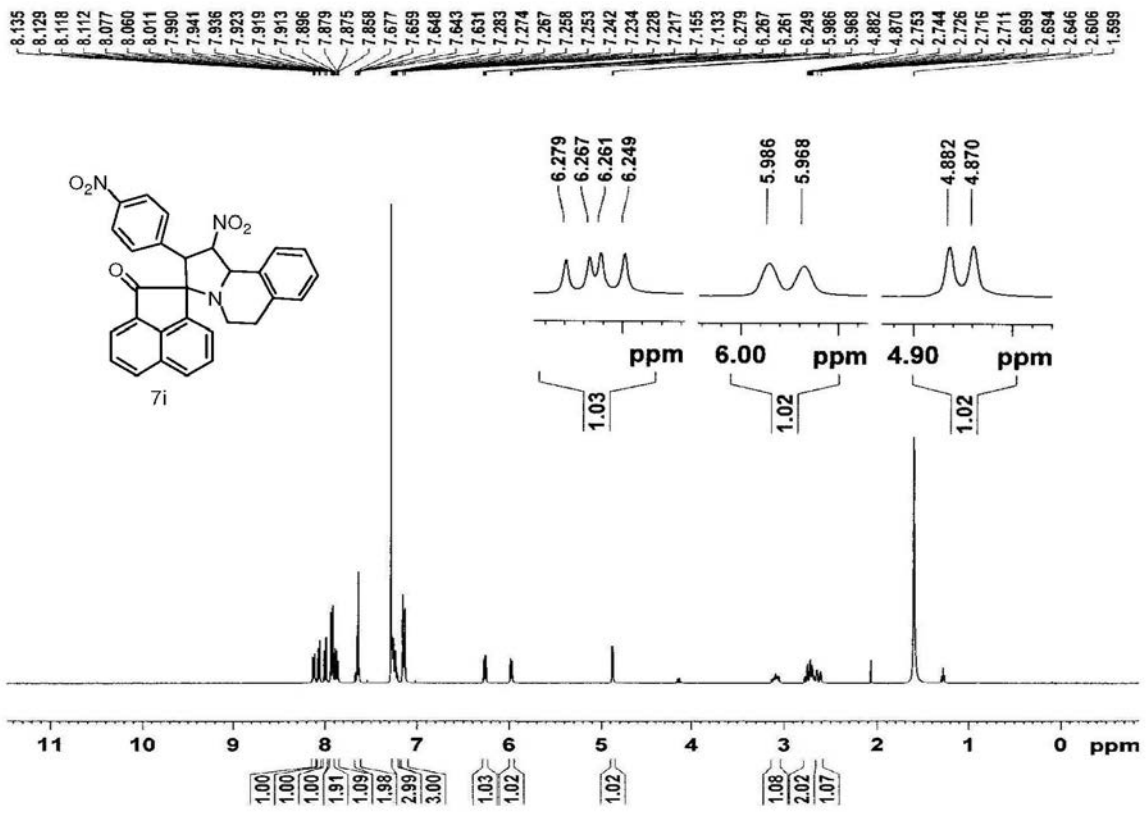

Figure S70. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7i**).

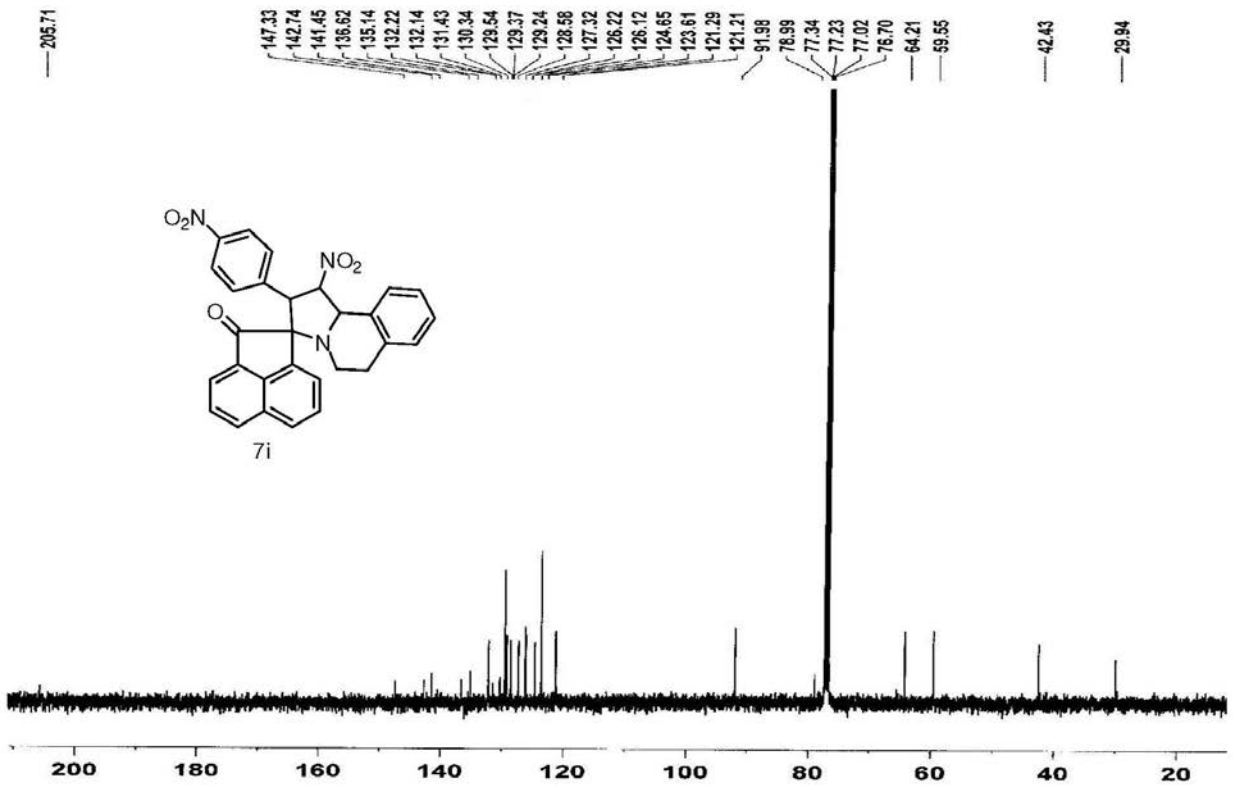

Figure S71. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7i**).

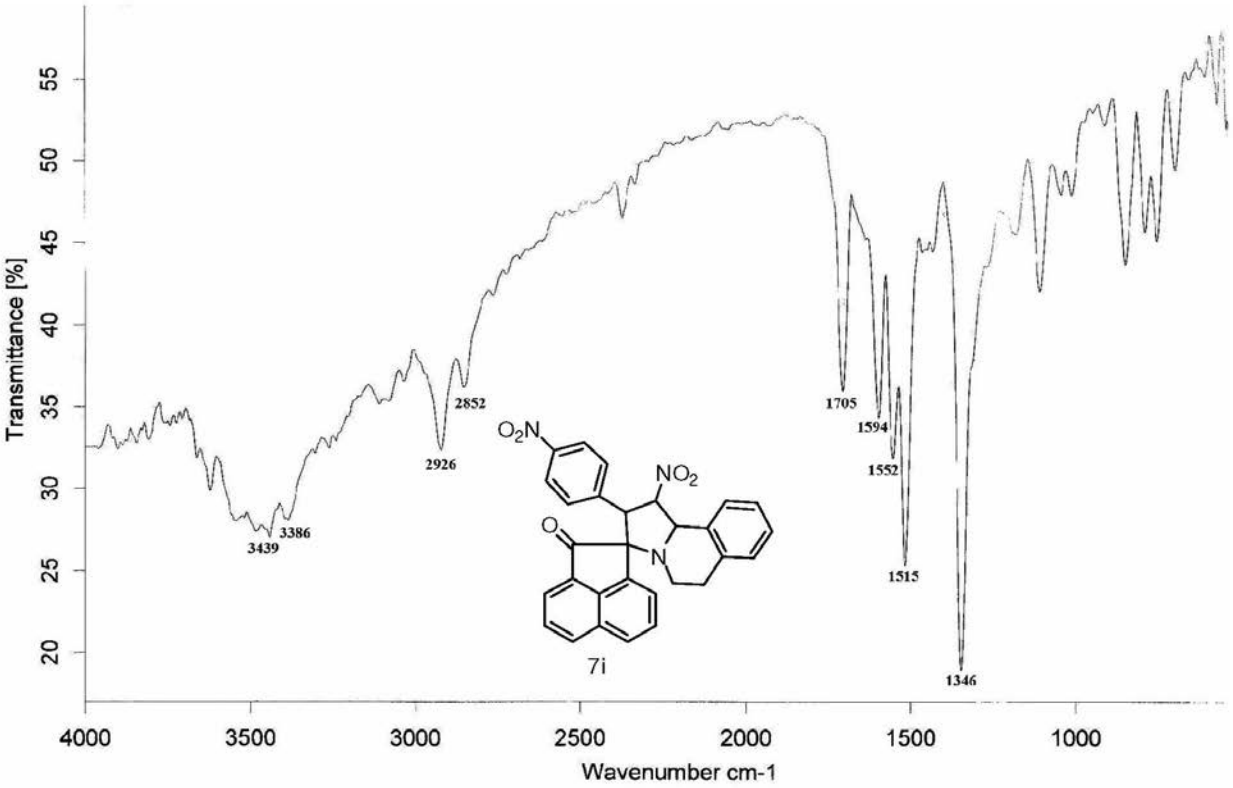

Figure S72. IR (KBr) of (**7i**).

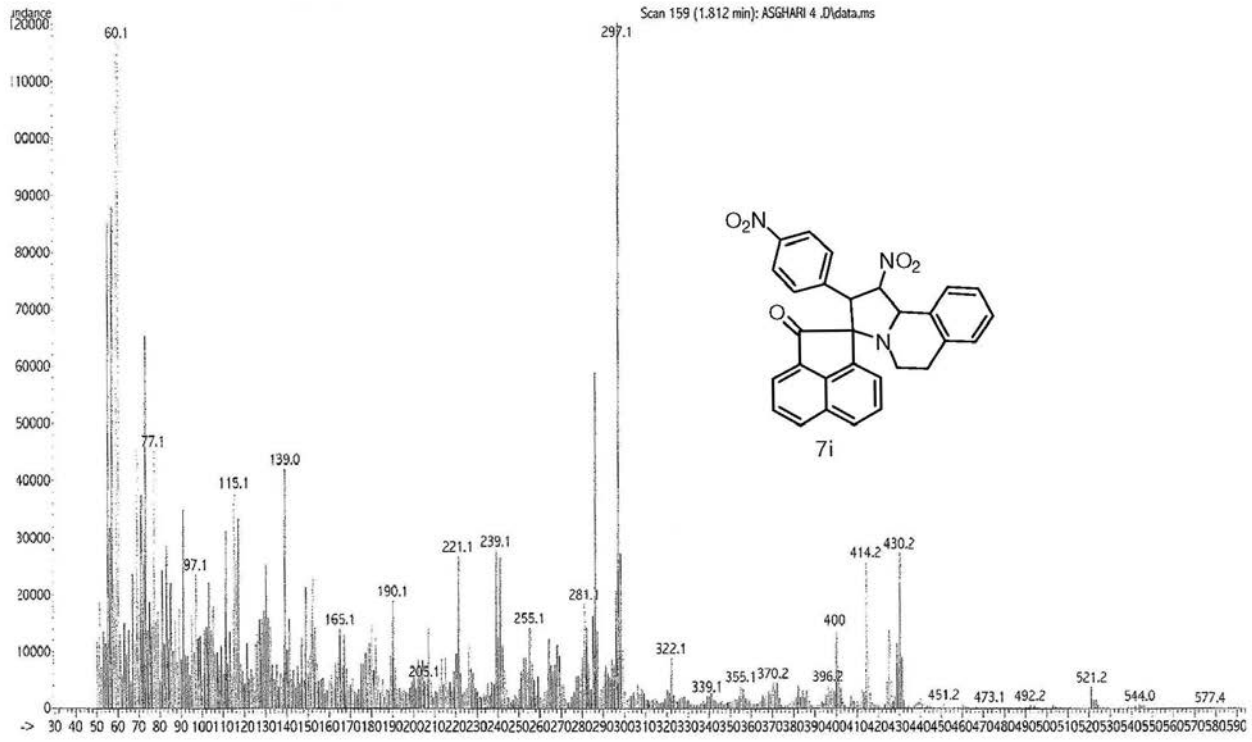

Figure S73. MS (70 eV) of (**7i**).

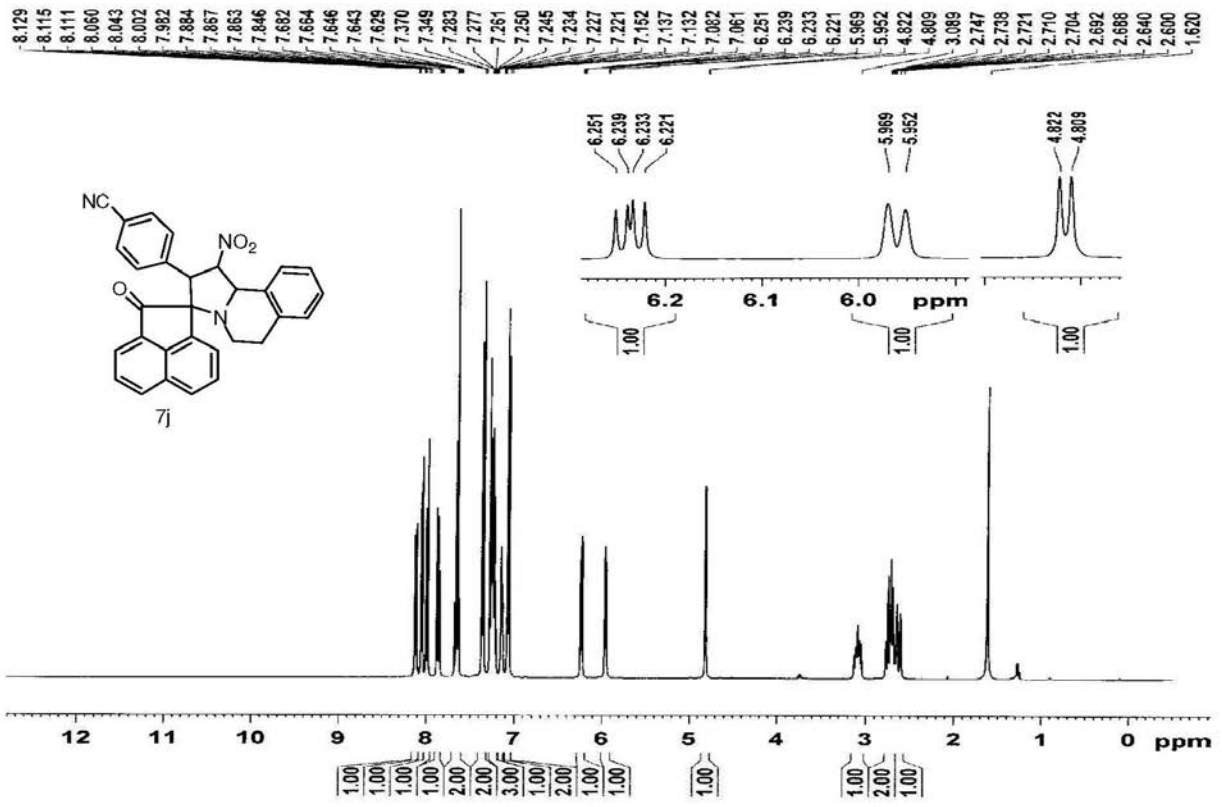

Figure S74. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7j**).

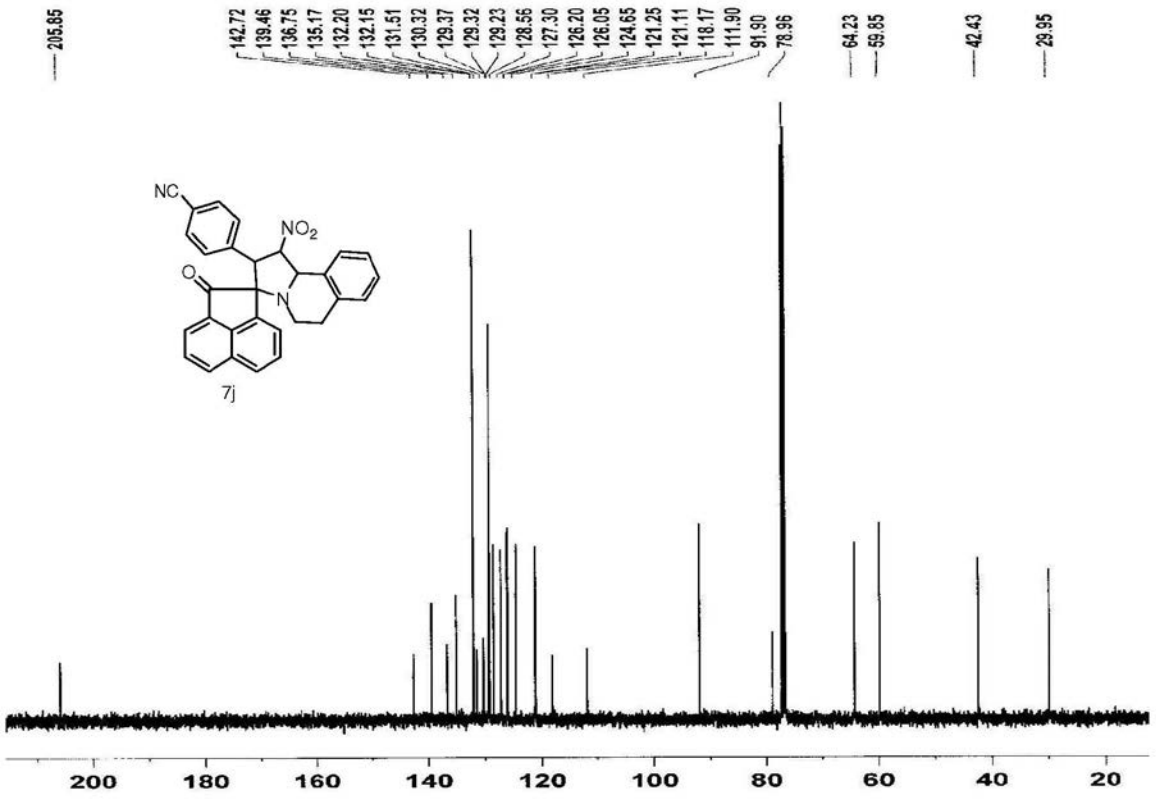

Figure S75. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7j**).

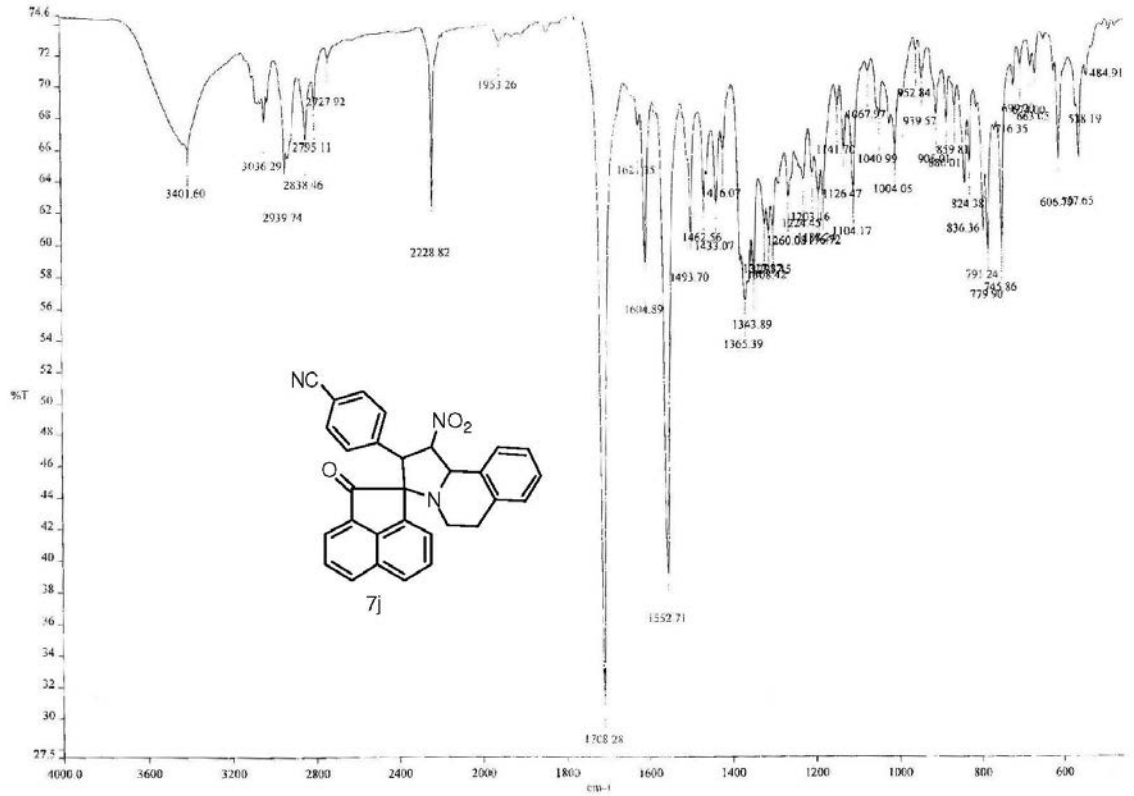

Figure S76. IR (KBr) of (**7j**).

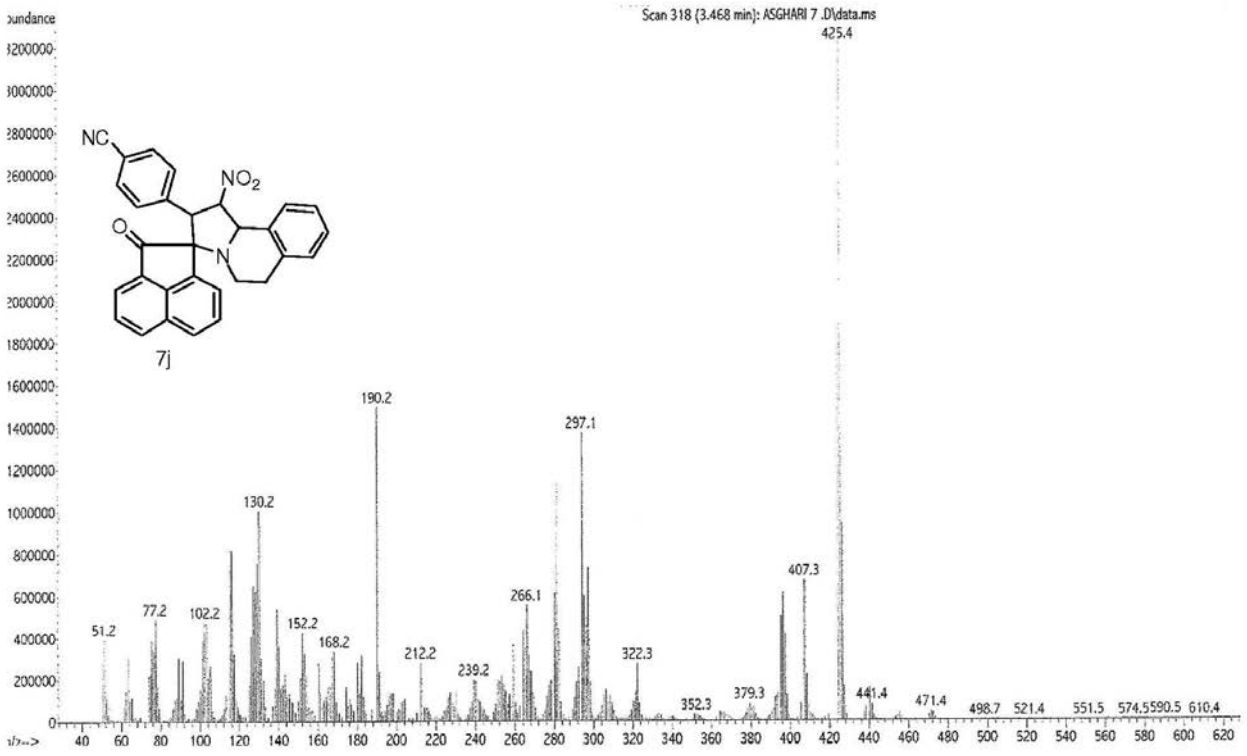

Figure S77. MS (70 eV) of (**7j**).

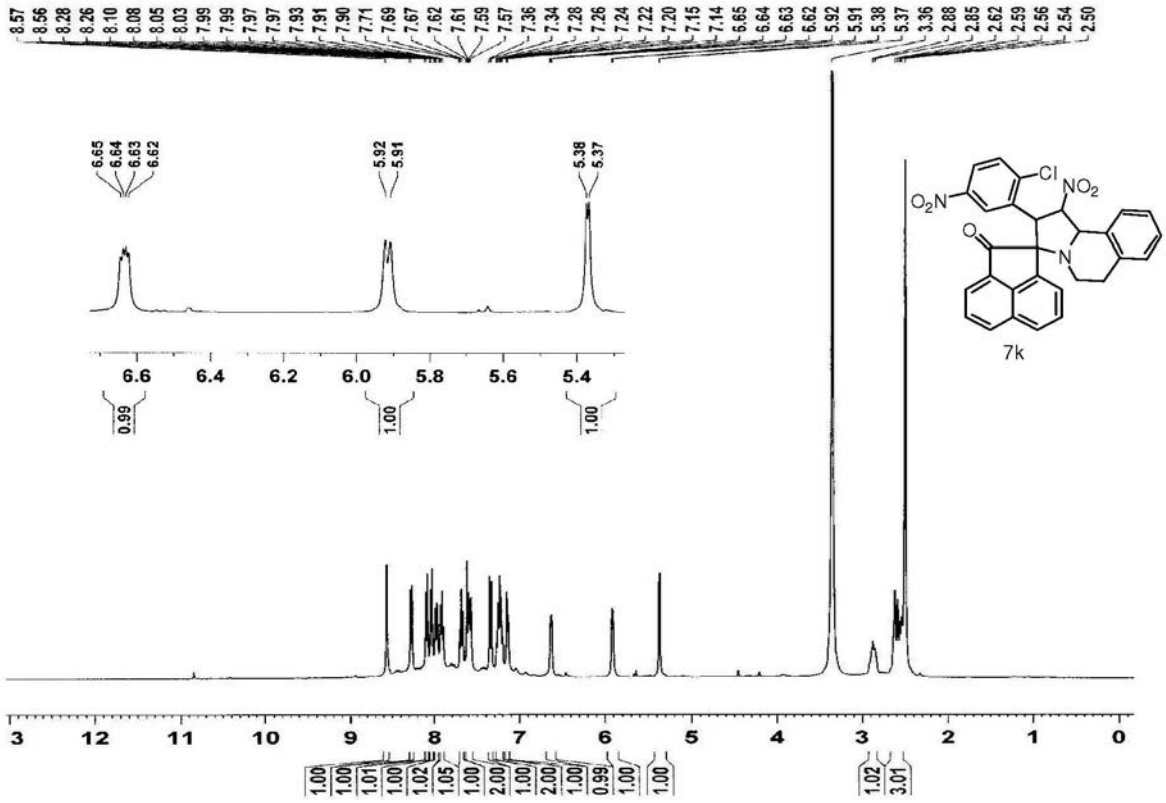

Figure S78. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7k**).

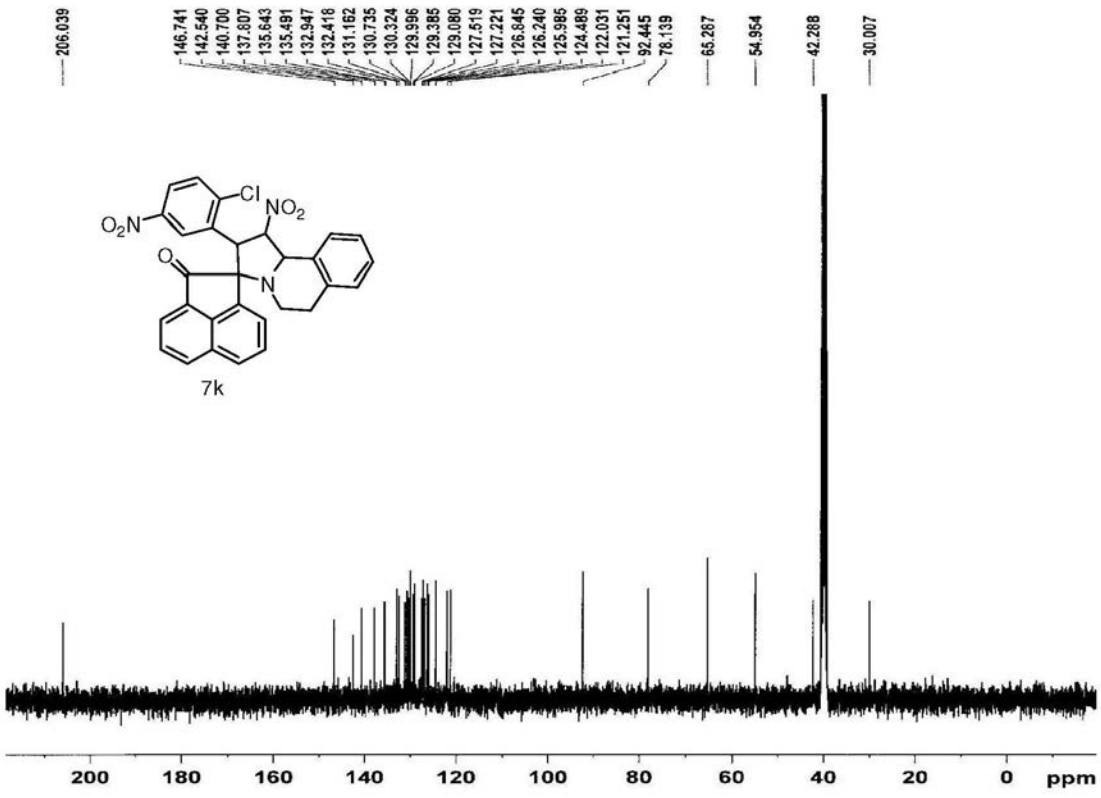

Figure S79. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7k**).

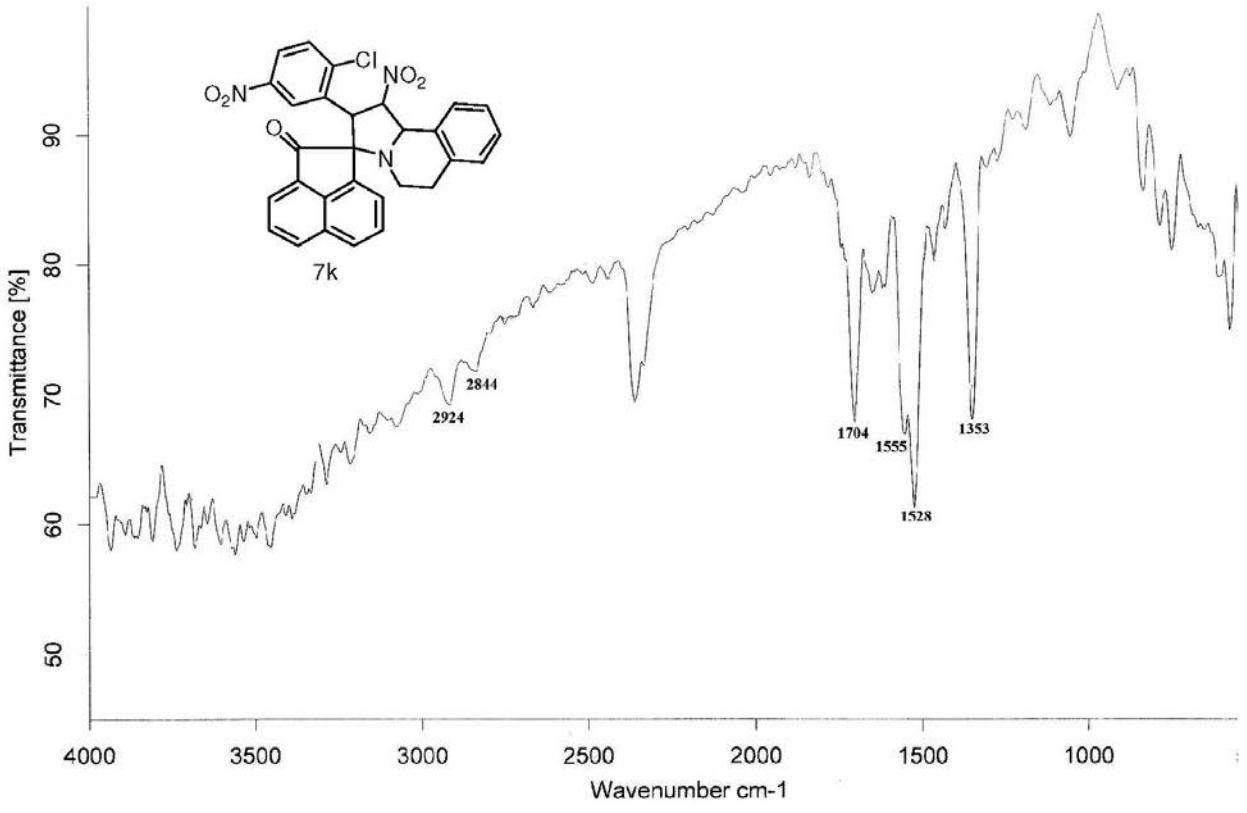

Figure S80. IR (KBr) of (**7k**).

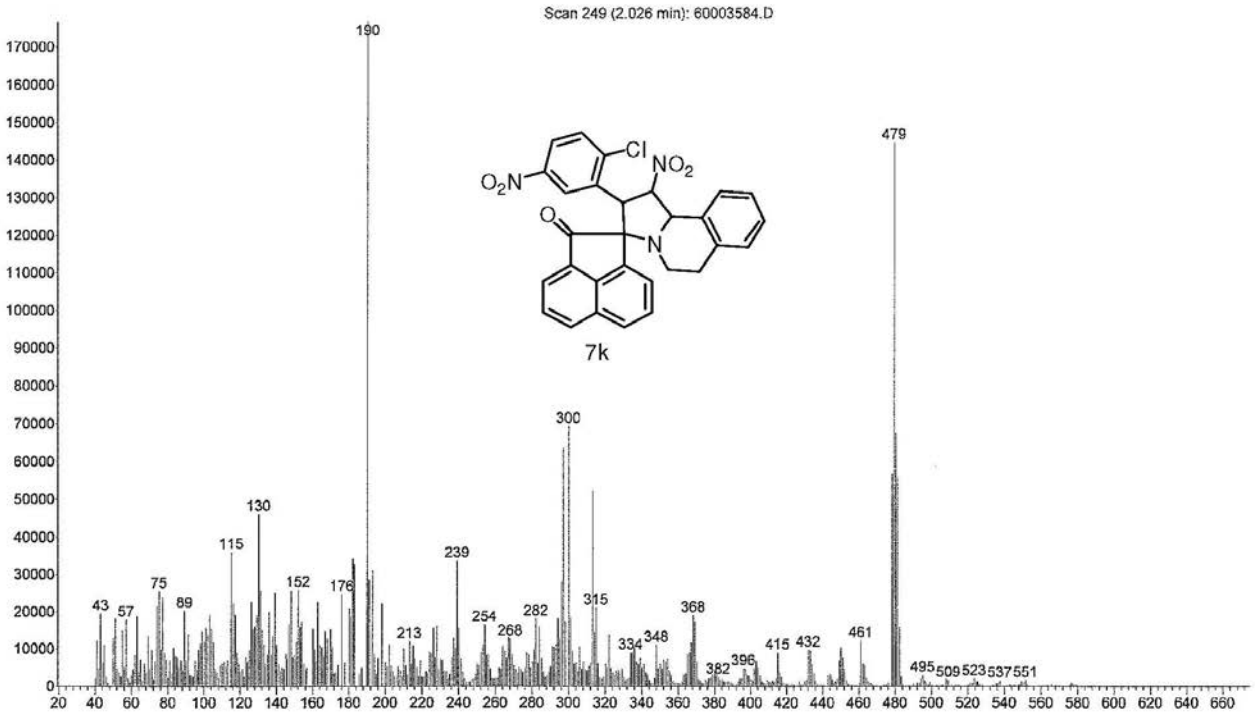

Figure S81. MS (70 eV) of (**7k**).

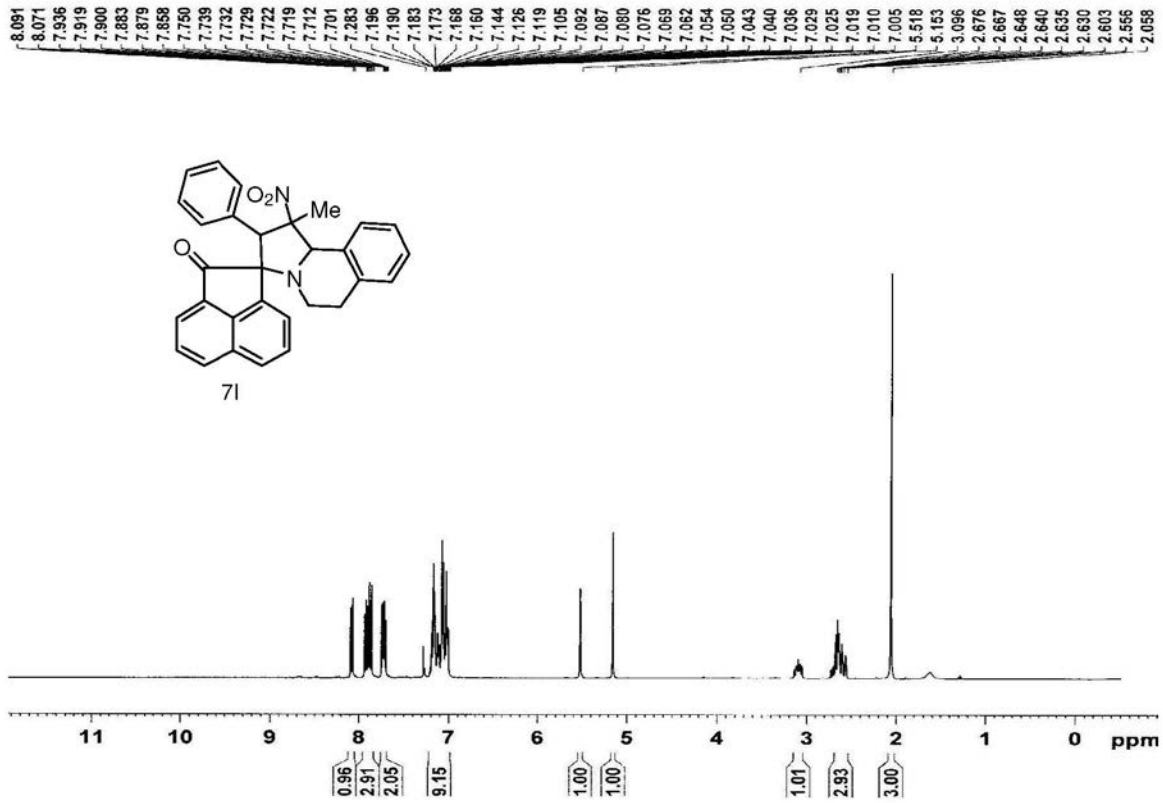

Figure S82. ^{1}H NMR (400 MHz, $CDCl_3$) of (**7l**).

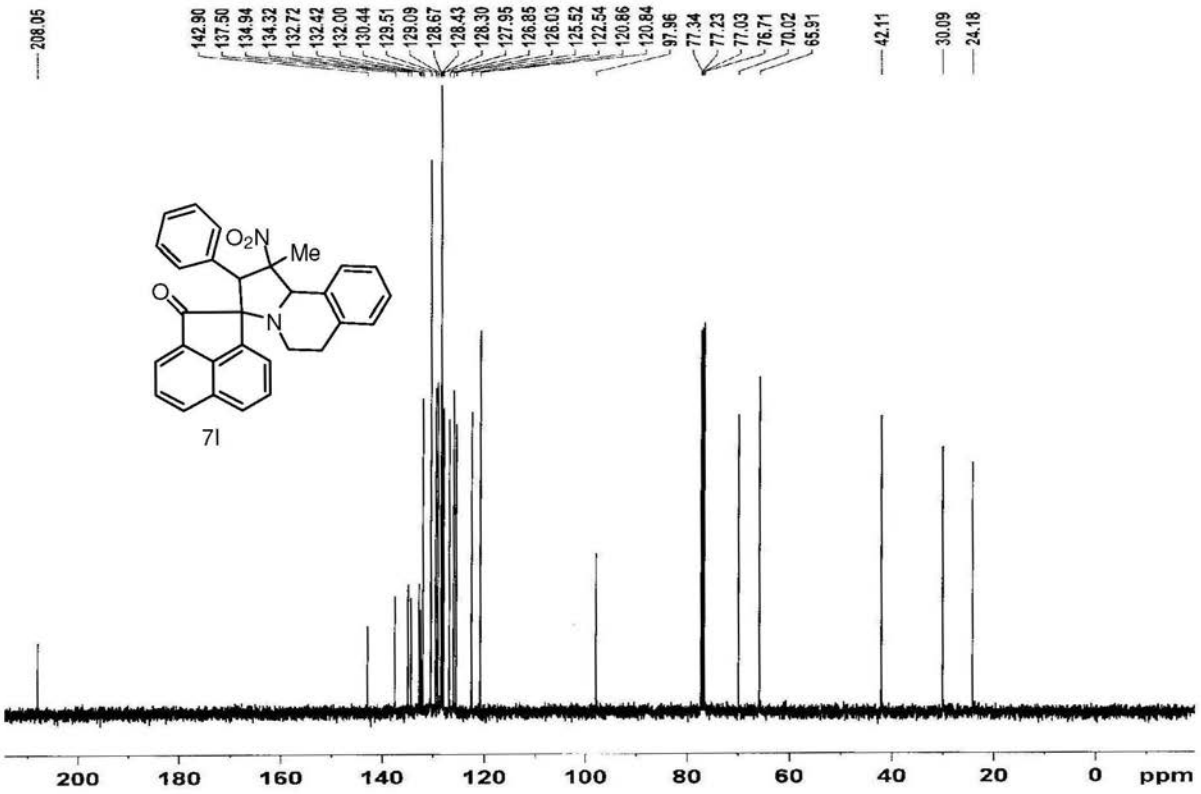

Figure S83. ^{13}C NMR (100 MHz, $CDCl_3$) of (**7l**).

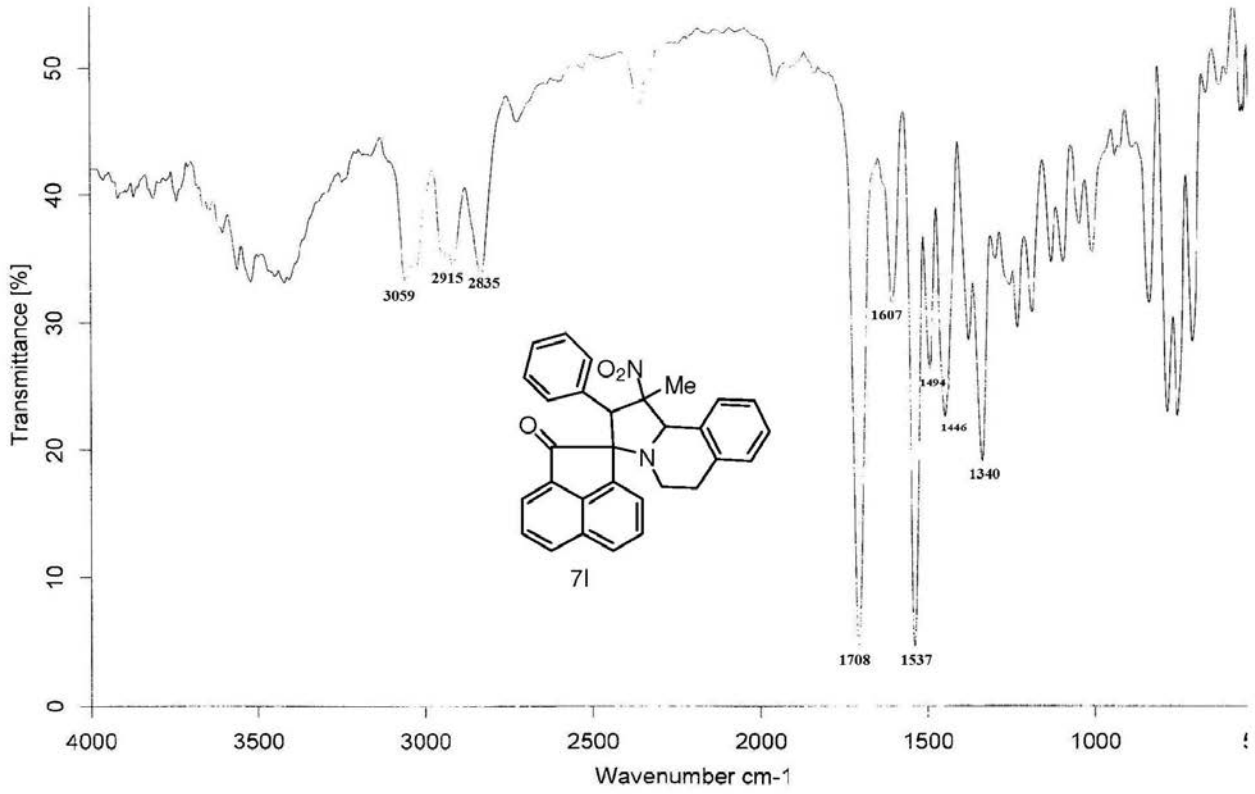

Figure S84. IR (KBr) of (**7l**).

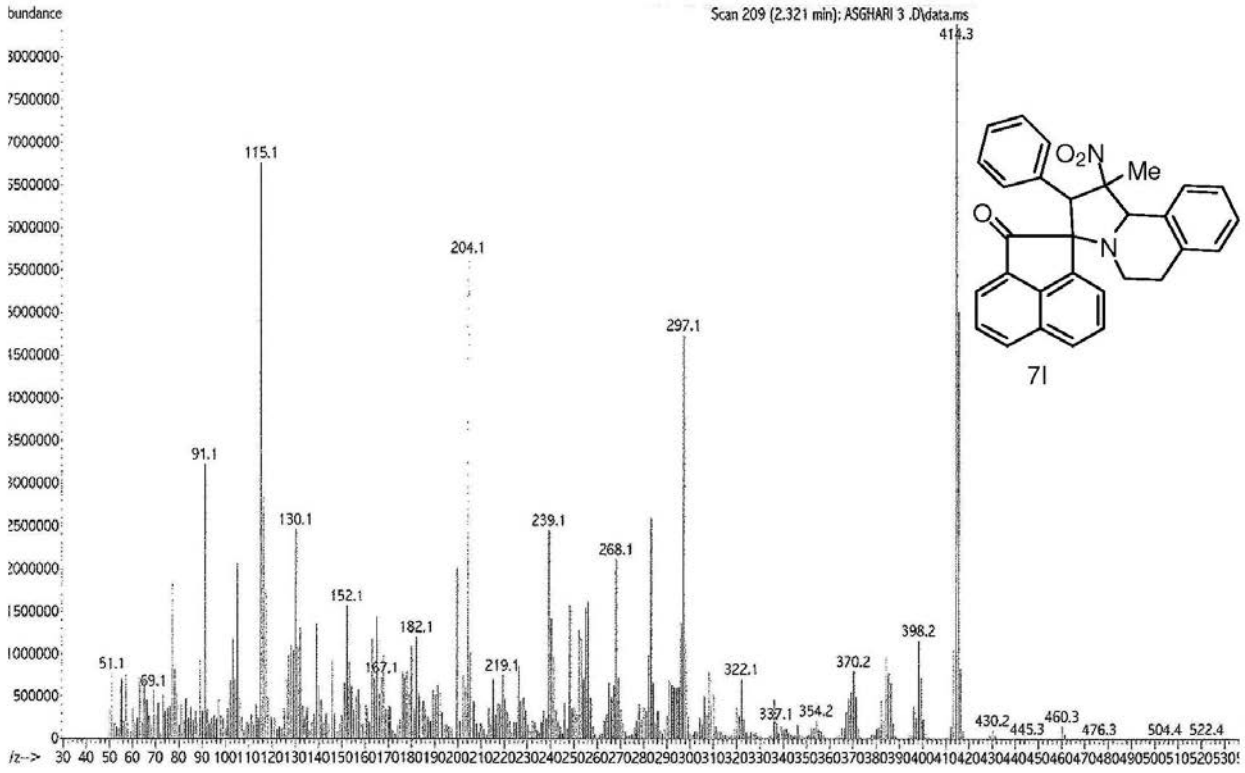

Figure S85. MS (70 eV) of (**7l**).