Supplementary Information

Ionic liquid coated sulfonated carbon@titania composites for the one-pot synthesis of indeno[1,2-*b*]indole-9,10-diones and 1*H*-pyrazolo[1,2-*b*]phthalazine-5,10-diones in aqueous media

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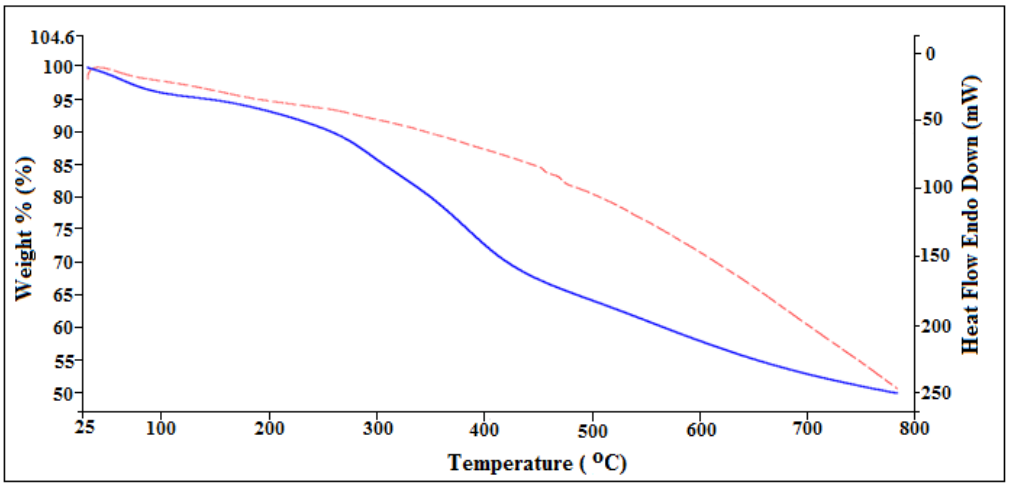
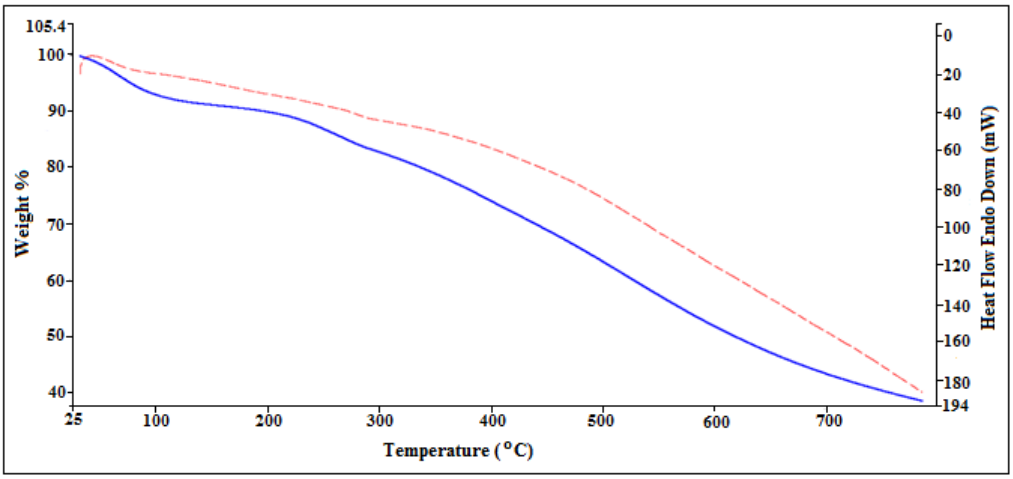
S1. TGA of (a) C@TiO_2-SO_3H-IL1; (b) C@TiO_2-SO_3H-IL2.

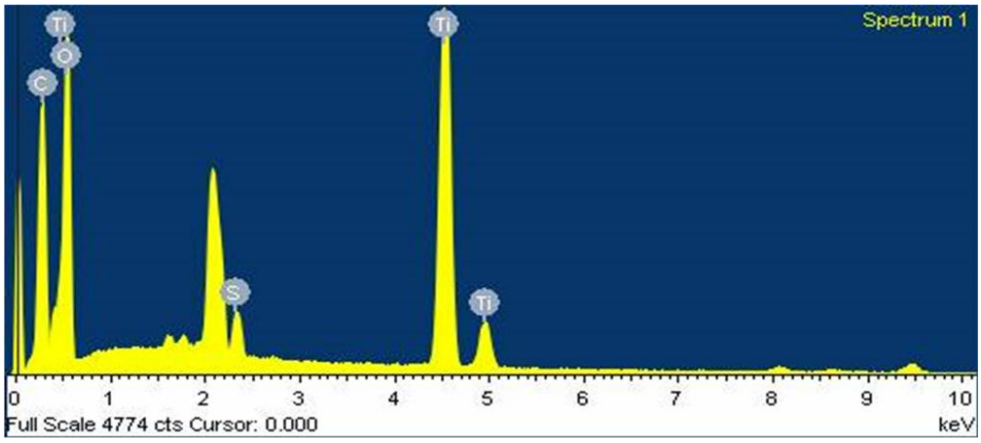


(a)

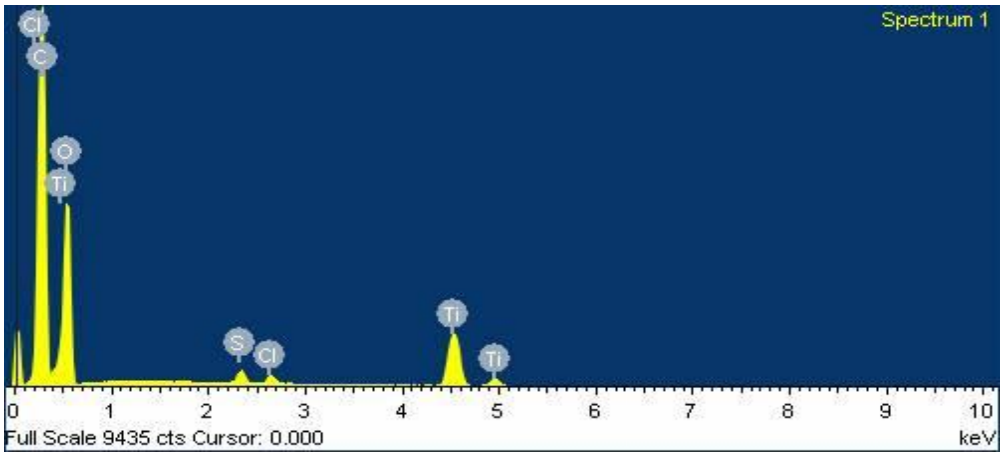


(b)

S2. EDX of (a) C@TiO_2-SO_3H; (b) C@TiO_2-SO_3H-IL1.

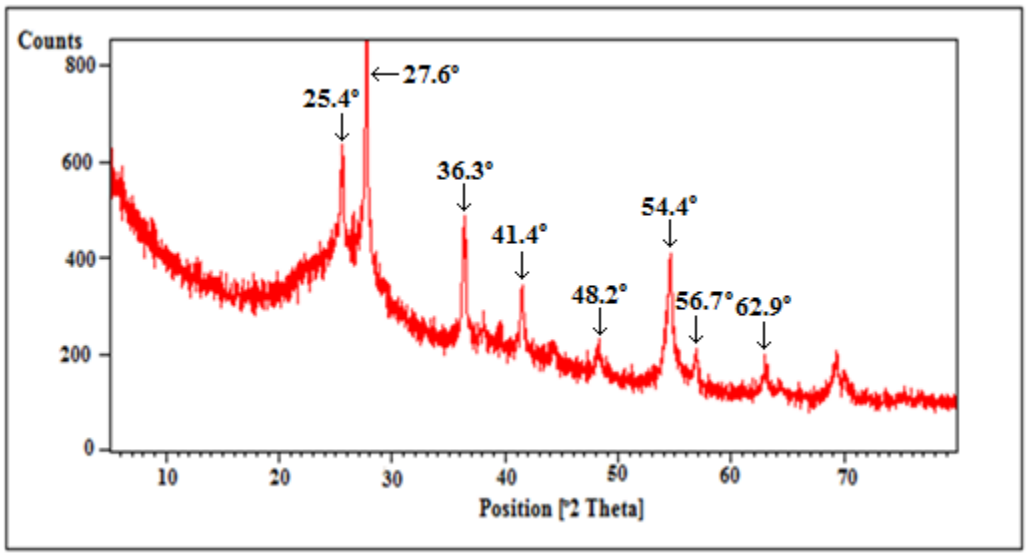


(a)

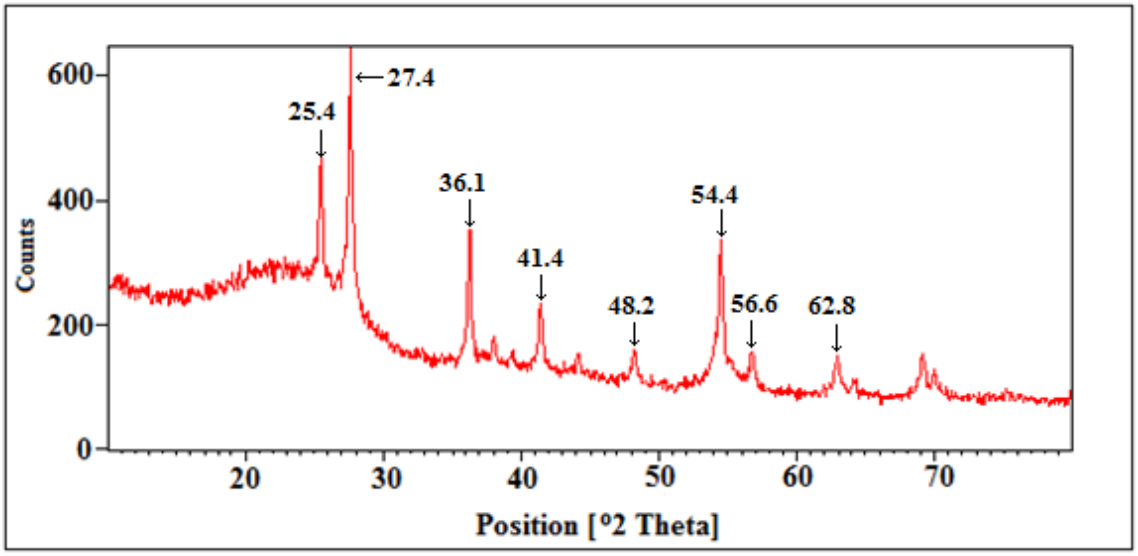


(b)

S3. XRD of (a) C@TiO_2-SO_3H; (b) C@TiO_2-SO_3H-IL1.



(a)

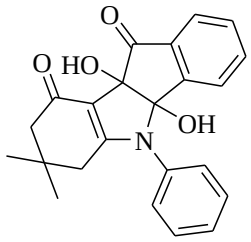


(b)

S4. FTIR, ^{1}H NMR, ^{13}C NMR and Mass spectral data of compounds

Spectral data of products listed in Table 6

4*b*,9*b*-Dihydroxy-7,7-dimethyl-5-phenyl-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



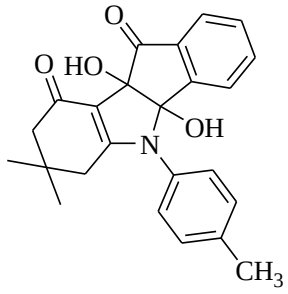
FTIR (KBr, ν_{max} in cm^{-1}): 3212 (OH stretch), 2924 (CH stretch), 1718 (C=O), 1548 (C=C);

^{1}H NMR (400 MHz, $CDCl_3$+DMSO-*d*$_6$): δ 0.90 (s, 3H, CH_3), 0.97 (s, 3H, CH_3), 1.80-1.84 (d, 1H, *J* = 16 Hz, CH_2), 1.92-1.96 (d, 1H, *J* = 16 Hz, CH_2), 2.13-2.17 (d, 1H, *J* = 16 Hz, CH_2), 2.30-2.34 (d, 1H, *J* = 16 Hz, CH_2), 5.98 (s, 1H, OH, exchangeable with D_2O), 6.64 (s, 1H, OH, exchangeable with D_2O), 7.21-7.25 (m, 3H, ArH), 7.44-7.50 (m, 5H, ArH), 7.69-7.71 (m, 1H, ArH);

^{13}C NMR (100 MHz, $CDCl_3$+DMSO-*d*$_6$): δ 27.2, 29.8, 33.9, 37.6, 51.6, 83.7, 97.1, 105.7, 123.5, 125.3, 128.3, 129.2, 129.8, 130.3, 134.9, 135.1, 136.3, 164.0, 190.1, 198.3;

MS (ESI): 376.15 $[M]^+$.

4*b*,9*b*-Dihydroxy-7,7-dimethyl-5-(*p*-tolyl)-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



FTIR (KBr, ν_{max} in cm^{-1}): 2962 (CH stretch), 1727 (C=O), 1544 (C=C);

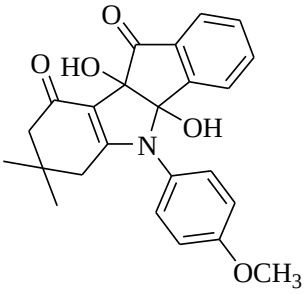
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 0.87 (s, 3H, CH_3), 0.95 (s, 3H, CH_3), 1.76-1.80 (d, 1H, *J* = 16 Hz, CH_2), 1.89-1.93 (d, 1H, *J* = 16 Hz, CH_2), 2.11-2.15 (d, 1H, *J* = 16 Hz, CH_2), 2.32-2.36 (d,

1H, *J* = 16 Hz, CH_2), 2.51 (s, 3H, CH_3), 6.67-6.69 (d, 1H, *J* = 8 Hz, ArH), 7.15-7.17 (d, 2H, *J* = 8 Hz, ArH), 7.29-7.31 (d, 2H, *J* = 8 Hz, ArH), 7.52-7.59 (m, 1H, ArH), 7.71-7.73 (d, 2H, *J* = 8 Hz, ArH);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 21.1, 27.0, 29.7, 33.9, 37.6, 51.7, 83.6, 97.2, 105.7, 123.6, 125.4, 129.7, 129.9, 130.6, 133.7, 135.1, 135.3, 137.9, 147.6, 164.0, 189.7, 197.9;

MS (ESI): 390.11 $[M]^+$.

4*b*,9*b*-Dihydroxy-5-(4-methoxyphenyl)-7,7-dimethyl-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



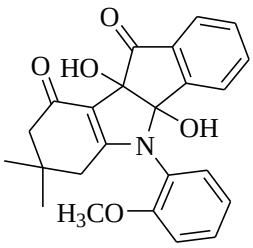
FTIR (KBr, ν_{max} in cm^{-1}): 3412 (OH stretch), 2943 (CH stretch), 1746 (C=O), 1520 (C=C);

^{1}H NMR (400 MHz, CD_3COCD_3): δ 0.97 (s, 3H, CH_3), 1.02 (s, 3H, CH_3), 1.97-2.38 (m, 4H, CH_2), 3.91 (s, 3H, OCH_3), 5.70 (s, 1H, OH, exchangeable with D_2O), 6.29 (s, 1H, OH, exchangeable with D_2O), 6.90-6.91 (d, 1H, *J* = 4 Hz, ArH), 7.06-7.08 (d, 2H, *J* = 8 Hz, ArH), 7.28-7.30 (d, 2H, *J* = 8 Hz, ArH), 7.58-7.65 (m, 2H, ArH), 7.80-7.82 (d, 1H, *J* = 8 Hz, ArH);

^{13}C NMR (400 MHz, CD_3COCD_3): δ 26.5, 27.4, 29.9, 33.8, 36.9, 50.9, 54.9, 83.0, 96.9, 105.8, 114.1, 123.5, 125.3, 128.4, 130.2, 130.9, 134.9, 148.1, 159.6, 164.4, 170.6, 190.7, 198.3;

MS (ESI): 406.5 $[M]^+$.

4*b*,9*b*-Dihydroxy-5-(2-methoxyphenyl)-7,7-dimethyl-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



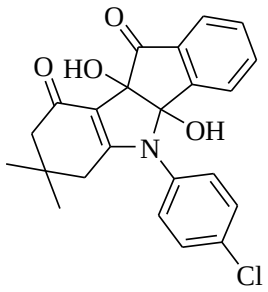
FTIR (KBr, ν_{max} in cm^{-1}): 3411 (OH stretch), 2842 (CH stretch), 1736 (C=O), 1523 (C=C);

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 0.76 (s, 3H, CH_3), 0.91 (s, 3H, CH_3), 1.88 (s, 2H, CH_2), 2.03 (s, 2H, CH_2), 3.11 (s, 3H, OCH_3), 5.90 (s, 1H, OH, exchangeable with D_2O), 6.51 (s, 1H, OH, exchangeable with D_2O), 7.01-7.03 (m, 1H, *J* = 8 Hz, ArH), 7.10-7.14 (m, 1H, ArH), 7.46-7.51 (m, 4H, ArH), 7.56-7.58 (d, 1H, *J* = 8 Hz, ArH), 7.70-7.72 (d, 1H, *J* = 8 Hz, ArH);

^{13}C NMR (400 MHz, DMSO-*d*$_6$): δ 28.1, 28.4, 33.5, 36.7, 49.1, 51.5, 55.3, 83.5, 96.5, 104.6, 112.4, 121.1, 123.6, 124.2, 124.9, 130.5, 131.0, 131.5, 134.8, 135.1, 148.1, 156.3, 166.8, 190.5, 198.7;

MS (ESI): 406.3 $[M]^+$.

4*b*,9*b*-Dihydroxy-5-(4-chlorophenyl)-7,7-dimethyl-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



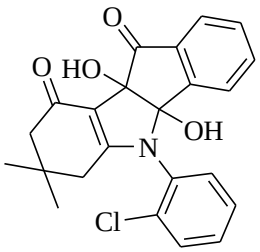
FTIR (KBr, ν_{max} in cm^{-1}): 3386 (OH stretch), 2950 (CH stretch), 1720 (C=O), 1545 (C=C);

^{1}H NMR (400 MHz, CD_3COCD_3): δ 1.00 (s, 3H, CH_3), 1.03 (s, 3H, CH_3), 1.97-1.99 (d, 1H, *J* = 8 Hz, CH_2), 2.01-2.03 (d, 1H, *J* = 8 Hz, CH_2), 2.22-2.26 (d, 1H, *J* = 16 Hz, CH_2), 2.44-2.48 (d, 1H, *J* = 16 Hz, CH_2), 5.68 (s, 1H, OH, exchangeable with D_2O), 6.40 (s, 1H, OH, exchangeable with D_2O), 6.89-6.91 (d, 1H, *J* = 8 Hz, ArH), 7.42-7.44 (d, 2H, *J* = 8 Hz, ArH), 7.56-7.63 (m, 4H, ArH), 7.80-7.82 (d, 1H, *J* = 8 Hz, ArH);

^{13}C NMR (100 MHz, CD_3COCD_3): δ 25.9, 28.9, 33.9, 37.2, 51.2, 83.4, 97.4, 106.2, 123.6, 125.0, 128.6, 129.2, 130.3, 131.0, 133.4, 134.9, 135.1, 135.3, 147.8, 163.7, 190.7;

MS (ESI): 410 $[M]^+$, 412 $[M+2]^+$.

4*b*,9*b*-Dihydroxy-5-(2-chlorophenyl)-7,7-dimethyl-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



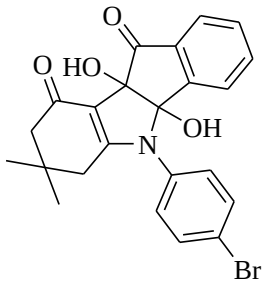
FTIR (KBr, ν_{max} in cm^{-1}): 3389 (OH stretch), 2979 (CH stretch), 1724 (C=O), 1542 (C=C);

^{1}H NMR (400 MHz,DMSO-*d*$_6$): δ 0.90 (s, 3H, CH_3), 1.02 (s, 3H, CH_3), 1.95-2.29 (m, 4H, CH_2), 5.65 (s, 1H, OH), 6.37 (s, 1H, OH), 7.01-7.03 (d, 1H, *J* = 8 Hz, ArH), 7.47-7.51 (t, 1H, *J* = 8 Hz, ArH), 7.59-7.64 (m, 4H, ArH), 7.73-7.75 (d, 1H, *J* = 8 Hz, ArH), 7.79-7.81 (d, 1H, *J* = 8 Hz, ArH);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 25.9, 28.9, 33.9, 37.2, 51.2, 83.4, 97.4, 106.2, 123.6, 125.0, 128.6, 129.2, 130.3, 131.0, 133.4, 134.9, 135.1, 147.8, 163.7, 190.7;

MS (ESI): 410.1 $[M]^+$, 412.3 $[M+2]^+$.

4*b*,9*b*-Dihydroxy-5-(4-bromophenyl)-7,7-dimethyl-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



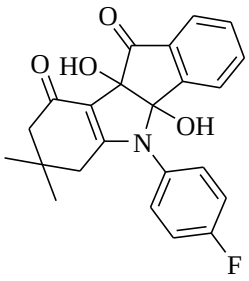
FTIR (KBr, ν_{max} in cm^{-1}): 3337 (OH stretch), 2945 (CH stretch), 1721 (C=O), 1547 (C=C);

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 1.12 (s, 3H, CH_3), 1.20 (s, 3H, CH_3), 2.12-2.43 (m, 4H, CH_2), 7.15-7.16 (d, 1H, *J* = 4 Hz, ArH), 7.42-7.44 (d, 2H, *J* = 8 Hz, ArH), 7.69-7.75 (m, 2H, ArH), 7.83-7.85 (d, 2H, *J* = 8 Hz, ArH), 8.04-8.05 (d, 1H, *J* = 4 Hz, ArH);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 26.5, 28.2, 29.8, 34.4, 38.2, 51.8, 82.6, 122.2, 124.7, 124.9, 130.8, 131.2, 132.7, 134.8, 135.1, 146.5, 164.8, 190.5, 198.1;

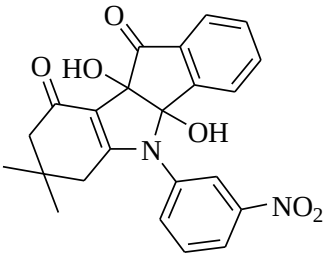
MS (ESI): 455 $[M]^+$, 457 $[M+2]^+$.

4*b*,9*b*-Dihydroxy-5-(4-fluorophenyl)-7,7-dimethyl-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



FTIR (KBr, ν_{max} in cm^{-1}): 3347 (OH stretch), 2935 (CH stretch), 1724 (C=O), 1548 (C=C);
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 0.88 (s, 3H, CH_3), 0.95 (s, 3H, CH_3), 1.76-1.80 (d, 1H, *J* = 16 Hz, CH_2), 1.89-1.93 (d, 1H, *J* = 16 Hz, CH_2), 2.11-2.15 (d, 1H, *J* = 16 Hz, CH_2), 2.35-2.39 (d, 1H, *J* = 16 Hz, CH_2), 6.06 (s, 1H, OH, exchangeable with D_2O), 6.66 (s, 1H, OH, exchangeable with D_2O), 7.33-7.37 (m, 5H, ArH), 7.54-7.61 (m, 2H, ArH), 7.72-7.74 (d, 1H, *J* = 8 Hz, ArH);
^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 27.0, 29.6, 33.9, 37.2, 51.4, 84.0, 96.9, 105.7, 116.2, 116.5, 123.7, 125.3, 130.7, 131.9, 132.0, 135.1, 135.5, 147.6, 160.7, 163.4, 164.0, 190.1, 198.0;
MS (ESI): 394.20 $[M]^+$.

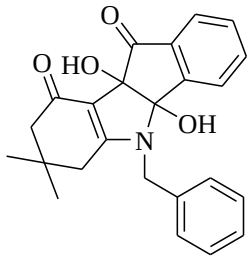
4*b*,9*b*-Dihydroxy-7,7-dimethyl-5-(3-nitrophenyl)-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



FTIR (KBr, ν_{max} in cm^{-1}): 3331 (OH stretch), 2939 (CH stretch), 1725 (C=O), 1536 (C=C);
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 0.90 (s, 3H, CH_3), 0.94 (s, 3H, CH_3), 2.11-2.30 (m, 4H, CH_2), 5.65 (s, 1H, OH), 6.22 (s, 1H, OH), 6.75-6.81 (m, 1H, ArH), 7.41-7.45 (m, 2H, ArH), 7.60-7.64 (t, 1H, *J* = 8 Hz, ArH), 7.79-7.81 (d, 2H, *J* = 8 Hz, ArH), 8.10-8.11 (d, 1H, *J* = 4 Hz, ArH), 8.27 (s, 1H, ArH);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 27.1, 28.9, 34.3, 39.7, 51.6, 82.7, 97.1, 106.3, 122.2, 124.2, 124.9, 130.5, 130.8, 135.1, 135.6, 135.9, 140.2, 147.5, 148.7, 164.1, 193.7, 197.3;
MS (ESI): 421 $[M]^+$.

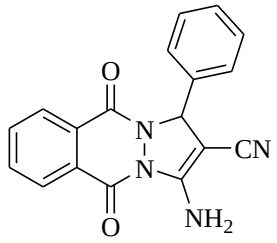
4*b*,9*b*-Dihydroxy-5-benzyl-7,7-dimethyl-4b,5,7,8-tetrahydroindeno[1,2-*b*]indole-9,10(6*H*,9b*H*)-dione



FTIR (KBr, ν_{max} in cm^{-1}): 3379 (OH stretch), 2956 (CH stretch), 1724 (C=O), 1556 (C=C);
^{1}H NMR (300 MHz, CD_3COCD_3): δ 1.19 (s, 3H, CH_3), 1.27 (s, 3H, CH_3), 2.10-2.22 (dd, 2H, *J* = 16 Hz, CH_2), 2.54-2.70 (dd, 2H, *J* = 16 Hz, CH_2), 4.54 (s, 2H, CH_2), 6.79-6.80 (d, 2H, *J* = 4 Hz, ArH), 7.03-7.10 (m, 3H, ArH), 7.49-7.51 (d, 1H, *J* = 8 Hz, ArH), 7.88-7.91 (t, 1H, *J* = 8 Hz, ArH), 7.98-8.02 (t, 1H, *J* = 8 Hz, ArH), 8.07-8.09 (d, 1H, *J* = 8 Hz, ArH);
^{13}C NMR (100 MHz, CD_3COCD_3): δ 28.0, 28.4, 33.9, 37.2, 50.7, 57.3, 77.7, 107.0, 122.7, 123.8, 126.9, 127.5, 128.8, 136.0, 136.3, 137.2, 140.3, 141.9, 169.1, 188.9, 195.1, 196.8;
MS (ESI): 390.40 $[M]^+$.
^{13}C NMR (100 MHz, CD_3COCD_3): δ 28.0, 28.4, 33.9, 37.2, 50.7, 57.3, 77.7, 107.0, 122.7, 123.8, 126.9, 127.5, 128.8, 136.0, 136.3, 137.2, 140.3, 141.9, 169.1, 188.9, 195.1, 196.8;
MS (ESI): 390.40 $[M]^+$.

Spectral data of products listed in Table 7

3-Amino-5,10-dihydro-5,10-dioxo-1-phenyl-1*H*-pyrazolo[1,2-*b*]phthalazin-2-carbonitrile



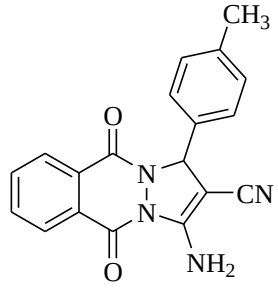
FTIR (KBr, ν_{max} in cm^{-1}): 3359 (NH stretch), 3190 (CH stretch), 2197 (C≡N), 1690 (C=O), 1558 (C=C);

^{1}H NMR (400 MHz, DMSO-d_6): δ 6.12 (s, 1H, CH), 7.27-7.48 (m, 5H, ArH), 7.94-8.28 (m, 4H, ArH), 8.39 (s, 2H, NH_2, exchangeable with D_2O);

^{13}C NMR (100 MHz, DMSO-d_6): δ 62.2, 63.5, 116.1, 126.9, 127.2, 127.9, 128.4, 128.8, 129.7, 134.2, 135.1, 138.7, 151.2, 154.2, 157.2;

MS (ESI): 317.10 $[M]^+$.

3-Amino-1-(4-methylphenyl)-5,10-dihydro-5,10-dioxo-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carbonitrile



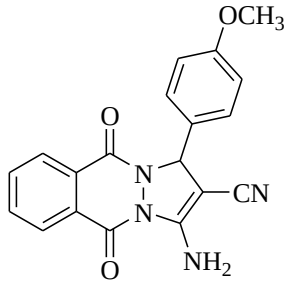
FTIR (KBr, ν_{max} in cm^{-1}): 3362 (NH stretch), 3060 (CH stretch), 2198 (C≡N), 1657 (C=O), 1565 (C=C);

^{1}H NMR (400 MHz, DMSO-d_6): δ 2.25 (s, 3H, CH_3), 6.09 (s, 1H, CH), 7.16-7.37 (m, 4H, ArH), 7.93-8.26 (m, 6H, ArH and NH_2, exchangeable with D_2O);

^{13}C NMR (100 MHz, DMSO-d_6): δ 21.1, 62.4, 64.3, 122.2, 123.4, 127.8, 127.2, 127.9, 128.5, 128.7, 130.3, 130.8, 133.3, 134.6, 135.0, 136.5, 153.0, 154.7, 157.0;

MS (ESI): 330 $[M]^+$.

3-Amino-1-(4-methoxy)-5,10-dioxo-5,10-dihydro-1*H*-pyrazolo-[1,2-*b*]phthalazine-2-carbonitrile



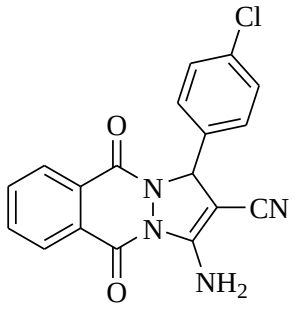
FTIR (KBr, ν_{max} in cm^{-1}): 3316 (NH stretch), 3016 (CH stretch), 2223 (C≡N), 1662 (C=O), 1557 (C=C);

^{1}H NMR (4000 MHz, DMSO-*d*$_6$): 3.74 (s, 3H, OCH_3), 6.09 (s, 1H, CH), 6.90-6.93 (d, 2H, *J* = 8 Hz, ArH), 7.36-7.39 (d, 2H, *J* = 12 Hz, ArH), 7.94-7.97 (m, 2H, ArH), 8.06-8.09 (m, 2H, ArH), 8.26 (s, 2H, NH_2, exchangeable with D_2O);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): 55.6, 61.9, 63.1, 114.3, 116.6, 127.1, 127.7, 128.9, 129.1, 130.4, 134.2, 135.2, 151.0, 153.9, 157.1, 159.7;

MS (ESI): 347.1$[M]^+$.

3-Amino-1-(4-chlorophenyl)-5,10-dioxo-5,10-dihydro-1*H*-pyrazolo-[1,2-*b*]phthalazine-2-carbonitrile



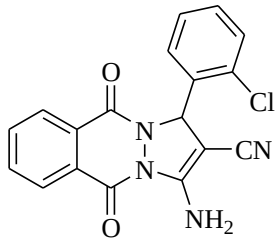
FTIR (KBr, ν_{max} in cm^{-1}): 3387 (NH stretch), 3107 (CH stretch), 2177 (C≡N), 1658 (C=O), 1562 (C=C);

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 6.11 (s, 1H, CH), 7.32-7.34 (d, 2H, *J* = 8 Hz, ArH), 7.41-7.43 (d, 2H, *J* = 8 Hz, ArH), 7.87-7.91 (m, 2H, ArH), 8.08-8.10 (d, 2H, *J* = 8 Hz, ArH), 8.26 (s, 2H, NH_2, exchangeable with D_2O);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 62.9, 116.4, 127.2, 127.7, 128.1, 128.8, 129.3, 129.4, 133.3, 133.9, 134.8, 142.2, 143.9, 151.2, 154.2, 157.1;

MS (ESI): 351.1 $[M]^+$, 353.3 $[M+2]^+$.

3-Amino-1-(2-chlorophenyl)-5,10-dioxo-5,10-dihydro-1*H*-pyrazolo-[1,2-*b*]phthalazine-2-carbonitrile



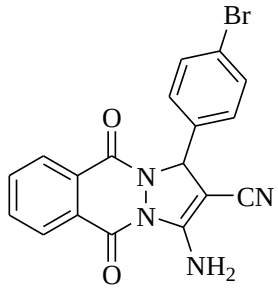
FTIR (KBr, ν_{max} in cm^{-1}): 3386 (NH stretch), 3076 (CH stretch), 2200 (C≡N), 1680 (C=O), 1524 (C=C);

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 6.44 (s, 1H, CH), 7.63-8.04 (m, 6H, ArH), 8.21-8.32 (m, 2H, ArH), 8.67 (s, 2H, NH_2, exchangeable with D_2O);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 58.9, 116.1, 124.7, 127.3, 127.8, 128.8, 129.4, 129.4, 131.0, 133.9, 134.5, 135.3, 137.9, 145.7, 151.9, 154.1, 157.2, 158.1;

MS (ESI): 351.1 $[M]^+$, 353.3 $[M+2]^+$.

3-Amino-1-(4-bromophenyl)-5,10-dioxo-5,10-dihydro-1*H*-pyrazolo-[1,2-*b*]phthalazine-2-carbonitrile



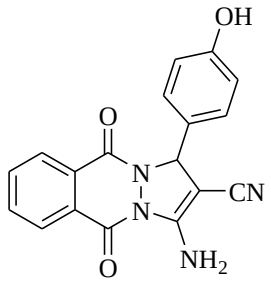
FTIR (KBr, ν_{max} in cm^{-1}): 3389 (NH stretch), 3106 (CH stretch), 2178 (C≡N), 1683 (C=O), 1536 (C=C);

^{1}H NMR (400 MHz, DMSO-d_6): δ 6.30 (s, 1H, CH), 6.42-6.44 (d, 2H, *J* = 8 Hz, ArH), 7.41-7.78 (m, 3H, ArH), 7.62-7.64 (d, 2H, *J* = 8 Hz, ArH), 7.87-8.21 (m, 3H, ArH and NH_2, exchangeable with D_2O);

^{13}C NMR (100 MHz, DMSO-d_6): δ 61.5, 83.6, 120.9, 126.7, 127.2, 128.7, 129.1, 130.5, 131.6, 133.7, 134.5, 138.8, 147.2, 153.1, 156.2, 164.1;

MS (ESI): 395.1 $[M]^+$, 397.0 $[M+2]^+$.

3-Amino-1-(4-hydroxyphenyl)-5,10-dihydro-5,10-dioxo-1*H*pyrazolo[1,2-*b*]phthalazine-2-carbonitrile



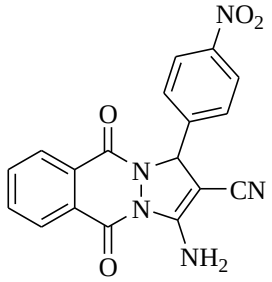
FTIR (KBr, ν_{max} in cm^{-1}): 3373 (NH stretch), 3060 (CH stretch), 2198 (C≡N), 1660 (C=O), 1578 (C=C);

^{1}H NMR (400 MHz, DMSO-d_6): δ 6.03 (s, 1H, CH), 6.72-6.74 (d, 1H, *J* = 8 Hz, ArH), 6.92-6.94 (d, 1H, *J* = 8 Hz, ArH), 7.21-7.23 (d, 1H, *J* = 8 Hz, ArH), 7.85-7.98 (m, 3H, ArH), 8.06-8.08 (m, 1H, ArH), 8.17 (s, 2H, NH_2, exchangeable with D_2O), 8.23-8.25 (m, 1H, ArH), 9.84 (bs, 1H, OH, exchangeable with D_2O);

^{13}C NMR (100 MHz, DMSO-d_6): δ 61.9, 63.3, 115.7, 117.1, 123.2, 127.1, 127.8, 128.7, 128.9, 134.4, 135.3, 151.0, 154.2, 157.1, 157.8, 160.9, 164.3;

MS (ESI): 333.30 $[M]^+$.

3-Amino-1-(4-nitrophenyl)-5,10-dioxo-5,10-dihydro-1*H*-pyrazolo-[1,2-*b*]phthalazine-2-carbonitrile



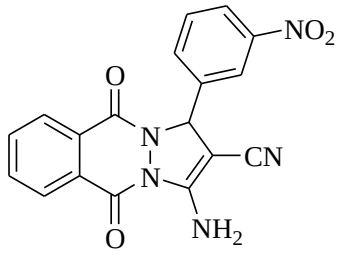
FTIR (KBr, ν_{max} in cm^{-1}): 3340 (NH stretch), 3079 (CH stretch), 2165 (C≡N), 1662 (C=O), 1560 (C=C);

^{1}H NMR (400 MHz, DMSO-d_6): δ 6.30 (s, 1H, CH), 7.82-7.84 (d, 2H, *J* = 8 Hz, ArH), 7.93-7.97 (m, 2H, ArH), 8.09-8.12 (m, 1H, ArH), 8.23 (s, 2H, NH_2, exchangeable with D_2O), 8.24-8.26 (d, 2H, *J* = 8 Hz, ArH), 8.26-8.29 (m, 1H, ArH);

^{13}C NMR (100 MHz, DMSO-d_6): 62.7, 116.7, 123.4, 126.7, 128.1, 128.8, 129.1, 129.7, 134.6, 134.9, 146.6, 148.0, 151.3, 151.5, 154.3, 156.9;

MS (ESI): 362.08 $[M]^+$.

3-Amino-1-(3-nitrophenyl)-5,10-dioxo-5,10-dihydro-1*H*-pyrazolo-[1,2-*b*]phthalazine-2-carbonitrile



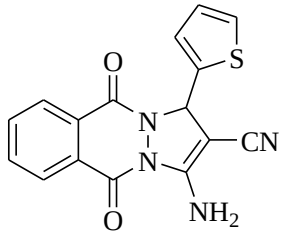
FTIR (KBr, ν_{max} in cm^{-1}): 3440 (NH stretch), 3079 (CH stretch), 2165 (C≡N), 1662 (C=O), 1520 (C=C);

^{1}H NMR (400 MHz, DMSO-d_6): δ 6.30 (s, 1H, CH), 7.66-7.70 (t, 1H, *J* = 8 Hz, ArH), 7.93-7.98 (m, 3H, ArH), 8.05-8.07 (d, 1H, *J* = 8 Hz, ArH), 8.13 (s, 2H, NH_2, exchangeable with D_2O), 8.18-8.20 (d, 1H, *J* = 8 Hz, ArH), 8.25-8.26 (d, 1H, *J* = 8 Hz, ArH), 8.34 (s, 1H, ArH);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): 60.6, 62.6, 116.4, 122.2, 123.9, 127.2, 127.8, 128.6, 129.2, 130.9, 134.2, 134.5, 135.3, 140.8, 148.4, 151.5, 154.5, 157.3;

MS (ESI): 362.8 $[M]^+$.

3-Amino-1-(thien-2-yl)-5,10-dioxo-5,10-dihydro-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carbonitrile



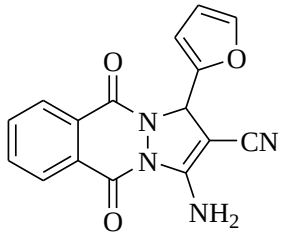
FTIR (KBr, ν_{max} in cm^{-1}): 3389 (NH stretch), 3075 (CH stretch), 2213 (C≡N), 1649 (C=O), 1488 (C=C);

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 6.29 (s, 1H, CH), 6.49-6.51 (d, 1H, *J* = 8 Hz, ArH), 6.65-6.67 (d, 1H, *J* = 8 Hz, ArH), 7.92-7.94 (t, 2H, *J* = 8 Hz, ArH), 8.09-8.14 (m, 4H, ArH and NH_2, exchangeable with D_2O), 8.21-8.26 (m, 1H, ArH) ;

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 57.1, 59.4, 110.7, 112.7, 118.3, 127.1, 127.9, 128.4, 134.7, 135.6, 143.4, 143.9, 150.1, 152.1, 154.6, 157.2;

MS (ESI): 323.01 $[M]^+$.

3-Amino-1-(furan-2-yl)-5,10-dioxo-5,10-dihydro-1*H*-pyrazolo[1,2-*b*]phthalazine-2-carbonitrile



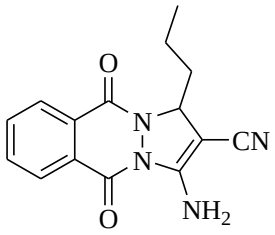
FTIR (KBr, ν_{max} in cm^{-1}): 3397 (NH stretch), 3058 (CH stretch), 2201 (C≡N), 1658 (C=O), 1485 (C=C);

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 6.32 (s, 1H, CH), 6.41-6.43 (d, 1H, *J* = 8 Hz, ArH), 6.59-6.61 (d, 1H, *J* = 8 Hz, ArH), 7.61-7.66 (m, 1H, ArH), 7.91-7.95 (t, 2H, *J* = 8 Hz, ArH), 8.07-8.12 (m, 3H, ArH and NH_2, exchangeable with D_2O), 8.20-8.24 (m, 1H, ArH);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 56.7, 58.9, 110.3, 111.5, 116.7, 127.2, 127.8, 128.9, 134.3, 135.3, 143.7, 143.8, 149.5, 151.2, 154.7, 157.1;

MS (ESI): 307.2 $[M]^+$.

3-Amino-1-propyl-5,10-dioxo-5,10-dihydro-1*H*-pyrazolo-[1,2-*b*]phthalazine-2-carbonitrile



FTIR (KBr, ν_{max} in cm^{-1}): 3395 (NH stretch), 3064 (CH stretch), 2826 (CH_2 stretch), 2201 (C≡N), 1658 (C=O), 1485 (C=C);

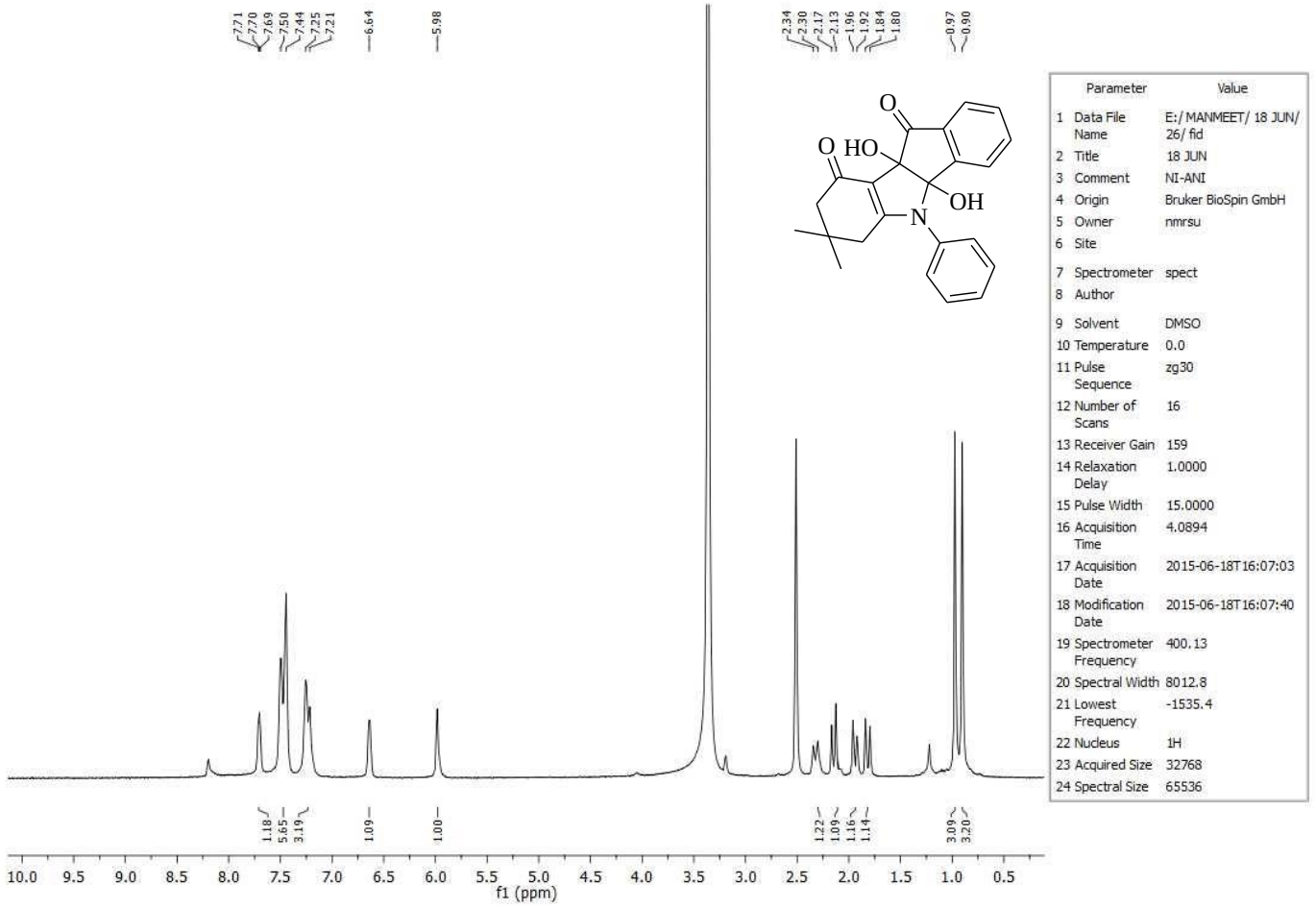
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 1.01-1.05 (t, 3H, *J* = 8 Hz, CH_3), 1.36-1.45 (m, 2H, CH_2), 1.60-1.67 (m, 2H, CH_2), 5.75-5.78 (t, 1H, *J* = 8 Hz, CH), 7.56-7.60 (t, 2H, *J* = 8 Hz, ArH), 8.14-8.22 (m, 4H, ArH and NH_2, exchangeable with D_2O);

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 18.1, 19.8, 36.2, 58.9, 117.7, 127.6, 127.9, 128.8, 134.2, 135.1, 140.6, 142.4, 145.6, 151.0, 154.3, 157.5;

MS (ESI): 307.2 $[M]^+$.

S5. Copies of ^{1}H and ^{13}C NMR spectra of some of the compounds synthesised in Table 6 and 7

^{1}H NMR spectra of entry 1, Table 6



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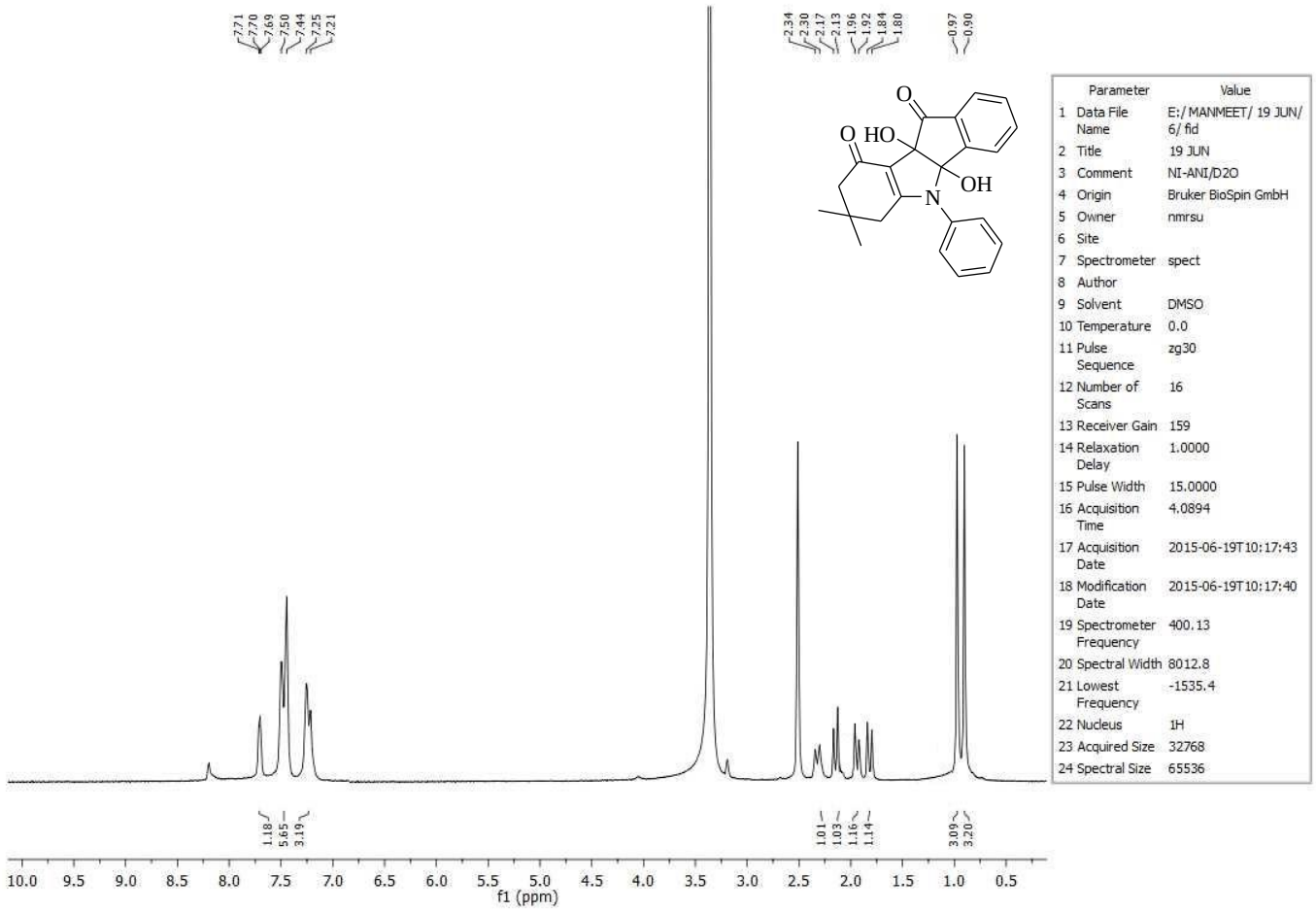
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	159
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2015-06-18T16:07:03
18	Modification Date	2015-06-18T16:07:40
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

D_2O of entry 1, Table 6



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5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	159
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
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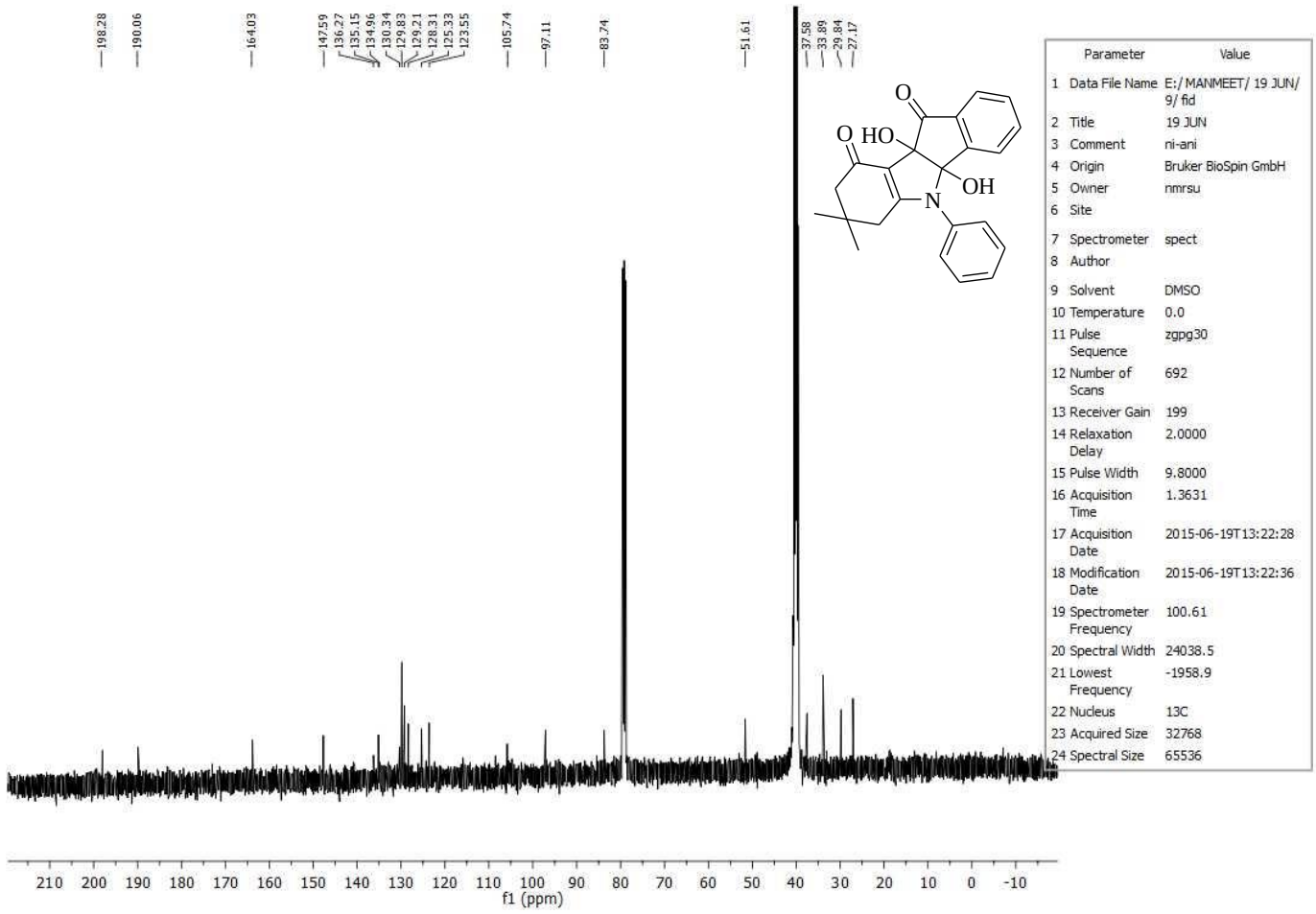
18	Modification Date	2015-06-19T10:17:40
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR spectra of entry 1, Table 6



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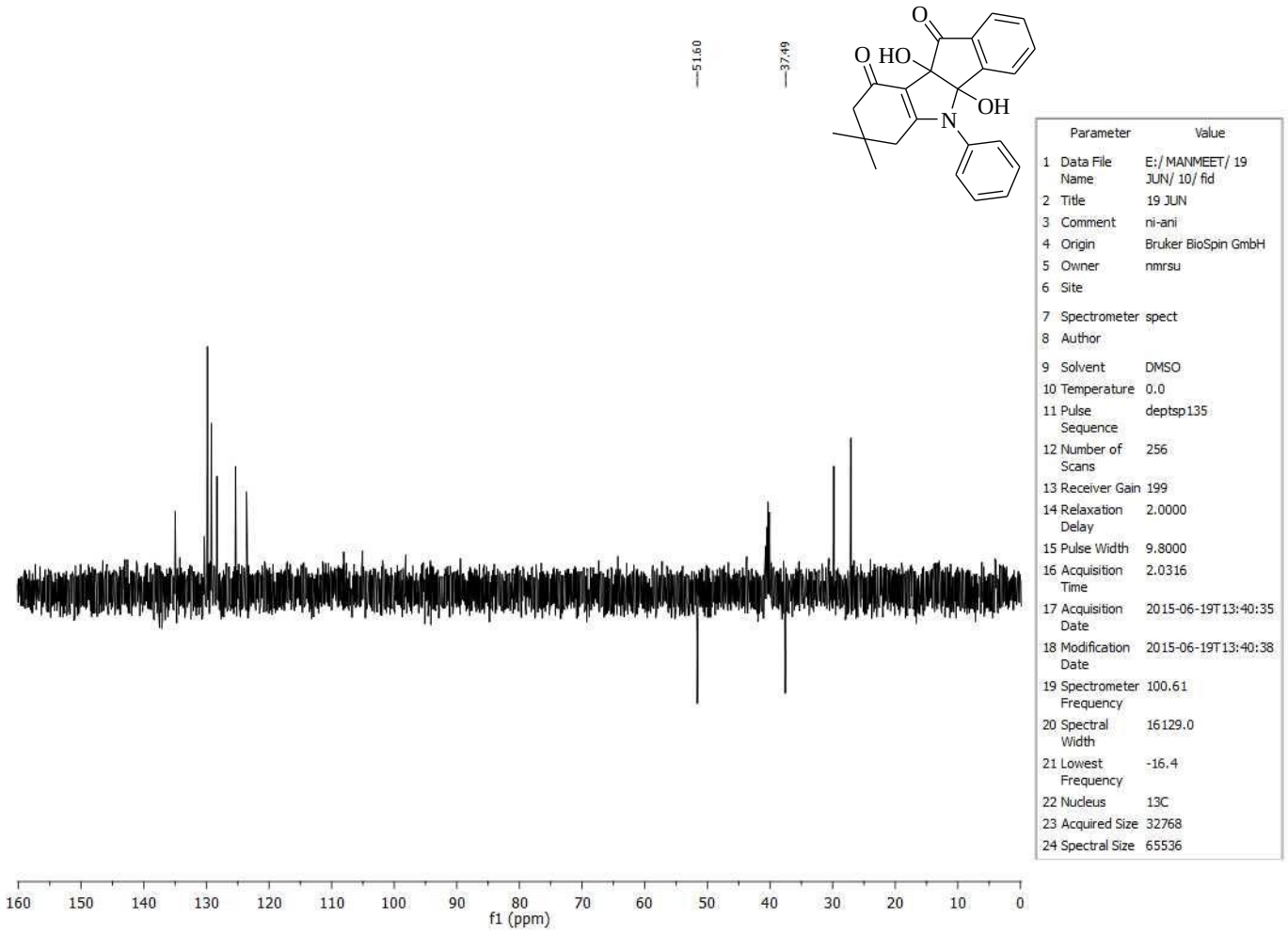
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Number of Scans	692
13	Receiver Gain	199
14	Relaxation Delay	2.0000
15	Pulse Width	9.8000
16	Acquisition Time	1.3631
17	Acquisition Date	2015-06-19T13:22:28
18	Modification Date	2015-06-19T13:22:36
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.9
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

DEPT of entry 1, Table 6



	Parameter	Value
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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
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12	Number of Scans	256
13	Receiver Gain	199
14	Relaxation Delay	2.0000
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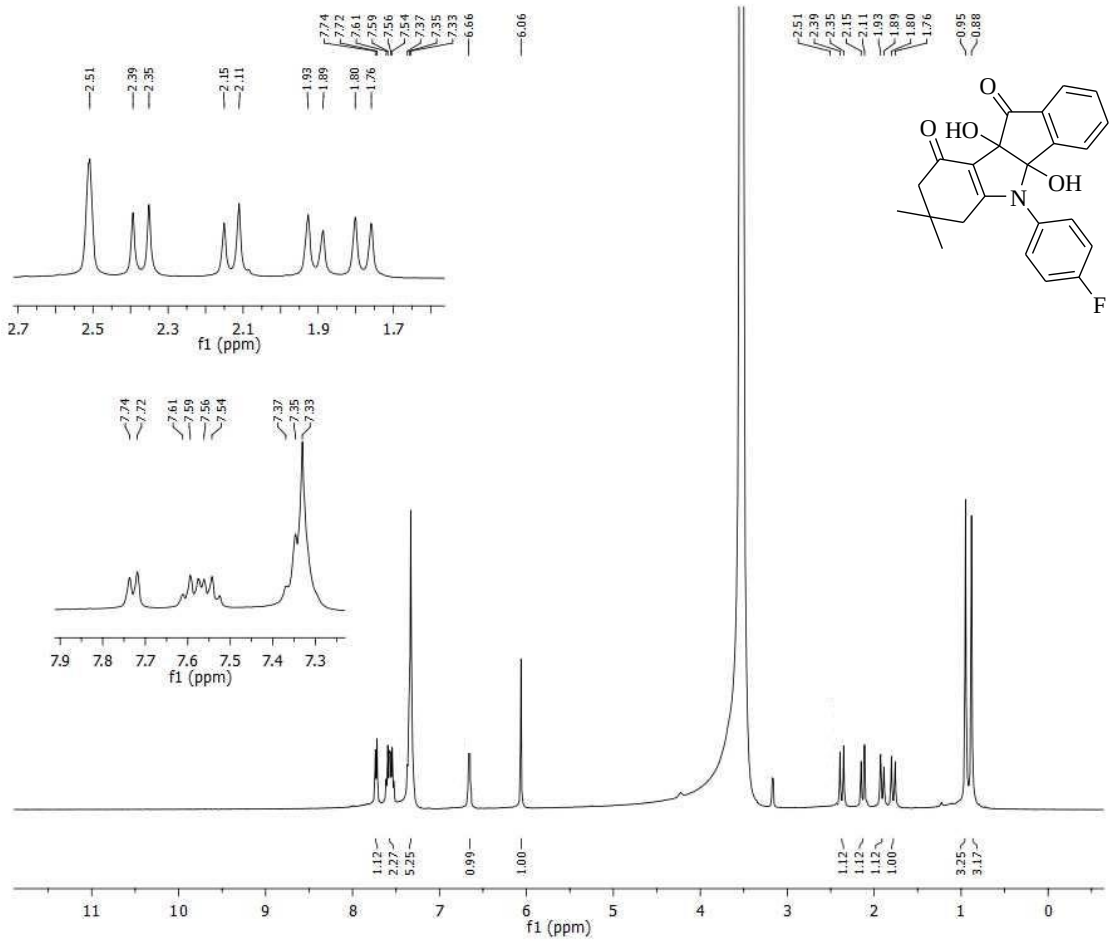
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR spectra of entry 8, Table 6



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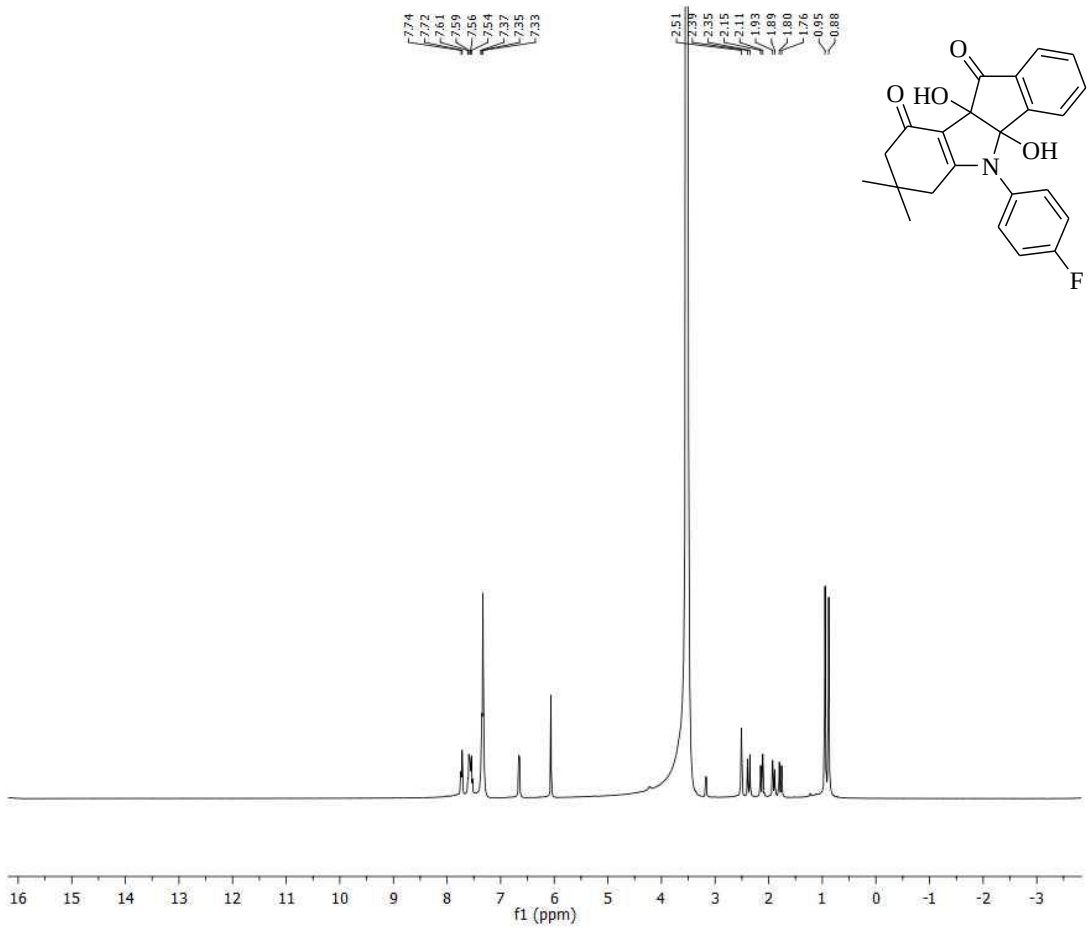
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	54
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2015-07-24T12 :55:56
18	Modification Date	2015-07-24T12 :55:58
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

D_2O of entry 8, Table 6



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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
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12	Number of Scans	16
13	Receiver Gain	54
14	Relaxation Delay	1.0000
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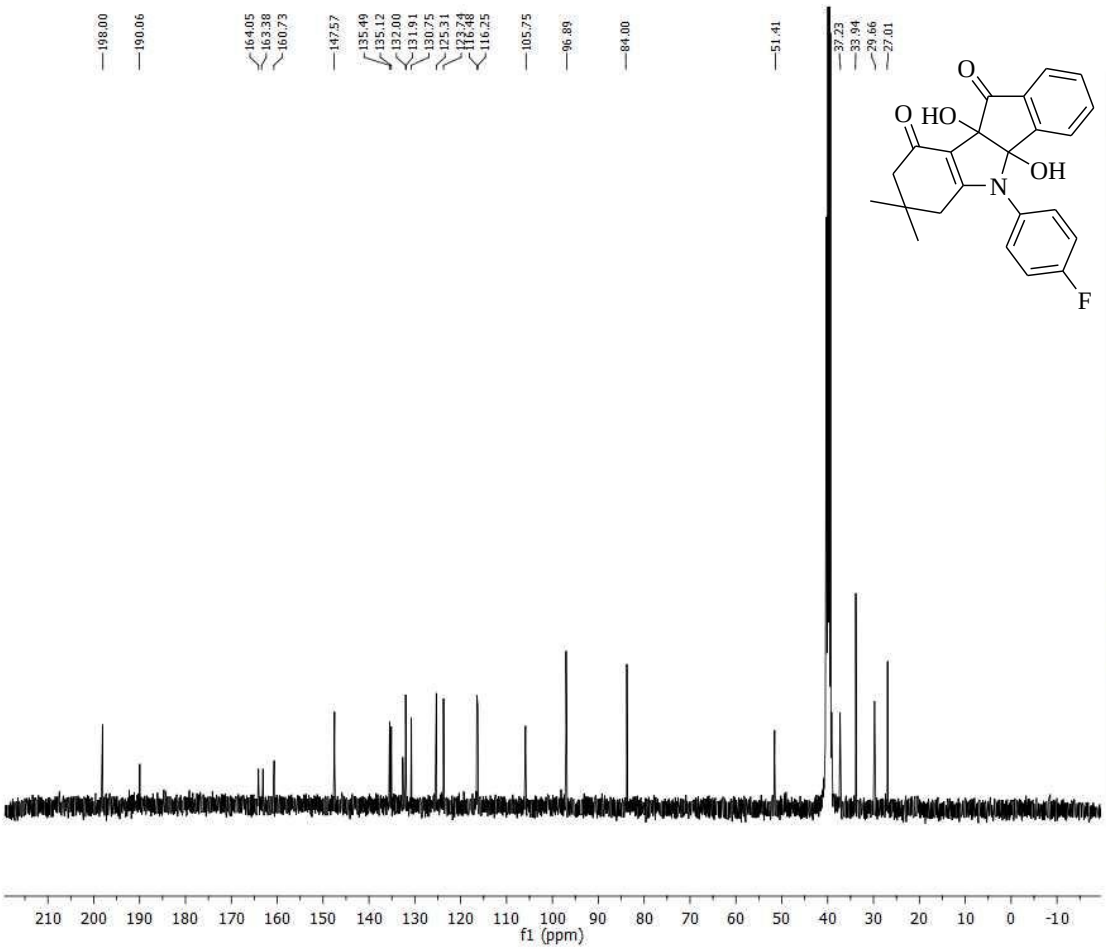
16	Acquisition Time	4.0894
17	Acquisition Date	2015-07-26T11 :55:59
18	Modification Date	2015-07-26T11 :55:59
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR spectra of entry 8, Table 6



	Parameter	Value
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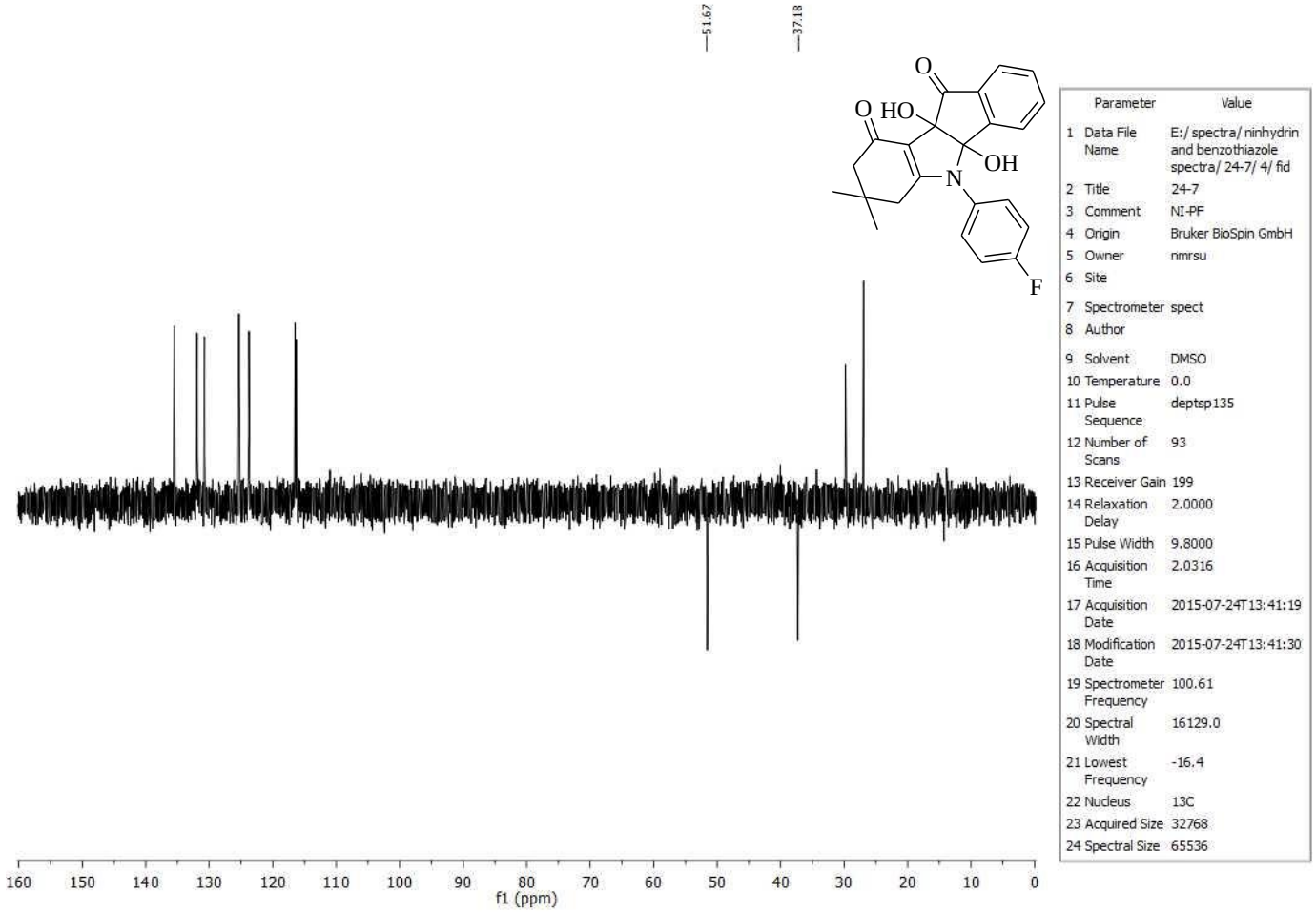
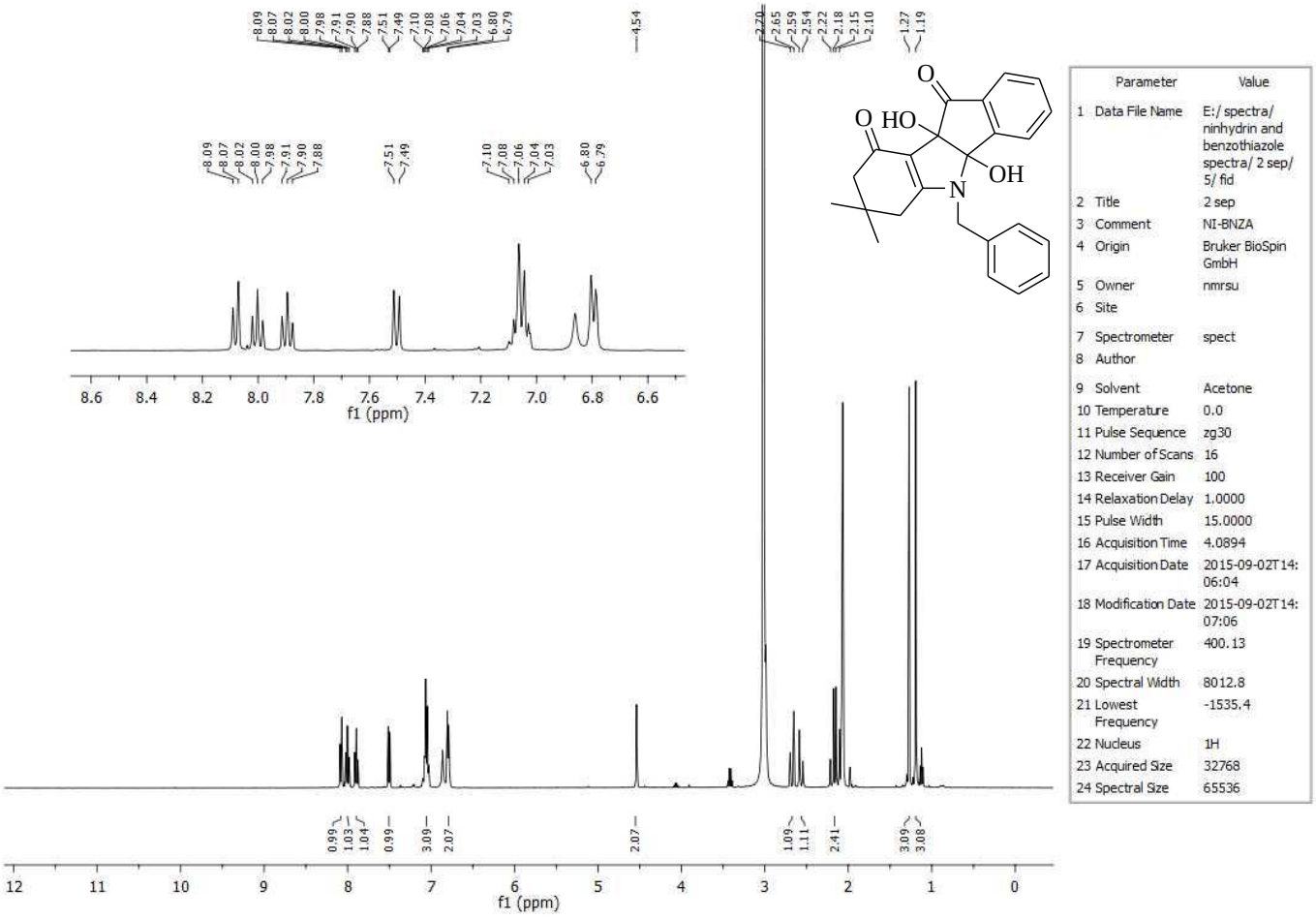
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Number of Scans	653
13	Receiver Gain	199
14	Relaxation Delay	2.0000
15	Pulse Width	9.8000
16	Acquisition Time	1.3631
17	Acquisition Date	2015-07-24T13:34:28
18	Modification Date	2015-07-24T13:34:30
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.9
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

DEPT of entry 8, Table 6



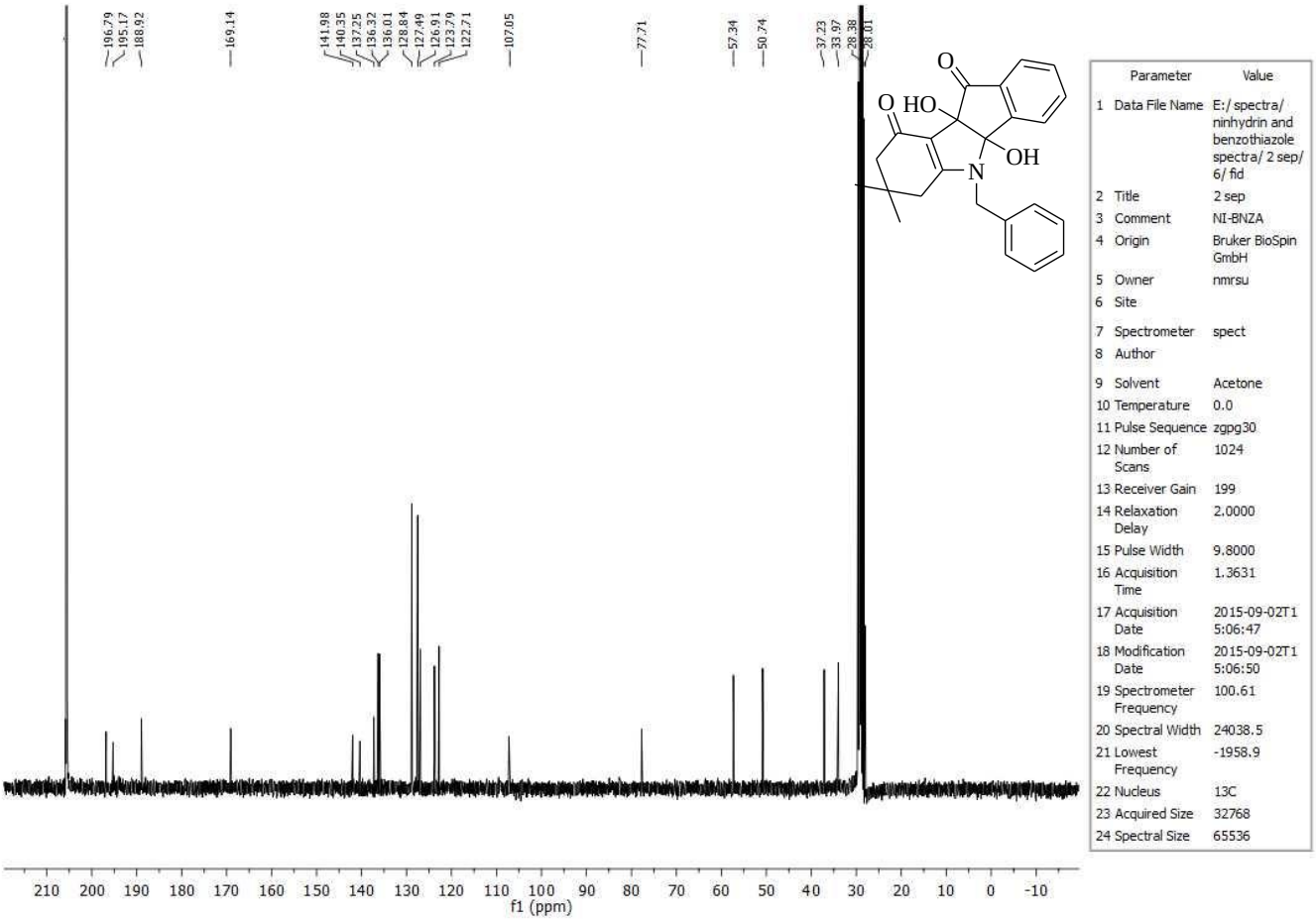
	Parameter	Value
1	Data File Name	E:/ spectra/ ninhydrin and benzothiazole spectra/ 24-7/ 4/ fid
2	Title	24-7
3	Comment	NI-PF
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	deptsp135
12	Number of Scans	93
13	Receiver Gain	199
14	Relaxation Delay	2.0000
15	Pulse Width	9.8000
16	Acquisition Time	2.0316
17	Acquisition Date	2015-07-24T13:41:19
18	Modification Date	2015-07-24T13:41:30
19	Spectrometer Frequency	100.61
20	Spectral Width	16129.0
21	Lowest Frequency	-16.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR spectra of entry 10, Table 6



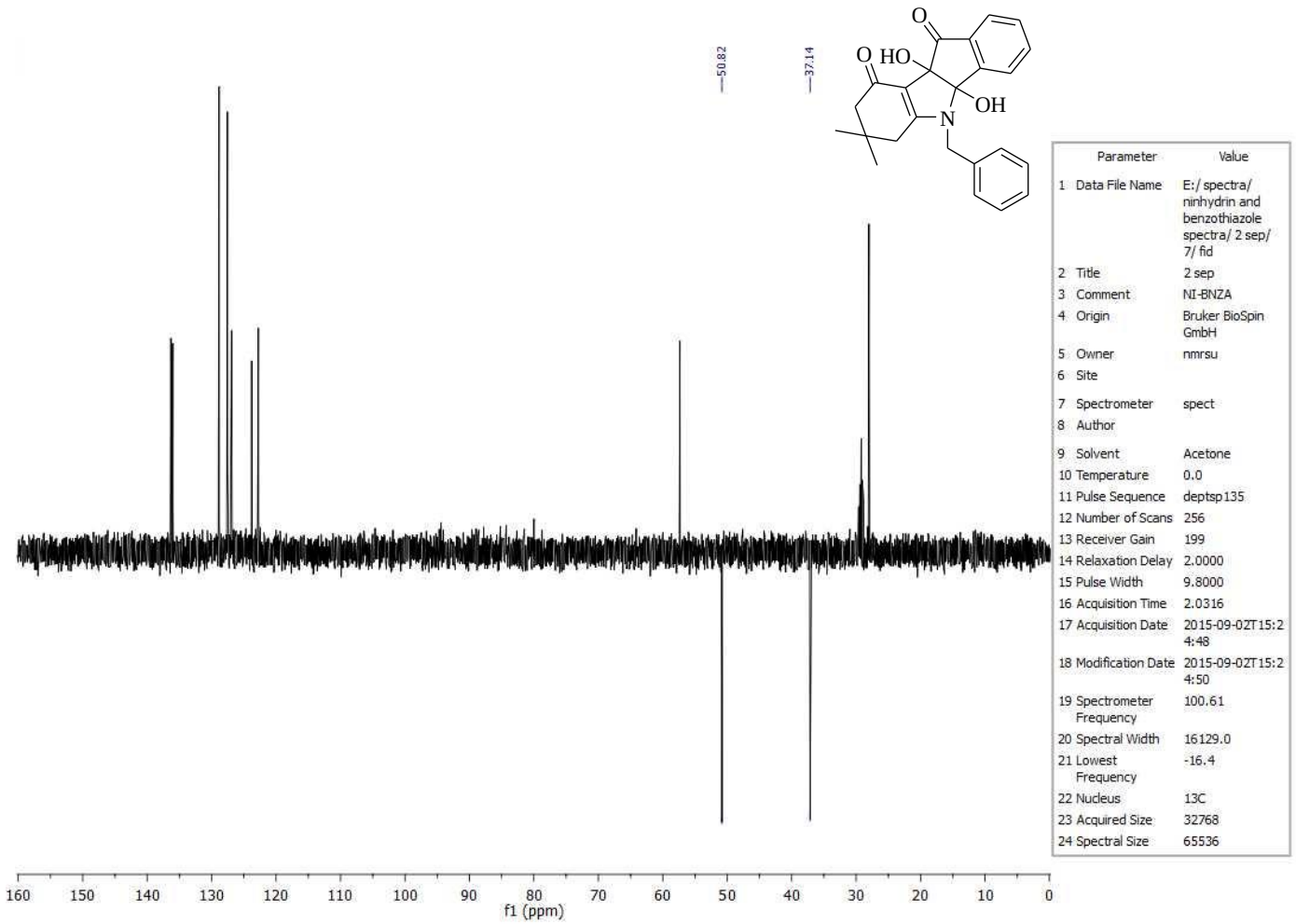
	Parameter	Value
1	Data File Name	E:/ spectra/ ninhydrin and benzothiazole spectra/ 2 sep/ 5/ fid
2	Title	2 sep
3	Comment	NI-BNZA
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	Acetone
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	100
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2015-09-02T14:06:04
18	Modification Date	2015-09-02T14:07:06
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR spectra of entry 10, Table 6



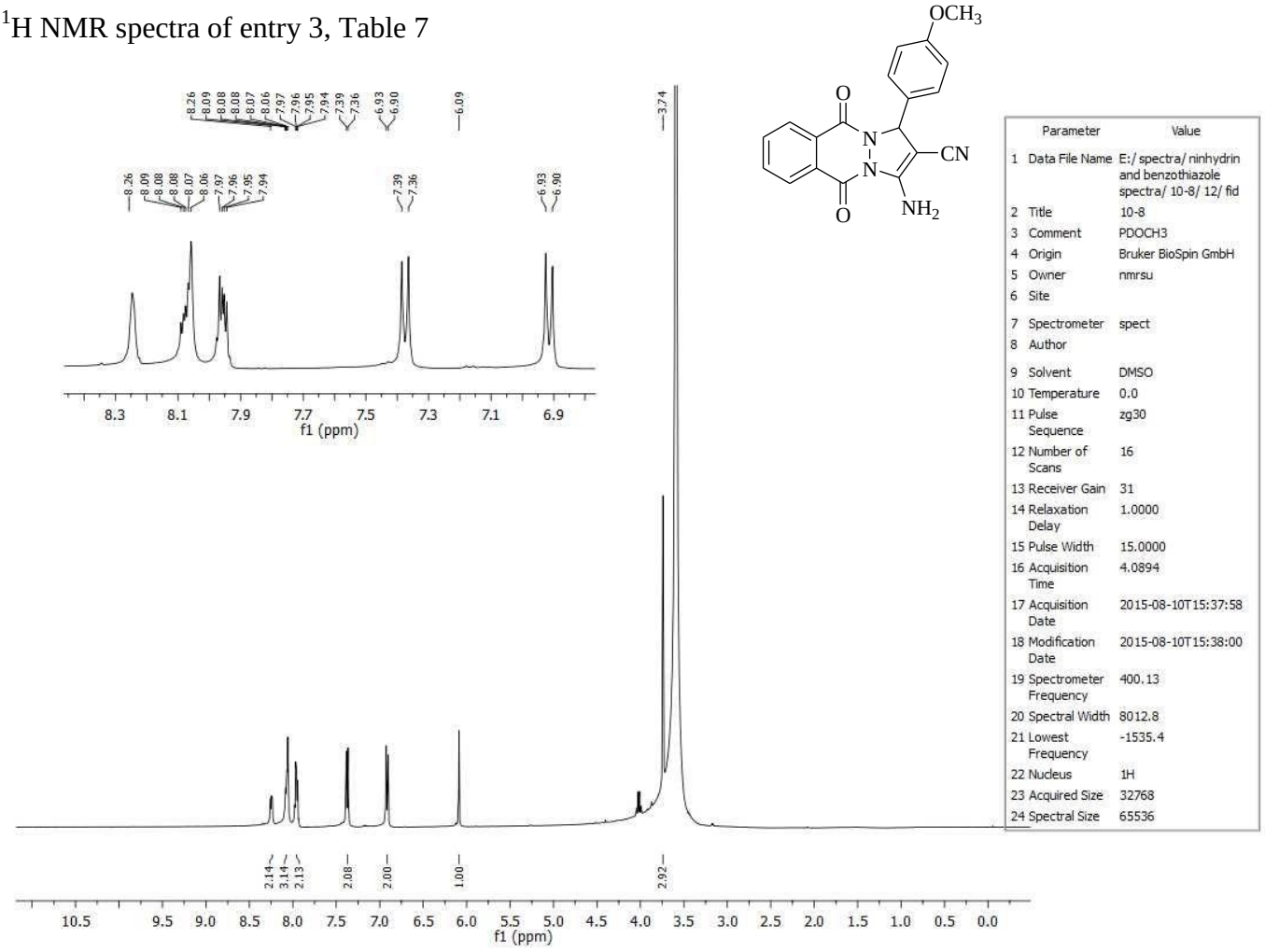
	Parameter	Value
1	Data File Name	E:/ spectra/ ninhydrin and benzothiazole spectra/ 2 sep/ 6/ fid
2	Title	2 sep
3	Comment	NI-BNZA
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	Acetone
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Number of Scans	1024
13	Receiver Gain	199
14	Relaxation Delay	2.0000
15	Pulse Width	9.8000
16	Acquisition Time	1.3631
17	Acquisition Date	2015-09-02T15:06:47
18	Modification Date	2015-09-02T15:06:50
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.9
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

DEPT of entry 10, Table 6



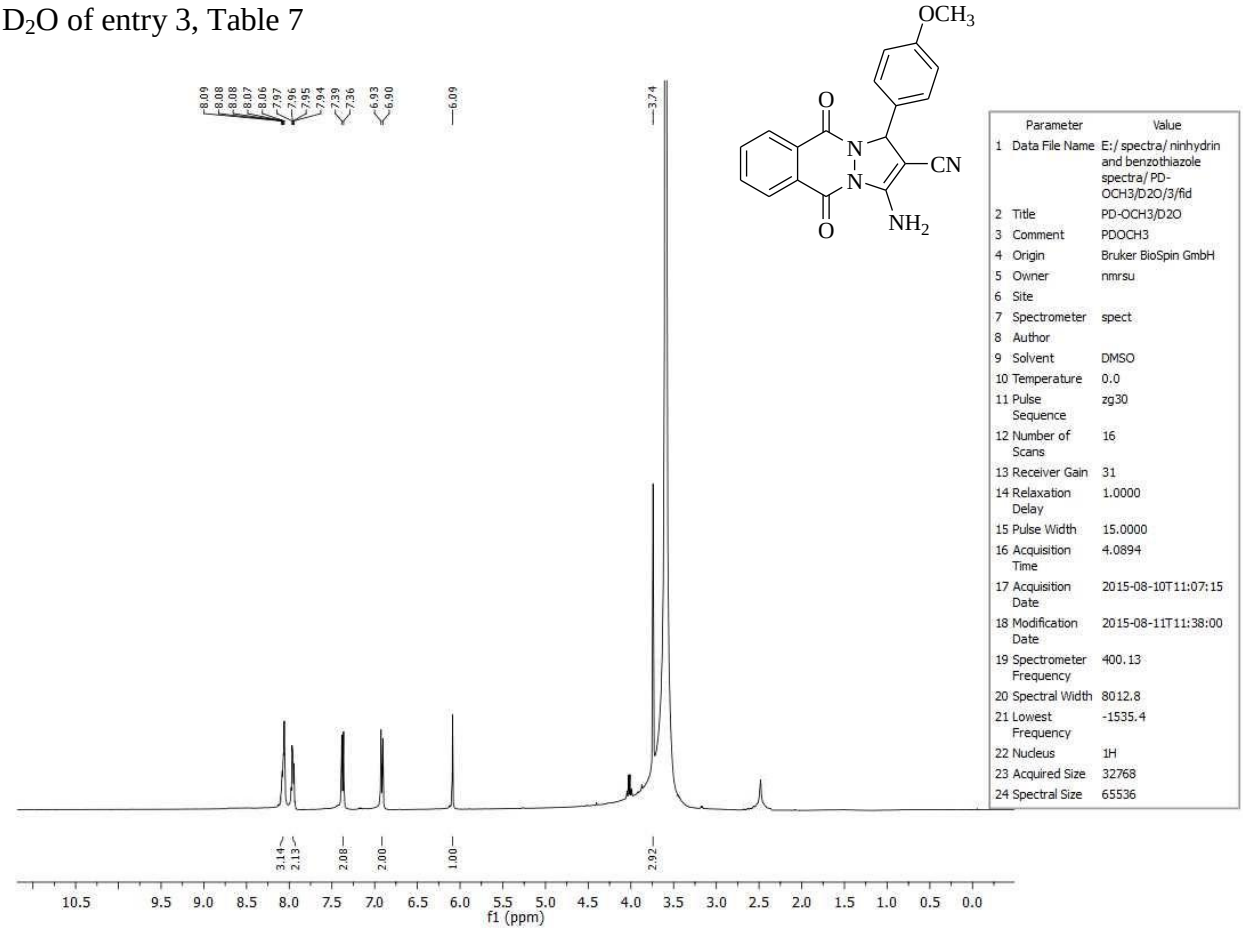
	Parameter	Value
1	Data File Name	E:/ spectra/ ninhydrin and benzothiazole spectra/ 2 sep/ 7/ fid
2	Title	2 sep
3	Comment	NI-BNZA
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	Acetone
10	Temperature	0.0
11	Pulse Sequence	deptsp135
12	Number of Scans	256
13	Receiver Gain	199
14	Relaxation Delay	2.0000
15	Pulse Width	9.8000
16	Acquisition Time	2.0316
17	Acquisition Date	2015-09-02T15:24:48
18	Modification Date	2015-09-02T15:24:50
19	Spectrometer Frequency	100.61
20	Spectral Width	16129.0
21	Lowest Frequency	-16.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR spectra of entry 3, Table 7



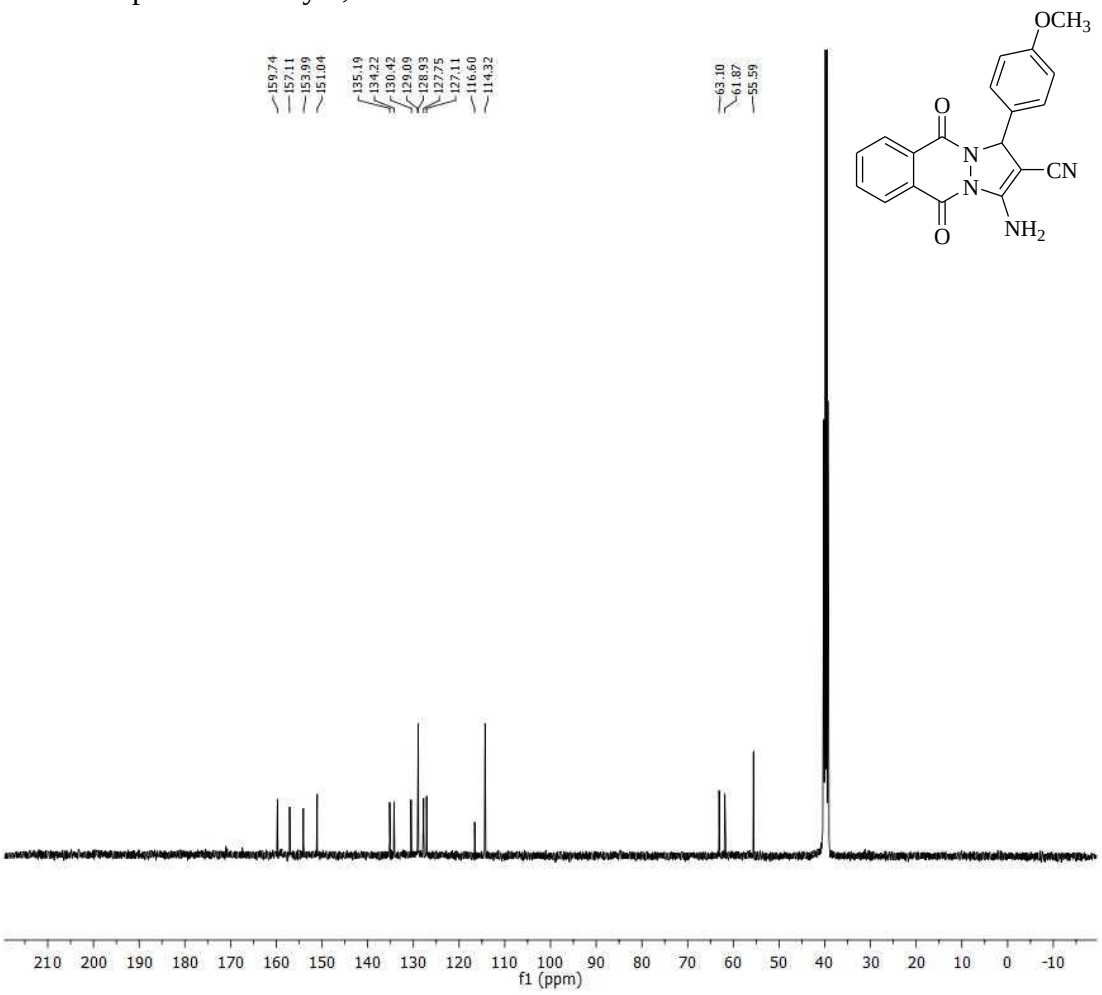
	Parameter	Value
1	Data File Name	E:/ spectra/ ninhydrin and benzothiazole spectra/ 10-8/ 12/ fid
2	Title	10-8
3	Comment	PDOCH3
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	31
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2015-08-10T15:37:58
18	Modification Date	2015-08-10T15:38:00
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

D_2O of entry 3, Table 7



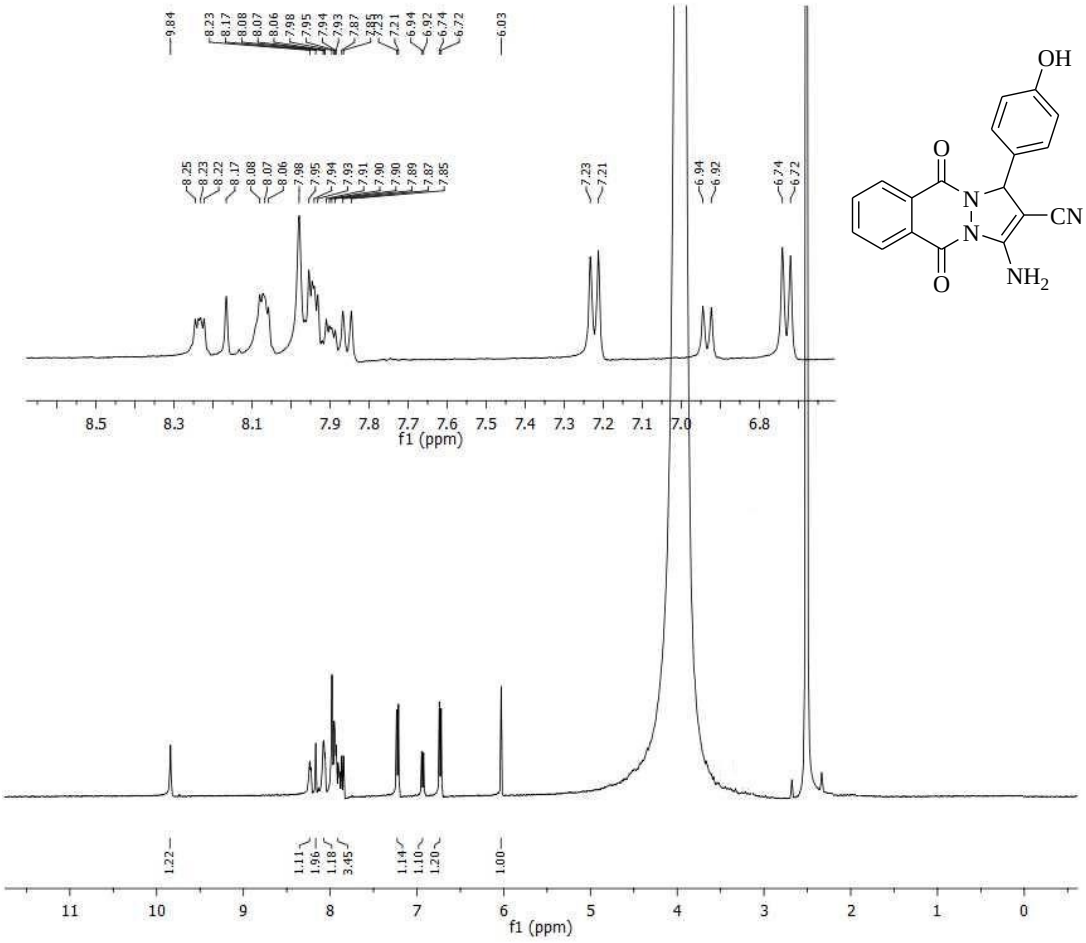
	Parameter	Value
1	Data File Name	E:/ spectra/ ninhydrin and benzothiazole spectra/ PD-OCH3/D2O/3/fid
2	Title	PD-OCH3/D2O
3	Comment	PDOCH3
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	31
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2015-08-10T11:07:15
18	Modification Date	2015-08-11T11:38:00
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR spectra of entry 3, Table 7



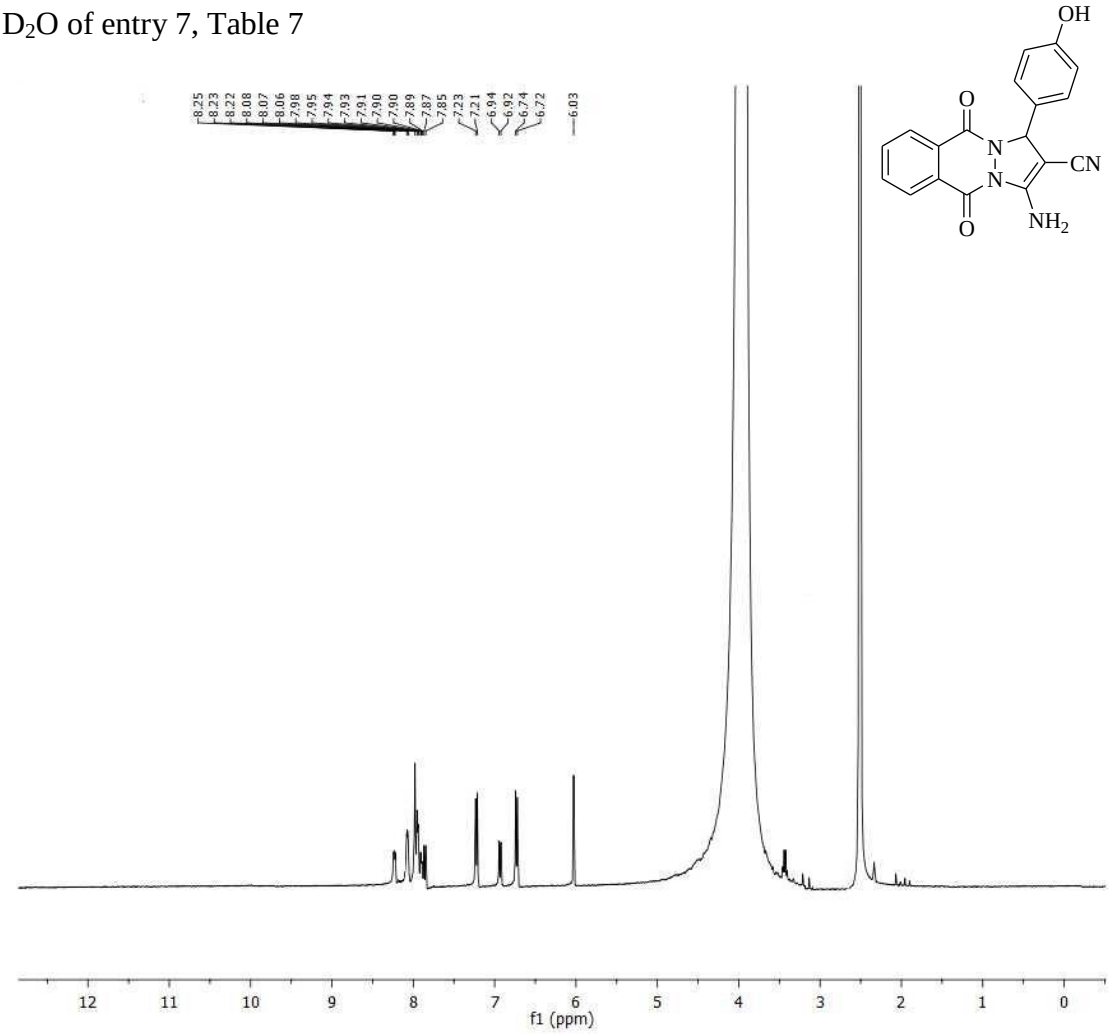
	Parameter	Value
1	Data File Name	E:/ spectra/ ninhydrin and benzothiazole spectra/ 10-8/ 13/ fid
2	Title	10-8
3	Comment	PDOCH3
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Number of Scans	824
13	Receiver Gain	199
14	Relaxation Delay	2.0000
15	Pulse Width	9.8000
16	Acquisition Time	1.3631
17	Acquisition Date	2015-08-10T15: 43:50
18	Modification Date	2015-08-10T16: 26:18
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.9
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR spectra of entry 7, Table 7



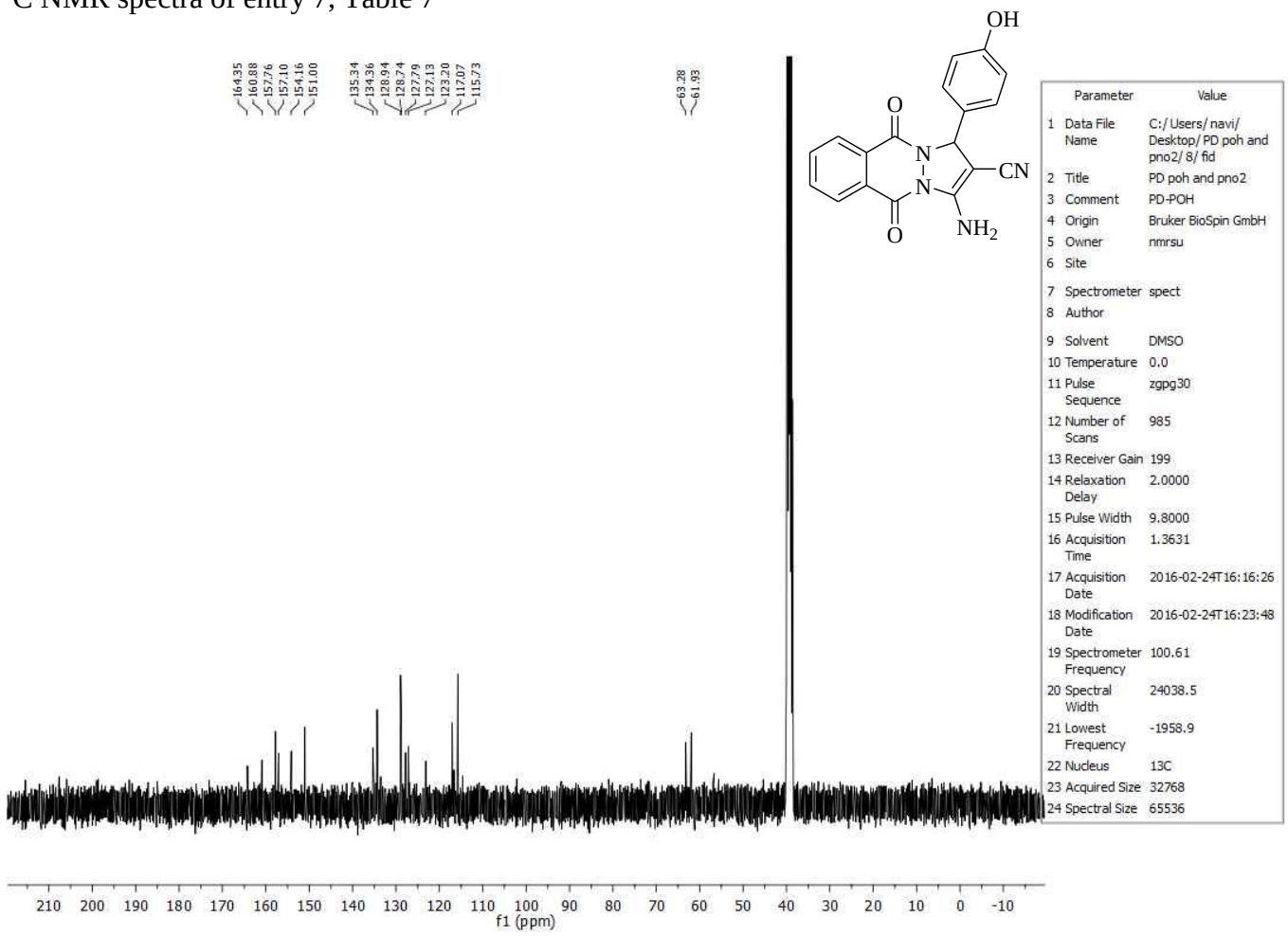
	Parameter	Value
1	Data File Name	C:/Users/navi/Desktop/PD poh and pno2/7/fid
2	Title	PD poh and pno2
3	Comment	PD-POH
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	14
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2016-02-24T15:26:43
18	Modification Date	2016-02-24T15:26:46
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

D_2O of entry 7, Table 7



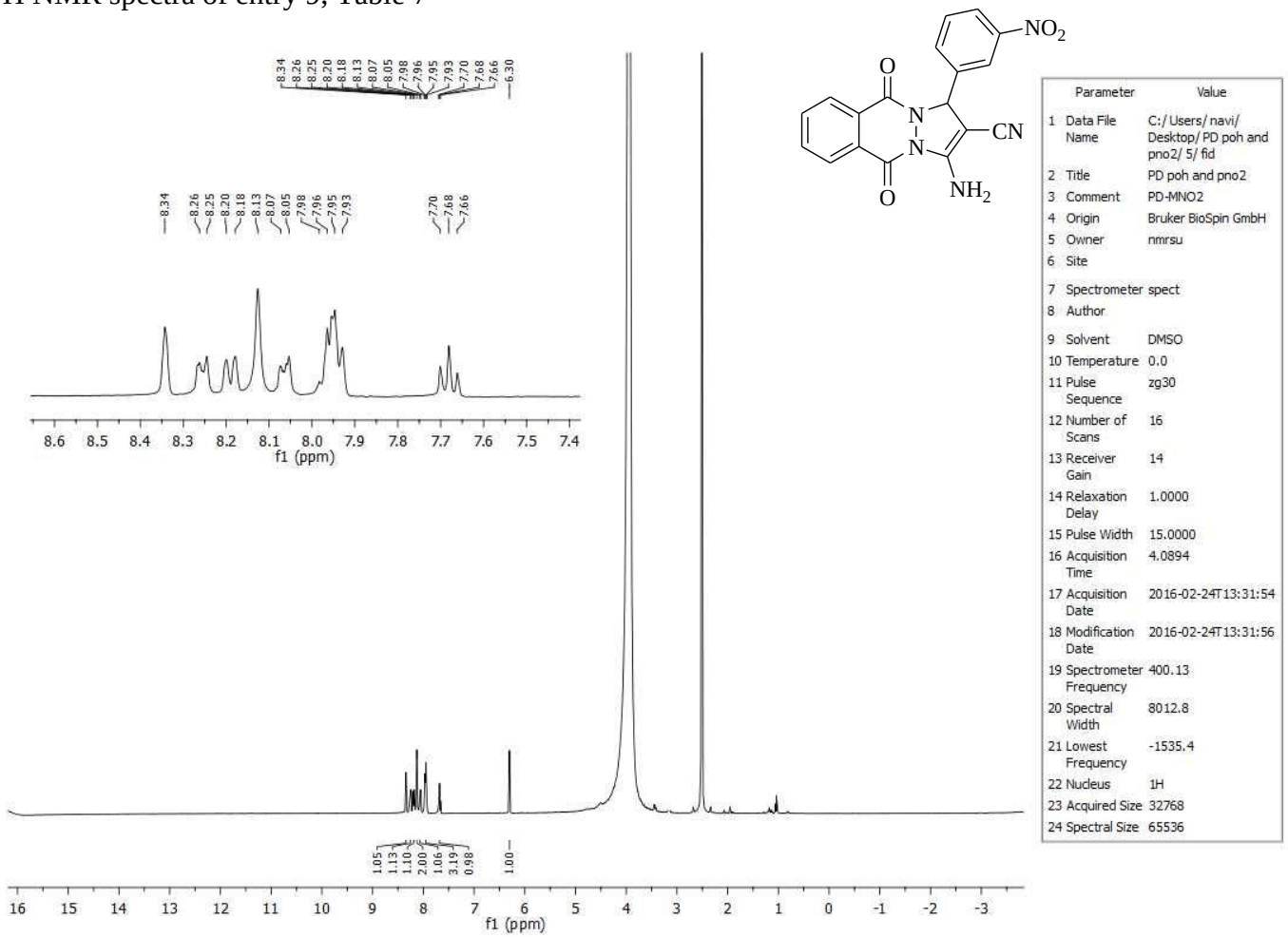
	Parameter	Value
1	Data File Name	C:/Users/navi/Desktop/PD poh and pno2/9/fid
2	Title	PD poh
3	Comment	PD-POH/D2O
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	14
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2016-02-25T11:16:32
18	Modification Date	2016-02-25T11:16:34
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR spectra of entry 7, Table 7



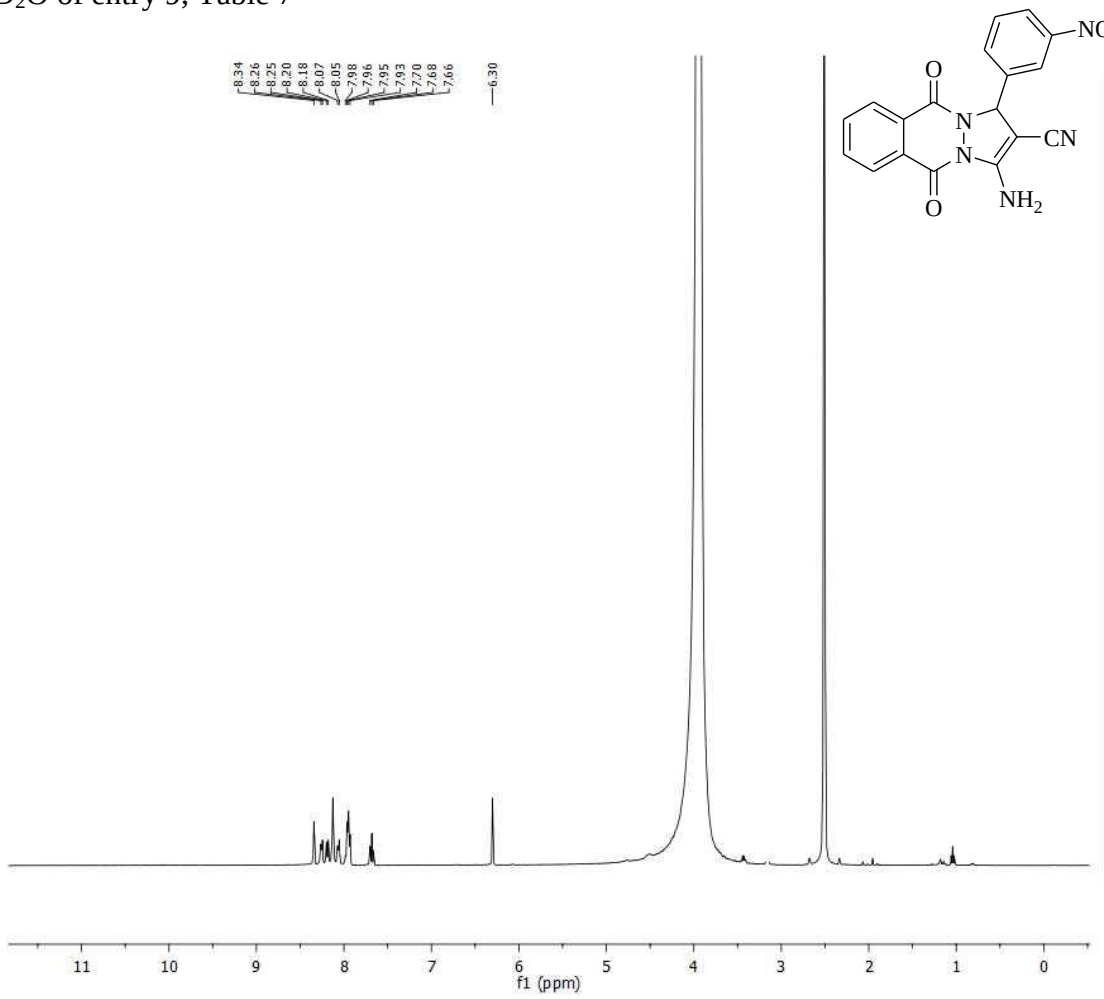
	Parameter	Value
1	Data File Name	C:/Users/navi/Desktop/PD poh and pno2/8/fid
2	Title	PD poh and pno2
3	Comment	PD-POH
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Number of Scans	985
13	Receiver Gain	199
14	Relaxation Delay	2.0000
15	Pulse Width	9.8000
16	Acquisition Time	1.3631
17	Acquisition Date	2016-02-24T16:16:26
18	Modification Date	2016-02-24T16:23:48
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.9
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR spectra of entry 9, Table 7



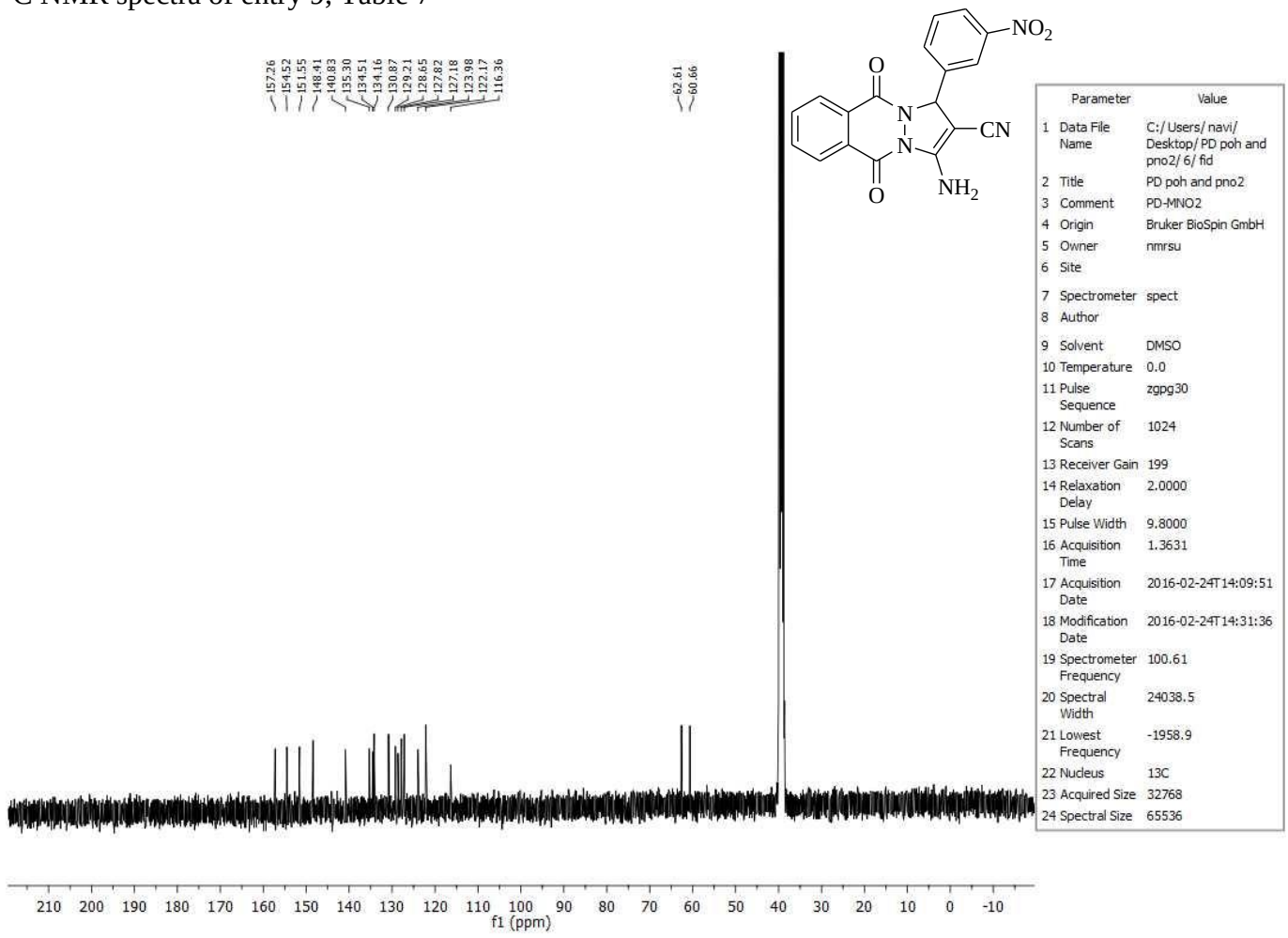
	Parameter	Value
1	Data File Name	C:/ Users/ navi/ Desktop/ PD poh and pno2/ 5/ fid
2	Title	PD poh and pno2
3	Comment	PD-MNO2
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	14
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2016-02-24T13:31:54
18	Modification Date	2016-02-24T13:31:56
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

D_2O of entry 9, Table 7



	Parameter	Value
1	Data File Name	C:/Users/navi/Desktop/PD poh and pno2/5/fid
2	Title	pno2/D2O
3	Comment	PD-MNO2/D2O
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	14
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2016-02-25T12:11:14
18	Modification Date	2016-02-25T12:11:16
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR spectra of entry 9, Table 7



	Parameter	Value
1	Data File Name	C:/ Users/ navi/ Desktop/ PD poh and pno2/ 6/ fid
2	Title	PD poh and pno2
3	Comment	PD-MNO2
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Number of Scans	1024
13	Receiver Gain	199
14	Relaxation Delay	2.0000
15	Pulse Width	9.8000
16	Acquisition Time	1.3631
17	Acquisition Date	2016-02-24T14:09:51
18	Modification Date	2016-02-24T14:31:36
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.9
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536