Supplementary material to:

D. Habibi, M.A. Zolfigol, M. Shiri and A. Sedaghat, *S. Afr. J. Chem.*, 2006, **59**, 93–96.

The references below refer to the reference list in the manuscript.

2-Methyl-6-nitro-phenol (1a**):**[28c]
IR (KBr) cm^{-1}: 3385 (OH, stretch), 3100 (Aromatic CH, stretch), 2926 (Aliphatic CH, stretch), 1607 (Aromatic C=C, stretch), 1542 (NO, unsym), 1462 (CH, bending), 1338 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 2.24 (3H, CH_3), 7.0 (1H, Ar), 7.30 (1H, Ar), 7.8 (1H, Ar), 10.80 (1H, OH).

2-Methyl-4-nitro-phenol (1b**):**[28c]
IR (KBr) cm^{-1}: 3374 (OH, stretch), 3088 (Aromatic CH, stretch), 2960 (Aliphatic CH, stretch), 1615 (Aromatic C=C, stretch), 1511 (NO, unsym), 1451 (CH, bending), 1311 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 2.30 (3H, CH_3), 6.80 (1H, Ar), 7.80–7.85 (2H, Ar), 10.92 (1H, OH).

3-Nitro-biphenyl-2-ol (2a**):**[41]
IR (KBr) cm^{-1}: 3450 (OH, stretch), 3095 (Aromatic CH, stretch), 1603 (Aromatic C=C, stretch), 1541 (NO, unsym), 1320 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 6.95–7.43 (7H, Ar), 7.99 (1H, Ar), 11.03 (1H, OH).

5-Nitro-biphenyl-2-ol (2b**):**[41]
IR (KBr) cm^{-1}: 3465 (OH, stretch), 3111 (Aromatic CH, stretch), 1608 (Aromatic C=C, stretch), 1554 (NO, unsym), 1339 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 7.45 (6H, Ar), 8.45(1H, Ar), 8.98 (1H, Ar), 11.51 (1H, OH).

2-Chloro-6-nitro-phenol (3a**):**[28c]
IR (KBr) cm^{-1}: 3256 (OH, stretch), 2926 (Aromatic CH, stretch), 1608 (Aromatic C=C, stretch), 1450, 1544 (NO, unsym), 1259 (NO, sym), 738 (C-Cl, stretch).

^{1}H NMR ($CDCl_3$): δ 6.89 (1H, Ar), 7.59 (1H, Ar), 7.94 (1H, Ar), 10.95 (1H, OH).

2-Chloro-4-nitro-phenol (3b**):**[28c]
IR (KBr) cm^{-1}: 3300 (OH, stretch), 3010 (Aromatic CH, stretch), 1595 (Aromatic C=C, stretch), 1535 (NO, unsym), 1295 (NO, sym), 735 (C-Cl, stretch).

^{1}H NMR ($CDCl_3$): δ 6.90 (1H, Ar), 7.9 (1H, Ar), 8.0 (1H, Ar), 10.7 (1H, OH).

2-Bromo-6-nitro-phenol (4a**):**[41]
IR (KBr) cm^{-1}: 3260 (OH, stretch), 3100 (Aromatic CH, stretch), 1614 (Aromatic C=C, stretch), 1521 (NO, unsym), 1333 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 7.0 (1H, Ar), 7.60 (1H, Ar), 7.90 (1H, Ar), 10.65 (1H, OH).

2-Bromo-4-nitro-phenol (4b**):**[36]
IR (KBr) cm^{-1}: 3281 (OH, stretch), 3093 (Aromatic CH, stretch), 1601 (Aromatic C=C, stretch), 1532 (NO, unsym), 1369 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 6.85 (1H, Ar), 7.93 (1H, Ar), 8.15 (1H, Ar), 10.31 (1H, OH).

2-Methoxy-6-nitro-phenol (5a**):**[24]
IR (KBr) cm^{-1}: 3413 (OH, stretch), 3093 (Aromatic CH, stretch), 2988 (Aliphatic CH, stretch), 1632 (Aromatic C=C, stretch), 1483 & 1501 (NO, unsym), 1464 (CH_3, bending), 1311 & 1373 (NO, sym), 1196 (C-O, stretch).

^{1}H NMR ($CDCl_3$): δ 3.80 (3H, CH_3), 6.90–6.95 (2H, Ar), 7.5 (1H, Ar), 10.98 (1H, OH).

2-Methoxy-4-nitro-phenol (5b**):**[24]
IR (KBr) cm^{-1}: 3408 (OH, stretch), 3097 (Aromatic CH, stretch), 2978 (Aliphatic CH, stretch), 1630 (Aromatic C=C, stretch), 1492 & 1517 (NO, unsym), 1444 (CH_3, bending), 1358 & 1369 (NO, sym), 1182 (C-O, stretch).

^{1}H NMR ($CDCl_3$): δ 3.79 (3H, CH_3), 6.83 (1H, Ar), 7.50–7.55 (2H, Ar), 10.91 (1H, OH).

3,6-Dimethyl-2-nitro-phenol (6a**):**[27]
IR (KBr) cm^{-1}: 3257 (OH, stretch), 3073 (Aromatic CH, stretch), 2968 (Aliphatic CH, stretch), 1608 (Aromatic C=C, stretch), 1513 (NO, unsym), 1469 (CH_3, bending), 1320 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 2.30 (6H, $2CH_3$), 6.70 (1H, Ar), 7.10 (1H, Ar), 10.18 (1H, OH).

2,5-Dimethyl-4-nitro-phenol (6b**):**[41]
IR (KBr) cm^{-1}: 3402 (OH, stretch), 3091 (Aromatic CH, stretch), 2981 (Aliphatic CH, stretch), 1616 (Aromatic C=C, stretch), 1521 (NO, unsym), 1477 (CH_3, bending), 1299 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 2.40 (6H, $2CH_3$), 6.7 (1H, Ar), 7.75 (1H, Ar), 11.04 (1H, OH).

4,5-Dimethyl-2-nitro-phenol (7a**):**[27]
IR (KBr) cm^{-1}: 3424 (OH, stretch), 3086 (Aromatic CH, stretch), 2926 (Aliphatic CH, stretch), 1633 (Aromatic C=C, stretch), 1514 (NO, unsym), 1465 (CH_3, bending), 1306 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 2.20 (6H, $2CH_3$), 6.63 (1H, Ar), 7.61 (1H, Ar), 10.52 (1H, OH).

3,4-Dimethyl-2-nitro-phenol (7b**):**[41]
IR (KBr) cm^{-1}: 3418 (OH, stretch), 3089 (Aromatic CH, stretch), 2937 (Aliphatic CH, stretch), 1609 (Aromatic C=C, stretch), 1516 (NO, unsym), 1473 (CH_3, bending), 1311 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 2.30 (6H, $2CH_3$), 6.70 (1H, Ar), 7.2 (1H, Ar), 10.49 (1H, OH).

3,5-Dimethyl-2-nitro-phenol (8a**):**[41]
IR (KBr) cm^{-1}: 3357 (OH, stretch), 3085 (Aromatic CH, stretch), 2929 (Aliphatic CH, stretch), 1596 (Aromatic C=C, stretch), 1510 (NO, unsym), 1470 (CH_3, bending), 1311 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 3.45 (6H, $2CH_3$), 7.88–7.99 (2H, Ar), 11.93 (1H, OH).

3,5-Dimethyl-4-nitro-phenol (8b**):**[41]
IR (KBr) cm^{-1}: 3250 (OH, stretch), 3080 (Aromatic CH, stretch), 2960 (Aliphatic CH, stretch), 1605 (Aromatic C=C, stretch), 1510 (NO, unsym), 1475 (CH_3, bending), 1315 (NO, sym).

^{1}H NMR ($CDCl_3$): δ 2.19 (6H, $2CH_3$), 6.59 (2H, Ar), 10.19 (1H, OH).