

Melamine nitrate (MN) : A novel and efficient reagent for regioselective nitration of phenols

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Table S1 The confirmation of the nitrophenol products

Entry ^a	Physical Property	¹ HNMR Shifts (600MHz, CDCl ₃)	MS m/s (%)	IR(KBr) ν , cm ⁻¹
1	buff solid	10.584 (s, 1H); 8.111 (d, J=8.4, 1H); 7.587 (t, J=6.6, 1H); 7.162 (d, J=8.4, 1H); 6.994 (t, J=7.8, 1H)	139 (M ⁺ , 100), 137 (40), 123 (35), 63 (50)	3436, 3235 (-OH); 1621, 1589, 1478 (Ar); 1531, 1376 (-NO ₂)
2	orange-yellow solid	10.336 (s, 1H); 7.505 (s, 1H); 7.215 (d, J=3, 1H); 7.091 (d, J=9.6, 1H); 3.828 (s, 3H)	169 (M ⁺ , 100)	3423, 3219 (-OH); 2921, 2855 (-CH ₃); 1589, 1482, 1433 (Ar); 1535, 1311 (-NO ₂)
3	yellow solid	10.426 (s, 1H); 7.887 (s, 1H); 7.390 (d, J=8.4, 1H); 7.048 (d, J=9, 1H); 2.339 (s, 3H)	153 (M ⁺ , 100), 152 (32), 137 (27)	3440, 3227 (-OH); 2921, 2855, 1384 (-CH ₃); 1629, 1585, 1486 (Ar); 1540, 1323 (-NO ₂)
4	yellow solid	10.585 (s, 1H); 8.329 (d, J=2.4, 1H); 7.839 (d, J=6.6, 1H); 7.563 (d, J=7.2, 2H); 7.470 (t, J=7.2, 2H); 7.392 (t, J=7.2, 1H); 7.247 (d, J=8.4, 1H)	215 (M ⁺ , 100)	3284 (-OH); 1634, 1580, 1478, 1450 (Ar); 1544, 1331 (-NO ₂)
5	yellow solid	10.623 (s, 1H); 7.653 (d, J=8.4, 1H); 7.244 (d, J=6.6, 1H); 6.910 (t, J=8.4, 1H); 5.828 (s, 1H)	155 (M ⁺ , 100), 107(57)	3485, 3432, 3227 (-OH); 1625, 1462 (Ar); 1548, 1356 (-NO ₂)
6	yellow solid	12.243 (s, 1H); 8.523 (d, J=8.4, 1H); 8.019 (d, J=9, 1H); 7.817 (d, J=7.8, 1H); 7.726 (t, J=7.2, 1H); 7.628 (t, J=8.4, 1H); 7.349 (d, J=9.6, 1H)	189 (M ⁺ , 100)	3419 (-OH); 1625, 1544, 1429 (Ar); 1585, 1384 (-NO ₂)
7	yellow solid	12.183 (s, 1H); 8.925 (d, J=9, 1H); 8.010 (d, J=9, 1H); 7.827 (d, J=7.8, 1H); 7.737 (t, J=7.8, 1H); 7.510 (t, J=7.8, 1H); 7.263 (d, J=9, 1H)	189 (M ⁺ , 100), 173 (40), 115 (27)	3415 (-OH); 1621, 1499, 1474 (Ar); 1540, 1380 (-NO ₂)
8 ^b	yellow solid	9.592 (s, 1H); 8.297 (s, 1H); 7.410 (s, 1H); 4.759 (s, 1H); 3.917 (s, 1H)	197(M ⁺ , 100), 196 (27)	3423, 3199 (-OH); 1687 (-C=O); 1613, 1576, 1470 (Ar); 1548, 1335 (-NO ₂)

^a. the entry order is the same as in table 2.^b. This compound is 3-Nitro-4-hydroxy-5-methoxybenzaldehyde which was dissolved in D₂O for

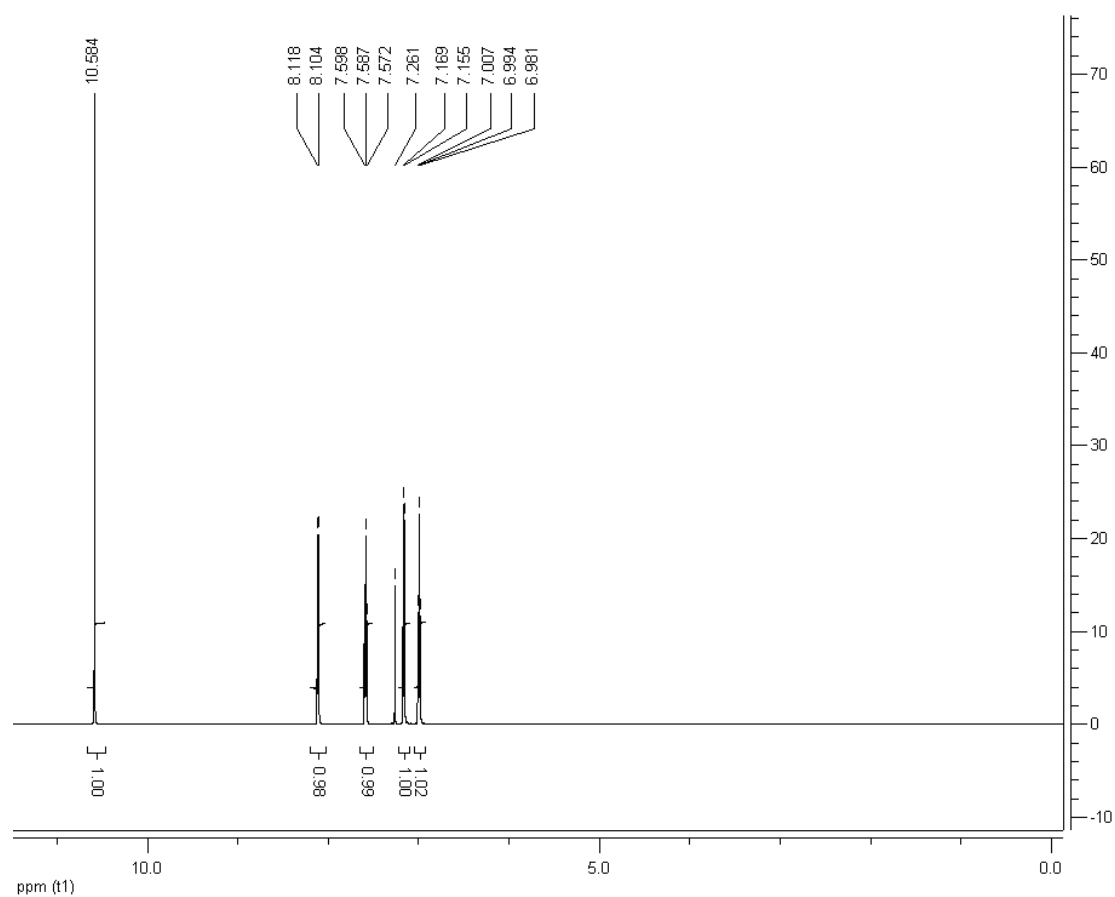


Figure S1 ^1H NMR of o-Nitrophenol

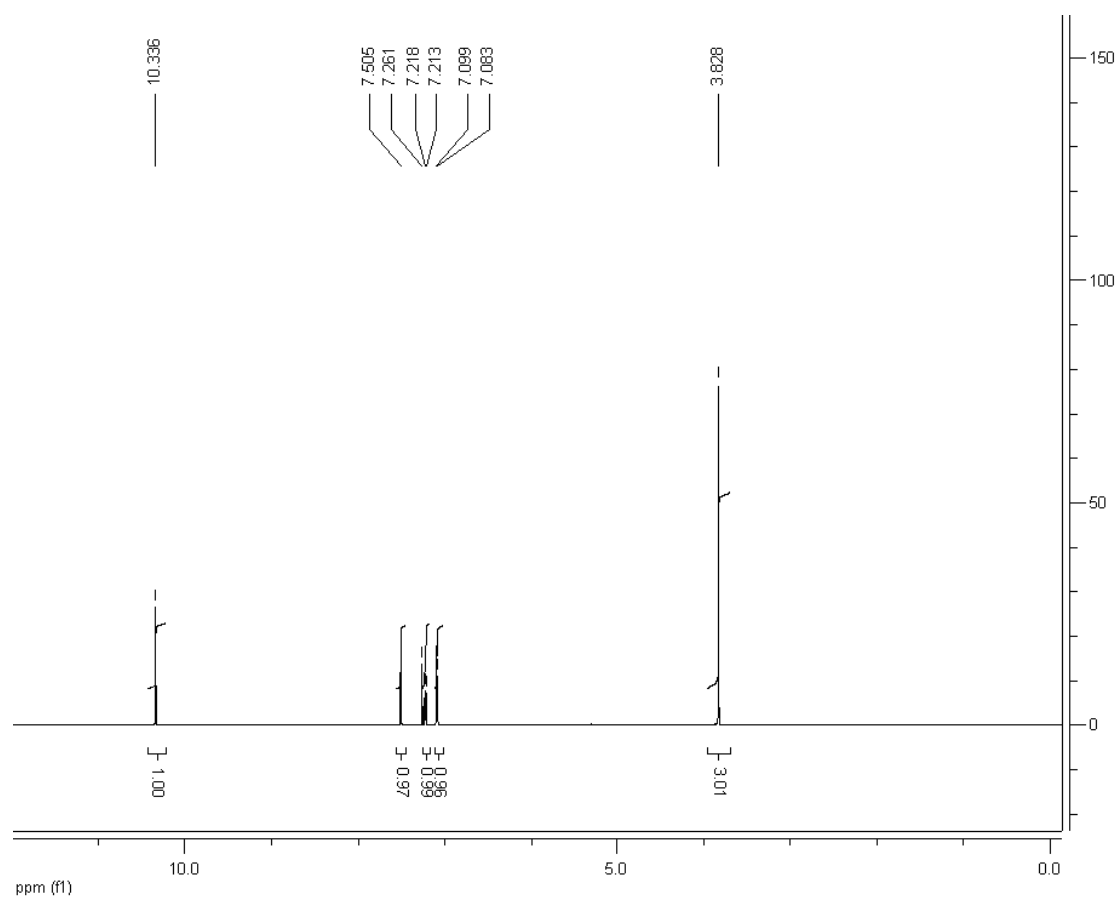


Figure S2 ¹H NMR of 4-Methoxy-2-nitrophenol

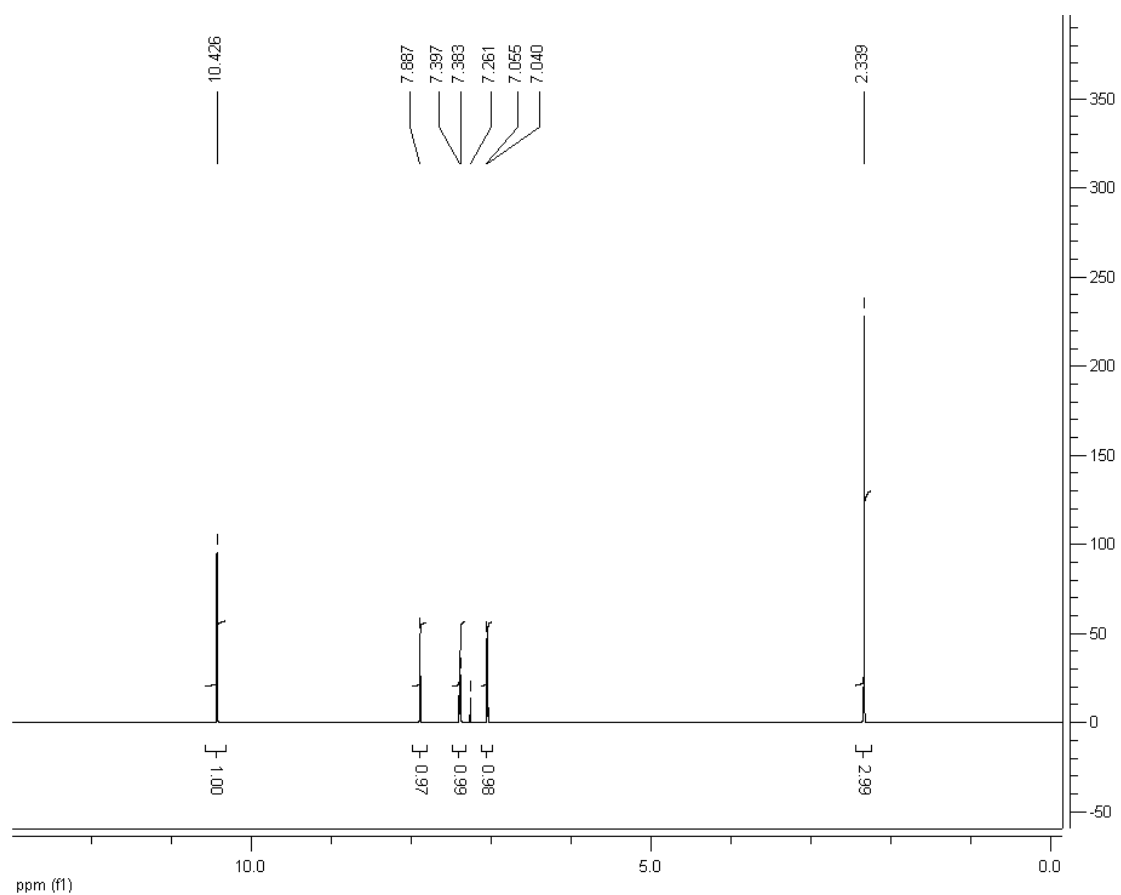


Figure S3. ¹H NMR of 4-Methyl-2-nitrophenol

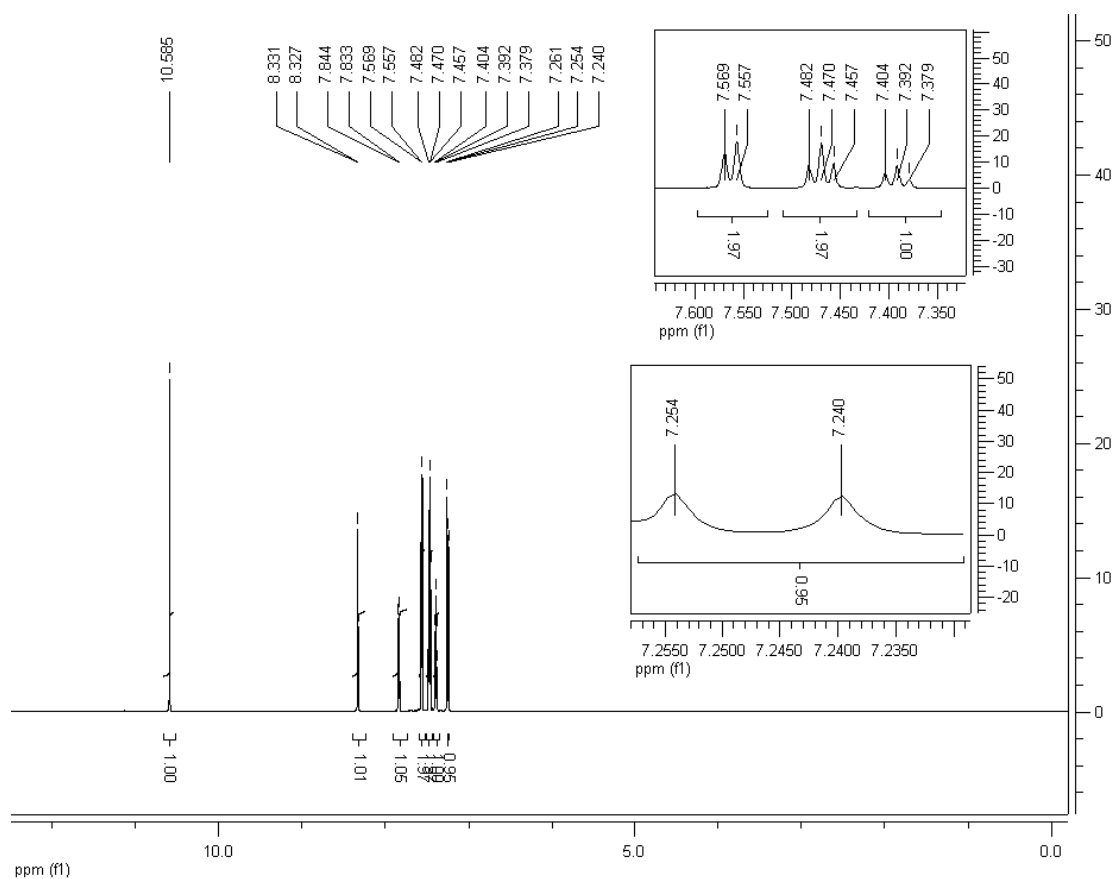


Figure S4. ^1H NMR of 4-Phenyl-2-nitrophenol

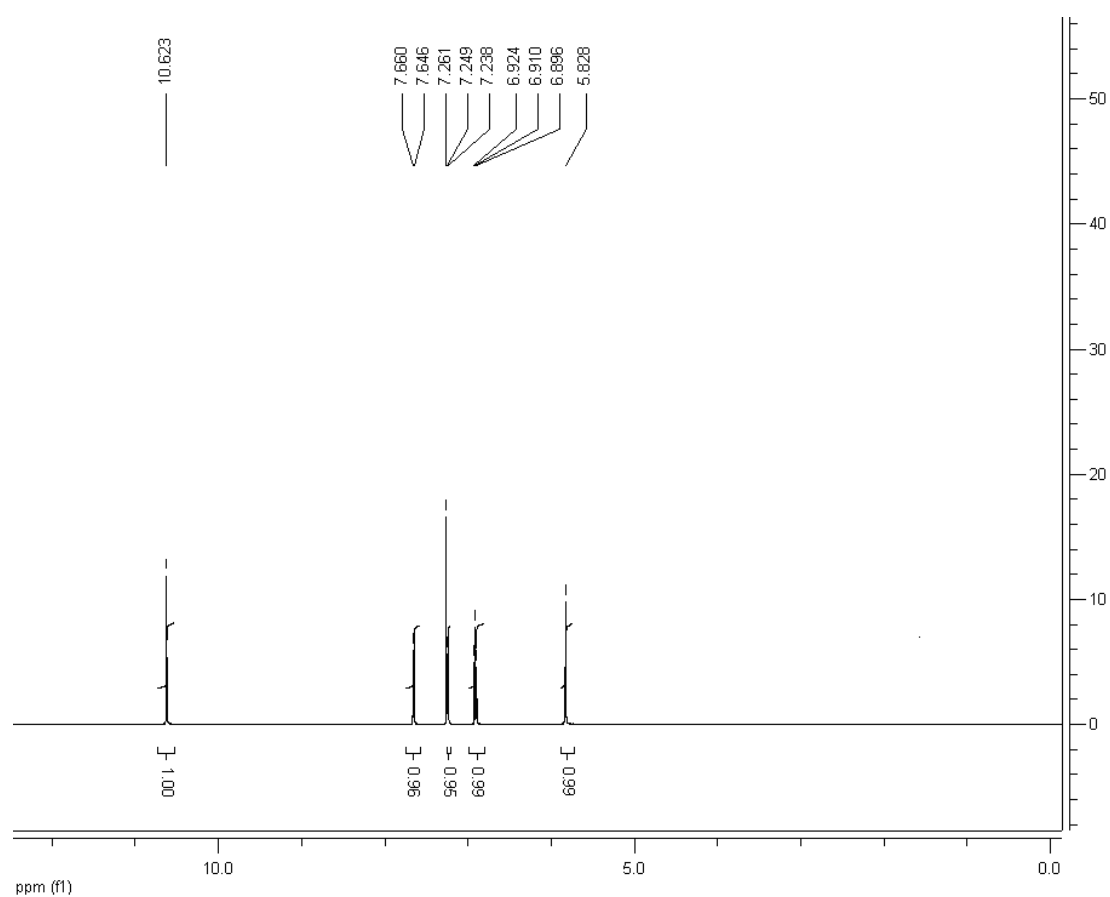


Figure S5. ¹H NMR of 3-nitro-1,2-benzenediol

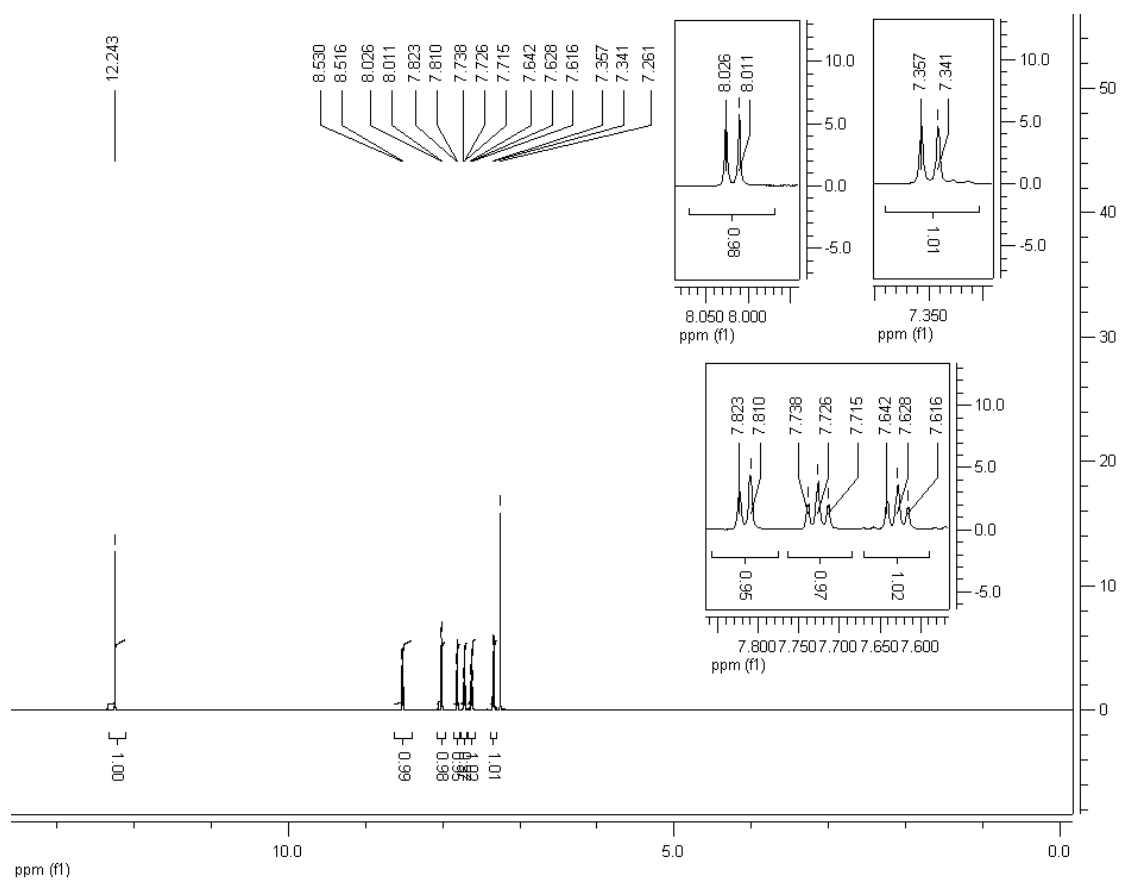


Figure S6. ^1H NMR of 2-Nitro-1-naphthol

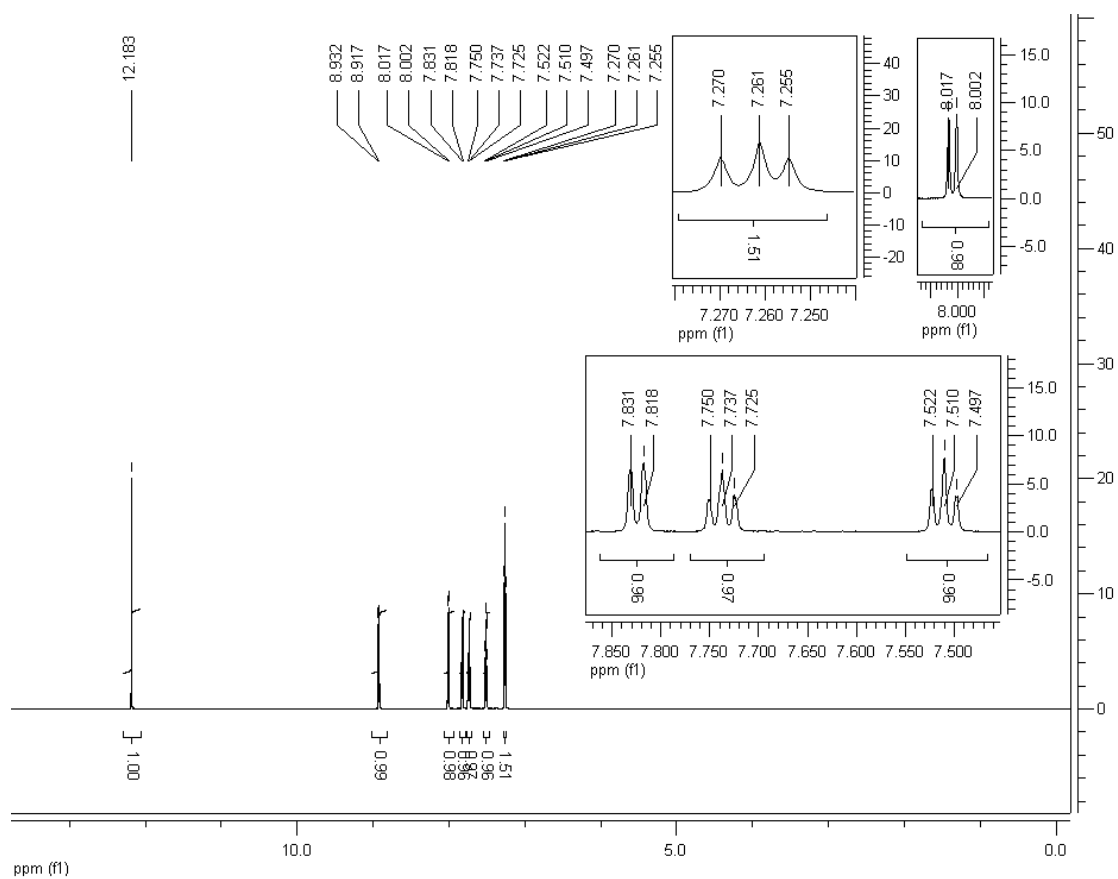


Figure S7. ^1H NMR of 1-Nitro-2-naphthol

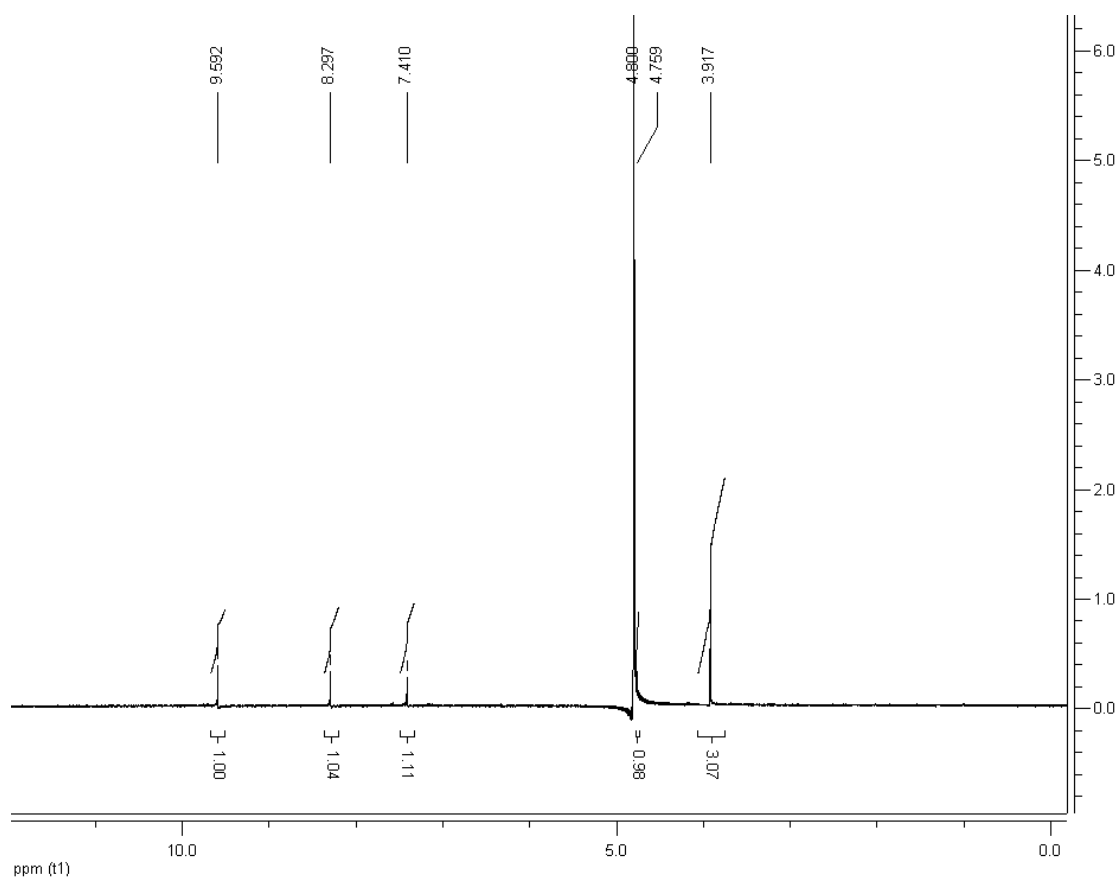


Figure S8. ¹H NMR of 3-Nitro-4-hydroxy-5-methoxybenzaldehyde

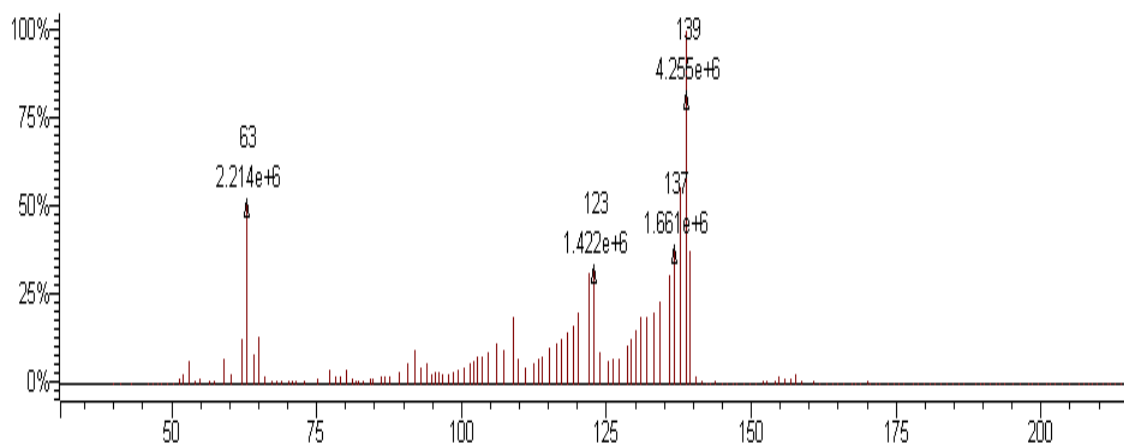


Figure S9. MS of o-Nitrophenol

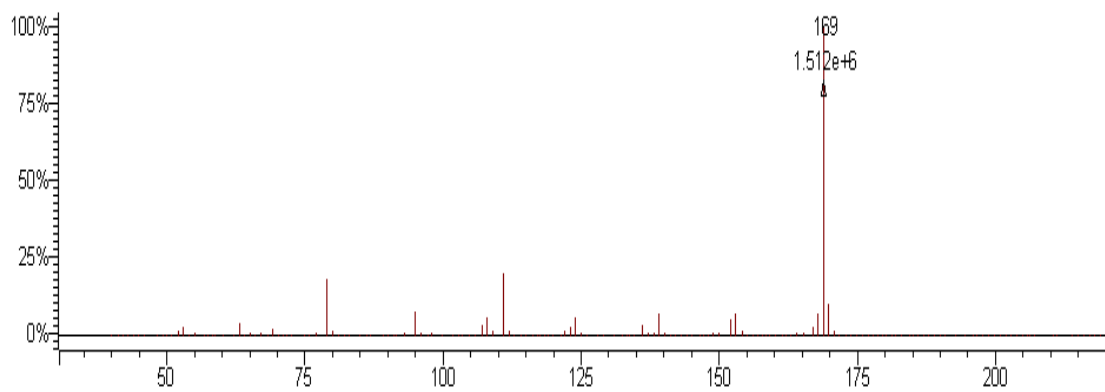


Figure S10. MS of 4-Methoxy-2-nitrophenol

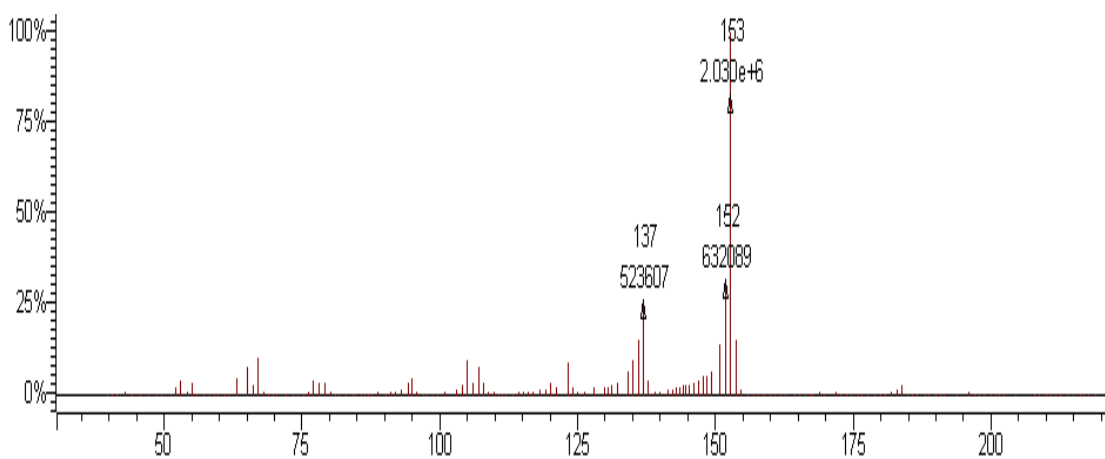


Figure S11. MS of 4-Methyl-2-nitrophenol

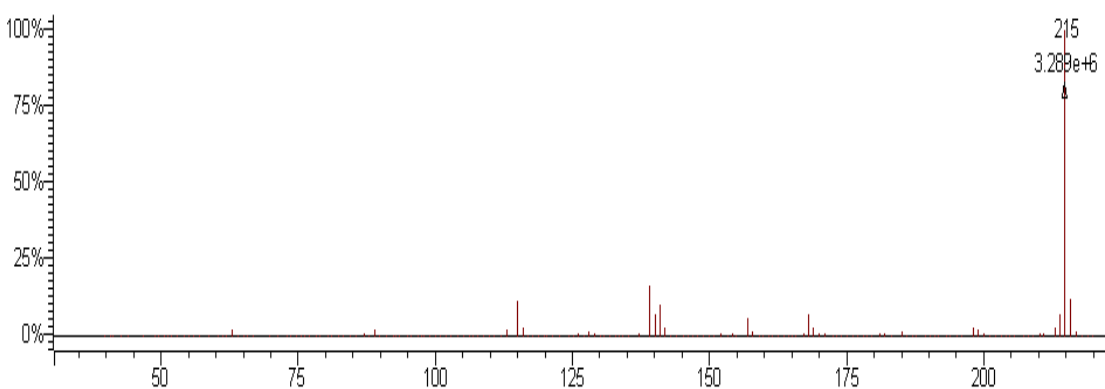


Figure S12. MS of 4-Phenyl-2-nitrophenol

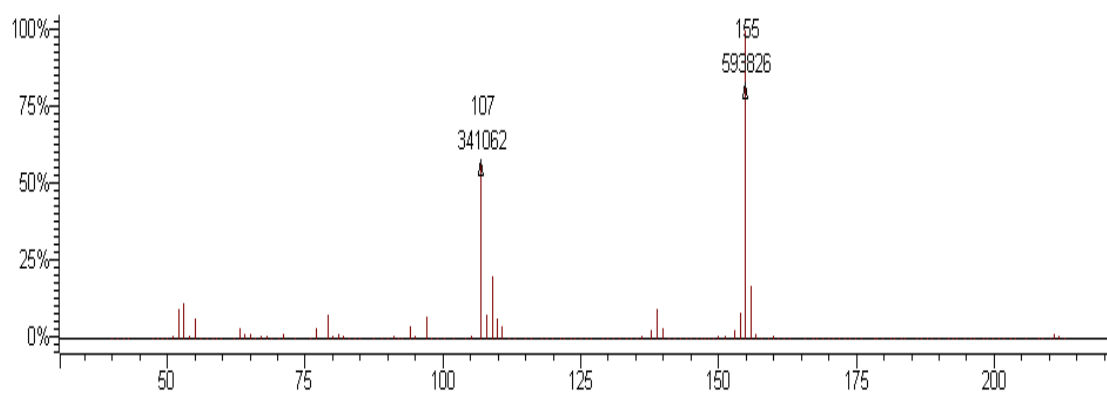


Figure S13. MS of 3-nitro-1,2-benzenediol

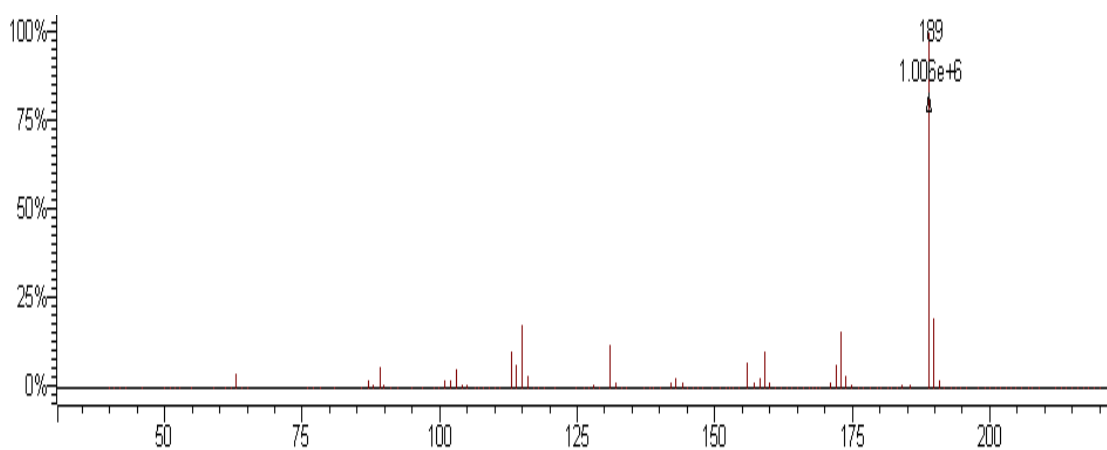


Figure S14. MS of 2-Nitro-1-naphthol

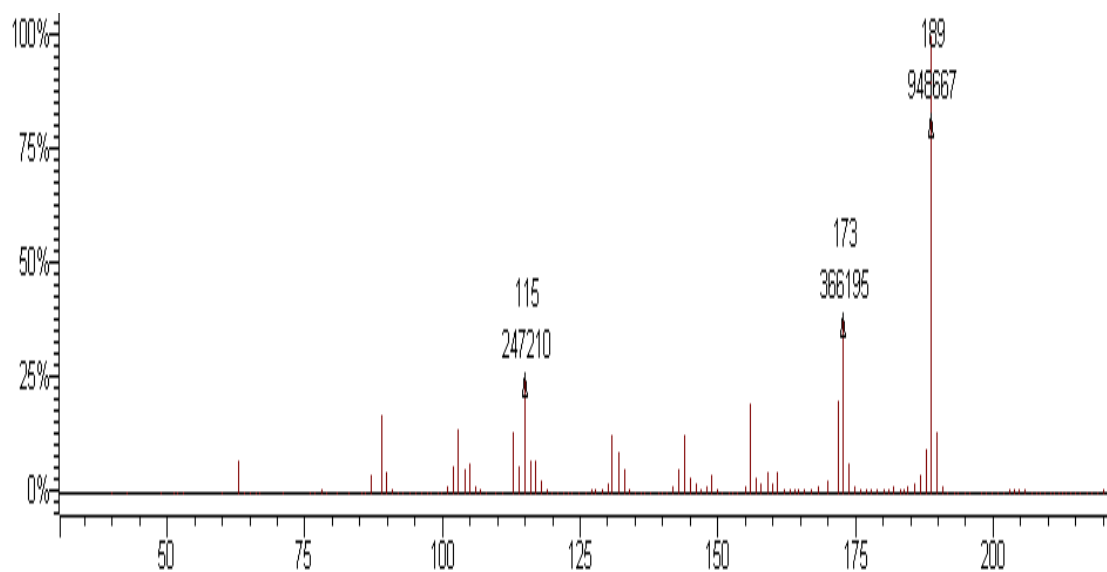


Figure S15. MS of 1-Nitro-2-naphthol

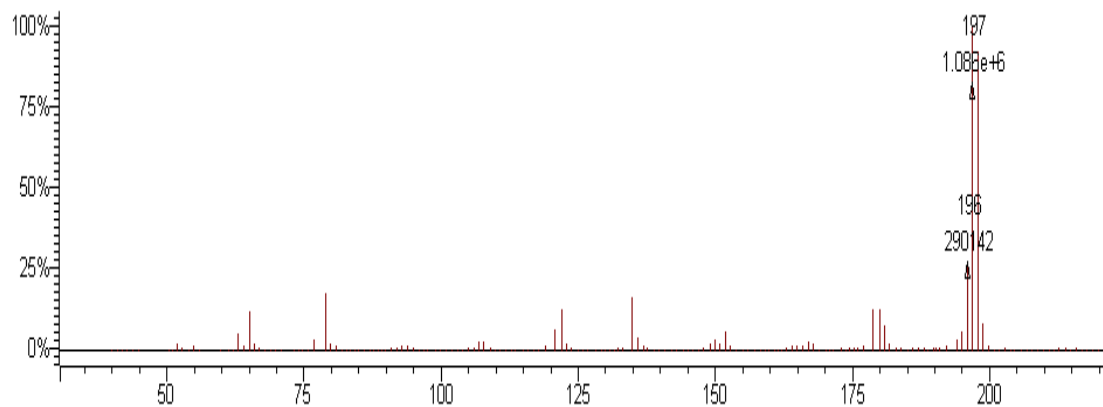


Figure S16. MS of 3-Nitro-4-hydroxy-5-methoxybenzaldehyde

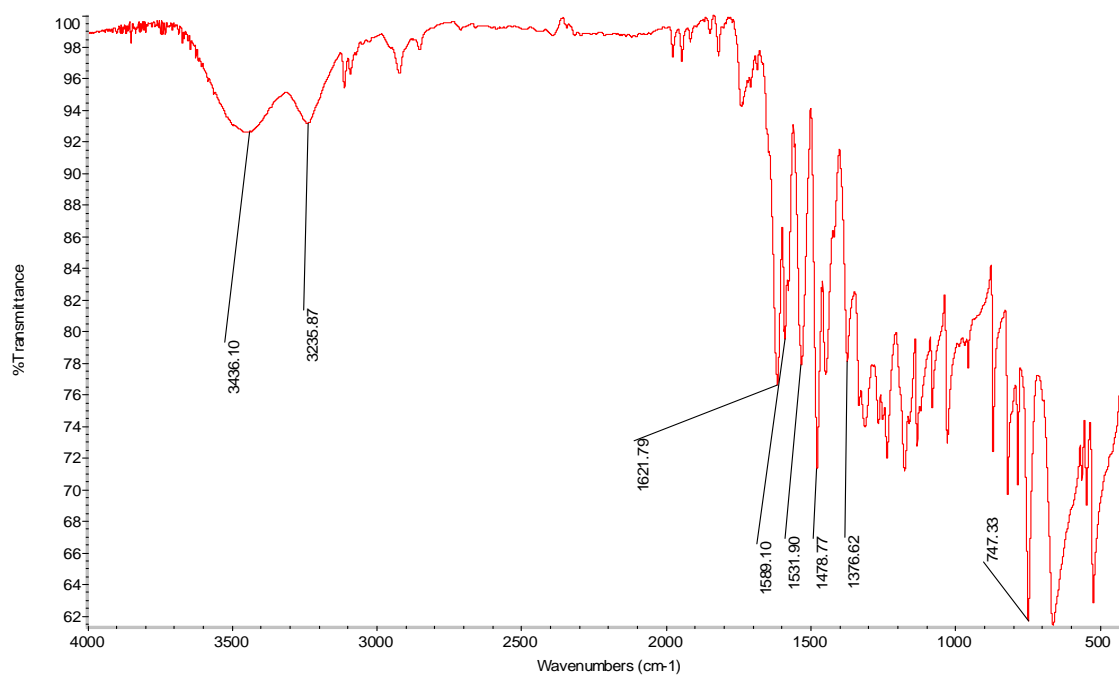


Figure S17. IR of o-Nitrophenol

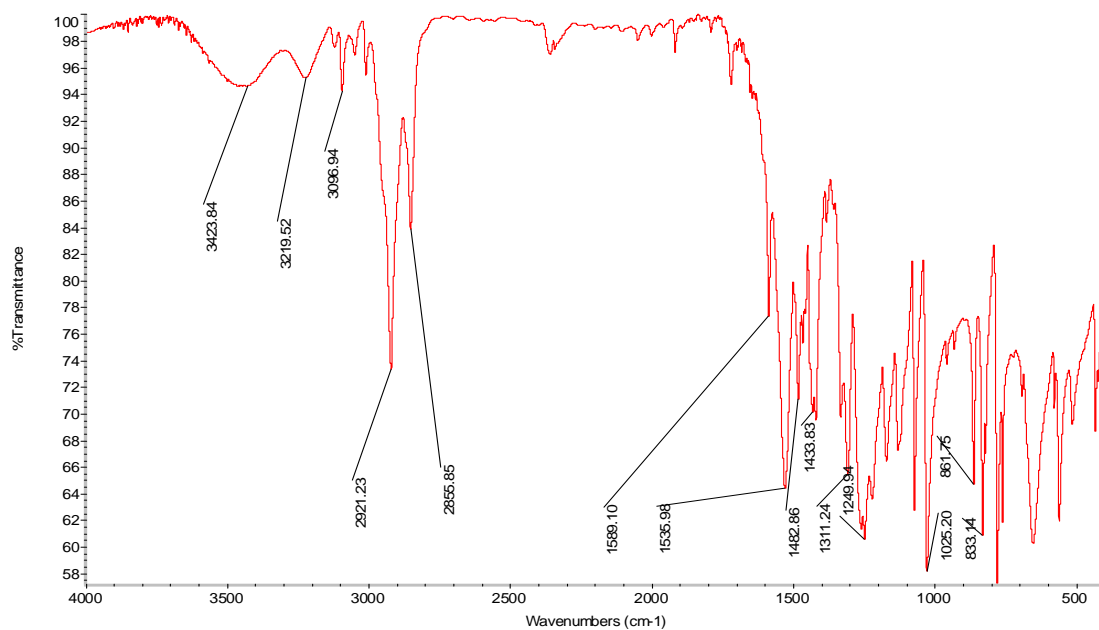


Figure S18. IR of 4-Methoxy-2-nitrophenol

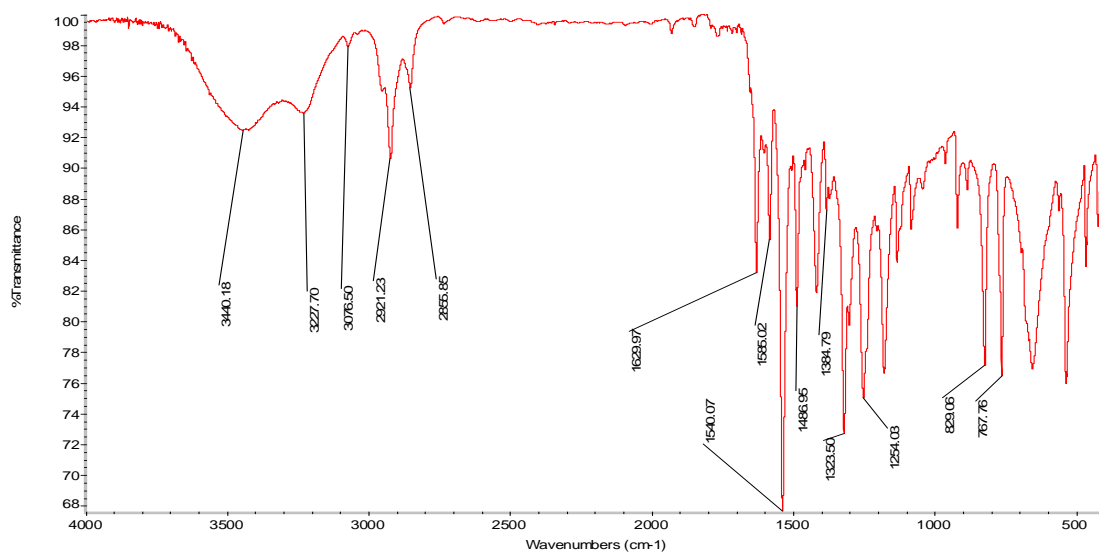


Figure S19. IR of 4-Methyl-2-nitrophenol

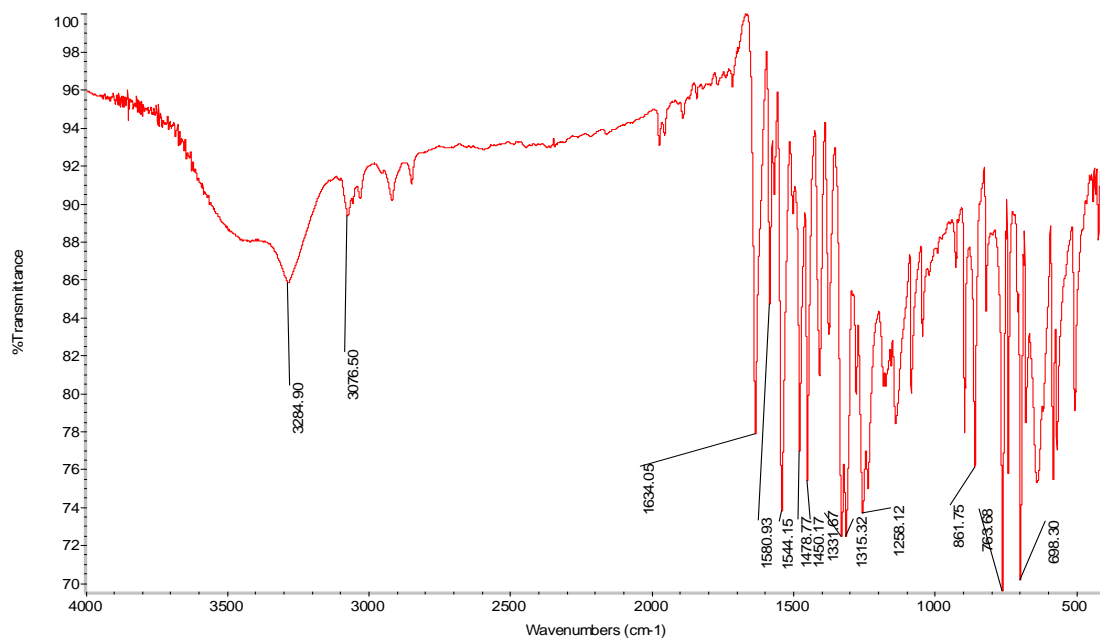


Figure S20. IR of 4-Phenyl-2-nitrophenol

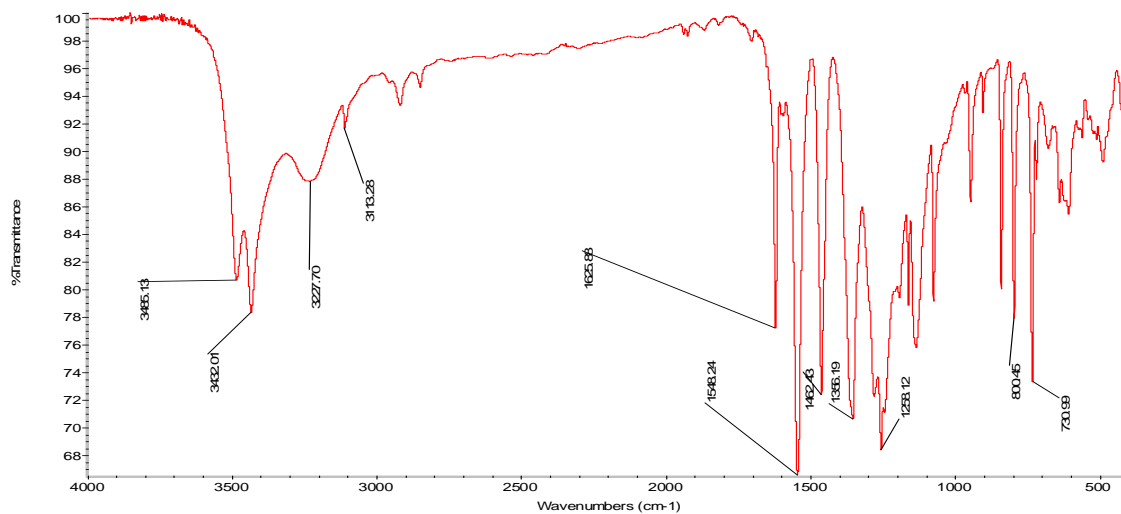


Figure S21. IR of 3-nitro-1,2-benzenediol

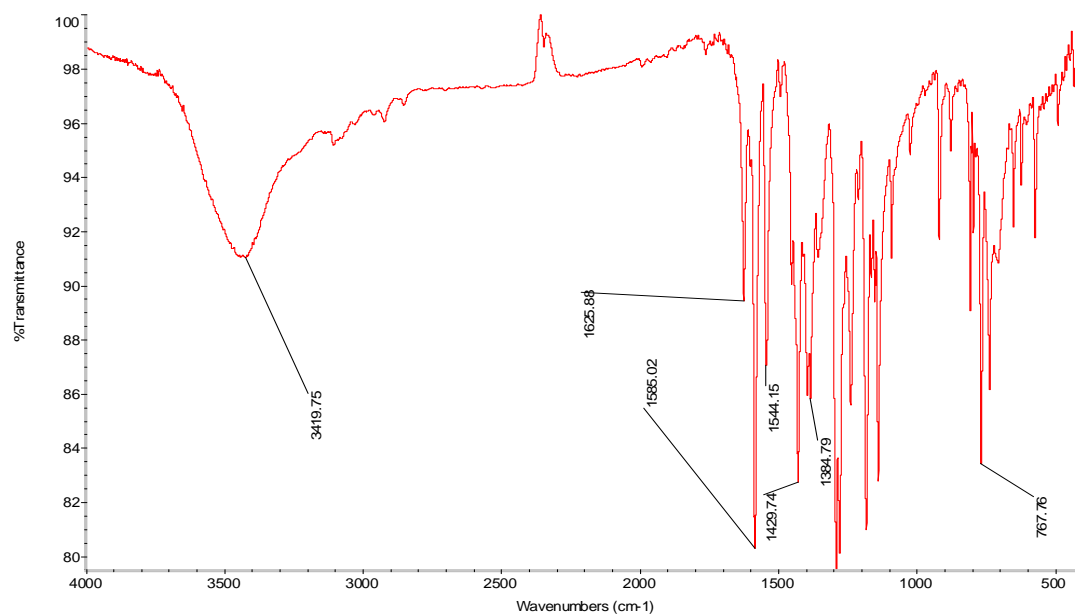


Figure S22. IR of 2-Nitro-1-naphthol

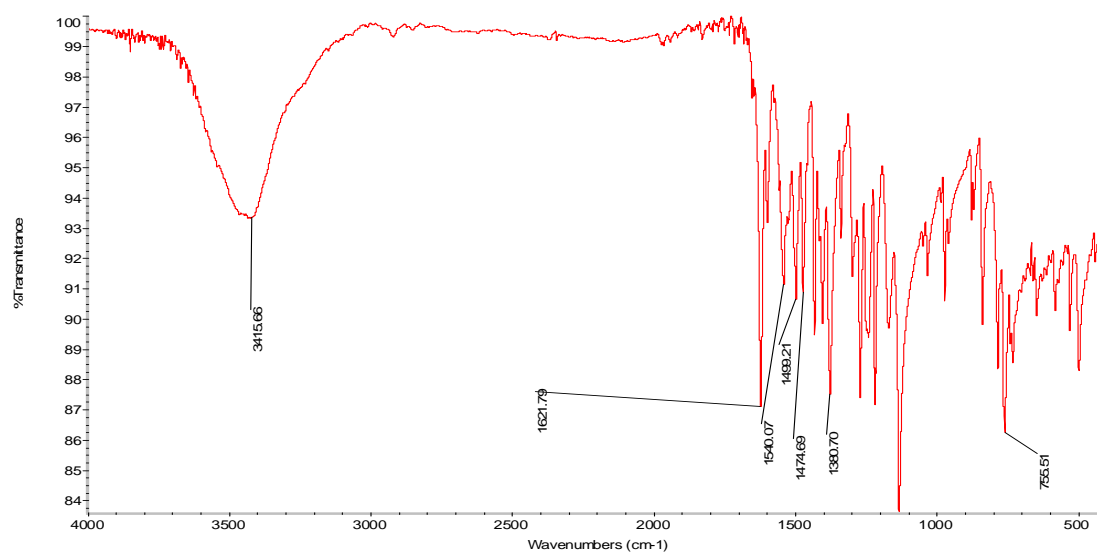


Figure S23. IR of 1-Nitro-2-naphthol

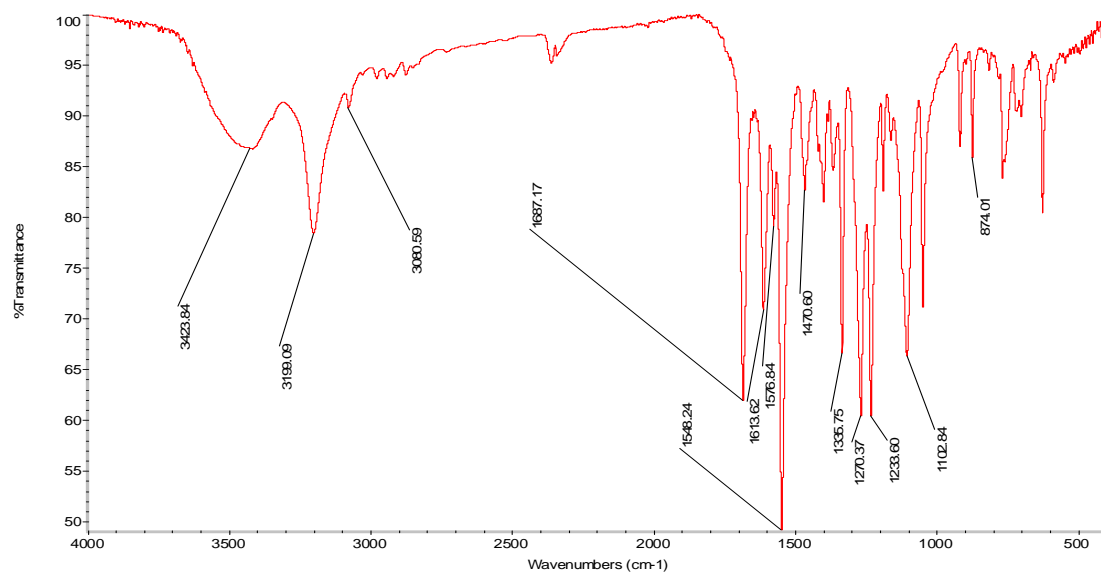


Figure S24. IR of 3-Nitro-4-hydroxy-5-methoxybenzaldehyde