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2-[6-(2-Hydroxyphenyl)-1,2,4,5-tetrazin-3-yl]phenol

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Hydrazine hydrate (99%, 5g, 100 mmol) was added to a solution of 2-cyanophenol (2 g, 16.8 mmol) in absolute ethanol (30 ml) under N₂ atmosphere, and the reaction mixture was refluxed for 12 h. During the course of the reaction, the color of the solution changed to yellow, and the yellow precipitate, 2-[6-(2-hydroxyphenyl)-1,4-dihydro-1,2,4,5-tetrazin-3-yl]phenol, produced was readily oxidized in air to 2-[6-(2-hydroxyphenyl)-1,2,4,5- tetrazin-3-yl]phenol (0.9 g, 40% yield), deep red crystals obtained from recrystallization from tetrahydrofuran.

¹H-NMR (300MHz, CDCl₃, d_{ppm}, J_{Hz}): 10.88 (2H, s), 8.66 (2H, d, J=8.1), 7.55 (2H, dd, J=7.2, 5.2), 7.16 (2H, d, J=7.2), 7.13 (2H, dd, J=8.2, 5.2).

IR (KBr, cm⁻¹): 523 (m), 560 (w), 590 (w), 681 (s), 713 (s), 744 (s), 838 (m), 875 (w), 948 (m), 1029 (w), 1050 (m), 1094 (m), 1127 (w), 1155 (m), 1233 (s), 1273 (w), 1331 (w), 1386 (s), 1418 (s), 1472 (m), 1485 (s), 1577 (s), 1616 (s), 3119 (m).

UV-Vis (in CH₃CN): 295 (e = $2.14 \times 104 \text{ mol}^{-1}\text{cm}^{-1}$), 355 (e = $1.86 \times 104 \text{ mol}^{-1}\text{cm}^{-1}$) and 534 nm (e = $3.96 \times 102 \text{ mol}^{-1}\text{cm}^{-1}$).

FAB-MS [M+]: 266.

Calcd: C, 63.15; H, 3.79; N, 21.04 %. Found: C, 63.0; H, 3.8; N, 21.1 %.

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