

Molecularly-Imprinted Polymeric Logic Gates Selective for Predetermined Input Chemical Species

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1) Preparation and assessment of the polymeric logic gates, P-AND and P-OR

A typical preparation procedure for P-AND: to methanol (2.5 mL) and chloroform (6.7 mL) were added 4-vinylpyridine (4.0 mmol), styrene (40 mmol), divinylbenzene (40 mmol), cobalt(II) acetate (2.0 mmol), 4,4,4-trifluoro-1-(2-naphthyl)-1,3-butanedione (TFNB) (2.0 mmol), and azobisisobutyronitrile (AIBN) (100 mg). After sparging with nitrogen gas, the mixture was placed in a water bath at 60 °C for 24 h. The resultant bulk polymer (P-AND) was ground in a mortar, sieved and packed in a stainless-steel column (50 x 4.6 mm, i.d.). The column was washed with methanol - acetic acid (8:2, v/v) and then with methanol.

A typical preparation procedure for P-OR: to chloroform (25 mL) were added methacrylic acid (4.94 mmol), 2-trifluoromethylacrylic acid (4.94 mmol), ethylene glycol dimethacrylate (69 mmol), cinchonidine (1.28 mmol), cinchonine (1.28 mmol), and azobisisobutyronitrile (AIBN) (100 mg). After sparging with nitrogen gas, the mixture was placed in a water bath at 60 °C for 24 h. The resultant bulk polymer (P-OR) was treated identically to P-AND, and subjected to chromatographic assessments.

Chromatographic assessments: Chromatography was conducted using a Waters HPLC system. For P-AND, methanol was used as an eluent with or without 1.0 mM of cobalt(II) acetate. For P-OR, acetonitrile, water, and acetic acid (90:5:5, v/v/v) were used as an eluent. The flow rate was 1.0 mL min⁻¹, and the detection by UV absorbance was at 255 nm (P-AND) and 280 nm (P-OR). The sample concentration was 0.5 mM, and its size was 20 μL.

Fluorescence spectra-based assessments: Fluorescence spectra of P-AND and P-OR were measured using a Hitachi spectrophotometer FP-4500. Fine particles (< 20 μm) of the polymers were incubated for 12 h with the corresponding input species (100 μM) in methanol-chloroform (P-AND) and chloroform (P-OR). After incubation, the polymer particles were filtered, dried and suspended with paraffin oil in a quartz cell (10 x 10 mm).

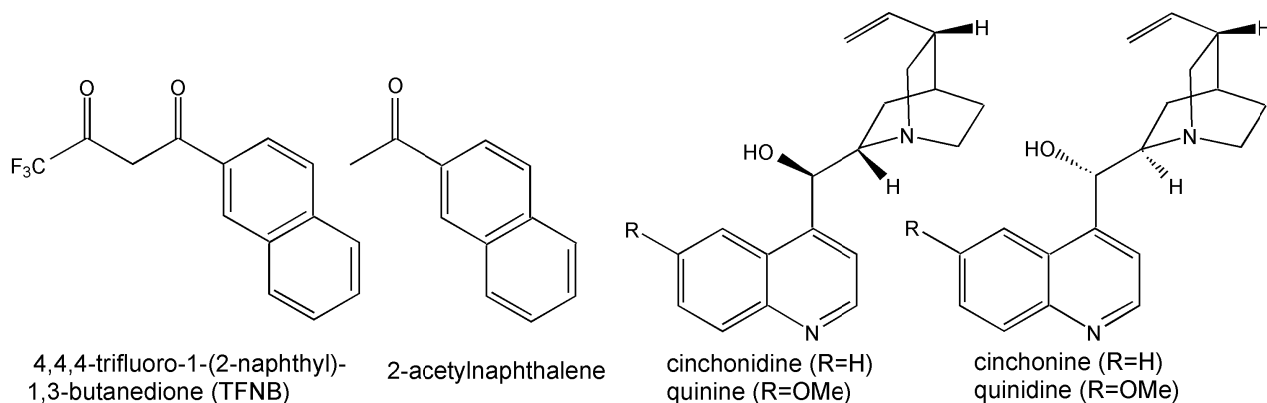


Fig. 1S Structures of the template molecules (input species) and fake input species.