Supplementary Information

6.1 NMR probe design

A custom designed NMR probe was employed featuring the integration of all subassemblies and providing the external connections for fluidics and NMR signal lines. The diameter was constrained by the MR unit, a 500 MHz wide bore system (Bruker) with a bore diameter of 72.9 mm. To provide flexibility for the fluidic interconnections we integrated a feedthrough system that enabled the integration of tubings of variable diameters and established the connections of the micro-detector with the external control and supply components. The probe was equipped with the required mechanical, electrical and fluidic connections to accommodate a commercial 3-axis micro gradient system. For final experimental installation, the gradient was slipped over the probe head and a tight mechanical locking mechanism ensured the rigid mounting of the probe head to the probe. The interface for the exchangeable NMR probe head provided the contacts for the ¹H RF channel. The probe was equipped with two additional high quality air trimmer capacitors (TG 092 Temex-Ceramics) that established a low loss interface between the 50 Ω transmission line and the RF resonator. A non-conducting glass fibre rod was mounted on each trimmer capacitor which enabled to conduct a final tuning and matching procedure once the final assembly was mounted into the MR scanner.

6.2 SABRE catalyst synthesis



Mes= 2,4,5-trimethylbenzene

Fig. 6 Reagents and conditions: (i) 1,3-bis(2,4,6-trimethylphenyl)-imidazol-2-ylidene, THF, r.t., 24 h

The SABRE catalyst used in this work is Ir(1,5-cyclooctadiene) (1,3-bis (2,4,6- trimethylphenyl) imidazolium) Cl (MW = 639.67 g/mol), in short 'Ir-IMes'. All starting materials and reagents were obtained from Sigma Aldrich and used as received. ¹H NMR and ¹³C NMR spectra were obtained using a Bruker spectrometer operating at 400 MHz. Chemical shifts are reported in ppm with the residual solvent peak as an internal standard.

315 mg (0.47 mM) of $[Ir(cod)Cl]_2$ was dissolved in 1 mL of THF. In a separate vial, 320 mg (1.05 mM) of 1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene was prepared in 7 mL of THF. This solution was mixed during a 5-minute period. The colour of the solution became dark orange. The reaction was stirred for 12 hours at room temperature under ambient condition. The solvent was removed by rotary vaporisation. The product was crystallised using 10 mL of absolute ethanol. The orange solid obtained (250 mg, 40%) was rinsed using 3 mL of hexane. ¹H NMR (400 MHz, MeOD-d₄) δ : 7.12 (d, 4H, Ar H), 6.92 (s, 2H, -NCHCHN-), 3.89 (m, 2H, COD CH), 2.97 (m, 2H, COD CH), 2.25 (s, 12H, Ar 2-Me), 2.18 (s, 6H, Ar 4-Me), 1.5-1.63 (m, 4H, COD CH2), 1.12-1.27 (m, 4H, COD CH2). ¹³C NMR (400 MHz, MeOD-d₄) δ : 136.08, 128.69, 125.70, 110.21, 103.99, 101.25, 100.81, 95.02, 55.81, 49.96, 16.98.

Sample insert example. Unmounted. (sealed off area in red)



Sample insert mounted inside the Helmholtz pair detector



Sample insert mounted and clamped to the fluidic connectors





Fig. 7 Top: Single scan, full ¹H-NMR spectra for a concentration series used in bulk solution SABRE chemosensing experiments. Bottom: close-up view of the unshielded region.



Fig. 8 Top: 128-scan, full ¹H-NMR spectra for a concentration series used in SABRE chemosensing experiments using the micro-polariser presented in this contribution. Bottom: close-up view of the unshielded region. Only *mtz* peaks are visible above the background.