Recognition of C$_{60}$ by Tetra- and Tri-Quinoxaline Cavitands

Francesco P. Ballistreri,*a Giovanna Brancatelli,b Nicola Demitri,c Silvano Geremia,b Dirk M. Guldi,d Michele Melchionna,b Andrea Pappalardo,a,c Maurizio Prato,b Gaetano A. Tomaselli,a Giuseppe Trusso Sfrazetto*·a

a Dipartimento di Scienze Chimiche, Università di Catania, Viale Andrea Doria 6, 95125 Catania, Italy

b Dipartimento di Scienze Chimiche e Farmaceutiche, Centro di Eccellenza in Biocristallografia, Università di Trieste, Via L. Giorgieri 1, Trieste, Italy

c Elettra - Sincrotrone Trieste, S. S. 14 Km 163.5 in Area Science Park, Basovizza, Trieste, Italy

d Department of Chemistry and Pharmacy and Intersciplinary Center for Molecular Materials, Friedrich-Alexander Universität Erlangen-Nürnberg, 91058, Erlangen, Germany

e I.N.S.T.M. UdR of Catania, Viale A. Doria 6, 95125 Catania, Italy

Supplementary Material
$^1$H NMR spectrum of **Octol** in acetone-$d_6$ (500 MHz, 27° C)

ESI-MS spectrum of **Octol**
$^1$H NMR spectrum of 1 in CDCl$_3$ (500 MHz, 27° C)

ESI-MS spectrum of 1
\textsuperscript{1}H NMR spectrum of 2 in CDCl\textsubscript{3}(500 MHz, 27\textdegree C)

ESI-MS spectrum of 2
Room temperature absorption spectra of cavitand 1 (2.14 × 10^{-5} M) in toluene as solvent upon adding variable concentration of C_{60} (0.21 × 10^{-5} – 3.21 × 10^{-5} M).

Room temperature absorption spectra of cavitand 2 (2.61 × 10^{-5} M) in toluene as solvent upon adding variable concentration of C_{60} (0.26 × 10^{-5} – 5.22 × 10^{-5} M).
$^1$H NMR stack plot of the signal decay (toluene-$d_8$, 1 mM, 298 K) as a function of the gradient strength (D) for the cavitand 1.

Fitting for the diffusion constant derived from the signal decays for the cavitand 1 (toluene-$d_8$, 1 mM, 298 K).
$^1$H NMR stack plot of the signal decay (toluene-$d_8$, 1 mM, 298 K) as a function of the gradient strength (D) for the supramolecular complex 1:1 between 1 and C$_{60}$.

Fitting for the diffusion constant derived from the signal decays for the supramolecular complex 1:1 between 1 and C$_{60}$ (toluene-$d_8$, 1 mM, 298 K).
EI-MS spectrum of the supramolecular complex 1:1 between 1 and C₆₀
Fluorescence titration between cavitand 1 and C$_{60}$

HypSpec output file:
Converged in 4 iterations with sigma = 0.078816

Log beta  value  stand. dev.
AB  5.2387  0.1422

Fluorescence titration between cavitand 2 and C$_{60}$

HypSpec output file:
Converged in 4 iterations with sigma = 0.095619

Log beta  value  stand. dev.
AB  4.9518  0.1424