Extremely effective separations of pyridine/picoline mixtures through supramolecular chemistry strategies employing (4*R*,5*R*)-bis(diphenylhydroxymethyl)-2-spiro-1'-cyclohexane-1,3-dioxolane as the host compound

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TADDOL6 NMR spectra

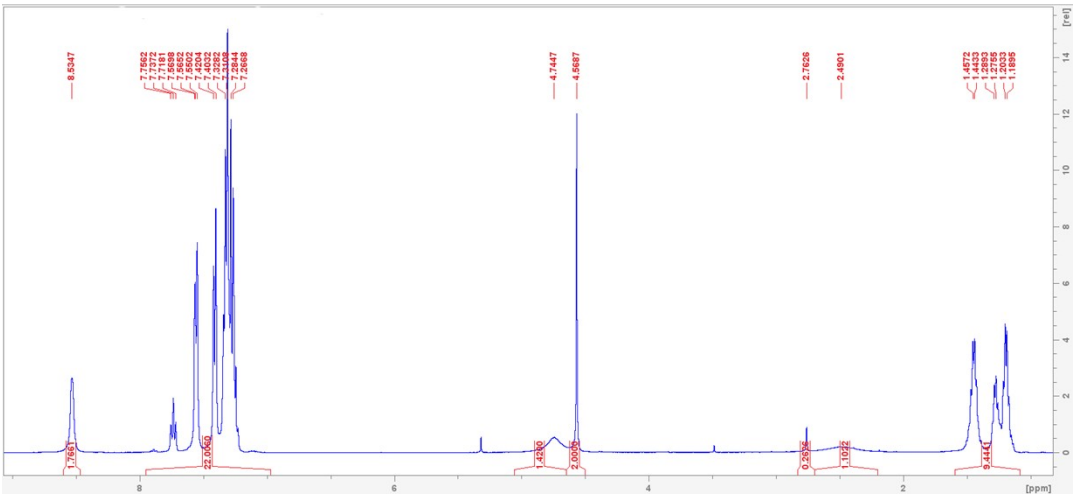


Figure S1 ^{1}H-NMR spectrum for equimolar binary PYR/2MP.

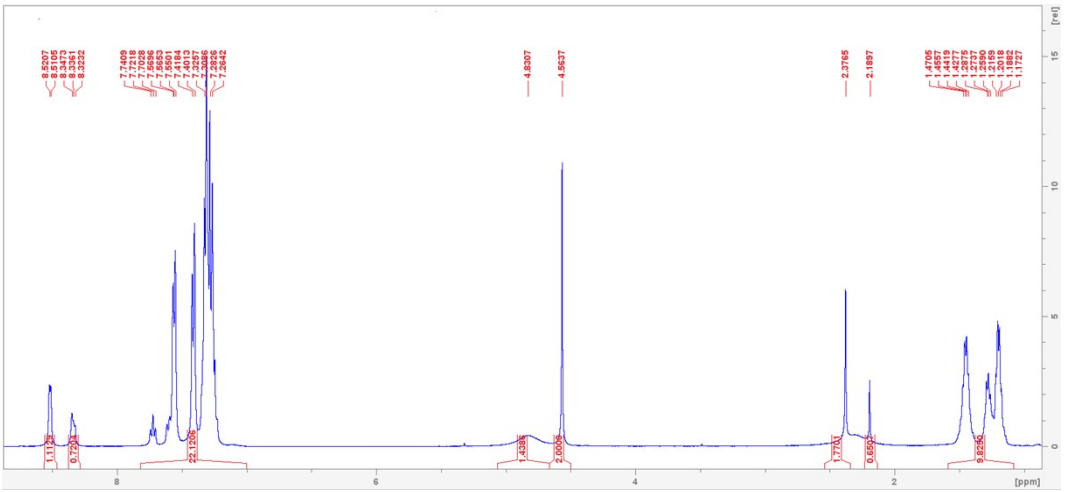


Figure S2 ^{1}H-NMR spectrum for equimolar binary PYR/3MP.

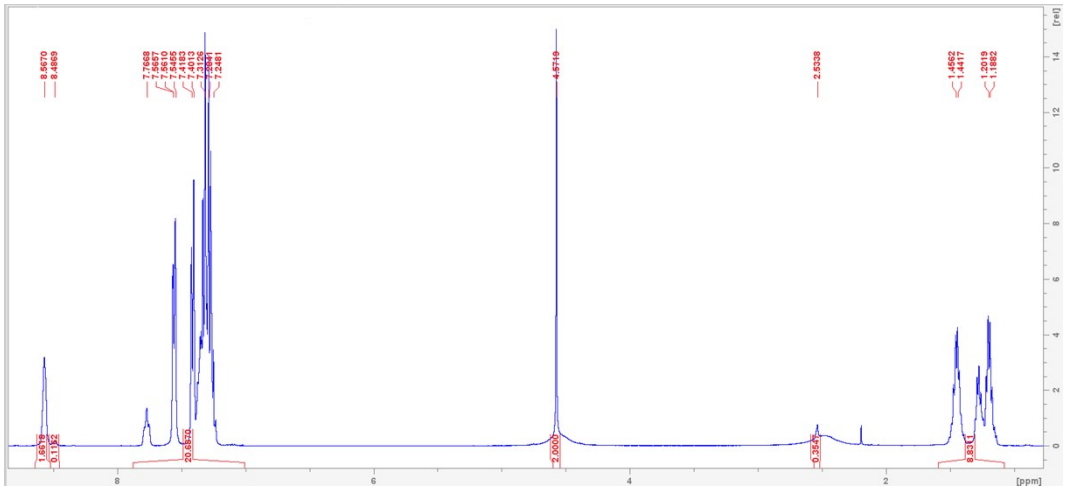


Figure S3 ^{1}H-NMR spectrum for equimolar binary PYR/4MP.

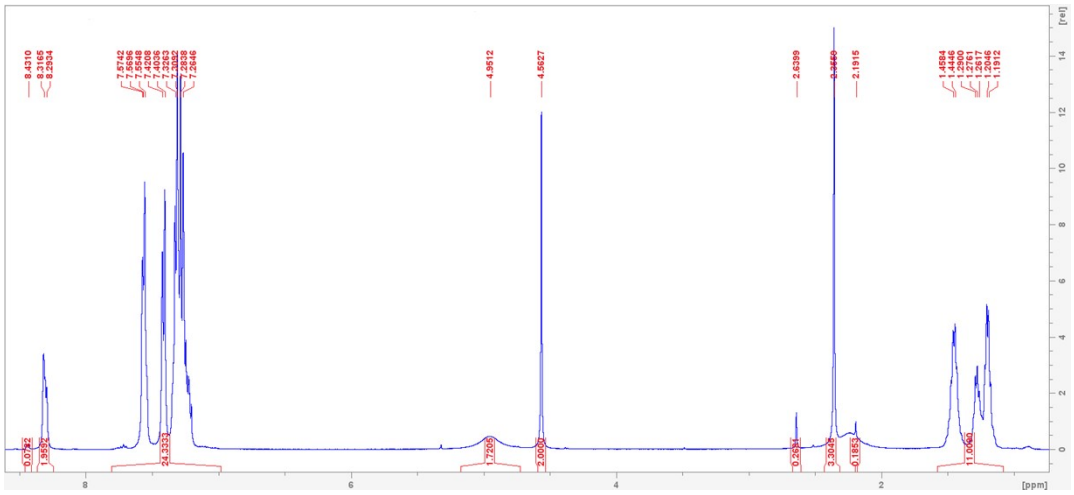


Figure S4 ^{1}H-NMR spectrum for equimolar binary 2MP/3MP.

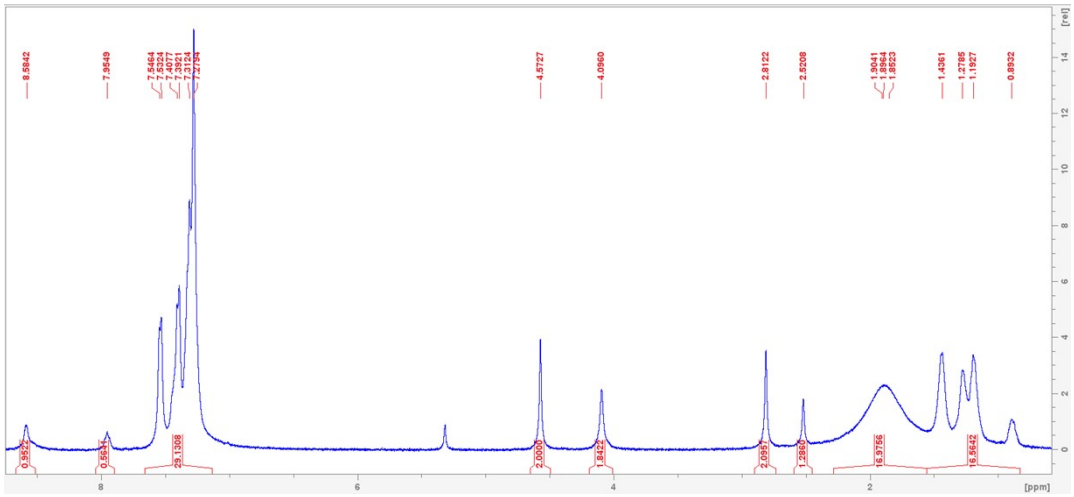


Figure S5 ^{1}H-NMR spectrum for equimolar binary 3MP/4MP.

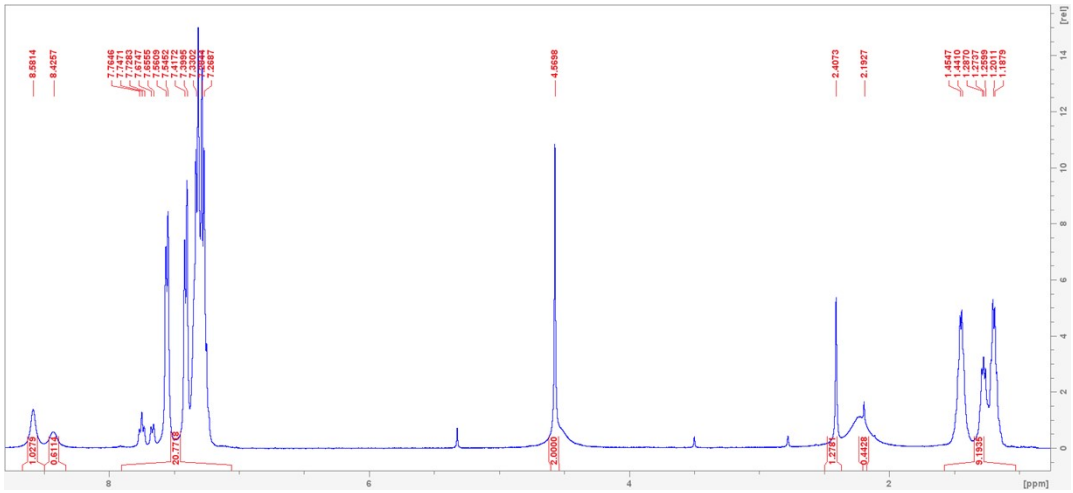


Figure S6 ^{1}H-NMR spectrum for equimolar ternary PYR/2MP/3MP.

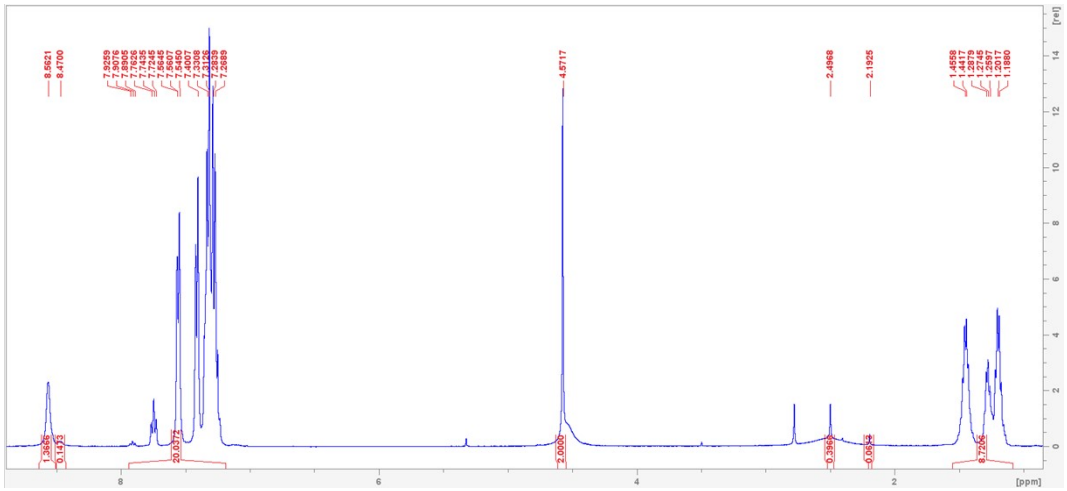


Figure S7 ^{1}H-NMR spectrum for equimolar ternary PYR/2MP/4MP.

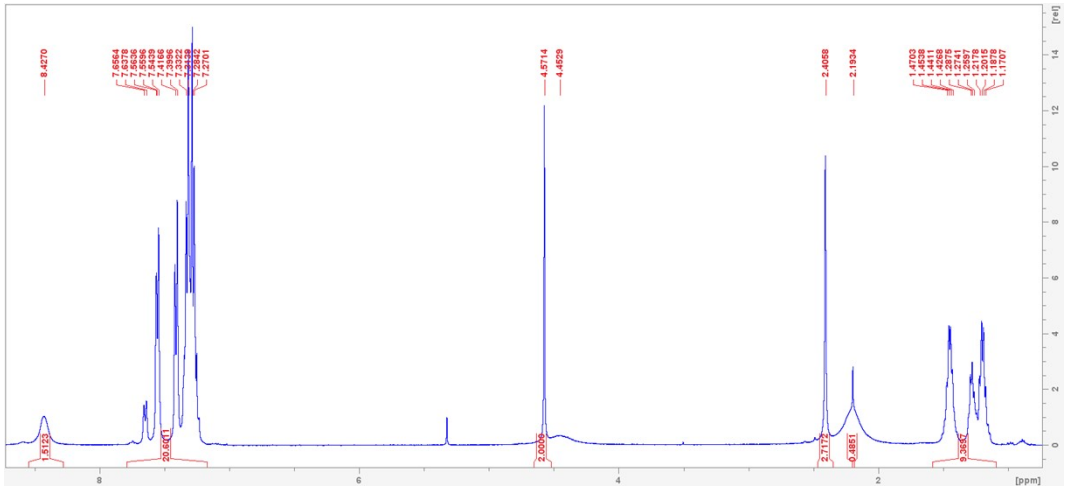


Figure S8 ^{1}H-NMR spectrum for equimolar ternary PYR/3MP/4MP.

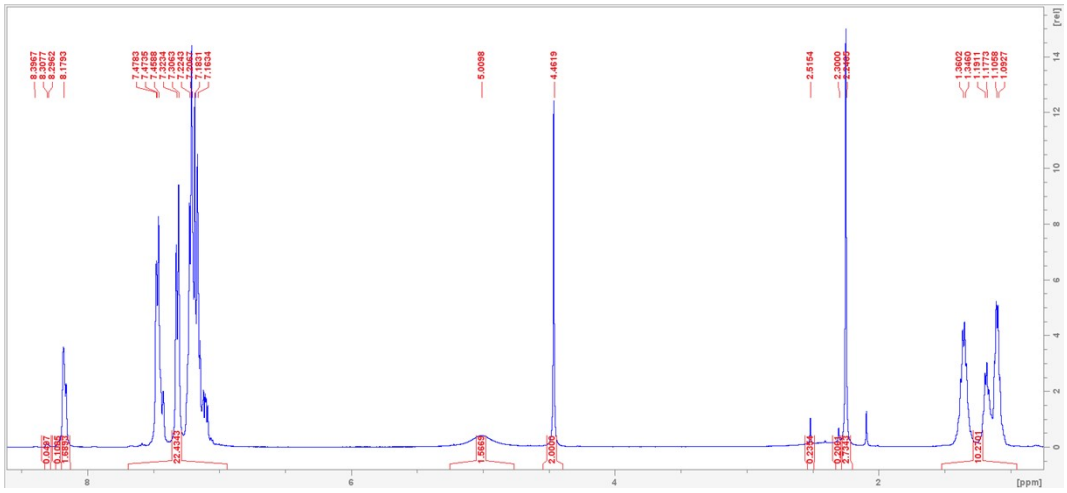


Figure S9 ^{1}H-NMR spectrum for equimolar ternary 2MP/3MP/4MP.

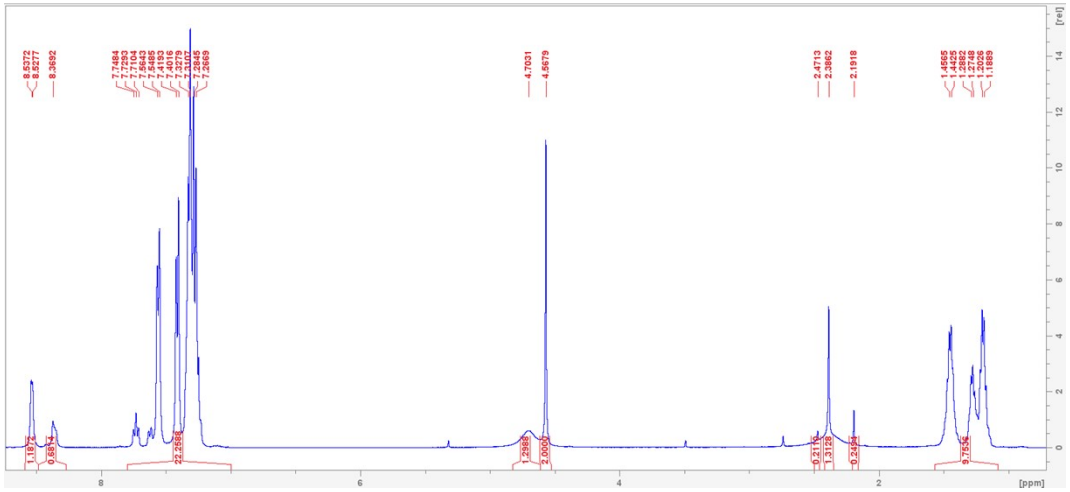
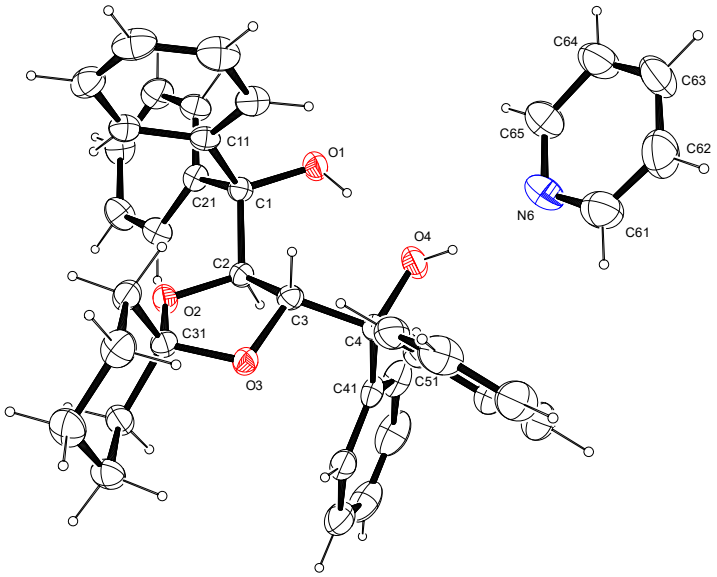
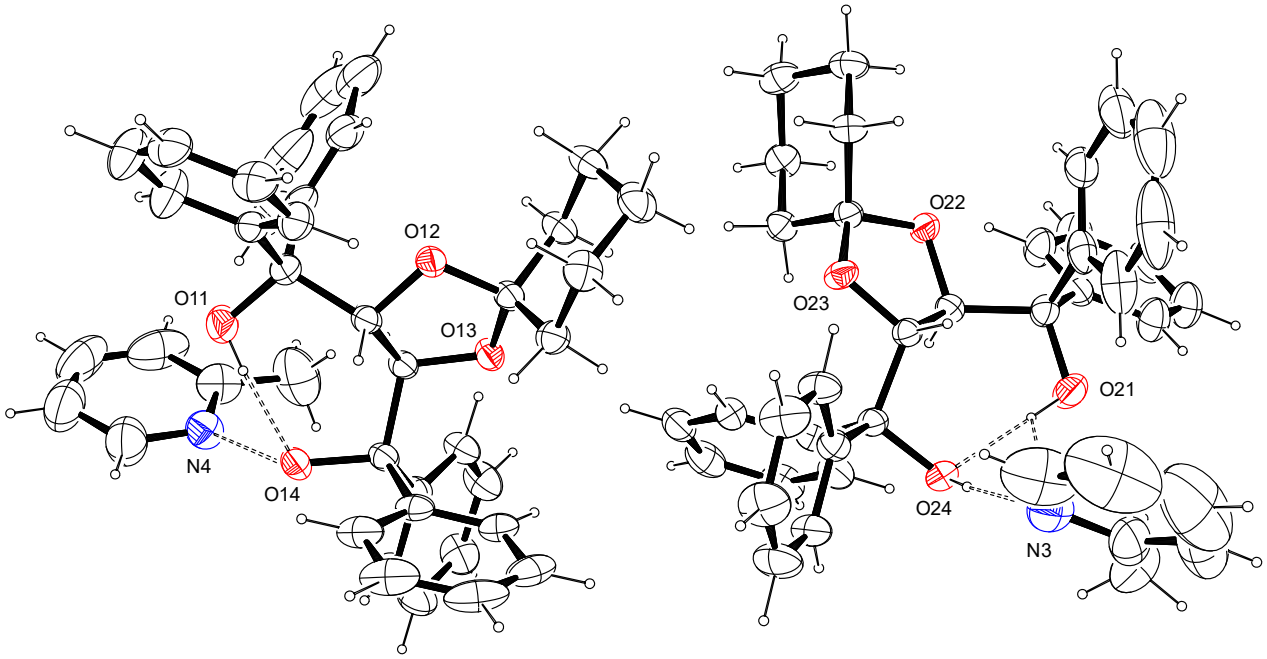


Figure S10 ^{1}H-NMR spectrum for equimolar quaternary PYR/2MP/3MP/4MP.

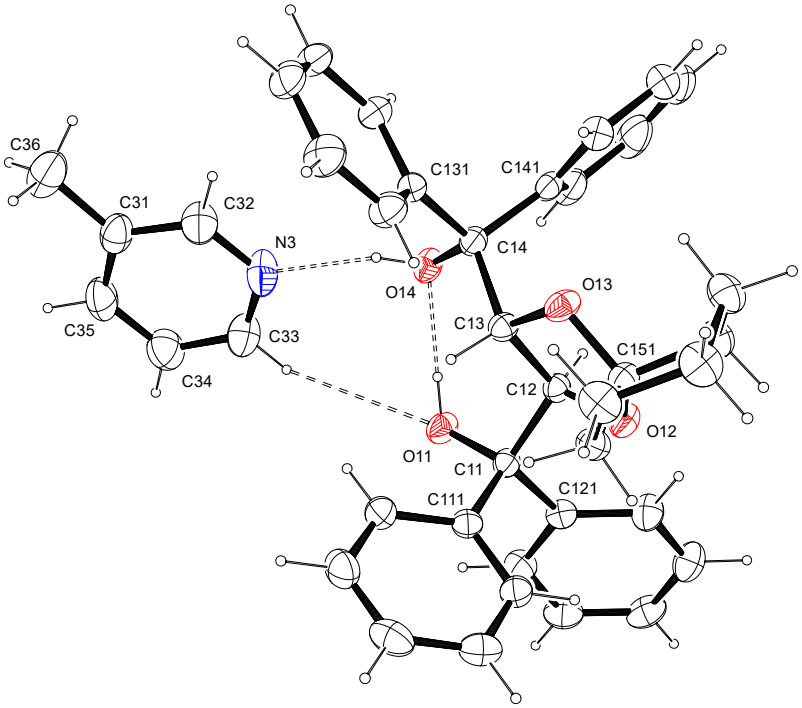
a)


C64
C63
C65
C62
N6
C61
C11
O1
C21
C1
O4
C2
O2
C3
C31
C4
O3
C41
C51

b)


O12
O11
O13
N4
O14
O22
O23
O21
O24
N3

c)



d)

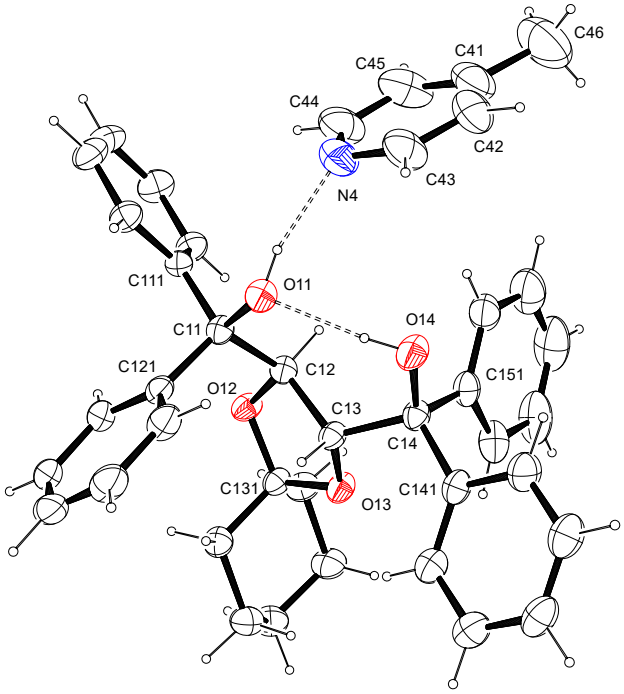


Figure S11 ORTEP diagrams for (a) TADDOL6·PYR, (b) TADDOL6·2MP, (c) TADDOL6·3MP and (d) TADDOL6·4MP.

Table S1 The (host)π···π(guest) stacking interactions, slippages and symmetry codes for complexes

Parameter	TADDOL6·PYR	TADDOL6·2MP	TADDOL6·3MP	TADDOL6·4MP
(host)π···π(guest)/Å	3.622(1)	-	3.735(1) 3.729(1)	-
(host) π···π (guest) slippage/Å	1.194	-	1.770 1.216	-
Symmetry codes	1+x, y, z	-	-1+x. y, z -1+x, y, z	-

TADDOL6·PYR, TADDOL6·2MP, TADDOL6·3MP an TADDOL6·4MP.

Table S2 The (host)H···π(guest) and (host)C–H···π(guest) interactions, the (host)C–H···π(guest) angles and the

Parameter	TADDOL6·PYR	TADDOL6·2MP	TADDOL6·3MP	TADDOL6·4MP
(host) H···π (guest)/Å	2.965 2.747	-	2.891	-
(host) C–H···π (guest)/Å	3.648(3) 3.639(3)	-	3.645(3)	-
(host) C–H···π (guest)/°	130 157	-	144	-
Symmetry codes	x, y, z -½+x, ½-y, 1-z	-	x, 1+y, 1+z	-

symmetry codes for complexes TADDOL6·PYR, TADDOL6·2MP, TADDOL6·3MP an TADDOL6·4MP.

Table S3 The (host)H···N(guest) and (host)O···N(guest) interactions, the (host)O–H···N(guest) angles and the

Parameter	TADDOL6·PYR	TADDOL6·2MP	TADDOL6·3MP	TADDOL6·4MP
(host)H···N(guest)/Å	1.91	1.88 1.78[a] 2.03[b]	1.87 1.88	1.91 1.91
(host)O···N(guest)/Å	2.713(3)	2.701(3) 2.564(8)[a] 2.791(4)[b]	2.660(3) 2.668(3)	2.730(3) 2.749(3)
(host)O–H···N(guest)/°	160	165 155[a] 151[b]	155 155	166 174
Symmetry codes	x, y, z	x, y, z	x, y, z	x, y, z
(host)H···O(host)[c]/Å	1.85	1.83 1.85	1.82 1.83	1.86 1.86
(host)O···O(host)[c]/Å	2.688(2)	2.664(3) 2.686(3)	2.663(2) 2.667(2)	2.749(2) 2.686(2)
(host)O–H···O(host)[c]/°	173	176 171	177 176	169 169

symmetry codes for complexes TADDOL6·PYR, TADDOL6·2MP, TADDOL6·3MP an TADDOL6·4MP.