1-Phenyl-3-(quinolin-5-yl)urea as a host for distinction of phthalic acid and terephthalic acid

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Abstract. Co-crystals of 1-phenyl-3-(quinolin-5-yl)urea (**1**) with terephthalic acid, adipic acid; and salts of **1** with phthalic acid, *p*-toluenesulphonic acids are prepared and structurally characterized. The reaction of phthalic acid and *p*-toluenesulphonic acid resulted in protonation of the host **1**, whereas the terephthalic acid and adipic acid interact with **1**, led to cocrystals with the host **1** through hydrogen bond interactions. The hydrogen bonds that appears in the urea taps of the host molecules **1** are lost while formation of salts; in such cases anions interacts with the urea portion of the host, while in the co-crystals the hydrogen bonded urea taps are retained. The salts are yellow in colour while the co-crystals are colourless; thereby the positional isomer phthalic acid can be distinguished from the terephthalic acid.

Keywords. 1-Phenyl-3-(quinolin-5-yl)urea; hydrogen bond; co-crystal; salt; visual distinction.

1. Introduction

The anion recognition property of urea derivatives are well-known in both in solid and in solution state.[1–5] Hosts having urea motif are useful for selective binding of carboxylic acids such as dibutylmalonic acid.[6] Owing to their versatile biological applications, design and synthesis of hosts for selective binding of carboxylic acids have gained interest in recent time.[7–12] There are several examples of hosts for dicarboxylic acids and their binding properties are explored in details.[13–22] Troger's base analogues have been reported to recognize dicarboxylic acids with different chain lengths.[23–28] Recently, it is shown that dicarboxylic acids form salts and co-crystals with pyridine hosts depending on the orientation of the acid groups.[29–35] Further to this conformational change in dicarboxylic acid by hosts have practical applications in memory devices.[36,37] Binding of the carboxylic acids to nitrogen containing hosts have great diversity[37,38] and upon such binding also leads to changes in the physical properties from the parent compounds.[38] We have shown that urea derivative 1-phenyl-3-(quinolin-5-yl)urea (**1**) is a good host in recognizing the *cis* and *trans* unsaturated acids.[39] In this report, we discuss structural features of salt and cocrystals of **1** with rigid and flexible carboxylic acids (scheme 1) and about visual distinction

of two positional isomers phthalic acid and terephthalic acid by this host.

2. Experimental

2.1 *Synthesis of 1-phenyl-3-(quinolin-5-yl)urea (**1**)*

5-Aminoquinoline (0.721 g, 5 mmol) was dissolved in dry dichloromethane (10 mL) and to this solution another solution of phenylisocyanate (0.54 mL, 5 mmol) in dichloromethane was added drop-wise and the mixture was stirred at room temperature for 3 h. The product formed was filtered and recrystallized from methanol. Yield: 78%. IR (KBr, cm^{-1}): 3280 (s), 3062 (m), 1641 (s), 1599 (s), 1557 (s), 1493 (s), 1449 (m), 1315 (m), 1249 (s), 1091 (w), 799 (m), 748 (m), 694 (m). ^{1}HNMR (DMSO-d_6, 400 MHz, ppm): 8.8 (3H, m), 8.4 (1H, d, J = 8.8 Hz), 8.0 (1H, d, J = 7.2 Hz), 7.6 (2H, m), 7.4 (3H, m), 7.2 (2H, m), 7.0 (1H, t, J = 7.2 Hz). ^{13}C NMR(DMSO-d_6, 100 MHz, ppm): 118.3, 118.9, 121.4, 121.9, 122.7, 124.5, 129.5, 130.1, 130.8, 135.4, 140.2, 148.8, 150.9, 153.5. LC-MS [M + 1]: 264.13.

2.2 *Synthesis of the salts and co-crystals of **1***

The compound **1** and the dicarboxylic acids (1:1) were dissolved in aqueous methanol. Slow evaporation of the solution results in colourless crystals of the co-crystals whereas in case of salts yellow coloured crystals were observed.

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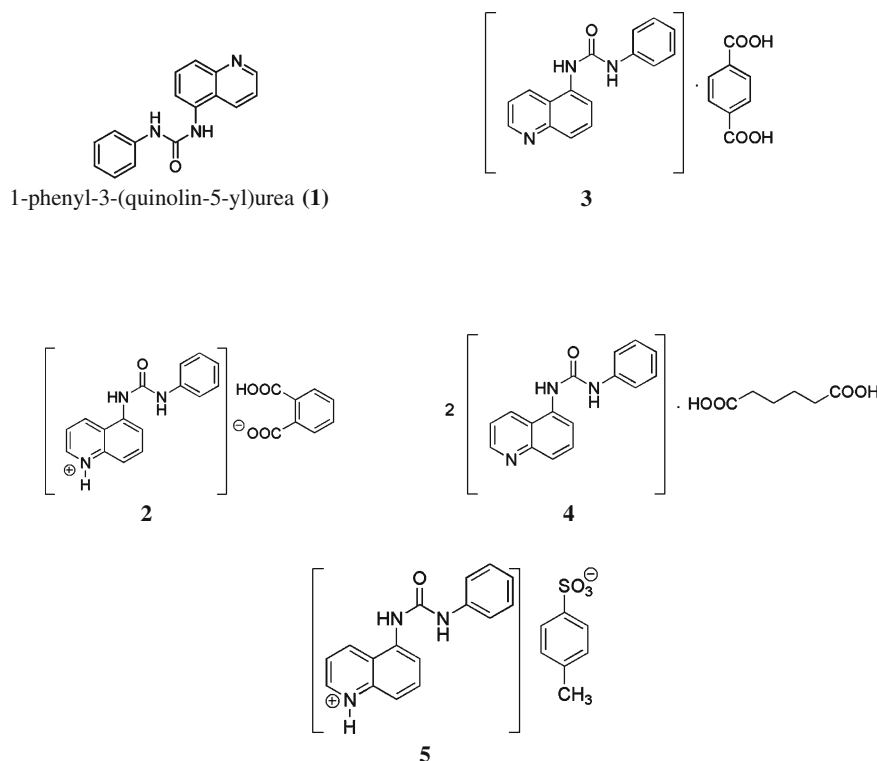
Scheme 1. The host and its salts and cocrystals.

2.2a *Salt of 1 with phthalic acid*: Isolated Yield: 69%. IR (KBr, cm^{-1}): 3444 (w), 2924 (w), 1695 (s), 1587 (m), 1535 (m), 1406 (m), 1284 (s), 1072 (m), 737 (m). ^{1}HNMR (DMSO-d_6, 400 MHz, ppm): 9.0 (1H, s), 8.9 (2H, m), 8.5 (1H, d, J = 7.6 Hz), 8.0 (2H, m), 7.6 (5H, m), 7.5 (3H, m), 7.3 (2H, d, J = 7.6 Hz), 7.0 (1H, d, J = 6.8 Hz). UV-vis {methanol, nm(ε)} 320 (1.3 × 10^4 cm^{-1}mol^{-1}); 400 (6 × 10^3 cm^{-1}mol^{-1}).

2.2b *Co-crystal of 1 with terephthalic acid*: Isolated Yield: 67%. IR (KBr, cm^{-1}): 3444 (w), 3266 (s), 2925(w), 1698 (s), 1637 (s), 1599 (s), 1562 (s), 1496 (m), 1275 (s), 1253 (m), 807 (m), 729 (m). ^{1}HNMR (DMSO-d_6, 400 MHz, ppm): 9.0 (1H, s), 8.9 (2H, m), 8.5 (1H, d, J = 8.8 Hz), 8.0 (5H, m), 7.7 (2H, m), 7.6 (1H, m), 7.5 (2H, d, J = 7.6 Hz), 7.3 (2H, t, J = 7.2 Hz), 7.0 (1H, t, J = 7.2 Hz). UV-vis {methanol, nm(ε)} 320 (1.6 × 10^4 cm^{-1}mol^{-1}).

2.2c *Co-crystal of 1 with adipic acid*: Isolated Yield: 74%. IR (KBr, cm^{-1}): 3436 (w), 3270 (s), 2945 (w), 1716 (s), 1639 (s), 1598 (s), 1561 (s), 1496 (m), 1258 (m), 1173 (m), 805 (m). ^{1}HNMR (DMSO-d_6, 400 MHz, ppm): 9.0 (1H, s), 8.9 (2H, m), 8.5 (1H, d, J = 8.4 Hz), 8.0 (1H, d, J = 6.8 Hz), 7.7 (2H, m), 7.6 (1H, m), 7.5 (2H, d, J = 8.0 Hz), 7.3 (2H, t, J = 8.0 Hz), 7.0 (1H, t, J = 7.2 Hz), 2.2 (2H, m), 1.5 (2H, m).

2.2d *p-Tolunesulphonate salt of 1*: The compound **1** and *p*-tolunesulphonic acids (1:1) were dissolved in aqueous methanol. Slow evaporation of the solution results in yellow coloured crystals of salt **5**. Isolated yield: 64%. IR (KBr, cm^{-1}): 3291 (w), 2922 (w), 1708 (s), 1637 (m), 1600 (m), 1539 (s), 1417 (m), 1366 (m), 1212 (s), 1165 (m), 1126 (m), 1033 (m), 1009 (m), 795 (m). ^{1}HNMR (DMSO-d_6, 400 MHz, ppm): 9.4 (1H, s), 9.2 (2H, m), 8.2 (1H, d, J = 7.6 Hz), 8.0 (2H, m), 7.8 (1H, d, J = 8.0 Hz), 7.5 (5H, m), 7.3 (2H, m), 7.1 (2H, d, J = 7.6 Hz), 7.0 (1H, t, J = 7.2 Hz), 2.2 (3H, s).

2.3 *X-ray crystallographic studies*

Diffraction data for compounds were collected at 296 K with Mo Kα radiation (λ = 0.71073 Å) using a Bruker Nonius SMART APEX CCD diffractometer equipped with graphite monochromator and Apex CD camera. The *SMART* software was used for data collection and also for indexing the reflections and determining the unit cell parameters. Data reduction and cell refinement were performed using *SAINT* software and the space groups of these crystals were determined from systematic absences by *XPREP* and further justified by the refinement results. The structures were solved by direct methods and refined by full-matrix least-square calculations using *SHELXTL* software. All the non-H

Table 1. Crystallographic parameters for **2–5**.

Compound no.	2	3	4	5
Formulae	$C_{24} H_{19} N_3 O_5$	$C_{20} H_{16} N_3 O_3$	$C_{19} H_{18} N_3 O_3$	$C_{23} H_{21} N_3 O_4 S$
CCDC no.				
Mol. wt.	429.42	346.36	336.36	435.49
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Monoclinic
Space group	Pbcn	$P2_1/c$	$P2_1/c$	C2/c
a/Å	12.545(2)	32.0957(11)	30.916(4)	35.284(2)
b/Å	12.547(2)	4.5387(2)	4.5580(5)	9.3485(6)
c/Å	26.0224(4)	11.8773(4)	12.1164(15)	13.8632(8)
α/°	90.00	90.00	90.00	90.00
β/°	90.00	99.816(2)	95.876(9)	111.403(5)
γ/°	90.00	90.00	90.00	90.00
V/Å^3	4096.2(12)	1704.87(11)	1698.4(4)	4257.5(4)
Z	8	4	4	8
Density/Mgm^{-3}	1.393	1.349	1.315	1.359
Abs. Coeff./mm^{-1}	0.099	0.093	0.091	0.188
Abs. correction	None	None	None	None
F(000)	1792	724	708	1824
Total no. of reflections	5101	4201	3088	3794
Reflections, $I > 2\sigma(I)$	2671	2510	1106	3167
Max. 2θ/°	28.33	28.40	25.25	25.25
Ranges (h, k, l)	$-16 \leq h \leq 15$ $-15 \leq k \leq 16$ $-33 \leq l \leq 34$	$-42 \leq h \leq 42$ $-5 \leq k \leq 5$ $-15 \leq l \leq 15$	$-34 \leq h \leq 37$ $-5 \leq k \leq 5$ $-13 \leq l \leq 14$	$-42 \leq h \leq 42$ $-8 \leq k \leq 11$ $-16 \leq l \leq 15$
Complete to 2θ (%)	99.6	98.9	99.8	98.3
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/Restraints/Parameters	5101/0/297	4201/0/236	3088/0/234	3794/0/353
Goof (F^2)	0.897	0.975	0.821	1.042
R indices [$I > 2\sigma(I)$],	0.0567	0.0454	0.0555	0.0450
R indices (all data),	0.1278	0.0790	0.1592	0.0532

atoms were refined in the anisotropic approximation against F^2 of all reflections. The H-atoms attached to heteroatoms in these crystals were located in the difference Fourier synthesis maps, and refined with isotropic displacement coefficients. The locations of acidic protons were justified by difference Fourier synthesis map and in the refinement these were allowed for as riding atoms. The Crystallographic parameters of the salts and cocrystals are listed in table 1.

3. Results and discussion

Phthalic acid forms a yellow coloured salt (**2**) with host **1**. The salt **2** crystallizes in the orthorhombic Pbcn space group with one protonated cation of **1** and a phthalate anion in the asymmetric unit (figure 1a). The urea tap motif is not observed in the structure of this salt, instead two hydrogen bond between the oxygen atom of the phthalate anion and the urea nitrogen atom is observed (N2-H2N····O4, N3-H3N····O5) (table 2). Another intermolecular hydrogen bond between the protonated nitrogen atom of the quinoline ring and the carboxylate group of phthalate anion (N1-H1N····O2) is also present in the crystal structure (figure 1b). The urea derivatives generally form planar urea tap motif and such motifs can be broken down by the presence of guest molecules or anions which may lead to the breakdown of the well-organized urea tap motifs.[40] In this particular case there is strong intra-molecular hydrogen bond interactions in the anion makes a cyclic structure within the anion and this moiety binds to the host and

it acts as acceptor for hydrogen bonding and breaks the urea taps. The role of electron withdrawing groups in retaining urea taps in lattice was studied earlier[41] and it has been shown that the orientation of the aromatic groups of urea can be controlled by the urea carboxylate interactions.[42]

Terephthalic acid forms a colourless co-crystal (**3**) with host **1**. The co-crystal **3** crystallizes in the monoclinic P2₁/c space group where the terephthalic acid molecule lies on an inversion centre with only half of the molecule contained in the crystallographic asymmetric unit (figure 2a). The urea tap motif of the host molecule is maintained in the co-crystal (N2-H2N····O1, N3-H3N····O1). Another intermolecular hydrogen bonding between the quinoline N atom and the carboxylic acid (O2-H2····N1) forms a bridge between two host molecules as shown in figure 2b. The hydrogen bond parameters are shown in table 3. In this case the terephthalic acids molecules are not capable of intra-molecular hydrogen bond it does not affect the urea taps and prefers to adopt a linear arrangement.

The pair of positional isomer namely phthalic acid and terephthalic acid can also be distinguished by virtue of their colour arising from the formation of salt and co-crystal. Phthalic acids forms a yellow coloured salt whereas terephthalic acid forms a colourless co-crystal. The quinoline derivatives generally show n–π* transition.[43] Upon protonation non-bonding electrons are no longer available; energy of these levels goes beneath the π-level. This helps in generating new transition π–π* transition and this transition occurs at a higher wavelength (400 nm) due to narrowing of energy among

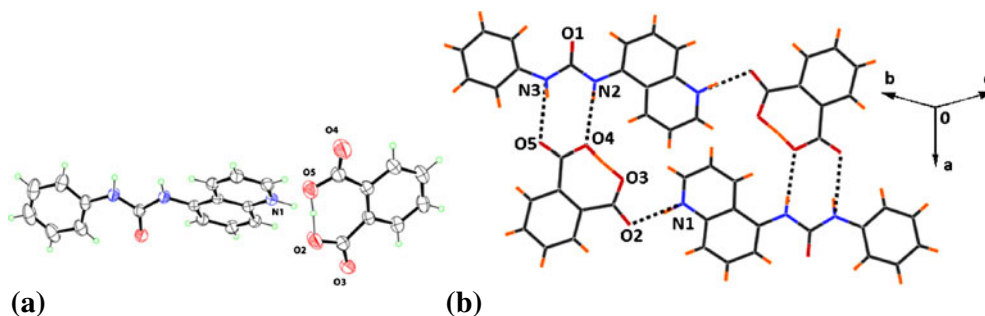**Figure 1.** (**a**) Asymmetric unit of **2** (ORTEP diagram drawn in 50% probability ellipsoid). (**b**) Hydrogen bonding network in **2**.

Table 2. Hydrogen bond distances and angles for compound **2**.

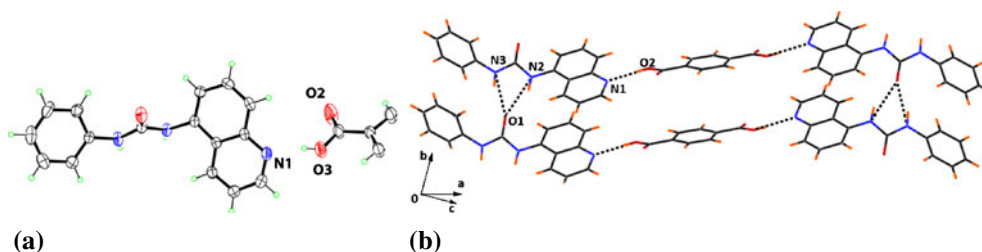| D-H····A	d_{D-H} (Å)	$d_{H····A}$ (Å)	$d_{D····A}$ (Å)	<D–H···· A (°)
N(1)-H(1N)····O(2) [x, −y, −1/2 + z]	1.05(3)	1.68(3)	2.714(2)	168(2)
N(2)-H(2N)····O(4) [−x, y, 1/2 − z]	0.86	2.16	3.015(3)	177
N(3)-H(3N)····O(5) [−x, y, 1/2 − z]	0.86	2.14	2.970(3)	163
O(3)-H(4A)····O(4)	1.25(4)	1.12(4)	2.367(3)	174(4)

Figure 2. (**a**) Asymmetric unit of **3** (ORTEP diagram drawn in 50% probability ellipsoid). (**b**) Hydrogen bonding network in **3**.

Table 3. Hydrogen bond distances and angles for compound **3**.

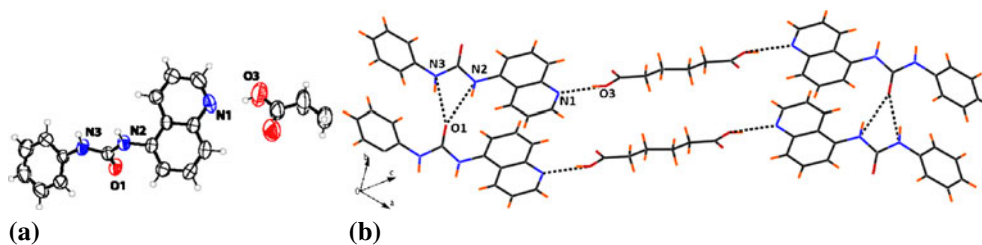| D-H····A	d_{D-H} (Å)	$d_{H····A}$ (Å)	$d_{D····A}$ (Å)	<D–H····A(°)
N(2)-H(2N)····O(1) [x, −1 + y, z]	0.86	2.10	2.864(1)	148
N(3)-H(3N)····O(1) [x, −1 + y, z]	0.86	1.98	2.779(2)	155
O(2)-H(2A)····N(1) [x, 3/2 − y, 1/2 + z]	0.82	1.89	2.697(2)	168

Figure 3. (**a**) Asymmetric unit of **4**. (ORTEP diagram drawn in 50% probability ellipsoid). (**b**) Hydrogen bonding network in **4**.

Table 4. Hydrogen bond distances and angles for compound **4**.

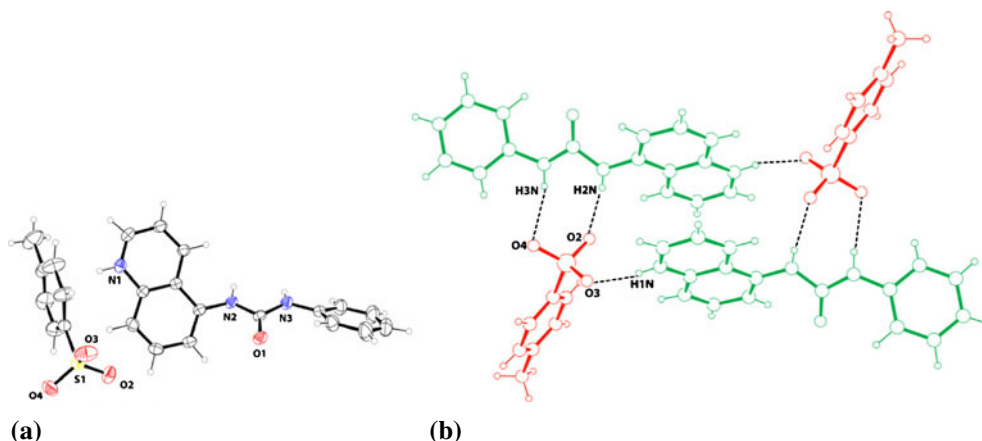| D-H····A	d_{D-H} (Å)	$d_{H····A}$ (Å)	$d_{D····A}$ (Å)	<D–H····A(°)
N(2)-H(2N)····O(1) [x, −1 + y, z]	0.85(2)	2.10(2)	2.870(3)	150(2)
N(3)-H(3N)····O(1) [x, −1 + y, z]	0.90(3)	1.98(3)	2.798(4)	150(2)
O(3)-H(3A)····N(1) [x, 3/2 − y, 1/2 + z]	0.82	1.92	2.707(5)	162

Figure 4. (**a**) Asymmetric unit of **5**. (**b**) Short range interactions in **5**.

the bonding and anti bonding π-orbitals. In order to confirm that this change in absorbance is from the host part, we have also studied the UV-visible spectra of the phthalic acid and terephthalic acid. Phthalic acid absorbs at 273 nm and on addition of base such as triethyl amine, no absorbance in the visible region is observed. Similarly, in the case of terephthalic acid which absorbs at 285 nm, no absorbance at the visible region is observed on addition of triethyl amine. Hence, the yellow colour of the salts is only because of the protonated form of the host **1**.

The host **1** forms a colourless co-crystal with adipic acid (**4**). The co-crystal **4** crystallizes in the space group monoclinic P2$_1$/c with half of the adipic acid molecule and a molecule of host **1** in the crystallographic asymmetric unit (figure 3). The co-crystal **4** forms an analogous structure with the other co-crystals by maintaining the urea tap hydrogen bonding interaction (N2-H2N····O1, N3-H3N····O1) (table 4). The carboxylic acid group of adipic acid form hydrogen bonds with the quinoline N atom (O3-H3····N1). The hydrogen bonded self-assembly of the co-crystal is shown in figure 3.

The salt **5** crystallizes in the space group monoclinic C2/c and exists as a Z$'$ = 1 structure with a total of two molecules in the crystallographic asymmetric unit (Z$''$ = 2). The asymmetric unit consists of a *p*-tolunesulphonate anion and a protonated **1** cation. In this structure also the urea tap motif is not observed, instead the urea H atoms are involved in an intermolecular hydrogen bond with the O atom of the *p*-tolunesulphonate anion (d$_{D-H···A}$ (Å), N2-H2N···O2, 2.904(2); N3-H3N···O4, 3.050(2) and <D-H···A (°), <N2-H2N···O2, 167(2); <N3-H3N···O4, 153(1)). Another oxygen atom O3 of the *p*-tolunesulphonate anion forms a hydrogen bond with the protonated quinoline nitrogen atom (d$_{D-H···A}$ (Å), N1-H1N···O3, 2.698(2) and <N1-H1N···O3, 156(2)). The asymmetric unit of **5** is shown in figure 4a along with the short range interactions in figure 4b.

The *p*-tolunesulphonate salt **5** shows a sharp peak at 1212 cm^{-1} characterestic of the *p*-tolunesulphonate anion. It may be mentioned that the type of supramolecular assembly formed by combination of carboxylic acids with pyridine depends on the difference in pKa values of each counterpart.[31] But in the case of acid–base complexes with similar pKa values, the amount of proton transfer in the solid state is not a predictable parameter as a continuum exists between the two extremes.[32] The terephthalic acid, phthalic acid, adipic acid and *p*-tolunesulphonic acids have pKa1 values 3.51, 2.98, 4.42, and 2.8, respectively. Thus, in the cases of the salt formation in solid and solution

states by phthalic acid and *p*-tolunesulphonic acids are reasonable and follow a predictive trend.

4. Conclusion

The present study thus shows that the host **1** is good for distinguishing two positional isomers of dicarboxylic acid namely phthalic acid and terephthalic acid. The protonation of quinoline unit allows the system to lose the self-assembling process by two N–H and one carbonyl oxygen of urea group of two neighbouring urea derivatives. These results also support the reasons provided on support of strong intra-molecular hydrogen bond interactions in visual distinction of maleic acid from fumeric acid by the same host.[39] The terephthalic acid being an industrially important substrate for polyester fibres and plastics, contamination of phthalic acid in such material is unwanted.[44] But the contaminant of terephthalic acid could be phthalic acid due to synthetic procedures, thus the presence of latter as impurity can be easily found out by using host **1** as an indicator.

Supplementary materials

The CIF data are deposited to Cambridge Crystallographic Database, CCDC Nos. are 854224-854226.

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