Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary information

Structural framework of biologically active coumarin derivatives. Crystal structures and Hirshfeld surface analysis

Magdalena Małecka,*[a] Elzbieta Budzisz[b]

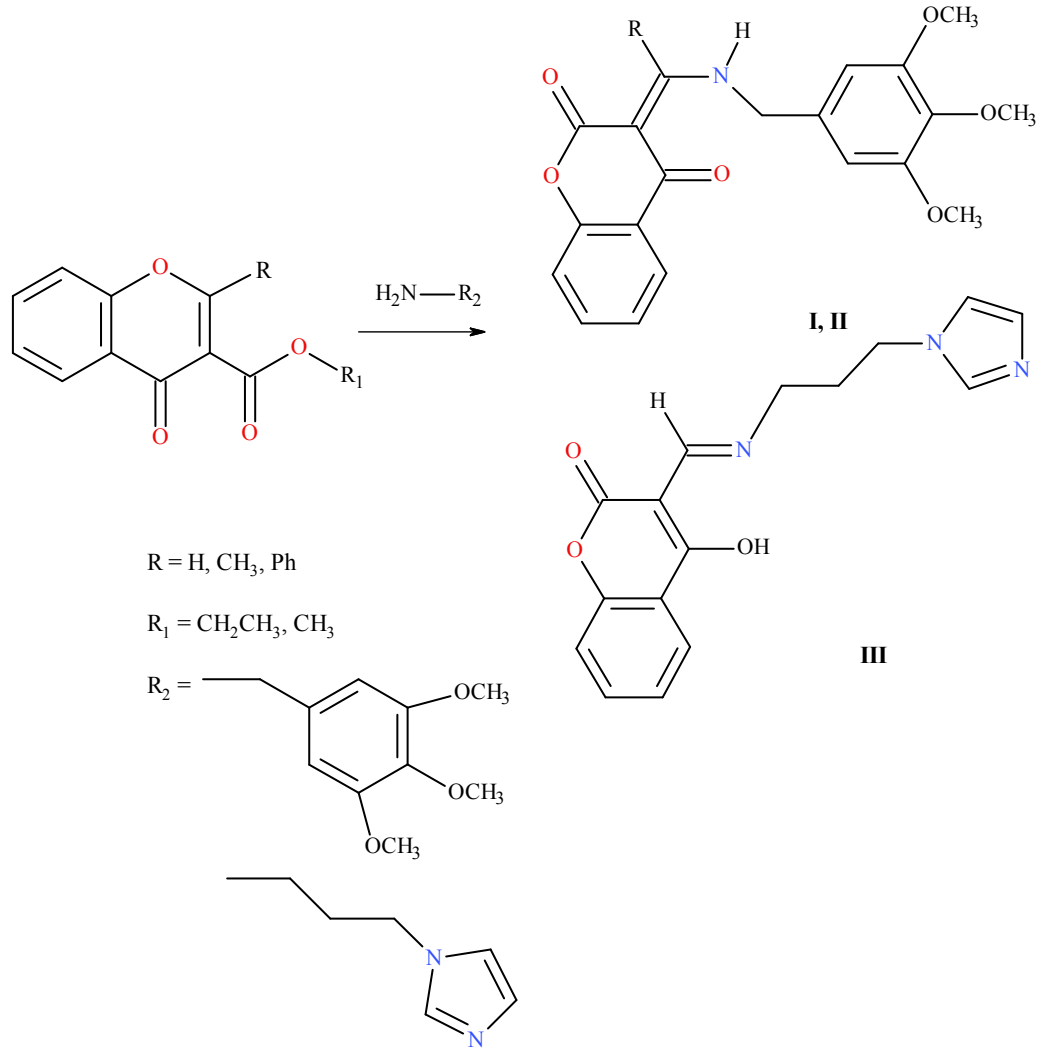
[a] *Structural Chemistry and Crystallography Group, University of Lodz, Pomorska 163/165, 90-236 Łódź, Poland. Tel: +48 42 635 57 41; E-mail: malecka@uni.lodz.pl*
[b] *Department of Cosmetic Raw Materials Chemistry, Medical University of Lodz, Muszyński 1, 90-151 Łódź, Poland. Tel: XX XXXX XXXX; E-mail: elzbieta.budzisz@umed.lodz.pl*

corresponding author email:malecka@uni.lodz.pl

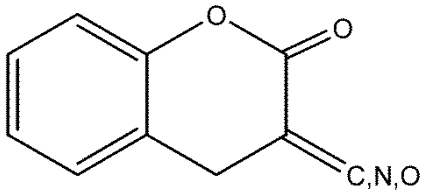
Table S1. Geometrical parameters (Å, °) for the C-H… π interactions and C-O…π for all derivatives.

	d(C-H)	d(H...Cg)	d(C...Cg)	<C-H…Cg	symmetry
compound (I)					
C351-H35C...Cg(3)	0.98	2.71	3.488(2)	137	1+x, y, z
C371-H37C...Cg(3)	0.98	2.90	3.787(2)	151	-1+x, y, z
C4-O4…Cg(2)	1.255 (2)	3.7072(16)	3.505(2)	70.98(11)	-1+x, y, z
compound (II)					
C371-H37C...Cg(4)	0.98	2.94	3.7487(17)	141	1+x, y, 1+z
C313-H313...Cg(2)	0.95	2.73	3.4237(19)	131	-x, -1/2+y, -1/2-z
compound (III)					
C7-H7…Cg(3)	0.95	2.75	3.5923(19)	148	-x, -1/2+y, -1/2-z
C4-O4…Cg(1)	1.258(2)	3.8460(17)	3.6638(19)	72.26(7)	1-x, -y, -z

Cg(1), Cg(2), Cg(3) are centroids of pyran ring, benzene ring from coumarin moiety and trimethoxy-benzene ring, respectively



Scheme S1. Scheme of the reaction for preparing comounds (I), (II), and (III)



Scheme 2. Scheme of query used in database CSD search

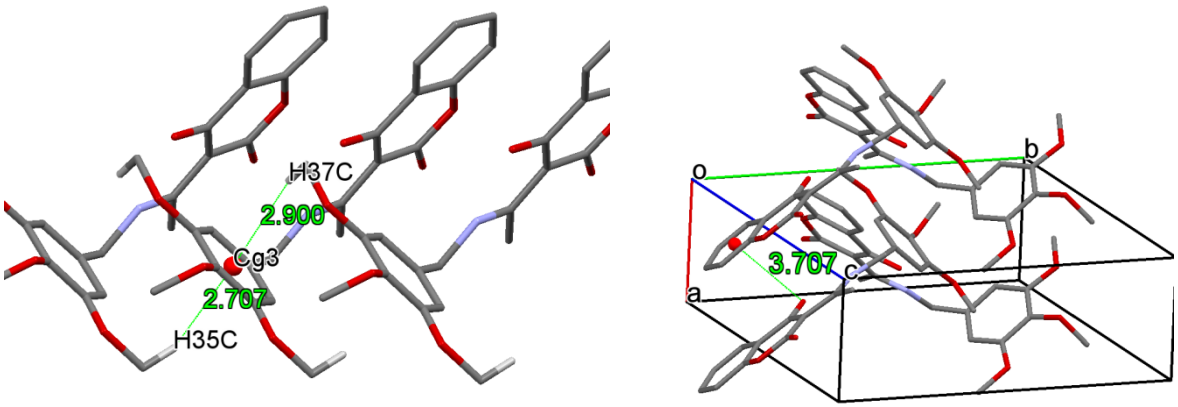


Figure S1 a) Molecules of (I) linked by C351-H35C…Cg3 (at 1+x, y, z) and C37C-H37C…Cg3 (at -1+x, y, z). Cg3 is a centroid of trimethoxybenzene ring. b) contact between C4=O4 group and π-ystem of benzene ring from benzopyran moiety.

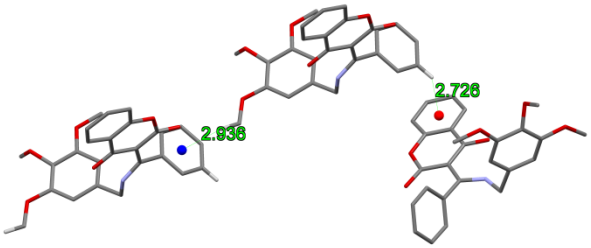


Figure S2. The perspective view of C-H...π interactions in crystal lattice of compound (II). The C313-H313.. Cg2 at –x,-1/2+y, -1/2-z forms chain along [010] direction. Cg2 is a centroid of benzene ring from coumarin moiety.

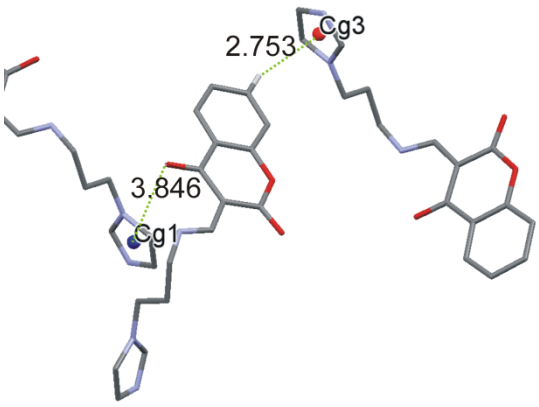


Figure S3. Two rows of molecules in (III) linked by C7-H7...Cg3 at –x, -½+y, -½-z interaction. Cg3 is a centroid of imidazole ring.

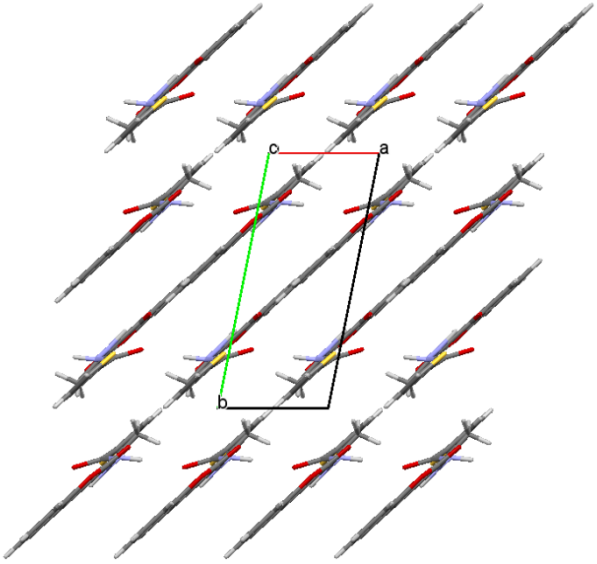


Figure S4. The layered structure of UPATAH.[32]