Phenoxy pendant isatins as potent α-glucosidase inhibitors: Reciprocal carbonyl···carbonyl interactions, antiparallel π···π stacking driven solid state self-assembly and biological evaluation

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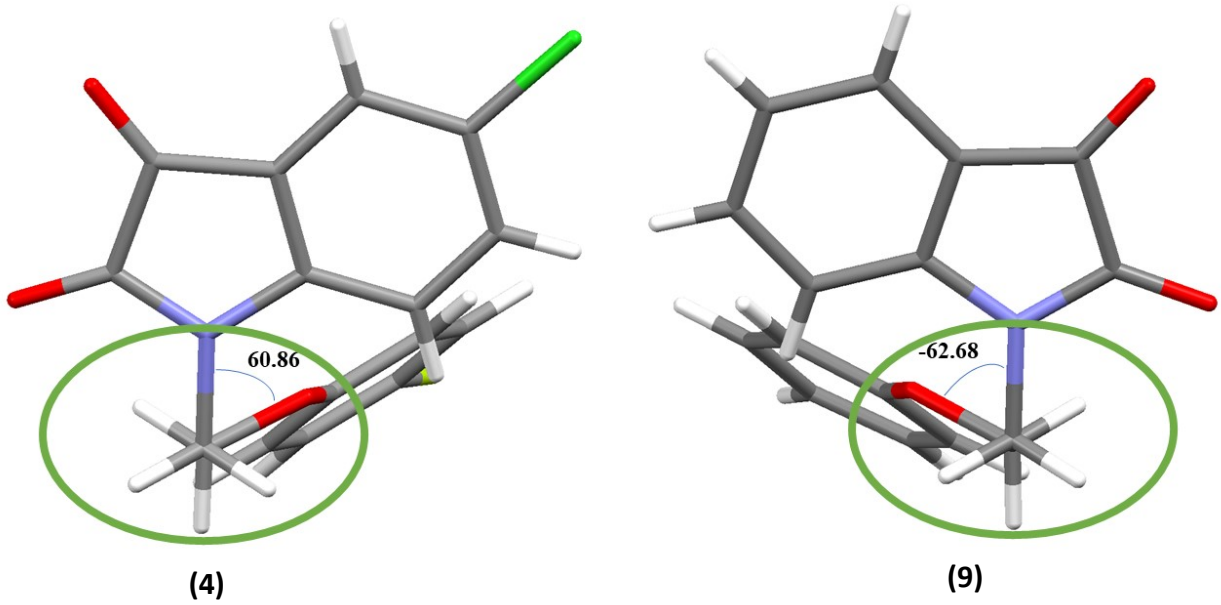

Fig. S1 Showing staggered gauche conformation of ethylene moity that is bridging two aryl rings of **4** and **9**

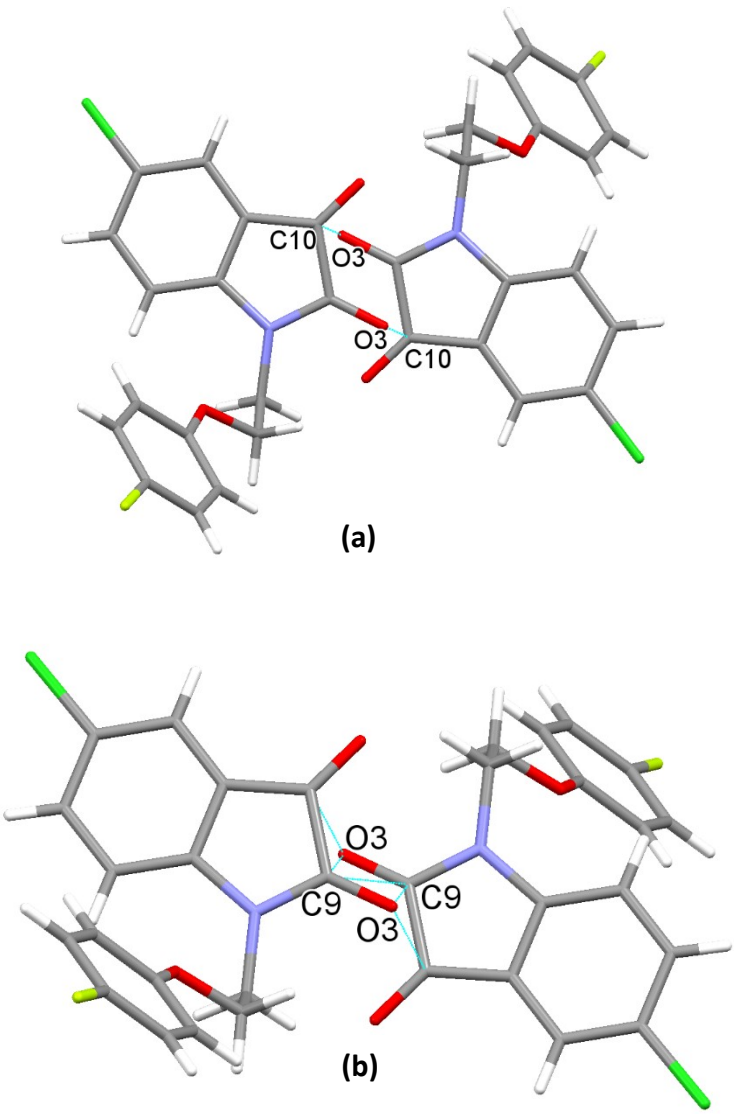

Fig. S2 Showing clear view of torsions of, a) one sided CO···CO [C=O···C=O (*T*) = -70.20° and ∠C =O···C = 102.94°]; b) a recently discovered reciprocal CO···CO [C=O···C=O (*T*) = 0° and ∠C=O···C = 85.00°] interactions of **4**.

Detailed geometric parameters of phenoxy pendant isatin 4; bond lengths (Å, bond angles (°) and torsion angles (°)derived from the X-ray crystallographic study

```
Cl1 C15 1.745(3) . ?
F1 C1 1.359(3) . ?
O2 C4 1.372(3) . ?
O2 C7 1.417(3) . ?
O3 C9 1.214(3) . ?
O4 C10 1.203(3) . ?
N1 C9 1.368(3) . ?
N1 C12 1.422(3) . ?
N1 C8 1.455(3) . ?
C1 C6 1.358(4) . ?
C1 C2 1.368(4) . ?
C2 C3 1.377(4) . ?
C3 C4 1.383(3) . ?
C4 C5 1.383(3) . ?
C5 C6 1.381(4) . ?
C7 C8 1.505(3) . ?
C9 C10 1.550(4) . ?
C10 C11 1.461(3) . ?
C11 C16 1.386(3) . ?
C11 C12 1.395(3) . ?
C12 C13 1.378(3) . ?
C13 C14 1.388(3) . ?
C14 C15 1.389(4) . ?
C15 C16 1.381(3) . ?

C4 O2 C7 118.66(18) . . ?
C9 N1 C12 110.60(19) . . ?
C9 N1 C8 123.16(19) . . ?
C12 N1 C8 126.14(19) . . ?
C6 C1 F1 119.1(3) . . ?
C6 C1 C2 122.6(2) . . ?
F1 C1 C2 118.3(3) . . ?
C1 C2 C3 118.8(3) . . ?
C2 C3 C4 119.7(2) . . ?
O2 C4 C3 115.0(2) . . ?
O2 C4 C5 124.6(2) . . ?
C3 C4 C5 120.4(2) . . ?
C6 C5 C4 119.6(2) . . ?
C1 C6 C5 118.9(2) . . ?
O2 C7 C8 107.11(19) . . ?
N1 C8 C7 112.9(2) . . ?
O3 C9 N1 127.2(2) . . ?
O3 C9 C10 126.7(2) . . ?
N1 C9 C10 106.17(19) . . ?
O4 C10 C11 131.1(2) . . ?
O4 C10 C9 123.7(2) . . ?
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C11 C10 C9 105.17(18) . . ?
C16 C11 C12 121.6(2) . . ?
C16 C11 C10 130.8(2) . . ?
C12 C11 C10 107.57(19) . . ?
C13 C12 C11 120.8(2) . . ?
C13 C12 N1 128.7(2) . . ?
C11 C12 N1 110.5(2) . . ?
C12 C13 C14 117.7(2) . . ?
C15 C14 C13 121.2(2) . . ?
C16 C15 C14 121.5(2) . . ?
C16 C15 Cl1 118.74(18) . . ?
C14 C15 Cl1 119.80(19) . . ?
C15 C16 C11 117.2(2) . . ?
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Detailed geometric parameters of phenoxy pendant isatin 9; bond lengths (Å, bond angles (°) and torsion angles (°)derived from the X-ray crystallographic study

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O1 C3 1.370(4) . ?
O1 C2 1.421(4) . ?
O2 C9 1.212(4) . ?
O3 C10 1.207(4) . ?
N1 C9 1.359(4) . ?
N1 C12 1.415(4) . ?
N1 C1 1.456(4) . ?
C1 C2 1.497(5) . ?
C1 H1A 0.9700 . ?
C1 H1B 0.9700 . ?
C2 H2A 0.9700 . ?
C2 H2B 0.9700 . ?
C3 C8 1.378(5) . ?
C3 C4 1.380(5) . ?
C4 C5 1.377(6) . ?
C4 H4 0.9300 . ?
C5 C6 1.380(7) . ?
C5 H5 0.9300 . ?
C6 C7 1.369(7) . ?
C6 H6 0.9300 . ?
C7 C8 1.392(5) . ?
C7 H7 0.9300 . ?
C8 H8 0.9300 . ?
C9 C10 1.554(5) . ?
C10 C11 1.453(5) . ?
C11 C16 1.387(5) . ?
C11 C12 1.391(5) . ?
C12 C13 1.374(5) . ?
C13 C14 1.389(5) . ?
C13 H13 0.9300 . ?
C14 C15 1.385(6) . ?
C14 H14 0.9300 . ?
C15 C16 1.382(5) . ?
C15 H15 0.9300 . ?
C16 H16 0.9300 . ?

C3 O1 C2 118.9(3) . . ?
C9 N1 C12 110.7(3) . . ?
C9 N1 C1 122.9(3) . . ?
C12 N1 C1 126.1(3) . . ?
N1 C1 C2 113.1(3) . . ?
N1 C1 H1A 109.0 . . ?
C2 C1 H1A 109.0 . . ?
N1 C1 H1B 109.0 . . ?
C2 C1 H1B 109.0 . . ?
H1A C1 H1B 107.8 . . ?
O1 C2 C1 107.1(3) . . ?
O1 C2 H2A 110.3 . . ?
C1 C2 H2A 110.3 . . ?
O1 C2 H2B 110.3 . . ?
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C1 C2 H2B 110.3 . . ?
H2A C2 H2B 108.5 . . ?
O1 C3 C8 124.5(3) . . ?
O1 C3 C4 114.6(3) . . ?
C8 C3 C4 120.9(4) . . ?
C5 C4 C3 119.4(4) . . ?
C5 C4 H4 120.3 . . ?
C3 C4 H4 120.3 . . ?
C4 C5 C6 120.7(5) . . ?
C4 C5 H5 119.6 . . ?
C6 C5 H5 119.6 . . ?
C7 C6 C5 119.2(4) . . ?
C7 C6 H6 120.4 . . ?
C5 C6 H6 120.4 . . ?
C6 C7 C8 121.2(4) . . ?
C6 C7 H7 119.4 . . ?
C8 C7 H7 119.4 . . ?
C3 C8 C7 118.5(4) . . ?
C3 C8 H8 120.8 . . ?
C7 C8 H8 120.8 . . ?
O2 C9 N1 127.0(3) . . ?
O2 C9 C10 126.9(3) . . ?
N1 C9 C10 106.1(3) . . ?
O3 C10 C11 131.7(3) . . ?
O3 C10 C9 123.4(3) . . ?
C11 C10 C9 104.9(3) . . ?
C16 C11 C12 120.3(3) . . ?
C16 C11 C10 132.0(3) . . ?
C12 C11 C10 107.7(3) . . ?
C13 C12 C11 121.6(3) . . ?
C13 C12 N1 127.9(3) . . ?
C11 C12 N1 110.6(3) . . ?
C12 C13 C14 117.3(3) . . ?
C12 C13 H13 121.3 . . ?
C14 C13 H13 121.3 . . ?
C15 C14 C13 122.1(4) . . ?
C15 C14 H14 119.0 . . ?
C13 C14 H14 119.0 . . ?
C16 C15 C14 119.8(3) . . ?
C16 C15 H15 120.1 . . ?
C14 C15 H15 120.1 . . ?
C15 C16 C11 118.9(4) . . ?
C15 C16 H16 120.6 . . ?
C11 C16 H16 120.6 . . ?

C9 N1 C1 C2 -91.2(4) . . . . ?
C12 N1 C1 C2 94.9(4) . . . . ?
C3 O1 C2 C1 -174.4(3) . . . . ?
N1 C1 C2 O1 -62.7(4) . . . . ?
C2 O1 C3 C8 -1.8(5) . . . . ?
C2 O1 C3 C4 178.3(3) . . . . ?
O1 C3 C4 C5 -177.3(4) . . . . ?
C8 C3 C4 C5 2.8(6) . . . . ?
C3 C4 C5 C6 0.0(7) . . . . ?
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C4 C5 C6 C7 -2.6(8) . . . . ?
C5 C6 C7 C8 2.5(7) . . . . ?
O1 C3 C8 C7 177.2(3) . . . . ?
C4 C3 C8 C7 -2.9(5) . . . . ?
C6 C7 C8 C3 0.2(6) . . . . ?
C12 N1 C9 O2 179.1(3) . . . . ?
C1 N1 C9 O2 4.4(5) . . . . ?
C12 N1 C9 C10 -0.1(3) . . . . ?
C1 N1 C9 C10 -174.8(3) . . . . ?
O2 C9 C10 O3 0.3(5) . . . . ?
N1 C9 C10 O3 179.5(3) . . . . ?
O2 C9 C10 C11 -178.4(3) . . . . ?
N1 C9 C10 C11 0.8(3) . . . . ?
O3 C10 C11 C16 0.9(6) . . . . ?
C9 C10 C11 C16 179.5(3) . . . . ?
O3 C10 C11 C12 -179.7(4) . . . . ?
C9 C10 C11 C12 -1.2(3) . . . . ?
C16 C11 C12 C13 0.1(5) . . . . ?
C10 C11 C12 C13 -179.4(3) . . . . ?
C16 C11 C12 N1 -179.4(3) . . . . ?
C10 C11 C12 N1 1.2(3) . . . . ?
C9 N1 C12 C13 179.9(3) . . . . ?
C1 N1 C12 C13 -5.6(5) . . . . ?
C9 N1 C12 C11 -0.7(3) . . . . ?
C1 N1 C12 C11 173.8(3) . . . . ?
C11 C12 C13 C14 -0.5(5) . . . . ?
N1 C12 C13 C14 178.8(3) . . . . ?
C12 C13 C14 C15 0.2(5) . . . . ?
C13 C14 C15 C16 0.6(6) . . . . ?
C14 C15 C16 C11 -1.1(5) . . . . ?
C12 C11 C16 C15 0.7(5) . . . . ?
C10 C11 C16 C15 -180.0(3) . . . . ?
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