Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting information

Supramolecular alleviation of cardiotoxicity of a small-molecule kinase inhibitor

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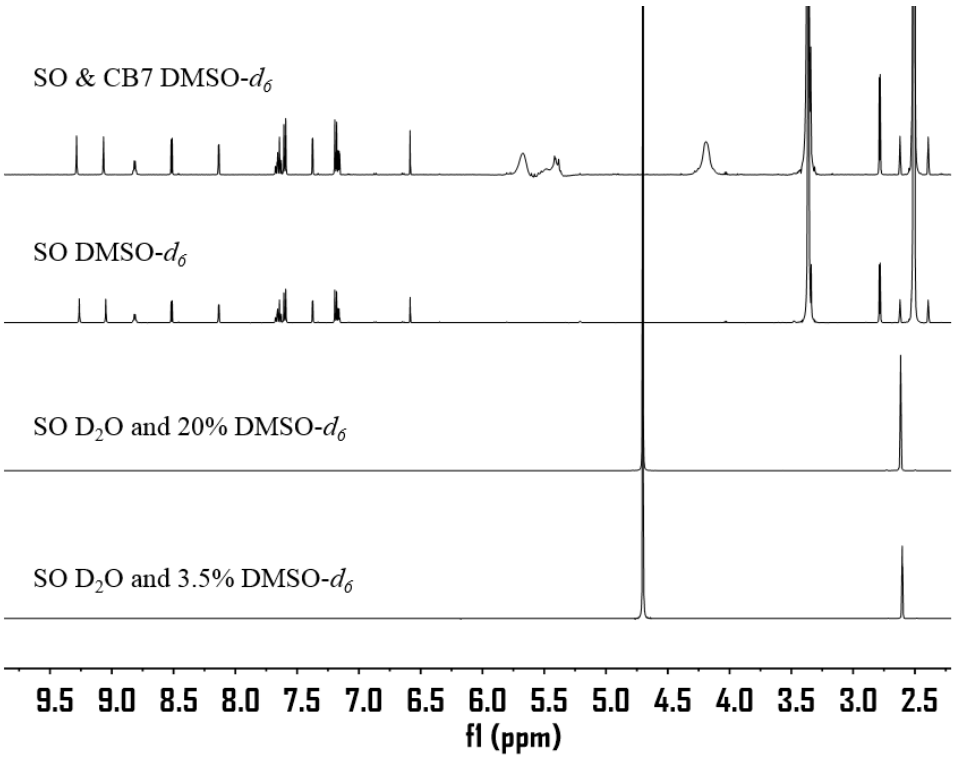


Fig. S1. The ^{1}H NMR spectra of SO in D_2O in the presence of various amounts of DMSO-d_6: 3.5 (v/v) % DMSO-d_6 (saturated SO); 20 v/v % DMSO-d_6 (saturated SO); 100% DMSO-d_6 (1 mM); and SO-CB[7] (1 mM SO in the presence of 1.2 mM CB[7]) in 100% DMSO-d_6.

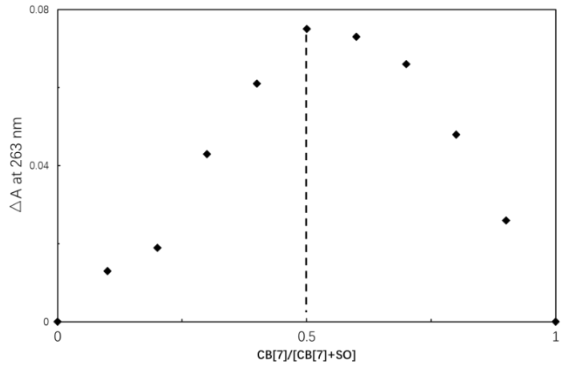


Fig. S2 Job plot indicating 1 : 1 host–guest complex stoichiometry for SO@CB[7] complex based on the continuous variation UV-visible titration monitored at 263 nm.

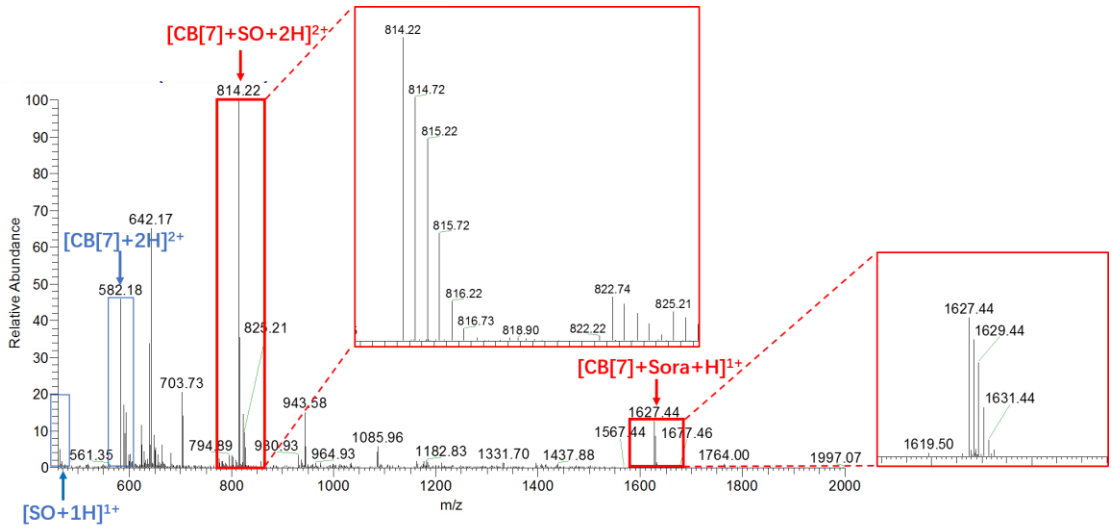


Fig. S3 ESI-MS spectrum of SO in the presence of CB[7]. The singlet charged peak at m/z = 1627.44 and a doublet charged peak at m/z = 814.22 are corresponding to the [SO+CB[7]+H]+ complex (calculated m/z = 1627.44) and [SO+CB[7]+2H]2+ complex (calculated m/z = 814.22).

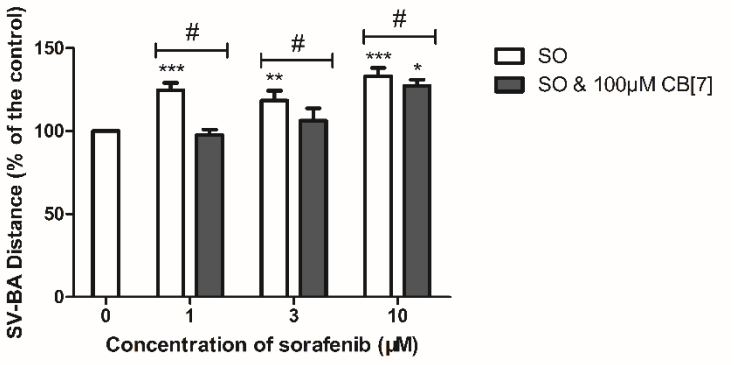


Fig. S4 Statistical analyses of SV–BA distance in SO treated group and SO@CB[7] complex treated group. $^{*}P < 0.05$, $^{**}P<0.01$, $^{***}P<0.001$ versus Control and $^{\#}P<0.05$ implies statistically significant difference between SO and SO@CB[7]. Data were plotted as mean ±

S.E.M. (n = 15-20) of three independent experiments.

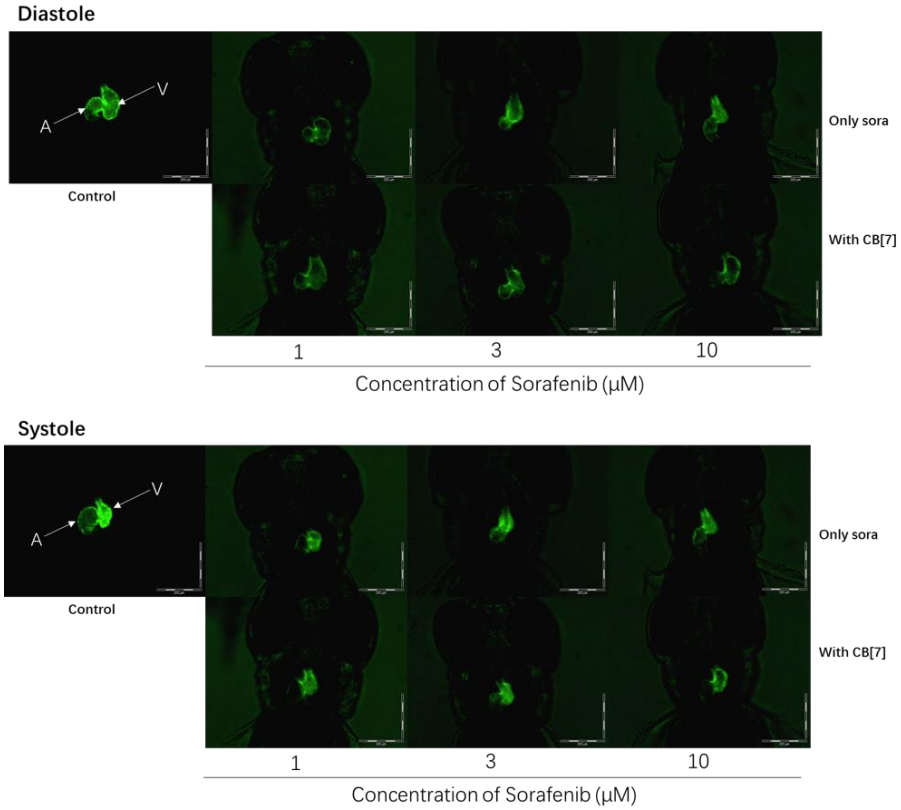


Fig. S5 Representative images of Tg(*cmlc2:*GFP) zebrafish heart after incubation in various concentrations of SO (1, 3, 10 μM) in the absence and in the presence of 100 μM CB[7]. A: Atrium, V: Ventricle. Scale bar: 200 mm.

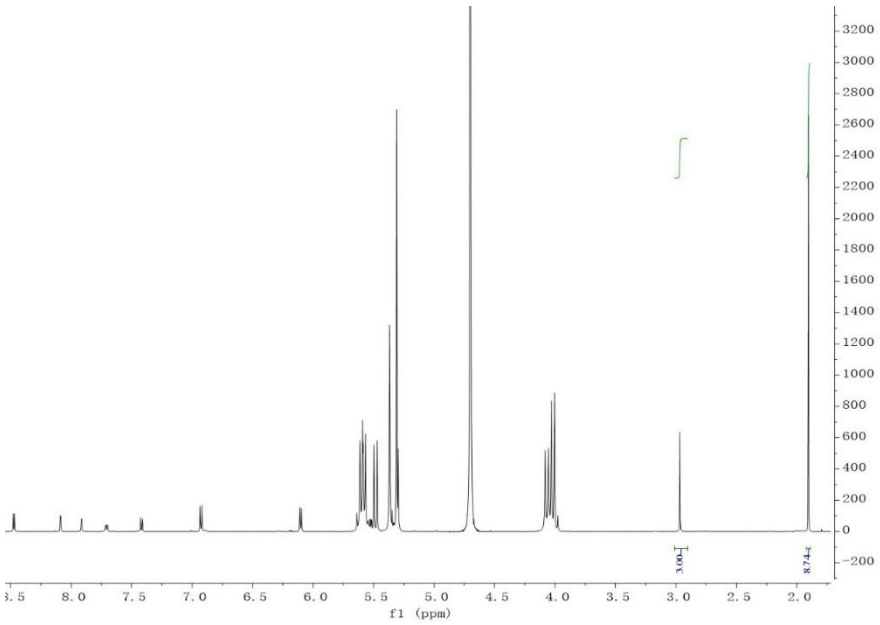
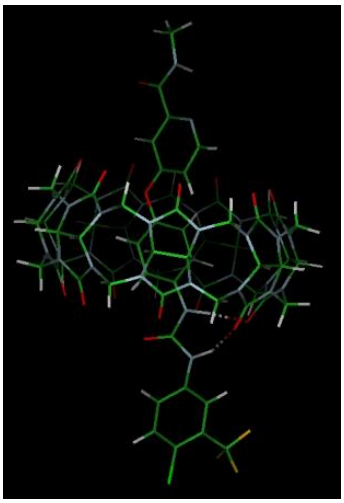


Fig. S6 Representative ^{1}H NMR integration results for the phase solubility experiment.

DFT calculations.

CB[7] inclusion complexes were first constructed using Chem3D considering 4 heights for the position of the host CB[7] along the skeleton of the SO guest. The minimized structures were then transported to the Gaussian interface (Gaussian09 Rev.D01) before DFT minimization by the B3LYP method (basis set 6-31G(d)) with a water continuum model (CPCM) to account as best as possible for solvation. The three most stable inclusion complexes are presented in Figure 4 of the paper (each separated by ≈ 1.4 kcal.mol^{-1} so within 2.8 kcal.mol^{-1}). Frequency calculations were performed to check that the structures correspond to true minima. Then BSSE calculations were performed to account for the basis set superposition errors. The atomic coordinates of the three minimized inclusion complexes are given hereafter as well as a table summarizing the energies of the inclusion complexes before BSSE calculations (water continuum model) and in vacuum (BSSE) providing the counterpoise corrected energies and the corrected complexation energies. Three other possibilities were considered for another conformation of the guest (relative positions of the pendant groups of the urea function) with three positions of CB[7] along this SO guest conformation and ended up with higher energy structures.

<u>Atomic coordinates of the inclusion complexes of SO with CB[7].</u>



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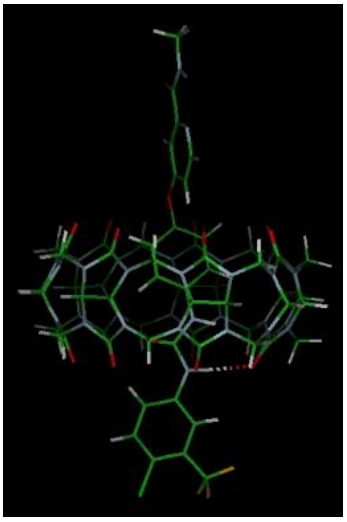

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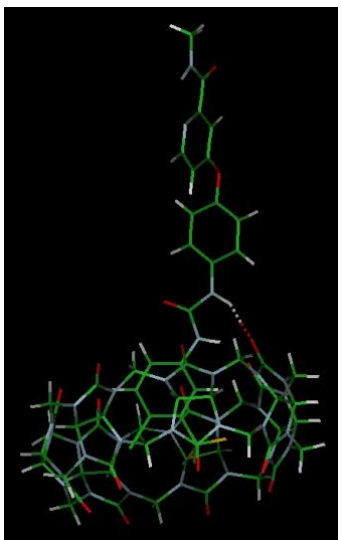

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Full names of some abbreviations:

1. RAF/MEK/ERK: a pathway of mitogen-activated protein kinase
2. VEGFR: Vascular endothelial growth factor receptor
3. PDGFR: Platelet-derived growth factor receptors
4. FLT: Fms-like tyrosine kinase
5. KIT: A name of gene sequence, which belongs to tyrosine kinases III family
6. ECG: Electrocardiograph