

Figure S1 Part of the crystal structure of 1, showing C-H $\cdots \mathrm{F}$ (viewed along the $a$ axis), represented by dashed lines. Symmetry codes: (ii) $-\mathrm{x}+1,-\mathrm{y}+2,-\mathrm{z}$.


Figure S2 Part of the crystal structure of 1, showing donating bifurcated $\mathrm{C}-\mathrm{H}^{\cdots} \mathrm{O}$ possible weak hydrogen bonds (viewed along the c axis), represented by dashed lines. Symmetry code: (iii) $\mathrm{x}-1, \mathrm{y}-1, \mathrm{z}$.


Figure S3 Part of the crystal structure of 2, viewed along [101], showing F $\cdots \mathrm{F}$ short contacts [2.704 (2) $\AA$ ] between adjacent symmetry-related molecules 1 . Symmetry code: (v) x, $-y+1 / 2$, $\mathrm{z}+1 / 2$.


Figure $\mathbf{S 4}{ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1}$ in DMSO- $d 6$. S denotes the residual solvent signal.


Figure S5 ${ }^{13} \mathrm{C}\left\{{ }^{\{1} \mathrm{H}\right\}$ NMR spectrum of $\mathbf{1}$ in DMSO- $d 6$. S denotes the residual solvent signal. The inset shows the aromatic region.


Figure S6 ${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{2}$ in DMSO- $d 6$. S denotes the residual solvent signal. The inset shows the aromatic region.


Figure $\mathbf{S 7} 7{ }^{13} \mathrm{C}\left\{{ }^{1} \mathrm{H}\right\}$ NMR spectrum of $\mathbf{2}$ in DMSO- $d 6$. S denotes the residual solvent signal. The inset shows the aromatic region.


Figure S8 Solid-state ATR-FT-IR spectrum of $\mathbf{1}$ at a resolution of $4 \mathrm{~cm}^{-1}$ ( 32 scans).


Figure S9 Solid-state ATR-FT-IR spectrum of $\mathbf{2}$ at a resolution of $4 \mathrm{~cm}^{-1}$ ( 32 scans).


Figure $\mathbf{S 1 0} \mathrm{ESI}^{-}$mass spectrum of $\mathbf{1}$ in methanol.


Figure $\mathbf{S 1 1} \mathrm{APCI}^{+}$mass spectrum of $\mathbf{2}$ in methanol.

