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**Supporting information for article:**

**A comparative experimental and theoretical investigation of hydrogen, halogen and  $\pi-\pi$  interactions in the solid-state supramolecular assembly of 2- and 4-formylphenyl arylsulfonates**

**Hina Andleeb, Imtiaz Khan, Antonio Bauzá, Muhammad Nawaz Tahir, Jim Simpson, Shahid Hameed and Antonio Frontera**

## **SUPPORTING INFORMATION**

### **A comparative experimental and theoretical investigation of hydrogen, halogen and $\pi \cdots \pi$ interactions in the solid-state supramolecular assembly of 2- and 4-formylphenyl arylsulfonates**

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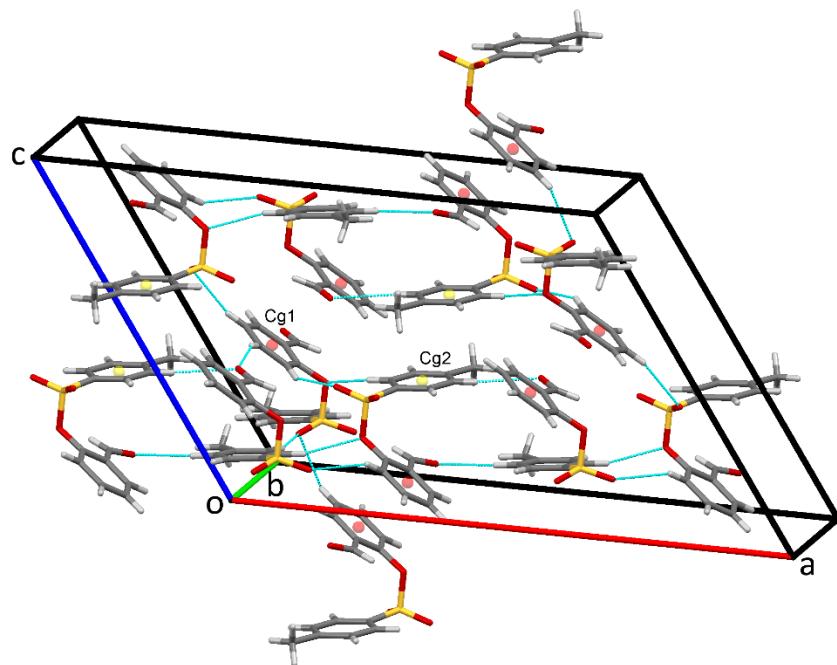
*Palma de Mallorca (Baleares), Spain*

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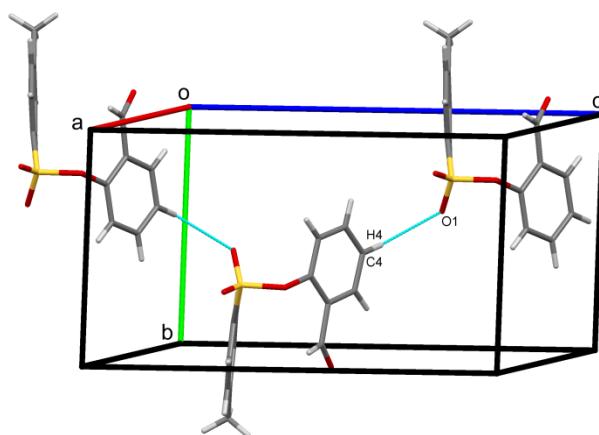
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<sup>†</sup>*School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, United Kingdom*

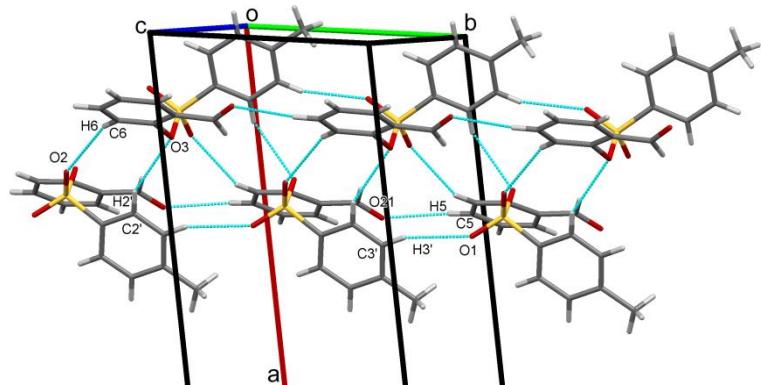
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**X-ray Crystallography**

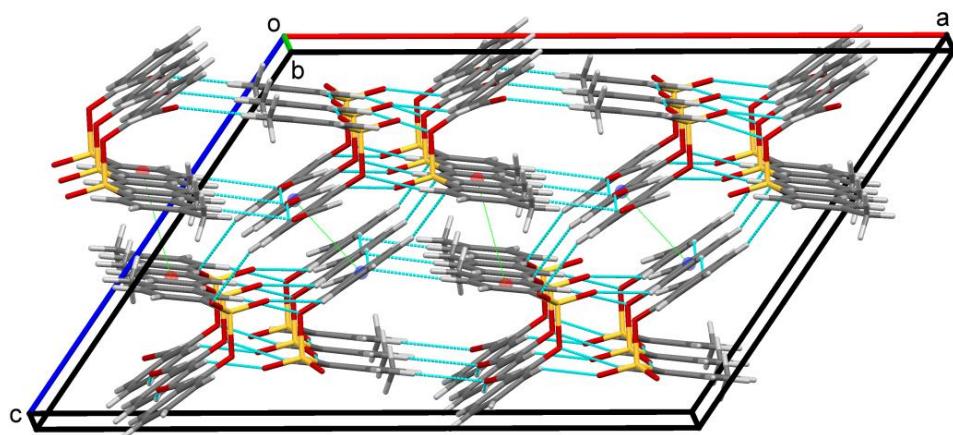
**Figure S1** Sheets of **3a** molecules in the *ac* plane.



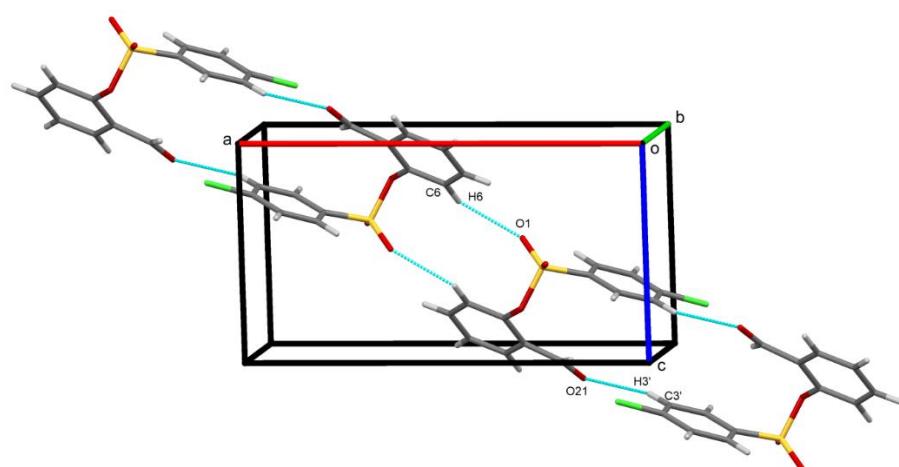
**Figure S2** Zig-zag chains of **3a** molecules along *c*. In this and subsequent Figures, hydrogen bonds are drawn as blue dashed lines.



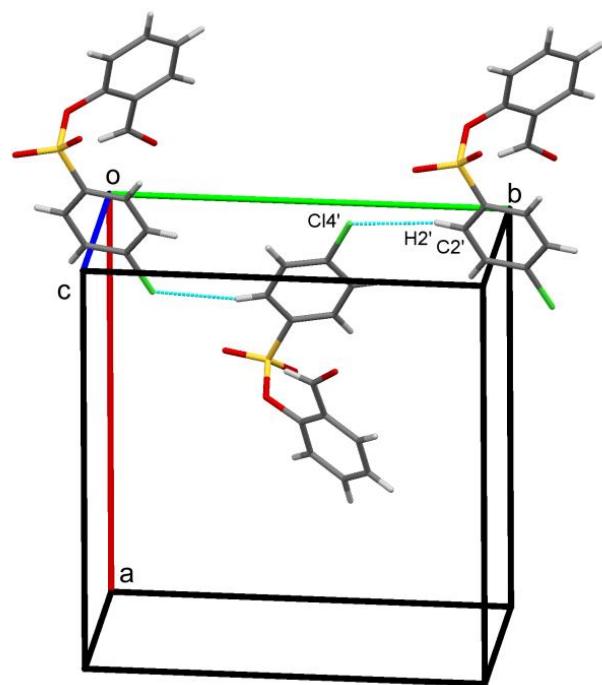
**Figure S3** Double chains of **3a** molecules along *b*.



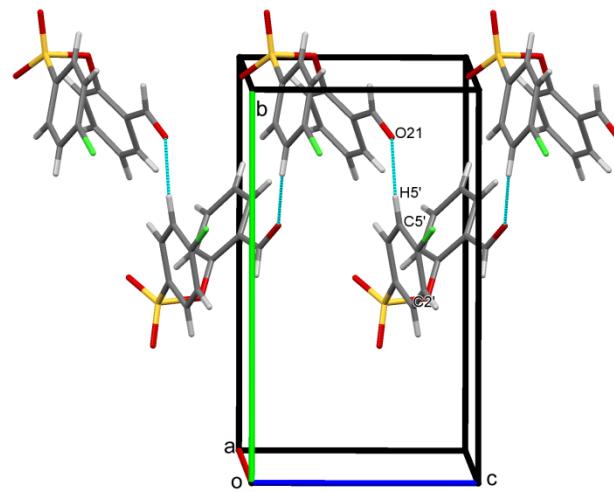
**Figure S4** Overall packing for **3a** viewed along the *b* axis direction. For clarity, only selected  $\pi \dots \pi$  contacts are shown.



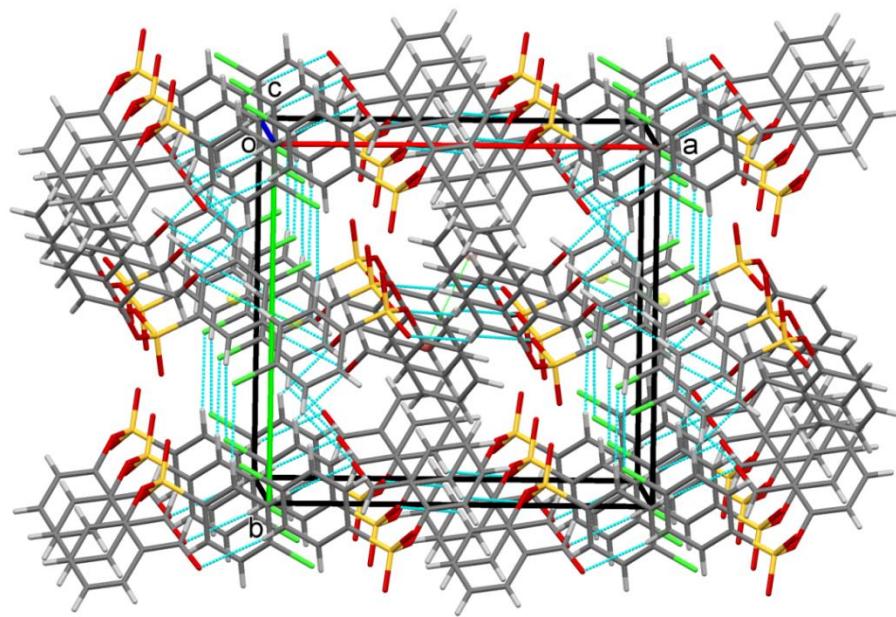
**Figure S5** Linked inversion dimers of compound **3b**.



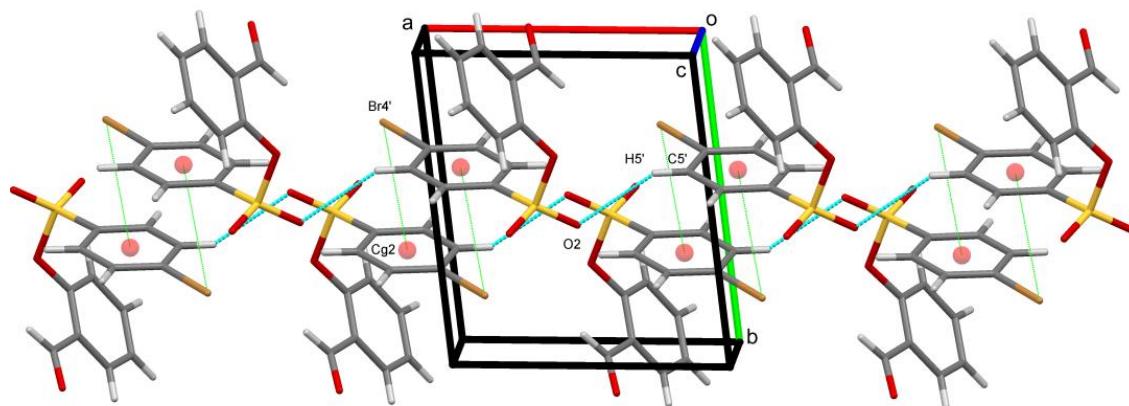
**Figure S6** Zig-zag chains of molecules of **3b** form along the *b* axis.



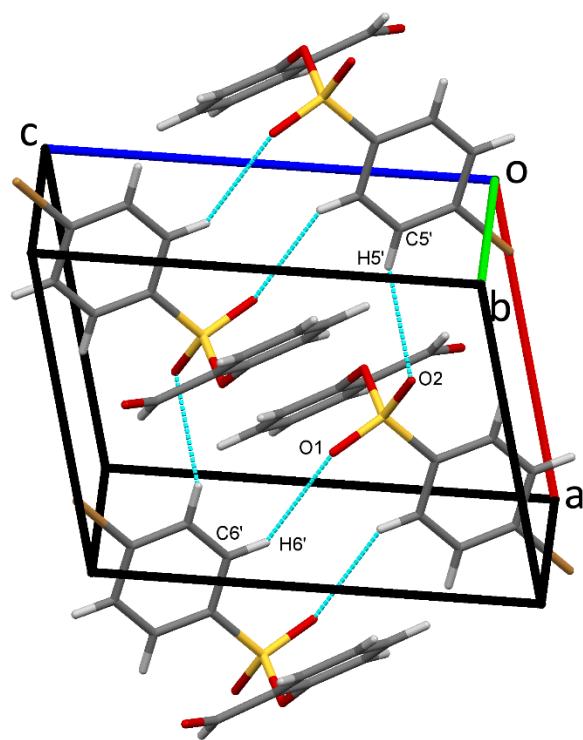
**Figure S7** Zig-zag chains of molecules of **3b** along the *c* axis.



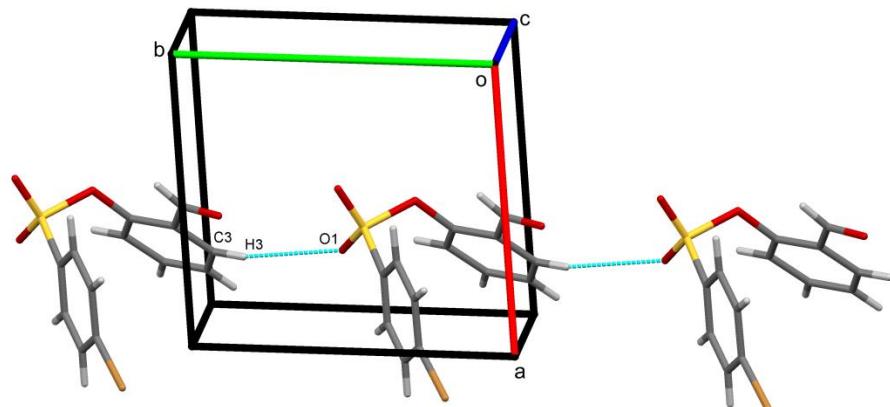
**Figure S8** Overall packing for **3b** viewed along the *c* axis direction.



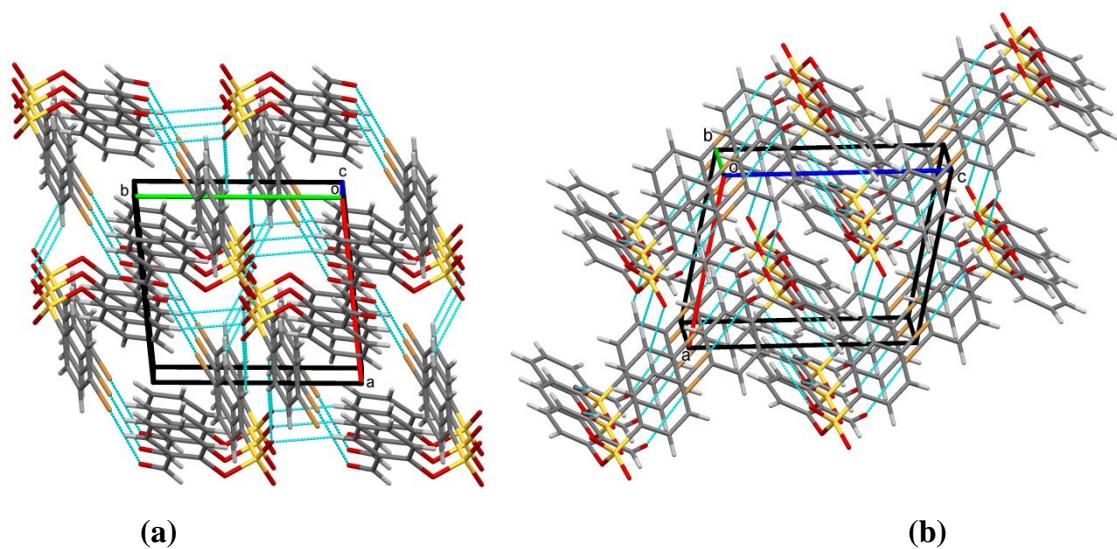
**Figure S9** Double C(6) chains of **3c** molecules along *a*. The Br...π contacts are shown as dotted green lines.



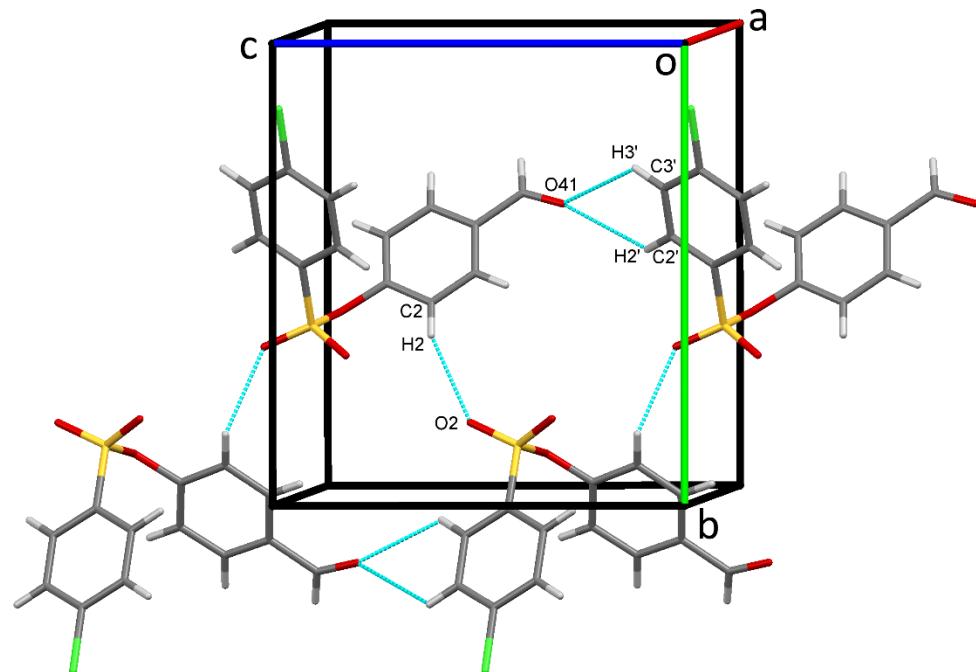
**Figure S10** Inversion dimers of **3c** molecules stacked along the *a* axis direction.



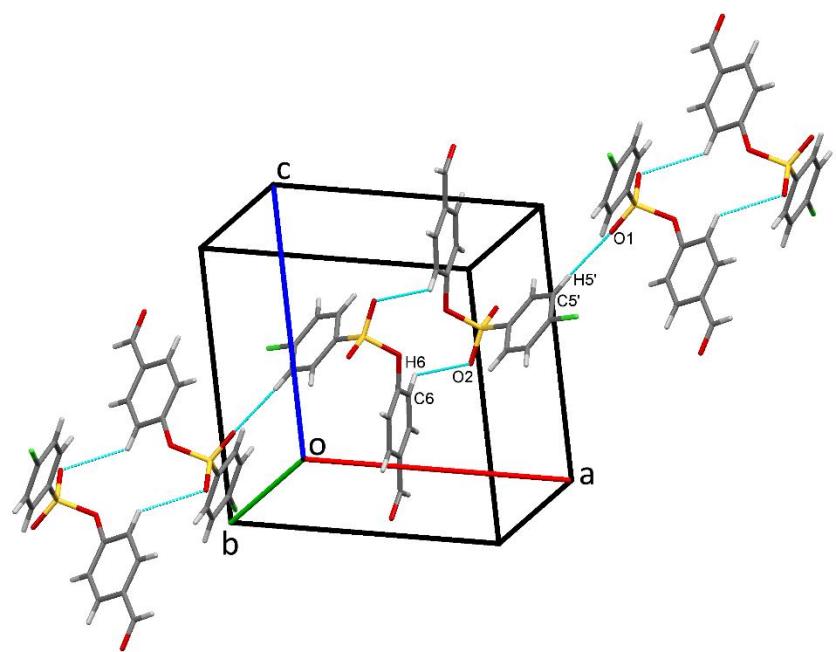
**Figure S11** *C*(7) chains of **3c** molecules along *b*.



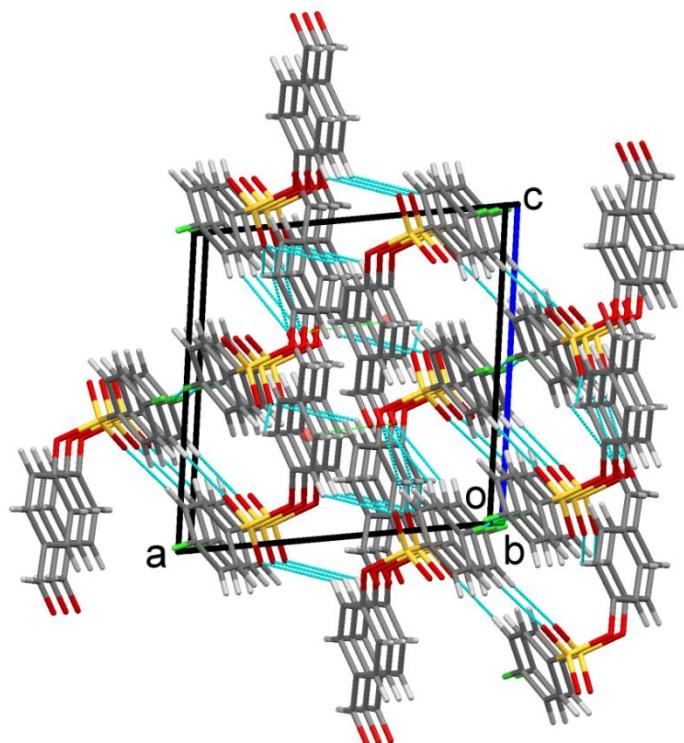
**Figure S12** Two views of the overall packing for **3c** (a) along the *b* and (b) along the *c* axis directions.



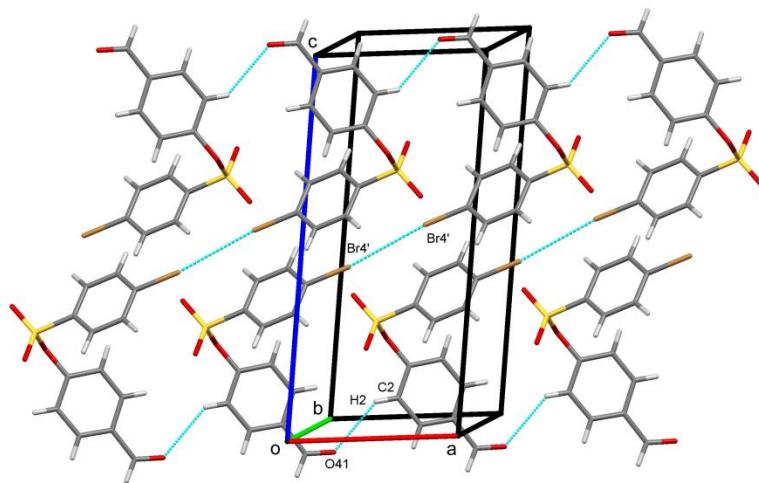
**Figure S13** Double chains of molecules of **4b** along *c*.



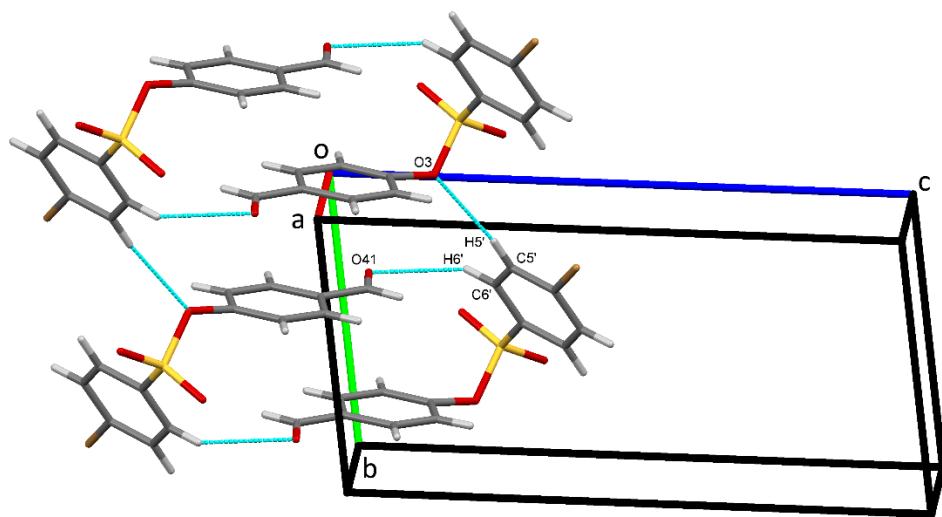
**Figure S14** Chains of inversion dimers of **4b** along the *ac* diagonal.



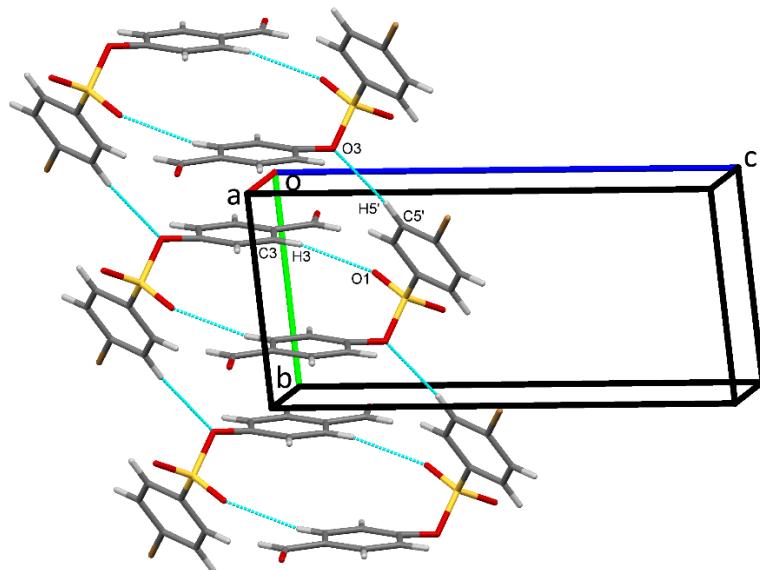
**Figure S15** Overall packing for **4b** viewed along the *b* axis direction.



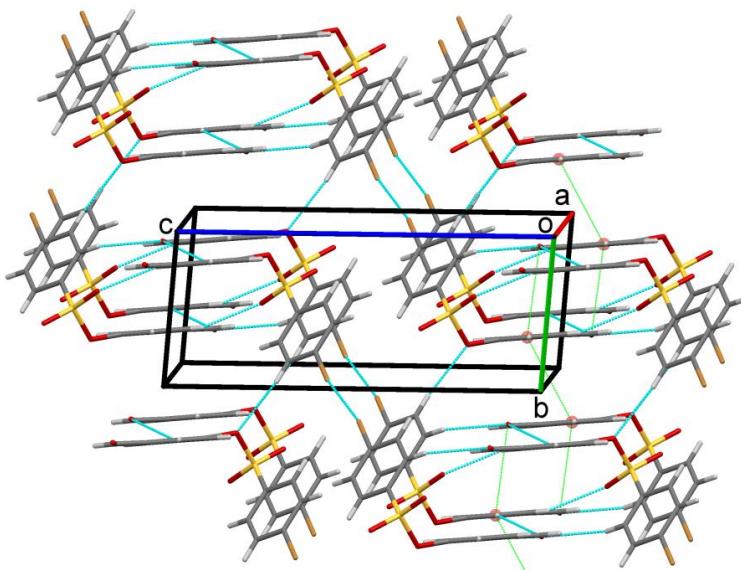
**Figure S16** Sheets of **4c** molecules parallel to (0 1 2).



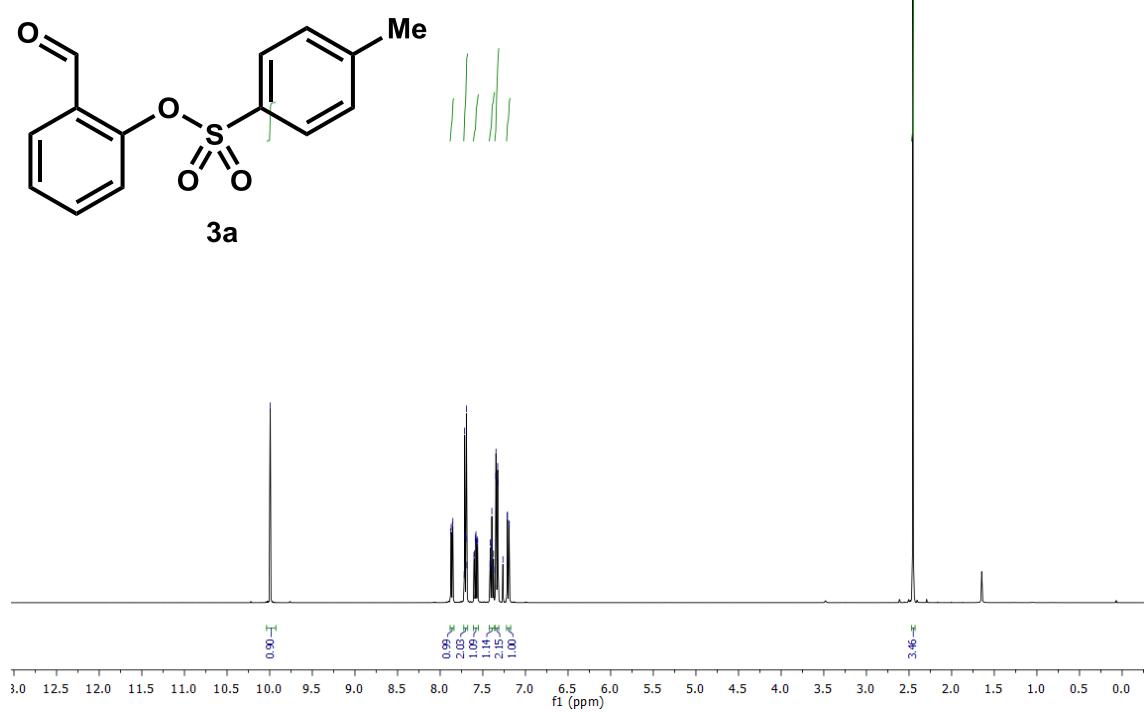
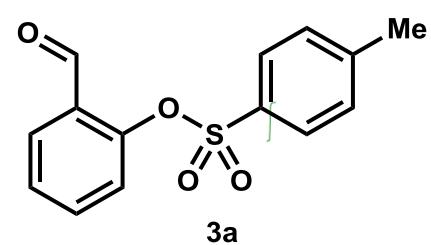
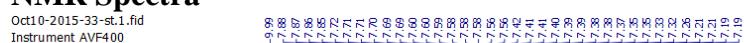
**Figure S17** C6'-H6'...O41 **4c** inversion dimers stacked along *b*.

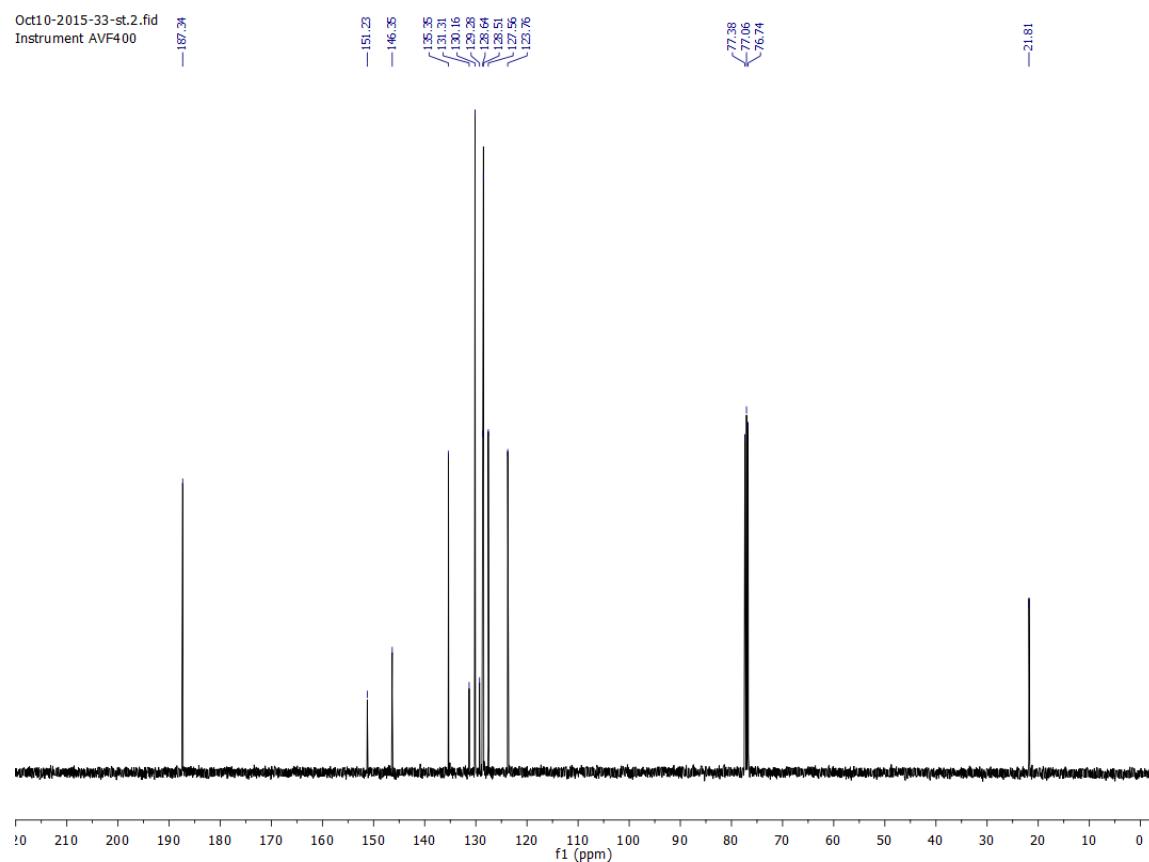


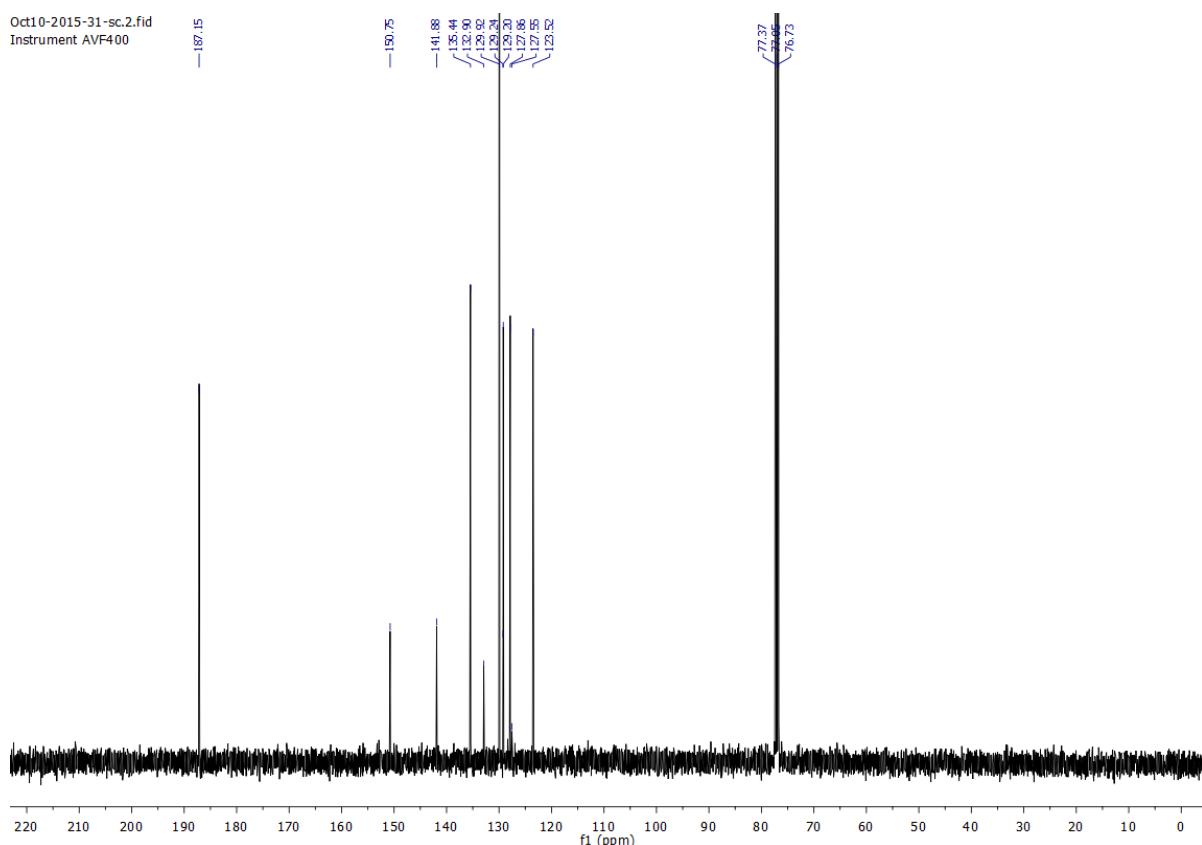
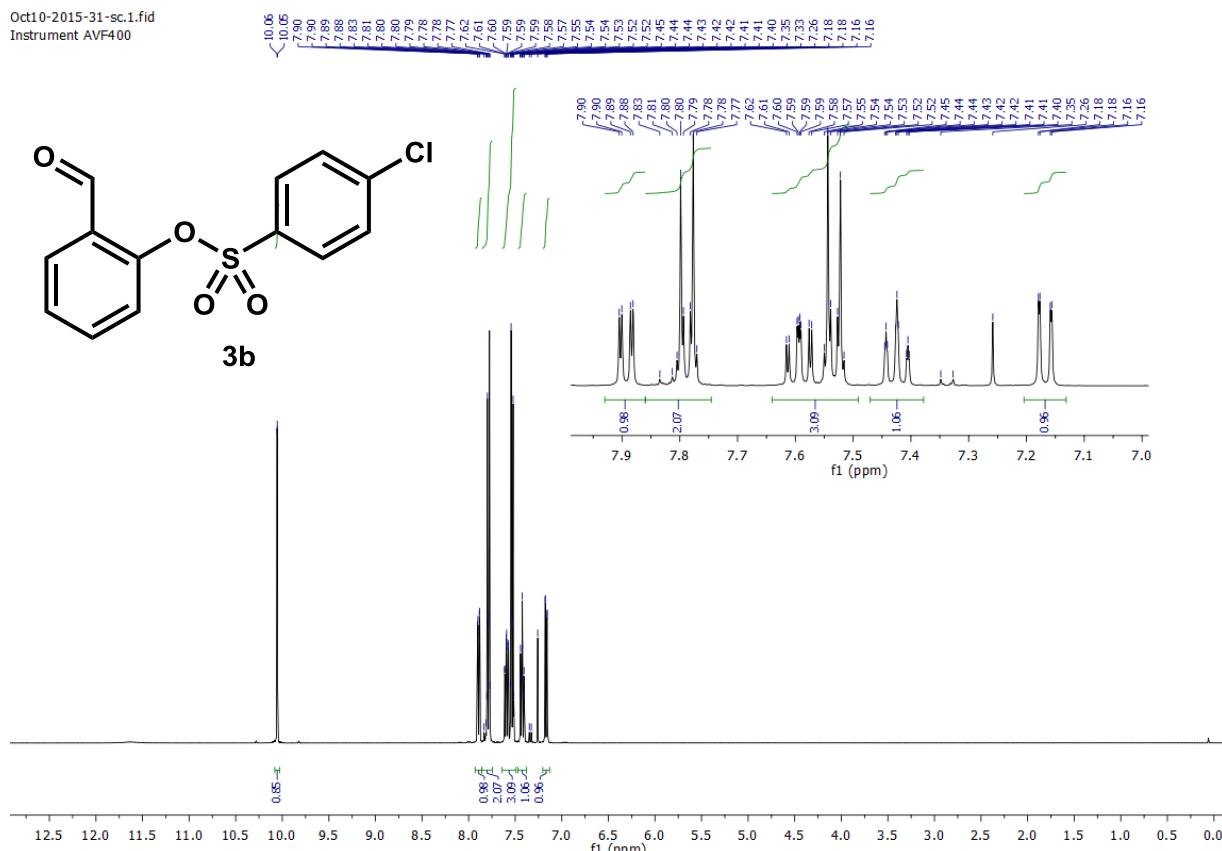
**Figure S18** C3-H3...O1 **4c** inversion dimers stacked along *b*.



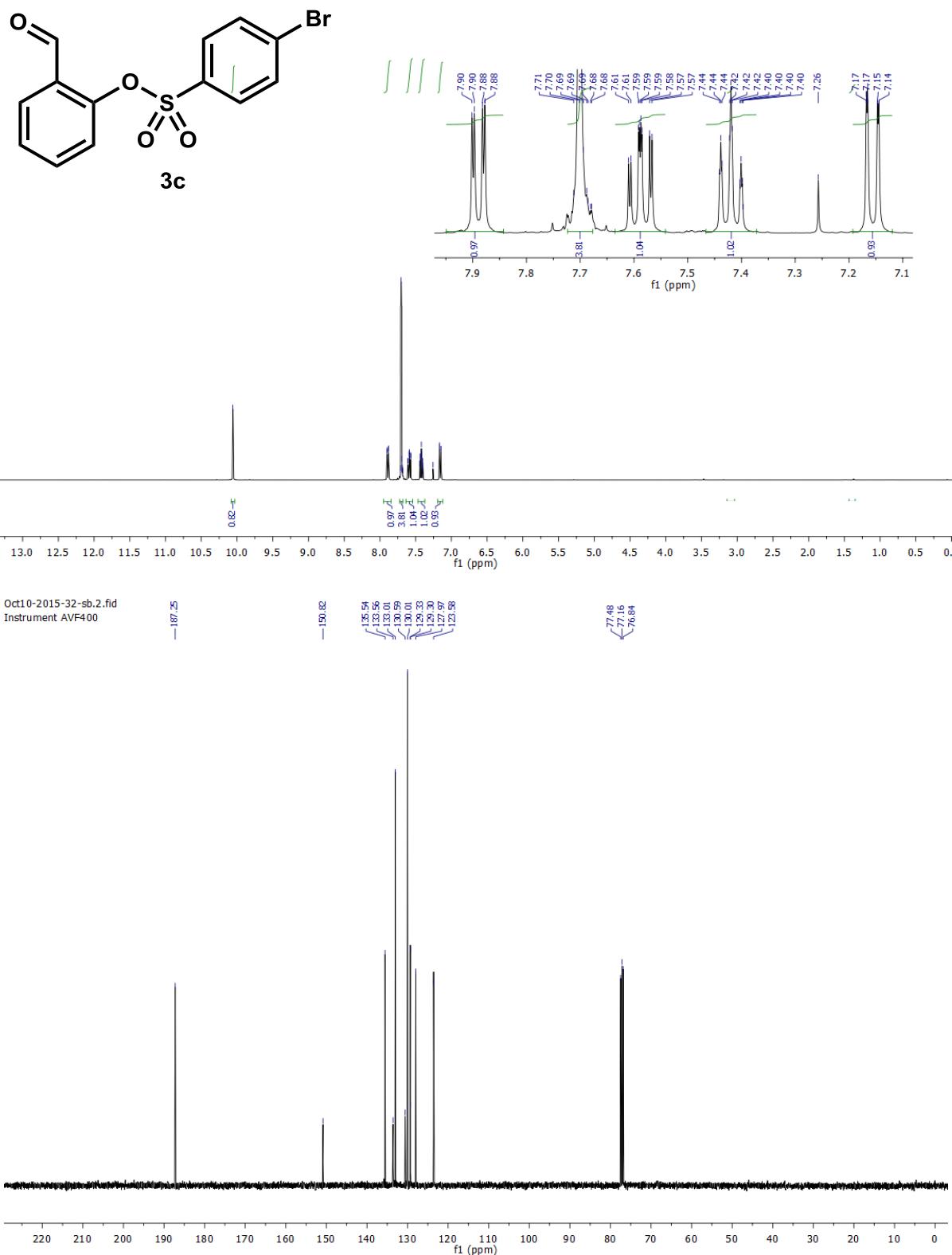
**Figure S19** Overall packing for **4c** viewed along the *a* axis direction with only selected  $\pi \dots \pi$  and  $\text{C}=\text{O} \dots \pi$  contacts shown.

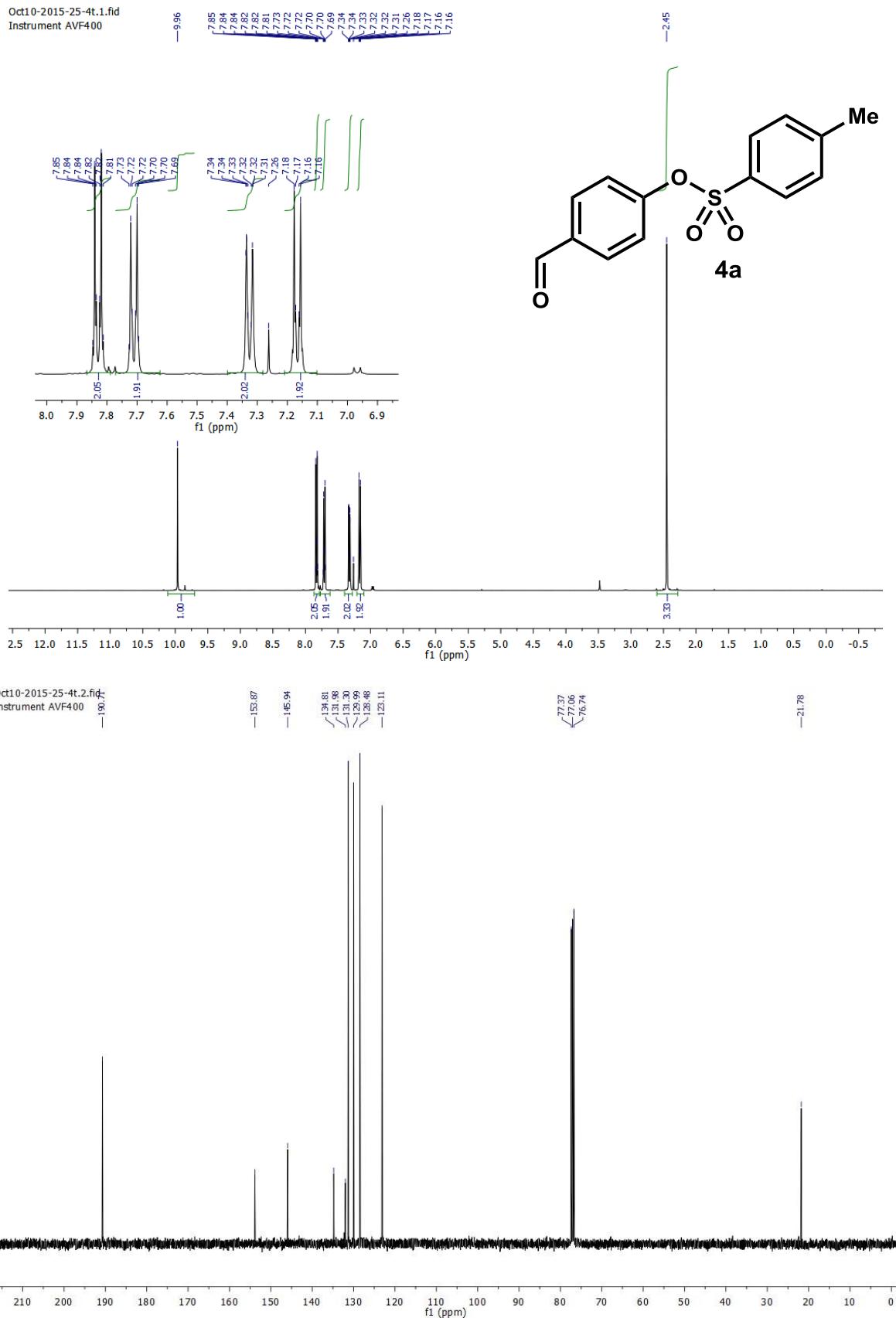
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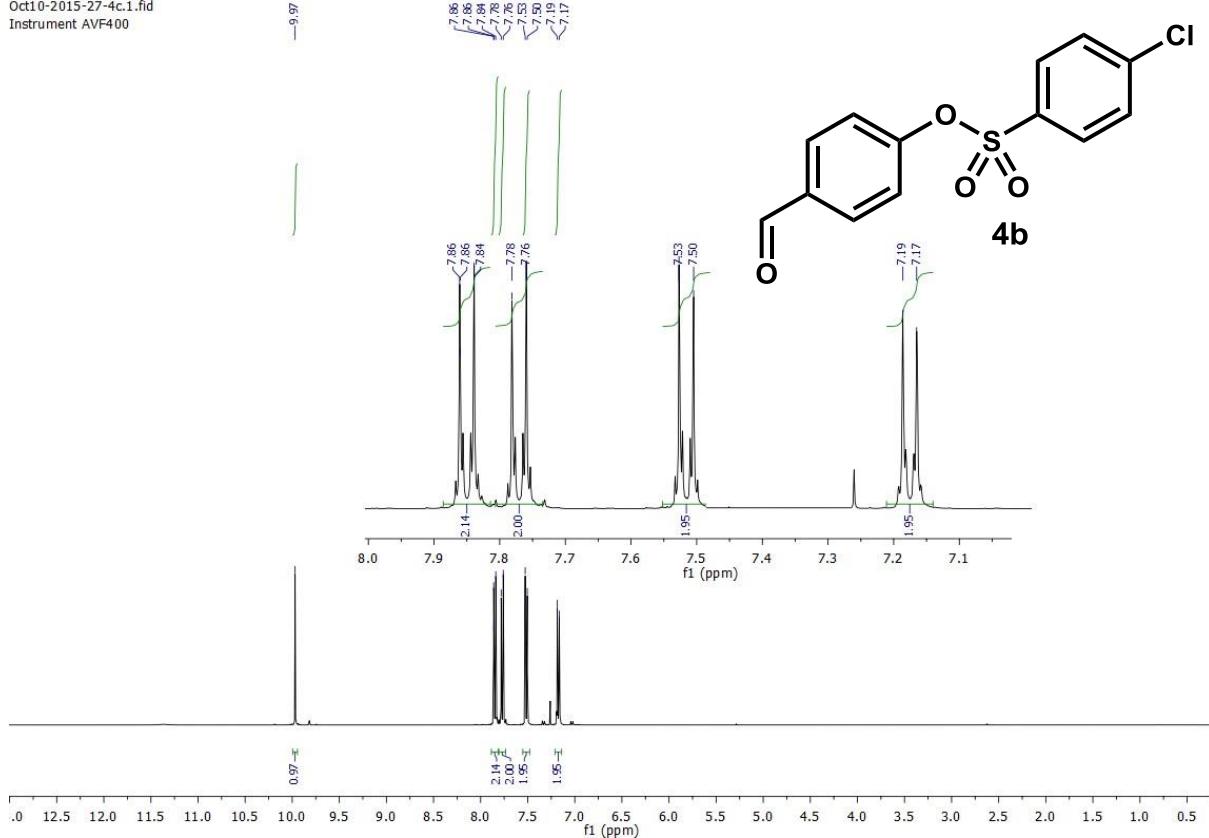


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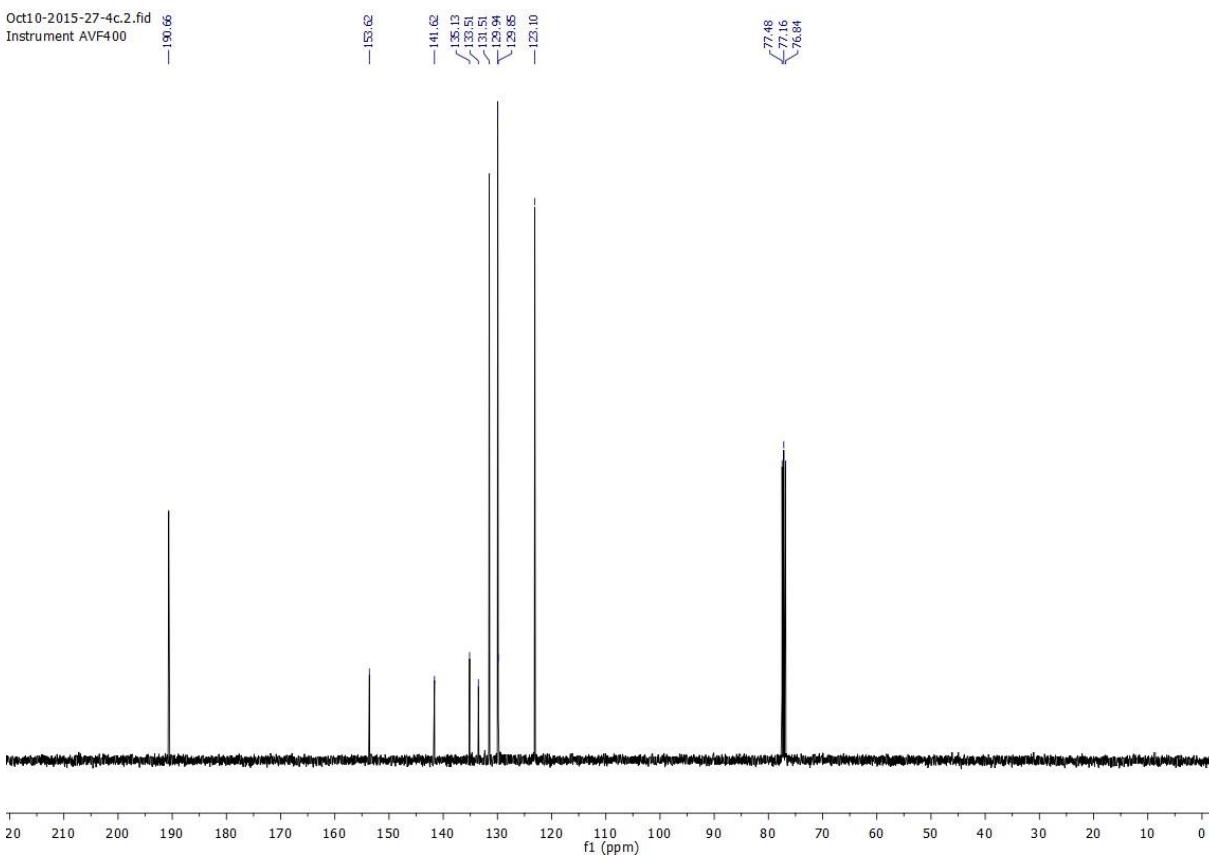


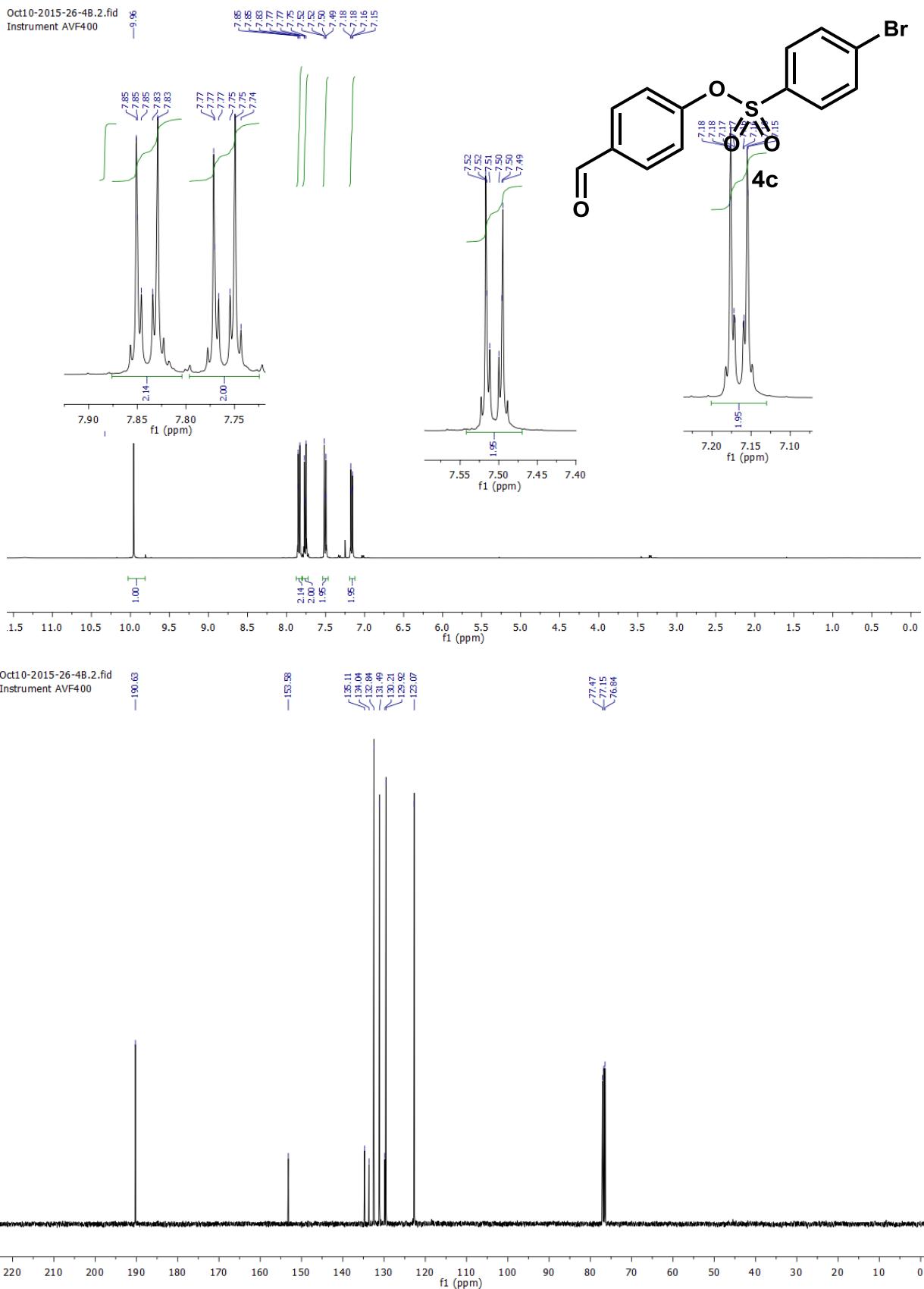


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## FTIR Spectra

