



STRUCTURAL  
CHEMISTRY

**Volume 76 (2020)**

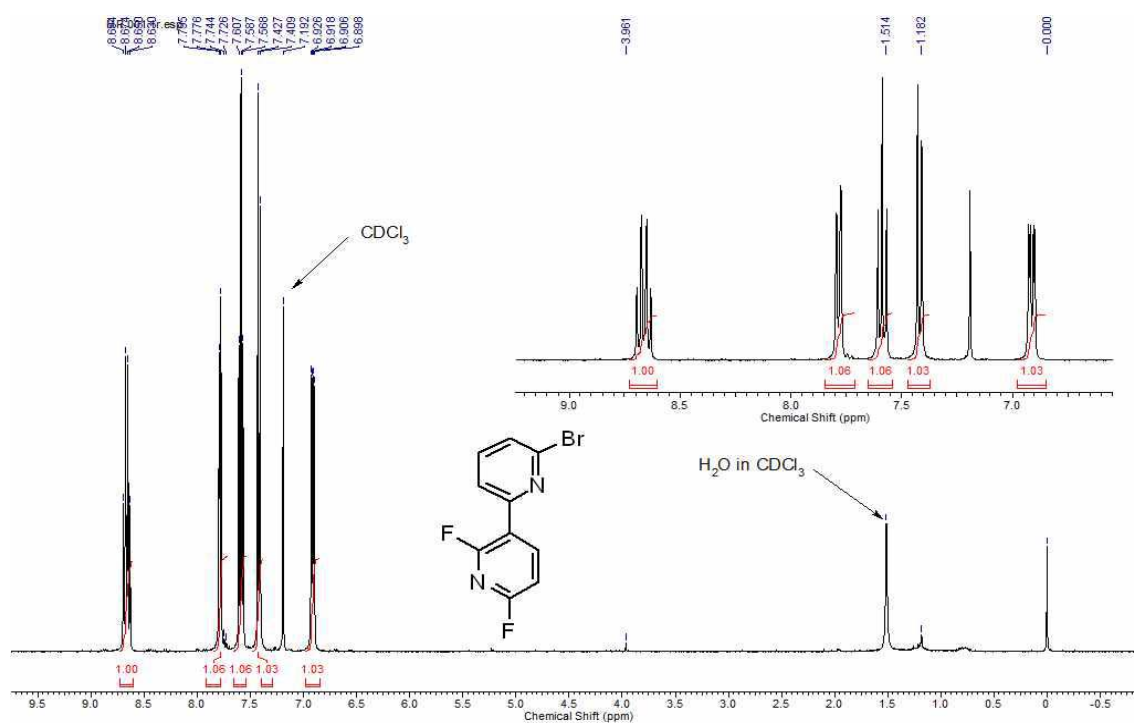
**Supporting information for article:**

**Structures and photophysical properties of two luminescent bipyridine compounds: 2',6'-difluoro-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine and 2',6'-dimethoxy-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine**

**Ki-Min Park, Kiyull Yang, Suk-Hee Moon and Youngjin Kang**

## Contents

- **Figure S1.**  $^1\text{H}$  NMR of **A** in  $\text{CDCl}_3$ .
- **Figure S2.**  $^1\text{H}$  NMR of **B** in  $\text{CDCl}_3$ .
- **Figure S3.**  $^1\text{H}$  NMR of **1** in  $\text{CDCl}_3$ .
- **Figure S4.**  $^{13}\text{C}$  NMR of **1** in  $\text{CDCl}_3$ .
- **Figure S5.**  $^1\text{H}$  NMR of **2** in  $\text{CDCl}_3$ .
- **Figure S6.**  $^{13}\text{C}$  NMR of **2** in  $\text{CDCl}_3$ .
- **Figure S7.** Mass data of **1**.
- **Figure S8.** Mass data of **2**.
- **Figure S9.** The two-dimensional fingerprint plots for the compounds (a) **1** and (b) **2**, and those delineated into overall,  $\text{H}\cdots\text{H}$ ,  $\text{H}\cdots\text{C}/\text{C}\cdots\text{H}$ ,  $\text{H}\cdots\text{F}/\text{F}\cdots\text{H}$ ,  $\text{H}\cdots\text{N}/\text{N}\cdots\text{H}$  and  $\text{H}\cdots\text{O}/\text{O}\cdots\text{H}$  contacts. Mass data of **2**. The  $d_i$  and  $d_e$  values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface contacts.
- **Figure S10.** Diagram showing the surfaces of HOMO and LUMO for **2**.



**Figure S1.**  $^1\text{H}$  NMR of A in  $\text{CDCl}_3$ .

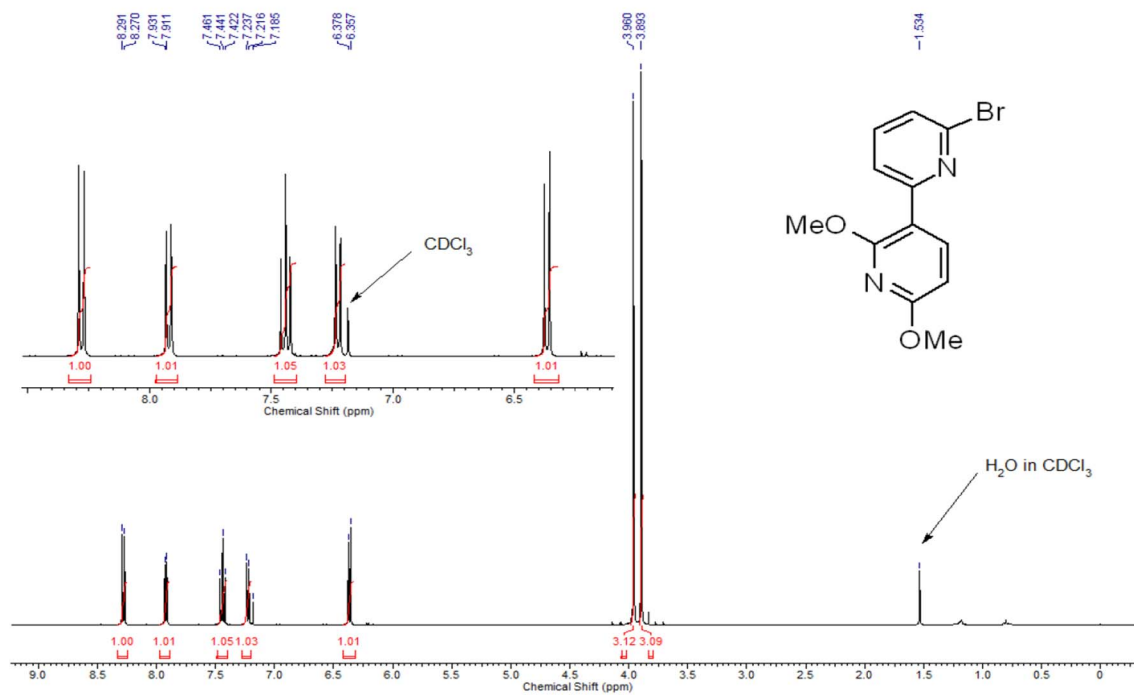
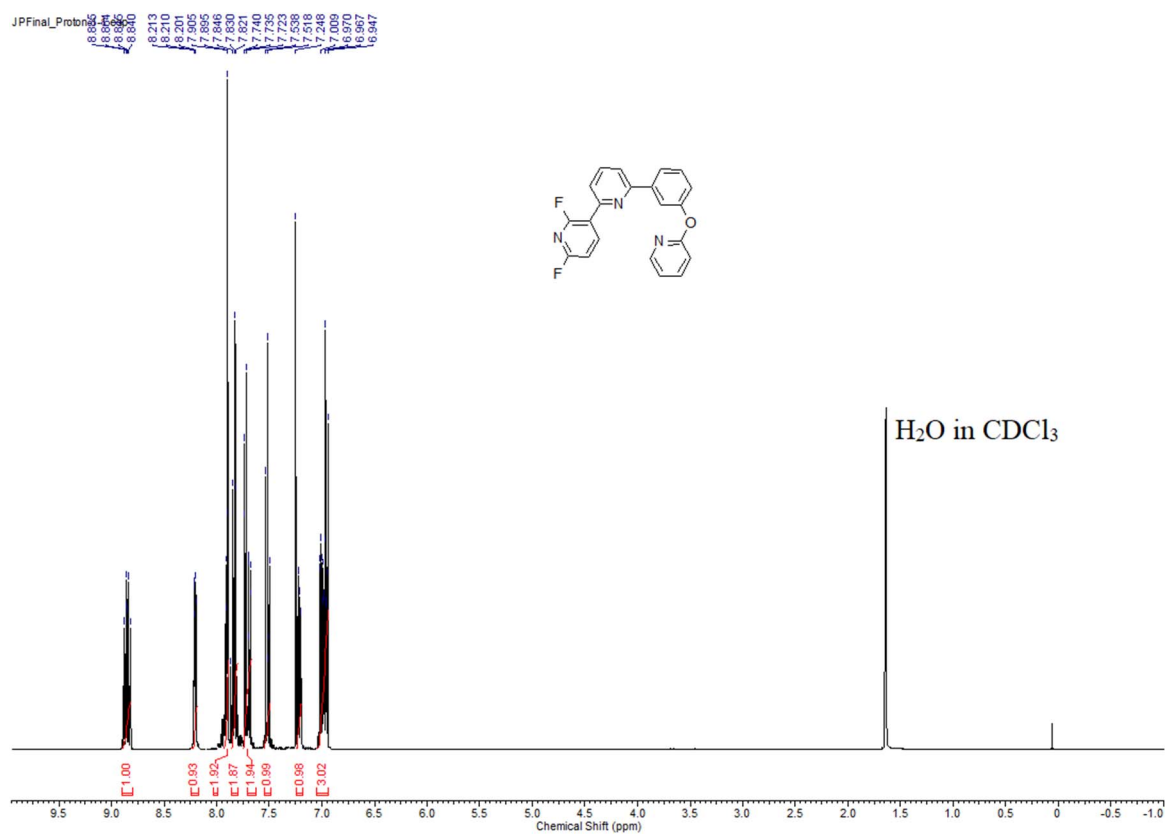
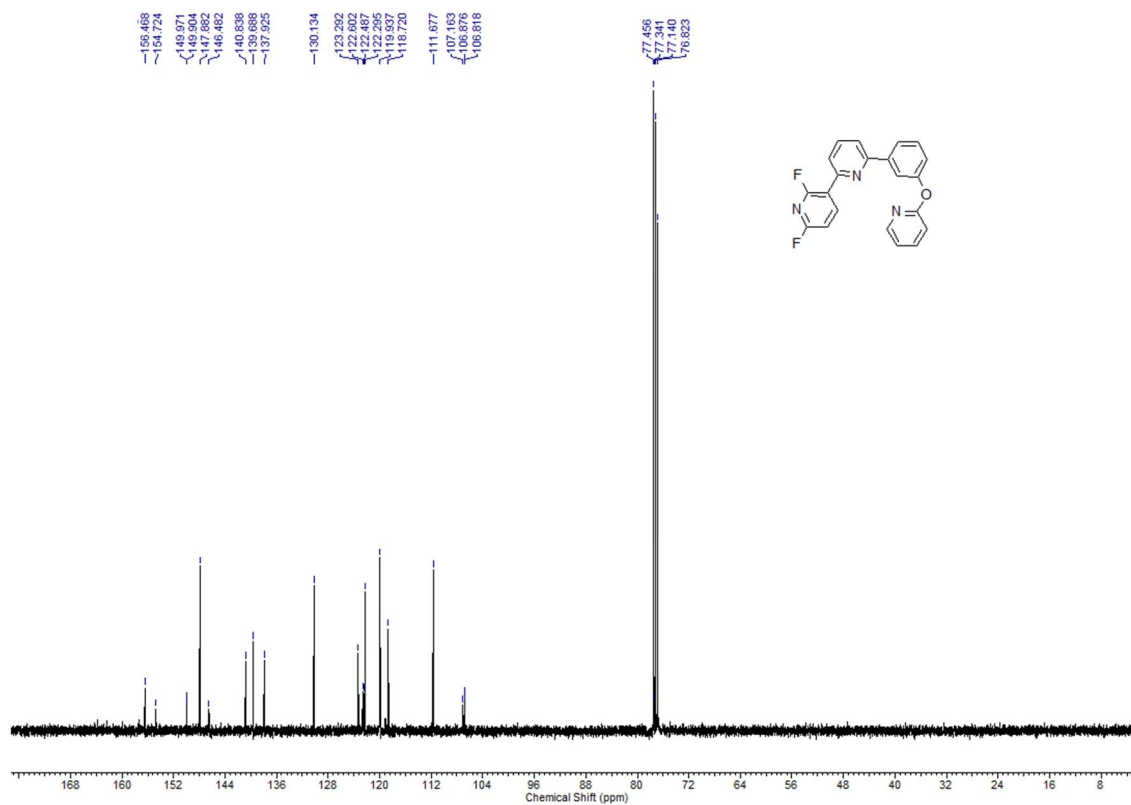
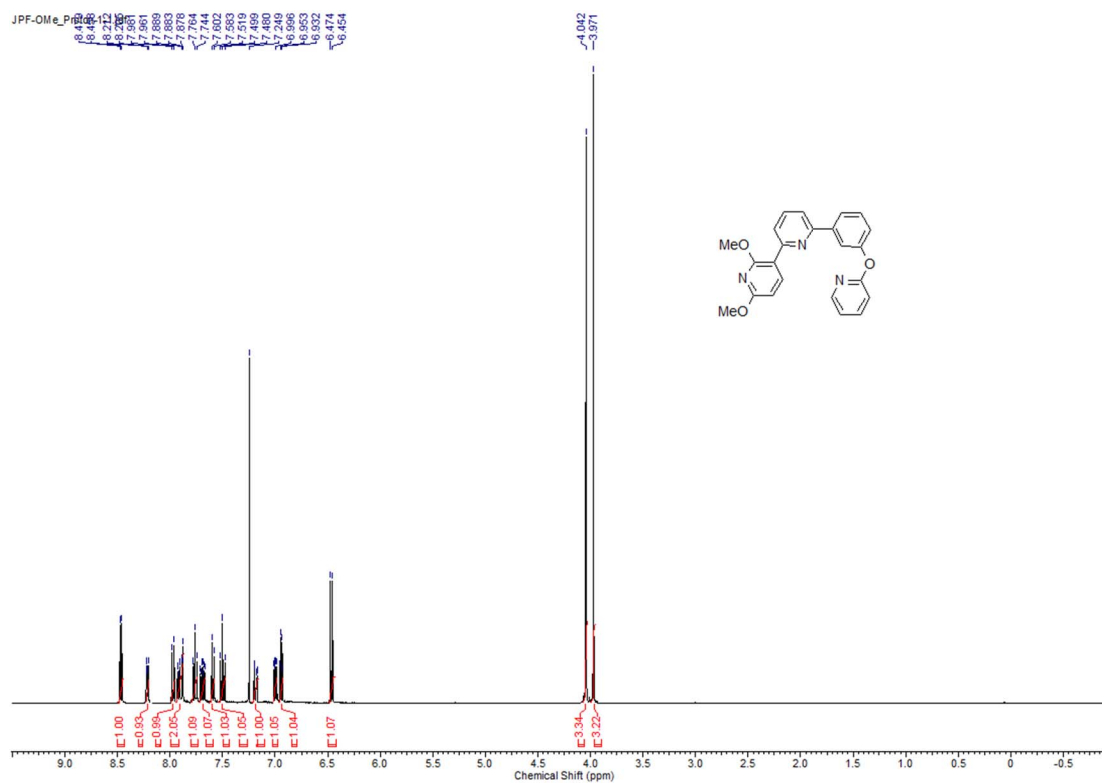


Figure S2.  $^1\text{H}$  NMR of **B** in  $\text{CDCl}_3$ .Figure S3.  $^1\text{H}$  NMR of **1** in  $\text{CDCl}_3$ 

**Figure S4.**  $^{13}\text{C}$  NMR of **1** in  $\text{CDCl}_3$ .

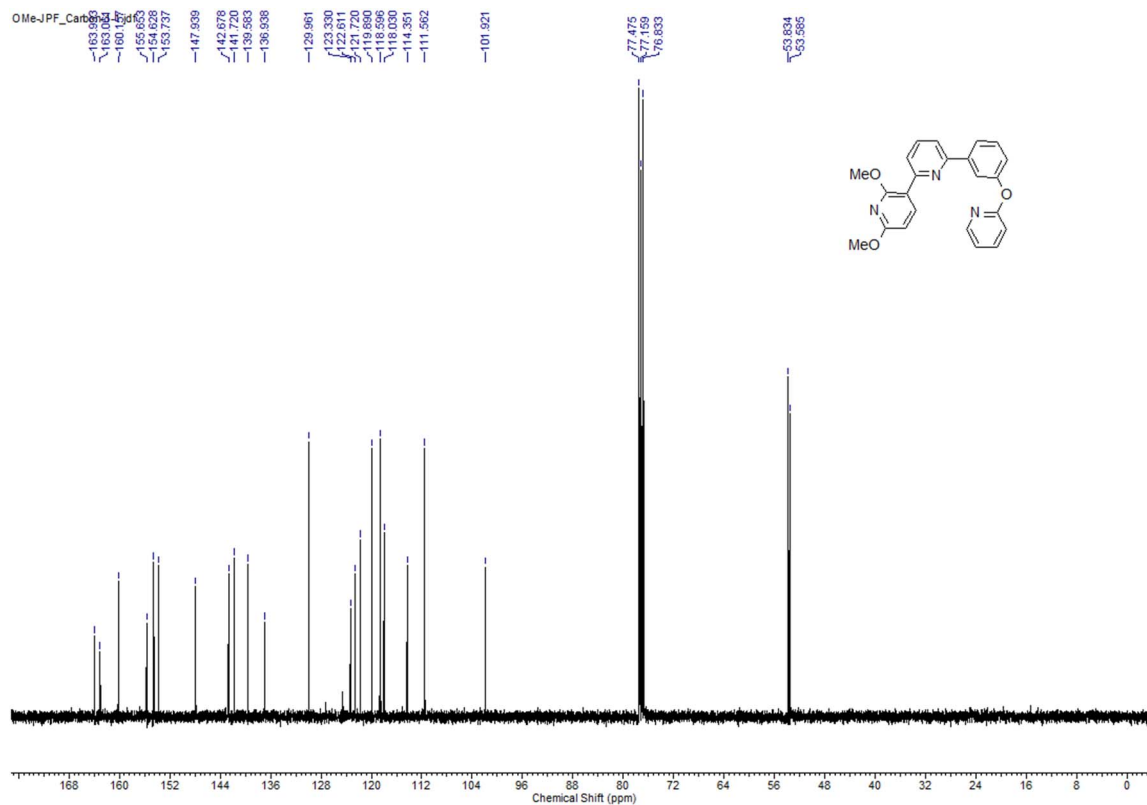


Figure S6.  $^{13}\text{C}$  NMR of **2** in  $\text{CDCl}_3$ .

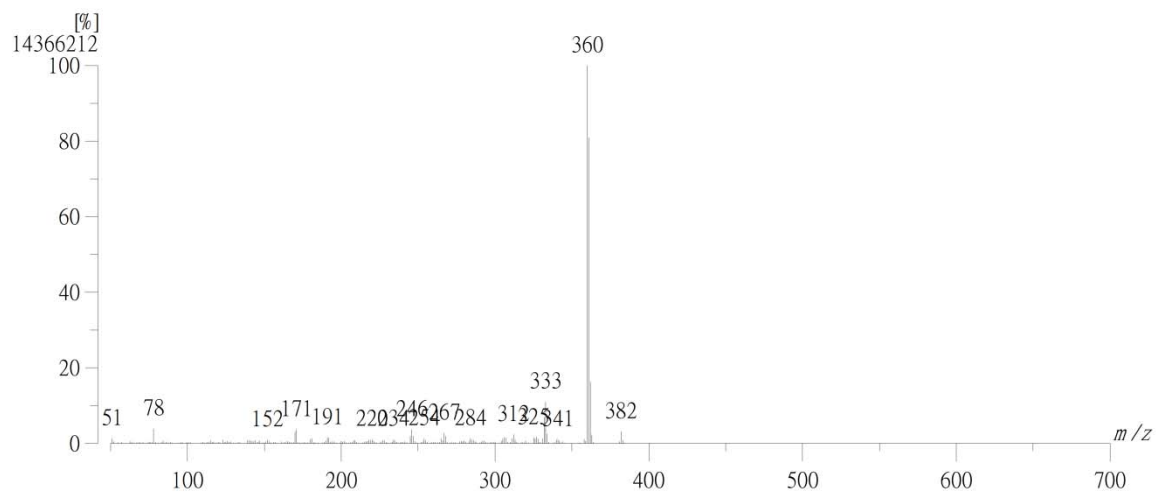


Figure S7. Mass data of **1**.

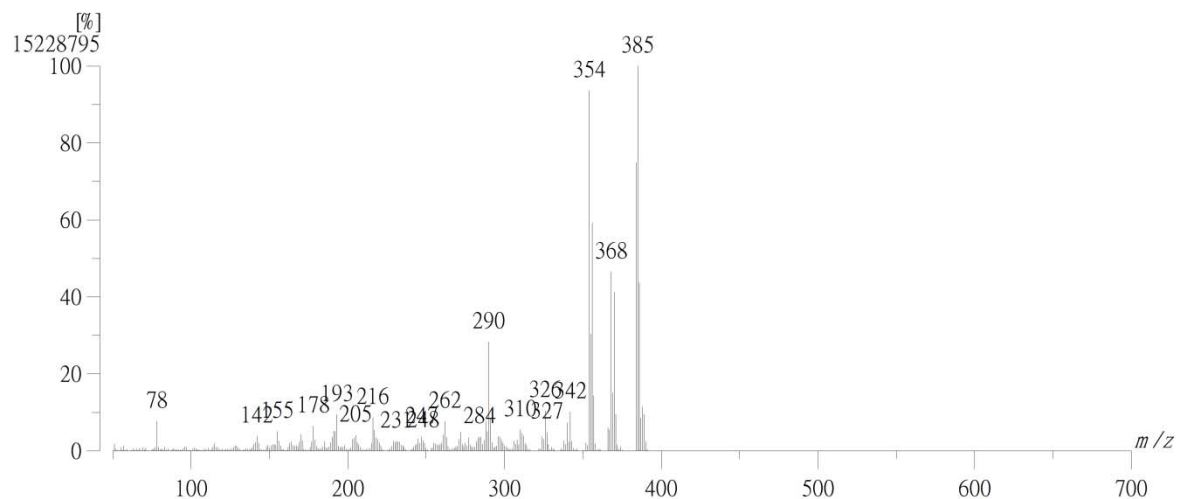
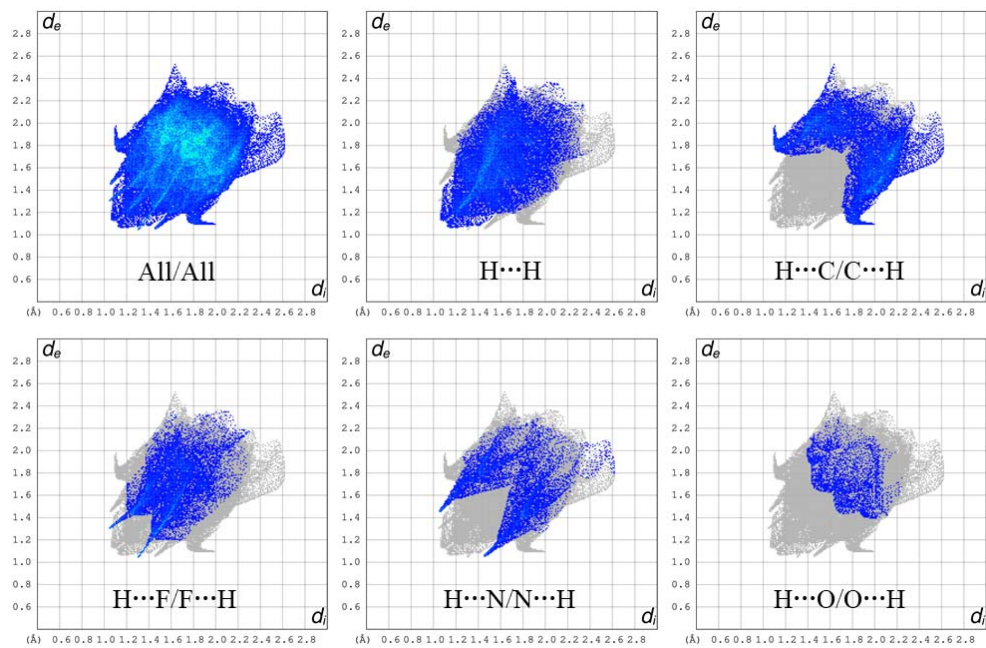
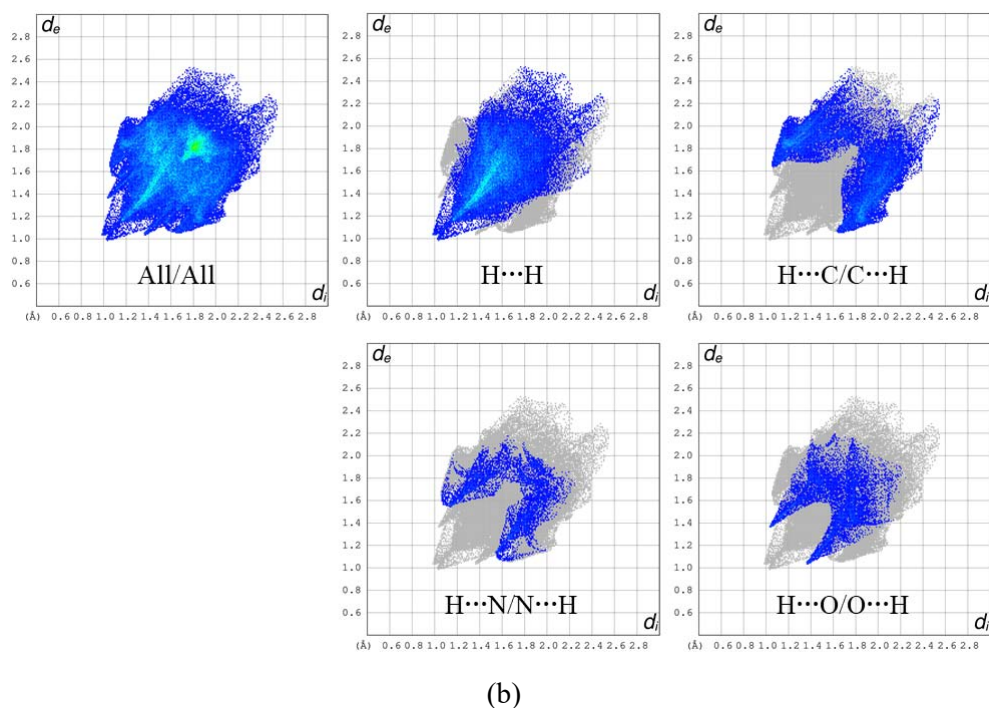


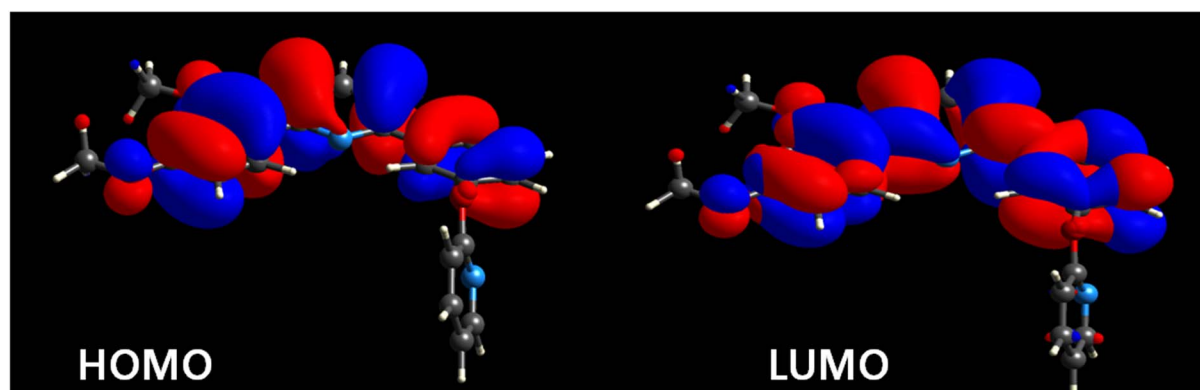
Figure S8. Mass data of 2.



(a)



**Figure S9.** The two-dimensional fingerprint plots for the compounds (a) **1** and (b) **2**, and those delineated into overall, H...H, H...C/C...H, H...F/F...H, H...N/N...H and H...O/O...H contacts. Mass data of **2**. The  $d_i$  and  $d_e$  values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface contacts.



**Figure S10.** Diagram showing the surfaces of HOMO and LUMO for **2**.