

Supporting Information

D-A-D 2*H*-benzo[*d*]1,2,3-triazole derivatives as p-type semiconductors in Organic Field-Effect Transistors (OFETs).

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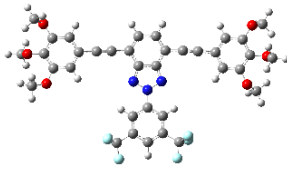
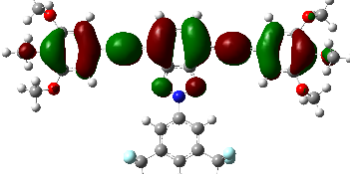
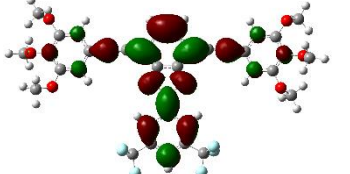

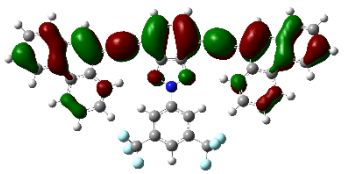
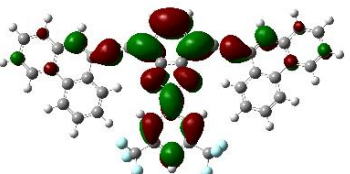
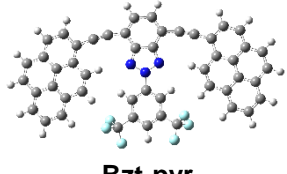
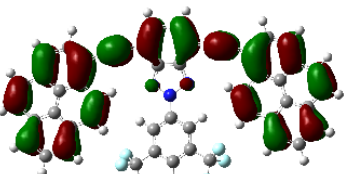
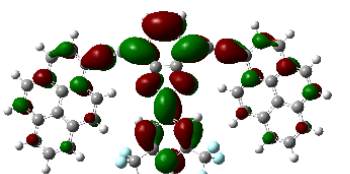
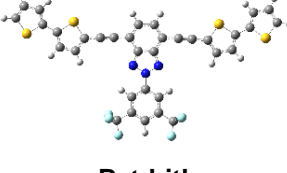
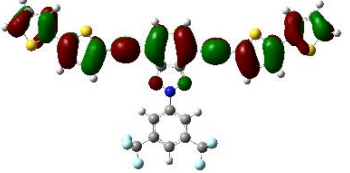
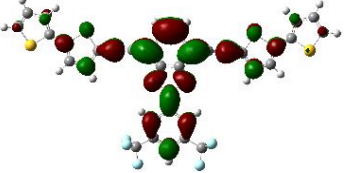
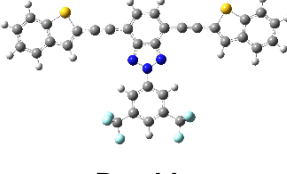
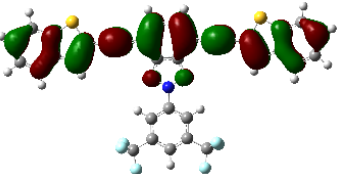
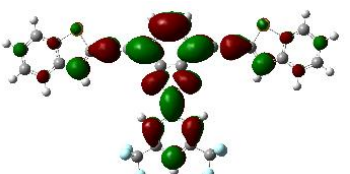
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1. Topology of frontier molecular orbitals.

COMPOUND	HOMO	LUMO	BAND GAP (eV)
 <p>Bzt-OCH₃</p>	 <p>-5.29 eV</p>	 <p>-2.48 eV</p>	2.81
 <p>Bzt-phe</p>	 <p>-5.29 eV</p>	 <p>-2.65 eV</p>	2.64
 <p>Bzt-pyr</p>	 <p>-5.07 eV</p>	 <p>-2.68 eV</p>	2.39
 <p>Bzt-bith</p>	 <p>-5.10 eV</p>	 <p>-2.71 eV</p>	2.39
 <p>Bzt-thbz</p>	 <p>-5.10 eV</p>	 <p>-2.83 eV</p>	2.27

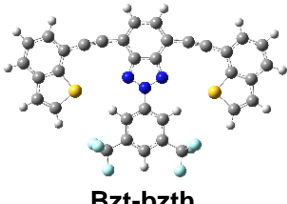
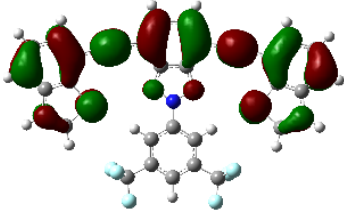
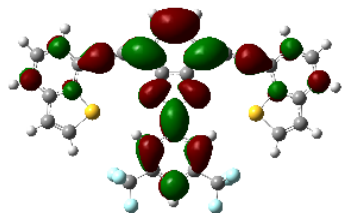
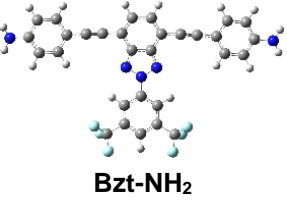
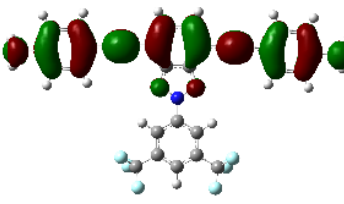
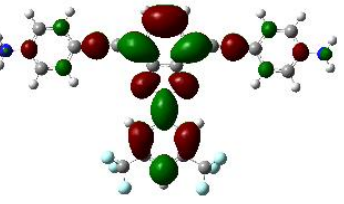
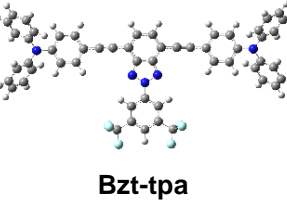
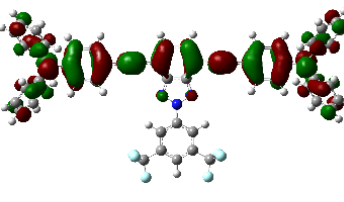
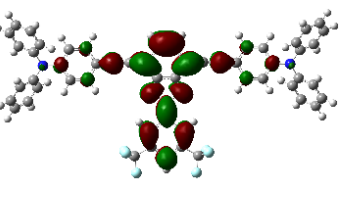
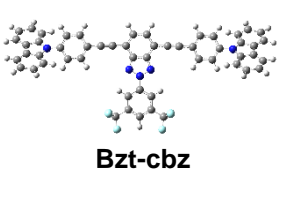
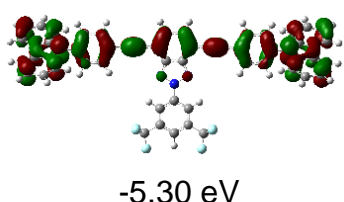
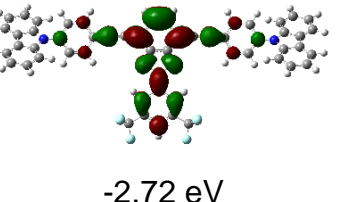
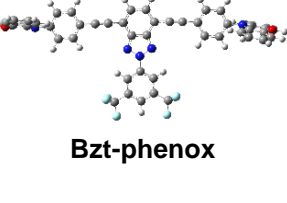
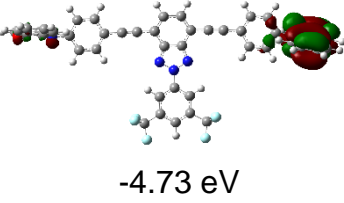
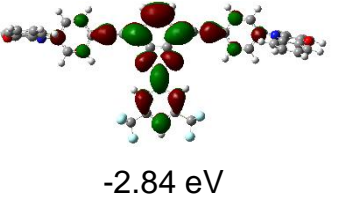
 <p>Bzt-bzth</p>	 <p>-5.41 eV</p>	 <p>-2.64 eV</p>	2.77
 <p>Bzt-NH₂</p>	 <p>-4.91 eV</p>	 <p>-2.43 eV</p>	2.48
 <p>Bzt-tpa</p>	 <p>-4.81 eV</p>	 <p>-2.42 eV</p>	2.39
 <p>Bzt-cbz</p>	 <p>-5.30 eV</p>	 <p>-2.72 eV</p>	2.58
 <p>Bzt-phenox</p>	 <p>-4.73 eV</p>	 <p>-2.84 eV</p>	1.89

Table S1. Topology of frontier molecular orbital computed at B3LYP/6-31G(d,p) of the synthesized compounds.

2. Emission spectra

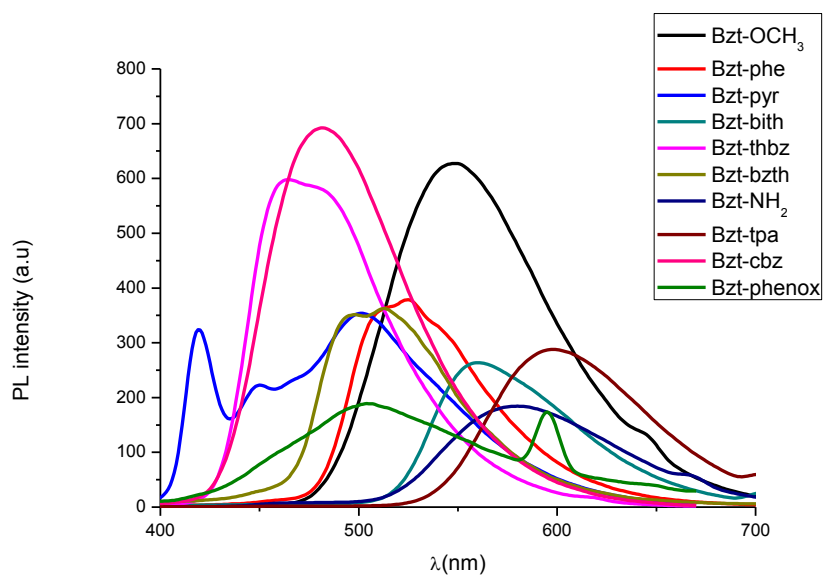


Figure S1. UV/Visible emission spectra of compounds **Bzt-Ar** (298 K, CHCl₃, 1 x 10⁻⁵ M)

3. CV Voltammograms

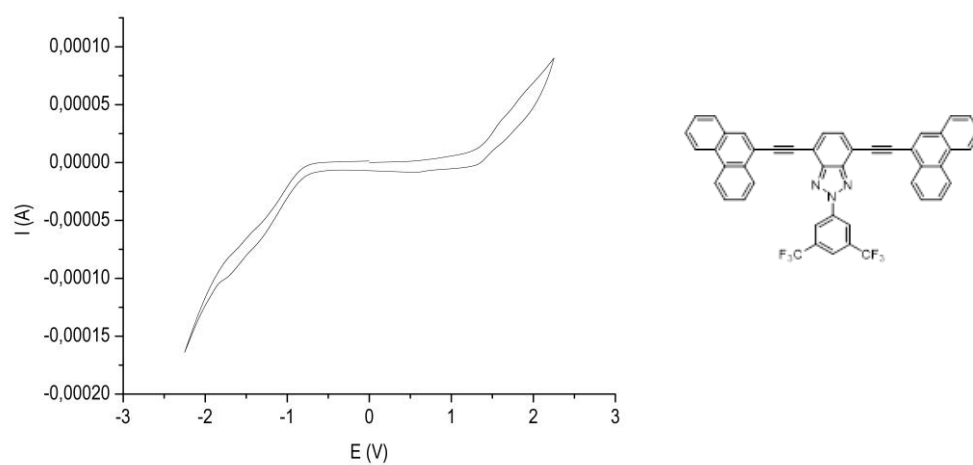


Figure S2. Cyclic Voltammograms of compound **Bzt-phe**.

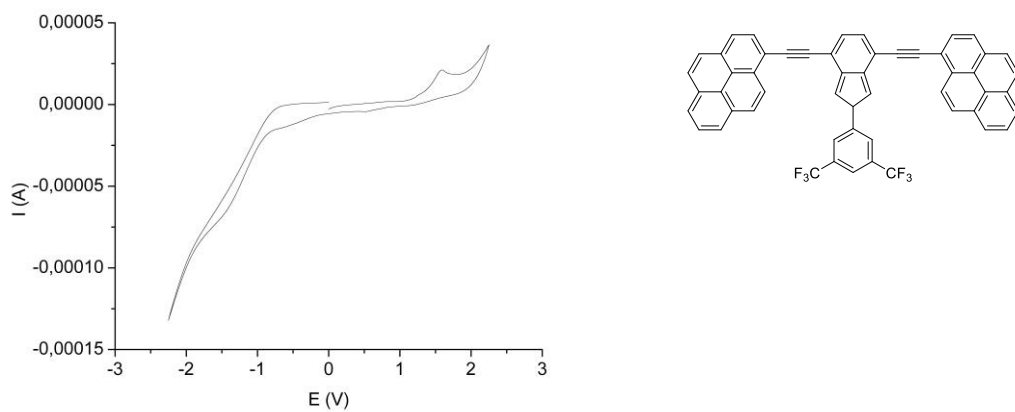


Figure S3. Cyclic Voltammograms of compound **Bzt-pyr**.

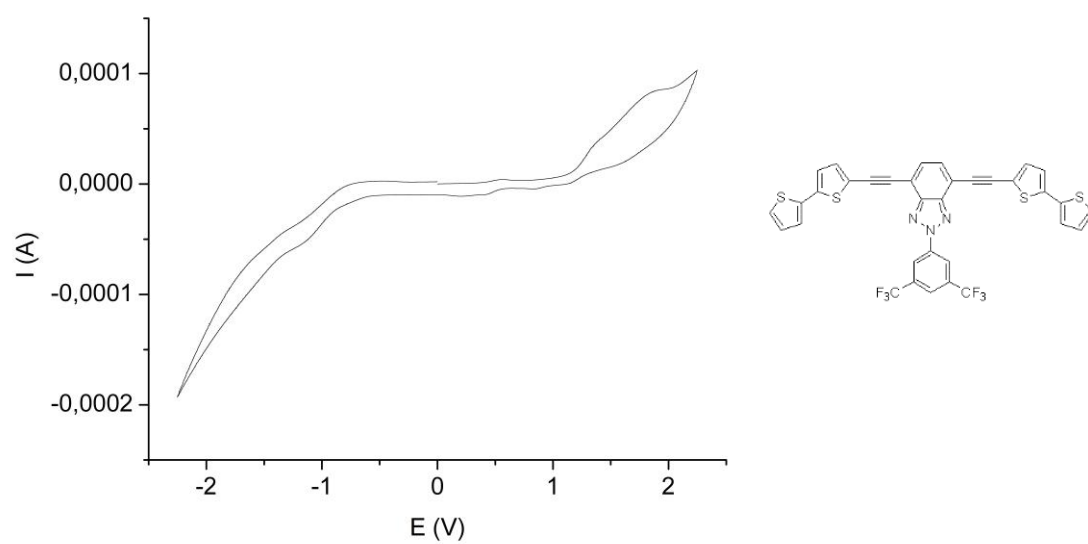


Figure S4. Cyclic Voltammograms of compound **Bzt-bith**.

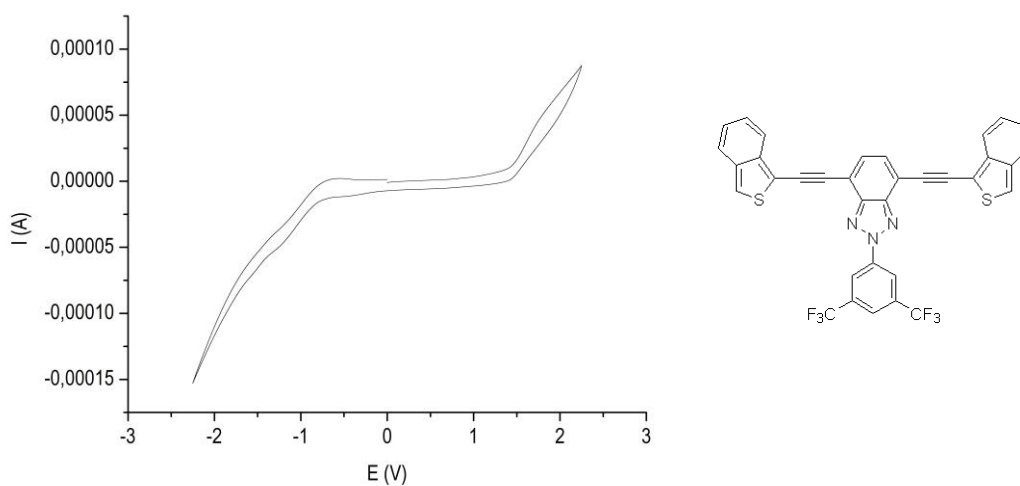


Figure S5. Cyclic Voltammograms of compound **Bzt-thbz**.

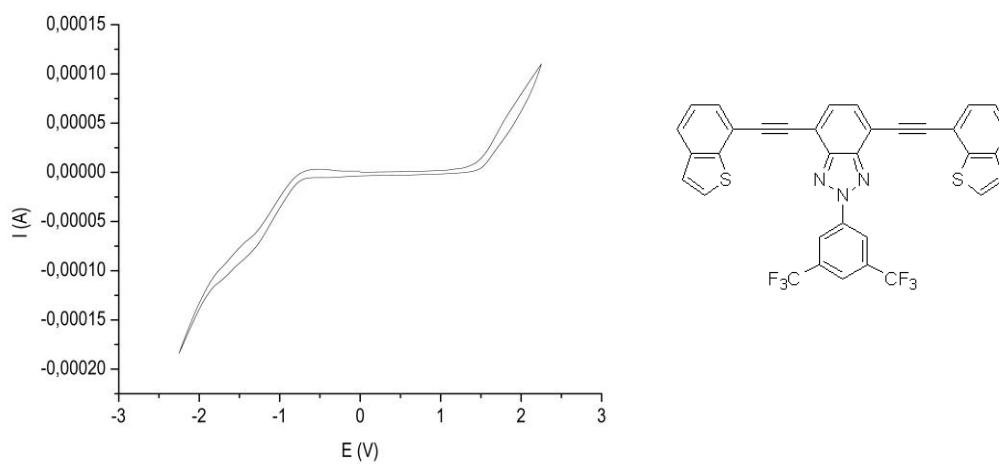


Figure S6. Cyclic Voltammograms of compound **Bzt-bzth**.

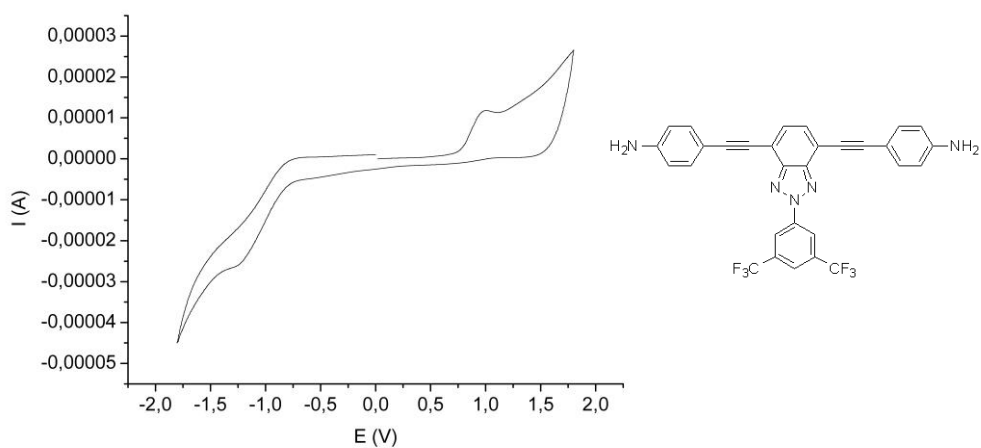


Figure S7. Cyclic Voltammograms of compound **Bzt-NH₂**.

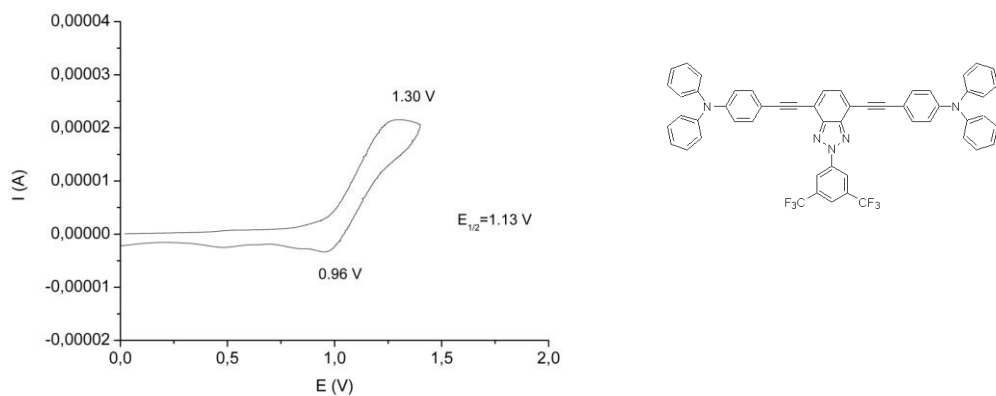


Figure S8. Cyclic Voltammograms of compound **Bzt-tpa**.

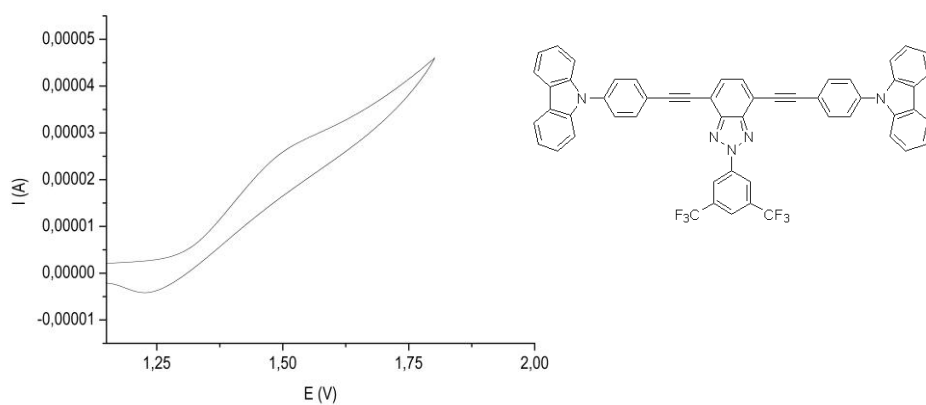


Figure S9. Cyclic Voltammograms of compound **Bzt-cbz**.

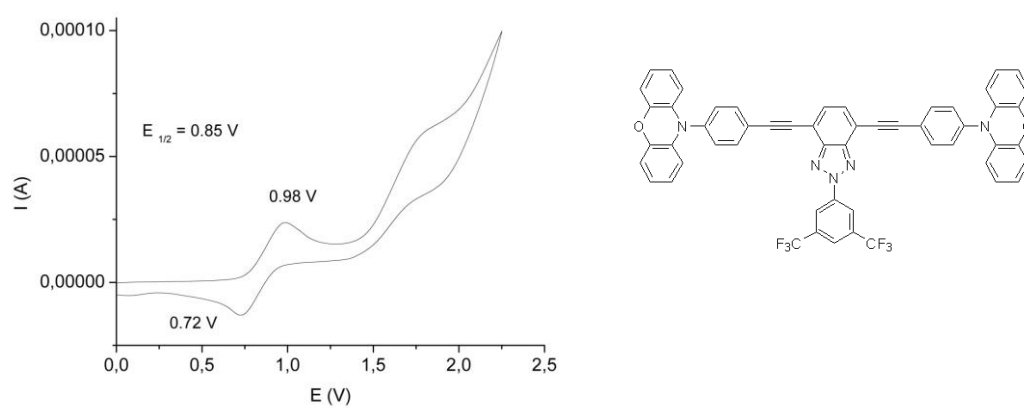


Figure S10. Cyclic Voltammograms of compound **Bzt-phenox**.

4. Theoretical and experimental Raman.

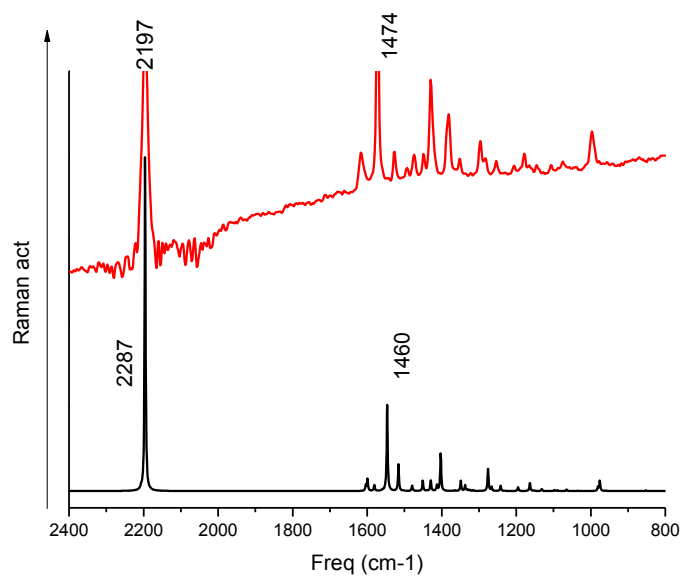


Figure S11. Comparison between experimental Raman spectra (red) and theoretical Raman spectra (black) for **Bzt-phe**. Theoretical data were calculated by B3LYP/6-31G(d,p).

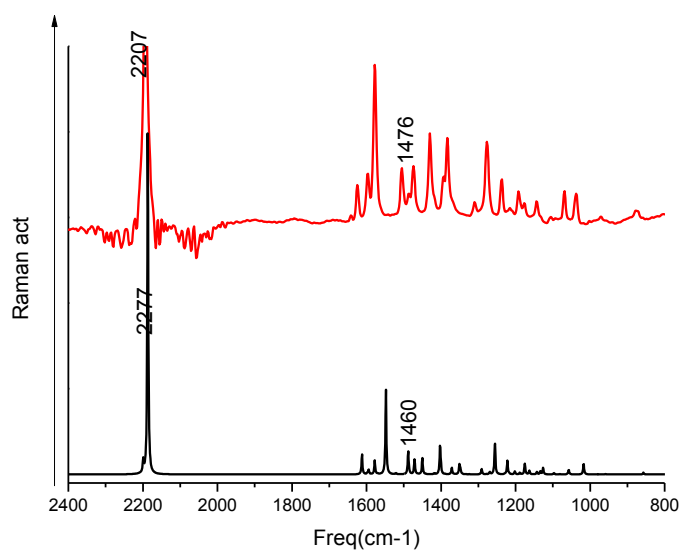


Figure S12. Comparison between experimental Raman spectra (red) and theoretical Raman spectra (black) for **Bzt-pyr**. Theoretical data were calculated by B3LYP/6-31G(d,p).

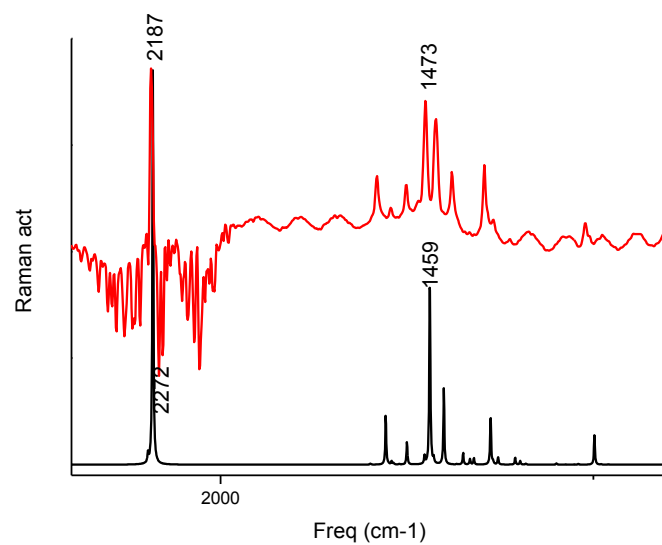


Figure S13. Comparison between experimental Raman spectra (red) and theoretical Raman spectra (black) for **Bzt-bith**. Theoretical data were calculated by B3LYP/6-31G(d,p).

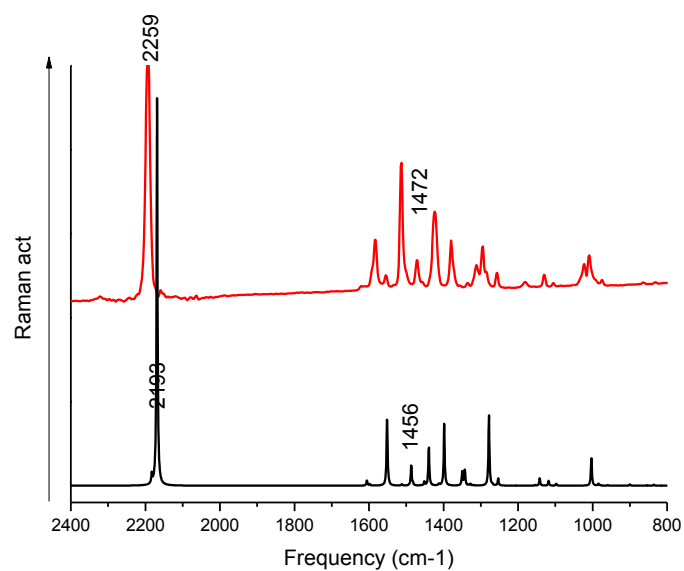


Figure S14. Comparison between experimental Raman spectra (red) and theoretical Raman spectra (black) for **Bzt-thbz**. Theoretical data were calculated by B3LYP/6-31G(d,p).

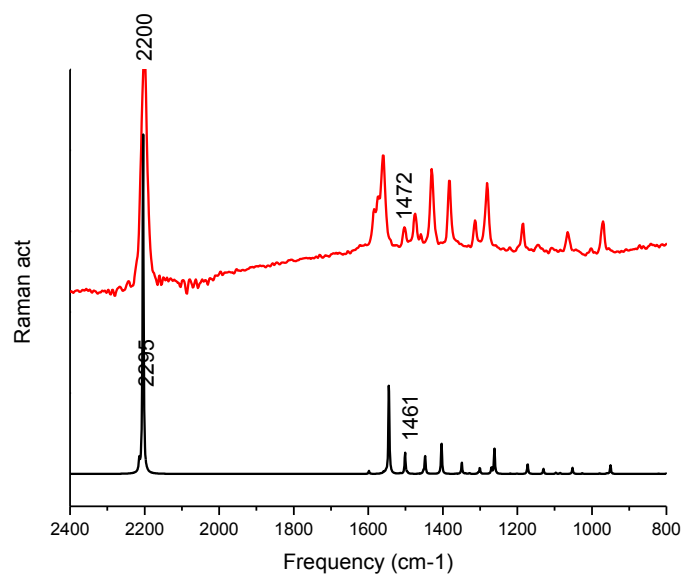


Figure S15. Comparison between experimental Raman spectra (red) and theoretical Raman spectra (black) for **Bzt-bzth**. Theoretical data were calculated by B3LYP/6-31G(d,p).

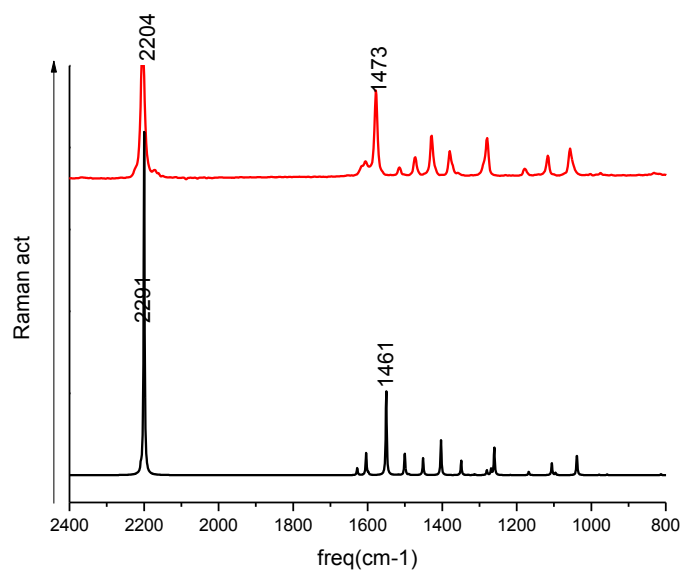


Figure S16. Comparison between experimental Raman spectra (red) and theoretical Raman spectra (black) for **Bzt-NH₂**. Theoretical data were calculated by B3LYP/6-31G(d,p).

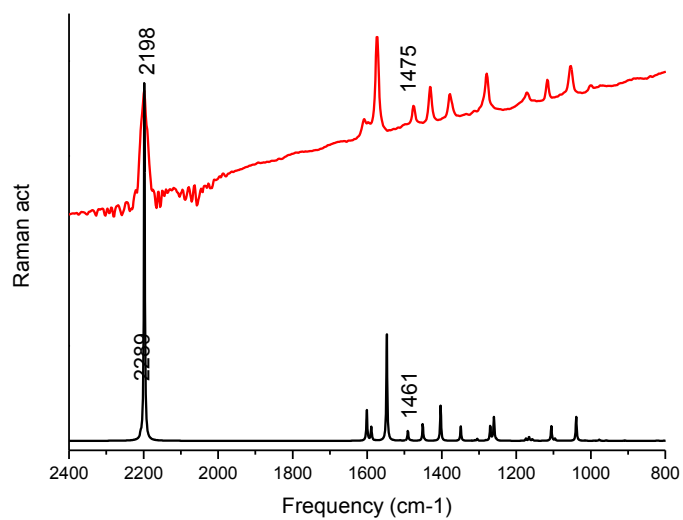


Figure S17. Comparison between experimental Raman spectra (red) and theoretical Raman spectra (black) for **Bzt-tpa**. Theoretical data were calculated by B3LYP/6-31G(d,p).

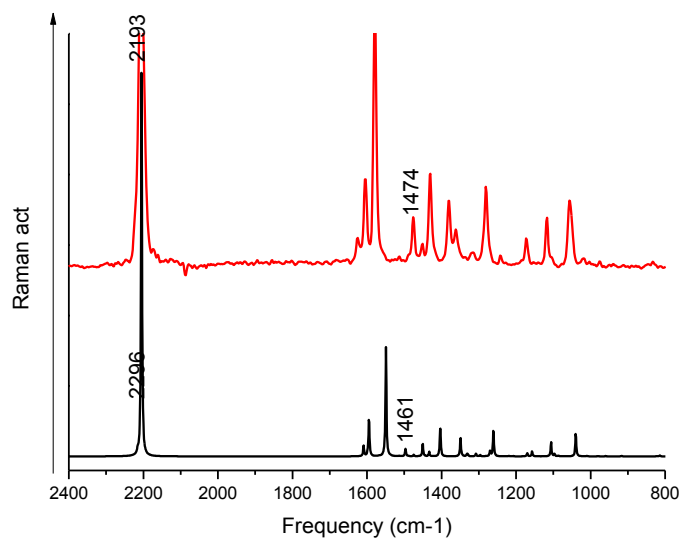


Figure S18. Comparison between experimental Raman spectra (red) and theoretical Raman spectra (black) for **Bzt-cbz**. Theoretical data were calculated by B3LYP/6-31G(d,p).

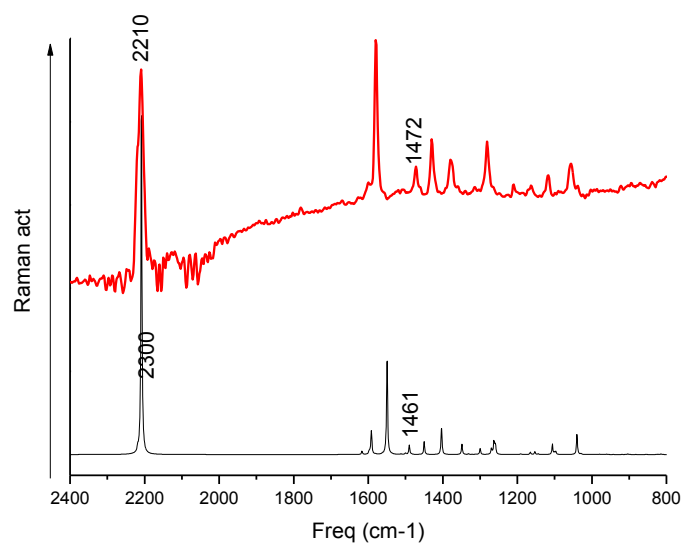


Figure S19. Comparison between experimental Raman spectra (red) and theoretical Raman spectra (black) for **Bzt-phenox**. Theoretical data were calculated by B3LYP/6-31G(d,p).