Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Synthesis of tunable, red fluorescent aggregation enhanced emissive organic fluorophores: Stimuli responsive high contrast off-on fluorescence switching

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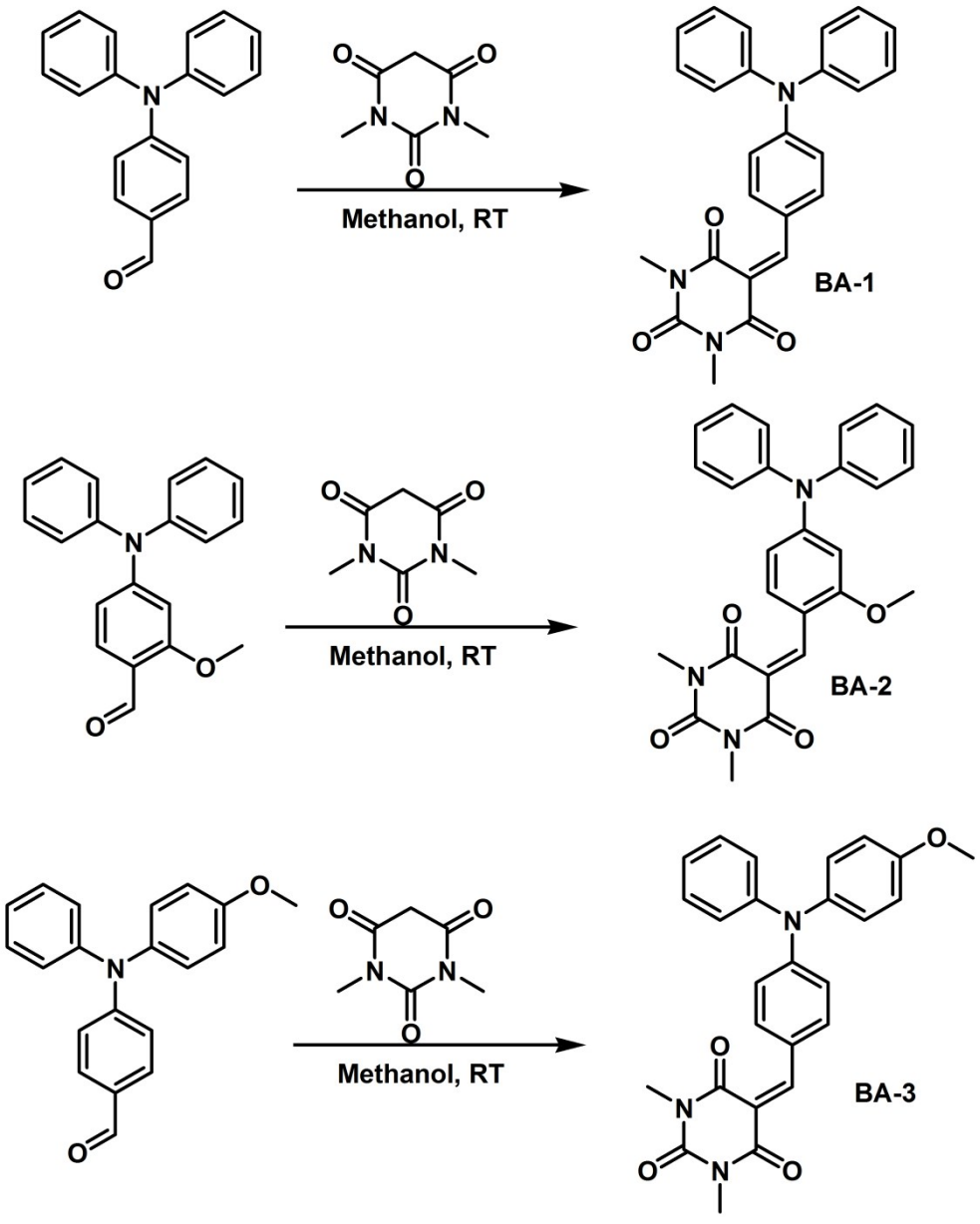
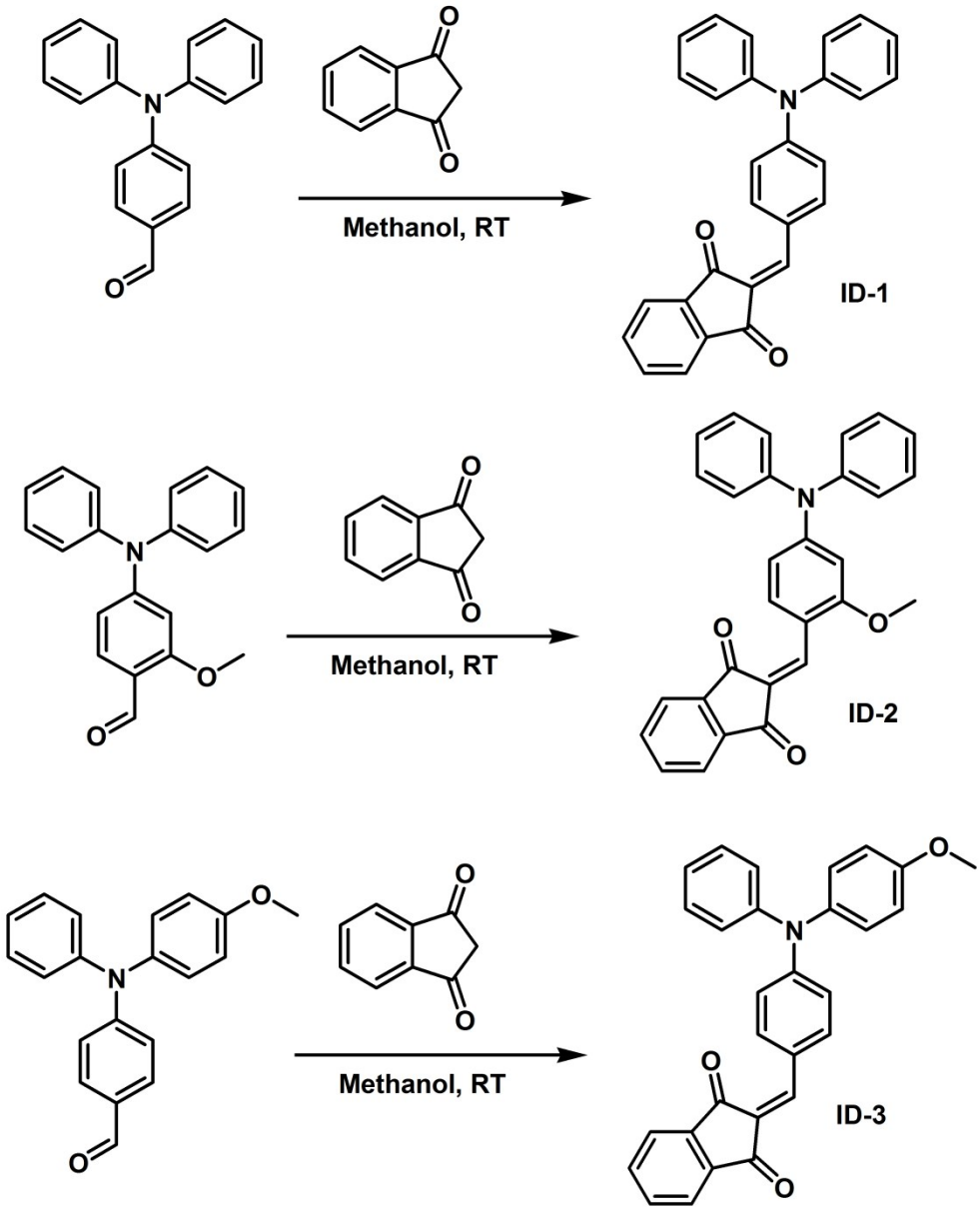
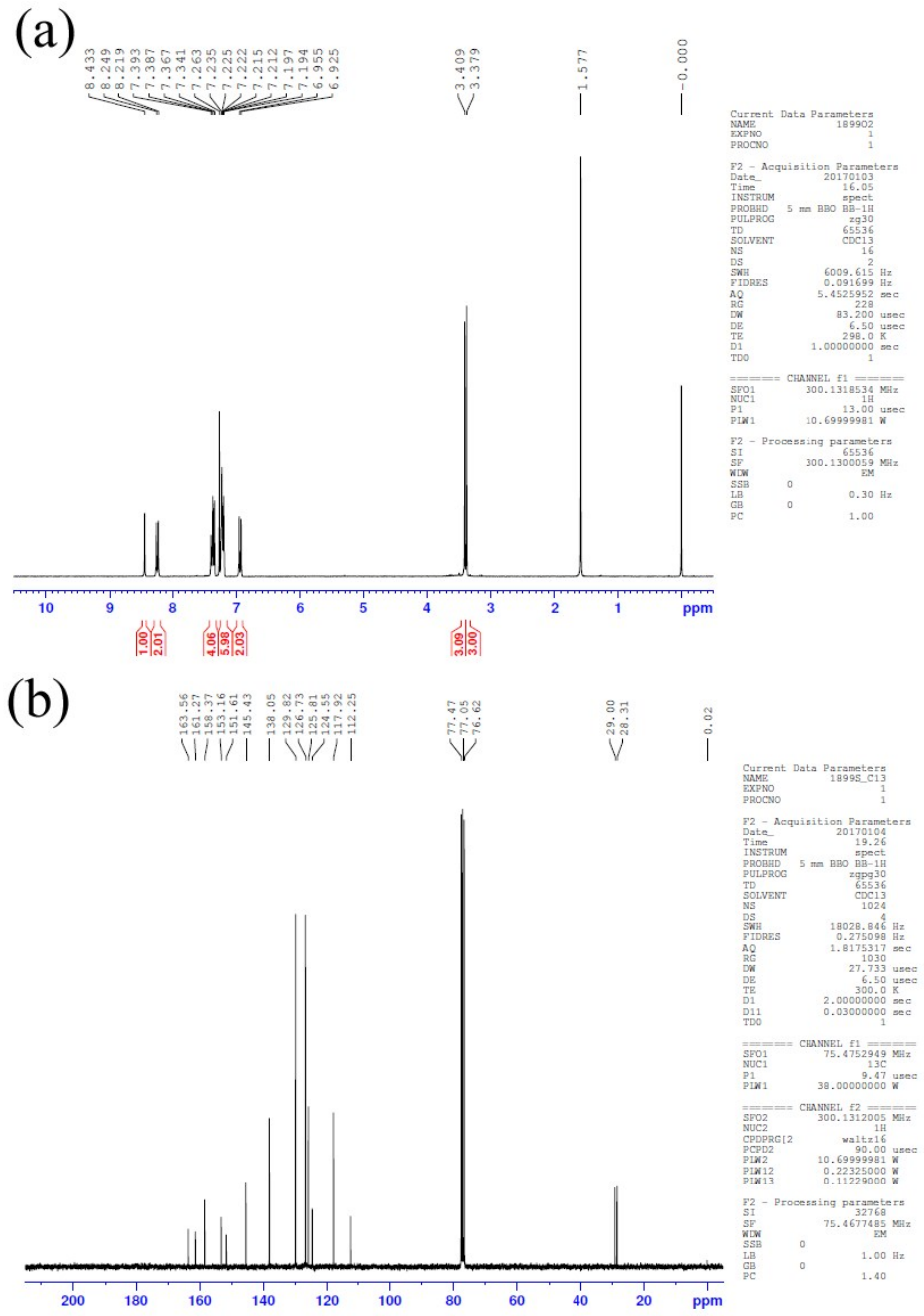


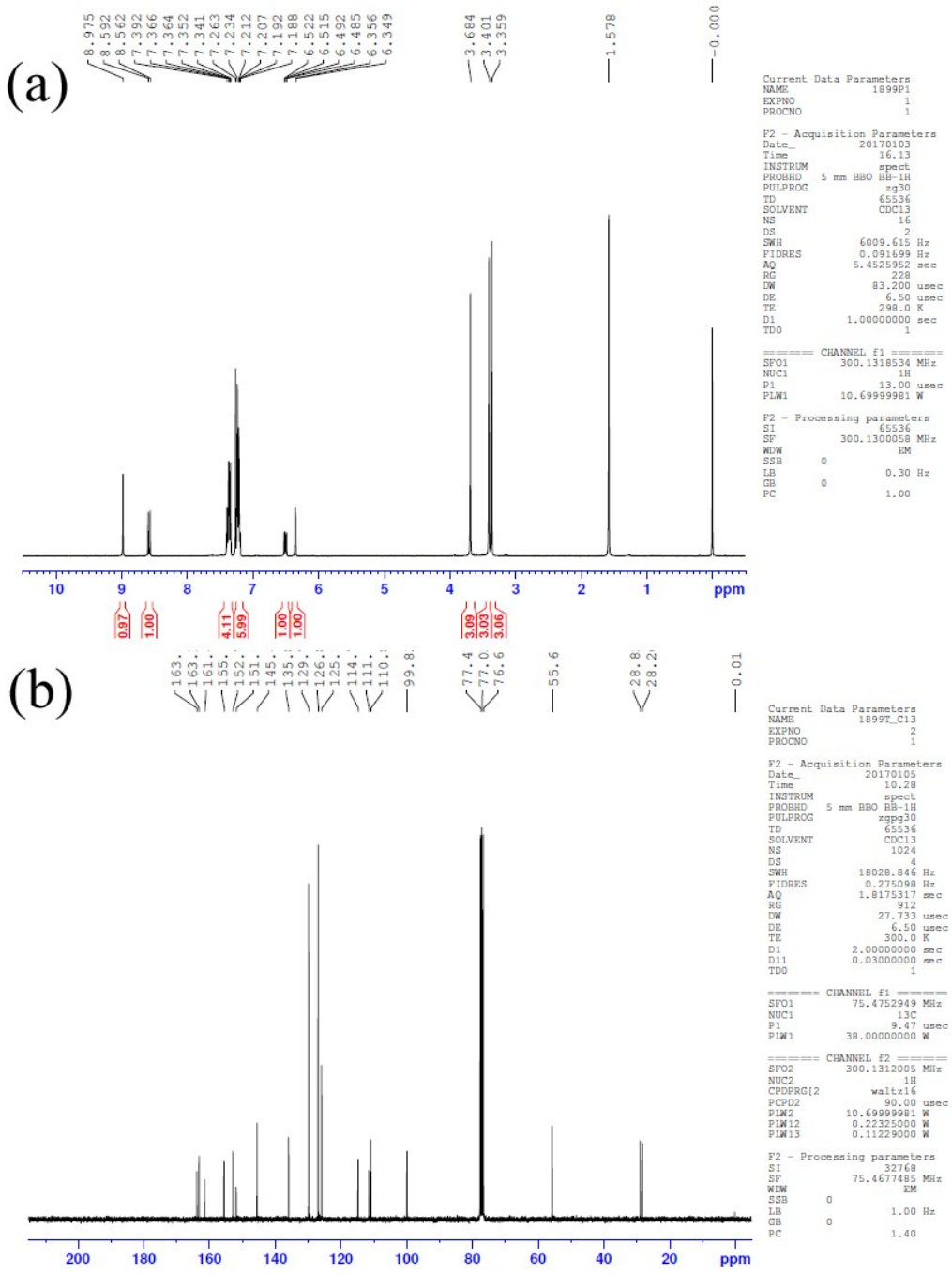
Scheme S1. Synthesis of BA compounds.



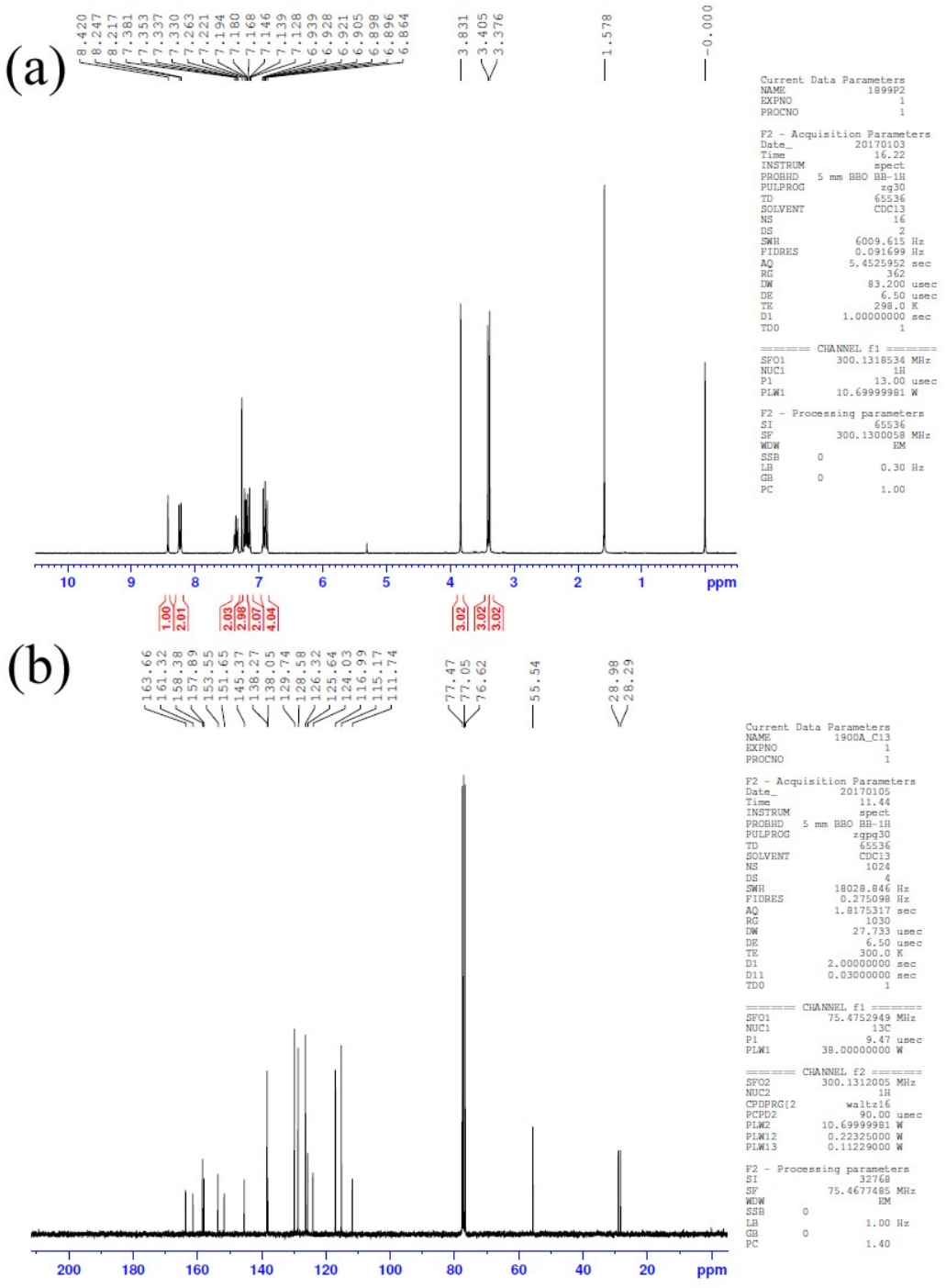
Scheme S2. Synthesis of ID compounds.



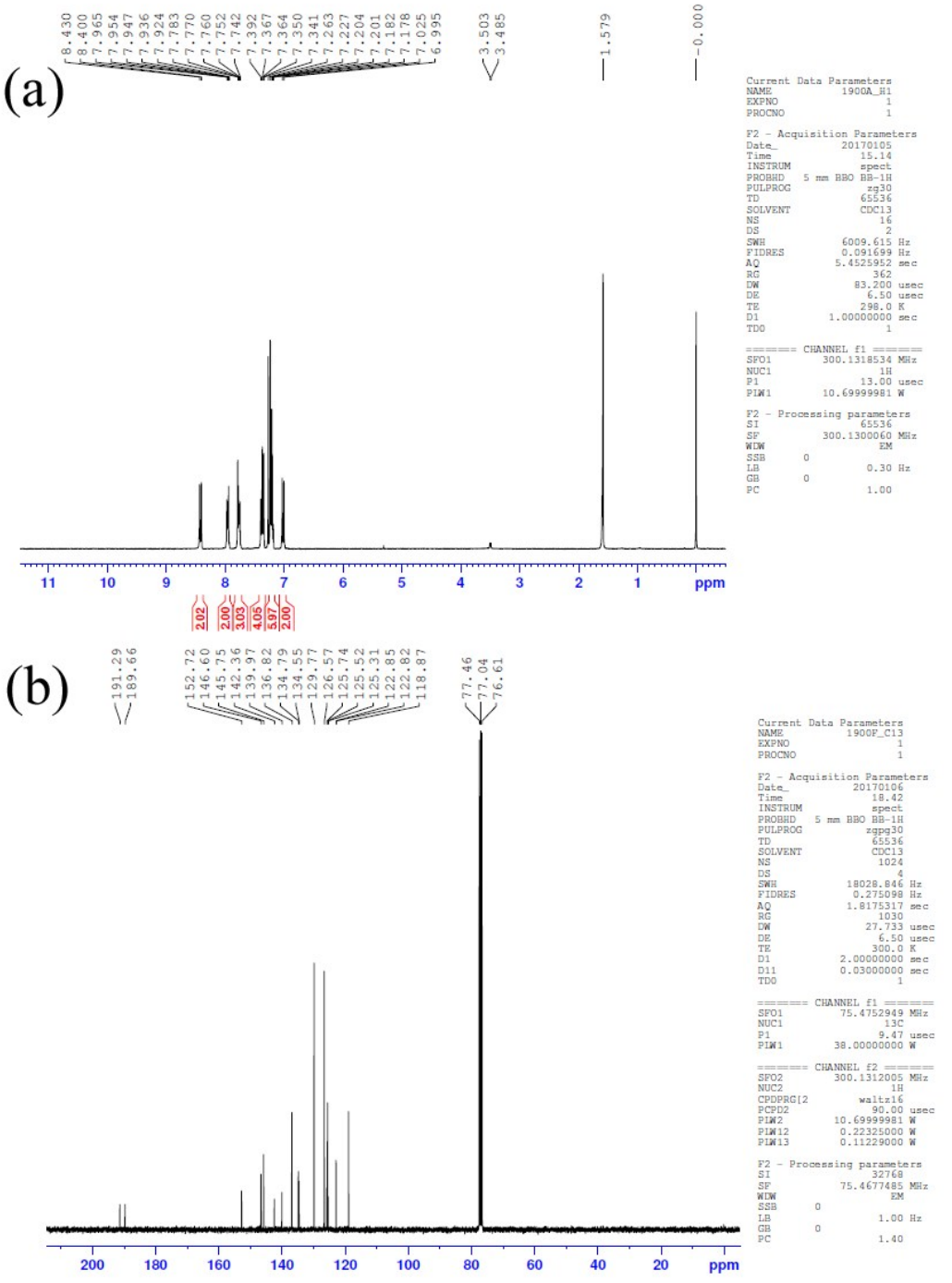
(a) ^{1}H and (b) ^{13}C-NMR spectra of BA-1.



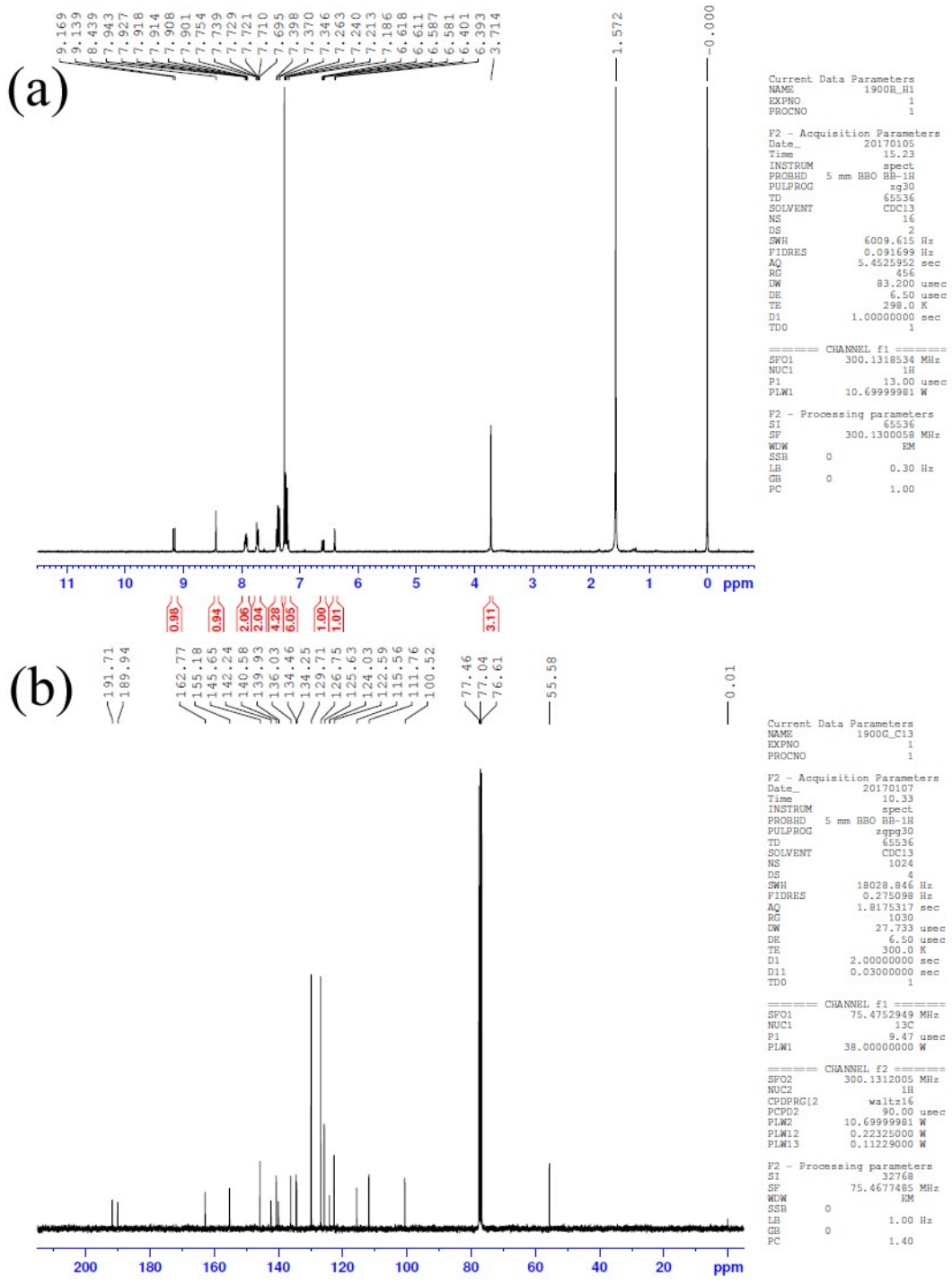
(a) ^{1}H and (b) ^{13}C-NMR spectra of BA-2.



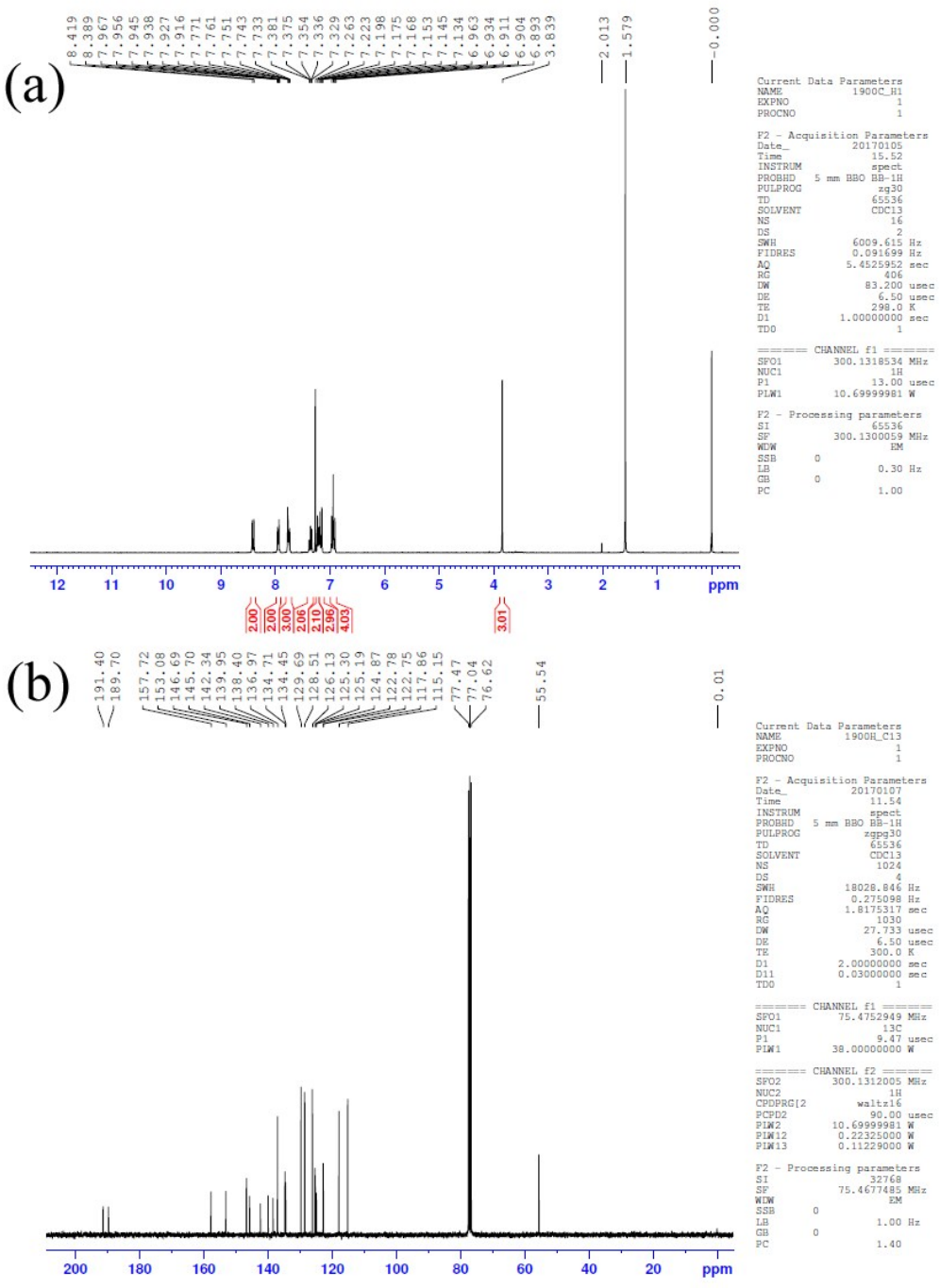
(a) ^{1}H and (b) ^{13}C-NMR spectra of BA-3.



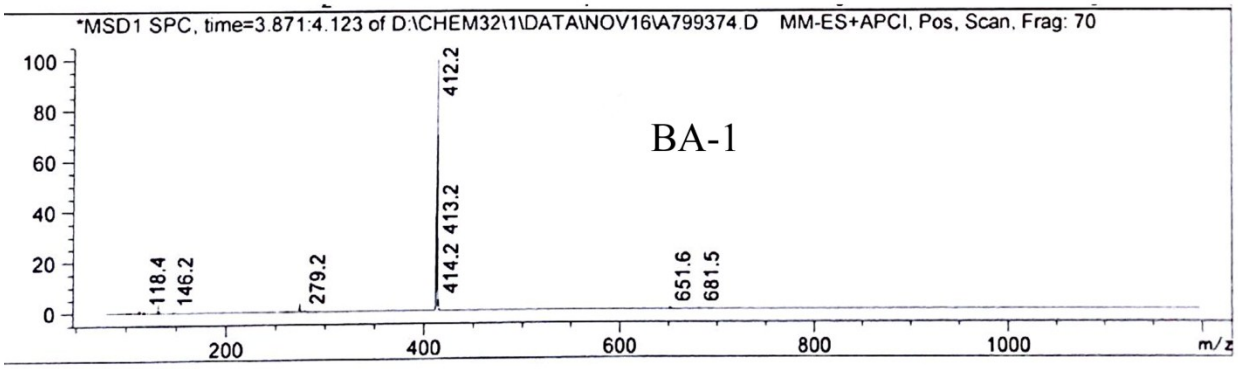
(a) ^{1}H and (b) ^{13}C-NMR spectra of ID-1.

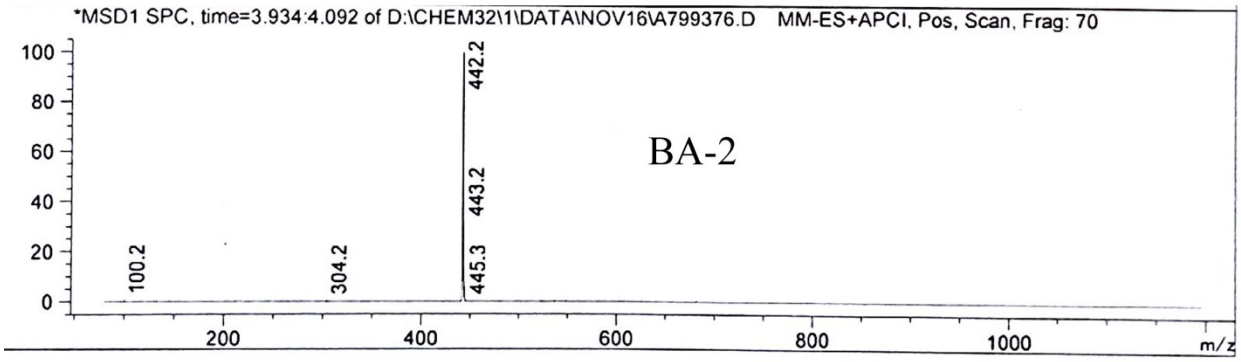


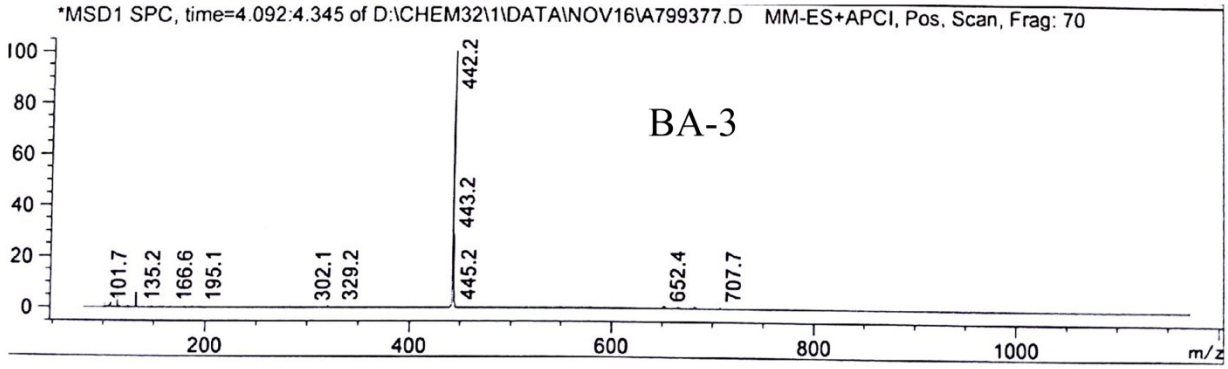
(a) *[1]H* and (b) *[13]C*-NMR spectra of ID-2.



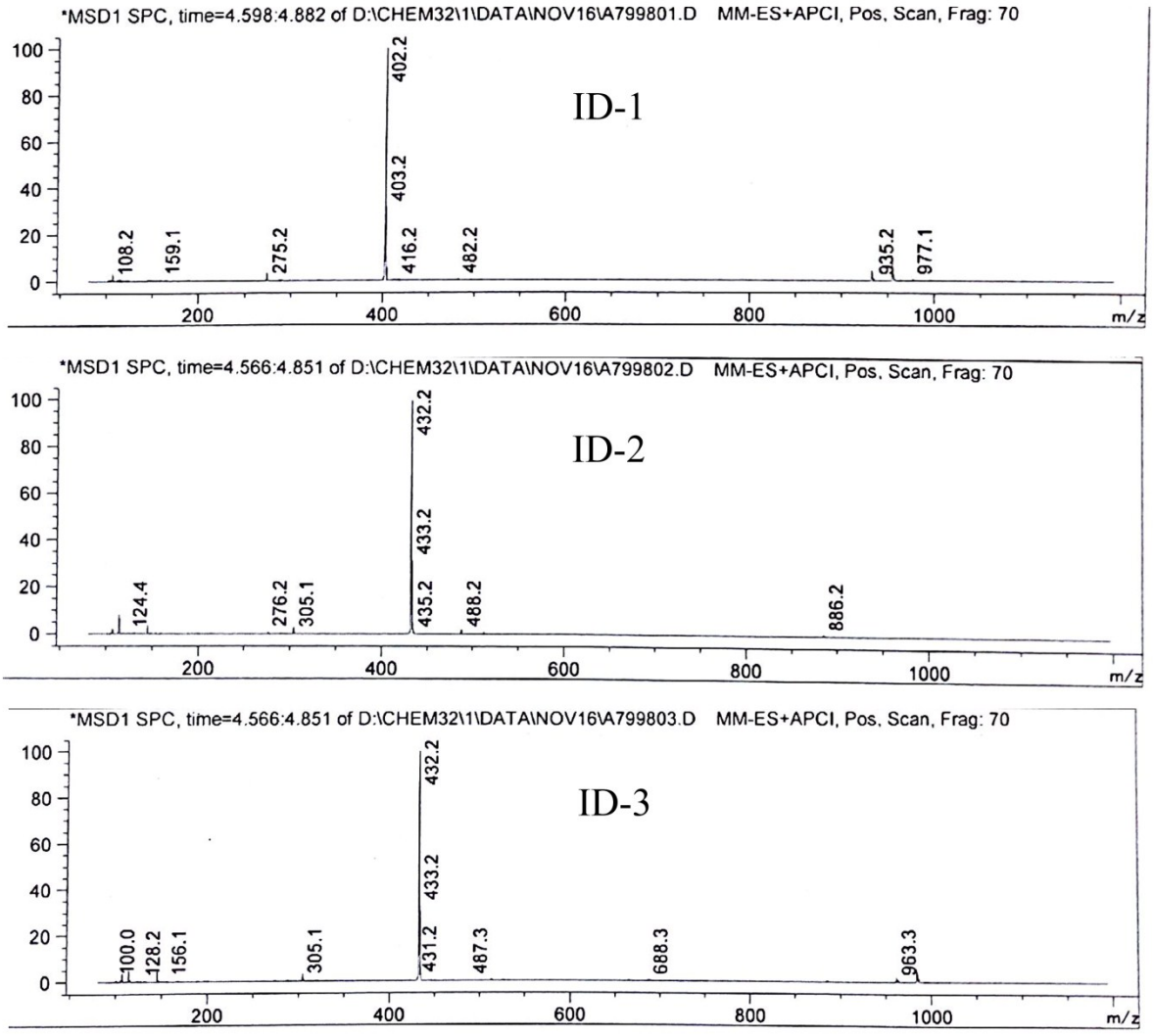
(a) ^{1}H and (b) ^{13}C-NMR spectra of ID-3.







Mass spectra of BA compounds.



Mass spectra of ID compounds.

Table S1. Quantum yields of BA and ID compounds in CH_3CN and CH_3CN-water mixture.

Solvents	BA-1 (Φ_f)	BA-2 (Φ_f)	BA-3 (Φ_f)	ID-1 (Φ_f)	ID-2 (Φ_f)	ID-3 (Φ_f)
CH_3CN	0.0008	0.0026	0.0012	0.00098	0.0016	0.0019
CH_3CN-Water	0.0231	0.080	0.032	0.0067	0.01	0.012

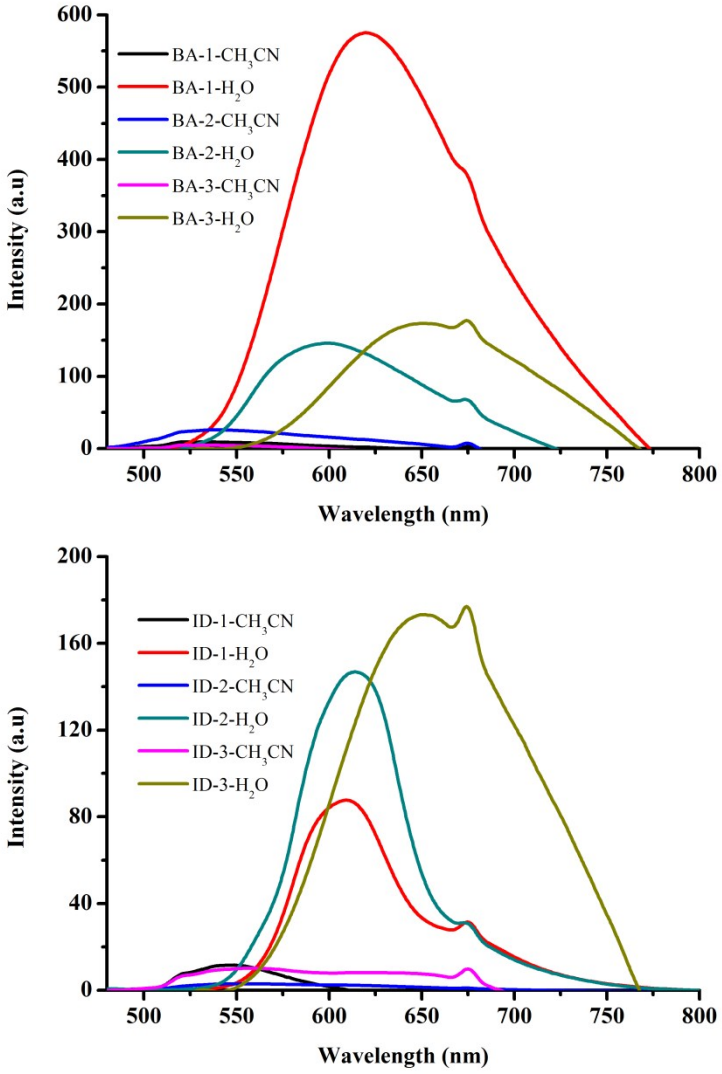


Fig. S1. Fluorescence spectra of BA and ID compounds in CH_3CN and CH_3CN-water mixture.

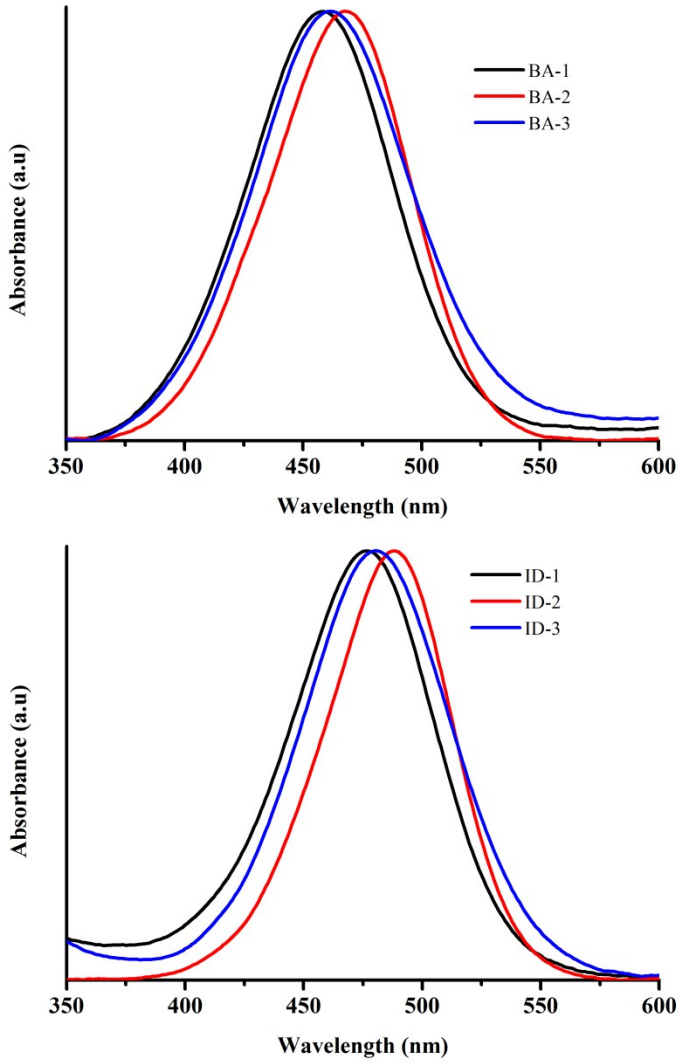


Fig. S2. Absorption spectra of BA and ID compounds in CH_3CN.

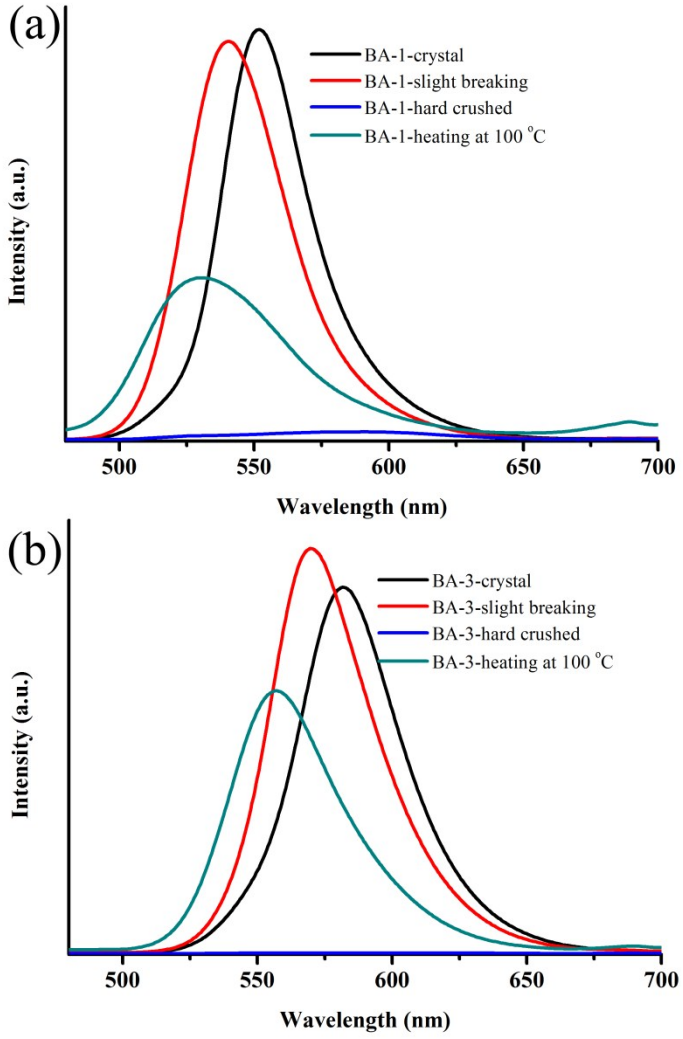


Fig. S3. Solid state fluorescence switching of (a) BA-1 and (b) BA-3 by external stimuli. (λ_{exc} = 370 nm).

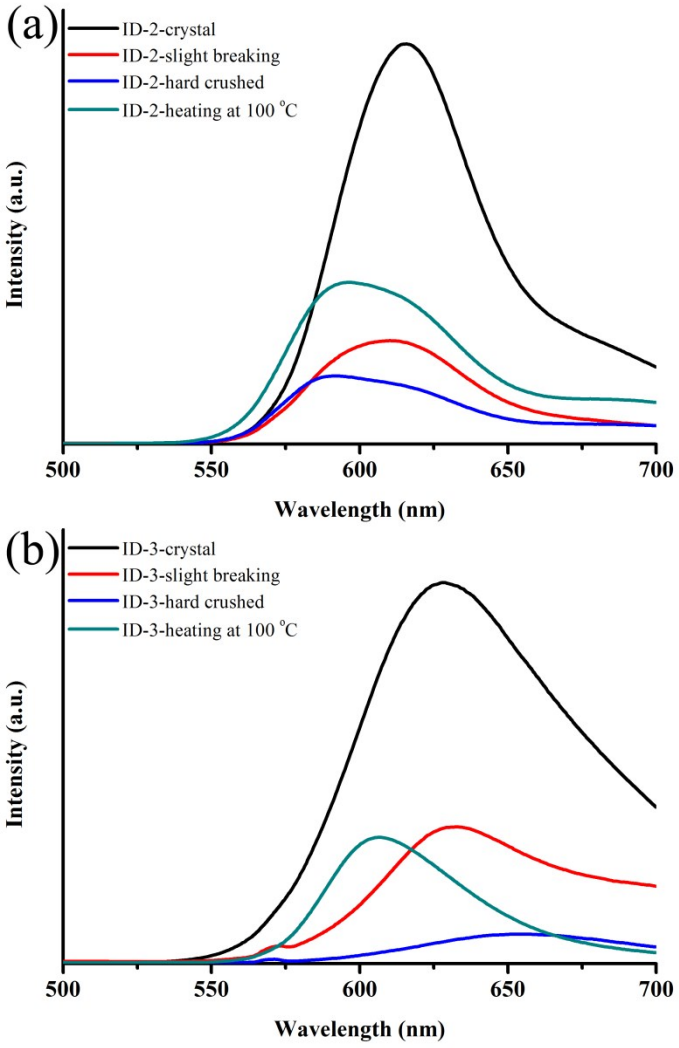


Fig. S4. Solid state fluorescence switching of (a) ID-2 and (b) ID-3 by external stimuli. (λ_{exc} = 370 nm).

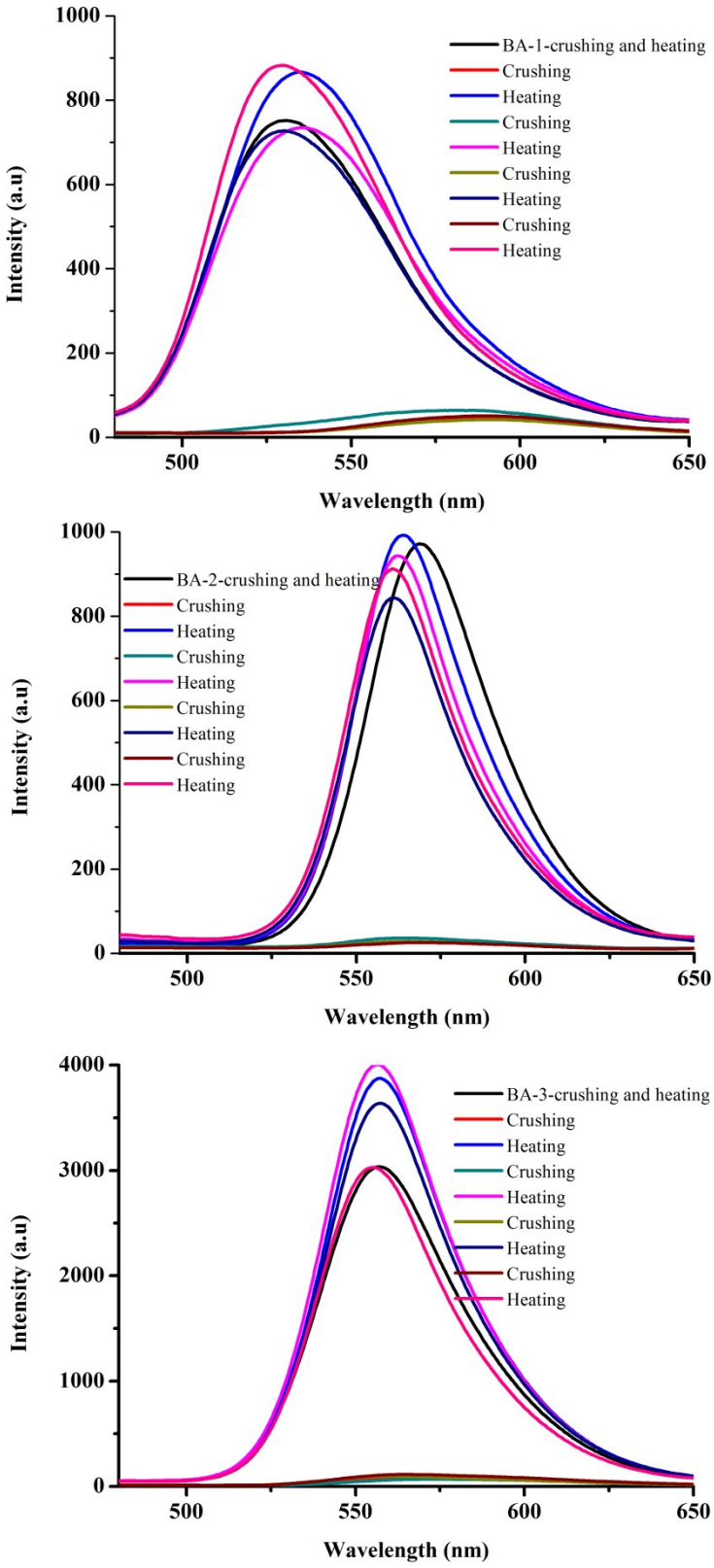


Fig. S5. Solid state fluorescence switching of BA-1-3 by strong crushing followed by heating. (λ_{exc} = 370 nm).

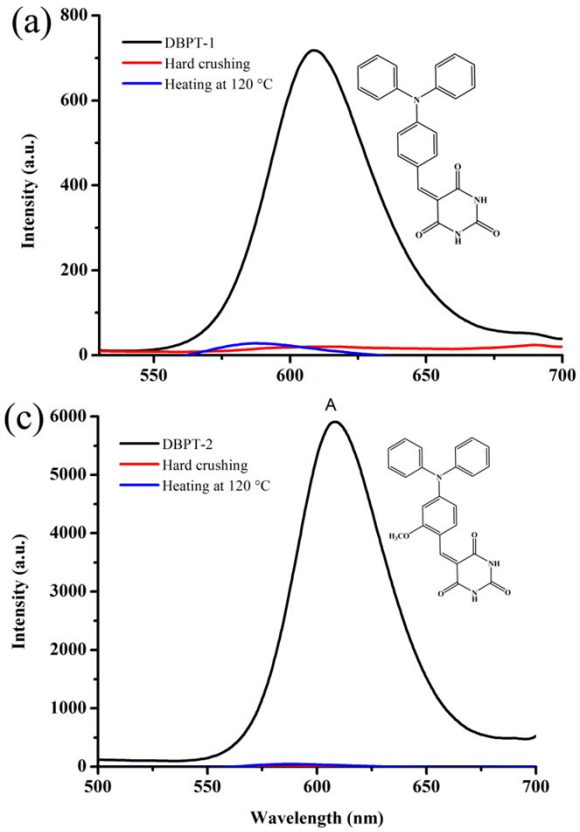


Fig. S6. Solid state fluorescence spectra of (a) DPBT-1 and (b) DPBT-2. (λ_{exc} = 370 nm).

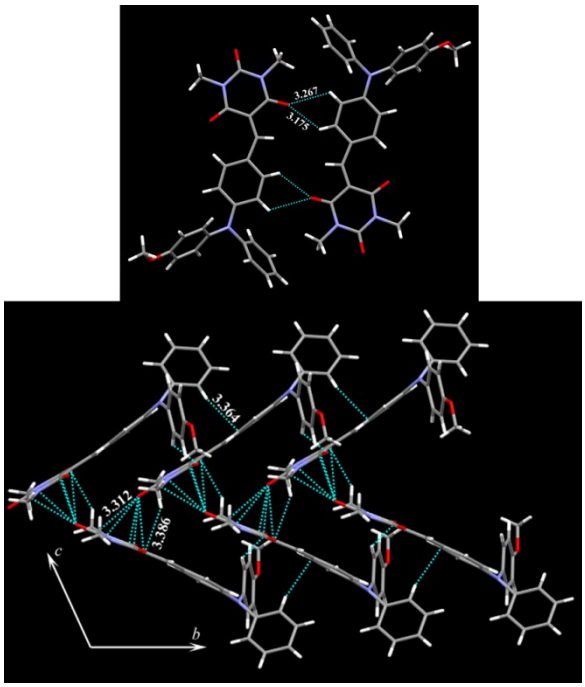


Fig. S7. Dimer formation via H-bonding interaction between oxygen of N-methyl barbituric acid and phenyl hydrogen and extended H-bonding interaction in the crystal lattice of BA-3. C (grey), N (blue), O (red), H (white). H-bonding interactions (broken line) distances are marked in Å.

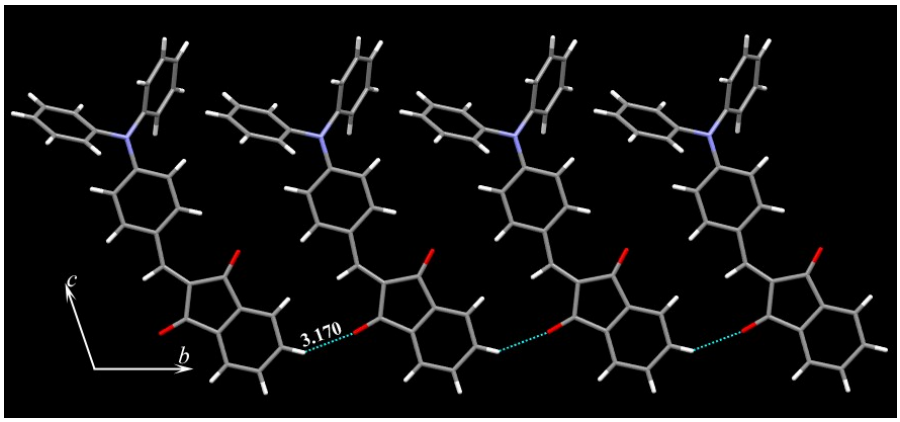


Fig. S8. H-bonding interaction between oxygen of indane dione and indane dione phenyl hydrogen in the crystal lattice of ID-1. C (grey), N (blue), O (red), H (white). H-bonding interactions (broken line) distances are marked in Å.

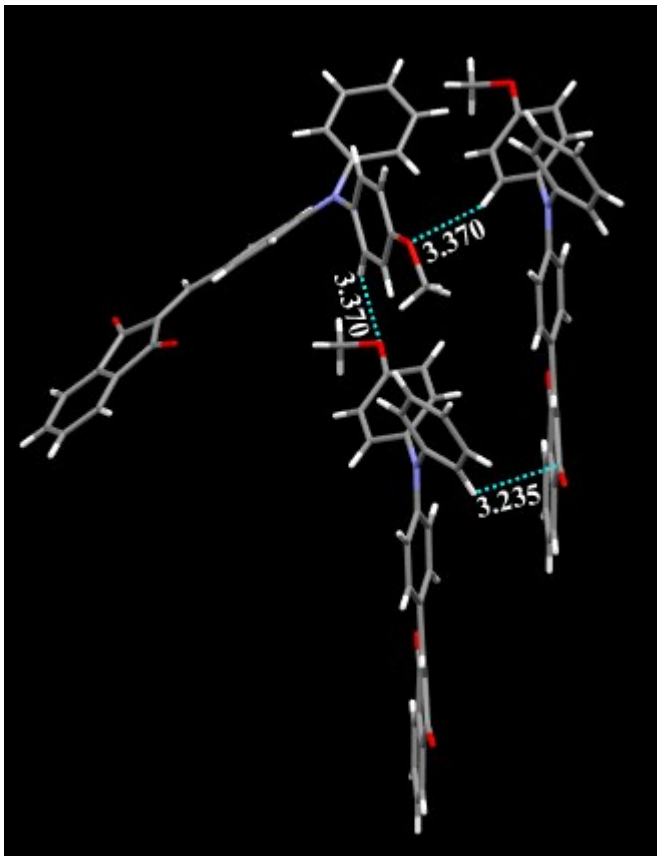


Fig. S9. H-bonding interactions in the crystal lattice of ID-3. C (grey), N (blue), O (red), H (white). H-bonding interactions (broken line) distances are marked in Å.

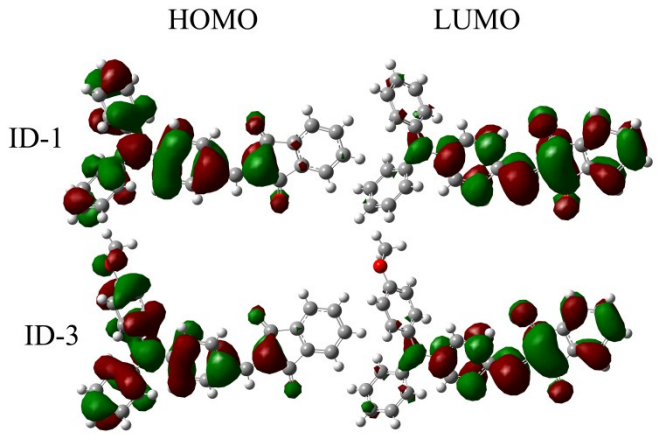


Fig. S10. Molecular orbital plots of the HOMOs and LUMOs of ID compounds.

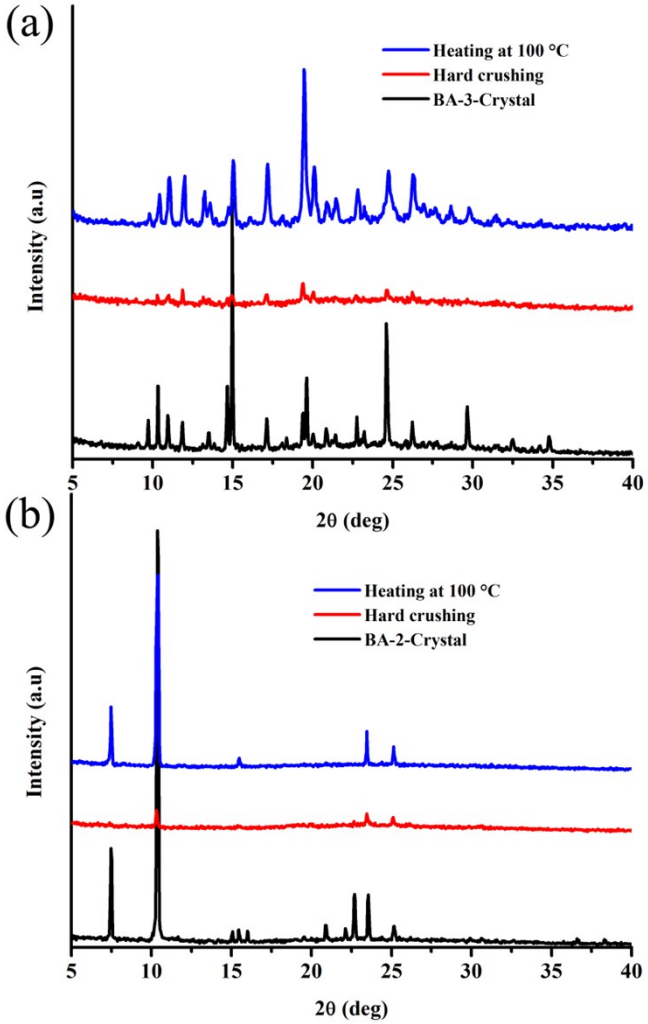


Fig. S11. PXRD pattern of (a) BA-2 and (b) BA-3 before, after hard crushing and heating.

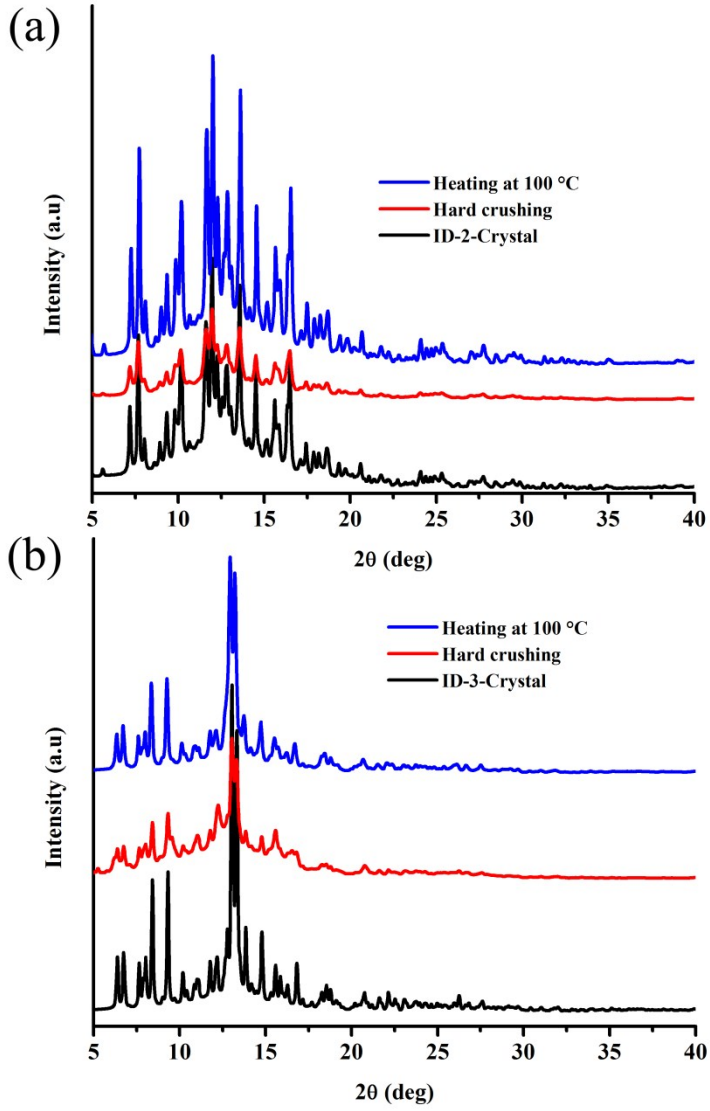


Fig. S12. PXRD pattern of (a) ID-2 and (b) ID-3 before, after hard crushing and heating.

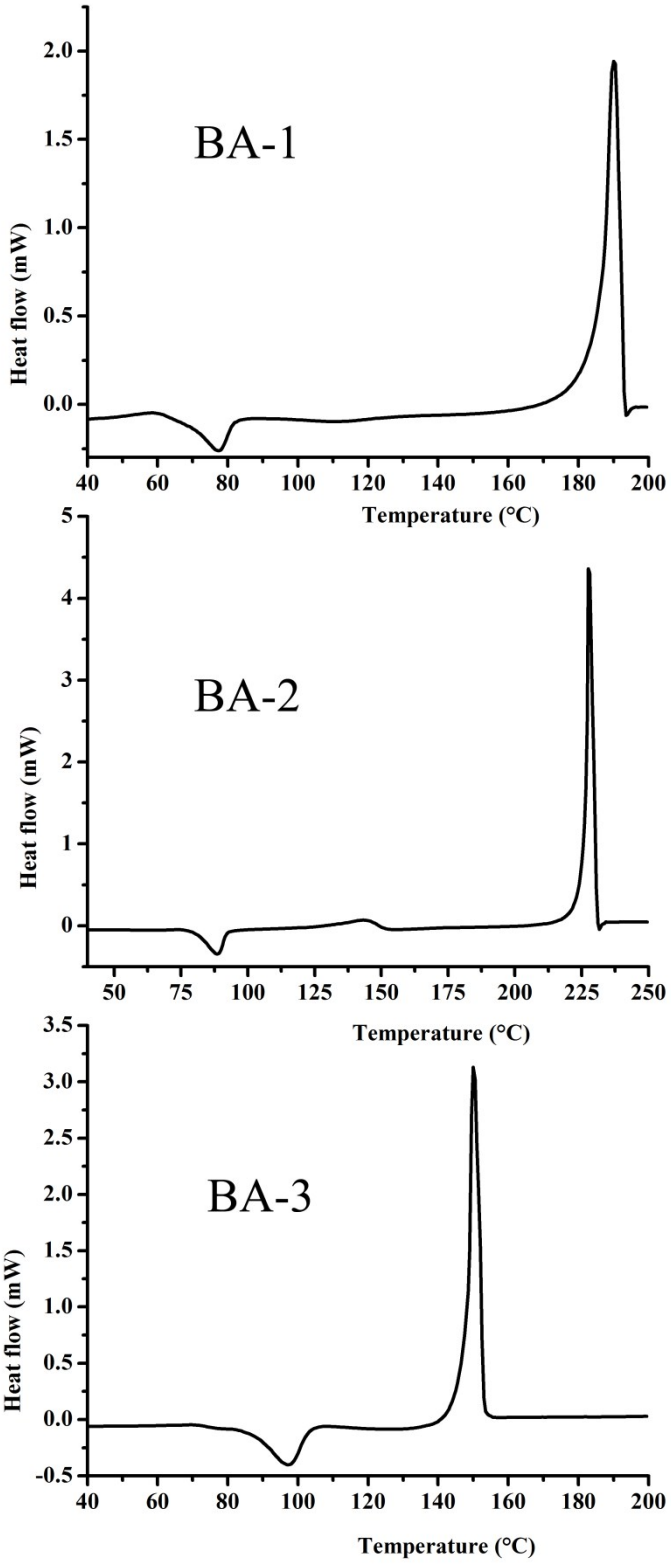


Fig. S13. DSC of BA-1-3.

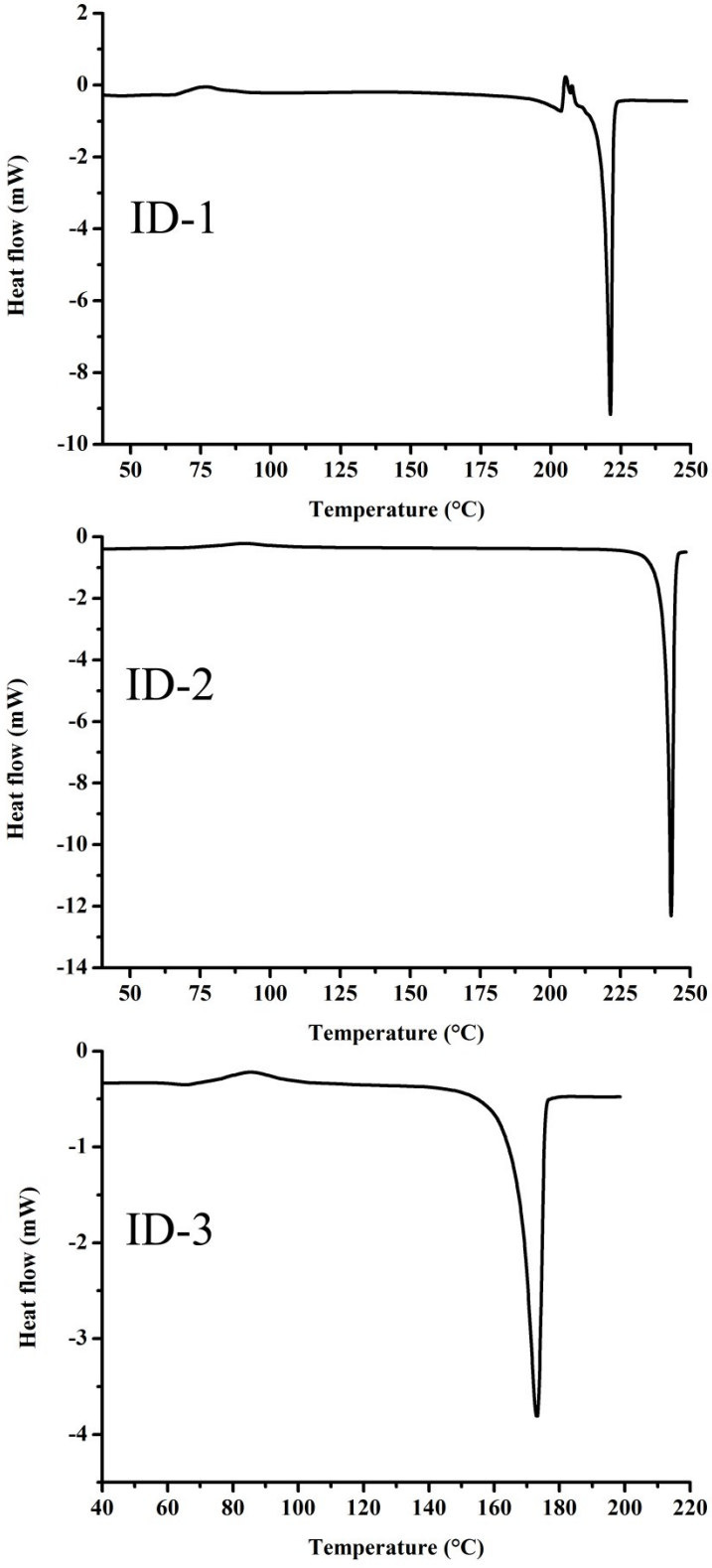


Fig. S14. DSC of ID-1-3.

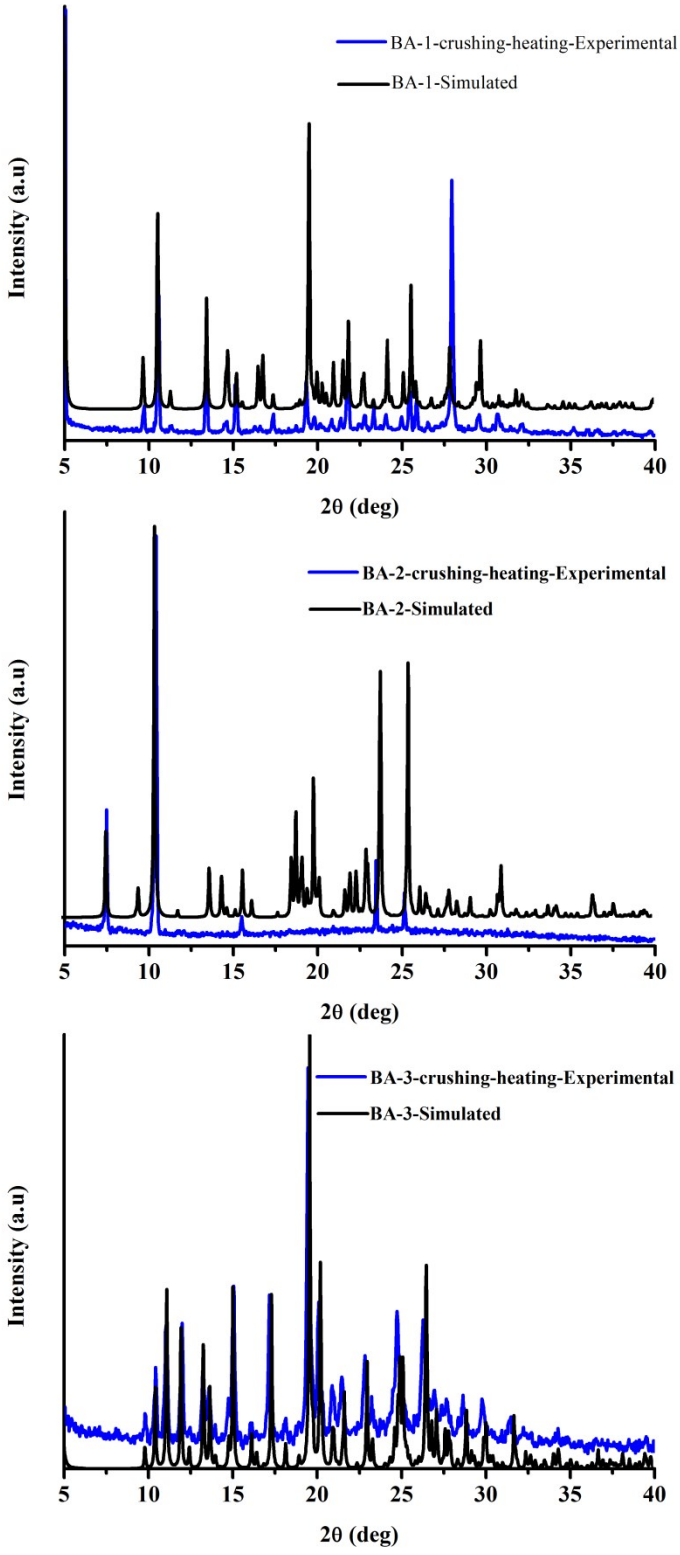


Fig. S15. PXRD pattern of (a) ID-2 and (b) ID-3 before, after hard crushing and heating.