Modulating some photophysical properties of cocrystals

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Supplementary data

Contents

1. Crystallographic data and crystal structures

1.1. Crystallographic data for 3DMABA cocrystals

Cocrystal	T2-3DMABA-PI	T2-3DMABA-PII	T3-3DMABA	T4-3DMABA	T5-3DMABA
Formula	$C_{17}H_{20}N_4O_5$	$C_{17}H_{20}N_4O_5$	$C_{18}H_{22}N_4O_5$	$C_{19}H_{24}N_4O_5$	$C_{20}H_{26}N_4O_5$
Dcalc./ g cm-3	1.341	1.374	1.314	1.335	1.347
μ/mm^{-1}	0.841	0.862	0.813	0.815	0.812
Formula Weight	360.37	360.37	374.39	388.42	402.45
Colour	light orange	orange	orange	Orange	orange
Shape	plate	plate	plate	plate	plate
Size/mm^3	0.28×0.04×0.00	0.13×0.06×0.02	0.33×0.08×0.02	0.19×0.14×0.06	0.16×0.12×0.04
T/K	200.00(10)	295.0(4)	200.0(1)	200(2)	200.00(10)
Crystal System	monoclinic	monoclinic	triclinic	triclinic	triclinic
Space Group	$P2_1/n$	$C2/c$	*P-1*	*P-1*	*P-1*
a/Å	16.7360(4)	24.8829(8)	6.21761(15)	6.35274(15)	6.42159(9)
b/Å	4.91439(11)	6.1032(2)	12.5048(4)	12.46903(18)	12.65205(14)
c/Å	21.9254(5)	23.3288(12)	12.7578(4)	12.9378(3)	13.02701(17)
α/°	90	90	79.345(2)	97.365316)	76.6124(10)
β/°	98.240(2)	100.391(4)	78.280(3)	103.862(2)	75.8298(12)
γ/°	90	90	80.4467(17)	99.5009(15)	80.7872(10)
V/Å^3	1784.68(7)	3484.7(2)	945.96(4)	966.16(4)	992.29(2)
Z	4	8	2	2	2
Z'	1	1	1	1	1
Wavelength/Å	1.54184	1.54184	1.54184	1.54184	1.54184
Radiation type	Cu Kα	Cu Kα	Cu Kα	Cu Kα	Cu Kα
θmin/°	3.116	3.612	3.582	3.574	3.572
θmax/°	80.512	80.128	80.089	80.154	79.934
Measured Refl.	13114	11779	17956	37103	20759
Independent Refl.	3662	3650	4064	4176	4253

1.2. Crystallographic data for 4ABA cocrystals

Cocrystal	T2-4ABA	T3-4ABA	T4-4ABA	T5-4ABA
Formula	$C_{15}H_{16}N_4O_5$	$C_{16}H_{18}N_4O_5$	$C_{17}H_{20}N_4O_5$	$C_{29}H_{37}N_7O_8$
Dcalc./ g cm-3	1.451	1.397	1.340	1.265
μ/mm^{-1}	0.939	0.890	0.841	0.782
Formula Weight	332.32	346.34	360.37	611.65
Colour	light yellow	yellow	yellow	light yellow
Shape	needle	irregular	plate	needle
Size/mm^3	0.29×0.01×0.01	0.16×0.12×0.11	0.15×0.11×0.03	0.10×0.02×0.02

T/K	200.00(10)	200.00(10)	295.9(3)	297(1)
Crystal System	monoclinic	triclinic	triclinic	monoclinic
Space Group	$P2_1/n$	*P-1*	*P-1*	$P2_1/n$
a/Å	12.5882(2)	5.8059(4)	6.15171(12)	20.1578(5)
b/Å	5.17490(7)	11.8005(10)	12.3495(4)	4.90086(14)
c/Å	23.3666(4)	12.9057(16)	12.6749(4)	32.5043(9)
α/°	90	73.991(9)	73.875(3)	90
β/°	91.8814(16)	78.882(9)	79.965(2)	90.875(2)
γ/°	90	78.277(7)	76.405(2)	90
V/Å^3	1521.34(4)	823.35(14)	892.97(4)	3210.75(15)
Z	4	2	2	4
Z'	1	1	1	1
Wavelength/Å	1.54184	1.54184	1.54184	1.54184
Radiation type	Cu Kα	Cu Kα	Cu Kα	Cu Kα
θmin/°	3.785	3.601	3.655	2.562
θmax/°	79.786	81.117	80.078	78.442
Measured Refl.	11401	11962	14844	24768
Independent Refl.	3225	3406	3854	6488

1.3. Crystal structures

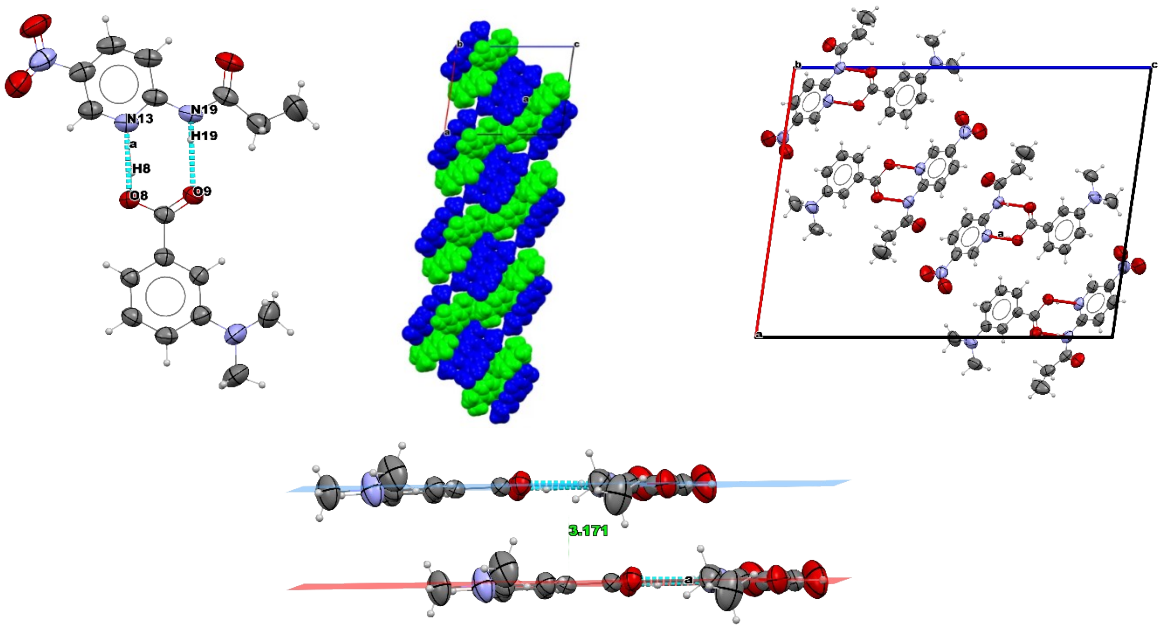

Figure S1. Crystal packing of T2-3DMABA-PI.

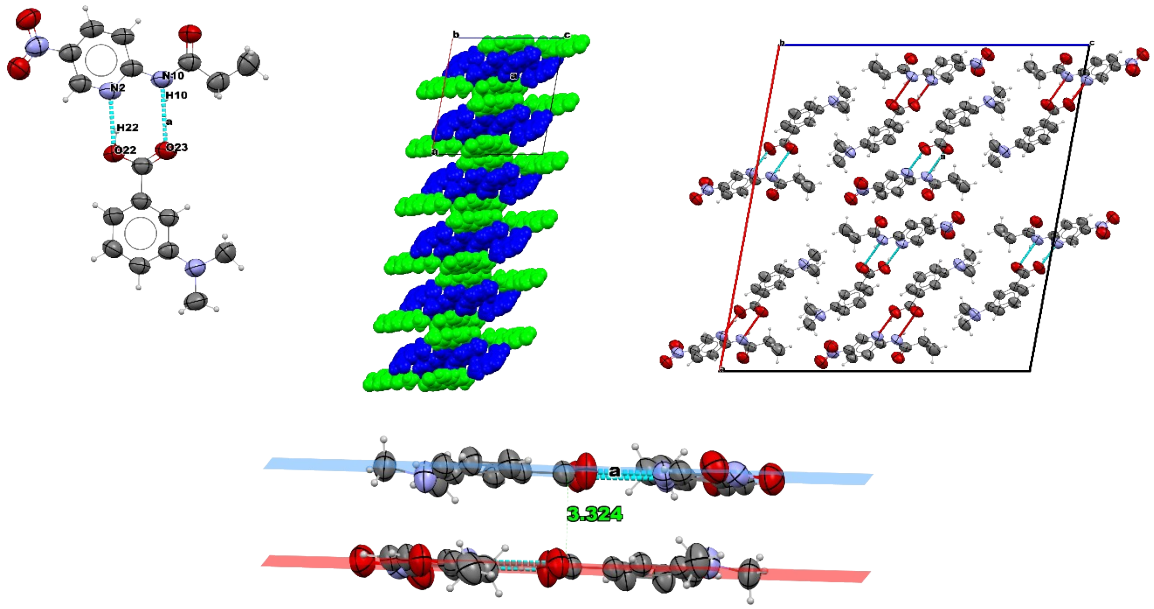

Figure S2. Crystal packing of T2-3DMABA – PII.

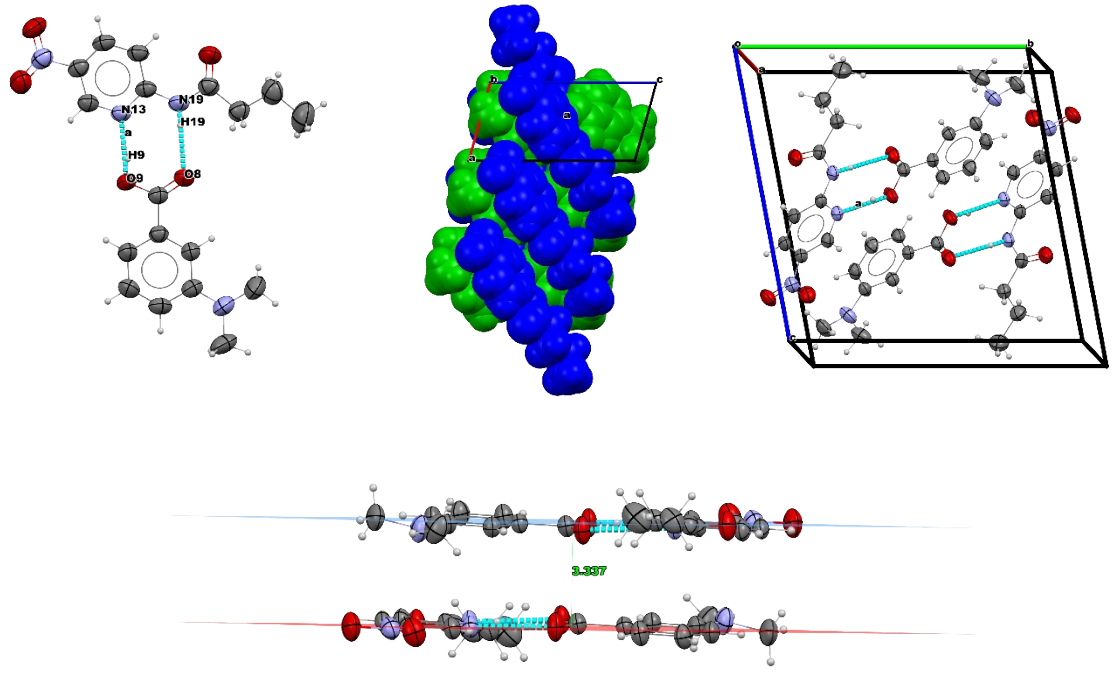

Figure S3. Crystal packing of T3-3DMABA.

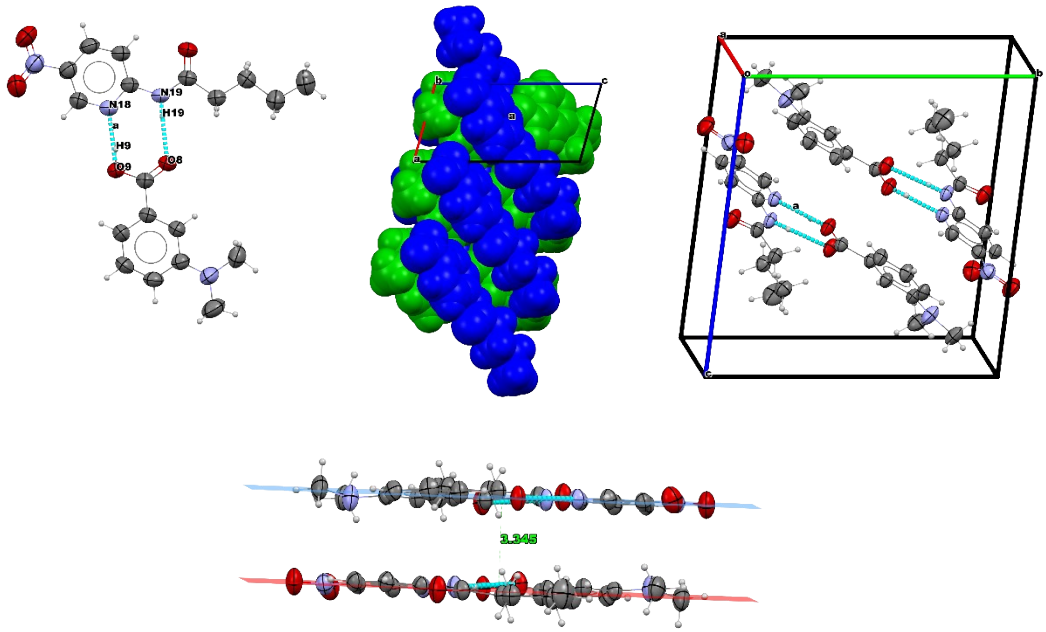

Figure S4. Crystal packing of T4-3DMABA.

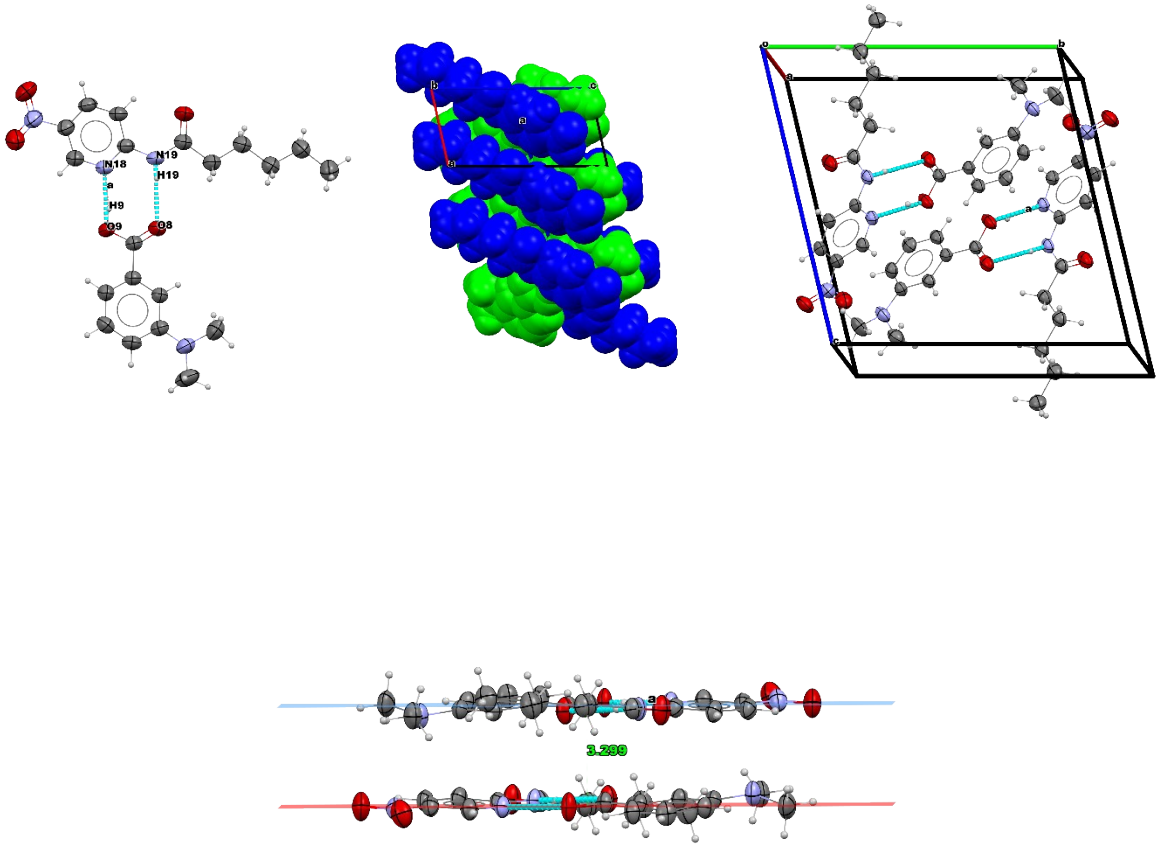

Figure S5. Crystal packing of T5-3DMABA.

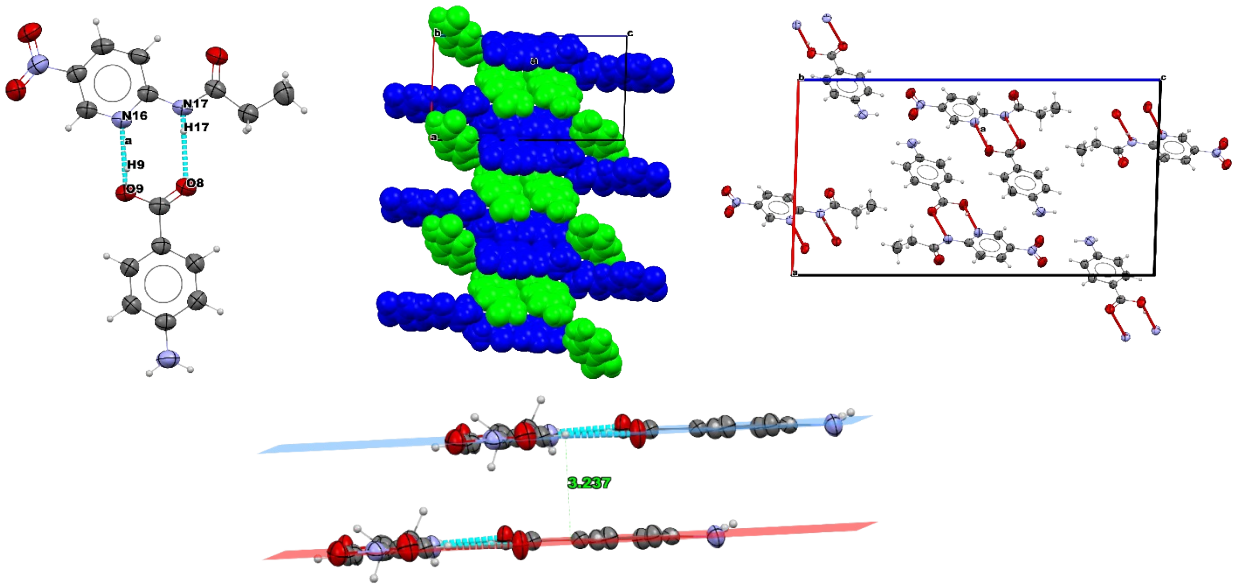

Figure S6. Crystal packing of T2-4ABA.

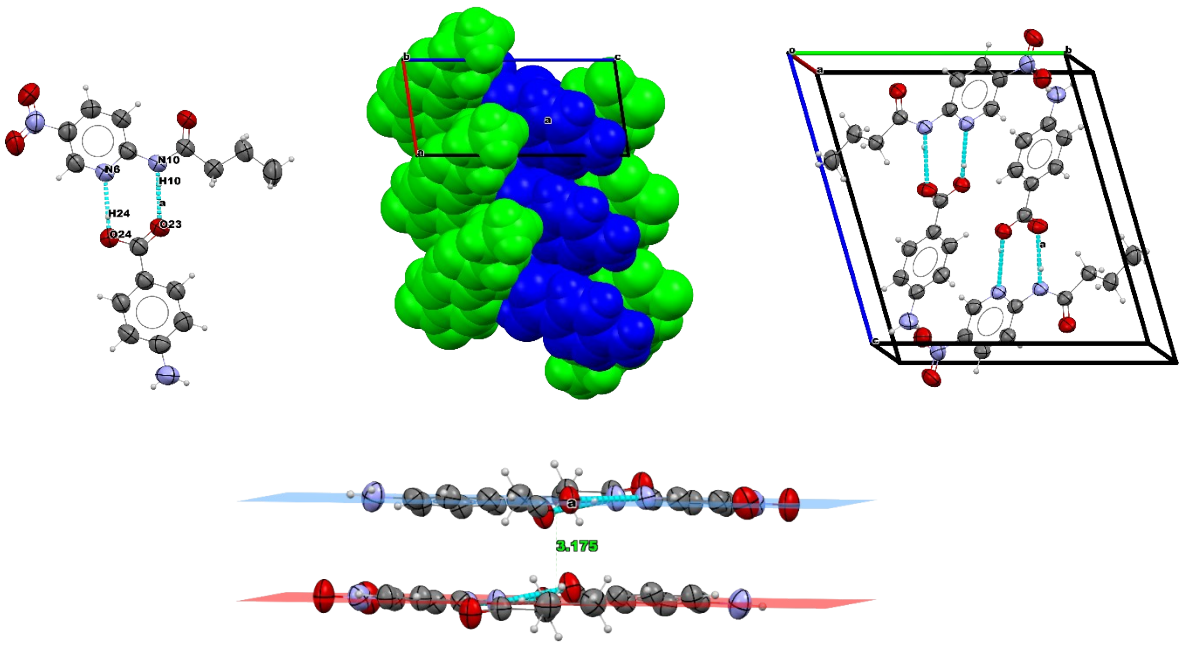

Figure S7. Crystal packing of T3-4ABA.

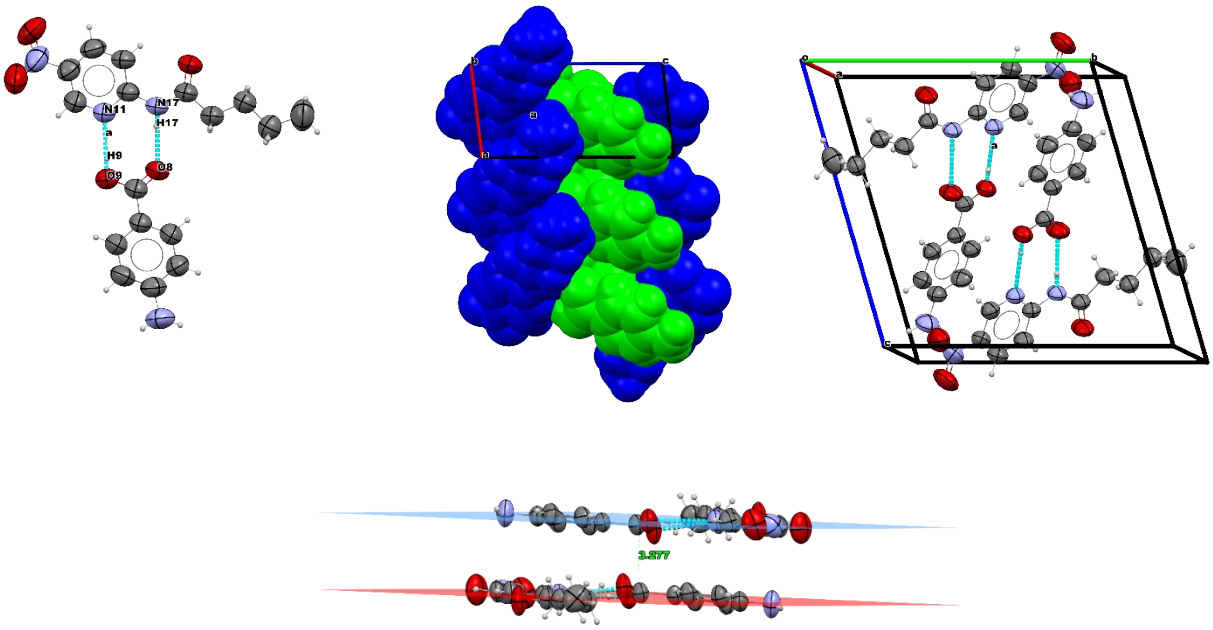

Figure S8. Crystal packing of T4-4ABA.

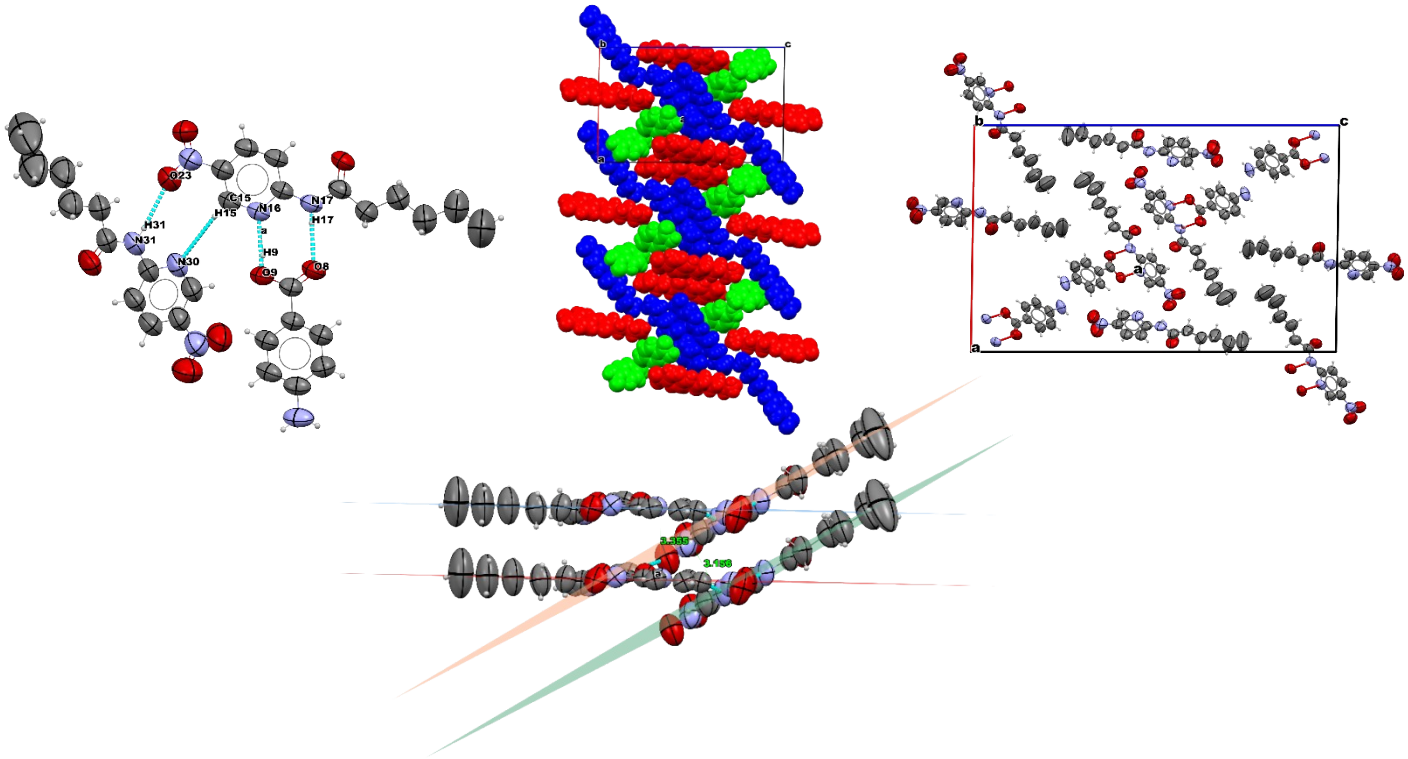

Figure S9. Crystal packing of T5-4ABA.

2. FTIR spectra

2.1 Starting materials

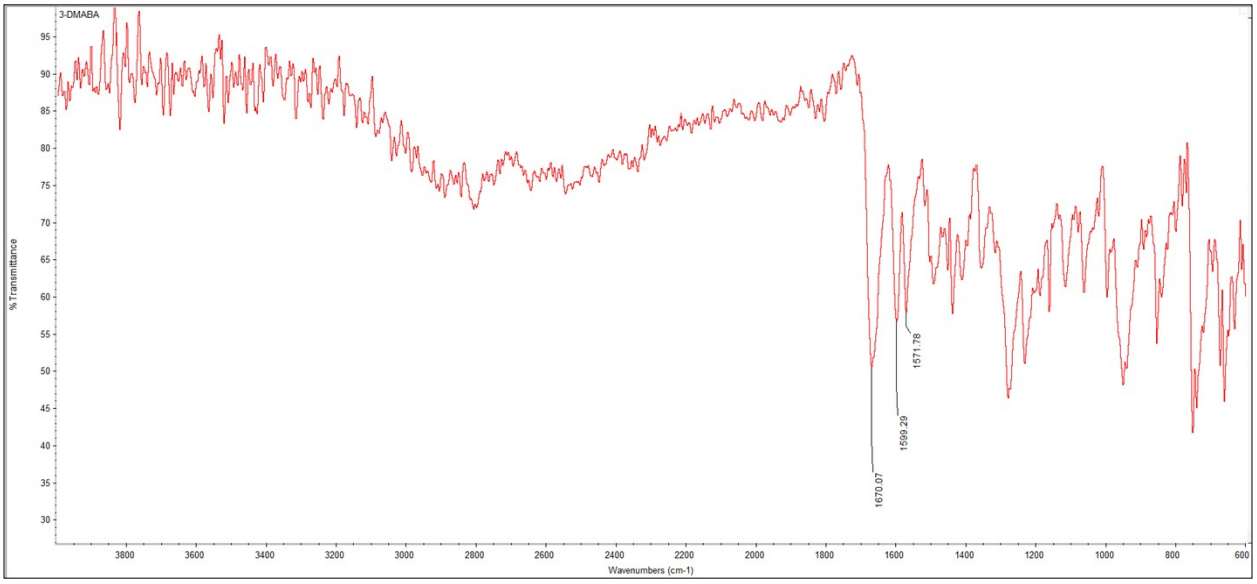

Figure S10. IR of 3DMABA.

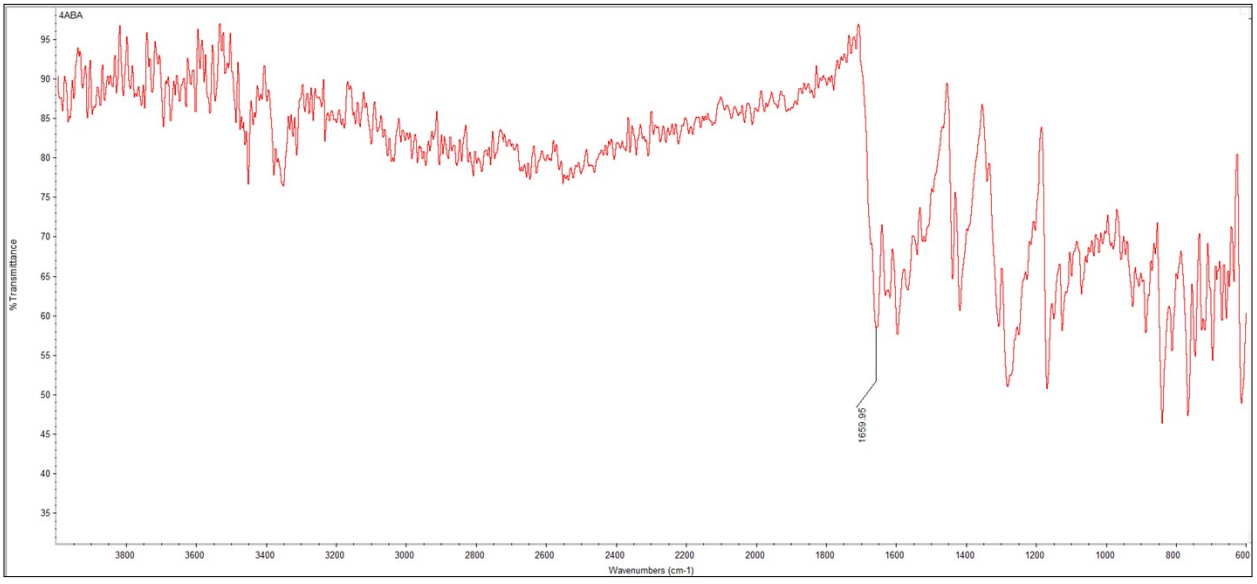

Figure S11. IR of 4ABA.

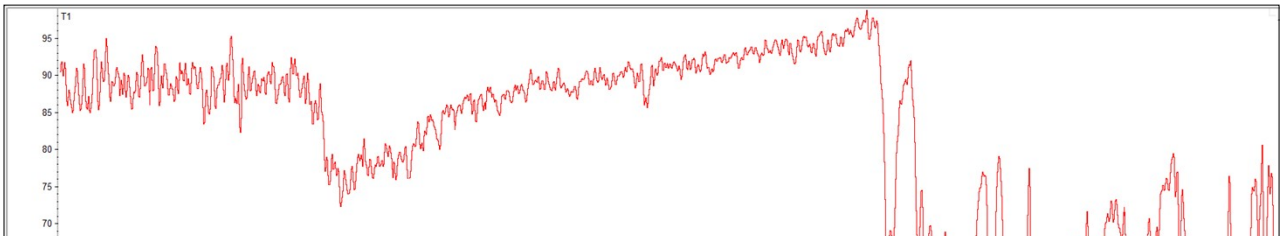

Figure S12. IR of T1.

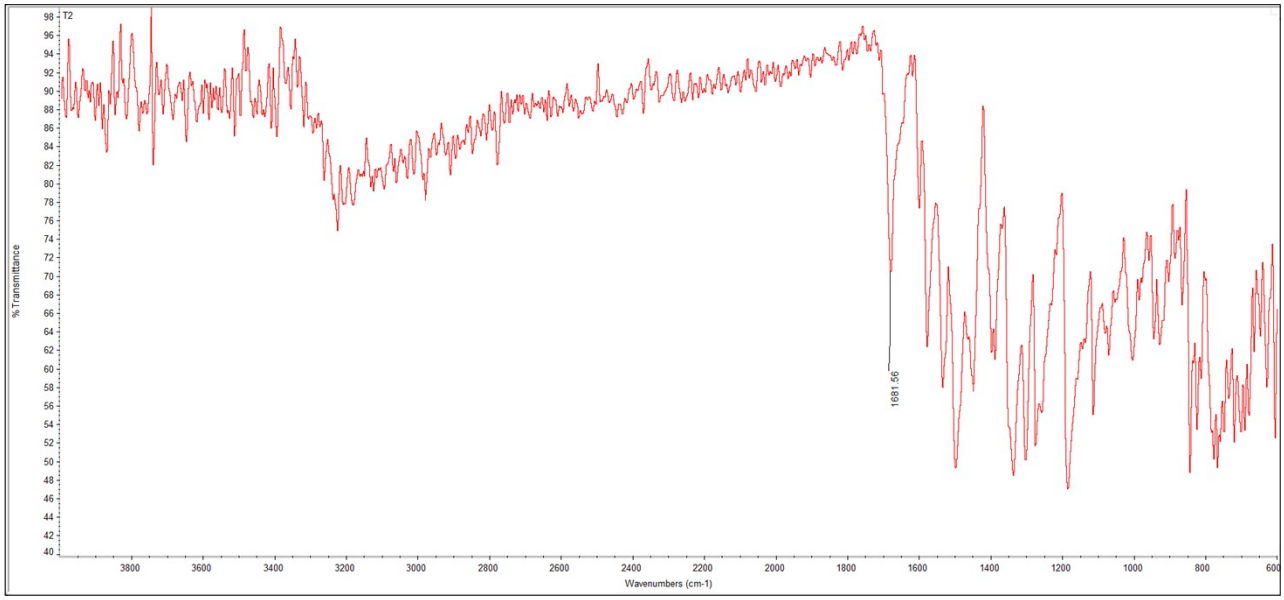

Figure S13. IR of T2.

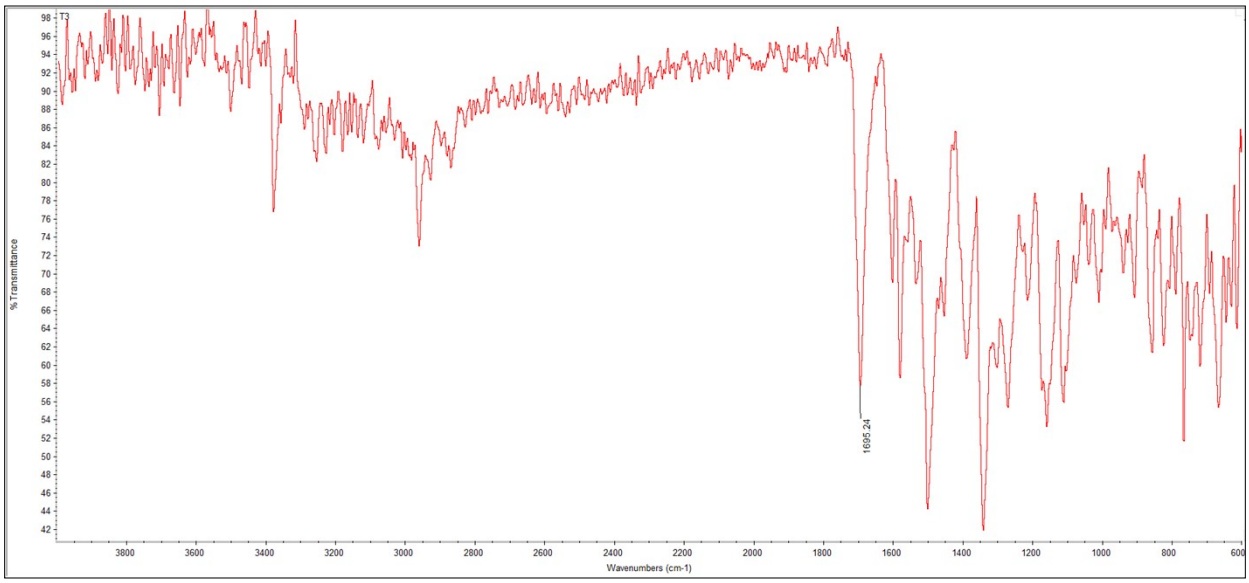

Figure S14. IR of T3.

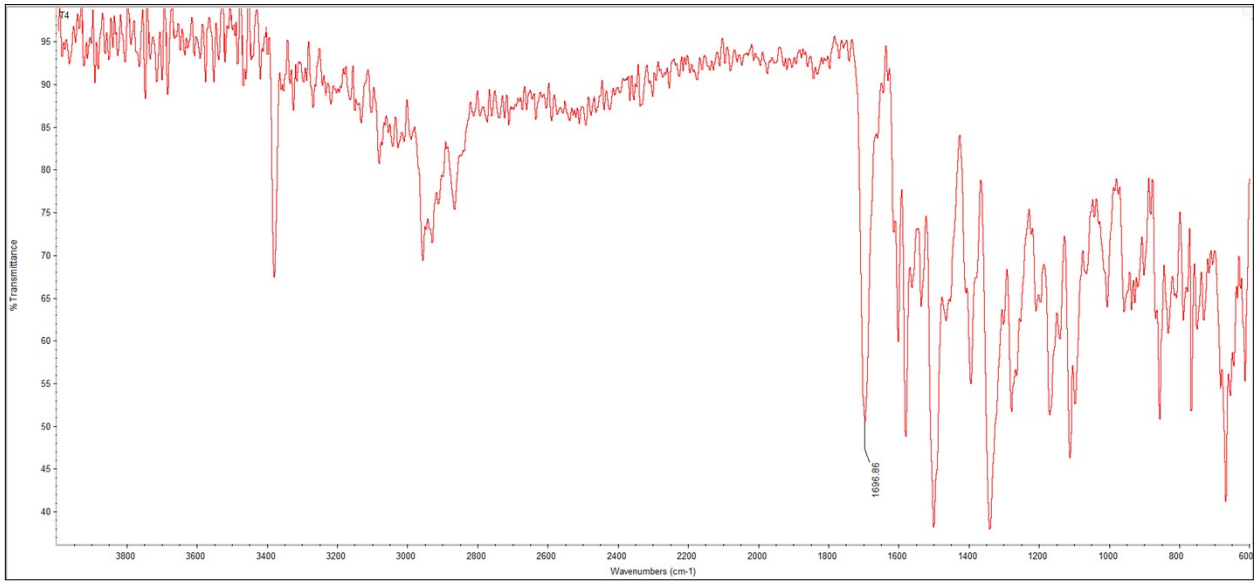

Figure S15. IR of T4.

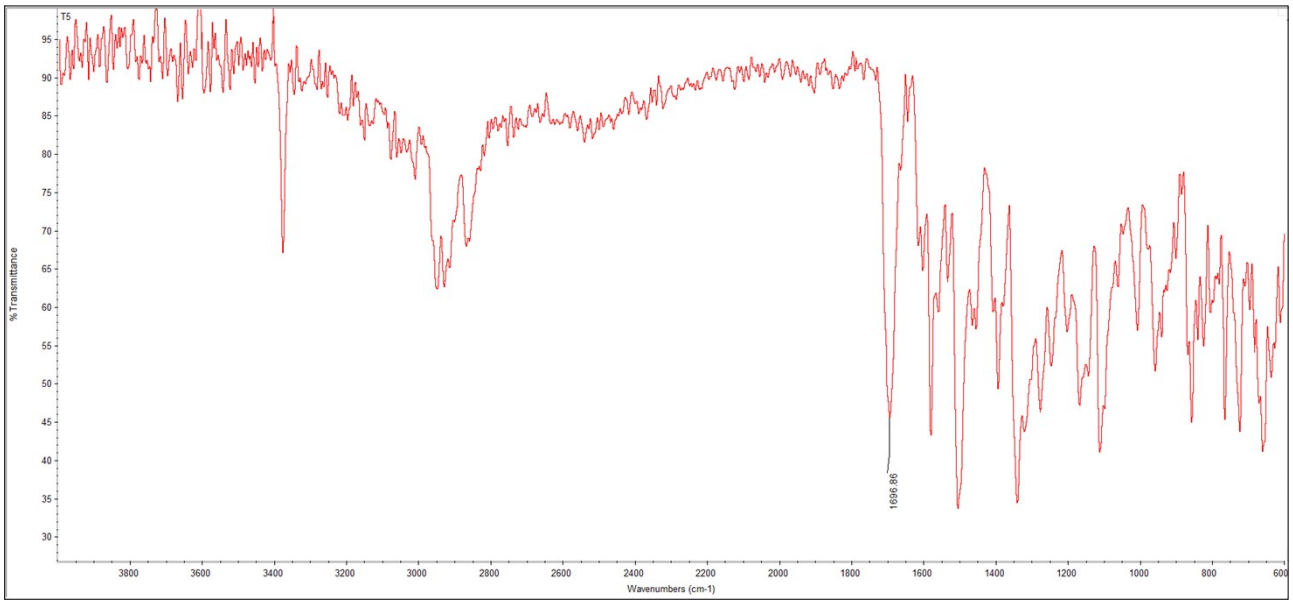

Figure S16. IR of T5.

2.2 Cocrystals with 3DMABA

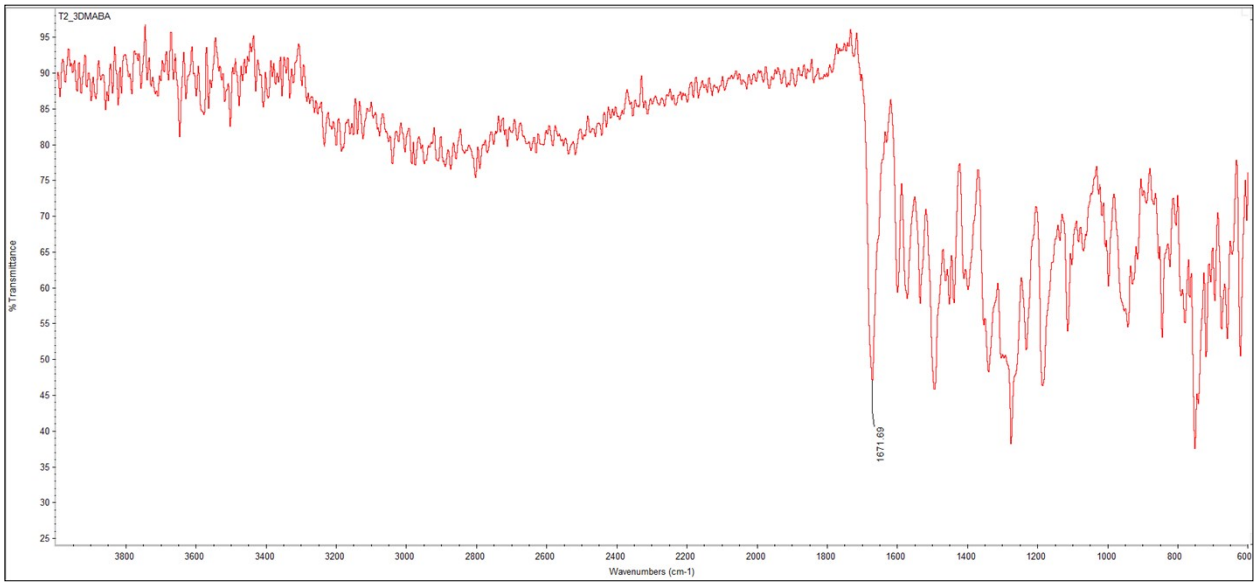

Figure S17. IR of T2-3DMABA.

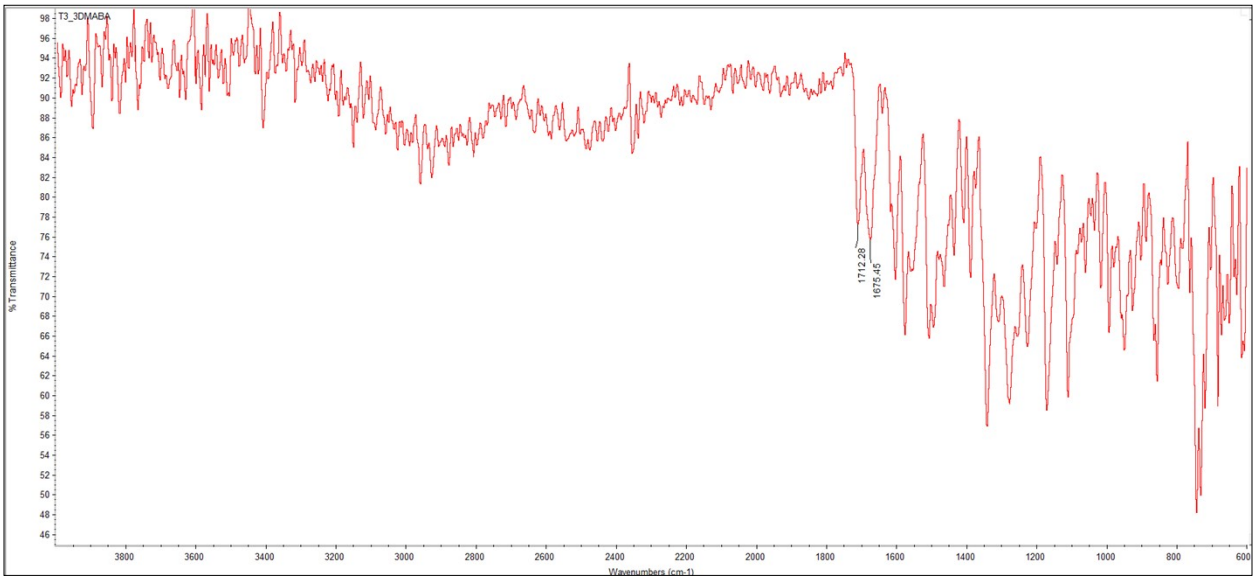

Figure S18. IR of T3-3DMABA.

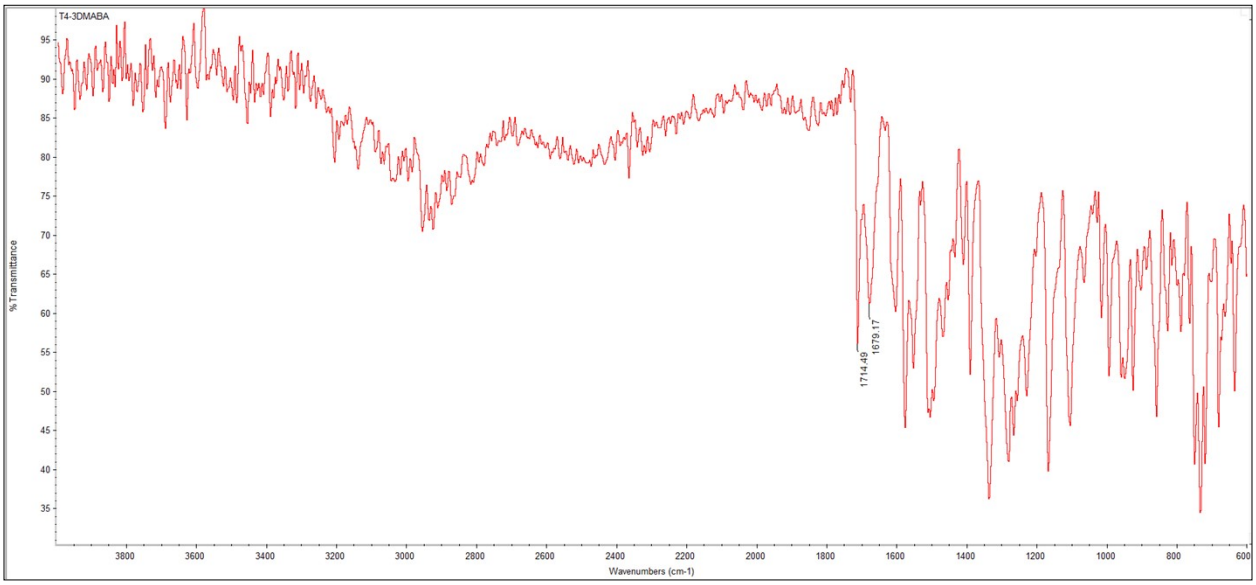

Figure S19. IR of T4-3DMABA.

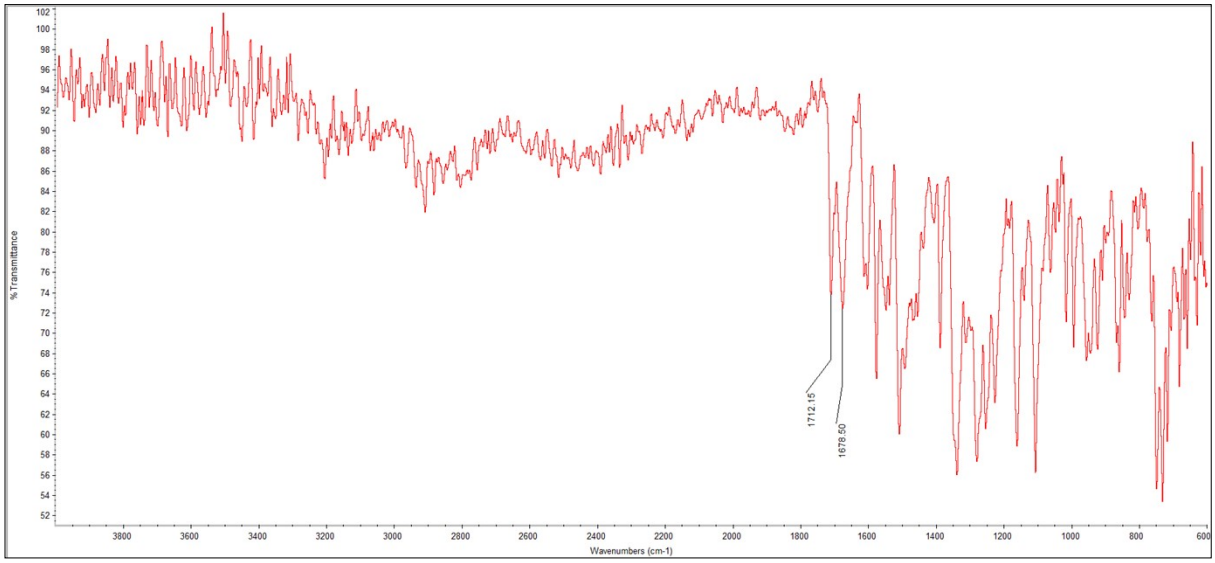

Figure S20. IR of T5-3DMABA.

2.3. Cocrystals with 4ABA

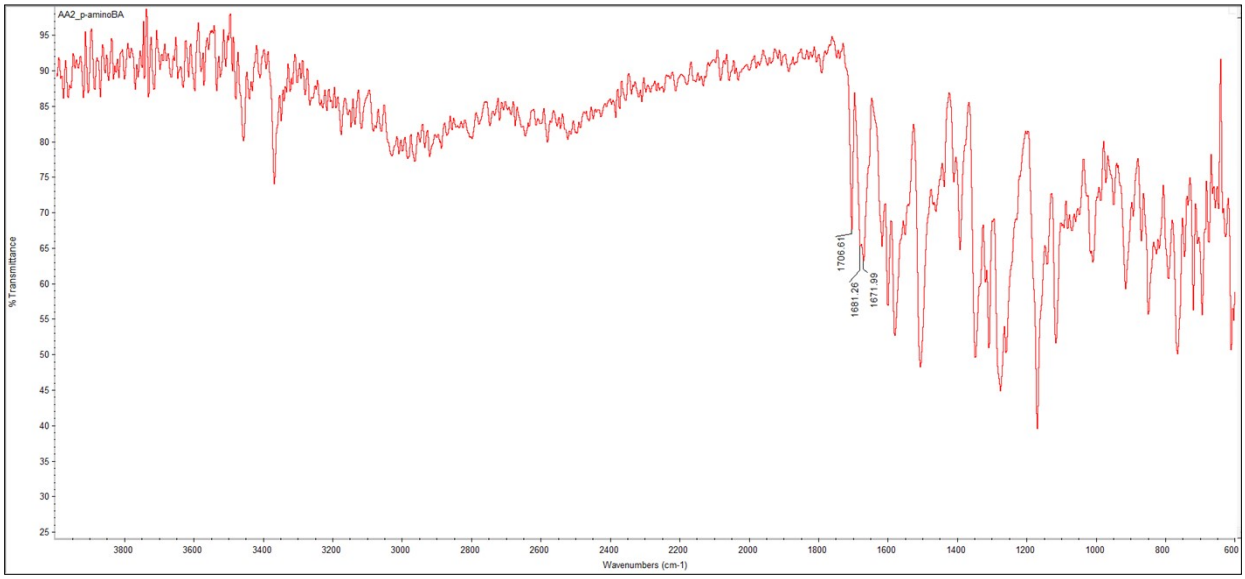

Figure S21. IR of T2-4ABA.

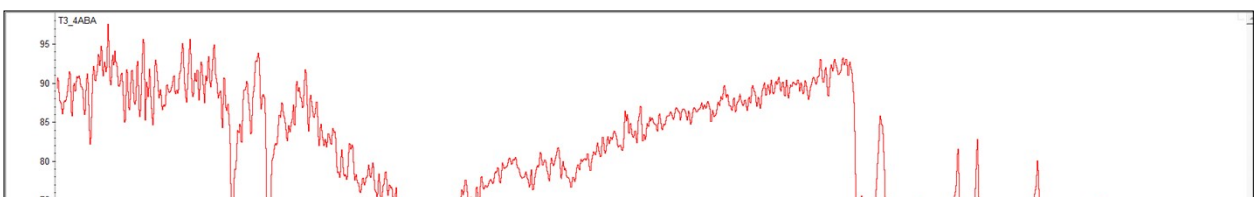

Figure S22. IR of T3-4ABA.

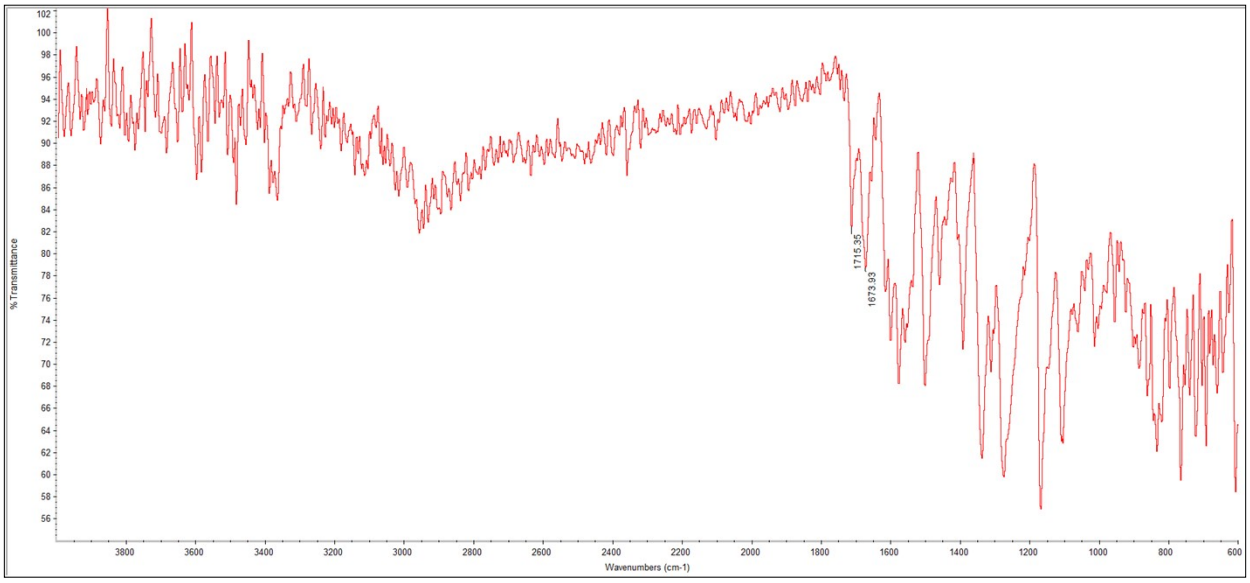

Figure S23. IR of T4-4ABA.

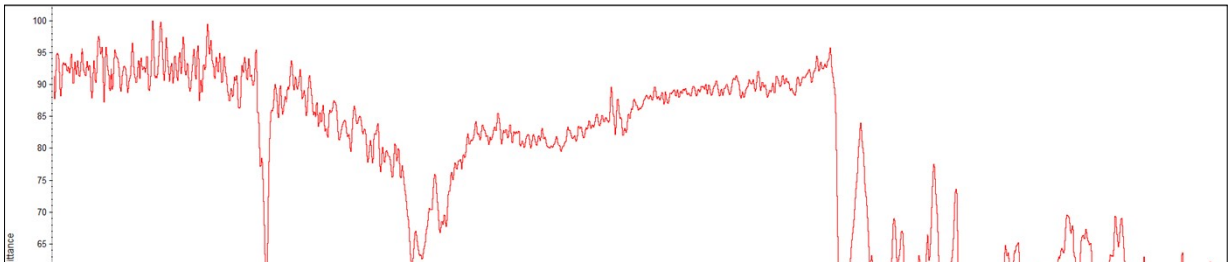

Figure S24. IR of T5-4ABA.

3. PXRD

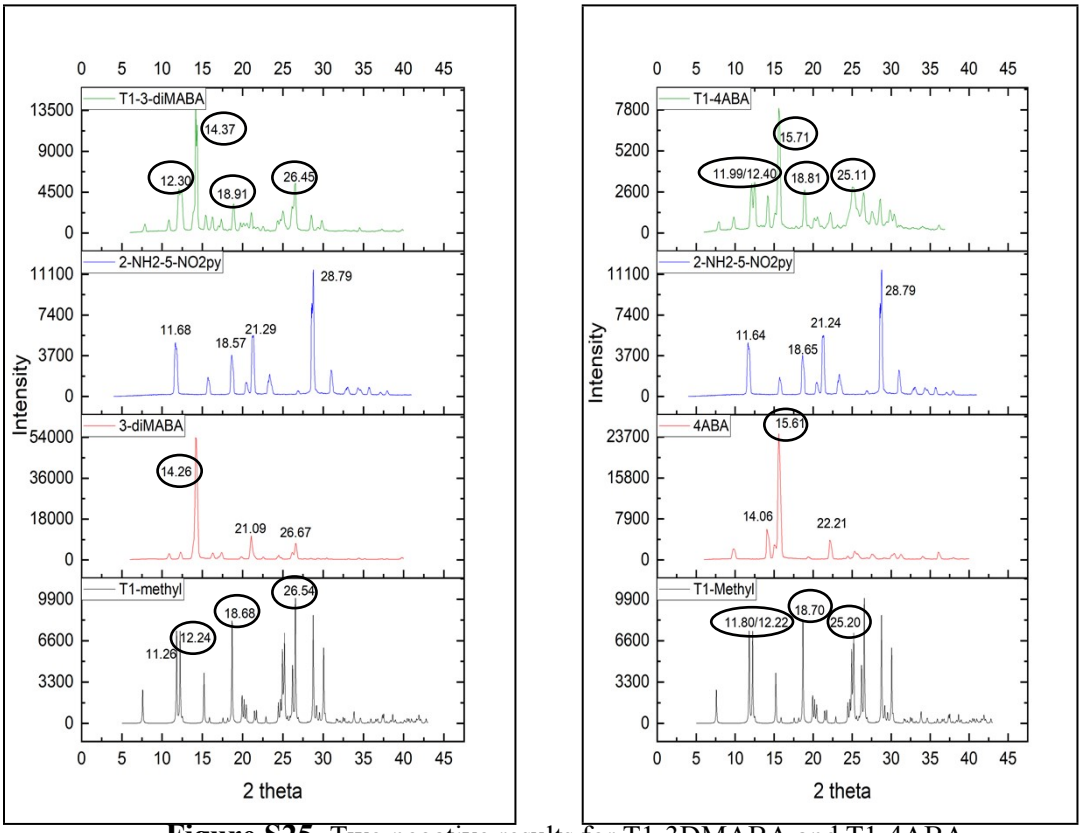

Figure S25. Two negative results for T1-3DMABA and T1-4ABA.

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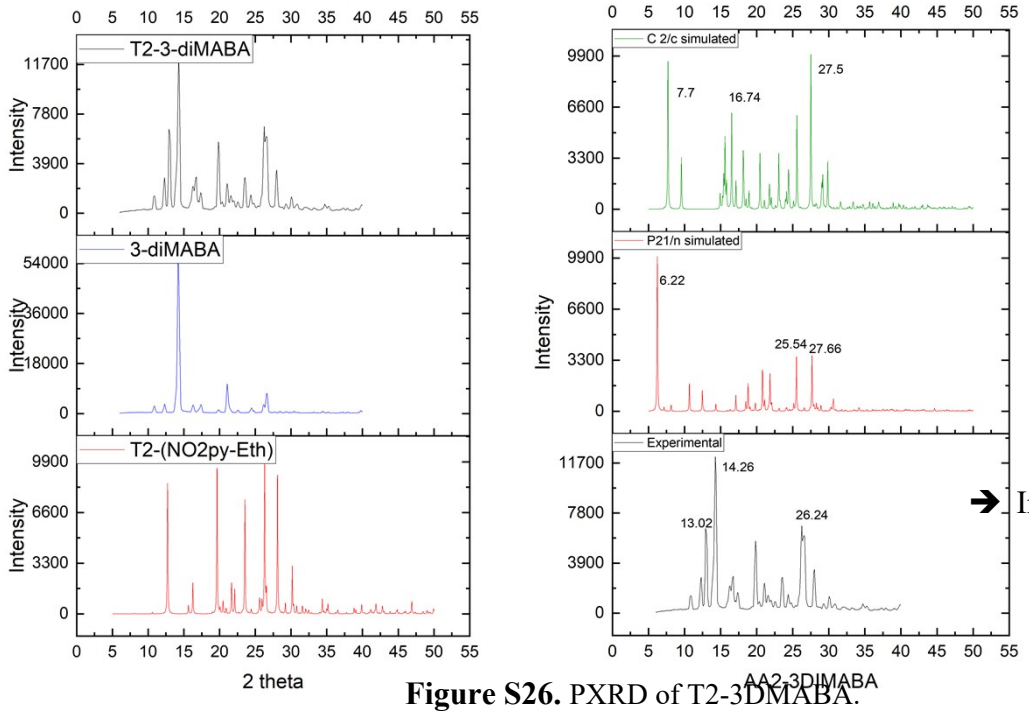
3.1 Cocrystals with 3DMABA



➔ Indication of third polymorph

Figure S26. PXRD of T2-3DMABA.

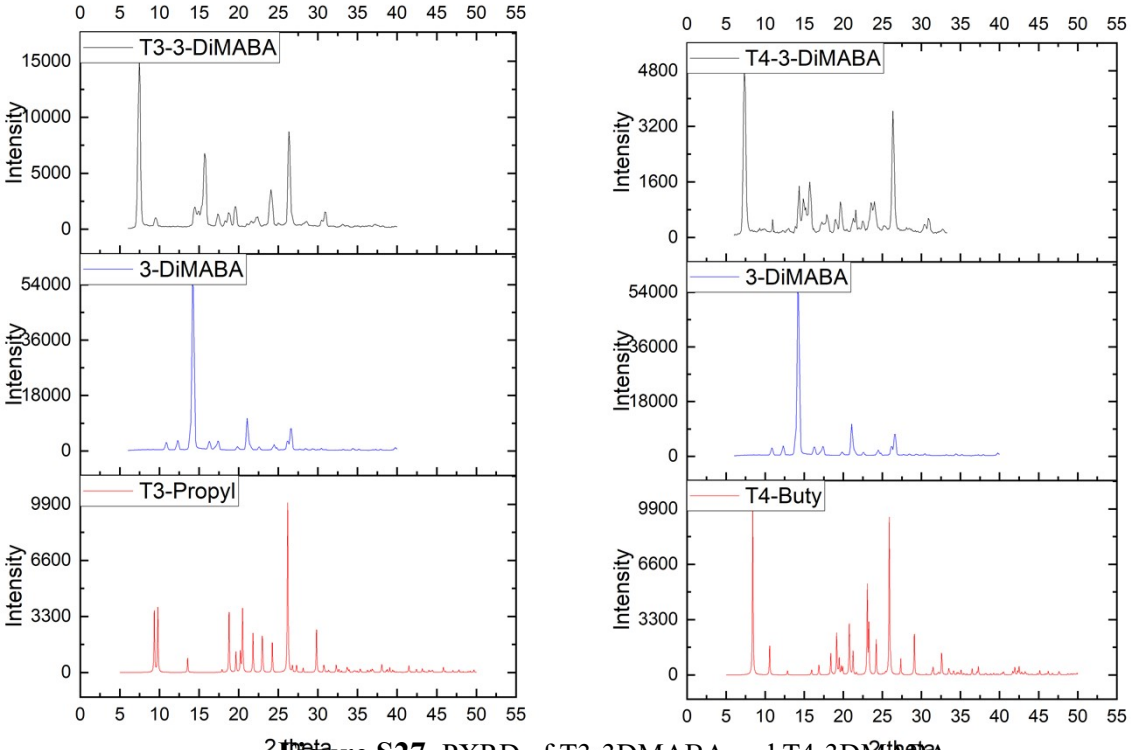


Figure S27. PXRD of T3-3DMABA and T4-3DMABA.

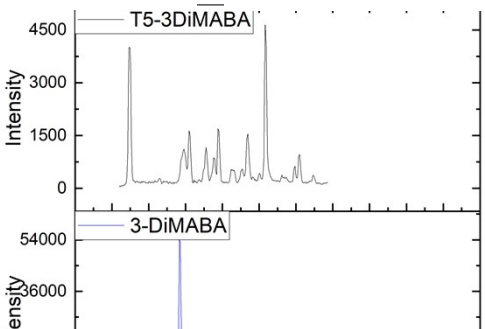


Figure S28. PXRD of T5-3DMABA.

3.2. Cocrystals with 4ABA

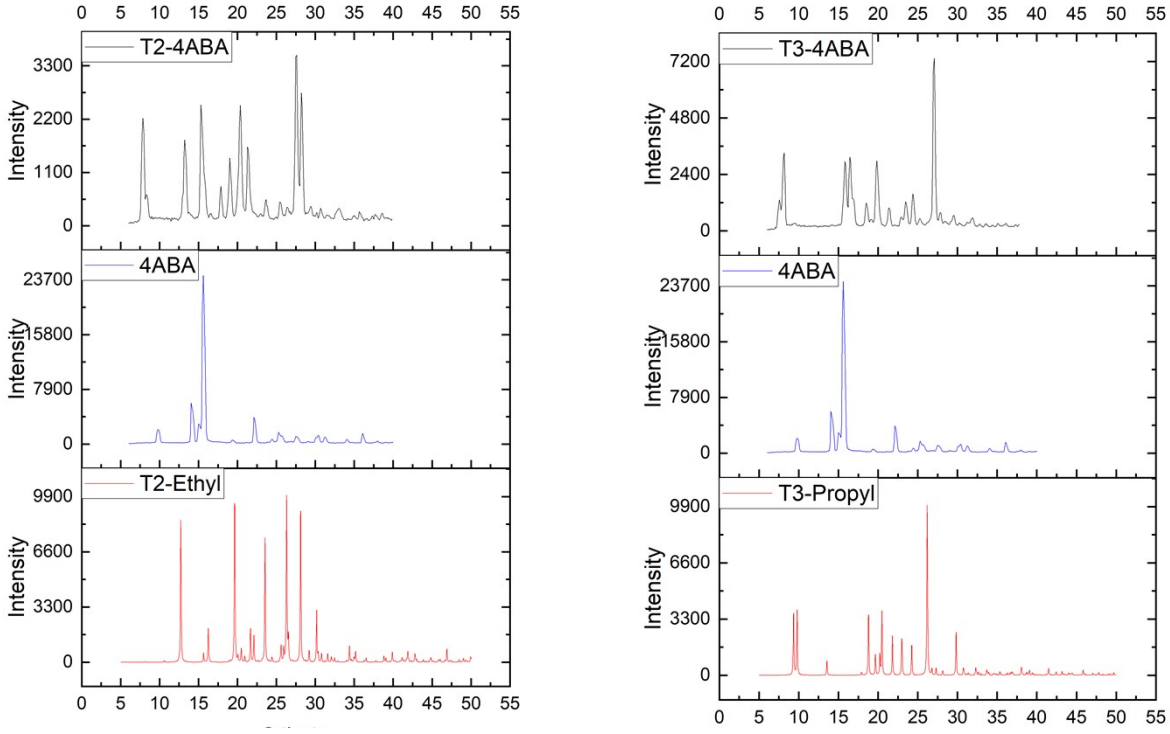


Figure S29. PXRD of T2-4ABA and T3-4ABA.

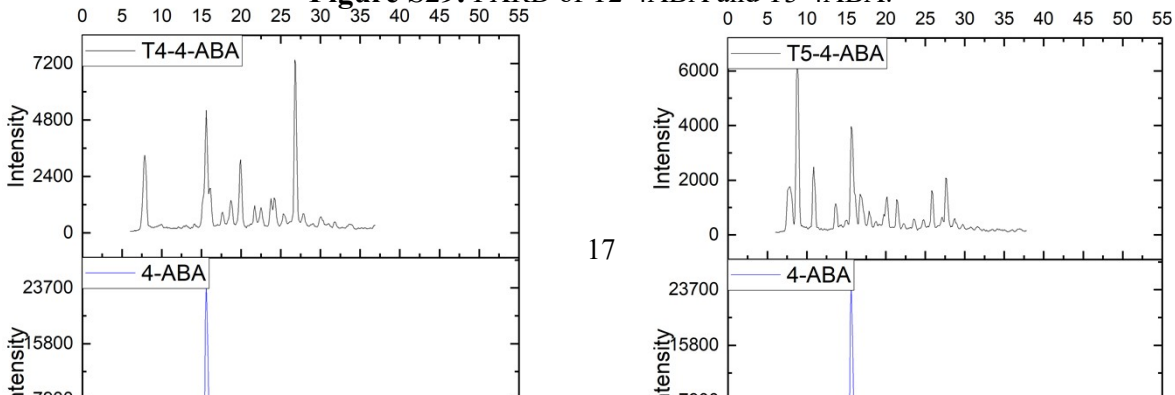


Figure S30. PXRD of T4-4ABA and T5-4ABA.

4. Solid-state UV-Visible spectra

4.1. Cocrystals with 3DMABA

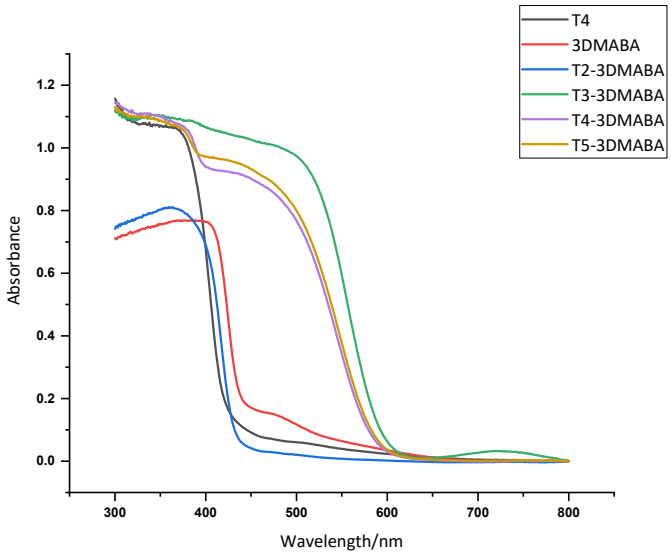


Figure S31. Solid-state UV-vis spectra for 3DMABA cocrystals.

4.2. Cocrystals with 4ABA

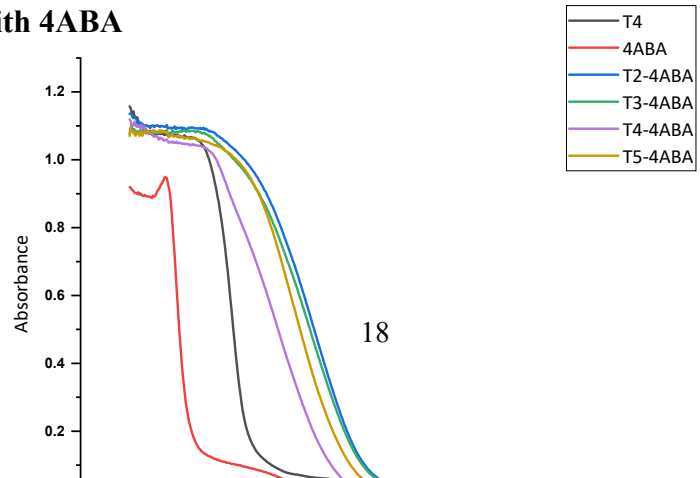
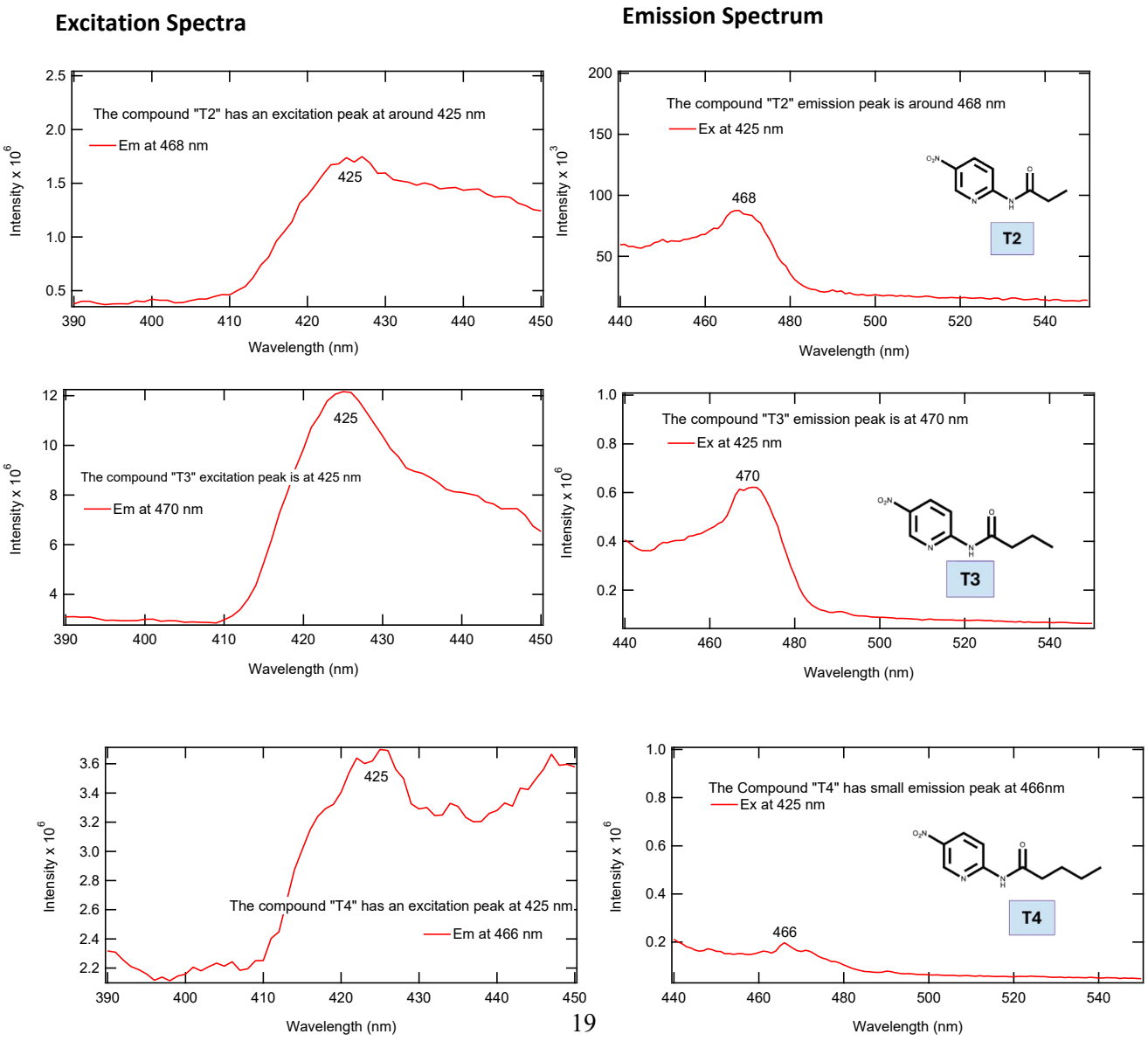
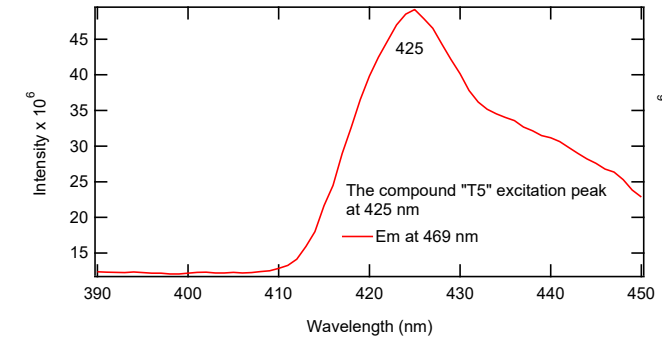


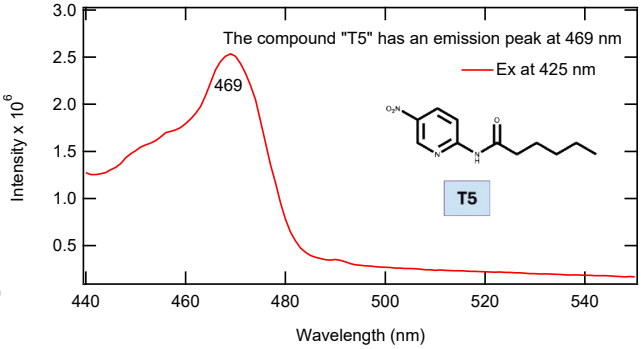
Figure S32. Solid-state UV-vis spectra for 4ABA cocrystals.

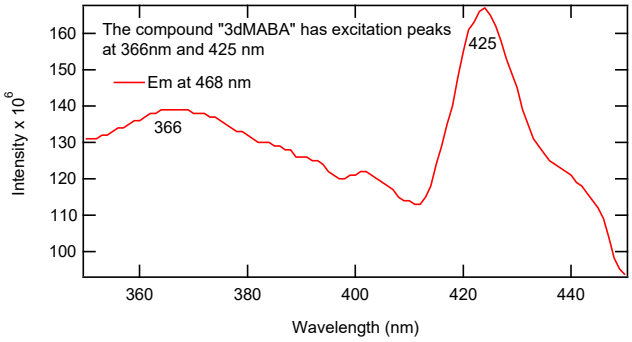
5. Photoluminescence studies

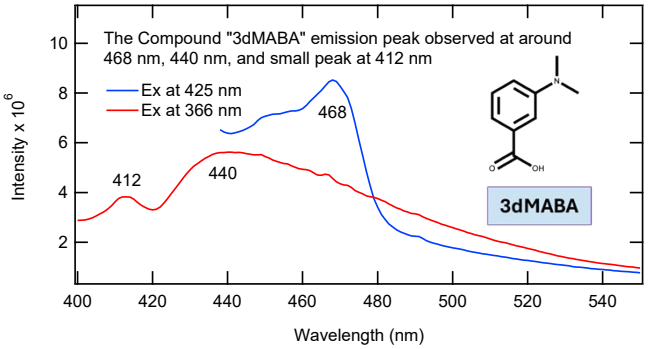
5.1. Starting materials:

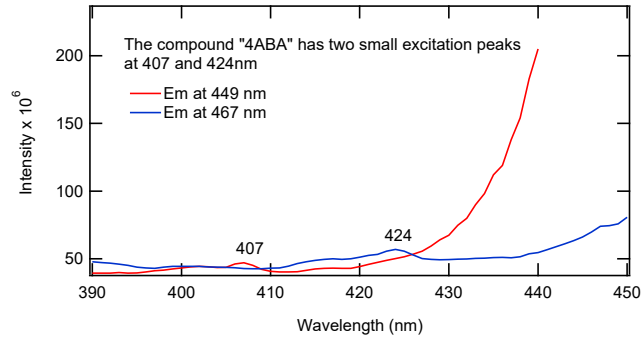


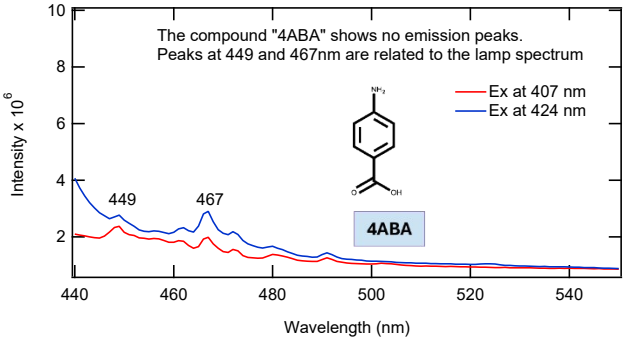




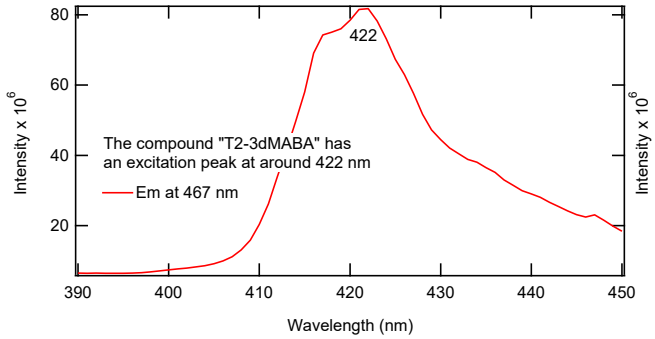


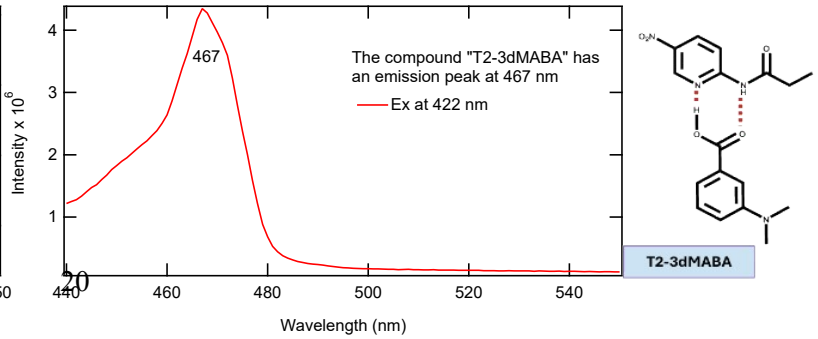


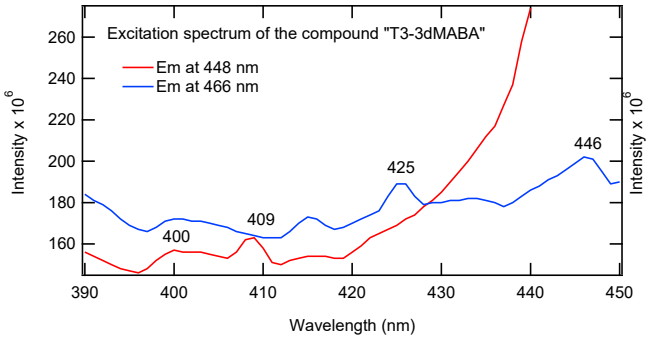


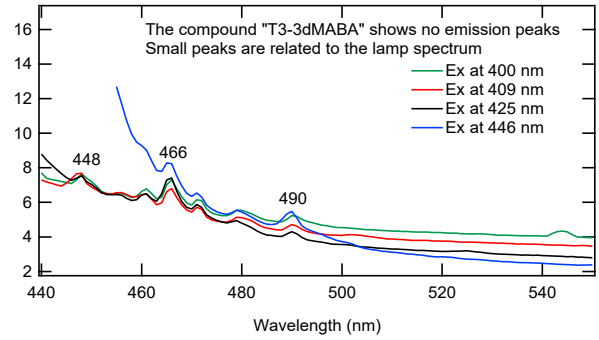


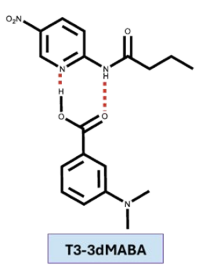
5.2. Cocrystals with 3DMABA

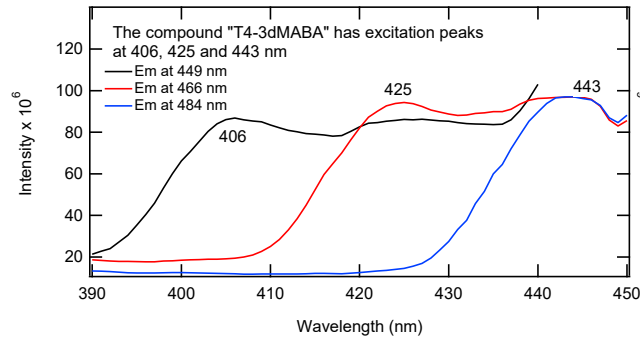


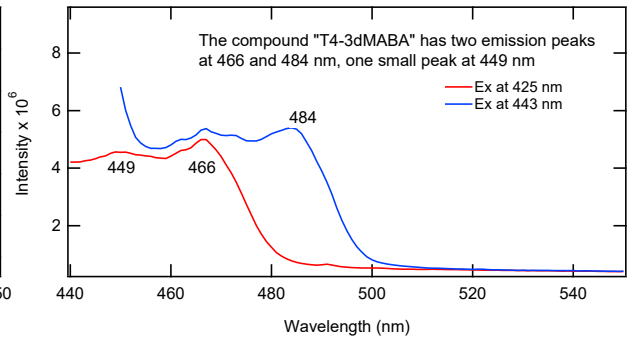


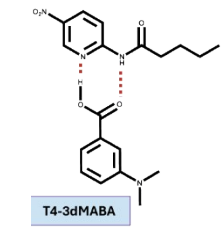


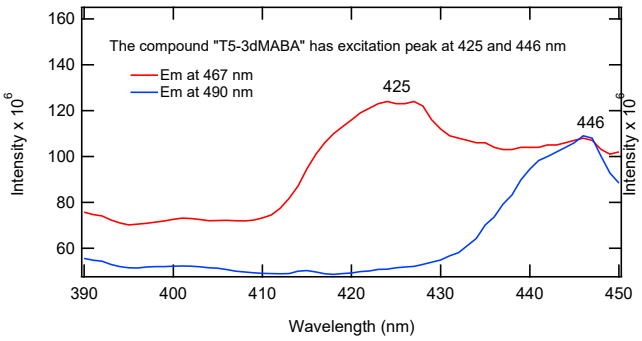


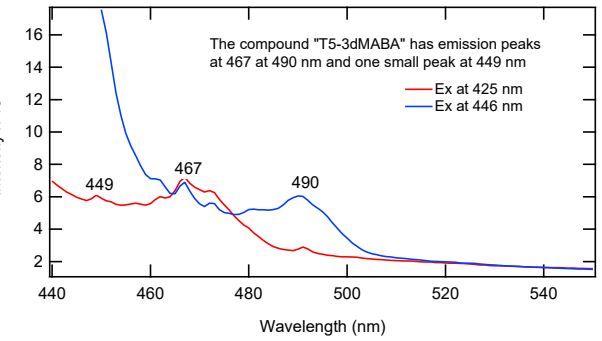


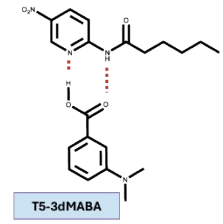




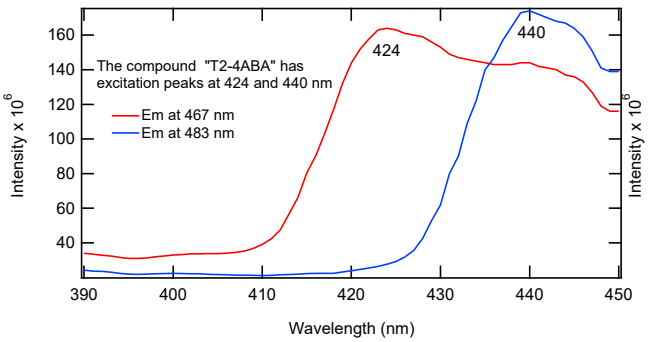


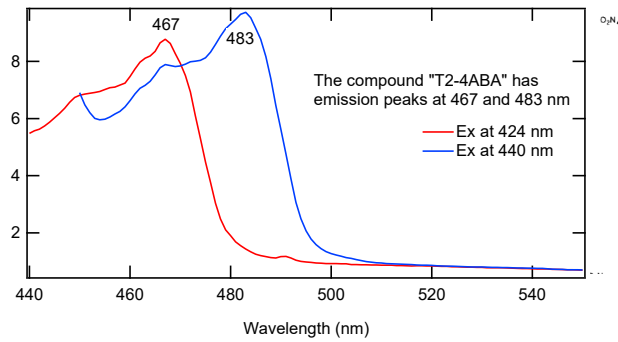


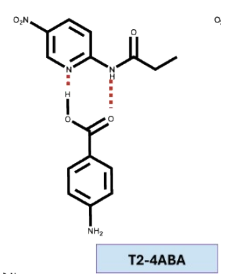


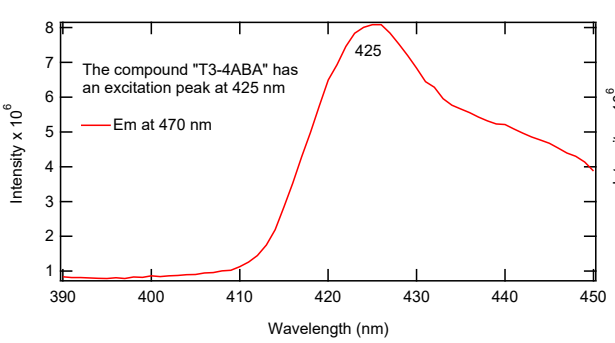


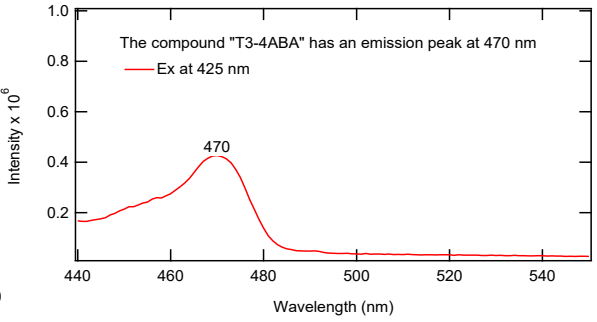
5.3. Cocrystals with 4ABA

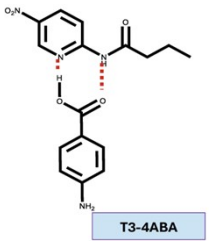


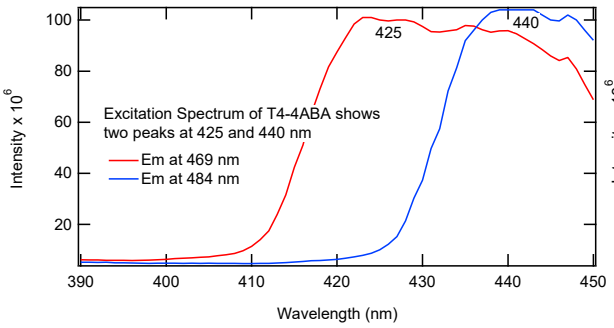


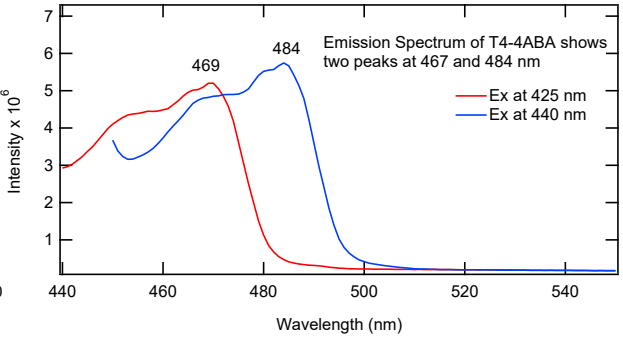


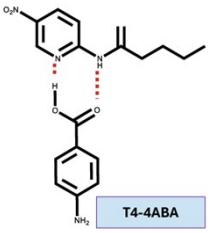


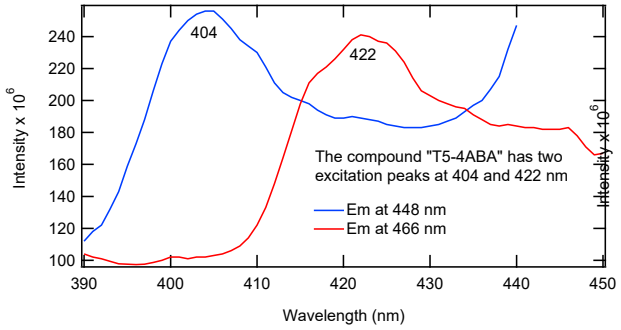


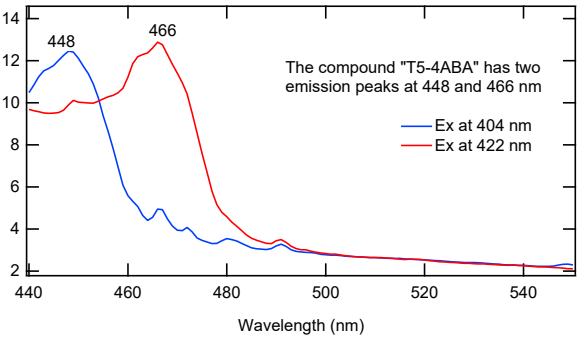


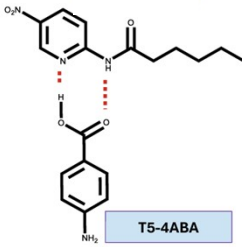




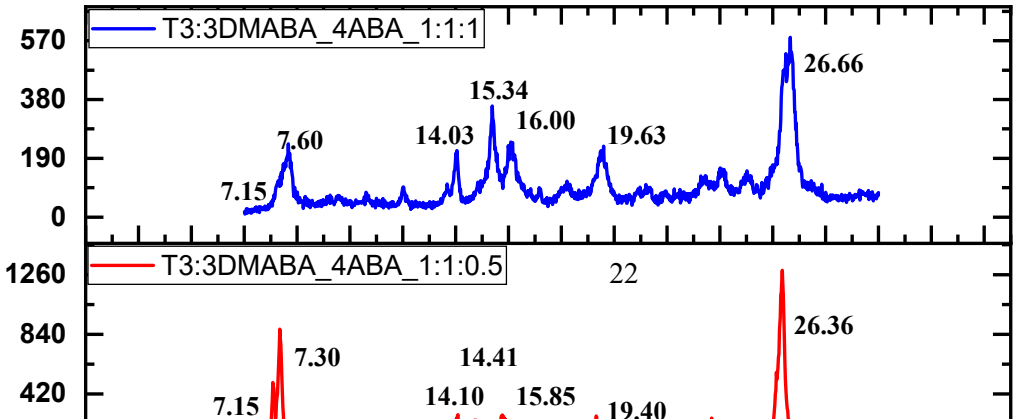


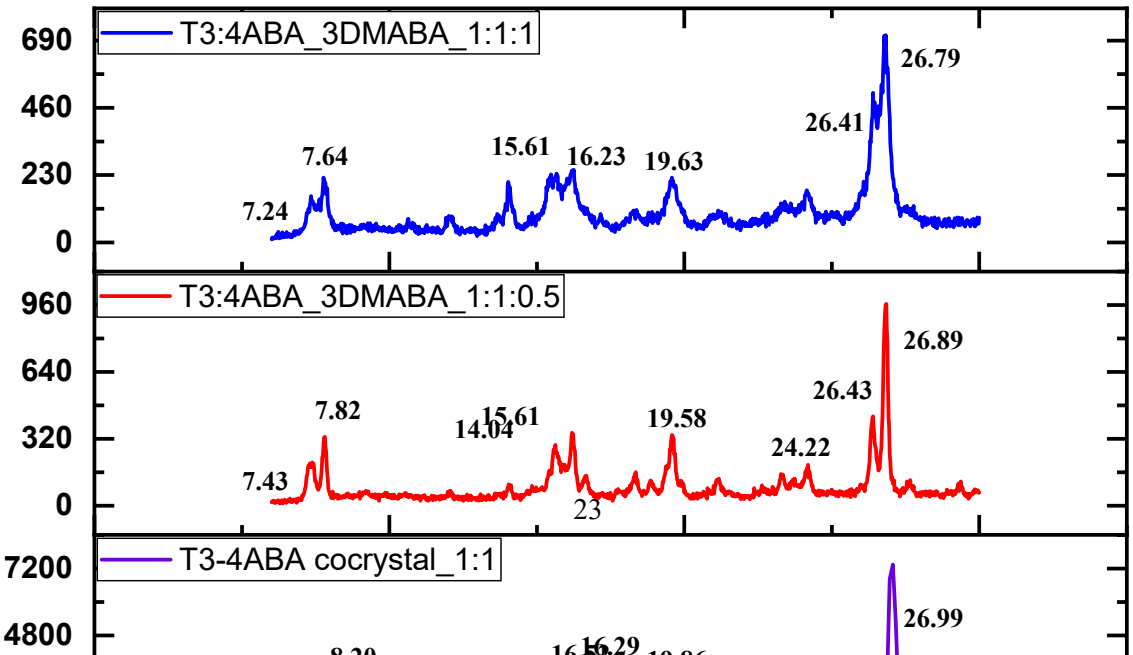






6. Solid-state replacement studies

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7.64
15.61
16.23
19.63
26.41
26.79
T3:4ABA_3DMABA_1:1:0.5
960
640
320
0
7.43
7.82
14.04
15.61
19.58
24.22
26.43
26.89
23
T3-4ABA cocrystal_1:1
7200
4800
26.99