

Supplementary Material

Control and interconversion of cocrystal stoichiometry in grinding: stepwise mechanism for the formation of a hydrogen-bonded cocrystal

Shyam Karki, Tomislav Friščić and William Jones*

Figure S1	PXRD patterns for screening experiments involving na and oxa in 1:1 stoichiometric ratio.	3
Figure S2	PXRD patterns for screening experiments involving na and oxa in 2:1 stoichiometric ratio.	4
Figure S3	PXRD patterns for screening experiments involving na and mal in 1:1 stoichiometric ratio.	5
Figure S4	PXRD patterns for screening experiments involving na and mal in 2:1 stoichiometric ratio.	6
Figure S5	PXRD patterns for screening experiments involving na and suc in 1:1 stoichiometric ratio.	7
Figure S6	PXRD patterns for screening experiments involving na and suc in 2:1 stoichiometric ratio.	8
Figure S7	PXRD patterns for screening experiments involving na and glu in 1:1 stoichiometric ratio.	9
Figure S8	PXRD patterns for screening experiments involving na and glu in 2:1 stoichiometric ratio.	10
Figure S9	PXRD patterns for screening experiments involving na and adi in 1:1 stoichiometric ratio.	11
Figure S10	PXRD patterns for screening experiments involving na and adi in 2:1 stoichiometric ratio.	12
Figure S11	PXRD patterns for screening experiments involving na and pim in 1:1 stoichiometric ratio.	13
Figure S12	PXRD patterns for screening experiments involving na and pim in 2:1 stoichiometric ratio.	14
Figure S13	PXRD patterns for screening experiments involving na and sub in 1:1 stoichiometric ratio.	15
Figure S14	PXRD patterns for screening experiments involving na and sub in 2:1 stoichiometric ratio.	16

	stoichiometric ratio.	
Figure S15	PXRD patterns for screening experiments involving na and aze in 1:1 stoichiometric ratio.	17
Figure S16	PXRD patterns for screening experiments involving na and aze in 2:1 stoichiometric ratio.	18
Figure S17	PXRD patterns for screening experiments involving na and seb in 1:1 stoichiometric ratio.	19
Figure S18	PXRD patterns for screening experiments involving na and seb in 2:1 stoichiometric ratio.	20
Figure S19	PXRD patterns for screening experiments involving na and fum in 1:1 stoichiometric ratio.	21
Figure S20	PXRD patterns for screening experiments involving na and fum in 2:1 stoichiometric ratio.	22
Figure S21	DSC thermogram for the cocrystallisation of na and mal from the melt in respective stoichiometric ratio 1:1.	23
Figure S22	DSC thermogram for the cocrystallisation of na and mal from the melt in respective stoichiometric ratio 2:1.	23
Figure S23	DSC thermogram for the cocrystallisation of na and suc from the melt in respective stoichiometric ratio 1:1.	24
Figure S24	DSC thermogram for the cocrystallisation of na and suc from the melt in respective stoichiometric ratio 2:1.	24
Figure S25	DSC thermogram for the cocrystallisation of na and glu from the melt in respective stoichiometric ratio 1:1.	25
Figure S26	DSC thermogram for the cocrystallisation of na and glu from the melt in respective stoichiometric ratio 2:1.	25
Figure S27	DSC thermogram for the cocrystallisation of na and adi from the melt in respective stoichiometric ratio 1:1.	26
Figure S28	DSC thermogram for the cocrystallisation of na and adi from the melt in respective stoichiometric ratio 2:1.	26
Figure S29	DSC thermogram for the cocrystallisation of na and pim from the melt in respective stoichiometric ratio 1:1.	27
Figure S30	DSC thermogram for the cocrystallisation of na and pim from the melt in respective stoichiometric ratio 2:1.	27
Figure S31	DSC thermogram for the cocrystallisation of na and sub from the melt in respective stoichiometric ratio 1:1.	28
Figure S32	DSC thermogram for the cocrystallisation of na and sub from the melt in respective stoichiometric ratio 2:1.	28
Figure S33	DSC thermogram for the cocrystallisation of na and aze from the melt in respective stoichiometric ratio 1:1.	29
Figure S34	DSC thermogram for the cocrystallisation of na and aze from the melt in respective stoichiometric ratio 2:1.	29
Figure S35	DSC thermogram for the cocrystallisation of na and seb from the melt in respective stoichiometric ratio 1:1.	30
Figure S36	DSC thermogram for the cocrystallisation of na and seb from the melt in respective stoichiometric ratio 2:1.	30

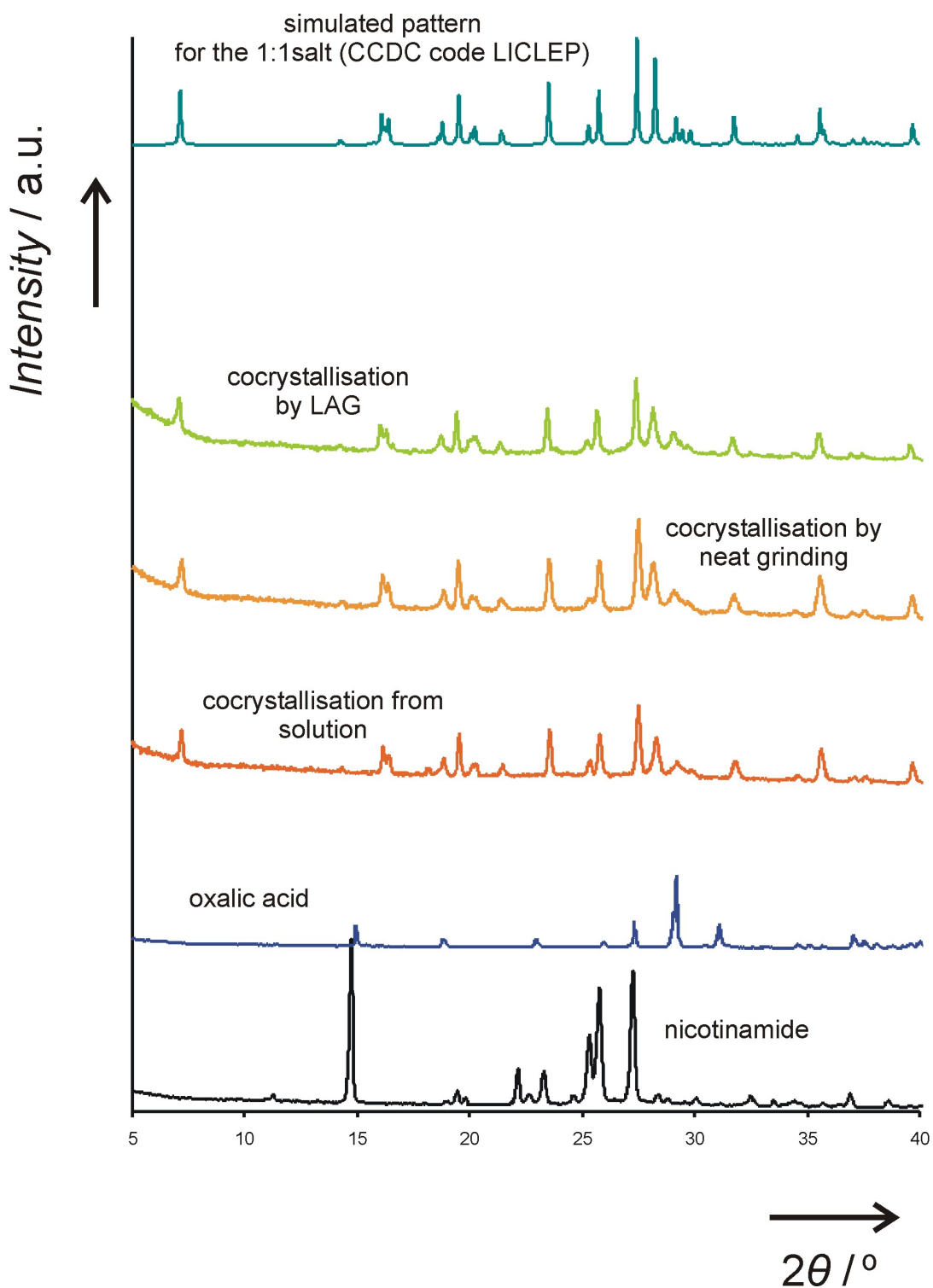


Figure S1. PXRD patterns for screening experiments involving **na** and **oxa** in 1:1 stoichiometric ratio. Screening from the melt was not performed due to the sensitivity of oxalic acid to elevated temperatures.

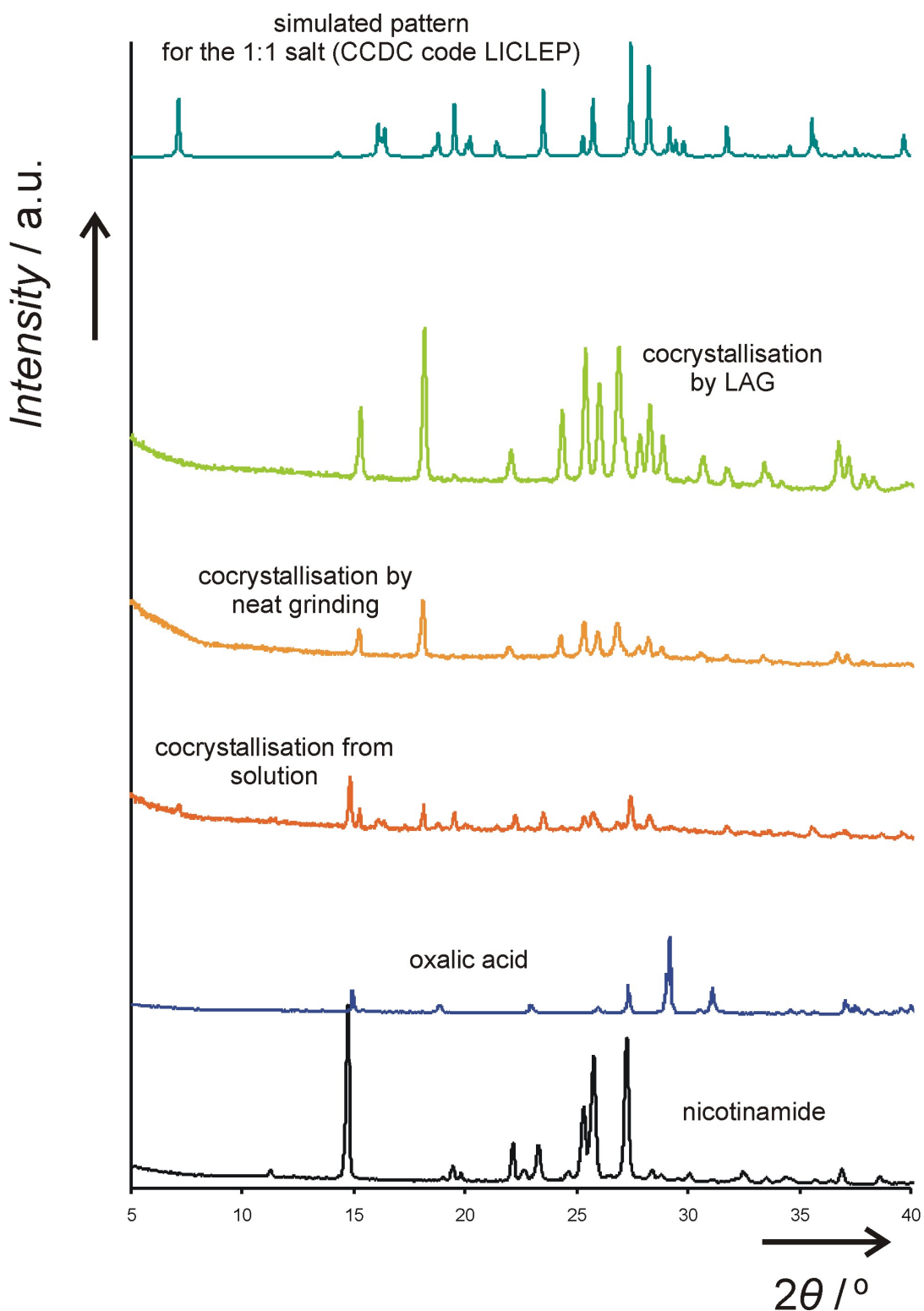


Figure S2. PXRD patterns for screening experiments involving **na** and **oxa** in 2:1 stoichiometric ratio. Screening from the melt was not performed due to the sensitivity of oxalic acid to elevated temperatures.

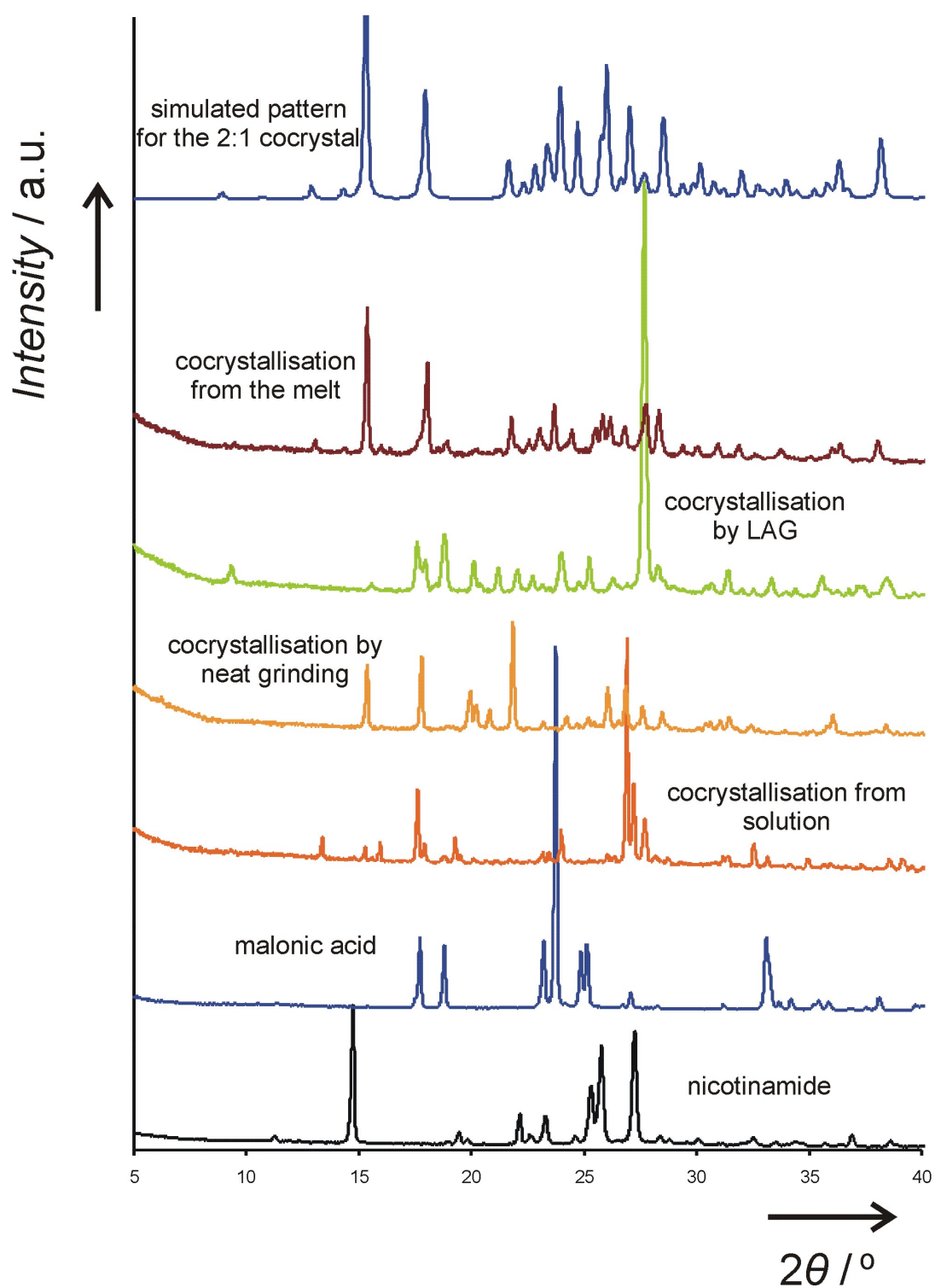


Figure S3. PXRD patterns for screening experiments involving **na** and **mal** in 1:1 stoichiometric ratio.

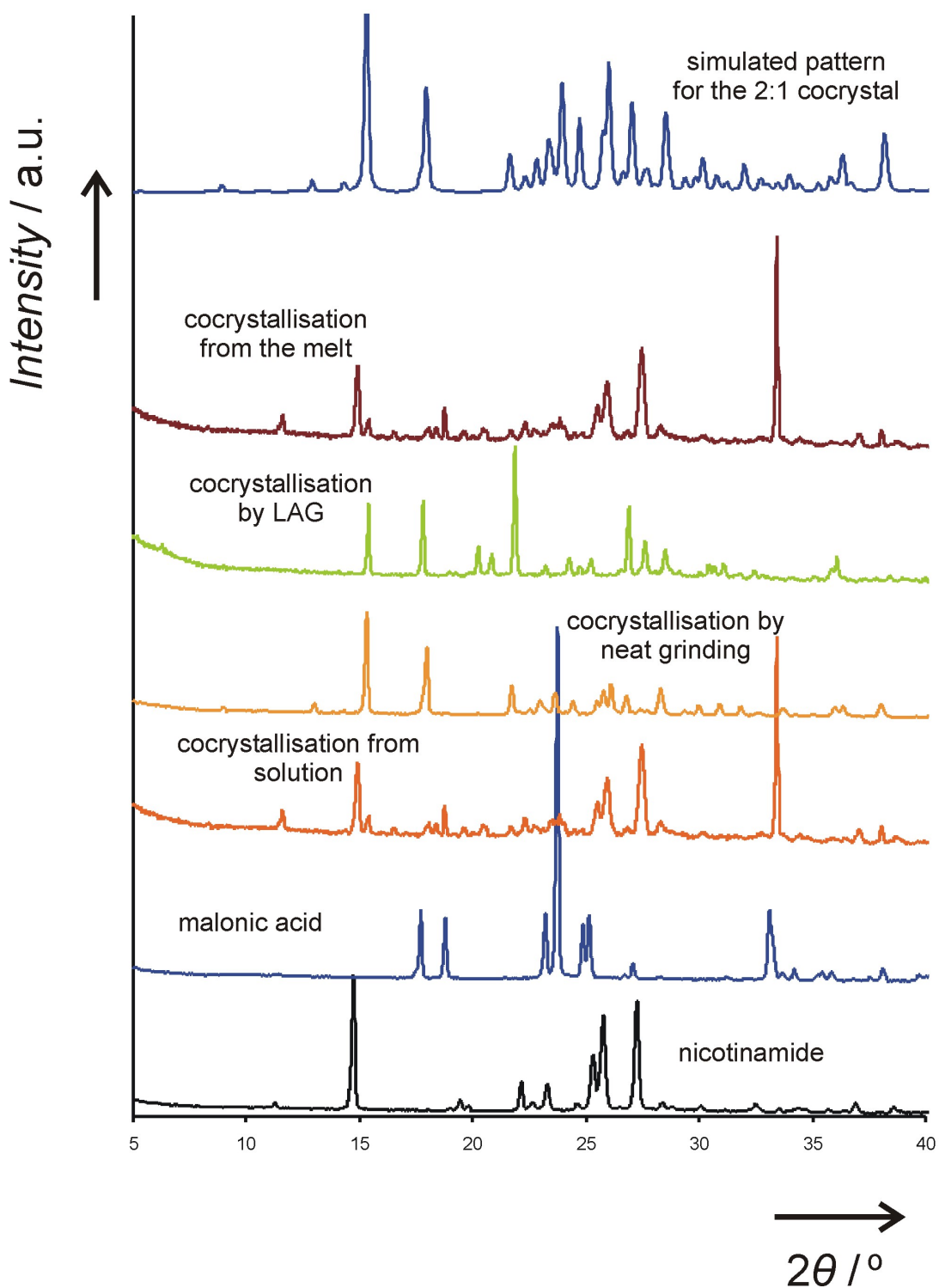


Figure S4. PXRD patterns for screening experiments involving **na** and **mal** in 2:1 stoichiometric ratio.

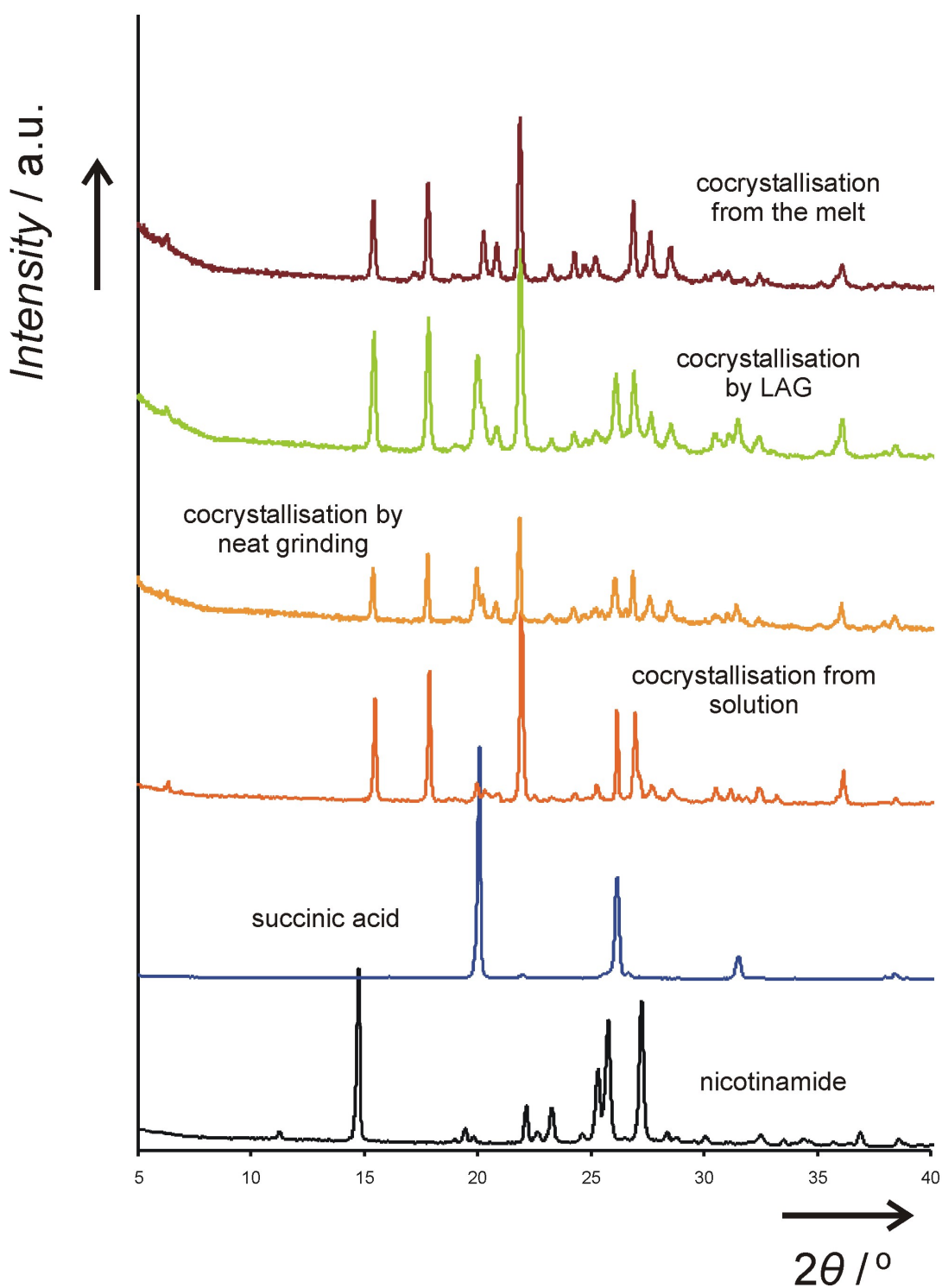


Figure S5. PXRD patterns for screening experiments involving **na** and **suc** in 1:1 stoichiometric ratio.

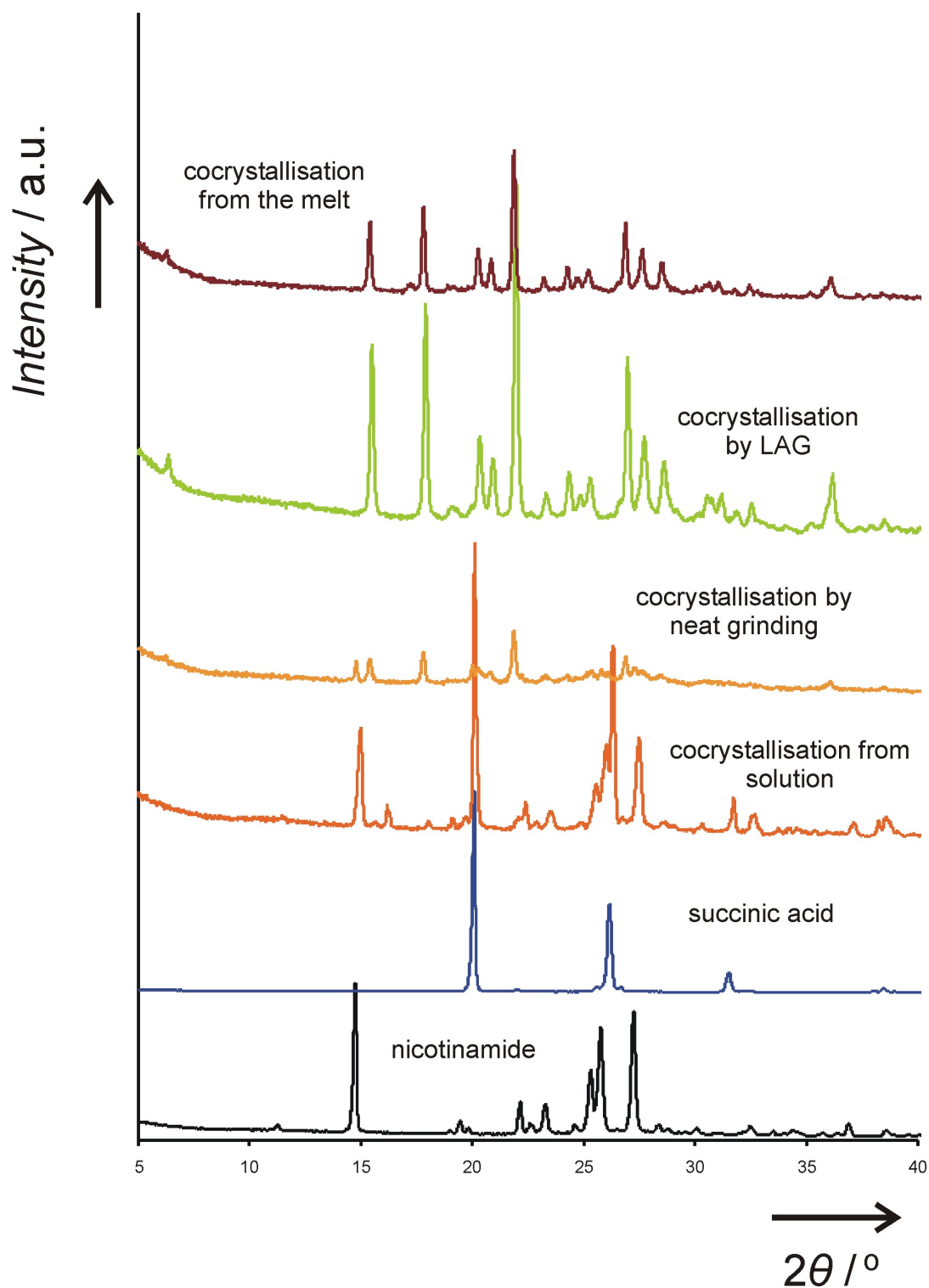


Figure S6. PXRD patterns for screening experiments involving **na** and **suc** in 2:1 stoichiometric ratio.

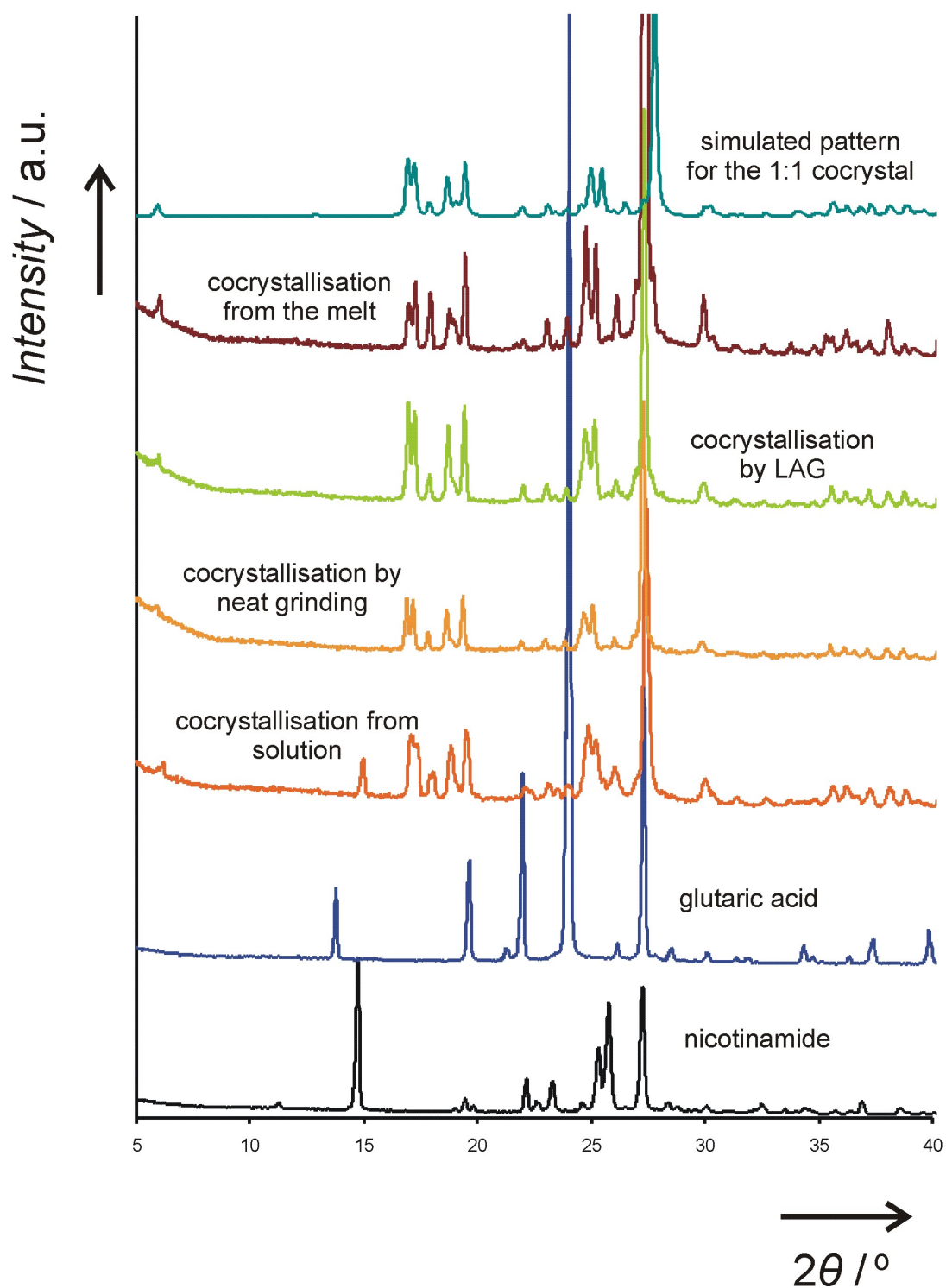


Figure S7. PXRD patterns for screening experiments involving **na** and **glu** in 1:1 stoichiometric ratio.

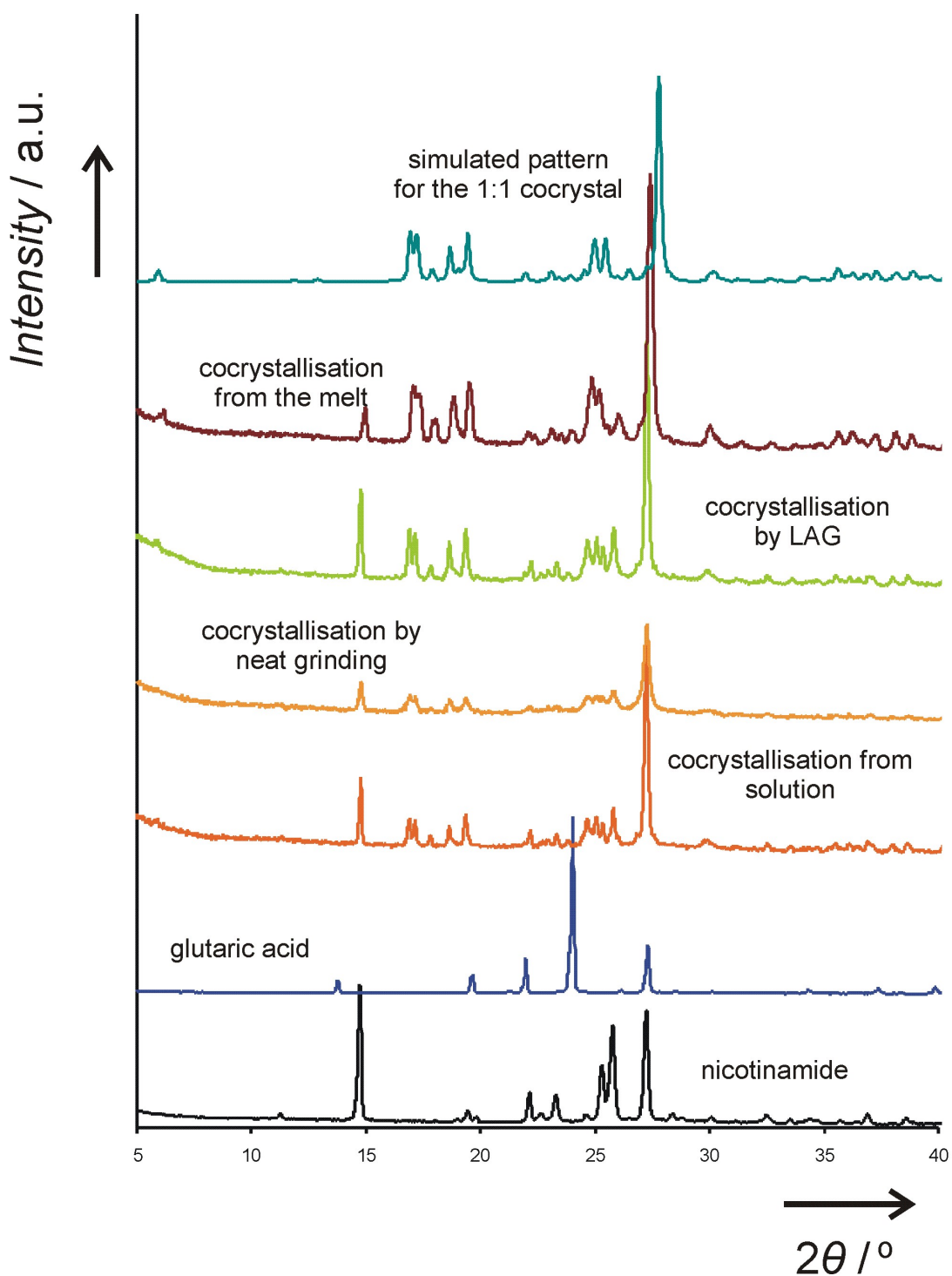


Figure S8. PXRD patterns for screening experiments involving **na** and **glu** in 2:1 stoichiometric ratio.

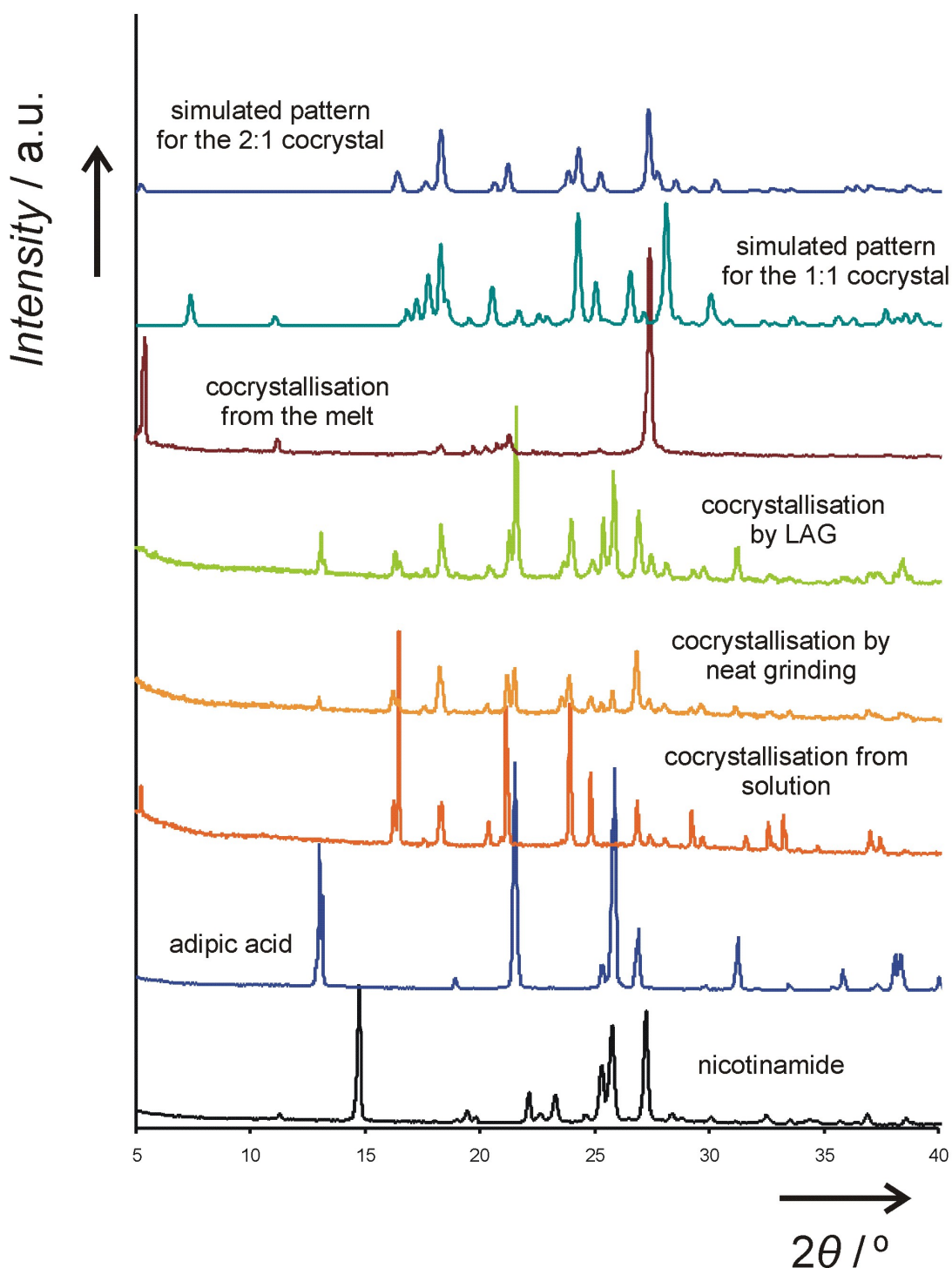


Figure S9. PXRD patterns for screening experiments involving **na** and **adi** in 1:1 stoichiometric ratio.

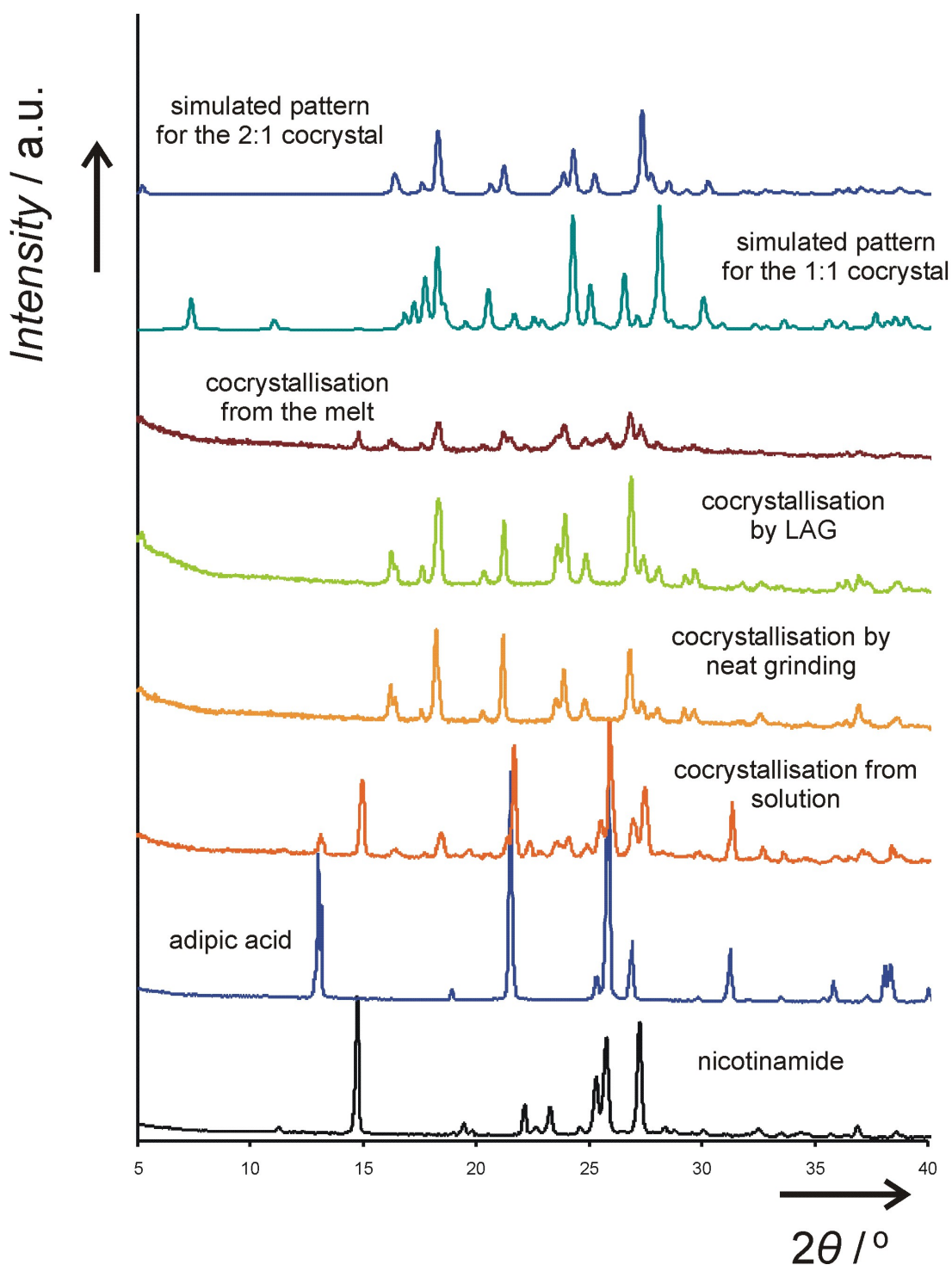


Figure S10. PXRD patterns for screening experiments involving **na** and **adi** in 2:1 stoichiometric ratio.

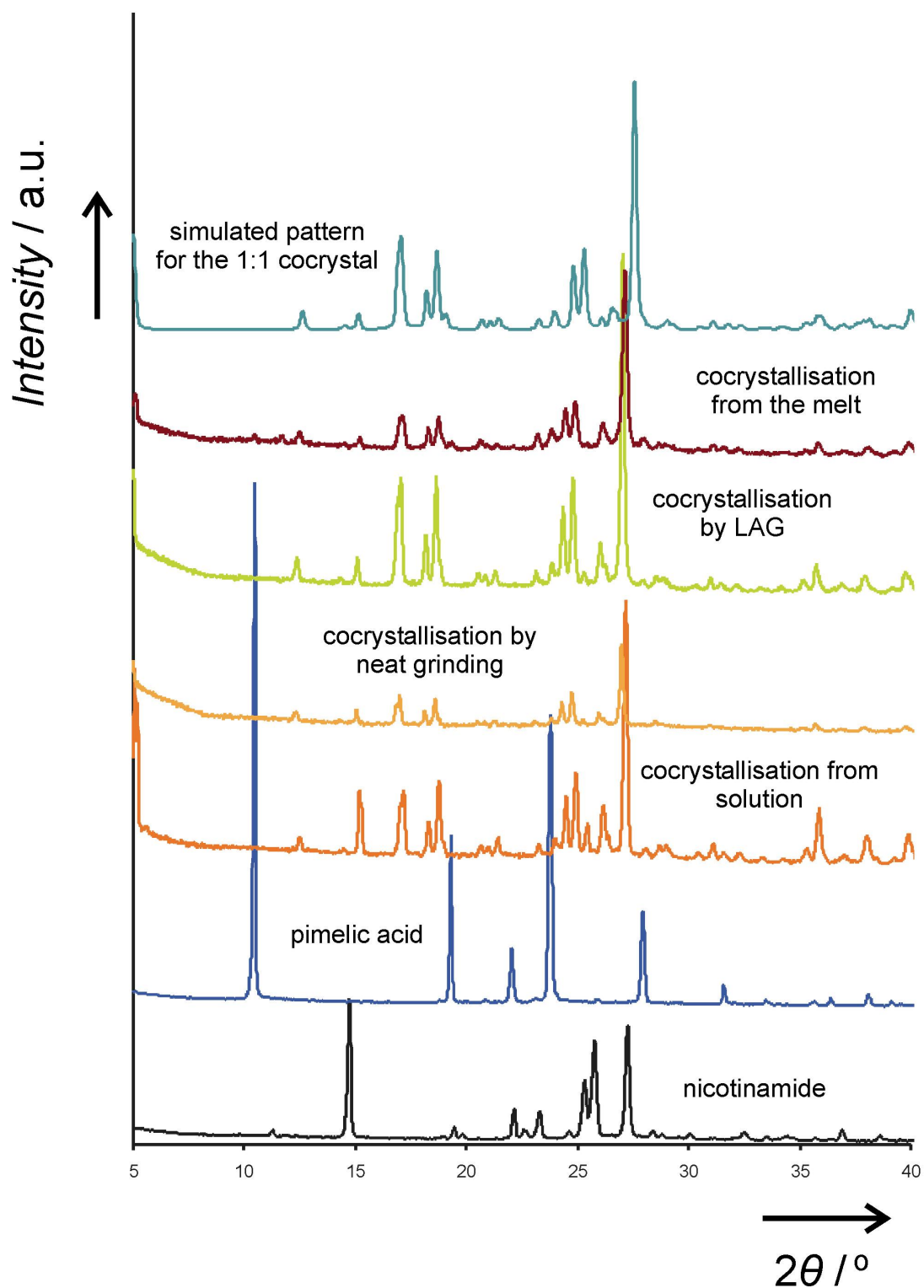


Figure S11. PXRD patterns for screening experiments involving **na** and **pim** in 1:1 stoichiometric ratio.

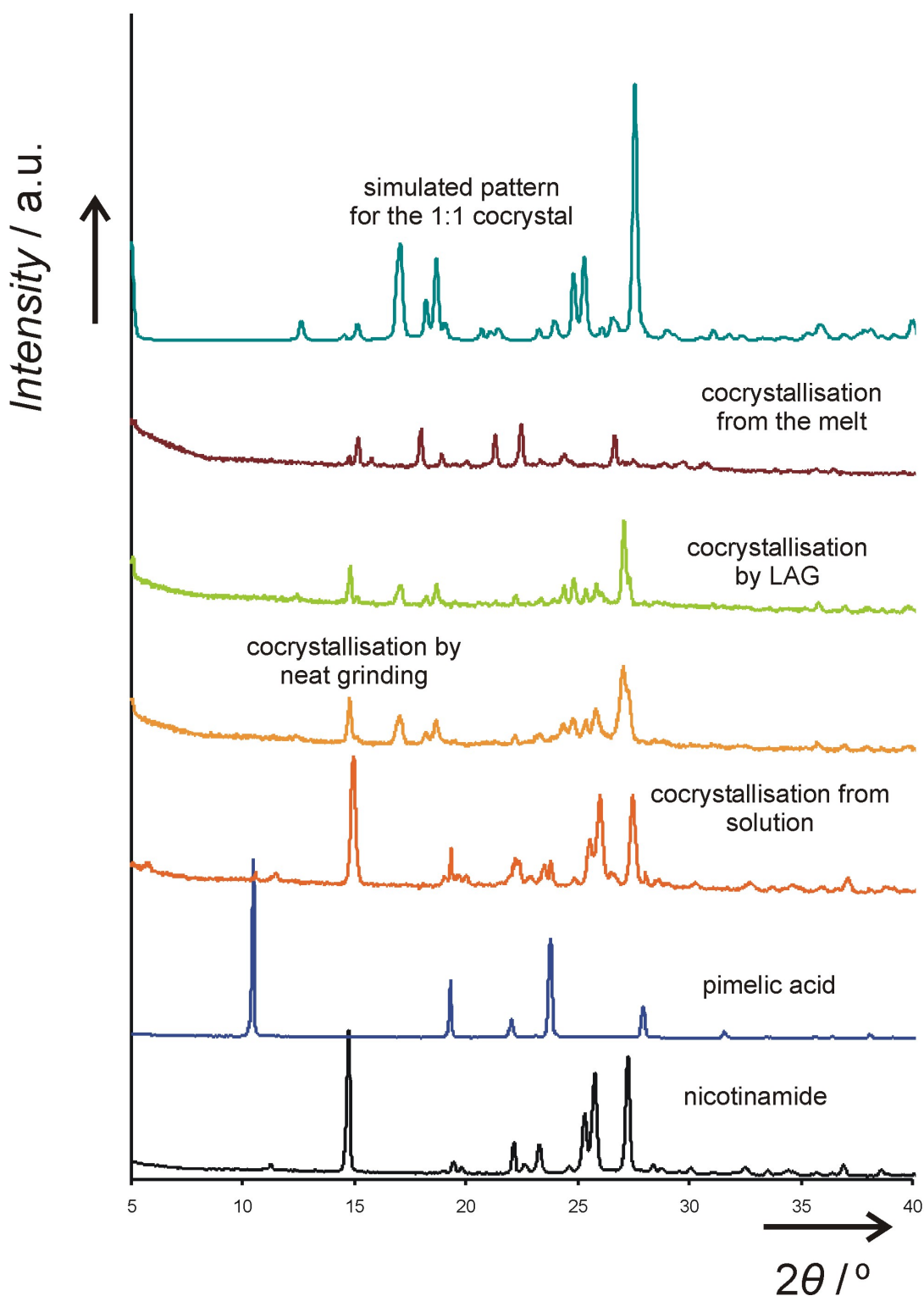


Figure S12. PXRD patterns for screening experiments involving **na** and **pim** in 2:1 stoichiometric ratio.

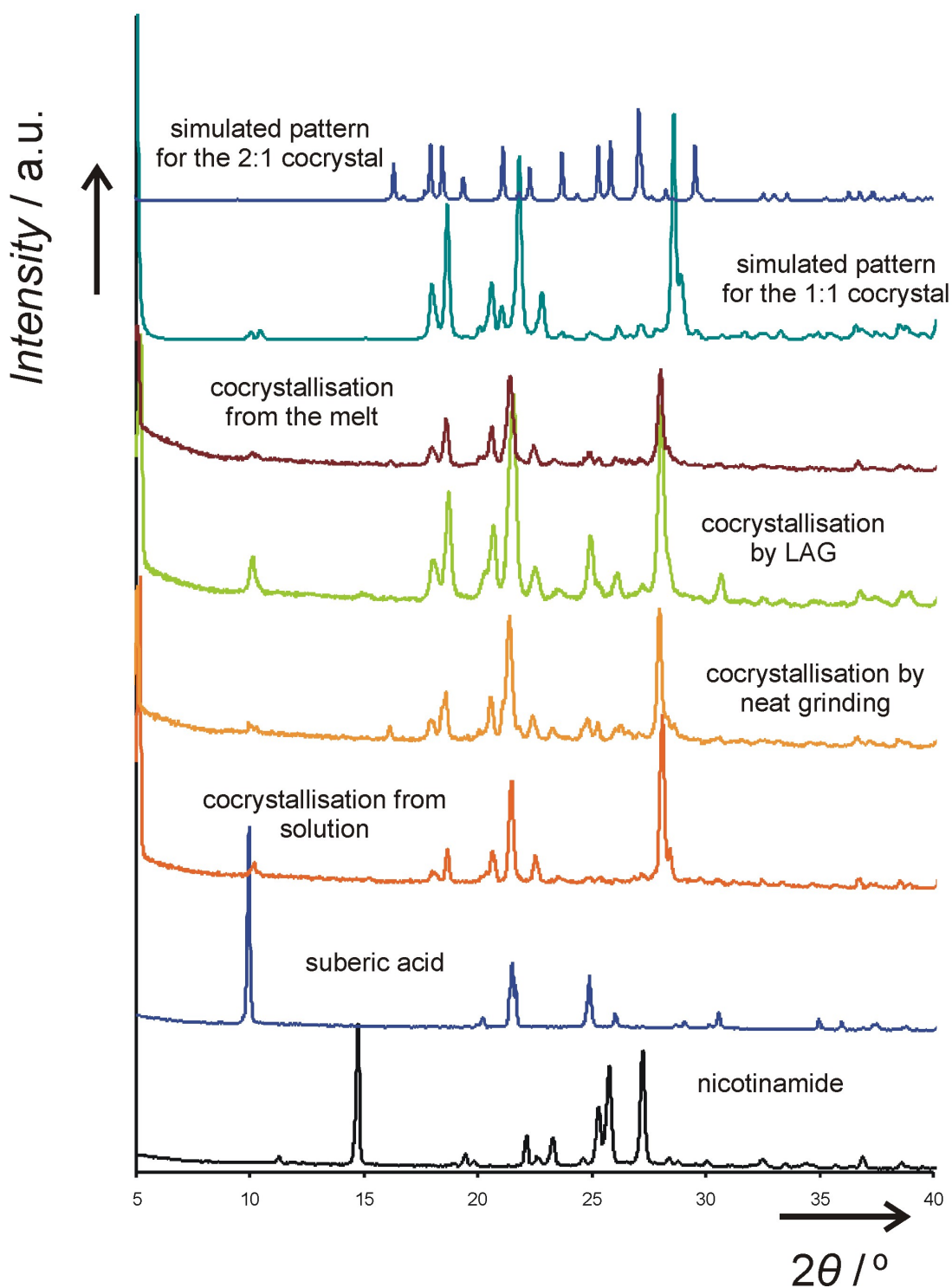


Figure S13. PXRD patterns for screening experiments involving **na** and **sub** in 1:1 stoichiometric ratio.

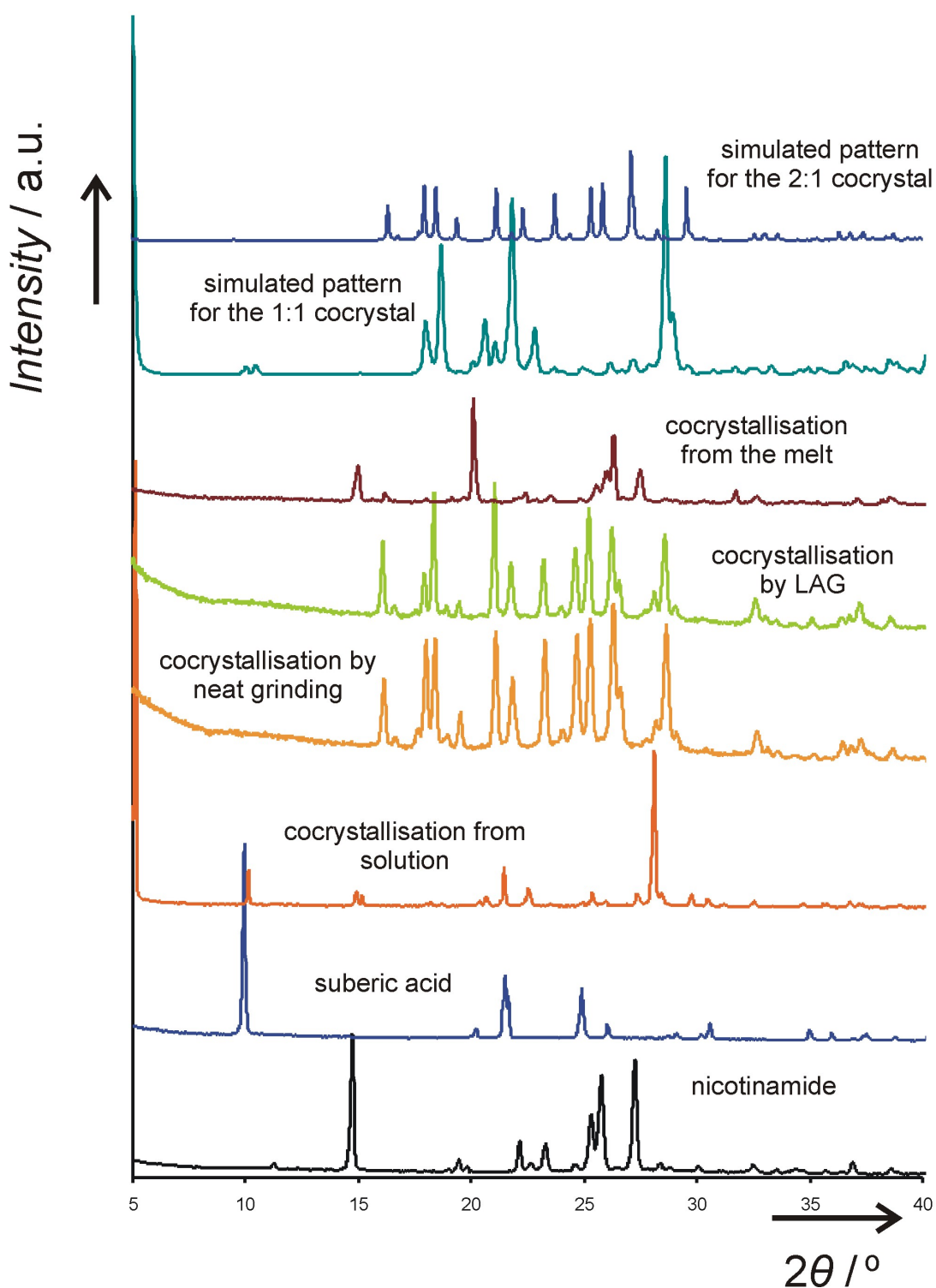


Figure S14. PXRD patterns for screening experiments involving **na** and **sub** in 2:1 stoichiometric ratio.

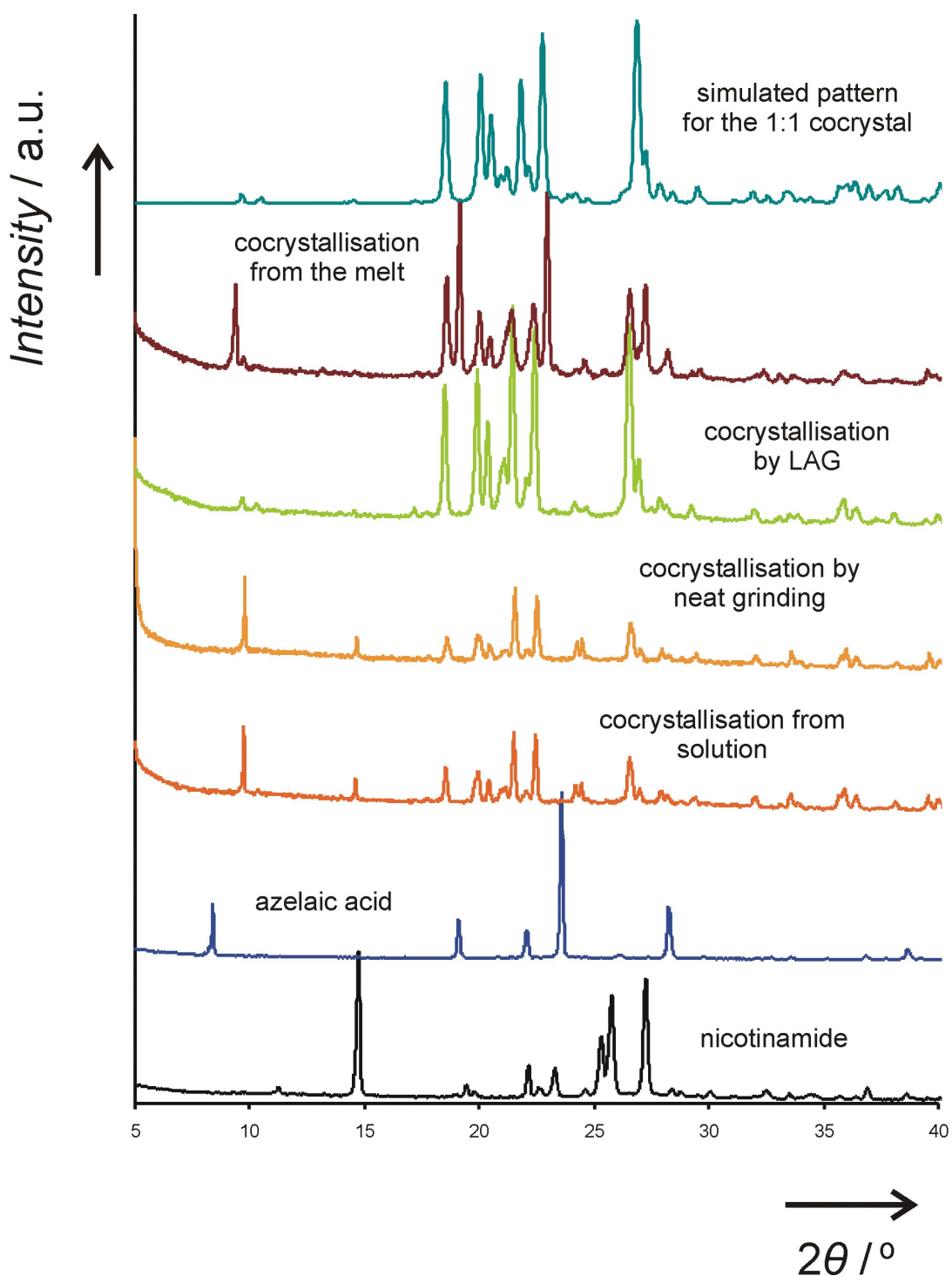


Figure S15. PXRD patterns for screening experiments involving **na** and **aze** in 1:1 stoichiometric ratio.

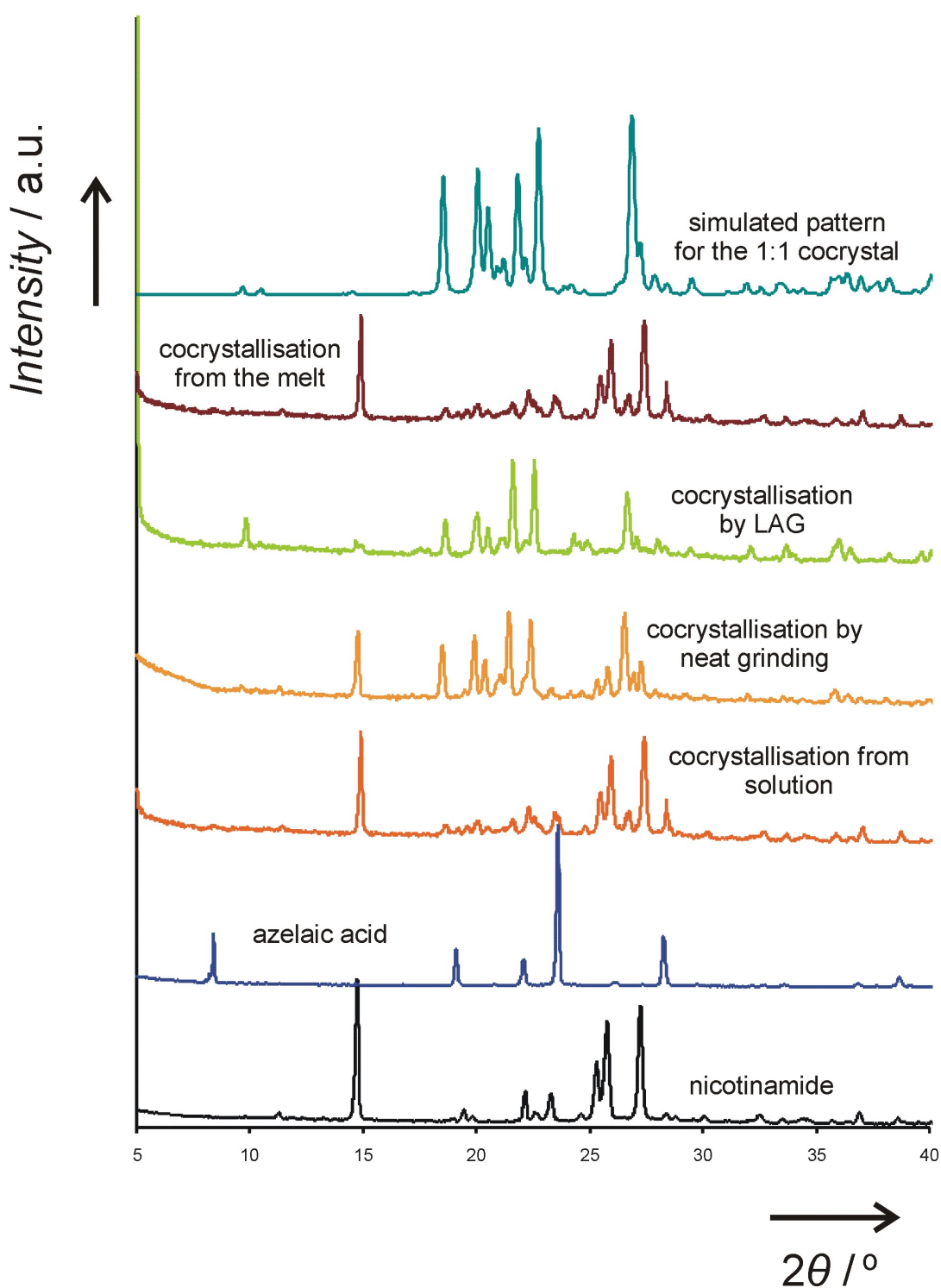


Figure S16. PXRD patterns for screening experiments involving **na** and **aze** in 2:1 stoichiometric ratio.

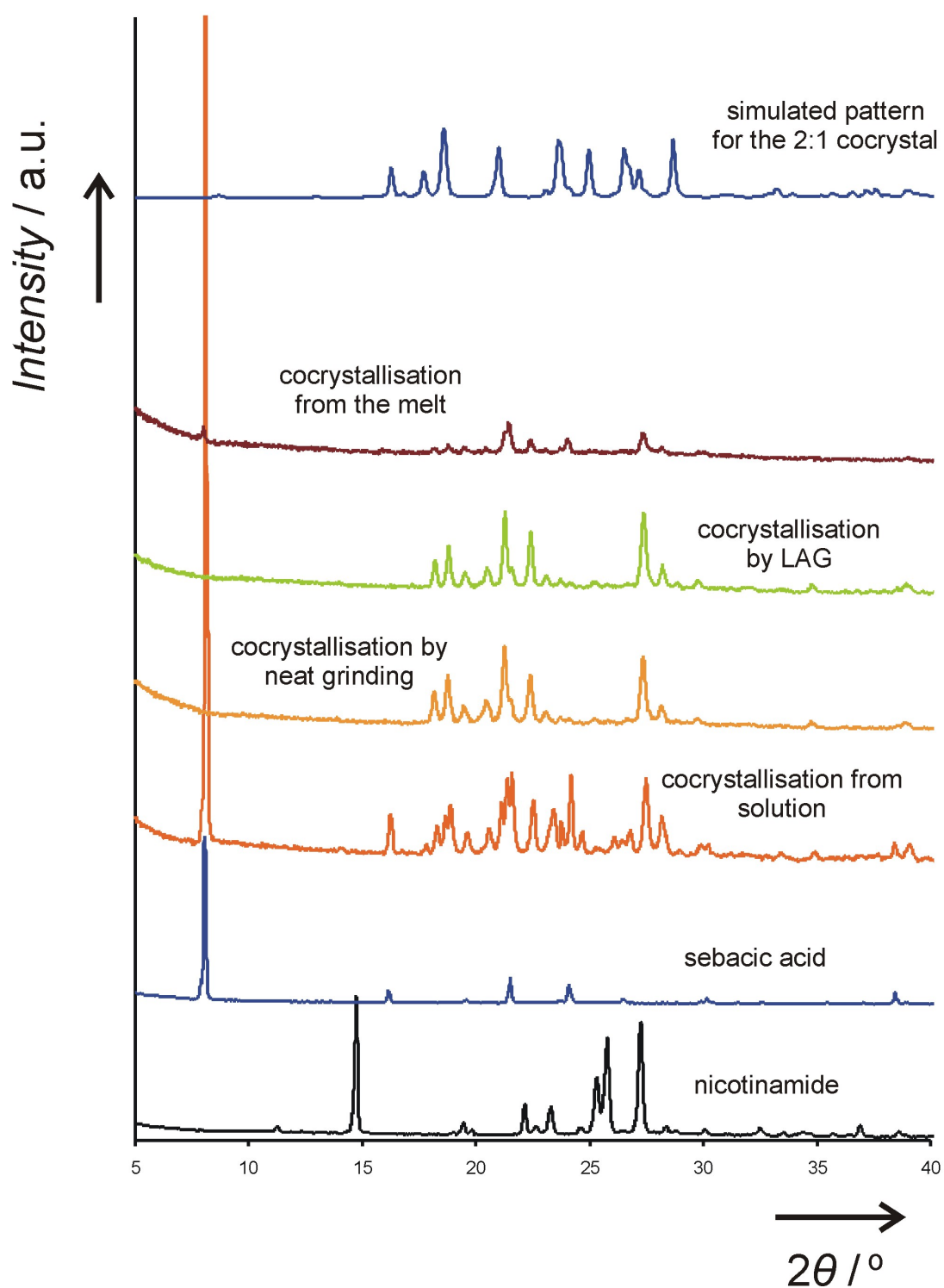


Figure S17. PXRD patterns for screening experiments involving **na** and **seb** in 1:1 stoichiometric ratio.

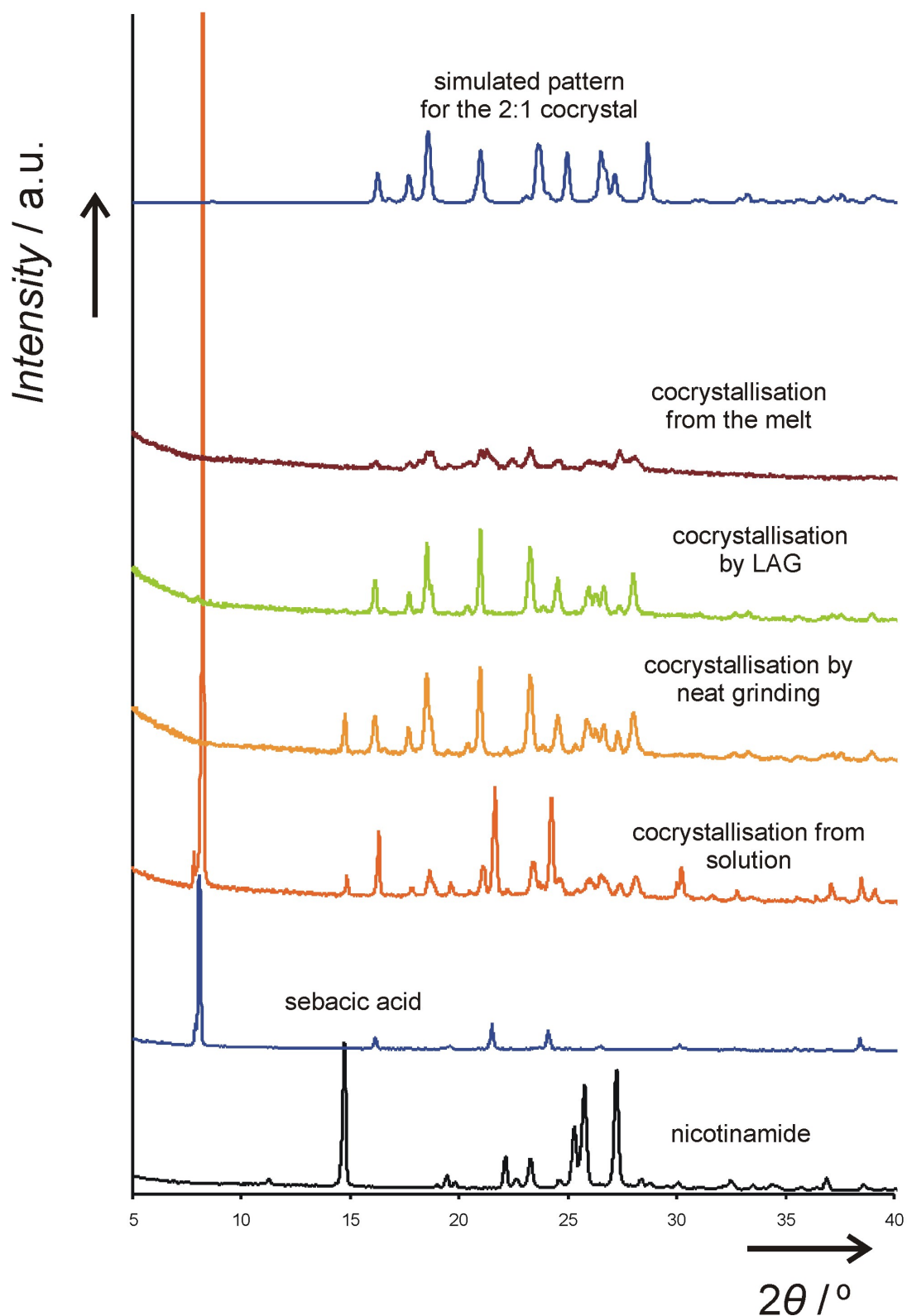


Figure S18. PXRD patterns for screening experiments involving **na** and **seb** in 2:1 stoichiometric ratio.

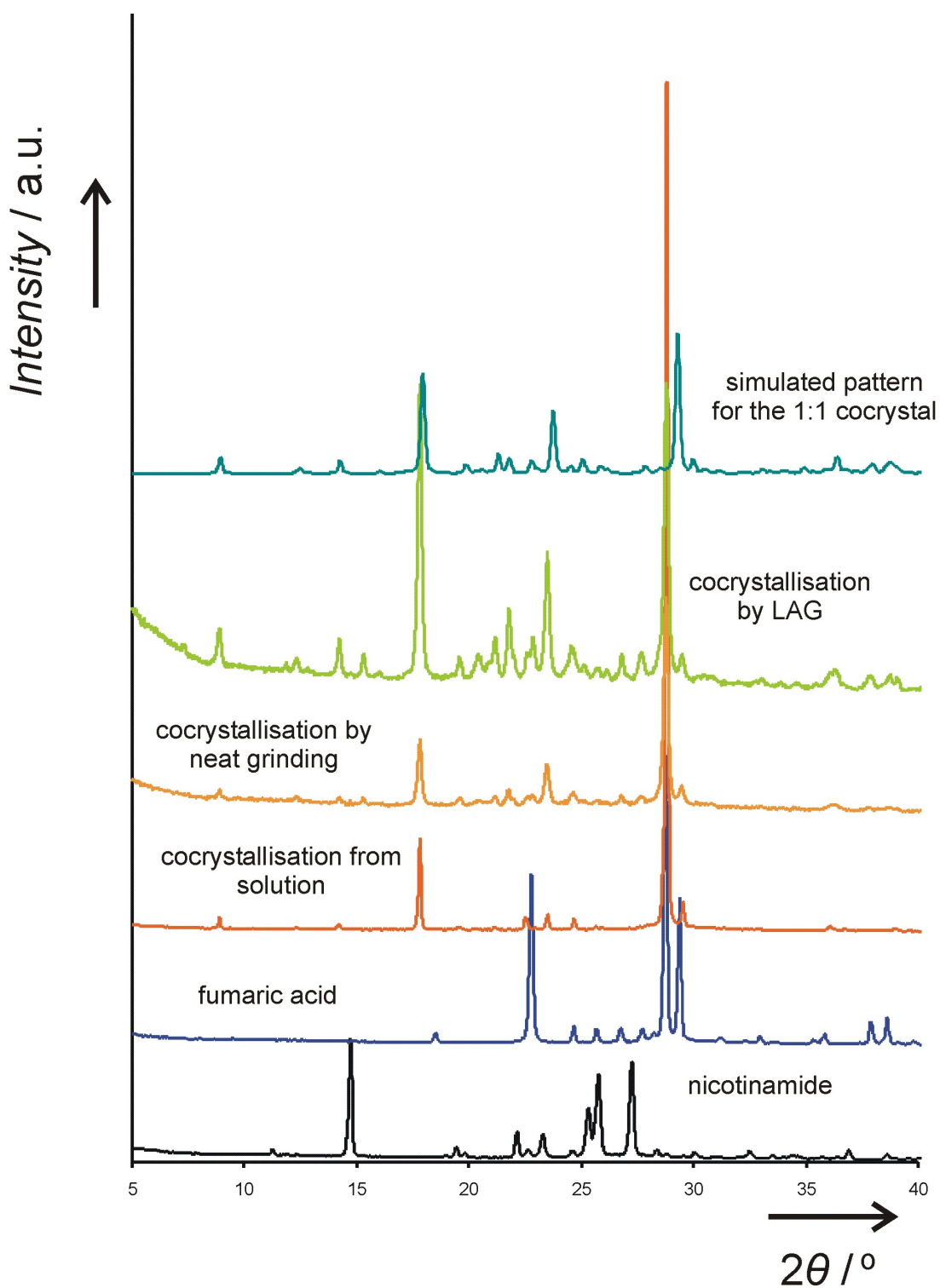


Figure S19. PXRD patterns for screening experiments involving **na** and **fum** in 1:1 stoichiometric ratio.

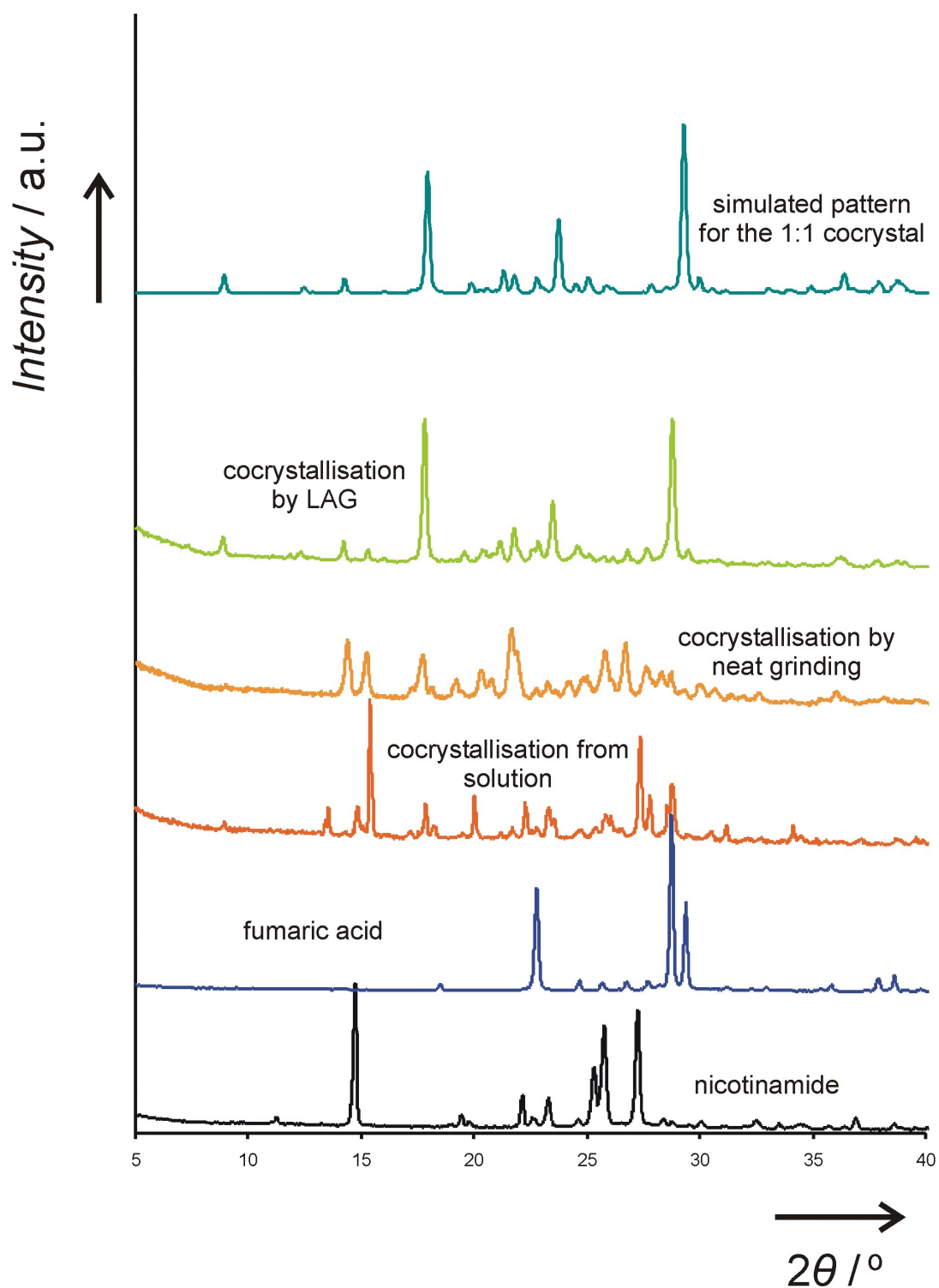


Figure S20. PXRD patterns for screening experiments involving **na** and **fum** in 2:1 stoichiometric ratio.

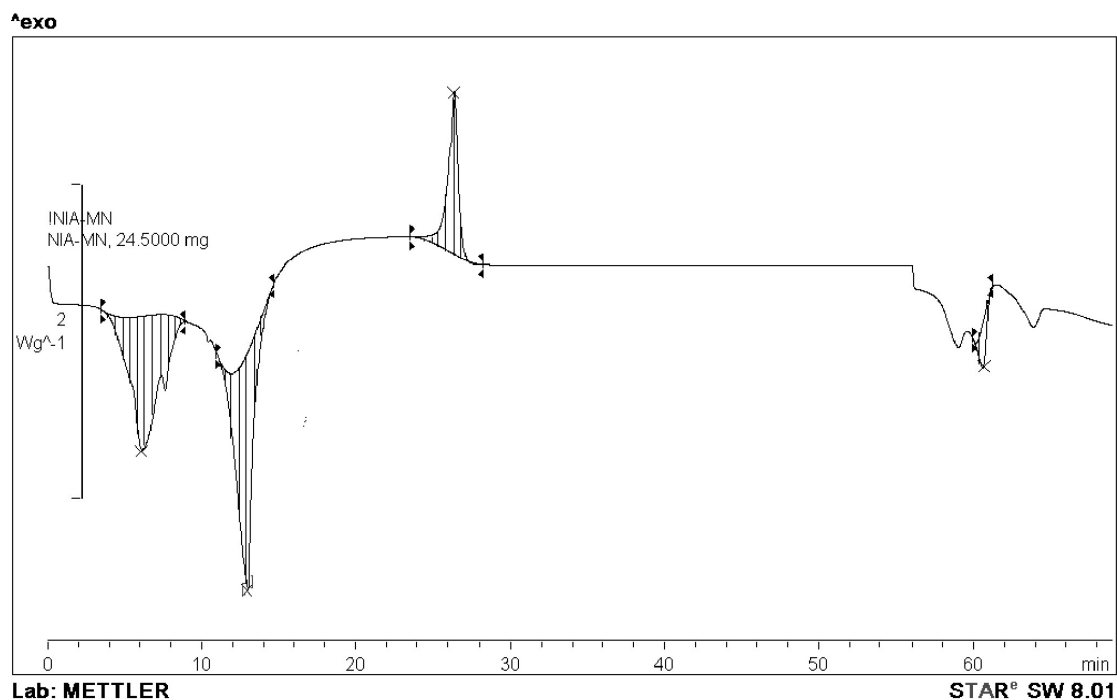


Figure S21. DSC thermogram for the cocrystallisation of **na** and **mal** from the melt in respective stoichiometric ratio 1:1.

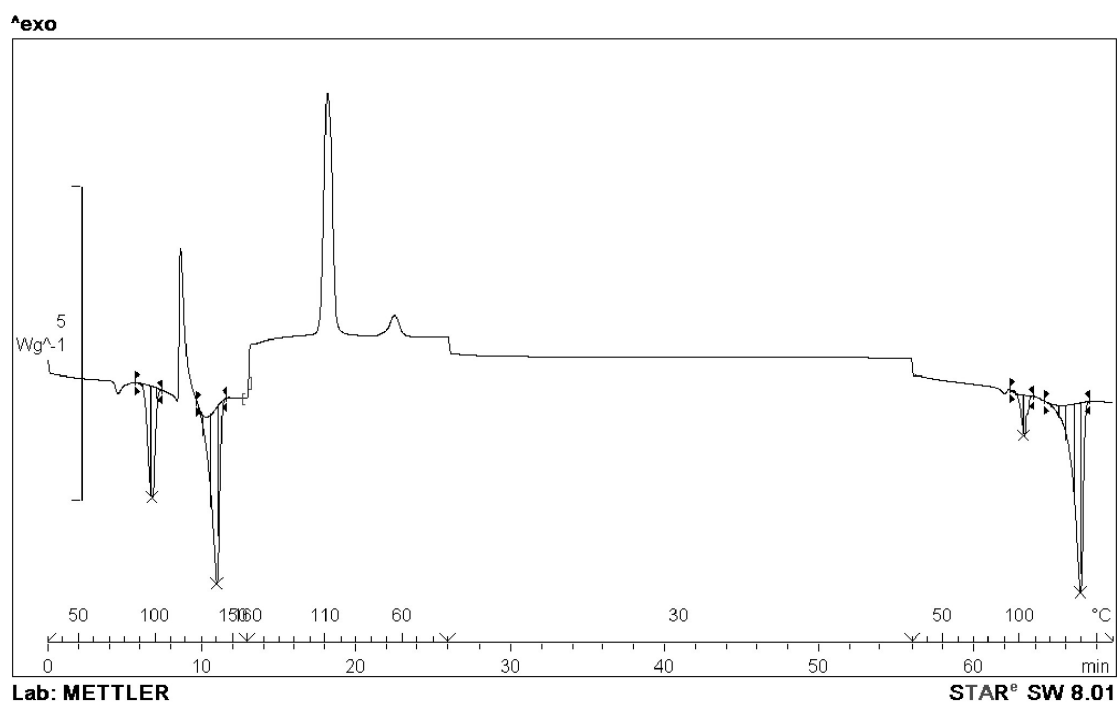


Figure S22. DSC thermogram for the cocrystallisation of **na** and **mal** from the melt in respective stoichiometric ratio 2:1.

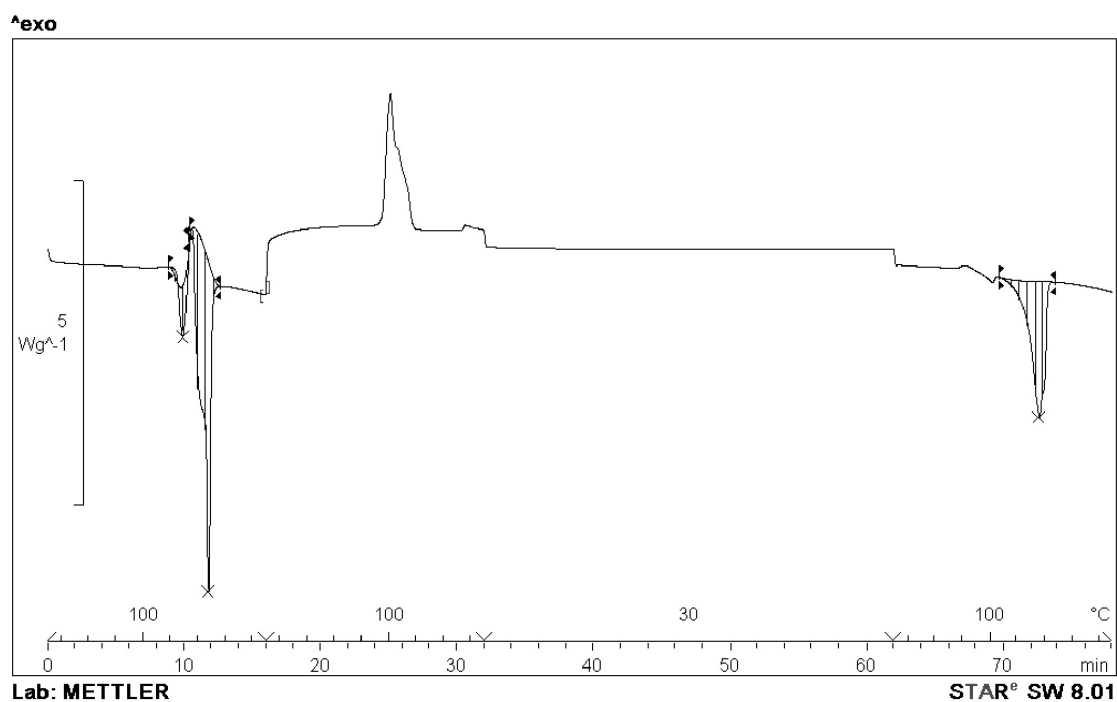


Figure S23. DSC thermogram for the cocrystallisation of **na** and **suc** from the melt in respective stoichiometric ratio 1:1.

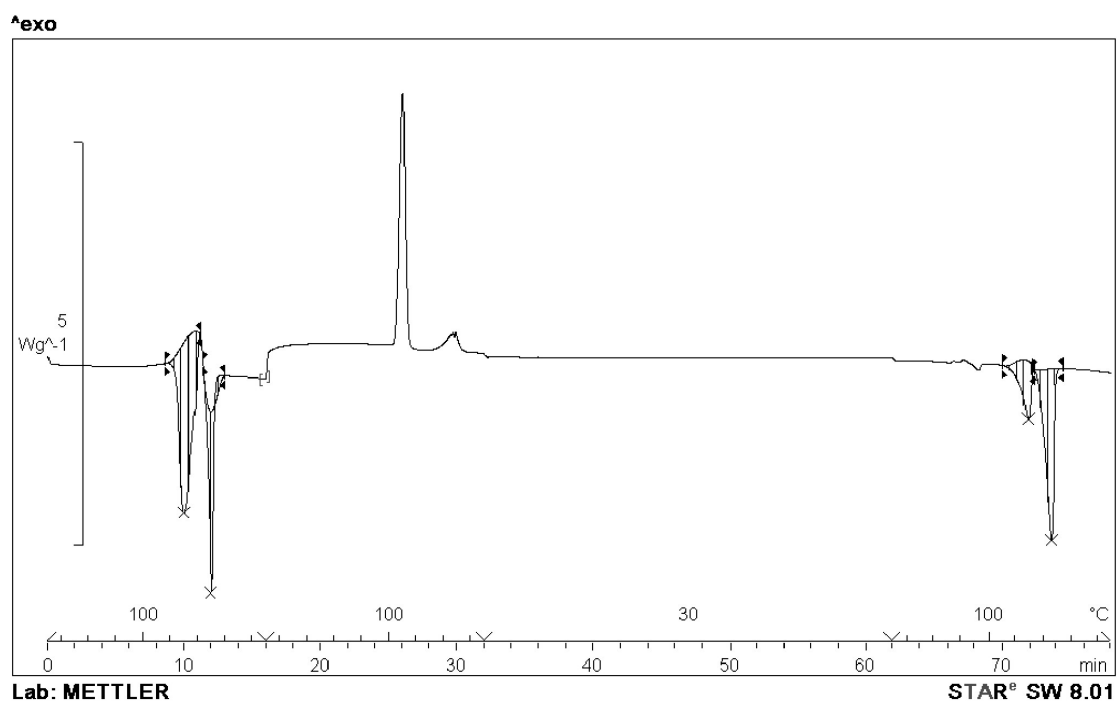


Figure S24. DSC thermogram for the cocrystallisation of **na** and **suc** from the melt in respective stoichiometric ratio 2:1.

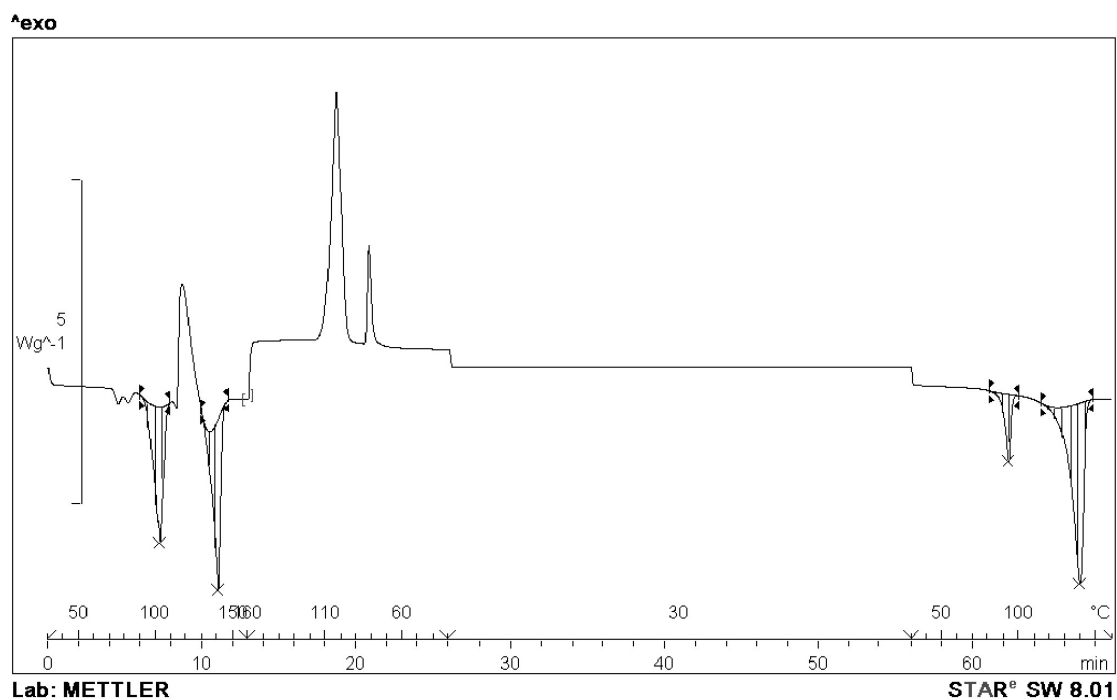


Figure S25. DSC thermogram for the cocrystallisation of **na** and **glu** from the melt in respective stoichiometric ratio 1:1.

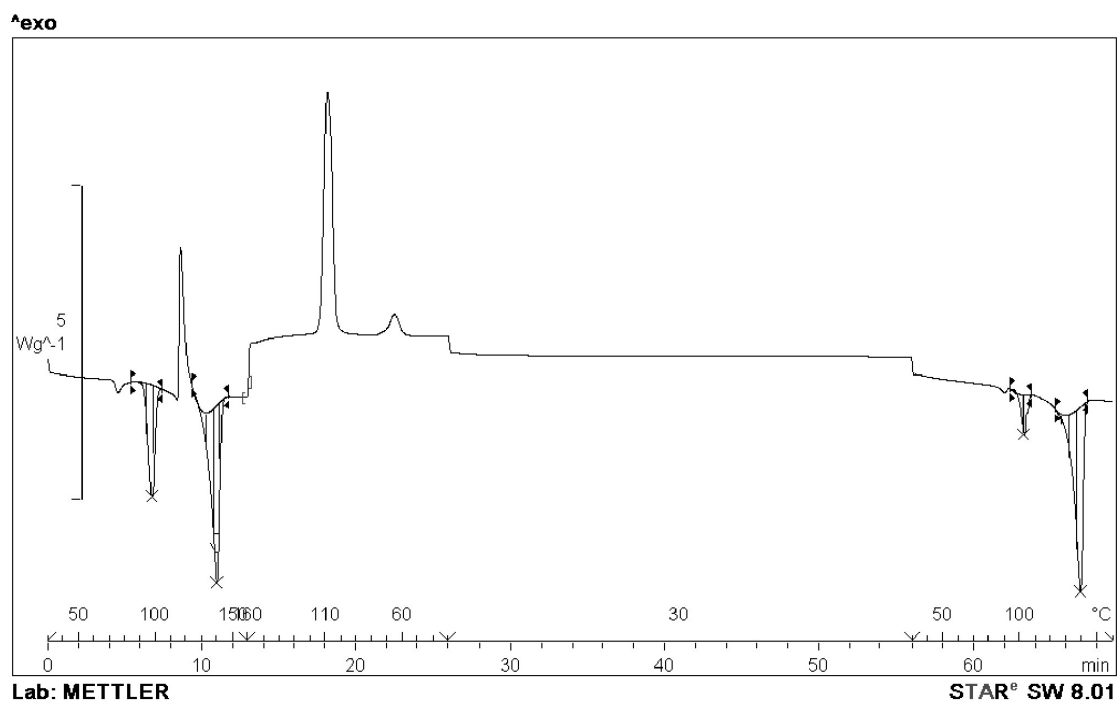
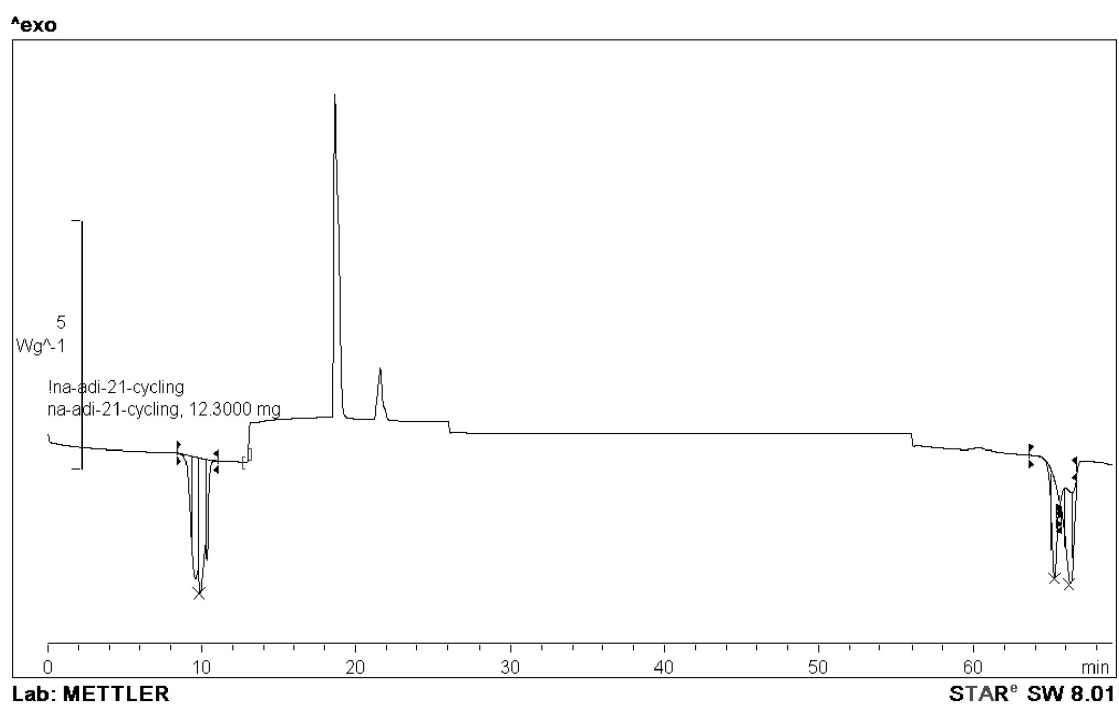
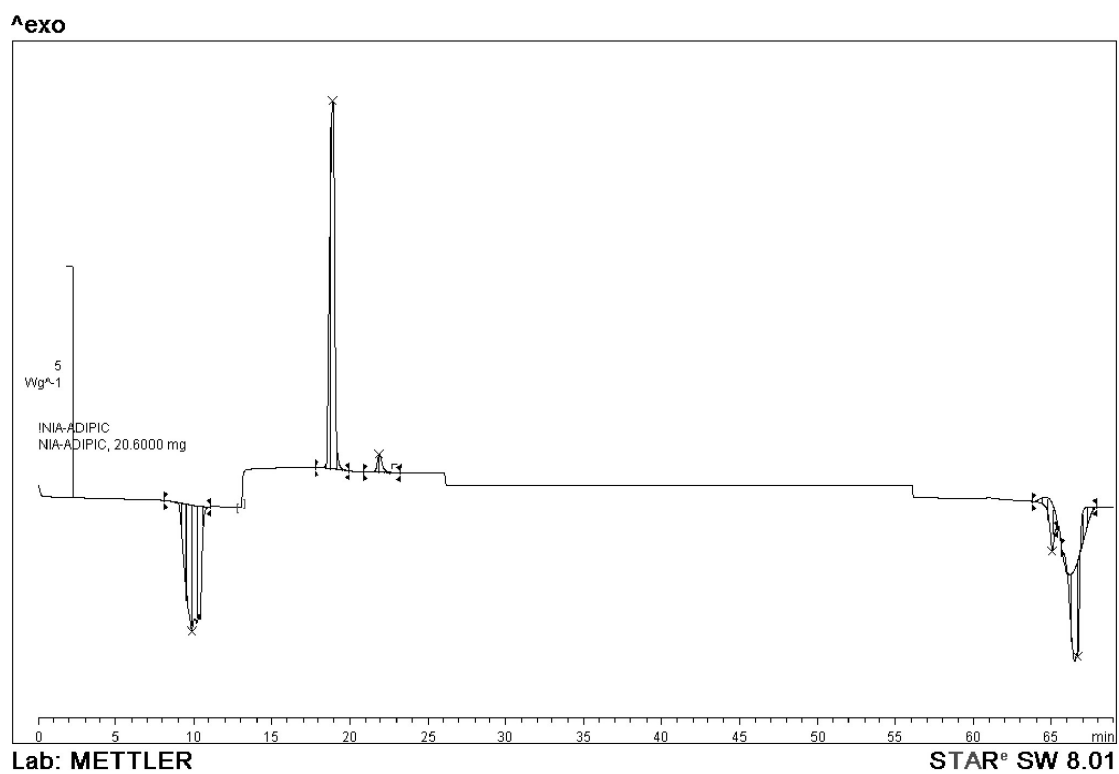


Figure 26. DSC thermogram for the cocrystallisation of **na** and **glu** from the melt in respective stoichiometric ratio 2:1.



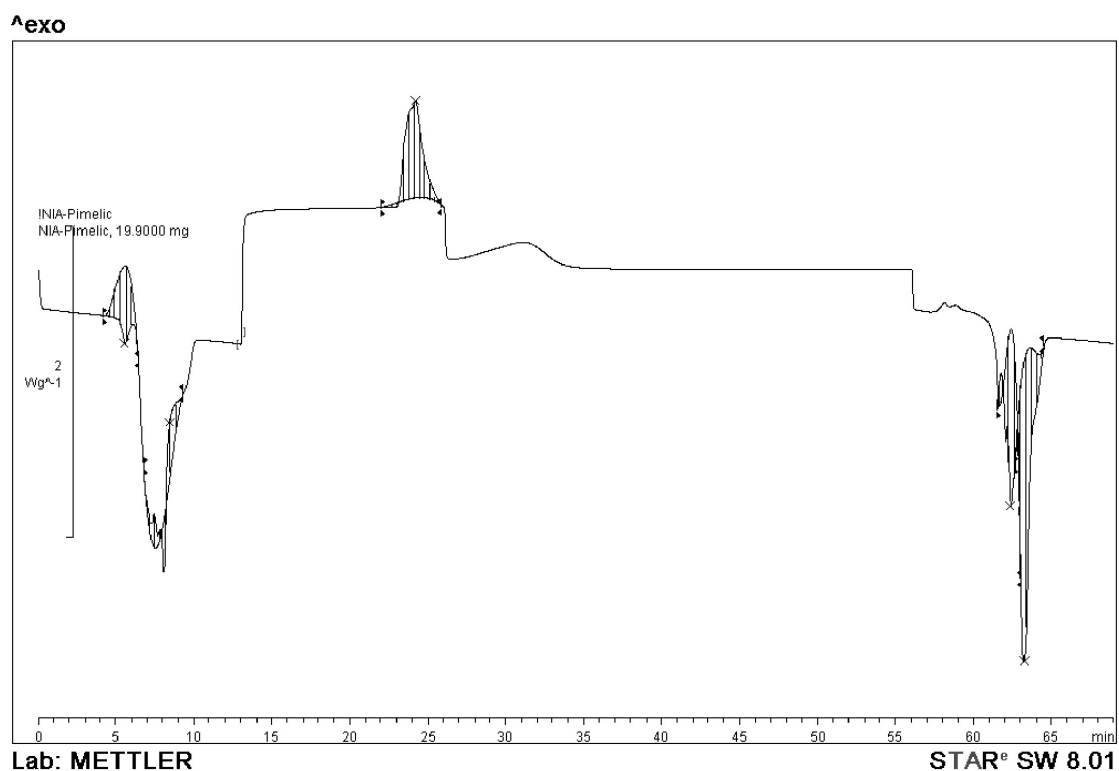


Figure S29. DSC thermogram for the cocrystallisation of **na** and **pim** from the melt in respective stoichiometric ratio 1:1.

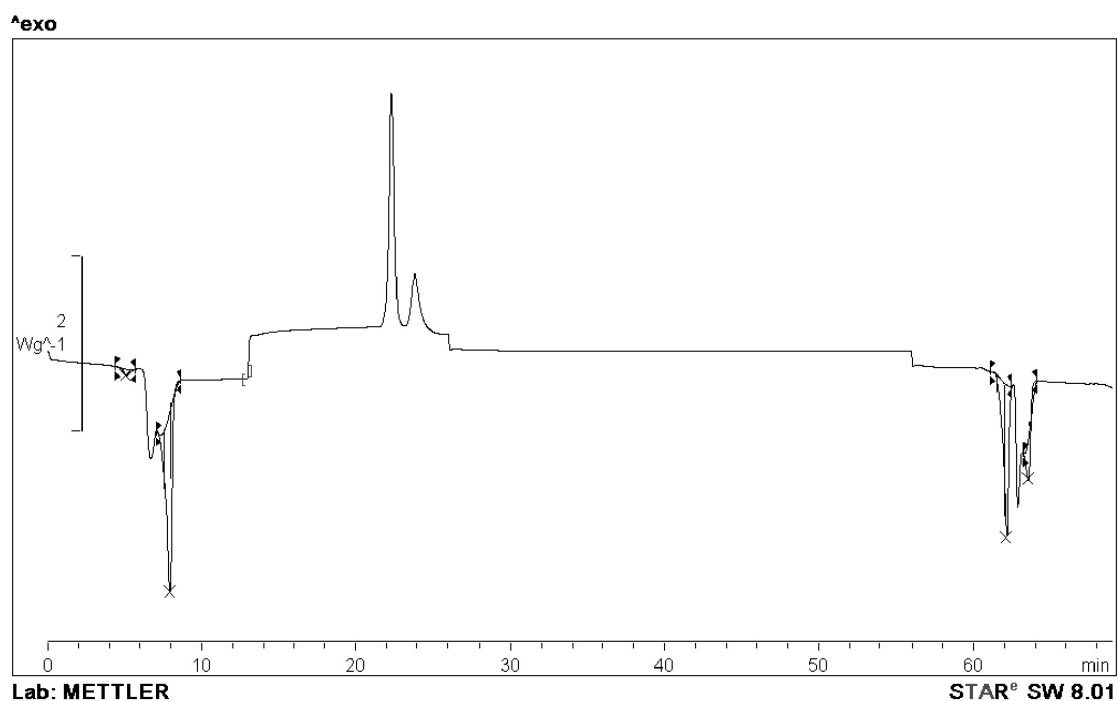


Figure S30. DSC thermogram for the cocrystallisation of **na** and **pim** from the melt in respective stoichiometric ratio 2:1.

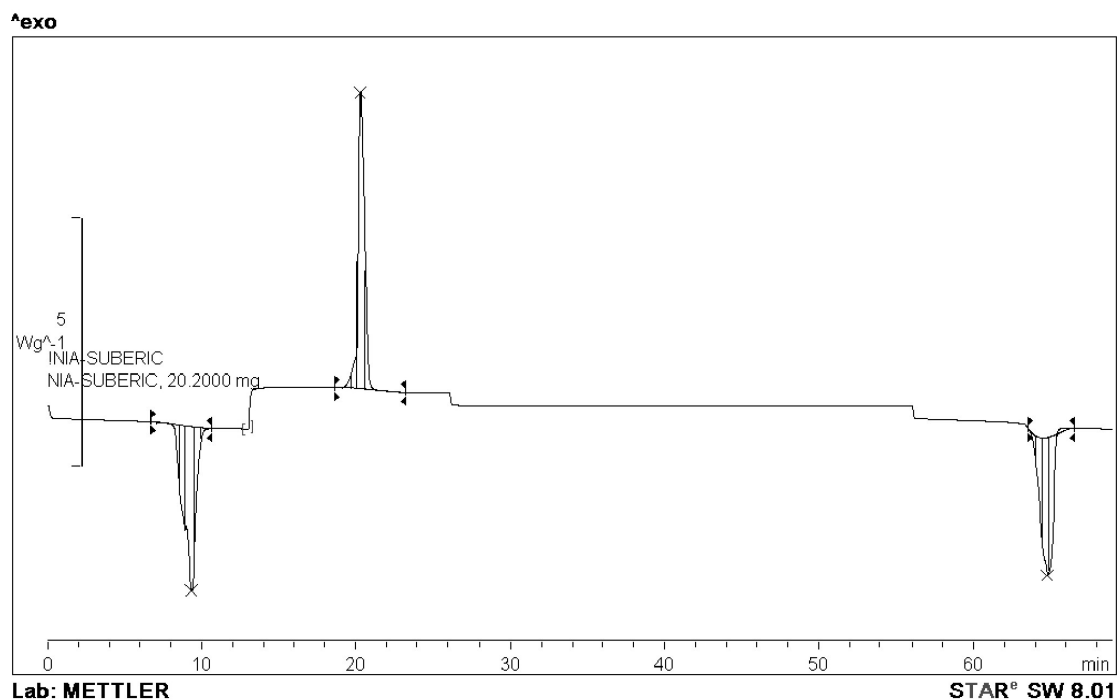


Figure S31. DSC thermogram for the cocrystallisation of **na** and **sub** from the melt in respective stoichiometric ratio 1:1.

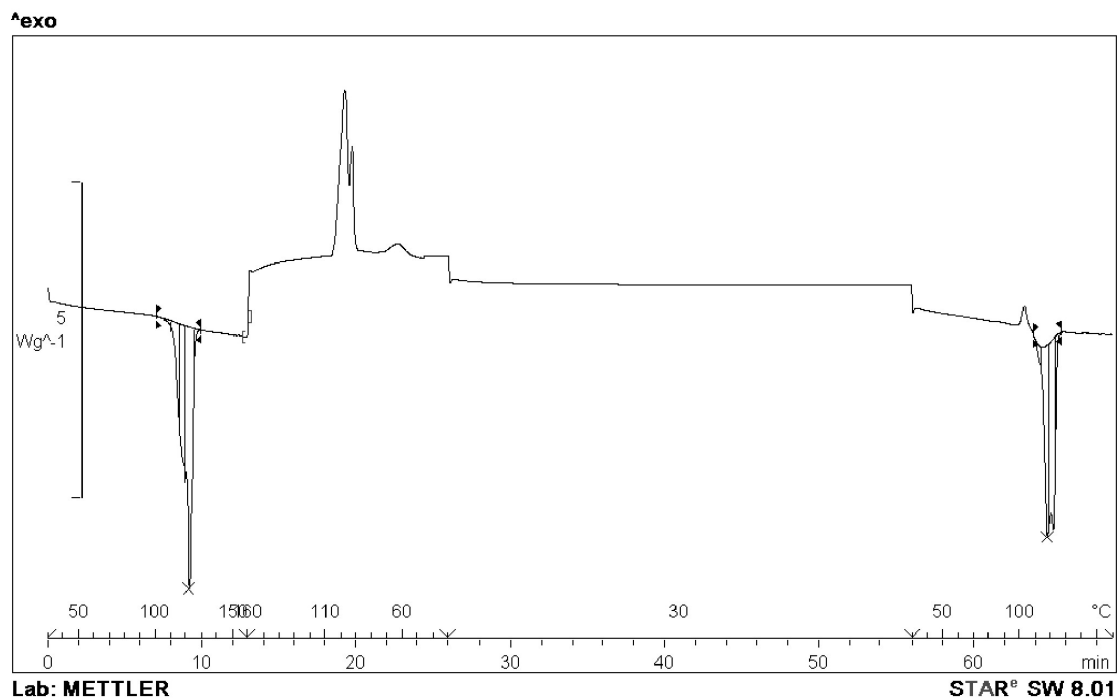


Figure S32. DSC thermogram for the cocrystallisation of **na** and **sub** from the melt in respective stoichiometric ratio 2:1.

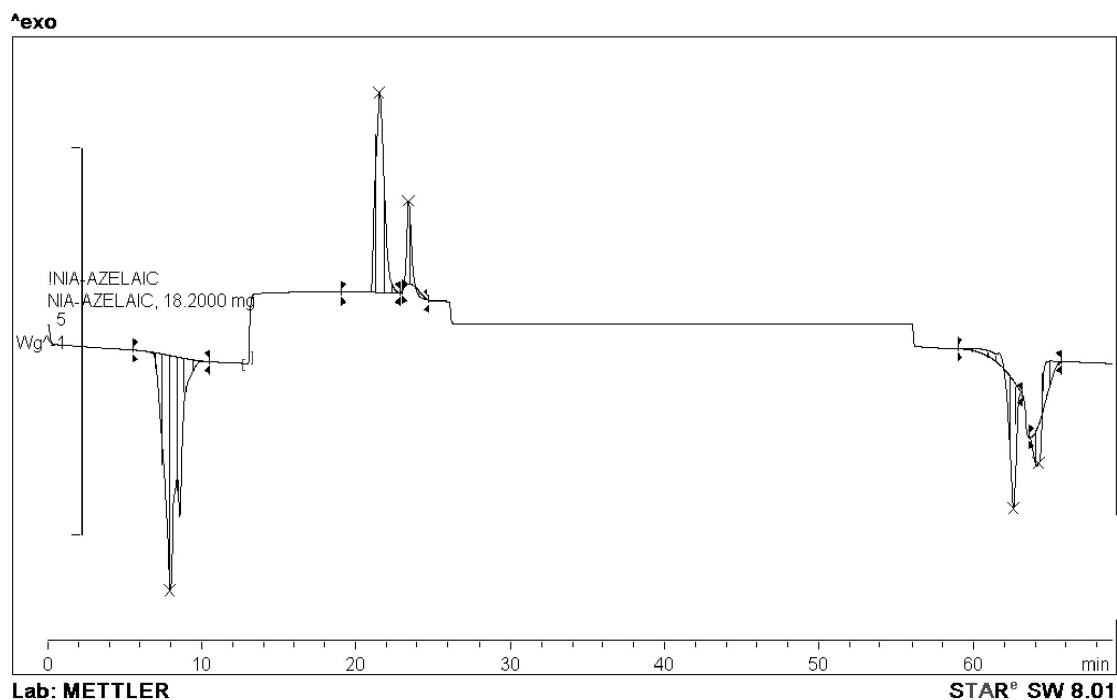


Figure S33. DSC thermogram for the cocrystallisation of **na** and **aze** from the melt in respective stoichiometric ratio 1:1.

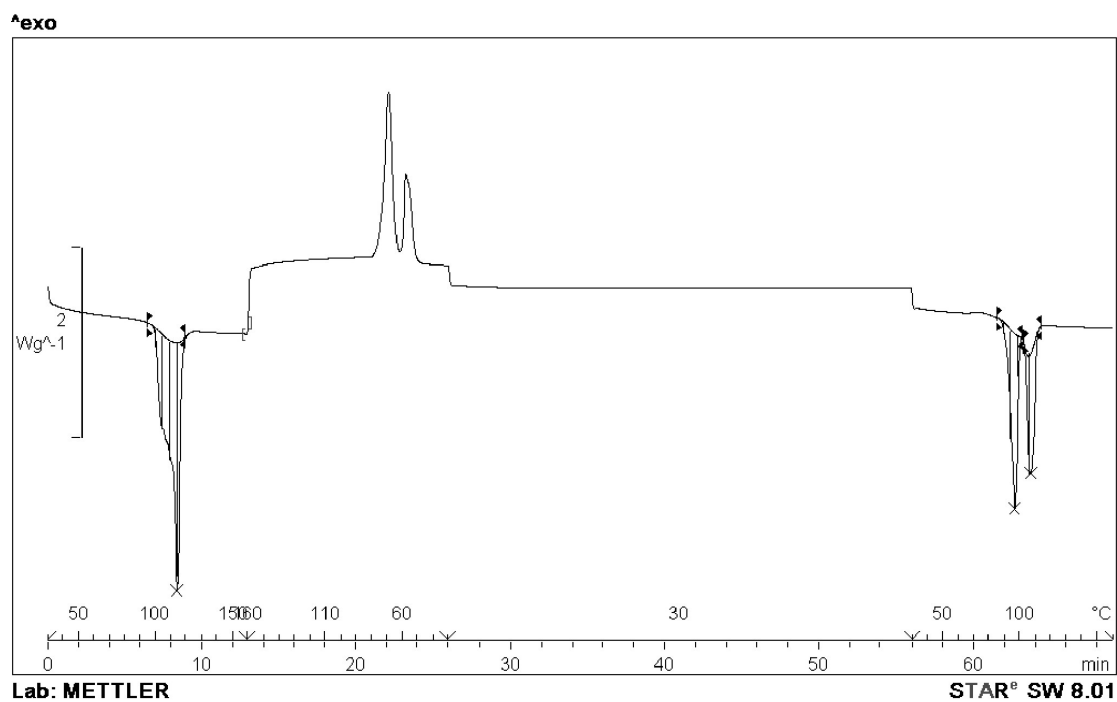


Figure S34. DSC thermogram for the cocrystallisation of **na** and **aze** from the melt in respective stoichiometric ratio 2:1.

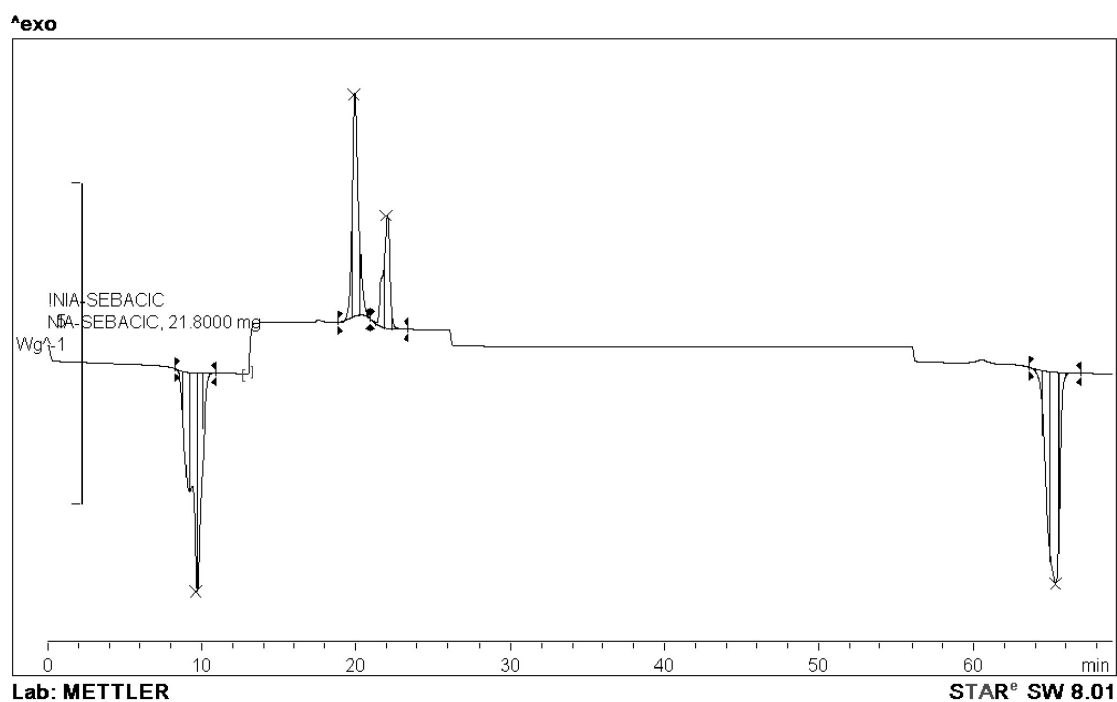


Figure S35. DSC thermogram for the cocrystallisation of **na** and **seb** from the melt in respective stoichiometric ratio 1:1.

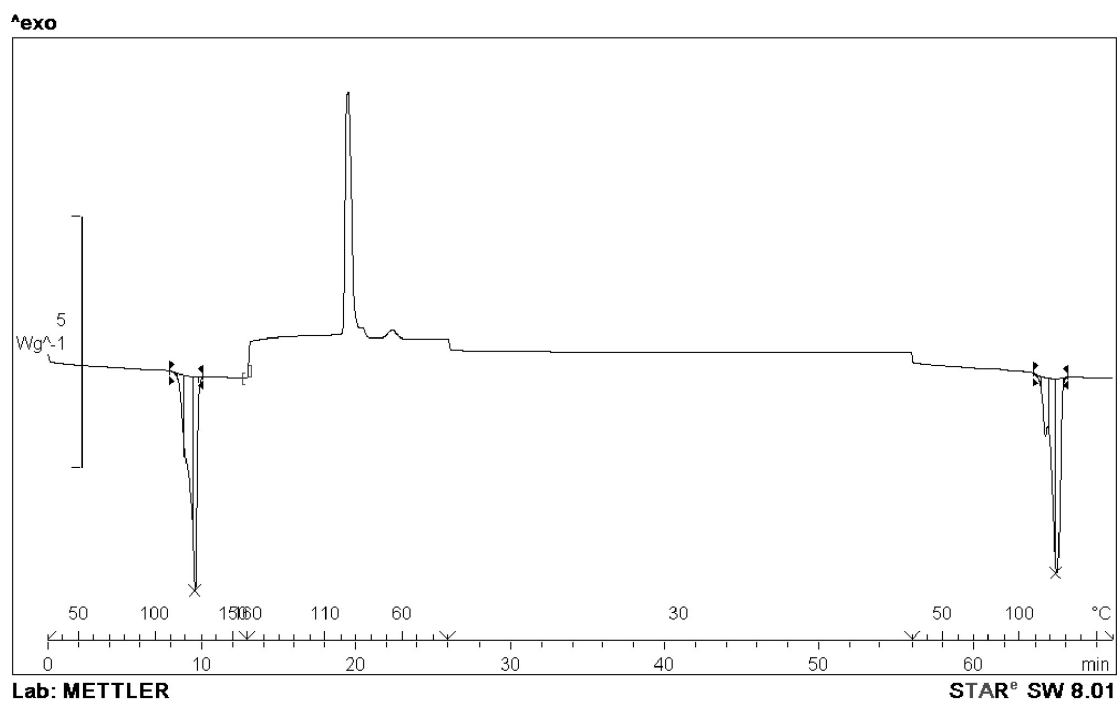


Figure S36. DSC thermogram for the cocrystallisation of **na** and **seb** from the melt in respective stoichiometric ratio 2:1.