Supporting Information to

"Disclosing the rich crystal chemistry of Lesinurad by ab-initio laboratory X-ray powder diffraction methods"

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Table S1. Comparison of diffraction peak positions for Lesinurad Forms 1, 2, 2 hT, 3.

Table S2. Chebyshev and hyperbolic coefficients describing the background contribution for Lesinurad Forms 1, 2, 2 hT, 3.

Table S3. Comparison of profile agreement factors for structureless (Le Bail) and Rietveld refinements for Lesinurad Forms 1, 2, 2 hT, 3. The final refined isotropic Debye-Waller (B_{iso}) factors are also reported in the last column (esd's in parentheses).

Figure S1. Comparison of the XRPD traces of Forms 2 (at RT, in blue) and 2 hT (in red, at 145°C)

Figure S2. STA traces for a) Form 1 b) Form 2 (and 2 hT) and c) Form 3. TG curve in blue and DSC curve in green.

Figure S3. FTIR spectra for a) Form 1 b) Form 2 and c) Form 3

Figure S4. Rietveld Refinement Plot for Form 2 hT (laboratory data in the range not affected by the aluminum sample holder of the temperature-controlled heating stage)

Figure S5. Rietveld Refinement Plots for Phases 1, 2, 2 hT and 3, shown in

Table S1. Comparison of diffraction peak positions for **Lesinurad Forms 1, 2, 2 hT, 3.**

Form 1	Form 2	Form 2 hT	Form 3
	7.98	8.05	7.96
6.81	9.66	10.10	9.63
10.33	10.46	10.87	10.08
12.95	11.93	11.52	11.48
13.53	12.55	12.49	11.67
13.64	12.92	12.93	11.91
14.40	13.80	13.48	12.41
15.29	15.42	14.48	12.98
15.89	16.17	15.78	13.53
16.10	16.46	16.09	13.56
16.72	18.20	18.40	14.40
18.53	18.73	18.46	14.54
18.82	18.99	19.14	15.15
19.57	19.49	19.46	15.34
19.97	19.82	19.70	15.44
20.53	20.38	20.28	15.97
20.78	21.01	20.79	16.27
21.34	21.35	21.41	16.90
22.33	21.92	21.85	17.40
22.74	22.30	22.06	17.56
23.08	22.46	22.64	17.87
23.21	23.04	22.82	18.10
25.03	23.39	23.16	18.29
25.50	23.99	23.26	18.85
25.51	24.00	23.68	19.10
26.00	24.21	24.23	19.34
26.29	24.56	24.51	19.57
26.63	25.11	24.62	19.99
26.77	25.44	24.85	20.25
27.27	26.03	25.13	20.49
27.54	26.48	25.65	20.87
28.23	26.73	25.84	20.99
28.42	27.82	26.03	21.11
28.81	28.01	26.39	21.45
29.02	28.04	26.67	21.81
29.36	29.16	28.03	22.50
29.67	29.57	28.12	22.91
	29.89	28.45	23.08

		29.49	23.18 23.53 23.76 24.05 24.85 25.34 25.48 26.13 26.24 26.33 26.63 26.78 27.32 27.50 28.13 28.16 28.42 28.57 28.95 29.05 29.19 29.33 29.81

Table S2. Chebyshev and hyperbolic coefficients describing the background contribution for Lesinurad Forms 1, 2, 2 hT, 3.

Form 1
-14588.162 28686.3747 -23499.8508 15961.0202 -9048.41594 4275.45912
-1486.33881 142.072721
One_on_X(770508.75691)

Form 2
14843.5369 -4884.98534 -2340.00021 2073.23506
One_on_X(22630.24045)

Form 2hT
1002.08273
One_on_X(195.19478)

Form 3
15535.4558 -6926.27656 -1063.18221 1661.53822 57.8126557
-1037.84961 1603.82253 -1482.88769 1174.34804 -409.012106
-262.47633 523.811023
One_on_X(0)

Table S3. Comparison of profile agreement factors R_p and R_{wp} for structureless (Le Bail) and Rietveld refinements for Lesinurad Forms 1, 2, 2 hT, 3. The final refined isotropic Debye-Waller (B_{iso}) factors are also reported in the last column (esd's in parentheses).

Form	R_p and R_{wp}, LeBail	R_p and R_{wp}, Rietveld	B_{iso}, Å^2
1	0.029, 0.048	0.058, 0.079	4.60(15)
2	0.035, 0.051	0.075, 0.102	6.00(13)
2 hT	0.078, 0.111	0.174, 0.192	9.1(8)
3	0.020, 0.037	0.066, 0.096	5.37(18)

Figure S1. Comparison of the XRPD traces of Forms 2 (at RT, in blue) and 2 hT (in red, at 145°C)

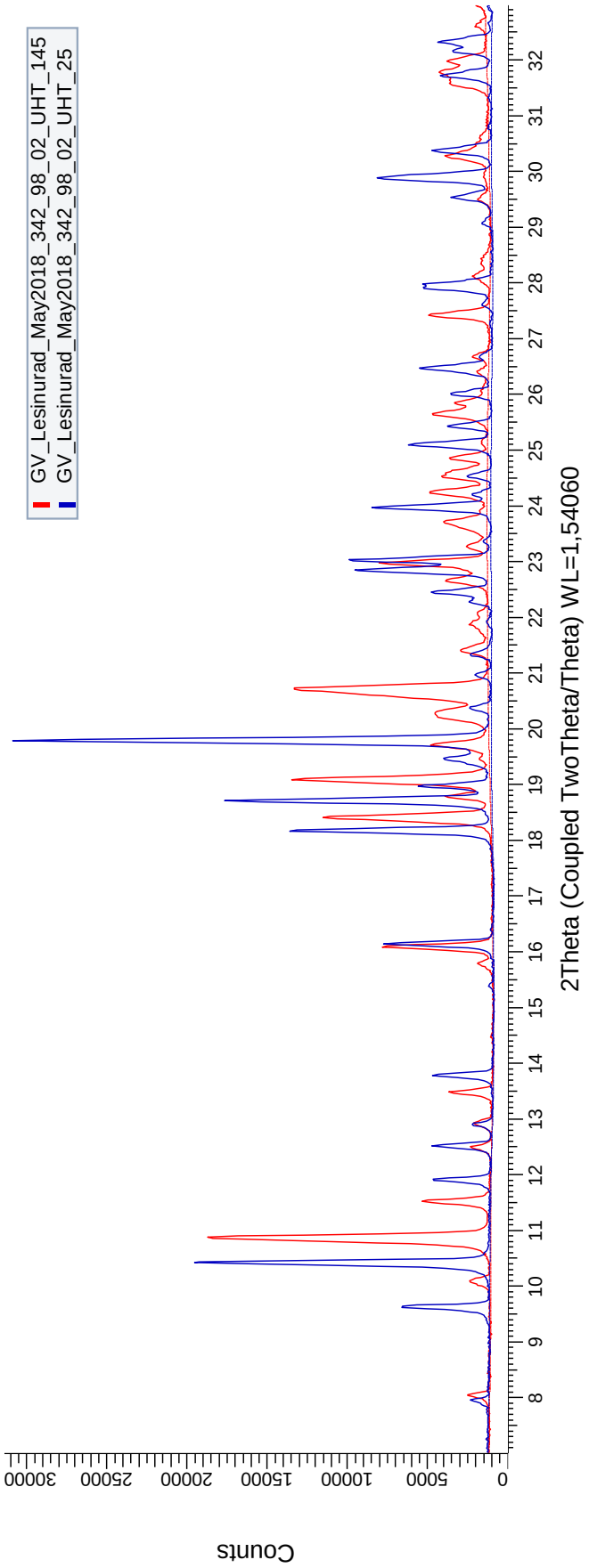


Figure S2. STA traces for a) Form 1 b) Form 2 (and 2 hT) and c) Form 3. TG curve in blue and DSC curve in green.

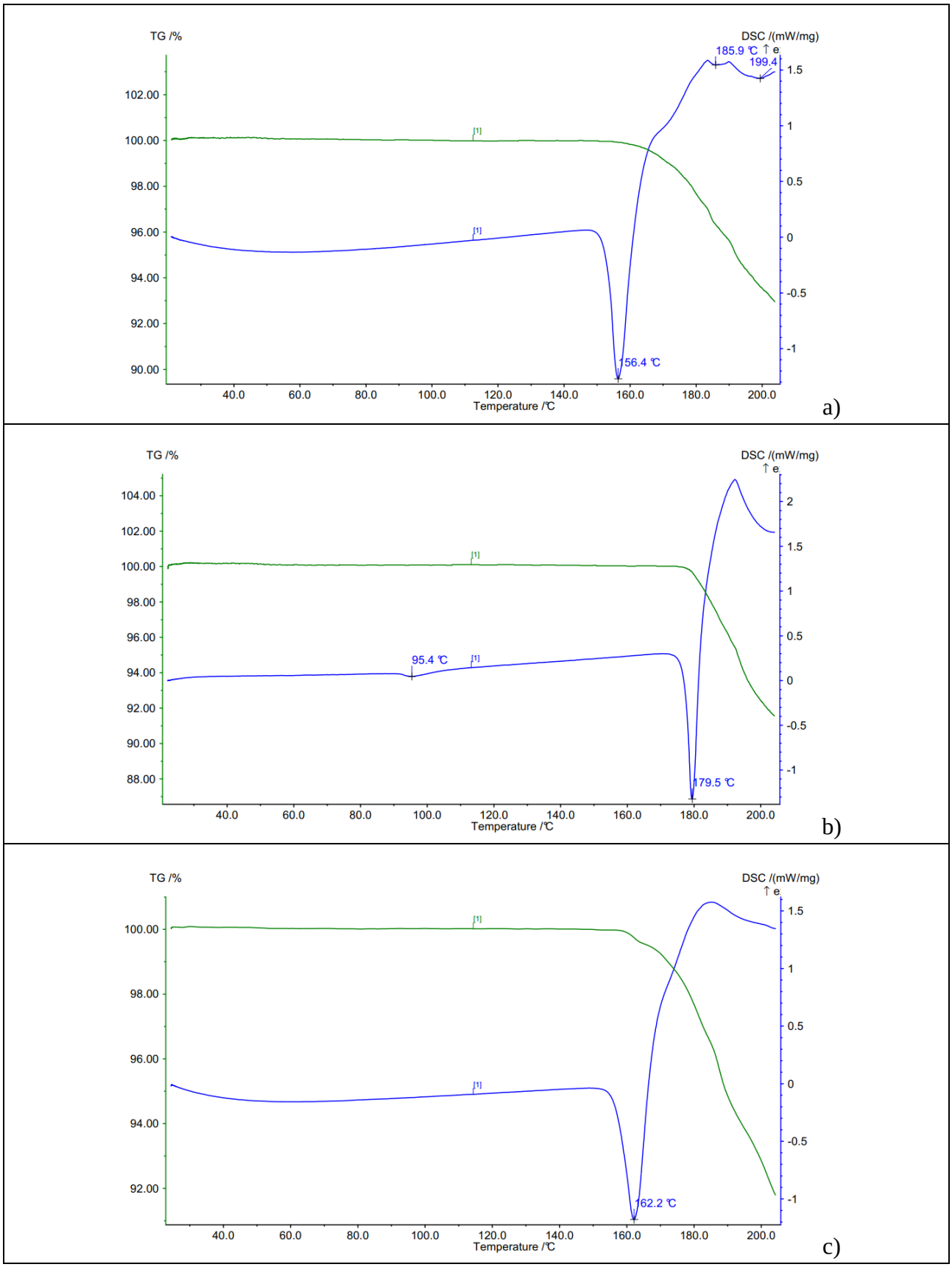


Figure S3. FTIR spectra for a) Form 1 b) Form 2 and c) Form 3

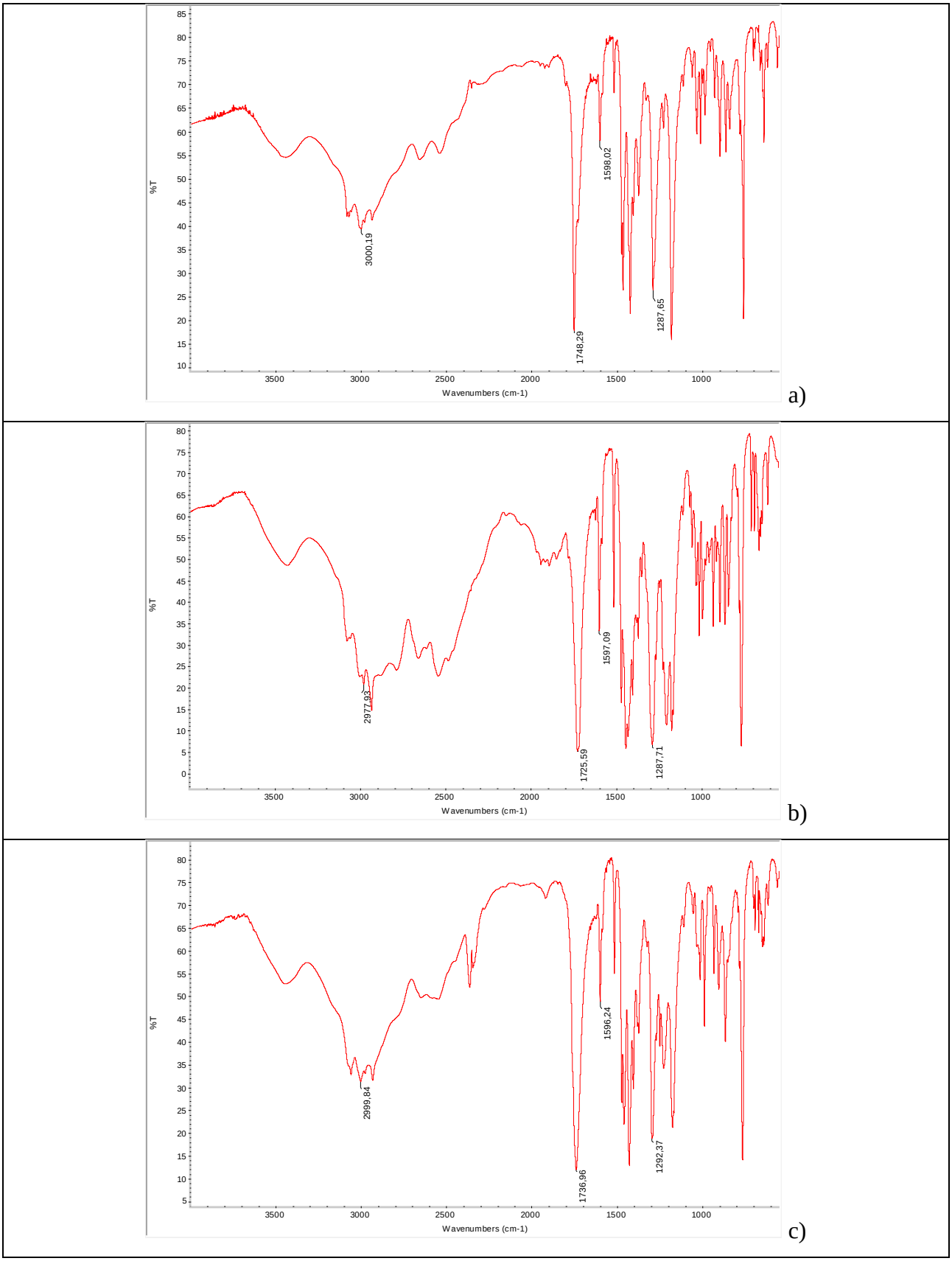


Figure S4. Rietveld Refinement Plot for Form 2 hT (laboratory data in the range not affected by the aluminum sample holder of the temperature-controlled heating stage)

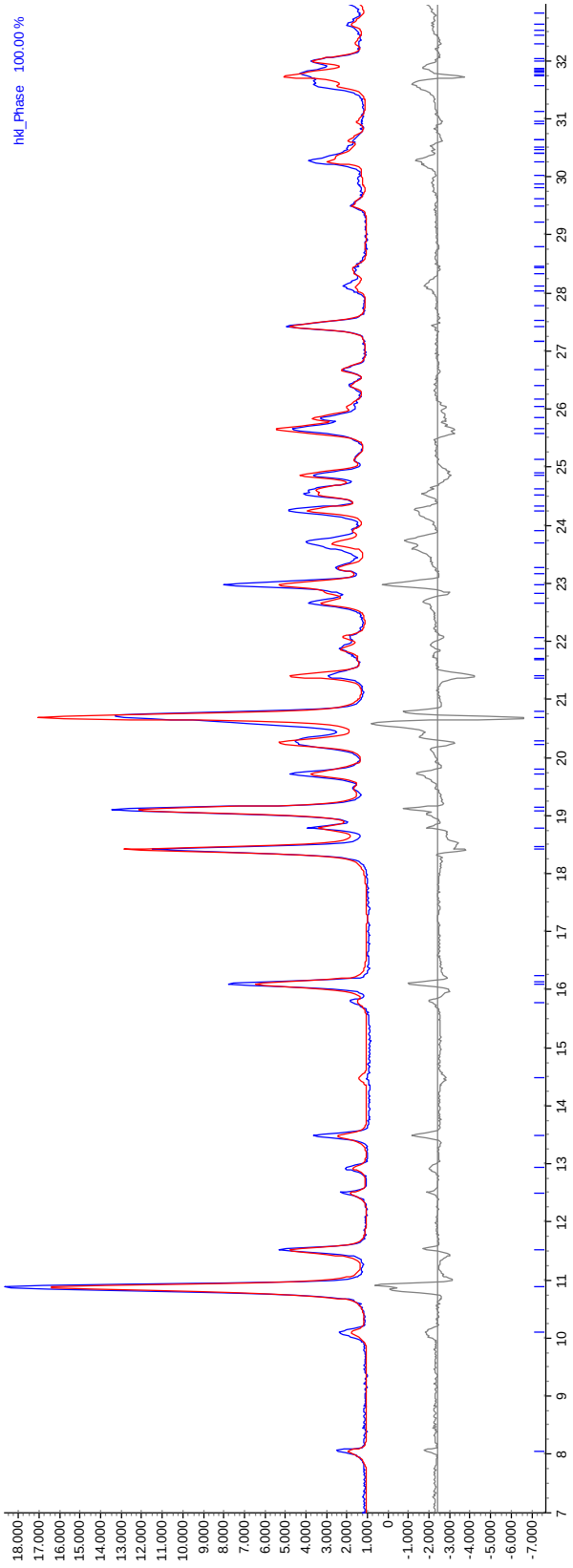
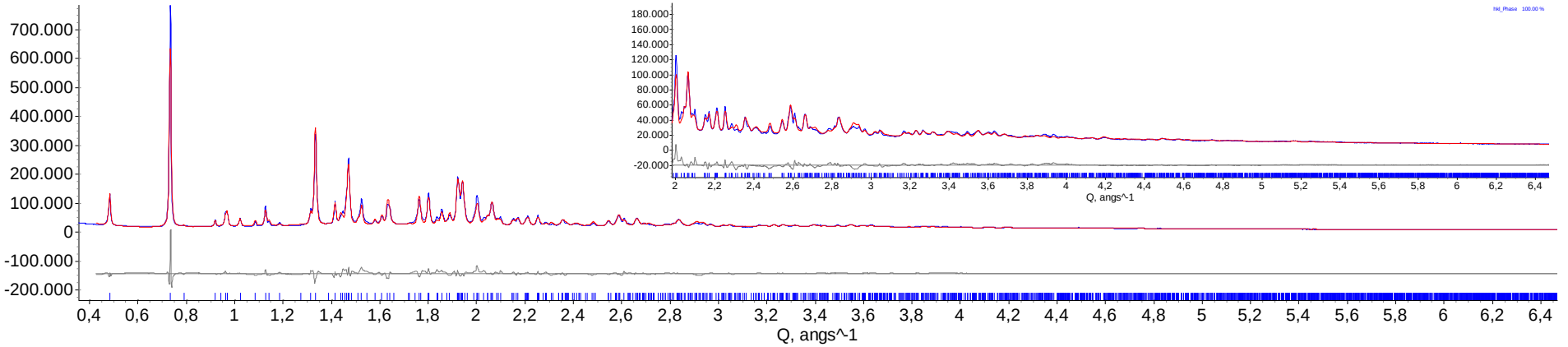
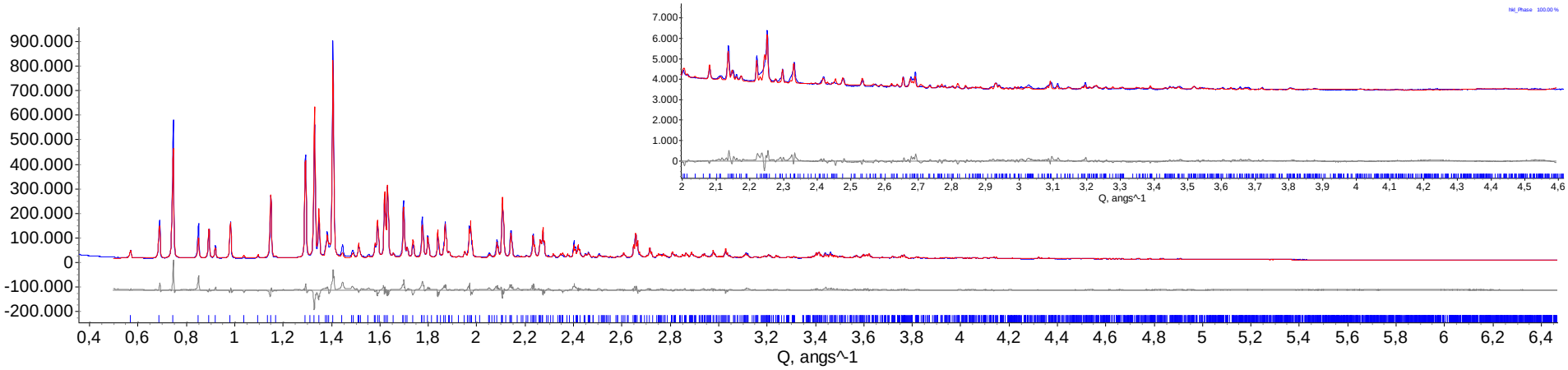


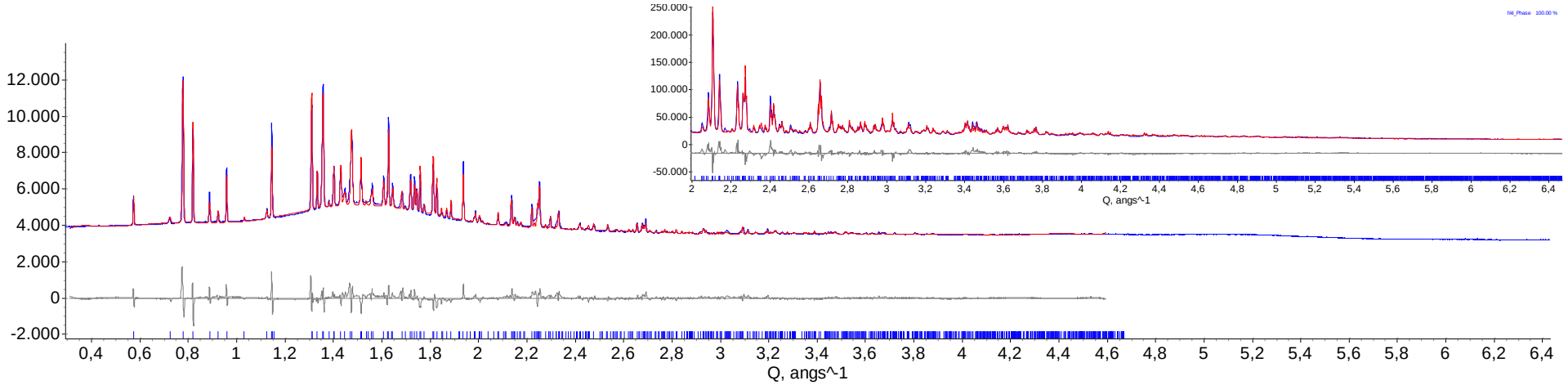
Figure S5. Rietveld Refinement Plots for Phases 1, 2, 2 hT and 3, shown in Form 1



Form 2



Form 2 hT



Form 3