Supplementary Information - Schmidtmann, Coster, Henry, Ting, Weller, Wilson: *Determining hydrogen positions in crystal engineered organic molecular complexes by joint neutron powder and single crystal X-ray diffraction*

Table S1 - Bond lengths (Å) involving hydrogen, from PND, and from single crystal X-ray data for comparison

Complex	Type	Bond	PND	SCXD
*PCP-2,6-Lutidine (**1**)*	C-H pyr	C8-H8	1.072(18)	0.982(15)
	C-H pyr	C9-H9	1.07(2)	0.962(16)
	C-H pyr	C10-H10	1.022(17)	0.946(14)
	C-H me	C12-H12A	1.100(17)	0.97(2)
	C-H me	C12-H12B	1.09(3)	0.97(2)
	C-H me	C12-H12C	1.01(2)	0.90(2)
	C-H me	C13-H13A	0.997(18)	0.936(18)
	C-H me	C13-H13B	1.041(19)	0.931(16)
	C-H me	C13-H13C	1.07(2)	0.905(17)
*PCP-2,4-Lutidine (**2**)*	C-H pyr	C8-H8	1.045(16)	0.933(17)
	C-H pyr	C10-H10	1.053(16)	0.989(17)
	C-H pyr	C11-H11	1.038(16)	0.886(16)
	C-H me	C12-H12A	1.004(17)	1.00(2)
	C-H me	C12-H12B	1.081(19)	0.92(2)
	C-H me	C12-H12C	1.075(19)	0.96(2)
	C-H me	C13-H13A	1.028(16)	0.93(2)
	C-H me	C13-H13B	1.16(2)	0.952(18)
	C-H me	C13-H13C	0.97(2)	0.955(16)
*IN2-OA-I (**3-I**)*	C-H pyr	C2-H2	1.040(16)	0.957(12)
	C-H pyr	C3-H3	1.076(15)	0.999(14)
	C-H pyr	C5-H4	1.035(16)	0.990(13)
	C-H pyr	C6-H5	1.055(16)	0.976(12)
	N-H amine	N2-H6	0.993(18)	0.918(13)
	N-H amine	N2-H7	0.996(18)	0.895(14)
*IN2-OA-II (**3-II**)*	C-H pyr	C2-H2	1.080(14)	0.983(12)
	C-H pyr	C3-H3	1.101(15)	0.986(14)
	C-H pyr	C5-H4	0.970(15)	0.974(13)
	C-H pyr	C6-H5	1.059(16)	0.968(14)
	N-H amine	N2-H6	0.986(14)	0.945(16)
	N-H amine	N2-H7	0.983(14)	0.929(14)
*IN2-dOA-80% (**3d**)*	C-H pyr	C2-H2	1.060(15)	0.960(13)
	C-H pyr	C3-H3	1.006(14)	0.967(13)
	C-H pyr	C5-H4	1.107(14)	0.952(12)
	C-H pyr	C6-H5	1.053(15)	0.948(14)
	N-D amine	N2-D6	1.027(11)	0.898(13)
	N-D amine	N2-D7	1.012(13)	0.953(14)

IN2-dOA-100%	C-H pyr	C2-H2	1.063(14)	
	C-H pyr	C3-H3	1.039(13)	
	C-H pyr	C5-H4	1.085(13)	
	C-H pyr	C6-H5	1.095(13)	
	N-D amine	N2-D6	1.045(7)	
	N-D amine	N2-D7	0.998(8)	
*35DNBAH-4-Picoline (**4**)*	C-H pyr	C3-H2	1.08(2)	0.957(15)
	C-H pyr	C5-H3	1.038(19)	0.952(16)
	C-H pyr	C7-H4	1.11(2)	0.952(16)
	C-H pyr	C8-H5	1.00(2)	0.966(17)
	C-H pyr	C9-H6	1.15(2)	0.945(17)
	C-H pyr	C11-H7	1.02(2)	0.965(16)
	C-H pyr	C12-H8	1.02(2)	0.951(17)
	C-H me	C13-H9	1.10(2)	0.97(2)
	C-H me	C13-H10	1.22(2)	0.95(2)
	C-H me	C13-H11	1.17(2)	0.971(19)
*35DNBAD-4-Picoline (**4d**)*	C-H pyr	C3-H2	1.05(2)	0.970(13)
	C-H pyr	C5-H3	1.030(18)	0.945(14)
	C-H pyr	C7-H4	1.06(2)	0.955(14)
	C-H pyr	C8-H5	0.99(2)	0.958(15)
	C-H pyr	C9-H6	0.98(2)	0.938(14)
	C-H pyr	C11-H7	1.08(2)	0.989(14)
	C-H pyr	C12-H8	1.03(2)	0.969(15)
	C-H me	C13-H9	0.98(2)	0.973(18)
	C-H me	C13-H10	1.08(2)	0.974(17)
	C-H me	C13-H11	1.00(2)	0.974(16)

Table S2 - Hydrogen bond lengths (Å), from PND, and from single crystal X-ray data for comparison

Complex	Bond	NPD	SXRD	SND	Bond	NPD	SXRD	SND
1	O1-H1	1.082(16)	0.88(2)		H1···N1	1.553(17)	1.75(2)	
2	N1-H1	1.063(17)	0.90(2)		H1···O1	1.600(17)	1.72(2)	
3-I	O1-H1	1.179(18)	1.25(2)	1.161(3)	H1···N1	1.397(16)	1.30(2)	1.398(3)
3-II	O1-H1	1.253(15)	1.20(2)	1.235(5)	H1···N1	1.287(15)	1.35(2)	1.313(6)
3d	N1-H1	1.064(8)	0.98(2)		H1···O1	1.846(8)	1.94(2)	
					H1···O2	1.939(8)	1.970(19)	
4	N3-H1	1.264(19)	1.19(2)		H1···O1	1.28(2)	1.33(2)	
4d	N3-D1	1.201(14)	1.125(18)		H1···O1	1.339(15)	1.395(18)	

Final Rietveld fits for refined neutron powder diffraction patterns

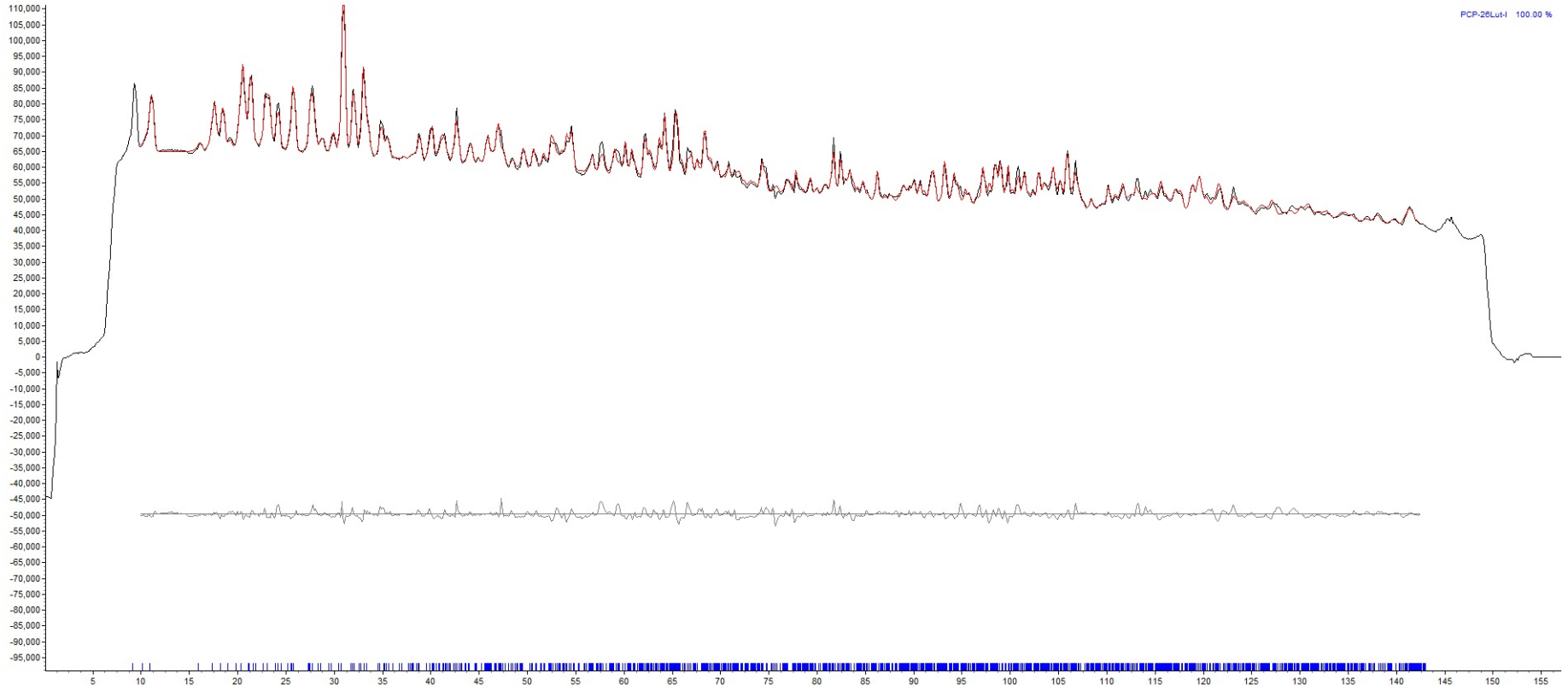

Figure S1 – pentachlorophenol – 2.6-lutidine (1:1) (**1**): RwP = 1.65%; GooF = 3.18

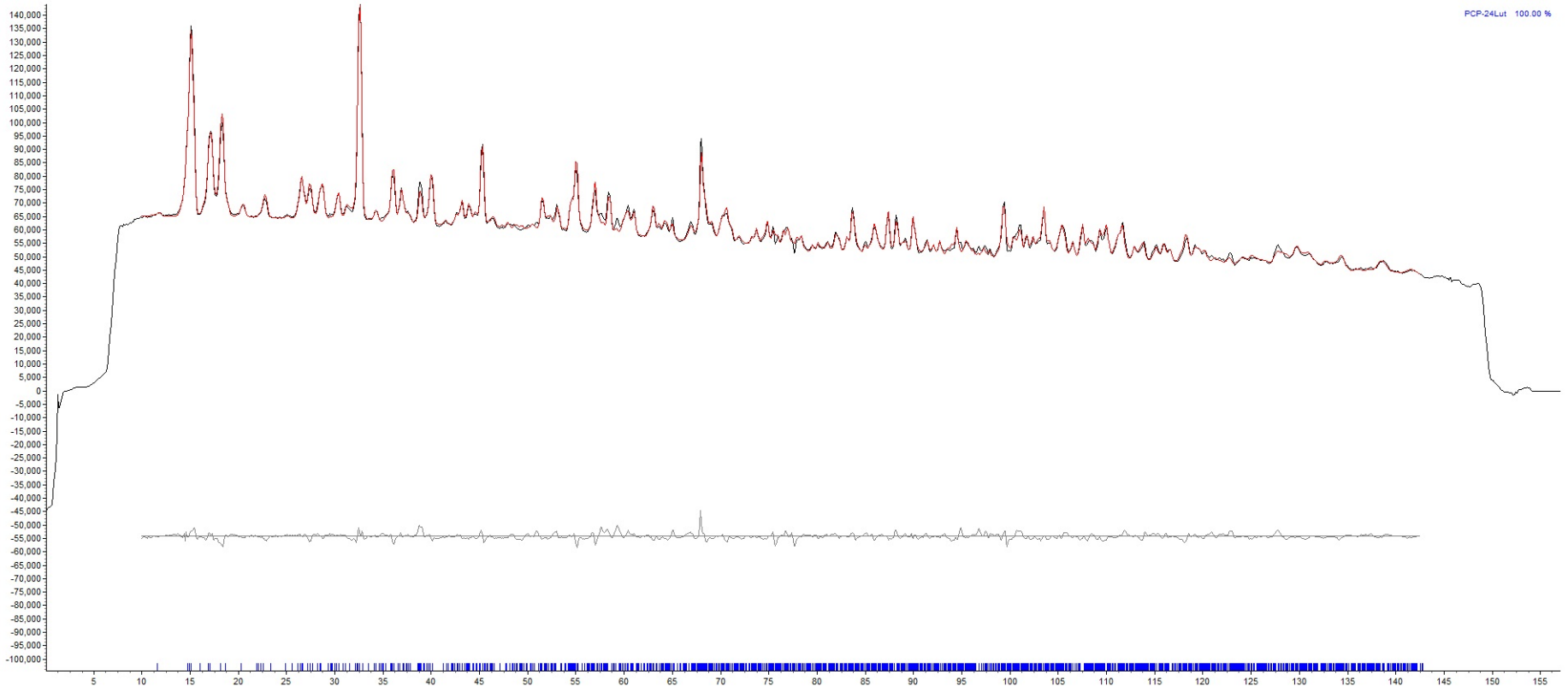

Figure S2 – pentachlorophenol – 2.4-lutidine (1:1) (**2**): RwP = 1.58%; GooF = 3.13

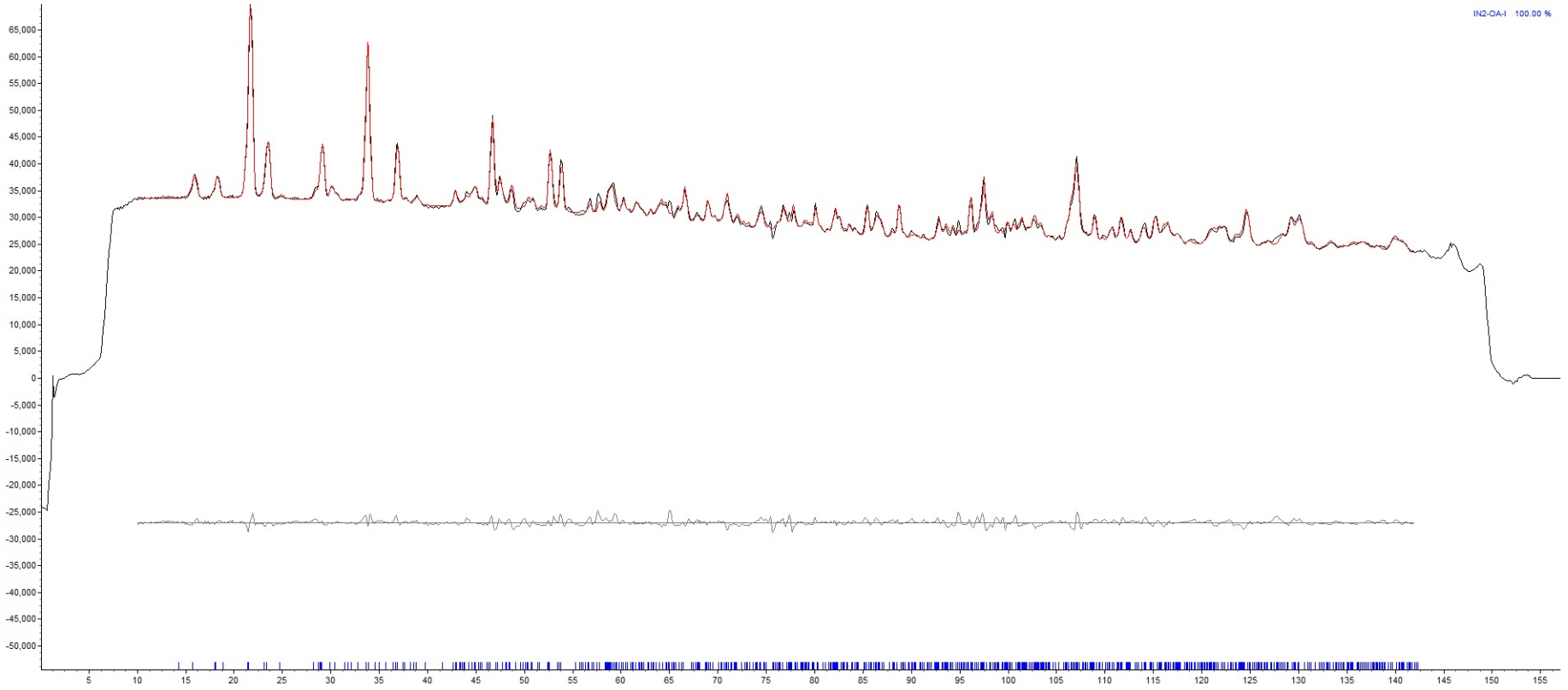

Figure S3 – isonicotinamide : oxalic acid (2:1) form I (**3-I**): RwP = 1.52%; GooF = 3.94

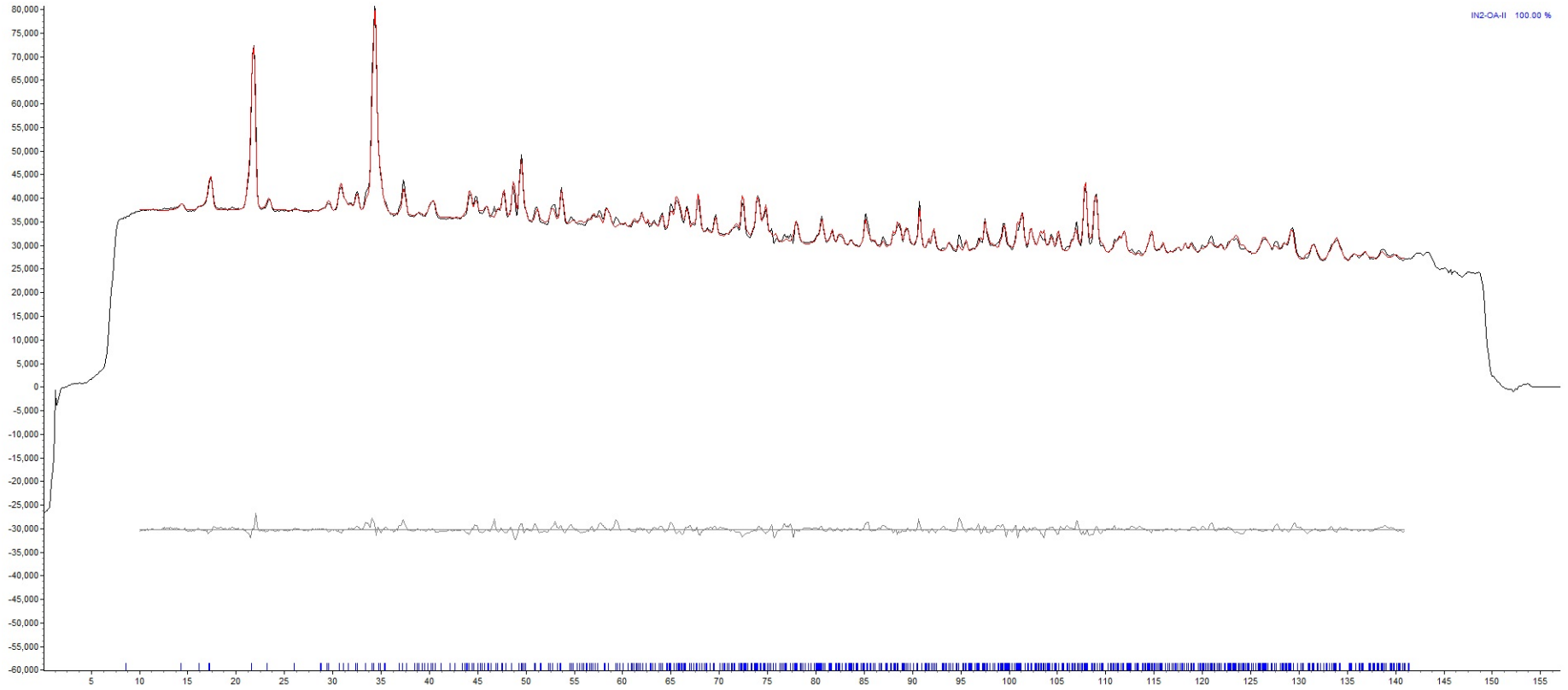

Figure S4 – isonicotinamide : oxalic acid (2:1) form II (**3-II**): RwP = 1.57%; GooF = 4.44

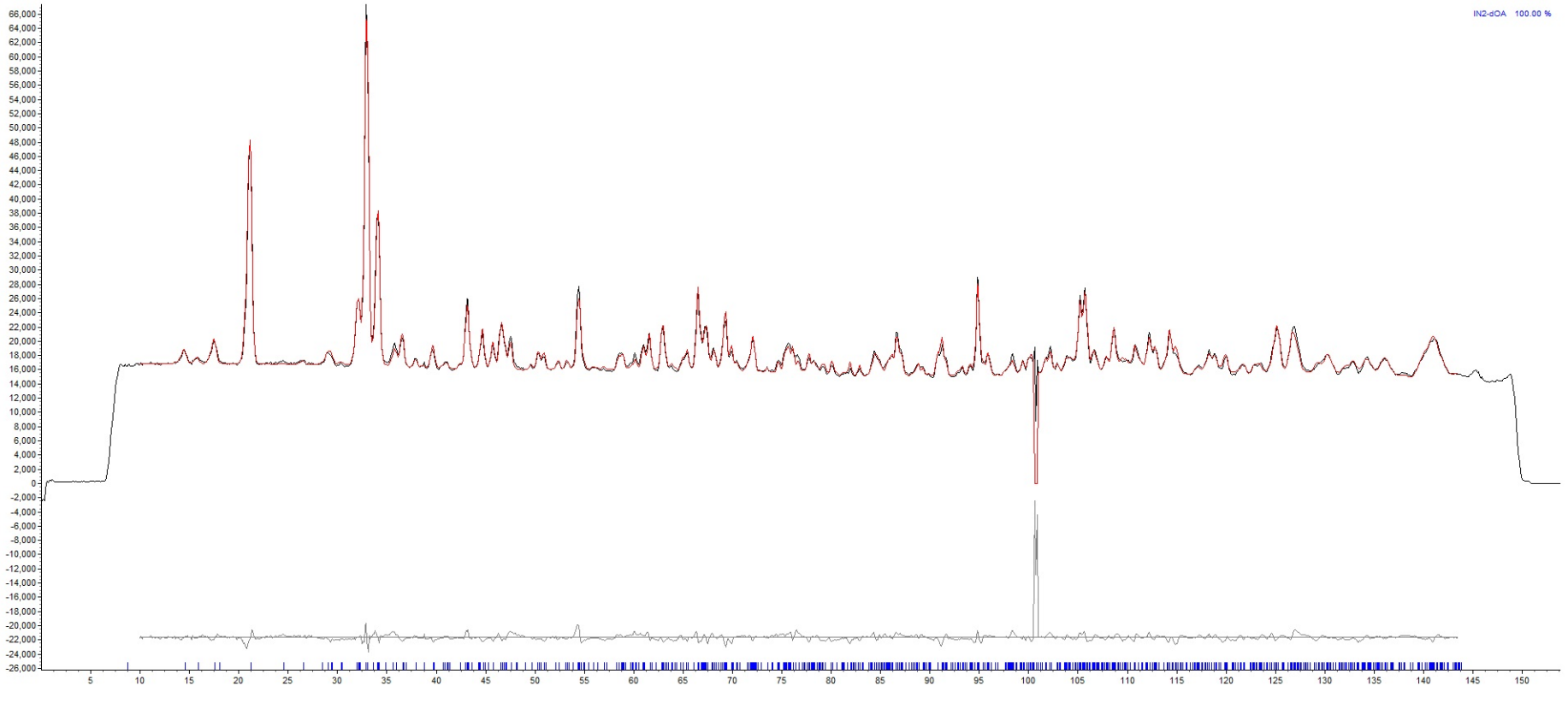

Figure S5 – isonicotinamide : oxalic acid (2:1) form I (**3d**) (deuterated, 70%D): RwP = 1.85%; GooF = 4.60. The dip in the spectrum represents a small excluded region in the fit due to data merging.

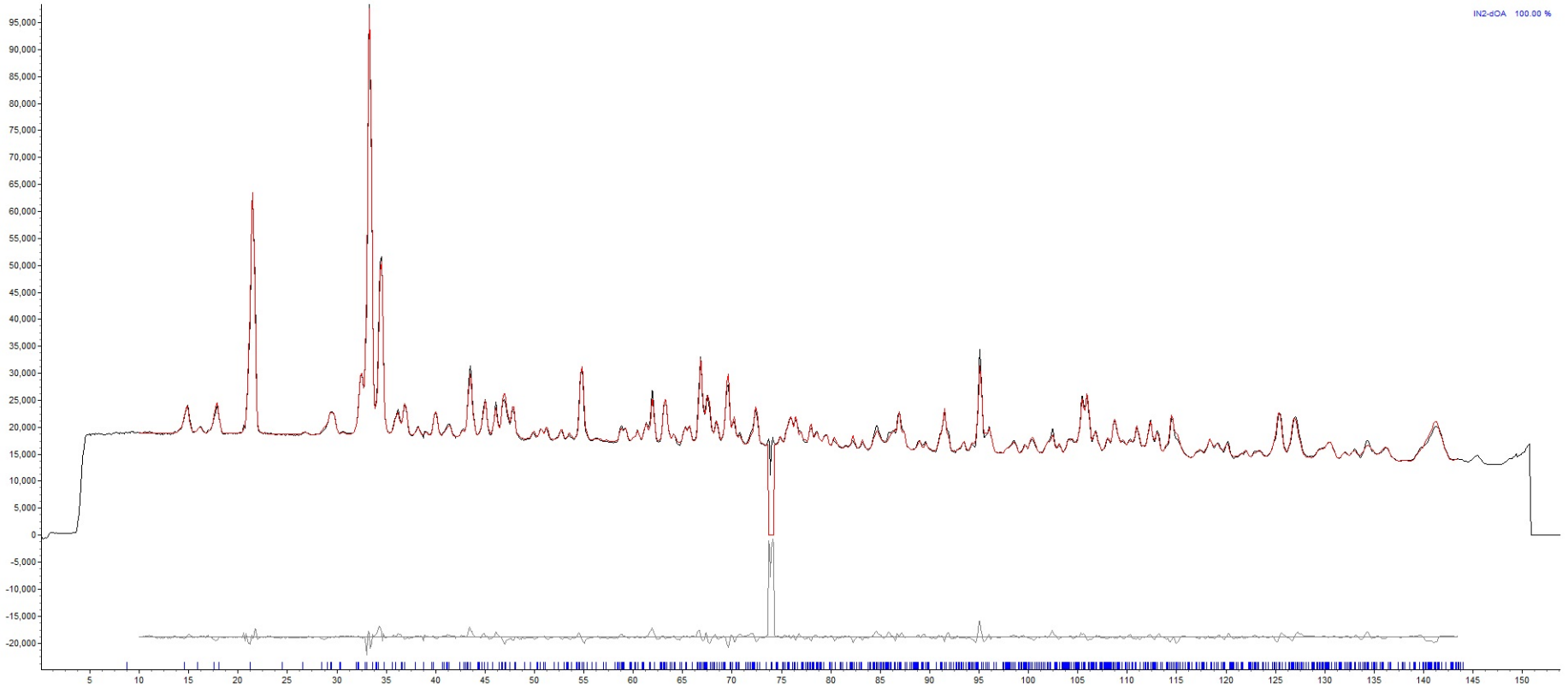

Figure S6 – isonicotinamide : oxalic acid (2:1) form I (**3d**) (deuterated, 100%D): RwP = 1.86%; GooF = 3.78. The dip in the spectrum represents a small excluded region in the fit due to data merging.

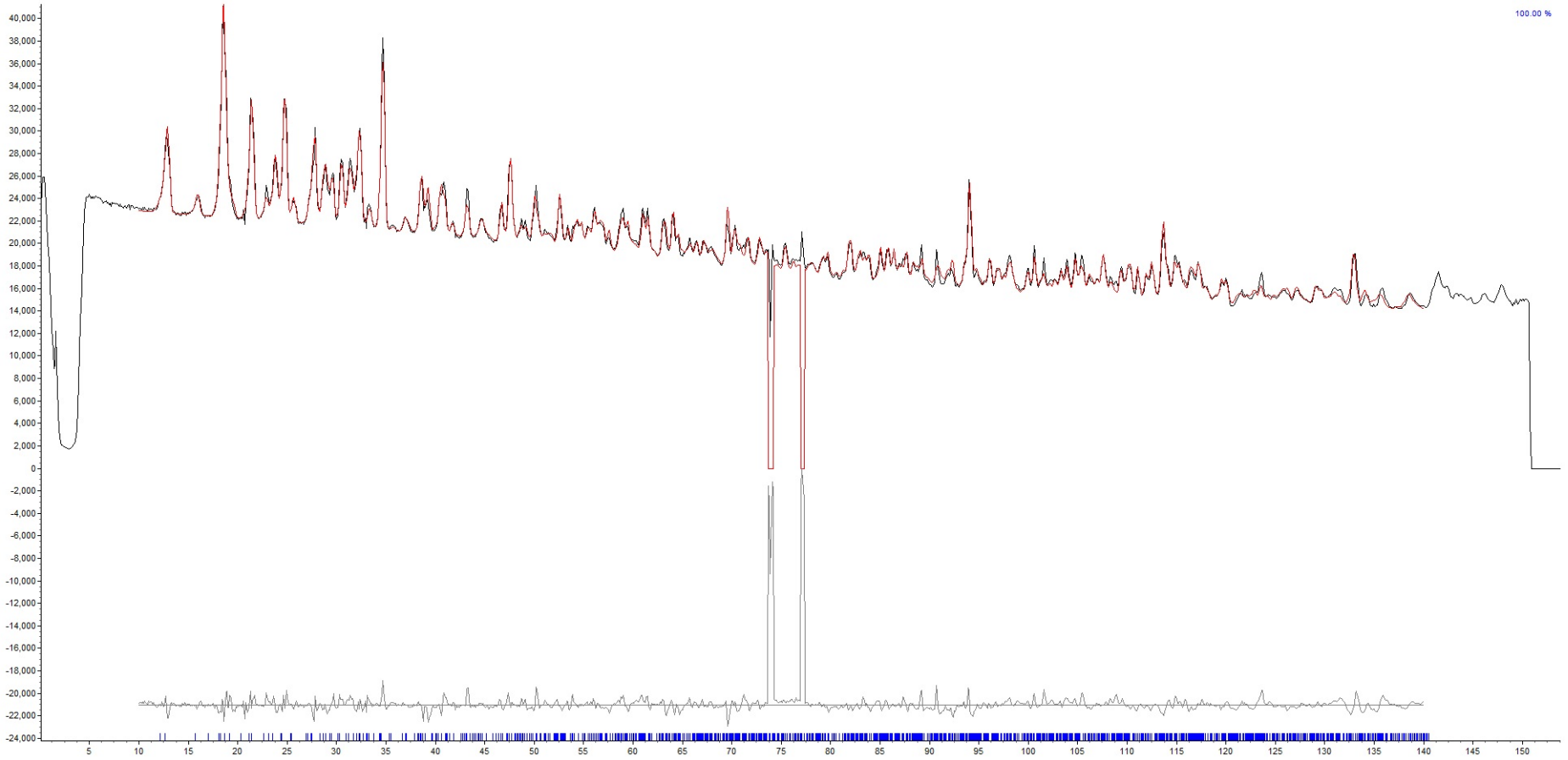

Figure S7 – 3,5-dinitrobenzoic acid : 4-methylpyridine (1:1) (**4**): RwP = 1.94%; GooF = 4.29. The dips in the spectrum represent small excluded regions in the fit due to data merging.

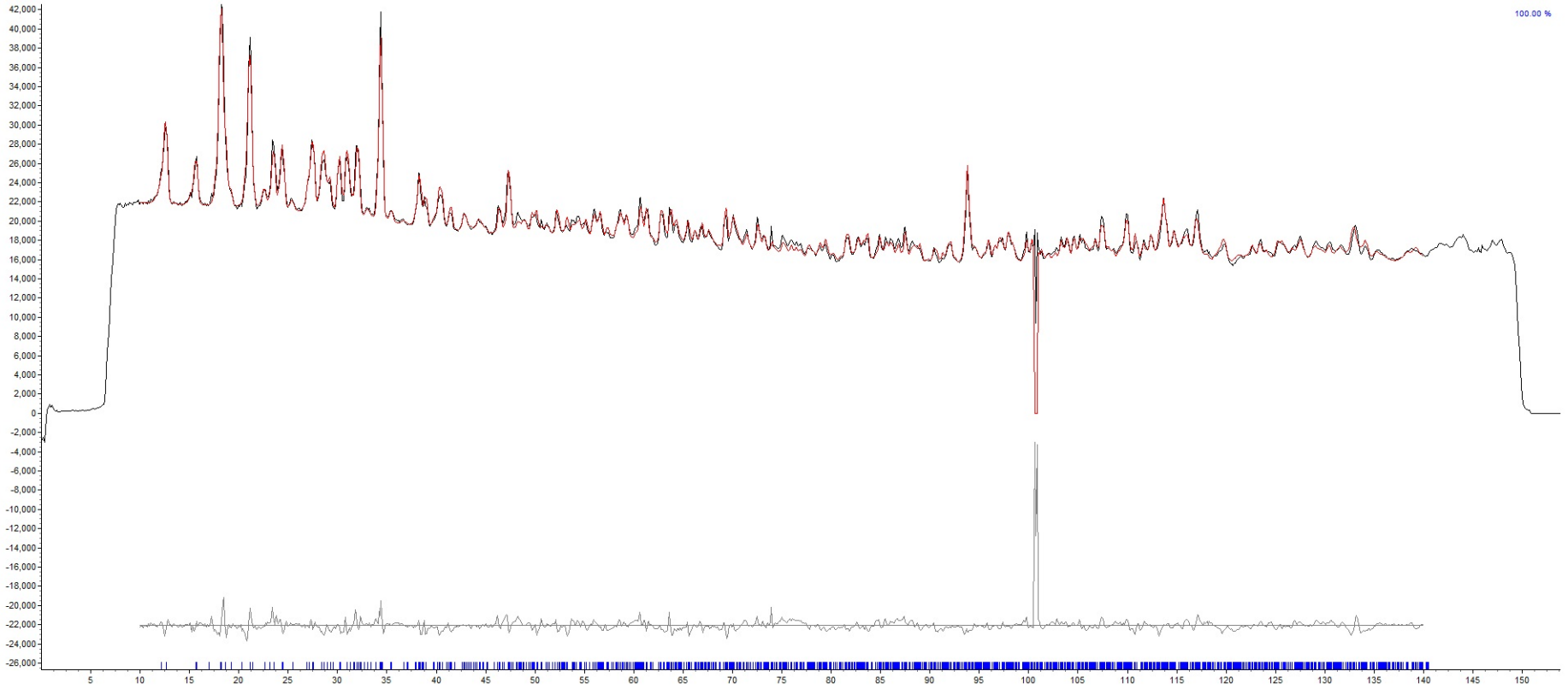

Figure S8 – 3,5-dinitrobenzoic acid : 4-methylpyridine (1:1) (**4d**) (deuterated, 80%D): RwP = 2.06%; GooF = 5.56. The dip in the spectrum represents a small excluded region in the fit due to data merging.