Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary information

Factors influencing stoichiometry and stability of Polyoxometalate – peptide complexes

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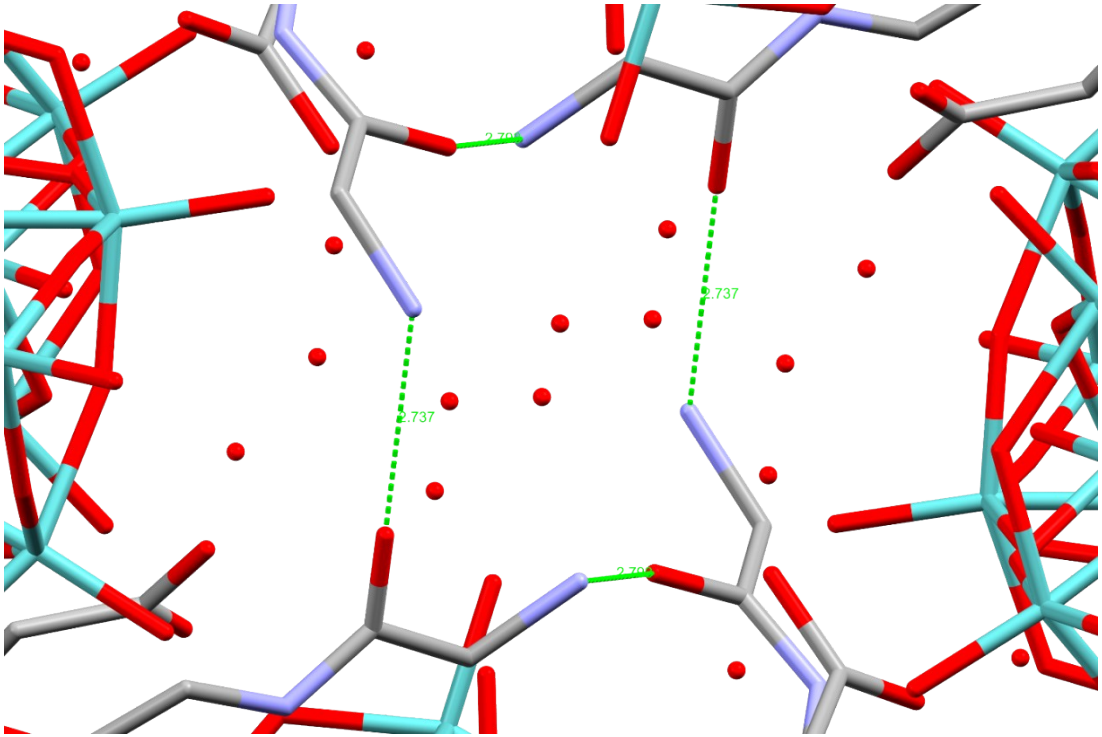

Figure S1. Ring structure between diglycines in **4**.

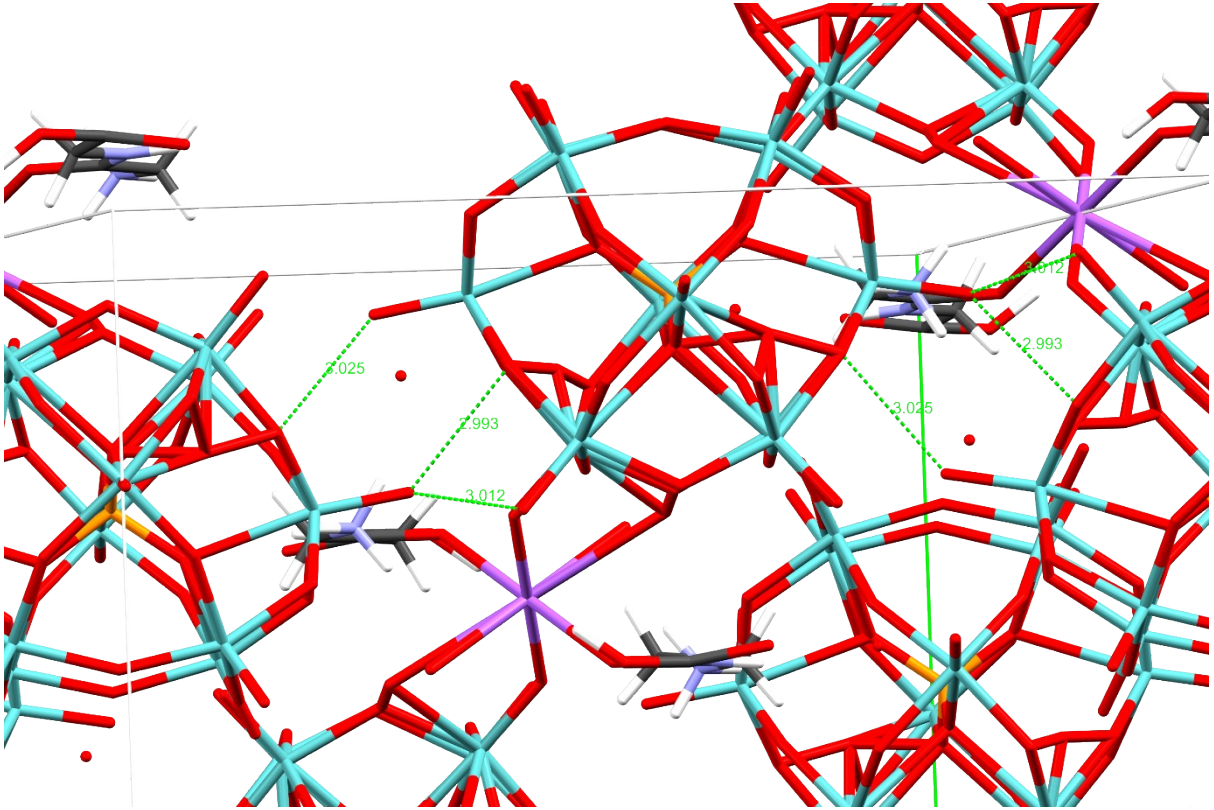

Figure S2. Contacts between POM oxygen in **6**.

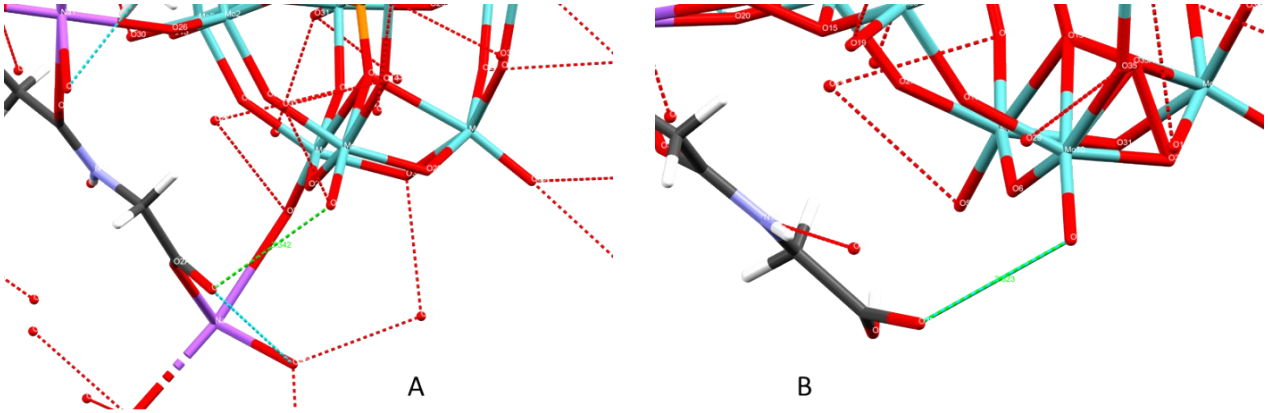

Figure S3. Distance between equivalent carboxyl groups in A) **5** and B) **6**, illustrating the small but significant differences caused by the presence of an extra Na^+ in **5**.

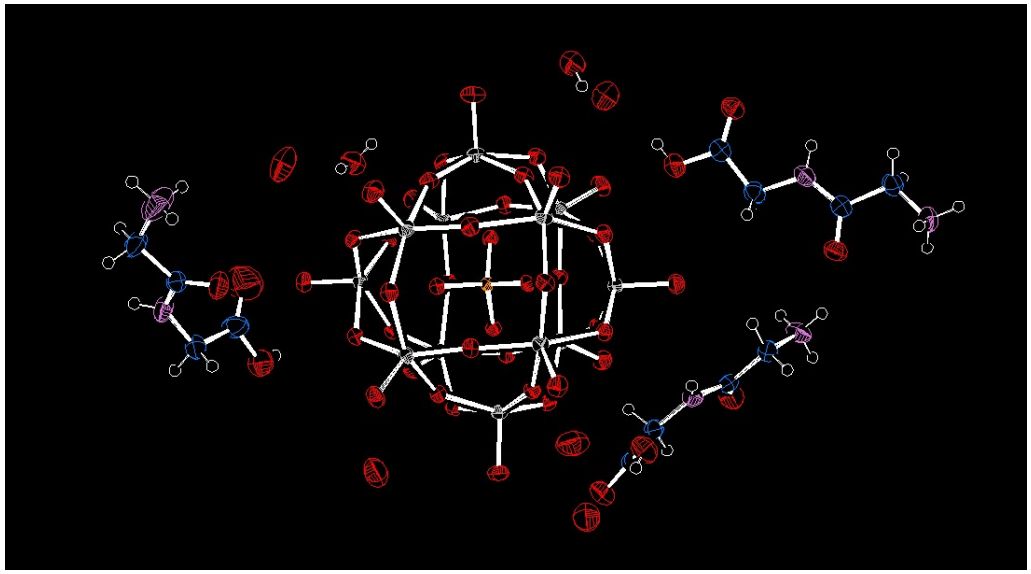

Figure S4. Thermal ellipsoidal diagram of 2

Comment [VK]: Björn, ange gärna % av probability for thermal ellipsoids.

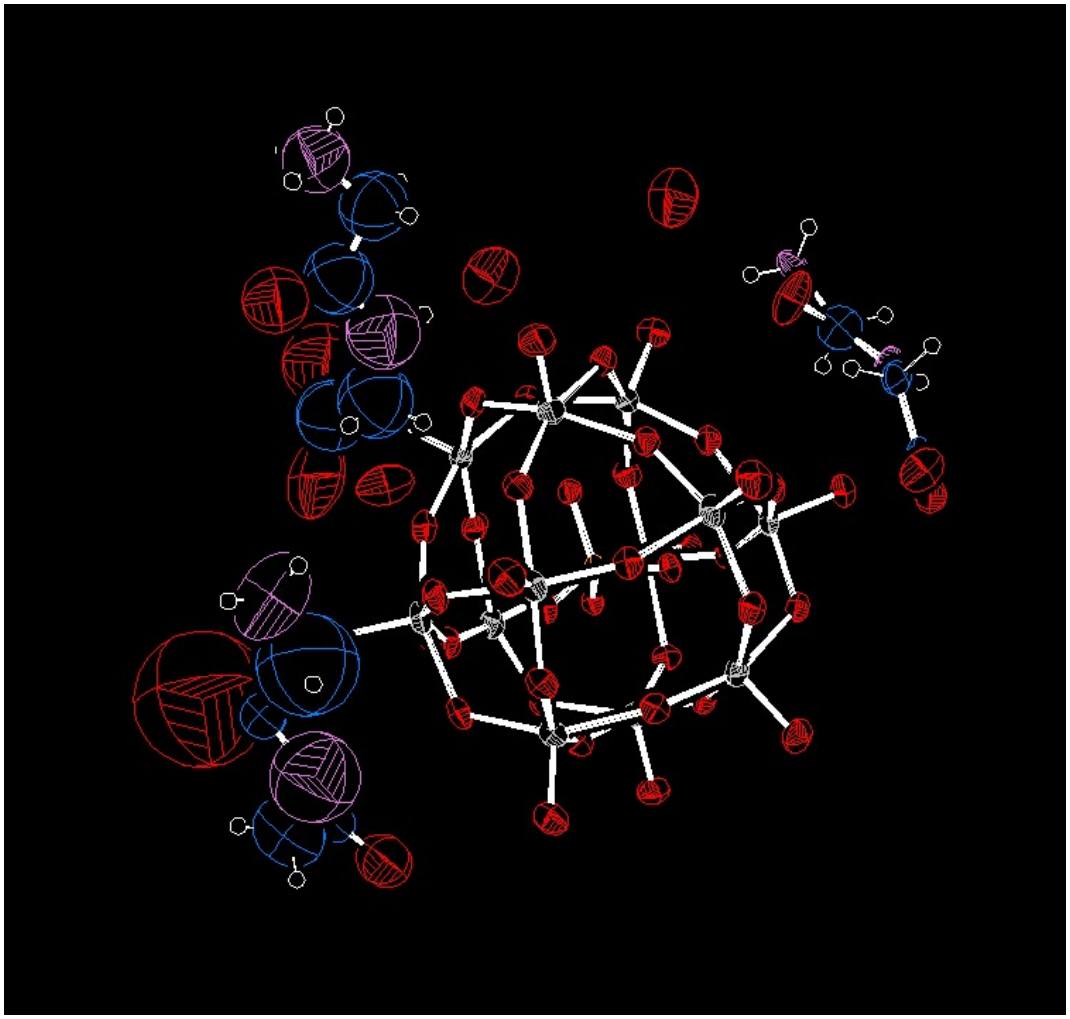

Figure S5. Thermal ellipsoidal diagram of **3**

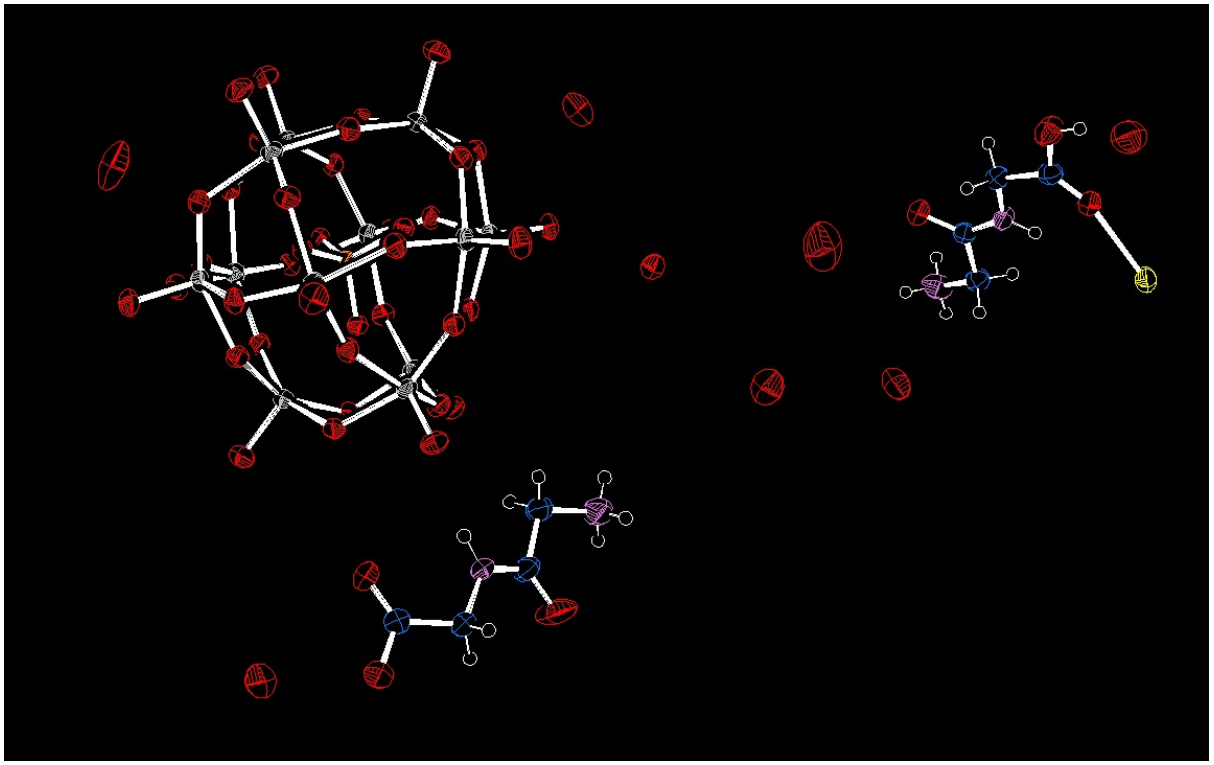

Figure S6. Thermal ellipsoidal diagram of **4**

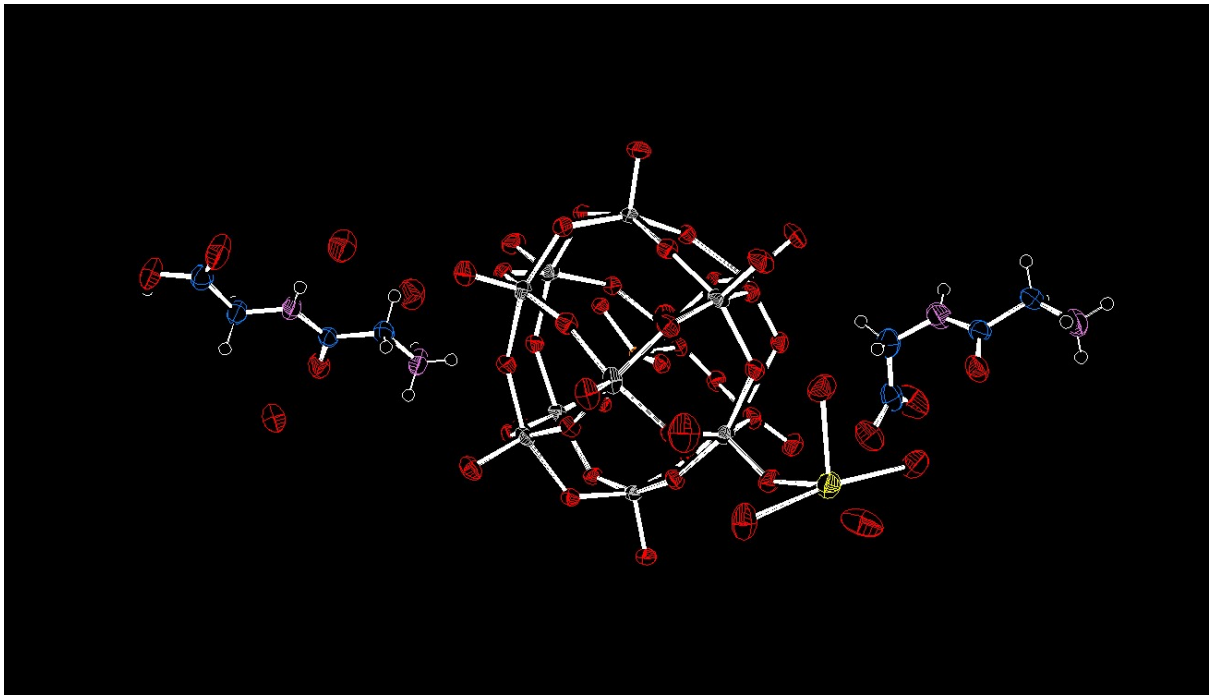

Figure S7. Thermal ellipsoidal diagram of **5**

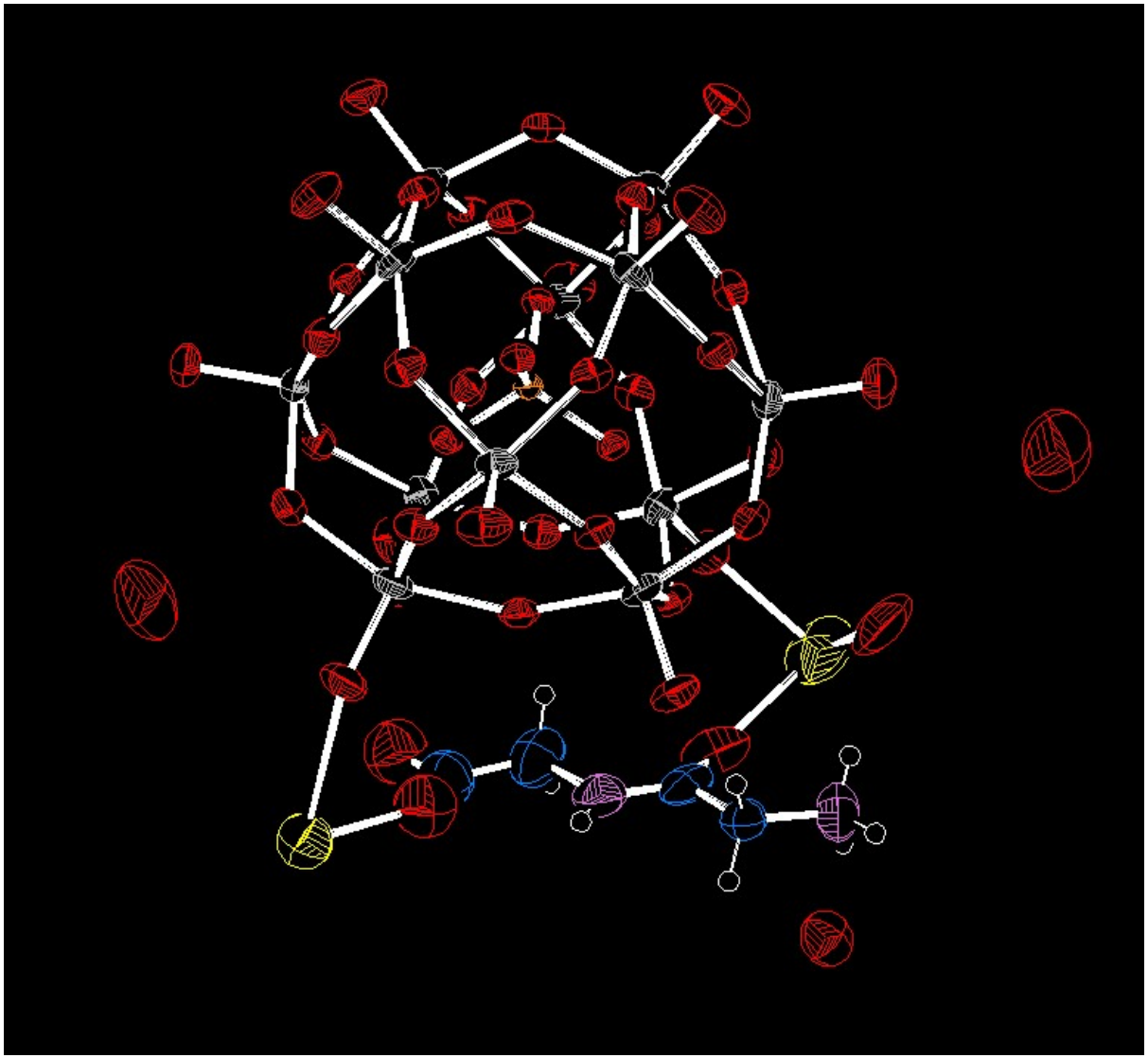

Figure S8. Thermal ellipsoidal diagram of **6**

Figure S9. Thermal ellipsoidal diagram of **7**

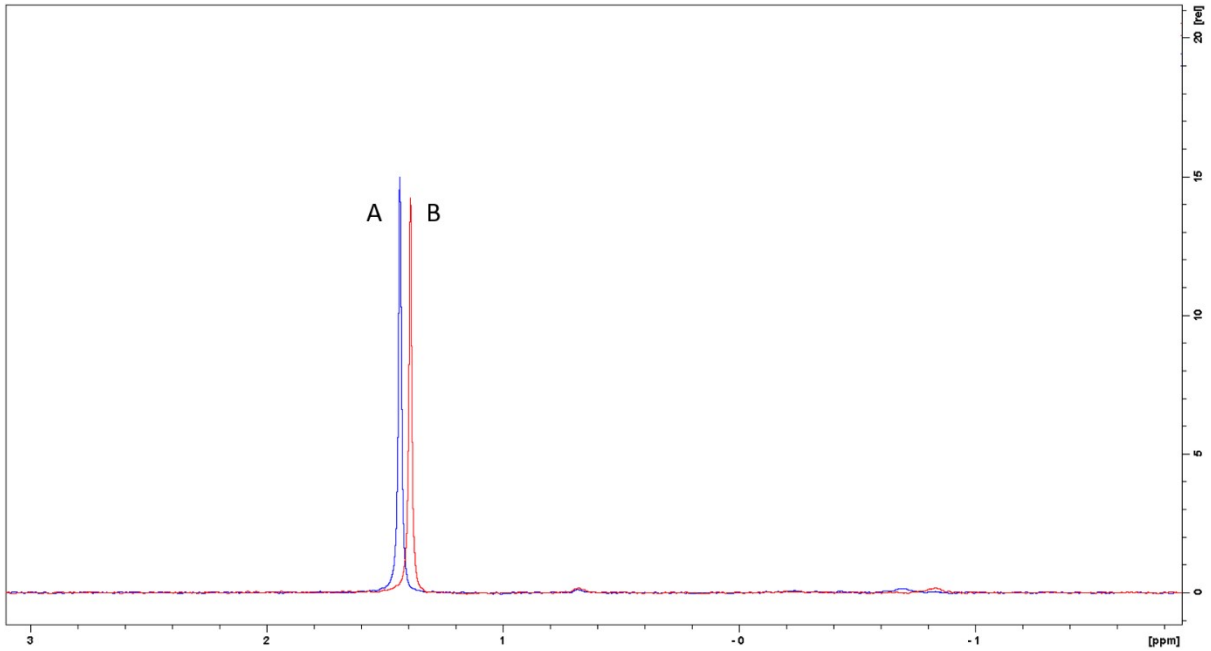

Figure S10. ^{31}P-NMR spectra of A: phosphomolybdate with diglycine at pH 6 and B: phosphomolybdate without diglycine at pH 6.

SEM

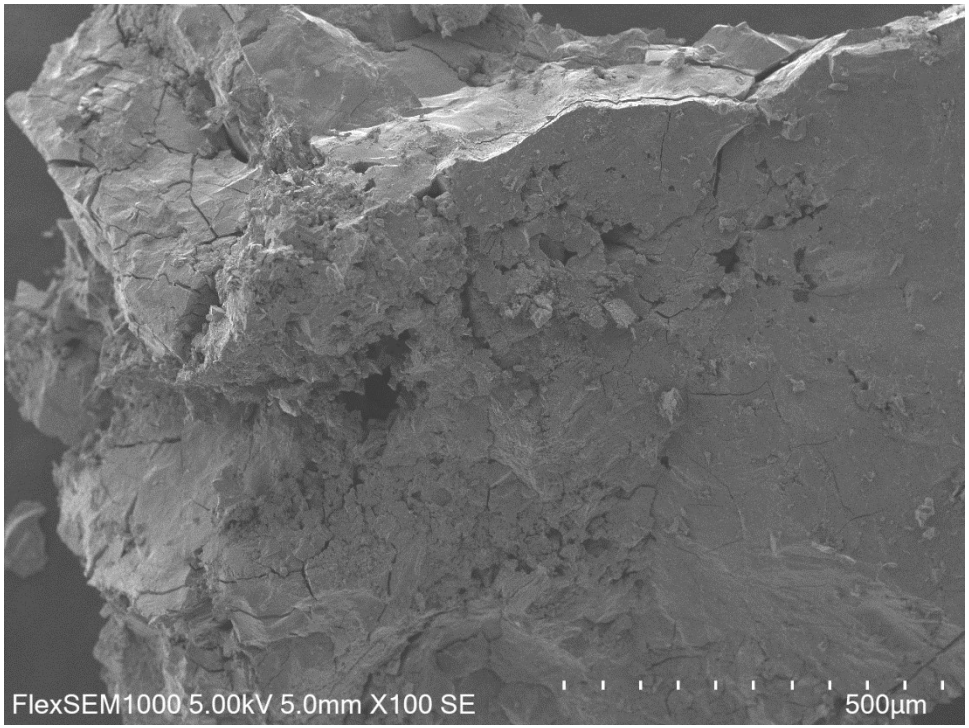

Figure S11. SEM image of **2**.

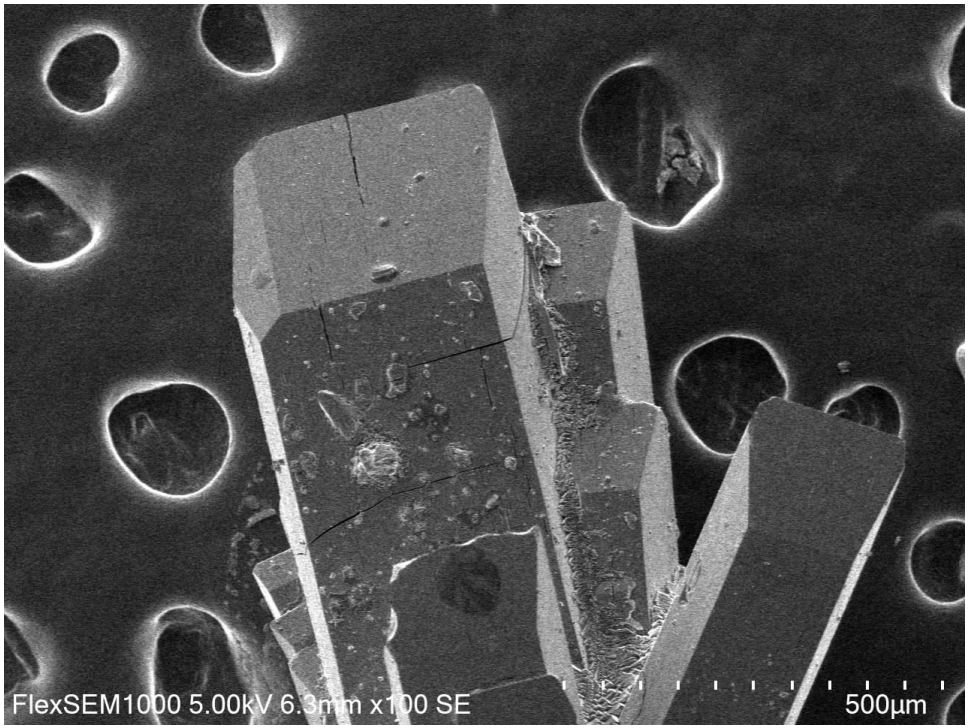

Figure S12. SEM image of **4**

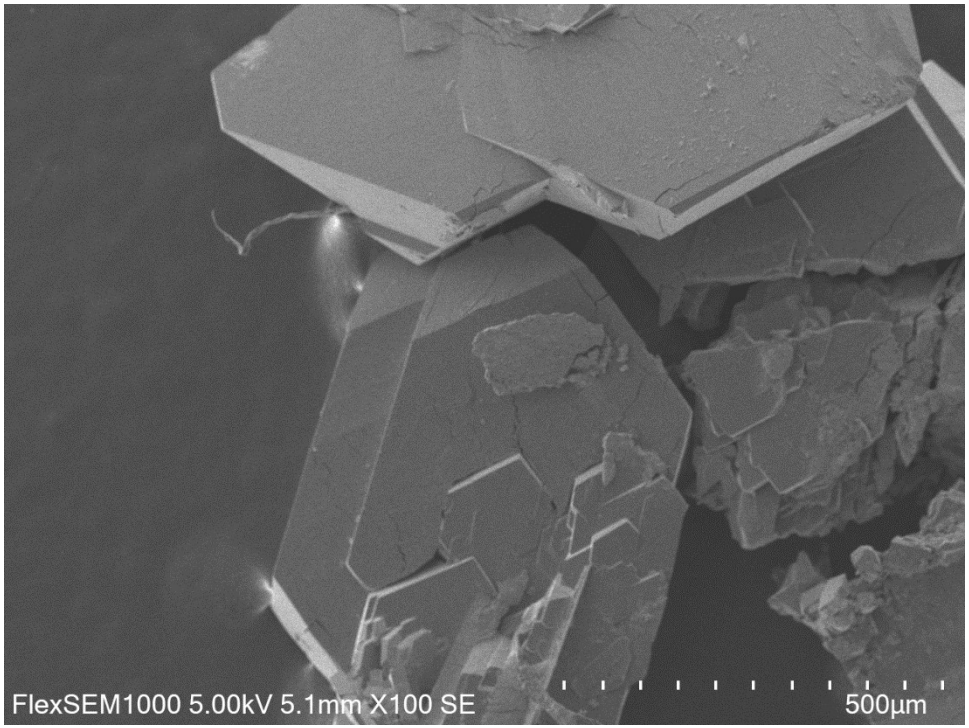

Figure S13. SEM image of **5**.

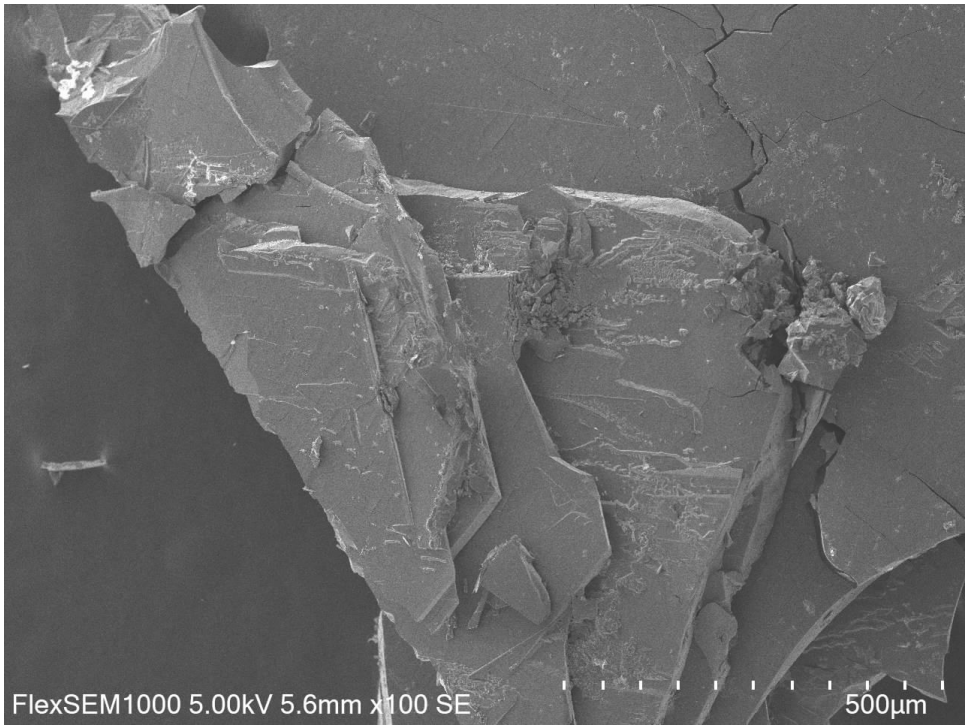

Figure S14. SEM image of **6**

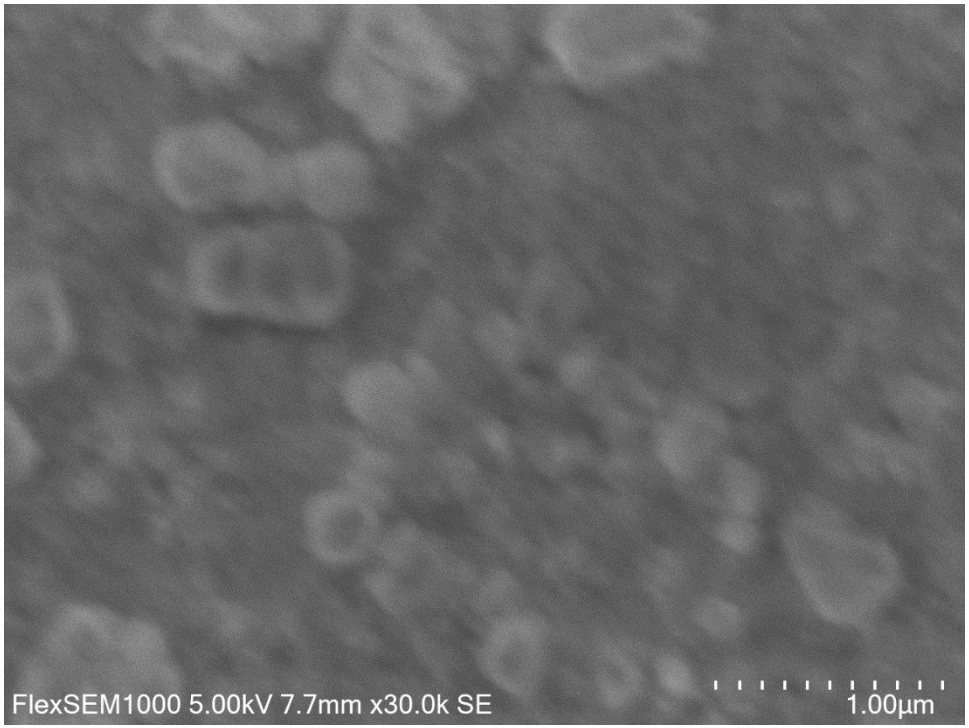

Figure S15. SEM image of ZrP, x30 000 magnification

EDS

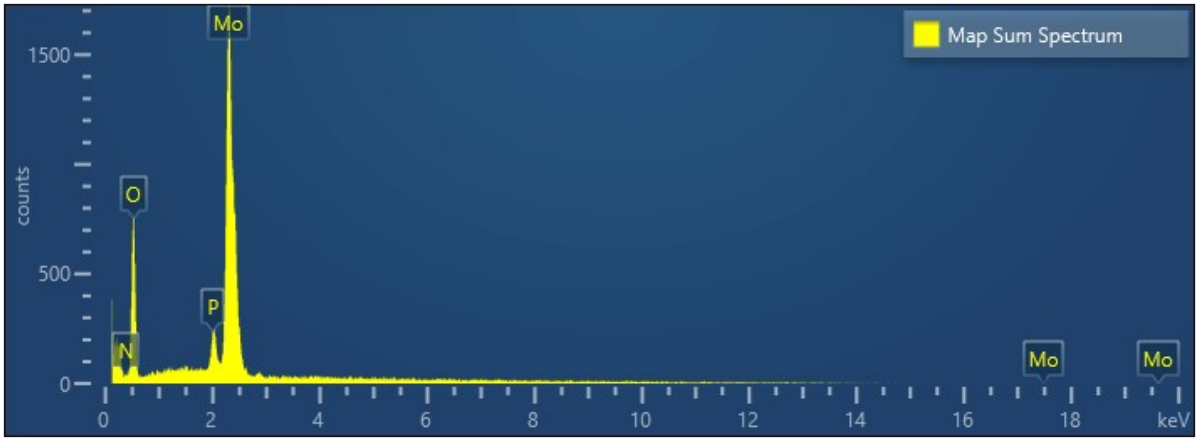

Figure S16. EDS spectrum of **2**.

Table S1. Elemental analysis of **2**.

Map Sum Spectrum				
Element	**Line Type**	**Weight %**	**Weight % Sigma**	**Atomic %**
O	K series	43.27	0.85	78.26
Mo	L series	53.18	0.91	16.04
P	K series	1.45	0.14	1.36
N	K series	2.10	1.09	4.34
Total		100.00		100.00

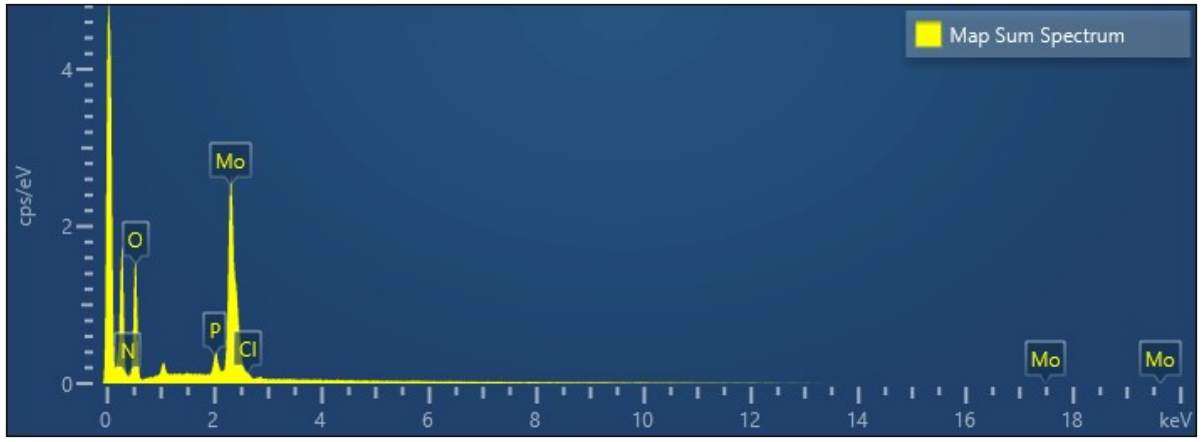

Figure S17. EDS spectrum of **4**

Table S2. Elemental analysis of **4**

Map Sum Spectrum				
Element	**Line Type**	**Weight %**	**Weight % Sigma**	**Atomic %**
Fe	K series	0.05	0.13	0.03
O	K series	47.65	0.37	82.36
Na	K series	1.76	0.10	2.12
Mo	L series	48.93	0.37	14.10
P	K series	1.24	0.07	1.10
N	K series	0.00	0.88	0.00

Cl	K series	0.37	0.07	0.29
Total		100.00		100.00

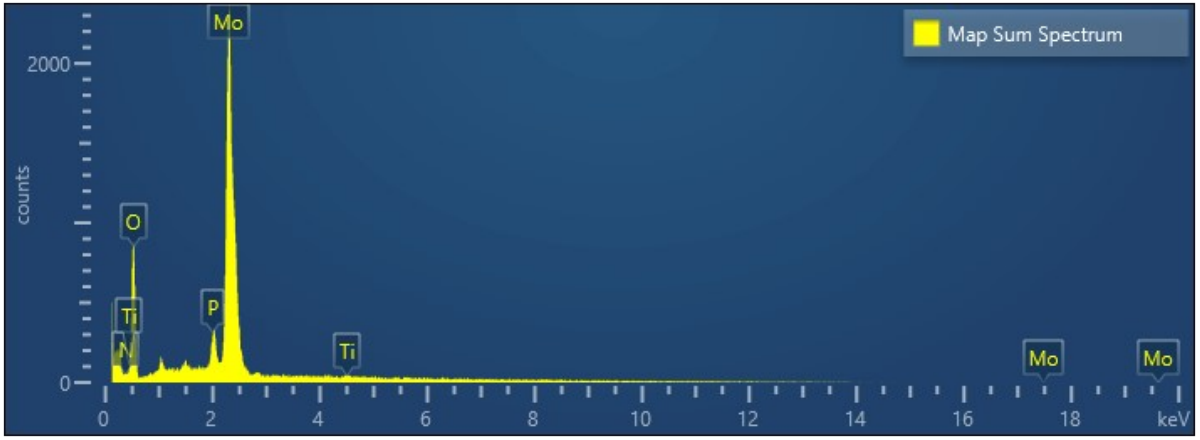

Figure S18. EDS spectrum of **5**.

Table S3. Elemental analysis of **5**.

Map Sum Spectrum				
Element	**Line Type**	**Weight %**	**Weight % Sigma**	**Atomic %**
O	K series	41.56	0.68	79.24
P	K series	1.41	0.13	1.39
Mo	L series	55.57	0.68	17.67

Na	K series	1.11	0.14	1.48
Ti	K series	0.35	0.15	0.23
N	K series	0.00	1.77	0.00
Total		100.00		100.00

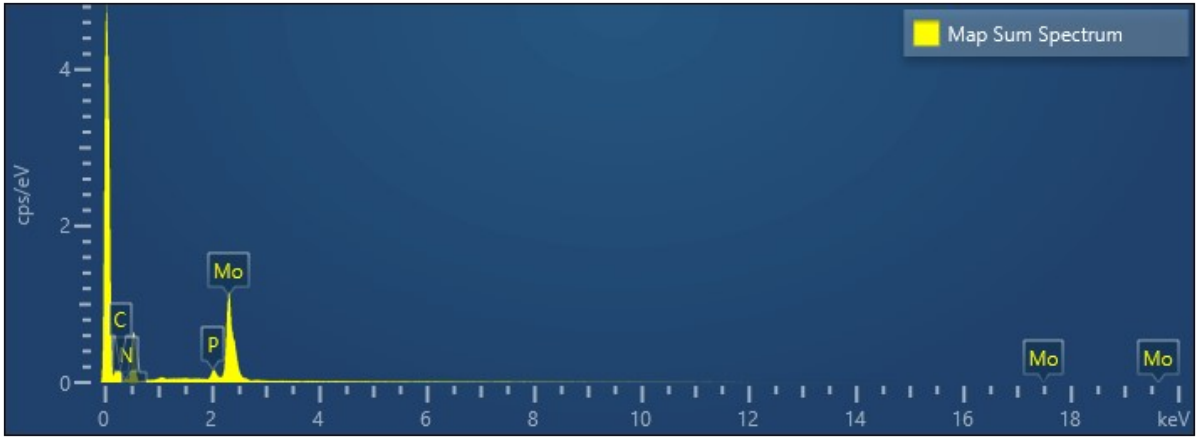

Figure S19. EDS spectrum of **6**

Table S4.Elemental analysis of **6**

Map Sum Spectrum				

Element	Line Type	Weight %	Weight % Sigma	Atomic %
O	K series	42.98	0.78	64.91
Mo	L series	43.47	0.78	10.95
P	K series	1.04	0.08	0.81
C	K series	7.26	1.17	14.60
N	K series	4.76	0.82	8.21
Na	K series	0.50	0.09	0.52
Total		100.00		100.00

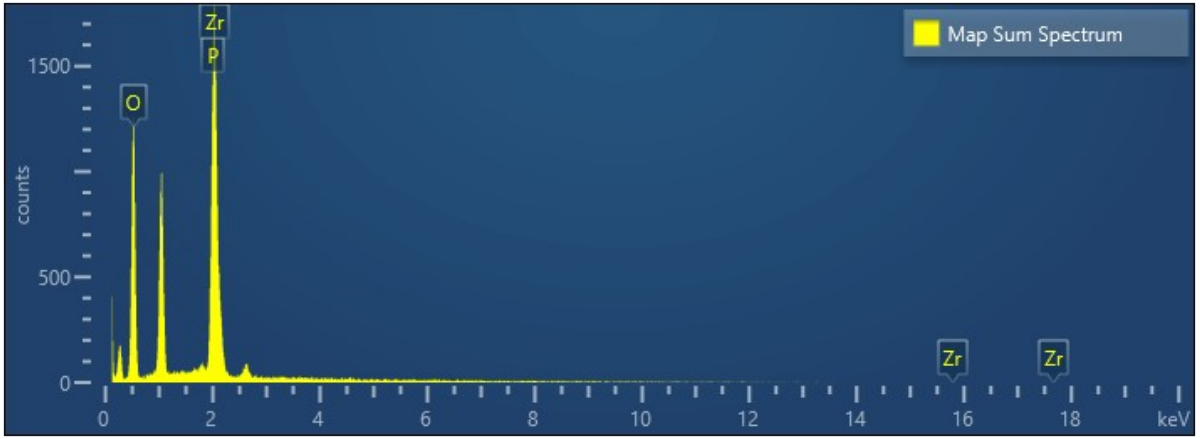

Figure S20. EDS spectrum of ZrP

Table S5. Elemental analysis of ZrP

Map Sum Spectrum				
Element	**Line Type**	**Weight %**	**Weight % Sigma**	**Atomic %**
O	K series	45.97	0.65	66.35
Na	K series	15.24	0.32	15.31
P	K series	16.36	0.38	12.19
Zr	L series	21.27	0.78	5.38
Cl	K series	1.17	0.12	0.76
Total		100.00		100.00

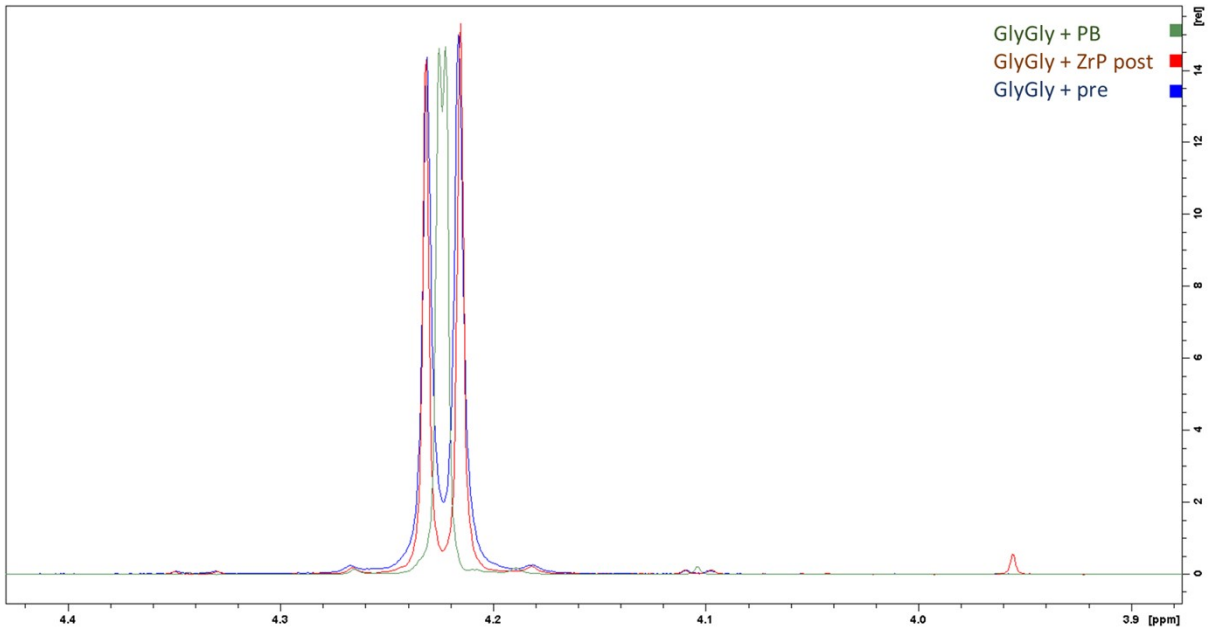

Figure S20. Overlaid ^{1}H-NMR spectra of samples with ZrP and GlyGly before (blue) and after incubation (red) and GlyGly with phosphate buffer after incubation (green). The signals at 4.23 and 4.21 ppm corresponds to diglycine. The peak at 3.95 ppm is unique to the incubated ZrP-GlyGly sample, and likely corresponds to monoglycine.

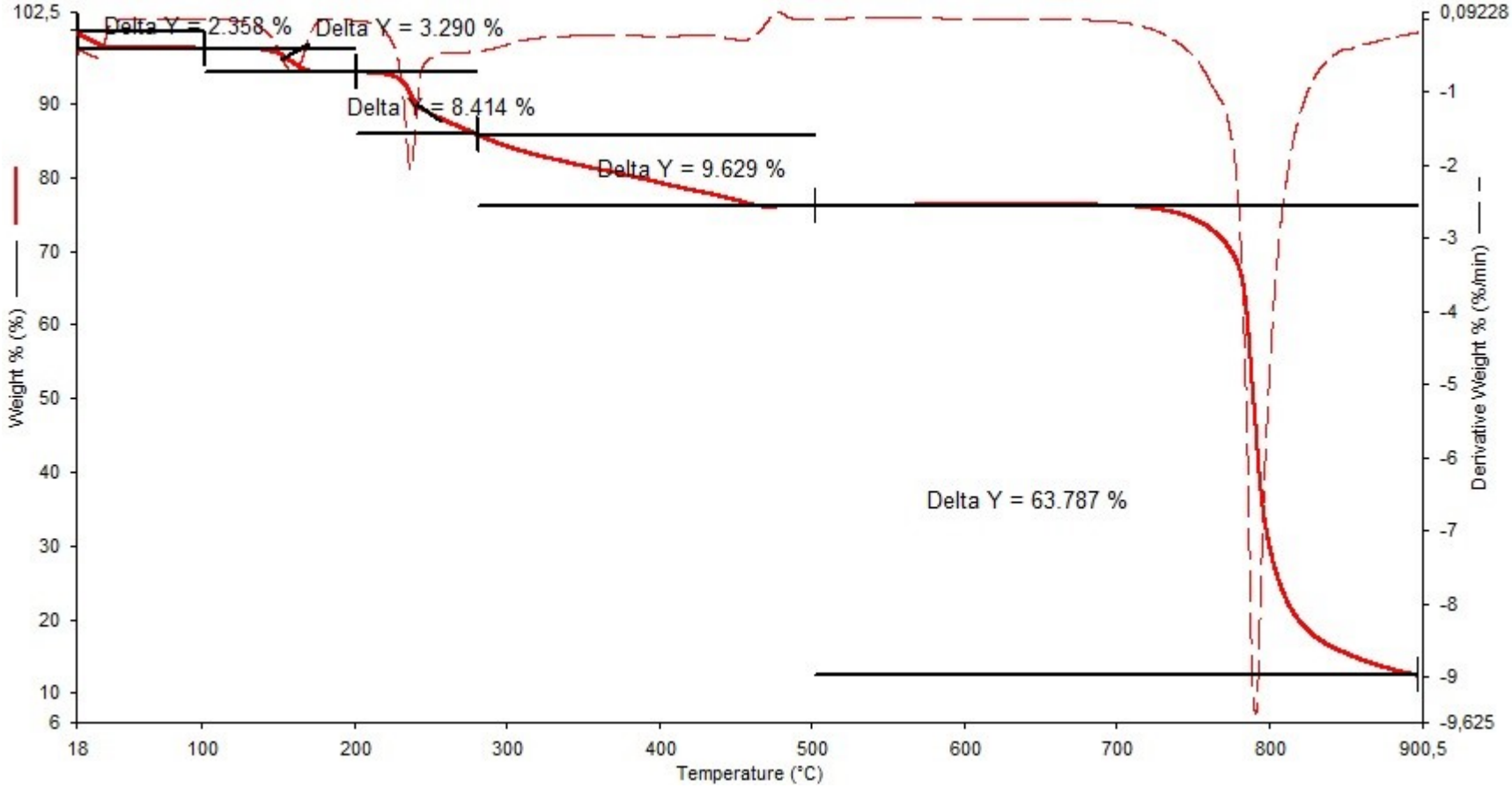

Figure S21. TGA of compound **1**.

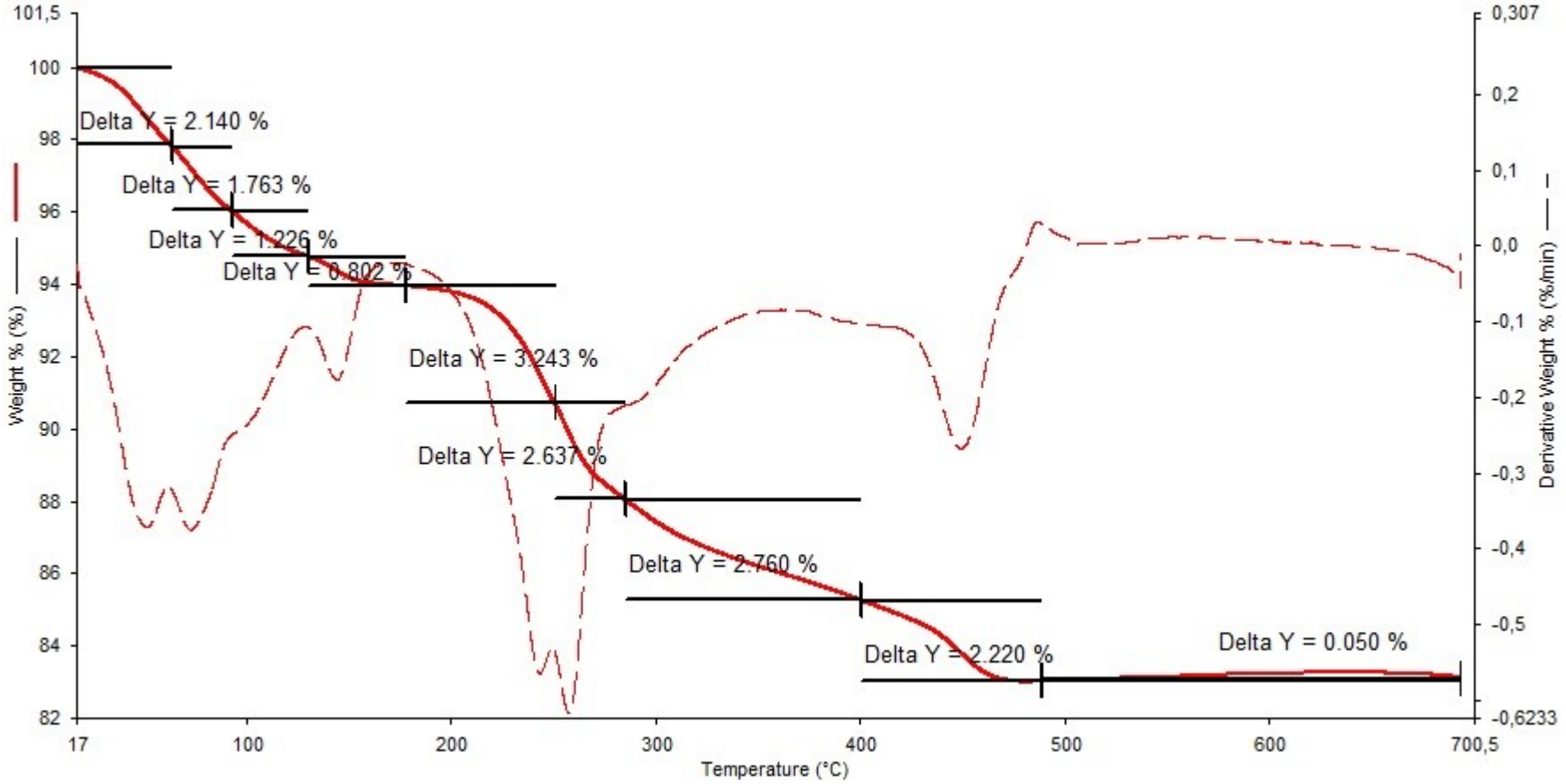

Figure S22. TGA of compound **2**.

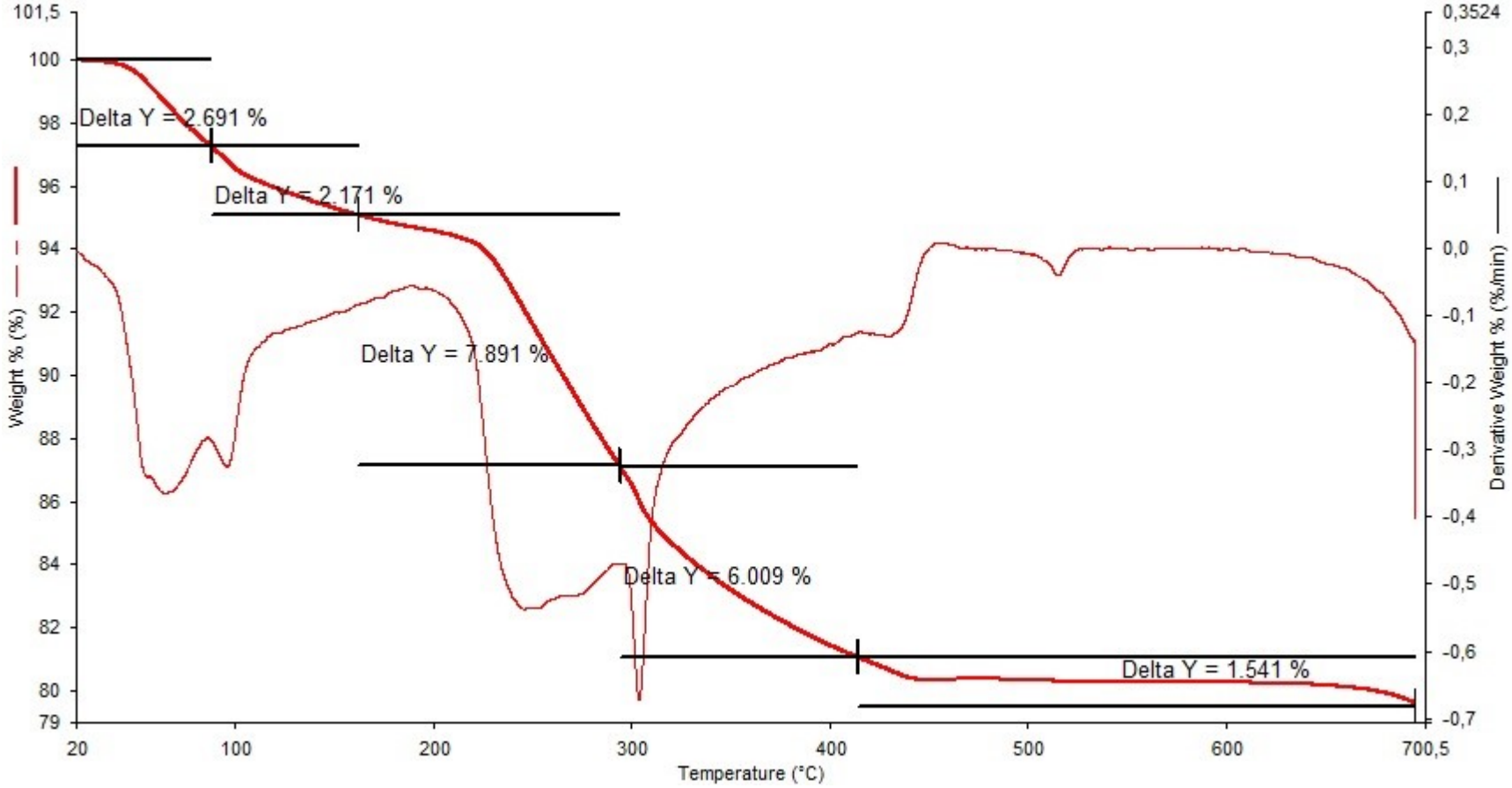

Figure S23. TGA of compound **3**.

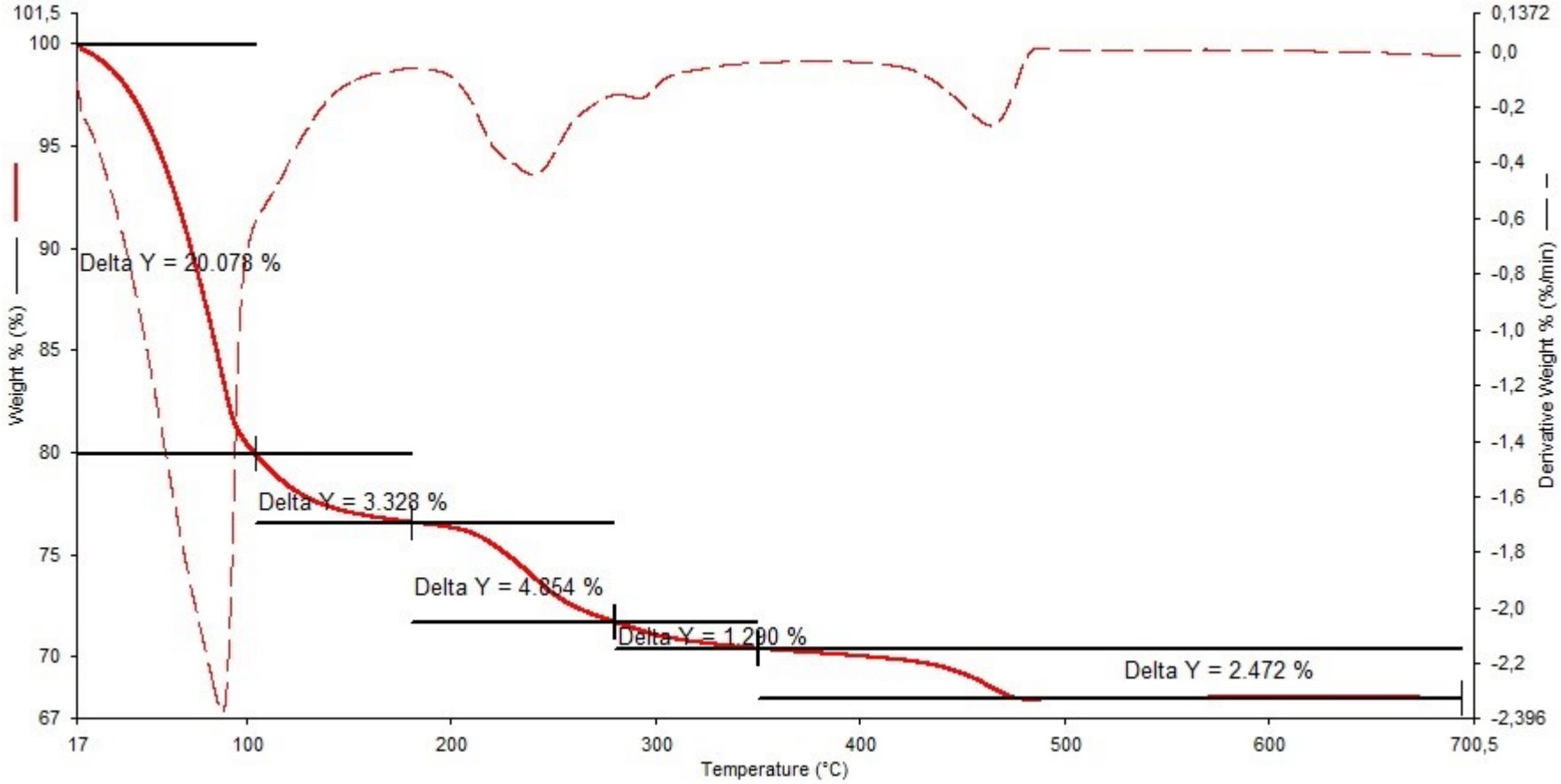

Figure S24. TGA of compound **4**.

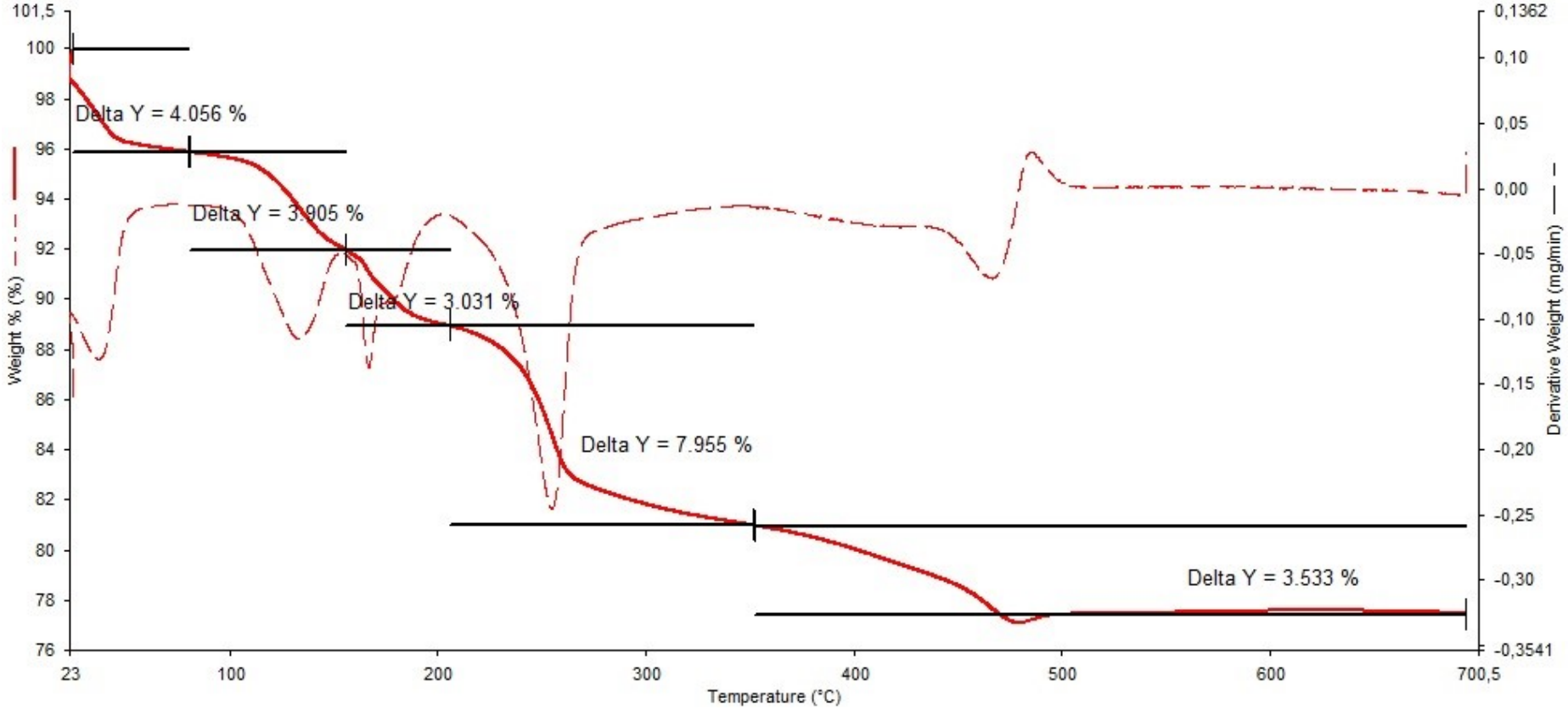

Figure S25. TGA of compound **6**.

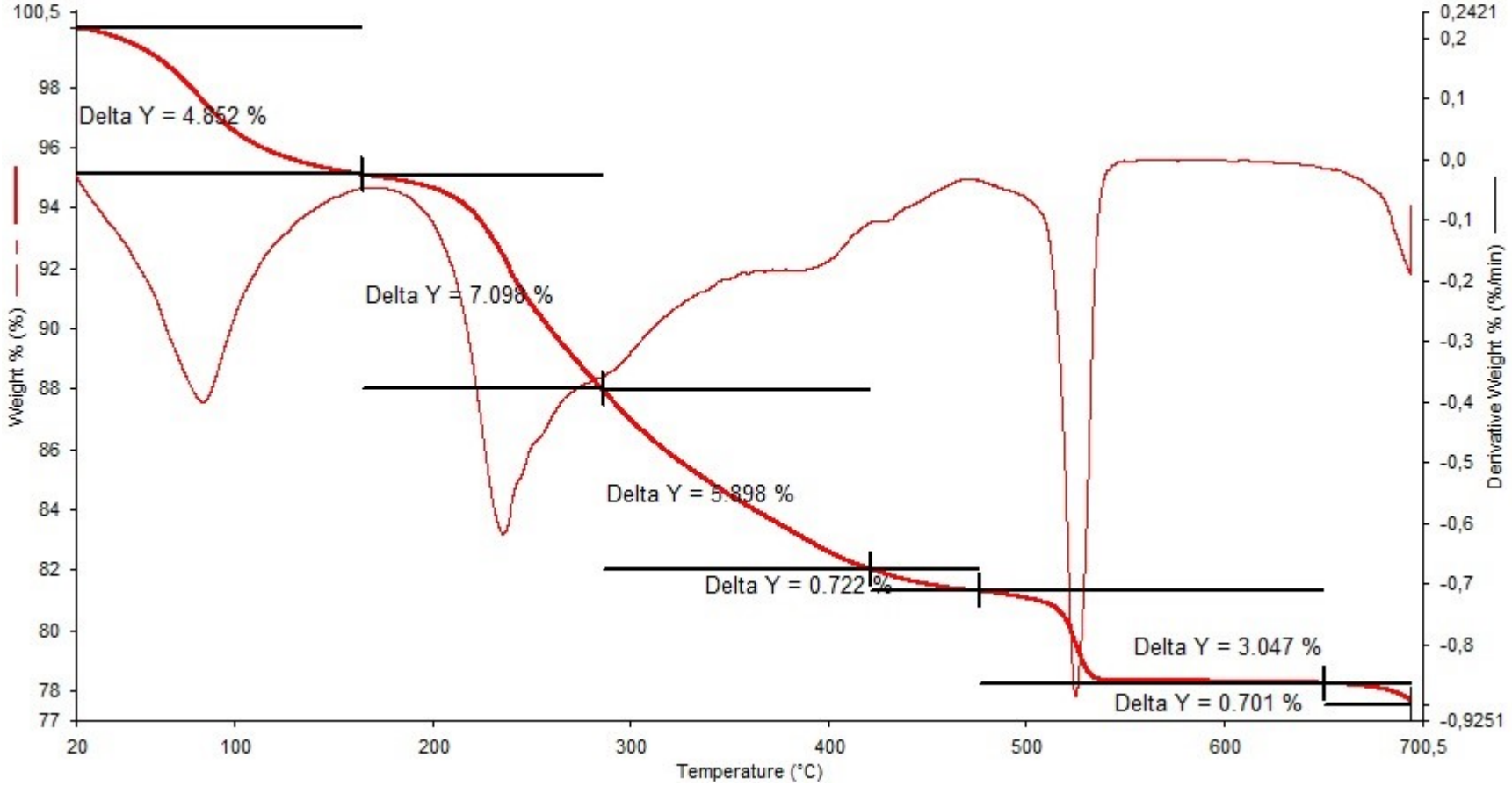

Figure S26. TGA of compound **7**.

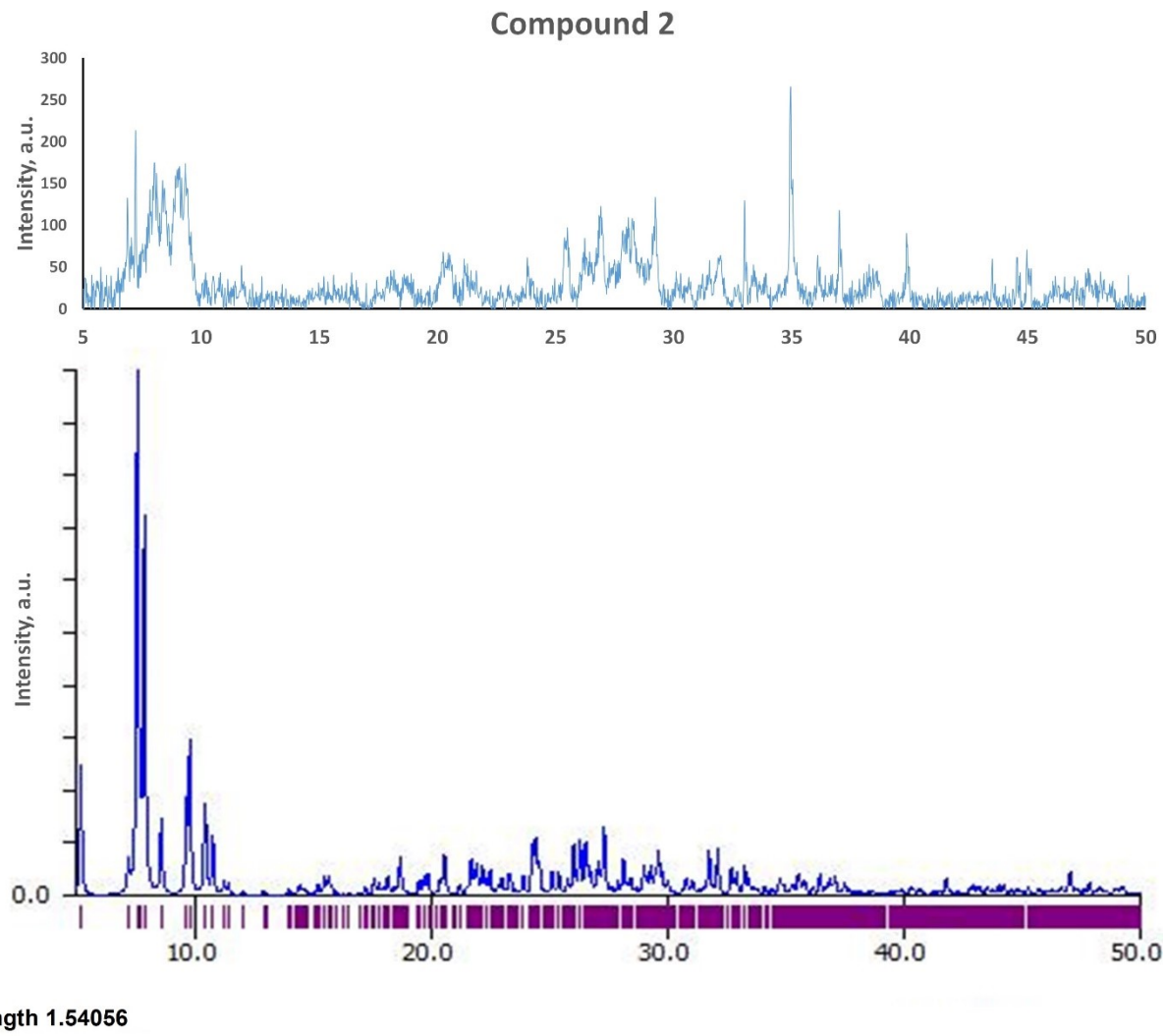

Figure S27. Experimental (above) and theoretically calculated powder patterns for compound **2**.

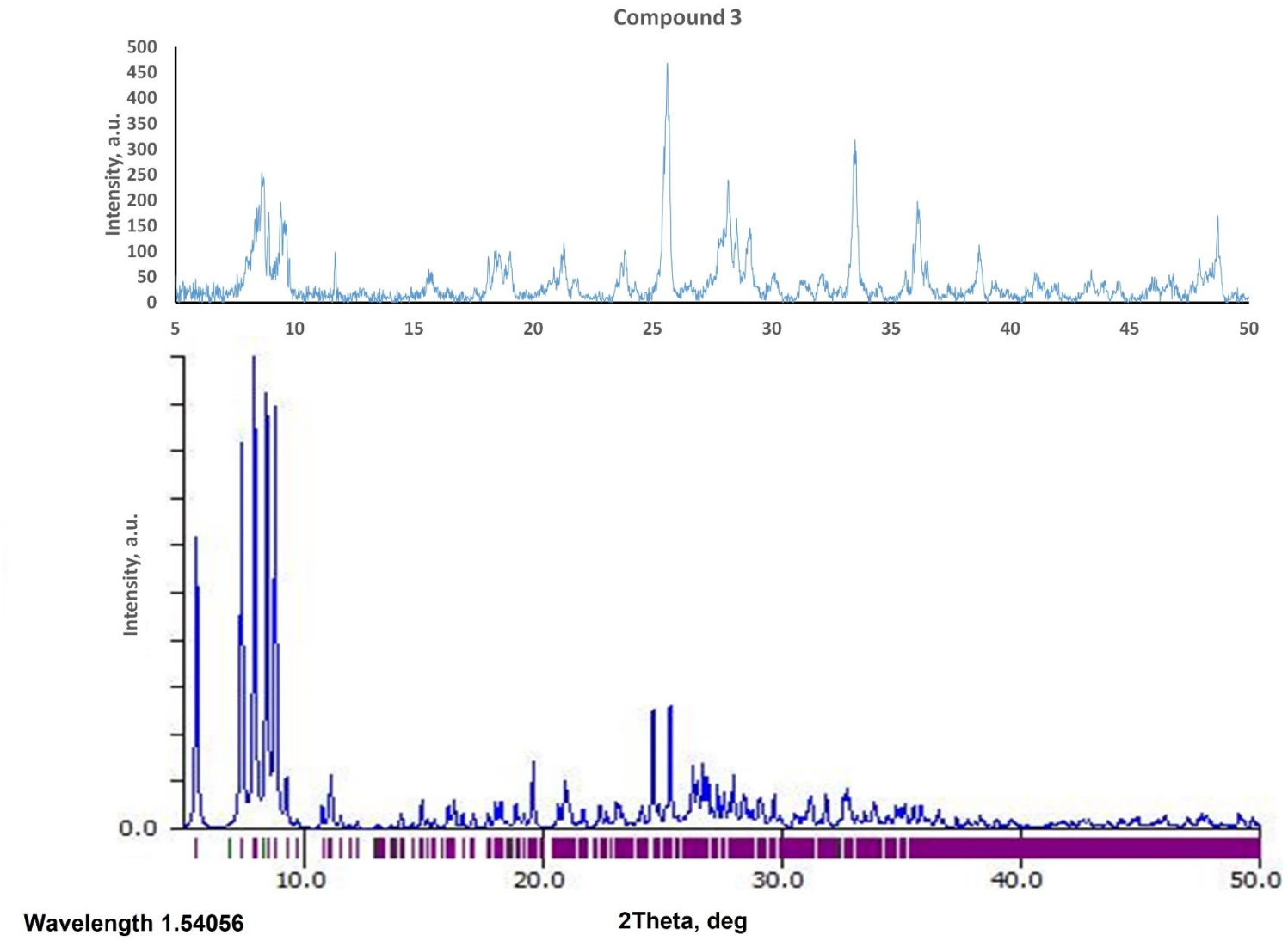

Figure S28. Experimental (above) and theoretically calculated powder patterns for compound **3**.

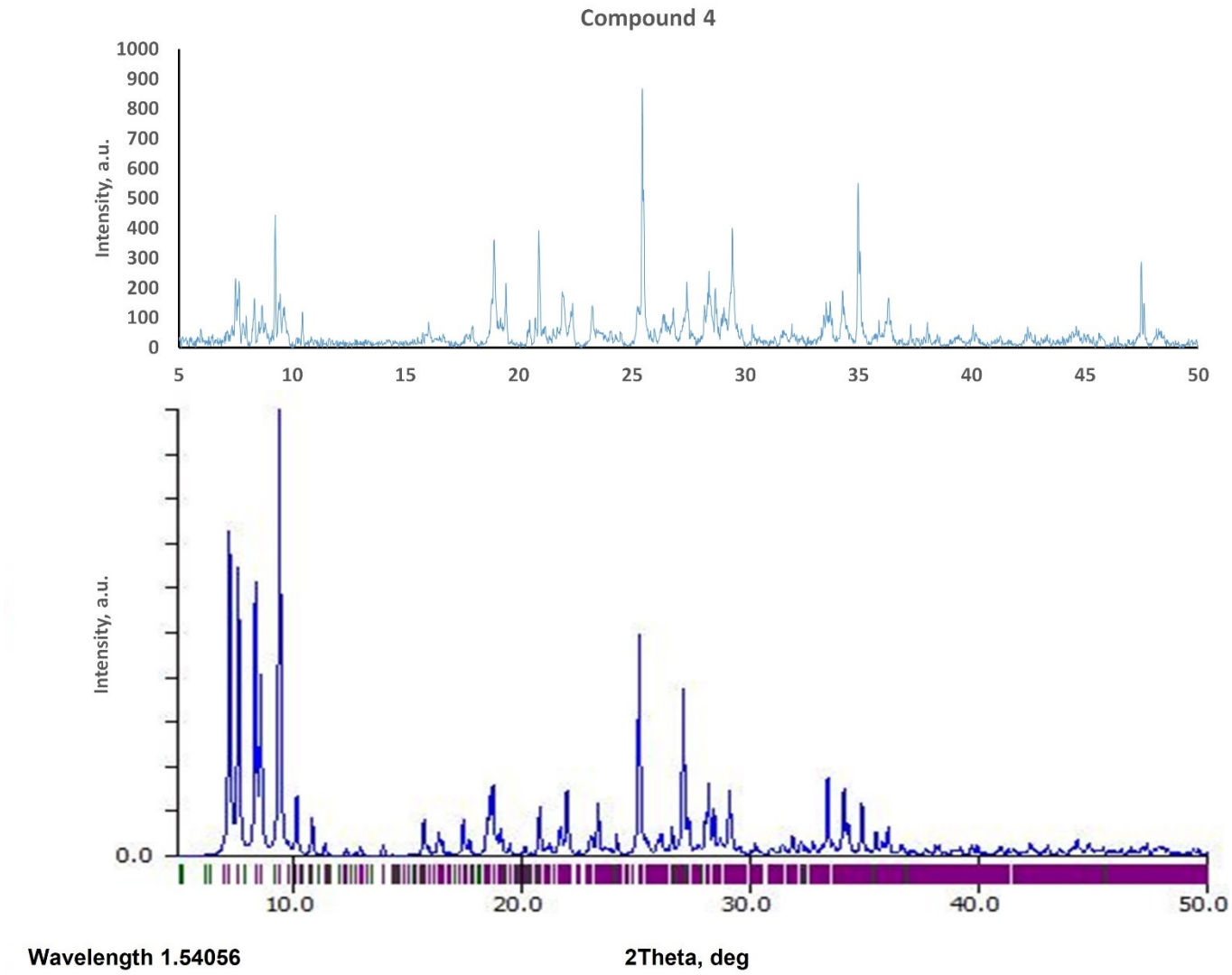

Figure S29. Experimental (above) and theoretically calculated powder patterns for compound **4**.

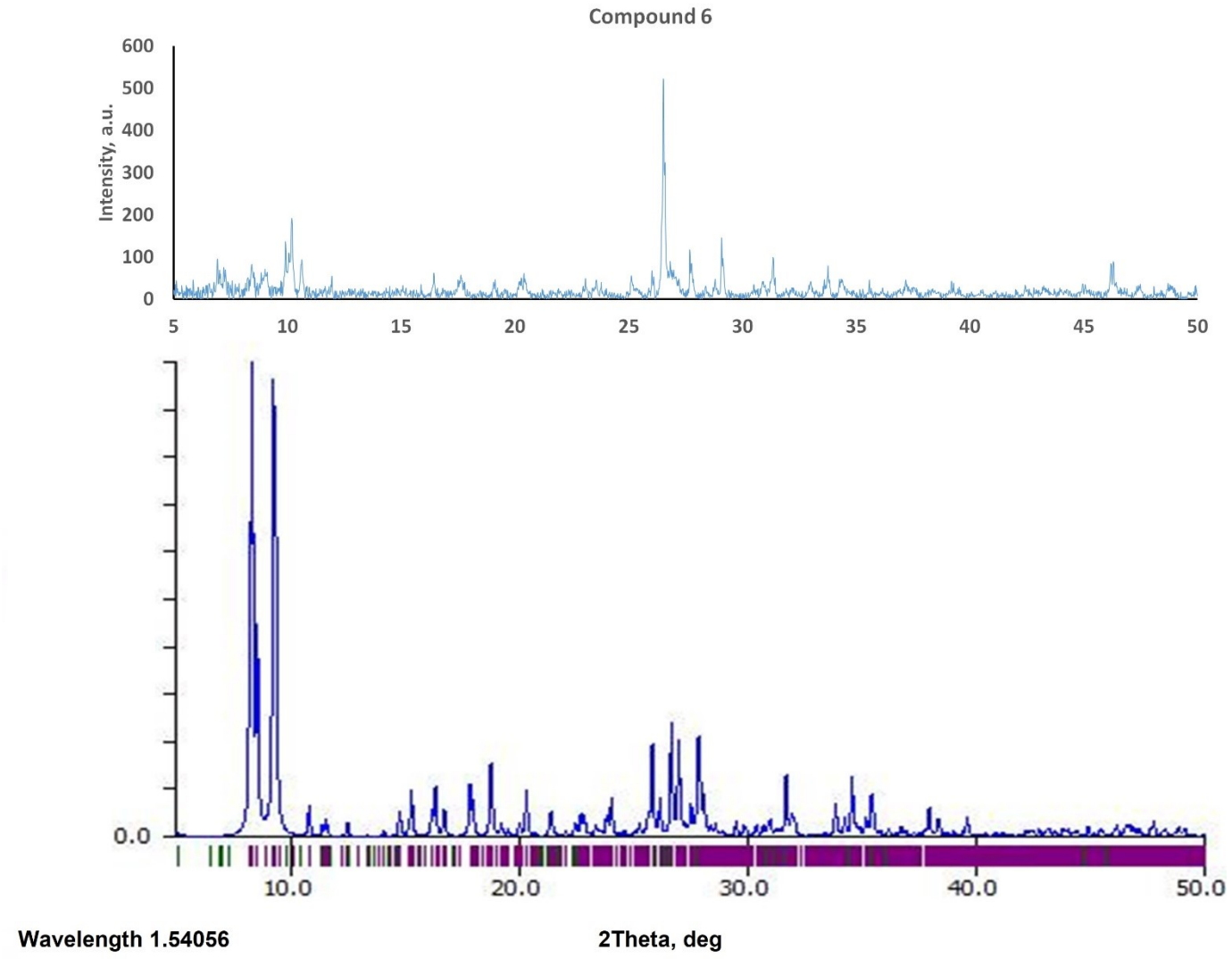

Figure S30. Experimental (above) and theoretically calculated powder patterns for compound **6**.

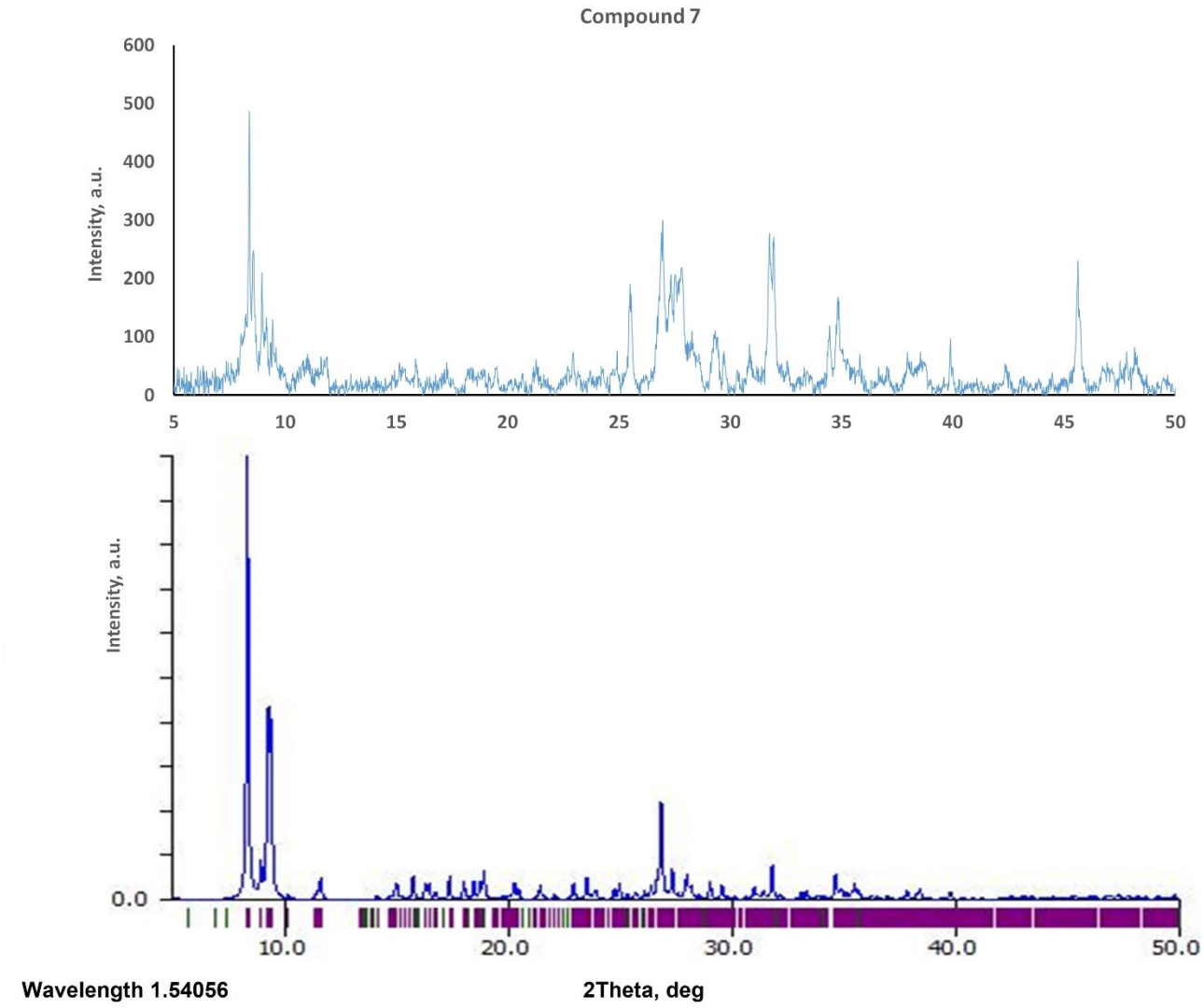

Figure S31. Experimental (above) and theoretically calculated powder patterns for compound **7**.