

TIHI Toolkit: A Peak Finder and Analyser for Spectroscopic Data

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Table S1: Performance comparison between *Tihi*, Spectragryph¹ and OriginPro² for the XRD spectrum of anatase.^{3,4} This table lists the experimental angles of incidence (θ), the angles detected by each tool, their absolute differences, and the percentage error relative to the experimental data. Missing data is indicated by asterisks (*). Abbreviations: Exp. for experimental, SG for Spectragryph.

Exp. Data	Tihi Results	Tihi Errors	SG Results	SG Errors	Origin Results	Origin Errors
25.23	25.24	0.01 (0.04%)	25.22	0.01 (0.04%)	24.08	1.15 (4.56%)
36.86	36.80	0.06 (0.16%)	36.83	0.03 (0.08%)	36.22	0.64 (1.74%)
37.72	37.66	0.06 (0.16%)	37.69	0.03 (0.08%)	37.96	0.24 (0.64%)
38.46	38.43	0.03 (0.08%)	38.43	0.04 (0.10%)	*	*
47.89	47.86	0.03 (0.06%)	47.85	0.04 (0.08%)	48.37	0.52 (1.09%)
53.77	53.70	0.07 (0.13%)	53.72	0.05 (0.09%)	53.57	0.20 (0.37%)
54.89	54.87	0.02 (0.04%)	54.85	0.05 (0.09%)	55.31	0.42 (0.77%)
61.92	62.02	0.10 (0.16%)	61.87	0.05 (0.08%)	60.51	1.41 (2.28%)
62.51	62.57	0.06 (0.10%)	62.46	0.06 (0.10%)	62.24	0.27 (0.43%)
68.59	68.59	0.00 (0.00%)	68.53	0.06 (0.09%)	*	*
70.05	70.24	0.19 (0.27%)	69.99	0.06 (0.09%)	70.91	0.86 (1.23%)
74.83	74.85	0.02 (0.03%)	74.76	0.07 (0.09%)	74.39	0.44 (0.59%)
75.78	75.54	0.24 (0.32%)	75.70	0.08 (0.11%)	76.12	0.34 (0.45%)
82.41	82.28	0.13 (0.16%)	82.33	0.08 (0.10%)	81.32	1.09 (1.32%)
82.87	82.52	0.35 (0.42%)	*	*	83.06	0.19 (0.23%)
Average Errors		0.09 (0.14%)	0.05 (0.09%)		0.60 (1.21%)	

Table S2: Performance comparison between *Tihi*, Spectragryph¹ and OriginPro² for the UV-Vis absorption spectrum of the petal tip of *Puya alpestris*⁵ flower. This table presents the peaks identified by Mizuno *et al.*,⁵ alongside the peaks detected by *Tihi*, Spectragryph and OriginPro, including their absolute differences and percentage errors relative to the experimental data. Missing data are indicated by asterisks (*). Abbreviations used: Exp. for experimental, SG for Spectragryph.

Exp. Data	Tihi Results	Tihi Errors	SG Results	SG Errors	Origin Results	Origin Errors
575	576	1 (0.17%)	*	*	535	40 (6.96%)
614	615	1 (0.16%)	610	4 (0.65%)	612	2 (0.33%)
679	675	4 (0.59%)	*	*	688	9 (1.33%)
Average Errors		2 (0.31%)	4 (0.65%)		17 (2.87%)	

References

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- (4) Horn, M. S. C. F.; Schwebdtfeger, C. F.; Meagher, E. P. Refinement of the structure of anatase at several temperatures. *Z. Kristallogr. Cryst. Mater.* **1972**, *136*, 273–281.
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