Table 4 | Computational cost and runtime (practicality) for MXene EIS fitting. Benchmark comparison of the three inference routes, classical nonlinear least squares (NLLS), continuous VQE/VQA (bounded decoding + COBYLA outer loop), and discrete QAOA (surrogate QUBO/Ising + γ–β search + best-shot decoding), reporting wall-time, number of objective evaluations, average time per evaluation, and sampling budget (shots = 4096 where applicable) in a fixed software/hardware environment (platform + Python/NumPy/SciPy versions and number of frequency points N). The table also summarizes scaling-relevant factors (e.g., O(N) circuit-model evaluation, dependence on angle-grid size for QAOA) and provides a practical breakdown highlighting the dominant QAOA costs from surrogate finite-difference construction, Ising-energy precomputation, and angle-evaluation/sampling.

Method	Algorithm	Wall-time (s)	Objective evals	Avg time / eval (s)	Shots	Key scaling	Notes	Breakdown
Classical NLLS	SciPy least_squares (TRF)	0.0139120839999691	6	0.002318680666661521	—	≈O(N_{freq}) per eval; convergence-dependent nfev	Deterministic baseline; direct complex residual fit	—
VQE/VQA (continuous)	COBYLA (bounded $u \in [0,1]^7$)	0.0100197649999813	53	0.0001890521698109691	4096	Hardware: O(shots·depth) per eval; here classical model O(N_{freq})	Continuous search; no discretization; optimizer settings affect n_{fev}	—
QAOA (discrete)	$p = 1$ + γ–β grid (25+81) + best-shot decode	269.58927698999923	99 (surrogate) + 106 (angles)	2.432 (per $\langle H \rangle$ eval)	4096	Angle-search ∝ #evals; qubits=7×bits; Δ sets local window	$\Delta = 0.08$; γ^*=2.8667, β^*=0.6676; reference implementation	Surrogate FD + energy precompute + 106 × $\langle H \rangle$ eval + sampling