

Supplementary Information for "Systematic Error Detection in the Database of Liquid Crystals (LiqCryst) Using Predictive Models"

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Table S1. Performance metrics for the three-class classification (achiral, chiral, and none) across individual LC phases.

Phases	N_V^a	accuracy [%]	recall	precision	F1 Score
N	18863	92.9	0.91	0.91	0.91
SmC	4382	96.8	0.82	0.84	0.83
SmF	266	99.8	0.73	0.82	0.77
Sml	233	99.7	0.72	0.74	0.73

^aThe numbers of molecules showing the specific phases.