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Artificial Neural Networks (ANNs) and Partial Least Squares (PLS) regression in the quantitative analysis of cocrystal formulations by Raman and ATR-FTIR spectroscopy

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Highlights

- Rational design of optimal ANN architecture is enabled by DOE.
- ANNs combined with ATR-FTIR spectroscopy showed improved fitting compared to Raman spectroscopy.
- ANN showed superior performance compared to PLS