

Accepted Manuscript

Title: 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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PII: S0731-7085(18)30801-X
DOI: <https://doi.org/10.1016/j.jpba.2018.06.004>
Reference: PBA 12008

To appear in: *Journal of Pharmaceutical and Biomedical Analysis*

Received date: 5-4-2018
Revised date: 1-6-2018
Accepted date: 2-6-2018

Please cite this article as: Barmpalexis P, Karagianni A, Nikolakakis I, Kachrimanis K, Artificial Neural Networks (ANNs) and Partial Least Squares (PLS) regression in the quantitative analysis of cocrystal formulations by Raman and ATR-FTIR spectroscopy, *Journal of Pharmaceutical and Biomedical Analysis* (2018), <https://doi.org/10.1016/j.jpba.2018.06.004>

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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

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