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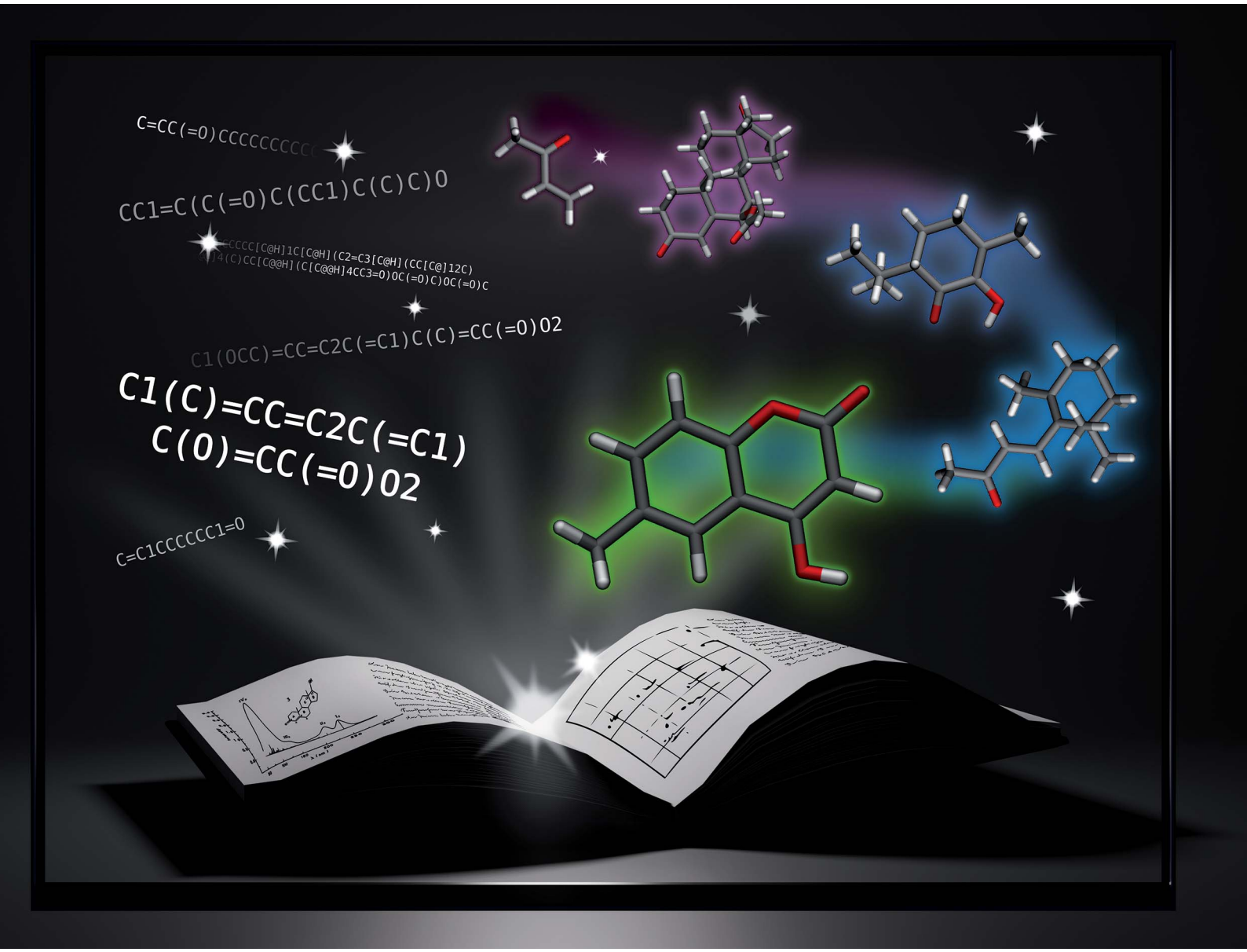
Digital Discovery

rsc.li/digitaldiscovery



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ROYAL SOCIETY OF CHEMISTRY

PAPER

Connor Forster and Carolin Müller

From handbooks to high-throughput: rule-based prediction of electronic absorption maxima from SMILES with ChromoPredict