



UNIVERSITY OF NAPOLI "FEDERICO II"

POLYTECHNIC AND SCIENCE SCHOOL

Department of Chemical Sciences

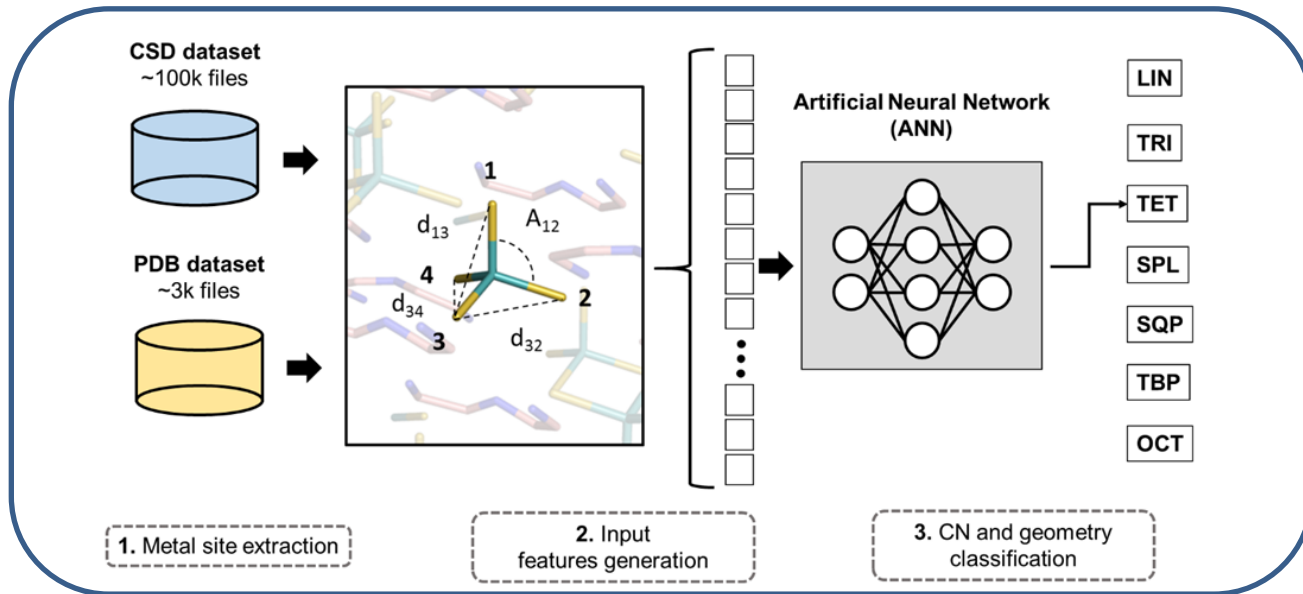
Ph.D. School in Chemical Sciences (XXXVII Cycle)



First year activity

Two artificial neural networks have been designed to perform coordination number and geometry classification of synthetic and biomolecular metal sites, obtained respectively from the CSD and PDB databases.

Ph.D. Student
Gianmattia
Sgueglia



Title:
Design of
modular
metalloenzymes
for sustainable
chemistry
through
machine
learning
techniques