






Supplementary information to:

Original article:

**MACHINE LEARNING APPROACHES TO STUDY THE STRUCTURE-
ACTIVITY RELATIONSHIPS OF LPxC INHIBITORS**

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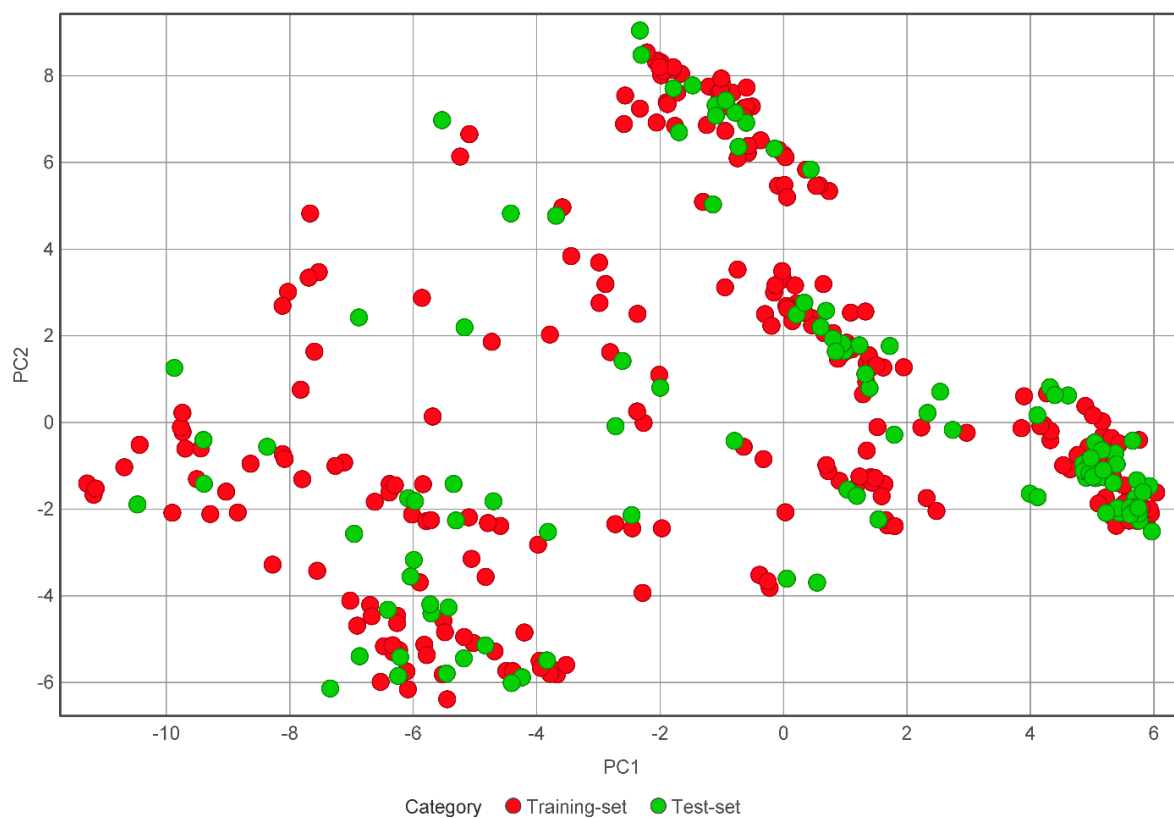
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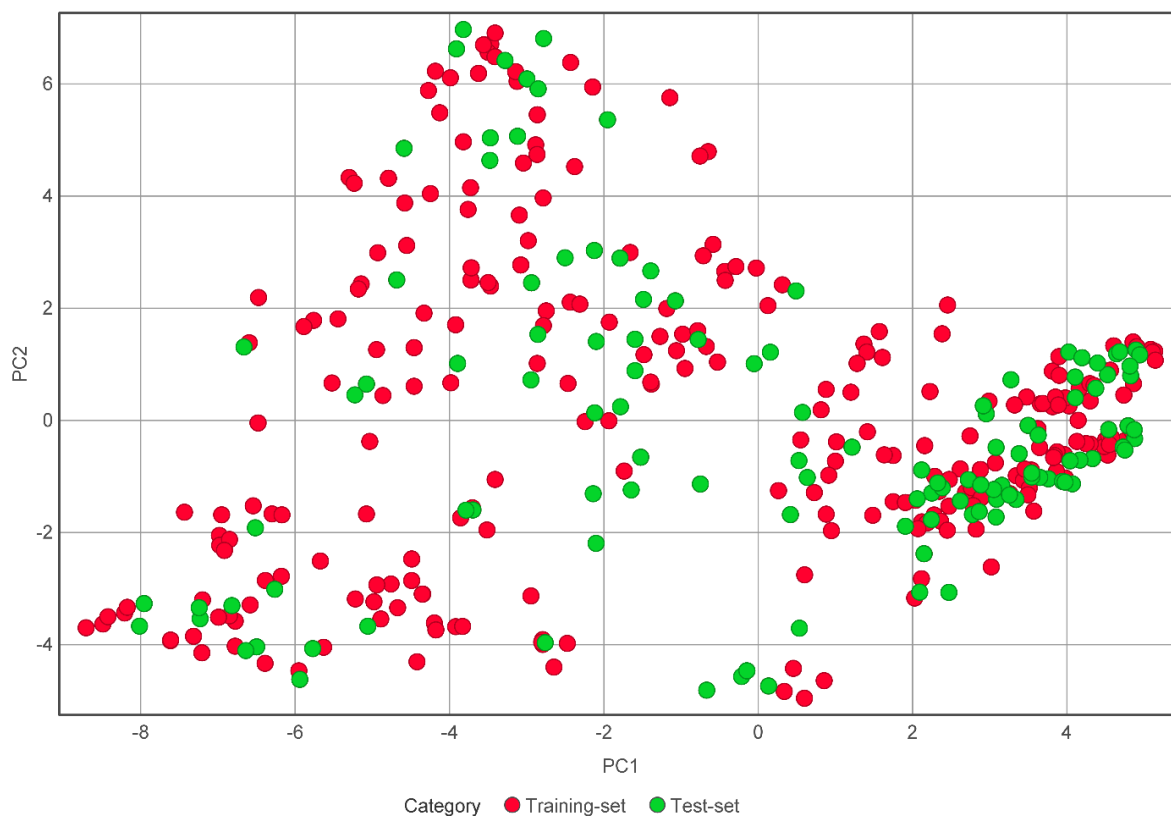
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<https://dx.doi.org/10.17179/excli2023-6356>

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Supplementary Figure 1A: Applicability domain illustration of models using PubChem fingerprint



Supplementary Figure 1B: Applicability domain illustration of models using MACCS fingerprint