The 2nd Joint Mini Workshop on Chemical Graph Learning

京都大学 総合生存学館 未来智慧研究会
京都大学 情報学研究科 離散数理研究室
京都大学 国際高等教育院 化学教室

京都工芸繊維大学
情報工学
視覚情報研究室

Quaid-i-Azam University Pakistan

日時 Time

15:30 - 19:00, Thu, Jan 30, 2025 (JST)

会場 Venue

Room 113, Higashiichijyou-Kan (京都大学東一条館)
Access: https://www.gsais.kyoto-u.ac.jp/access/

15:30 – 15:35, Opening Remark by Prof. Liang Zhao

Talk 1 15:35 – 16:00, 成田 光伸 (NARITA, Koshin), Fundamental Study on the Extraction of Common Substructures of Compounds through Fragmentation (Talk in Japanese)

Talk 2 16:00 – 16:25, 武木田 真生 (TAKEKIDA, Mao), An Experimental Comparison of Molecular Inference Frameworks: Generative AIs and mol-infer

Talk 3 16:25 – 16:50, 朱 見深 (ZHU, Jianshen), Towards Environment-Sensitive Molecular Inference via Mixed Integer Linear Programming

Break Time: 16:50 – 17:00

Talk 4 17:00 – 17:25, 李 楊和璞 (LI, Yanghepu), CRoCExplainer: A Tool to Explain Graph Learning with Improved Connectedness Representation

Talk 5 17:25 – 17:50, 左 振宇 (ZUO, Zhenyu), Automatic Identification of Significant Chemical Substructures with Graph Neural Networks

Break Time: 17:50 – 17:55

Talk 6 (online) 17:55 – 18:20, Kanwal Bibi, On the Prediction Performance of Random Forest for QSPR Using Mol-infer

Talk 7 (online) 18:20 – 18:45, Raveena Rai, From Single to Multi-Property QSPR: Evolving Mol-infer

18:45 – 19:00, Comments, ending Remark, and group photo

WWW https://aw.gsais.kyoto-u.ac.jp/activities/wcgl-20250130