講演会の御案内

Novel selective small-molecule inhibitors of C_4 photosynthesis: A structural and computational biology approach to combat C_4 weeds in arable crops

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日時　　平成 29 年 11 月 9 日（木）16 時～18 時
場所　　すずかけ台キャンパス　R1 棟　第三会議室

Weeds are a major challenge for global food production. Most weeds use C4 photosynthesis, whereas the majority of crops use the C3 photosynthetic pathway. Structural and biochemical studies in our lab have identified highly specific and selective inhibitors of C4 key enzymes Phosphoenolpyruvate Carboxylase (PEPC) and Pyruvate Phosphate Dikinase (PPDK) catalyzing essential reactions of the C4 photosynthetic pathway. Specific inhibitors for PEPC were identified in comparative docking studies on crystal structures of PEPCs from the C3 model Flaveria pringlei and the C4 model Flaveria trinervia [1-5]. Novel PPDK inhibitors were identified from screening of a chemical library [6] and recent structural studies on Flaveria PPDKs that identified novel conformational intermediates in the catalytic cycle of this intriguing molecular machine performing one of the largest single domain movements known today [7-8]. The compounds identified by our studies are among the most effective PEPC and PPDK inhibitors described today. Moreover, recent physiological studies on leaf tissues of a C4 model plant [6] and studies on whole plants [4] confirmed in vivo inhibition of C4 driven photosynthesis by these substances. Consequently, the novel small molecule inhibitors identified in in our structural and computational studies provide new lead structures for the development of selective herbicides and highlight novel modes of action against C4 weeds.

[1] Paulus, J.K.et al.(2013) Nature Communications 4:1518.
[2] Paulus, J.K., et al.(2013) Mol. Plant 6: 1996-1999.
[3] Paulus, J.K., et al. (2014) FEBS Lett. 588: 2101-2106.
[4] Nguyen, G.T.T., et al. (2016) Sci. Rep. 6: 27333. doi: 10.1038/srep27333.
[5] Dick, M., et al. (2017) FEBS Lett. doi: 10.1002/1873-3468.12842.
[6] Minges, A. and Groth, G. (2017) PLoS ONE 12:e0181139. doi:10.1371/journal.pone.0181139.
[7] Minges, A.et al.(2017) Sci. Rep. 7: 45389. doi: 10.1038/srep45389.
[8] Minges, A.et al. (2017) Protein Science 26:1667-1673. doi:10.1002/pro.3184.

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