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Rational drug design in photopharmacology

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Stellingen

Behorende bij het proefschrift
Rational drug design in photopharmacology
door
Piermichele Kobauri

1. After showing numerous proof-of-concept studies, photopharmacology should now aim at applications in real-world scenarios by attracting pharmaceutical industry's attention.
2. Explicitly declared "hopes" are hardly valid scientific hypotheses. The photopharmacology community could use more appropriate terms, such as "working hypotheses" or "educated guesses". Alternatively, we can introduce the neologism "hopethesis".
Angew. Chem., Int. Ed., 2013, **52**, 9845–9848 and *ACS Med. Chem. Lett.*, 2019, **10**, 1341–1345
3. Electronic differences between (*E*)- and (*Z*)-azobenzene offer underexplored opportunities for molecular design in photopharmacology.
Chapter 3 and 4
4. Docking scores cannot be treated as a meaningful approximation of binding free energies.
J. Am. Chem. Soc., 2021, **143**, 736–743
5. Chemistry, and science in general, would greatly benefit from closer collaborations between experimentalists and theorists, instead of sterile superiority claims and constant skirmishes.
6. Research groups pay a publication fee to publish articles, whose access requires a costly subscription paid by universities. In the reviewing process, referees work on a voluntary basis, while all the profit goes to publishing companies. Inexplicably, there are only limited collective movements in academia that fights such unfair practice.
7. It is more valuable to have an idea about why something is not working as expected than to have no idea about why something works.
8. Computational drug design not only saves time and money in the early stages of drug discovery, but it can also make the pharmaceutical industry more sustainable, thereby helping in the fight against global warming.
9. Workaholicism should not be praised as it currently – and toxically – is in academic settings. Negligence of work-life balance in academia is a serious threat to the mental health of too many researchers in academia.
Nat. Biotechnol., 2018, **36**, 282–284
10. To counteract the ongoing reproducibility crisis in science, it is necessary to dedicate more laboratories around the world to the replication and validation of scientific results, following the example of the Center for Open Science. In an ideal evolution of the current publishing process, peer review could be expanded with concomitant peer replication.
eLife, 2021, 10:e67995

11. On closer inspection, photopharmacology is a form of molecular enlightenment.
12. Scientific writing tends to be uncreative and repetitive. Short sentences are clear yet boring.
13. Every chemical reaction is a nanoscopic choreography, in which molecules are the dancers, temperature is the rhythm, and the solvent is the dance floor.