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Computational studies of influenza hemagglutinin

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Propositions

accompanying the dissertation

COMPUTATIONAL STUDIES OF INFLUENZA HEMAGGLUTININ. HOW DOES IT MEDIATE MEMBRANE FUSION?

by

Sander Boonstra

1. To enable a quantitative comparison of membrane-fusion energy barriers between different assays, a collaborative approach is needed, involving experimental and computational studies that use the same system parameters. (Chapter 2)
2. In molecular dynamics simulations, a small change in the water model, not significantly influencing bulk water properties, can have a dramatic effect on peptide folding characteristics. (Chapter 3)
3. A network of salt bridges in the globular bottom of hemagglutinin governs its stability against mechanical unfolding. (Chapter 4)
4. The amount of free energy that each hemagglutinin can contribute to membrane fusion is $34 k_B T$. (Chapter 5)
5. When curing diseases, measures to reduce overpopulation become disproportionately more important.
6. Climate change, overpopulation and urbanization, factors that cause the ongoing destruction of flora and fauna, are driven by the trend to maximize economic or personal gain and can therefore only be fought effectively by governmental interference, through world-wide regulations and international collaboration.
7. Overzealous teachers make lazy students; efficient education means teaching just enough.

Stellingen

behorende bij het proefschrift

COMPUTATIONAL STUDIES OF INFLUENZA HEMAGGLUTININ. HOW DOES IT MEDIATE MEMBRANE FUSION?

door

Sander Boonstra

1. Om activeringsenergieën uit verschillende studies van membraanfusie kwantitatief te kunnen vergelijken is meer samenwerking nodig, zodat de parameters van zowel experimentele als rekenkundige onderzoeken op elkaar kunnen worden afgestemd. (Hoofdstuk 2)
2. In moleculaire dynamica simulaties kan een kleine verandering in het gebruikte watermodel, waarbij de bulkeigenschappen van het water niet significant veranderen, een dramatisch effect hebben op de structurele eigenschappen van peptides. (Hoofdstuk 3)
3. Een netwerk van zoutbruggen reguleert de stabiliteit van de bolvormige onderkant van hemagglutinine tegen mechanisch ontvouwen. (Hoofdstuk 4)
4. De hoeveelheid vrije energie die beschikbaar is voor membraanfusie is $34 k_B T$ per hemagglutinine. (Hoofdstuk 5)
5. Met het genezen van ziekten worden maatregelen om overbevolking te verminderen onevenredig veel belangrijker.
6. Klimaatverandering, overbevolking en verstedelijking, factoren die de voortdurende vernietiging van flora en fauna veroorzaken, worden gedreven door de trend om economisch of persoonlijk gewin te maximaliseren en kunnen daarom alleen effectief worden bestreden door de inmenging van overheden, met wereldwijde regelgeving en internationale samenwerking.
7. Studenten worden lui van overijverige docenten; om efficiënt les te geven moet je het doceren doseren.