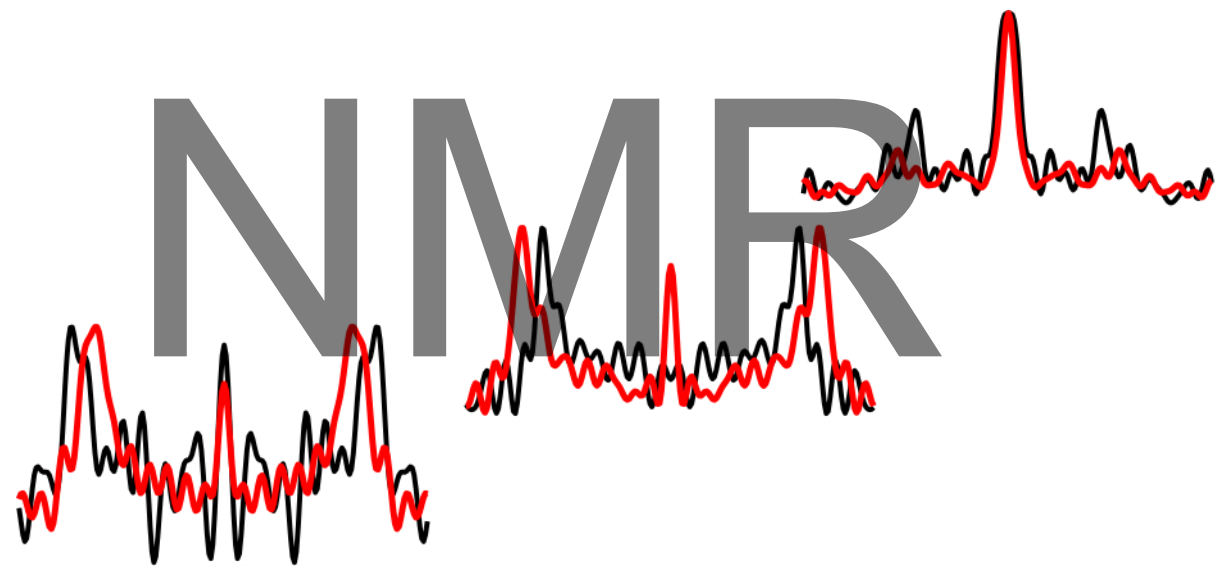
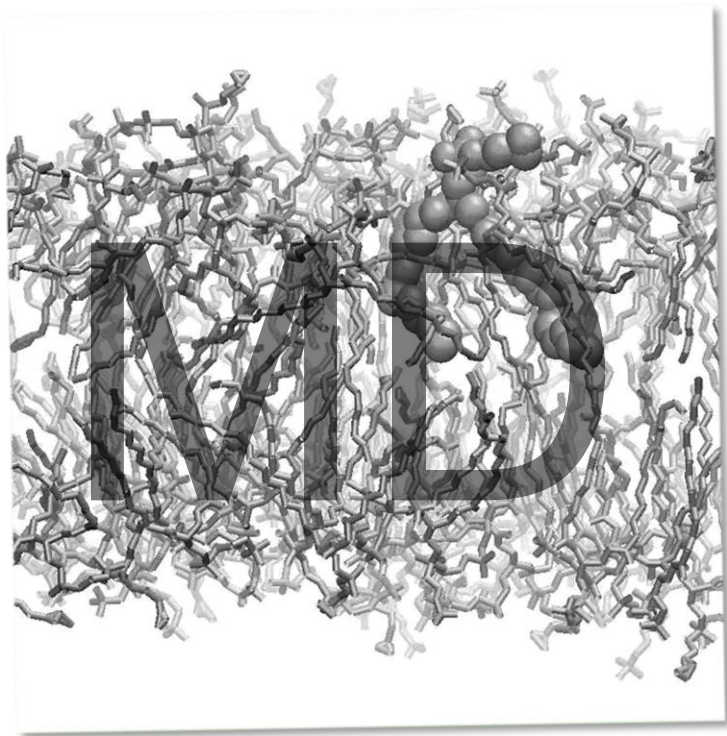


High-fidelity Biomolecular Modelling



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Nov 25th 2024

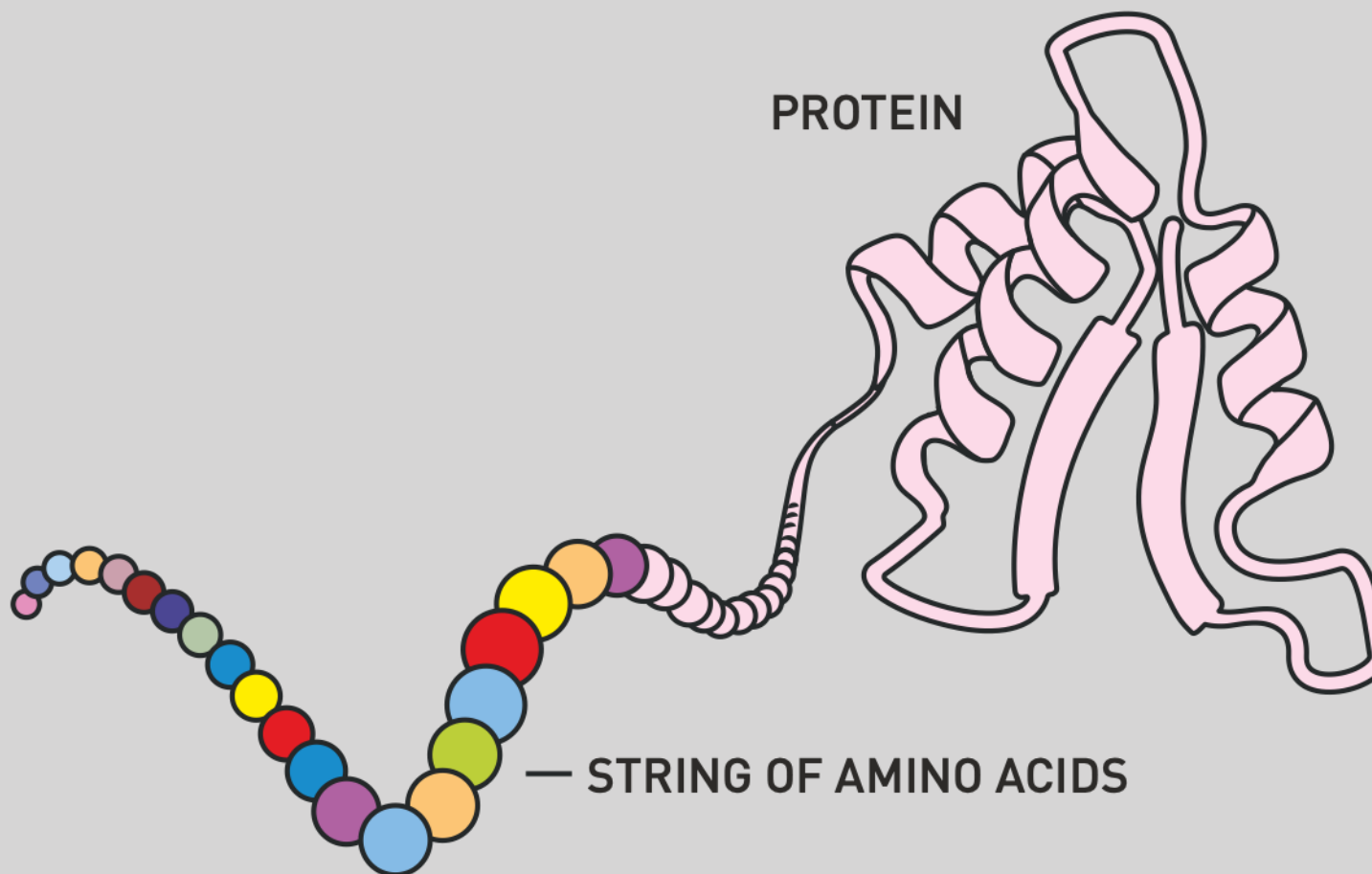


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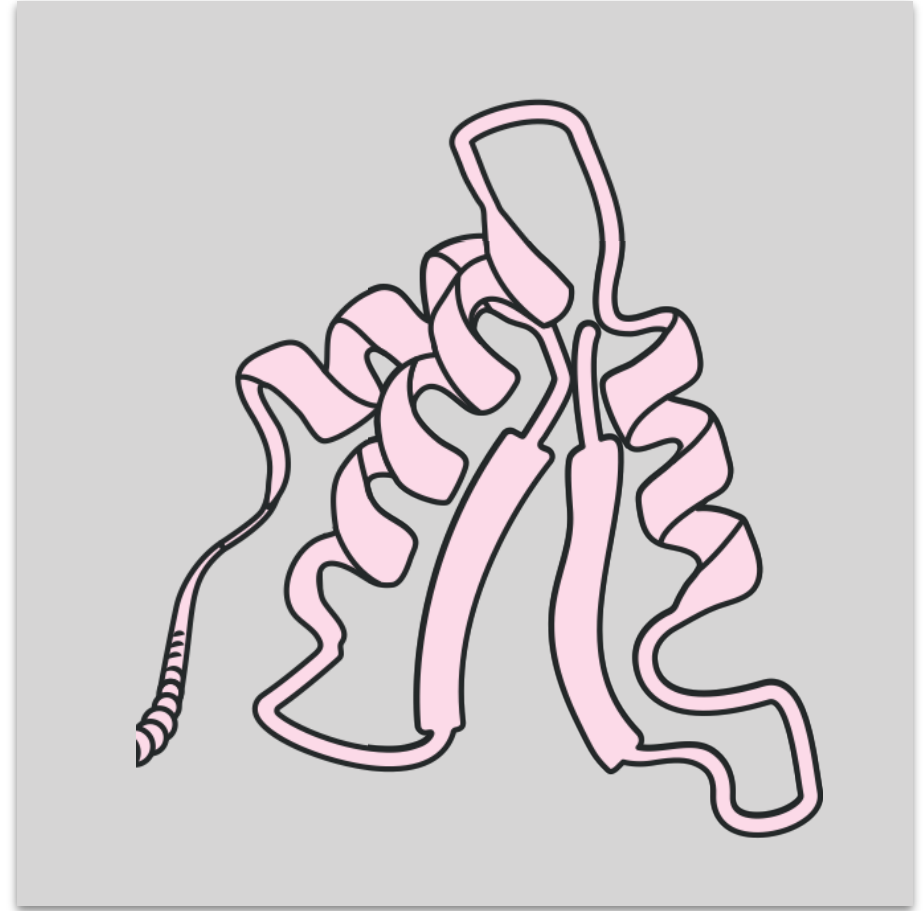
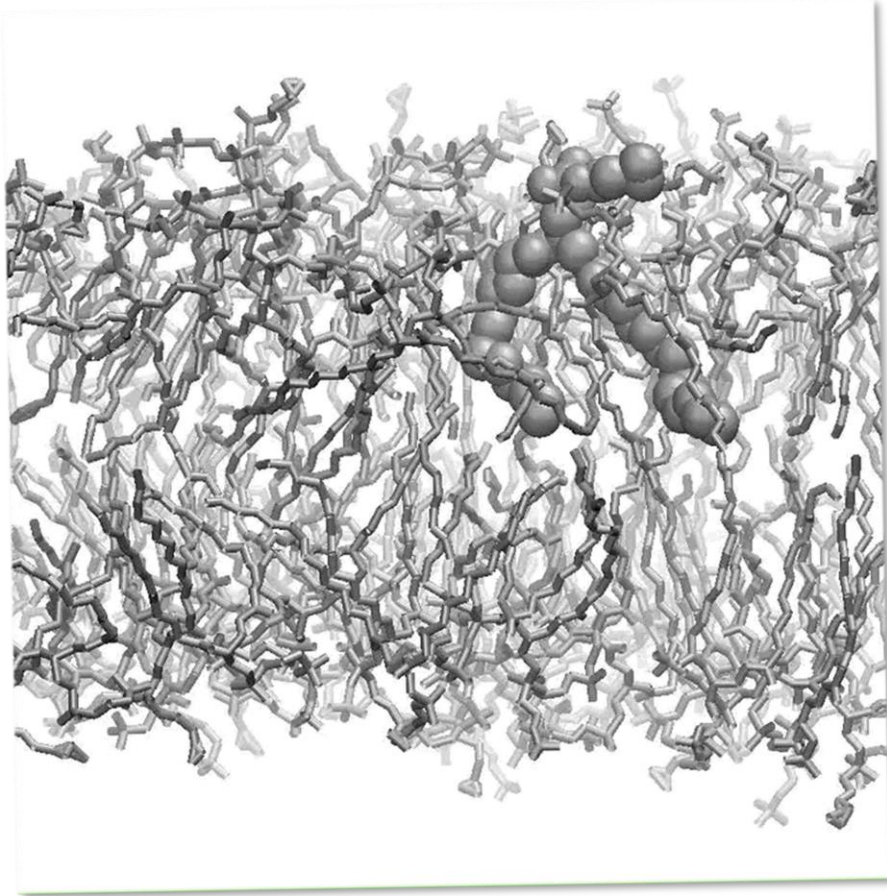
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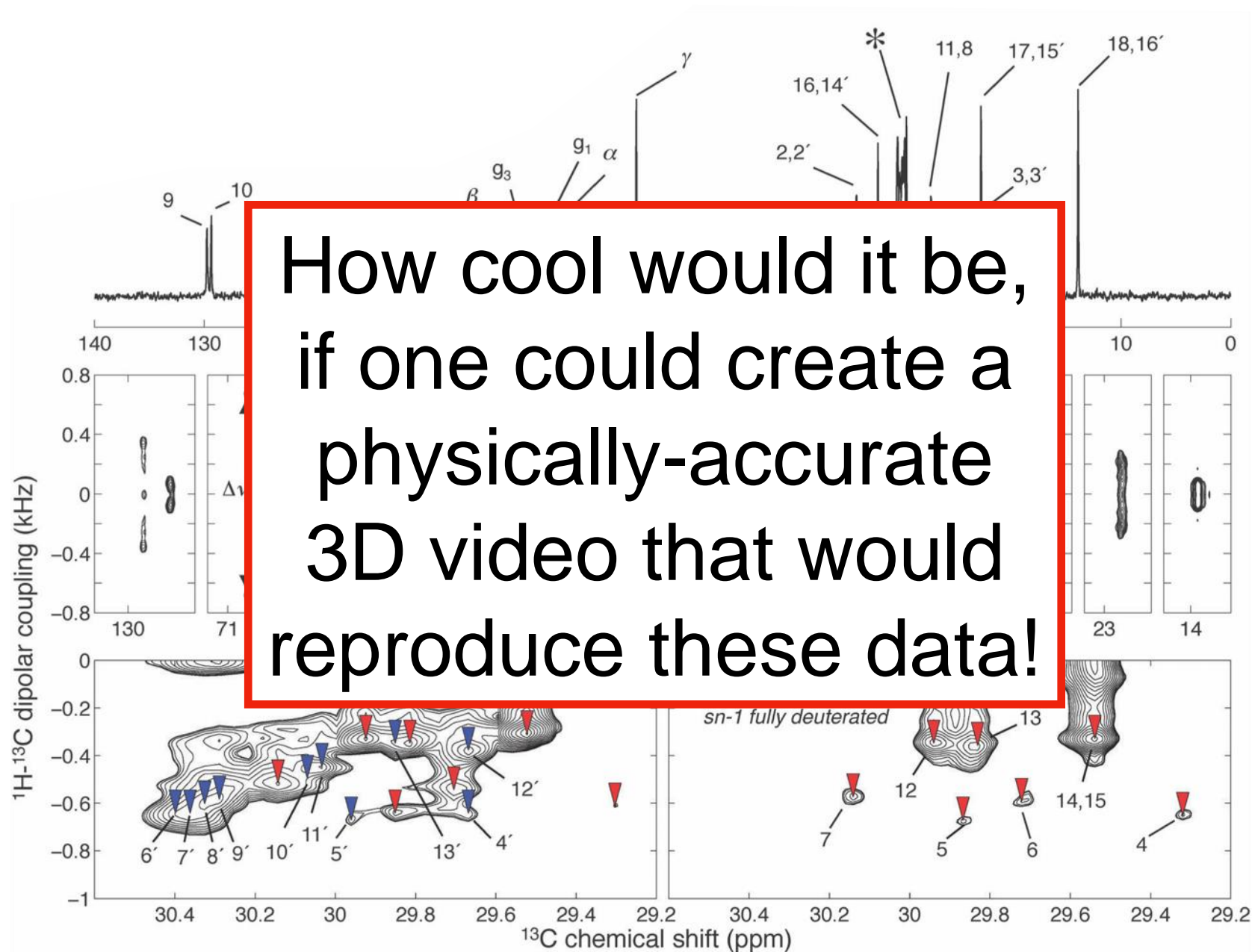
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“for protein **structure** prediction”

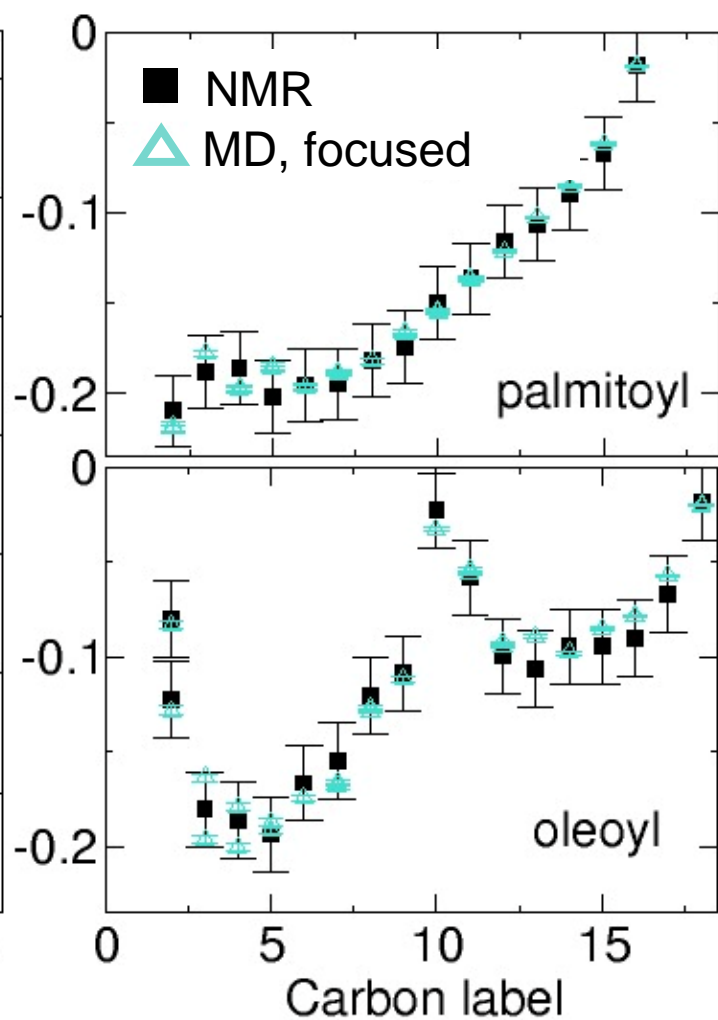
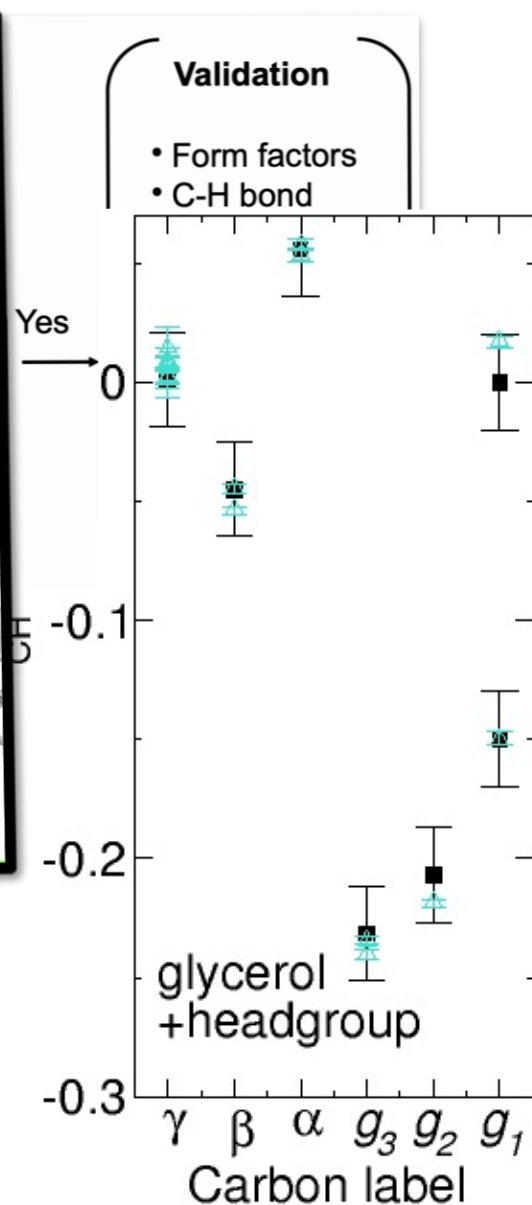
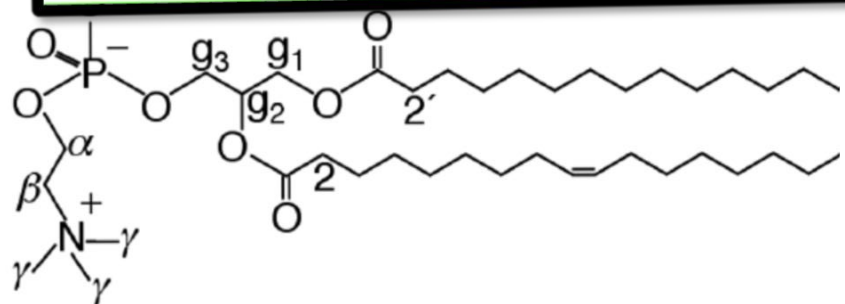
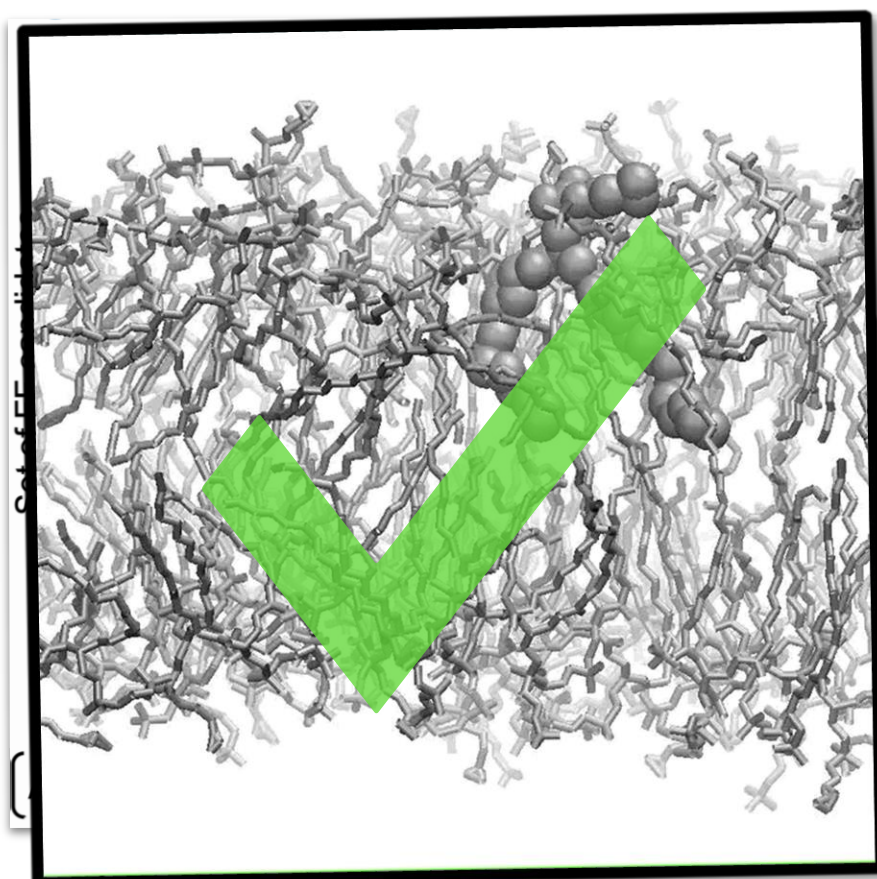
But how about motion?



NMR experiments detect such motion...
but the data are far from intuitive



“Autofocused” MD simulations



Take home

1

NMR provides ample high-precision data on the dynamics of biomolecules.

2

We can “autofocus” all-atom MD simulations to reproduce these NMR data.

3

NMR + autofocused MD
= Ångström-resolution microscopy

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