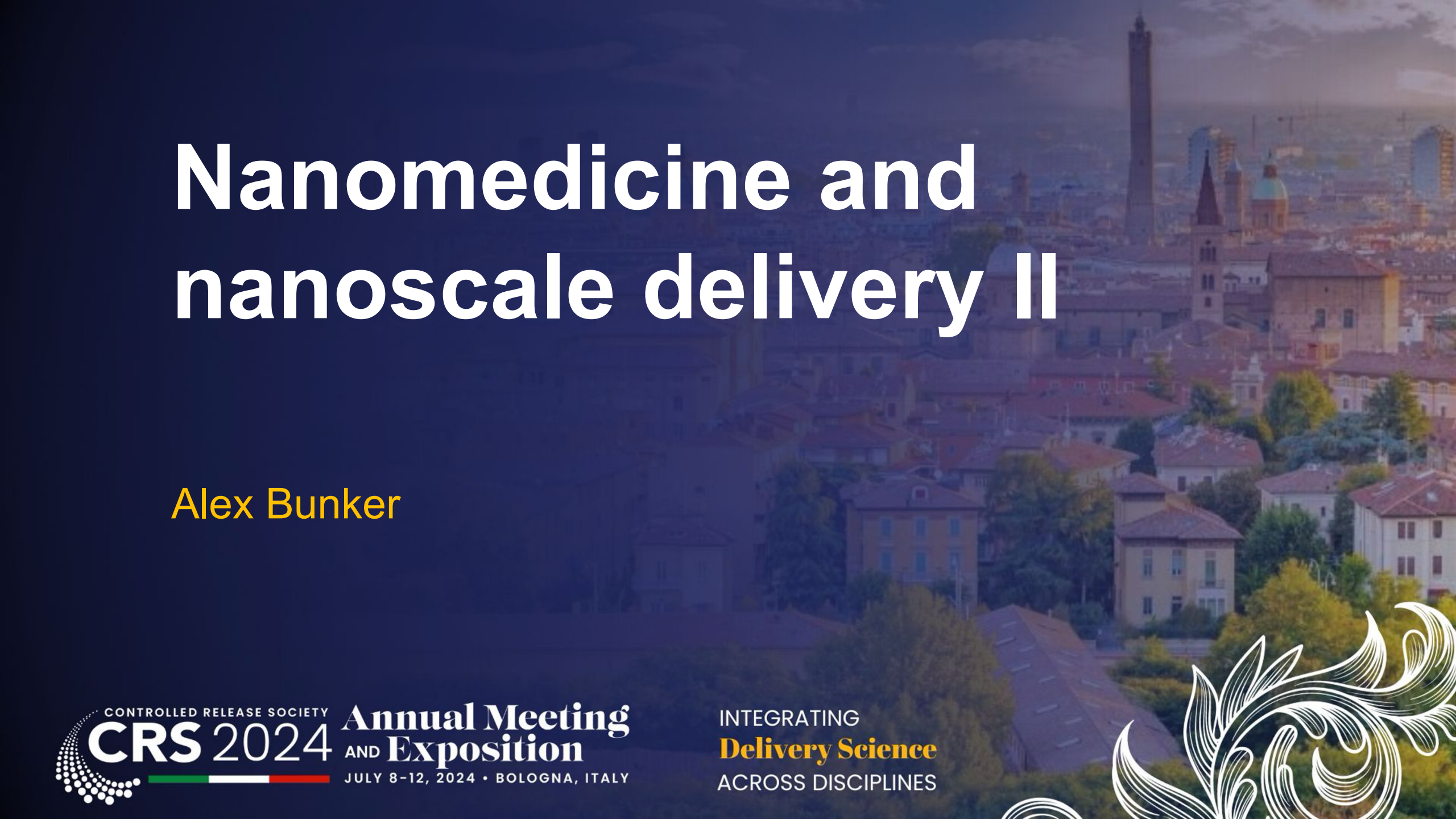
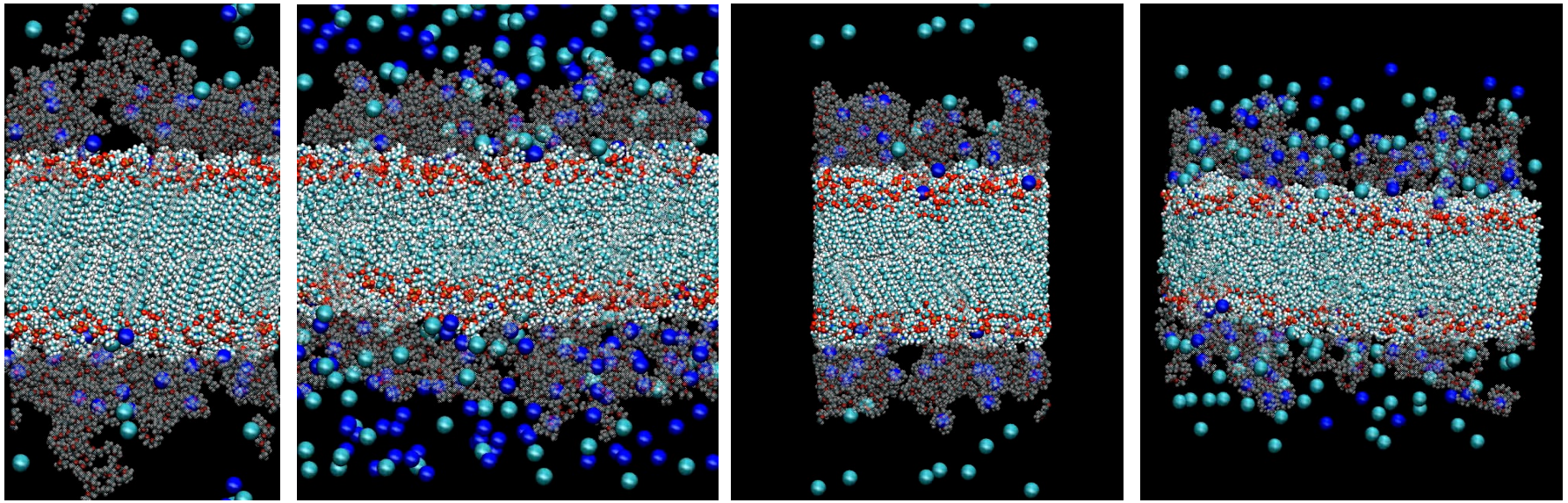
Nanomedicine and nanoscale delivery II

Alex Bunker



CRS2011 in National Harbor, USA…

- I presented my first work in this journey:
  - Molecular dynamics (MD) simulation of lipid membranes
  - mature tool in biophysics → drug delivery liposome development
  - PEGylated membrane → Doxil formation
  - Looked at formulation, targeting ligands, drugs in membrane…

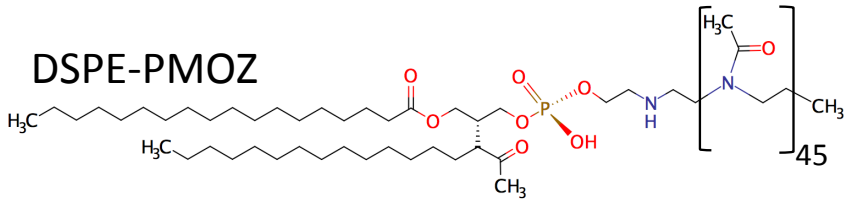


- PEG gold standard but not perfect
  - Active search for alternatives
  - Our start was developing mechanistic understanding of PEG
  - One very promising avenue is oxyzene-oxazoline scaffold

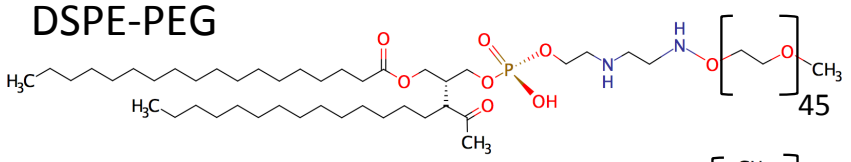
Polymer coatings other than PEG

- Oxazoline-oxyzene scaffold is very promising
- Modelled liposome membranes with poly eth- and poly methoxazoline

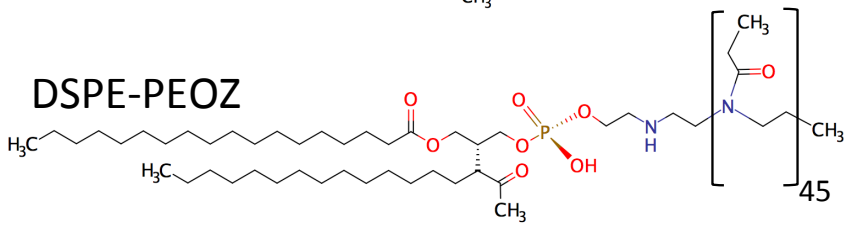
DSPE-PMOZ

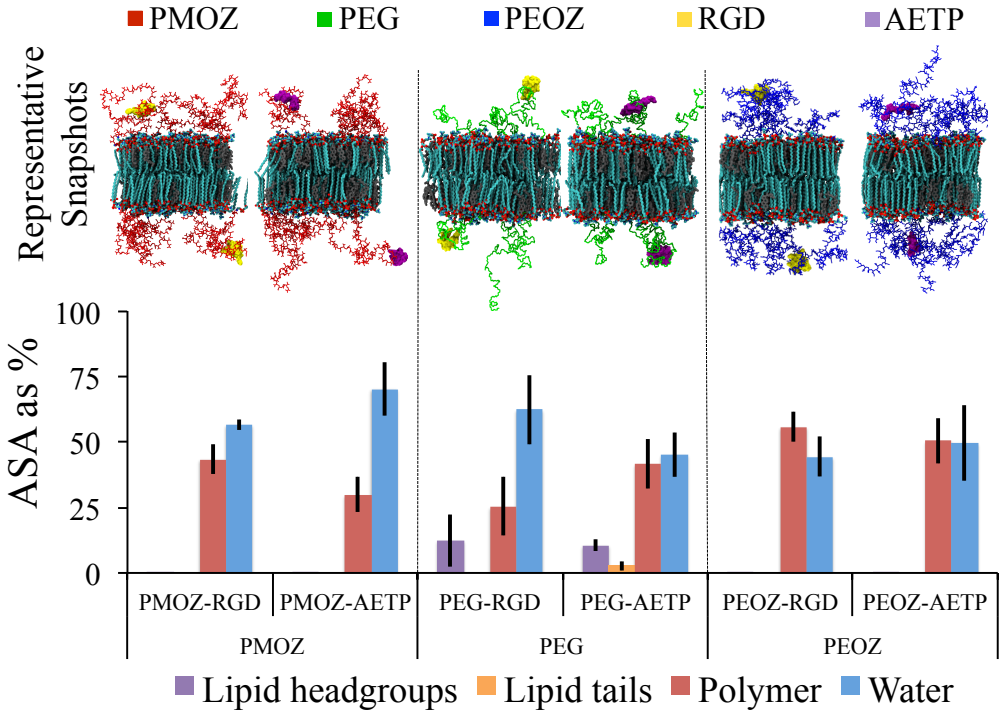


DSPE-PEG



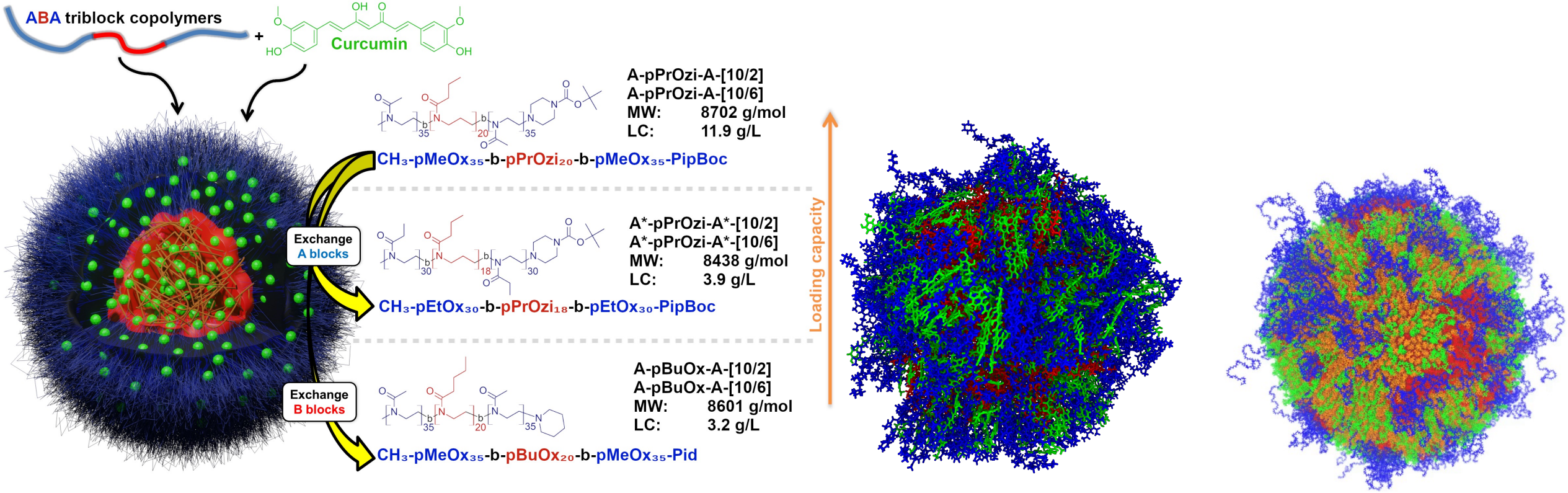
DSPE-PEOZ





And nanoparticles other than liposomes

- And we have gone on to simulate:
- Polymeric micelles and lipid nanoparticles
- Used both MD and machine learning for design of polymeric micelles
- Lipid nanoparticle simulation requires pre-exascale GPU resourcs



Pharmaceutical Biophysics group:

THANK YOU!!

References:

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