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Structure Detail Resolution of Pharmaceutical Drug Carriers by Contrast Variation: Deuterium-SANS and (A)SAXS

Pharmaceutical nanocarriers are complexes composed of frame materials, e.g. lipids or polymers, and medically active materials, such as bio-chemical drugs or biological agents, e.g. proteins or mRNA. The structure is the key to the medical application and safety. The formulation depends on the application pathway, which may be oral (tablets, capsules), pulmonary (inhalation), intramuscular (tissue injection), parenteral (blood injection), or intracranial (brain injection). Success, patient security and structure issues increase in this sequence.

The structure determination by solution scattering and imaging of neutrons and synchrotron X-rays is enforced by specific component labeling by contrast variation, i.e. deuteration in SANS, magnetic material scattering, or heavy metal scattering, absorption and fluorescence (ASAXS, imaging), in combination with DLS as µm size range extension. The neutron contrast variation of pharmaceutical and bio-medical samples in solution follows two strategies: solvent deuteration, mostly with D2O, or material deuteration, e.g. of lipids, proteins or mRNA.

We have investigated the structure and development of pharmaceutical nanocarriers in original form (static) and upon simulated application (dynamic, space-time resolved) by contrast labeling via selective deuteration and lanthanide complexes. The studies were done by SANS (ILL-D11, MLZ-KWS2), and SAXS, ASAXS (DESY-EMBL-P12, ESRF-ID01, BESSY-SAXS-9T) with lipid and polymer frame carriers and surface modification by an artificial protein shell for specific bio-targeting, e.g. in cancer therapy. The application of the complementary neutron and synchrotron X-ray methods combines the detection of deuterated lipids and mRNA without radiation damage with high resolution scattering, focusing and flux.

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