Analysis of vesicular medicines structure by small-angle X-ray scattering

V.A. Chausova, A.V. Shulenina, G.S. Peters, Yu.A. Tereshkina,
E.G. Tikhonova, P. Selyshchev, M.A. Kiselev

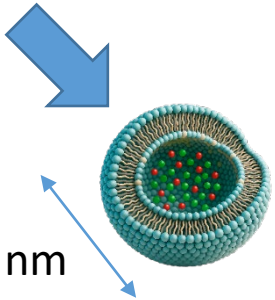
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Subject:

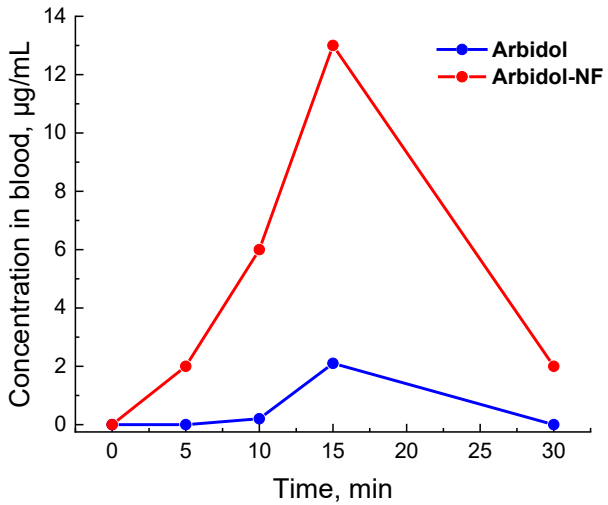


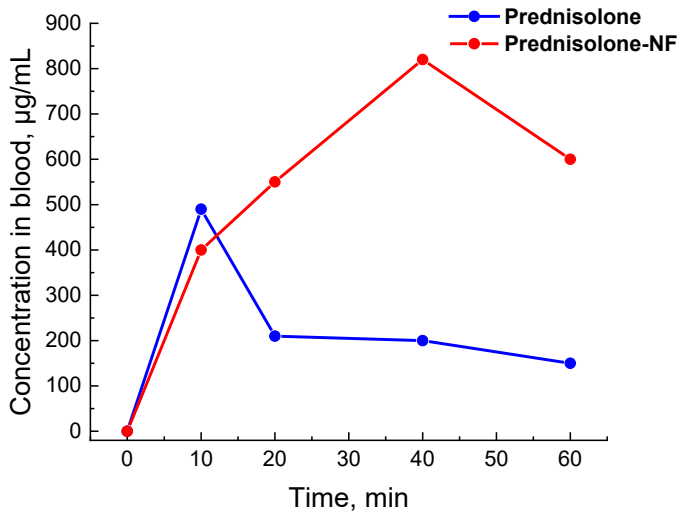


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30-40 nm

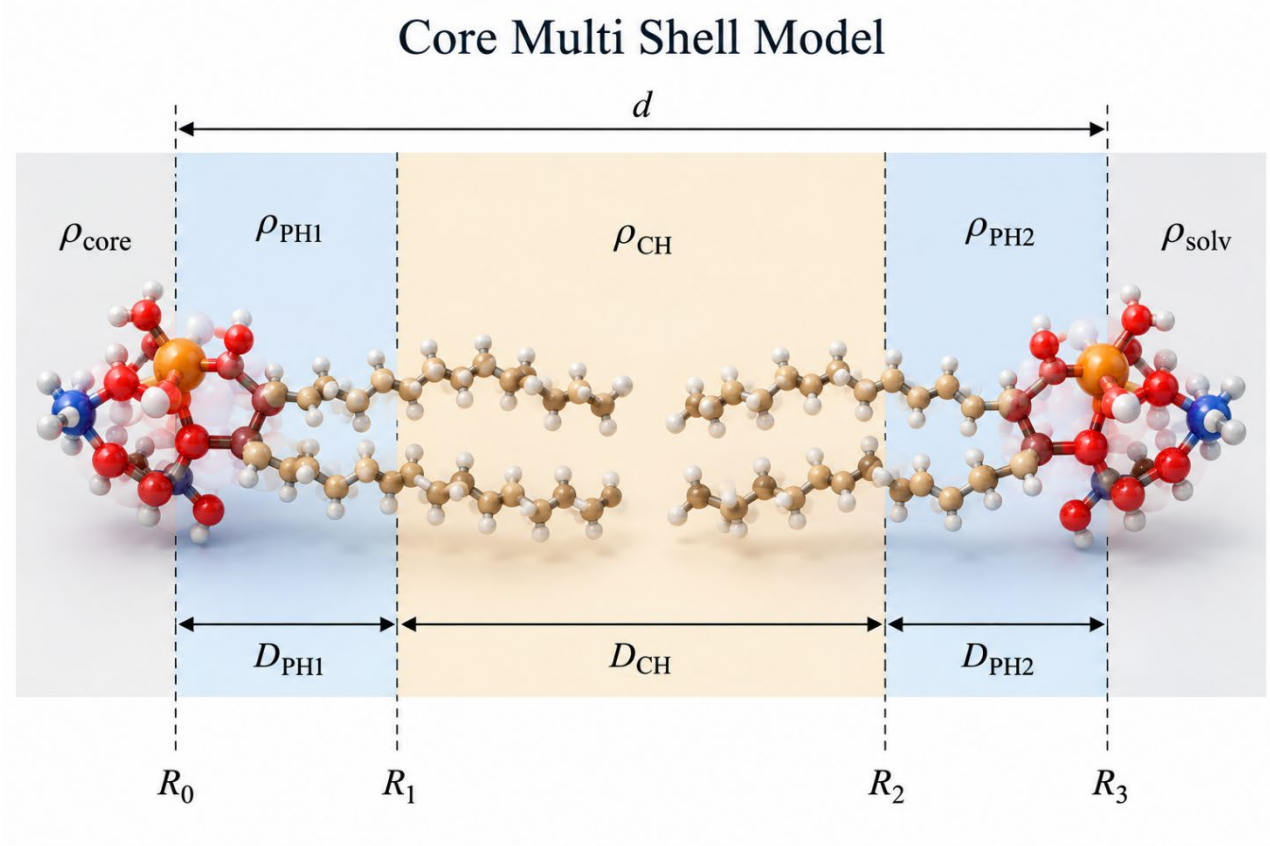




Changes in arbidol and prednisolone levels in rat blood after oral administration «NANOSYSTEM FOR DRUG TRANSPORT BASED ON PHOSPHOLIPIDS» (ibmc.msk.ru)

Key idea: determination of the structure of the "phospholipid transport nanosystem + biologically active substance" system and establishment of the relationship between system composition and structural features

Method:



ρ_{core}, ρ_{solv} – scattering length density (SLD) in core and solvent

ρ_{PH}, ρ_{CH} – SLD values in the hydrophilic heads and hydrophobic tails regions

R_0 – inner radius

Samples:



Vitaphospholip
Berberine-NF
Arbidol-NF

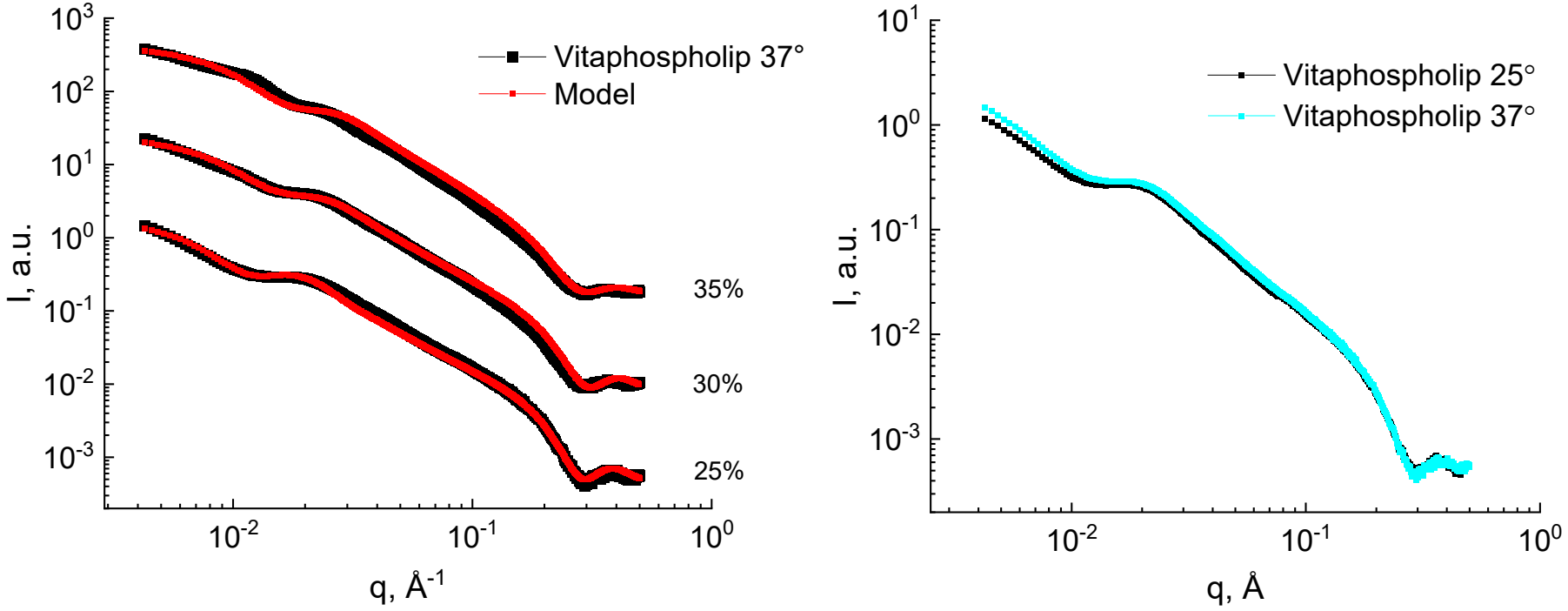
S80 phosphatidylcholine content ≈ 73–79%



Arbidol-NF

S100 phosphatidylcholine content ≈ 94%

Vitaphospholip:

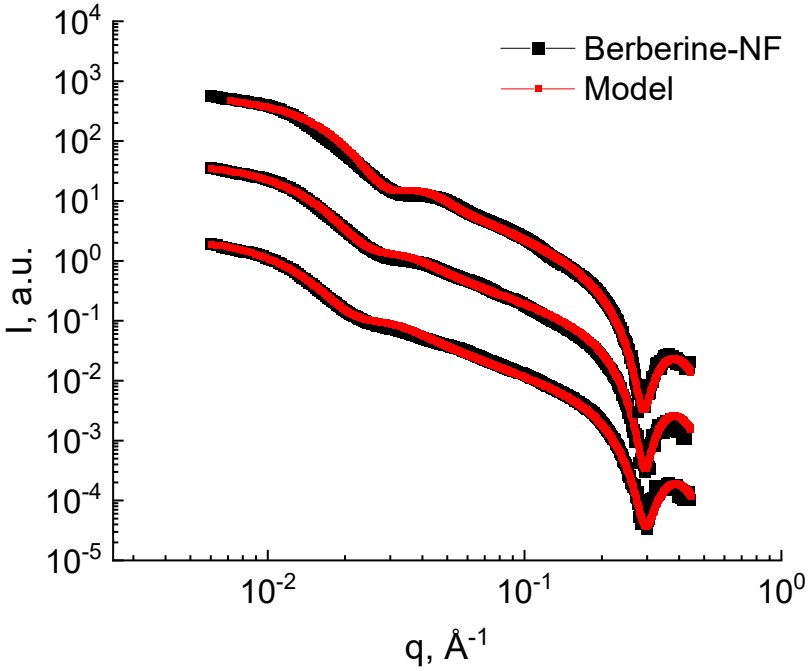


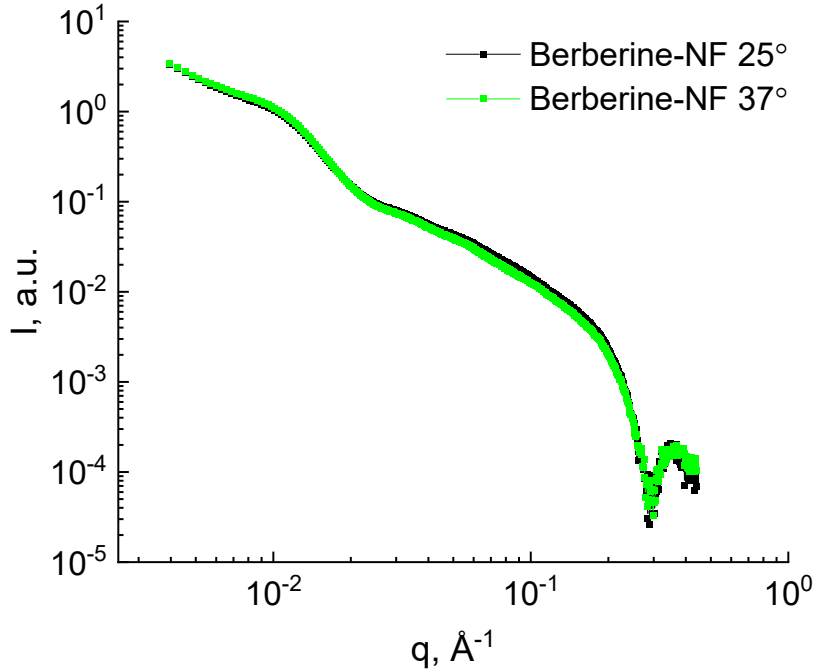


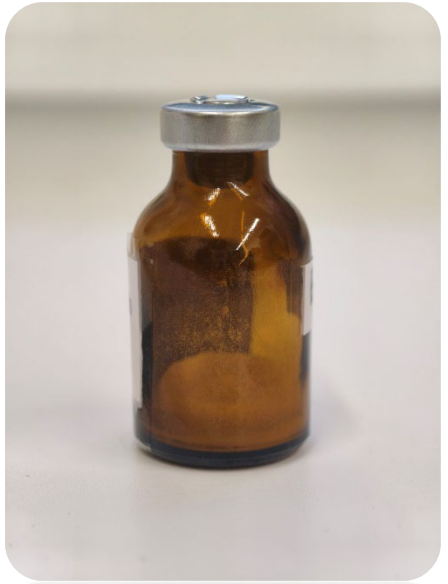
Small-angle x-ray scattering curves from Vitaphospholip and product appearance

Concentration, %	ρ_{core}, 10^{-6} Å^{-2}	R, Å	ρ_{PH1}, 10^{-6} Å^{-2}	D_{PH1}, Å	ρ_{CH}, 10^{-6} Å^{-2}	D_{CH}, Å	ρ_{PH2}, 10^{-6} Å^{-2}	D_{PH2}, Å	ρ_{solv}, 10^{-6} Å^{-2}
25	10.4 ± 0.2	159.3 ± 2.2	11.2 ± 0.1	9 (fix)	8.2 (fix)	21.9 ± 1.0	10.8 ± 0.1	9 (fix)	10.2 ± 0.1
30	10.5 ± 0.2	110.4 ± 1.5	11.2 ± 0.2	8.1 ± 1.9	8.2 (fix)	20.7 ± 0.6	10.9 ± 0.1	8.0 ± 1.1	10.2 ± 0.1
35	10.8 ± 0.3	98.5 ± 5.9	11.2 ± 0.1	9.0 ± 2.1	8.2 (fix)	21.9 ± 0.4	10.8 ± 0.1	9.1 ± 1.0	10.4 ± 0.1

Berberine-NF:



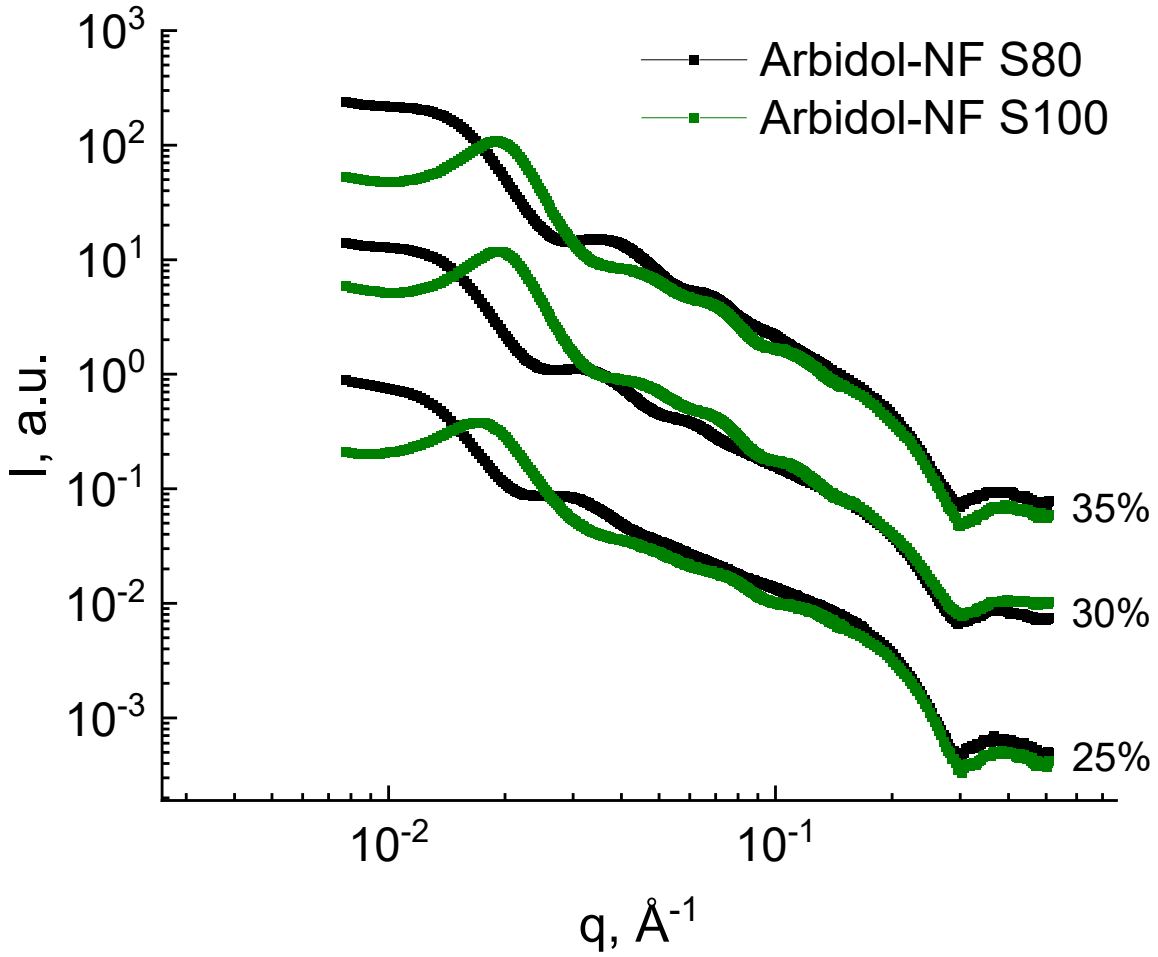




Small-angle x-ray scattering curves from Berberine-NF and product appearance

Concentration, %	ρ_{core}, 10^{-6} Å^{-2}	R, Å	ρ_{PH1}, 10^{-6} Å^{-2}	D_{PH1}, Å	ρ_{CH}, 10^{-6} Å^{-2}	D_{CH}, Å	ρ_{PH2}, 10^{-6} Å^{-2}	D_{PH2}, Å	ρ_{solv}, 10^{-6} Å^{-2}
25	10.08 ± 0.03	94.5 ± 21.2	10.8 ± 0.1	9 (fix)	8.82 (fix)	21.8 ± 0.7	10.6 ± 0.1	9 (fix)	10.04 (fix)
30	10.19 ± 0.01	84.7 ± 8.9	10.7 ± 0.1	11.5 ± 2.2	8.82 (fix)	21.7 ± 0.6	10.6 ± 0.1	8 ± 1.0	10.19 (fix)
35	10.33 ± 0.03	87.6 ± 6.7	10.8 ± 0.1	10.2 ± 2.9	8.82 (fix)	21.9 ± 0.6	10.5 ± 0.6	9 ± 1.2	10.37 ± 0.13

Arbidol-NF:



Key points:

- changes in composition

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changes in characteristic particle dimensions,

and

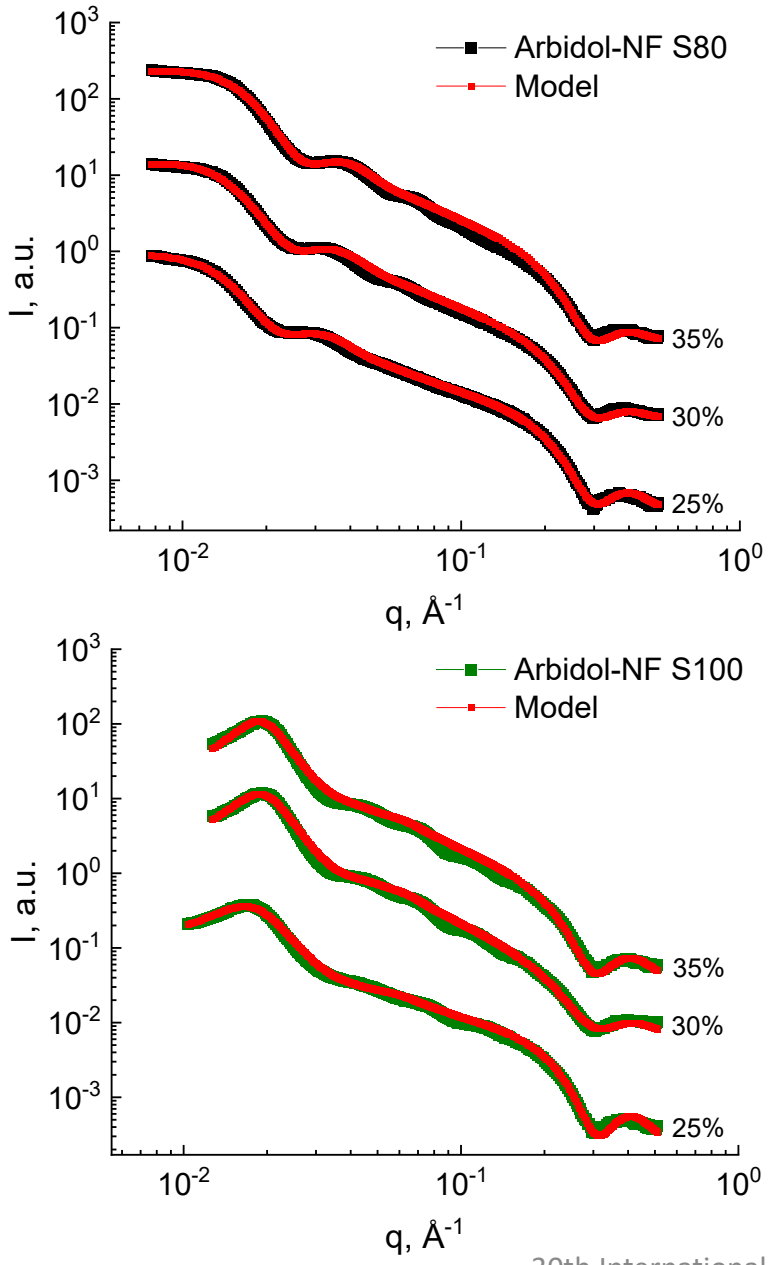
- emergence of inter-vesicular interaction

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necessity of introducing a structure factor

Comparison of small-angle x-ray scattering curves for Arbidol-NF formulations based on soybean phospholipids S80 and S100

Arbidol-NF:



	S80			S100		
Conc., %	25	30	35	25	30	35
$\rho_{core,}$ 10^{-6} Å^{-2}	10.07 ± 0.04	10.21 ± 0.05	10.31 (fix)	10.05 ± 0.15	10.16 (fix)	10.31 (fix)
R, Å	103.8 ± 8.5	90.0 ± 4.3	82.1 ± 7.1	51.0 ± 9.2	55.3 ± 5.2	50,1 ± 5.4
$\rho_{PH1,}$ 10^{-6} Å^{-2}	10.4 ± 0.2	10.4 ± 0.1	10.7 ± 0.1	10.73 ± 0.43	10.3 ± 0.2	10.2 ± 3.9
D_{PH1}, Å	9 (fix)	10.1 ± 1.4	10.7 ± 2.7	8.2 ± 1.3	6.4 ± 5.8	8.1 ± 3.8
$\rho_{CH,}$ 10^{-6} Å^{-2}	8.99 ± 0.1	8.69 ± 0.08	8.87 ± 0.05	9.1 ± 0.1	9.2 ± 0.1	9.3 ± 0.1
D_{CH}, Å	21.0 ± 1.5	19.9 ± 1.1	19.9 ± 0.7	20.9 ± 2.8	20.9 ± 1.3	21.2 ± 2.5
$\rho_{PH2,}$ 10^{-6} Å^{-2}	10.7 ± 0.2	10.16 ± 0.1	10.6 ± 0.1	10.5 ± 0.3	10.6 ± 0.1	10.6 ± 0.1
D_{PH2}, Å	9 (fix)	11.1 ± 2.0	10.9 ± 1.8	8.0 ± 1.9	7.6 ± 5.0	7.9 ± 2.8
$\rho_{solv,}$ 10^{-6} Å^{-2}	10.03 (fix)	10.6 ± 0.2	10.31(fix)	10.03 (fix)	10.16 (fix)	10.31 (fix)
Charge, e	20	60	20	60	50	58
Salt, M	0.001	0.002	0.001	0.002	0.001	0.001
Dielelectric const	73	68	65	72	68	65

Small-angle x-ray scattering curves from Arbidol-NF

Conclusions:

- Vitaphospholip demonstrated an increased scattering length density inside and outside the vesicles, as well as a decrease in the inner radius with increasing concentration.

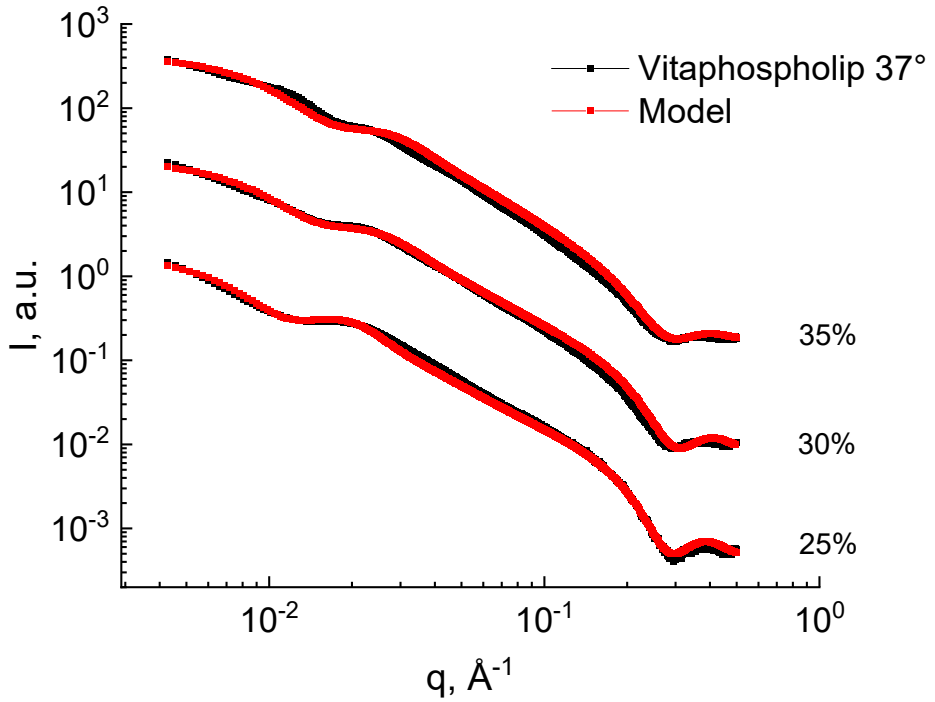
- In the case of Berberine-NF, stability of the size is observed, as well as, like in the case of vitaphospholip, the preservation of the hydrophobic tail region.

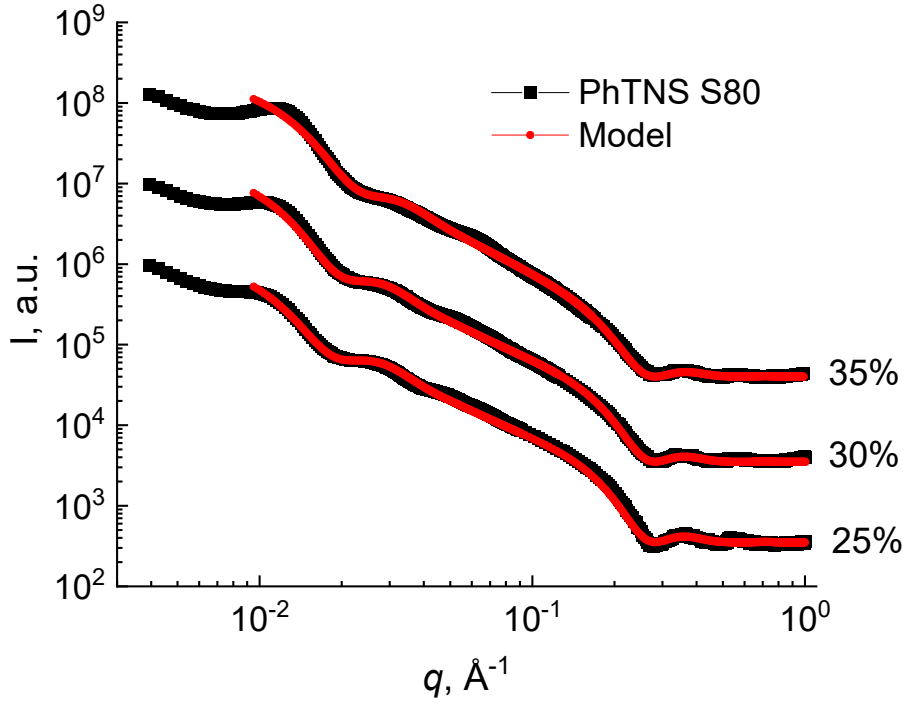
- Arbidol-NF was studied with varying levels of phosphatidylcholine, and the samples demonstrate changes in the size and internal structure of the bilayer, as well as the emergence of intervesicular interaction.

Thank you for your attention!

varvara@jinr.ru

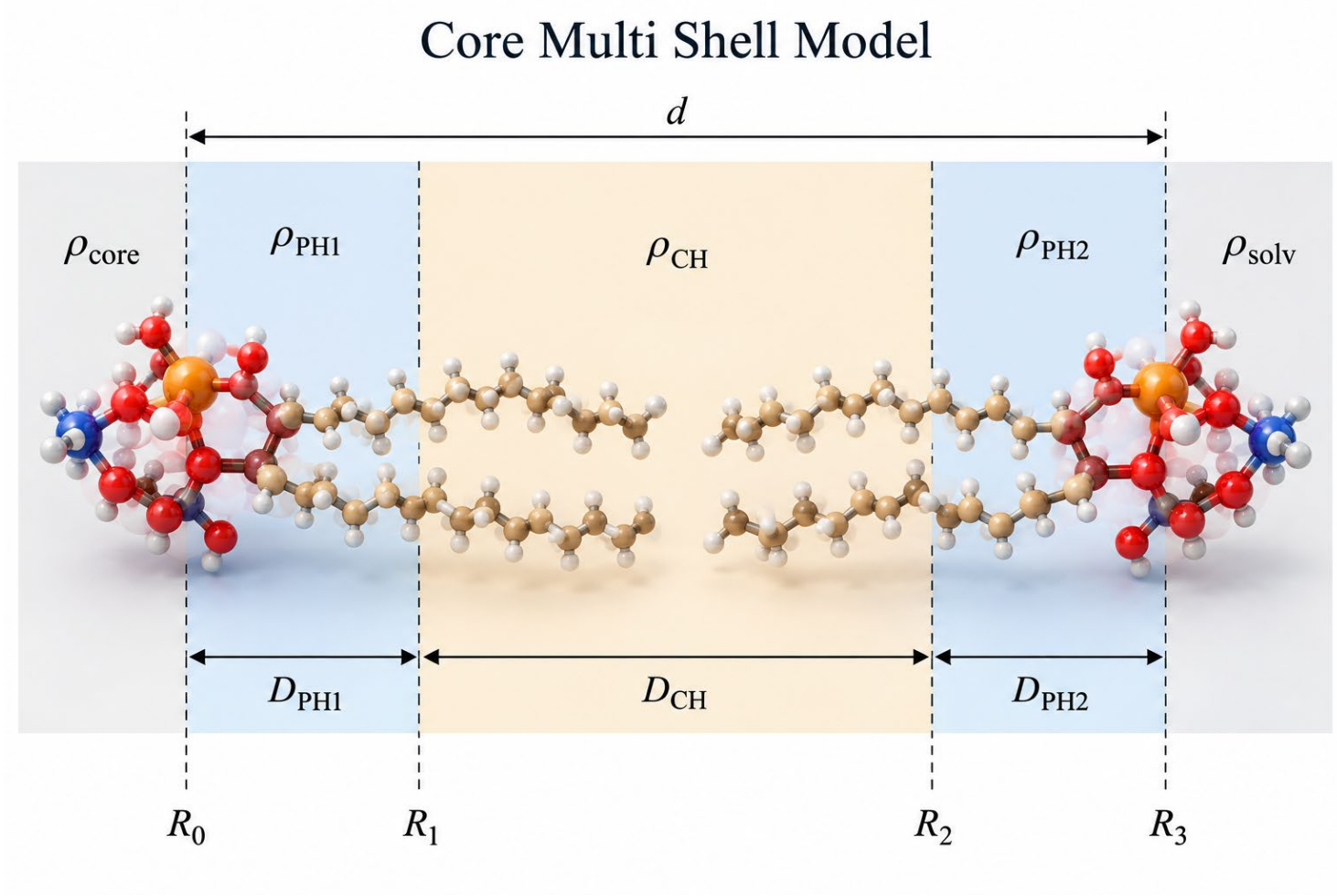
Comparison Vitaphospholip and PhTNS





Conc., %	R, Å	d, Å
25	159.3	39.9
30	110.4	36.8
35	98.5	40

Conc., %	R, Å	d, Å
25	115	46
30	115	46
35	95	46



$$\frac{d\Sigma}{d\Omega}(q, R_0, R_1, R_2, R_3) = \frac{Scale}{V} F^2(q, R_0, R_1, R_2, R_3) + Bg,$$

$$\begin{aligned} &F(q) \\ &= \frac{3}{V_v}[V_0(\rho_0 - \rho_1)]P(q, R_0) \\ &+ V_1(\rho_1 - \rho_2)[V_1 P(q, R_1) - V_0 P(q, R_0)] \\ &+ V_2(\rho_2 - \rho_3)[V_2 P(q, R_2) - V_1 P(q, R_1)] \\ &+ V_3(\rho_3 - \rho_p)[V_3 P(q, R_3) - V_2 P(q, R_2)] \end{aligned}$$

$$P(q, R_i) = \frac{[\sin(qR_i) - qR_i cos(qR_i)]}{(qR_i)^3}$$

Structure Factor "Hayter MSA":

$$S(q) = \frac{1}{1 - \frac{24\phi}{\left(\frac{qD}{2}\right)^3}\left[A cos\left(\frac{qD}{2}\right) - B sin\left(\frac{qD}{2}\right)\right]}$$