

Supporting material for

Characterisation of the membrane affinity of an isoniazide peptide conjugate by tensiometry, atomic force microscopy and sum-frequency vibrational spectroscopy, using a phospholipid Langmuir monolayer model

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Table S1. Fitting parameters for the sum-frequency *ssp* spectra of Phospholipon on pure water and for Phospholipon after INH peptide conjugate penetration at 15 and 20 mN/m.

	CH ₂ (s)	CH ₃ (s)	CH ₂ (as)	CH ₃ (FR)	CH ₃ (as)	A_{NR}	φ_{NR} (radian)
ω_m (cm ⁻¹)	2850	2878	2900	2938	2961		
Γ_m (cm ⁻¹)	15	6.7	15	8.5	10		
Area/molecule (Å ²)							
Phospholipon spread onto pure water subphase							
40	2.56	7.14	0.93	6.76	-3.11	0.07	-0.99
41	2.48	6.99	0.84	6.52	-3.23	0.08	-1.05
41	2.60	6.88	0.94	6.47	-3.10	0.08	-1.23
42	2.87	6.31	0.99	5.97	-2.76	0.09	-1.28
44	2.78	6.47	1.01	6.36	-2.77	0.09	-1.21
45	2.99	6.29	1.12	6.15	-2.74	0.09	-1.29
50	3.37	5.74	1.30	5.81	-2.62	0.10	-1.47
52	3.58	5.40	1.36	5.46	-2.33	0.11	-1.49
59	3.58	4.68	1.11	4.69	-2.05	0.11	-1.57
62	3.81	4.42	1.11	4.55	-2.13	0.11	-1.58
70	3.86	3.80	1.45	4.05	-1.66	0.12	-1.61
86	4.30	2.87	1.40	3.29	-1.36	0.12	-1.63
98	2.46	1.29	2.37	2.09	-1.26	0.11	-2.13
108	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Phospholipon following penetration of INH peptide conjugate at 15 mN/m							
52	2.61	6.29	0.71	6.14	-2.85	-0.05	1.62
52	3.03	6.61	0.82	6.35	-2.69	0.02	-1.20
59	3.03	5.82	1.02	5.56	-2.15	-0.02	0.84
66	2.74	5.16	1.38	4.96	-1.79	-0.04	0.45
71	2.53	4.47	1.45	4.27	-1.93	-0.06	0.08
81	1.91	3.63	1.23	3.47	-2.69	-0.12	-0.39
95	1.74	3.23	2.70	3.18	0.34	-0.11	0.42
110	0.84	2.44	2.20	2.46	-1.09	-0.15	0.04
Phospholipon following penetration of INH peptide conjugate at 20 mN/m							
50	2.41	6.39	1.24	6.17	-2.75	0.06	-1.39
50	2.63	6.40	0.67	6.28	-2.82	0.02	-1.48
52	2.73	6.37	0.77	6.17	-2.64	0.02	-1.90
56	2.80	5.78	1.19	5.74	-2.31	-0.03	0.64
62	2.55	5.00	1.44	5.01	-2.03	-0.05	0.10
72	1.87	3.63	0.82	3.71	-2.90	-0.11	-0.52
80	1.46	3.64	1.00	3.57	-2.75	-0.12	-0.38
90	1.24	3.12	1.49	3.00	-2.04	-0.13	-0.18
98	1.05	2.85	2.48	2.70	0.84	-0.12	0.41
109	0.57	2.03	2.68	2.20	1.12	-0.13	0.65