SUPPORTING INFORMATION

THIACALIX[4]ARENE-FUNCTIONALIZED VESICLES AS PHOSPHORESCENT INDICATORS FOR PYRIDOXINE DETECTION IN AQUEOUS SOLUTION

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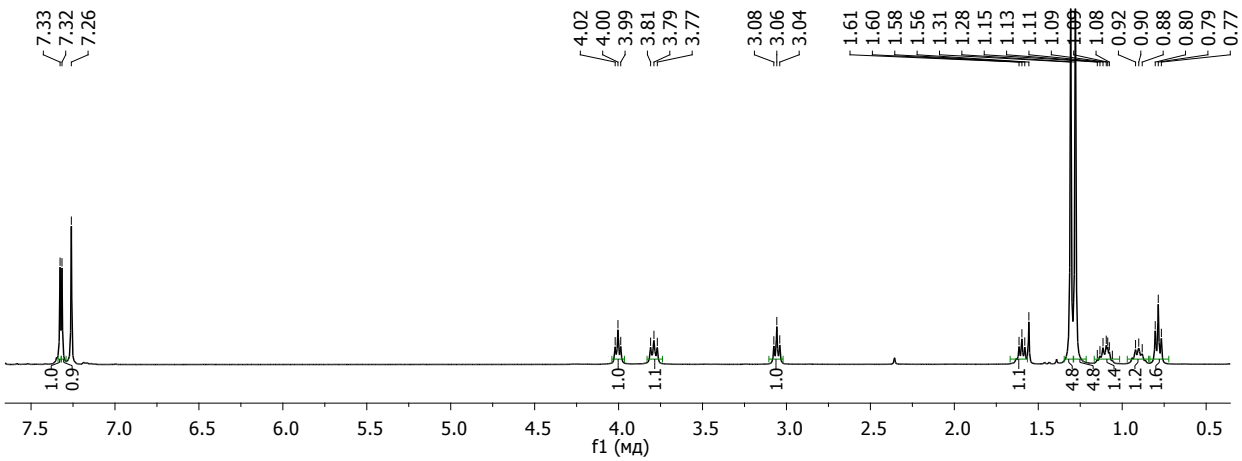
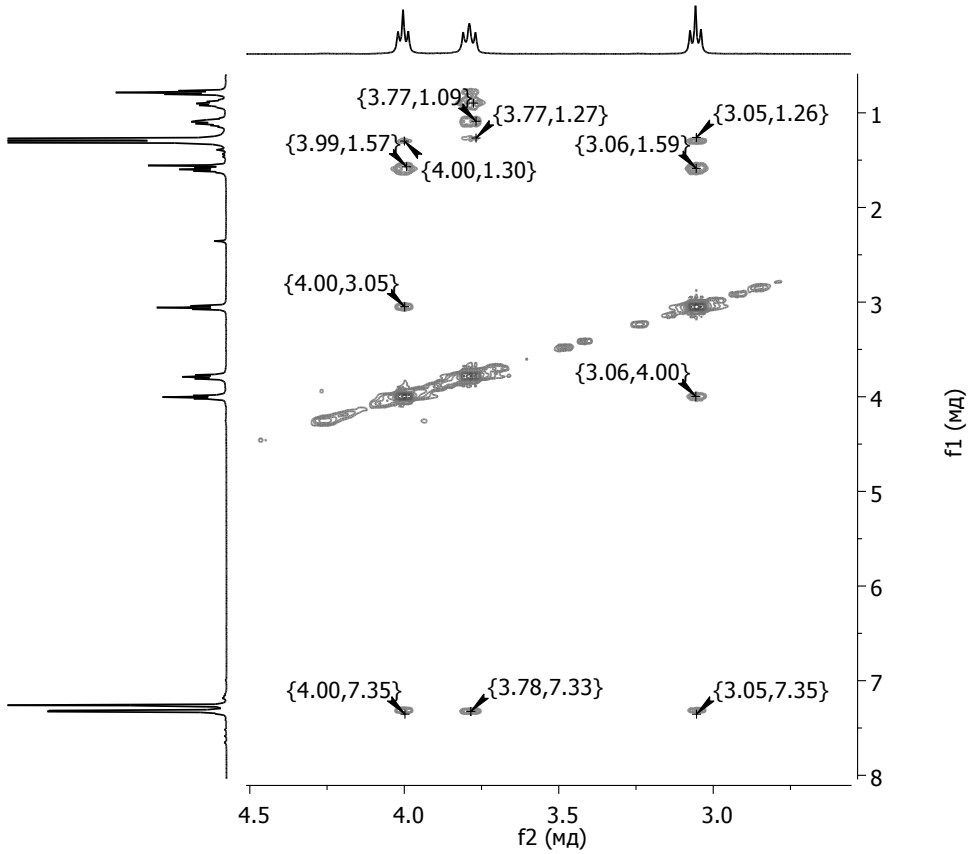
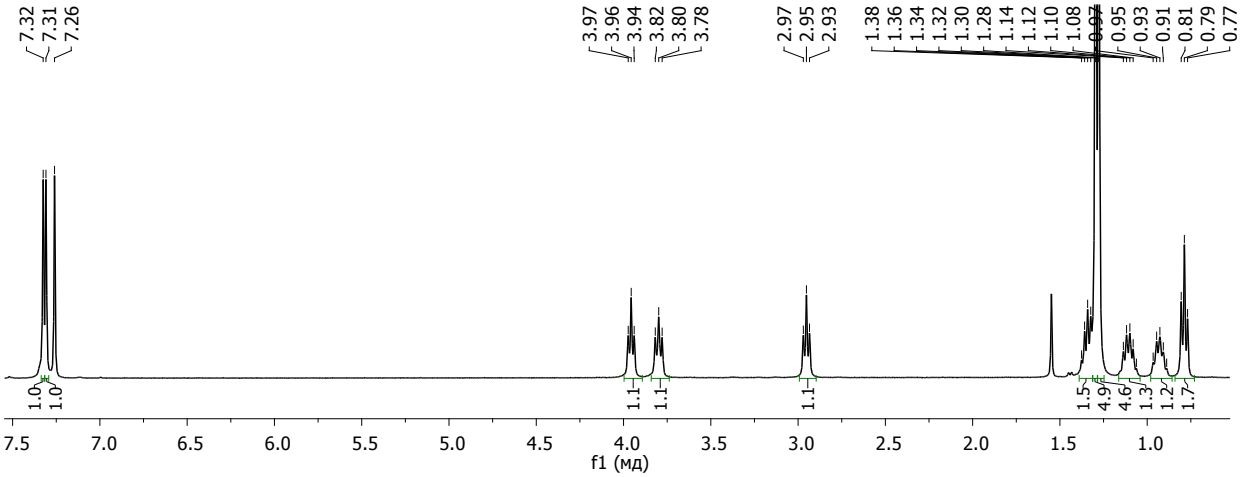
NMR SPECTRA OF COMPOUNDS 5-13



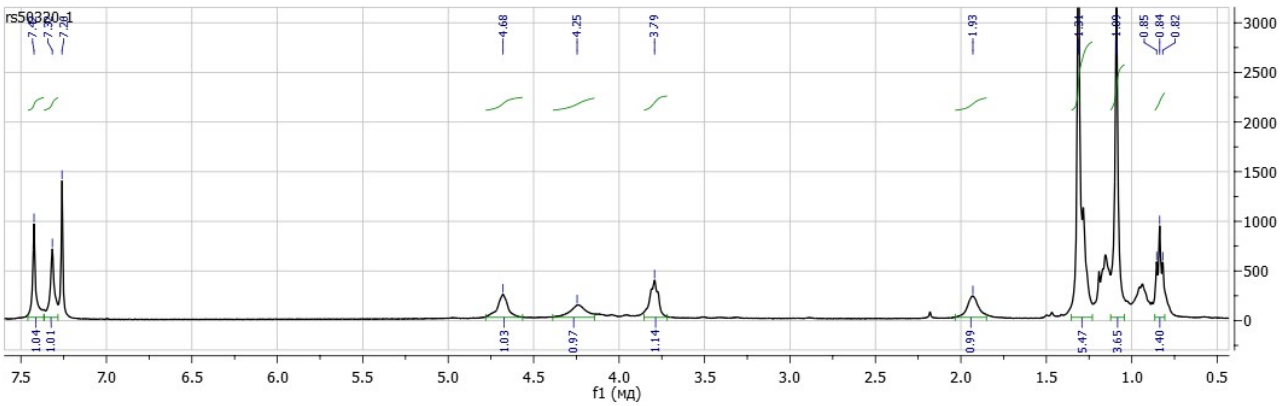
5,11,17,23-Tetra-*tert*-butyl-25,27-dibutyloxy-26,28-di-3-bromopropyloxy-2,8,14,20-tetrathiacalix[4]arene **5** ^{1}H NMR ($CDCl_3$)



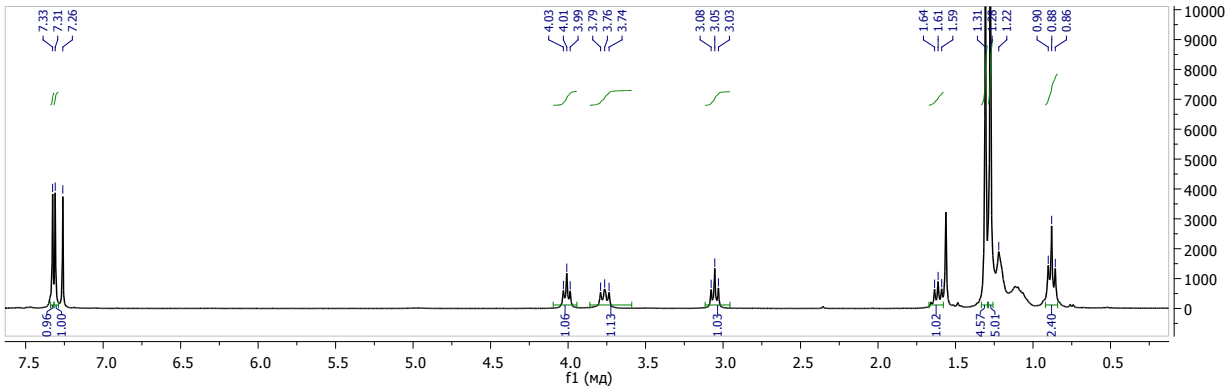
5,11,17,23-Tetra-*tert*-butyl-25,27-dibutyloxy-26,28-di-3-bromopropyloxy-2,8,14,20-tetrathiacalix[4]arene **5** 2D NOESY NMR ($CDCl_3$)



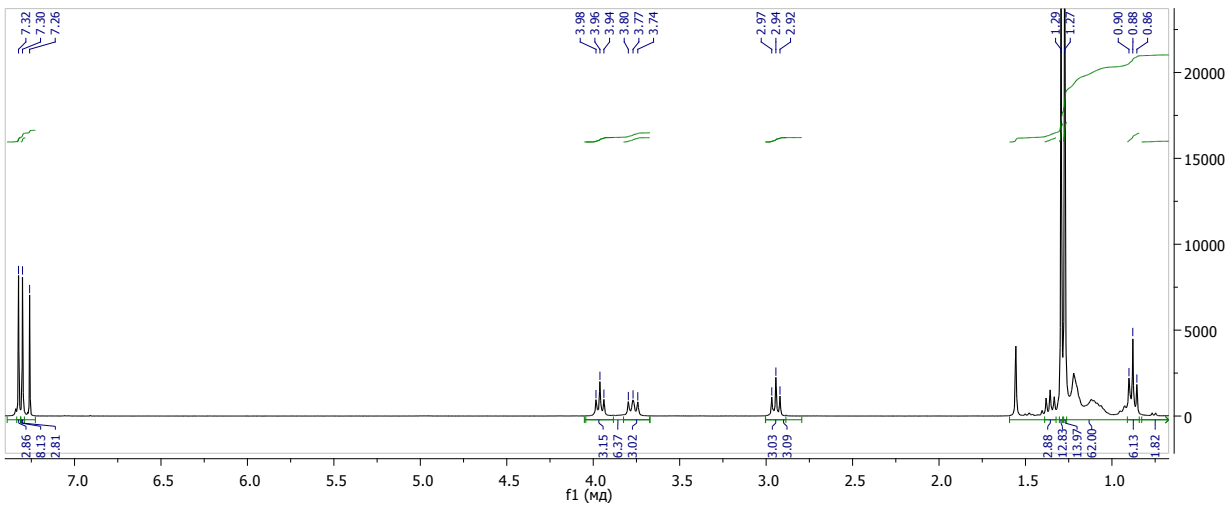
5,11,17,23-Tetra-*tert*-butyl-25,27-dibutyloxy-26,28-di-3-azidopropyloxy-2,8,14,20-tetrathiacalix[4]arene 8



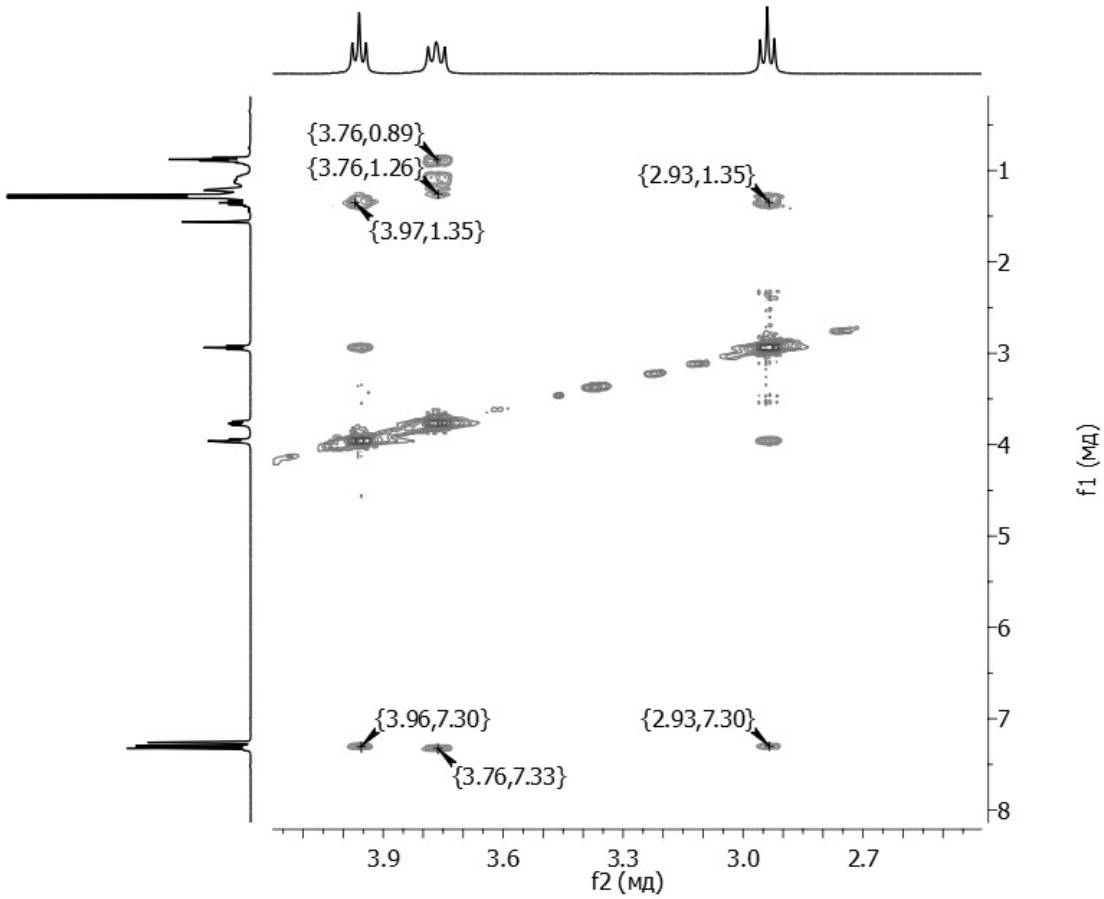
5,11,17,23-Tetra-*tert*-butyl-25,27-dibutyloxy-26,28-bis[3-(4,5-dicarboxy-1,2,3-triazol-1-yl)propyloxy]-2,8,14,20-tetrathiacalix[4]arene 11 ^{1}H NMR ($CDCl_3$)



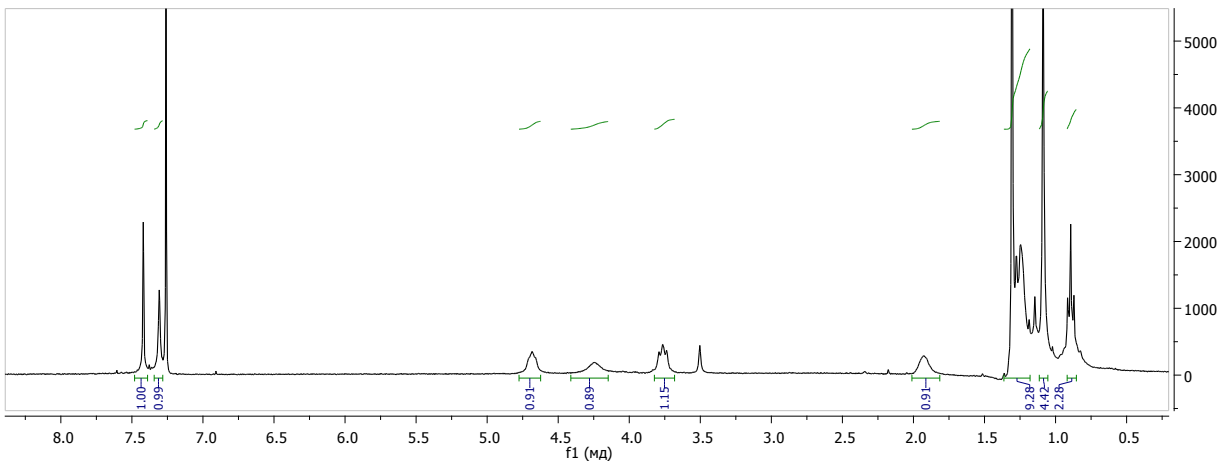
5,11,17,23-Tetra-*tert*-butyl-25,27-dioctyloxy-26,28-di-3-bromopropyloxy-2,8,14,20-tetrathiacalix[4]arene **6** ^{1}H NMR ($CDCl_3$)



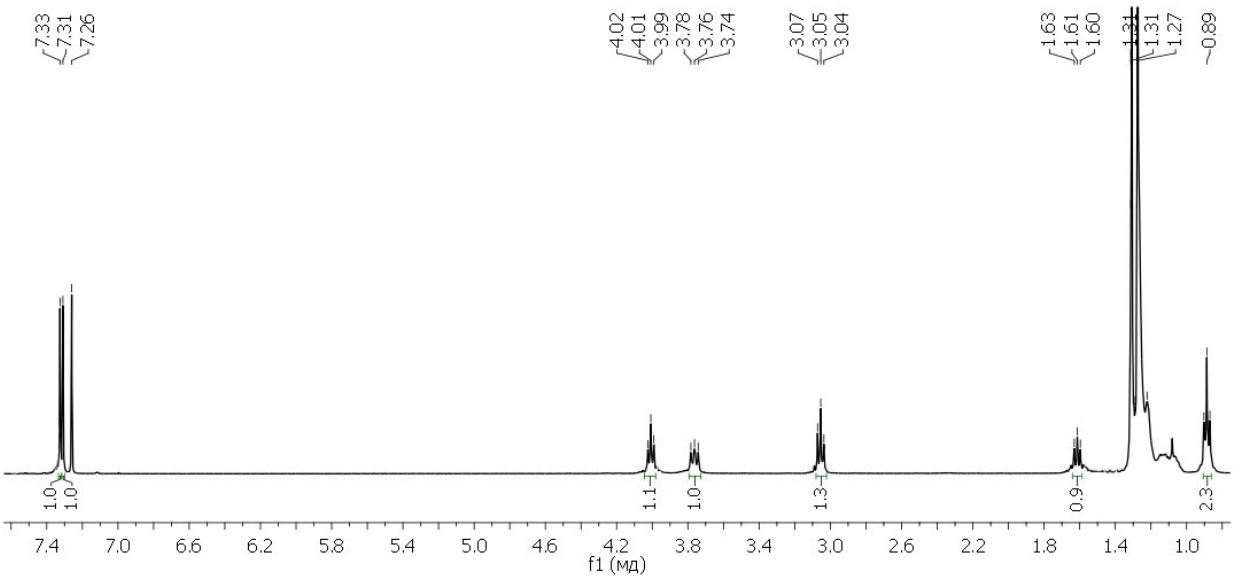
5,11,17,23-Tetra-*tert*-butyl-25,27-dioctyloxy-26,28-di-3-azidopropyloxy-2,8,14,20-tetrathiacalix[4]arene **9** ^{1}H NMR ($CDCl_3$)



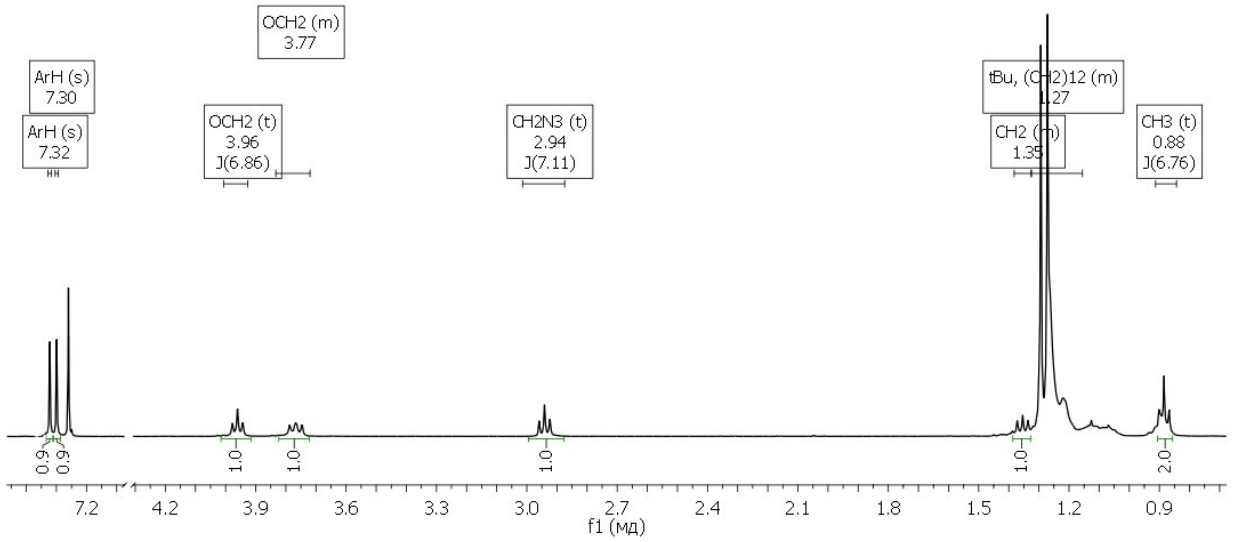
5,11,17,23-Tetra-*tert*-butyl-25,27-dioctyloxy-26,28-di-3-azidopropyloxy-2,8,14,20-tetrathiacalix[4]arene **9** 2D NOESY NMR ($CDCl_3$)



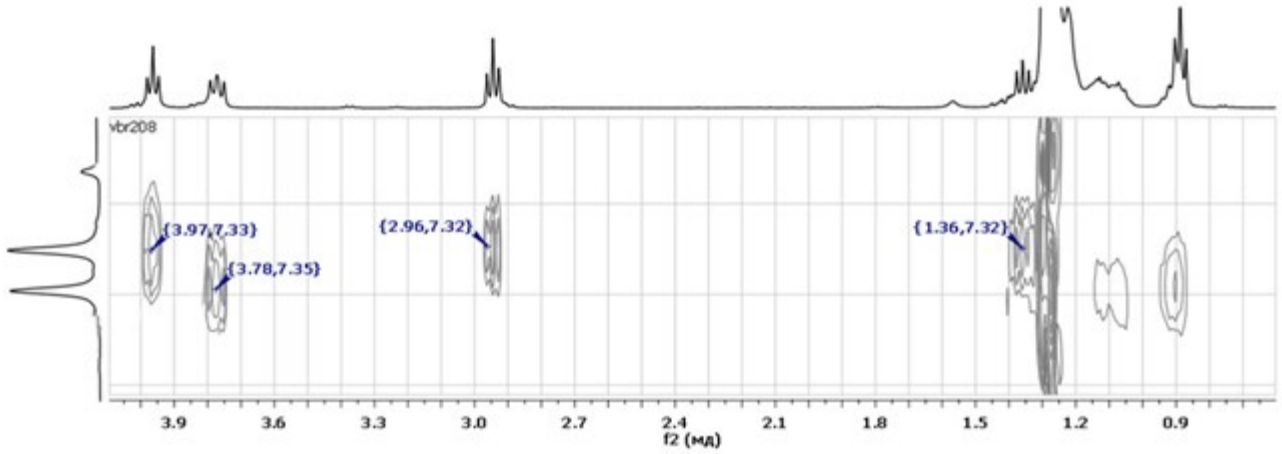
5,11,17,23-Tetra-tert-butyl-25,27-dioctyloxy-26,28- bis[3-(4,5-dicarboxy-1,2,3-triazol-1-yl) propoxy]-]-2,8,14,20-tetrathiacalix[4]arene 12 ^{1}H NMR ($CDCl_3$)



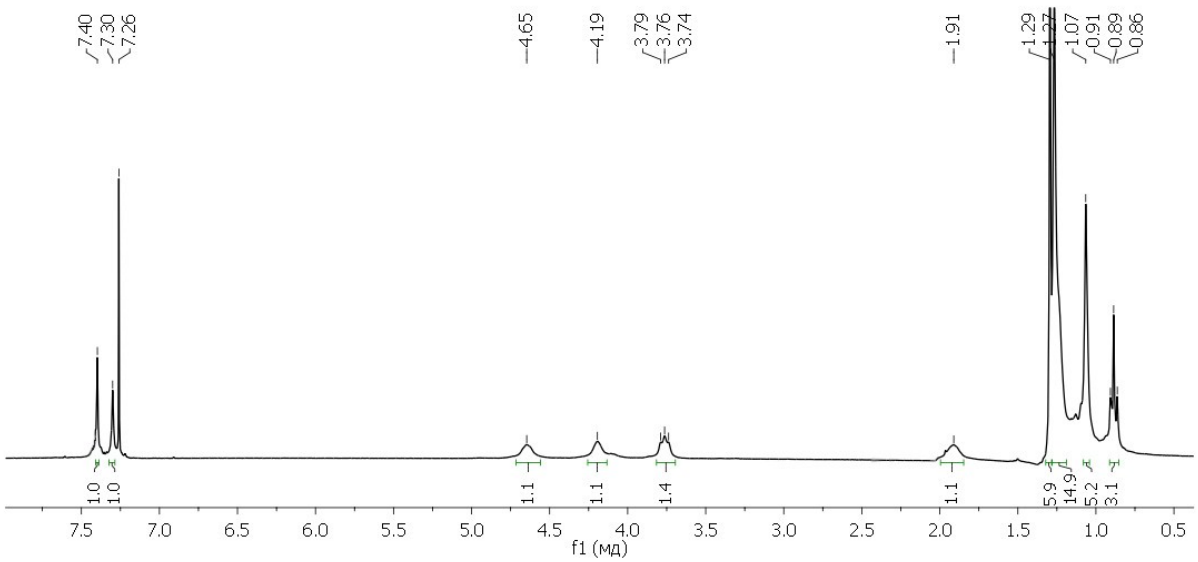
5,11,17,23-Tetra-*tert*-butyl-25,27-ditetradecyloxy-26,28-di-3-bromopropyloxy-2,8,14,20-tetrathiacalix[4]arene **7** ^{1}H NMR ($CDCl_3$)



5,11,17,23-Tetra-*tert*-butyl-25,27-ditetradecyloxy-26,28-di-3-azidopropyloxy-2,8,14,20-tetrathiacalix[4]arene **10** ^{1}H NMR ($CDCl_3$)

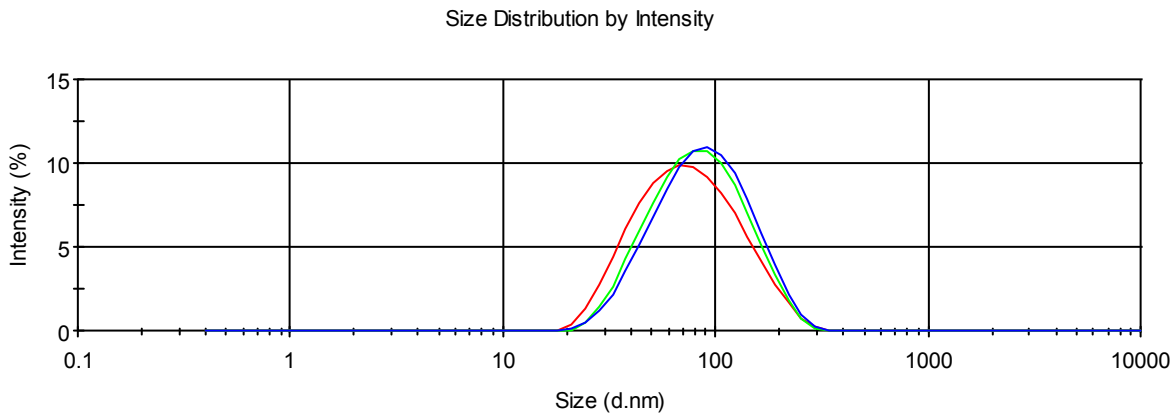


5,11,17,23-Tetra-*tert*-butyl-25,27-ditetradecyloxy-26,28-di-3-azidopropyloxy-2,8,14,20-tetrathiacalix[4]arene **10** 2D NOESY NMR ($CDCl_3$)



5,11,17,23-Tetra-tert-butyl-25,27-ditetradecyloxy-26,28- bis [3-(4,5-dicarboxy-1,2,3-triazol-1-yl) propyloxy]-2,8,14,20-tetrathiacalix[4]arene 13 ^{1}H NMR ($CDCl_3$)

DLS data



CA4_DPPC, C(CA4) = 0,07 mM C(DPPC) = 0,7 mM; C(TRIS) = 20mM; C(NaCl) = 150 mM; pH = 7,4

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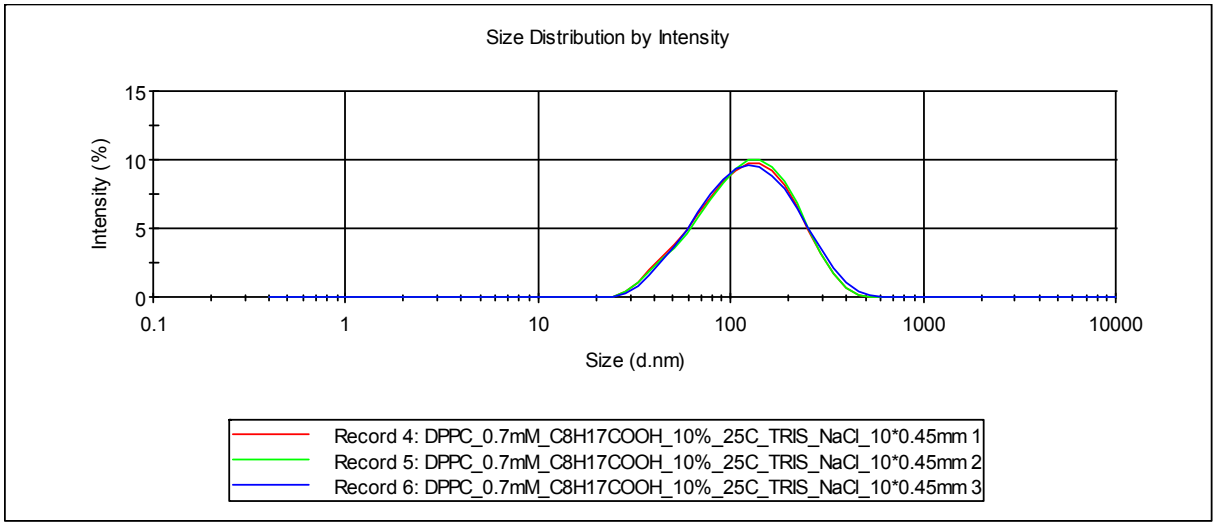
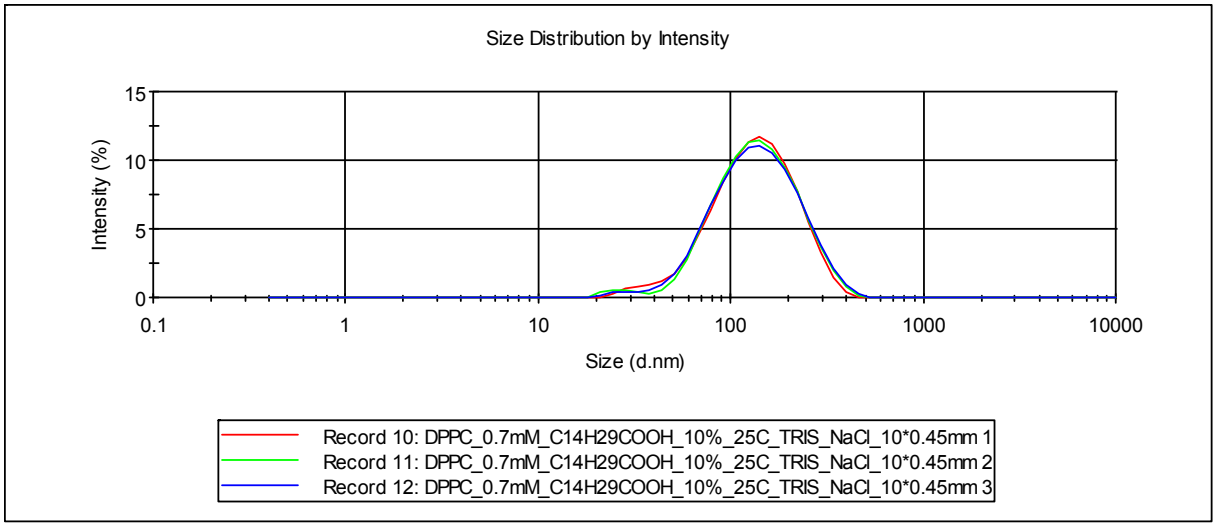
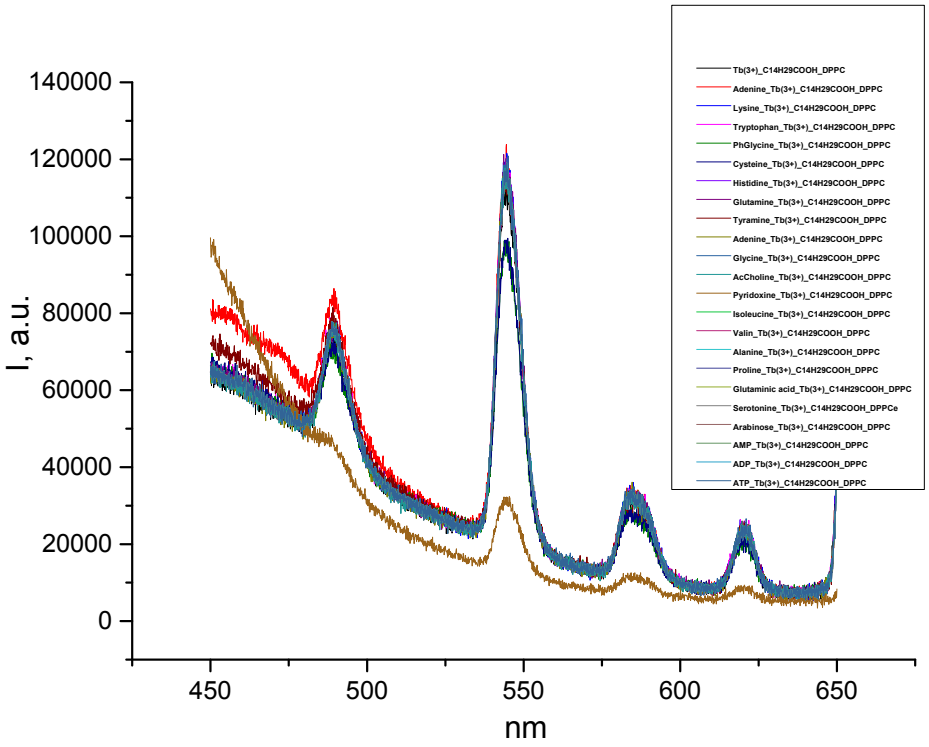


CA8_DPPC, C(CA8) = 0,07 mM C(DPPC) = 0,7 mM; C(TRIS) = 20mM; C(NaCl) = 150 mM; pH = 7,4

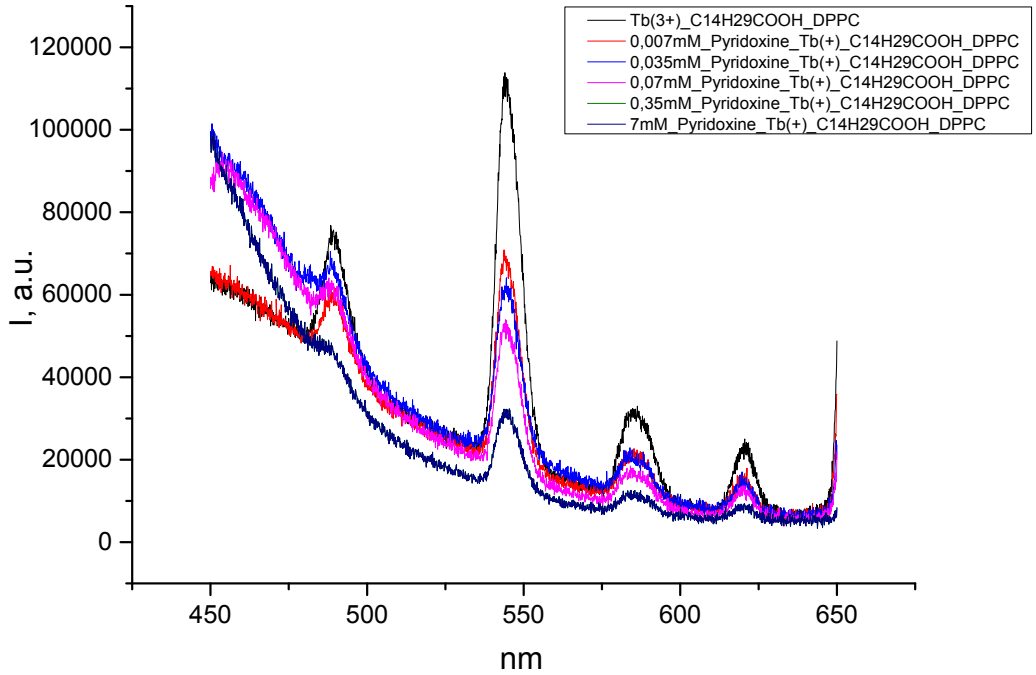


CA14_DPPC, C(CA14) = 0,07 mM C(DPPC) = 0,7 mM; C(TRIS) = 20mM; C(NaCl) = 150 mM; pH = 7,4

Luminescence data

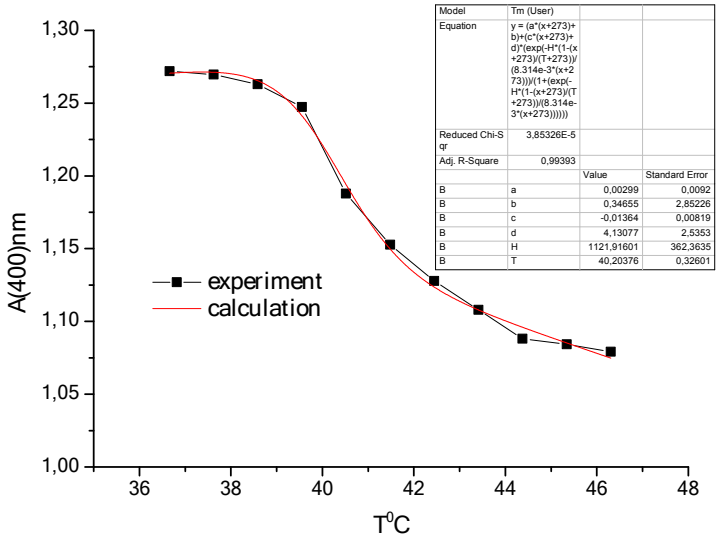


Luminescence spectra of DPPC-CA14-Tb(III) vesicles after addition of organic analyte molecules. C[CA14] = 0,07 mM; C[DPPC] = 0,7 mM; C[Tb] = 0,07 mM; C[TRIS] = 20mM; C[NaCl] = 150 mM; pH = 7,4, C[org. guest] = 0.35 mM.



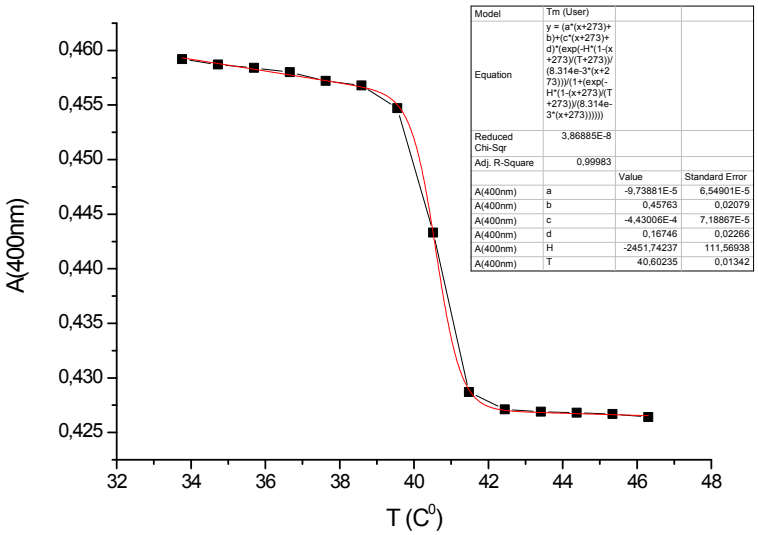
Luminescence spectra of DPPC-CA14-Tb(III) vesicles vs pyridoxine*HCl concentration. C[CA14] = 0,07 mM; C[DPPC] = 0,7 mM; C[Tb] = 0,7 mM; C[TRIS] = 20mM; C[NaCl] = 150 mM; pH = 7,4, C[pyridoxine] = 0,0007-7 mM.

T_m plots



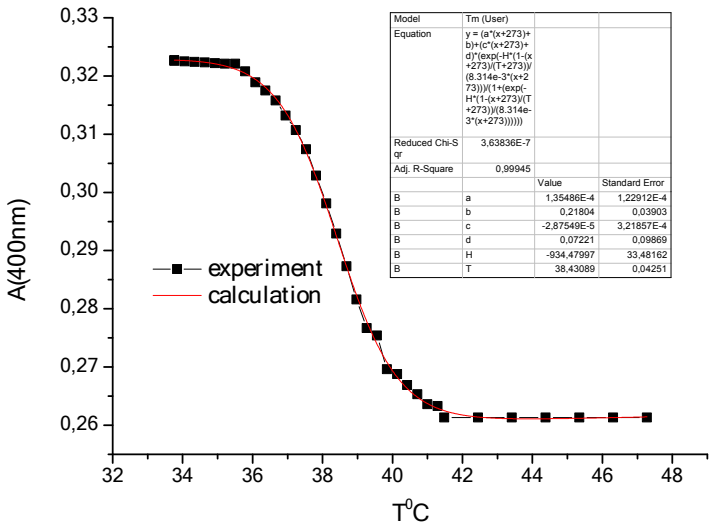
Model	Tm (User)		
Equation	y = (a*(x+273)+b)+(c*(x+273)+d)*(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273)))/(1+(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273)))))		
Reduced Chi-Sqr	3,85326E-5		
Adj. R-Square	0,99393		
		Value	Standard Error
B	a	0,00299	0,0092
B	b	0,34655	2,85226
B	c	-0,01364	0,00819
B	d	4,13077	2,5353
B	H	1121,91601	362,3635
B	T	40,20376	0,32601

T_m plot of CA-4 (10 mol%)_DPPC vesicles, C(DPPC) = 0.7 mM; C(TRIS) = 20 mM; C(NaCl) = 150 mM; pH = 7.4



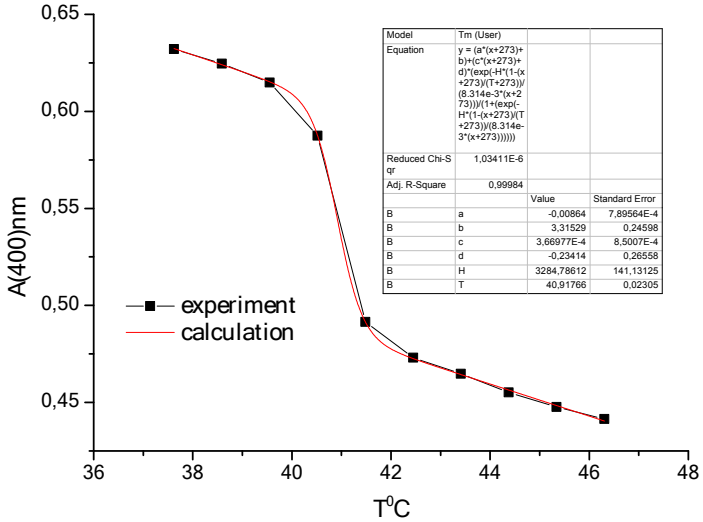
Model	Tm (User)		
Equation	y = (a*(x+273)+b)+(c*(x+273)+d)*(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273)))/(1+(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273)))))		
Reduced Chi-Sqr	3,86885E-8		
Adj. R-Square	0,99983		
		Value	Standard Error
A(400nm)	a	-9,73881E-5	6,54901E-5
A(400nm)	b	0,45763	0,02079
A(400nm)	c	-4,43006E-4	7,18867E-5
A(400nm)	d	0,16746	0,02266
A(400nm)	H	-2451,74237	111,56938
A(400nm)	T	40,60235	0,01342

T_m plot of CA-4 (1 mol%)_DPPC vesicles, C(DPPC) = 0.7 mM; C(TRIS) = 20 mM; C(NaCl) = 150 mM; pH = 7.4



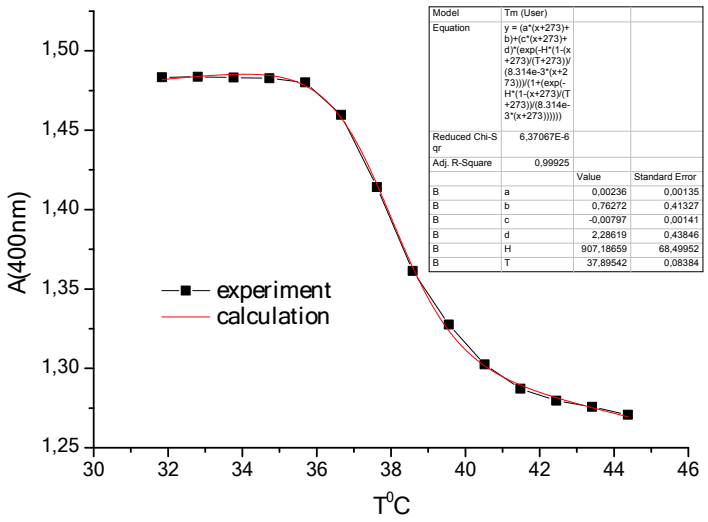
Model	Tm (User)		
Equation	y = (a*(x+273)+b)+(c*(x+273)+d)*(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273)))/(1+(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273))))))		
Reduced Chi-Sqr	3,63836E-7		
Adj. R-Square	0,99945		
		Value	Standard Error
B	a	1,35486E-4	1,22912E-4
B	b	0,21804	0,03903
B	c	-2,87549E-5	3,21857E-4
B	d	0,07221	0,09869
B	H	-934,47997	33,48162
B	T	38,43089	0,04251

T_m plot of CA-8 (10 mol%)_DPPC vesicles, C(DPPC) = 0.7 mM; C(TRIS) = 20 mM; C(NaCl) = 150 mM; pH = 7.4



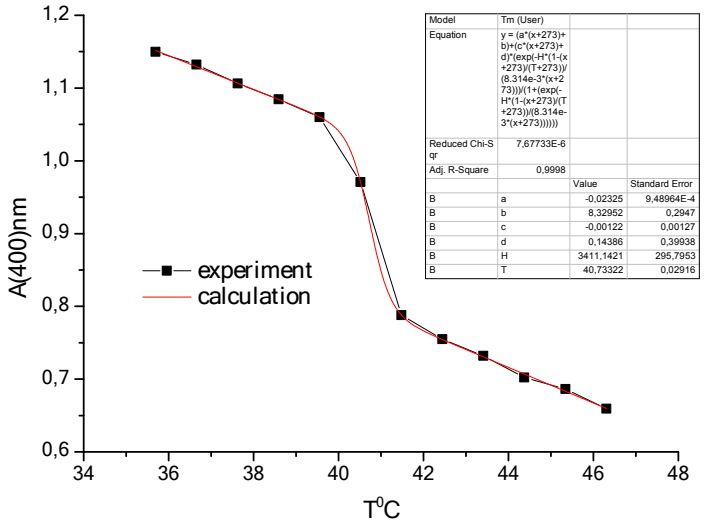
Model	Tm (User)		
Equation	y = (a*(x+273)+b)+(c*(x+273)+d)*(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273)))/(1+(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273))))))		
Reduced Chi-Sqr	1,03411E-6		
Adj. R-Square	0,99984		
		Value	Standard Error
B	a	-0,00864	7,89564E-4
B	b	3,31529	0,24598
B	c	3,66977E-4	8,5007E-4
B	d	-0,23414	0,26558
B	H	3284,78612	141,13125
B	T	40,91766	0,02305

T_m plot of CA-8 (1 mol%)_DPPC vesicles, C(DPPC) = 0.7 mM; C(TRIS) = 20 mM; C(NaCl) = 150 mM; pH = 7.4



Model	Tm (User)		
Equation	y = (a*(x+273)+b)+(c*(x+273)+d)*(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273)))/(1+(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273))))))		
Reduced Chi-Sqr	6,37067E-6		
Adj. R-Square	0,99925		
		Value	Standard Error
B	a	0,00236	0,00135
B	b	0,76272	0,41327
B	c	-0,00797	0,00141
B	d	2,28619	0,43846
B	H	907,18659	68,49952
B	T	37,89542	0,08384

T_m plot of CA-14 (10 mol%)_DPPC vesicles, C(DPPC) = 0.7 mM; C(TRIS) = 20 mM; C(NaCl) = 150 mM; pH = 7.4



Model	Tm (User)		
Equation	y = (a*(x+273)+b)+(c*(x+273)+d)*(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273)))/(1+(exp(-H*(1-(x+273)/(T+273))/(8.314e-3*(x+273)))))		
Reduced Chi-Sqr	7,67733E-6		
Adj. R-Square	0,9998		
		Value	Standard Error
B	a	-0,02325	9,48964E-4
B	b	8,32952	0,2947
B	c	-0,00122	0,00127
B	d	0,14386	0,39938
B	H	3411,1421	295,7953
B	T	40,73322	0,02916

T_m plot of CA-14 (1 mol%)_DPPC vesicles, C(DPPC) = 0.7 mM; C(TRIS) = 20 mM; C(NaCl) = 150 mM; pH = 7.4