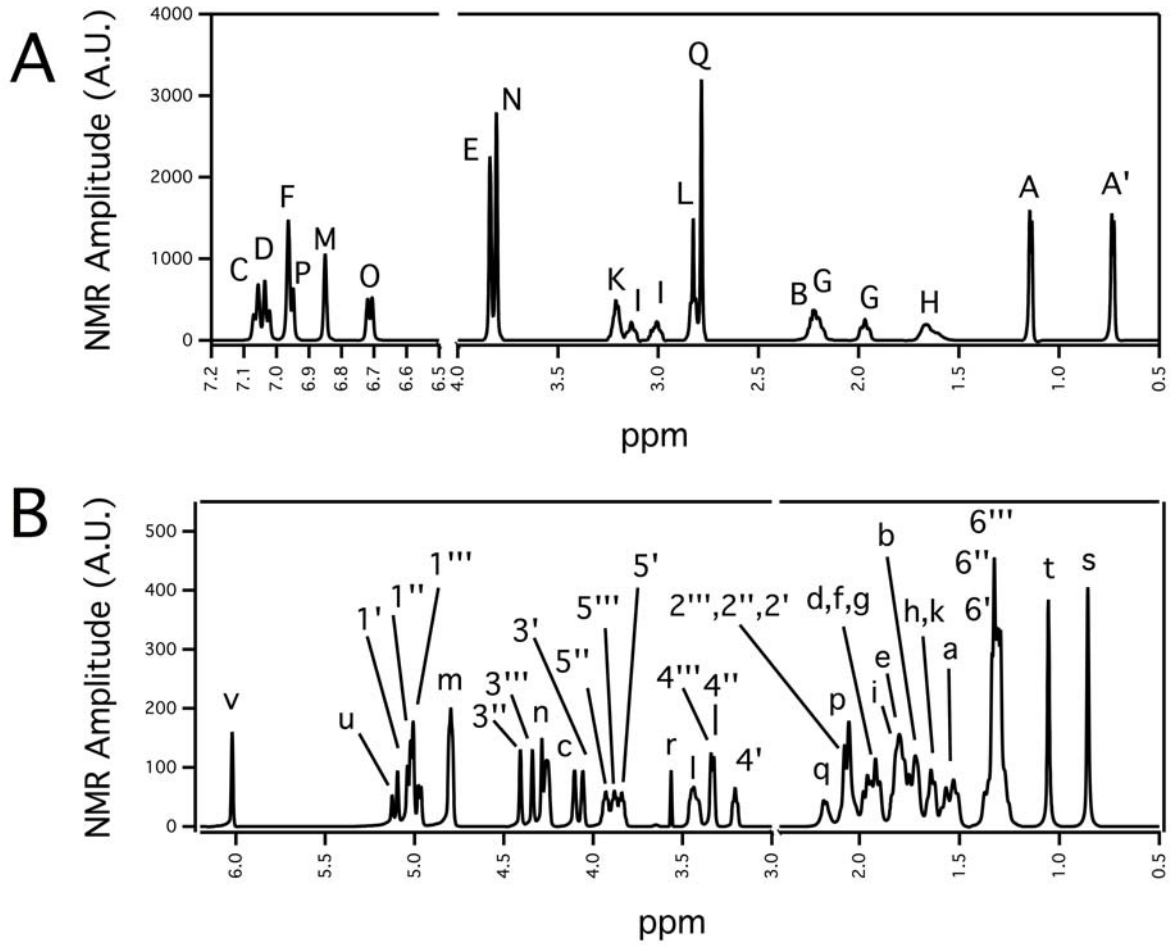
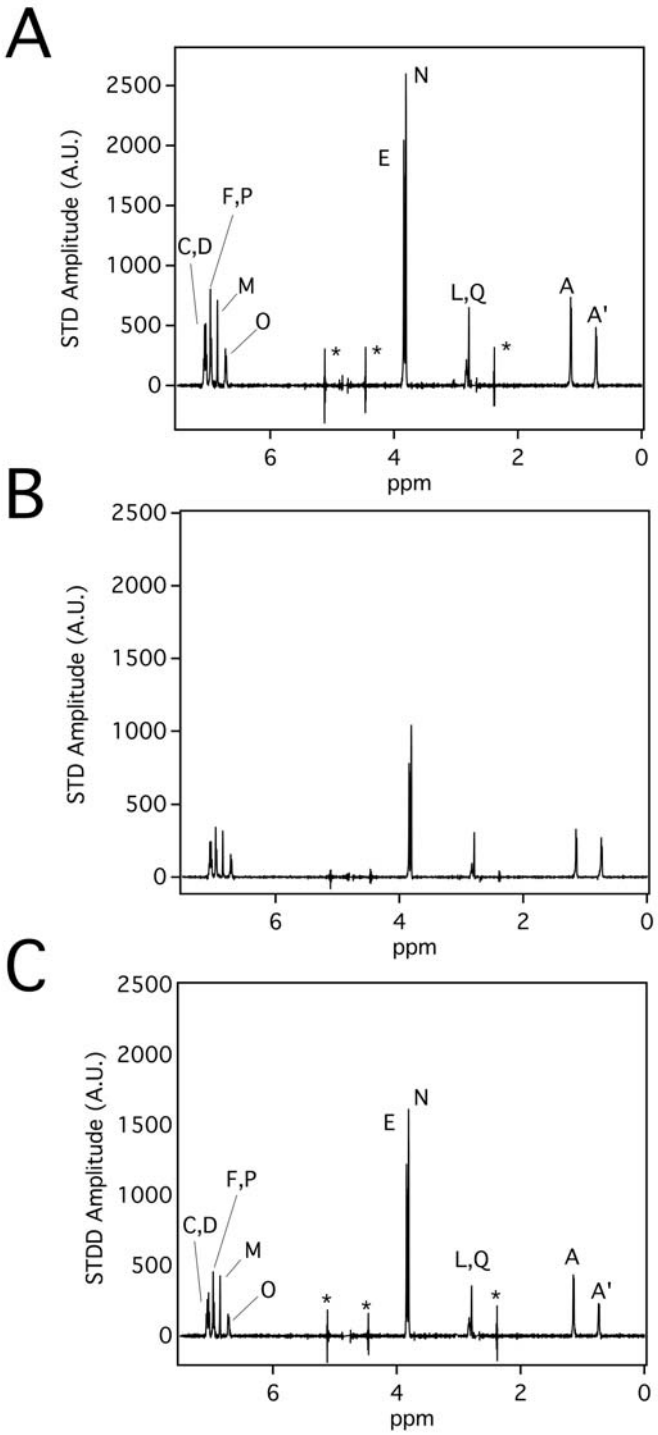
Supplementary Information



Supplementary Figure 1. ^{1}H proton NMR assignments for 1 mM verapamil in 100 mM KPi, pD 7.4 and 200 mM digoxin in d^{6}-DMSO.

Results

^{1}H proton NMR assignments for verapamil and digoxin. Figs. S1A and S1B show the ^{1}H NMR peak assignments for verapamil and digoxin, respectively. The verapamil and digoxin ^{1}H NMR peak assignments from this study were virtually identical to previous assignments [1-3]. Hydroxyl protons of digoxin were not visible in the ^{1}H proton NMR spectrum because of exchange broadening.



Supplementary Figure 2. Subtraction of background STD contributions from the saturation transfer between liposome and verapamil. A) STD NMR spectrum of 1 mM verapamil with 1 µM of the mouse Pgp transporter in proteoliposomes. B) STD NMR of 1 mM verapamil and liposomes in the absence of Pgp. C) STDD NMR of 1mM verapamil with with1 µM of the mouse Pgp transporter in proteoliposomes. The peaks denoted with an * are subtraction artifacts.

Supplementary Table 1. Fitting parameters and their averages used for fitting the ATPase activity curves with verapamil and digoxin.

verapamil, µM	0 – 500				0	4	8	125	
digoxin, µM	0	125	250	500	0 - 250				Average
V_{MAX0} [b]	526	506	543	560	641	451	605	470	538 ± 64
K_{D1} [a] V_{MAX1} [b]	1.83 3000	1.00 2500	3.00 3100	1.00 3164	- -	1.72 2500	1.85 2536	3.27 2500	1.95 ± 0.89 2757 ± 313
K_{D2} [a] V_{MAX2} [b]	211 1100	150 900	150 800	221 800	- -	250 808	175 1062	150 800	187 ± 41 896 ± 132
K_{D3} [a] V_{MAX3} [b]	- -	171 1993	120 1708	288 2077	239 1983	220 1703	207 2200	200 2200	206 ± 53 1981 ± 207
K_{D4} [a] K_{D5} [a] $V_{MAX4,5}$ [b]	- -	231 1.00 0.00	207 5.00 84.5	309 1.00 5.85	- -	208 4.52 43.9	394 3.92 292	400 5.00 300	292 ± 89 3.41 ± 1.91 121 ± 139
R- Correlation	0.994	0.992	0.968	0.921	0.994	0.986	0.909	0.704[c]	

[a] In units of µM
[b] In units of nmol min^{-1} mg^{-1}
[c] $X^2 = 2.05$

References

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