

Supplementary Materials

Properties of Therapeutic Deep Eutectic Solvents of L-Arginine and Ethambutol for Tuberculosis Treatment

Filipa Santos ¹, Maria Inês P.S. Leitão ² and Ana Rita C. Duarte ^{1,*}

¹ LAQV, REQUIMTE, Departamento de Química da Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal; mfca.santos@campus.fct.unl.pt

² ITQB—Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Estação Agronómica Nacional, Av. Da Repúblíca, 2780-157 Oeiras, Portugal; inesleitao@itqb.unl.pt

* Correspondence: aduarte@fct.unl.pt; Tel.: +351-212-949-680

Table S1. Different eutectic systems prepared, during optimization process.

Component A	Component B	Component C	Molar Ratio	Visual Aspect
Citric Acid	L-Arginine		1:1; 1:2; 2:1	White Solid
Citric Acid	L-Arginine	H ₂ O	1:1:3; 1:2:3; 2:1:3	White Solid
Citric Acid	L-Arginine	H ₂ O	1:1:5; 1:2:5	Transparent viscous liquid with white precipitate
Citric Acid	Ethambutol		1:1; 1:2; 2:1; 5:2; 7:3 1:2:4; 2:1:6; 4:1:4; 4:1:5; 4:1:7; 4:1:9; 5:1:2; 5:1:4; 5:1:9	White Solid
Citric Acid	Ethambutol	H ₂ O	1:1:6	White Solid
Citric Acid	Ethambutol	H ₂ O	1:1:6	Transparent viscous liquid with white precipitate

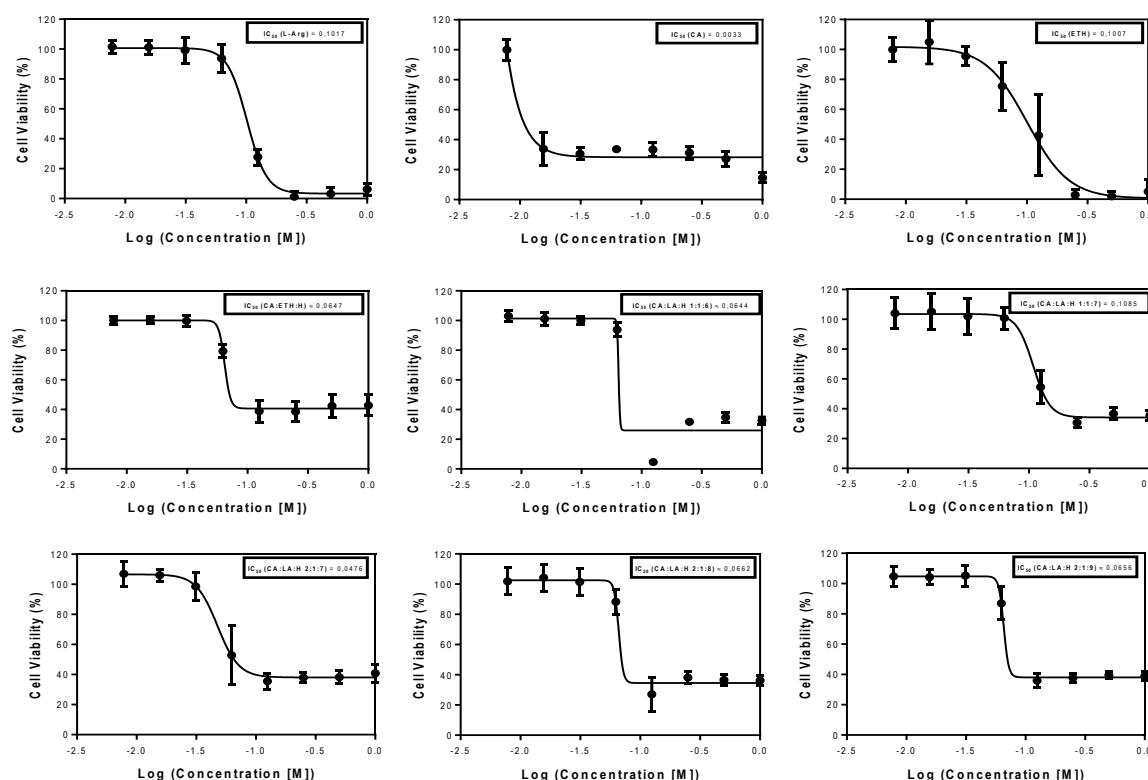


Figure S1. IC₅₀ graphs with log concentrations and cell viability used to determine IC₅₀.

Table S2. ^1H and ^{13}C NMR chemical shifts.

Compound	Chemical Shift ^1H (ppm)						Chemical Shift ^{13}C (ppm)			
	-CH ₂	-CH ₂	-COH	-COH	-OH	-NH	-C=O	2 x -C=O	-COH	2 x -CH ₂
Citric Acid	2,75	2,65	12,37	5,15	-	-	174,83	171,58	72,74	43,01
Ethambutol	-	-	-	-	9,24	5,40	-	-	-	-
Citric Acid:Ethambutol:H ₂ O (2:1:10)	2,75	2,65	12,34	5,15	9,14	5,40	174,67	171,45	72,59	42,82
Citric Acid:L-Arginine:H ₂ O (1:1:6)	2,57	2,50	-	-	-	-	177,34	172,09	71,87	44,50
Citric Acid:L-Arginine:H ₂ O (1:1:7)	2,58	2,51	-	-	-	-	176,97	171,70	71,67	44,29
Citric Acid:L-Arginine:H ₂ O (2:1:7)	2,64	2,56	-	-	-	-	176,12	171,52	71,99	43,72
Citric Acid:L-Arginine:H ₂ O (2:1:8)	2,66	2,57	-	-	-	-	176,02	171,65	72,14	43,66
Citric Acid:L-Arginine:H ₂ O (2:1:9)	2,65	2,56	-	-	-	-	176,28	171,82	72,22	43,82