

Table S1: Exact masses of NAT22 and its metabolites generated by microsomes from different mammals were obtained after LC-ESI-MS/MS.

Table S2: Docking energy (ordered by best interaction energy) and types of intermolecular interactions observed between the ligands and the cTXNPx enzyme.

Supplementary Table S1: Exact masses of NAT22 and its metabolites generated by microsomes from different mammals were obtained after LC-ESI-MS/MS.

Analyte (E)	Accurate mass (m/z)	Human		Dog		Rat		Mouse		Molecular Formula
		Exact mass (m/z)	Error (ppm)	Exact mass (m/z)	Error (ppm)	Exact mass (m/z)	Error (ppm)	Exact mass (m/z)	Error (ppm)	
NAT22	344,11286	344,11230	1,63	344,11206	2,32	344,11191	2,76	344,11218	1,98	C ₁₈ H ₁₇ NO ₆
M1	346,09213	346,09186	2,92	346,09149	1,85	346,09186	0,78	346,09171	1,21	C ₁₇ H ₁₅ NO ₇
M2	316,08156	316,08112	1,39	316,08099	1,80	316,08081	2,37	316,08145	0,35	C ₁₆ H ₁₃ NO ₆
M3	346,09213	346,09189	0,69	346,09143	2,02	346,09140	2,11	346,09164	1,42	C ₁₇ H ₁₅ NO ₇
M4	330,09721	330,09680	1,24	330,09641	2,42	330,09637	2,54	330,09650	2,15	C ₁₇ H ₁₅ NO ₆
M5	360,10778	360,10745	0,92	360,10690	2,44	360,10687	2,53	360,10709	1,92	C ₁₈ H ₁₇ NO ₇
M6	346,09213	346,09180	0,95	346,09140	2,11	346,09131	2,37	-	-	C ₁₇ H ₁₅ NO ₇
M7	330,09721	330,09708	0,39	330,09644	2,33	330,09659	1,88	330,09677	1,33	C ₁₇ H ₁₅ NO ₆

Supplementary Table S2: Docking energy (ordered by best interaction energy) and types of intermolecular interactions observed between the ligands and the cTXNPx enzyme.

Ligands	Docking energy (kcal/mol)	H-bond	Pi-sigma	Pi-alkyl	Alkyl	Van der Waals
M2	-6,045	Gln-289	-	Pro-188	-	Pro-186, Glu-187, Ser-191, Val-192, Phe-196, Phe-247, Leu-245 , Pro-249 , Lys-293, Gly-294
M4	-5,970	Gln-289	-	Pro-188	Pro-249	Pro-186, Glu-187, Ser-191, Val-192, Phe-196, Phe-247, Leu-245, Thr-248 , Lys-293, Gly-294
NAT22	-5,964	Gln-289	Thr-248	Pro-188	Leu-245, Pro-249	Pro-186, Glu-187, Ser-191, Val-192, Phe-196, Phe-247, Lys-293, Gly-294
M7	-5,927	Gln-289	-	Pro-188	Leu-245	Pro-186, Glu-187, Ser-191, Val-192, Phe-196, Phe-247, Thr-248 , Lys-293, Pro-249 , Gly-294
M3	-5,886	Gln-289	-	Pro-188	Pro-188, Pro-249	Glu-187, Ser-191, Val-192, Phe-196, Leu-245, Phe-247, Thr-248, Lys-293, Gly-294
M1	-5,851	Gln-289	Thr-248	Pro-188	-	Pro-186, Glu-187, Ser-191, Val-192, Phe-196, Phe-247, Pro-249, Lys-293, Gly-294
M6	-5,841	Gln-289	-	Pro-188	Leu-245	Pro-186, Glu-187, Ser-191, Val-192, Phe-196, Phe-247, Thr-248, Lys-293, Pro-249, Gly-294
M5	-5,831	Gln-289	-	Pro-188	Pro-186, Leu-245, Pro-249	Glu-187, Ser-191, Val-197, Phe-196, Phe-247, Thr-248, Lys-293, Gly-294