

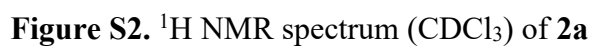
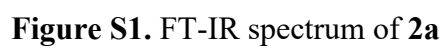
Silver-*N*-heterocyclic complexes against *Leishmania major*: *In vitro*, *in vivo*, and *in-silico* therapeutic activities

**Neslihan Şahin ^{1,2}, Zübeyda Akın Polat ³, Derya Gül Gülpınar ³, Ahmet Duran Ataş ³,
Elvan Üstün ^{4,*}, İsmail Özdemir ⁵ and David Sémeril ^{6,*}**

- 1 Malatya Turgut Özal University, Faculty of Engineering and Natural Sciences, Department of Engineering Basic Sciences, 44900 Malatya, Türkiye
- 2 Cumhuriyet University, Faculty of Education, Department of Science Education, 58040 Sivas, Türkiye
- 3 Cumhuriyet University, Department of Medical Parasitology, School of Medicine, 58140 Sivas, Türkiye
- 4 Ordu University, Faculty of Art and Science, Department of Chemistry, 52200 Ordu, Türkiye
- 5 İnönü University, Faculty of Art and Science, Department of Chemistry, 44280 Malatya, Türkiye
- 6 Strasbourg University, Synthèse Organométallique et Catalyse, UMR-CNRS 7177, 67008 Strasbourg, France

Supporting Information

Content		Page
Figure S1	FT-IR spectrum of 2a	3
Figure S2	¹ H NMR spectrum of 2a	3
Figure S3	¹³ C{ ¹ H} NMR spectrum of 2a	4
Figure S4	FT-IR spectrum of 2b	4
Figure S5	¹ H NMR spectrum of 2b	5
Figure S6	¹³ C{ ¹ H} NMR spectrum of 2b	6
Figure S7	¹ H NMR spectra of 2b at different time intervals	6
Figure S8	Interaction details and residues of 1a against LaGP63	8
Figure S9	Interaction details and residues of 1b against LaGP63	8
Figure S10	Interaction details and residues of 2a against LaGP63	9
Figure S11	Interaction details and residues of 2b against LaGP63	9
Figure S12	Interaction details and residues of 1a against LaARG	10
Figure S13	Interaction details and residues of 1b against LaARG	10
Figure S14	Interaction details and residues of 2a against LaARG	11
Figure S15	Interaction details and residues of 2b against LaARG	11
Figure S16	Interaction details and residues of 1a against <i>N</i> -myristoyltransferase	12
Figure S17	Interaction details and residues of 1b against <i>N</i> -myristoyltransferase	12
Figure S18	Interaction details and residues of 2b against <i>N</i> -myristoyltransferase	13
Figure S19	Interaction details and residues of 2b against <i>N</i> -myristoyltransferase	13
Figure S20	Interaction details and residues of 1a against farnesyl diphosphate synthase	14
Figure S21	Interaction details and residues of 1b against farnesyl diphosphate synthase	14
Figure S22	Interaction details and residues of 2a against farnesyl diphosphate synthase	15
Figure S23	Interaction details and residues of 2b against farnesyl diphosphate synthase	15



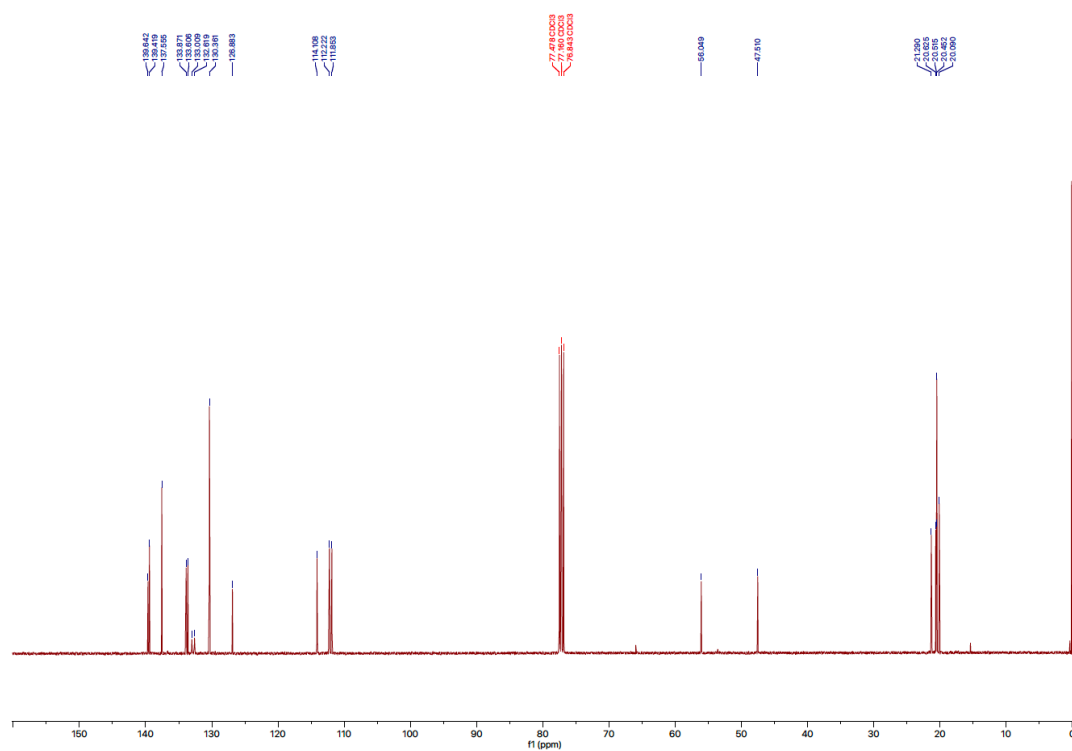


Figure S3. ¹³C{¹H} NMR spectrum (CDCl₃) of **2a**

Chloro[1-methallyl-3-(4-chlorobenzyl)-5,6-dimethylbenzimidazole-2-ylidene]silver(I) (2b)

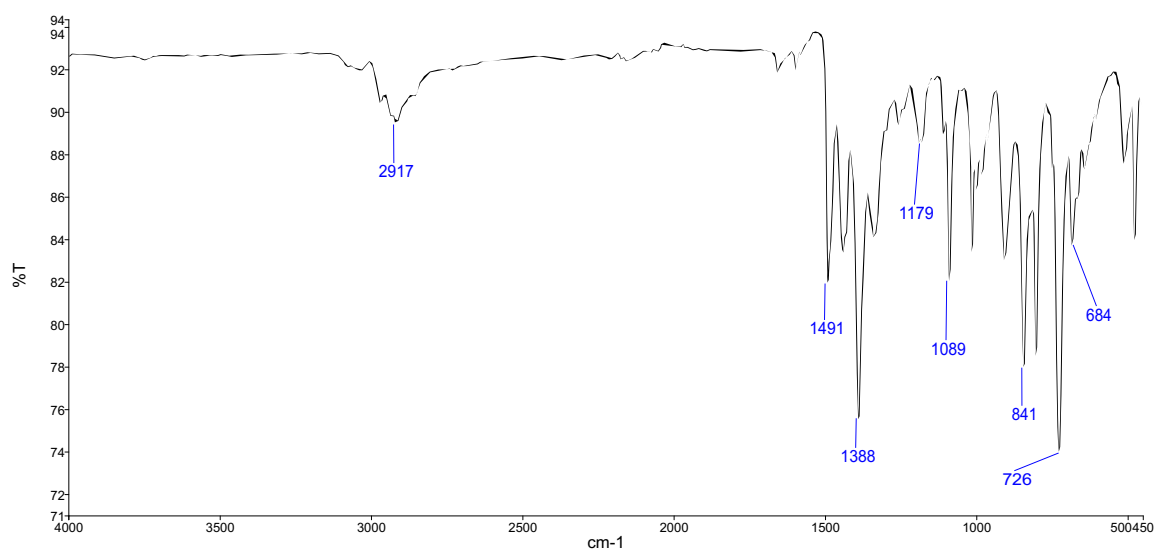
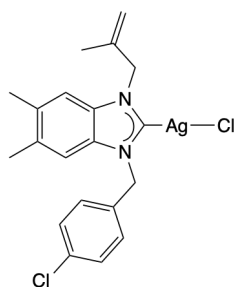


Figure S4. FT-IR spectrum of **2b**

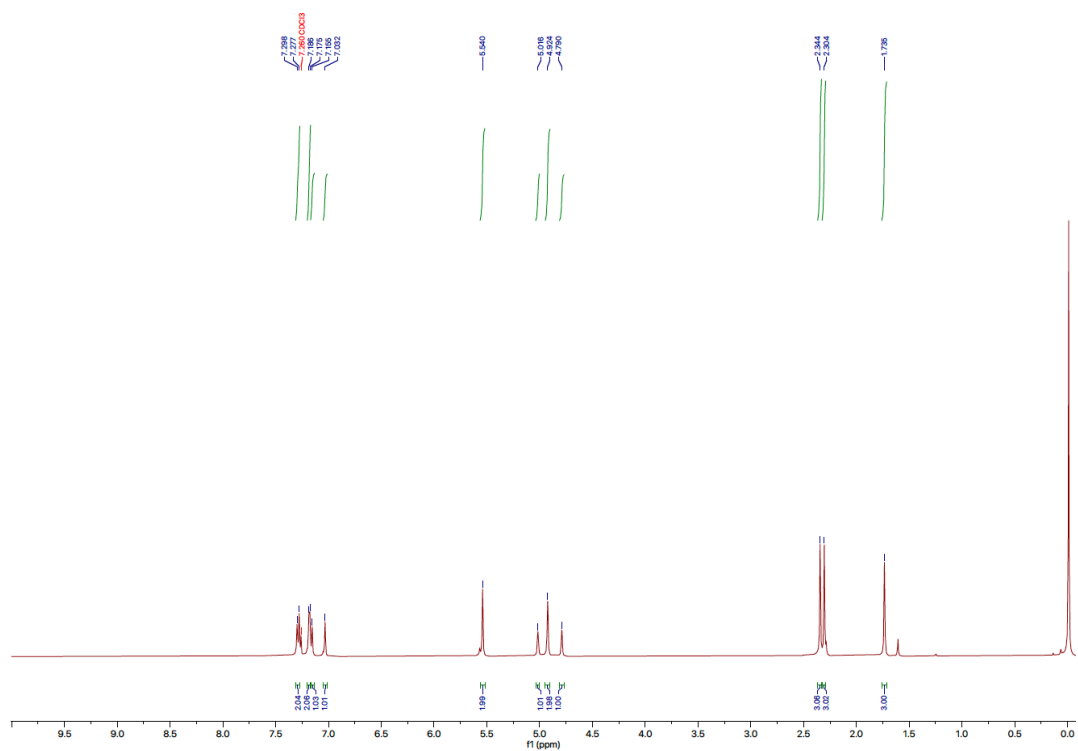


Figure S5. ¹H NMR spectrum (CDCl₃) of **2b**

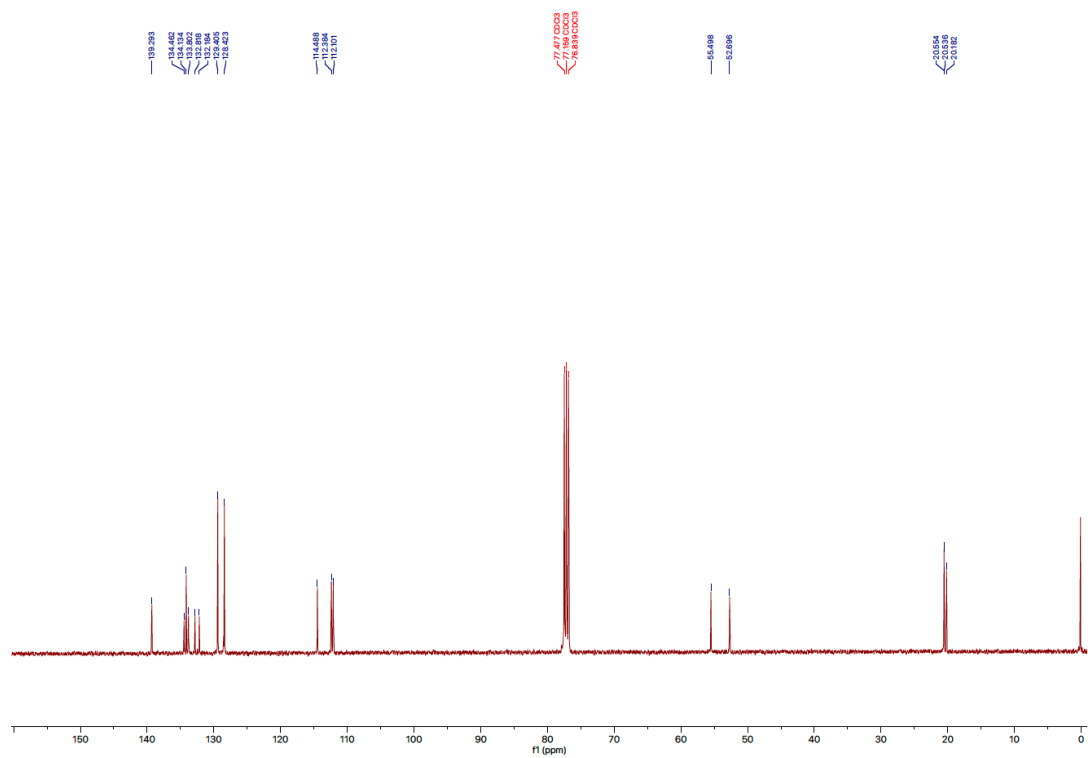


Figure S6. ¹³C {¹H} NMR spectrum (CDCl₃) of **2b**

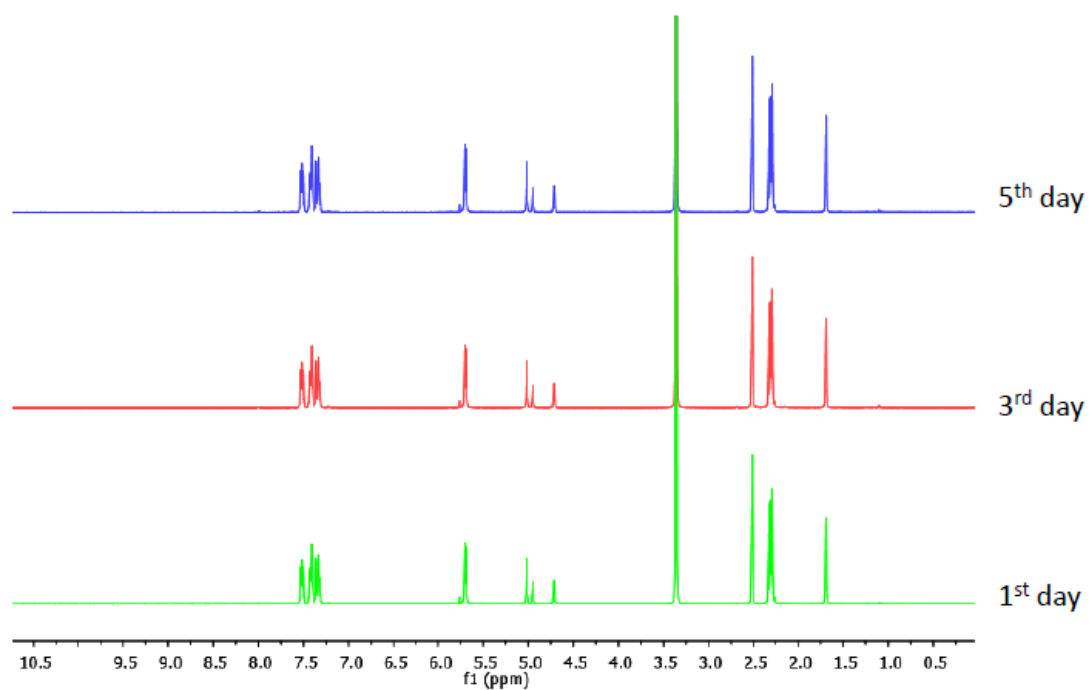


Figure S7. ^1H NMR spectra of **2b** at different time intervals

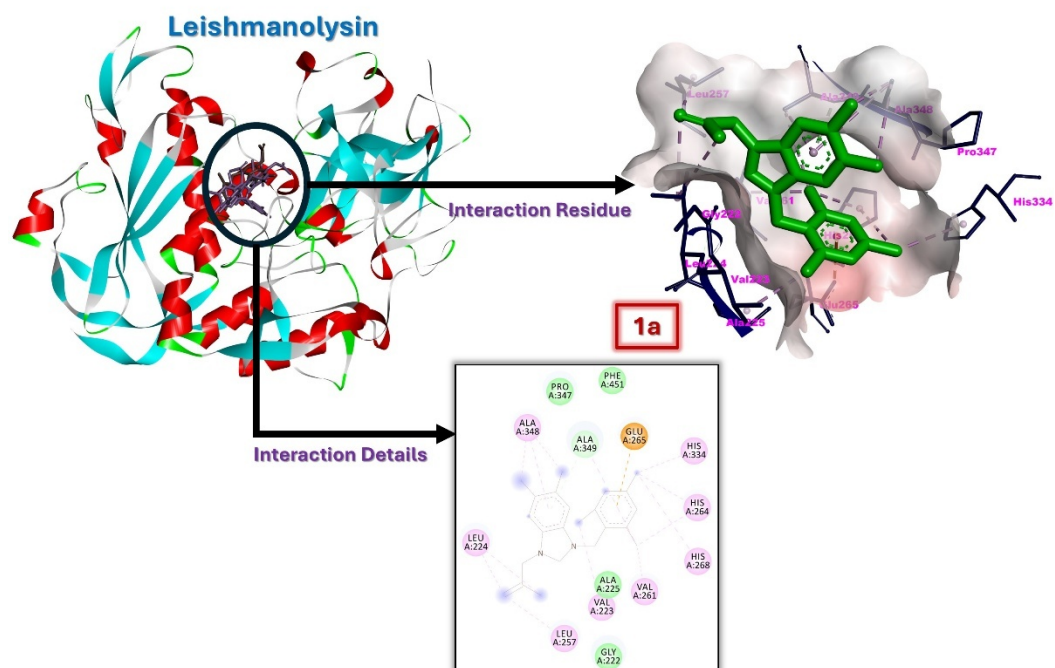


Figure S8. Interaction details and residues of **1a** against LaGP63

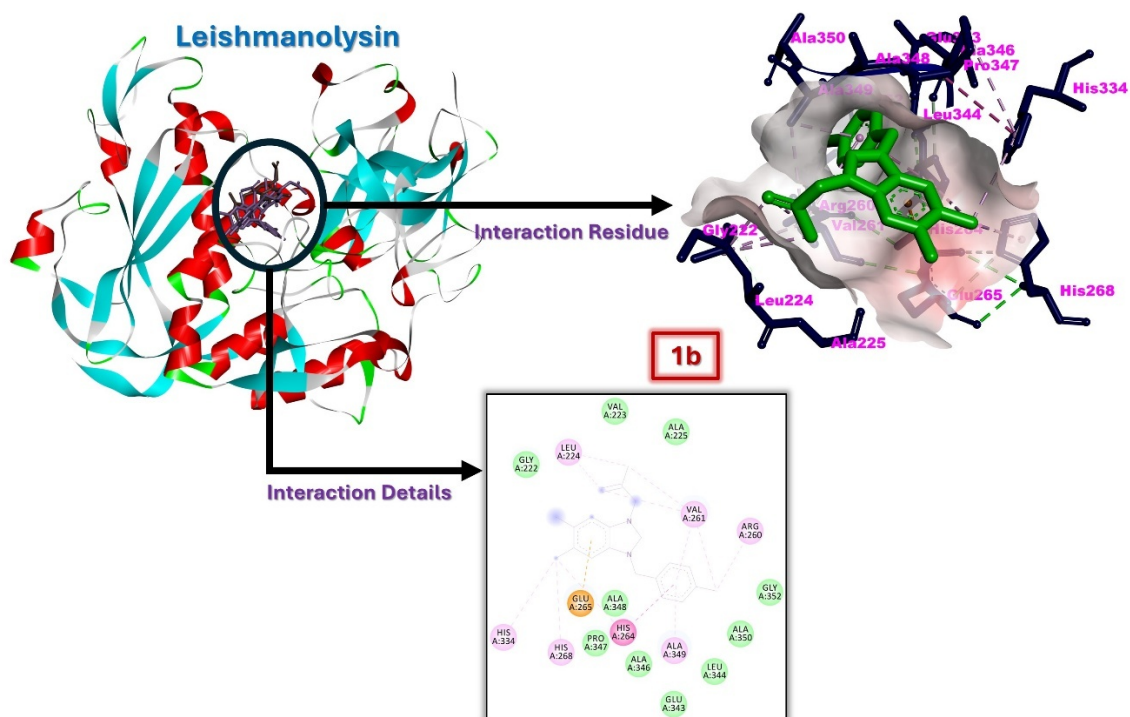


Figure S9. Interaction details and residues of **1b** against LaGP63

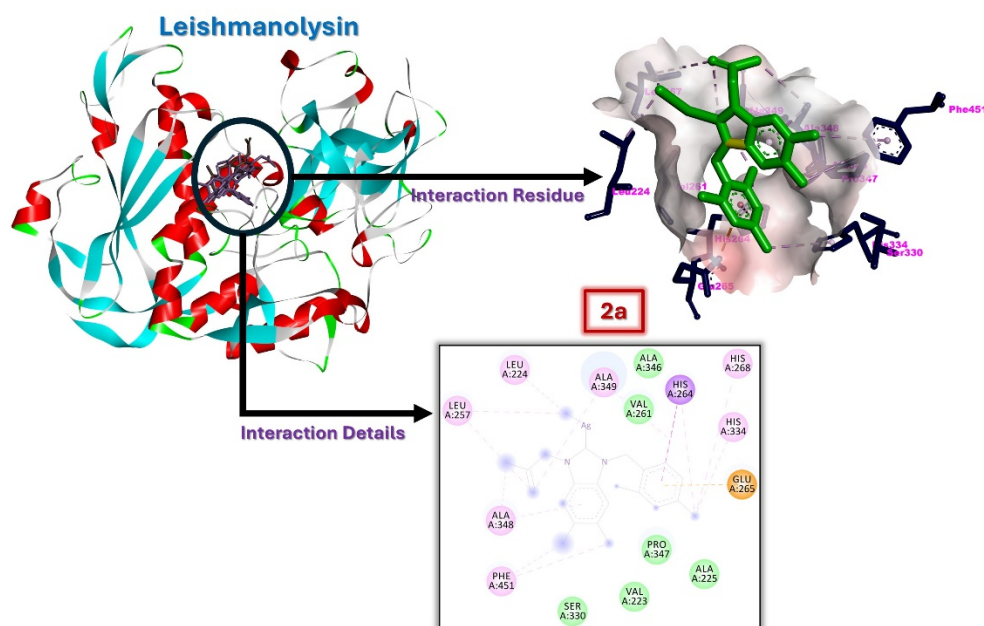


Figure 10. Interaction details and residues of **2a** against LaGP63

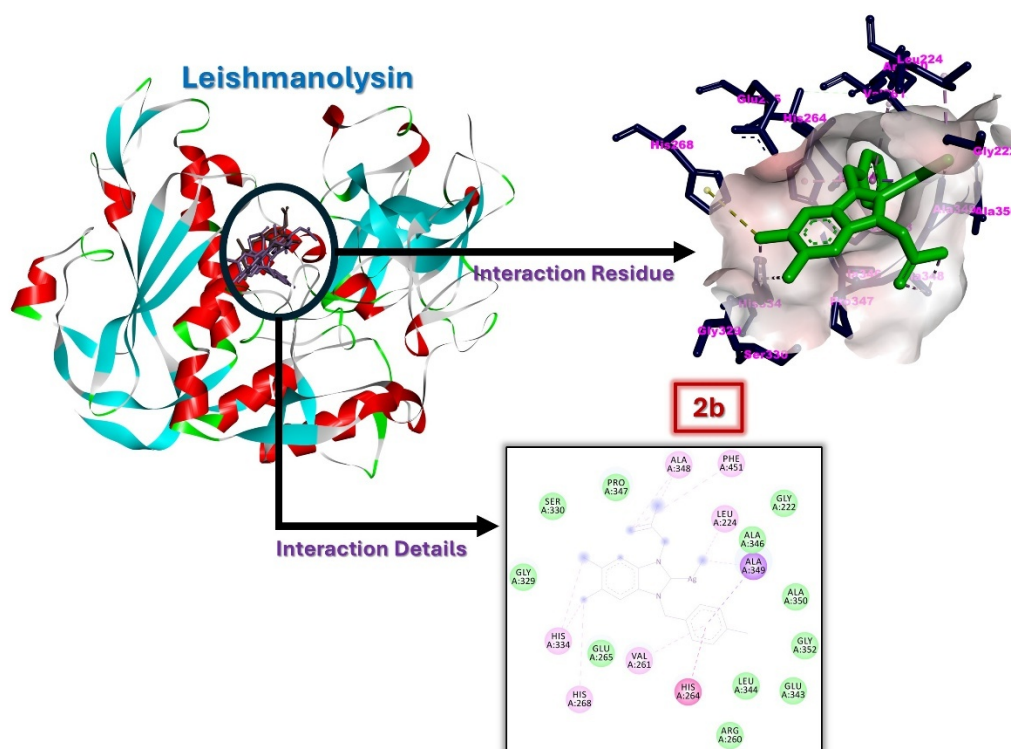


Figure S11. Interaction details and residues of **2b** against LaGP63

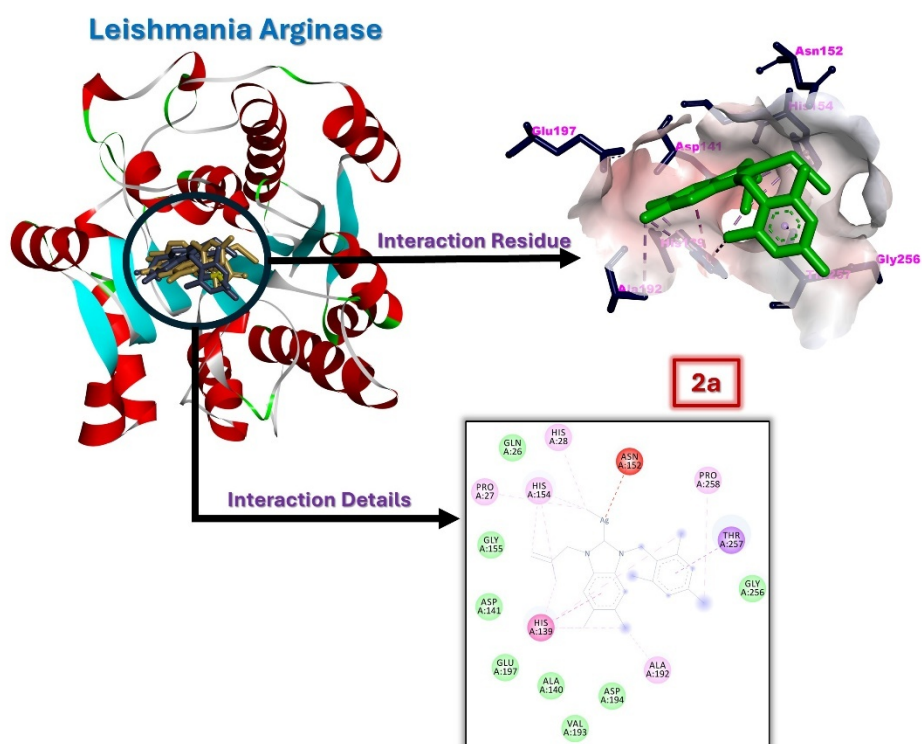


Figure S14. Interaction details and residues of **2b** against LaARG

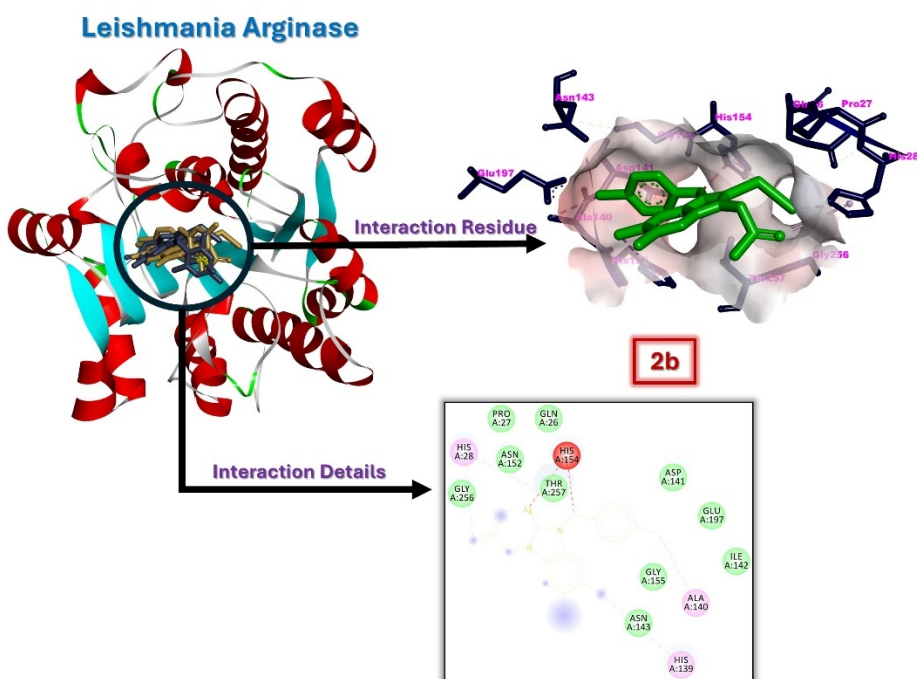


Figure S15. Interaction details and residues of **2b** against LaARG

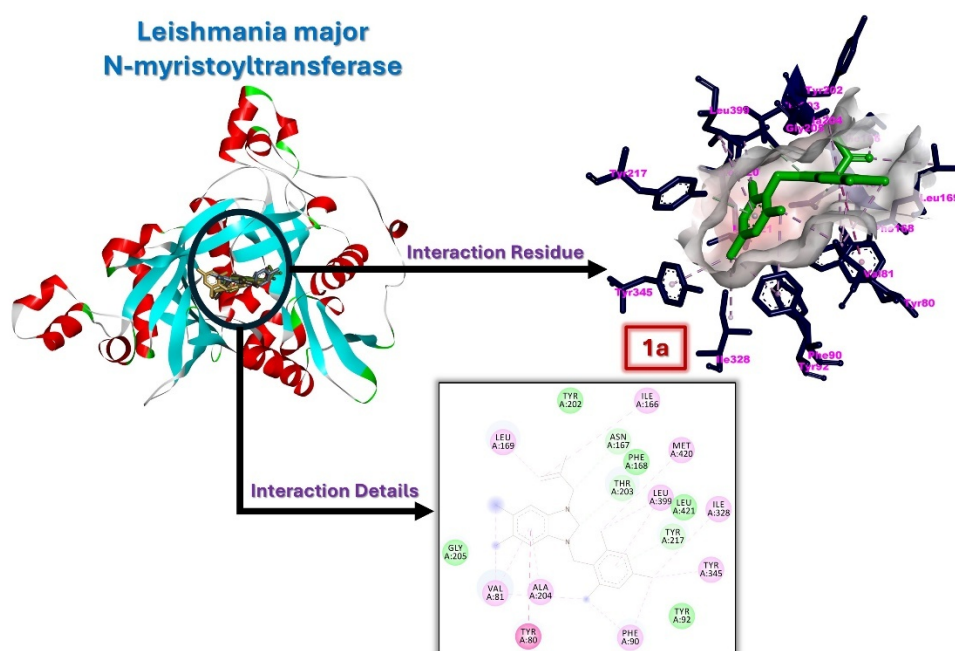


Figure S16. Interaction details and residues of **1a** against *N*-myristoyltransferase

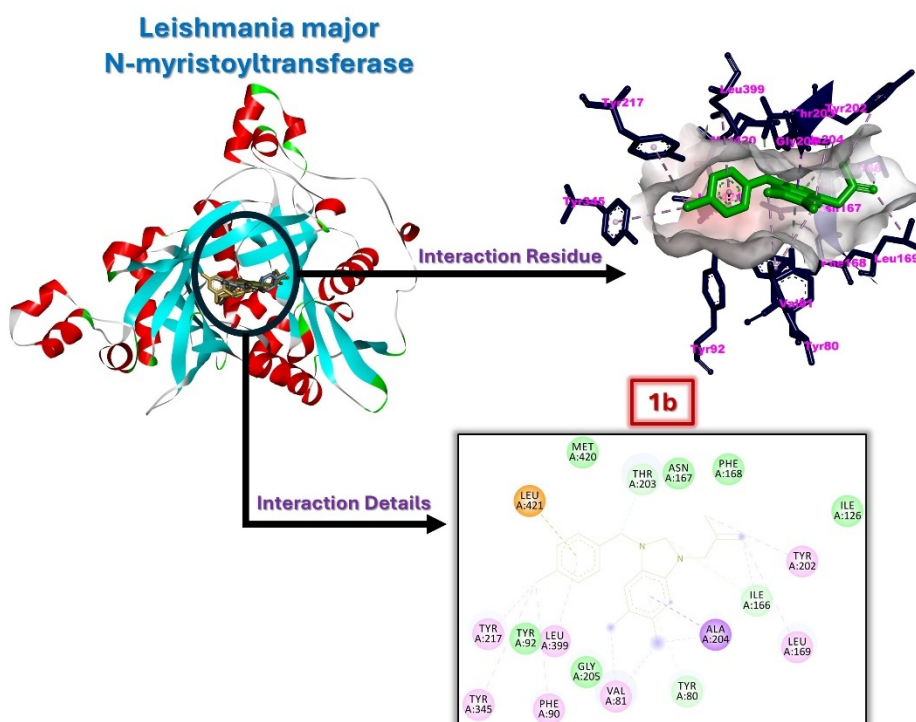


Figure S17. Interaction details and residues of **1b** against *N*-myristoyltransferase

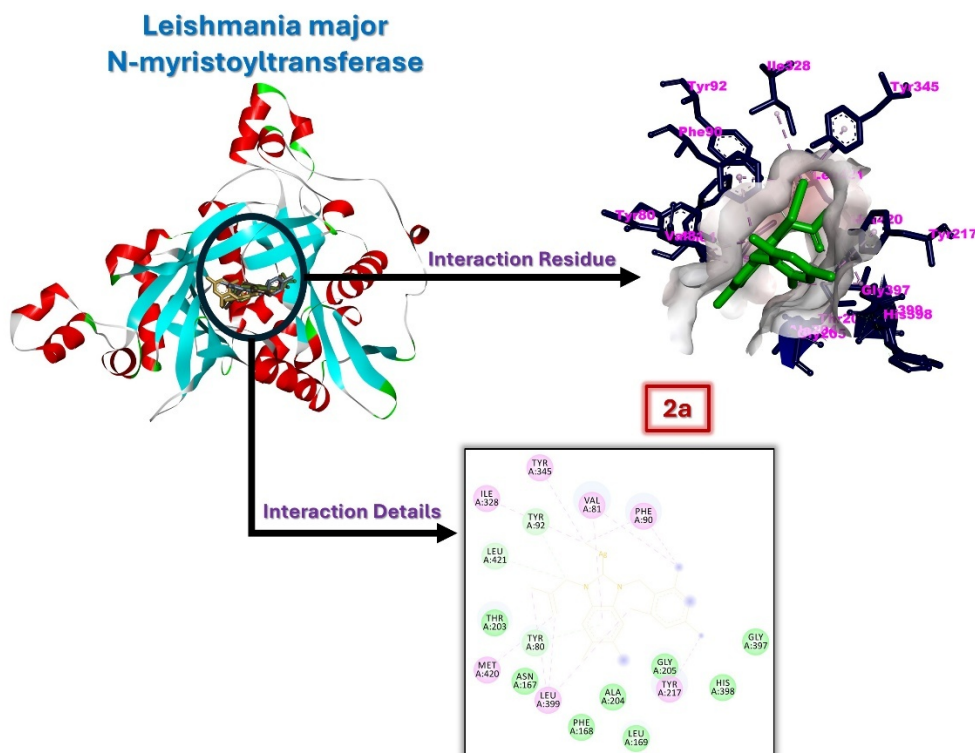


Figure S18. Interaction details and residues of **2a** against *N*-myristoyltransferase

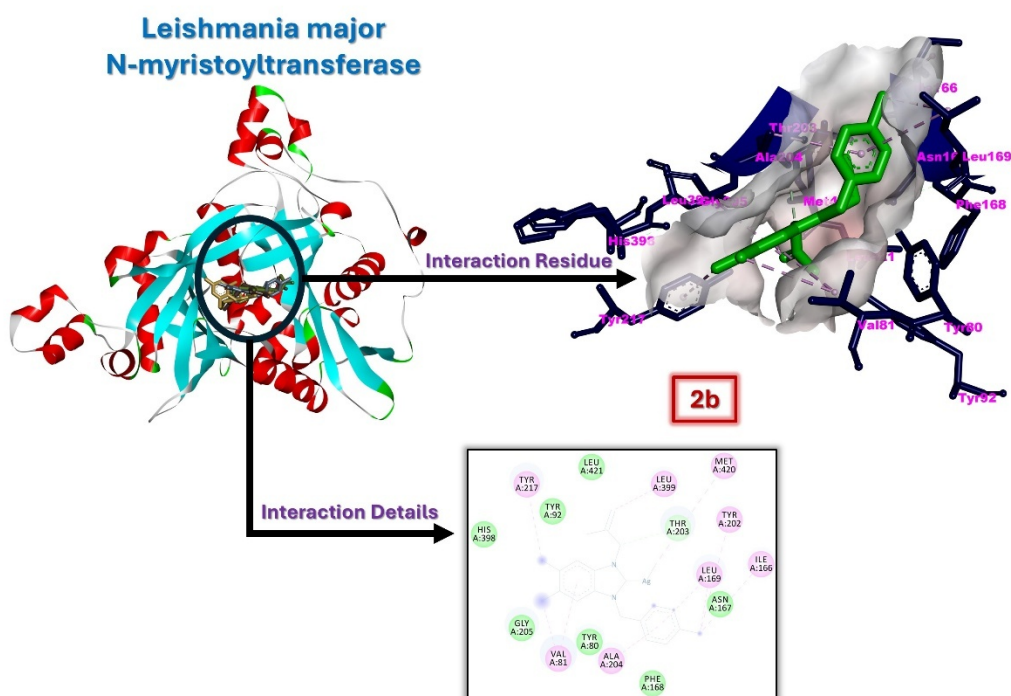


Figure S19. Interaction details and residues of **2b** against *N*-myristoyltransferase

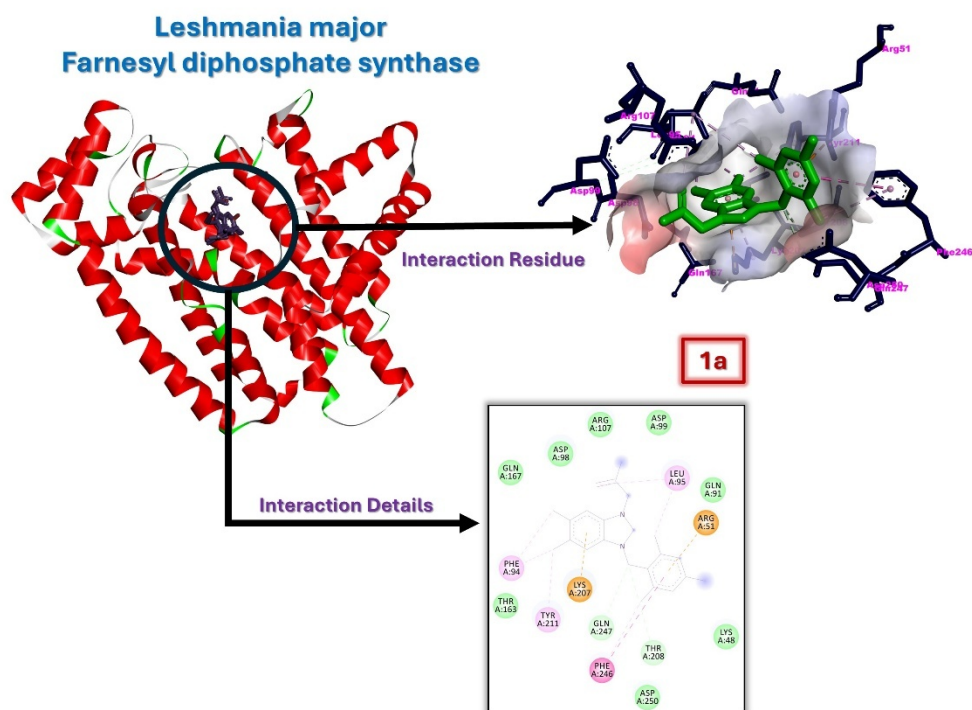


Figure S20. Interaction details and residues of **1a** against farnesyl diphosphate synthase

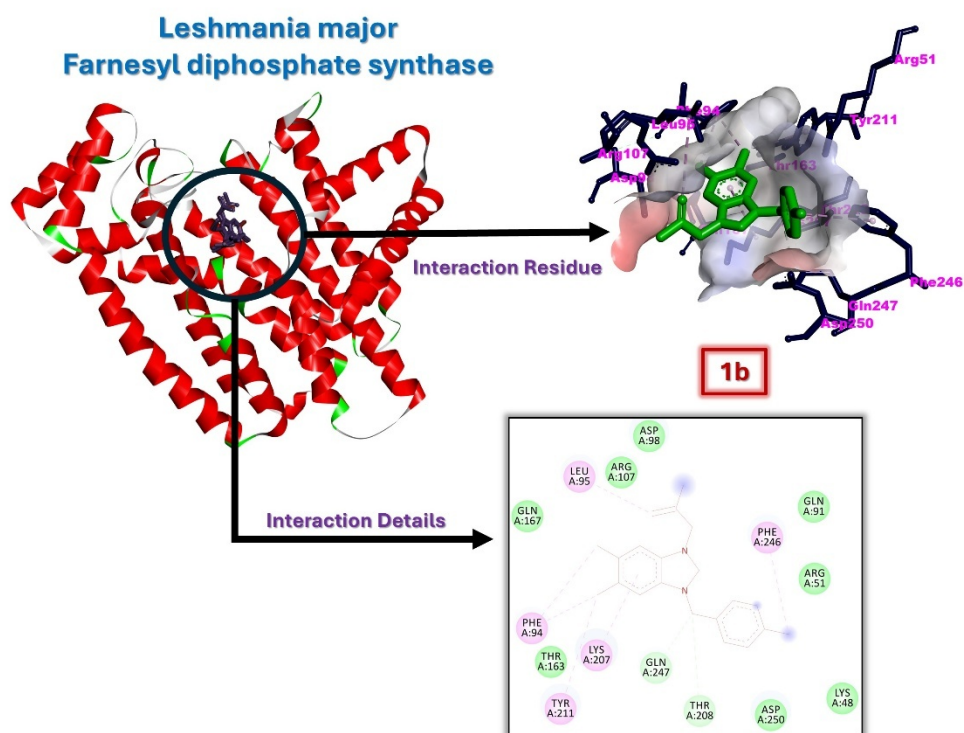


Figure S21. Interaction details and residues of **1b** against farnesyl diphosphate synthase

