

Supplementary Material

Enhancing Giardicidal Activity and Aqueous Solubility through the Development of “RetroABZ”, a Regioisomer of Albendazole: In Vitro, In Vivo, and In Silico Studies [†]

Carlos Martínez-Conde ¹, Blanca Colín-Lozano ¹, Abraham Gutiérrez-Hernández ¹, Emanuel Hernández-Núñez ², Lilián Yépez-Mulia ³, Luis Fernando Colorado-Pablo ⁴, Rodrigo Aguayo-Ortiz ⁴, Jaime Escalante ⁵, Julio C. Rivera-Leyva ¹, Jessica Nayelli Sánchez-Carranza ¹, Elizabeth Barbosa-Cabrera ⁶ and Gabriel Navarrete-Vazquez ^{1,*}

¹ Facultad de Farmacia, Universidad Autónoma del Estado de Morelos, Cuernavaca 62209, Morelos, Mexico; mcc_ff@uaem.mx (C.M.-C.); clbi_ff@uaem.mx (B.C.-L.); ghaa_ff@uaem.mx (A.G.-H.); julio.rivera@uaem.mx (J.C.R.-L.); jessica.sanchez@uaem.mx (J.N.S.-C.)

² Departamento de Recursos del Mar, Centro de Investigación y de Estudios Avanzados, IPN, Unidad Mérida, Merida 97310, Yucatán, Mexico; emanuel.hernandez@cinvestav.mx

³ Unidad de Investigación Médica en Enfermedades Infecciosas y Parasitarias, Unidad Médica de Alta Especialidad-Hospital de Pediatría, Centro Médico Nacional Siglo XXI, Instituto Mexicano del Seguro Social, Mexico City 06720, Mexico; lilianyepez@yahoo.com

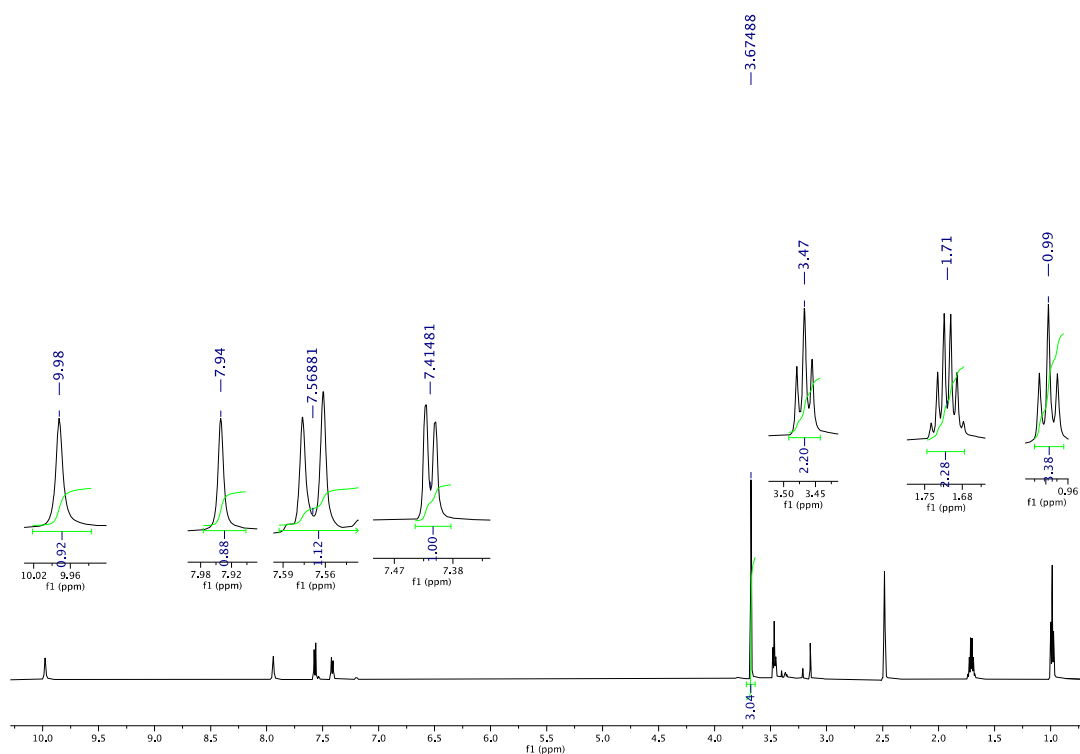
⁴ Departamento de Farmacia, Facultad de Química, Universidad Nacional Autónoma de México, Mexico City 04510, Mexico; fernando1303@comunidad.unam.mx (L.F.C.-P.); rodaguayo@comunidad.unam.mx (R.A.-O.)

⁵ Centro de Investigaciones Químicas-IICBA, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Cuernavaca 62209, Morelos, Mexico; jaime@uaem.mx

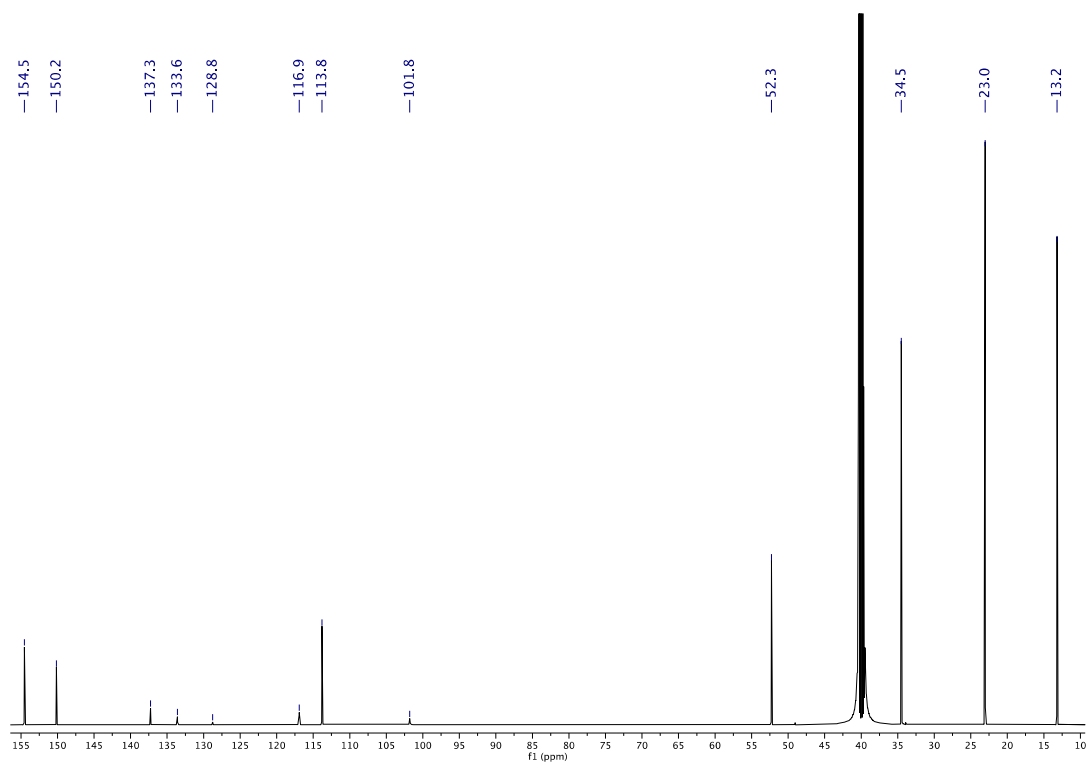
⁶ Sección de Estudios de Posgrado e Investigación, Escuela Superior de Medicina, IPN, Mexico City 11340, Mexico; rebc78@yahoo.com.mx

* Correspondence: gabriel_navarrete@uaem.mx; Tel.: +52-777-329-7089 (ext. 2322)

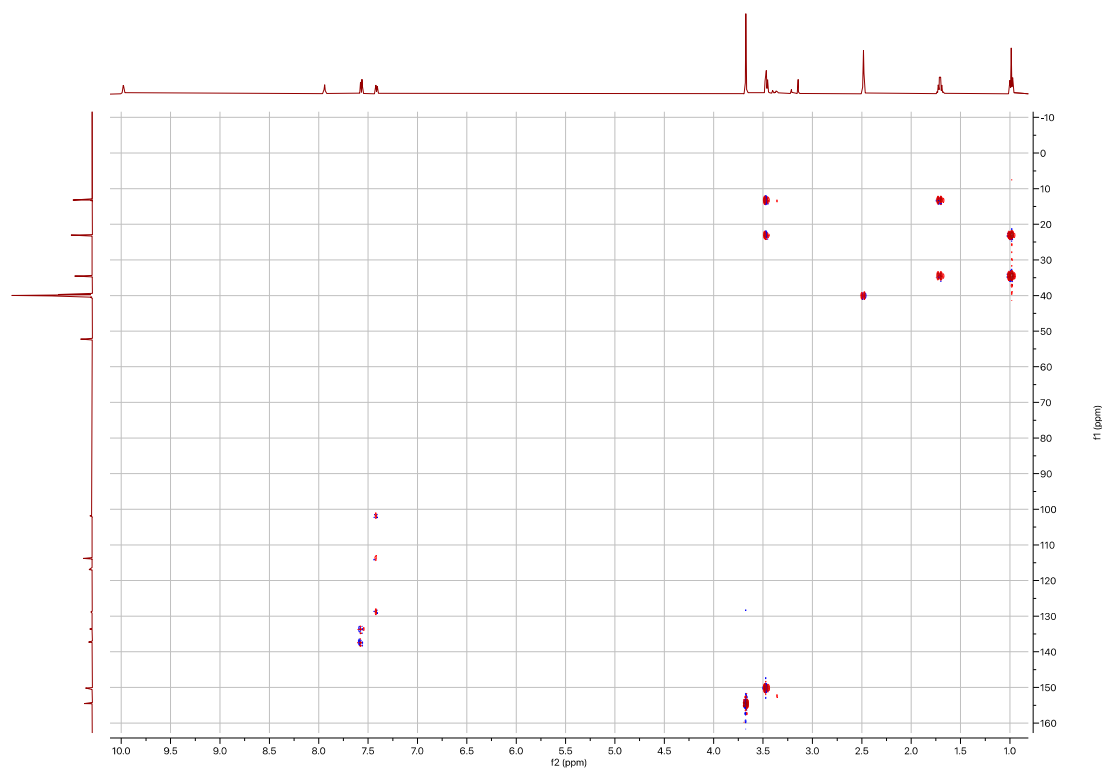
[†] Taking in part of the Ph.D. thesis of C. Martínez-Conde.



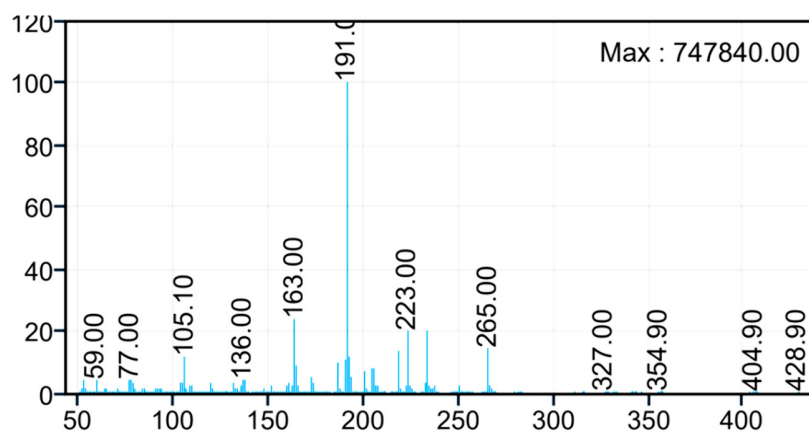
¹H NMR: Methyl (2-(propylthio)-1H-benzo[d]imidazol-5-yl)carbamate (RetroABZ, 1)



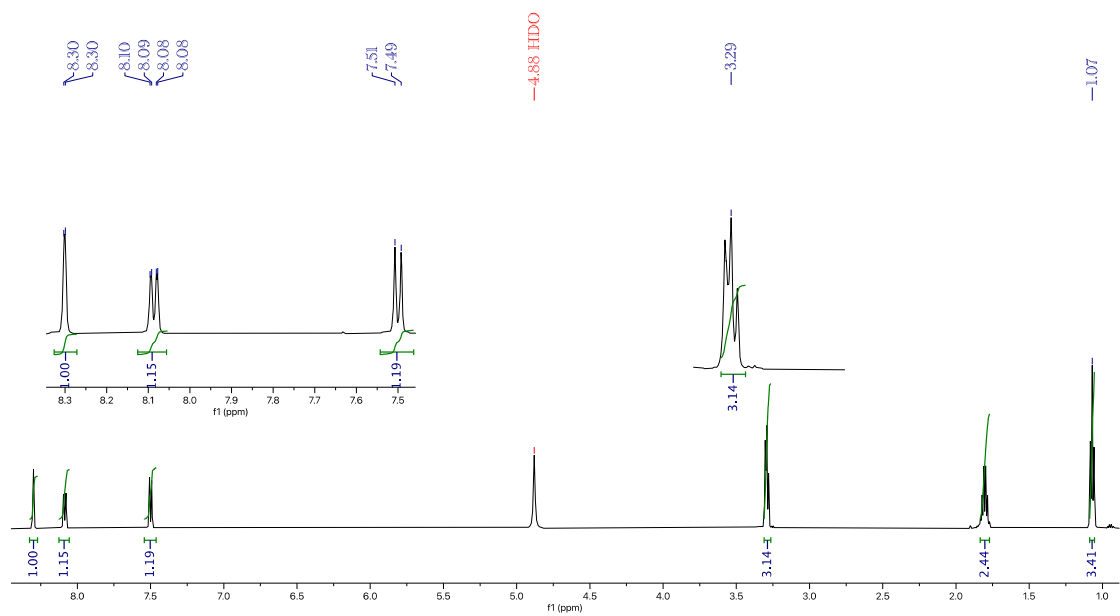
¹³C NMR: Methyl (2-(propylthio)-1H-benzo[d]imidazol-5-yl)carbamate (RetroABZ, 1)



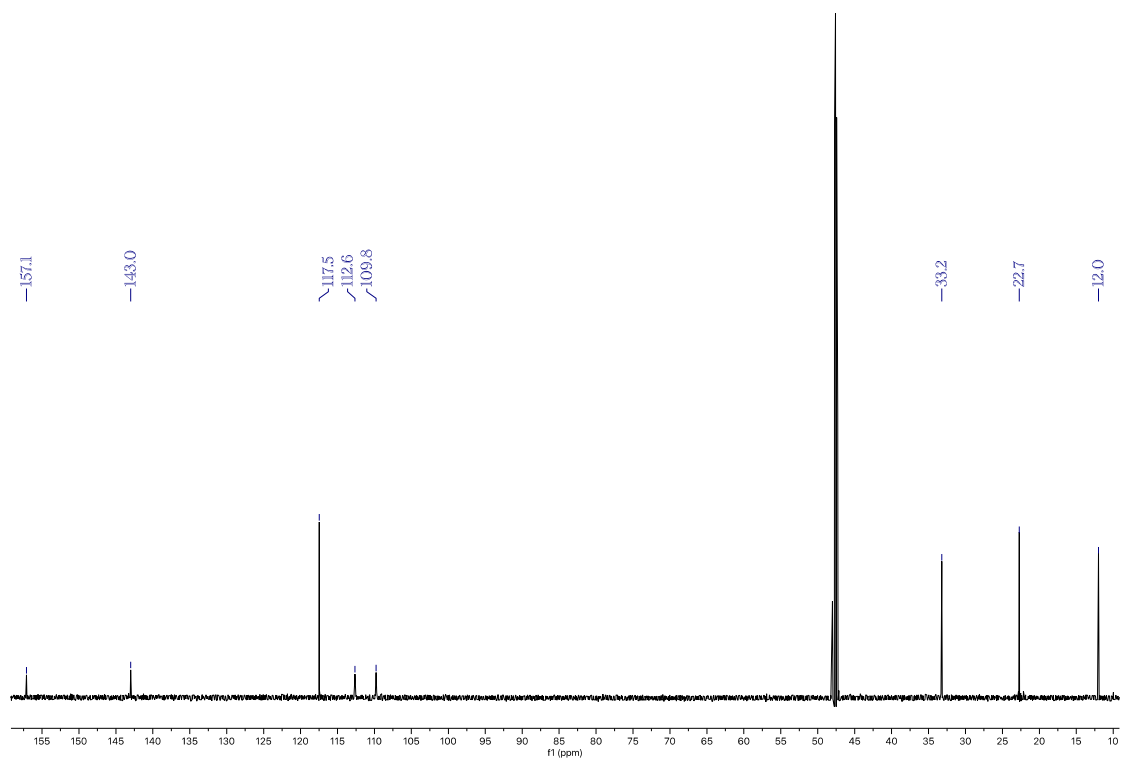
HMBC, Methyl (2-(propylthio)-1H-benzo[d]imidazol-5-yl)carbamate (**RetroABZ, 1**)



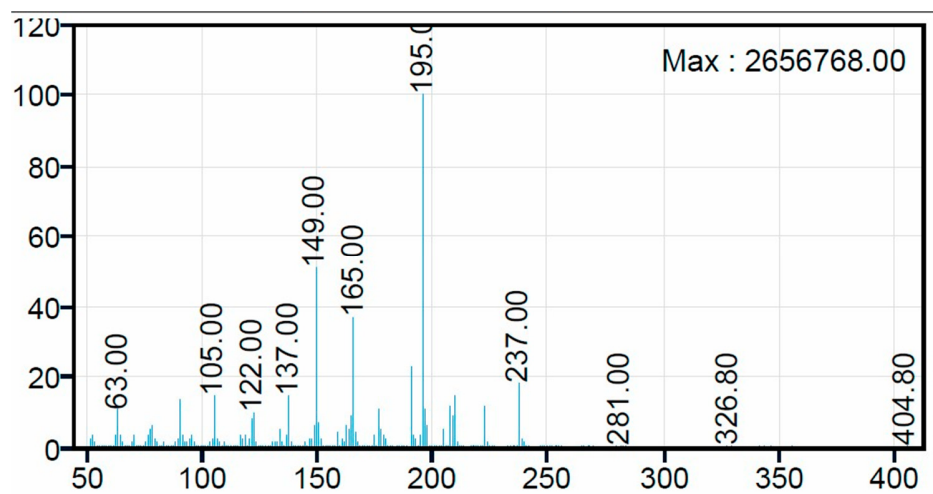
MS: m/z (% rel. Int), Methyl (2-(propylthio)-1H-benzo[d]imidazol-5-yl)carbamate (**RetroABZ, 1**)



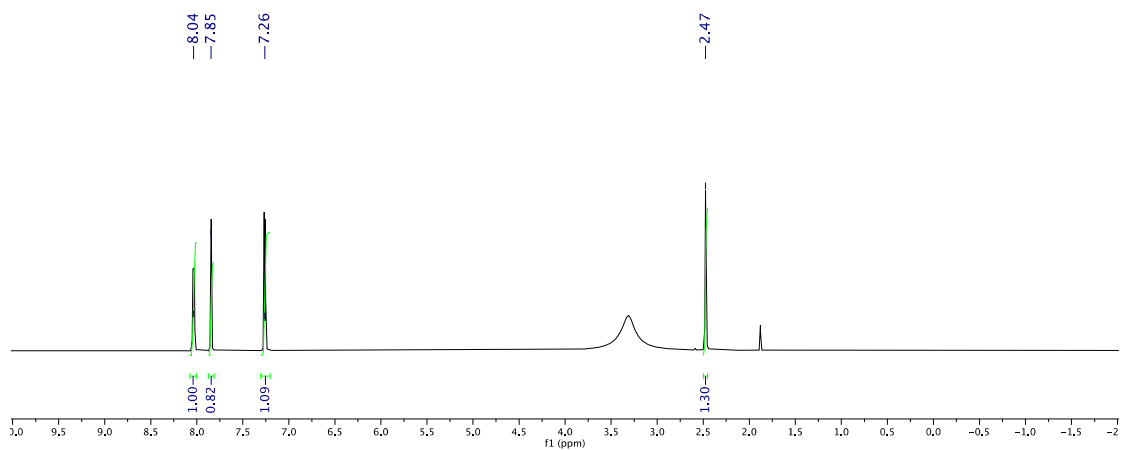
¹H NMR, 5-Nitro-2-(propylthio)-1H-benzo[d]imidazole



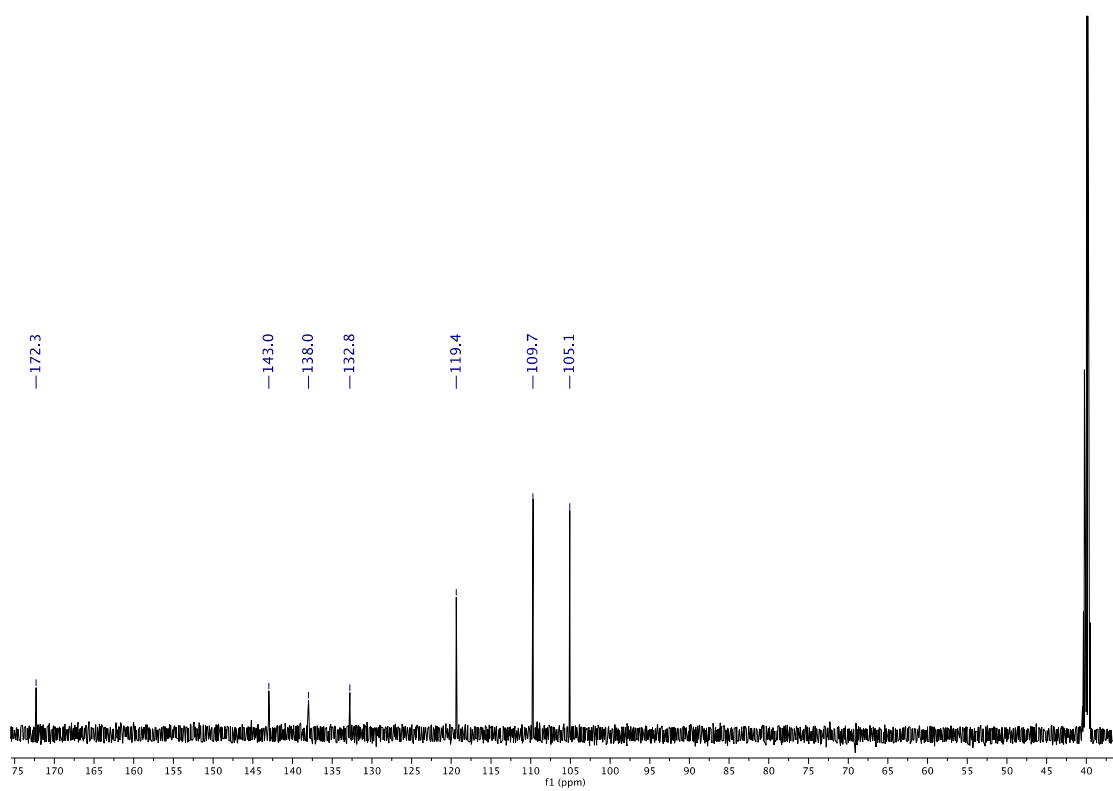
¹³C NMR, 5-Nitro-2-(propylthio)-1H-benzo[d]imidazole



MS: m/z (% rel. Int), 5-Nitro-2-(propylthio)-1H-benzo[d]imidazole



¹H NMR, 5-Nitro-1H-benzo[d]imidazole-2-thiol (**2**)



¹³C NMR, 5-Nitro-1H-benzo[d]imidazole-2-thiol (**2**)