

Supporting Information

Nature-inspired 1-phenylpyrrolo[2,1-*a*]isoquinoline scaffold for novel antiproliferative agents circumventing P-glycoprotein-dependent multidrug resistance

Alisa A. Nevskaya ^{1a}, Rosa Purgatorio ², Tatiana Borisova ^{1a}, Alexey V. Varlamov ^{1a}, Lada V. Anikina ³, Arina Obydennik ^{1a}, Elena Yu. Nevskaya ^{1b}, Mauro Niso ², Nicola A. Colabufo², Antonio Carrieri ², Marco Catto ², Modesto de Candia ², Leonid G. Voskressensky ^{1a} and Cosimo D. Altomare ^{2*}

¹ ^aOrganic Chemistry Department, ^bGeneral and Inorganic Chemistry Department, Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklaya St., 117198 Moscow, Russian Federation

² Department of Pharmacy-Pharmaceutical Sciences, University of Bari Aldo Moro, Via E. Orabona 4, 70125 Bari, Italy

³ Institute of Physiologically Active Compounds of the FSBI of the Federal Research Center for Problems of Chemical Physics and Medicinal Chemistry of the RAS, 1 Severnyi Proezd, 142432 Chernogolovka, Russian Federation

* Correspondence: cosimodamiano.altomare@uniba.it

Table of content

¹ H and ¹³ C-NMR of 4b	Figure S1	Page 2
¹ H and ¹³ C-NMR of 5a	Figure S2	Page 3
¹ H and ¹³ C-NMR of 5b	Figure S3	Page 4
¹ H and ¹³ C-NMR of 6c	Figure S4	Page 5
¹ H and ¹³ C-NMR of 6d	Figure S5	Page 6
¹ H and ¹³ C-NMR of 7	Figure S6	Page 7
¹ H and ¹³ C-NMR of 8a	Figure S7	Page 8
¹ H and ¹³ C-NMR of 8b	Figure S8	Page 9
¹ H and ¹³ C-NMR of 8b'	Figure S9	Page 10

Figure S1: ^1H and ^{13}C -NMR of (1-(4-methoxyphenyl)-8,9-dimethoxy-5,6-dihydropyrrolo[2,1-*a*]isoquinoline-2-carbaldehyde (**4b**)

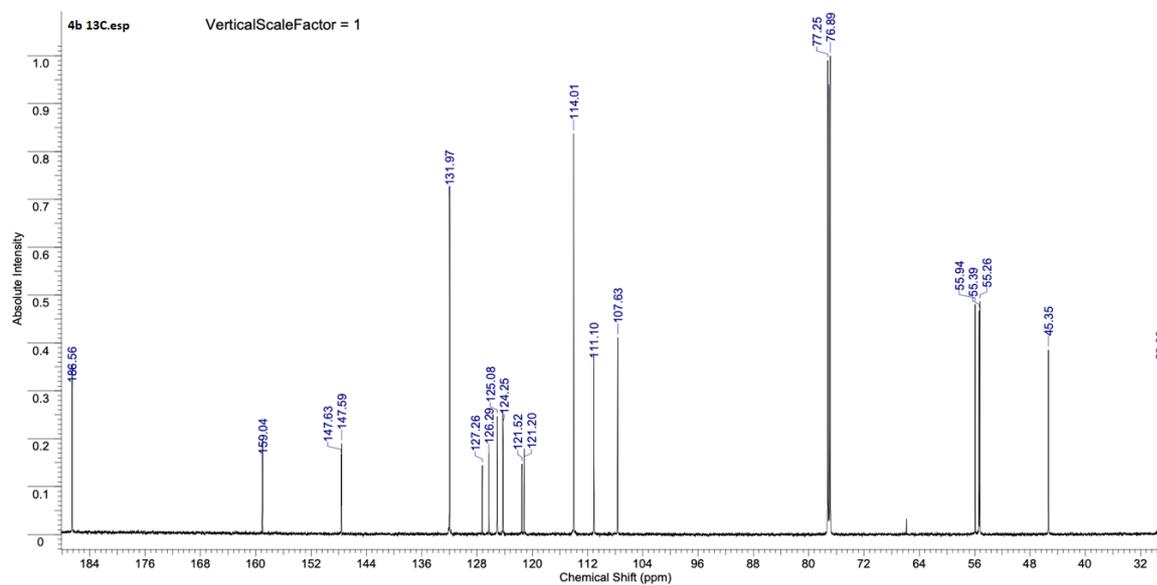
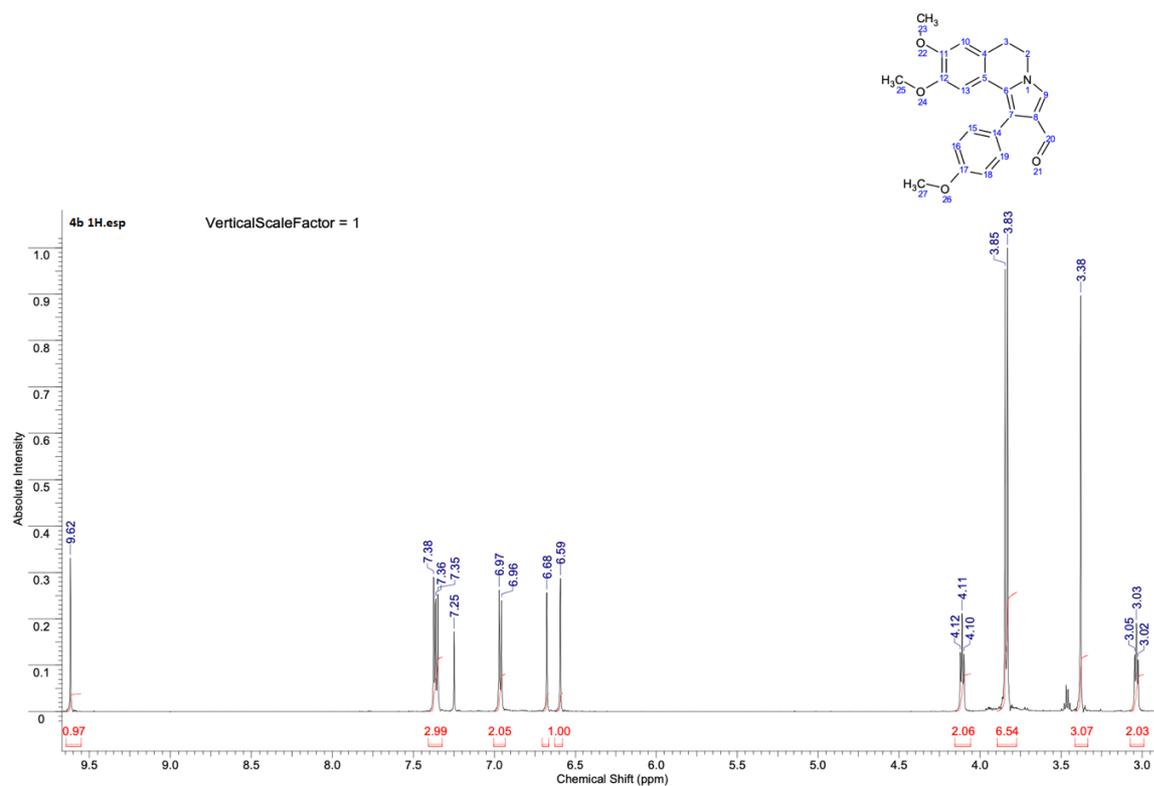


Figure S2: ^1H and ^{13}C -NMR of 1-(4-chlorophenyl)-8,9-dimethoxy-5,6-dihydropyrrolo[2,1-*a*]isoquinoline-2-carboxylic acid (**5a**)

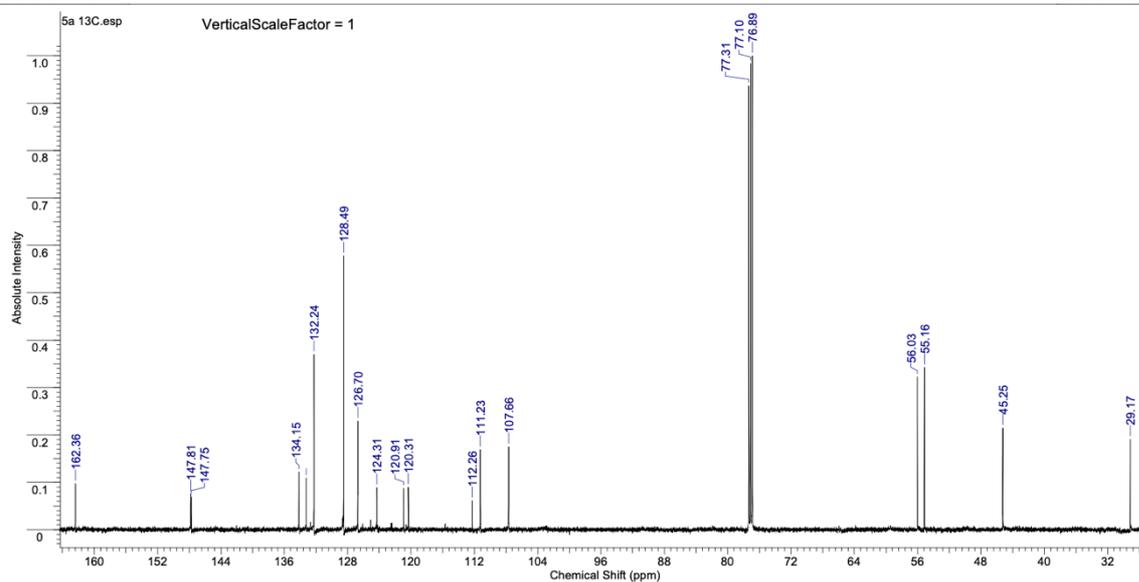
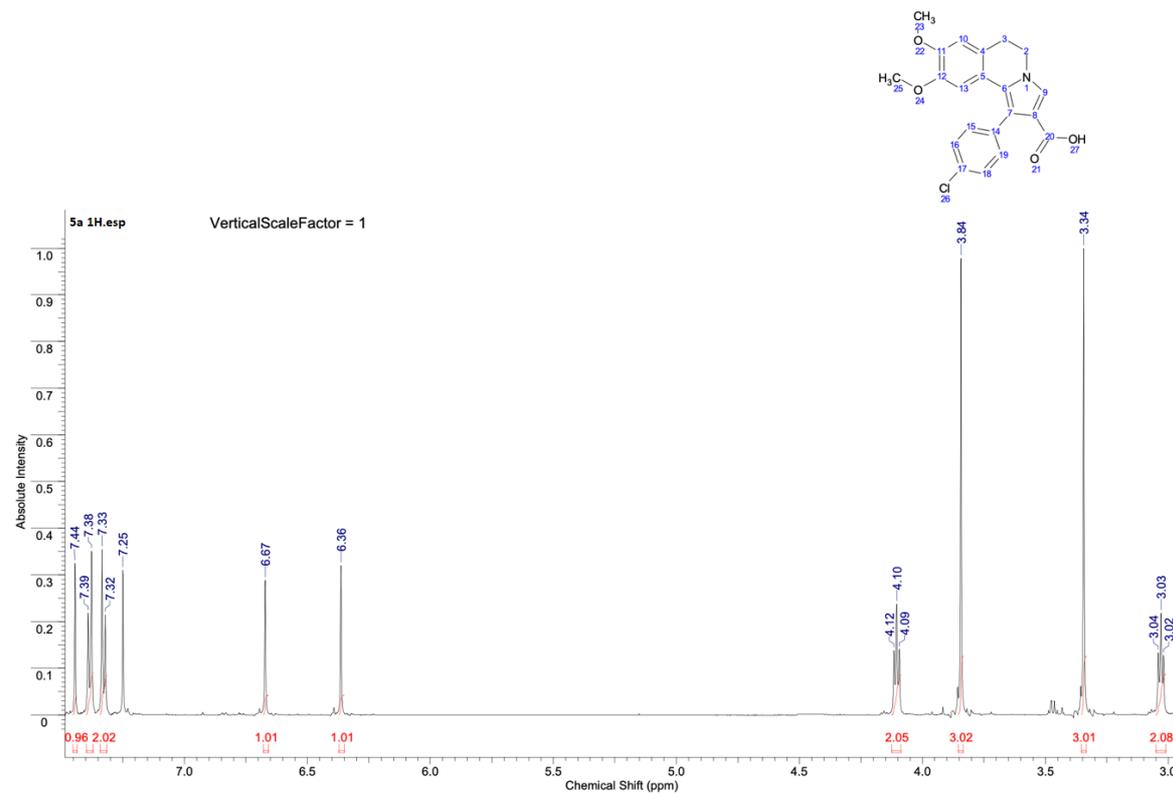


Figure S3: ^1H and ^{13}C -NMR of 1-(3,4-diethoxyphenyl)-8,9-diethoxy-5,6-dihydropyrrolo[2,1-*a*]isoquinoline-2-carboxylic acid (**5b**)

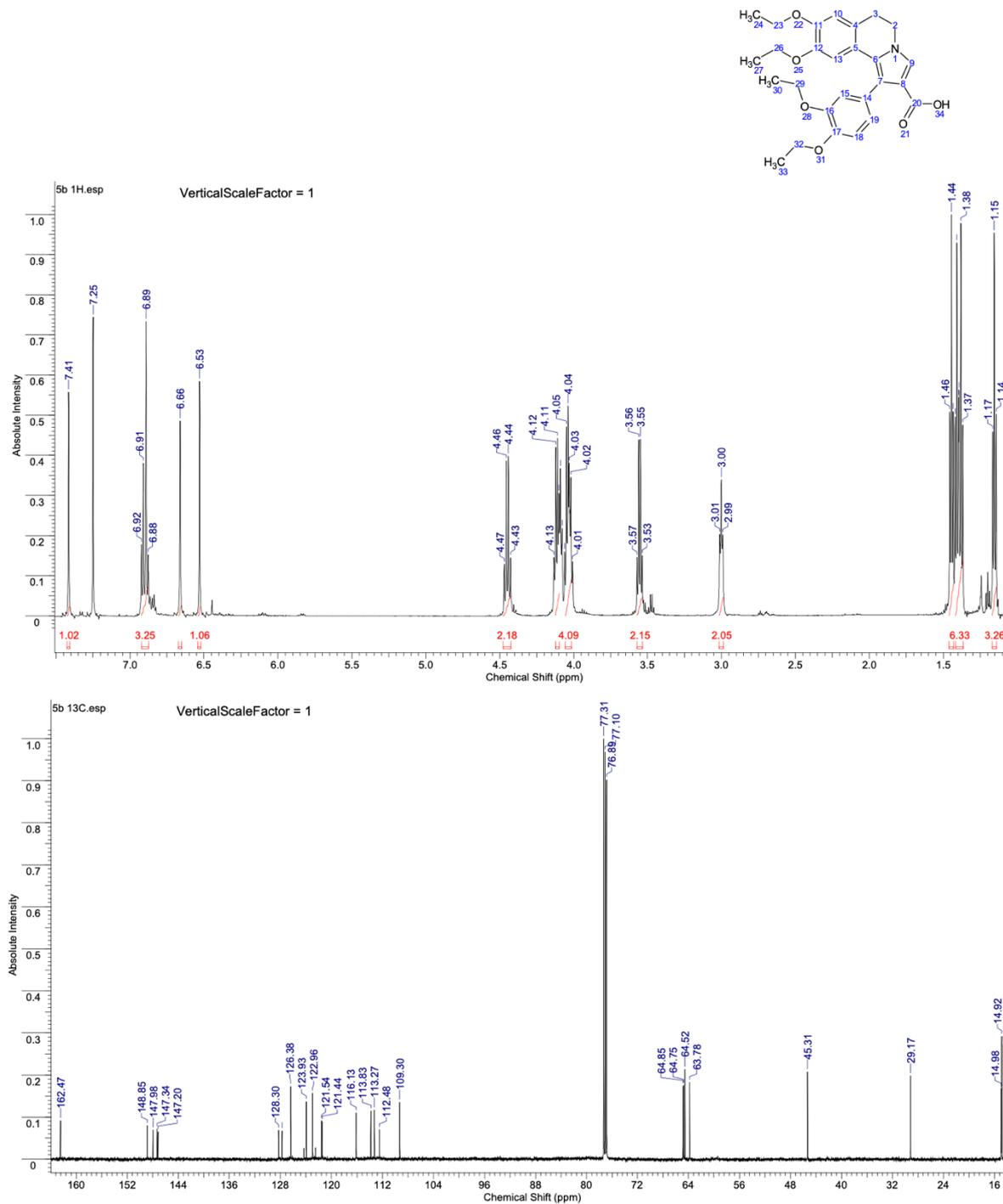


Figure S4: ^1H and ^{13}C -NMR of 1-(3,4-diethoxyphenyl)-8,9-diethoxy-3-methyl-5,6-dihydropyrrolo[2,1-*a*]isoquinoline-2-carbonitrile (**6c**)

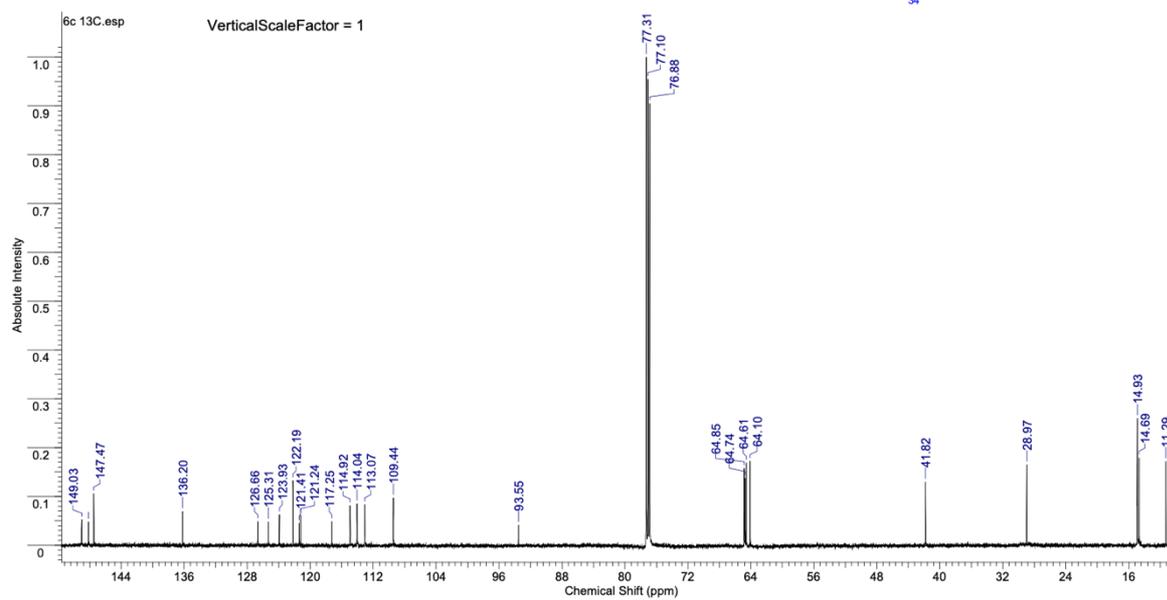
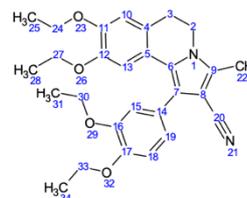
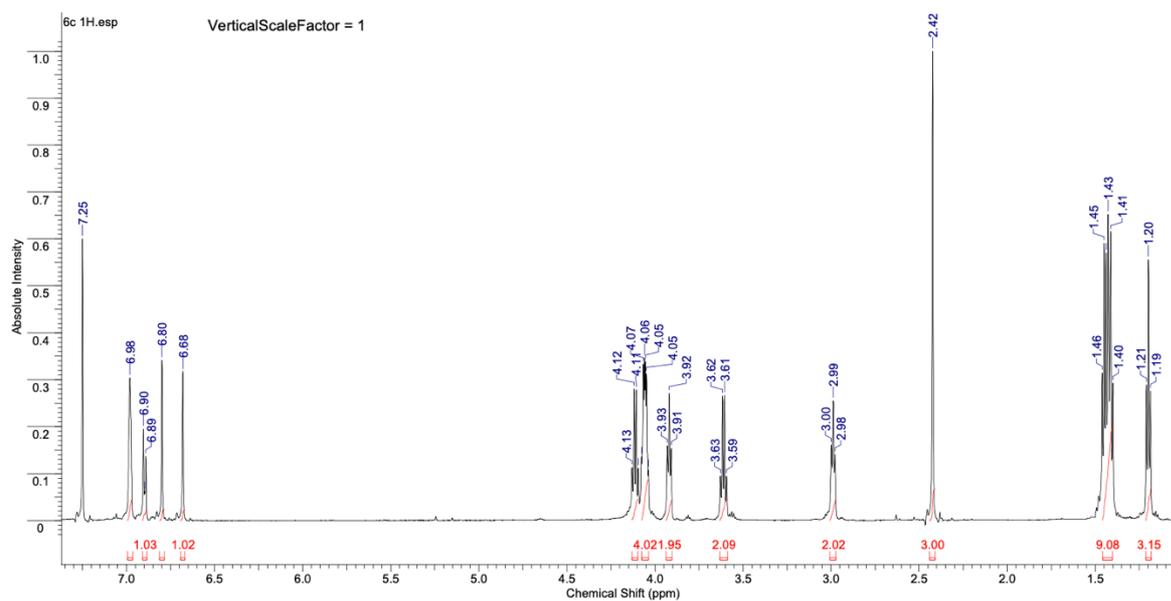


Figure S5: ^1H and ^{13}C -NMR of 1-(3,4-diethoxyphenyl)-8,9-diethoxy-3-phenyl-5,6-dihydropyrrolo[2,1-*a*]isoquinoline-2-carbonitrile (**6d**)

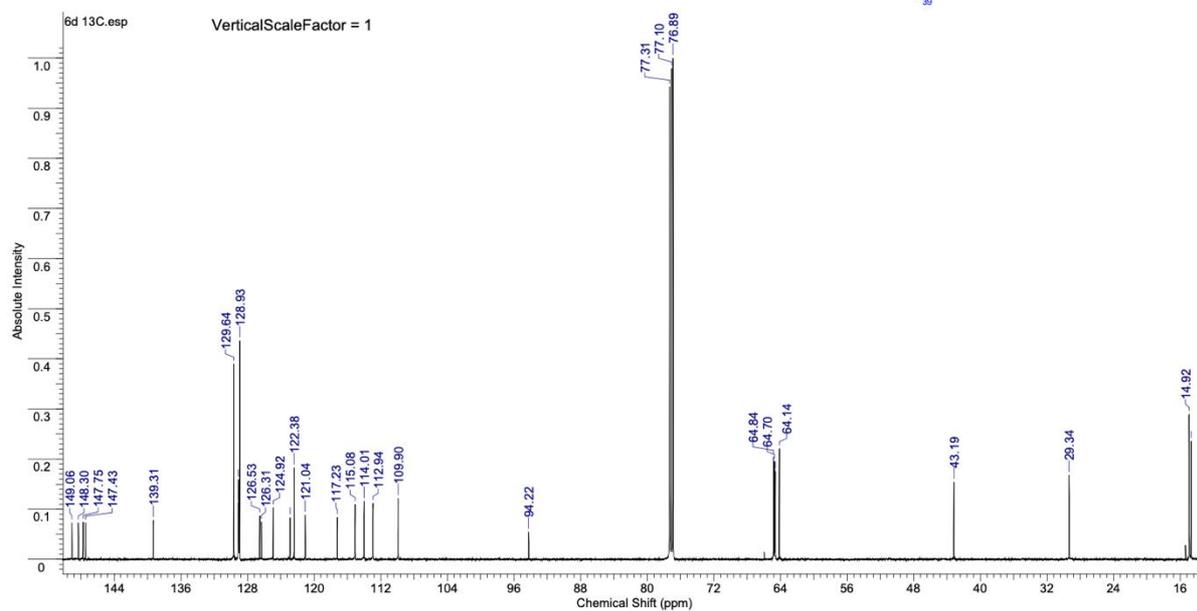
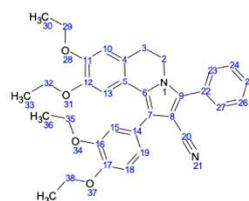
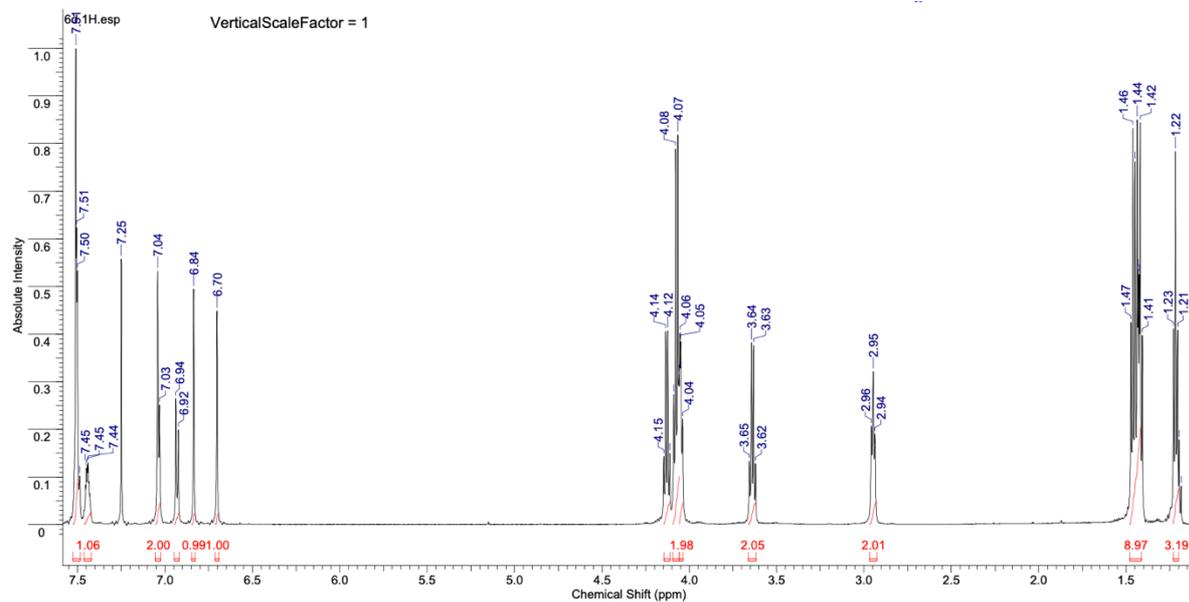


Figure S6: ^1H and ^{13}C -NMR of ethyl 1-(3,4-diethoxyphenyl)-8,9-diethoxy-5,6-dihydro pyrrolo[2,1-*a*]isoquinoline-2-carboxylate (**7**)

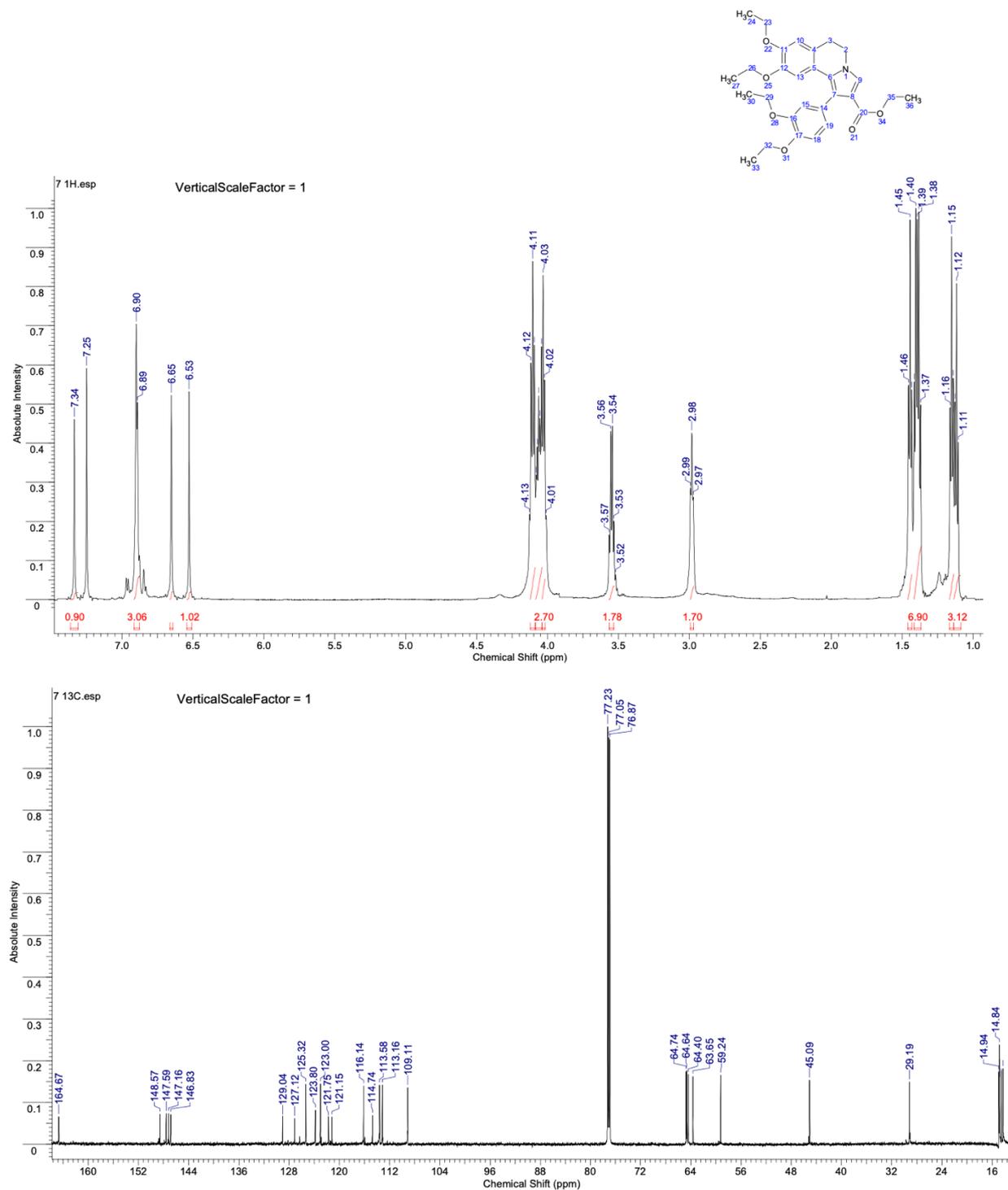


Figure S7: ^1H and ^{13}C -NMR of 8,9-dimethoxy-1-(4-methoxyphenyl)-2-(morpholin-4-ylmethyl)-5,6-dihydropyrrolo[2,1-*a*]isoquinoline (**8a**)

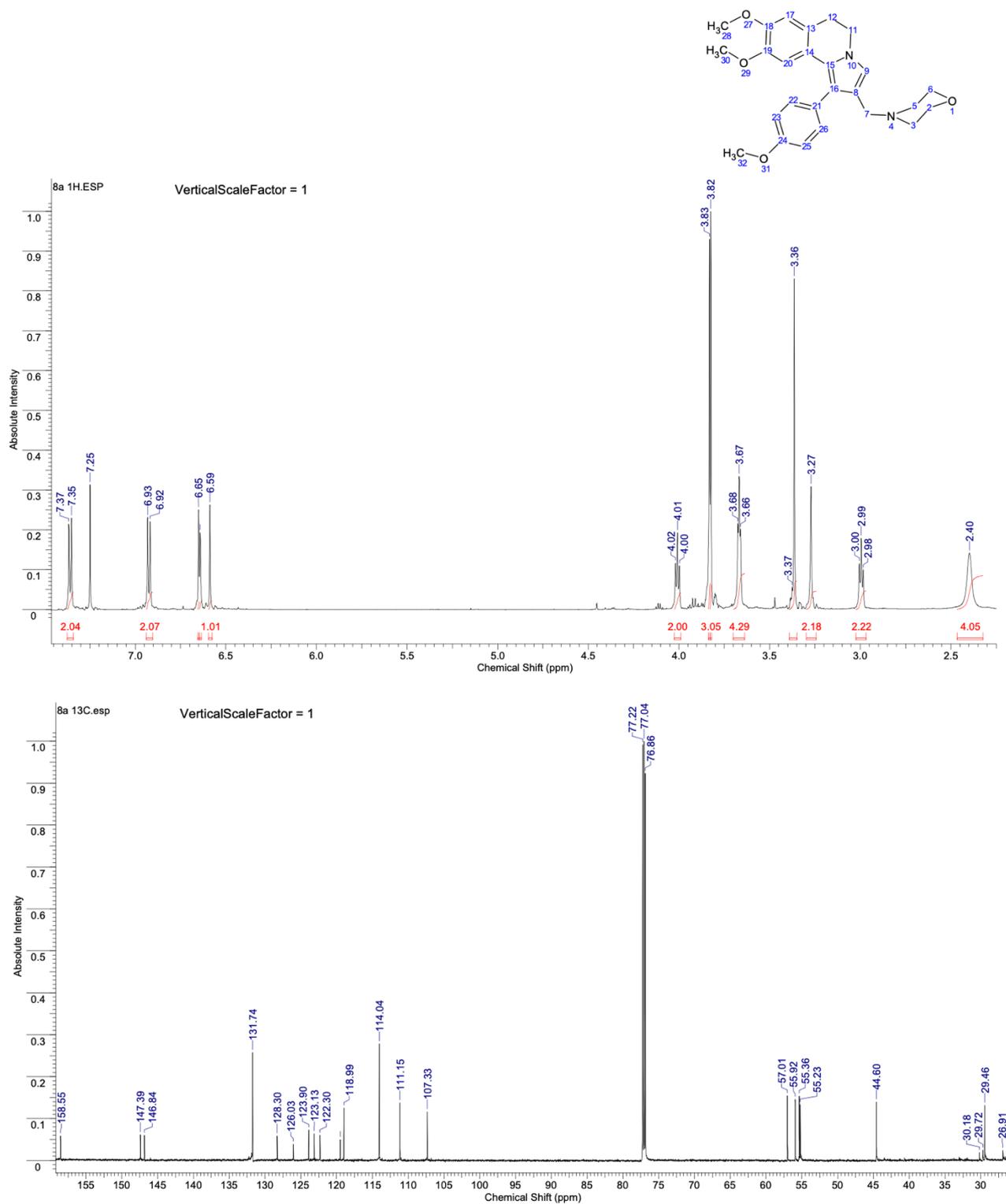


Figure S8: ^1H and ^{13}C -NMR of 1-(3,4-diethoxyphenyl)-8,9-diethoxy-2-(morpholin-4-ylmethyl)-5,6-dihydropyrrolo[2,1-*a*]isoquinoline (**8b**)

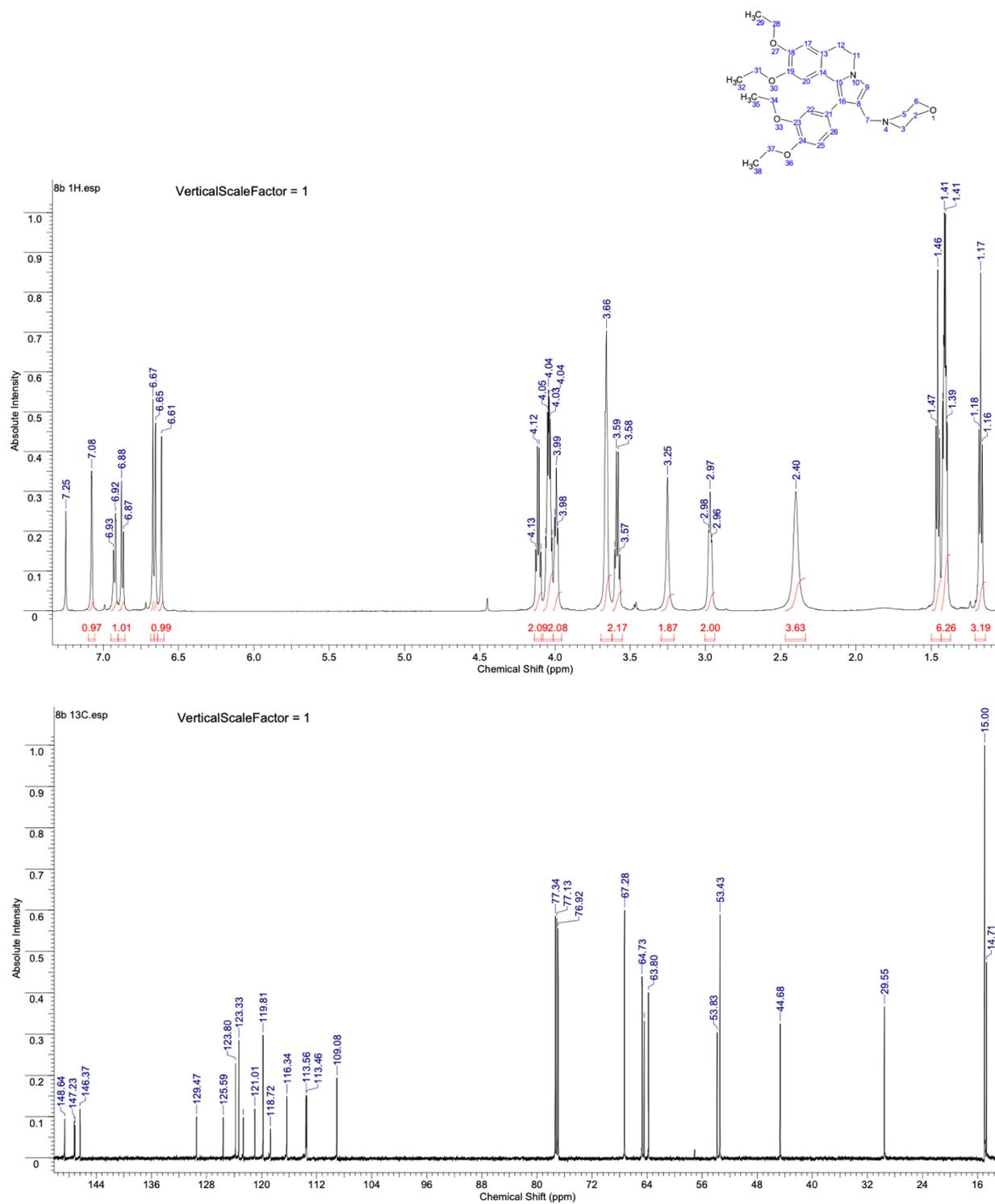


Figure S9: ^1H and ^{13}C -NMR of 4-[[1-(3,4-diethoxyphenyl)-8,9-diethoxy-5,6-dihydropyrrolo[2,1-*a*]isoquinolin-2-yl)methyl]morpholin-4-ium chloride (**8b'**)

