

Supporting Information

A concise and free-metal access to lactone annelated pyrrolo[2,1-*a*]isoquinoline derivatives via a 1,2-rearrangement step

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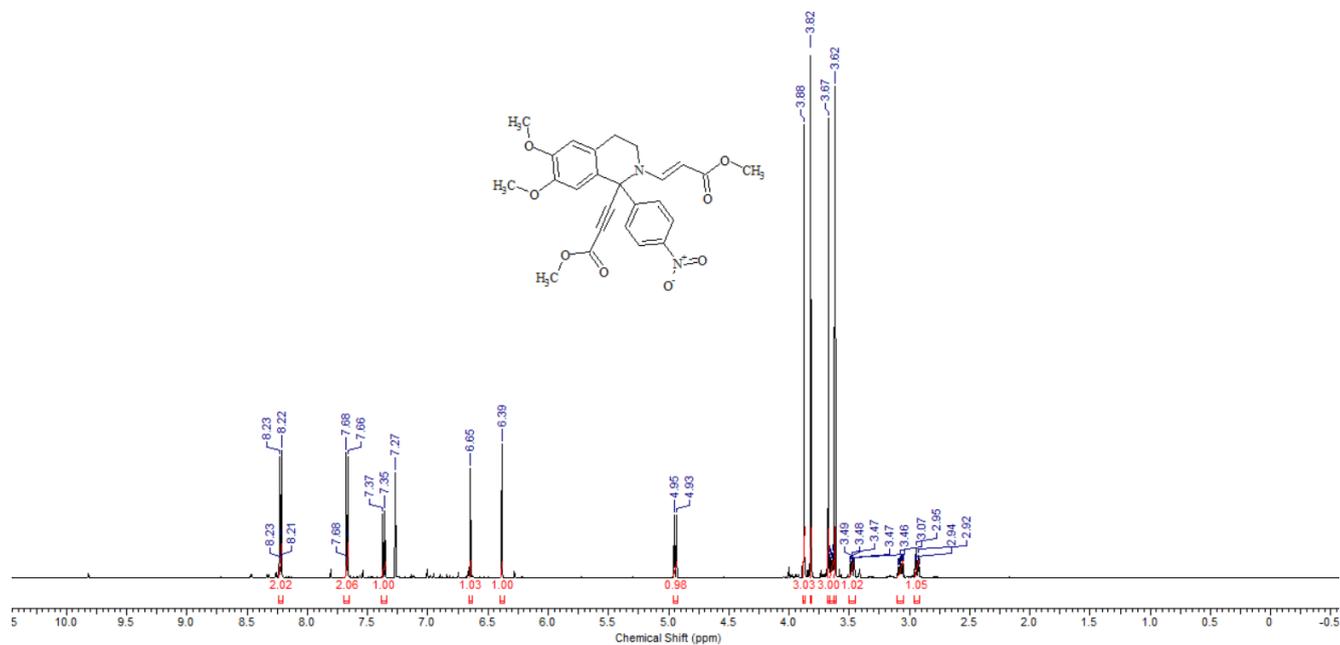
Table S1**X-ray Structure Determination of Compound 3a**

Compound	3a
Empirical formula	C ₁₉ H ₂₁ NO ₆
Formula weight	359
Temperature/K	295
Crystal system	triclinic
Space group	P $\bar{1}$ (2)
a, Å	7.6475(7)
b, Å	9.1412(9)
c, Å	13.9957(11)
α , °	104.356(4)
β , °	92.863(4)
γ , °	108.263(4)
Volume, Å ³	891.399
Z	2
R-Factor (%)	4.81
deposit CCDC	2156399

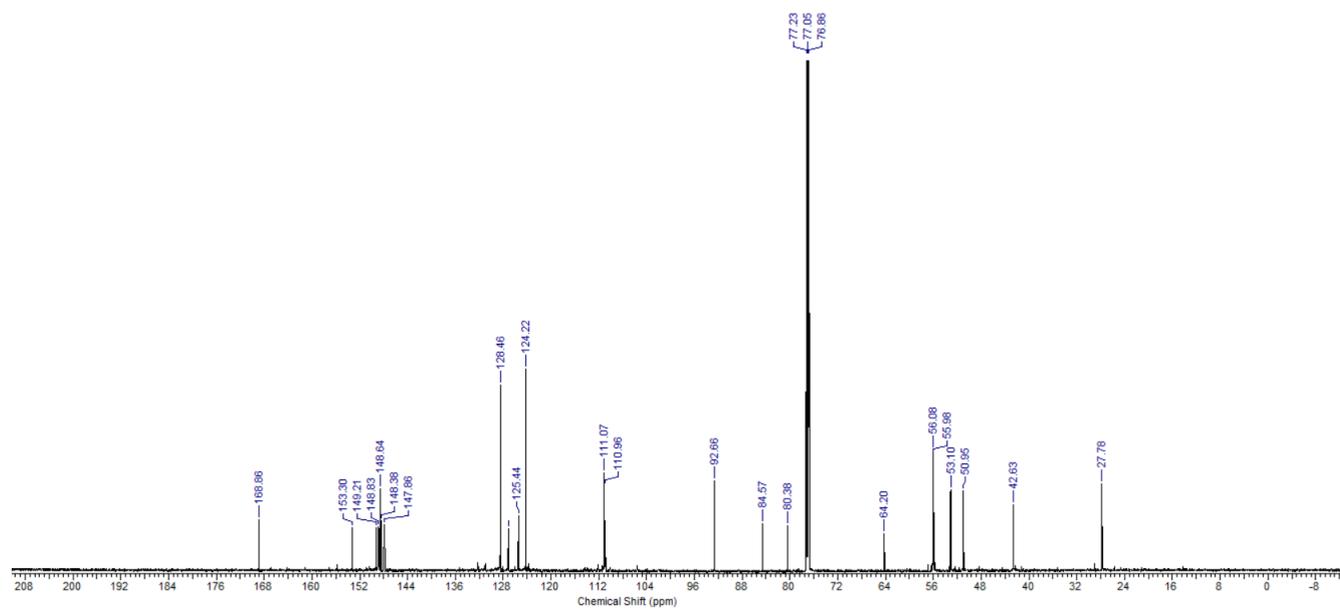
Copies of ^1H and ^{13}C NMR spectra

Methyl (2*E*)-3-[6,7-dimethoxy-1-(3-methoxy-3-oxoprop-1-yn-1-yl)-1-(4-nitrophenyl)-3,4-dihydroisoquinolin-2(1*H*)-yl]prop-2-enoate **1g**

^1H NMR (600 MHz, CDCl_3):

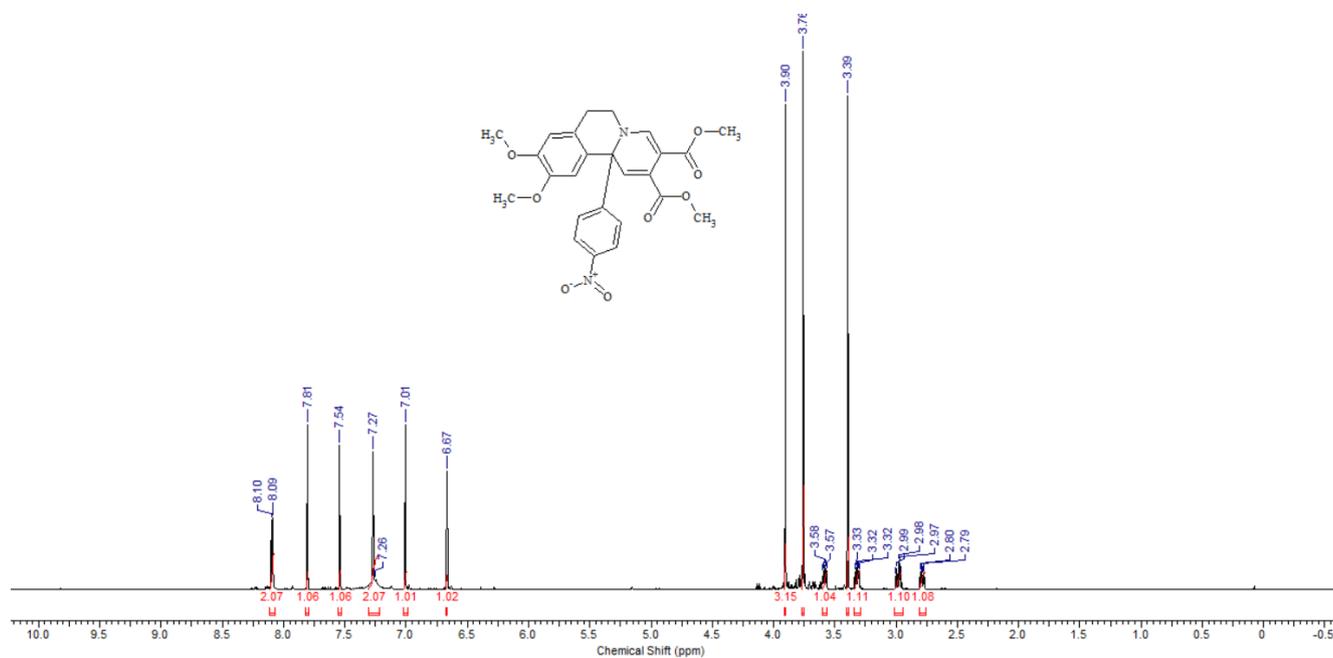


^{13}C NMR (150 MHz, CDCl_3):

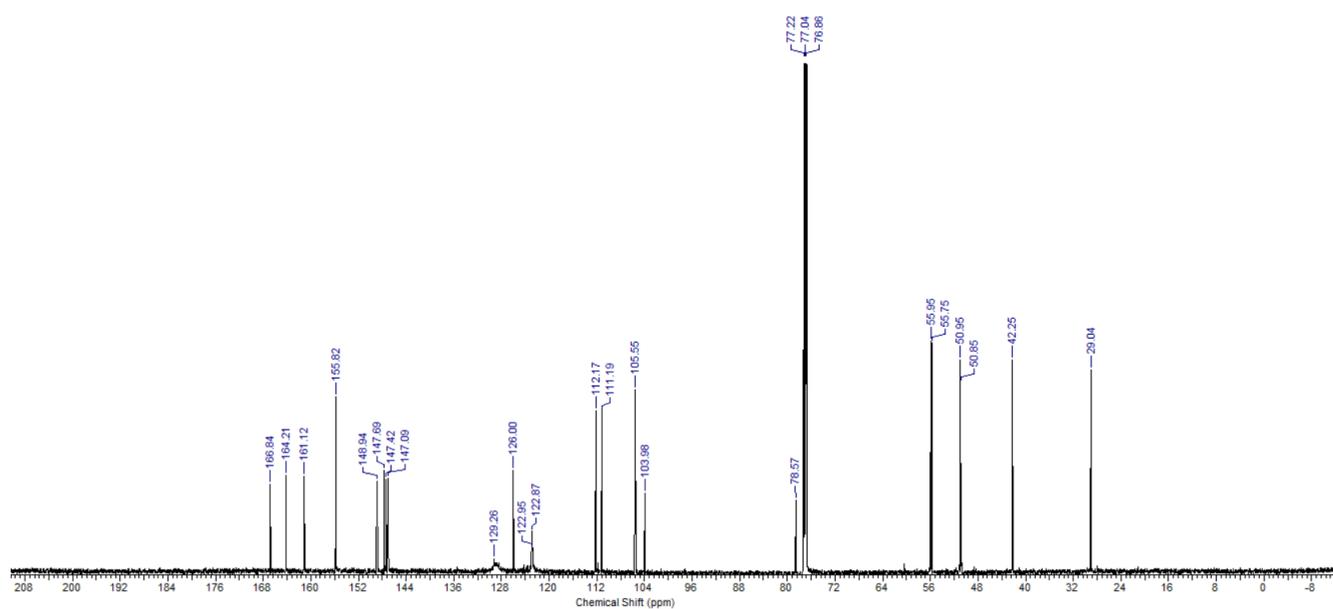


Dimethyl 11b-(4-nitrophenyl)-9,10-dimethoxy-7,11b-dihydro-6H-pyrido[2,1-a]isoquinoline-2,3-dicarboxylate 2g

^1H NMR (600 MHz, CDCl_3):

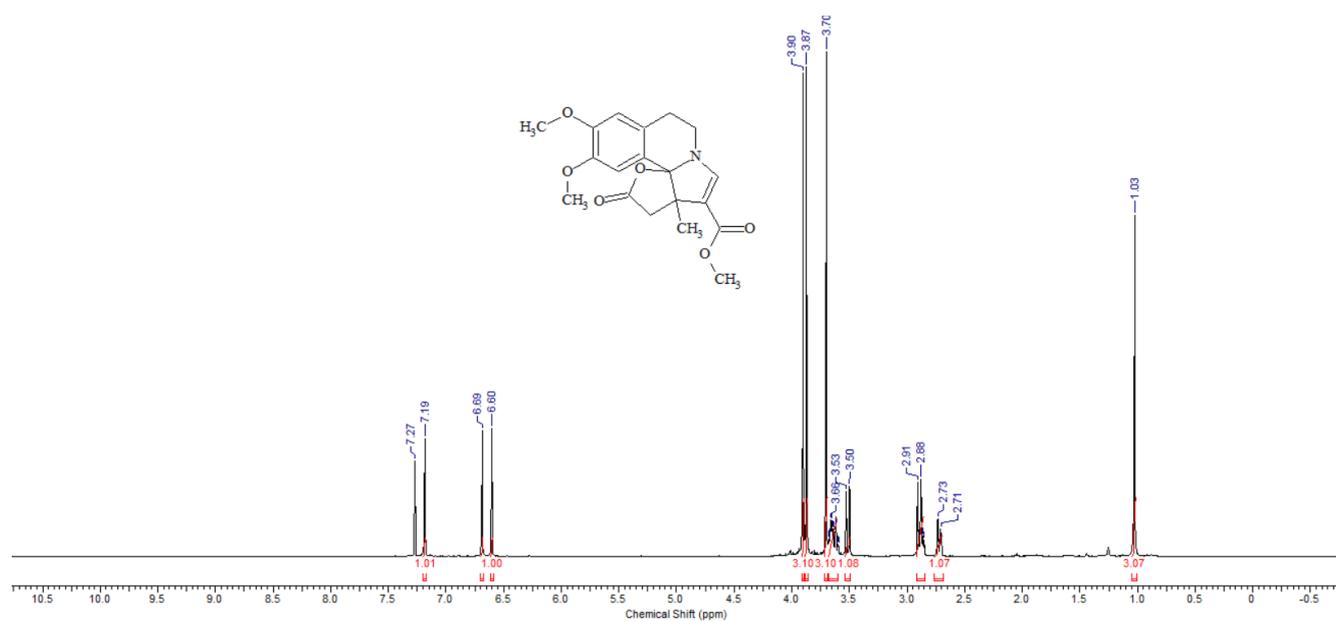


^{13}C NMR (150 MHz, CDCl_3):

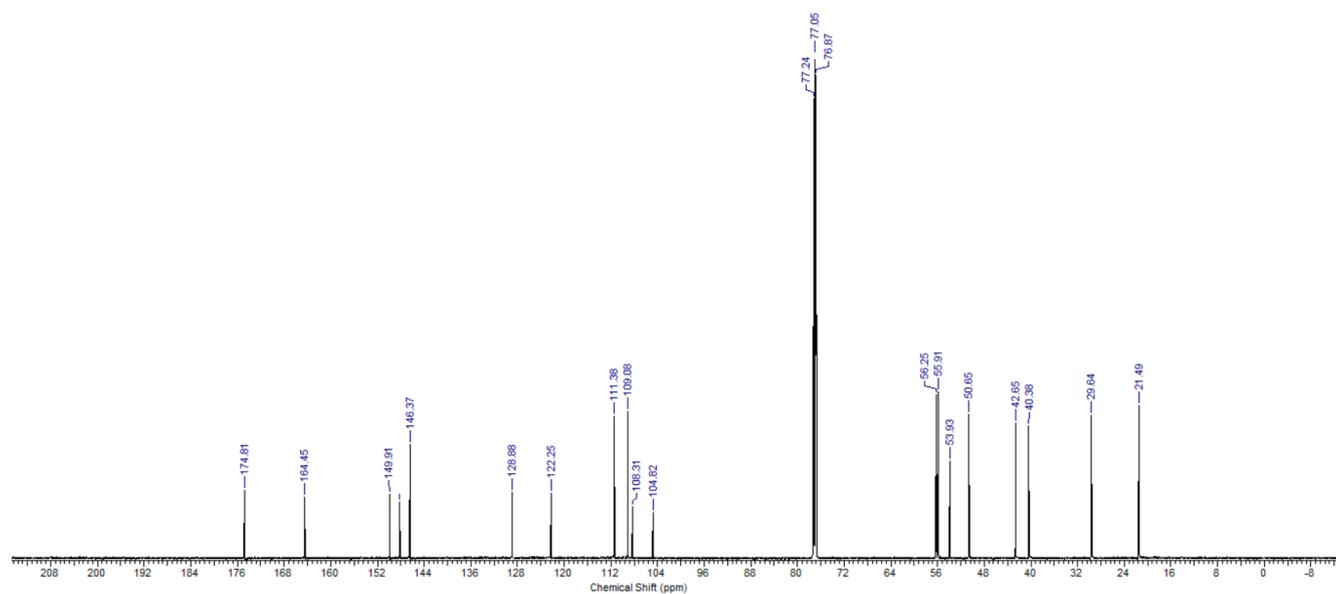


Methyl 10,11-dimethoxy-3a-methyl-2-oxo-3,3a,7,8-tetrahydro-2H-furo[2',3':2,3]pyrrolo[2,1-a]isoquinoline-4-carboxylate 3a

^1H NMR (600 MHz, CDCl_3):

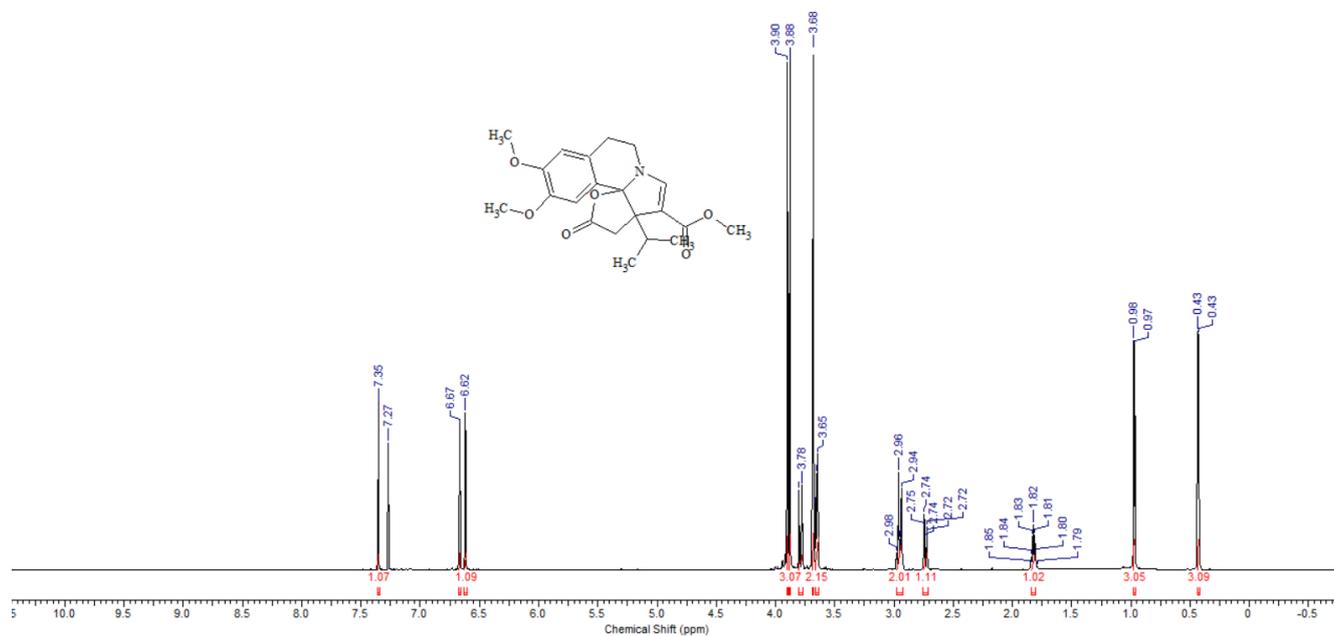


^{13}C NMR (150 MHz, CDCl_3):

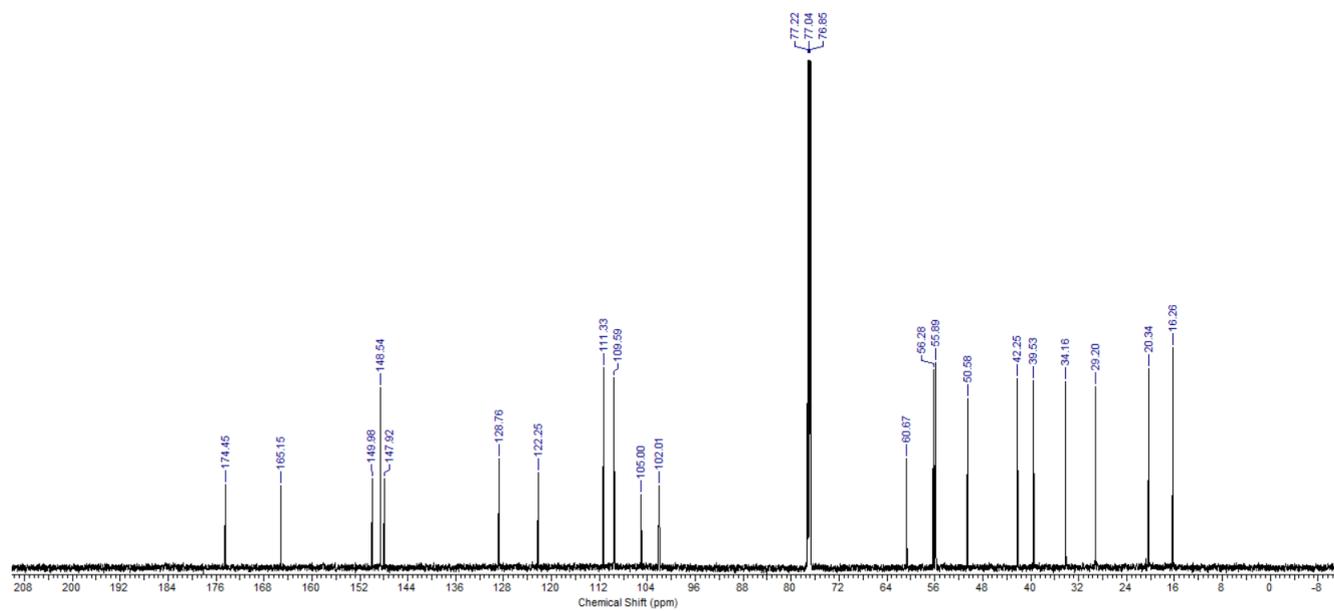


Methyl 10,11-dimethoxy-2-oxo-3a-(propan-2-yl)-3,3a,7,8-tetrahydro-2H-furo[2',3':2,3]pyrrolo[2,1-a]isoquinoline-4-carboxylate 3b

^1H NMR (600 MHz, CDCl_3):

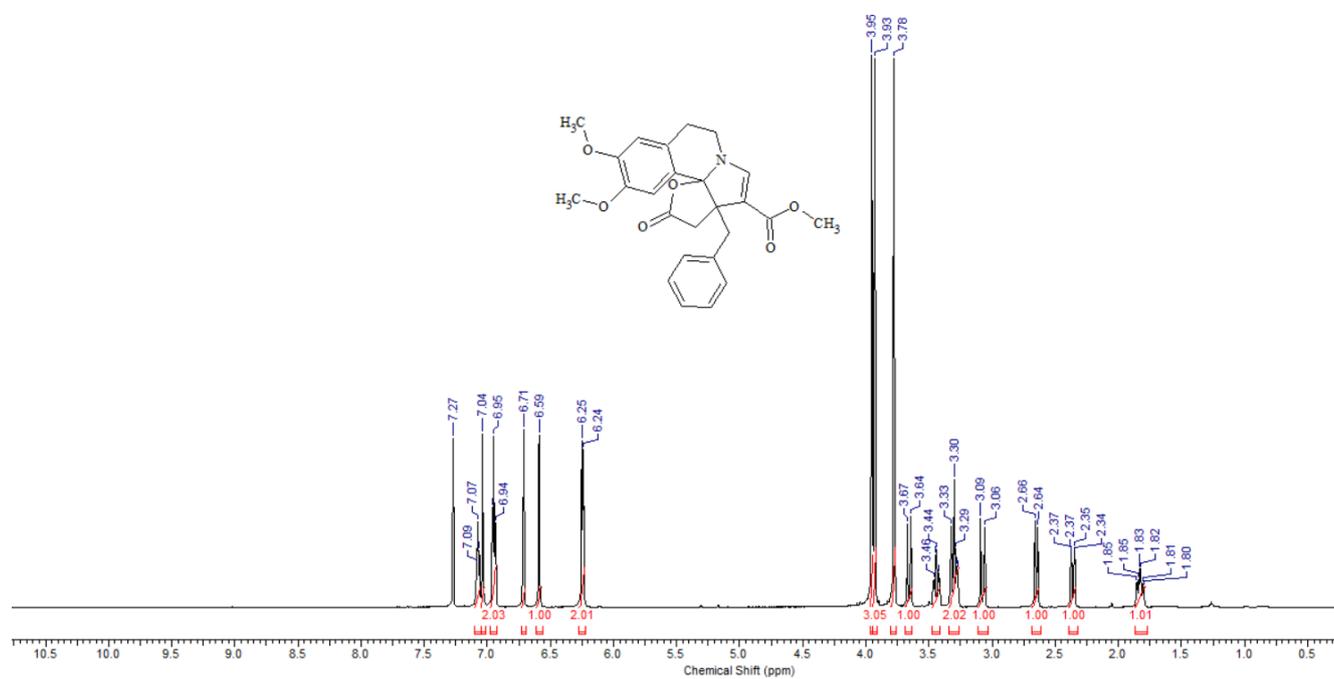


^{13}C NMR (150 MHz, CDCl_3):

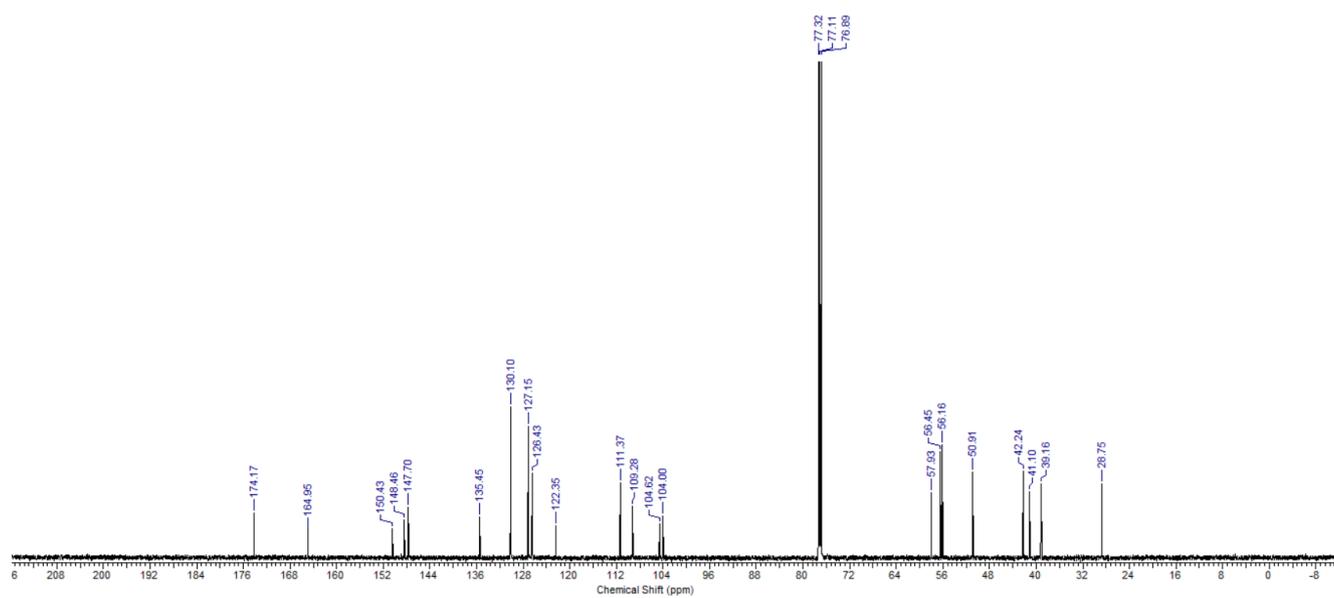


Methyl 3a-benzyl-10,11-dimethoxy-2-oxo-3,3a,7,8-tetrahydro-2H-furo[2',3':2,3]pyrrolo[2,1-a]isoquinoline-4-carboxylate 3c

^1H NMR (600 MHz, CDCl_3):

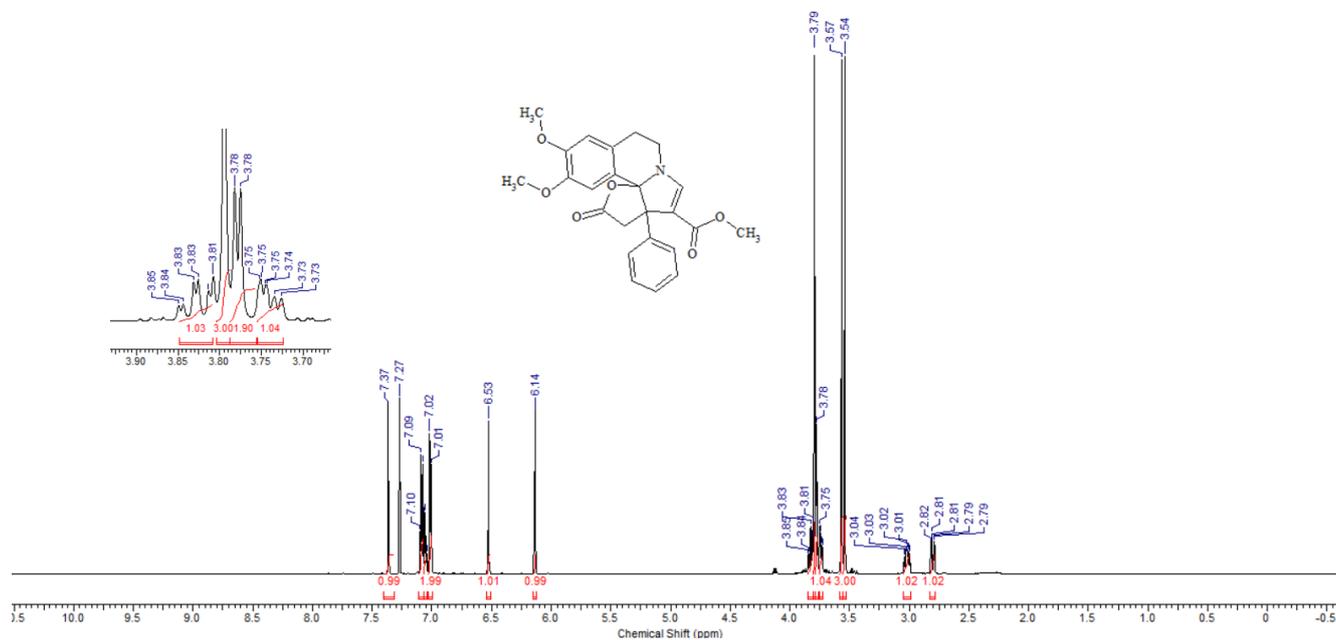


^{13}C NMR (150 MHz, CDCl_3):

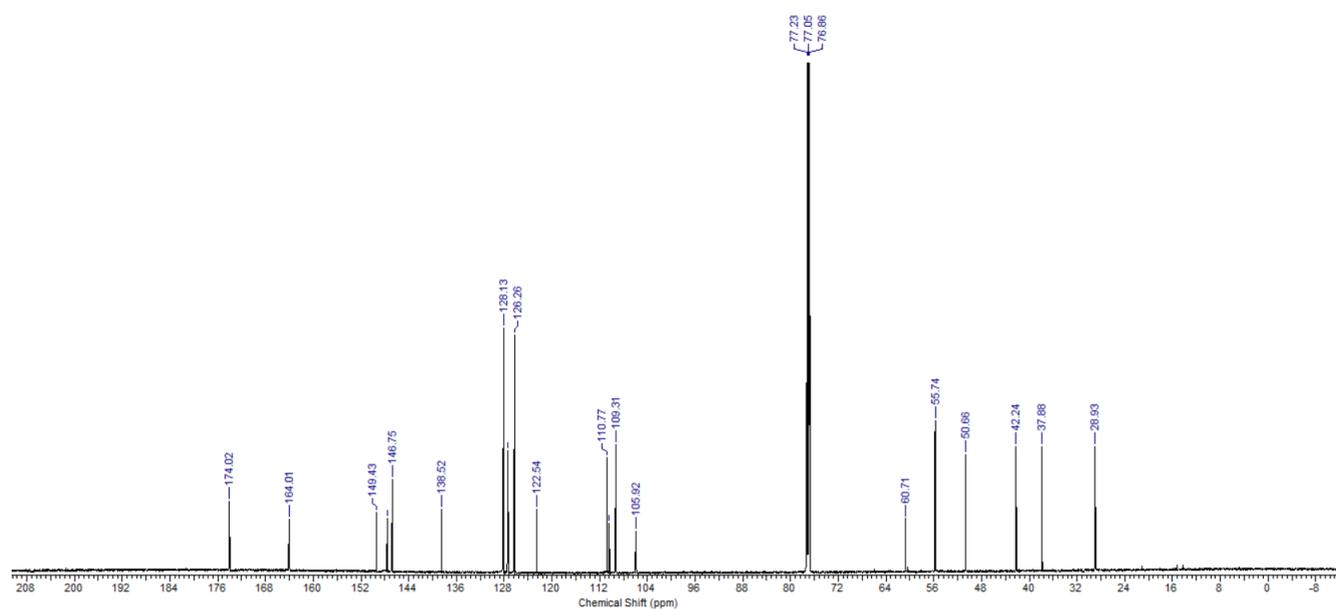


Methyl 10,11-dimethoxy-2-oxo-3a-phenyl-3,3a,7,8-tetrahydro-2H-furo[2',3':2,3]pyrrolo[2,1-a]isoquinoline-4-carboxylate 3d

^1H NMR (600 MHz, CDCl_3):

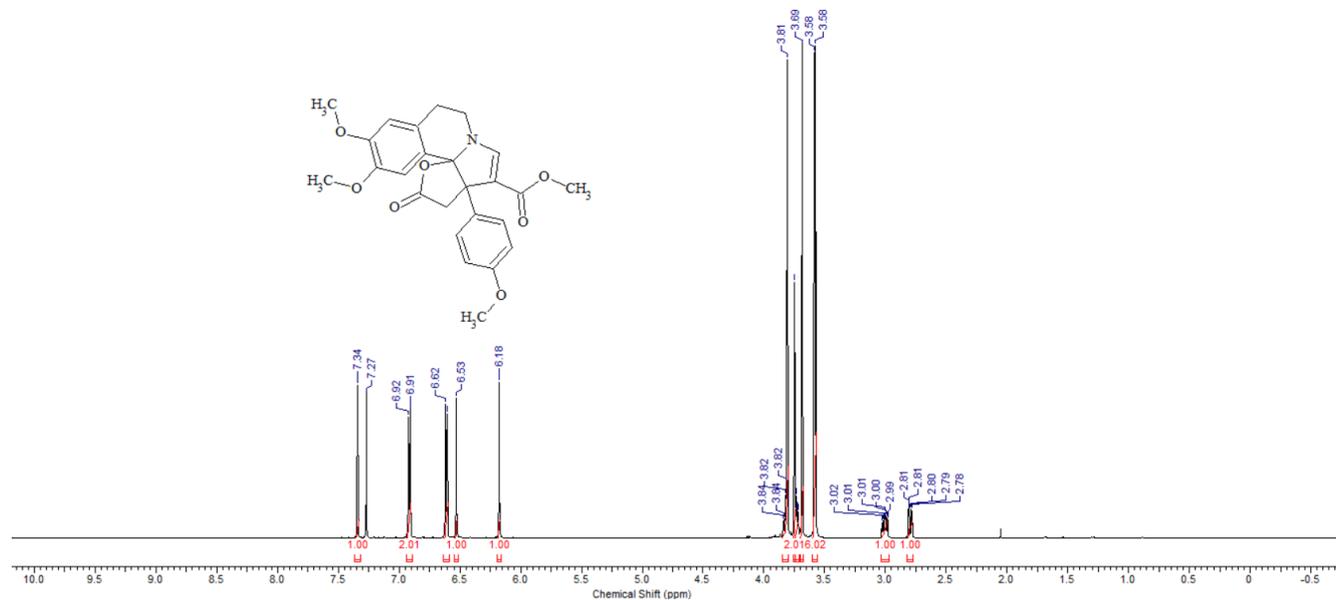


^{13}C NMR (150 MHz, CDCl_3):

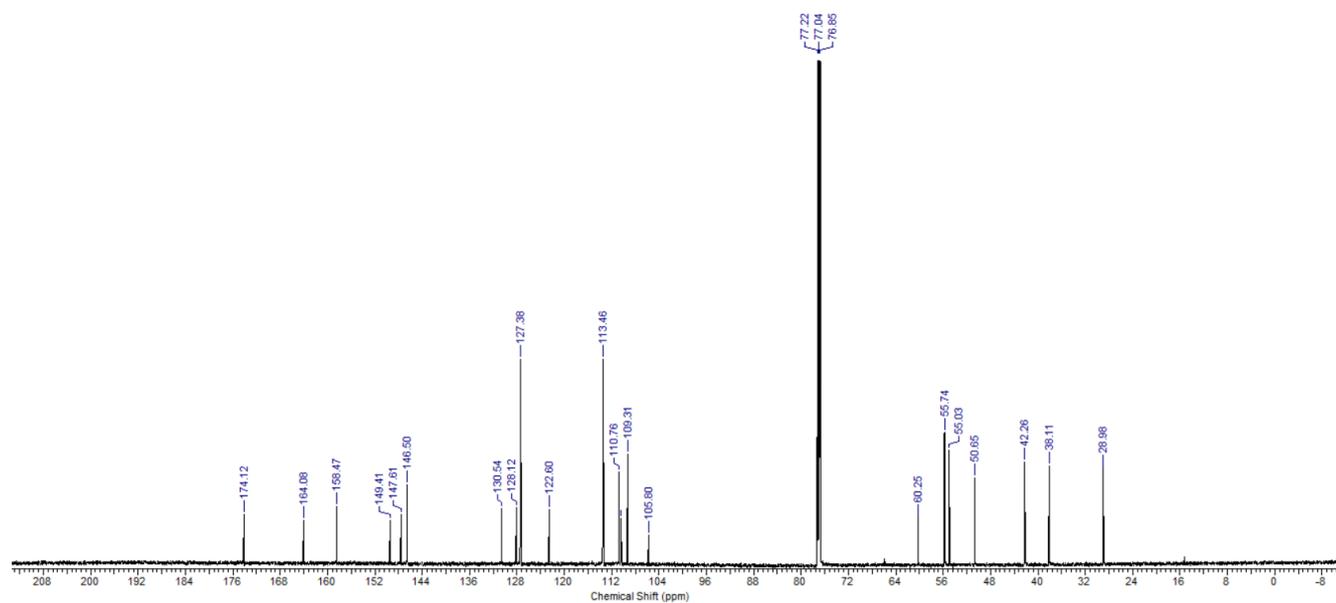


Methyl 10,11-dimethoxy-3a-(4-methoxyphenyl)-2-oxo-3,3a,7,8-tetrahydro-2H-furo[2',3':2,3]pyrrolo[2,1-a]isoquinoline-4-carboxylate 3e

^1H NMR (600 MHz, CDCl_3):

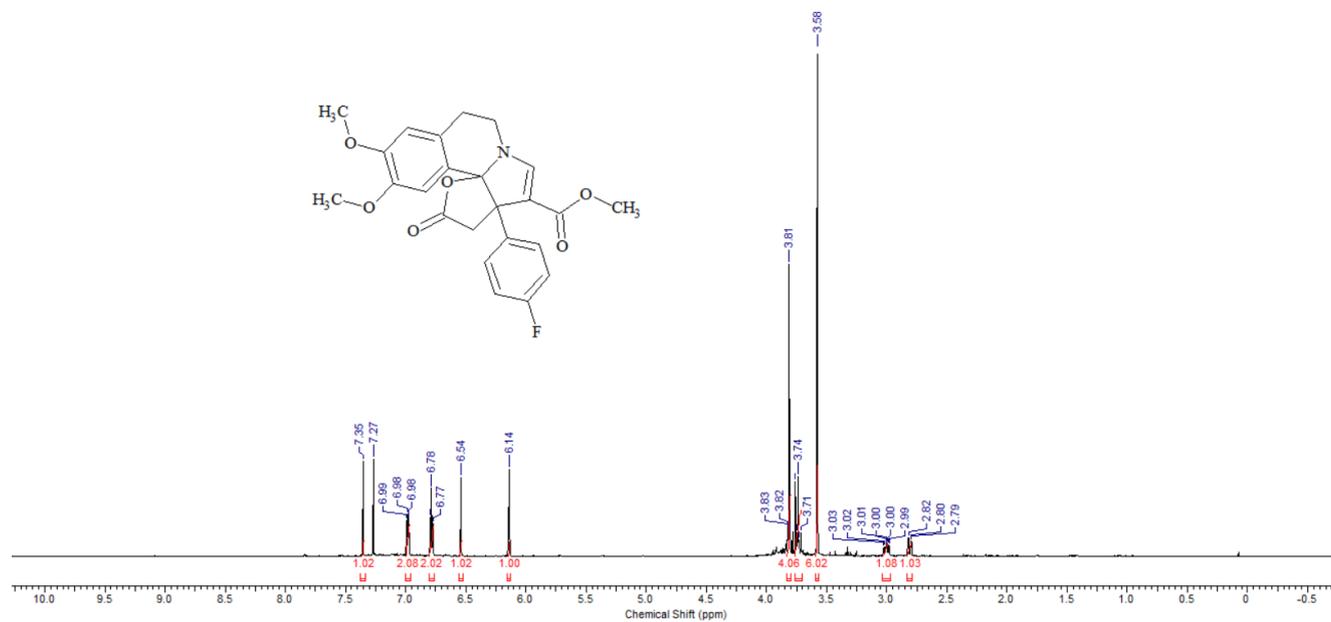


^{13}C NMR (150 MHz, CDCl_3):

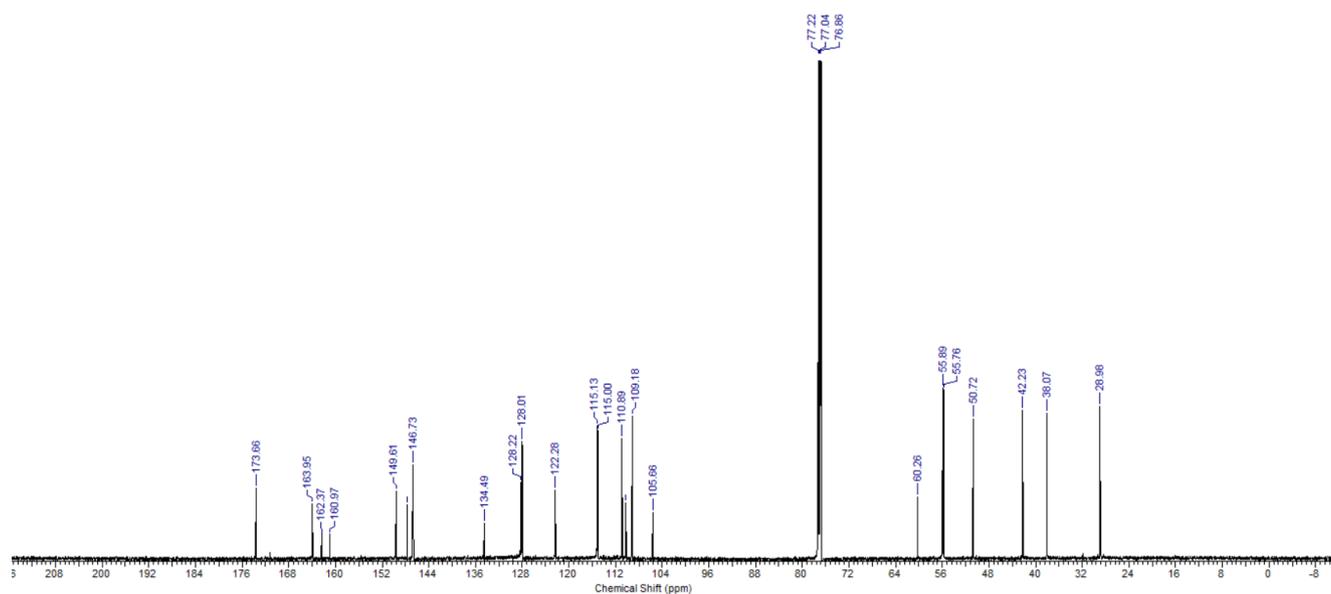


Methyl 3a-(4-fluorophenyl)-10,11-dimethoxy-2-oxo-3,3a,7,8-tetrahydro-2H-furo[2',3':2,3]pyrrolo[2,1-a]isoquinoline-4-carboxylate 3f

^1H NMR (600 MHz, CDCl_3):

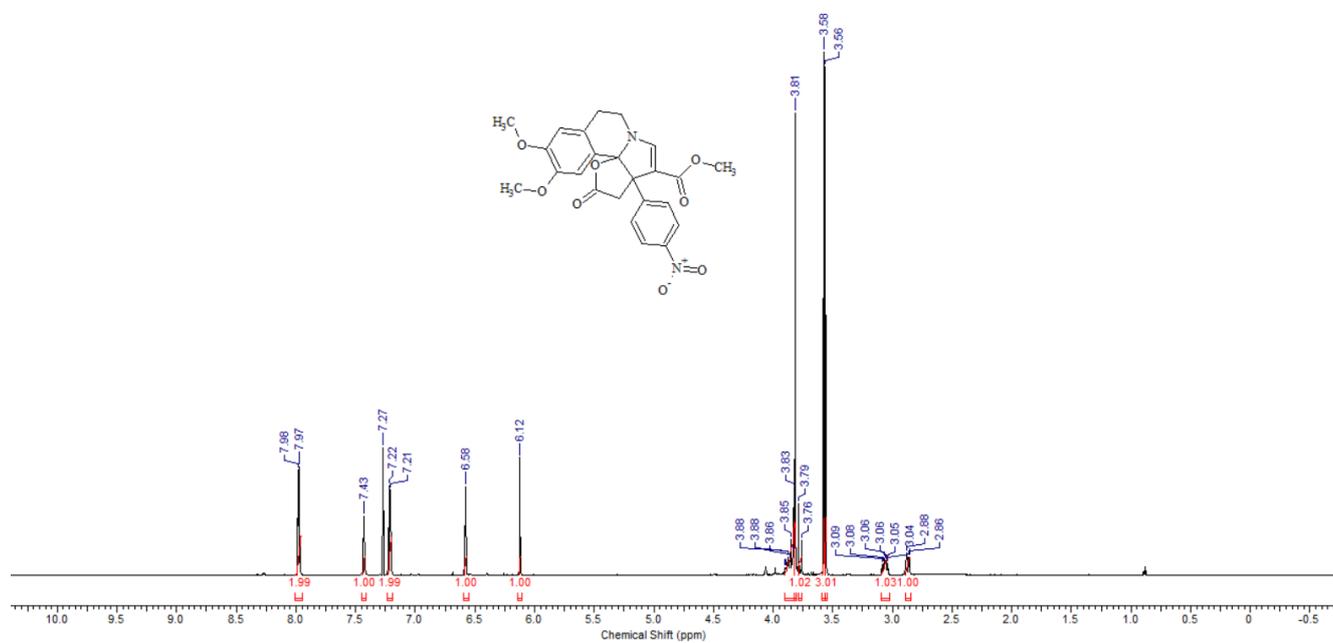


^{13}C NMR (150 MHz, CDCl_3):

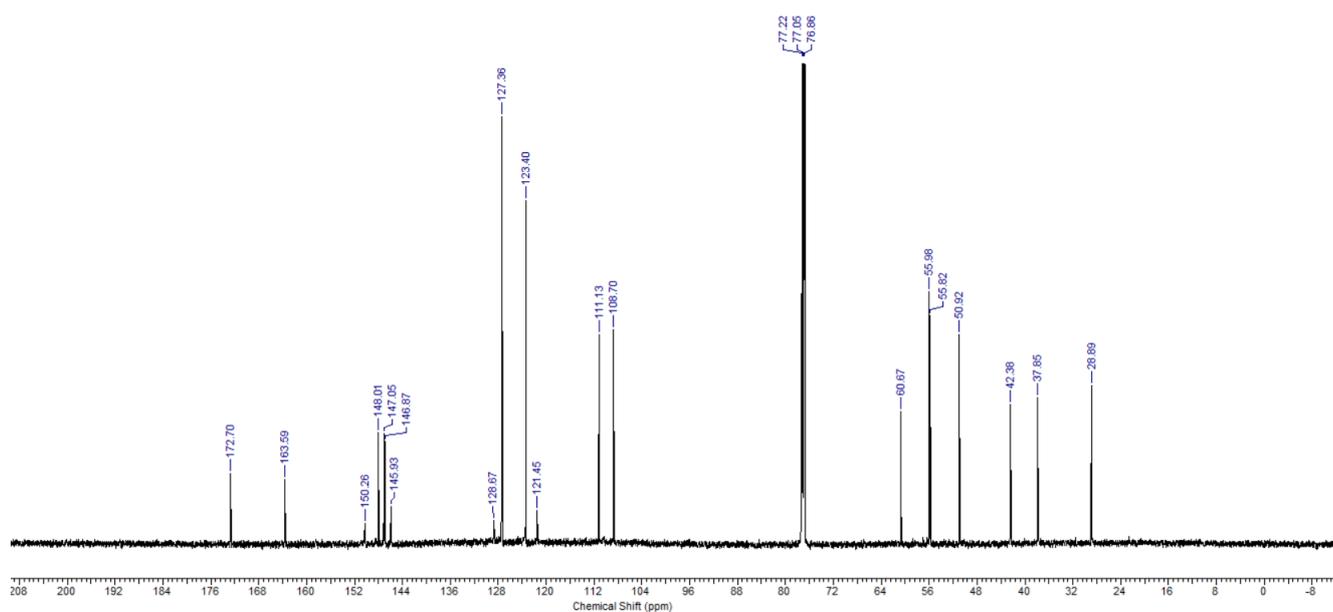


Methyl 10,11-dimethoxy-3a-(4-nitrophenyl)-2-oxo-3,3a,7,8-tetrahydro-2H-furo[2',3':2,3]pyrrolo[2,1-a]isoquinoline-4-carboxylate 3g

^1H NMR (600 MHz, CDCl_3):

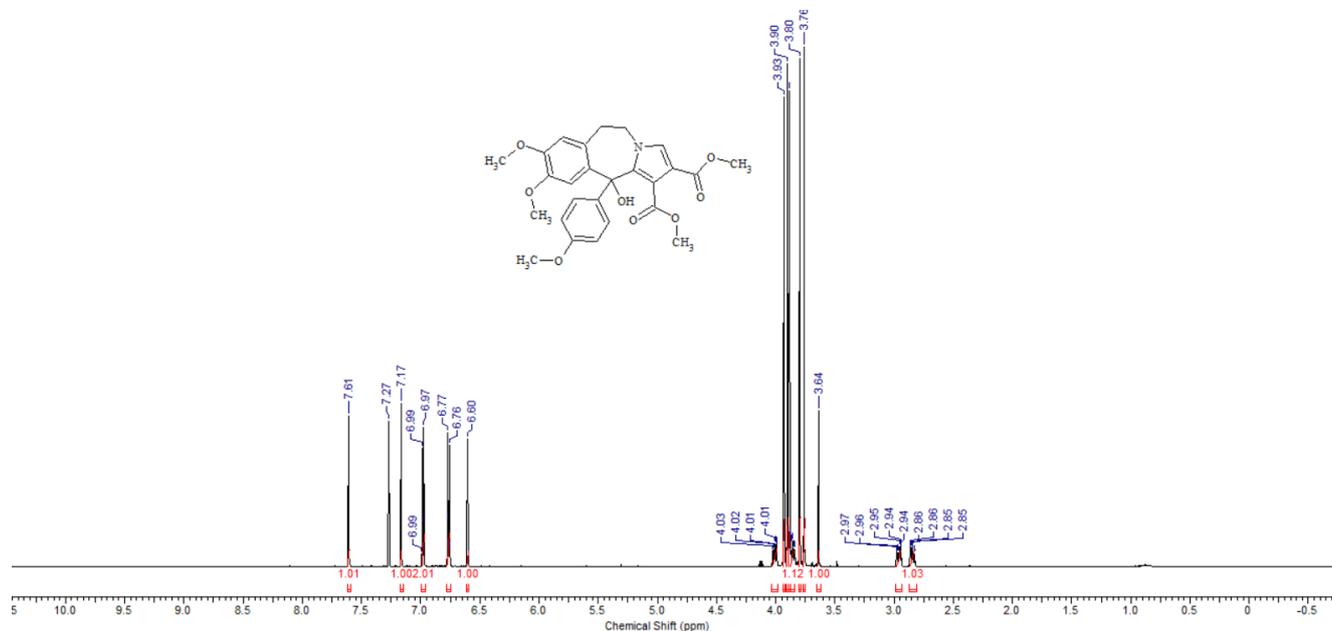


^{13}C NMR (150 MHz, CDCl_3):

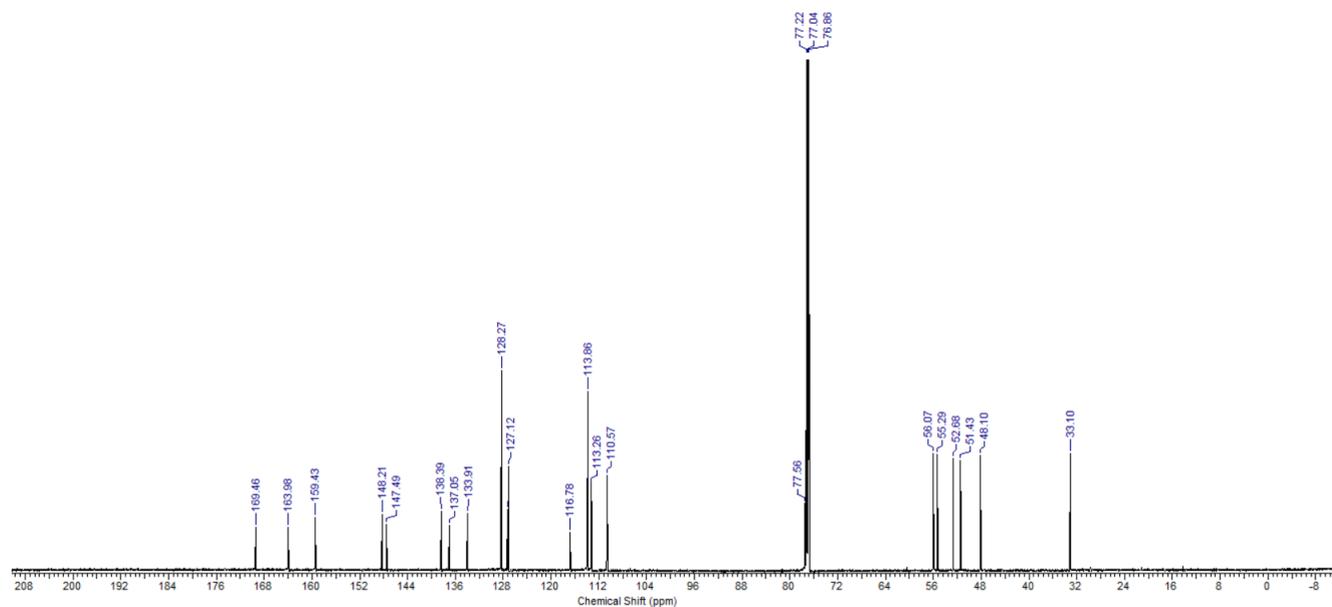


Dimethyl 11-hydroxy-8,9-dimethoxy-11-(4-methoxyphenyl)-6,11-dihydro-5H-pyrrolo[2,1-*b*][3]benzazepine-1,2-dicarboxylate **5a**

^1H NMR (600 MHz, CDCl_3):

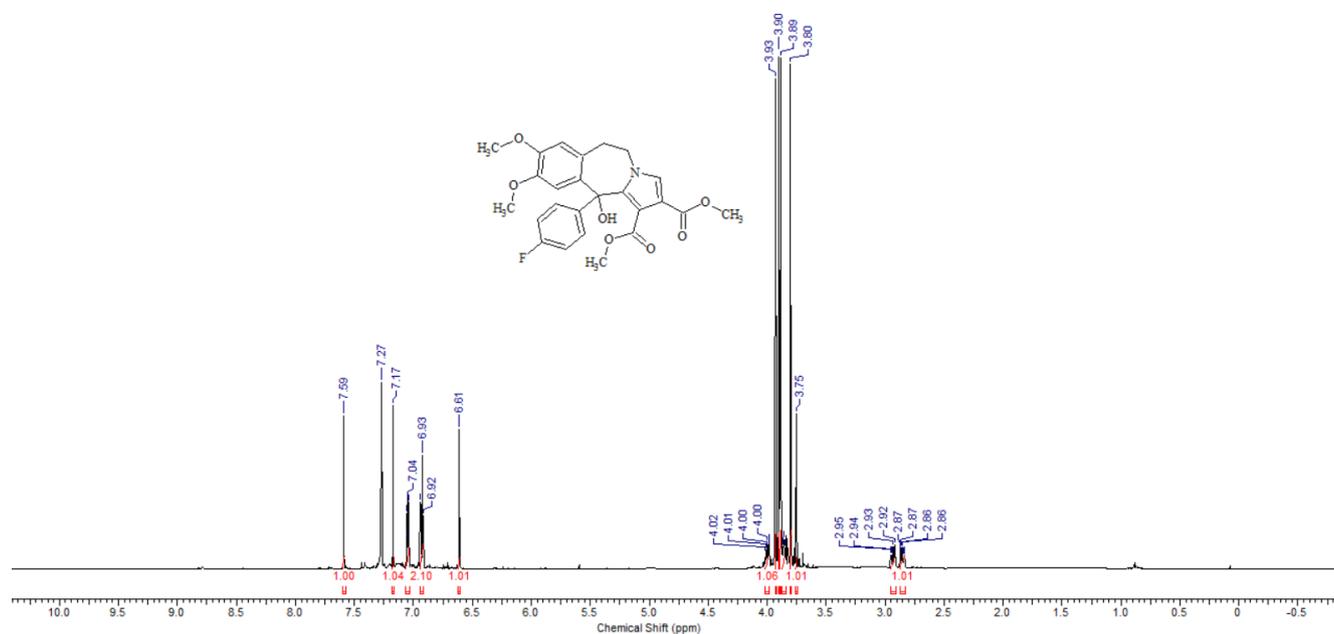


^{13}C NMR (150 MHz, CDCl_3):

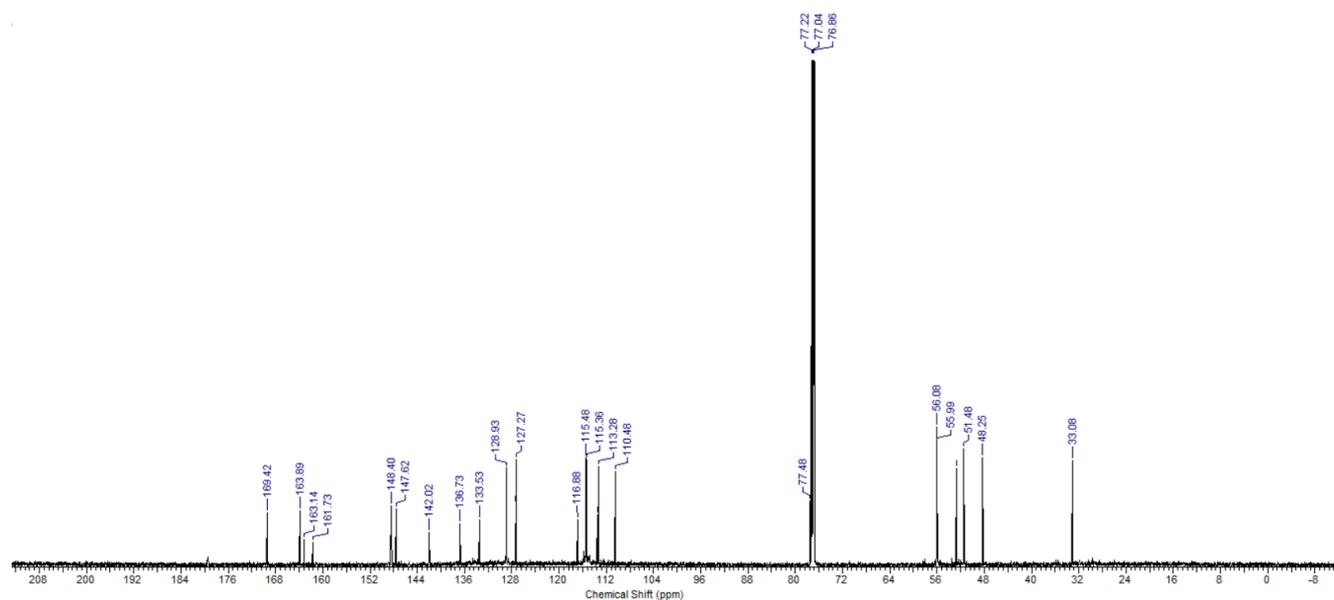


Dimethyl 11-(4-fluorophenyl)-11-hydroxy-8,9-dimethoxy-6,11-dihydro-5H-pyrrolo[2,1-*b*][3]benzazepine-1,2-dicarboxylate 5b

^1H NMR (600 MHz, CDCl_3):

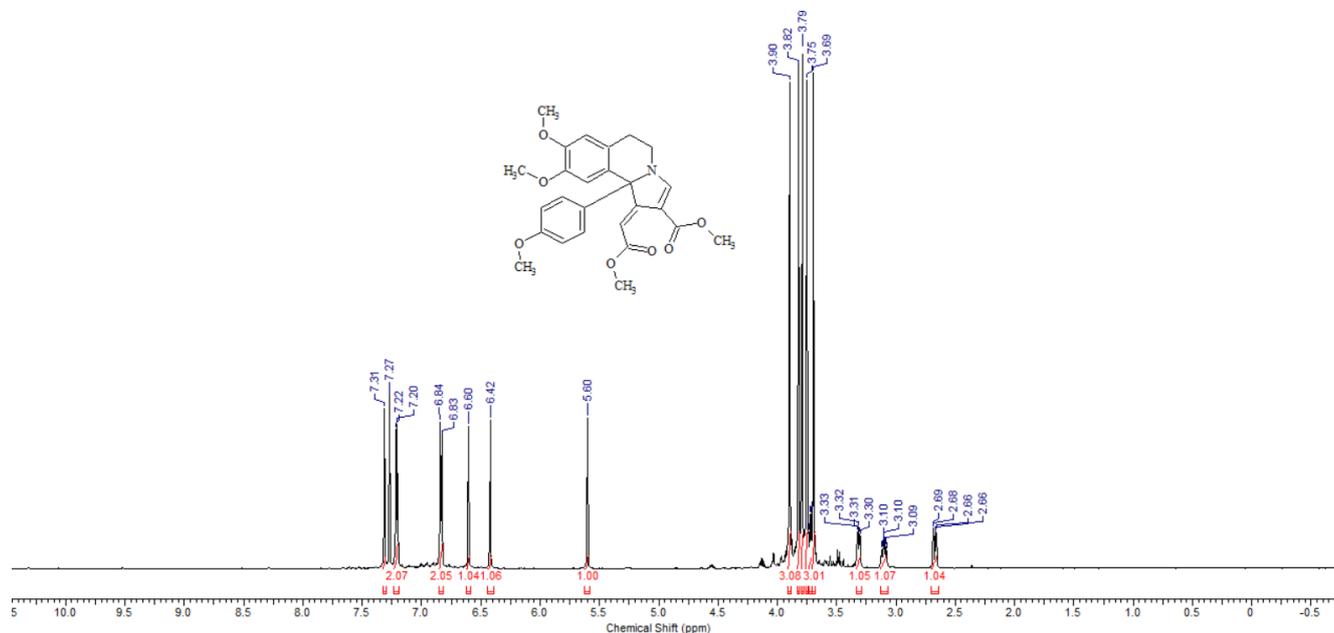


^{13}C NMR (150 MHz, CDCl_3):

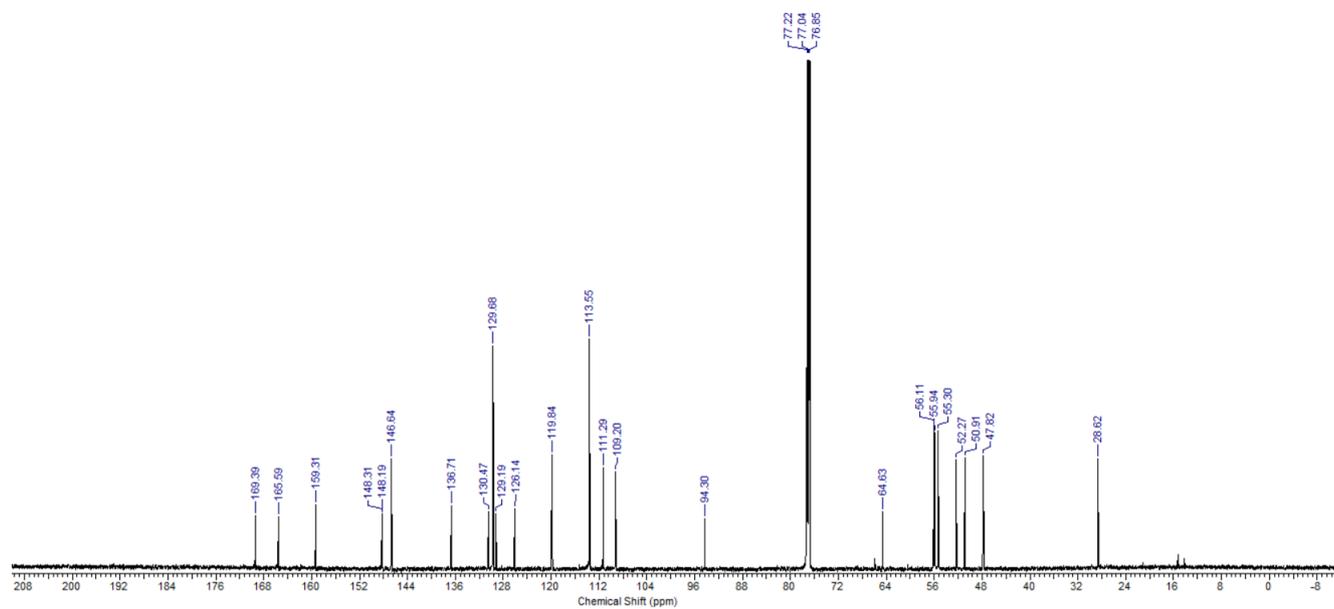


Methyl (1E)-8,9-dimethoxy-1-(2-methoxy-2-oxoethylidene)-10b-(4-methoxyphenyl)-1,5,6,10b-tetrahydropyrrolo[2,1-a]isoquinoline-2-carboxylate 6a

^1H NMR (600 MHz, CDCl_3):

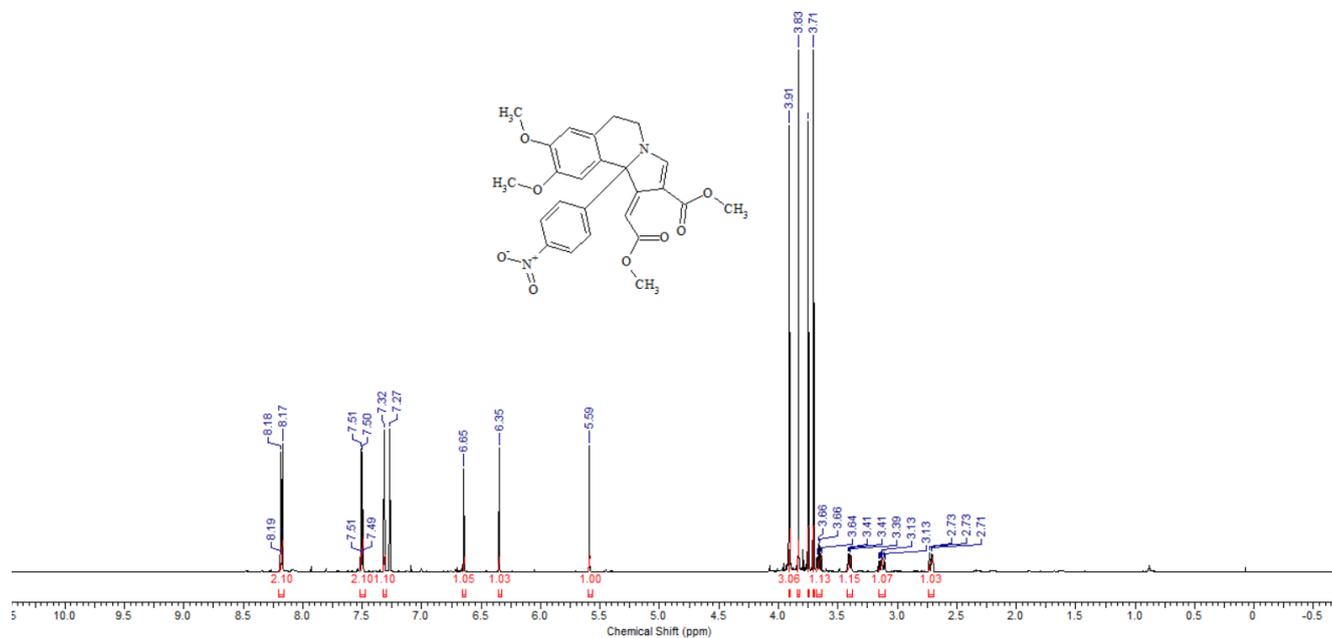


^{13}C NMR (150 MHz, CDCl_3):

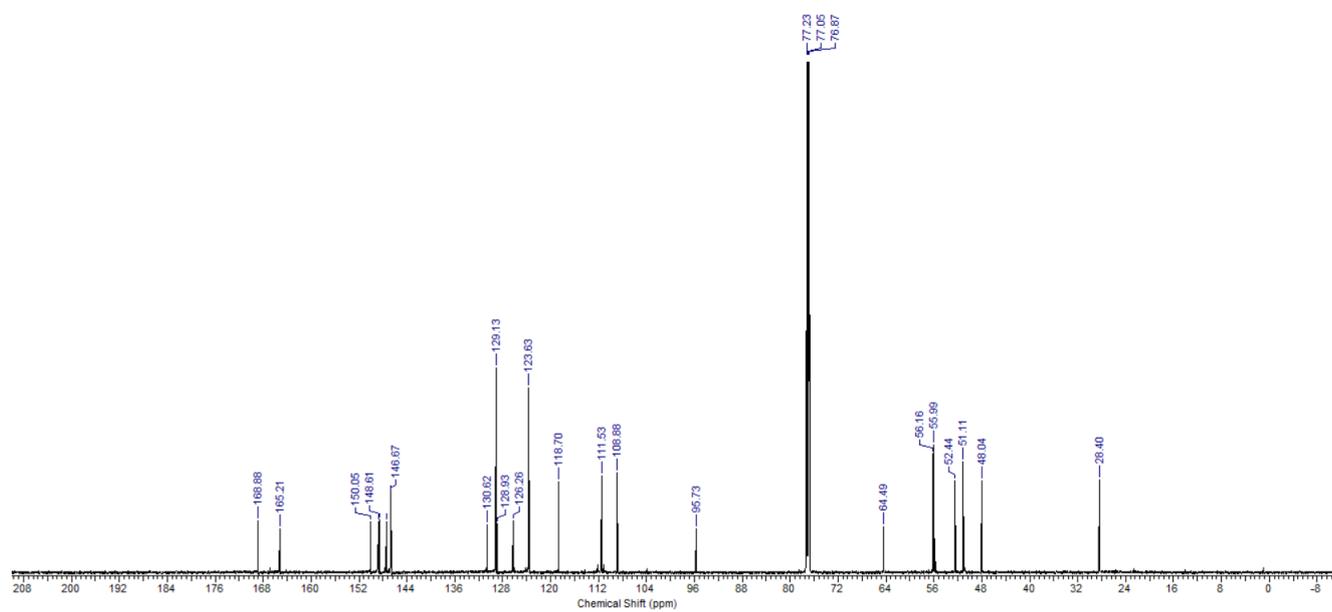


Methyl (1E)-8,9-dimethoxy-1-(2-methoxy-2-oxoethylidene)-10b-(4-nitrophenyl)-1,5,6,10b-tetrahydropyrrolo[2,1-a]isoquinoline-2-carboxylate 6b

^1H NMR (600 MHz, CDCl_3):



^{13}C NMR (150 MHz, CDCl_3):



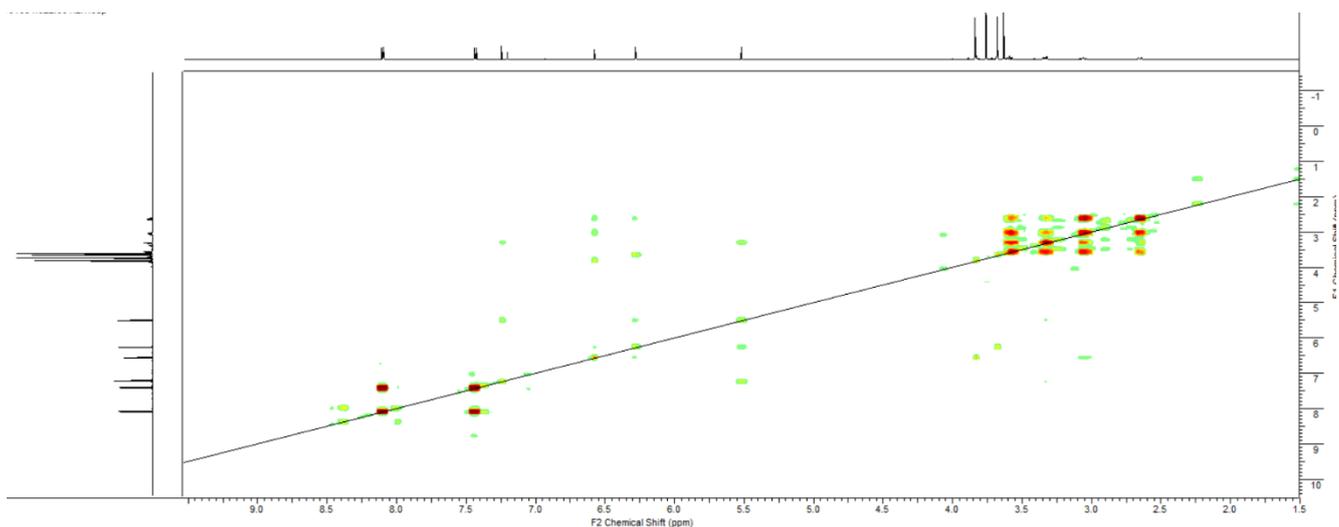


Figure S1. NOESY spectrum of **6b** in CDCl₃.

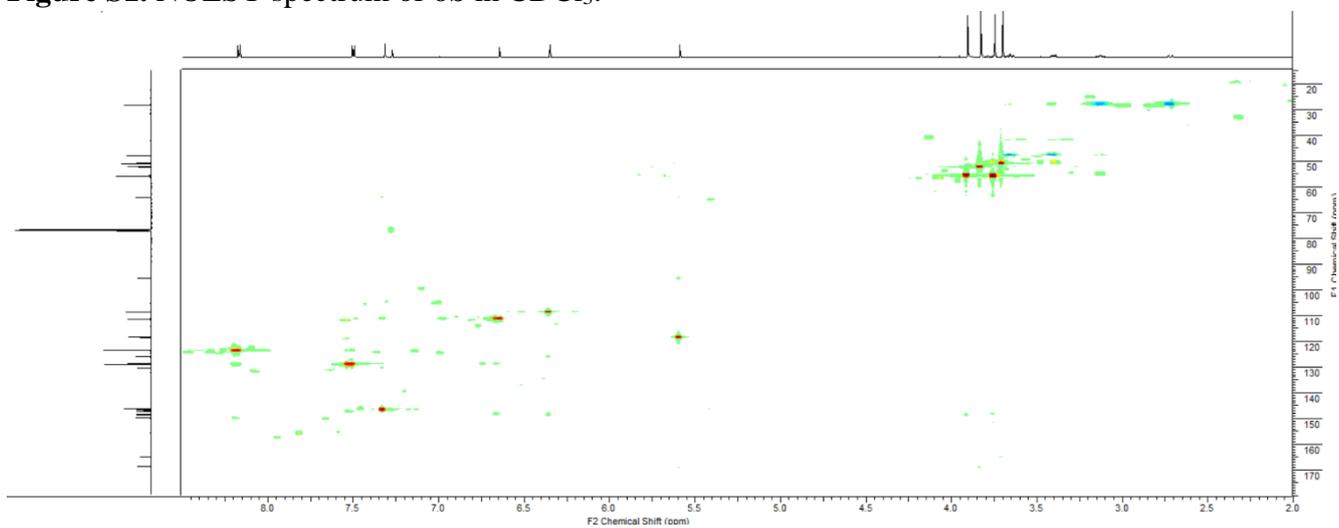


Figure S2. HMQC 1H-13C spectrum of **6b** in CDCl₃.

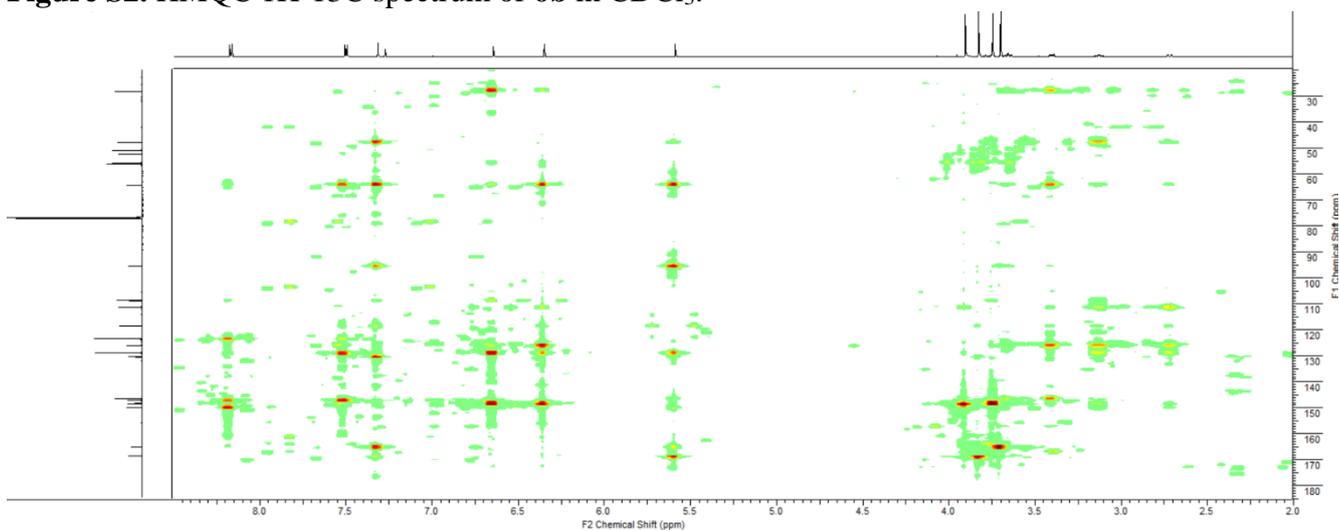


Figure S3. HMBC 1H-13C spectrum of **6b** in CDCl₃.