

Supporting information for:

Computer-aided structure-based optimization of 4,5,6,7-tetrahydrobenzo[d]thiazole-2,6-diamine derivatives as DNA gyrase B inhibitors

Lucas J. Gutierrez,^{a,b} Marcela Vettorazzi,^{a,c} Jaka Dernovšek,^d Martina Durcik,^d Lucija Peterlin Mašič,^d Tihomir Tomašič*^d and Ricardo D. Enriz*^{a,b}.

^a Universidad Nacional de San Luis, Facultad de Química, Bioquímica y Farmacia, Ejército de los Andes 950, 5700 San Luis, Argentina.

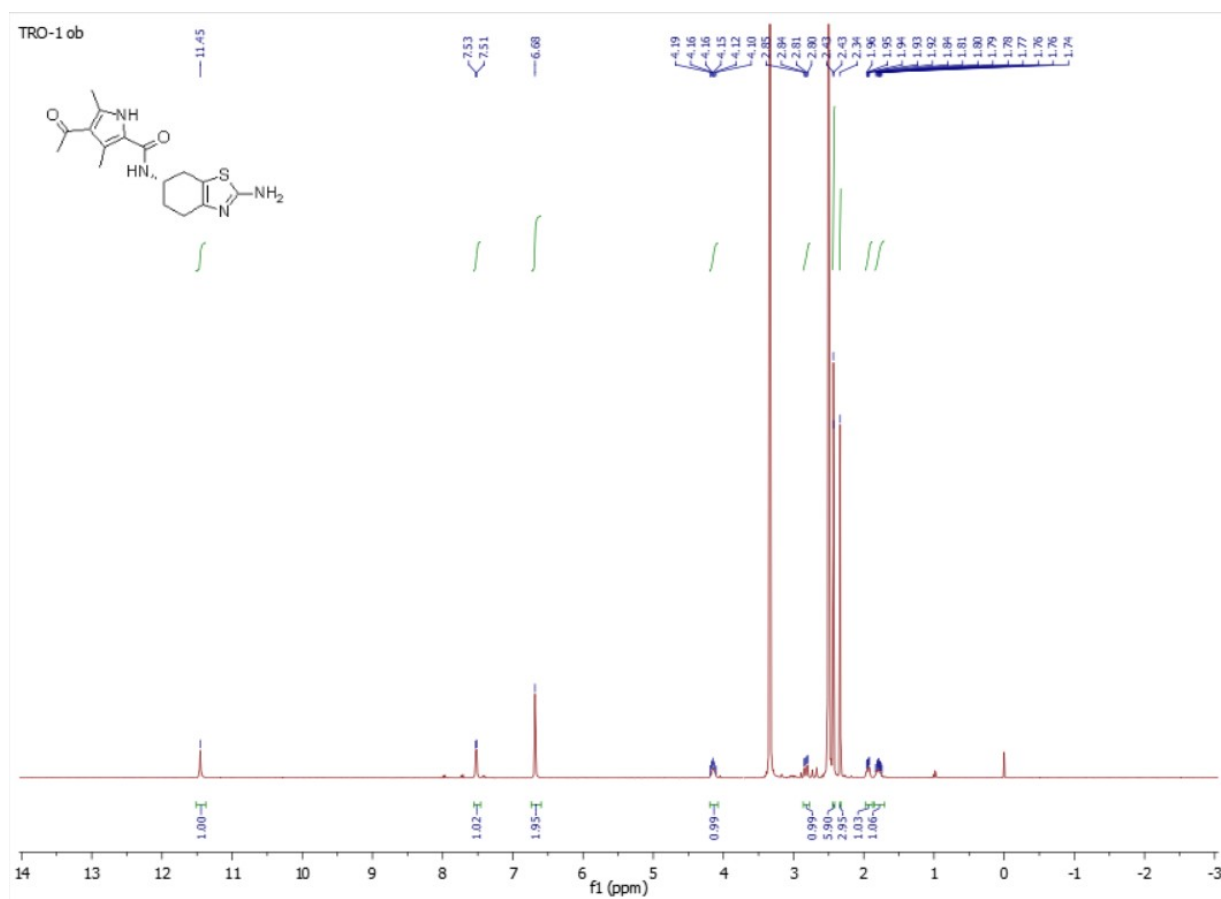
^b IMIBIO-CONICET, UNSL, Ejército de los Andes 950, 5700 San Luis, Argentina.

^c IMASL-CONICET, UNSL, Ejército de los Andes 950, 5700 San Luis, Argentina.

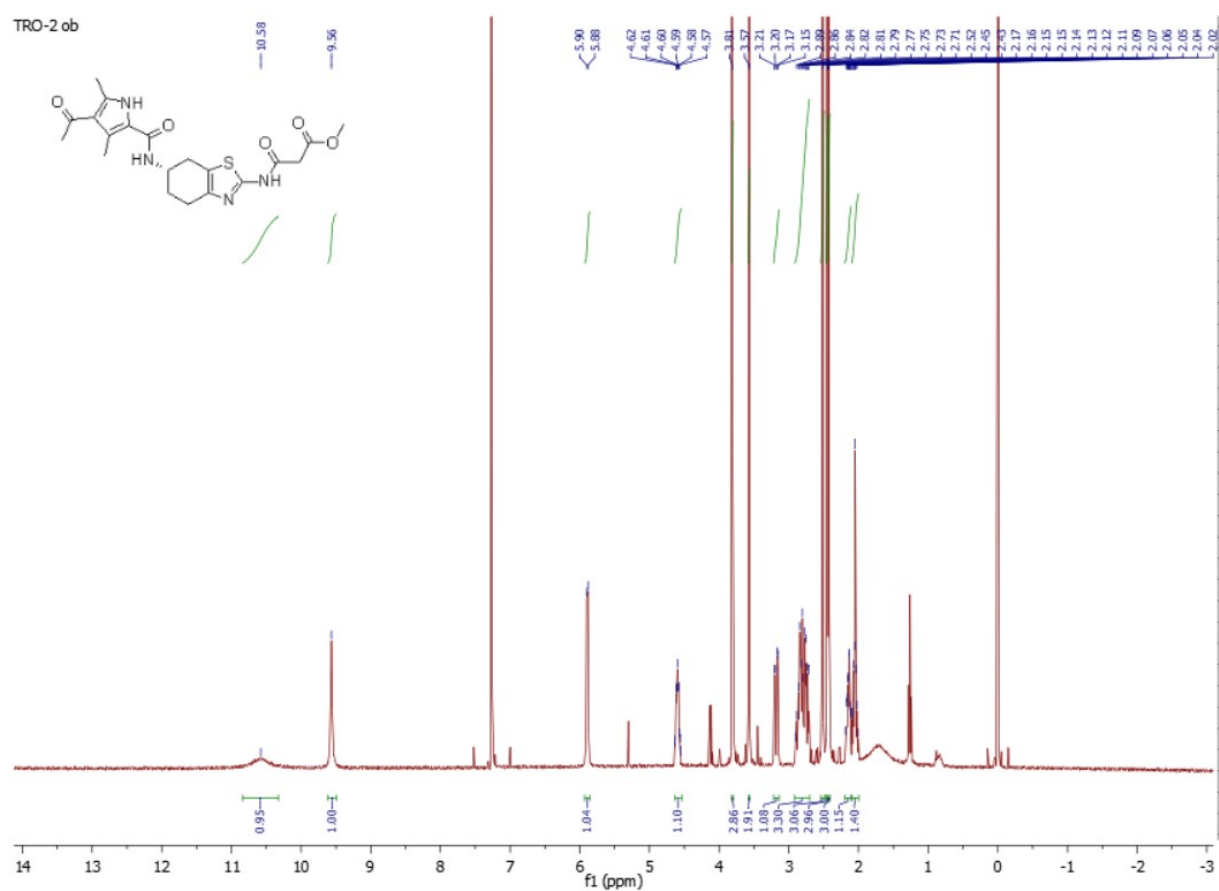
^d University of Ljubljana, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Aškerčeva cesta 7, 1000 Ljubljana, Slovenia.

† denriz@unsl.edu.ar; tihomir.tomasic@ffa.uni-lj.si

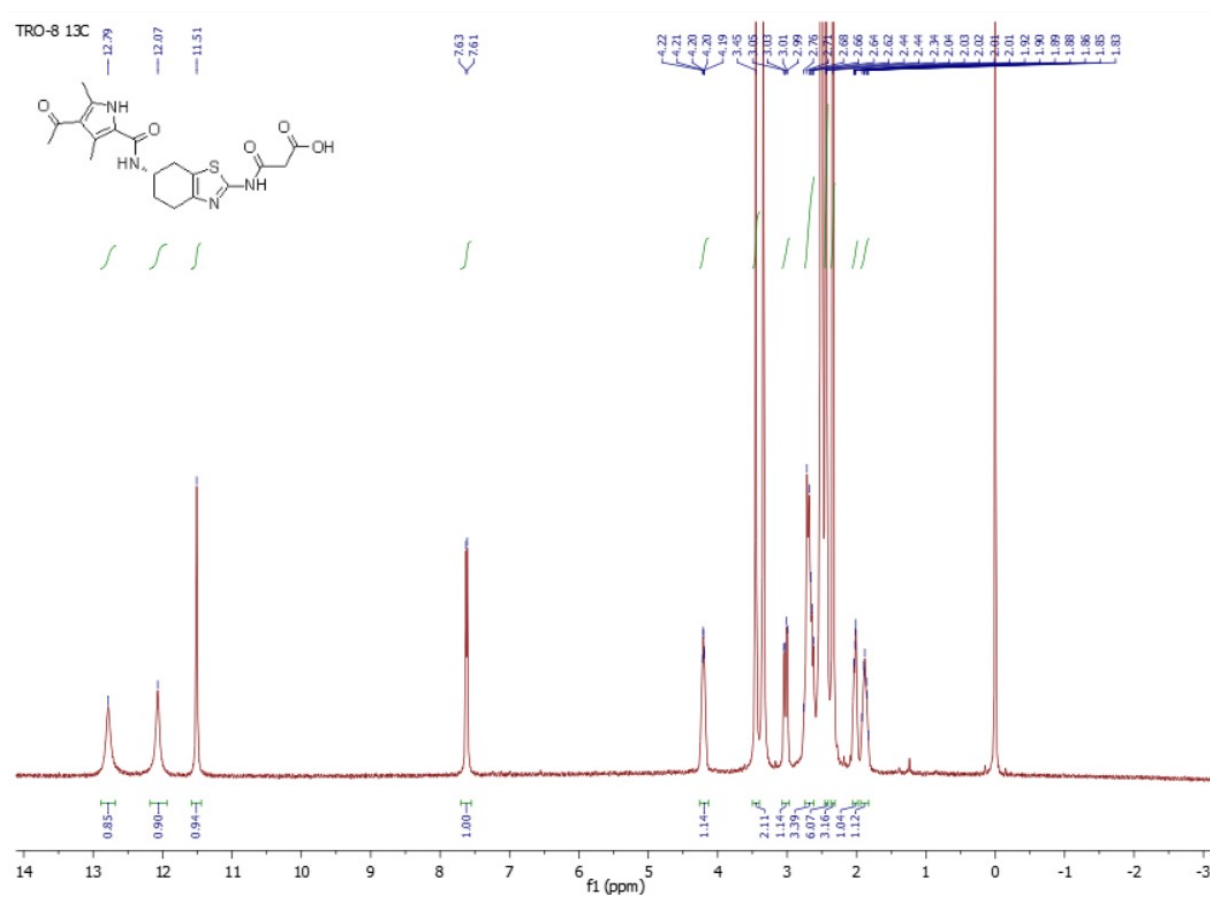
¹H NMR spectrum for compound 11b



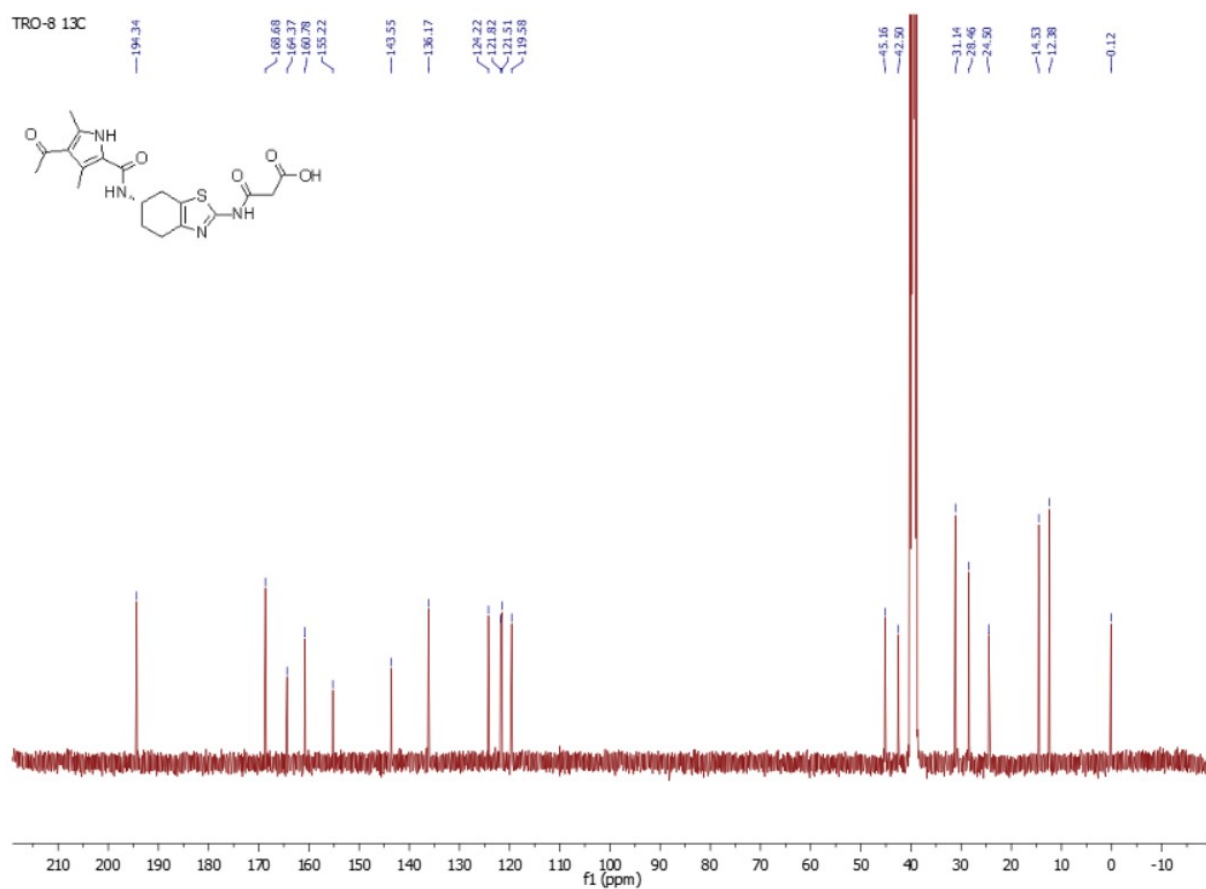
¹H NMR spectrum for compound 11c



¹H NMR spectrum for compound 11



¹³C NMR spectrum for compound 11

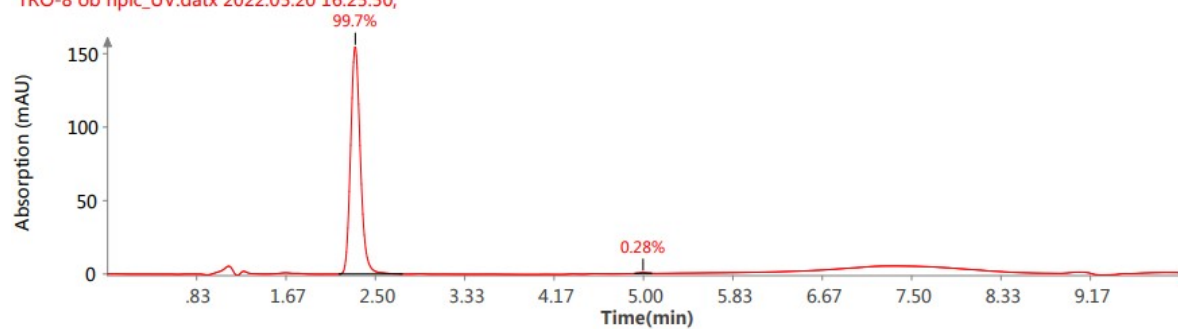


HPLC chromatogram for compound 11

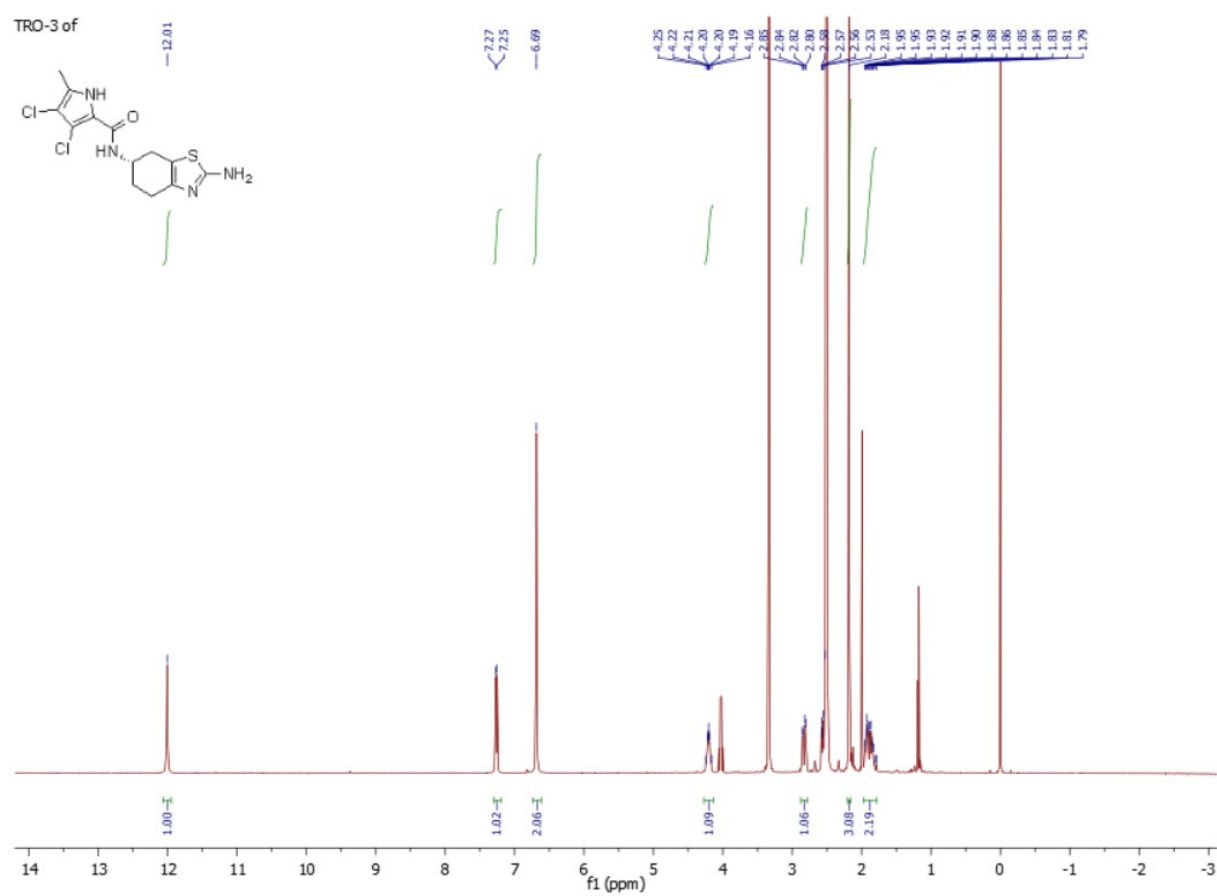
HPLC t_r =2,31 min (99.7% purity)

VWD: Signal A, 254 nm

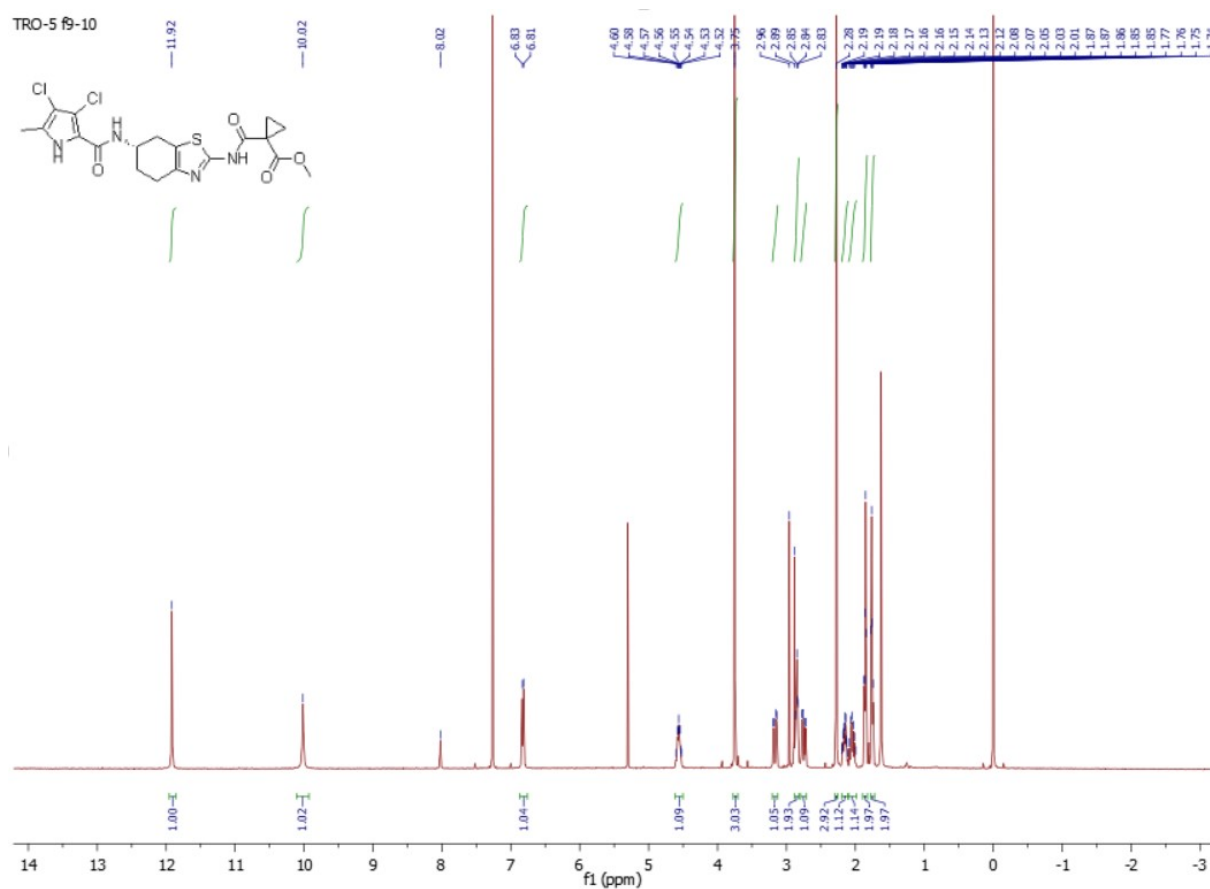
TRO-8 ob hplc_UV.datx 2022.05.20 16:25:50;



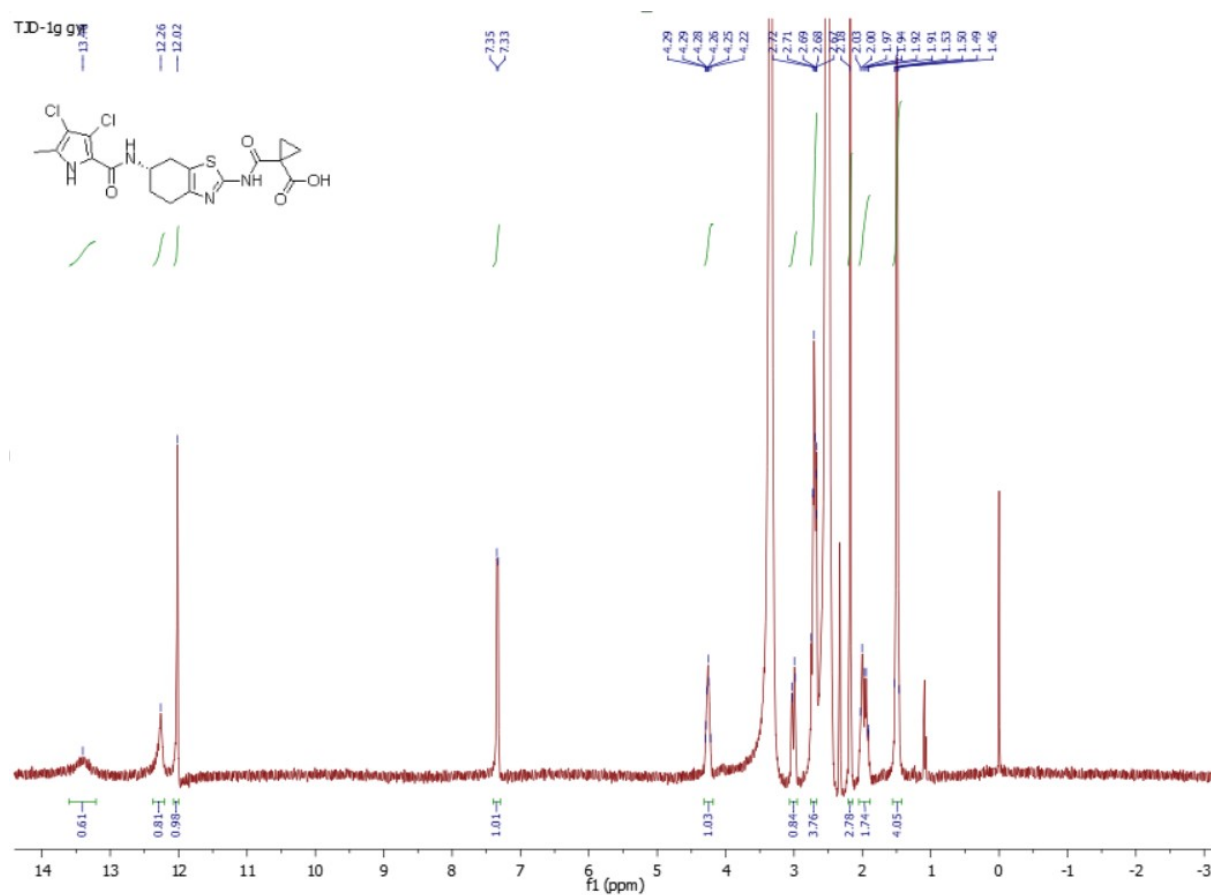
¹H NMR spectrum for compound 12b



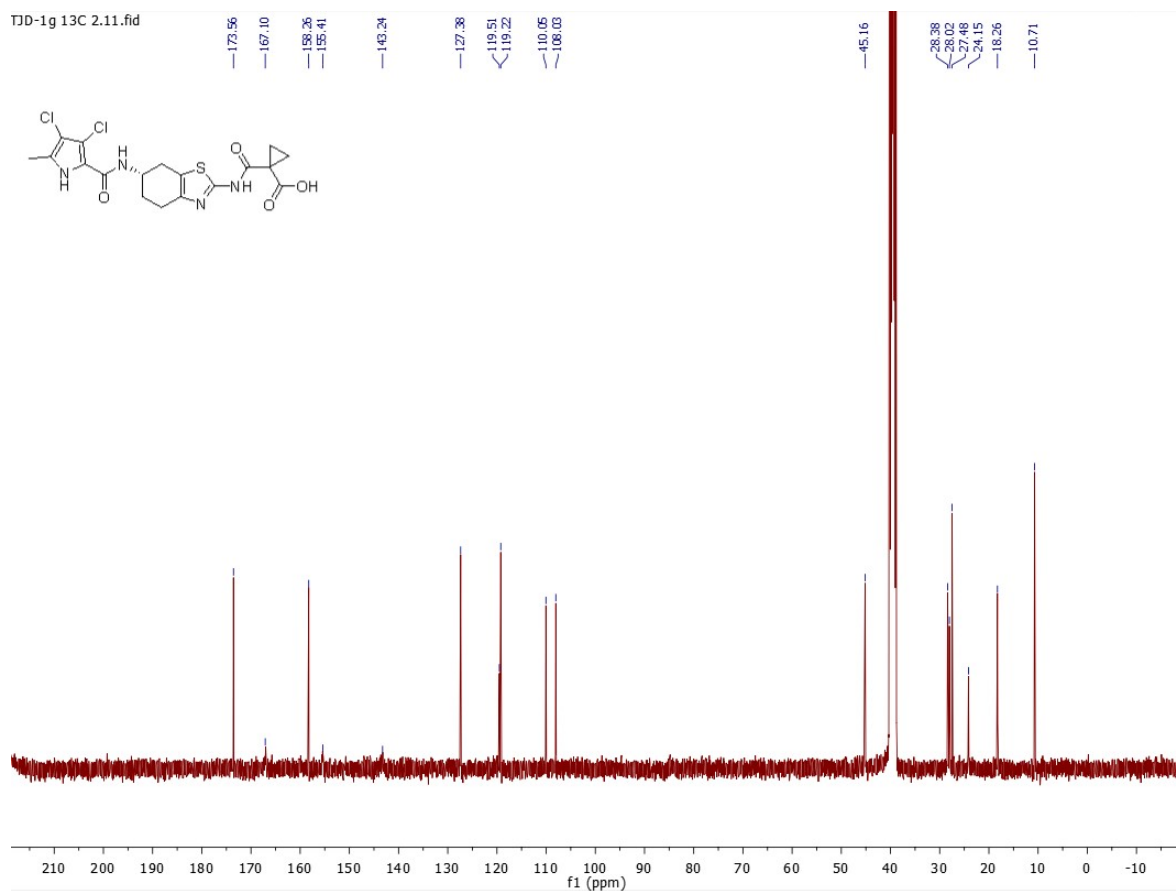
¹H NMR spectrum for compound 12c



¹H NMR spectrum for compound 12



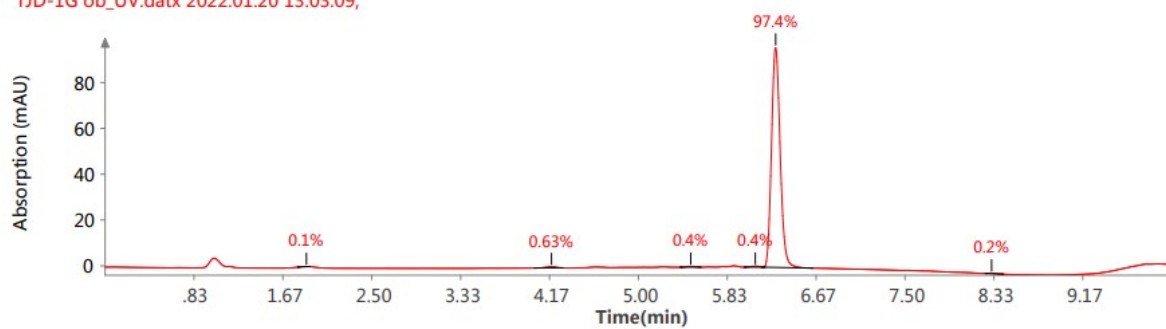
¹³C NMR spectrum for compound 12



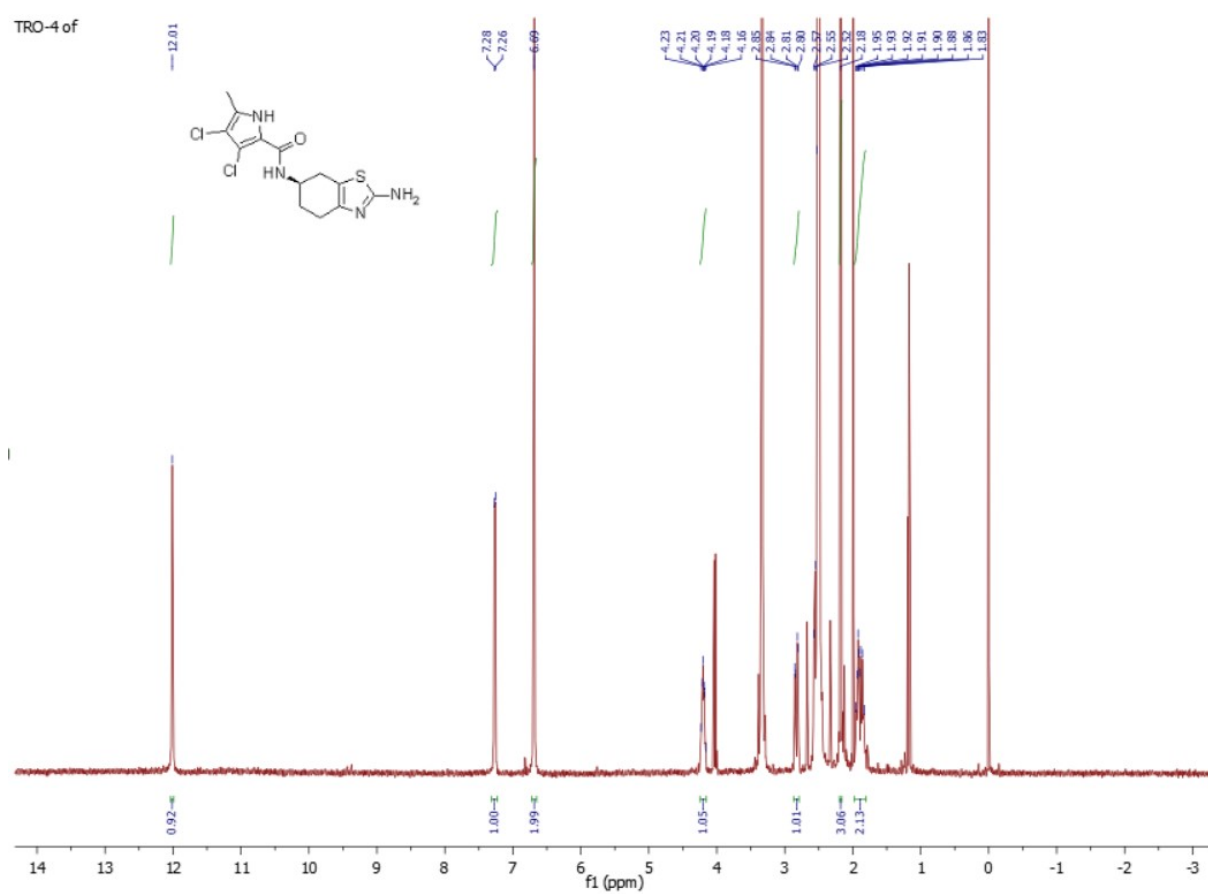
HPLC chromatogram for compound 12

HPLC: t_r = 6,28 min (97.4% at 254 nm)

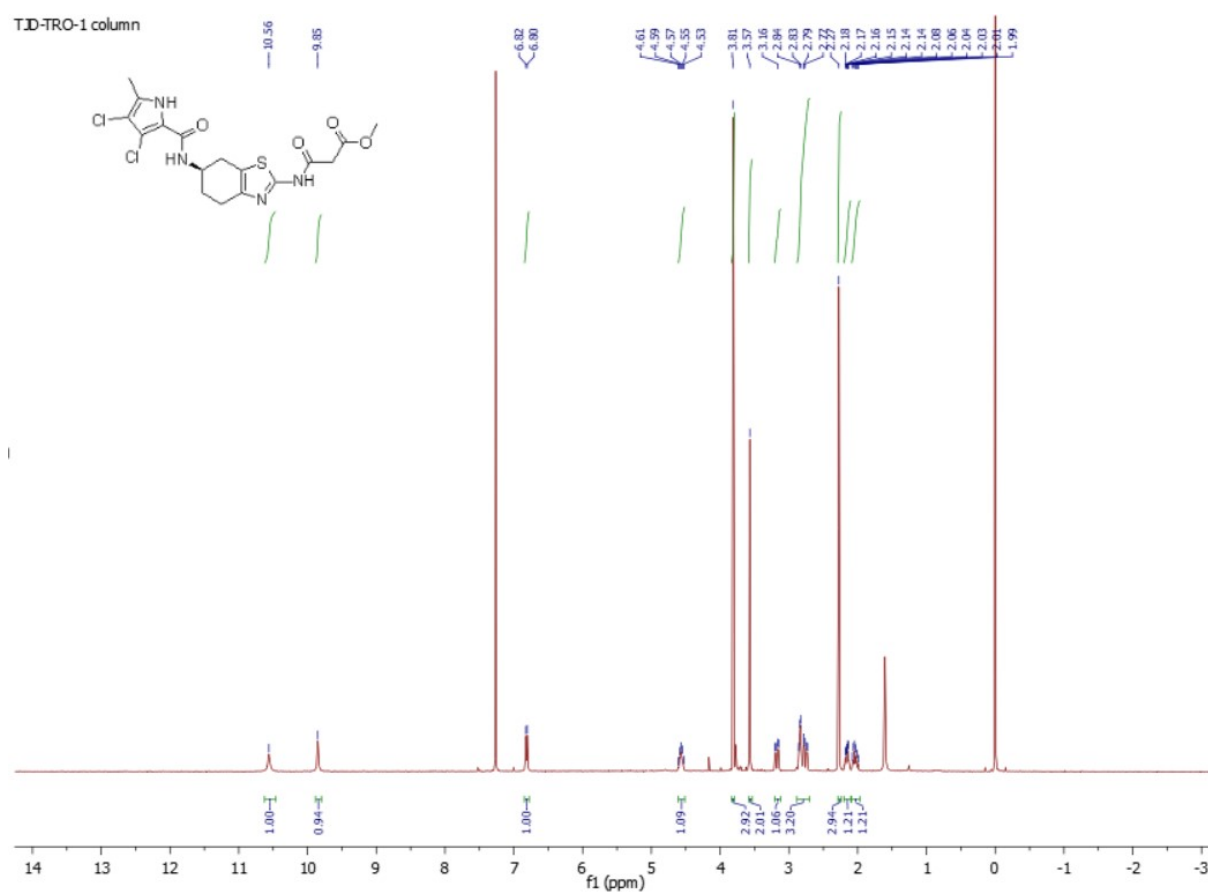
VWD: Signal A, 254 nm
TJD-1G ob_UV.datx 2022.01.20 13:03:09;



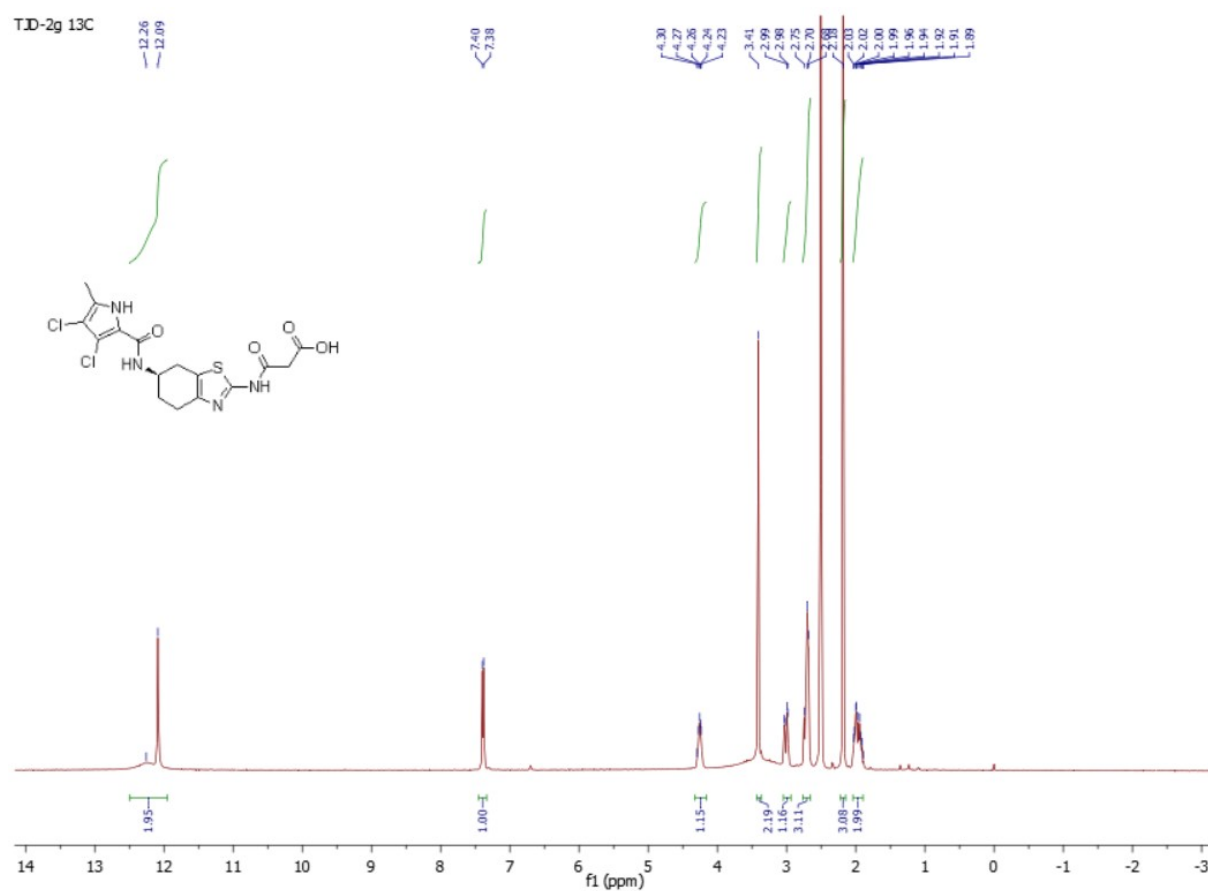
¹H NMR spectrum for compound 13b



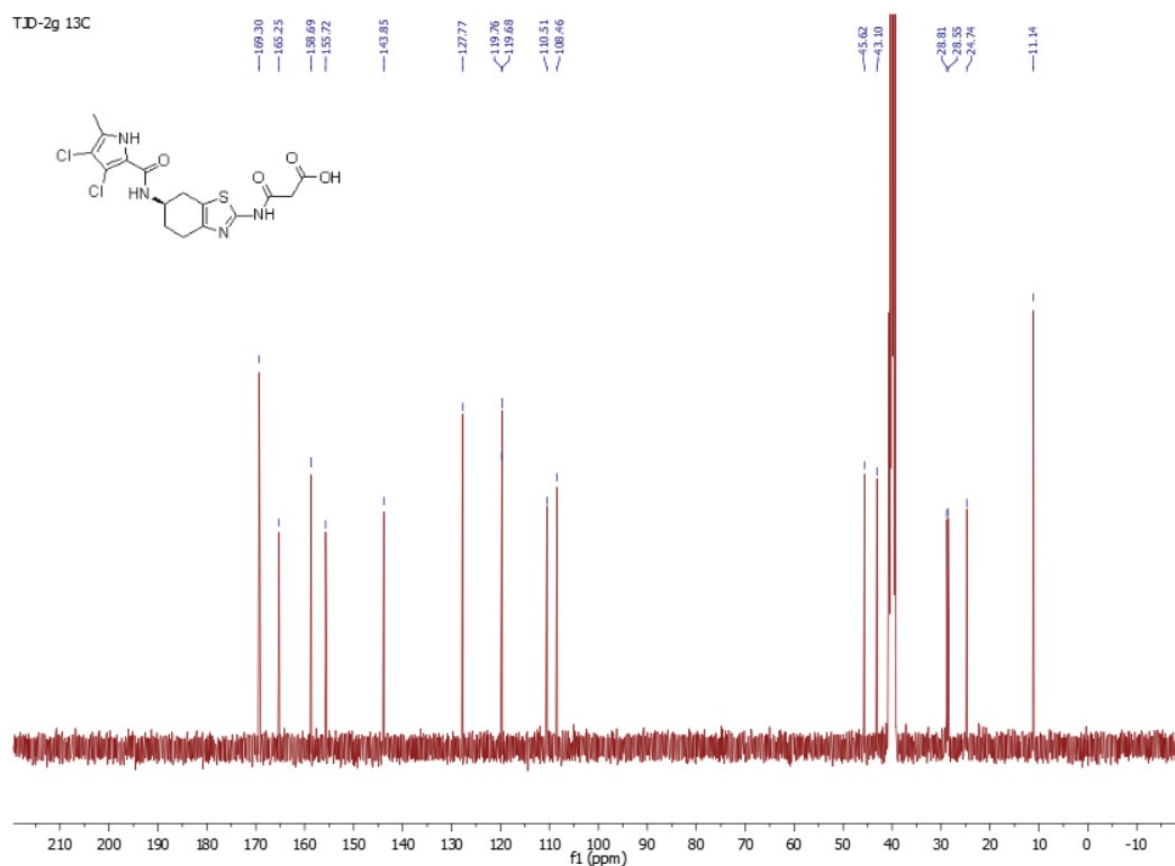
¹H NMR spectrum for compound 13c



¹H NMR spectrum for compound 13



¹³C NMR spectrum for compound 13



HPLC chromatogram for compound 13

HPLC: t_r = 5.52 min (96.8% at 254 nm)

VWD: Signal A, 254 nm

TJD-2g ob_UV.datx 2022.02.16 13:27:00;

