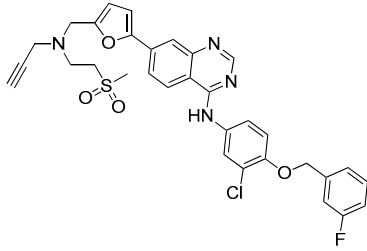


***Closo*-carboranyl- and Metallacarboranyl[1,2,3]triazolyl-decorated Lapatinib-scaffold for Cancer Therapy Combining Tyrosine Kinase Inhibition and Boron Neutron Capture Therapy**

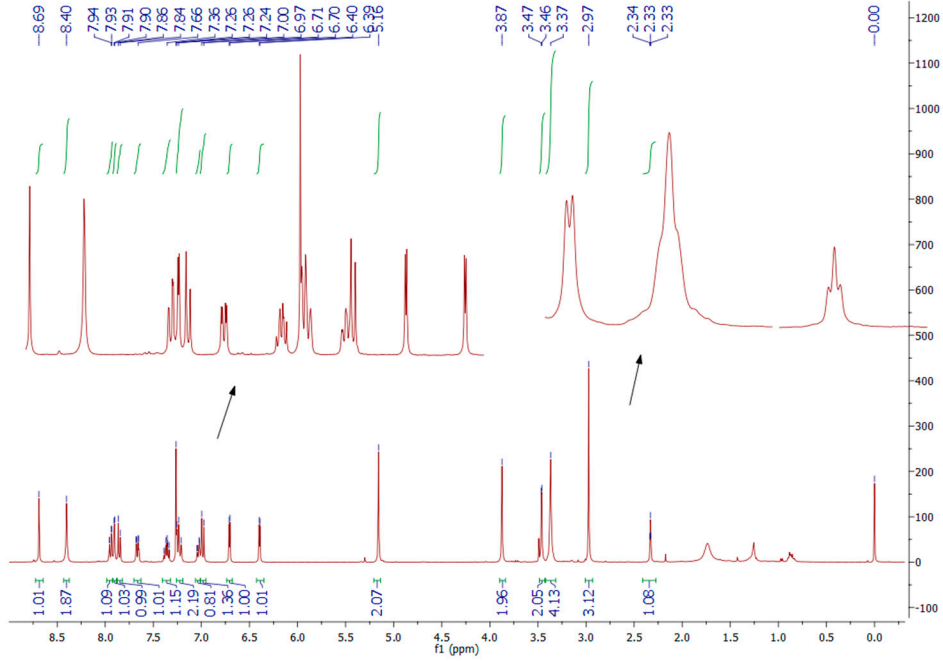
Marcos Couto, Catalina Alamón, María Fernanda García, Mariángeles Kovacs, Emiliano Trias, Susana Nieves, Emiliano Pozzi, Paula Curotto, Silvia Thorp, María Alejandra Dagrosa, Francesc Teixidor, Clara Viñas and Hugo Cerecetto

Supplementary Material

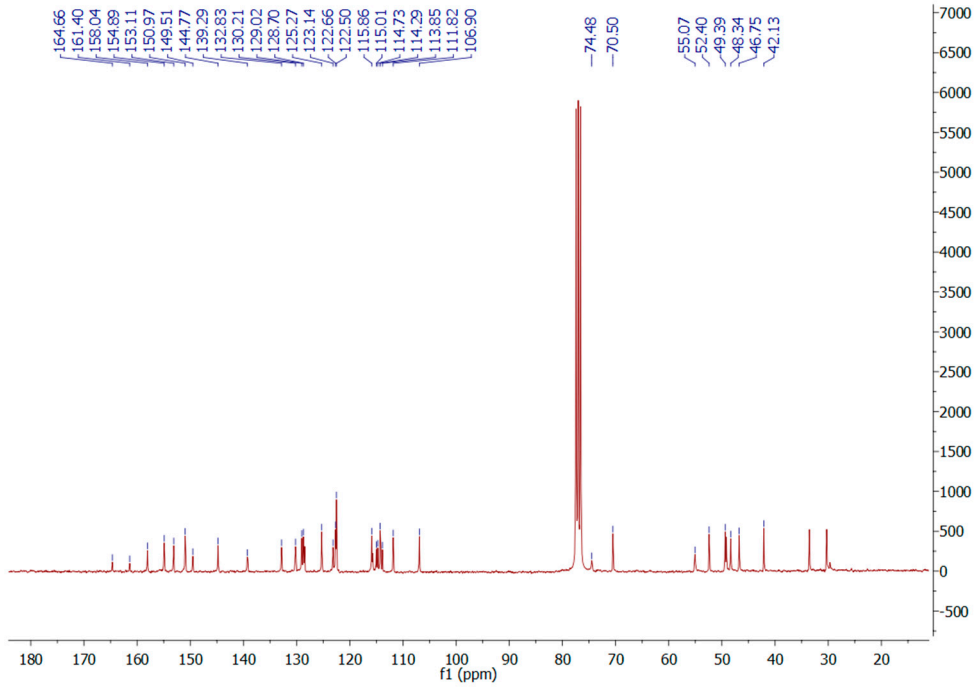
Spectra developed compoundspages 2–15
Figure S1page 16
Figure S2page 17

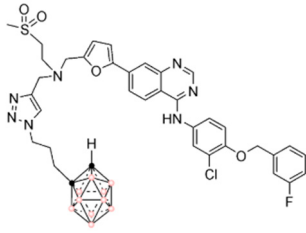


¹H-NMR

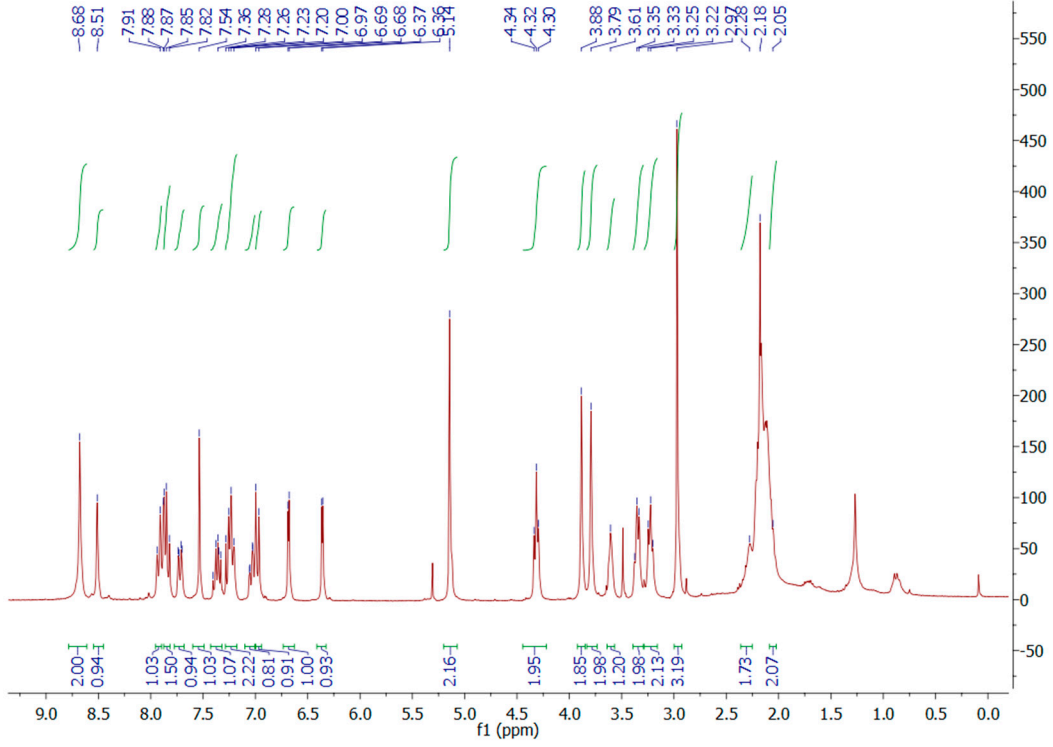


¹³C-NMR

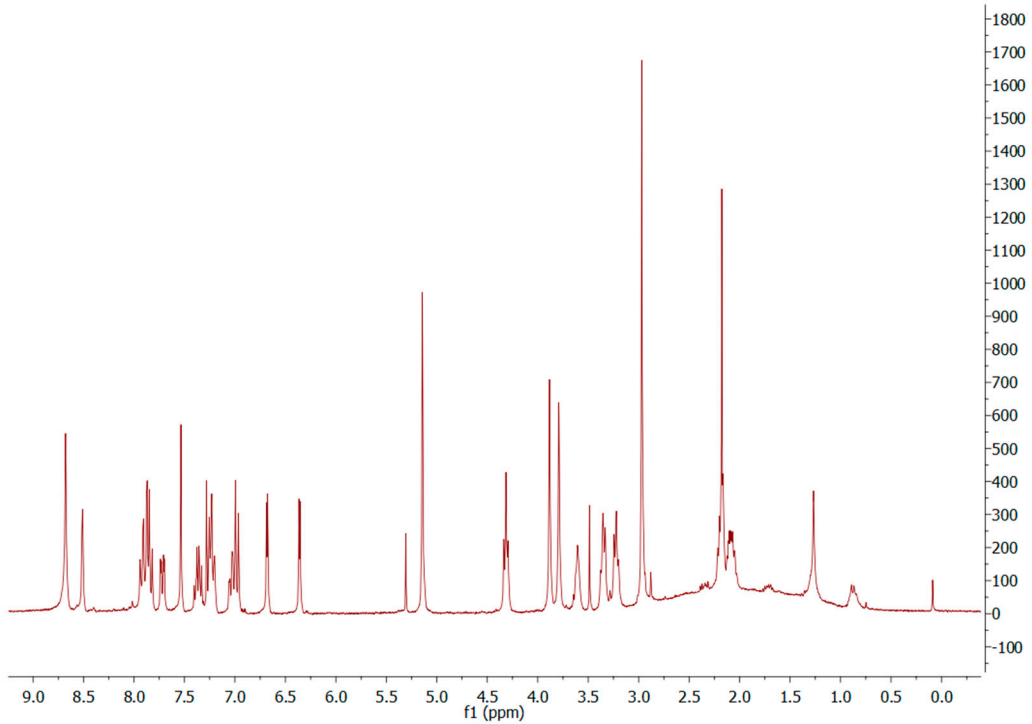




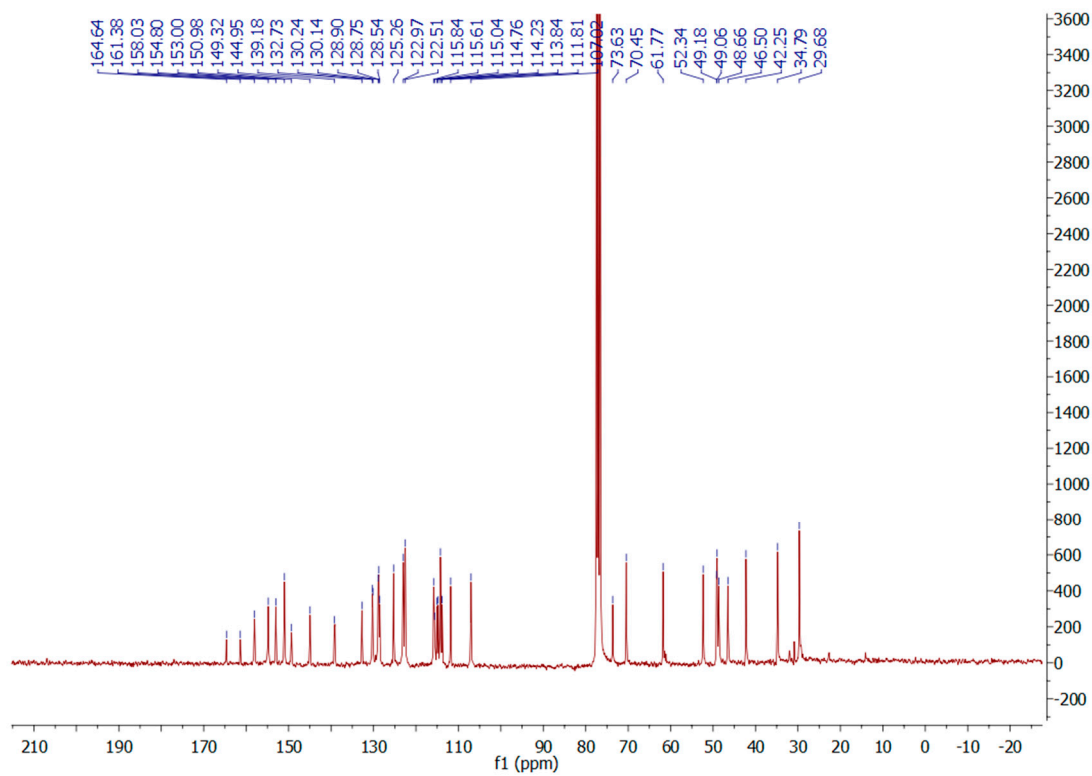
$^1\text{H}\{^{11}\text{B}\}$ -NMR



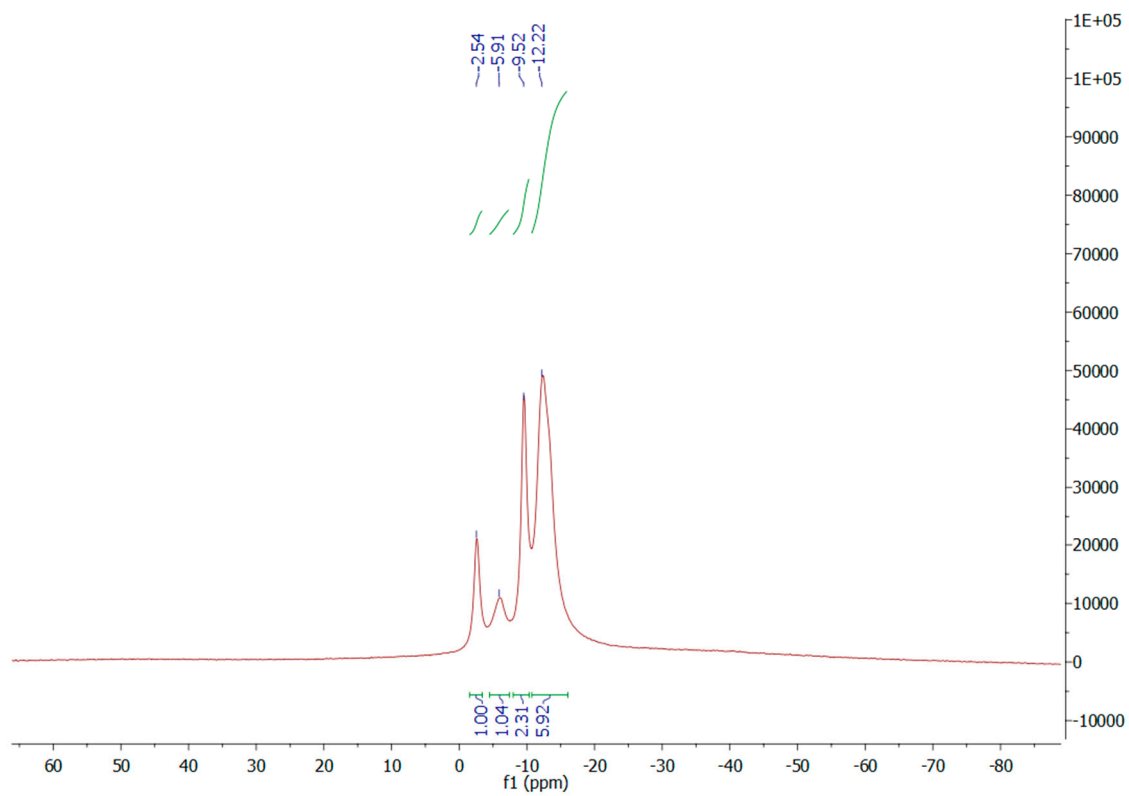
^1H -NMR

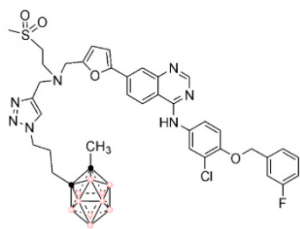


^{13}C -NMR

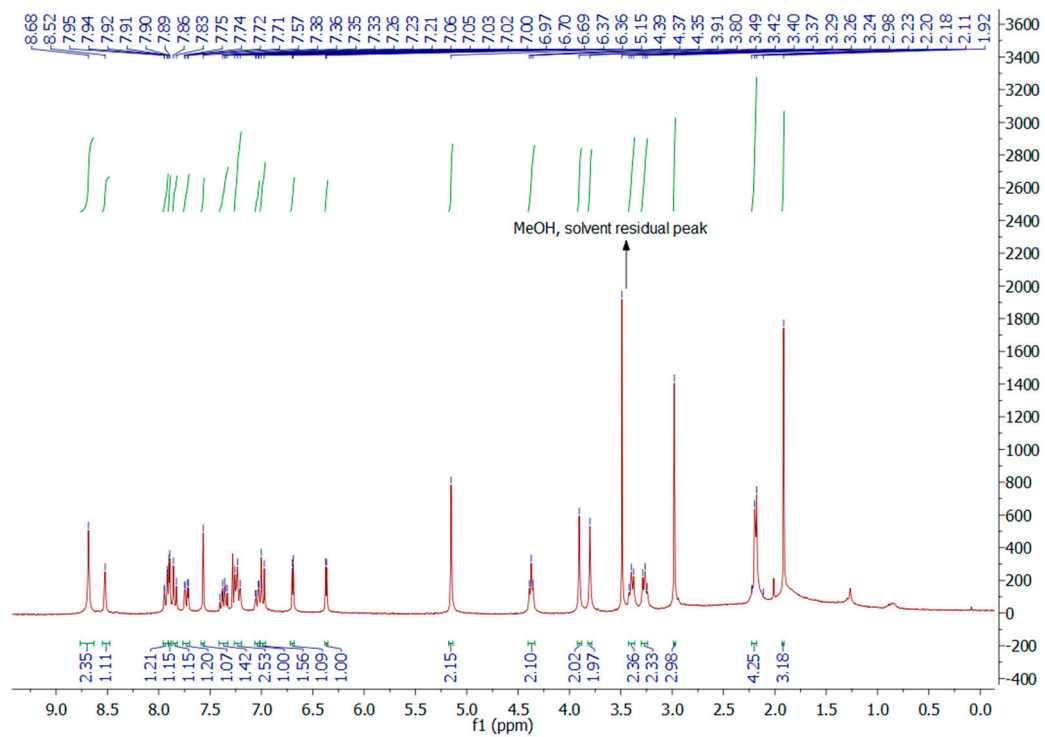


$^{11}\text{B}\{^1\text{H}\}$ -NMR

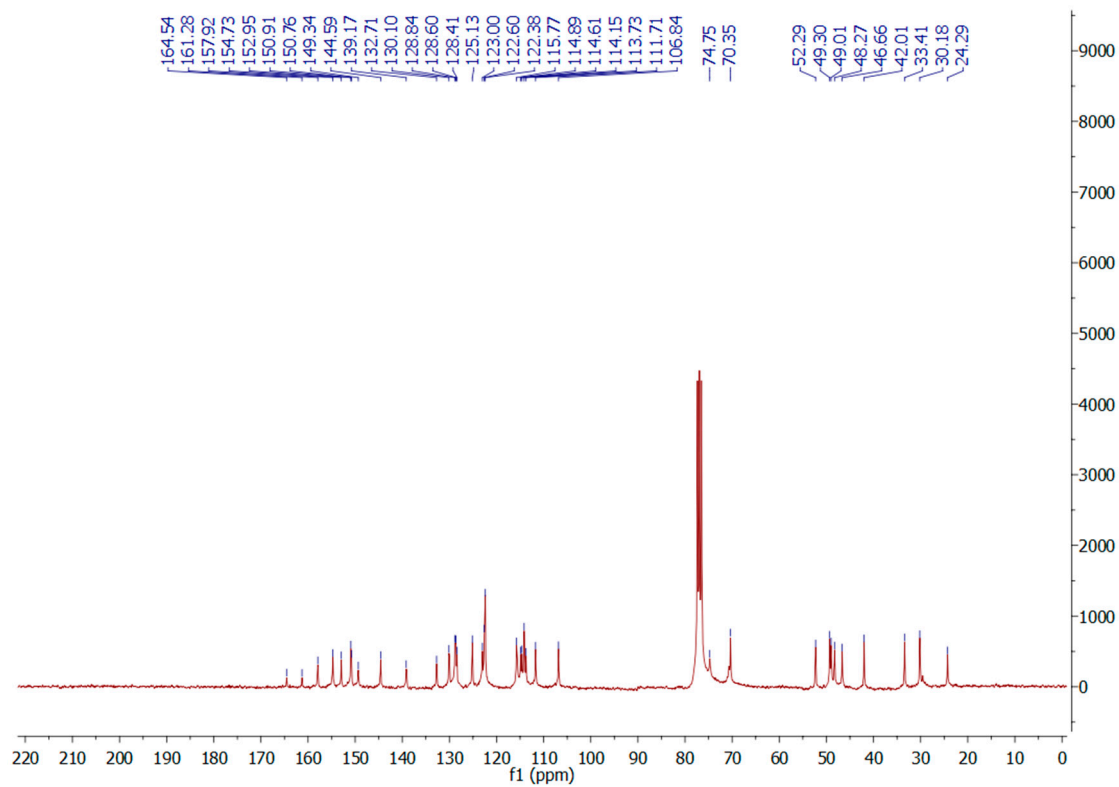




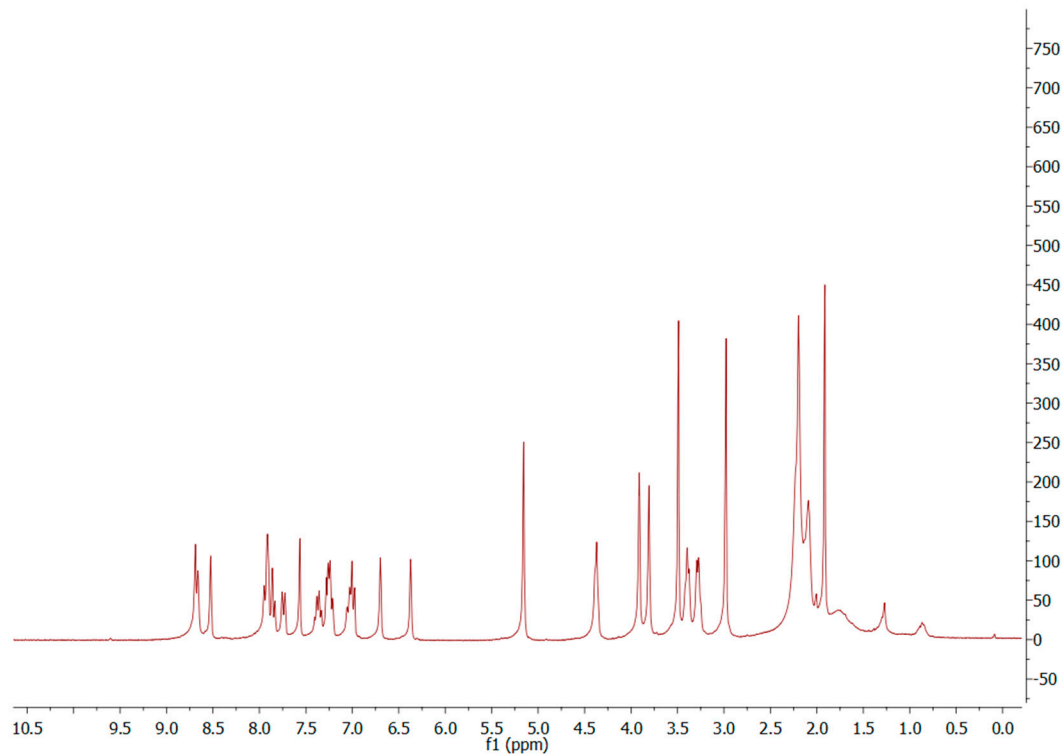
¹H-NMR



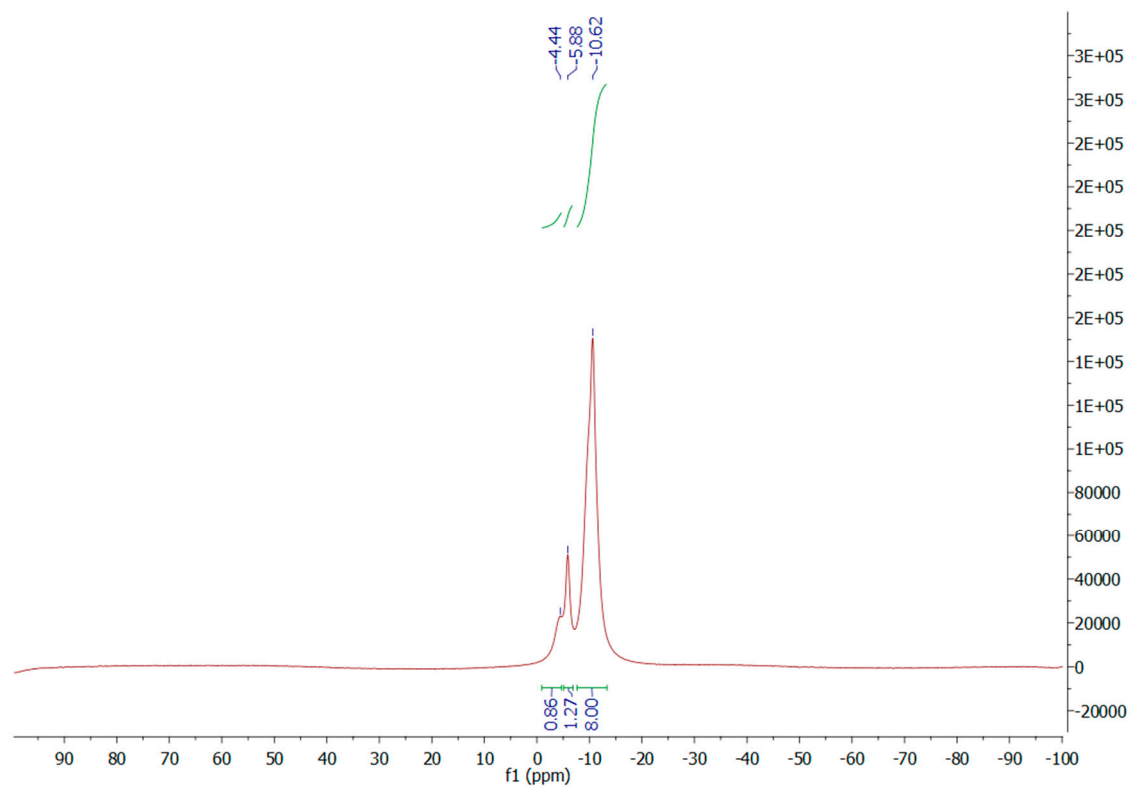
¹³C-NMR

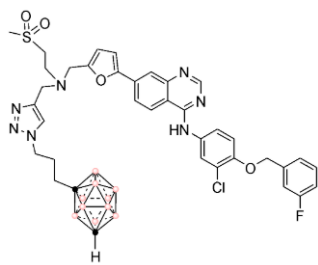


$^1\text{H}\{^{11}\text{B}\}$ -NMR

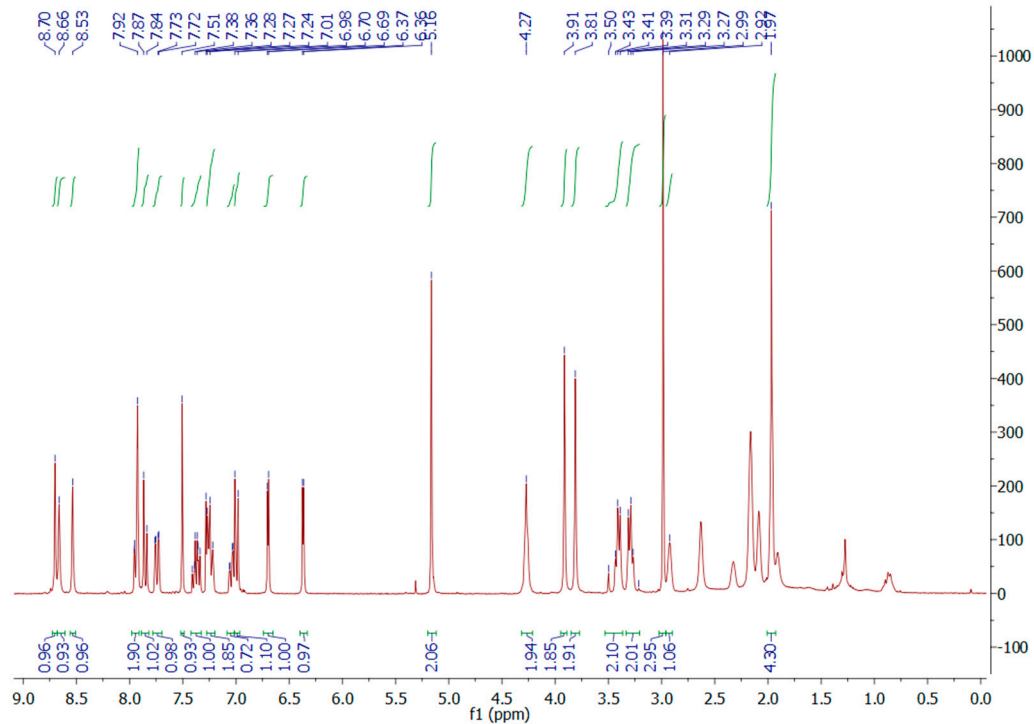


$^{11}\text{B}\{^1\text{H}\}$ -NMR

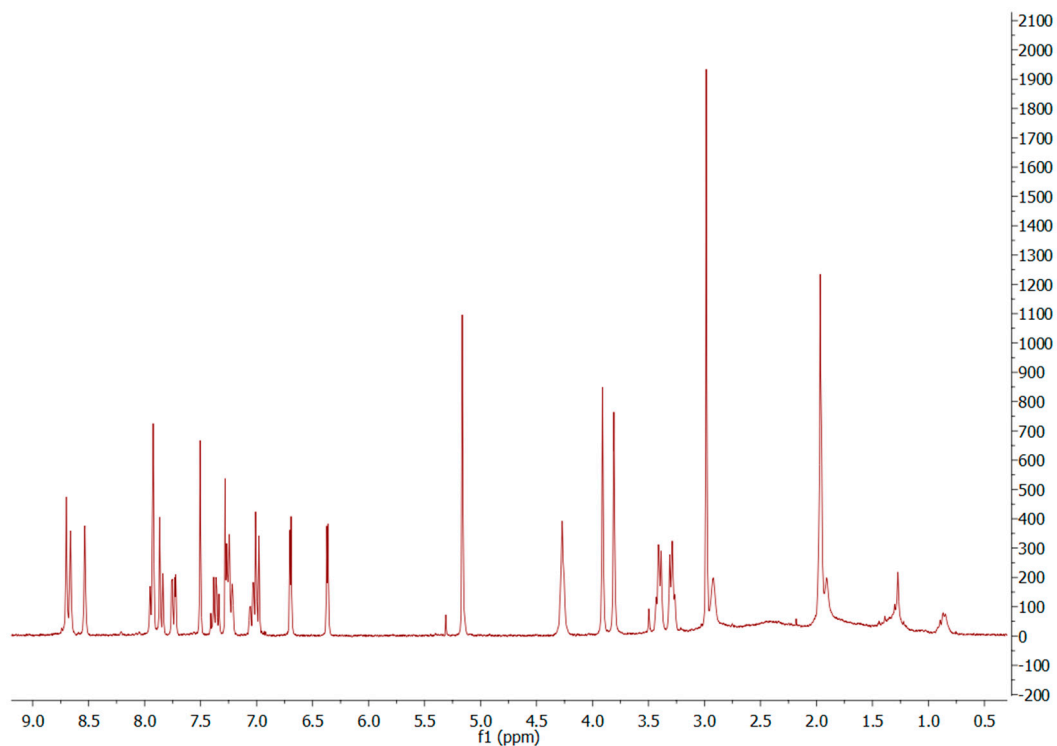




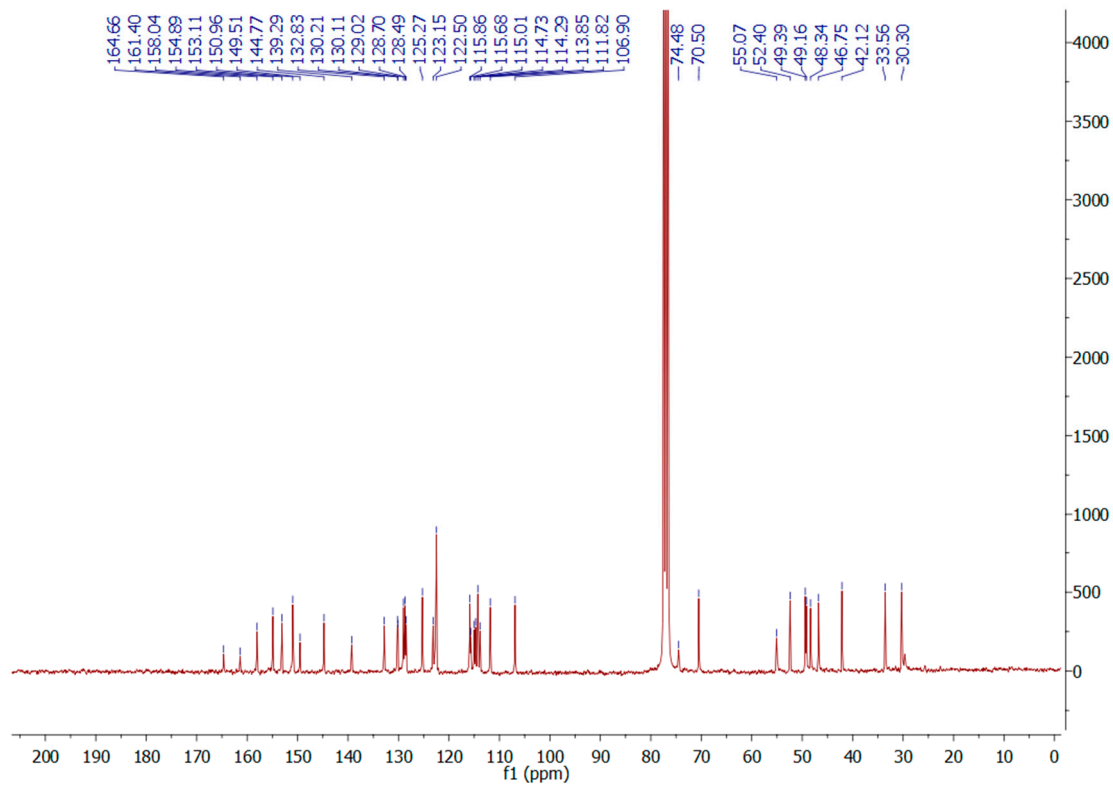
$^1\text{H}\{^{11}\text{B}\}$ -NMR



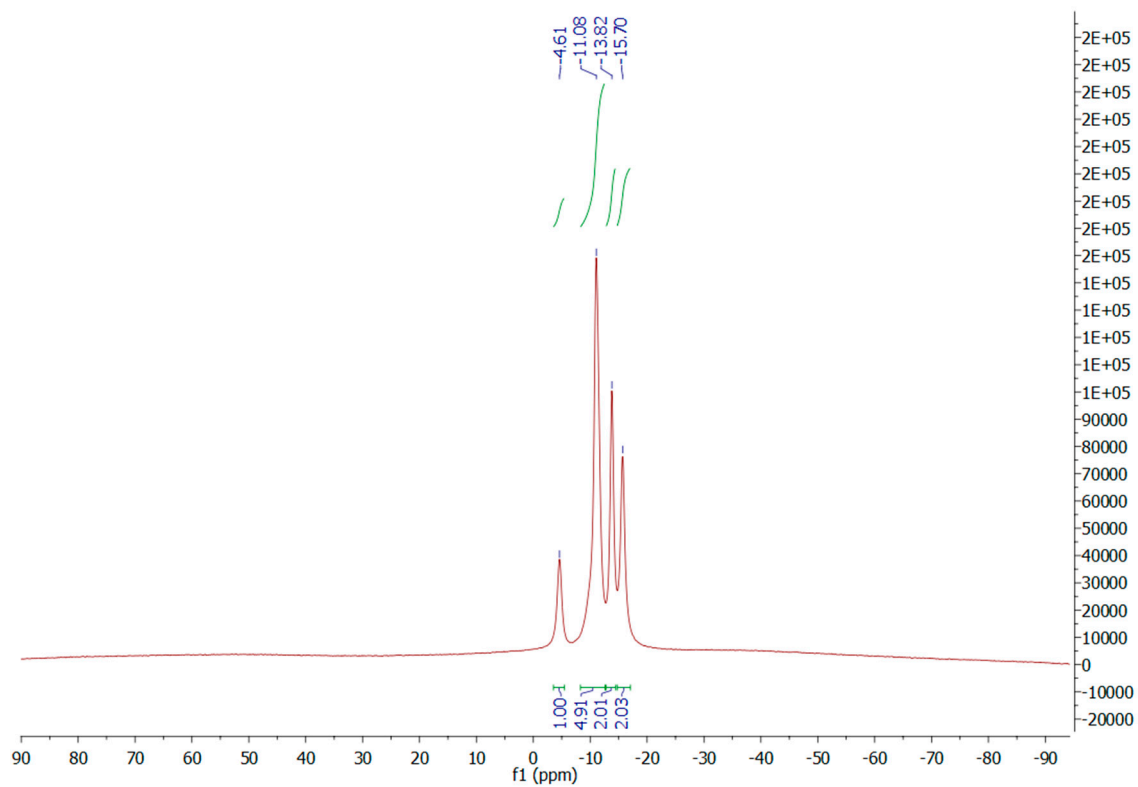
^1H -NMR



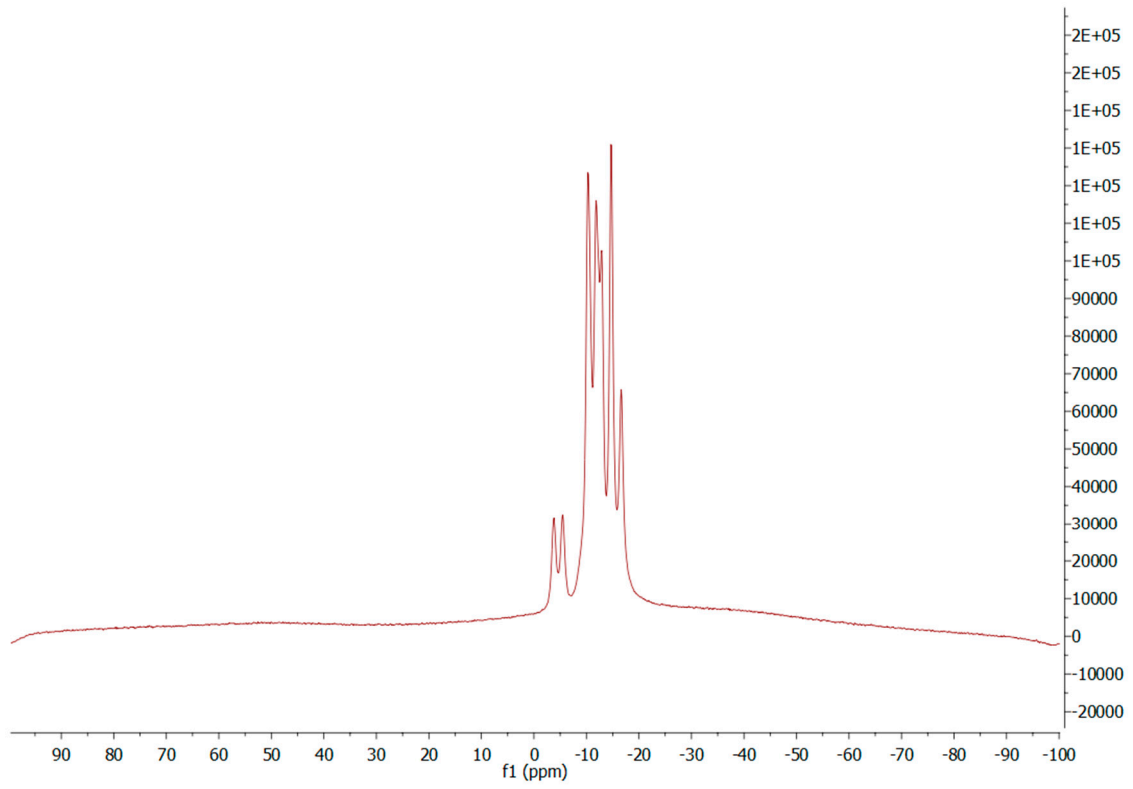
^{13}C -NMR

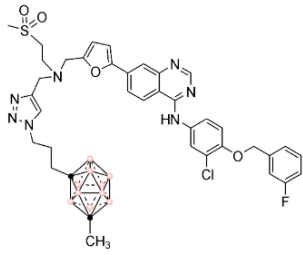


$^{11}\text{B}\{^1\text{H}\}$ -NMR

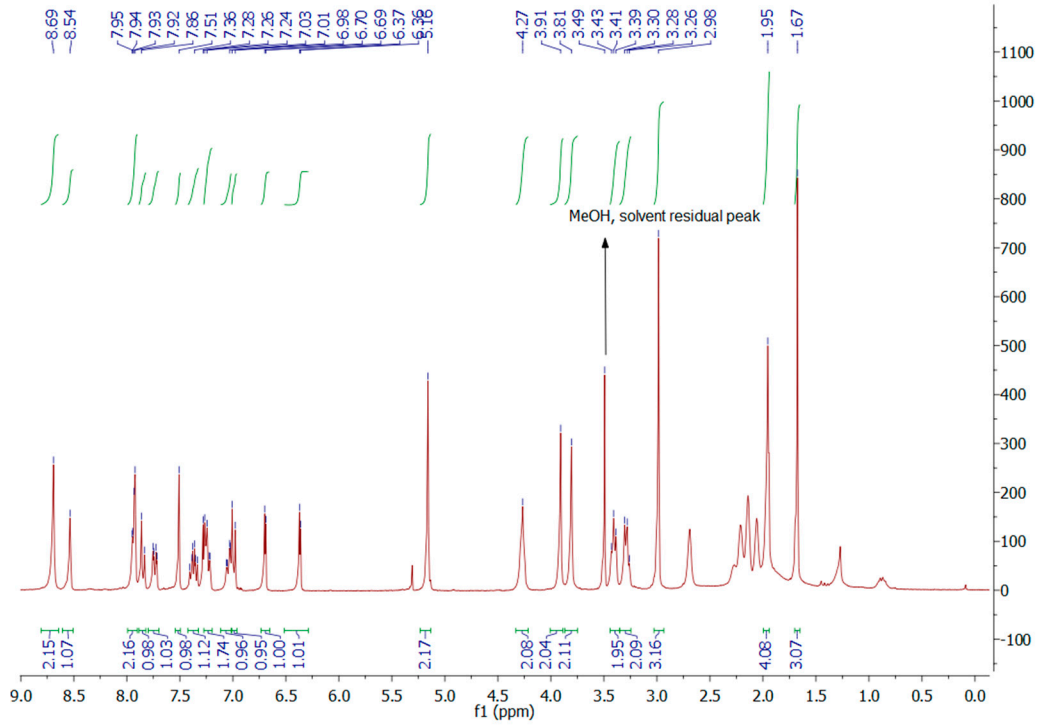


¹¹B-NMR

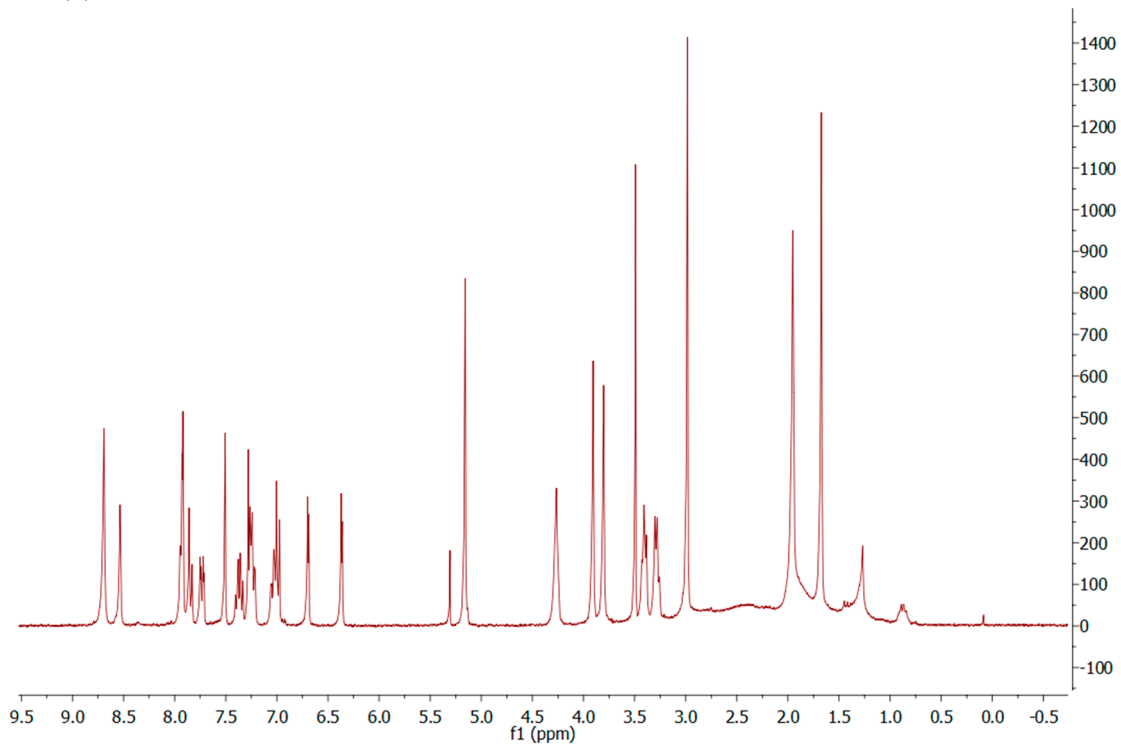




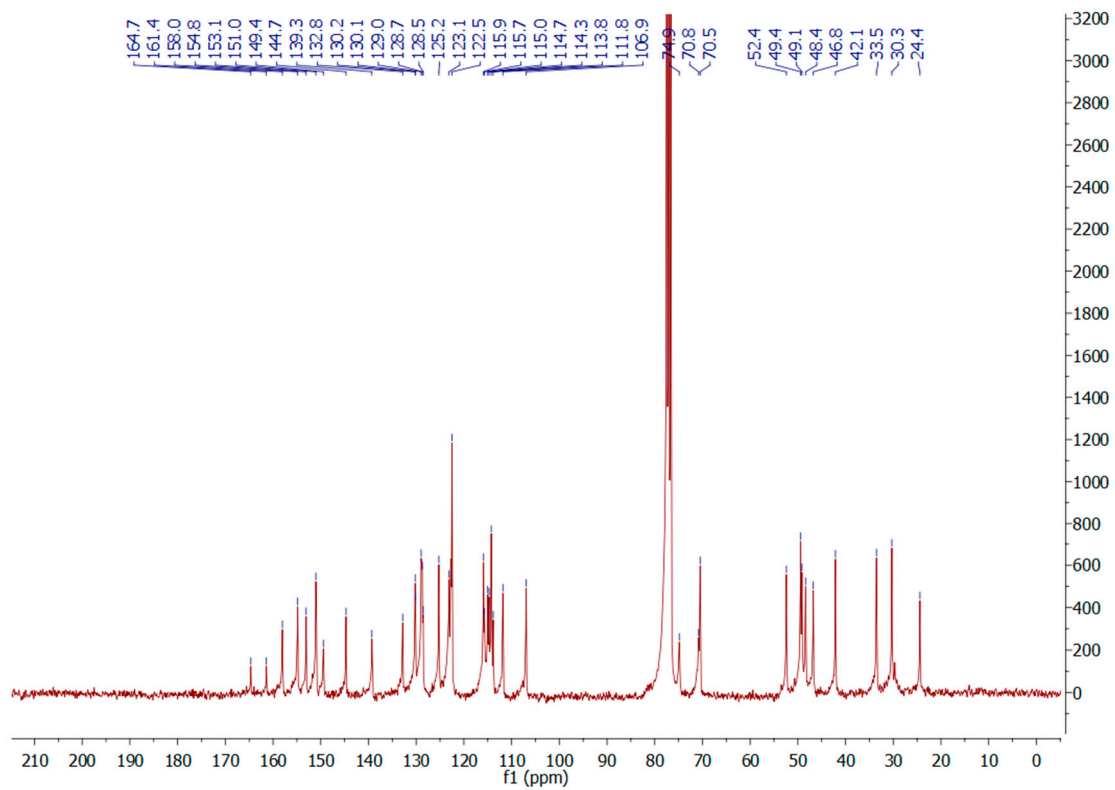
$^1\text{H}\{^{11}\text{B}\}$ -NMR



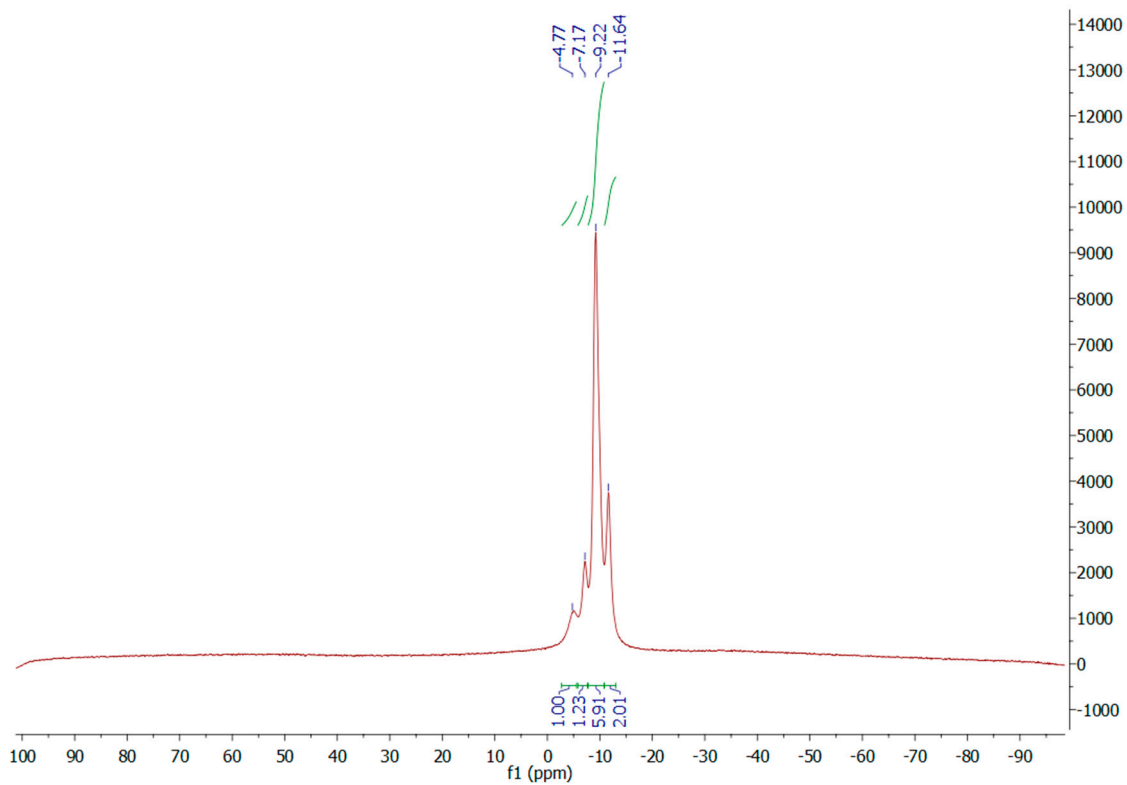
^1H -NMR



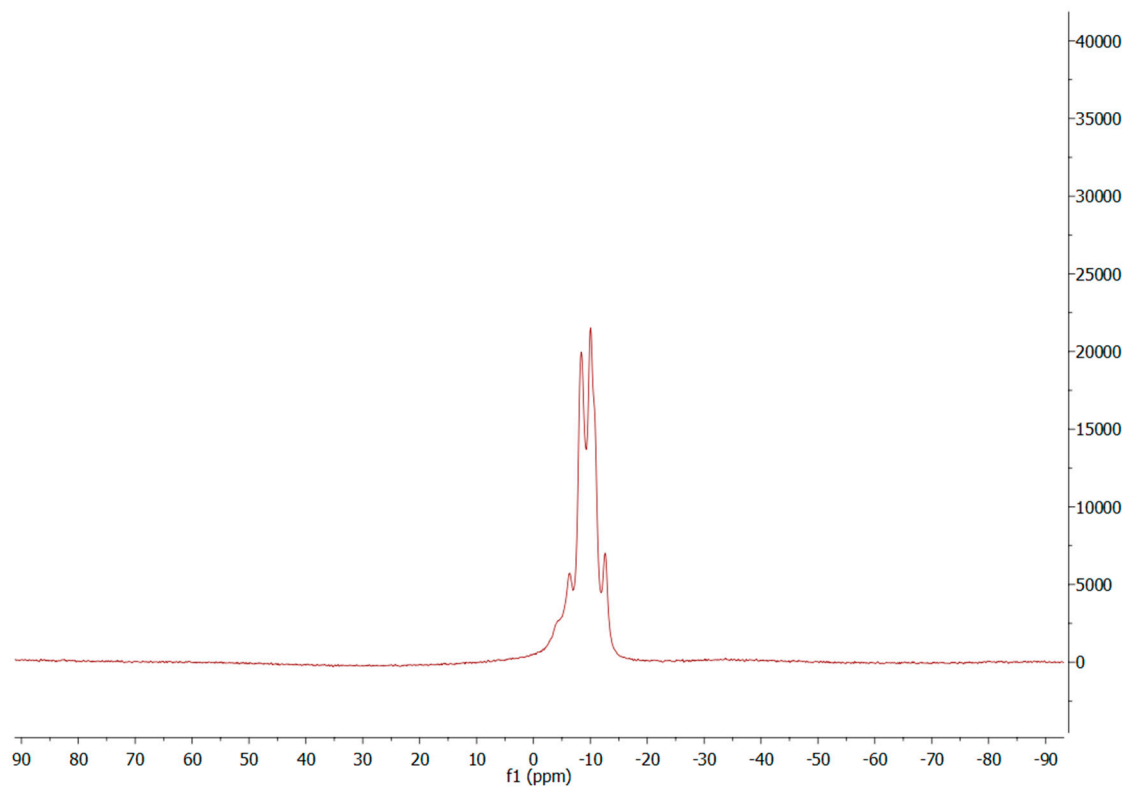
^{13}C -NMR

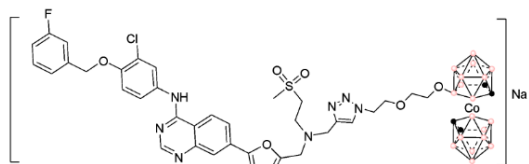


$^{11}\text{B}\{^1\text{H}\}$ -NMR

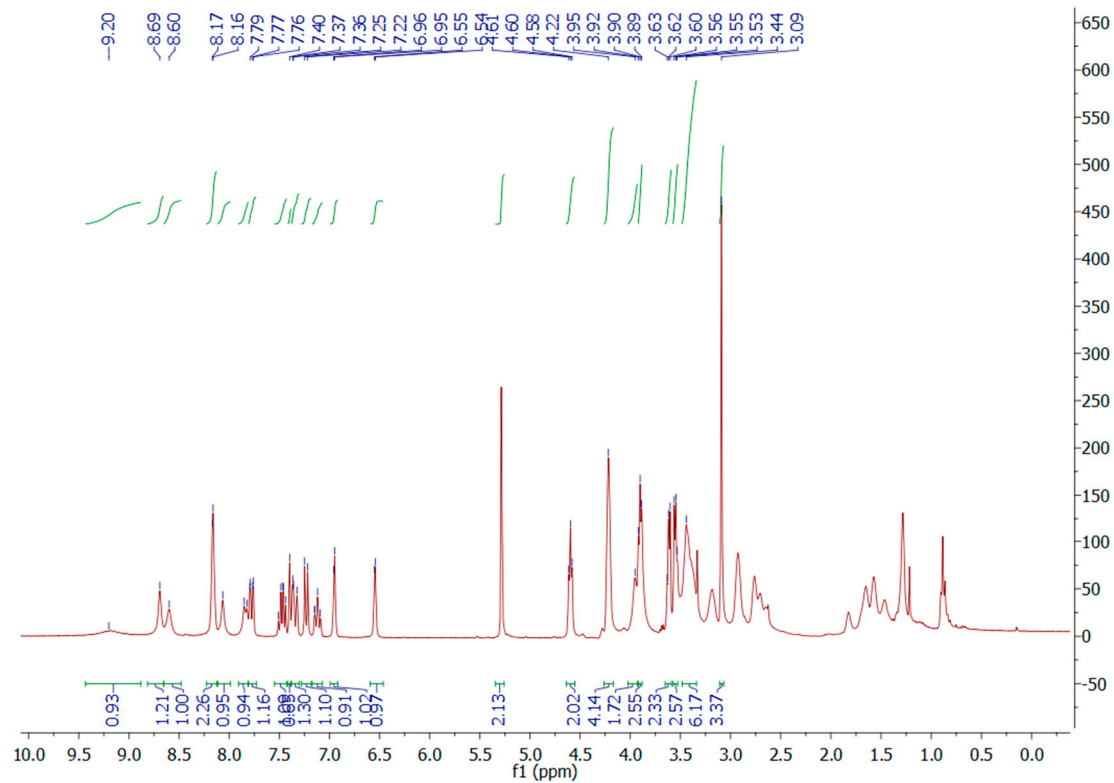


¹¹B-NMR

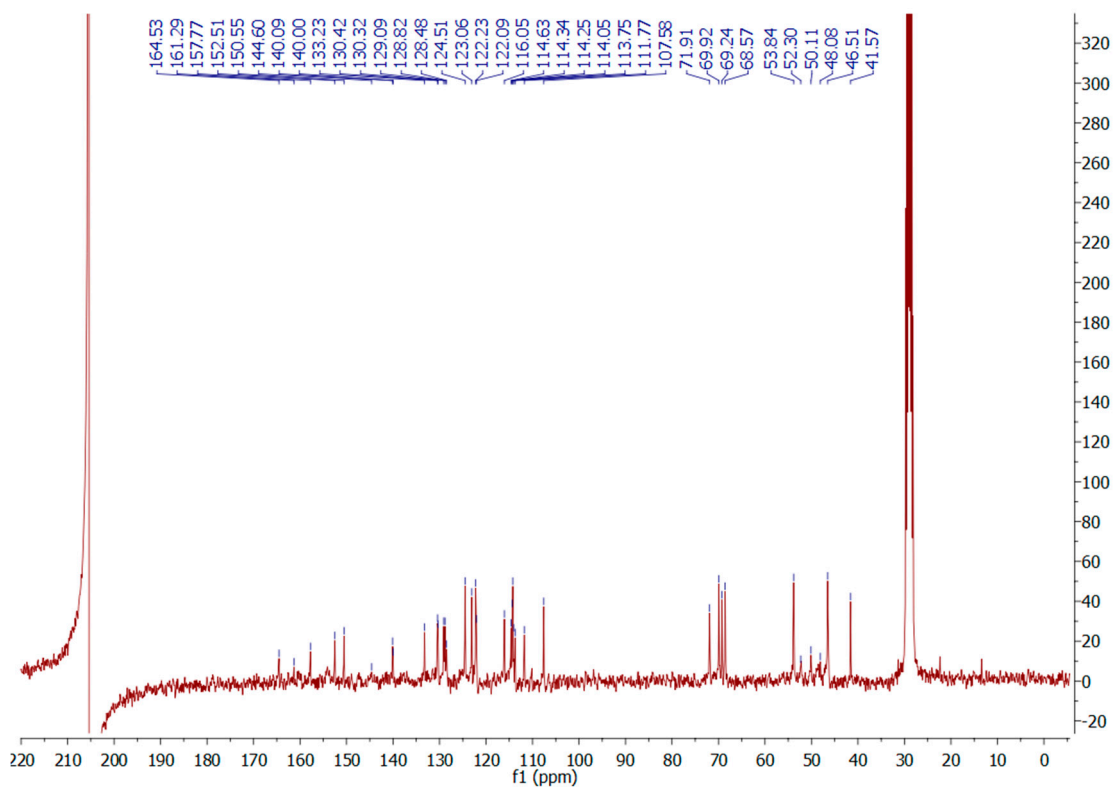




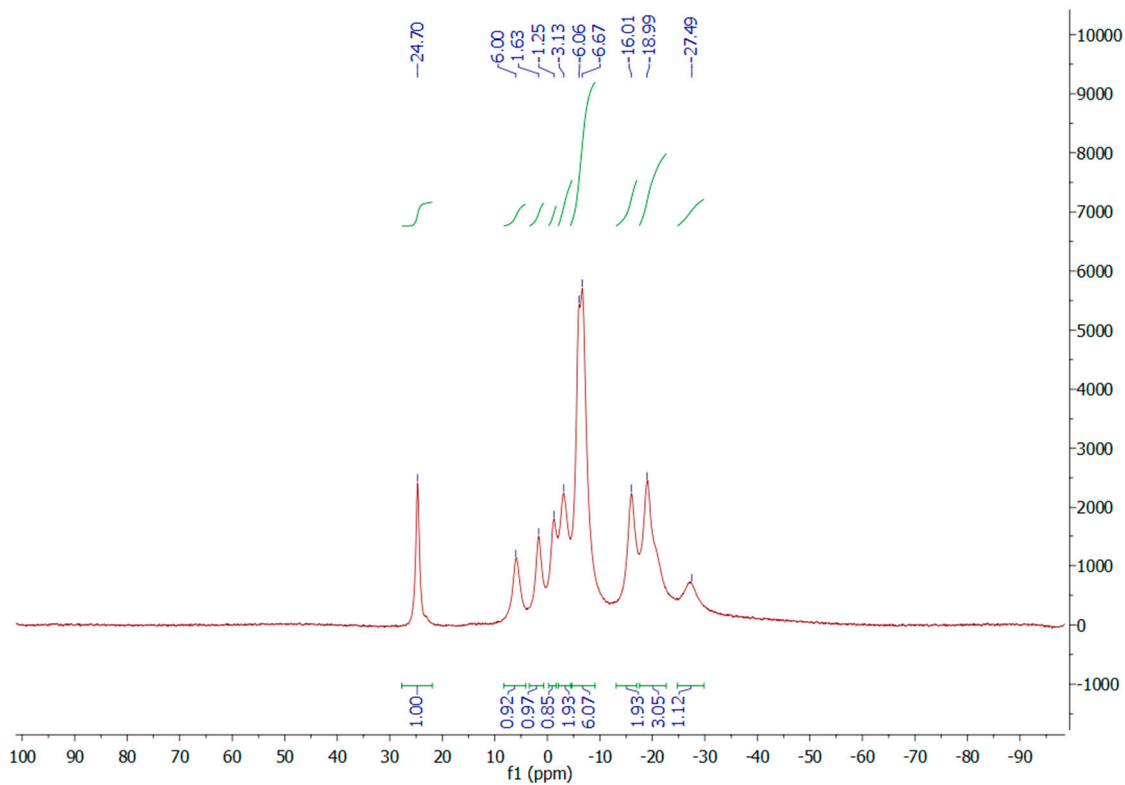
$^1\text{H}\{^{11}\text{B}\}$ -NMR



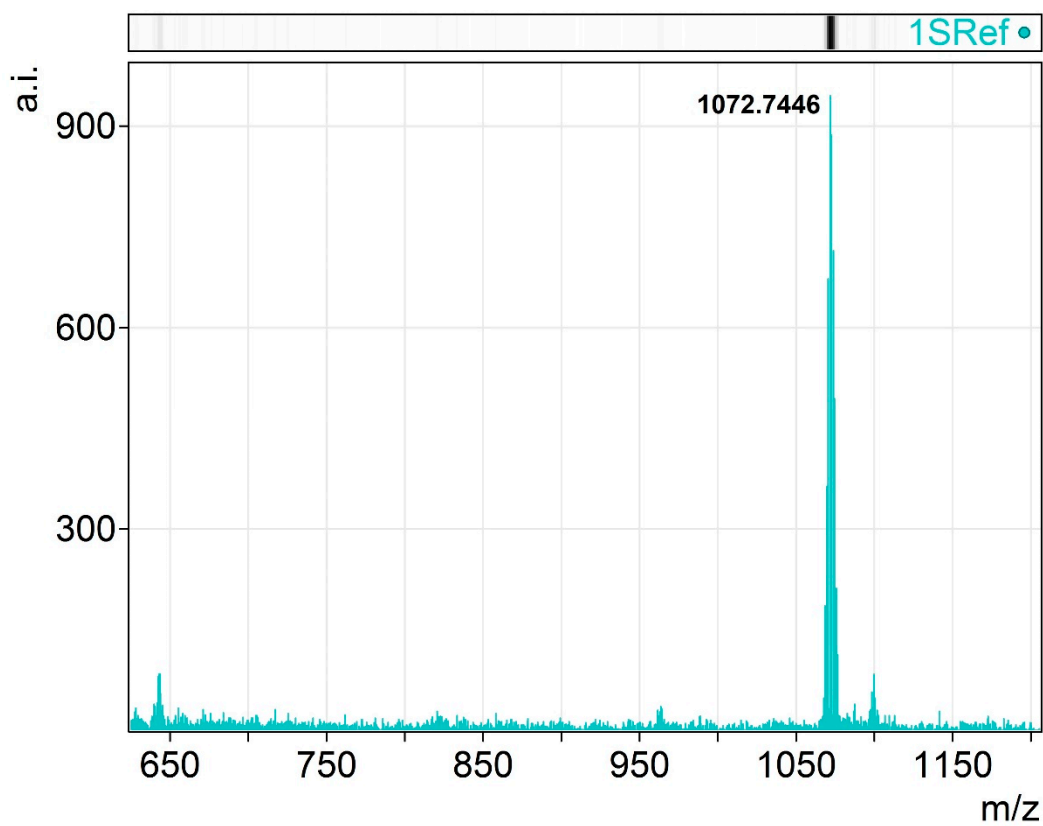
^{13}C -NMR

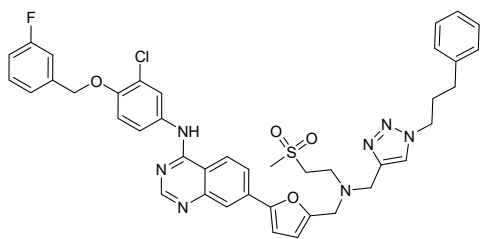


$^{11}\text{B}\{^1\text{H}\}$ -NMR

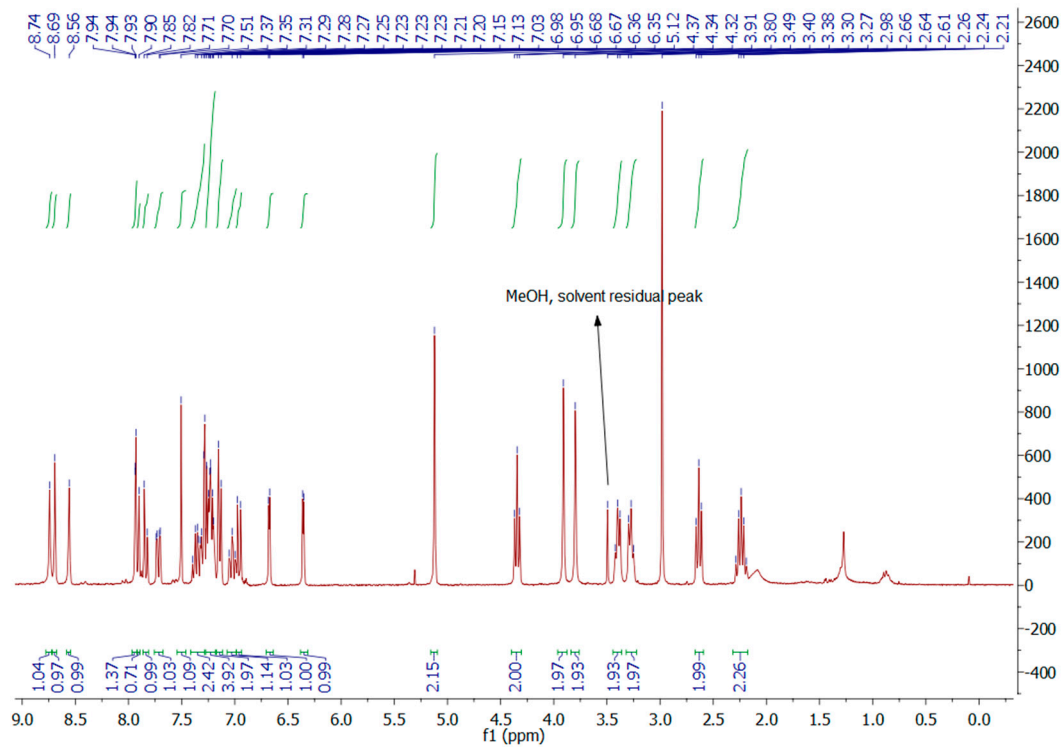


MALDI-TOF-MS

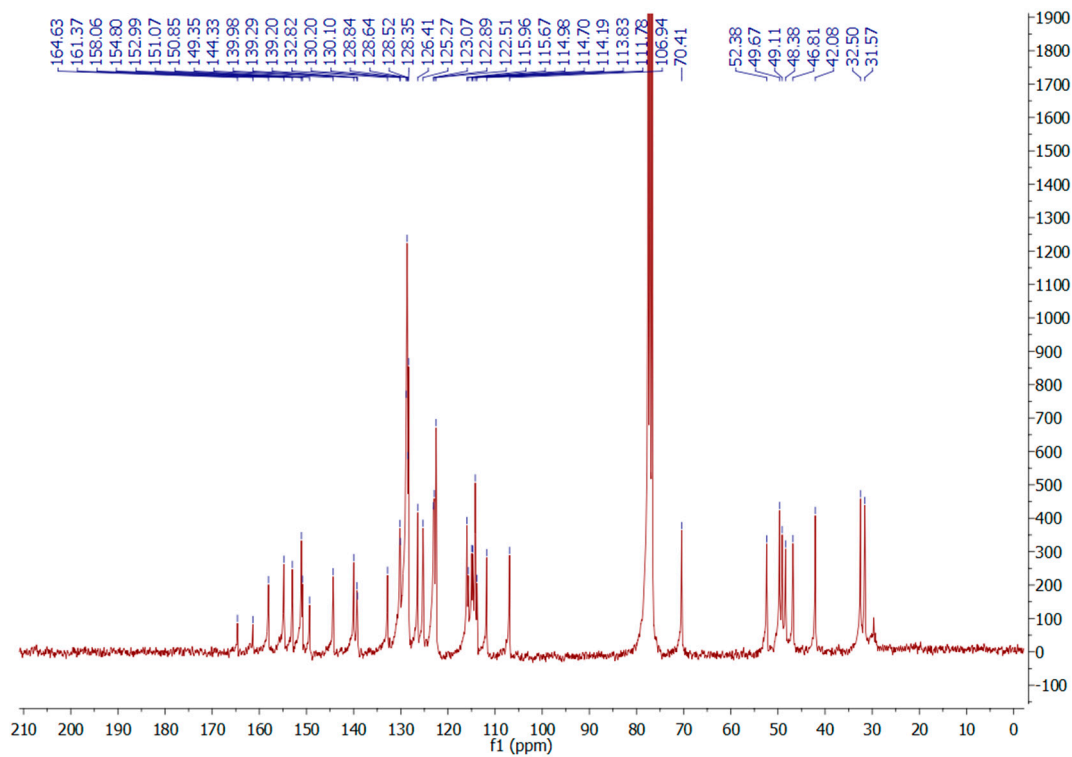




¹H-NMR



¹³C-NMR



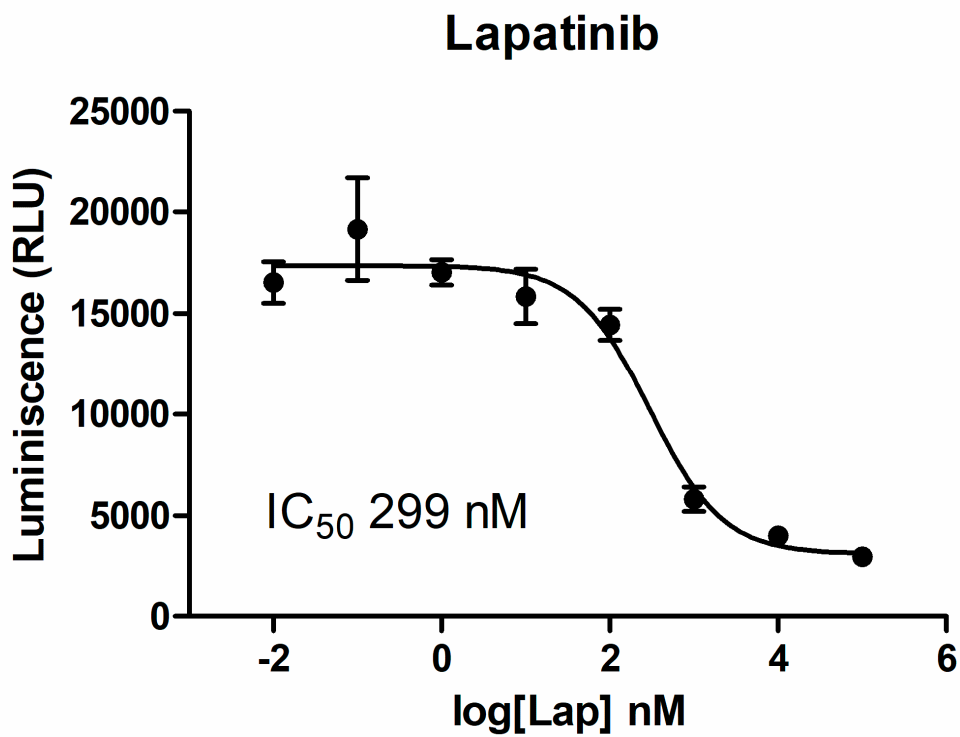
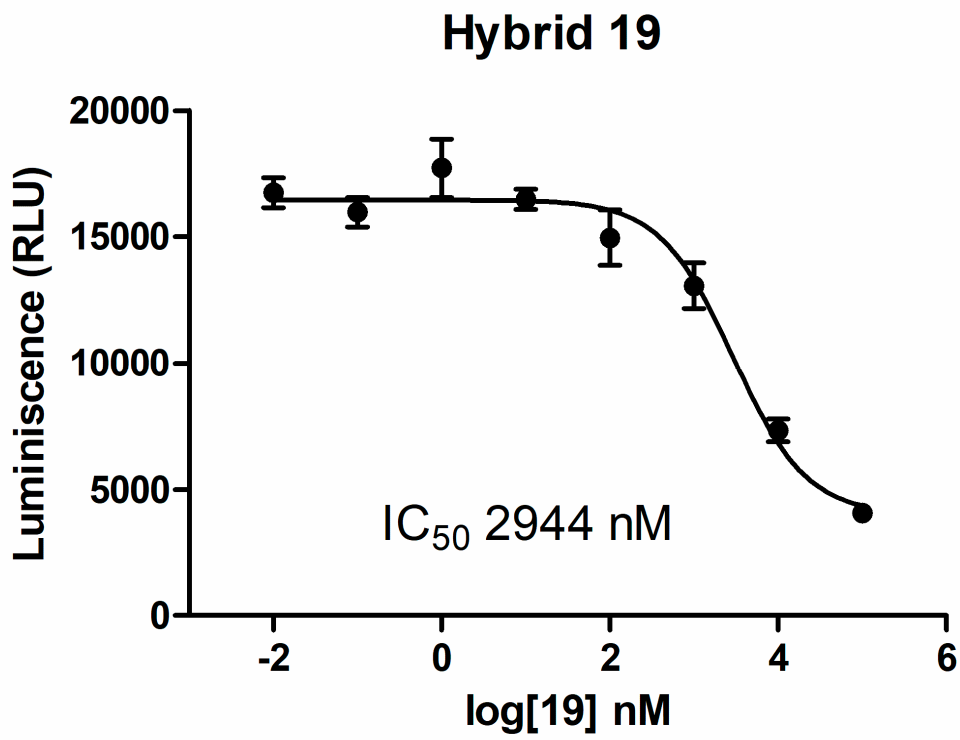


Figure S1. EGFR inhibition. Dose-response curves for hybrid, 19 and Lap.

Lapatinib

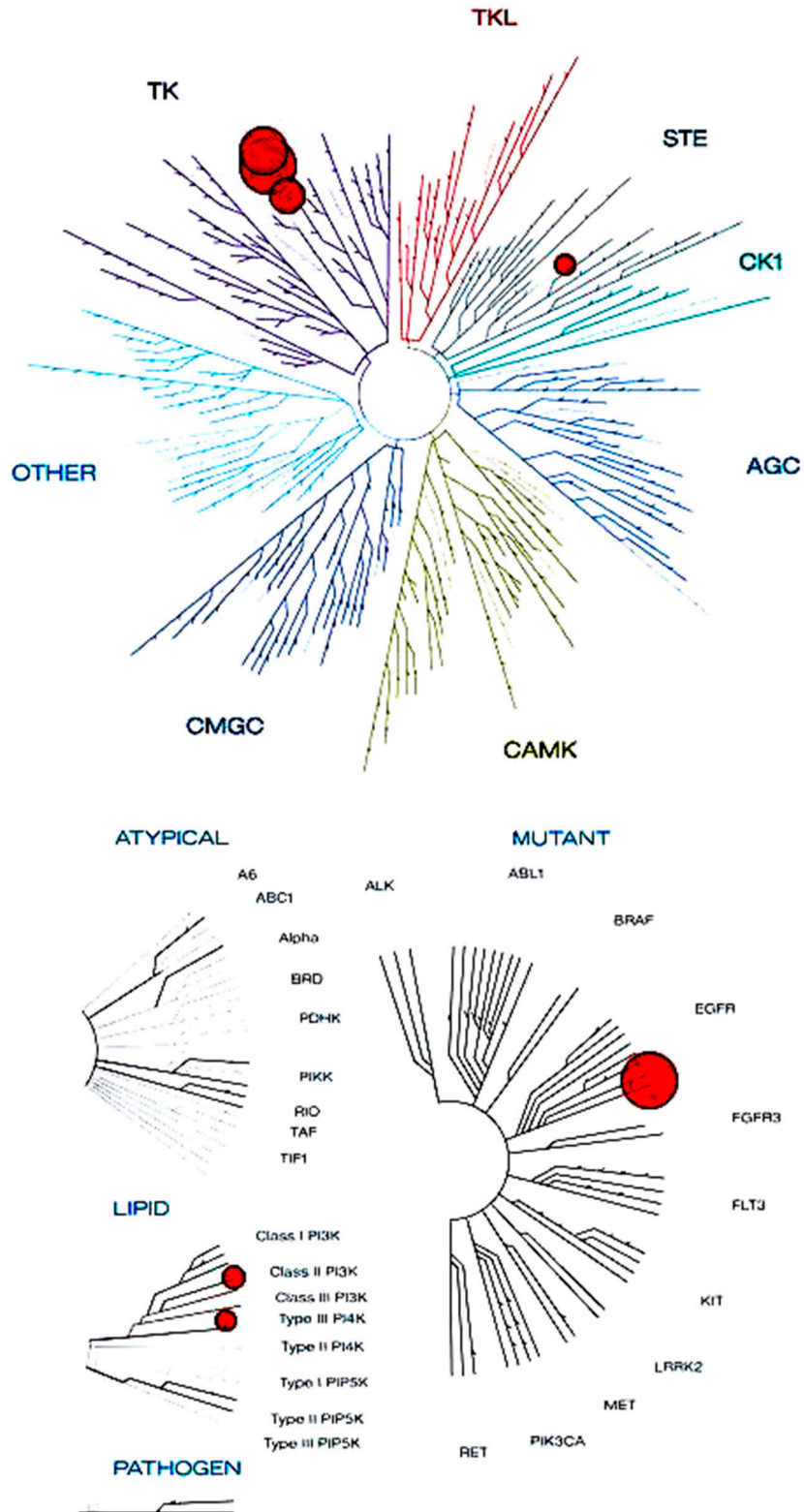


Figure S2. Profile of Lap against 468 protein kinases. Relative binding affinities are indicated by red circles in a phylogenetic kinome tree for wild-type enzymes and atypical/mutant/lipo/pathogen variants.. Image generated using TREEspot™ Software Tool (KINOMEScan®, a division of DiscoverX Corporation, © DISCOVERX CORPORATION 2010).