

Supplementary Material

Development of (4-phenylamino)quinazoline Alkylthiourea Derivatives as Novel NF- κ B Inhibitors

Sarah S. Darwish ^{1,2,†}, Po-Jen Chen ^{3,†}, Mostafa M. Hamed ^{4,†}, Reem A. Wagdy ¹, Shun-Hua Chen ⁵, Ashraf H. Abadi ¹, Mohammad Abdel-Halim ¹, Tsong-Long Hwang ^{6,7,8,9,*} and Matthias Engel ^{10,*}

¹ Department of Pharmaceutical Chemistry, Faculty of Pharmacy and Biotechnology, German University in Cairo, 11835 Cairo, Egypt; s.same@gaf.edu.eg (S.S.D.); reem.ahmed-afifi@guc.edu.eg (R.A.W.); ashraf.abadi@guc.edu.eg (A.H.A.); mohammad.abdel-halim@guc.edu.eg (M.A.-H.)

² School of Life and Medical Sciences, University of Hertfordshire hosted by Global Academic Foundation, New Administrative Capital, 11578 Cairo, Egypt

³ Department of Medical Research, E-Da Hospital, Kaohsiung City 824005, Taiwan; littlep@hotmail.com

⁴ Drug design and optimization, Helmholtz Institute for Pharmaceutical Research Saarland (HIPS), Helmholtz Centre for Infection Research, Saarland University Campus, 66123 Saarbrücken, Germany; mostafa.hamed@helmholtz-hips.de

⁵ School of Nursing, Fooyin University, Kaohsiung 831, Taiwan; ft104@fy.edu.tw

⁶ Graduate Institute of Natural Products, College of Medicine, Chang Gung University, Taoyuan 333, Taiwan

⁷ Research Center for Chinese Herbal Medicine, Graduate Institute of Health Industry Technology, College of Human Ecology, Chang Gung University of Science and Technology, Taoyuan 333, Taiwan

⁸ Department of Anesthesiology, Chang Gung Memorial Hospital, Taoyuan 333, Taiwan

⁹ Department of Chemical Engineering, Ming Chi University of Technology, New Taipei City 243, Taiwan

¹⁰ Pharmaceutical and Medicinal Chemistry, Saarland University, Campus C2.3, 66123 Saarbrücken, Germany

† These authors contributed equally to this work.

* Correspondence: htl@mail.cgu.edu.tw (T.-L.H.); ma.engel@mx.uni-saarland.de (M.E.); Tel.: +886-3-2118506 (T.-L.H.); +49-681-302-70312 (M.E.); Fax: +886-3-2118506 (T.-L.H.); +49-681-302-70308 (M.E.)

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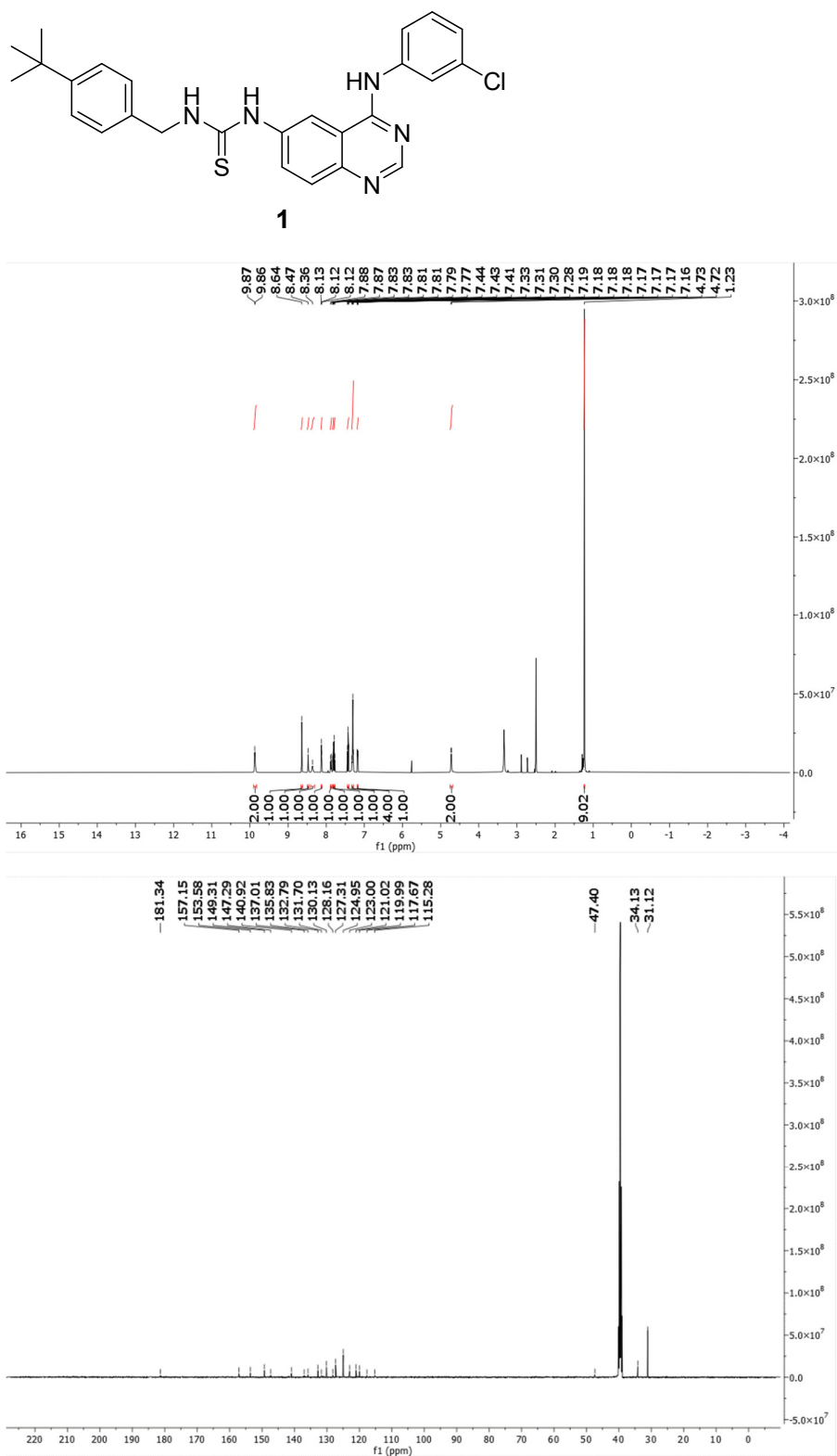
1. Table S1
2. ¹H-NMR (500 MHz, DMSO) and ¹³C-NMR (126 MHz, DMSO) spectra of newly synthesized compounds.

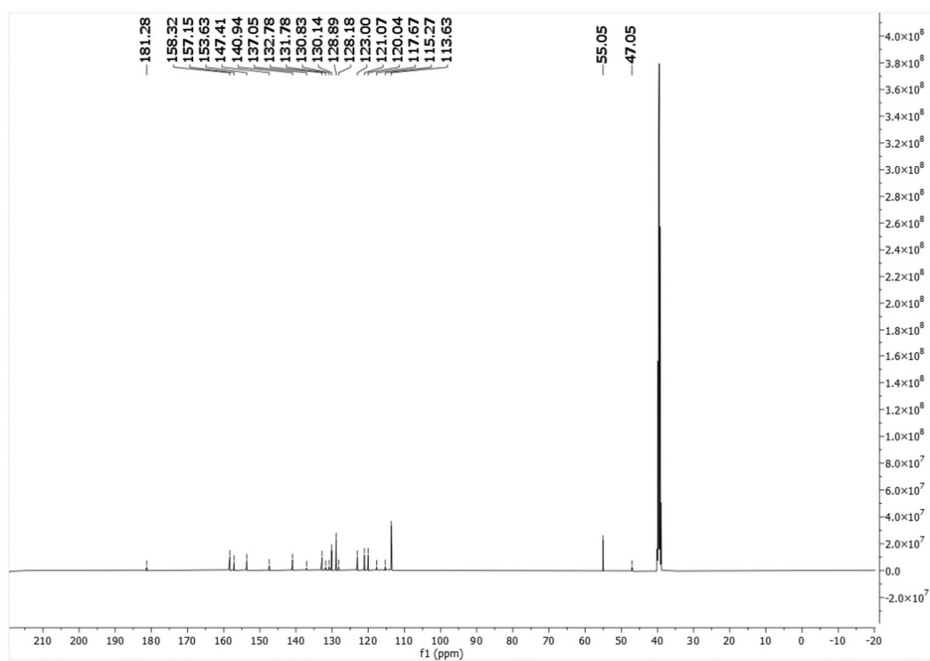
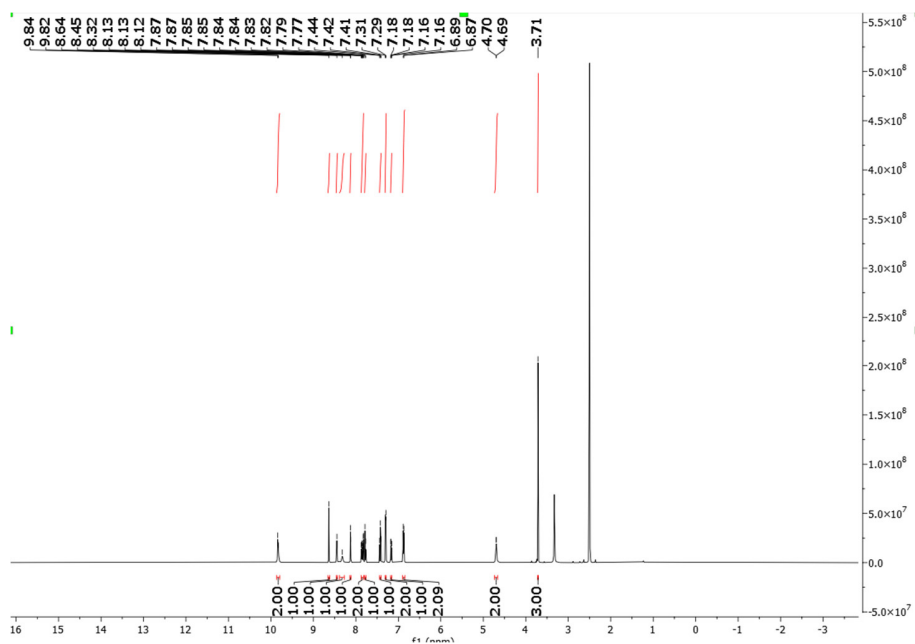
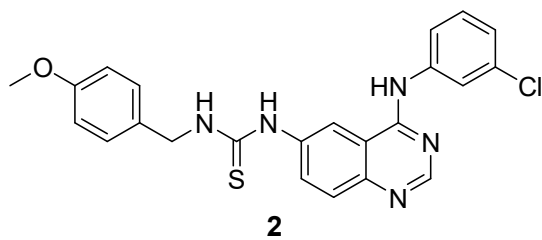
Table S1. Selectivity profiling of compound **19** against the protein kinases known to regulate the NF- κ B pathway

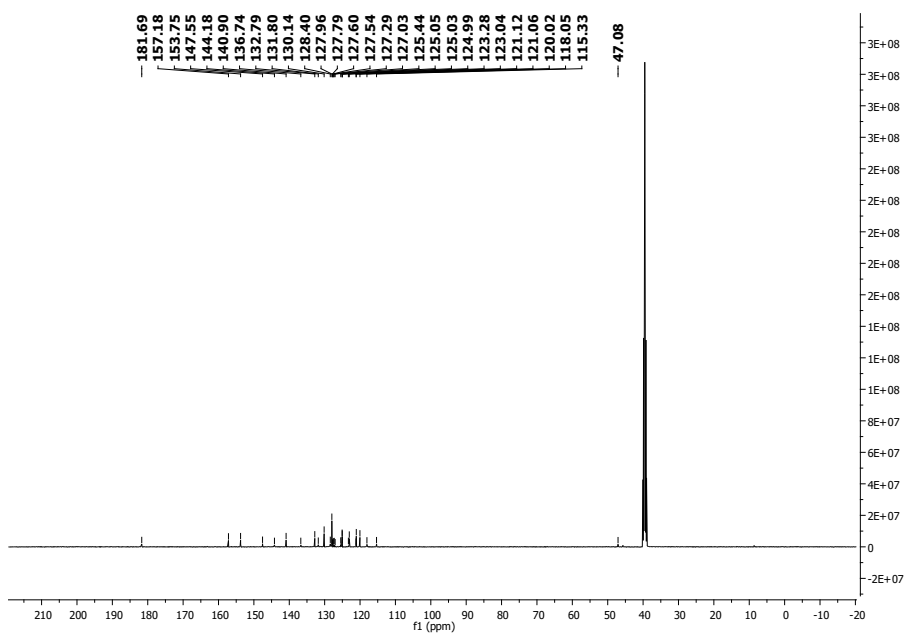
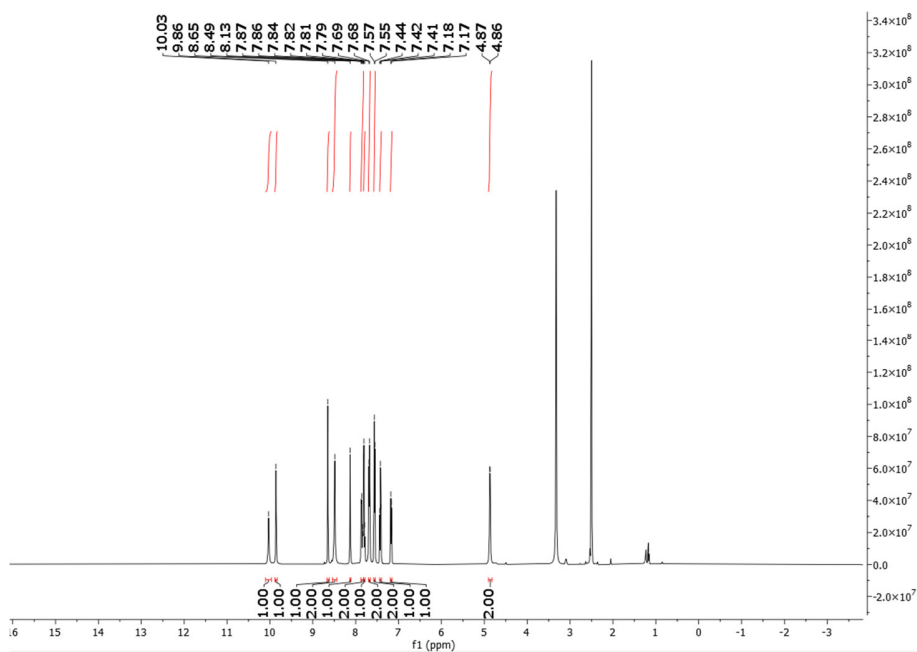
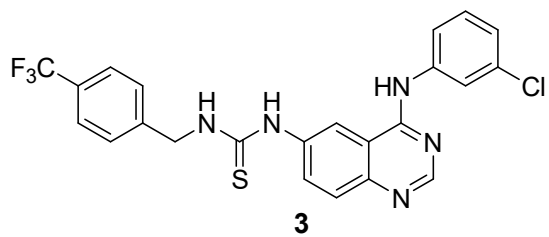
kinase	% Inhibition at 2 μ M ^a
	19
CHUK (IKK alpha)	6
IRAK1	2
MAP3K14 (NIK)	9
MAP3K7/MAP3K7IP1 (TAK1-TAB1)	3
RIPK2	29
GSK3B (GSK3 beta)	4
IKBKB (IKK beta)	3
IKBKE (IKK epsilon)	3
IRAK4	5
MAPK14 (p38 alpha)	4
MAPK3 (ERK1)	2
PRKCI (PKC iota)	n.i.
PRKCQ (PKC theta)	n.i.
PRKCZ (PKC zeta)	3
RPS6KA1 (RSK1)	1
TBK1	8

^aScreenings were performed as a service at Thermo Fisher Scientific at an ATP concentration of 100 μ M. n.i., no inhibition. Data represent mean values of duplicates that differed by less than 7%.

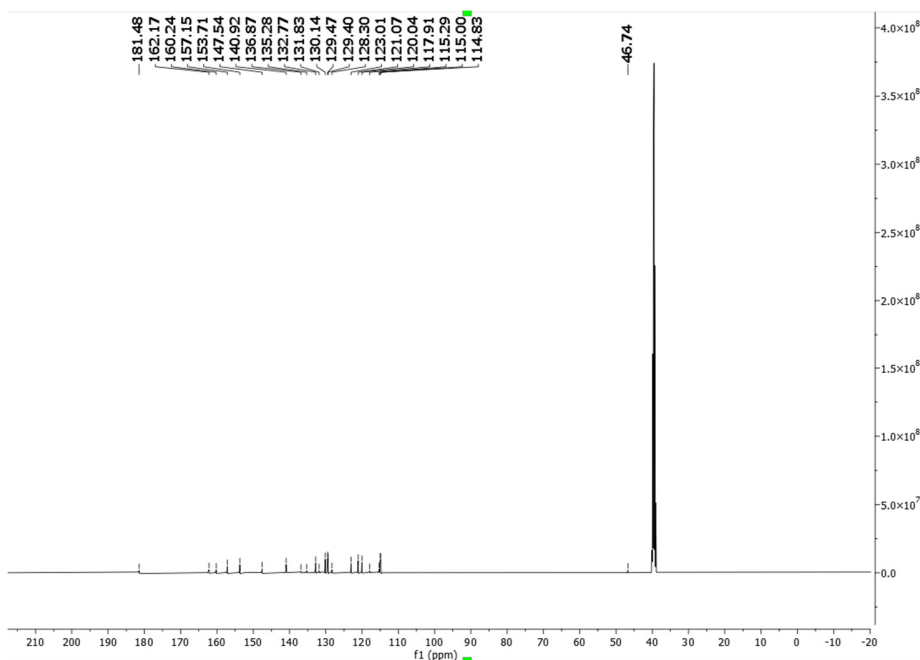
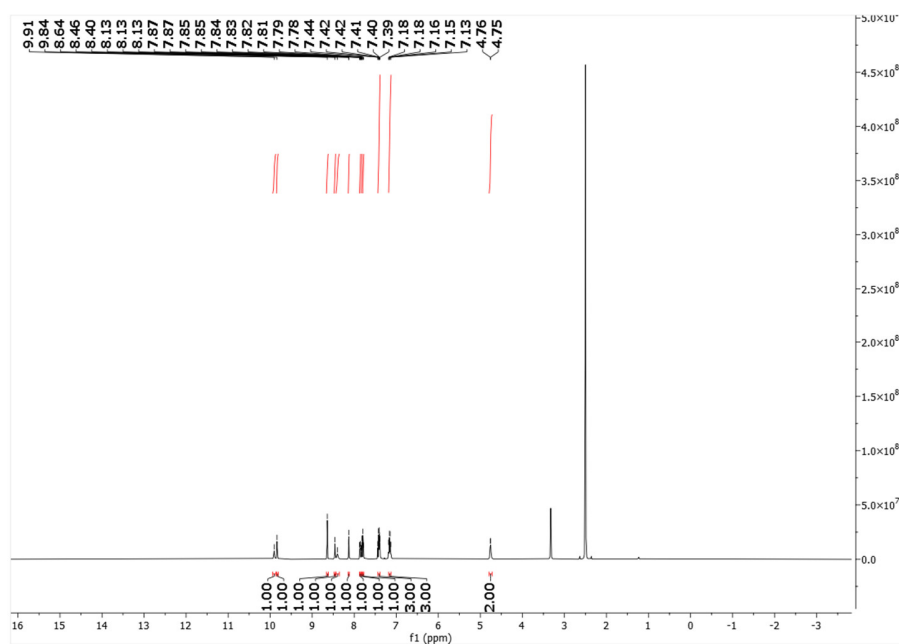
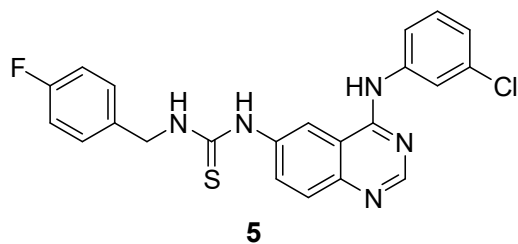
Figure S1 ^1H -NMR (500 MHz, DMSO) and ^{13}C -NMR (126 MHz, DMSO) spectra

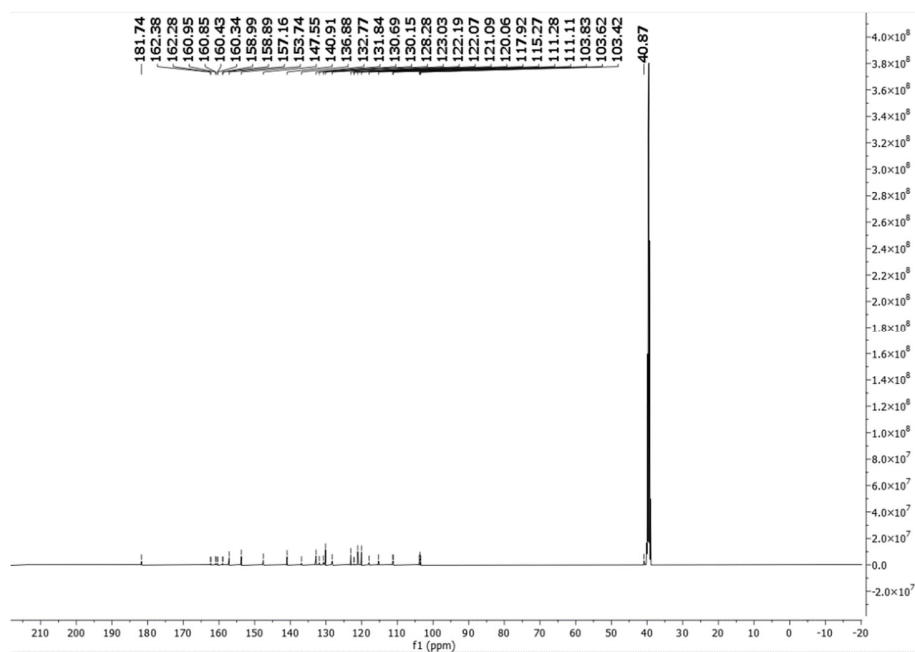
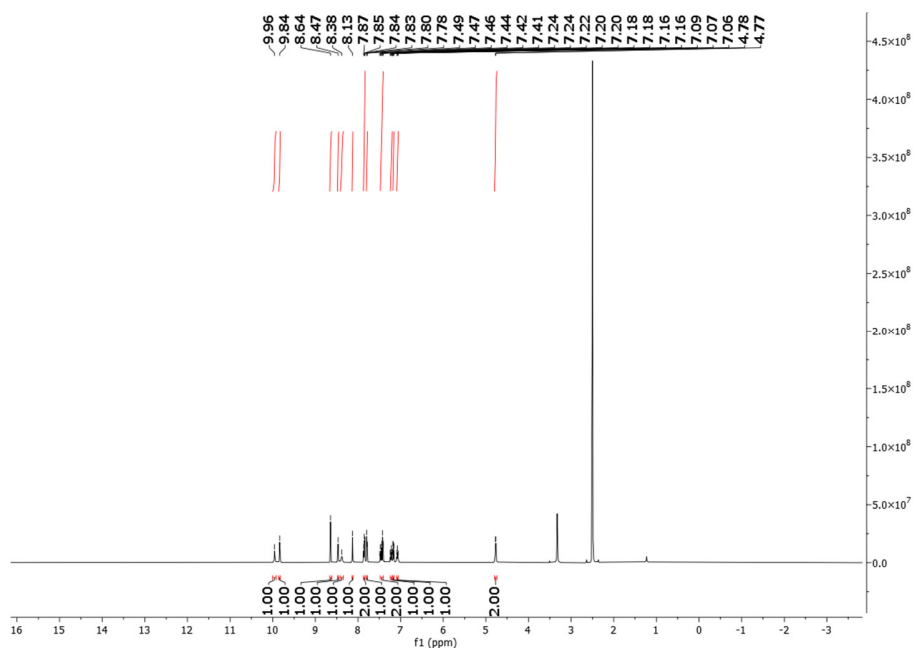
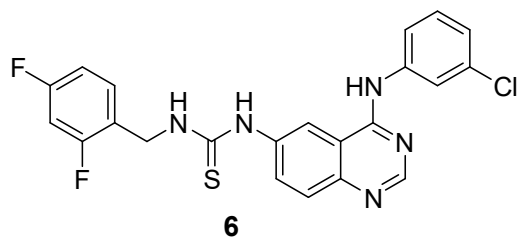


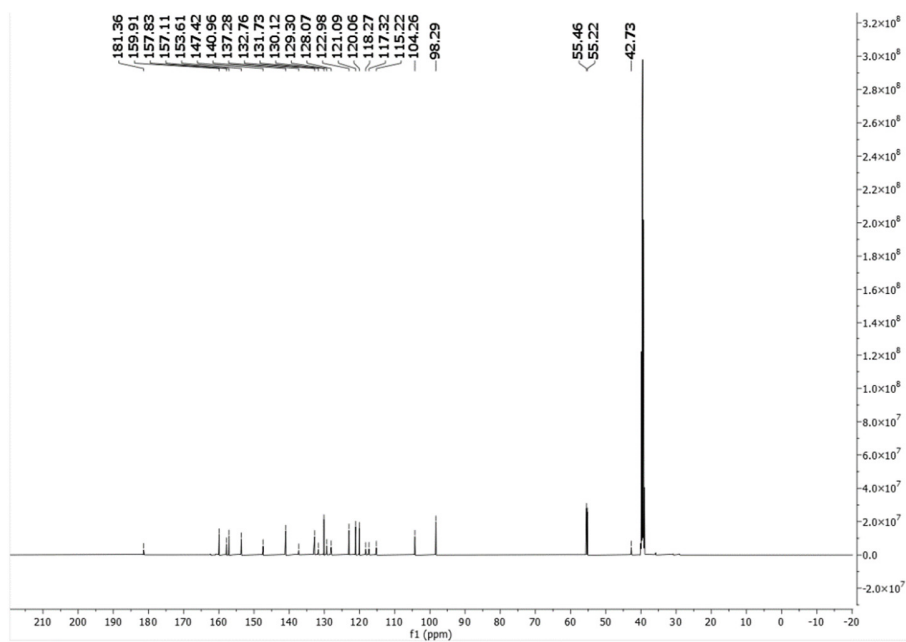
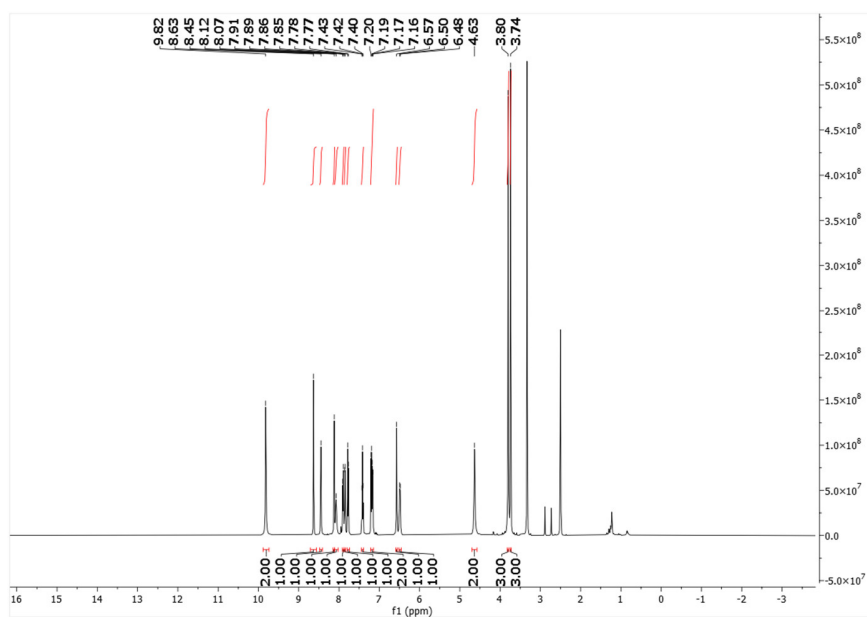
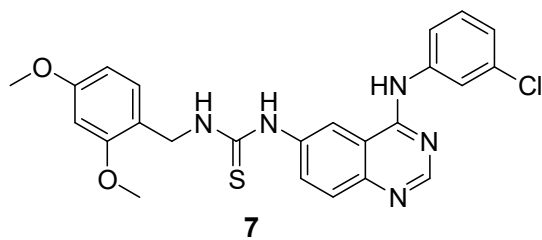


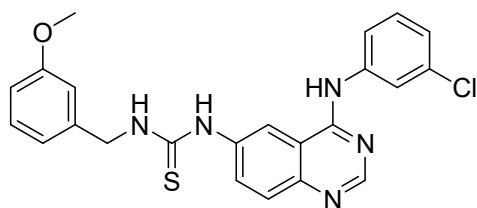




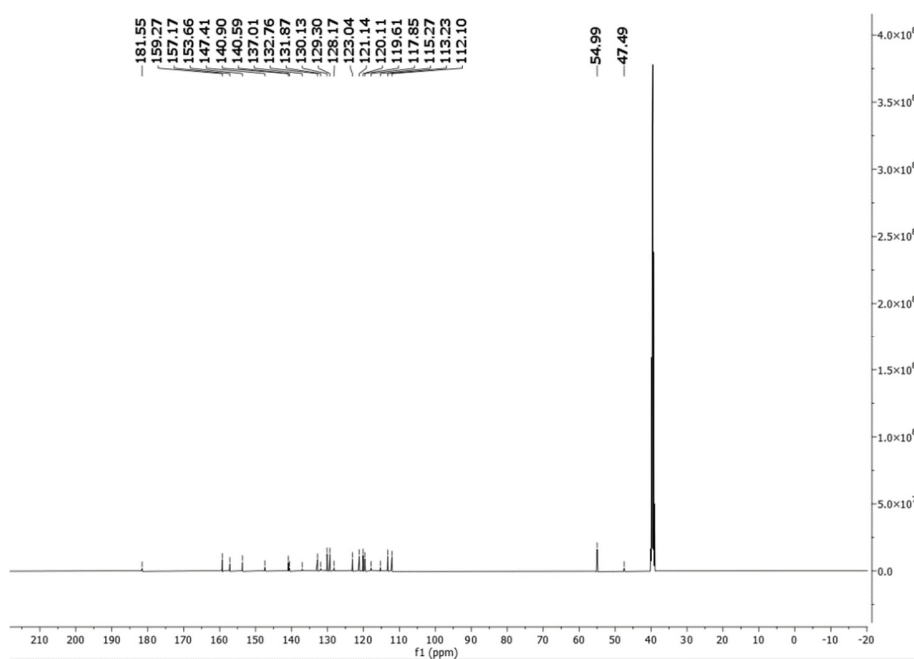
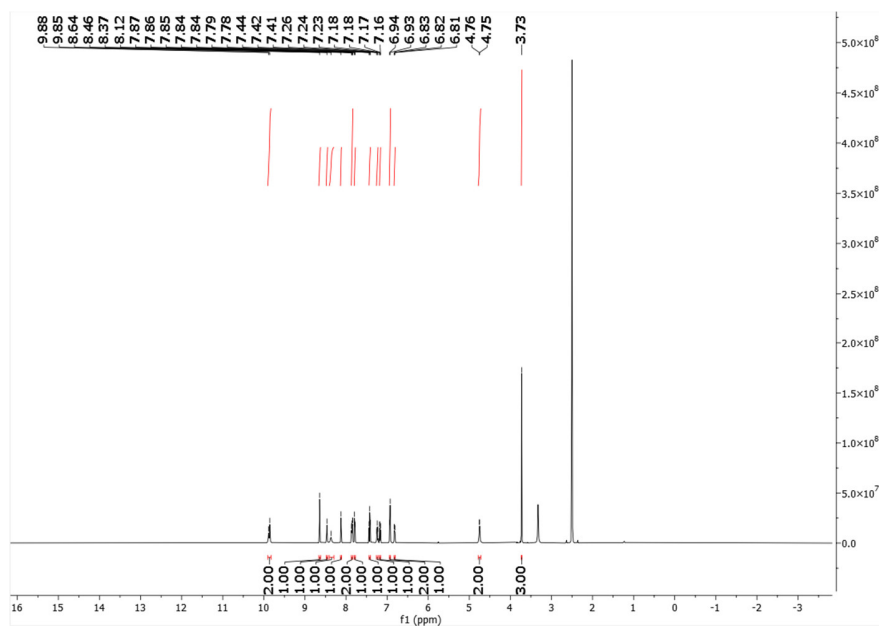


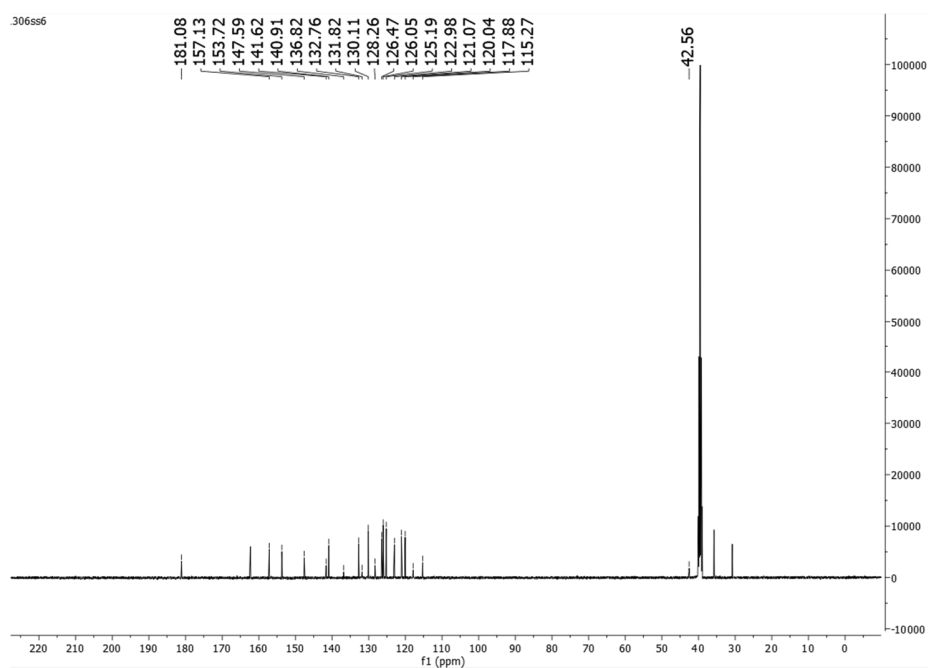
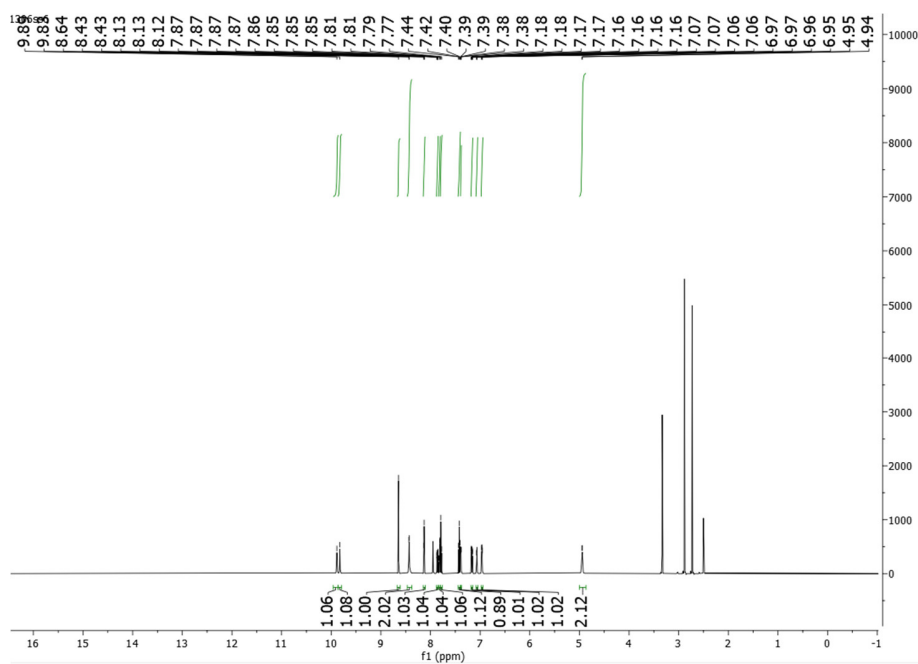
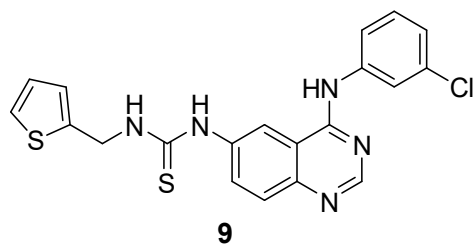


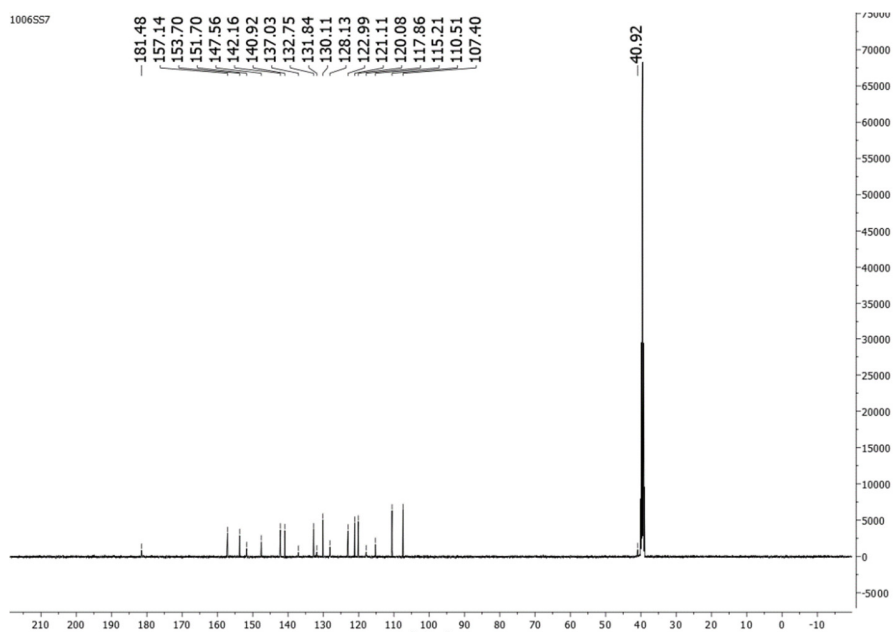
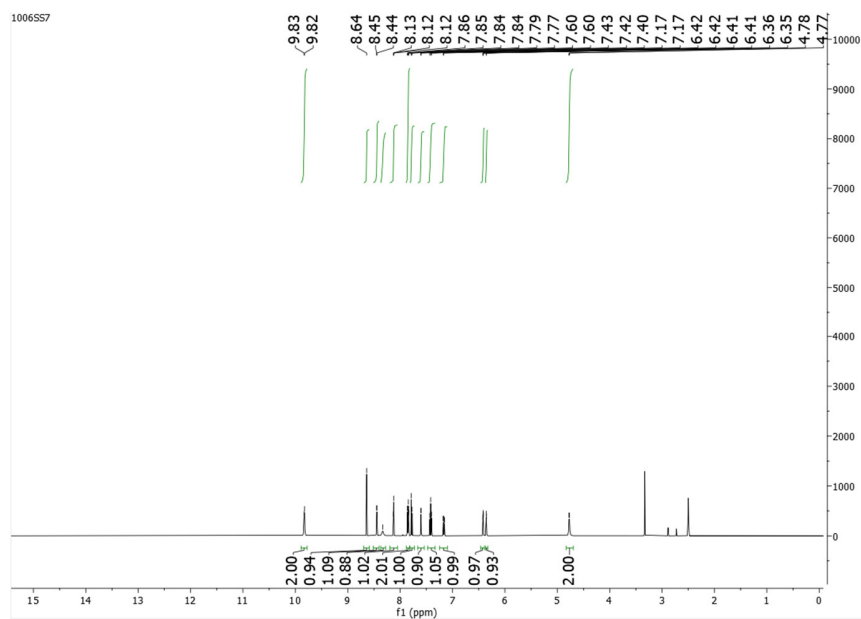
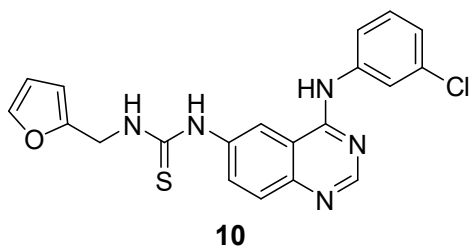


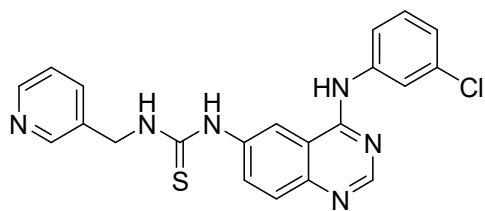


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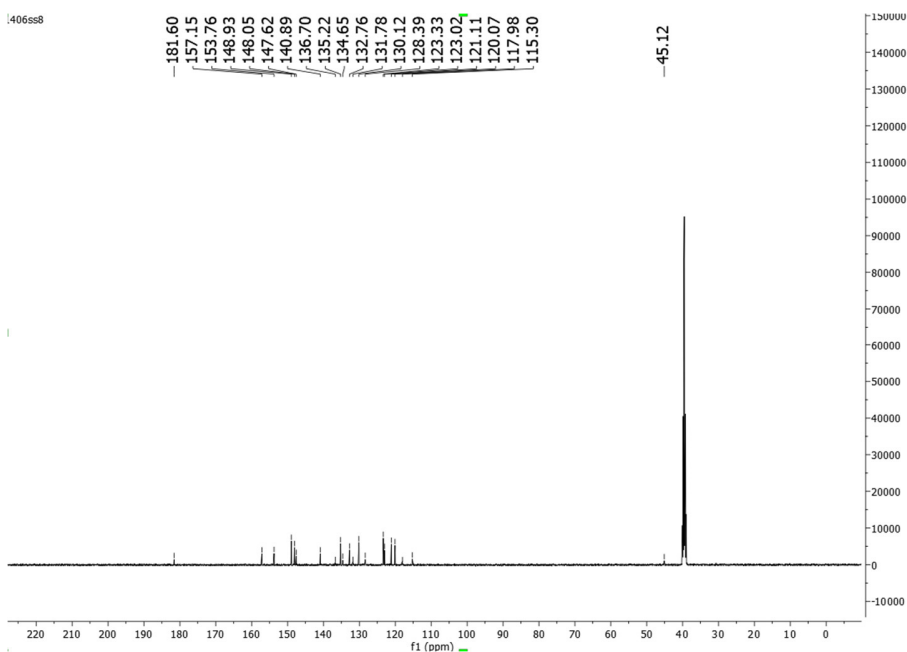
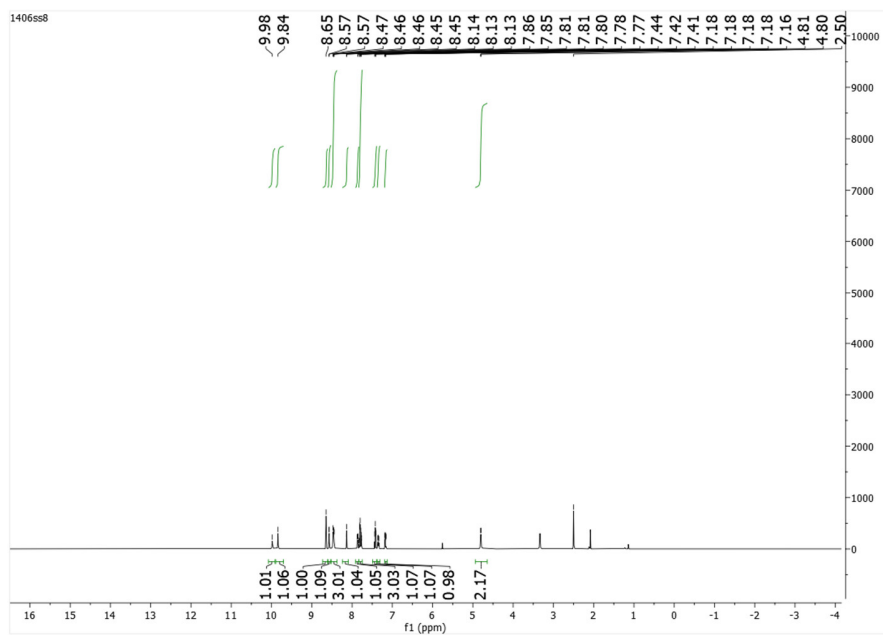


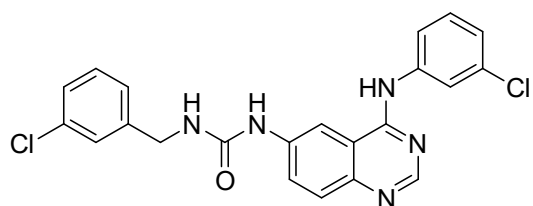




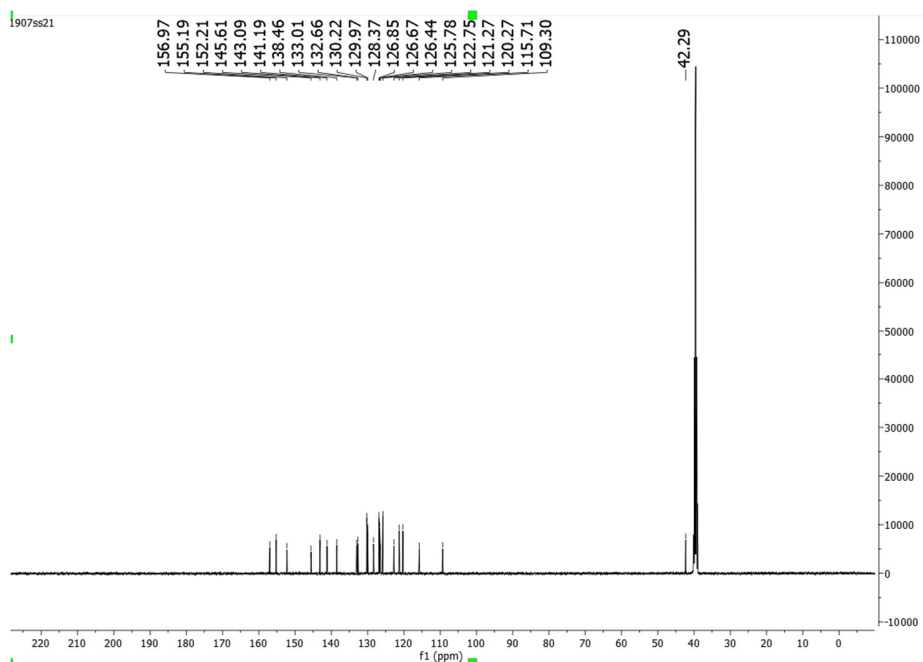
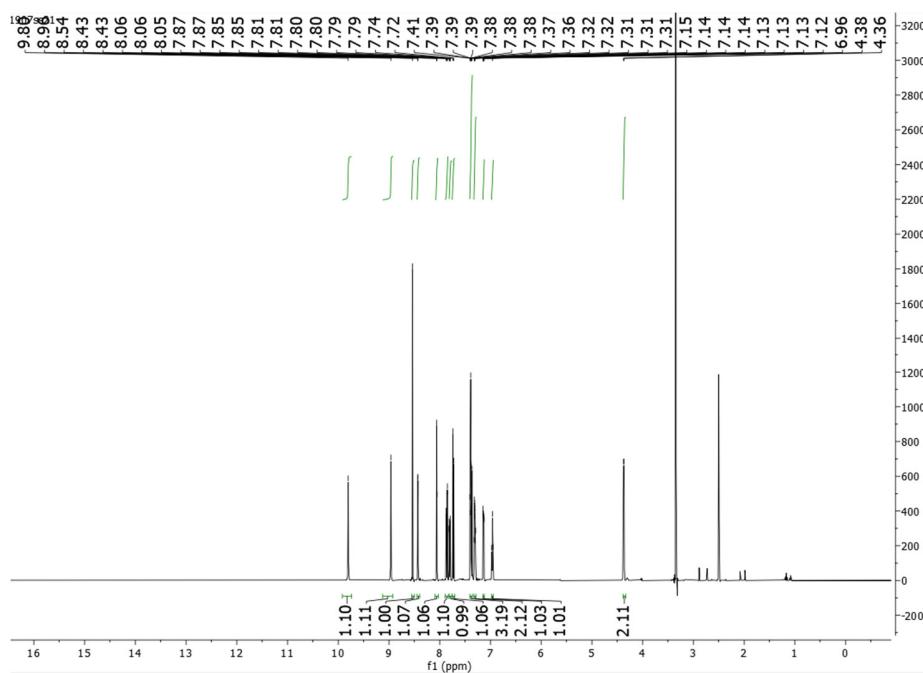


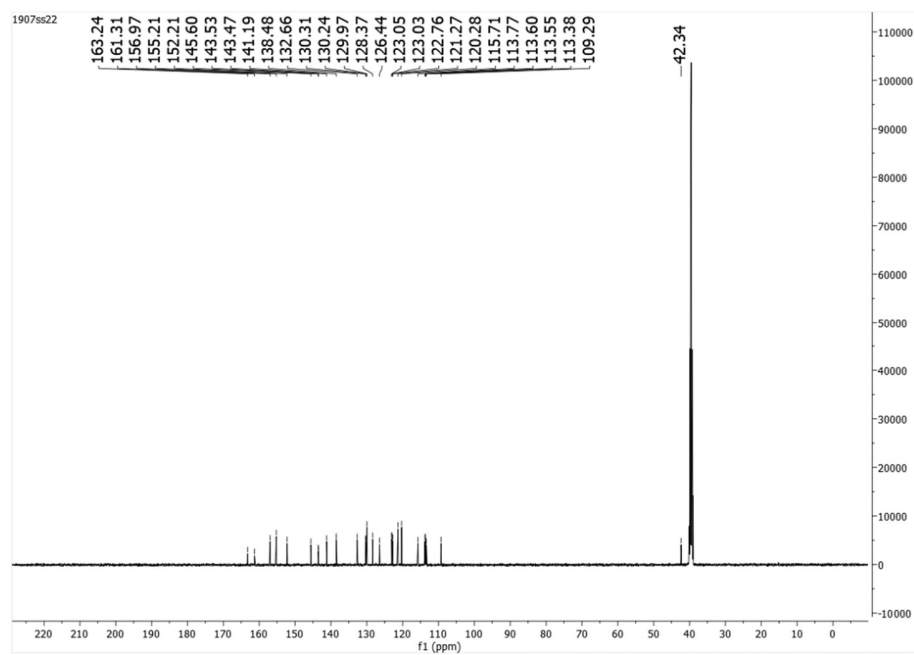
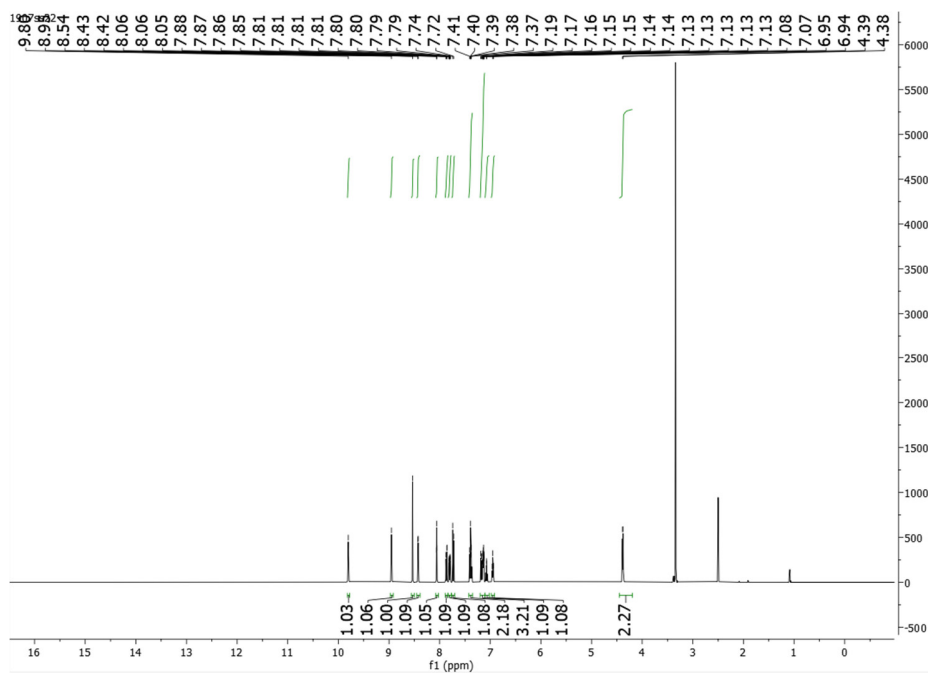
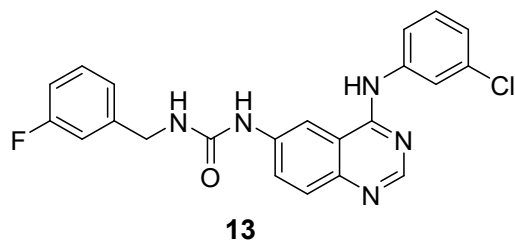
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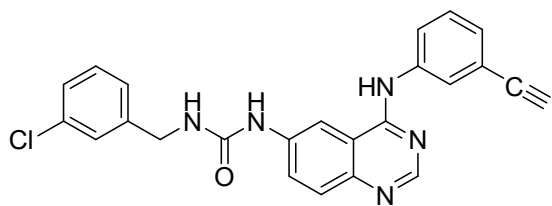




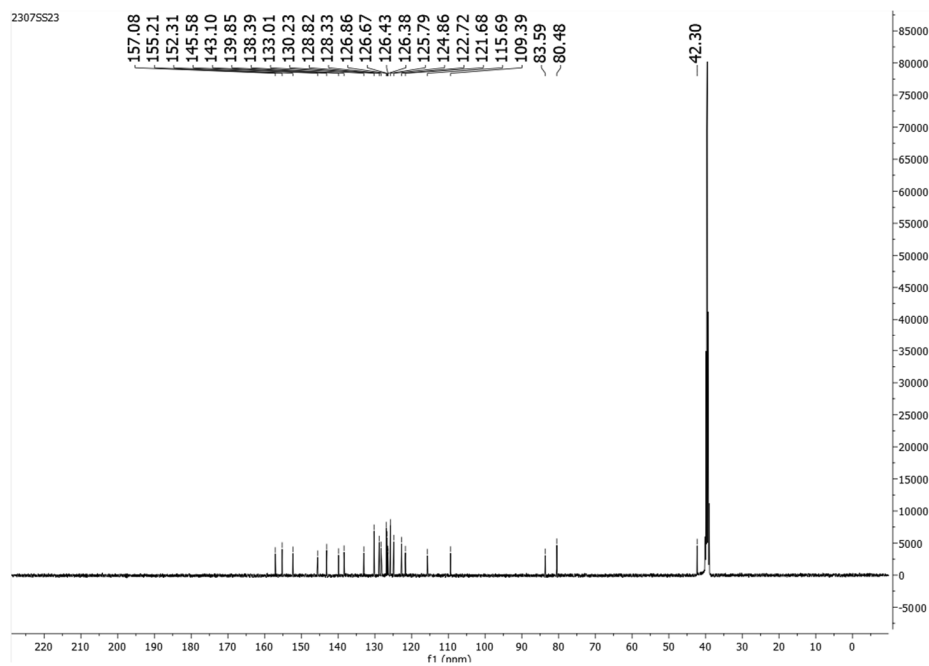
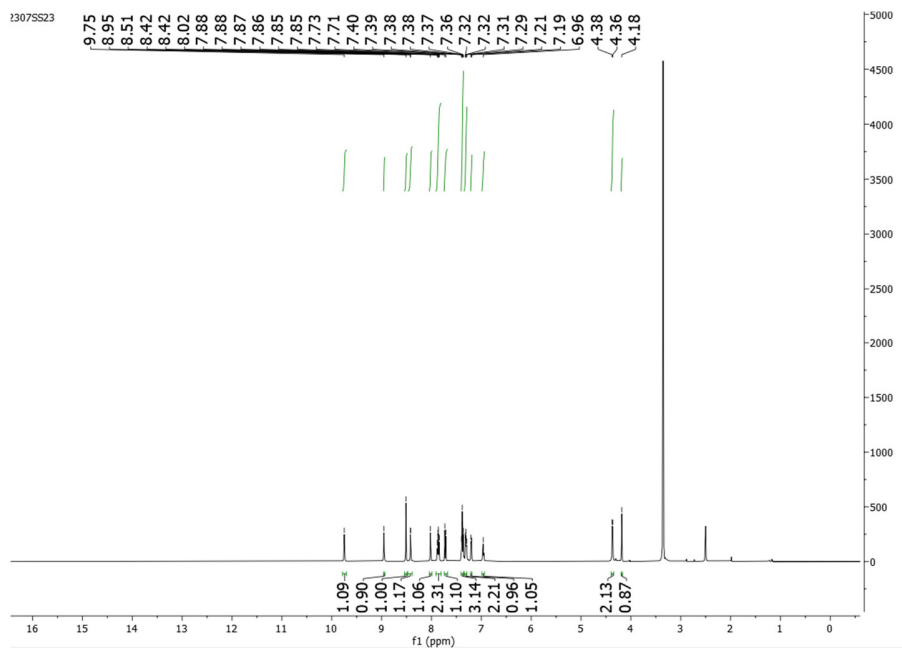
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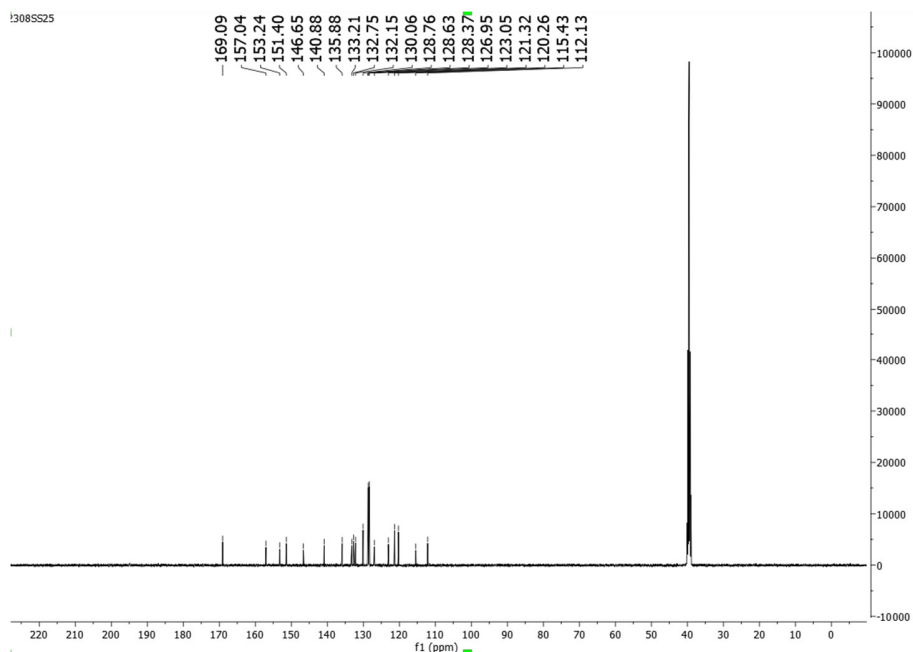
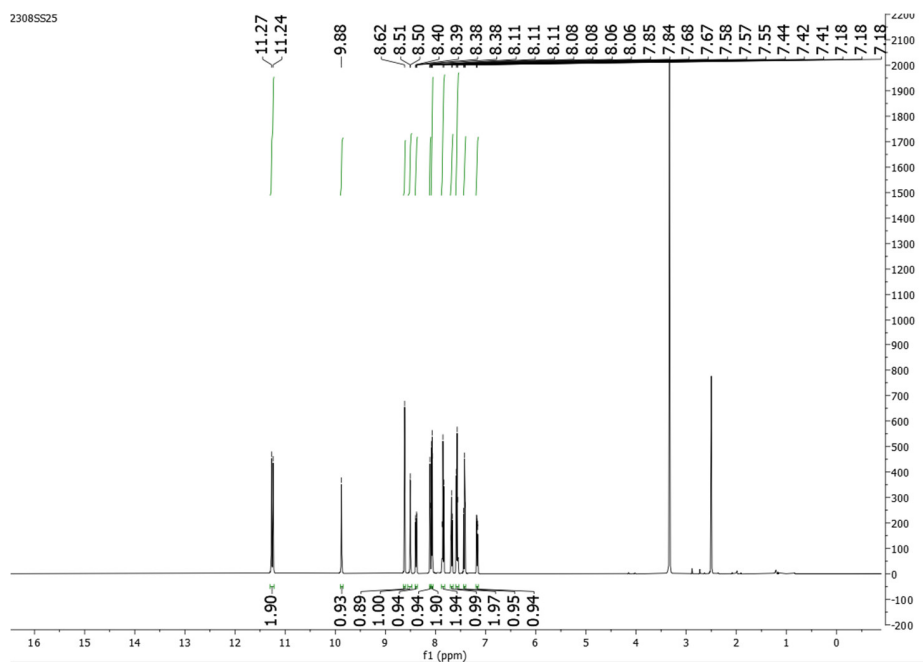
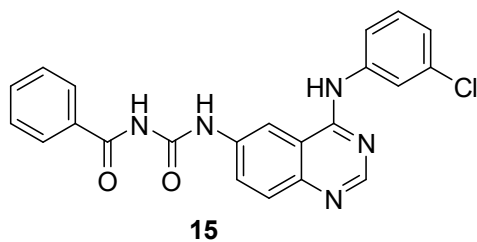


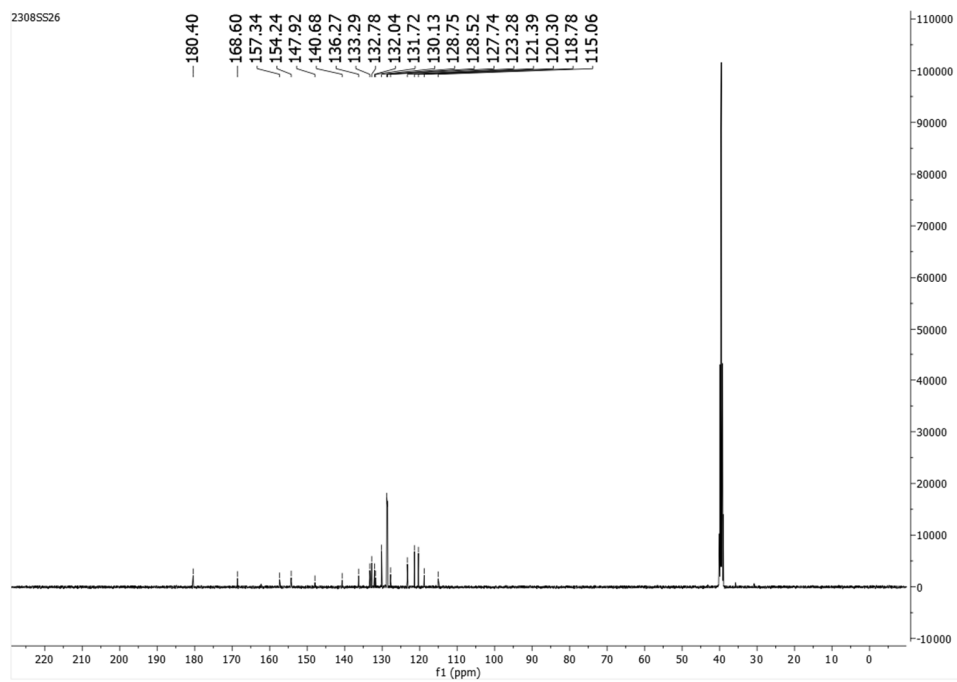
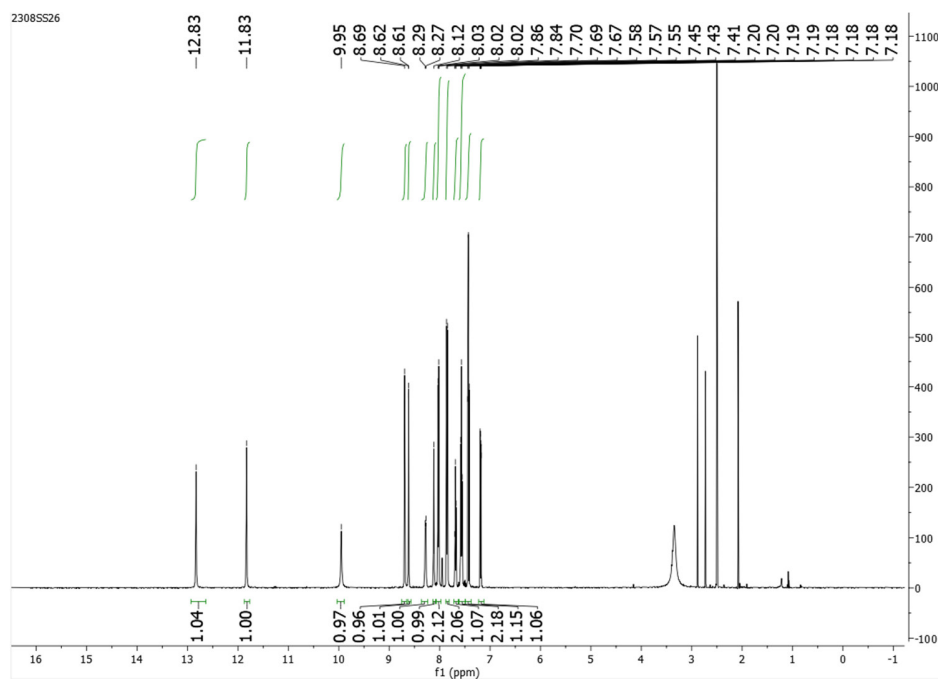
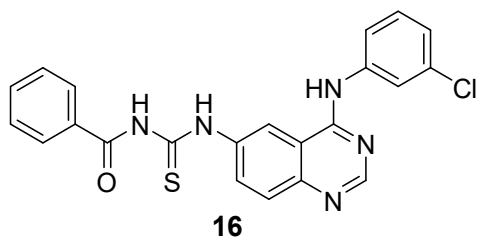


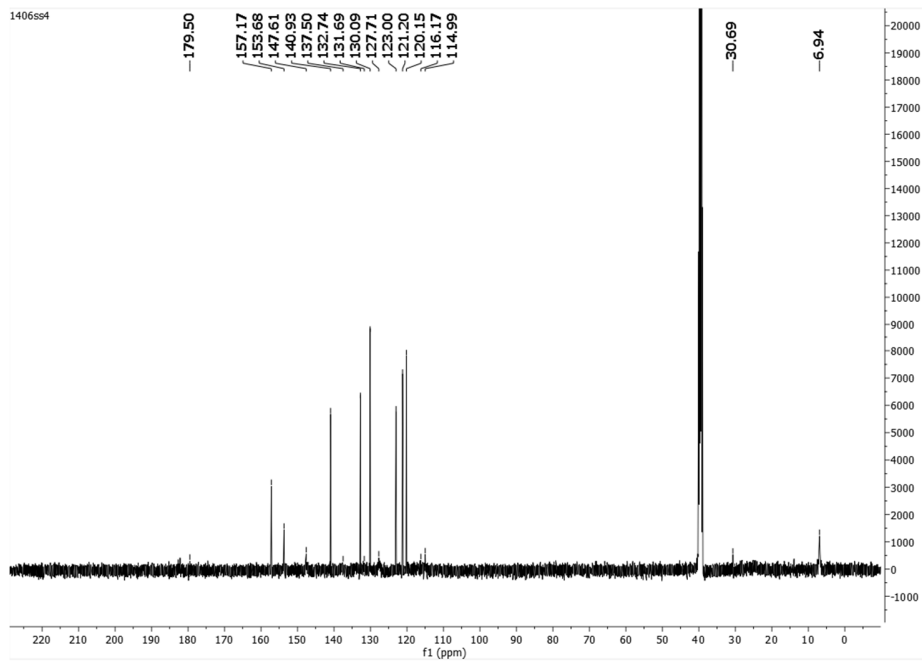
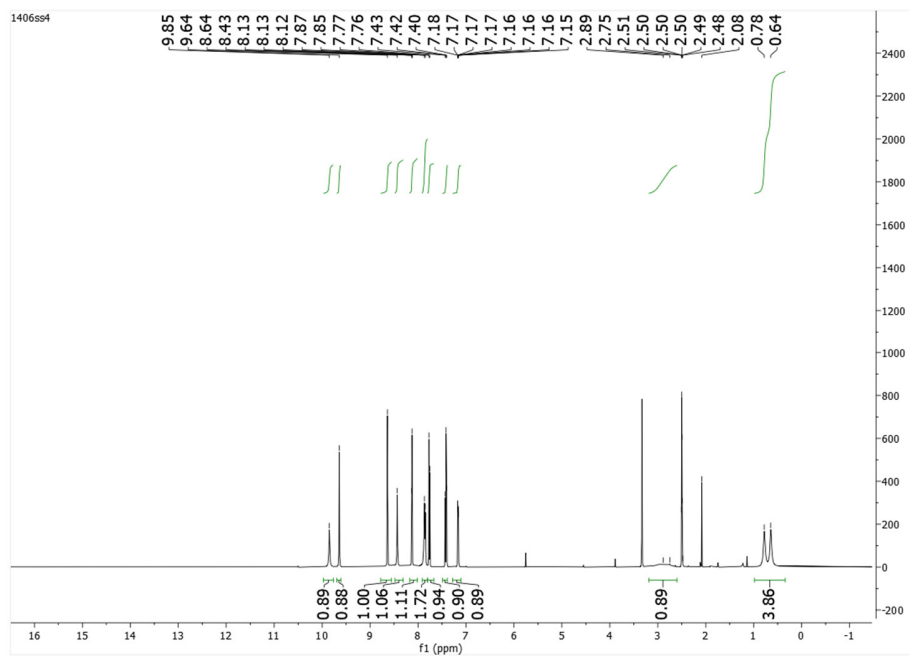
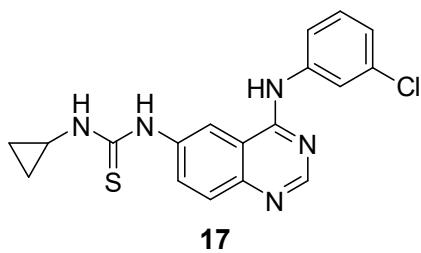


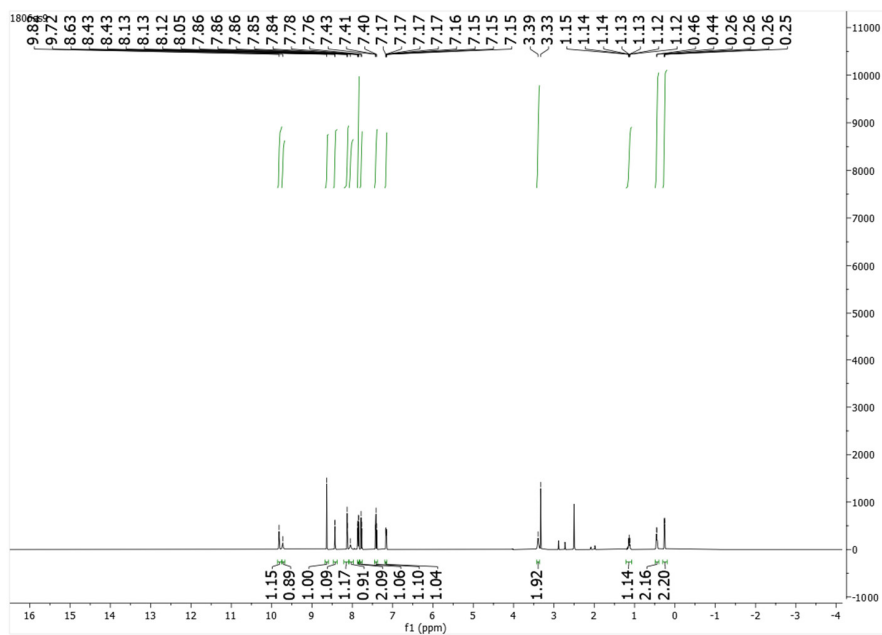
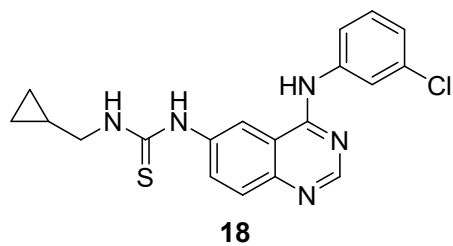
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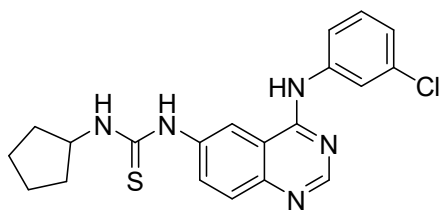












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