

SUPPORTING INFORMATION

Synthesis and antiviral activity of conjugates of chloro-containing *N*-heterocycles with *N*-aminosulfonyl glutamic acids

**A. Yu. Vigorov,^{a,*} I. A. Nizova,^a A. A. Tumashov,^a M. A. Ezhikova,^a M. I. Kodess,^a
V. L. Andronova,^b G. A. Galegov,^b V. V. Zarubaev,^c Ya. L. Esaulkova,^c G. L. Levit,^a and
V. P. Krasnov^{a,*}**

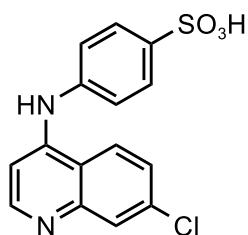
^a*I. Ya. Postovsky Institute of Organic Synthesis, Ural Branch of the Russian Academy of Sciences, 22/20 ul. S. Kovalevskoj, 620066 Yekaterinburg, Russian Federation.*

Fax: +7 (343) 374 1189; e-mail: ca@ios.uran.ru

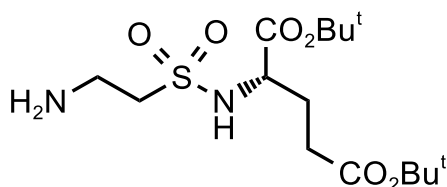
^b*D. I. Ivanovsky Institute of Virology, Gamaleya National Research Center for Epidemiology and Microbiology, Ministry of Health of the Russian Federation, 16 ul. Gamalei, 123098 Moscow, Russian Federation*

^c*Saint Petersburg Pasteur Research Institute of Epidemiology and Microbiology, 14 ul. Mira, 197101 Saint Petersburg, Russian Federation*

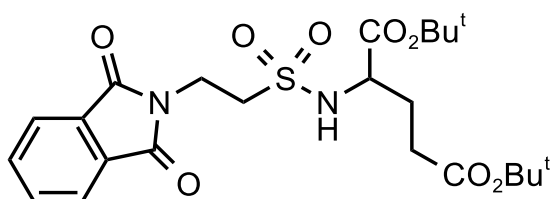
Experimental. Synthesis of some starting compounds



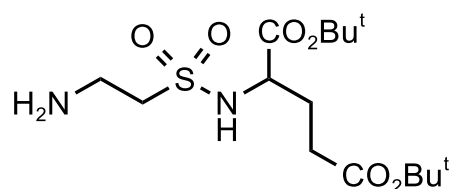
N-(7-Chloroquinolin-4-yl)-4-aminobenzenesulfonic acid, hydrate (12) was obtained according US Patent 3933829. Yield 46%, light gray crystals, mp > 360 °C. ^1H NMR spectrum (500 MHz, DMSO- d_6): 6.87 (d, 1H, H(3)_{Quin}, $J_{3-2} = 7.0$ Hz); 7.44 (d, 2H, H_{Ar}, $J = 8.4$ Hz); 7.79 (d, 2H, H_{Ar}, $J = 8.4$ Hz); 7.91 (dd, 1H, H(6)_{Quin}, $J_{6-5} = 9.1$ Hz, $J_{6-8} = 2.0$ Hz); 8.01 (d, 1H, H(8)_{Quin}, $J_{8-6} = 2.0$ Hz); 8.56 (d, 1H, H(2)_{Quin}, $J_{2-3} = 7.0$ Hz); 8.72 (d, 1H, H(5)_{Quin}, $J_{5-6} = 9.1$ Hz); 10.94 (s, 1H, NH). Signal of SO₃H-group is not detected. ^{13}C NMR spectrum could not be registered due to the low solubility of this compound in both DMSO- d_6 and D₂O+NaOD. Found (%): C, 51.88; H, 3.54; Cl 10.43; N, 7.84; S, 9.14. C₁₅H₁₁ClN₂O₃ • 0.75 H₂O. Calculated (%): C, 51.73; H, 3.62; Cl 10.18; N, 8.04; S, 9.20.



Di-tert-butyl N-(2-aminoethanesulfonyl)-(S)-glutamate [(S)-13] was obtained according [A. Yu. Vigorov, E. B. Gorbunov, M. A. Ezhikova, M. I. Kodess, D. V. Belyaev, D. V. Vakhrusheva, G. L. Levit, V. P. Krasnov, *Russ. Chem. Bull.*, 2022, **71**, 2685]. White solid, mp 94–95 °C (Et₂O).



Di-tert-butyl N-(2-phthalimidoethanesulfonyl)-(RS)-glutamate was obtained similarly to the corresponding (S)-isomer [A. Yu. Vigorov, E. B. Gorbunov, M. A. Ezhikova, M. I. Kodess, D. V. Belyaev, D. V. Vakhrusheva, G. L. Levit, V. P. Krasnov, *Russ. Chem. Bull.*, 2022, **71**, 2685]. The yield of crude product 92%. The yield after crystallization from 95% aq. EtOH 80%. White solid, mp 128–130 °C (EtOH).



Di-*tert*-butyl *N*-(2-aminoethanesulfonyl)-(*RS*)-glutamate [(*RS*)-13] was obtained similarly to the corresponding (*S*)-isomer [A. Yu. Vigorov, E. B. Gorbunov, M. A. Ezhikova, M. I. Kodess, D. V. Belyaev, D. V. Vakhrusheva, G. L. Levit, V. P. Krasnov, *Russ. Chem. Bull.*, 2022, **71**, 2685]. White solid, mp 74–75 °C (Et₂O).

NMR Spectra

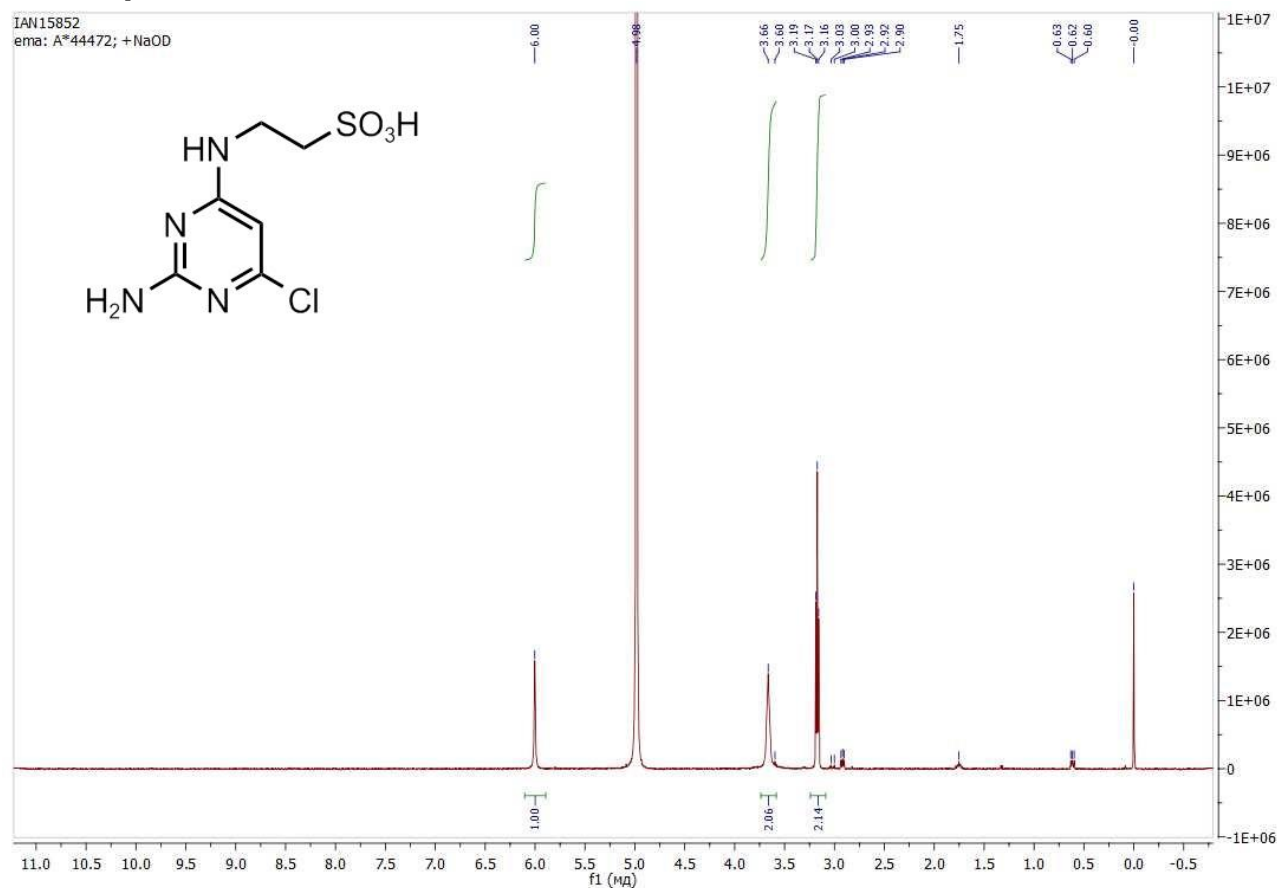


Figure S1. ^1H NMR spectrum of compound **8** (500 MHz, $\text{D}_2\text{O}+\text{NaON}$). Internal standard DSS.

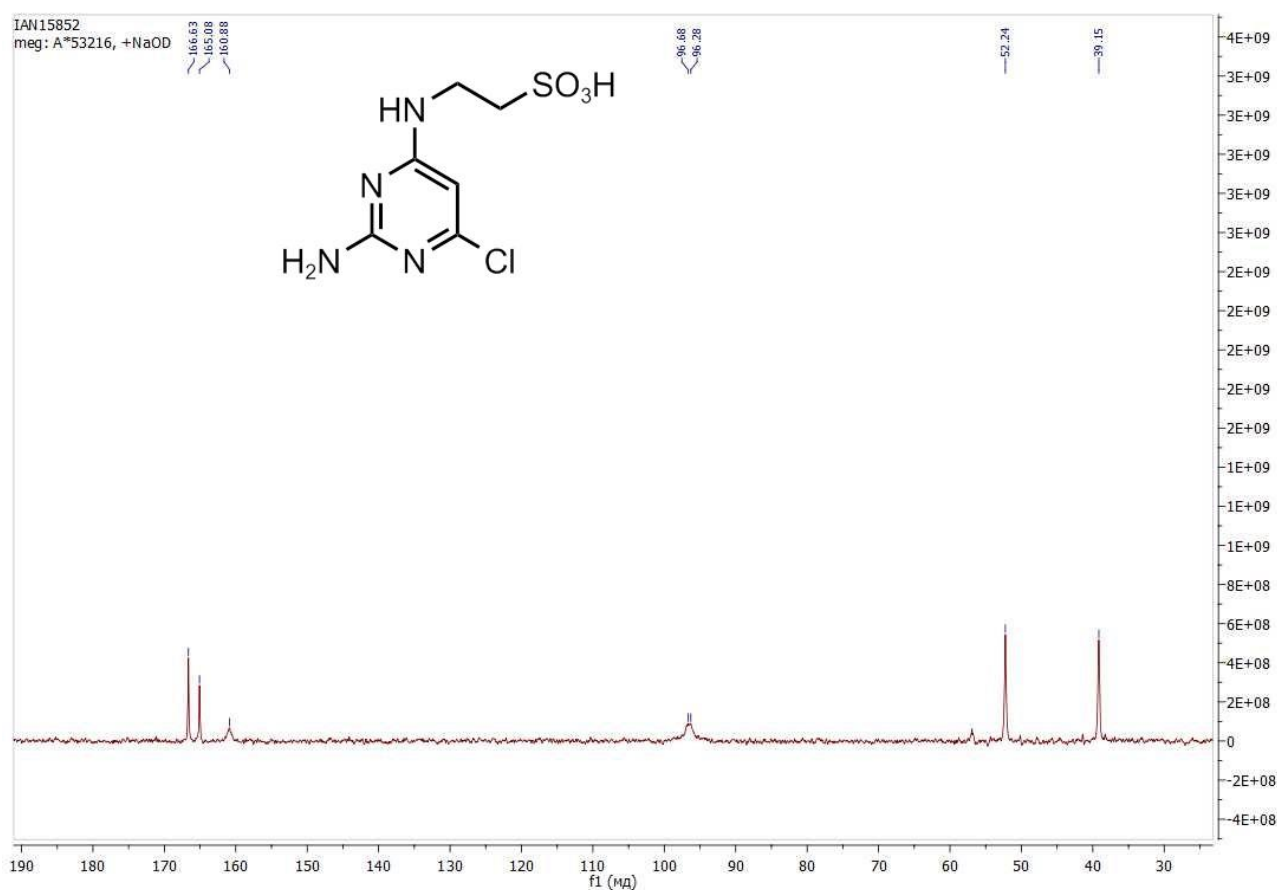


Figure S2. ^{13}C NMR spectrum of compound **8** (126 MHz, $\text{D}_2\text{O}+\text{NaON}$). Internal standard DSS.

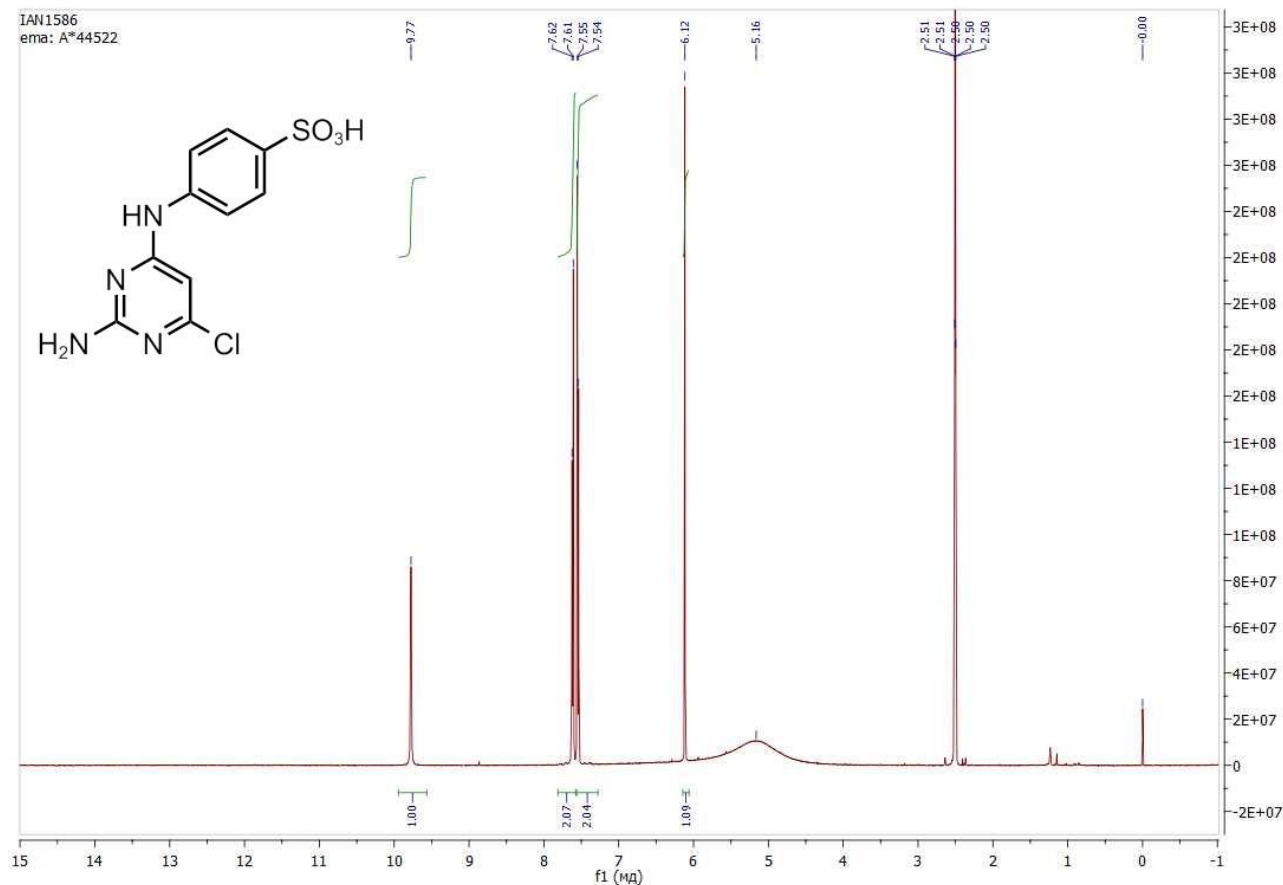


Figure S3. ^1H NMR spectrum of compound **9** (500 MHz, DMSO-d_6). Internal standard TMS.

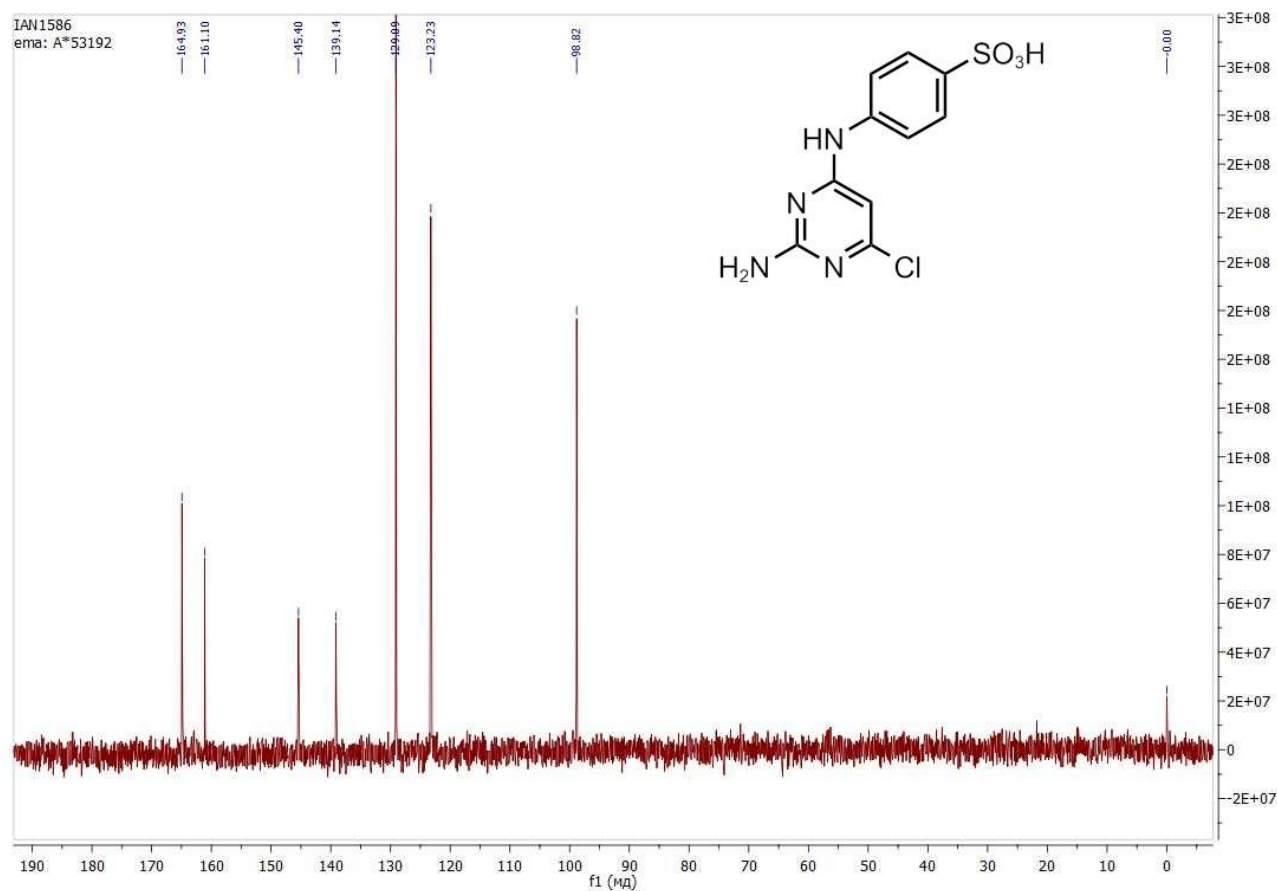


Figure S4. ^{13}C NMR spectrum of compound **9** (126 MHz, DMSO-d_6). Internal standard TMS.

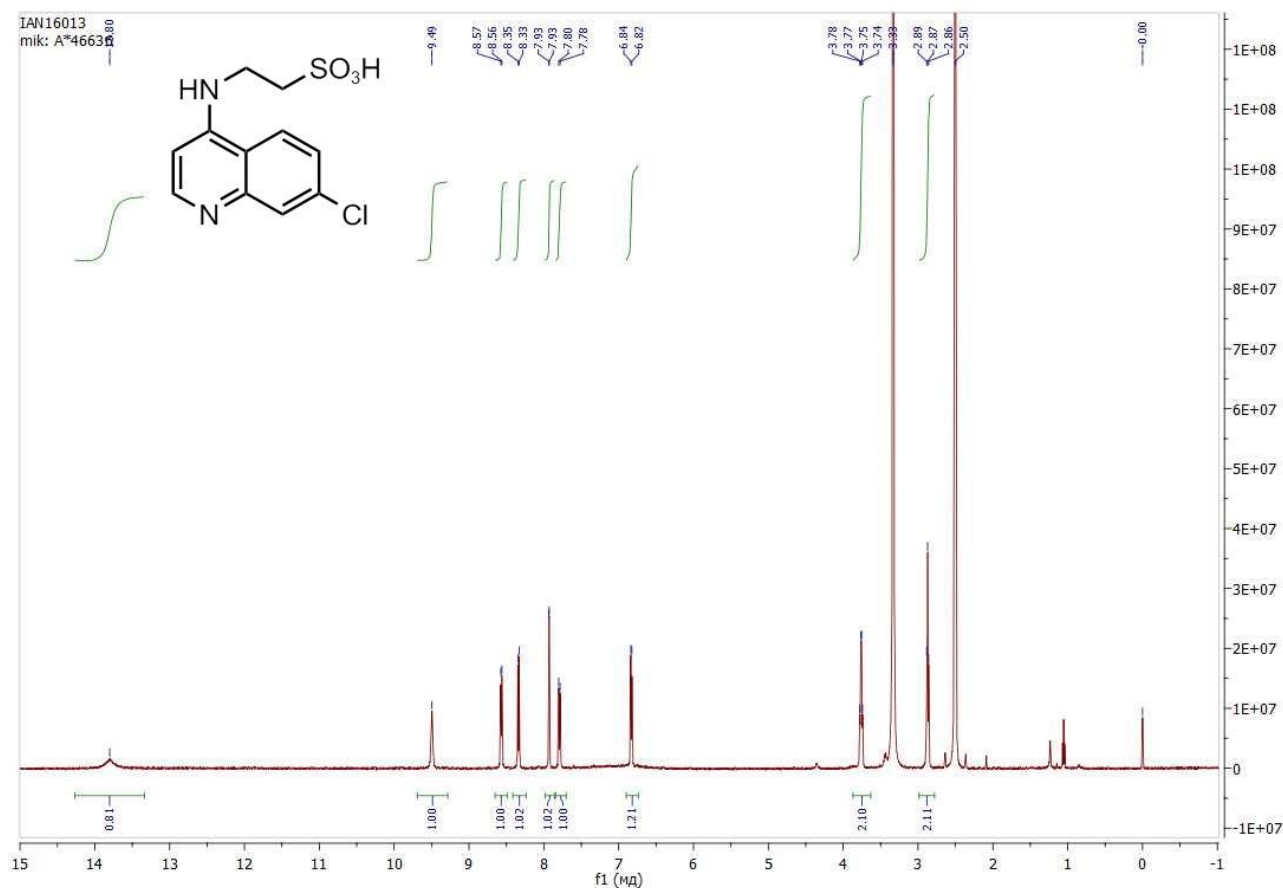


Figure S5. ¹H NMR spectrum of compound **11** (500 MHz, DMSO-d₆). Internal standard TMS.

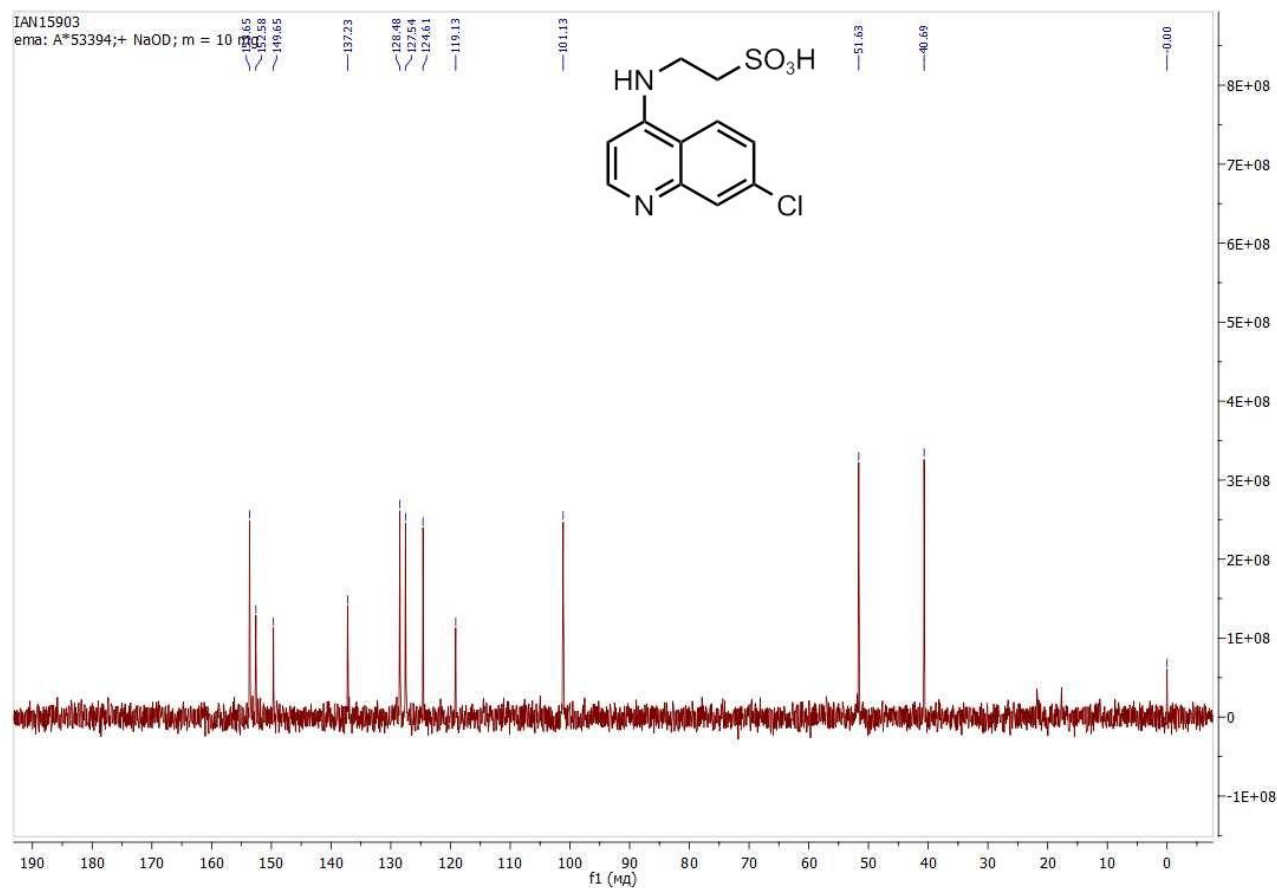


Figure S6. ¹³C NMR spectrum of compound **11** (126 MHz, D₂O+NaON). Internal standard DSS.

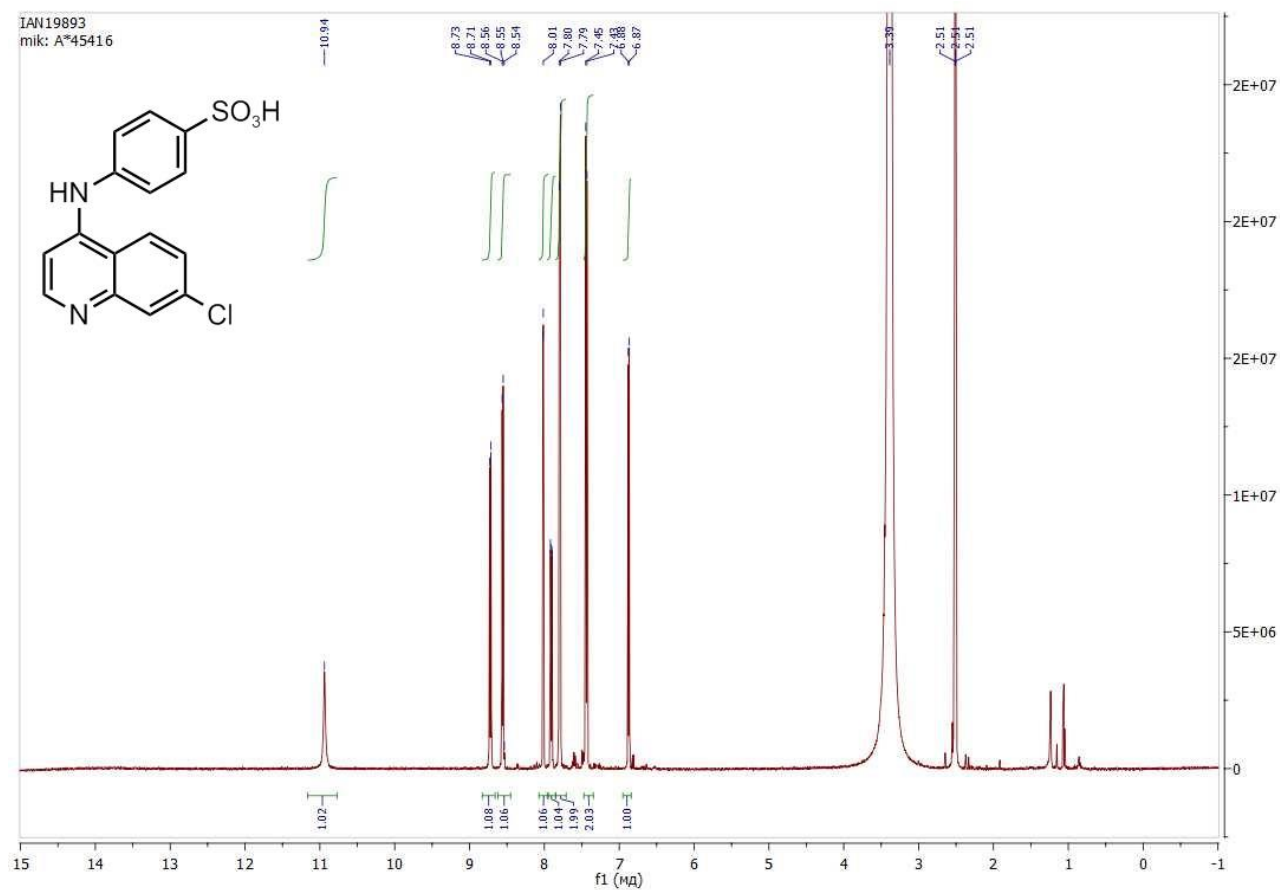


Figure S7. ^1H NMR spectrum of compound **12** (500 MHz, DMSO-d_6). Internal standard TMS.

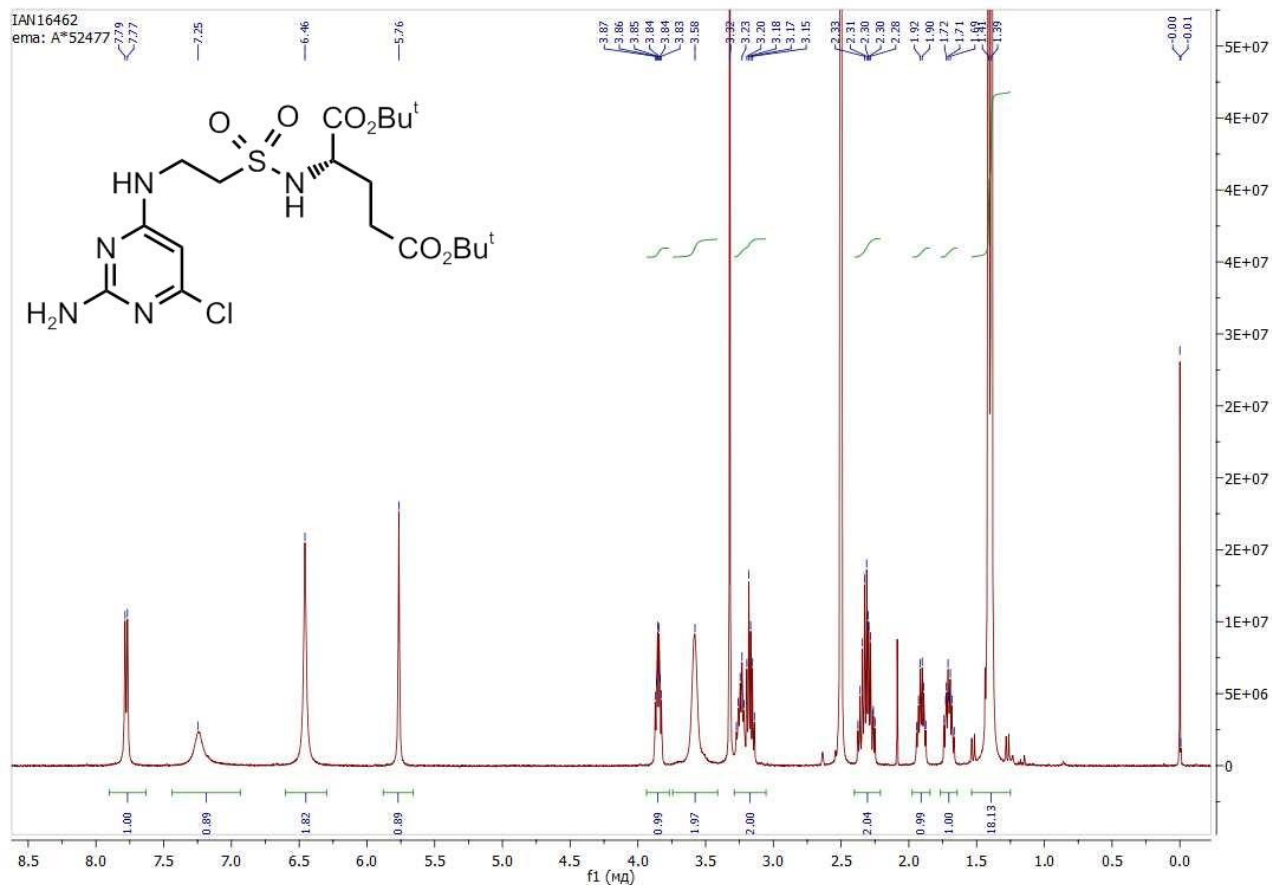


Figure S8. ¹H NMR spectrum of compound (S)-14 (500 MHz, DMSO-d₆). Internal standard TMS.

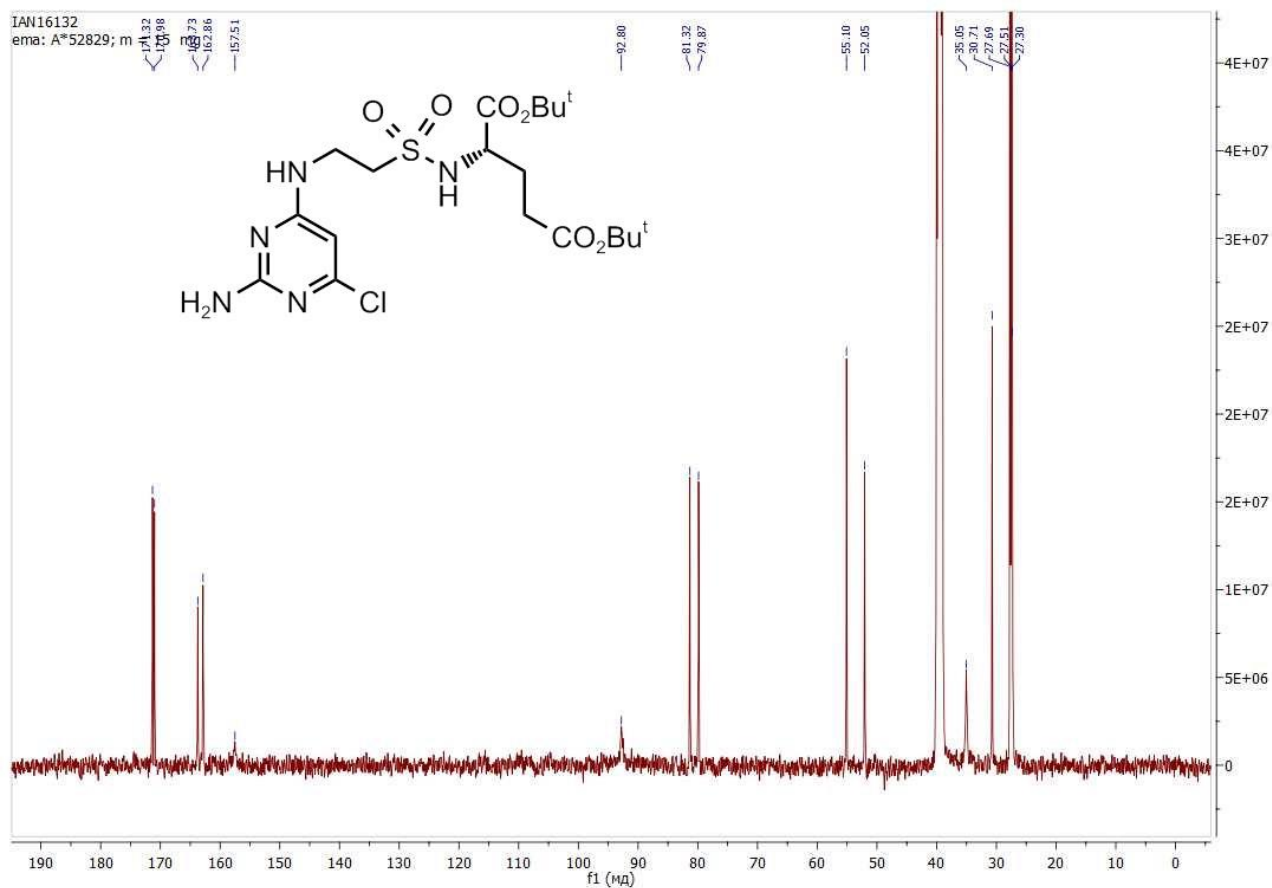


Figure S9. ¹³C NMR spectrum of compound (S)-14 (126 MHz, DMSO-d₆). Internal standard TMS.

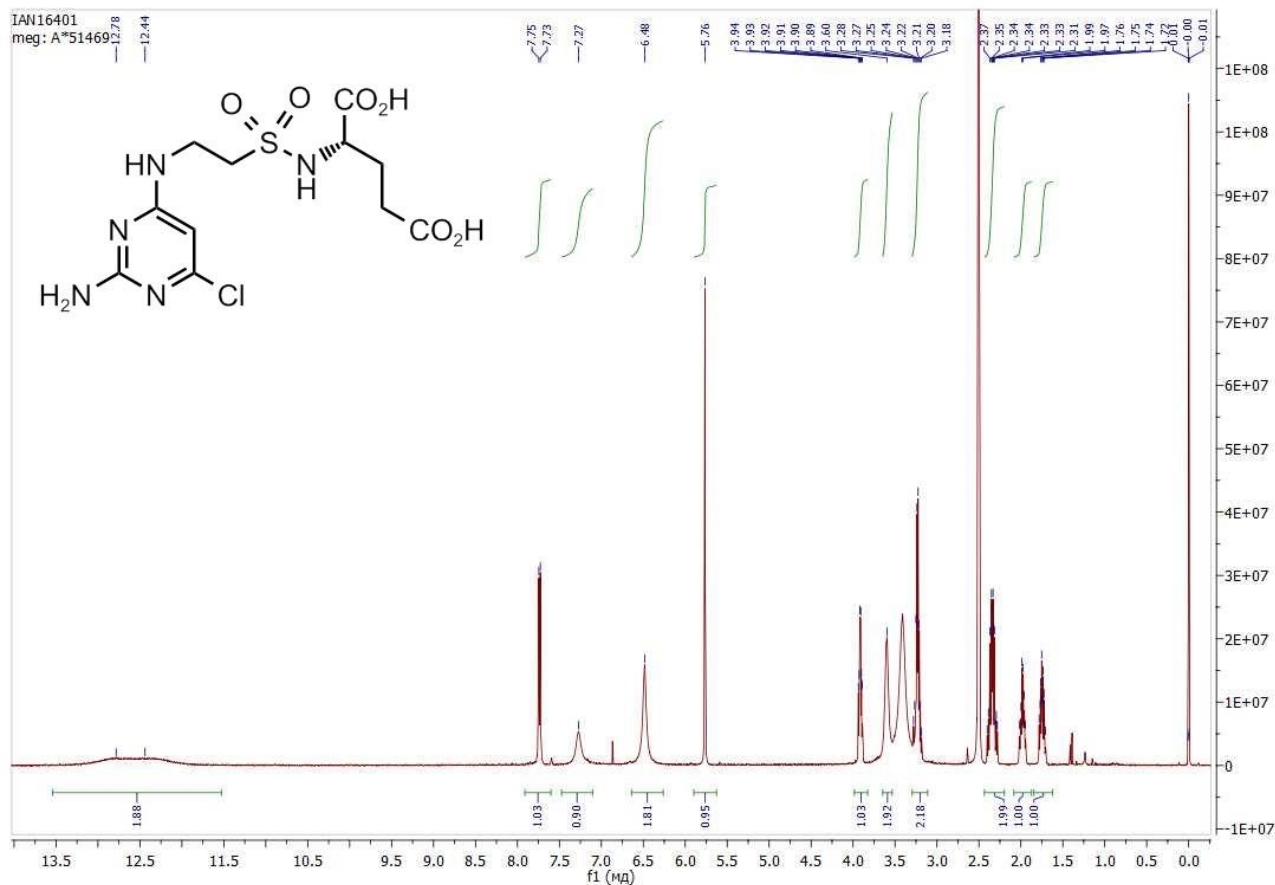


Figure S10. ^1H NMR spectrum of compound (S)-15 (500 MHz, DMSO-d_6). Internal standard TMS.

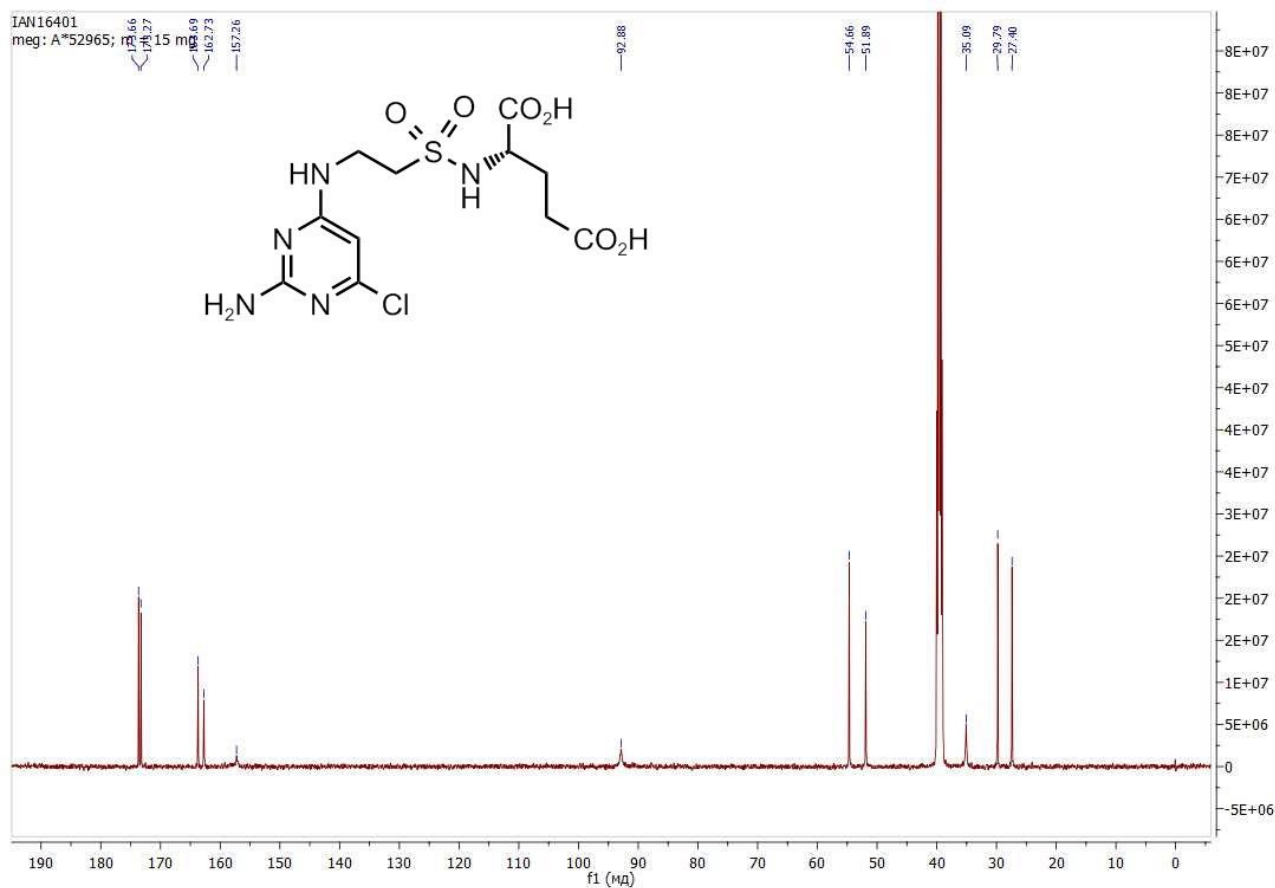


Figure S11. ^{13}C NMR spectrum of compound (S)-15 (126 MHz, DMSO-d_6). Internal standard TMS.

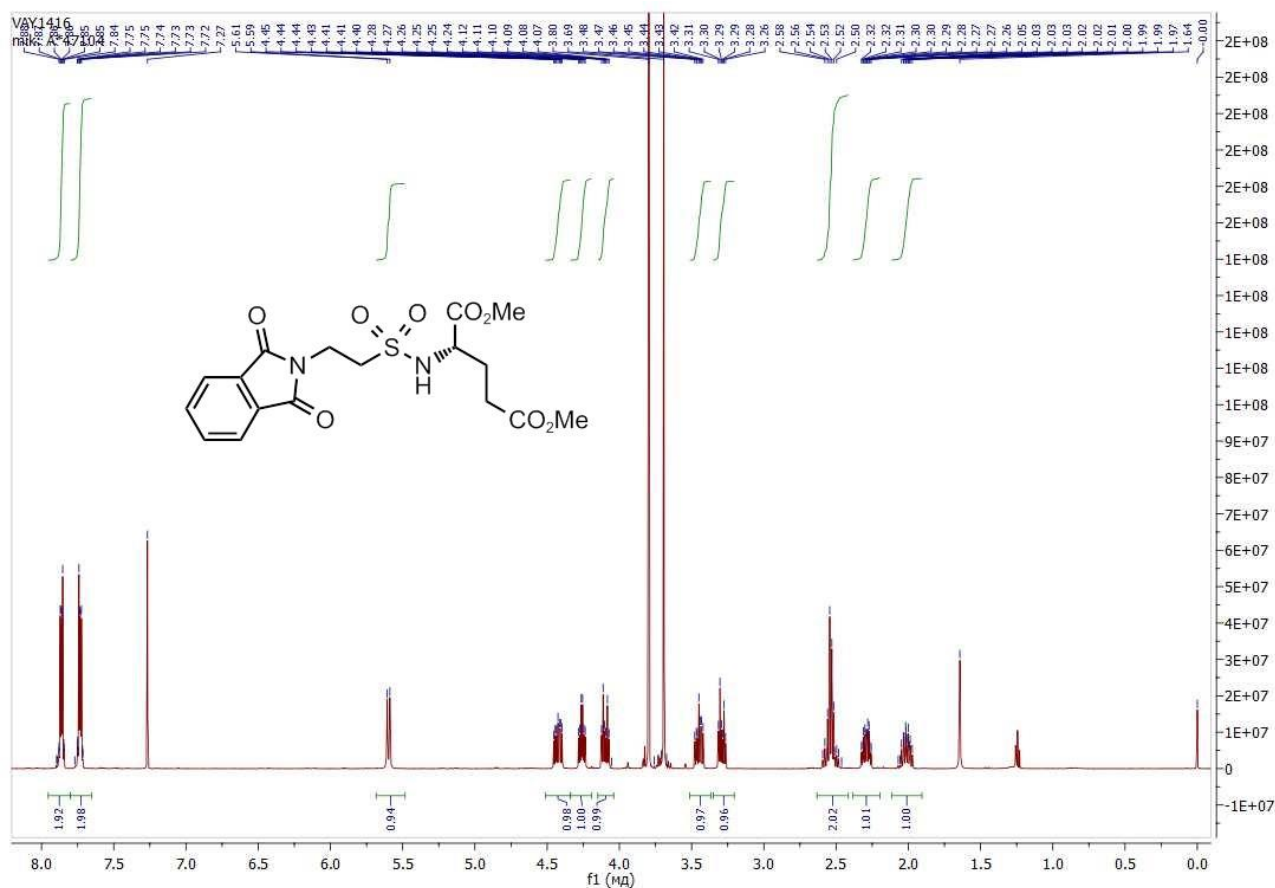


Figure S12. ¹H NMR spectrum of compound (S)-16 (500 MHz, CDCl₃). Internal standard TMS.

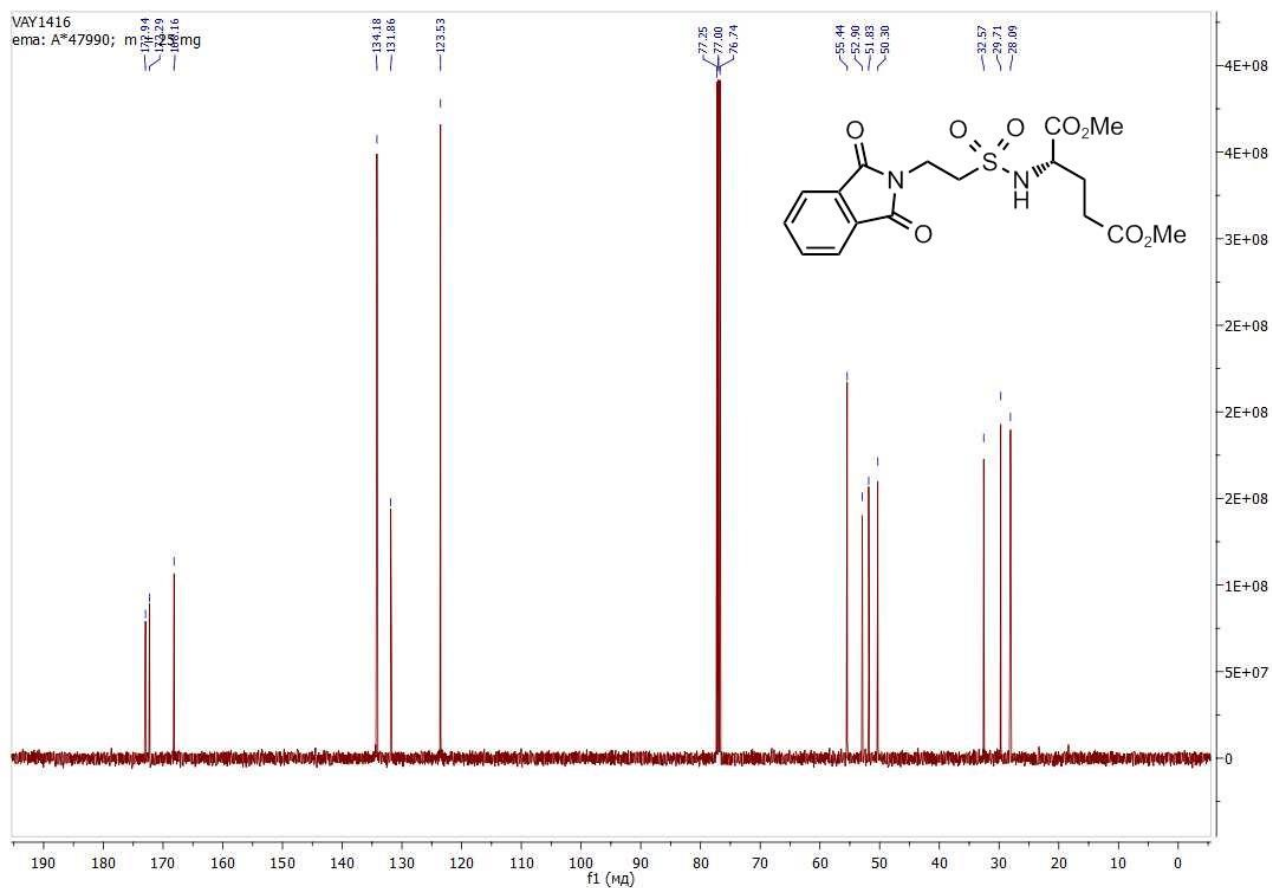


Figure S13. ¹³C NMR spectrum of compound (S)-16 (126 MHz, CDCl₃). Internal standard TMS.

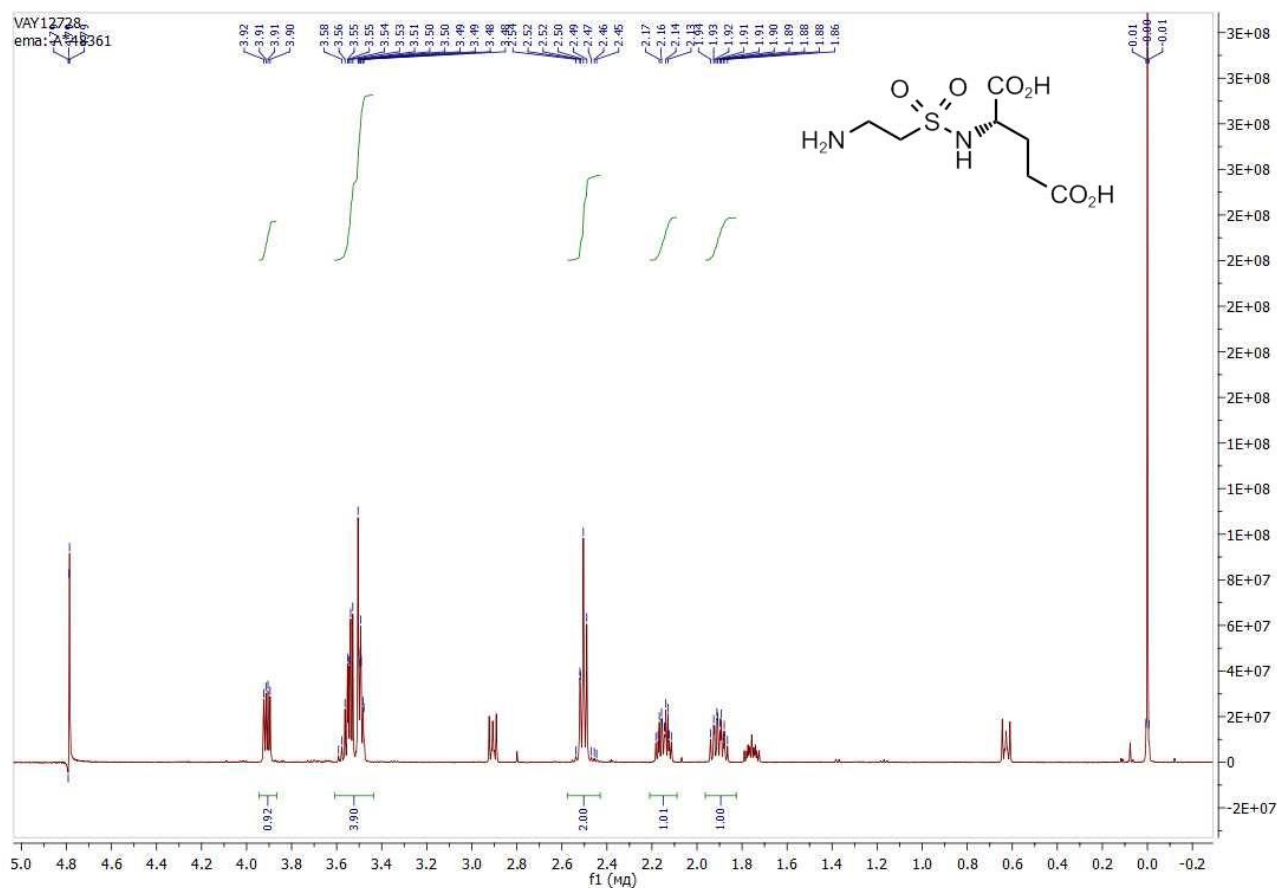


Figure S14. ^1H NMR spectrum of compound **17** (500 MHz, D_2O). Internal standard DSS.

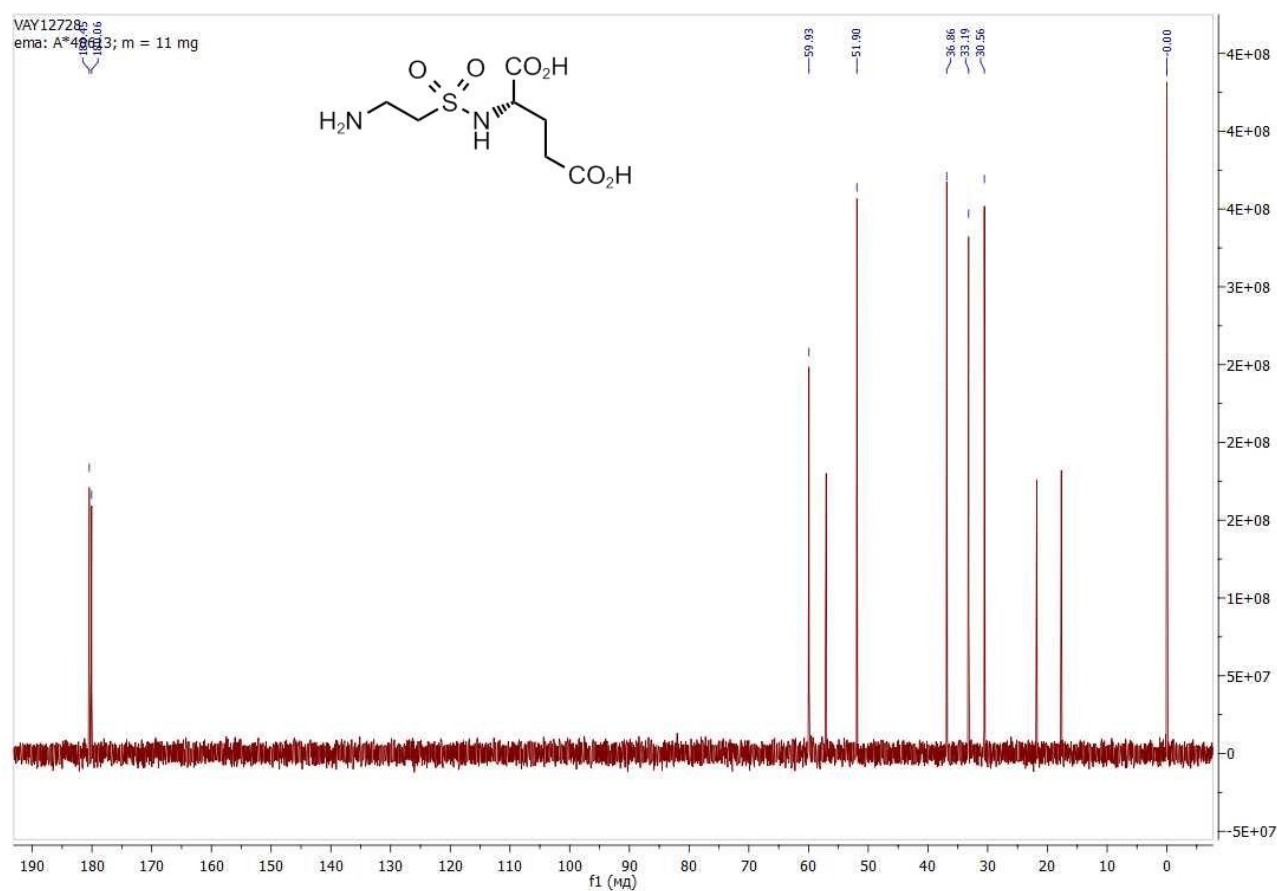


Figure S15. ^{13}C NMR spectrum of compound **17** (126 MHz, D_2O). Internal standard DSS.

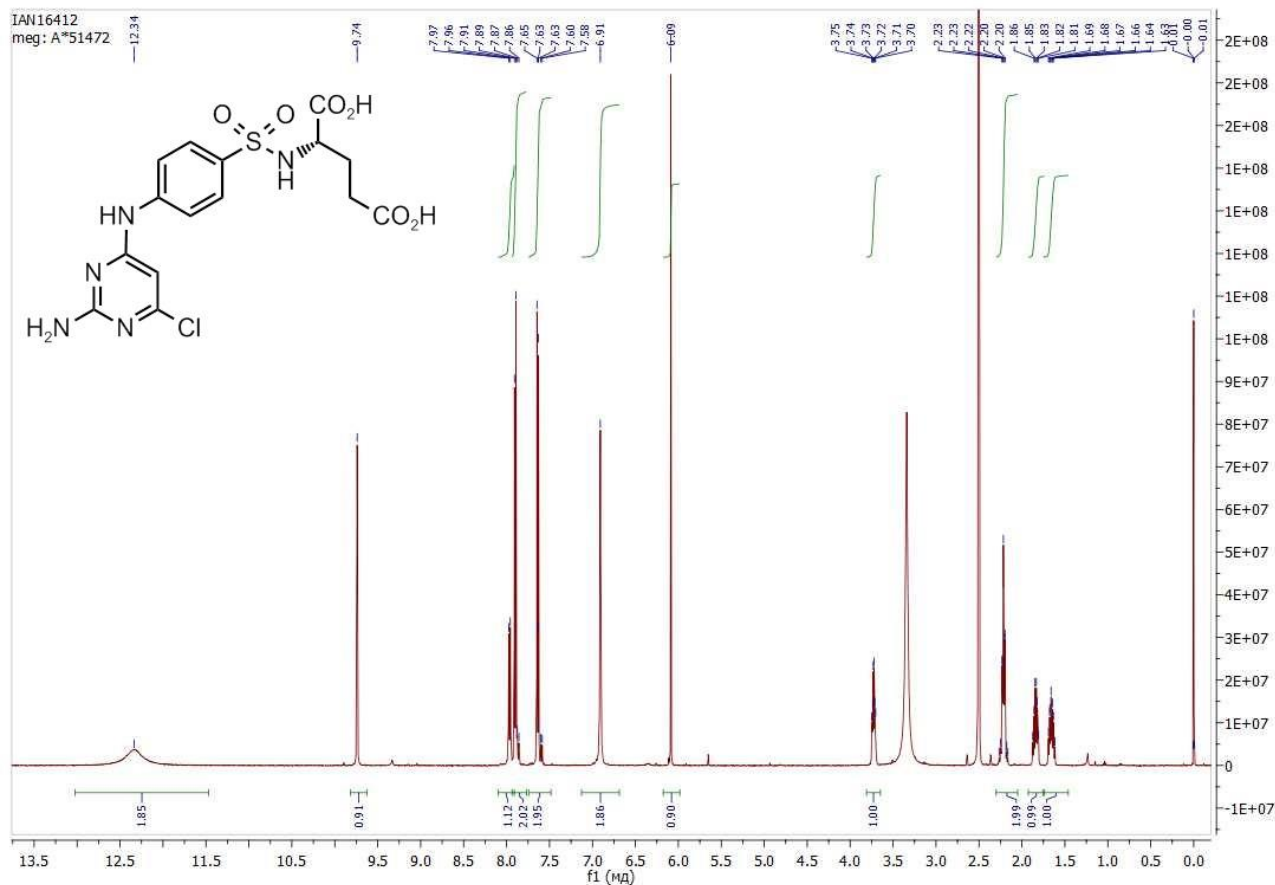


Figure S16. ^1H NMR spectrum of compound (S)-19 (500 MHz, DMSO-d_6). Internal standard TMS.

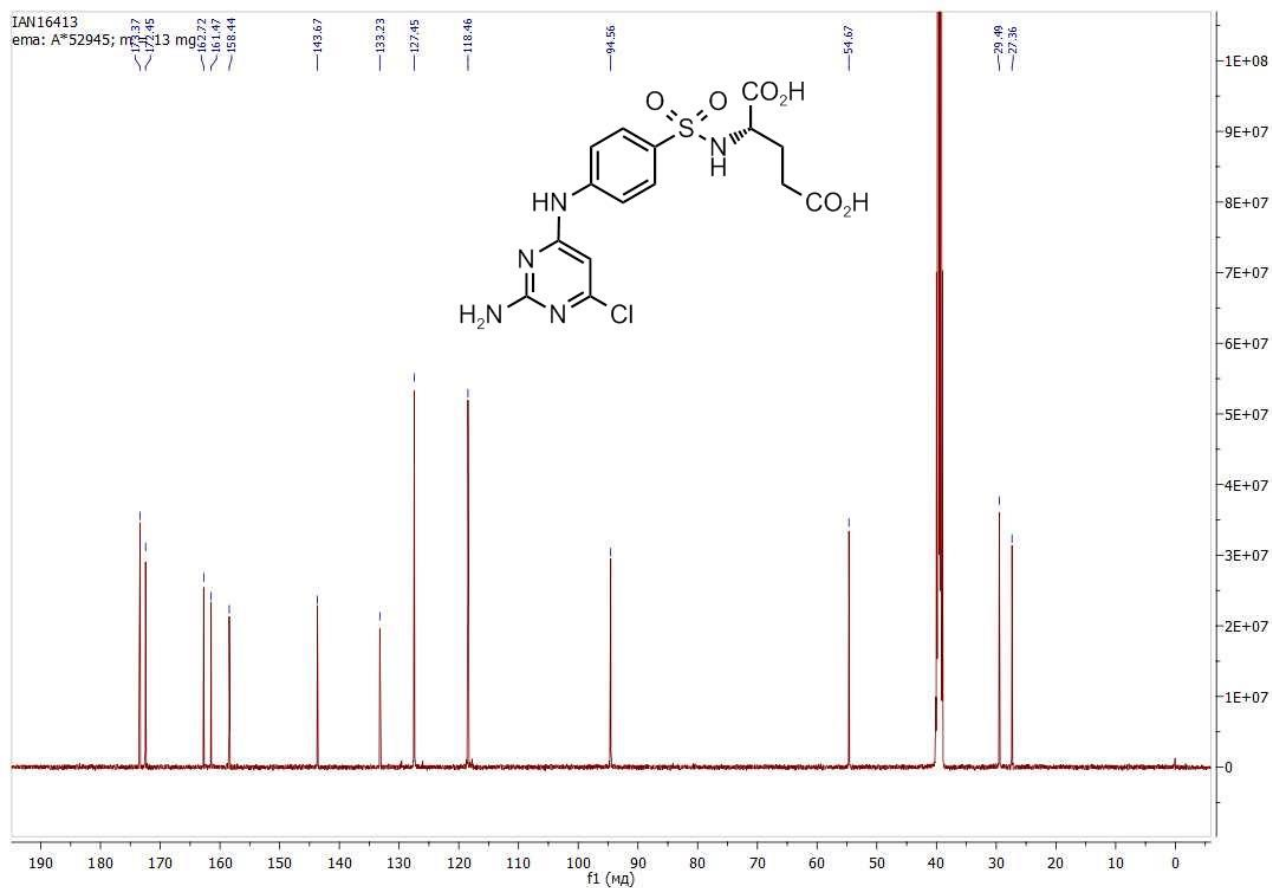


Figure S17. ^{13}C NMR spectrum of compound (S)-19 (126 MHz, DMSO-d_6). Internal standard TMS.

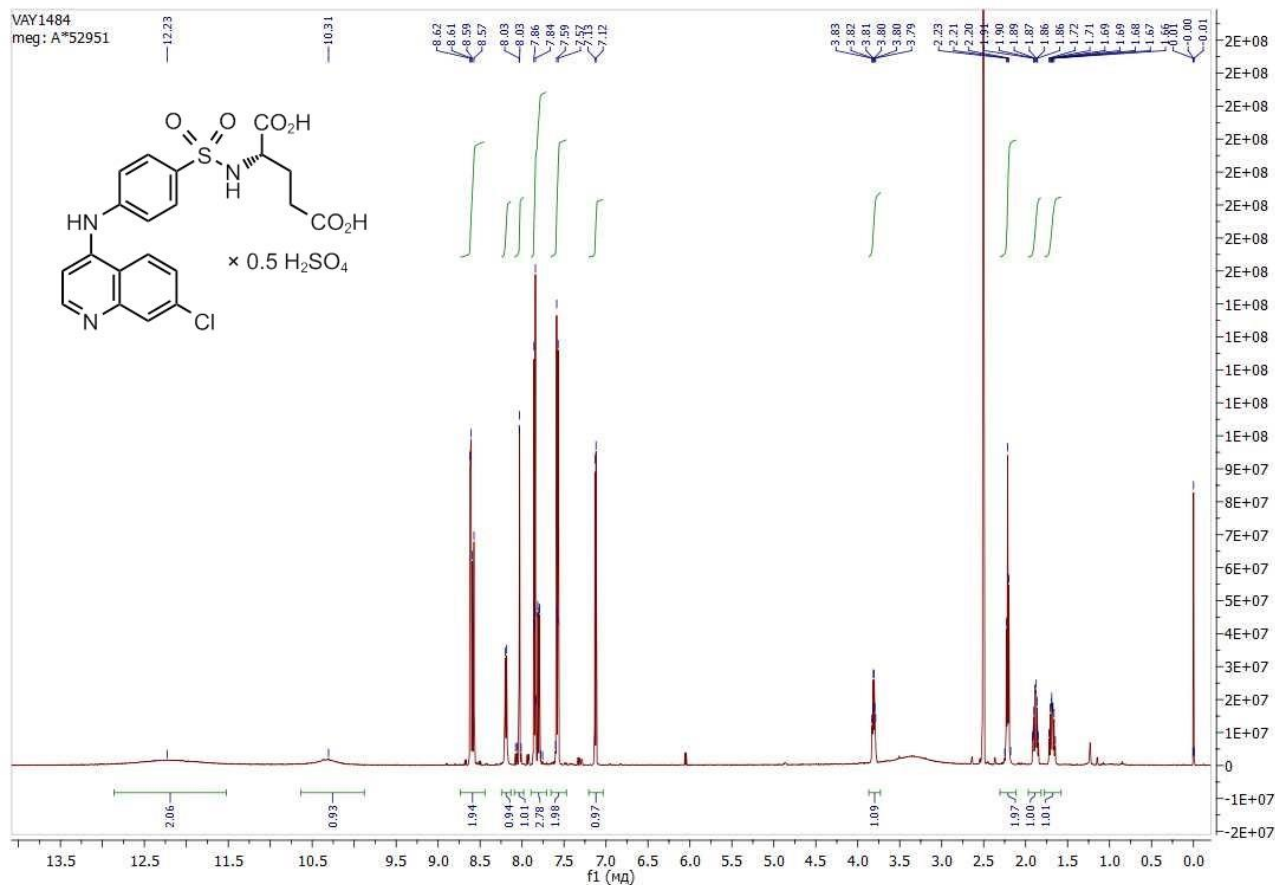


Figure S18. ¹H NMR spectrum of compound (S)-20 (500 MHz, DMSO-d₆). Internal standard TMS.

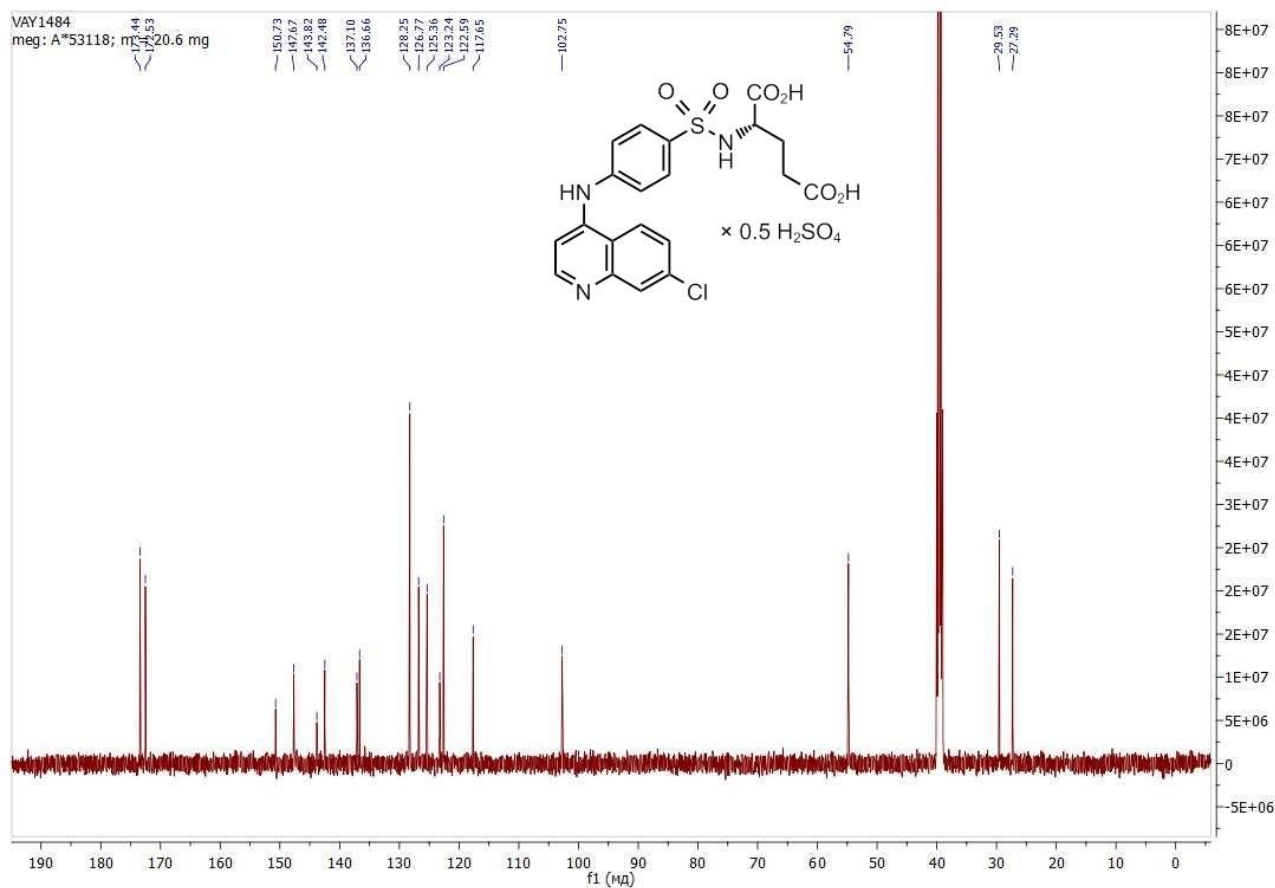


Figure S19. ¹³C NMR spectrum of compound (S)-20 (126 MHz, DMSO-d₆). Internal standard TMS.

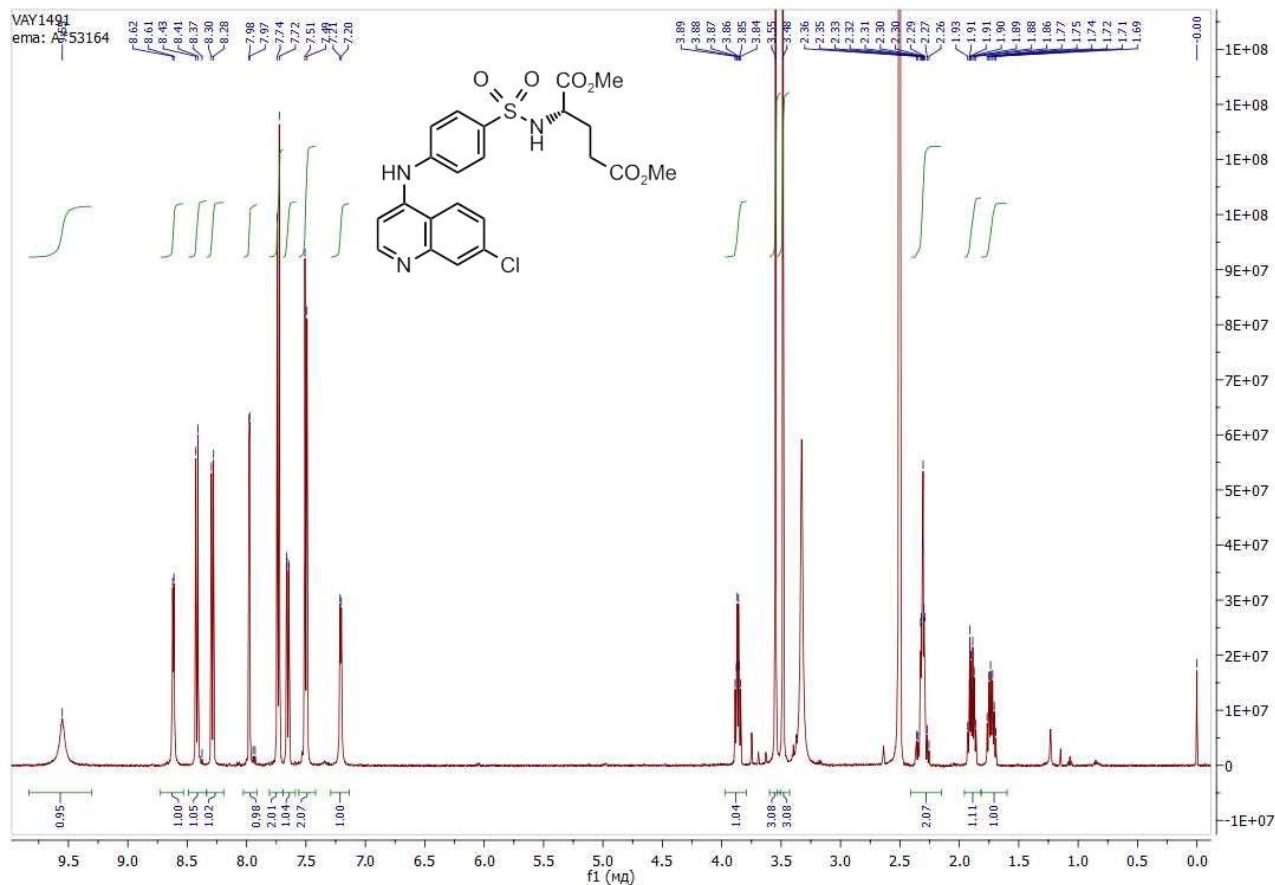


Figure S20. ¹H NMR spectrum of compound (S)-21 (500 MHz, DMSO-d₆). Internal standard TMS.

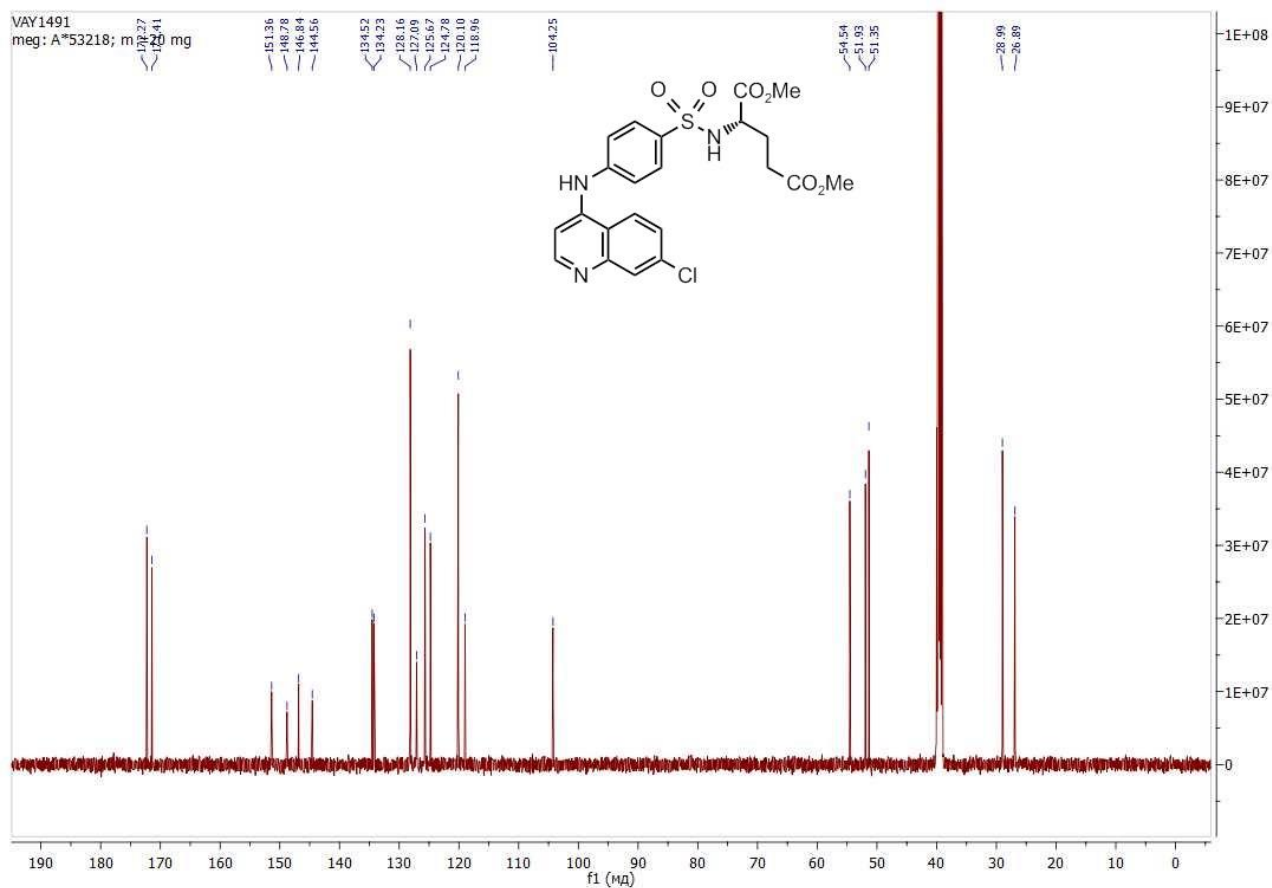


Figure S21. ¹³C NMR spectrum of compound (S)-21 (126 MHz, DMSO-d₆). Internal standard TMS.

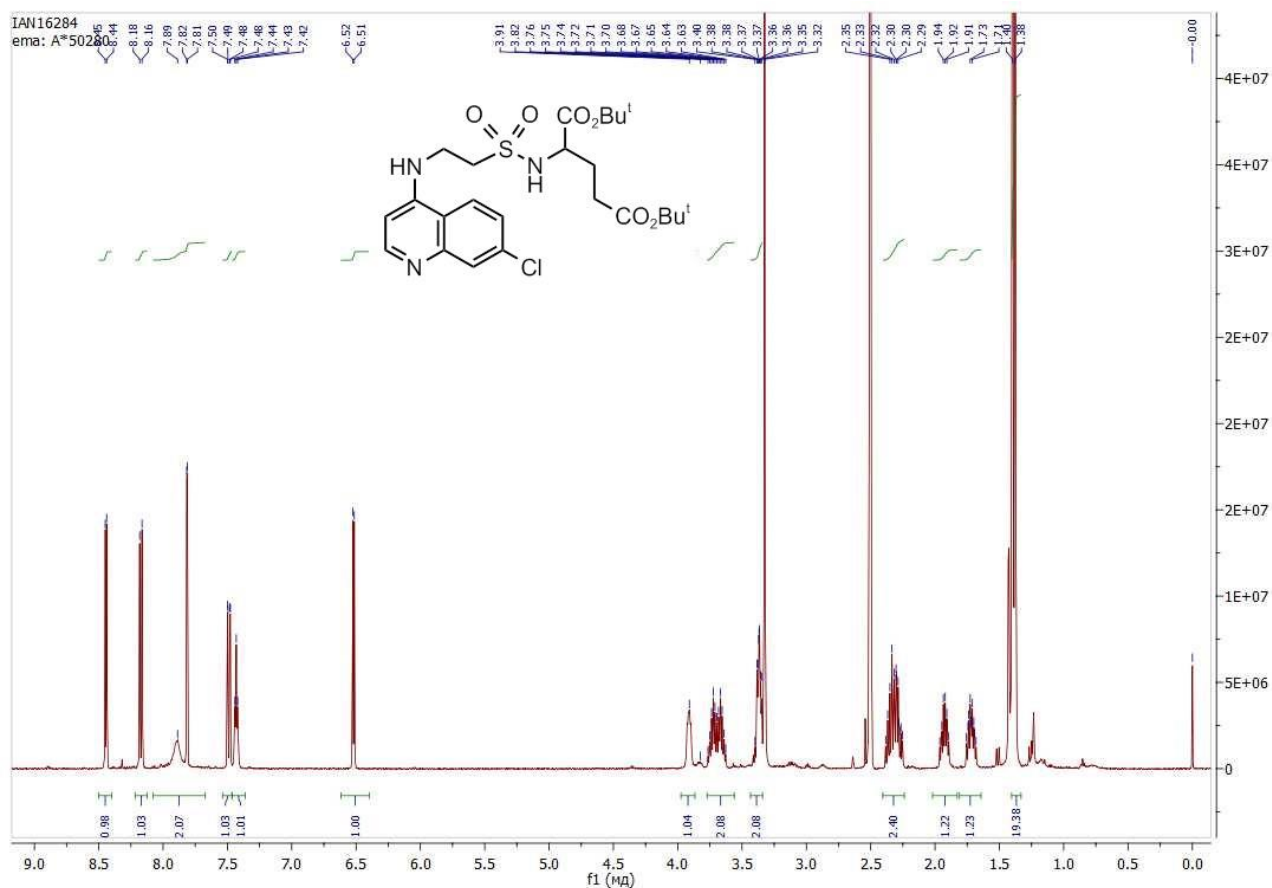


Figure S22. ^1H NMR spectrum of compound (RS)-22 (500 MHz, DMSO- d_6). Internal standard TMS.

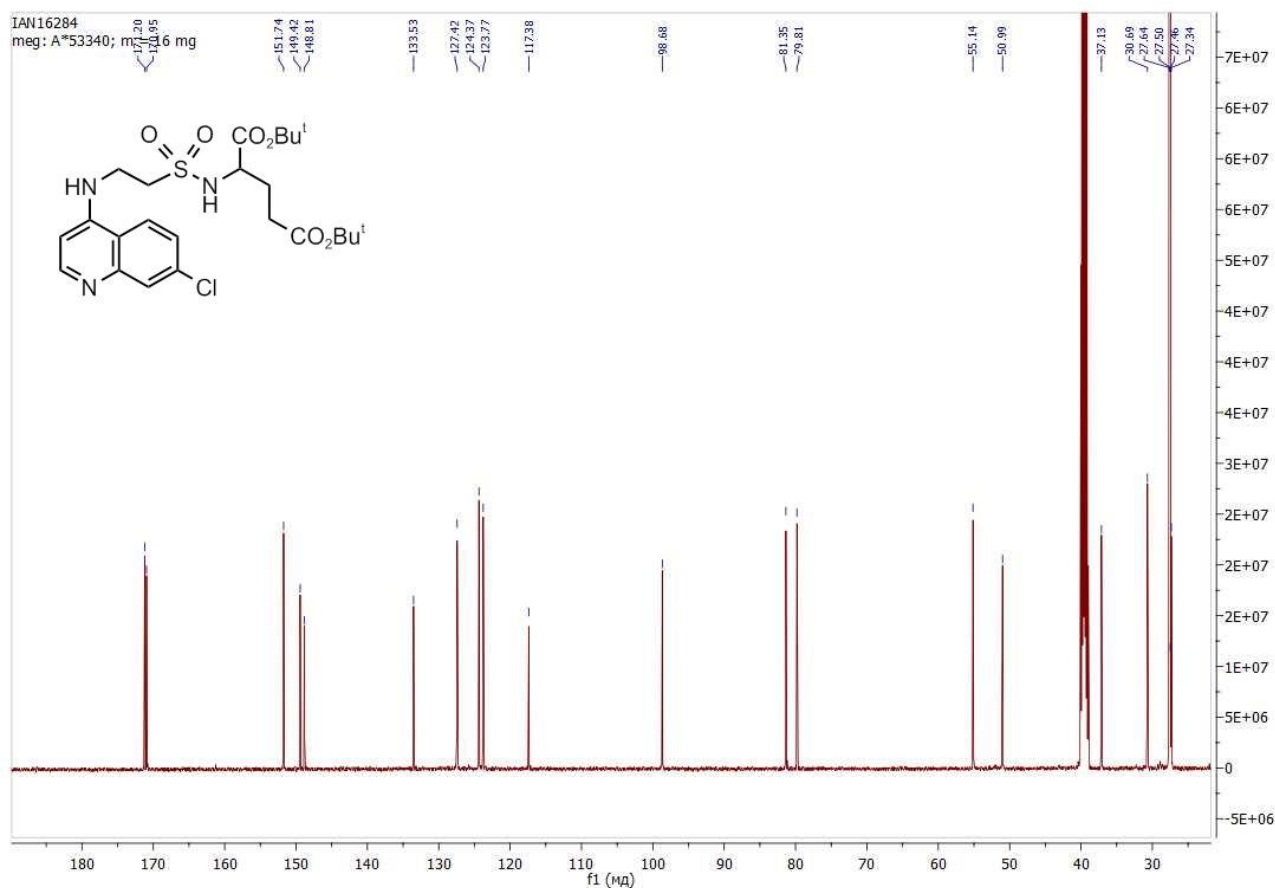


Figure S23. ^{13}C NMR spectrum of compound (RS)-22 (126 MHz, DMSO- d_6). Internal standard TMS.

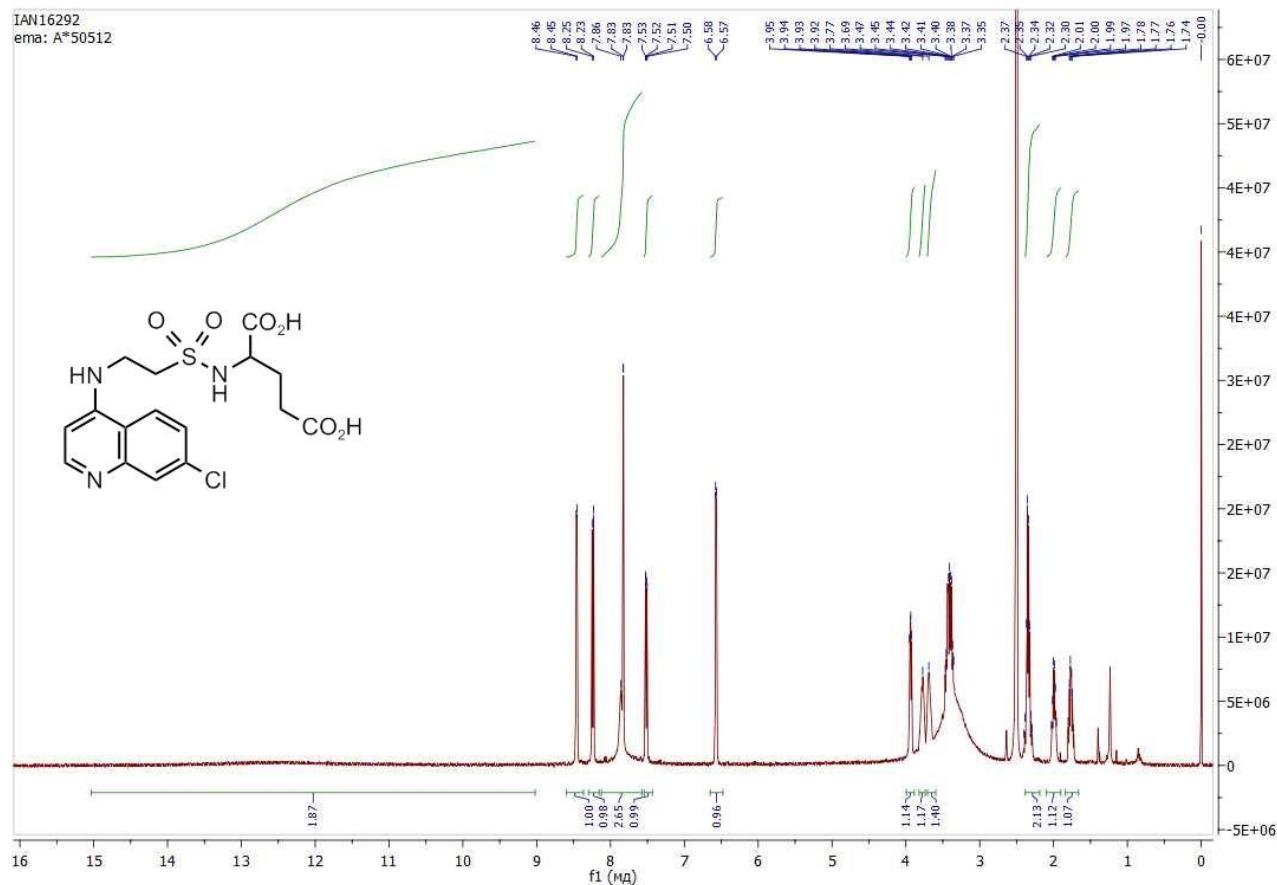


Figure S24. ¹H NMR spectrum of compound (RS)-23 (500 MHz, DMSO-d₆). Internal standard TMS.

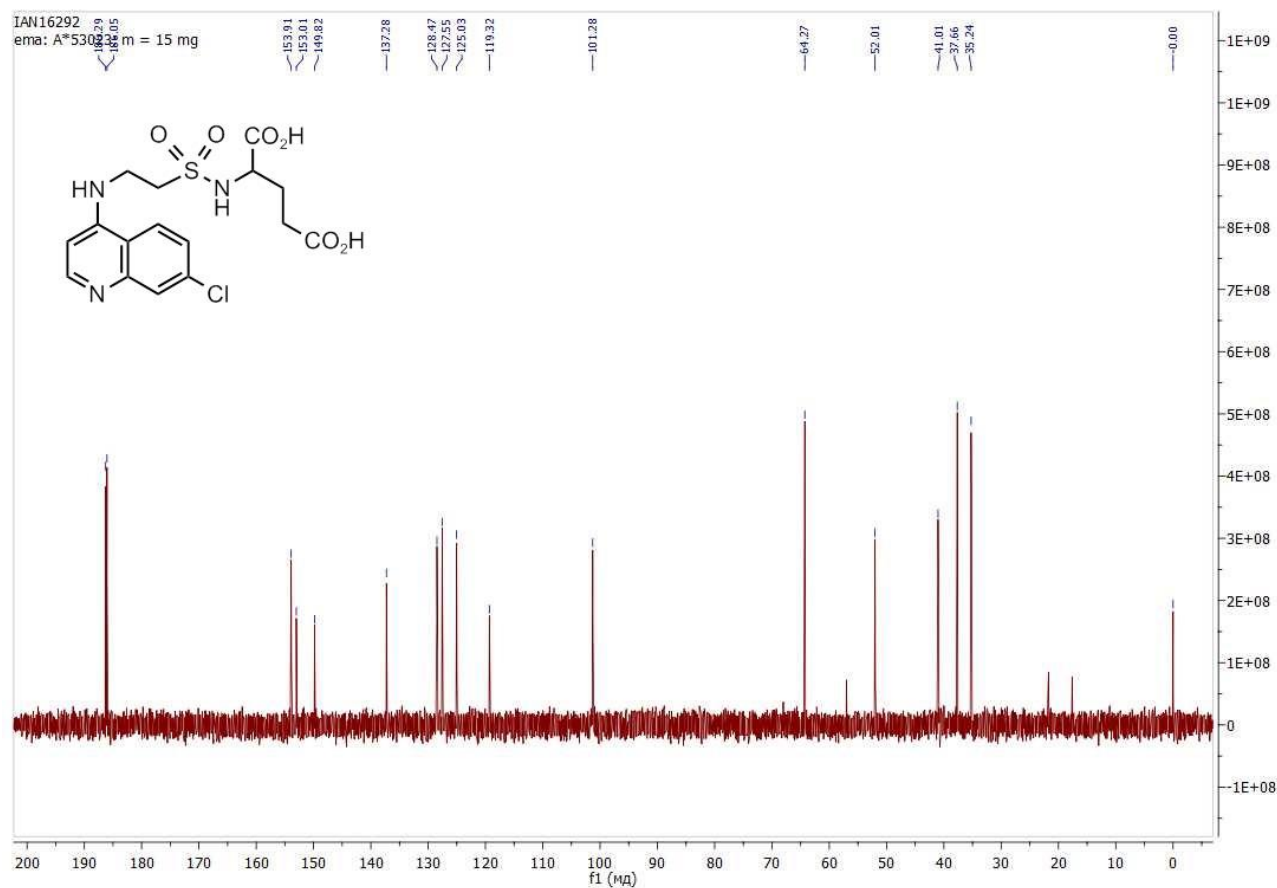


Figure S25. ¹³C NMR spectrum of compound (RS)-23 (126 MHz, D₂O+NaOD). Internal standard DSS.