

Electronic Supplementary Information

5-Selenocyanato and 5-trifluoromethanesulfonyl derivatives of 2'-deoxyuridine: synthesis, radiation and computational chemistry as well as cytotoxicity †

Samanta Makurat,^{a,‡} Magdalena Zdrowowicz,^{a,‡} Lidia Chomicz-Mańka,^{a,‡} Witold Kozak,^{a,‡} Illia E. Serdiuk,^b Paweł Wityk,^a Alicja Kawecka,^a Marta Sosnowska^a and Janusz Rak*

^a Department of Chemistry, University of Gdańsk, Wita Stwosza 63, 80-308 Gdańsk, Poland. E-mail: janusz.rak@ug.edu.pl

^b Faculty of Mathematics, Physics and Informatics, University of Gdańsk, Wita Stwosza 57, 80-308 Gdańsk, Poland.

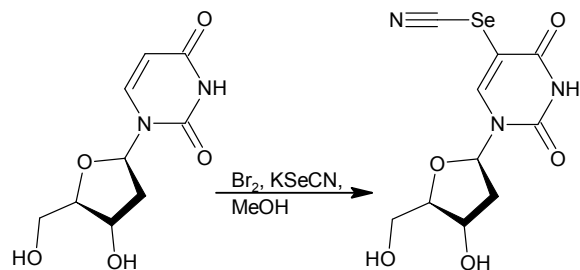
† Electronic supplementary information (ESI) available. See DOI:

‡ These authors contributed equally to this work.

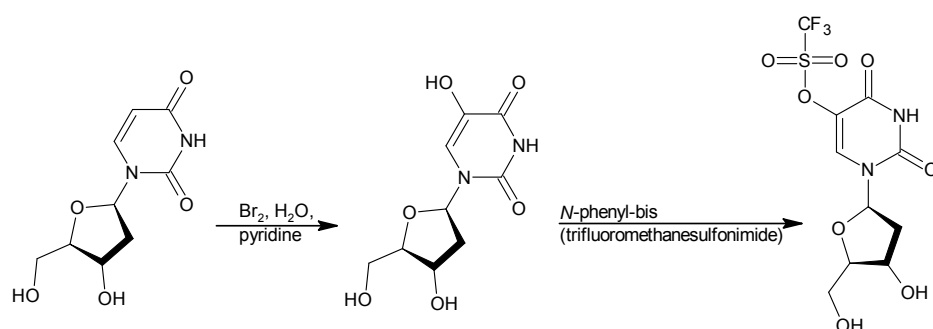
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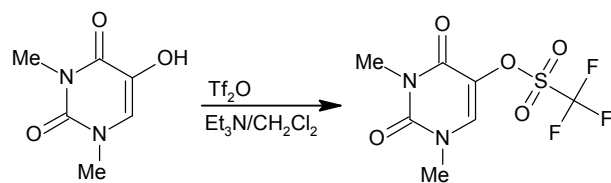
Synthesis schemes for studied analogs



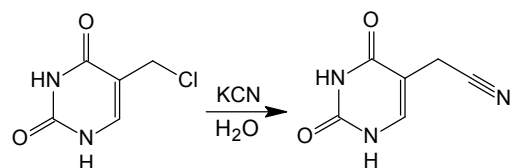
Scheme S1 Synthetic route for 5-selenocyanato-2'-deoxyuridine.



Scheme S2 Synthetic route for 5-trifluoromethanesulfonyl-2'-deoxyuridine.



Scheme S3 Synthetic route for 1,3-dimethyl-5-trifluoromethanesulfonyluracil.



Scheme S4 Synthetic route for 5-cyanomethyluracil.

Identification of radiolysis products for 5-selenocyanato-2'-deoxyuridine (SeCNdU)

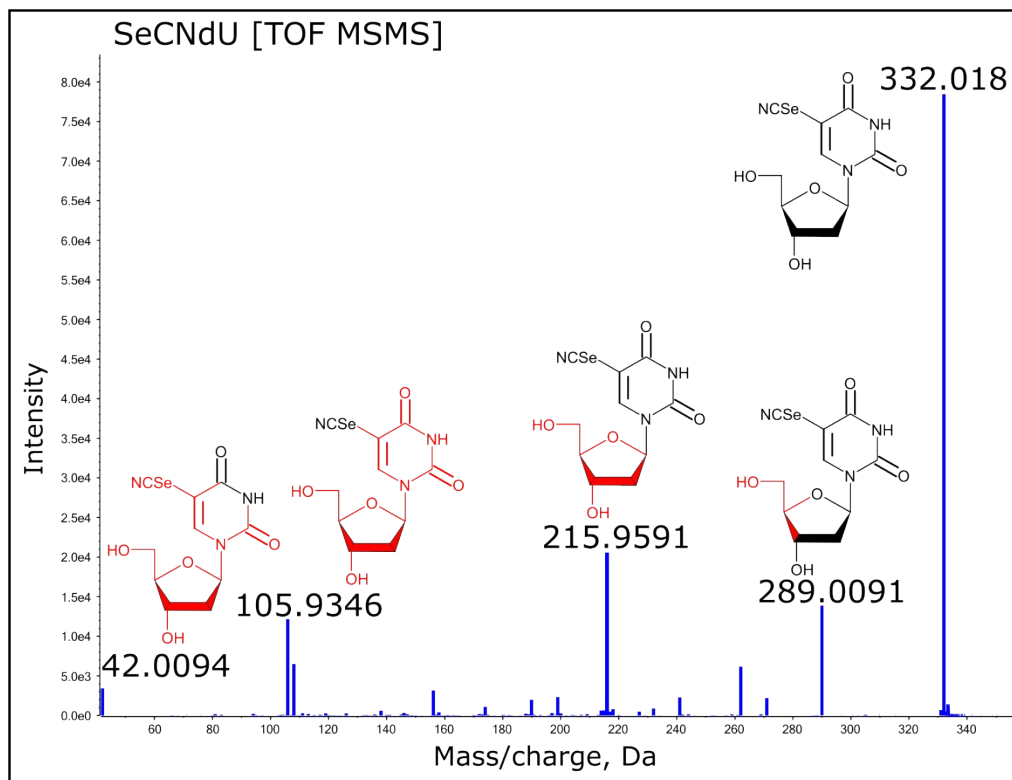


Fig. S1 MS/MS spectrum (in negative ionization mode) of SeCNdU and ion identities.

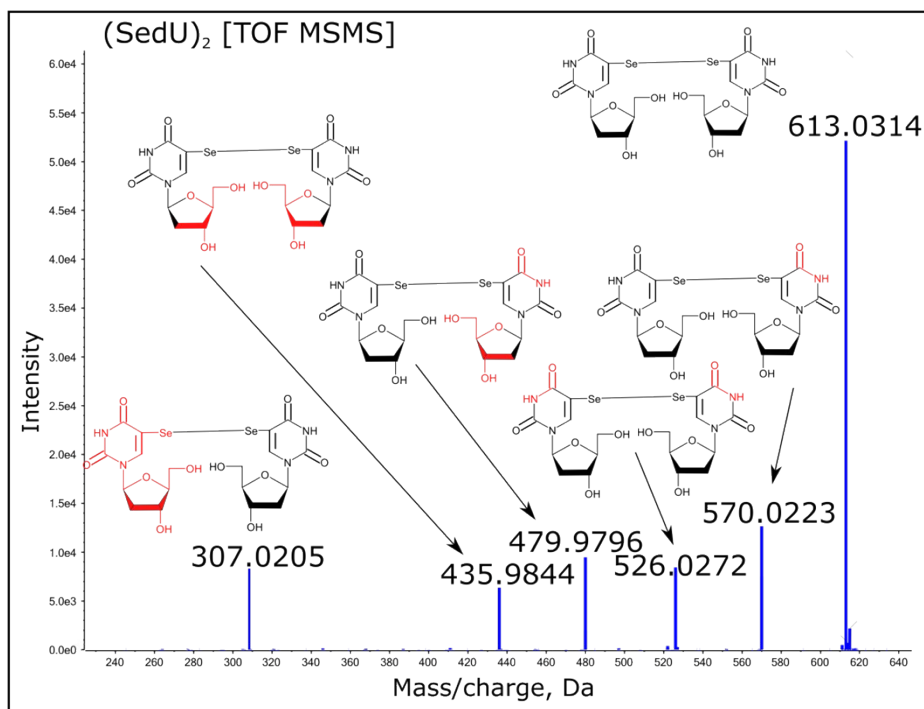


Fig. S2 MS/MS spectrum (in negative ionization mode) of dU-Se-Se-dU and ion identities.

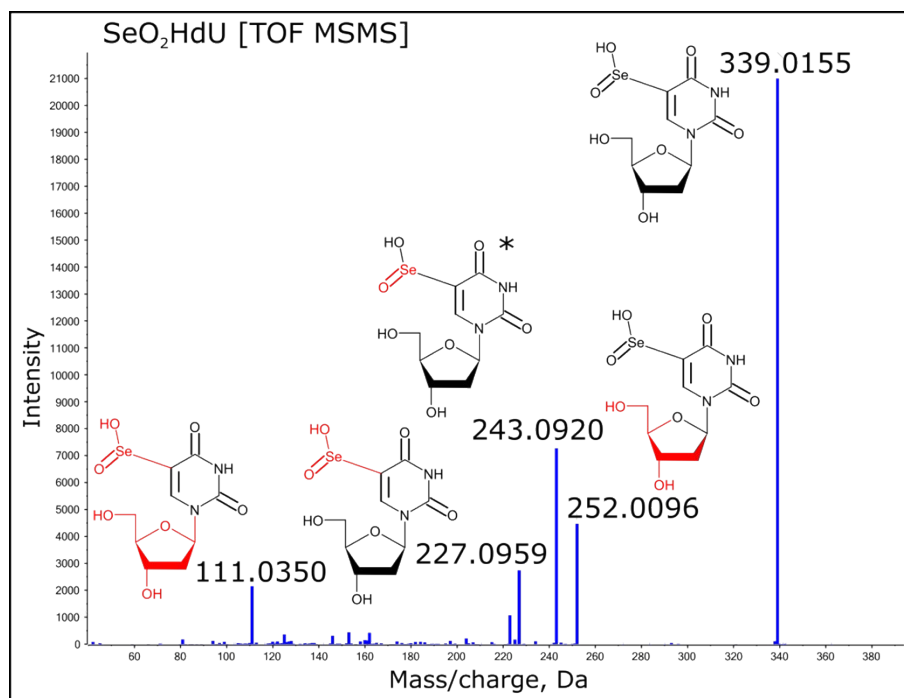


Fig. S3 MS/MS spectrum (in negative ionization mode) of SeO₂HdU and ion identities.

*This fragmentation may result from the possible [2,3]-sigmatropic rearrangement for α,β -unsaturated selenoorganic compounds [A. Nakamura and M. Nakada, *Synthesis*, 2013, **45**, 1421–1451].

Identification of radiolysis products for 5-trifluoromethanesulfonyl-2'-deoxyuridine (OTfdu)

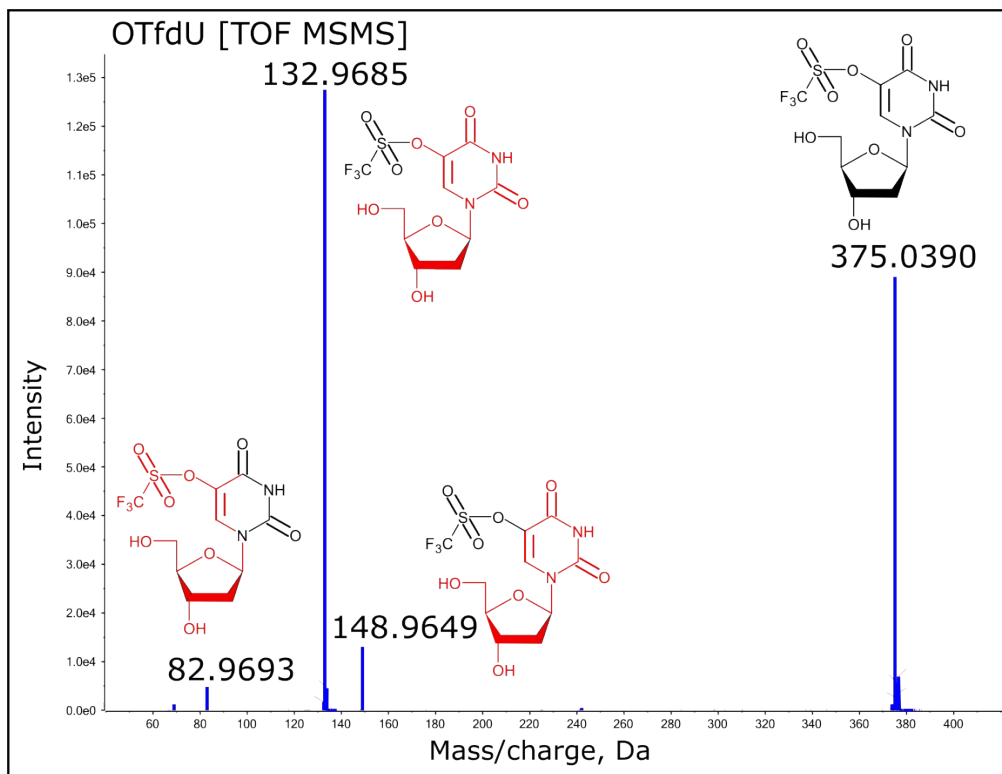


Fig. S4 MS/MS spectrum (in negative ionization mode) of OTfdu and ion identities.

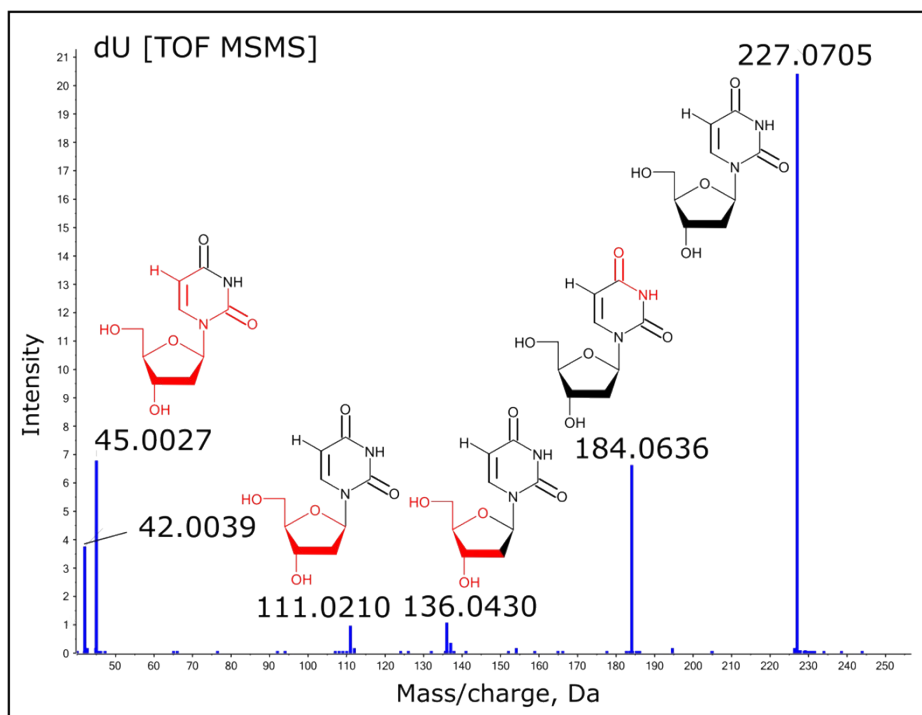


Fig. S5 MS/MS spectrum (in negative ionization mode) of dU and ion identities.

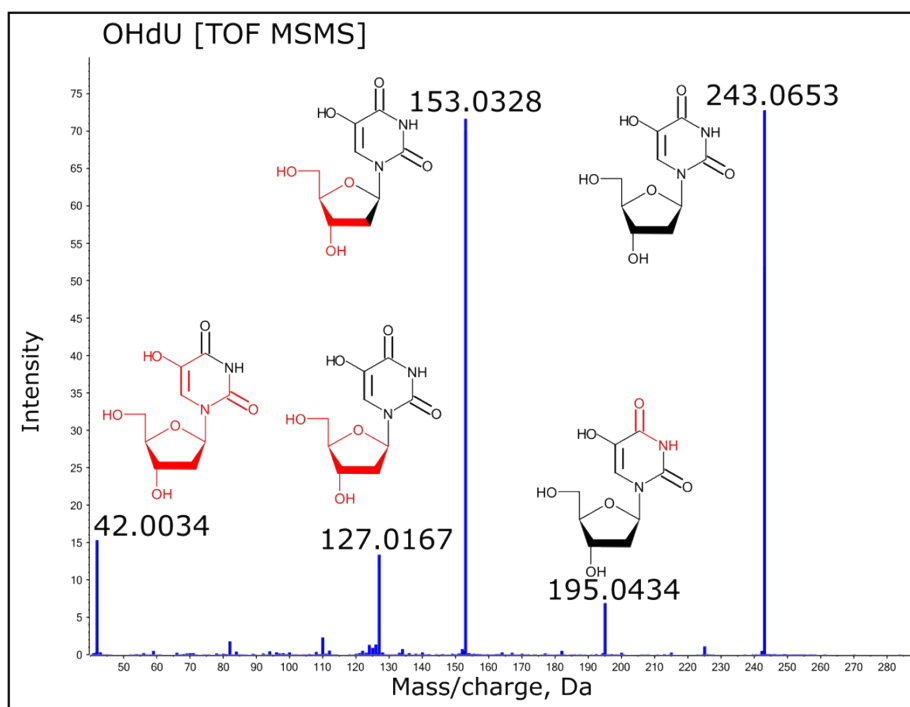


Fig. S6 MS/MS spectrum (in negative ionization mode) of OHdU and ion identities.

NMR spectra of synthesized analogs

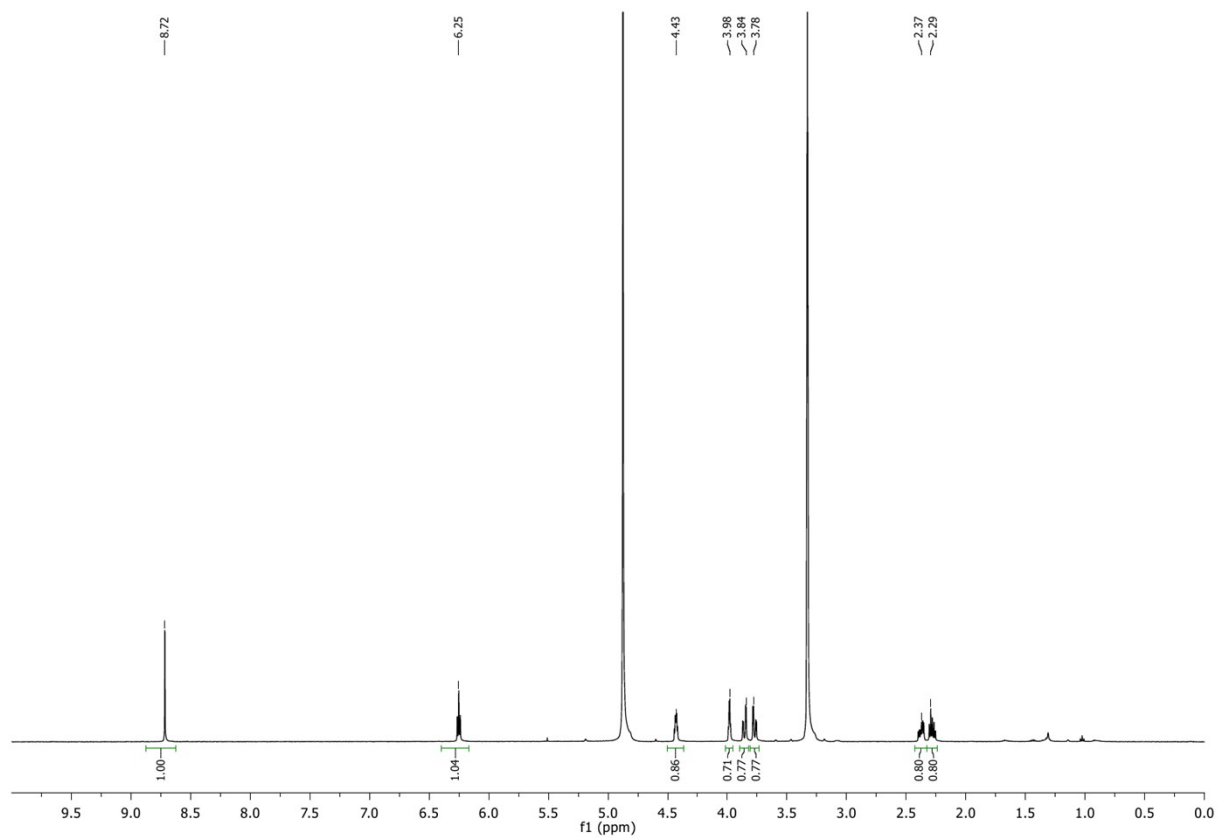


Fig. S7 ^1H NMR spectrum of SeCNdU.

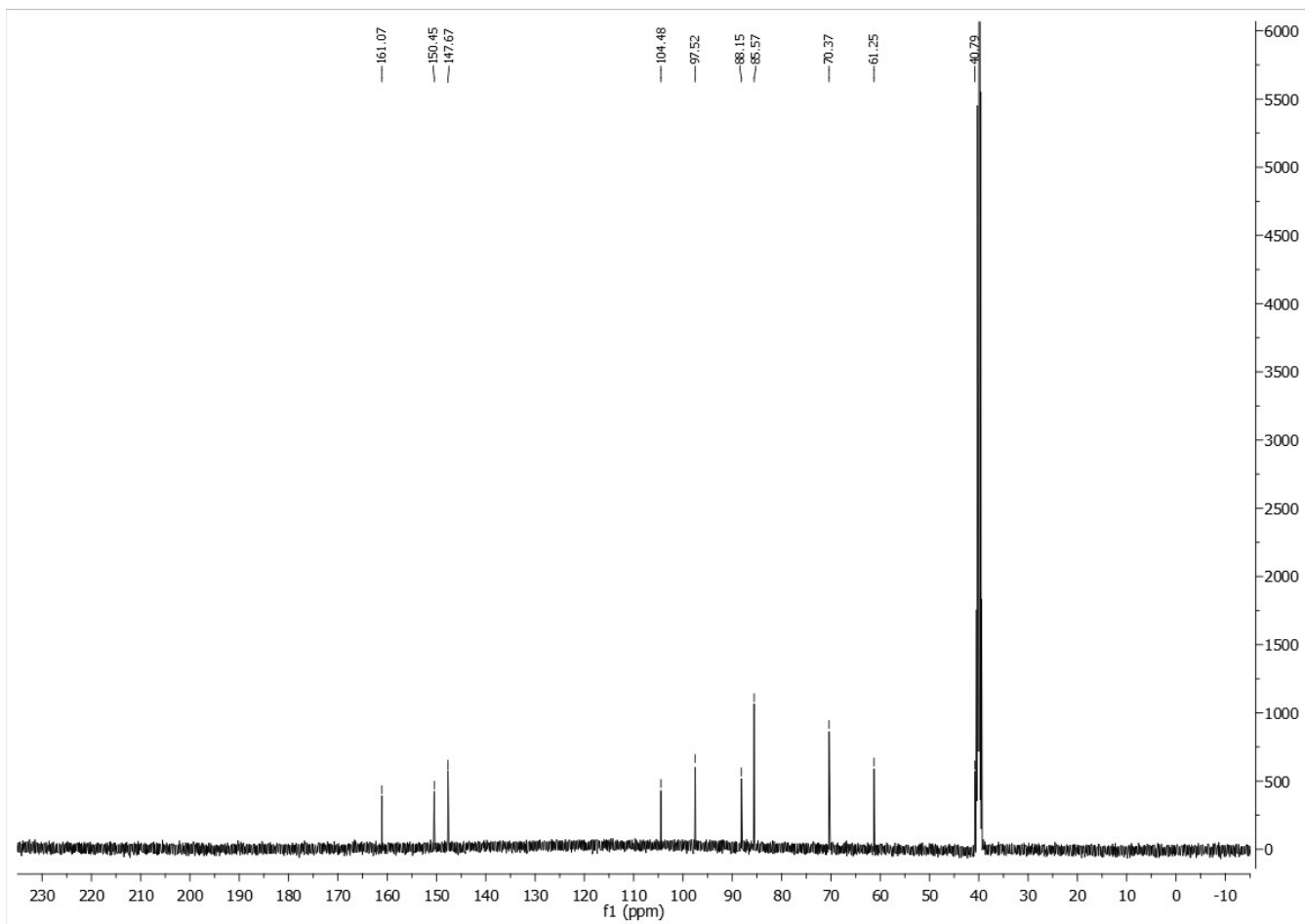


Fig. S8 ^{13}C NMR spectrum of SeCNdU.

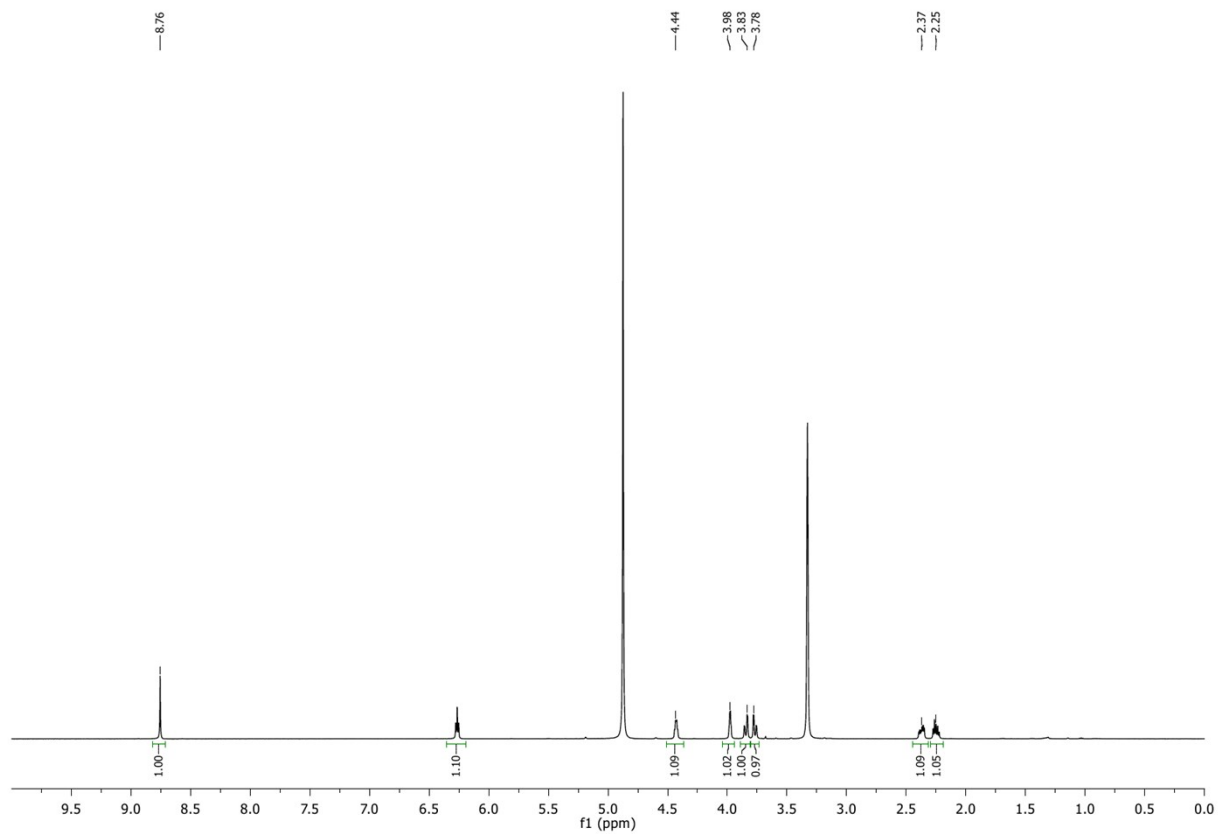


Fig. S9 ^1H NMR spectrum of OTfdU.

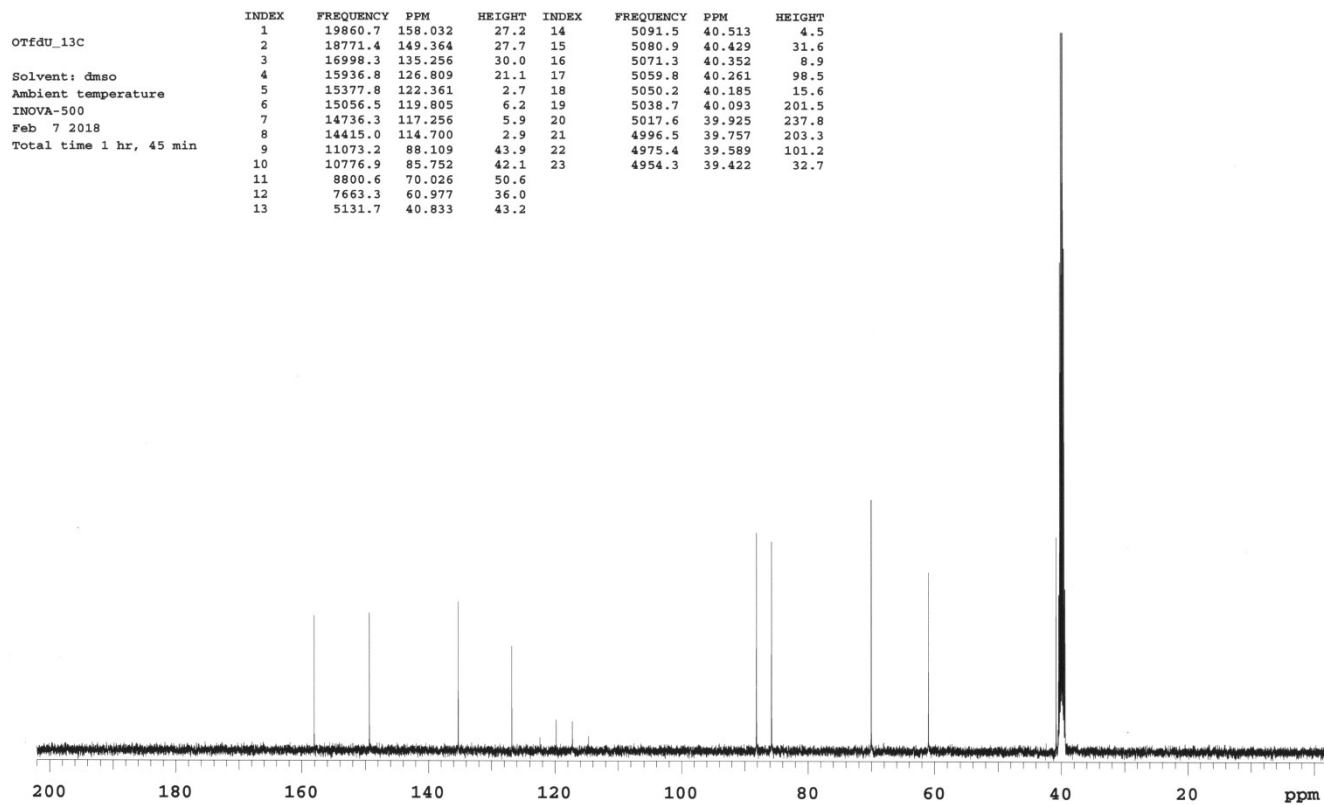


Fig. S10 ^{13}C NMR spectrum of OTfdU.

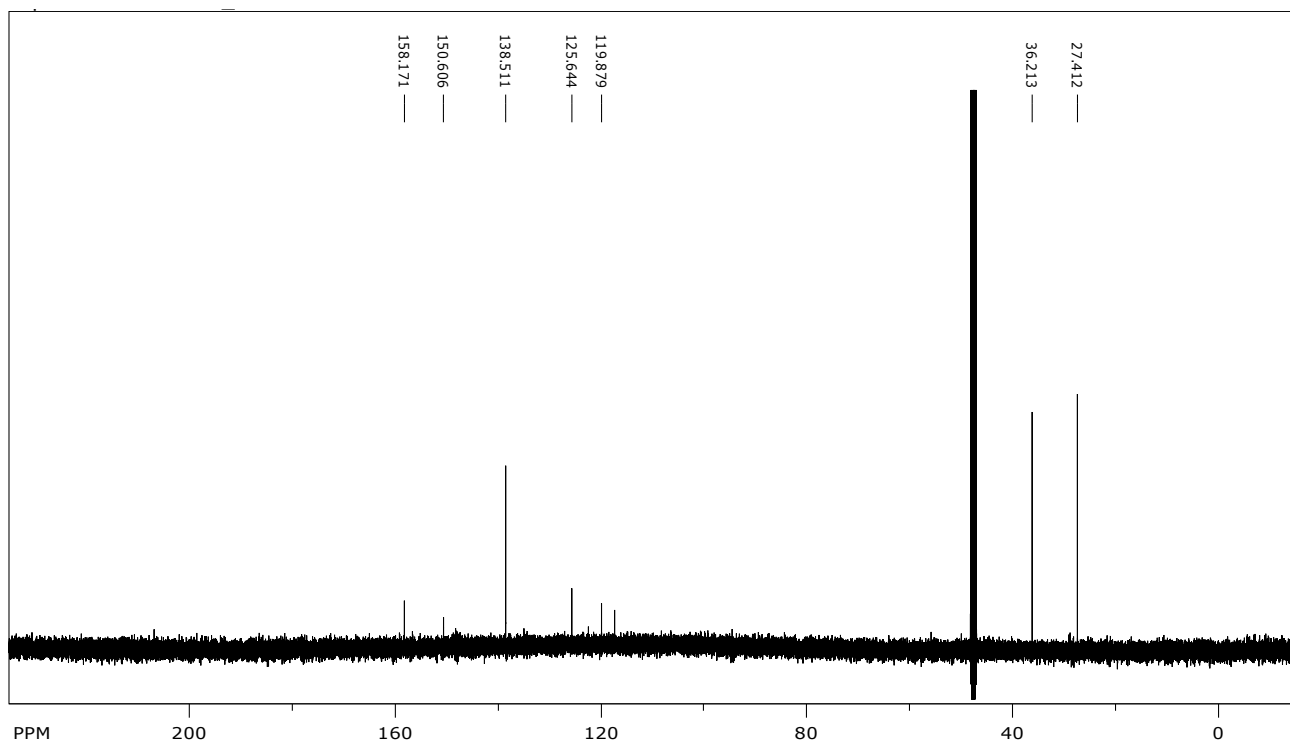


Fig. S11 ¹³C NMR spectrum of OTfDMU.

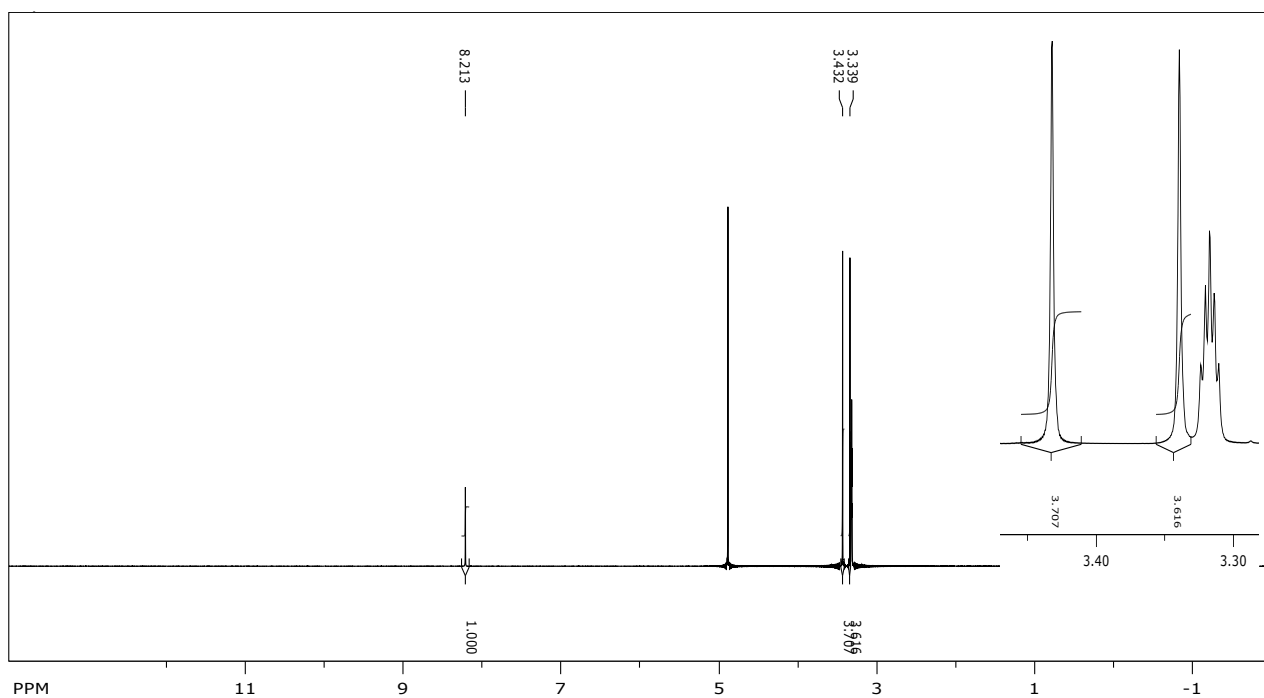


Fig. S12 ¹H NMR spectrum of OTfDMU.

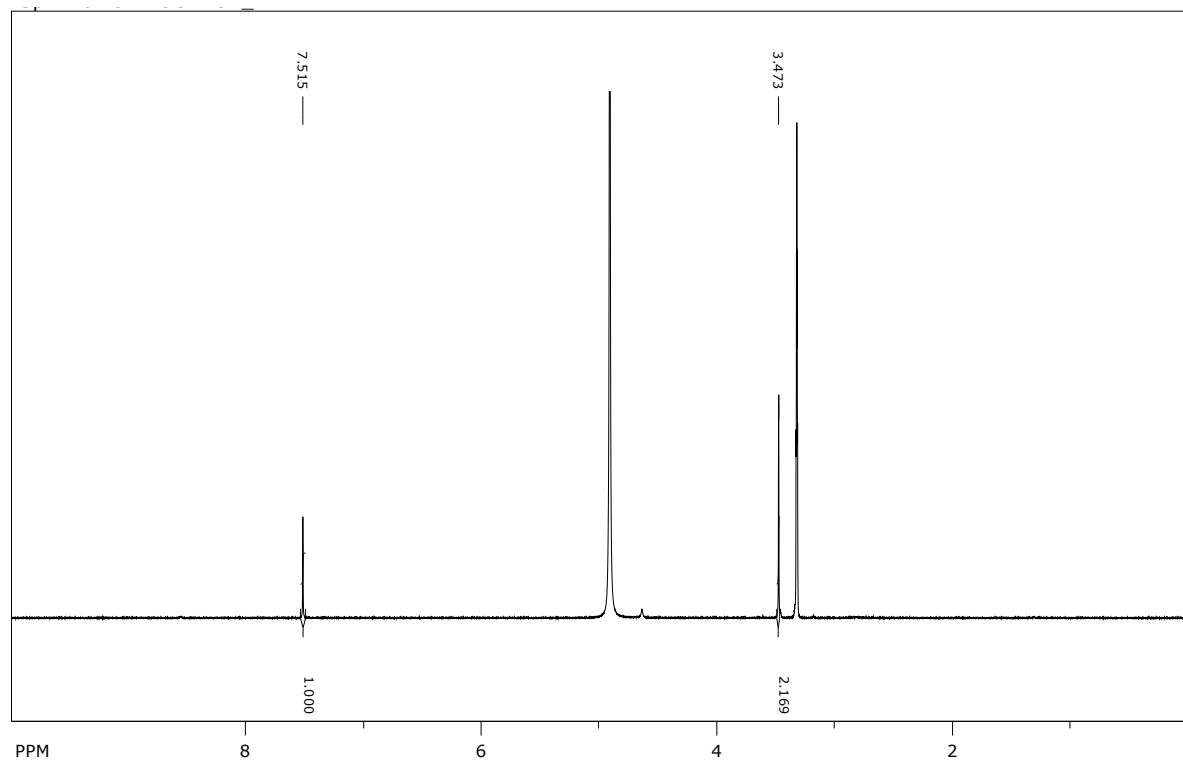


Fig. S13 ^1H NMR spectrum of CH_2CNU .

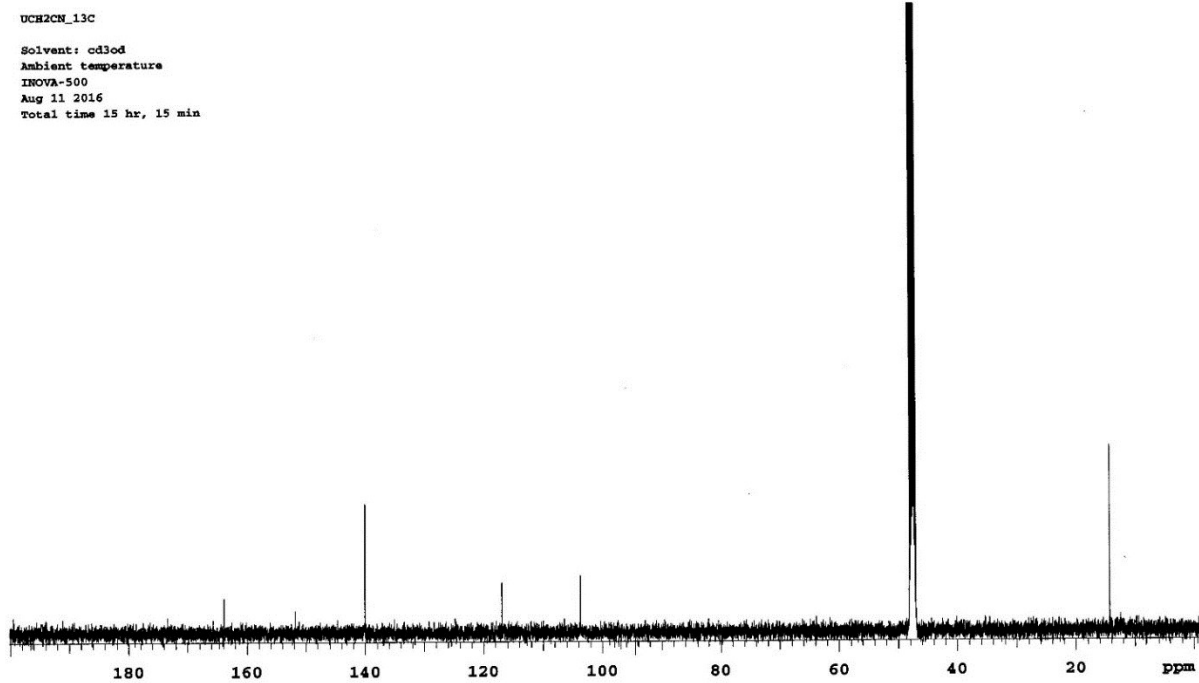


Fig. S14 ^{13}C NMR spectrum of CH_2CNU .