

SUPPLEMENTARY INFORMATION

(Thio)substituted-1,4-benzoquinones: Synthesis, Electrochemistry, DFT

Calculations and Potential Antiproliferative Effect Against

MDAMB- 231 Cells

Aysecik Kacmaz,^{a*} Elif Turker Acar,^b Gulden Atun,^b Zuhall Hamurcu^c

^a *Dr. A. Kacmaz*, Department of Chemistry, Division of Organic Chemistry, Istanbul University- Cerrappasa, Avcılar, Istanbul 34320, Turkey

^b *Dr. E. T. Acar, Prof. G. Atun*, Department of Chemistry, Division of Physical Chemistry, Istanbul University- Cerrahpasa, Avcılar, Istanbul 34320, Turkey

^c *Z. Hamurcu*, Department of Medical Biology, Faculty of Medicine, Erciyes University, Kayseri, Turkey

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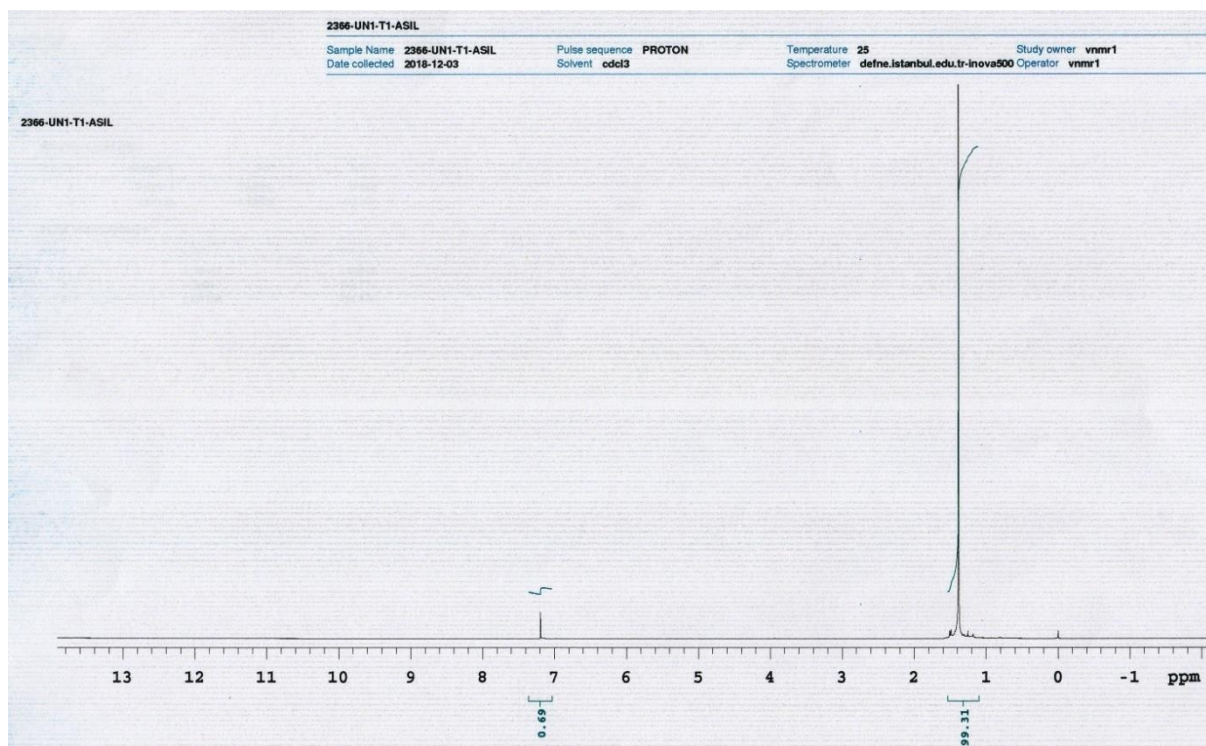


Figure S 1. The ^1H NMR spectrum of **5**

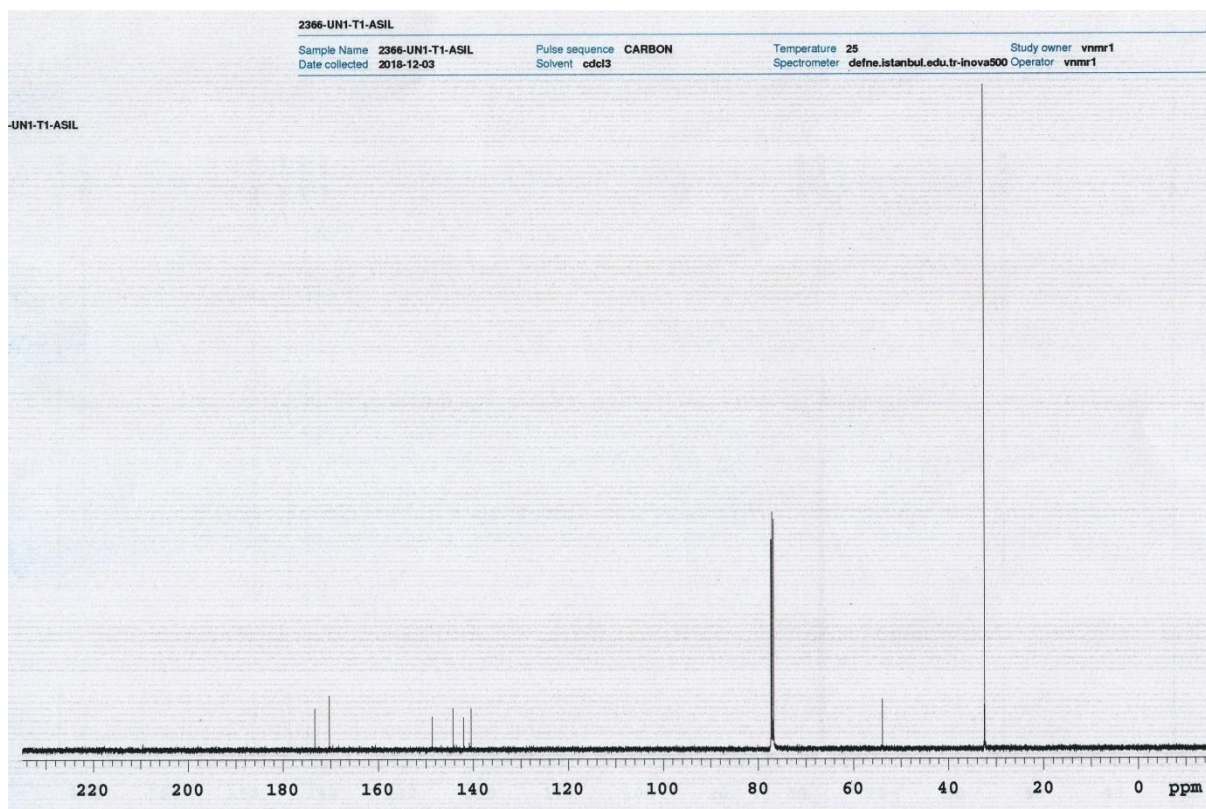


Figure S 2. The ^{13}C NMR spectrum of **5**

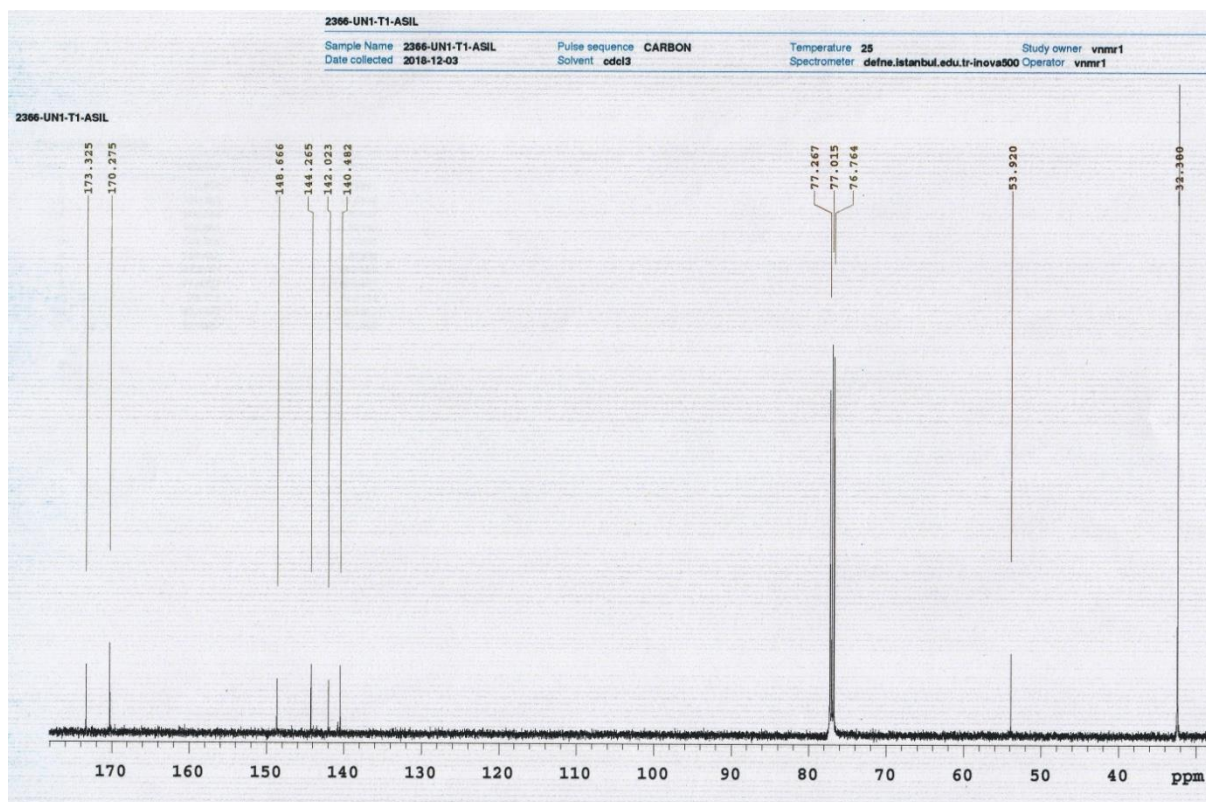


Figure S 3. The ^{13}C NMR spectrum of 5

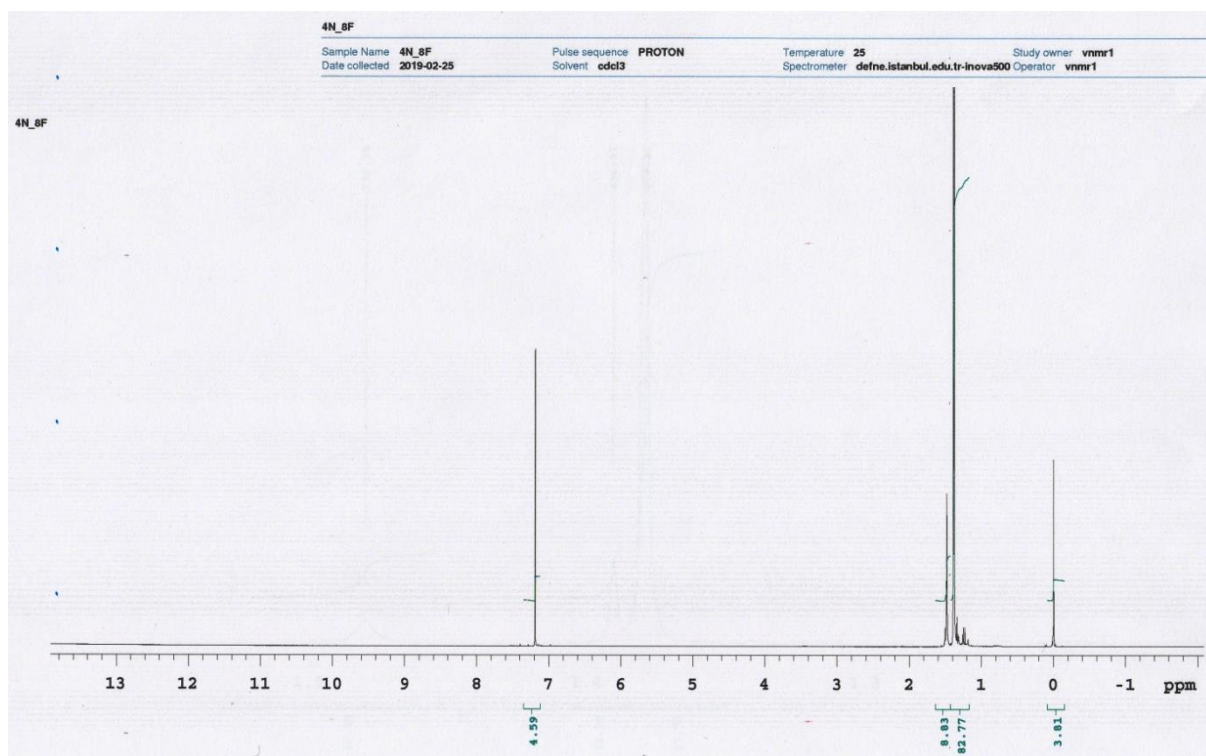


Figure S 4. The ^1H NMR spectrum of 6

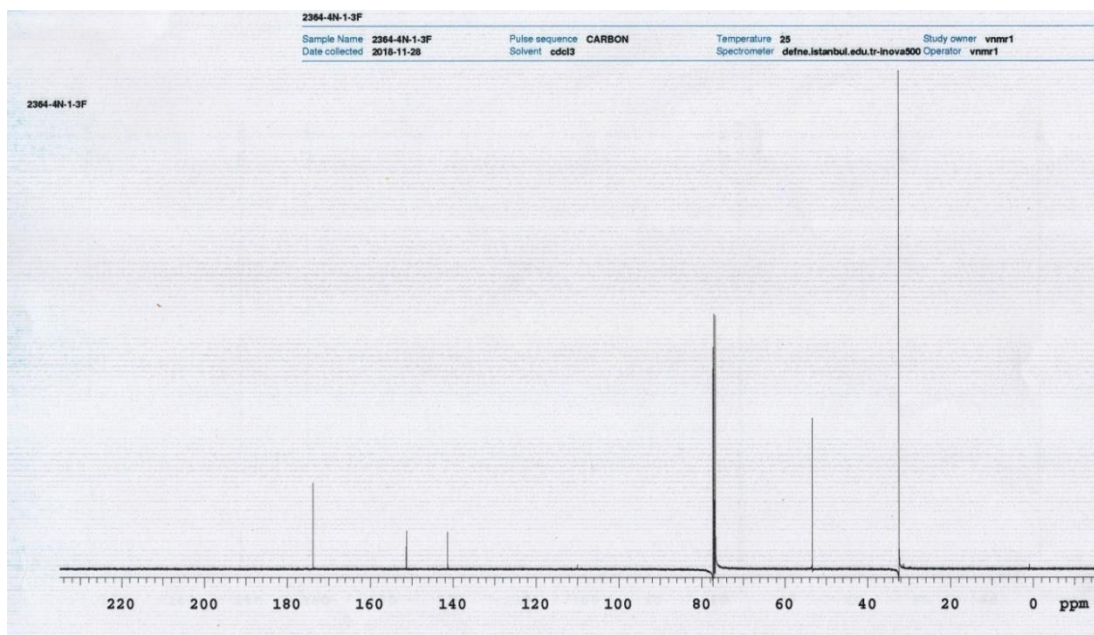


Figure S 5. The ¹³C NMR spectrum of 6

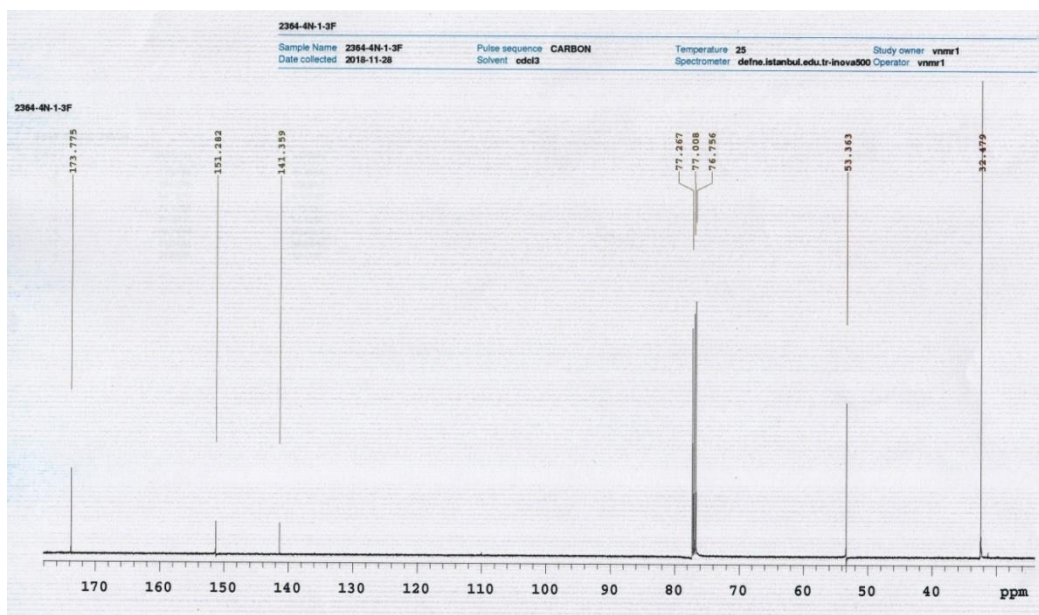


Figure S 6. The ¹³C NMR spectrum of 6

PROTON_01
2533_UN12F

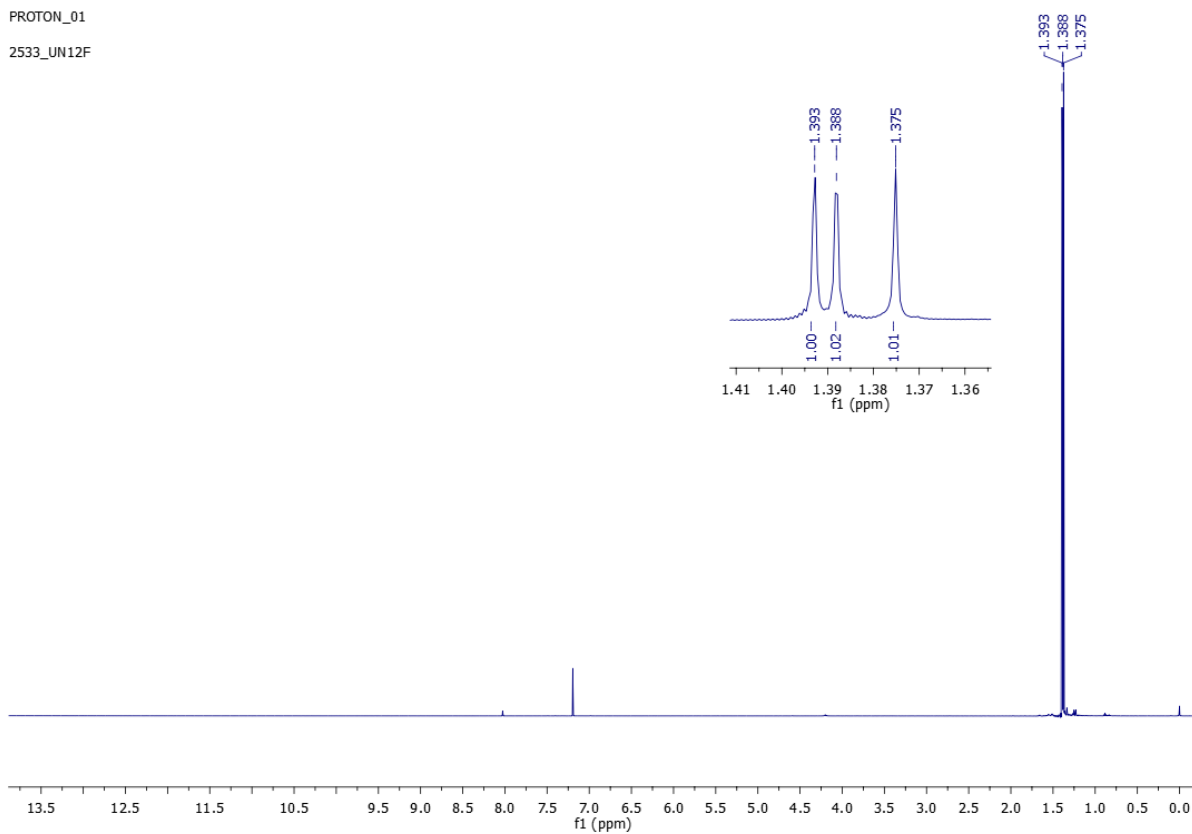


Figure S 7. The ^1H NMR spectrum of **7**

CARBON_01
2533_UN12F

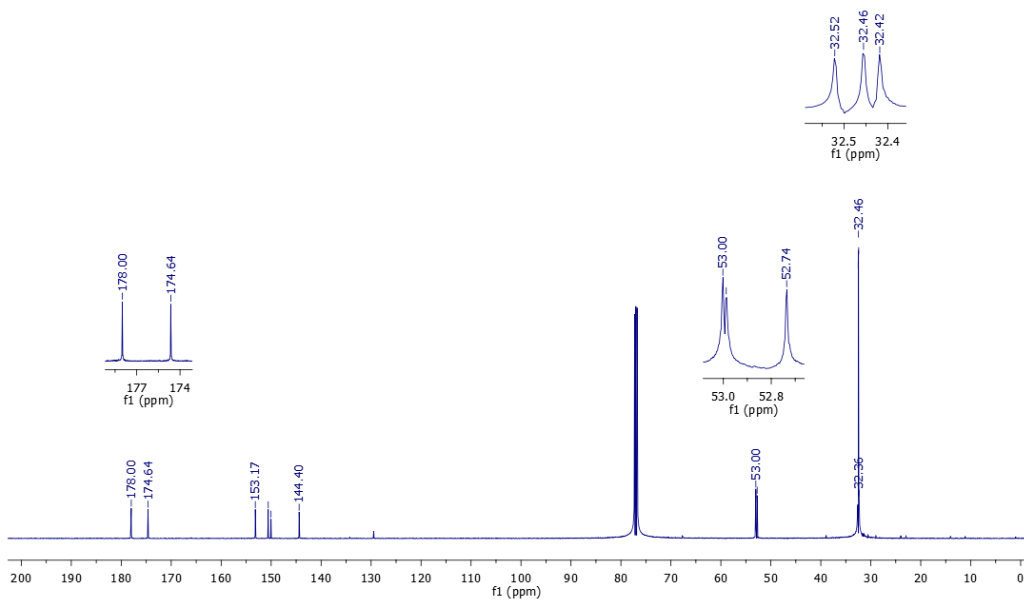


Figure S 8. The ^{13}C NMR spectrum of **7**

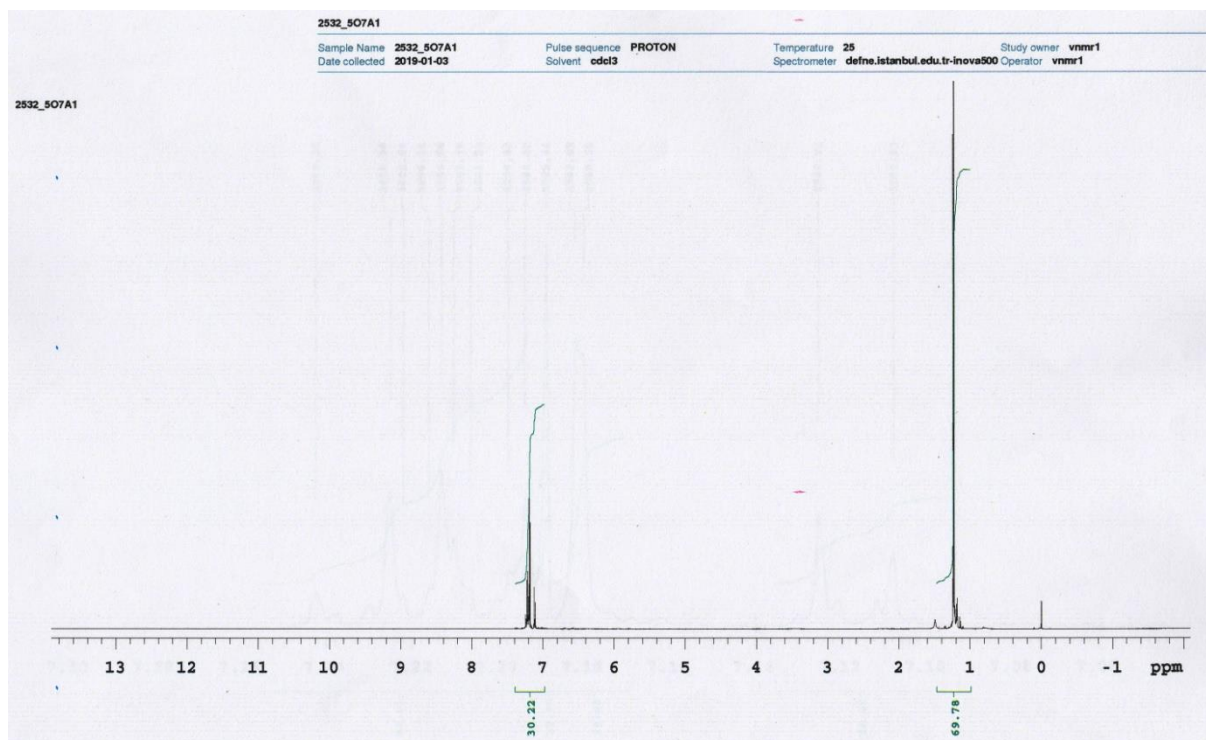


Figure S 9. The ^1H NMR spectrum of **8**

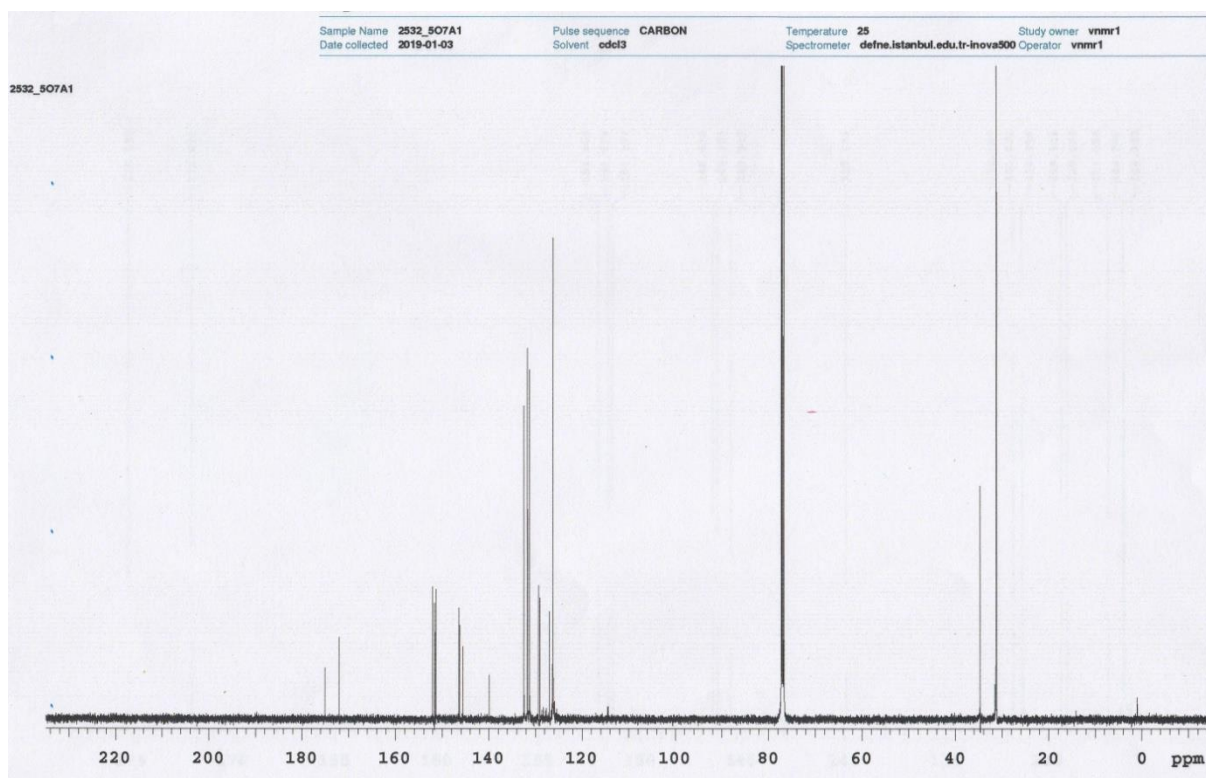


Figure S 10. The ^{13}C NMR spectrum of **8**

PROTON_01
TC_SP_A1

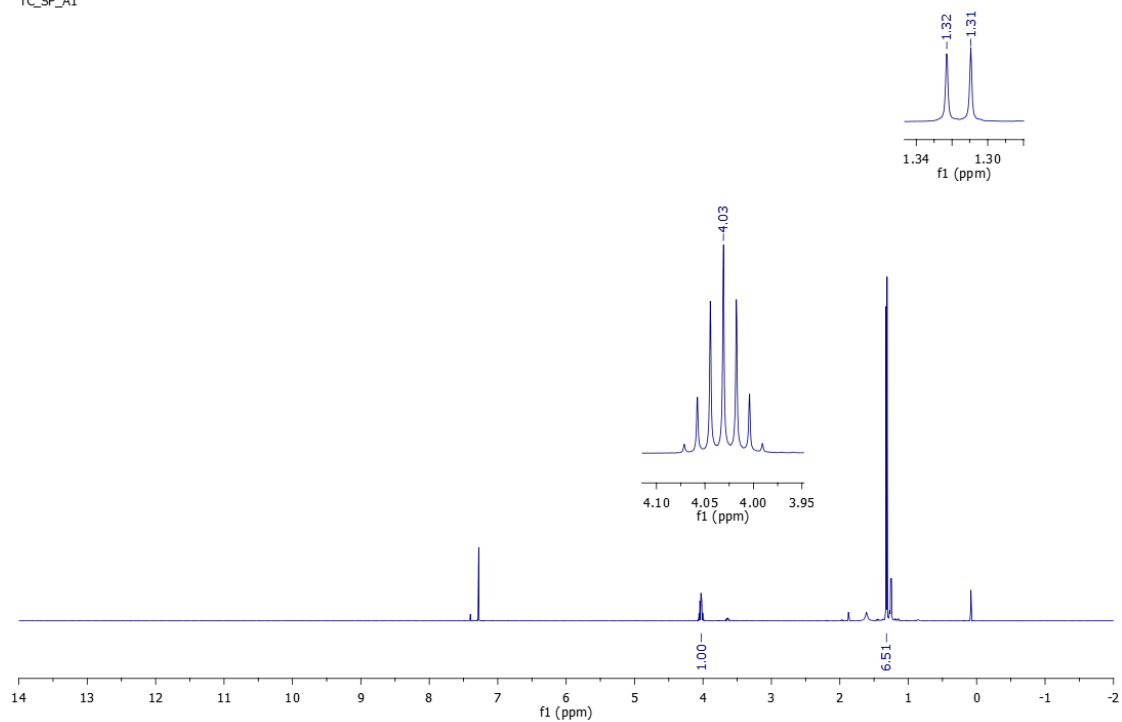


Figure S 11. The ^1H NMR spectrum of **9**

CARBON_01
TC_SP_A1

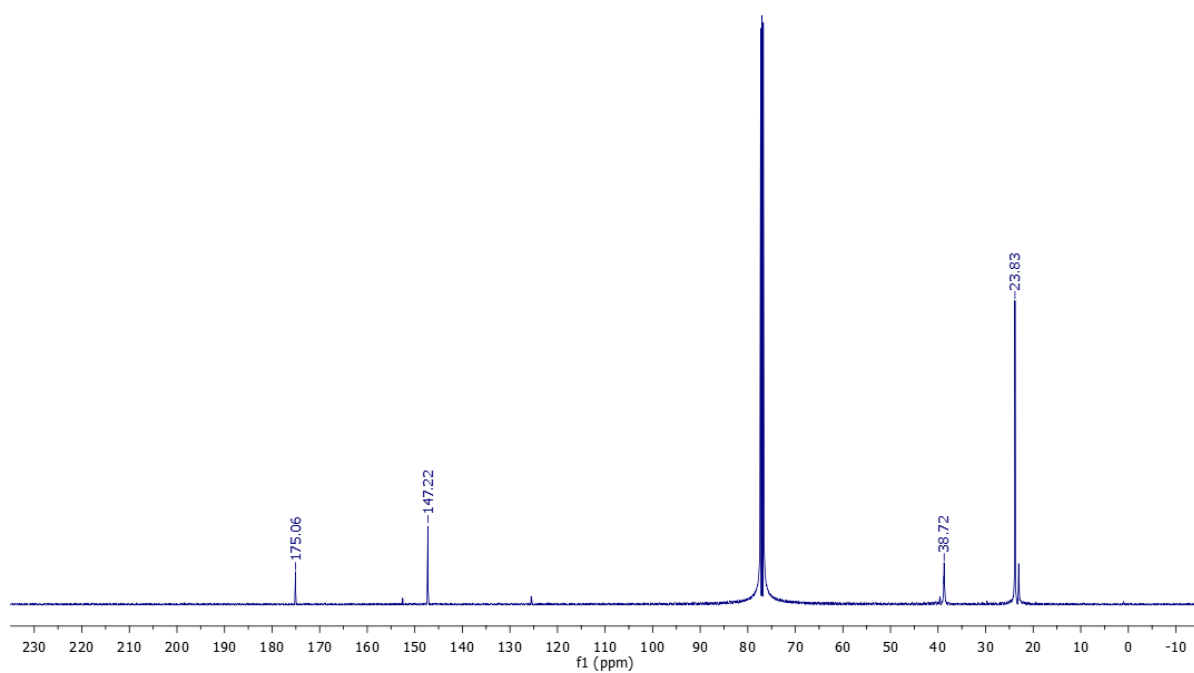


Figure S 12. The ^{13}C NMR spectrum of **9**

un-1-t1 #940-950 RT: 12.31-12.44 AV: 11 NL: 1.58E5
T: - c ESI Full ms [50.00-600.00]

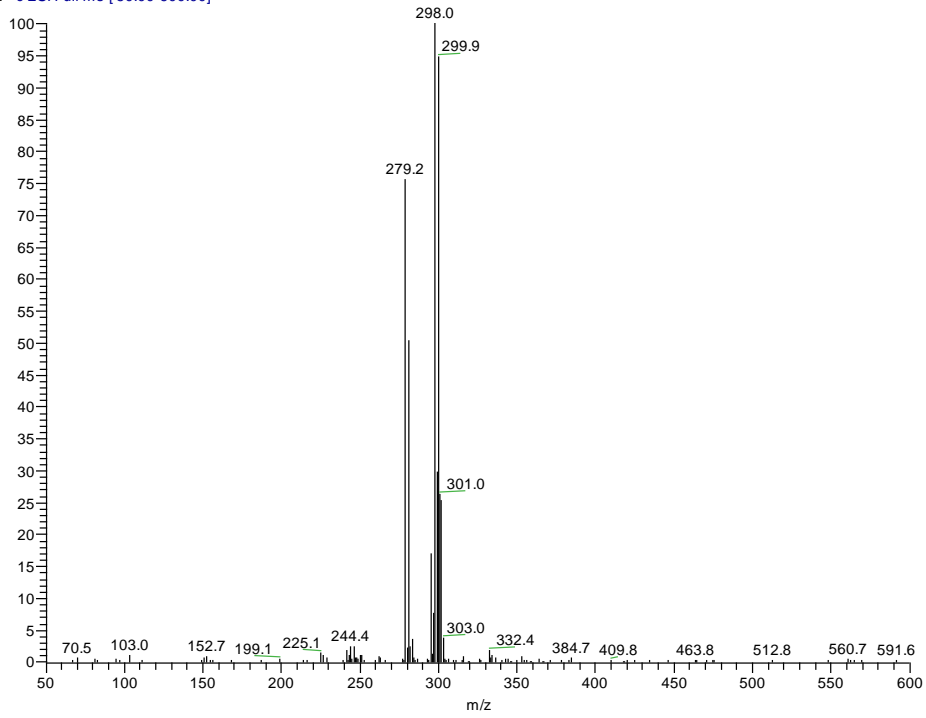


Figure S 13. Mass spectrum of 5

un-8-f#1635-1646 RT: 16.65-16.79 AV: 12 NL: 3.53E4
T: - c ESI Full ms [50.00-600.00]

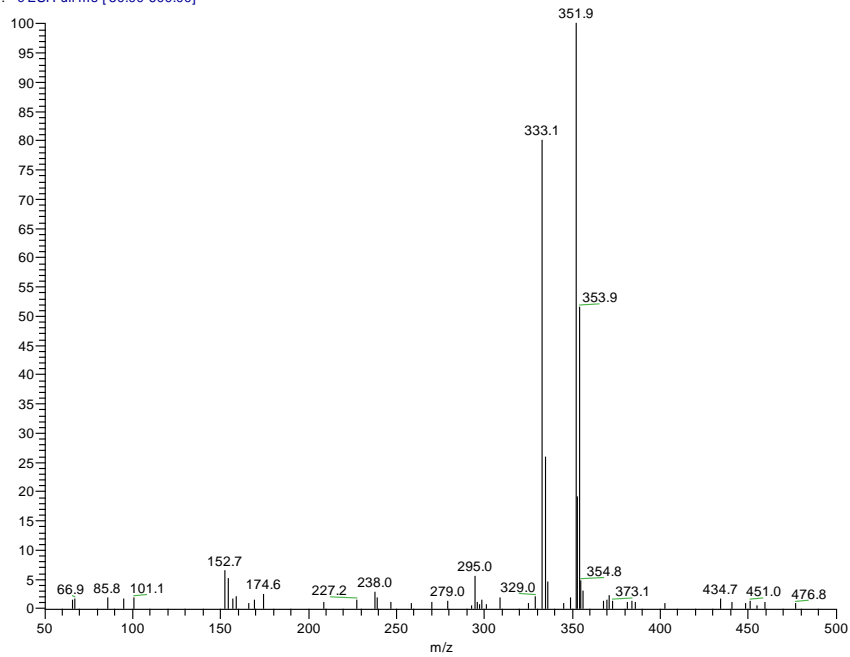


Figure S 14. Mass spectrum of 6

un-12f_190121080229 #1036-1041 RT: 13.95-14.01 AV: 6 NI: 3.07E7
T: + c ESI Full ms [50.00-800.00]

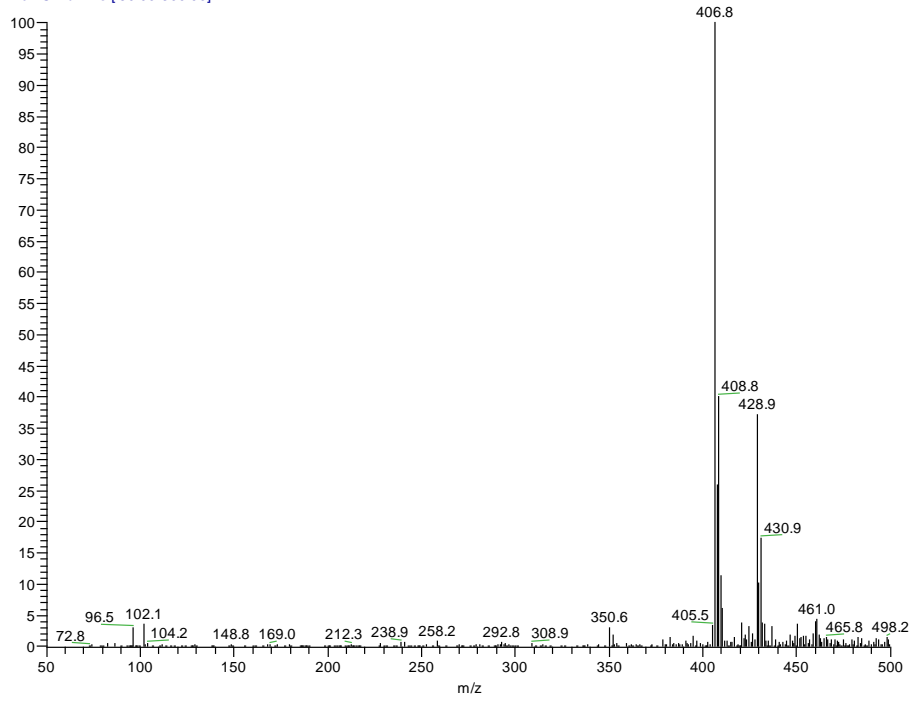


Figure S 15. Mass spectrum of 7

pca #372-373 RT: 4.97-4.99 AV: 2 NL: 9.93E4
T: - c ESI Full ms [50.00-2000.00]

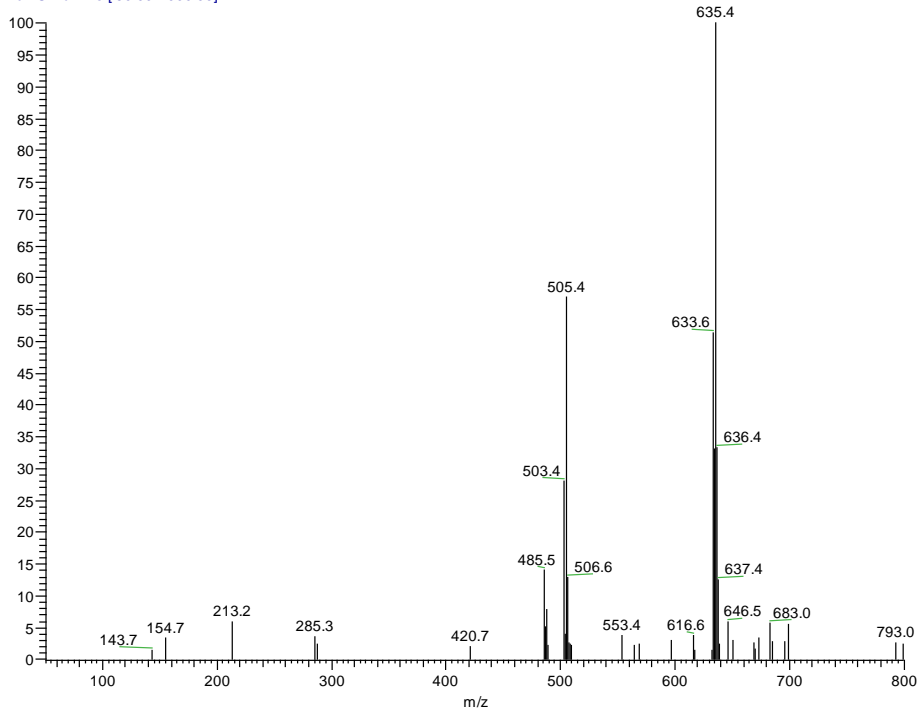


Figure S 16. Mass spectrum of 8

tc-sp_180817142641 #91 RT: 2.51 AV: 1 NL: 2.10E7
T: + c ESI Full ms [50.00-2000.00]

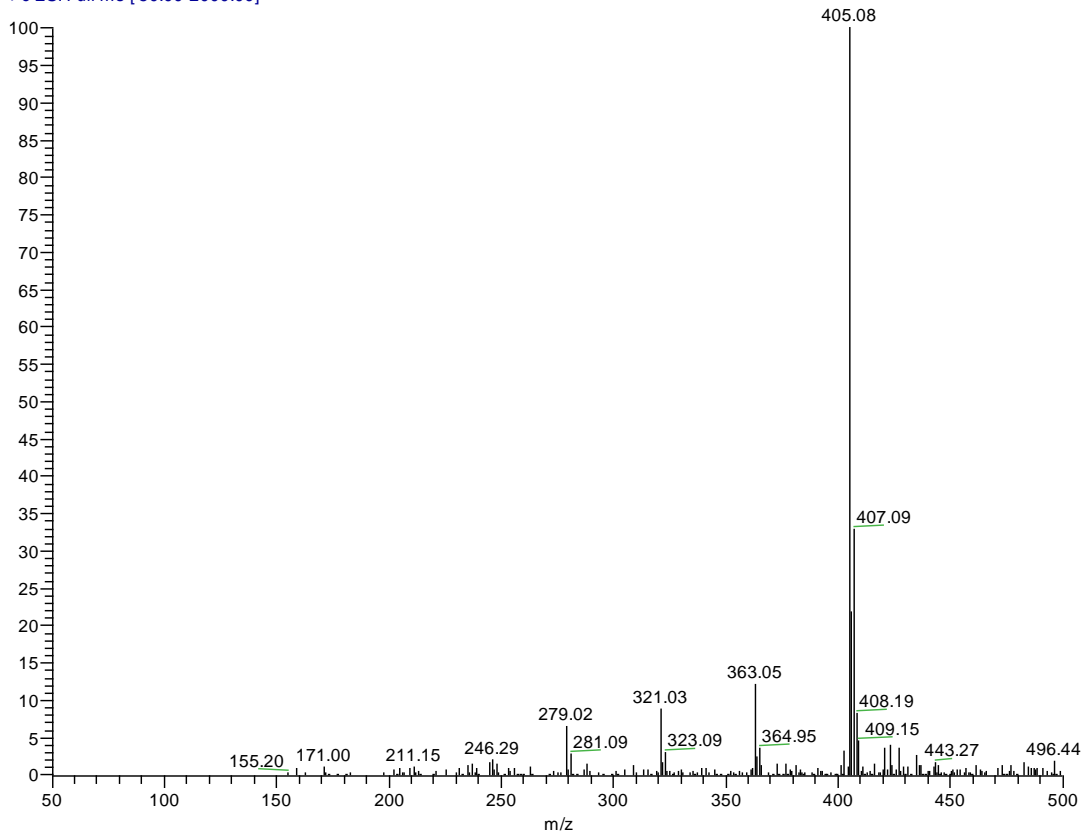


Figure S 17. Mass spectrum of 9