Synthesis of 3-aryl-3-(furan-2-yl)propanoic acid derivatives, and study of their antimicrobial activity

Mikhail V. Kalyaev,[a] Dmitry S. Ryabukhin,[a,b] Marina A. Borisova,[a] Alexander Yu. Ivanov,[c] Irina A. Boyarskaya,[d] Kristina E. Borovkova,[e] Lia R. Nikiforova,[e] Julia V. Salmova,[e] Nikolay V. Ul'yanovskii,[f] Dmitry S. Kosyakov,[f] Aleksander V. Vasilyev*[a,d]

[a]Department of Chemistry, Saint Petersburg State Forest Technical University, Institutsky per., 5, Saint Petersburg, 194021, Russia

[b]All-Russia Research Institute for Food Additives – Branch of V.M. Gorbatov Federal Research Center for Food Systems of RAS, Liteyniy pr., 55, Saint Petersburg, 191014, Russia

[c]Center for Magnetic Resonance, Research Park, Saint Petersburg State University, Universitetskiy pr., 26, Saint Petersburg, Petrodvoretz, 198504, Russia

[d]Department of Organic Chemistry, Institute of Chemistry, Saint Petersburg State University, Universitetskaya nab., 7/9, Saint Petersburg, 199034, Russia

[e]Research and manufacturing company «Home of Pharmacy», Zavodskaya st., 3-245, Kuzmolovskiy t.s., Leningrad oblast, 188663, Russia

[f]Core Facility Center "Arktika", Northern (Arctic) Federal University, nab. Severnoy Dviny, 17, Arkhangelsk, 163002, Russia.

*Corresponding author: A.V. Vasilyev; e-mails: *aleksvasil@mail.ru; a.vasilyev@spbu.ru*

Contents

1. ^{1}H and ^{13}C NMR spectra of compounds **1** and **2**……S2

2. Results of study of oligomeric compounds by liquid chromatography-high-resolution mass-spectrometry……S27

3. Study of biological activity of compounds **1** and **2**……S32

4. ^{1}H and ^{13}C NMR spectra of cations **Ae** and **Ah** in TfOH……S35

5. Data of DFT calculations of compounds **1** and species **A-C**……S38

1. ^{1}H and ^{13}C NMR spectra of compounds 1and 2

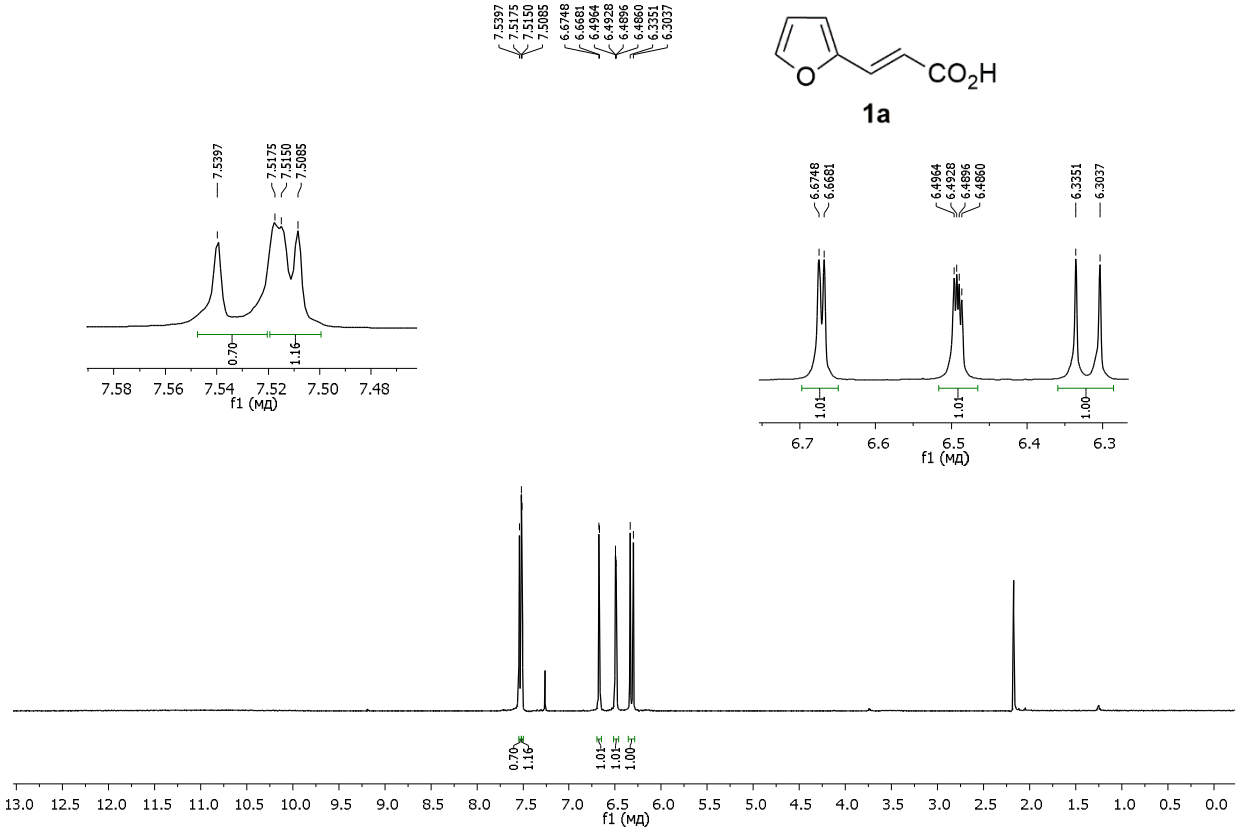


Figure S1. ^{1}H NMR spectrum of compound **1a** (500 MHz, $CDCl_3$).

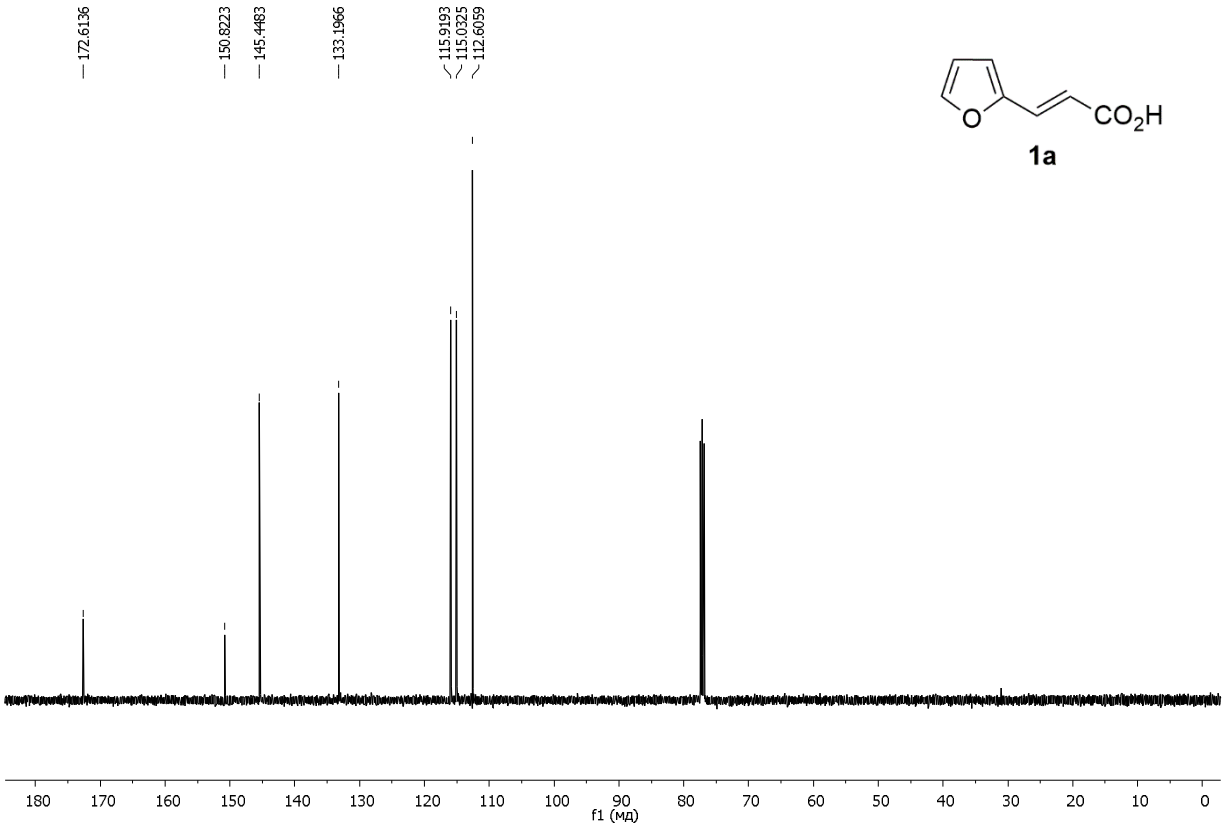


Figure S2. ^{13}C NMR spectrum of compound **1a** (125 MHz, $CDCl_3$).

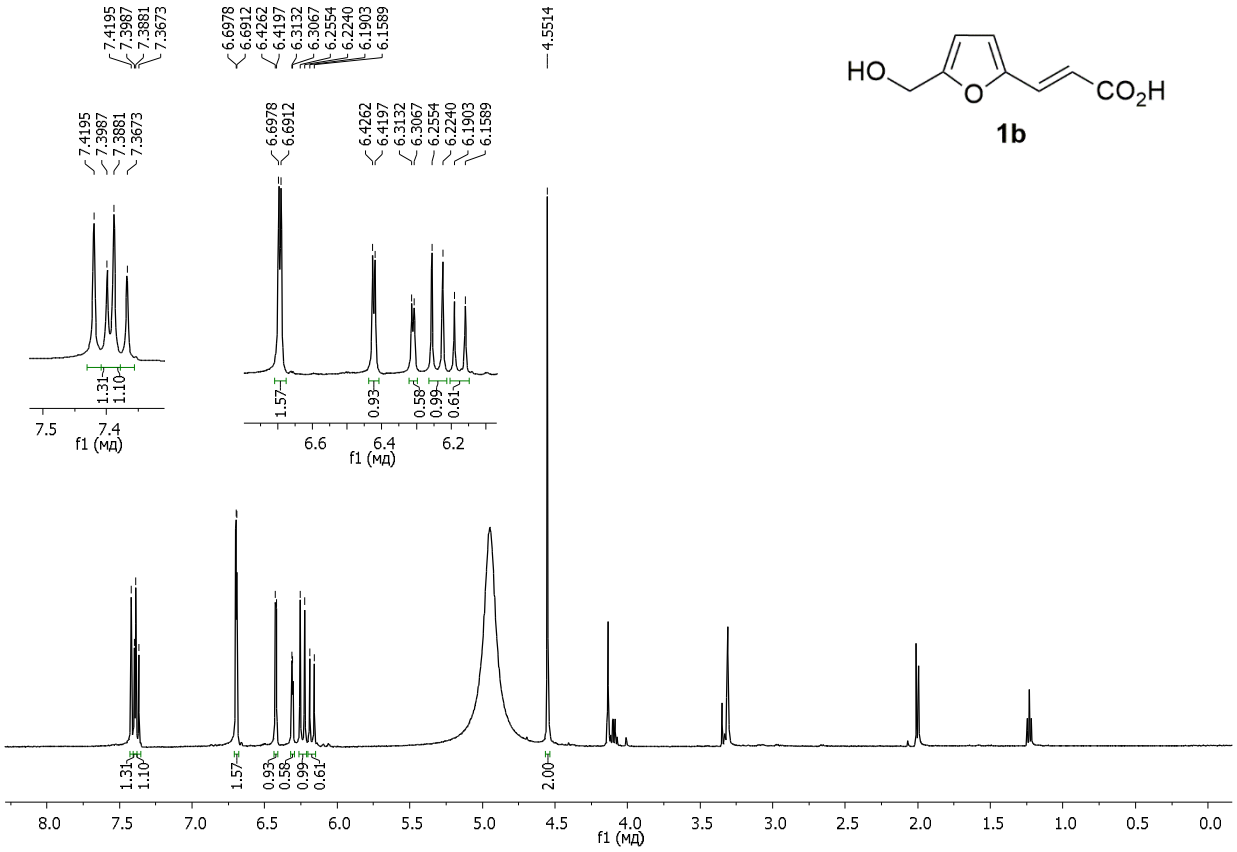


Figure S3. ^{1}H NMR spectrum of compounds E-/Z-**1b** (500 MHz, CD_3OD).

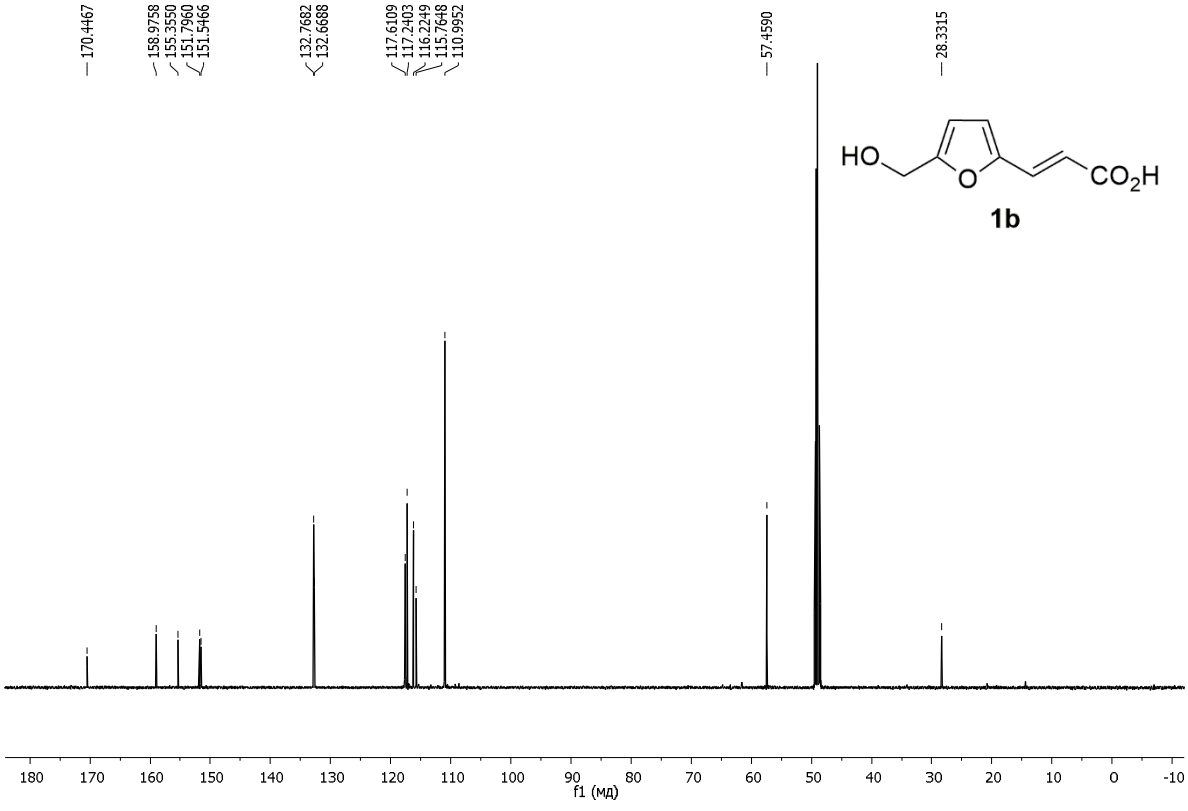


Figure S4. ^{13}C NMR spectrum of compounds E-/Z-**1b** (125 MHz, CD_3OD).

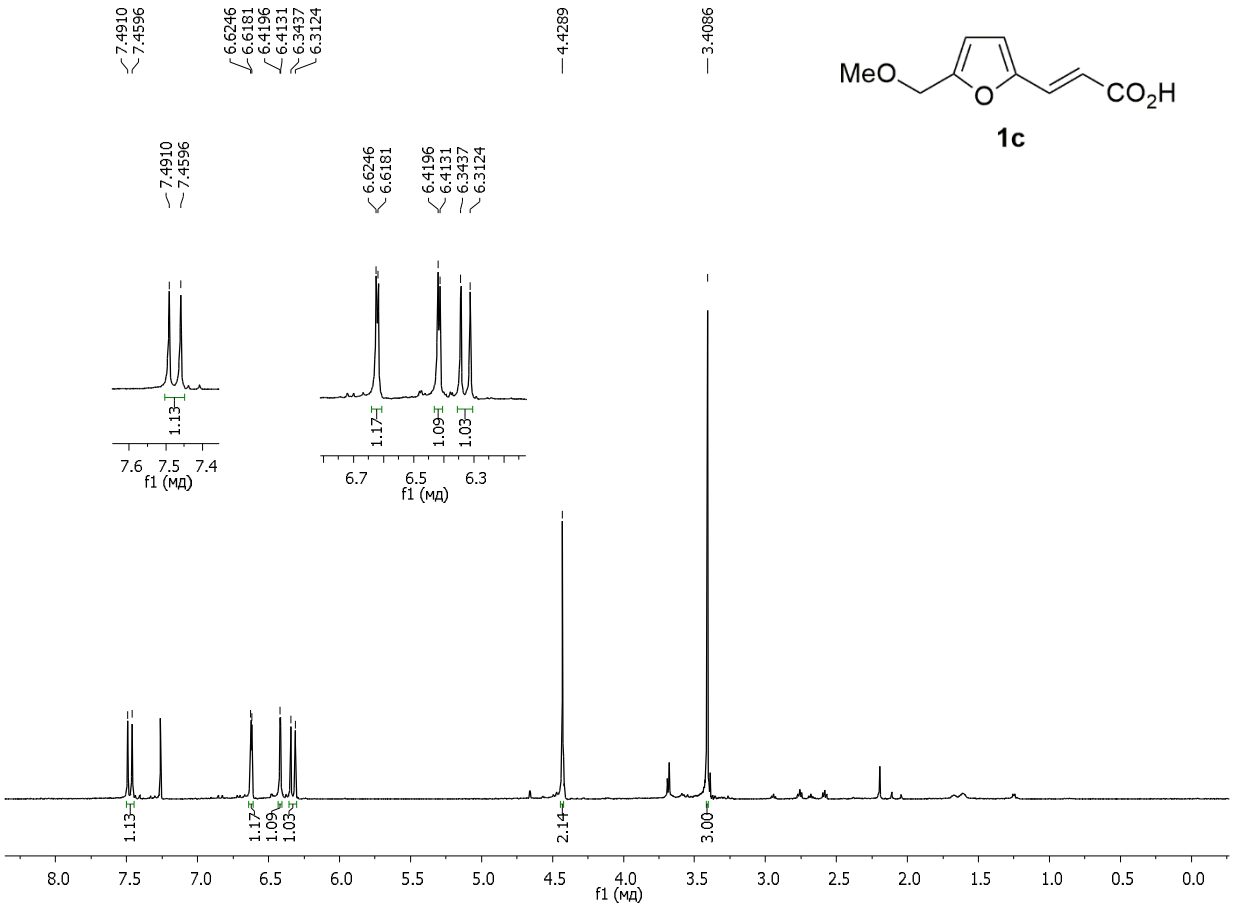


Figure S5. ^{1}H NMR spectrum of compound **1c** (500 MHz, $CDCl_3$).

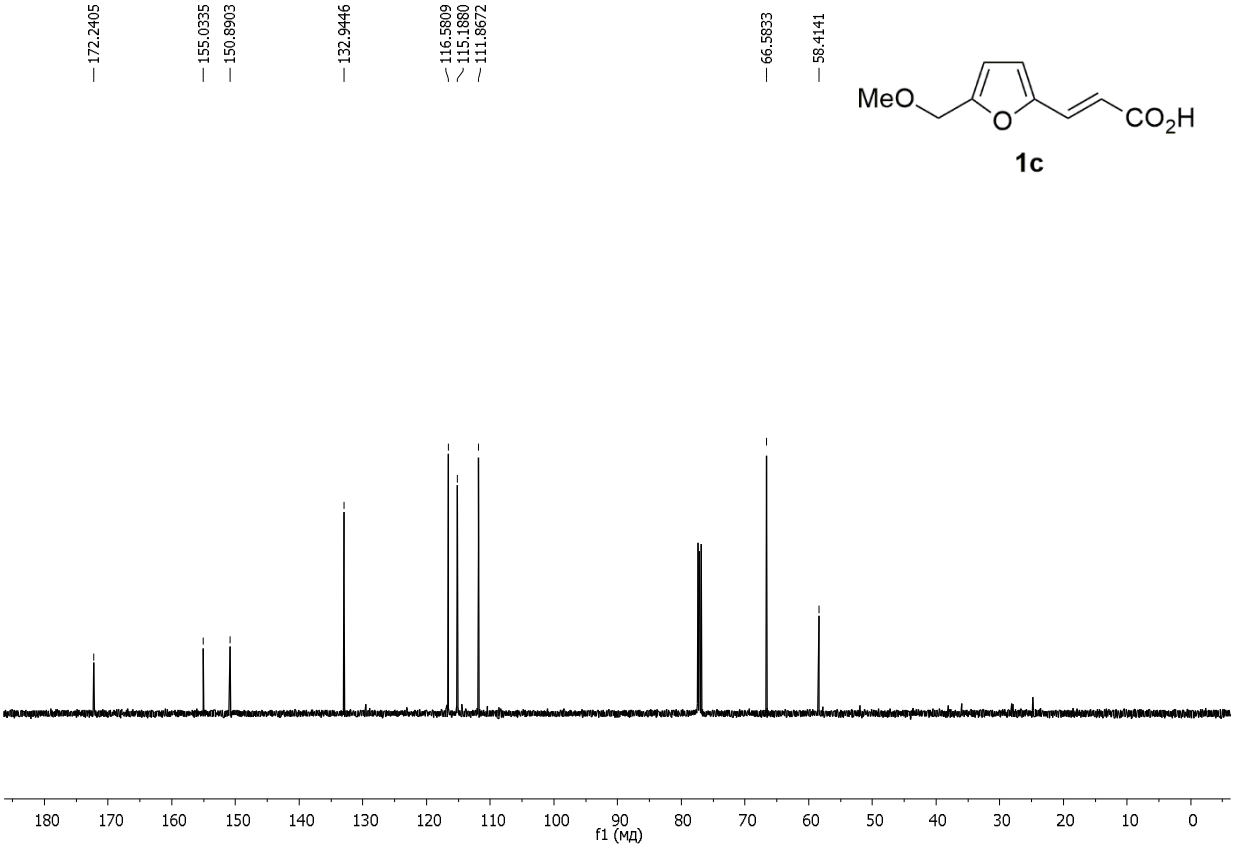


Figure S6. ^{13}C NMR spectrum of compound **1c** (125 MHz, $CDCl_3$).

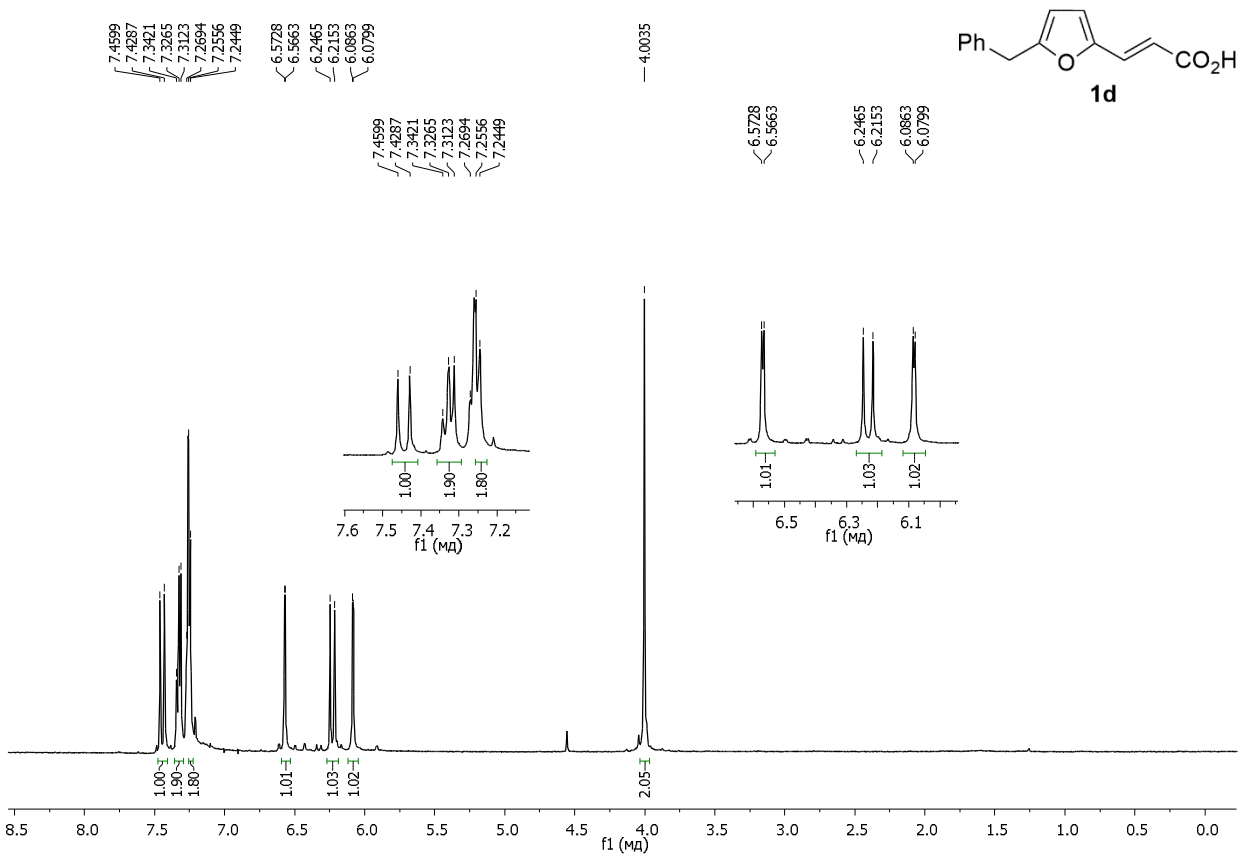


Figure S7. ^{1}H NMR spectrum of compound **1d** (500 MHz, $CDCl_3$).

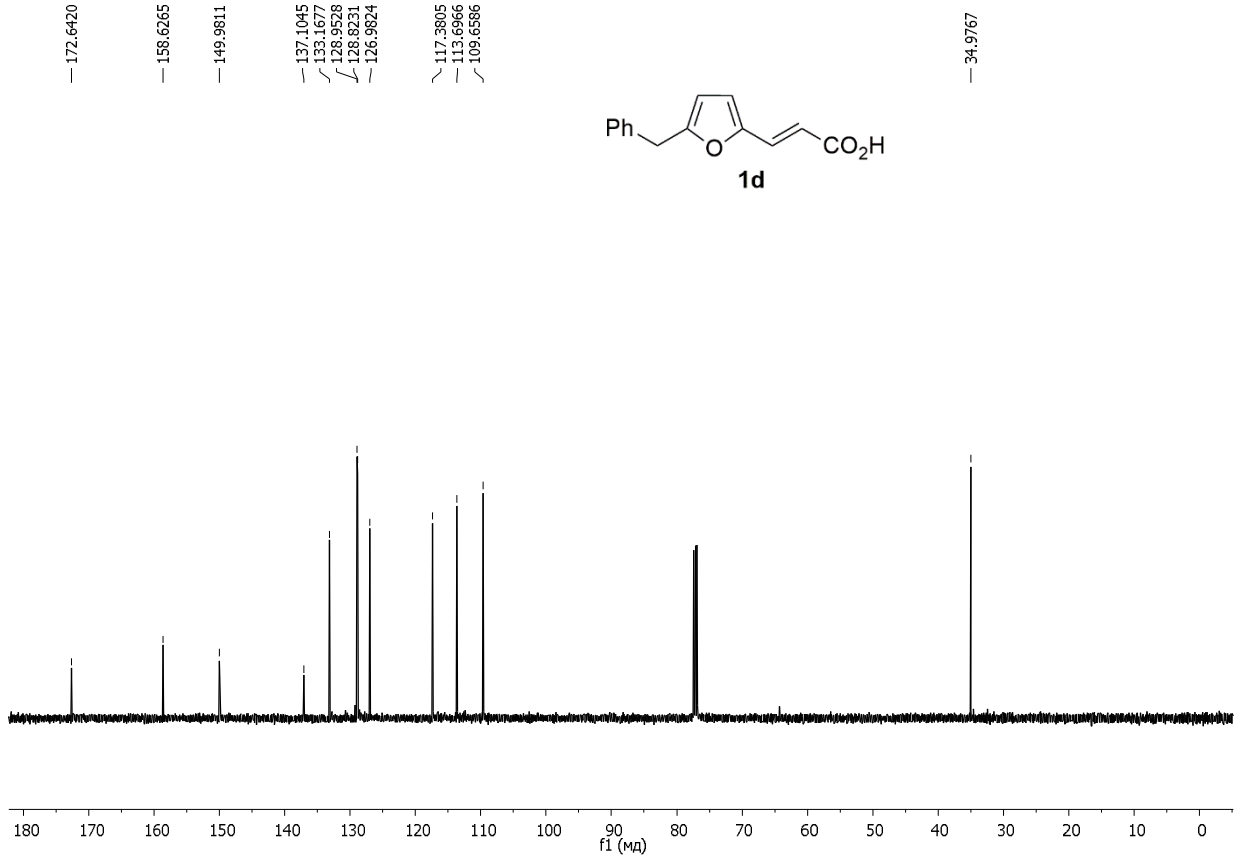


Figure S8. ^{13}C NMR spectrum of compound **1d** (125 MHz, $CDCl_3$).

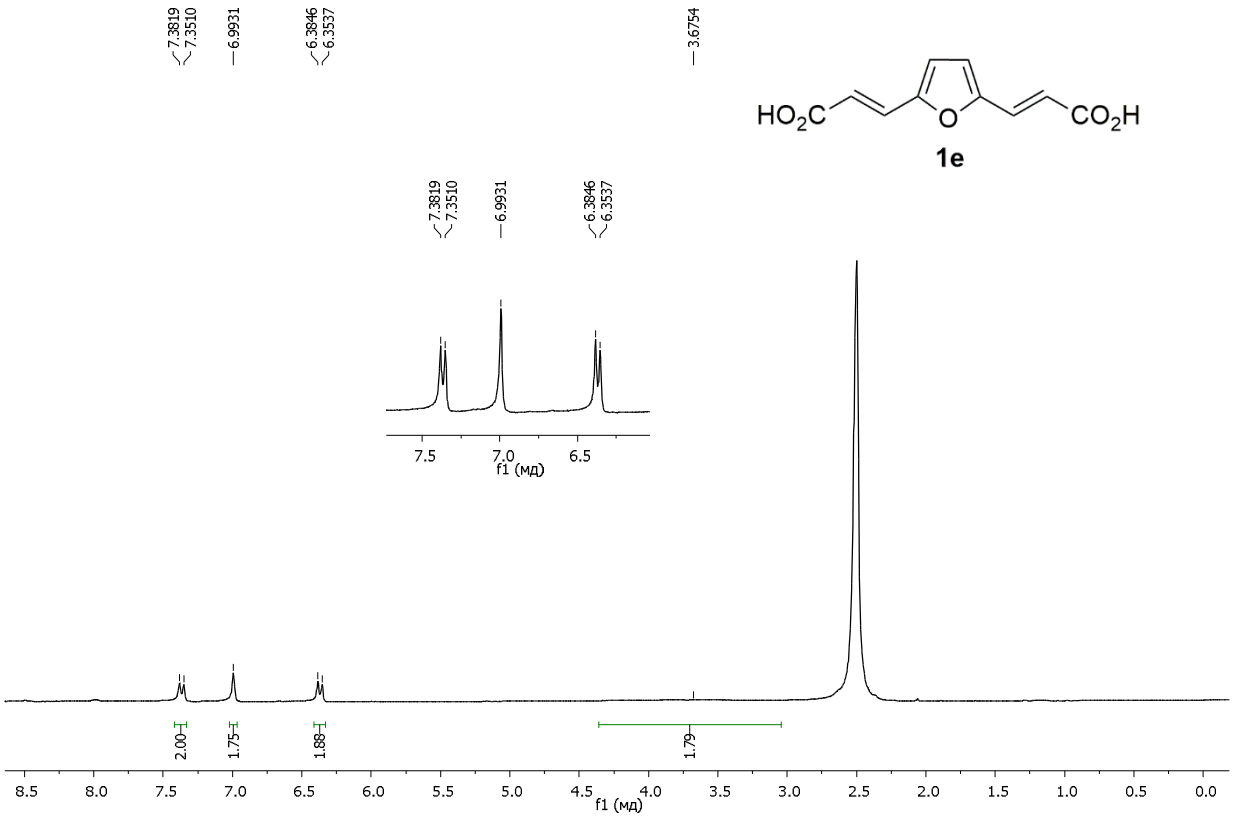


Figure S9. ^{1}H NMR spectrum of compound **1e** (500 Hz, $(CD_3)_2SO$)

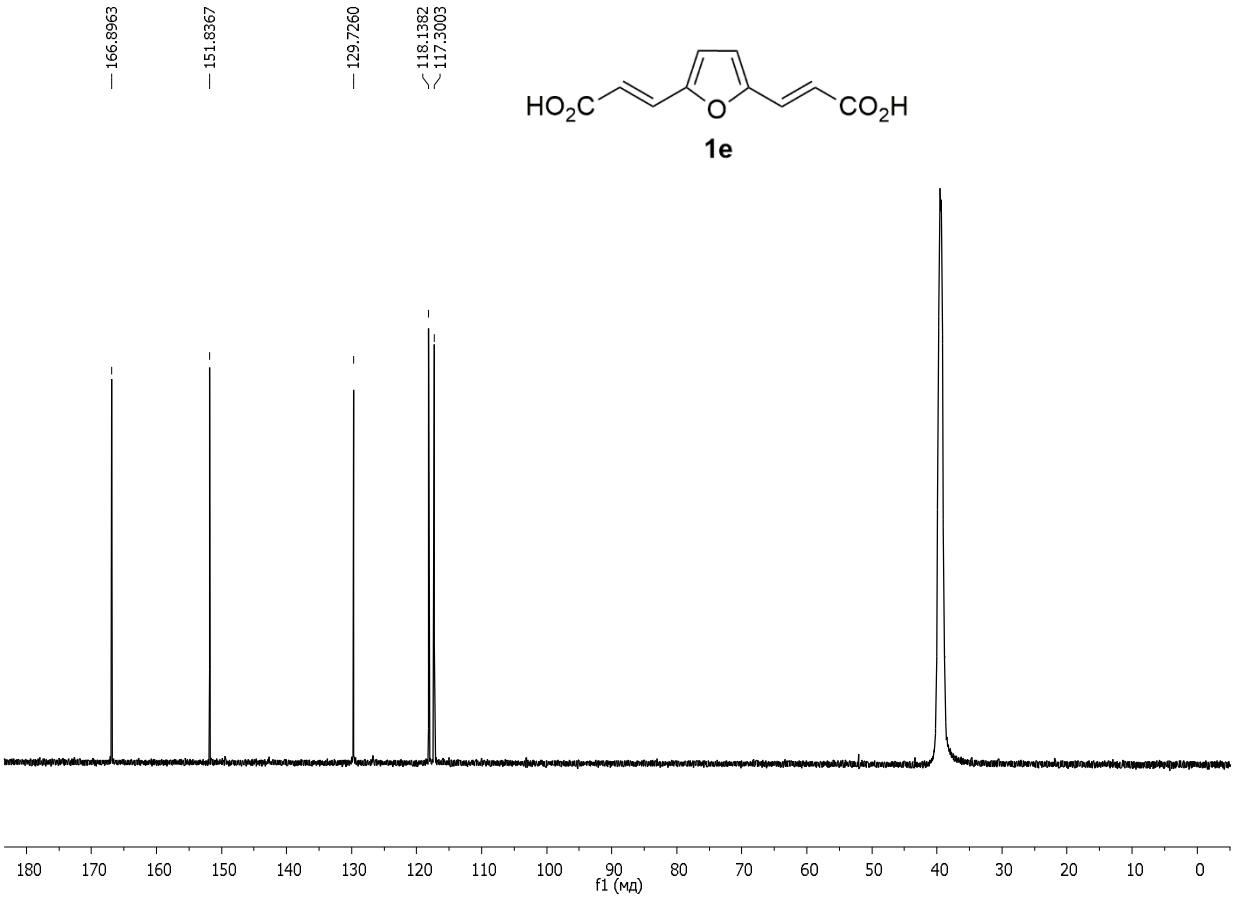


Figure S10. ^{13}C NMR spectrum of compound **1e** (125 Hz, $(CD_3)_2SO$)

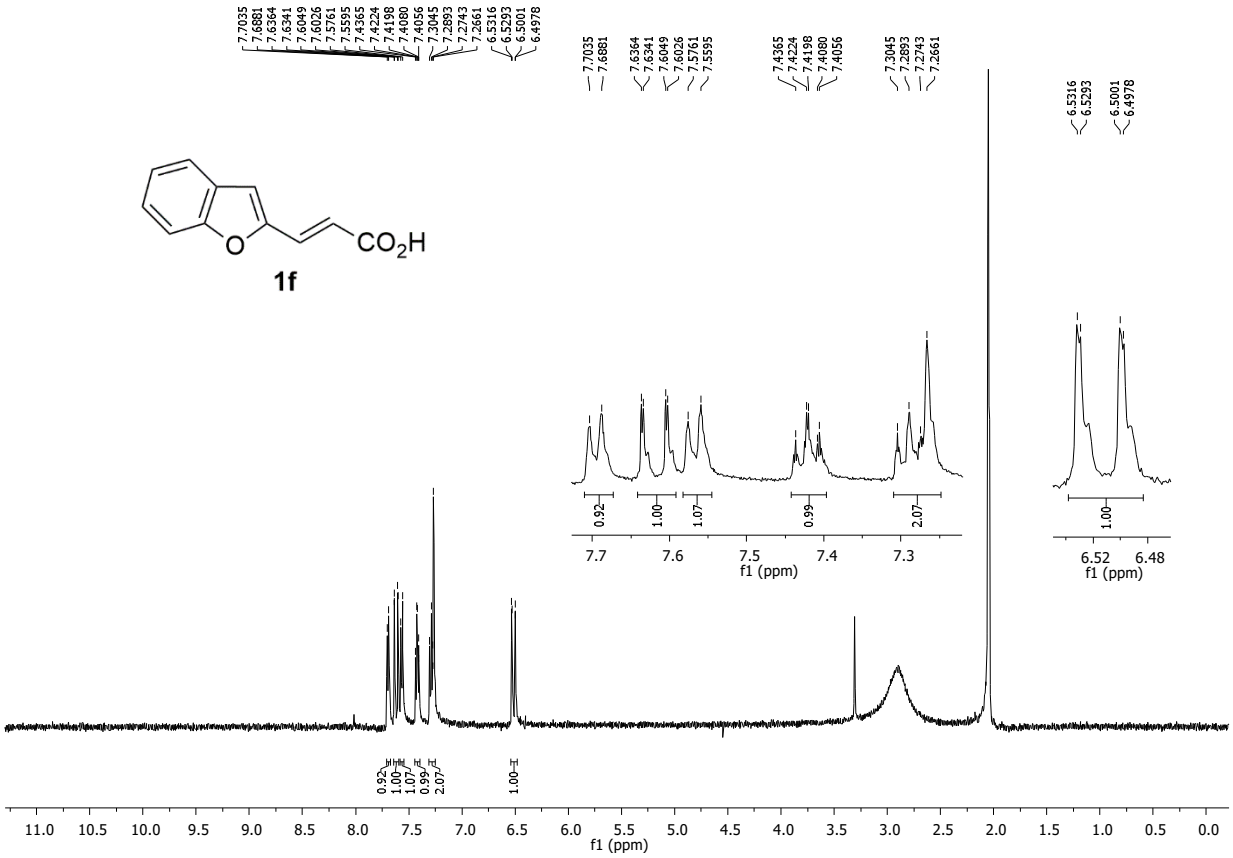


Figure S11. ^{1}H NMR spectrum of compound **1f** (500 Hz, $(CD_3)_2CO$)

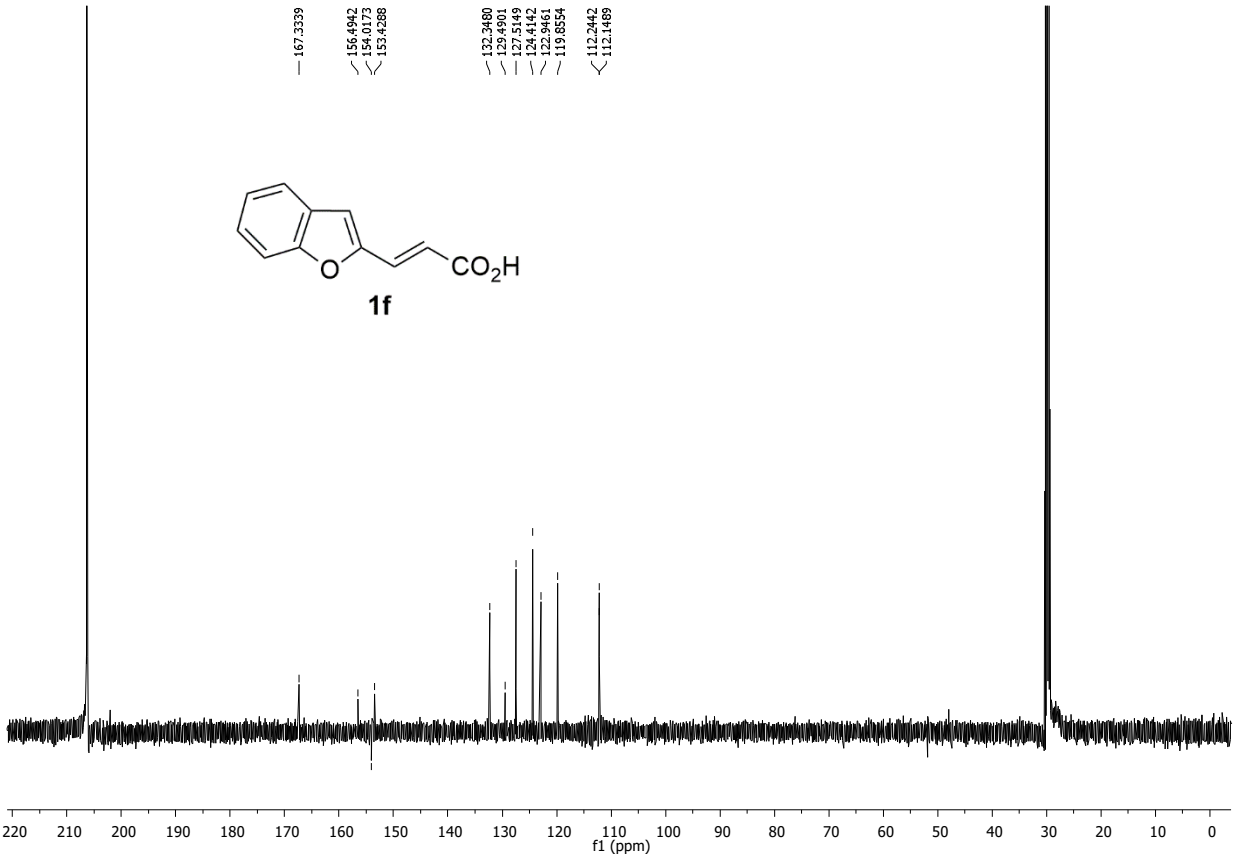


Figure S12. ^{13}C NMR spectrum of compound **1f** (125 Hz, $(CD_3)_2SO$)

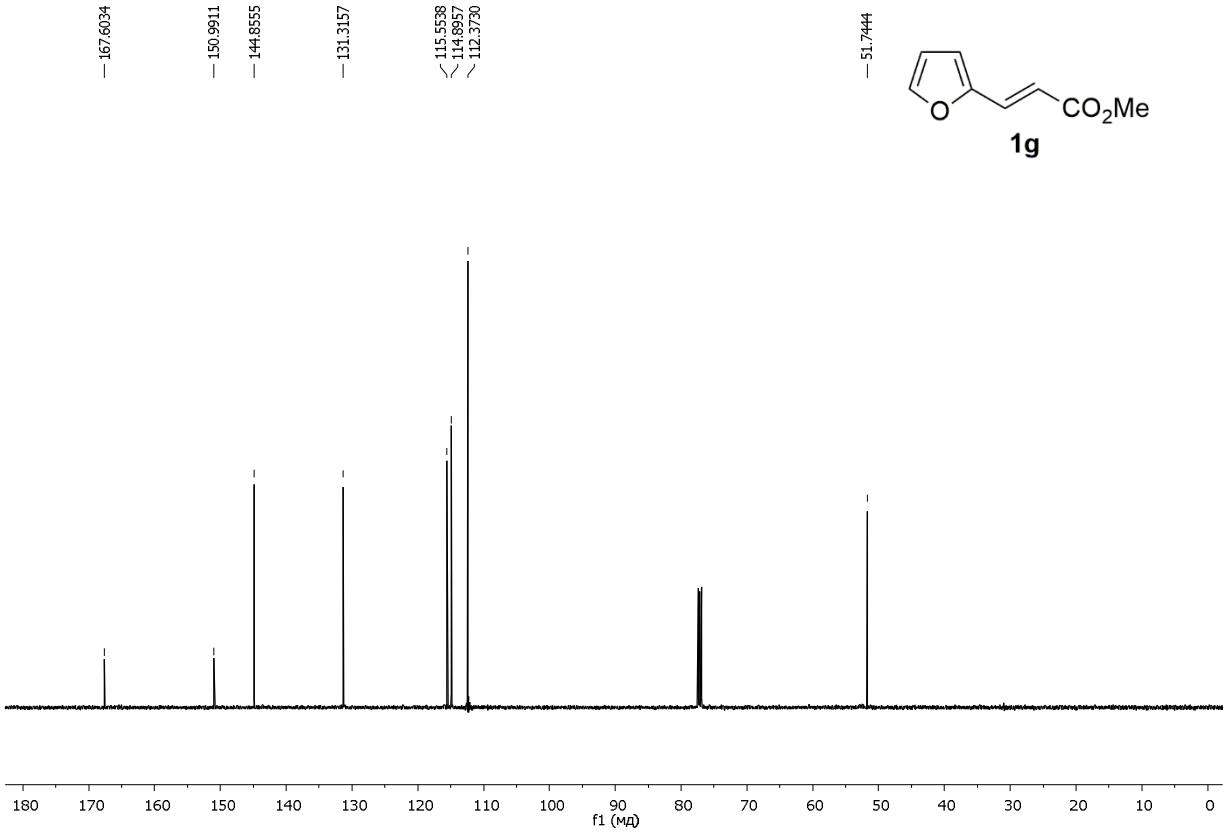


Figure S13. ^{1}H NMR spectrum of compound **1g** (500 MHz, $CDCl_3$).

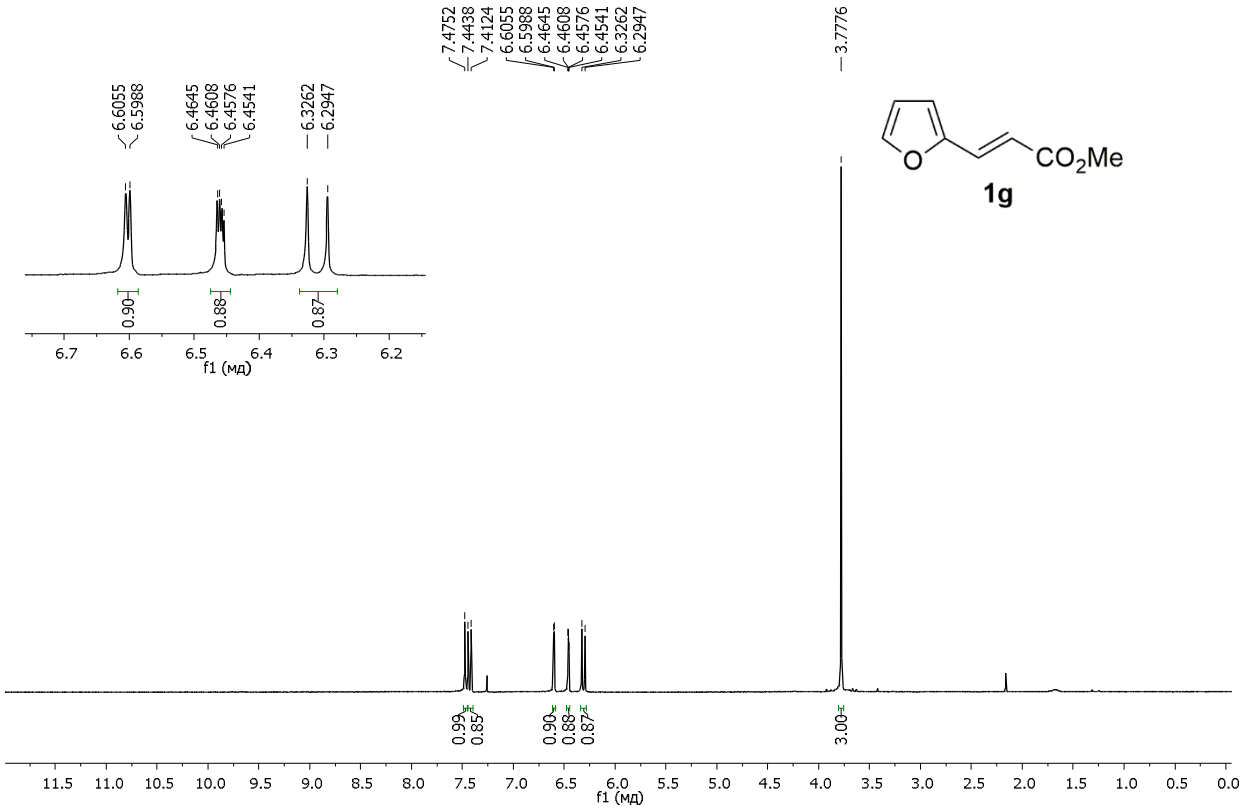


Figure S14. ^{13}C NMR spectrum of compound **1g** (125 MHz, $CDCl_3$).

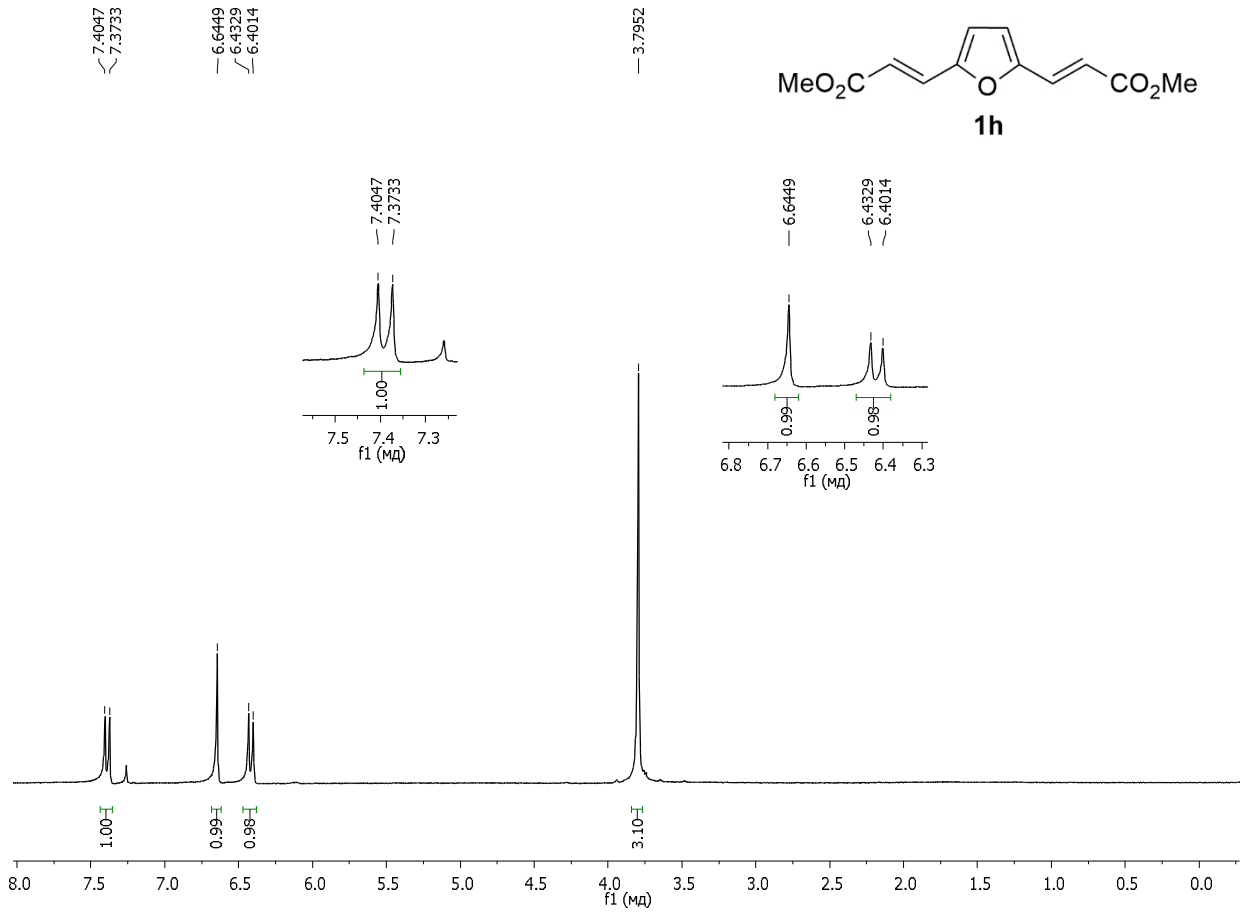


Figure S15. ^{1}H NMR spectrum of compound **1h** (500 MHz, $CDCl_3$).

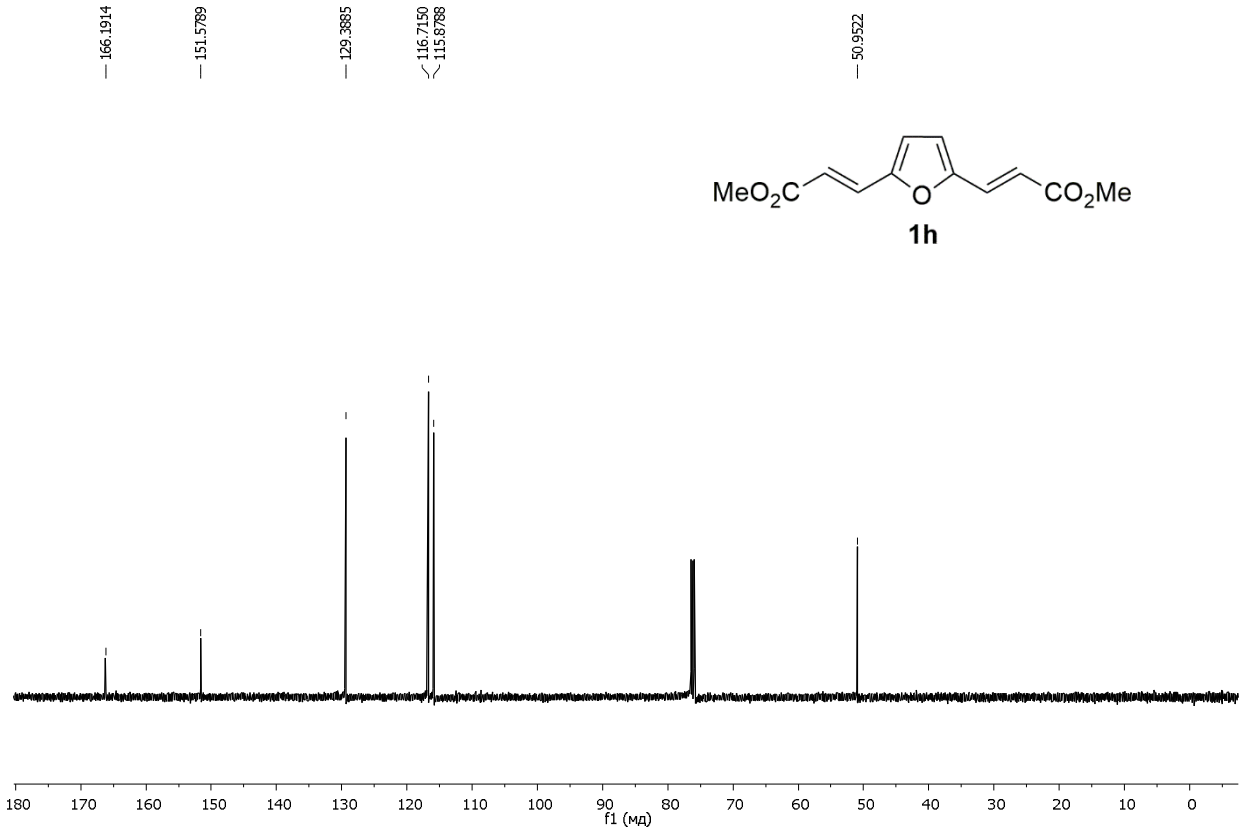


Figure S16. ^{13}C NMR spectrum of compound **1h** (125 MHz, $CDCl_3$).

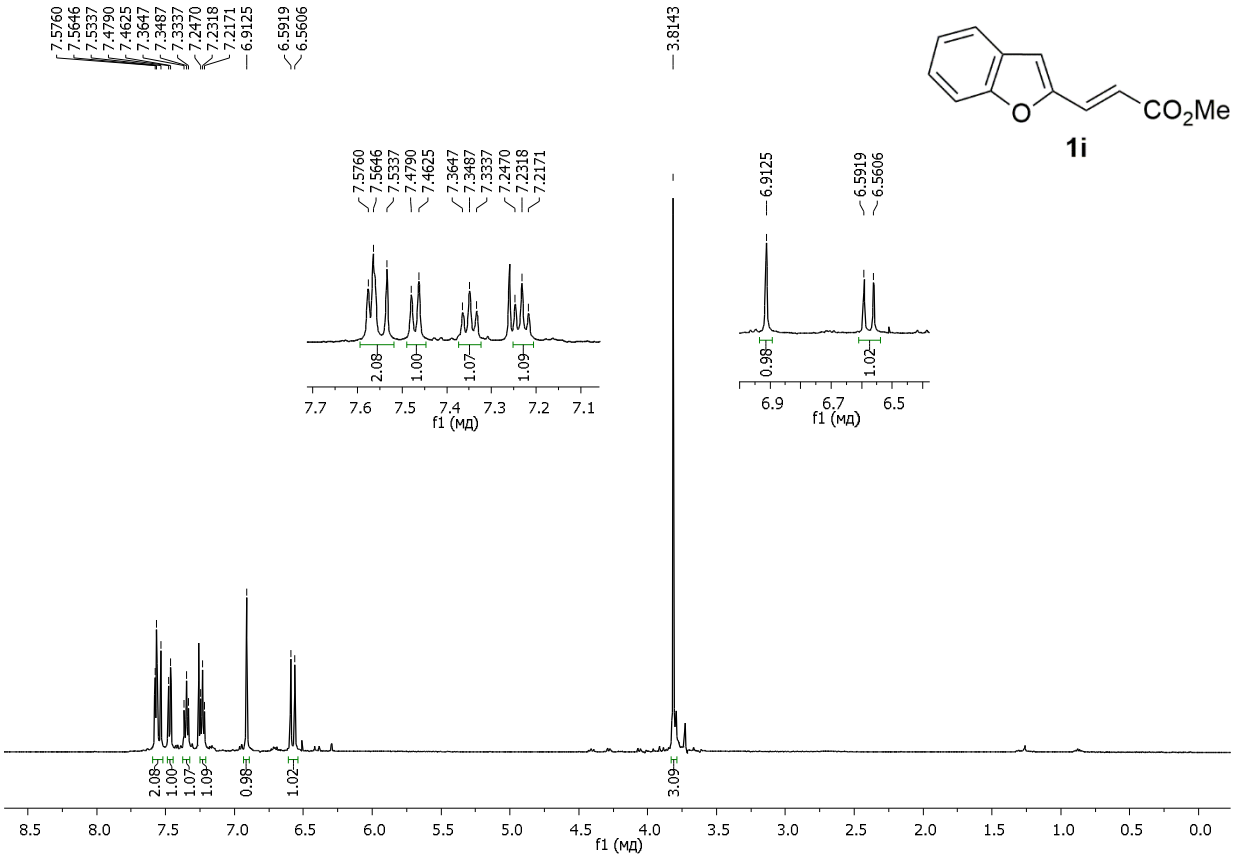


Figure S17. ^{1}H NMR spectrum of compound **1i** (500 MHz, $CDCl_3$).

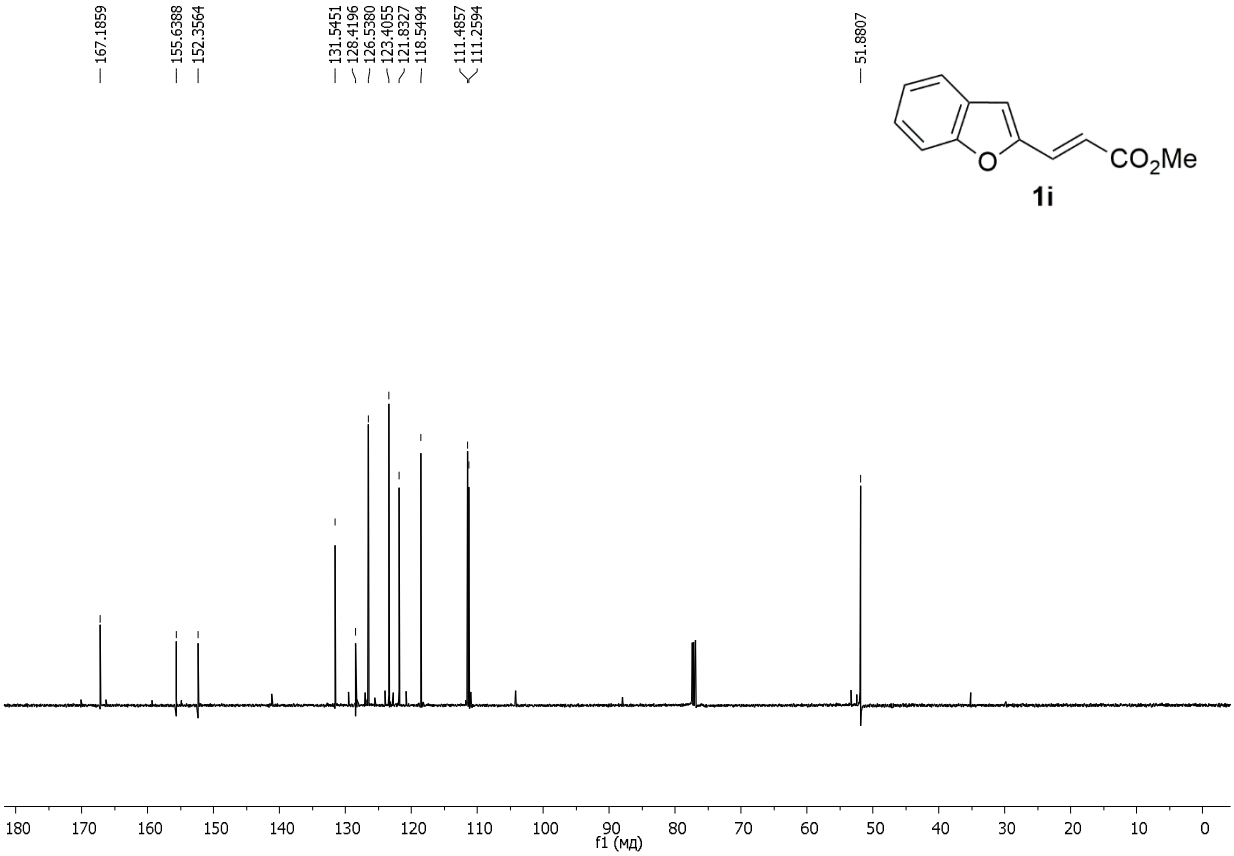


Figure S18. ^{13}C NMR spectrum of compound **1i** (125 MHz, $CDCl_3$).

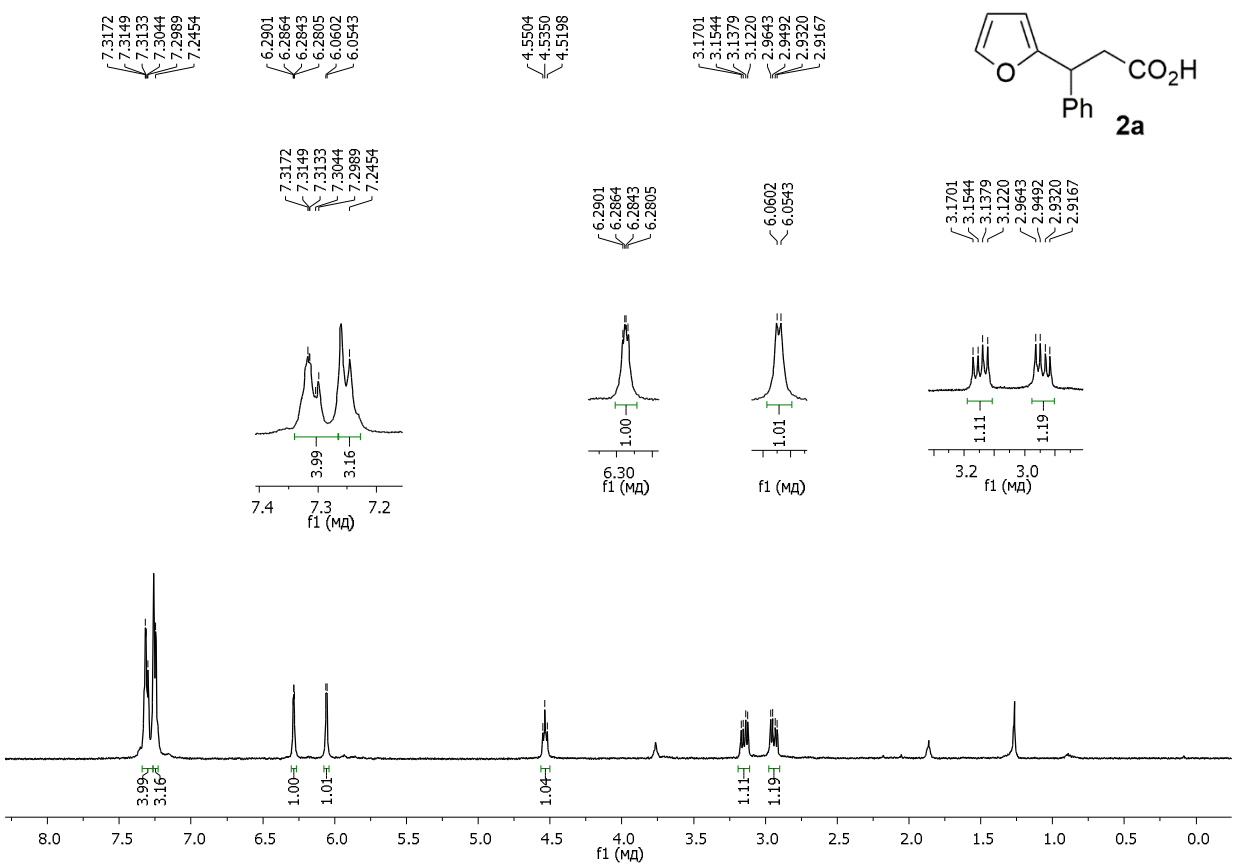


Figure S19. ^{1}H NMR spectrum of compound **2a** (500 MHz, $CDCl_3$).

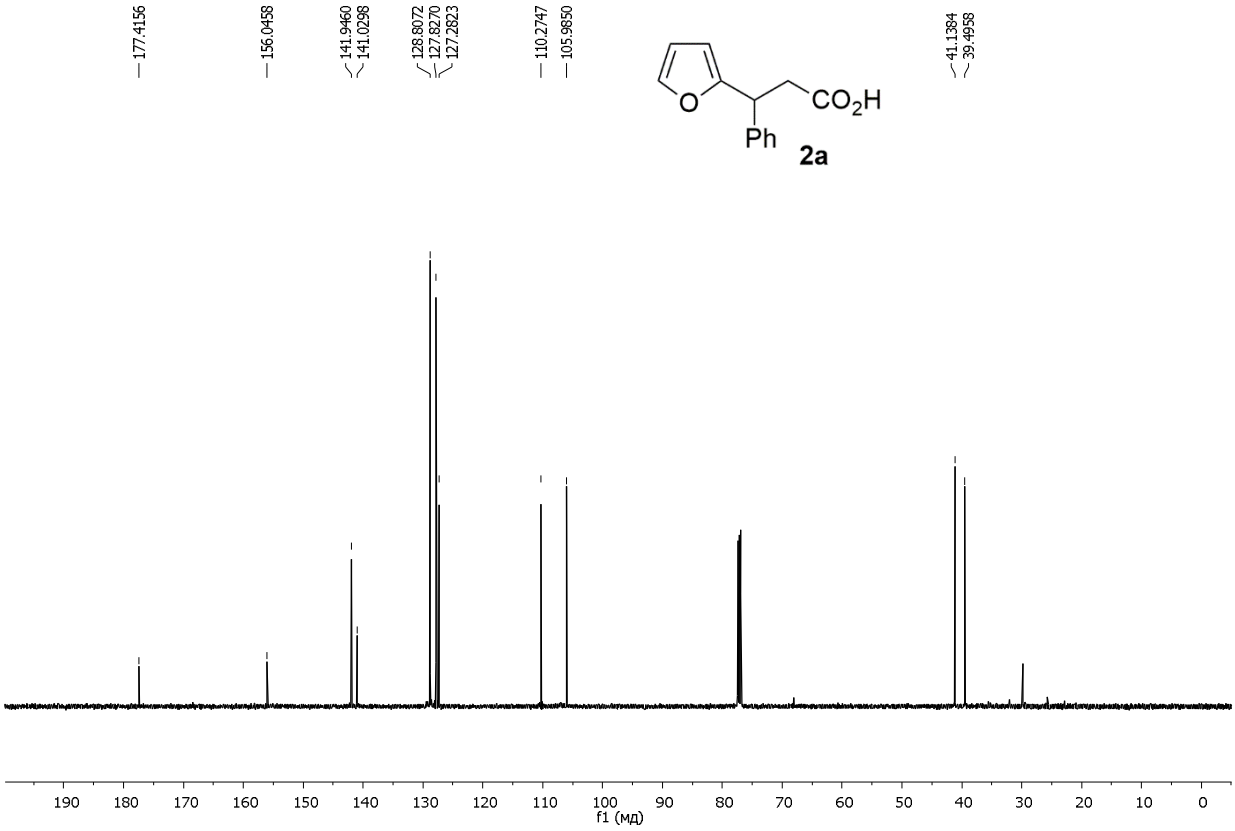


Figure S20. ^{13}C NMR spectrum of compound **2a** (125 MHz, $CDCl_3$).

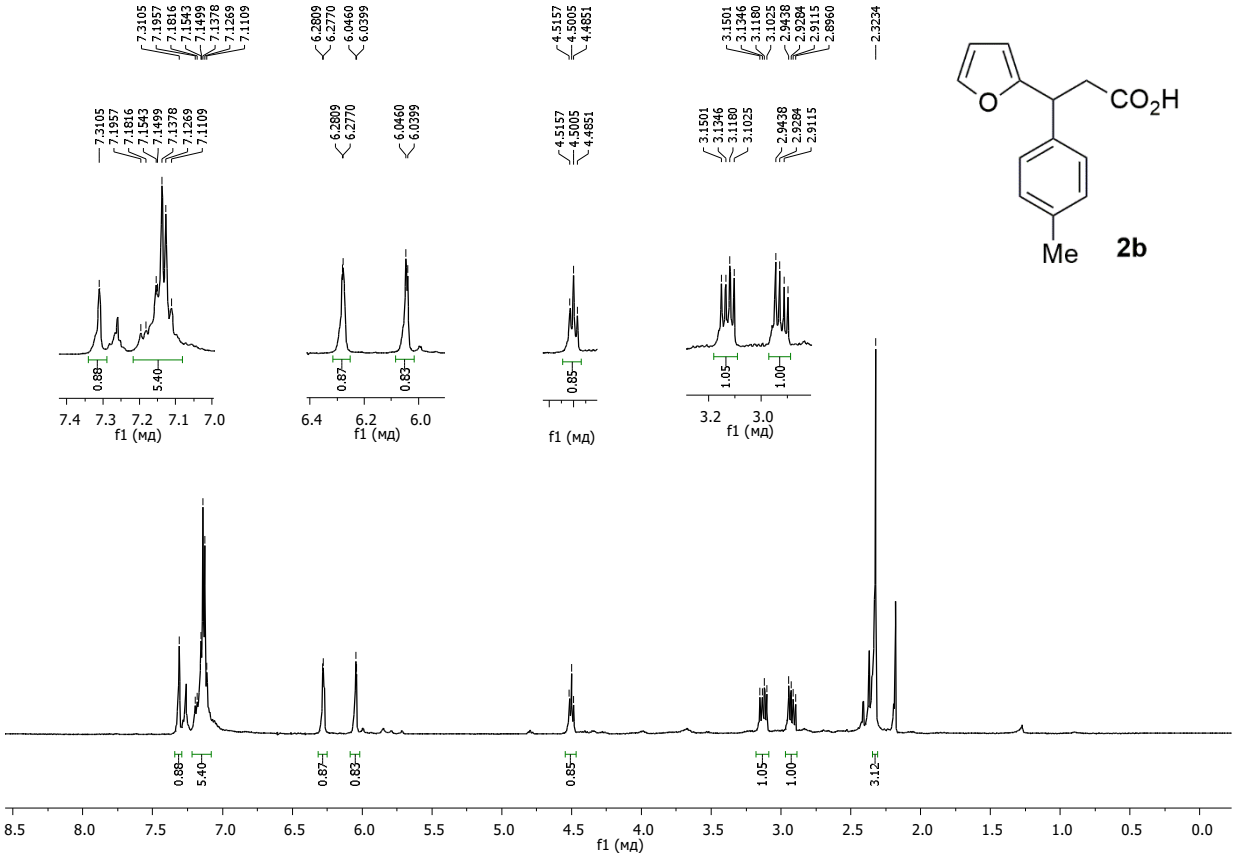


Figure S21. ^{1}H NMR spectrum of compound **2b** (500 MHz, $CDCl_3$).

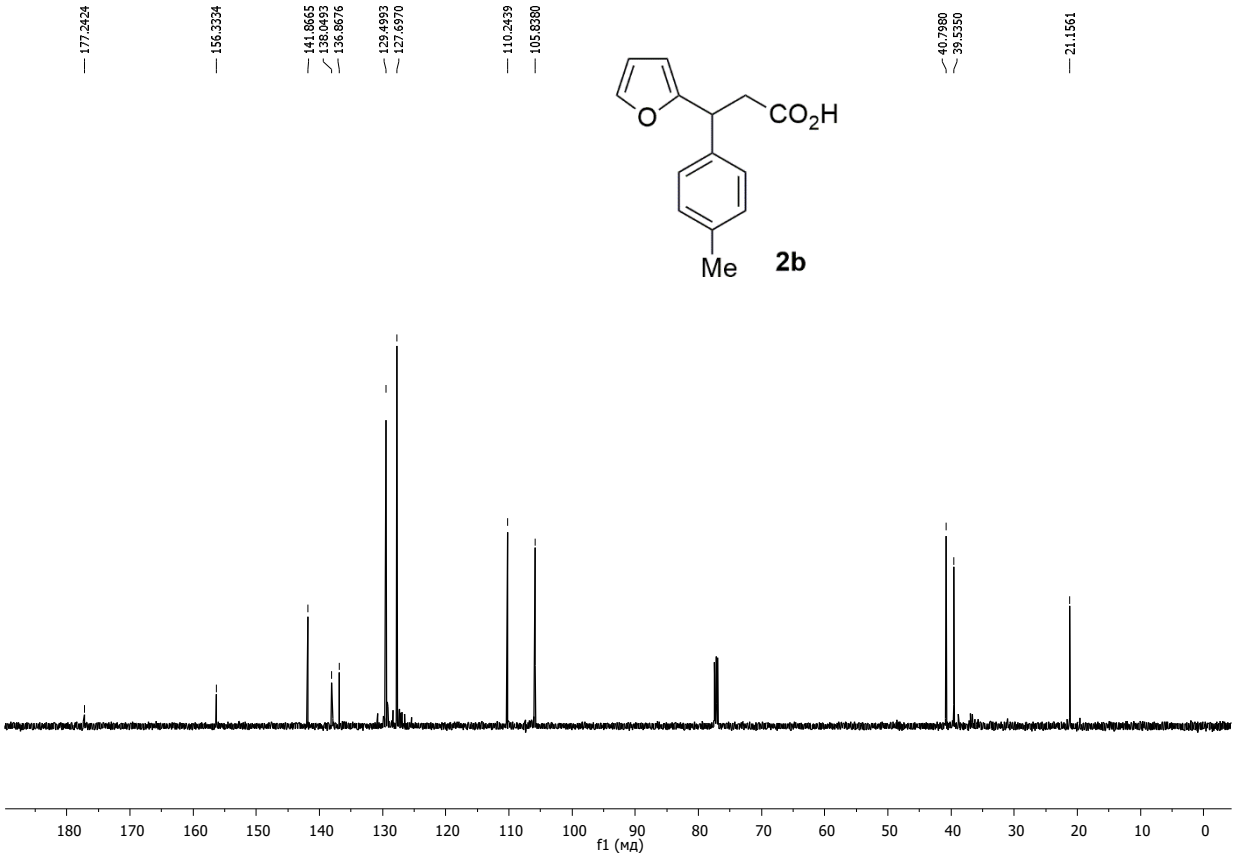


Figure S22. ^{13}C NMR spectrum of compound **2b** (125 MHz, $CDCl_3$).

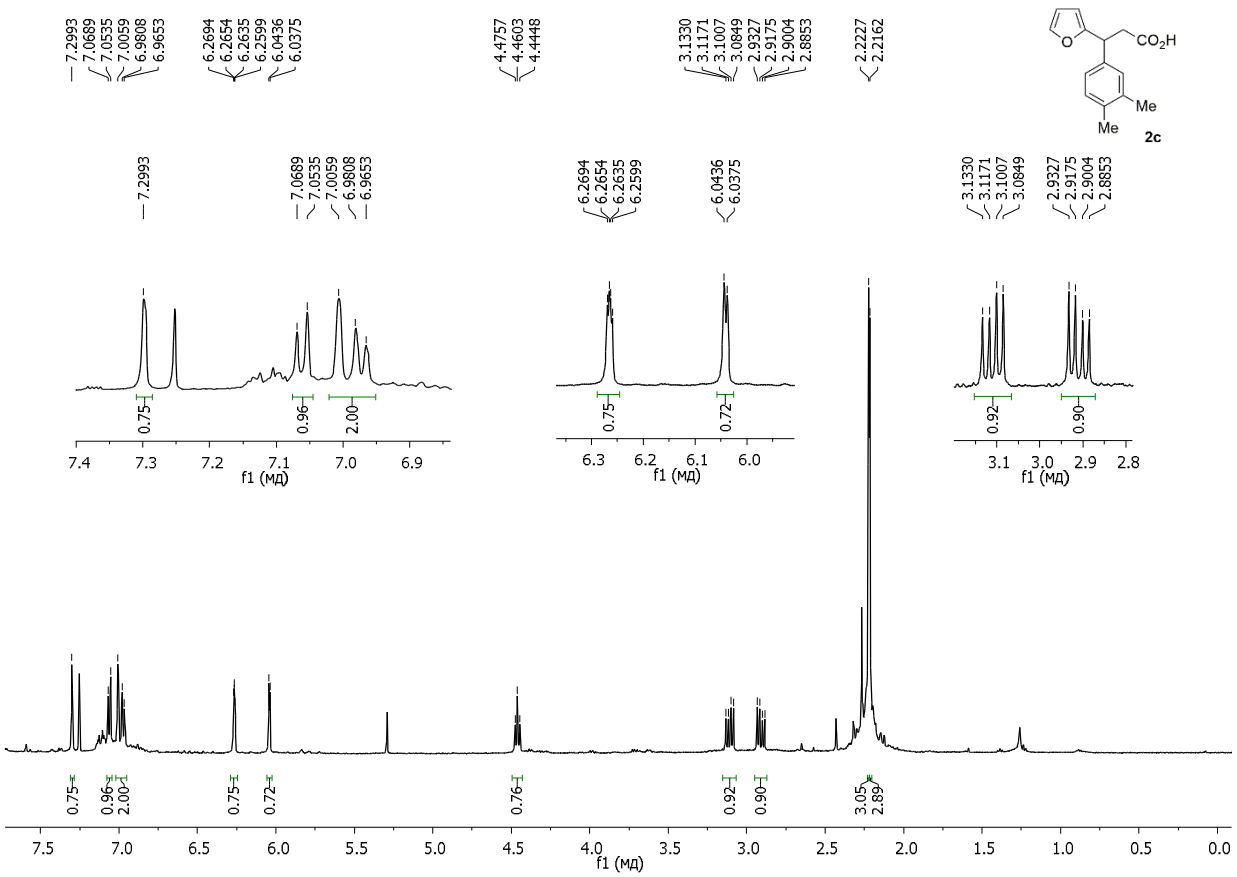


Figure S23. ^{1}H NMR spectrum of compound **2c** (500 MHz, $CDCl_3$).

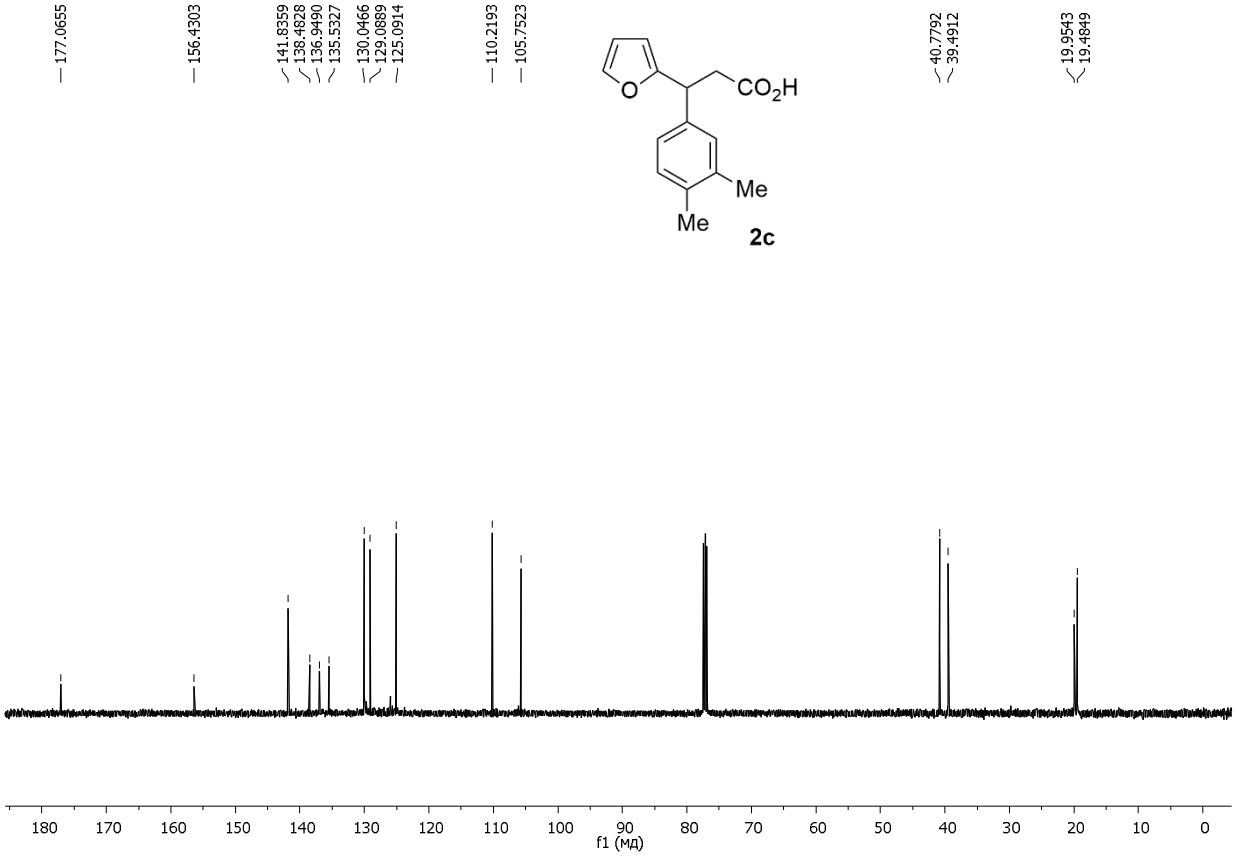


Figure S24. ^{13}C NMR spectrum of compound **2c** (125 MHz, $CDCl_3$).

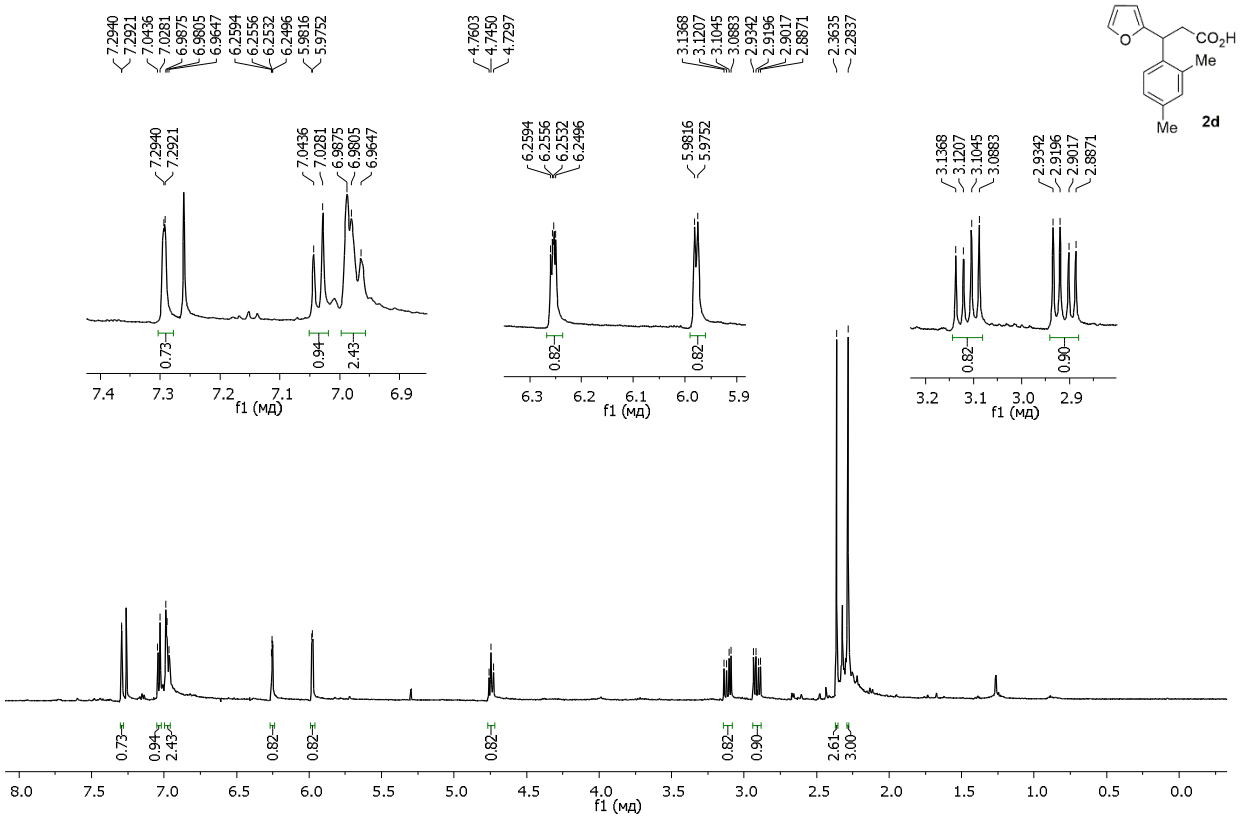


Figure S25. ^{1}H NMR spectrum of compound **2d** (500 MHz, $CDCl_3$).

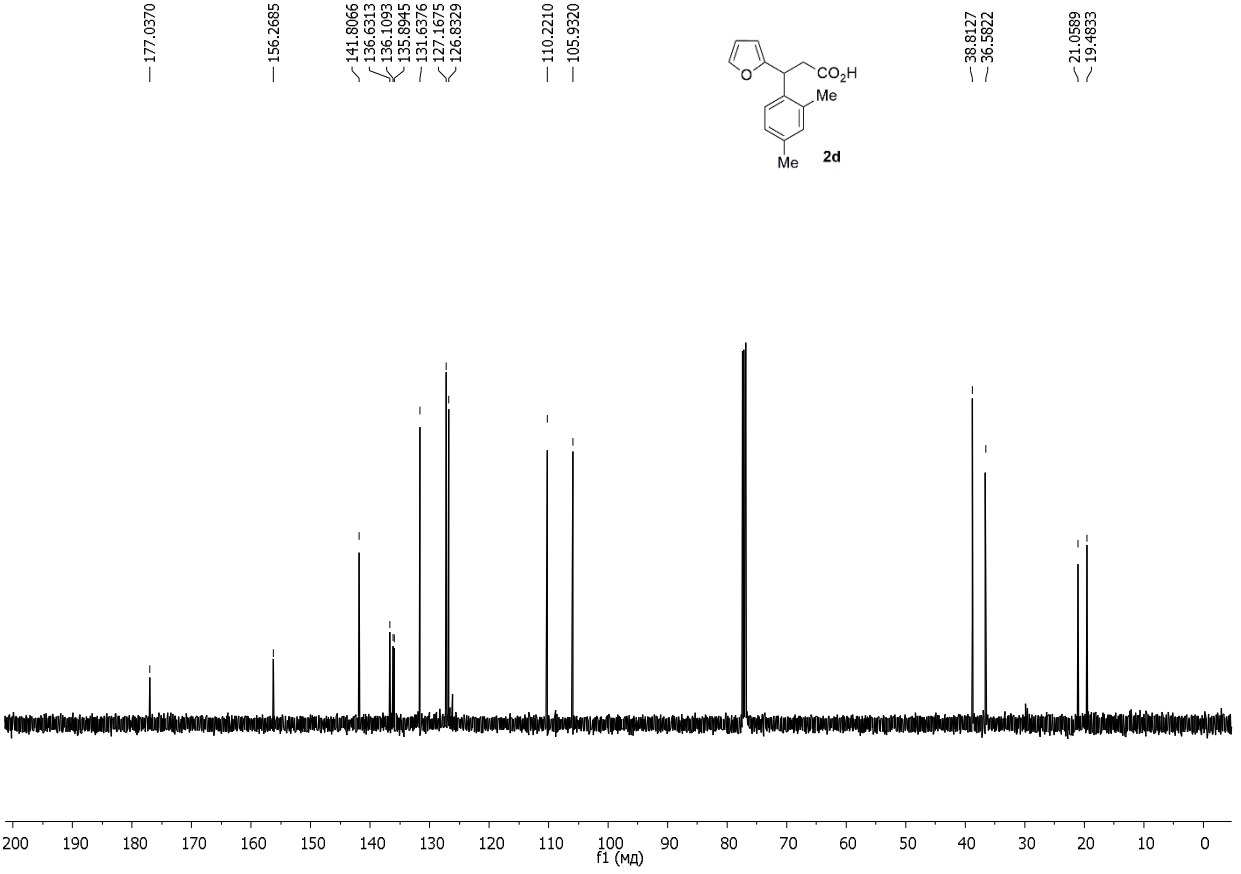


Figure S26. ^{13}C NMR spectrum of compound **2d** (125 MHz, $CDCl_3$).

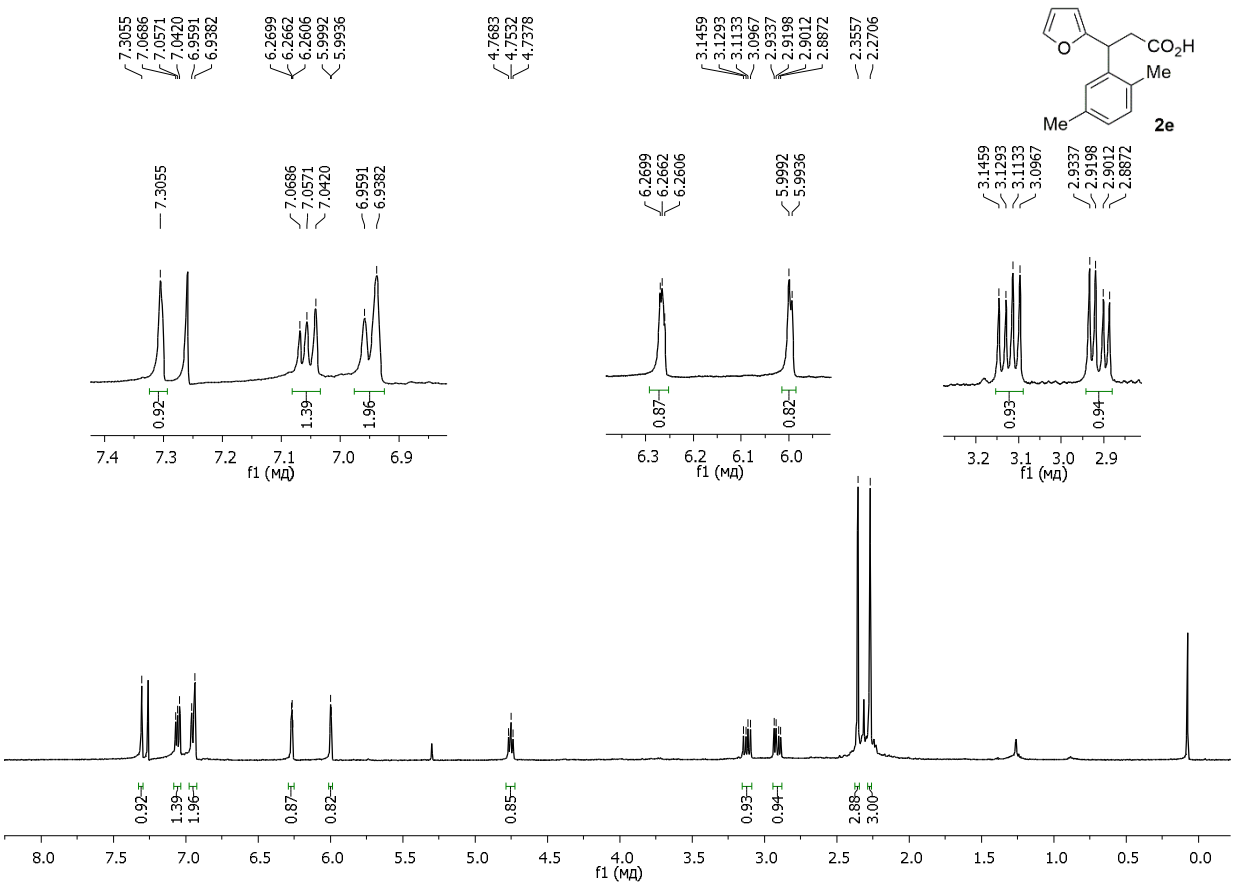


Figure S27. ^{1}H NMR spectrum of compound **2e** (500 MHz, $CDCl_3$).

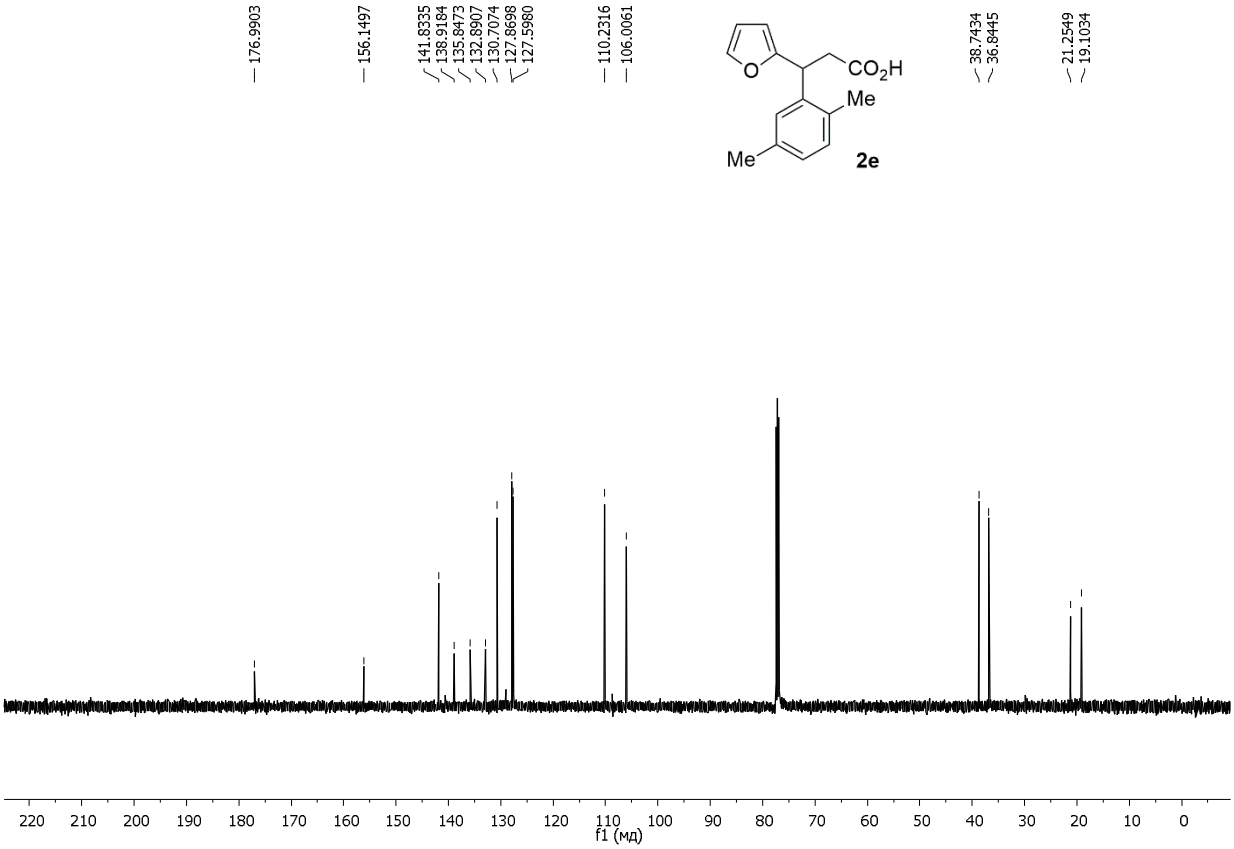


Figure S28. ^{13}C NMR spectrum of compound **2e** (125 MHz, $CDCl_3$).

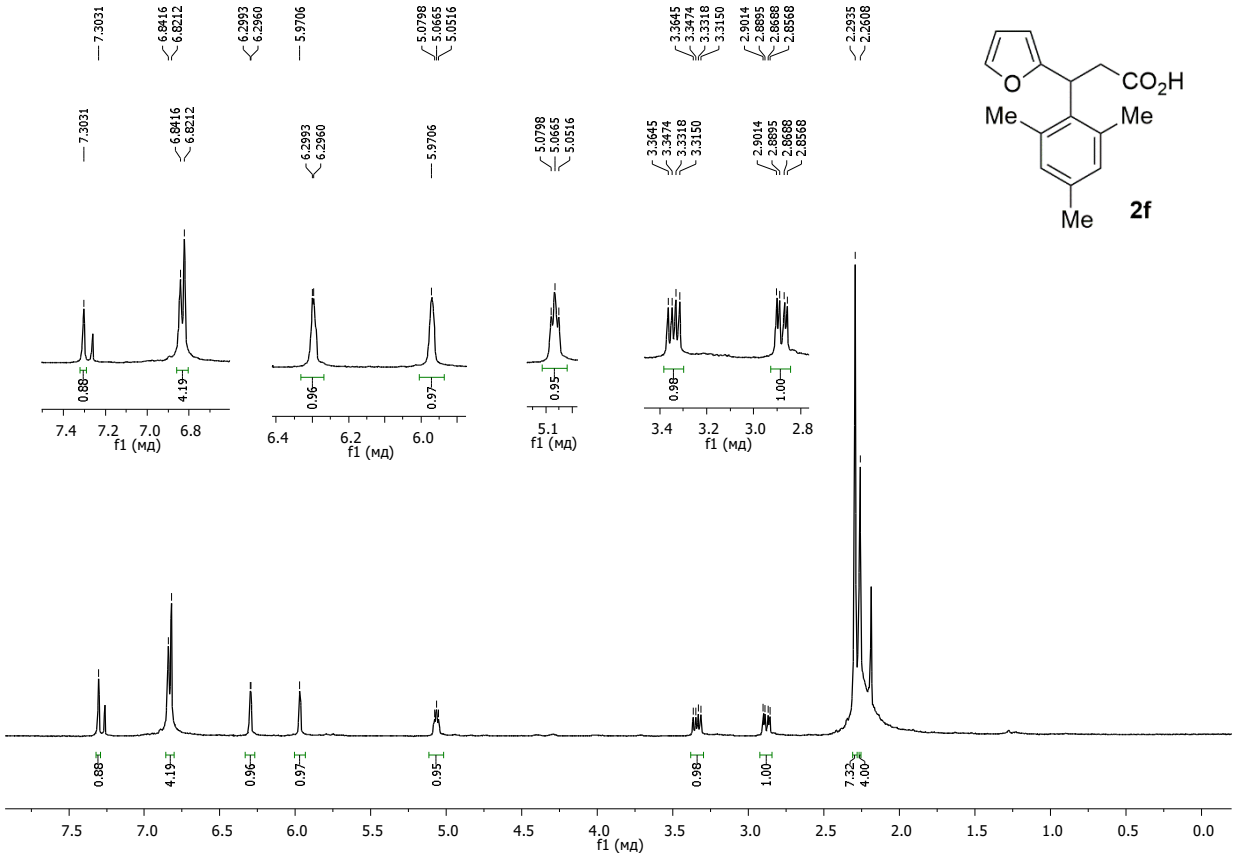


Figure S29. ^{1}H NMR spectrum of compound **2f** (500 MHz, $CDCl_3$).

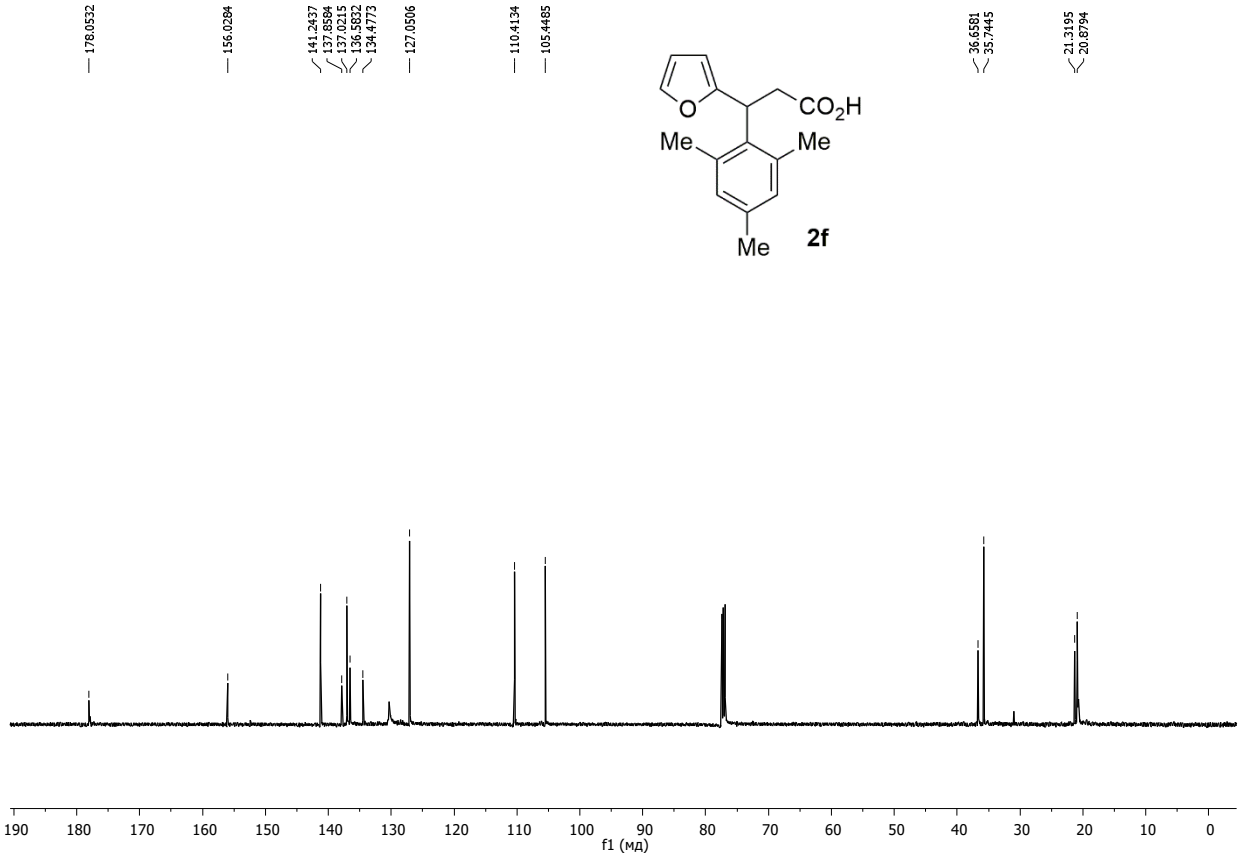


Figure S30. ^{13}C NMR spectrum of compound **2f** (125 MHz, $CDCl_3$).

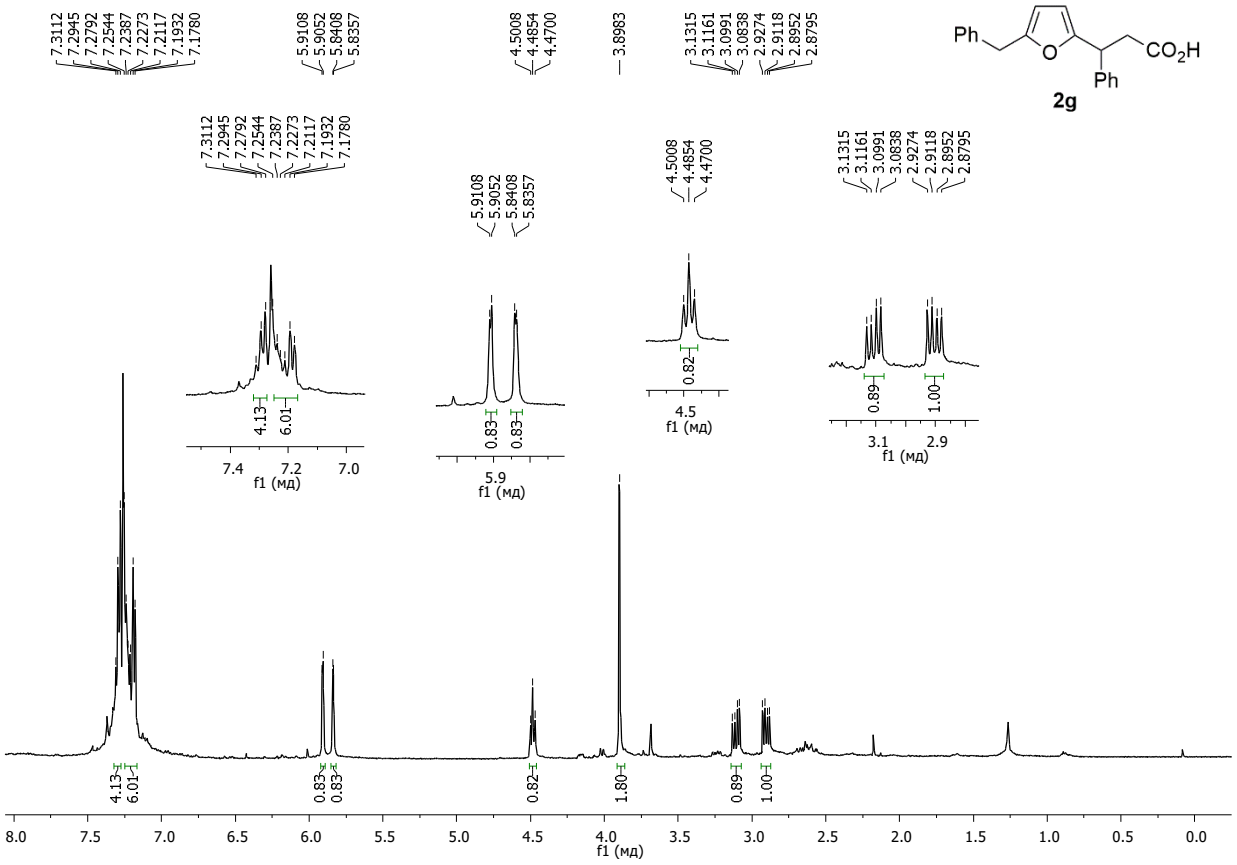


Figure S31. ^{1}H NMR spectrum of compound **2g** (500 MHz, $CDCl_3$).

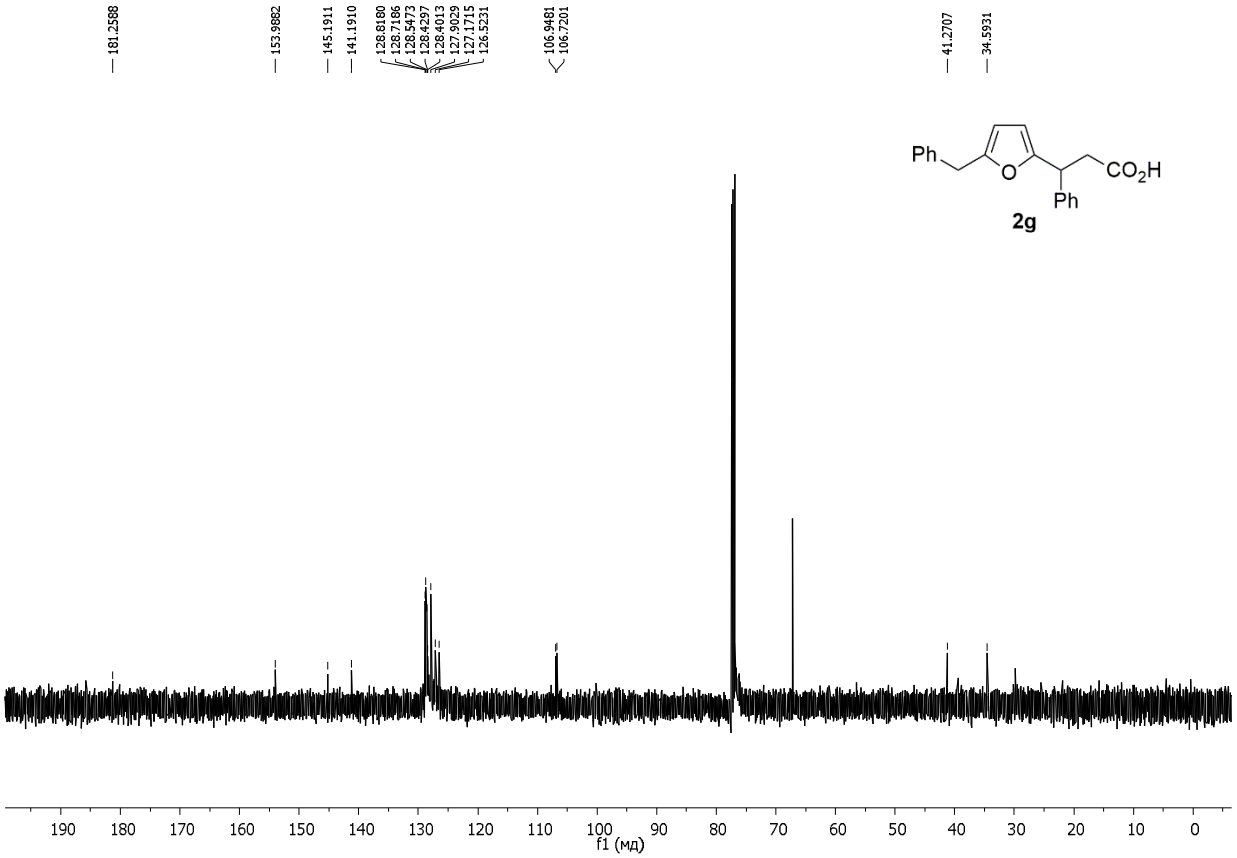


Figure S32. ^{13}C NMR spectrum of compound **2g** (125 MHz, $CDCl_3$).

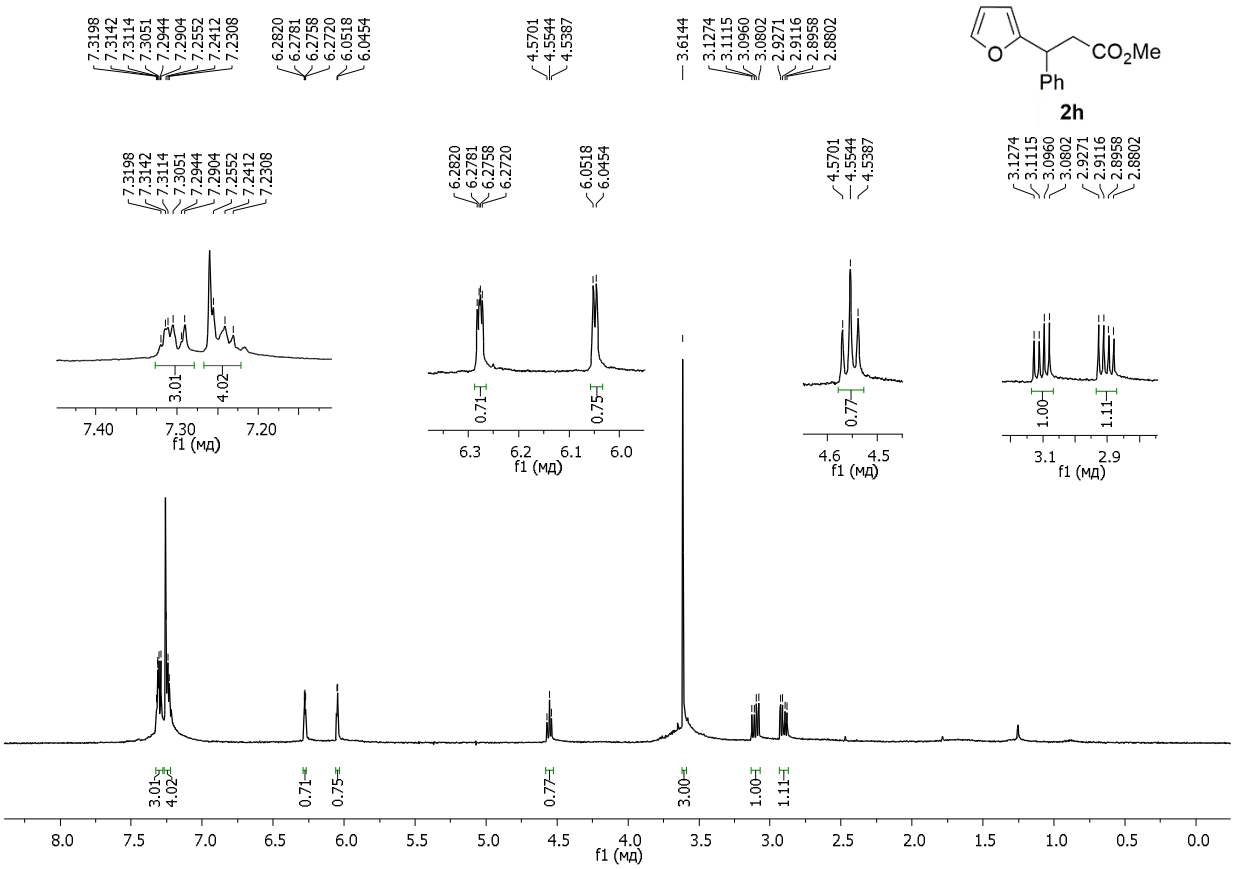


Figure S33. ^{1}H NMR spectrum of compound **2h** (500 MHz, $CDCl_3$).

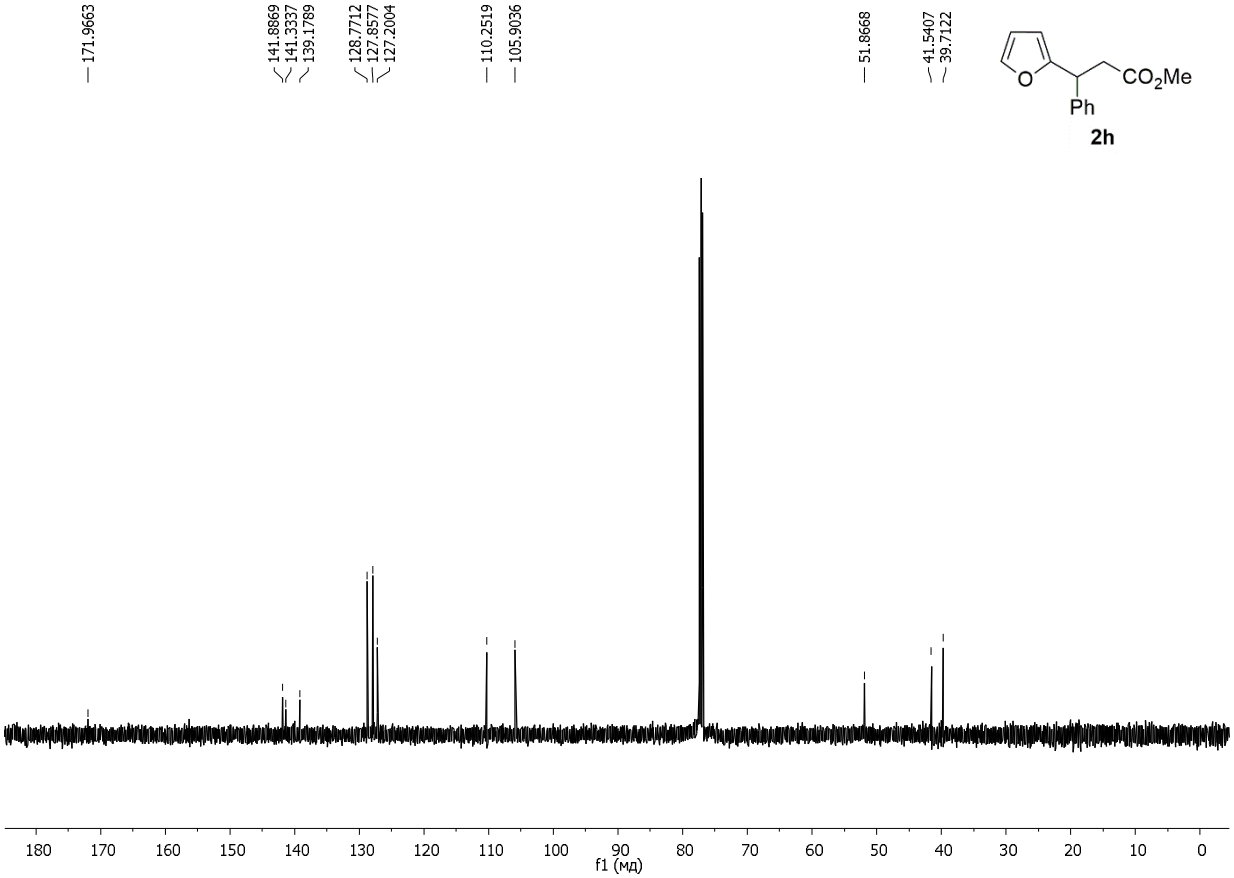


Figure S34. ^{13}C NMR spectrum of compound **2h** (125MHz, $CDCl_3$).

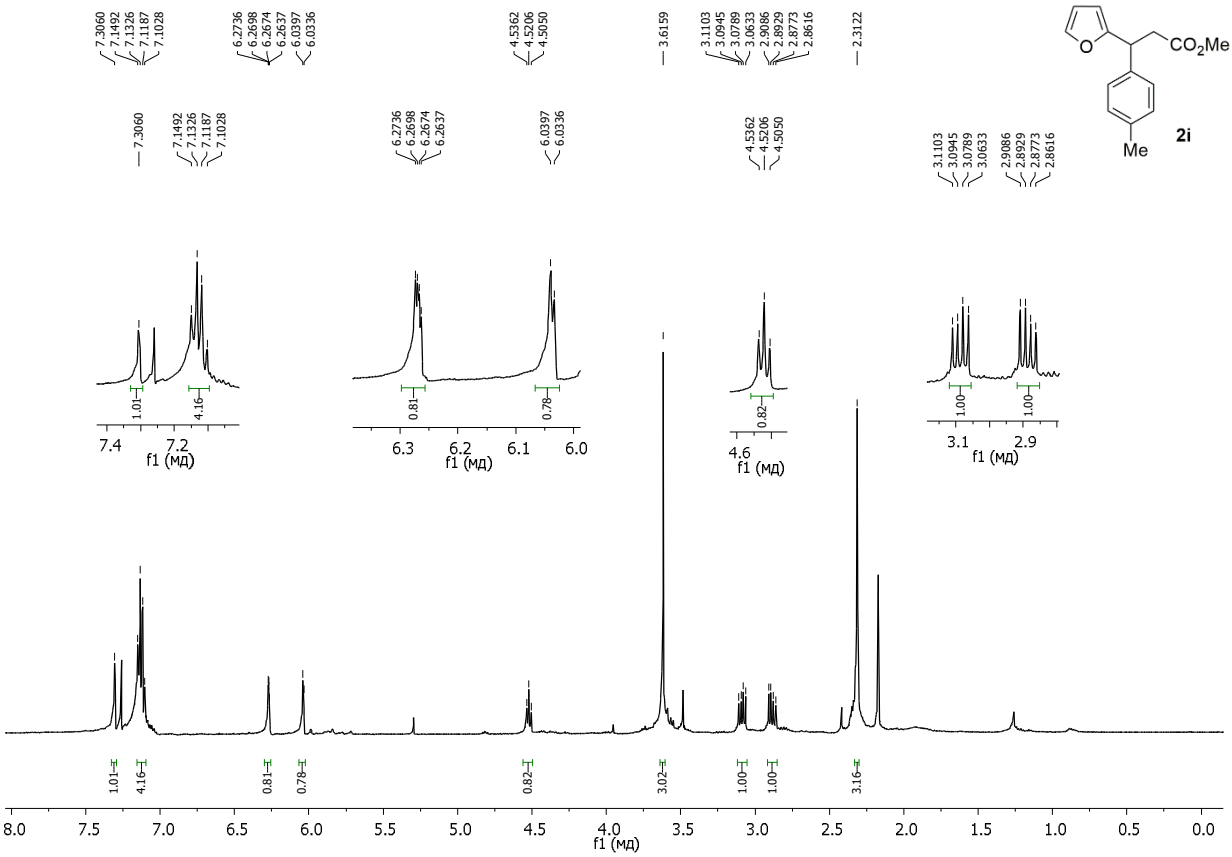


Figure S35. ^{1}H NMR spectrum of compound **2i** (500 MHz, $CDCl_3$).

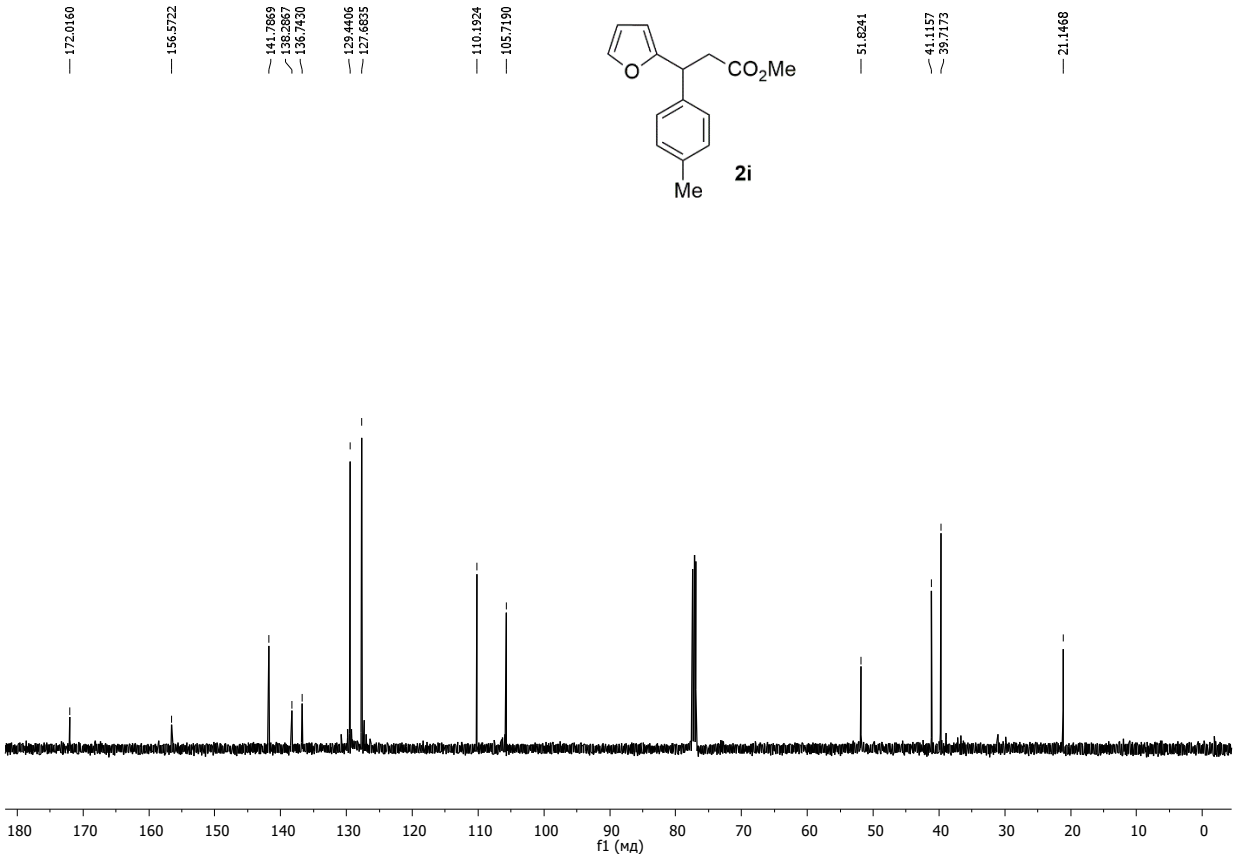


Figure S36. ^{13}C NMR spectrum of compound **2i** (125 MHz, $CDCl_3$).

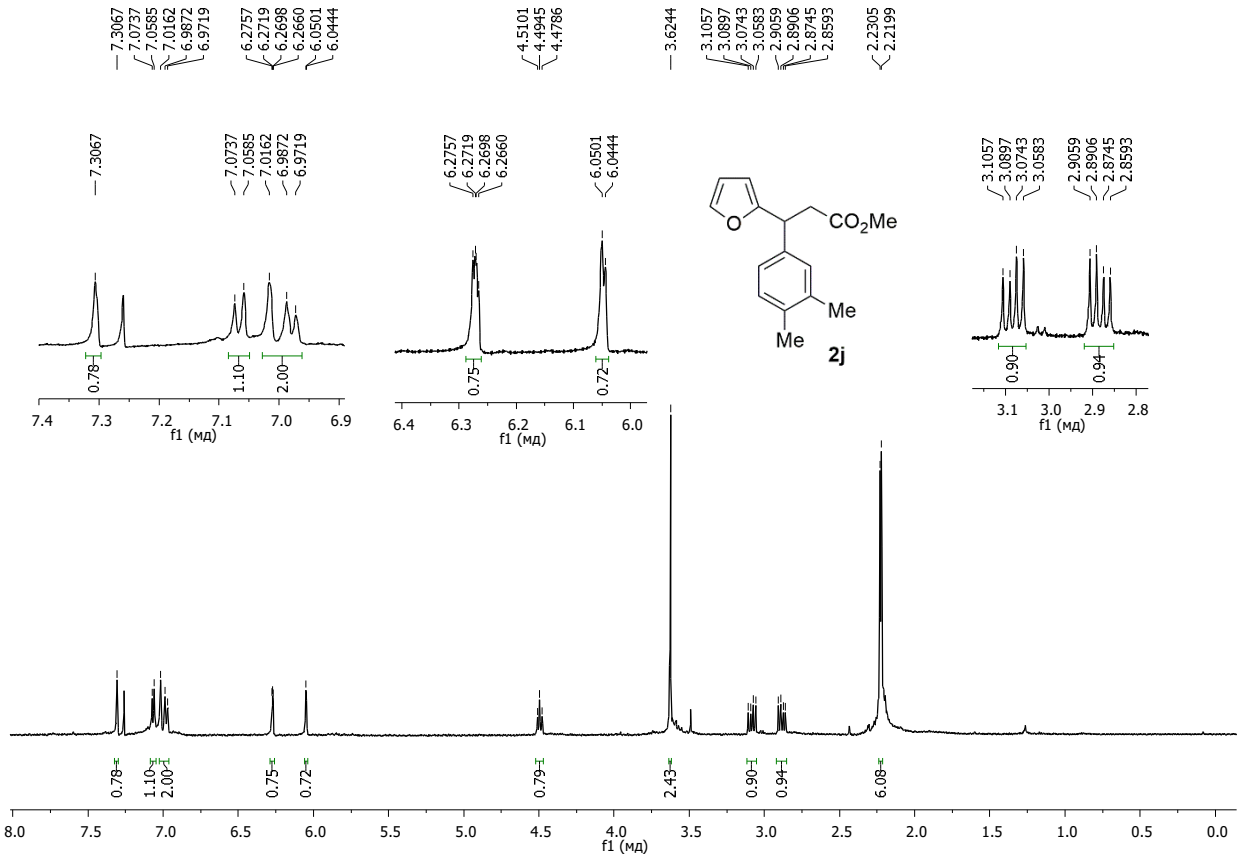


Figure S37. ^{1}H NMR spectrum of compound **2j** (500 MHz, $CDCl_3$).

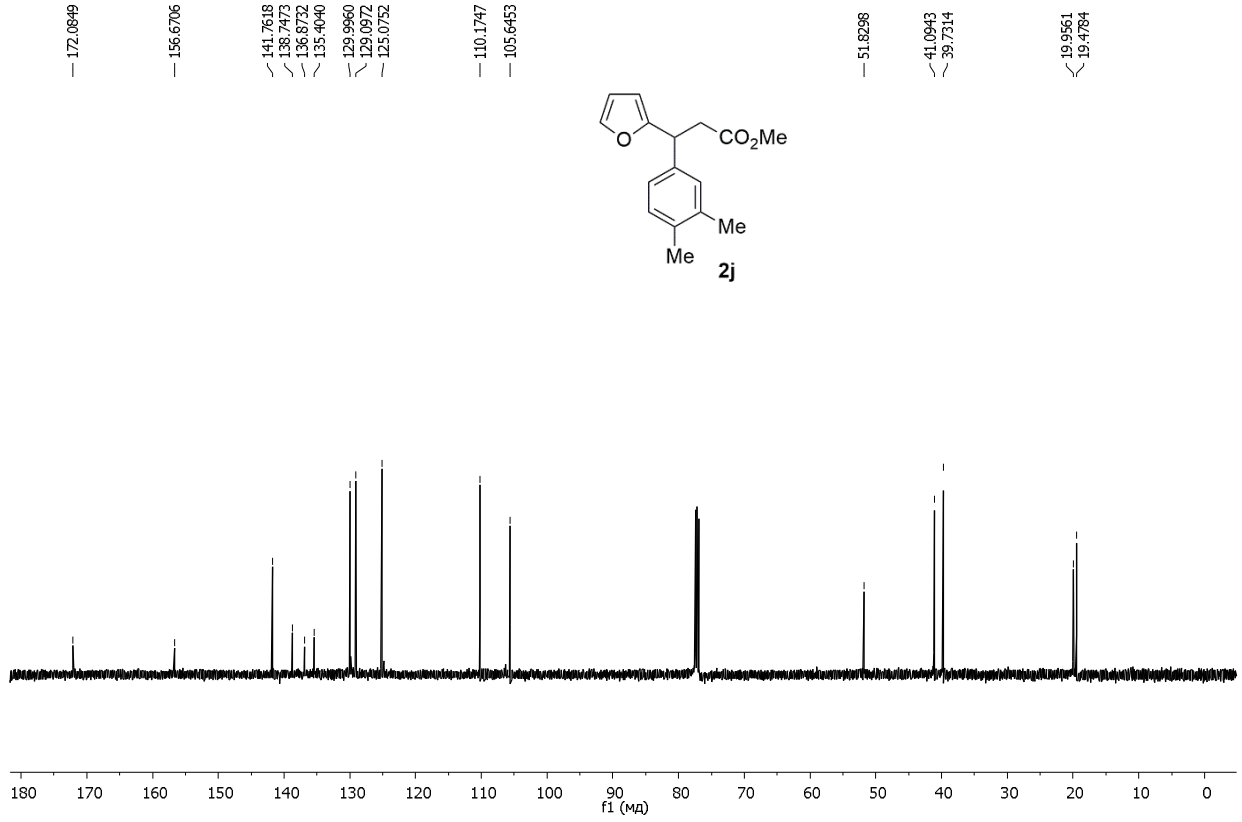


Figure S38. ^{13}C NMR spectrum of compound **2j** (125 MHz, $CDCl_3$).

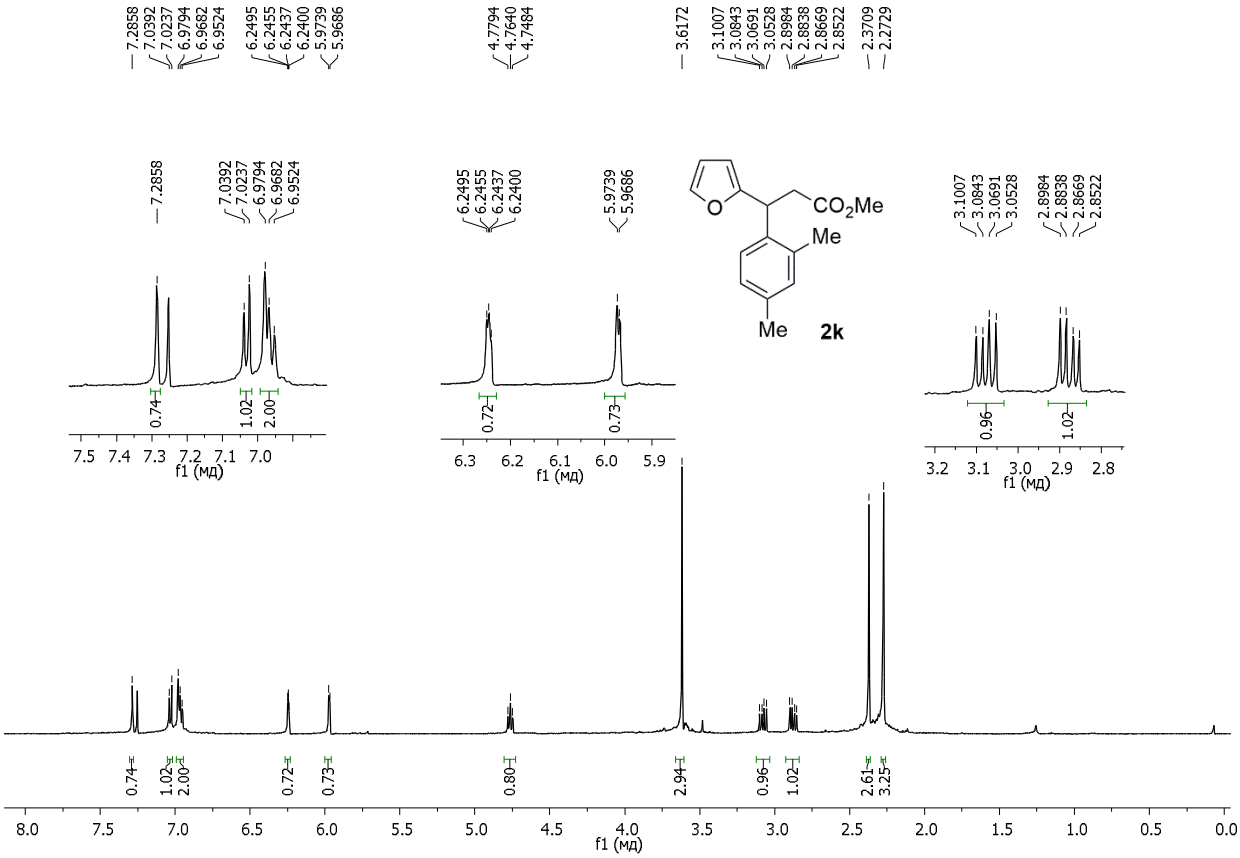


Figure S39. ^{1}H NMR spectrum of compound **2k** (500 MHz, $CDCl_3$).

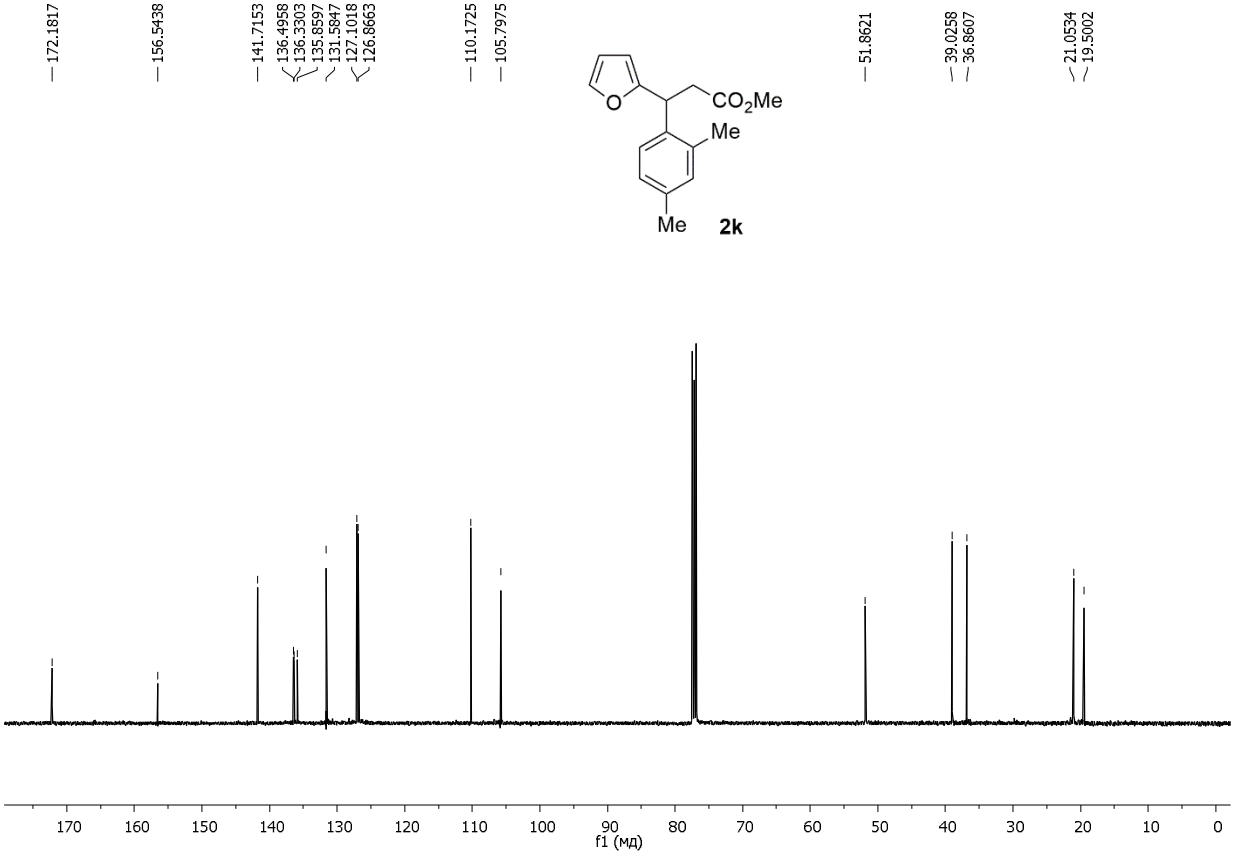


Figure S40. ^{13}C NMR spectrum of compound **2k** (125 MHz, $CDCl_3$).

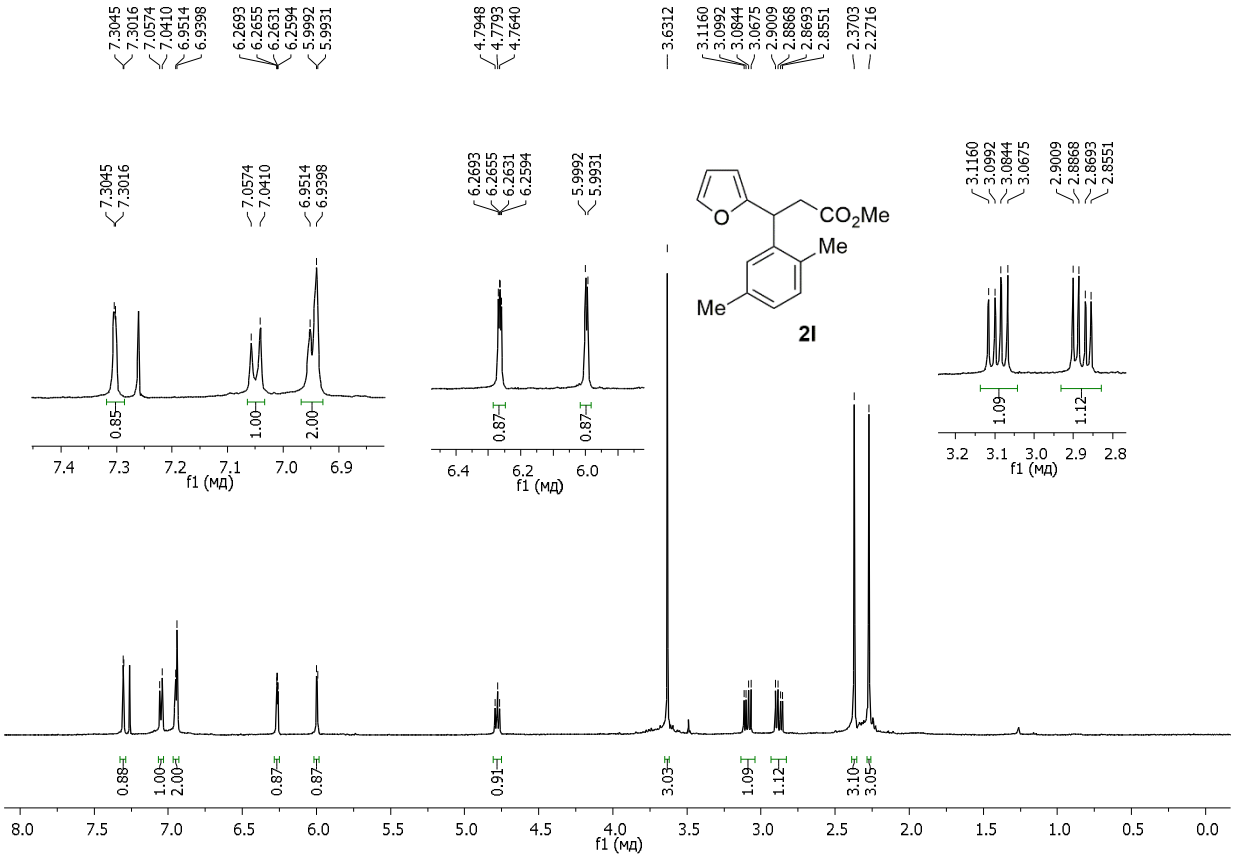


Figure S41. ^{1}H NMR spectrum of compound **2l** (500 MHz, $CDCl_3$).

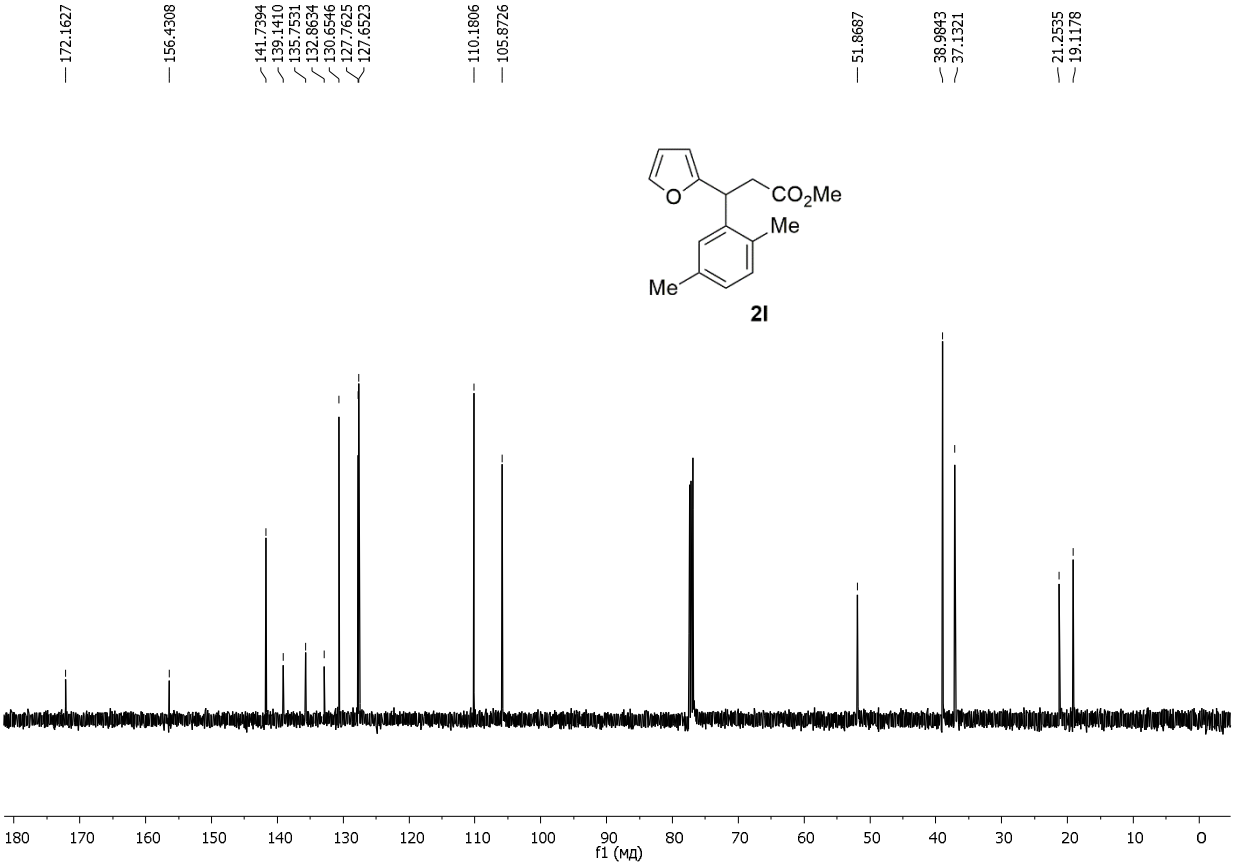


Figure S42. ^{13}C NMR spectrum of compound **2l** (125 MHz, $CDCl_3$).

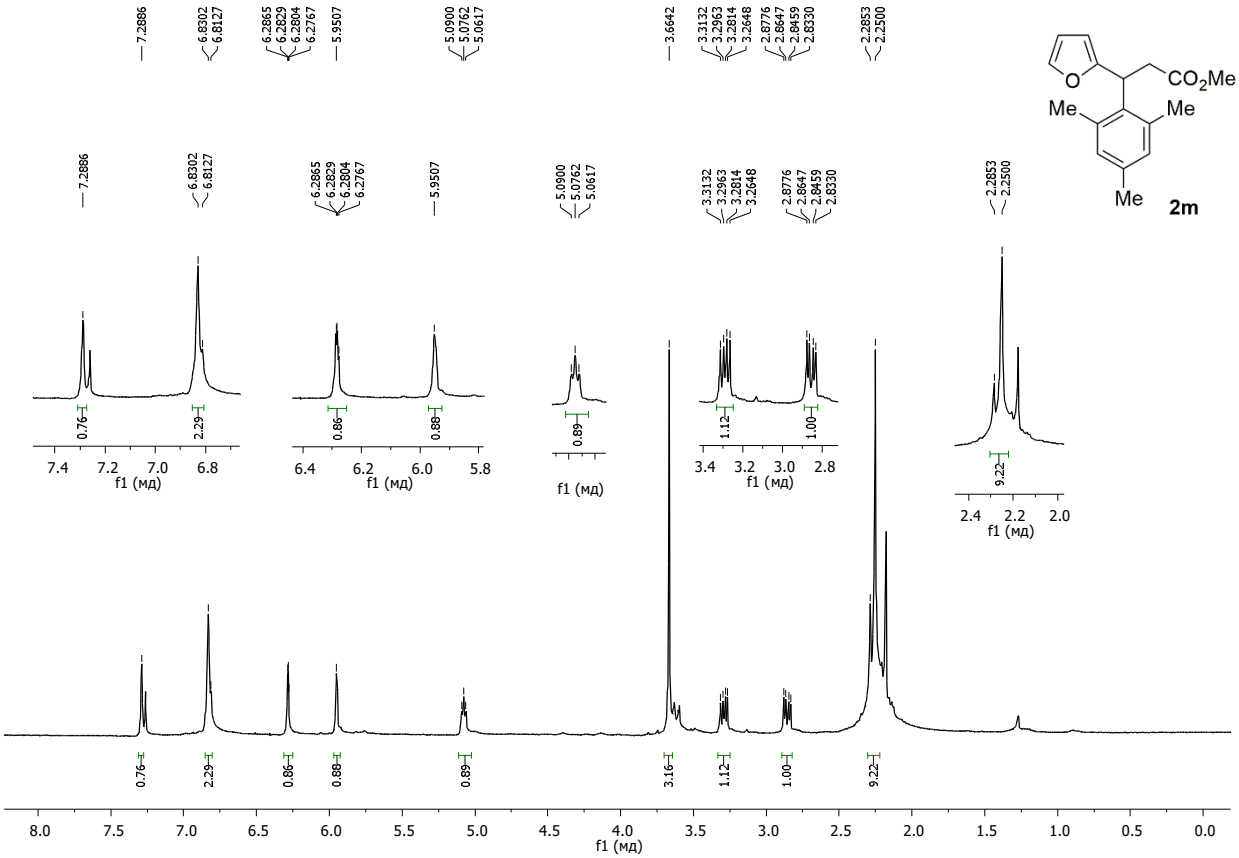


Figure S43. ^{1}H NMR spectrum of compound **2m** (500 MHz, $CDCl_3$).

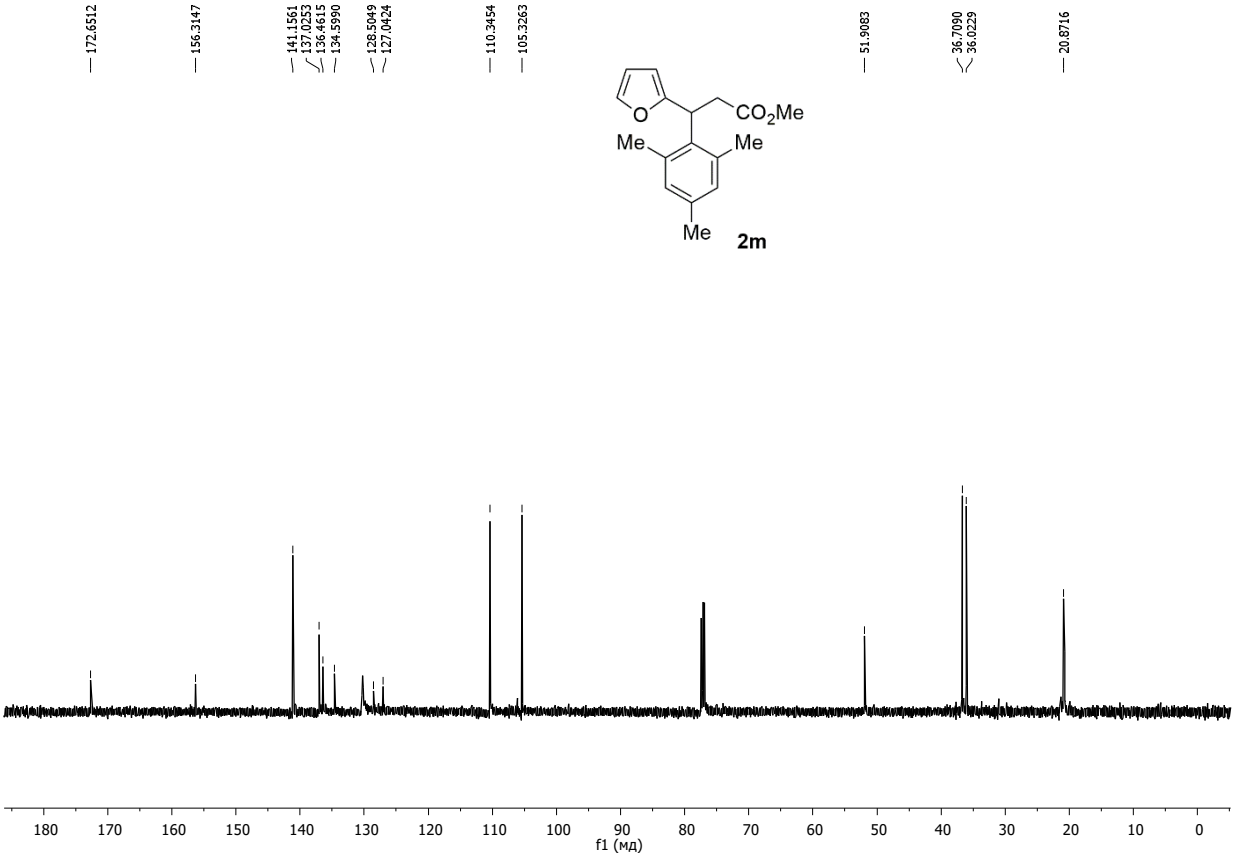


Figure S44. ^{13}C NMR spectrum of compound **2m** (125 MHz, $CDCl_3$).

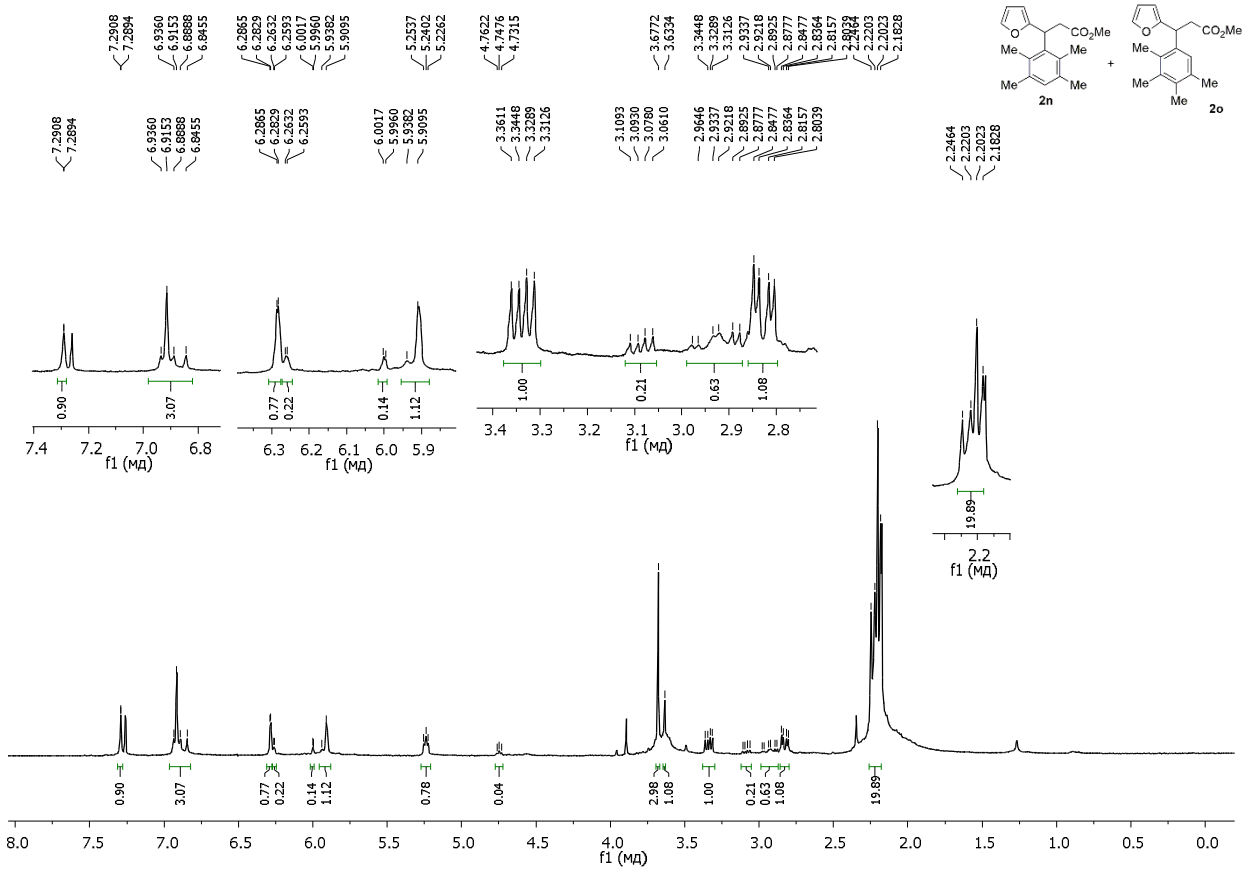


Figure S45. ^{1}H NMR spectrum of compound **2n** and **2o** (500 MHz, $CDCl_3$).

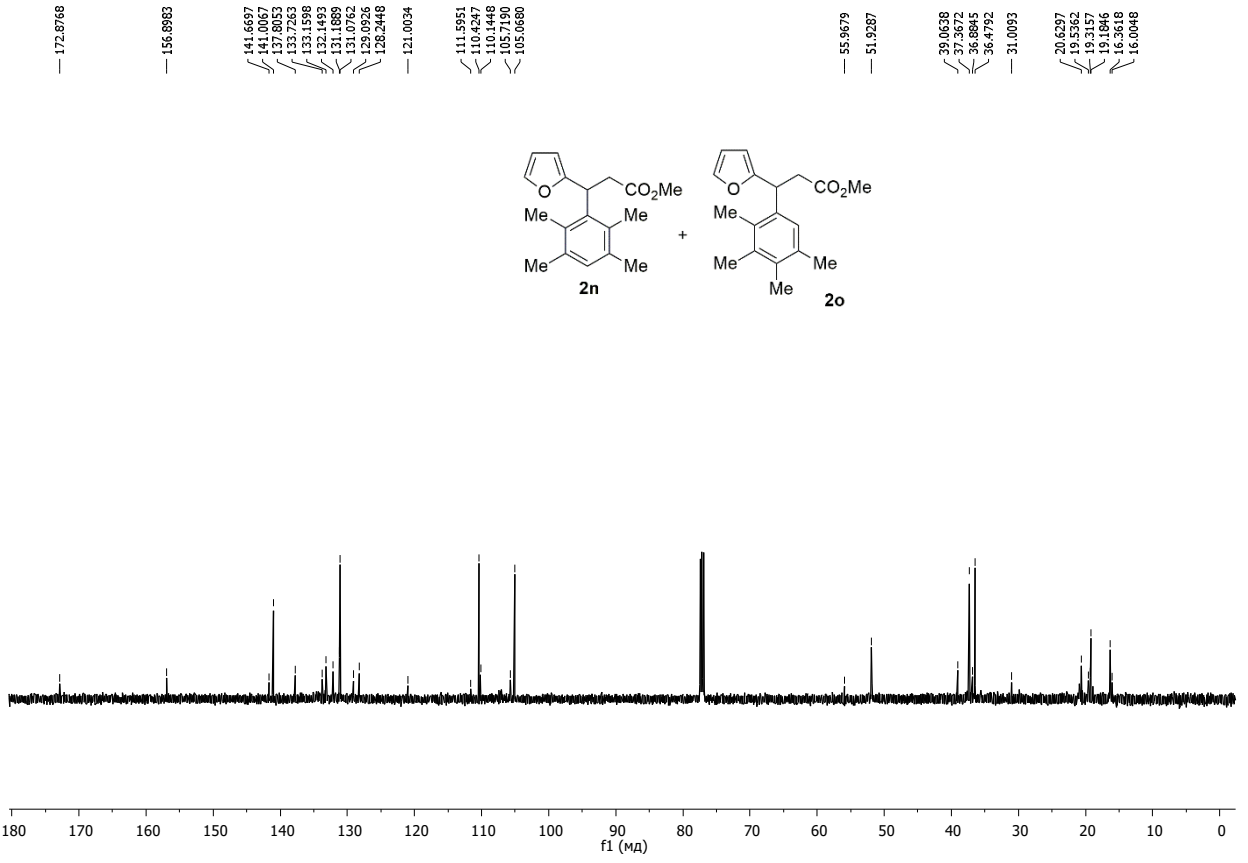


Figure S46. ^{13}C NMR spectrum of compounds **2n** and **2o** (125 MHz, $CDCl_3$).

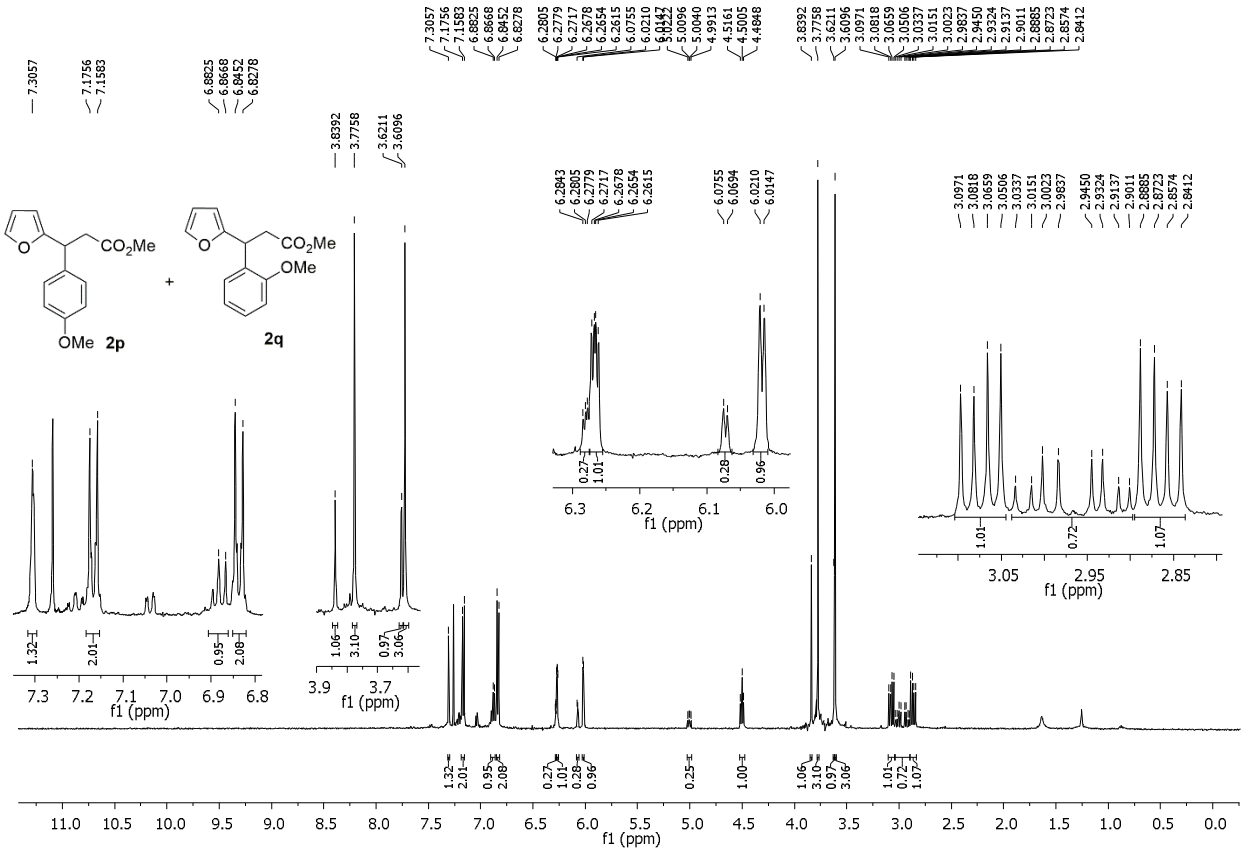


Figure S47. ^{1}H NMR spectrum of compounds **2p** and **2q** (500 MHz, $CDCl_3$).

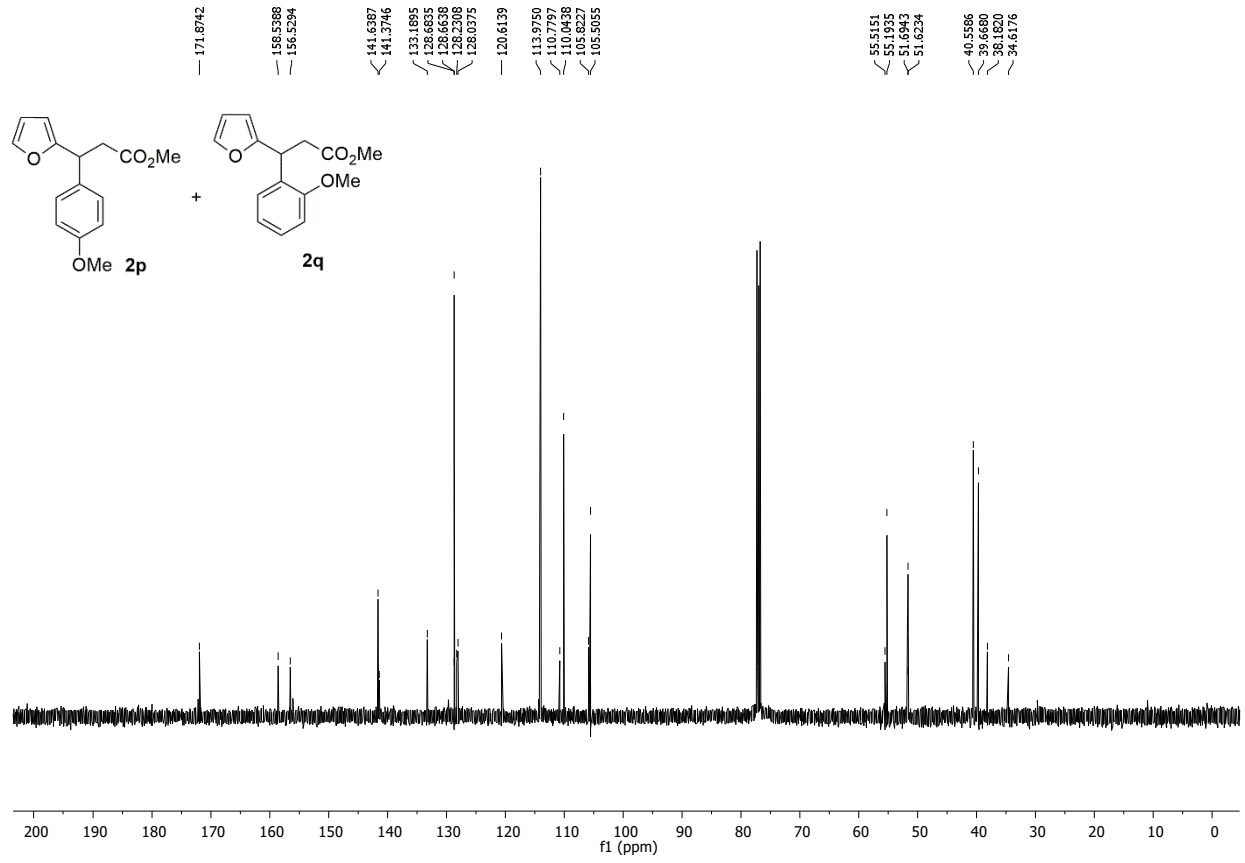


Figure S48. ^{13}C NMR spectrum of compounds **2p** and **2q** (125 MHz, $CDCl_3$).

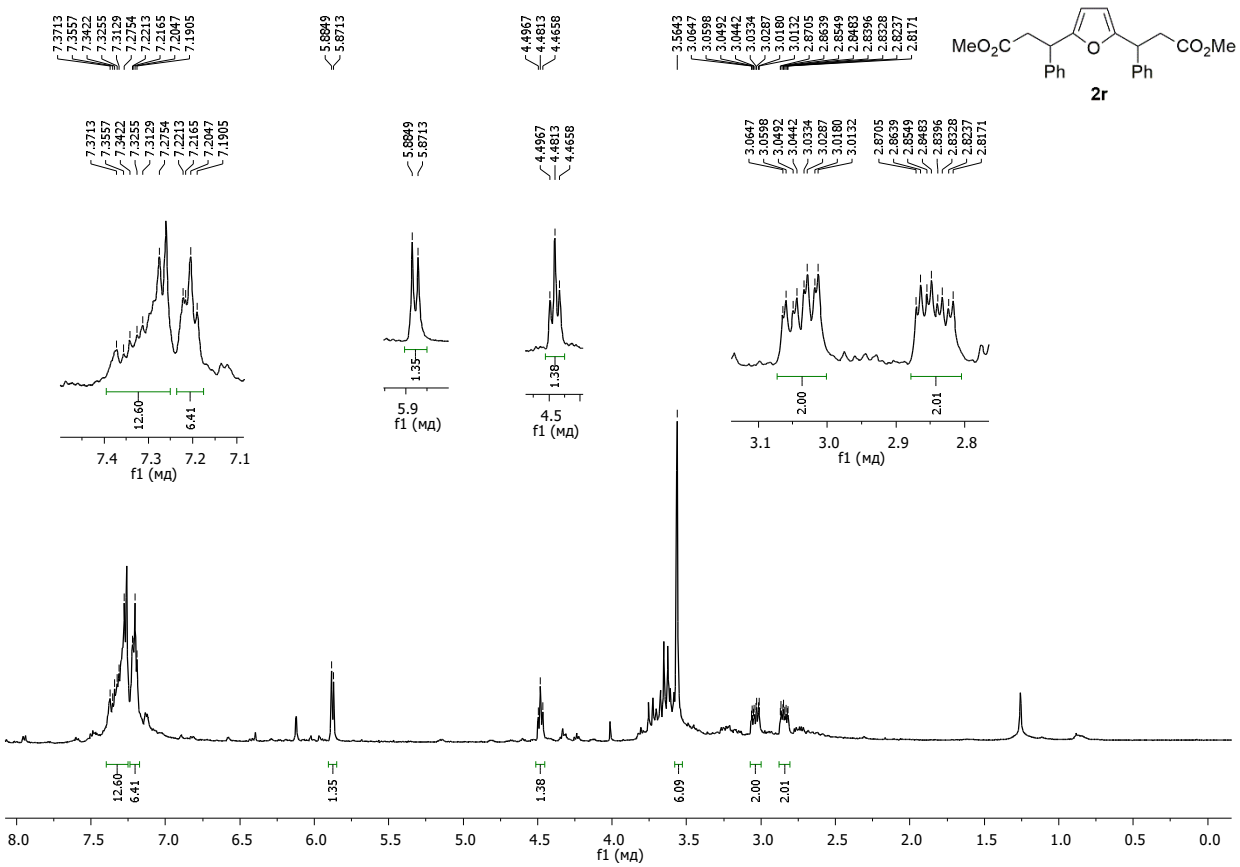


Figure S49. ^{1}H NMR spectrum of equimolar mixture of diastereomers of compound **2r** (500 MHz, $CDCl_3$).

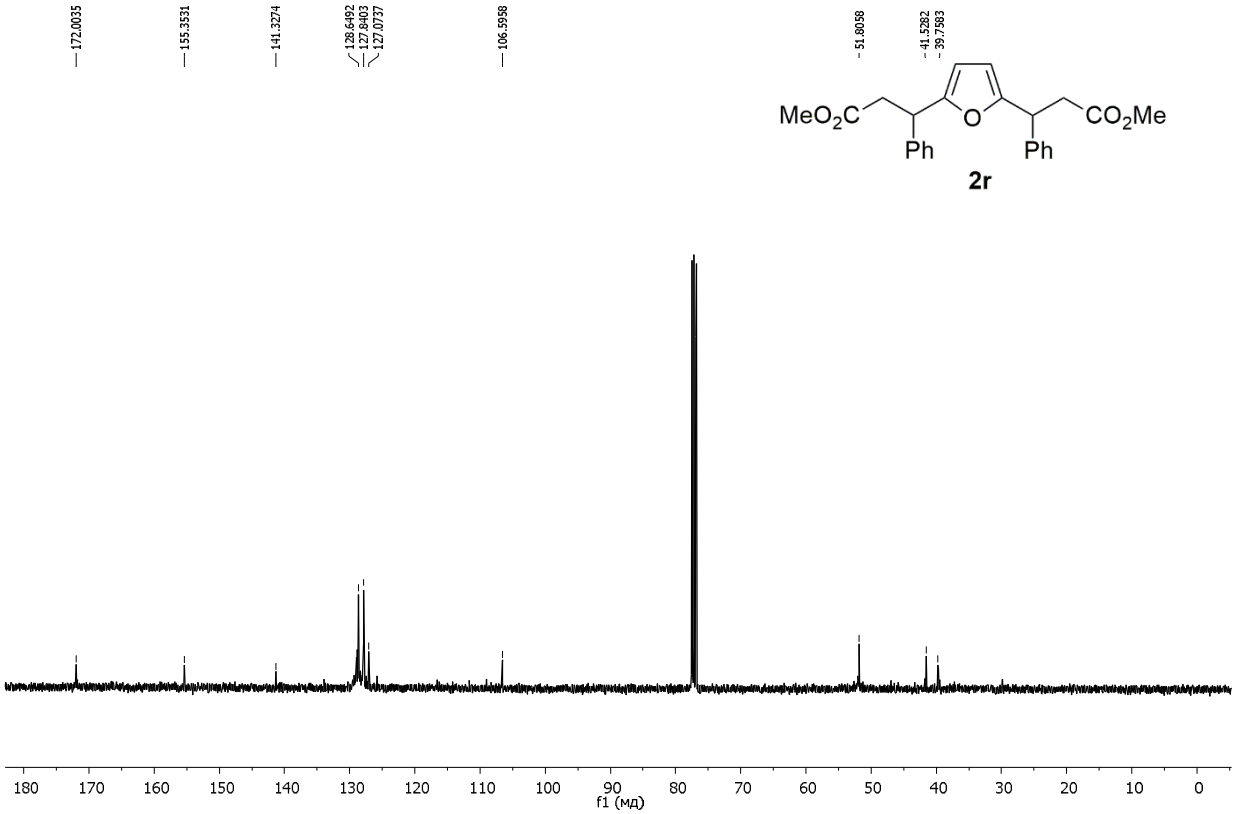


Figure S50. ^{13}C NMR spectrum of equimolar mixture of diastereomers of compound **2r** (125MHz, $CDCl_3$).

2. Results of study of oligomeric compounds by liquid chromatography-high-resolution mass-spectrometry

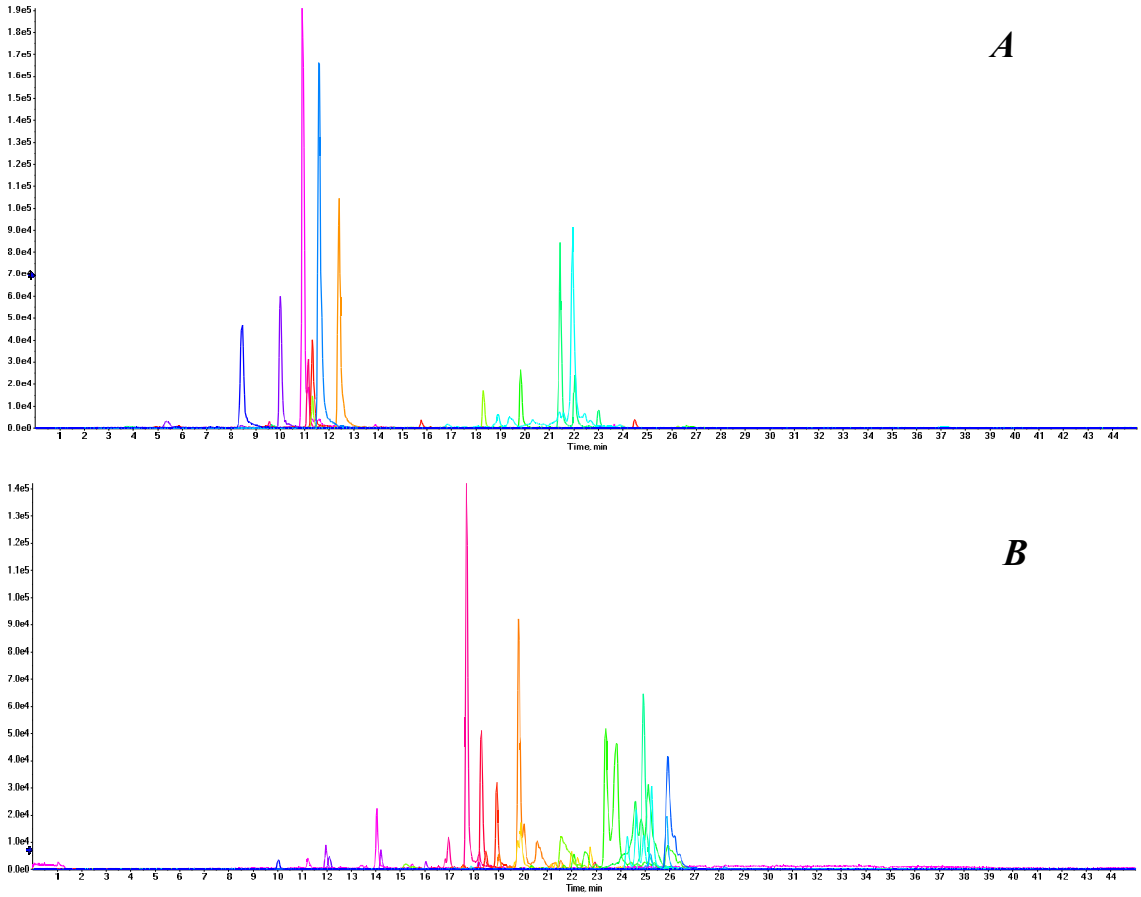


Figure S51.Reconstructed extracted ion chromatograms (XIC) of the products of **1a**(A) and **1b**(B) reactions with benzene in H_2SO_4

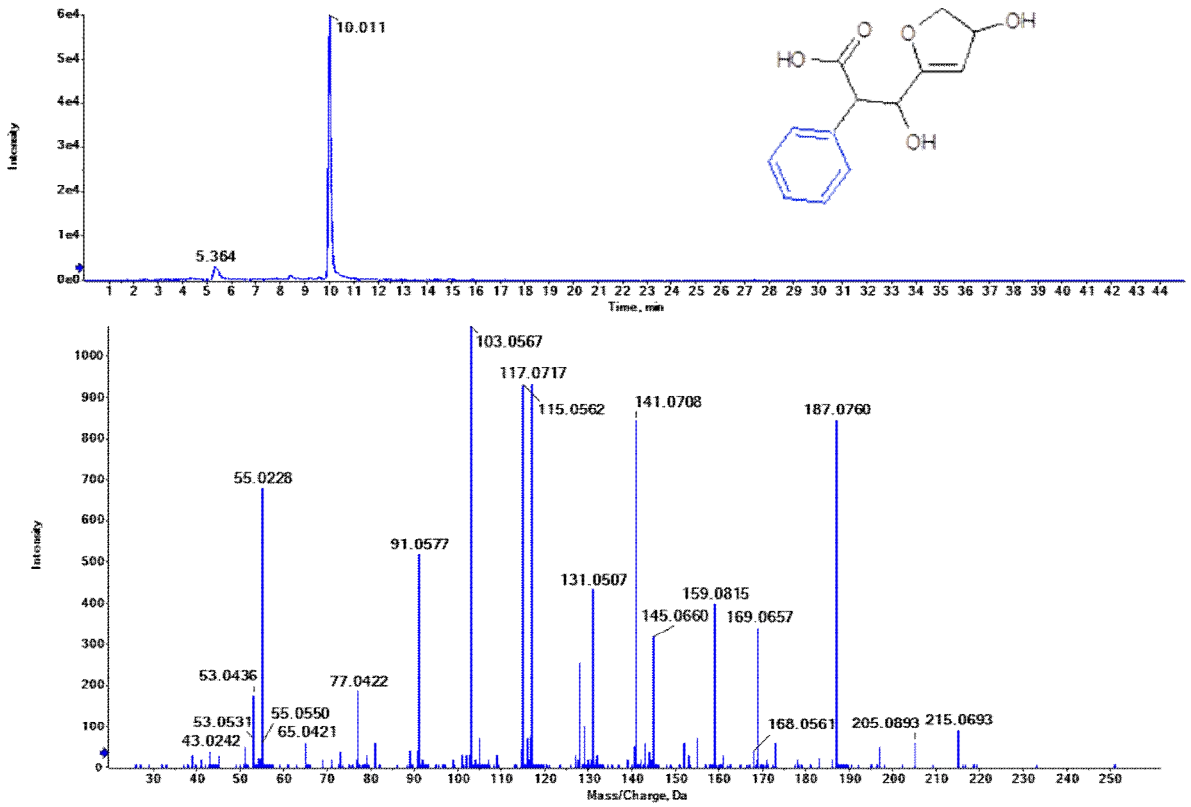


Figure S52. Accurate mass XIC chromatogram, tentative structural formula and MS/MS spectrum of the product of **1a** interaction with benzene in sulfuric acid medium with elemental composition $C_{13}H_{14}O_5$

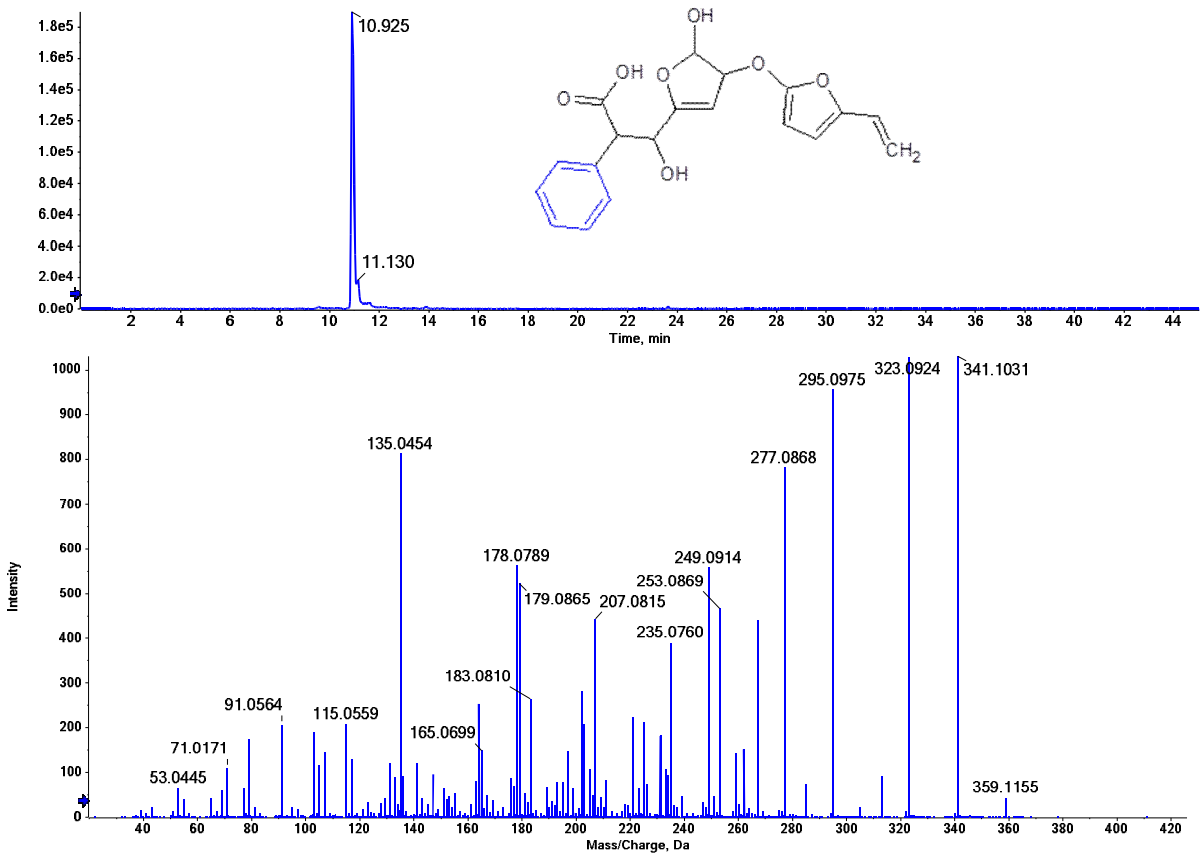


Figure S53. Accurate mass XIC chromatogram, tentative structural formula and MS/MS spectrum of the product of **1a** interaction with benzene in sulfuric acid medium with elemental composition $C_{19}H_{18}O_7$

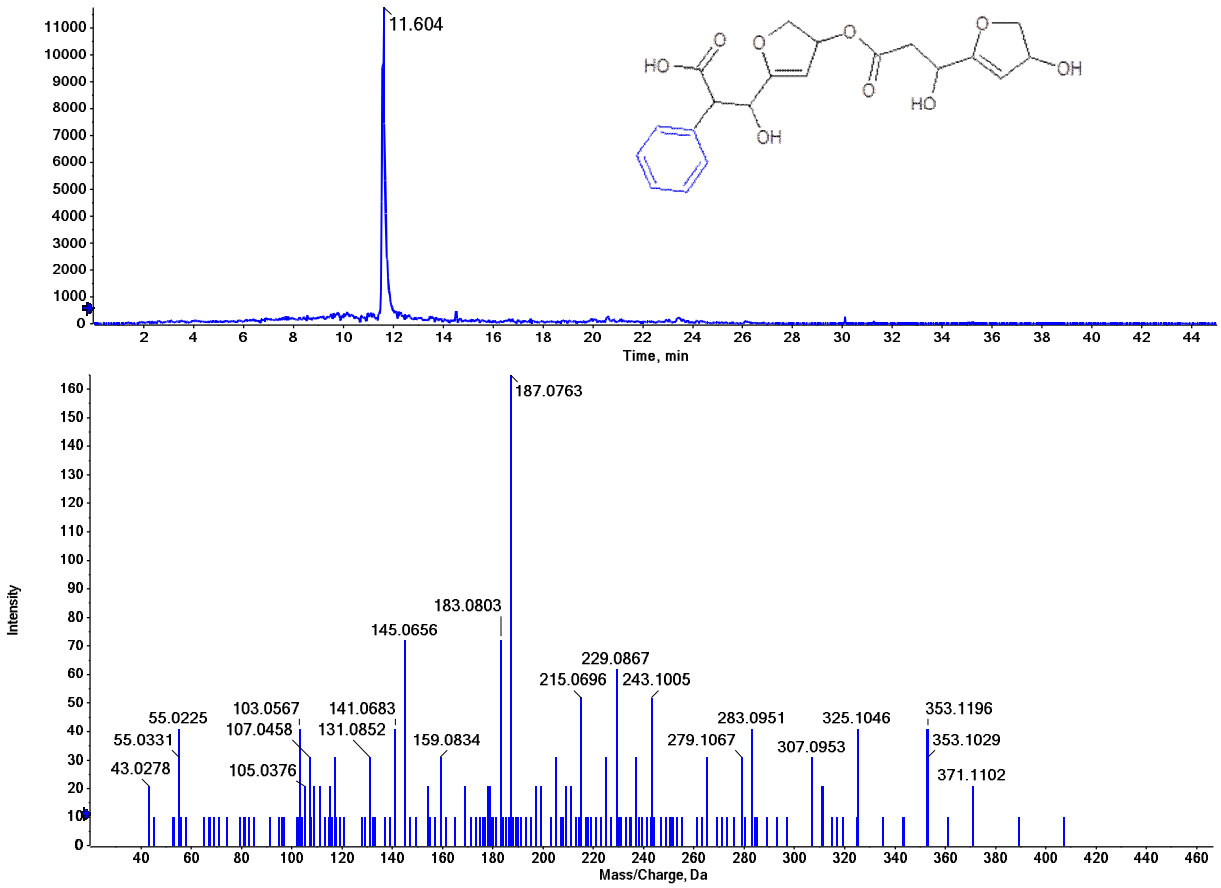


Figure S54. Accurate mass XIC chromatogram, tentative structural formula and MS/MS spectrum of the product of **1a** interaction with benzene in sulfuric acid medium with elemental composition $C_{20}H_{22}O_9$

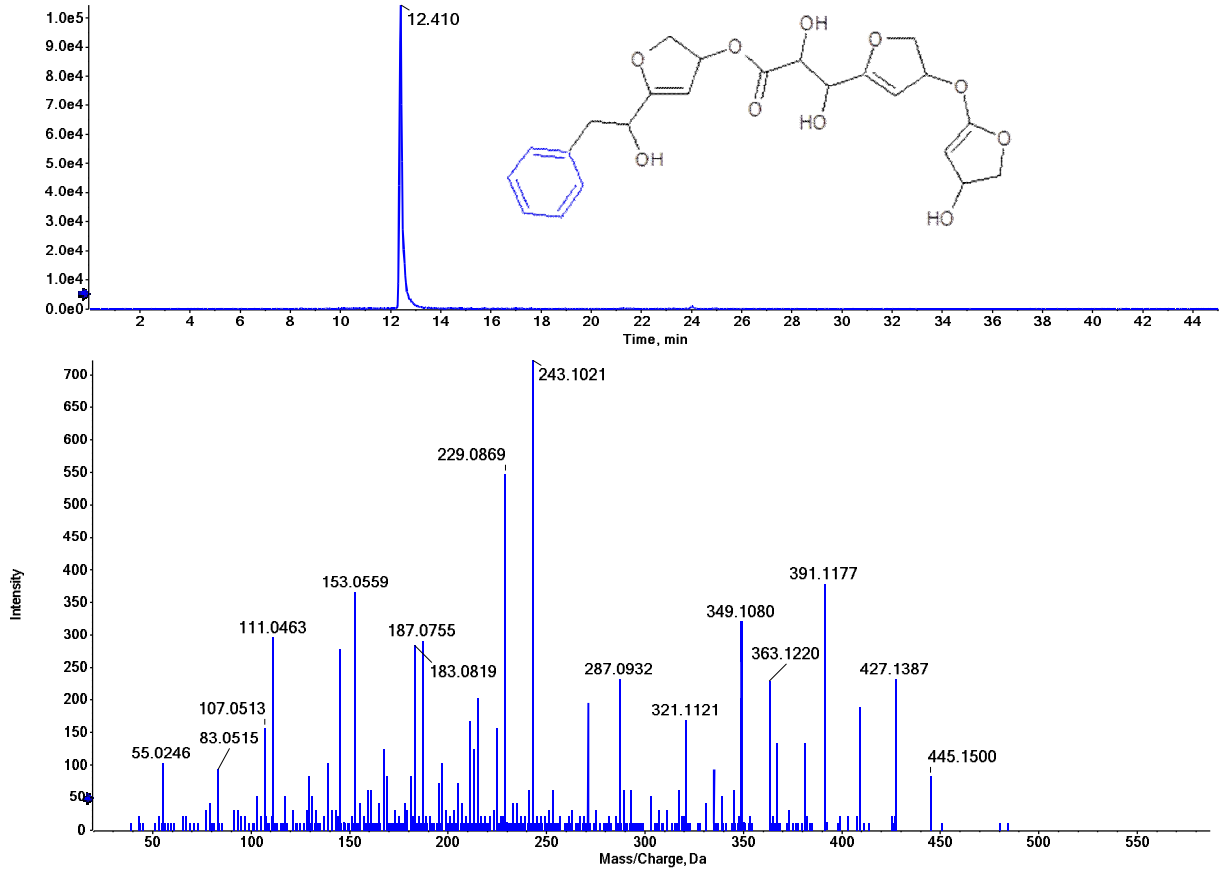


Figure S55. Accurate mass XIC chromatogram, tentative structural formula and MS/MS spectrum of the product of **1a** interaction with benzene in sulfuric acid medium with elemental composition $C_{23}H_{26}O_{10}$

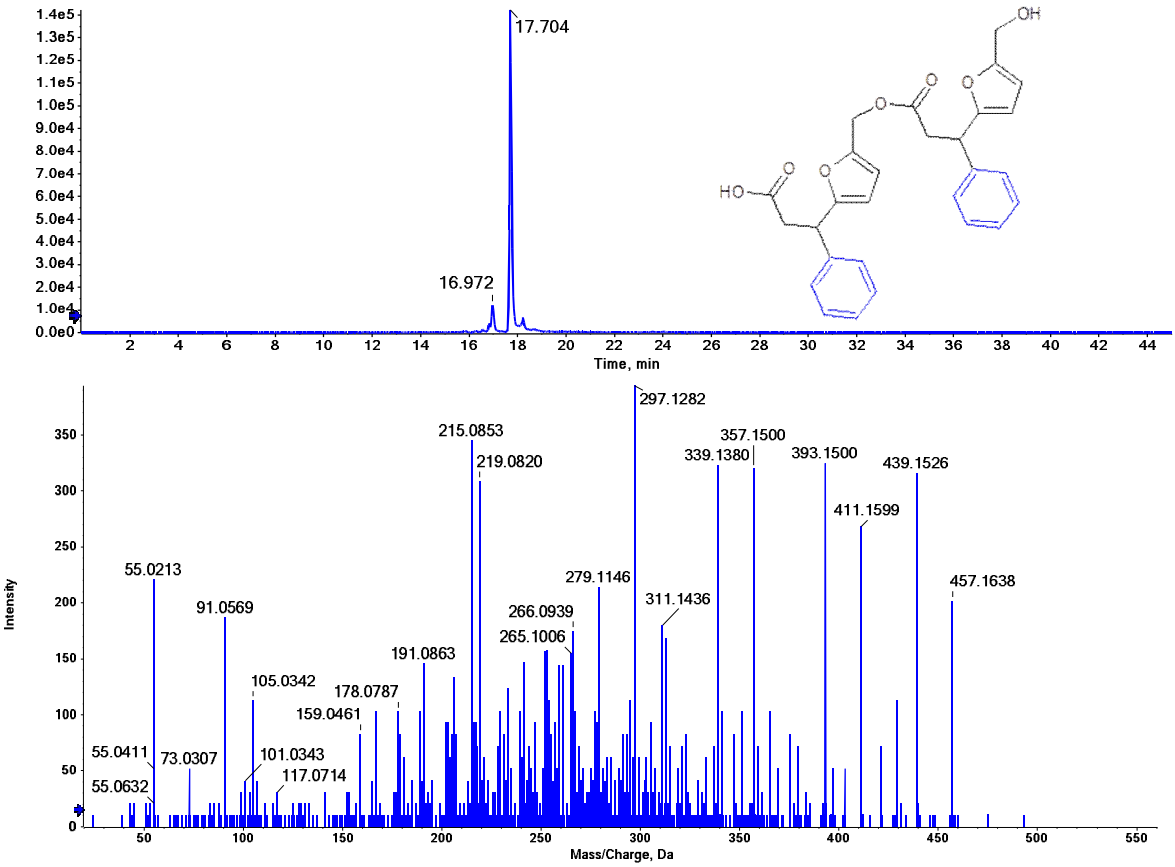


Figure S56. Accurate mass XIC chromatogram, tentative structural formula and MS/MS spectrum of the product of **1b** interaction with benzene in sulfuric acid medium with elemental composition $C_{28}H_{26}O_7$

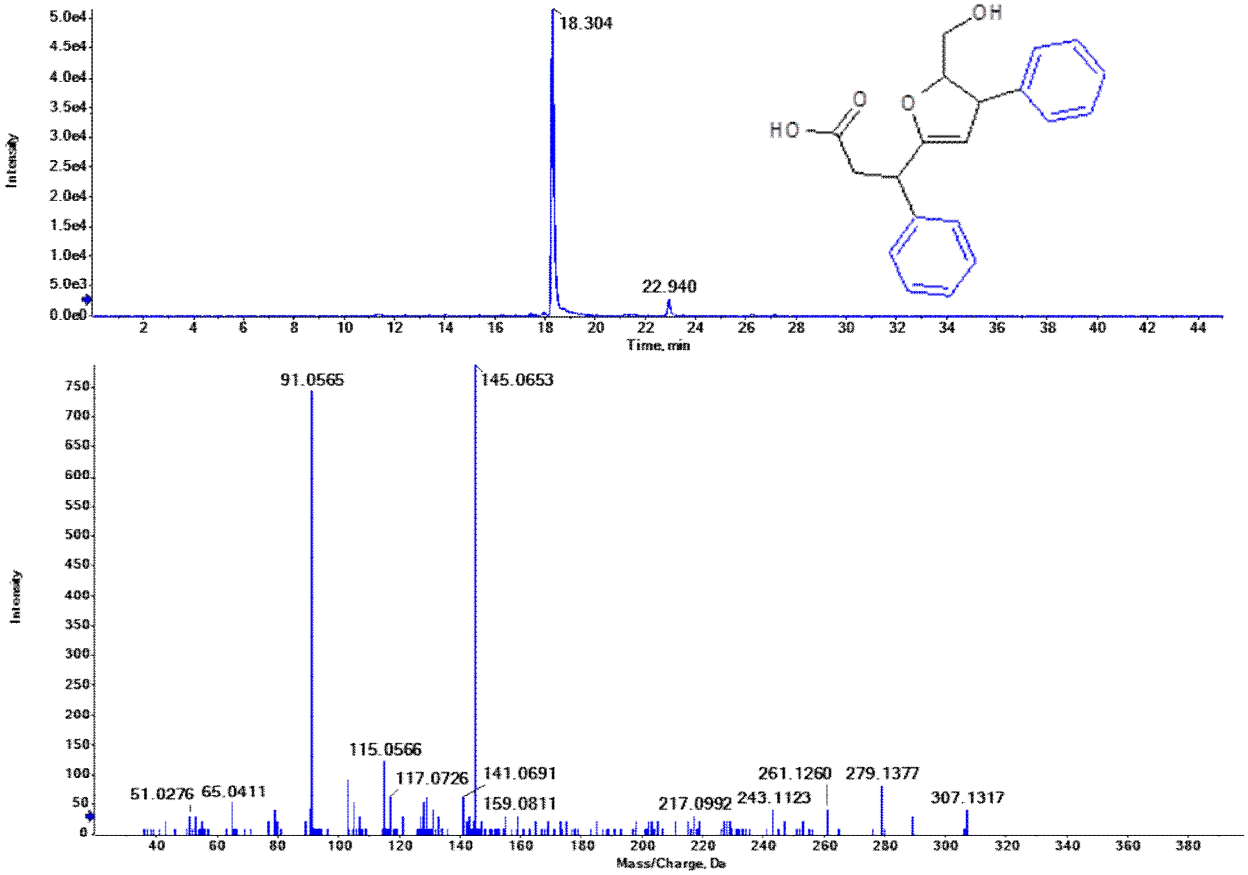


Figure S57. Accurate mass XIC chromatogram, tentative structural formula and MS/MS spectrum of the product of **1b** interaction with benzene in sulfuric acid medium with elemental composition $C_{20}H_{20}O_4$

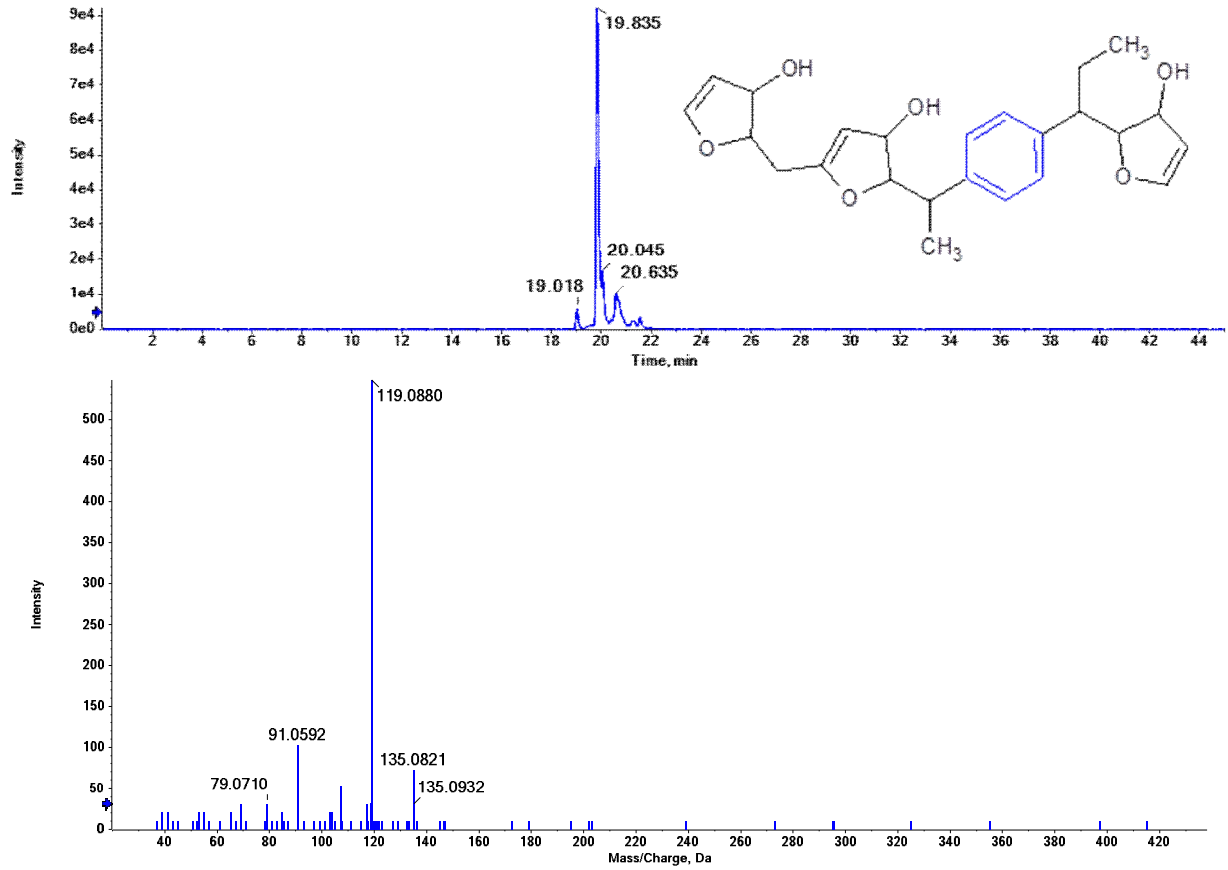


Figure S58. Accurate mass XIC chromatogram, tentative structural formula and MS/MS spectrum of the product of **1b** interaction with benzene in sulfuric acid medium with elemental composition $C_{24}H_{30}O_6$

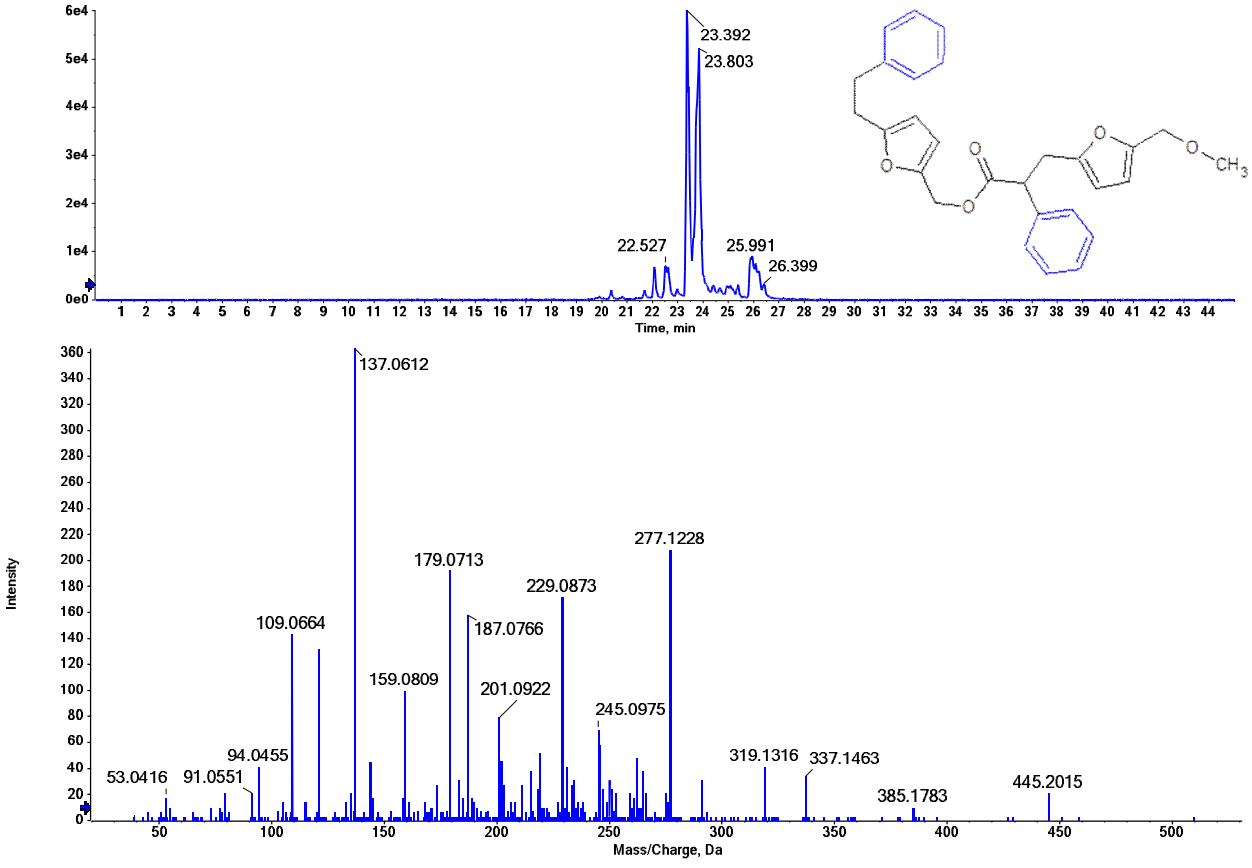


Figure S59. Accurate mass XIC chromatogram, tentative structural formula and MS/MS spectrum of the product of **1b** interaction with benzene in sulfuric acid medium with elemental composition $C_{28}H_{28}O_5$

3. Study of biological activity of compounds 1 and 2

MICs of furan compounds against *Escherichia coli* ATCC 25922, *Staphylococcus aureus* ATCC 29213, *Candida albicans* ATCC 10231 were determined using broth microdilution as described in ISO 20776-1:2019 and ISO 16256:2021. Stock solutions of furan compounds in neat (pure) DMSO were prepared in sterile tubes and used on the same day. Two-fold dilutions of the furan compounds in the appropriate culture medium were added to the wells of a 96-well plate. The final concentrations of the test substances (after inoculation) were 256, 128, 64, 32, 16, 8, 4, 2, 1 μg/ml. Solutions of furan compounds were added to the wells of the plates, 50 μl per well for *S. aureus* and *E. coli*, 100 μl for *C. albicans*.

RPMI-1640 medium, buffered with MOPS [3-(N-morpholino)propanesulfonic acid] containing l-glutamine and lacking sodium bicarbonate was used for *C. albicans*. The medium for *E. coli* and *S. aureus* was Mueller-Hinton broth. The fungus inoculum was prepared in the test medium and adjusted to match the turbidity of a 0.5 McFarland standard. A 1:100 dilution followed by a 1:20 dilution was performed for the yeast strain to obtain a final inoculum ranging from 0.5 to 2.5 x 10^3 CFU/ml. Then, 100 μl of fungal inoculum was added to each well containing furan compounds.

Bacterial inoculums were prepared in sterile sodium chloride solution and adjusted to 0.5 McFarland standard. A volume of 50 μl of this suspension was diluted in 10 ml of Mueller-Hinton broth until a concentration of approximately 5 × 10^5 CFU/ml was reached. Of this suspension, 50 μl was inoculated into each furan compounds-containing wells.

To ensure that the inoculum contained the required number of cells, the viability of the inoculum suspensions was counted. 100 μl of the inoculum was taken from the growth control tube immediately after inoculation and diluted in 9.9 ml of sodium chloride solution. 100 μl of this dilution was applied to the surface of a suitable agar plate (Sabouraud dextrose agar plate for *C. albicans*, Trypticase soy agar plate for *S. aureus*, *E. coli*) which were then incubated overnight.

After inoculation, the plates were incubated at 37 °C for 18 h for bacterial strains, 22 h for *C. albicans*. The susceptibility to furans was assessed on the basis of visual observation of growth the strains in the culture media. The minimal inhibitory concentration (MIC) is the lowest concentration of an antimicrobial that inhibits visible growth of a bacterial culture under a defined set of experimental conditions.

After incubation in the thermostat of agar plates with dose control inoculum, the number of cells contained in the wells of the plates was counted, taking into account the dilution with the test objects.

The number of cells, contained in the wells, was counted after incubation (with control of inoculum dose) taking into account the dilution with test objects. The number of culturable bacteria present per 1 ml of culture (CFU/ml) was 5.1×10^5 for *E. coli*, 4.9×10^5 for *S. aureus*, and 1.0×10^3 for *C.albicans*. Thus, control of the inoculum dose confirmed the required number of cells inoculated into the wells of the bacterial plate, ranging from $2x10^5$ CFU/ml to $8x10^5$ CFU/ml. For yeast-like microorganisms ranging from 0.5×10^3 to 2.5×10^3 CFU/ml.

The results were read in the presence of sufficient growth of the test organism (i.e. turbidity in the positive growth control) and the absence of growth in the uninoculated control. The amount of growth in each well was compared with the amount of growth in the positive growth control and the MIC was recorded as the lowest concentration of agent that completely inhibited growth according to Figure S60.

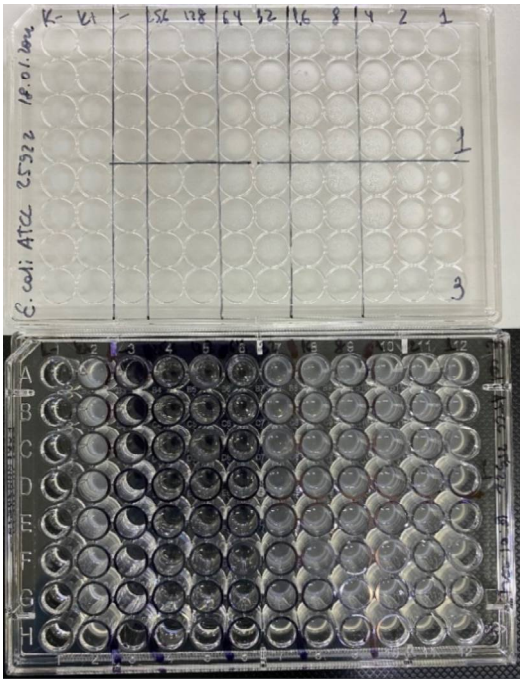


Figure S60. Plate inoculated with *E. coli* in the presence of test objects №1 and №3.

The results of the evaluation of the antimicrobial activity of the test objects are shown in Table S1.

Table S1. Evaluation of the antimicrobial activity of the test objects

Compounds	MIC, μg/ml		
	E. coli	*S. aureus*	*C. albicans*
2d	64	64	64
1a	64	128	64
3h	64	128	64
1g	64	128	64
1b	64	128	64
2e	128	128	64
2a	128	128	64
2k	128	128	64

2l	64	128	64
2p+2q	64	128	64
2j	128	128	64
2g	64	128	64
1e	64	128	64
1h	64	128	64
1d	128	128	64
1c	64	128	64
1f	64	128	64
1i	64	128	64
2i	64	>256	64
2m	64	>256	64
2n+2o	128	128	64
2b	128	128	64
2f	64	128	64
2r	>256	>256	64

4. ^{1}H and ^{13}C NMR spectra of cations Ae and Ah in TfOH

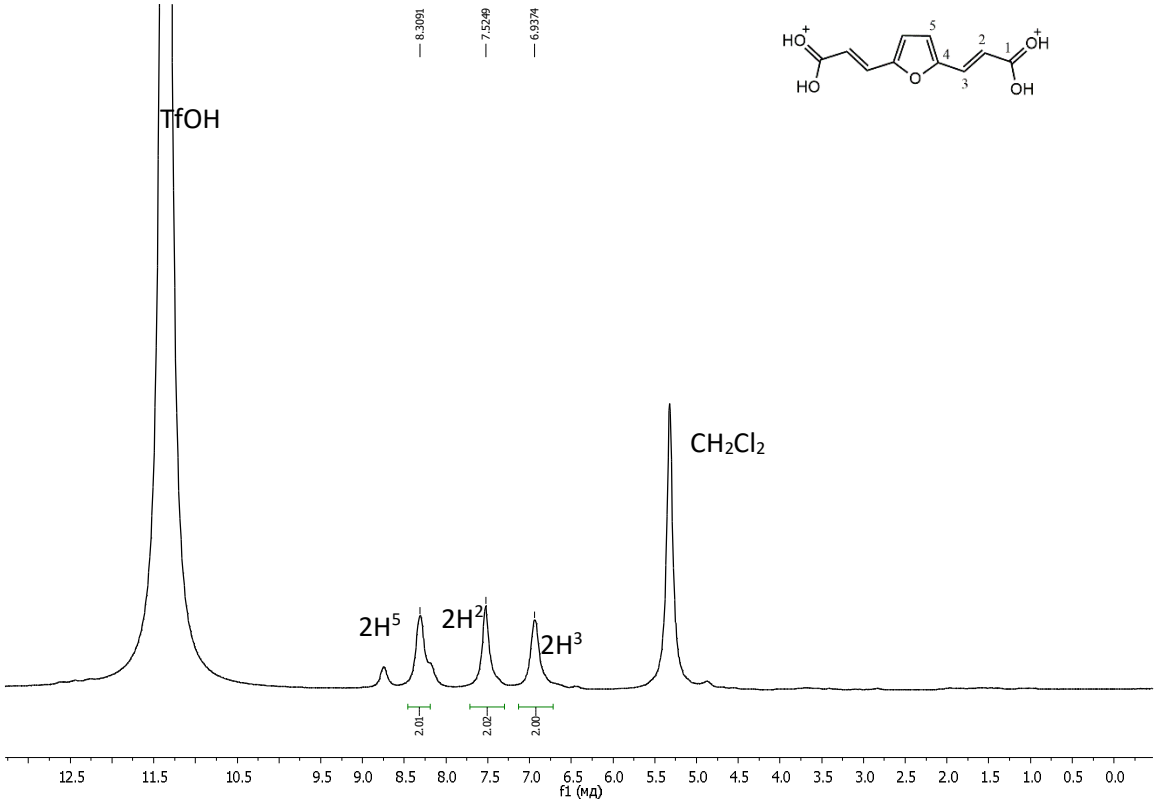


Figure S61. ^{1}H NMR spectrum of cation **Aa** in TFOH at room temperature (CH_2Cl_2 as internal standard, 400 MHz).

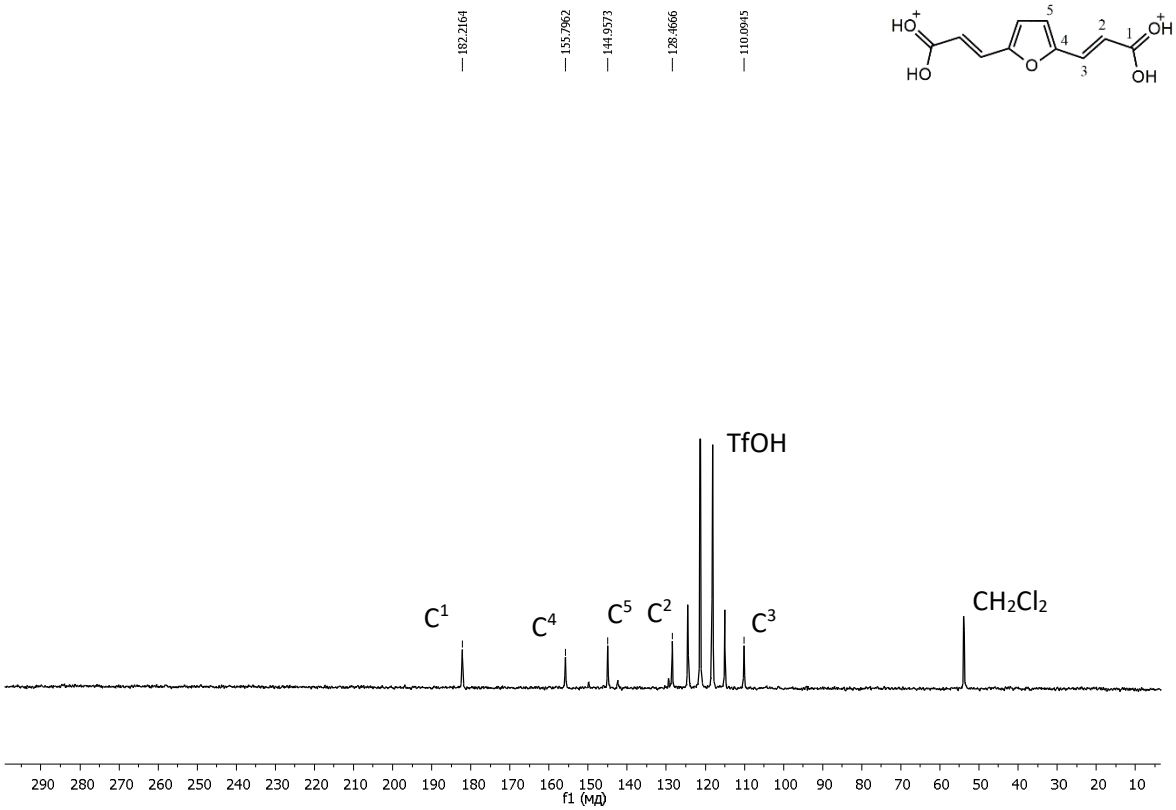


Figure S62. ^{13}C NMR spectrum of cation **Aa** in TfOH at room temperature (CH_2Cl_2 as internal standard, 100 MHz).

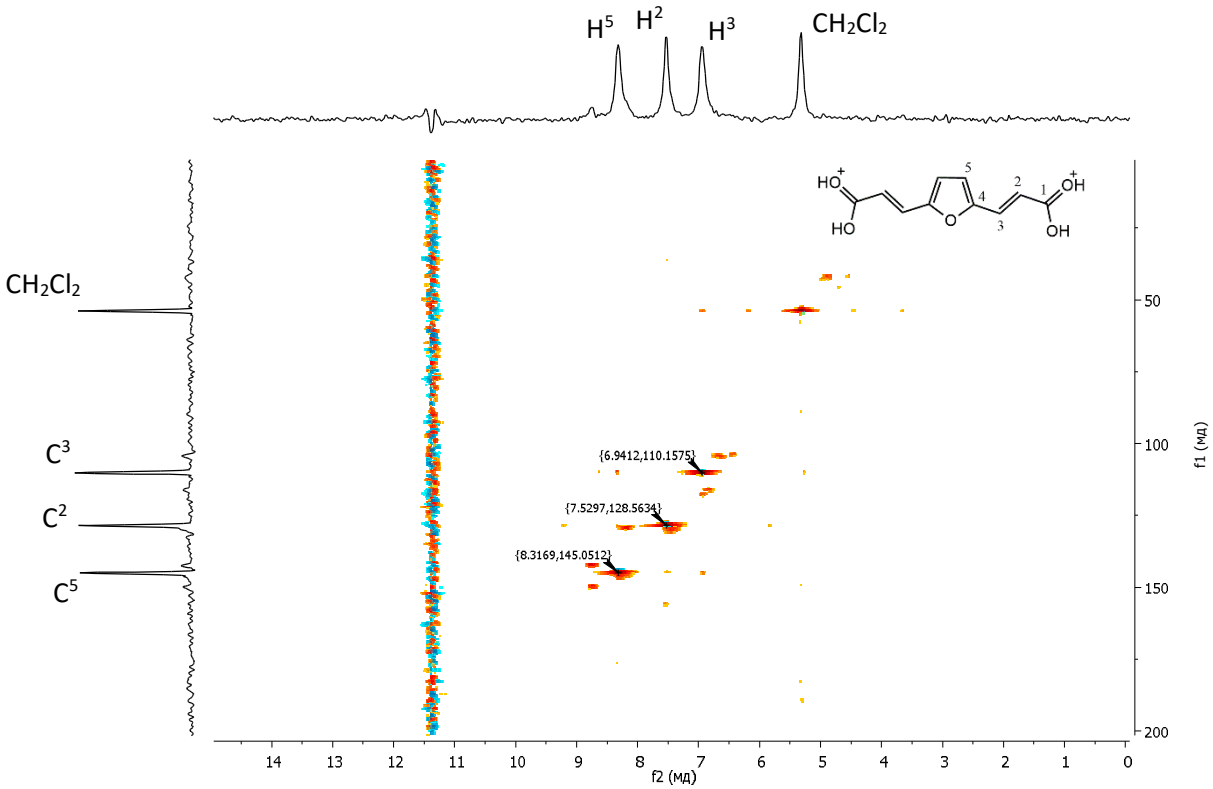


Figure S63. $^{1}H–^{13}C$ HSQC spectrum of cation **Aa** in TFOH at room temperature (CH_2Cl_2 as internal standard).

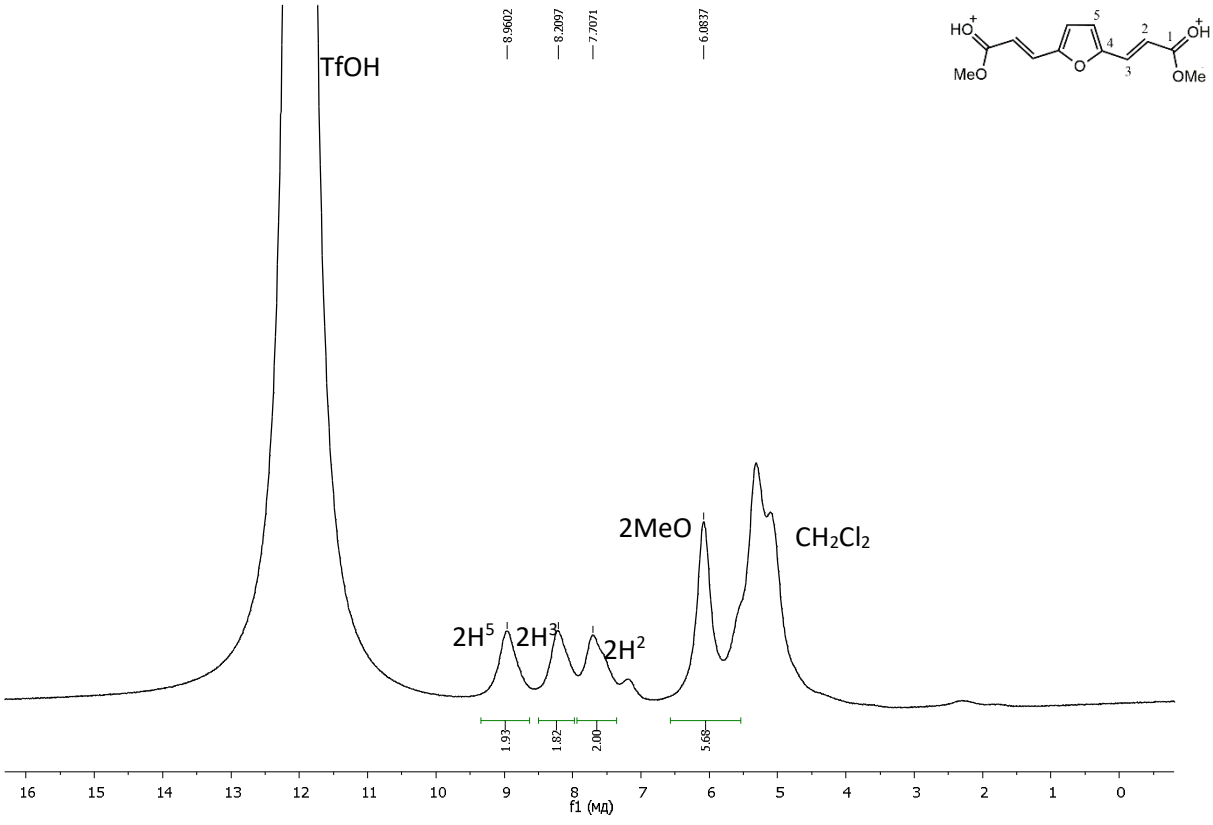


Figure S64. ^{1}H NMR spectrum of cation **Ah** in TFOH at room temperature (CH_2Cl_2 as internal standard, 400 MHz).

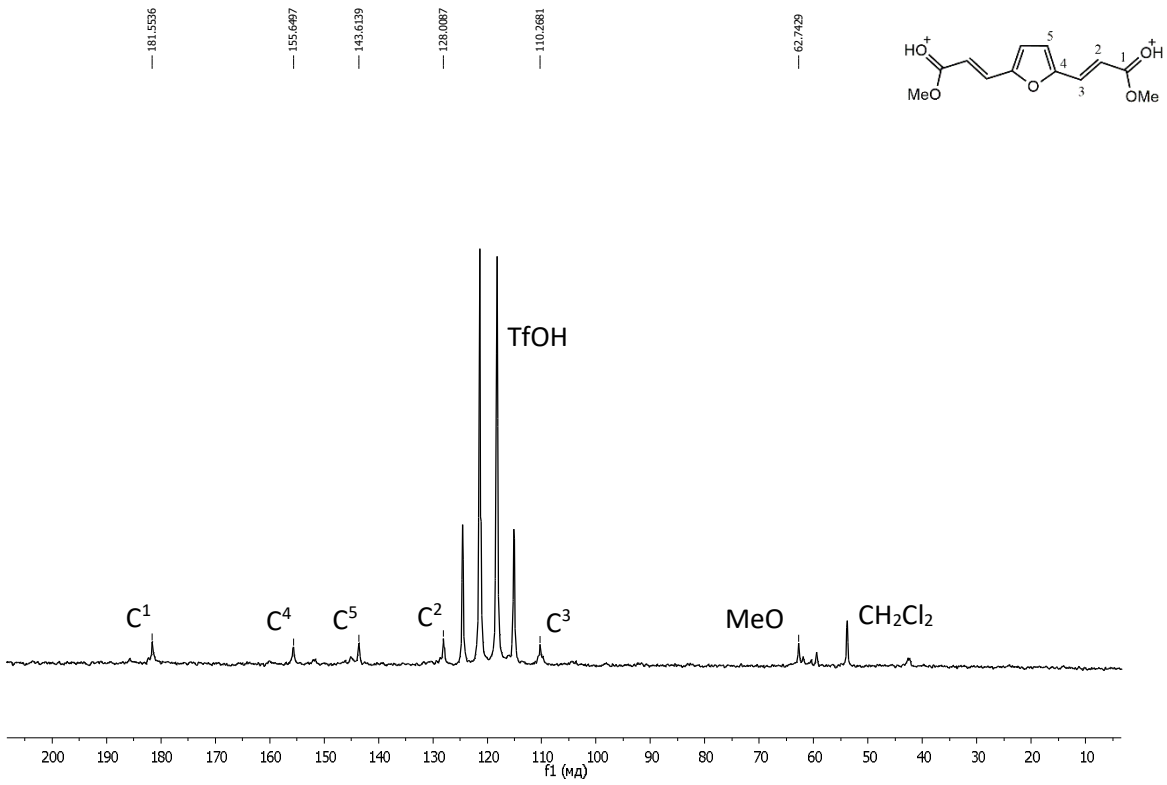


Figure S65. ^{13}C NMR spectrum of cation **Aa** in TfOH at room temperature (CH_2Cl_2 as internal standard, 100 MHz).

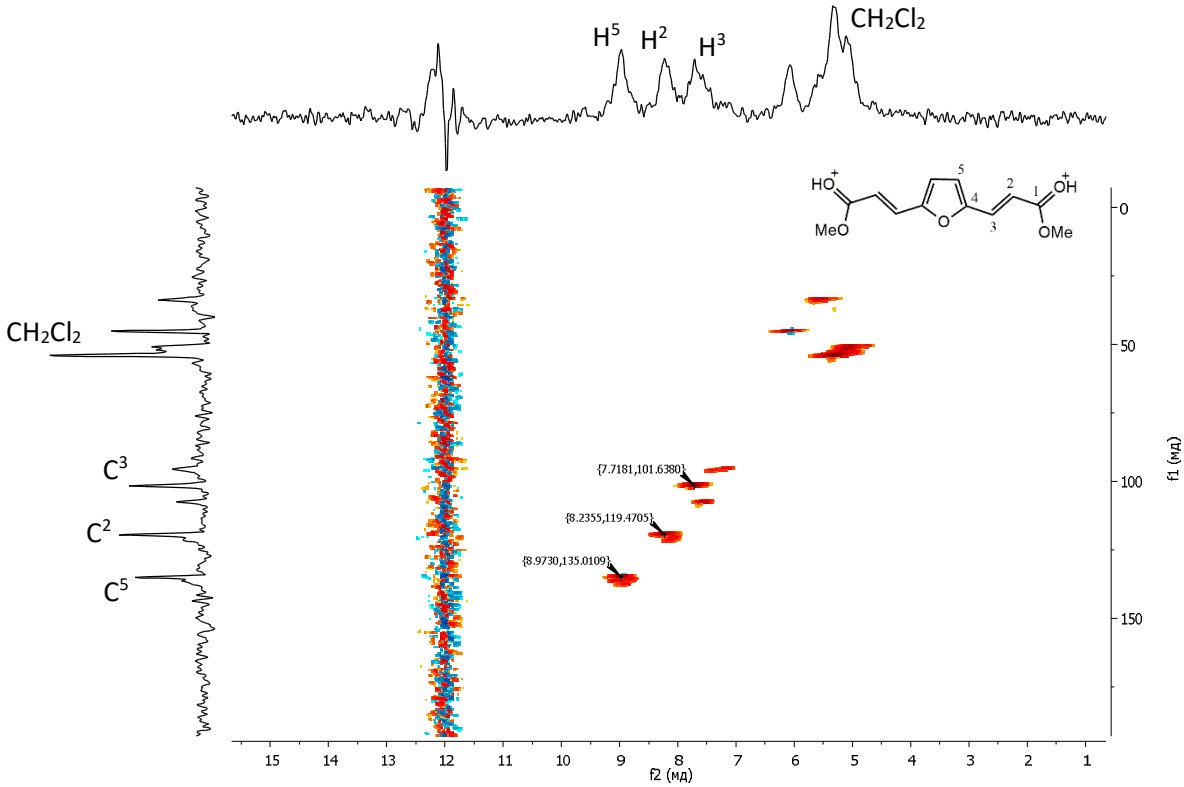


Figure S66. $^{1}H–^{13}C$ HSQC spectrum of cation **Ah** in TFOH at room temperature (CH_2Cl_2 as internal standard).

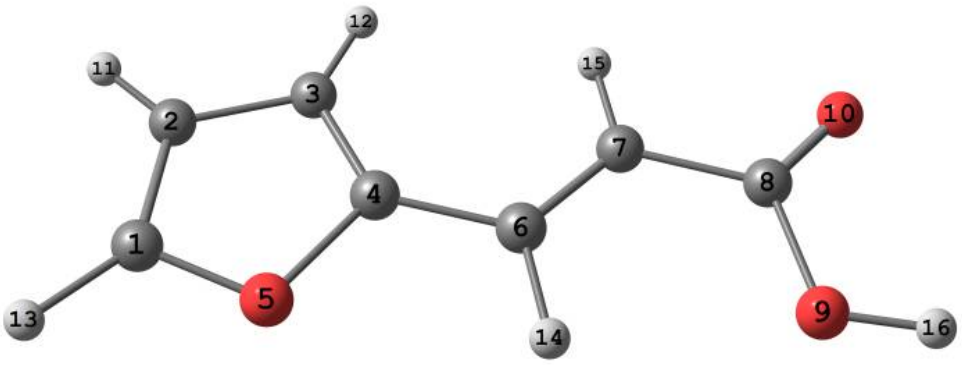
5. Data of DFT calculations of compounds 1 and species A-C

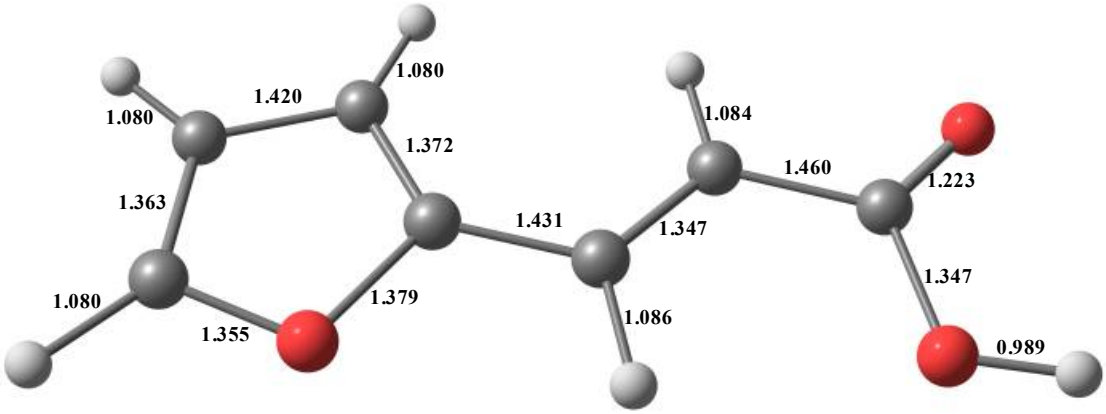
Compound 1a

Energy E(B3LYP) = -496.19161622 h, G^{298} = -496.110577 h, μ=4.70 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-3.027947	-1.366141	0.000000
2	C	-2.224016	-2.466232	0.000000
3	C	-0.888102	-1.983538	0.000000
4	C	-0.958886	-0.613335	0.000000
5	O	-2.284495	-0.233441	0.000000
6	C	0.000000	0.448866	0.000000
7	C	1.337883	0.289522	0.000000
8	C	2.289653	1.397185	0.000000
9	O	1.734516	2.624064	0.000000
10	O	3.502506	1.236274	0.000000
11	H	-2.549587	-3.495557	0.000000
12	H	0.017125	-2.572778	0.000000
13	H	-4.099510	-1.233439	0.000000
14	H	-0.418832	1.450835	0.000000
15	H	1.794946	-0.693384	0.000000
16	H	2.464129	3.291187	0.000000





Summary of Natural Population Analysis:

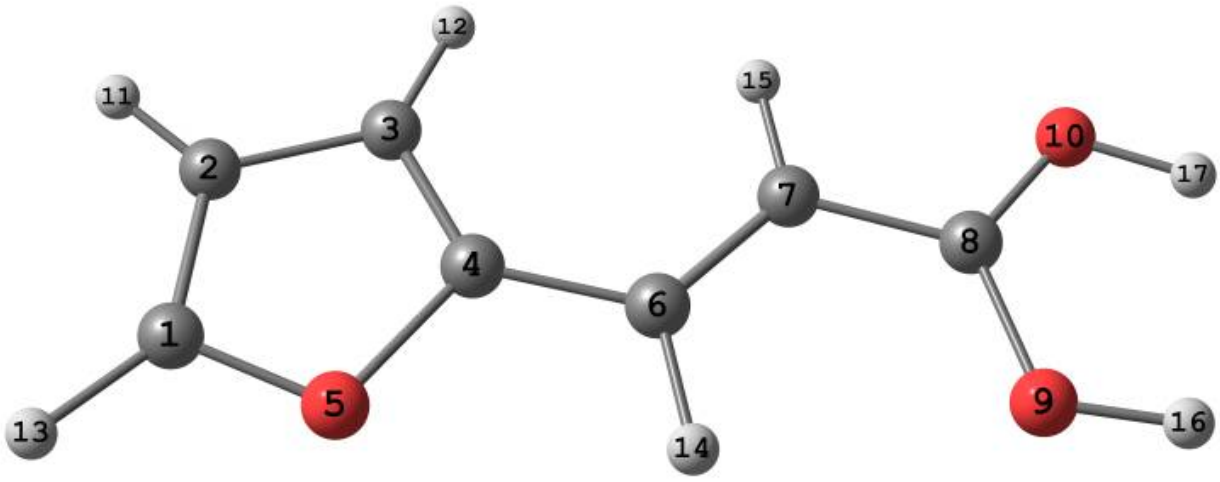
		Natural Population				
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.14732	1.99908	3.82860	0.02499	5.85268
C	2	-0.30733	1.99916	4.28940	0.01877	6.30733
C	3	-0.24174	1.99903	4.22559	0.01712	6.24174
C	4	0.23379	1.99893	3.74256	0.02472	5.76621
O	5	-0.46982	1.99973	6.44562	0.02448	8.46982
C	6	-0.15432	1.99904	4.13504	0.02025	6.15432
C	7	-0.31694	1.99899	4.29750	0.02045	6.31694
C	8	0.78286	1.99936	3.17937	0.03841	5.21714
O	9	-0.72431	1.99975	6.70199	0.02257	8.72431
O	10	-0.68539	1.99975	6.65927	0.02637	8.68539
H	11	0.24677	0.00000	0.75174	0.00150	0.75323
H	12	0.24755	0.00000	0.75094	0.00151	0.75245
H	13	0.22557	0.00000	0.77299	0.00144	0.77443
H	14	0.24433	0.00000	0.75338	0.00229	0.75567
H	15	0.23138	0.00000	0.76636	0.00226	0.76862
H	16	0.54030	0.00000	0.45665	0.00305	0.45970
* Total *		0.00000	19.99281	51.75702	0.25018	72.00000

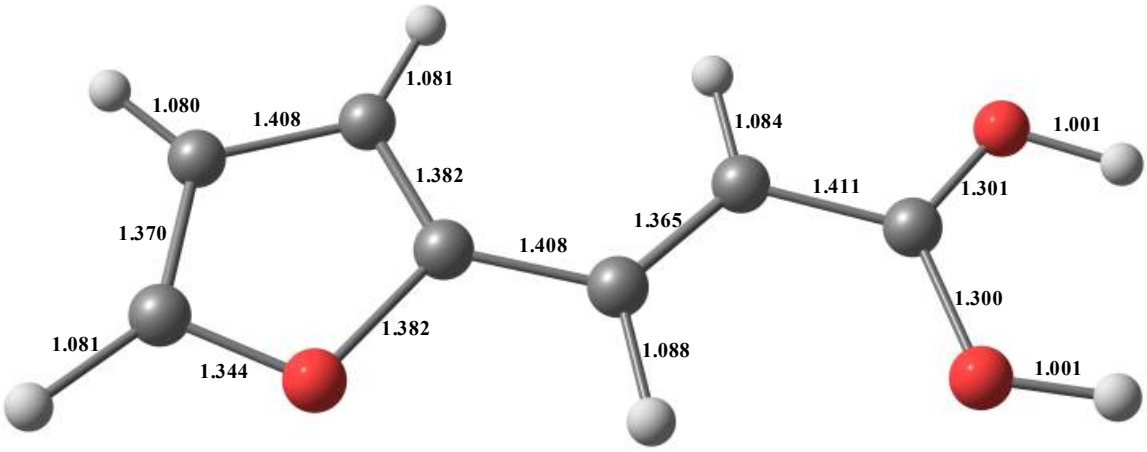
Aa

Energy E(B3LYP) = -496.618181837 h, G^{298} = -496.526579 h, μ=8.55 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-3.317050	-0.560987	-0.007732
2	C	-3.252289	0.807760	0.007338
3	C	-1.882605	1.135313	0.012156
4	C	-1.183261	-0.056741	0.000311
5	O	-2.087054	-1.101940	-0.011663
6	C	0.181271	-0.403138	-0.000794
7	C	1.215630	0.487248	-0.001413
8	C	2.561920	0.063782	-0.000418
9	O	2.862023	-1.201046	0.018913
10	O	3.478979	0.986465	-0.016317
11	H	-4.092403	1.485983	0.014379
12	H	-1.447214	2.124812	0.024337
13	H	-4.145838	-1.255051	-0.016987
14	H	0.394128	-1.469853	-0.002799
15	H	1.059464	1.559565	-0.005482
16	H	3.848952	-1.369610	0.012928
17	H	4.409633	0.616897	-0.010523





Summary of Natural Population Analysis:

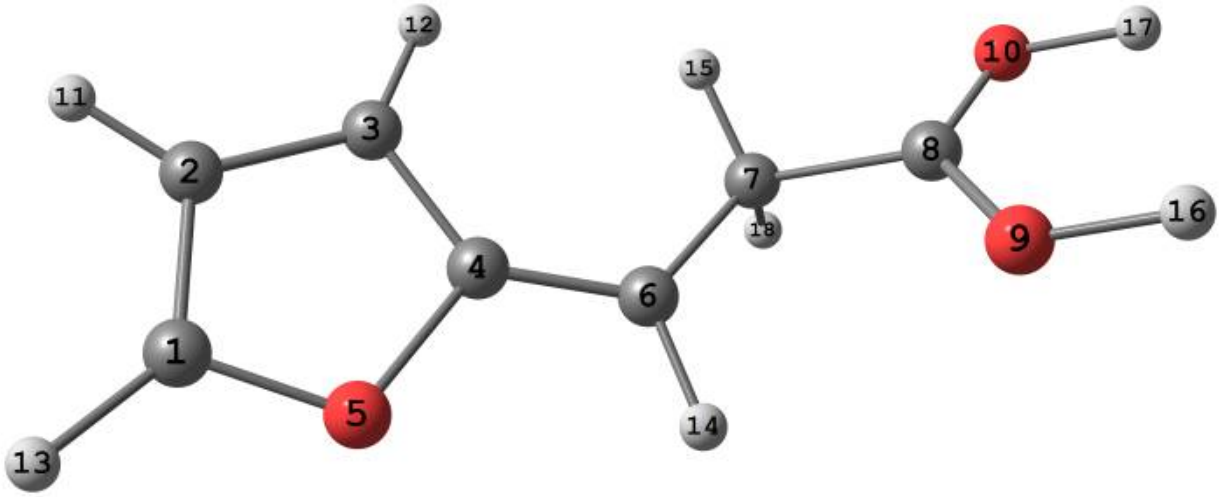
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	0.20254	1.99911	3.77398	0.02437	5.79746
C	2	-0.30190	1.99917	4.28414	0.01859	6.30190
C	3	-0.18516	1.99904	4.16950	0.01662	6.18516
C	4	0.21780	1.99893	3.75934	0.02393	5.78220
O	5	-0.45231	1.99972	6.42819	0.02440	8.45231
C	6	-0.07691	1.99905	4.05898	0.01888	6.07691
C	7	-0.35467	1.99901	4.33509	0.02057	6.35467
C	8	0.82651	1.99922	3.14489	0.02938	5.17349
O	9	-0.64670	1.99970	6.62277	0.02423	8.64670
O	10	-0.63609	1.99970	6.61199	0.02439	8.63609
H	11	0.25603	0.00000	0.74249	0.00148	0.74397
H	12	0.25687	0.00000	0.74169	0.00144	0.74313
H	13	0.23420	0.00000	0.76443	0.00137	0.76580
H	14	0.25691	0.00000	0.74100	0.00209	0.74309
H	15	0.25697	0.00000	0.74115	0.00189	0.74303
H	16	0.57425	0.00000	0.42304	0.00271	0.42575
H	17	0.57167	0.00000	0.42566	0.00267	0.42833
* Total *		1.00000	19.99265	51.76833	0.23902	72.00000

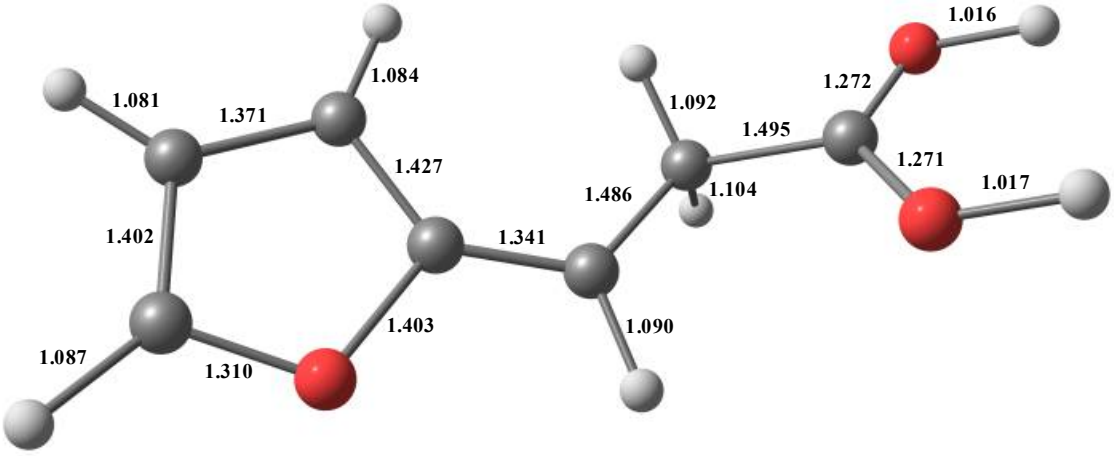
Ba

Energy E(B3LYP) = -497.007336659 h, G^{298} = -496.906348 h, μ=7.35 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.258420	-0.501921	-0.135622
2	C	3.099554	0.867914	-0.387335
3	C	1.769372	1.135311	-0.188885
4	C	1.141770	-0.090732	0.185016
5	O	2.133381	-1.082946	0.199758
6	C	-0.110654	-0.451767	0.501286
7	C	-1.249070	0.499328	0.592692
8	C	-2.511468	0.022422	-0.050065
9	O	-2.544681	-1.155137	-0.528300
10	O	-3.477003	0.849887	-0.061858
11	H	3.886554	1.549302	-0.680344
12	H	1.268459	2.091272	-0.294336
13	H	4.141532	-1.134949	-0.175888
14	H	-0.288749	-1.499107	0.747269
15	H	-1.030739	1.495595	0.201742
16	H	-3.437798	-1.417157	-0.938407
17	H	-4.323638	0.497463	-0.498420
18	H	-1.496734	0.639817	1.659068





Summary of Natural Population Analysis:

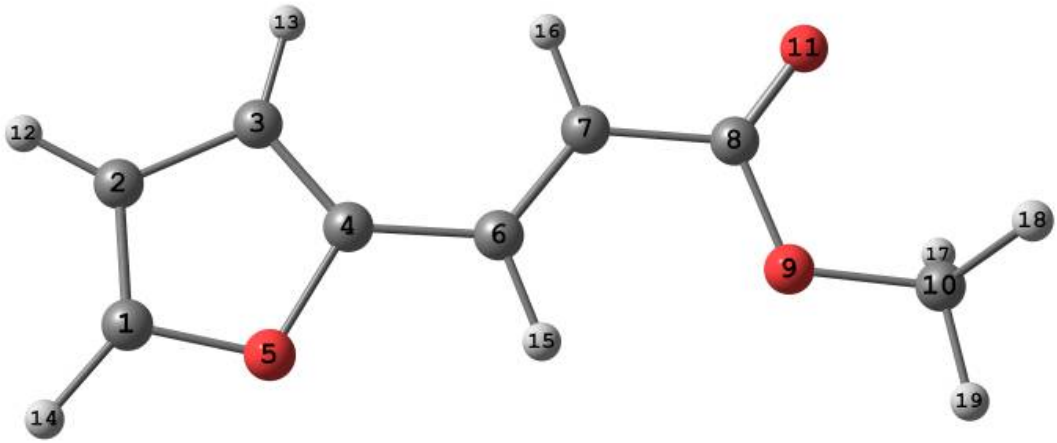
Natural Population

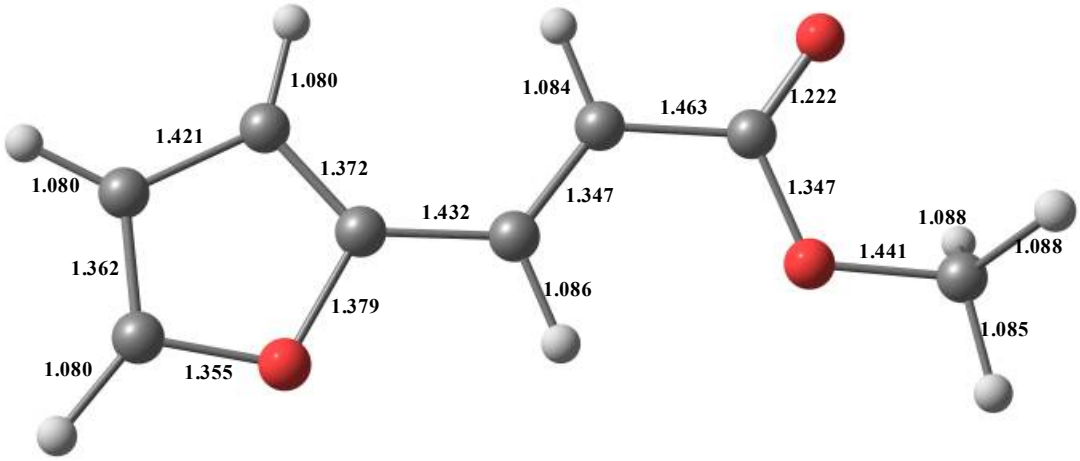
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.38115	1.99921	3.59599	0.02364	5.61885
C	2	-0.27540	1.99916	4.25781	0.01843	6.27540
C	3	-0.07009	1.99906	4.05440	0.01663	6.07009
C	4	0.22676	1.99882	3.75198	0.02244	5.77324
O	5	-0.41138	1.99971	6.38624	0.02543	8.41138
C	6	0.02001	1.99897	3.96280	0.01821	5.97999
C	7	-0.54328	1.99911	4.52438	0.01979	6.54328
C	8	0.94165	1.99944	3.02790	0.03101	5.05835
O	9	-0.59868	1.99967	6.57423	0.02478	8.59868
O	10	-0.59553	1.99967	6.57079	0.02507	8.59553
H	11	0.28358	0.00000	0.71504	0.00138	0.71642
H	12	0.28120	0.00000	0.71722	0.00158	0.71880
H	13	0.26204	0.00000	0.73676	0.00120	0.73796
H	14	0.28167	0.00000	0.71636	0.00198	0.71833
H	15	0.29133	0.00000	0.70703	0.00164	0.70867
H	16	0.60282	0.00000	0.39464	0.00254	0.39718
H	17	0.59948	0.00000	0.39794	0.00258	0.40052
H	18	0.32266	0.00000	0.67576	0.00158	0.67734
* Total *		2.00000	19.99281	51.76727	0.23992	72.00000

Compound 1g
Energy E(B3LYP) = -535.494711806 h, G^{298} = -535.387039 h, μ=4.49 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.654663	-0.789203	0.000338
2	C	3.752951	0.569535	-0.000016
3	C	2.421545	1.065770	-0.000371
4	C	1.589160	-0.024609	-0.000099
5	O	2.354477	-1.171886	0.000496
6	C	0.170757	-0.218445	-0.000174
7	C	-0.751044	0.763225	-0.000712
8	C	-2.195979	0.534422	-0.000080
9	O	-2.550297	-0.765577	-0.000874
10	C	-3.963929	-1.042715	0.000092
11	O	-3.016884	1.439070	0.001160
12	H	4.666974	1.144003	-0.000098
13	H	2.112975	2.100772	-0.000781
14	H	4.385631	-1.583744	0.000656
15	H	-0.153134	-1.254943	0.000365
16	H	-0.468562	1.810045	-0.001180
17	H	-4.432215	-0.626482	0.889606
18	H	-4.433555	-0.625521	-0.888265
19	H	-4.045219	-2.124867	-0.000422





Summary of Natural Population Analysis:

Natural Population

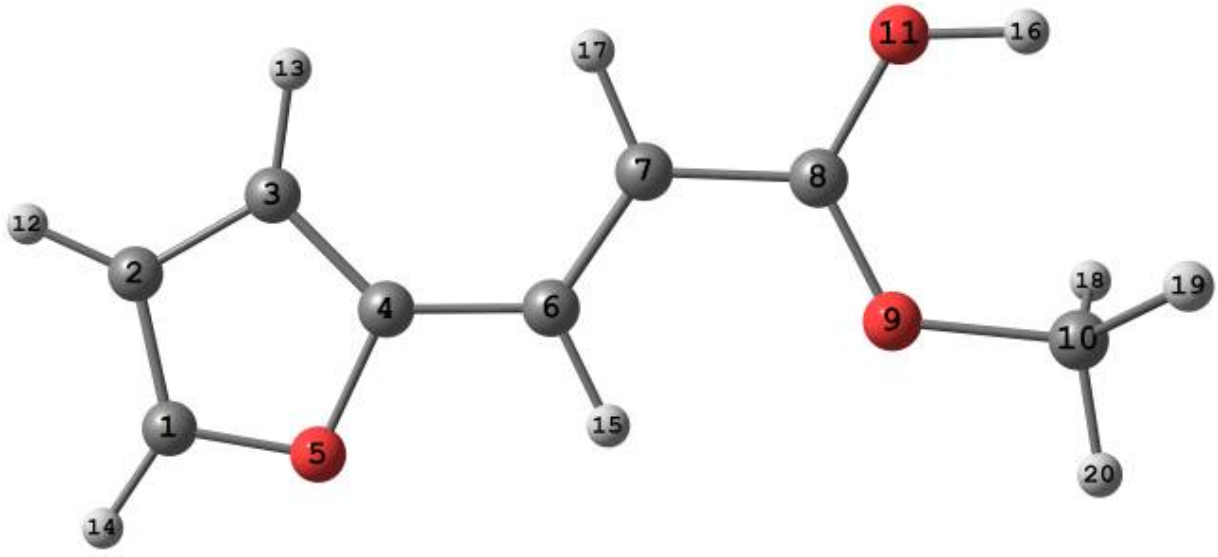
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.14555	1.99908	3.83036	0.02501	5.85445
C	2	-0.30739	1.99916	4.28946	0.01876	6.30739
C	3	-0.24383	1.99902	4.22771	0.01709	6.24383
C	4	0.23528	1.99893	3.74128	0.02452	5.76472
O	5	-0.47044	1.99973	6.44639	0.02433	8.47044
C	6	-0.15582	1.99903	4.13735	0.01944	6.15582
C	7	-0.30778	1.99900	4.28833	0.02045	6.30778
C	8	0.78951	1.99931	3.17455	0.03664	5.21049
O	9	-0.56433	1.99971	6.54068	0.02394	8.56433
C	10	-0.21221	1.99923	4.19888	0.01411	6.21221
O	11	-0.67152	1.99975	6.64624	0.02553	8.67152
H	12	0.24643	0.00000	0.75208	0.00150	0.75357
H	13	0.24716	0.00000	0.75133	0.00151	0.75284
H	14	0.22521	0.00000	0.77334	0.00145	0.77479
H	15	0.24375	0.00000	0.75396	0.00229	0.75625
H	16	0.23134	0.00000	0.76651	0.00215	0.76866
H	17	0.18806	0.00000	0.80984	0.00210	0.81194
H	18	0.18808	0.00000	0.80982	0.00210	0.81192
H	19	0.19296	0.00000	0.80570	0.00135	0.80704
* Total *		0.00000	21.99195	57.74380	0.26424	80.00000

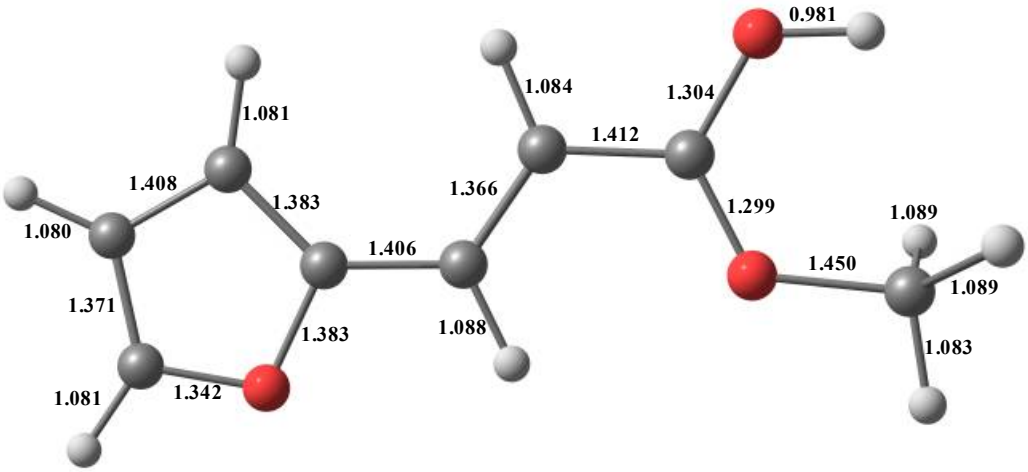
Ag

Energy E(B3LYP) = -535.909938855 h, G^{298} = -535.79194 h, μ=6.39 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.681990	-0.772453	0.000535
2	C	3.763278	0.596304	-0.000275
3	C	2.436657	1.067150	-0.000519
4	C	1.613783	-0.044387	-0.000024
5	O	2.402890	-1.179576	0.000234
6	C	0.222178	-0.248223	0.000099
7	C	-0.718432	0.742032	-0.000081
8	C	-2.101234	0.458342	-0.000063
9	O	-2.504275	-0.776231	-0.000711
10	C	-3.907734	-1.141872	-0.000090
11	O	-2.903702	1.485679	0.000784
12	H	4.670926	1.181039	-0.000549
13	H	2.108563	2.097250	-0.001050
14	H	4.433635	-1.549608	0.000994
15	H	-0.097881	-1.287737	0.000296
16	H	-3.873545	1.335166	0.000318
17	H	-0.455278	1.793313	-0.000147
18	H	-4.388373	-0.762545	0.900589
19	H	-4.389376	-0.761921	-0.899969
20	H	-3.910893	-2.225294	-0.000429





Summary of Natural Population Analysis:

Natural Population

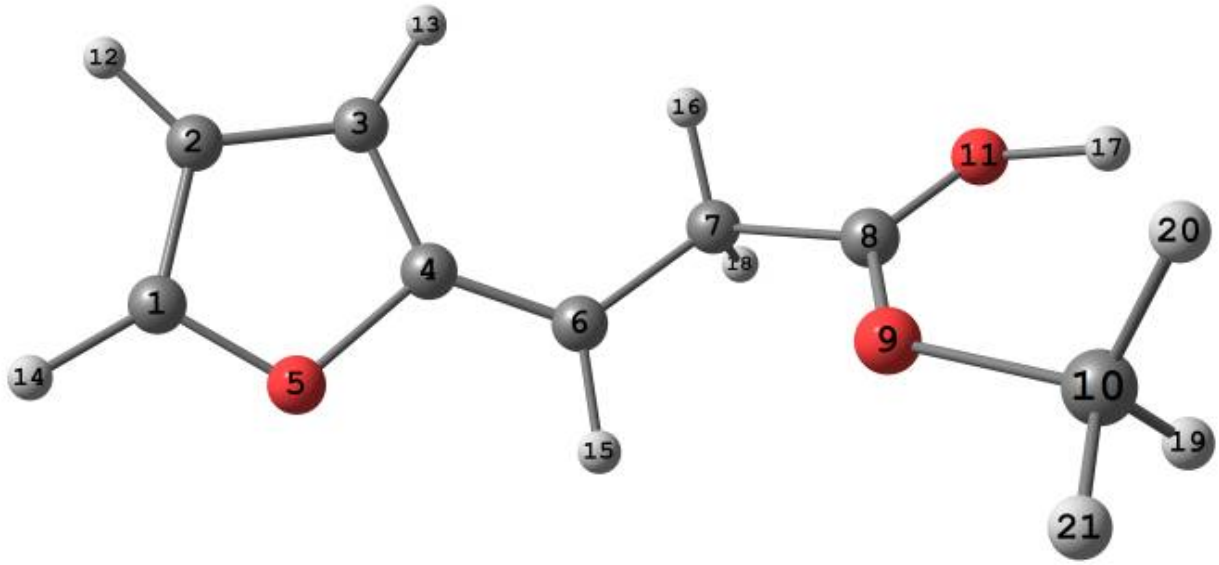
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.20571	1.99912	3.77080	0.02437	5.79429
C	2	-0.30155	1.99917	4.28380	0.01859	6.30155
C	3	-0.18296	1.99904	4.16734	0.01658	6.18296
C	4	0.21843	1.99893	3.75887	0.02377	5.78157
O	5	-0.45159	1.99972	6.42738	0.02448	8.45159
C	6	-0.07519	1.99904	4.05725	0.01889	6.07519
C	7	-0.34671	1.99902	4.32651	0.02118	6.34671
C	8	0.83186	1.99914	3.14134	0.02766	5.16814
O	9	-0.48790	1.99965	6.46419	0.02406	8.48790
C	10	-0.23111	1.99920	4.21921	0.01269	6.23111
O	11	-0.63119	1.99969	6.60751	0.02399	8.63119
H	12	0.25641	0.00000	0.74211	0.00147	0.74359
H	13	0.25729	0.00000	0.74127	0.00145	0.74271
H	14	0.23459	0.00000	0.76405	0.00136	0.76541
H	15	0.25715	0.00000	0.74035	0.00250	0.74285
H	16	0.55556	0.00000	0.44179	0.00264	0.44444
H	17	0.25827	0.00000	0.73983	0.00190	0.74173
H	18	0.20496	0.00000	0.79334	0.00170	0.79504
H	19	0.20500	0.00000	0.79330	0.00170	0.79500
H	20	0.22295	0.00000	0.77584	0.00121	0.77705
* Total *		1.00000	21.99172	57.75609	0.25219	80.00000

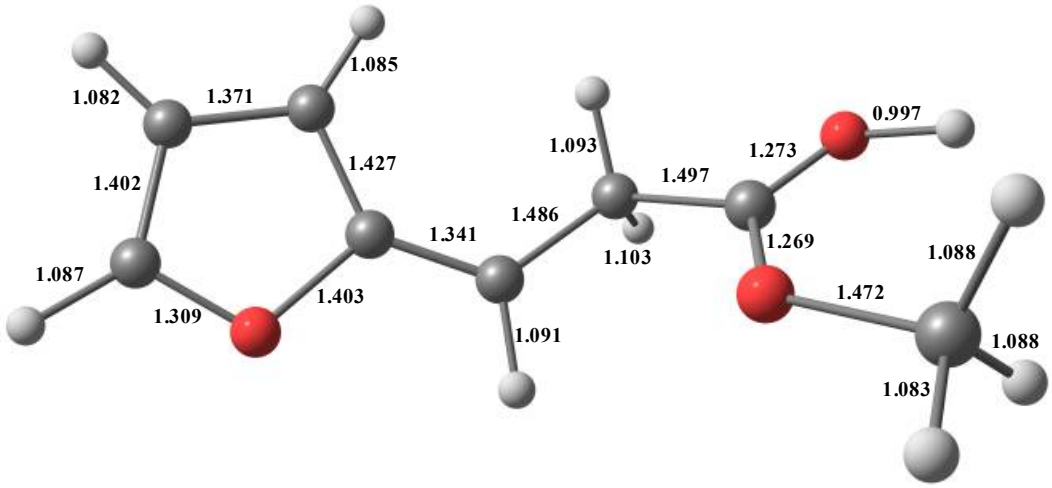
Bg

Energy E(B3LYP) = -536.298620401 h, G^{298} = -536.169898 h, μ=4.10 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.567431	0.731844	0.047186
2	C	3.524406	-0.519977	0.677754
3	C	2.242934	-0.979121	0.514343
4	C	1.527193	0.013046	-0.220941
5	O	2.417991	1.065454	-0.482752
6	C	0.271761	0.127290	-0.677970
7	C	-0.756634	-0.937434	-0.546361
8	C	-2.106636	-0.456469	-0.112018
9	O	-2.241590	0.780538	0.135422
10	C	-3.506583	1.399168	0.563015
11	O	-2.993185	-1.366117	-0.034189
12	H	4.351214	-0.998620	1.184641
13	H	1.829346	-1.915850	0.871959
14	H	4.382231	1.443414	-0.064082
15	H	0.009922	1.036152	-1.221050
16	H	-0.469021	-1.752063	0.123712
17	H	-3.928196	-1.175410	0.253884
18	H	-0.907468	-1.398799	-1.536484
19	H	-4.249241	1.245942	-0.216532
20	H	-3.805502	0.958276	1.511163
21	H	-3.262247	2.447867	0.674881





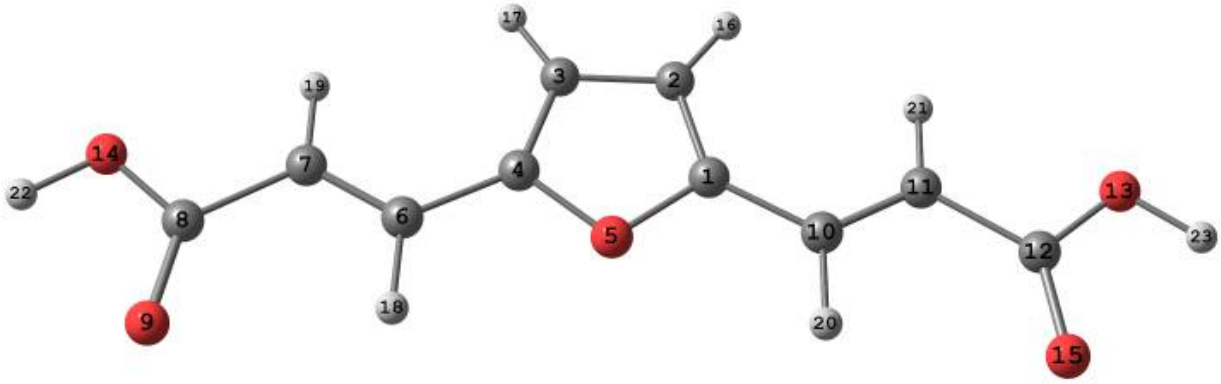
Summary of Natural Population Analysis:

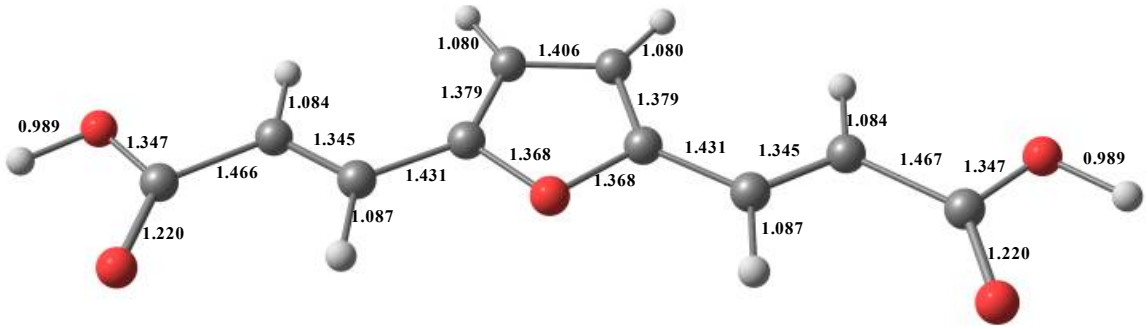
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	0.38226	1.99921	3.59486	0.02366	5.61774
C	2	-0.27501	1.99916	4.25741	0.01844	6.27501
C	3	-0.07047	1.99906	4.05475	0.01666	6.07047
C	4	0.22751	1.99881	3.75102	0.02266	5.77249
O	5	-0.41117	1.99971	6.38579	0.02567	8.41117
C	6	0.01836	1.99897	3.96429	0.01839	5.98164
C	7	-0.53610	1.99912	4.51683	0.02015	6.53610
C	8	0.95159	1.99934	3.02027	0.02880	5.04841
O	9	-0.44403	1.99961	6.42181	0.02261	8.44403
C	10	-0.22775	1.99920	4.21462	0.01393	6.22775
O	11	-0.59676	1.99965	6.57287	0.02425	8.59676
H	12	0.28377	0.00000	0.71484	0.00138	0.71623
H	13	0.28144	0.00000	0.71697	0.00159	0.71856
H	14	0.26217	0.00000	0.73663	0.00120	0.73783
H	15	0.28171	0.00000	0.71592	0.00237	0.71829
H	16	0.29327	0.00000	0.70502	0.00171	0.70673
H	17	0.58933	0.00000	0.40814	0.00253	0.41067
H	18	0.32040	0.00000	0.67795	0.00165	0.67960
H	19	0.21887	0.00000	0.77981	0.00132	0.78113
H	20	0.21883	0.00000	0.77985	0.00132	0.78117
H	21	0.23179	0.00000	0.76719	0.00101	0.76821
* Total *		2.00000	21.99184	57.75685	0.25131	80.00000

Compound 1e
Energy E(B3LYP) = -762.280625947 h, G^{298} = -762.160726 h, μ=6.38 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.104502	0.357988	0.000128
2	C	0.703227	1.676870	0.000188
3	C	-0.703271	1.676852	-0.000065
4	C	-1.104497	0.357952	-0.000398
5	O	0.000000	-0.448606	-0.000276
6	C	-2.374732	-0.300209	-0.000628
7	C	-3.567140	0.322248	-0.000126
8	C	-4.819476	-0.440717	-0.000016
9	O	-4.919658	-1.656507	-0.000803
10	C	2.374726	-0.300174	0.000411
11	C	3.567135	0.322283	-0.000016
12	C	4.819532	-0.440717	0.000287
13	O	5.893364	0.372512	-0.001273
14	O	-5.893346	0.372547	0.000910
15	O	4.919635	-1.656503	0.001626
16	H	1.354344	2.538797	0.000478
17	H	-1.354400	2.538768	-0.000059
18	H	-2.345710	-1.386908	-0.001035
19	H	-3.652732	1.402989	0.000531
20	H	2.345703	-1.386873	0.000911
21	H	3.652761	1.403022	-0.000779
22	H	-6.710229	-0.185795	0.000882
23	H	6.710275	-0.185797	-0.000993





Summary of Natural Population Analysis:

Natural Population

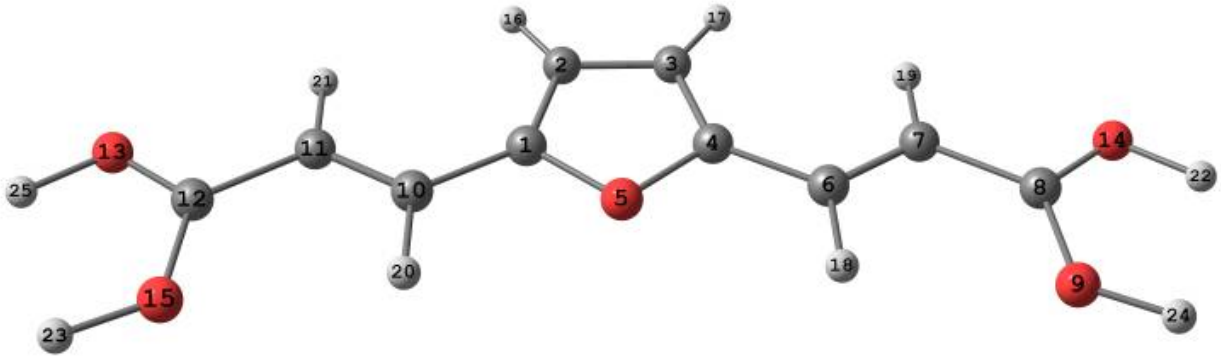
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.27035	1.99894	3.70686	0.02385	5.72965
C	2	-0.23927	1.99904	4.22322	0.01701	6.23927
C	3	-0.23926	1.99904	4.22321	0.01701	6.23926
C	4	0.27035	1.99894	3.70686	0.02385	5.72965
O	5	-0.45841	1.99970	6.43478	0.02393	8.45841
C	6	-0.16993	1.99906	4.14710	0.02376	6.16993
C	7	-0.31097	1.99887	4.28284	0.02927	6.31097
C	8	0.82744	1.99941	3.13622	0.03692	5.17256
O	9	-0.69516	1.99975	6.66400	0.03142	8.69516
C	10	-0.16996	1.99906	4.14714	0.02376	6.16996
C	11	-0.31094	1.99887	4.28281	0.02927	6.31094
C	12	0.82745	1.99941	3.13621	0.03692	5.17255
O	13	-0.72290	1.99975	6.69725	0.02590	8.72290
O	14	-0.72292	1.99975	6.69727	0.02590	8.72292
O	15	-0.69516	1.99975	6.66400	0.03142	8.69516
H	16	0.25191	0.00000	0.74656	0.00153	0.74809
H	17	0.25191	0.00000	0.74656	0.00153	0.74809
H	18	0.24711	0.00000	0.75068	0.00221	0.75289
H	19	0.23240	0.00000	0.76560	0.00200	0.76760
H	20	0.24711	0.00000	0.75068	0.00221	0.75289
H	21	0.23240	0.00000	0.76561	0.00200	0.76760
H	22	0.53960	0.00000	0.45745	0.00295	0.46040
H	23	0.53961	0.00000	0.45744	0.00295	0.46039
* Total *		0.00274	29.98936	77.59035	0.41755	107.99726

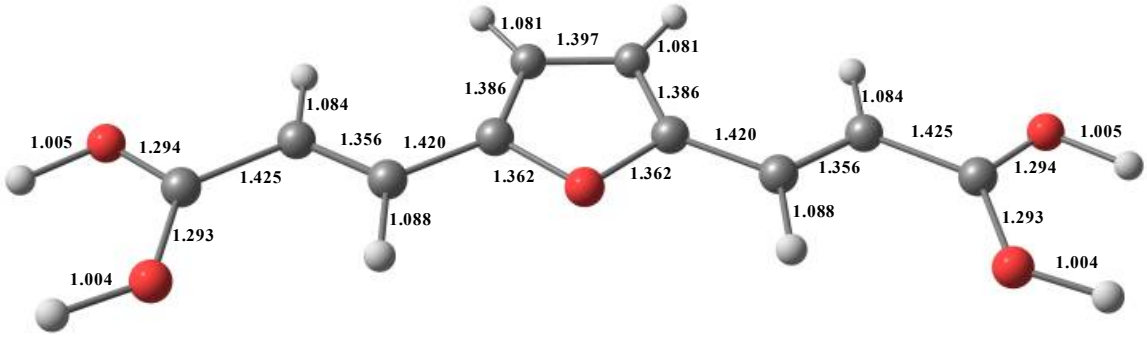
Ae

Energy E(B3LYP) = -763.12469868 h, G^{298} = -762.984781 h, μ=4.31 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.097662	0.391170	-0.000629
2	C	-0.698742	1.718785	-0.001036
3	C	0.698746	1.718784	-0.000960
4	C	1.097661	0.391167	-0.000503
5	O	-0.000001	-0.414992	-0.000341
6	C	2.359204	-0.260455	-0.000088
7	C	3.553581	0.381253	0.000224
8	C	4.784350	-0.337673	0.000386
9	O	4.782355	-1.630375	-0.000810
10	C	-2.359206	-0.260448	-0.000376
11	C	-3.553583	0.381259	0.000265
12	C	-4.784351	-0.337673	0.000398
13	O	-5.873687	0.360056	0.001539
14	O	5.873683	0.360062	0.001722
15	O	-4.782349	-1.630375	-0.000483
16	H	-1.352022	2.580297	-0.001449
17	H	1.352029	2.580294	-0.001290
18	H	2.324942	-1.347665	0.000098
19	H	3.641212	1.462131	0.000426
20	H	-2.324952	-1.347659	-0.000677
21	H	-3.641216	1.462136	0.000817
22	H	6.707506	-0.200657	0.001705
23	H	-5.703770	-2.030120	-0.000068
24	H	5.703778	-2.030118	-0.000293
25	H	-6.707507	-0.200668	0.001618





Summary of Natural Population Analysis:

Natural Population

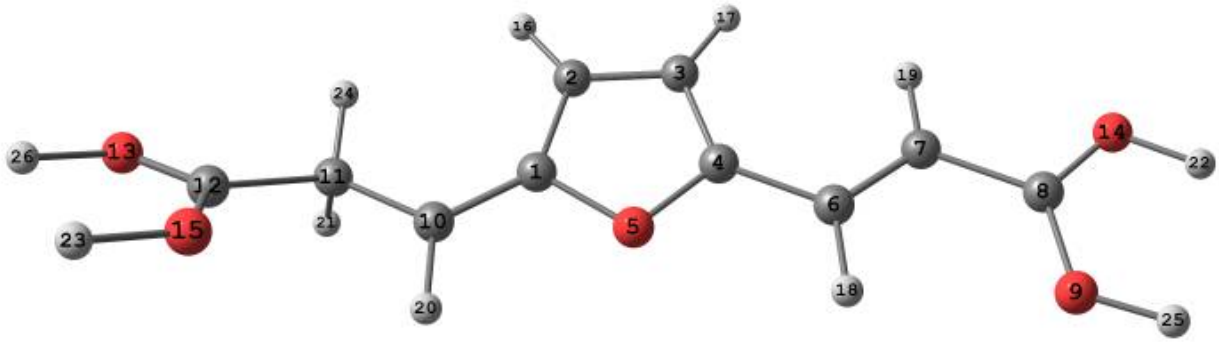
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.27527	1.99897	3.70058	0.02518	5.72473
C	2	-0.20378	1.99904	4.18635	0.01839	6.20378
C	3	-0.20337	1.99904	4.18613	0.01820	6.20337
C	4	0.28100	1.99896	3.69565	0.02438	5.71900
O	5	-0.43646	1.99970	6.41200	0.02477	8.43646
C	6	-0.13737	1.99914	4.10038	0.03784	6.13737
C	7	-0.24064	1.99889	4.22150	0.02025	6.24064
C	8	0.86035	1.99936	3.11423	0.02605	5.13965
O	9	-0.64263	1.99970	6.61432	0.02862	8.64263
C	10	-0.12436	1.99893	4.08694	0.03849	6.12436
C	11	-0.24578	1.99890	4.22467	0.02222	6.24578
C	12	0.85978	1.99936	3.11434	0.02652	5.14022
O	13	-0.63324	1.99971	6.60346	0.03007	8.63324
O	14	-0.63350	1.99971	6.60358	0.03022	8.63350
O	15	-0.64266	1.99970	6.61436	0.02860	8.64266
H	16	0.26459	0.00000	0.73374	0.00167	0.73541
H	17	0.26455	0.00000	0.73380	0.00165	0.73545
H	18	0.26282	0.00000	0.73510	0.00207	0.73718
H	19	0.25190	0.00000	0.74412	0.00399	0.74810
H	20	0.26133	0.00000	0.73629	0.00238	0.73867
H	21	0.25296	0.00000	0.74327	0.00377	0.74704
H	22	0.57884	0.00000	0.41840	0.00276	0.42116
H	23	0.58115	0.00000	0.41614	0.00270	0.41885
H	24	0.58116	0.00000	0.41614	0.00271	0.41884
H	25	0.57881	0.00000	0.41840	0.00279	0.42119
* Total *		2.01073	29.98911	77.57388	0.42628	107.98927

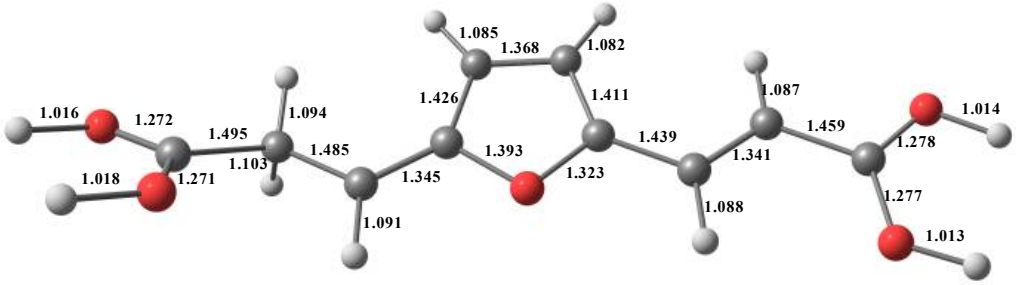
Be

Energy E(B3LYP) = -763.503051513 h, G^{298} = -763.354135 h, μ=4.09 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.104910	0.296007	0.246846
2	C	0.702204	1.620823	-0.093864
3	C	-0.662042	1.617865	-0.199209
4	C	-1.076190	0.296782	0.073594
5	O	-0.043398	-0.487116	0.337223
6	C	-2.374892	-0.321908	0.111747
7	C	-3.499465	0.368017	-0.129950
8	C	-4.807182	-0.277730	-0.088982
9	O	-4.875087	-1.523581	0.182872
10	C	2.289076	-0.296827	0.484791
11	C	3.587902	0.422640	0.499896
12	C	4.719799	-0.323475	-0.129922
13	O	5.857900	0.240918	-0.075415
14	O	-5.810128	0.474125	-0.337536
15	O	4.477511	-1.445900	-0.675666
16	H	1.367701	2.464321	-0.242002
17	H	-1.308666	2.450238	-0.445761
18	H	-2.391169	-1.384050	0.348212
19	H	-3.516538	1.428476	-0.367875
20	H	2.280057	-1.360012	0.727724
21	H	3.881892	0.590747	1.549736
22	H	-6.703461	-0.004311	-0.301377
23	H	5.292989	-1.902300	-1.078505
24	H	3.551282	1.414474	0.040047
25	H	-5.818282	-1.894202	0.189570
26	H	6.605089	-0.284111	-0.521283





Summary of Natural Population Analysis:

Natural Population

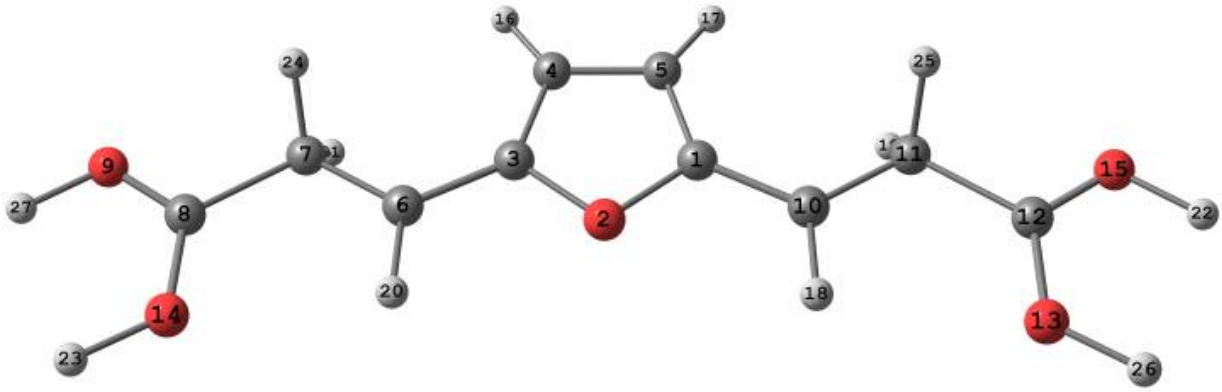
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.23870	1.99883	3.74064	0.02183	5.76130
C	2	-0.07413	1.99906	4.05823	0.01684	6.07413
C	3	-0.23245	1.99904	4.21401	0.01940	6.23245
C	4	0.46789	1.99905	3.50802	0.02505	5.53211
O	5	-0.40839	1.99968	6.38306	0.02565	8.40839
C	6	-0.18834	1.99912	4.15261	0.03662	6.18834
C	7	-0.12249	1.99889	4.10473	0.01888	6.12249
C	8	0.88975	1.99946	3.08479	0.02601	5.11025
O	9	-0.61050	1.99969	6.58203	0.02878	8.61050
C	10	0.01440	1.99902	3.96799	0.01859	5.98560
C	11	-0.53408	1.99899	4.51681	0.01829	6.53408
C	12	0.93950	1.99945	3.02997	0.03107	5.06050
O	13	-0.59527	1.99967	6.57061	0.02499	8.59527
O	14	-0.60031	1.99970	6.57027	0.03034	8.60031
O	15	-0.59851	1.99967	6.57394	0.02490	8.59851
H	16	0.28380	0.00000	0.71464	0.00156	0.71620
H	17	0.28582	0.00000	0.71240	0.00177	0.71418
H	18	0.28299	0.00000	0.71499	0.00202	0.71701
H	19	0.26570	0.00000	0.73038	0.00392	0.73430
H	20	0.28640	0.00000	0.71175	0.00185	0.71360
H	21	0.32146	0.00000	0.67643	0.00212	0.67854
H	22	0.59636	0.00000	0.40101	0.00263	0.40364
H	23	0.60334	0.00000	0.39414	0.00251	0.39666
H	24	0.29439	0.00000	0.70357	0.00204	0.70561
H	25	0.59849	0.00000	0.39893	0.00258	0.40151
H	26	0.59998	0.00000	0.39747	0.00256	0.40002
* Total *		3.00450	29.98930	77.61341	0.39279	107.99550

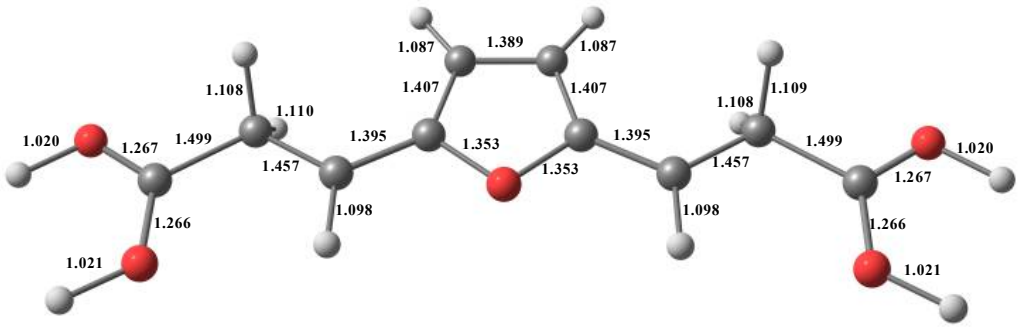
Ce

Energy E(B3LYP) = -763.81729201 h, G^{298} = -763.659391 h, μ=2.87 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.081903	0.375339	-0.014139
2	O	0.000161	-0.436368	-0.018067
3	C	1.082119	0.375370	-0.008656
4	C	0.694580	1.727420	0.001037
5	C	-0.694484	1.727417	-0.003458
6	C	2.325867	-0.256397	-0.004426
7	C	3.592628	0.462362	0.030214
8	C	4.834110	-0.377242	0.006750
9	O	5.923035	0.270548	0.003560
10	C	-2.325614	-0.256376	-0.016211
11	C	-3.592532	0.462937	-0.013602
12	C	-4.833859	-0.377025	0.004589
13	O	-4.706307	-1.636776	0.022221
14	O	4.705747	-1.637025	-0.009650
15	O	-5.923238	0.270009	0.006044
16	H	1.351229	2.593793	0.009189
17	H	-1.351180	2.593771	0.002233
18	H	-2.301743	-1.353670	-0.024019
19	H	-3.635029	1.170830	0.838050
20	H	2.302014	-1.353639	-0.019002
21	H	3.630984	1.111882	0.929664
22	H	-6.760600	-0.312401	0.022289
23	H	5.585911	-2.155106	-0.025158
24	H	3.648557	1.200102	-0.794133
25	H	-3.644934	1.144224	-0.887719
26	H	-5.586715	-2.154506	0.037411
27	H	6.760860	-0.311208	-0.014265





Summary of Natural Population Analysis:

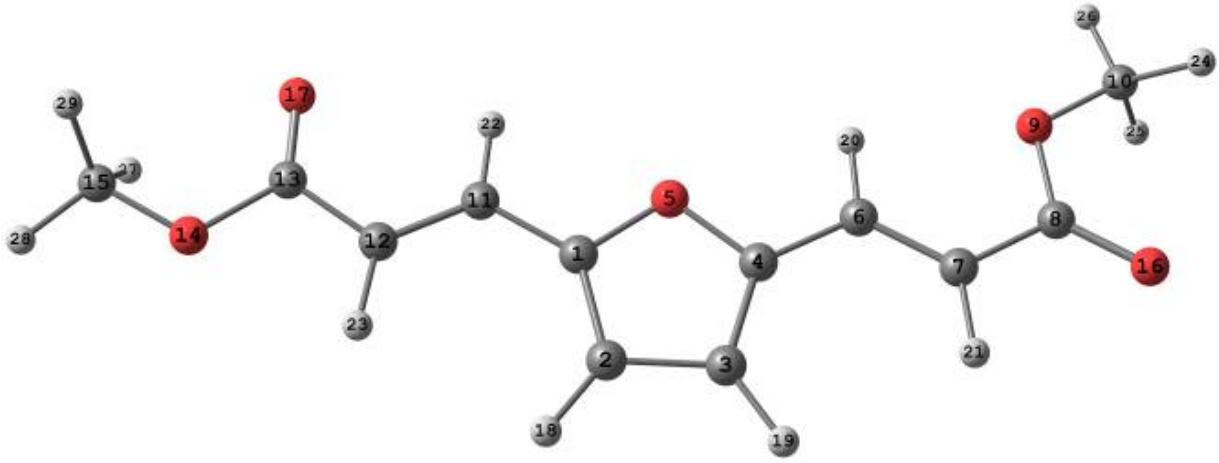
Natural Population

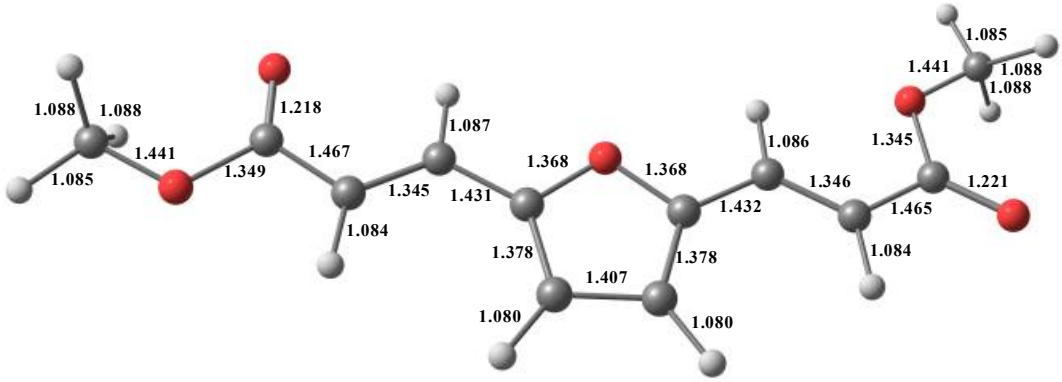
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.27550	1.99898	3.70228	0.02324	5.72450
C	2	-0.07795	1.99907	4.05980	0.01907	6.07795
C	3	-0.07590	1.99908	4.05967	0.01714	6.07590
C	4	0.28150	1.99897	3.69721	0.02232	5.71850
O	5	-0.36135	1.99968	6.33659	0.02508	8.36135
C	6	0.24362	1.99911	3.73967	0.01760	5.75638
C	7	-0.59595	1.99896	4.57936	0.01763	6.59595
C	8	0.93706	1.99947	3.03230	0.03116	5.06294
O	9	-0.59175	1.99966	6.56694	0.02515	8.59175
C	10	0.22413	1.99902	3.74956	0.02729	5.77587
C	11	-0.51537	1.99897	4.49152	0.02488	6.51537
C	12	0.91776	1.99954	3.04721	0.03548	5.08224
O	13	-0.58753	1.99968	6.56242	0.02543	8.58753
O	14	-0.58024	1.99966	6.55549	0.02509	8.58024
O	15	-0.59849	1.99968	6.57422	0.02460	8.59849
H	16	0.30634	0.00000	0.69200	0.00167	0.69366
H	17	0.30658	0.00000	0.69188	0.00154	0.69342
H	18	0.30709	0.00000	0.69099	0.00192	0.69291
H	19	0.36111	0.00000	0.63686	0.00202	0.63889
H	20	0.30592	0.00000	0.69193	0.00215	0.69408
H	21	0.35715	0.00000	0.63771	0.00514	0.64285
H	22	0.60894	0.00000	0.38860	0.00246	0.39106
H	23	0.61488	0.00000	0.38251	0.00260	0.38512
H	24	0.35071	0.00000	0.64408	0.00521	0.64929
H	25	0.36467	0.00000	0.63331	0.00203	0.63533
H	26	0.61387	0.00000	0.38370	0.00243	0.38613
H	27	0.61002	0.00000	0.38740	0.00257	0.38998
* Total *		4.00235	29.98953	77.61521	0.39291	107.99765

Compound 1h
Energy E(B3LYP) = -840.887057444 h, G^{298} = -840.714184 h, μ=3.23 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.044988	0.528149	-0.004258
2	C	0.717597	1.866966	-0.005914
3	C	-0.687499	1.945563	-0.006260
4	C	-1.161453	0.651275	-0.004891
5	O	-0.103315	-0.215051	-0.003918
6	C	-2.464830	0.058256	-0.003802
7	C	-3.622943	0.744124	0.001726
8	C	-4.948896	0.120361	0.005682
9	O	-4.924814	-1.224783	-0.008712
10	C	-6.204434	-1.887626	-0.004319
11	C	2.273582	-0.205334	-0.001944
12	C	3.503886	0.338092	-0.001327
13	C	4.700258	-0.510932	0.002189
14	O	5.822555	0.238359	0.001147
15	C	7.070977	-0.481833	0.004612
16	O	-5.987037	0.762277	0.021050
17	O	4.719256	-1.728940	0.005774
18	H	1.415388	2.691522	-0.006686
19	H	-1.289190	2.842667	-0.007463
20	H	-2.481528	-1.027490	-0.006728
21	H	-3.644170	1.828265	0.006616
22	H	2.175855	-1.287990	-0.000103
23	H	3.662324	1.410573	-0.003210
24	H	-6.762730	-1.628292	0.892738
25	H	-6.778882	-1.608739	-0.885159
26	H	-5.978833	-2.948906	-0.018036
27	H	7.149707	-1.106762	-0.882503
28	H	7.843902	0.279657	0.003420
29	H	7.147600	-1.101773	0.895412





Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	0.27042	1.99894	3.70700	0.02365	5.72958
C	2	-0.24023	1.99904	4.22431	0.01689	6.24023
C	3	-0.24163	1.99903	4.22557	0.01703	6.24163
C	4	0.26624	1.99895	3.71058	0.02422	5.73376
O	5	-0.46002	1.99970	6.43608	0.02423	8.46002
C	6	-0.16016	1.99884	4.13983	0.02148	6.16016
C	7	-0.28237	1.99886	4.26196	0.02154	6.28237
C	8	0.78756	1.99932	3.17692	0.03620	5.21244
O	9	-0.56207	1.99971	6.53767	0.02468	8.56207
C	10	-0.21259	1.99923	4.19927	0.01409	6.21259
C	11	-0.17053	1.99906	4.15009	0.02138	6.17053
C	12	-0.28410	1.99883	4.26404	0.02123	6.28410
C	13	0.78555	1.99934	3.17464	0.04046	5.21445
O	14	-0.54969	1.99973	6.53341	0.01655	8.54969
C	15	-0.21529	1.99923	4.20153	0.01454	6.21529
O	16	-0.66499	1.99975	6.63989	0.02534	8.66499
O	17	-0.67119	1.99974	6.64567	0.02578	8.67119
H	18	0.25145	0.00000	0.74702	0.00153	0.74855
H	19	0.25164	0.00000	0.74682	0.00154	0.74836
H	20	0.24580	0.00000	0.75179	0.00242	0.75420
H	21	0.23210	0.00000	0.76569	0.00222	0.76790
H	22	0.24640	0.00000	0.75119	0.00241	0.75360
H	23	0.23348	0.00000	0.76435	0.00217	0.76652
H	24	0.18882	0.00000	0.80911	0.00207	0.81118
H	25	0.18887	0.00000	0.80907	0.00206	0.81113
H	26	0.19375	0.00000	0.80489	0.00136	0.80625

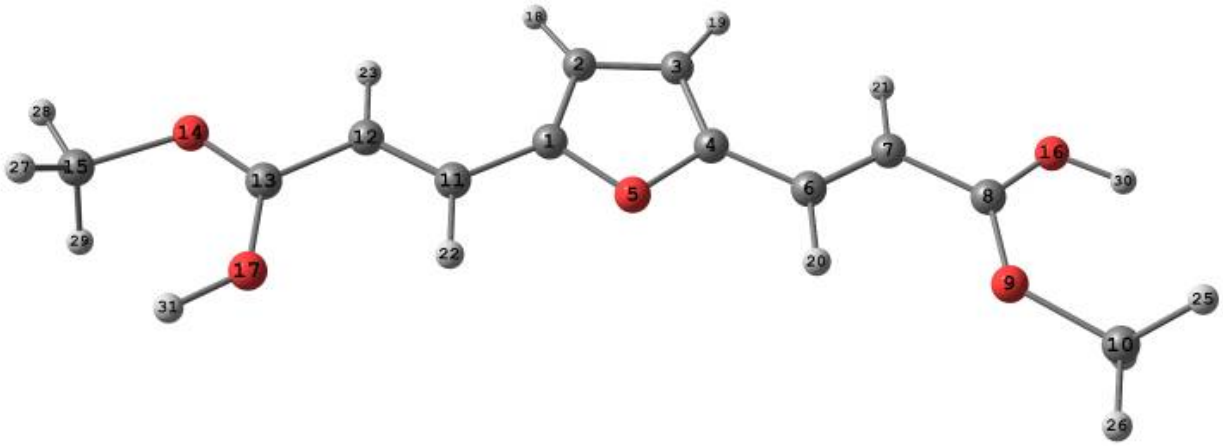
H	27	0.18949	0.00000	0.80866	0.00185	0.81051
H	28	0.19385	0.00000	0.80484	0.00131	0.80615
H	29	0.18947	0.00000	0.80868	0.00185	0.81053
* Total *		0.00003	33.98732	89.60056	0.41210	123.99997

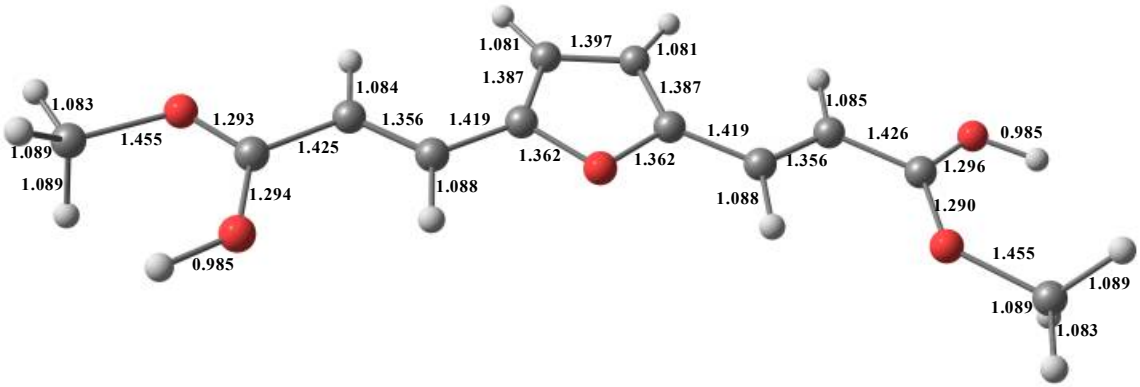
Ah

Energy E(B3LYP) = -841.708370748 h, G^{298} = -841.514366 h, μ=2.87 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.047205	-0.508174	-0.002621
2	C	-0.713583	-1.854029	-0.001823
3	C	0.681643	-1.922570	-0.001179
4	C	1.145209	-0.615515	-0.001580
5	O	0.088518	0.243333	-0.002669
6	C	2.436911	-0.027275	-0.001035
7	C	3.596068	-0.731190	0.000819
8	C	4.868142	-0.086432	0.001283
9	O	4.921753	1.202932	-0.001347
10	C	6.173899	1.943872	0.001154
11	C	-2.274370	0.204859	-0.002991
12	C	-3.499142	-0.377984	-0.001976
13	C	-4.694929	0.397945	-0.000879
14	O	-5.802517	-0.268350	0.002652
15	C	-7.107521	0.374923	0.005534
16	O	5.899524	-0.870637	0.004496
17	O	-4.608966	1.688740	-0.001709
18	H	-1.408198	-2.682566	-0.001592
19	H	1.291883	-2.815133	-0.000376
20	H	2.458862	1.060274	-0.002046
21	H	3.624823	-1.815316	0.002168
22	H	-2.186103	1.288867	-0.003684
23	H	-3.640393	-1.453168	-0.001000
24	H	6.738326	1.703230	0.900566
25	H	6.736786	1.710680	-0.901164
26	H	5.875372	2.985031	0.005798
27	H	-7.221403	0.972135	-0.897710
28	H	-7.816244	-0.444083	0.012665
29	H	-7.213547	0.980791	0.903982
30	H	6.807853	-0.489036	0.003673
31	H	-5.425234	2.239575	-0.000890





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.27696	1.99897	3.69928	0.02479	5.72304
C	2	-0.20260	1.99904	4.18533	0.01823	6.20260
C	3	-0.20252	1.99905	4.18514	0.01834	6.20252
C	4	0.28254	1.99896	3.69410	0.02440	5.71746
O	5	-0.43612	1.99970	6.41153	0.02489	8.43612
C	6	-0.13821	1.99914	4.09988	0.03919	6.13821
C	7	-0.23160	1.99891	4.21012	0.02256	6.23160
C	8	0.88217	1.99927	3.09436	0.02420	5.11783
O	9	-0.48621	1.99965	6.45730	0.02927	8.48621
C	10	-0.23457	1.99921	4.21884	0.01653	6.23457
C	11	-0.11701	1.99893	4.08628	0.03180	6.11701
C	12	-0.22474	1.99887	4.20489	0.02098	6.22474
C	13	0.82089	1.99927	3.14549	0.03435	5.17911
O	14	-0.46255	1.99965	6.43936	0.02355	8.46255
C	15	-0.23368	1.99920	4.22161	0.01287	6.23368
O	16	-0.63472	1.99970	6.60276	0.03227	8.63472
O	17	-0.62854	1.99967	6.60558	0.02329	8.62854
H	18	0.26497	0.00000	0.73342	0.00161	0.73503
H	19	0.26482	0.00000	0.73349	0.00169	0.73518
H	20	0.26325	0.00000	0.73425	0.00250	0.73675
H	21	0.25252	0.00000	0.74315	0.00433	0.74748
H	22	0.26217	0.00000	0.73548	0.00235	0.73783
H	23	0.25430	0.00000	0.74157	0.00414	0.74570
H	24	0.20809	0.00000	0.78987	0.00204	0.79191
H	25	0.20838	0.00000	0.78959	0.00203	0.79162
H	26	0.22546	0.00000	0.77324	0.00129	0.77454
H	27	0.20908	0.00000	0.78921	0.00171	0.79092

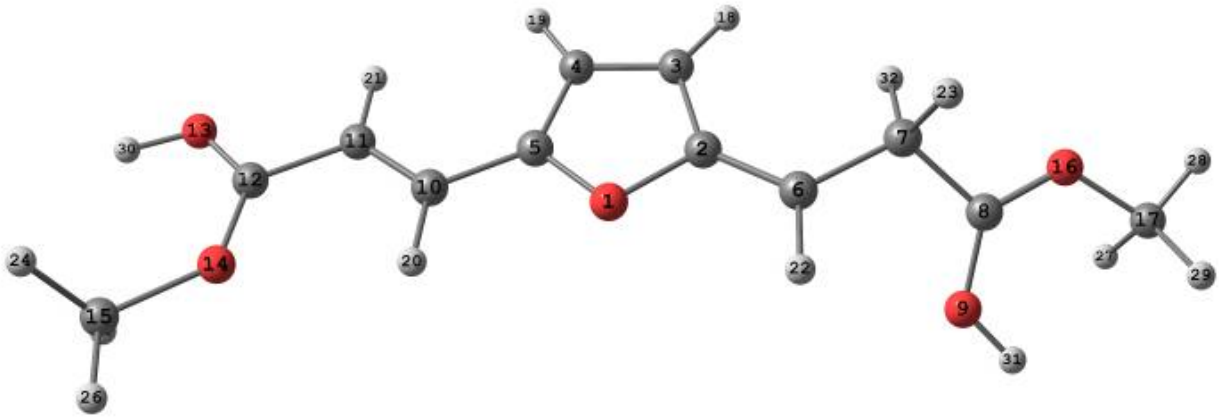
H	28	0.22549	0.00000	0.77335	0.00116	0.77451
H	29	0.20887	0.00000	0.78942	0.00172	0.79113
H	30	0.56425	0.00000	0.43302	0.00273	0.43575
H	31	0.56670	0.00000	0.43043	0.00286	0.43330
* Total *		2.00783	33.98720	89.55132	0.45365	123.99217

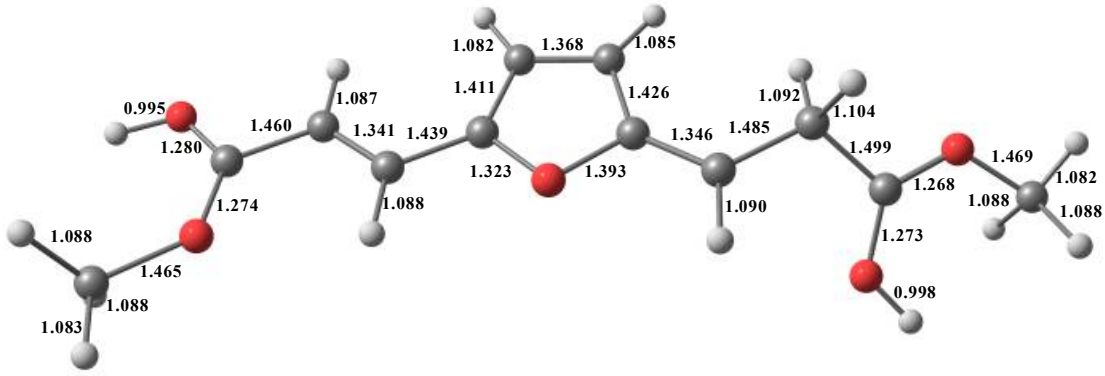
Bh

Energy E(B3LYP) = -842.085368228 h, G^{298} = -841.880944 h, μ=2.21 D

Cartesian coordinates, Å

N	atom	x	y	z
1	O	-0.131740	-0.373248	0.348377
2	C	1.058216	0.350352	0.326147
3	C	0.736183	1.709420	0.038202
4	C	-0.621620	1.783527	-0.111175
5	C	-1.113252	0.476798	0.092506
6	C	2.204066	-0.311422	0.570542
7	C	3.528934	0.352185	0.666638
8	C	4.656527	-0.379528	0.004242
9	O	4.399014	-1.512326	-0.515238
10	C	-2.445248	-0.066631	0.073639
11	C	-3.517245	0.698334	-0.181627
12	C	-4.868964	0.145535	-0.192333
13	O	-5.790254	0.990948	-0.464614
14	O	-5.013071	-1.093784	0.066096
15	C	-6.311453	-1.771890	0.101115
16	O	5.769584	0.227560	0.036575
17	C	7.015576	-0.289618	-0.545416
18	H	1.448564	2.522415	-0.050591
19	H	-1.214939	2.660018	-0.338000
20	H	-2.532794	-1.131850	0.278549
21	H	-3.459153	1.762979	-0.393537
22	H	2.140736	-1.383743	0.758405
23	H	3.805358	0.414451	1.733803
24	H	-6.922188	-1.320111	0.880041
25	H	-6.776269	-1.694187	-0.879687
26	H	-6.069351	-2.799824	0.339410
27	H	6.867823	-0.435946	-1.612982
28	H	7.740723	0.490084	-0.350526
29	H	7.280391	-1.213634	-0.036659
30	H	-6.748163	0.725915	-0.499628
31	H	5.102362	-2.072193	-0.949626
32	H	3.538317	1.380035	0.296569





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
O	1	-0.40868	1.99968	6.38309	0.02591	8.40868
C	2	0.23907	1.99883	3.73960	0.02250	5.76093
C	3	-0.07432	1.99906	4.05844	0.01682	6.07432
C	4	-0.23291	1.99903	4.21412	0.01976	6.23291
C	5	0.46238	1.99905	3.51286	0.02571	5.53762
C	6	0.02546	1.99899	3.95762	0.01794	5.97454
C	7	-0.53801	1.99912	4.51913	0.01977	6.53801
C	8	0.95046	1.99934	3.02058	0.02961	5.04954
O	9	-0.59927	1.99965	6.57583	0.02380	8.59927
C	10	-0.17662	1.99890	4.13833	0.03938	6.17662
C	11	-0.11951	1.99891	4.09790	0.02270	6.11951
C	12	0.91349	1.99936	3.06273	0.02443	5.08651
O	13	-0.60614	1.99968	6.57446	0.03199	8.60614
O	14	-0.45679	1.99964	6.42857	0.02858	8.45679
C	15	-0.23113	1.99921	4.21382	0.01809	6.23113
O	16	-0.44175	1.99961	6.41919	0.02294	8.44175
C	17	-0.22682	1.99920	4.21366	0.01396	6.22682
H	18	0.28380	0.00000	0.71458	0.00162	0.71620
H	19	0.28579	0.00000	0.71236	0.00185	0.71421
H	20	0.28171	0.00000	0.71569	0.00260	0.71829
H	21	0.26709	0.00000	0.72898	0.00392	0.73291
H	22	0.28223	0.00000	0.71578	0.00199	0.71777
H	23	0.32485	0.00000	0.67331	0.00185	0.67515
H	24	0.21687	0.00000	0.78141	0.00172	0.78313
H	25	0.21636	0.00000	0.78191	0.00173	0.78364
H	26	0.23071	0.00000	0.76816	0.00113	0.76929

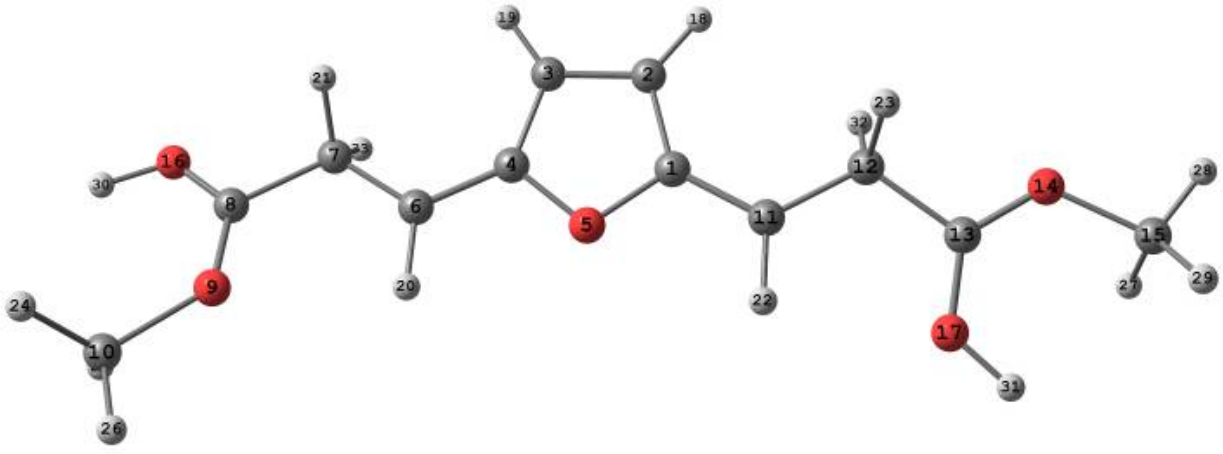
H	27	0.21749	0.00000	0.78120	0.00131	0.78251
H	28	0.23101	0.00000	0.76800	0.00099	0.76899
H	29	0.21803	0.00000	0.78068	0.00129	0.78197
H	30	0.58465	0.00000	0.41270	0.00264	0.41535
H	31	0.59267	0.00000	0.40485	0.00249	0.40733
H	32	0.29285	0.00000	0.70514	0.00201	0.70715
* Total *		3.00504	33.98725	89.57470	0.43302	123.99496

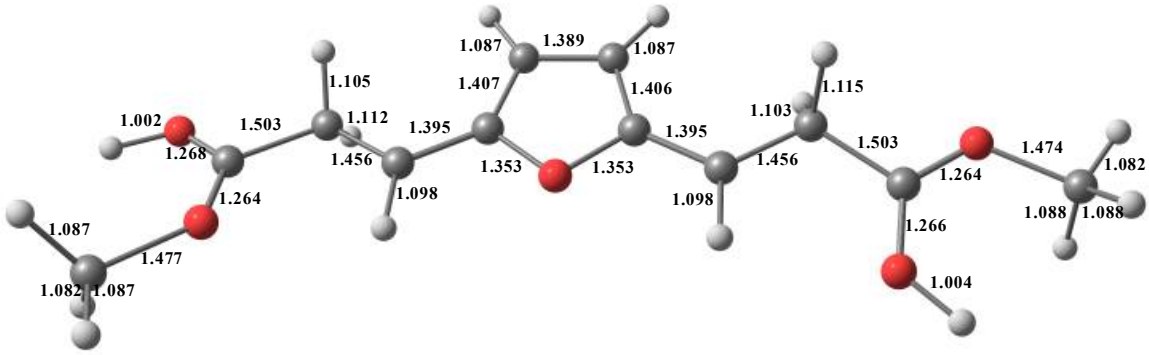
Ch

Energy E(B3LYP) = -842.399291665 h, G^{298} = -842.191548 h, μ=1.29 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.018300	-0.482640	0.081840
2	C	-0.697009	-1.850369	0.146243
3	C	0.688916	-1.921047	0.087236
4	C	1.140716	-0.592729	-0.011412
5	O	0.100688	0.272223	-0.011443
6	C	2.412655	-0.028637	-0.105622
7	C	3.634835	-0.816018	-0.189331
8	C	4.932916	-0.063967	-0.104612
9	O	4.876088	1.171857	0.153470
10	C	6.057429	2.047915	0.291030
11	C	-2.228993	0.209962	0.085263
12	C	-3.525197	-0.436904	0.233037
13	C	-4.734736	0.420632	-0.014021
14	O	-5.831310	-0.196244	0.110303
15	C	-7.159337	0.414406	-0.078579
16	O	5.952873	-0.791518	-0.298511
17	O	-4.530580	1.633832	-0.314614
18	H	-1.393835	-2.681335	0.221531
19	H	1.302530	-2.818159	0.114517
20	H	2.448543	1.068035	-0.145461
21	H	3.655362	-1.633227	0.554457
22	H	-2.154716	1.301276	-0.005819
23	H	-3.592738	-0.816905	1.278630
24	H	6.649183	1.690501	1.130184
25	H	6.609007	2.029550	-0.645881
26	H	5.634281	3.024809	0.486624
27	H	-7.230538	0.773551	-1.102613
28	H	-7.848532	-0.399258	0.107388
29	H	-7.276622	1.213490	0.649693
30	H	6.889560	-0.437275	-0.262946
31	H	-5.268814	2.288983	-0.500904
32	H	-3.610443	-1.359829	-0.364941
33	H	3.622322	-1.369024	-1.154539





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.28252	1.99897	3.69674	0.02178	5.71748
C	2	-0.07538	1.99908	4.05935	0.01695	6.07538
C	3	-0.07544	1.99907	4.05928	0.01709	6.07544
C	4	0.27702	1.99897	3.70183	0.02217	5.72298
O	5	-0.36252	1.99968	6.33664	0.02620	8.36252
C	6	0.24529	1.99894	3.73509	0.02068	5.75471
C	7	-0.59013	1.99896	4.57306	0.01811	6.59013
C	8	0.94875	1.99937	3.02327	0.02862	5.05125
O	9	-0.44768	1.99961	6.41894	0.02913	8.44768
C	10	-0.20216	1.99919	4.18644	0.01652	6.20216
C	11	0.23516	1.99912	3.74843	0.01728	5.76484
C	12	-0.58626	1.99896	4.56891	0.01839	6.58626
C	13	0.94761	1.99937	3.02381	0.02922	5.05239
O	14	-0.42905	1.99961	6.40706	0.02238	8.42905
C	15	-0.22384	1.99920	4.21095	0.01369	6.22384
O	16	-0.58555	1.99964	6.56228	0.02363	8.58555
O	17	-0.59691	1.99964	6.57331	0.02397	8.59691
H	18	0.30661	0.00000	0.69185	0.00153	0.69339
H	19	0.30681	0.00000	0.69165	0.00154	0.69319
H	20	0.31461	0.00000	0.68333	0.00206	0.68539
H	21	0.35176	0.00000	0.64603	0.00221	0.64824
H	22	0.31488	0.00000	0.68304	0.00208	0.68512
H	23	0.37642	0.00000	0.62137	0.00222	0.62358
H	24	0.21877	0.00000	0.77984	0.00138	0.78123
H	25	0.21776	0.00000	0.78084	0.00141	0.78224

H	26	0.23001	0.00000	0.76880	0.00119	0.76999
H	27	0.22134	0.00000	0.77740	0.00126	0.77866
H	28	0.23339	0.00000	0.76563	0.00098	0.76661
H	29	0.22133	0.00000	0.77741	0.00126	0.77867
H	30	0.60080	0.00000	0.39666	0.00254	0.39920
H	31	0.60685	0.00000	0.39076	0.00239	0.39315
H	32	0.34734	0.00000	0.65046	0.00220	0.65266
H	33	0.37076	0.00000	0.62687	0.00237	0.62924
* Total *		4.00087	33.98739	89.61732	0.39442	123.99913