

Supplementary data

Two new glucoside derivatives of truxinic and cinnamic acids from *Lavandula angustifolia* Mill

Gulnigar Ablikim^{a,b}, Khayrulla Bobakulov^{a, c}, Jun Li^a, Nigary Yadikar^{d*}, H.A. Aisa^{a*}

^a State Key Laboratory Basis of Indigenous Medicinal Plants Resource Utilization, and Key Laboratory of Plants Resources and Chemistry of Arid Zone, Xinjiang Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, South Beijing Rd 40-1, Urumqi 830011, P. R. China, e-mail: haji@ms.xjb.ac.cn

^b University of Chinese Academy of Sciences, Beijing 100039, P. R. China

^c Department of Physical Methods of Research, Acad. S.Yu. Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan, 77, M.Ulugbek str., 100170, Tashkent, Uzbekistan, e-mail: khayrulla@rambler.ru

^d College of Food Science and Pharmaceutical Science, Xinjiang Agricultural University, Urumqi, China. E-mail: nigary0115@sina.com

* Corresponding author: Prof. H.A. Aisa, South Beijing Rd 40-1, Urumqi 830011, P. R. China, e-mail: haji@ms.xjb.ac.cn

A phytochemical investigations on the *n*-butanol fraction of *Lavandula angustifolia* Mill residues resulted in the isolation of ten compounds, including two new ones, 4,4'-dimethoxy-2,2'-di-*O*- β -D-glucopyranosyl-truxinate (**1**) and 2-(β -D-glucosyloxy)-*trans*-cinnamic acid butyl ester (**2**), along with eight known compounds. The structures of compounds were confirmed by 1D, 2D NMR and HR-ESI-MS techniques and comparison with published data. The NMR data for **3** were attributed for the first time. All isolated compounds were evaluated for their antioxidant and anti-hypoglycaemic activities. Among them, compounds **4** and **5** showed strong anti-oxidant activities against DPPH with IC₅₀ values of 12.99 and 31.74 μ M, respectively. Compound **5** exhibited moderate inhibitory activity against PTP1B with an IC₅₀ value of 31.28 μ M.

Keywords: *Lavandula angustifolia* Mill; chemical constituents; structure elucidation; antioxidant activity; PTP1B; truxinic acid derivative; cinnamic acid esters.

Content:

Figure S1. HR-ESI-MS spectrum of compound **1**

Figure S2. ^1H NMR (600 MHz) spectrum of compound **1** in DMSO-*d*₆

Figure S3. ^{13}C NMR (150 MHz) spectrum of compound **1** in DMSO-*d*₆

Figure S4. ^1H - ^1H COSY spectrum of compound **1** in DMSO-*d*₆

Figure S5. HSQC spectrum of compound **1** in DMSO-*d*₆

Figure S6. HMBC spectrum of compound **1** in DMSO-*d*₆

Figure S7. NOESY spectrum of compound **1** in DMSO-*d*₆

Figure S8. Expanded region of NOESY spectrum of compound **1** in DMSO-*d*₆

Figure S9. HR-ESI-MS spectrum of compound **2**

Figure S10. ^1H NMR (400 MHz) spectrum of compound **2** in CD₃OD

Figure S11. ^{13}C NMR (100 MHz) spectrum of compound **2** in CD₃OD

Figure S12. ^1H - ^1H COSY spectrum of compound **2** in CD₃OD

Figure S13. HSQC spectrum of compound **2** in CD₃OD

Figure S14. HMBC spectrum of compound **2** in CD₃OD

Figure S15. HR-ESI-MS spectrum of compound **3**

Figure S16. ^1H NMR (600 MHz) spectrum of compound **3** in DMSO-*d*₆

Figure S17. ^{13}C NMR (150 MHz) spectrum of compound **3** in DMSO-*d*₆

Figure S18. ^1H - ^1H COSY spectrum of compound **3** in DMSO-*d*₆

Figure S19. HSQC spectrum of compound **3** in DMSO-*d*₆

Figure S20. HMBC spectrum of compound **3** in DMSO-*d*₆

Figure S21. Key HMBC correlations of compound **1**

Figure S22. Key NOESY correlations of compound **1**

Figure S23. Key HMBC correlations of compound **2**

Table S1. ^1H and ^{13}C NMR Data of compounds **1-3** (δ , ppm, 600 MHz for ^1H and 150 MHz for ^{13}C)

D14-26-4-1 #18 RT: 0.16 AV: 1 SB: 29 0.39-0.94 NL: 1.61E9
T: FTMS - p ESI Full ms [100.0000-1500.0000]

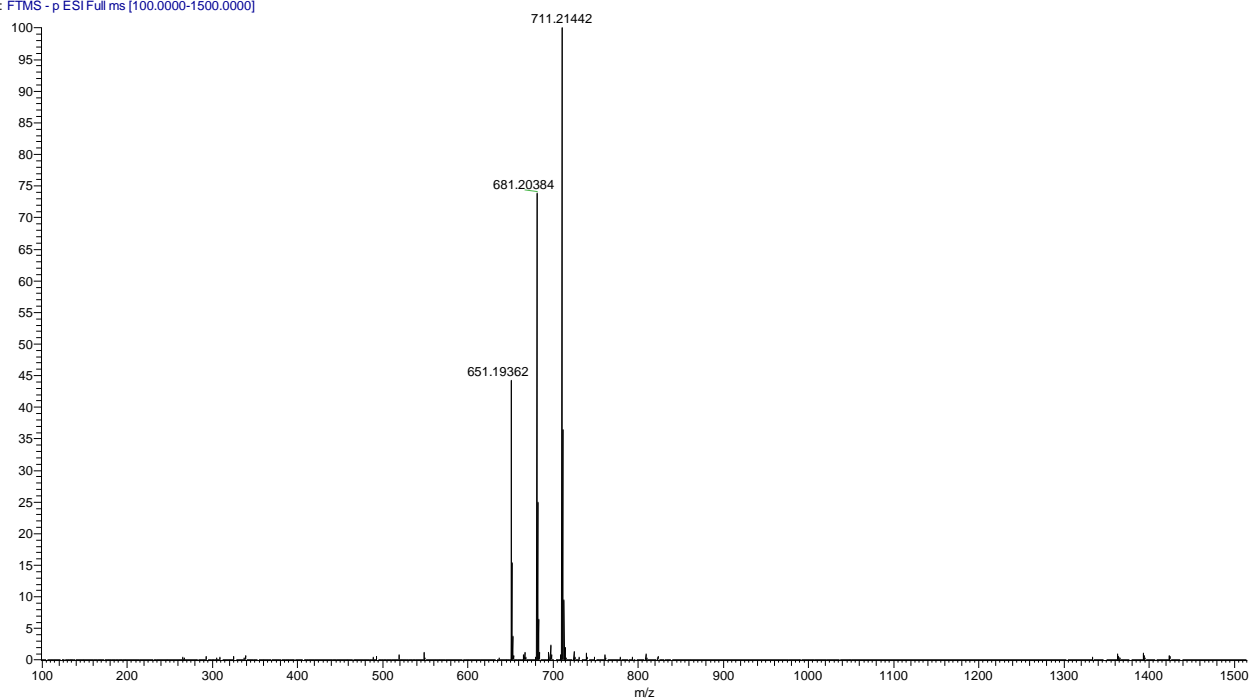


Figure S1. HR-ESI-MS spectrum of compound **1**

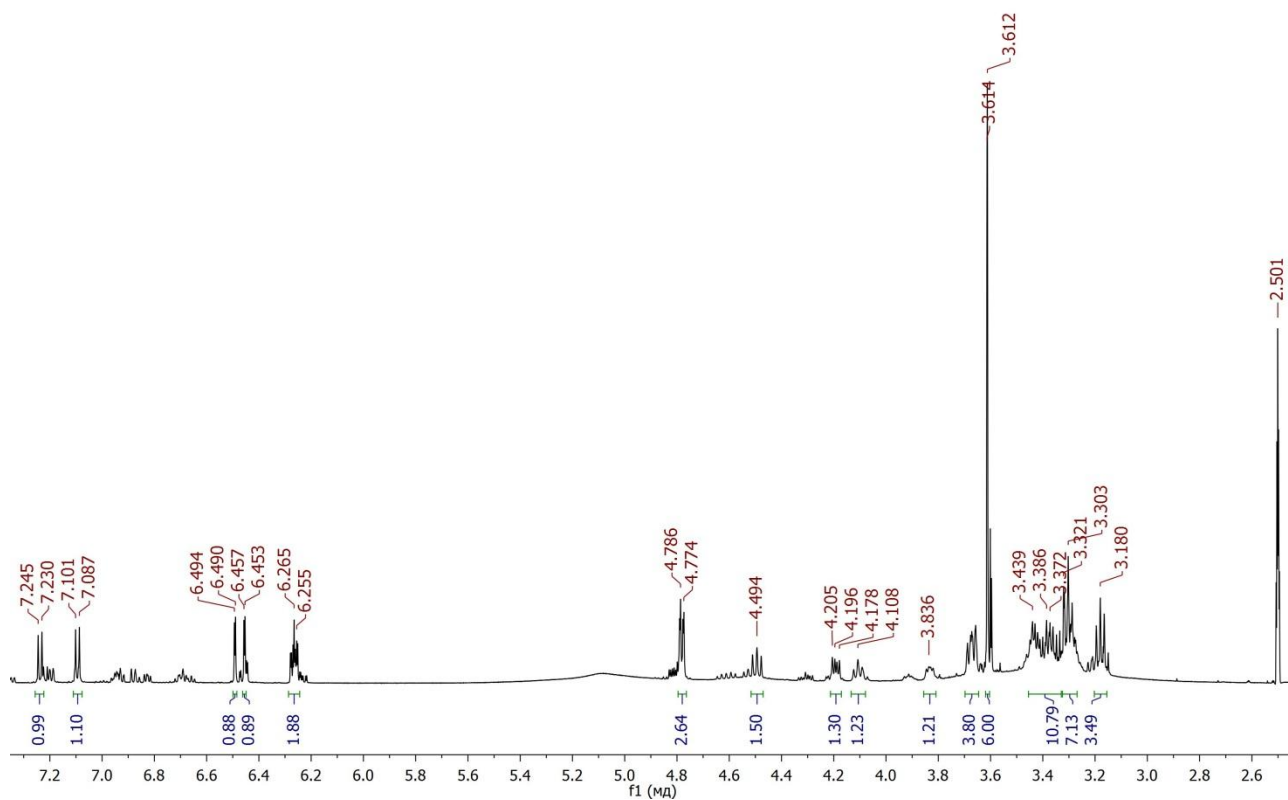


Figure S2. ¹H NMR (600 MHz) spectrum of compound **1** in DMSO-*d*₆

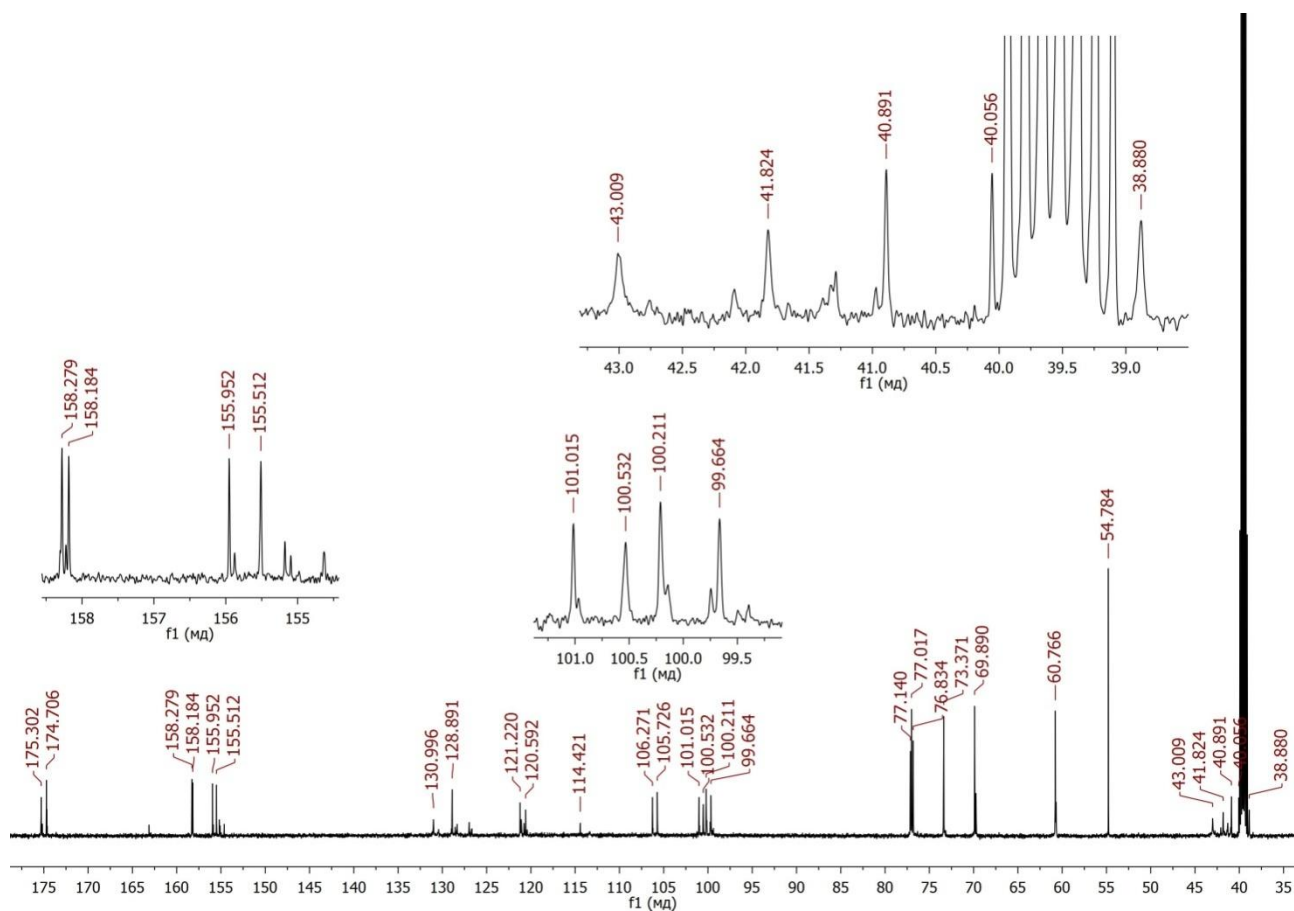


Figure S3. ¹³C NMR (150 MHz) spectrum of compound **1** in DMSO-*d*₆

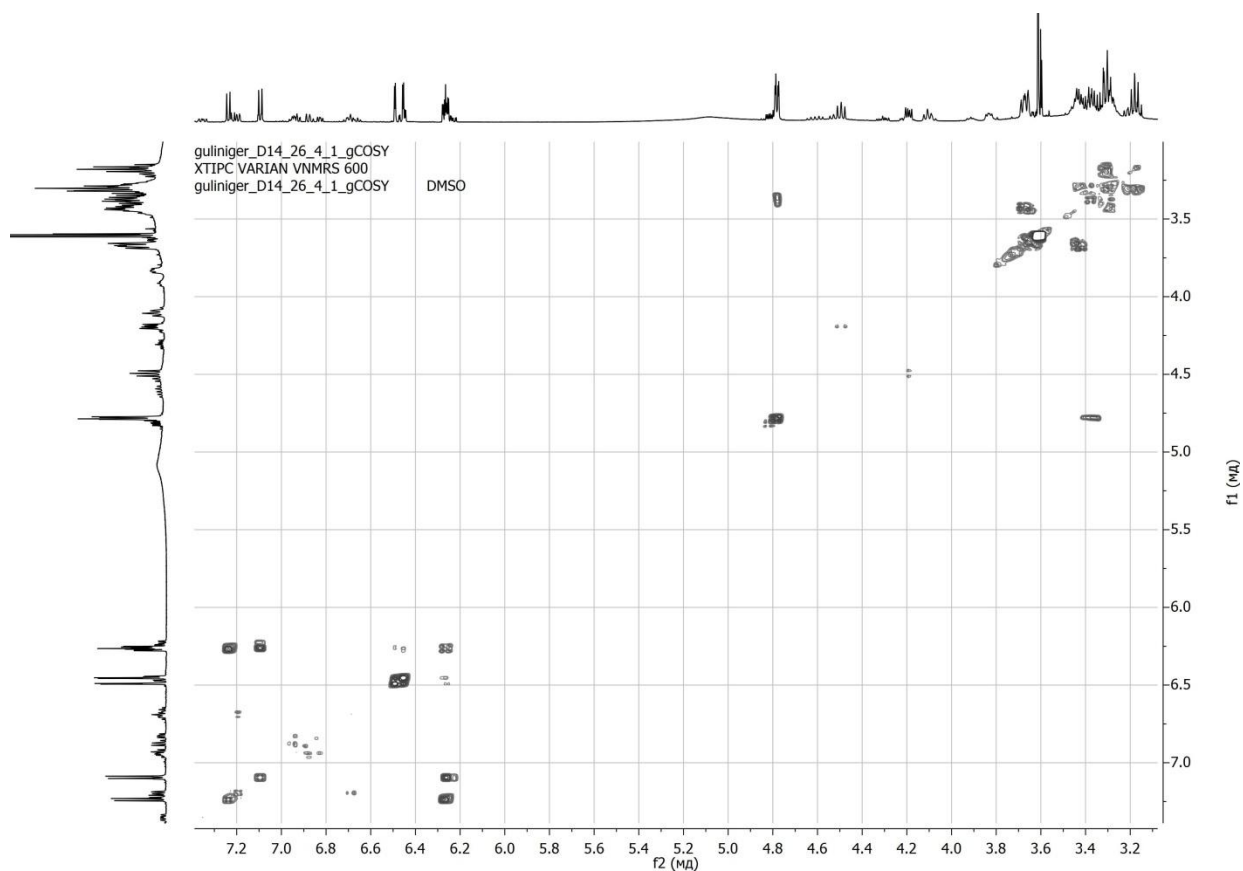


Figure S4. ¹H-¹H COSY spectrum of compound **1** in DMSO-*d*₆

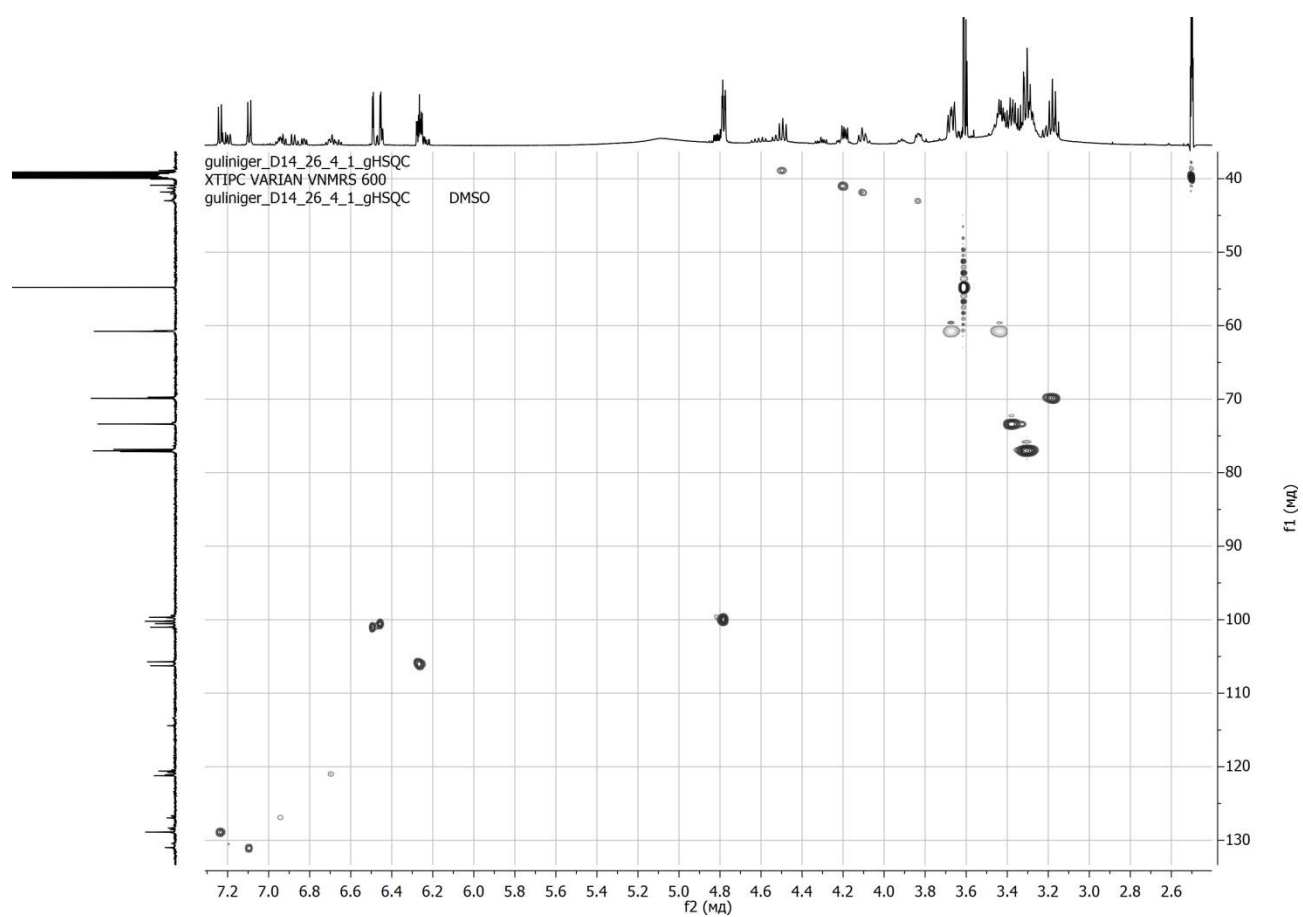


Figure S5. HSQC spectrum of compound **1** in DMSO-*d*₆

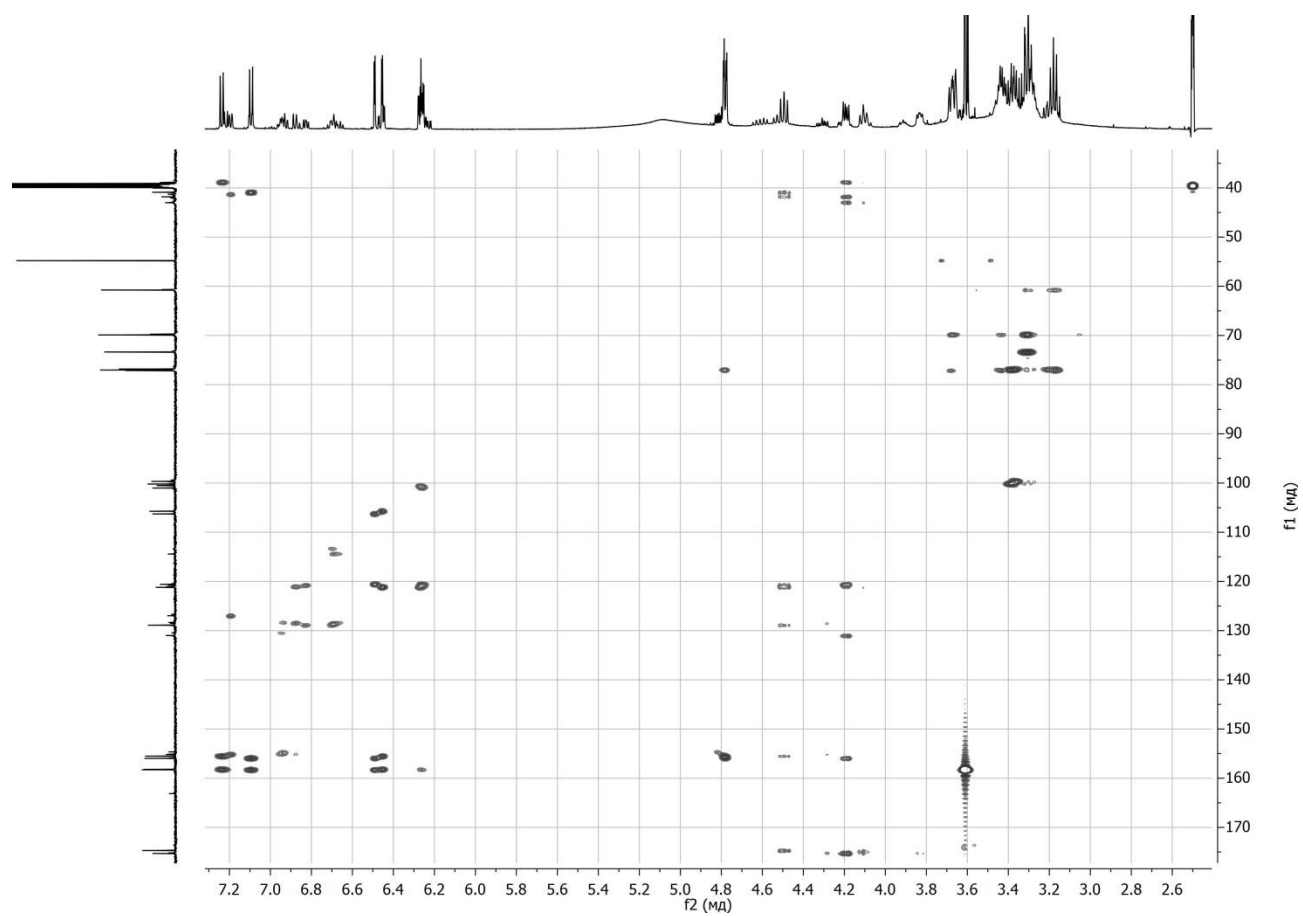


Figure S6. HMBC spectrum of compound **1** in DMSO-*d*₆

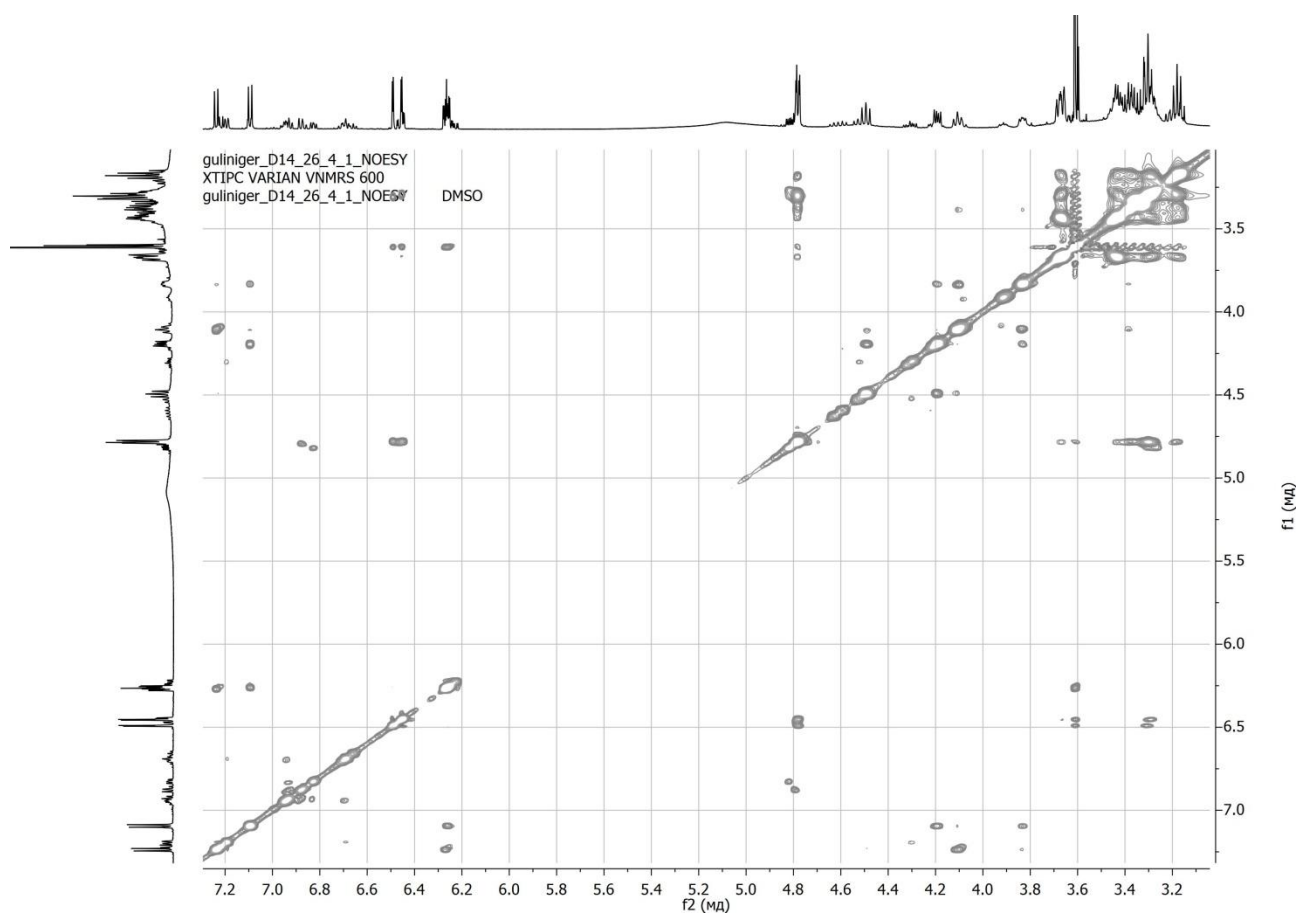


Figure S7. NOESY spectrum of compound **1** in DMSO-*d*₆

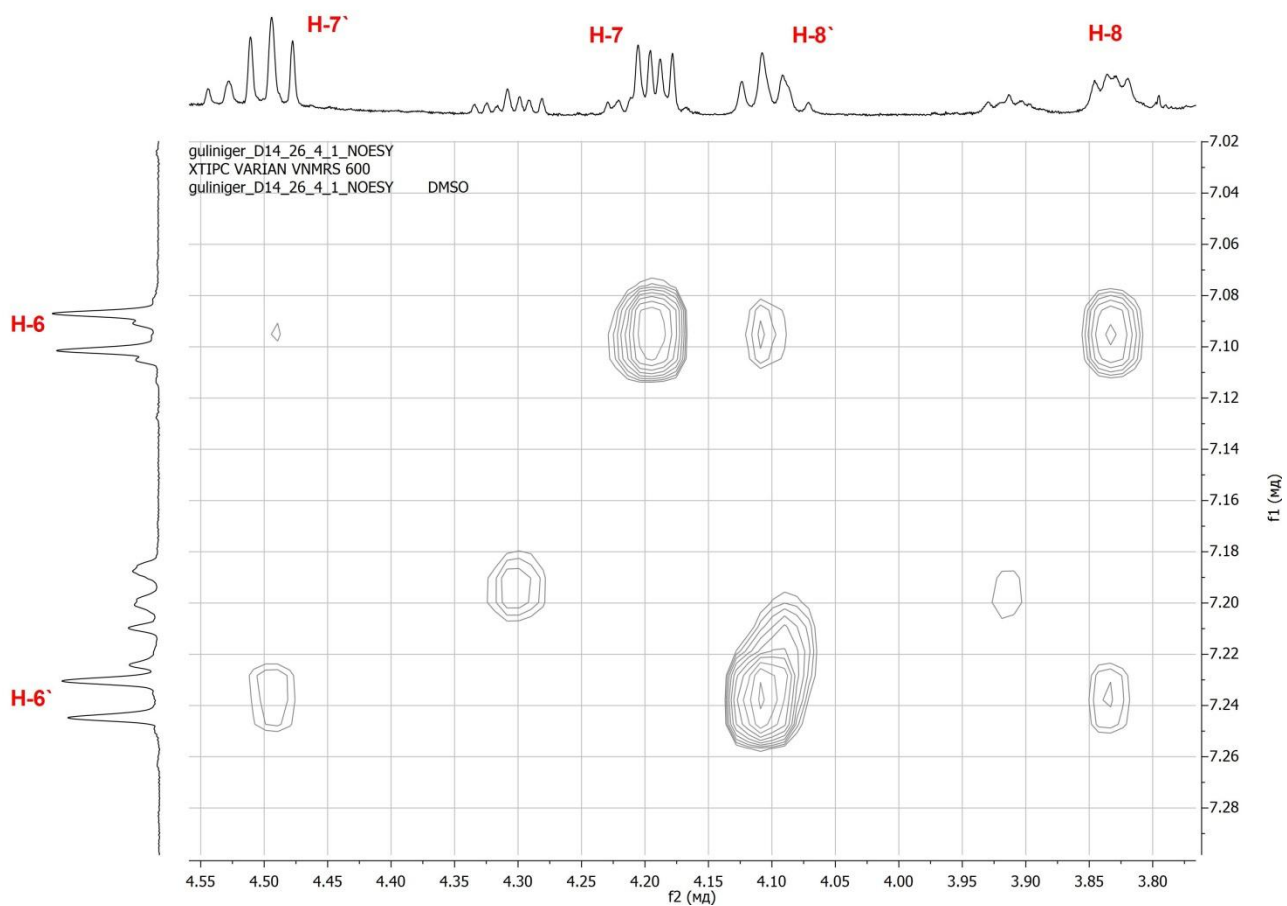


Figure S8. Expanded region of NOESY spectrum of compound **1** in DMSO-*d*₆

G26-7 #19 RT: 0.18 AV: 1 SB: 13 0.45-0.71 NL: 5.49E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]

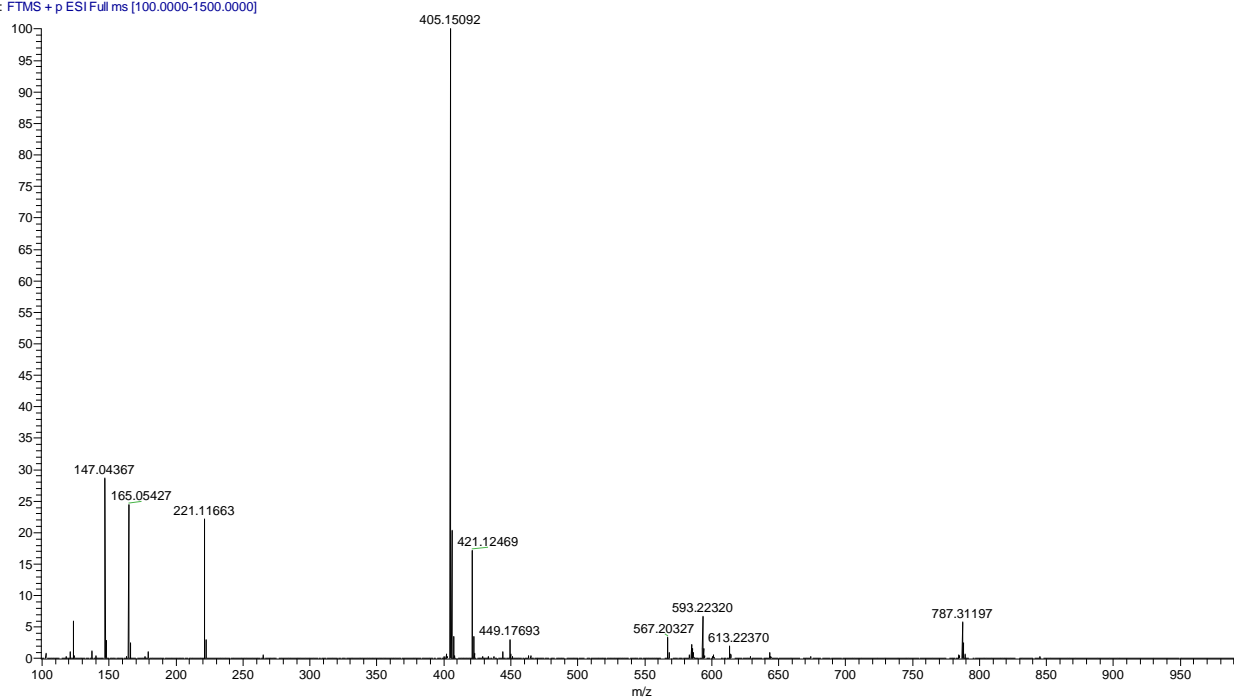


Figure S9. HR-ESI-MS spectrum of compound **2**

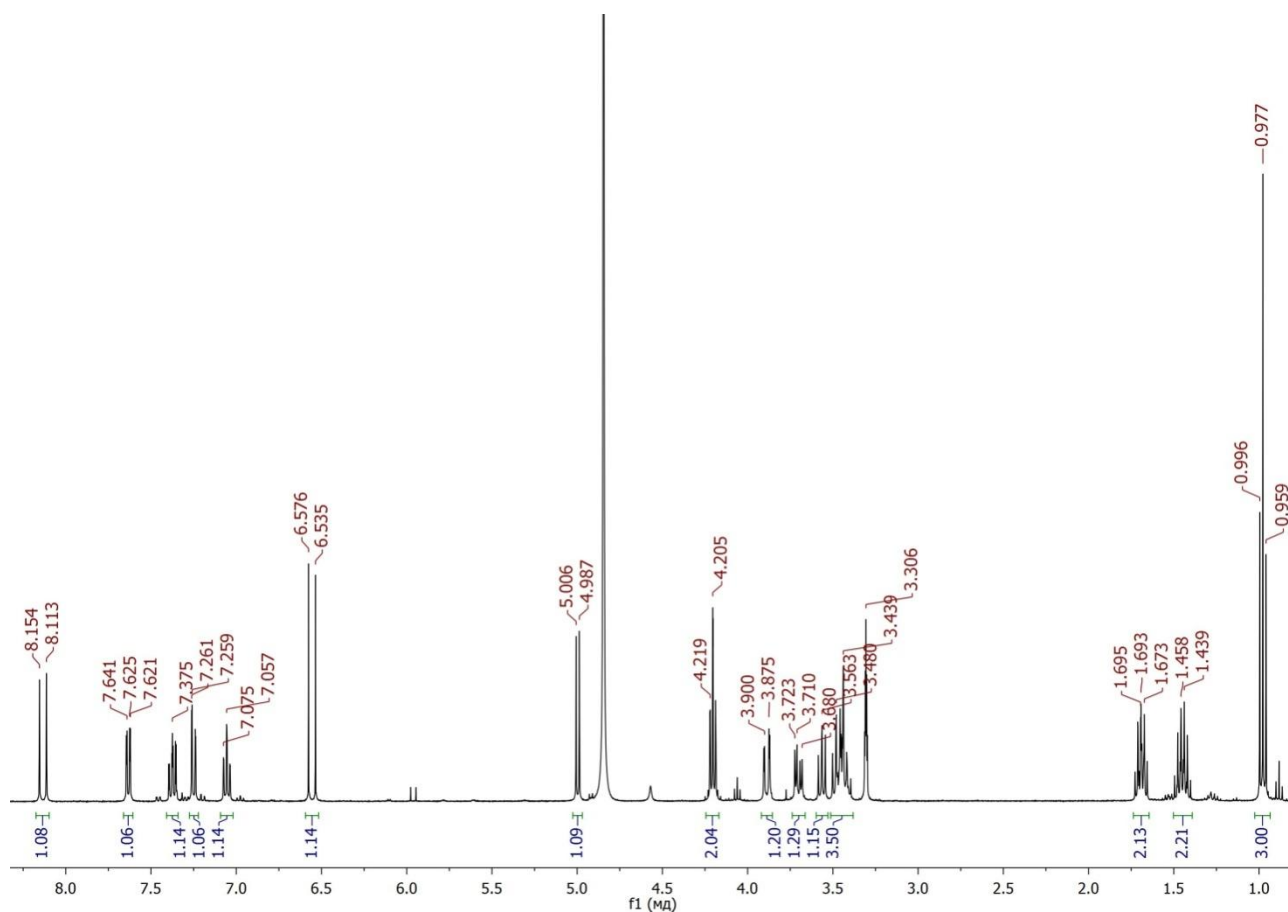


Figure S10. ^1H NMR (600 MHz) spectrum of compound **2** in CD_3OD

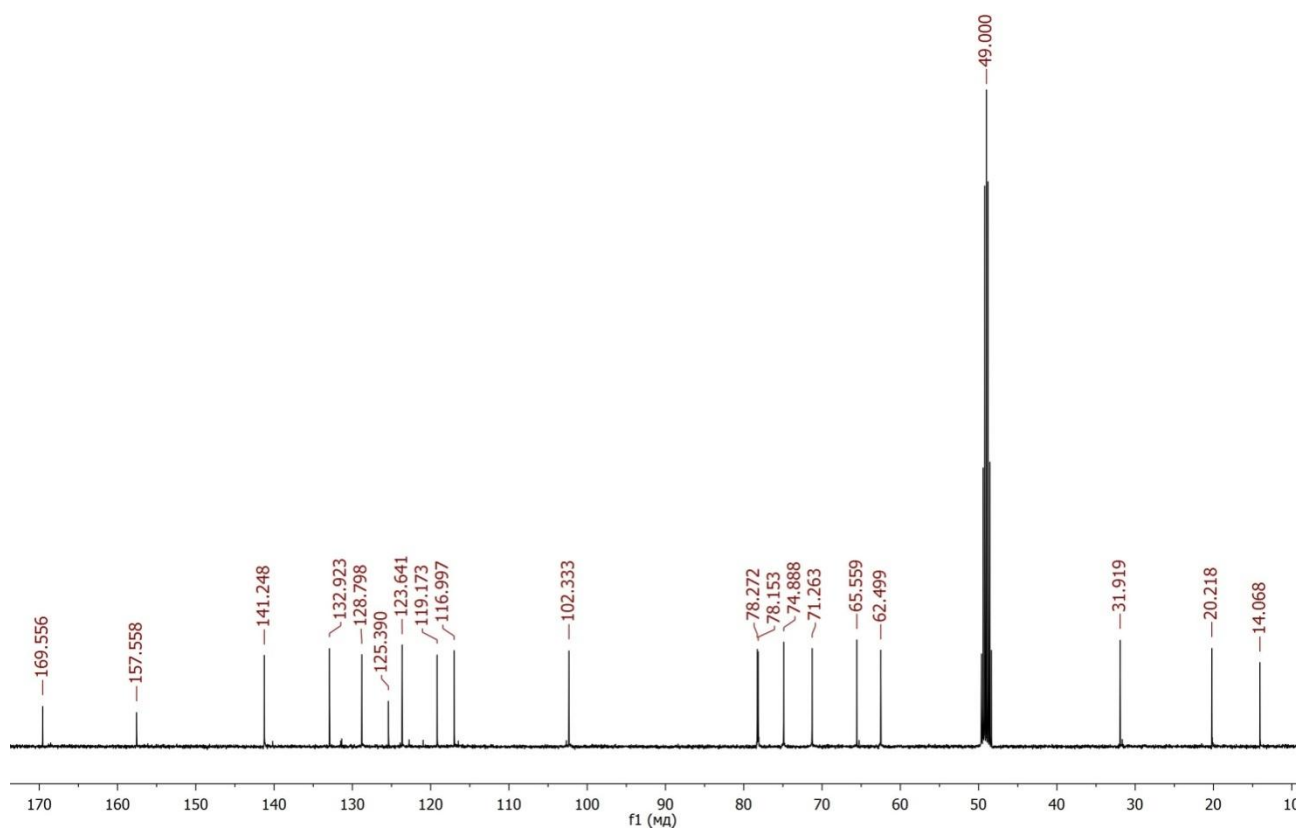


Figure S11. ^{13}C NMR (150 MHz) spectra of compound **2** in CD_3OD

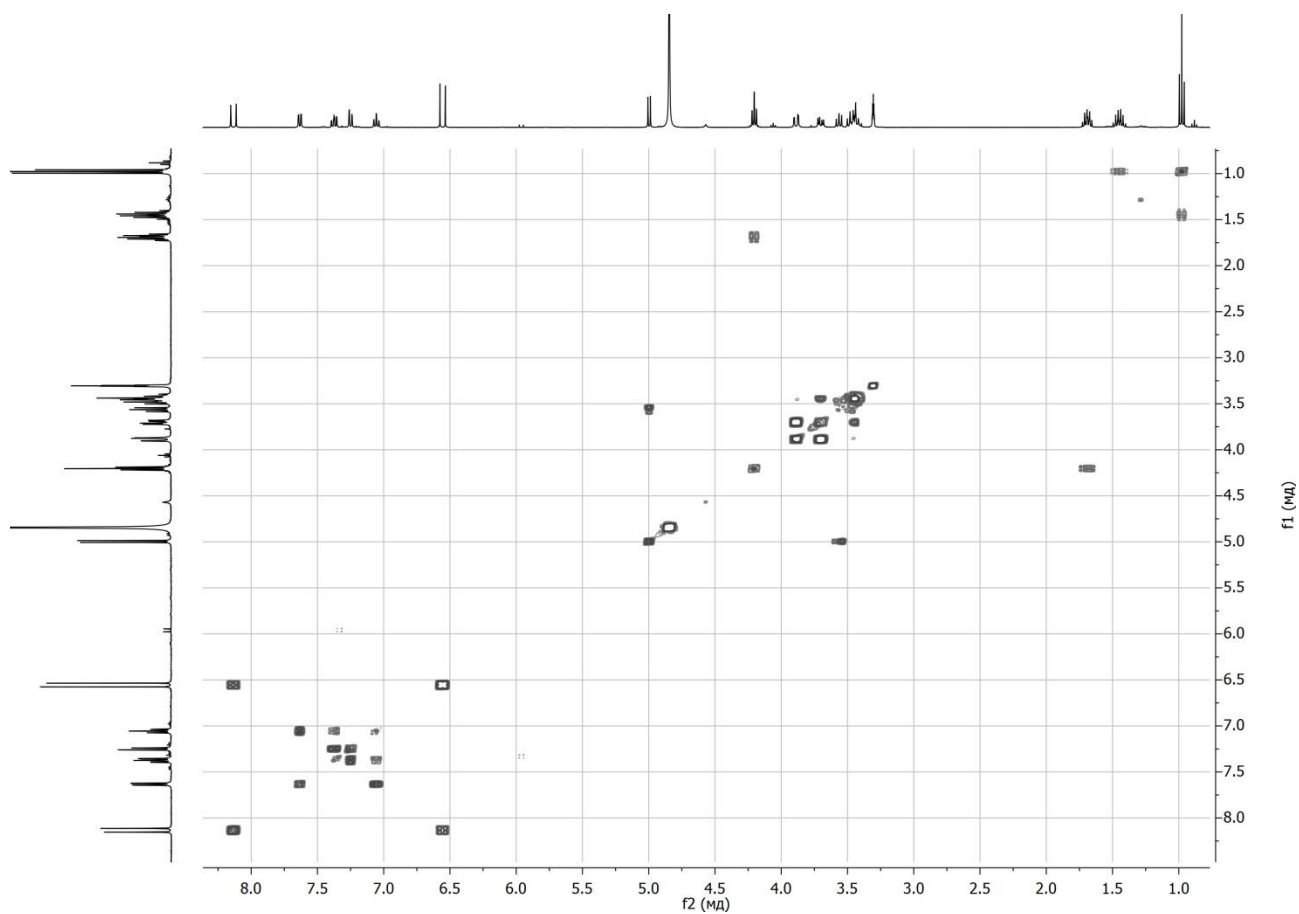


Figure S12. ^1H - ^1H COSY spectrum of compound **2** in CD_3OD

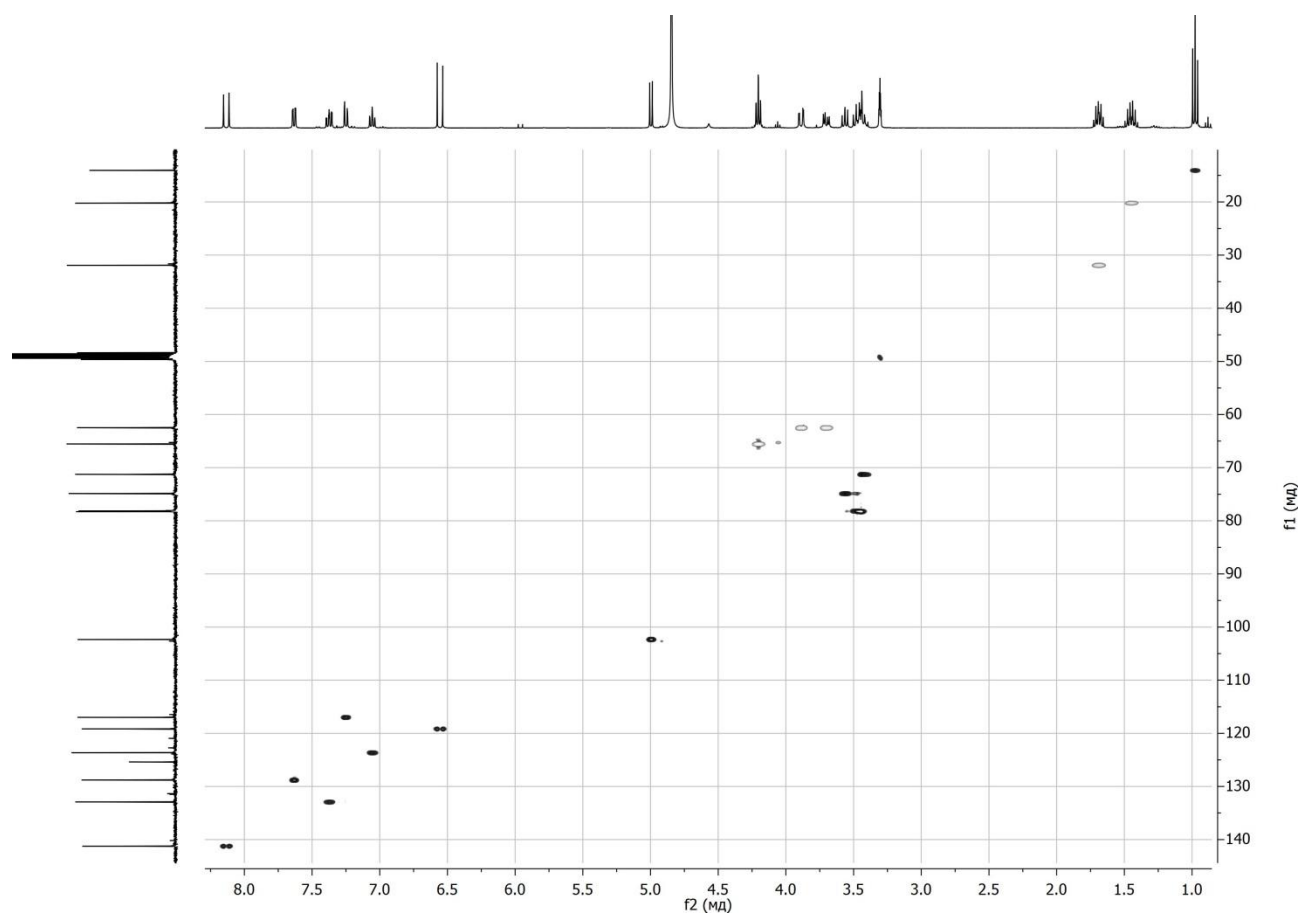


Figure S13. HSQC spectrum of compound **2** in CD₃OD

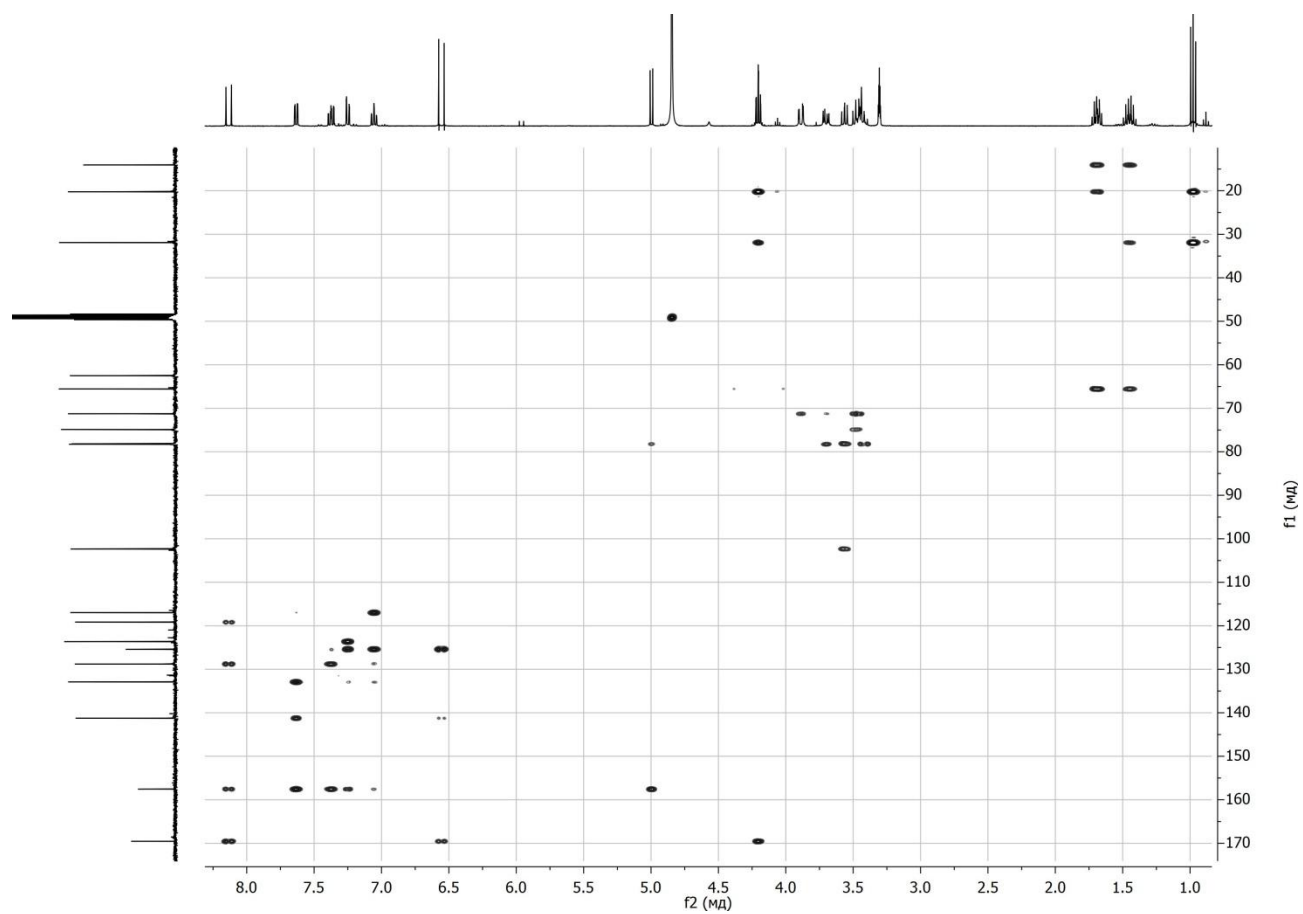


Figure S14. HMBC spectrum of compound **2** in CD₃OD

G1-9_181119133058 #15 RT: 0.14 AV: 1 SB: 22 0.36-0.78 NL: 2.39E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

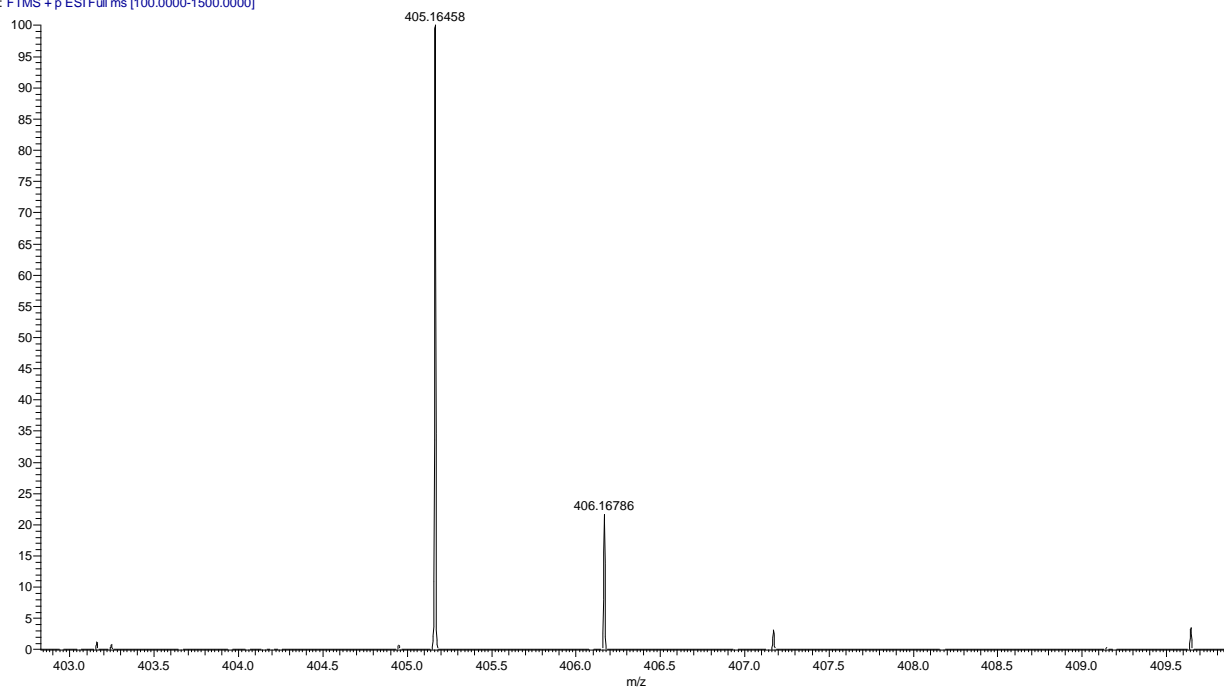


Figure S15. HR-ESI-MS spectrum of compound **3**

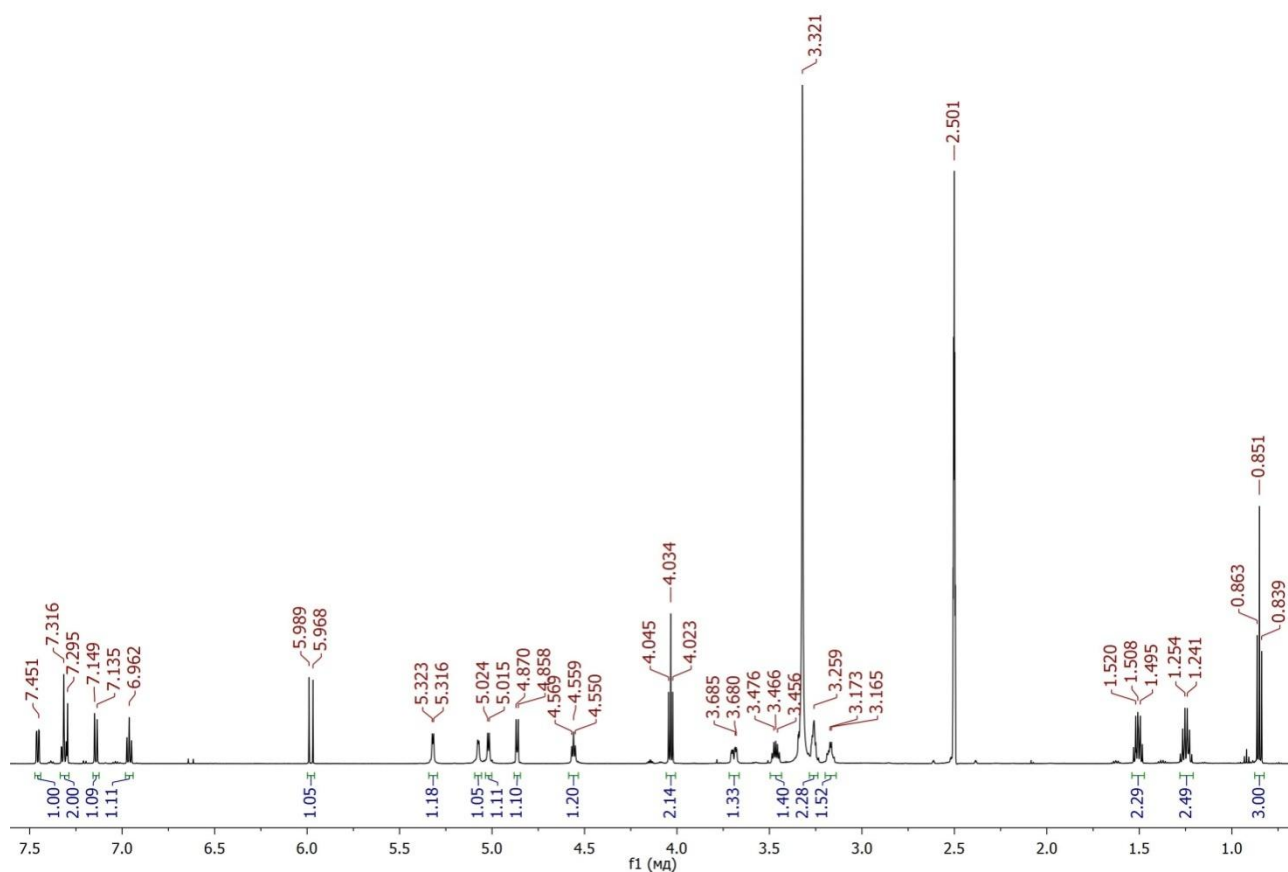


Figure S16. ¹H NMR (600 MHz) spectrum of compound **3** in DMSO-*d*₆

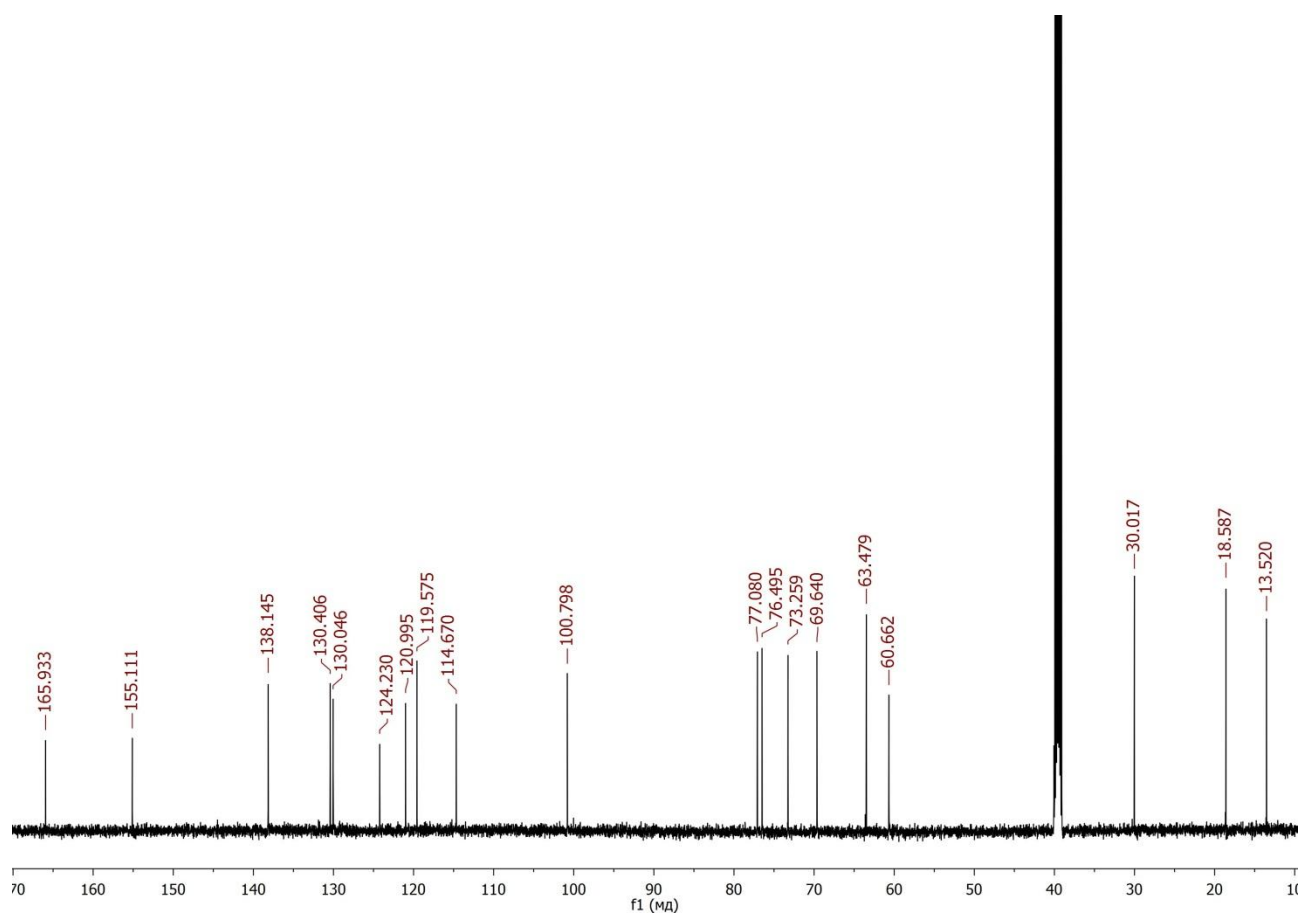


Figure S17. ^{13}C NMR (150 MHz) spectrum of compound **3** in $\text{DMSO-}d_6$

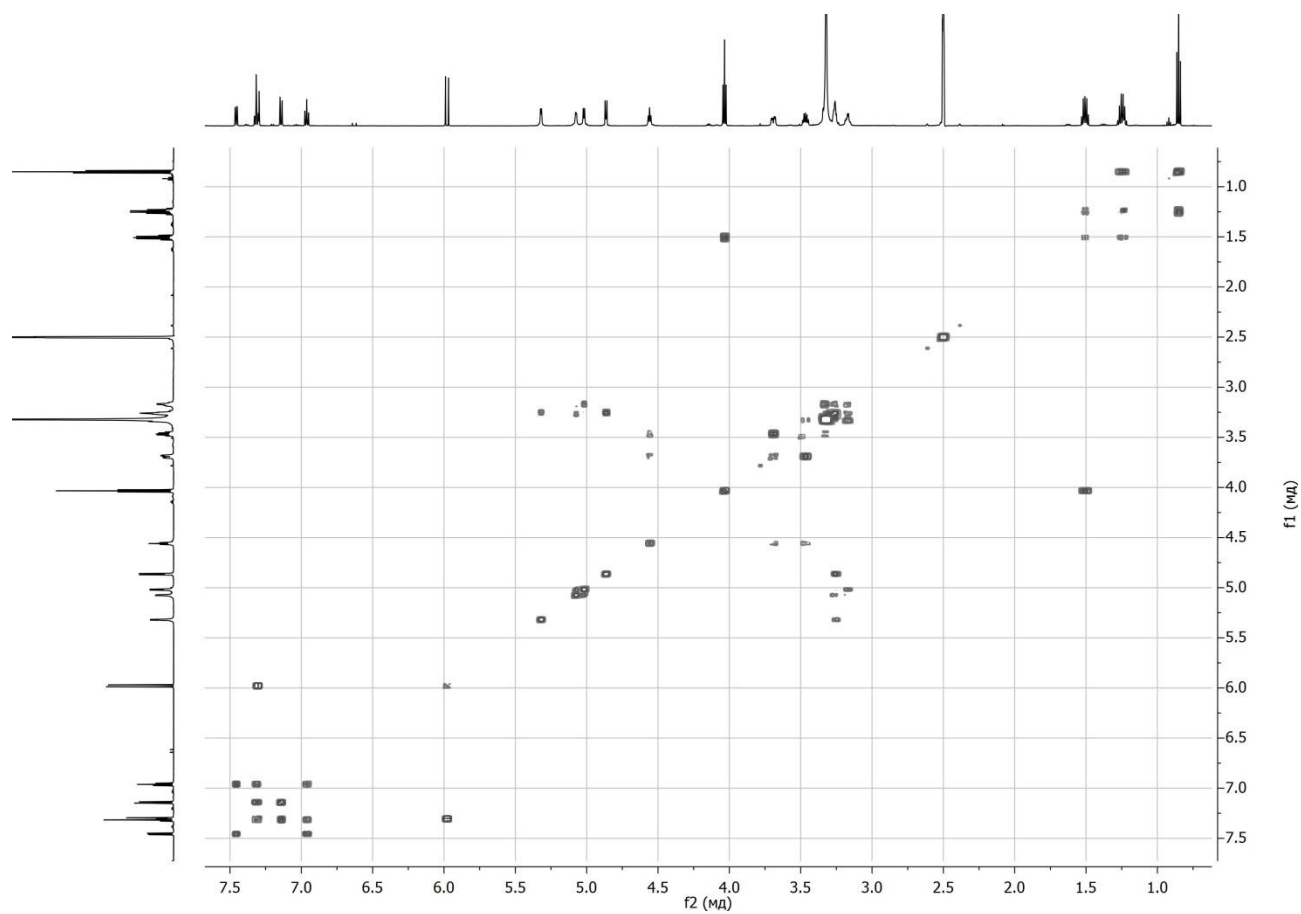


Figure S18. ^1H - ^1H COSY spectrum of compound **3** in $\text{DMSO-}d_6$

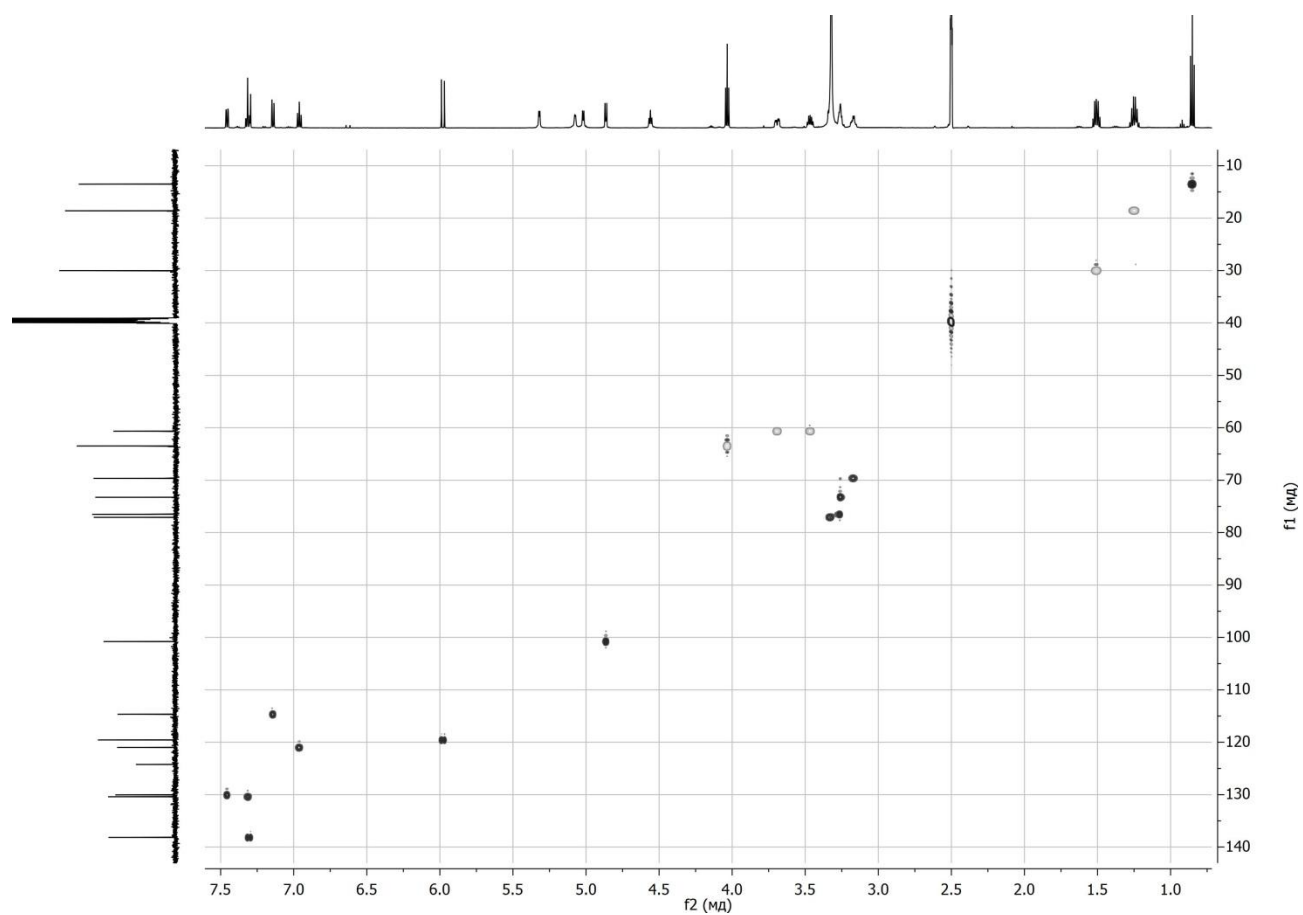


Figure S19. HSQC spectrum of compound **3** in DMSO-*d*₆

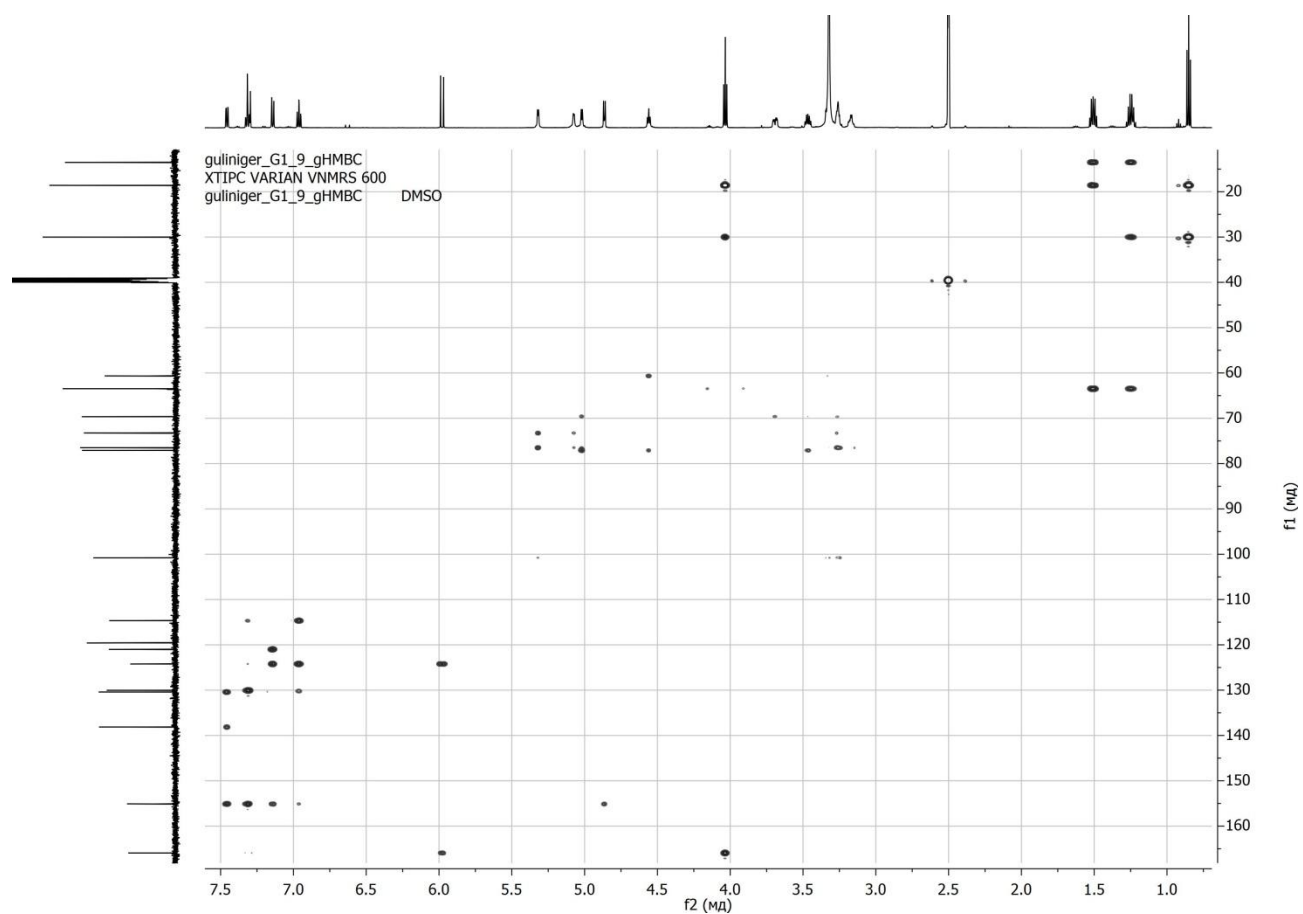


Figure S20. HMBC spectrum of compound **3** in DMSO-*d*₆

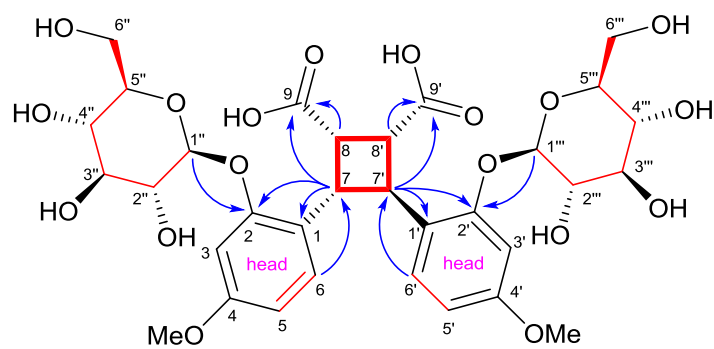


Figure S21. key HMBC correlations of compound **1**

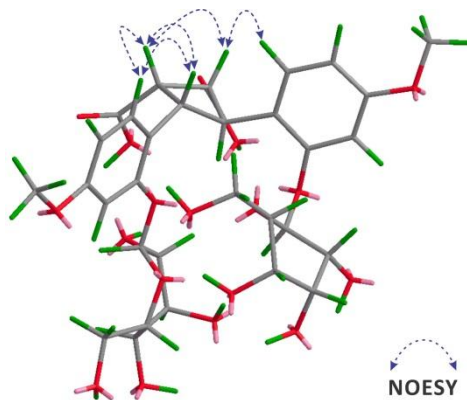


Figure S22. Key NOESY correlations of compound **1**

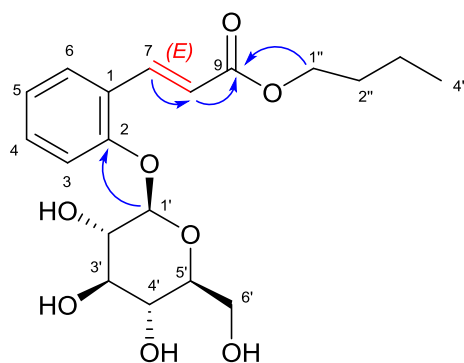


Figure S23. HMBC correlations of compound **2**

Table S1. ¹H and ¹³C NMR Data of compounds **1-3** (δ, ppm, 600 MHz for ¹H and 150 MHz for ¹³C)

No	1 *		2 **		3 *	
	δ _C	δ _H (J/Hz)	δ _C	δ _H (J/Hz)	δ _C	δ _H (J/Hz)
1	120.59		125.39		124.23	
2	155.95		157.56		155.11	
3	101.02	6.49, d, (2.4)	117.00	7.25, dd, (8.5, 1.1)	114.67	7.14, d, (8.2)
4	158.28		132.97	7.37, ddd, (8.8, 7.3, 1.7)	130.05	7.31, m
5	106.27	6.26, dd, (8.6, 2.4)	123.64	7.06, dd, (7.8, 7.3)	121.00	6.96, m
6	130.99	7.09, d, (8.6)	128.80	7.63, dd, (7.8, 1.7)	130.41	7.46, dd, (7.7, 1.4)
7	40.89	4.19, dd, (10.2, 5.8)	141.25	8.13, d, (16.3)	138.15	7.31, d, (12.5)
8	43.01	3.83, dd, (10.2, 5.8)	119.17	6.56, d, (16.3)	119.58	5.98, d, (12.5)
9	175.30		169.56		165.93	
1'	121.22		102.33	5.00, d, (7.7)	100.80	4.86, d, (7.4)
2'	155.51		74.89	3.56, dd (8.7, 7.7)	73.26	3.26, m
3'	100.53	6.46, d, (2.4)	78.15	3.48, m	75.50	3.26, m
4'	158.18		71.26	3.44, m	69.64	3.17, m
5'	105.73	6.27, dd, (8.6, 2.4)	78.27	3.45, m	77.08	3.33, m
6'	128.89	7.24, d, (8.6)	62.50	3.70, dd, (12.0, 5.1)	60.66	3.47, m
				3.89, dd, (12.0, 2.0)		3.69, ddd, (11.6, 4.9, 1.7)
7'	38.88	4.49, t, (10.0)				
8'	41.82	4.11, t, (10.0)				
9'	174.71					
1''	100.21	4.78, d, (7.6)	65.56	4.20, td, (6.6, 0.9)	63.48	4.03, t, (6.6)
2''	73.37	3.38, m	31.92	1.69, m	30.02	1.51, m
3''	77.01	3.30, m	20.22	1.46, m	18.59	1.25, m
4''	69.89	3.18, m	14.07	0.98, t, (7.4)	13.52	0.85, t, (7.4)
5''	77.14	3.30, m				
6''	60.77	3.43, dd, (11.5, 5.6)				
		3.67, m				
1'''	99.66	4.78, d, (7.6)				
2'''	73.37	3.38, m				
3'''	76.83	3.30, m				
4'''	69.89	3.18, m				
5'''	77.02	3.30, m				
6'''	60.77	3.43, dd, (11.5, 5.6)				
		3.67, m				
4-OCH ₃	54.78	3.61, s				
4'-OCH ₃	54.78	3.61, s				
2-OH					5.32, d, (4.6)	
3-OH					5.07, d, (4.0)	
4-OH					5.02, d, (5.3)	
6-OH					4.56, t, (5.8)	

* - in DMSO-*d*₆; ** - in CD₃OD