Molbank
Supporting Information

Synthesis and Anti-Inflammatory Activity of (*Z*)-4-(2-(3-Oxopiperazin-2-ylidene)acetyl)benzoic Acid

Maksim V. Dmitriev, Ekaterina E. Khramtsova, Danila Y. Apuskin, Alexander I. Andreev, Ilya I. Kovalenko, Irina V. Mashevskaya and Andrey N. Maslivets *

Department of Chemistry, Perm State University, ul. Bukireva, 15, 614990 Perm, Russia
** Correspondence: koh2@psu.ru*

Table of contents

1. X-ray analysis

Table S1. Crystal data and structure refinement for piron and compound **3**.

Compound	**Piron**	**3**
CCDC	2314647	2314648
Empirical formula	$C_{13}H_{14}N_2O_2$	$C_{26}H_{24}N_6O_5$
Formula weight	230.26	500.51
Temperature, K	295(2)	293(2)
Crystal system	monoclinic	monoclinic
Space group	C2/c	$P2_1/c$
a, Å	24.996(6)	11.589(3)
b, Å	5.2350(8)	25.450(5)
c, Å	18.116(3)	8.4635(17)
α, °	90	90
β, °	91.106(18)	99.40(2)
γ, °	90	90
Volume, $Å^3$	2370.1(8)	2462.8(10)
Z	8	4
Density (calculated), g/cm^3	1.291	1.350
Absorption coefficient, mm^{-1}	0.089	0.096
F(000)	976.0	1048.0
Crystal size, mm^3	0.5 × 0.25 × 0.12	0.56 × 0.41 × 0.06
Radiation	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection, °	6.522 to 58.774	5.836 to 58.826
Index ranges	-23 ≤ h ≤ 33, -6 ≤ k ≤ 7, -24 ≤ l ≤ 23	-15 ≤ h ≤ 11, -35 ≤ k ≤ 23, -11 ≤ l ≤ 11
Reflections collected	9992	13980
Independent reflections	2930 [R_{int} = 0.0331, R_{sigma} = 0.0259]	5819 [R_{int} = 0.0309, R_{sigma} = 0.0426]
Data/restraints/parameters	2930/5/182	5819/0/353
Goodness-of-fit on F^2	1.029	1.009
Final R indexes [I>=2σ (I)]	R_1 = 0.0561, wR_2 = 0.1490	R_1 = 0.0583, wR_2 = 0.1318
Final R indexes [all data]	R_1 = 0.0747, wR_2 = 0.1685	R_1 = 0.0946, wR_2 = 0.1546
Largest diff. peak/hole, $eÅ^{-3}$	0.17/-0.18	0.28/-0.28

2. Copies of ^{1}H and ^{13}C NMR Spectra

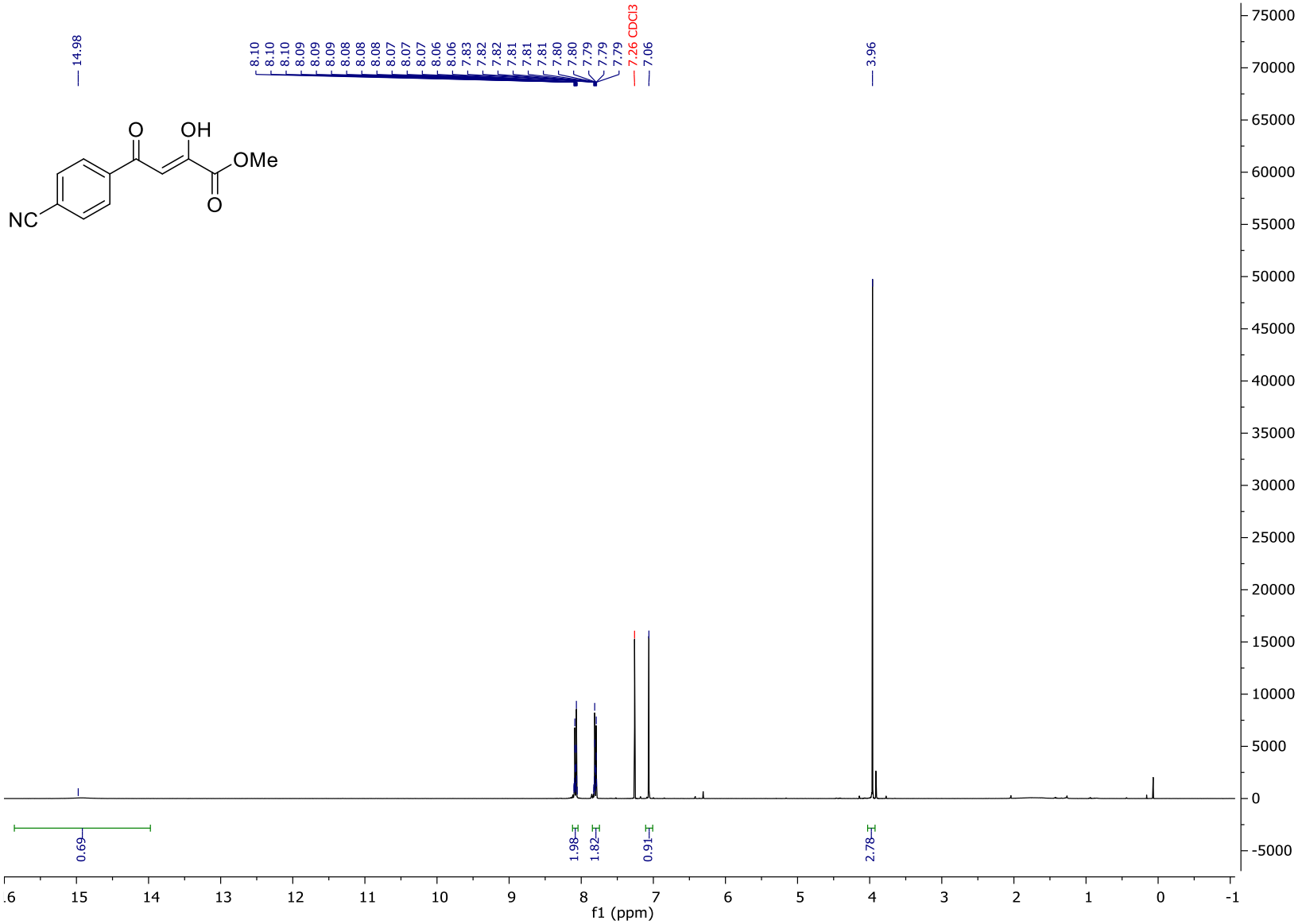

Figure S1. *^{1}H NMR spectrum of compound **2**.*

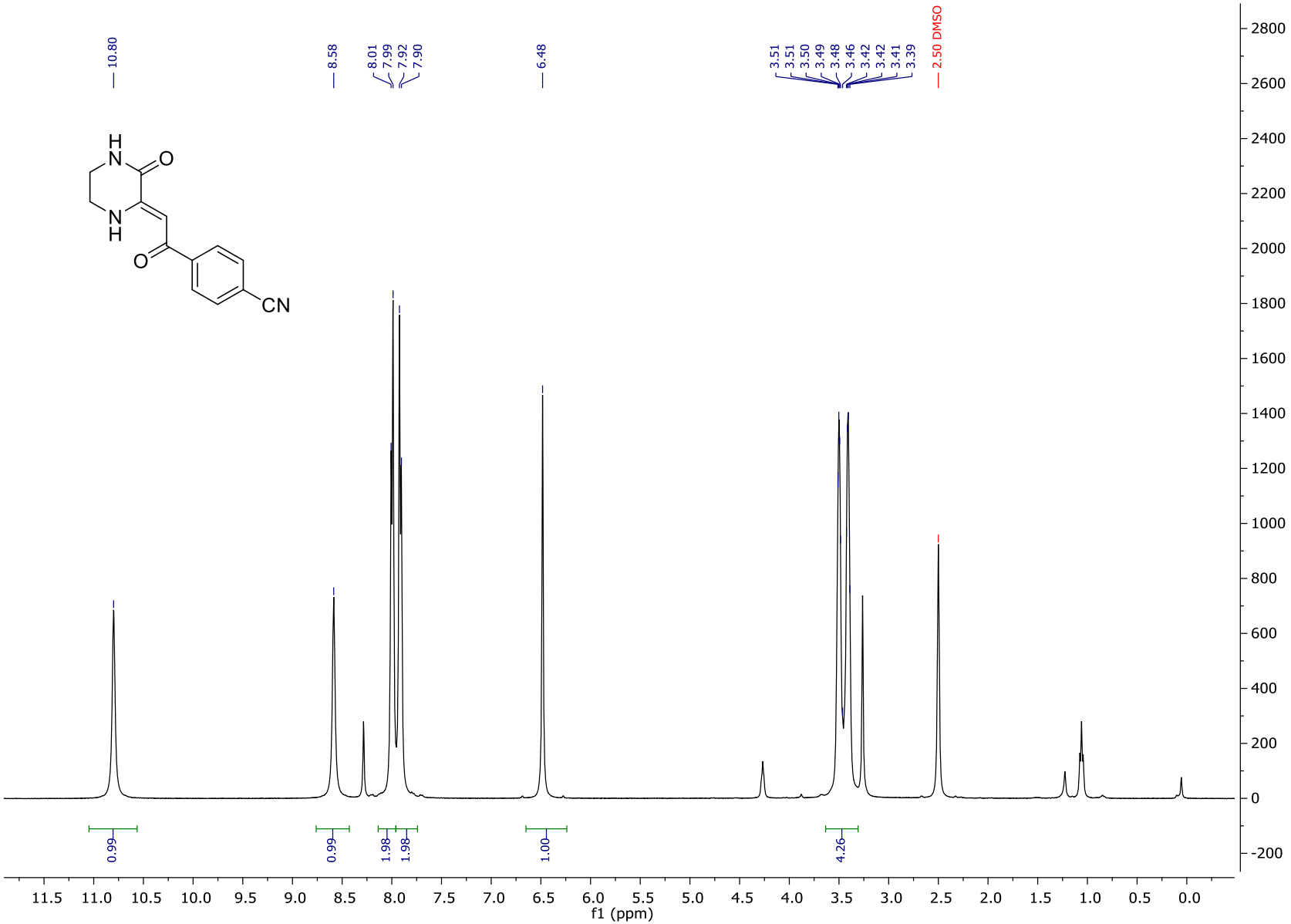

Figure S2. *^{1}H NMR spectrum of compound **3**.*

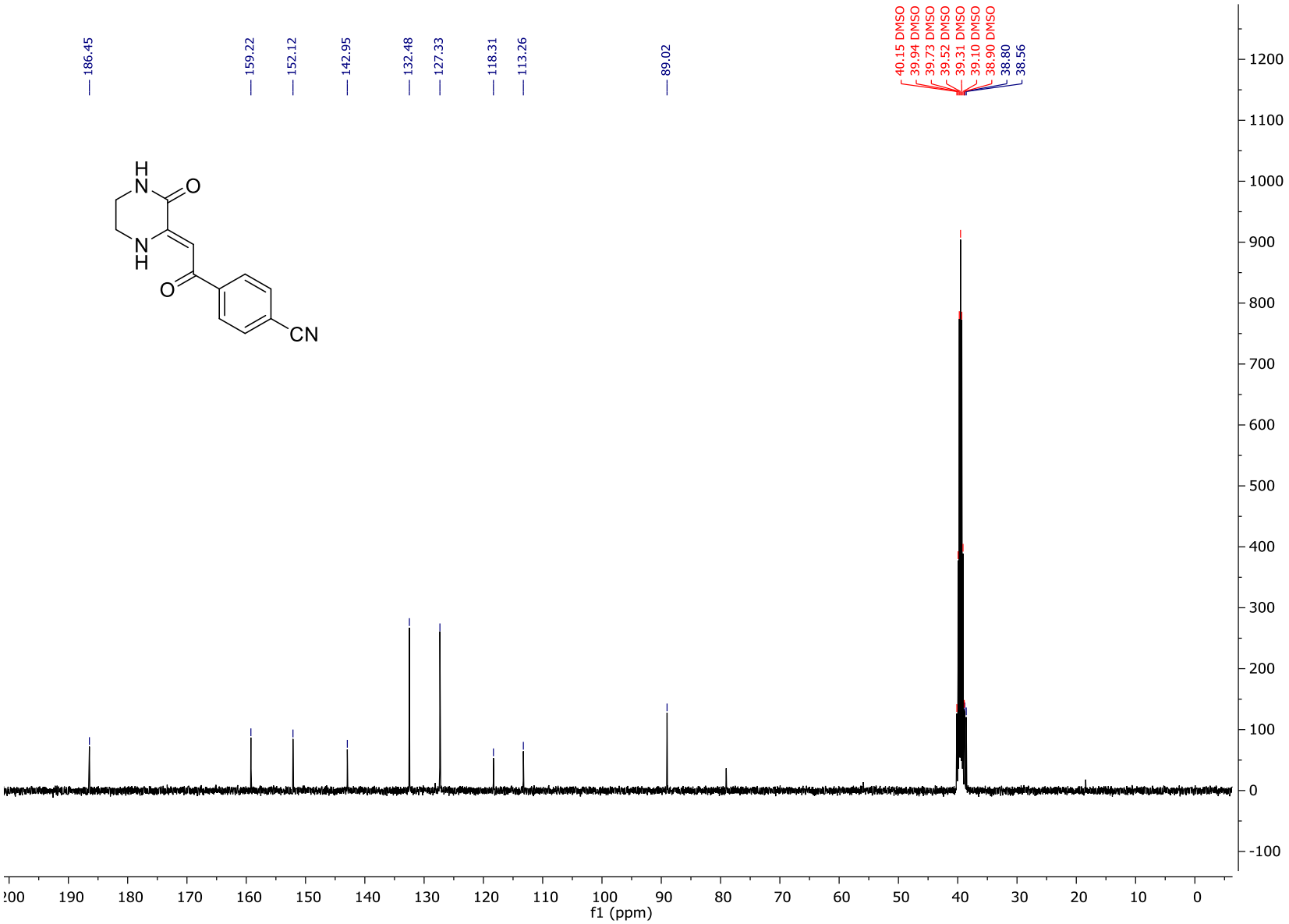

Figure S3. *^{13}C NMR spectrum of compound **3**.*

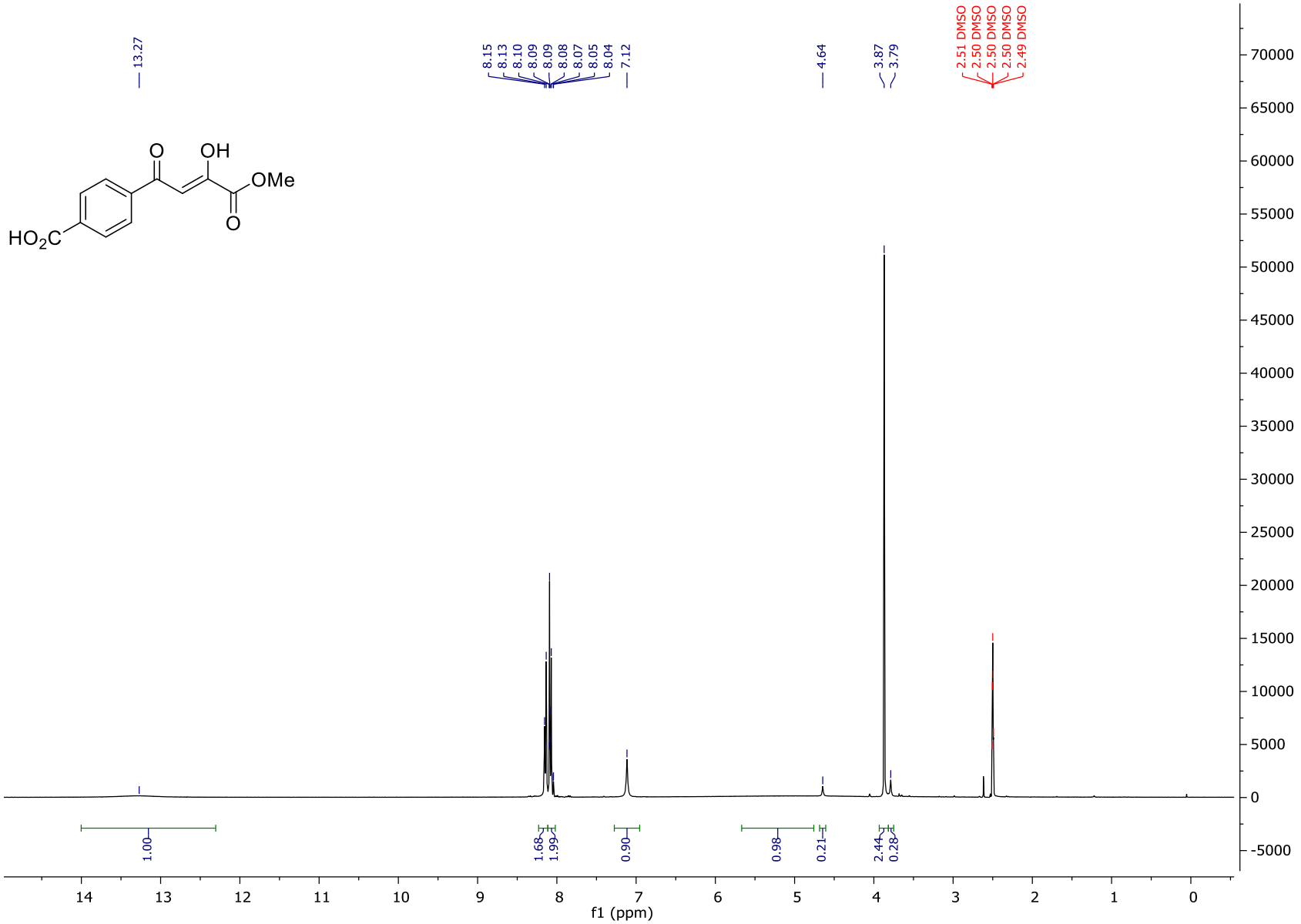

Figure S4. *^{1}H NMR spectrum of compound **4**.*

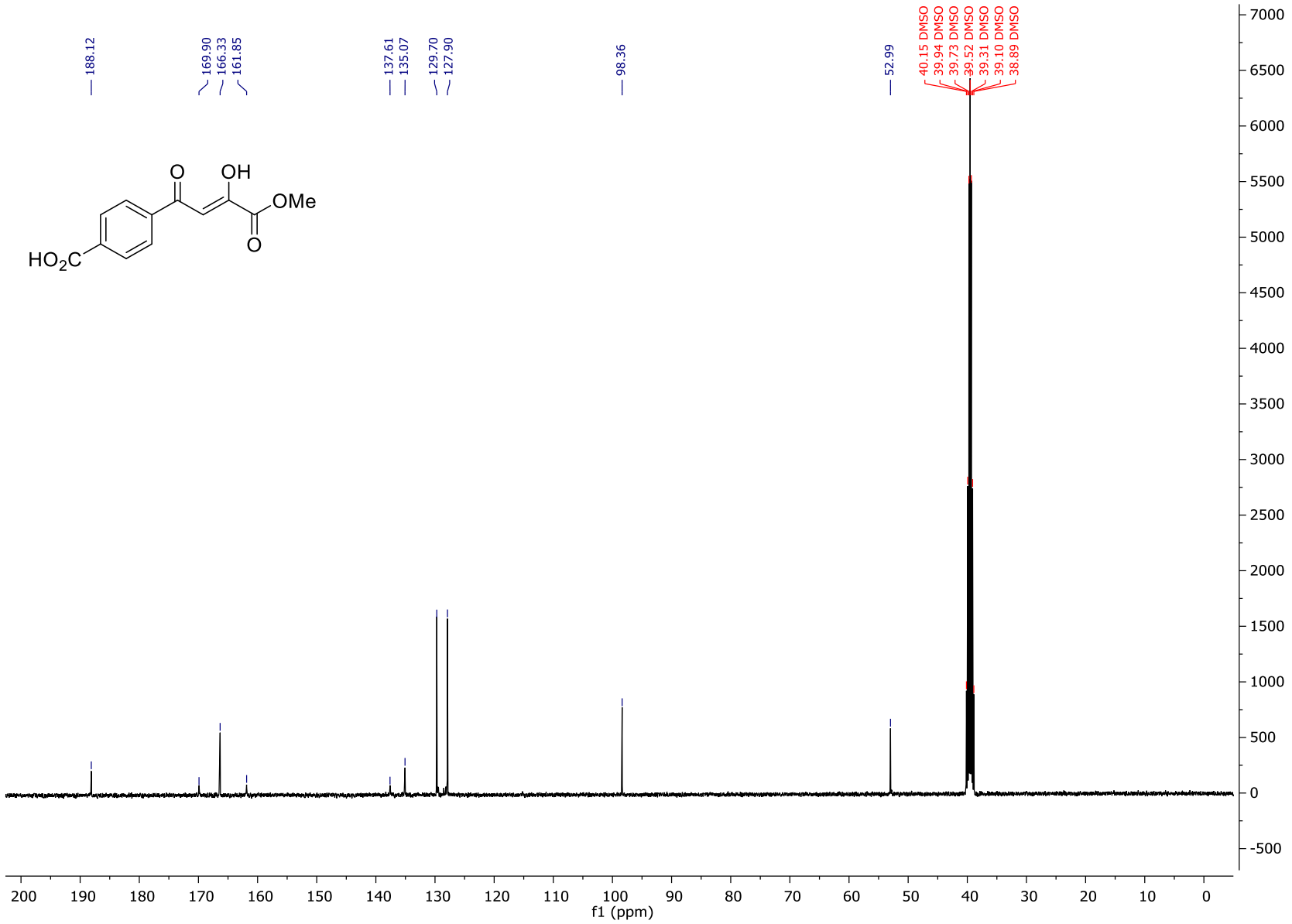

Figure S5. *^{13}C NMR spectrum of compound **4**.*

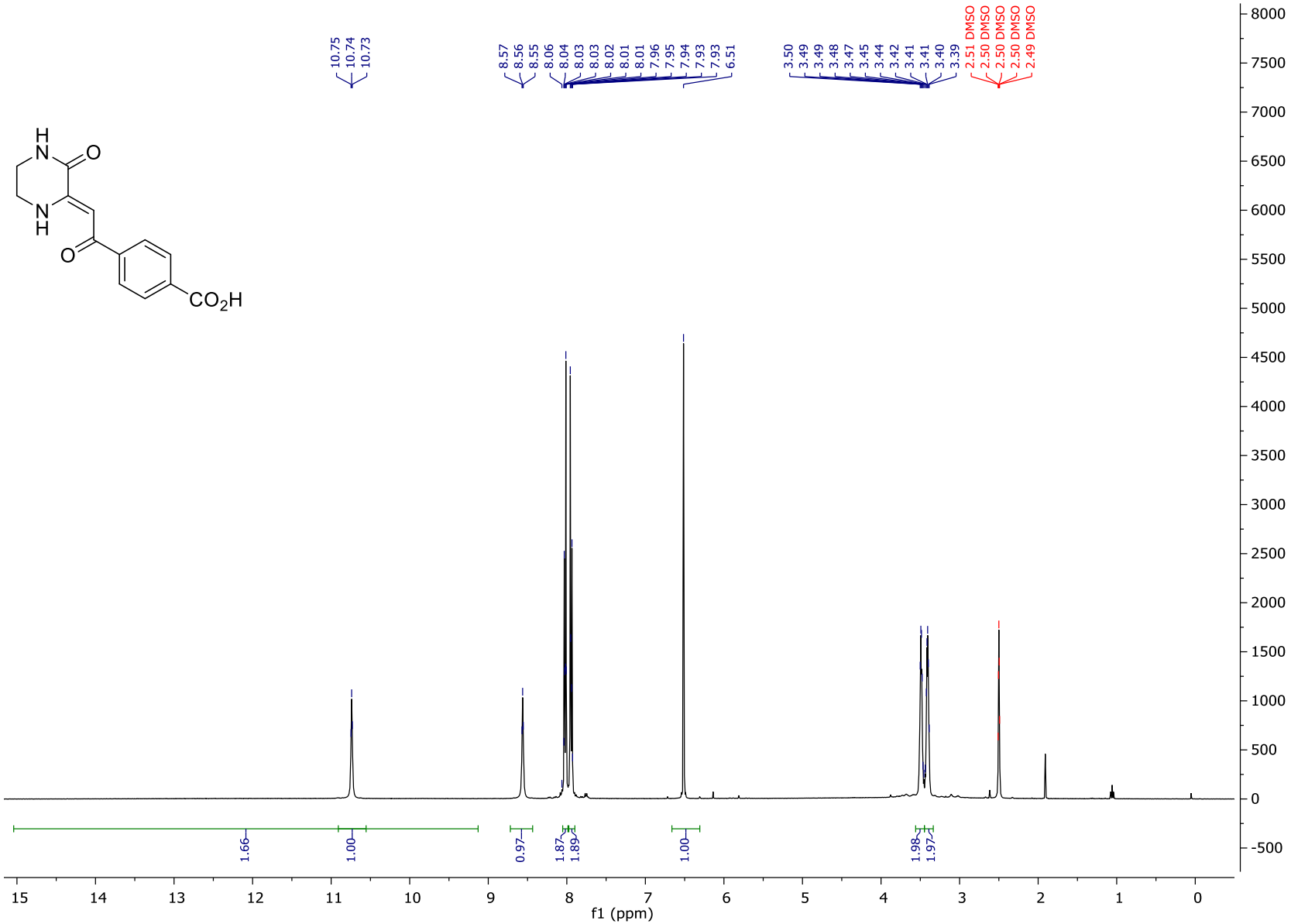

Figure S6. *^{1}H NMR spectrum of compound **1**.*

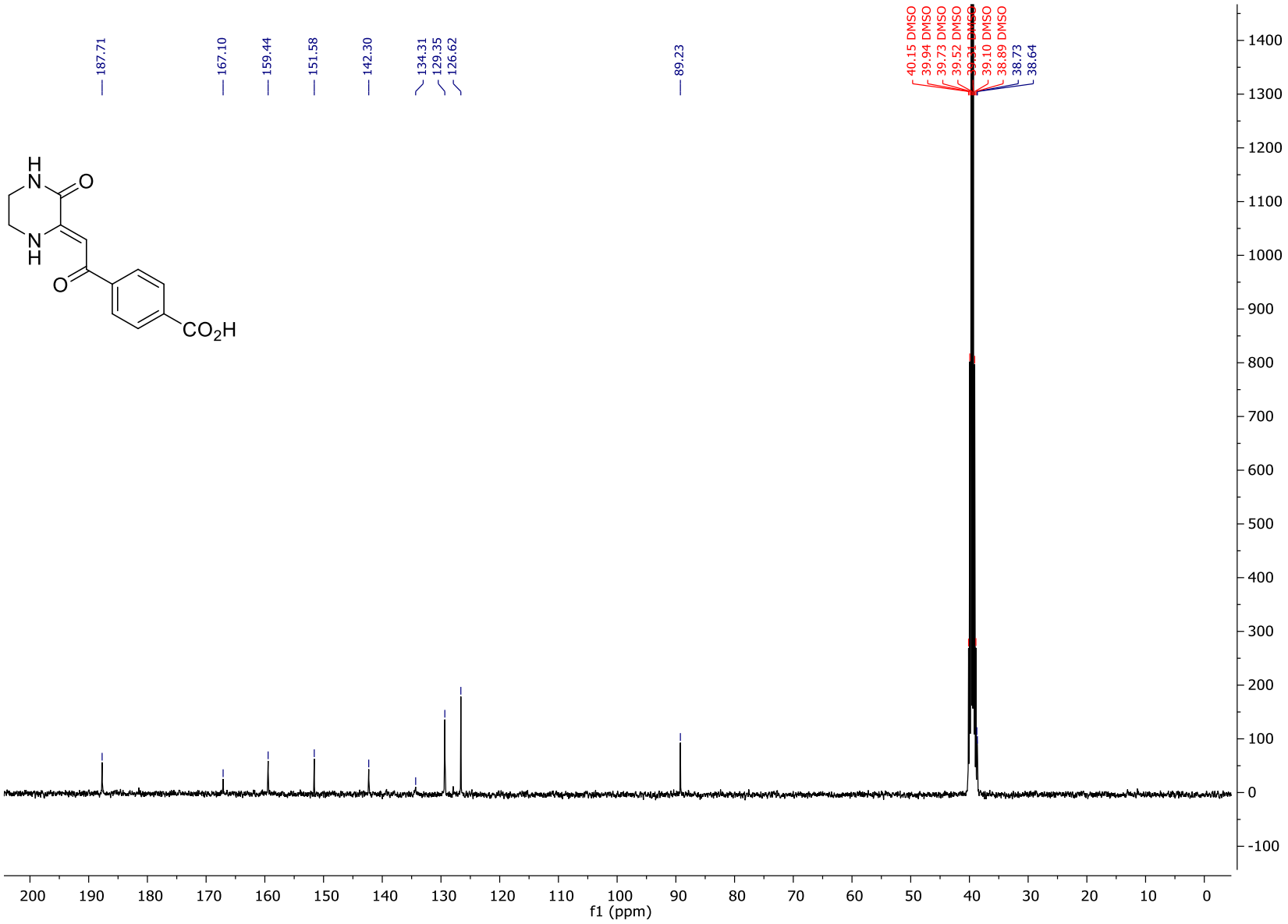

Figure S7. *^{13}C NMR spectrum of compound* ***1***