## **Supporting Information**

Org. Commun. 16:3 (2023) 152-165

## Novel oxalamide derivatives for COXs expression and breast cancer: design, synthesis, biological evaluation, and docking studies

## Burak Kuzu 1,2, Ceylan Hepokur 3 and Oztekin Algul 1,4

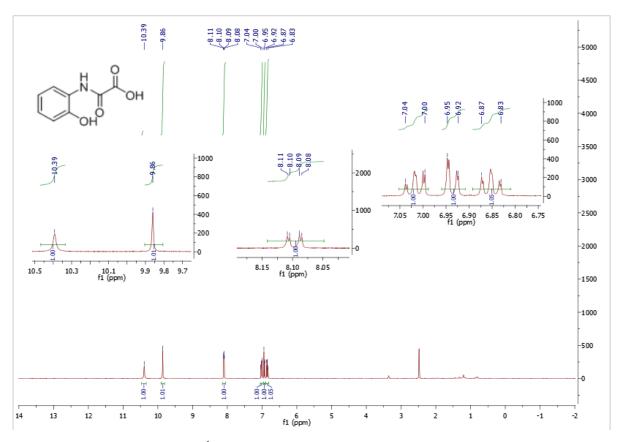
<sup>&</sup>lt;sup>4</sup> Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Erzincan Binali Yildirim University, Erzincan, 24100, Türkiye

Table of Contents	Page
Figure S1: <sup>1</sup> H-NMR (400 MHz, d <sub>6</sub> -DMSO) Spectrum of 4	2
Figure S2: $^{13}$ C-NMR (100 MHz, $d_6$ -DMSO) Spectrum of 4	2
Figure S3: ${}^{1}\text{H-NMR}$ (400 MHz, $d_{6}$ -DMSO) Spectrum of 6a	3
<b>Figure S4:</b> $^{13}$ C-NMR (100 MHz, $d_6$ -DMSO) Spectrum of <b>6a</b>	3
Figure S5: <sup>1</sup> H-NMR (400 MHz, d <sub>6</sub> -DMSO) Spectrum of <b>6b</b>	4
<b>Figure S6:</b> $^{13}$ C-NMR (100 MHz, $d_6$ -DMSO) Spectrum of <b>6b</b>	4
Figure S7: ${}^{1}\text{H-NMR}$ (400 MHz, $d_{6}\text{-DMSO}$ ) Spectrum of 6c	5
<b>Figure S8:</b> $^{13}$ C-NMR (100 MHz, $d_6$ -DMSO) Spectrum of <b>6c</b>	5
<b>Figure S9:</b> $^{1}$ H-NMR (400 MHz, $d_{6}$ -DMSO) Spectrum of <b>6d</b>	6
Figure S10: $^{13}$ C-NMR (100 MHz, $d_6$ -DMSO) Spectrum of 6d	6
Figure S11: <sup>1</sup> H-NMR (400 MHz, d <sub>6</sub> -DMSO) Spectrum of <b>7a</b>	7
Figure S12: $^{13}$ C-NMR (100 MHz, $d_6$ -DMSO) Spectrum of 7a	7
Figure S13: <sup>1</sup> H-NMR (400 MHz, d <sub>6</sub> -DMSO) Spectrum of <b>7b</b>	8
<b>Figure S14:</b> $^{13}$ C-NMR (100 MHz, $d_6$ -DMSO) Spectrum of <b>7b</b>	8
Figure S15: ${}^{1}$ H-NMR (400 MHz, $d_{6}$ -DMSO) Spectrum of 7c	9
Figure S16: $^{13}$ C-NMR (100 MHz, $d_6$ -DMSO) Spectrum of 7c	9
Figure S17: <sup>1</sup> H-NMR (400 MHz, d <sub>6</sub> -DMSO) Spectrum of 7d	10
Figure S18: $^{13}$ C-NMR (100 MHz, $d_6$ -DMSO) Spectrum of 7d	10

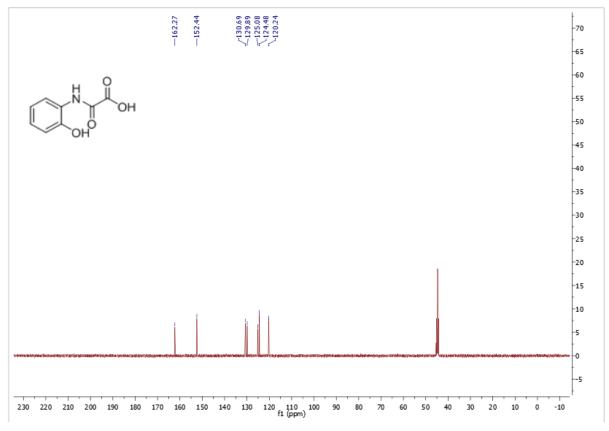
<sup>&</sup>lt;sup>1</sup> Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Mersin University, Mersin, 33169, Türkiye

<sup>&</sup>lt;sup>2</sup> Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Van Yuzuncu Yil University, Van, 65080, Türkiye

<sup>&</sup>lt;sup>3</sup> Department of Basic Pharmaceutical Sciences, Division of Biochemistry, Faculty of Pharmacy, Cumhuriyet University, Sivas, 58100, Türkiye



**Figure S1:**  $^{1}$ H-NMR (400 MHz,  $d_{6}$ -DMSO) Spectrum of **4** 



**Figure S2:**  $^{13}$ C-NMR (100 MHz,  $d_6$ -DMSO) Spectrum of **4** © 2023 ACG Publications. All rights reserved.

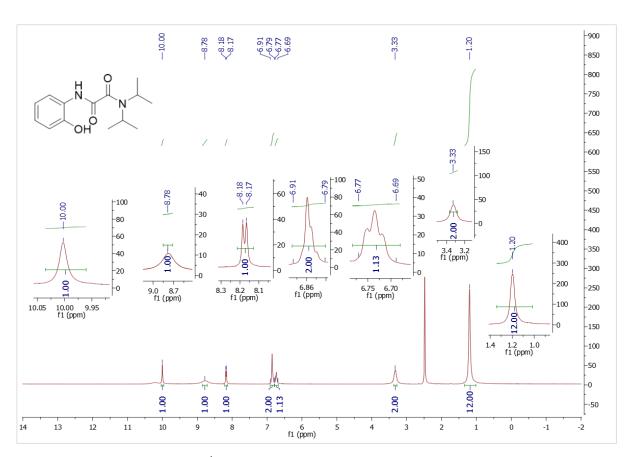
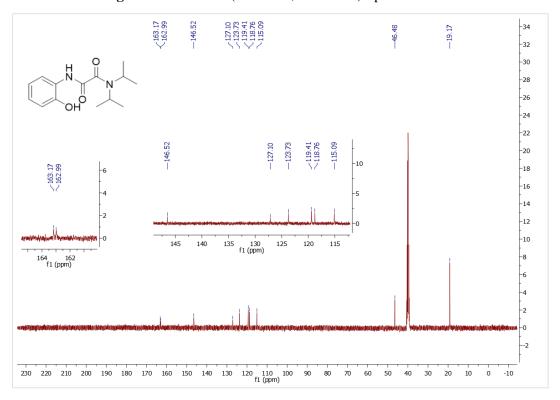


Figure S3: <sup>1</sup>H-NMR (400 MHz, d<sub>6</sub>-DMSO) Spectrum of 6a



**Figure S4:**  $^{13}$ C-NMR (100 MHz,  $d_6$ -DMSO) Spectrum of **6a** 

© 2023 ACG Publications. All rights reserved.

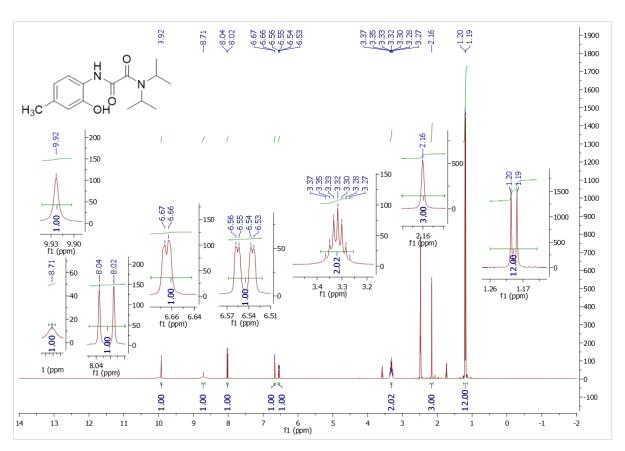
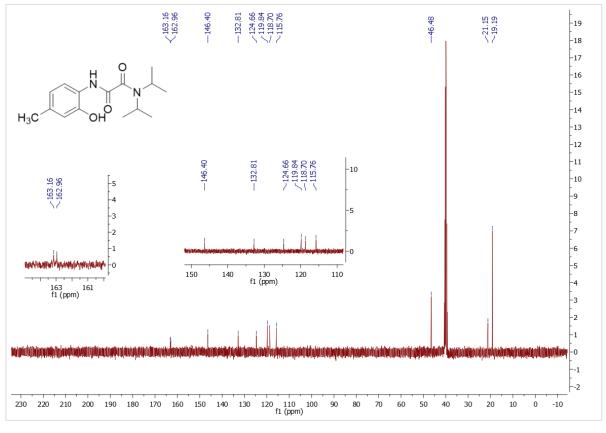


Figure S5: <sup>1</sup>H-NMR (400 MHz, d<sub>6</sub>-DMSO) Spectrum of **6b** 



**Figure S6:**  $^{13}$ C-NMR (100 MHz,  $d_6$ -DMSO) Spectrum of **6b** © 2023 ACG Publications. All rights reserved.

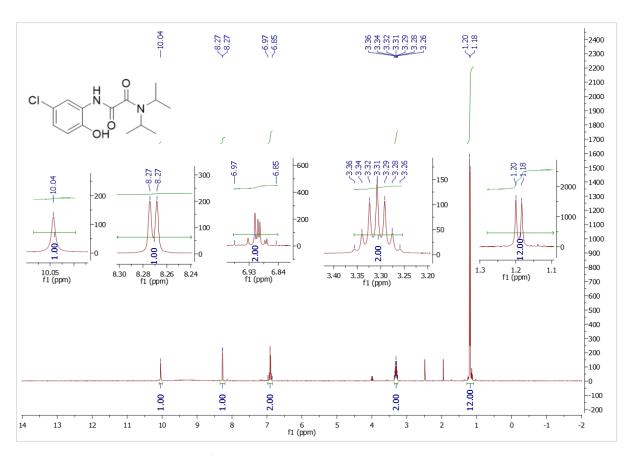
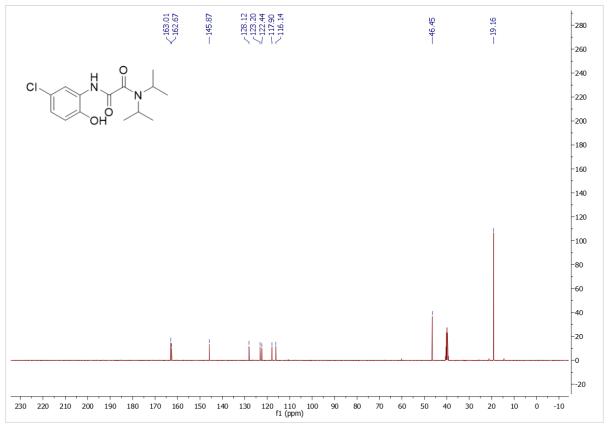


Figure S7: <sup>1</sup>H-NMR (400 MHz, d<sub>6</sub>-DMSO) Spectrum of 6c



**Figure S8:**  $^{13}$ C-NMR (100 MHz,  $d_6$ -DMSO) Spectrum of **6c** © 2023 ACG Publications. All rights reserved.

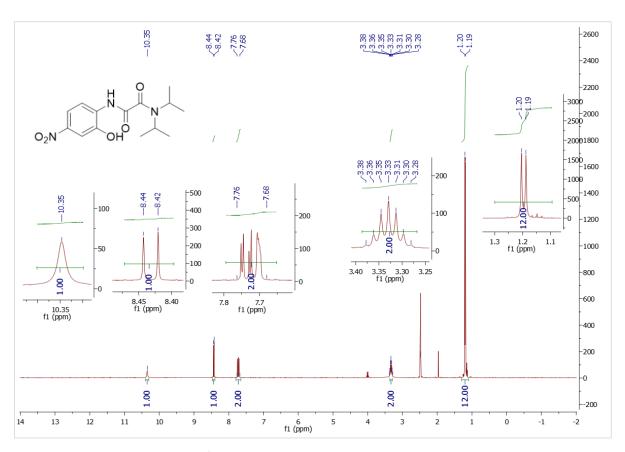
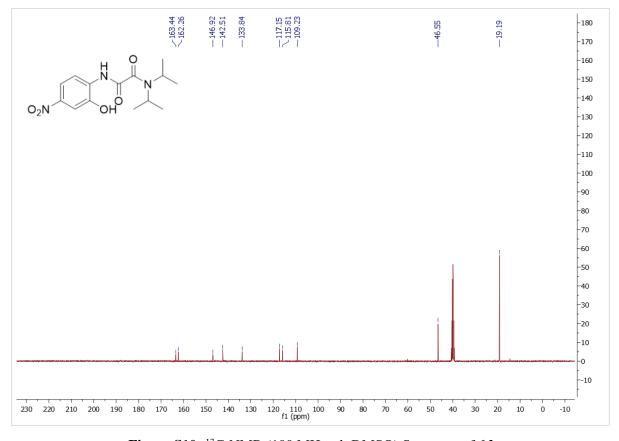


Figure S9: <sup>1</sup>H-NMR (400 MHz, d<sub>6</sub>-DMSO) Spectrum of 6d



**Figure S10:**  $^{13}$ C-NMR (100 MHz,  $d_6$ -DMSO) Spectrum of **6d** © 2023 ACG Publications. All rights reserved.

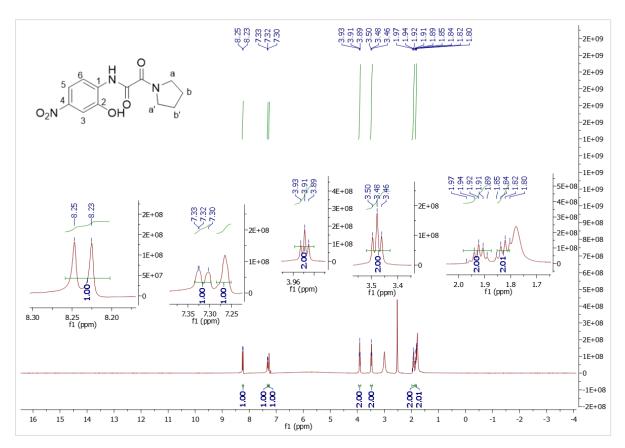
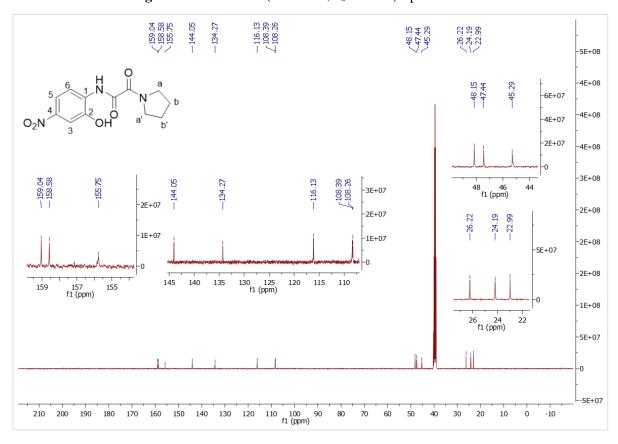
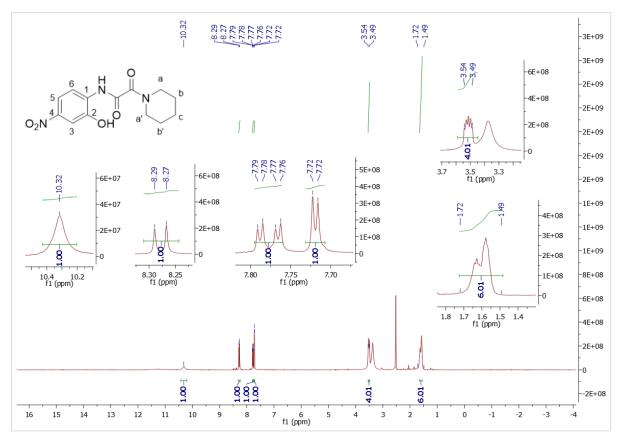


Figure S11: <sup>1</sup>H-NMR (400 MHz, d<sub>6</sub>-DMSO) Spectrum of 7a

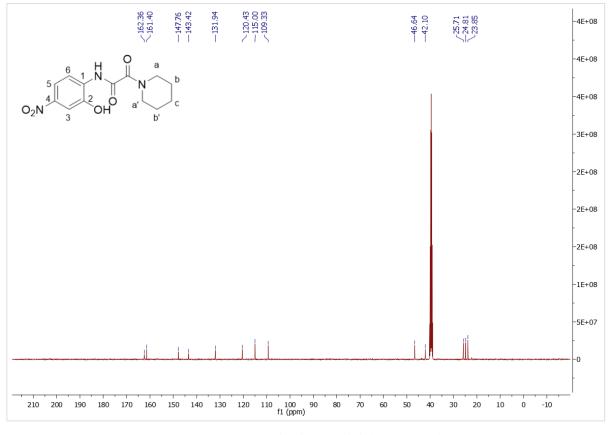


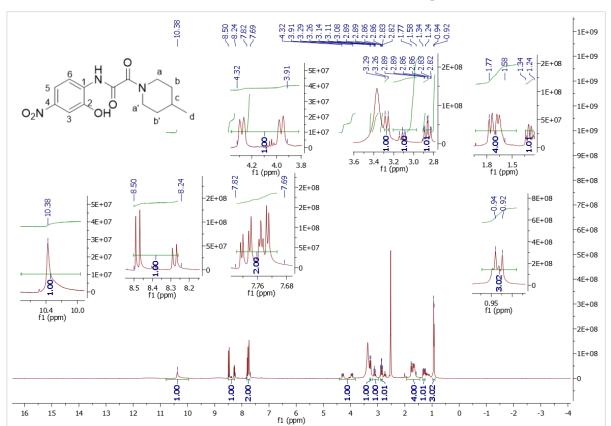
© 2023 ACG Publications. All rights reserved.

Figure S12:  ${}^{13}\text{C-NMR}$  (100 MHz,  $d_6$ -DMSO) Spectrum of 7a



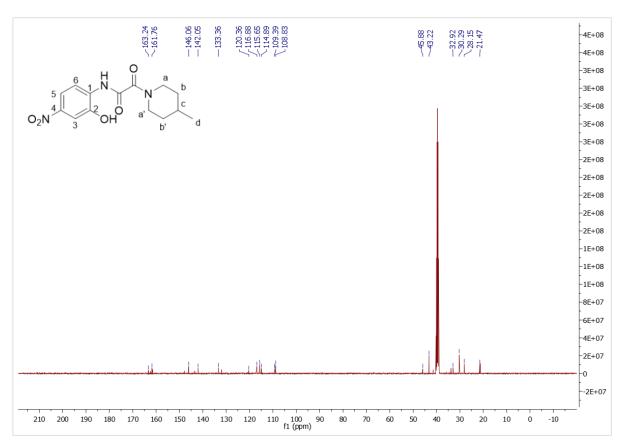
**Figure S13:**  $^{1}$ H-NMR (400 MHz,  $d_{6}$ -DMSO) Spectrum of **7b** 



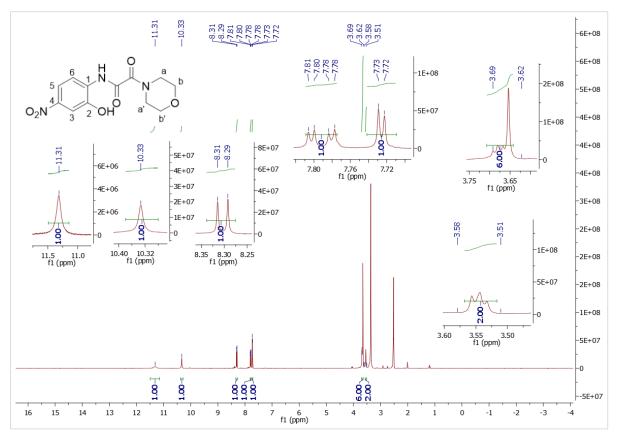


**Figure S14:**  $^{13}$ C-NMR (100 MHz,  $d_6$ -DMSO) Spectrum of **7b** 

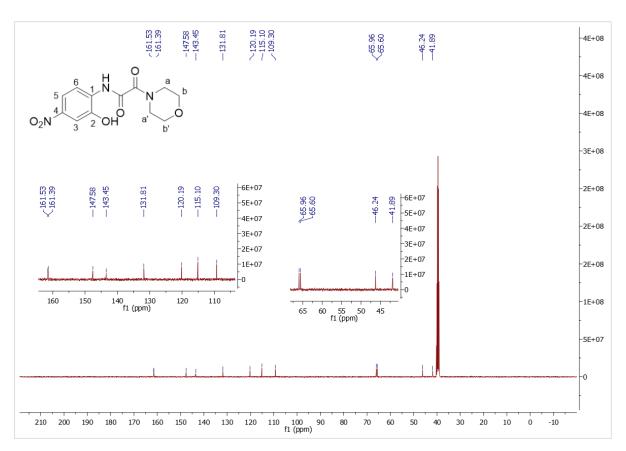
Figure S15:  ${}^{1}$ H-NMR (400 MHz,  $d_{6}$ -DMSO) Spectrum of 7c



**Figure S16:**  $^{13}$ C-NMR (100 MHz,  $d_6$ -DMSO) Spectrum of **7c** 



**Figure S17:** <sup>1</sup>H-NMR (400 MHz, *d*<sub>6</sub>-DMSO) Spectrum of **7a** © 2023 ACG Publications. All rights reserved.



**Figure S18:**  $^{13}$ C-NMR (100 MHz,  $d_6$ -DMSO) Spectrum of **7d**