**Investigations on crystal structure of a novel 3-((4,6-dimethylpyrimidin-2-yl)amino)isobenzofuran-1(3*H*)-one, and related theoretical studies.**

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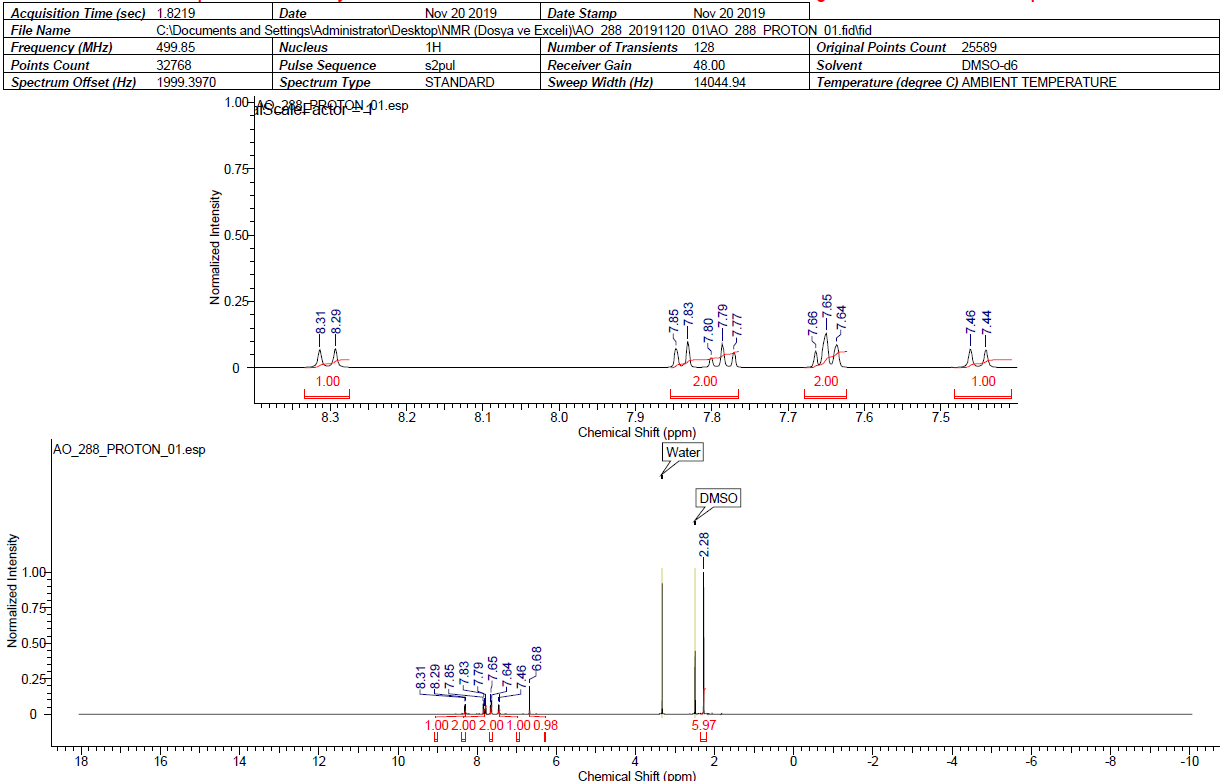
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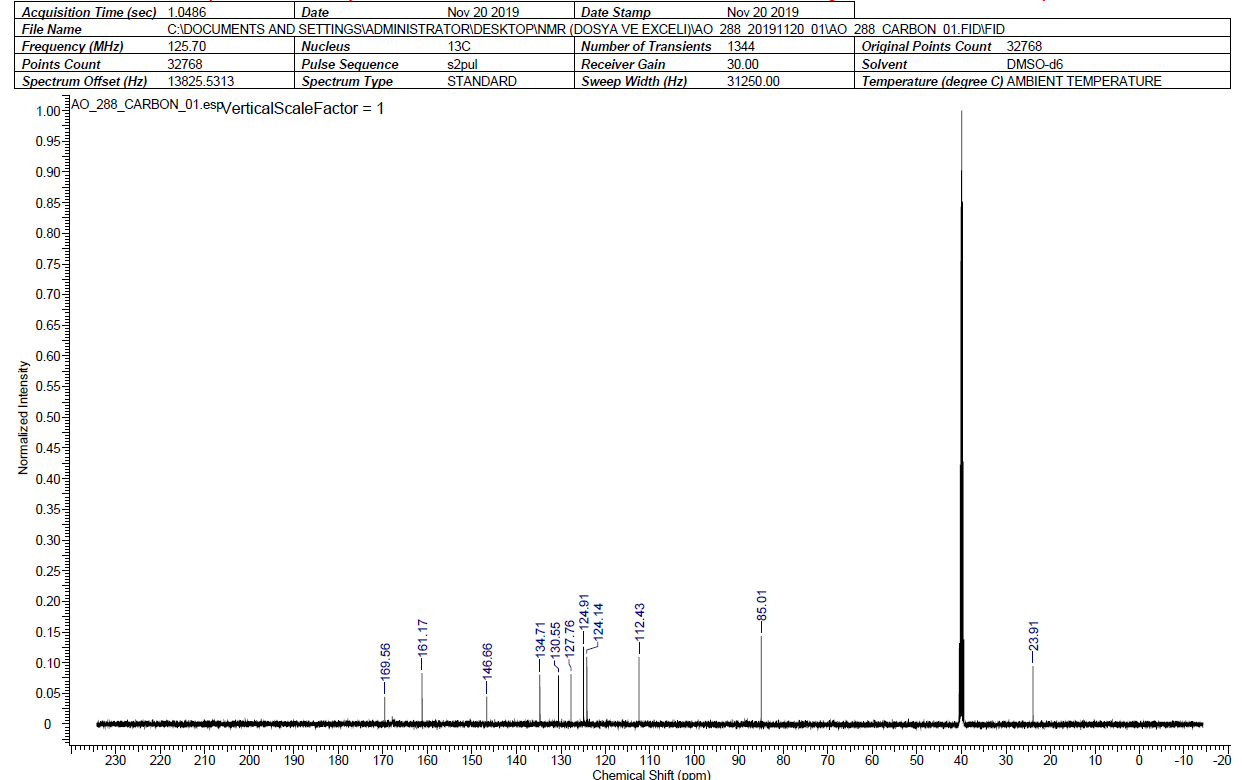
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**Fig. S2.** **13**C**-**NMR spectrum of 3-((4,6-dimethylpyrimidin-2-yl)amino)isobenzofuran-1(3*H*)-one (**1**)inDMSO-d*6* **…………………………………………………………………… 3**

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**Fig. S1. 1**H**-**NMR spectrum of 3-((4,6-dimethylpyrimidin-2-yl)amino)isobenzofuran-1(3*H*)-one (**1**)inDMSO-d6



**Fig. S2.** **13**C**-**NMR spectrum of 3-((4,6-dimethylpyrimidin-2-yl)amino)isobenzofuran-1(3*H*)-one (**1**)inDMSO-d6