The crystal structure of 6-methacryloylbenzo[\textit{d}][1,3]dioxol-5-yl 4-nitrobenzenesulfonate, \textit{C}_{17}\textit{H}_{13}\textit{NO}_{8}\textit{S}

Abstract
\textit{C}_{17}\textit{H}_{13}\textit{NO}_{8}\textit{S}, monoclinic, \textit{P}2\textit{1}/\textit{c} (no. 14), \textit{a} = 17.7630(4) Å, \textit{b} = 7.04725(16) Å, \textit{c} = 13.7187(3) Å, \textit{β} = 102.748(2)°, \textit{V} = 1674.97(7) Å³, \textit{Z} = 4, \textit{R}_{\text{gt}}(\textit{F}) = 0.0557, \textit{wR}_{\text{ref}}(\textit{F}^2) = 0.1652, \textit{T} = 273 K.

The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material
Sulfonate derivatives were prepared according to the method reported previously [5–6]. To a mixture of 1-(6-hydroxybenzo[\textit{d}][1,3]dioxol-5-yl)-2-methylprop-2-en-1-one (103 mg, 0.5 mmol) and 4-nitrobenzenesulfonyl chloride (144 mg, 0.65 mmol) in dry DCM (5 mL) was added 4-dimethylaminopyridine (DMAP, 12 mg, 0.1 mmol) and stirred uniformly at room temperature in a round-bottomed flask. Then a solution of Et\textsubscript{3}N (0.1 mL, 0.75 mmol) dissolved in dried DCM (0.5 mL) was dropwise added into the above mixture and continued to stir until the reaction was completed according to TLC detection. Subsequently, H\textsubscript{2}O (10 mL) was added into the reaction, and extracted with DCM (2 × 20 mL). Then organic phase was combined, washed by saturated brine (2 × 20 mL), and dried over anhydrous Na\textsubscript{2}SO\textsubscript{4}. After filtration and removal of the solvent, the residue was purified by column chromatography on silica gel to obtain the title compound 131 mg (yield 67 %). Suitable crystals for X-ray diffraction measurements were obtained from DCM.

2 Experimental details
Coordinates of hydrogen atoms were included using constraints or restraints. Their \textit{U}_{iso} values were set to 1.2\textit{U}_{eq} or 1.5\textit{U}_{eq} of the parent atoms.

3 Comment
Sulfonate derivatives containing a kakuol moiety are potential for development of new potential fungicidal candidates [6].
In recent years, kakuol and its derivative have aroused the great interest of many agricultural chemists because of their remarkable antifungal activity [7–8]. As displayed in figure, there is one molecule in the asymmetric unit of the title compound. The bond distance of $C7–O3$ is $1.215(3)$ Å, which is similar to the $C–O$ bond length [9–10], indicating the $C–O$ bond is double bond. The bond lengths of $C1–O4$, $C3–O1$, $C9–O1$, $C4–O2$, and $C9–O2$ in the title molecule are $1.418(3)$ Å, $1.371(3)$ Å, $1.439(4)$ Å, $1.370(3)$ Å, and $1.413(3)$ Å, respectively, which are obviously single bonds.

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**References**