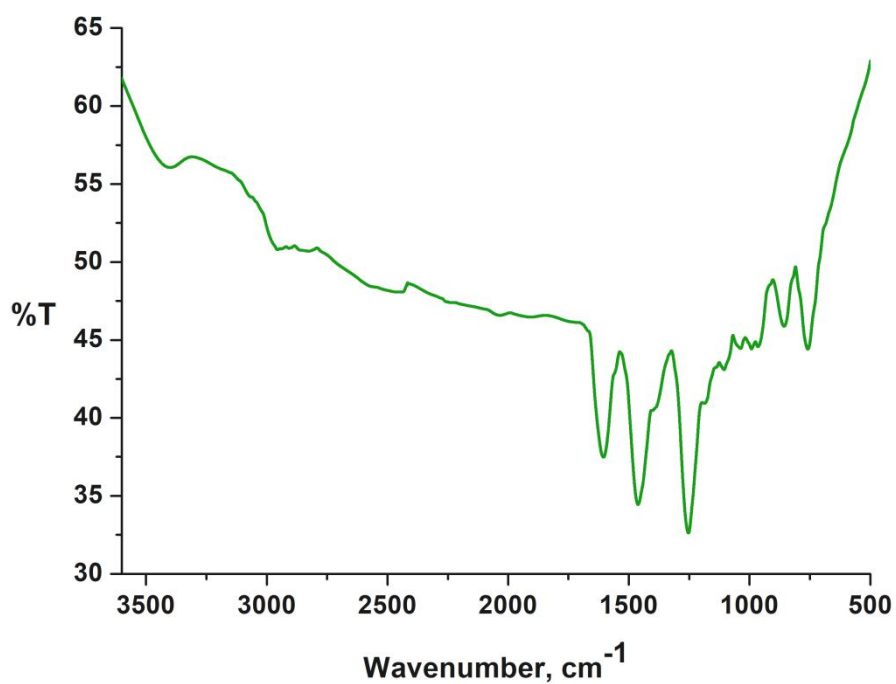


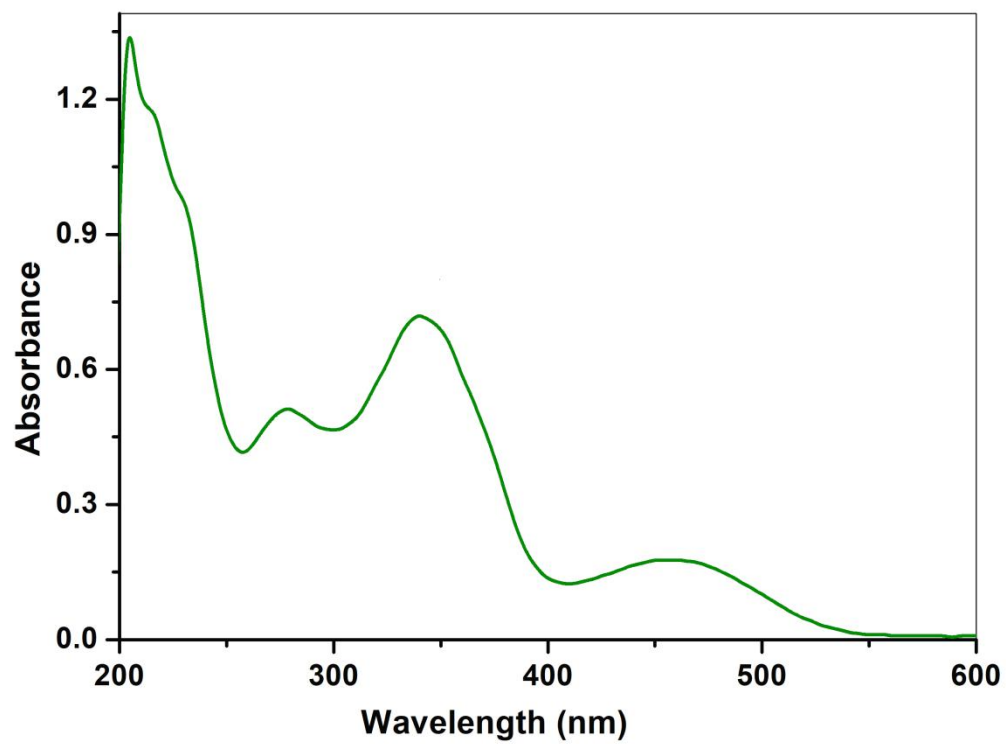
# Synthesis, X-ray Structure and Evaluation of Bactericidal Activity of an o-vanilin Functionalized Schiff Base

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## Supporting Information



**Fig. S1.** FT-IR spectrum of the Schiff base



**Fig. S2.** UV-Vis spectrum of the Schiff base in MeCN

P11-1H

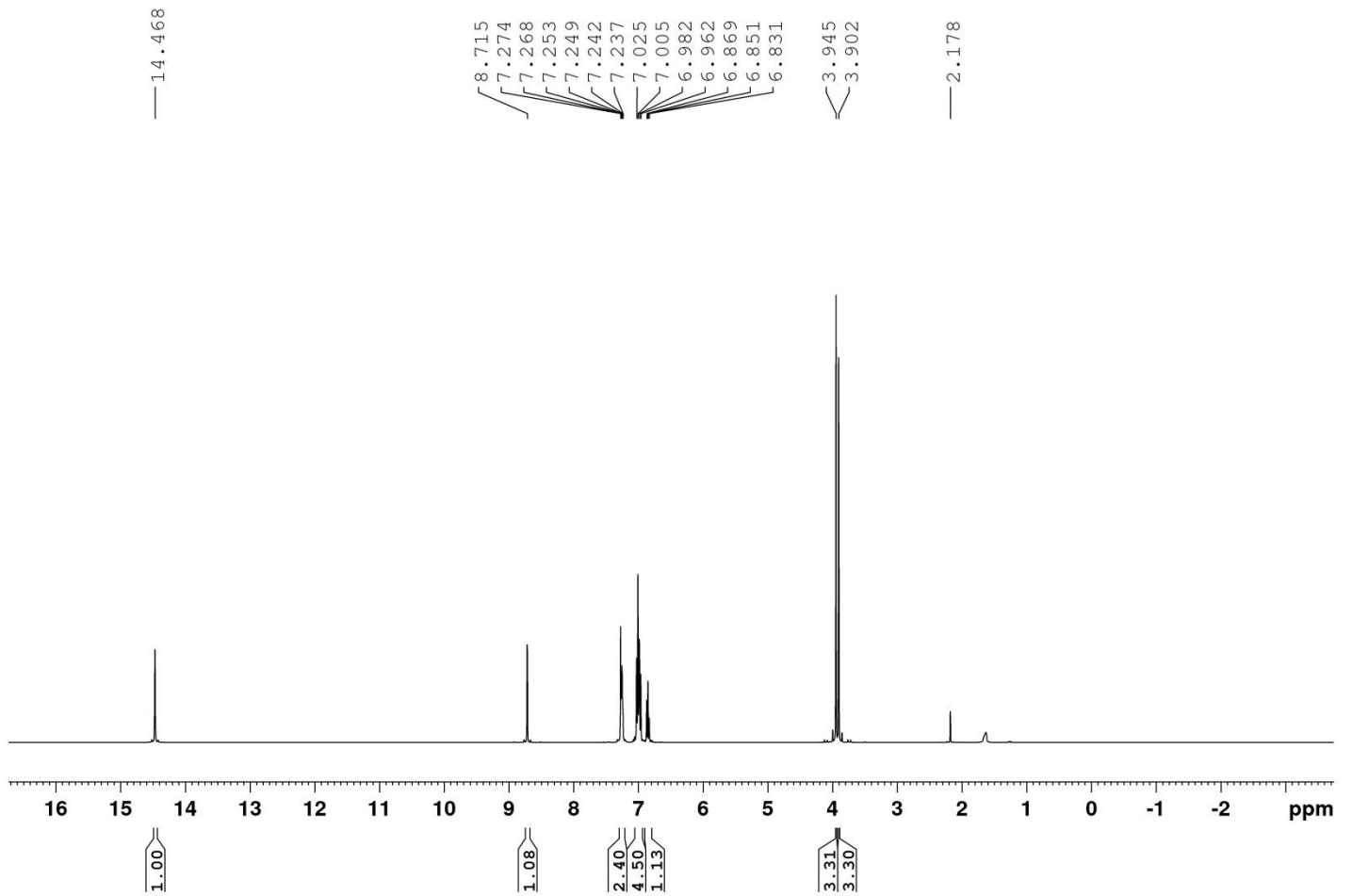
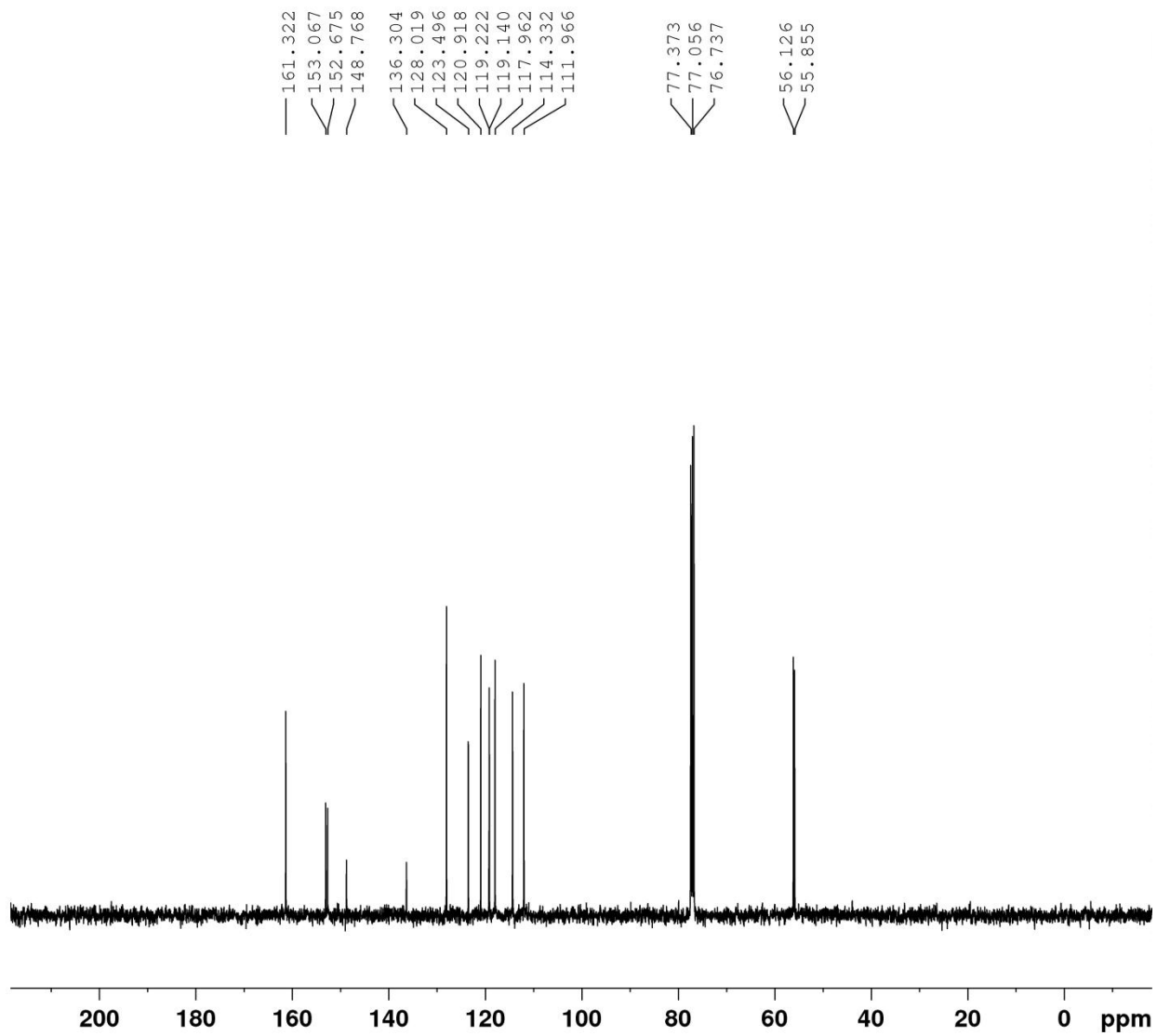
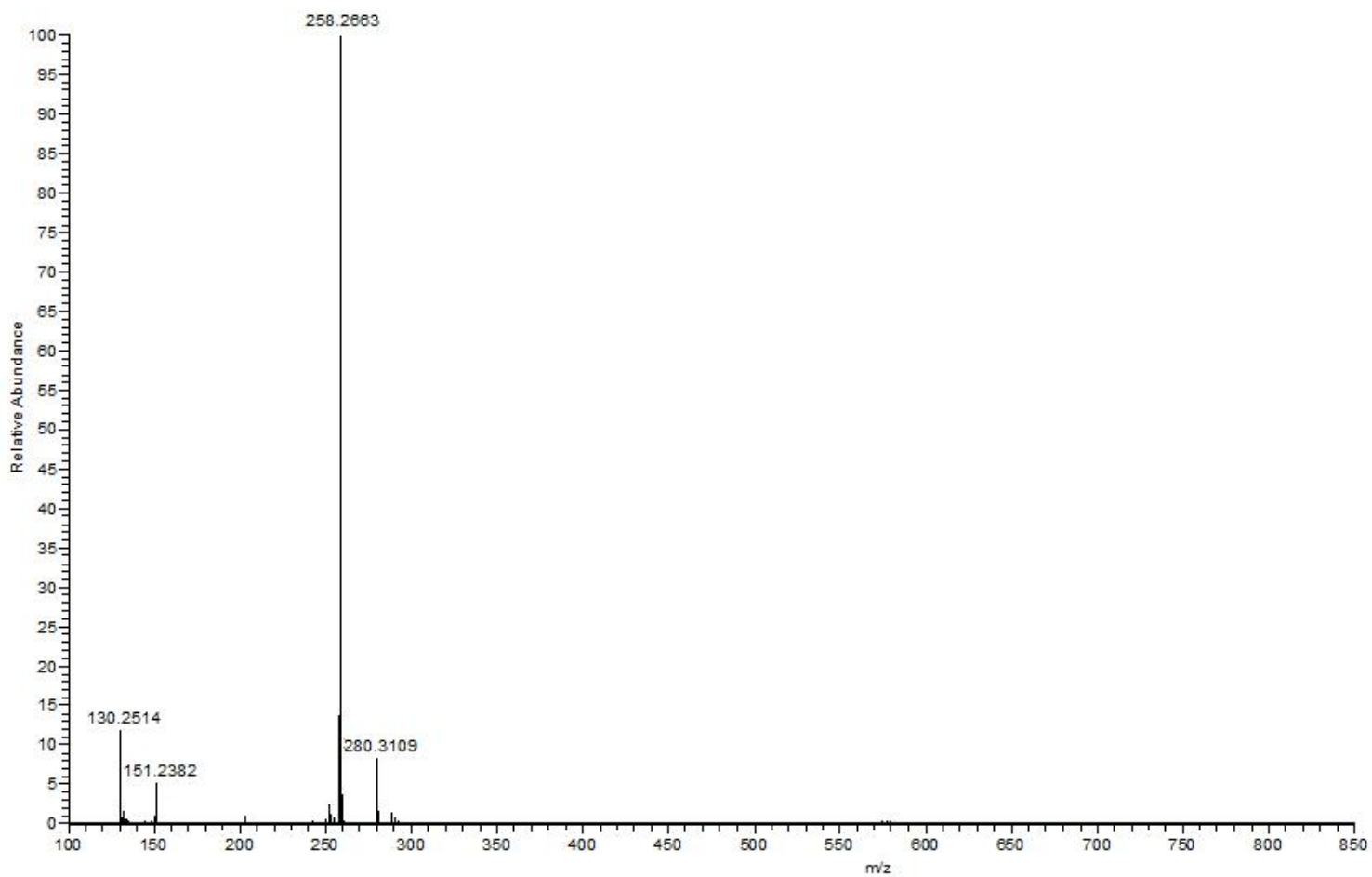


Fig. S3.  $^1\text{H}$  NMR spectrum of the Schiff base in  $\text{CDCl}_3$ .

P11-13C



**Fig. S4.**  $^{13}\text{C}$  NMR spectrum of the Schiff base in  $\text{CDCl}_3$ .



**Fig. S5.** Mass spectrum of the Schiff base in MeCN

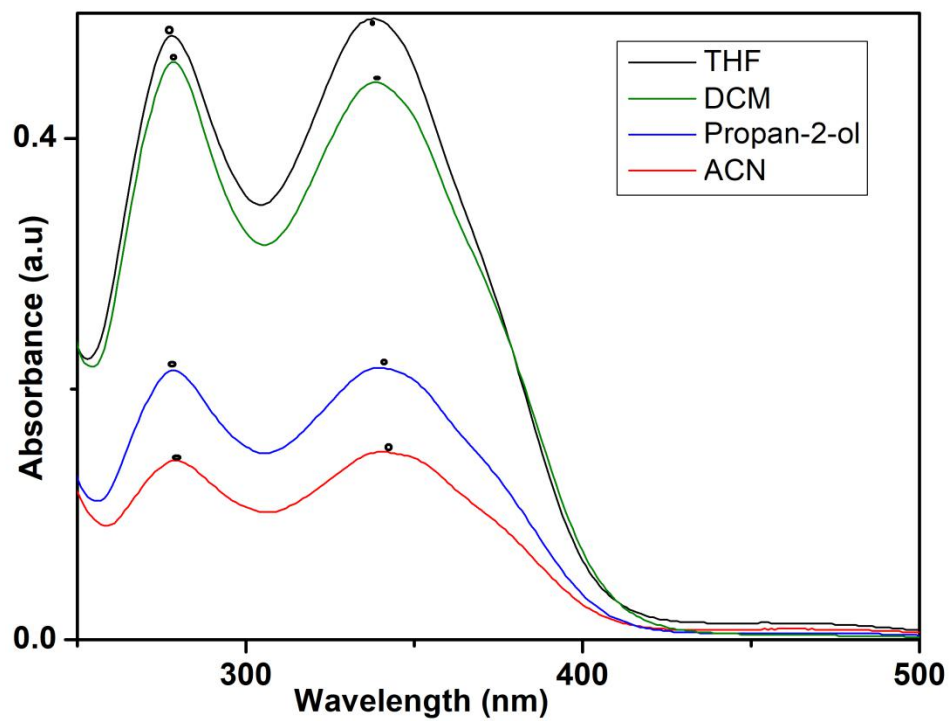


Fig. S6. UV-Vis spectra of the Schiff base in different solvent media

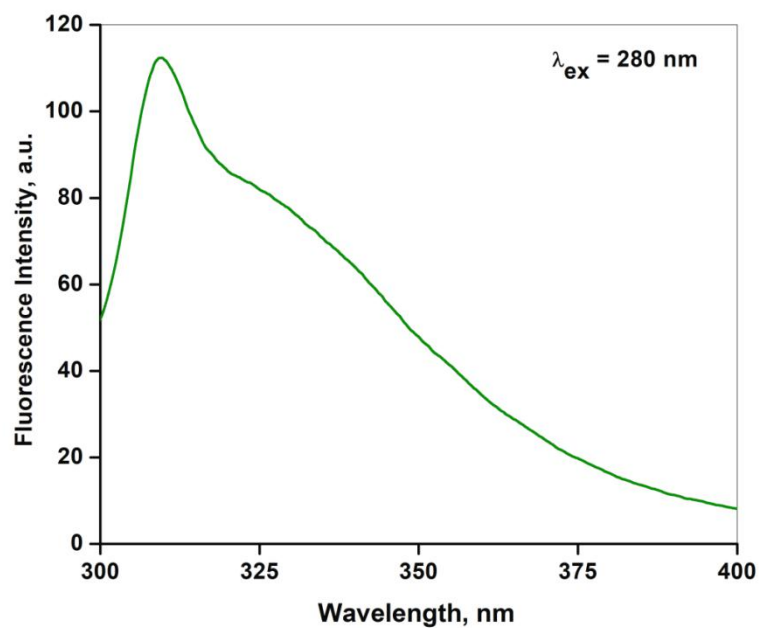


Fig. S7. Fluorescence spectrum of the Schiff base in MeCN



**Fig. S8.** *In vitro* antimicrobial activity of the Schiff base against *Shigella flexneri* by agar well diffusion method. Concentrations were loaded consecutively in increasing gradient: a) 1 mM, b) 2.5 mM, c) 5 mM and d) 10 mM. Only DMSO is loaded in the center well (e).

**Table S1** Geometrical parameters of C-H...O hydrogen bonds ( $\text{\AA}$ ,  $^\circ$ ) involved in the supramolecular construction in **L**. D = donor, A = acceptor ( $\text{\AA}$ ,  $^\circ$ )

Compound	D-H...A	D-H	H...A	D...A	$\angle$ D-H-A
<b>L</b>	C12-H12...O3	0.93( $\text{\AA}$ )	2.64( $\text{\AA}$ )	3.52( $\text{\AA}$ )	156

**Table S2.** Percentage share of the interaction of each atom with other atoms when they are in or out of the Hirshfeld surface

Atom Position	% of Surface occupy
All-in All-out	100
All-in O-out	8.5
All-in N-out	1.0
All-in C-out	13.3
All-in H-out	77.2
O-in All-out	10.1
N-in All-out	1.6
C-in All-out	19.3
H-in All-out	69.1