Supplementary Materials: Design and Stereochemical Research (DFT, ECD and Crystal Structure) of Novel Bedaquiline Analogs as Potent Antituberculosis Agents

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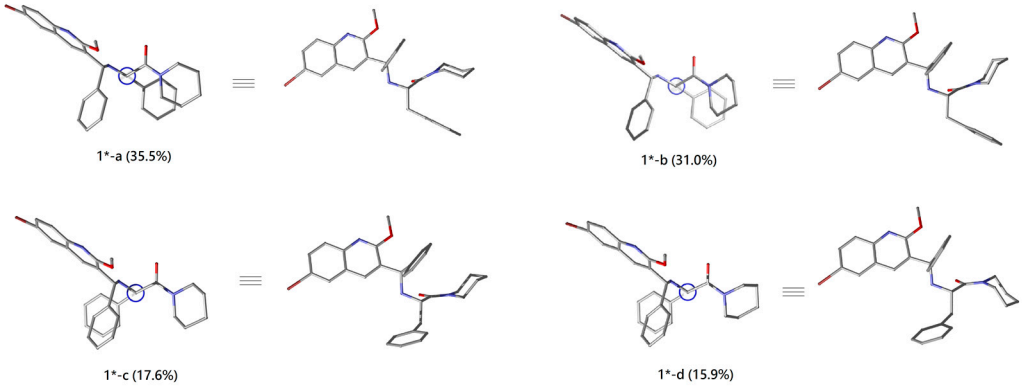

Figure S1. Relative stable conformers of **1***. All conformers are shown as "Newman Projections" by viewing along the C10-N13 bond axis.

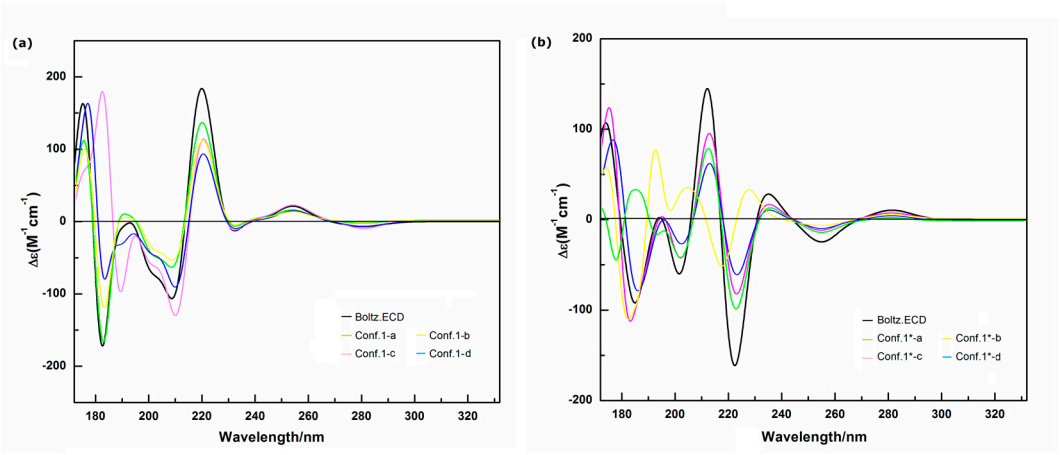

Figure S2. Calculated ECD spectra of individual conformers of (**a**) **1** and (**b**) **1***.

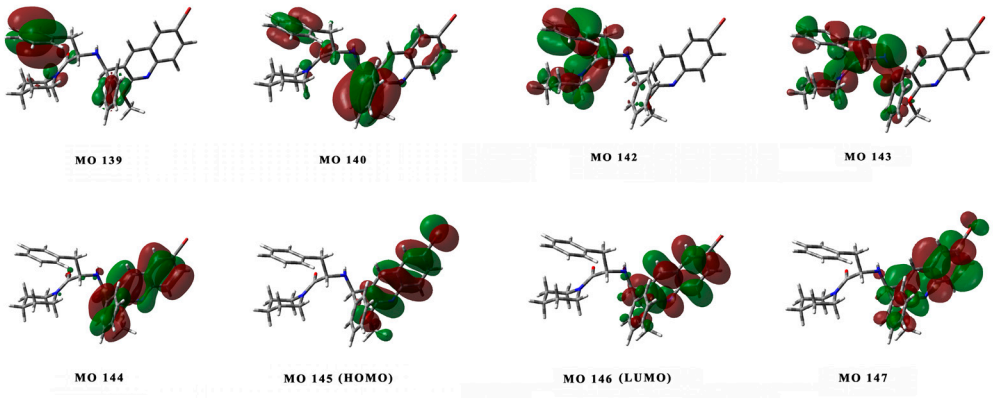

Figure S3. Molecular orbitals involved in the electronic transitions of **1***.

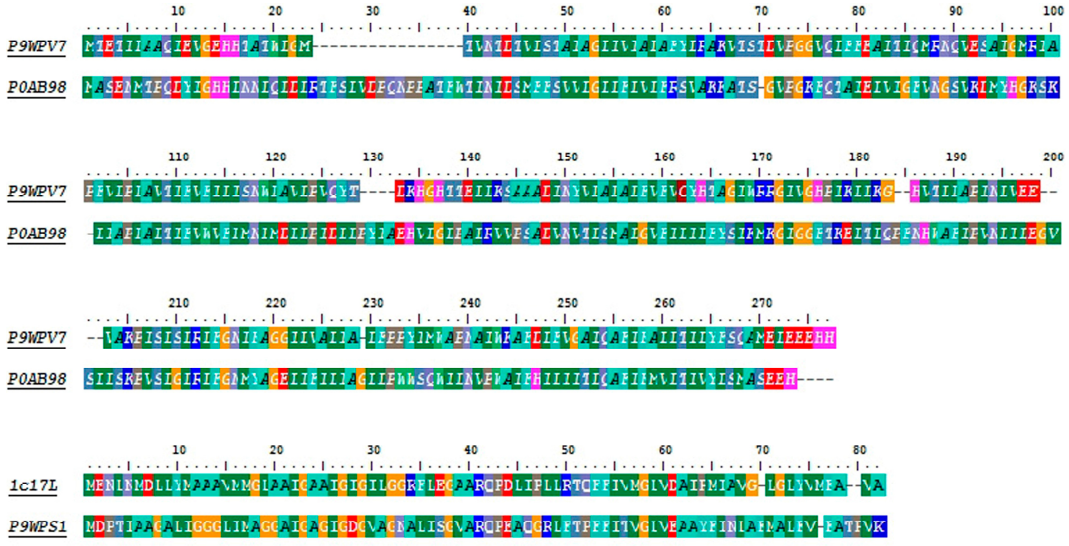

Figure S4. Alignments of the a-subunits (atpB gene) above and c-subunits (atpE gene) below of *Mycobacterium tuberculosis* and *Escherichia coli*. Sequence numbering in the a-subunits is different (upper numbers are for *Mycobacterium tuberculosis* lower numbers for *Escherichia coli*) The c-subunit sequence numbering is the same for these species.

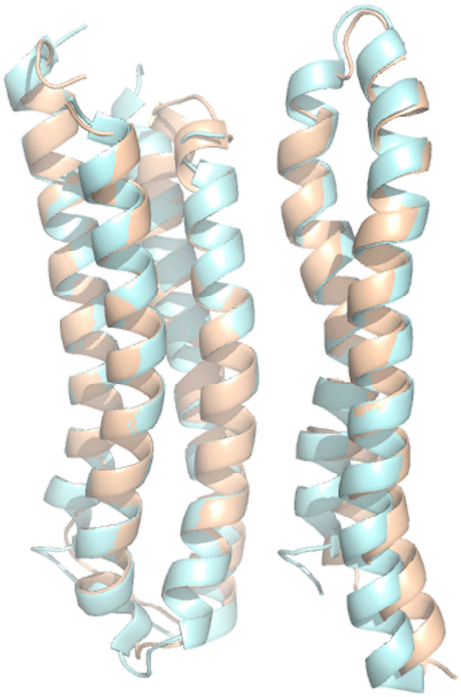

Figure S5. Superimpose for a- and c-subunits of *Escherichia coli* (carbon atoms indicated in blue) and homology model of *Mycobacterium tuberculosis* (carbon atoms indicated in brown).

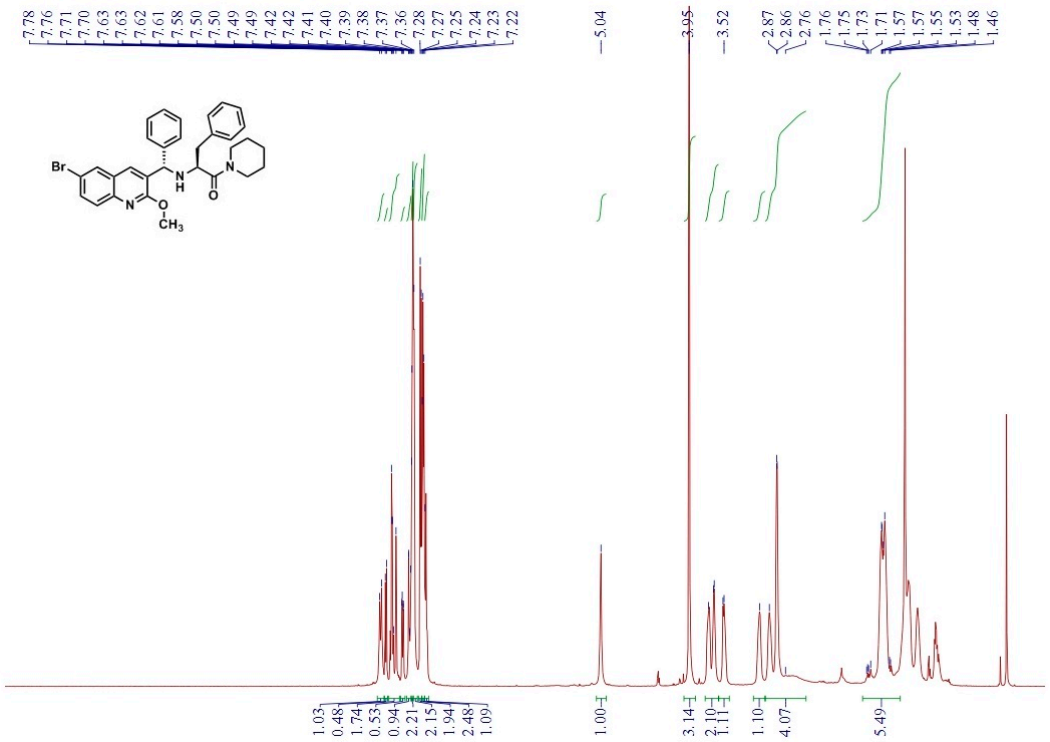

Figure S6. [1]H-NMR spectrum of compound **1**.

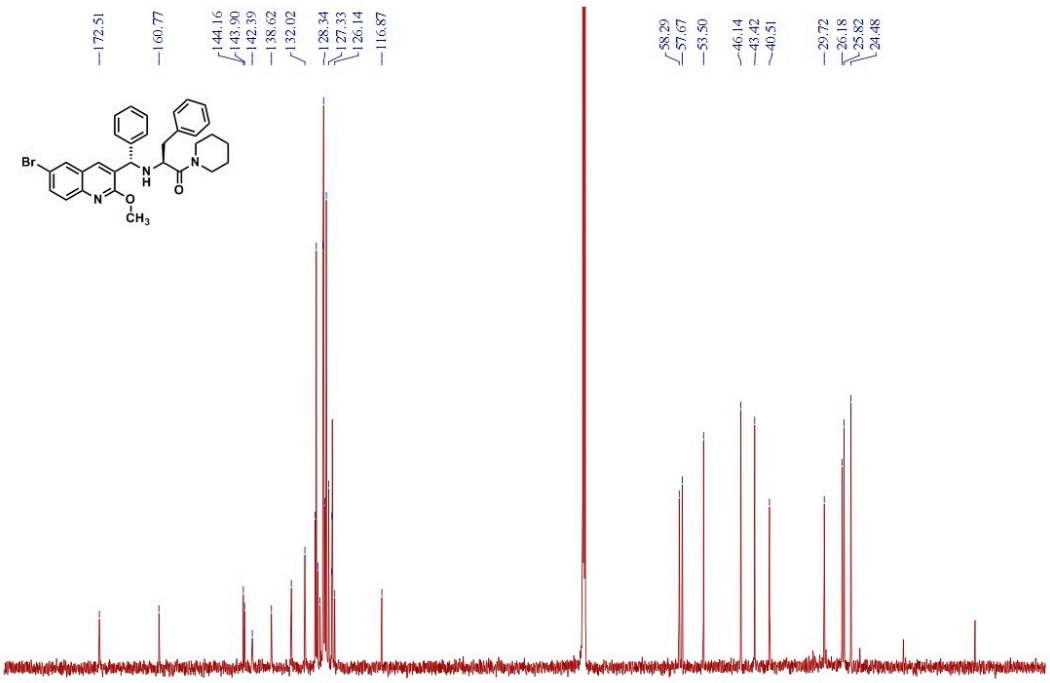

Figure S7. [13]C-NMR spectrum of compound **1**.

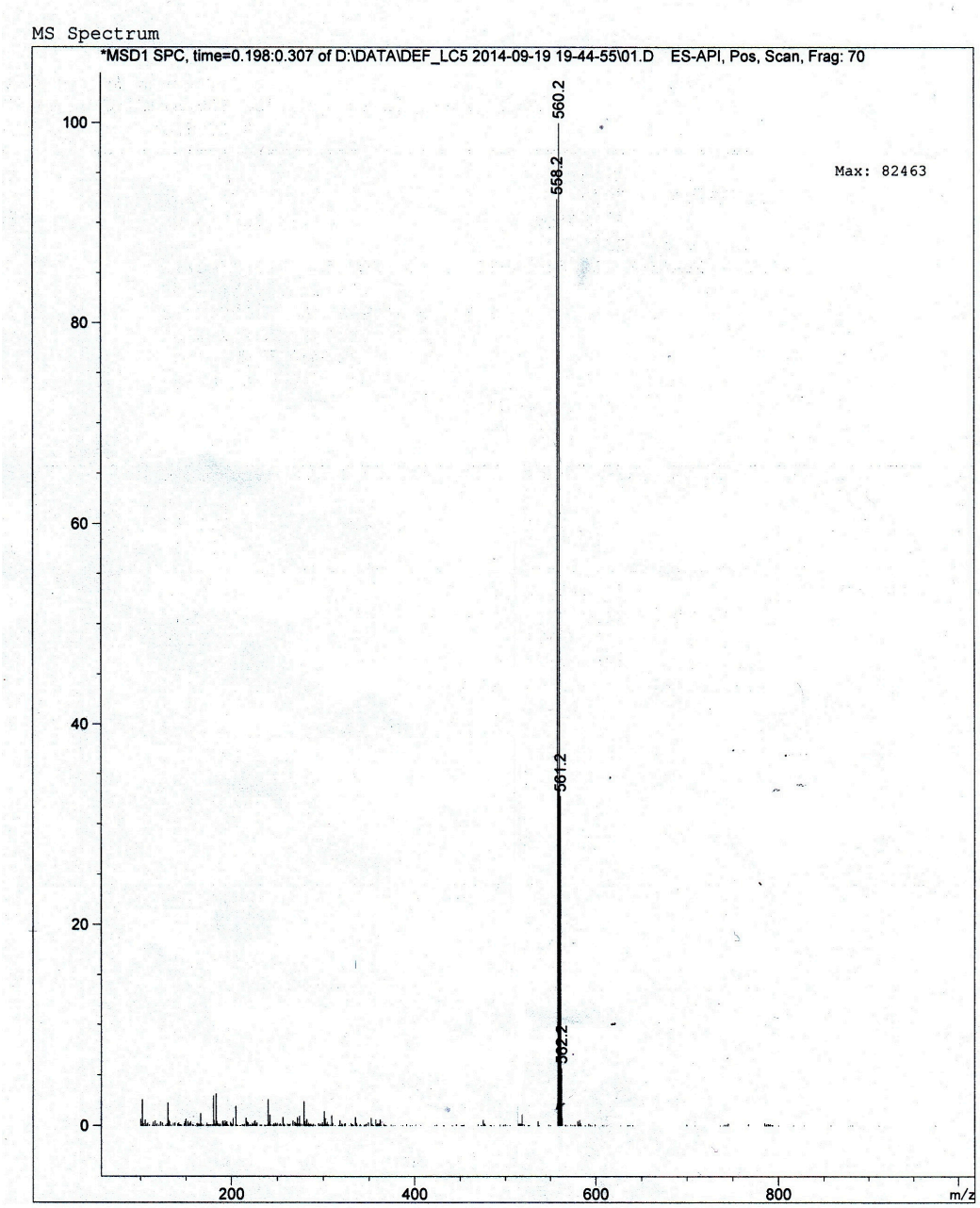

Figure S8. MS spectrum of compound **1**.

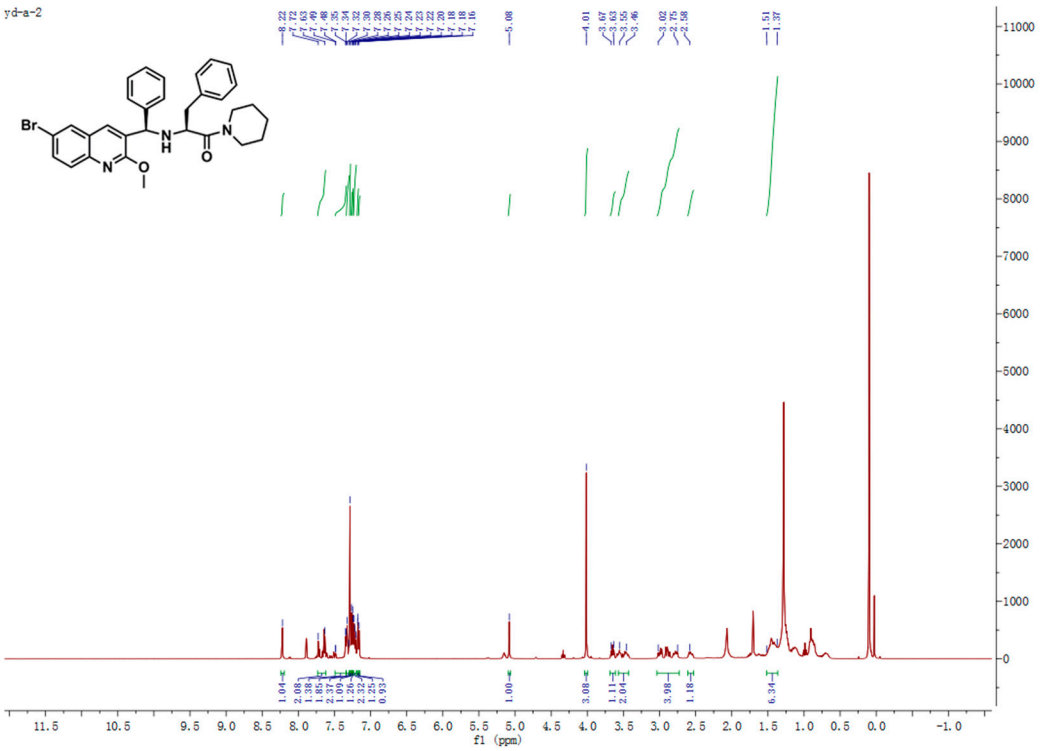

Figure S9. ^{1}H-NMR spectrum of **1***.

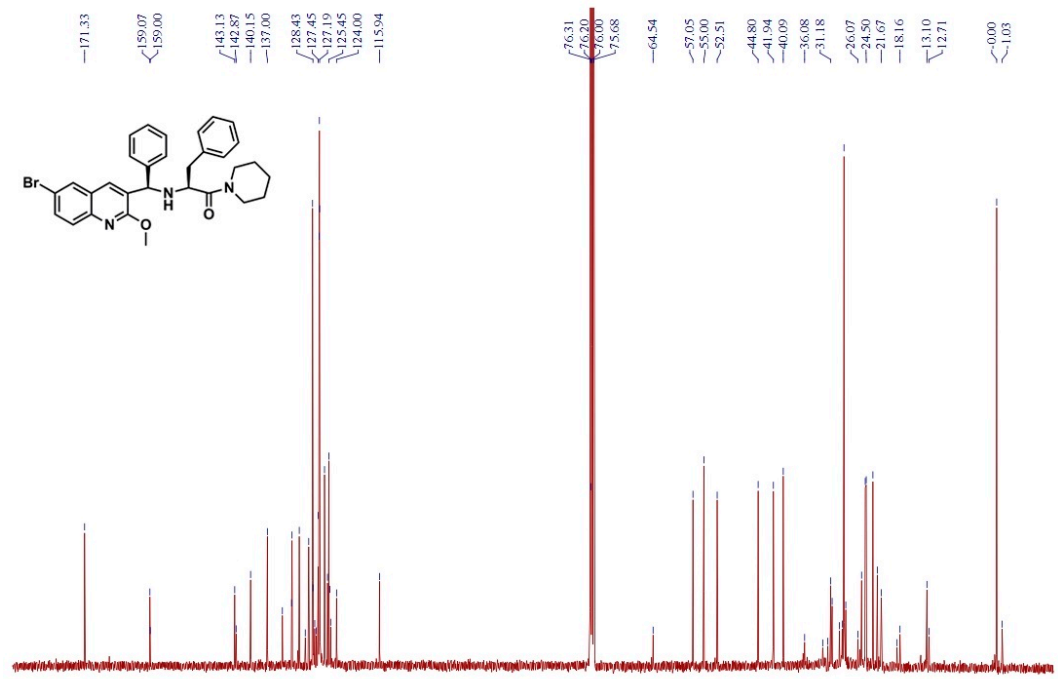

Figure S10. ^{13}C-NMR spectrum of **1***.

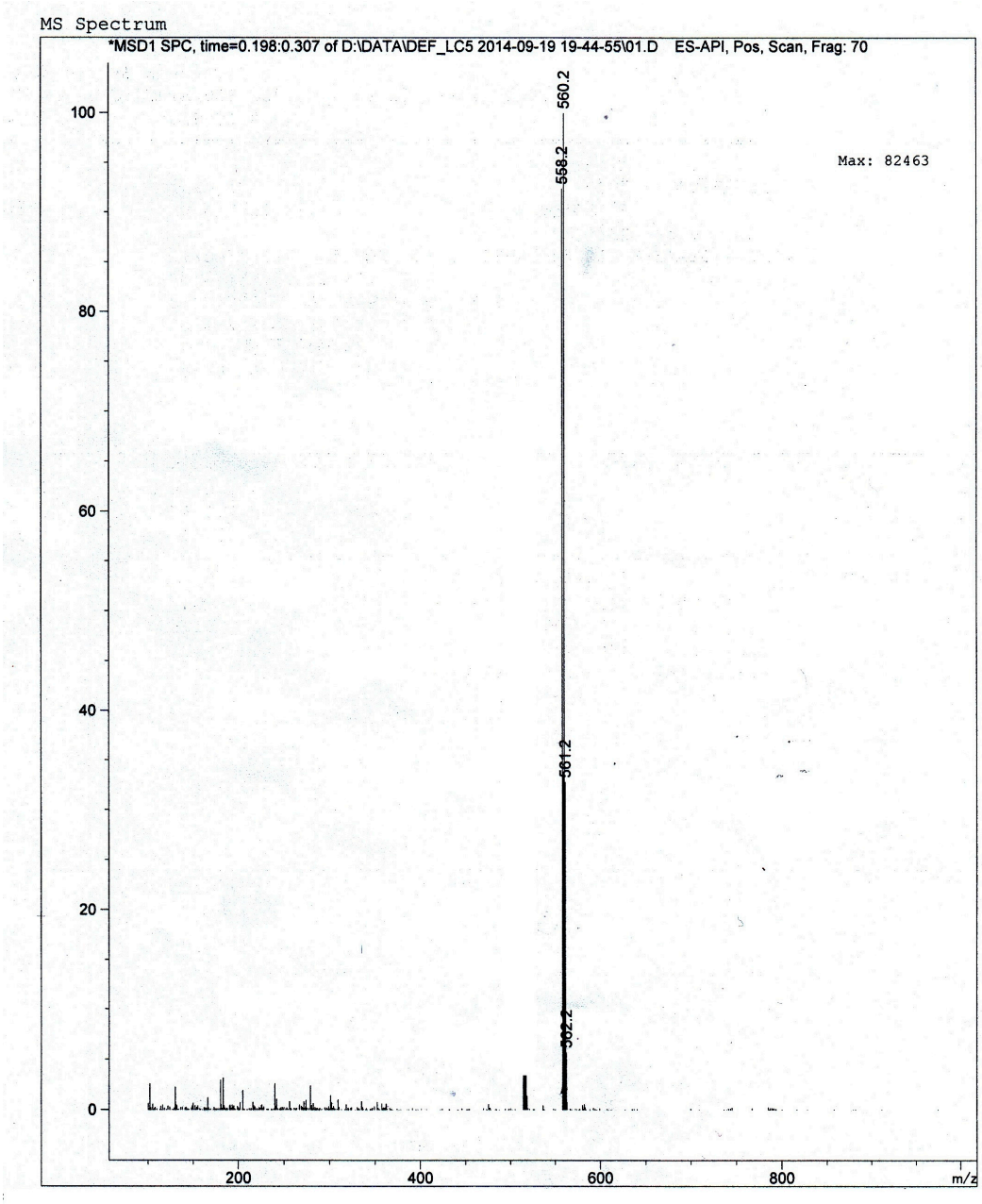

Figure S11. MS spectrum of **1***.

Table S1. Gibbs free energies (*G*), relative Gibbs free energies (Δ *G*) [a] and Boltzmann weighting factor (*P*%) [b] of compound **1*** conformers by using the DFT/B3LYP/6-311++G(2d,p) method.

Conf.	*G* (kcal/mol)	Δ*G* (kcal/mol)	P_i%
1*-a	−2566110.008	0	35.5
1*-b	−2566109.930	0.078	31.0
1*-c	−2566109.597	0.410	17.6
1*-d	−2566109.535	0.473	15.9

[a] which related to the most stable conformer; [b] Boltzmann weighting factor (P_i%) based on Δ *G*.