11*H*-indeno[1,2-*b*]quinoxalin-11-one 2-(4-ethylbenzylidene)hydrazone

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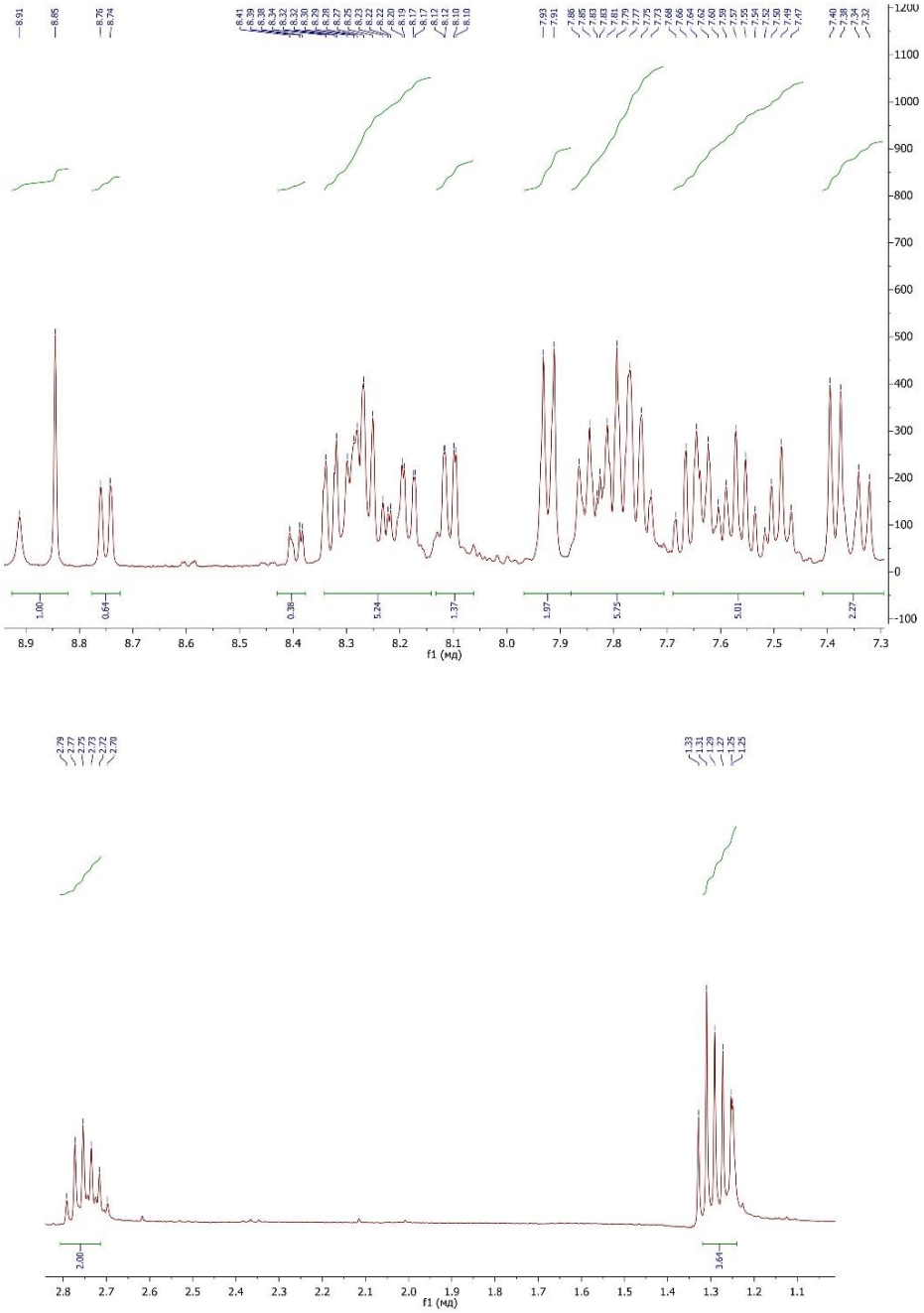


Figure S1. The [1]H NMR spectrum of recrystallized compound **3**

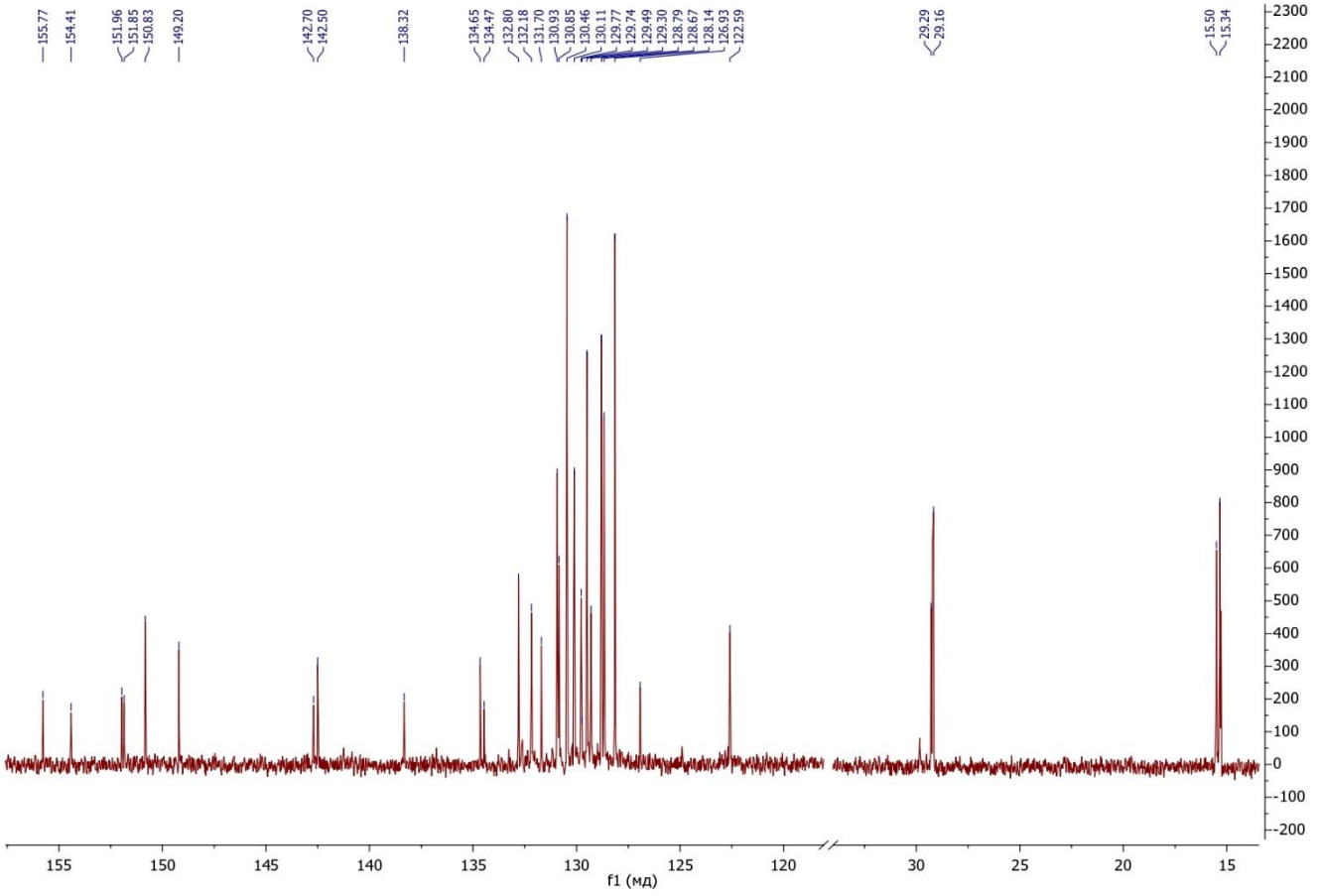
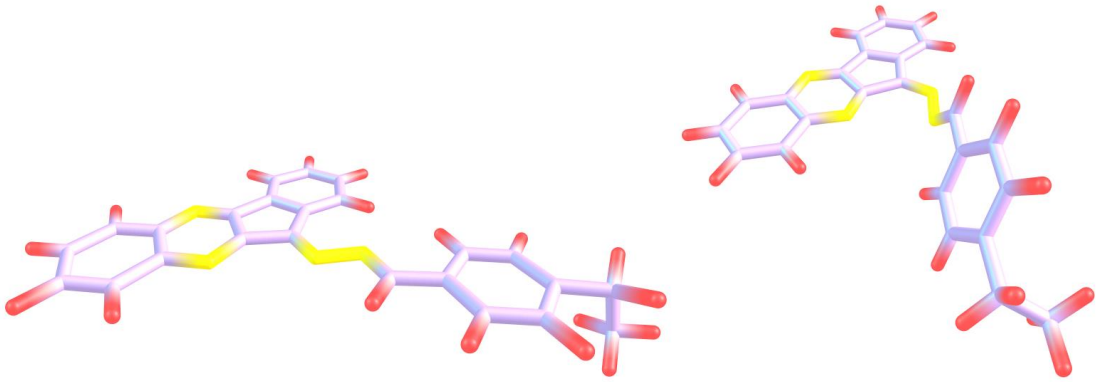
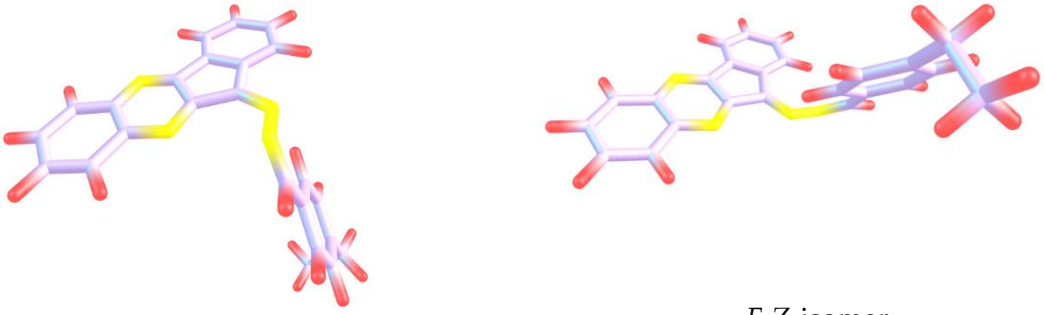


Figure S2. The ^{13}C NMR spectrum of compound **3.**



E,*E*-isomer
0 kJ/mol

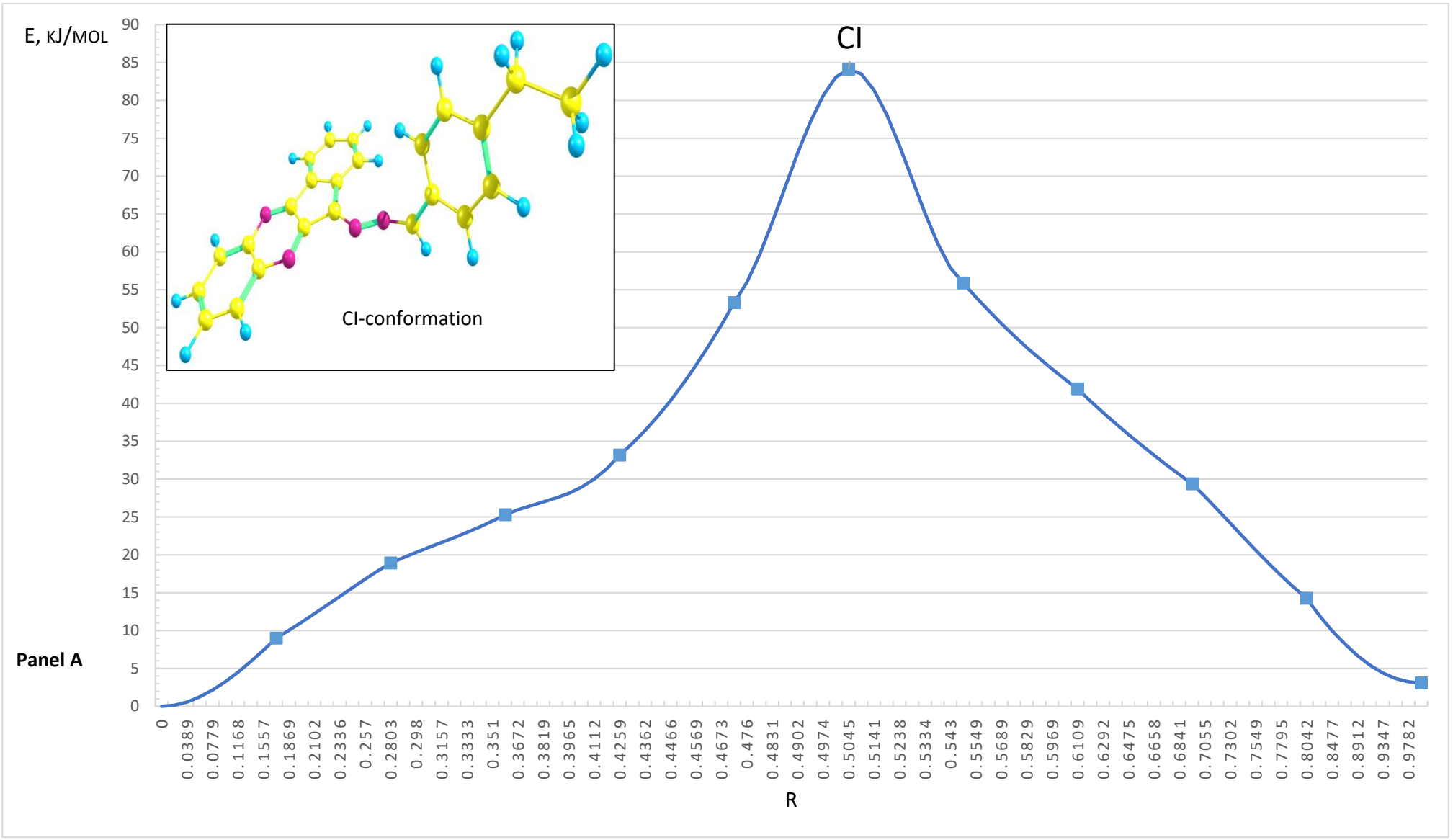
Z,*E*-isomer
3.16 kJ/mol



Z,*Z*-isomer
7.13 kJ/mol

E,*Z*-isomer
4.91 kJ/mol

Figure S3. The structures of *E*,*E*-, *Z*,*E*-, *E*,*Z*-, and *Z*,*Z*-isomers of compound **3** optimized by the DFT method with B3LYP/G functional and ma-def2-SVP basis set. The solvent (chloroform) was accounted for with the use of CPCM model. The torsion angles about double C=N bonds of the azine moiety do not exceed 5° for *E*,*E*-, *Z*,*E*-, *E*,*Z*-isomers and are within 7.5-8.5° for *Z*,*Z*-isomer. The C=N-N=C torsion angles equal 179, 124, 127, and 121° for *E*,*E*-, *Z*,*E*-, *E*,*Z*-, and *Z*,*Z*-isomers, respectively. The ethyl-substituted phenyl ring is nearly coplanar with the adjacent CH=N fragment (torsion within 0.2-3.8°). Calculated Gibbs energies at 298.15 K are shown with respect to *E*,*E*-isomer.


E, KJ/MOL
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
CI
CI-conformation
0
0.0389
0.0779
0.1168
0.1557
0.1869
0.2102
0.2336
0.257
0.2803
0.298
0.3157
0.3333
0.351
0.3672
0.3819
0.3965
0.4112
0.4259
0.4362
0.4466
0.4569
0.4673
0.476
0.4831
0.4902
0.4974
0.5045
0.5141
0.5238
0.5334
0.543
0.5549
0.5689
0.5829
0.5969
0.6109
0.6292
0.6475
0.6658
0.6841
0.7055
0.7302
0.7549
0.7795
0.8042
0.8477
0.8912
0.9347
0.9782
R

Panel A

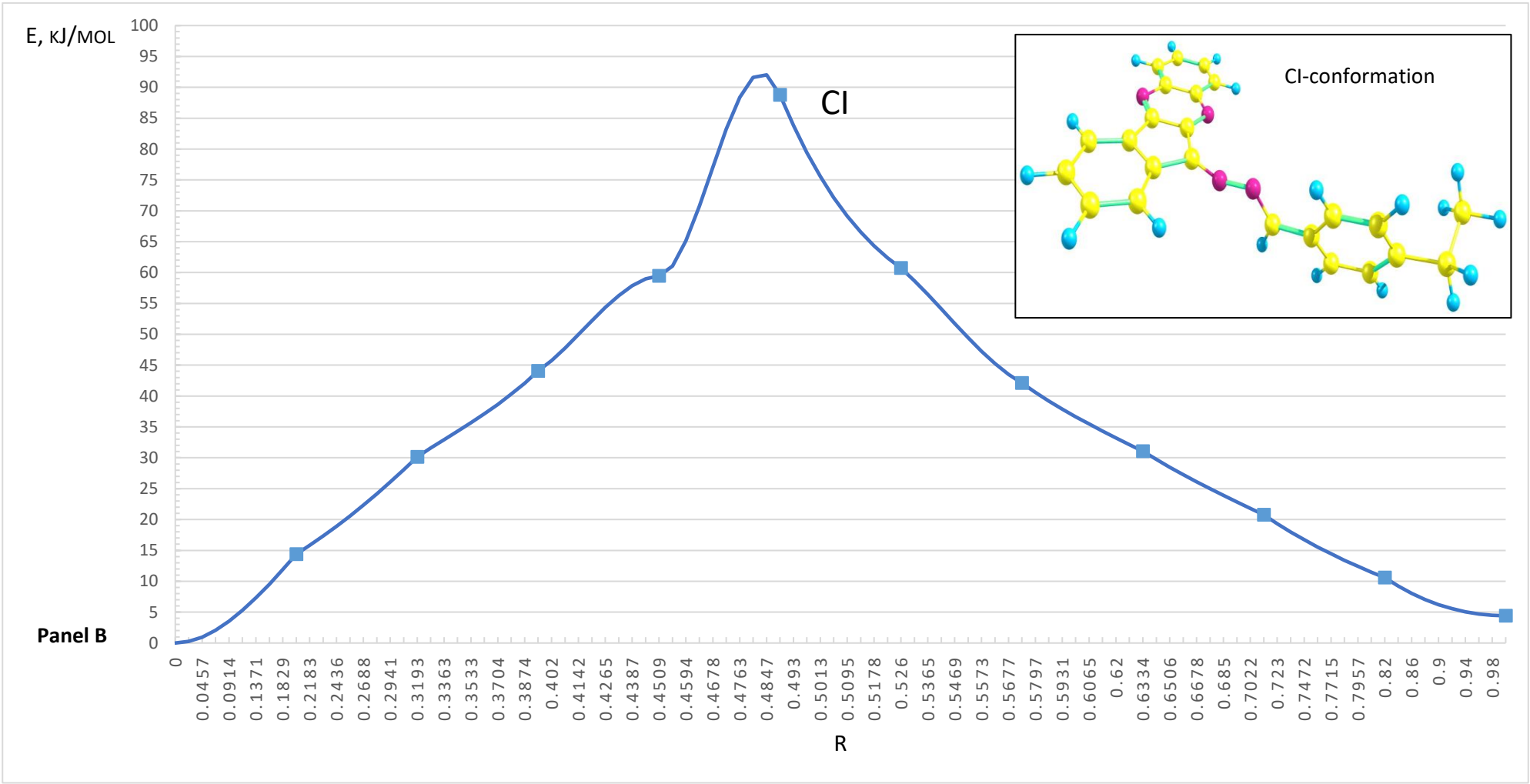
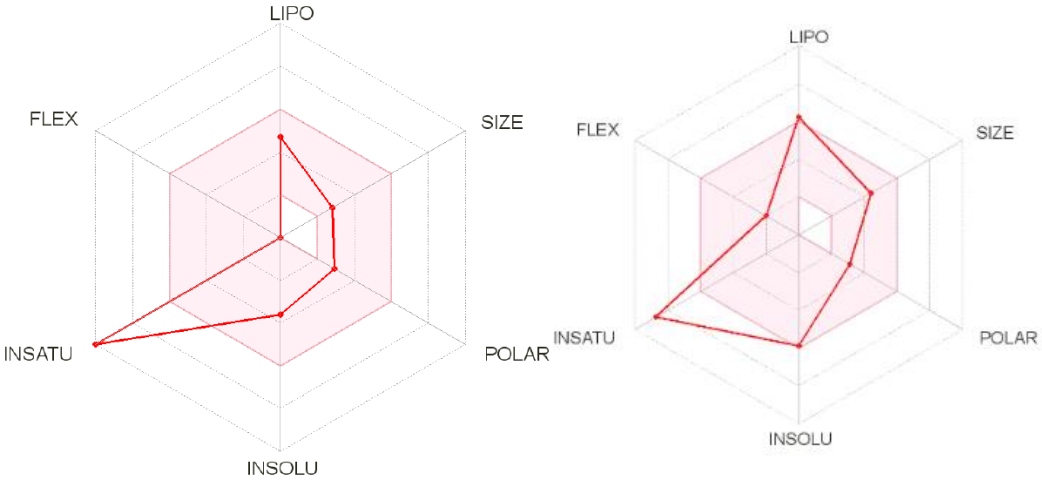


Figure S4. The energy diagrams (cubic polynomial interpolation curves from ORCA 5.0 output) and the climbing image (CI) conformations for *E*,*E* ⇄ *Z*,*E* (Panel A) and *E*,*E* ⇄ *E*,*Z* (Panel B) isomerization of compound **3**. R- relative reaction coordinate. The intermediate images are shown as squares on the energy diagrams. The N-N=C valence angles at the nitrogen centers of inversion in the CI conformations are equal to 160.9° (Panel A) and 157.9° (Panel B).



SP600125 **Compound 3**

Figure S5. Bioavailability radar plots of compound **3** and **SP600125**. The plots depict the LIPO (lipophilicity), SIZE (molecular weight), POLAR (polarity), INSOLU (insolubility), INSATU (unsaturation), and FLEX (rotatable bond flexibility) parameters.