# Conformational, thermodynamic, and spectroscopic features of benzothiazole derivatives via computational approaches

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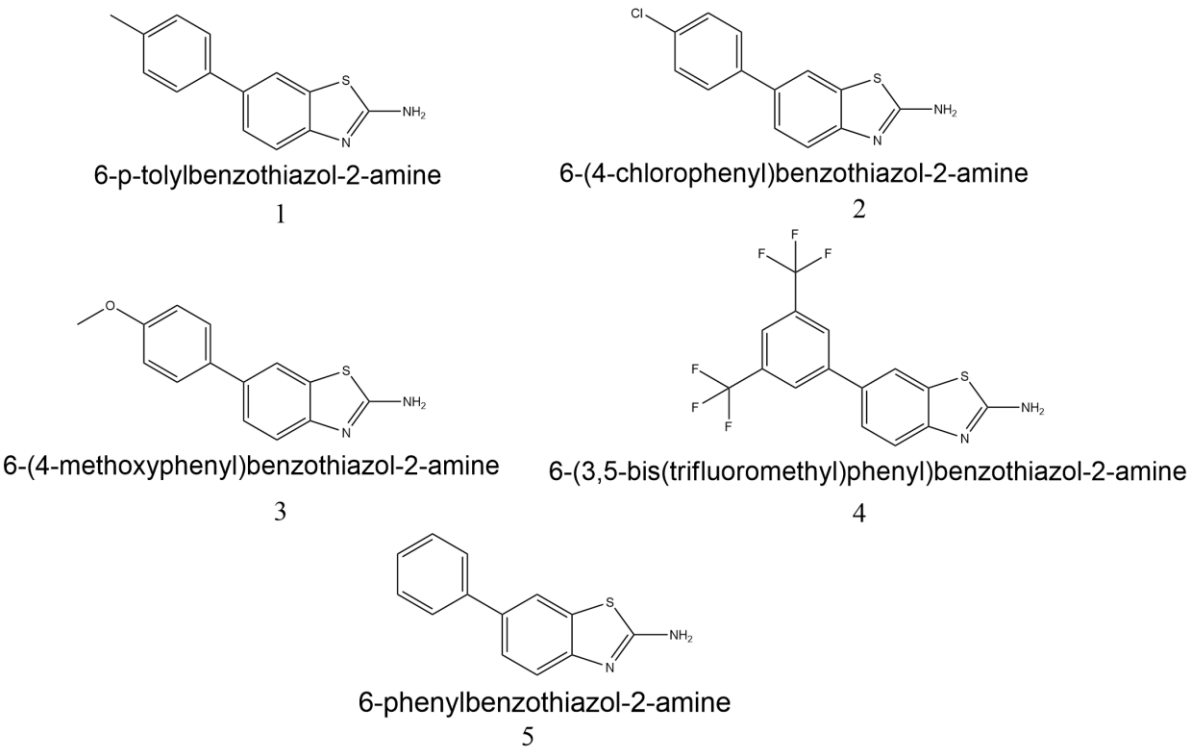


**Figure S1:** Structure with IUPAC names of Benzothiazole derivatives

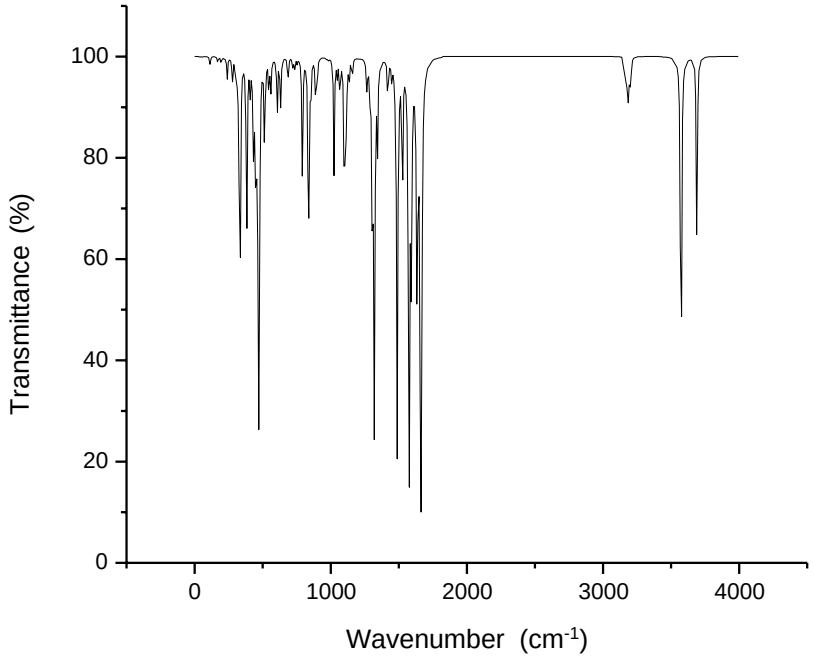


**Figure S2:** IR spectrum of **2**

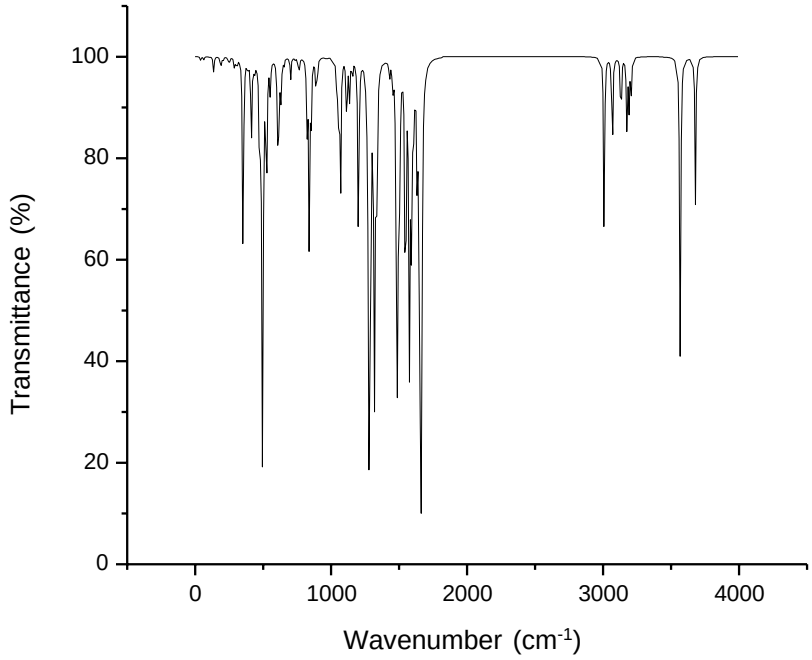


**Figure S3:** IR spectrum of **3**

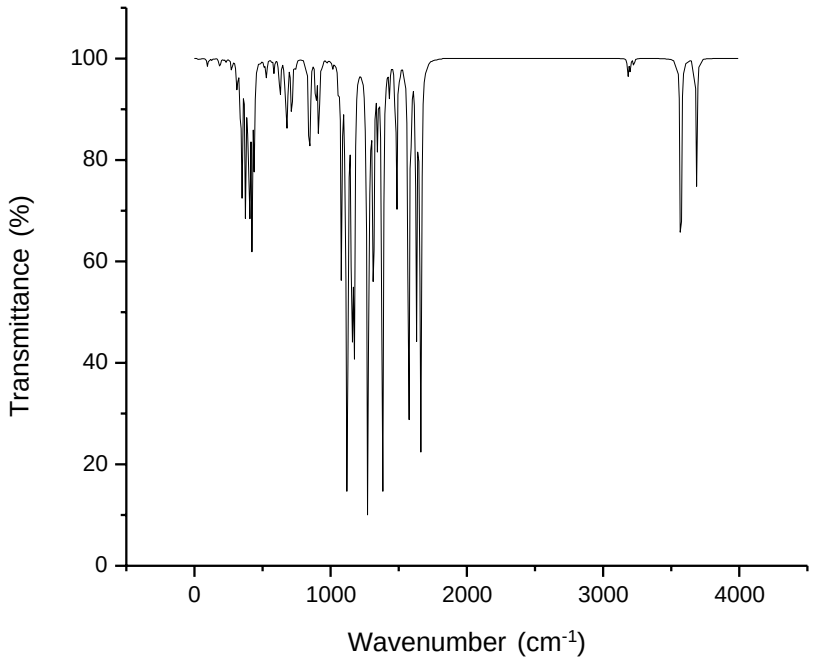


**Figure S4:** IR spectrum of **4**

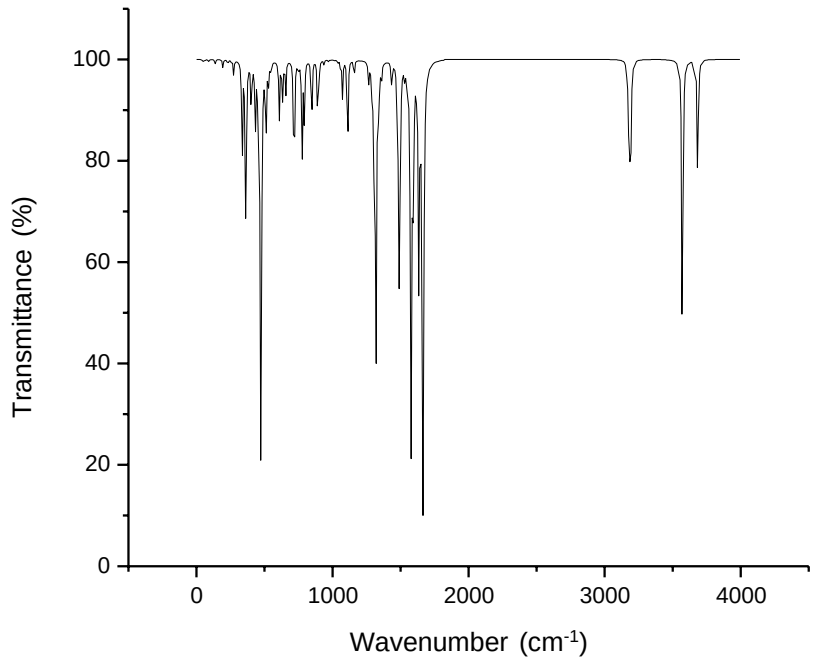


**Figure S5:** IR spectrum of **5**

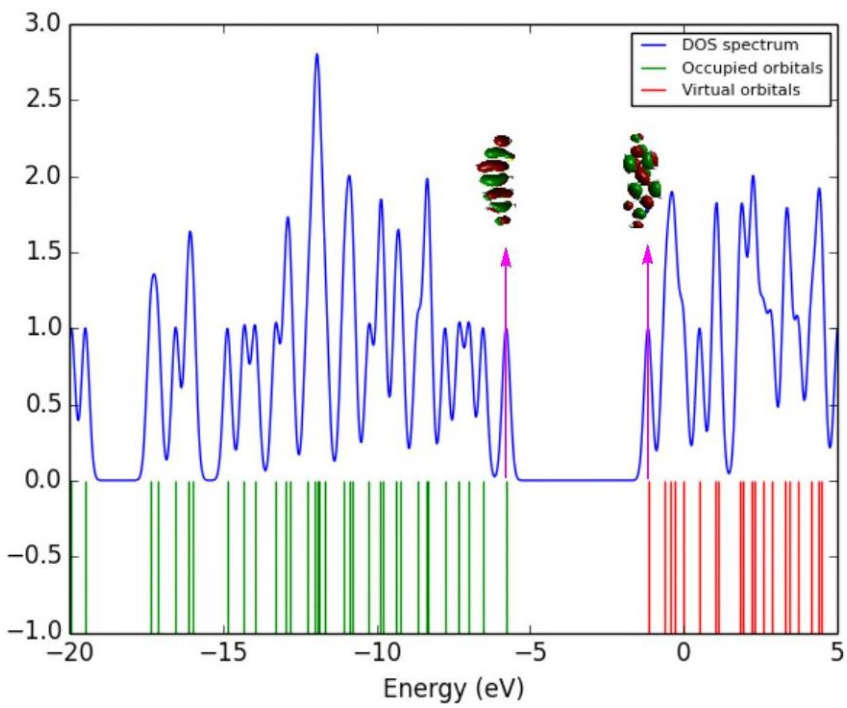


**Figure S6:** DOS Spectrum of **2** calculated from GaussSum

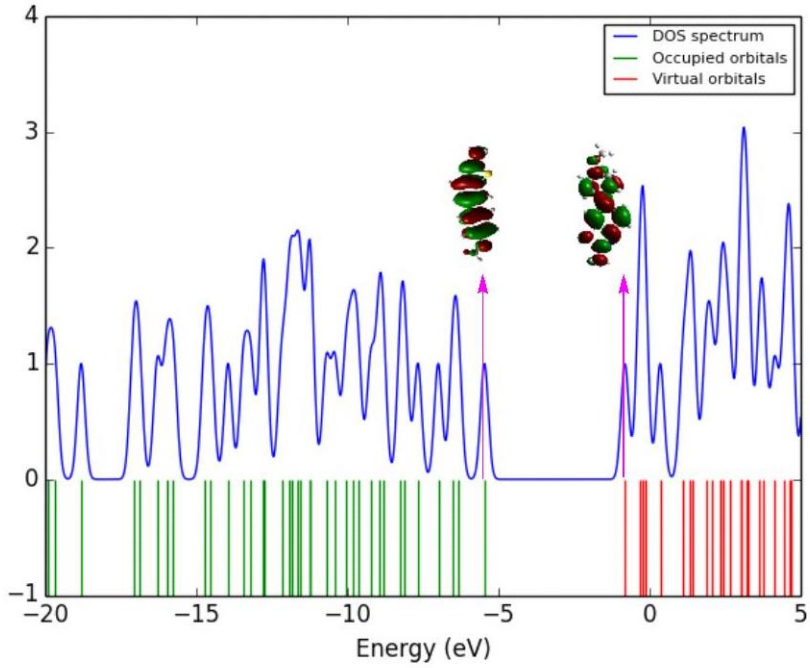


**Figure S7:** DOS Spectrum of **3** calculated from GaussSum

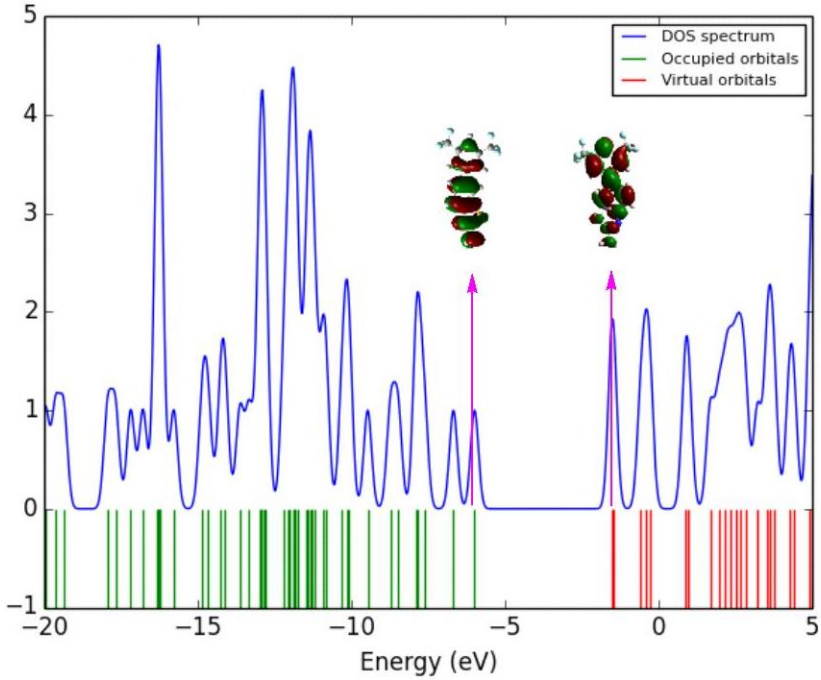


**Figure S8:** DOS Spectrum of **4** calculated from GaussSum

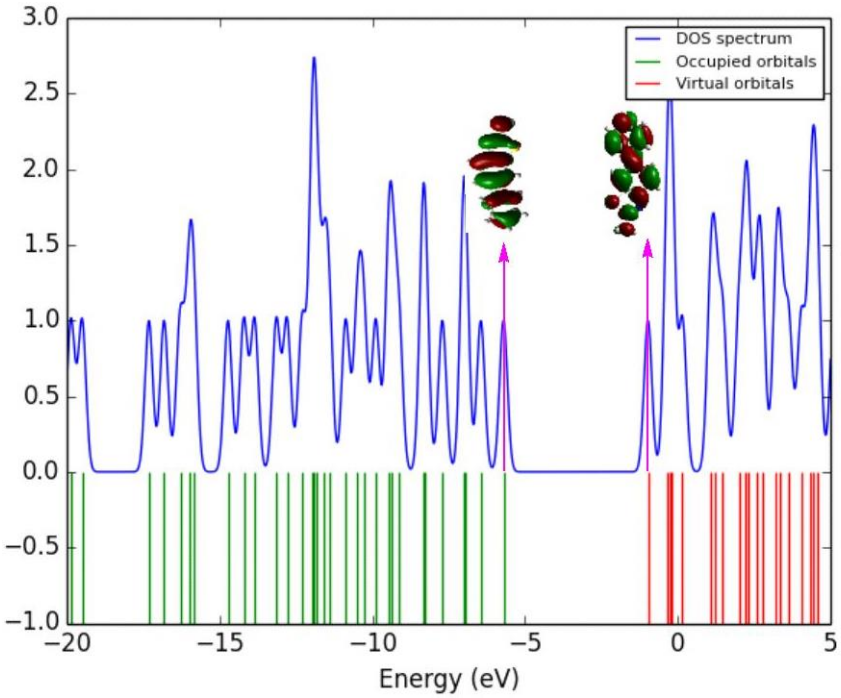


**Figure S9:** DOS Spectrum of **5** calculated from GaussSum

**Table S1:** The chemical shifts of $^{1}H$ and $^{13}C$-NMR calculated by the GIAO method at B3LYP/6-311G (d,p)/$SMD_{Chloroform}$ level of theory and the experimental chemical shifts published by us (*Molecules* **2013**, *18*, 8845-8857; doi:10.3390/molecules18088845)

| **Position of H-atom** | **Compound 1** | | **Compound 2** | | **Compound 3** | | **Compound 4** | | **Compound 5** | |
|---|---|---|---|---|---|---|---|---|---|---|
| | **Calc** | **Exp** | **Calc** | **Exp** | **Calc** | **Exp** | **Calc** | **Exp** | **Calc** | **Exp** |
| 4 | 7.68 | 8.11 | 7.67 | 7.59 | 7.66 | 7.38 | 7.74 | 8.08 | 7.90 | 7.59 |
| 5 | 7.58 | 8.11 | 7.55 | 7.59 | 7.54 | 7.38 | 7.69 | 8.08 | 7.59 | 7.32-7.57 |
| 7 | 7.87 | 7.30-7.70 | 7.87 | 7.26-7.43 | 7.85 | 7.38 | 7.98 | 8.22 | 7.69 | 7.32-7.57 |
| 2' | 7.64 | 7.30-7.70 | 7.65 | 7.26-7.43 | 7.67 | 7.40-7.56 | 8.22 | 7.55-7.86 | 7.68 | 7.32-7.57 |
| 3' | 7.51 | 7.30-7.70 | 7.52 | 7.26-7.43 | 6.92 | 7.40-7.56 | – | – | 7.66 | 7.32-7.57 |
| 4' | – | – | – | – | – | | 8.05 | 7.55-7.86 | 7.53 | 7.32-7.57 |
| 5' | 7.50 | 7.30-7.70 | 7.52 | 7.26-7.43 | 7.17 | 7.40-7.56 | – | – | 7.66 | 7.32-7.57 |
| 6' | 7.58 | 7.30-7.70 | 7.60 | 7.26-7.43 | 7.60 | 7.40-7.56 | 8.16 | 7.55-7.86 | 7.73 | 7.32-7.57 |
| **Position of C-atom** | | | | | | | | | | |
| $C_2$ | 170.5 | 167.85 | 170.9 | 167.48 | 170.6 | 167.73 | 171.5 | 168.50 | 170.8 | 167.85 |
| $C_{3a}$ | 155.7 | 149.17 | 156.4 | 150.02 | 155.2 | 149.39 | 157.3 | 152.02 | 155.9 | 147.61 |
| $C_4$ | 122.6 | 119.20 | 122.7 | 119.27 | 122.6 | 118.13 | 123.1 | 116.06 | 122.7 | 118.70 |
| $C_5$ | 129.4 | 128.69 | 129.4 | 128.51 | 128.9 | 128. | 129.6 | 129.73 | 129.6 | 128.56 |
| $C_6$ | 141.8 | 140.81 | 139.9 | 134.96 | 141.6 | 134.67 | 137.9 | 134.5 | 134.8 | 132.24 |
| $C_7$ | 123.2 | 128.57 | 123.3 | 123.42 | 122.8 | 122.96 | 123.8 | 123.05 | 123.5 | 123.57 |
| $C_{7a}$ | 141.9 | 140.8 | 141.9 | 140.51 | 141.9 | 141.49 | 142.3 | 139.04 | 141.8 | 141.61 |
| $C_{1'}$ | 145.1 | 145.96 | 146.9 | 141.03 | 139.2 | 131.88 | 139.9 | 132.03 | 128.3 | 128.68 |
| $C_{2'}$ | 131.6 | 132.81 | 133.1 | 128.91 | 132.8 | 132.28 | 133.8 | 124.72 | 131.8 | 129.57 |
| $C_{3'}$ | 133.1 | 135.72 | 133.0 | 129.32 | 134.7 | 131.45 | 136.3 | 132.03 | 132.6 | 132.01 |
| $C_{4'}$ | 143.0 | 140.0 | 144.9 | 132.01 | 165.2 | 149.39 | 124.3 | 122.06 | 130.6 | 129.07 |
| $C_{5'}$ | 133.1 | 135.72 | 133.0 | 128.91 | 130.9 | 123.37 | 136.1 | 124.72 | 132.6 | 132.01 |
| $C_{6'}$ | 131.4 | 132.81 | 133.8 | 134.96 | 132.7 | 132.28 | 133.1 | 128.05 | 131.5 | 129.68 |