**Fig S1.** Screened structures of cyclohexanone derivatives utilized for this DFT study.

   

H11 H21 H22 H23

  

H31 H32 H33

  

H41 H42 H43



H51

**Table S1.** HOMO – LUMO result of free optimized structure of cyclohexanone derivatives

|  |  |  |  |
| --- | --- | --- | --- |
| **Compound** | **HOMO (eV)** | **LUMO (eV)** | **Eg (eV)** |
| H1 | -5.422 | -1.735 | 3.687 |
| H2 | -5.833 | -2.386 | 3.447 |
| H3 | -6.055 | -3.133 | 2.922 |
| H4 | -6.305 | -4.303 | 2.002 |
| H5 | -6.368 | -5.816 | 0.552 |

**Table S3.** HOMO – LUMO result of optimized structure of cyclohexanone derivatives fine-tuned with EDG.

|  |  |  |  |
| --- | --- | --- | --- |
| **Compound** | **HOMO (eV)** | **LUMO (eV)** | **Eg (eV)** |
| H1-EDG | -5.344 | -1.832 | 3.512 |
| H2-EDG | -4.534 | -2.453 | 2.081 |
| H3-EDG | -6.008 | -3.051 | 2.957 |
| H4-EDG | -6.307 | -4.257 | 2.050 |
| H5-EDG | -6.379 | -5.607 | 0.772 |

**Table S2.** HOMO – LUMO result of optimized structure of cyclohexanone derivatives structurally designed with EWG.

|  |  |  |  |
| --- | --- | --- | --- |
| **Compound** | **HOMO (eV)** | **LUMO (eV)** | **Eg (eV)** |
| H1-EWG | -5.825 | -2.094 | 3.731 |
| H2-EWG | -6.106 | -2.804 | 3.302 |
| H3-EWG | -6.352 | -3.465 | 2.887 |
| H4-EWG | -6.542 | -4.638 | 1.904 |
| H5-EWG | -6.621 | -6.089 | 0.532 |

**Table S4.** Second order perturbation energy of the fock matrix analysis for free optimized structure of cyclohexanone derivatives.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Donor (ἰ) | Acceptor (j) | E(2) (kcal/mol) | E(j) – E(ἰ) (a.u) | F(ἰ,j) (a.u) |
| H1 | LP(2) O17 | σ\*C2 – C3 | 18.71 | 0.53 | 0.090 |
| H2 | LP(2) O16 | σ\*C2 – C3 | 19.95 | 0.53 | 0.093 |
| H3 | LP(2) O15 | σ\*C5 – C6 | 19.49 | 0.53 | 0.092 |
| H4 | LP(2) O14 | σ\*C1 – C2 | 22.02 | 0.51 | 0.091 |
| H5 | LP(2) O11 | σ\*C1 – C2 | 23.31 | 0.50 | 0.097 |

**Table S5.** Second order perturbation energy of the Fock matrix analysis for optimized structure of cyclohexanone derivatives fine-tuned with EDG.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Donor (ἰ) | Acceptor (j) | E(2) (kcal/mol) | E(j) – E(ἰ) (a.u) | F(ἰ,j) (a.u) |
| H1-EDG | LP(2) O16 | σ\*C2 – C3 | 19.35 | 0.53 | 0.091 |
| H2-EDG | LP(2) O15 | σ\*C2 – C3 | 19.88 | 0.53 | 0.093 |
| H3-EDG | LP(2) O14 | σ\*C5 – C6 | 22.53 | 0.50 | 0.096 |
| H4-EDG | LP(2) O13 | σ\*C1 – C2 | 22.53 | 0.50 | 0.095 |
| H5-EDG | LP(2) O10 | σ\*C1 – C2 | 22.80 | 0.50 | 0.096 |

**Table S6.** Second order perturbation energy of the Fock matrix analysis for optimized structure of cyclohexanone derivatives structurally designed with EWG

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Donor (ἰ) | Acceptor (j) | E(2) (kcal/mol) | E(j) – E(ἰ) (au) | F(ἰ,j) (au) |
| H1-EWG | LP(2) O16 | σ\*C1 – C2 | 19.53 | 0.53 | 0.091 |
| H2-EWG | LP(2) O15 | σ\*C2 – C3 | 20.28 | 0.52 | 0.093 |
| H3-EWG | LP(2) O14 | σ\*C5 – C6 | 20.44 | 0.52 | 0.094 |
| H4-EWG | LP(2) O13 | σ\*C1 – C2 | 22.18 | 0.51 | 0.095 |
| H5-EWG | π\*C4 – O8 | π\*C3 – O12 | 33.95 | 0.01 | 0.061 |

**Table S7.** Binding Energy of the studied cyclohexanone derivates in free optimized state, with EDG and EWG.

|  |  |
| --- | --- |
| **Free optimized state** | |
| **Compound** | **Binding Energy (kcal/mol)** |
| H1-Li | -17.74 |
| H2-Li | -16.14 |
| H3-Li | -52.33 |
| H4-Li | -76.28 |
| H5-Li | -92.55 |
| **With EDG** | |
| **Compound** | **Binding Energy (kcal/mol)** |
| H1-Li-EDG | -18.07 |
| H2-Li-EDG | -14.86 |
| H3-Li-EDG | -51.16 |
| H4-Li-EDG | -73.06 |
| H5-Li-EDG | -87.06 |
| **With EWG** | |
| **Compound** | **Binding Energy (kcal/mol)** |
| H1-Li-EWG | -19.63 |
| H2-Li-EWG | -44.89 |
| H3-Li-EWG | -59.09 |
| H4-Li-EWG | -78.84 |
| H5-Li-EWG | -94.38 |