Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# High-Performance Carbon Dioxide Capture and Storage by Multi-Functional Sphingosine Kinase Inhibitors through a $CO_2$-philic Membrane

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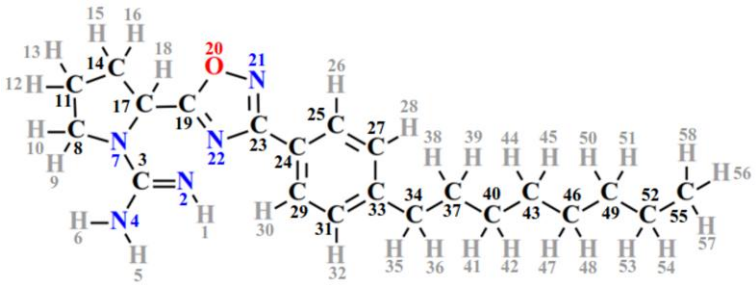

**Scheme S1.** The schematic structure of SphKI molecule with atom labeling; carbon, hydrogen, nitrogen and oxygen labeled by black, gray, blue and red colors, respectively.

**Table S1.** Atom type and LJ parameters for SphKI molecule.

| Atom type | σ [nm] | ε [kJ/mol] |
|---|---|---|
| 1 | 0.363487 | 0.209200 |
| 2 | 0.329632 | 0.836800 |
| 3 | 0.329632 | 0.836800 |
| 4 | 0.363487 | 0.209200 |
| 5 | 0.355005 | 0.292880 |
| 6 | 0.040001 | 0.192464 |
| 7 | 0.329632 | 0.836800 |
| 8 | 0.356359 | 0.460240 |
| 9 | 0.329632 | 0.836800 |
| 10 | 0.040001 | 0.192464 |
| 11 | 0.387541 | 0.230120 |
| 12 | 0.235197 | 0.092048 |
| 13 | 0.329632 | 0.836800 |

**Table S2.** Atom label, atom type and charges for SphKI molecule.

| Atom number | Atom type | Charge [e] | Atom number | Atom type | Charge [e] |
|---|---|---|---|---|---|
| 1 | 1 | 0.382 | 30 | 12 | 0.272 |
| 2 | 2 | -0.897 | 31 | 12 | -0.233 |
| 3 | 3 | 0.631 | 32 | 12 | 0.261 |
| 4 | 4 | -0.921 | 33 | 12 | -0.018 |
| 5 | 5 | 0.447 | 34 | 11 | -0.499 |
| 6 | 5 | 0.440 | 35 | 12 | 0.265 |
| 7 | 5 | -0.536 | 36 | 12 | 0.264 |
| 8 | 5 | -0.270 | 37 | 11 | -0.484 |
| 9 | 5 | 0.267 | 38 | 12 | 0.245 |
| 10 | 5 | 0.248 | 39 | 12 | 0.245 |
| 11 | 6 | -0.497 | 40 | 11 | -0.476 |
| 12 | 7 | 0.260 | 41 | 12 | 0.241 |
| 13 | 8 | 0.275 | 42 | 12 | 0.241 |
| 14 | 9 | -0.476 | 43 | 11 | -0.477 |
| 15 | 10 | 0.280 | 44 | 12 | 0.240 |
| 16 | 10 | 0.265 | 45 | 12 | 0.240 |
| 17 | 9 | -0.123 | 46 | 11 | -0.478 |
| 18 | 11 | 0.284 | 47 | 12 | 0.239 |
| 19 | 12 | 0.594 | 48 | 12 | 0.239 |
| 20 | 12 | -0.336 | 49 | 11 | -0.479 |
| 21 | 11 | -0.182 | 50 | 12 | 0.238 |
| 22 | 12 | -0.535 | 51 | 12 | 0.238 |
| 23 | 12 | 0.344 | 52 | 11 | -0.489 |
| 24 | 11 | -0.122 | 53 | 12 | 0.240 |
| 25 | 12 | -0.198 | 54 | 12 | 0.240 |
| 26 | 12 | 0.269 | 55 | 11 | -0.710 |
| 27 | 11 | -0.260 | 56 | 12 | 0.239 |
| 28 | 12 | 0.262 | 57 | 12 | 0.246 |
| 29 | 13 | -0.222 | 58 | 12 | 0.239 |

**Table S3.** LJ parameters and charges for $CO_2$ molecule.

| | **C atom** | **O atom** |
|---|---|---|
| **q (e)** | 0.6512 | -0.3256 |
| **ε (kJ/mol)** | 0.2340 | 0.6683 |
| **σ (nm)** | 0.2800 | 0.3028 |

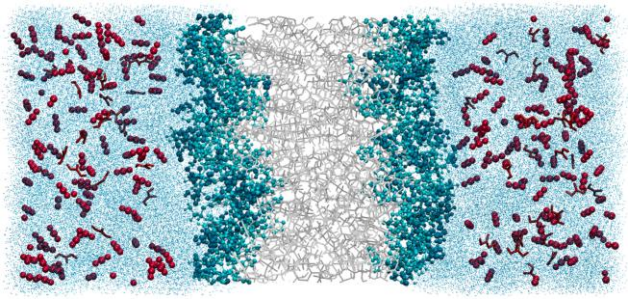

**Figure S1.** The initial simulation box (before a simulation run) for $CO_2$-SphKI system. $CO_2$, $H_2CO_3$ and water molecules are colored in light red (CPK format), dark red (licorice format) and cyan (point format), respectively. Ions are left invisible.

## Local Nucleophilicity

The electrophilic ($P_k^+$) and nucleophilic ($P_k^-$) Parr functions of a molecule can be described by conceptual density functional theory, which are given by the following equations:

$$P^- (r) = \rho_s^{rc} (r) \qquad \text{for electrophilic attacks} \qquad (1)$$

$$P^+ (r) = \rho_s^{ra} (r) \qquad \text{for nucleophilic attacks} \qquad (2)$$

where $\rho_s^{rc}$ (r) is the atomic spin density at the "r" atom of the radical cation (charge = +1; multiplicity = 2) and $\rho_s^{ra}$ (r) is the atomic spin density at the "r" atom of the radical anion (charge = -1; multiplicity = 2). With the optimized neutral molecular structure at hand, each atomic spin density gathered at the different atoms of the radical cation (rc) and the radical anion (ra), which provides the local electrophilic and nucleophilic Parr functions of the neutral molecule. In this study, nucleophilic ($P_k^-$) Parr function was obtained at the UM06-2X/6-31+G** computational level (single point energy).

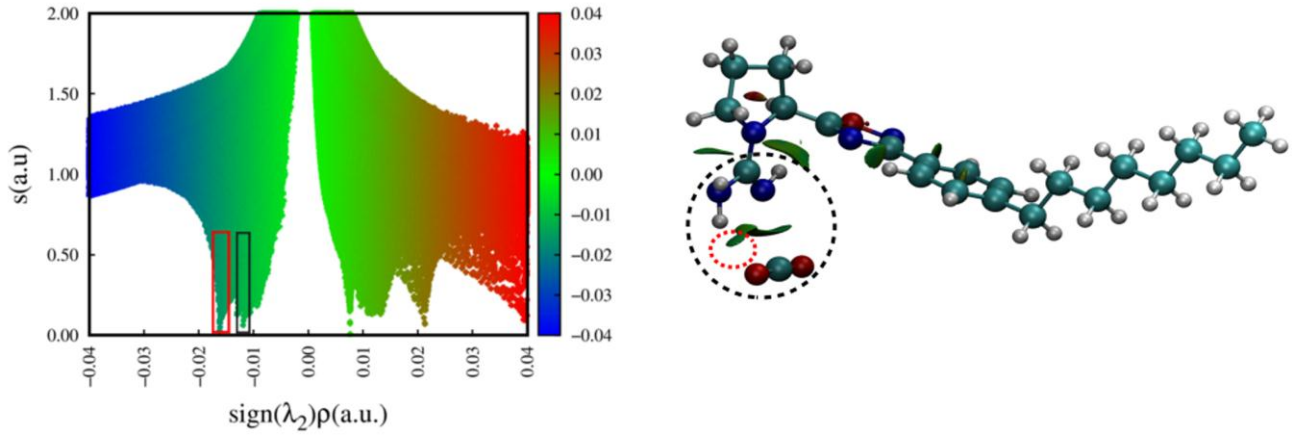


**Figure S2.** (left) M06-2X/6-31+G** 2D plot of RDG, s(r), versus sign ($\lambda_2$)ρ(r) for complex 1 (C1). (right) NCI 3D isosurfaces of C1 generated by NCIPLOT 3.0 program and visualized by VMD 1.9.

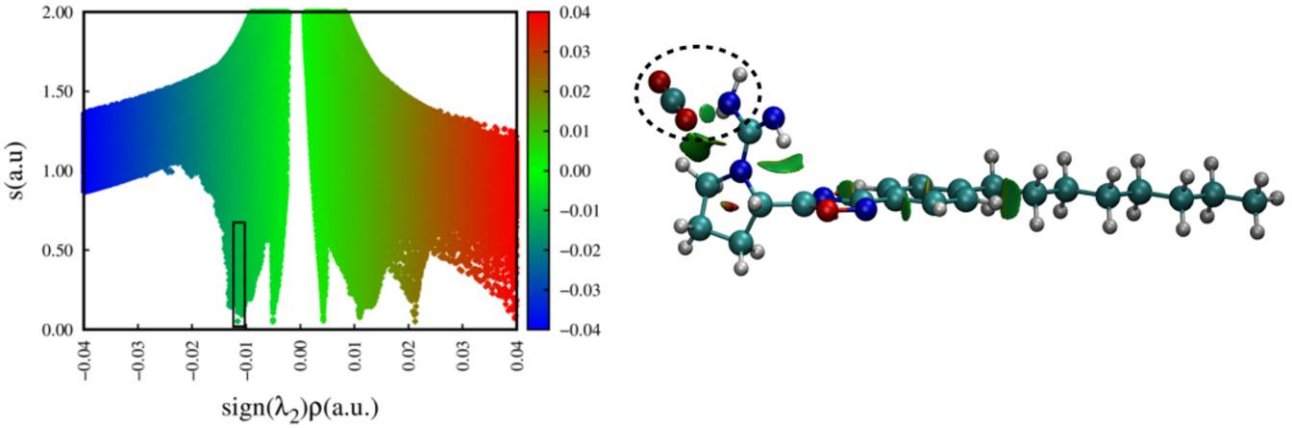


**Figure S3.** (left) M06-2X/6-31+G** 2D plot of RDG, s(r), versus sign ($\lambda_2$)ρ(r) for complex 2 (C2). (right) NCI 3D isosurfaces of C2 generated by NCIPLOT 3.0 program and visualized by VMD 1.9.

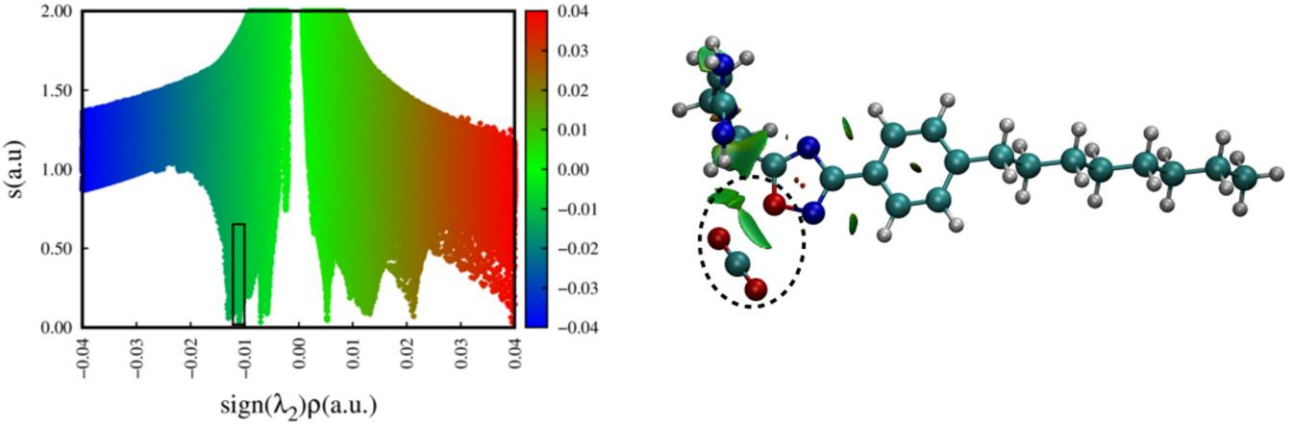


**Figure S4.** (left) M06-2X/6-31+G** 2D plot of RDG, s(r), versus sign ($\lambda_2$)ρ(r) for complex 5 (C5). (right) NCI 3D isosurfaces of C5 generated by NCIPLOT 3.0 program and visualized by VMD 1.9.

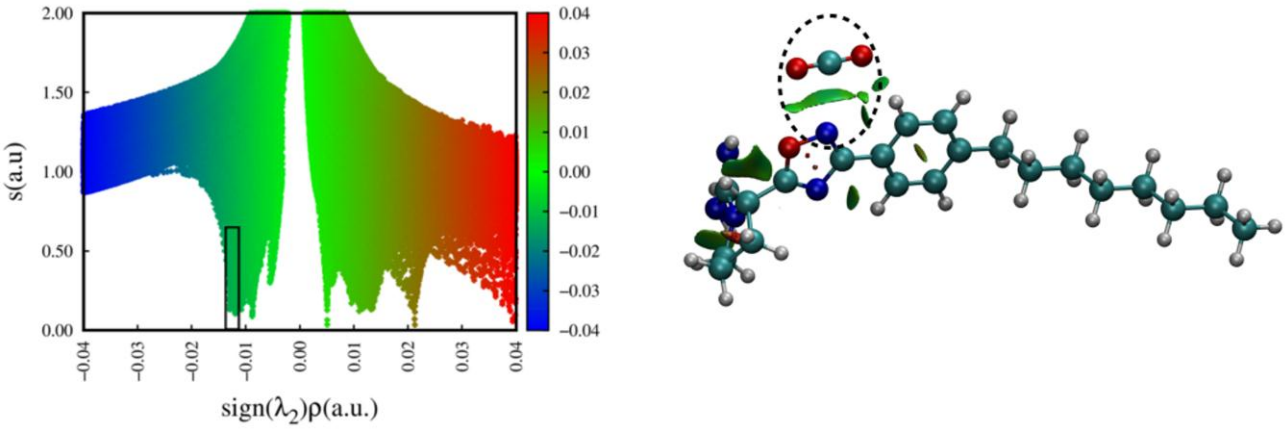


**Figure S5.** (left) M06-2X/6-31+G** 2D plot of RDG, s(r), versus sign ($\lambda_2$)ρ(r) for complex 6 (C6). (right) NCI 3D isosurfaces of C6 generated by NCIPLOT 3.0 program and visualized by VMD 1.9.

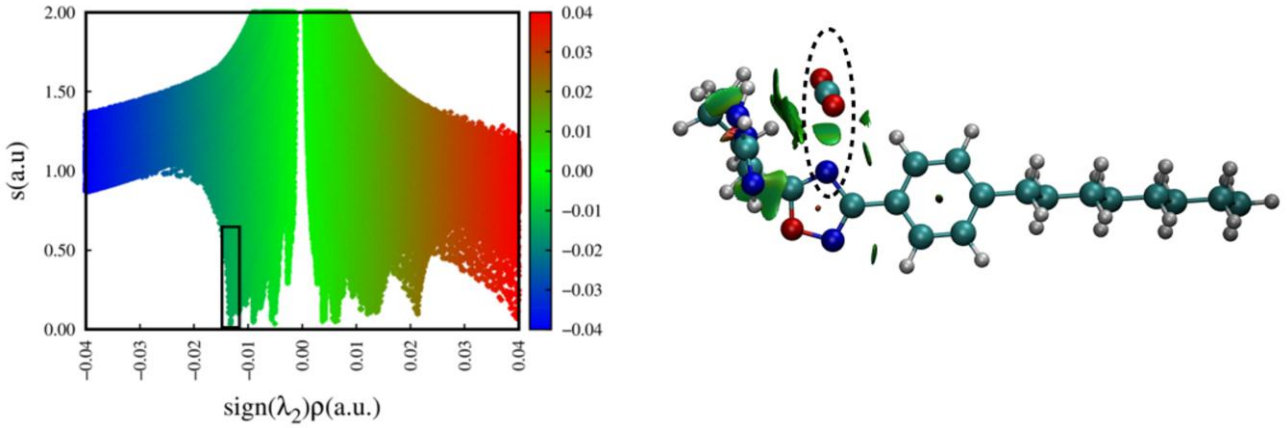


**Figure S6.** (left) M06-2X/6-31+G** 2D plot of RDG, s(r), versus sign ($\lambda_2$)ρ(r) for complex 7 (C7). (right) NCI 3D isosurfaces of C7 generated by NCIPLOT 3.0 program and visualized by VMD 1.9.

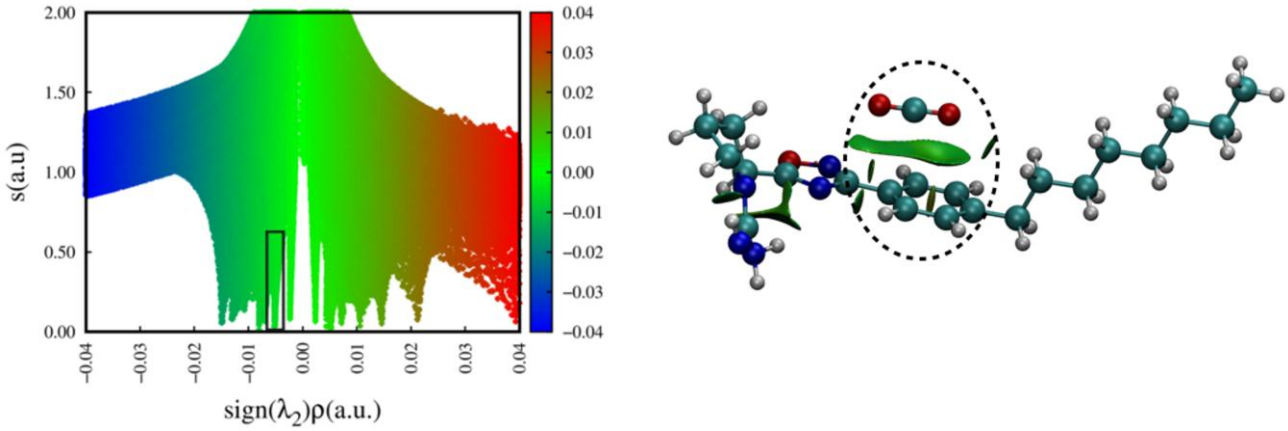


**Figure S7.** (left) M06-2X/6-31+G** 2D plot of RDG, s(r), versus sign ($\lambda_2$)ρ(r) for complex 8 (C8). (right) NCI 3D isosurfaces of C8 generated by NCIPLOT 3.0 program and visualized by VMD 1.9.

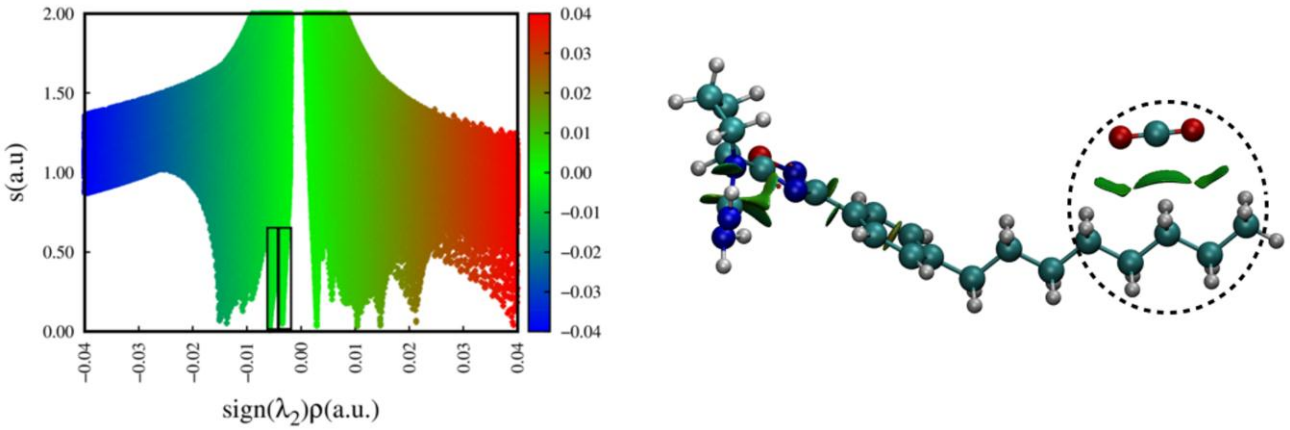


**Figure S8.** (left) M06-2X/6-31+G** 2D plot of RDG, s(r), versus sign ($\lambda_2$)ρ(r) for complex 9 (C9). (right) NCI 3D isosurfaces of C9 generated by NCIPLOT 3.0 program and visualized by VMD 1.9.

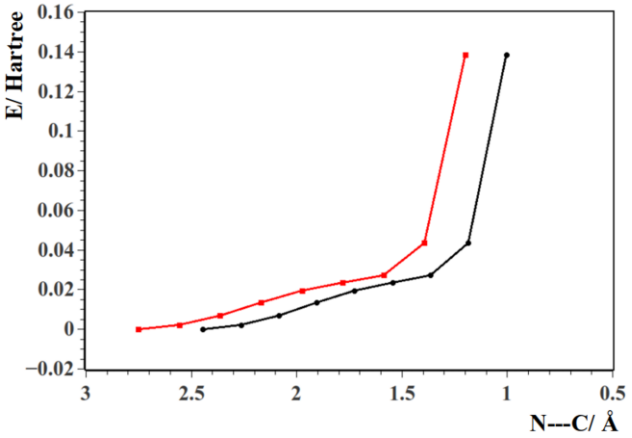


**Figure S9.** The two potential energy surface scan (PES) curves of N2-C($CO_2$) (black) and N3-C($CO_2$) (red) obtained by DFT calculations.

**Table S4.** Thermodynamic data, in Hartree (including unique imaginary frequency of TS, in $cm^{-1}$) of the located stationary points in the SphKI(N1)-$CO_2$ reaction at 25°C.

| Stationary points | Sum of electronic and zero-point correction energies (Hartree) | Thermal correction to Gibbs free energy (Hartree) | Imaginary frequency ($cm^{-1}$) |
|---|---|---|---|
| **SphKI + $CO_2$** | -1355.456854 | 0.448457 | - |
| **TS** | -1355.452631 | 0.450518 | -263.1 |
| **SphKI-$CO_2$** | -1355.473419 | 0.454373 | - |