**Supplementary Material**

**Table S1.** Some thermodynamics parameters for amide-1 isomer of MAAP.

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| --- | --- |
| Parameters |  B3LYP/6-31++G(d,p) |
|  | Amide-1  |
| Thermal total energy. (kcal/mol) | 200.245 |
| Vibrational energy. (kcal/mol)  | 198.468 |
| Zero point vibrational energy. (kcal/mol) | 188.102 |
| Total Entropy. (kcal/mol.K) | 145.587 |
| Heat capacity. (kcal/mol.K) | 72.714 |
| Dipole moment (Debye) | 2.543 |
| Rotational constant (GHz) |  |
| a | 0.827 |
| b | 0.171 |
| c | 0.147 |