**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 |