|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  |  |  |  |
| **Conformers** | **Δφ** | **Δψ** | **Δχ1** | **Δχ2** |
| **βL)a g+ (** | -2.0 | 0.1 | 1.7 | 0.0 |
| **βL)a g- (** | -2.3 | 0.6 | 1.3 | 0.0 |
| **βL)g- g-(** | -0.5 | 2.1 | 0.6 | -0.4 |
| **γL)g+ g+ (** | 0.2 | -5.3 | 1.7 | 8.1 |
| **γL)g+ g-)** | 1.6 | -2.7 | 1.8 | 0.4 |
| **γL)a g+(** | 0.8 | -2.3 | 0.3 | 0.1 |
| **γL)a g-(** | 0.3 | 1.1 | 0.3 | 4.3 |
| **γD)a g+(** | 0.2 | 0.3 | 0.7 | 1.0 |
| **γD)a a (** | 0.1 | 0.4 | 0.8 | -1.0 |
| **γD)a g-(** | 0.6 | -7.3 | -1.0 | -0.9 |
| **γD)g- g+)** | 0.3 | -0.3 | -0.6 | 0.2 |
| **γD)g- g-)** | 0.0 | 0.8 | 0.1 | -1.6 |
| **δD)g+ g+ (** | 3.4 | 2.3 | -0.5 | -1.8 |
| **δD)g+ g-(** | 2.6 | 1.5 | -0.2 | -1.1 |
| **δD)a g+(** | 0.6 | 2.4 | 1.7 | -1.4 |
| **δD)a g-)** | 0.3 | 1.4 | 1.3 | 0.1 |
| **εD )a g+(** | 0.7 | -1.4 | 0.1 | 0.5 |
| **εD )a a(** | -1.2 | -2.6 | 1.2 | 0.8 |
| **εD )g- g+(** | 2.8 | -2.1 | -0.9 | 0.4 |
|  |  |  |  |  |

**Table S3: The gaps between the dihedral angles of 19 commun structures of the systems HCO-L-Tyrosine-NH2 and HCO-L-Phenylalanine-NH2 detected at the MNC/AM1**