|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Conformations** | **φ****C2-N3-C4-C5** | **ψ****N3-C4-C5-N6** | **χ1****N3-C4-C12-C14** | **χ2****C4-C12-C14-C15** | **χ3****H27-O24-C17-C16** | **ΔHf** **)Kcalmol-1(** | **Δ )ΔHf(****)Kcalmol-1(** |
|  |
| **αD)g+ g-(** | 27.3 | 52.4 | 43.8 | -100.6 | 178.9 | -97.917740 | 7.14 |
|
| **βL)g+g+ (** | -150.2 | 145.3 | 30.6 | 58 .9 | -179.2 | -102.052803 | 3.00 |
| **βL)a g+ (** | -148.8 | 170.9 | -142.9 | 65.4 | -178.7 | -103.225380 | 1.83 |
| **βL)a g- (** | -148.5 | 171.0 | -143.5 | -116.0 | 1.7 | -103.224808 | 1.84 |
| **βL)g- g-(** | -119.7 | 134.2 | -57.0 | -31.6 | -179.9 | -102.665298 | 2.39 |
|
| **γL)g+ g+ (** | -82.5 | 55.3 | 41.0 | 86.4 | -179.4 | -104.902924 | 0.16 |
| **γL)g+ g-)** | -82.5 | 55.4 | 41.1 | -94.5 | 1.4 | -104.905060 | 0.15 |
| **γL)a g+(** | -80.2 | 72.6 | -155.9 | 89.4 | 0.1 | -103.979950 | 1.08 |
| **γL)a g-(** | -82.1 | 71.7 | -155.2 | -90.9 | -179.8 | -103.989449 | 1.07 |
| **γL)g- g+(** | -84.8 | 65.2 | -56.6 | 103.0 | -0.9 | -105.061569 | 0.00 |
| **γL)g- g-(** | -84.4 | 65.9 | -56.1 | -77.0 | 179.1 | -105.048922 | 0.01 |
| **γD)a g+(** | 75.6 | -65.3 | -166.9 | 69.4 | 2.3 | -102.401909 | 2.65 |
| **γD)a a (** | 77.6 | -54.7 | -129.6 | 130.7 | -179.3 | -102.635551 | 2.42 |
| **γD)a g-(** | 77.8 | -54.5 | -131.0 | -50.6 | 179.4 | -102.805450 | 2.25 |
| **γD)g- g+)** | 75.9 | -62.3 | -69.4 | 110.0 | -1.3 | -102.428558 | 2.63 |
| **γD)g- g-)** | 75.5 | -61.6 | -69.1 | -71.6 | 178.5 | -104.425468 | 0.63 |
| **δD)g+ g+ (** | -111.8 | -51.1 | 48.8 | 97.6 | -2.8 | -101.686378 | 3.37 |
| **δD)g+ g-(** | -111.3 | -50.5 | 49.2 | -84.0 | 2.0 | -101.726463 | 3.33 |
| **δD)a g+)** | -128.5 | -67.1 | -176.8 | 63.6 | 178.2 | -100.070488 | 4.99 |
| **δD)a g-)** | -129.0 | -68.2 | -177.3 | -117 .4 | -2.3 | -100.069321 | 4.99 |
| **δD)g- g-)** | -114.2 | -46.4 | -66.2 | -14.6 | 178.2 | -100.958000 | 4.10 |
| **εD )a g+(** | 92.6 | -159.6 | -151.8 | 57.4 | -178.9 | -100.128181 | 4.93 |
| **εD )a a(** | 93.5 | -153.0 | -153.6 | -126.5 | 0.4 | -100.125420 | 4.94 |
| **εD )g- g+(** | 82.0 | 167.3 | -64.3 | 105.5 | -179 .7 | -98.624420 | 6.43 |
| **αL)g- g+(** | -102.5 | -0.1 | -93.5 | 75.1 | -7.4 | -100.016762 | 5.04 |
| **αL)g- g-(** | -103.7 | -1.2 | -59.8 | -69.1 | 179.0 | -102.250122 | 2.81 |

a torsion angles in degrees

**Table S1: Torsion angles (a), heats of formationΔHf and relative heats of formation  Δ )ΔHf( of 26 structures of HCO-L-Tyr-NH2 located at MNC/AM1**