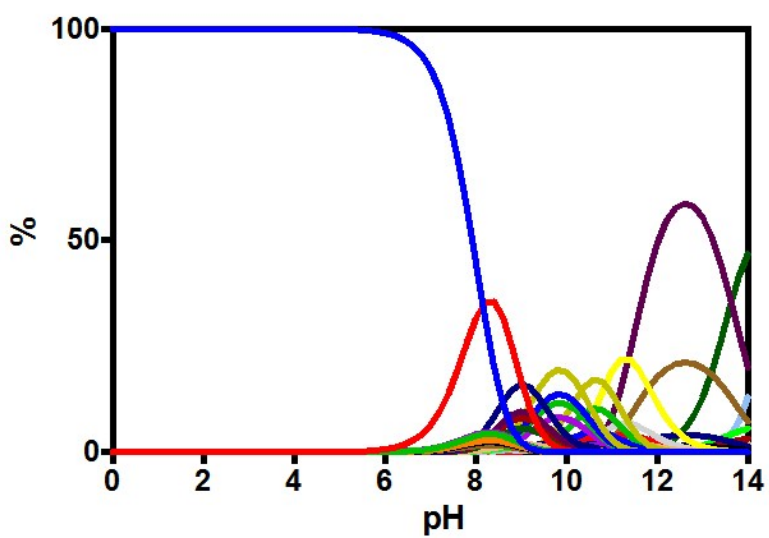
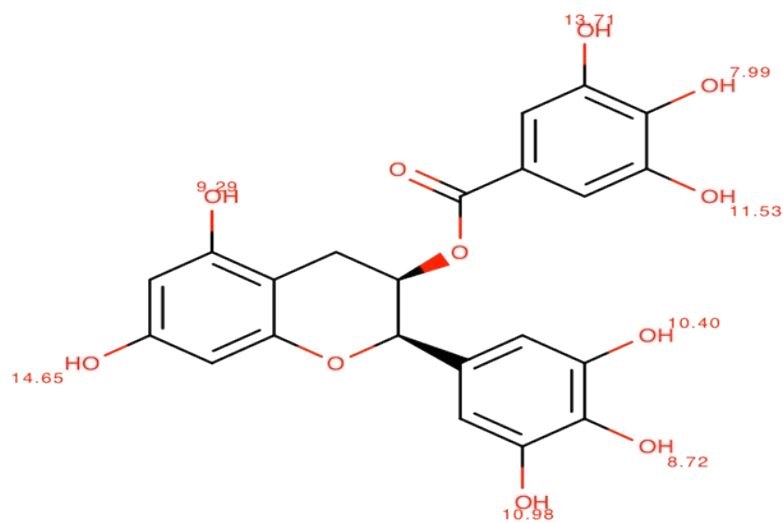


Supplementary Fig. 1



Supplementary Table 1. Calculated pK_a values of β -Lg . The pK_a values of amino acid residues of β -Lg compared to the predicted values at different pH.

| Residue | pKa | pK model |
|-----------|-------|----------|
| ASP 11 A | 3.81 | 3.80 |
| ASP 28 A | 2.73 | 3.80 |
| ASP 33 A | 4.25 | 3.80 |
| ASP 53 A | 3.80 | 3.80 |
| ASP 64 A | 3.98 | 3.80 |
| ASP 85 A | 3.90 | 3.80 |
| ASP 96 A | 3.87 | 3.80 |
| ASP 98 A | 2.35 | 3.80 |
| ASP 129 A | 3.41 | 3.80 |
| ASP 130 A | 4.07 | 3.80 |
| ASP 137 A | 3.57 | 3.80 |
| GLU 44 A | 6.70 | 4.50 |
| GLU 45 A | 4.58 | 4.50 |
| GLU 51 A | 4.61 | 4.50 |
| GLU 55 A | 3.67 | 4.50 |
| GLU 62 A | 3.76 | 4.50 |
| GLU 65 A | 4.63 | 4.50 |
| GLU 74 A | 5.01 | 4.50 |
| GLU 89 A | 7.79 | 4.50 |
| GLU 108 A | 4.31 | 4.50 |
| GLU 112 A | 4.71 | 4.50 |
| GLU 114 A | 4.95 | 4.50 |
| GLU 127 A | 4.41 | 4.50 |
| GLU 131 A | 4.77 | 4.50 |
| GLU 134 A | 4.34 | 4.50 |
| GLU 157 A | 4.11 | 4.50 |
| GLU 158 A | 4.99 | 4.50 |
| ILE 162 A | 3.44 | 3.20 |
| HIS 146 A | 6.35 | 6.50 |
| HIS 161 A | 4.54 | 6.50 |
| TYR 20 A | 11.85 | 10.00 |
| TYR 42 A | 10.80 | 10.00 |
| TYR 99 A | 10.10 | 10.00 |
| TYR 102 A | 12.62 | 10.00 |
| LYS 8 A | 10.46 | 10.50 |
| LYS 14 A | 10.55 | 10.50 |

| | | |
|-----------|-------|-------|
| LYS 47 A | 11.05 | 10.50 |
| LYS 60 A | 9.32 | 10.50 |
| LYS 69 A | 11.10 | 10.50 |
| LYS 70 A | 10.44 | 10.50 |
| LYS 75 A | 10.43 | 10.50 |
| LYS 77 A | 10.44 | 10.50 |
| LYS 83 A | 10.36 | 10.50 |
| LYS 91 A | 10.45 | 10.50 |
| LYS 100 A | 11.18 | 10.50 |
| LYS 101 A | 10.71 | 10.50 |
| LYS 135 A | 10.59 | 10.50 |
| LYS 138 A | 10.25 | 10.50 |
| LYS 141 A | 10.36 | 10.50 |
| ARG 40 A | 12.49 | 12.50 |
| ARG 124 A | 11.35 | 12.50 |
| ARG 148 A | 12.73 | 12.50 |
| N+ 1 A | 8.32 | 8.00 |

Pk_a values were calculated by the Propka method. A: β -Lg A-chain.