**S2 Table.** The average energy values determined during the 50 ns of MD simulations of *Ca*DPP III – RRNA complex using ff14SB and the parameters required for aMD simulations. All values are given in kcal mol-1. *E*r and *E*a values are 1.0 and 0.1 kcal mol-1, respectively.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | ***Ca*DPP III – RRNA** | ***Ca*DPP III – GRNA** | ***Ca*DPPIII – GPNA** | ***Ca*DPPIII – GFNA** |
| $\overbar{E\_{pot}}$a | -199640 | -199500 | -212451 | -212296 |
| $\overbar{E\_{dih}}$a | 7090 | 7071 | 7085 | 7078 |
| $$E\_{threshP}$$ | -192988 | -192855 | -205407 | -205257 |
| $$α\_{P}$$ | 6651 | 6644 | 7044 | 7039 |
| $$E\_{threshD}$$ | 7631 | 7614 | 7625 | 7618 |
| $$α\_{D}$$ | 108 | 108 | 108 | 108 |

aAverage potential and dihedral energies.