

Table 1. *In silico* evaluation of CoQ10 and CoQ10 Ac by ADMETlab 3.0.

| | Property | Value | Decision | Comment |
|----------|---------------------|--------|----------|---|
| CoQ10 | Caco-2 Permeability | -4.688 | ● | Optimal: higher than -5.15 Log unit |
| | PAMPA | 0.0 | ● | <ul style="list-style-type: none"> ■ The experimental data for Peff was logarithmically transformed (logPeff). ■ Molecules with log Peff values below 2.0 were classified as low-permeability (Category 0), while those with log Peff values exceeding 2.5 were classified as high-permeability (Category 1). |
| | BBB | 0.0 | ● | <ul style="list-style-type: none"> ■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; ■ The output value is the probability of being BBB+ |
| CoQ10 Ac | Caco-2 Permeability | -4.751 | ● | Optimal: higher than -5.15 Log unit |
| | PAMPA | 0.0 | ● | <ul style="list-style-type: none"> ■ The experimental data for Peff was logarithmically transformed (logPeff). ■ Molecules with log Peff values below 2.0 were classified as low-permeability (Category 0), while those with log Peff values exceeding 2.5 were classified as high-permeability (Category 1). |
| | BBB | 0.0 | ● | <ul style="list-style-type: none"> ■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; ■ The output value is the probability of being BBB+ |

For Caco-2 permeability, empirical decision: > -5.15: excellent (green); otherwise: poor (red); for PAMPA, empirical decision: 0-0.3: excellent (green); 0.3-0.7: medium (yellow); 0.7-1.0: poor (red); for BBB penetration, empirical decision: 0-0.3: excellent (green); 0.3-0.7: medium (yellow); 0.7-1.0: poor (red).