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多巴胺在 POPC 磷脂双层膜中扩散和透过过程的分子动力学模拟

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Molecular Dynamics Simulation of Dopamine Diffusion within and Permeation through POPC Phospholipid Bilayer Membrane

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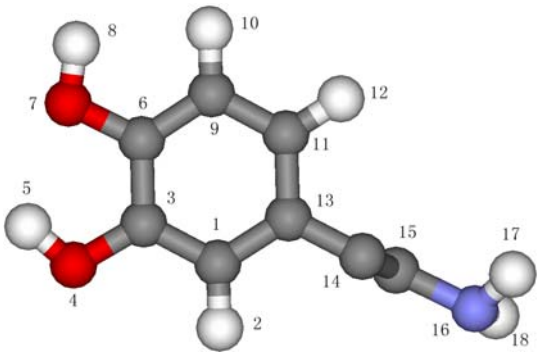


图S1　多巴胺分子结构和标记的原子或原子团序号用于书写其力场参数

Fig.S1　Structure of dopamine and its atom labels used to write its molecular dynamic parameters.

```
[ moleculetype ]
; Name dopamine
DOP          3
[ atoms ]
;     nr         type    resnr resid    atom    cgnr      charge        mass
       1          CR6        1    DOP        CAF        1    -0.006    12.0110
       2          HCR        1    DOP        HAF        1     0.006     1.0080
       3          CR6        1    DOP        CAA        2     0.082    12.0110
       4           OA        1    DOP        OAJ        2    -0.112    15.9994
       5           HO        1    DOP        HAL        2     0.030     1.0080
       6          CR6        1    DOP        CAB        3     0.082    12.0110
       7           OA        1    DOP        OAI        3    -0.112    15.9994
       8           HO        1    DOP        HAK        3     0.030     1.0080
       9          CR6        1    DOP        CAC        4    -0.010    12.0110
      10          HCR        1    DOP        HAC        4     0.003     1.0080
      11          CR6        1    DOP        CAD        5    -0.011    12.0110
      12          HCR        1    DOP        HAD        5     0.003     1.0080
      13          CR6        1    DOP        CAE        6    -0.061    12.0110
      14          CH2        1    DOP        CAG        6     0.005    14.0270
      15          CH2        1    DOP        CAH        6     0.007    14.0270
      16           NT        1    DOP        NAK        6     0.064    14.0067
      17            H        1    DOP        HAN        6     0.005     1.0080
      18            H        1    DOP        HAO        6     0.005     1.0080

[ bonds ]
; ai    aj    fu        c0, c1, ...
    1     2     2        0.109    12300000.0        0.109    12300000.0 ;    CAF    HAF
    3     1     2        0.139    10800000.0        0.139    10800000.0 ;    CAA    CAF
   13     1     2        0.139    10800000.0        0.139    10800000.0 ;    CAE    CAF
    3     4     2        0.136    10200000.0        0.136    10200000.0 ;    CAA    OAJ
    3     6     2        0.139    10800000.0        0.139    10800000.0 ;    CAA    CAB
    4     5     2        0.100    15700000.0        0.100    15700000.0 ;    OAJ    HAL
    6     7     2        0.136    10200000.0        0.136    10200000.0 ;    CAB    OAI
```

```
  6    9    2      0.139   10800000.0      0.139   10800000.0 ;    CAB   CAC
  7    8    2      0.100   15700000.0      0.100   15700000.0 ;    OAI   HAK
  9   10    2      0.109   12300000.0      0.109   12300000.0 ;    CAC   HAC
  9   11    2      0.139   10800000.0      0.139   10800000.0 ;    CAC   CAD
 11   12    2      0.109   12300000.0      0.109   12300000.0 ;    CAD   HAD
 13   11    2      0.139   10800000.0      0.139   10800000.0 ;    CAE   CAD
 13   14    2      0.139    8660000.0      0.139    8660000.0 ;    CAE   CAG
 14   15    2      0.153    7150000.0      0.153    7150000.0 ;    CAG   CAH
 15   16    2      0.147    8710000.0      0.147    8710000.0 ;    CAH   NAK
 16   17    2      0.100   18700000.0      0.100   18700000.0 ;    NAK   HAN
 16   18    2      0.100   18700000.0      0.100   18700000.0 ;    NAK   HAO

[ pairs ]
; ai    aj    fu       c0, c1, ...
  1     5     1                                                  ;    CAF   HAL
  1     7     1                                                  ;    CAF   OAI
  1     9     1                                                  ;    CAF   CAC
  1    12     1                                                  ;    CAF   HAD
  1    15     1                                                  ;    CAF   CAH
  2     4     1                                                  ;    HAF   OAJ
  2     6     1                                                  ;    HAF   CAB
  2    11     1                                                  ;    HAF   CAD
  2    14     1                                                  ;    HAF   CAG
  3     8     1                                                  ;    CAA   HAK
  3    10     1                                                  ;    CAA   HAC
  3    11     1                                                  ;    CAA   CAD
  3    14     1                                                  ;    CAA   CAG
  4     7     1                                                  ;    OAJ   OAI
  4     9     1                                                  ;    OAJ   CAC
  4    13     1                                                  ;    OAJ   CAE
  5     6     1                                                  ;    HAL   CAB
  6    12     1                                                  ;    CAB   HAD
  6    13     1                                                  ;    CAB   CAE
  7    10     1                                                  ;    OAI   HAC
  7    11     1                                                  ;    OAI   CAD
  8     9     1                                                  ;    HAK   CAC
  9    14     1                                                  ;    CAC   CAG
 10    12     1                                                  ;    HAC   HAD
 10    13     1                                                  ;    HAC   CAE
 11    15     1                                                  ;    CAD   CAH
 12    14     1                                                  ;    HAD   CAG
 13    16     1                                                  ;    CAE   NAK
 14    17     1                                                  ;    CAG   HAN
 14    18     1                                                  ;    CAG   HAO
```

[angles]

; ai aj ak fu c0, c1, ...

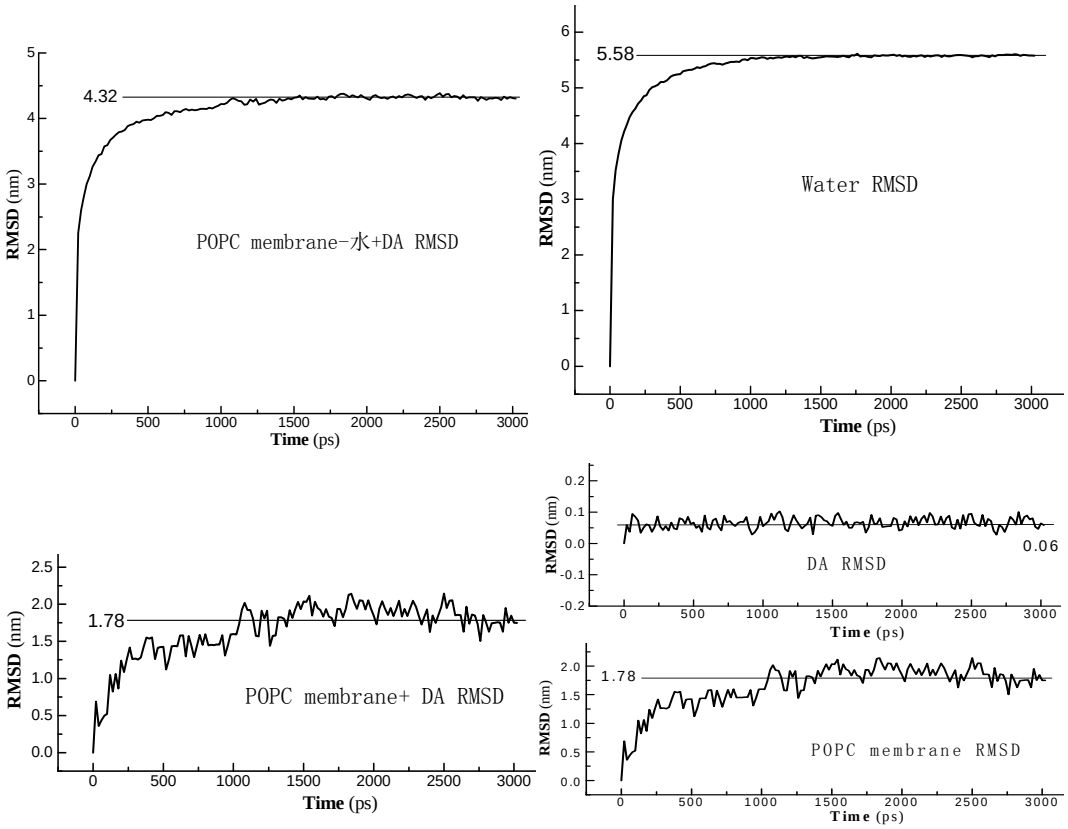
2	1	3	2	120.0	505.0	120.0	505.0	;	HAF	CAF	CAA
2	1	13	2	120.0	505.0	120.0	505.0	;	HAF	CAF	CAE
3	1	13	2	120.0	505.0	120.0	505.0	;	CAA	CAF	CAE
1	3	4	2	120.0	560.0	120.0	560.0	;	CAF	CAA	OAJ
1	3	6	2	120.0	560.0	120.0	560.0	;	CAF	CAA	CAB
4	3	6	2	115.0	610.0	115.0	610.0	;	OAJ	CAA	CAB
3	4	5	2	109.5	450.0	109.5	450.0	;	CAA	OAJ	HAL
3	6	7	2	115.0	610.0	115.0	610.0	;	CAA	CAB	OAI
3	6	9	2	120.0	560.0	120.0	560.0	;	CAA	CAB	CAC
7	6	9	2	120.0	560.0	120.0	560.0	;	OAI	CAB	CAC
6	7	8	2	109.5	450.0	109.5	450.0	;	CAB	OAI	HAK
6	9	10	2	120.0	505.0	120.0	505.0	;	CAB	CAC	HAC
6	9	11	2	120.0	505.0	120.0	505.0	;	CAB	CAC	CAD
10	9	11	2	120.0	505.0	120.0	505.0	;	HAC	CAC	CAD
9	11	12	2	120.0	505.0	120.0	505.0	;	CAC	CAD	HAD
9	11	13	2	120.0	505.0	120.0	505.0	;	CAC	CAD	CAE
12	11	13	2	120.0	505.0	120.0	505.0	;	HAD	CAD	CAE
1	13	11	2	120.0	560.0	120.0	560.0	;	CAF	CAE	CAD
1	13	14	2	120.0	560.0	120.0	560.0	;	CAF	CAE	CAG
11	13	14	2	120.0	560.0	120.0	560.0	;	CAD	CAE	CAG
13	14	15	2	109.5	520.0	109.5	520.0	;	CAE	CAG	CAH
14	15	16	2	111.0	530.0	111.0	530.0	;	CAG	CAH	NAK
15	16	17	2	109.5	425.0	109.5	425.0	;	CAH	NAK	HAN
15	16	18	2	109.5	425.0	109.5	425.0	;	CAH	NAK	HAO
17	16	18	2	109.5	380.0	109.5	380.0	;	HAN	NAK	HAO

[dihedrals]

; ai aj ak al fu c0, c1, m, ...

1	13	3	2	2	0.0	167.4	0.0	167.4	; imp	CAF	CAE	CAA HAF
3	1	4	6	2	0.0	167.4	0.0	167.4	; imp	CAA	CAF	OAJ CAB
6	9	7	3	2	0.0	167.4	0.0	167.4	; imp	CAB	CAC	OAI CAA
9	6	11	10	2	0.0	167.4	0.0	167.4	; imp	CAC	CAB	CAD HAC
11	9	13	12	2	0.0	167.4	0.0	167.4	; imp	CAD	CAC	CAE HAD
13	14	11	1	2	0.0	167.4	0.0	167.4	; imp	CAE	CAG	CAD CAF
16	15	17	18	2	35.3	334.8	35.3	334.8	; imp	NAK	CAH	HAN

```
HAO
   1    3    6    9    2        0.0    209.3        0.0    209.3    ; imp    CAF    CAA    CAB
CAC
   3    6    9   11    2        0.0    209.3        0.0    209.3    ; imp    CAA    CAB    CAC
CAD
   6    9   11   13    2        0.0    209.3        0.0    209.3    ; imp    CAB    CAC    CAD
CAE
   9   11   13    1    2        0.0    209.3        0.0    209.3    ; imp    CAC    CAD    CAE
CAF
  11   13    1    3    2        0.0    209.3        0.0    209.3    ; imp    CAD    CAE    CAF
CAA
  13    1    3    6    2        0.0    209.3        0.0    209.3    ; imp    CAE    CAF    CAA
CAB
   1    3    4    5    1      180.0      7.1 2      180.0      7.1 2 ; dih    CAF    CAA    OAJ    HAL
   3    6    7    8    1      180.0      7.1 2      180.0      7.1 2 ; dih    CAA    CAB    OAI    HAK
  15   14   13    1    1        0.0      1.0 6        0.0      1.0 6 ; dih    CAH    CAG    CAE    CAF
  16   15   14   13    1        0.0      5.9 3        0.0      5.9 3 ; dih    NAK    CAH    CAG    CAE
```



图S2　3 ns分子动力学模拟取得的POPC膜-水+DA体系和各个组成体系的RMSD随分子动力学模拟时间变化曲线

Fig.S2　RMSD *vs* MD time for POPC-H_2O+DA membrane, H_2O backbone, POPC+DA, POPC membrane and DA backbones within 3 ns of simulation