Supporting Information

Tanshinones Inhibit Amyloid Aggregation by Amyloid-β Peptide, Disaggregate Amyloid Fibrils, and Protect Cultured Cells

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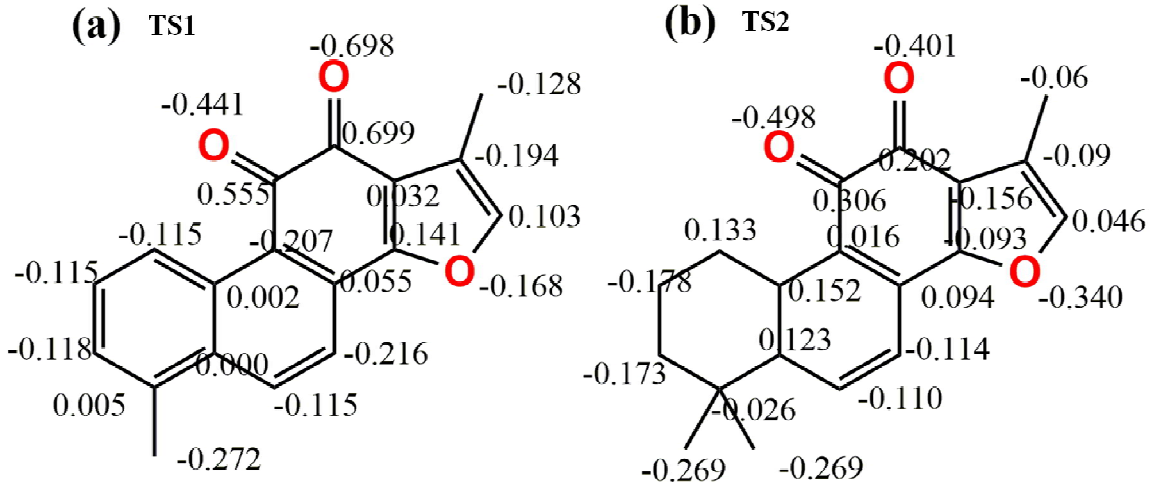
Running Title: Tanshinones inhibit the aggregation and cytotoxicity of Aβ

Keywords: Aβ, amyloid, Tanshinone, Alzheimer disease

Figure S1. A complete set of force field parameters for (a) Tanshinone (TS1) and (b) Tanshinone IIA (TS2) in CHARMM27 format.

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* Toppar stream file
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36 1

MASS   302 CZ61    12.01100
MASS   299 CZ51    12.01100
MASS   296 CZ25    12.01100
MASS   366 OZ50    15.99940
MASS   361 OZ23    15.99940
MASS   320 CZ33    12.01100
MASS   302 CK61    12.01100
MASS   316 CK32    12.01100
MASS   311 CK30    12.01100
MASS   296 CK25    12.01100
MASS   299 CK51    12.01100
MASS   366 OK50    15.99940
MASS   320 CK33    12.01100
MASS   361 OK23    15.99940
MASS   257 HGA2     1.00800
MASS   277 HZ61     1.00800
MASS   275 HZ52     1.00800
MASS   258 HGA3     1.00800


RESI TS1         0.000
GROUP
ATOM C1     CZ61   -0.115
ATOM C2     CZ61   -0.118
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```
ATOM C3     CZ61    0.005
ATOM C4     CZ61    0.000
ATOM C5     CZ61    0.002
ATOM C6     CZ61   -0.115
ATOM C7     CZ61   -0.115
ATOM C8     CZ61   -0.216
ATOM C9     CZ61    0.055
ATOM C10    CZ61   -0.207
ATOM C11    CZ51    0.141
ATOM C12    CZ51    0.032
ATOM C13    CZ25    0.699
ATOM C14    CZ25    0.555
ATOM O1     OZ50   -0.168
ATOM C15    CZ51    0.103
ATOM C16    CZ51   -0.194
ATOM O2     OZ23   -0.698
ATOM O3     OZ23   -0.441
ATOM C17    CZ33   -0.272
ATOM C18    CZ33   -0.228
ATOM H1     HZ61    0.115
ATOM H2     HZ61    0.115
ATOM H3     HZ61    0.115
ATOM H4     HZ61    0.115
ATOM H5     HZ61    0.115
ATOM H6     HZ52    0.180
ATOM H9     HGA3    0.090
ATOM H10    HGA3    0.090
ATOM H11    HGA3    0.090
ATOM H12    HGA3    0.090
ATOM H13    HGA3    0.090
ATOM H14    HGA3    0.090


BOND H13  C18
BOND H10  C17
BOND O2   C13
BOND H14  C18
BOND H1   C1
BOND H2   C2
BOND C18  C16
BOND C18  H12
BOND C2   C1
BOND C2   C3
BOND C1   C6
BOND H11  C17
BOND C17  C3
BOND C17  H9
BOND H6   C15
BOND C16  C15
BOND C16  C12
```

```
BOND C6   H3
BOND C6   C5
BOND C13  C12
BOND C13  C14
BOND C3   C4
BOND C15  O1
BOND C4   C5
BOND C4   C7
BOND O1   C11
BOND C12  C11
BOND C11  C9
BOND C5   C10
BOND C10  C9
BOND C10  C14
BOND H4   C7
BOND C7   C8
BOND C8   C9
BOND C8   H5
BOND C14  O3

IMPR C13    C14    C12    O2
IMPR C14    C13    C10    O3
```

RESI TS2 0.000

```
GROUP
ATOM C1     CK61    0.152
ATOM C2     CK61    0.123
ATOM C3     CK61   -0.110
ATOM C4     CK61   -0.114
ATOM C5     CK61    0.094
ATOM C6     CK61    0.016
ATOM C7     CK32    0.133
ATOM C8     CK32   -0.178
ATOM C9     CK32   -0.173
ATOM C10    CK30   -0.026
ATOM C11    CK25    0.306
ATOM C12    CK25    0.202
ATOM C13    CK51   -0.156
ATOM C14    CK51   -0.093
ATOM C15    CK51    0.046
ATOM C16    CK51   -0.090
ATOM O1     OK50   -0.340
ATOM C17    CK33   -0.060
ATOM C18    CK33   -0.269
ATOM C19    CK33   -0.269
ATOM O2     OK23   -0.498
ATOM O3     OK23   -0.401
ATOM H1     HZ61    0.115
ATOM H2     HZ61    0.115
ATOM H3     HGA2    0.090
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ATOM H4     HGA2    0.090
ATOM H5     HGA2    0.090
ATOM H6     HGA2    0.090
ATOM H7     HGA2    0.090
ATOM H8     HGA2    0.090
ATOM H9     HZ52    0.125
ATOM H10    HGA3    0.090
ATOM H11    HGA3    0.090
ATOM H12    HGA3    0.090
ATOM H13    HGA3    0.090
ATOM H14    HGA3    0.090
ATOM H15    HGA3    0.090
ATOM H16    HGA3    0.090
ATOM H17    HGA3    0.090
ATOM H18    HGA3    0.090

BOND H14  C18
BOND H7   C9
BOND H15  C18
BOND C18  H13
BOND C18  C10
BOND H3   C7
BOND H11  C17
BOND O2   C11
BOND C9   C10
BOND C9   H8
BOND C9   C8
BOND C11  C6
BOND C11  C12
BOND C5   C6
BOND C5   C4
BOND C5   C14
BOND C6   C1
BOND C3   C4
BOND C3   C2
BOND C3   H1
BOND C4   H2
BOND C2   C1
BOND C2   C10
BOND C1   C7
BOND C10  C19
BOND C13  C14
BOND C13  C12
BOND C13  C16
BOND C14  O1
BOND O1   C15
BOND C12  O3
BOND C7   C8
BOND C7   H4
BOND C15  C16
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BOND C15  H9
BOND C16  C17
BOND C17  H12
BOND C17  H10
BOND H5   C8
BOND C8   H6
BOND C19  H17
BOND C19  H16
BOND C19  H18

IMPR C11    C12    C6     O2
IMPR C12    C11    C13    O3

END
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BONDS

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CZ25   CZ25    300.00     1.4800
CZ25   CZ51    254.00     1.4600
CZ51   CZ61    400.00     1.4360
CZ33   HGA3    322.00     1.1110
CZ51   CZ33    229.63     1.5000
CZ51   CZ51    410.00     1.3600
CZ51   HZ52    375.00     1.0830
CZ51   OZ50    450.00     1.3610
CZ25   CZ61    254.00     1.5000
CZ61   CZ61    305.00     1.3750
CZ61   CZ33    230.00     1.4900
CZ61   HZ61    340.00     1.0800
CZ25   OZ23    700.00     1.2300
CK25   CK25    300.00     1.4800
CK25   CK51    254.00     1.4600
CK51   CK61    300.00     1.4360
CK61   CK30    230.00     1.4900
CK33   HGA3    322.00     1.1110
CK51   CK33    229.63     1.5000
CK51   CK51    410.00     1.3600
CK51   HZ52    375.00     1.0830
CK51   OK50    450.00     1.3710
CK25   CK61    254.00     1.4600
CK61   CK61    305.00     1.3750
CK61   CK33    230.00     1.4900
CK61   HZ61    340.00     1.0800
CK25   OK23    700.00     1.2300
CK30   CK33    222.50     1.5380
CK32   HGA2    309.00     1.1110
CK32   CK32    222.50     1.5300
CK51   CK32    229.63     1.5000
CK61   CK32    230.00     1.4900
CK30   CK32    222.50     1.5380
```

ANGLES

CZ25	CZ25	CZ51	40.00	117.20		
CZ25	CZ25	CZ61	40.00	117.20		
CZ25	CZ25	OZ23	95.00	121.50		
CZ51	CZ25	OZ23	70.00	121.30		
CZ25	CZ51	CZ51	45.80	130.00		
CZ51	CZ51	CZ61	45.80	130.00		
CZ61	CZ51	OZ50	65.00	127.80		
CZ51	CZ61	CZ61	36.00	120.00		
CZ61	CZ61	CZ61	40.00	120.00	35.00	2.41620
CZ61	CZ61	HZ61	30.00	120.00	22.00	2.15250
CZ61	CZ61	CZ33	45.80	120.00		
CZ25	CZ61	CZ61	45.00	120.00		
CZ51	CZ51	OZ50	130.00	111.70		
CZ51	OZ50	CZ51	100.00	106.00		
CZ51	CZ51	CZ51	90.00	107.20		
CZ61	CZ25	OZ23	70.00	124.30		
CZ51	CZ51	HZ52	22.00	130.00	15.00	2.21500
CZ51	CZ51	CZ33	45.80	130.00		
OZ50	CZ51	HZ52	50.00	118.30		
CZ61	CZ33	HGA3	49.30	107.50		
CZ51	CZ33	HGA3	55.00	109.50		
CK25	CK25	CK51	40.00	117.20		
CK25	CK25	CK61	40.00	117.20		
CK25	CK25	OK23	95.00	121.50		
CK51	CK25	OK23	70.00	121.30		
CK51	CK51	CK61	45.80	130.00		
CK61	CK51	OK50	65.00	127.80		
CK51	CK61	CK61	36.00	120.00		
CK61	CK61	CK30	45.80	120.00		
CK61	CK30	CK32	51.80	107.50		
CK61	CK30	CK33	51.80	107.50		
CK61	CK61	CK61	40.00	120.00	35.00	2.41620
CK61	CK61	HZ61	30.00	120.00	22.00	2.15250
CK61	CK61	CK33	45.80	120.00		
CK25	CK61	CK61	45.00	120.00		
CK51	CK51	OK50	130.00	111.70		
CK51	OK50	CK51	100.00	106.00		
CK30	CK33	HGA3	33.43	110.10	22.53	2.17900
CK30	CK32	HGA2	26.50	110.10	22.53	2.179
CK30	CK32	CK32	58.35	113.50	11.16	2.561
CK32	CK32	HGA2	26.50	110.10	22.53	2.17900
CK61	CK61	CK32	45.80	120.00		
CK61	CK32	CK32	51.80	107.50		
CK61	CK32	HGA2	49.30	107.50		
HGA2	CK32	HGA2	35.50	109.00	5.40	1.802
CK32	CK30	CK33	58.35	113.50	11.16	2.561
CK61	CK25	OK23	70.00	121.30		
CK51	CK51	CK51	90.00	107.20		
CK51	CK51	HZ52	22.00	130.00	15.00	2.21500

OK50	CK51	HZ52	50.00	118.30		
CK51	CK51	CK33	45.80	130.00		
CK51	CK33	HGA3	55.00	109.50		
HGA3	CK33	HGA3	35.50	108.40	5.40	1.80200
CK33	CK30	CK33	58.35	113.50	11.16	2.561

DIHEDRALS

CZ51	CZ25	CZ25	CZ61	8.4000	2	180.00
CZ51	CZ25	CZ25	OZ23	6.4000	2	0.00
CZ61	CZ25	CZ25	OZ23	3.4000	2	0.00
OZ23	CZ25	CZ25	OZ23	2.3000	2	180.00
CZ25	CZ25	CZ51	CZ51	5.5850	2	180.00
OZ23	CZ25	CZ51	CZ51	3.5850	2	180.00
CZ25	CZ25	CZ61	CZ61	2.5850	2	180.00
CZ25	CZ51	CZ51	CZ51	2.0000	2	180.00
CZ25	CZ51	CZ51	CZ61	3.0000	2	180.00
CZ25	CZ51	CZ51	CZ33	4.9000	2	180.00
CZ25	CZ51	CZ51	OZ50	8.5000	2	180.00
CZ51	CZ51	CZ51	CZ61	5.0000	2	180.00
CZ51	CZ51	CZ51	CZ33	4.0000	2	180.00
CZ33	CZ51	CZ51	OZ50	3.0000	2	180.00
CZ51	CZ51	CZ61	CZ61	3.0000	2	180.00
OZ50	CZ51	CZ61	CZ61	3.0000	2	180.00
CZ61	CZ51	OZ50	CZ51	10.5000	2	180.00
CZ25	CZ61	CZ61	CZ51	3.1000	2	180.00
CZ51	CZ61	CZ61	CZ61	5.1000	2	180.00
CZ51	CZ61	CZ61	HZ61	5.4000	2	180.00
CZ61	CZ61	CZ61	CZ61	3.1000	2	180.00
CZ61	CZ61	CZ61	HZ61	4.2000	2	180.00
CZ61	CZ61	CZ33	HGA3	0.0020	6	0.00
CZ61	CZ61	CZ61	CZ33	3.1000	2	180.00
CZ25	CZ61	CZ61	CZ61	3.1000	2	180.00
OZ23	CZ25	CZ61	CZ61	2.5850	2	180.00
CZ51	CZ51	CZ51	CZ51	15.0000	2	0.00
CZ51	CZ51	CZ51	OZ50	8.5000	2	180.00
CZ51	CZ51	CZ51	HZ52	1.5000	2	180.00
CZ51	CZ51	OZ50	CZ51	12.5000	2	180.00
CZ51	CZ51	CZ33	HGA3	0.0000	3	0.00
HZ52	CZ51	OZ50	CZ51	3.8000	2	180.00
CZ33	CZ51	CZ51	HZ52	1.0000	2	180.00
CZ33	CZ61	CZ61	HZ61	2.4000	2	180.00
HZ61	CZ61	CZ61	HZ61	2.4000	2	180.00
CK51	CK25	CK25	CK61	8.4000	2	180.00
CK51	CK25	CK25	OK23	6.4000	2	0.00
CK61	CK25	CK25	OK23	3.4000	2	0.00
OK23	CK25	CK25	OK23	2.3000	2	180.00
CK25	CK25	CK51	CK51	5.5850	2	180.00
OK23	CK25	CK51	CK51	3.5850	2	180.00
CK25	CK25	CK61	CK61	2.5850	2	180.00
CK25	CK51	CK51	CK51	2.0000	2	180.00

CK25	CK51	CK51	CK61	2.0000	2	180.00
CK25	CK51	CK51	CK33	4.9000	2	180.00
CK25	CK51	CK51	OK50	8.5000	2	180.00
CK51	CK51	CK51	CK61	2.0000	2	180.00
CK51	CK51	CK51	CK33	4.0000	2	180.00
CK33	CK51	CK51	OK50	3.0000	2	180.00
CK51	CK51	CK61	CK61	1.0000	2	180.00
OK50	CK51	CK61	CK61	1.0000	2	180.00
CK61	CK51	OK50	CK51	10.5000	2	180.00
CK25	CK61	CK61	CK51	3.1000	2	180.00
CK25	CK61	CK61	CK32	2.4000	2	180.00
CK51	CK61	CK61	CK61	3.1000	2	180.00
CK51	CK61	CK61	HZ61	2.4000	2	180.00
CK61	CK61	CK61	CK30	3.1000	2	180.00
CK30	CK61	CK61	CK32	2.4000	2	180.00
CK30	CK61	CK61	HZ61	2.4000	2	180.00
CK61	CK61	CK30	CK32	0.2300	2	180.00
CK61	CK61	CK30	CK33	0.2300	2	180.00
CK61	CK30	CK32	CK32	0.0400	3	0.00
CK61	CK30	CK32	HGA2	0.0000	3	0.00
CK61	CK30	CK33	HGA3	0.0400	3	0.00
CK61	CK61	CK61	CK61	3.1000	2	180.00
CK61	CK61	CK61	HZ61	4.2000	2	180.00
CK61	CK61	CK33	HGA3	0.0020	6	0.00
CK61	CK61	CK61	CK33	3.1000	2	180.00
CK25	CK61	CK61	CK61	3.1000	2	180.00
OK23	CK25	CK61	CK61	2.5850	2	180.00
CK51	CK51	CK51	CK51	15.0000	2	180.00
CK51	CK51	CK51	OK50	8.5000	2	180.00
CK51	CK51	CK51	HZ52	1.5000	2	180.00
CK51	CK51	OK50	CK51	12.5000	2	180.00
CK51	CK51	CK33	HGA3	0.0000	3	0.00
HZ52	CK51	OK50	CK51	3.8000	2	180.00
CK33	CK51	CK51	HZ52	1.0000	2	180.00
CK33	CK61	CK61	HZ61	2.4000	2	180.00
HZ61	CK61	CK61	HZ61	2.4000	2	180.00
CK61	CK32	CK32	CK32	0.0400	3	0.00
CK61	CK32	CK32	HGA2	0.0400	3	0.00
CK61	CK61	CK32	CK32	0.2300	2	180.00
CK61	CK61	CK32	HGA2	0.0020	6	0.00
CK61	CK61	CK61	CK32	3.1000	2	180.00
CK30	CK32	CK32	CK32	0.1950	3	0.00
CK32	CK32	CK32	HGA2	0.1950	3	0.00
CK33	CK30	CK32	CK32	0.2000	3	0.00
CK32	CK30	CK33	HGA3	0.1600	3	0.00
CK30	CK32	CK32	HGA2	0.1950	3	0.00
CK33	CK30	CK32	HGA2	0.1950	3	0.00
CK33	CK30	CK33	HGA3	0.1600	3	0.00
HGA2	CK32	CK32	HGA2	0.2200	3	0.00

IMPROPERS

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CZ25   CZ25   CZ61   OZ23       6.0000  0     0.00
CZ25   CZ25   CZ51   OZ23       6.0000  0     0.00
CK25   CK25   CK51   OK23       6.0000  0     0.00
CK25   CK25   CK61   OK23       6.0000  0     0.00

NONBONDED nbxmod  5 atom cdiel fshift vatom vdistance vfswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5

CZ61     0.0       -0.0700     1.9924
CZ51     0.0       -0.0500     2.1000
CZ25     0.0       -0.0900     2.0000
OZ23     0.0       -0.0500     1.7000   0.0 -0.12 1.40
OZ50     0.0       -0.1200     1.7000
HZ61     0.0       -0.0300     1.3582
HGA3     0.0       -0.0240     1.3400
CZ33     0.0       -0.0780     2.0500   0.0 -0.01 1.9
HZ52     0.0       -0.0460     0.9000
CK61     0.0       -0.0700     1.9924
CK51     0.0       -0.0500     2.1000
CK25     0.0       -0.0900     2.0000
OK23     0.0       -0.0500     1.7000   0.0 -0.12 1.40
OK50     0.0       -0.1200     1.7000
CK33     0.0       -0.0780     2.0500   0.0 -0.01 1.9
CK30     0.0       -0.0320     2.0000   0.0 -0.01 1.9
HGA2     0.0       -0.0350     1.3400
CK32     0.0       -0.0560     2.0100   0.0 -0.01 1.9

HBOND CUTHB 0.5

END
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