Supporting Information for

Original article

High-throughput screening for amyloid-*β* binding natural small-molecules based on the combinational use of biolayer interferometry and UHPLC–DAD-Q/TOF-MS/MS

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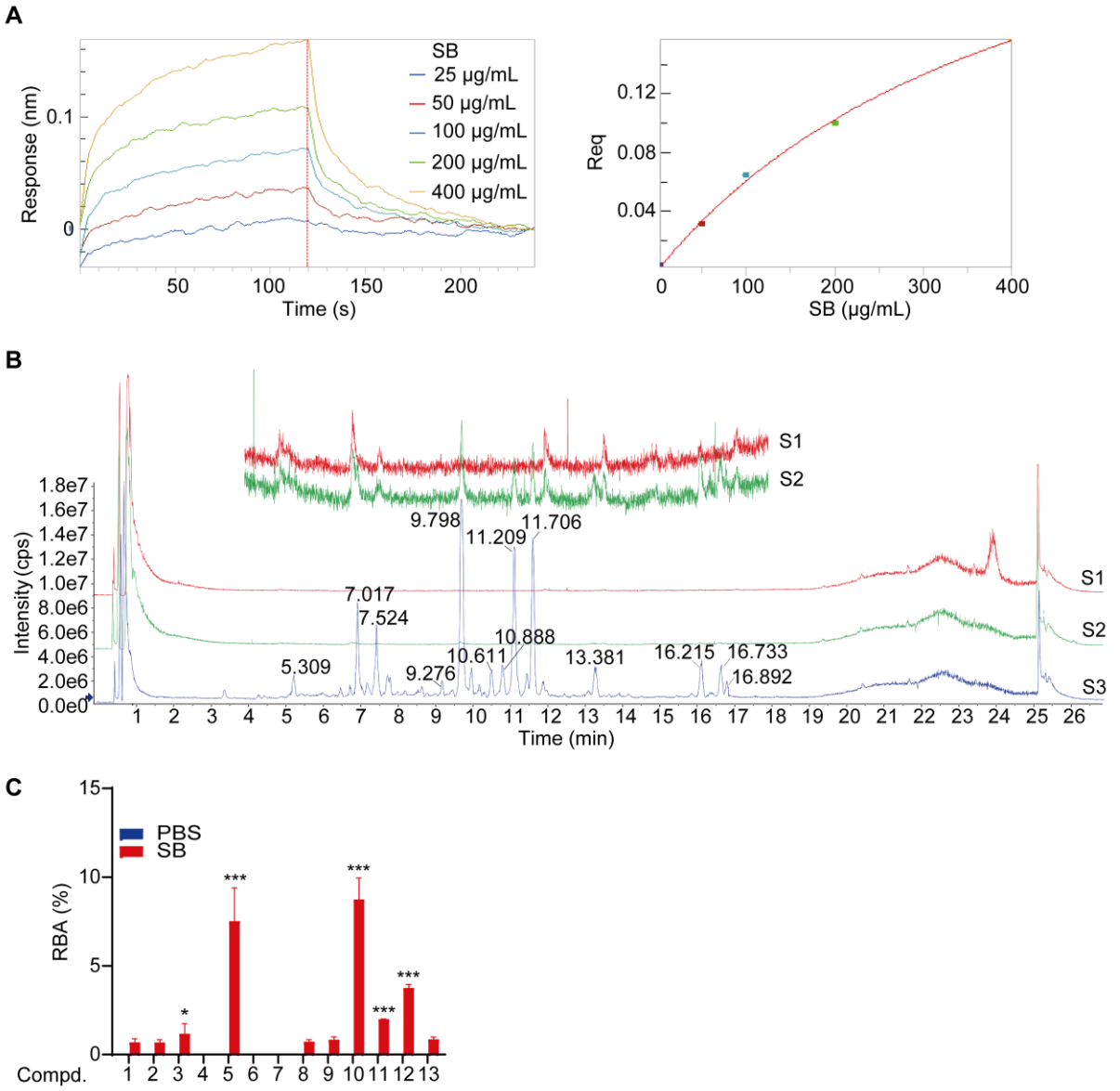

Figure S1 Screening of Aβ binding components in SB by the combinational use of BLI and UHPLC−DAD-Q/TOF-MS/MS. (A) Real-time kinetic binding sensorgrams of different concentrations of SB increasing from 25 to 400 μg/mL were shown. Response (nm) indicates the optical thickness on the SA biosensor layer. The equilibrium binding signal (Req) revealed by the flattened curve is reached. (B) The total ion chromatograms (TICs) were recorded by UHPLC−DAD-Q/TOF-MS/MS instrument. S1: The dissociation buffer without SB extract; S2: The dissociation buffer with SB extract; S3: SB extract used for the BLI assay. (C) The bar chart indicates the RBA of the detected components in SB. All data are representative of at least three independent experiments and are presented as mean ± SD. n=3. *P < 0.05, ***P < 0.001 compared with the components without RBA.

Table S1 The binding affinity (K_D), association rate constant (K_{on}), and dissociation rate constant (K_{dis}) of SB to Aβ_{1-42}.

TCM	K_D (μg/mL)	K_{on} (L/mol·s)	K_{dis} (1/s)
SB extract	199	6.18×10^{2}	1.23×10^{-1}

Table S2 The main detected components in SB and their RBA (%) with Aβ.

Compd.	RT (min)	$[M-H]^-$	Formula	MW	Chemical name	RBA (%)
1	5.309	303.0613	$C_{15}H_{12}O_7$	304	(2*R*,3*R*)-3,5,7,2′,6′-pentahydroxyflavanone	0.69
2	7.017	547.1647	$C_{26}H_{28}O_{13}$	548	Chrysin 6-*C*-arabinose-8-*C*-glucose	0.67
3	7.524	547.1653	$C_{26}H_{28}O_{13}$	548	Chrysin 6-*C*-glucose-8-*C*-arabinose	1.17
4	9.276	475.1049	$C_{22}H_{20}O_{12}$	476	Hispidulin 7-glucuronide	0
5	9.798	445.0936	$C_{21}H_{18}O_{11}$	446	Baicalin	7.52
6	10.611	445.0933	$C_{21}H_{18}O_{11}$	446	Norwogonin 7-*O*-*β*-D-glucuronide (5,8-dihydroxyflavone 7-*O*-*β*-D-glucuronide)	0
7	10.888	475.1051	$C_{22}H_{20}O_{12}$	476	5,7,8-Tetrahydroxyflavone; 6-Me ether,7-*O*-*β*-D-glucuronopyranoside	0
8	11.209	459.1092	$C_{22}H_{20}O_{11}$	460	Oroxyloside	0.73
9	11.706	459.1087	$C_{22}H_{20}O_{11}$	460	Wogonoside	0.83
10	13.381	269.0553	$C_{15}H_{10}O_5$	270	Baicalein	8.74
11	16.215	283.0711	$C_{16}H_{12}O_5$	284	Wogonin	1.99
12	16.733	373.1106	$C_{19}H_{18}O_8$	374	Skullcapflavone II	3.76
13	16.892	283.0711	$C_{16}H_{12}O_5$	284	Oroxylin A	0.85

Note: RT, retention time; MW, molecular weight; RBA, relative binding amount.