Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Fullerene derivatives act as inhibitors of Leukocyte Common Antigen based on Molecular Dynamics Simulations

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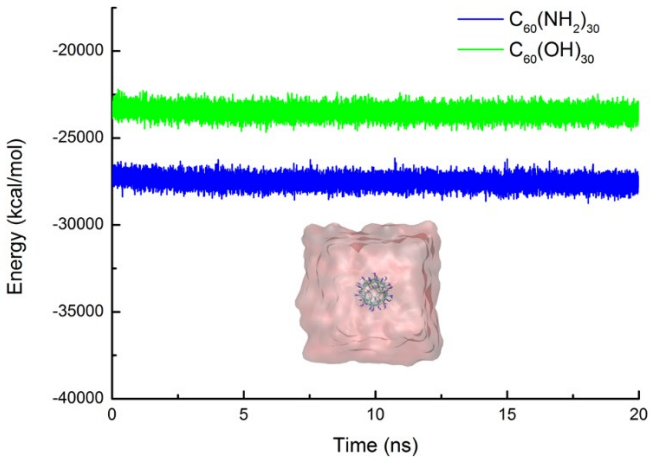

Figure S1. The energy of $C_{60}(NH_2)_{30}$/$C_{60}(OH)_{30}$ in a water box during 20 ns simulation.

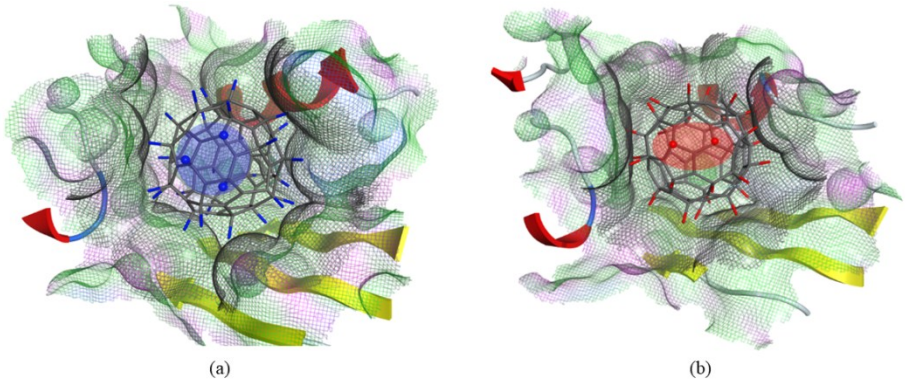

Figure S2. The grid of interactions (gray region) between (a) $C_{60}(NH_2)_{30}$, (b)$C_{60}(OH)_{30}$ and CD45. The surfaces of their binding pockets are colored by H-Bonding regions (purple), hydrophobic regions (green), and polar regions (blue). Functional groups that are not involved in interaction are specifically marked by translucent regions.

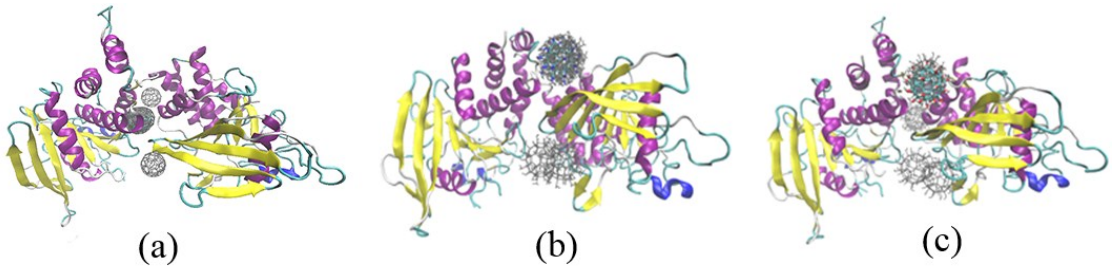

Figure S3. Docking poses of (a) CD45+C_{60}, (b) CD45+$C_{60}(NH_2)_{30}$, and (c) CD45+$C_{60}(OH)_{30}$ (top 50 docking poses). For each system, the docking pose with the highest docking score is represented by licorice and colored by atom name, and the

remaining 49 docking poses are colored in gray. The CD45 is shown with NewCartoon representation, where alpha-helix, beta-sheet, and random coil are shown in purple, yellow, and blue, respectively.

Table S1. The calculated pKa values of all hisdines.

Hisdines	pKa values
H609	6.977
H761	5.353
H788	7.254
H797	6.934
H804	7.286
H827	6.883
H881	7.152
H901	7.228
H905	6.816
H936	6.134
H1041	6.628
H1083	5.150
H1143	6.788

Table S2. The probability of residues that directly interact with $C_{60}(NH_2)_{30}$ and $C_{60}(OH)_{30}$.

	$C_{60}(NH_2)_{30}$	$C_{60}(OH)_{30}$
Q760	95.2%	100%
K762	100%	100%
C764	100%	42.4%
Y767	100%	92.6%
I769	100%	93.5%
K771	100%	98.1%
T787	100%	85.0%
I789	99.6%	89.7%
R811	92.6%	100%
R812	100%	100%
V813	98.5%	93.6%
A815	100%	100%
F816	100%	100%
S817	30.2%	100%
F819	99.9%	0%
F820	99.7%	0%

E894	65.2%	65.4%
N896	86.5%	96.5%
T1166	99.6%	91.6%
E1167	100%	100%
E1168	100%	100%
V1169	100%	100%

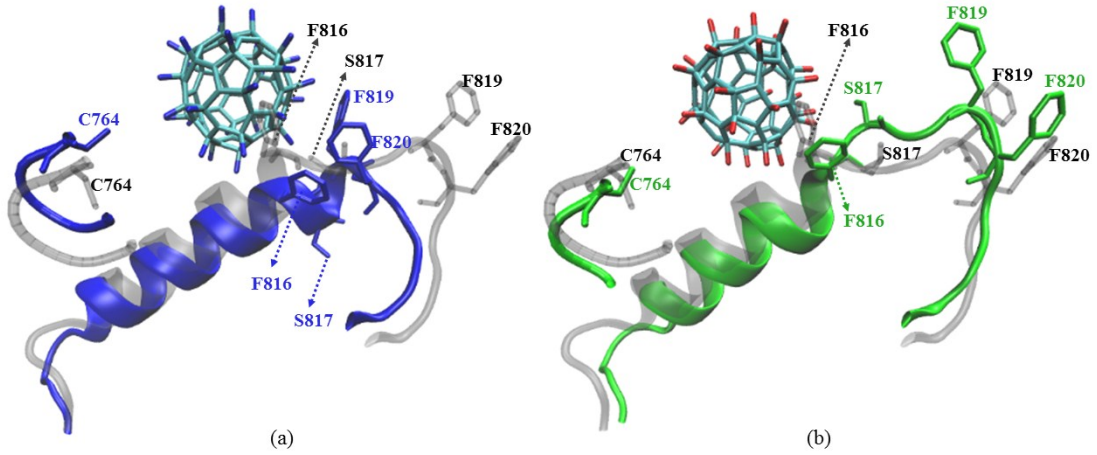

Figure S4. Comparison of the segment (C764 to D766, P800 to I824) of CD45 in crystal structure (gray) with the structure bound with $C_{60}(NH_2)_{30}$ (blue), and $C_{60}(OH)_{30}$ (green). C764, F816, S817, F819 and F820 are represented in relative colors.

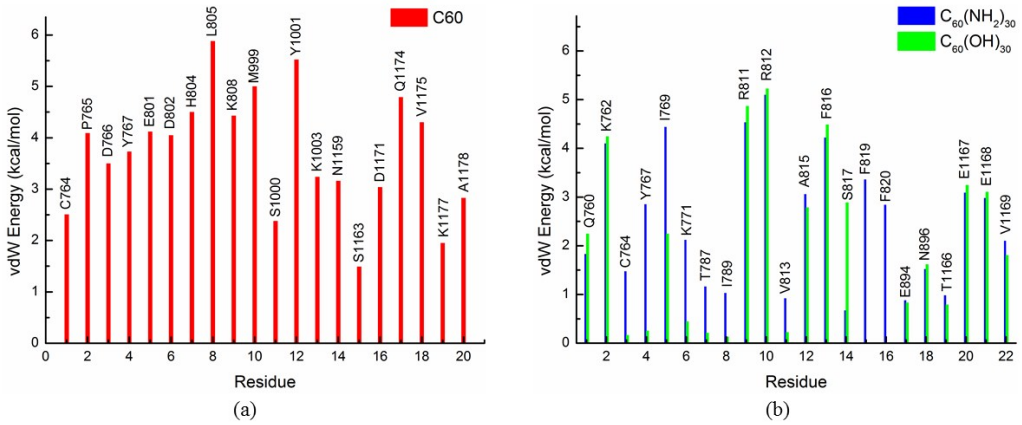

Figure S5. The vdW energy between every residue of binding pocket and C_{60} (red) $C_{60}(NH_2)_{30}$ (blue), $C_{60}(OH)_{30}$ (green).

Table S3. The full name and the abbreviation of amino acids

Full name	Abbreviation
Gly	G
Ala	A
Val	V
Leu	L
Ile	I
Phe	F
Pro	P
Ser	S
Thr	T
His	H
Trp	W
Cys	C
Asp	D
Glu	E
Lys	K
Tyr	Y
Met	M
Asn	N
Gln	Q
Arg	R