Supporting Information

for

Unusual hydrogen bonds pattern for contribution a supramolecular assembly: Conformational study, Hirshfeld surface analysis and density functional calculations of a new steroid derivative.

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Table S1. The ring puckering parameters of compound **I**.

Molecule	Ring	Q(2) (Å)	Q(3) (Å)	Φ (2) (°)	Q (Å)	θ (°)
IA	*A*	0.023 (3)	-0.568 (3)	63.3 (7)	0.568 (3)	179.7 (3)
	B	0.016 (3)	-0.563 (3)	107.8 (1)	0.562 (3)	180.0 (3)
	C	0.111 (3)	-0.578 (3)	99.0 (1)	0.589 (3)	169.0 (3)
	D	0.364 (3)		34.2 (5)		
IB	*A*	0.040 (3)	-0.563 (3)	119.0 (4)	0.565 (3)	176.0 (3)
	B	0.049 (3)	-0.588 (3)	92.8 (3)	0.588 (3)	175.4 (3)
	C	0.128 (3)	-0.561 (3)	84.7 (1)	0.576 (3)	167.1 (3)
	D	0.375 (3)		31.1 (5)		
IC	*A*	0.051 (3)	-0.563 (3)	91.1 (4)	0.565 (3)	174.8 (3)
	B	0.007 (3)	-0.567 (3)	155.0 (2)	0.567 (3)	180.0 (3)
	C	0.101 (3)	-0.579 (3)	97.0 (2)	0.587 (3)	170.1 (3)
	D	0.371 (3)		30.9 (5)		

Table S2. Experimental X-ray and theoretical bond lengths (Å) of compound **I**.

Parameters*	Experimental			Calculated	
	Molecule IA	Molecule IB	Molecule IC	[a]M06-2X/ 6-31++G(d.p)	[b]M06-2X/ 6-311++G(d.p)
Cl-C17	1.721(3)	1.720(3)	1.715(4)	1,729	1,729
O1-C21	1.334(4)	1.342(3)	1.340(4)	1,346	1,344
O1-C3	1.460 (3)	1.463(3)	1.459(3)	1,441	1,441
O2-C21	1.208(4)	1.201(3)	1.202(5)	1,208	1,202
O3-C18	1.204(5)	1.202(4)	1.210(6)	1,214	1,207
C1-C2	1.527(4)	1.526(3)	1.532(4)	1,533	1,533
C1-C10	1.542(4)	1.536(4)	1.537(4)	1,544	1,543
C2-C3	1.516(5)	1.510(4)	1.504(5)	1,522	1,521
C3-C4	1.513(4)	1.506(4)	1.508(4)	1,519	1,517
C4-C5	1.525(3)	1.537(3)	1.531(4)	1,531	1,530
C5-C6	1.502(4)	1.519(4)	1.507(4)	1,529	1,528
C5-C10	1.549(4)	1.545(4)	1.548(4)	1,556	1,555
C6-C7	1.519(3)	1.531(4)	1.515(4)	1,528	1,527
C7-C8	1.523(4)	1.525(4)	1.517(4)	1,531	1,530
C8-C14	1.515(3)	1.510(3)	1.517(3)	1,520	1,519
C8-C9	1.552(3)	1.545(4)	1.548(3)	1,552	1,552
C9-C11	1.544(4)	1.535(4)	1.544(4)	1,545	1,544
C9-C10	1.553(3)	1.556(3)	1.554(3)	1,557	1,556
C10-C20	1.537(4)	1.536(4)	1.537(4)	1,539	1,538
C11-C12	1.535(3)	1.540(3)	1.531(3)	1,541	1,540
C12-C13	1.524(4)	1.517(4)	1.518(4)	1,527	1,526
C13-C17	1.507(3)	1.512(3)	1.513(4)	1,513	1,511
C13-C19	1.540(4)	1.546(4)	1.542(4)	1,544	1,543
C13-C14	1.549(4)	1.537(4)	1.544(4)	1,546	1,545
C14-C15	1.534(3)	1.541(4)	1.534(4)	1,537	1,536
C15-C16	1.509(4)	1.507(4)	1.505(5)	1,518	1,517
C16-C17	1.347(4)	1.326(4)	1.344(5)	1,346	1,342
C16-C18	1.460(4)	1.467(4)	1.462(4)	1.468	1.467
C18-H	1.030(4)	1.050(3)	1.040(6)	1.106	1.104
C21-C22	1.501(4)	1.493(4)	1.499(4)	1.505	1.504
$MD = \sum \lvert x_{exp} - x^{a}{}_{theor} \rvert / N$	**0.009**	**0.010**	**0.009**		
$MD = \sum \lvert x_{exp} - x^{b}{}_{theor} \rvert / N$	**0.008**	**0.008**	**0.008**		

* The structure parameters are in accordance with the atom numbering scheme given in Figure

In *MD* (mean deviation) expression: x = bond lengths and N= 30.

[a]M06-2X/6-31++G(d,p)

[b]M06-2X/6-311++G(d,p)

Table S3. Experimental X-ray and theoretical angles (°) of compound **I**.

Parameters*	Experimental			Calculated	
	Molecule IA	Molecule IB	Molecule IC	[a]M06-2X/ 6-31++G(d.p)	[b]M06-2X/ 6-311++G(d.p)
C21-O1-C3	117.5(3)	117.1(2)	117.7(3)	117,0	117,1
C2-C-C10	114.0(2)	113.7(2)	113.7(2)	113,6	113,6
C3-C2-C1	110.9(3)	110.7(2)	111.8(3)	110,8	110,8
O1-C3-C4	111.2(2)	106.6(2)	110.7(2)	107,1	107,1
O1-C3-C2	106.3(3)	109.8(2)	106.0(3)	110,6	110,6
C4-C3-C2	111.9(3)	112.9(2)	112.8(3)	111,5	111,6
C3-C4-C5	110.4(2)	111.1(2)	110.5(2)	110,3	110,2
C6-C5-C4	113.0(2)	111.8(2)	112.4(2)	112,1	112,1
C6-C5-C10	113.6(2)	112.2(2)	113.1(2)	112,3	112,3
C4-C5-C10	113.2(2)	112.9(2)	113.0(2)	113,0	113,0
C5-C6-C7	111.9(2)	111.6(3)	111.8(2)	112,1	110,8
C6-C7-C8	111.5(2)	111.9(2)	111.0(2)	112,1	112,0
C14-C8-C7	112.5(2)	112.3(2)	112.3(2)	111,8	111,7
C14-C8-C9	107.5(2)	108.6(2)	107.9(2)	107,4	107,3
C7-C8-C9	111.3(2)	110.0(2)	111.5(2)	110,0	111,0
C11-C9-C8	112.3(2)	113.6(2)	111.9(2)	113,0	113,0
C11-C9-C10	113.8(2)	114.0(2)	114.0(2)	113,7	113,7
C8-C9-C10	112.4(2)	111.3(2)	112.4(2)	112,1	112,0
C20-C10-C1	109.5(2)	109.2(2)	109.6(2)	109,1	109,1
C20-C10-C5	111.7(2)	112.1(2)	112.0(2)	111,8	111,9
C1-C10-C5	106.8(2)	106.6(2)	106.2(2)	107,6	107,6
C20-C10-C9	110.7(2)	110.8(2)	110.5(2)	111,0	111,0
C1-C10-C9	110.1(2)	110.7(2)	110.3(2)	110,2	110,1
C5-C10-C9	107.9(2)	107.4(2)	108.0(2)	107,1	107,1
C12-C11-C9	115.1(2)	114.9(2)	115.1(2)	114,5	114,4
C13-C12-C11	109.9(2)	109.7(2)	109.7(2)	109,8	109,8
C17-C13-C12	118.2(2)	118.7(2)	118.6(2)	118,7	118,6
C17-C13-C19	106.4(2)	106.2(2)	106.2(2)	106,2	106,2
C12-C13-C19	111.5(2)	111.7(3)	111.1(2)	110,8	111,0
C17-C13-C14	98.7(2)	98.5(2)	98.6(2)	98,8	98,7
C12-C13-C14	107.5(2)	107.6(2)	107.8(2)	108,2	108,2
C19-C13-C14	114.2(2)	113.6(3)	114.3(3)	113,8	113,8
C8-C14-C15	123.2(2)	122.0(2)	122.6(2)	122,2	122,3
C8-C14-C13	112.2(2)	112.4(2)	112.2(2)	112,2	112,1
C15-C14-C13	104.7(2)	104.0(2)	104.4(2)	104,5	104,5
C16-C15-C14	100.9(2)	100.8(2)	100.8(3)	100,8	100,8
C17-C16-C18	125.2(3)	126.2(3)	125.0(4)	126,5	126,5
C17-C16-C15	109.7(2)	110.0(2)	110.3(3)	109,9	109,9
C18-C16-C15	125.1(3)	123.8(2)	124.7(4)	126,6	123,6
O3-C18-C16	124.8(4)	124.6(2)	123.5(5)	122,6	122,7
O3-C18-H	121.0(2)	121.8(18)	124.0(3)	121,0	121,1
C16-C18-H	114.0(2)	113.7(18)	112.0(3)	116,4	116,2
C16-C17-C13	112.9(2)	112.6(2)	111.9(3)	112,2	112,3
C16-C17-Cl	126.3(2)	126.9(2)	126.4(2)	126,6	126,6
C13-C17-Cl	120.6(2)	120.1(2)	121.3(3)	120,9	120,8
O2-C21-O1	123.7(3)	122.8(2)	123.9(3)	123,6	123,7
O2-C21-C22	125.4(4)	124.9(3)	124.9(4)	125,2	125,3
O1-C21-C22	110.9(4)	112.3(3)	111.2(4)	111,2	111,0
$MD = \sum \left\| x_{exp} - x^{a}{}_{theor} \right\| / N$	**0.69**	**0.55**	**0.79**		

$MD = \sum \left\| x_{exp} - x^{b}_{theor} \right\| / N$	**0.66**	**0.52**	**0.77**

* The structure parameters are in accordance with the atom numbering scheme given in Figure

In *MD* (mean deviation) expression: x = angles and N= 48.

[a]M06-2X/6-31++G(d,p)

[b]M06-2X/6-311++G(d,p)

Table S4. Experimental X-ray and theoretical torsion angles (°) of compound **I**

Parameters*	Experimental			Calculated	
	Molecule IA	Molecule IB	Molecule IC	[a]M06-2X/ 6-31++G(d.p)	[b]M06-2X/ 6-311++G(d.p)
C10-C1-C2-C3	55.1(4)	56,2(3)	54.4(4)	55.4	55.1
C21-O1-C3-C4	81.9(3)	160.1(2)	77.3(3)	157.5	157.2
C21-O1-C3-C2	-156.1(3)	-77.3(3)	-160(3)	-80.8	-80.9
C1-C2-C3-O1	-175.7(2)	-171.6(2)	-173(2)	-174.5	-174.7
C1-C2-C3-C4	-54.2(4)	-52.8(3)	-51.8(4)	-55.4	-55.5
O1-C3-C4-C5	174.3(2)	173.7(2)	172(2)	177.7	177.9
C2-C3-C4-C5	55.7(3)	53(3)	53.4(4)	56.5	56.7
C3-C4-C5-C6	171.1(3)	176.6(3)	172.7(3)	174.2	174.3
C3-C4-C5-C10	-58.0(3)	-55.9(3)	-57.8(3)	-57.6	-57.6
C4-C5-C6-C7	-172.8(2)	-175.9(3)	-173.2(3)	-173.3	-173.3
C10-C5-C6-C7	56.5(3)	56.1(4)	57.3(3)	63.4	58.3
C5-C6-C7-C8	-54.5(3)	-53.8(4)	-55.9(4)	-54.5	-54.6
C6-C7-C8-C14	174.5(2)	175.7(3)	176(2)	173.3	173.3
C6-C7-C8-C9	53.8(3)	54.6(4)	54.7(3)	53.4	53.6
C14-C8-C9-C11	51.3(3)	47.9(3)	51.3(3)	51.6	51.7
C7-C8-C9-C11	174.9(2)	171.2(2)	175.1(2)	174.3	174.3
C14-C8-C9-C10	-178.8(2)	-178.2(2)	-179(2)	-178,4	-178,3
C7-C8-C9-C10	-55.2(3)	-58.5(3)	-55.2(3)	-55,9	-56,0
C2-C1-C10-C20	66.8(3)	64.6(3)	65.7(4)	67,6	67,6
C2-C1-C10-C5	-54.4(3)	-56.7(3)	-55.5(3)	-53,9	-54,0
C2-C1-C10-C9	-171.3(3)	-173.2(2)	-172.3(3)	-170,3	-170,4
C6-C5-C10-C20	66.7(3)	64(3)	67(3)	63,4	63,3
C4-C5-C10-C20	-64(3)	-63.3(3)	-62.2(3)	-64,7	-64,7
C6-C5-C10-C1	-173.6(2)	-176.5(3)	-173.4(2)	-176,9	-176,9
C4-C5-C10-C1	55.8(3)	56.1(3)	57.5(3)	55,0	55,1
C6-C5-C10-C9	-55.2(3)	-57.9(3)	-55(3)	-58,5	-58,6
C4-C5-C10-C9	174.1(19)	174.8(2)	175.9(2)	173,4	173,4
C11-C9-C10-C20	60.7(3)	66.5(3)	59.3(3)	64,4	64,3
C8-C9-C10-C20	-68.4(3)	-63.6(3)	-69.3(3)	-65,3	-65,3
C11-C9-C10-C1	-60.6(3)	-54.7(3)	-62.2(3)	-56,5	-56,6
C8-C9-C10-C1	170.3(2)	175.1(2)	169.2(2)	173,8	173,8
C11-C9-C10-C5	-176.8(3)	-170.7(2)	-177.9(2)	-173,3	-173,3
C8-C9-C10-C5	54.1(3)	59.1(3)	53.5(3)	57,1	57,1
C8-C9-C11-C12	-48.3(3)	-45.5(4)	-49.2(3)	-48,9	-48,9
C10-C9-C11-C12	-177.4(2)	-174.5(2)	-178(2)	-178,0	-178,0
C9-C11-C12-C13	51.2(3)	50.8(3)	52.2(3)	51,2	51,2
C11-C12-C13-C17	-167.7(2)	-169.3(3)	-168.3(3)	-168,6	-168,5
C11-C12-C13-C19	68.6(3)	66.7(3)	68.3(3)	68,2	68,2
C11-C12-C13-C14	-57.3(3)	-58.7(3)	-57.6(3)	-57,3	-57,3
C7-C8-C14-C15	48.7(3)	54.2(3)	50(4)	51,6	51,7
C9-C8-C14-C15	171.6(2)	176.1(2)	173.2(3)	173,6	173,7
C7-C8-C14-C13	175.1(2)	178.6(2)	175.4(2)	176,9	176,8
C9-C8-C14-C13	-61.9(3)	-59.5(3)	-61.3(3)	-61,1	-61,3
C17-C13-C14-C8	-170.4(19)	-169.7(2)	-170.6(2)	170,2	170,1
C12-C13-C14-C8	66.3(3)	66.4(3)	65.5(3)	65,7	65,8
C19-C13-C14-C8	-58(3)	-57.8(3)	-58.5(3)	-58,0	-58,1
C17-C13-C14-C15	-34.4(2)	-35.9(2)	-35.7(3)	-35,7	-35,7
C12-C13-C14-C15	-157.8(2)	-159.7(2)	-159.6(2)	-159,8	-159,7

C19-C13-C14-C15	78.0(3)	76(3)	76.4(3)	76,5	76,4
C8-C14-C15-C16	164.0(2)	162.7(2)	163.1(3)	162,7	162,6
C13-C14-C15-C16	34.3(3)	34.5(3)	34.3(3)	34,1	34,1
C14-C15-C16-C17	-20.7(3)	-19.3(3)	-19.2(4)	-19,0	-19,0
C14-C15-C16-C18	157.7(3)	162.3(3)	160.2(3)	162,6	162,6
C17-C16-C18-O3	178.6(3)	175.5(3)	178.7(4)	176,7	176,8
C15-C16-C18-O3	0.4(5)	2.6(5)	-0.5(7)	1,5	1,4
C18-C16-C17-C13	180.0(3)	174.2(3)	176.6(3)	174,2	174,2
C15-C16-C17-C13	-1.6(3)	-4.1(4)	-4.1(4)	-4,2	-4,2
C18-C16-C17-Cl	5.8(3)	1.0(5)	3.9(5)	0,2	0,3
C15-C16-C17-Cl	-175.8(2)	-177.3(2)	-176.7(2)	-178,1	-178,1
C12-C13-C17-C16	138.1(3)	141.1(3)	140.9(3)	141,5	141,5
C19-C13-C17-C16	-95.7(3)	-92.2(3)	-93.3(3)	-92,9	-92,9
C14-C13-C17-C16	22.8(3)	25.6(3)	25.1(3)	25,2	25,2
C12-C13-C17-Cl	-47.4(3)	-45.2(3)	-46(4) (3)	-44,1	-44,2
C19-C13-C17-Cl	78.8(3)	81.5(3)	79.8(3)	81,4	81,4
C14-C13-C17-Cl	-162.69(19)	-160.8(2)	-161.8(2)	-160,5	-160,6
C3-O1-C21-O2	-0.7(3)	-3.6(4)	1.9(5)	0,0	0,0
C3-O1-C21-C22	178.8(3)	175.5(2)	179.4(3)	179,9	179,7
$MD = \sum \left\| x_{exp} - x^{a}{}_{theor} \right\| / N$	**4.01**	**1.66**	**4.05**		
$MD = \sum \left\| x_{exp} - x^{b}{}_{theor} \right\| / N$	**3.93**	**1.59**	**3.96**		

* The structure parameters are in accordance with the atom numbering scheme given in Figure

In *MD* (mean deviation) expression: x = torsion angles and N= 67.

[a]M06-2X/6-31++G(d,p)

[b]M06-2X/6-311++G(d,p)

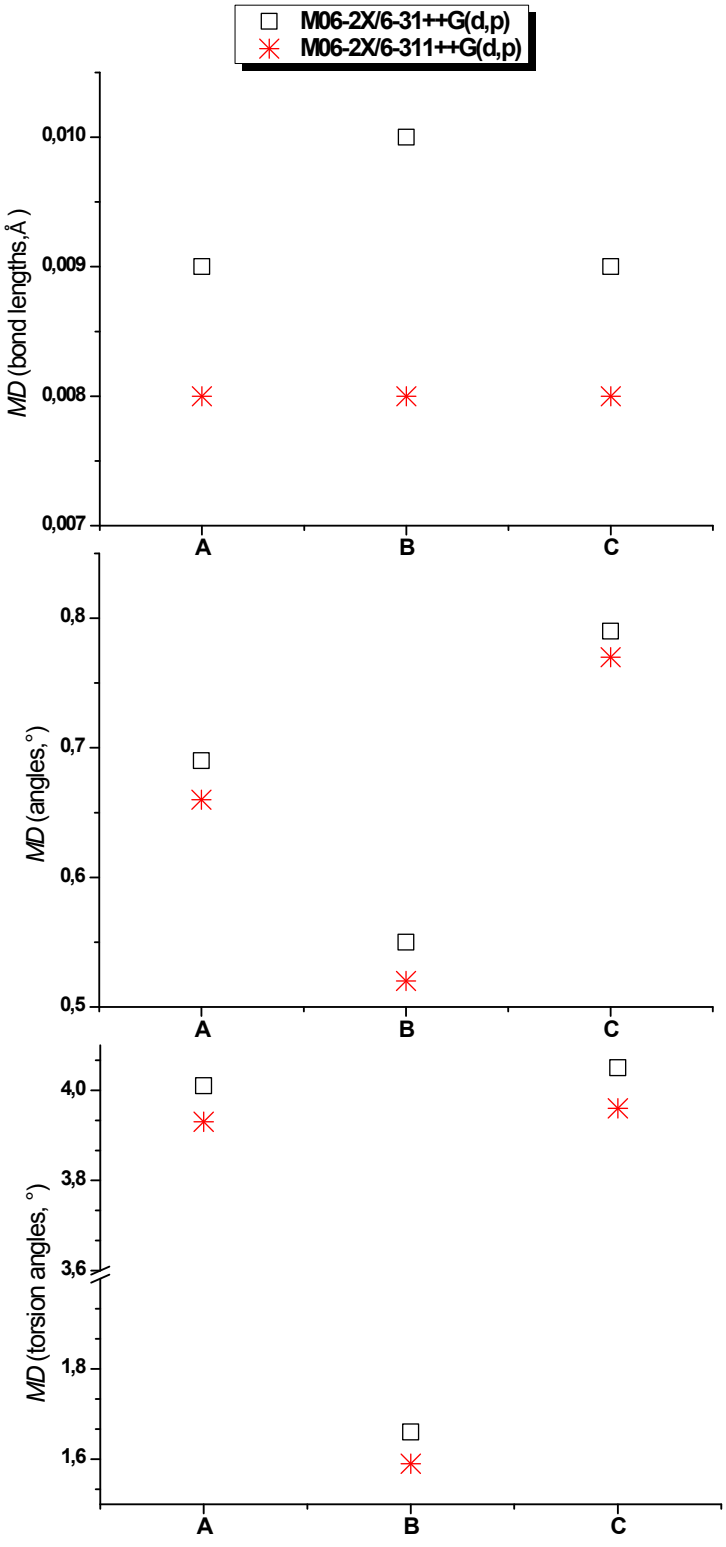

Figure S1. Mean deviations (*MD*) values of bond lengths, bond angles and torsion angles

Table S5. Relationship of C17-C16-C18-H torsion angle with C18-H distance (d_{C18-H}) and stretching vibrational frequencies of C18-H (ν_{C18-H}).

Torsion angle C17-C16-C18-H (°)	**d_{C18-H} (Å)**	**ν_{C-H} (cm^{-1})**
0	1.1058	2790.37
90	1.1092	2731.15
180	1.1102	2727.56

*Scale factor = 0.94 for M06-2X/6-31+G(d,p) level of theory taken from: M. Alecu, J. Zheng, Y. Zhao and D. G. Truhlar. Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. *J. Chem. Theory Comput.,* **2010***, 6,*. 2872-2887.

Table S6. Relative contributions to the Hirshfeld surface area for the intermolecular contacts of the three molecules in title compound **I**.

Interactions	% Hirshfeld surface area		
	Molecule IA	Molecule IB	Molecule IC
H···H	64.1	66.1	66.3
H···Cl	9.2	8.5	8.6
H···O	19.8	17.9	19.5
H···C	3.6	3.8	3.4

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_symmetry_equiv_pos_as_xyz
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3 1/2+x,1/2-y,-z
4 -x,1/2+y,1/2-z
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H2B H 0.4744 0.1507 0.2565
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H4B H 0.9488 0.1386 0.2369
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H7B H 0.9131 0.1287 0.1216
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#END