

Table S1: The geometrical parameters of estrogens in gas phase, active site and the QM/MM minimized structure calculated at B3LYP/6-311G** level of theory.

Bonds	Estrone			Bonds	17 β -estradiol			Bonds	Estriol		
	GP	Docking	QM/MM		GP	Docking	QM/MM		GP	Docking	QM/MM
C(2)–C(1)	1.387	1.387	1.388	C(2)–C(1)	1.387	1.387	1.387	C(2)–C(1)	1.387	1.386	1.379
C(3)–C(2)	1.403	1.402	1.399	C(1)–C(6)	1.394	1.393	1.397	C(3)–C(2)	1.403	1.403	1.403
C(3)–C(4)	1.406	1.407	1.403	C(3)–C(2)	1.403	1.402	1.4	C(3)–C(4)	1.406	1.405	1.398
C(4)–C(5)	1.399	1.398	1.395	C(3)–C(4)	1.406	1.407	1.396	C(4)–C(5)	1.399	1.399	1.395
C(5)–C(6)	1.390	1.391	1.4	C(4)–C(5)	1.399	1.399	1.387	C(5)–C(6)	1.390	1.39	1.394
C(1)–C(6)	1.394	1.394	1.404	C(5)–C(6)	1.390	1.391	1.401	C(1)–C(6)	1.394	1.395	1.405
C(7)–C(3)	1.530	1.53	1.507	C(7)–C(3)	1.530	1.529	1.505	C(7)–C(3)	1.530	1.529	1.5
C(8)–C(7)	1.552	1.549	1.547	C(8)–C(7)	1.551	1.552	1.546	C(8)–C(7)	1.551	1.551	1.543
C(8)–C(9)	1.530	1.531	1.519	C(7)–C(11)	1.546	1.546	1.534	C(8)–C(9)	1.531	1.531	1.519
C(9)–C(10)	1.529	1.529	1.515	C(8)–C(9)	1.531	1.529	1.518	C(9)–C(10)	1.529	1.529	1.517
C(10)–C(4)	1.518	1.518	1.496	C(9)–C(10)	1.529	1.528	1.515	C(10)–C(4)	1.518	1.517	1.495
C(7)–C(11)	1.547	1.547	1.534	C(10)–C(4)	1.518	1.518	1.494	C(7)–C(11)	1.546	1.547	1.531
C(12)–C(11)	1.543	1.542	1.534	C(12)–C(11)	1.542	1.541	1.531	C(12)–C(11)	1.543	1.541	1.525
C(13)–C(12)	1.530	1.535	1.531	C(13)–C(12)	1.535	1.537	1.532	C(13)–C(12)	1.535	1.535	1.528
C(13)–C(18)	1.551	1.545	1.53	C(13)–C(14)	1.549	1.549	1.549	C(13)–C(14)	1.551	1.551	1.548
C(14)–C(13)	1.548	1.549	1.551	C(13)–C(15)	1.541	1.54	1.559	C(13)–C(18)	1.543	1.542	1.53
C(14)–C(8)	1.528	1.53	1.521	C(13)–C(18)	1.543	1.543	1.53	C(14)–C(8)	1.527	1.527	1.521
C(14)–C(17)	1.541	1.541	1.529	C(14)–C(8)	1.528	1.529	1.52	C(13)–C(15)	1.546	1.547	1.548
C(13)–C(15)	1.531	1.539	1.561	C(14)–C(17)	1.542	1.541	1.527	C(15)–C(16)	1.541	1.54	1.567
C(15)–C(16)	1.540	1.554	1.556	C(15)–C(16)	1.554	1.555	1.553	C(17)–C(16)	1.548	1.548	1.551
C(17)–C(16)	1.546	1.558	1.531	C(17)–C(16)	1.557	1.558	1.533	C(14)–C(17)	1.543	1.544	1.525
O(1)–C(6)	1.367	1.369	1.365	O(1)–C(6)	1.368	1.368	1.364	O(1)–C(6)	1.367	1.368	1.362
O(2)–C(15)	1.205	1.212	1.225	O(2)–C(15)	1.424	1.425	1.401	O(2)–C(15)	1.425	1.426	1.403
								O(3)–C(16)	1.426	1.426	1.409

Bond angles (°)

O(1)–C(6)–C(5)	122.9	122.8	123.1	O(1)–C(6)–C(1)	117.8	117.7	117.2	O(1)–C(6)–C(5)	122.9	122.9	121.1
O(1)–C(6)–C(1)	117.7	117.8	117.1	O(1)–C(6)–C(5)	122.9	122.8	122.9	O(1)–C(6)–C(1)	117.8	117.7	117.9
O(2)–C(15)–C(13)	126.5	111.4	112.8	O(2)–C(15)–C(13)	111.3	111.4	111.6	O(2)–C(15)–C(13)	117.3	117.3	117.3
O(2)–C(15)–C(16)	125.5	114.3	112.2	O(2)–C(15)–C(16)	114.3	114.3	112.3	O(2)–C(15)–C(16)	109.1	109.1	112.4
								O(3)–C(16)–C(15)	112.8	112.8	114.6
								O(3)–C(16)–C(17)	109.9	109.9	111.1
Torsion angles (°)											
C(2)–C(1)–C(6)–O(1)	-179.9	-179.9	-179.4	C(4)–C(5)–C(6)–O(1)	179.9	179.9	179.4	C(2)–C(1)–C(6)–O(1)	-179.8	179.9	179.5
C(4)–C(5)–C(6)–O(1)	179.9	179.9	179.9	C(2)–C(1)–C(6)–O(1)	-179.9	-179.8	-179.8	C(4)–C(5)–C(6)–O(1)	179.8	179.9	179.4
C(12)–C(13)–C(15)–O(2)	33.3	78	82.3	C(14)–C(13)–C(15)–O(2)	-166.0	-166	-161.3	C(12)–C(13)–C(15)–O(2)	79.5	79.5	76.2
C(14)–C(13)–C(15)–O(2)	151.6	-166	163.2	C(12)–C(13)–C(15)–O(2)	78.1	78.1	83.7	C(14)–C(13)–C(15)–O(2)	-165.1	-165.1	-167.9
O(2)–C(15)–C(16)–C(17)	-175.4	145.1	-145.2	C(18)–C(13)–C(15)–O(2)	-46.8	-46.8	-41.5	O(2)–C(15)–C(16)–C(17)	153.3	153.3	-153.5
C(18)–C(13)–C(15)–O(2)	-89.6	-46.9	-43.4	O(2)–C(15)–C(16)–C(17)	145.1	145.2	141.4	C(18)–C(13)–C(15)–O(2)	-45.8	-45.8	-48.1
								C(13)–C(15)–C(16)–O(3)	147.1	147.2	149.3
								C(14)–C(17)–C(16)–O(3)	-120.2	-120.2	-122.7
								O(2)–C(15)–C(16)–O(3)	-86.5	-86.5	-83.7

Table S2: The topological properties of electron density of estrogens. First line: QM/MM minimized structure, Second line: Experimental, Third line: Gas phase.

Bonds	Estrone		Bonds	17 β -Estradiol		Bonds	Estriol	
	$\rho_{bcp}(r)$	$\nabla^2\rho_{bcp}(r)$		$\rho_{bcp}(r)$	$\nabla^2\rho_{bcp}(r)$		$\rho_{bcp}(r)$	$\nabla^2\rho_{bcp}(r)$
C(1)–C(2)	2.097	-20.9	C(1)–C(2)	2.097	-20.8	C(1)–C(2)	2.13	-21.5
EXP	2.146	-17.7	EXP	2.165	-19.1	EXP A	2.125	-18.7
GP	2.101	-20.9	GP	2.1	-20.9	B	2.165	-20.3
C(2)–C(3)	2.064	-20.1	C(2)–C(3)	2.073	-20.3	GP	2.1	-20.9
	2.053	-17.0		2.134	-19.0	C(2)–C(3)	2.048	-19.8
	2.048	-19.8		2.049	-19.8		2.065	-17.7
C(3)–C(4)	2.047	-19.6	C(3)–C(4)	2.056	-19.8		2.107	-18.3
	2.101	-18.7		2.092	-17.2		2.048	-19.8
	2.039	-19.4		2.039	-19.4	C(3)–C(4)	2.062	-19.9
C(4)–C(5)	2.078	-20.4	C(4)–C(5)	2.075	-20.3		2.122	-18.5
	2.146	-18.7		2.086	-16.7		2.101	-17.8
	2.057	-20.0		2.057	-20.0		2.039	-19.4
C(5)–C(6)	2.085	-20.8	C(5)–C(6)	2.08	-20.6	C(4)–C(5)	2.077	-20.4
	2.13	-19.1		2.21	-18.7		2.145	-19.2
	2.111	-21.2		2.111	-21.2		2.072	-18.0
C(1)–C(6)	2.056	-20.2	C(1)–C(6)	2.057	-20.1		2.058	-20.0
	2.152	-19.3		2.195	-18.7	C(5)–C(6)	2.107	-21.2
	2.108	-21.4		2.108	-21.4		2.194	-20.9
C(3)–C(7)	1.711	-14.5	C(3)–C(7)	1.717	-14.6		2.189	-20.2
	1.7	-10.6		1.621	-9.0		2.111	-21.2
	1.635	-13.1		1.634	-13.1	C(1)–C(6)	2.061	-20.3
C(7)–C(8)	1.604	-12.5	C(7)–C(8)	1.607	-12.5		2.204	-21.4
	1.598	-8.7		1.601	-8.5		2.138	-19.5
	1.585	-12.1		1.589	-12.2		2.109	-21.4
C(8)–C(9)	1.68	-13.8	C(8)–C(9)	1.681	-13.9	C(3)–C(7)	1.736	-14.9
	1.684	-10.4		1.625	-9.0		1.661	-10.5
	1.639	-13.1		1.638	-13.1		1.671	-10.9
C(9)–C(10)	1.684	-14.0	C(9)–C(10)	1.684	-14.0		1.635	-13.1
	1.672	-10.0		1.643	-9.2	C(7)–C(8)	1.615	-12.7
	1.635	-13.2		1.635	-13.2		1.554	-8.5
C(4)–C(10)	1.749	-15.3	C(4)–C(10)	1.754	-15.4		1.565	-8.7
	1.681	-11.1		1.711	-10.6		1.588	-12.2
	1.674	-13.9		1.674	-13.9	C(8)–C(9)	1.679	-13.8
C(7)–C(11)	1.629	-13.0	C(7)–C(11)	1.628	-12.9		1.619	-9.5
	1.652	-9.9		1.612	-8.8		1.659	-10.9
	1.586	-12.2		1.59	-12.3		1.638	-13.1
C(11)–C(12)	1.62	-12.9	C(11)–C(12)	1.63	-13.0	C(9)–C(10)	1.674	-13.9
	1.607	-9.1		1.586	-9.1		1.634	-10.3
	1.59	-12.4		1.593	-12.4		1.631	-10.7
C(12)–C(13)	1.644	-13.2	C(12)–C(13)	1.643	-13.1		1.635	-13.2
	1.657	-10.2		1.672	-10.4	C(4)–C(10)	1.746	-15.2

	1.639	-13.1		1.632	-13.0		1.699	-11.4
C(13)–C(14)	1.6	-12.2	C(13)–C(14)	1.607	-12.4		1.676	-10.5
	1.606	-9.1		1.597	-8.5		1.675	-13.9
	1.606	-12.3		1.605	-12.3	C(7)–C(11)	1.639	-13.1
C(14)–C(8)	1.678	-13.7	C(14)–C(8)	1.682	-13.8		1.534	-8.7
	1.691	-11.1		1.616	-9.3		1.613	-9.2
	1.651	-13.3		1.651	-13.3		1.589	-12.3
C(13)–C(15)	1.59	-12.2	C(13)–C(15)	1.598	-12.3	C(11)–C(12)	1.647	-13.3
	1.759	-12.0		1.585	-8.6		1.587	-8.8
	1.691	-13.8		1.652	-13.3		1.572	-8.9
C(15)–C(16)	1.599	-12.4	C(15)–C(16)	1.607	-12.6		1.59	-12.4
	1.687	-10.5		1.638	-8.5	C(12)–C(13)	1.655	-13.3
	1.645	-13.1		1.601	-12.4		1.63	-10.6
C(16)–C(17)	1.629	-13.0	C(16)–C(17)	1.624	-12.9		1.642	-10.3
	1.56	-8.2		1.518	-7.5		1.631	-12.9
	1.583	-12.2		1.546	-11.6	C(13)–C(14)	1.611	-12.4
C(14)–C(17)	1.643	-13.1	C(14)–C(17)	1.647	-13.2		1.622	-10.1
	1.62	-9.2		1.59	-8.1		1.602	-8.9
	1.601	-12.3		1.6	-12.4		1.598	-12.2
C(13)–C(18)	1.625	-12.9	C(13)–C(18)	1.625	-12.9	C(14)–C(8)	1.676	-13.7
	1.553	-8.5		1.637	-9.7		1.727	-11.6
	1.546	-11.5		1.585	-12.2		1.706	-11.5
C(6)–O(1)	1.916	-9.3	C(6)–O(1)	1.922	-9.3		1.652	-13.3
	2.036	-15.9		2.065	-17.9	C(13)–C(15)	1.62	-12.6
	1.908	-9.0		1.904	-9.0		1.685	-11.7
C(15)–O(2)	2.771	1.1	C(15)–O(2)	1.804	-12.0		1.65	-10.5
	2.856	-17.6		1.654	-5.2		1.631	-12.8
	2.781	0.3		1.707	-11.6	C(15)–C(16)	1.597	-12.4
C(1)–H(1)	1.843	-21.9	C(1)–H(1)	1.838	-21.8		1.655	-10.7
	1.843	-16.8		1.895	-18.2		1.69	-11.3
	1.897	-23.2		1.896	-23.1		1.685	-14.0
C(2)–H(2)	1.822	-21.4	C(2)–H(2)	1.821	-21.2	C(16)–C(17)	1.613	-12.8
	1.916	-18.6		1.87	-18.4		1.565	-9.3
	1.911	-23.5		1.911	-23.5		1.596	-9.6
C(5)–H(5)	1.809	-21.1	C(5)–H(5)	1.807	-21.0		1.617	-12.9
	1.867	-17.7		1.771	-15.6	C(14)–C(17)	1.657	-13.3
	1.862	-22.3		1.861	-22.2		1.595	-8.6
C(7)–H(7)	1.719	-18.7	C(7)–H(7)	1.719	-18.7		1.557	-8.6
	1.772	-14.9		1.832	-16.4		1.598	-12.3
	1.835	-21.4		1.833	-21.3	C(13)–C(18)	1.626	-12.9
C(8)–H(8)	1.756	-19.6	C(8)–H(8)	1.754	-19.6		1.591	-10.4
	1.783	-15.2		1.773	-15.8		1.605	-10.5
	1.848	-21.7		1.849	-21.7		1.588	-12.2
C(9)–H(9A)	1.774	-20.0	C(9)–H(9A)	1.774	-20.0	C(6)–O(1)	1.955	-10.8
	1.819	-14.7		1.935	-17.6		2.033	-20.3
	1.858	-22.0		1.858	-22.0		2.033	-19.9

C(9)–H(9B)	1.795	-20.5	C(9)–H(9B)	1.799	-20.6		2.485	-60.7
	1.77	-14.4		1.833	-15.9	C(15)–O(2)	1.764	-9.9
	1.844	-21.7		1.843	-21.6		1.849	-13.9
C(10)–H(10A)	1.759	-19.7	C(10)–H(10A)	1.763	-19.8		1.774	-12.6
	1.841	-17.1		1.876	-15.3		1.693	-11.0
	1.854	-21.9		1.852	-21.9	C(16)–O(3)	1.745	-10.1
C(10)–H(10B)	1.79	-20.4	C(10)–H(10B)	1.787	-20.4		1.73	-10.0
	1.847	-16.8		1.681	-11.6		1.632	-8.1
	1.836	-21.5		1.836	-21.5		1.714	-12.2
C(11)–H(11A)	1.8	-20.6	C(11)–H(11A)	1.799	-20.6	C(1)–H(1)	1.788	-20.7
	1.808	-15.9		1.805	-16.0		1.896	-17.2
	1.855	-21.9		1.856	-21.9		1.851	-16.6
C(11)–H(11B)	1.797	-20.6	C(11)–H(11B)	1.791	-20.4		1.896	-23.1
	1.819	-16.7		1.876	-17.0	C(2)–H(2)	1.809	-20.9
	1.866	-22.1		1.863	-22.1		1.845	-16.4
C(12)–H(12A)	1.779	-20.1	C(12)–H(12A)	1.777	-20.1		1.871	-16.3
	1.844	-15.4		1.803	-15.2		1.91	-23.4
	1.851	-21.8		1.839	-21.5	C(5)–H(5)	1.834	-21.5
C(12)–H(12B)	1.793	-20.5	C(12)–H(12B)	1.793	-20.5		1.908	-17.2
	1.815	-14.9		1.83	-15.9		1.834	-15.7
	1.863	-22.1		1.858	-22.0		1.862	-22.2
C(14)–H(14)	1.754	-19.5	C(14)–H(14)	1.747	-19.4	C(7)–H(7)	1.748	-19.4
	1.81	-15.9		1.857	-16.9		1.762	-14.8
	1.838	-21.4		1.838	-21.4		1.787	-15.6
C(16)–H(16A)	1.8	-20.6	C(15)–H(15)	1.786	-20.2		1.835	-21.3
	1.774	-13.7		2.007	-20.7	C(8)–H(8)	1.778	-20.2
	1.846	-21.8		1.884	-22.6		1.839	-16.5
C(16)–H(16B)	1.781	-20.2	C(16)–H(16A)	1.803	-20.7		1.766	-15.8
	1.779	-13.7		1.889	-16.8		1.847	-21.6
	1.839	-21.6		1.854	-21.9	C(9)–H(9A)	1.786	-20.3
C(17)–H(17A)	1.786	-20.2	C(16)–H(16B)	1.801	-20.7		1.836	-16.9
	1.769	-14.1		1.764	-14.7		1.837	-15.6
	1.868	-22.2		1.862	-22.0		1.86	-22.0
C(17)–H(17B)	1.779	-20.2	C(17)–H(17A)	1.788	-20.3	C(9)–H(9B)	1.778	-20.1
	1.789	-14.8		1.857	-15.6		1.837	-17.0
	1.858	-22.0		1.865	-22.2		1.78	-14.1
C(18)–H(18A)	1.804	-20.7	C(17)–H(17B)	1.779	-20.2		1.844	-21.7
	1.817	-14.8		1.722	-13.1	C(10)–H(10A)	1.746	-19.3
	1.855	-21.9		1.857	-21.9		1.7	-12.1
C(18)–H(18B)	1.822	-21.2	C(18)–H(18A)	1.803	-20.6		1.829	-15.5
	1.792	-14.7		1.886	-15.1		1.853	-21.9
	1.851	-21.8		1.865	-22.2	C(10)–H(10B)	1.774	-20.0
C(18)–H(18C)	1.791	-20.4	C(18)–H(18B)	1.786	-20.3		1.824	-14.0
	1.791	-13.8		1.924	-15.3		1.771	-14.9
	1.859	-22.0		1.856	-21.9		1.836	-21.5
O(1)–H(6)	2.35	-60.5	C(18)–H(18C)	1.818	-21.1	C(11)–H(11A)	1.775	-19.9

2.656	-48.4		1.805	-13.8		1.805	-15.4
2.485	-60.7		1.849	-21.8		1.669	-11.8
		O(1)–H(6)	2.344	-60.4		1.857	-21.9
			2.595	-51.8	C(11)–H(11B)	1.787	-20.3
			2.486	-60.7		1.744	-14.1
		O(2)–H(3)	2.522	-64.4		1.789	-13.8
			2.797	-59.9		1.864	-22.1
			2.493	-59.6	C(12)–H(12A)	1.803	-20.8
						1.791	-13.6
						1.795	-13.4
						1.839	-21.5
					C(12)–H(12B)	1.805	-20.8
						1.788	-13.3
						1.671	-11.1
						1.841	-21.6
					C(14)–H(14)	1.731	-19.0
						1.849	-17.0
						1.816	-16.3
						1.846	-21.5
					C(16)–H(16)	1.843	-21.7
						1.894	-21.5
						1.933	-22.9
						1.902	-23.0
					C(17)–H(17A)	1.796	-20.5
						1.851	-19.9
						1.854	-20.0
						1.872	-22.3
					C(17)–H(17B)	1.784	-20.2
						1.845	-19.2
						1.86	-20.5
						1.855	-21.9
					C(18)–H(18A)	1.783	-20.1
						1.903	-21.2
						1.913	-21.8
						1.856	-21.9
					C(18)–H(18B)	1.813	-20.9
						1.912	-21.4
						1.939	-22.6
						1.851	-21.8
					C(18)–H(18C)	1.825	-21.2
						1.891	-21.0
						1.901	-20.7
						1.858	-22.0
					O(1)–H(6)	2.353	-59.1
						2.099	-31.2
						2.033	-34.2

	2.485	-60.7
O(2)–H(4)	2.479	-61.4
	2.284	-37.7
	2.326	-39.1
	2.491	-59.7
O(3)–H(3)	2.545	-63.0
	2.187	-32.2
	2.396	-43.5
	2.484	-59.5

Table S3: Atomic charges and Volumes of estrogens for QM/MM minimized and gas phase molecule.

Atoms	17 β -Estradiol						Atoms	Estriol						Atoms	Estrone					
	Gas Phase			QM/MM				Gas Phase			QM/MM				Gas Phase			QM/MM		
	MPA	AIM	V	MPA	AIM	V		MPA	AIM	V	MPA	AIM	V		MPA	AIM	V	MPA	AIM	V
O(1)	-0.366	-1.07	17.09	-0.466	-1.19	17.19	O(1)	-0.366	-1.07	17.09	-0.386	-1.15	17.21	O(1)	-0.365	-1.07	19.41	-0.469	-1.18	17.04
O(2)	-0.409	-1.06	16.79	-0.422	-0.96	16.98	O(2)	-0.413	-1.06	16.86	-0.426	-1.12	16.95	O(2)	-0.297	-1.11	17.08	-0.263	-0.88	16.84
C(1)	-0.085	-0.01	12.35	-0.168	-0.06	12.68	O(3)	-0.409	-1.05	16.97	-0.392	-1.07	16.27	C(1)	-0.084	-0.01	12.33	-0.152	-0.03	12.03
C(2)	-0.068	-0.01	11.96	-0.094	-0.03	12.15	C(1)	-0.085	-0.01	12.35	-0.154	0.02	12.68	C(2)	-0.068	-0.01	11.96	-0.068	-0.03	12.33
C(3)	-0.016	-0.02	10.45	-0.018	-0.02	10.96	C(2)	-0.068	-0.01	11.97	-0.117	-0.02	12.01	C(3)	-0.018	-0.03	10.46	-0.024	-0.02	10.62
C(4)	-0.076	-0.01	10.26	-0.064	-0.02	10.49	C(3)	-0.018	-0.02	10.45	0.011	-0.01	10.96	C(4)	-0.076	-0.01	10.25	-0.111	-0.01	10.43
C(5)	-0.113	-0.03	12.26	-0.105	-0.02	13.62	C(4)	-0.076	-0.01	10.24	-0.099	0.01	10.49	C(5)	-0.113	-0.03	12.26	-0.082	-0.03	12.38
C(6)	0.164	0.49	9.02	0.183	0.5	9.12	C(5)	-0.113	-0.03	12.25	-0.119	-0.02	13.62	C(6)	0.165	0.49	9.01	0.186	0.5	9.13
C(7)	-0.158	0.05	7.1	-0.178	0.03	6.89	C(6)	0.165	0.49	9.02	0.108	0.52	9.12	C(7)	-0.159	0.05	7.12	-0.168	0.03	6.94
C(8)	-0.148	0.05	6.79	-0.147	0.04	6.75	C(7)	-0.157	0.05	7.11	-0.186	0.04	6.88	C(8)	-0.15	0.05	6.85	-0.145	0.04	6.72
C(9)	-0.169	0.05	8.28	-0.203	0.03	8.34	C(8)	-0.147	0.05	6.82	-0.142	0.04	6.73	C(9)	-0.17	0.05	8.29	-0.2	0.02	8.17
C(10)	-0.175	0.05	8.57	-0.165	0.08	8.46	C(9)	-0.168	0.05	8.31	-0.218	0.03	8.46	C(10)	-0.177	0.05	8.56	-0.161	0.04	8.42
C(11)	-0.185	0.04	8.12	-0.187	0.02	8.17	C(10)	-0.175	0.05	8.58	-0.164	0.02	8.47	C(11)	-0.186	0.04	8.15	-0.184	0.04	8.9
C(12)	-0.113	0.04	7.74	-0.134	0.03	7.81	C(11)	-0.185	0	8.36	-0.189	0.02	8.08	C(12)	-0.108	0.05	8.16	-0.144	0.02	8.18
C(13)	-0.292	0.06	7.01	-0.299	0.05	6.11	C(12)	-0.124	0.03	8.27	-0.109	0.03	8.15	C(13)	-0.31	0.02	6.3	-0.282	0.04	6.49
C(14)	-0.163	0.04	6.71	-0.175	0.03	6.67	C(13)	-0.311	0.04	7.08	-0.362	0.04	6.02	C(14)	-0.155	0.04	6.76	-0.177	0.03	6.67
C(15)	0.125	0.49	6.26	0.134	0.53	6.3	C(14)	-0.18	0.04	6.75	-0.189	0.02	6.61	C(15)	0.262	0.99	6.61	0.113	0.72	6.15
C(16)	-0.211	0.02	8.86	-0.218	0.01	8.84	C(15)	0.132	0.47	6.1	0.111	0.48	6.17	C(16)	-0.222	-0.02	9.29	-0.225	-0.01	8.77
C(17)	-0.151	0.03	8.6	-0.167	0.01	8.4	C(16)	0.038	0.5	6.31	0.028	0.49	6.38	C(17)	-0.17	0.03	8.64	-0.17	0.01	8.41
C(18)	-0.215	0.01	9.43	-0.214	0	9.36	C(17)	-0.112	0.03	8.27	-0.126	0.01	8.39	C(18)	-0.229	0.01	9.65	-0.213	0.01	9.48
H(1)	0.096	0.03	7.28	0.135	0.02	7.01	C(18)	-0.206	0.01	9.47	-0.211	-0.01	9.34	H(1)	0.098	0.03	7.27	0.13	0.06	6.79
H(2)	0.084	0.01	6.88	0.104	0.01	5.92	H(1)	0.096	0.03	7.28	0.155	0.01	7.05	H(2)	0.085	0.01	6.87	0.094	0.03	7.04
H(3)	0.235	0.54	3.57	0.261	0.59	2.67	H(2)	0.083	0.01	6.89	0.094	0	5.95	H(5)	0.07	-0.01	7.54	0.079	0.02	9.26
H(5)	0.068	-0.01	7.55	0.084	-0.01	7.74	H(3)	0.238	0.54	3.61	0.245	0.55	3.15	H(6)	0.245	0.56	3.44	0.302	0.64	1.6
H(6)	0.244	0.56	3.44	0.305	0.6	2.43	H(4)	0.239	0.54	3.4	0.289	0.55	2.49	H(7)	0.123	-0.02	7.24	0.121	-0.02	5.96

