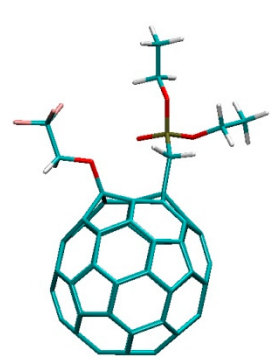
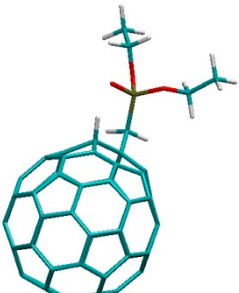
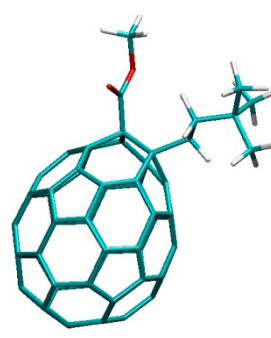



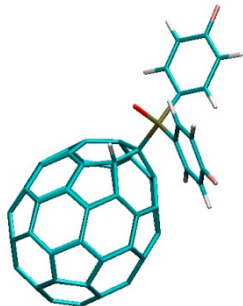
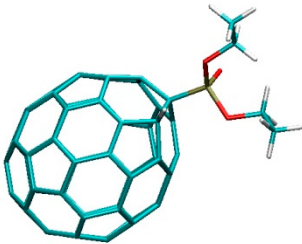
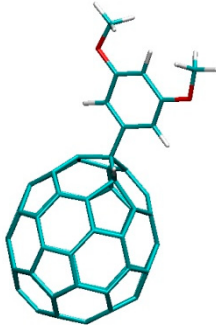
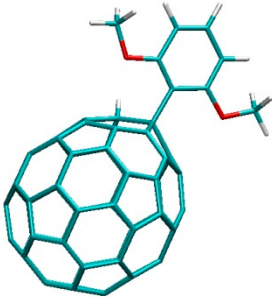

Supplementary materials

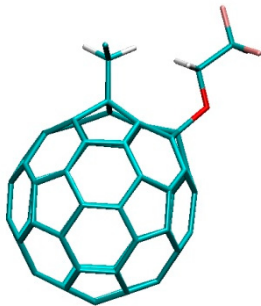
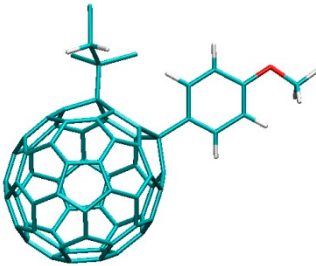
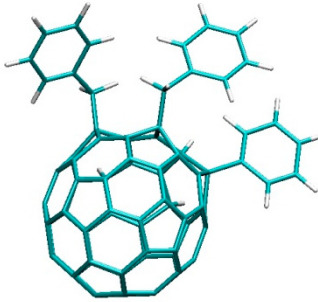
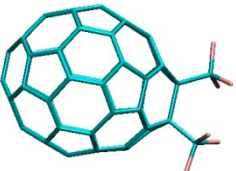
## The Immobilization of ChEMBL474807 Molecule Using Different Classes of Nanostructures

Przemysław Czeleń \* and Beata Szefler

**Table S1.** Description of functionalized C<sub>60</sub> fullerene derivatives (FF\_X) used during docking stage.

FF_1	CID_11332103	
	<u>C<sub>67</sub>H<sub>14</sub>F<sub>3</sub>O<sub>4</sub>P</u>	
	1-(diethoxyphosphorylmethyl)-7-(2,2,2-trifluoroethoxy)(C <sub>60</sub> -I <sub>h</sub> ) [5,6]fullerene	
FF_2	CID_11468612	
	<u>C<sub>65</sub>H<sub>13</sub>O<sub>3</sub>P</u>	
	9-(diethoxyphosphorylmethyl)-1 <i>H</i> -(C <sub>60</sub> -I <sub>h</sub> ) [5,6]fullerene	
FF_3	CID_16146387	
	<u>C<sub>67</sub>H<sub>16</sub>O<sub>2</sub>Si</u>	
	methyl 9-(2-trimethylsilylethyl)(C <sub>60</sub> -I <sub>h</sub> ) [5,6]fullerene-1-carboxylate	
FF_4	CID_16150529	
	<u>C<sub>70</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub></u>	

	1- <i>N</i> ,1- <i>N</i> ,9- <i>N</i> ,9- <i>N</i> -tetraethyl( $C_{60}$ - $I_h$ )[5,6]fullerene-1,9-dicarboxamide	
FF_5	CID_16156307	
	<u>C<sub>72</sub>H<sub>9</sub>F<sub>2</sub>OP</u>	
	9-bis(4-fluorophenyl)phosphoryl-1 <i>H</i> -( $C_{60}$ - $I_h$ )[5,6]fullerene	
FF_6	CID_53469305	
	<u>C<sub>64</sub>H<sub>11</sub>O<sub>3</sub>P</u>	
	9-diethoxyphosphoryl-1 <i>H</i> -( $C_{60}$ - $I_h$ )[5,6]fullerene	
FF_7	CID_71618962	
	<u>C<sub>68</sub>H<sub>10</sub>O<sub>2</sub></u>	
	9-(3,5-dimethoxyphenyl)-1 <i>H</i> -( $C_{60}$ - $I_h$ )[5,6]fullerene	
FF_8	CID_71619055	
	<u>C<sub>68</sub>H<sub>10</sub>O<sub>2</sub></u>	
	9-(2,6-dimethoxyphenyl)-1 <i>H</i> -( $C_{60}$ - $I_h$ )[5,6]fullerene	
FF_9	CID_71619159	
	<u>C<sub>68</sub>H<sub>10</sub>O<sub>2</sub></u>	

	9-(2,4-dimethoxyphenyl)-1 <i>H</i> -(C <sub>60</sub> -I <sub>h</sub> )[5,6]fullerene	
FF_10	CID_101218232	
	<u>C<sub>63</sub>H<sub>4</sub>ClF<sub>3</sub>O</u>	
	1-(chloromethyl)-7-(2,2,2-trifluoroethoxy)(C <sub>60</sub> -I <sub>h</sub> )[5,6]fullerene	
FF_11	CID_101218236	
	<u>C<sub>69</sub>H<sub>9</sub>Cl<sub>3</sub>O</u>	
	1-(4-methoxyphenyl)-7-(1,1,2-trichloroethyl)(C <sub>60</sub> -I <sub>h</sub> )[5,6]fullerene	
FF_12	CID_101266715	
	<u>C<sub>80</sub>H<sub>22</sub></u>	
	12,15-dibenzyl-9-phenyl-6,18-dihydro-1 <i>H</i> -(C <sub>60</sub> -I <sub>h</sub> )[5,6]fullerene	
FF_13	CID_101382121	
	C62F6	
	1,9-bis(trifluoromethyl)(C <sub>60</sub> -I <sub>h</sub> )[5,6]fullerene	

**Table S2.** Description of cube rhombellanes (Core) and functionalized structures with external layer (C-rbl). Value chem. type define chemical bond type characteristic for specific layer of considered molecule (core–molecular core; ex. shell–external layer of the nanomolecule).

Nanostructure Name	Atoms Quantity					Chem. Type core/ex. shell	Structure Type
	All	C	H	O	N		
144 ex_ex/in_ex	144	48	84	24	0	Ether	Core
156 ex_ex/in_ex	156	48	84	36	0	Ether	Core
308 a4 / b4	308	100	124	84	0	Ether/Ester	C-rbl
360 a / b	360	168	108	84	0	Ether/Ester	C-rbl
372AB	372	180	120	60	12	Ether/Amide; Ester	C-rbl
396	396	192	132	72	0	Ether/Ester	C-rbl
420	420	192	156	48	24	Ether/Amide	C-rbl
444	444	192	180	48	24	Ether/Amide	C-rbl
456	456	192	180	60	24	Ether/Amide	C-rbl
ADA_132	132	60	60	12	0	Ether	ADA/rbl



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