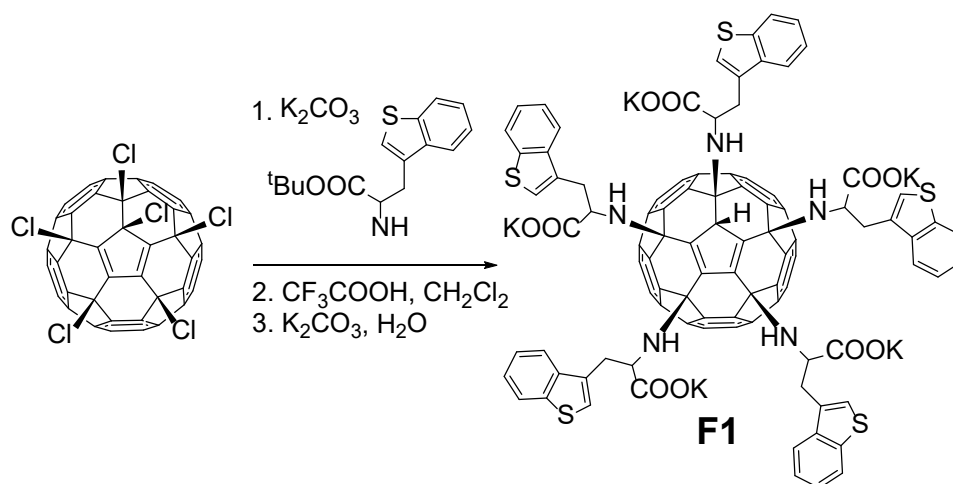


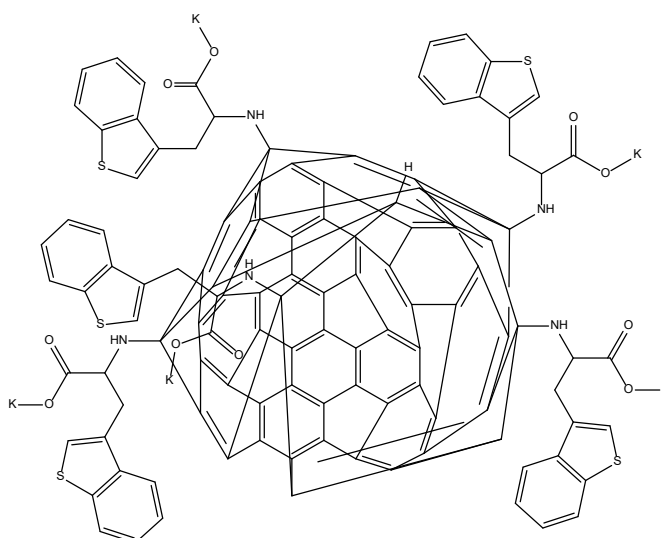
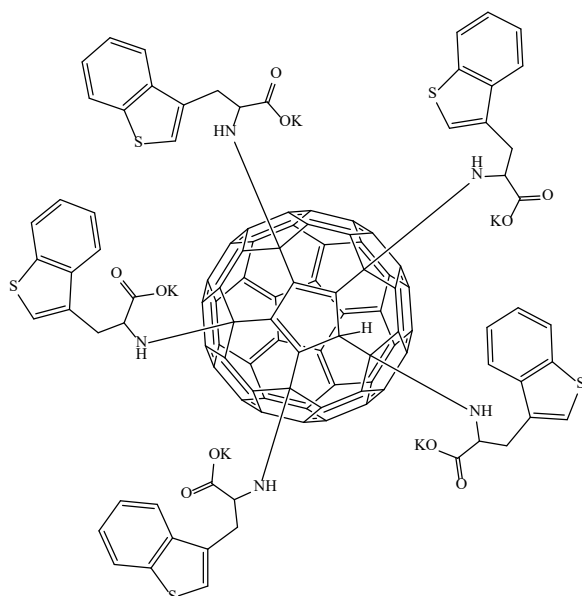
Supplementary 1

Molecular formula of fullerene derivative F1 and method for the synthesis of compound F1 from [1].



Compound F1 SMILES

```
[H]C12C3(NC(CC4=CSC5=C4C=CC=C5)C(O[K])=O)C6=C7C8(NC(CC9=CSC%10=C9C=CC=C%10)C(O[K])=O)C%11=C%12C%13=C(C%14=C(C%15=C%13%16)C%17=C%18C%19=C%20C(C%21=C%22%23)=C%17C%15=C%22C%24=C%16C%12(NC(CC%25=CSC%26=C%25C=CC=C%26)C(O[K])=O)C%27=C81)C%28=C%11C7=C%29C%30=C%28C%14=C%18C(C%19=C%31C%32=C%20C%21=C%33C%34=C%23C%24(NC(CC%35=CSC%36=C%35C=CC=C%36)C(O[K])=O)C%27=C2C%34(NC(CC%37=CSC%38=C%37C=CC=C%38)C(O[K])=O)C%39=C3%40)=C%30C%41=C%31C(C%32=C%39%33)=C%40C6=C%29%41
```



[H]C12C3(NC(CC4=CSC5=C4C=CC=C5)C(O[K])=O)C6=C7C8(NC(CC9=CSC%10=C9C=CC=C%10)C(O[K])=O)C%11=C%12C%13=C(C%14=C(C%15=C%13%16)C%17=C%18C%19=C%20C(C%21=C%22%23)=C%17C%15=C%22C%24=C%16C%12(NC(CC%25=CSC%26=C%25C=CC=C%26)C(O[K])=O)C%27=C81)C%28=C%11C7=C%29C%30=C%28C%14=C%18C(C%19=C%31C%32=C%20C%21=C%33C%34=C%23C%24(NC(CC%35=CSC%36=C%35C=CC=C%36)C(O[K])=O)C%27=C2C%34(NC(CC%37=CSC%38=C%37C=CC=C%38)C(O[K])=O)C%39=C3%40)=C%30C%41=C%31C(C%32=C%39%33)=C%40C6=C%29%41

[1] Huang HJ, Chetyrkina M, Wong CW, Kraevaya OA, Zhilenkov AV, Voronov II, *et al.* Identification of potential descriptors of water-soluble fullerene derivatives responsible for antitumor effects on lung cancer cells via QSAR analysis. Computational and Structural Biotechnology Journal. 2021; 19: 812–825.