**Supplementary**

**Table S1**. The 1-(3-nitrobenzoiloksimetil)-5-fluorourasil derivatives structure

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| **No.** | **IUPAC Name** | **2D structure** | **3D structure** |
|  | 1-(3-nitrobenzoiloksimetil)-5-fluorourasil  (NB5FU) |  |  |
| 1 | (E)-(5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-4-(phenyldiazenyl)benzoate  (NB5FU1) |  |  |
| 2 | (E)-(5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-4-(phenyldiazenyl)benzoate  (NB5FU2) |  |  |
| 3 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-(dimethylamino)-3-nitrobenzoate (NB5FU3) |  |  |
| 4 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2-(chloromethyl)-5-nitrobenzoate (NB5FU4) |  |  |
| 5 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-5-(trifluoromethyl)benzoate  (NB5FU5) |  |  |
| 6 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-acetoxy-5-nitrobenzoate (NB5FU6) |  |  |
| 7 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-(methylthio)-3-nitrobenzoate (NB5FU7) |  |  |
| 8 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-2-(trifluoromethyl)benzoate  (NB5FU8) |  |  |
| 9 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-5-(trifluoromethoxy)benzoate  (NB5FU9) |  |  |
| 10 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-4-(trifluoromethylthio)benzoate  (NB5FU10) |  |  |
| 11 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-4-(trifluoromethoxy)benzoate  (NB5FU11) |  |  |
| 12 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-(chlorosulfonyl)-3-nitrobenzoate (NB5FU12) |  |  |
| 13 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-(difluoromethylthio)-3-nitrobenzoate (NB5FU13) |  |  |
| 14 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-(difluoromethoxy)-3-nitrobenzoate (NB5FU14) |  |  |
| 15 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-2,6-bis(trifluoromethyl)benzoate  (NB5FU15) |  |  |
| 16 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2-fluoro-3-nitro-5-(trifluoromethyl)benzoate  (NB5FU16) |  |  |
| 17 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-2,5-bis(trifluoromethyl)benzoate  (NB5FU17) |  |  |
| 18 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-fluoro-3-nitro-2-(trifluoromethyl)benzoate  (NB5FU18) |  |  |
| 19 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2-fluoro-3-nitro-4-(trifluoromethyl)benzoate  (NB5FU19) |  |  |
| 20 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-fluoro-5-nitro-4-(trifluoromethyl)benzoate  (NB5FU20) |  |  |
| 21 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-fluoro-5-nitro-2-(trifluoromethyl)benzoate  (NB5FU21) |  |  |
| 22 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 5-fluoro-3-nitro-2-(trifluoromethyl)benzoate  (NB5FU22) |  |  |
| 23 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 5-nitro-2,4-bis(trifluoromethyl)benzoate  (NB5FU23) |  |  |
| 24 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-2,6-bis(trifluoromethyl)benzoate  (NB5FU24) |  |  |
| 25 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2-chloro-3-nitro-4-(trifluoromethyl)benzoate  (NB5FU25) |  |  |
| 26 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,5-dichloro-4-methoxy-3-nitrobenzoat (NB5FU26) |  |  |
| 27 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-chloro-2-fluoro-5-nitro-6-(trifluoromethyl)benzoate  (NB5FU27) |  |  |
| 28 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-chloro-2-fluoro-5-nitro-4-(trifluoromethyl)benzoate  (NB5FU28) |  |  |
| 29 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2-fluoro-3-nitro-4-(trifluoromethyl)benzoate  (NB5FU29) |  |  |
| 30 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 5-chloro-3-nitro-2-(trifluoromethyl)benzoate  (NB5FU30) |  |  |
| 31 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-4-(1,2,3-thiadiazol-4-yl)benzoate (NB5FU31) |  |  |
| 32 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-methyl-3-nitro-5-(trifluoromethyl)benzoate  (NB5FU32) |  |  |
| 33 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-4-(1H-pyrazol-1-yl)benzoate  (NB5FU33) |  |  |
| 34 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-(bromomethyl)-3-nitrobenzoate (NB5FU34) |  |  |
| 35 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,3,4,6-tetrafluoro-5-nitrobenzoate (NB5FU35) |  |  |
| 36 | (NB5FU36) |  |  |
| 37 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-ethyl-3-nitrobenzoate (NB5FU37) |  |  |
| 38 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2-cyano-3-nitrobenzoate (NB5FU38) |  |  |
| 39 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-cyano-5-nitrobenzoate (NB5FU39) |  |  |
| 40 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-cyano-3-nitrobenzoate (NB5FU40) |  |  |
| 41 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-4-propylbenzoate (NB5FU41) |  |  |
| 42 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-iodo-3-nitrobenzoate (NB5FU42) |  |  |
| 43 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-butyl-3-nitrobenzoate (NB5FU43) |  |  |
| 44 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-heptyl-3-nitrobenzoate (NB5FU44) |  |  |
| 45 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-hexyl-3-nitrobenzoate (NB5FU45) |  |  |
| 46 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-4-octylbenzoate (NB5FU46) |  |  |
| 47 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-decyl-3-nitrobenzoate (NB5FU47) |  |  |
| 48 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-butoxy-3-nitrobenzoate (NB5FU48) |  |  |
| 49 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,4-dimethyl-3-nitrobenzoate (NB5FU49) |  |  |
| 50 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,4-difluoro-3-nitrobenzoate (NB5FU50) |  |  |
| 51 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3,4-difluoro-5-nitrobenzoate (NB5FU51) |  |  |
| 52 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,4,6-trimethyl-3-nitrobenzoate (NB5FU52) |  |  |
| 53 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,4,5-trifluoro-3-nitrobenzoate (NB5FU53) |  |  |
| 54 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-chloro-3,5-dinitrobenzoate (NB5FU54) |  |  |
| 55 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,3,4-trifluoro-5-nitrobenzoate (NB5FU55) |  |  |
| 56 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2-chloro-3,4-dinitrobenzoate (NB5FU56) |  |  |
| 57 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,4,6-trichloro-3-nitrobenzoate (NB5FU57) |  |  |
| 58 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,3,4-trimethoxy-5-nitrobenzoate (NB5FU58) |  |  |
| 59 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3,4-dimethoxy-5-nitrobenzoate (NB5FU59) |  |  |
| 60 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,3,4-trinitrobenzoate (NB5FU60) |  |  |
| 61 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,4-dimethoxy-3-nitrobenzoate (NB5FU61) |  |  |
| 62 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-methyl-3,5-dinitrobenzoate (NB5FU62) |  |  |
| 63 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2-chloro-4-fluoro-3-nitrobenzoate (NB5FU63) |  |  |
| 64 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-fluoro-3-methyl-5-nitrobenzoate (NB5FU64) |  |  |
| 65 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,3-difluoro-5-nitrobenzoate (NB5FU65) |  |  |
| 66 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,4-difluoro-5-nitrobenzoate (NB5FU66) |  |  |
| 67 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,6-difluoro-4-methoxy-3-nitrobenzoate (NB5FU67) |  |  |
| 68 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 2,5-dichloro-4-methoxy-3-nitrobenzoate (NB5FU68) |  |  |
| 69 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-chloro-2,5-difluoro-3-nitrobenzoate (NB5FU69) |  |  |
| 70 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-chloro-4-fluoro-5-nitrobenzoate (NB5FU70) |  |  |
| 71 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-fluoro-4-methoxy-5-nitrobenzoate (NB5FU71) |  |  |
| 72 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-fluoro-4-methyl-5-nitrobenzoate (NB5FU72) |  |  |
| 73 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-bromo-2-fluoro-3-nitrobenzoate (NB5FU73) |  |  |
| 74 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-bromo-3-methyl-5-nitrobenzoate (NB5FU74) |  |  |
| 75 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-chloro-2,5-difluoro-3-nitrobenzoate (NB5FU75) |  |  |
| 76 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-fluoro-3-nitro-5-(trifluoromethyl)benzoate (NB5FU76) |  |  |
| 77 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 4-(fluorosulfonyl)-3-nitrobenzoate (NB5FU77) |  |  |
| 78 | (5-fluoro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl 3-nitro-4-(thiophen-2-yl)benzoate (NB5FU78) |  |  |