Structural, Hirshfeld surface and *in vitro* cytotoxicity evaluation of five newN-aryl-N'*-*alkoxycarbonyl thiocarbamide derivatives

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**Figure S 1.** Comparative *in vitro* cytotoxicity of compounds **1−5** for a panel of seven human cancer cell lines; Cervical (**2008** and **C13\*),** Colorectal (**HT29** and **HCT116**) and Ovarian carcinoma (**A2780**, **A2780/CP** and **IGROV-1**

**Table S1 :** Decomposed fingerprint plots for various interactions in compounds **2** and **5.**

|  |  |  |
| --- | --- | --- |
| Compound 2 |  | Compound 5 |
| Interactions | **Decomposed fingerprint plots** | **Interactions** | **Decomposed fingerprint plots** |
|  |  |  |  |
| C⋯C | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_CC_4.9.png | **C⋯C** | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_2\C2_CC_1.2.png |
| H⋯H | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_HH_23.3.png |  | **H⋯H** | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_2\C2_HH_40.6.png |
| C⋯H | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_CH_9.4.png |  | **C⋯H** | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_2\C2_CH_13.0.png |
| O⋯H | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_OH_10.3.png |  | **O⋯H** | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_2\C2_OH_22.9.png |
| S⋯H | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_SH_11.1.png |  | **N⋯H** | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_2\C2_NH_4.2.png |
| C⋯Cl | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_CCl_1.6.png |  | **S⋯H** | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_2\C2_SH_8.8.png |
| Cl⋯ Cl | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_ClCl_3.5.png |  |  | **C⋯O** | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_2\C2_CO_2.5.png |
| Cl⋯H | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_ClH_26.6.png |  |  | **S⋯O** | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_2\C2_SO_1.6.png |
| C⋯S | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_CS_1.5.png |  |  | **O⋯O** | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_2\C2_OO_1.7.png |
| S⋯O | F:\NCL_All_Data\Vol_D\SKP\Paper_3\HFS\Compound_1\C1_SO_2.0.png |  |  |  |  |

**Table S 2:** IC50 values (µM) for the compounds **1−5** against seven human cancer cell lines; (cervical **2008** and **C13\*),** (colorectal **HT29** and **HCT116**) and (ovarian carcinoma **A2780, A2780/CP** and **IGROV-1)**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Compounds | 2008 | C13\* | HT29 | HCT116 | A2780 | A2780/CP | IGROV-1 |
| **1** | 24.5±0.4 | 22.7±0.5 | 33.2±1 | 32.6±0.5 | 40.3±0.6 | 38.3±0.2  | 26.7±0.5 |
| **2** | 21.5±0.3 | 20.6±0.7 | 29.1±0.5 | 31.5±0.3 | 36.4±0.7 | 34.2±0.4 | 25.4±0.6 |
| **3** | 22.4±1 | 23.3±0.5 | 30.6±0.4 | 30.7±0.4 | 37.1±0.2 | 35.3±0.4 | 28.4±0.4 |
| **4** | 29.1±0.6 | 25.4±0.3 | 33.6±0.5 | 32.1±0.9 | 30.1±0.8 | 34.5±0.2 | 23.8±0.5 |
| **5** | 18.2±5 | 19.2±0.3 | 21.2±0.5 | 25.1±0.4 | 32.5±0.6 | 31.4±0.5 | 24.1±3  |
| **5-FU** | 4.1±0.3 | 8.5±0.5 | 15.2±2.1 | 13.5±1.8 | 5.5±0.3 | 12.8±0.5 | 5.1±0.2 |