*Table S1. Structural features of chiral pentaamines bis-cyclic guanidines and bis-cyclic thioureas*

** **

**(A) (B)**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Scaffold A** | | | | |
| Compound No. | R1 | R2 | R3 | R4 |
| 1 |  | -H | -H |  |
| 2 |  | -H | -H |  |
| 3 |  | -H | -H |  |
| 5 |  | -H | -H |  |
| **Scaffold B** | | | | |
| 6 |  | -NH | -NH |  |
| 7 |  | -NH | -NH |  |
| 8 |  | -NH | -NH |  |
| 9 |  | -NH | -NH |  |
| 10 |  | -NH | -NH |  |
| 11 |  | -NH | -NH |  |
| 12 |  | -NH | -NH |  |
| 13 |  | -NH | -NH |  |
| 14 |  | -NH | -NH |  |
| 15 |  | -NH | -NH |  |
| 16 |  | -NH | -NH |  |
| 17 |  | -NH | -NH |  |
| 18 |  | -S | -S |  |
| 19 |  | -S | -S | -Isopropyl |

*Table S2. Structural features of bis-cyclic piperazines*

****

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound No. | R1 | R2 | | R3 | R4 |
| 4 |  |  | | -H | -H |
| 20 |  |  | | -H | -H |
| 21 |  |  | | -H | -H |
| 22 |  |  | | -H | -H |
| 23 |  |  | | -H | -H |
| 24 |  |  | | -H | -H |
| 25 |  |  | | -H | -H |
| 26 |  |  | | -H | -H |
| 27 |  |  | | -H | -H |
| 28 |  |  | | -H | -H |
| 29 |  |  | | -H | -H |
| 30 |  |  | | -H | -H |
| 32 |  |  | | -H | -H |
| 33 |  |  | | -H | -H |
| 34 |  | -Isopropyl | | -H | -H |
| 35 |  | -n-butane | | -H | -H |
| 36 |  |  | | -H | -H |
| 37 |  |  | | -H | -H |
| 38 | -n-heptane |  | | -H | -H |
| 39 |  |  | | -H | -H |
| 40 |  |  | | -H | -H |
| 41 |  | -2-methyl propane | | -H | -H |
| 42 |  |  | | -H | -H |
| 44 |  |  | | -H | -H |
| 45 |  |  | | -H | -H |
| 46 |  |  | | -H | -H |
| 47 |  |  | | -H | -H |
| 48 |  |  | | -H | -H |
| 49 |  |  | | -H | -H |
| 50 |  |  | | -H | -H |
| 51 |  |  | | -H | -H |
| 52 | -2-methyl-butane |  | | -H | -H |
| 53 |  |  | | -H | -H |
| 54 |  |  | | -H | -H |
| 55 |  |  | | -H | -H |
| 56 |  |  | | -H | -H |
| 57 |  |  | | -H | -H |
| compound no. 31 | | | compound no. 43 | | |

*Table S3. Structural features of quinolylhydrazones*

 

A B

|  |  |  |  |
| --- | --- | --- | --- |
| Compound No | R | R’ | Ar |
| **Scaffold A** | | | |
| 58 | CH3 | 6-nOC4H9 |  |
| 59 | H | 6-Cyclohexyl |  |
| 60 | CH3 | 6-Cyclohexyl |  |
| 61 | H | 7-Cl |  |
| 62 | CH3 | 7-Cl |  |
| 63 | C6H5 | 6-OCH3 |  |
| 64 | CH3 | 7-OC2H5 |  |
| 65 | CH3 | 6-nC4H9 |  |
| 66 | H | 6-nOC4H9 |  |
| **Scaffold B** | | | |
| 67 | H | H | 4-OCH3-naphthyl |
| 68 | H | 7-OC2H5 | 4-N(C2H5)2-C6H4 |
| 69 | CH3 | 7-OC2H5 | 2-OCH3-naphthyl |
| 70 | CH3 | 7-OC2H5 | 4-OCH3-naphthyl |
| 71 | CH3 | 7-OC2H5 | 4-N(C2H5)2-C6H4 |
| 72 | H | 6-nC4H9 | 4-OCH3-naphthyl |
| 73 | CH3 | 6-nC4H9 | 4-OCH3-naphthyl |
| 74 | H | 7-OCH3 | 2-OCH3-naphthyl |
| 75 | CH3 | 6-nC4H9 | 3,4-(OCH2O)-C6H3 |
| 76 | H | 6-nOC4H9 | 4-OCH3-naphthyl |
| 77 | CH3 | 6-nOC4H9 | 4-OCH3-naphthyl |
| 78 | H | 6-Cyclohexyl | 4-OCH3-naphthyl |
| 79 | H | 6-Cyclohexyl | 1-C6H5-2,5-CH3-3-pyrrolyl |
| 80 | CH3 | 6-Cyclohexyl | C6H5 |
| 81 | CH3 | 6-Cyclohexyl | 4-N(C2H5)2-C6H4 |
| 82 | CH3 | 6-Cyclohexyl | 4-OCH3-naphthyl |
| 83 | CH3 | 6-Cyclohexyl | 1-C6H5-2,5-CH3-3-pyrrolyl |
| 84 | H | 7-OCH3 | 4-OCH3-naphthyl |
| 85 | H | 7Cl | 4-OCH3-naphthyl |
| 86 | CH3 | 7Cl | 2-OCH3-naphthyl |
| 87 | CH3 | 7Cl | 4-OCH3-naphthyl |
| 88 | CH3 | 7Cl | 4-N(C2H5)2-C6H4 |
| 89 | CH3 | 6F | 4-OCH3-naphthyl |
| 90 | H | 7-OCH3 | 4-N(C2H5)2-C6H4 |
| 91 | CH3 | 7-OCH3 | 2-OCH3-naphthyl |
| 92 | CH3 | 7-OCH3 | 3,4-(OCH2O)-C6H3 |
| 93 | CH3 | 8-OCH3 | 4-OCH3-naphthyl |