

Supplementary Materials

Novel reversible inhibitors of xanthine oxidase targeting the active site of the enzyme

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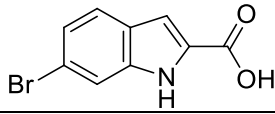
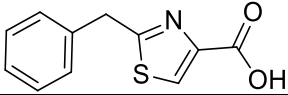
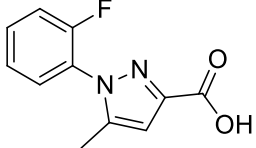
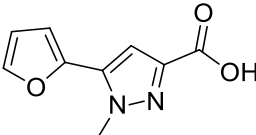
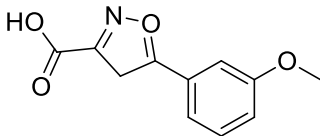
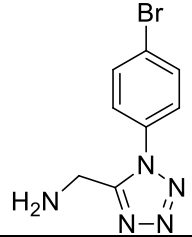
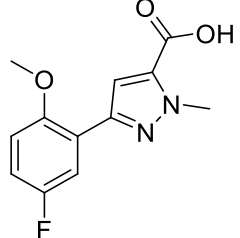
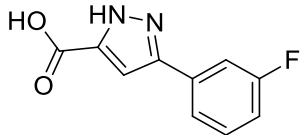
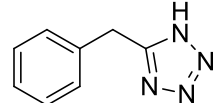
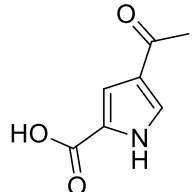
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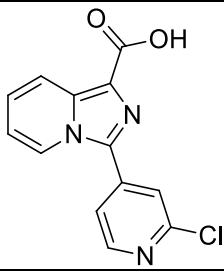

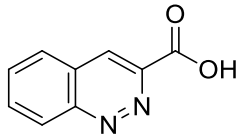
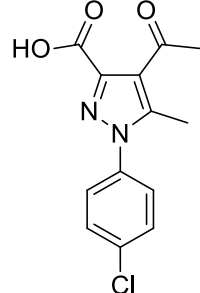
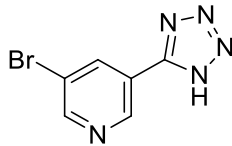
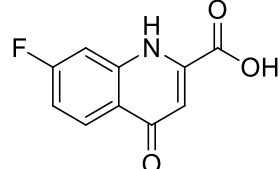
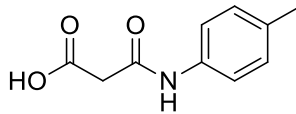
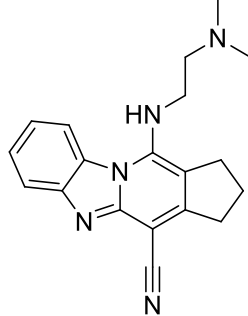
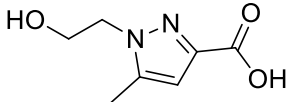
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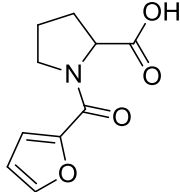
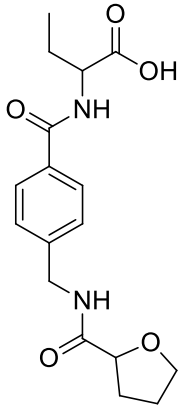
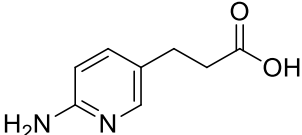
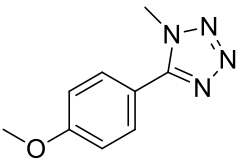
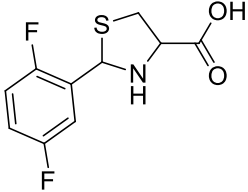
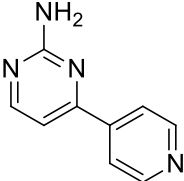
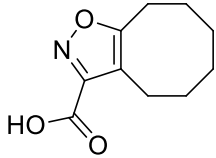
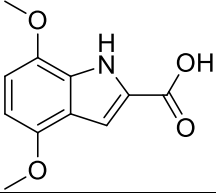
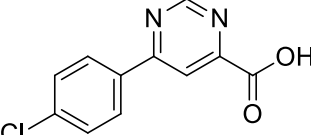
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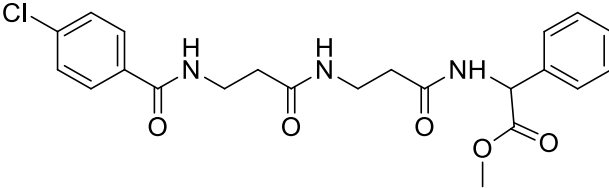
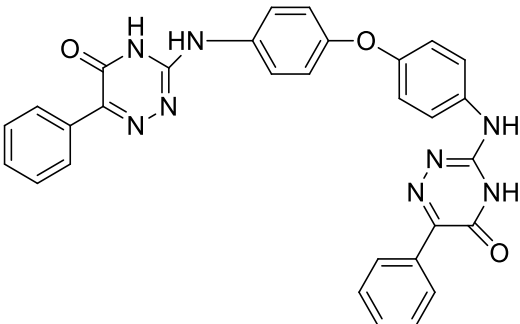
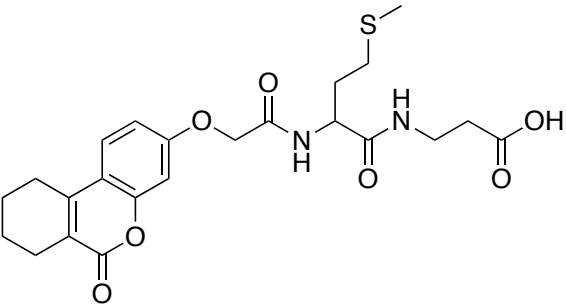
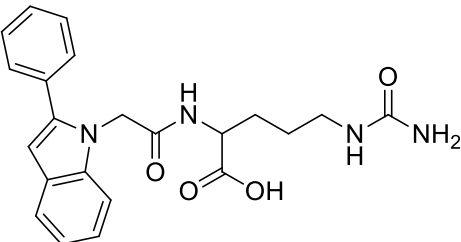
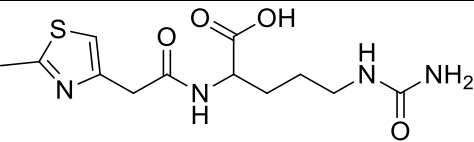
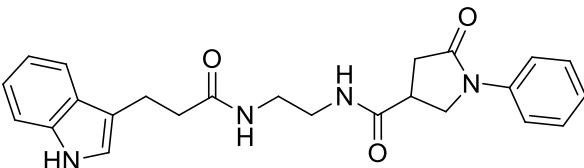
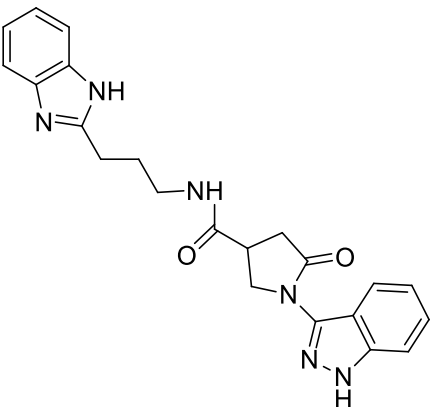
† R.R. and C.C. equally contributed to this paper.

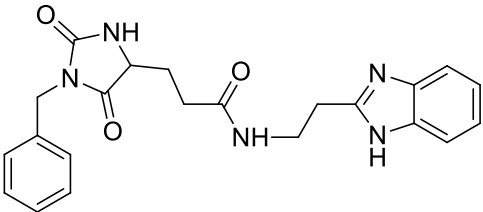
Table S1. Compounds ALS-1→36 identified by virtual screening [46].

| N. | Approach | ID | Structure |
|----|----------|--------|--|
| 1 | LBVS | ALS-1 |  |
| 2 | LBVS | ALS-2 |  |
| 3 | LBVS | ALS-3 |  |
| 4 | LBVS | ALS-4 |  |
| 5 | LBVS | ALS-5 |  |
| 6 | LBVS | ALS-6 |  |
| 7 | LBVS | ALS-7 |  |
| 8 | LBVS | ALS-8 |  |
| 9 | LBVS | ALS-9 |  |
| 10 | LBVS | ALS-10 |  |

| | | | |
|----|------|--------|--|
| 11 | LBVS | ALS-11 |  |
| 12 | LBVS | ALS-12 |  |
| 13 | LBVS | ALS-13 |  |
| 14 | LBVS | ALS-14 |  |
| 15 | LBVS | ALS-15 |  |
| 16 | LBVS | ALS-16 |  |
| 17 | LBVS | ALS-17 |  |
| 18 | SBVS | ALS-18 |  |
| 19 | LBVS | ALS-19 |  |

| | | | |
|----|------|--------|--|
| 20 | LBVS | ALS-20 |  |
| 21 | SBVS | ALS-21 |  |
| 22 | LBVS | ALS-22 |  |
| 23 | LBVS | ALS-23 |  |
| 24 | LBVS | ALS-24 |  |
| 25 | LBVS | ALS-25 |  |
| 26 | LBVS | ALS-26 |  |
| 27 | LBVS | ALS-27 |  |
| 28 | LBVS | ALS-28 |  |

| | | | |
|----|------|--------|--|
| 29 | SBVS | ALS-29 |  |
| 30 | SBVS | ALS-30 |  |
| 31 | SBVS | ALS-31 |  |
| 32 | SBVS | ALS-32 |  |
| 33 | SBVS | ALS-33 |  |
| 34 | SBVS | ALS-34 |  |
| 35 | SBVS | ALS-35 |  |

| | | | |
|----|------|--------|--|
| 36 | SBVS | ALS-36 |  <p>The chemical structure of ALS-36 is a complex molecule featuring a benzimidazole moiety linked via a methylene group to a secondary amide. This amide is connected to a 1-phenyl-1H-imidazole-2-carboxamide derivative through a three-carbon chain. The structure includes a benzimidazole ring system, a methylene bridge, a secondary amide group, a three-carbon linker, and a 1-phenyl-1H-imidazole-2-carboxamide moiety.</p> |
|----|------|--------|--|