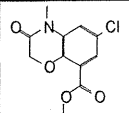
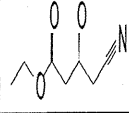
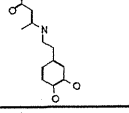
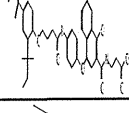
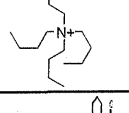
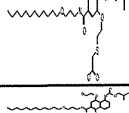
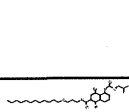
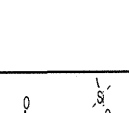
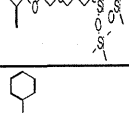
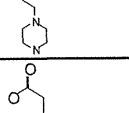
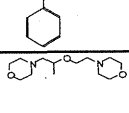
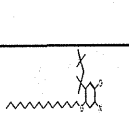
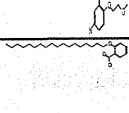
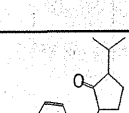
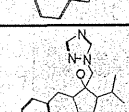
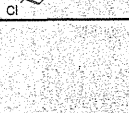
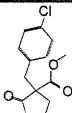
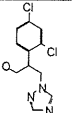
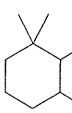
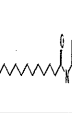
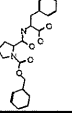
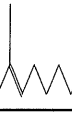
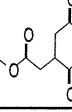
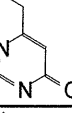
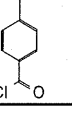
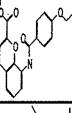
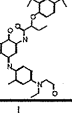
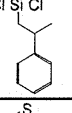
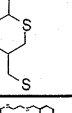



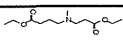
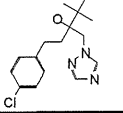
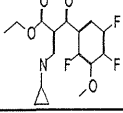
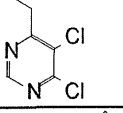
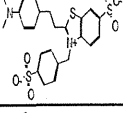

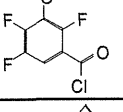
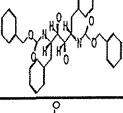
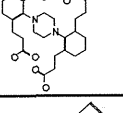
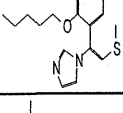
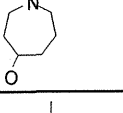
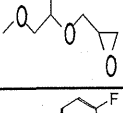
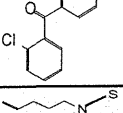
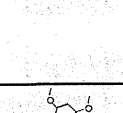
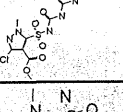
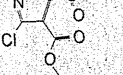


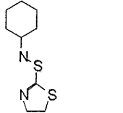
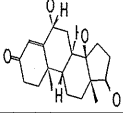
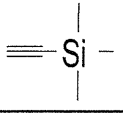
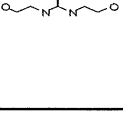
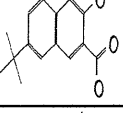
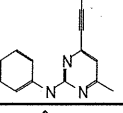
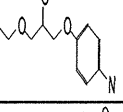
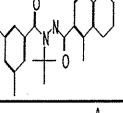

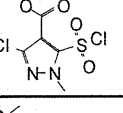
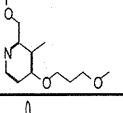
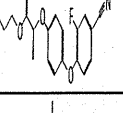
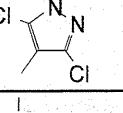
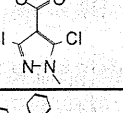
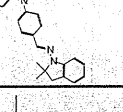
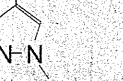
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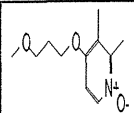
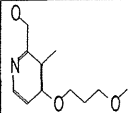
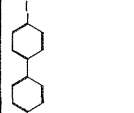
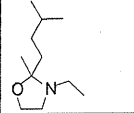
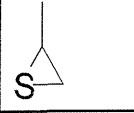
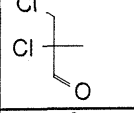
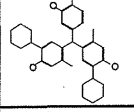
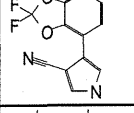
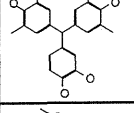
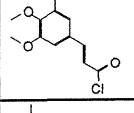
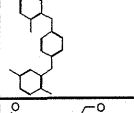
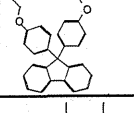
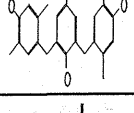
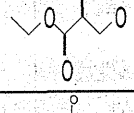
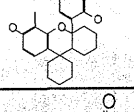
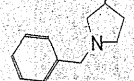
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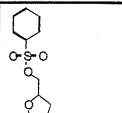
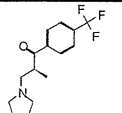
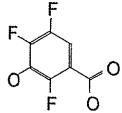
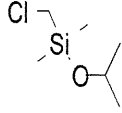
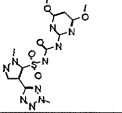
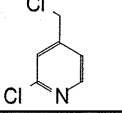
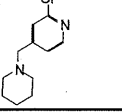
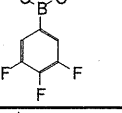
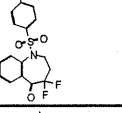
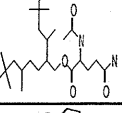
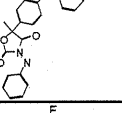
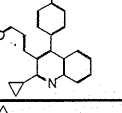
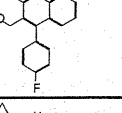
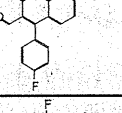
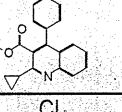
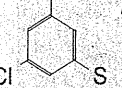
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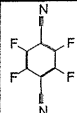
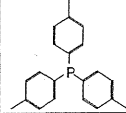
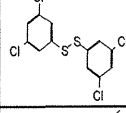
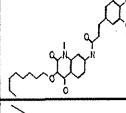
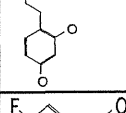
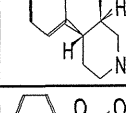
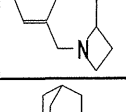
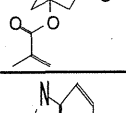
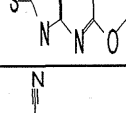
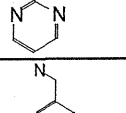
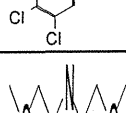
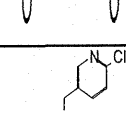
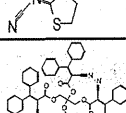
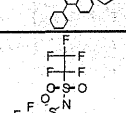
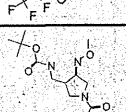

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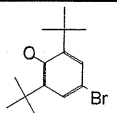
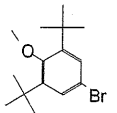
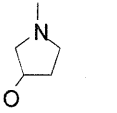
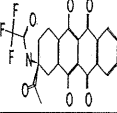
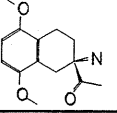
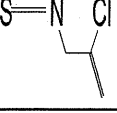
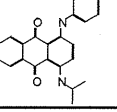
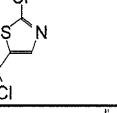
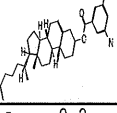
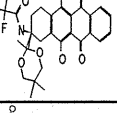
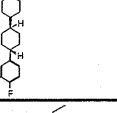
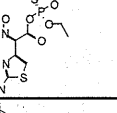
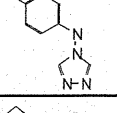
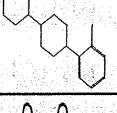
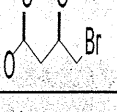
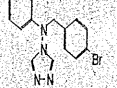
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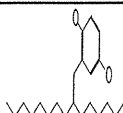
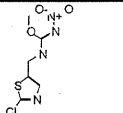
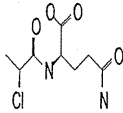
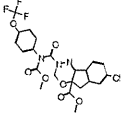
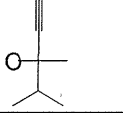
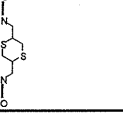
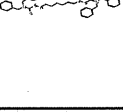
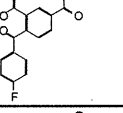
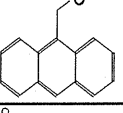
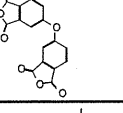
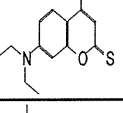
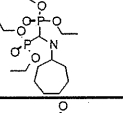
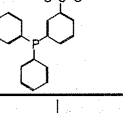
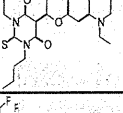
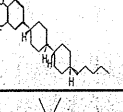
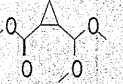
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| 807 |  | 364.2685 | C | - | JP.143807-66-3 | - | - | - |
| 808 |  | 332.2663 | C | - | JP.10578-34-4 | - | - | - |
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| 814 |  | 390.3305 | C | - | JP.113840-79-2 | - | - | - |
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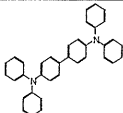
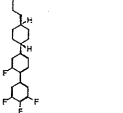
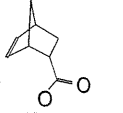
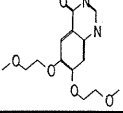
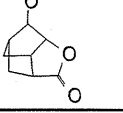
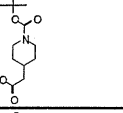
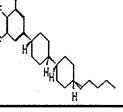
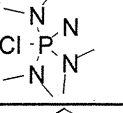
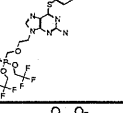
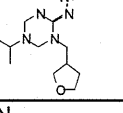
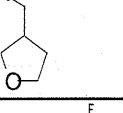
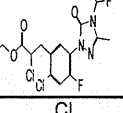
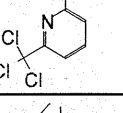
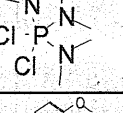
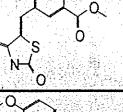
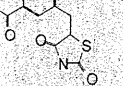
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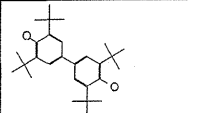
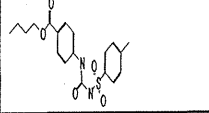
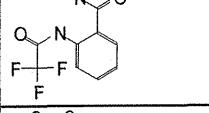
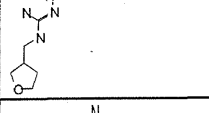
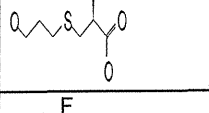
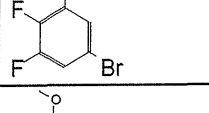
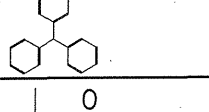
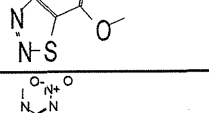
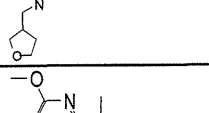
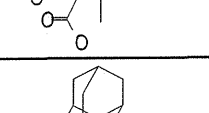
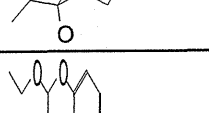
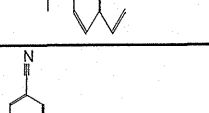
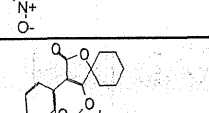
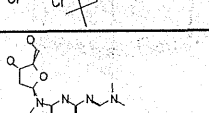
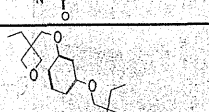
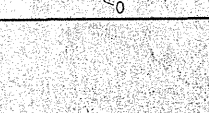
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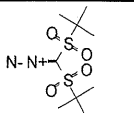
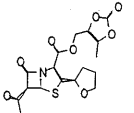
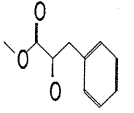
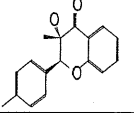
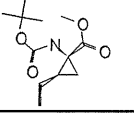
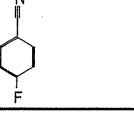
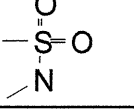
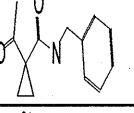
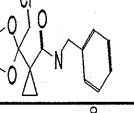
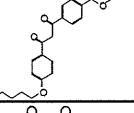
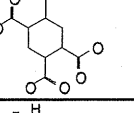
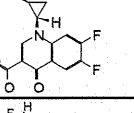
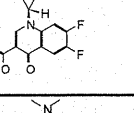
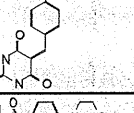
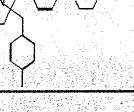
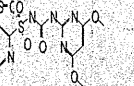
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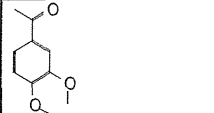
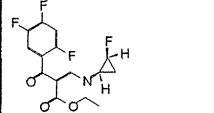
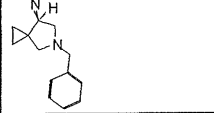
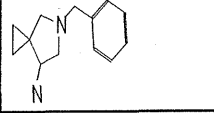
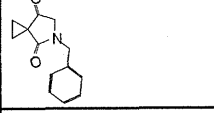
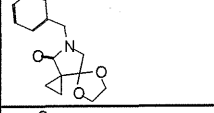
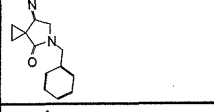
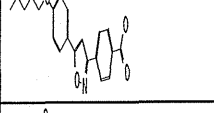
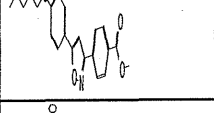
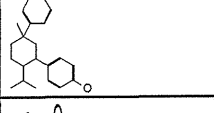
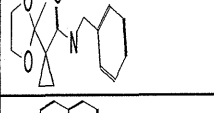
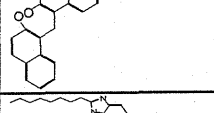
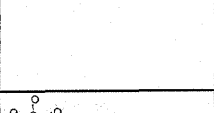
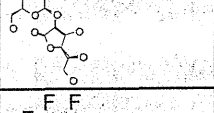
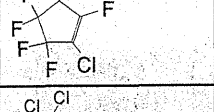

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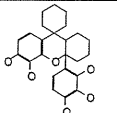
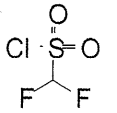
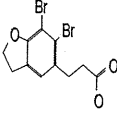
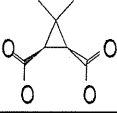
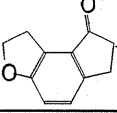
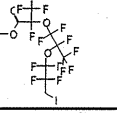
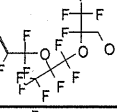
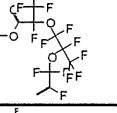
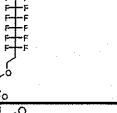
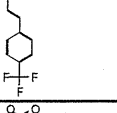
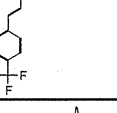
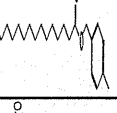
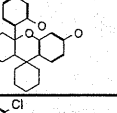
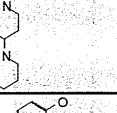
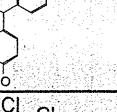
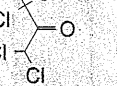
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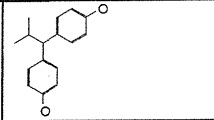
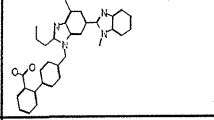
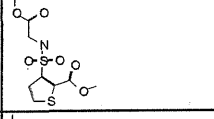
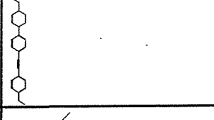
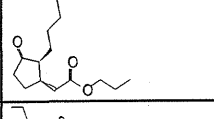
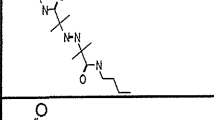
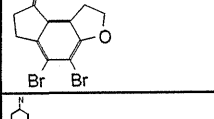
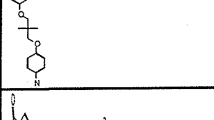
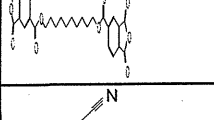
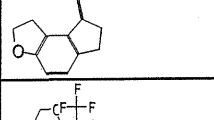
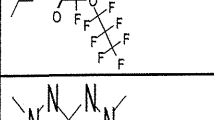
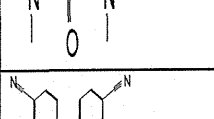
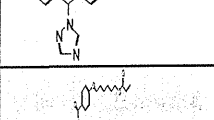
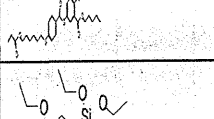
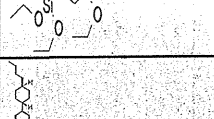

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| 988 |  | 274.2154 | C | - | JP.112809-51-5 | + | + | + |
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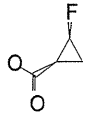
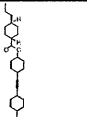
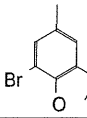
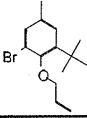
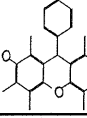
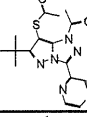
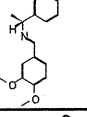
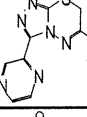
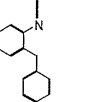
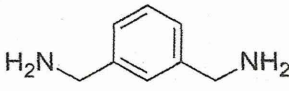
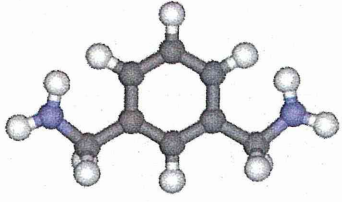
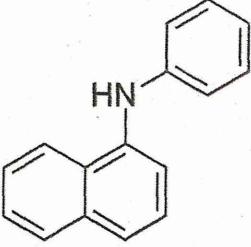
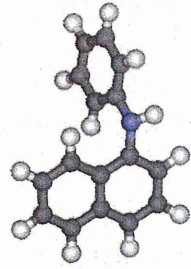
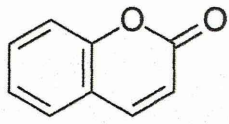
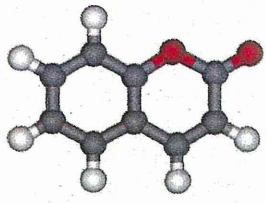
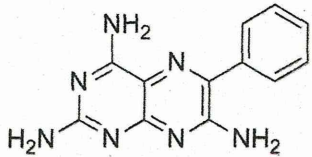
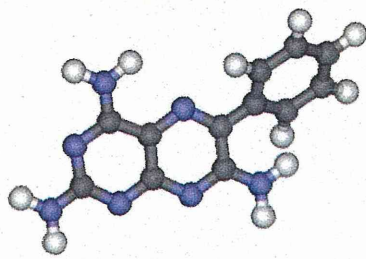
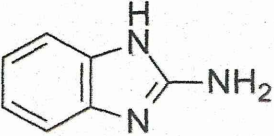
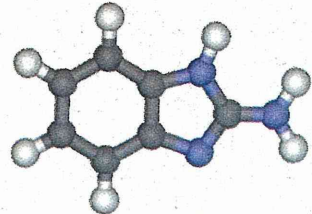
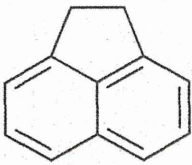
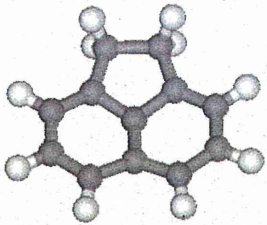
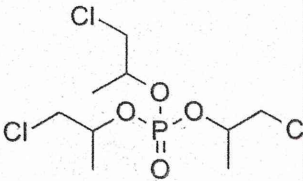
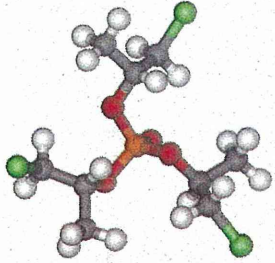
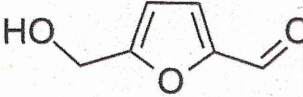
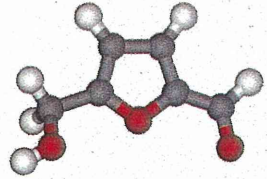
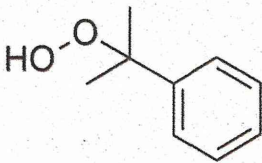
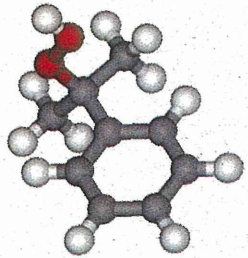
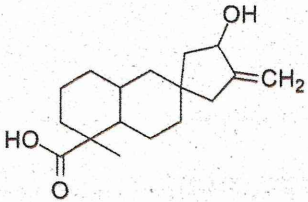
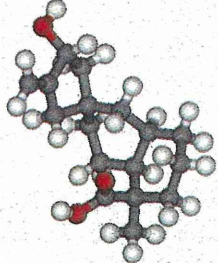
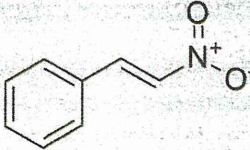
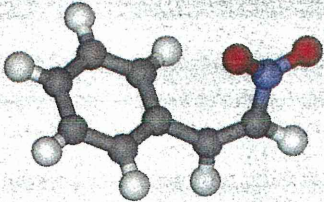
| | | | | | | | | |
|------|---|----------|---|---|----------------|---|---|---|
| 992 |  | 99.03999 | C | - | JP.127199-14-8 | - | - | - |
| 993 |  | 334.2822 | C | - | JP.128060-75-3 | + | - | - |
| 994 |  | 228.0211 | C | - | JP.1516-93-4 | - | - | - |
| 995 |  | 264.0532 | A | + | JP.188021-38-7 | - | - | - |
| 996 |  | 348.2657 | C | - | JP.153164-65-9 | + | + | + |
| 997 |  | 340.2752 | C | - | JP.110130-88-6 | + | + | + |
| 998 |  | 251.1953 | C | - | JP.13156-95-1 | + | + | + |
| 999 |  | 260.2336 | C | - | JP.110675-26-8 | + | - | - |
| 1000 |  | 198.1559 | C | - | JP.146446-96-0 | - | + | + |

表 12

今までの予測モデルで必ず誤分類される化合物

| | Name | Structure | 3D Structure |
|---|--------------------------|---|--|
| 1 | m-xylylenediamine |  |  |
| 2 | N-phenyl-1-naphthylamine |  |  |
| 3 | coumarin |  |  |
| 4 | triamterene |  |  |
| 5 | 2-aminobenzimidazole |  |  |

| | | | |
|----|----------------------------------|---|---|
| 6 | acenaphthene |  |  |
| 7 | tris(1-chloro-2-propyl)phosphate |  |  |
| 8 | 5-hydroxymethylfurfural |  |  |
| 9 | cumene hydroperoxide |  |  |
| 10 | steviol |  |  |
| 11 | beta-nitrostyrene |  |  |