Model ranks patent pathway as top-1: Example 3

ASKCOS pathway, score: -24.012, ranking: 39, group: 9
ASKCOS pathway, score: -23.910, ranking: 34, group: 8
ASKCOS pathway, score: -22.954, ranking: 22, group: 7
ASKCOS pathway, score: -22.864, ranking: 20, group: 6
ASKCOS pathway, score: -22.666, ranking: 16, group: 5
ASKCOS pathway, score: -20.830, ranking: 10, group: 4
ASKCOS pathway, score: -20.054, ranking: 8, group: 3
ASKCOS pathway, score: -17.056, ranking: 3, group: 2
ASKCOS pathway, score: -16.869, ranking: 2, group: 1

Model ranks patent pathway as top-1: Example 3
Model ranks patent pathway as top-1: Example 4

[Diagram of pathway]

Piatachio pathway, score: 6.927, ranking: 1, Patent No: US06509359B1

[Diagram of pathway]
Model ranks patent pathway as top-1: Example 5
Model ranks patent pathway as top-1: Example 7
Model ranks patent pathway as top-1: Example 8
Model ranks patent pathway as top-1: Example 9
Model ranks patent pathway as top-1: Example 10
Model ranks patent pathway as top-1: Example 11

Model ranks patent pathway as top-1: Example 11
Model ranks patent pathway as top-1: Example 12
Model ranks patent pathway as top-1: Example 13

[Diagrams of pathways with scores and rankings]
Model ranks patent pathway as top-1: Example 15
Model ranks patent pathway as top-1: Example 16
Model ranks patent pathway as top-1: Example 17
Model ranks patent pathway as top-1: Example 20

ASKCOS pathway, score: -19.342, ranking: 13, group: 9
ASKCOS pathway, score: -19.286, ranking: 12, group: 8
ASKCOS pathway, score: -19.116, ranking: 11, group: 7
ASKCOS pathway, score: -19.070, ranking: 10, group: 6
ASKCOS pathway, score: -18.696, ranking: 8, group: 5
ASKCOS pathway, score: -18.385, ranking: 5, group: 4
ASKCOS pathway, score: -17.078, ranking: 4, group: 3
ASKCOS pathway, score: -15.842, ranking: 3, group: 2
ASKCOS pathway, score: -15.831, ranking: 2, group: 1

Piatachio pathway, score: -6.376, ranking: 1, Patent No: EP2760834B1
Model ranks patent pathway as top-1: Example 21
Model ranks patent pathway as top-1: Example 22
Model ranks patent pathway as top-1: Example 23
Model ranks patent pathway as top-1: Example 24
Model ranks patent pathway as top-1: Example 25
Model ranks patent pathway as top-1: Example 27

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Piatachio pathway, score: 1.503, ranking: 1, Patent No: US10064848

Model ranks patent pathway as top-1: Example 27
Model ranks patent pathway as top-1: Example 28


Model ranks patent pathway as top-1: Example 28
Model ranks patent pathway as top-1: Example 29

ASKCOS pathway, score: -17.495, ranking: 56, group: 9

ASKCOS pathway, score: -17.345, ranking: 52, group: 8

ASKCOS pathway, score: -16.348, ranking: 29, group: 7

ASKCOS pathway, score: -15.865, ranking: 24, group: 6

ASKCOS pathway, score: -15.287, ranking: 17, group: 5

ASKCOS pathway, score: -14.397, ranking: 10, group: 4

ASKCOS pathway, score: -13.942, ranking: 5, group: 3

ASKCOS pathway, score: -13.710, ranking: 3, group: 2

ASKCOS pathway, score: -12.198, ranking: 2, group: 1

Piatachio pathway, score: -1.763, ranking: 1, Patent No: US06762205B1

Model ranks patent pathway as top-1: Example 29
Model ranks patent pathway as top-1: Example 30
Model ranks patent pathway as top-1: Example 31

ASKCOS pathway, score: -23.925, ranking: 16, group: 9

ASKCOS pathway, score: -22.799, ranking: 15, group: 8

ASKCOS pathway, score: -22.124, ranking: 11, group: 7

ASKCOS pathway, score: -21.571, ranking: 8, group: 6

ASKCOS pathway, score: -21.408, ranking: 6, group: 5

ASKCOS pathway, score: -21.033, ranking: 5, group: 4

ASKCOS pathway, score: -20.996, ranking: 4, group: 3

ASKCOS pathway, score: -20.753, ranking: 3, group: 2

ASKCOS pathway, score: -20.408, ranking: 2, group: 1


Model ranks patent pathway as top-1: Example 31
Model ranks patent pathway as top-1: Example 32
Model ranks patent pathway as top-1: Example 33

**ASKCOS pathway, score: -29.310, ranking: 8, group: 3**

**ASKCOS pathway, score: -27.770, ranking: 3, group: 2**

**ASKCOS pathway, score: -27.207, ranking: 2, group: 1**

**Piatachio pathway, score: -12.247, ranking: 1, Patent No: US05747487A**

Model ranks patent pathway as top-1: Example 33
Model ranks patent pathway as top-1: Example 34
Model ranks patent pathway as top-1: Example 35

\[
\text{ASKCOS pathway, score: } -27.999, \text{ ranking: 10, group: 9}
\]

\[
\text{ASKCOS pathway, score: } -27.947, \text{ ranking: 9, group: 8}
\]

\[
\text{ASKCOS pathway, score: } -27.853, \text{ ranking: 8, group: 7}
\]

\[
\text{ASKCOS pathway, score: } -27.636, \text{ ranking: 7, group: 6}
\]

\[
\text{ASKCOS pathway, score: } -27.532, \text{ ranking: 6, group: 5}
\]

\[
\text{ASKCOS pathway, score: } -27.191, \text{ ranking: 5, group: 4}
\]

\[
\text{ASKCOS pathway, score: } -27.163, \text{ ranking: 4, group: 3}
\]

\[
\text{ASKCOS pathway, score: } -23.321, \text{ ranking: 3, group: 2}
\]

\[
\text{ASKCOS pathway, score: } -18.925, \text{ ranking: 2, group: 1}
\]

\[
\text{Piatachio pathway, score: } -14.450, \text{ ranking: 1, Patent No: US20080004295A1}
\]

\[
\text{Model ranks patent pathway as top-1: Example 35}
\]
Model ranks patent pathway as top-1: Example 36
Model ranks patent pathway as top-1: Example 37
Model ranks patent pathway as top-1: Example 38

Piatachio pathway, score: -1.413, ranking: 1, Patent No: US20180009797A1

Example 38
Model ranks patent pathway as top-1: Example 39
Model ranks patent pathway as top-1: Example 40
Model ranks patent pathway as top-1: Example 41


ASKCOS pathway, score: -32.913, ranking: 12, group: 9

ASKCOS pathway, score: -32.581, ranking: 9, group: 8

ASKCOS pathway, score: -32.377, ranking: 8, group: 7

ASKCOS pathway, score: -31.328, ranking: 7, group: 6

ASKCOS pathway, score: -30.651, ranking: 6, group: 5

ASKCOS pathway, score: -29.827, ranking: 5, group: 4

ASKCOS pathway, score: -27.854, ranking: 4, group: 3

ASKCOS pathway, score: -27.812, ranking: 3, group: 2

ASKCOS pathway, score: -26.300, ranking: 2, group: 1
Model ranks patent pathway as top-1: Example 42

\[
\text{ASKCOS pathway, score: } -22.276, \text{ ranking: 9, group: 8}
\]

\[
\text{ASKCOS pathway, score: } -21.967, \text{ ranking: 8, group: 7}
\]

\[
\text{ASKCOS pathway, score: } -21.625, \text{ ranking: 7, group: 6}
\]

\[
\text{ASKCOS pathway, score: } -21.335, \text{ ranking: 6, group: 5}
\]

\[
\text{ASKCOS pathway, score: } -19.138, \text{ ranking: 5, group: 4}
\]

\[
\text{ASKCOS pathway, score: } -18.380, \text{ ranking: 4, group: 3}
\]

\[
\text{ASKCOS pathway, score: } -17.624, \text{ ranking: 3, group: 2}
\]

\[
\text{ASKCOS pathway, score: } -11.793, \text{ ranking: 2, group: 1}
\]

\[
\text{Piatachio pathway, score: 0.343, ranking: 1, Patent No: US10308637}
\]
Model ranks patent pathway as top-1: Example 44

- ASKCOS pathway, score: -16.502, ranking: 24, group: 9
- ASKCOS pathway, score: -16.098, ranking: 17, group: 8
- ASKCOS pathway, score: -16.037, ranking: 16, group: 7
- ASKCOS pathway, score: -15.720, ranking: 14, group: 6
- ASKCOS pathway, score: -15.642, ranking: 12, group: 5
- ASKCOS pathway, score: -15.637, ranking: 11, group: 4
- ASKCOS pathway, score: -15.396, ranking: 8, group: 3
- ASKCOS pathway, score: -13.791, ranking: 3, group: 2
- ASKCOS pathway, score: -12.764, ranking: 2, group: 1

- Piatachio pathway, score: -0.381, ranking: 1, Patent No: US20030207868A1
Model ranks patent pathway as top-1: Example 45
Model ranks patent pathway as top-1: Example 46
Model ranks patent pathway as top-1: Example 47

\[
\text{ASKCOS pathway, score: } -20.900, \text{ ranking: 29, group: 9}
\]
\[
\text{ASKCOS pathway, score: } -20.795, \text{ ranking: 27, group: 8}
\]
\[
\text{ASKCOS pathway, score: } -20.551, \text{ ranking: 25, group: 7}
\]
\[
\text{ASKCOS pathway, score: } -20.352, \text{ ranking: 24, group: 6}
\]
\[
\text{ASKCOS pathway, score: } -20.037, \text{ ranking: 20, group: 5}
\]
\[
\text{ASKCOS pathway, score: } -19.881, \text{ ranking: 19, group: 4}
\]
\[
\text{ASKCOS pathway, score: } -19.437, \text{ ranking: 16, group: 3}
\]
\[
\text{ASKCOS pathway, score: } -18.583, \text{ ranking: 10, group: 2}
\]
\[
\text{ASKCOS pathway, score: } -16.343, \text{ ranking: 2, group: 1}
\]

\[
\text{Piatachio pathway, score: } -12.786, \text{ ranking: 1, Patent No: US2010027883A1}
\]

\[
\text{Model ranks patent pathway as top-1: Example 47}
\]
Model ranks patent pathway as top-1: Example 48
Model ranks patent pathway as top-1: Example 49
Model ranks patent pathway as top-1: Example 50
Model ranks patent pathway not as top-1: Example 1

ASKCOS pathway, score: -16.918, ranking: 23, group: 8

ASKCOS pathway, score: -16.884, ranking: 21, group: 7

ASKCOS pathway, score: -15.926, ranking: 16, group: 6

ASKCOS pathway, score: -15.882, ranking: 15, group: 5

ASKCOS pathway, score: -15.284, ranking: 11, group: 4

ASKCOS pathway, score: -15.251, ranking: 10, group: 3

ASKCOS pathway, score: -14.984, ranking: 6, group: 2

ASKCOS pathway, score: -14.231, ranking: 2, group: 1

ASKCOS pathway, score: -13.773, ranking: 1, group: 0


Model ranks patent pathway not as top-1: Example 1
Model ranks patent pathway not as top-1: Example 3
Model ranks patent pathway not as top-1: Example 4
Model ranks patent pathway not as top-1: Example 6

ASKCOS pathway, score: -20.792, ranking: 39, group: 9

ASKCOS pathway, score: -19.911, ranking: 26, group: 8

ASKCOS pathway, score: -19.192, ranking: 15, group: 7

ASKCOS pathway, score: -18.929, ranking: 12, group: 6

ASKCOS pathway, score: -18.646, ranking: 9, group: 5

ASKCOS pathway, score: -18.040, ranking: 5, group: 4

ASKCOS pathway, score: -17.859, ranking: 4, group: 3

ASKCOS pathway, score: -17.803, ranking: 3, group: 2

ASKCOS pathway, score: -16.492, ranking: 1, group: 0

Piatachio pathway, score: -17.728, ranking: 2, Patent No: US20190002402A1

Model ranks patent pathway not as top-1: Example 6
Model ranks patent pathway not as top-1: Example 7
Model ranks patent pathway not as top-1: Example 9

ASKCOS pathway, score: -18.669, ranking: 16, group: 9

ASKCOS pathway, score: -18.414, ranking: 15, group: 8

ASKCOS pathway, score: -18.376, ranking: 14, group: 7

ASKCOS pathway, score: -17.338, ranking: 7, group: 6

ASKCOS pathway, score: -17.228, ranking: 6, group: 5

ASKCOS pathway, score: -16.591, ranking: 5, group: 4

ASKCOS pathway, score: -15.758, ranking: 4, group: 3

ASKCOS pathway, score: -14.090, ranking: 2, group: 1

ASKCOS pathway, score: -13.110, ranking: 1, group: 0

Model ranks patent pathway not as top-1: Example 10

- ASKCOS pathway, score: -37.385, ranking: 267, group: 9
- ASKCOS pathway, score: -36.164, ranking: 252, group: 8
- ASKCOS pathway, score: -34.496, ranking: 231, group: 7
- ASKCOS pathway, score: -34.387, ranking: 228, group: 6
- ASKCOS pathway, score: -34.264, ranking: 226, group: 5
- ASKCOS pathway, score: -30.689, ranking: 170, group: 4
- ASKCOS pathway, score: -25.466, ranking: 26, group: 2
- ASKCOS pathway, score: -23.528, ranking: 8, group: 1
- ASKCOS pathway, score: -21.656, ranking: 1, group: 0