



STRUCTURAL
BIOLOGY

Volume 77 (2021)

Supporting information for article:

Complex crystal structure determination and anti-non-small-cell lung cancer activity of the Hsp90^N inhibitor Debio0932

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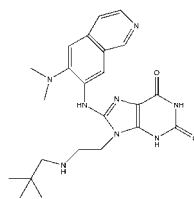
Table S1 Molecular docking data of Debio0932 and its new derivatives.

Name	Total score	Cscore	Molecular structure	Total score increment
D	7.8	5		
D13	10.4	5		↑2.6
D15	9.5	5		↑1.7
D25	9.2	5		↑1.4
D12	8.7	4		↑0.9
D7	8.4	4		↑0.6
D1	8.1	5		↑0.3

D24

8.0

3

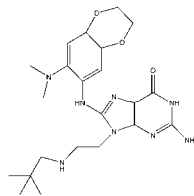


↑0.2

D9

7.9

4

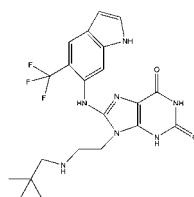


↑0.1

D28

7.9

5

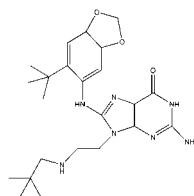


↑0.1

D2

7.8

4

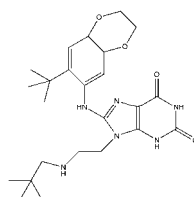


0.0

D11

7.8

3

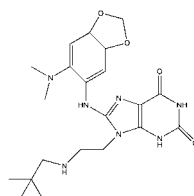


0.0

D6

7.7

4

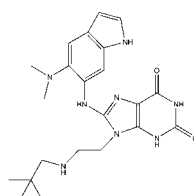


↓0.1

D30

7.7

3

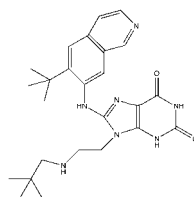


↓0.1

D23

7.7

5

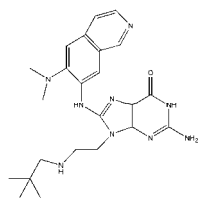


↓0.1

D21

7.6

3

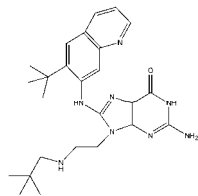


↓0.2

D14

7.6

5

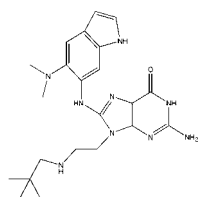


↓0.2

D27

7.5

5

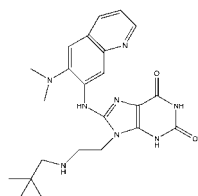


↓0.3

D18

7.5

3

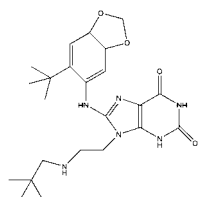


↓0.3

D5

7.1

5

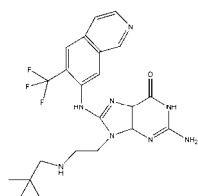


↓0.7

D19

7.0

4

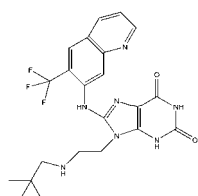


↓0.8

D16

7.0

4

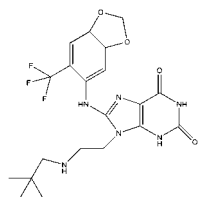


↓0.8

D4

6.9

2

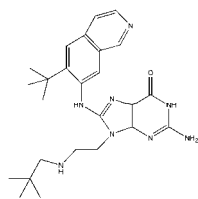


↓0.9

D20

6.8

4

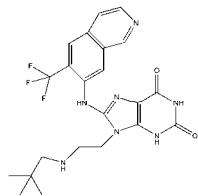


↓1.0

D22

6.8

5

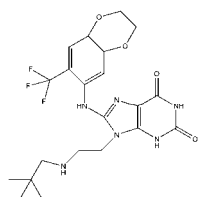


↓1.0

D10

6.7

5

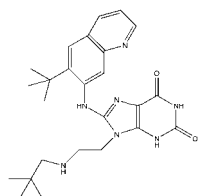


↓1.1

D17

6.7

4

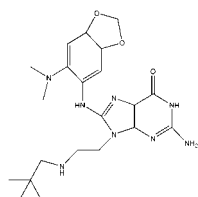


↓1.1

D3

6.6

4

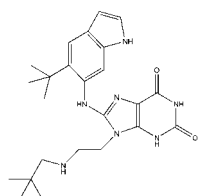


↓1.2

D29

6.2

2

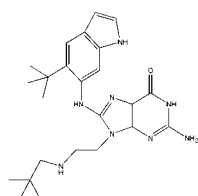


↓1.6

D26

6.0

5

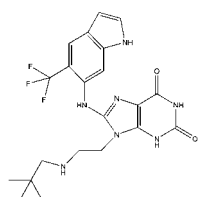


↓1.8

D8

5.9

5



↓1.9

Annotation: The red means new derivatives with increased Total score values compared with Debio0932 determined by molecular docking with software SYBYL-X 2.0 and the blue means ones with decreased Total score values.

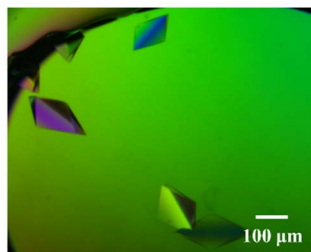


Figure S1 Complex crystals of Hsp90^N-Debio0932. The complex crystals of Hsp90^N-Debio0932 (220 μm×130 μm×50 μm) were gained after 3~5 days at 4°C by the hanging drop method.