**Supplementary Table S1.** Docking cluster, element, fullfitneess, estimate ΔG between 2Y9X and pinostrobin using SwissDock.

| Cluster | Element | FullFitness (kcal/mol) | Estimated ΔG (kcal/mol) | Cluster | Element | FullFitness (kcal/mol) | Estimated ΔG (kcal/mol) | Cluster | Element | FullFitness (kcal/mol) | Estimated ΔG (kcal/mol) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | -940.18 | -6.48 | 10 | 0 | -936.46 | -6.71 | 21 | 5 | -933.61 | -5.8 |
| 0 | 1 | -940.18 | -6.48 | 10 | 1 | -916.21 | -5.64 | 21 | 6 | -933.61 | -5.8 |
| 0 | 2 | -938.88 | -6.28 | 11 | 0 | -936.05 | -6.47 | 21 | 7 | -933.58 | -5.79 |
| 0 | 3 | -938.88 | -6.28 | 11 | 1 | -936.03 | -6.45 | 22 | 0 | -933.93 | -6.24 |
| 0 | 4 | -937.53 | -6.12 | 11 | 2 | -935.93 | -6.45 | 22 | 1 | -933.86 | -6.25 |
| 0 | 5 | -937.53 | -6.12 | 11 | 3 | -935.93 | -6.45 | 22 | 2 | -933.85 | -6.26 |
| 0 | 6 | -937.53 | -6.12 | 11 | 4 | -933.76 | -5.98 | 22 | 3 | -933.81 | -6.24 |
| 0 | 7 | -937.53 | -6.12 | 11 | 5 | -933.62 | -6 | 22 | 4 | -933.58 | -6.22 |
| 1 | 0 | -940.08 | -7.5 | 11 | 6 | -933.41 | -5.97 | 22 | 5 | -929.12 | -6.26 |
| 1 | 1 | -939.94 | -7.48 | 11 | 7 | -933.41 | -5.97 | 22 | 6 | -927.83 | -5.82 |
| 1 | 2 | -939.85 | -7.49 | 11 | 8 | -933.27 | -6.21 | 22 | 7 | -927.74 | -5.87 |
| 1 | 3 | -939.43 | -7.48 | 11 | 9 | -932.92 | -5.96 | 23 | 0 | -933.9 | -6.27 |
| 1 | 4 | -939.11 | -7.46 | 11 | 10 | -932.76 | -5.92 | 23 | 1 | -933.86 | -6.27 |
| 1 | 5 | -931.88 | -6.53 | 11 | 11 | -932.67 | -5.92 | 23 | 2 | -933.84 | -6.25 |
| 1 | 6 | -931.5 | -6.92 | 11 | 12 | -932.65 | -5.93 | 23 | 3 | -931.07 | -6.43 |
| 2 | 0 | -937.93 | -7.2 | 12 | 0 | -935.7 | -6.26 | 23 | 4 | -930.61 | -6.24 |
| 2 | 1 | -933.86 | -6.52 | 12 | 1 | -935.67 | -6.25 | 23 | 5 | -930.6 | -6.46 |
| 2 | 2 | -933.8 | -6.5 | 12 | 2 | -935.6 | -6.23 | 23 | 6 | -930.55 | -6.46 |
| 2 | 3 | -933.71 | -6.5 | 12 | 3 | -930.39 | -5.75 | 23 | 7 | -930.55 | -6.24 |
| 2 | 4 | -923.01 | -5.37 | 12 | 4 | -929.84 | -5.66 | 24 | 0 | -933.76 | -5.86 |
| 2 | 5 | -922.98 | -5.37 | 12 | 5 | -929.53 | -5.61 | 24 | 1 | -933.47 | -5.83 |
| 2 | 6 | -922.97 | -5.36 | 12 | 6 | -929.34 | -5.61 | 24 | 2 | -933.47 | -5.83 |
| 2 | 7 | -921.46 | -5.33 | 12 | 7 | -929.2 | -5.58 | 24 | 3 | -933.45 | -5.83 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 0 | -937.83 | -6.51 | 13 | 0 | -935.46 | -5.88 | 24 | 4 | -933.45 | -5.83 |
| 3 | 1 | -936.12 | -6.39 | 13 | 1 | -935.46 | -5.88 | 24 | 5 | -933.45 | -5.83 |
| 3 | 2 | -936.12 | -6.39 | 13 | 2 | -935.46 | -5.88 | 24 | 6 | -933.45 | -5.83 |
| 3 | 3 | -936.12 | -6.39 | 13 | 3 | -935.46 | -5.88 | 24 | 7 | -933.45 | -5.83 |
| 3 | 4 | -935.67 | -6.36 | 13 | 4 | -935.46 | -5.88 | 25 | 0 | -933.43 | -6.06 |
| 3 | 5 | -935.67 | -6.36 | 13 | 5 | -935.45 | -5.88 | 25 | 1 | -933.43 | -6.06 |
| 3 | 6 | -935.67 | -6.36 | 13 | 6 | -935.45 | -5.88 | 25 | 2 | -933.43 | -6.06 |
| 3 | 7 | -935.67 | -6.36 | 13 | 7 | -935.45 | -5.88 | 25 | 3 | -933.4 | -6.07 |
| 4 | 0 | -937.22 | -6.58 | 14 | 0 | -935.32 | -6.53 | 25 | 4 | -933.4 | -6.07 |
| 4 | 1 | -937.13 | -6.57 | 14 | 1 | -935.3 | -6.53 | 25 | 5 | -933.4 | -6.07 |
| 4 | 2 | -937.03 | -6.56 | 14 | 2 | -929.03 | -5.86 | 25 | 6 | -933.27 | -6.05 |
| 4 | 3 | -936.98 | -6.55 | 14 | 3 | -927.09 | -6.39 | 25 | 7 | -933.27 | -6.05 |
| 4 | 4 | -936.64 | -6.55 | 14 | 4 | -924.84 | -5.78 | 26 | 0 | -933.43 | -6.55 |
| 4 | 5 | -931.18 | -6.18 | 14 | 5 | -924.12 | -5.82 | 26 | 1 | -933.05 | -6.58 |
| 4 | 6 | -930.67 | -6.16 | 14 | 6 | -923.32 | -5.51 | 26 | 2 | -932.18 | -6.6 |
| 4 | 7 | -930.58 | -6.14 | 14 | 7 | -921.23 | -5.87 | 26 | 3 | -927.48 | -5.95 |
| 5 | 0 | -937.21 | -6.24 | 15 | 0 | -935.28 | -6.58 | 26 | 4 | -926.58 | -6.16 |
| 5 | 1 | -937.21 | -6.24 | 15 | 1 | -935.25 | -6.58 | 26 | 5 | -925.11 | -6.07 |
| 5 | 2 | -937.17 | -6.24 | 15 | 2 | -935.25 | -6.58 | 27 | 0 | -933.35 | -5.79 |
| 5 | 3 | -937.17 | -6.24 | 15 | 3 | -927.83 | -6.07 | 27 | 1 | -933.35 | -5.79 |
| 5 | 4 | -937.16 | -6.24 | 15 | 4 | -927.83 | -6.07 | 27 | 2 | -933.35 | -5.79 |
| 5 | 5 | -937.16 | -6.24 | 15 | 5 | -925.22 | -5.87 | 27 | 3 | -933.35 | -5.79 |
| 5 | 6 | -937.16 | -6.24 | 15 | 6 | -924.86 | -5.81 | 27 | 4 | -933.33 | -5.79 |
| 5 | 7 | -937.16 | -6.24 | 15 | 7 | -924.86 | -5.81 | 27 | 5 | -933.33 | -5.79 |
| 5 | 8 | -933.73 | -6.05 | 16 | 0 | -934.95 | -5.79 | 27 | 6 | -933.33 | -5.79 |
| 5 | 9 | -933.49 | -6.05 | 16 | 1 | -934.95 | -5.79 | 27 | 7 | -933.33 | -5.79 |
| 5 | 10 | -933.32 | -6.05 | 16 | 2 | -934.76 | -5.75 | 28 | 0 | -933.2 | -6.58 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 0 | -937.15 | -6.73 | 16 | 3 | -934.76 | -5.75 | 28 | 1 | -933.19 | -6.58 |
| 6 | 1 | -936.99 | -6.72 | 16 | 4 | -934.76 | -5.75 | 28 | 2 | -933.18 | -6.59 |
| 6 | 2 | -936.87 | -6.71 | 16 | 5 | -933.77 | -5.67 | 28 | 3 | -933.18 | -6.57 |
| 6 | 3 | -936.79 | -6.71 | 16 | 6 | -933.77 | -5.67 | 28 | 4 | -932.93 | -6.66 |
| 6 | 4 | -929.35 | -6.25 | 16 | 7 | -933.77 | -5.67 | 28 | 5 | -931.65 | -6.83 |
| 6 | 5 | -929.33 | -6.26 | 17 | 0 | -934.78 | -6.49 | 28 | 6 | -931.64 | -6.82 |
| 6 | 6 | -929.33 | -6.26 | 17 | 1 | -934.71 | -6.51 | 29 | 0 | -932.6 | -6.47 |
| 6 | 7 | -929.3 | -6.27 | 17 | 2 | -934.66 | -6.5 | 29 | 1 | -932.6 | -6.47 |
| 7 | 0 | -936.92 | -6.14 | 17 | 3 | -934.65 | -6.49 | 29 | 2 | -932.6 | -6.47 |
| 7 | 1 | -936.92 | -6.14 | 17 | 4 | -933.98 | -6.38 | 29 | 3 | -932.6 | -6.47 |
| 7 | 2 | -936.92 | -6.14 | 17 | 5 | -933.93 | -6.42 | 29 | 4 | -932.6 | -6.47 |
| 7 | 3 | -936.92 | -6.14 | 17 | 6 | -933.9 | -6.42 | 29 | 5 | -932.51 | -6.46 |
| 7 | 4 | -936.91 | -6.14 | 17 | 7 | -933.75 | -6.38 | 29 | 6 | -932.51 | -6.46 |
| 7 | 5 | -936.91 | -6.14 | 18 | 0 | -934.67 | -6.4 | 29 | 7 | -932.51 | -6.46 |
| 7 | 6 | -936.91 | -6.14 | 18 | 1 | -934.53 | -6.39 | 29 | 8 | -929.96 | -6.03 |
| 7 | 7 | -936.79 | -6.13 | 18 | 2 | -934.45 | -6.39 | 29 | 9 | -929.02 | -6.03 |
| 8 | 0 | -936.8 | -6.66 | 18 | 3 | -933.78 | -6.29 | 30 | 0 | -931.24 | -6 |
| 8 | 1 | -935.89 | -6.54 | 18 | 4 | -930.83 | -6 | 31 | 0 | -930.54 | -6.16 |
| 8 | 2 | -935.82 | -6.54 | 18 | 5 | -930.1 | -5.93 | 31 | 1 | -927.88 | -5.94 |
| 8 | 3 | -935.57 | -6.52 | 18 | 6 | -929.27 | -6.03 | 31 | 2 | -926.91 | -6 |
| 8 | 4 | -935.48 | -6.54 | 18 | 7 | -928.21 | -5.85 | 32 | 0 | -927 | -6.09 |
| 8 | 5 | -934.8 | -6.45 | 19 | 0 | -934.18 | -6.05 | 33 | 0 | -923.94 | -5.95 |
| 8 | 6 | -934 | -6.38 | 19 | 1 | -934.18 | -6.05 | 33 | 1 | -921.56 | -7.07 |
| 8 | 7 | -933.3 | -6.4 | 19 | 2 | -934.18 | -6.05 | 33 | 2 | -919.93 | -6.32 |
| 9 | 0 | -936.6 | -6.52 | 19 | 3 | -934.18 | -6.05 | 33 | 3 | -908.27 | -5.03 |
| 9 | 1 | -936.59 | -6.54 | 19 | 4 | -934 | -6.06 | 33 | 4 | -897.72 | -4.85 |
| 9 | 2 | -936.51 | -6.51 | 19 | 5 | -933 | -6.11 | 33 | 5 | -897.72 | -4.84 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| 9 | 3 | -936.44 | -6.51 | 19 | 6 | -933 | -6.11 | 34 | 0 | -912.73 | -5.73 |
| 9 | 4 | -936.42 | -6.53 | 19 | 7 | -933 | -6.11 | 34 | 0 | -912.73 | -5.73 |
| 9 | 5 | -935.99 | -6.46 | 20 | 0 | -934 | -6.38 | | | | |
| 9 | 6 | -935.8 | -6.47 | 20 | 1 | -933.99 | -6.38 | | | | |
| 9 | 7 | -935.8 | -6.47 | 20 | 2 | -933.43 | -6.4 | | | | |
| 9 | 8 | -935.8 | -6.44 | 20 | 3 | -933.38 | -6.4 | | | | |
| 9 | 9 | -935.8 | -6.44 | 20 | 4 | -931.26 | -6.21 | | | | |
| 9 | 10 | -934.7 | -6.22 | 21 | 0 | -933.94 | -5.82 | | | | |
| 9 | 11 | -934.26 | -6.16 | 21 | 1 | -933.89 | -5.81 | | | | |
| 9 | 12 | -933.28 | -6.43 | 21 | 2 | -933.89 | -5.81 | | | | |
| 9 | 13 | -933.23 | -6.47 | 21 | 3 | -933.62 | -5.8 | | | | |
| 9 | 14 | -933.18 | -6.47 | 21 | 4 | -933.62 | -5.8 | | | | |