Supplementary Information

Table 1. Estimated and predicted free energy upon binding of paclitaxel and epothilone analogs to tubulin; kcal/mol.

Compd	K_{exp}(μM)	K_{pred}(μM)	Kp/Ke	ΔG_{exp}	ΔG_{pred}	ΔΔG	Ref
Training set [a]							
1	15	14	0.9	-6.5	-6.5	0.0	d
2	7.5	6.9	0.9	-6.9	-6.9	0.0	e
3	60	46	0.8	-5.7	-5.8	-0.1	e
4	4.4	3.8	0.9	-7.2	-7.3	-0.1	f
5	7.6	7.4	1.0	-6.9	-6.9	0.0	e
6	11	19	1.7	-6.6	-6.3	0.3	g
7	3000	2300	0.8	-3.4	-3.5	-0.1	h
8	4500	4700	1.1	-3.1	-3.1	0.0	i
9	4500	3700	0.8	-3.1	-3.2	0.1	j
13	120	140	1.1	-5.2	-5.1	0.1	k
14	710	570	0.8	-4.2	-4.3	-0.1	k
15	3400	4100	1.2	-3.3	-3.2	0.1	k
17	4.0	3.3	0.8	-7.2	-7.3	0.1	d
19	22	65	2.8	-6.2	-5.6	0.6	d
26	39	26	0.7	-5.9	-6.1	-0.2	d
Test set [b]							
10	18	11	0.7	-6.4	-6.6	-0.2	e
11	90	150	1.6	-5.4	-5.1	0.3	f
12	260	830	3.2	-4.8	-4.1	0.7	e
16	14	12	0.9	-6.5	-6.6	-0.1	d
18	71% [b]	22			-6.3		l
20	17% [b]	1400			-3.8		l
21	0.5% [b,c]	1300			-3.9		m
22	51% [b]	75			-5.5		l
23	13% [b]	6200			-3.0		l
24	25	29	1.2	-6.2	-6.1	0.1	d
25	3.3	14	4.1	-7.3	-6.5	0.8	d
17'	4.0	180000[d]	45000	-7.2	-1.0	-6.2	n

[a] slope=0.26, intercept=1.79, R=0.99, rms=0.19 Kcal / mol,

[b] Percentage of tubulin polymerization from Ref. 5f,

[c] Relative to 16. [d] Epothilone B with thiazole ring matched to paclitaxel's C-10 Oac,

[d] Ref. 5g,

[e] Ref. 12,

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[l] Ref. 5f,

[m] Ref. 5n,

[n] Ref. 21.

20 Amino Acid Minireceptor, pdb coordinates.

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HEADER    PROTEIN                         12-MAR-99
COMPND    TAXOL_MINIRECEPTOR
AUTHOR    GENERATED BY SYBYL, A PRODUCT OF TRIPOS ASSOCIATES, INC.
SEQRES   1     1  ARG
SEQRES   1     1  GLU
SEQRES   1     1  VAL
SEQRES   1     1  HID
SEQRES   1     1  ILE
SEQRES   1     1  CYS
SEQRES   1     1  VAL
SEQRES   1     1  VAL
SEQRES   1     1  ILE
SEQRES   1     1  GLU
SEQRES   1     1  PHE
SEQRES   1     1  PHE
SEQRES   1     1  TYR
SEQRES   1     1  VAL
SEQRES   1     1  ARG
SEQRES   1     1  SER
SEQRES   1     1  LEU
SEQRES   1     1  ASN
SEQRES   1     1  GLY
SEQRES   1     1  PRO
SEQRES   1     1  LEU
ATOM      1  N   ARG     4     -3.298  -1.072   3.529  1.00  0.00
ATOM      2  CA  ARG     4      -2.423  -1.695   2.544  1.00  0.00
ATOM      3  C   ARG     4     -1.054  -1.982   3.185  1.00  0.00
ATOM      4  O   ARG     4     -0.680  -3.135   3.409  1.00  0.00
ATOM      5  CB  ARG     4      -2.353  -0.837   1.259  1.00  0.00
ATOM      6  CG  ARG     4      -3.644  -0.555   0.459  1.00  0.00
ATOM      7  CD  ARG     4      -3.553   0.263  -0.828  1.00  0.00
ATOM      8  NE  ARG     4      -4.862   0.467  -1.455  1.00  0.00
ATOM      9  CZ  ARG     4      -5.465  -0.415  -2.276  1.00  0.00
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ATOM     10  NH1 ARG     4      -4.772  -1.459  -2.780  1.00  0.00
ATOM     11  NH2 ARG     4      -6.760  -0.218  -2.589  1.00  0.00
ATOM     12  HN  ARG     4      -3.539  -1.593   4.359  1.00  0.00
ATOM     13  HA  ARG     4      -2.874  -2.675   2.267  1.00  0.00
ATOM     14  HB1 ARG     4      -1.932   0.151   1.551  1.00  0.00
ATOM     15  HB2 ARG     4      -1.646  -1.349   0.567  1.00  0.00
ATOM     16  HG1 ARG     4      -4.081  -1.542   0.187  1.00  0.00
ATOM     17  HG2 ARG     4      -4.340  -0.017   1.139  1.00  0.00
ATOM     18  HD1 ARG     4      -3.112   1.257  -0.591  1.00  0.00
ATOM     19  HD2 ARG     4      -2.892  -0.272  -1.548  1.00  0.00
ATOM     20  HNE ARG     4      -5.341   1.325  -1.216  1.00  0.00
ATOM     21  HN11ARG     4      -5.122  -1.998  -3.562  1.00  0.00
ATOM     22  HN12ARG     4      -3.875  -1.709  -2.387  1.00  0.00
ATOM     23  HN21ARG     4      -7.262  -0.755  -3.288  1.00  0.00
ATOM     24  HN22ARG     4      -7.289   0.512  -2.119  1.00  0.00
TER      25      ARG     4
ATOM     26  N   GLU     5      -5.378   1.690   3.960  1.00  0.00
ATOM     27  CA  GLU     5      -6.462   0.991   4.621  1.00  0.00
ATOM     28  C   GLU     5      -6.062   0.651   6.064  1.00  0.00
ATOM     29  O   GLU     5      -6.858   0.123   6.843  1.00  0.00
ATOM     30  CB  GLU     5      -6.865  -0.260   3.823  1.00  0.00
ATOM     31  CG  GLU     5      -7.259  -0.045   2.352  1.00  0.00
ATOM     32  CD  GLU     5      -7.396  -1.302   1.500  1.00  0.00
ATOM     33  OE1 GLU     5      -8.099  -2.236   1.944  1.00  0.00
ATOM     34  OE2 GLU     5      -6.792  -1.304   0.406  1.00  0.00
ATOM     35  HN  GLU     5      -4.810   1.166   3.296  1.00  0.00
ATOM     36  HA  GLU     5      -7.339   1.674   4.659  1.00  0.00
ATOM     37  HB1 GLU     5      -6.004  -0.965   3.840  1.00  0.00
ATOM     38  HB2 GLU     5      -7.733  -0.725   4.340  1.00  0.00
ATOM     39  HG1 GLU     5      -8.237   0.484   2.338  1.00  0.00
ATOM     40  HG2 GLU     5      -6.482   0.600   1.884  1.00  0.00
TER      41      GLU     5
ATOM     42  N   VAL     6     -15.799   3.398   1.162  1.00  0.00
ATOM     43  CA  VAL     6     -14.414   2.980   0.932  1.00  0.00
ATOM     44  C   VAL     6     -13.751   3.957  -0.053  1.00  0.00
ATOM     45  O   VAL     6     -14.418   4.597  -0.863  1.00  0.00
ATOM     46  CB  VAL     6     -14.352   1.494   0.491  1.00  0.00
ATOM     47  CG1 VAL     6     -14.991   0.626   1.578  1.00  0.00
ATOM     48  CG2 VAL     6     -15.087   1.252  -0.834  1.00  0.00
ATOM     49  HN  VAL     6     -16.197   4.099   0.555  1.00  0.00
ATOM     50  HA  VAL     6     -13.876   3.064   1.902  1.00  0.00
ATOM     51  HB  VAL     6     -13.286   1.199   0.373  1.00  0.00
ATOM     52  HG1 VAL     6     -14.760  -0.446   1.391  1.00  0.00
ATOM     53  HG2 VAL     6     -14.592   0.925   2.572  1.00  0.00
ATOM     54  HG3 VAL     6     -16.095   0.775   1.569  1.00  0.00
ATOM     55  HG4 VAL     6     -15.050   0.170  -1.097  1.00  0.00
ATOM     56  HG5 VAL     6     -16.148   1.573  -0.735  1.00  0.00
ATOM     57  HG6 VAL     6     -14.602   1.844  -1.642  1.00  0.00
TER      58      VAL     6
ATOM     59  N   HID     7      -9.596  -7.773   6.064  1.00  0.00
ATOM     60  CA  HID     7      -9.237  -6.475   5.492  1.00  0.00
ATOM     61  C   HID     7      -9.607  -5.377   6.501  1.00  0.00
ATOM     62  O   HID     7     -10.698  -5.372   7.069  1.00  0.00
ATOM     63  CB  HID     7      -9.858  -6.275   4.081  1.00  0.00
ATOM     64  CG  HID     7      -9.614  -7.374   3.074  1.00  0.00
ATOM     65  ND1 HID     7      -8.500  -8.114   3.072  1.00  0.00
ATOM     66  CD2 HID     7     -10.382  -7.838   2.033  1.00  0.00
ATOM     67  CE1 HID     7      -8.569  -9.001   2.067  1.00  0.00
ATOM     68  NE2 HID     7      -9.711  -8.873   1.391  1.00  0.00
ATOM     69  HN  HID     7     -10.571  -8.032   6.093  1.00  0.00
ATOM     70  HA  HID     7      -8.131  -6.461   5.374  1.00  0.00
ATOM     71  HB1 HID     7     -10.960  -6.170   4.205  1.00  0.00
ATOM     72  HB2 HID     7      -9.441  -5.331   3.661  1.00  0.00
ATOM     73  HND HID     7      -7.733  -7.996   3.730  1.00  0.00
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ATOM     74  HE  HID     7      -7.786  -9.736   1.832  1.00  0.00
ATOM     75  HD  HID     7     -11.373  -7.449   1.751  1.00  0.00
TER      76      HID     7
ATOM     77  N   ILE     8     -18.590  -4.536   4.285  1.00  0.00
ATOM     78  CA  ILE     8     -18.080  -3.167   4.362  1.00  0.00
ATOM     79  C   ILE     8     -19.252  -2.196   4.143  1.00  0.00
ATOM     80  O   ILE     8     -20.367  -2.603   3.819  1.00  0.00
ATOM     81  CB  ILE     8     -16.883  -2.944   3.398  1.00  0.00
ATOM     82  CG1 ILE     8     -17.365  -2.764   1.943  1.00  0.00
ATOM     83  CG2 ILE     8     -16.017  -1.752   3.844  1.00  0.00
ATOM     84  CD1 ILE     8     -18.214  -3.880   1.317  1.00  0.00
ATOM     85  HN  ILE     8     -19.556  -4.676   4.028  1.00  0.00
ATOM     86  HA  ILE     8     -17.708  -3.011   5.399  1.00  0.00
ATOM     87  HB  ILE     8     -16.245  -3.855   3.431  1.00  0.00
ATOM     88  HG1 ILE     8     -15.217  -1.560   3.096  1.00  0.00
ATOM     89  HG2 ILE     8     -16.657  -0.845   3.942  1.00  0.00
ATOM     90  HG3 ILE     8     -15.556  -1.978   4.831  1.00  0.00
ATOM     91  HG4 ILE     8     -17.968  -1.830   1.907  1.00  0.00
ATOM     92  HG5 ILE     8     -16.460  -2.642   1.307  1.00  0.00
ATOM     93  HD1 ILE     8     -18.317  -3.711   0.220  1.00  0.00
ATOM     94  HD2 ILE     8     -17.726  -4.864   1.495  1.00  0.00
ATOM     95  HD3 ILE     8     -19.224  -3.886   1.785  1.00  0.00
TER      96      ILE     8
ATOM     97  N   CYS     9     -15.347  -1.999  -5.699  1.00  0.00
ATOM     98  CA  CYS     9     -15.247  -2.415  -4.302  1.00  0.00
ATOM     99  C   CYS     9     -14.733  -1.253  -3.440  1.00  0.00
ATOM    100  O   CYS     9     -13.561  -0.884  -3.495  1.00  0.00
ATOM    101  CB  CYS     9     -14.371  -3.678  -4.183  1.00  0.00
ATOM    102  SG  CYS     9     -14.982  -5.064  -5.186  1.00  0.00
ATOM    103  HN  CYS     9     -14.529  -1.612  -6.148  1.00  0.00
ATOM    104  HA  CYS     9     -16.269  -2.676  -3.947  1.00  0.00
ATOM    105  HB1 CYS     9     -13.340  -3.426  -4.513  1.00  0.00
ATOM    106  HB2 CYS     9     -14.349  -3.995  -3.115  1.00  0.00
ATOM    107  HSG CYS     9     -14.127  -5.597  -5.193  1.00  0.00
TER     108      CYS     9
ATOM    109  N   VAL    10      -8.268   2.654  -1.251  1.00  0.00
ATOM    110  CA  VAL    10      -8.971   2.794  -2.527  1.00  0.00
ATOM    111  C   VAL    10      -9.567   4.208  -2.621  1.00  0.00
ATOM    112  O   VAL    10      -9.591   4.956  -1.645  1.00  0.00
ATOM    113  CB  VAL    10     -10.003   1.654  -2.720  1.00  0.00
ATOM    114  CG1 VAL    10     -11.065   1.756  -1.623  1.00  0.00
ATOM    115  CG2 VAL    10     -10.693   1.720  -4.089  1.00  0.00
ATOM    116  HN  VAL    10      -8.375   3.382  -0.560  1.00  0.00
ATOM    117  HA  VAL    10      -8.212   2.698  -3.337  1.00  0.00
ATOM    118  HB  VAL    10      -9.480   0.675  -2.625  1.00  0.00
ATOM    119  HG1 VAL    10     -11.824   0.953  -1.754  1.00  0.00
ATOM    120  HG2 VAL    10     -10.581   1.651  -0.626  1.00  0.00
ATOM    121  HG3 VAL    10     -11.563   2.749  -1.681  1.00  0.00
ATOM    122  HG4 VAL    10     -11.372   0.848  -4.213  1.00  0.00
ATOM    123  HG5 VAL    10     -11.283   2.662  -4.161  1.00  0.00
ATOM    124  HG6 VAL    10      -9.925   1.710  -4.892  1.00  0.00
TER     125      VAL    10
ATOM    126  N   VAL    11     -15.071  -8.424   6.047  1.00  0.00
ATOM    127  CA  VAL    11     -14.594  -8.861   4.733  1.00  0.00
ATOM    128  C   VAL    11     -13.090  -9.175   4.822  1.00  0.00
ATOM    129  O   VAL    11     -12.324  -8.450   5.456  1.00  0.00
ATOM    130  CB  VAL    11     -14.965  -7.827   3.639  1.00  0.00
ATOM    131  CG1 VAL    11     -16.487  -7.761   3.513  1.00  0.00
ATOM    132  CG2 VAL    11     -14.432  -6.423   3.964  1.00  0.00
ATOM    133  HN  VAL    11     -14.429  -7.934   6.653  1.00  0.00
ATOM    134  HA  VAL    11     -15.120  -9.811   4.488  1.00  0.00
ATOM    135  HB  VAL    11     -14.535  -8.160   2.669  1.00  0.00
ATOM    136  HG1 VAL    11     -16.772  -7.029   2.723  1.00  0.00
ATOM    137  HG2 VAL    11     -16.881  -8.766   3.246  1.00  0.00
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ATOM    138  HG3 VAL    11     -16.927  -7.445   4.486  1.00  0.00
ATOM    139  HG4 VAL    11     -14.566  -5.754   3.084  1.00  0.00
ATOM    140  HG5 VAL    11     -14.988  -6.008   4.835  1.00  0.00
ATOM    141  HG6 VAL    11     -13.351  -6.487   4.221  1.00  0.00
TER     142      VAL    11
ATOM    143  N   ILE    12      -3.209  -7.012 -12.995  1.00  0.00
ATOM    144  CA  ILE    12      -1.928  -7.714 -13.063  1.00  0.00
ATOM    145  C   ILE    12      -2.038  -9.014 -12.250  1.00  0.00
ATOM    146  O   ILE    12      -2.954  -9.190 -11.446  1.00  0.00
ATOM    147  CB  ILE    12      -0.746  -6.799 -12.636  1.00  0.00
ATOM    148  CG1 ILE    12      -0.437  -5.744 -13.718  1.00  0.00
ATOM    149  CG2 ILE    12      -1.017  -6.130 -11.275  1.00  0.00
ATOM    150  CD1 ILE    12      -1.560  -4.785 -14.138  1.00  0.00
ATOM    151  HN  ILE    12      -3.962  -7.434 -12.474  1.00  0.00
ATOM    152  HA  ILE    12      -1.761  -8.000 -14.125  1.00  0.00
ATOM    153  HB  ILE    12       0.156  -7.440 -12.522  1.00  0.00
ATOM    154  HG1 ILE    12      -0.153  -5.495 -10.985  1.00  0.00
ATOM    155  HG2 ILE    12      -1.932  -5.498 -11.350  1.00  0.00
ATOM    156  HG3 ILE    12      -1.181  -6.914 -10.503  1.00  0.00
ATOM    157  HG4 ILE    12       0.406  -5.122 -13.342  1.00  0.00
ATOM    158  HG5 ILE    12      -0.114  -6.292 -14.630  1.00  0.00
ATOM    159  HD1 ILE    12      -1.151  -3.981 -14.790  1.00  0.00
ATOM    160  HD2 ILE    12      -2.343  -5.348 -14.693  1.00  0.00
ATOM    161  HD3 ILE    12      -2.018  -4.328 -13.231  1.00  0.00
TER     162      ILE    12
ATOM    163  N   GLU    13      -2.049  -4.539  -3.984  1.00  0.00
ATOM    164  CA  GLU    13      -0.663  -4.679  -4.383  1.00  0.00
ATOM    165  C   GLU    13      -0.035  -3.295  -4.593  1.00  0.00
ATOM    166  O   GLU    13       0.304  -2.590  -3.642  1.00  0.00
ATOM    167  CB  GLU    13      -0.546  -5.564  -5.637  1.00  0.00
ATOM    168  CG  GLU    13      -0.961  -7.036  -5.483  1.00  0.00
ATOM    169  CD  GLU    13      -0.678  -7.944  -6.675  1.00  0.00
ATOM    170  OE1 GLU    13      -0.563  -7.413  -7.802  1.00  0.00
ATOM    171  OE2 GLU    13      -0.581  -9.166  -6.435  1.00  0.00
ATOM    172  HN  GLU    13      -2.612  -5.385  -3.922  1.00  0.00
ATOM    173  HA  GLU    13      -0.116  -5.181  -3.555  1.00  0.00
ATOM    174  HB1 GLU    13      -1.187  -5.115  -6.428  1.00  0.00
ATOM    175  HB2 GLU    13       0.516  -5.544  -5.967  1.00  0.00
ATOM    176  HG1 GLU    13      -0.416  -7.451  -4.605  1.00  0.00
ATOM    177  HG2 GLU    13      -2.054  -7.062  -5.287  1.00  0.00
TER     178      GLU    13
ATOM    179  N   PHE    14      -6.615   1.997  -9.375  1.00  0.00
ATOM    180  CA  PHE    14      -6.965   2.036  -7.968  1.00  0.00
ATOM    181  C   PHE    14      -5.797   2.650  -7.201  1.00  0.00
ATOM    182  O   PHE    14      -4.864   3.163  -7.823  1.00  0.00
ATOM    183  CB  PHE    14      -7.297   0.626  -7.461  1.00  0.00
ATOM    184  CG  PHE    14      -8.355  -0.117  -8.244  1.00  0.00
ATOM    185  CD1 PHE    14      -7.984  -0.915  -9.342  1.00  0.00
ATOM    186  CD2 PHE    14      -9.708  -0.013  -7.878  1.00  0.00
ATOM    187  CE1 PHE    14      -8.964  -1.611 -10.069  1.00  0.00
ATOM    188  CE2 PHE    14     -10.689  -0.709  -8.605  1.00  0.00
ATOM    189  CZ  PHE    14     -10.317  -1.507  -9.702  1.00  0.00
ATOM    190  HN  PHE    14      -5.679   2.306  -9.612  1.00  0.00
ATOM    191  HA  PHE    14      -7.860   2.684  -7.838  1.00  0.00
ATOM    192  HB1 PHE    14      -6.360   0.023  -7.489  1.00  0.00
ATOM    193  HB2 PHE    14      -7.647   0.713  -6.407  1.00  0.00
ATOM    194  HD1 PHE    14      -6.924  -0.992  -9.632  1.00  0.00
ATOM    195  HE1 PHE    14      -8.673  -2.236 -10.927  1.00  0.00
ATOM    196  HZ1 PHE    14     -11.086  -2.052 -10.272  1.00  0.00
ATOM    197  HE2 PHE    14     -11.748  -0.629  -8.316  1.00  0.00
ATOM    198  HD2 PHE    14     -10.000   0.614  -7.021  1.00  0.00
TER     199      PHE    14
ATOM    200  N   PHE    15     -12.726  -9.947   0.814  1.00  0.00
ATOM    201  CA  PHE    15     -13.876 -10.679   1.309  1.00  0.00
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ATOM    202  C   PHE    15     -13.378 -11.957   1.979  1.00  0.00
ATOM    203  O   PHE    15     -13.990 -13.012   1.805  1.00  0.00
ATOM    204  CB  PHE    15     -14.852 -10.983   0.164  1.00  0.00
ATOM    205  CG  PHE    15     -15.254  -9.797  -0.682  1.00  0.00
ATOM    206  CD1 PHE    15     -15.080  -9.839  -2.077  1.00  0.00
ATOM    207  CD2 PHE    15     -15.801  -8.652  -0.077  1.00  0.00
ATOM    208  CE1 PHE    15     -15.459  -8.741  -2.867  1.00  0.00
ATOM    209  CE2 PHE    15     -16.179  -7.552  -0.868  1.00  0.00
ATOM    210  CZ  PHE    15     -16.007  -7.597  -2.262  1.00  0.00
ATOM    211  HN  PHE    15     -12.720  -9.744  -0.179  1.00  0.00
ATOM    212  HA  PHE    15     -14.398 -10.055   2.069  1.00  0.00
ATOM    213  HB1 PHE    15     -14.372 -11.734  -0.505  1.00  0.00
ATOM    214  HB2 PHE    15     -15.777 -11.419   0.606  1.00  0.00
ATOM    215  HD1 PHE    15     -14.648 -10.734  -2.551  1.00  0.00
ATOM    216  HE1 PHE    15     -15.324  -8.775  -3.961  1.00  0.00
ATOM    217  HZ1 PHE    15     -16.303  -6.735  -2.881  1.00  0.00
ATOM    218  HE2 PHE    15     -16.611  -6.656  -0.394  1.00  0.00
ATOM    219  HD2 PHE    15     -15.934  -8.615   1.015  1.00  0.00
TER     220      PHE    15
ATOM    221  N   TYR    16      -2.854 -11.170   3.349  1.00  0.00
ATOM    222  CA  TYR    16      -1.886 -10.821   2.327  1.00  0.00
ATOM    223  C   TYR    16      -0.541 -11.431   2.713  1.00  0.00
ATOM    224  O   TYR    16      -0.202 -11.453   3.898  1.00  0.00
ATOM    225  CB  TYR    16      -1.795  -9.297   2.175  1.00  0.00
ATOM    226  CG  TYR    16      -1.090  -8.763   0.944  1.00  0.00
ATOM    227  CD1 TYR    16      -1.655  -8.960  -0.330  1.00  0.00
ATOM    228  CD2 TYR    16       0.136  -8.086   1.066  1.00  0.00
ATOM    229  CE1 TYR    16      -1.002  -8.469  -1.475  1.00  0.00
ATOM    230  CE2 TYR    16       0.787  -7.592  -0.076  1.00  0.00
ATOM    231  CZ  TYR    16       0.218  -7.782  -1.349  1.00  0.00
ATOM    232  OH  TYR    16       0.846  -7.303  -2.460  1.00  0.00
ATOM    233  HN  TYR    16      -2.475 -11.515   4.224  1.00  0.00
ATOM    234  HA  TYR    16      -2.215 -11.260   1.358  1.00  0.00
ATOM    235  HB1 TYR    16      -2.835  -8.901   2.167  1.00  0.00
ATOM    236  HB2 TYR    16      -1.256  -8.905   3.066  1.00  0.00
ATOM    237  HD1 TYR    16      -2.608  -9.500  -0.430  1.00  0.00
ATOM    238  HE1 TYR    16      -1.447  -8.623  -2.470  1.00  0.00
ATOM    239  HOH TYR    16       1.723  -6.949  -2.286  1.00  0.00
ATOM    240  HE2 TYR    16       1.744  -7.058   0.023  1.00  0.00
ATOM    241  HD2 TYR    16       0.586  -7.943   2.061  1.00  0.00
TER     242      TYR    16
ATOM    243  N   VAL    17      -5.981  -5.269   9.511  1.00  0.00
ATOM    244  CA  VAL    17      -6.121  -5.824   8.163  1.00  0.00
ATOM    245  C   VAL    17      -5.912  -7.346   8.224  1.00  0.00
ATOM    246  O   VAL    17      -5.366  -7.871   9.181  1.00  0.00
ATOM    247  CB  VAL    17      -5.189  -5.089   7.163  1.00  0.00
ATOM    248  CG1 VAL    17      -5.592  -3.614   7.102  1.00  0.00
ATOM    249  CG2 VAL    17      -3.725  -5.183   7.575  1.00  0.00
ATOM    250  HN  VAL    17      -5.401  -5.760  10.175  1.00  0.00
ATOM    251  HA  VAL    17      -7.169  -5.646   7.836  1.00  0.00
ATOM    252  HB  VAL    17      -5.317  -5.539   6.154  1.00  0.00
ATOM    253  HG1 VAL    17      -5.013  -3.095   6.306  1.00  0.00
ATOM    254  HG2 VAL    17      -6.681  -3.536   6.880  1.00  0.00
ATOM    255  HG3 VAL    17      -5.390  -3.130   8.087  1.00  0.00
ATOM    256  HG4 VAL    17      -3.093  -4.617   6.850  1.00  0.00
ATOM    257  HG5 VAL    17      -3.587  -4.754   8.591  1.00  0.00
ATOM    258  HG6 VAL    17      -3.401  -6.254   7.583  1.00  0.00
TER     259      VAL    17
ATOM    260  N   ARG    18      -7.371 -20.672  -7.020  1.00  0.00
ATOM    261  CA  ARG    18      -7.690 -19.256  -7.139  1.00  0.00
ATOM    262  C   ARG    18      -6.641 -18.430  -6.372  1.00  0.00
ATOM    263  O   ARG    18      -6.914 -17.876  -5.306  1.00  0.00
ATOM    264  CB  ARG    18      -9.149 -18.988  -6.700  1.00  0.00
ATOM    265  CG  ARG    18      -9.657 -17.534  -6.583  1.00  0.00
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ATOM    267  NE  ARG    18     -11.407 -15.858  -6.018  1.00  0.00
ATOM    268  CZ  ARG    18     -10.921 -15.011  -5.090  1.00  0.00
ATOM    269  NH1 ARG    18     -10.078 -15.456  -4.135  1.00  0.00
ATOM    270  NH2 ARG    18     -11.308 -13.721  -5.136  1.00  0.00
ATOM    271  HN  ARG    18      -7.294 -21.076  -6.099  1.00  0.00
ATOM    272  HA  ARG    18      -7.609 -18.982  -8.214  1.00  0.00
ATOM    273  HB1 ARG    18      -9.808 -19.503  -7.435  1.00  0.00
ATOM    274  HB2 ARG    18      -9.276 -19.457  -5.698  1.00  0.00
ATOM    275  HG1 ARG    18      -8.973 -17.006  -5.881  1.00  0.00
ATOM    276  HG2 ARG    18      -9.575 -17.079  -7.594  1.00  0.00
ATOM    277  HD1 ARG    18     -11.795 -17.776  -6.795  1.00  0.00
ATOM    278  HD2 ARG    18     -11.196 -17.732  -5.080  1.00  0.00
ATOM    279  HNE ARG    18     -12.017 -15.501  -6.739  1.00  0.00
ATOM    280  HN11ARG    18      -9.824 -14.884  -3.342  1.00  0.00
ATOM    281  HN12ARG    18      -9.693 -16.390  -4.195  1.00  0.00
ATOM    282  HN21ARG    18     -10.951 -12.999  -4.517  1.00  0.00
ATOM    283  HN22ARG    18     -12.004 -13.425  -5.813  1.00  0.00
TER     284      ARG    18
ATOM    285  N   SER    19       1.154 -14.021  -3.816  1.00  0.00
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ATOM    287  C   SER    19      -0.727 -15.440  -4.484  1.00  0.00
ATOM    288  O   SER    19      -0.595 -16.644  -4.705  1.00  0.00
ATOM    289  CB  SER    19      -0.891 -13.803  -2.523  1.00  0.00
ATOM    290  OG  SER    19      -1.870 -14.546  -1.791  1.00  0.00
ATOM    291  HN  SER    19       1.474 -14.205  -4.757  1.00  0.00
ATOM    292  HA  SER    19       0.372 -15.554  -2.621  1.00  0.00
ATOM    293  HB1 SER    19      -0.268 -13.213  -1.814  1.00  0.00
ATOM    294  HB2 SER    19      -1.404 -13.112  -3.229  1.00  0.00
ATOM    295  HOG SER    19      -2.469 -13.923  -1.366  1.00  0.00
TER     296      SER    19
ATOM    297  N   LEU    20      -8.988 -15.607  -1.472  1.00  0.00
ATOM    298  CA  LEU    20      -7.636 -15.069  -1.514  1.00  0.00
ATOM    299  C   LEU    20      -7.423 -14.106  -0.335  1.00  0.00
ATOM    300  O   LEU    20      -6.654 -14.384   0.585  1.00  0.00
ATOM    301  CB  LEU    20      -7.413 -14.407  -2.876  1.00  0.00
ATOM    302  CG  LEU    20      -6.088 -13.680  -3.218  1.00  0.00
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ATOM    304  CD2 LEU    20      -6.156 -13.059  -4.613  1.00  0.00
ATOM    305  HN  LEU    20      -9.122 -16.551  -1.138  1.00  0.00
ATOM    306  HA  LEU    20      -6.917 -15.914  -1.412  1.00  0.00
ATOM    307  HB1 LEU    20      -7.538 -15.206  -3.638  1.00  0.00
ATOM    308  HB2 LEU    20      -8.225 -13.653  -2.996  1.00  0.00
ATOM    309  HG  LEU    20      -5.956 -12.853  -2.484  1.00  0.00
ATOM    310  HD1 LEU    20      -3.951 -14.050  -3.373  1.00  0.00
ATOM    311  HD2 LEU    20      -4.796 -14.978  -2.059  1.00  0.00
ATOM    312  HD3 LEU    20      -5.006 -15.469  -3.791  1.00  0.00
ATOM    313  HD4 LEU    20      -5.270 -12.407  -4.783  1.00  0.00
ATOM    314  HD5 LEU    20      -6.175 -13.867  -5.379  1.00  0.00
ATOM    315  HD6 LEU    20      -7.085 -12.454  -4.704  1.00  0.00
TER     316      LEU    20
ATOM    317  N   ASN    21      -2.984  -1.593  -5.314  1.00  0.00
ATOM    318  CA  ASN    21      -2.847  -0.140  -5.248  1.00  0.00
ATOM    319  C   ASN    21      -4.144   0.461  -4.694  1.00  0.00
ATOM    320  O   ASN    21      -5.245   0.033  -5.033  1.00  0.00
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ATOM    322  CG  ASN    21      -2.304   1.951  -6.715  1.00  0.00
ATOM    323  OD1 ASN    21      -2.240   2.658  -5.717  1.00  0.00
ATOM    324  ND2 ASN    21      -2.220   2.473  -7.938  1.00  0.00
ATOM    325  HN  ASN    21      -3.908  -1.996  -5.359  1.00  0.00
ATOM    326  HA  ASN    21      -2.033   0.092  -4.527  1.00  0.00
ATOM    327  HB1 ASN    21      -1.441  -0.007  -6.881  1.00  0.00
ATOM    328  HB2 ASN    21      -3.189   0.108  -7.365  1.00  0.00
ATOM    329  HND1ASN    21      -2.176   3.478  -8.017  1.00  0.00
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TER     331      ASN    21
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ATOM    333  CA  GLY    22      -0.591  -4.675   0.501  1.00  0.00
ATOM    334  C   GLY    22       0.805  -4.065   0.382  1.00  0.00
ATOM    335  O   GLY    22       1.275  -3.425   1.324  1.00  0.00
ATOM    336  HN  GLY    22      -0.724  -4.838   2.615  1.00  0.00
ATOM    337  HA1 GLY    22      -0.741  -5.395  -0.334  1.00  0.00
ATOM    338  HA2 GLY    22      -1.345  -3.861   0.427  1.00  0.00
TER     339      GLY    22
ATOM    340  N   PRO    23      -2.725 -12.865  -9.245  1.00  0.00
ATOM    341  CA  PRO    23      -2.038 -12.036  -8.245  1.00  0.00
ATOM    342  C   PRO    23      -1.803 -12.976  -7.071  1.00  0.00
ATOM    343  O   PRO    23      -2.848 -13.245  -6.433  1.00  0.00
ATOM    344  CB  PRO    23      -2.920 -10.837  -7.887  1.00  0.00
ATOM    345  CG  PRO    23      -4.202 -10.988  -8.709  1.00  0.00
ATOM    346  CD  PRO    23      -4.051 -12.284  -9.509  1.00  0.00
ATOM    347  HD1 PRO    23      -4.159 -12.077 -10.574  1.00  0.00
ATOM    348  HD2 PRO    23      -4.818 -12.997  -9.203  1.00  0.00
ATOM    349  HG1 PRO    23      -5.071 -11.048  -8.049  1.00  0.00
ATOM    350  HG2 PRO    23      -4.317 -10.138  -9.383  1.00  0.00
ATOM    351  HB1 PRO    23      -3.152 -10.832  -6.819  1.00  0.00
ATOM    352  HB2 PRO    23      -2.410  -9.908  -8.146  1.00  0.00
ATOM    353  HA  PRO    23      -1.076 -11.699  -8.631  1.00  0.00
TER     354      PRO    23
ATOM    355  N   LEU    24      -6.449 -13.719   4.296  1.00  0.00
ATOM    356  CA  LEU    24      -5.219 -13.323   3.637  1.00  0.00
ATOM    357  C   LEU    24      -5.575 -12.236   2.625  1.00  0.00
ATOM    358  O   LEU    24      -6.662 -11.663   2.704  1.00  0.00
ATOM    359  CB  LEU    24      -4.462 -14.534   3.026  1.00  0.00
ATOM    360  CG  LEU    24      -3.088 -14.366   2.328  1.00  0.00
ATOM    361  CD1 LEU    24      -2.361 -15.697   2.165  1.00  0.00
ATOM    362  CD2 LEU    24      -3.248 -13.674   0.976  1.00  0.00
ATOM    363  HN  LEU    24      -7.255 -13.125   4.126  1.00  0.00
ATOM    364  HA  LEU    24      -4.557 -12.866   4.405  1.00  0.00
ATOM    365  HB1 LEU    24      -4.307 -15.259   3.856  1.00  0.00
ATOM    366  HB2 LEU    24      -5.146 -14.981   2.268  1.00  0.00
ATOM    367  HG  LEU    24      -2.459 -13.712   2.973  1.00  0.00
ATOM    368  HD1 LEU    24      -1.365 -15.531   1.694  1.00  0.00
ATOM    369  HD2 LEU    24      -2.224 -16.171   3.162  1.00  0.00
ATOM    370  HD3 LEU    24      -2.966 -16.375   1.522  1.00  0.00
ATOM    371  HD4 LEU    24      -2.249 -13.500   0.517  1.00  0.00
ATOM    372  HD5 LEU    24      -3.860 -14.314   0.302  1.00  0.00
ATOM    373  HD6 LEU    24      -3.766 -12.700   1.118  1.00  0.00
TER     374      LEU    24
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Taxol Conformation in the Minireceptor, mol2 format

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#       Creating user name:     minmin
#       Creation time:          Fri Mar 12 11:04:55 1999

#       Modifying user name:    minmin
#       Modification time:      Fri Mar 12 11:04:55 1999

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tax.mol2
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SMALL
NO_CHARGES


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     5 CT       -11.1400  -10.0260   -5.5710 C.3      1 <1>        0.0000
     6 CT       -11.8040  -10.0390   -6.9480 C.3      1 <1>        0.0000
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    18 CT       -10.8170   -4.1130   -6.8990 C.3      1 <1>        0.0000
    19 CT        -9.2280  -10.0820   -8.3300 C.3      1 <1>        0.0000
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    21 OE        -7.3770   -8.4130   -5.0140 O.3      1 <1>        0.0000
    22 OE       -10.0480   -8.3360   -4.1180 O.3      1 <1>        0.0000
    23 OE       -10.3930  -11.1900   -5.2980 O.3      1 <1>        0.0000
    24 OH       -11.9500   -9.1020   -9.1050 O.3      1 <1>        0.0000
    25 O         -9.0920   -8.1050  -10.1040 O.2      1 <1>        0.0000
    26 OE        -9.8840   -5.5200  -10.1050 O.3      1 <1>        0.0000
    27 OE        -9.3190   -3.9020   -4.5670 O.3      1 <1>        0.0000
    28 CT        -9.5590   -2.7500   -2.5080 C.3      1 <1>        0.0000
    29 OH        -8.8770   -1.7330   -1.7930 O.3      1 <1>        0.0000
    30 CT        -9.8060   -3.9430   -1.5690 C.3      1 <1>        0.0000
    31 C        -10.9170   -3.7920   -0.5400 C.ar     1 <1>        0.0000
    32 C        -11.4790   -2.5390   -0.2130 C.ar     1 <1>        0.0000
    33 C        -12.5050   -2.4380    0.7450 C.ar     1 <1>        0.0000
    34 C        -12.9790   -3.5900    1.3940 C.ar     1 <1>        0.0000
    35 C        -12.4220   -4.8410    1.0860 C.ar     1 <1>        0.0000
    36 C        -11.3970   -4.9370    0.1270 C.ar     1 <1>        0.0000
    37 N         -8.5940   -4.2340   -0.8140 N.am     1 <1>        0.0000
    38 O         -7.7450   -5.6480   -2.3220 O.2      1 <1>        0.0000
    39 C         -6.2560   -9.1390   -4.9080 C.2      1 <1>        0.0000
    40 O         -5.5900   -9.5010   -5.8420 O.2      1 <1>        0.0000
    41 C         -5.9640   -9.4490   -3.4830 C.ar     1 <1>        0.0000
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42	C	-6.7420	-8.9240	-2.4240	C.ar	1 <1>	0.0000
43	C	-6.4390	-9.2310	-1.0850	C.ar	1 <1>	0.0000
44	C	-5.3510	-10.0660	-0.7830	C.ar	1 <1>	0.0000
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46	C	-4.8740	-10.2830	-3.1600	C.ar	1 <1>	0.0000
47	CT	-11.3840	-7.1890	-2.5830	C.3	1 <1>	0.0000
48	H	-8.4500	-3.7090	0.0330	H	1 <1>	0.0000
49	HO	-11.8480	-8.3300	-9.6790	H	1 <1>	0.0000
50	HO	-7.9930	-2.0810	-1.6210	H	1 <1>	0.0000
51	C	-8.6690	-3.1090	-3.7050	C.2	1 <1>	0.0000
52	O	-7.5490	-2.6870	-3.8400	O.2	1 <1>	0.0000
53	C	-11.1380	-7.5720	-4.0340	C.2	1 <1>	0.0000
54	O	-11.8390	-7.2650	-4.9610	O.2	1 <1>	0.0000
55	C	-7.6500	-5.0780	-1.2390	C.2	1 <1>	0.0000
56	C	-6.4620	-5.3000	-0.3760	C.ar	1 <1>	0.0000
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59	C	-4.1730	-5.7630	1.2320	C.ar	1 <1>	0.0000
60	C	-5.2630	-5.0410	1.7470	C.ar	1 <1>	0.0000
61	C	-6.3990	-4.8130	0.9490	C.ar	1 <1>	0.0000
62	HC	-5.3880	-6.4010	-1.8890	H	1 <1>	0.0000
63	HC	-3.3900	-6.8160	-0.4860	H	1 <1>	0.0000
64	HC	-3.3010	-5.9420	1.8460	H	1 <1>	0.0000
65	HC	-5.2300	-4.6650	2.7610	H	1 <1>	0.0000
66	HC	-7.2300	-4.2720	1.3750	H	1 <1>	0.0000
67	HC	-7.3060	-8.6160	-7.0640	H	1 <1>	0.0000
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71	HC	-12.8860	-9.9820	-6.8150	H	1 <1>	0.0000
72	HC	-11.8180	-7.9640	-7.4240	H	1 <1>	0.0000
73	HC	-10.9080	-6.2020	-8.4570	H	1 <1>	0.0000
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75	HC	-8.4330	-6.2270	-4.6810	H	1 <1>	0.0000
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77	HC	-7.1540	-6.2610	-9.9520	H	1 <1>	0.0000
78	HC	-5.7410	-6.5810	-8.9410	H	1 <1>	0.0000
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83	HC	-11.1900	-3.9710	-7.9120	H	1 <1>	0.0000
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88	HC	-9.3940	-10.8720	-7.6090	H	1 <1>	0.0000
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97	HC	-10.9650	-5.9020	-0.0950	H	1 <1>	0.0000
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  112 HC      -11.0010   -4.0370  -11.9520 H       1 <1>       0.0000
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Epothilone Conformation in the Minireceptor, mol2 format

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#       Creation time:          Fri Mar 12 11:04:55 1999

#       Modifying user name:    minmin
#       Modification time:      Fri Mar 12 11:04:55 1999

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NO_CHARGES


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     17 OE        -9.7990   -5.9530   -2.8030 O.3      1 <1>        0.0000
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      30 C       -11.5870   -1.8300    1.8200 C.2     1 <1>       0.0000
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      68 HC       -4.9530   -6.6800   -0.2200 H       1 <1>       0.0000
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