Supporting Information.

# A Robust and Cost-Efficient Scheme for Accurate Conformational Energies of Organic Molecules

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## *Table S1. Table forming the basis of Figure 2.*

| Method | PBE-D3 | MNDO | AM1 | RM1 | PM3 | PM6 | PM7 | QM | DFTB3 | GFN-xTB | GFN2-xTB | MMFF94 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Q3 | 0.996 | 0.785 | 0.848 | 0.866 | 0.839 | 0.897 | 0.920 | 0.975 | 0.976 | 0.961 | 0.971 | 0.962 |
| Q1 | 0.980 | -0.097 | 0.150 | 0.534 | 0.460 | 0.285 | 0.537 | 0.902 | 0.833 | 0.839 | 0.874 | 0.800 |
| max | 1.000 | 0.967 | 0.971 | 0.983 | 0.976 | 0.985 | 0.998 | 0.997 | 0.994 | 0.979 | 0.993 | 0.987 |
| min | 0.926 | -0.920 | -0.951 | -0.786 | -0.887 | -0.314 | -0.294 | 0.264 | 0.185 | -0.153 | 0.340 | 0.586 |
| median | 0.990 | 0.523 | 0.669 | 0.709 | 0.726 | 0.614 | 0.760 | 0.949 | 0.922 | 0.916 | 0.927 | 0.918 |
| Worst compound | 18crown6 | ProstaglandinE1 | Liu_catal | Glufosinate | Glufosinate | Cryptand222 | Glufosinate | UH232 | 18crown6 | XylitolPentanit | 18crown6 | Cimetidine |
| Best compound | Isradipine | Bispidin | Triacetin | Knoevenagel_cond | Indomethacin | Indomethacin | Indomethacin | Isradipine | Indomethacin | Isradipine | Cembrene | XylitolPentanit |
| median Opt | | 0.655 | 0.598 | 0.753 | 0.514 | 0.631 | 0.599 | 0.864 | 0.895 | 0.853 | 0.879 | 0.878 |
| | | | | | **Pearson correlation coefficient (ρ)[a]** | | | | | | | |
| 18crown6 | 0.93 | 0.48 | 0.41 | 0.47 | 0.17 | 0.14 | 0.15 | 0.84 | 0.19 | 0.26 | 0.34 | 0.67 |
| Artemizinin | 1.00 | 0.73 | 0.82 | 0.80 | 0.84 | 0.85 | 0.90 | 0.96 | 0.95 | 0.96 | 0.97 | 0.90 |
| Atropine | 1.00 | -0.19 | 0.40 | 0.71 | 0.74 | 0.56 | 0.83 | 0.97 | 0.99 | 0.87 | 0.97 | 0.90 |
| Bispidin | 1.00 | 0.97 | 0.75 | 0.86 | 0.79 | 0.57 | 0.62 | 0.99 | 0.98 | 0.94 | 0.96 | 0.96 |
| Cembrene | 1.00 | 0.95 | 0.96 | 0.98 | 0.96 | 0.96 | 0.94 | 0.98 | 0.98 | 0.98 | 0.99 | 0.98 |
| Cimetidine | 1.00 | -0.90 | 0.48 | 0.43 | -0.15 | 0.57 | 0.64 | 0.97 | 0.97 | 0.98 | 0.93 | 0.59 |
| Cryptand222 | 0.97 | 0.76 | 0.15 | 0.22 | 0.21 | -0.31 | -0.26 | 0.36 | 0.58 | 0.57 | 0.66 | 0.74 |
| Dapiprazole | 0.99 | 0.64 | 0.56 | 0.29 | 0.51 | -0.25 | 0.09 | 0.87 | 0.94 | 0.76 | 0.86 | 0.61 |
| Eperisone | 0.99 | 0.71 | 0.85 | 0.74 | 0.83 | 0.63 | 0.69 | 0.97 | 0.92 | 0.90 | 0.91 | 0.82 |
| Fotemustin | 0.99 | 0.28 | -0.04 | 0.47 | 0.53 | 0.48 | 0.68 | 0.93 | 0.90 | 0.90 | 0.89 | 0.93 |
| GABA | 0.96 | -0.36 | 0.08 | 0.87 | 0.46 | 0.77 | 0.88 | 0.98 | 0.82 | 0.96 | 0.95 | 0.97 |
| Gemcitabine | 0.98 | 0.10 | 0.67 | 0.54 | 0.64 | 0.59 | 0.70 | 0.84 | 0.92 | 0.94 | 0.86 | 0.92 |
| Glufosinate | 0.98 | -0.83 | -0.78 | -0.79 | -0.89 | 0.04 | -0.29 | 0.94 | 0.90 | 0.66 | 0.93 | 0.91 |
| Indometacin | 0.97 | 0.52 | 0.92 | 0.94 | 0.98 | 0.98 | 1.00 | 0.96 | 0.99 | 0.96 | 0.98 | 0.97 |
| Isradipine | 1.00 | 0.38 | 0.91 | 0.91 | 0.50 | 0.93 | 1.00 | 1.00 | 0.99 | 0.98 | 0.98 | 0.98 |
| Knoevenagel_cond | 0.99 | 0.95 | 0.97 | 0.98 | 0.96 | 0.91 | 0.95 | 0.98 | 0.91 | 0.92 | 0.92 | 0.92 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Liu_catal | 1.00 | -0.86 | -0.95 | 0.68 | -0.22 | 0.08 | 0.76 | 0.93 | 0.90 | 0.97 | 0.99 | 0.96 |
| Mannosulfan | 0.98 | 0.86 | 0.39 | 0.70 | 0.08 | 0.61 | 0.75 | 0.90 | 0.88 | 0.94 | 0.86 | 0.93 |
| N_iprit | 0.97 | 0.94 | 0.92 | 0.77 | 0.90 | 0.70 | 0.08 | 0.99 | 0.61 | 0.94 | 0.92 | 0.84 |
| Oseltamivir | 1.00 | 0.95 | 0.69 | 0.89 | 0.84 | 0.35 | 0.76 | 0.98 | 0.98 | 0.84 | 0.89 | 0.96 |
| Pantoprazole | 0.94 | 0.72 | 0.68 | 0.86 | 0.76 | 0.89 | 0.87 | 0.90 | 0.95 | 0.96 | 0.97 | 0.72 |
| Propranolol | 0.99 | -0.10 | -0.04 | 0.77 | 0.49 | 0.61 | 0.89 | 0.92 | 0.97 | 0.93 | 0.95 | 0.96 |
| ProstaglandinE1 | 1.00 | -0.92 | -0.84 | -0.07 | -0.48 | 0.97 | 0.97 | 0.97 | 0.98 | 0.98 | 0.98 | 0.88 |
| Pyridoxalphosphate | 0.98 | -0.72 | -0.34 | 0.64 | 0.28 | 0.82 | 0.76 | 0.93 | 0.95 | 0.84 | 0.92 | 0.77 |
| Quinuclidinyl | 0.99 | 0.42 | 0.59 | 0.69 | 0.88 | 0.51 | 0.83 | 0.96 | 0.99 | 0.84 | 0.97 | 0.95 |
| RAMBO | 1.00 | 0.82 | -0.12 | -0.42 | 0.76 | 0.05 | 0.73 | 0.94 | 0.30 | 0.65 | 0.76 | 0.93 |
| RH34 | 0.98 | 0.30 | 0.82 | 0.87 | 0.73 | 0.73 | 0.83 | 0.95 | 0.92 | 0.96 | 0.93 | 0.94 |
| Rolipram | 0.96 | 0.34 | 0.85 | 0.66 | 0.56 | -0.17 | 0.22 | 0.55 | 0.74 | 0.52 | 0.87 | 0.77 |
| Rosmaridiphenol | 1.00 | 0.67 | 0.84 | 0.80 | 0.83 | 0.95 | 0.96 | 0.95 | 0.98 | 0.95 | 0.98 | 0.92 |
| Takemoto | 0.99 | -0.32 | 0.79 | 0.94 | 0.95 | 0.93 | 0.92 | 0.99 | 0.90 | 0.98 | 0.97 | 0.92 |
| Triacetin | 1.00 | 0.79 | 0.97 | 0.96 | 0.92 | 0.92 | 0.97 | 0.99 | 0.97 | 0.93 | 0.97 | 0.98 |
| Tsogoeva | 0.99 | -0.69 | -0.33 | 0.06 | -0.15 | 0.29 | 0.54 | 0.72 | 0.73 | 0.84 | 0.68 | 0.95 |
| UH232 | 0.99 | 0.83 | 0.94 | 0.98 | 0.94 | 0.92 | 0.93 | 0.26 | 0.98 | 0.89 | 0.96 | 0.98 |
| VX | 0.98 | 0.79 | 0.85 | 0.68 | 0.52 | 0.88 | 0.43 | 0.95 | 0.83 | 0.62 | 0.66 | 0.65 |
| WAY100635 | 1.00 | 0.39 | 0.59 | 0.53 | 0.63 | -0.07 | 0.31 | 0.84 | 0.92 | 0.85 | 0.88 | 0.80 |
| XylitolPentanit | 0.99 | 0.72 | 0.38 | 0.55 | 0.78 | -0.09 | 0.37 | 0.73 | 0.69 | -0.15 | 0.86 | 0.99 |
| shiepox_depox | 0.99 | 0.56 | 0.80 | 0.83 | 0.74 | 0.90 | 0.93 | 0.96 | 0.83 | 0.87 | 0.90 | 0.78 |

[a] Correlation coefficient is calculated with respect to DLPNO-CCSD(T)/cc-pVTZ coformational energies

## *Table S2. Table forming the basis of Figure 3.*

| Method | PBE-D3 | MNDO | AM1 | RM1 | PM3 | PM6 | PM7 | QM | DFTB3 | GFN-xTB | GFN2-xTB | MMFF94 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Q3 | 0.96 | 5.38 | 4.21 | 3.08 | 3.86 | 3.90 | 3.10 | 2.35 | 2.41 | 2.41 | 2.04 | 3.43 |
| Q1 | 0.45 | 2.21 | 1.90 | 1.60 | 1.83 | 1.79 | 1.53 | 0.78 | 1.20 | 1.29 | 0.94 | 1.98 |
| max | 1.60 | 33.44 | 10.18 | 7.31 | 8.16 | 9.58 | 6.05 | 6.53 | 4.97 | 4.46 | 4.22 | 6.15 |
| min | 0.20 | 1.19 | 0.81 | 0.63 | 0.59 | 0.70 | 0.70 | 0.24 | 0.50 | 0.57 | 0.67 | 0.61 |
| median | 0.61 | 3.51 | 2.90 | 2.46 | 2.96 | 2.66 | 2.25 | 1.35 | 1.71 | 1.82 | 1.52 | 2.69 |
| Worst compound | GABA | ProstaglandinE1 | Glufosinate | Glufosinate | Glufosinate | 18crown6 | 18crown6 | Cryptand222 | RAMBO | 18crown6 | RAMBO | Oseltamivir |
| Best compound | Rosmaridiphenol | Cembrene | Indometacin | Indometacin | UH232 | Rosmaridiphenol | Rosmaridiphenol | Isradipine | Indometacin | RH34 | GABA | Liu_catal |
| median Opt | | 2.78 | 2.99 | 2.79 | 3.30 | 2.93 | 2.44 | 2.20 | 2.15 | 1.86 | 1.62 | 2.36 |
| **Mean absolute error in conformational energy (MAE)[a]** | | | | | | | | | | | | |
| 18crown6 | 0.7 | 7.0 | 3.0 | 2.6 | 3.6 | 9.6 | 6.1 | 4.2 | 2.6 | 4.5 | 3.3 | 1.5 |
| Artemizinin | 0.5 | 2.2 | 2.5 | 2.0 | 4.4 | 2.7 | 2.4 | 1.0 | 2.9 | 2.2 | 2.0 | 3.1 |
| Atropine | 1.0 | 5.4 | 4.8 | 3.8 | 4.9 | 4.9 | 2.7 | 2.1 | 2.0 | 1.9 | 2.0 | 1.6 |
| Bispidin | 0.4 | 1.6 | 3.2 | 1.7 | 2.3 | 4.1 | 3.5 | 2.7 | 1.7 | 1.7 | 1.2 | 5.2 |
| Cembrene | 0.5 | 1.2 | 2.6 | 1.6 | 3.1 | 3.4 | 3.1 | 1.0 | 2.4 | 2.0 | 1.5 | 2.6 |
| Cimetidine | 0.4 | 6.0 | 3.4 | 3.3 | 4.6 | 3.2 | 4.1 | 1.5 | 1.4 | 1.3 | 1.7 | 3.0 |
| Cryptand222 | 0.9 | 6.7 | 3.1 | 3.0 | 2.7 | 6.0 | 5.4 | 6.5 | 2.3 | 2.4 | 2.4 | 3.6 |
| Dapiprazole | 0.5 | 2.9 | 4.2 | 4.2 | 3.5 | 4.3 | 3.8 | 1.4 | 3.6 | 3.7 | 3.6 | 3.1 |
| Eperisone | 0.4 | 1.8 | 1.3 | 1.5 | 1.7 | 1.8 | 1.8 | 0.7 | 1.2 | 1.4 | 0.9 | 2.9 |
| Fotemustin | 0.5 | 4.8 | 2.9 | 2.5 | 2.6 | 2.8 | 2.8 | 2.5 | 1.6 | 1.9 | 1.4 | 3.6 |
| GABA | 1.6 | 4.9 | 3.6 | 1.2 | 2.1 | 2.0 | 1.6 | 0.7 | 1.1 | 1.3 | 0.7 | 2.3 |
| Gemcitabine | 0.6 | 3.4 | 2.4 | 3.2 | 3.1 | 2.6 | 1.9 | 2.4 | 1.0 | 0.9 | 1.2 | 0.9 |
| Glufosinate | 1.0 | 14.8 | 10.2 | 7.3 | 8.2 | 3.3 | 4.0 | 4.1 | 1.2 | 2.7 | 1.9 | 1.4 |
| Indometacin | 0.7 | 1.9 | 0.8 | 0.6 | 1.2 | 0.8 | 1.0 | 0.6 | 0.5 | 1.8 | 0.7 | 2.0 |
| Isradipine | 0.5 | 5.1 | 2.8 | 2.7 | 5.0 | 2.5 | 1.2 | 0.2 | 0.5 | 1.6 | 1.3 | 2.0 |
| Knoevenagel_cond | 1.1 | 3.6 | 1.9 | 0.9 | 1.8 | 2.9 | 2.0 | 0.5 | 3.3 | 2.5 | 2.5 | 2.7 |
| Liu_catal | 0.5 | 8.7 | 4.7 | 3.3 | 3.9 | 4.1 | 2.0 | 0.9 | 3.7 | 2.1 | 2.4 | 0.6 |
| Mannosulfan | 1.2 | 5.4 | 4.2 | 3.0 | 4.9 | 3.7 | 2.5 | 5.0 | 4.2 | 2.4 | 2.0 | 3.2 |
| N_iprit | 1.4 | 1.3 | 2.1 | 1.5 | 0.7 | 1.4 | 2.0 | 0.4 | 1.7 | 1.2 | 1.5 | 4.0 |
| Oseltamivir | 1.0 | 1.6 | 3.9 | 2.2 | 5.0 | 4.3 | 4.1 | 0.8 | 3.1 | 3.5 | 3.7 | 6.1 |
| Pantoprazole | 0.9 | 6.2 | 2.4 | 1.7 | 1.7 | 1.4 | 2.4 | 2.6 | 0.9 | 1.7 | 1.0 | 3.6 |
| Propranolol | 0.3 | 3.4 | 3.3 | 2.1 | 2.5 | 2.0 | 1.0 | 0.8 | 1.3 | 0.7 | 0.9 | 3.1 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ProstaglandinE1 | 1.0 | 33.4 | 9.6 | 5.6 | 6.6 | 1.1 | 3.0 | 3.9 | 1.6 | 1.0 | 0.8 | 3.3 |
| Pyridoxalphosphate | 1.2 | 8.1 | 4.4 | 2.4 | 3.8 | 2.1 | 3.1 | 1.9 | 2.7 | 1.8 | 2.3 | 2.5 |
| Quinuclidinyl | 0.5 | 5.0 | 3.2 | 2.7 | 3.0 | 3.1 | 2.3 | 1.0 | 1.3 | 1.9 | 0.9 | 2.4 |
| RAMBO | 0.6 | 1.3 | 4.4 | 4.7 | 3.8 | 4.5 | 3.2 | 0.7 | 5.0 | 4.3 | 4.2 | 5.5 |
| RH34 | 0.4 | 2.4 | 1.7 | 1.4 | 1.5 | 1.5 | 1.2 | 1.3 | 1.0 | 0.6 | 0.8 | 1.0 |
| Rolipram | 1.1 | 3.1 | 1.4 | 1.5 | 1.7 | 1.9 | 1.5 | 1.3 | 1.9 | 1.4 | 0.8 | 2.0 |
| Rosmaridiphenol | 0.2 | 4.1 | 1.2 | 2.5 | 1.8 | 0.7 | 0.7 | 1.5 | 0.8 | 0.9 | 0.7 | 4.5 |
| Takemoto | 0.8 | 4.6 | 2.5 | 2.7 | 2.2 | 2.5 | 1.5 | 0.5 | 1.5 | 2.1 | 1.6 | 1.4 |
| Triacetin | 0.5 | 2.6 | 1.4 | 1.6 | 3.0 | 2.1 | 1.1 | 1.7 | 2.4 | 1.6 | 1.4 | 2.2 |
| Tsogoeva | 0.6 | 10.0 | 7.5 | 2.8 | 3.3 | 3.1 | 2.2 | 2.5 | 1.7 | 1.7 | 1.8 | 3.2 |
| UH232 | 0.8 | 1.5 | 0.9 | 2.0 | 0.6 | 1.7 | 1.4 | 2.1 | 1.0 | 1.1 | 1.1 | 4.5 |
| VX | 0.4 | 3.0 | 0.9 | 1.6 | 1.1 | 0.8 | 1.6 | 0.8 | 1.3 | 1.3 | 0.9 | 1.5 |
| WAY100635 | 0.3 | 3.5 | 4.4 | 4.1 | 4.1 | 4.6 | 3.9 | 1.8 | 1.8 | 3.1 | 2.4 | 2.4 |
| XylitolPentanit | 0.7 | 3.0 | 2.9 | 3.1 | 1.8 | 3.9 | 2.6 | 1.8 | 1.9 | 3.7 | 1.5 | 2.2 |
| shiepox_depox | 0.3 | 1.9 | 1.7 | 1.5 | 2.0 | 0.9 | 0.9 | 0.8 | 1.7 | 1.0 | 1.2 | 3.4 |

[a] Mean absolute error is calculated with respect to DLPNO-CCSD(T)/cc-pVTZ coformational energies

## *Table S3. Table forming the basis of Figure 4.*

| **Symmetry** | **CCSD(T)** | **PBE-D3** | **MNDO** | **AM1** | **RM1** | **PM3** | **PM6** | **PM7** | **QM** | **DFTB3** | **GFN-xTB** | **GFN2-xTB** | **MMFF94** | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $S_6$ | 0.0 | 0.0 | 10.5 | 0.0 | 0.0 | 2.0 | 2.1 | 1.8 | 0.0 | 2.8 | 0.0 | 0.0 | 0.6 | |
| $C_i$ | 0.2 | 0.9 | 3.9 | 5.1 | 3.3 | 6.2 | 13.2 | 8.4 | 5.5 | 1.1 | 5.4 | 4.5 | 0.6 | |
| $D_{3d}$ | 4.3 | 2.7 | 0.0 | 13.2 | 12.1 | 11.1 | 34.4 | 23.2 | 6.8 | 9.2 | 21.4 | 16.4 | 8.8 | |
| $C_2$ | 2.0 | 2.6 | 6.2 | 4.0 | 1.7 | 3.9 | 9.6 | 6.3 | 7.0 | 2.6 | 5.3 | 4.5 | 1.8 | |
| $C_s$ | 2.4 | 2.7 | 8.1 | 7.4 | 7.5 | 7.2 | 14.3 | 10.4 | 7.4 | 3.6 | 6.9 | 5.7 | 3.7 | |
| $C_3$ | 3.0 | 3.9 | 6.2 | 3.0 | 2.6 | 5.2 | 6.9 | 5.1 | 8.8 | 0.0 | 2.4 | 2.9 | 0.0 | |
| $D_2$ | 5.0 | 5.0 | 18.4 | 2.4 | 1.4 | 0.0 | 0.0 | 0.0 | 8.7 | 2.9 | 1.2 | 1.1 | 4.7 | |
| $C_{2h}$ | 6.4 | 8.1 | 17.0 | 6.8 | 7.0 | 6.6 | 9.4 | 6.5 | 12.5 | 1.3 | 5.1 | 6.0 | 4.5 | |
| | **Energy difference** $\Delta\Delta E = (E_{D_{3d}}^{method} - E_{D_2/S_6}^{method}) - (E_{D_{3d}}^{DLPNO-CCSD(T)} - E_{D_2/S_6}^{DLPNO-CCSD(T)})$ **(kcal/mol)** | | | | | | | | | | | | | |
| | PBE-D3 | MNDO | AM1 | RM1 | PM3 | PM6 | PM7 | QM | DFTB3 | GFN-xTB | GFN2-xTB | MMFF94 | MM3 | |
| $\Delta\Delta E(D_{3d}\text{-}D_2)$ | -1.6 | -17.7 | 11.5 | 11.4 | 11.8 | 35.1 | 23.9 | -1.2 | 7.01 | 20.8 | 16.1 | 6.4 | -12.7 | |
| $\Delta\Delta E(D_{3d}\text{-}S_6)$ | -1.6 | -14.8 | 8.9 | 7.8 | 4.8 | 28 | 17.1 | 2.5 | 2.13 | 17.1 | 12.1 | 5.1 | -12.2 | |

## *Table S4. Table forming the basis of Figure 5.*

| Method | MNDO | AM1 | RM1 | PM3 | PM6 | PM7 | QM | DFTB3 | GFN-xTB | GFN2-xTB | MMFF94 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Q3 | 24 | 18 | 13 | 18 | 22 | 21 | 11 | 8 | 13 | 9 | 9 |
| Q1 | 16 | 7 | 7 | 8 | 7 | 10 | 3 | 4 | 5 | 3 | 5 |
| max | 52 | 32 | 42 | 37 | 35 | 45 | 27 | 23 | 26 | 18 | 19 |
| min | 9 | 4 | 2 | 5 | 3 | 3 | 2 | 2 | 2 | 1 | 3 |
| median | 20 | 13 | 10 | 12 | 13 | 12 | 7 | 6 | 7 | 5 | 7 |
| Worst compound | Pantoprazole | Pantoprazole | Pyridoxalphosphate | Pyridoxalphosphate | Gemcitabine | Pyridoxalphosphate | RH34 | Gemcitabine | VX | Fotemustin | Pyridoxalphosphate |
| Best compound | Liu_catal | UH232 | Bispidin | Knoevenagel_cond | WAY100635 | Bispidin | Bispidin | Bispidin | Atropine | Atropine | 18crown6 |
| **Mean absolute deviation in rotatble bond dihedral (MAE)[a]** | | | | | | | | | | | |
| 18crown6 | 10 | 9 | 10 | 12 | 26 | 17 | 6 | 5 | 18 | 5 | 3 |
| Artemizinin | 14 | 7 | 8 | 10 | 7 | 10 | 7 | 5 | 5 | 5 | 7 |
| Atropine | 15 | 9 | 4 | 8 | 5 | 3 | 3 | 2 | 2 | 1 | 4 |
| Bispidin | 16 | 15 | 2 | 7 | 4 | 3 | 2 | 2 | 2 | 1 | 4 |
| Cembrene | 21 | 9 | 12 | 9 | 11 | 11 | 2 | 2 | 5 | 5 | 3 |
| Cimetidine | 24 | 13 | 9 | 16 | 12 | 14 | 6 | 8 | 6 | 6 | 12 |
| Cryptand222 | 17 | 10 | 10 | 16 | 29 | 29 | 13 | 5 | 10 | 9 | 4 |
| Dapiprazole | 17 | 7 | 6 | 6 | 8 | 13 | 5 | 2 | 3 | 2 | 6 |
| Eperisone | 23 | 18 | 11 | 12 | 21 | 21 | 8 | 5 | 5 | 5 | 6 |
| Fotemustin | 29 | 19 | 23 | 22 | 22 | 23 | 11 | 18 | 22 | 18 | 9 |
| GABA | 13 | 8 | 7 | 6 | 7 | 10 | 3 | 4 | 2 | 3 | 5 |
| Gemcitabine | 23 | 16 | 16 | 21 | 35 | 23 | 9 | 23 | 18 | 10 | 9 |
| Glufosinate | 16 | 23 | 16 | 20 | 11 | 10 | 8 | 7 | 6 | 5 | 7 |
| Indometacin | 35 | 25 | 18 | 22 | 28 | 26 | 8 | 12 | 15 | 8 | 6 |
| Isradipine | 30 | 6 | 11 | 24 | 5 | 12 | 12 | 3 | 3 | 3 | 15 |
| Knoevenagel_cond | 16 | 5 | 6 | 5 | 11 | 5 | 6 | 4 | 10 | 3 | 5 |
| Liu_catal | 9 | 12 | 6 | 7 | 5 | 10 | 6 | 6 | 3 | 2 | 5 |
| Mannosulfan | 28 | 16 | 19 | 14 | 20 | 18 | 17 | 8 | 14 | 14 | 14 |
| N_iprit | 17 | 6 | 10 | 8 | 13 | 13 | 3 | 10 | 6 | 8 | 9 |
| Oseltamivir | 23 | 5 | 7 | 10 | 11 | 8 | 2 | 3 | 5 | 2 | 5 |
| Pantoprazole | 52 | 32 | 33 | 35 | 31 | 24 | 12 | 16 | 12 | 14 | 18 |
| Propranolol | 28 | 7 | 10 | 12 | 16 | 17 | 3 | 6 | 7 | 3 | 8 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ProstaglandinE1 | 15 | 7 | 6 | 8 | 7 | 6 | 3 | 4 | 4 | 2 | 5 |
| Pyridoxalphosphate | 46 | 24 | 42 | 37 | 32 | 45 | 15 | 10 | 23 | 14 | 19 |
| Quinuclidinyl | 16 | 17 | 7 | 11 | 15 | 12 | 8 | 6 | 6 | 3 | 13 |
| RAMBO | 18 | 14 | 7 | 15 | 12 | 8 | 3 | 7 | 5 | 5 | 5 |
| RH34 | 24 | 18 | 12 | 10 | 18 | 19 | 27 | 8 | 11 | 10 | 14 |
| Rolipram | 33 | 18 | 13 | 20 | 18 | 18 | 12 | 11 | 13 | 7 | 15 |
| Rosmaridiphenol | 9 | 7 | 8 | 7 | 7 | 6 | 7 | 5 | 6 | 4 | 10 |
| Takemoto | 20 | 12 | 9 | 11 | 12 | 10 | 10 | 7 | 9 | 8 | 6 |
| Triacetin | 14 | 14 | 10 | 8 | 24 | 22 | 12 | 5 | 16 | 12 | 8 |
| Tsogoeva | 26 | 16 | 12 | 18 | 14 | 12 | 9 | 12 | 11 | 8 | 8 |
| UH232 | 22 | 4 | 7 | 6 | 6 | 7 | 3 | 4 | 8 | 6 | 3 |
| VX | 23 | 22 | 25 | 14 | 26 | 21 | 6 | 7 | 26 | 13 | 9 |
| WAY100635 | 19 | 5 | 9 | 8 | 3 | 6 | 2 | 3 | 3 | 2 | 7 |
| XylitolPentanit | 13 | 13 | 8 | 15 | 19 | 12 | 25 | 7 | 10 | 17 | 7 |
| shiepox_depox | 22 | 23 | 19 | 24 | 23 | 26 | 5 | 8 | 15 | 9 | 8 |

[a] Mean absolute error is calculated with respect to corresponding PBE-D3/def2-tzvp dihedrals

# Tabulated relative conformational energies (kcal/mol)

***Table S5. Tabulated relative conformational energies (kcal/mol) obtained with SP DLPNO-CCSD(T)/cc-pVTZ, PBE-D3/def2-tzvp, AM1, MNDO, PM3, PM6, PM7, RM1, QM, MMFF94, DFTB3, GFN-xTB, GFN2-xTB.***

| | № | DLPNO/TZ | PBE-D3 | AM1 | MNDO | PM3 | PM6 | PM7 | RM1 | QM | MMFF94 | DFTB3 | GFN-xTB | GFN2-xTB |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18crown6 | 1 | 0.0 | 0.0 | 0.0 | 10.5 | 2.0 | 2.1 | 1.8 | 0.0 | 0.0 | 0.6 | 2.8 | 0.0 | 0.0 |
| 18crown6 | 2 | 0.2 | 0.9 | 5.1 | 3.9 | 6.2 | 13.2 | 8.4 | 3.3 | 5.5 | 0.6 | 1.1 | 5.4 | 4.5 |
| 18crown6 | 3 | 4.3 | 2.7 | 13.2 | 0.0 | 11.1 | 34.4 | 23.2 | 12.1 | 6.8 | 8.8 | 9.2 | 21.4 | 16.4 |
| 18crown6 | 4 | 2.0 | 2.6 | 4.0 | 6.2 | 3.9 | 9.6 | 6.3 | 1.7 | 7.0 | 1.8 | 2.6 | 5.3 | 4.5 |
| 18crown6 | 5 | 2.4 | 2.7 | 7.4 | 8.1 | 7.2 | 14.3 | 10.4 | 7.5 | 7.4 | 3.7 | 3.6 | 6.9 | 5.7 |
| 18crown6 | 6 | 3.0 | 3.9 | 3.0 | 6.2 | 5.2 | 6.9 | 5.1 | 2.6 | 8.8 | 0.0 | 0.0 | 2.4 | 2.9 |
| 18crown6 | 7 | 5.0 | 5.0 | 2.4 | 18.4 | 0.0 | 0.0 | 0.0 | 1.4 | 8.7 | 4.7 | 2.9 | 1.2 | 1.1 |
| 18crown6 | 8 | 6.4 | 8.1 | 6.8 | 17.0 | 6.6 | 9.4 | 6.5 | 7.0 | 12.5 | 4.5 | 1.3 | 5.1 | 6.0 |
| Artemizinin | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Artemizinin | 2 | 7.4 | 7.0 | 4.3 | 6.3 | 0.8 | 5.1 | 5.3 | 5.0 | 9.1 | 12.9 | 4.9 | 6.1 | 5.5 |
| Artemizinin | 3 | 8.2 | 7.3 | 10.1 | 8.2 | 4.6 | 8.8 | 8.5 | 11.5 | 9.0 | 9.5 | 6.8 | 7.0 | 7.7 |
| Artemizinin | 4 | 7.7 | 7.2 | 5.8 | 5.2 | 4.0 | 4.1 | 4.5 | 5.7 | 8.0 | 9.7 | 4.6 | 4.4 | 5.4 |
| Artemizinin | 5 | 10.0 | 9.0 | 7.0 | 5.5 | 5.0 | 6.9 | 6.9 | 9.0 | 10.2 | 11.7 | 5.7 | 7.5 | 7.3 |
| Artemizinin | 6 | 10.3 | 9.6 | 7.9 | 8.1 | 6.6 | 6.6 | 6.2 | 9.5 | 9.9 | 13.3 | 5.8 | 7.2 | 7.1 |
| Artemizinin | 7 | 11.3 | 11.0 | 8.4 | 11.4 | 5.2 | 8.6 | 8.9 | 10.0 | 14.8 | 20.3 | 8.2 | 8.9 | 8.9 |
| Artemizinin | 8 | 11.2 | 11.0 | 6.3 | 3.9 | 5.0 | 5.9 | 7.3 | 6.2 | 11.9 | 13.5 | 7.3 | 7.4 | 8.3 |
| Atropine | 1 | 0.0 | 0.0 | 0.0 | 9.6 | 0.4 | 0.1 | 0.0 | 1.3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Atropine | 2 | 1.5 | 0.7 | 1.5 | 9.6 | 1.2 | 0.6 | 1.0 | 2.4 | 0.5 | 2.3 | 0.4 | 2.2 | 0.6 |
| Atropine | 3 | 2.9 | 2.3 | 1.2 | 3.3 | 0.0 | 0.0 | 1.4 | 0.0 | 4.3 | 0.5 | 2.5 | 4.3 | 2.1 |
| Atropine | 4 | 8.1 | 7.2 | 0.2 | 0.0 | 0.4 | 1.6 | 4.9 | 2.0 | 13.2 | 6.2 | 6.3 | 7.1 | 5.7 |
| Atropine | 5 | 9.6 | 8.5 | 1.0 | 5.2 | 2.2 | 2.2 | 5.5 | 4.7 | 12.7 | 9.4 | 6.8 | 6.9 | 6.4 |
| Atropine | 6 | 11.6 | 10.5 | 2.0 | 8.3 | 3.5 | 1.8 | 5.3 | 5.3 | 13.1 | 10.3 | 7.5 | 6.6 | 7.1 |
| Atropine | 7 | 11.6 | 9.9 | 2.9 | 5.5 | 3.5 | 2.4 | 6.5 | 4.7 | 15.3 | 9.3 | 8.1 | 9.1 | 8.3 |
| Atropine | 8 | 8.7 | 6.7 | 6.6 | 11.5 | 4.4 | 6.5 | 9.7 | 7.9 | 9.4 | 12.6 | 6.2 | 10.3 | 7.7 |
| Bispidin | 1 | 0.0 | 0.0 | 2.1 | 0.0 | 2.1 | 3.9 | 2.6 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Bispidin | 2 | 3.4 | 3.0 | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.3 | 4.6 | 4.0 | 1.6 | 1.4 | 1.6 |
| Bispidin | 3 | 4.1 | 3.9 | 7.0 | 3.8 | 6.2 | 8.4 | 7.6 | 4.9 | 6.8 | 11.2 | 3.9 | 3.9 | 4.4 |
| Bispidin | 4 | 4.3 | 4.4 | 11.1 | 3.6 | 8.5 | 12.8 | 11.4 | 7.5 | 6.7 | 10.1 | 4.2 | 5.1 | 5.4 |
| Bispidin | 5 | 5.2 | 4.7 | 7.0 | 4.3 | 5.4 | 7.4 | 6.4 | 5.5 | 8.5 | 10.3 | 3.7 | 4.1 | 4.6 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Bispidin | 6 | 11.3 | 10.6 | 8.0 | 8.6 | 7.4 | 6.1 | 5.8 | 7.3 | 15.7 | 19.1 | 7.8 | 6.9 | 8.6 |
| Bispidin | 7 | 11.5 | 10.9 | 12.2 | 8.9 | 10.1 | 11.2 | 10.3 | 10.2 | 15.4 | 18.8 | 8.1 | 8.3 | 9.6 |
| Bispidin | 8 | 11.9 | 11.5 | 16.6 | 9.5 | 13.2 | 16.5 | 15.0 | 13.1 | 15.3 | 19.4 | 8.6 | 9.9 | 11.0 |
| Cembrene | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Cembrene | 2 | 3.0 | 2.8 | 1.5 | 2.2 | 2.0 | 1.6 | 2.0 | 1.9 | 3.6 | 3.3 | 2.6 | 2.6 | 2.7 |
| Cembrene | 3 | 3.8 | 3.2 | 1.7 | 2.5 | 0.8 | 1.4 | 0.9 | 2.7 | 1.8 | 6.1 | 2.4 | 1.6 | 2.2 |
| Cembrene | 4 | 6.0 | 5.6 | 2.1 | 4.1 | 2.3 | 1.7 | 3.0 | 3.0 | 5.1 | 6.7 | 3.8 | 4.8 | 4.7 |
| Cembrene | 5 | 6.0 | 5.8 | 3.4 | 8.2 | 2.0 | 1.9 | 1.2 | 4.5 | 4.6 | 9.1 | 3.2 | 3.8 | 4.2 |
| Cembrene | 6 | 9.5 | 8.8 | 5.0 | 7.8 | 6.0 | 5.0 | 6.3 | 6.7 | 8.4 | 12.1 | 5.6 | 6.7 | 7.5 |
| Cembrene | 7 | 10.4 | 9.7 | 7.1 | 11.0 | 6.4 | 5.7 | 6.2 | 9.3 | 9.7 | 16.7 | 7.2 | 7.9 | 8.2 |
| Cembrene | 8 | 12.5 | 11.1 | 9.4 | 13.5 | 7.3 | 6.4 | 6.9 | 10.3 | 11.4 | 17.9 | 7.1 | 8.1 | 9.3 |
| Cimetidine | 1 | 0.0 | 0.0 | 0.0 | 11.8 | 5.3 | 1.0 | 4.9 | 1.6 | 0.0 | 3.4 | 0.0 | 0.0 | 0.0 |
| Cimetidine | 2 | 2.2 | 2.4 | 0.9 | 11.4 | 5.7 | 1.8 | 2.7 | 2.1 | 3.1 | 3.0 | 0.8 | 1.9 | 1.6 |
| Cimetidine | 3 | 5.2 | 5.4 | 1.9 | 6.6 | 3.1 | 0.0 | 0.0 | 2.1 | 6.0 | 0.0 | 5.2 | 3.3 | 3.0 |
| Cimetidine | 4 | 8.1 | 7.6 | 0.6 | 5.6 | 0.0 | 0.3 | 3.2 | 0.0 | 8.6 | 4.0 | 6.8 | 5.0 | 4.0 |
| Cimetidine | 5 | 5.6 | 6.0 | 4.9 | 11.3 | 9.2 | 6.4 | 11.8 | 7.2 | 6.8 | 7.9 | 4.0 | 4.8 | 4.8 |
| Cimetidine | 6 | 6.4 | 7.2 | 1.7 | 6.5 | 4.4 | 0.5 | 4.4 | 1.6 | 9.2 | 7.0 | 5.0 | 5.1 | 3.5 |
| Cimetidine | 7 | 6.0 | 6.3 | 5.7 | 10.0 | 10.3 | 6.8 | 10.0 | 6.9 | 5.7 | 12.0 | 3.3 | 4.6 | 3.4 |
| Cimetidine | 8 | 13.4 | 14.1 | 4.2 | 0.0 | 5.2 | 9.4 | 18.1 | 7.2 | 18.9 | 11.8 | 11.1 | 11.8 | 13.0 |
| Cryptand222 | 1 | 0.0 | 0.0 | 3.4 | 7.5 | 6.4 | 14.1 | 12.0 | 9.5 | 0.0 | 7.5 | 5.2 | 4.0 | 1.6 |
| Cryptand222 | 2 | 1.0 | 1.5 | 3.7 | 0.0 | 2.0 | 9.8 | 8.2 | 2.9 | 9.8 | 0.1 | 1.3 | 2.8 | 1.6 |
| Cryptand222 | 3 | 0.4 | 1.6 | 2.9 | 6.5 | 1.4 | 7.3 | 6.1 | 1.5 | 9.5 | 0.0 | 0.0 | 1.6 | 0.2 |
| Cryptand222 | 4 | 2.5 | 3.0 | 5.3 | 2.6 | 3.1 | 11.7 | 10.0 | 5.6 | 11.1 | 2.7 | 1.8 | 3.7 | 2.5 |
| Cryptand222 | 5 | 3.2 | 4.7 | 0.2 | 15.3 | 1.9 | 0.0 | 0.0 | 1.4 | 8.3 | 1.9 | 0.3 | 0.0 | 0.0 |
| Cryptand222 | 6 | 5.9 | 6.9 | 0.0 | 13.5 | 0.0 | 0.5 | 0.1 | 0.0 | 16.1 | 1.8 | 0.7 | 2.7 | 1.2 |
| Cryptand222 | 7 | 4.9 | 6.2 | 5.2 | 15.9 | 2.4 | 4.7 | 3.8 | 5.4 | 13.0 | 6.7 | 1.8 | 1.1 | 1.2 |
| Cryptand222 | 8 | 9.9 | 8.9 | 5.5 | 18.2 | 6.7 | 9.6 | 8.9 | 9.6 | 7.6 | 22.6 | 10.2 | 8.9 | 5.2 |
| Dapiprazole | 1 | 0.0 | 0.0 | 0.8 | 2.2 | 1.1 | 6.3 | 4.1 | 2.3 | 0.0 | 1.0 | 0.0 | 0.3 | 0.1 |
| Dapiprazole | 2 | 2.3 | 2.1 | 0.9 | 0.0 | 1.9 | 6.5 | 6.3 | 2.1 | 2.9 | 0.0 | 1.5 | 2.4 | 1.4 |
| Dapiprazole | 3 | 5.3 | 4.4 | 0.7 | 3.5 | 2.7 | 4.6 | 5.4 | 1.5 | 5.3 | 2.6 | 1.8 | 2.1 | 1.7 |
| Dapiprazole | 4 | 5.2 | 5.0 | 0.0 | 2.0 | 0.0 | 2.0 | 2.9 | 0.0 | 4.7 | 2.4 | 2.5 | 1.8 | 2.1 |
| Dapiprazole | 5 | 4.8 | 4.4 | 2.9 | 9.1 | 3.8 | 2.3 | 0.0 | 2.9 | 0.3 | 10.2 | 1.5 | 0.0 | 0.0 |
| Dapiprazole | 6 | 8.8 | 7.6 | 0.3 | 5.8 | 0.3 | 0.0 | 1.4 | 0.5 | 7.2 | 4.8 | 3.1 | 2.2 | 2.4 |
| Dapiprazole | 7 | 10.5 | 9.6 | 3.8 | 6.0 | 5.3 | 6.6 | 7.5 | 3.5 | 10.9 | 5.7 | 3.4 | 5.3 | 5.2 |
| Dapiprazole | 8 | 9.5 | 9.6 | 4.9 | 11.2 | 5.4 | 5.0 | 4.5 | 4.8 | 6.3 | 11.2 | 4.2 | 3.8 | 4.8 |
| Eperisone | 1 | 0.0 | 0.1 | 0.7 | 0.0 | 0.3 | 2.3 | 2.4 | 1.2 | 0.5 | 0.0 | 1.2 | 0.7 | 1.4 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Eperisone | 2 | 0.9 | 0.0 | 0.0 | 1.7 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 6.4 | 0.0 | 0.0 | 0.0 |
| Eperisone | 3 | 1.3 | 0.9 | 1.6 | 4.4 | 1.3 | 2.3 | 2.6 | 2.0 | 1.2 | 5.3 | 1.2 | 2.1 | 2.2 |
| Eperisone | 4 | 3.5 | 3.1 | 4.4 | 2.1 | 2.4 | 4.1 | 5.1 | 6.1 | 2.9 | 6.4 | 3.1 | 3.9 | 4.1 |
| Eperisone | 5 | 5.0 | 4.0 | 2.4 | 3.1 | 1.6 | 1.3 | 2.3 | 3.8 | 3.8 | 9.5 | 2.4 | 3.3 | 2.9 |
| Eperisone | 6 | 5.9 | 6.0 | 4.9 | 3.7 | 4.6 | 6.9 | 6.8 | 5.1 | 6.9 | 8.4 | 4.9 | 4.4 | 6.0 |
| Eperisone | 7 | 6.0 | 6.1 | 5.1 | 3.7 | 4.3 | 6.9 | 6.8 | 5.1 | 6.8 | 8.7 | 5.2 | 4.3 | 6.2 |
| Eperisone | 8 | 7.8 | 7.8 | 4.4 | 4.8 | 3.0 | 3.9 | 4.4 | 4.0 | 8.0 | 9.0 | 5.1 | 4.3 | 6.5 |
| Fotemustin | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 2.5 | 2.8 | 0.0 | 0.0 | 0.0 | 2.8 | 1.0 | 2.0 |
| Fotemustin | 2 | 0.2 | 1.1 | 14.6 | 6.4 | 5.6 | 4.4 | 3.2 | 6.7 | 0.1 | 1.6 | 0.0 | 0.0 | 0.0 |
| Fotemustin | 3 | 3.8 | 2.8 | 4.8 | 13.2 | 2.6 | 0.0 | 0.0 | 4.9 | 0.5 | 4.8 | 1.7 | 1.6 | 2.2 |
| Fotemustin | 4 | 4.4 | 4.9 | 4.1 | 11.2 | 0.9 | 6.8 | 2.5 | 1.1 | 1.4 | 4.1 | 4.2 | 2.7 | 4.4 |
| Fotemustin | 5 | 5.2 | 4.9 | 4.6 | 11.7 | 5.9 | 3.9 | 2.8 | 7.5 | 2.0 | 13.5 | 2.8 | 2.5 | 3.6 |
| Fotemustin | 6 | 7.5 | 7.3 | 7.3 | 10.4 | 5.1 | 6.7 | 5.0 | 7.1 | 5.0 | 10.3 | 5.6 | 3.6 | 6.2 |
| Fotemustin | 7 | 9.0 | 8.5 | 4.7 | 5.7 | 5.7 | 3.4 | 5.2 | 5.7 | 4.4 | 16.9 | 7.1 | 6.1 | 6.5 |
| Fotemustin | 8 | 9.7 | 10.2 | 7.4 | 6.6 | 5.5 | 8.1 | 7.8 | 6.4 | 6.5 | 17.1 | 8.4 | 9.0 | 11.7 |
| GABA | 1 | 0.3 | 0.0 | 11.2 | 14.4 | 4.0 | 4.0 | 2.5 | 2.3 | 0.2 | 0.0 | 3.4 | 0.8 | 0.8 |
| GABA | 2 | 0.0 | 0.6 | 10.4 | 15.9 | 5.1 | 4.7 | 2.9 | 3.2 | 0.0 | 0.6 | 2.2 | 1.8 | 1.3 |
| GABA | 3 | 0.0 | 2.3 | 1.9 | 0.6 | 1.7 | 1.5 | 1.0 | 0.6 | 1.3 | 2.1 | 0.0 | 0.0 | 0.0 |
| GABA | 4 | 1.4 | 3.4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 2.9 | 4.7 | 0.6 | 0.6 | 0.1 |
| GABA | 5 | 2.3 | 4.4 | 1.8 | 2.0 | 3.2 | 2.5 | 1.6 | 2.8 | 2.3 | 3.9 | 1.3 | 1.9 | 1.5 |
| GABA | 6 | 5.1 | 7.0 | 6.8 | 2.3 | 4.3 | 7.2 | 7.1 | 5.3 | 6.2 | 8.8 | 5.2 | 7.7 | 5.6 |
| GABA | 7 | 5.3 | 7.3 | 7.0 | 5.7 | 6.0 | 7.2 | 6.8 | 6.5 | 5.6 | 9.0 | 4.9 | 7.8 | 6.0 |
| GABA | 8 | 6.9 | 8.5 | 7.3 | 3.5 | 4.6 | 7.7 | 7.7 | 7.0 | 7.8 | 10.3 | 5.8 | 9.1 | 6.6 |
| Gemcitabine | 1 | 0.0 | 0.0 | 3.2 | 6.4 | 0.1 | 0.0 | 0.0 | 1.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Gemcitabine | 2 | 2.2 | 2.4 | 0.0 | 2.1 | 0.0 | 0.3 | 1.9 | 0.0 | 5.8 | 3.9 | 3.1 | 2.4 | 2.1 |
| Gemcitabine | 3 | 3.1 | 4.1 | 2.6 | 0.0 | 1.6 | 2.8 | 4.1 | 1.9 | 6.3 | 2.5 | 3.4 | 3.5 | 4.6 |
| Gemcitabine | 4 | 5.2 | 4.9 | 2.3 | 3.0 | 2.1 | 1.7 | 3.3 | 2.1 | 8.4 | 6.1 | 3.9 | 3.6 | 3.2 |
| Gemcitabine | 5 | 4.7 | 5.8 | 4.1 | 7.4 | 3.6 | 4.4 | 5.4 | 3.5 | 7.4 | 3.6 | 6.4 | 5.8 | 7.2 |
| Gemcitabine | 6 | 6.9 | 6.8 | 4.0 | 9.7 | 0.8 | 3.7 | 4.4 | 2.2 | 5.2 | 7.8 | 7.3 | 6.1 | 5.5 |
| Gemcitabine | 7 | 7.0 | 7.7 | 3.4 | 8.3 | 2.5 | 0.8 | 2.2 | 1.8 | 8.9 | 6.6 | 8.5 | 6.3 | 7.6 |
| Gemcitabine | 8 | 9.3 | 10.6 | 6.4 | 1.0 | 2.9 | 3.7 | 5.5 | 2.4 | 11.8 | 7.4 | 7.8 | 7.3 | 7.8 |
| Glufosinate | 1 | 0.0 | 0.0 | 22.6 | 36.2 | 18.5 | 6.5 | 5.0 | 20.3 | 0.0 | 0.0 | 0.0 | 1.3 | 0.0 |
| Glufosinate | 2 | 1.7 | 2.4 | 16.5 | 23.2 | 14.2 | 3.0 | 4.7 | 9.0 | 5.6 | 3.9 | 4.4 | 0.0 | 1.3 |
| Glufosinate | 3 | 1.9 | 2.9 | 14.3 | 19.0 | 12.9 | 4.0 | 4.4 | 6.2 | 5.3 | 2.0 | 4.5 | 0.1 | 2.1 |
| Glufosinate | 4 | 3.1 | 4.4 | 10.0 | 15.4 | 4.6 | 0.0 | 1.2 | 9.1 | 1.2 | 4.4 | 4.0 | 6.6 | 2.4 |
| Glufosinate | 5 | 7.1 | 7.3 | 13.2 | 17.5 | 7.7 | 6.0 | 7.0 | 8.2 | 12.5 | 5.9 | 7.1 | 5.1 | 4.7 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Glufosinate | 6 | 8.3 | 8.6 | 11.6 | 13.6 | 3.3 | 7.8 | 4.9 | 4.7 | 15.8 | 7.5 | 8.6 | 5.7 | 5.6 |
| Glufosinate | 7 | 7.6 | 9.9 | 0.0 | 0.0 | 0.1 | 2.3 | 0.0 | 0.0 | 13.1 | 10.7 | 6.7 | 3.4 | 3.4 |
| Glufosinate | 8 | 8.7 | 10.7 | 1.0 | 0.4 | 0.0 | 1.9 | 0.5 | 0.4 | 14.2 | 11.6 | 6.9 | 4.5 | 4.1 |
| Indometacin | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Indometacin | 2 | 1.4 | 1.3 | 0.7 | 2.0 | 0.6 | 1.1 | 1.7 | 1.6 | 0.7 | 3.2 | 1.0 | 1.8 | 1.1 |
| Indometacin | 3 | 3.4 | 1.7 | 5.4 | 7.6 | 3.0 | 4.6 | 4.1 | 5.3 | 4.5 | 4.9 | 2.6 | 6.0 | 4.6 |
| Indometacin | 4 | 3.6 | 2.2 | 6.0 | 8.5 | 3.2 | 4.8 | 4.3 | 5.7 | 4.6 | 7.0 | 2.8 | 7.2 | 5.1 |
| Indometacin | 5 | 5.2 | 4.8 | 6.2 | 3.6 | 3.8 | 6.5 | 6.7 | 5.7 | 4.8 | 7.4 | 5.1 | 7.4 | 6.3 |
| Indometacin | 6 | 6.0 | 5.4 | 6.4 | 6.1 | 4.4 | 6.9 | 7.7 | 6.2 | 5.2 | 8.7 | 5.2 | 8.0 | 6.2 |
| Indometacin | 7 | 6.5 | 6.0 | 6.5 | 4.1 | 4.3 | 7.2 | 7.8 | 6.4 | 6.0 | 8.6 | 6.0 | 8.4 | 7.4 |
| Indometacin | 8 | 7.3 | 6.6 | 7.3 | 6.0 | 4.9 | 7.8 | 8.8 | 7.3 | 6.7 | 9.9 | 6.7 | 9.3 | 7.7 |
| Isradipine | 1 | 0.0 | 0.0 | 0.8 | 2.0 | 0.9 | 0.8 | 0.0 | 1.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Isradipine | 2 | 0.1 | 0.2 | 1.0 | 2.5 | 1.3 | 1.1 | 0.7 | 1.3 | 0.3 | 0.6 | 0.0 | 0.2 | 0.2 |
| Isradipine | 3 | 3.3 | 3.1 | 0.0 | 0.0 | 0.0 | 0.0 | 2.1 | 0.0 | 2.8 | 6.3 | 3.0 | 1.4 | 0.9 |
| Isradipine | 4 | 4.6 | 4.4 | 1.0 | 0.0 | 0.8 | 1.4 | 4.0 | 1.4 | 4.6 | 6.9 | 5.5 | 3.4 | 2.5 |
| Isradipine | 5 | 4.6 | 4.4 | 1.0 | 0.0 | 0.8 | 1.4 | 4.0 | 1.4 | 4.6 | 6.9 | 5.5 | 3.4 | 2.5 |
| Isradipine | 6 | 10.3 | 9.2 | 7.6 | 3.8 | 2.5 | 8.1 | 8.3 | 8.3 | 10.4 | 13.4 | 9.8 | 12.8 | 9.1 |
| Isradipine | 7 | 9.9 | 8.9 | 6.0 | 2.1 | 1.2 | 7.1 | 8.3 | 6.6 | 9.7 | 13.4 | 9.6 | 12.7 | 8.1 |
| Isradipine | 8 | 12.0 | 11.0 | 8.3 | 2.5 | 1.3 | 8.9 | 9.4 | 8.0 | 12.9 | 13.0 | 10.9 | 15.1 | 11.6 |
| Knoevenagel_cond | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.8 | 0.0 | 0.0 | 0.0 | 0.0 | 0.5 | 1.1 | 0.8 |
| Knoevenagel_cond | 2 | 3.4 | 1.7 | 1.3 | 8.9 | 3.2 | 0.0 | 1.2 | 4.8 | 4.3 | 1.7 | 0.3 | 0.0 | 0.0 |
| Knoevenagel_cond | 3 | 4.2 | 3.1 | 1.7 | 6.8 | 1.8 | 1.8 | 1.5 | 3.4 | 3.4 | 2.5 | 0.0 | 1.0 | 0.4 |
| Knoevenagel_cond | 4 | 5.8 | 4.9 | 2.6 | 6.9 | 3.1 | 1.3 | 1.9 | 5.5 | 6.7 | 2.8 | 2.7 | 2.6 | 3.3 |
| Knoevenagel_cond | 5 | 4.9 | 4.5 | 2.4 | 7.0 | 2.5 | 1.5 | 2.7 | 5.3 | 6.1 | 0.3 | 3.1 | 2.8 | 3.3 |
| Knoevenagel_cond | 6 | 7.5 | 5.9 | 5.3 | 9.8 | 6.1 | 4.3 | 5.1 | 8.3 | 7.3 | 8.2 | 3.5 | 4.6 | 3.7 |
| Knoevenagel_cond | 7 | 8.9 | 7.7 | 7.7 | 14.9 | 6.2 | 6.2 | 8.2 | 9.6 | 9.0 | 14.1 | 5.2 | 7.6 | 7.2 |
| Knoevenagel_cond | 8 | 12.6 | 10.8 | 11.1 | 22.1 | 9.7 | 9.8 | 10.9 | 15.5 | 12.6 | 17.3 | 6.8 | 9.6 | 10.4 |
| Liu_catal | 1 | 0.0 | 0.0 | 6.6 | 14.0 | 2.2 | 0.4 | 0.0 | 1.4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Liu_catal | 2 | 2.4 | 2.6 | 5.8 | 9.4 | 0.9 | 0.6 | 3.3 | 0.0 | 3.0 | 1.4 | 0.8 | 0.9 | 1.2 |
| Liu_catal | 3 | 2.6 | 2.9 | 6.9 | 11.3 | 1.9 | 1.3 | 4.1 | 0.9 | 3.2 | 3.2 | 0.6 | 0.9 | 1.5 |
| Liu_catal | 4 | 3.9 | 3.8 | 4.9 | 15.1 | 0.0 | 0.0 | 2.1 | 0.2 | 5.2 | 5.2 | 0.3 | 1.2 | 1.6 |
| Liu_catal | 5 | 3.9 | 3.9 | 4.9 | 13.6 | 0.1 | 0.0 | 2.4 | 0.2 | 5.2 | 5.4 | 0.5 | 1.4 | 1.7 |
| Liu_catal | 6 | 5.9 | 6.9 | 1.4 | 3.9 | 2.2 | 0.1 | 1.8 | 3.7 | 4.1 | 6.0 | 0.8 | 3.8 | 2.2 |
| Liu_catal | 7 | 8.4 | 9.6 | 0.2 | 0.4 | 1.1 | 0.6 | 5.8 | 2.8 | 7.4 | 8.3 | 1.6 | 5.5 | 4.0 |
| Liu_catal | 8 | 8.7 | 10.1 | 0.0 | 0.0 | 0.9 | 0.9 | 5.5 | 3.0 | 7.8 | 8.3 | 2.0 | 5.6 | 4.2 |
| Mannosulfan | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 5.5 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Mannosulfan | 2 | 2.0 | 2.0 | 1.8 | 4.5 | 6.2 | 1.8 | 2.3 | 4.0 | 3.7 | 0.7 | 1.9 | 1.4 | 4.4 |
| Mannosulfan | 3 | 3.5 | 2.7 | 1.0 | 6.2 | 0.0 | 1.1 | 3.3 | 1.5 | 11.7 | 4.7 | 1.3 | 3.1 | 6.0 |
| Mannosulfan | 4 | 7.8 | 4.8 | 6.5 | 20.1 | 3.5 | 6.4 | 9.6 | 5.8 | 13.7 | 13.1 | 1.9 | 4.0 | 4.8 |
| Mannosulfan | 5 | 2.6 | 1.8 | 5.1 | 12.0 | 5.6 | 5.7 | 8.0 | 6.0 | 2.7 | 8.3 | 0.9 | 1.5 | 3.9 |
| Mannosulfan | 6 | 9.7 | 9.3 | 0.9 | 13.7 | 7.7 | 0.9 | 5.4 | 9.0 | 19.2 | 8.7 | 2.7 | 4.2 | 9.1 |
| Mannosulfan | 7 | 11.2 | 9.3 | 0.0 | 12.9 | 4.8 | 4.4 | 7.4 | 4.6 | 22.3 | 15.3 | 5.1 | 8.9 | 10.7 |
| Mannosulfan | 8 | 14.7 | 11.8 | 7.5 | 25.1 | 4.6 | 8.0 | 10.2 | 7.5 | 18.1 | 22.0 | 4.0 | 9.1 | 8.8 |
| N_iprit | 1 | 0.0 | 0.0 | 0.3 | 0.0 | 0.0 | 0.2 | 3.0 | 0.1 | 0.0 | 0.0 | 2.1 | 0.0 | 0.8 |
| N_iprit | 2 | 1.1 | 0.1 | 0.0 | 1.9 | 1.3 | 1.5 | 3.0 | 0.5 | 1.1 | 3.6 | 0.0 | 0.5 | 0.0 |
| N_iprit | 3 | 1.6 | 0.7 | 0.1 | 1.2 | 1.2 | 0.0 | 1.9 | 0.0 | 1.6 | 5.0 | 3.1 | 0.9 | 0.9 |
| N_iprit | 4 | 2.2 | 0.4 | 0.2 | 3.3 | 2.0 | 1.4 | 0.0 | 0.4 | 1.3 | 9.0 | 5.2 | 0.7 | 0.5 |
| N_iprit | 5 | 2.2 | 0.9 | 0.4 | 4.2 | 2.1 | 4.0 | 3.4 | 2.5 | 2.1 | 7.0 | 0.4 | 1.0 | 1.3 |
| N_iprit | 6 | 3.4 | 1.9 | 0.4 | 5.3 | 1.8 | 0.0 | 2.5 | 0.5 | 3.0 | 5.7 | 2.5 | 1.1 | 1.2 |
| N_iprit | 7 | 3.3 | 1.1 | 1.0 | 6.3 | 5.1 | 4.0 | 1.9 | 2.8 | 3.0 | 10.6 | 2.5 | 2.9 | 1.4 |
| N_iprit | 8 | 7.7 | 5.3 | 3.0 | 9.1 | 6.6 | 5.4 | 3.0 | 3.6 | 6.1 | 12.7 | 5.5 | 4.9 | 4.7 |
| Oseltamivir | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 3.2 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.5 | 0.0 |
| Oseltamivir | 2 | 2.6 | 1.8 | 1.4 | 1.4 | 0.2 | 4.2 | 1.7 | 2.5 | 3.1 | 8.0 | 1.8 | 2.4 | 1.0 |
| Oseltamivir | 3 | 4.2 | 3.7 | 0.1 | 7.8 | 0.0 | 0.0 | 0.0 | 2.3 | 2.2 | 8.6 | 1.4 | 0.0 | 0.2 |
| Oseltamivir | 4 | 6.4 | 5.2 | 4.8 | 6.0 | 2.7 | 7.9 | 5.5 | 6.7 | 7.3 | 10.1 | 4.1 | 5.5 | 5.1 |
| Oseltamivir | 5 | 8.1 | 6.7 | 0.8 | 9.1 | 1.2 | 3.3 | 1.9 | 3.8 | 7.0 | 17.6 | 4.5 | 3.6 | 2.4 |
| Oseltamivir | 6 | 8.5 | 7.6 | 4.8 | 9.9 | 3.1 | 3.6 | 3.2 | 5.1 | 8.2 | 13.6 | 5.0 | 3.1 | 4.1 |
| Oseltamivir | 7 | 11.6 | 10.4 | 2.1 | 11.9 | 2.2 | 4.2 | 4.4 | 6.3 | 11.9 | 19.6 | 5.7 | 6.0 | 5.4 |
| Oseltamivir | 8 | 12.8 | 10.6 | 9.1 | 18.0 | 4.8 | 6.0 | 5.1 | 10.3 | 14.1 | 25.9 | 6.6 | 6.4 | 6.3 |
| Pantoprazole | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 4.7 | 0.0 | 4.9 | 0.0 | 0.0 | 2.5 | 0.0 |
| Pantoprazole | 2 | 4.7 | 1.8 | 7.8 | 13.6 | 2.6 | 6.5 | 6.7 | 1.6 | 8.9 | 5.5 | 4.6 | 7.4 | 2.6 |
| Pantoprazole | 3 | 1.1 | 1.3 | 6.4 | 5.4 | 4.1 | 4.5 | 5.3 | 3.8 | 1.7 | 5.3 | 0.9 | 3.3 | 0.3 |
| Pantoprazole | 4 | 4.5 | 5.2 | 3.0 | 3.5 | 3.1 | 2.8 | 7.9 | 2.7 | 8.9 | 1.7 | 5.2 | 6.5 | 4.8 |
| Pantoprazole | 5 | 0.6 | 2.4 | 7.5 | 14.3 | 6.7 | 1.1 | 0.0 | 3.6 | 0.0 | 9.6 | 2.2 | 0.0 | 1.1 |
| Pantoprazole | 6 | 8.2 | 7.3 | 8.6 | 15.7 | 8.8 | 7.2 | 10.3 | 9.8 | 11.1 | 11.6 | 5.2 | 9.2 | 5.8 |
| Pantoprazole | 7 | 7.2 | 7.0 | 8.3 | 13.1 | 7.2 | 6.0 | 6.5 | 6.4 | 8.7 | 12.7 | 6.9 | 9.1 | 6.3 |
| Pantoprazole | 8 | 11.1 | 11.0 | 10.3 | 19.6 | 10.6 | 9.2 | 12.6 | 12.0 | 13.0 | 14.0 | 9.6 | 12.0 | 10.1 |
| Propranolol | 1 | 0.5 | 0.1 | 4.9 | 3.4 | 0.6 | 1.8 | 2.3 | 0.6 | 1.0 | 0.0 | 0.0 | 0.9 | 0.0 |
| Propranolol | 2 | 0.0 | 0.0 | 4.1 | 8.2 | 1.0 | 0.0 | 0.0 | 1.2 | 0.0 | 3.7 | 0.4 | 0.0 | 0.6 |
| Propranolol | 3 | 1.9 | 2.2 | 0.0 | 1.7 | 0.7 | 0.8 | 2.8 | 0.0 | 0.6 | 2.7 | 0.8 | 2.3 | 1.7 |
| Propranolol | 4 | 3.0 | 3.2 | 1.1 | 0.8 | 0.5 | 1.5 | 3.9 | 1.1 | 3.0 | 5.2 | 1.5 | 3.2 | 2.0 |
| Propranolol | 5 | 1.3 | 0.5 | 6.2 | 3.9 | 1.9 | 5.1 | 4.8 | 2.2 | 0.5 | 2.8 | 1.9 | 3.7 | 2.3 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Propranolol | 6 | 5.9 | 5.6 | 2.4 | 0.0 | 0.0 | 3.5 | 5.8 | 1.5 | 5.8 | 9.9 | 4.3 | 6.1 | 4.4 |
| Propranolol | 7 | 6.8 | 6.6 | 4.9 | 2.0 | 1.8 | 4.7 | 6.8 | 3.8 | 7.5 | 12.2 | 4.9 | 6.8 | 6.7 |
| Propranolol | 8 | 7.6 | 7.3 | 3.9 | 8.3 | 4.1 | 4.0 | 6.5 | 4.4 | 4.8 | 14.5 | 5.2 | 5.9 | 5.5 |
| ProstaglandinE1 | 1 | 0.0 | 0.1 | 9.5 | 48.8 | 4.4 | 0.0 | 1.5 | 0.8 | 0.0 | 0.0 | 1.3 | 0.6 | 0.2 |
| ProstaglandinE1 | 2 | 0.1 | 0.0 | 11.5 | 54.4 | 5.9 | 0.7 | 1.5 | 2.5 | 0.6 | 1.3 | 0.5 | 0.0 | 0.0 |
| ProstaglandinE1 | 3 | 0.9 | 0.5 | 12.6 | 58.4 | 4.3 | 0.9 | 0.0 | 3.8 | 1.3 | 2.0 | 0.0 | 0.0 | 0.6 |
| ProstaglandinE1 | 4 | 1.1 | 1.2 | 12.6 | 58.6 | 4.4 | 1.6 | 0.1 | 3.3 | 1.9 | 3.6 | 0.8 | 1.1 | 1.4 |
| ProstaglandinE1 | 5 | 9.7 | 11.4 | 8.8 | 34.1 | 4.8 | 8.6 | 11.0 | 5.5 | 17.5 | 7.2 | 10.9 | 10.2 | 11.3 |
| ProstaglandinE1 | 6 | 12.8 | 14.5 | 5.0 | 18.7 | 5.5 | 11.1 | 18.1 | 4.0 | 15.4 | 5.4 | 14.4 | 12.9 | 12.0 |
| ProstaglandinE1 | 7 | 9.8 | 11.5 | 0.0 | 5.3 | 0.0 | 13.1 | 17.9 | 1.1 | 19.9 | 5.9 | 14.9 | 14.4 | 12.8 |
| ProstaglandinE1 | 8 | 14.6 | 16.5 | 0.6 | 0.0 | 1.1 | 13.4 | 18.8 | 0.0 | 23.7 | 6.5 | 16.5 | 15.5 | 14.4 |
| Pyridoxalphosphate | 1 | 0.0 | 0.0 | 5.4 | 13.6 | 2.9 | 2.9 | 6.9 | 3.2 | 0.0 | 0.8 | 0.0 | 2.6 | 0.7 |
| Pyridoxalphosphate | 2 | 2.0 | 2.0 | 3.6 | 13.4 | 0.0 | 0.2 | 1.1 | 0.0 | 1.5 | 2.2 | 0.2 | 1.3 | 0.8 |
| Pyridoxalphosphate | 3 | 3.1 | 2.7 | 6.4 | 15.2 | 2.7 | 0.0 | 0.0 | 2.3 | 1.0 | 2.8 | 0.2 | 0.0 | 0.0 |
| Pyridoxalphosphate | 4 | 4.9 | 7.4 | 0.0 | 10.0 | 1.0 | 5.2 | 9.6 | 5.1 | 1.7 | 0.0 | 2.4 | 5.2 | 3.5 |
| Pyridoxalphosphate | 5 | 5.8 | 7.6 | 7.1 | 12.8 | 8.0 | 3.6 | 7.3 | 11.6 | 1.9 | 0.8 | 1.8 | 5.0 | 2.2 |
| Pyridoxalphosphate | 6 | 8.4 | 9.5 | 4.1 | 12.5 | 2.1 | 7.5 | 10.9 | 6.3 | 6.0 | 7.7 | 5.3 | 6.1 | 5.4 |
| Pyridoxalphosphate | 7 | 9.3 | 10.8 | 1.4 | 8.1 | 1.7 | 5.9 | 12.4 | 5.7 | 7.2 | 6.6 | 5.1 | 6.6 | 5.9 |
| Pyridoxalphosphate | 8 | 10.2 | 12.8 | 3.5 | 0.0 | 5.5 | 7.9 | 12.3 | 8.7 | 9.6 | 15.5 | 7.3 | 12.3 | 8.6 |
| Quinuclidinyl | 1 | 0.0 | 0.0 | 4.3 | 6.3 | 0.7 | 2.4 | 0.5 | 1.8 | 0.0 | 1.1 | 0.0 | 0.0 | 0.0 |
| Quinuclidinyl | 2 | 0.4 | 0.3 | 4.7 | 5.5 | 0.7 | 3.5 | 1.4 | 1.8 | 1.2 | 0.0 | 0.2 | 0.3 | 0.4 |
| Quinuclidinyl | 3 | 2.8 | 3.4 | 0.0 | 1.7 | 0.0 | 0.0 | 0.0 | 0.6 | 2.1 | 2.2 | 2.5 | 1.7 | 2.9 |
| Quinuclidinyl | 4 | 4.4 | 4.7 | 4.1 | 0.0 | 0.7 | 3.3 | 2.2 | 0.0 | 5.3 | 7.5 | 3.7 | 4.9 | 4.8 |
| Quinuclidinyl | 5 | 6.8 | 6.0 | 8.8 | 12.2 | 5.1 | 4.4 | 5.1 | 7.3 | 5.2 | 9.1 | 4.8 | 2.8 | 4.3 |
| Quinuclidinyl | 6 | 8.8 | 8.8 | 4.5 | 8.2 | 4.5 | 2.1 | 4.7 | 6.0 | 6.6 | 9.8 | 7.1 | 4.5 | 7.1 |
| Quinuclidinyl | 7 | 8.6 | 7.0 | 13.4 | 19.7 | 4.6 | 9.4 | 9.9 | 10.8 | 9.6 | 15.1 | 6.0 | 9.9 | 8.1 |
| Quinuclidinyl | 8 | 11.0 | 10.5 | 8.1 | 5.2 | 4.8 | 5.2 | 6.6 | 4.9 | 10.6 | 14.9 | 8.0 | 7.4 | 8.8 |
| RAMBO | 1 | 0.0 | 0.0 | 3.8 | 0.0 | 0.0 | 1.5 | 0.0 | 3.6 | 0.0 | 0.0 | 0.9 | 0.0 | 0.0 |
| RAMBO | 2 | 5.0 | 4.5 | 0.0 | 4.6 | 2.2 | 0.0 | 0.4 | 1.0 | 2.4 | 10.0 | 0.0 | 0.4 | 0.4 |
| RAMBO | 3 | 6.2 | 5.2 | 1.9 | 3.8 | 2.4 | 4.0 | 4.5 | 2.2 | 5.6 | 13.8 | 0.9 | 2.9 | 2.6 |
| RAMBO | 4 | 5.5 | 5.0 | 0.1 | 6.3 | 1.6 | 0.5 | 1.7 | 0.0 | 4.9 | 14.1 | 0.8 | 1.3 | 0.9 |
| RAMBO | 5 | 6.0 | 5.4 | 3.0 | 4.1 | 2.4 | 2.5 | 3.6 | 1.7 | 6.4 | 10.8 | 0.2 | 1.3 | 1.4 |
| RAMBO | 6 | 6.6 | 5.6 | 2.4 | 8.3 | 2.3 | 0.6 | 2.7 | 1.9 | 5.8 | 14.1 | 1.3 | 1.2 | 1.6 |
| RAMBO | 7 | 7.2 | 6.6 | 2.4 | 5.7 | 1.2 | 0.7 | 2.5 | 1.1 | 7.2 | 12.0 | 0.9 | 1.1 | 1.3 |
| RAMBO | 8 | 8.1 | 7.4 | 3.7 | 6.3 | 2.2 | 1.7 | 3.7 | 2.7 | 7.7 | 14.1 | 1.6 | 1.9 | 2.7 |
| RH34 | 1 | 0.0 | 0.0 | 1.4 | 3.7 | 2.2 | 3.8 | 2.8 | 1.9 | 1.0 | 0.0 | 0.0 | 0.9 | 0.6 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| RH34 | 2 | 0.4 | 0.4 | 0.0 | 2.3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.4 | 0.7 | 0.0 | 0.0 |
| RH34 | 3 | 2.7 | 2.2 | 0.7 | 1.6 | 0.0 | 0.5 | 0.6 | 1.0 | 3.7 | 0.9 | 2.1 | 1.2 | 1.1 |
| RH34 | 4 | 1.2 | 1.5 | 5.5 | 6.5 | 3.3 | 2.3 | 1.4 | 4.4 | 1.8 | 3.0 | 1.5 | 0.3 | 1.3 |
| RH34 | 5 | 4.0 | 4.5 | 4.2 | 5.3 | 4.1 | 4.9 | 2.6 | 5.2 | 2.8 | 4.0 | 6.8 | 4.1 | 5.7 |
| RH34 | 6 | 3.8 | 4.7 | 5.7 | 0.0 | 2.3 | 5.9 | 5.3 | 3.7 | 4.6 | 4.1 | 7.0 | 3.9 | 5.4 |
| RH34 | 7 | 6.4 | 5.9 | 8.0 | 4.8 | 5.1 | 6.3 | 7.0 | 7.9 | 9.0 | 7.9 | 7.0 | 6.3 | 6.3 |
| RH34 | 8 | 7.0 | 6.5 | 8.4 | 6.7 | 5.1 | 6.0 | 6.5 | 8.4 | 10.1 | 9.3 | 7.4 | 6.5 | 6.9 |
| Rolipram | 1 | 0.0 | 0.0 | 0.5 | 2.6 | 0.0 | 2.2 | 1.3 | 0.7 | 1.6 | 1.6 | 0.0 | 0.5 | 0.0 |
| Rolipram | 2 | 1.2 | 1.1 | 1.0 | 0.0 | 0.0 | 2.5 | 1.9 | 1.1 | 2.6 | 0.9 | 0.2 | 0.9 | 0.7 |
| Rolipram | 3 | 0.4 | 1.6 | 0.0 | 3.5 | 0.7 | 1.1 | 0.6 | 0.0 | 0.2 | 1.1 | 3.3 | 0.0 | 1.5 |
| Rolipram | 4 | 0.4 | 1.8 | 0.2 | 3.2 | 1.0 | 1.4 | 0.9 | 0.1 | 0.0 | 1.3 | 3.7 | 0.3 | 1.8 |
| Rolipram | 5 | 3.2 | 5.4 | 0.4 | 0.1 | 1.3 | 1.8 | 2.5 | 0.9 | 0.9 | 0.0 | 7.3 | 2.6 | 4.3 |
| Rolipram | 6 | 4.4 | 5.5 | 1.9 | 0.6 | 0.4 | 3.1 | 3.1 | 0.6 | 3.8 | 6.0 | 5.6 | 2.5 | 3.7 |
| Rolipram | 7 | 4.1 | 5.0 | 2.0 | 8.9 | 1.3 | 0.9 | 1.0 | 2.5 | 3.7 | 7.9 | 4.2 | 0.8 | 2.9 |
| Rolipram | 8 | 4.4 | 6.2 | 2.1 | 7.5 | 1.6 | 0.0 | 0.0 | 1.8 | 1.0 | 8.2 | 6.7 | 0.3 | 4.0 |
| Rosmaridiphenol | 1 | 0.0 | 0.0 | 0.0 | 4.0 | 0.4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Rosmaridiphenol | 2 | 2.1 | 2.2 | 0.7 | 0.0 | 0.0 | 2.3 | 2.1 | 0.1 | 3.5 | 1.1 | 2.9 | 3.2 | 3.0 |
| Rosmaridiphenol | 3 | 1.4 | 1.7 | 5.1 | 10.6 | 5.9 | 4.0 | 2.7 | 2.9 | 1.6 | 5.5 | 1.5 | 1.4 | 2.2 |
| Rosmaridiphenol | 4 | 4.7 | 4.8 | 2.9 | 5.2 | 2.8 | 4.1 | 4.4 | 2.2 | 6.9 | 5.2 | 4.0 | 4.8 | 4.9 |
| Rosmaridiphenol | 5 | 6.0 | 6.0 | 5.0 | 9.3 | 6.7 | 6.6 | 5.8 | 2.8 | 8.9 | 14.1 | 5.2 | 4.8 | 5.2 |
| Rosmaridiphenol | 6 | 7.0 | 7.4 | 6.6 | 13.5 | 9.4 | 8.1 | 7.1 | 3.4 | 10.2 | 16.4 | 6.4 | 6.2 | 6.6 |
| Rosmaridiphenol | 7 | 7.1 | 7.1 | 8.2 | 11.3 | 8.4 | 7.4 | 5.3 | 5.0 | 6.6 | 12.8 | 5.6 | 4.9 | 6.1 |
| Rosmaridiphenol | 8 | 8.7 | 9.4 | 8.2 | 11.8 | 9.6 | 8.5 | 6.8 | 3.9 | 10.0 | 15.6 | 7.1 | 6.7 | 7.3 |
| Takemoto | 1 | 1.7 | 0.3 | 5.0 | 6.3 | 0.0 | 0.8 | 0.0 | 0.0 | 0.0 | 1.1 | 4.0 | 0.8 | 0.4 |
| Takemoto | 2 | 0.0 | 0.0 | 0.0 | 5.2 | 1.3 | 0.0 | 1.6 | 0.3 | 0.3 | 0.0 | 0.0 | 0.0 | 0.0 |
| Takemoto | 3 | 3.8 | 2.4 | 3.9 | 2.4 | 2.1 | 1.2 | 2.7 | 3.0 | 3.7 | 2.1 | 3.2 | 2.1 | 2.5 |
| Takemoto | 4 | 4.4 | 3.5 | 2.6 | 3.4 | 4.3 | 1.4 | 1.2 | 0.9 | 4.3 | 3.9 | 3.9 | 3.1 | 2.7 |
| Takemoto | 5 | 7.6 | 6.4 | 3.5 | 0.0 | 5.3 | 4.9 | 7.7 | 4.1 | 7.5 | 6.9 | 5.1 | 5.0 | 4.9 |
| Takemoto | 6 | 6.9 | 7.2 | 4.9 | 7.4 | 4.3 | 6.1 | 7.6 | 5.0 | 7.1 | 4.6 | 6.4 | 3.7 | 6.2 |
| Takemoto | 7 | 11.1 | 10.1 | 6.5 | 0.3 | 6.9 | 5.9 | 10.0 | 6.3 | 10.0 | 6.7 | 6.7 | 6.5 | 7.5 |
| Takemoto | 8 | 11.4 | 11.4 | 7.2 | 5.7 | 8.0 | 6.6 | 8.8 | 6.5 | 10.7 | 12.4 | 10.4 | 8.7 | 9.6 |
| Triacetin | 1 | 0.0 | 0.0 | 0.0 | 1.5 | 0.1 | 0.3 | 0.0 | 0.5 | 0.0 | 0.0 | 0.3 | 0.2 | 0.0 |
| Triacetin | 2 | 0.8 | 1.0 | 0.1 | 0.0 | 0.0 | 0.3 | 0.2 | 0.1 | 2.3 | 1.4 | 0.0 | 0.6 | 0.3 |
| Triacetin | 3 | 2.5 | 2.5 | 2.6 | 2.3 | 2.0 | 1.8 | 2.0 | 2.5 | 3.8 | 4.0 | 0.2 | 1.3 | 0.7 |
| Triacetin | 4 | 3.6 | 3.7 | 0.8 | 1.8 | 0.4 | 0.0 | 1.1 | 0.0 | 5.3 | 1.9 | 1.0 | 0.0 | 1.5 |
| Triacetin | 5 | 4.5 | 4.4 | 3.1 | 6.1 | 3.3 | 0.5 | 1.7 | 2.5 | 4.9 | 5.7 | 0.9 | 0.4 | 1.2 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Triacetin | 6 | 8.7 | 7.9 | 6.4 | 1.6 | 2.7 | 7.6 | 8.8 | 6.5 | 12.7 | 11.7 | 6.3 | 9.5 | 8.8 |
| Triacetin | 7 | 9.0 | 8.1 | 8.4 | 6.3 | 4.5 | 7.2 | 9.0 | 7.9 | 10.3 | 13.8 | 6.6 | 9.1 | 8.4 |
| Triacetin | 8 | 14.2 | 12.7 | 10.7 | 9.1 | 6.7 | 9.1 | 11.9 | 11.8 | 17.3 | 18.8 | 9.8 | 11.4 | 11.9 |
| Tsogoeva | 1 | 0.0 | 0.0 | 9.8 | 21.8 | 6.3 | 1.1 | 0.0 | 3.7 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Tsogoeva | 2 | 2.5 | 2.3 | 13.0 | 16.3 | 5.1 | 5.3 | 4.5 | 4.7 | 4.5 | 4.1 | 2.7 | 5.4 | 2.7 |
| Tsogoeva | 3 | 1.4 | 1.9 | 11.2 | 16.1 | 5.1 | 3.3 | 1.9 | 2.2 | 3.8 | 2.5 | 2.8 | 3.7 | 2.7 |
| Tsogoeva | 4 | 2.5 | 3.4 | 12.8 | 11.6 | 3.4 | 5.3 | 4.1 | 1.6 | 7.8 | 4.8 | 5.3 | 7.0 | 4.9 |
| Tsogoeva | 5 | 4.8 | 6.3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.8 | 0.0 | 7.4 | 11.6 | 1.8 | 4.9 | 2.3 |
| Tsogoeva | 6 | 6.5 | 6.4 | 15.6 | 12.8 | 4.6 | 8.9 | 7.6 | 5.2 | 11.3 | 10.2 | 6.1 | 10.4 | 6.5 |
| Tsogoeva | 7 | 7.2 | 7.6 | 8.2 | 11.0 | 7.2 | 4.3 | 4.7 | 7.3 | 7.6 | 9.2 | 4.3 | 7.4 | 4.3 |
| Tsogoeva | 8 | 9.6 | 11.0 | 4.8 | 4.0 | 3.6 | 3.7 | 3.9 | 0.9 | 7.4 | 17.9 | 6.3 | 9.7 | 4.7 |
| UH232 | 1 | 0.0 | 0.0 | 1.1 | 1.3 | 0.0 | 2.0 | 1.8 | 0.0 | 1.6 | 0.0 | 0.0 | 0.7 | 0.4 |
| UH232 | 2 | 1.1 | 0.8 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 2.4 | 2.5 | 0.5 | 1.2 | 0.0 |
| UH232 | 3 | 1.9 | 1.1 | 2.8 | 0.5 | 1.8 | 3.8 | 3.2 | 3.6 | 0.0 | 6.0 | 0.7 | 0.0 | 0.8 |
| UH232 | 4 | 2.4 | 2.1 | 3.2 | 3.1 | 2.1 | 3.6 | 3.1 | 3.7 | 2.8 | 5.1 | 2.1 | 1.9 | 2.0 |
| UH232 | 5 | 3.8 | 2.8 | 4.6 | 1.8 | 3.4 | 5.5 | 5.3 | 6.2 | 0.9 | 8.5 | 2.4 | 2.1 | 2.3 |
| UH232 | 6 | 4.4 | 3.1 | 5.7 | 7.7 | 5.6 | 6.0 | 4.9 | 6.6 | 2.6 | 12.9 | 2.9 | 3.9 | 3.2 |
| UH232 | 7 | 5.1 | 3.9 | 6.3 | 6.7 | 4.8 | 8.1 | 7.8 | 8.9 | 1.7 | 11.9 | 3.5 | 3.2 | 3.9 |
| UH232 | 8 | 6.2 | 4.8 | 6.2 | 6.5 | 4.9 | 7.6 | 8.1 | 9.6 | 2.7 | 14.0 | 4.5 | 4.4 | 4.6 |
| VX | 1 | 0.0 | 0.0 | 0.5 | 0.0 | 0.5 | 0.0 | 1.2 | 0.3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 |
| VX | 2 | 1.9 | 1.2 | 0.0 | 0.4 | 1.2 | 0.7 | 1.9 | 0.0 | 1.0 | 1.7 | 1.0 | 1.0 | 0.0 |
| VX | 3 | 1.7 | 1.6 | 2.5 | 3.8 | 2.6 | 2.1 | 3.1 | 3.0 | 1.1 | 3.2 | 1.8 | 2.6 | 2.6 |
| VX | 4 | 2.6 | 2.1 | 3.4 | 4.6 | 4.2 | 1.7 | 3.6 | 6.0 | 2.7 | 5.6 | 1.0 | 1.7 | 2.8 |
| VX | 5 | 2.4 | 2.7 | 3.2 | 9.4 | 2.5 | 3.1 | 4.3 | 0.7 | 1.4 | 1.1 | 1.9 | 2.3 | 1.8 |
| VX | 6 | 4.0 | 3.3 | 3.2 | 5.1 | 0.0 | 2.8 | 0.0 | 4.4 | 3.0 | 4.8 | 1.9 | 1.0 | 4.2 |
| VX | 7 | 4.3 | 3.8 | 5.5 | 7.0 | 4.2 | 2.9 | 2.6 | 7.2 | 3.5 | 7.5 | 1.8 | 1.9 | 4.0 |
| VX | 8 | 5.3 | 5.1 | 5.4 | 12.8 | 4.5 | 4.9 | 6.8 | 4.3 | 3.5 | 3.2 | 2.4 | 3.2 | 2.2 |
| WAY100635 | 1 | 0.0 | 0.0 | 1.6 | 5.9 | 1.2 | 6.1 | 7.1 | 2.3 | 0.0 | 2.4 | 0.0 | 0.6 | 0.0 |
| WAY100635 | 2 | 3.6 | 4.1 | 0.0 | 0.0 | 0.0 | 4.1 | 9.0 | 0.8 | 6.3 | 0.0 | 3.0 | 2.8 | 3.5 |
| WAY100635 | 3 | 5.7 | 5.7 | 0.1 | 1.5 | 0.0 | 2.8 | 7.7 | 0.0 | 6.9 | 2.3 | 2.9 | 2.8 | 3.0 |
| WAY100635 | 4 | 6.7 | 7.1 | 1.0 | 6.7 | 0.5 | 1.7 | 7.3 | 1.0 | 8.1 | 2.9 | 6.6 | 3.6 | 4.0 |
| WAY100635 | 5 | 8.4 | 8.1 | 5.7 | 7.5 | 5.7 | 9.2 | 13.8 | 7.8 | 10.4 | 8.0 | 5.1 | 6.4 | 7.4 |
| WAY100635 | 6 | 5.2 | 5.6 | 3.9 | 17.7 | 4.9 | 0.0 | 0.0 | 3.0 | 0.9 | 7.0 | 2.7 | 0.0 | 0.5 |
| WAY100635 | 7 | 10.6 | 11.4 | 4.0 | 9.9 | 4.9 | 3.9 | 9.0 | 4.9 | 9.6 | 9.0 | 9.5 | 6.5 | 8.1 |
| WAY100635 | 8 | 12.4 | 12.4 | 4.2 | 12.1 | 4.9 | 2.9 | 8.7 | 4.4 | 10.8 | 9.9 | 8.2 | 6.4 | 7.2 |
| XylitolPentanit | 1 | 0.0 | 0.0 | 0.1 | 3.8 | 0.6 | 3.1 | 0.0 | 0.5 | 0.0 | 0.4 | 1.8 | 2.0 | 1.1 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| XylitolPentanit | 2 | 1.0 | 1.6 | 2.0 | 4.0 | 2.8 | 4.8 | 1.4 | 1.3 | 1.9 | 0.0 | 0.0 | 1.3 | 0.0 |
| XylitolPentanit | 3 | 2.9 | 3.3 | 0.6 | 0.0 | 0.0 | 6.1 | 1.6 | 0.2 | 6.7 | 4.1 | 3.0 | 6.2 | 2.6 |
| XylitolPentanit | 4 | 4.0 | 4.5 | 1.1 | 6.1 | 2.1 | 3.0 | 1.7 | 0.3 | 3.7 | 5.7 | 2.6 | 0.0 | 2.0 |
| XylitolPentanit | 5 | 3.8 | 5.2 | 0.0 | 1.9 | 2.3 | 4.3 | 1.8 | 0.0 | 2.3 | 5.3 | 1.7 | 0.7 | 1.8 |
| XylitolPentanit | 6 | 5.5 | 6.7 | 5.2 | 3.6 | 8.5 | 12.2 | 7.0 | 3.9 | 0.6 | 7.8 | 6.1 | 6.8 | 7.1 |
| XylitolPentanit | 7 | 7.3 | 8.1 | 0.0 | 13.3 | 5.5 | 0.0 | 0.0 | 0.9 | 6.6 | 12.6 | 3.5 | 0.1 | 4.5 |
| XylitolPentanit | 8 | 8.9 | 9.9 | 3.4 | 11.2 | 7.8 | 3.3 | 3.3 | 3.3 | 10.8 | 13.4 | 4.2 | 0.5 | 7.5 |
| shiepox_depox | 1 | 0.0 | 0.0 | 0.8 | 5.0 | 1.1 | 0.0 | 0.0 | 1.0 | 0.4 | 1.4 | 0.0 | 0.0 | 0.0 |
| shiepox_depox | 2 | 0.5 | 0.3 | 1.8 | 3.3 | 1.3 | 1.4 | 0.7 | 1.5 | 0.1 | 0.0 | 1.1 | 1.3 | 1.3 |
| shiepox_depox | 3 | 1.3 | 2.0 | 0.1 | 0.5 | 0.5 | 1.7 | 0.7 | 0.0 | 0.9 | 7.6 | 0.5 | 0.6 | 0.2 |
| shiepox_depox | 4 | 1.7 | 2.3 | 0.0 | 0.0 | 0.0 | 1.4 | 0.4 | 0.1 | 0.0 | 6.2 | 0.9 | 1.2 | 0.9 |
| shiepox_depox | 5 | 3.7 | 3.8 | 1.4 | 5.5 | 2.4 | 1.7 | 2.0 | 1.8 | 5.0 | 9.8 | 0.6 | 1.2 | 1.2 |
| shiepox_depox | 6 | 4.8 | 4.6 | 3.6 | 5.0 | 2.0 | 4.8 | 4.8 | 4.0 | 4.7 | 6.0 | 3.1 | 4.4 | 3.5 |
| shiepox_depox | 7 | 5.1 | 5.0 | 2.1 | 3.4 | 2.2 | 3.0 | 2.8 | 2.3 | 5.0 | 8.7 | 1.7 | 2.7 | 2.8 |
| shiepox_depox | 8 | 6.6 | 6.7 | 4.9 | 7.6 | 2.3 | 5.1 | 5.8 | 5.2 | 8.2 | 10.5 | 2.9 | 7.0 | 5.7 |

***Table S6. Tabulated relative conformational energies (kcal/mol) obtained with SP DLPNO-CCSD(T)/cc-pVTZ and PBE-D3/def2-tzvp on PBE-D3/def2-tzvp geometries and OPT AM1, MNDO, PM3, PM6, PM7, RM1, QM, MMFF94, DFTB3, GFN-xTB, GFN2-xTB starting from PBE-D3/def2-tzvp geometries.***

| | № | DLPNO/TZ | PBE-D3 | AM1 | MNDO | PM3 | PM6 | PM7 | RM1 | QM1 | MMFF94 | DFTB3 | GFN-xTB | GFN2-xTB |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18crown6 | 1 | 0.0 | 0.0 | 0.0 | 1.5 | 0.4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.0 | 0.0 |
| 18crown6 | 2 | 0.2 | 0.9 | 7.2 | 0.0 | 7.9 | 4.6 | 6.4 | 8.9 | 7.6 | 1.4 | 1.0 | 7.2 | 6.3 |
| 18crown6 | 3 | 4.3 | 2.7 | 11.4 | 1.4 | 12.8 | 14.7 | 16.1 | 18.0 | 9.6 | 10.3 | 9.2 | 8.0 | 16.6 |
| 18crown6 | 4 | 2.0 | 2.6 | 5.3 | 2.7 | 4.4 | 1.9 | 6.9 | 6.7 | 6.9 | 2.7 | 2.7 | 4.3 | 5.9 |
| 18crown6 | 5 | 2.4 | 2.7 | 6.5 | 2.3 | 7.0 | 6.3 | 7.7 | 10.3 | 8.5 | 4.8 | 3.0 | 7.2 | 5.8 |
| 18crown6 | 6 | 3.0 | 3.9 | 5.4 | 1.8 | 0.4 | 6.7 | 7.7 | 3.7 | 11.2 | 1.4 | 0.0 | 4.8 | 4.6 |
| 18crown6 | 7 | 5.0 | 5.0 | 3.5 | 7.9 | 0.0 | 1.5 | 3.6 | 4.4 | 8.9 | 6.6 | 2.3 | 2.9 | 1.7 |
| 18crown6 | 8 | 6.4 | 8.1 | 9.1 | 5.0 | 7.8 | 0.5 | 11.4 | 11.2 | 14.5 | 5.4 | 2.1 | 8.0 | 8.5 |
| Artemizinin | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Artemizinin | 2 | 7.4 | 7.0 | 4.8 | 0.0 | 0.9 | 5.5 | 5.5 | 3.6 | 10.6 | 10.7 | 5.0 | 5.7 | 5.4 |
| Artemizinin | 3 | 8.2 | 7.3 | 4.8 | 0.0 | 0.9 | 5.5 | 5.5 | 3.6 | 9.2 | 9.1 | 5.0 | 6.5 | 7.2 |
| Artemizinin | 4 | 7.7 | 7.2 | 4.6 | 3.4 | 3.6 | 3.7 | 4.3 | 4.6 | 7.9 | 9.4 | 4.7 | 4.3 | 5.2 |
| Artemizinin | 5 | 10.0 | 9.0 | 5.7 | 5.9 | 4.6 | 6.4 | 6.4 | 8.0 | 8.5 | 11.6 | 5.8 | 7.5 | 7.0 |
| Artemizinin | 6 | 10.3 | 9.6 | 5.7 | 5.9 | 6.5 | 6.3 | 6.0 | 8.4 | 8.5 | 13.0 | 5.7 | 7.1 | 6.8 |
| Artemizinin | 7 | 11.3 | 11.0 | 8.1 | 6.7 | 5.6 | 9.0 | 9.5 | 9.4 | 16.5 | 17.2 | 8.3 | 8.7 | 8.8 |
| Artemizinin | 8 | 11.2 | 11.0 | 6.9 | 3.4 | 3.6 | 6.9 | 4.3 | 6.2 | 13.3 | 12.4 | 7.6 | 4.3 | 5.2 |
| Atropine | 1 | 0.0 | 0.0 | 0.1 | 1.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Atropine | 2 | 1.5 | 0.7 | 1.2 | 2.8 | 1.2 | 0.8 | 1.1 | 1.5 | 0.8 | 2.3 | 0.3 | 2.3 | 0.8 |
| Atropine | 3 | 2.9 | 2.3 | 1.1 | 2.5 | 0.3 | 1.3 | 2.6 | 0.8 | 4.9 | 0.5 | 2.9 | 4.6 | 2.4 |
| Atropine | 4 | 8.1 | 7.2 | 0.1 | 0.8 | 0.4 | 2.2 | 5.9 | 2.4 | 15.5 | 5.1 | 7.3 | 7.4 | 6.2 |
| Atropine | 5 | 9.6 | 8.5 | 0.0 | 0.0 | 0.3 | 2.3 | 5.6 | 3.3 | 14.3 | 8.1 | 7.6 | 6.9 | 6.7 |
| Atropine | 6 | 11.6 | 10.5 | 2.8 | 3.3 | 1.2 | 2.3 | 5.3 | 3.9 | 14.1 | 8.1 | 8.2 | 6.4 | 7.0 |
| Atropine | 7 | 11.6 | 9.9 | 4.3 | 6.3 | 2.6 | 3.3 | 7.2 | 5.0 | 16.9 | 8.7 | 8.8 | 9.3 | 8.6 |
| Atropine | 8 | 8.7 | 6.7 | 5.3 | 7.8 | 0.3 | 7.2 | 9.9 | 6.3 | 9.4 | 12.1 | 6.5 | 10.3 | 7.8 |
| Bispidin | 1 | 0.0 | 0.0 | 1.0 | 0.0 | 0.8 | 2.9 | 2.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Bispidin | 2 | 3.4 | 3.0 | 0.0 | 2.1 | 0.0 | 0.0 | 0.0 | 0.8 | 4.8 | 4.9 | 1.5 | 1.3 | 1.5 |
| Bispidin | 3 | 4.1 | 3.9 | 5.9 | 3.8 | 4.7 | 7.1 | 6.9 | 5.0 | 7.5 | 10.3 | 3.9 | 3.8 | 4.7 |
| Bispidin | 4 | 4.3 | 4.4 | 1.0 | 2.7 | 6.2 | 10.9 | 10.7 | 7.3 | 7.4 | 8.1 | 4.2 | 5.1 | 5.9 |
| Bispidin | 5 | 5.2 | 4.7 | 5.0 | 3.9 | 3.9 | 6.0 | 5.9 | 5.2 | 9.1 | 9.9 | 3.7 | 4.2 | 4.9 |
| Bispidin | 6 | 11.3 | 10.6 | 7.1 | 7.5 | 5.5 | 5.4 | 5.6 | 7.5 | 16.4 | 19.3 | 7.8 | 6.8 | 8.7 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Bispidin | 7 | 11.5 | 10.9 | 2.2 | 2.7 | 7.4 | 9.7 | 9.7 | 9.8 | 16.0 | 17.9 | 8.1 | 8.2 | 9.7 |
| Bispidin | 8 | 11.9 | 11.5 | 12.1 | 6.8 | 9.7 | 14.2 | 14.1 | 12.2 | 15.9 | 17.1 | 8.5 | 9.7 | 11.2 |
| Cembrene | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.6 | 0.0 | 0.2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Cembrene | 2 | 3.0 | 2.8 | 1.1 | 0.5 | 2.1 | 1.7 | 2.1 | 1.5 | 3.5 | 3.0 | 2.8 | 2.5 | 3.0 |
| Cembrene | 3 | 3.8 | 3.2 | 1.2 | 2.9 | 1.2 | 1.1 | 0.0 | 2.2 | 1.7 | 6.0 | 2.4 | 1.8 | 2.1 |
| Cembrene | 4 | 6.0 | 5.6 | 1.2 | 0.0 | 1.2 | 1.3 | 2.9 | 1.7 | 5.0 | 6.9 | 3.8 | 5.1 | 4.9 |
| Cembrene | 5 | 6.0 | 5.8 | 2.7 | 7.8 | 0.0 | 1.3 | 0.7 | 3.3 | 4.3 | 8.2 | 2.7 | 3.8 | 4.1 |
| Cembrene | 6 | 9.5 | 8.8 | 4.4 | 3.8 | 2.8 | 4.6 | 5.5 | 4.8 | 8.2 | 11.2 | 5.7 | 6.4 | 7.4 |
| Cembrene | 7 | 10.4 | 9.7 | 5.9 | 9.3 | 3.2 | 5.0 | 5.4 | 9.0 | 9.4 | 14.8 | 6.9 | 7.9 | 8.4 |
| Cembrene | 8 | 12.5 | 11.1 | 7.7 | 6.9 | 4.6 | 6.0 | 6.1 | 8.4 | 11.1 | 15.9 | 7.1 | 8.3 | 9.3 |
| Cimetidine | 1 | 0.0 | 0.0 | 0.0 | 0.6 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 4.3 | 0.0 | 0.0 | 0.0 |
| Cimetidine | 2 | 2.2 | 2.4 | 0.9 | 0.0 | 1.9 | 1.8 | 1.6 | 1.1 | 3.6 | 3.1 | 0.8 | 2.0 | 2.1 |
| Cimetidine | 3 | 5.2 | 5.4 | 2.1 | 1.5 | 3.0 | 1.3 | 0.0 | 1.0 | 5.9 | 0.0 | 5.3 | 3.7 | 4.0 |
| Cimetidine | 4 | 8.1 | 7.6 | 3.7 | 2.3 | 2.2 | 2.2 | 2.6 | 0.9 | 8.9 | 4.8 | 7.0 | 5.5 | 5.0 |
| Cimetidine | 5 | 5.6 | 6.0 | 3.2 | 0.8 | 1.4 | 5.1 | 5.7 | 4.6 | 6.4 | 9.6 | 3.9 | 5.3 | 5.2 |
| Cimetidine | 6 | 6.4 | 7.2 | 3.3 | 1.1 | 2.3 | 1.8 | 4.0 | 2.8 | 9.8 | 6.9 | 4.2 | 4.4 | 2.9 |
| Cimetidine | 7 | 6.0 | 6.3 | 2.2 | 1.2 | 1.7 | 3.7 | 6.7 | 1.6 | 4.9 | 6.5 | 3.0 | 4.3 | 3.8 |
| Cimetidine | 8 | 13.4 | 14.1 | 5.8 | 1.8 | 3.9 | 8.4 | 2.7 | 7.2 | 19.9 | 15.1 | 11.9 | 11.5 | 13.9 |
| Cryptand222 | 1 | 0.0 | 0.0 | 0.9 | 0.8 | 10.8 | 7.3 | 3.8 | 4.7 | 0.0 | 6.7 | 3.2 | 1.1 | 0.0 |
| Cryptand222 | 2 | 1.0 | 1.5 | 3.9 | 0.0 | 0.0 | 1.6 | 2.9 | 2.7 | 18.9 | 0.2 | 1.3 | 2.0 | 3.8 |
| Cryptand222 | 3 | 0.4 | 1.6 | 3.9 | 1.4 | 9.4 | 4.2 | 4.4 | 1.8 | 18.4 | 0.0 | 0.4 | 1.8 | 2.7 |
| Cryptand222 | 4 | 2.5 | 3.0 | 2.8 | 0.7 | 7.4 | 2.9 | 0.9 | 0.5 | 7.7 | 1.5 | 1.8 | 1.5 | 2.4 |
| Cryptand222 | 5 | 3.2 | 4.7 | 0.0 | 4.1 | 4.1 | 0.0 | 2.2 | 1.3 | 15.4 | 1.1 | 0.0 | 0.6 | 0.7 |
| Cryptand222 | 6 | 5.9 | 6.9 | 0.3 | 3.6 | 5.3 | 0.5 | 1.1 | 0.0 | 25.4 | 1.3 | 0.9 | 3.0 | 2.9 |
| Cryptand222 | 7 | 4.9 | 6.2 | 6.0 | 5.1 | 4.8 | 2.5 | 0.0 | 1.6 | 15.5 | 4.9 | 1.7 | 0.0 | 1.5 |
| Cryptand222 | 8 | 9.9 | 8.9 | 4.1 | 5.2 | 5.7 | 3.2 | 4.6 | 5.6 | 6.5 | 18.8 | 8.4 | 7.5 | 5.5 |
| Dapiprazole | 1 | 0.0 | 0.0 | 1.5 | 0.1 | 1.6 | 4.8 | 3.5 | 1.0 | 0.0 | 1.4 | 0.0 | 0.0 | 0.0 |
| Dapiprazole | 2 | 2.3 | 2.1 | 1.4 | 0.0 | 2.1 | 5.6 | 3.7 | 1.0 | 6.0 | 0.0 | 1.7 | 2.6 | 1.6 |
| Dapiprazole | 3 | 5.3 | 4.4 | 0.6 | 2.4 | 1.1 | 3.3 | 6.1 | 0.9 | 8.4 | 2.9 | 2.2 | 2.5 | 2.1 |
| Dapiprazole | 4 | 5.2 | 5.0 | 0.5 | 1.9 | 1.0 | 2.6 | 2.3 | 0.0 | 7.7 | 2.5 | 2.7 | 2.3 | 2.1 |
| Dapiprazole | 5 | 4.8 | 4.4 | 1.2 | 4.6 | 1.6 | 1.9 | 0.9 | 2.8 | 1.2 | 9.4 | 0.9 | 0.0 | 0.1 |
| Dapiprazole | 6 | 8.8 | 7.6 | 0.0 | 4.1 | 0.0 | 0.0 | 0.0 | 0.6 | 10.2 | 4.8 | 3.4 | 2.8 | 2.4 |
| Dapiprazole | 7 | 10.5 | 9.6 | 2.4 | 3.7 | 4.7 | 5.4 | 4.9 | 3.5 | 13.7 | 5.8 | 3.7 | 6.0 | 5.3 |
| Dapiprazole | 8 | 9.5 | 9.6 | 2.7 | 3.4 | 4.3 | 3.5 | 5.2 | 3.9 | 8.3 | 9.8 | 4.7 | 3.8 | 4.8 |
| Eperisone | 1 | 0.0 | 0.1 | 1.2 | 0.0 | 0.9 | 2.0 | 2.8 | 1.4 | 4.3 | 0.0 | 1.5 | 0.6 | 1.9 |
| Eperisone | 2 | 0.9 | 0.0 | 0.0 | 1.7 | 0.0 | 0.0 | 0.0 | 0.8 | 2.9 | 5.7 | 0.0 | 0.0 | 0.0 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Eperisone | 3 | 1.3 | 0.9 | 0.8 | 0.0 | 1.9 | 0.0 | 0.0 | 0.0 | 0.0 | 4.6 | 1.2 | 0.8 | 2.6 |
| Eperisone | 4 | 3.5 | 3.1 | 3.3 | 2.2 | 1.1 | 3.0 | 3.9 | 2.7 | 6.5 | 3.6 | 3.1 | 3.3 | 3.9 |
| Eperisone | 5 | 5.0 | 4.0 | 1.9 | 3.6 | 0.2 | 0.4 | 2.1 | 2.5 | 4.5 | 8.9 | 2.7 | 3.0 | 3.0 |
| Eperisone | 6 | 5.9 | 6.0 | 3.2 | 2.1 | 3.6 | 1.9 | 3.5 | 5.2 | 10.7 | 7.0 | 5.1 | 4.5 | 6.5 |
| Eperisone | 7 | 6.0 | 6.1 | 2.9 | 2.0 | 4.5 | 1.8 | 2.2 | 5.5 | 10.5 | 7.4 | 5.5 | 4.3 | 6.7 |
| Eperisone | 8 | 7.8 | 7.8 | 3.2 | 2.1 | 3.6 | 1.9 | 3.2 | 4.3 | 11.8 | 8.2 | 5.5 | 4.3 | 6.8 |
| Fotemustin | 1 | 0.0 | 0.0 | 0.6 | 0.0 | 0.0 | 0.0 | 5.8 | 0.0 | 5.9 | 0.0 | 6.3 | 2.4 | 3.6 |
| Fotemustin | 2 | 0.2 | 1.1 | 6.3 | 2.5 | 6.2 | 0.2 | 6.6 | 4.3 | 4.3 | 1.0 | 5.6 | 3.2 | 0.0 |
| Fotemustin | 3 | 3.8 | 2.8 | 0.0 | 2.8 | 2.9 | 0.6 | 3.1 | 2.1 | 5.4 | 3.5 | 3.9 | 4.2 | 3.8 |
| Fotemustin | 4 | 4.4 | 4.9 | 5.2 | 2.2 | 2.9 | 7.0 | 0.0 | 0.1 | 6.1 | 4.5 | 0.0 | 0.0 | 1.3 |
| Fotemustin | 5 | 5.2 | 4.9 | 3.6 | 3.3 | 2.5 | 2.4 | 1.8 | 4.9 | 0.0 | 10.7 | 6.7 | 6.2 | 4.6 |
| Fotemustin | 6 | 7.5 | 7.3 | 5.9 | 2.6 | 2.0 | 1.2 | 8.7 | 4.2 | 9.6 | 10.4 | 10.2 | 7.1 | 4.4 |
| Fotemustin | 7 | 9.0 | 8.5 | 4.1 | 2.3 | 2.7 | 1.9 | 2.9 | 4.9 | 8.5 | 14.3 | 9.5 | 8.2 | 5.8 |
| Fotemustin | 8 | 9.7 | 10.2 | 4.2 | 3.0 | 2.1 | 3.2 | 10.0 | 4.4 | 6.0 | 15.8 | 13.7 | 10.6 | 11.8 |
| GABA | 1 | 0.3 | 0.0 | 5.7 | 3.7 | 1.2 | 4.1 | 2.4 | 2.0 | 0.1 | 0.0 | 2.5 | 0.4 | 0.8 |
| GABA | 2 | 0.0 | 0.6 | 5.7 | 3.4 | 3.3 | 4.4 | 3.1 | 2.4 | 0.0 | 1.3 | 1.8 | 1.5 | 1.4 |
| GABA | 3 | 0.0 | 2.3 | 1.6 | 0.4 | 1.6 | 1.3 | 1.1 | 1.1 | 2.1 | 2.6 | 0.0 | 0.0 | 0.0 |
| GABA | 4 | 1.4 | 3.4 | 0.0 | 0.7 | 0.0 | 0.0 | 0.0 | 0.4 | 3.9 | 5.6 | 0.5 | 0.4 | 0.1 |
| GABA | 5 | 2.3 | 4.4 | 1.4 | 0.0 | 2.4 | 2.0 | 0.2 | 0.0 | 2.9 | 4.4 | 1.3 | 2.0 | 1.4 |
| GABA | 6 | 5.1 | 7.0 | 6.6 | 4.4 | 3.3 | 7.7 | 7.9 | 5.6 | 6.7 | 8.6 | 5.6 | 7.5 | 5.7 |
| GABA | 7 | 5.3 | 7.3 | 6.9 | 4.7 | 3.5 | 7.9 | 7.7 | 6.4 | 5.8 | 9.3 | 5.0 | 7.8 | 6.0 |
| GABA | 8 | 6.9 | 8.5 | 7.0 | 4.3 | 3.2 | 8.2 | 2.4 | 6.7 | 8.2 | 10.1 | 5.8 | 8.9 | 6.6 |
| Gemcitabine | 1 | 0.0 | 0.0 | 2.3 | 0.0 | 0.2 | 0.0 | 0.0 | 1.4 | 0.0 | 0.6 | 0.0 | 0.0 | 0.0 |
| Gemcitabine | 2 | 2.2 | 2.4 | 0.7 | 0.8 | 0.0 | 1.4 | 2.8 | 1.2 | 4.7 | 0.7 | 3.4 | 1.4 | 2.4 |
| Gemcitabine | 3 | 3.1 | 4.1 | 2.1 | 1.0 | 0.7 | 1.4 | 3.9 | 1.2 | 6.3 | 0.0 | 3.4 | 2.2 | 4.2 |
| Gemcitabine | 4 | 5.2 | 4.9 | 2.9 | 3.2 | 0.5 | 4.0 | 5.6 | 3.5 | 7.1 | 0.9 | 4.2 | 2.9 | 2.4 |
| Gemcitabine | 5 | 4.7 | 5.8 | 4.9 | 2.6 | 2.3 | 1.4 | 5.0 | 5.0 | 7.4 | 1.9 | 6.9 | 7.3 | 7.9 |
| Gemcitabine | 6 | 6.9 | 6.8 | 0.0 | 0.4 | 0.5 | 0.3 | 1.4 | 0.0 | 3.8 | 8.5 | 0.0 | 1.5 | 5.7 |
| Gemcitabine | 7 | 7.0 | 7.7 | 4.0 | 2.3 | 0.9 | 0.7 | 5.7 | 3.9 | 8.6 | 5.2 | 6.9 | 7.3 | 8.1 |
| Gemcitabine | 8 | 9.3 | 10.6 | 4.7 | 0.7 | 3.4 | 0.9 | 0.0 | 2.8 | 11.9 | 6.2 | 3.3 | 8.4 | 3.1 |
| Glufosinate | 1 | 0.0 | 0.0 | 8.1 | 7.7 | 6.8 | 3.2 | 1.5 | 4.5 | 0.0 | 0.0 | 0.0 | 2.5 | 0.0 |
| Glufosinate | 2 | 1.7 | 2.4 | 0.0 | 1.9 | 4.4 | 0.0 | 0.4 | 3.8 | 6.8 | 5.1 | 4.8 | 0.0 | 2.3 |
| Glufosinate | 3 | 1.9 | 2.9 | 2.4 | 0.9 | 8.9 | 0.5 | 1.8 | 3.7 | 5.5 | 2.7 | 4.0 | 1.6 | 3.1 |
| Glufosinate | 4 | 3.1 | 4.4 | 5.7 | 3.8 | 2.8 | 1.2 | 0.9 | 7.3 | 2.0 | 5.3 | 5.6 | 7.4 | 3.7 |
| Glufosinate | 5 | 7.1 | 7.3 | 4.4 | 4.0 | 1.5 | 4.2 | 4.2 | 6.2 | 5.5 | 5.9 | 8.0 | 6.7 | 6.0 |
| Glufosinate | 6 | 8.3 | 8.6 | 6.0 | 4.8 | 1.5 | 6.3 | 0.3 | 4.1 | 17.5 | 7.8 | 9.4 | 7.7 | 7.0 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Glufosinate | 7 | 7.6 | 9.9 | 0.6 | 0.0 | 0.0 | 3.3 | 0.0 | 0.0 | 15.4 | 11.6 | 8.0 | 5.3 | 4.9 |
| Glufosinate | 8 | 8.7 | 10.7 | 1.2 | 0.8 | 0.2 | 2.8 | 0.0 | 0.5 | 16.4 | 12.7 | 8.1 | 5.9 | 5.6 |
| Indometacin | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Indometacin | 2 | 1.4 | 1.3 | 1.4 | 0.4 | 1.1 | 1.5 | 2.3 | 1.8 | 2.1 | 3.2 | 1.5 | 2.4 | 1.7 |
| Indometacin | 3 | 3.4 | 1.7 | 4.8 | 5.0 | 1.0 | 5.0 | 4.6 | 3.8 | 5.0 | 3.9 | 3.1 | 6.8 | 5.2 |
| Indometacin | 4 | 3.6 | 2.2 | 5.2 | 4.9 | 1.2 | 5.0 | 5.0 | 4.1 | 4.0 | 6.2 | 3.5 | 7.7 | 5.1 |
| Indometacin | 5 | 5.2 | 4.8 | 4.4 | 4.3 | 0.7 | 4.5 | 3.8 | 6.0 | 5.9 | 7.1 | 6.0 | 6.2 | 7.0 |
| Indometacin | 6 | 6.0 | 5.4 | 5.2 | 3.9 | 1.0 | 5.2 | 5.3 | 4.4 | 6.3 | 8.2 | 6.1 | 7.7 | 6.8 |
| Indometacin | 7 | 6.5 | 6.0 | 4.8 | 4.2 | 0.8 | 5.0 | 4.6 | 3.8 | 7.0 | 8.3 | 3.1 | 6.7 | 8.0 |
| Indometacin | 8 | 7.3 | 6.6 | 5.3 | 4.4 | 1.2 | 5.2 | 5.5 | 4.3 | 7.6 | 9.9 | 3.8 | 7.8 | 4.8 |
| Isradipine | 1 | 0.0 | 0.0 | 0.7 | 0.6 | 0.3 | 1.8 | 0.0 | 2.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Isradipine | 2 | 0.1 | 0.2 | 0.8 | 1.3 | 0.6 | 2.0 | 0.0 | 2.5 | 0.0 | 0.6 | 0.2 | 0.3 | 0.2 |
| Isradipine | 3 | 3.3 | 3.1 | 0.0 | 2.0 | 1.4 | 0.0 | 0.7 | 0.0 | 4.1 | 5.3 | 3.3 | 1.3 | 0.7 |
| Isradipine | 4 | 4.6 | 4.4 | 0.8 | 2.2 | 1.3 | 1.2 | 2.1 | 0.7 | 6.4 | 7.3 | 6.1 | 3.4 | 2.5 |
| Isradipine | 5 | 4.6 | 4.4 | 0.8 | 2.2 | 1.3 | 1.2 | 2.1 | 0.7 | 6.4 | 7.6 | 6.1 | 3.4 | 2.5 |
| Isradipine | 6 | 10.3 | 9.2 | 6.7 | 5.2 | 0.0 | 7.9 | 7.4 | 6.9 | 0.0 | 12.0 | 9.5 | 11.9 | 8.5 |
| Isradipine | 7 | 9.9 | 8.9 | 5.5 | 0.0 | 1.6 | 7.3 | 6.5 | 6.1 | 10.4 | 13.6 | 9.8 | 12.3 | 8.0 |
| Isradipine | 8 | 12.0 | 11.0 | 7.8 | 8.8 | 2.0 | 9.7 | 8.6 | 9.2 | 13.9 | 15.9 | 11.1 | 14.7 | 11.2 |
| Knoevenagel_cond | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.6 | 0.0 | 0.0 | 0.0 | 0.5 | 0.0 | 1.2 |
| Knoevenagel_cond | 2 | 3.4 | 1.7 | 0.8 | 5.8 | 1.6 | 0.0 | 0.0 | 1.6 | 4.0 | 2.6 | 0.0 | 0.8 | 0.0 |
| Knoevenagel_cond | 3 | 4.2 | 3.1 | 1.3 | 3.5 | 2.0 | 1.8 | 1.2 | 2.2 | 3.0 | 3.0 | 0.0 | 1.2 | 0.4 |
| Knoevenagel_cond | 4 | 5.8 | 4.9 | 2.1 | 5.5 | 3.2 | 1.0 | 1.5 | 3.9 | 7.2 | 3.8 | 2.6 | 3.6 | 3.3 |
| Knoevenagel_cond | 5 | 4.9 | 4.5 | 1.2 | 3.7 | 2.0 | 0.0 | 1.9 | 2.5 | 4.8 | 1.2 | 2.4 | 2.5 | 3.4 |
| Knoevenagel_cond | 6 | 7.5 | 5.9 | 3.5 | 6.9 | 5.8 | 3.1 | 2.9 | 4.7 | 6.2 | 7.9 | 1.4 | 3.2 | 3.5 |
| Knoevenagel_cond | 7 | 8.9 | 7.7 | 6.3 | 1.6 | 1.1 | 6.4 | 7.7 | 7.4 | 7.9 | 13.5 | 5.3 | 8.5 | 7.4 |
| Knoevenagel_cond | 8 | 12.6 | 10.8 | 8.2 | 2.2 | 5.5 | 7.8 | 9.1 | 12.8 | 10.7 | 17.5 | 6.3 | 9.7 | 10.3 |
| Liu_catal | 1 | 0.0 | 0.0 | 0.3 | 0.2 | 1.6 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Liu_catal | 2 | 2.4 | 2.6 | 1.3 | 0.0 | 1.9 | 1.0 | 3.5 | 0.4 | 3.1 | 1.3 | 1.0 | 0.6 | 1.3 |
| Liu_catal | 3 | 2.6 | 2.9 | 2.6 | 1.2 | 2.9 | 2.0 | 4.5 | 1.5 | 3.4 | 3.2 | 0.9 | 0.7 | 1.6 |
| Liu_catal | 4 | 3.9 | 3.8 | 0.3 | 3.7 | 1.1 | 1.0 | 2.5 | 0.6 | 5.6 | 4.6 | 0.6 | 1.1 | 1.8 |
| Liu_catal | 5 | 3.9 | 3.9 | 0.0 | 2.5 | 0.0 | 0.9 | 2.7 | 0.8 | 5.6 | 4.8 | 0.8 | 1.3 | 1.9 |
| Liu_catal | 6 | 5.9 | 6.9 | 0.1 | 1.9 | 3.6 | 2.6 | 3.5 | 3.9 | 4.6 | 7.0 | 2.9 | 4.0 | 2.8 |
| Liu_catal | 7 | 8.4 | 9.6 | 0.1 | 1.1 | 2.1 | 3.1 | 5.7 | 4.0 | 8.1 | 8.7 | 3.4 | 5.5 | 4.6 |
| Liu_catal | 8 | 8.7 | 10.1 | 0.1 | 1.4 | 2.3 | 3.5 | 5.7 | 4.1 | 7.9 | 9.3 | 3.6 | 5.7 | 4.9 |
| Mannosulfan | 1 | 0.0 | 0.0 | 1.7 | 2.9 | 2.0 | 0.5 | 1.6 | 0.0 | 8.8 | 0.0 | 0.7 | 0.3 | 0.0 |
| Mannosulfan | 2 | 2.0 | 2.0 | 2.3 | 2.2 | 2.3 | 3.6 | 0.9 | 2.5 | 13.6 | 2.0 | 2.6 | 1.9 | 6.3 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Mannosulfan | 3 | 3.5 | 2.7 | 2.3 | 5.6 | 0.0 | 1.1 | 2.2 | 3.9 | 0.0 | 5.3 | 0.0 | 0.4 | 3.3 |
| Mannosulfan | 4 | 7.8 | 4.8 | 3.1 | 11.2 | 3.2 | 7.8 | 9.1 | 2.7 | 12.7 | 7.8 | 3.5 | 1.9 | 5.6 |
| Mannosulfan | 5 | 2.6 | 1.8 | 6.1 | 8.7 | 3.8 | 8.8 | 6.0 | 6.7 | 6.7 | 9.0 | 1.4 | 0.0 | 2.3 |
| Mannosulfan | 6 | 9.7 | 9.3 | 3.6 | 3.8 | 1.1 | 1.7 | 3.2 | 5.1 | 22.0 | 8.2 | 4.0 | 1.0 | 9.3 |
| Mannosulfan | 7 | 11.2 | 9.3 | 2.6 | 0.0 | 3.3 | 0.4 | 0.0 | 7.3 | 31.3 | 13.2 | 6.1 | 8.3 | 12.2 |
| Mannosulfan | 8 | 14.7 | 11.8 | 0.0 | 10.9 | 4.9 | 0.0 | 7.7 | 10.3 | 27.2 | 19.3 | 4.0 | 6.7 | 9.9 |
| N_iprit | 1 | 0.0 | 0.0 | 0.9 | 0.0 | 0.7 | 2.0 | 6.7 | 2.1 | 0.0 | 0.0 | 6.2 | 0.8 | 1.3 |
| N_iprit | 2 | 1.1 | 0.1 | 0.2 | 1.3 | 0.7 | 3.1 | 5.9 | 3.3 | 0.9 | 3.1 | 1.6 | 0.8 | 0.3 |
| N_iprit | 3 | 1.6 | 0.7 | 0.0 | 1.4 | 0.2 | 0.7 | 4.4 | 1.4 | 1.3 | 3.4 | 6.8 | 0.8 | 1.1 |
| N_iprit | 4 | 2.2 | 0.4 | 0.0 | 2.4 | 0.0 | 0.0 | 0.6 | 0.0 | 0.6 | 9.0 | 5.0 | 0.0 | 0.0 |
| N_iprit | 5 | 2.2 | 0.9 | 0.9 | 2.6 | 1.3 | 2.4 | 4.5 | 3.0 | 1.8 | 8.2 | 0.0 | 1.0 | 1.4 |
| N_iprit | 6 | 3.4 | 1.9 | 0.0 | 1.4 | 0.1 | 0.9 | 0.0 | 2.1 | 2.6 | 7.1 | 6.3 | 1.4 | 1.2 |
| N_iprit | 7 | 3.3 | 1.1 | 0.1 | 2.7 | 0.6 | 2.4 | 2.2 | 2.7 | 2.1 | 11.1 | 4.4 | 1.6 | 0.9 |
| N_iprit | 8 | 7.7 | 5.3 | 2.0 | 4.1 | 2.8 | 3.4 | 2.6 | 3.0 | 5.2 | 13.1 | 9.2 | 3.8 | 1.4 |
| Oseltamivir | 1 | 0.0 | 0.0 | 0.0 | 0.3 | 4.3 | 2.6 | 0.5 | 0.3 | 0.0 | 0.0 | 0.0 | 1.5 | 0.3 |
| Oseltamivir | 2 | 2.6 | 1.8 | 1.3 | 1.9 | 0.0 | 2.8 | 0.7 | 0.8 | 4.0 | 7.7 | 1.9 | 3.0 | 1.6 |
| Oseltamivir | 3 | 4.2 | 3.7 | 0.1 | 4.5 | 1.8 | 0.0 | 0.0 | 0.0 | 1.5 | 8.2 | 0.9 | 0.0 | 0.0 |
| Oseltamivir | 4 | 6.4 | 5.2 | 4.5 | 5.5 | 4.3 | 3.3 | 4.9 | 4.9 | 7.6 | 9.8 | 3.9 | 6.3 | 5.6 |
| Oseltamivir | 5 | 8.1 | 6.7 | 0.9 | 5.7 | 1.0 | 1.5 | 1.3 | 0.8 | 6.8 | 17.2 | 3.9 | 4.0 | 1.9 |
| Oseltamivir | 6 | 8.5 | 7.6 | 3.9 | 4.7 | 3.1 | 2.3 | 2.2 | 2.0 | 7.7 | 13.2 | 4.6 | 3.3 | 4.3 |
| Oseltamivir | 7 | 11.6 | 10.4 | 2.1 | 4.3 | 0.0 | 3.9 | 2.2 | 4.0 | 12.6 | 18.3 | 5.5 | 6.7 | 5.9 |
| Oseltamivir | 8 | 12.8 | 10.6 | 7.7 | 0.0 | 4.7 | 4.8 | 3.9 | 7.0 | 14.6 | 23.5 | 5.9 | 7.0 | 6.4 |
| Pantoprazole | 1 | 0.0 | 0.0 | 0.2 | 0.1 | 0.0 | 0.0 | 4.6 | 0.0 | 9.4 | 0.0 | 4.7 | 3.2 | 0.7 |
| Pantoprazole | 2 | 4.7 | 1.8 | 4.5 | 0.7 | 3.7 | 3.7 | 5.8 | 3.6 | 13.0 | 5.1 | 6.6 | 5.5 | 1.8 |
| Pantoprazole | 3 | 1.1 | 1.3 | 0.0 | 0.0 | 0.1 | 3.1 | 3.8 | 3.0 | 0.3 | 4.6 | 0.0 | 2.4 | 0.0 |
| Pantoprazole | 4 | 4.5 | 5.2 | 0.8 | 0.0 | 0.4 | 0.6 | 6.7 | 1.1 | 2.8 | 1.2 | 9.3 | 7.5 | 1.6 |
| Pantoprazole | 5 | 0.6 | 2.4 | 2.2 | 0.1 | 2.1 | 0.1 | 0.0 | 1.4 | 0.0 | 6.3 | 6.6 | 0.0 | 1.5 |
| Pantoprazole | 6 | 8.2 | 7.3 | 1.9 | 0.4 | 0.7 | 4.2 | 0.5 | 0.1 | 14.8 | 12.1 | 8.6 | 8.1 | 5.4 |
| Pantoprazole | 7 | 7.2 | 7.0 | 5.6 | 0.5 | 0.9 | 0.4 | 5.5 | 1.1 | 4.5 | 8.2 | 8.9 | 5.6 | 2.7 |
| Pantoprazole | 8 | 11.1 | 11.0 | 1.9 | 0.4 | 0.8 | 0.4 | 0.5 | 1.1 | 16.0 | 12.9 | 14.2 | 11.8 | 10.2 |
| Propranolol | 1 | 0.5 | 0.1 | 1.4 | 0.0 | 1.4 | 0.7 | 2.9 | 0.2 | 1.6 | 0.0 | 0.0 | 0.9 | 0.0 |
| Propranolol | 2 | 0.0 | 0.0 | 1.3 | 1.1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 3.4 | 0.3 | 0.0 | 0.4 |
| Propranolol | 3 | 1.9 | 2.2 | 0.0 | 0.8 | 2.1 | 1.6 | 4.3 | 0.6 | 1.2 | 2.8 | 1.2 | 2.6 | 1.7 |
| Propranolol | 4 | 3.0 | 3.2 | 1.6 | 0.2 | 1.7 | 1.0 | 3.6 | 1.6 | 3.8 | 5.0 | 1.5 | 3.4 | 2.0 |
| Propranolol | 5 | 1.3 | 0.5 | 2.7 | 0.1 | 2.7 | 0.7 | 2.9 | 1.4 | 1.0 | 2.6 | 1.9 | 3.3 | 2.2 |
| Propranolol | 6 | 5.9 | 5.6 | 2.4 | 2.3 | 1.5 | 1.0 | 3.6 | 1.7 | 6.6 | 5.0 | 1.5 | 3.4 | 4.4 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Propranolol | 7 | 6.8 | 6.6 | 4.9 | 1.5 | 3.8 | 2.0 | 5.0 | 2.3 | 8.3 | 11.9 | 5.1 | 3.5 | 6.5 |
| Propranolol | 8 | 7.6 | 7.3 | 3.2 | 2.8 | 4.3 | 2.9 | 6.7 | 5.6 | 4.4 | 14.3 | 5.0 | 5.8 | 5.3 |
| ProstaglandinE1 | 1 | 0.0 | 0.1 | 0.0 | 0.2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 1.4 | 0.6 | 0.2 |
| ProstaglandinE1 | 2 | 0.1 | 0.0 | 1.1 | 1.7 | 0.6 | 0.5 | 0.1 | 1.5 | 0.3 | 1.2 | 0.3 | 0.0 | 0.0 |
| ProstaglandinE1 | 3 | 0.9 | 0.5 | 1.6 | 6.1 | 2.7 | 0.8 | 0.8 | 2.0 | 1.3 | 2.2 | 0.0 | 0.6 | 0.5 |
| ProstaglandinE1 | 4 | 1.1 | 1.2 | 2.3 | 5.6 | 1.6 | 1.9 | 1.4 | 2.5 | 2.1 | 3.6 | 1.2 | 1.6 | 1.6 |
| ProstaglandinE1 | 5 | 9.7 | 11.4 | 6.3 | 3.9 | 3.2 | 8.0 | 13.4 | 3.1 | 19.1 | 7.5 | 12.2 | 11.2 | 11.5 |
| ProstaglandinE1 | 6 | 12.8 | 14.5 | 3.7 | 0.0 | 7.4 | 9.3 | 16.4 | 2.6 | 17.2 | 6.0 | 15.6 | 13.2 | 12.4 |
| ProstaglandinE1 | 7 | 9.8 | 11.5 | 4.7 | 0.6 | 1.8 | 11.2 | 15.0 | 2.1 | 23.5 | 8.5 | 14.7 | 15.1 | 13.8 |
| ProstaglandinE1 | 8 | 14.6 | 16.5 | 3.8 | 0.3 | 2.9 | 12.7 | 17.9 | 1.3 | 26.9 | 9.4 | 17.7 | 16.6 | 15.2 |
| Pyridoxalphosphate | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 5.1 | 0.0 | 0.3 | 1.2 | 2.1 | 0.4 | 2.3 | 1.5 |
| Pyridoxalphosphate | 2 | 2.0 | 2.0 | 1.2 | 2.0 | 1.2 | 6.8 | 0.5 | 0.0 | 0.0 | 1.9 | 0.0 | 0.0 | 0.0 |
| Pyridoxalphosphate | 3 | 3.1 | 2.7 | 2.5 | 1.1 | 1.1 | 7.2 | 1.8 | 1.2 | 1.2 | 3.8 | 0.9 | 0.3 | 0.9 |
| Pyridoxalphosphate | 4 | 4.9 | 7.4 | 3.2 | 0.5 | 6.0 | 10.8 | 4.3 | 1.8 | 3.2 | 1.1 | 3.3 | 2.1 | 4.9 |
| Pyridoxalphosphate | 5 | 5.8 | 7.6 | 4.2 | 2.2 | 4.2 | 0.0 | 9.3 | 1.9 | 2.6 | 1.1 | 0.7 | 4.0 | 1.6 |
| Pyridoxalphosphate | 6 | 8.4 | 9.5 | 5.7 | 1.1 | 7.4 | 16.6 | 8.1 | 3.4 | 7.0 | 0.0 | 5.6 | 5.2 | 5.7 |
| Pyridoxalphosphate | 7 | 9.3 | 10.8 | 4.0 | 0.1 | 6.8 | 15.1 | 0.6 | 2.1 | 8.7 | 1.2 | 5.8 | 7.0 | 6.4 |
| Pyridoxalphosphate | 8 | 10.2 | 12.8 | 7.2 | 1.1 | 3.6 | 11.9 | 8.0 | 1.8 | 10.6 | 16.6 | 7.9 | 9.4 | 9.9 |
| Quinuclidinyl | 1 | 0.0 | 0.0 | 1.1 | 0.6 | 0.0 | 0.1 | 0.0 | 0.2 | 0.0 | 0.9 | 0.0 | 0.0 | 0.0 |
| Quinuclidinyl | 2 | 0.4 | 0.3 | 1.2 | 0.8 | 0.8 | 0.8 | 0.9 | 0.6 | 0.8 | 0.0 | 0.4 | 0.5 | 0.5 |
| Quinuclidinyl | 3 | 2.8 | 3.4 | 0.0 | 0.0 | 0.2 | 0.0 | 1.7 | 0.0 | 2.1 | 2.3 | 2.0 | 2.0 | 3.1 |
| Quinuclidinyl | 4 | 4.4 | 4.7 | 3.8 | 1.6 | 1.4 | 3.7 | 4.0 | 0.9 | 5.2 | 4.2 | 3.5 | 5.2 | 4.5 |
| Quinuclidinyl | 5 | 6.8 | 6.0 | 5.4 | 8.5 | 5.0 | 2.5 | 4.3 | 4.9 | 5.1 | 8.5 | 4.5 | 3.3 | 4.2 |
| Quinuclidinyl | 6 | 8.8 | 8.8 | 4.2 | 6.0 | 4.6 | 1.9 | 5.4 | 4.0 | 6.2 | 9.5 | 6.1 | 4.5 | 7.0 |
| Quinuclidinyl | 7 | 8.6 | 7.0 | 10.2 | 0.6 | 1.7 | 8.4 | 10.1 | 8.2 | 9.3 | 14.1 | 6.3 | 10.4 | 8.1 |
| Quinuclidinyl | 8 | 11.0 | 10.5 | 8.1 | 8.0 | 5.6 | 6.0 | 8.0 | 5.1 | 10.4 | 11.0 | 7.6 | 7.5 | 8.4 |
| RAMBO | 1 | 0.0 | 0.0 | 2.6 | 0.0 | 0.0 | 0.9 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| RAMBO | 2 | 5.0 | 4.5 | 1.3 | 8.0 | 5.1 | 2.4 | 2.2 | 1.0 | 3.9 | 8.9 | 2.0 | 0.0 | 3.6 |
| RAMBO | 3 | 6.2 | 5.2 | 0.0 | 8.1 | 1.9 | 0.0 | 5.0 | 2.3 | 8.0 | 12.9 | 3.1 | 2.4 | 5.9 |
| RAMBO | 4 | 5.5 | 5.0 | 0.6 | 8.2 | 1.3 | 2.0 | 2.6 | 0.3 | 7.0 | 12.8 | 2.9 | 0.7 | 4.1 |
| RAMBO | 5 | 6.0 | 5.4 | 4.1 | 8.8 | 5.0 | 4.7 | 5.5 | 2.0 | 9.0 | 9.6 | 2.4 | 1.1 | 4.8 |
| RAMBO | 6 | 6.6 | 5.6 | 3.2 | 11.0 | 3.8 | 2.7 | 4.0 | 1.6 | 8.0 | 12.7 | 3.2 | 0.5 | 4.7 |
| RAMBO | 7 | 7.2 | 6.6 | 3.4 | 9.4 | 3.3 | 3.3 | 4.5 | 1.1 | 9.7 | 10.9 | 3.1 | 0.8 | 4.6 |
| RAMBO | 8 | 8.1 | 7.4 | 4.2 | 8.8 | 3.5 | 3.7 | 5.1 | 2.5 | 10.2 | 9.6 | 3.6 | 1.2 | 5.5 |
| RH34 | 1 | 0.0 | 0.0 | 1.6 | 0.0 | 0.5 | 5.0 | 6.0 | 0.8 | 0.7 | 0.0 | 0.0 | 0.7 | 0.8 |
| RH34 | 2 | 0.4 | 0.4 | 0.0 | 1.4 | 0.0 | 0.0 | 0.0 | 0.0 | 11.8 | 0.4 | 0.7 | 0.0 | 0.0 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| RH34 | 3 | 2.7 | 2.2 | 2.1 | 1.8 | 0.3 | 0.3 | 4.5 | 1.1 | 16.1 | 1.5 | 2.0 | 1.0 | 1.3 |
| RH34 | 4 | 1.2 | 1.5 | 6.3 | 1.8 | 3.7 | 4.7 | 5.4 | 3.7 | 12.9 | 2.2 | 1.3 | 0.3 | 1.2 |
| RH34 | 5 | 4.0 | 4.5 | 5.0 | 0.5 | 3.5 | 6.8 | 6.2 | 3.6 | 11.3 | 3.8 | 2.6 | 3.8 | 5.4 |
| RH34 | 6 | 3.8 | 4.7 | 6.8 | 1.2 | 2.9 | 8.1 | 2.9 | 3.5 | 0.0 | 3.8 | 2.1 | 3.9 | 5.5 |
| RH34 | 7 | 6.4 | 5.9 | 2.1 | 1.4 | 2.2 | 6.9 | 8.3 | 5.5 | 16.2 | 5.3 | 6.9 | 4.6 | 5.3 |
| RH34 | 8 | 7.0 | 6.5 | 2.0 | 1.4 | 2.3 | 3.6 | 8.3 | 0.7 | 14.6 | 2.9 | 7.2 | 4.6 | 5.7 |
| Rolipram | 1 | 0.0 | 0.0 | 0.5 | 0.0 | 0.7 | 2.4 | 3.0 | 1.0 | 0.4 | 1.7 | 0.0 | 2.3 | 0.0 |
| Rolipram | 2 | 1.2 | 1.1 | 0.6 | 0.0 | 0.6 | 2.4 | 2.9 | 0.9 | 1.6 | 1.6 | 0.0 | 2.1 | 0.0 |
| Rolipram | 3 | 0.4 | 1.6 | 0.0 | 0.1 | 0.4 | 0.5 | 1.3 | 0.2 | 0.8 | 0.0 | 1.4 | 0.0 | 0.3 |
| Rolipram | 4 | 0.4 | 1.8 | 0.2 | 0.0 | 0.7 | 0.5 | 1.3 | 0.2 | 0.6 | 0.3 | 1.4 | 0.0 | 0.3 |
| Rolipram | 5 | 3.2 | 5.4 | 0.0 | 0.0 | 1.1 | 2.1 | 3.2 | 0.0 | 0.0 | 0.1 | 6.9 | 4.0 | 4.0 |
| Rolipram | 6 | 4.4 | 5.5 | 1.5 | 0.0 | 0.1 | 2.9 | 3.0 | 0.7 | 4.9 | 7.1 | 5.2 | 3.8 | 3.5 |
| Rolipram | 7 | 4.1 | 5.0 | 1.2 | 0.0 | 0.1 | 0.0 | 0.0 | 1.0 | 4.5 | 7.2 | 1.8 | 0.4 | 1.8 |
| Rolipram | 8 | 4.4 | 6.2 | 1.3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.2 | 0.8 | 6.9 | 1.8 | 0.4 | 2.7 |
| Rosmaridiphenol | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Rosmaridiphenol | 2 | 2.1 | 2.2 | 0.5 | 0.1 | 0.1 | 1.9 | 1.8 | 0.6 | 3.6 | 1.6 | 3.4 | 3.1 | 2.5 |
| Rosmaridiphenol | 3 | 1.4 | 1.7 | 3.8 | 2.8 | 3.5 | 3.5 | 2.8 | 2.0 | 0.0 | 4.3 | 1.2 | 0.9 | 1.7 |
| Rosmaridiphenol | 4 | 4.7 | 4.8 | 3.1 | 3.5 | 3.6 | 4.6 | 5.2 | 3.7 | 7.2 | 5.1 | 4.4 | 5.0 | 5.2 |
| Rosmaridiphenol | 5 | 6.0 | 6.0 | 5.2 | 5.0 | 7.4 | 6.9 | 6.5 | 4.2 | 8.9 | 11.7 | 5.5 | 4.9 | 5.4 |
| Rosmaridiphenol | 6 | 7.0 | 7.4 | 6.1 | 7.1 | 8.6 | 7.8 | 6.8 | 4.7 | 10.3 | 15.2 | 6.8 | 5.9 | 6.1 |
| Rosmaridiphenol | 7 | 7.1 | 7.1 | 5.2 | 4.3 | 6.4 | 6.2 | 4.8 | 4.7 | 3.6 | 8.8 | 4.7 | 4.3 | 5.9 |
| Rosmaridiphenol | 8 | 8.7 | 9.4 | 7.7 | 7.0 | 8.1 | 8.6 | 6.3 | 4.8 | 5.4 | 15.4 | 7.5 | 6.7 | 7.1 |
| Takemoto | 1 | 1.7 | 0.3 | 1.0 | 1.6 | 0.4 | 0.0 | 0.0 | 0.0 | 0.0 | 2.7 | 2.3 | 1.2 | 0.4 |
| Takemoto | 2 | 0.0 | 0.0 | 0.0 | 3.3 | 0.3 | 1.7 | 3.4 | 1.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.0 |
| Takemoto | 3 | 3.8 | 2.4 | 1.9 | 3.3 | 0.0 | 1.4 | 3.6 | 2.5 | 3.4 | 4.0 | 3.3 | 2.8 | 2.8 |
| Takemoto | 4 | 4.4 | 3.5 | 2.4 | 4.0 | 2.5 | 2.6 | 2.4 | 2.4 | 4.6 | 5.3 | 3.7 | 3.1 | 3.0 |
| Takemoto | 5 | 7.6 | 6.4 | 0.9 | 0.0 | 2.6 | 1.5 | 4.9 | 4.7 | 5.6 | 6.8 | 2.8 | 2.1 | 1.8 |
| Takemoto | 6 | 6.9 | 7.2 | 7.6 | 6.6 | 5.4 | 4.5 | 7.9 | 7.2 | 5.8 | 5.8 | 6.0 | 4.6 | 6.5 |
| Takemoto | 7 | 11.1 | 10.1 | 2.6 | 2.3 | 6.3 | 2.5 | 5.9 | 3.5 | 7.8 | 7.6 | 6.8 | 2.9 | 4.0 |
| Takemoto | 8 | 11.4 | 11.4 | 3.8 | 2.5 | 8.9 | 3.4 | 3.8 | 4.7 | 4.8 | 12.8 | 4.1 | 3.7 | 3.6 |
| Triacetin | 1 | 0.0 | 0.0 | 0.2 | 0.0 | 0.0 | 1.6 | 0.5 | 0.0 | 0.0 | 0.0 | 0.1 | 1.7 | 1.4 |
| Triacetin | 2 | 0.8 | 1.0 | 0.1 | 0.7 | 0.5 | 0.5 | 0.3 | 1.0 | 3.4 | 1.3 | 0.0 | 1.9 | 0.0 |
| Triacetin | 3 | 2.5 | 2.5 | 0.0 | 1.9 | 2.4 | 0.2 | 0.3 | 3.6 | 4.7 | 3.9 | 0.4 | 2.5 | 2.1 |
| Triacetin | 4 | 3.6 | 3.7 | 0.0 | 2.8 | 1.1 | 0.0 | 0.0 | 0.8 | 5.9 | 2.0 | 1.2 | 0.0 | 0.3 |
| Triacetin | 5 | 4.5 | 4.4 | 0.0 | 4.2 | 0.9 | 0.3 | 0.5 | 2.7 | 5.3 | 5.1 | 1.2 | 3.2 | 2.5 |
| Triacetin | 6 | 8.7 | 7.9 | 5.7 | 5.0 | 1.1 | 4.9 | 5.5 | 7.7 | 13.1 | 11.9 | 7.1 | 7.3 | 8.2 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Triacetin | 7 | 9.0 | 8.1 | 7.2 | 6.3 | 2.0 | 7.7 | 10.2 | 7.6 | 10.7 | 13.2 | 6.9 | 11.9 | 9.8 |
| Triacetin | 8 | 14.2 | 12.7 | 8.7 | 0.3 | 4.8 | 6.9 | 8.9 | 3.0 | 0.8 | 2.6 | 6.6 | 10.1 | 8.4 |
| Tsogoeva | 1 | 0.0 | 0.0 | 4.5 | 3.5 | 3.9 | 0.2 | 0.0 | 0.9 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Tsogoeva | 2 | 2.5 | 2.3 | 4.9 | 2.8 | 2.9 | 1.4 | 1.9 | 2.1 | 5.5 | 3.1 | 2.3 | 3.0 | 2.5 |
| Tsogoeva | 3 | 1.4 | 1.9 | 5.2 | 3.0 | 2.9 | 1.4 | 2.1 | 1.9 | 4.6 | 2.2 | 2.7 | 3.2 | 1.8 |
| Tsogoeva | 4 | 2.5 | 3.4 | 5.6 | 2.1 | 1.9 | 2.6 | 3.8 | 3.3 | 9.0 | 5.2 | 1.1 | 6.1 | 3.6 |
| Tsogoeva | 5 | 4.8 | 6.3 | 0.0 | 0.0 | 0.0 | 0.0 | 1.2 | 0.0 | 9.6 | 12.1 | 2.0 | 4.5 | 1.9 |
| Tsogoeva | 6 | 6.5 | 6.4 | 6.8 | 3.9 | 2.2 | 3.4 | 5.0 | 4.6 | 9.4 | 9.9 | 5.2 | 7.5 | 4.5 |
| Tsogoeva | 7 | 7.2 | 7.6 | 5.6 | 5.3 | 4.0 | 4.3 | 5.5 | 4.1 | 9.2 | 7.5 | 4.8 | 7.0 | 4.4 |
| Tsogoeva | 8 | 9.6 | 11.0 | 1.2 | 3.1 | 1.0 | 2.7 | 4.0 | 1.9 | 9.0 | 12.7 | 4.4 | 8.0 | 4.1 |
| UH232 | 1 | 0.0 | 0.0 | 1.3 | 2.1 | 0.0 | 2.1 | 2.0 | 0.4 | 2.0 | 0.0 | 0.0 | 0.4 | 0.4 |
| UH232 | 2 | 1.1 | 0.8 | 0.0 | 0.0 | 1.0 | 0.0 | 0.0 | 0.0 | 3.0 | 2.4 | 0.3 | 1.3 | 0.3 |
| UH232 | 3 | 1.9 | 1.1 | 2.6 | 5.0 | 3.3 | 3.8 | 2.6 | 3.2 | 0.0 | 5.4 | 0.6 | 0.0 | 0.9 |
| UH232 | 4 | 2.4 | 2.1 | 2.8 | 2.8 | 0.8 | 3.3 | 2.4 | 0.9 | 3.4 | 4.9 | 2.1 | 1.5 | 2.1 |
| UH232 | 5 | 3.8 | 2.8 | 3.7 | 5.5 | 3.9 | 4.7 | 3.8 | 4.8 | 0.8 | 7.6 | 2.5 | 2.0 | 2.3 |
| UH232 | 6 | 4.4 | 3.1 | 3.0 | 5.3 | 4.0 | 4.0 | 1.6 | 4.5 | 1.9 | 9.6 | 0.4 | 0.2 | 0.0 |
| UH232 | 7 | 5.1 | 3.9 | 4.5 | 5.4 | 4.7 | 5.6 | 5.1 | 6.5 | 1.4 | 10.5 | 3.4 | 2.8 | 3.5 |
| UH232 | 8 | 6.2 | 4.8 | 4.8 | 3.9 | 4.7 | 5.1 | 5.4 | 7.9 | 2.4 | 12.9 | 4.6 | 2.3 | 3.9 |
| VX | 1 | 0.0 | 0.0 | 0.6 | 0.0 | 2.4 | 0.0 | 1.4 | 0.0 | 0.2 | 0.0 | 0.2 | 0.0 | 0.2 |
| VX | 2 | 1.9 | 1.2 | 0.0 | 0.3 | 0.0 | 0.1 | 1.7 | 1.3 | 0.0 | 2.9 | 0.9 | 1.0 | 0.0 |
| VX | 3 | 1.7 | 1.6 | 1.6 | 2.0 | 3.6 | 1.7 | 3.2 | 1.1 | 0.9 | 1.4 | 0.6 | 0.4 | 0.6 |
| VX | 4 | 2.6 | 2.1 | 5.1 | 2.9 | 3.5 | 1.7 | 0.7 | 1.7 | 2.6 | 3.7 | 0.0 | 1.3 | 2.6 |
| VX | 5 | 2.4 | 2.7 | 4.8 | 0.0 | 5.5 | 4.3 | 4.7 | 2.0 | 1.4 | 0.7 | 1.4 | 1.7 | 2.1 |
| VX | 6 | 4.0 | 3.3 | 4.0 | 3.3 | 4.1 | 2.6 | 0.0 | 0.9 | 2.7 | 6.0 | 0.9 | 1.2 | 2.8 |
| VX | 7 | 4.3 | 3.8 | 1.4 | 6.4 | 2.4 | 4.3 | 0.2 | 1.5 | 3.7 | 6.8 | 1.3 | 2.4 | 3.6 |
| VX | 8 | 5.3 | 5.1 | 5.5 | 3.5 | 5.1 | 4.6 | 6.3 | 5.1 | 3.4 | 3.1 | 2.1 | 4.2 | 2.6 |
| WAY100635 | 1 | 0.0 | 0.0 | 1.1 | 0.9 | 1.4 | 5.0 | 7.2 | 2.0 | 0.0 | 3.0 | 0.0 | 1.0 | 0.0 |
| WAY100635 | 2 | 3.6 | 4.1 | 0.3 | 0.0 | 0.7 | 3.3 | 9.3 | 0.0 | 7.8 | 0.0 | 1.9 | 3.0 | 3.3 |
| WAY100635 | 3 | 5.7 | 5.7 | 0.0 | 1.0 | 0.8 | 2.7 | 8.4 | 0.6 | 8.6 | 1.8 | 1.7 | 3.2 | 2.9 |
| WAY100635 | 4 | 6.7 | 7.1 | 0.1 | 2.0 | 0.0 | 0.8 | 6.7 | 1.1 | 9.9 | 2.0 | 6.8 | 4.3 | 4.4 |
| WAY100635 | 5 | 8.4 | 8.1 | 5.3 | 3.3 | 4.7 | 7.2 | 12.6 | 5.8 | 11.4 | 8.7 | 4.7 | 6.7 | 6.9 |
| WAY100635 | 6 | 5.2 | 5.6 | 0.7 | 6.9 | 1.6 | 0.0 | 0.0 | 0.0 | 0.5 | 4.2 | 2.0 | 0.0 | 0.1 |
| WAY100635 | 7 | 10.6 | 11.4 | 2.3 | 5.4 | 3.3 | 2.6 | 6.2 | 4.1 | 10.6 | 8.2 | 8.3 | 6.7 | 7.7 |
| WAY100635 | 8 | 12.4 | 12.4 | 2.4 | 6.6 | 1.8 | 2.5 | 8.3 | 4.3 | 11.5 | 9.4 | 7.7 | 6.5 | 6.6 |
| XylitolPentanit | 1 | 0.0 | 0.0 | 2.5 | 0.5 | 1.4 | 3.1 | 0.1 | 1.5 | 1.6 | 0.0 | 1.2 | 1.5 | 0.0 |
| XylitolPentanit | 2 | 1.0 | 1.6 | 5.1 | 0.0 | 2.6 | 3.1 | 0.0 | 4.4 | 2.4 | 0.2 | 0.0 | 1.3 | 1.3 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| XylitolPentanit | 3 | 2.9 | 3.3 | 2.1 | 0.2 | 0.0 | 0.1 | 1.0 | 3.7 | 8.9 | 4.6 | 1.3 | 2.1 | 3.1 |
| XylitolPentanit | 4 | 4.0 | 4.5 | 2.0 | 3.5 | 3.0 | 2.9 | 1.3 | 0.0 | 13.2 | 5.5 | 0.8 | 0.0 | 3.2 |
| XylitolPentanit | 5 | 3.8 | 5.2 | 2.1 | 2.8 | 5.1 | 6.0 | 2.5 | 2.7 | 0.0 | 4.3 | 0.3 | 0.6 | 3.9 |
| XylitolPentanit | 6 | 5.5 | 6.7 | 6.1 | 1.5 | 3.0 | 7.6 | 4.3 | 3.2 | 3.8 | 5.3 | 4.4 | 2.6 | 5.8 |
| XylitolPentanit | 7 | 7.3 | 8.1 | 1.1 | 12.7 | 1.3 | 0.0 | 0.2 | 1.7 | 2.9 | 11.0 | 2.6 | 0.5 | 7.8 |
| XylitolPentanit | 8 | 8.9 | 9.9 | 0.0 | 5.0 | 1.8 | 1.9 | 2.4 | 5.1 | 14.0 | 12.8 | 2.2 | 0.6 | 6.2 |
| shiepox_depox | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.0 | 0.2 | 1.2 | 1.8 | 0.0 | 0.0 | 0.0 |
| shiepox_depox | 2 | 0.5 | 0.3 | 0.0 | 0.0 | 0.1 | 0.0 | 0.0 | 0.4 | 0.9 | 0.0 | 1.0 | 0.0 | 1.0 |
| shiepox_depox | 3 | 1.3 | 2.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 | 0.3 | 6.5 | 0.4 | 0.9 | 0.0 |
| shiepox_depox | 4 | 1.7 | 2.3 | 0.0 | 0.0 | 0.1 | 0.0 | 0.0 | 0.3 | 0.0 | 6.0 | 0.9 | 0.9 | 0.6 |
| shiepox_depox | 5 | 3.7 | 3.8 | 1.2 | 2.7 | 0.4 | 1.4 | 2.0 | 0.9 | 7.0 | 8.1 | 0.7 | 0.0 | 1.1 |
| shiepox_depox | 6 | 4.8 | 4.6 | 1.2 | 2.7 | 0.3 | 1.4 | 2.0 | 0.9 | 6.4 | 5.8 | 2.2 | 0.0 | 0.6 |
| shiepox_depox | 7 | 5.1 | 5.0 | 1.2 | 2.7 | 0.3 | 1.4 | 2.0 | 0.9 | 6.9 | 7.0 | 2.0 | 0.0 | 1.1 |
| shiepox_depox | 8 | 6.6 | 6.7 | 1.2 | 2.7 | 0.0 | 6.8 | 2.0 | 0.9 | 8.9 | 8.7 | 3.5 | 7.3 | 5.6 |