

| Host | Host conc (mM) | Guest conc (mM) | Run number | K (M ⁻¹) | ΔG (KJ/mol) | ΔH (KJ/mol) | ΔS (J/mol/K) |
|---------|----------------|-----------------|---------------|----------------------|---------------------|---------------------|----------------------|
| b-CD | 2.5 | 37.5 | bCDt4mch1 | 2025.31 ± 68.11 | -19.00 ± 0.08 | -10.90 ± 0.44 | 26.97 ± 1.51 |
| | 2.5 | 37.5 | bCDt4mch2 | 2098.64 ± 66.95 | -19.09 ± 0.08 | -10.53 ± 0.47 | 28.52 ± 1.58 |
| MGLab8 | 2 | 40 | MGLab8t4mch1 | 244.18 ± 13.89 | -13.72 ± 0.14 | -9.18 ± 1.40 | 15.13 ± 4.68 |
| | 2.3 | 40 | MGLab8t4mch2 | 286.54 ± 14.93 | -14.12 ± 0.13 | -5.89 ± 0.52 | 27.42 ± 1.78 |
| MGLab24 | 2 | 45 | MGLab24t4mch1 | 276.83 ± 13.59 | -14.03 ± 0.12 | -7.76 ± 0.82 | 20.92 ± 2.79 |
| | 2 | 45 | MGLab24t4mch2 | 286.54 ± 14.95 | -14.12 ± 0.15 | -5.89 ± 0.54 | 27.42 ± 1.80 |
| MGLab9 | 1.8 | 45 | MGLab9t4mch1 | 221.08 ± 12.72 | -13.47 ± 0.14 | -10.49 ± 1.80 | 9.93 ± 6.01 |
| | 1.8 | 45 | MGLab9t4mch2 | 203.13 ± 10.87 | -13.26 ± 0.13 | -12.44 ± 2.65 | 2.72 ± 8.87 |
| MGLab23 | 1.6 | 47 | MGLab23t4mch1 | 236.64 ± 11.99 | -13.64 ± 0.12 | -9.88 ± 1.68 | 12.55 ± 5.60 |
| | 1.5 | 50 | MGLab23t4mch2 | 210.20 ± 10.99 | -13.35 ± 0.13 | -13.01 ± 4.18 | 1.10 ± 13.94 |
| MGLab19 | 4 | 77 | MGLab19t4mch1 | 199.60 ± 8.02 | -13.22 ± 0.10 | -9.17 ± 0.73 | 13.48 ± 2.46 |
| | 4 | 77 | MGLab19t4mch2 | 228.31 ± 8.82 | -13.55 ± 0.10 | -8.05 ± 0.52 | 18.35 ± 1.78 |
| | 3.8 | 80 | MGLab21t4mch3 | 123.47 ± 6.44 | -12.02 ± 0.13 | -14.14 ± 2.04 | -7.07 ± 6.83 |
| MGLab35 | 4.5 | 74 | MGLab34t4mch1 | 2103.19 ± 65.42 | -19.09 ± 0.08 | -17.87 ± 0.72 | 4.08 ± 2.41 |
| | 4.5 | 74 | MGLab34t4mch2 | 2442.72 ± 73.46 | -19.47 ± 0.08 | -19.78 ± 0.83 | -1.05 ± 2.77 |
| MGLab34 | 3.5 | 80 | MGLab35t4mch1 | 570.79 ± 17.8 | -15.84 ± 0.08 | -15.14 ± 0.74 | 2.32 ± 2.48 |
| | 3.5 | 80 | MGLab35t4mch2 | 775.47 ± 23.66 | -16.60 ± 0.08 | -15.98 ± 0.72 | 2.09 ± 2.41 |
| | 3.5 | 80 | MGLab35t4mch3 | 880.96 ± 27.44 | -16.92 ± 0.08 | -16.04 ± 0.74 | 2.93 ± 2.47 |
| MGLab36 | 3.5 | 80 | MGLab36t4mch4 | 197.68 ± 7.63 | -13.19 ± 0.1 | -13.55 ± 1.14 | -1.19 ± 3.83 |
| | 3 | 80 | MGLab36t4mch5 | 274.18 ± 11.11 | -14.01 ± 0.1 | -12.20 ± 0.93 | 5.63 ± 3.43 |
| | 3.5 | 80 | MGLab36t4mch6 | 207.65 ± 8.29 | -13.32 ± 0.10 | -11.66 ± 0.81 | 5.52 ± 2.73 |

| ΔS (J/mol/K) | Unc. In ΔS (J/mol/K) | T ΔS (kJ/mol) | Unc in T ΔS (J/m N | T (K)= | 300.15 |
|----------------------|------------------------------|-----------------------|----------------------------|-----------------|--------|
| 26.97 | 1.51 | 8.0950455 | 0.4532265 | 0.86 \pm 0.03 | |
| 28.52 | 1.58 | 8.560278 | 0.474237 | 0.89 \pm 0.03 | |
| 15.13 | 4.68 | 4.5412695 | 1.404702 | 0.78 \pm 0.09 | |
| 27.42 | 1.78 | 8.230113 | 0.534267 | 1.00 \pm 0.07 | |
| 20.92 | 2.79 | 6.279138 | 0.8374185 | 0.83 \pm 0.07 | |
| 27.42 | 1.8 | 8.230113 | 0.54027 | 1.00 \pm 0.09 | |
| 9.93 | 6.01 | 2.9804895 | 1.8039015 | 0.82 \pm 0.12 | |
| 2.72 | 8.87 | 0.816408 | 2.6623305 | 0.79 \pm 0.13 | |
| 12.55 | 5.6 | 3.7668825 | 1.68084 | 0.81 \pm 0.11 | |
| 1.1 | 13.94 | 0.330165 | 4.184091 | 0.70 \pm 0.15 | |
| 13.48 | 2.46 | 4.046022 | 0.738369 | 0.81 \pm 0.05 | |
| 18.35 | 1.78 | 5.5077525 | 0.534267 | 0.85 \pm 0.04 | |
| -7.07 | 6.83 | -2.1220605 | 2.0500245 | 0.76 \pm 0.09 | |
| 4.08 | 2.41 | 1.224612 | 0.7233615 | 0.94 \pm 0.03 | |
| -1.05 | 2.77 | -0.3151575 | 0.8314155 | 0.76 \pm 0.02 | |
| 2.32 | 2.48 | 0.696348 | 0.744372 | 0.83 \pm 0.03 | |
| 2.09 | 2.41 | 0.6273135 | 0.7233615 | 0.80 \pm 0.03 | |
| 2.93 | 2.47 | 0.8794395 | 0.7413705 | 0.81 \pm 0.03 | |
| -1.19 | 3.83 | -0.3571785 | 1.1495745 | 0.81 \pm 0.05 | |
| 5.63 | 3.43 | 1.6898445 | 1.0295145 | 0.76 \pm 0.05 | |
| 5.52 | 2.73 | 1.656828 | 0.8194095 | 0.93 \pm 0.05 | |