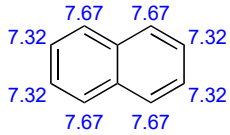
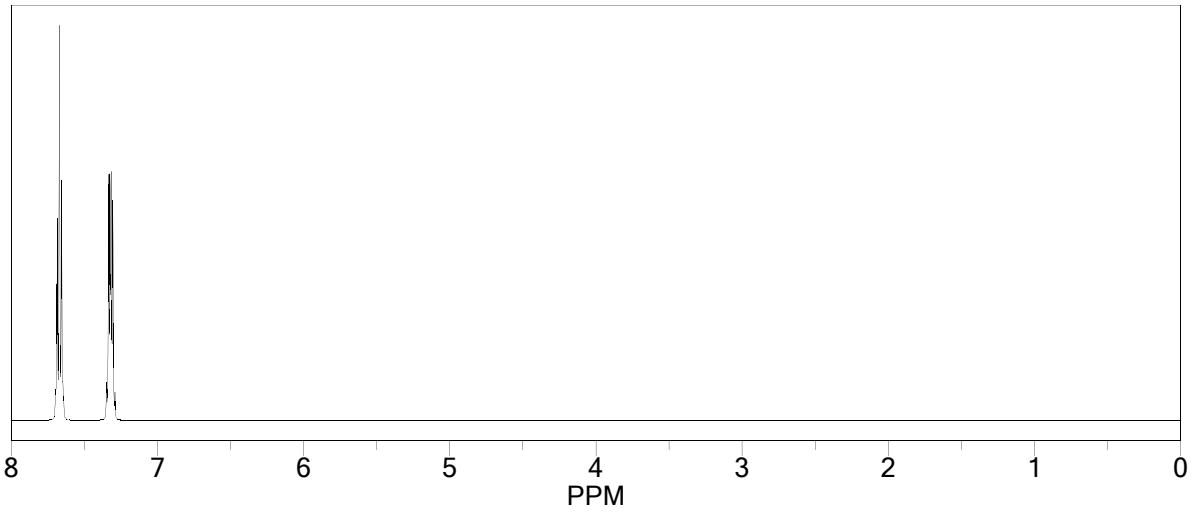
# ChemNMR $^1$H Estimation




Estimation quality is indicated by color: good, medium, rough




Protocol of the H-1 NMR Prediction:

| Node | Shift | Base + Inc. | Comment (ppm rel. to TMS) |
|---|---|---|---|
| CH | 7.67 | 7.67 | naphthalene |
| CH | 7.67 | 7.67 | naphthalene |
| CH | 7.67 | 7.67 | naphthalene |
| CH | 7.67 | 7.67 | naphthalene |
| CH | 7.32 | 7.32 | naphthalene |
| CH | 7.32 | 7.32 | naphthalene |
| CH | 7.32 | 7.32 | naphthalene |
| CH | 7.32 | 7.32 | naphthalene |

1H NMR Coupling Constant Prediction

| shift | atom index | coupling partner, constant and vector |
|---|---|---|
| 7.67 | 3 | |
| | 2 | 7.5 H-C*C-H |
| | 7 | 1.5 H-C*C*C-H |
| | 1 | 1.5 H-C*CH*C-H |
| 7.67 | 6 | |
| | 1 | 7.5 H-C*C-H |
| | 10 | 1.5 H-C*C*C-H |
| | 2 | 1.5 H-C*CH*C-H |
| 7.67 | 7 | |
| | 8 | 7.5 H-C*C-H |
| | 3 | 1.5 H-C*C*C-H |
| | 9 | 1.5 H-C*CH*C-H |
| 7.67 | 10 | |
| | 9 | 7.5 H-C*C-H |
| | 6 | 1.5 H-C*C*C-H |
| | 8 | 1.5 H-C*CH*C-H |
| 7.32 | 8 | |
| | 7 | 7.5 H-C*C-H |
| | 9 | 7.5 H-C*C-H |
| | 10 | 1.5 H-C*CH*C-H |
| 7.32 | 9 | |
| | 10 | 7.5 H-C*C-H |
| | 8 | 7.5 H-C*C-H |
| | 7 | 1.5 H-C*CH*C-H |
| 7.32 | 1 | |
| | 6 | 7.5 H-C*C-H |

| | | | | |
|---|---|---|---|---|
| | | 2 | 7.5 | H-C*C-H |
| | | 3 | 1.5 | H-C*CH*C-H |
| 7.32 | 2 | | | |
| | | 3 | 7.5 | H-C*C-H |
| | | 1 | 7.5 | H-C*C-H |
| | | 6 | 1.5 | H-C*CH*C-H |