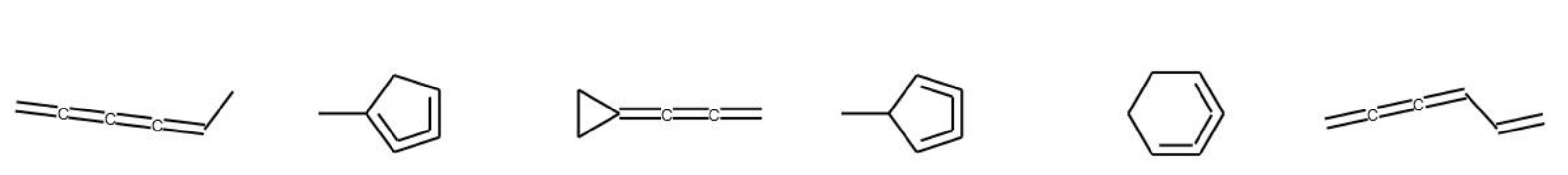
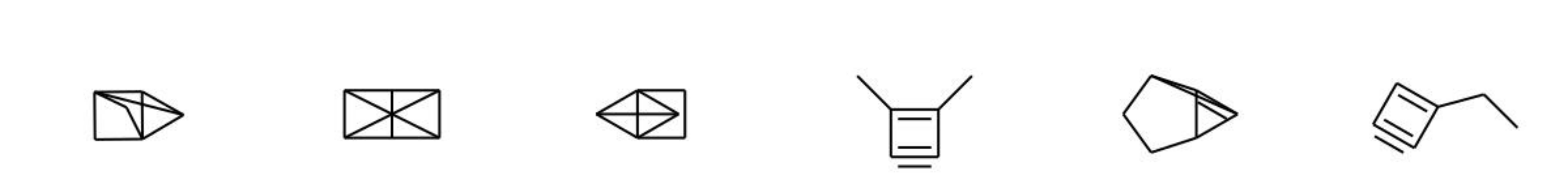
CCC12C3=C1C32, nan, False | CC1=C2C(C)=C12, 6.642, False | CC12C3C14CC324, 111.6, False | CC1C23C4C2C143, 109.9, False | CC1=C=C=C1C, 21.67, False | CCC1=C=C=C1, 21.62, False

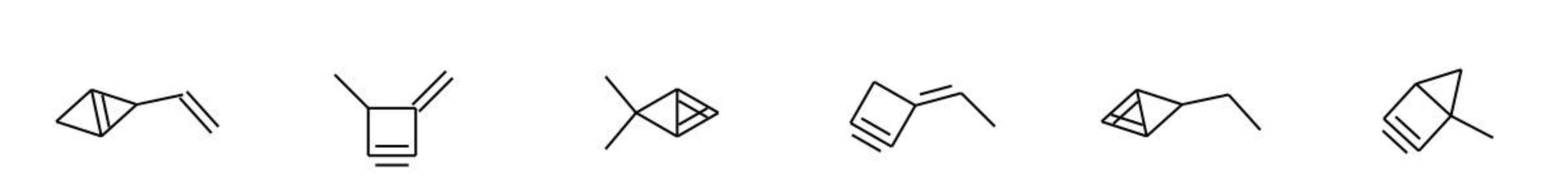


C=C=C=C=CC, 0.002, True | CC1=C=C=CC1, 15.28, False | C=C=C=C1CC1, 14.55, False | CC1C=C=C=C1, 15.34, False | C1=C=CCCC=1, 10.01, True | C=C=C=CC=C, 0.054, True

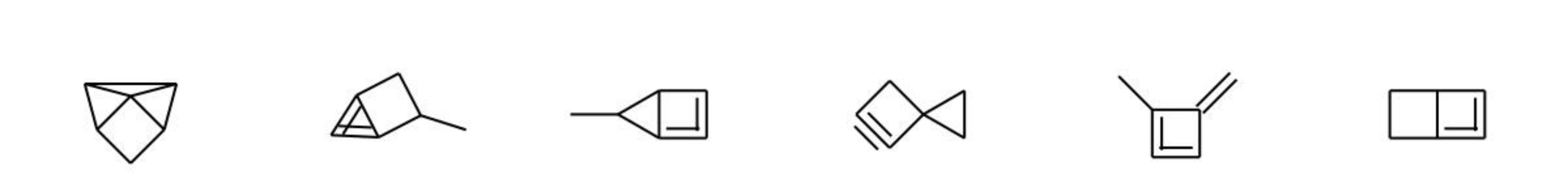
C1C2C3C4C3C124, 82.39, False | CC1C2=C=C1C2, nan, False | CC1=C=C2CC12, 39.26, False | C1=C2CCC=1C2, nan, False | CC12C=C=C1C2, 39.71, False | C12C3C1C1C2C31, 64.98, False



C1C23CC14C2C34, 89.66, False | C12C3C4C1C3C24, nan, False | C1CC23C4C2C143, 96.55, False | CC1=C(C)C#C1, 20.73, False | C1CC2C3=C2C13, nan, False | CCC1=CC#C1, 20.81, False

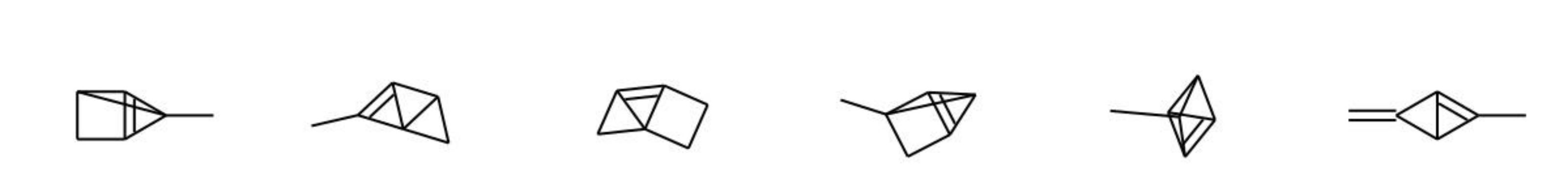


C=CC1C2=C1C2, 26.58, False | C=C1C#CC1C, 21.71, False | CC1(C)C2=C=C21, 31.05, False | CC=C1C#CC1, 21.57, False | CCC1C2=C=C21, 28.67, False | CC12C#CC1C2, 46.19, False

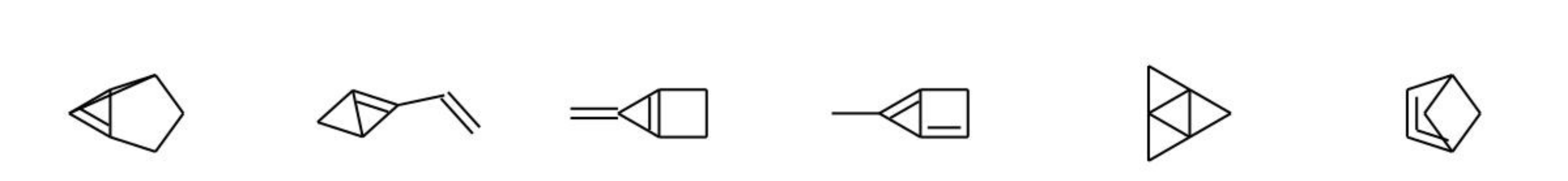


C1C2C3C4C1C234, 70.60, False | CC1CC2=C=C21, 44.02, False | CC1C2=C=CC21, 39.63, False | C1#CC2(C1)CC2, 48.67, False | C=C1C=C=C1C, 8.781, True | C1=CC2CCC=12, nan, False

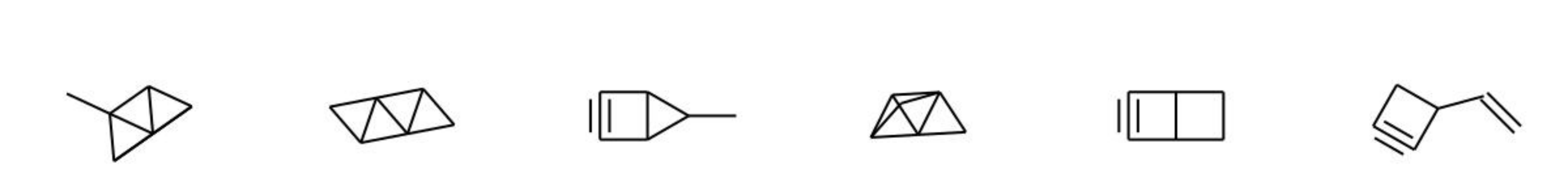
C=CC1=C=CC1, 10.22, True | CC=C=C1C=C1, 0.297, True | C1=CCC2CC=12, 26.91, False | CC1=C=CC=C1, 8.432, True | CCC1=C2C=C21, 6.602, False | CC1C2=C3CC321, 79.09, False



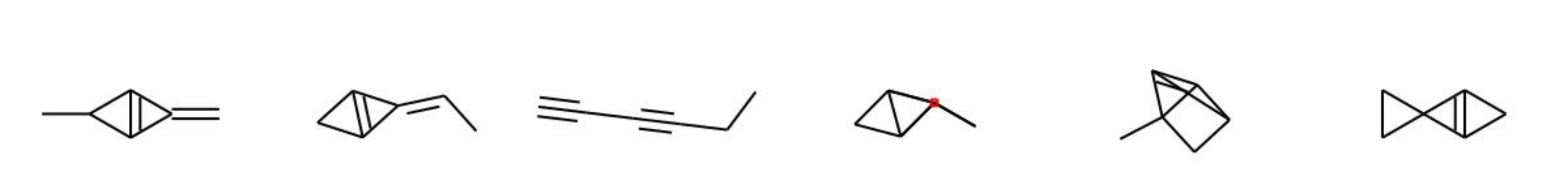
CC12C3=C1C2C3, nan, False | CC1=C2C3CC123, 51.78, False | C1CC23CC2=C13, 45.92, False | CC12CC3=C1C32, nan, False | CC1C2=C3C2C31, nan, False | C=C1C2=C(C)C12, 23.94, False



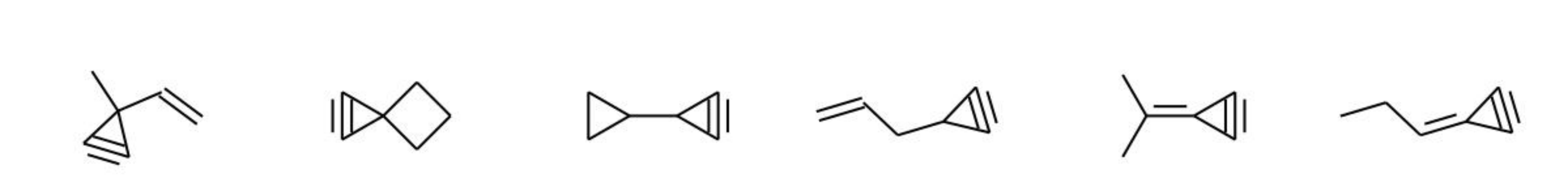
C1CC2C3=C1C32, nan, False | C=CC1=C2CC12, 33.43, False | C=C1C2=C1CC2, 30.22, False | CC1=C2CC=C12, 27.43, False | C1C23CC24CC134, 86.07, False | C1=CC2CC=1C2, nan, False



CC12C3C4C1C432, 94.60, False | C1C2C13C1CC213, 85.59, False | CC1C2C#CC12, 47.76, False | C1C2C3C14CC234, 78.72, False | C1#CC2CCC12, nan, False | C=CC1C#CC1, 23.86, False

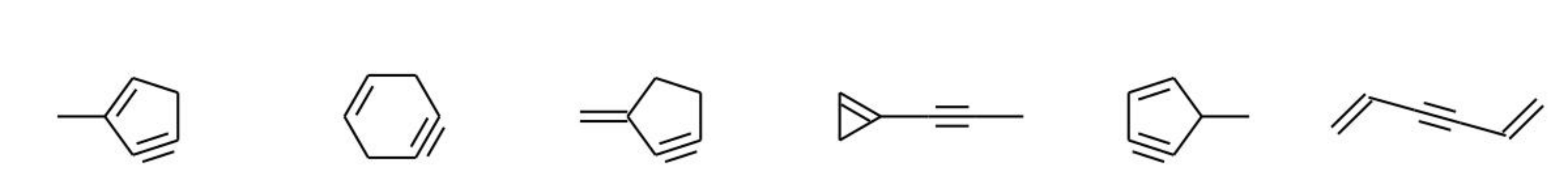


C=C1C2=C1C2C, 17.99, False | CC=C1C2=C1C2, 17.07, False | C#CC#CCC, -0.00, True | C1C2C34CC23C14, 78.00, False | CC12CC3C1=C32, nan, False | C1C2=C1C21CC1, 47.73, False

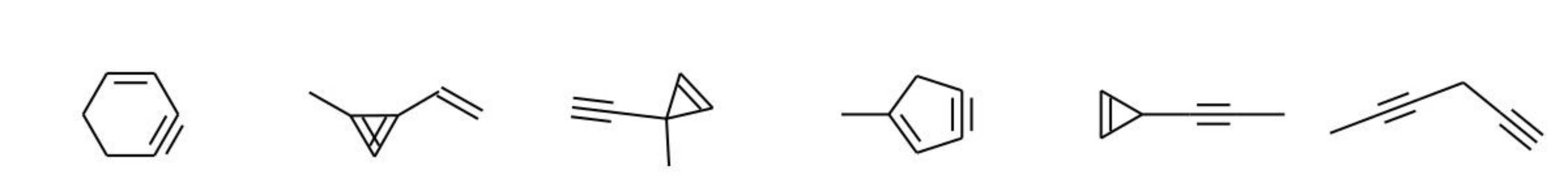


C=CC1(C)C#C1, 41.93, False | C1#CC12CCC2, 49.07, False | C1#CC1C1CC1, 63.92, False | C=CCC1C#C1, 41.66, False | CC(C)=C1C#C1, 32.93, False | CCC=C1C#C1, 32.91, False

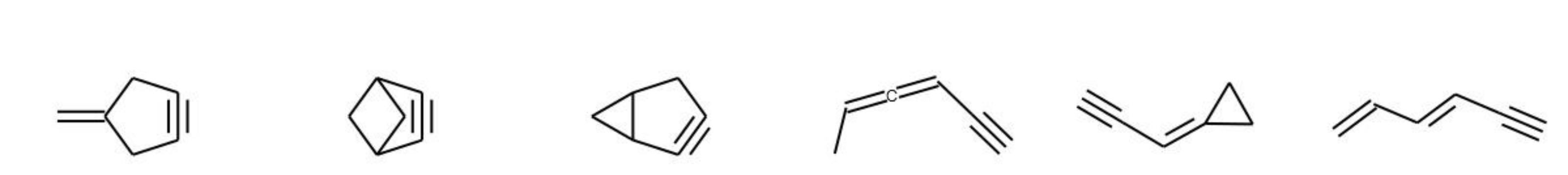
CC1CC12C#C2, 65.90, False | C=C(C)C1C#C1, 41.64, False | CC=CC1C#C1, 41.53, False | CC1C2C3=C2C31, nan, False | CC#CC#CC, -0.07, True | C1C2C3C4C2C134, 71.52, False



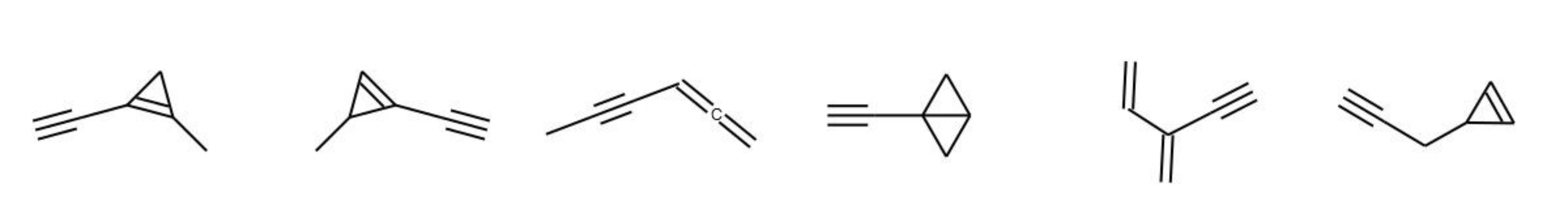
CC1=CCC#C1, 14.71, False | C1#CCC=CC1, 8.894, False | C=C1C#CCC1, 13.79, False | CC#CC1=CC1, 8.303, False | CC1C#CC=C1, 14.66, False | C=CC#CC=C, 0.048, True



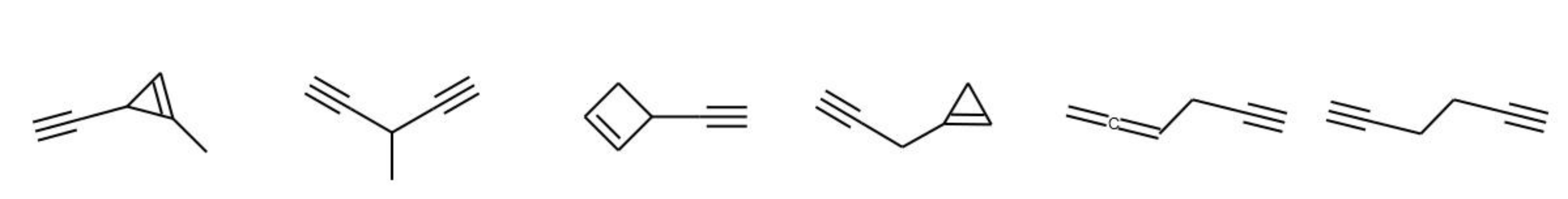
C1#CCCC=C1, 9.572, True | C=CC1=C=C1C, 16.30, False | C#CC1(C)C=C1, 8.754, True | CC1=CC#CC1, 14.71, False | CC#CC1C=C1, 8.365, False | C#CCC#CC, -0.07, True



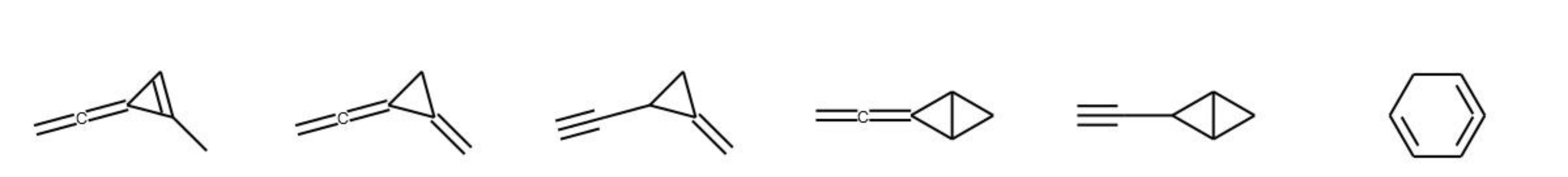
C=C1CC#CC1, 12.87, False | C1#CC2CC1C2, 27.46, False | C1#CC2CC2C1, 35.30, False | C#CC=C=CC, -0.04, True | C#CC=C1CC1, 14.53, False | C#CC=CC=C, 0.165, True



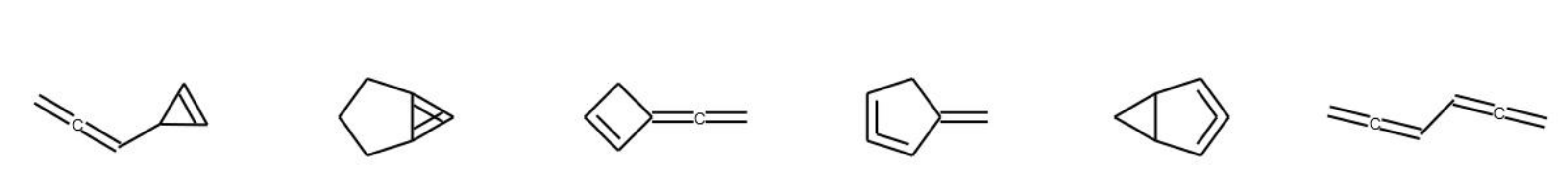
C#CC1=C(C)C1, 8.359, True | C#CC1=CC1C, 8.589, False | C=C=CC#CC, -0.08, True | C#CC12CC1C2, 43.42, False | C#CC(=C)C=C, 0.341, True | C#CCC1C=C1, 8.547, True



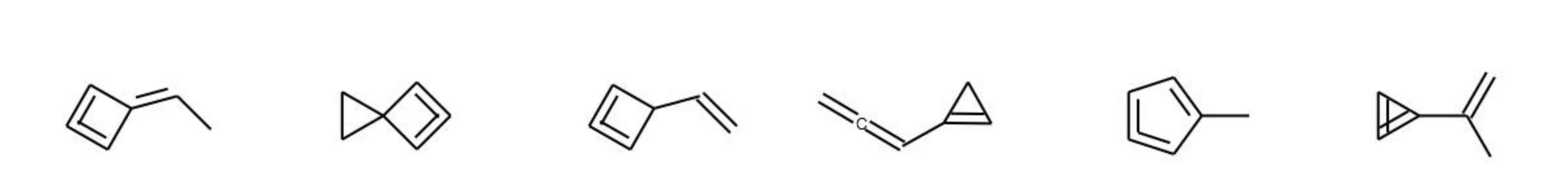
C#CC1C=C1C, 8.423, True | C#CC(C)C#C, 0.041, True | C#CC1C=CC1, 3.541, True | C#CCC1=CC1, 8.285, True | C#CCC=C=C, 0.007, True | C#CCCC#C, 0.102, True



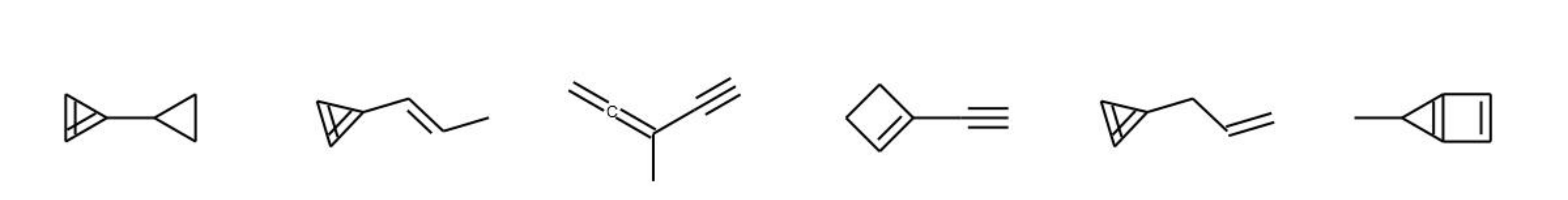
C=C=C1C=C1C, 0.305, True | C=C=C1CC1=C, 6.930, False | C#CC1CC1=C, 14.66, False | C=C=C1C2CC12, 35.83, False | C#CC1C2CC12, 43.31, False | C1=CC=CCC=1, 4.333, True



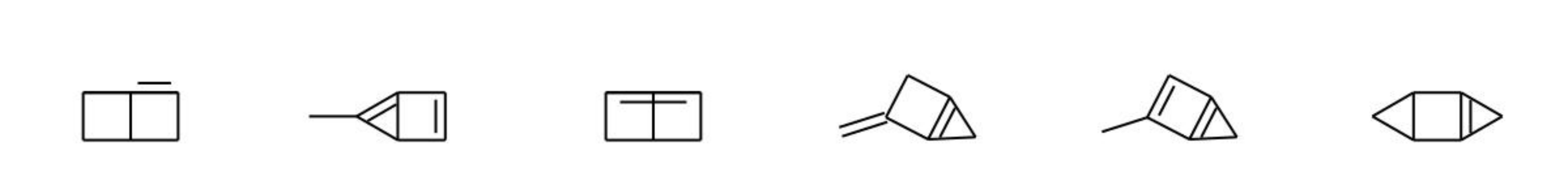
C=C=CC1C=C1, 8.464, False | C1=C2CCCC=12, 26.09, False | C=C=C1C=CC1, 1.561, True | C=C1C=C=CC1, 7.349, True | C1=CC2CC2C=1, 29.50, False | C=C=CC=C=C, 0.119, True



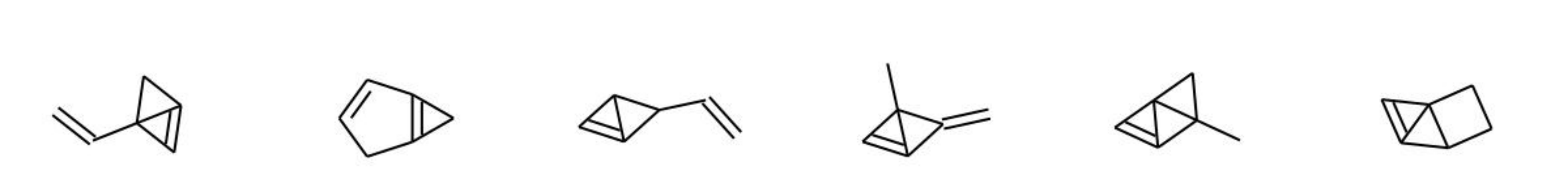
CC=C1C=C=C1, 8.817, True | C1=CC2(C=1)CC2, 34.71, False | C=CC1C=C=C1, 10.47, True | C=C=CC1=CC1, 8.280, False | CC1=CC=C=C1, 8.498, True | C=C(C)C1=C=C1, 16.52, False



C1=CC=1C1CC1, 44.77, False | CC=CC1=C=C1, 16.53, False | C#CC(C)=C=C, 0.004, True | C#CC1=CCC1, 3.417, True | C=CCC1=C=C1, 16.45, False | CC1C2=C1C=C2, 39.78, False

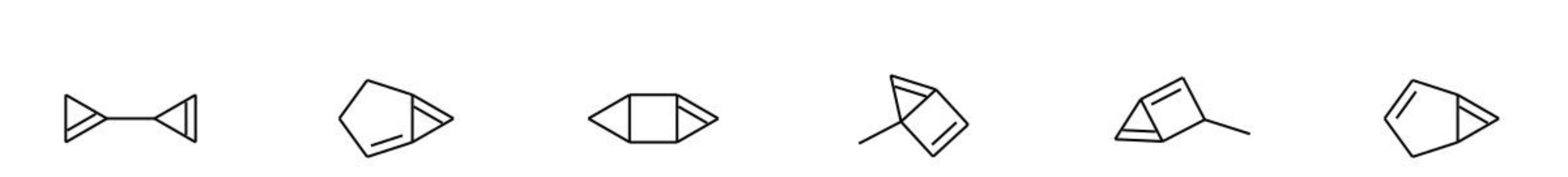


C1C2=C3C1CC23, nan, False | CC1=C2C=CC12, 21.08, False | C1C2=C3CC1C23, nan, False | C=C1CC2=C1C2, 37.50, False | CC1=CC2=C1C2, 39.51, False | C1C2=C1C1CC21, 62.89, False

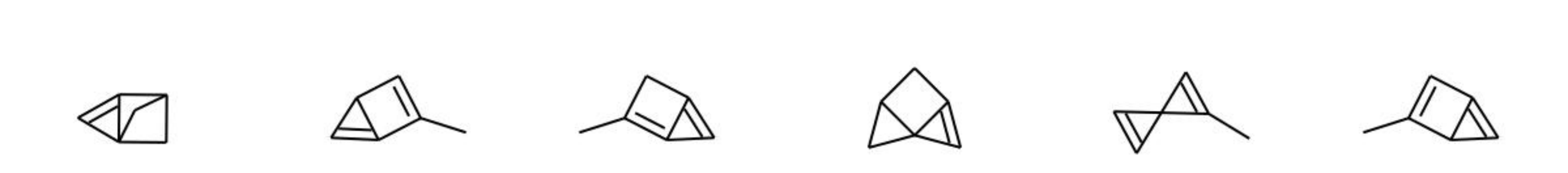


C=CC12C=C1C2, 34.02, False | C1=CC2=C(C1)C2, 21.31, False | C=CC1C2=CC21, 33.18, False | C=C1C2=CC12C, 26.10, False | CC12CC13C=C23, 52.47, False | C1=C2C3CCC123, 40.28, False

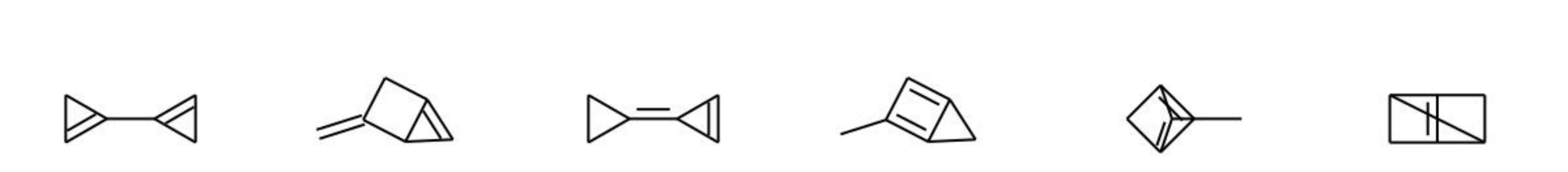
CC=C1C2=CC12, 23.95, False | C1=C2C1C21CC1, 55.29, False | CC1C2C3=CC312, 52.20, False | C=CC1=CC1=C, 0.294, True | C1=CC2C=C2C1, 14.01, False | C=C1CC2C=C12, 20.39, False



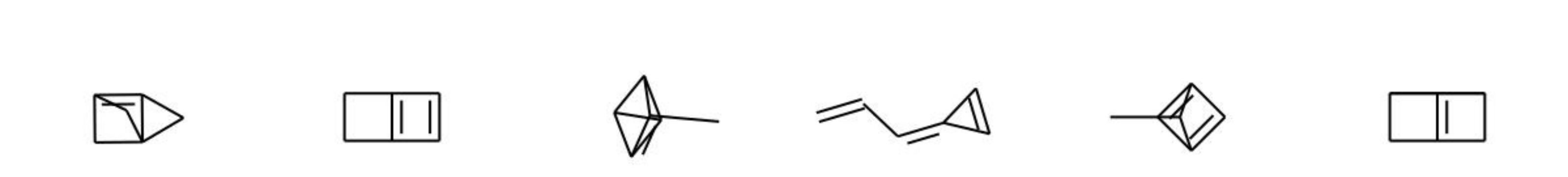
C1=CC1C1=CC1, 27.70, False | C1=C2C=C2CC1, 11.01, False | C1=C2C1C1CC21, 43.44, False | CC12C=CC1=C2, 21.64, False | CC1C=C2C=C21, 27.52, False | C1=CC2=CC2C1, 14.90, False



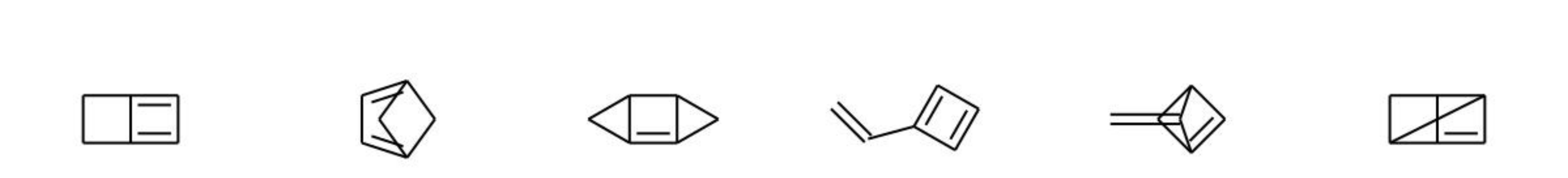
C1=C2C3CC12C3, nan, False | CC1=CC2C=C12, 21.18, False | CC1=C2C=C2C1, 27.46, False | C1=C2CC3CC123, 45.12, False | C1=CC12C=C2, 18.97, False | CC1=CC2=CC12, 21.10, False



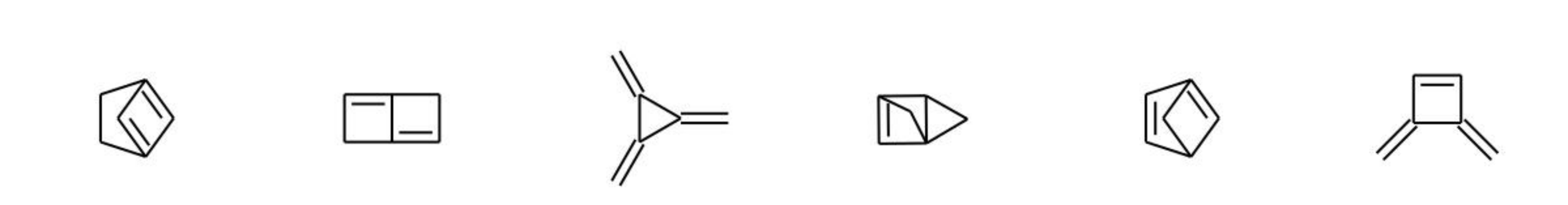
C1=C(C2=CC2)C1, 36.58, False | C=C1CC2=CC12, 22.41, False | C1=CC1=C1CC1, 29.41, False | CC1=C2CC2=C1, 36.03, False | CC1=C2C=C1C2, nan, False | C1C2=C3CC2C13, nan, False



C1C2=C3CC13C2, nan, False | C1=CC2=C1CC2, 9.368, True | CC1=C2C3C1C23, nan, False | C=CC=C1C=C1, 0.382, True | CC1C2=CC1=C2, nan, False | C1C2=C3C1C3C2, nan, False

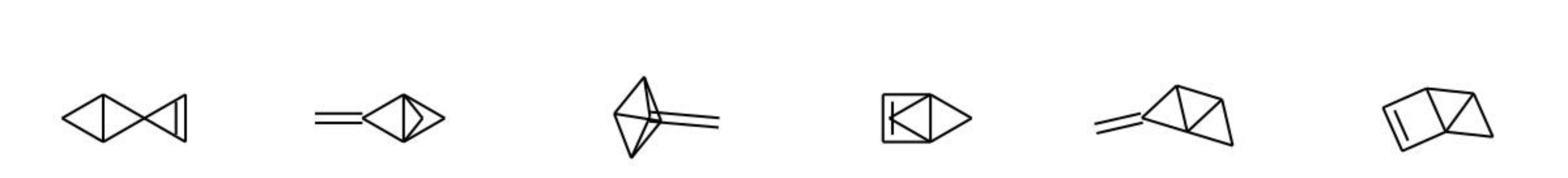


C1=C2CCC2=C1, 10.38, True | C1=C2CC(=C1)C2, nan, False | C1C2=C3CC3C12, 50.70, False | C=CC1=CC=C1, 0.009, True | C=C1C2=CC1C2, nan, False | C1=C2C3CC2C13, nan, False

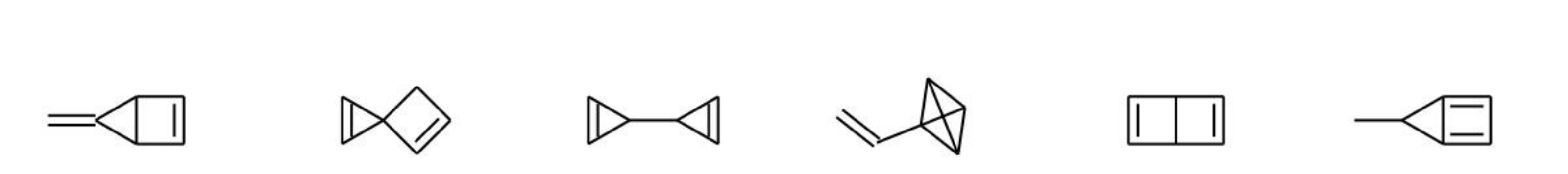


C1=C2C=C1CC2, nan, False | C1=C2CC=C2C1, 10.85, True | C=C1C(=C)C1=C, -0.11, True | C1=C2CC13CC23, nan, False | C1=CC2C=C1C2, nan, False | C=C1C=CC1=C, 0.066, True

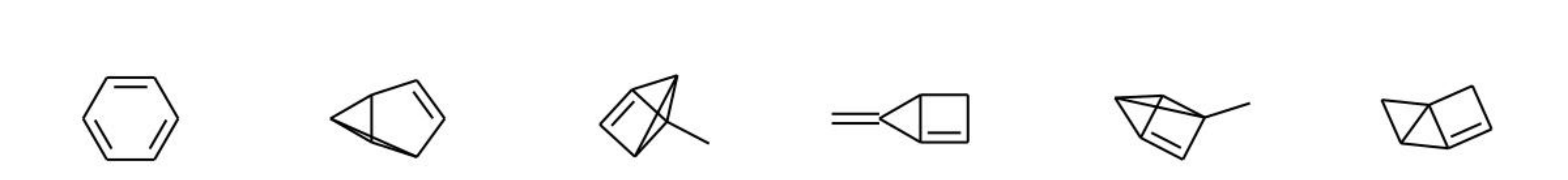
C=C1CC12C=C2, 25.34, False | C=C1C=CC=C1, 2.452, True | C1=C2C=C(C1)C2, nan, False | C1=CC2CC=C12, nan, False | C=C1C2C(=C)C12, 27.95, False | C1=C2CC3C1C23, nan, False



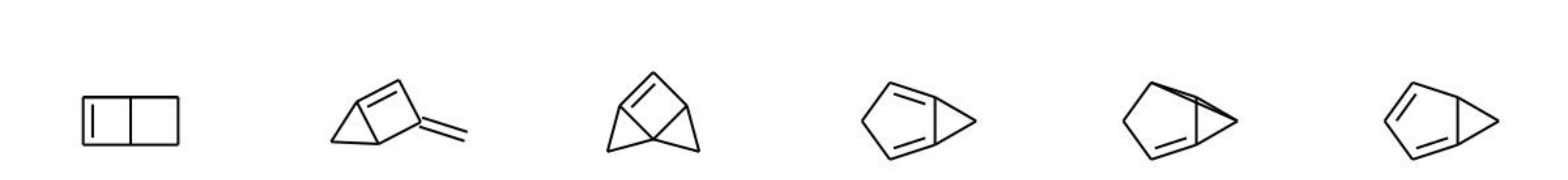
C1=CC12C1CC12, 53.52, False | C=C1C23CC12C3, 58.51, False | C=C1C2C3C1C23, 57.91, False | C1=CC23CC12C3, 46.09, False | C=C1C2C3CC132, 57.78, False | C1=CC23CC2C13, 47.02, False



C=C1C2C=CC12, 17.85, False | C1=CC2(C=C2)C1, 14.05, False | C1=CC1C1C=C1, 16.91, False | C=CC12C3C1C32, 93.59, False | C1=CC2C=CC12, nan, False | CC1C2=CC=C21, 36.26, False



c1ccccc1, 0.878, True | C1=CC2C3C1C23, 48.21, False | CC12C3=CC1C32, nan, False | C=C1C2=CCC12, 19.45, False | CC12C=C3C1C32, nan, False | C1=C2C3CC23C1, 48.30, False



C1=C2C3CC1C23, nan, False | C=C1C=C2CC12, 26.53, False | C1=C2CC23CC13, 49.31, False | C1=C2CC2=CC1, 20.01, False | C1=C2C3C(C1)C23, nan, False | C1=CC2CC2=C1, 22.11, False