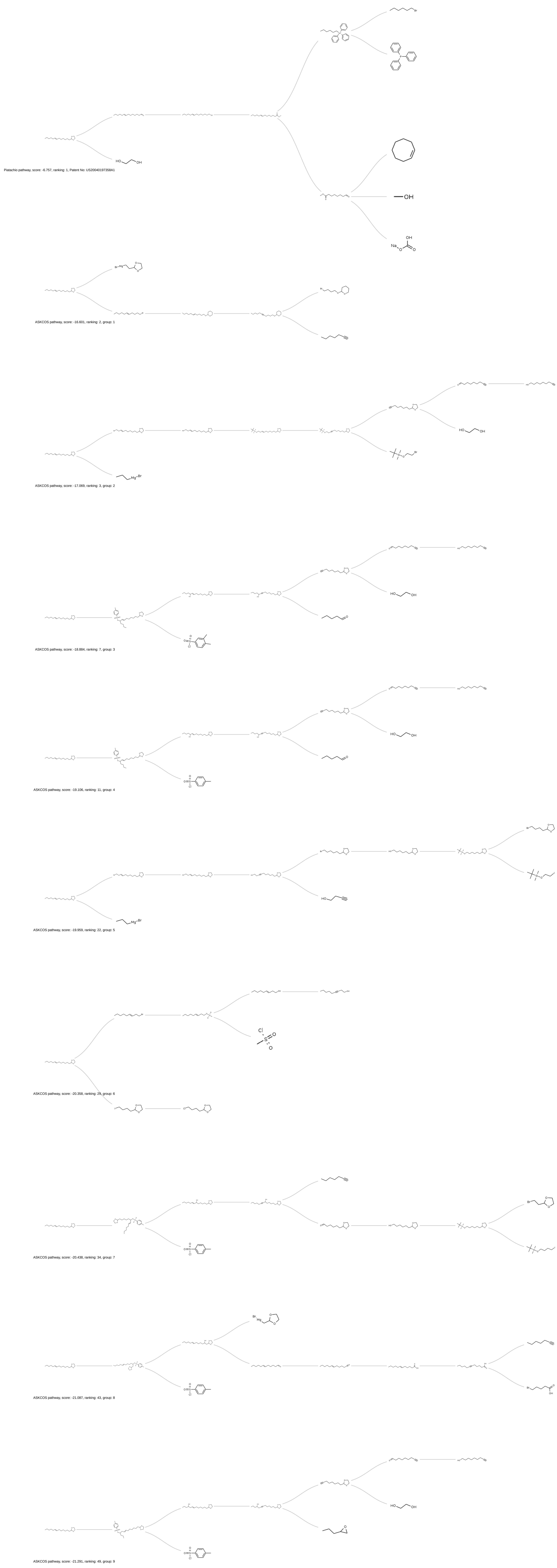
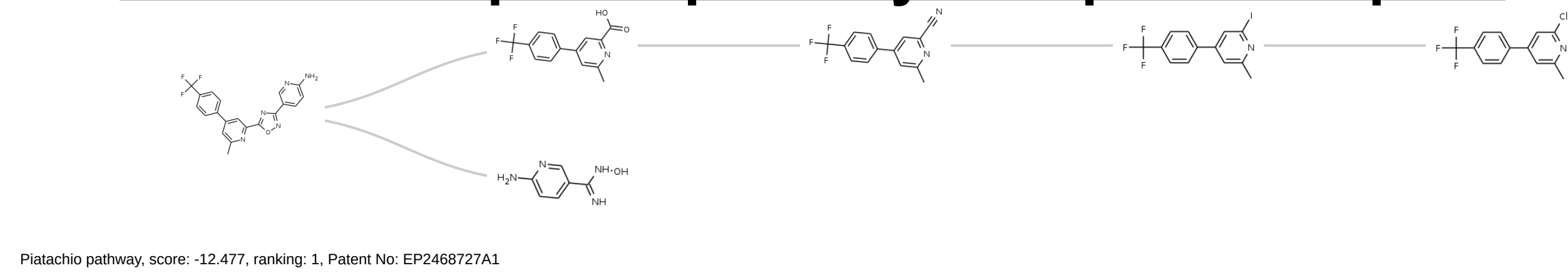


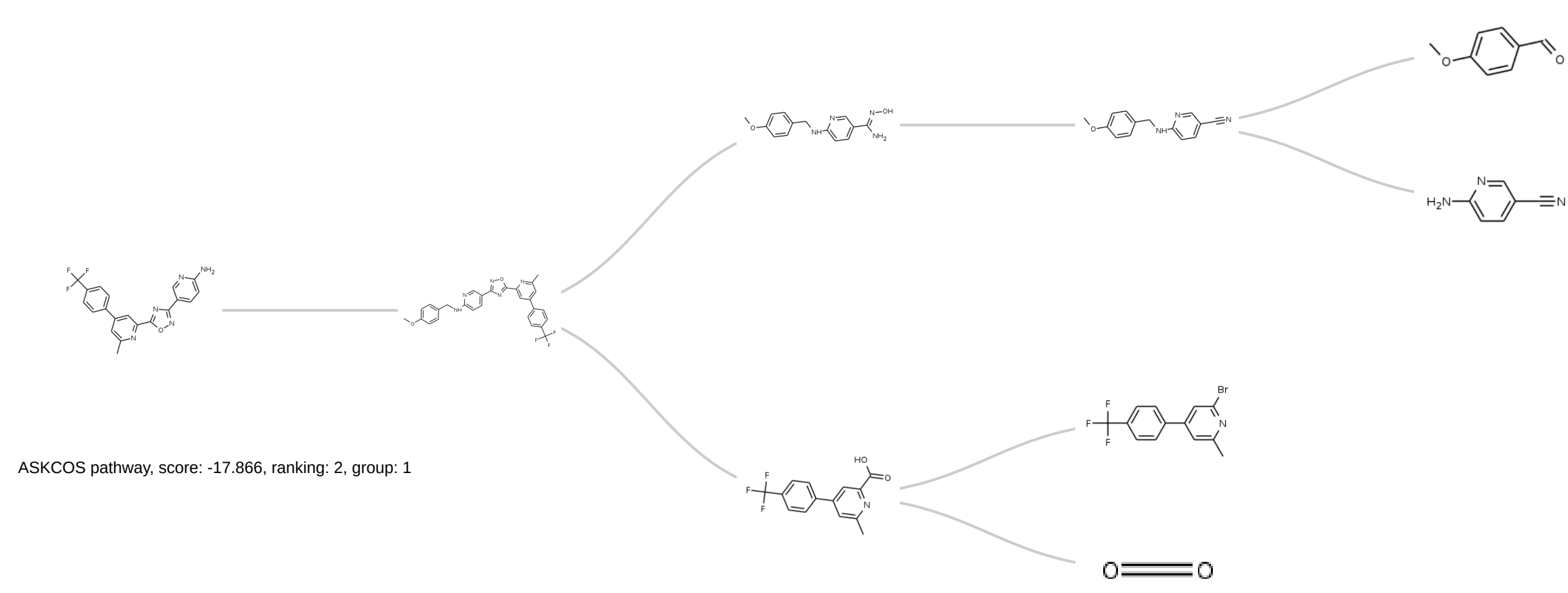
### Model ranks patent pathway as top-1: Example 1



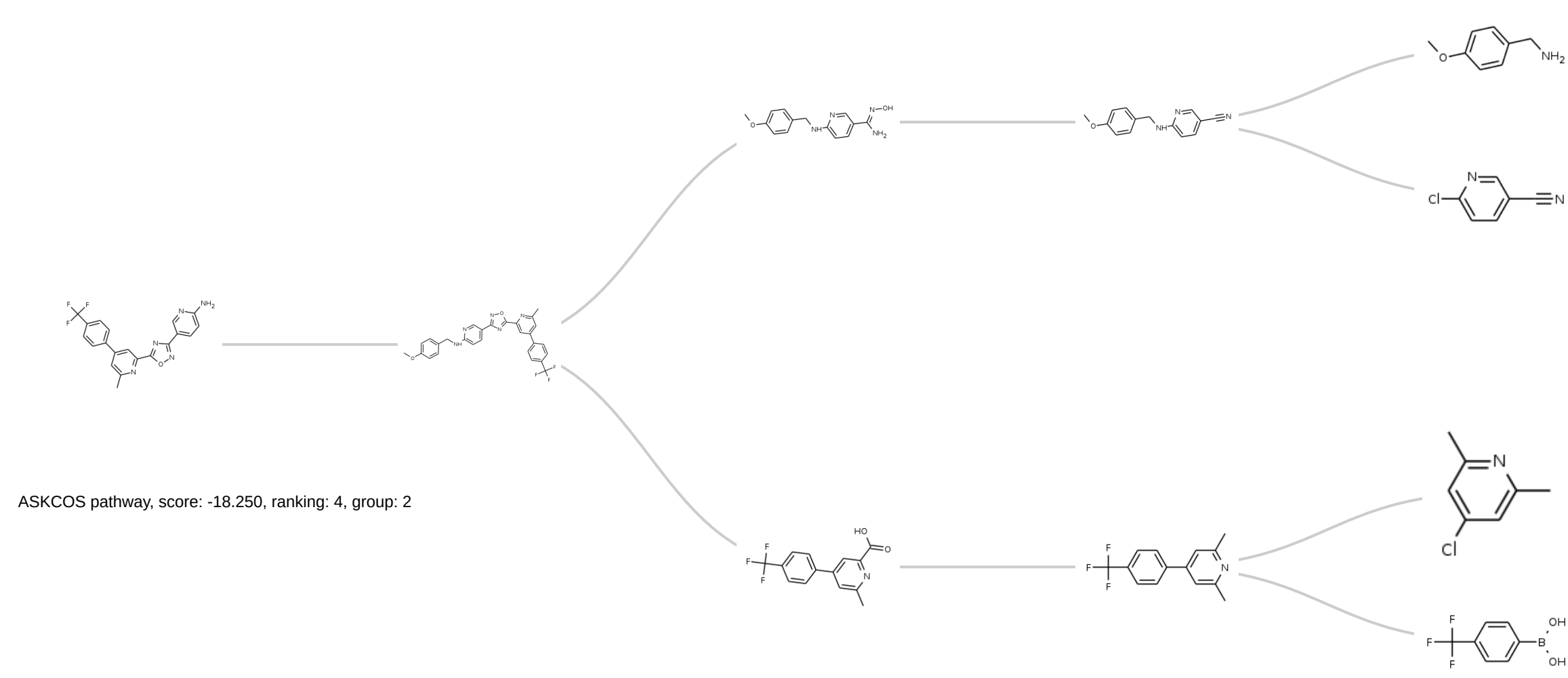
## Model ranks patent pathway as top-1: Example 2



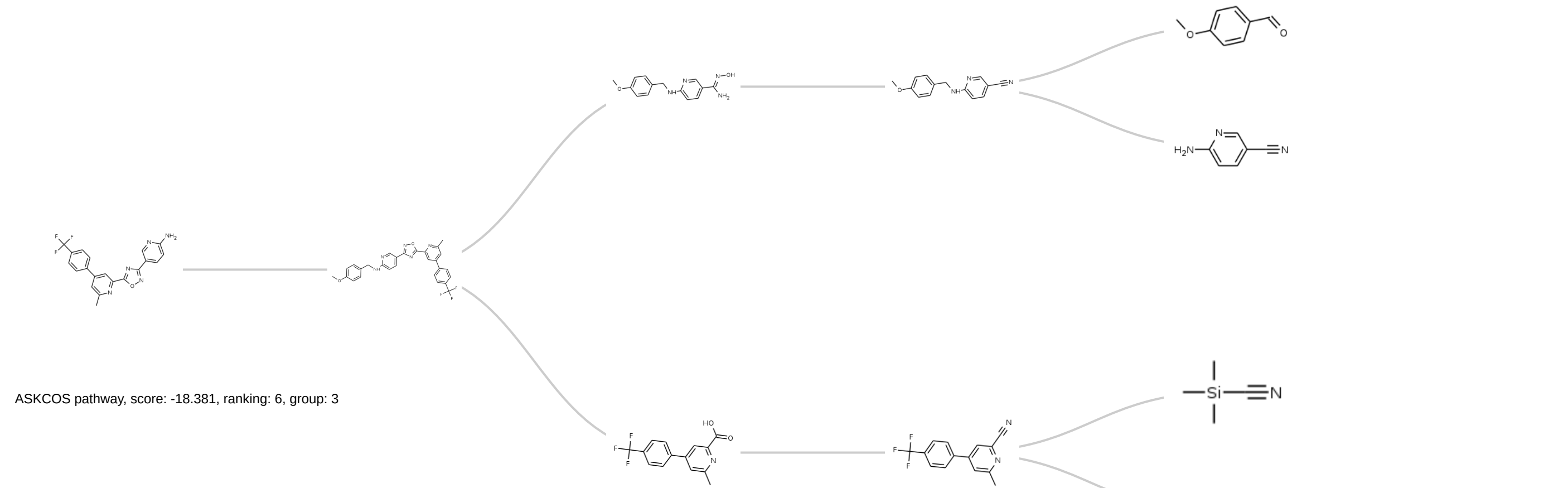
Patato pathway score: -12.477, ranking: 1, Patent No: EP2468727A1



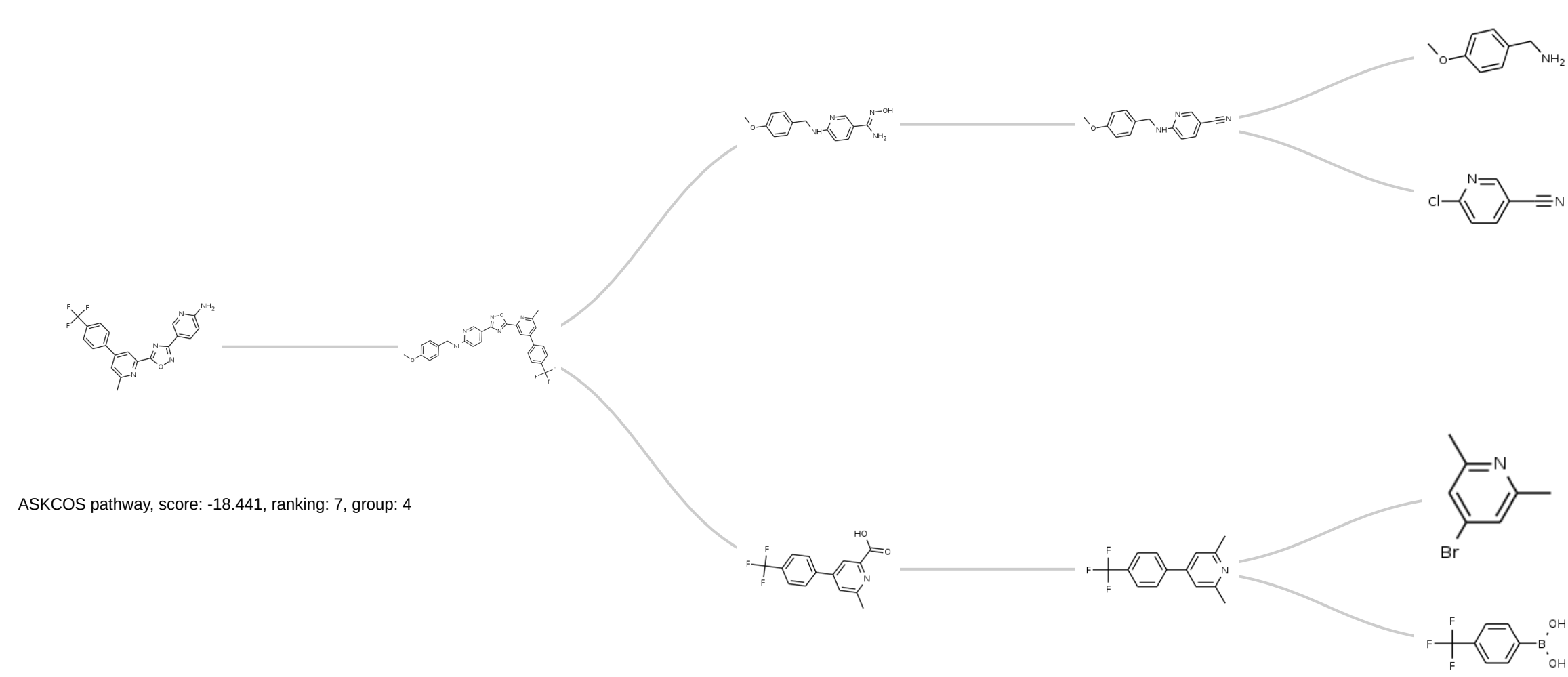
ASKCOS pathway score: -17.856, ranking: 2, group: 1



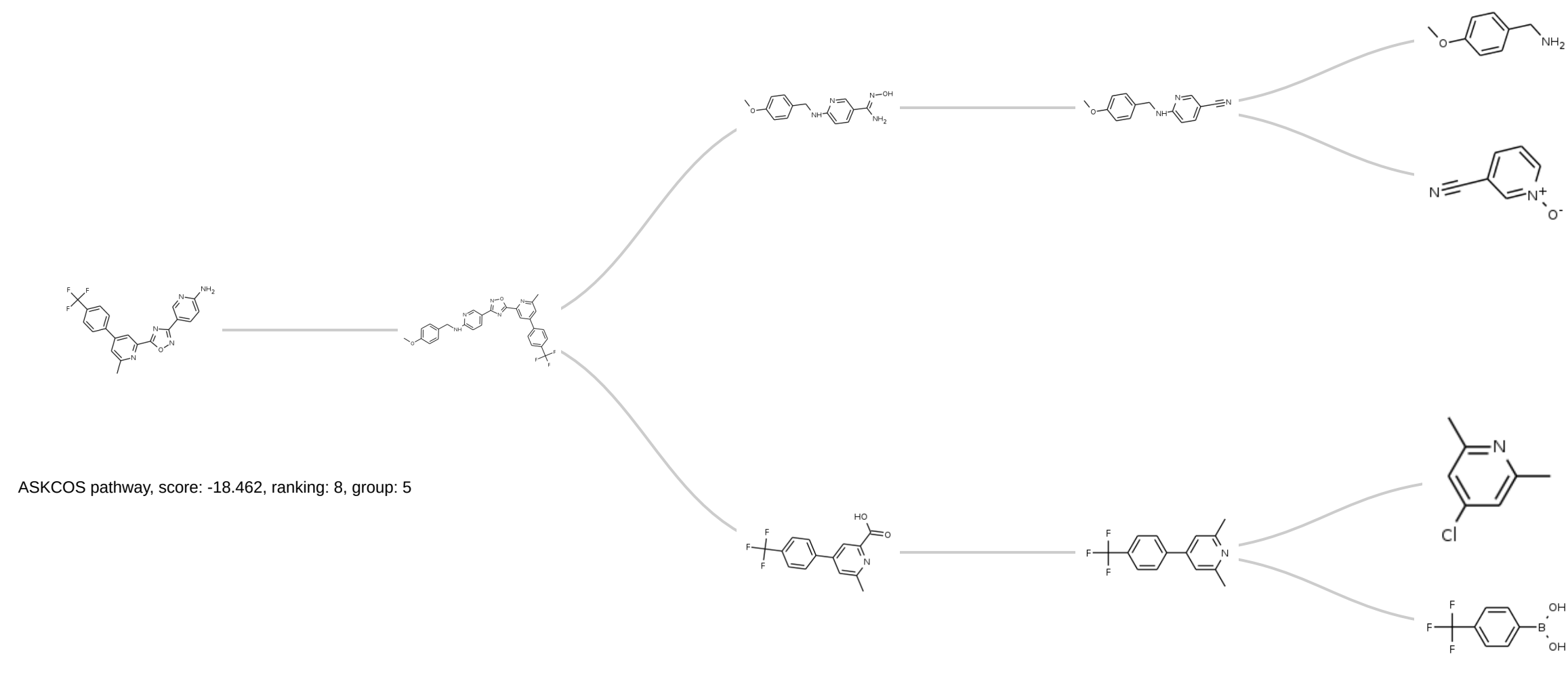
ASKCOS pathway score: -18.250, ranking: 4, group: 2



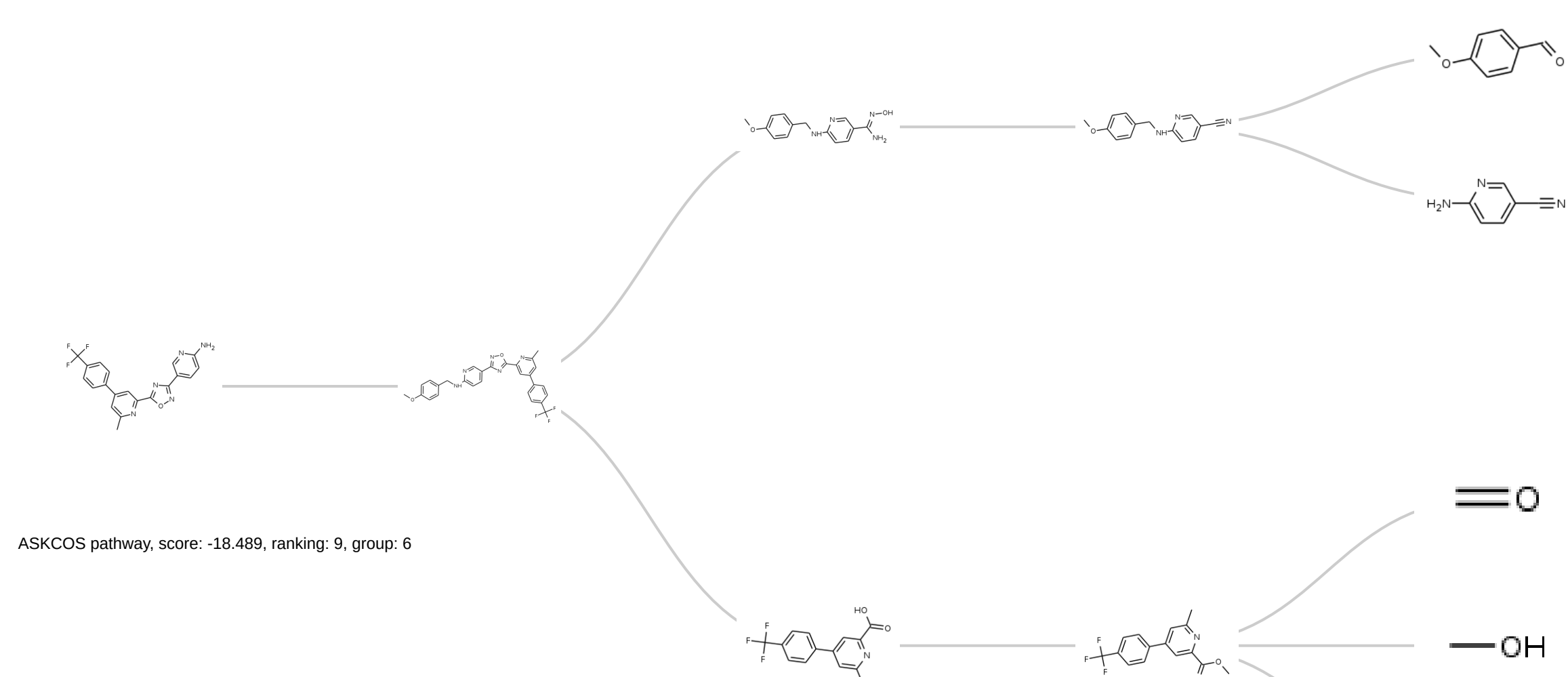
ASKCOS pathway score: -18.351, ranking: 6, group: 3



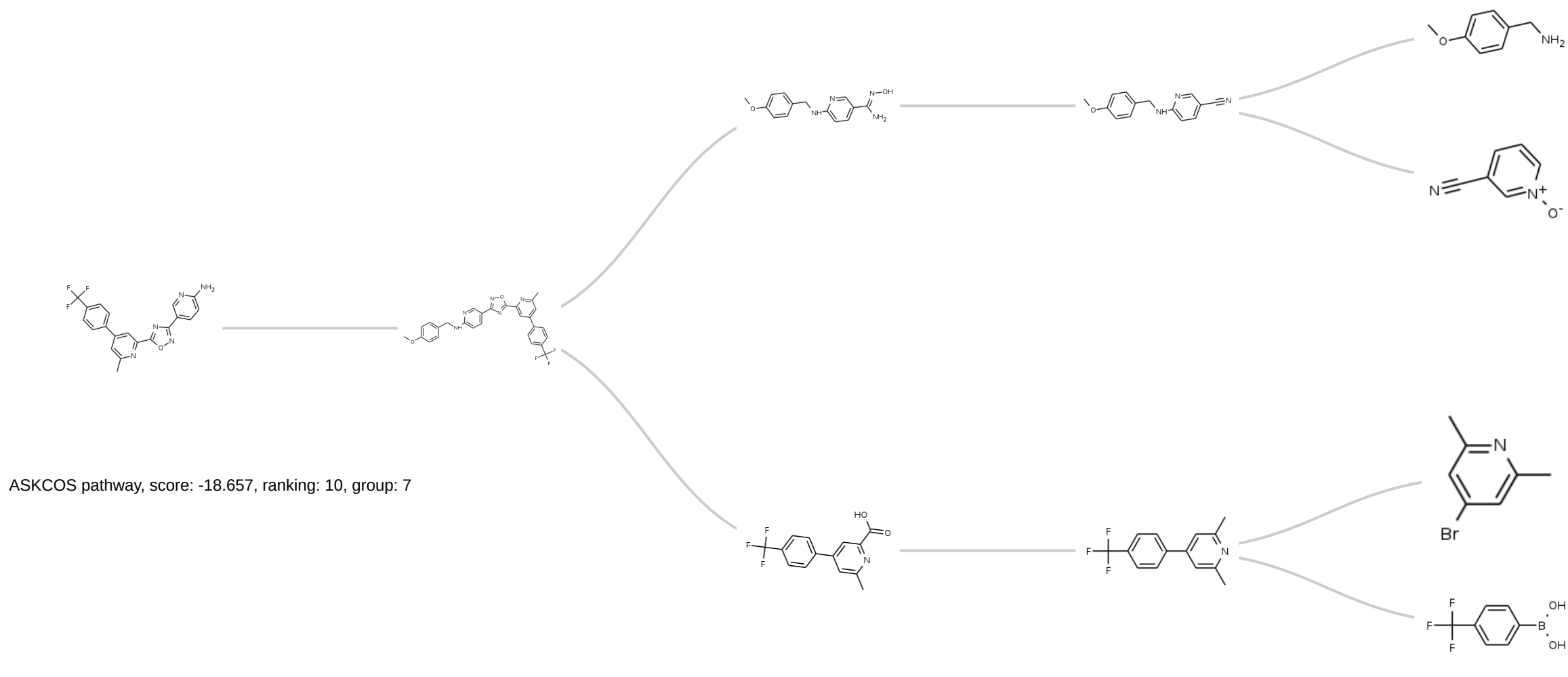
ASKCOS pathway score: -18.441, ranking: 7, group: 4



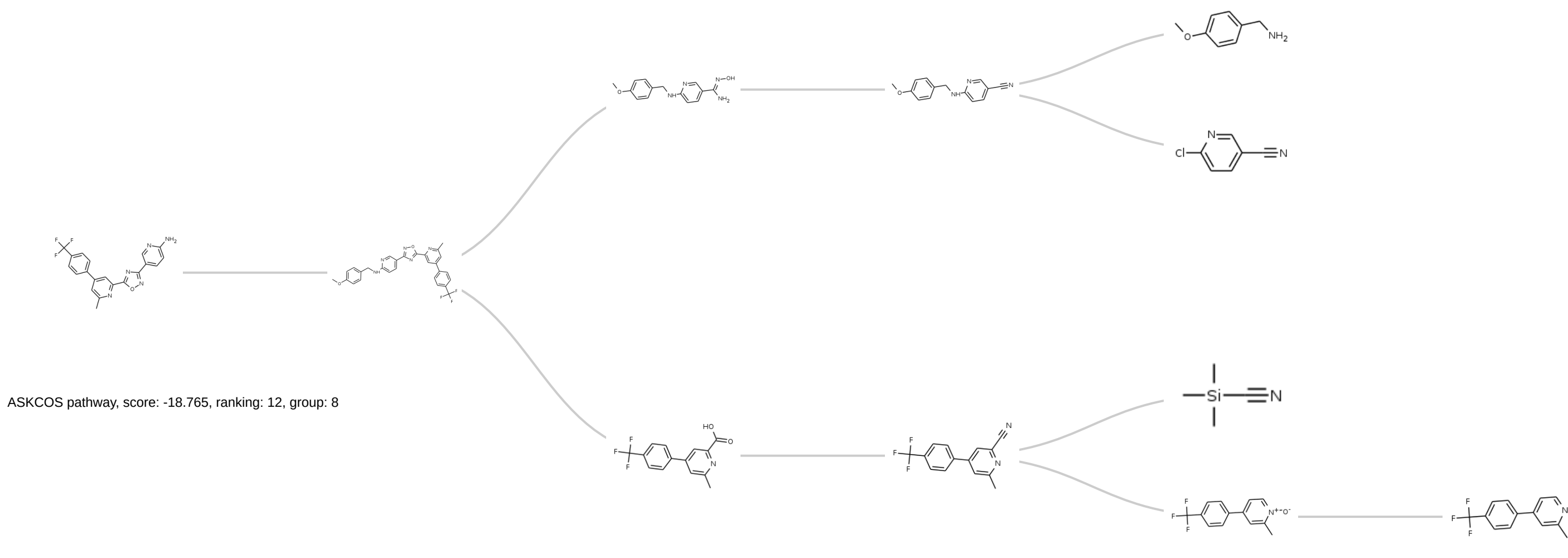
ASKCOS pathway score: -18.462, ranking: 8, group: 5



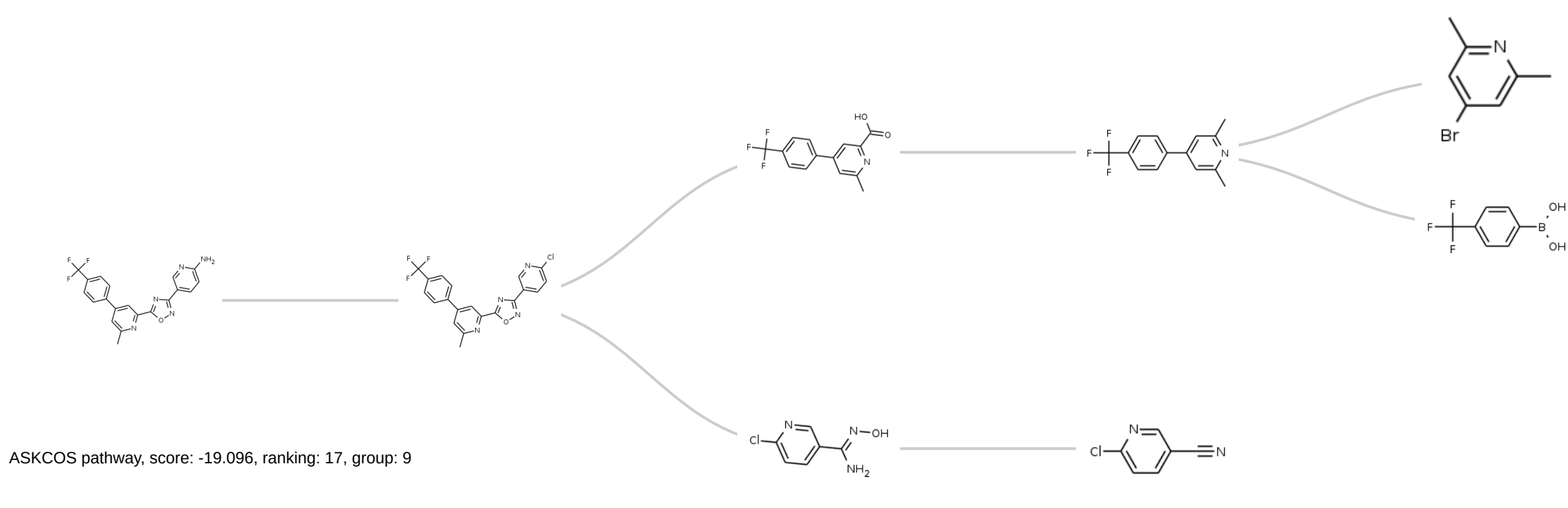
ASKCOS pathway score: -18.489, ranking: 9, group: 6



ASKCOS pathway score: -18.657, ranking: 10, group: 7

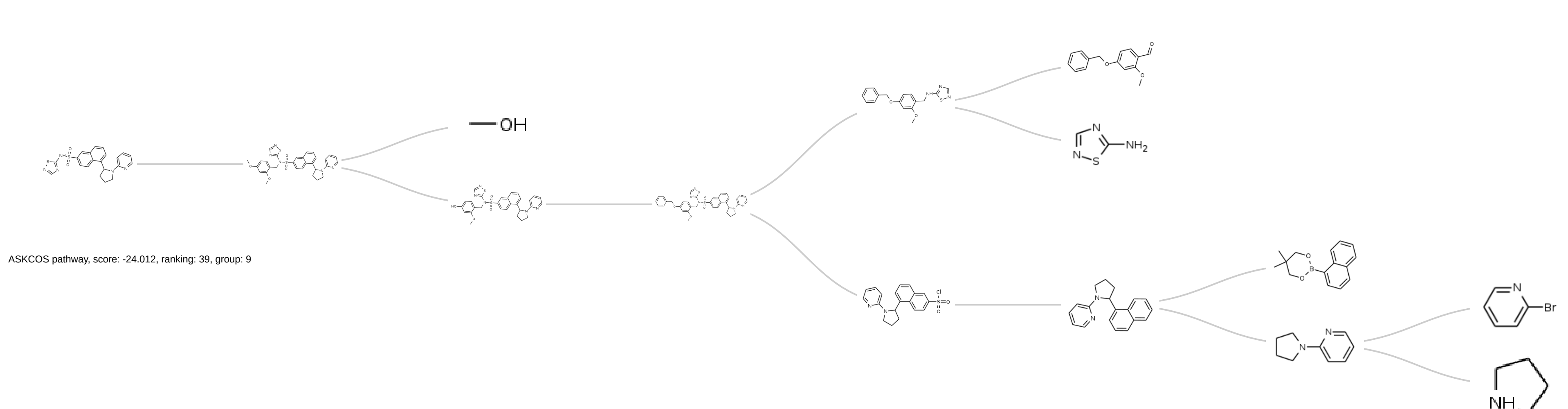
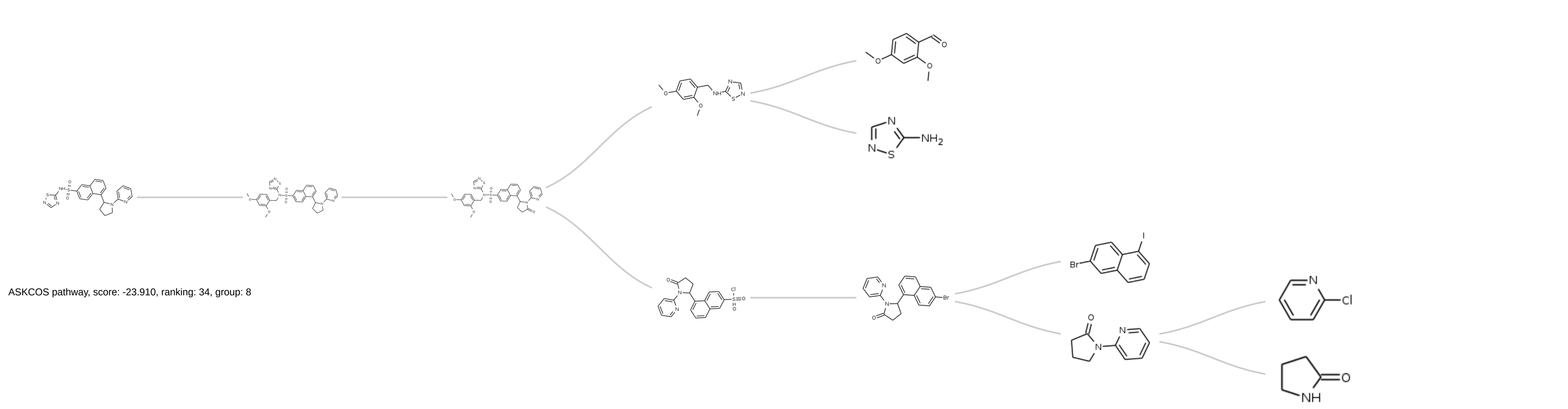
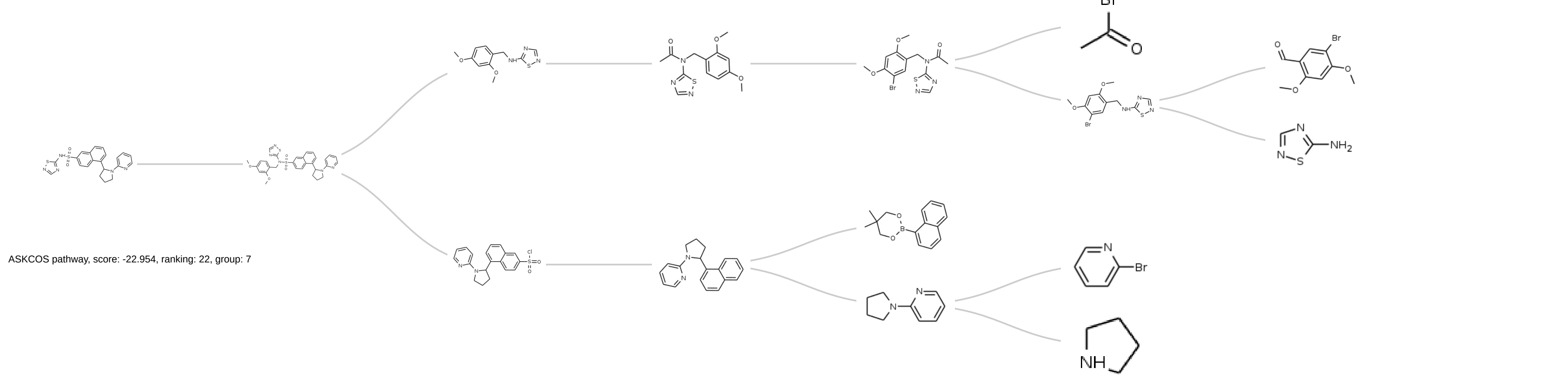
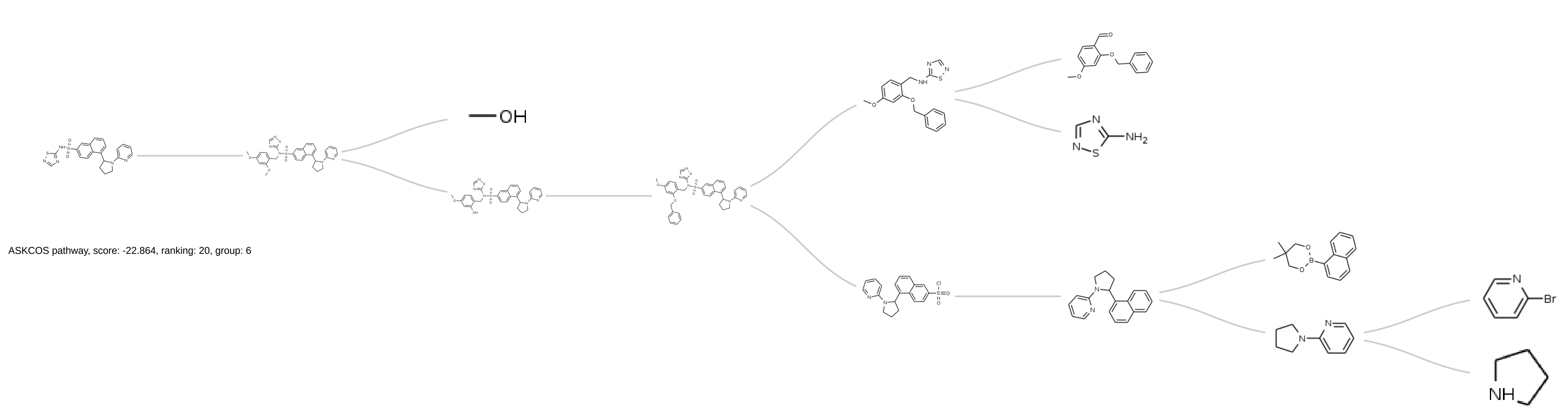
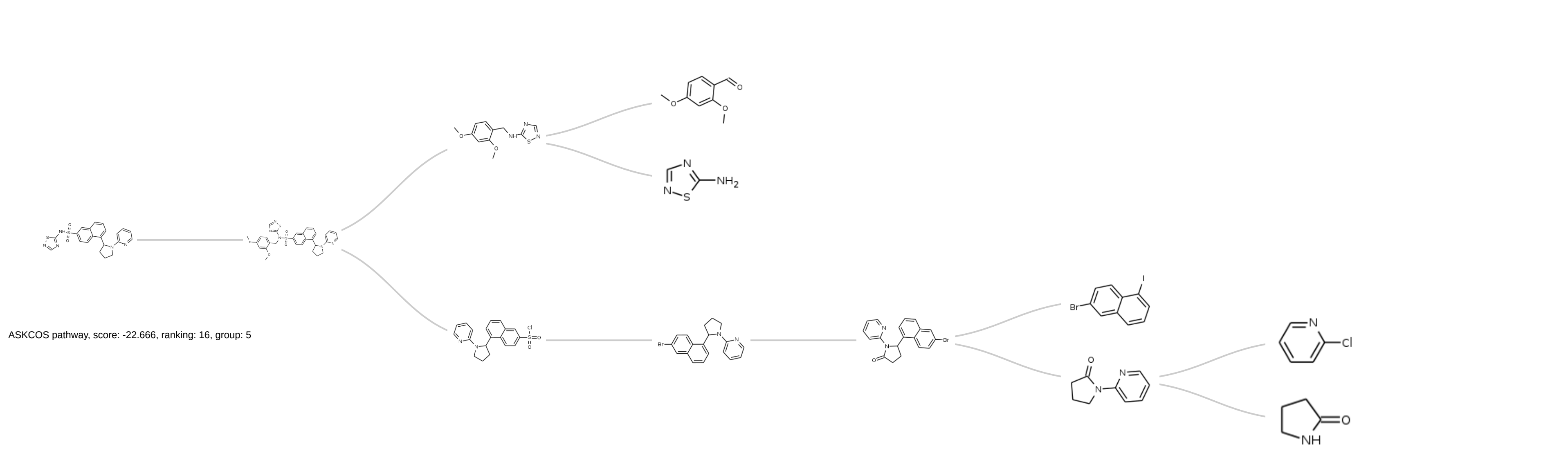
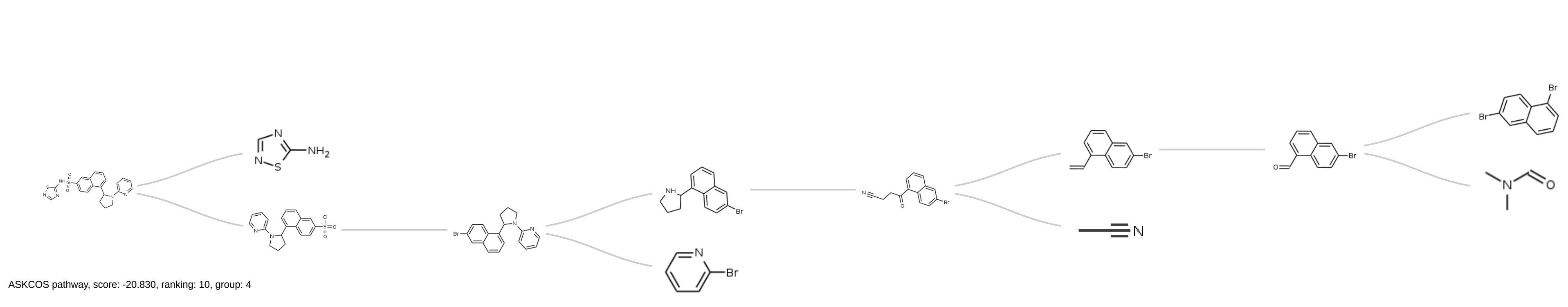
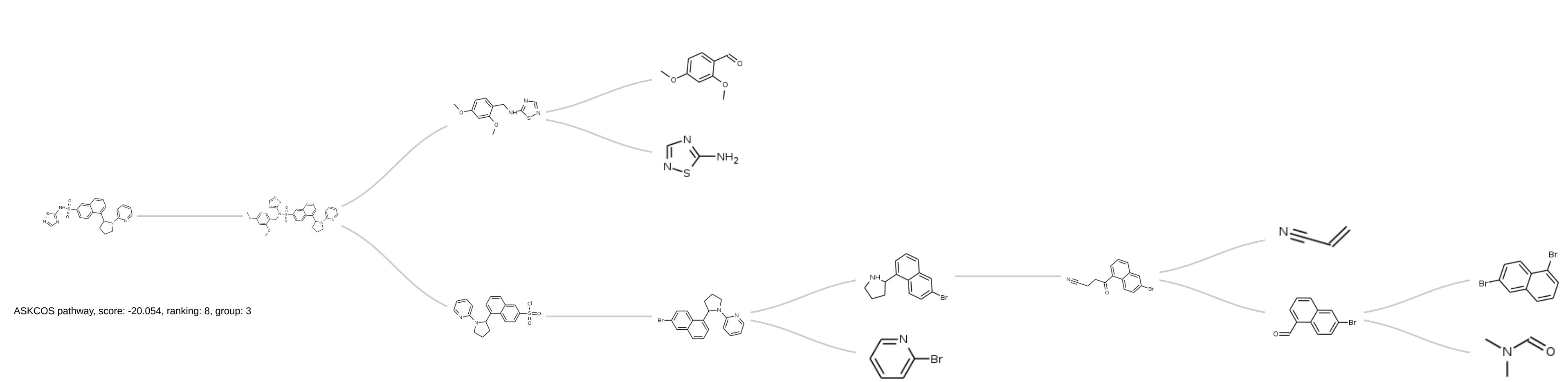
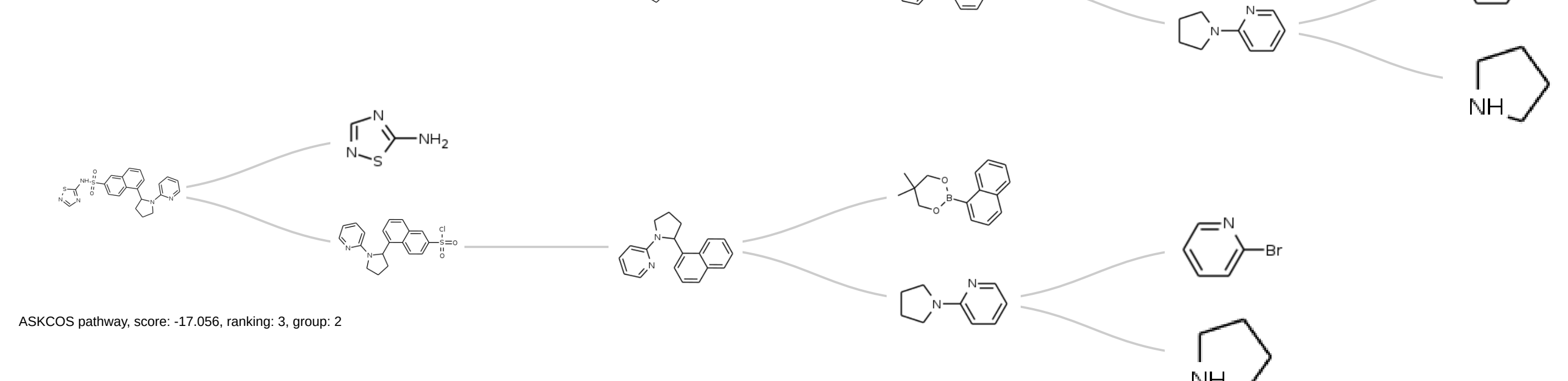
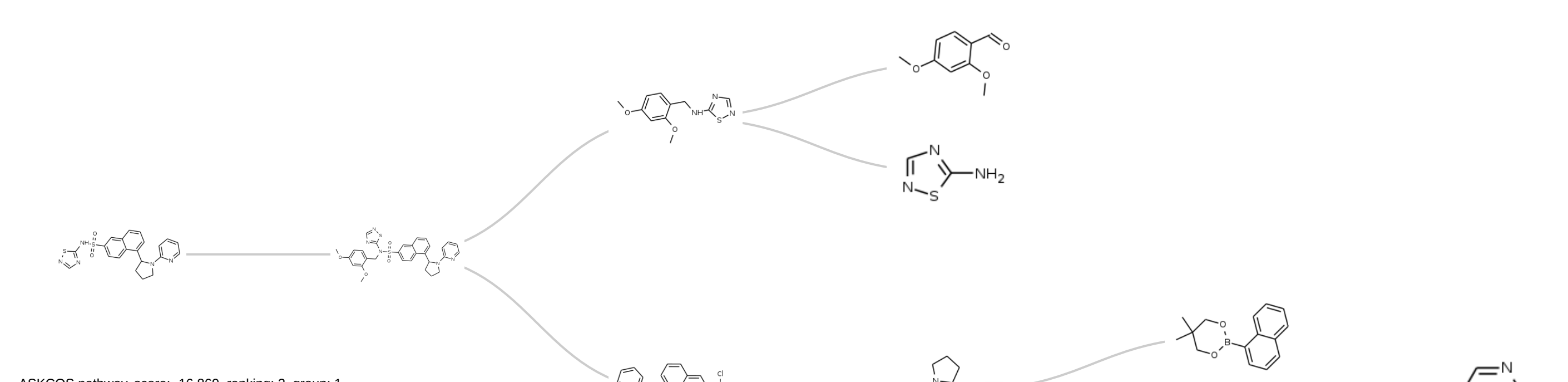
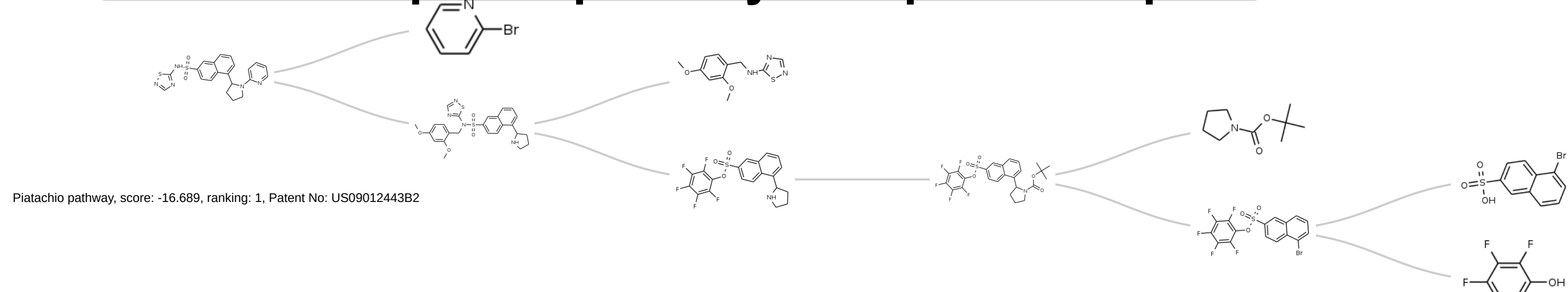


ASKCOS pathway score: -18.765, ranking: 12, group: 8

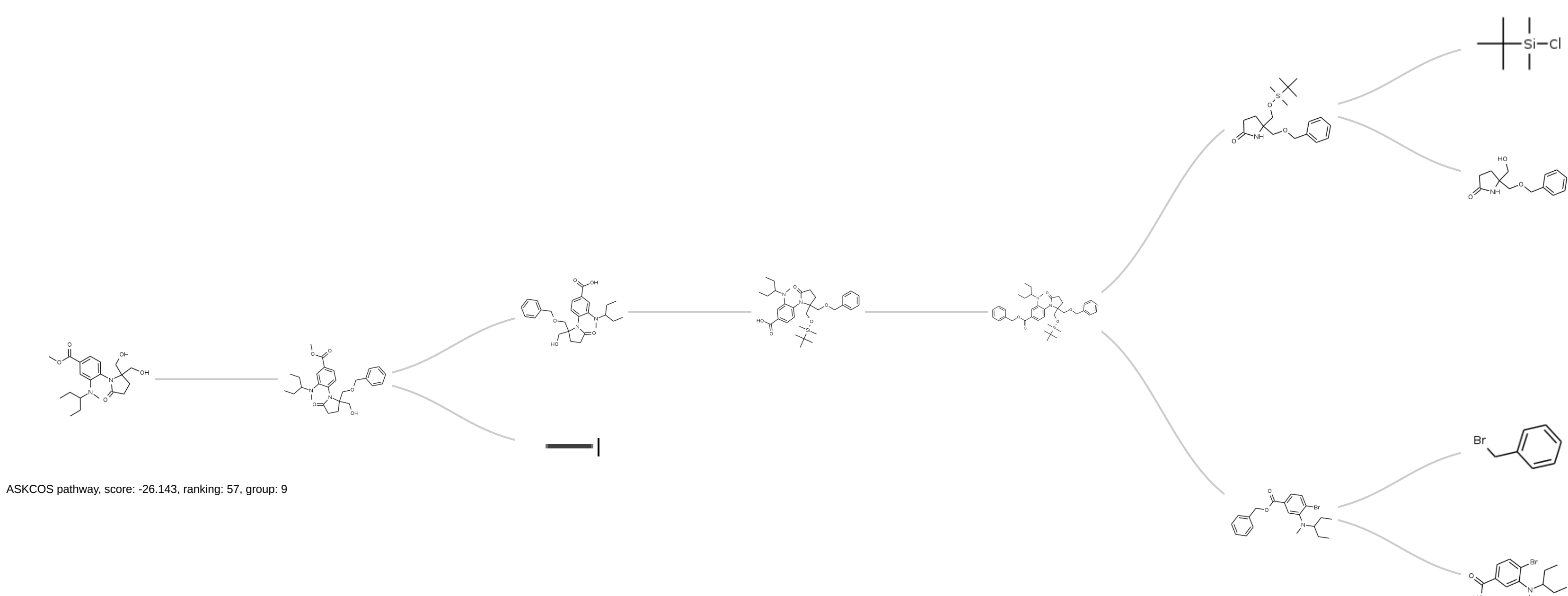
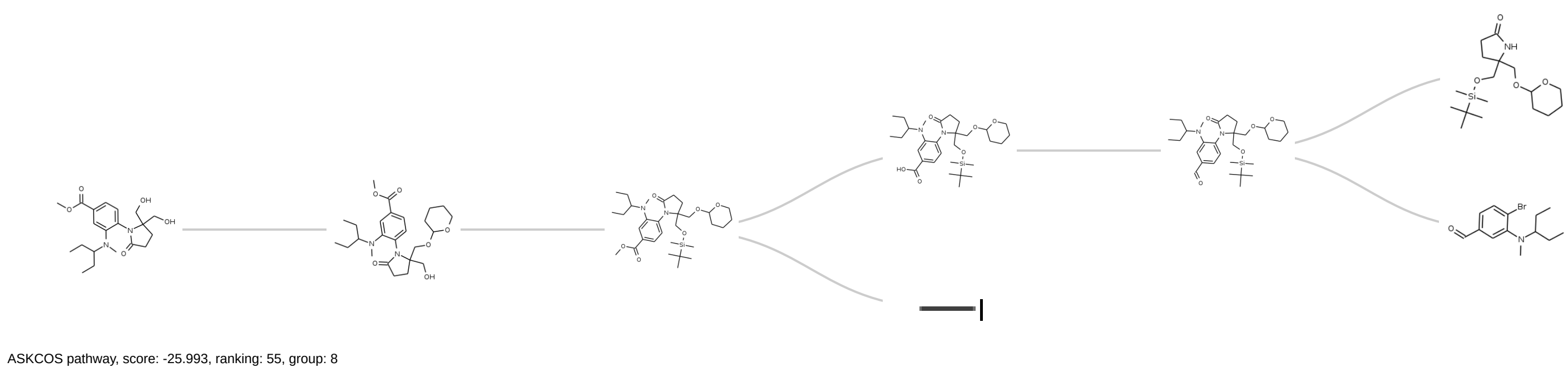
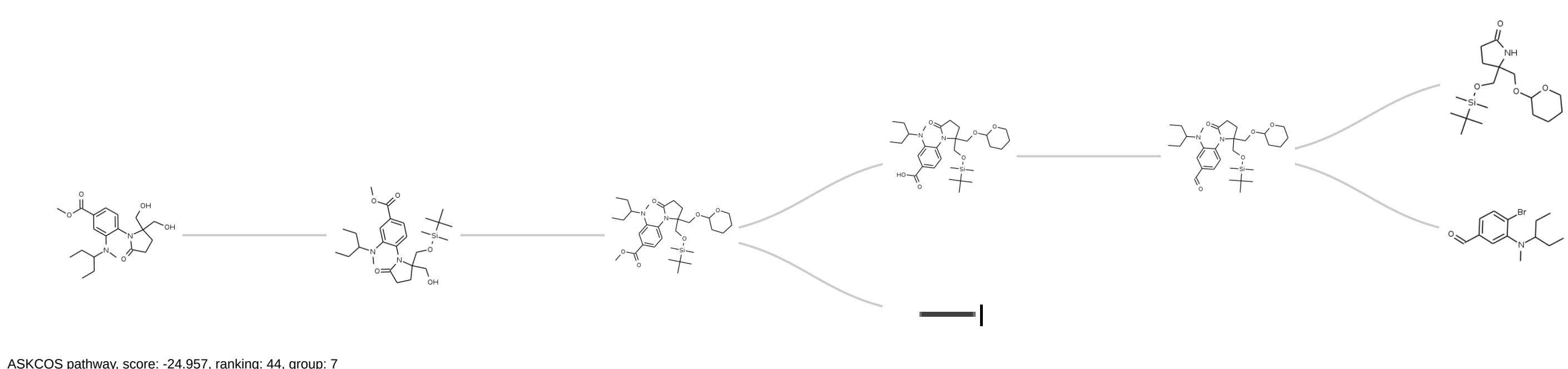
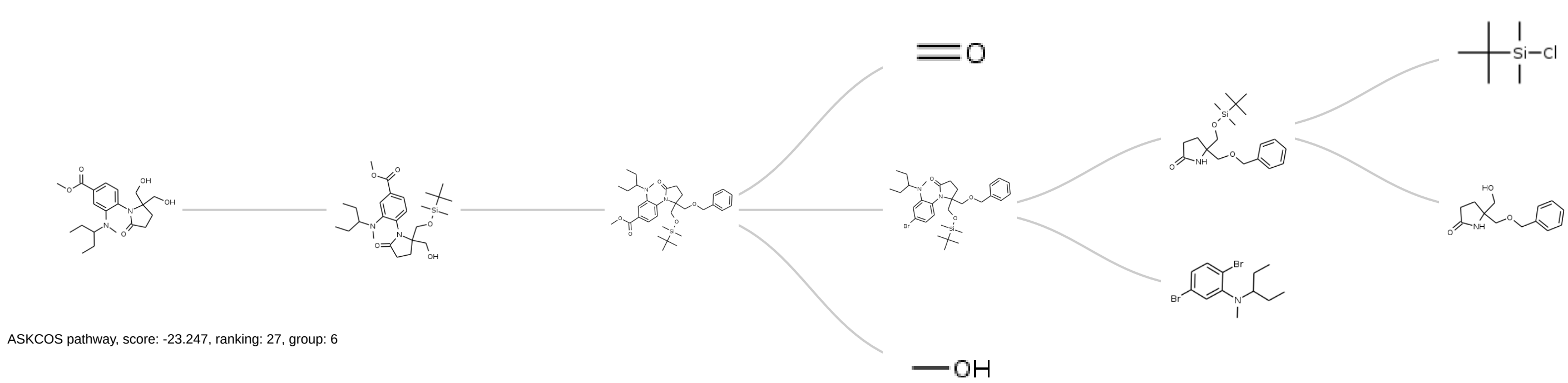
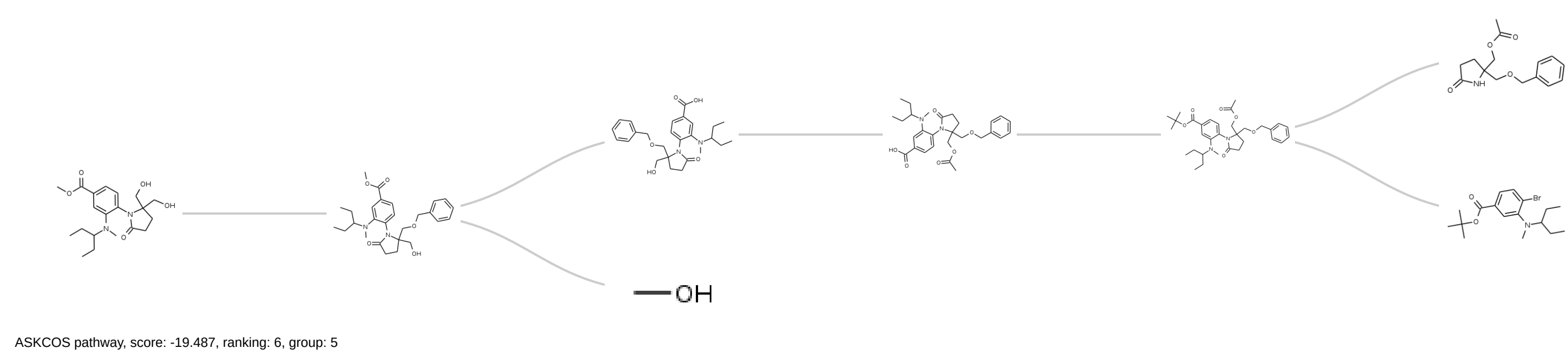
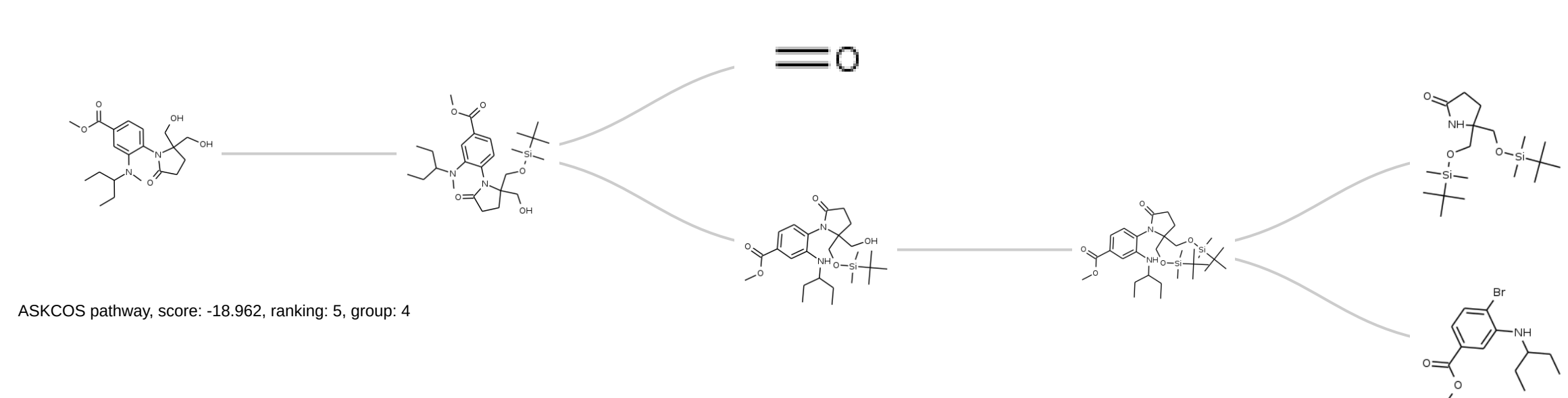
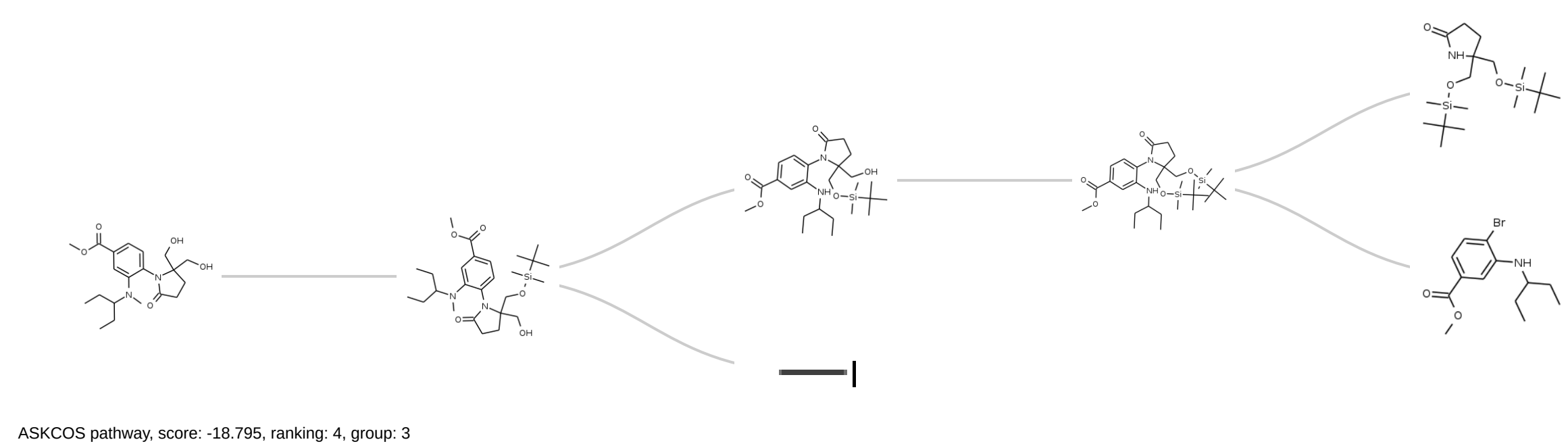
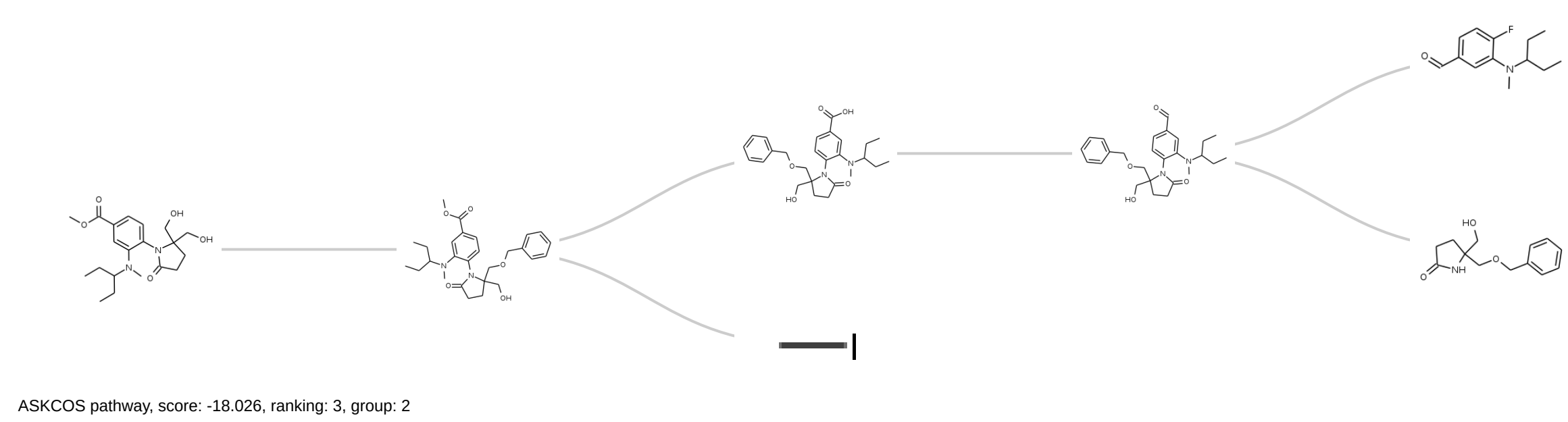
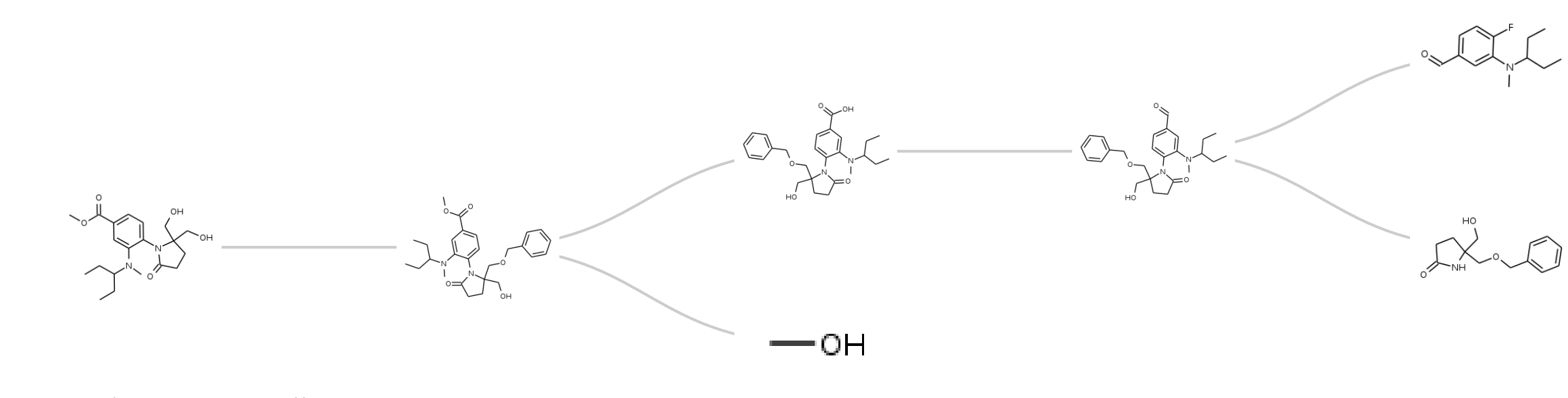
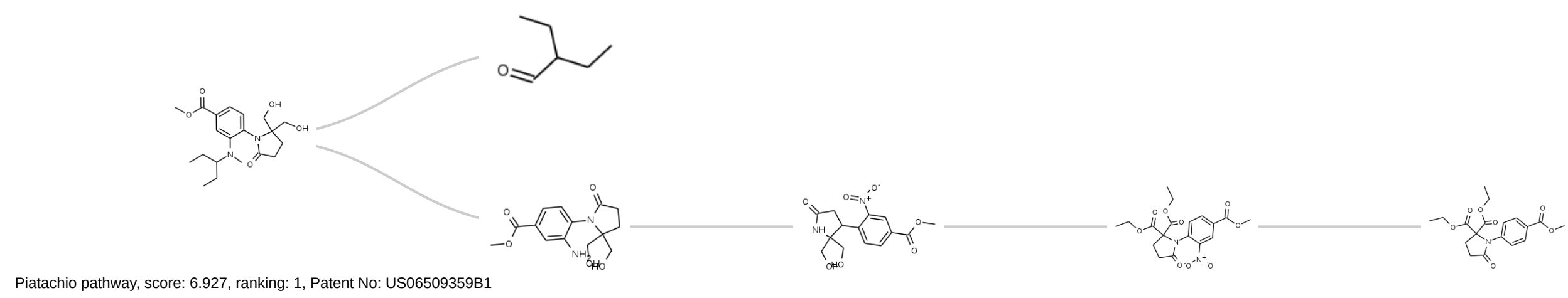


ASKCOS pathway score: -19.095, ranking: 17, group: 9

### Model ranks patent pathway as top-1: Example 3

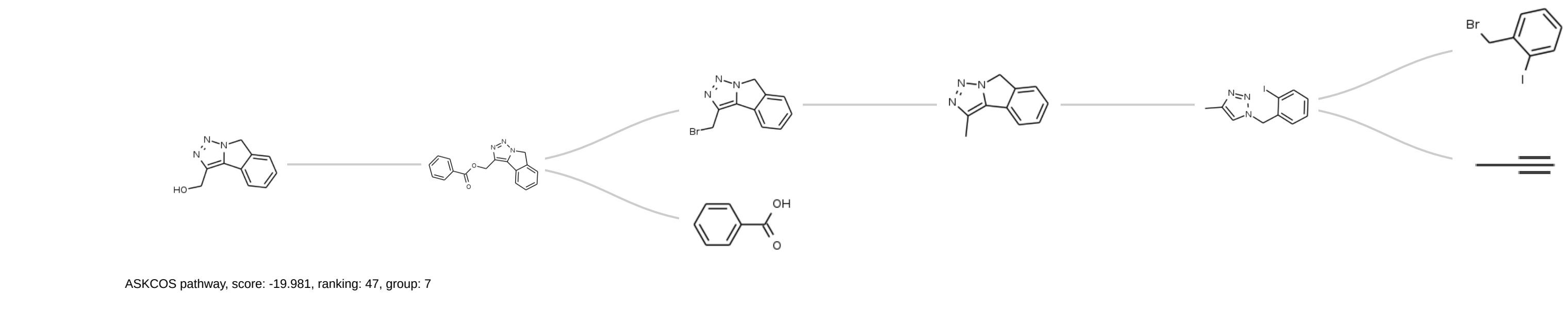
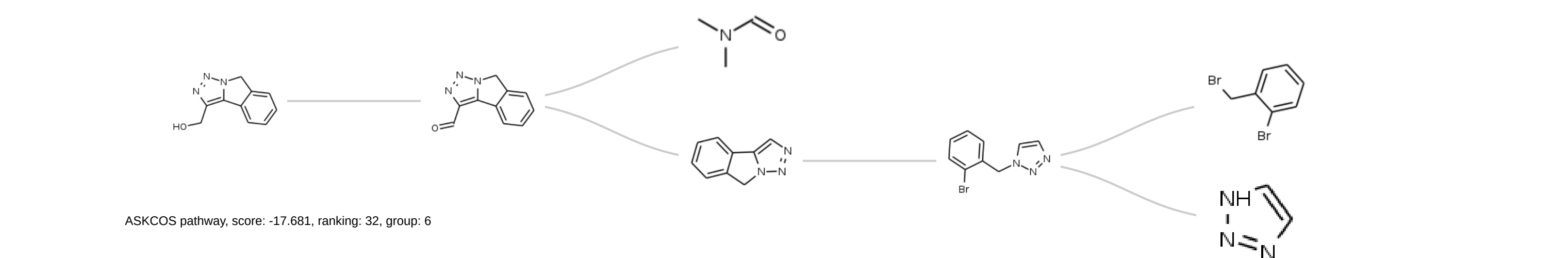
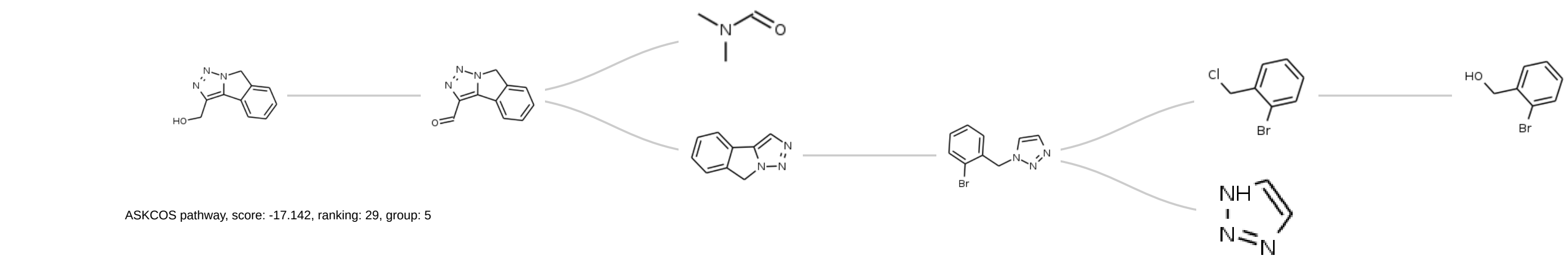
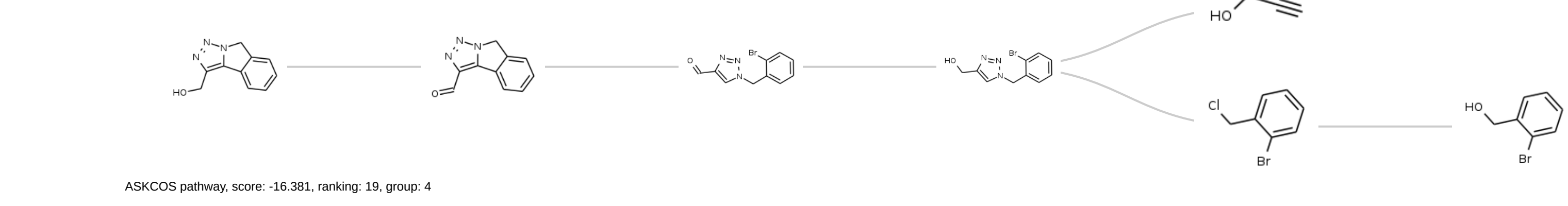
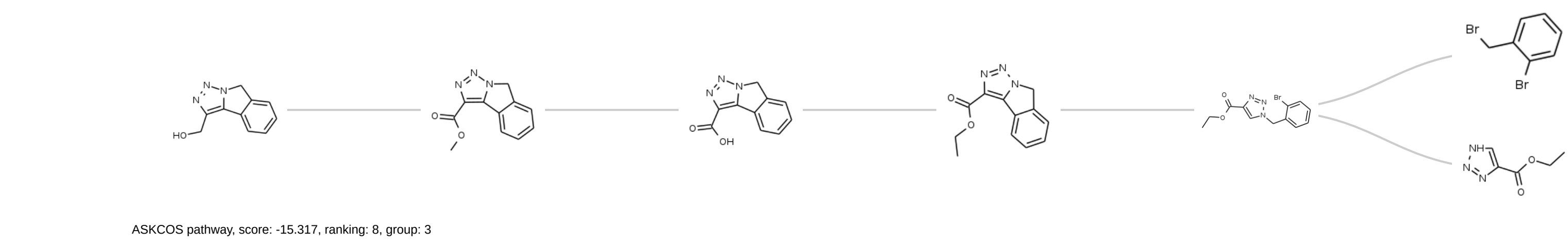
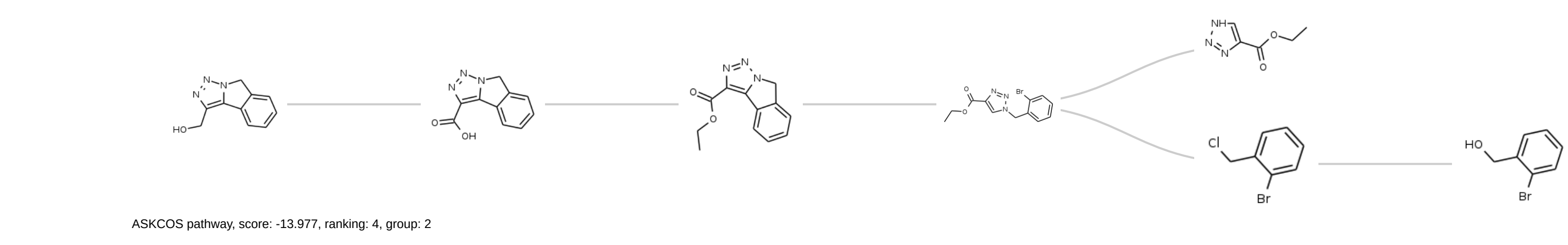
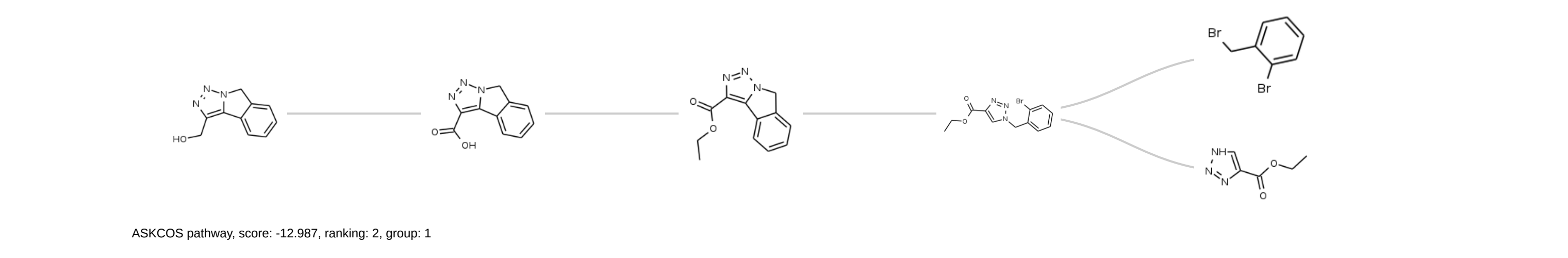
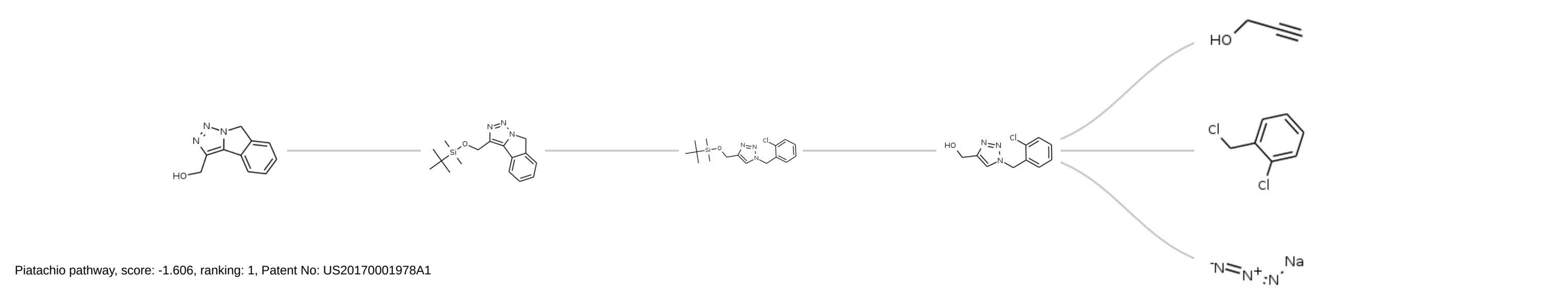


# Model ranks patent pathway as top-1: Example 4

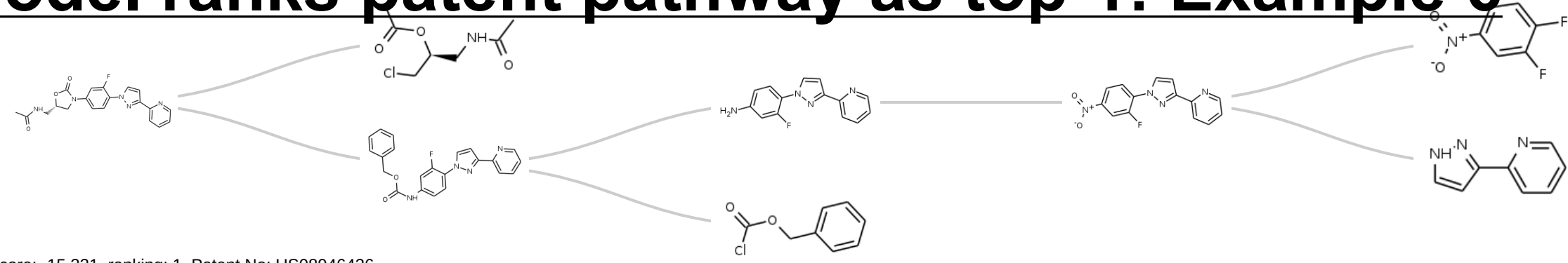




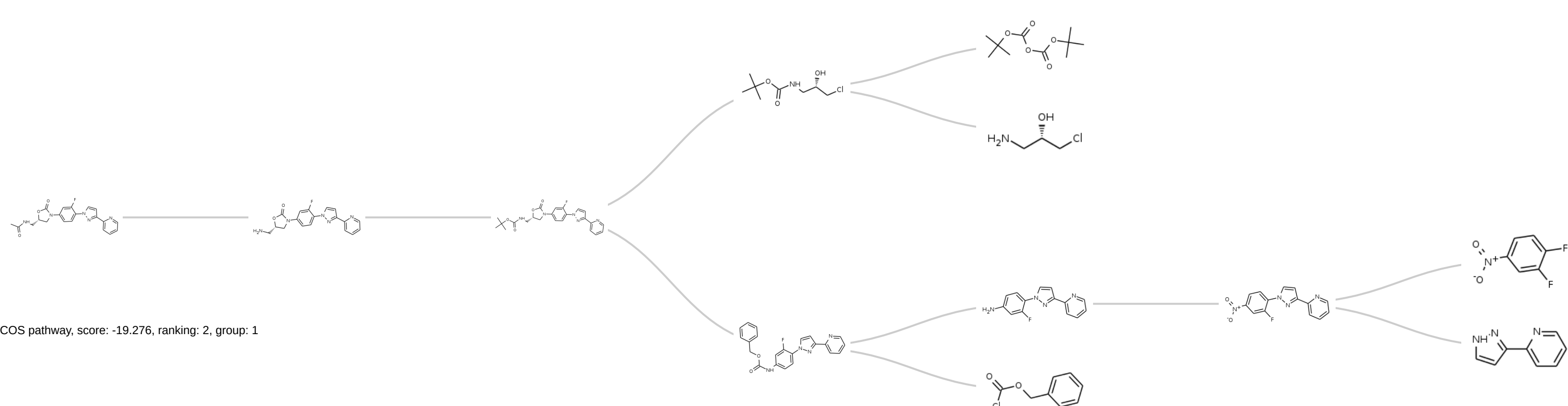
# Model ranks patent pathway as top-1: Example 5



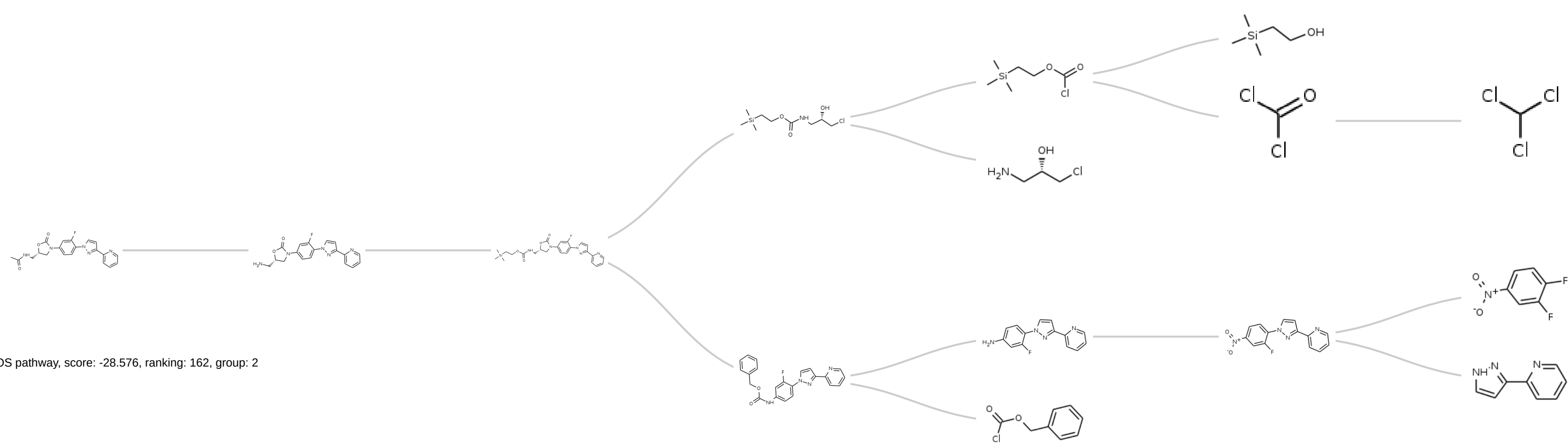
# Model ranks patent pathway as top-1: Example 6



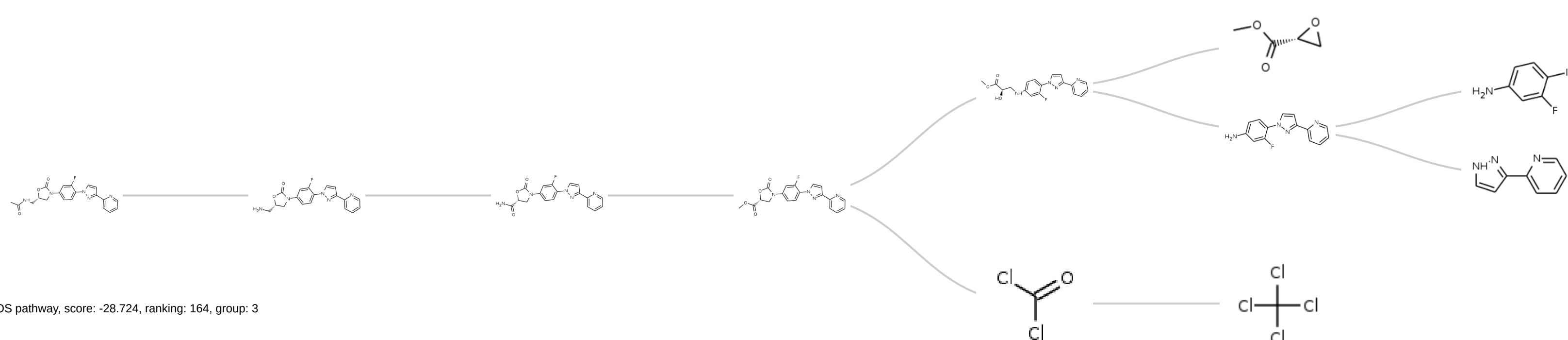
Patent pathway, score: -15.531, ranking: 1, Patent no: US0984636



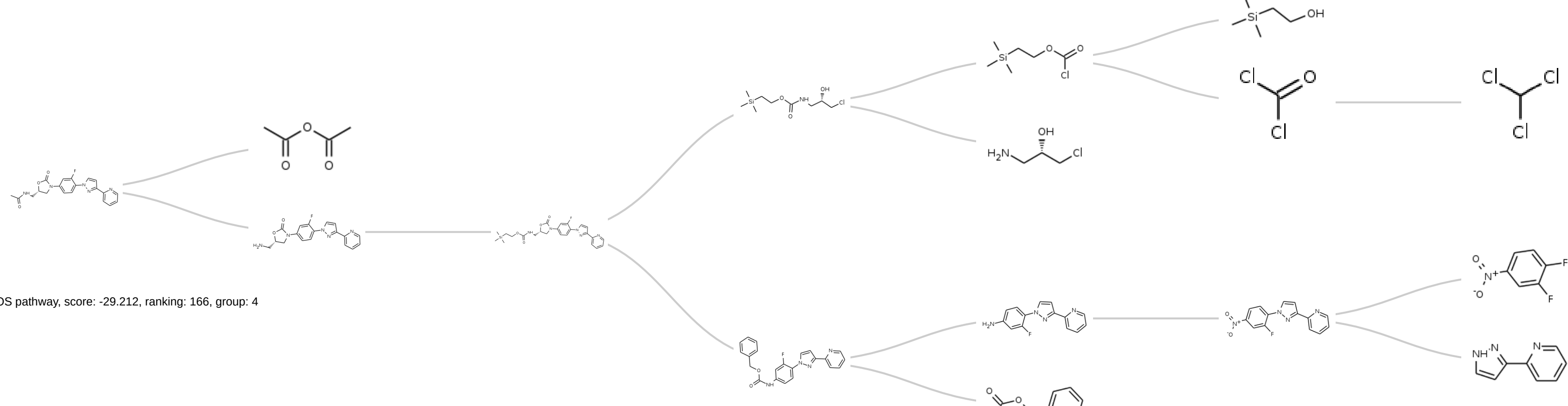
ASKCOS pathway, score: -19.276, ranking: 2, group: 1



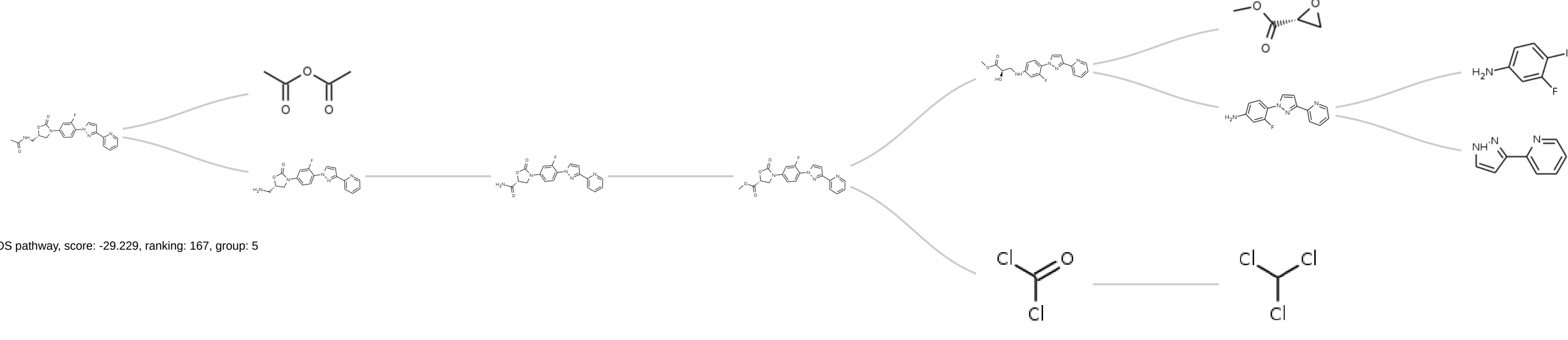
ASKCOS pathway, score: -28.576, ranking: 162, group: 2



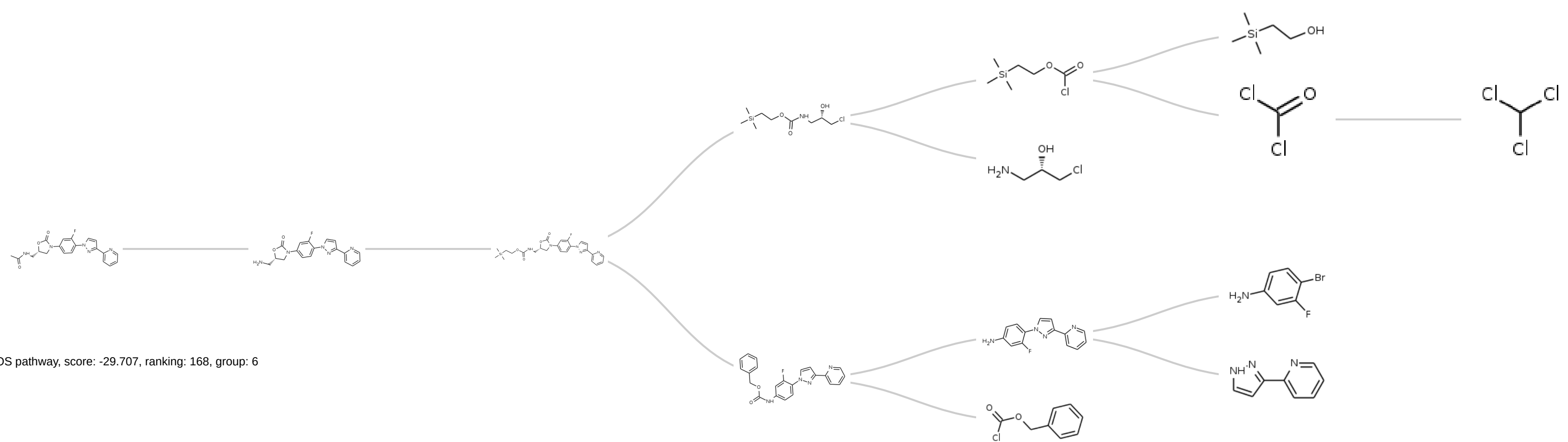
ASKCOS pathway, score: -28.724, ranking: 164, group: 3



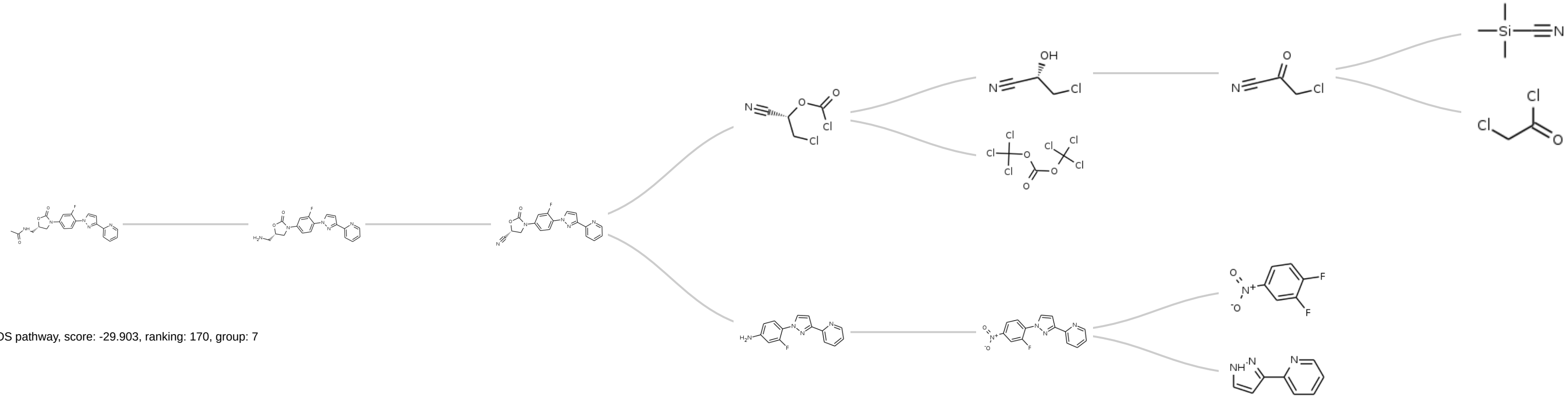
ASKCOS pathway, score: -29.212, ranking: 166, group: 4



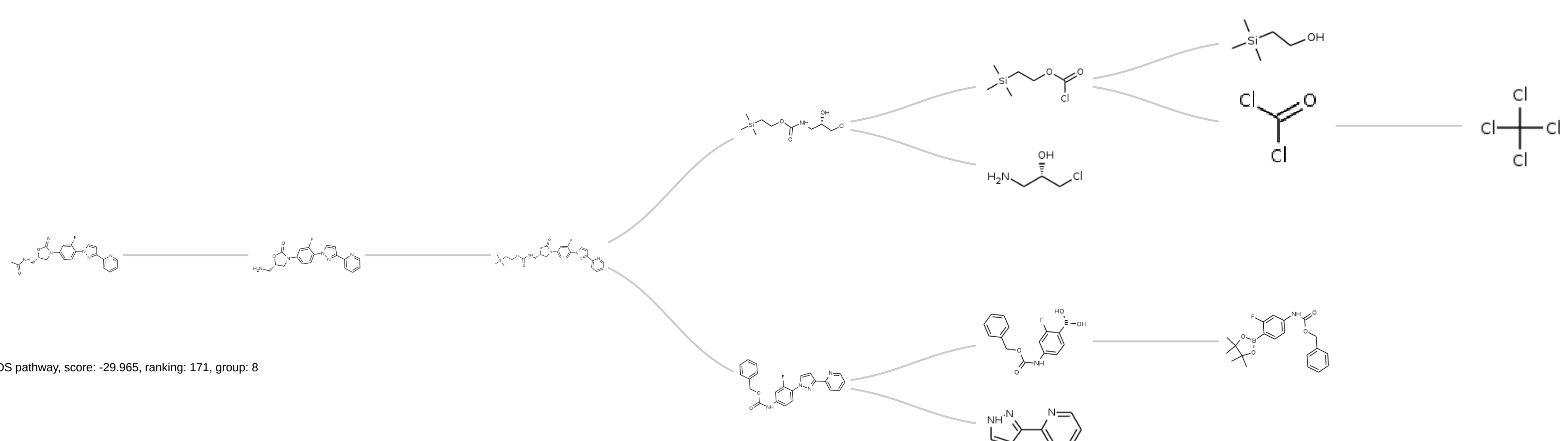
ASKCOS pathway, score: -29.229, ranking: 167, group: 5



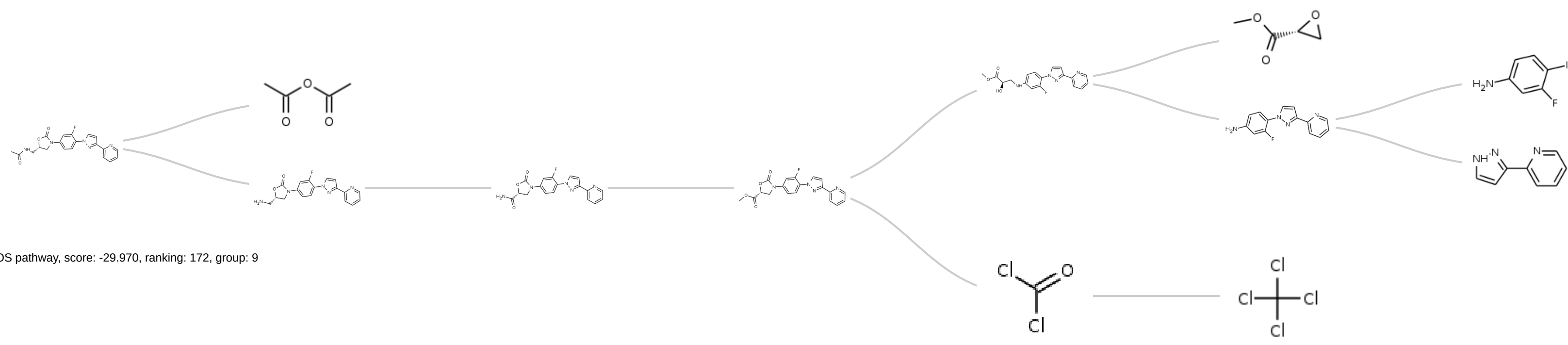
ASKCOS pathway, score: -29.707, ranking: 168, group: 6



ASKCOS pathway, score: -29.953, ranking: 170, group: 7

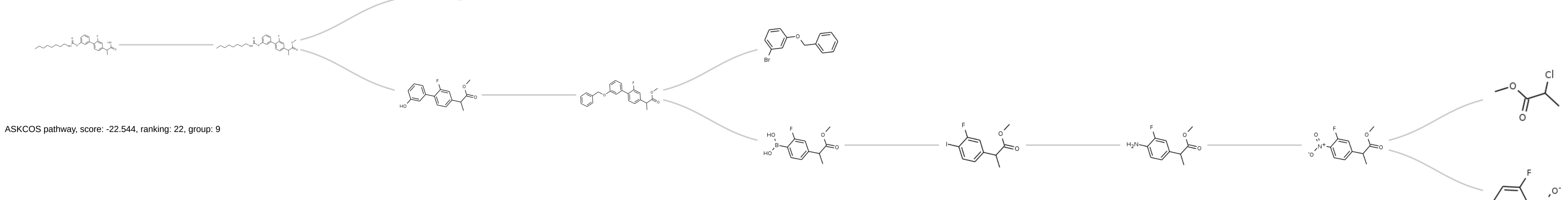
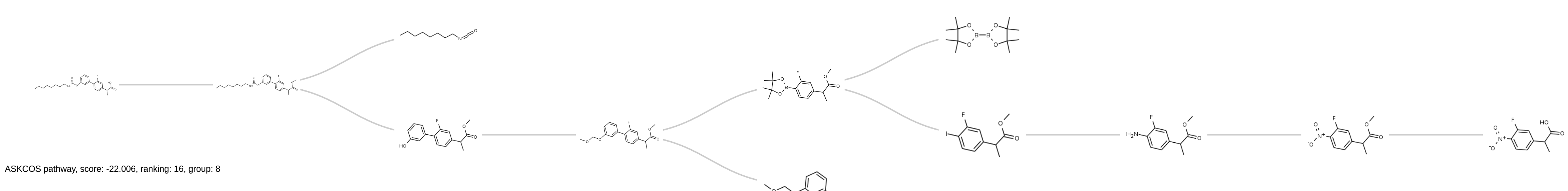
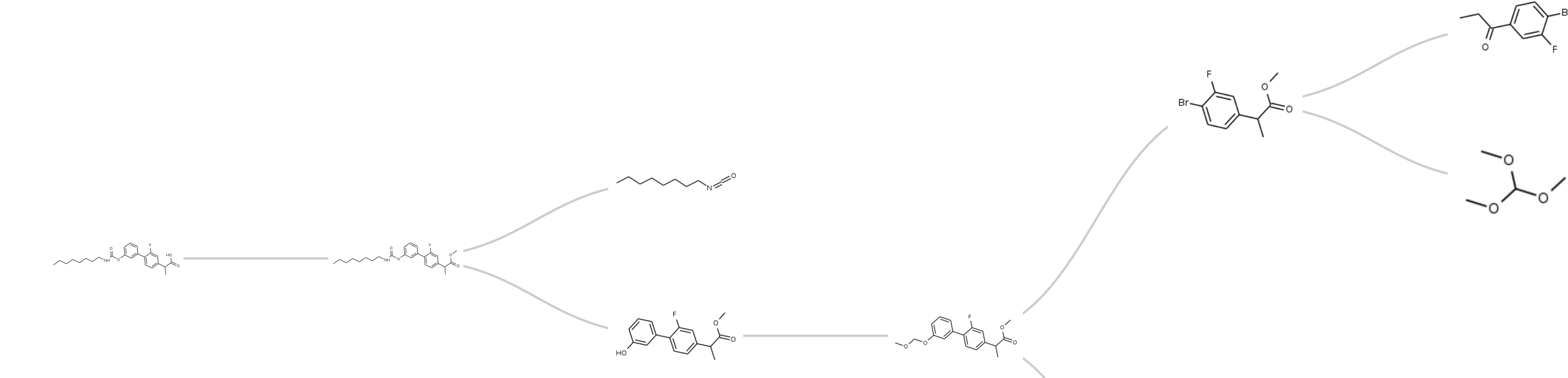
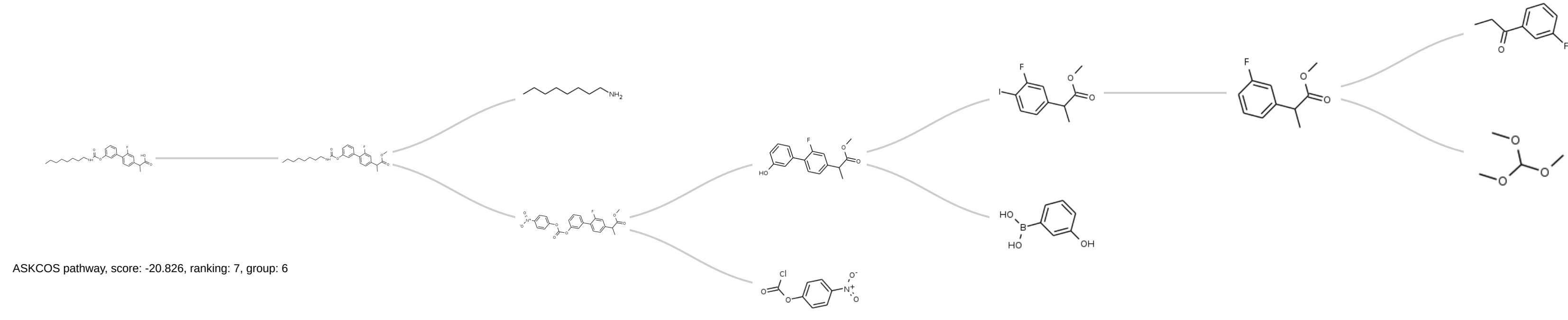
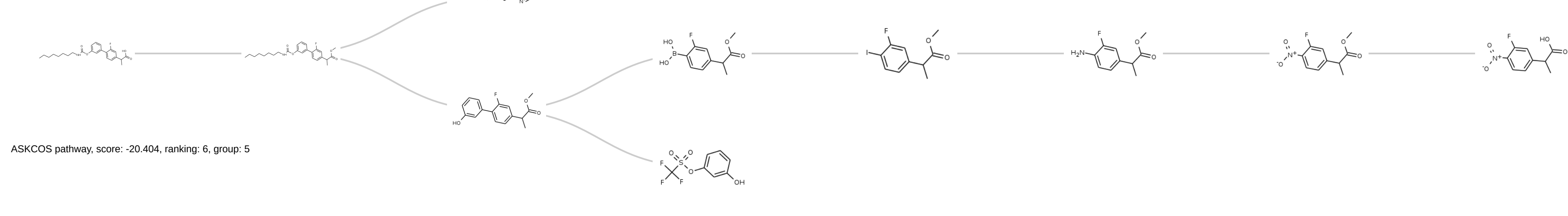
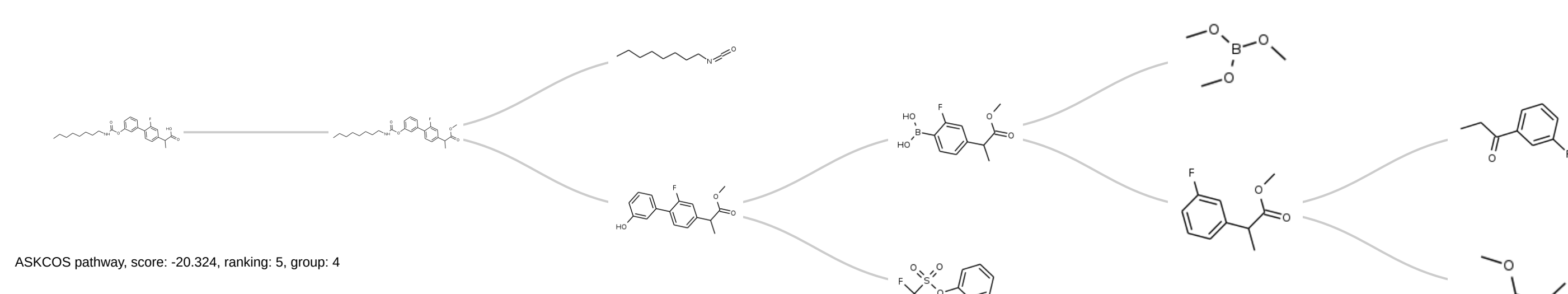
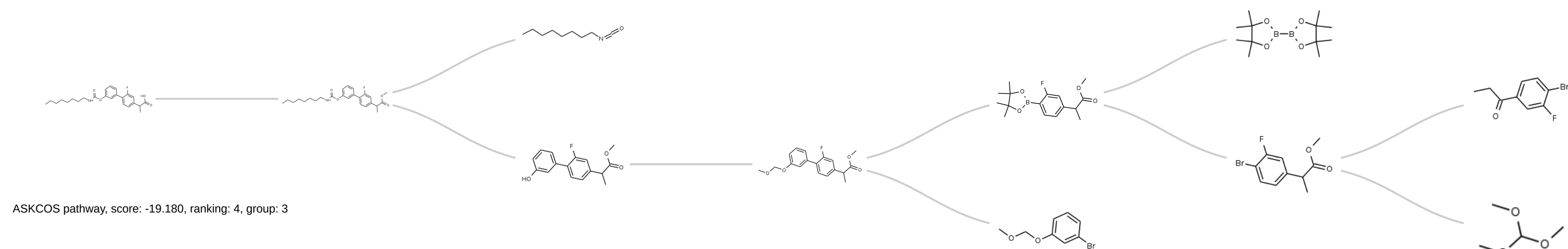
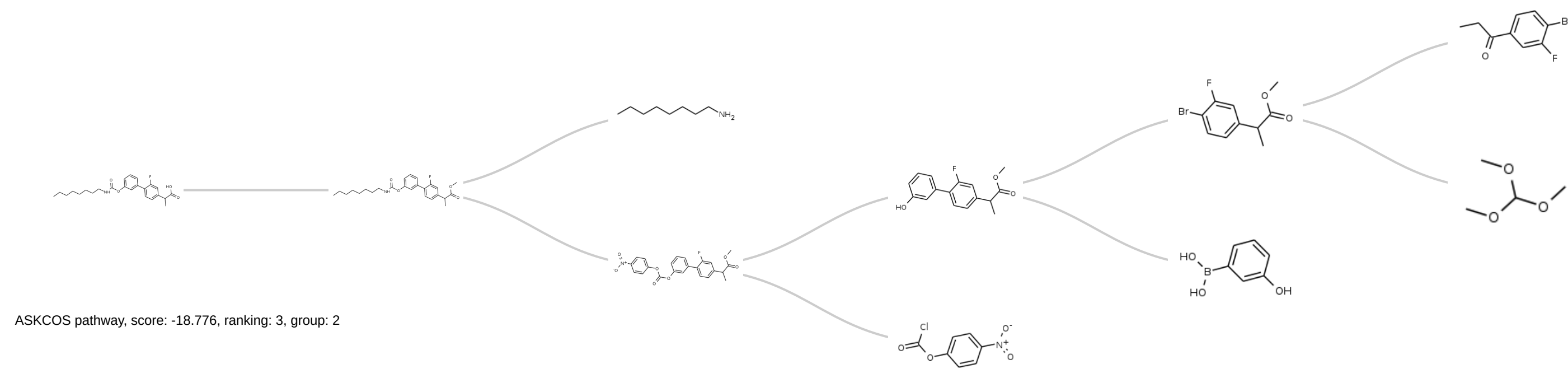
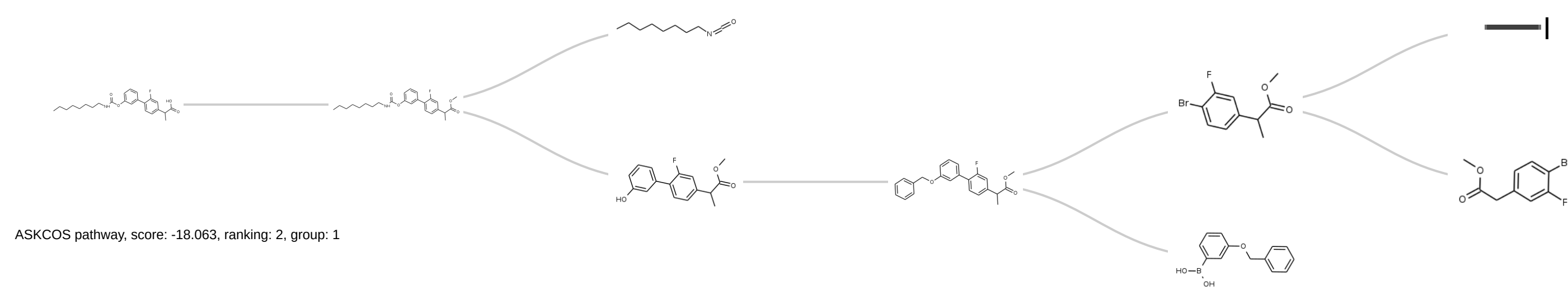
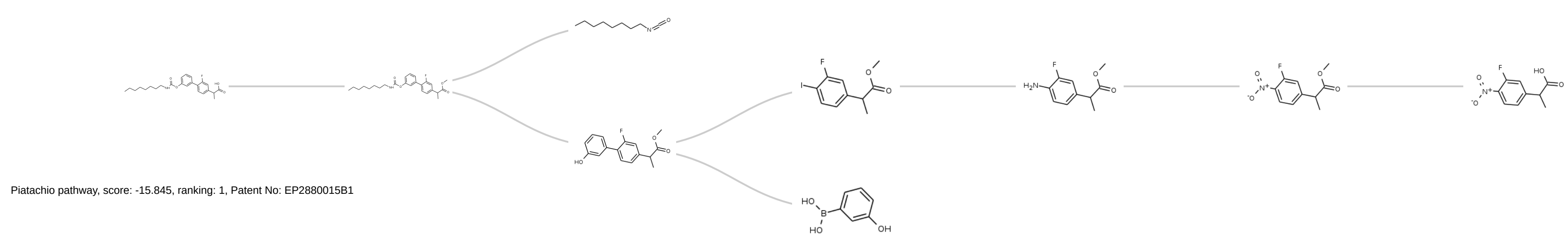


ASKCOS pathway, score: -29.965, ranking: 171, group: 8



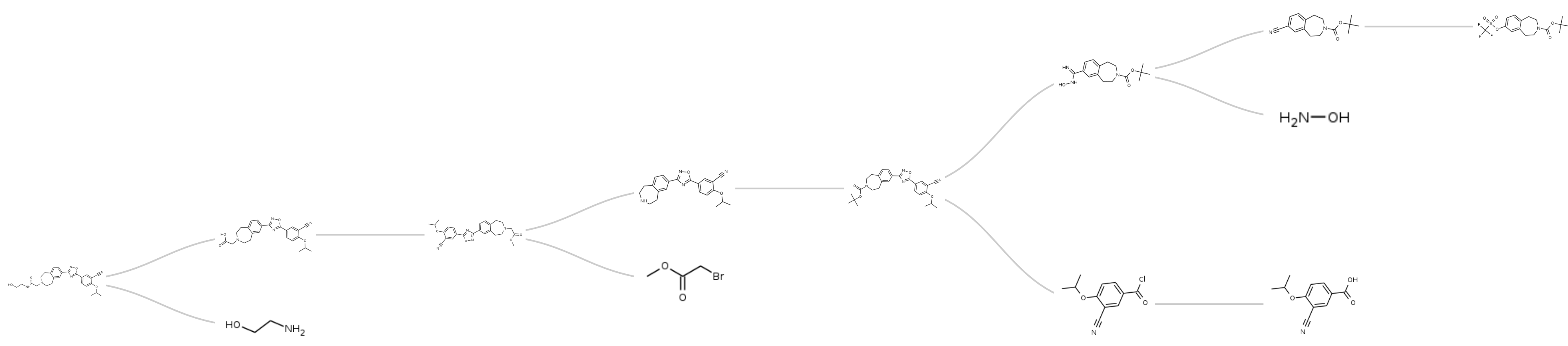
ASKCOS pathway, score: -29.970, ranking: 172, group: 9

# Model ranks patent pathway as top-1: Example 7

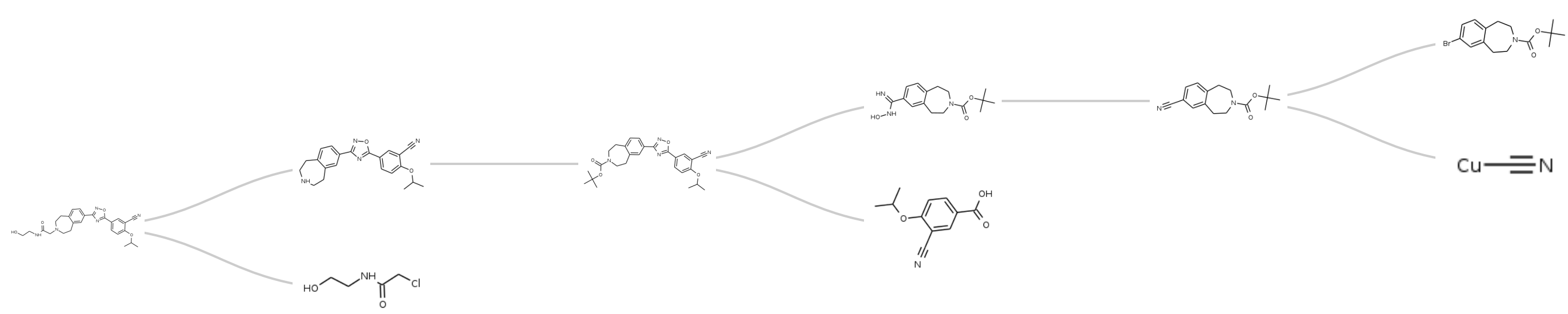




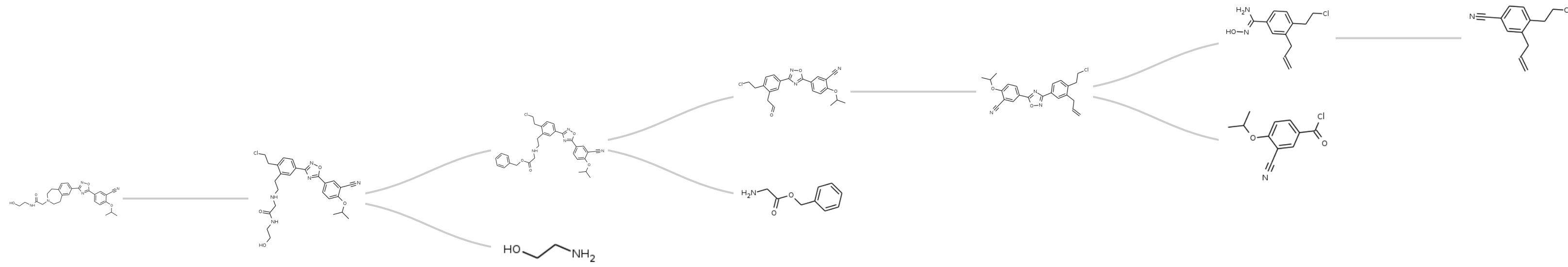
# Model ranks patent pathway as top-1: Example 9



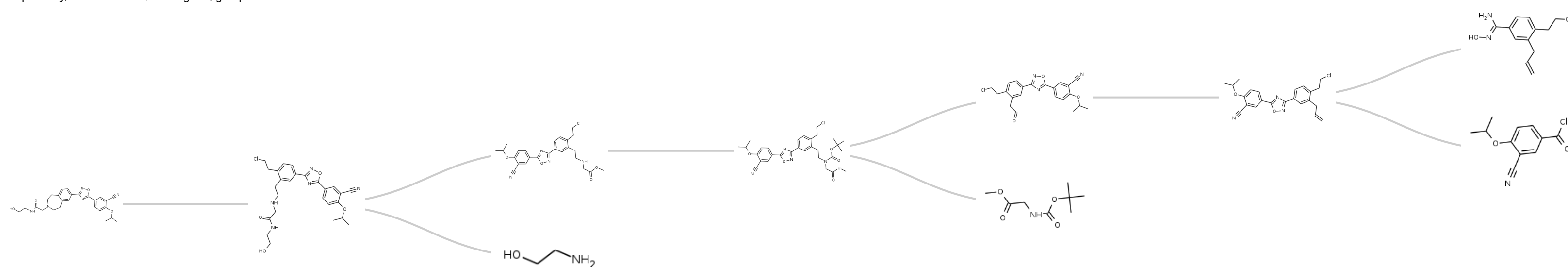
Patatcho pathway, score: -6.187, ranking: 1, Patent No: US2012015108A1



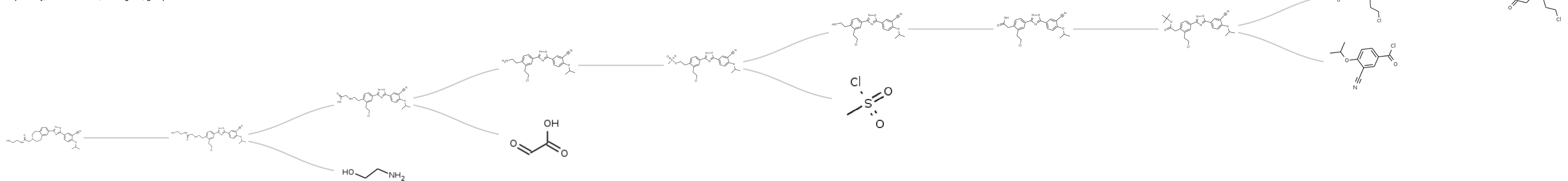
ASKCOS pathway, score: -11.898, ranking: 2, group: 1



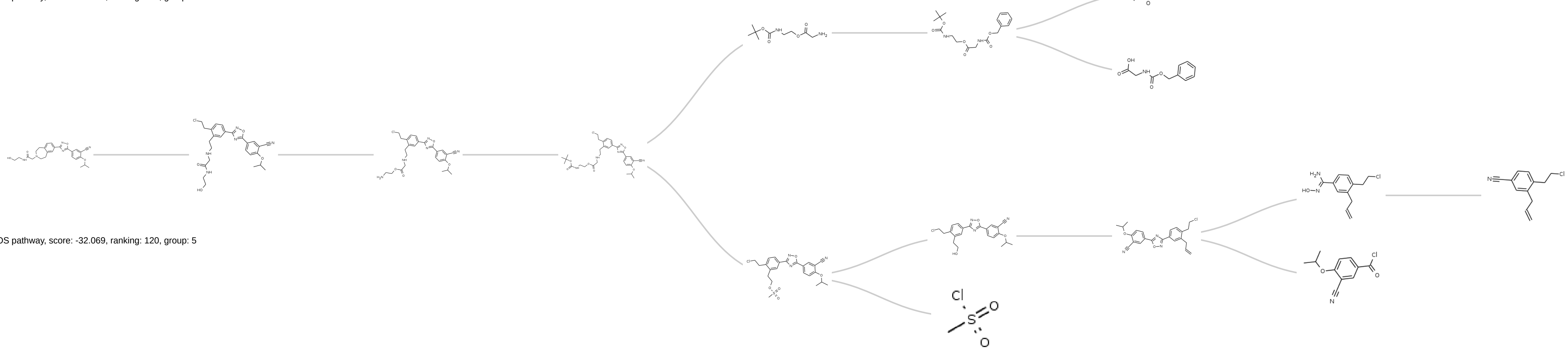
ASKCOS pathway, score: -25.233, ranking: 45, group: 2



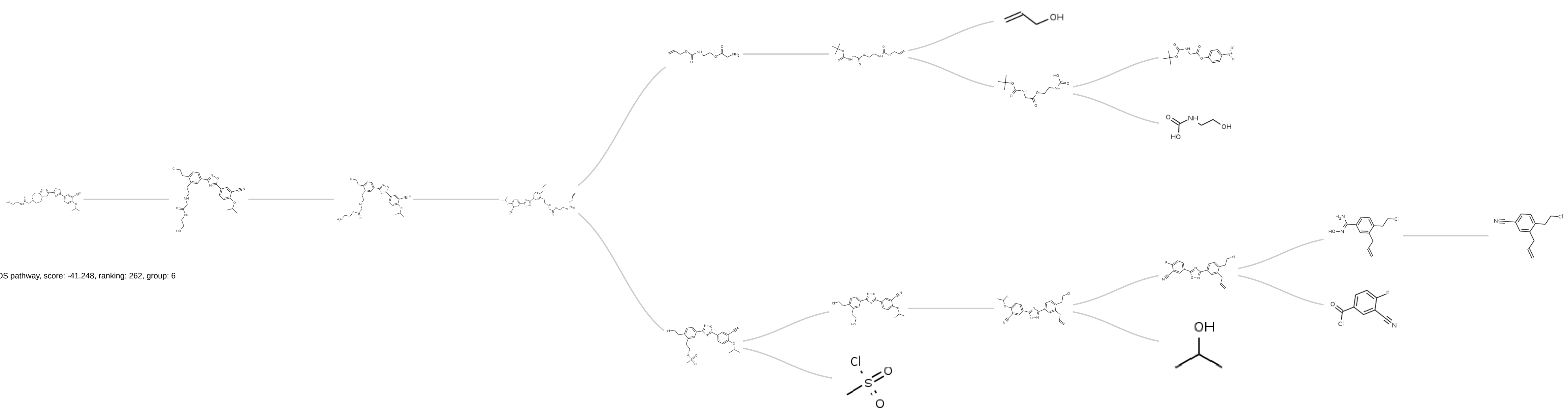
ASKCOS pathway, score: -25.371, ranking: 45, group: 3



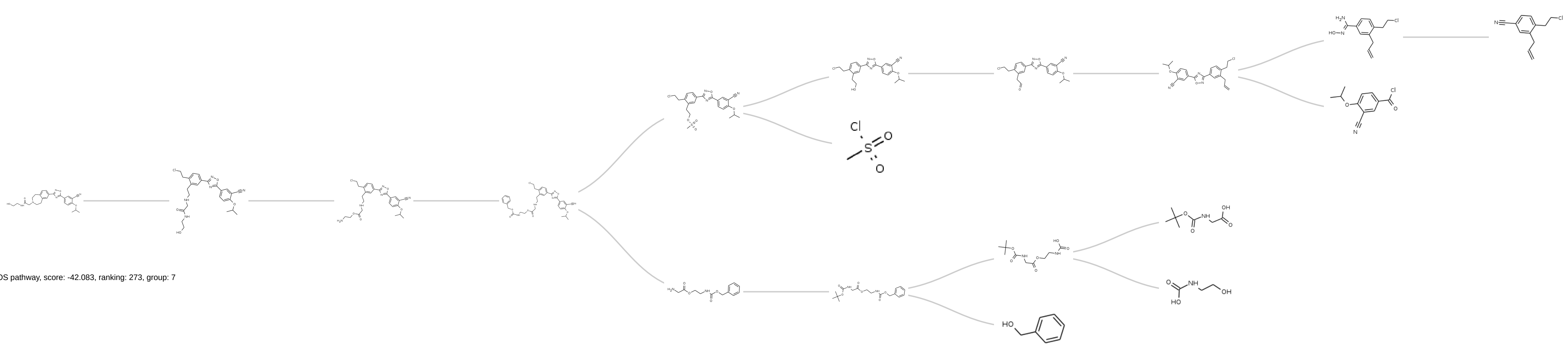
ASKCOS pathway, score: -31.666, ranking: 105, group: 4



ASKCOS pathway, score: -32.069, ranking: 120, group: 5



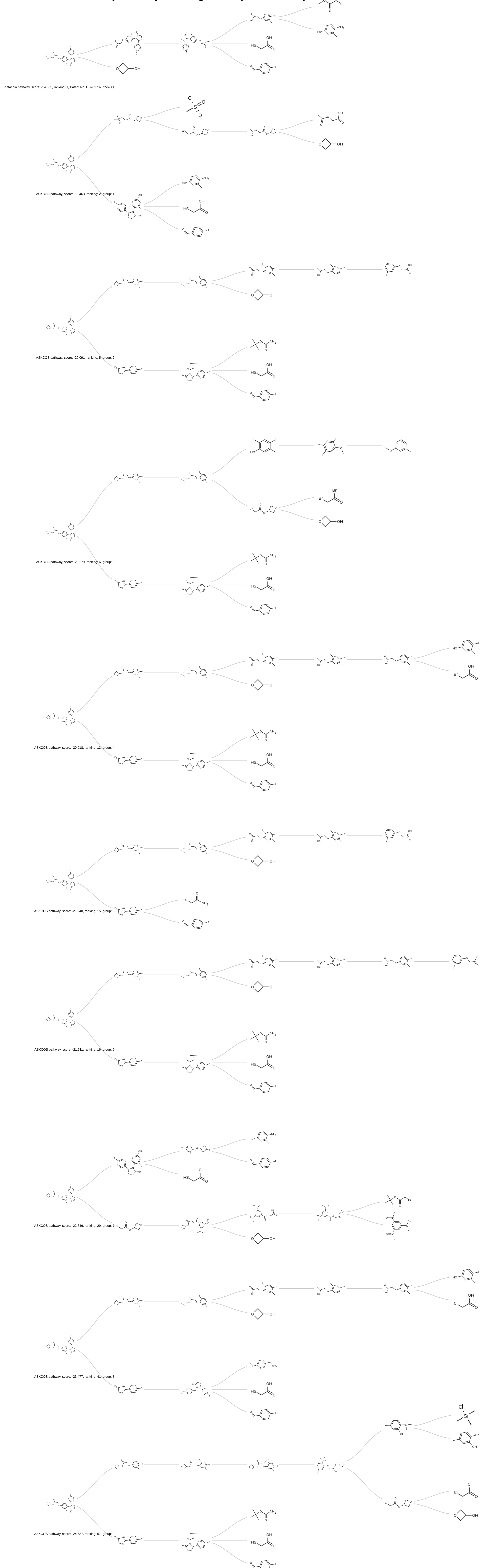
ASKCOS pathway, score: -41.248, ranking: 262, group: 6



ASKCOS pathway, score: -42.083, ranking: 273, group: 7

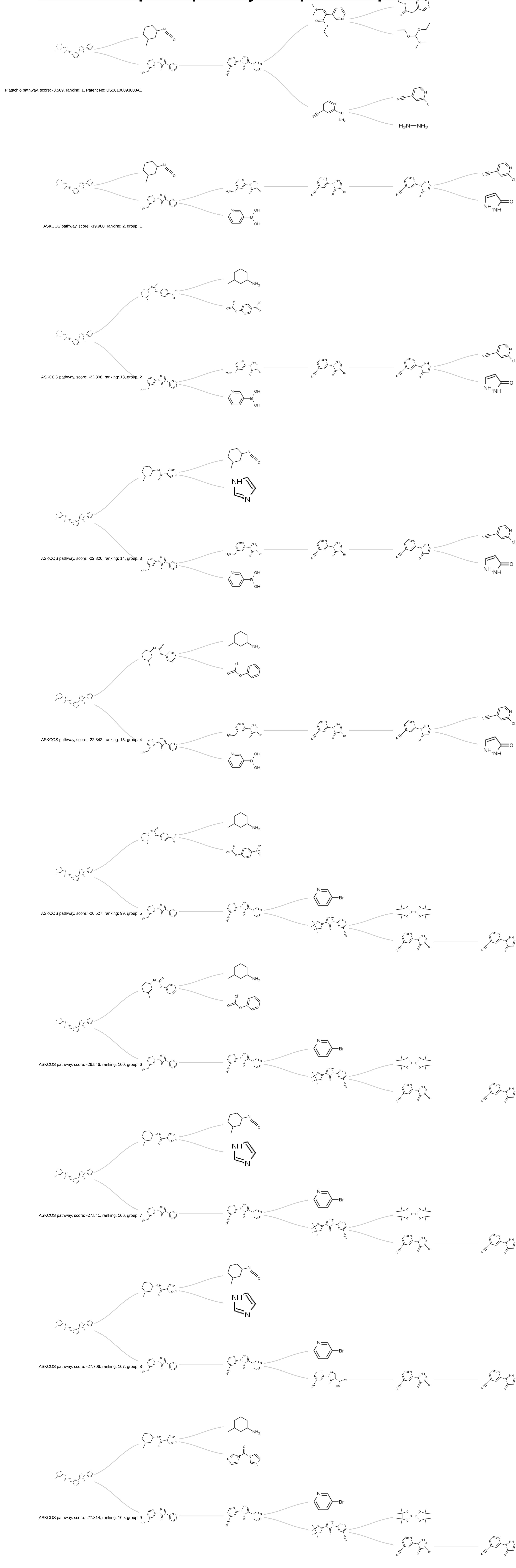


# Model ranks patent pathway as top-1: Example 10

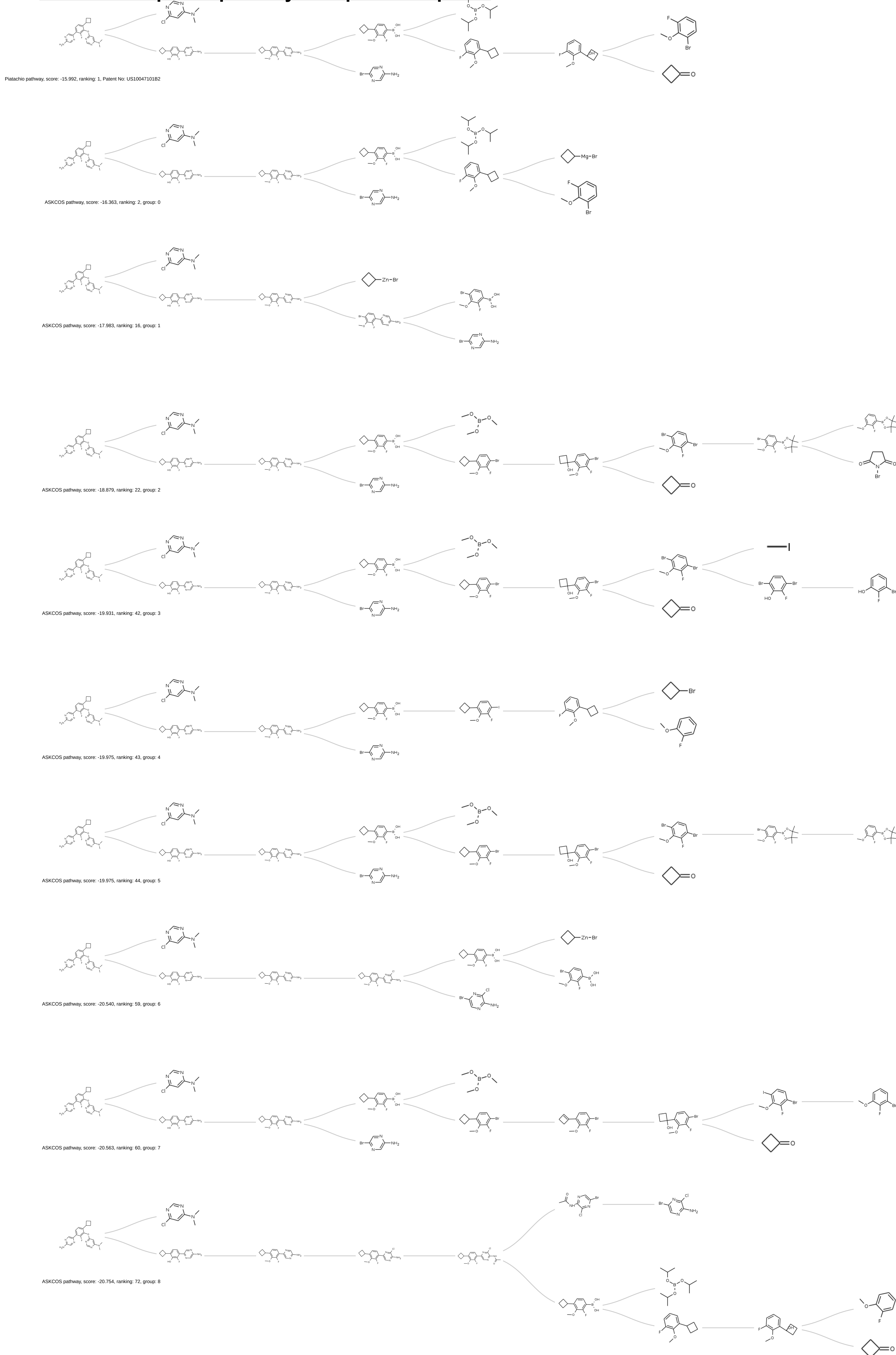




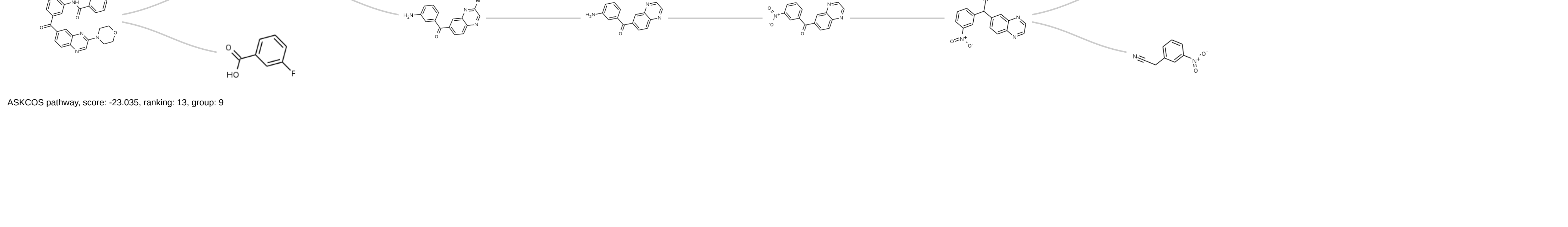
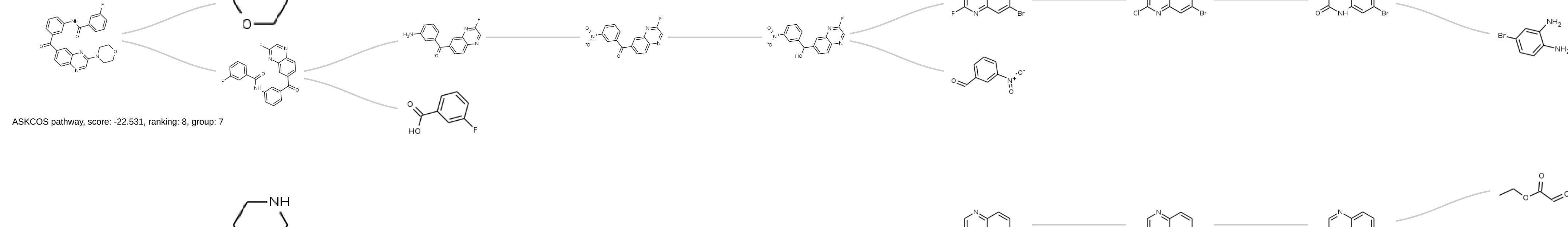
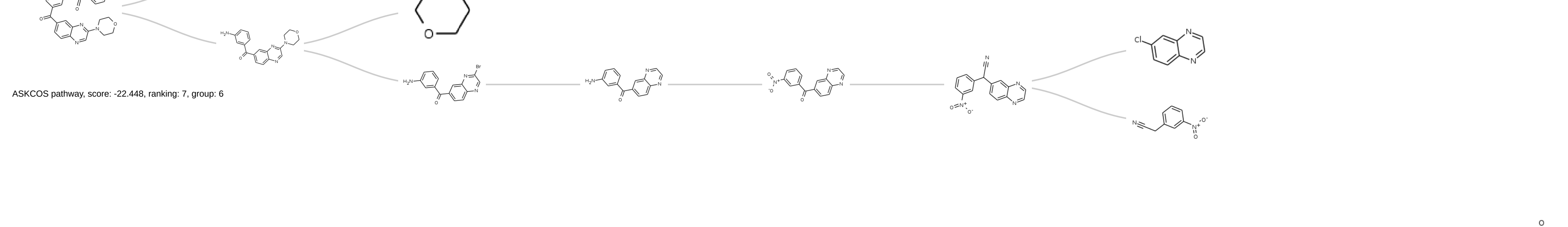
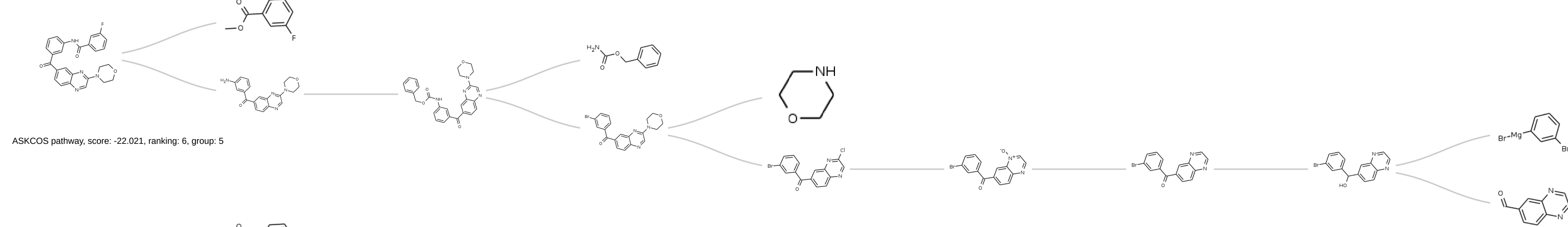
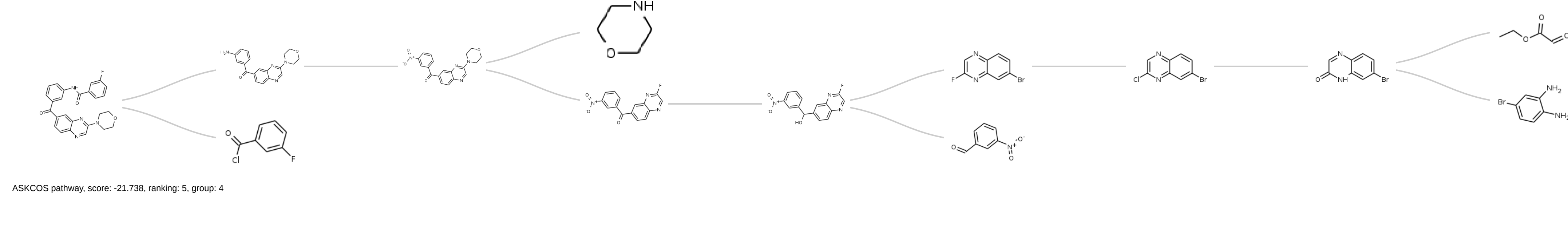
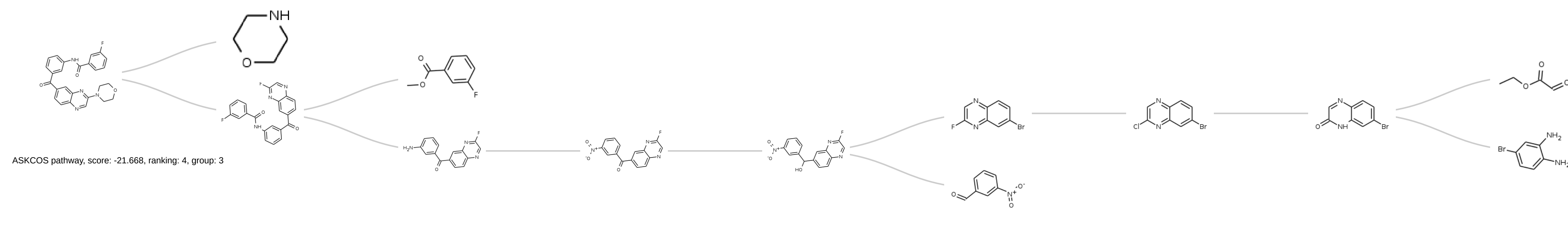
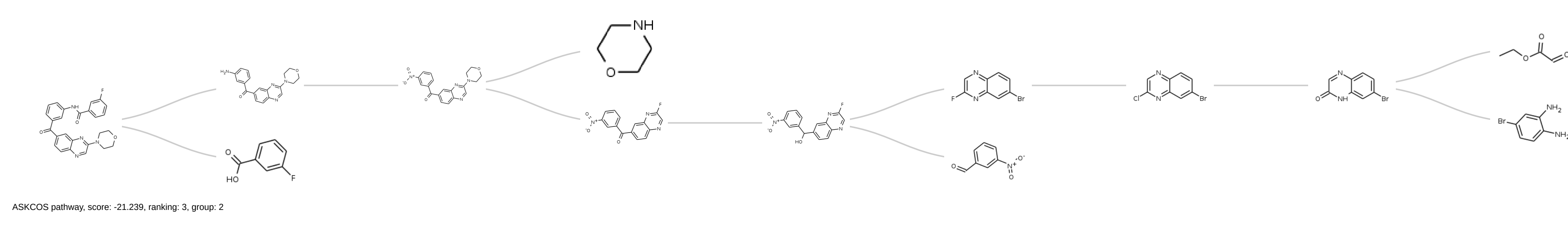
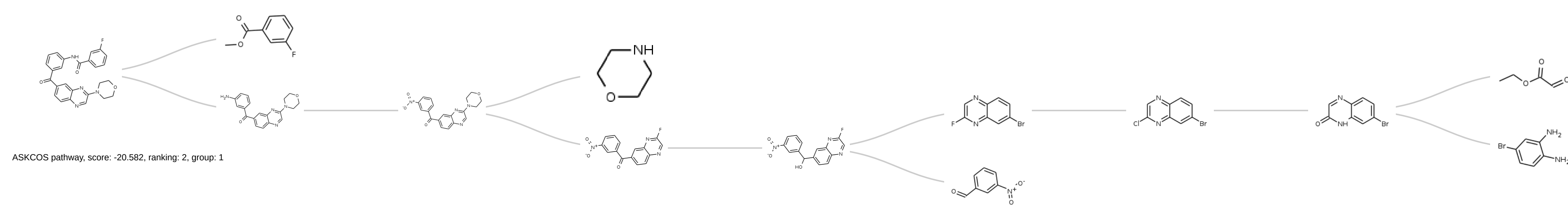
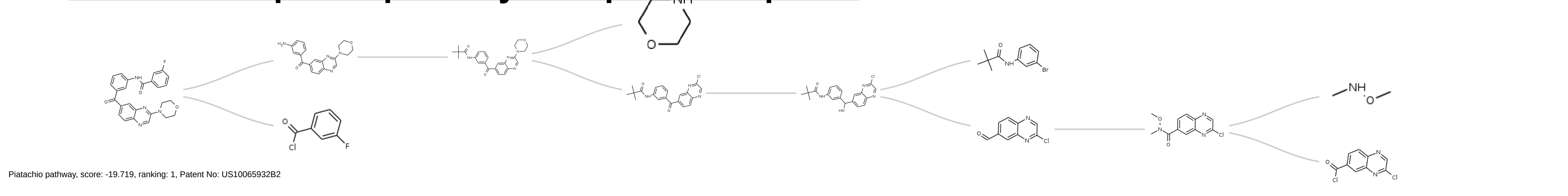
# Model ranks patent pathway as top-1: Example 11



# Model ranks patent pathway as top-1: Example 12

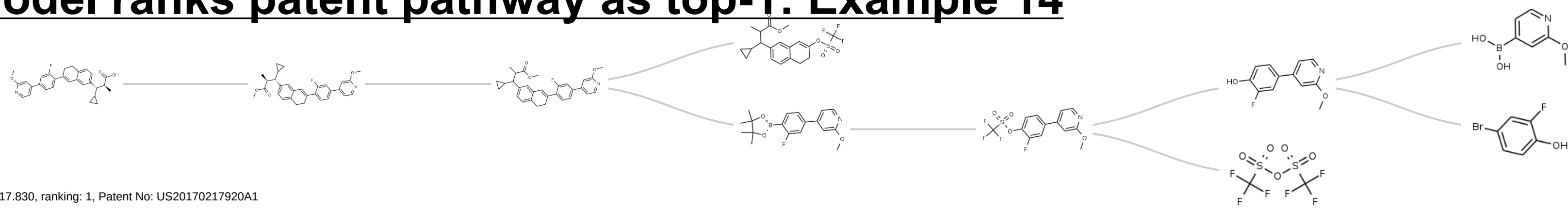


### Model ranks patent pathway as top-1: Example 13

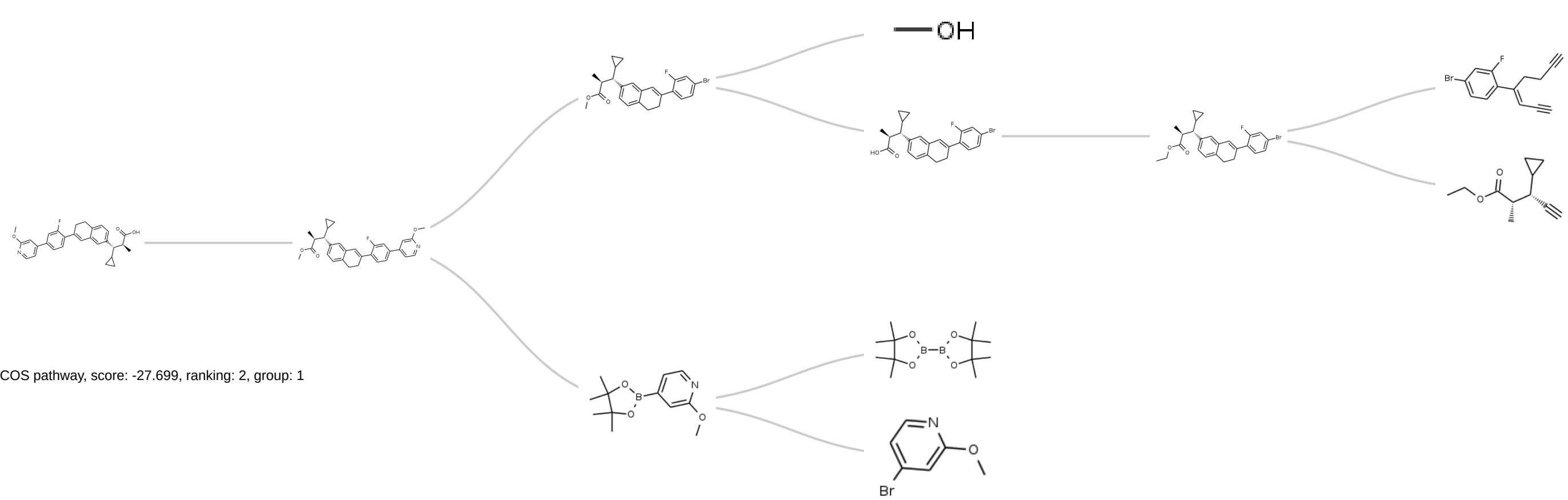


# Model ranks patent pathway as top-1: Example 14

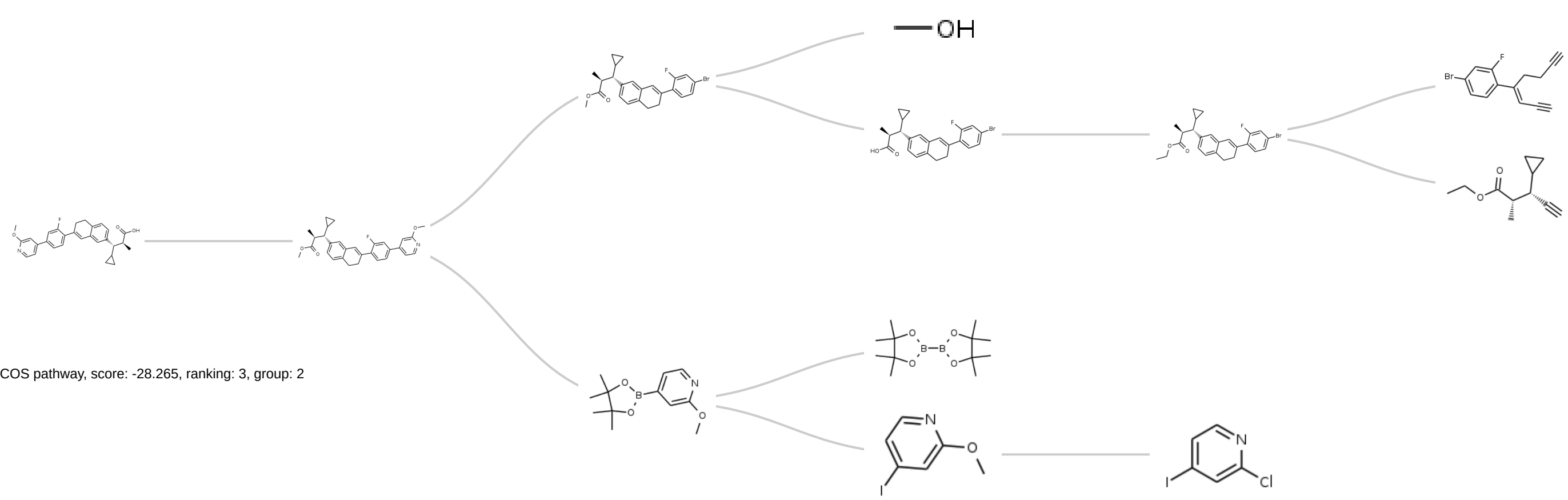
Platzho pathway score: -17.830, ranking: 1, Patent No: US2017021900A1



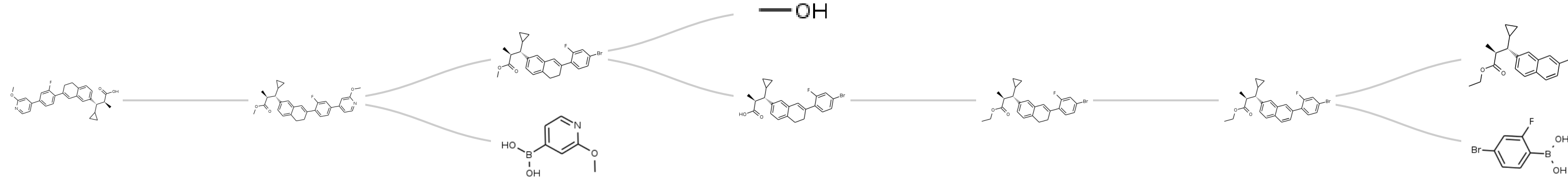
ASKCOS pathway score: -27.659, ranking: 2, group: 1



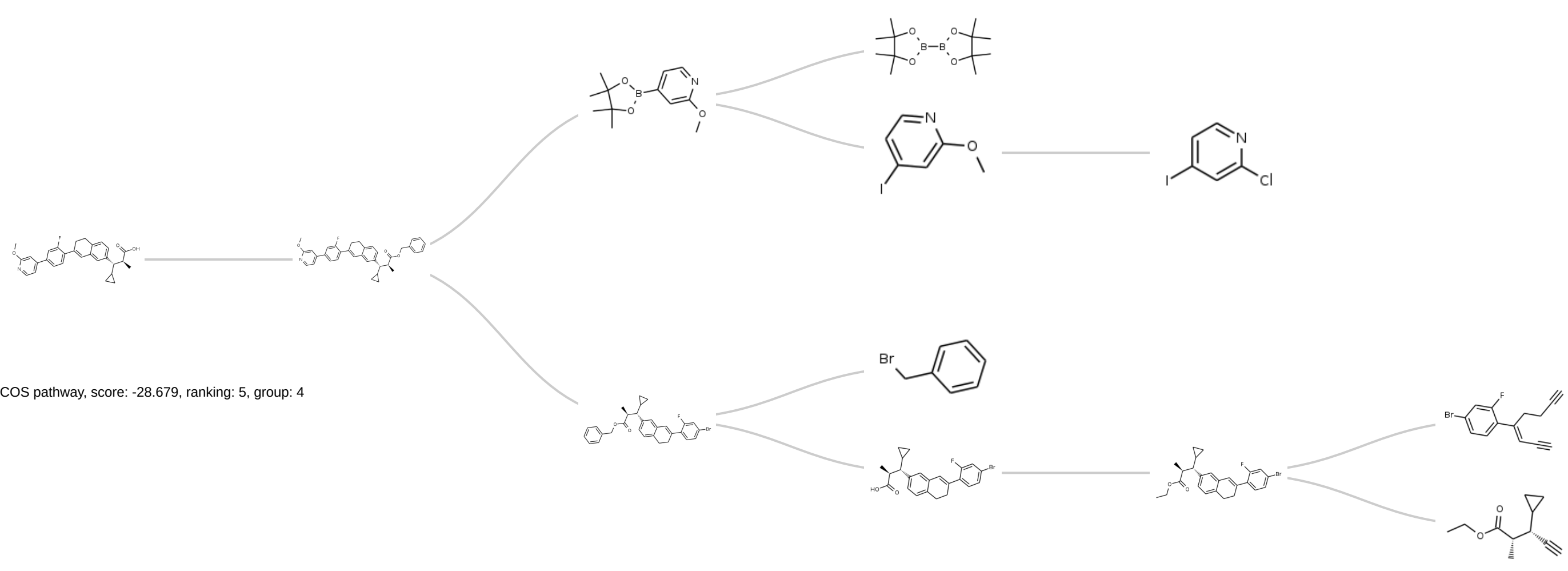
ASKCOS pathway score: -28.266, ranking: 3, group: 2



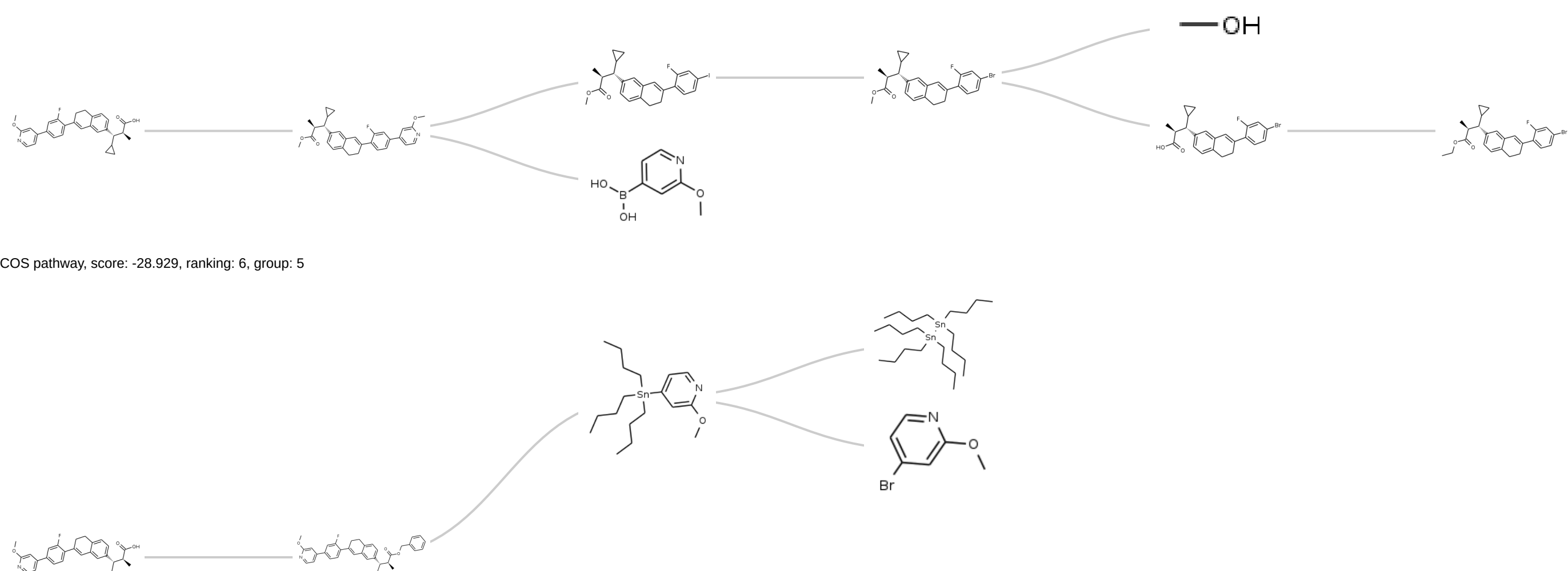
ASKCOS pathway score: -28.316, ranking: 4, group: 3



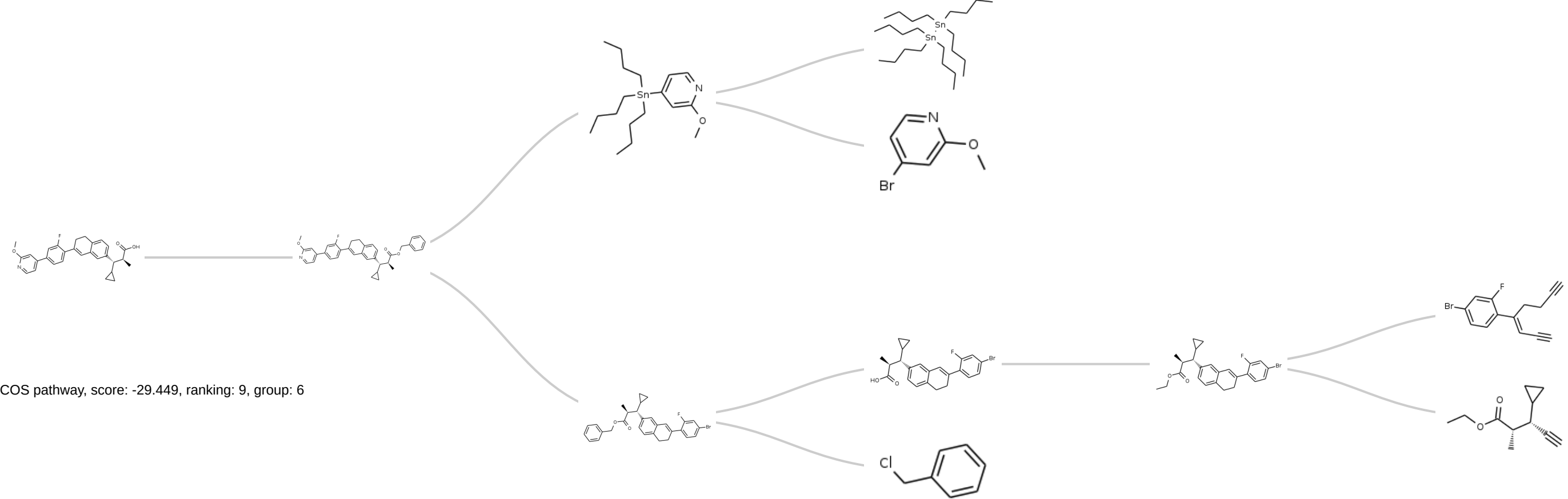
ASKCOS pathway score: -28.679, ranking: 5, group: 4



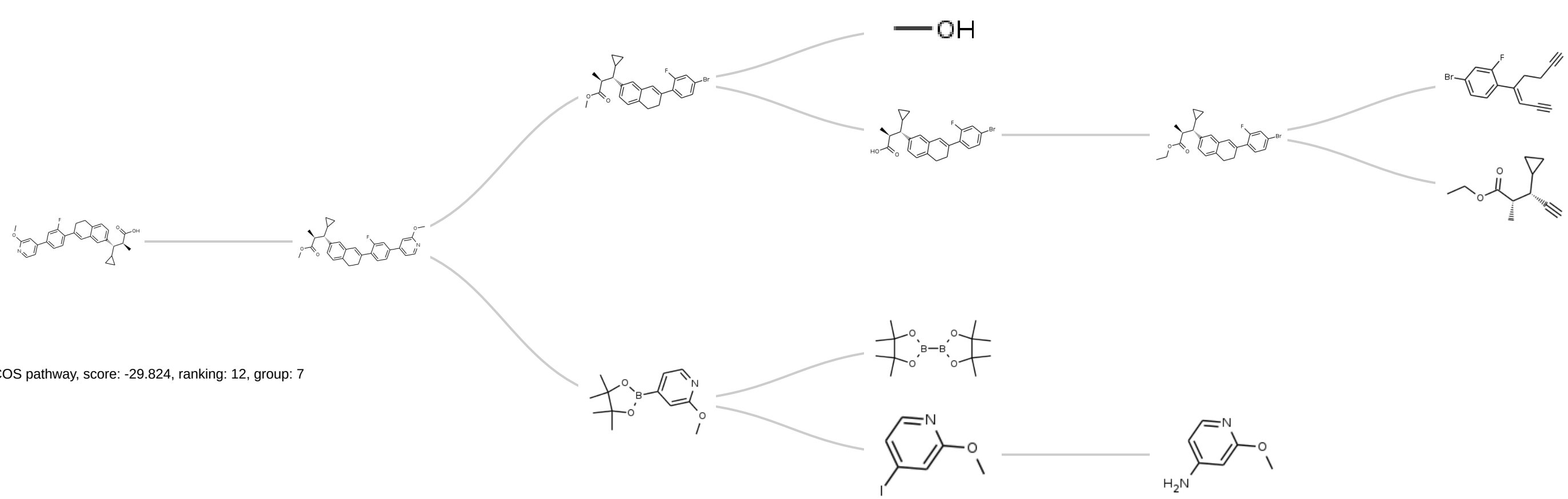
ASKCOS pathway score: -28.929, ranking: 6, group: 5



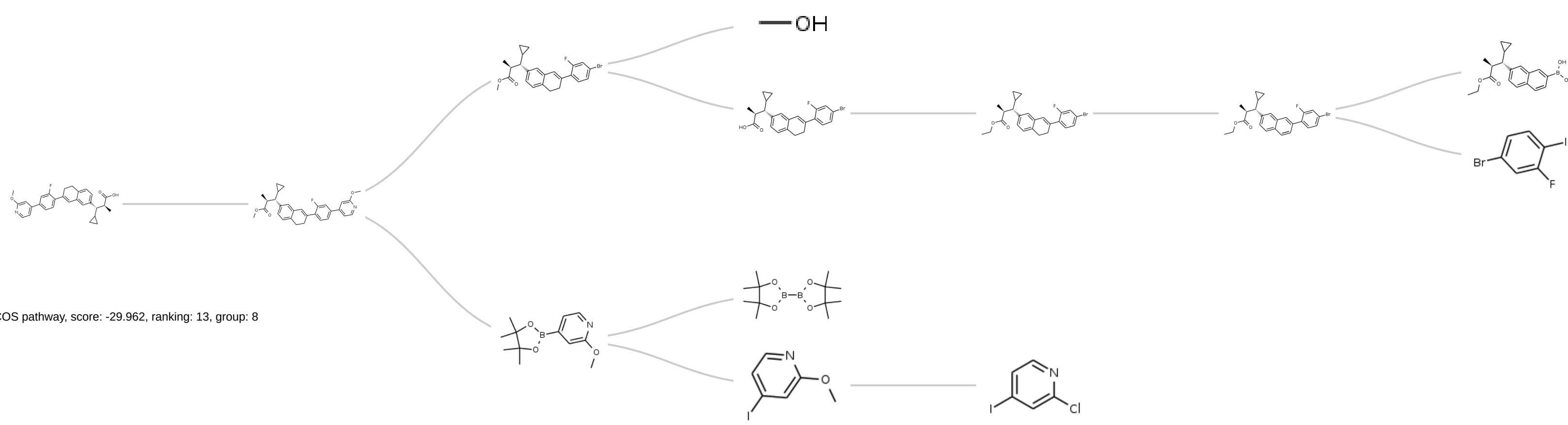
ASKCOS pathway score: -29.449, ranking: 9, group: 6



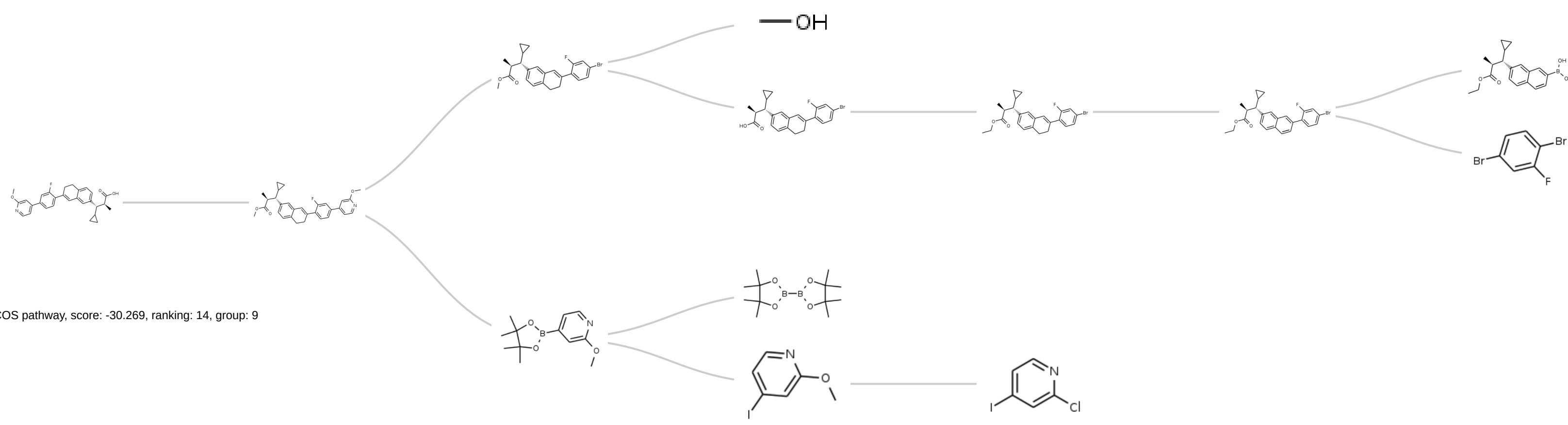
ASKCOS pathway score: -29.824, ranking: 12, group: 7



ASKCOS pathway score: -29.962, ranking: 13, group: 8



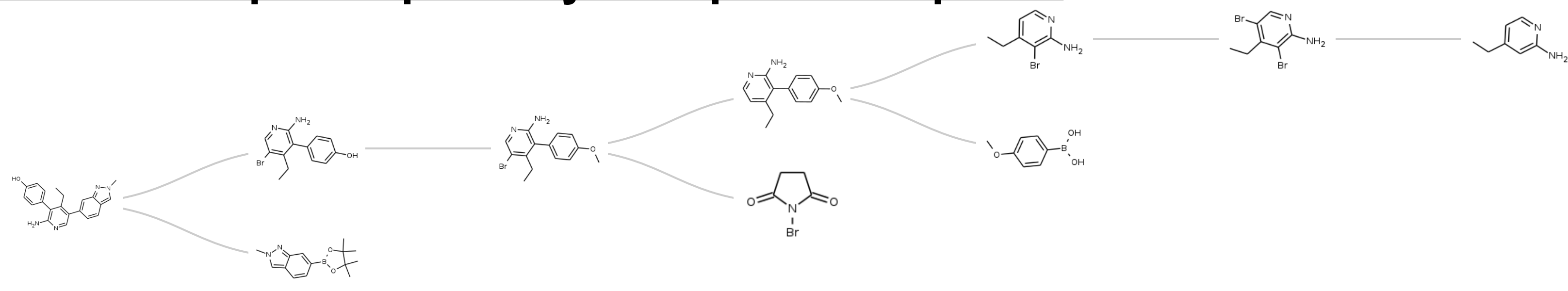
ASKCOS pathway score: -30.269, ranking: 14, group: 9



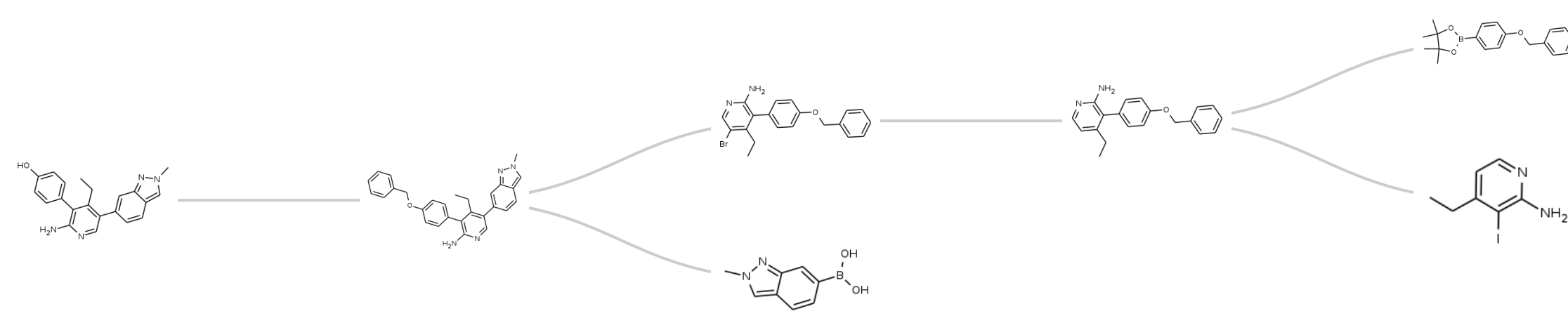




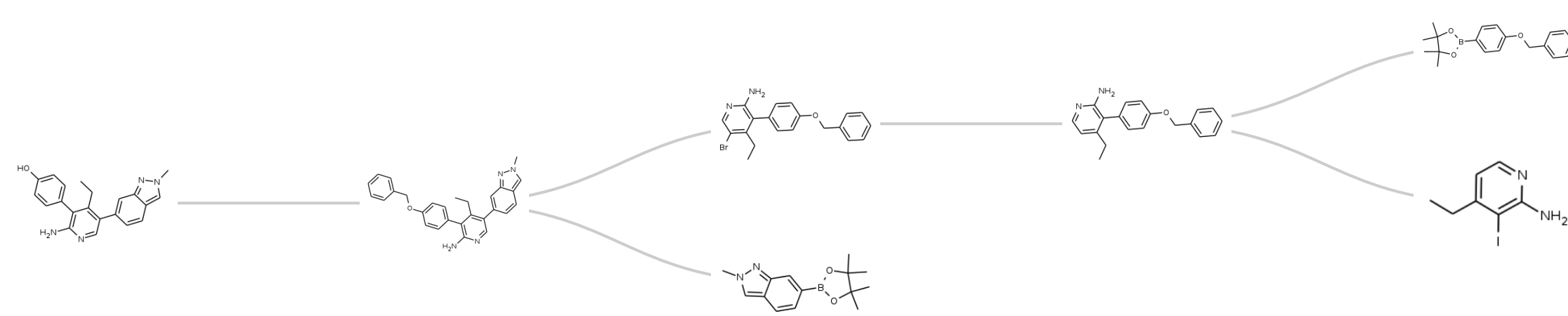
# Model ranks patent pathway as top-1: Example 16



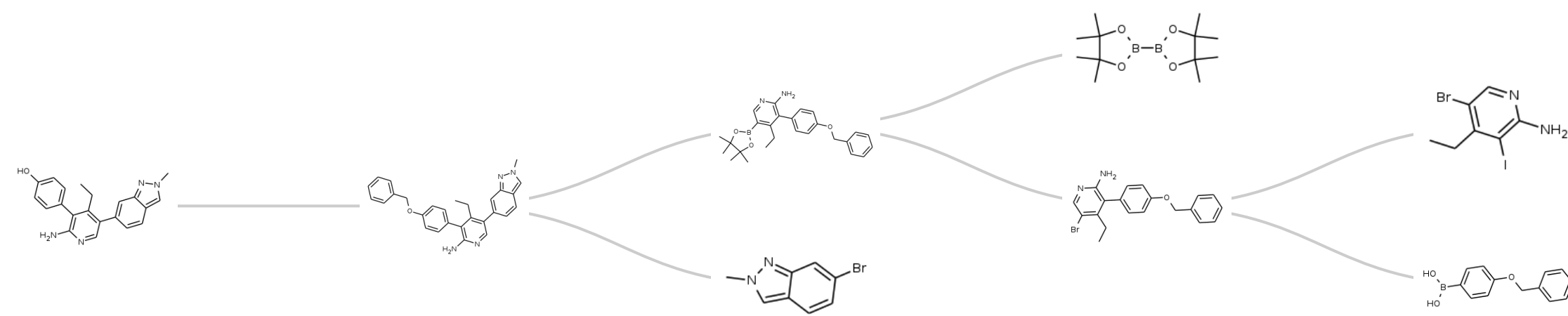
Patent pathway score: -11.915, ranking: 1, Patent No: US09073999



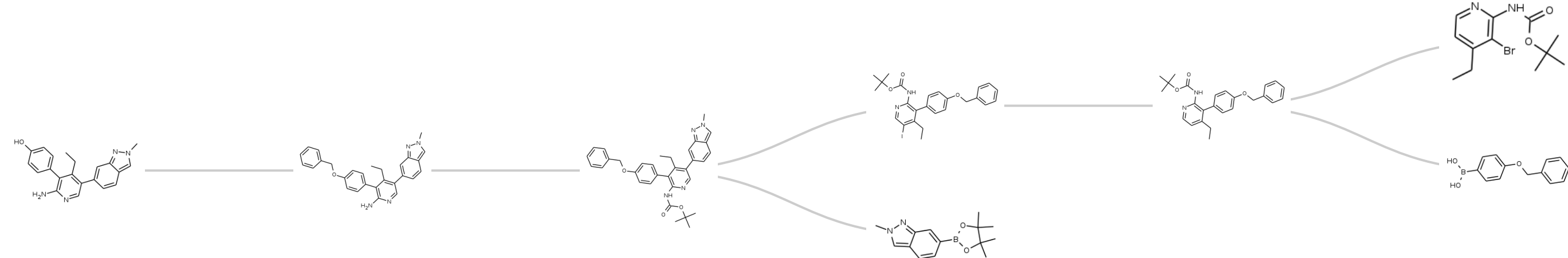
ASKCOS pathway score: -17.347, ranking: 2, group: 1



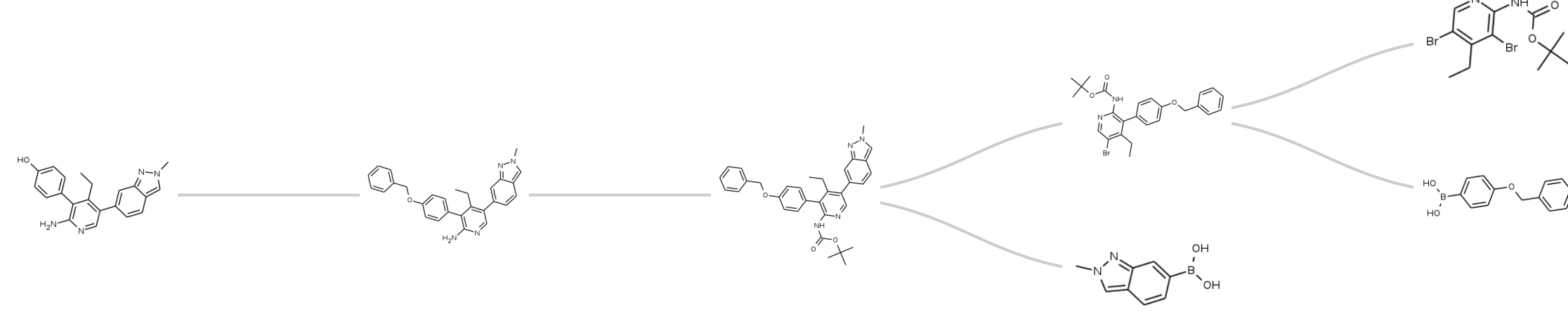
ASKCOS pathway score: -18.007, ranking: 3, group: 2



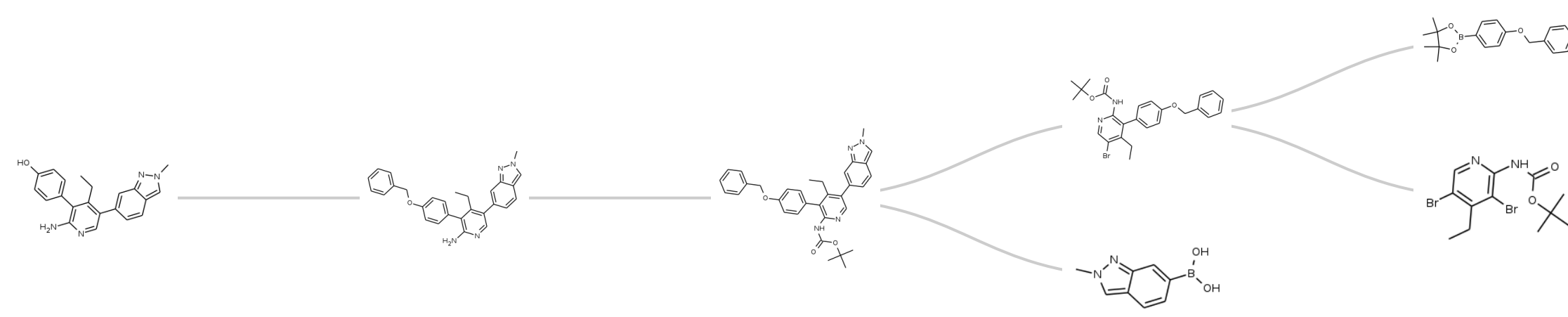
ASKCOS pathway score: -18.564, ranking: 4, group: 3



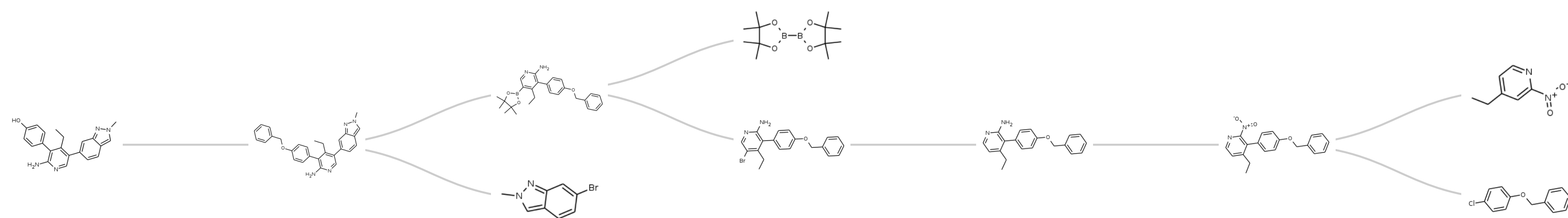
ASKCOS pathway score: -19.499, ranking: 9, group: 4



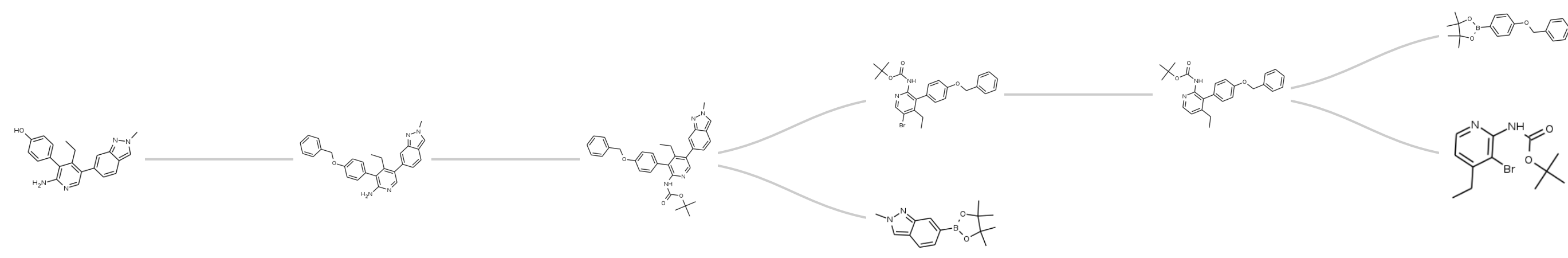
ASKCOS pathway score: -19.539, ranking: 10, group: 5



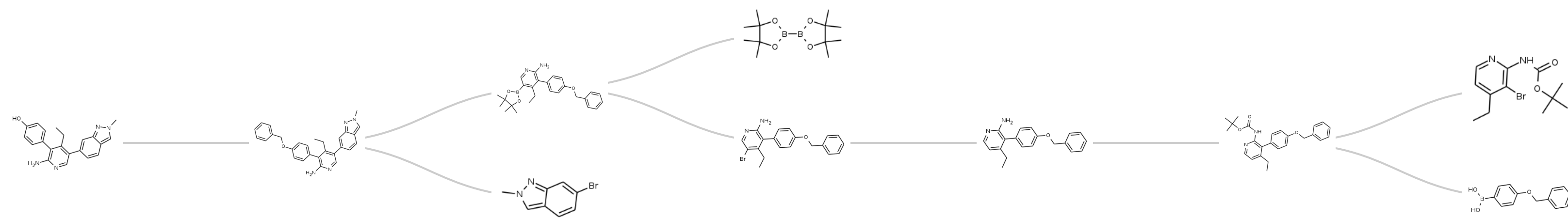
ASKCOS pathway score: -20.171, ranking: 13, group: 6



ASKCOS pathway score: -20.520, ranking: 17, group: 7



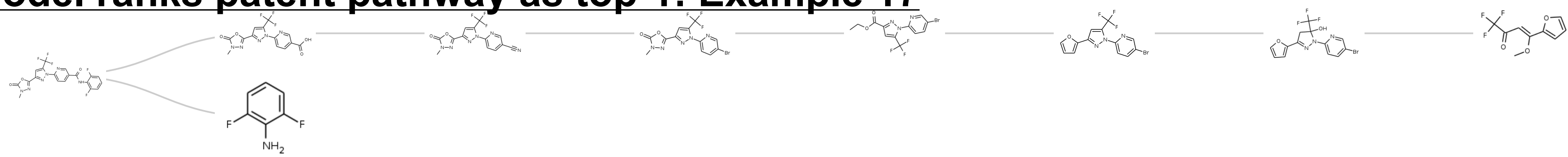
ASKCOS pathway score: -20.759, ranking: 19, group: 8



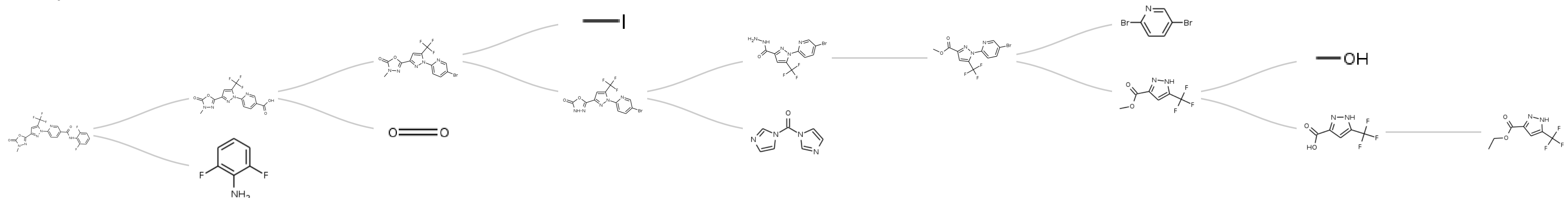
ASKCOS pathway score: -20.827, ranking: 21, group: 9



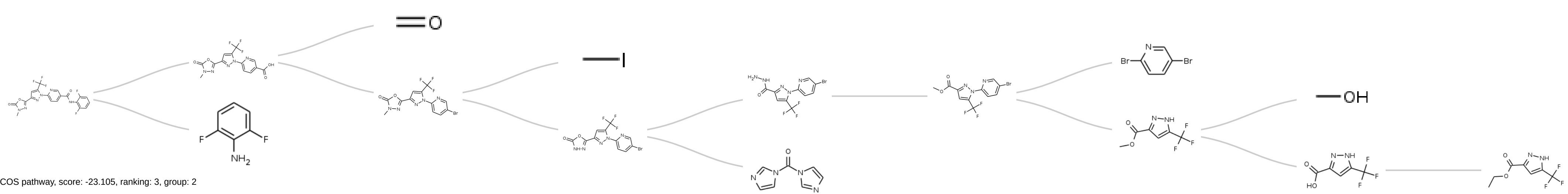
# Model ranks patent pathway as top-1: Example 17



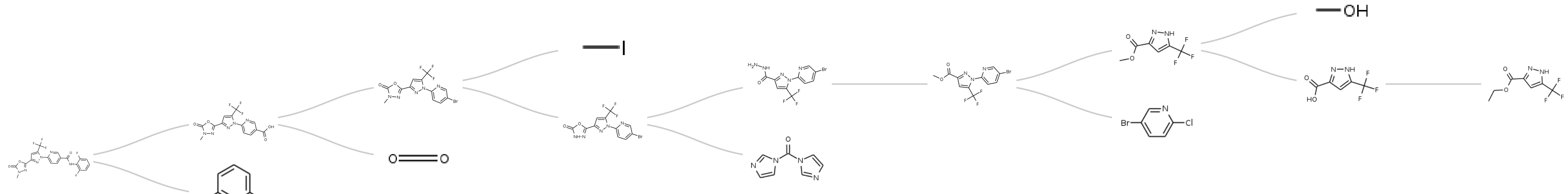
ASKCOS pathway score: -14.001, ranking: 1, Patent No: US2015011925A1



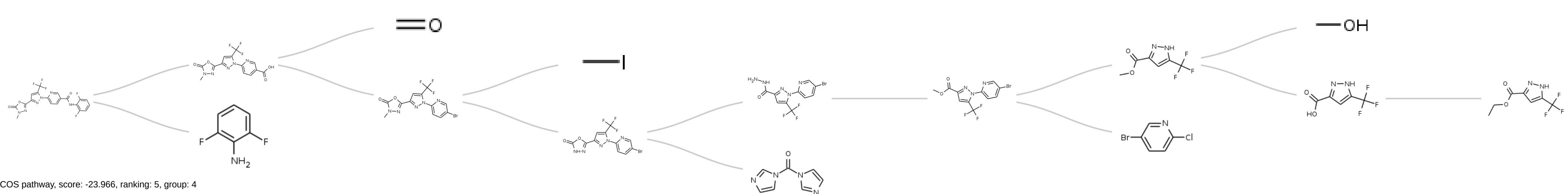
ASKCOS pathway score: -23.066, ranking: 2, group: 1



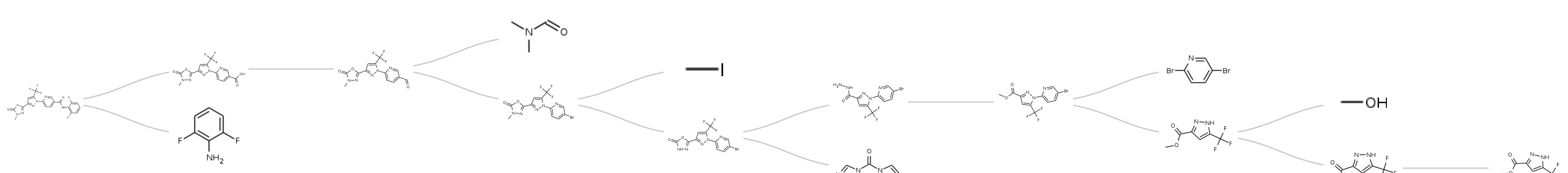
ASKCOS pathway score: -23.105, ranking: 3, group: 2



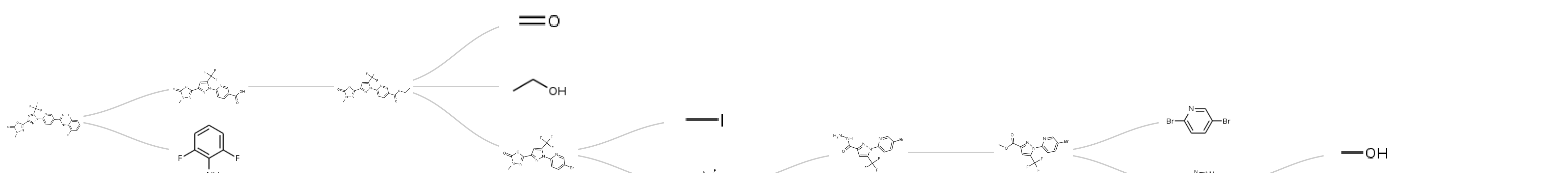
ASKCOS pathway score: -23.890, ranking: 4, group: 3



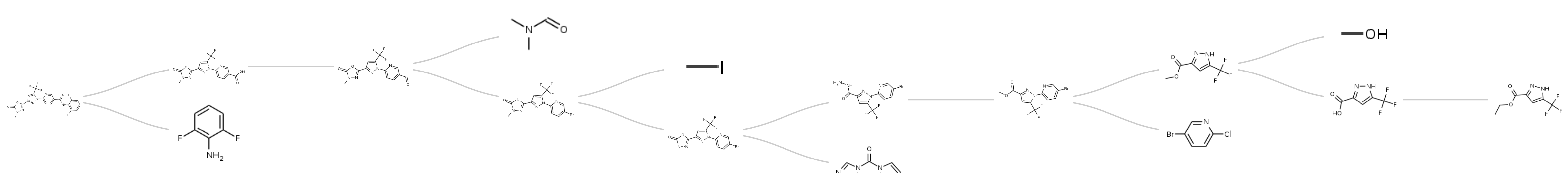
ASKCOS pathway score: -23.966, ranking: 5, group: 4



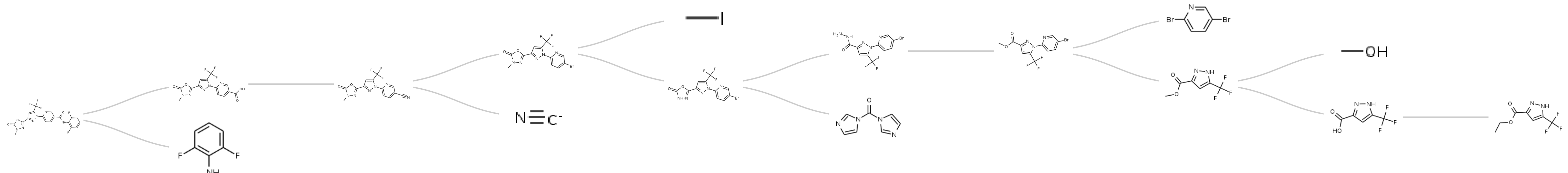
ASKCOS pathway score: -24.547, ranking: 6, group: 5



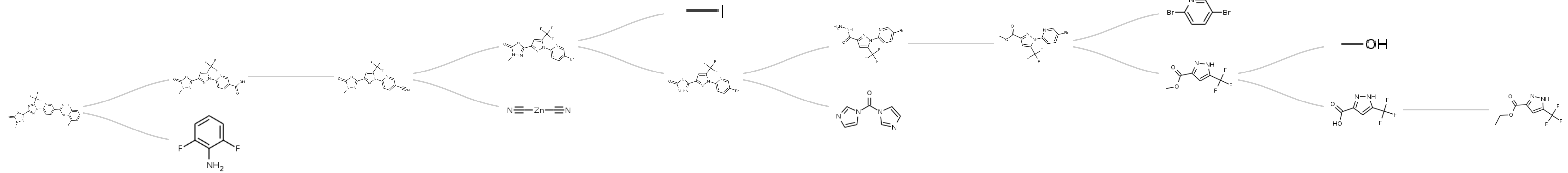
ASKCOS pathway score: -24.896, ranking: 7, group: 6



ASKCOS pathway score: -25.368, ranking: 8, group: 7

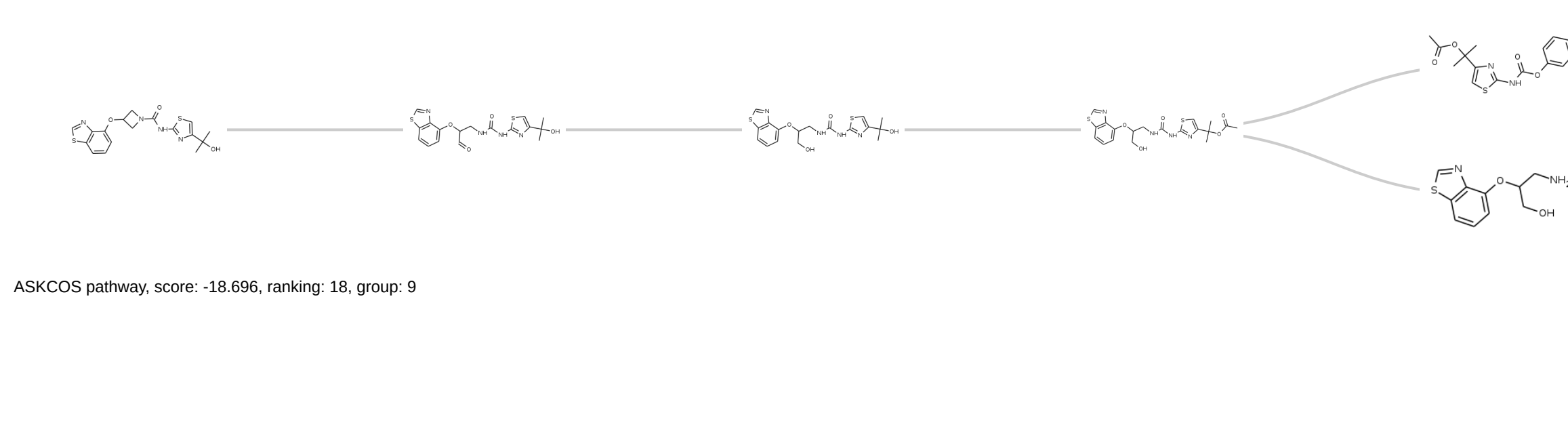
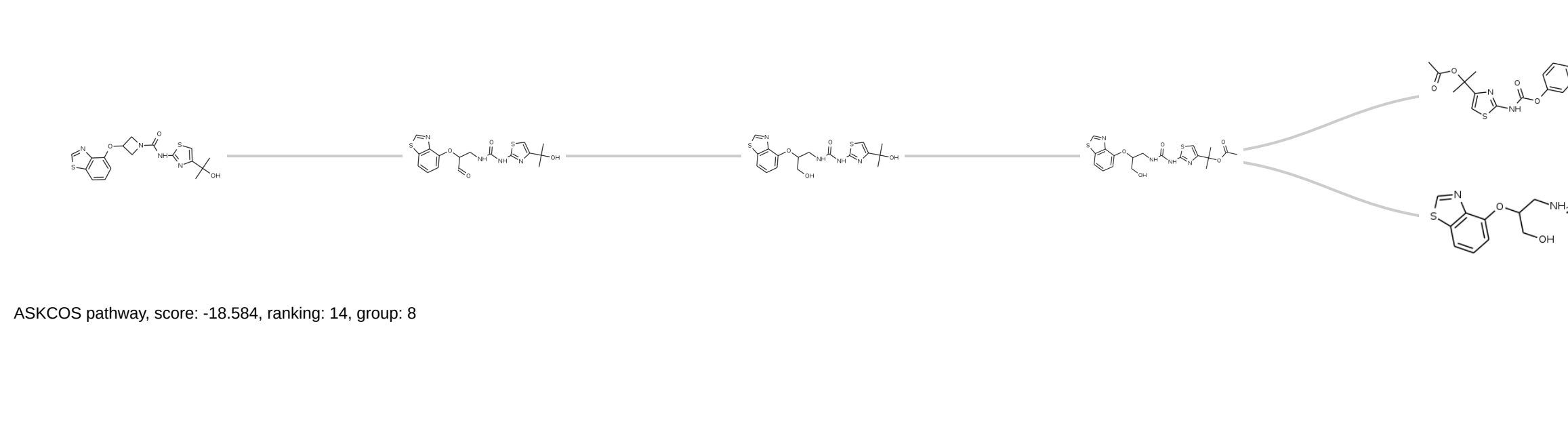
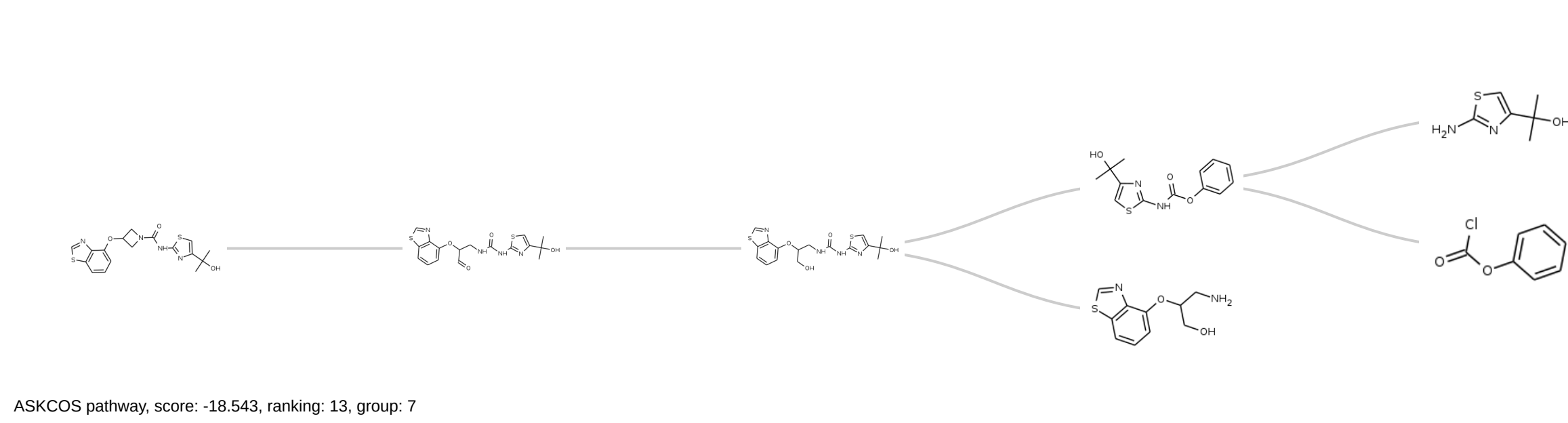
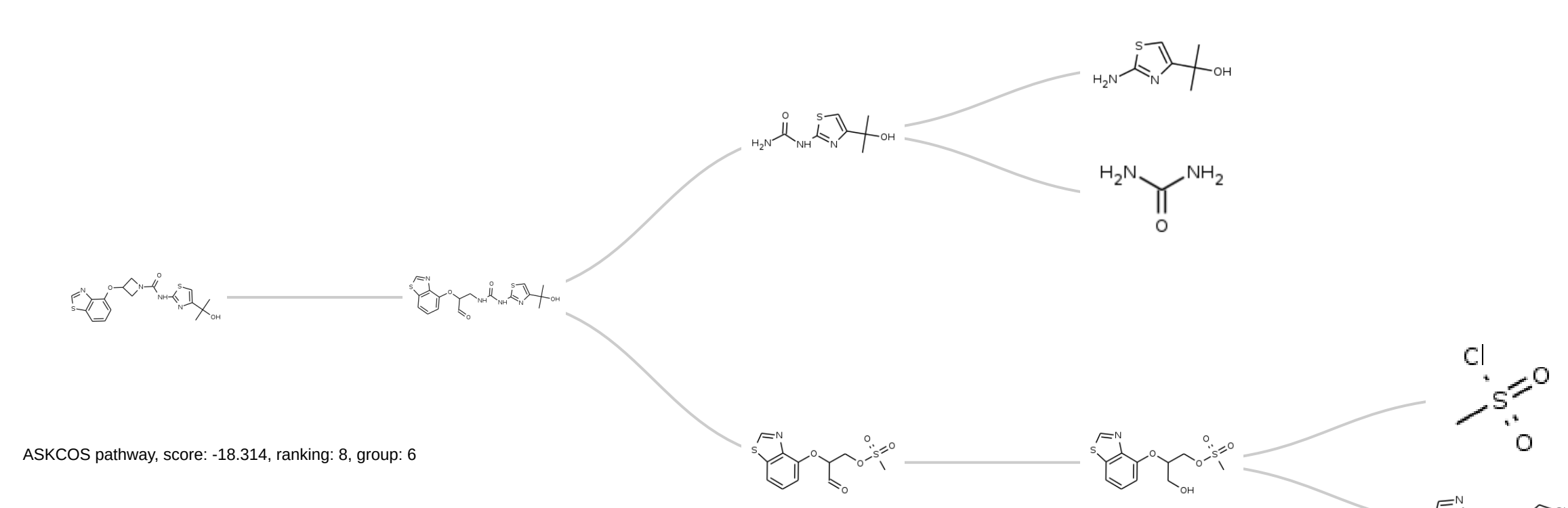
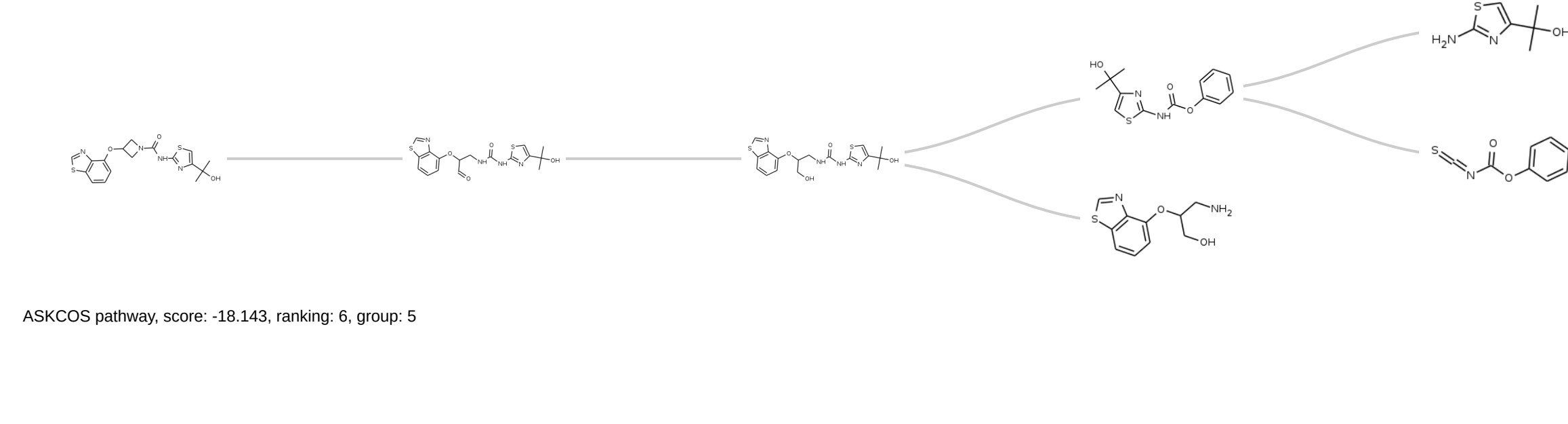
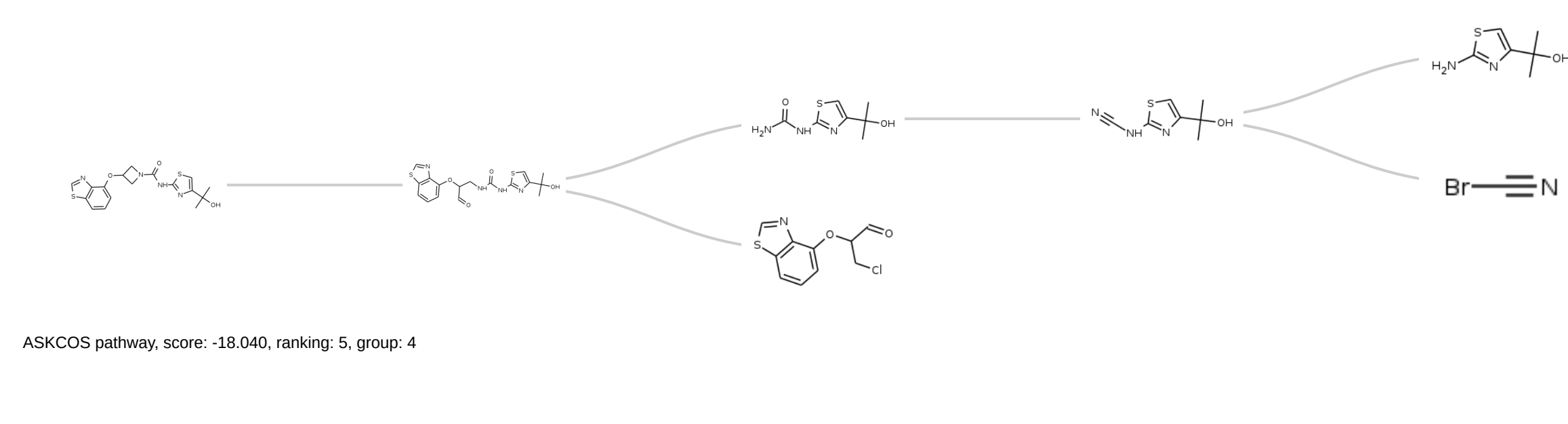
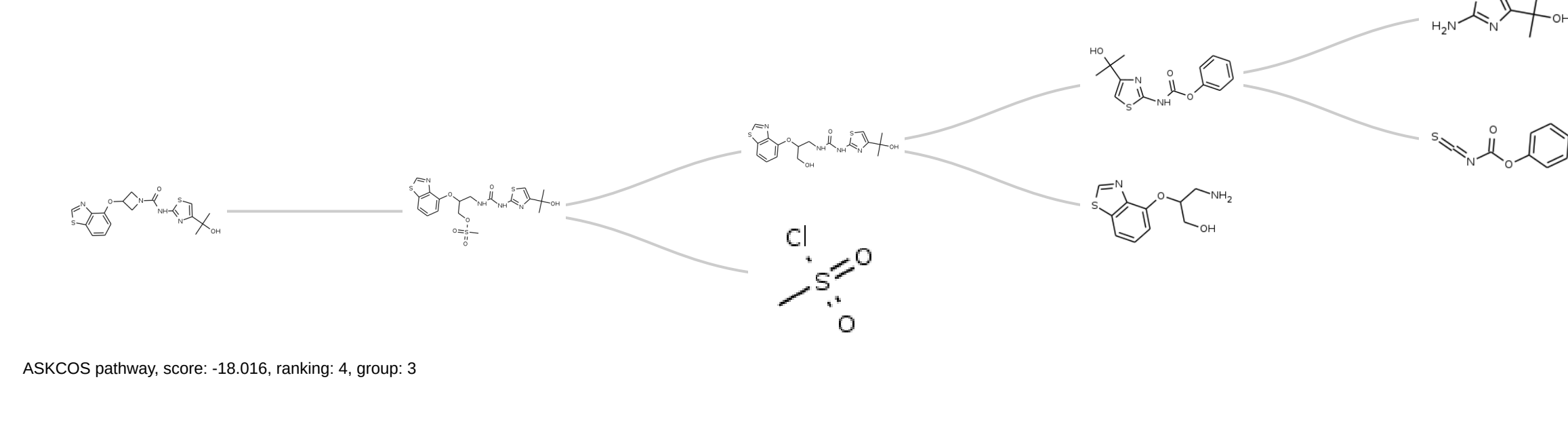
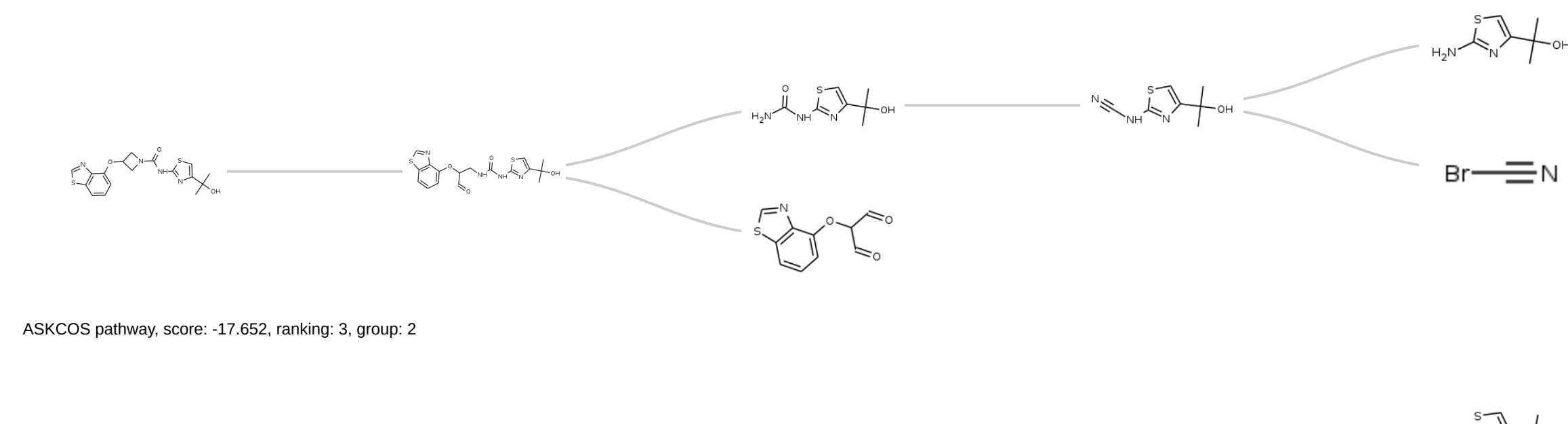
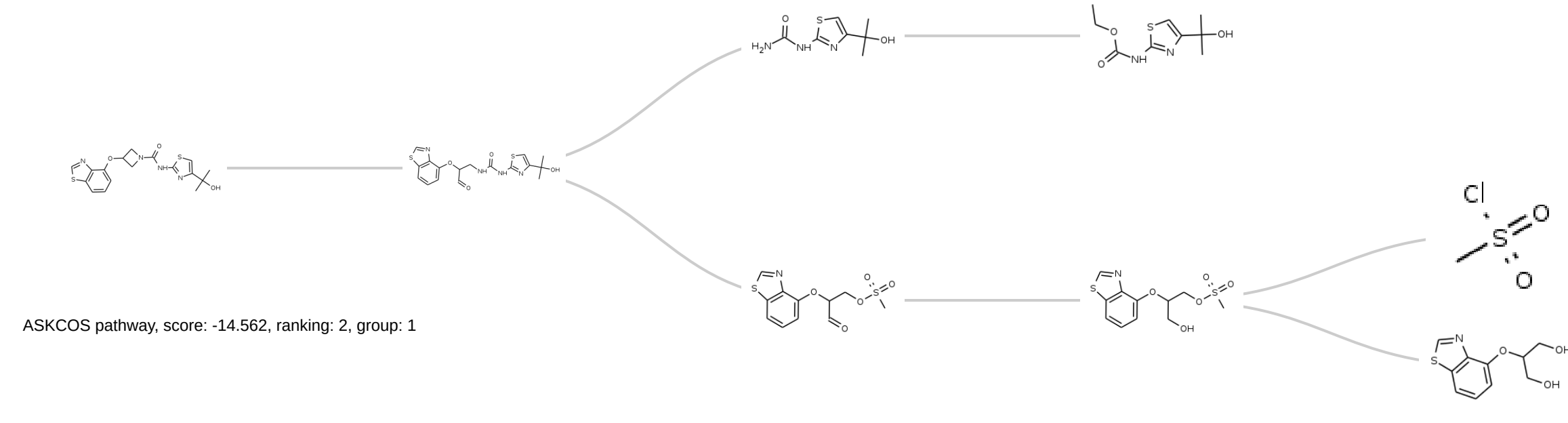
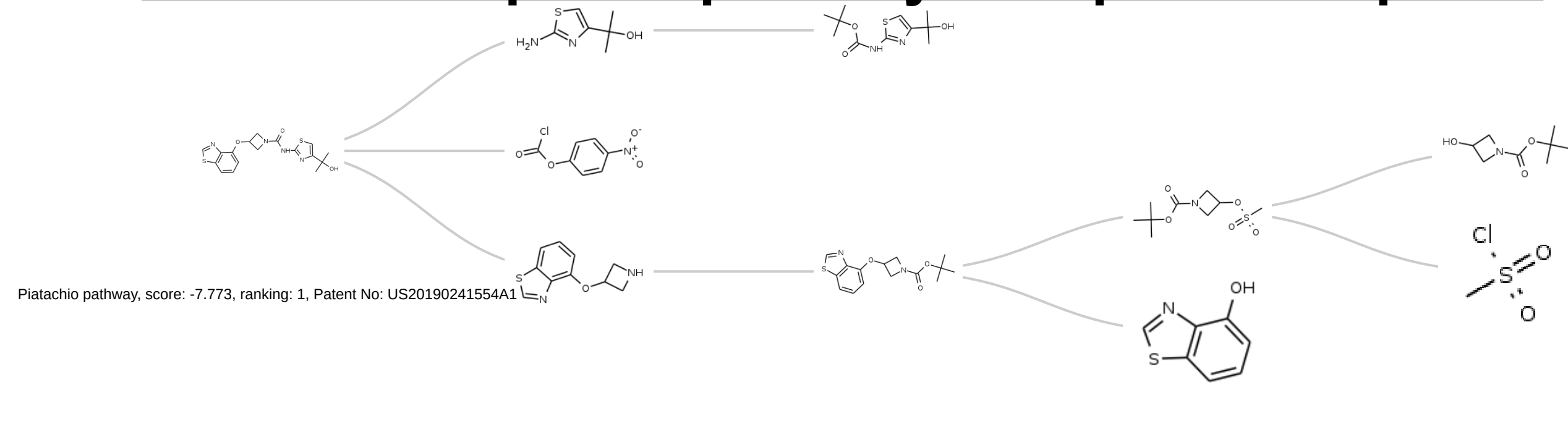


ASKCOS pathway score: -25.376, ranking: 9, group: 8

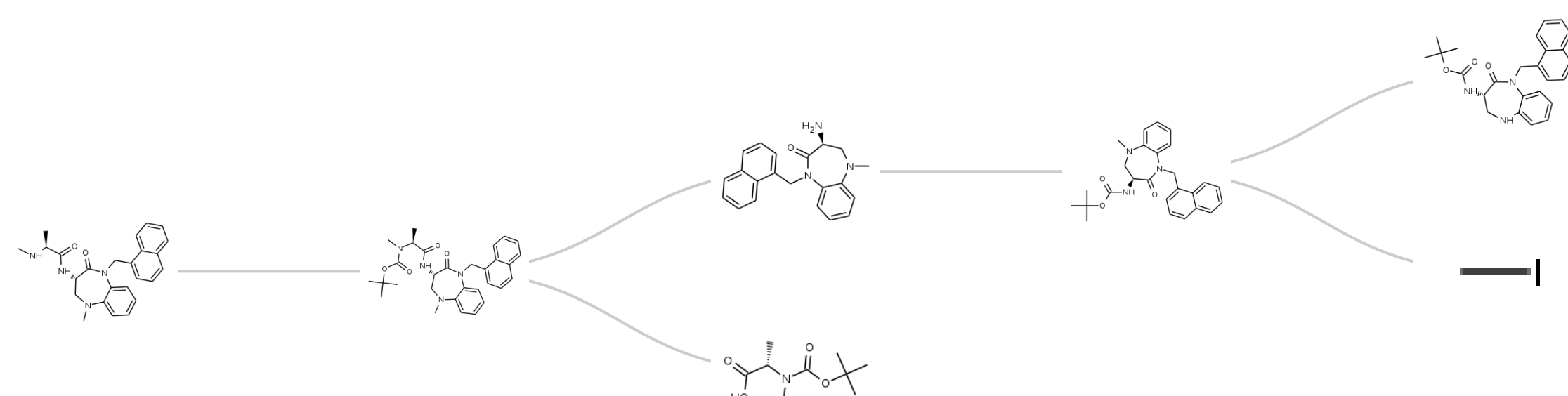


ASKCOS pathway score: -25.378, ranking: 10, group: 9

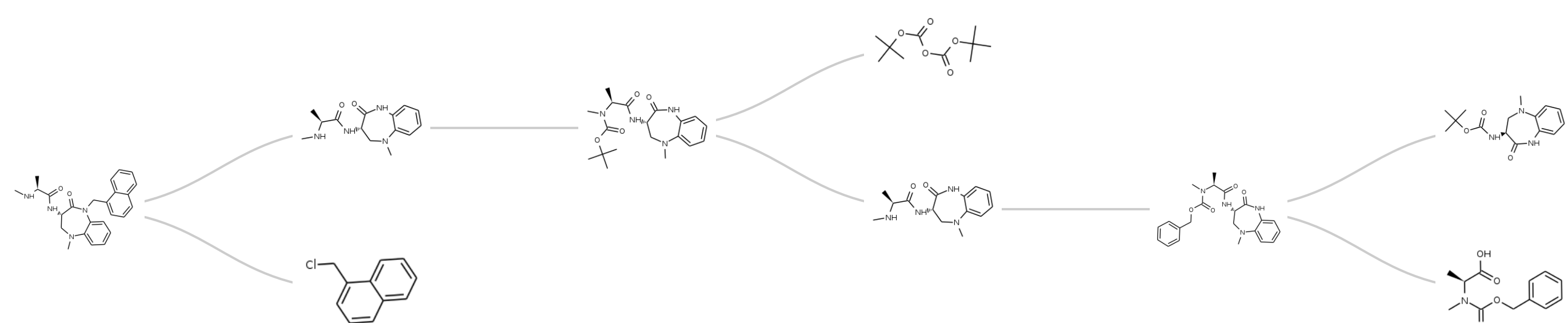
# Model ranks patent pathway as top-1: Example 18



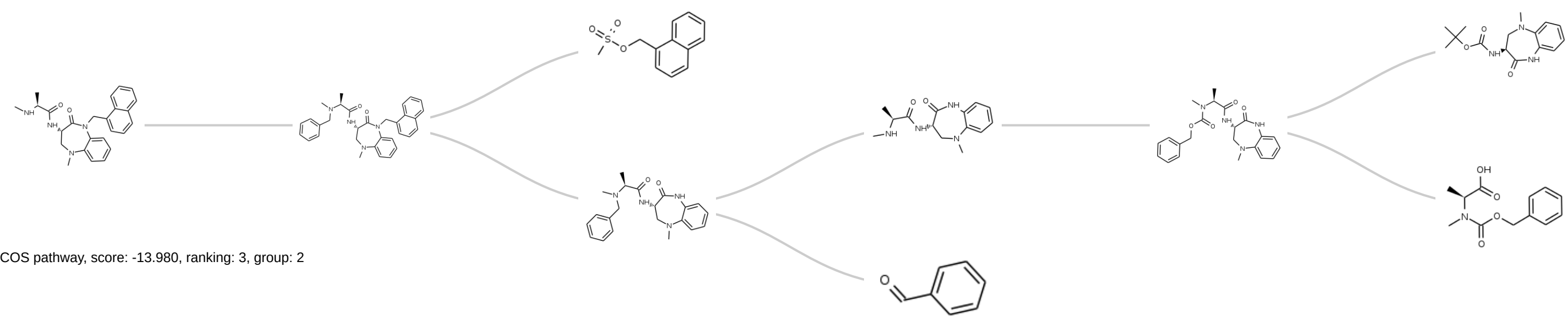
**Model ranks patent pathway as top-1: Example 19**



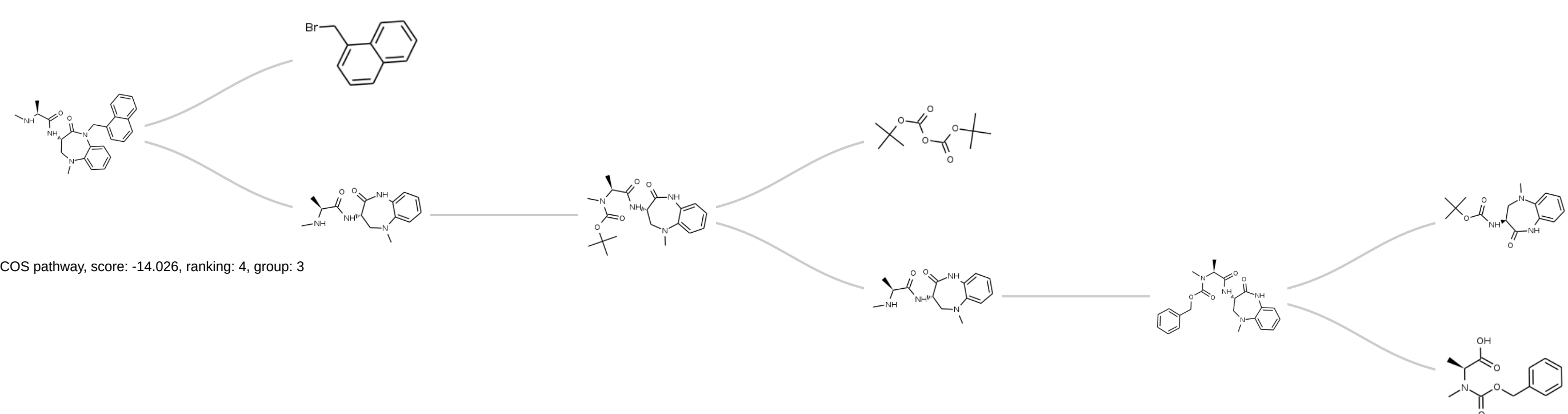
Platzho pathway, score: -12.956, ranking: 1, Patent No: US20160272596A1



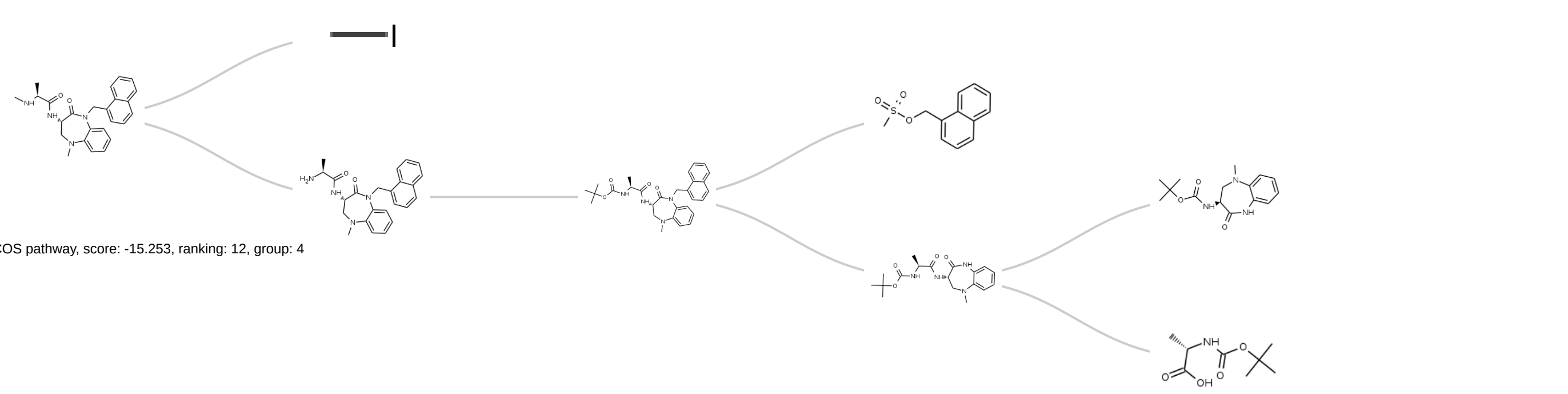
ASKCOS pathway, score: -13.743, ranking: 2, group: 1



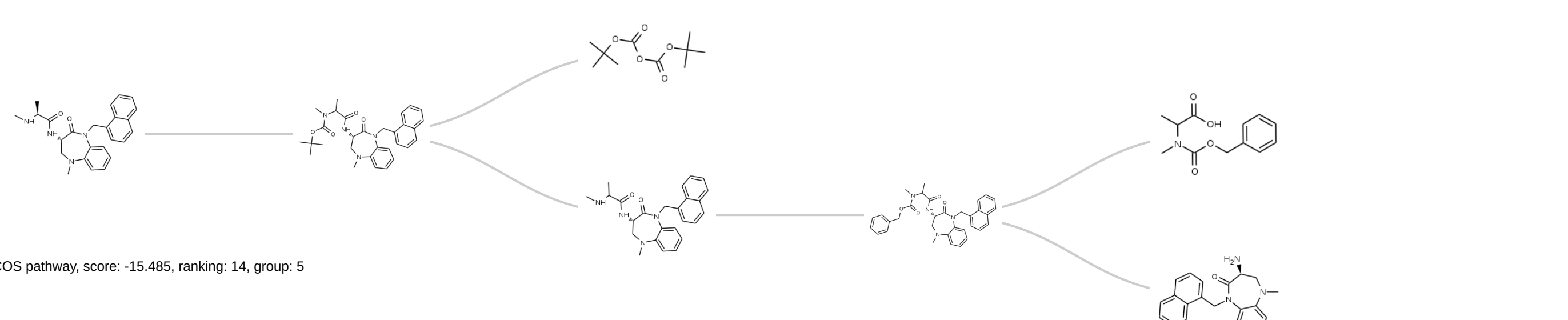
ASKCOS pathway, score: -13.980, ranking: 3, group: 2



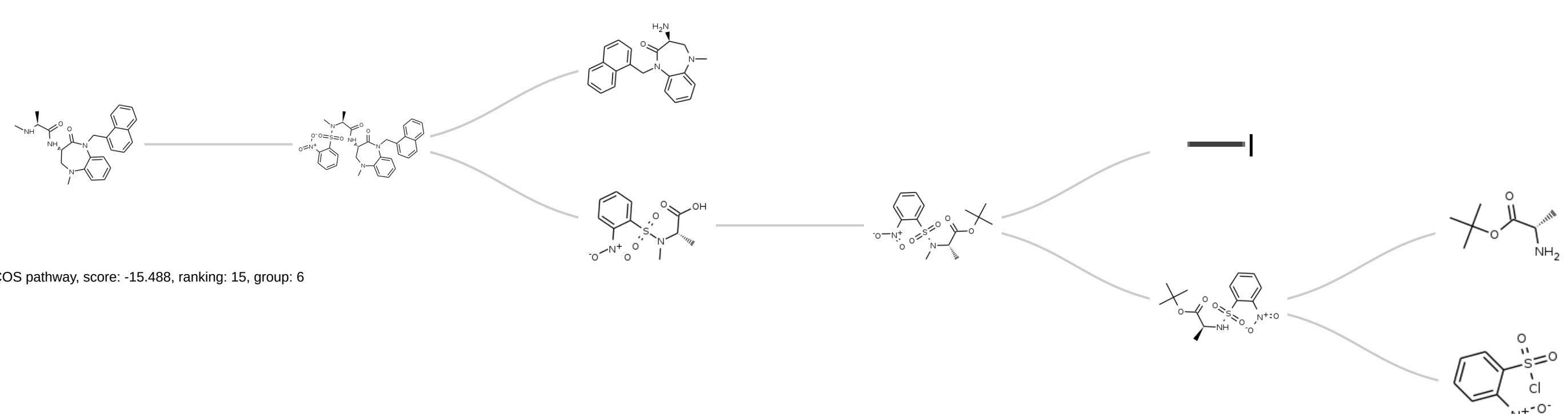
ASKCOS pathway, score: -14.026, ranking: 4, group: 3



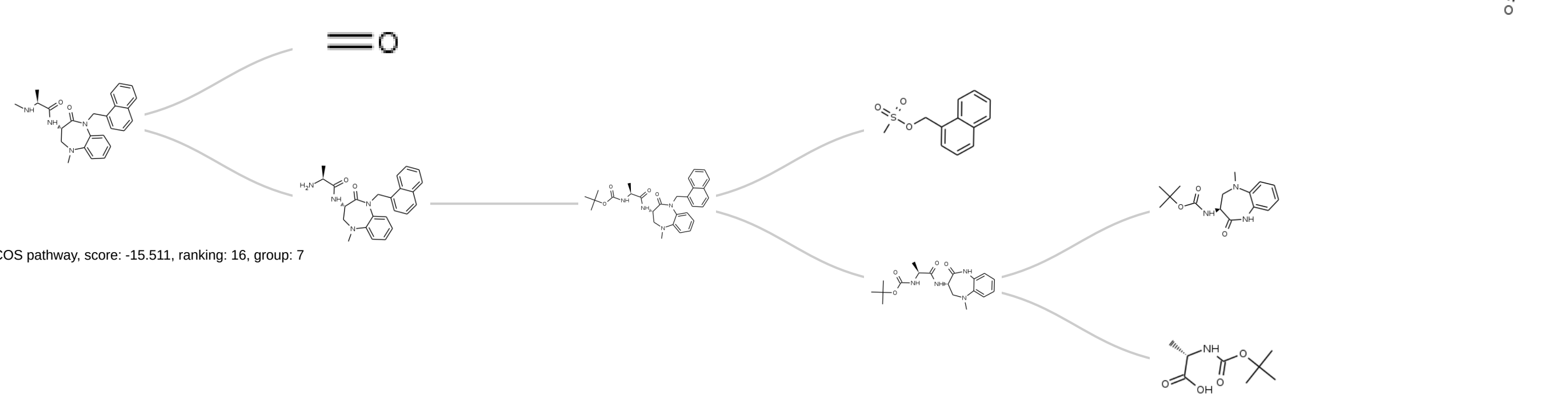
ASKCOS pathway, score: -15.253, ranking: 12, group: 4



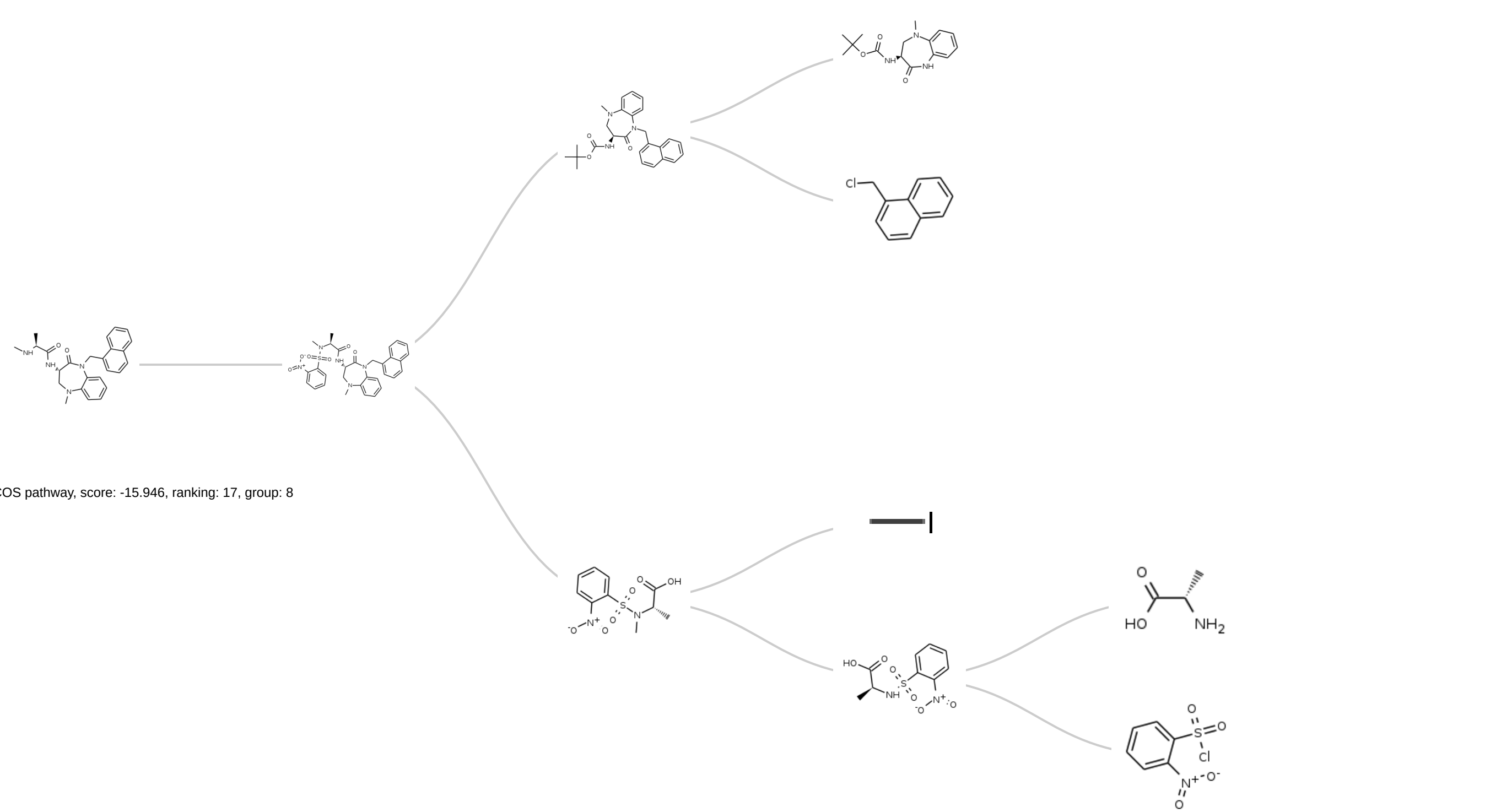
ASKCOS pathway, score: -15.485, ranking: 14, group: 5



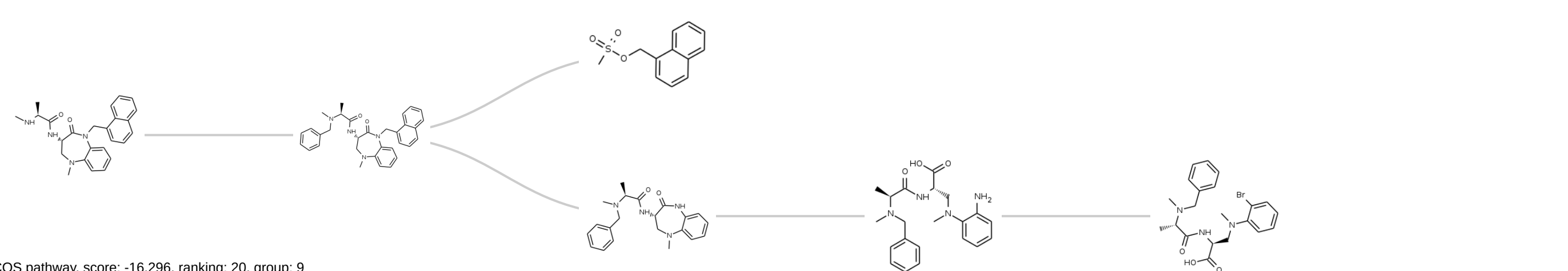
ASKCOS pathway, score: -15.488, ranking: 15, group: 6



ASKCOS pathway, score: -15.511, ranking: 16, group: 7

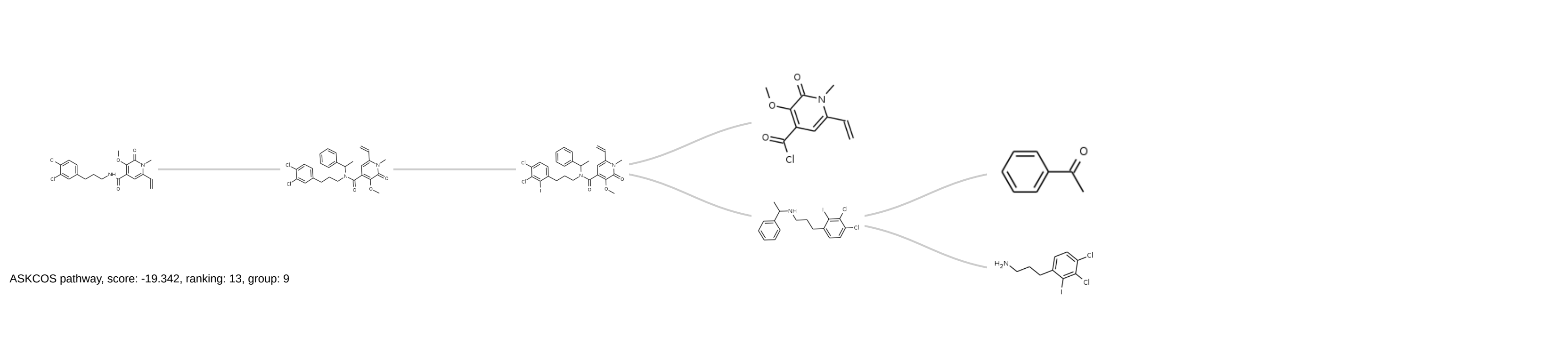
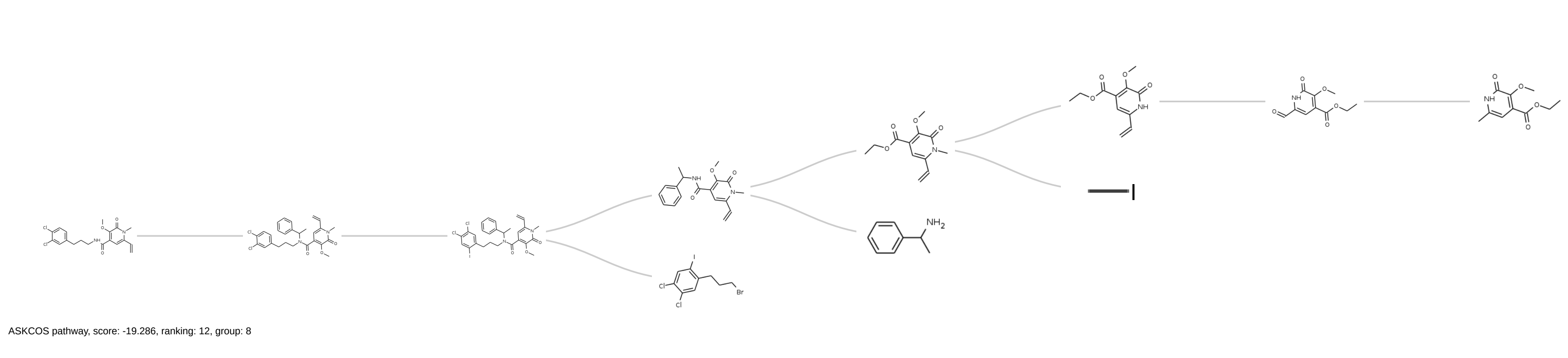
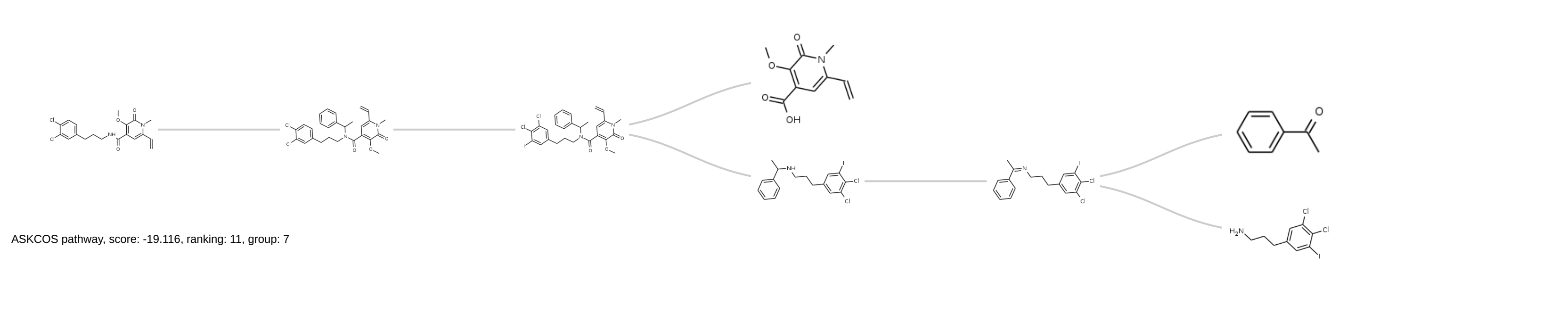
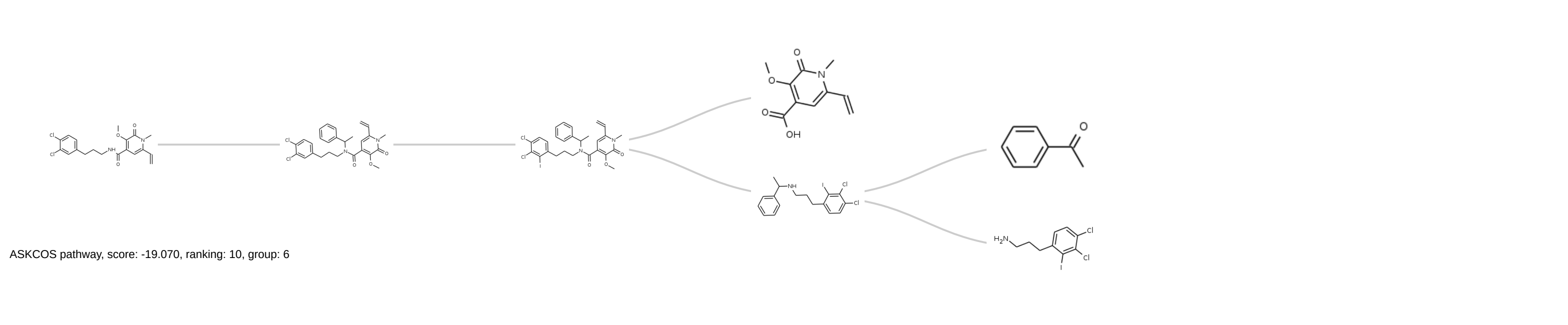
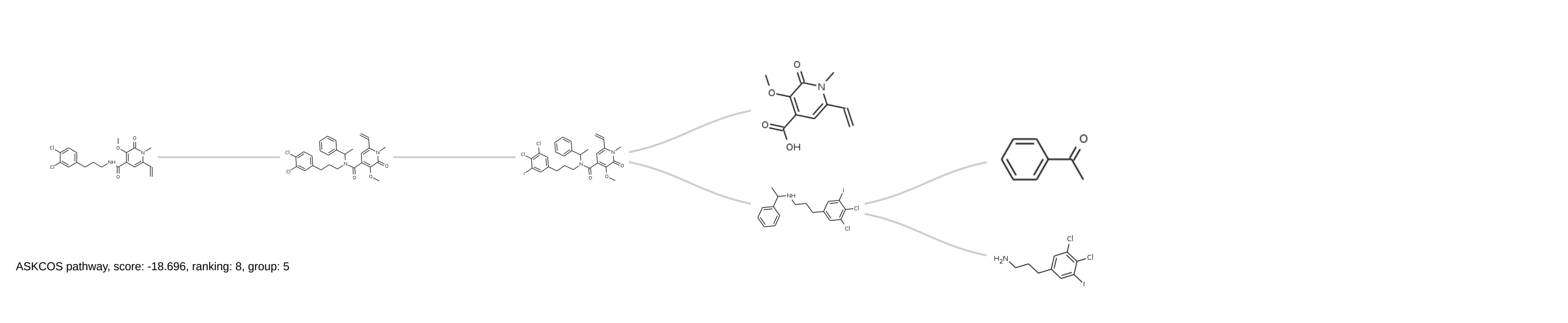
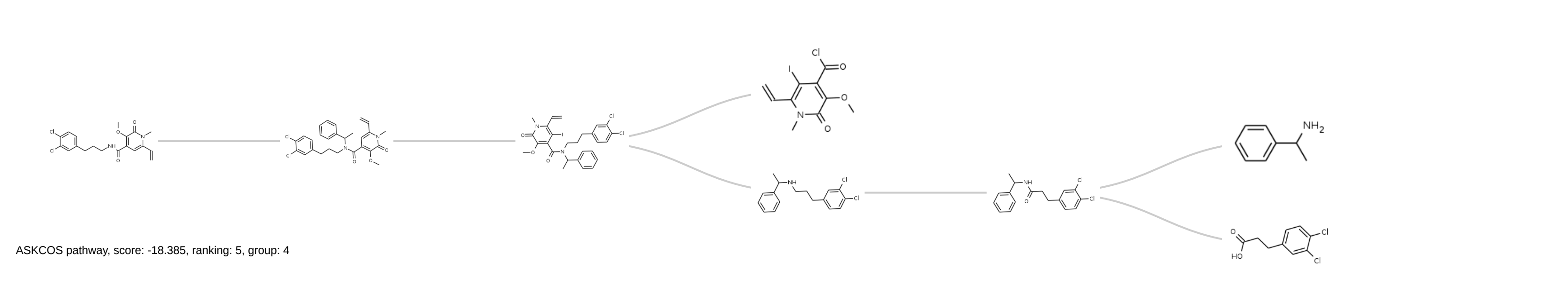
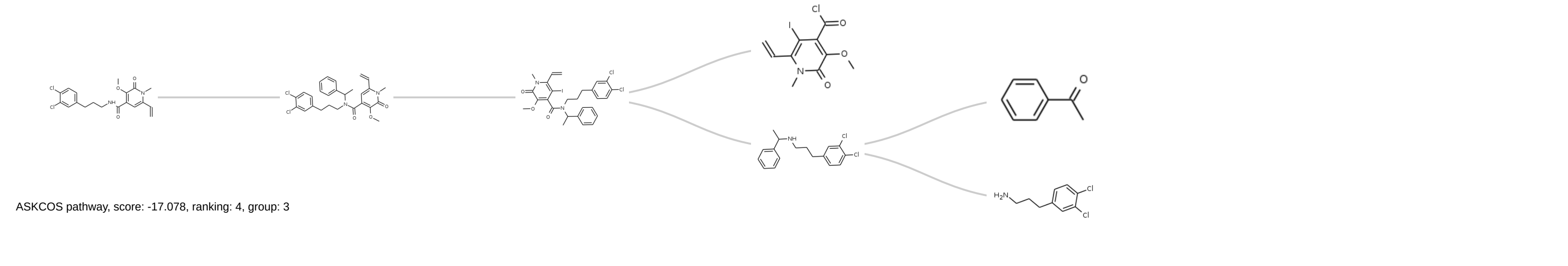
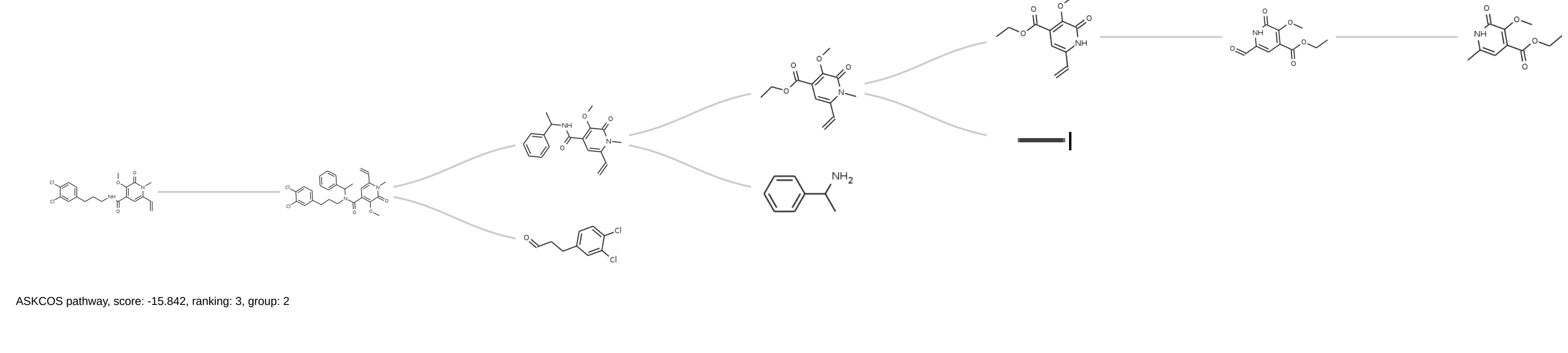
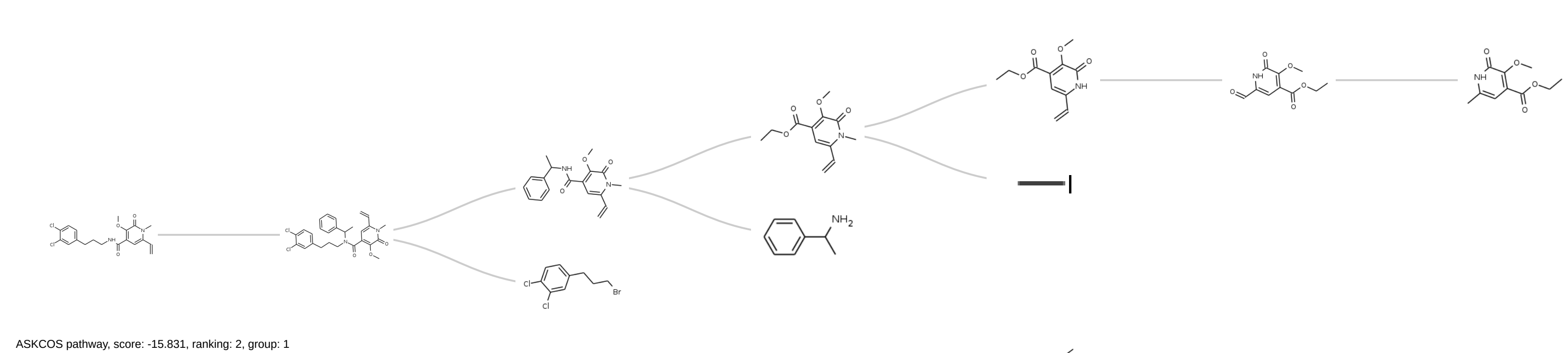
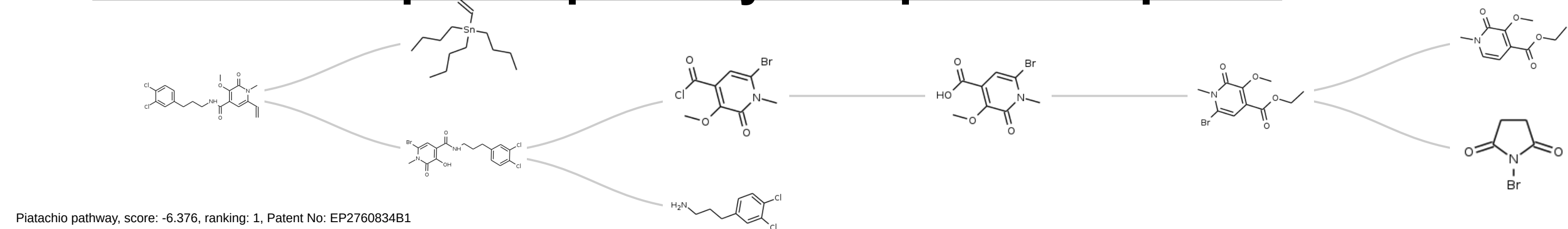


ASKCOS pathway, score: -15.946, ranking: 17, group: 8



ASKCOS pathway, score: -16.296, ranking: 20, group: 9

# Model ranks patent pathway as top-1: Example 20

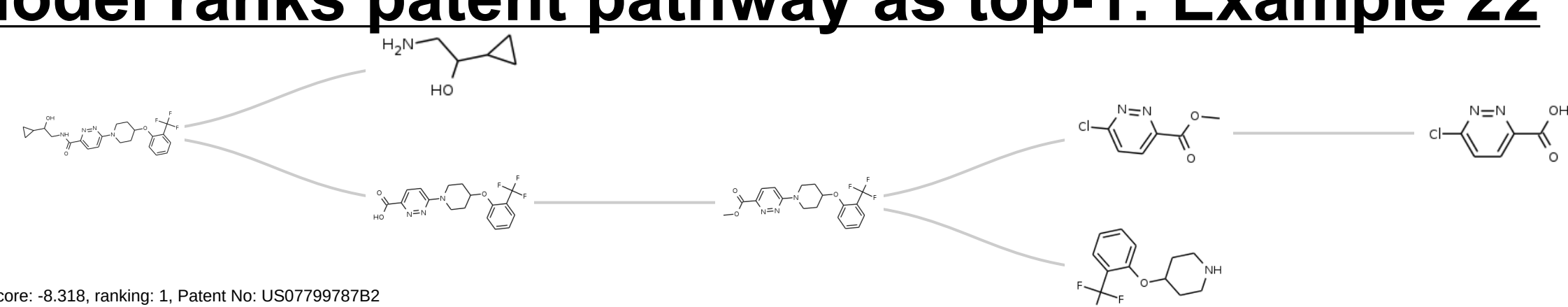




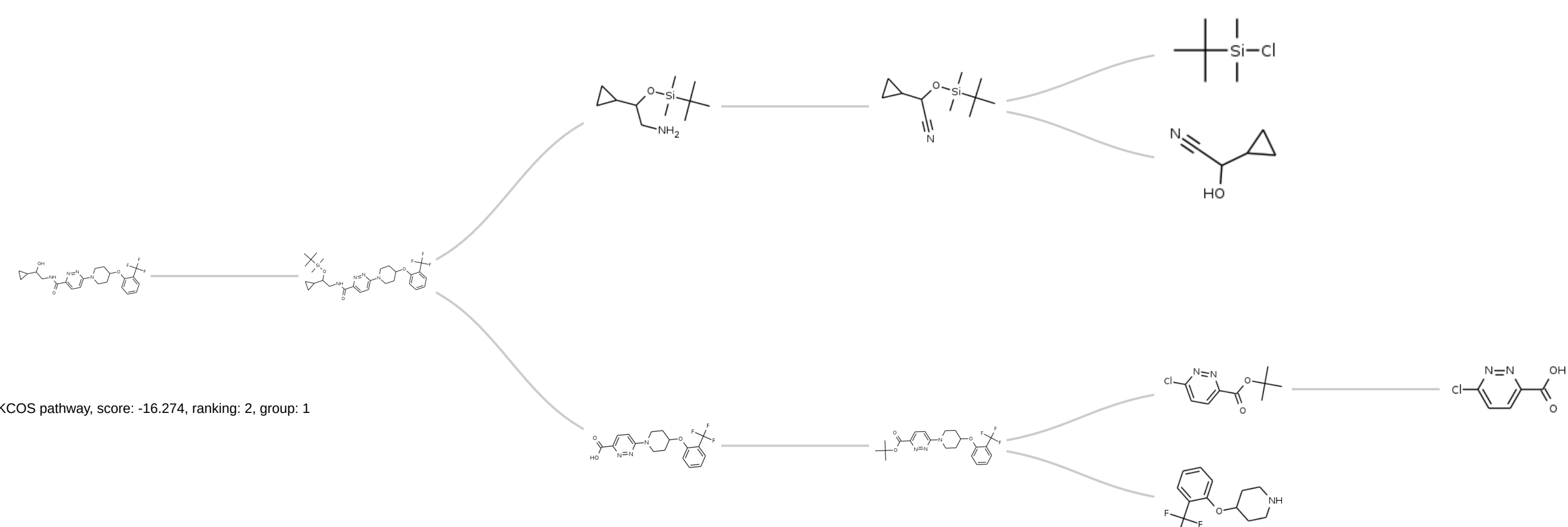


# Model ranks patent pathway as top-1: Example 22

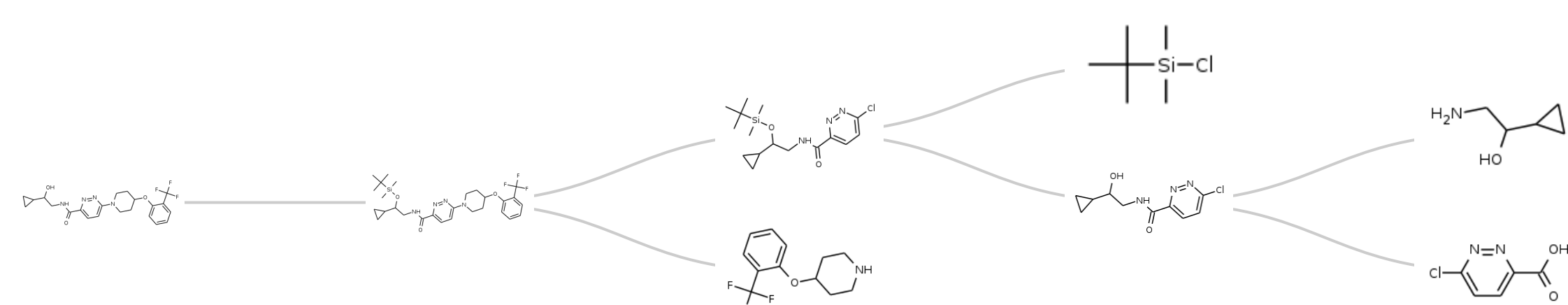
PatInfo pathway, score: -8.318, ranking: 1, Patent No: US07799787B2



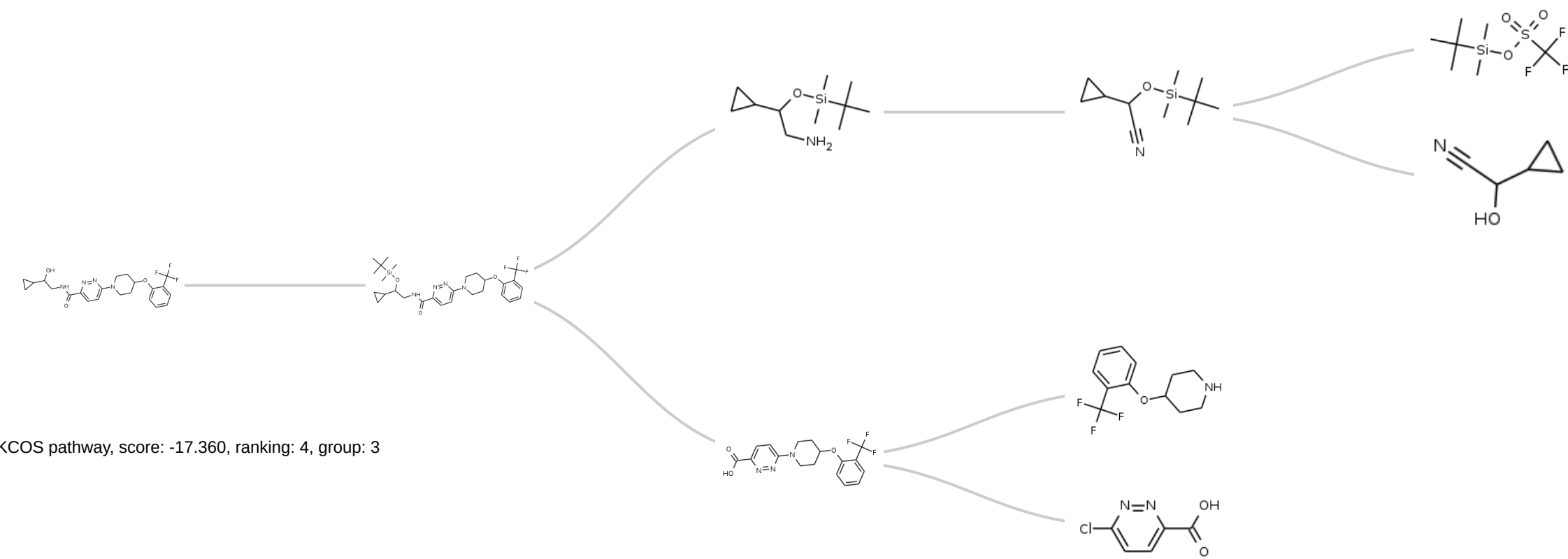
ASKCOS pathway, score: -16.274, ranking: 2, group: 1



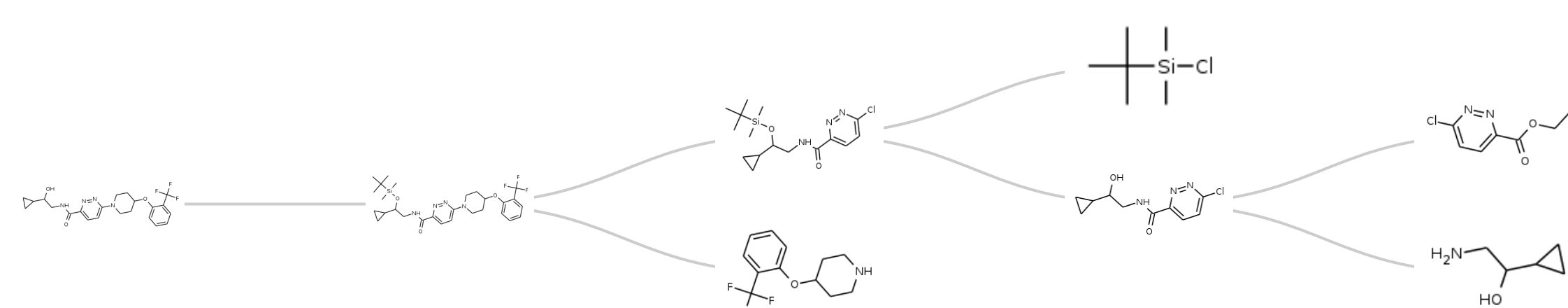
ASKCOS pathway, score: -16.700, ranking: 3, group: 2



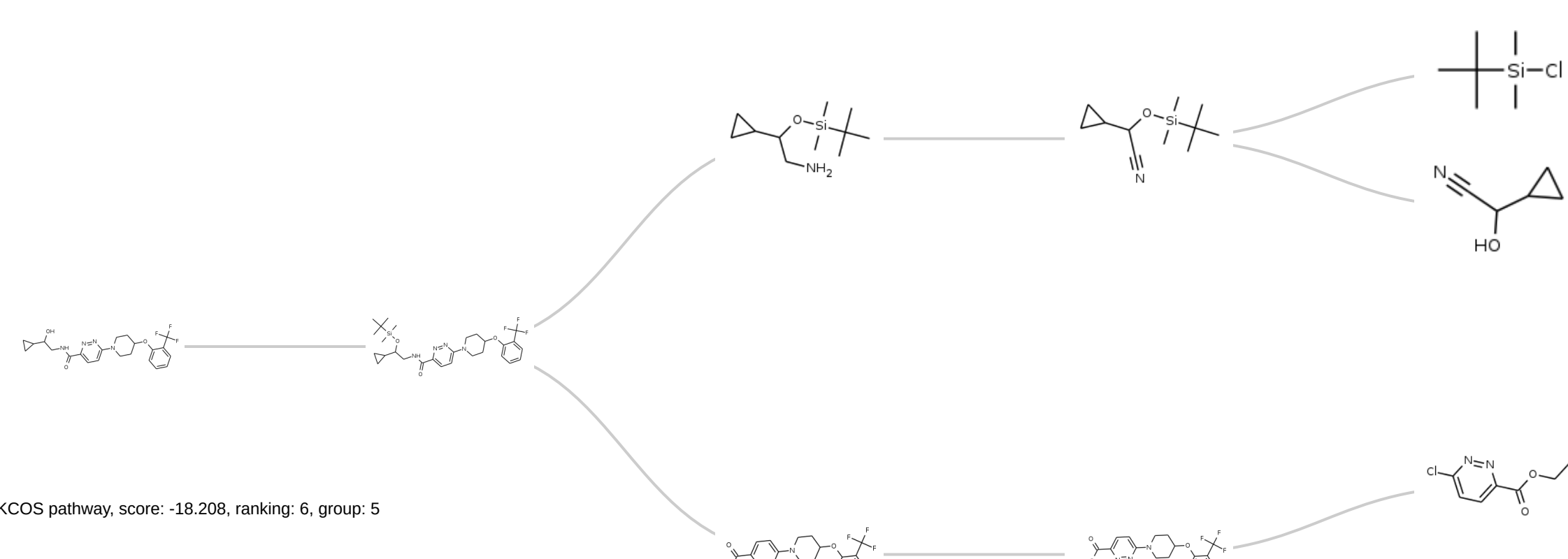
ASKCOS pathway, score: -17.350, ranking: 4, group: 3



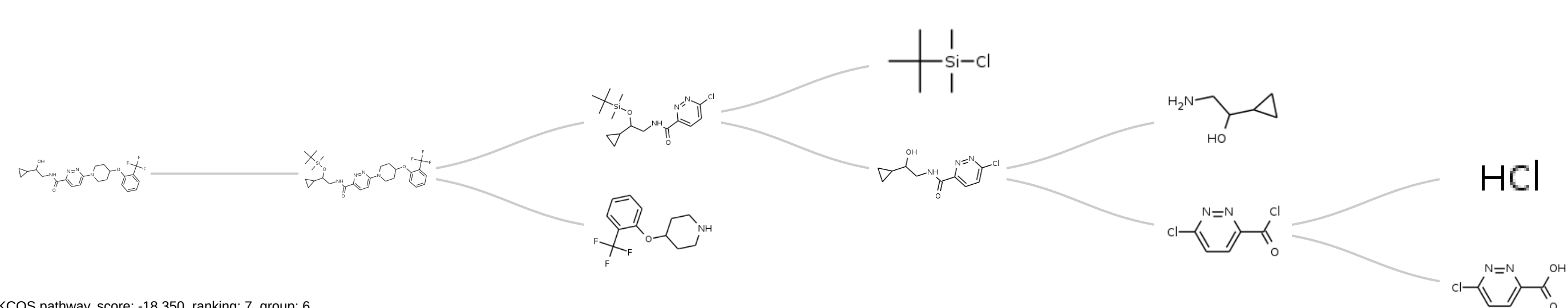
ASKCOS pathway, score: -18.005, ranking: 5, group: 4



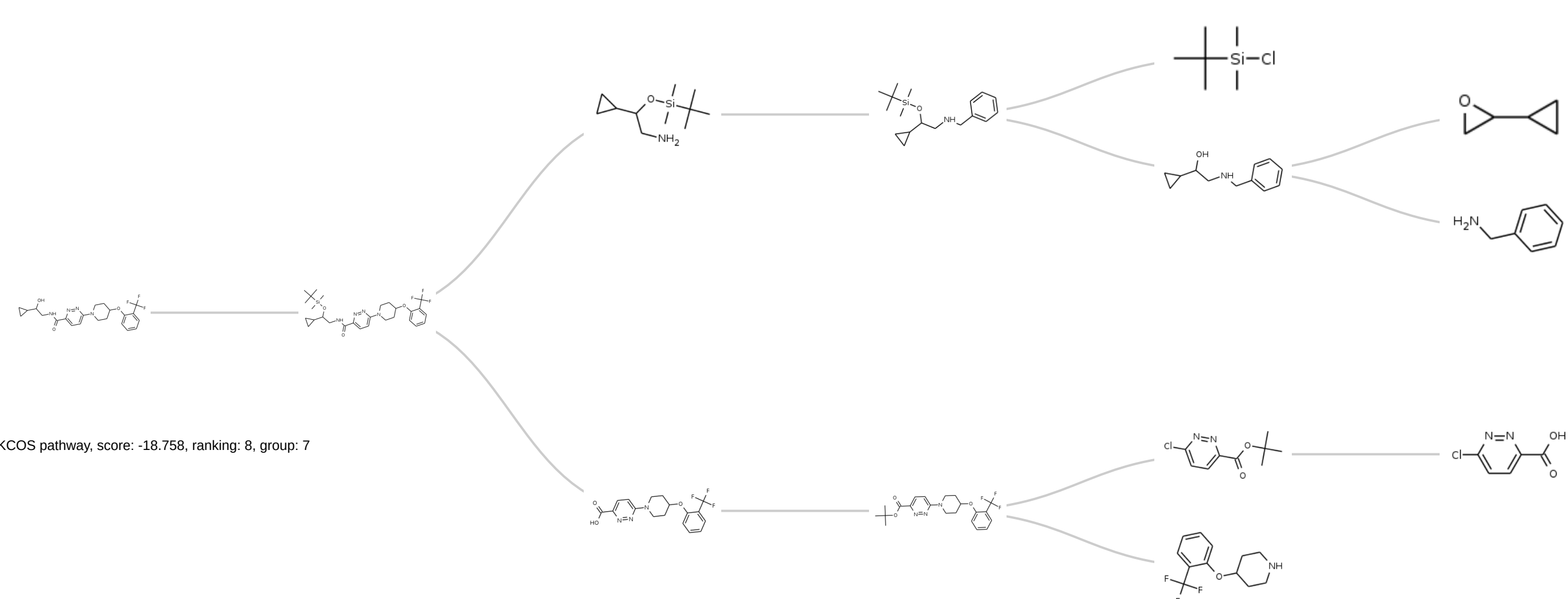
ASKCOS pathway, score: -18.208, ranking: 6, group: 5



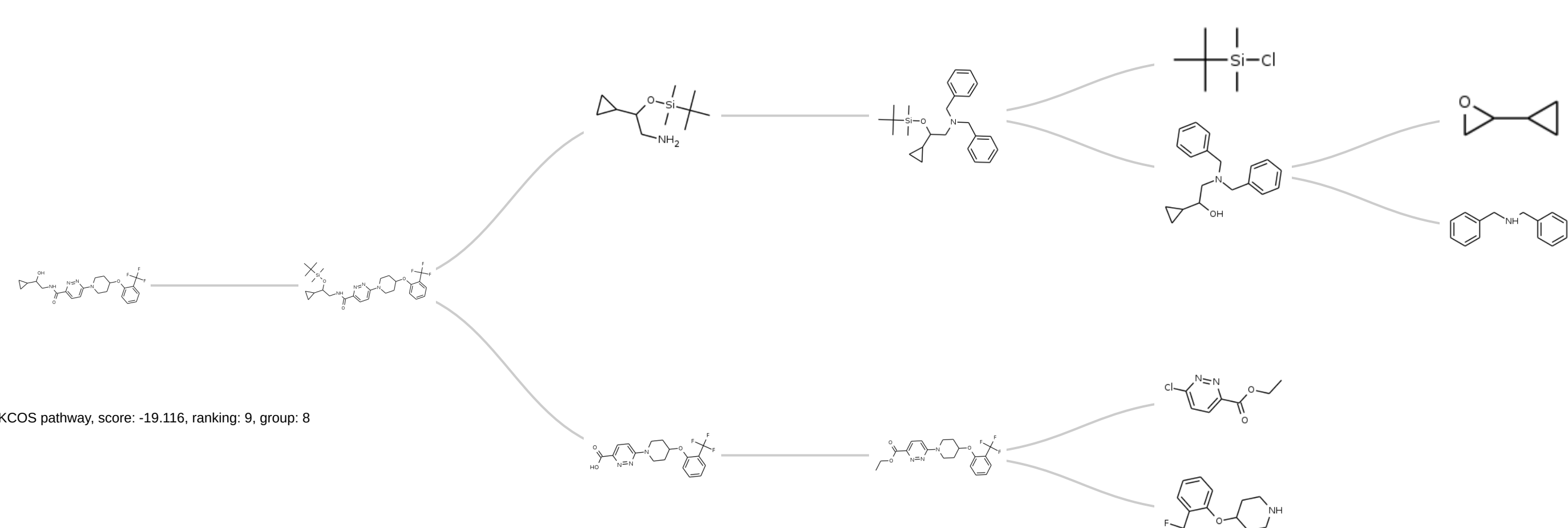
ASKCOS pathway, score: -18.350, ranking: 7, group: 6



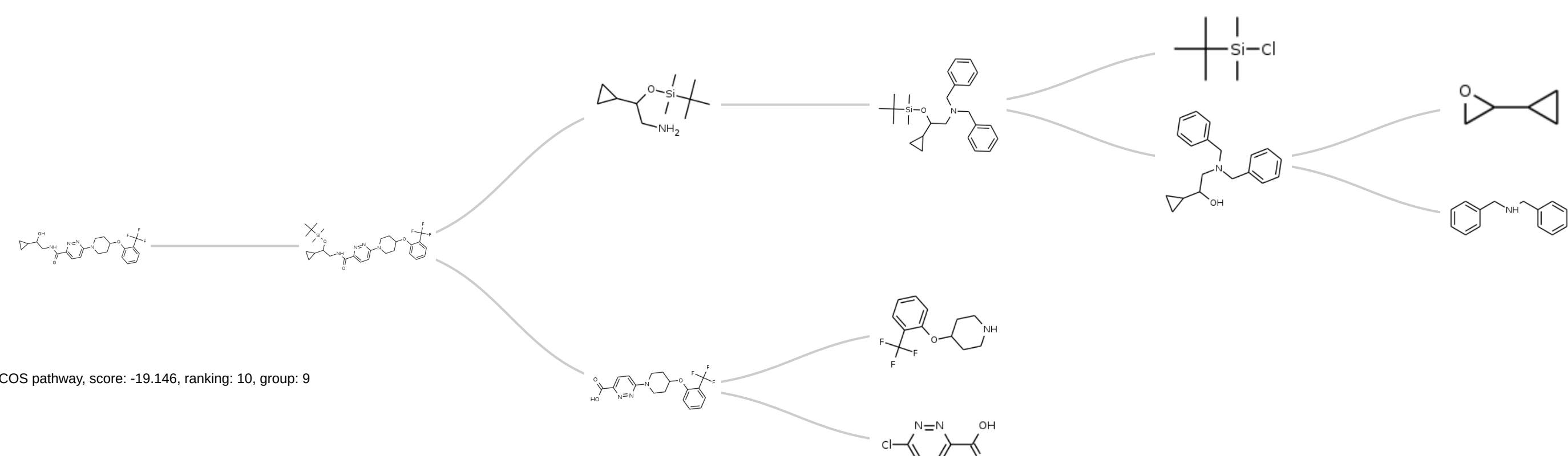
ASKCOS pathway, score: -18.758, ranking: 8, group: 7



ASKCOS pathway, score: -19.116, ranking: 9, group: 8

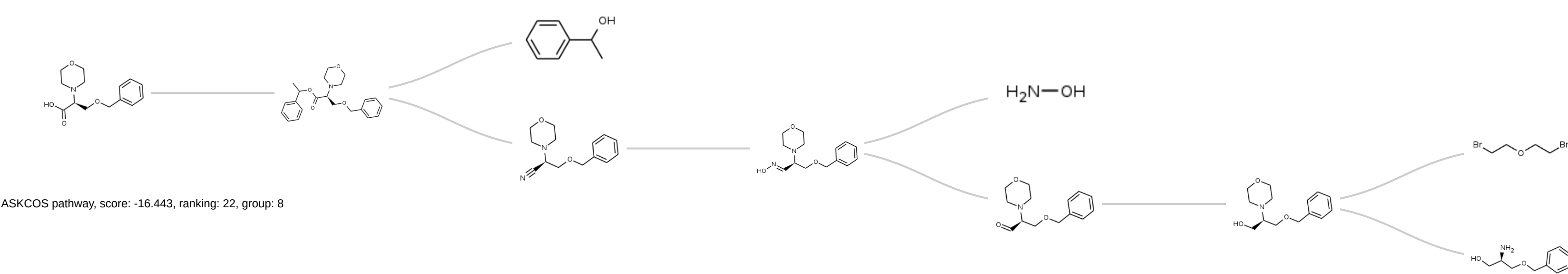
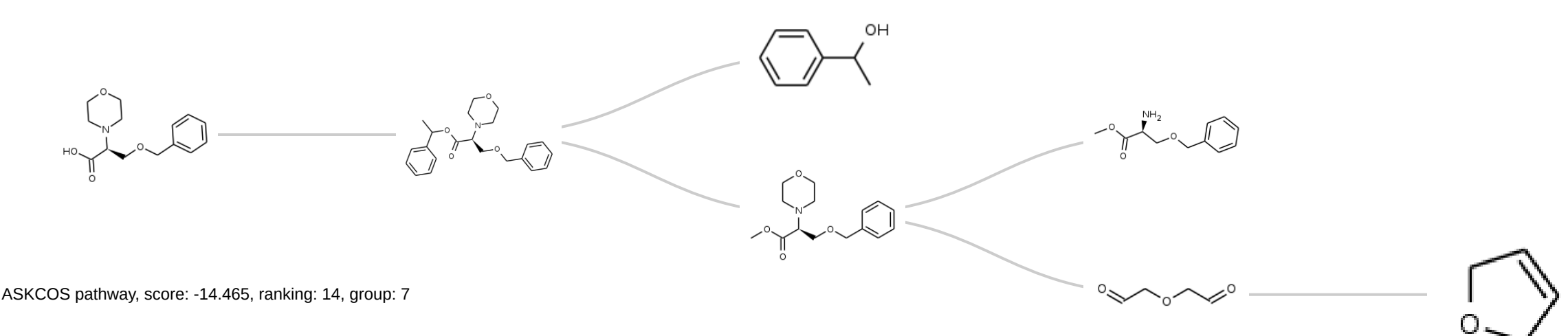
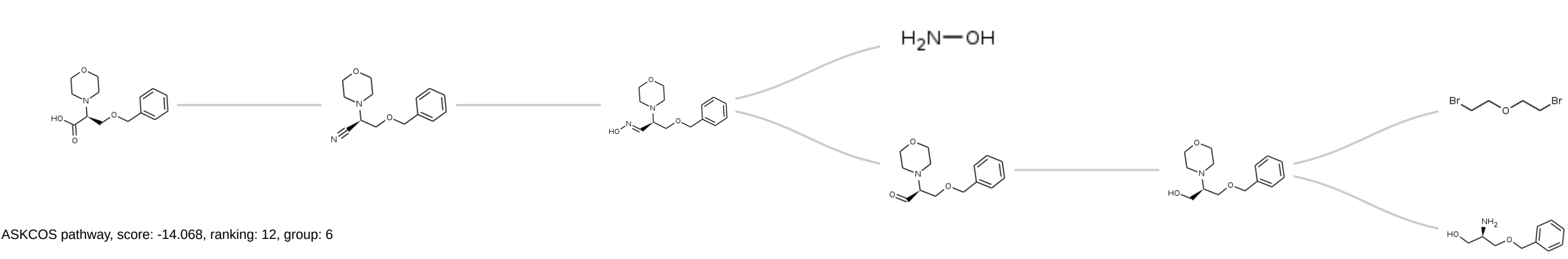
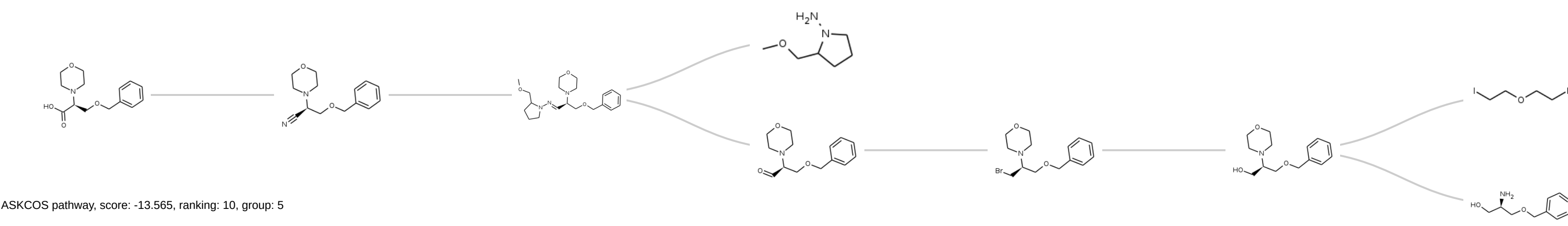
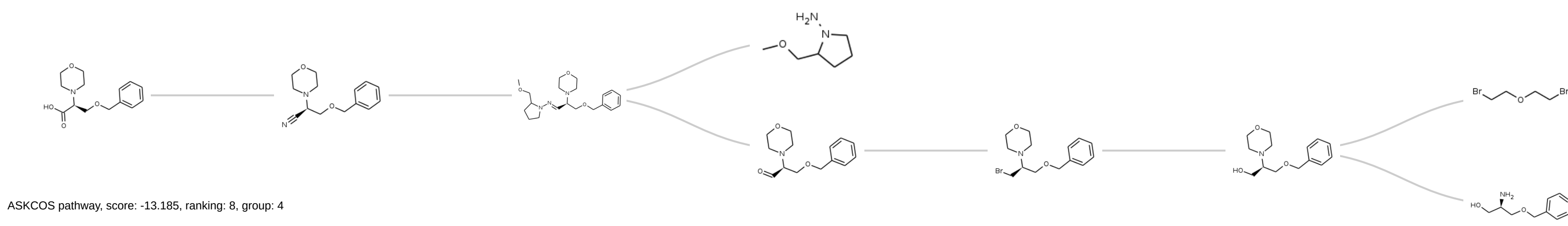
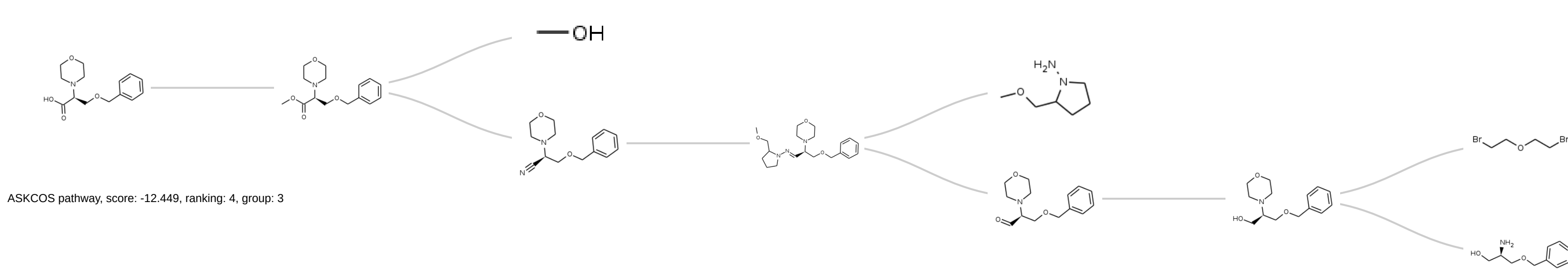
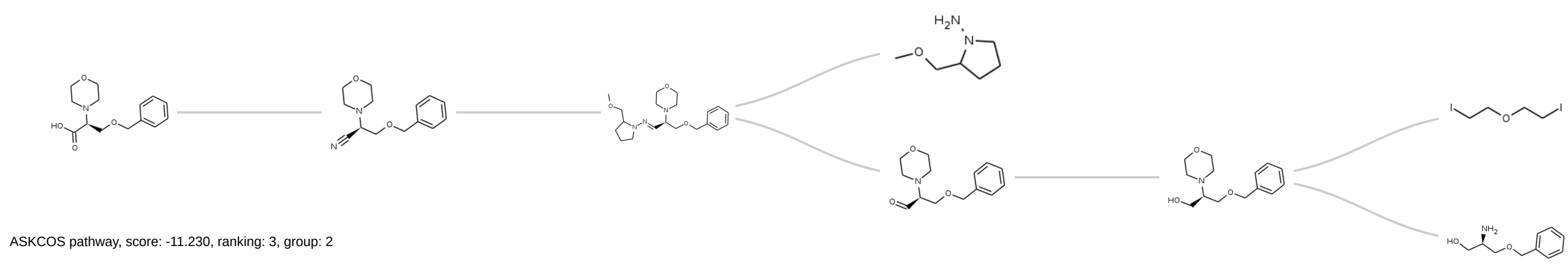
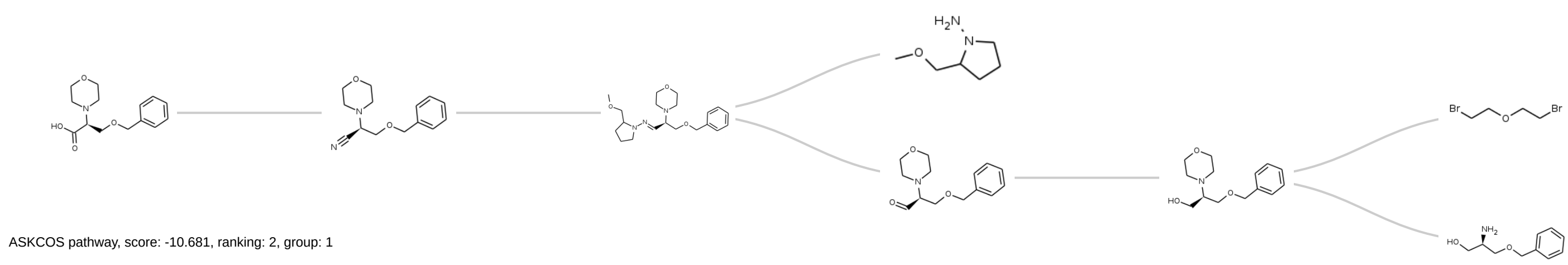
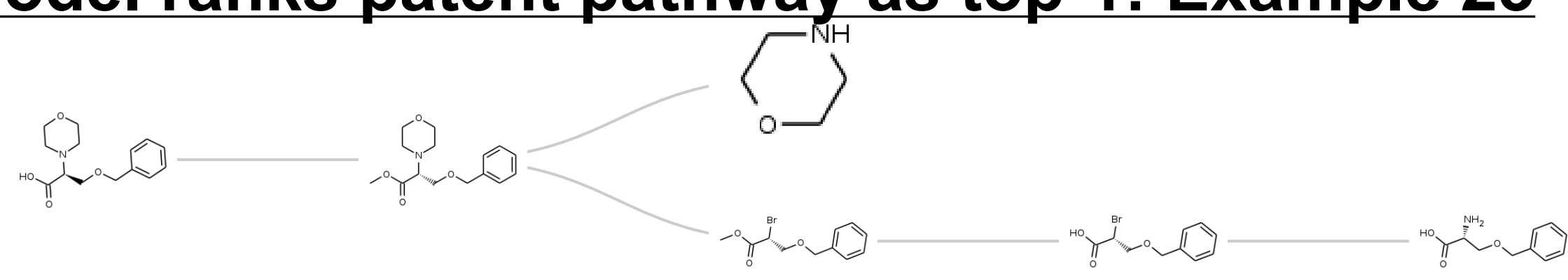


ASKCOS pathway, score: -19.146, ranking: 10, group: 9

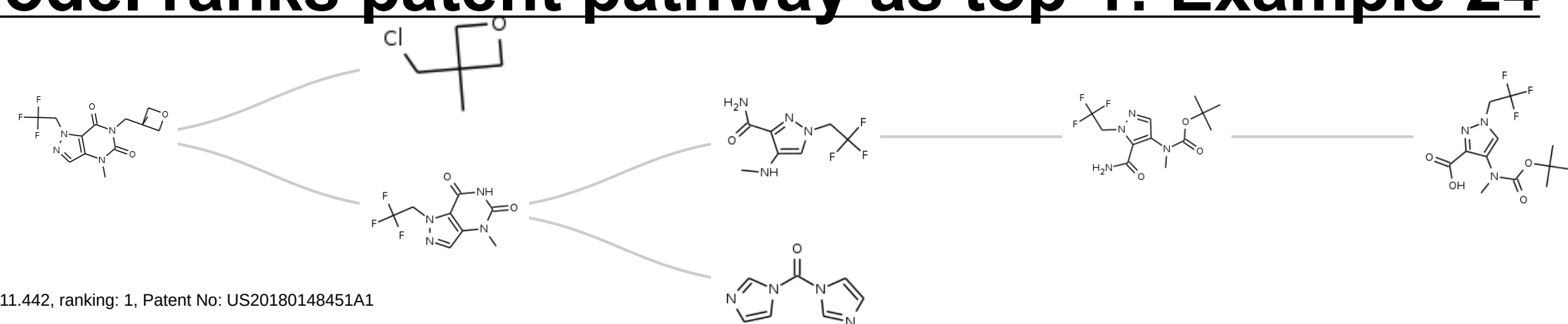




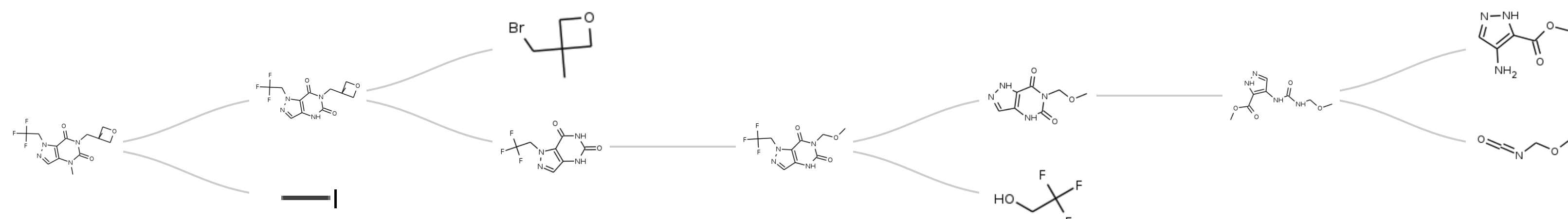
### Model ranks patent pathway as top-1: Example 23



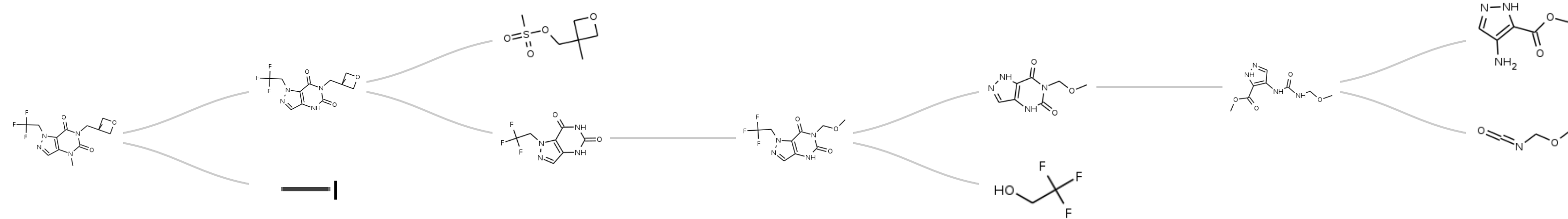
# Model ranks patent pathway as top-1: Example 24



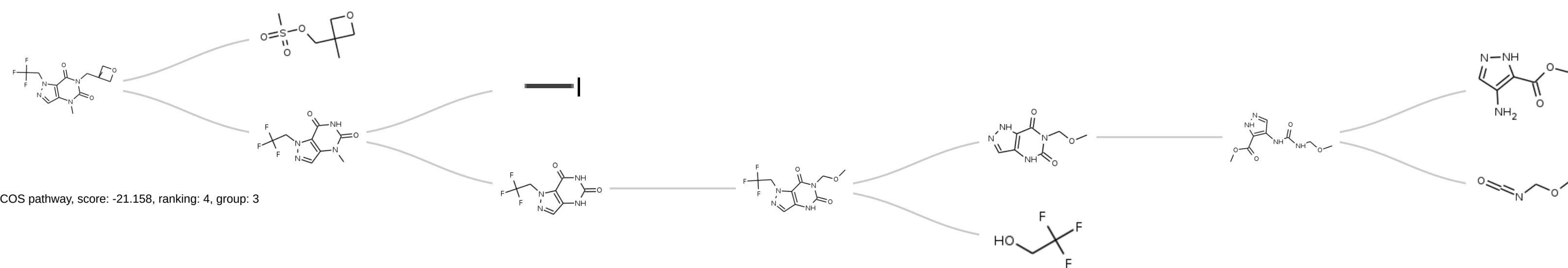
PatInfo pathway score: -11.442, ranking: 1, Patent No: US20180148451A1



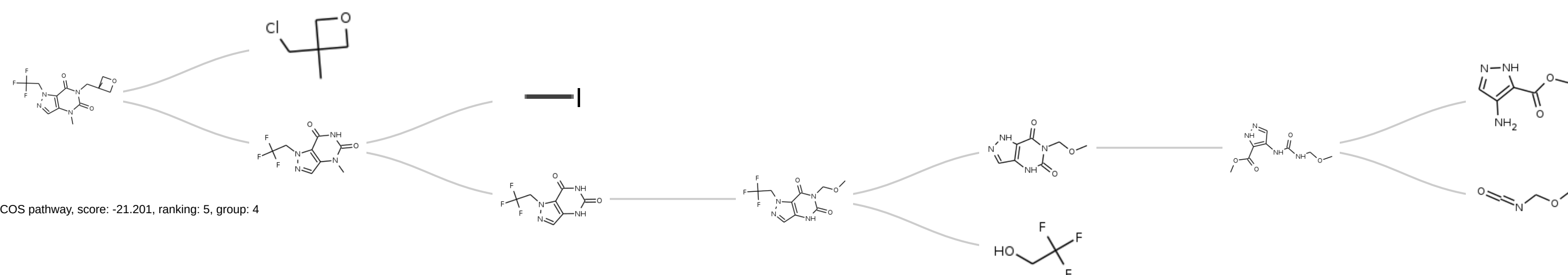
ASKCOS pathway score: -16.806, ranking: 2, group: 1



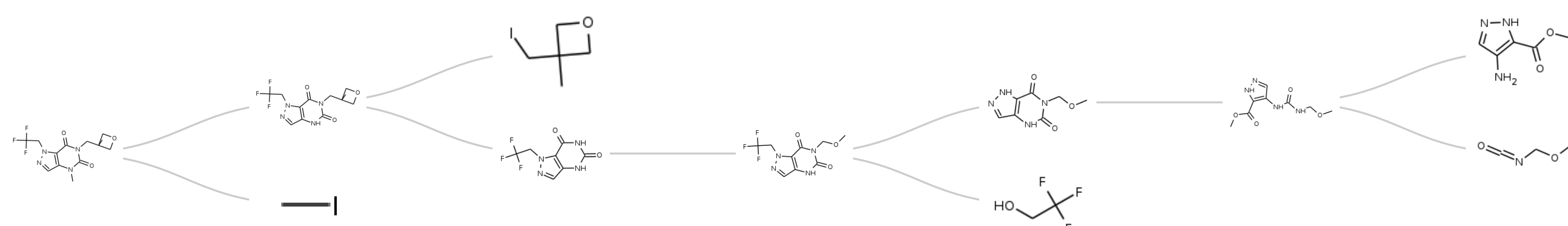
ASKCOS pathway score: -17.307, ranking: 3, group: 2



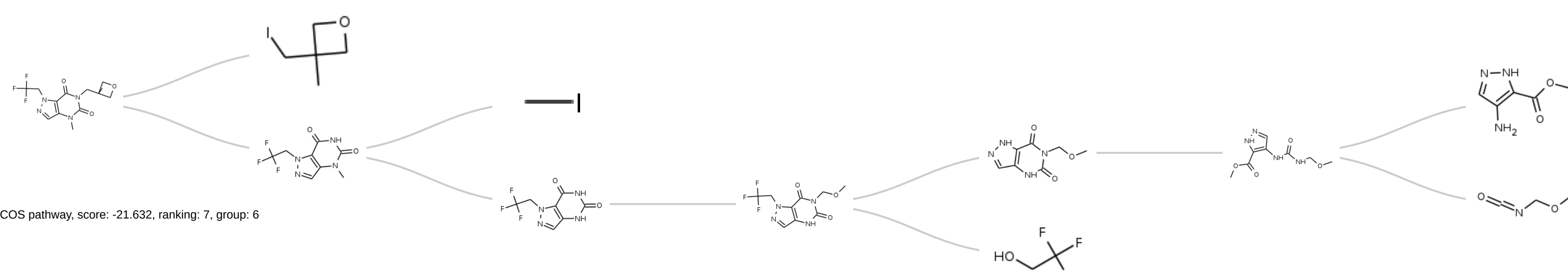
ASKCOS pathway score: -21.158, ranking: 4, group: 3



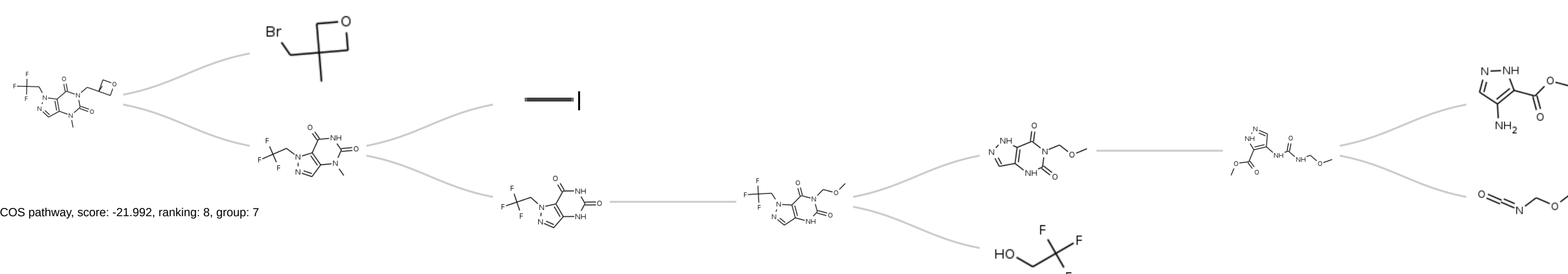
ASKCOS pathway score: -21.201, ranking: 5, group: 4



ASKCOS pathway score: -21.570, ranking: 6, group: 5

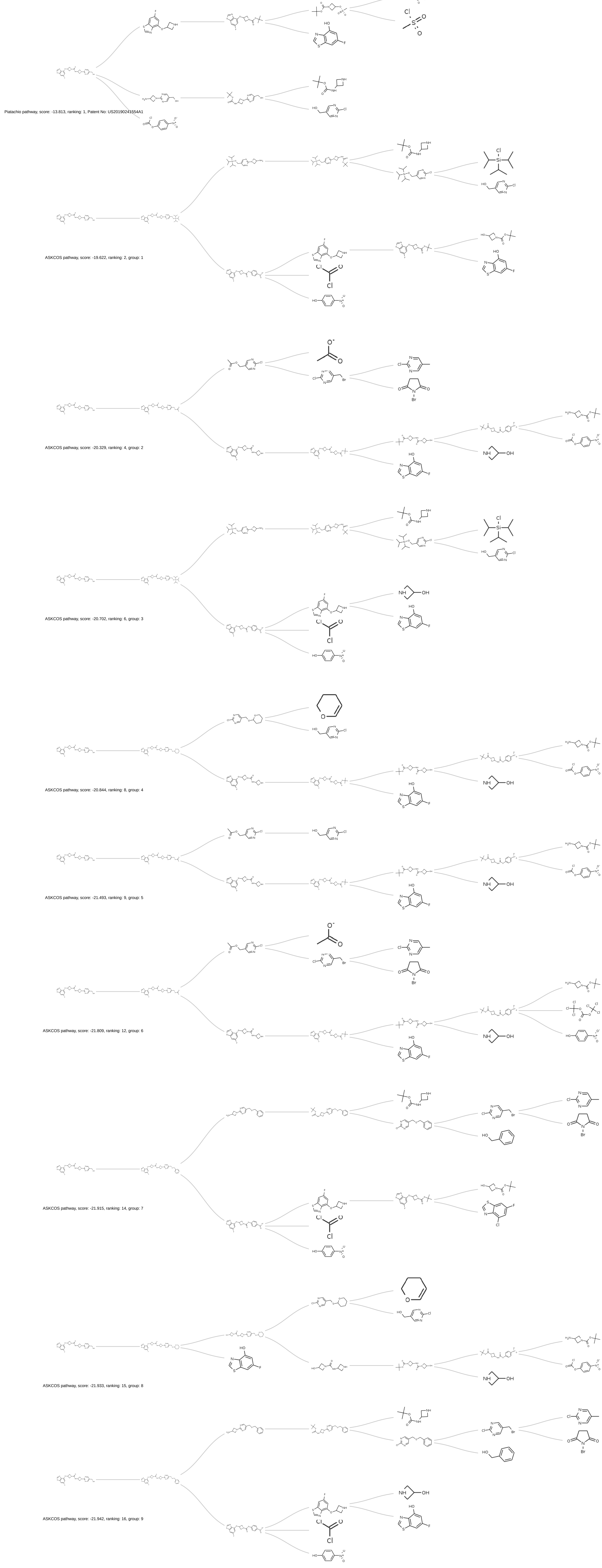


ASKCOS pathway score: -21.632, ranking: 7, group: 6

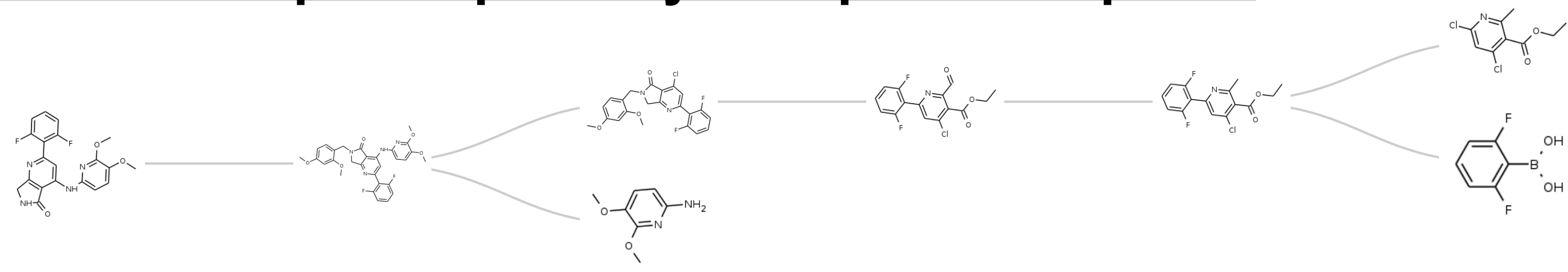


ASKCOS pathway score: -21.992, ranking: 8, group: 7

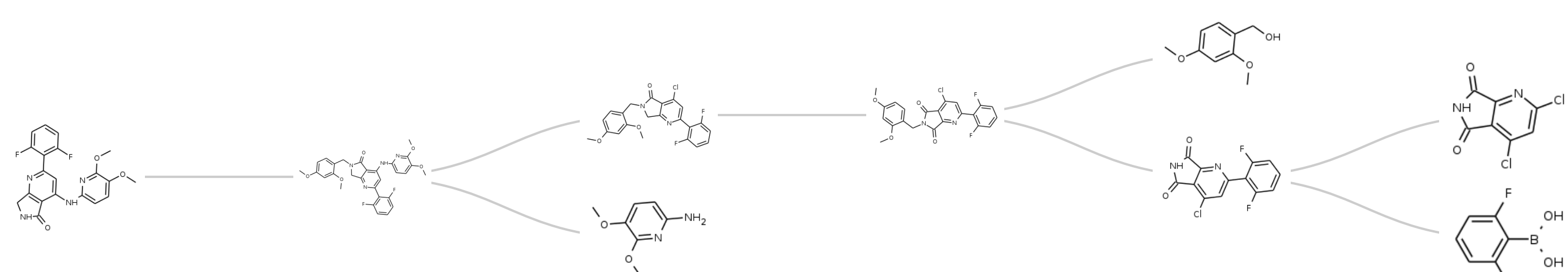
# Model ranks patent pathway as top-1: Example 25



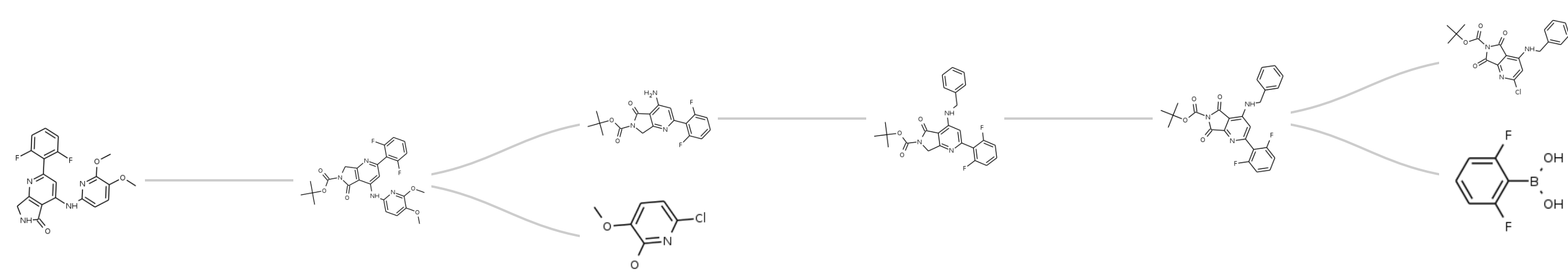
# Model ranks patent pathway as top-1: Example 26



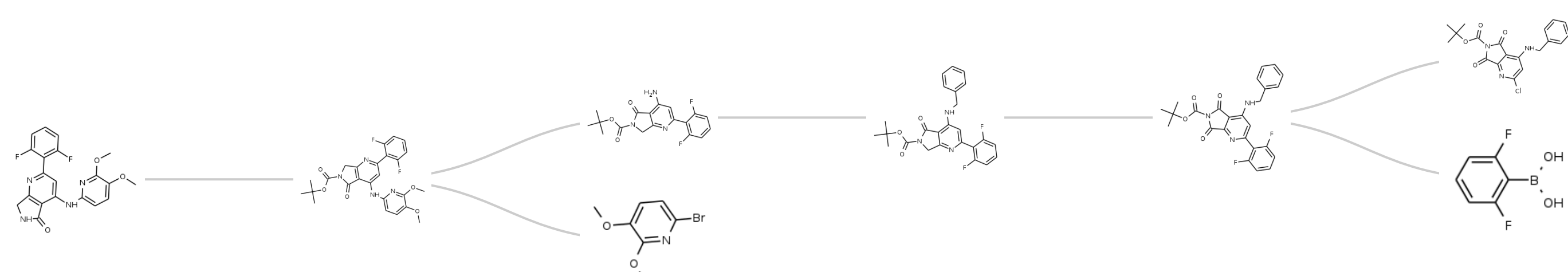
ASKCOS pathway score: -16.356, ranking: 2, group: 1



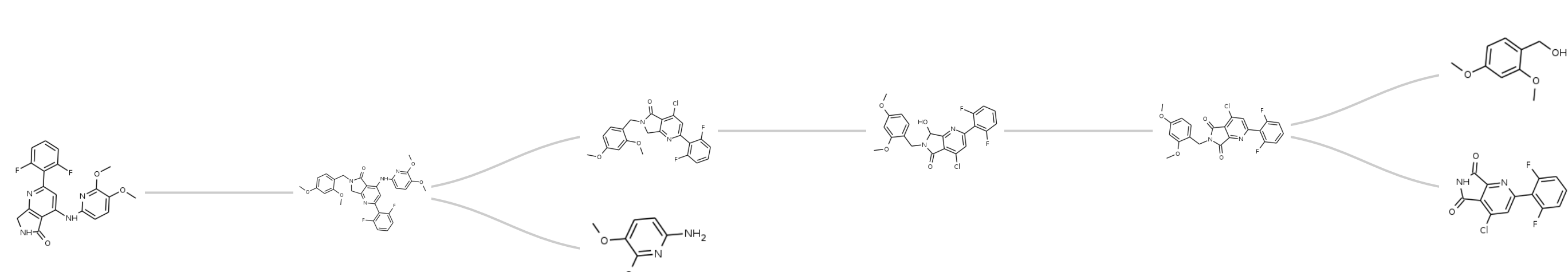
ASKCOS pathway score: -16.468, ranking: 3, group: 2



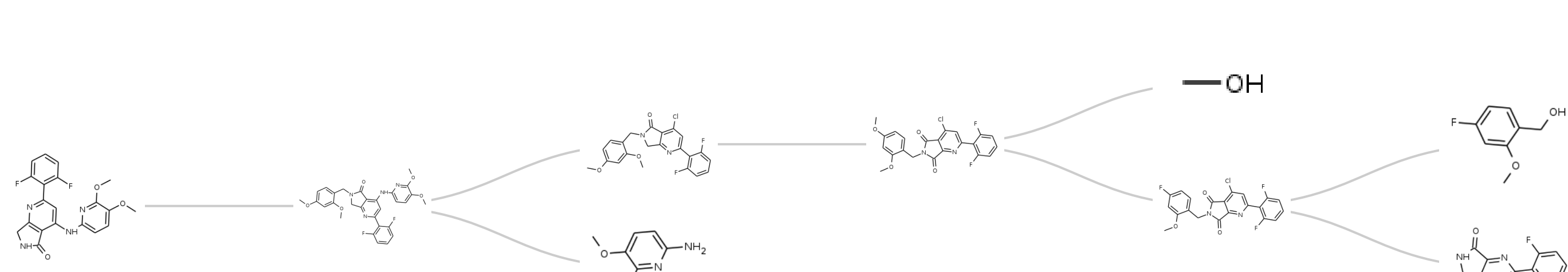
ASKCOS pathway score: -17.779, ranking: 4, group: 3



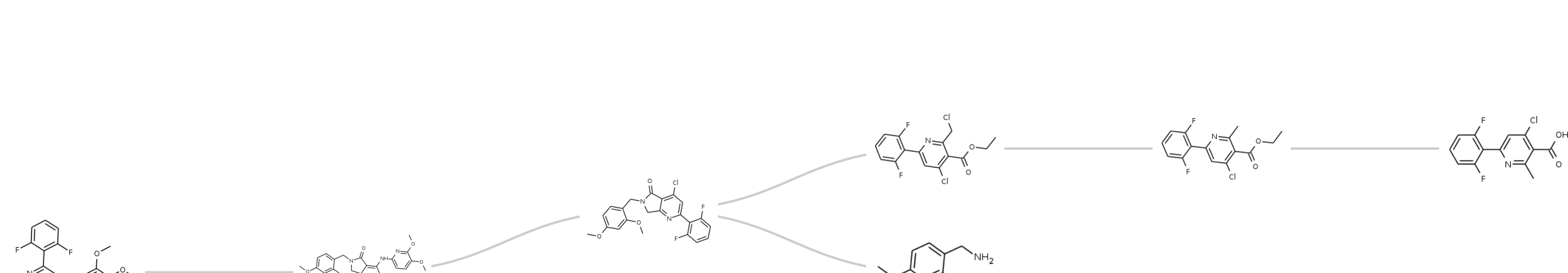
ASKCOS pathway score: -18.897, ranking: 5, group: 4



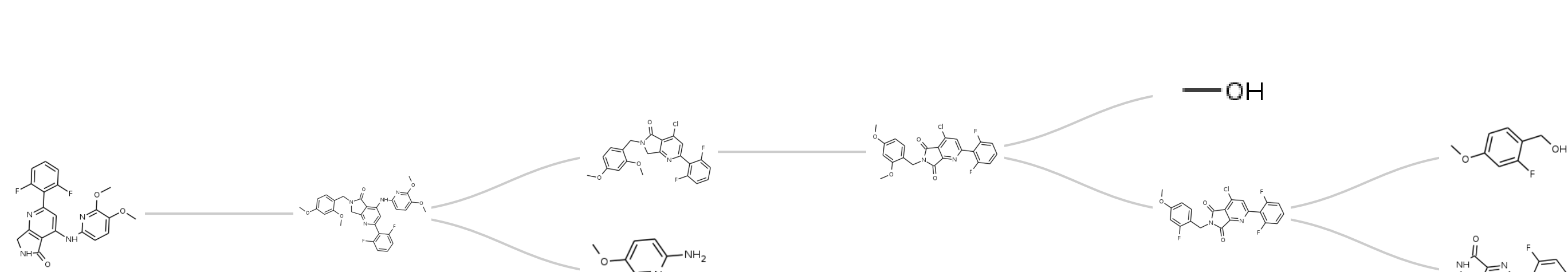
ASKCOS pathway score: -19.023, ranking: 6, group: 5



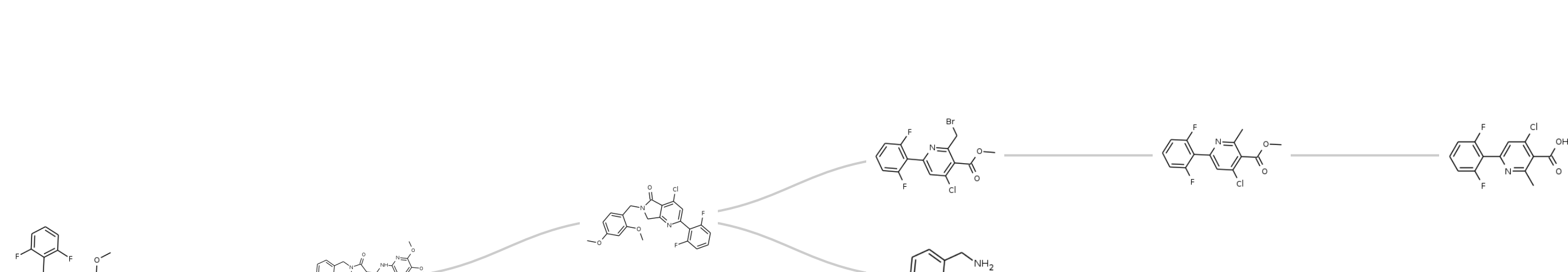
ASKCOS pathway score: -19.479, ranking: 7, group: 6



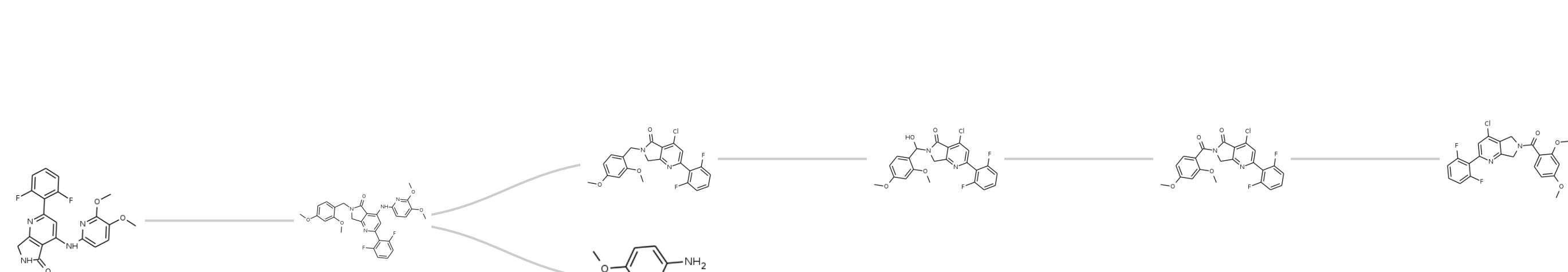
ASKCOS pathway score: -19.482, ranking: 8, group: 7



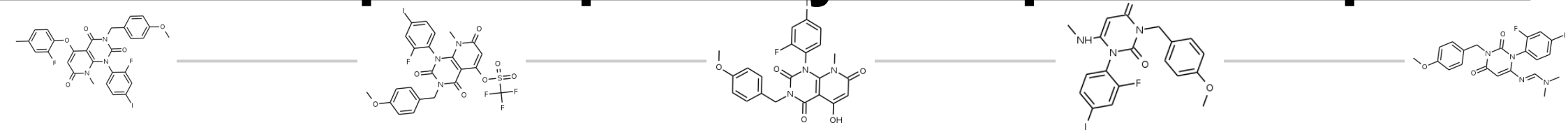
ASKCOS pathway score: -20.894, ranking: 16, group: 8



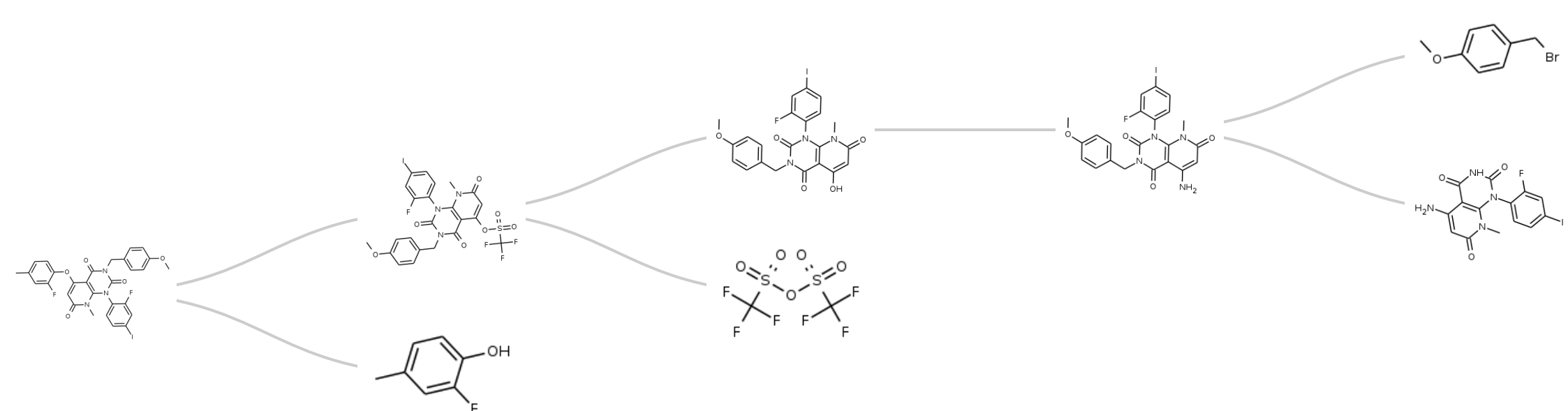
ASKCOS pathway score: -21.178, ranking: 19, group: 9



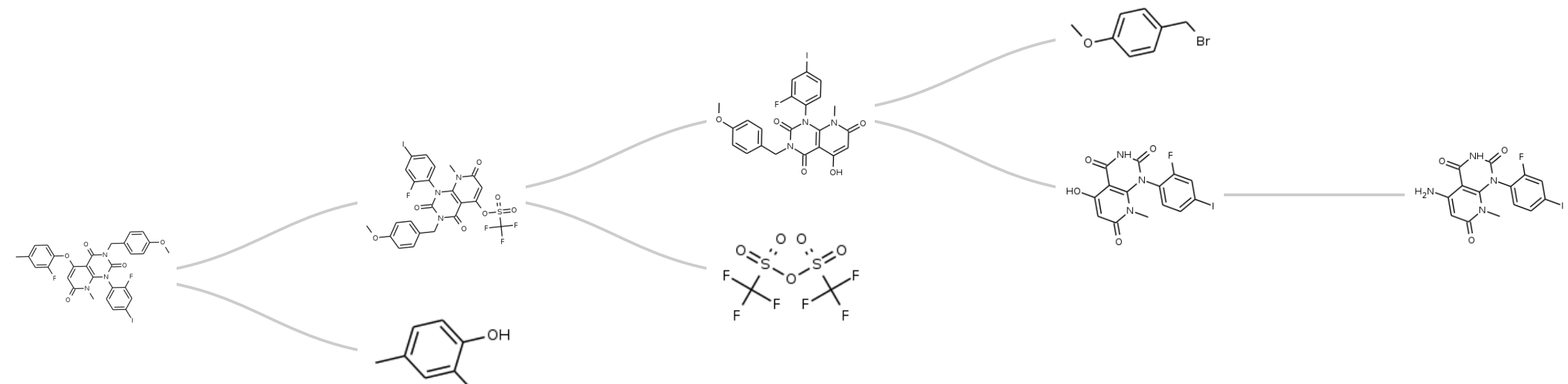
# Model ranks patent pathway as top-1: Example 27



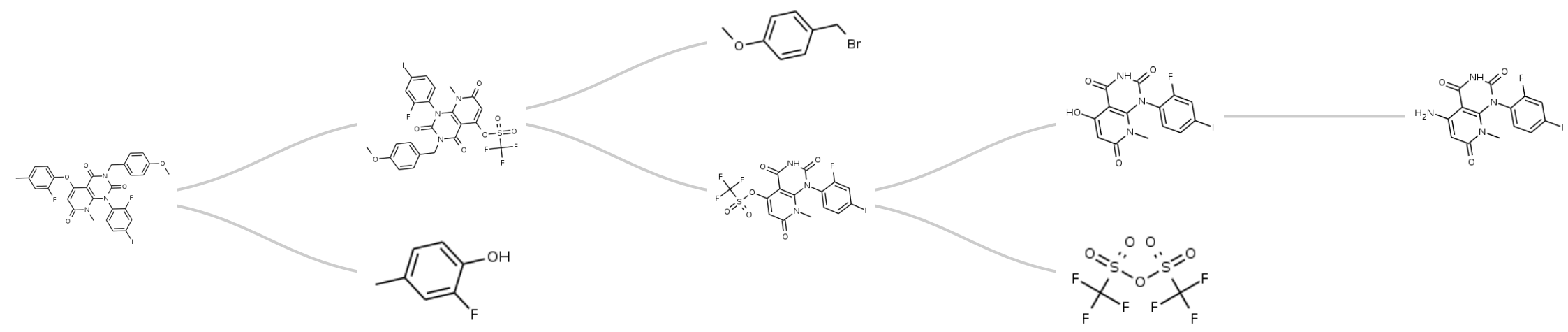
Patent pathway: score: 1.503, ranking: 1, Patent No: US10064848



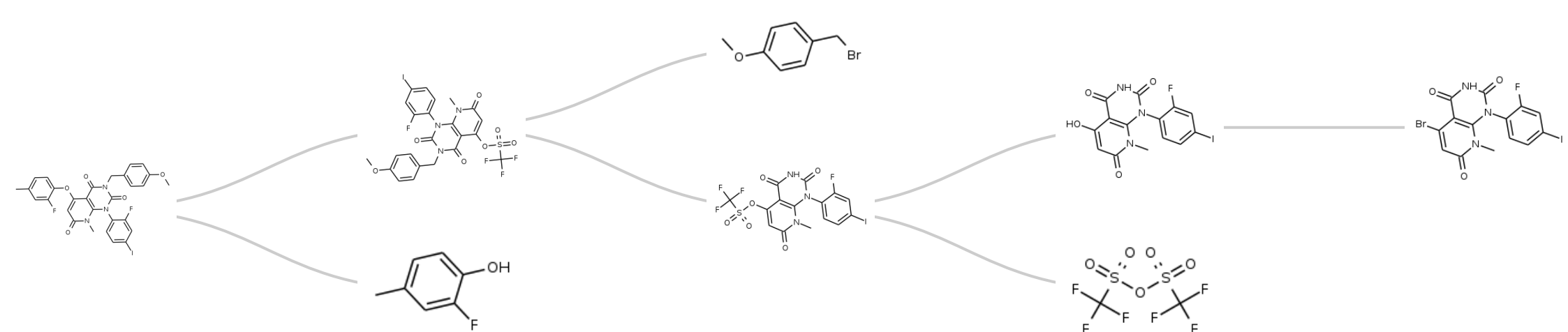
ASKCOS pathway: score: -17.367, ranking: 2, group: 1



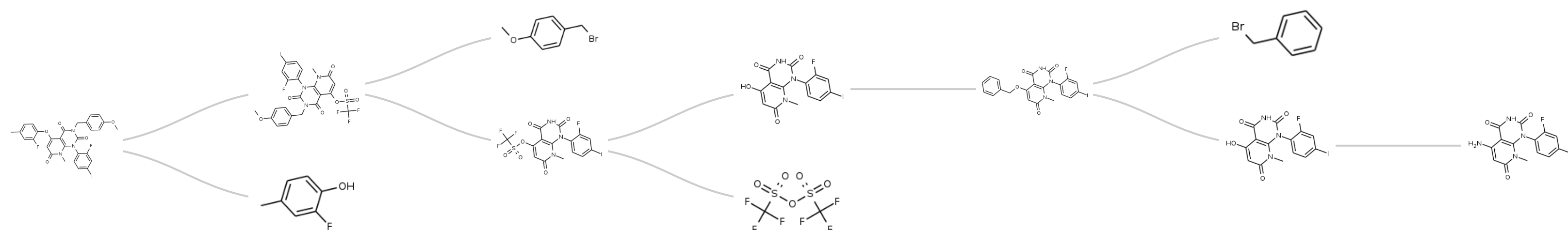
ASKCOS pathway: score: -18.055, ranking: 3, group: 2



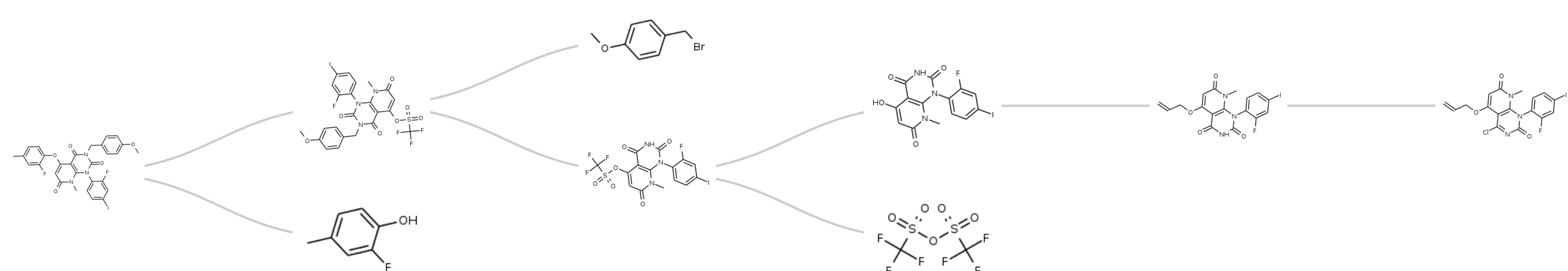
ASKCOS pathway: score: -18.070, ranking: 4, group: 3



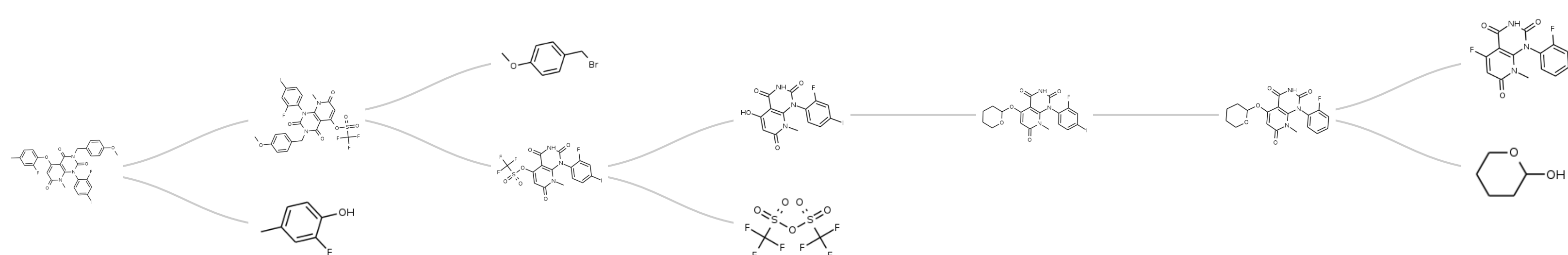
ASKCOS pathway: score: -18.211, ranking: 5, group: 4



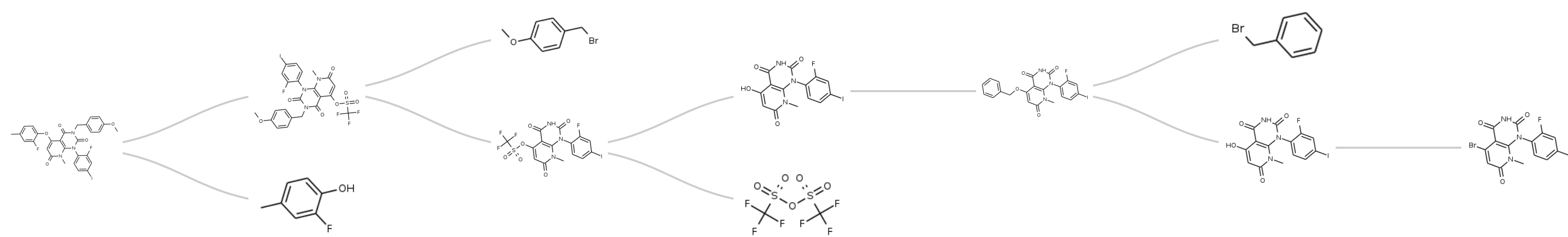
ASKCOS pathway: score: -20.907, ranking: 16, group: 5



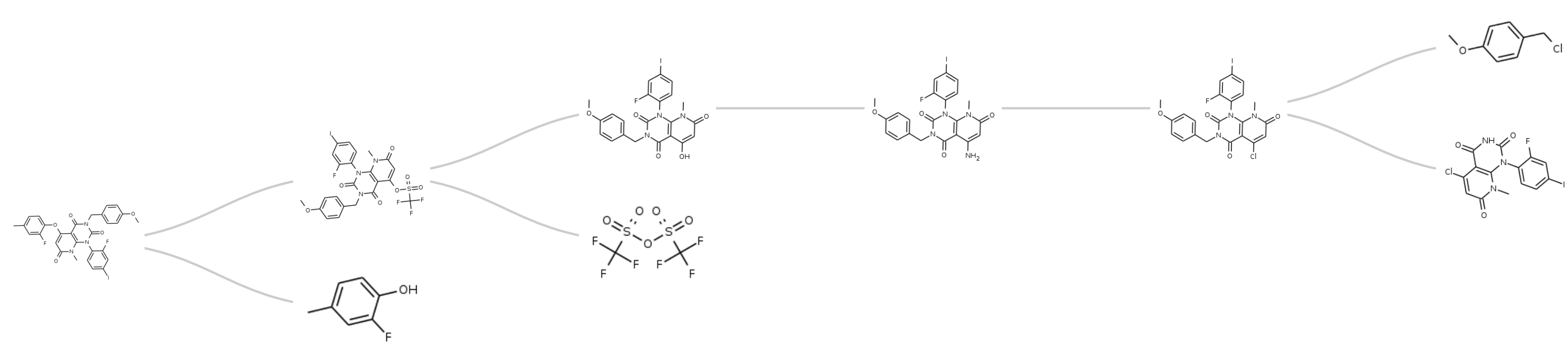
ASKCOS pathway: score: -20.919, ranking: 17, group: 6



ASKCOS pathway: score: -21.134, ranking: 19, group: 7



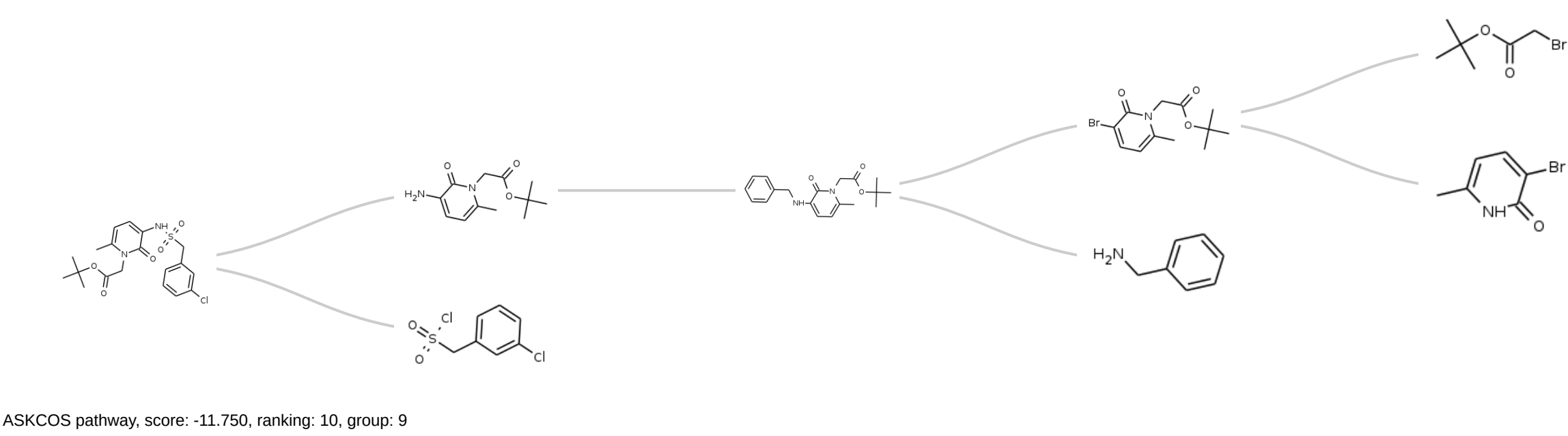
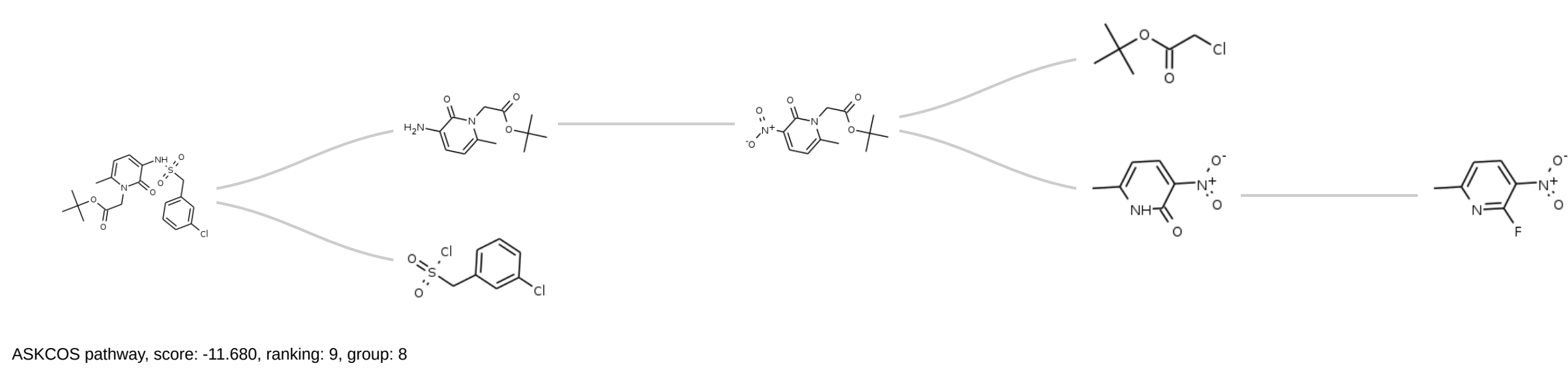
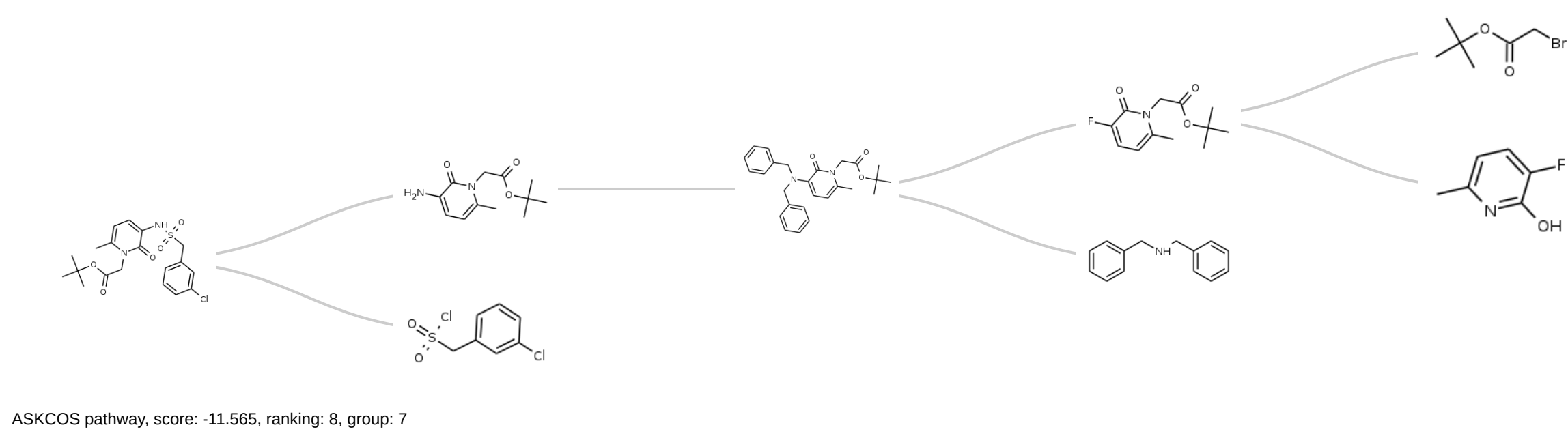
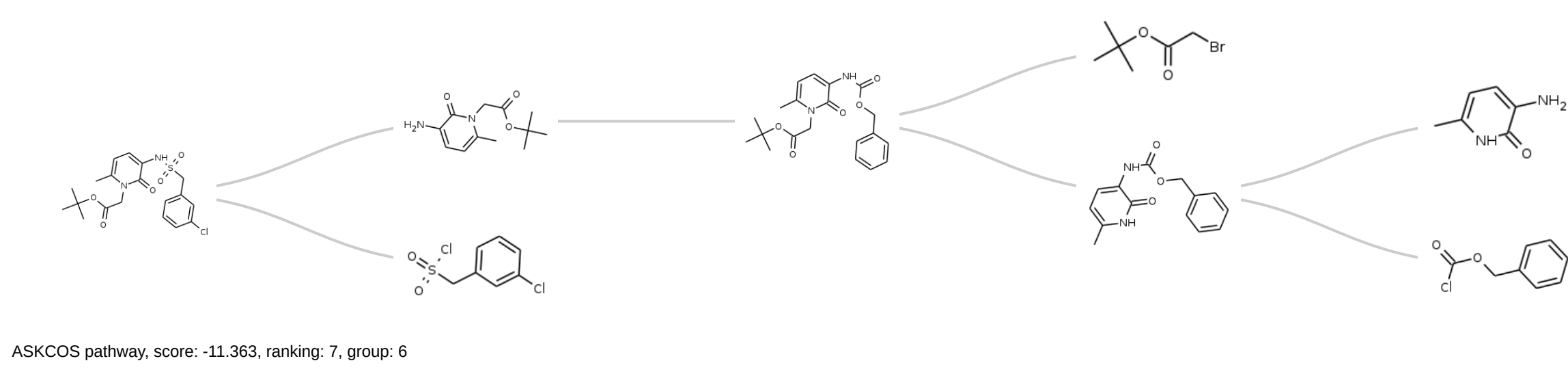
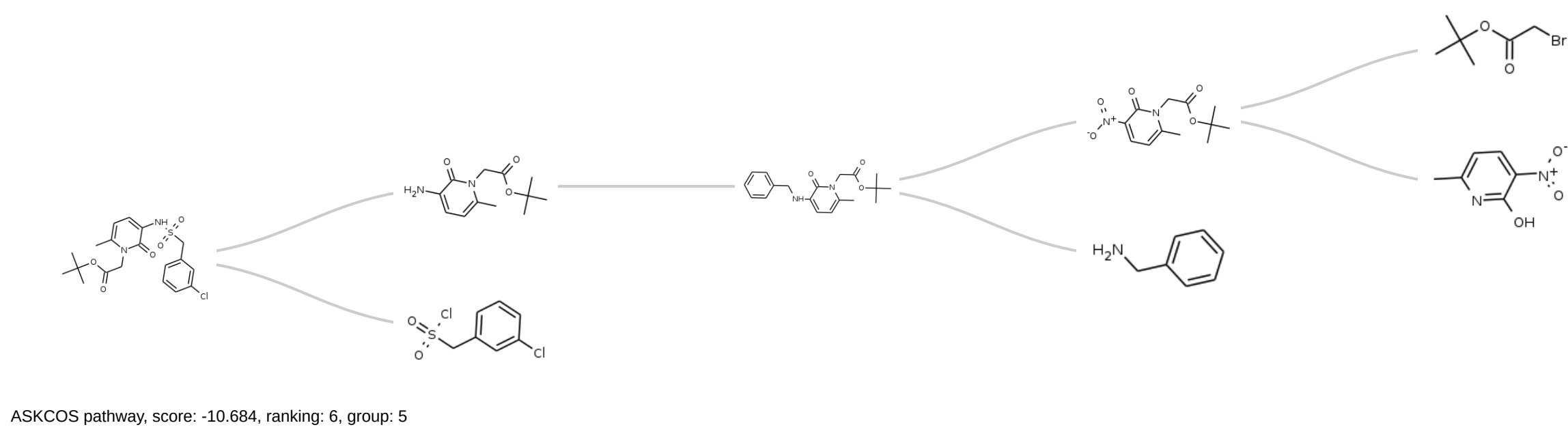
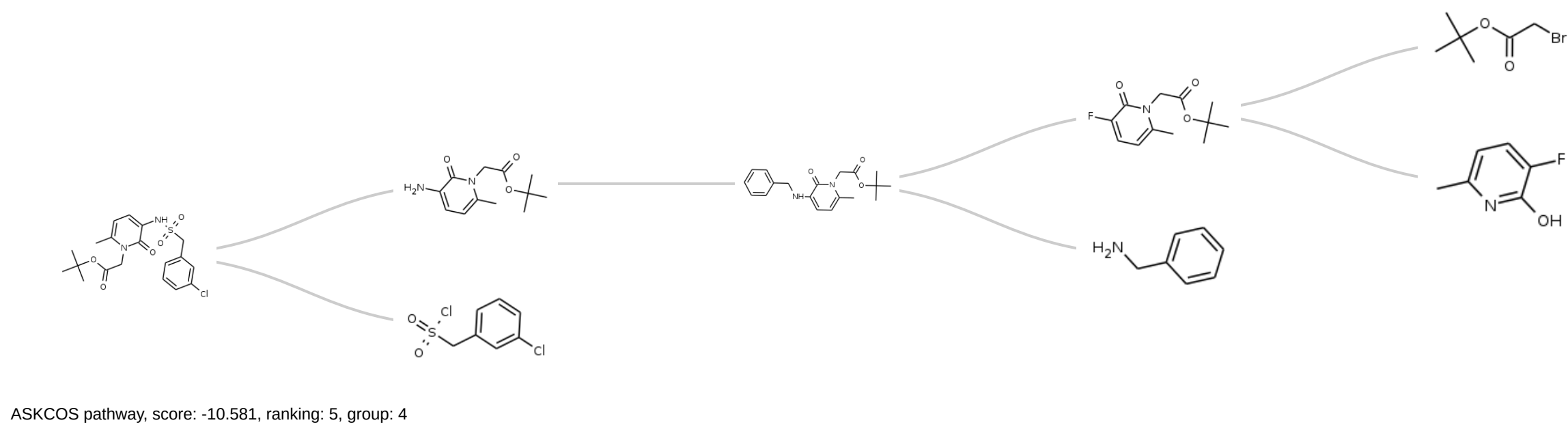
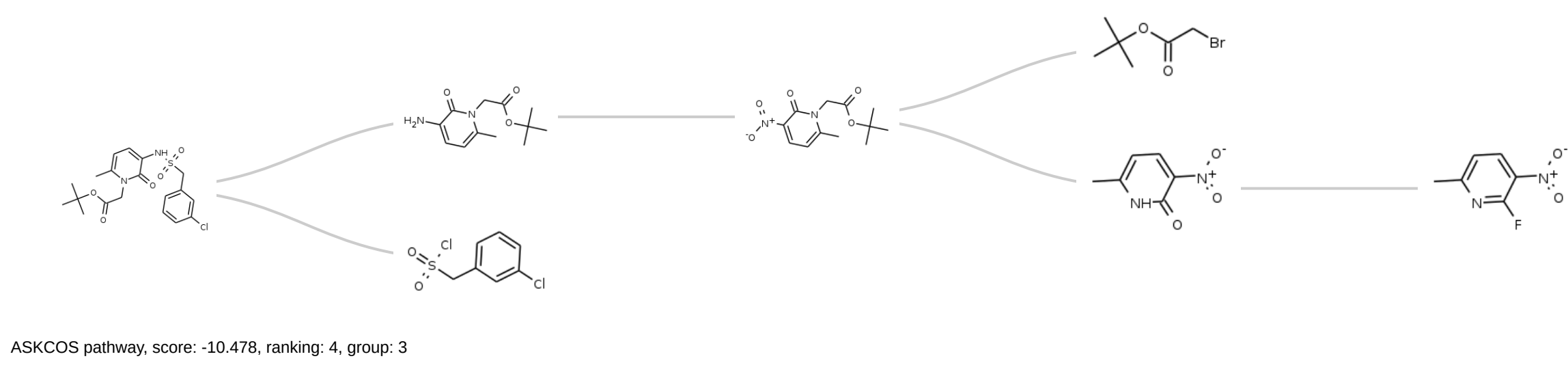
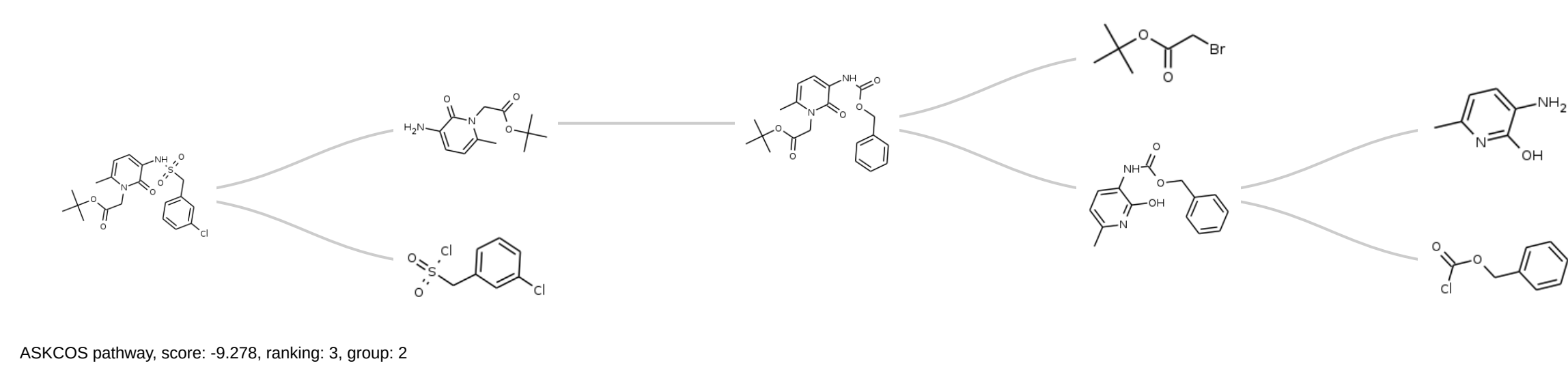
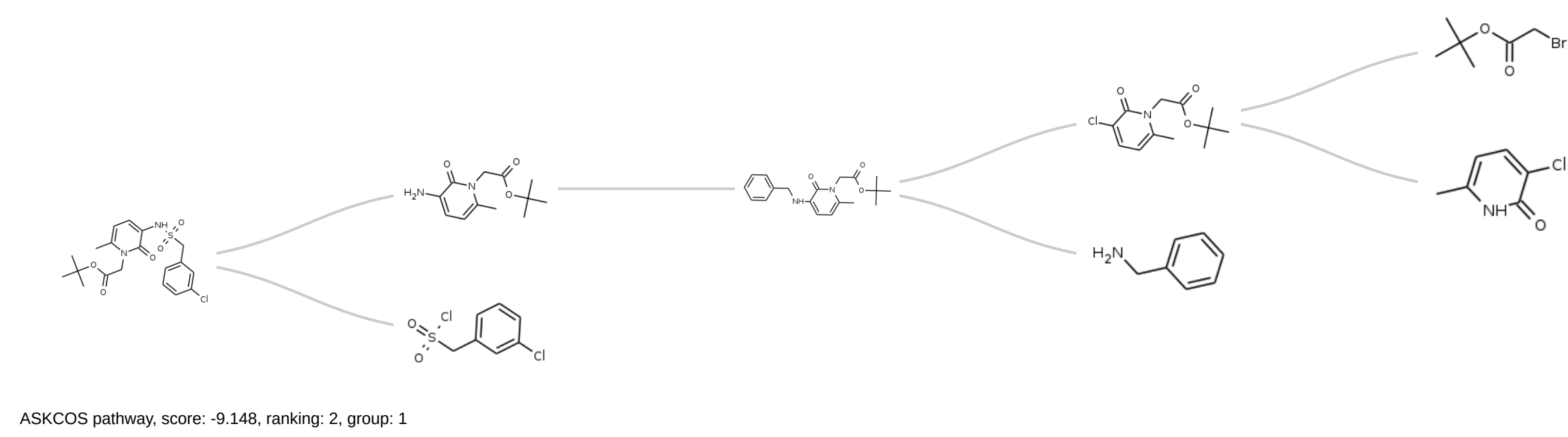
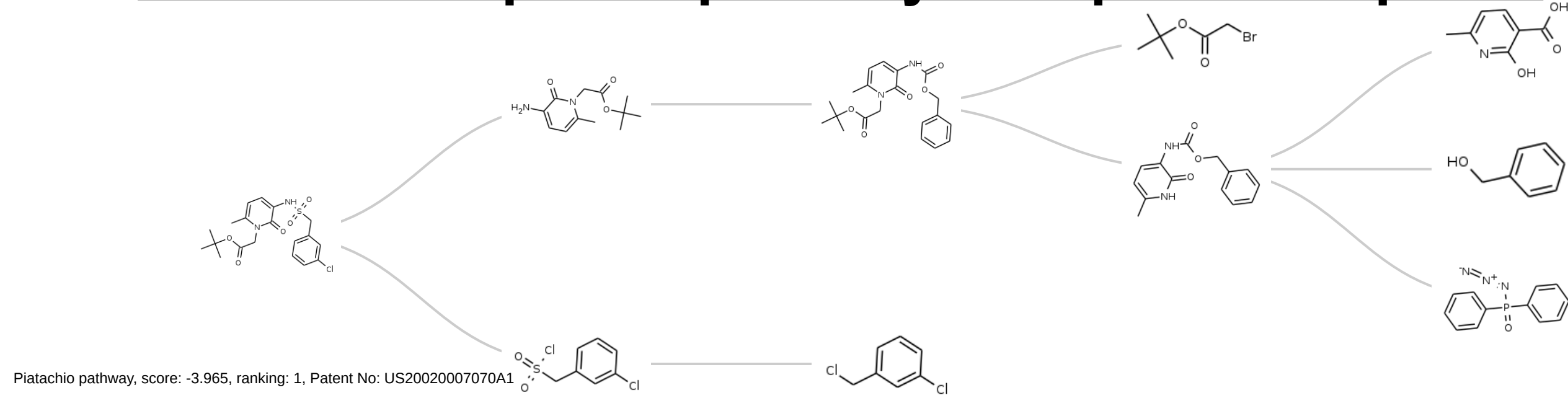
ASKCOS pathway: score: -21.148, ranking: 20, group: 8



ASKCOS pathway: score: -21.272, ranking: 21, group: 9

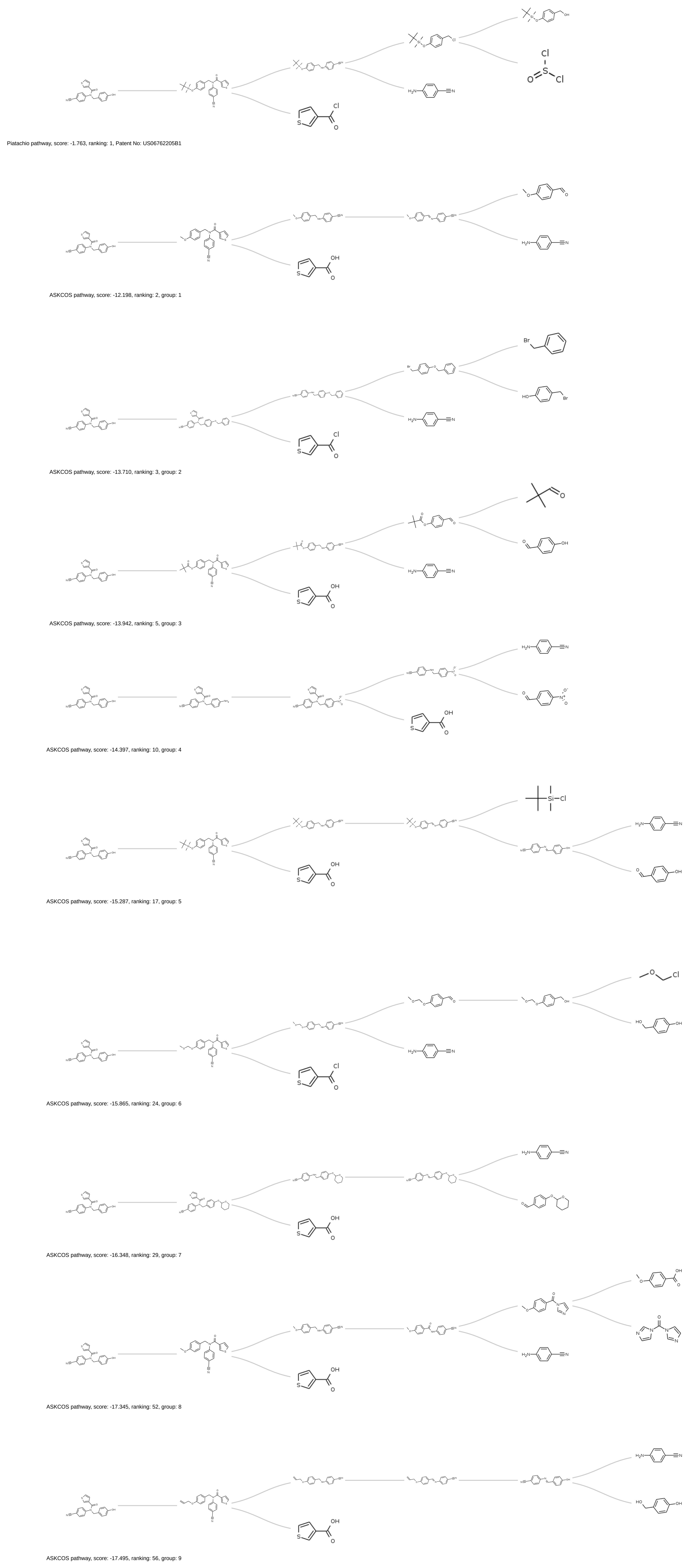


# Model ranks patent pathway as top-1: Example 28

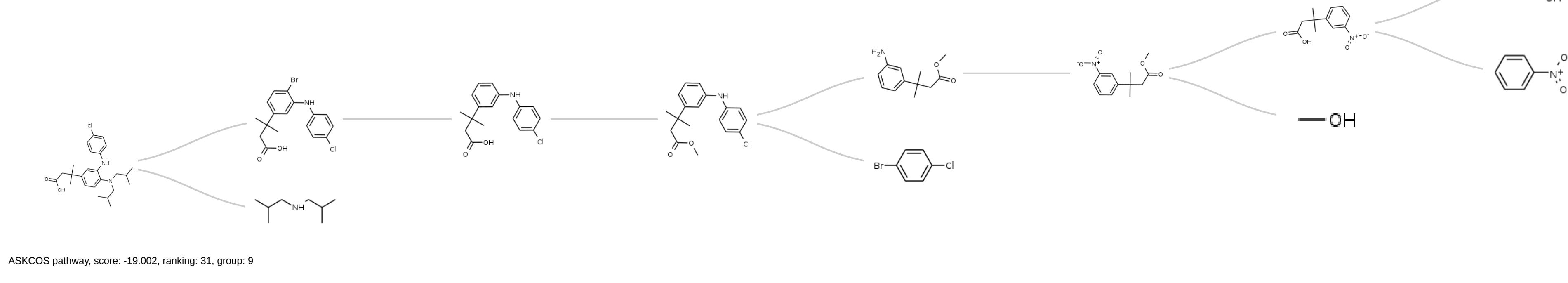
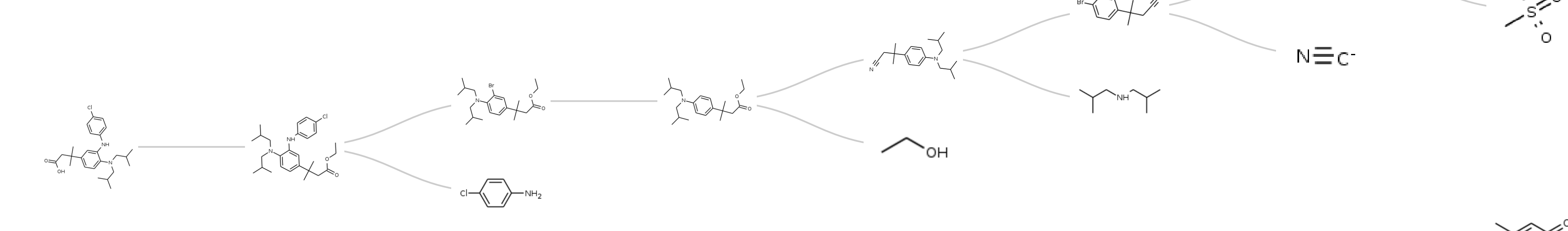
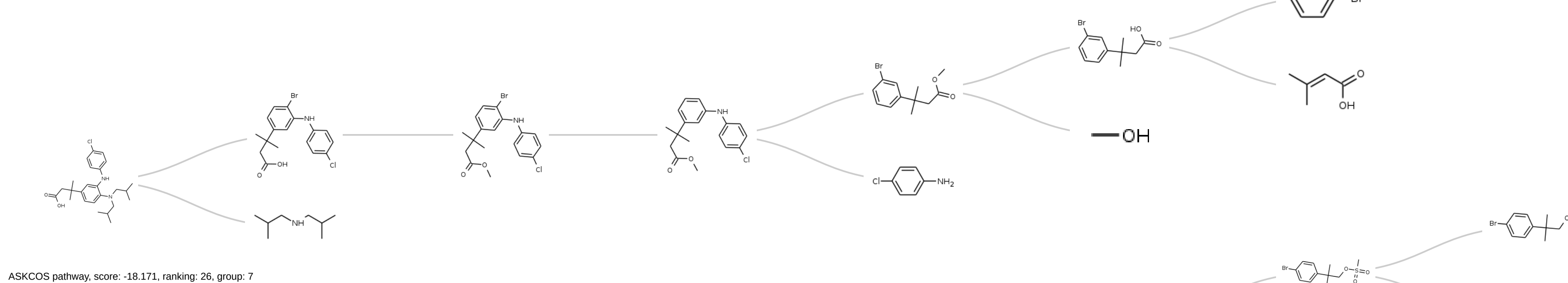
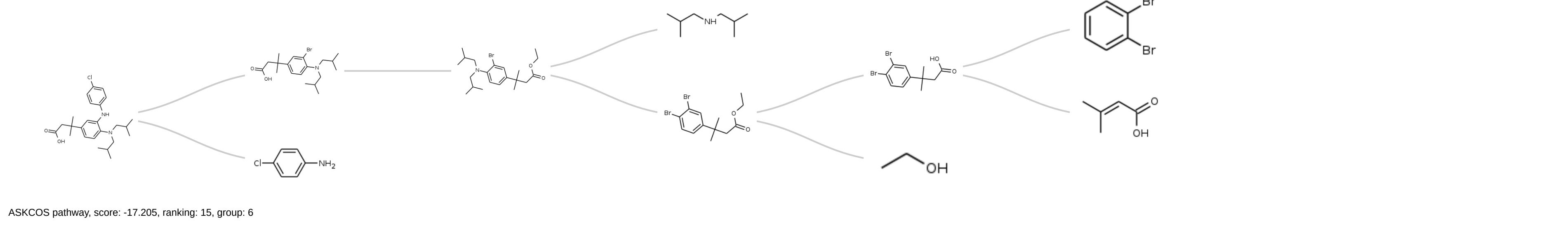
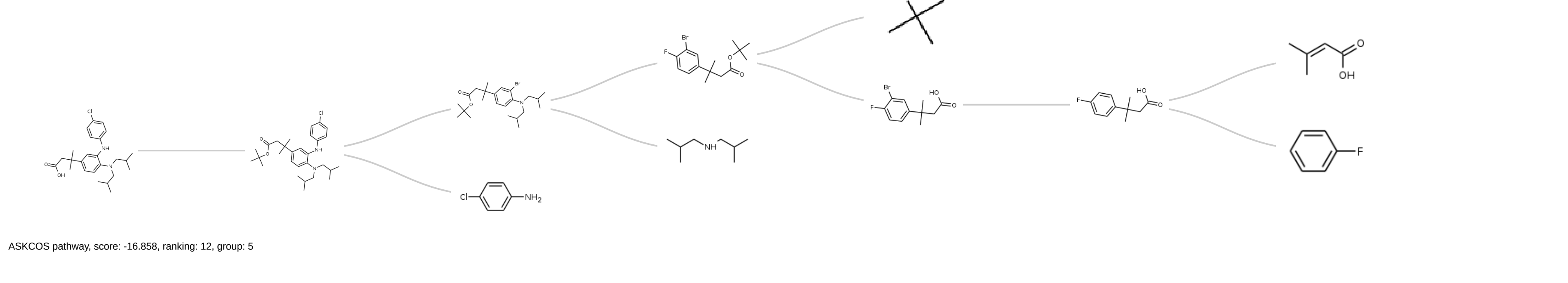
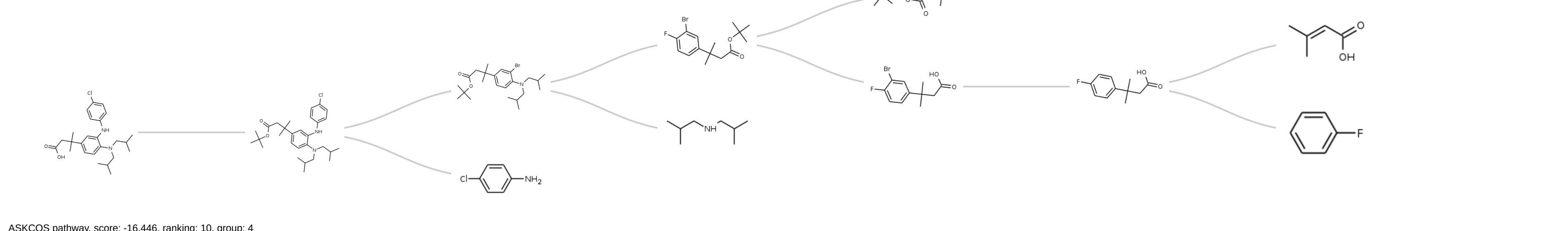
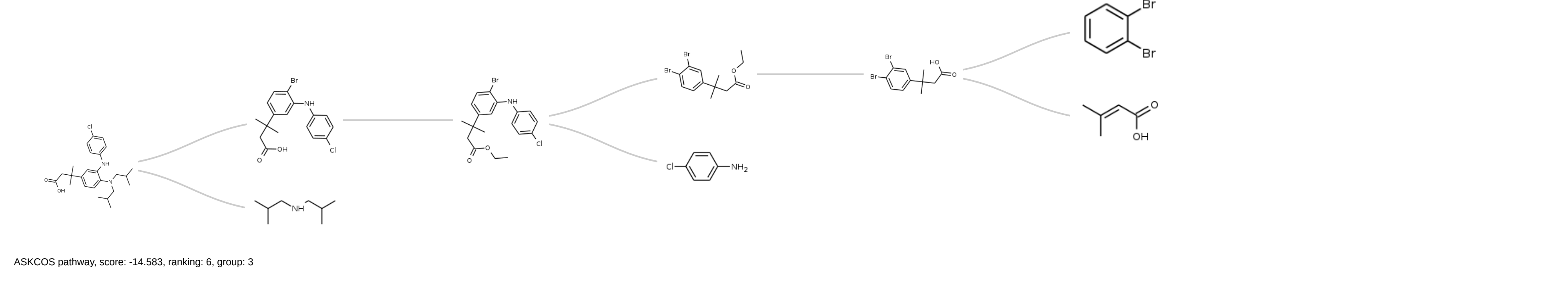
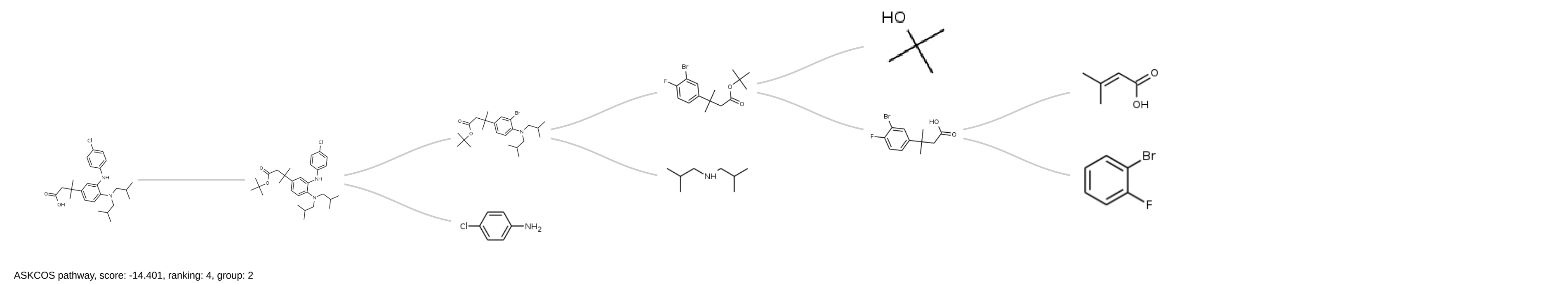
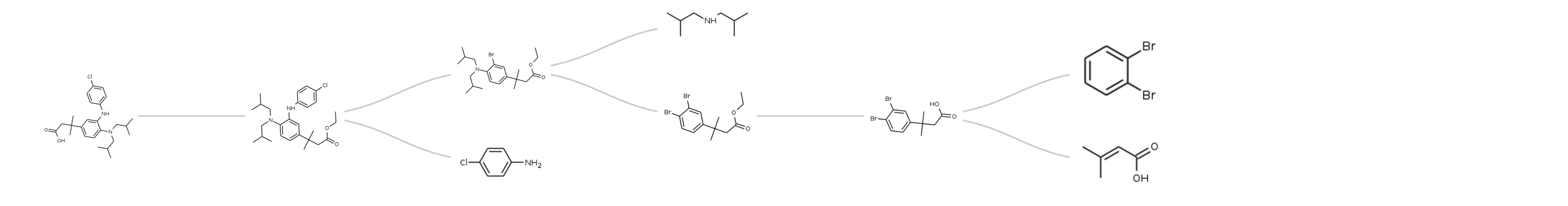
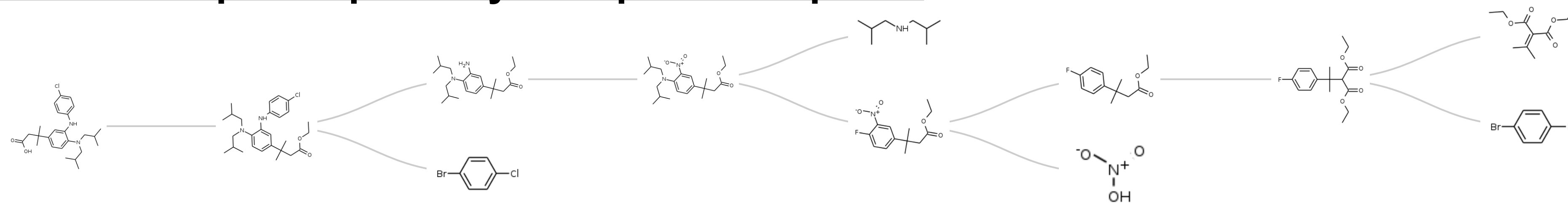




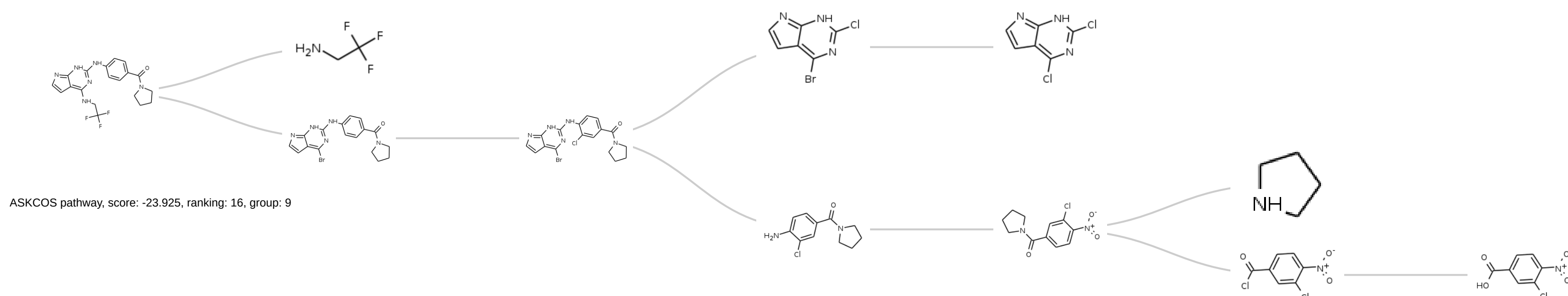
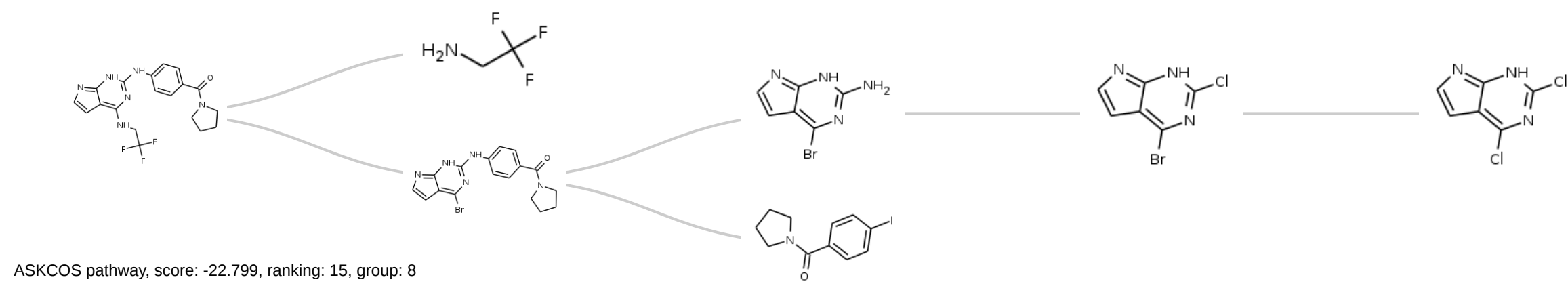
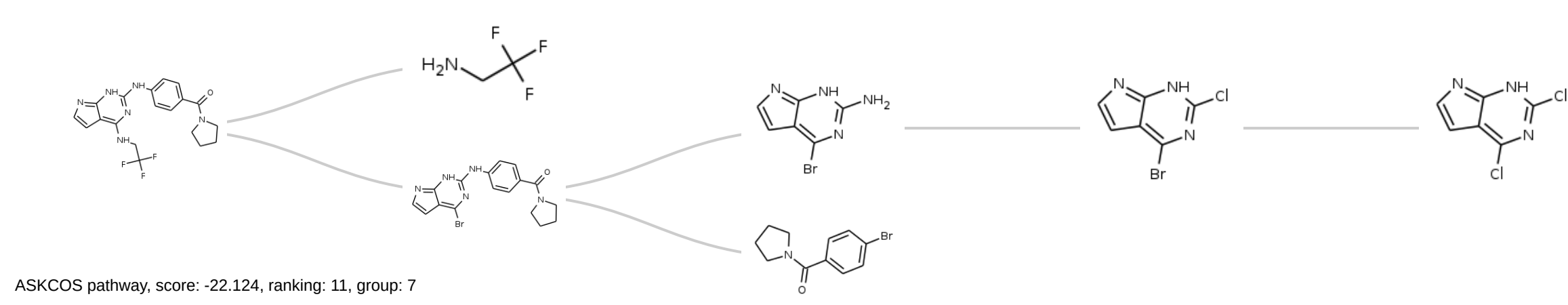
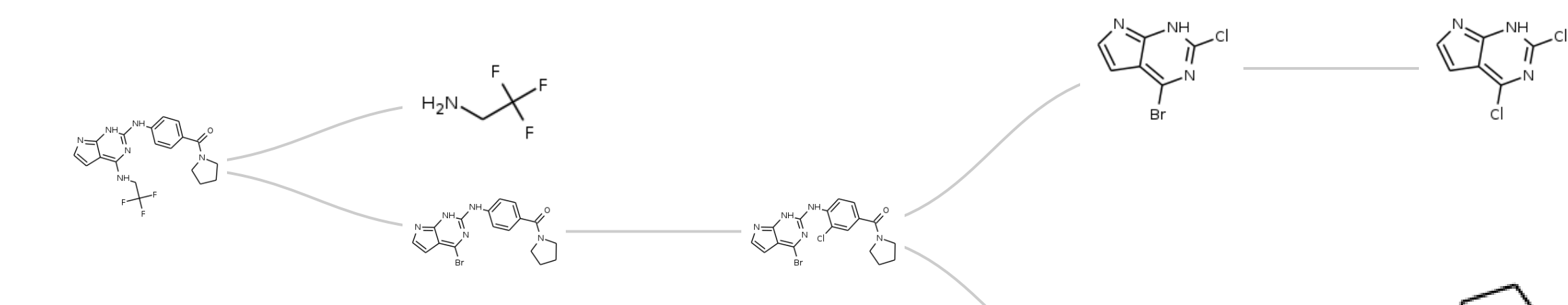
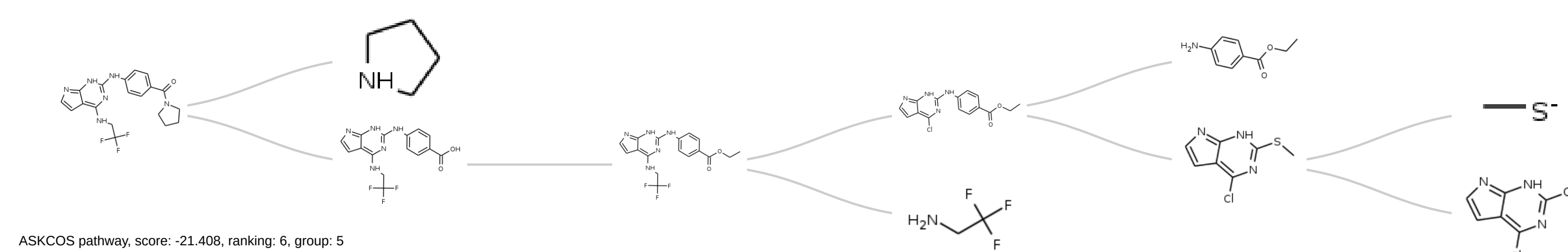
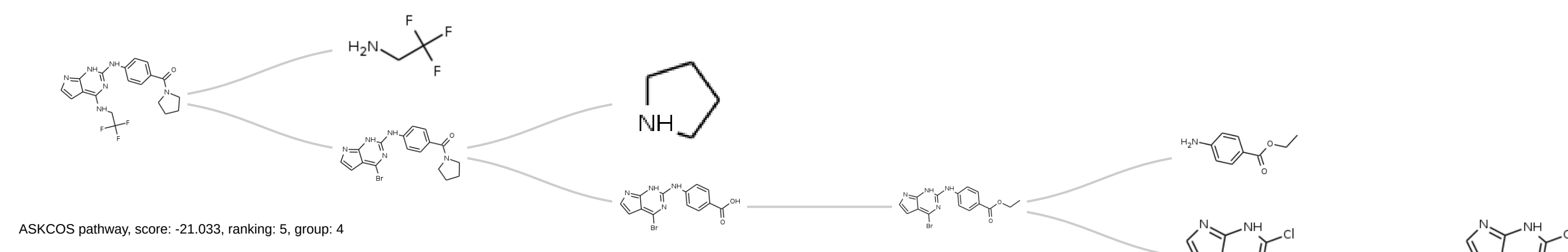
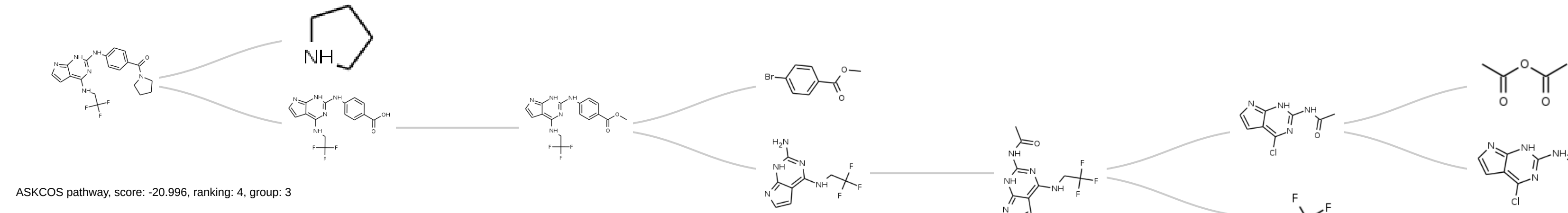
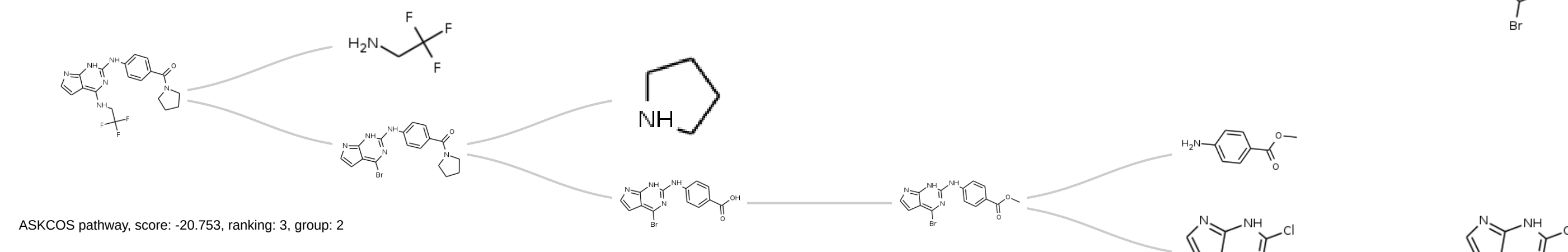
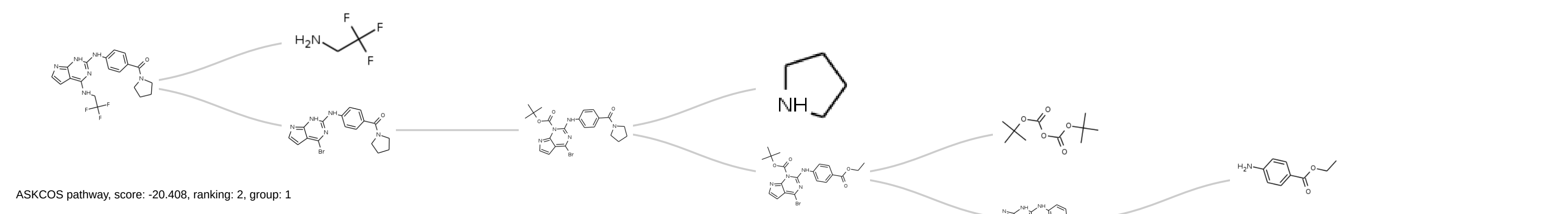
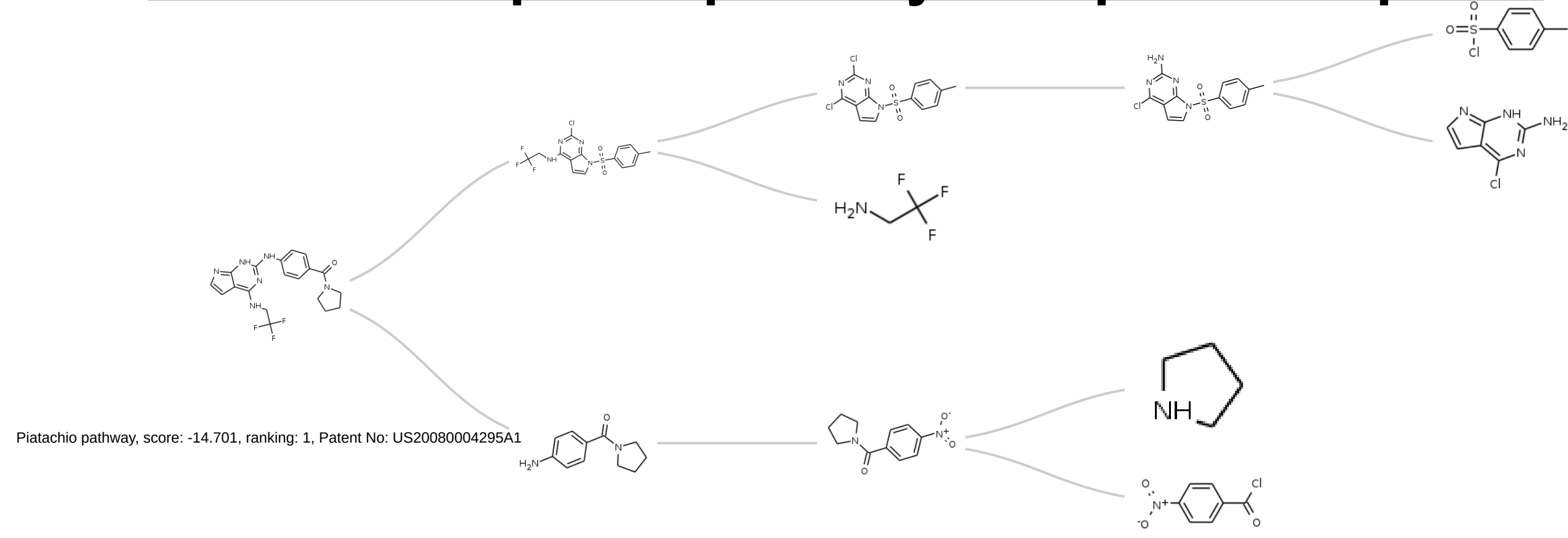
# Model ranks patent pathway as top-1: Example 29



# Model ranks patent pathway as top-1: Example 30

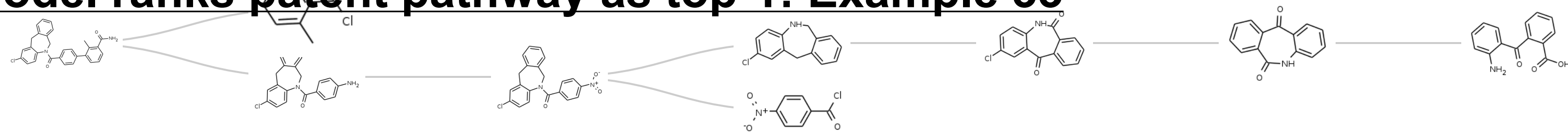


# Model ranks patent pathway as top-1: Example 31

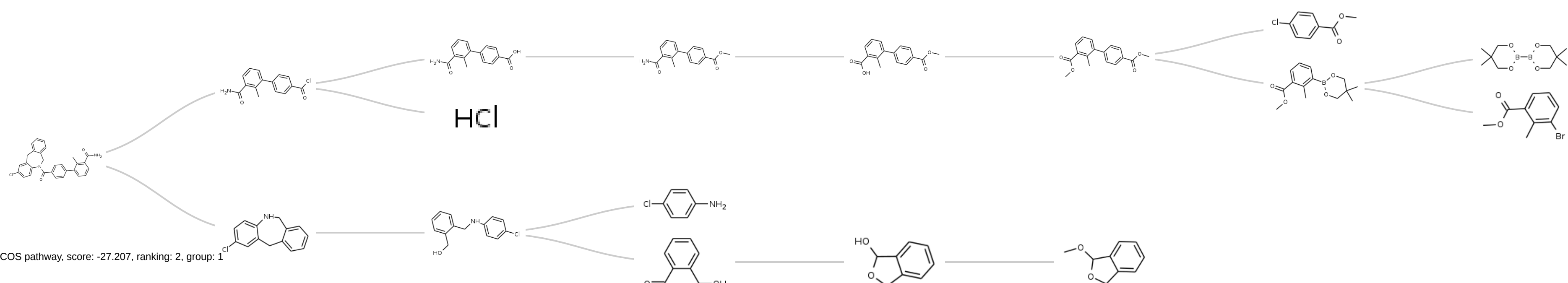




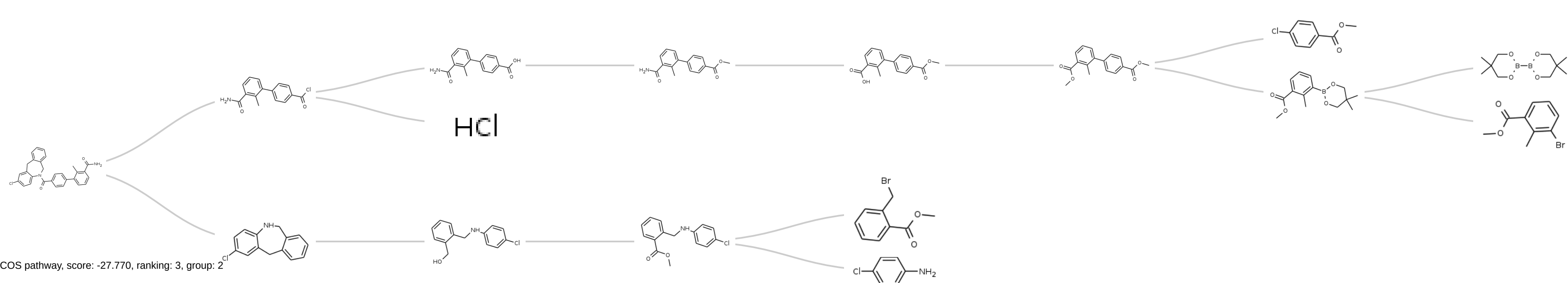
### Model ranks patent pathway as top-1: Example 33



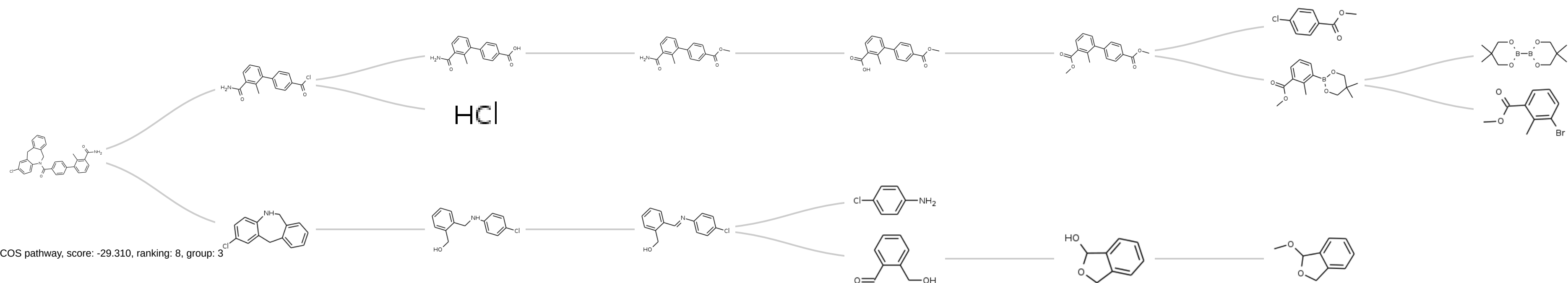
Patent pathway, score: -12.247, ranking: 1, Patent No: US0514747A



ASKCOS pathway, score: -27.207, ranking: 2, group: 1



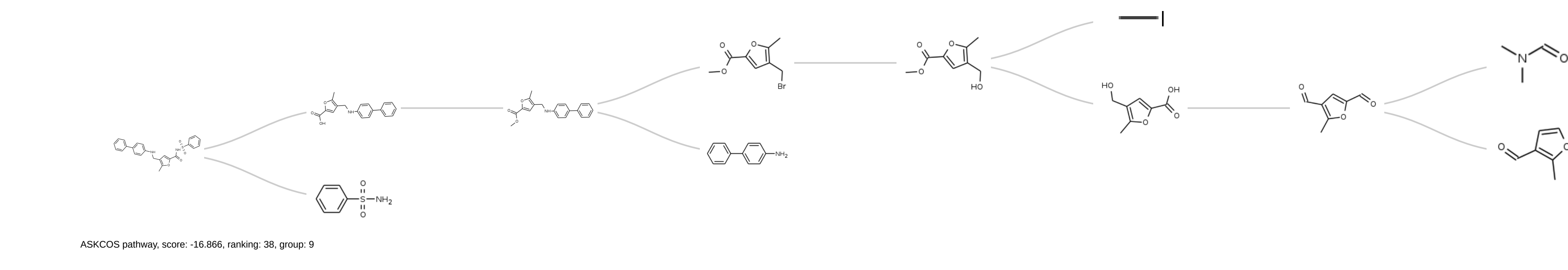
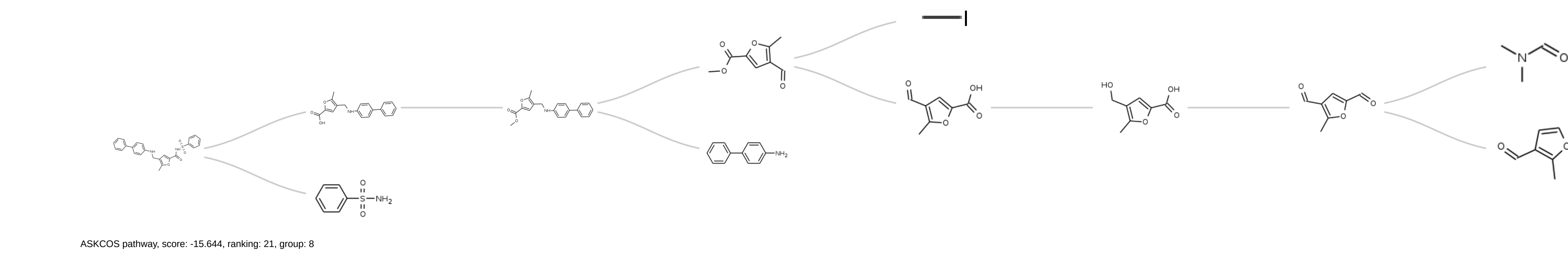
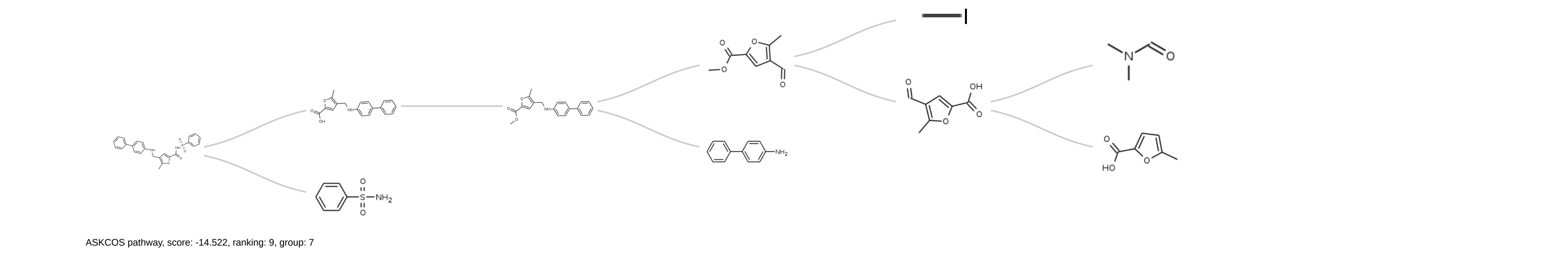
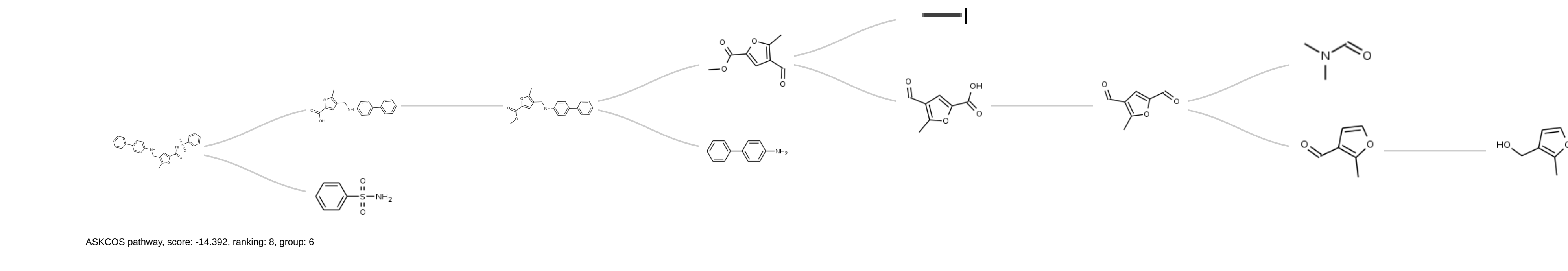
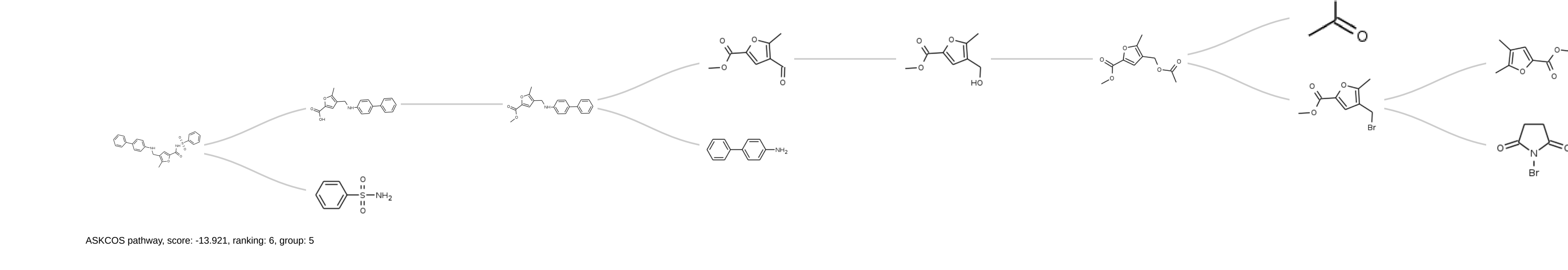
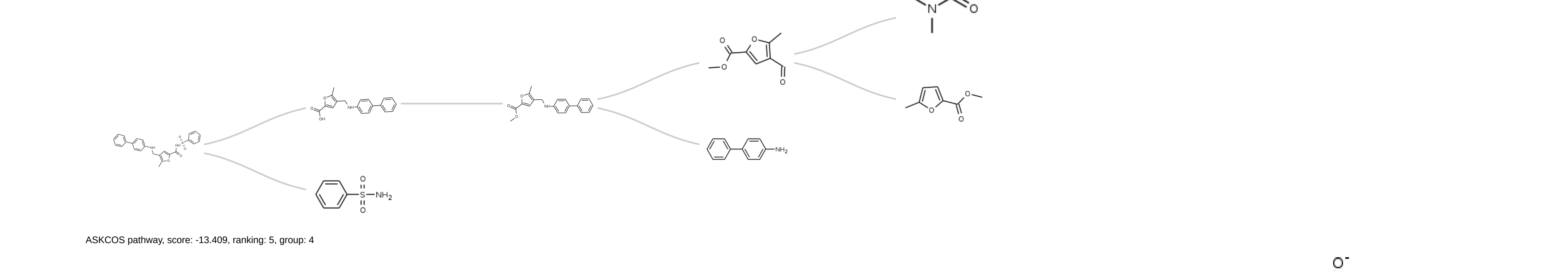
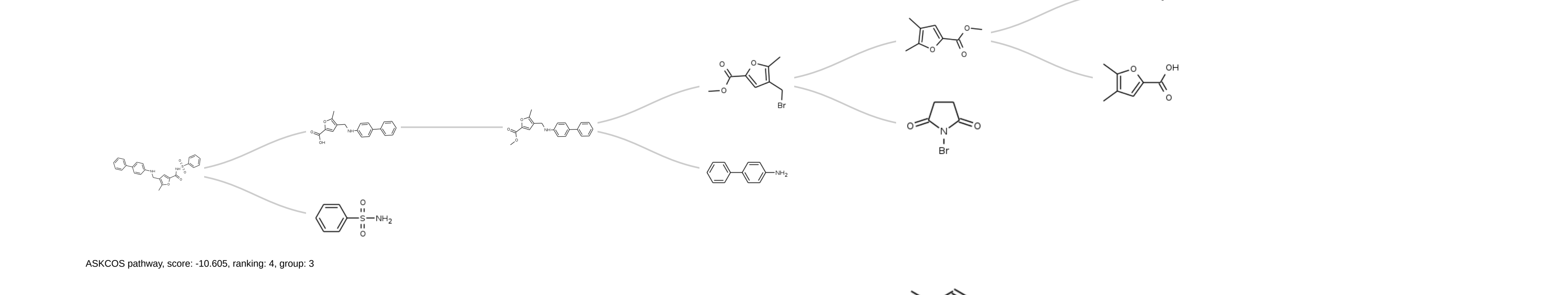
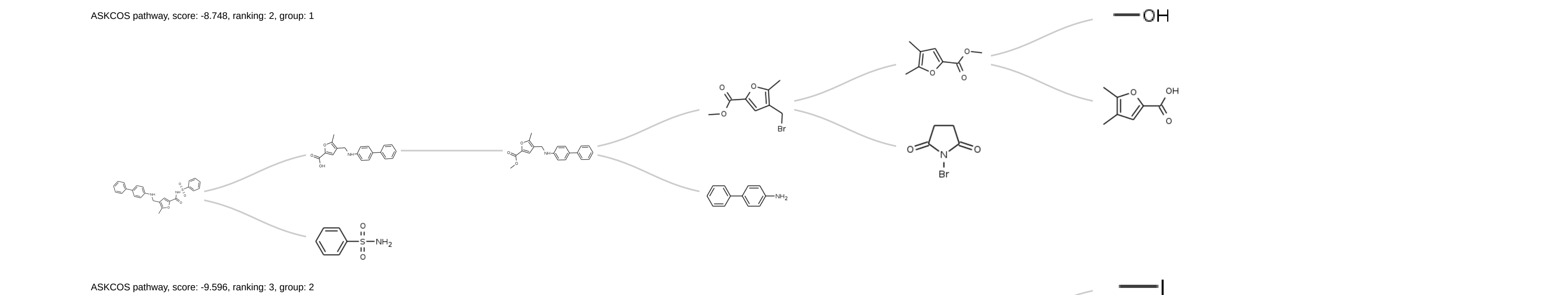
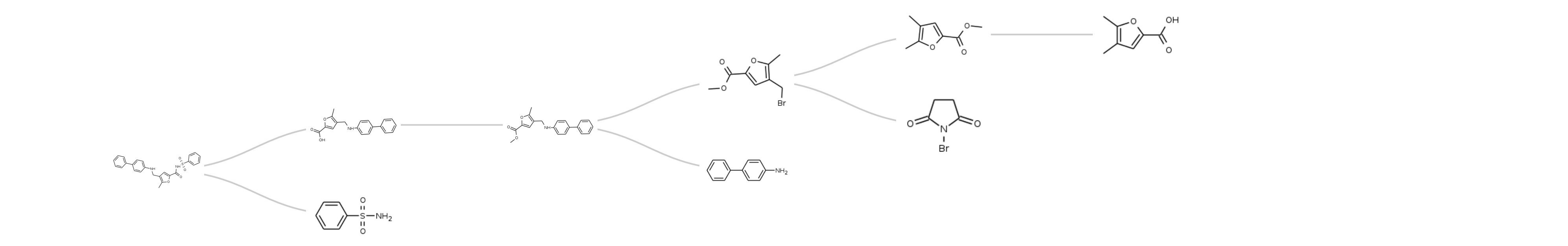
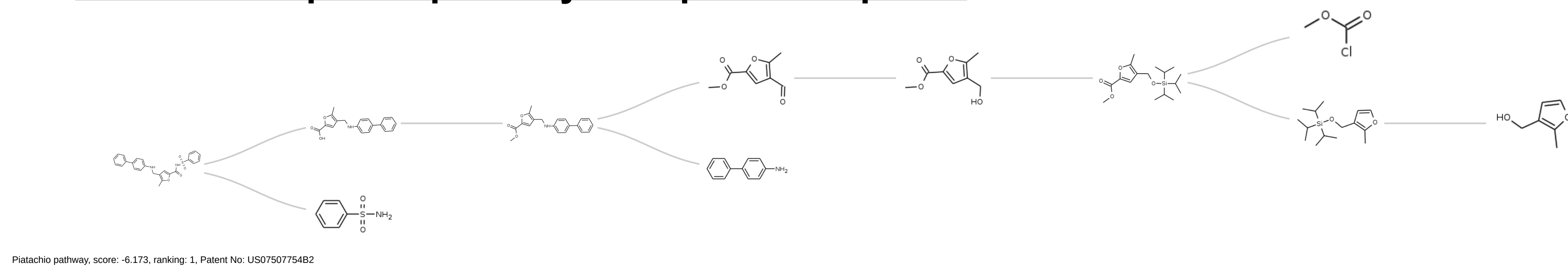
ASKCOS pathway, score: -27.770, ranking: 3, group: 2



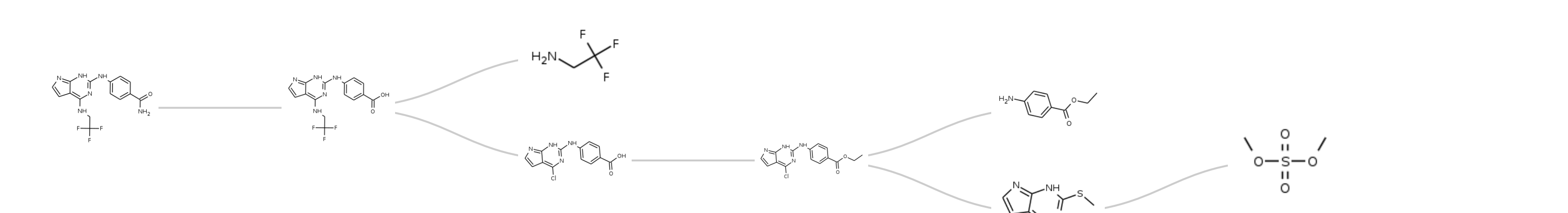
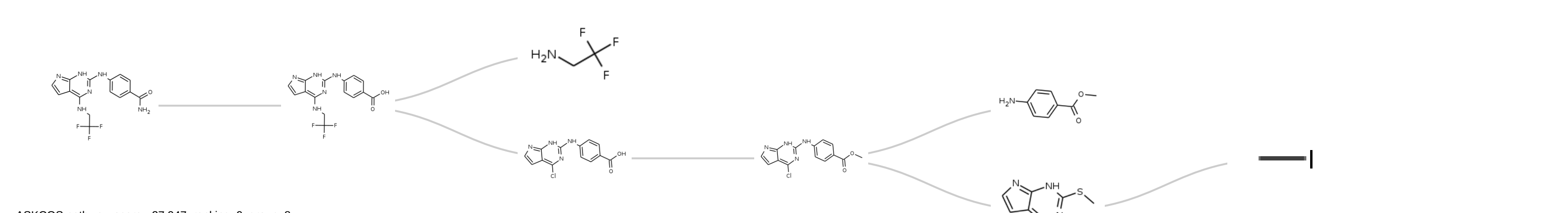
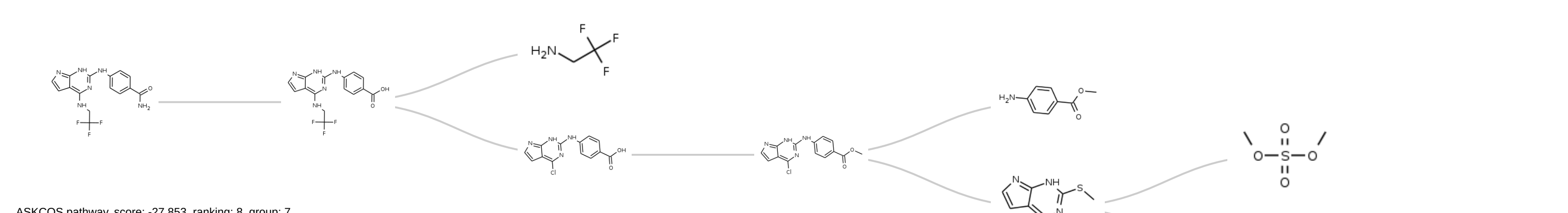
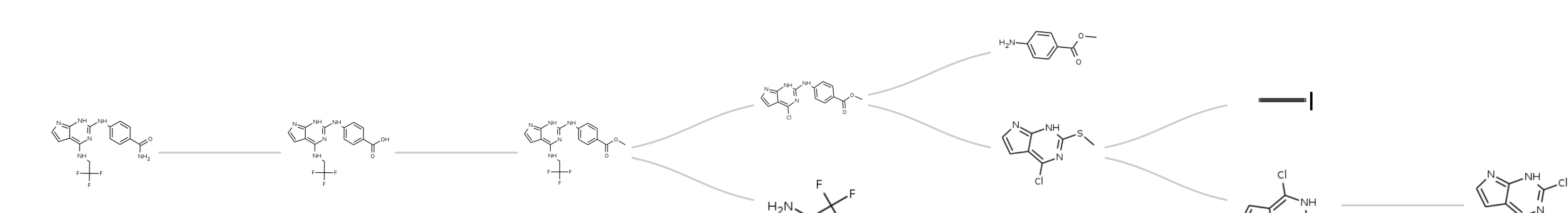
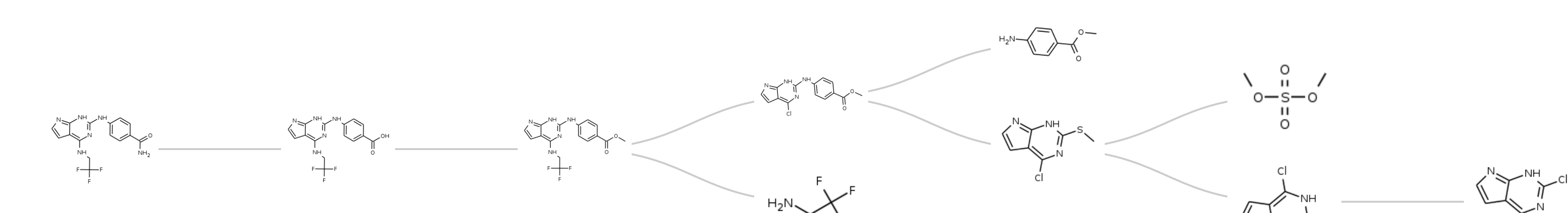
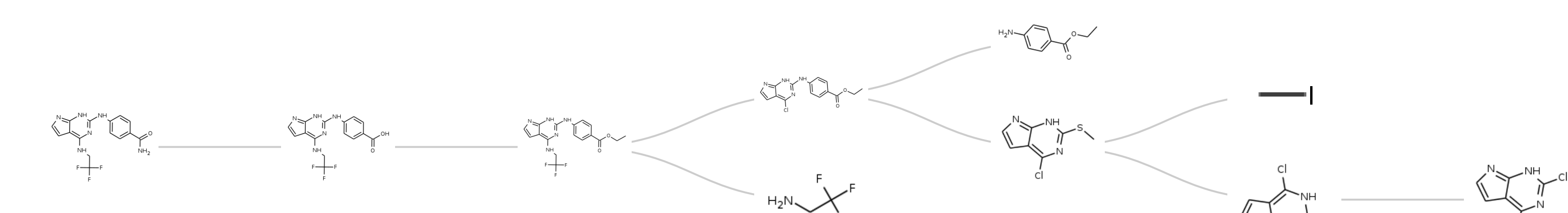
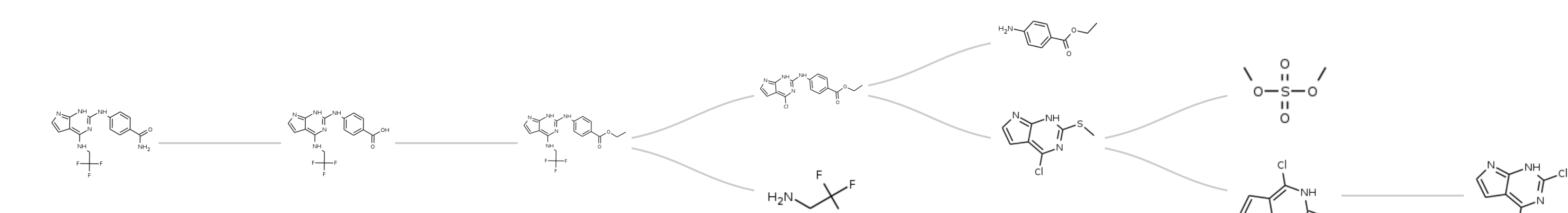
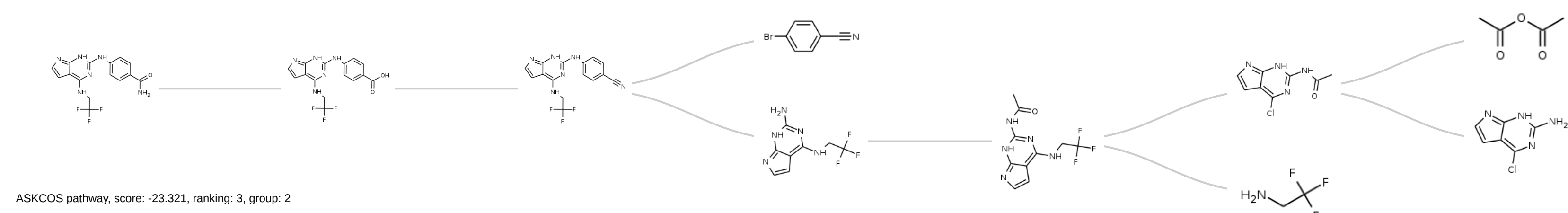
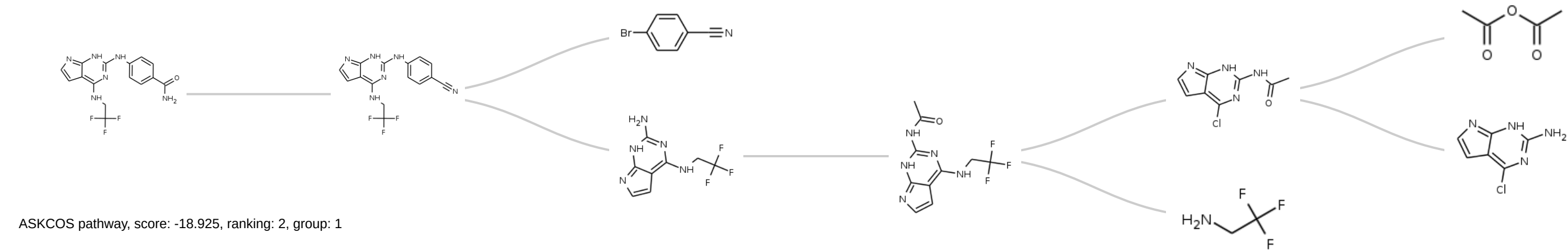
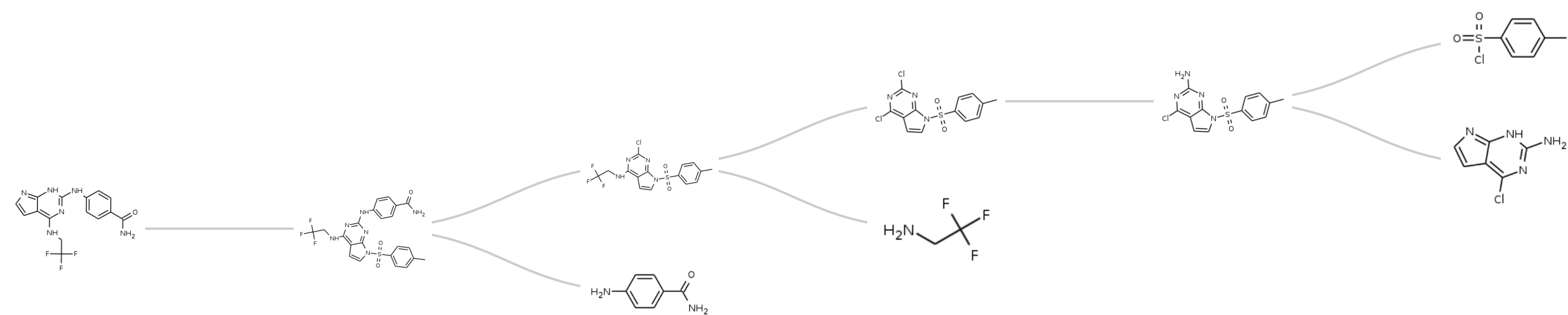
ASKCOS pathway, score: -29.310, ranking: 8, group: 3



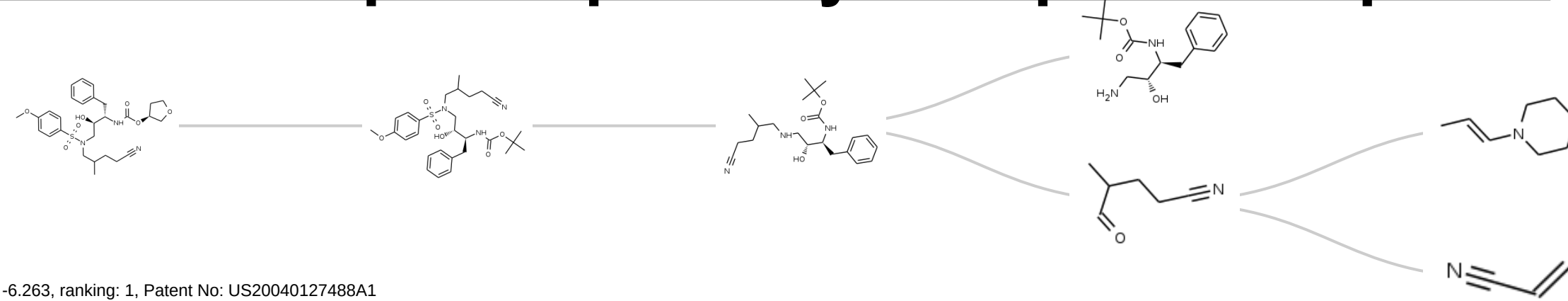
# Model ranks patent pathway as top-1: Example 34



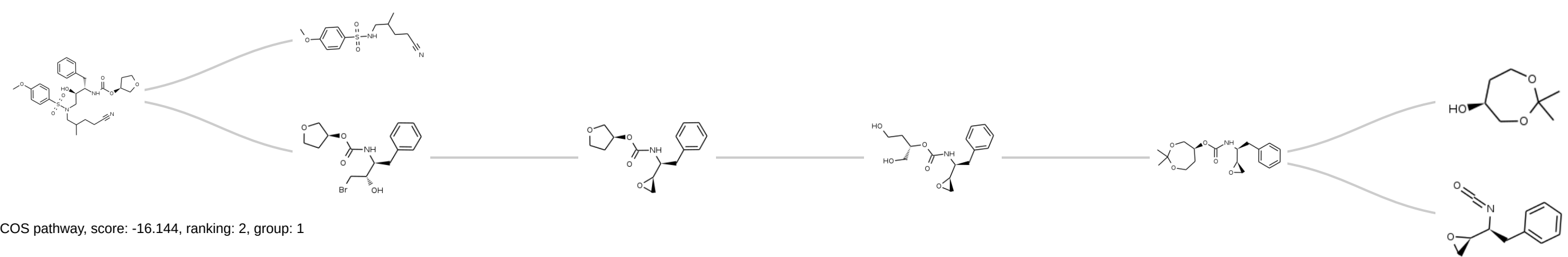
# Model ranks patent pathway as top-1: Example 35



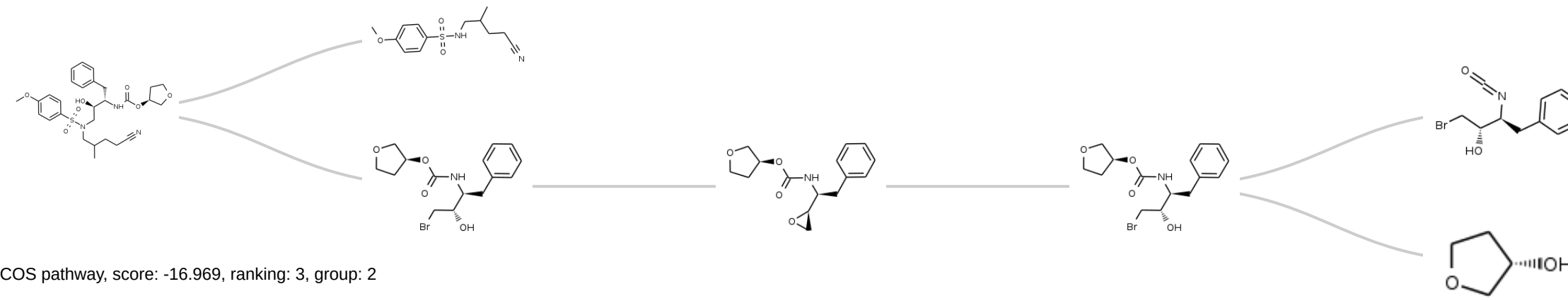
### Model ranks patent pathway as top-1: Example 36



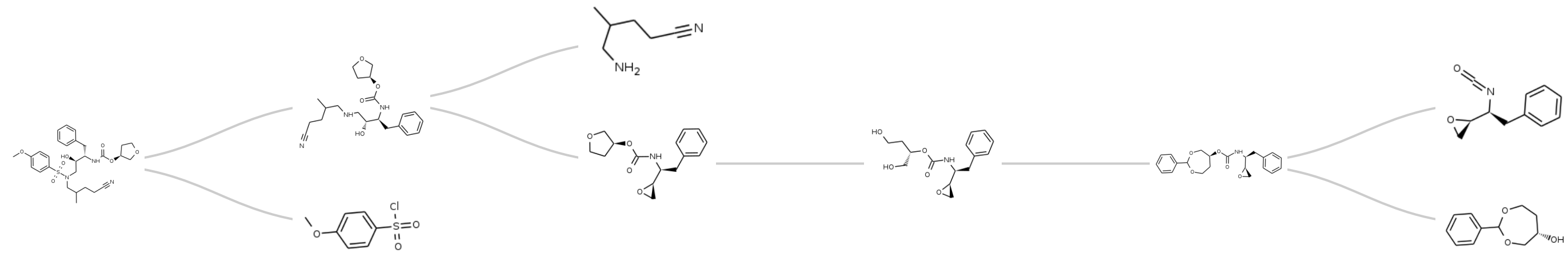
Patent pathway score: -6.263, ranking: 1, Patent No: US20060327488A1



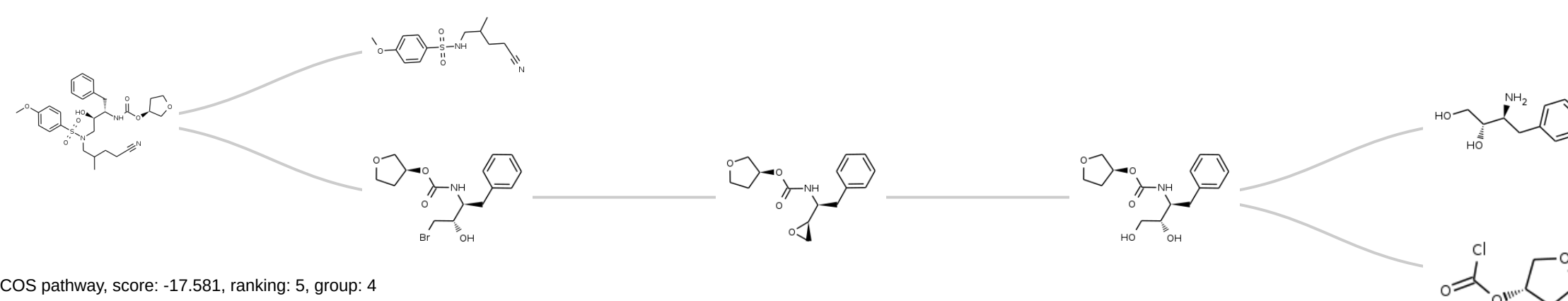
ASKCOS pathway score: -16.144, ranking: 2, group: 1



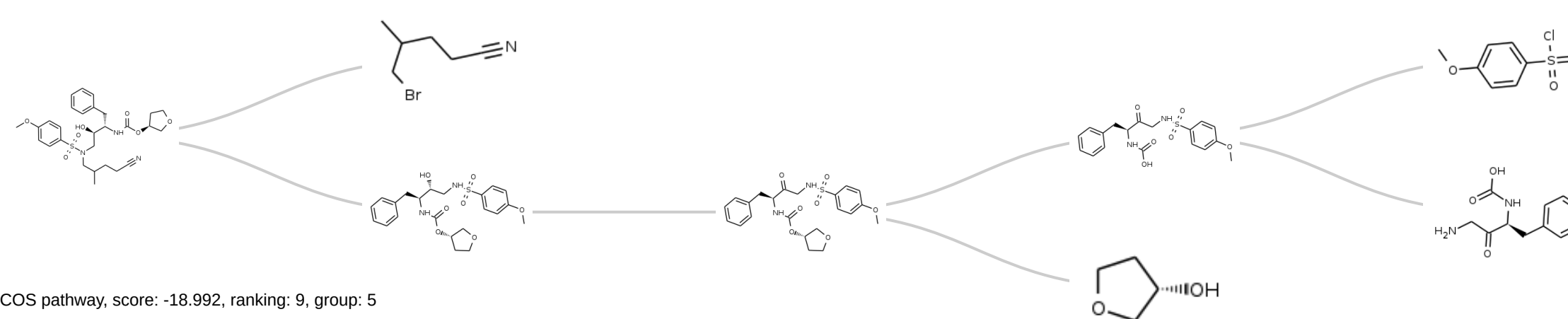
ASKCOS pathway score: -16.969, ranking: 3, group: 2



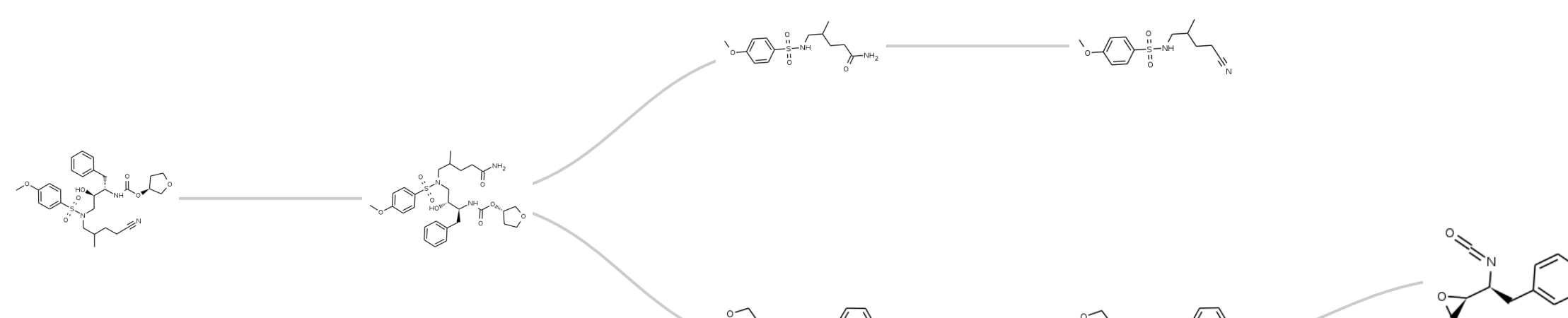
ASKCOS pathway score: -17.381, ranking: 4, group: 3



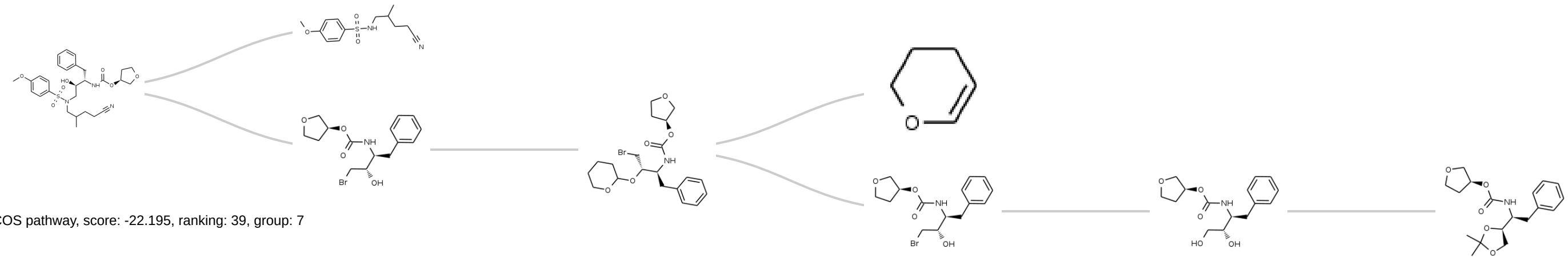
ASKCOS pathway score: -17.581, ranking: 5, group: 4



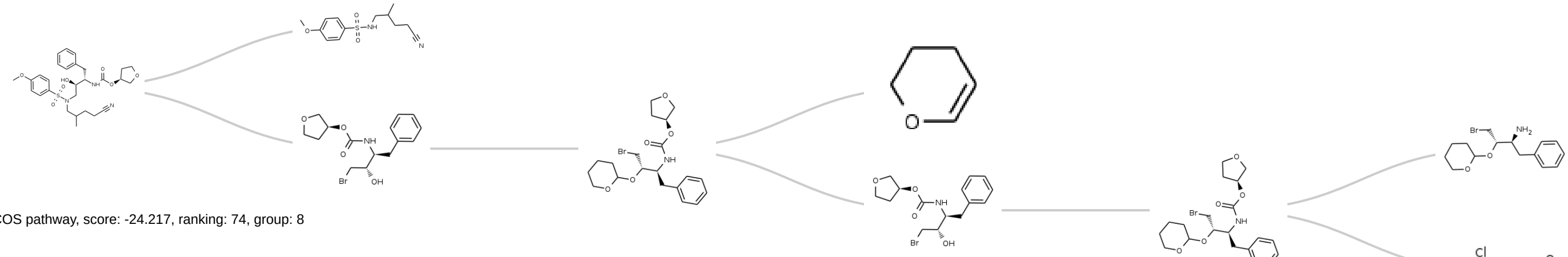
ASKCOS pathway score: -18.992, ranking: 9, group: 5



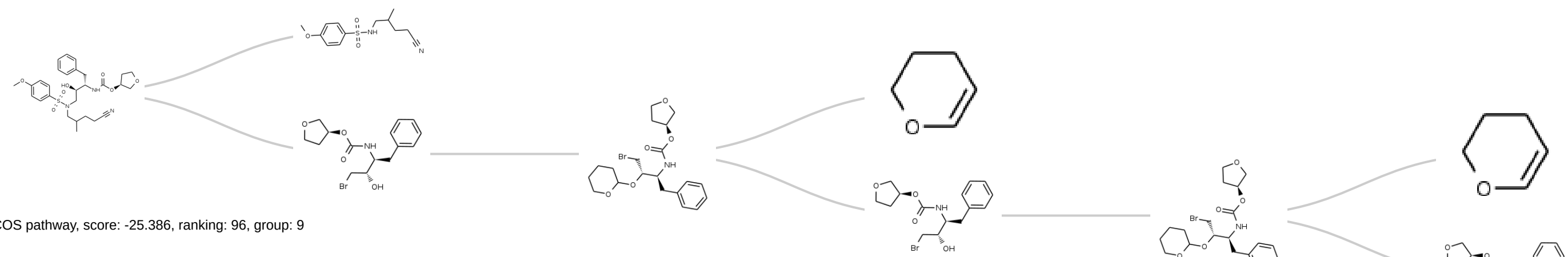
ASKCOS pathway score: -19.685, ranking: 14, group: 6



ASKCOS pathway score: -22.195, ranking: 39, group: 7

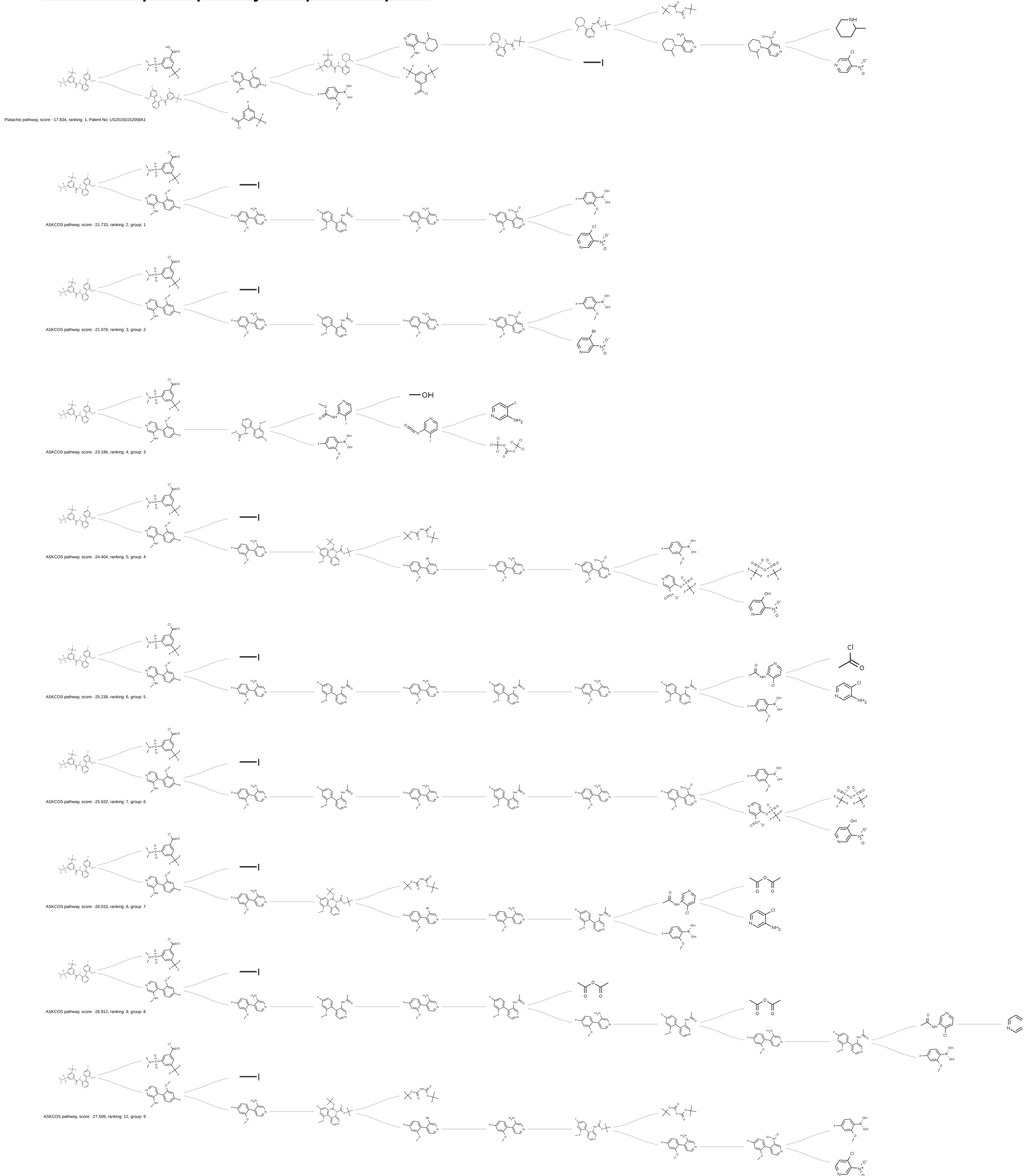


ASKCOS pathway score: -24.217, ranking: 74, group: 8

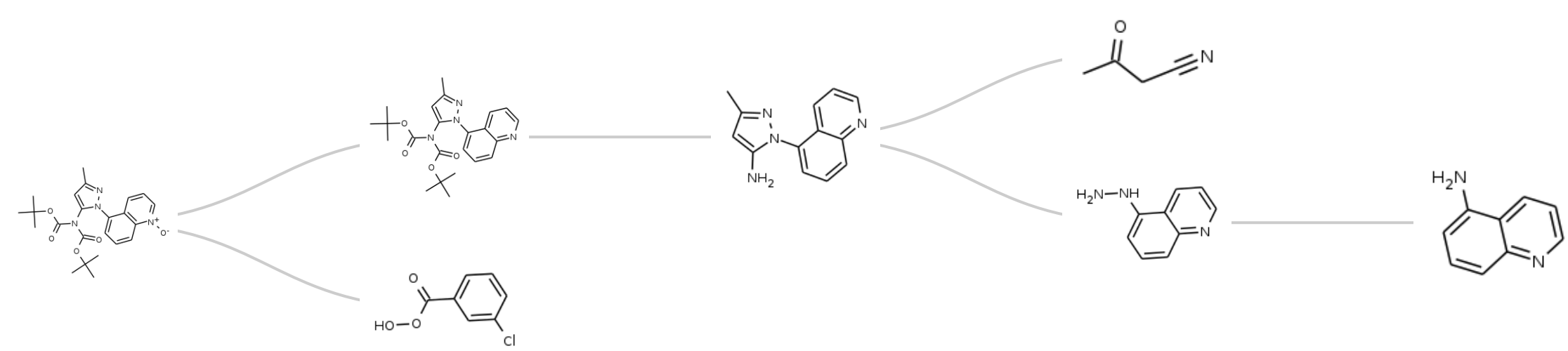


ASKCOS pathway score: -25.396, ranking: 96, group: 9

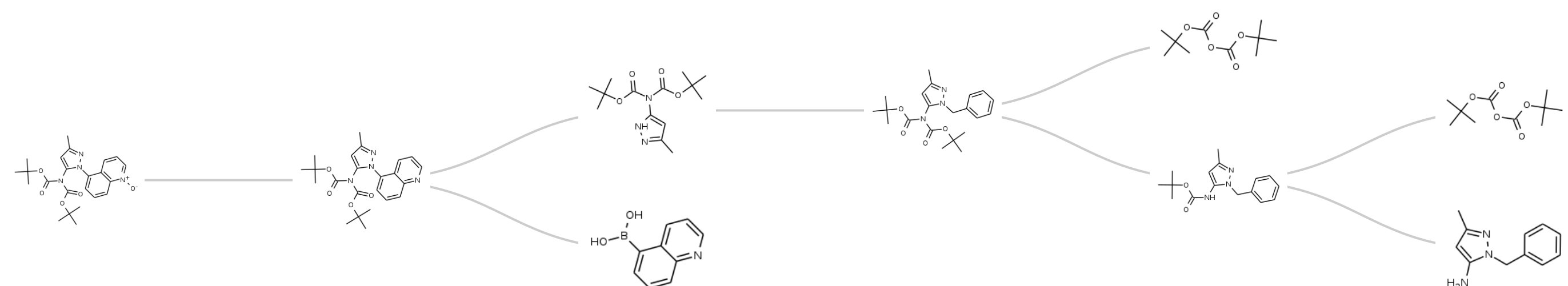
**Model ranks patent pathway as top-1: Example 37**



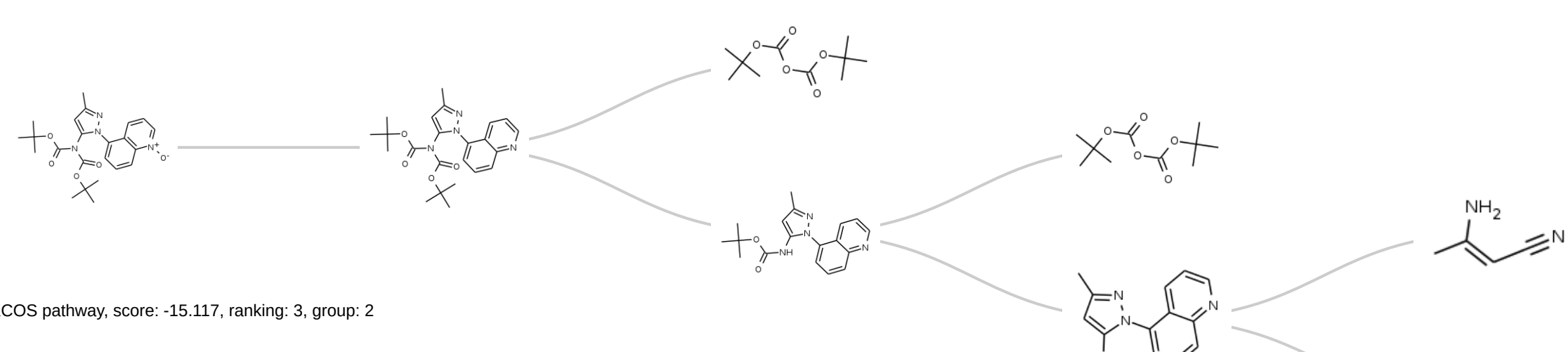
**Model ranks patent pathway as top-1: Example 38**



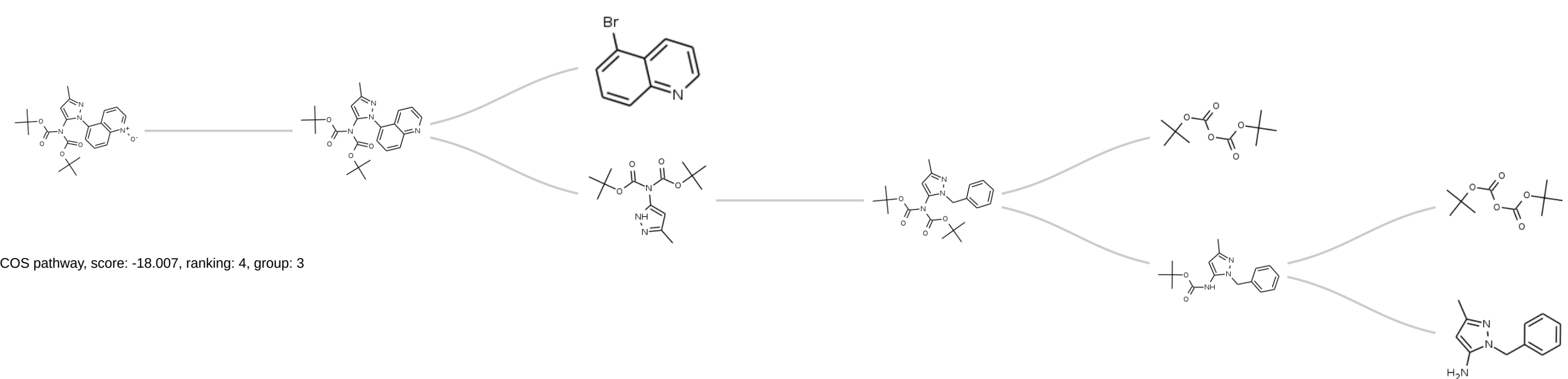
Patatcho pathway, score: -1.413, ranking: 1, Patent No: US20180099797A1



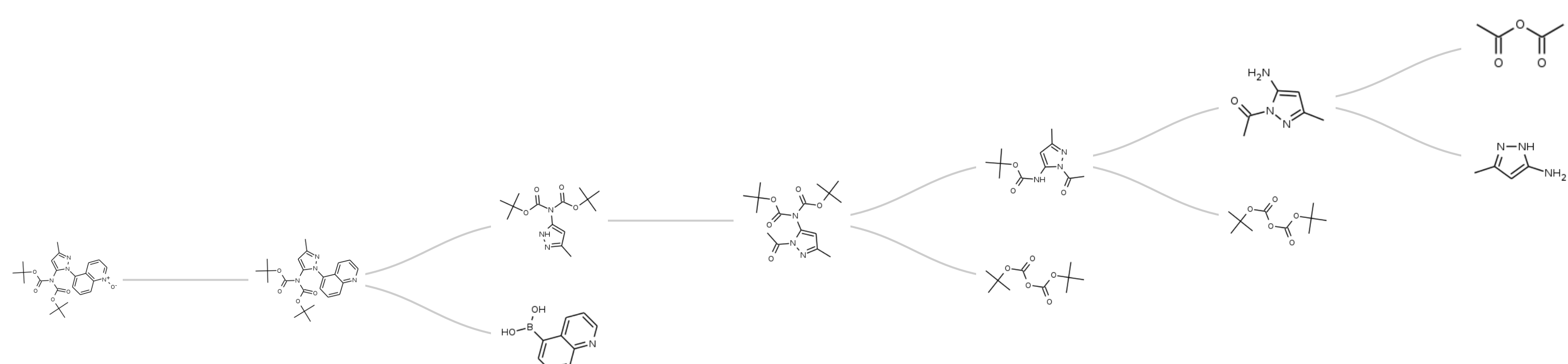
ASKCOS pathway, score: -14.936, ranking: 2, group: 1



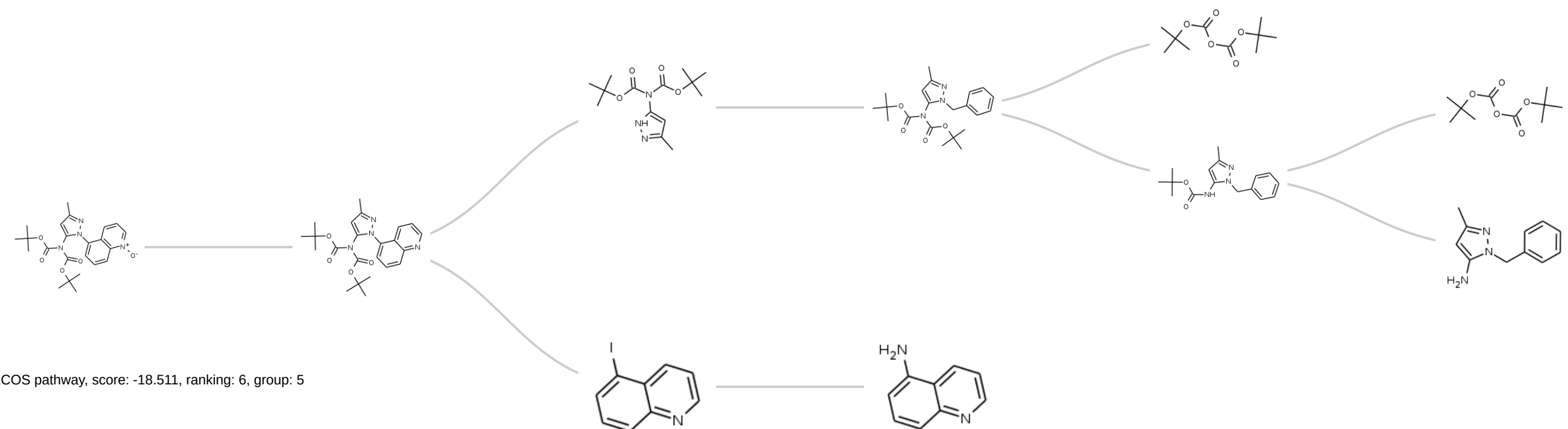
ASKCOS pathway, score: -15.117, ranking: 3, group: 2



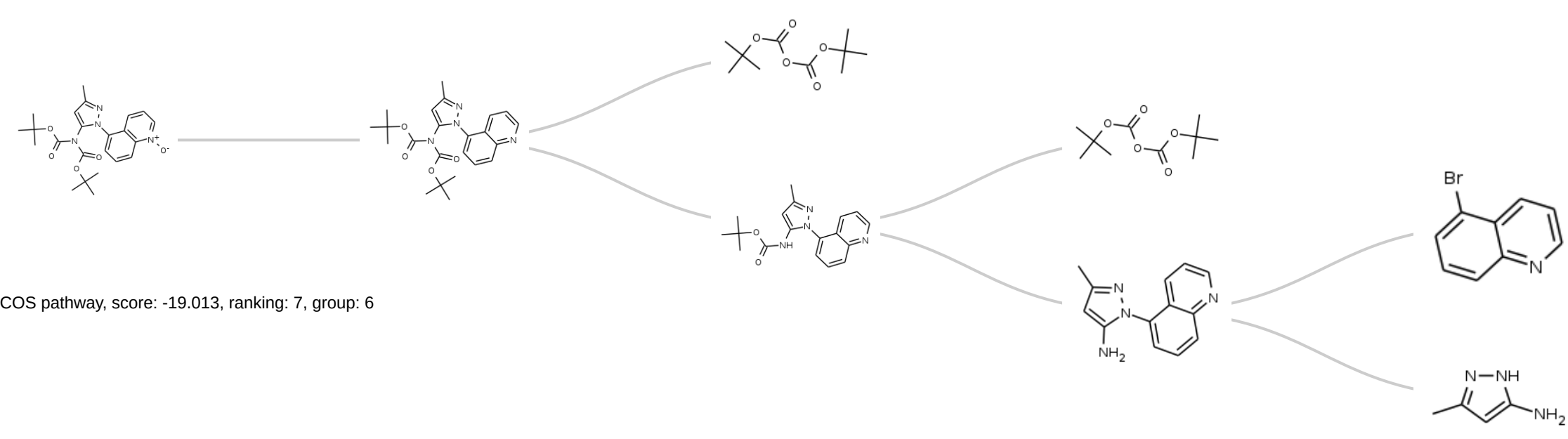
ASKCOS pathway, score: -18.007, ranking: 4, group: 3



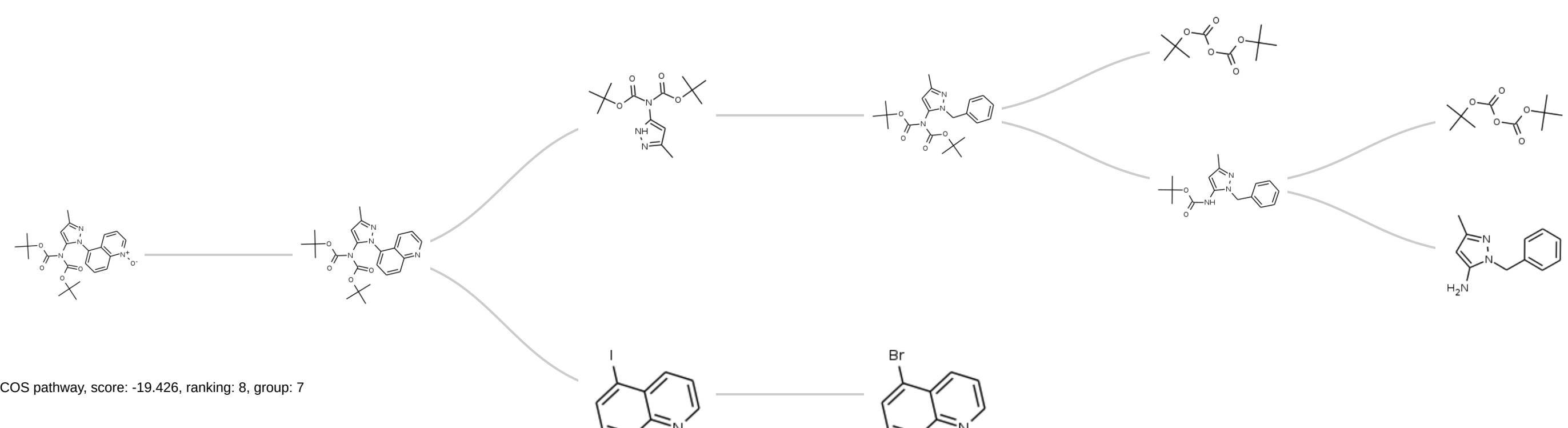
ASKCOS pathway, score: -18.241, ranking: 5, group: 4



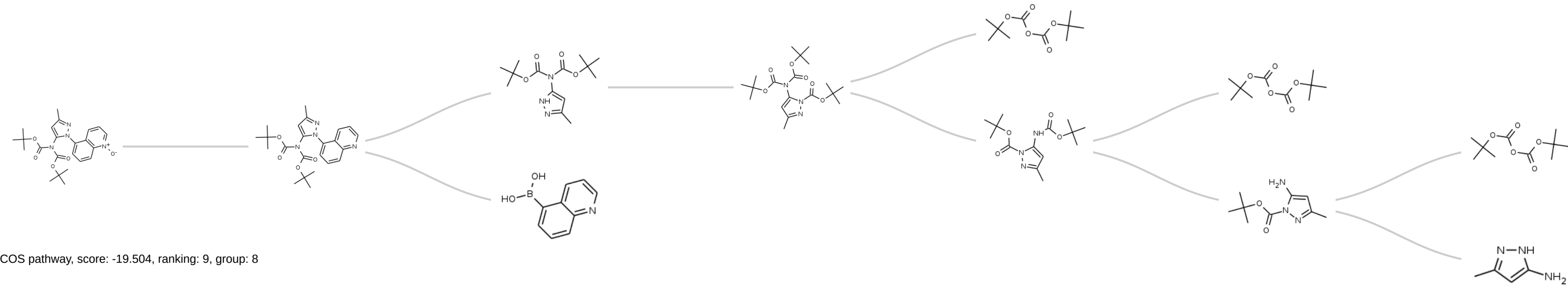
ASKCOS pathway, score: -18.511, ranking: 6, group: 5



ASKCOS pathway, score: -19.013, ranking: 7, group: 6



ASKCOS pathway, score: -19.426, ranking: 8, group: 7



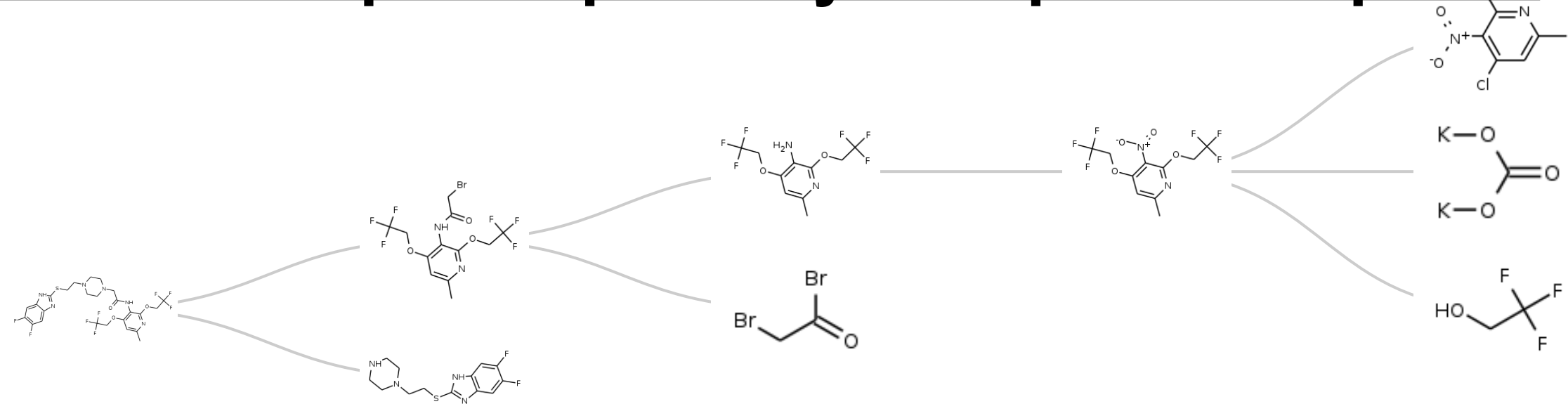
ASKCOS pathway, score: -19.504, ranking: 9, group: 8



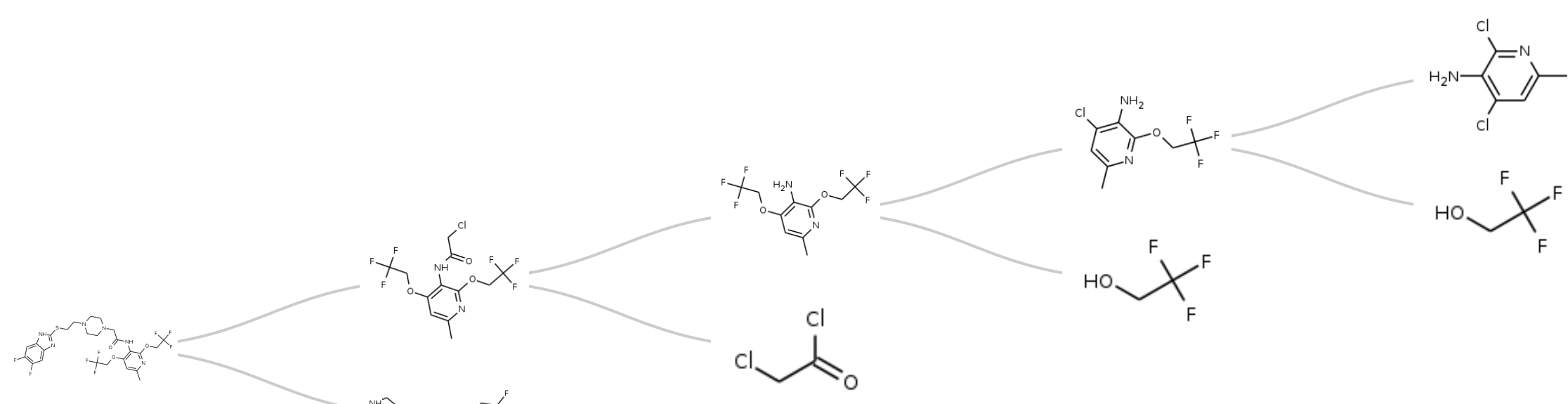
ASKCOS pathway, score: -21.465, ranking: 15, group: 9



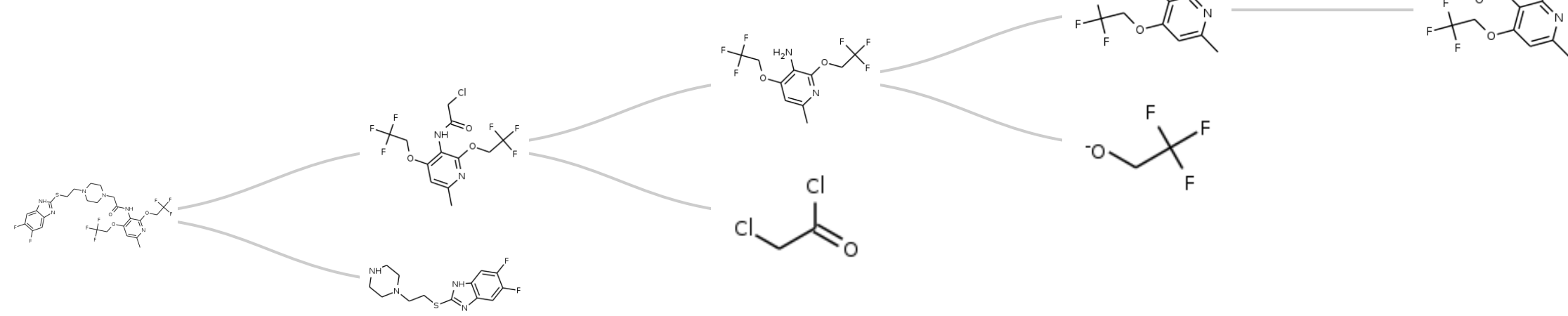
# Model ranks patent pathway as top-1: Example 39



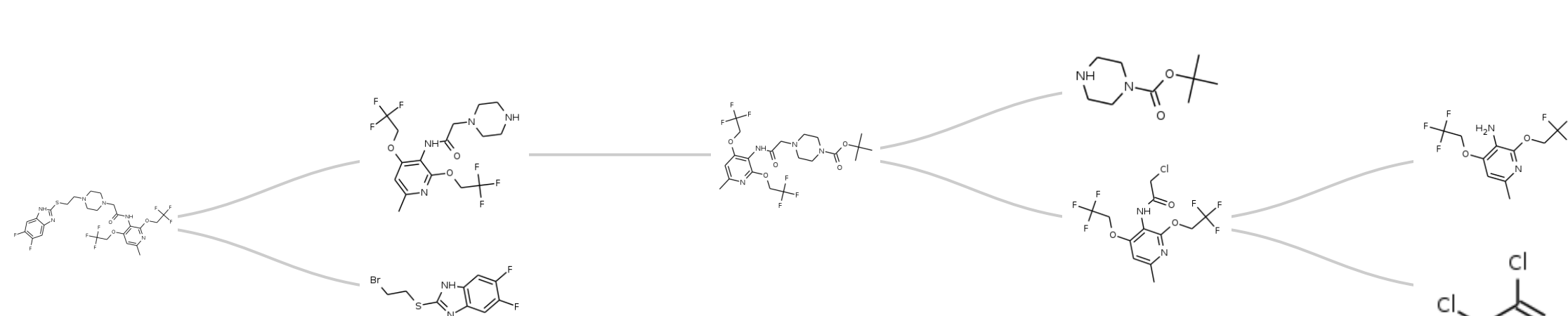
Platacho pathway, score: -10.059, ranking: 1, Patent No: US2005002006A1



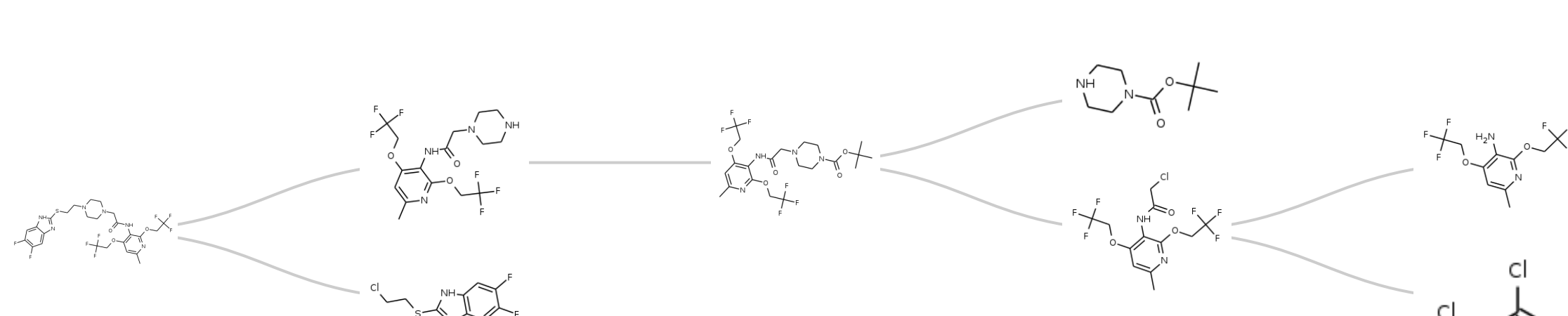
ASKCOS pathway, score: -15.964, ranking: 2, group: 1



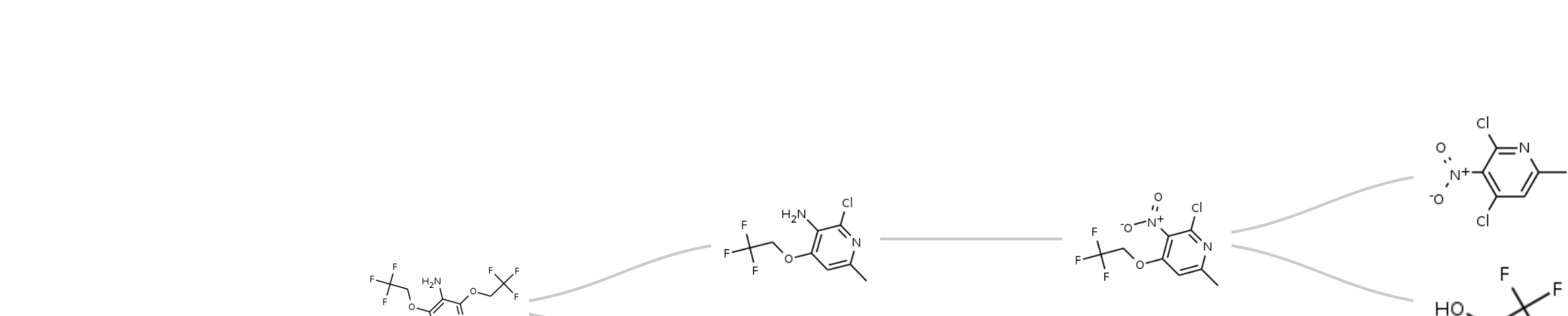
ASKCOS pathway, score: -16.027, ranking: 3, group: 2



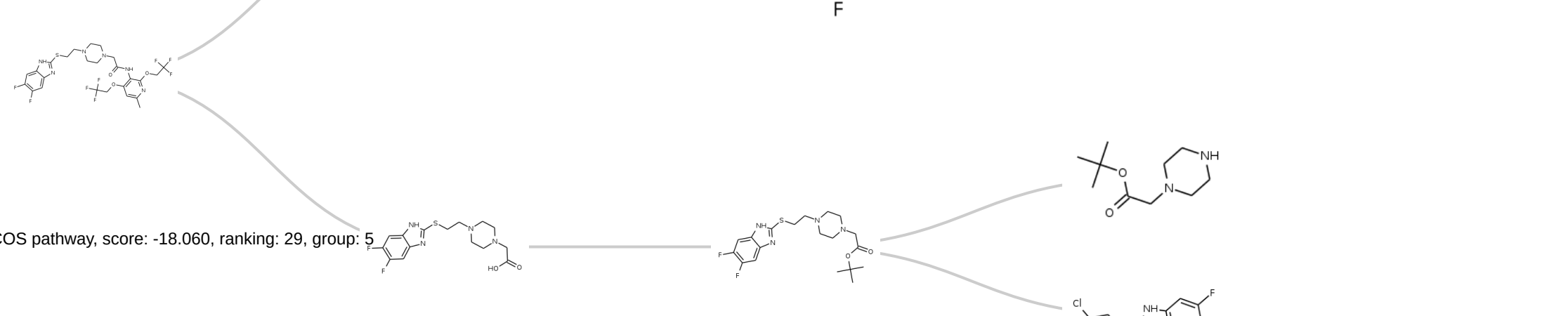
ASKCOS pathway, score: -16.660, ranking: 7, group: 3



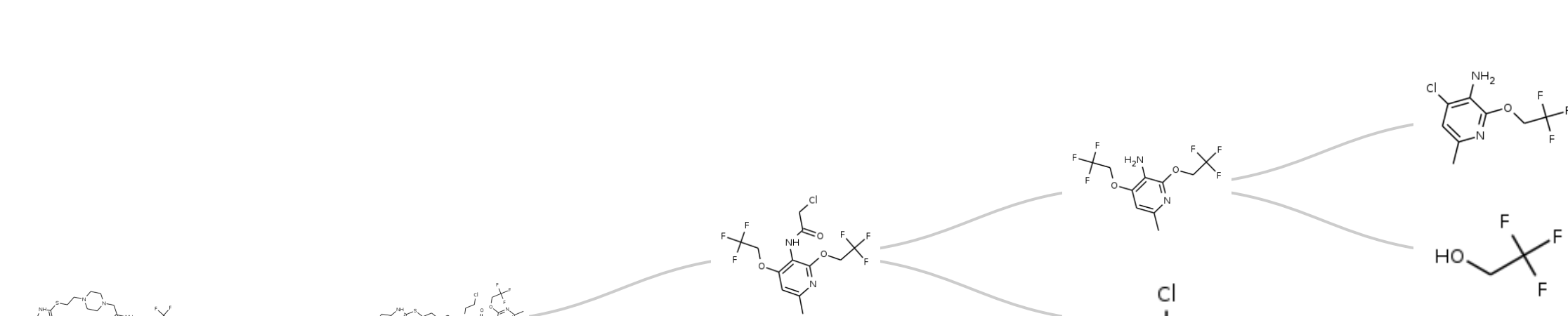
ASKCOS pathway, score: -16.862, ranking: 10, group: 4



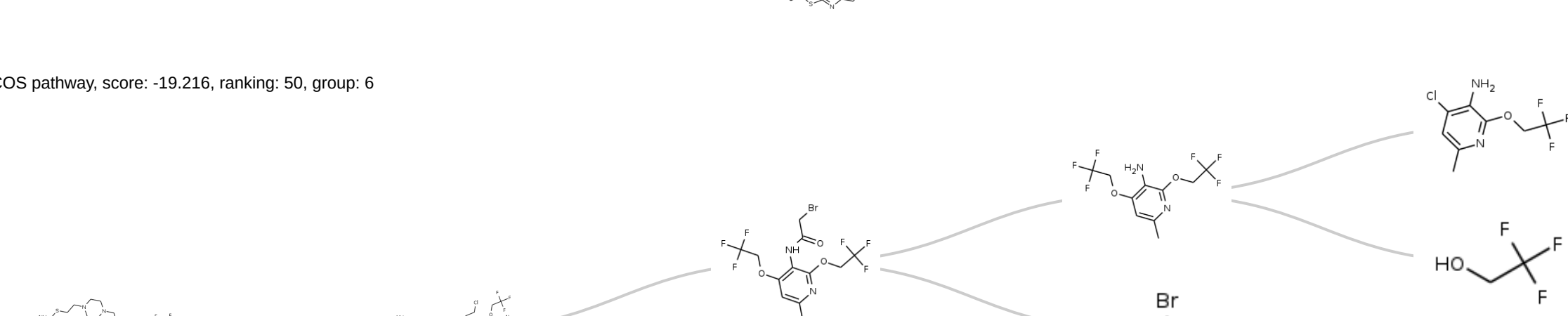
ASKCOS pathway, score: -18.050, ranking: 29, group: 5



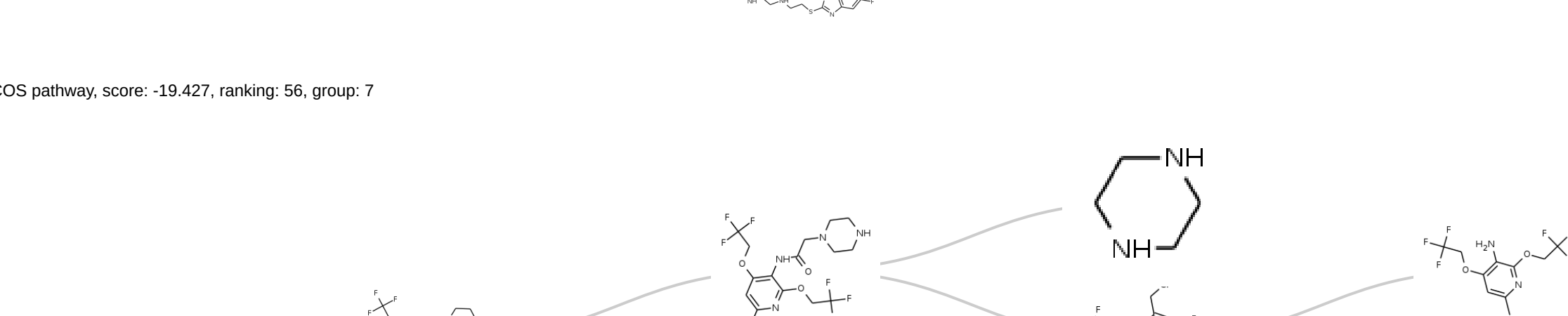
ASKCOS pathway, score: -19.216, ranking: 50, group: 6



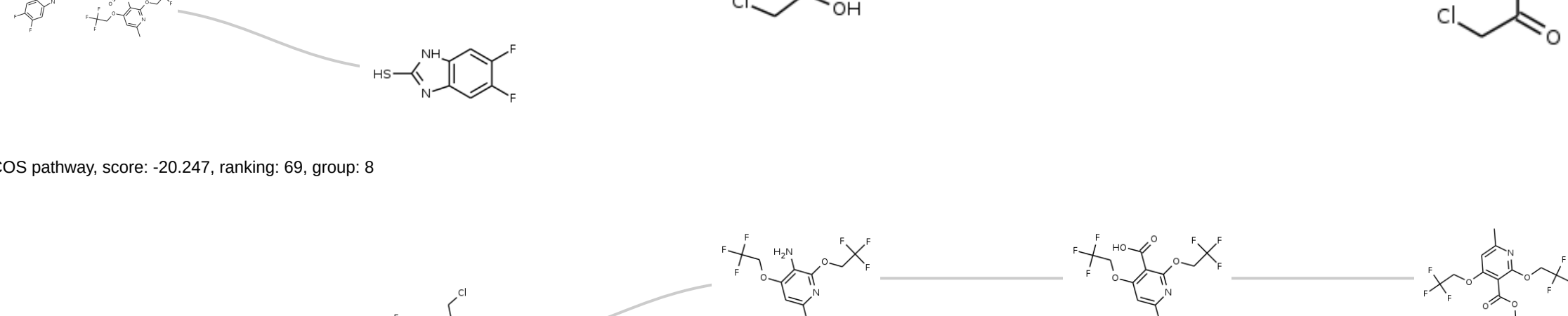
ASKCOS pathway, score: -19.427, ranking: 56, group: 7



ASKCOS pathway, score: -20.247, ranking: 69, group: 8



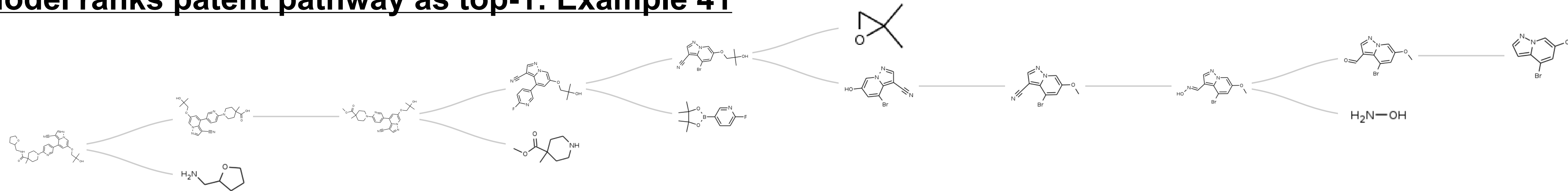
ASKCOS pathway, score: -20.847, ranking: 81, group: 9



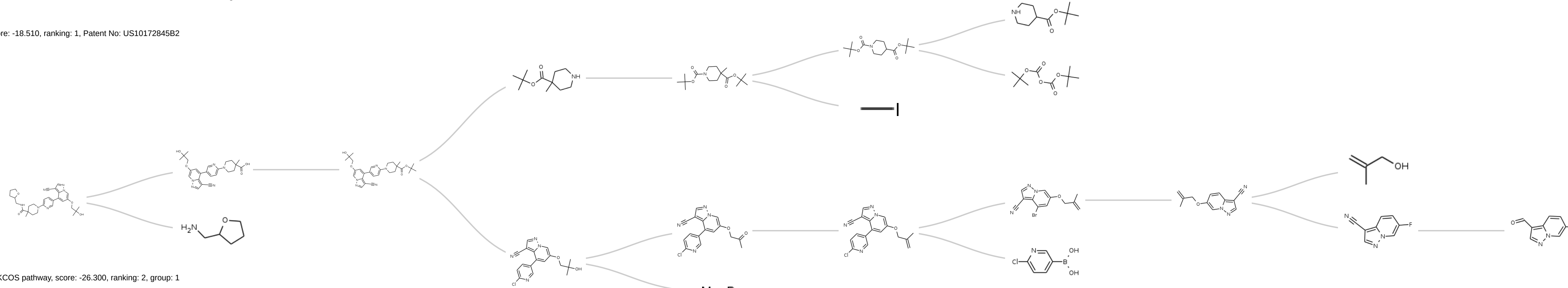


# Model ranks patent pathway as top-1: Example 41

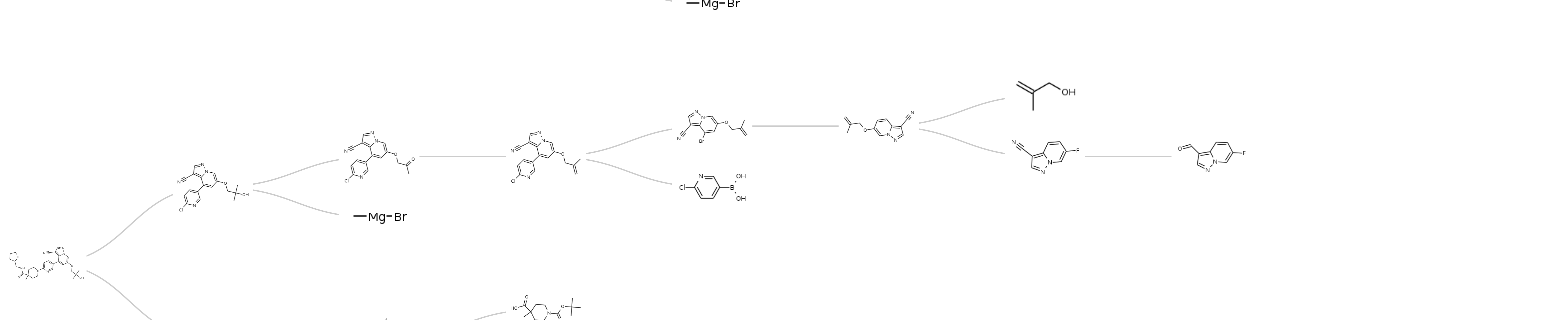
Patascho pathway, score: -18.510, ranking: 1, Patent No: US10172846B2



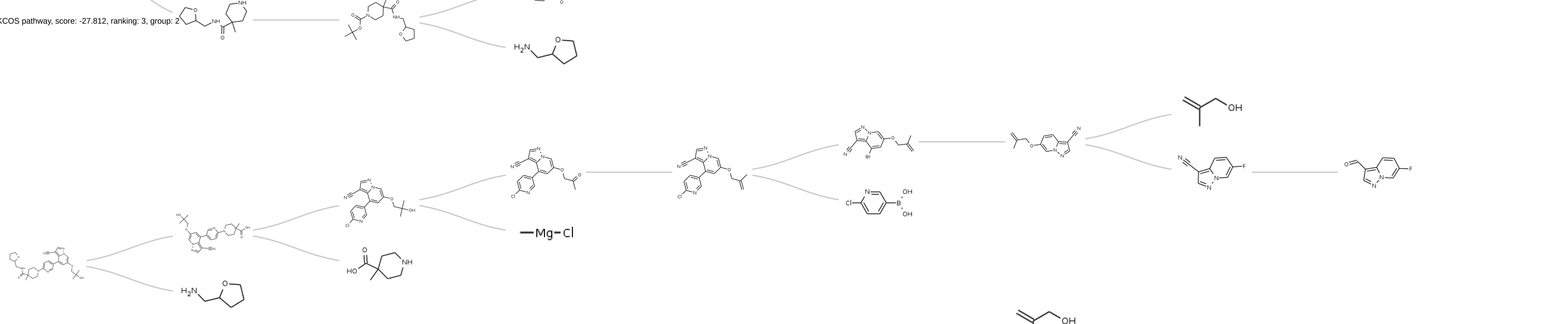
ASKCOS pathway, score: -26.300, ranking: 2, group: 1



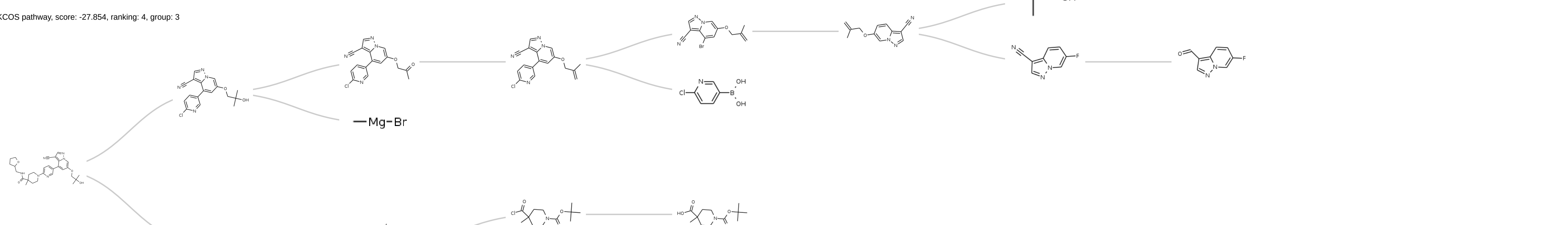
ASKCOS pathway, score: -27.812, ranking: 3, group: 3



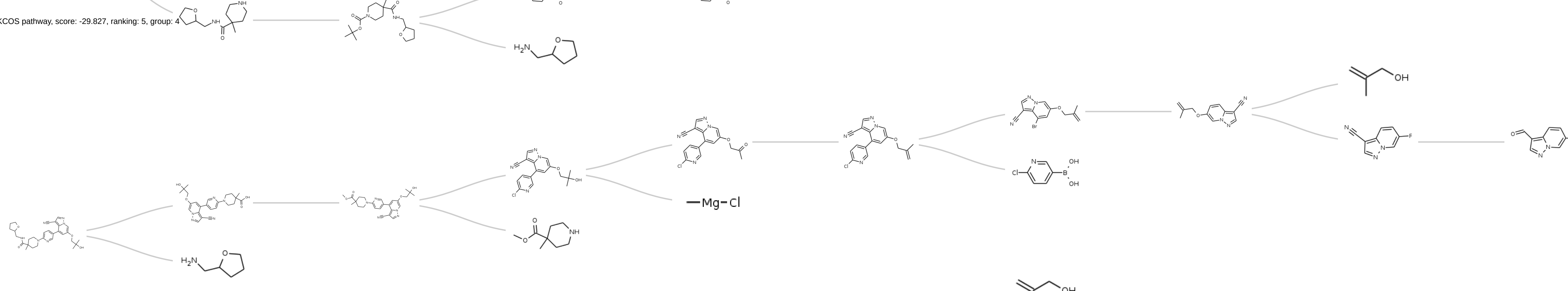
ASKCOS pathway, score: -27.854, ranking: 4, group: 3



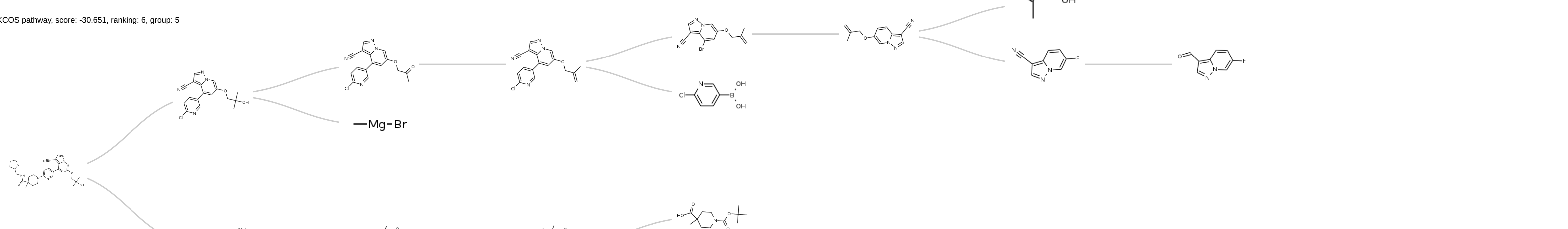
ASKCOS pathway, score: -29.827, ranking: 5, group: 5



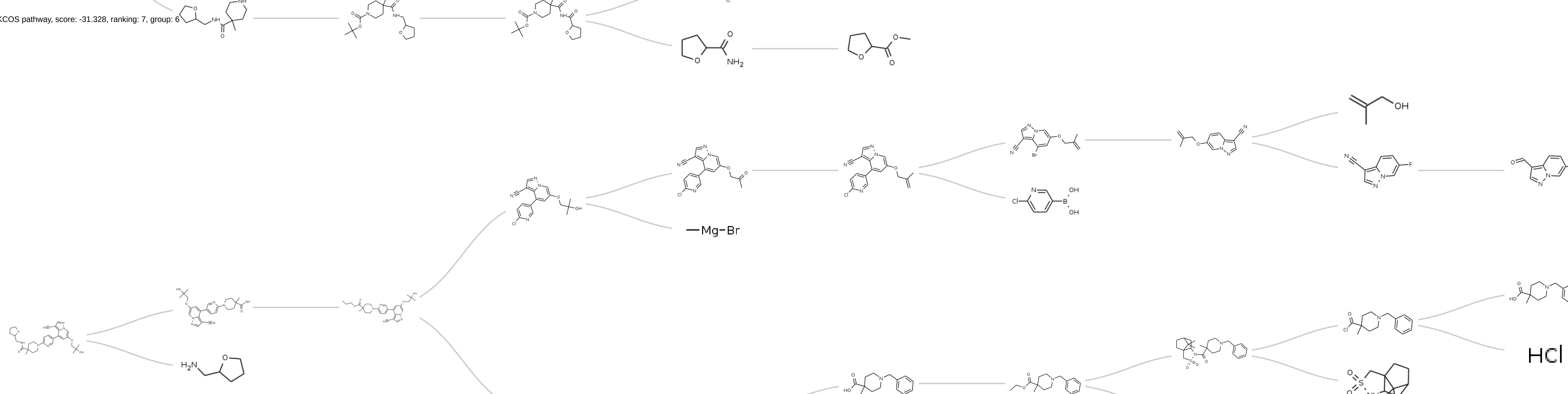
ASKCOS pathway, score: -30.651, ranking: 6, group: 5



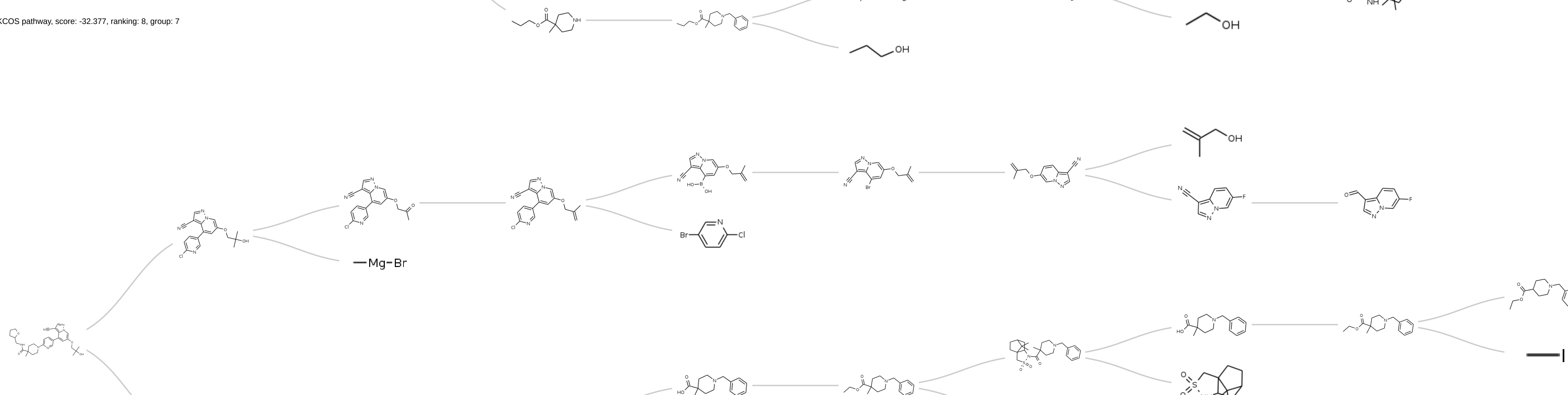
ASKCOS pathway, score: -31.328, ranking: 7, group: 7



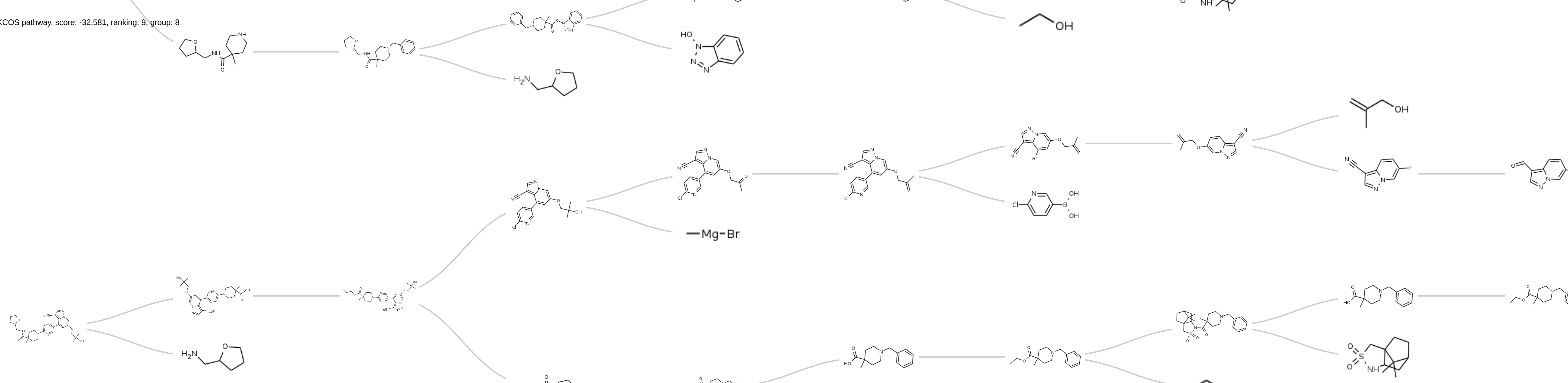
ASKCOS pathway, score: -32.377, ranking: 8, group: 7



ASKCOS pathway, score: -32.551, ranking: 9, group: 8

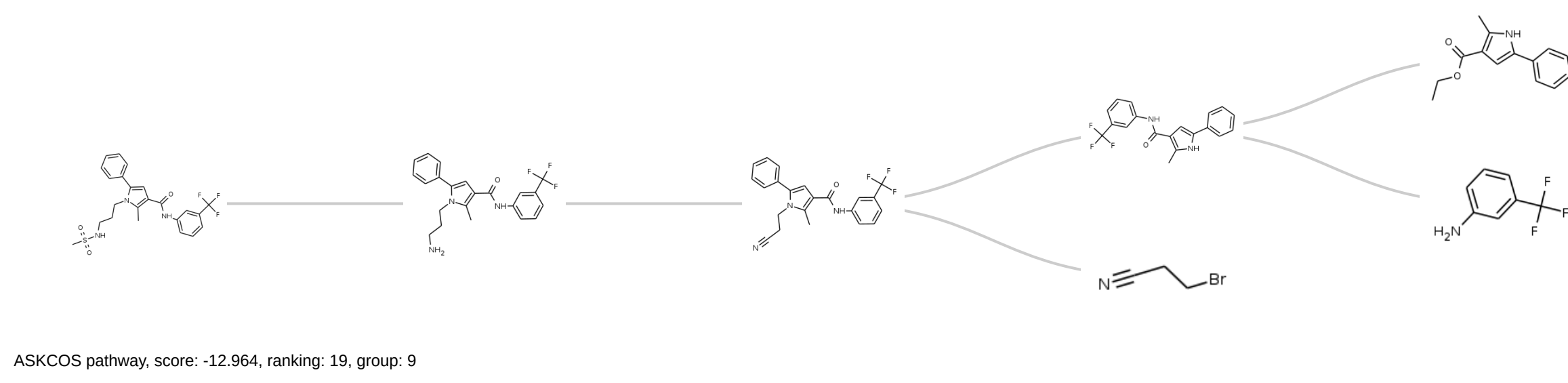
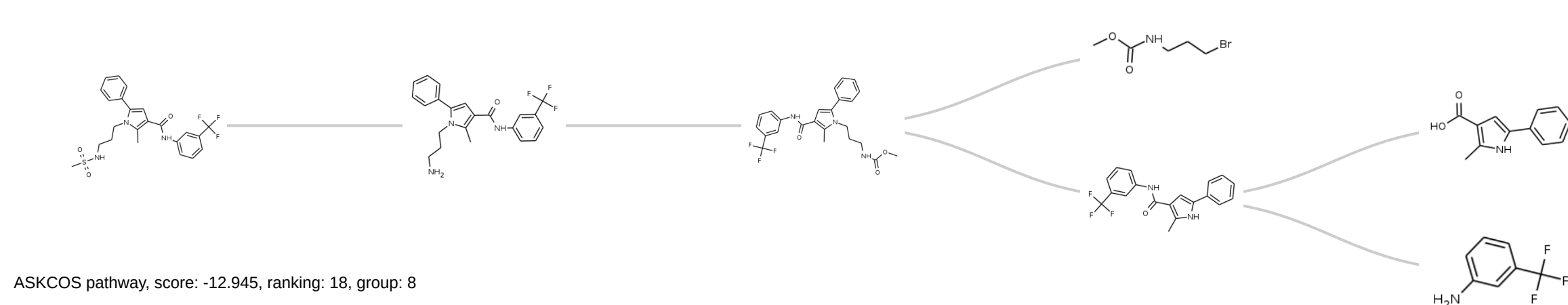
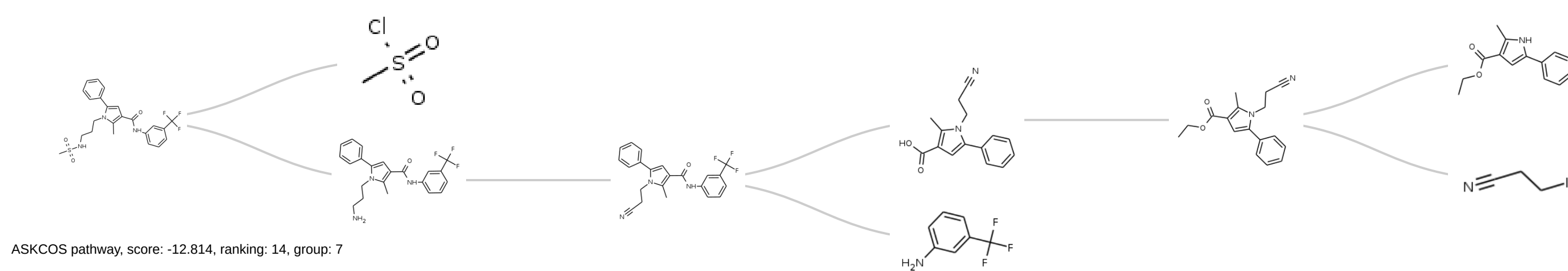
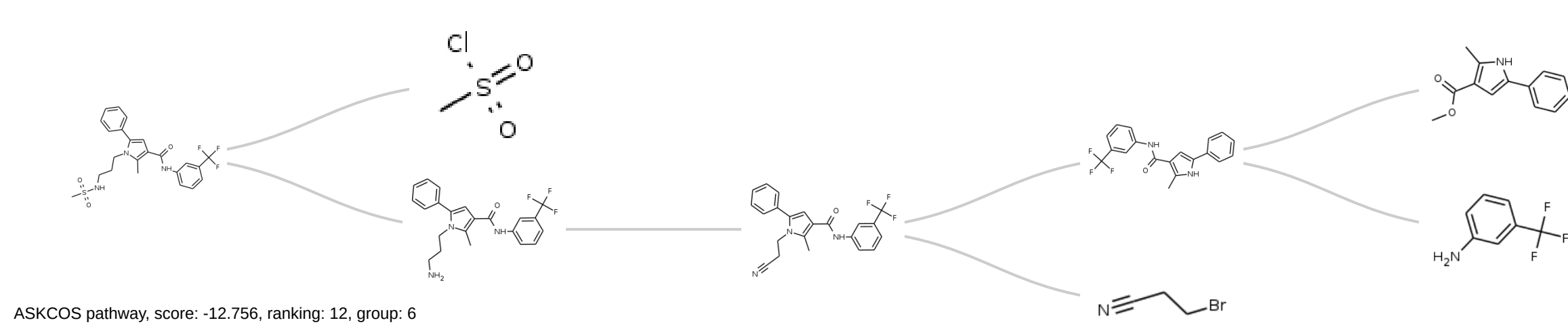
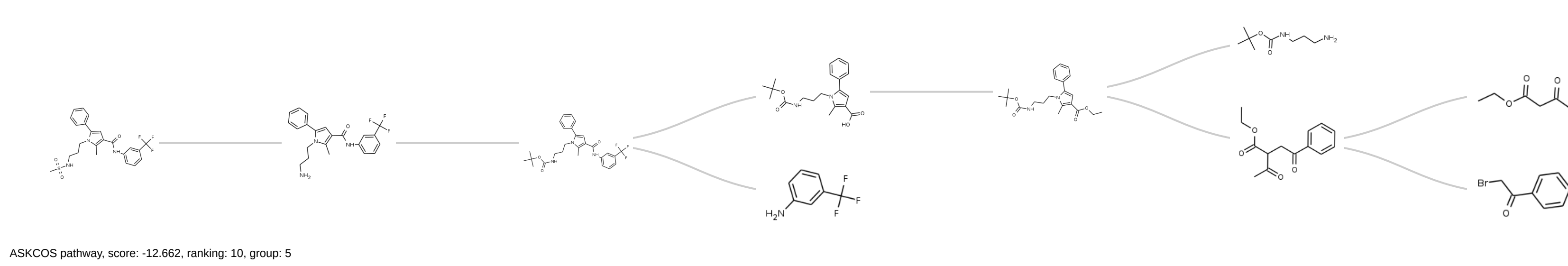
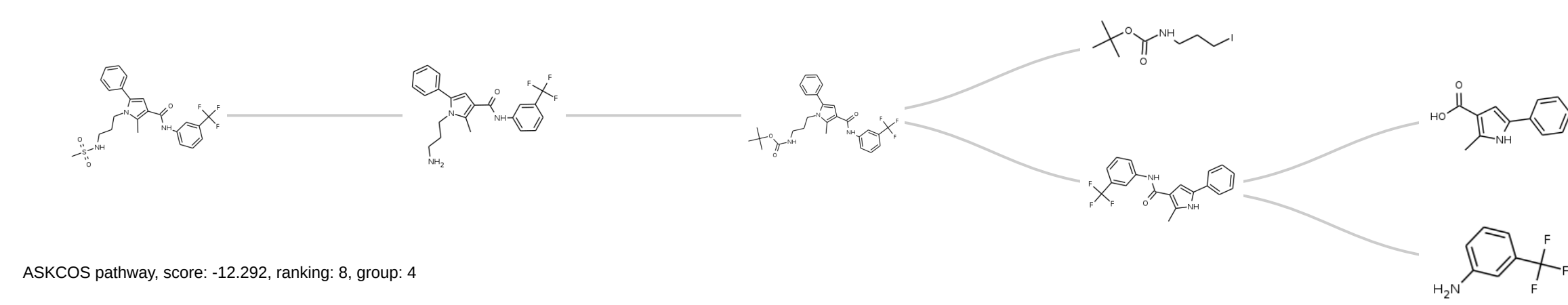
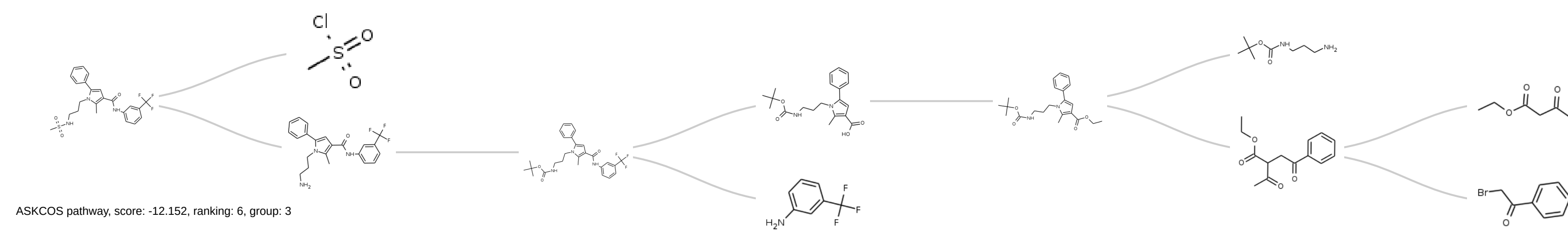
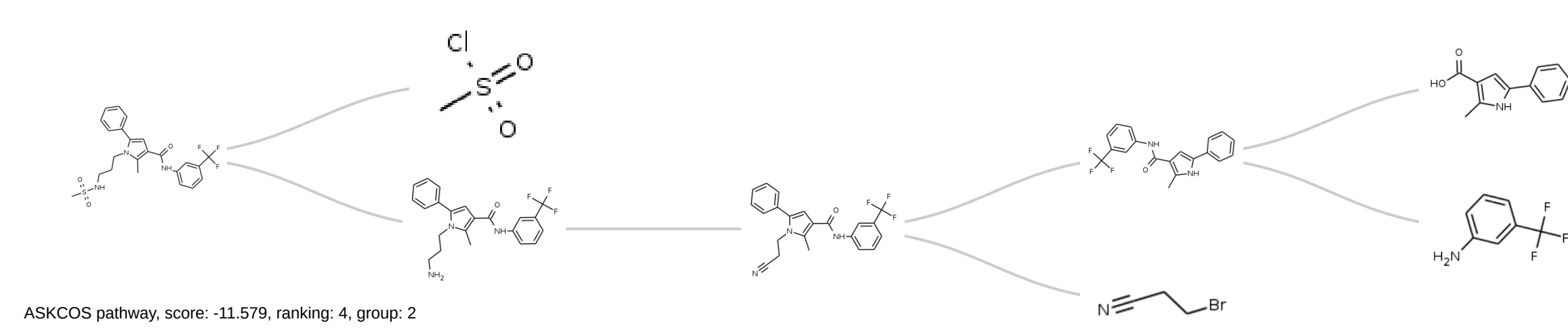
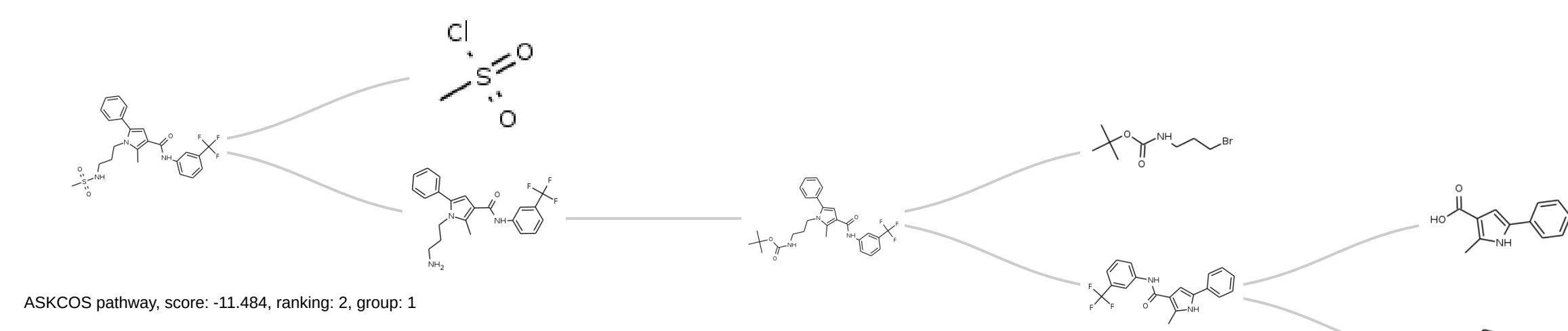
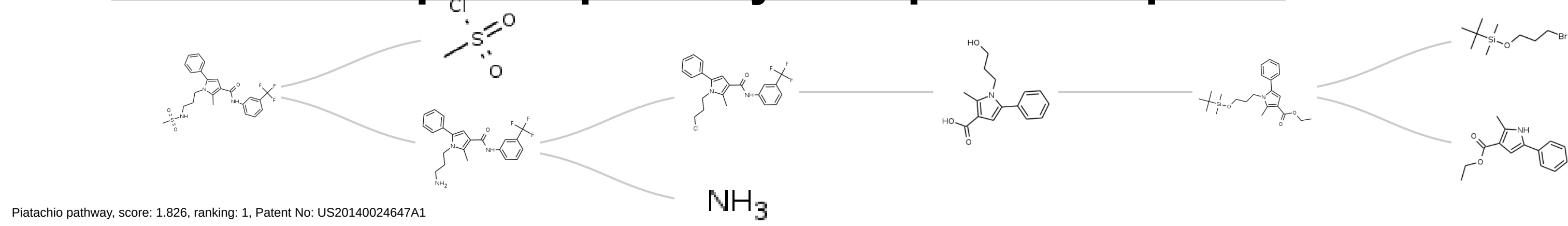


ASKCOS pathway, score: -32.913, ranking: 12, group: 9





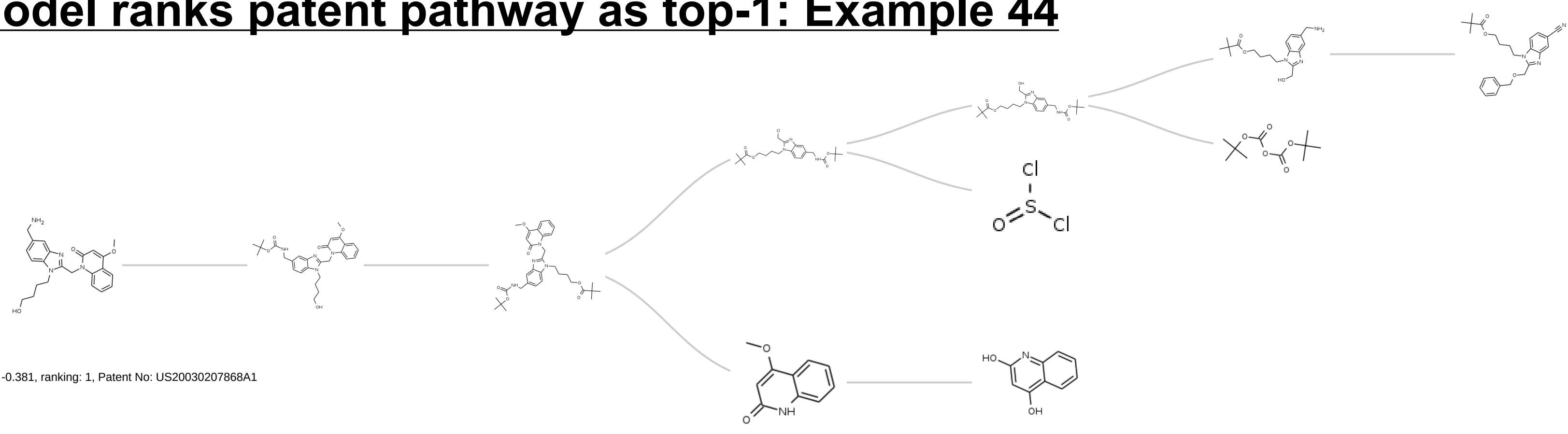
### Model ranks patent pathway as top-1: Example 43



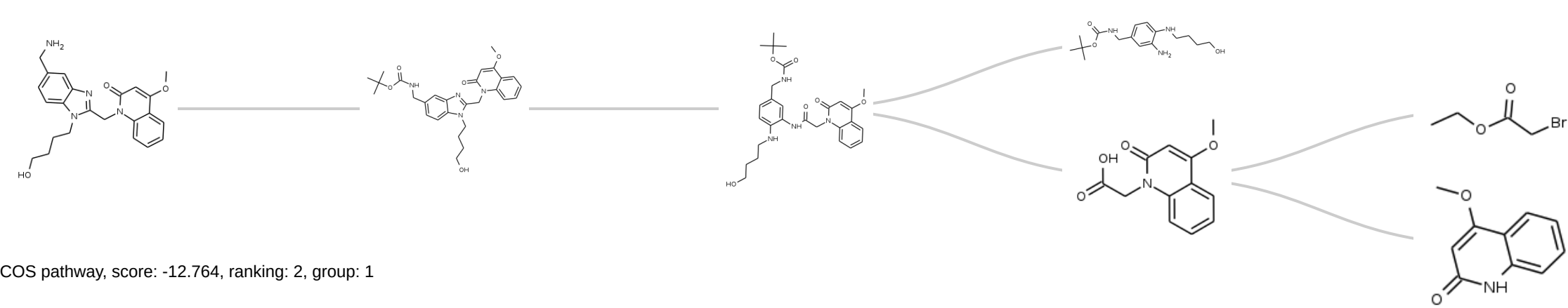


# Model ranks patent pathway as top-1: Example 44

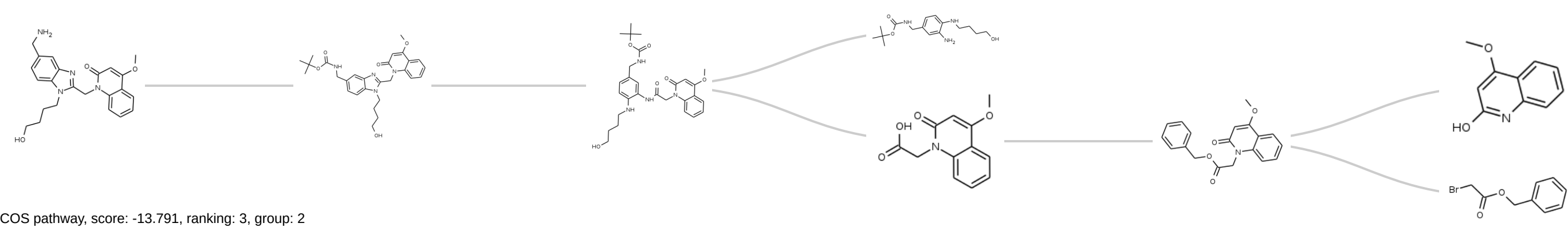
Patango pathway, score: -0.351, ranking: 1, Patent No: US20030207856A1



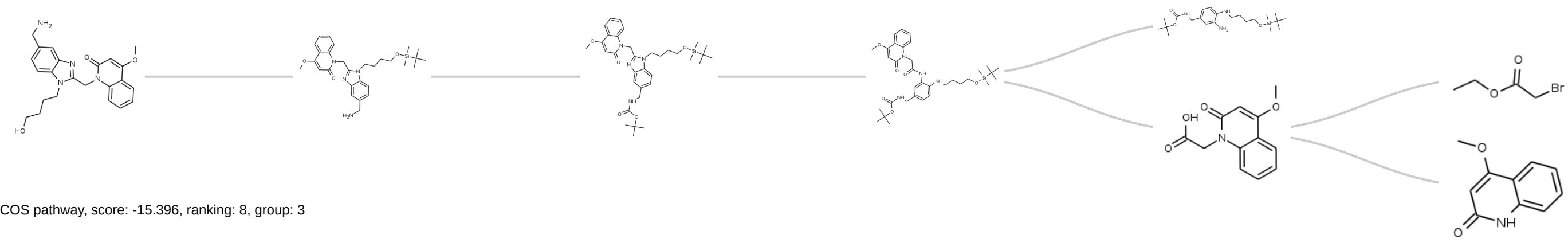
ASKCOS pathway, score: -12.764, ranking: 2, group: 1



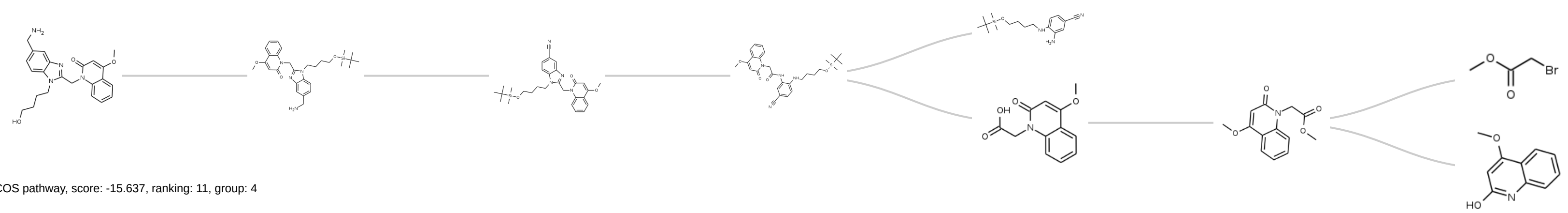
ASKCOS pathway, score: -13.701, ranking: 3, group: 2



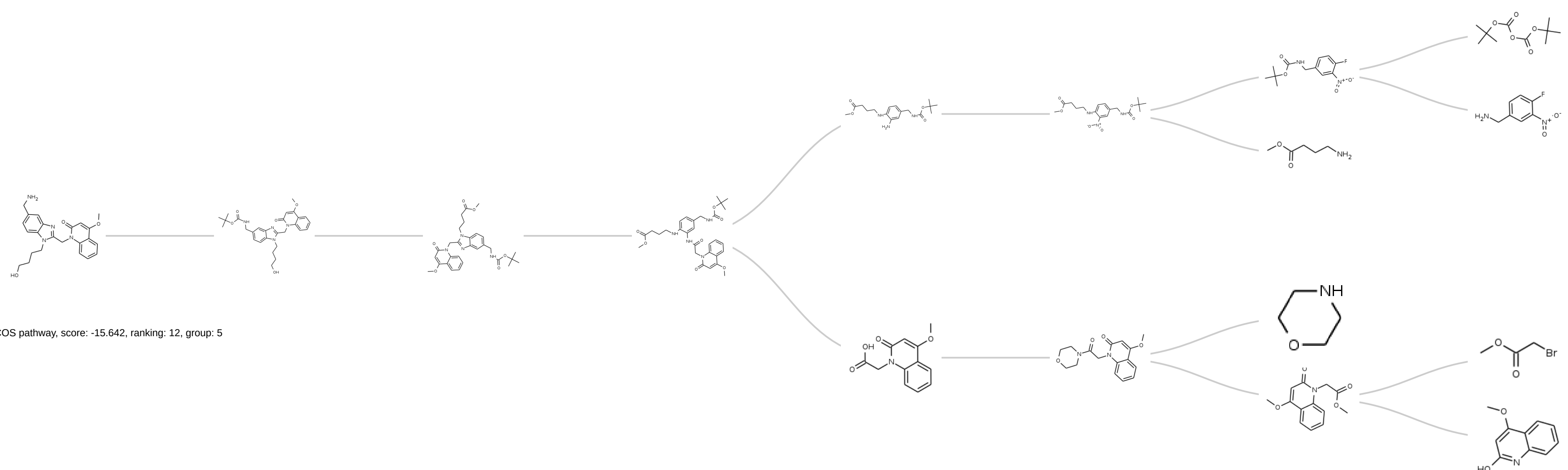
ASKCOS pathway, score: -15.936, ranking: 8, group: 3



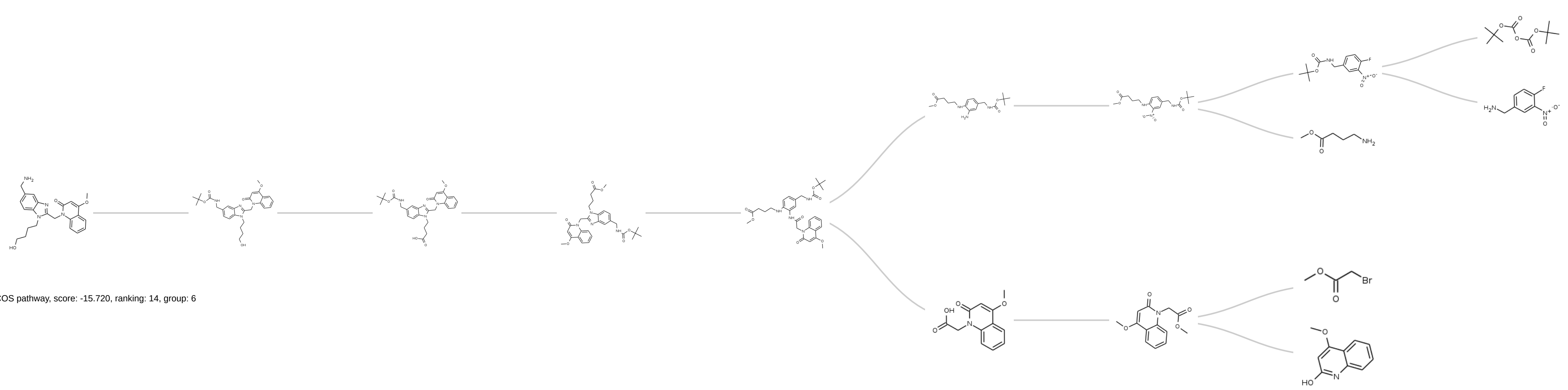
ASKCOS pathway, score: -15.637, ranking: 11, group: 4



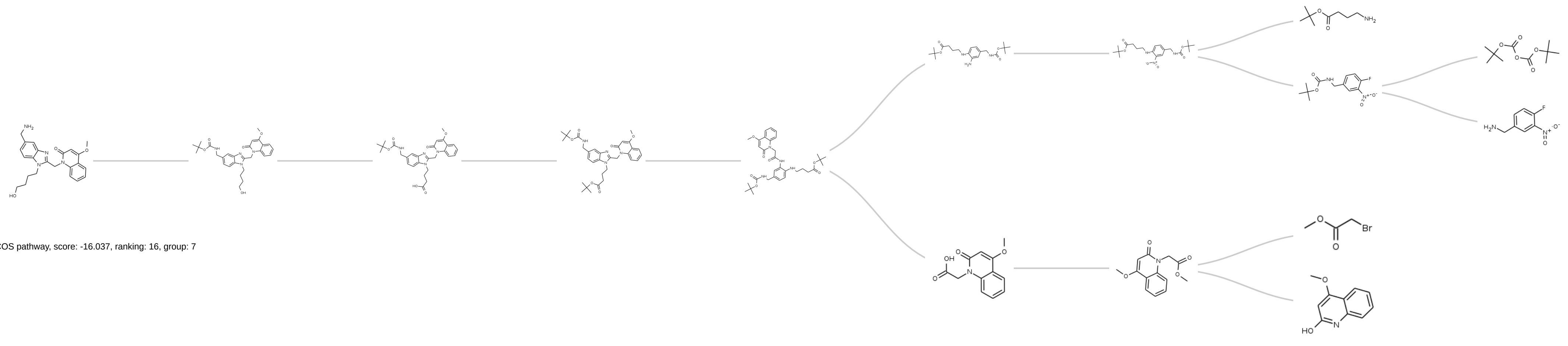
ASKCOS pathway, score: -15.642, ranking: 12, group: 5



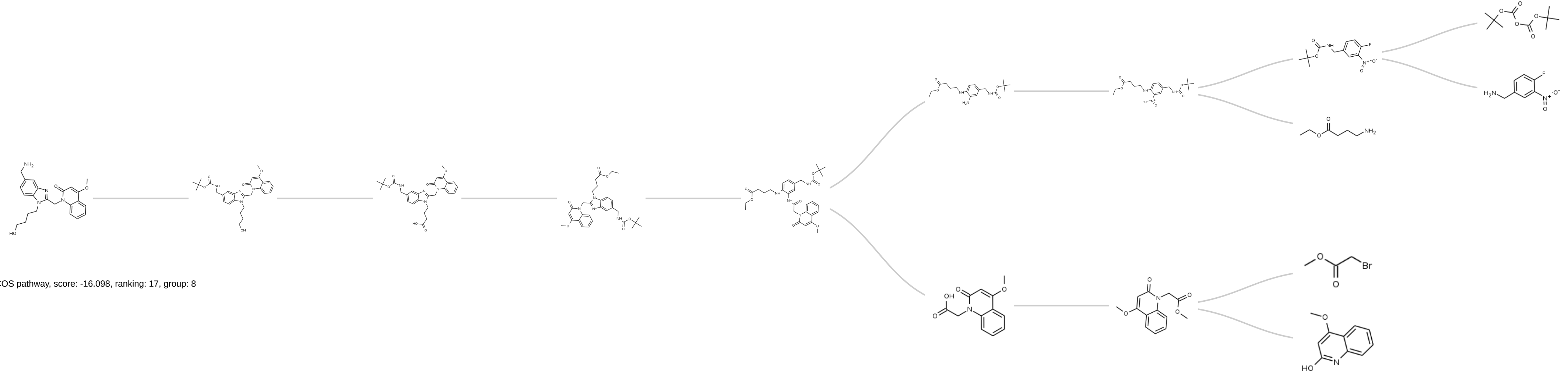
ASKCOS pathway, score: -15.720, ranking: 14, group: 6



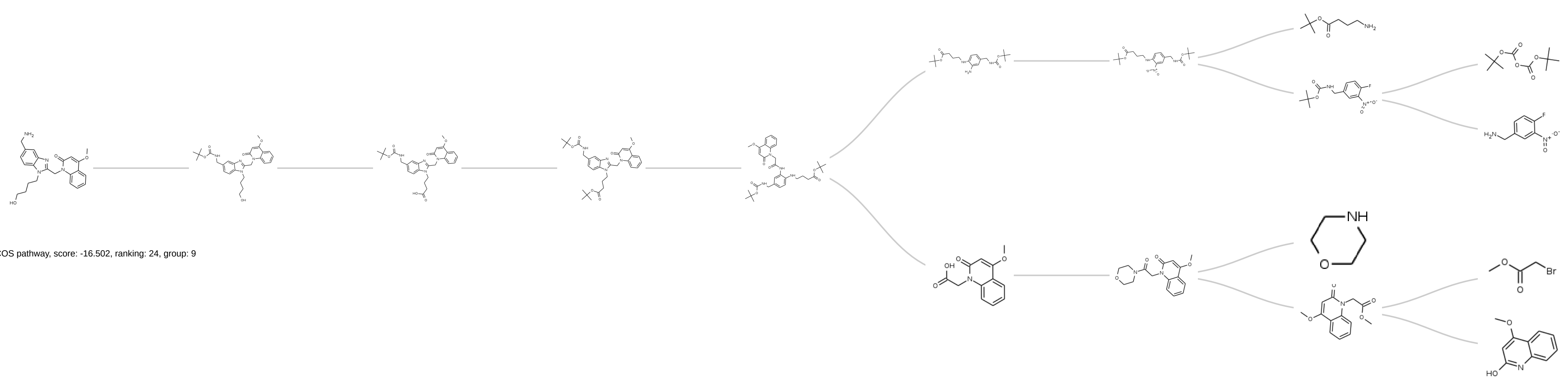
ASKCOS pathway, score: -16.037, ranking: 16, group: 7



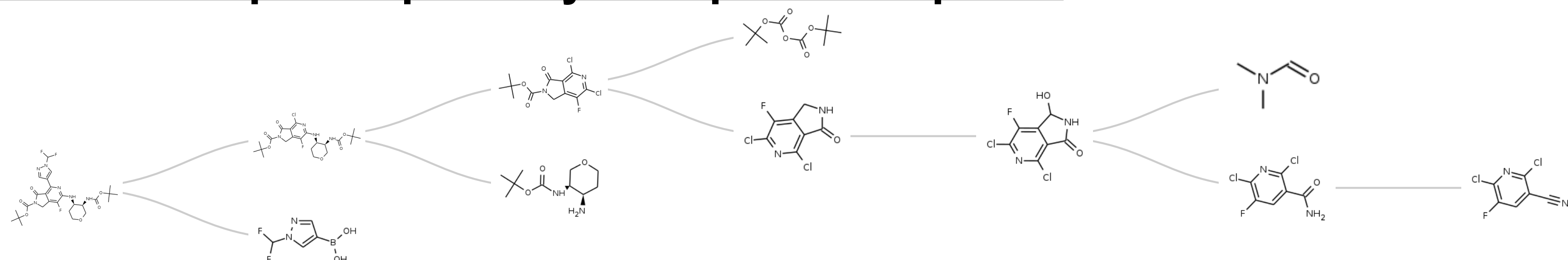
ASKCOS pathway, score: -16.098, ranking: 17, group: 8



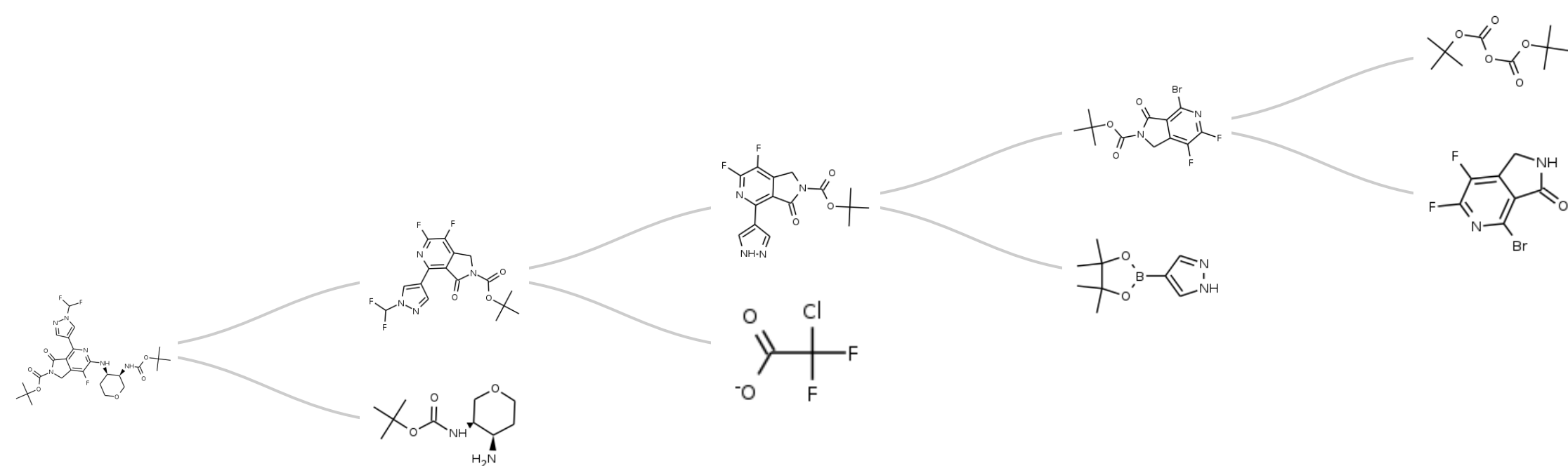
ASKCOS pathway, score: -16.502, ranking: 24, group: 9



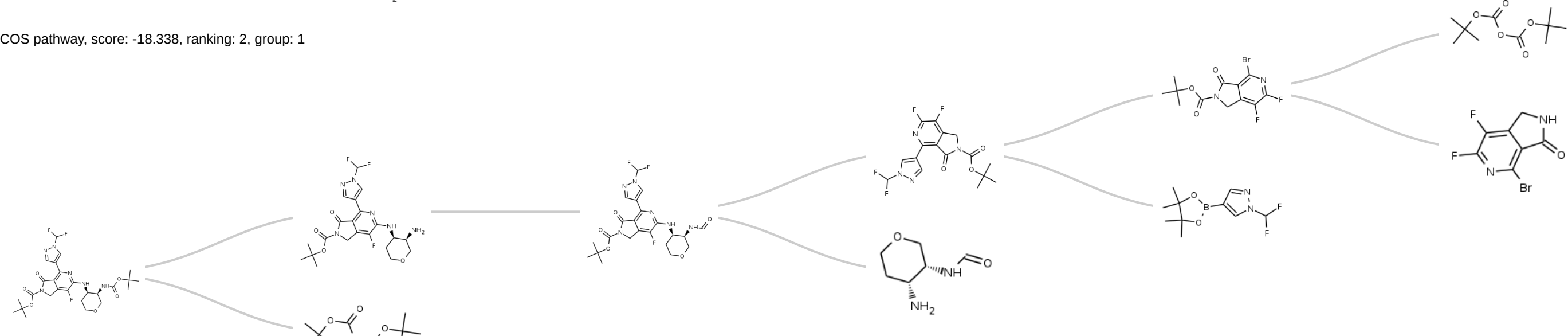
# Model ranks patent pathway as top-1: Example 45



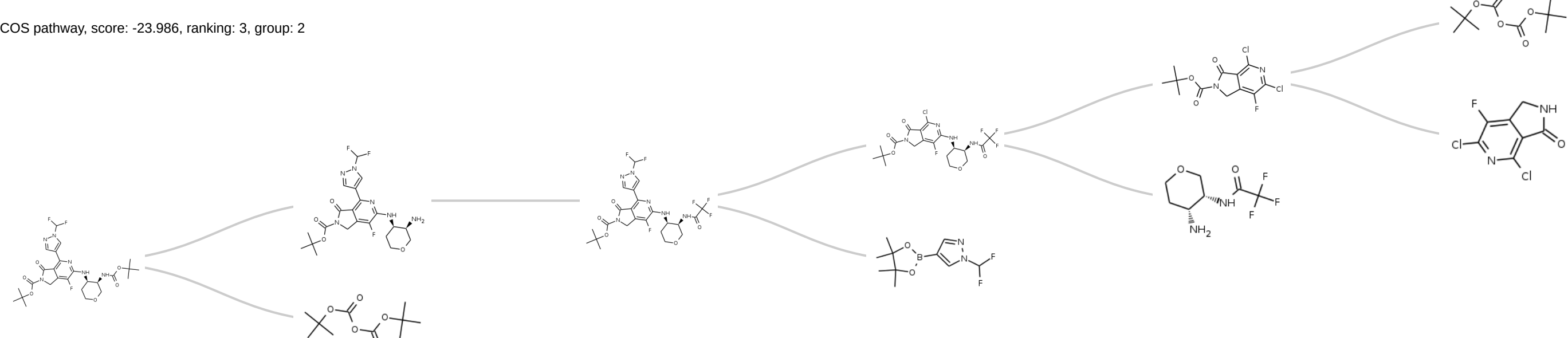
Patcho pathway, score: -12.616, ranking: 1, Patent No: US20110152279A1



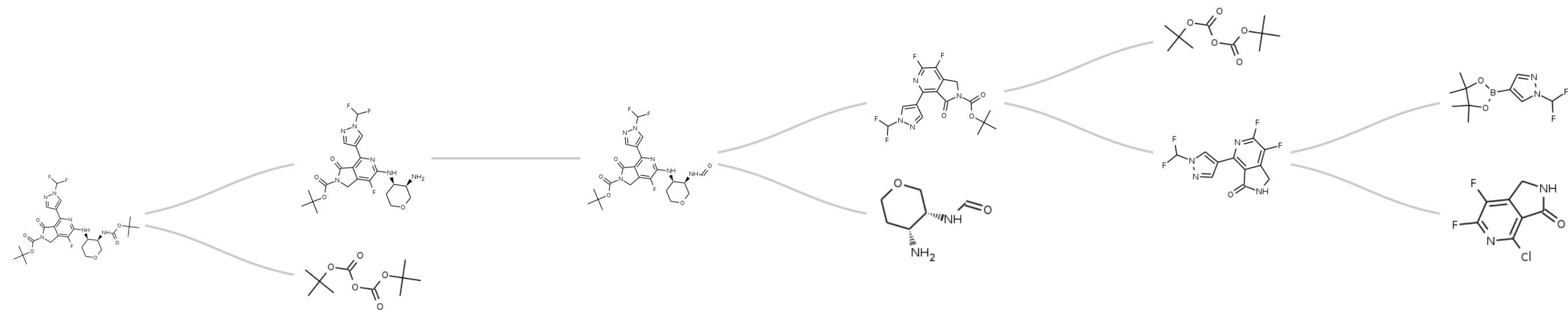
ASKCOS pathway, score: -18.338, ranking: 2, group: 1



ASKCOS pathway, score: -23.996, ranking: 3, group: 2

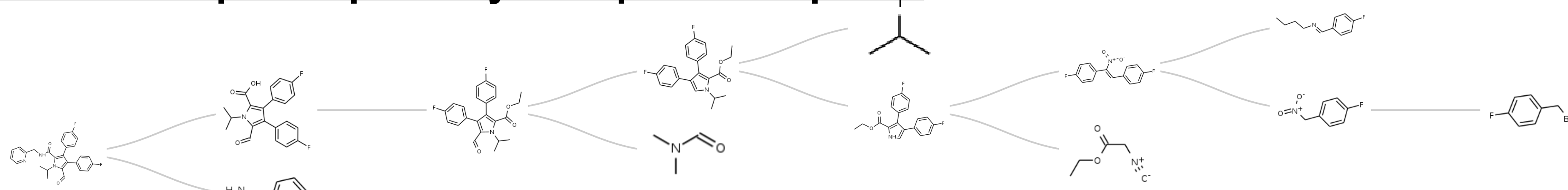


ASKCOS pathway, score: -24.753, ranking: 6, group: 3

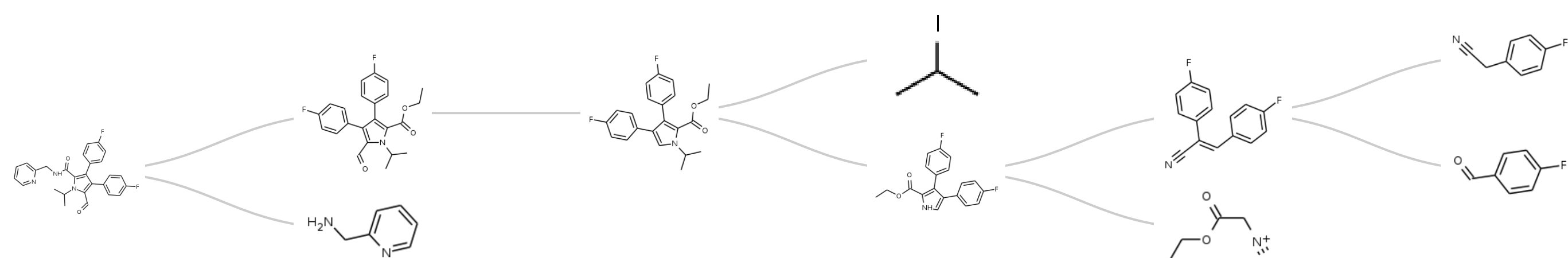


ASKCOS pathway, score: -27.769, ranking: 19, group: 4

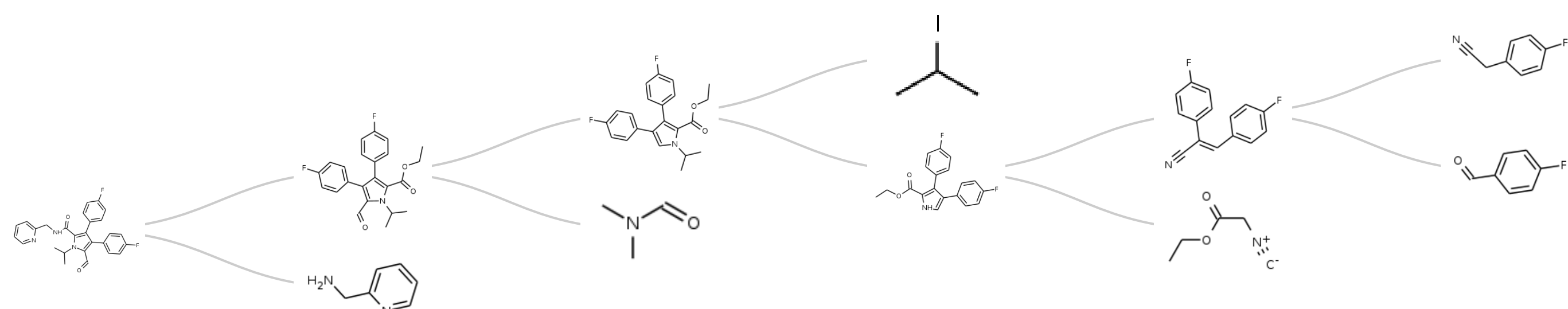
# Model ranks patent pathway as top-1: Example 46



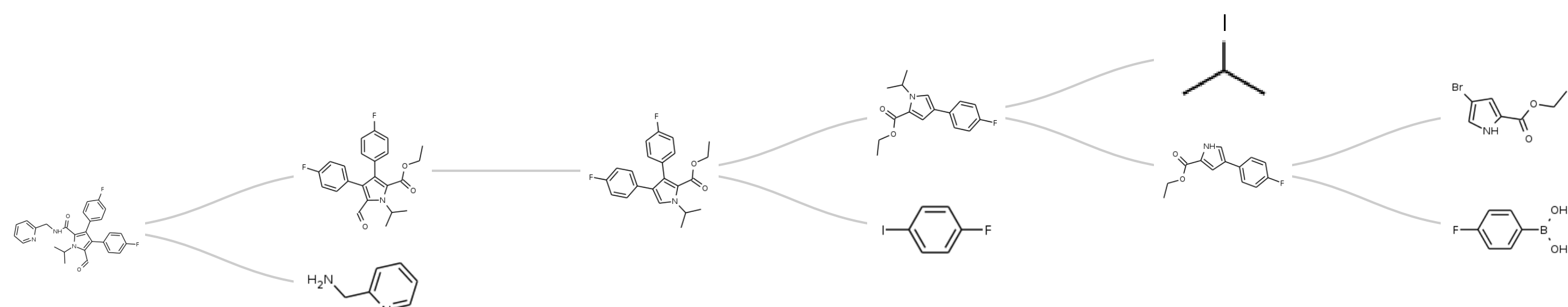
Phazho pathway, score: -12.498, ranking: 1, Patent No: US2009154042A1



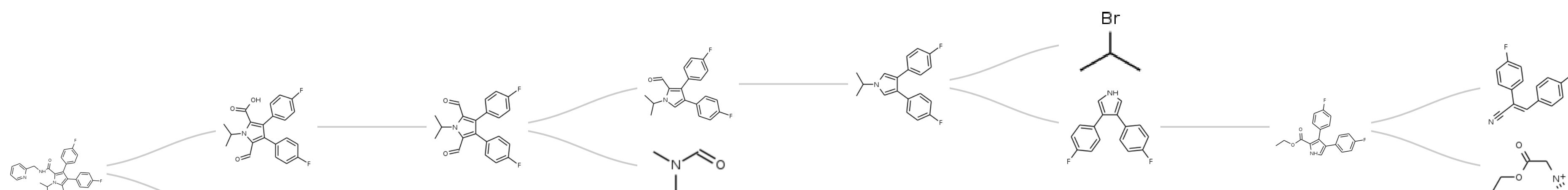
ASKCOS pathway, score: -13.426, ranking: 2, group: 1



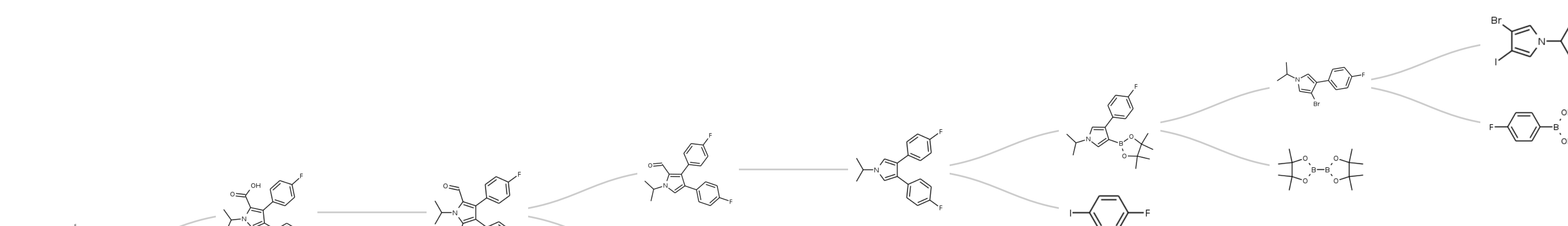
ASKCOS pathway, score: -13.554, ranking: 3, group: 2



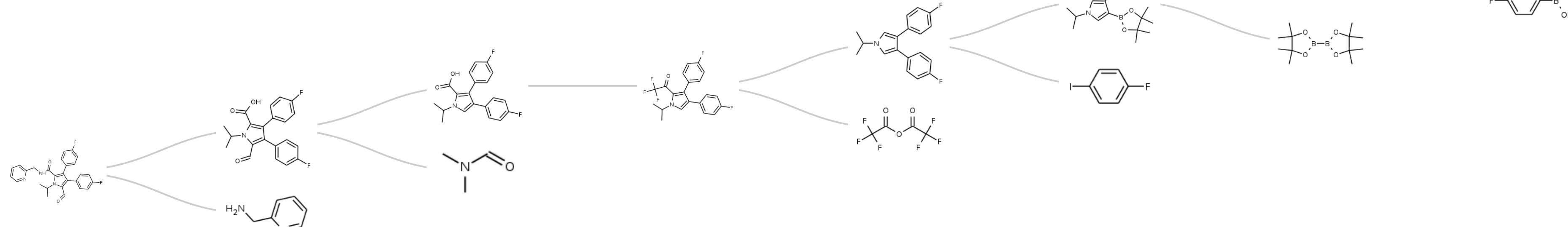
ASKCOS pathway, score: -18.741, ranking: 17, group: 3



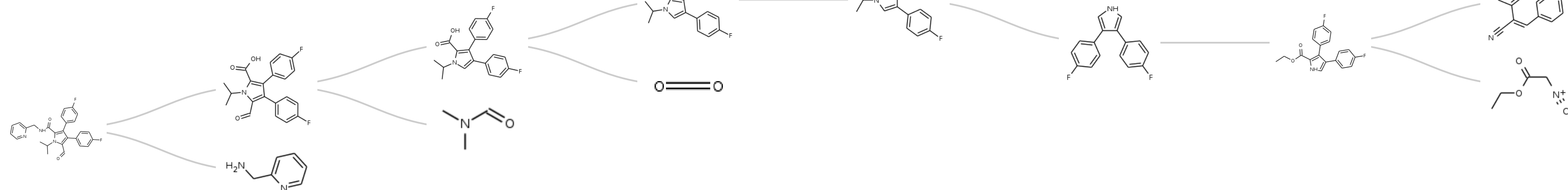
ASKCOS pathway, score: -19.026, ranking: 20, group: 4



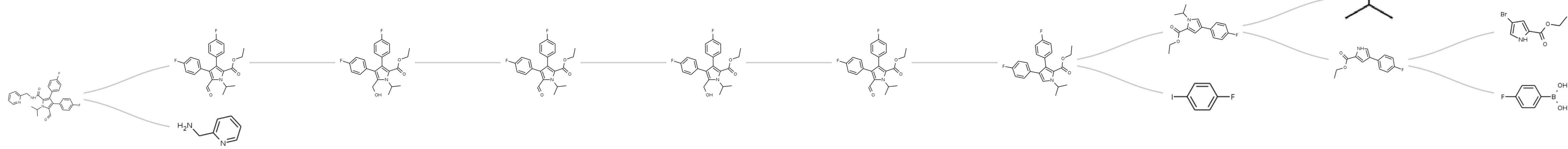
ASKCOS pathway, score: -20.423, ranking: 36, group: 5



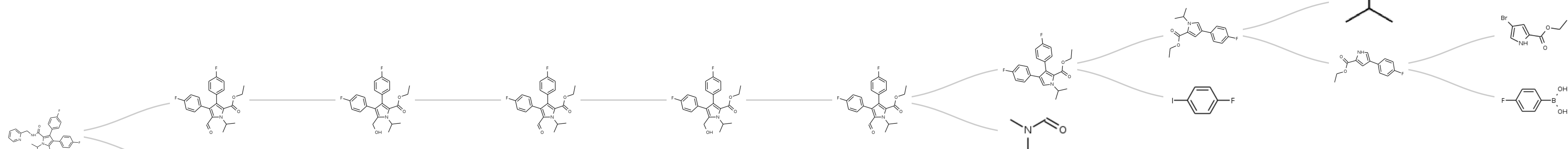
ASKCOS pathway, score: -21.339, ranking: 47, group: 6



ASKCOS pathway, score: -21.863, ranking: 57, group: 7

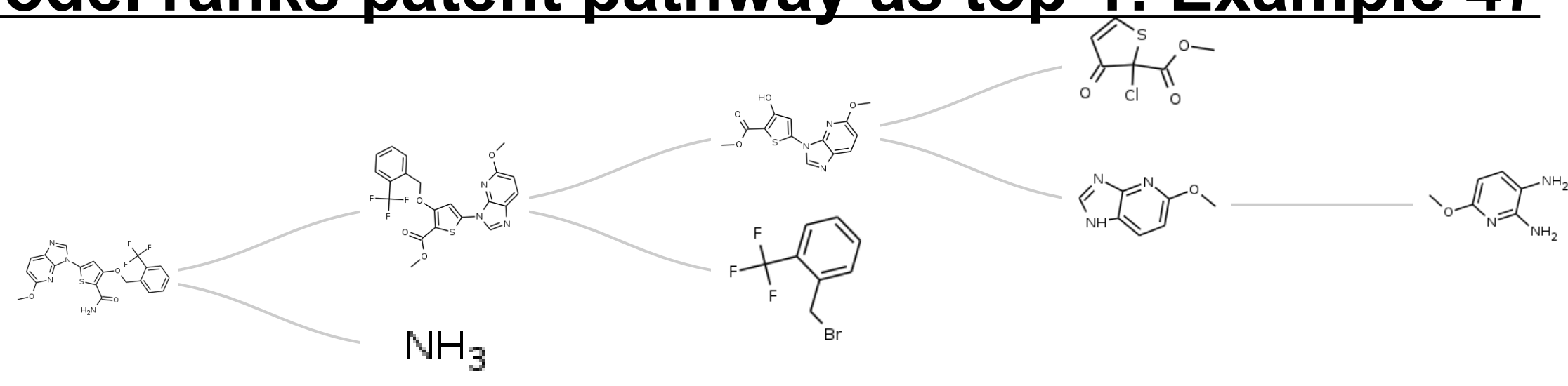


ASKCOS pathway, score: -22.229, ranking: 62, group: 8

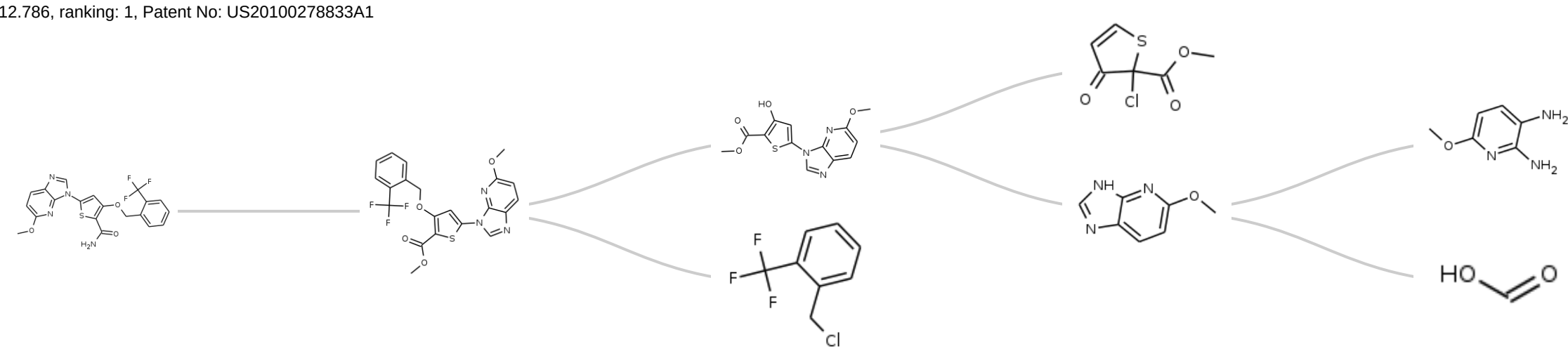


ASKCOS pathway, score: -22.348, ranking: 63, group: 9

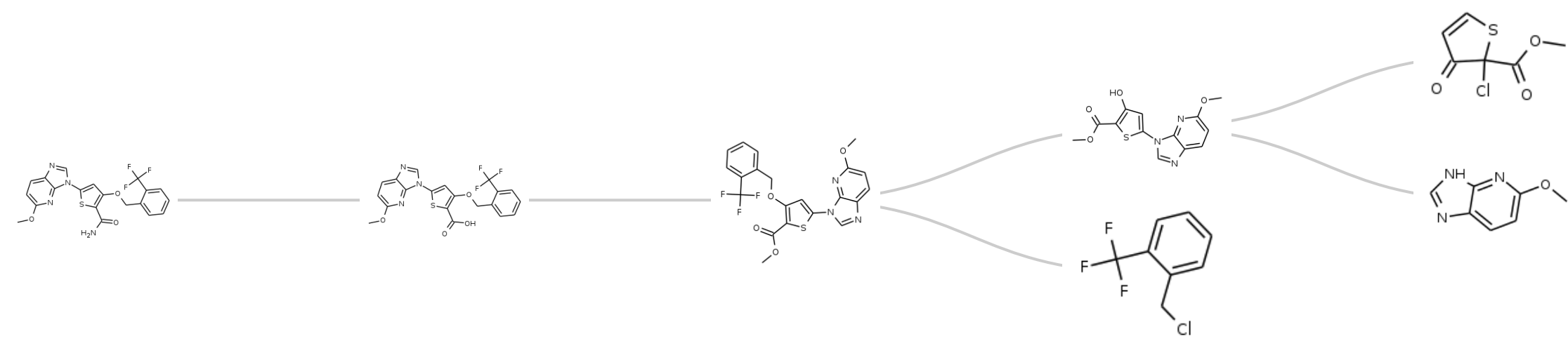
# Model ranks patent pathway as top-1: Example 47



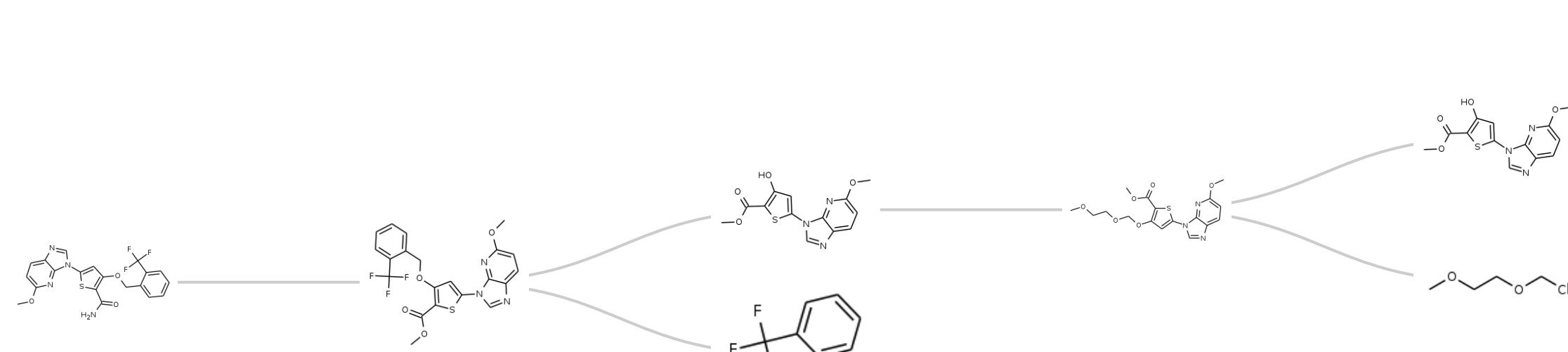
Pubchem pathway score: -12.796, ranking: 1, Patent No: US2010027833A1



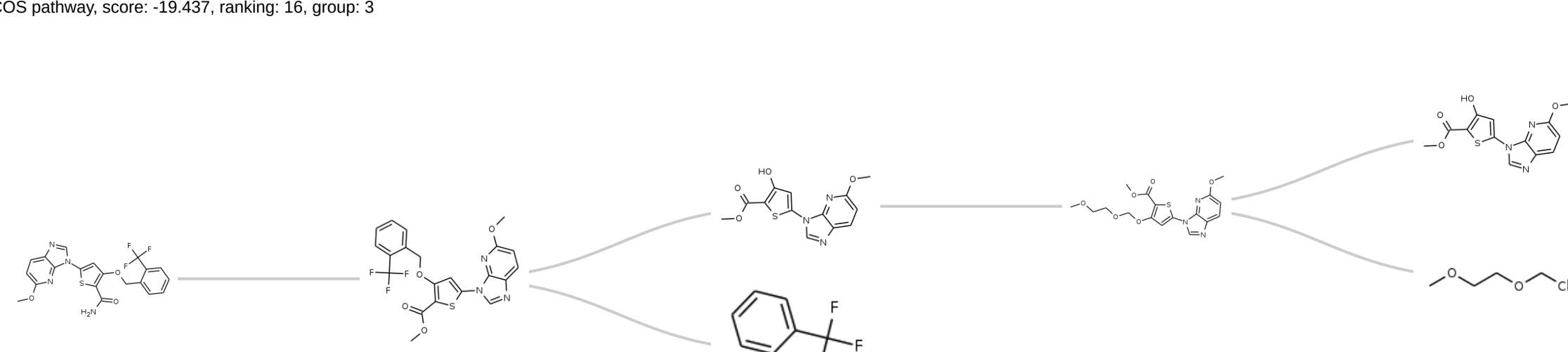
ASKCOS pathway score: -16.343, ranking: 2, group: 1



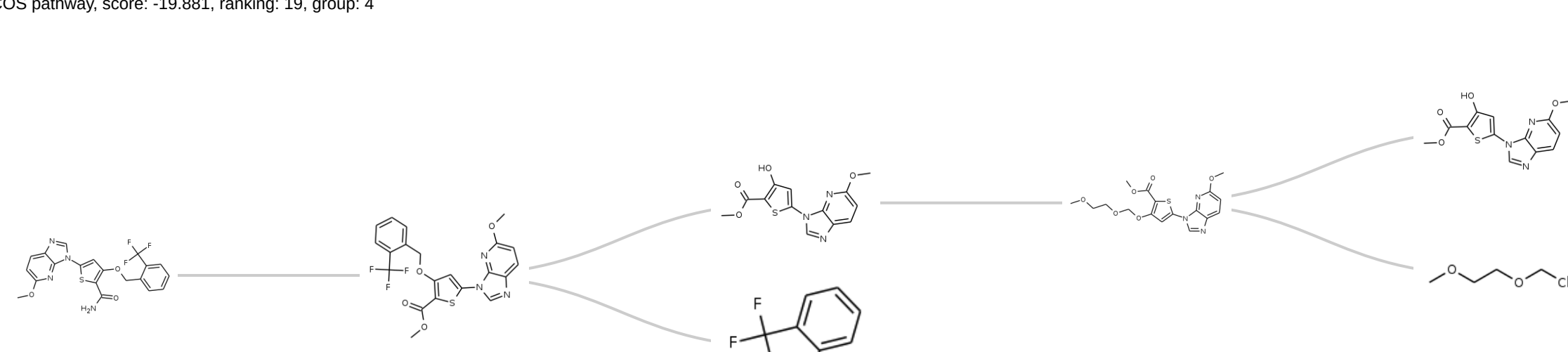
ASKCOS pathway score: -18.583, ranking: 10, group: 2



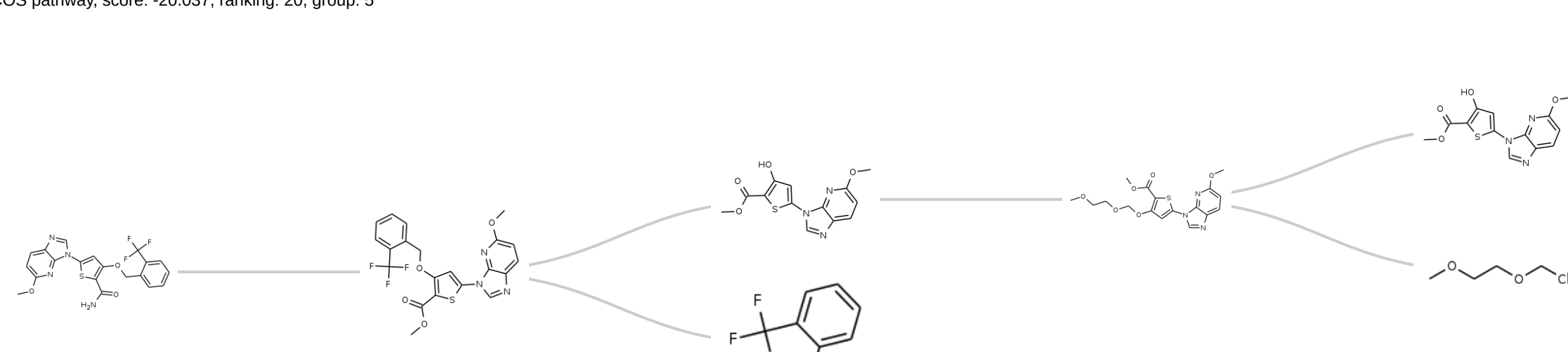
ASKCOS pathway score: -18.437, ranking: 15, group: 3



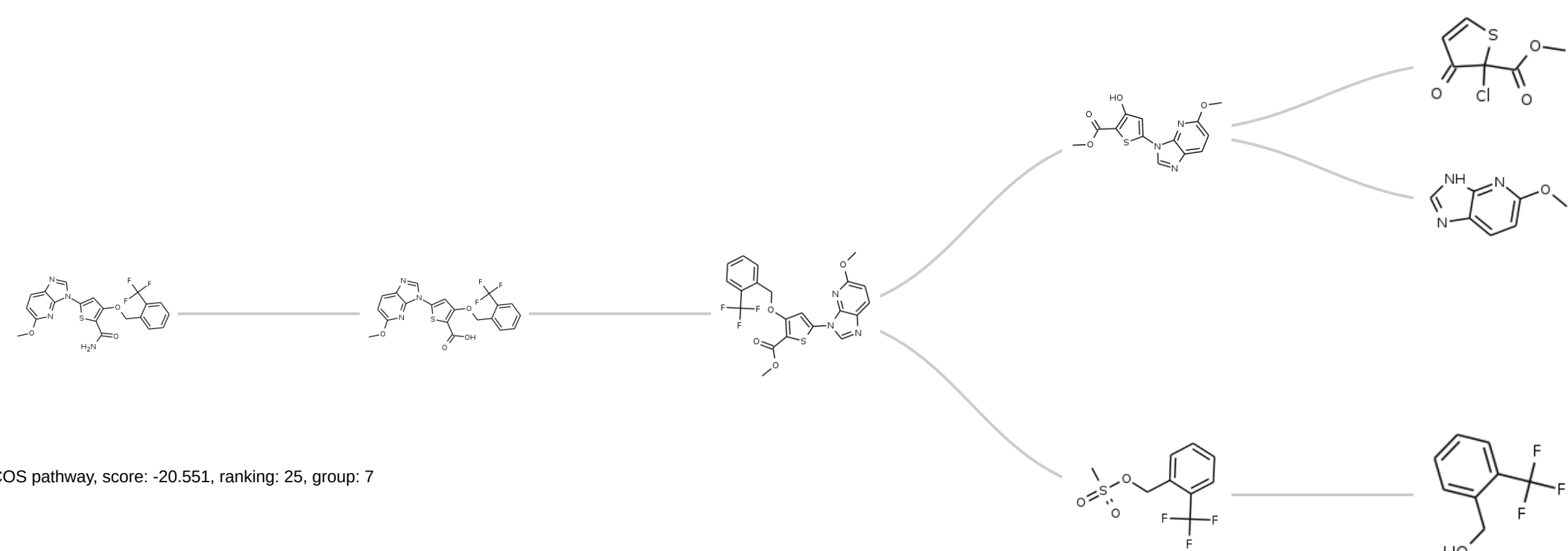
ASKCOS pathway score: -19.881, ranking: 19, group: 4



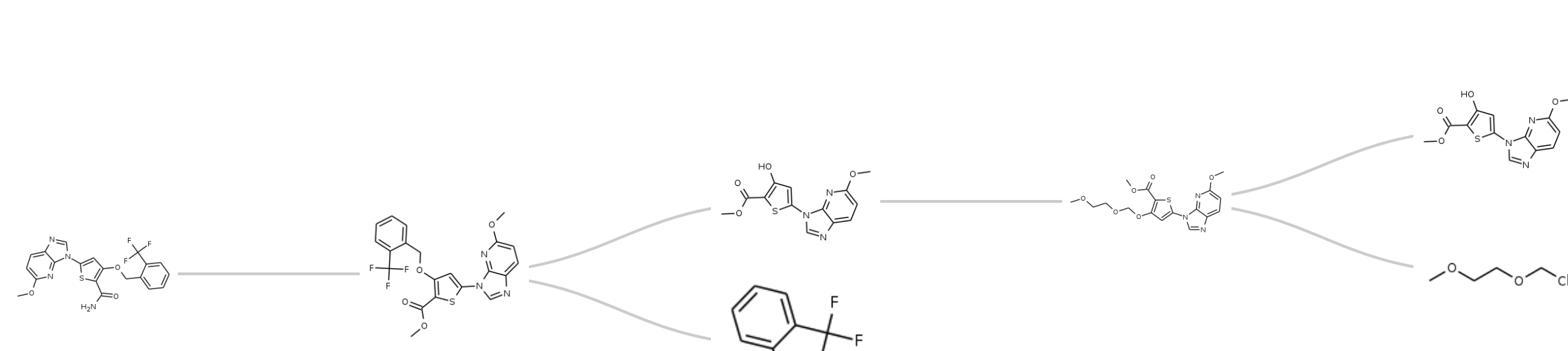
ASKCOS pathway score: -20.037, ranking: 20, group: 5



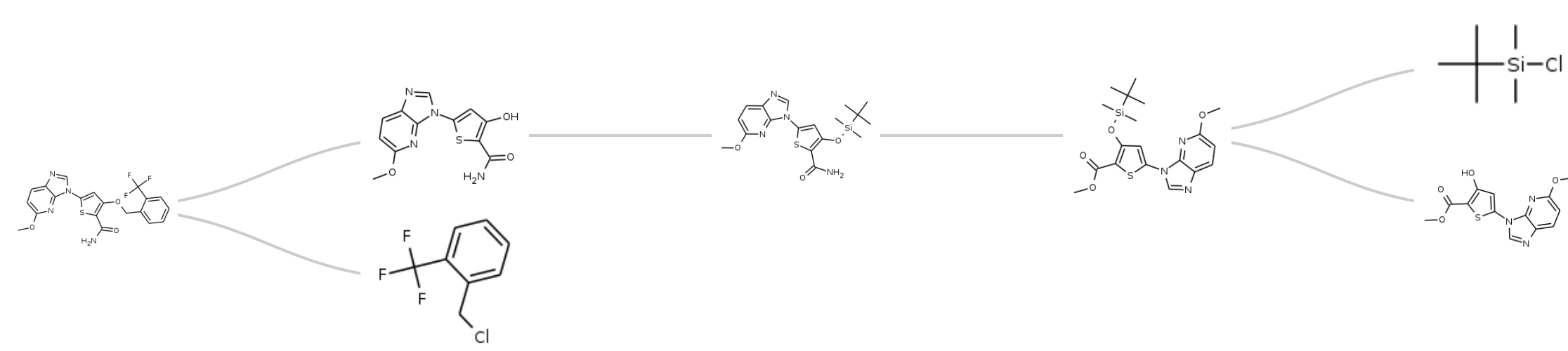
ASKCOS pathway score: -20.352, ranking: 24, group: 6



ASKCOS pathway score: -20.551, ranking: 25, group: 7



ASKCOS pathway score: -20.795, ranking: 27, group: 8

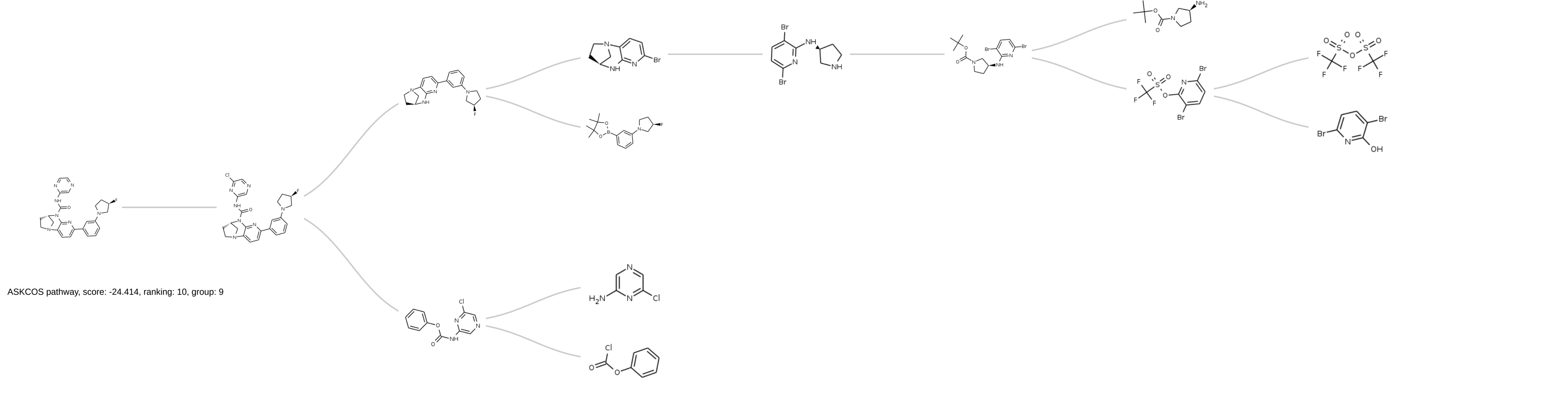
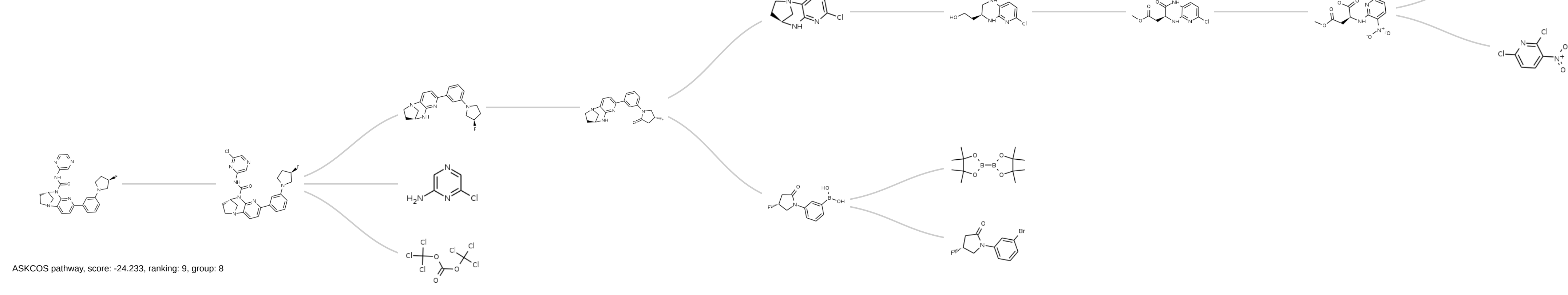
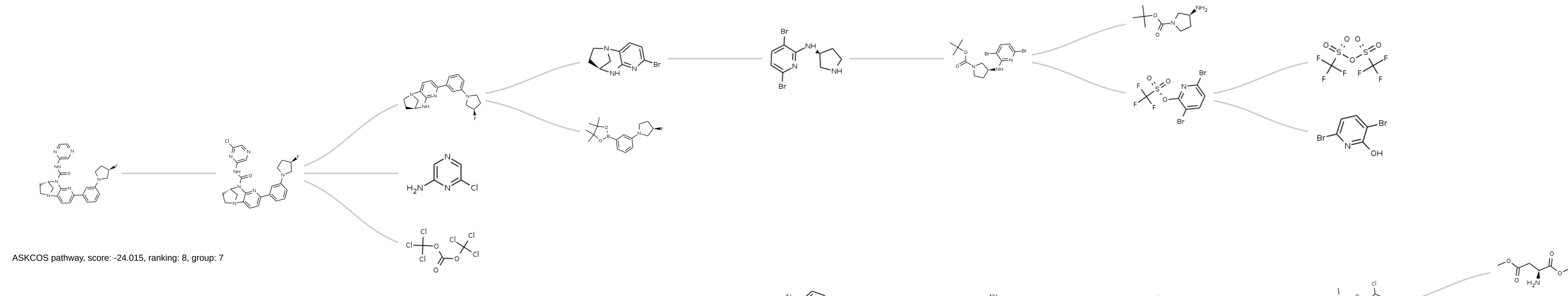
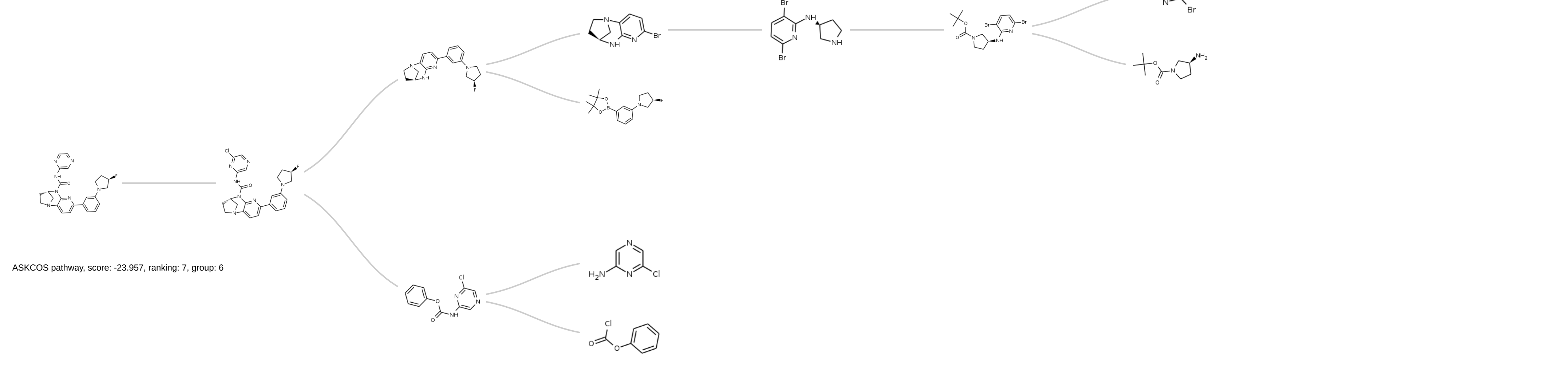
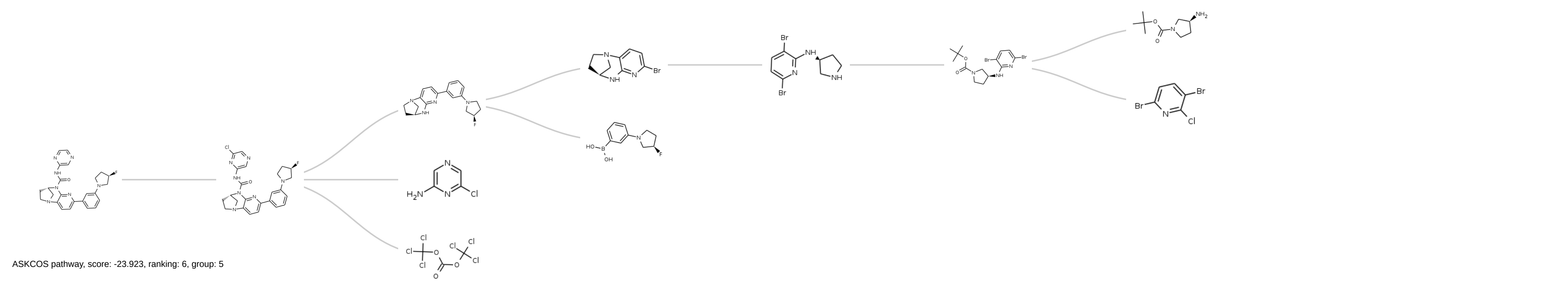
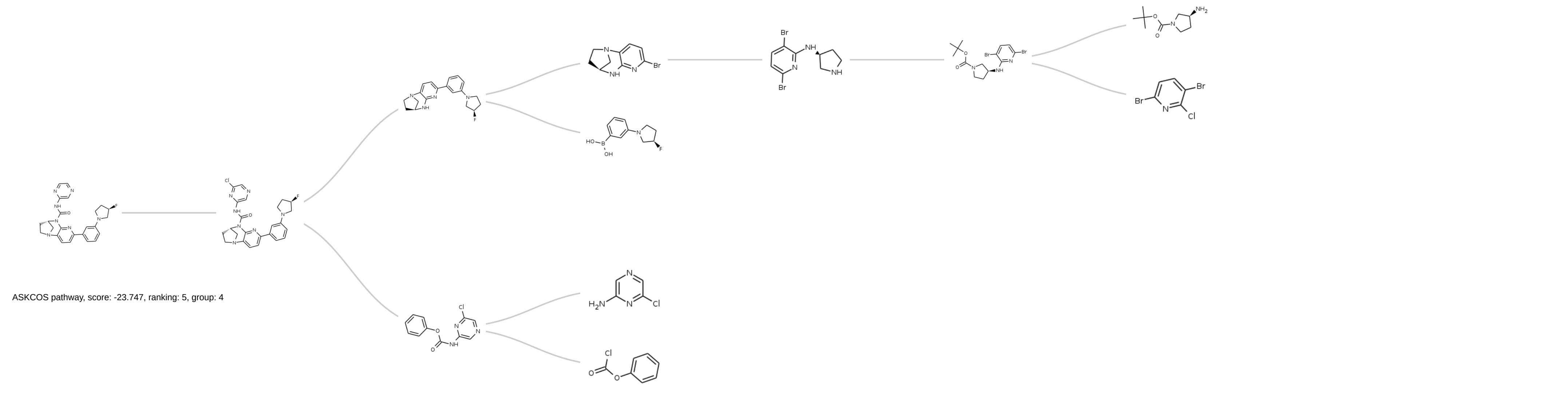
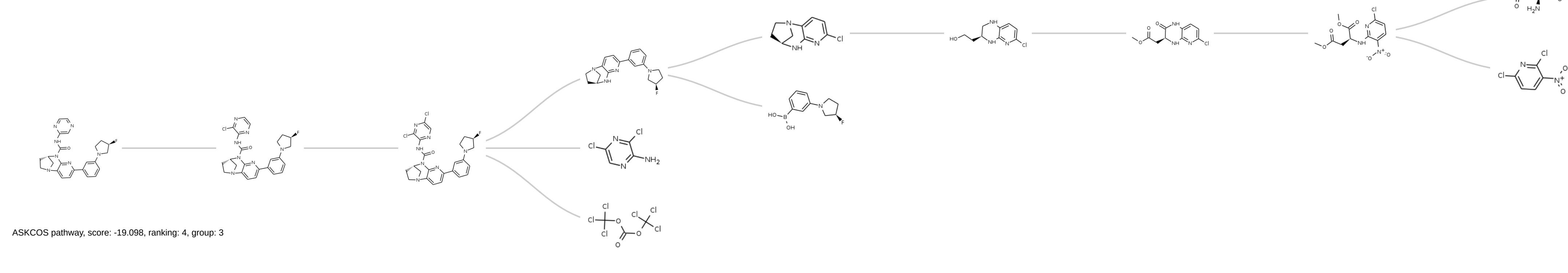
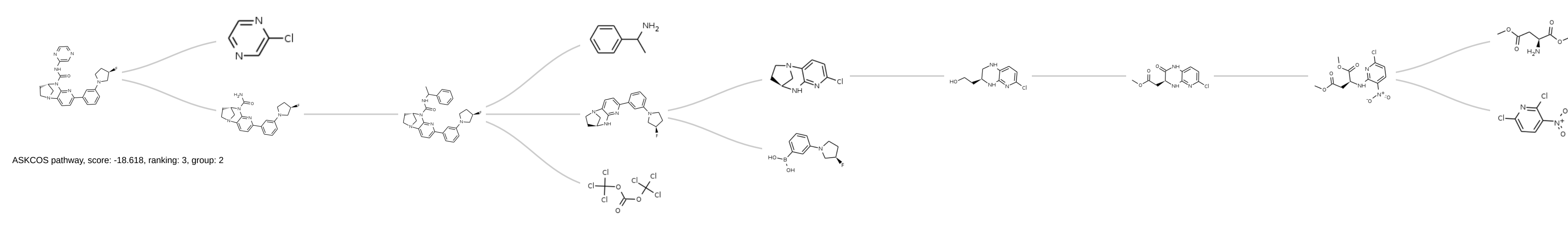
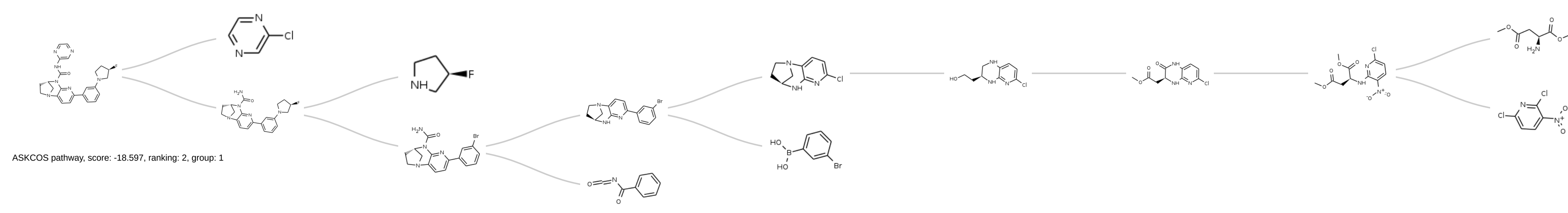
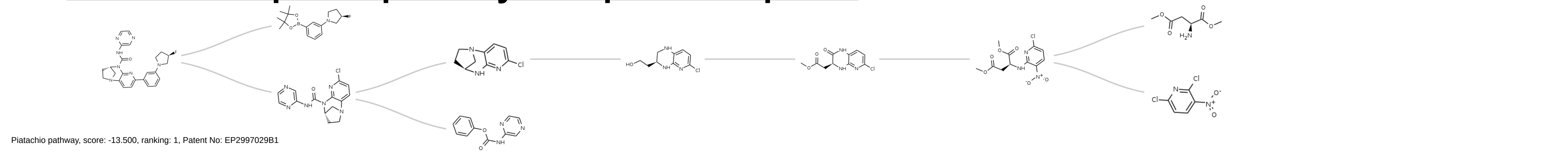


ASKCOS pathway score: -20.900, ranking: 29, group: 9



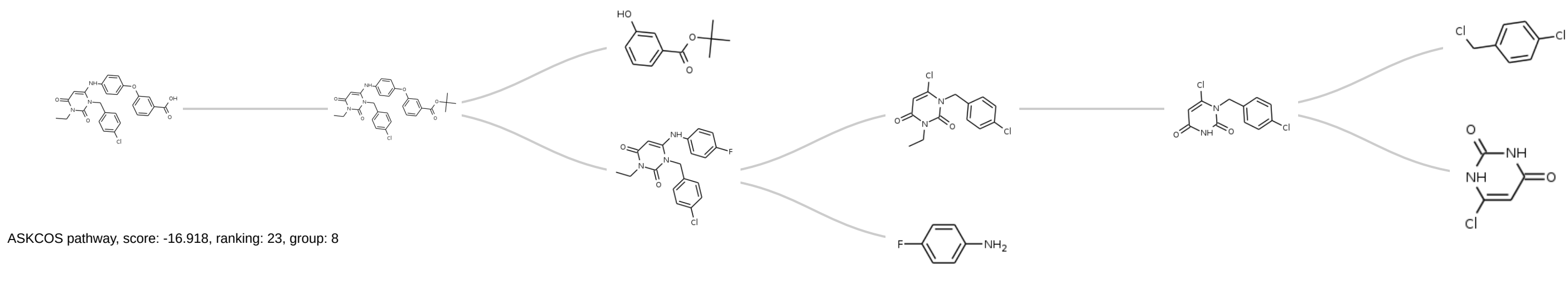
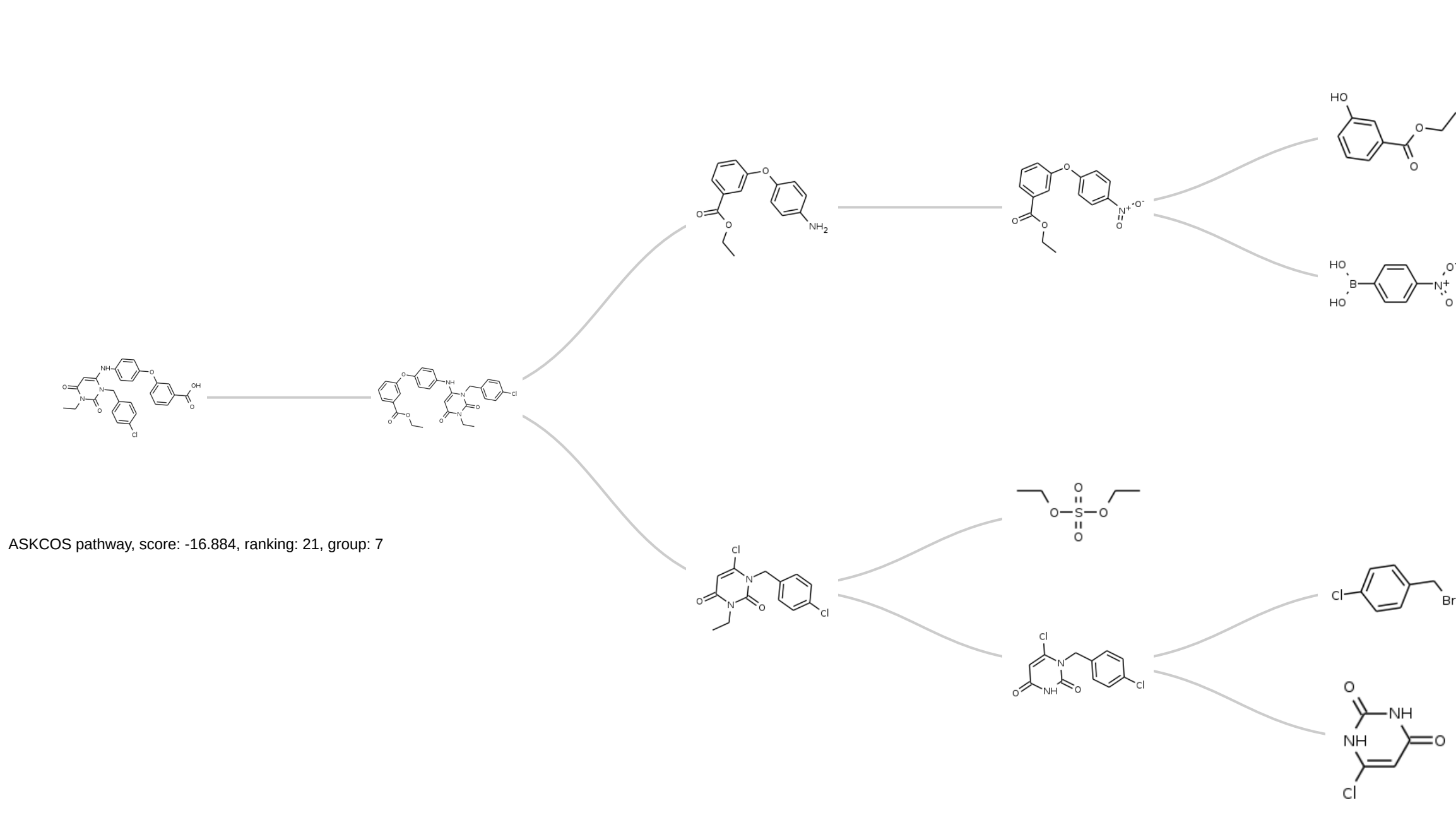
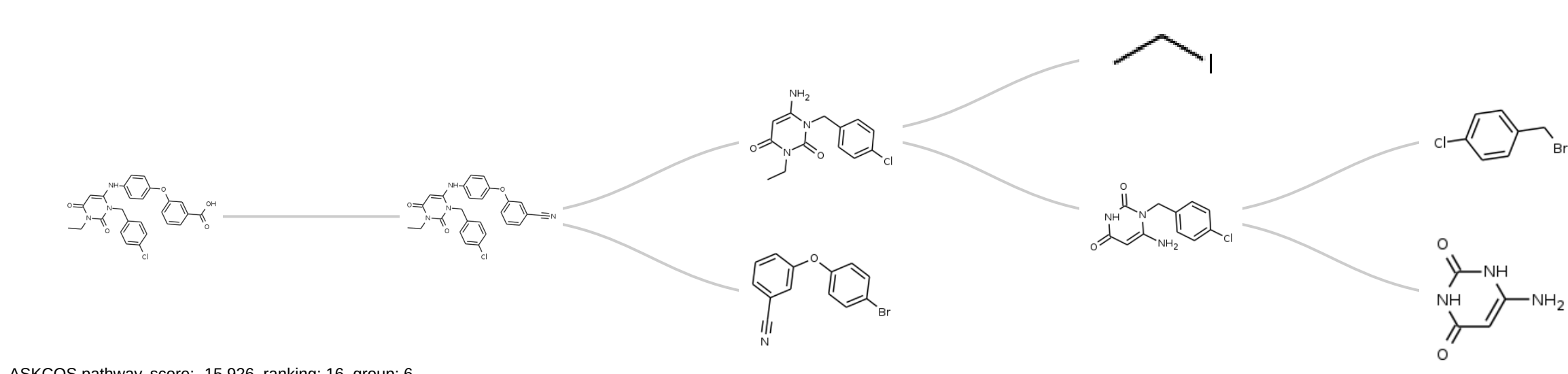
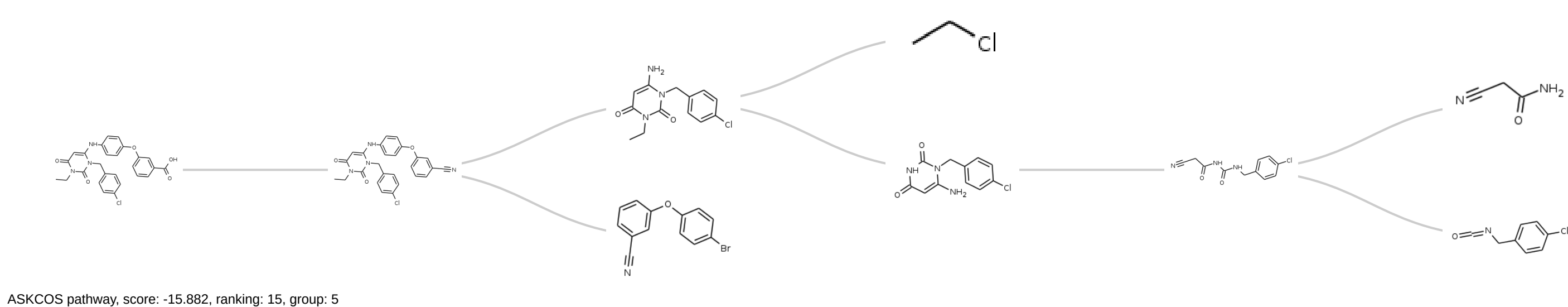
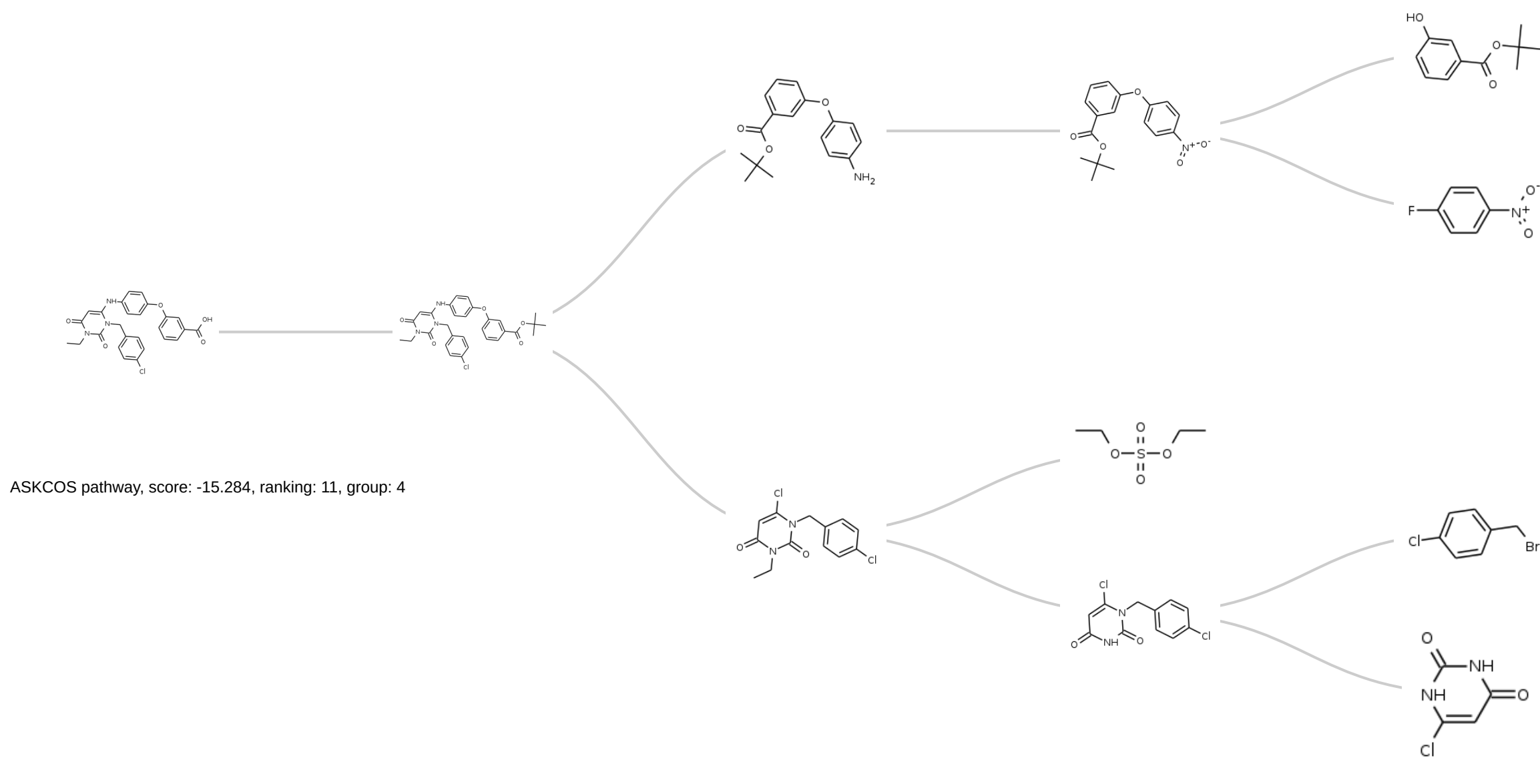
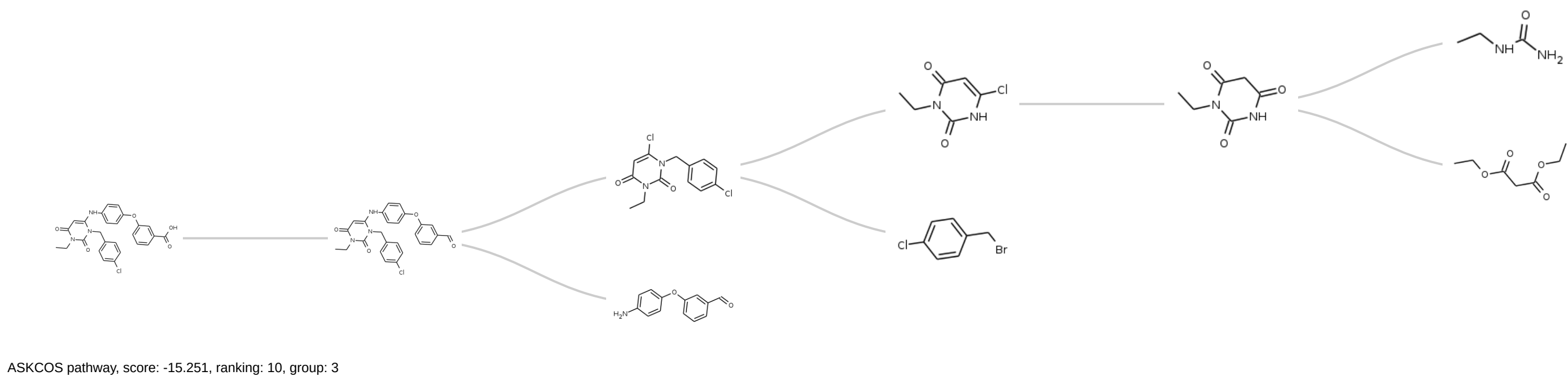
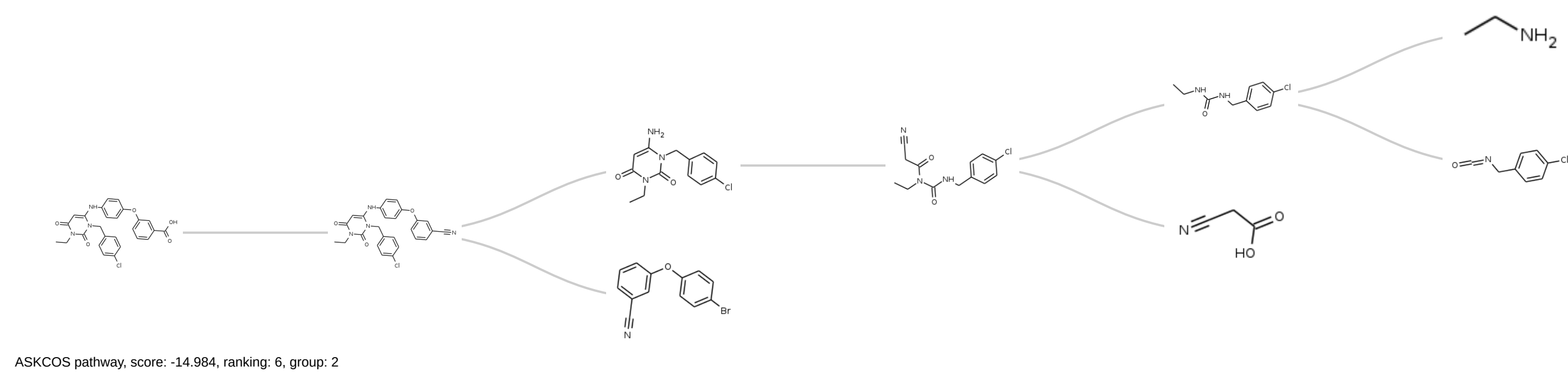
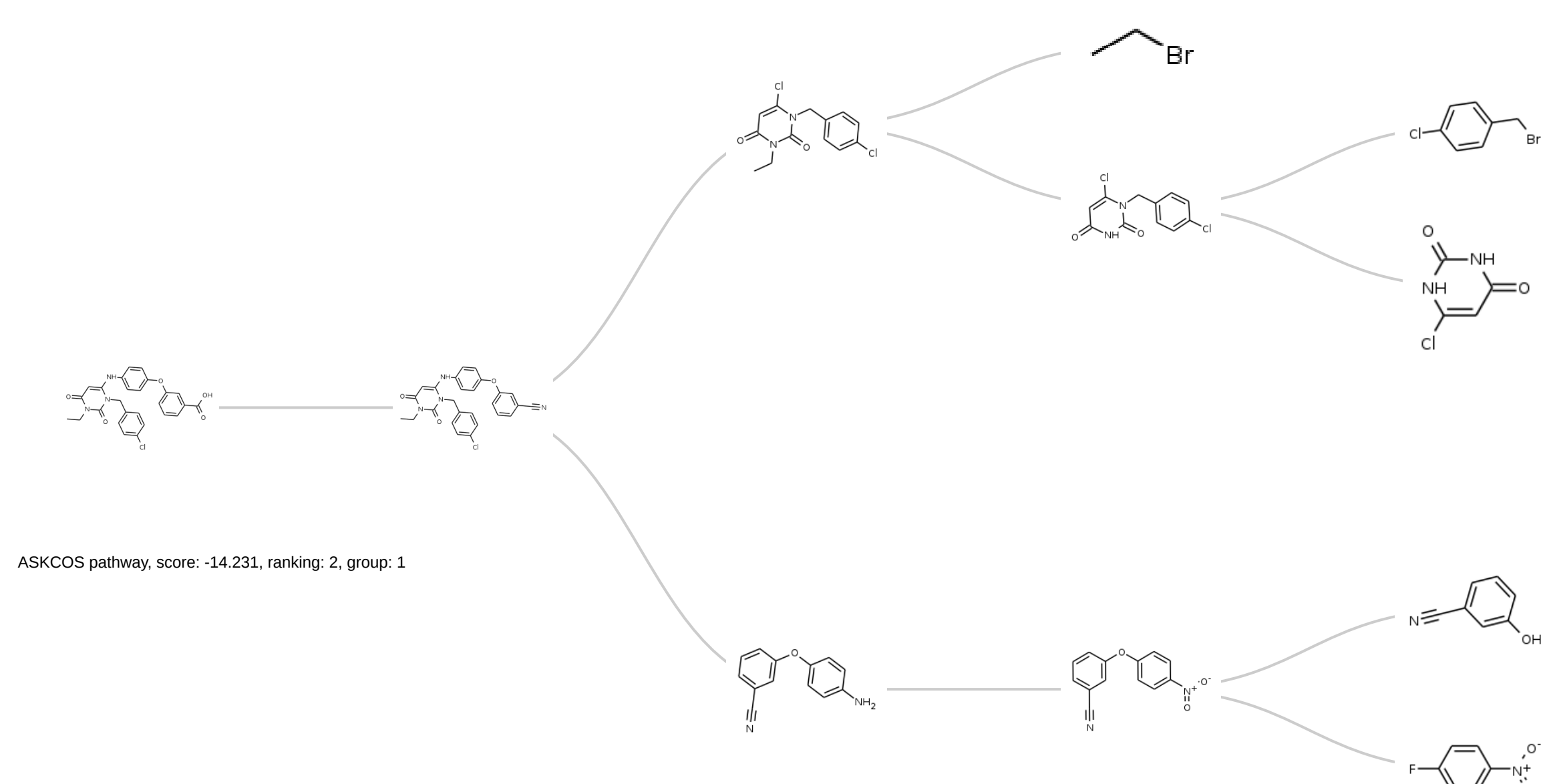
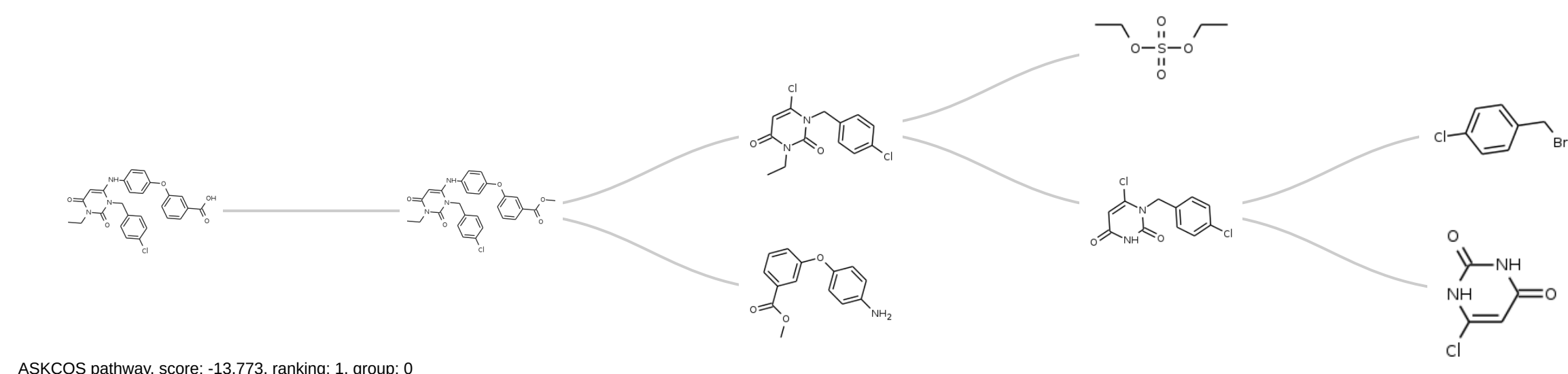
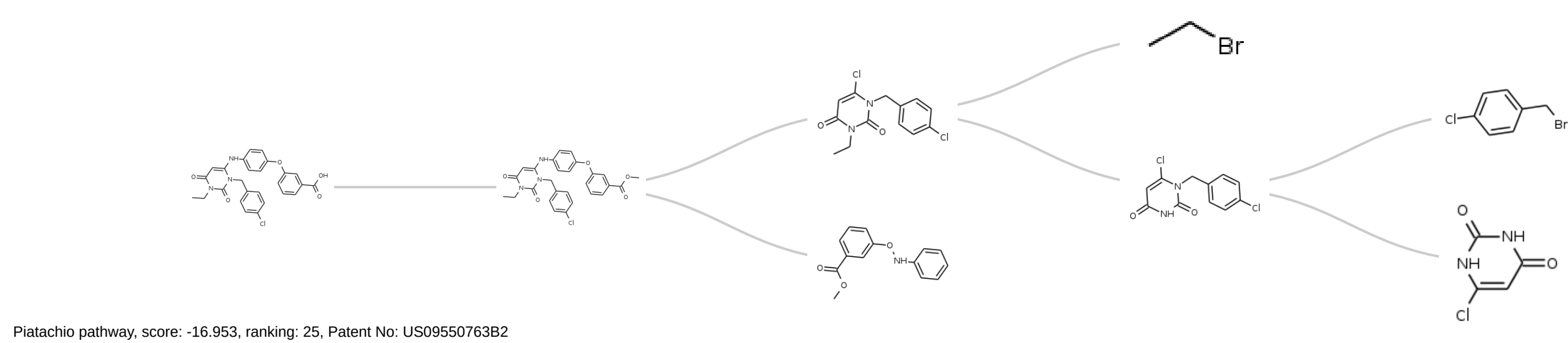


# Model ranks patent pathway as top-1: Example 49



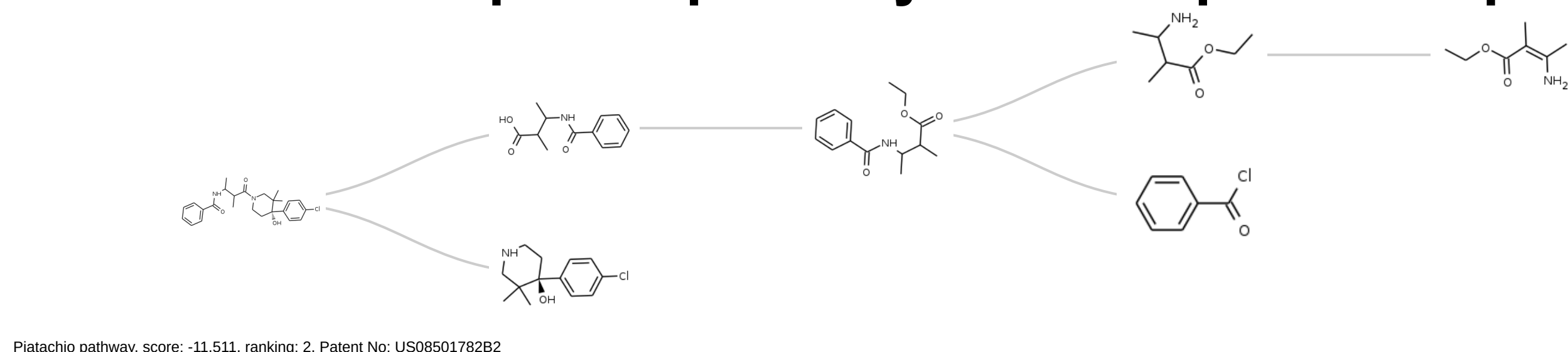


# Model ranks patent pathway not as top-1: Example 1

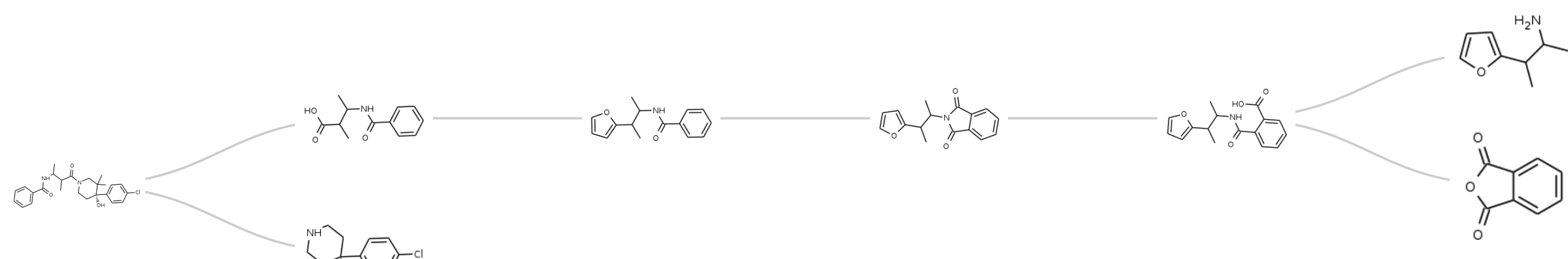




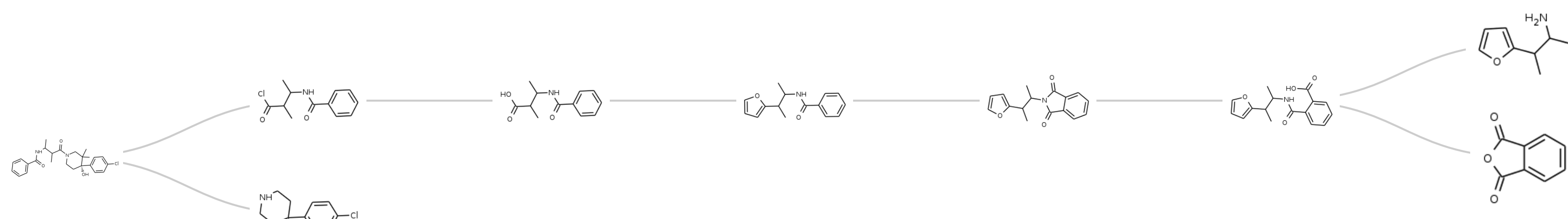
### Model ranks patent pathway not as top-1: Example 3



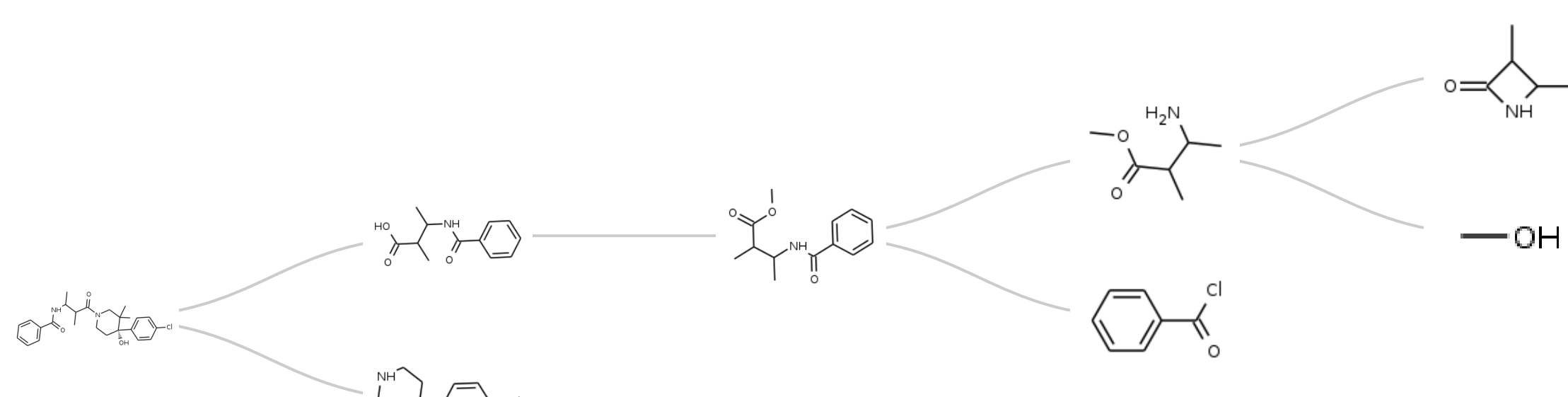
Patent pathway, score: -11.511, ranking: 2, Patent No: US06501762B2



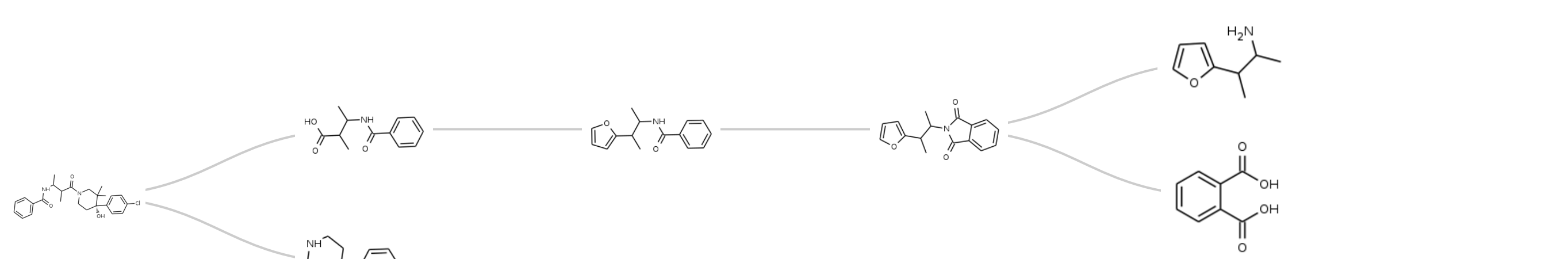
ASKCOS pathway, score: -8.654, ranking: 1, group: 0



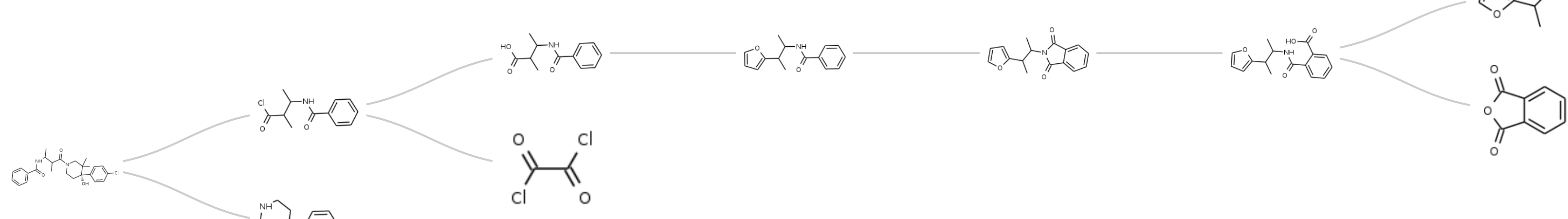
ASKCOS pathway, score: -11.728, ranking: 3, group: 2



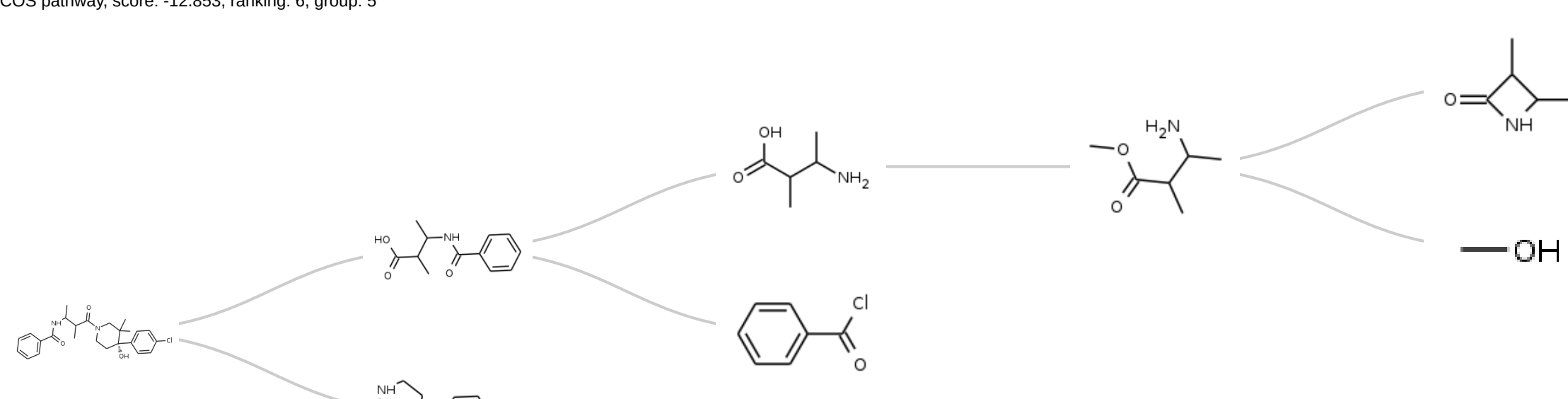
ASKCOS pathway, score: -11.906, ranking: 4, group: 3



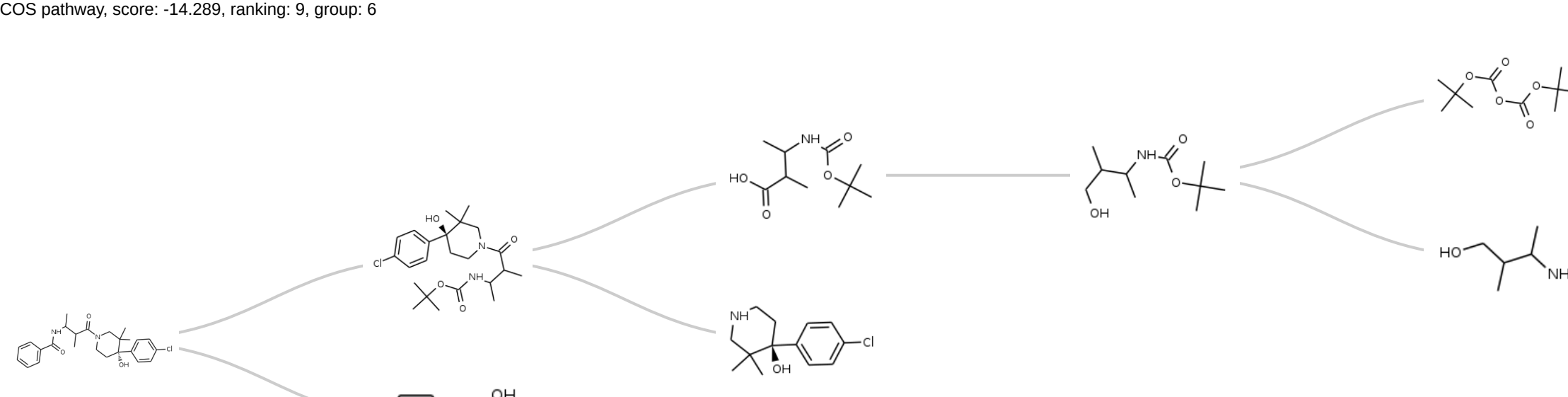
ASKCOS pathway, score: -12.242, ranking: 5, group: 4



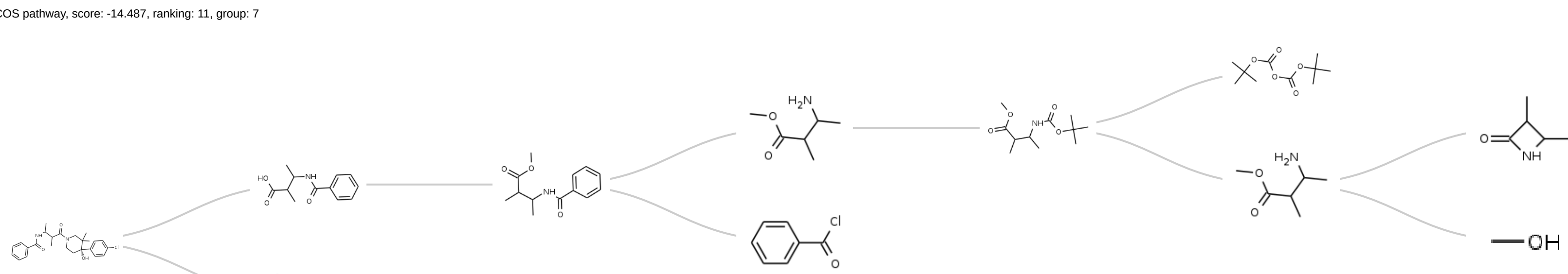
ASKCOS pathway, score: -12.853, ranking: 6, group: 5



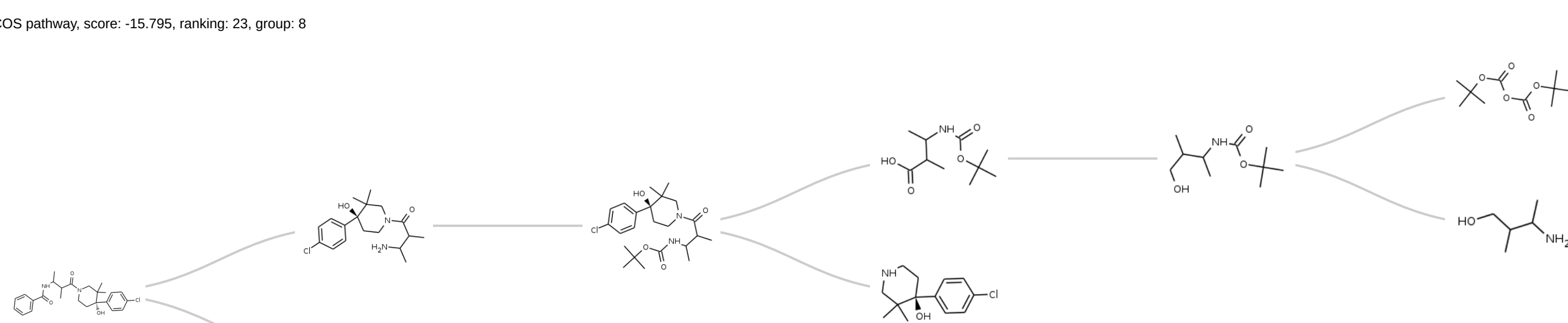
ASKCOS pathway, score: -14.289, ranking: 9, group: 6



ASKCOS pathway, score: -14.487, ranking: 11, group: 7



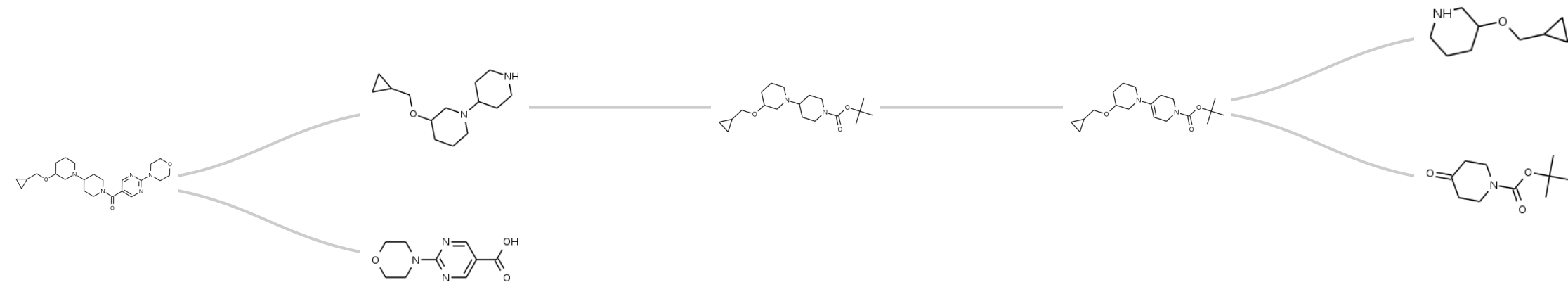
ASKCOS pathway, score: -15.195, ranking: 23, group: 8



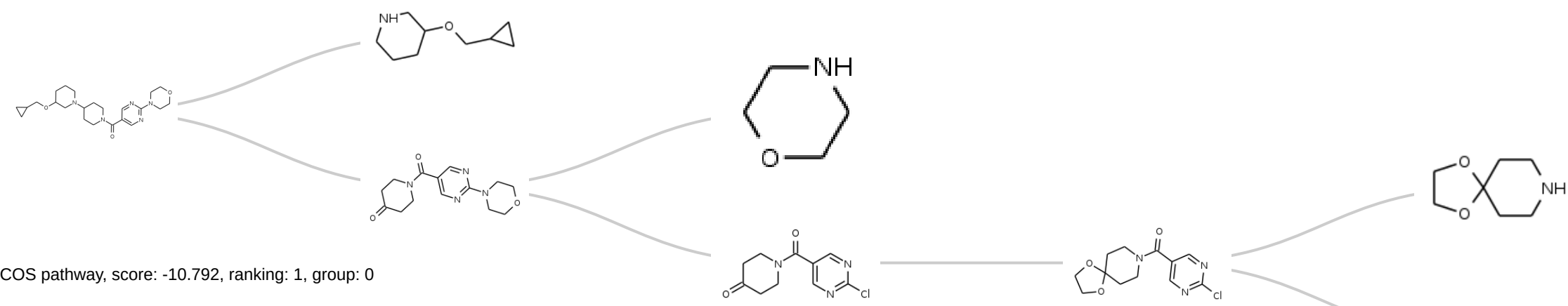
ASKCOS pathway, score: -16.159, ranking: 32, group: 9



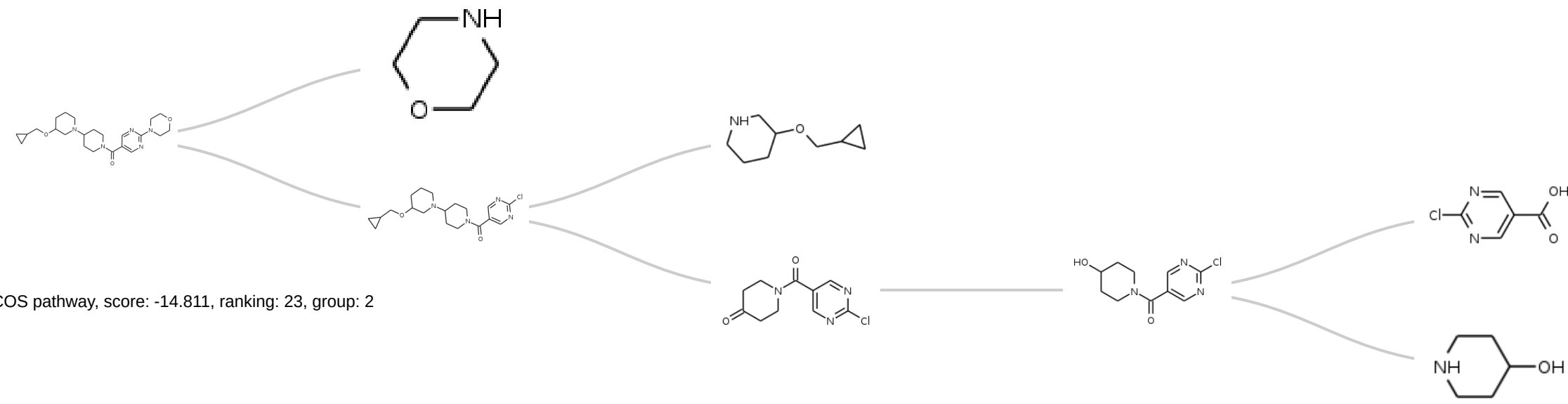
# Model ranks patent pathway not as top-1: Example 4



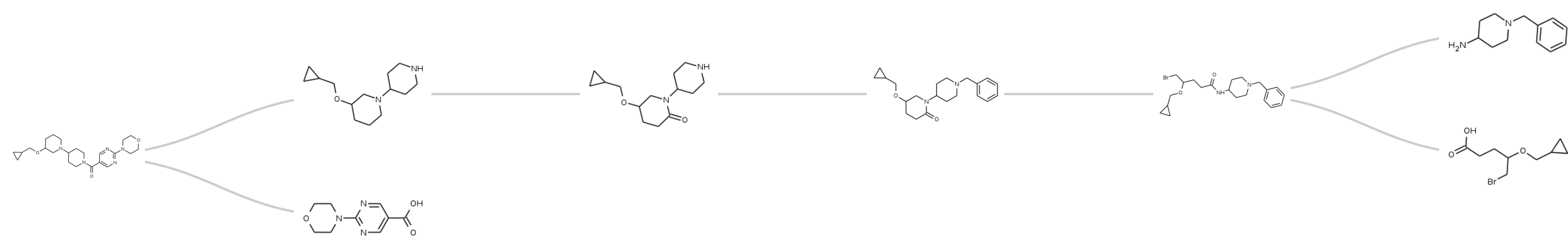
Platacho pathway, score: -14.512, ranking: 21, Patent No: US0962419B2



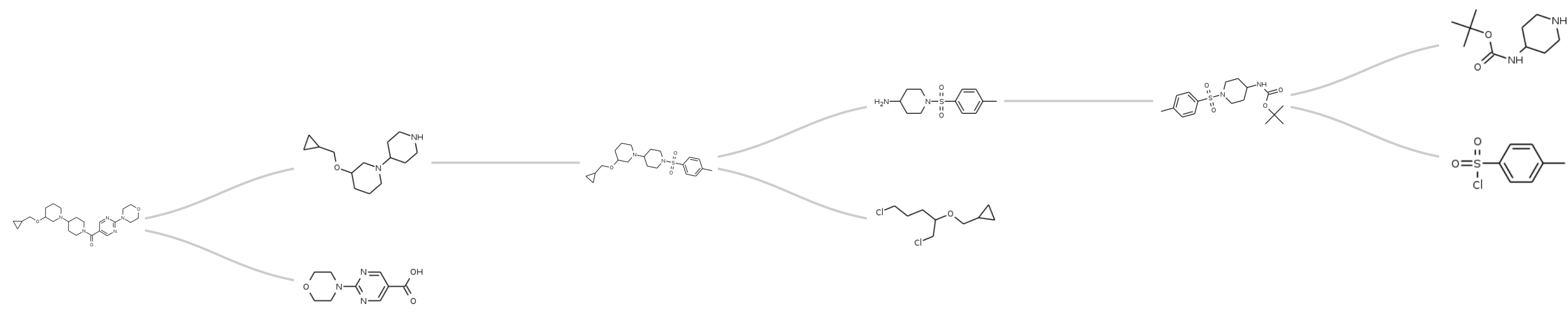
ASKCOS pathway, score: -10.792, ranking: 1, group: 0



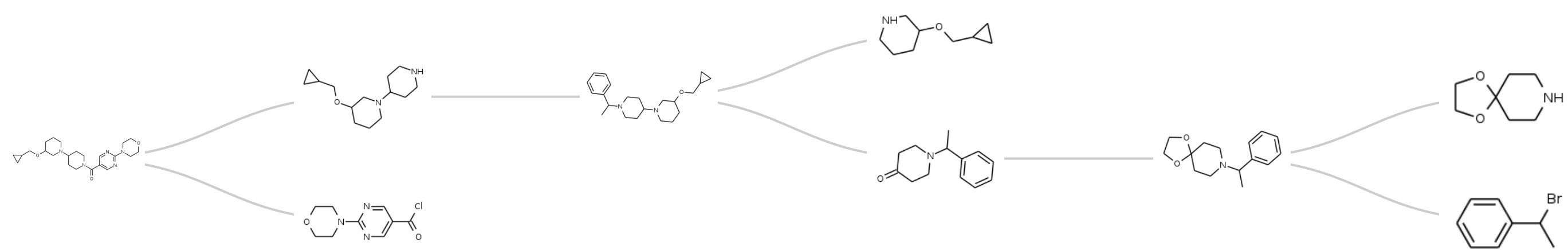
ASKCOS pathway, score: -14.811, ranking: 23, group: 2



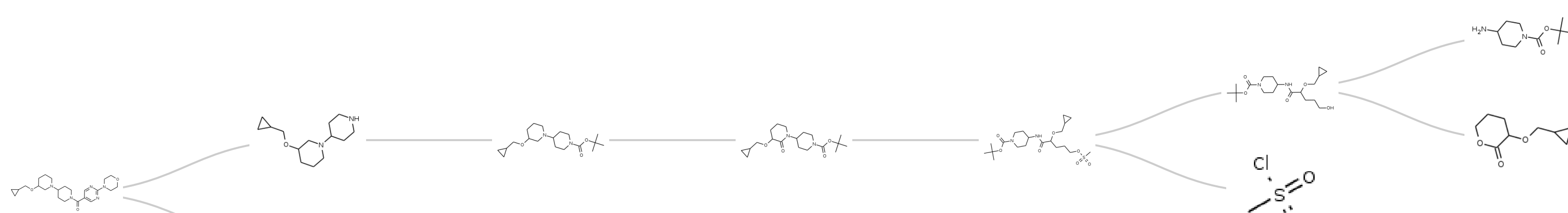
ASKCOS pathway, score: -15.423, ranking: 26, group: 3



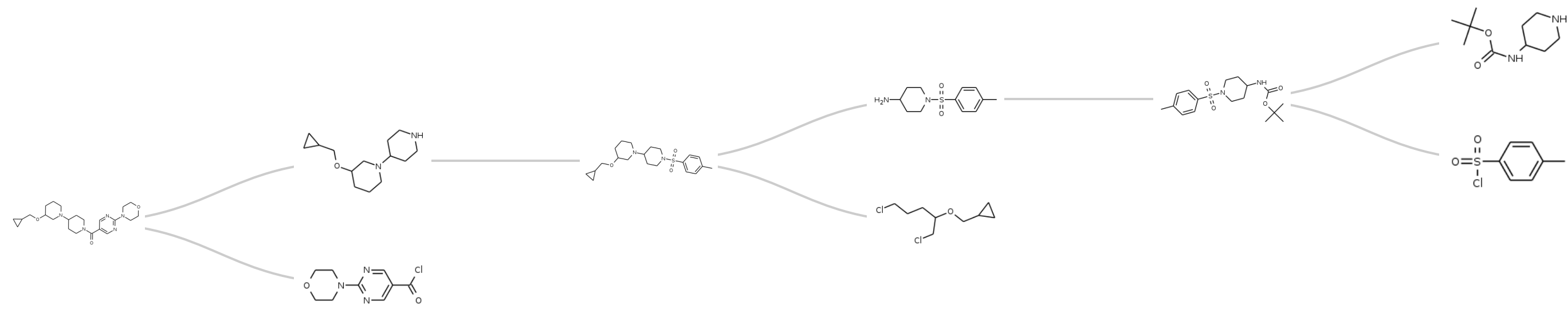
ASKCOS pathway, score: -15.627, ranking: 27, group: 4



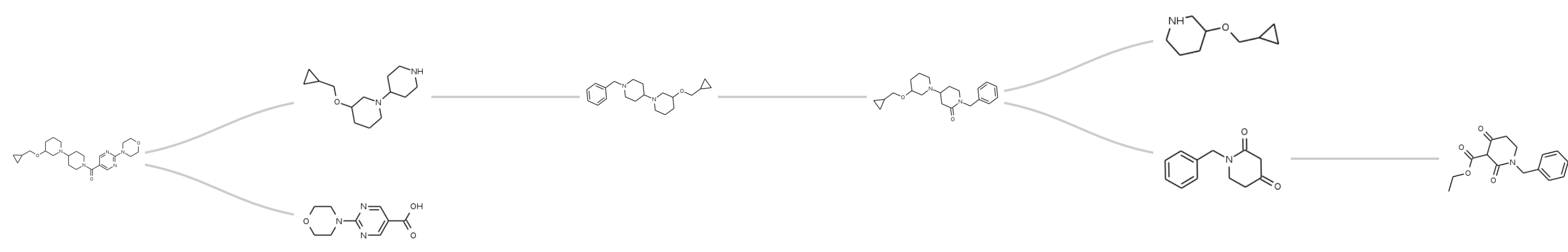
ASKCOS pathway, score: -16.227, ranking: 30, group: 5



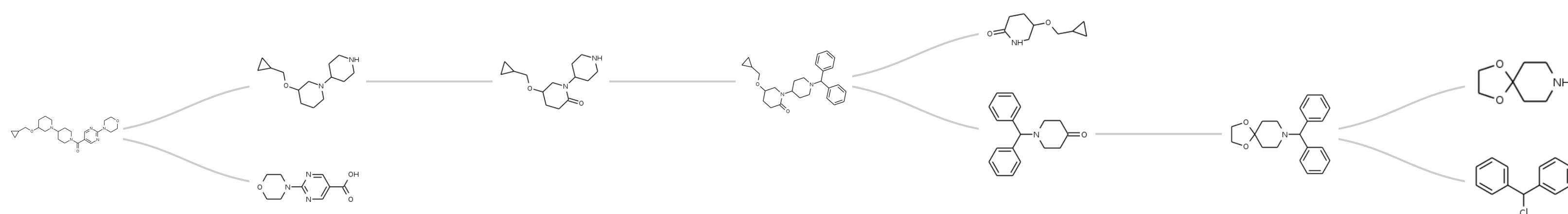
ASKCOS pathway, score: -16.512, ranking: 31, group: 6



ASKCOS pathway, score: -16.710, ranking: 33, group: 7

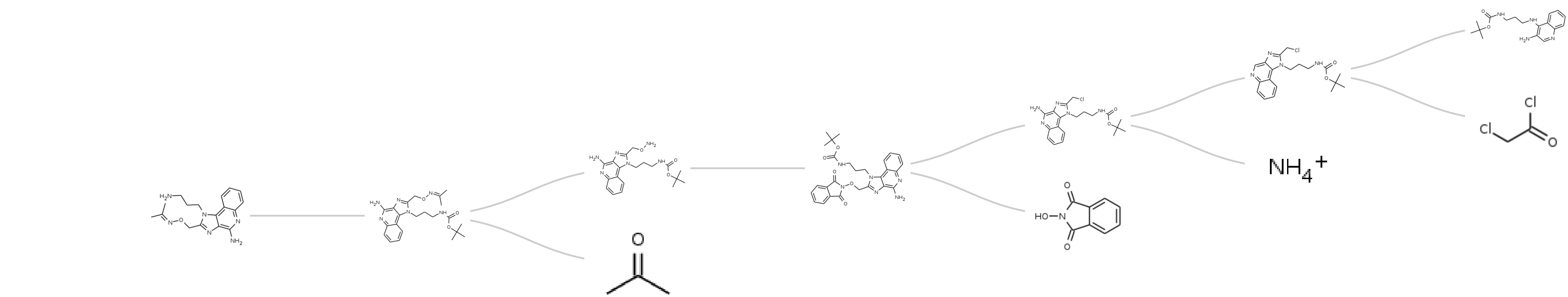


ASKCOS pathway, score: -17.024, ranking: 40, group: 8

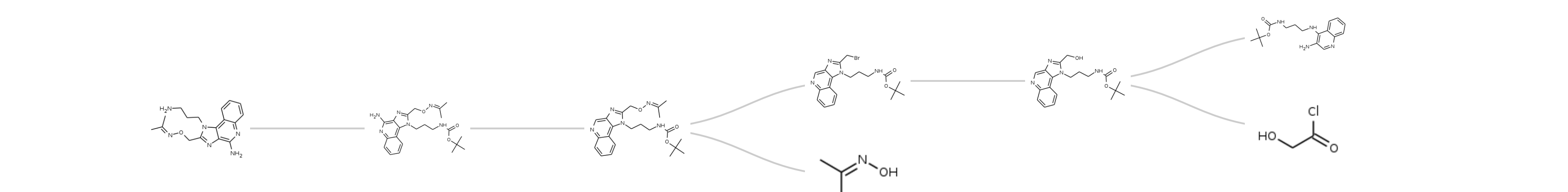


ASKCOS pathway, score: -17.975, ranking: 51, group: 9

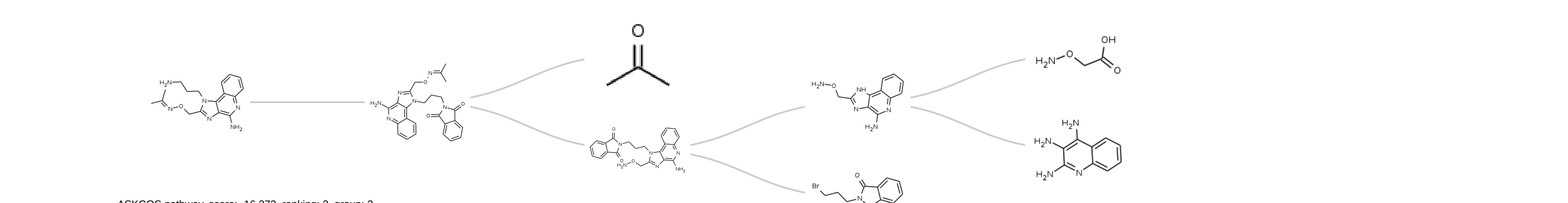
# Model ranks patent pathway not as top-1: Example 5



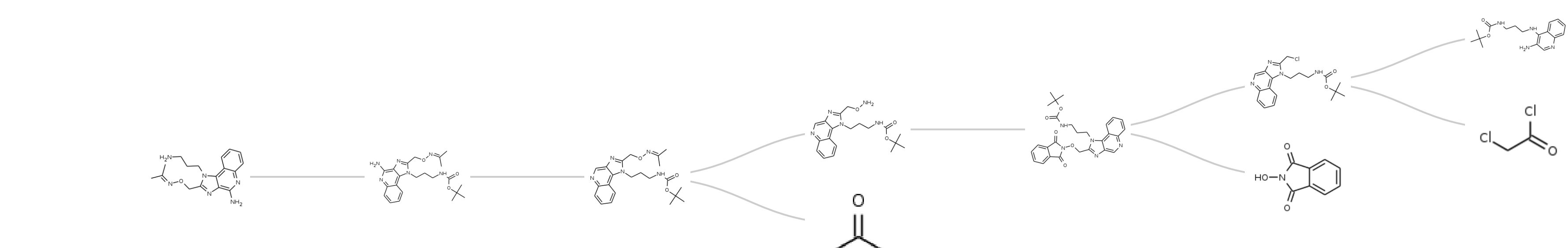
Patacho pathway, score: -16.024, ranking: 2, Patent No: US2009042925A1



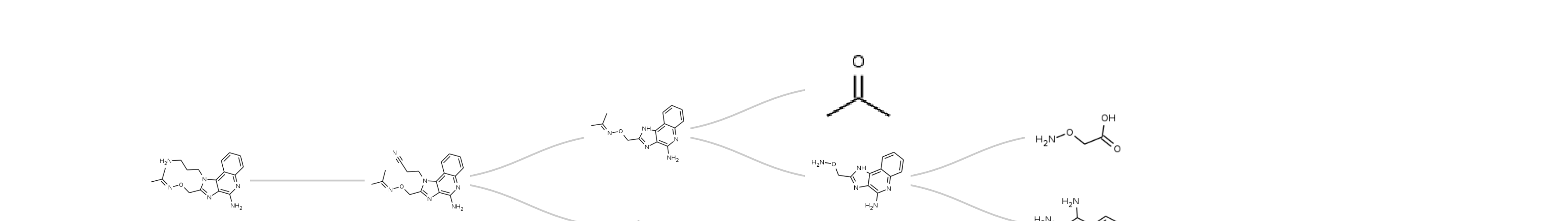
ASKCOS pathway, score: -15.201, ranking: 1, group: 0



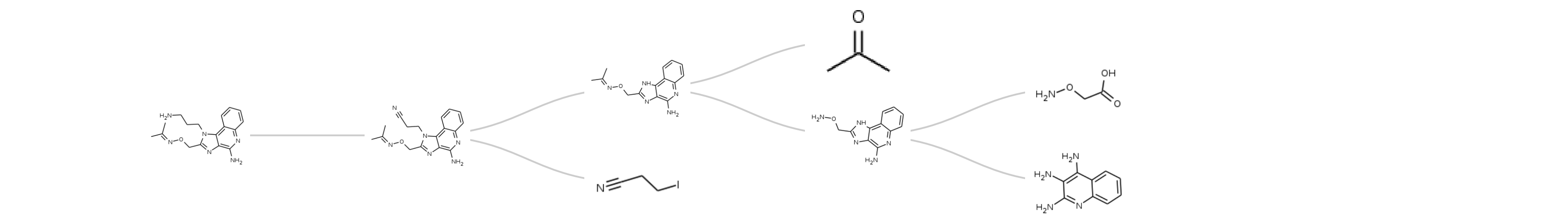
ASKCOS pathway, score: -16.372, ranking: 3, group: 2



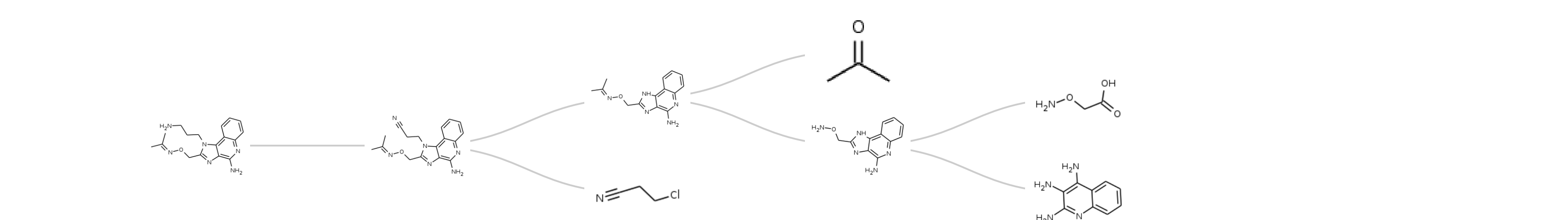
ASKCOS pathway, score: -16.554, ranking: 4, group: 3



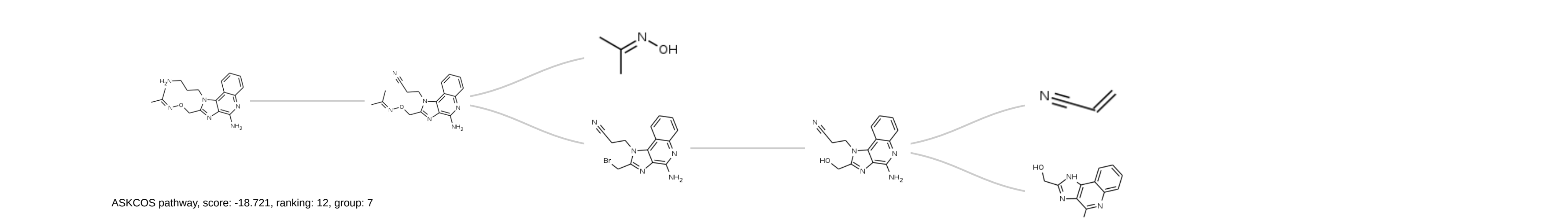
ASKCOS pathway, score: -17.659, ranking: 6, group: 4



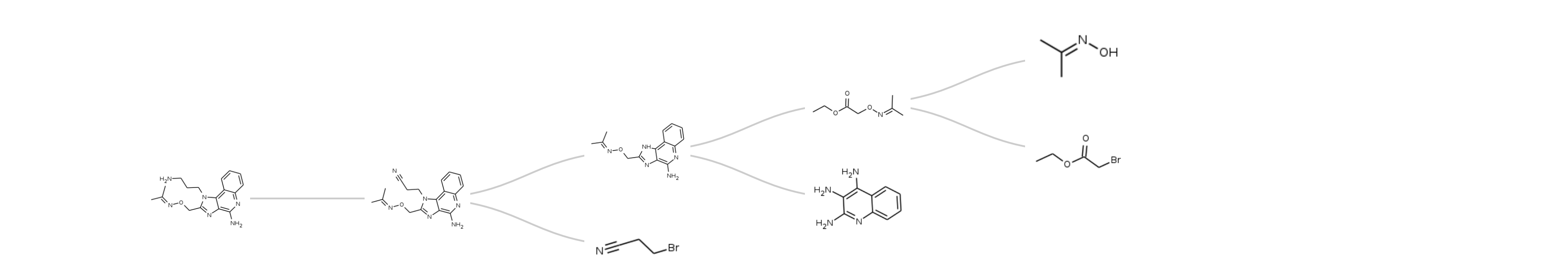
ASKCOS pathway, score: -17.856, ranking: 7, group: 5



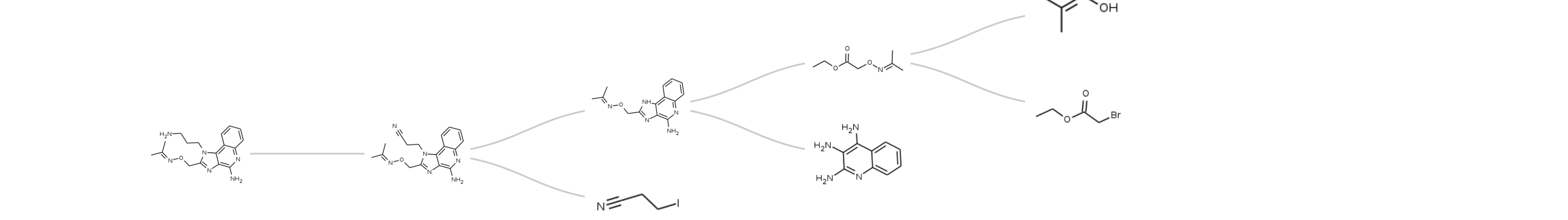
ASKCOS pathway, score: -17.950, ranking: 8, group: 6



ASKCOS pathway, score: -18.721, ranking: 12, group: 7

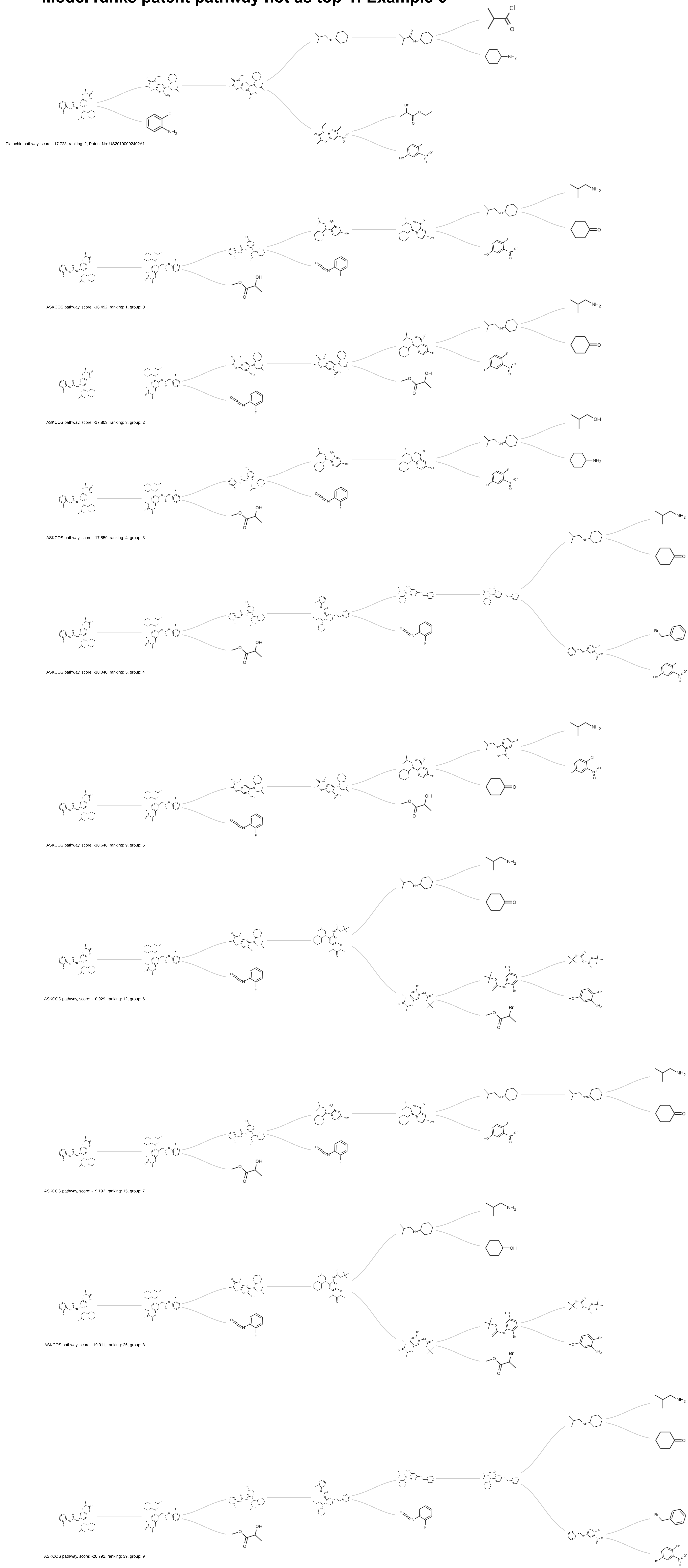


ASKCOS pathway, score: -18.798, ranking: 13, group: 8

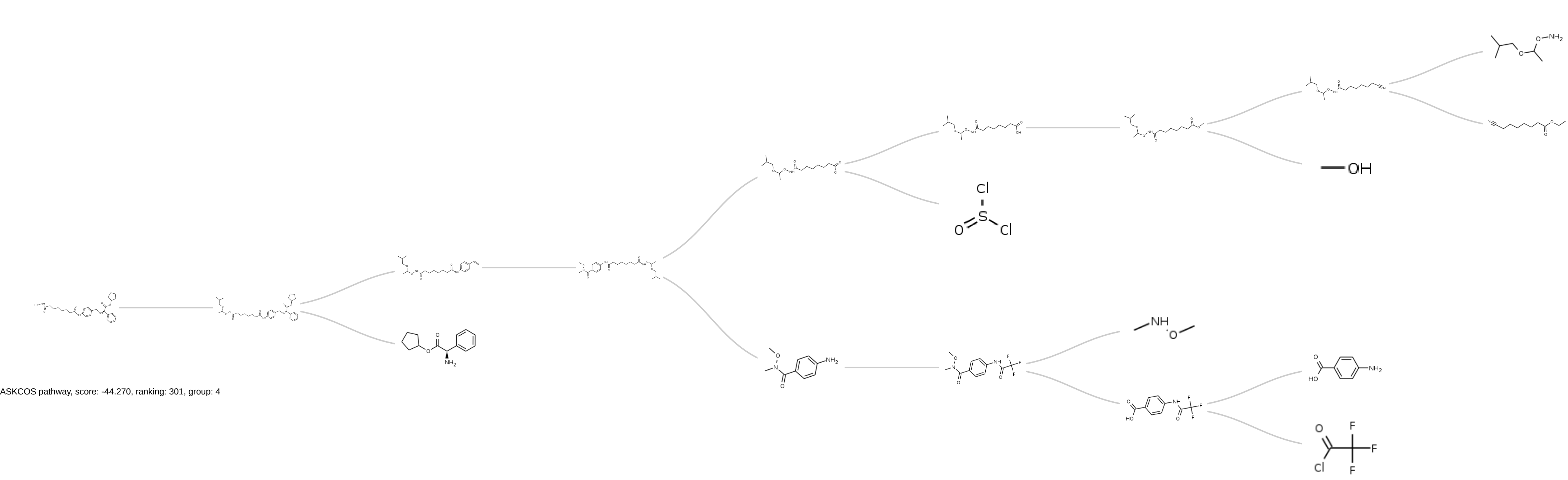
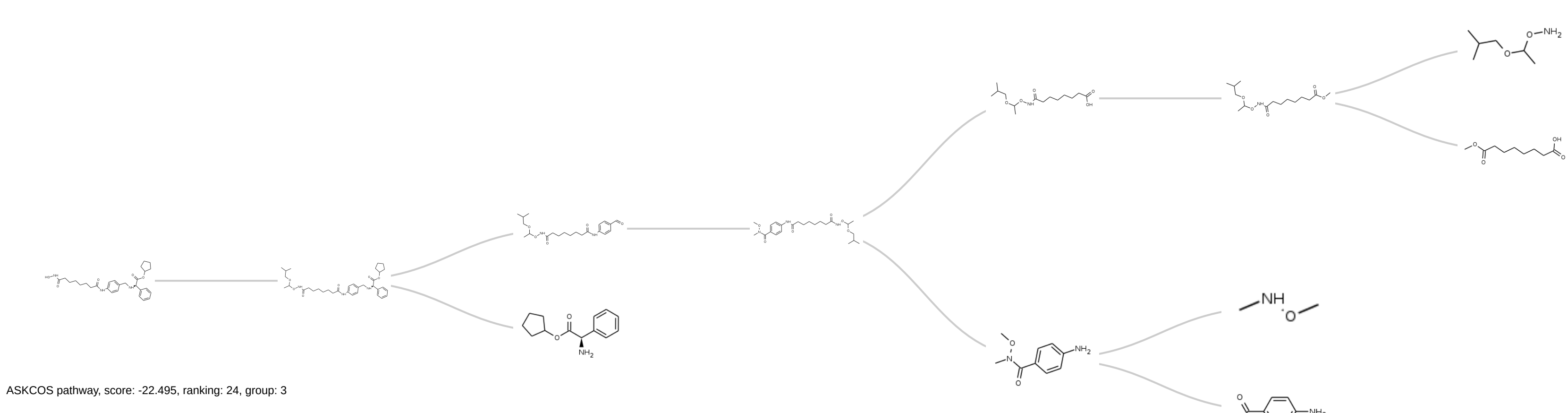
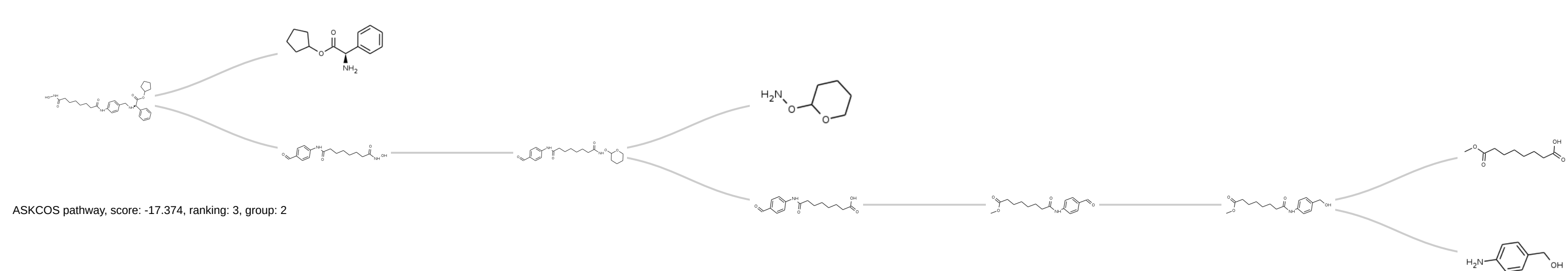
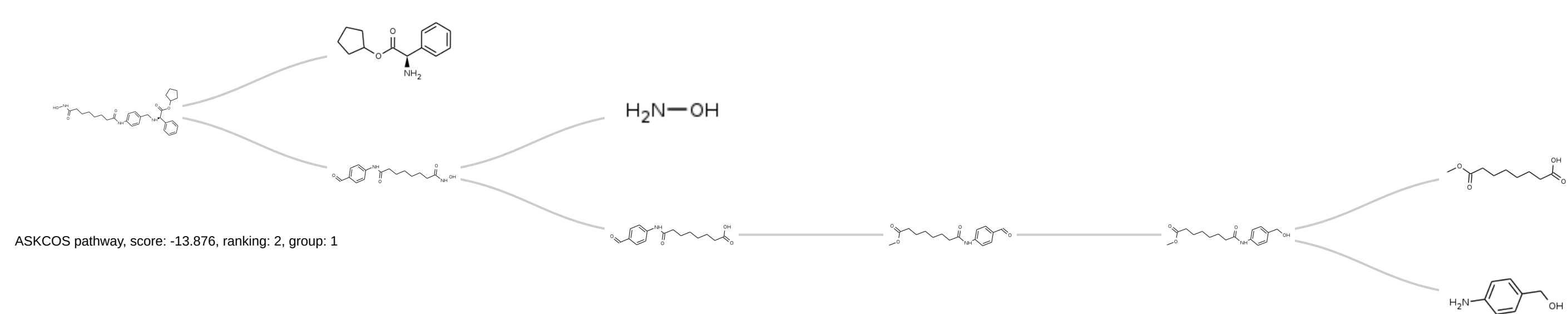
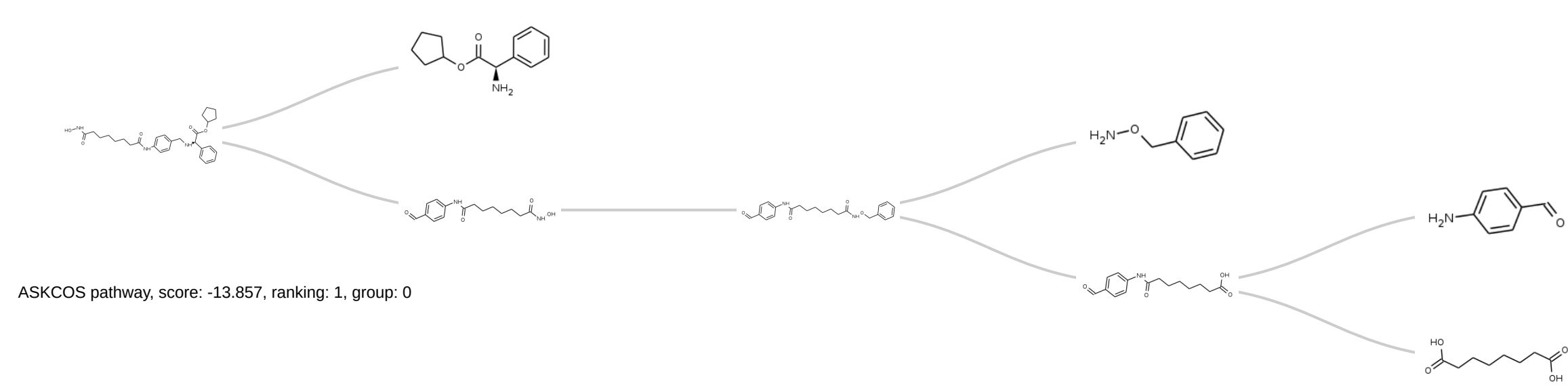
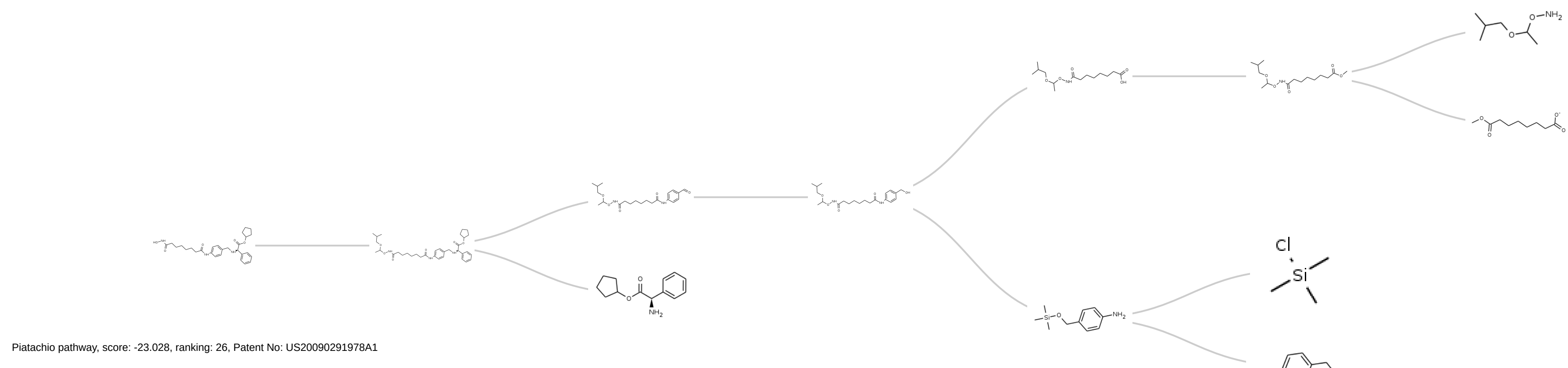


ASKCOS pathway, score: -18.977, ranking: 14, group: 9

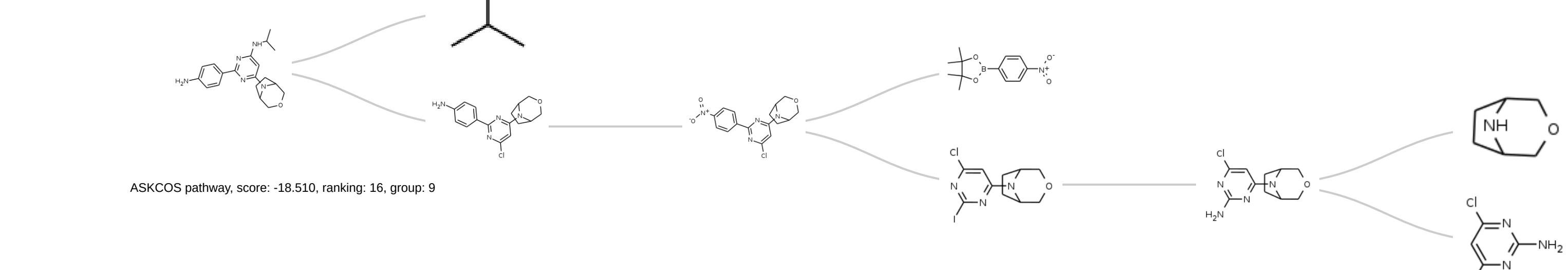
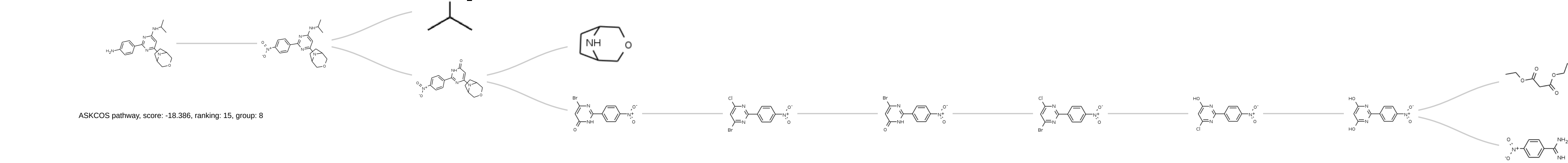
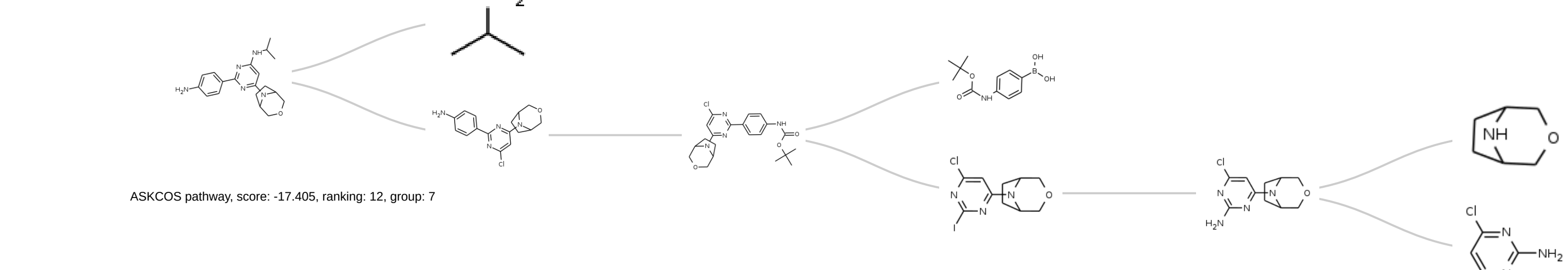
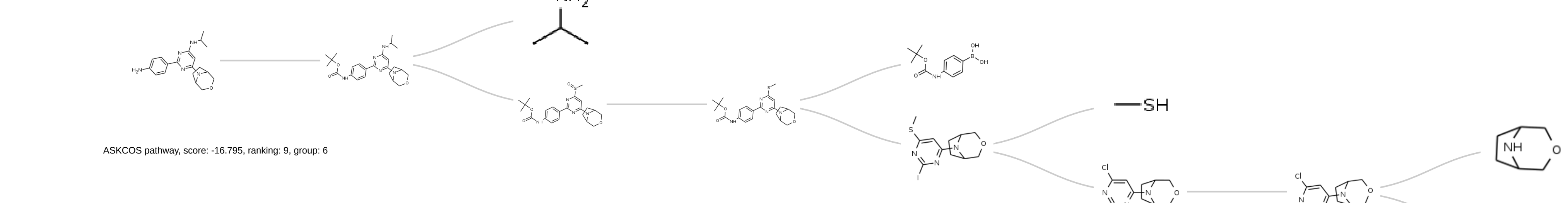
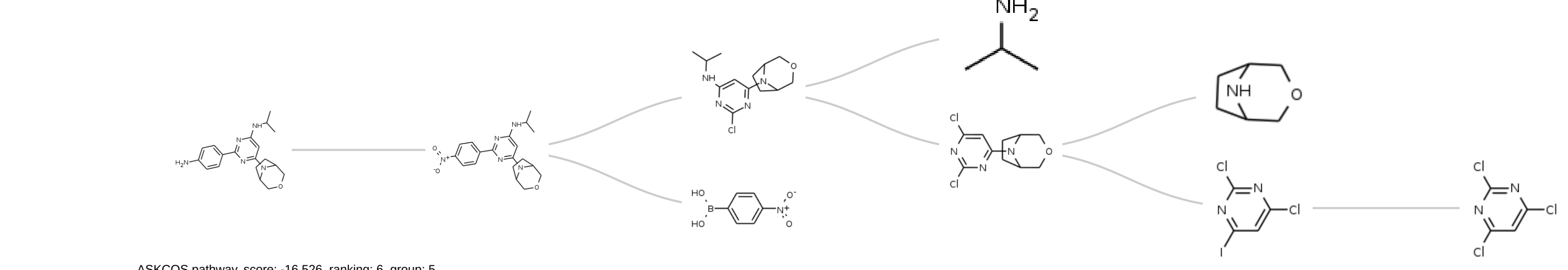
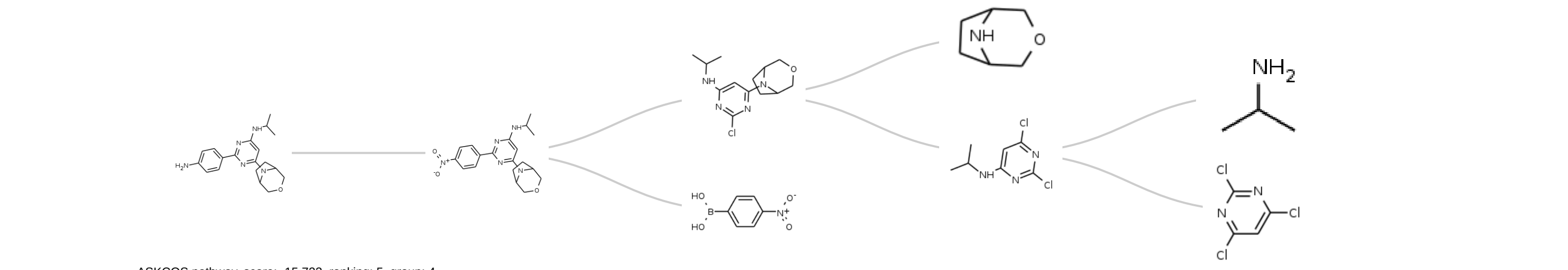
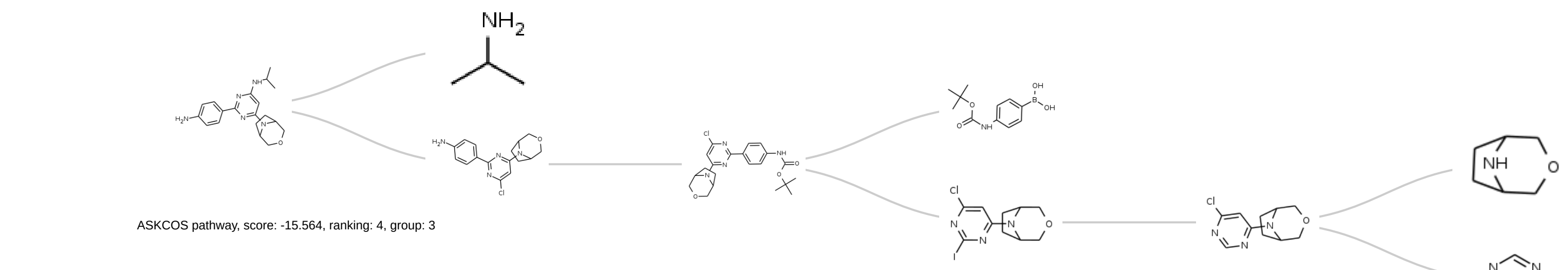
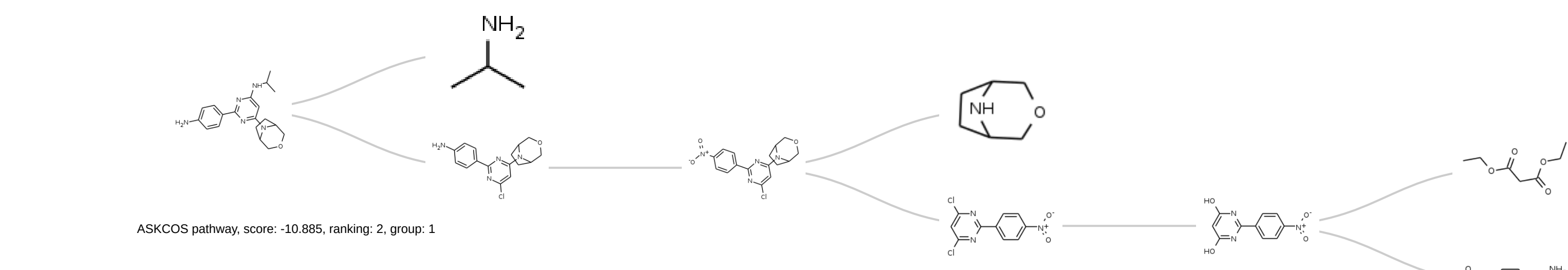
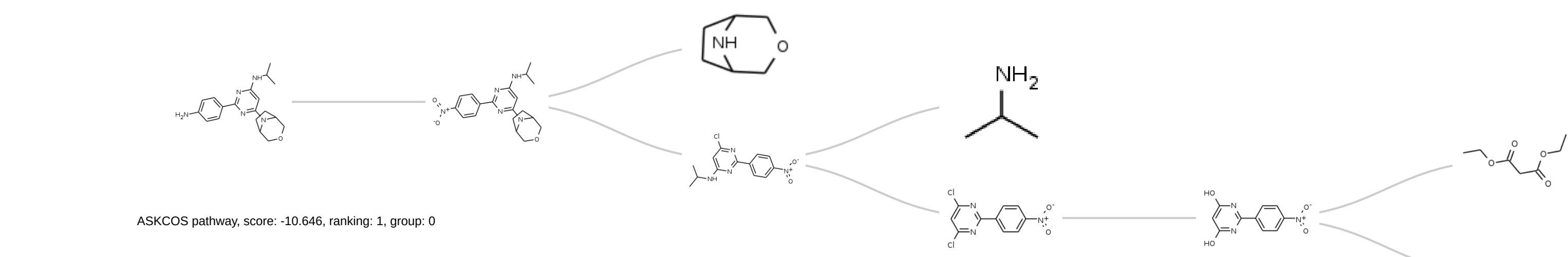
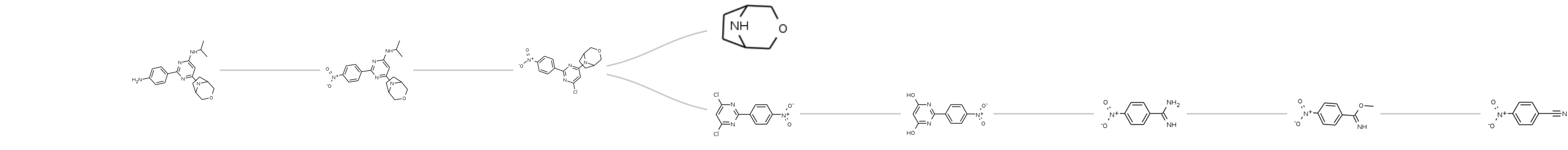
# Model ranks patent pathway not as top-1: Example 6



# Model ranks patent pathway not as top-1: Example 7



# Model ranks patent pathway not as top-1: Example 8







# Model ranks patent pathway not as top-1: Example 10

