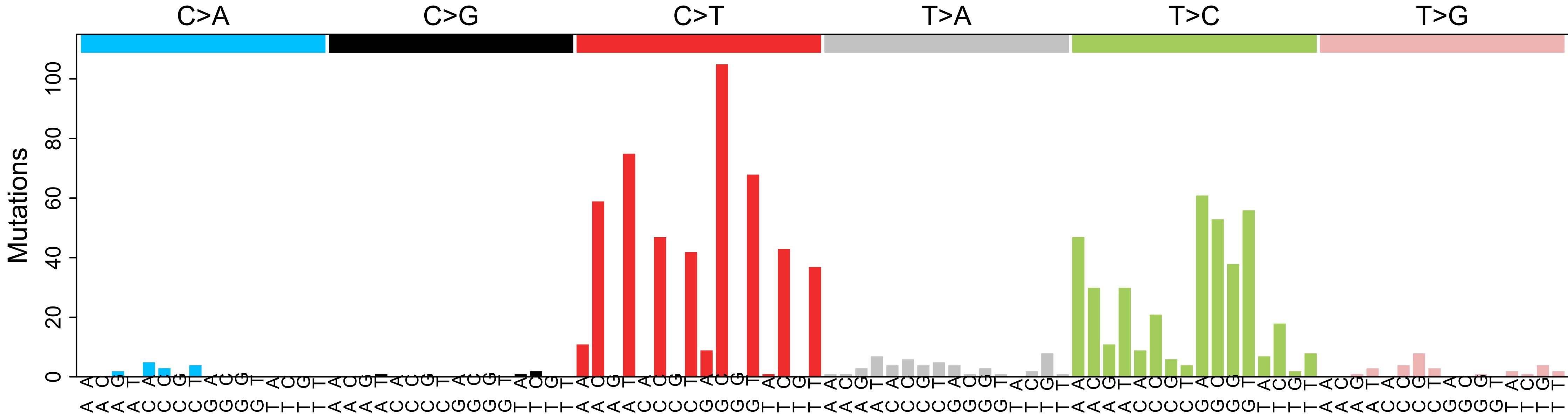
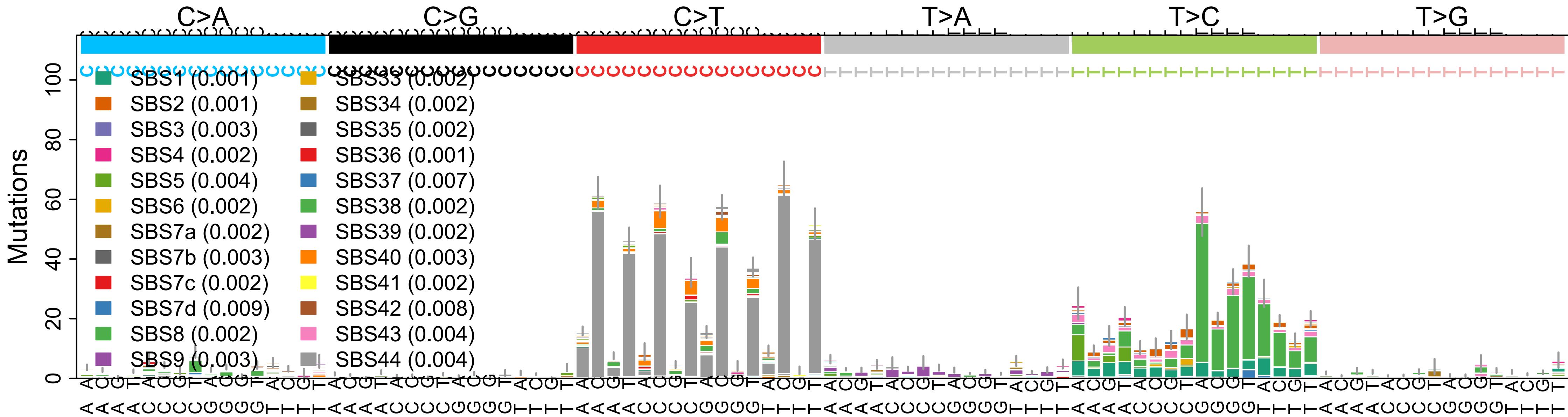


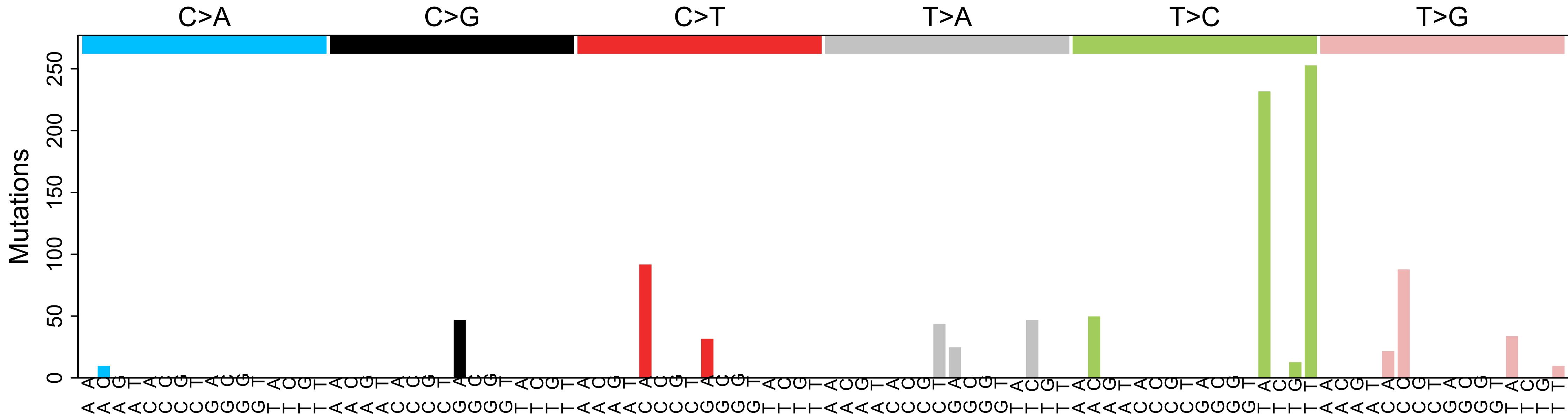
1_2_dimethylhydrazine_9cffdc696a32 (996 mutations)



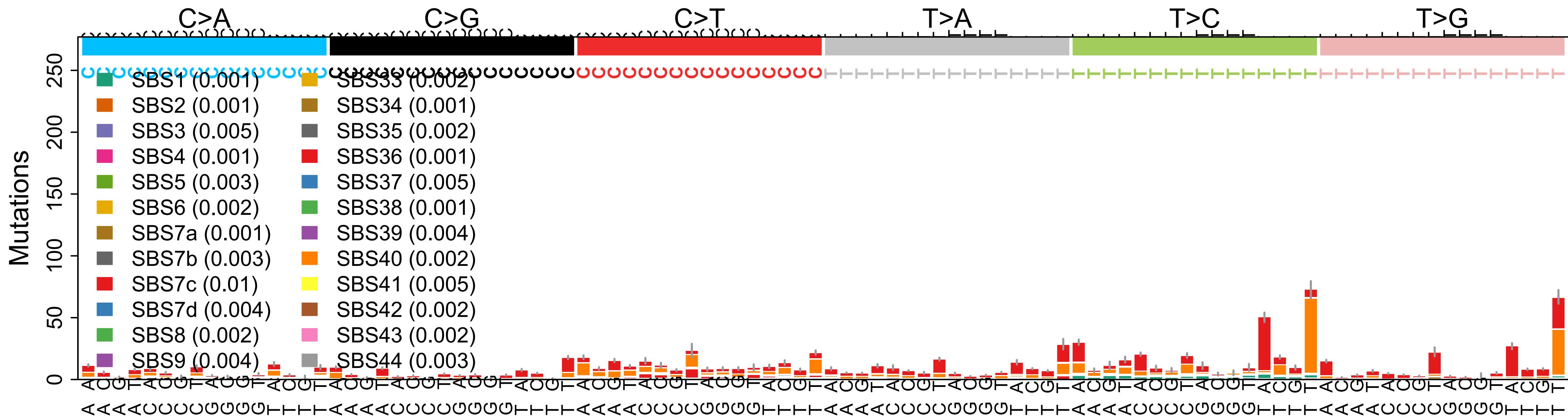
Reconstructed spectrum (cosine similarity = 0.904)



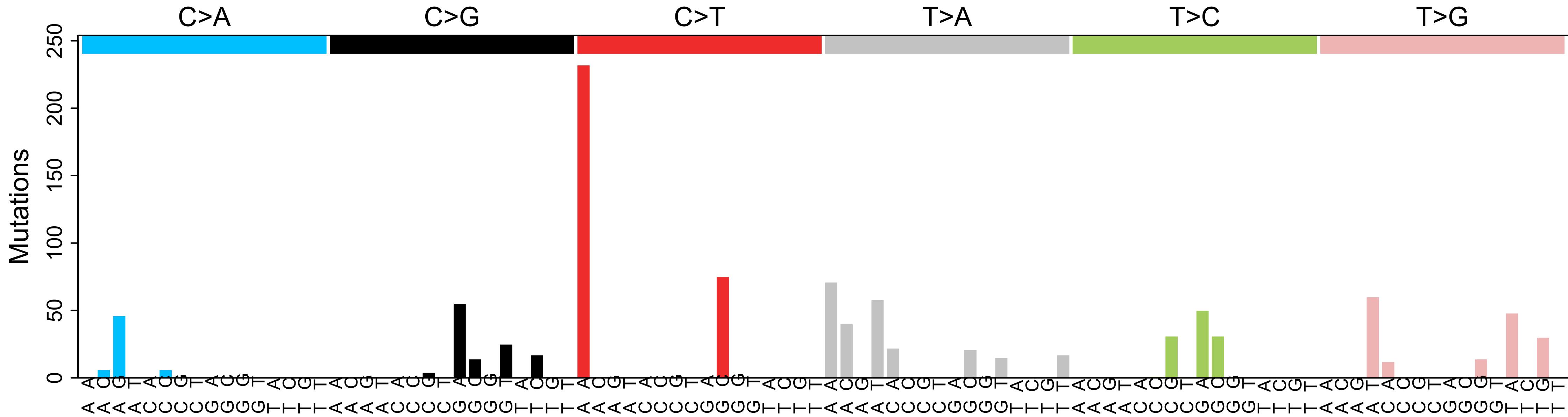
1_2_dimethylhydrazine_ef5d55b18c9c (1,001 mutations)



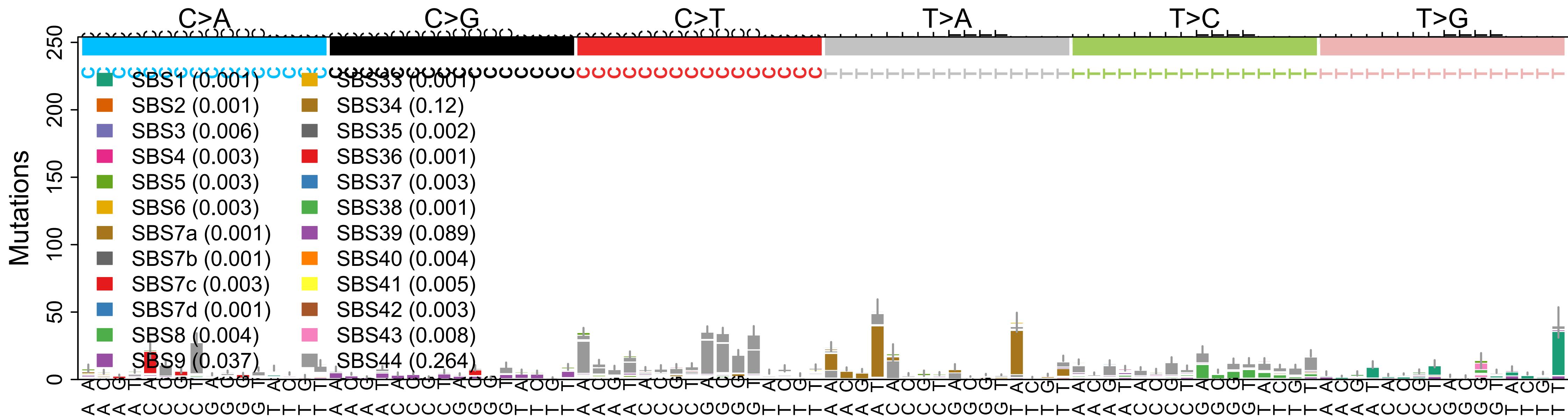
Reconstructed spectrum (cosine similarity = 0.616)



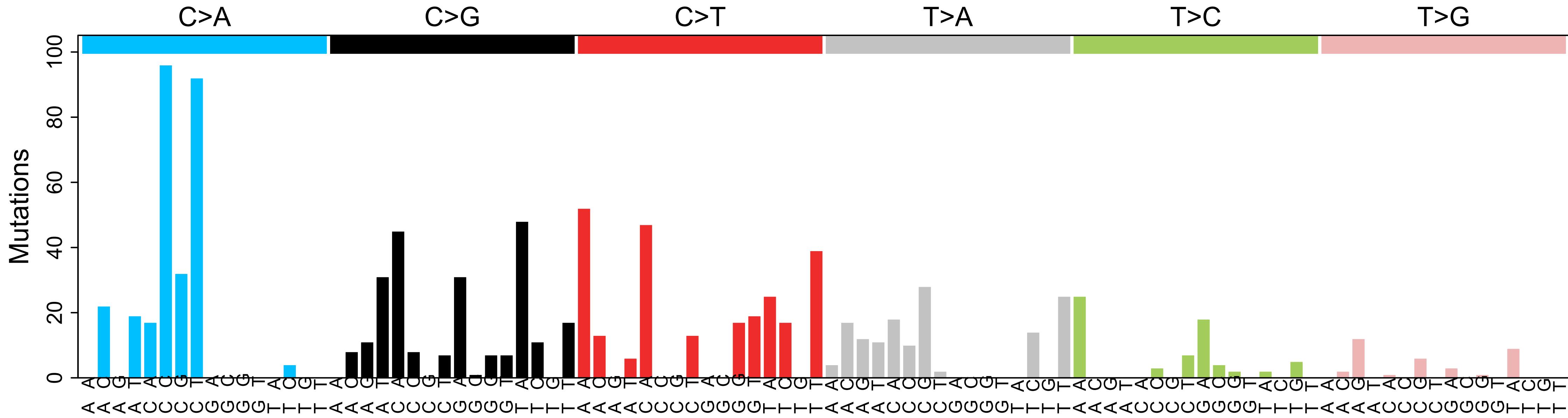
1_4_benzoquinone_2d25052e44b1 (1,001 mutations)



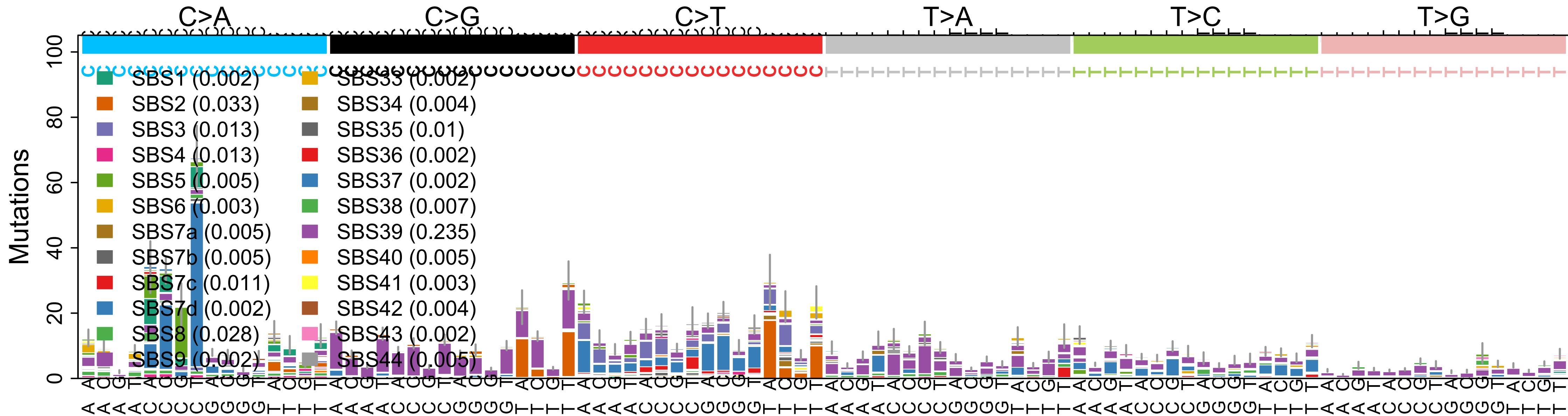
Reconstructed spectrum (cosine similarity = 0.492)



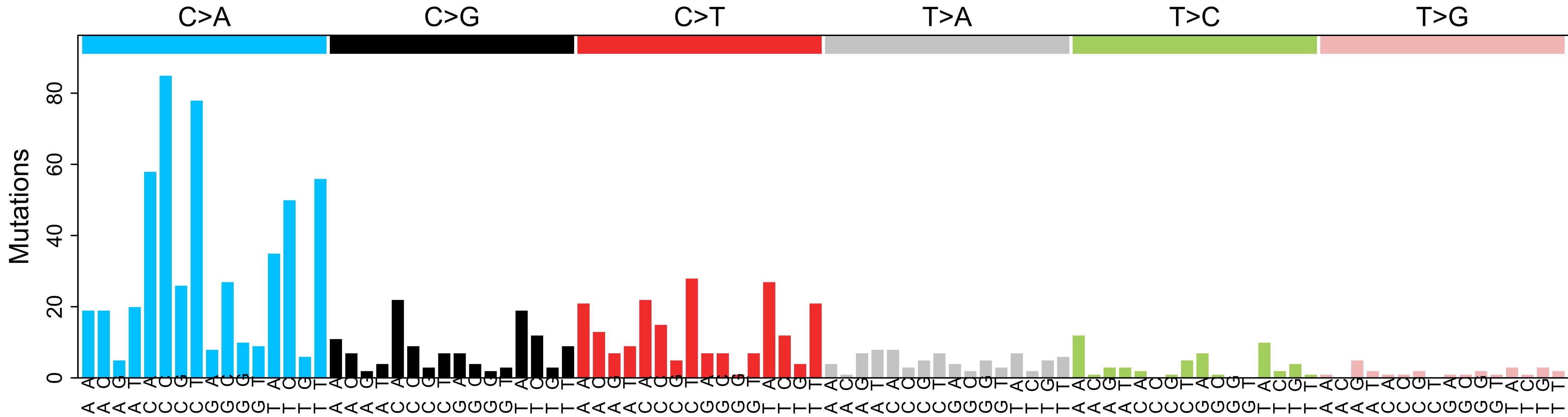
1_6_dinitropyrene_77c0ec6159e4 (1,003 mutations)



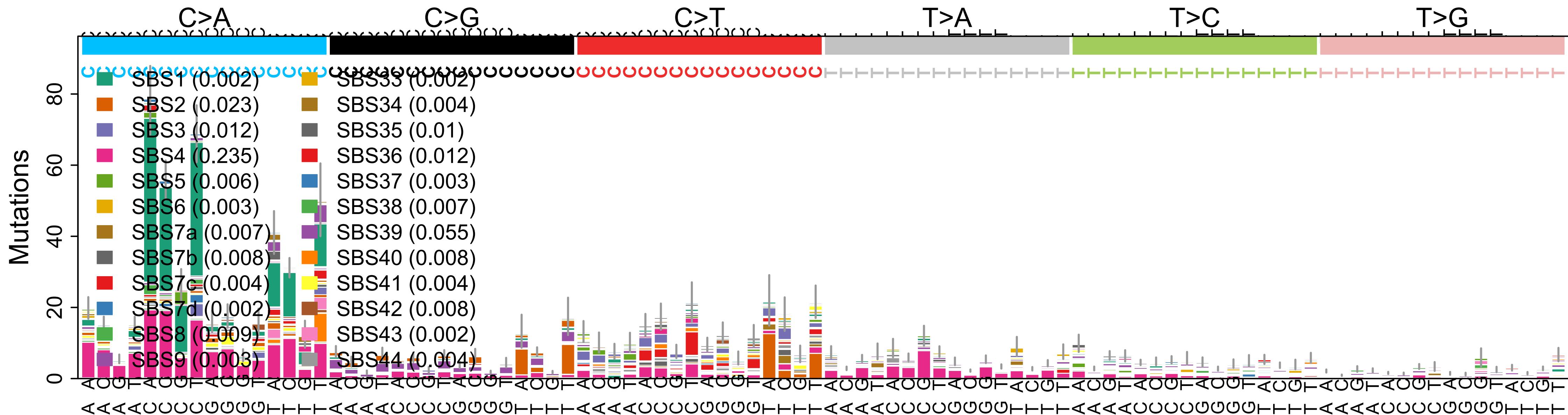
Reconstructed spectrum (cosine similarity = 0.792)



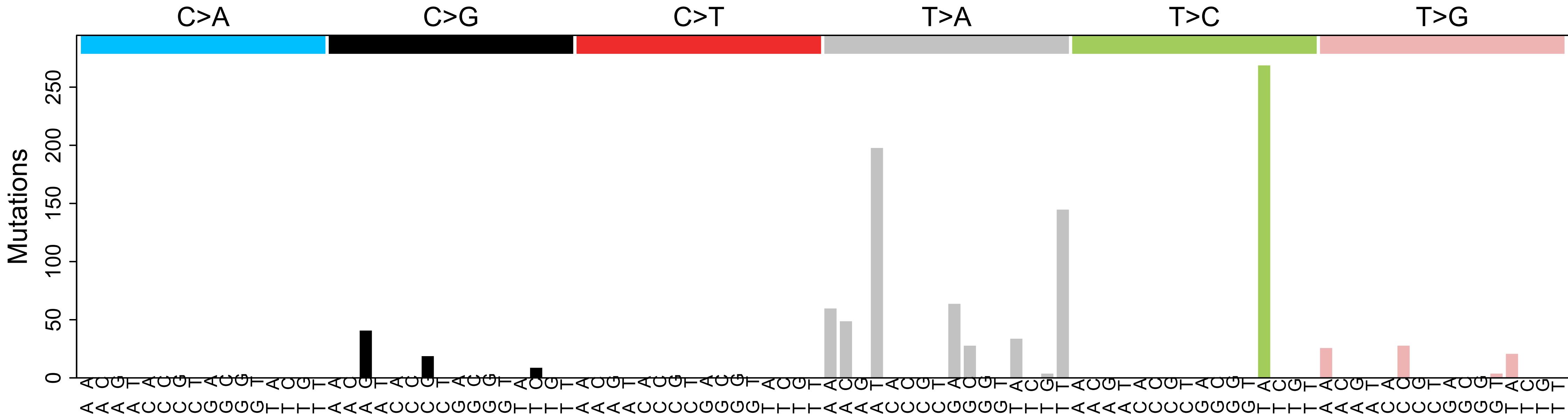
1_8_dinitropyrene_da7ddba98e4a (996 mutations)



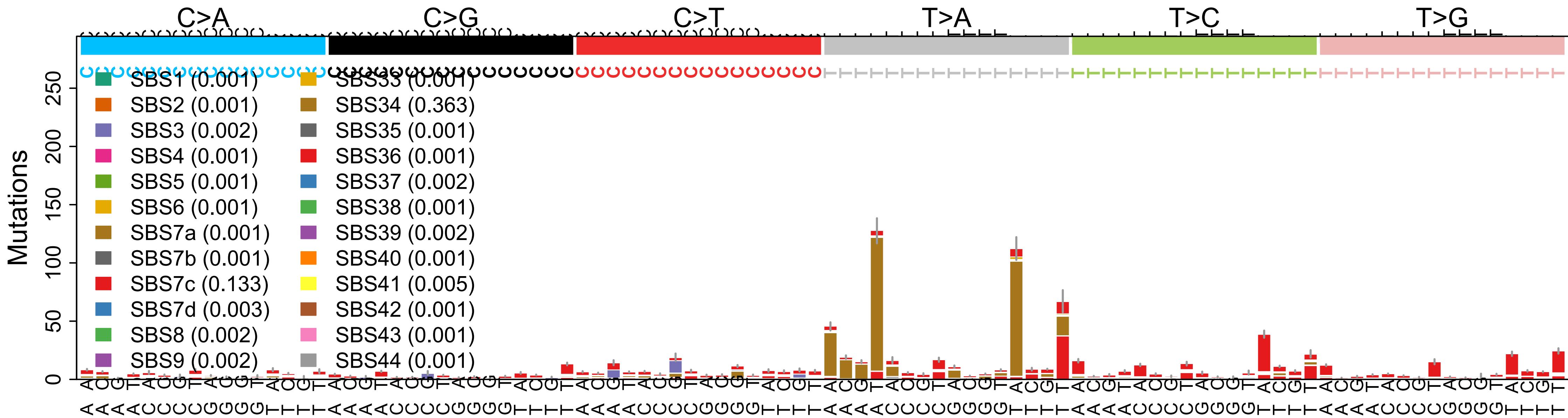
Reconstructed spectrum (cosine similarity = 0.95)



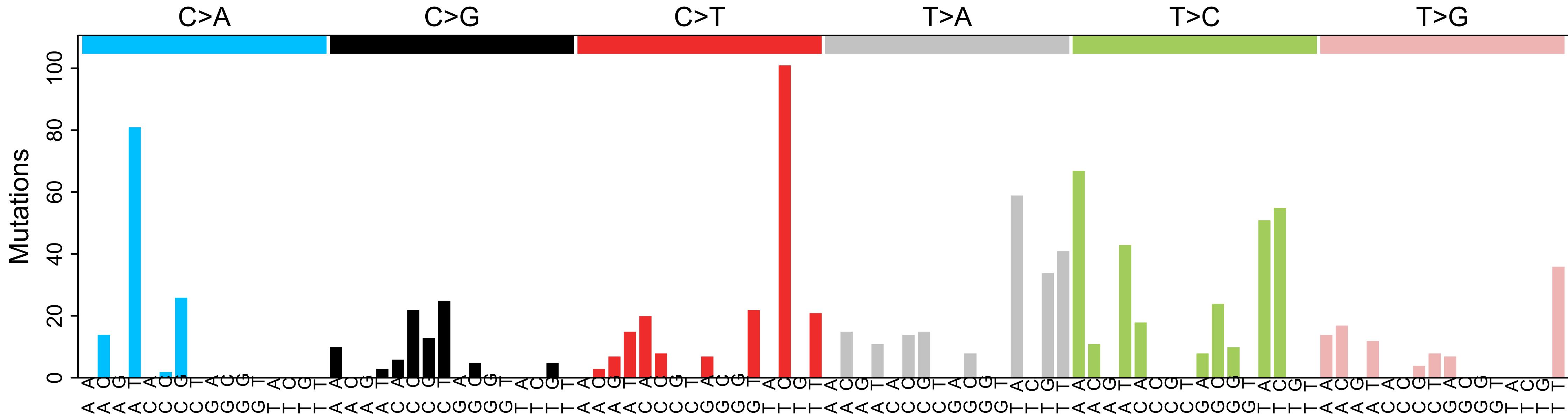
1_nitropyrene_2c37b07dec5a (999 mutations)



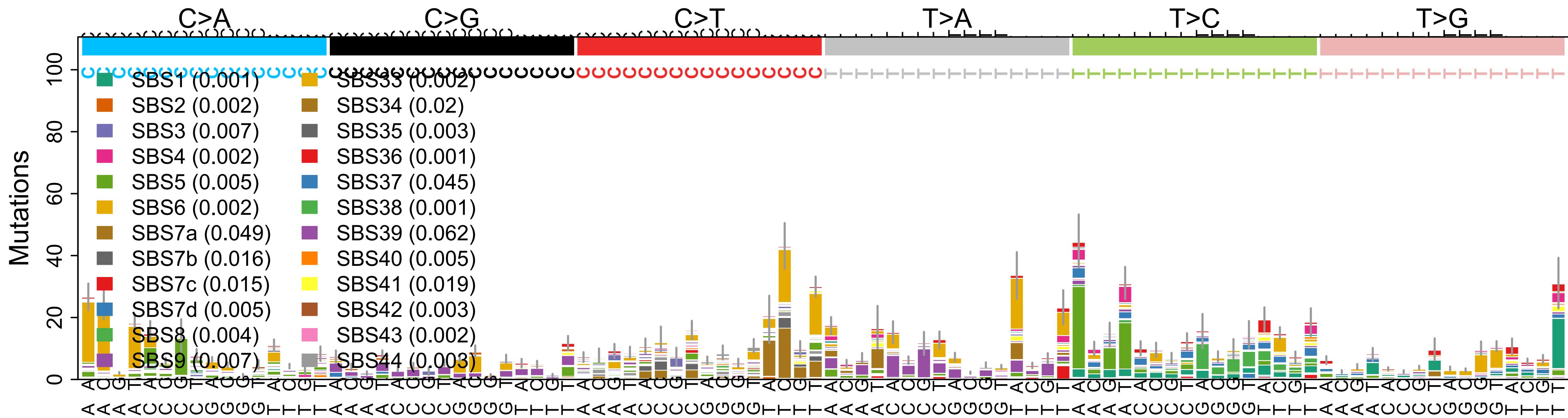
Reconstructed spectrum (cosine similarity = 0.682)



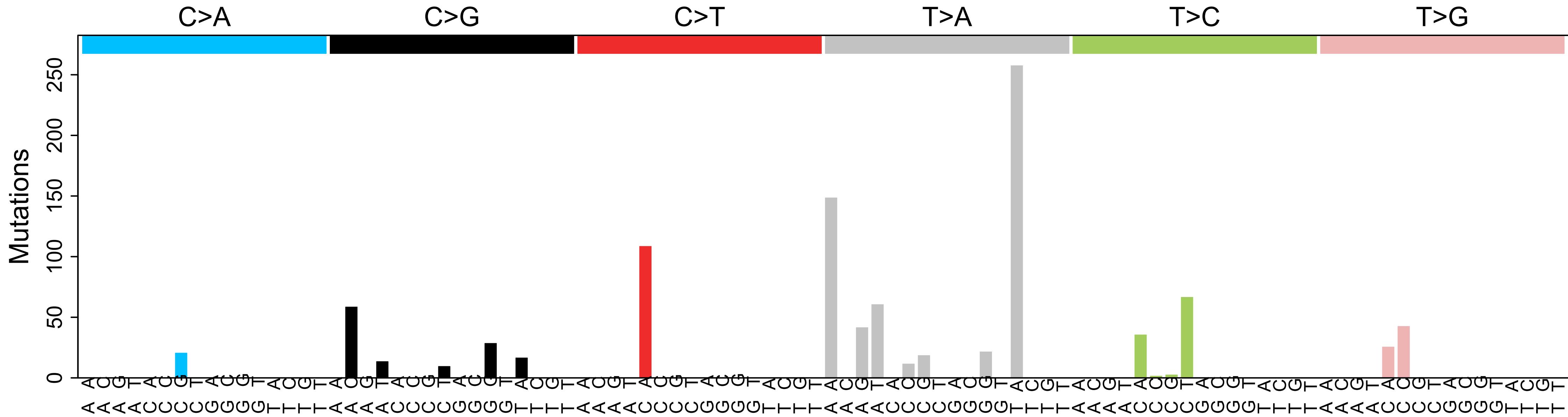
2_6_dimethylaniline_3de14f6a14d9 (998 mutations)



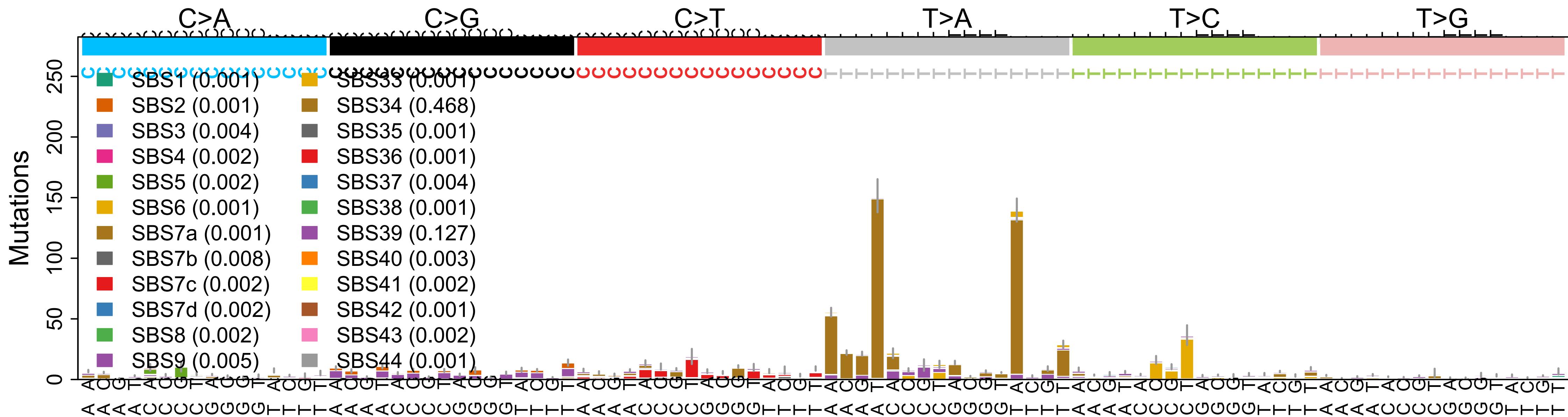
Reconstructed spectrum (cosine similarity = 0.745)



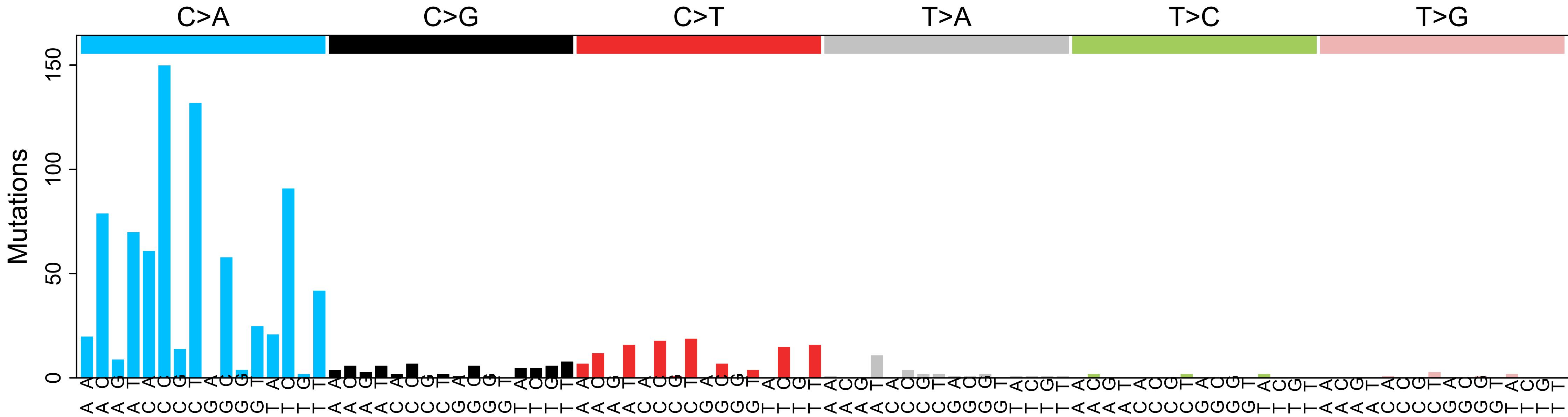
2_6_dimethylaniline_42d3abf9de65 (999 mutations)



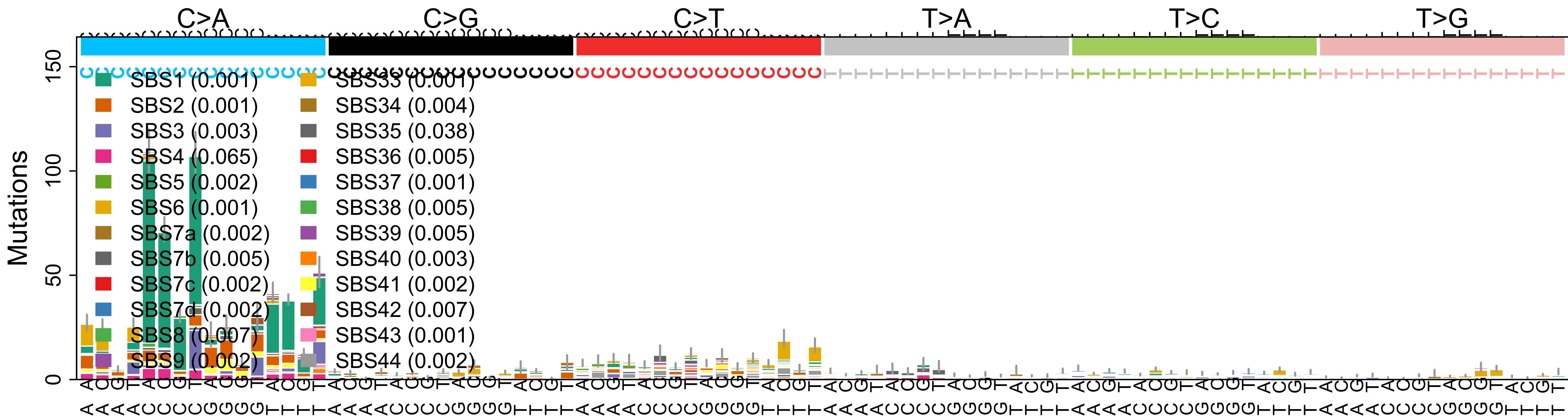
Reconstructed spectrum (cosine similarity = 0.749)



2_amino_1_methyl_6_phenylimidazo4_5_bpyridine_d8aa29785596 (996 mutations)



Reconstructed spectrum (cosine similarity = 0.852)



2_amino_3_8_dimethylimidazo4_5_fquinoxaline_d2762690cb73 (1,000 mutations)

C>A

C>G

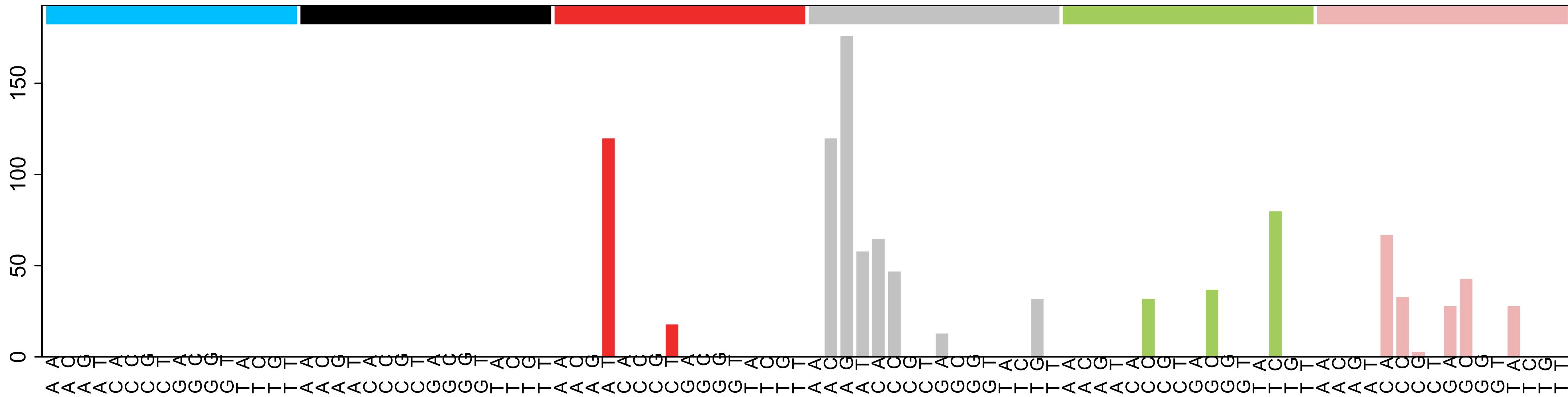
C>T

T>A

T>C

T>G

Mutations



Reconstructed spectrum (cosine similarity = 0.419)

C>A

C>G

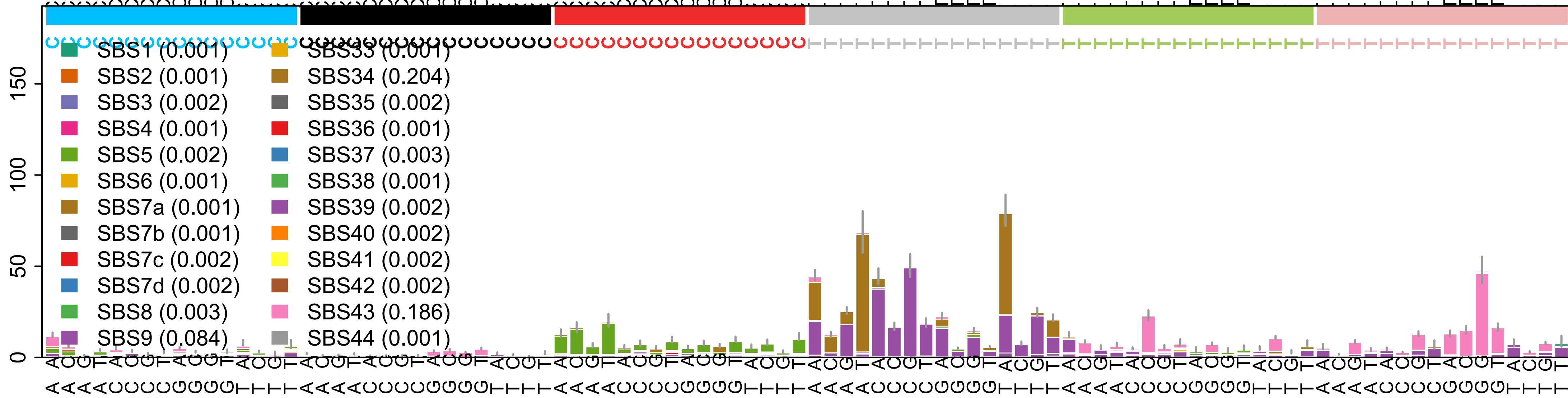
C>T

T>A

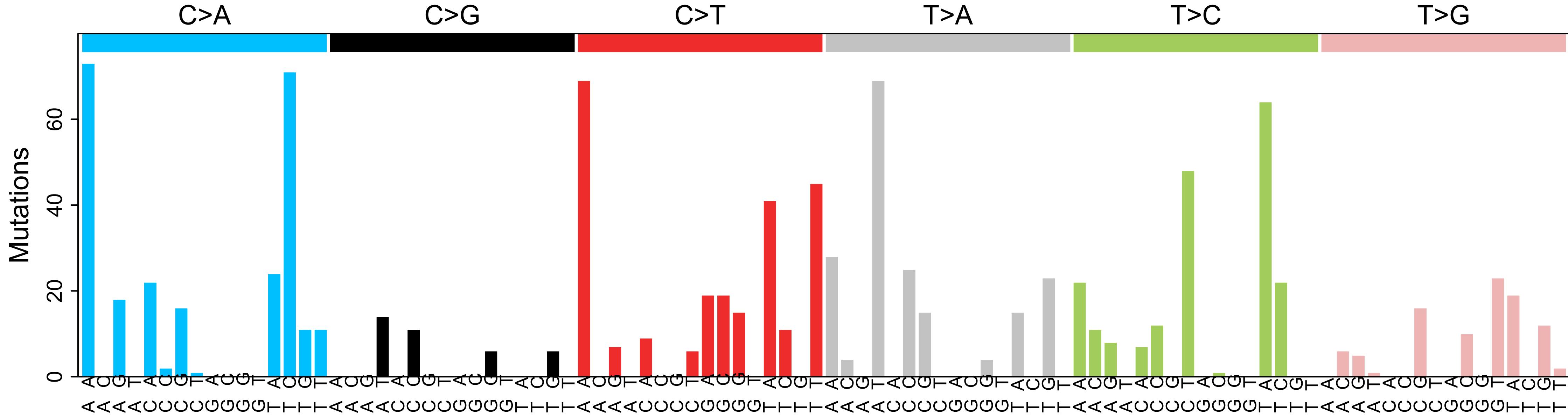
T>C

T>G

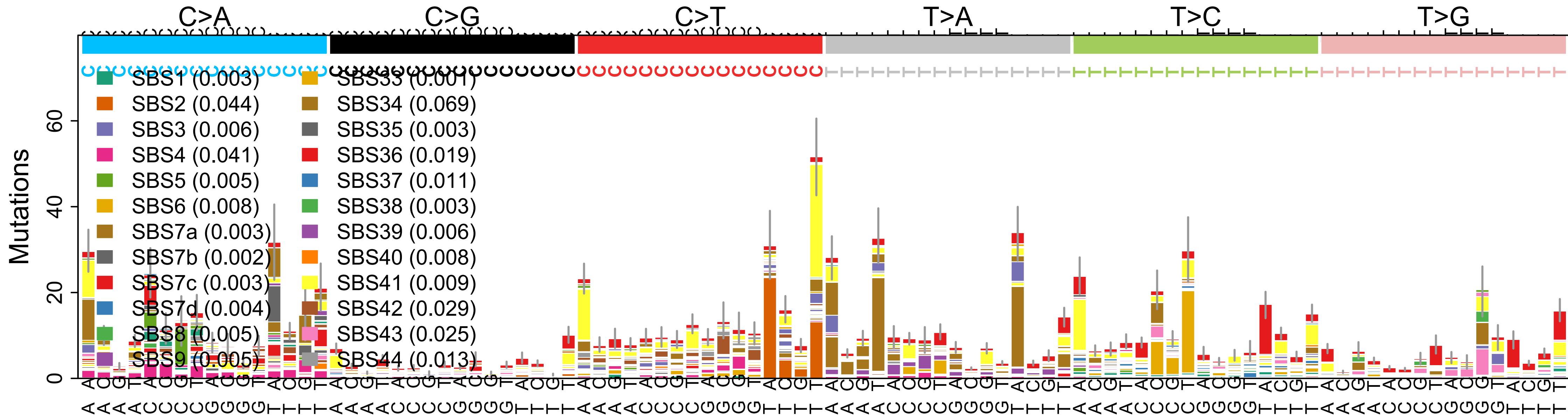
Mutations



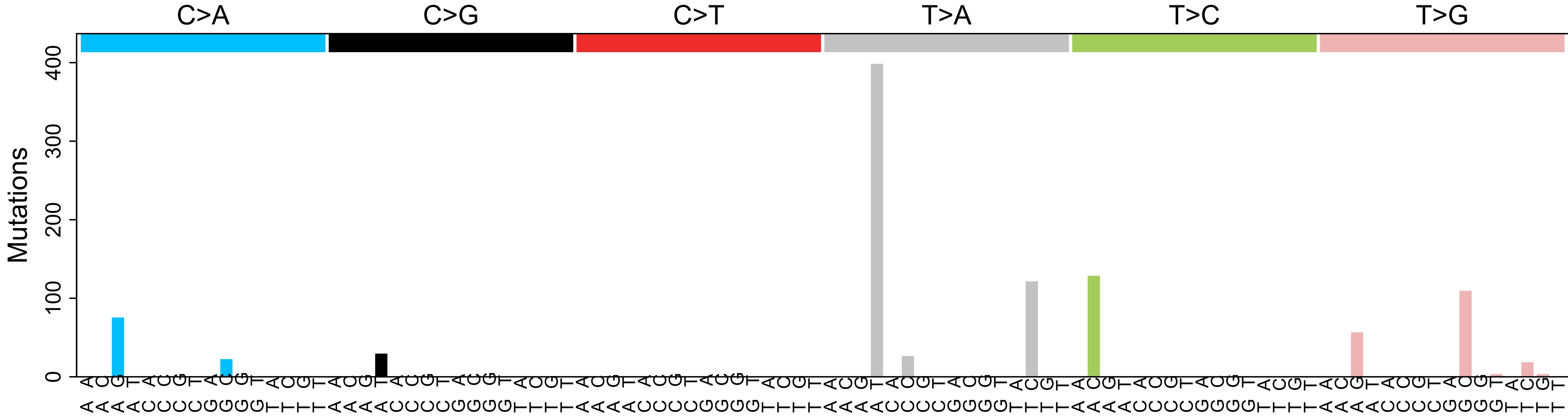
2_amino_3_methyl_9h_pyrido2_3_bindole_f10529056af1 (999 mutations)



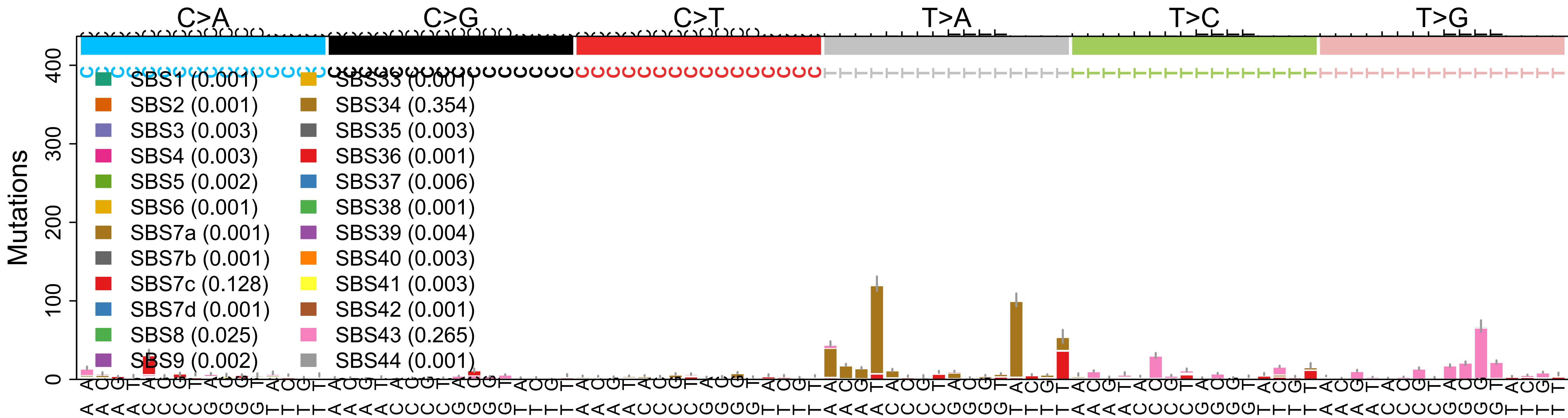
Reconstructed spectrum (cosine similarity = 0.745)



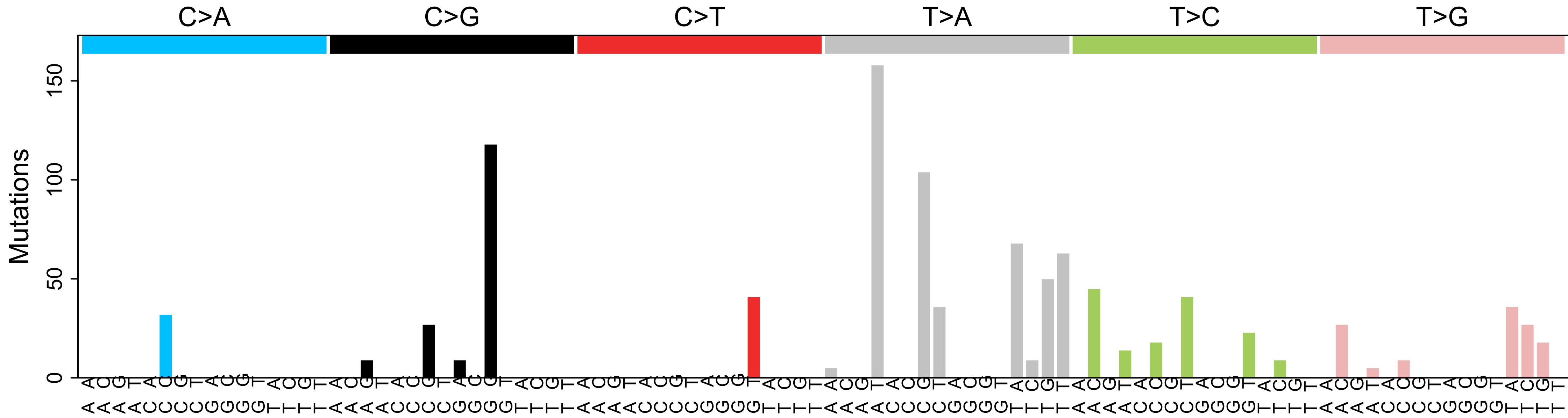
2_amino_3_methylimidazo4_5_fquinoline_0e3b1136946a (1,000 mutations)



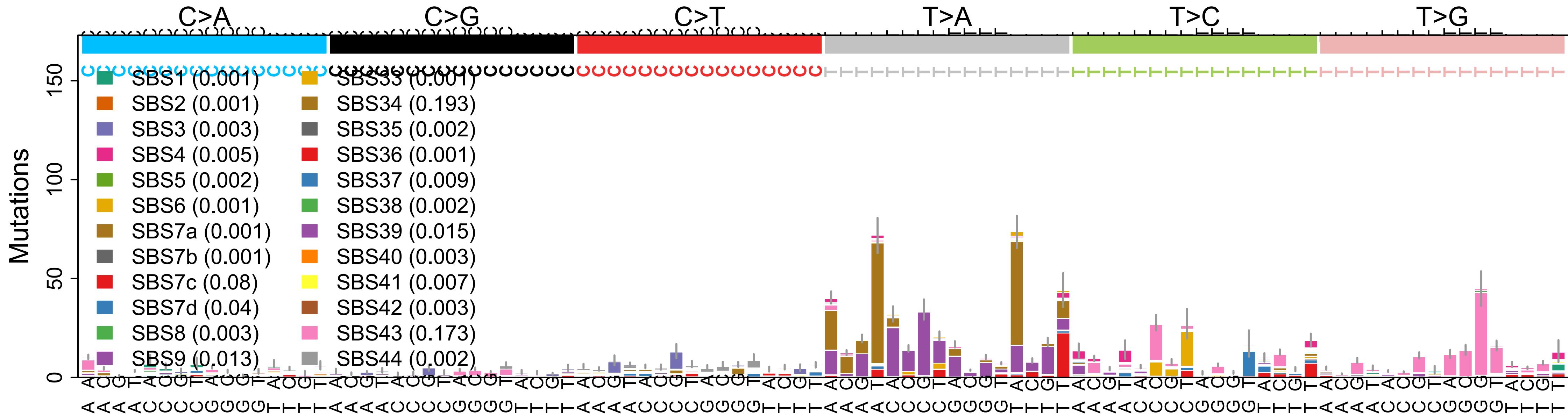
Reconstructed spectrum (cosine similarity = 0.575)



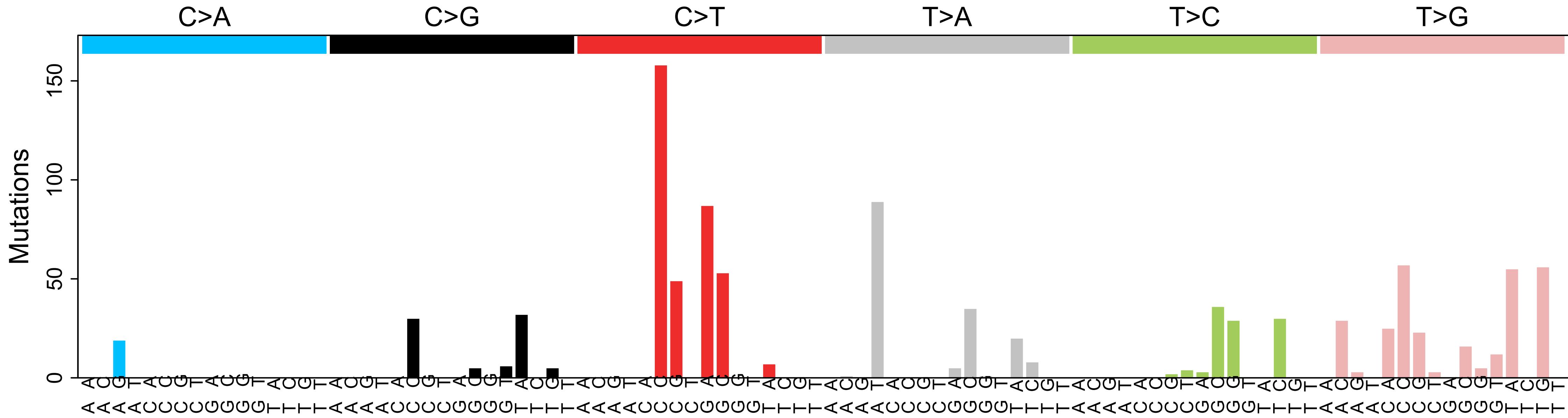
2_naphthylamine_0678c60a05a6 (1,001 mutations)



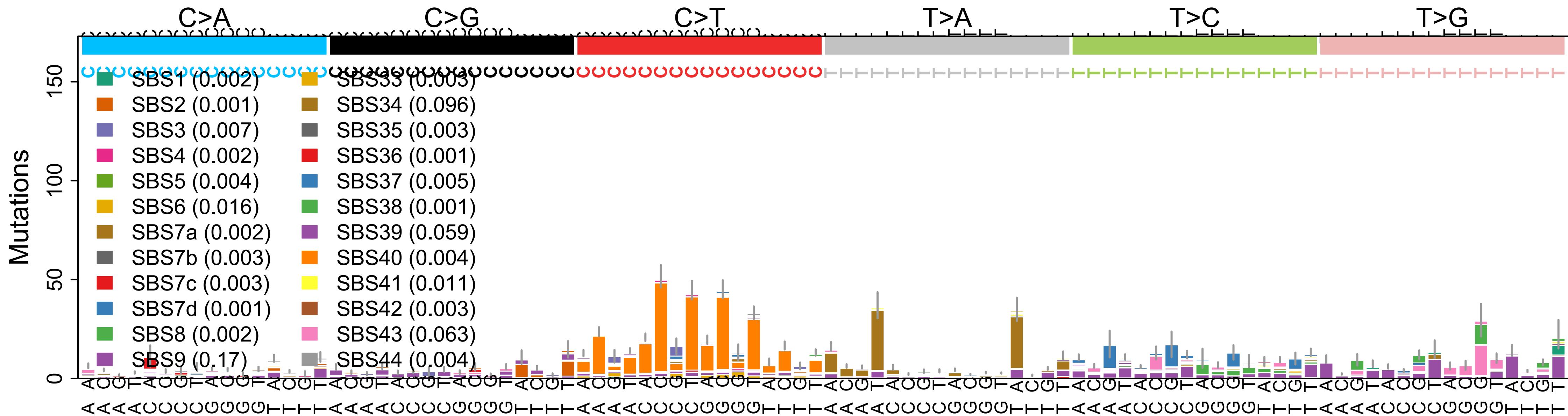
Reconstructed spectrum (cosine similarity = 0.663)



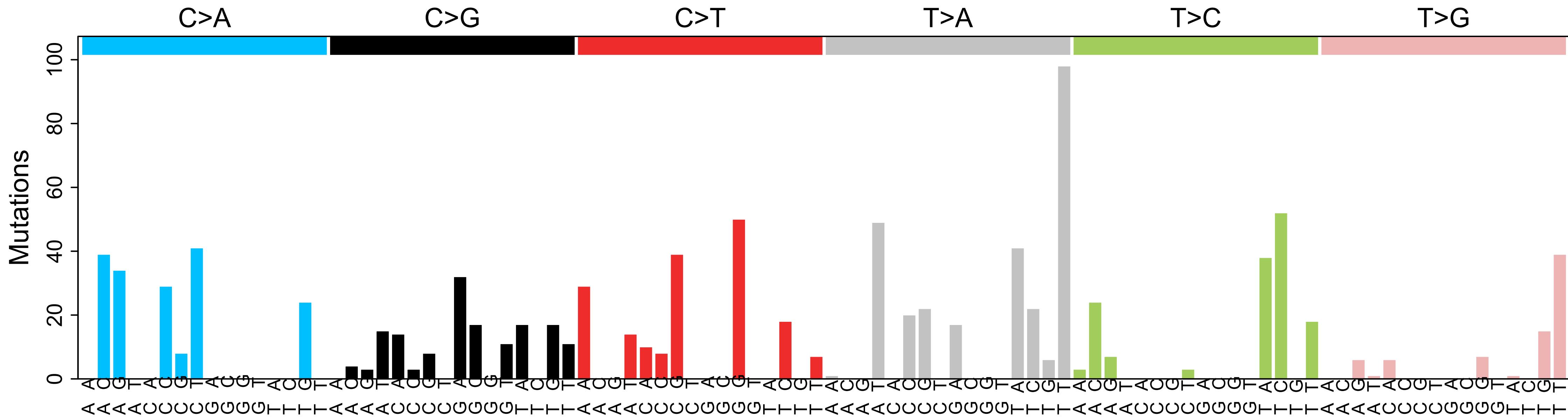
2_naphthylamine_8d0ae6c5590e (998 mutations)



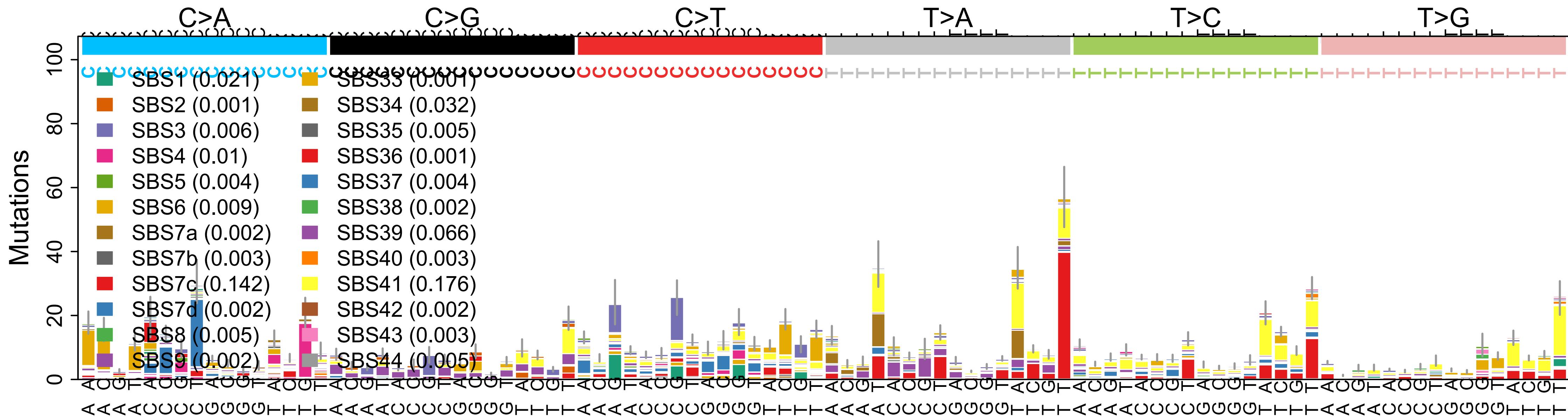
Reconstructed spectrum (cosine similarity = 0.597)



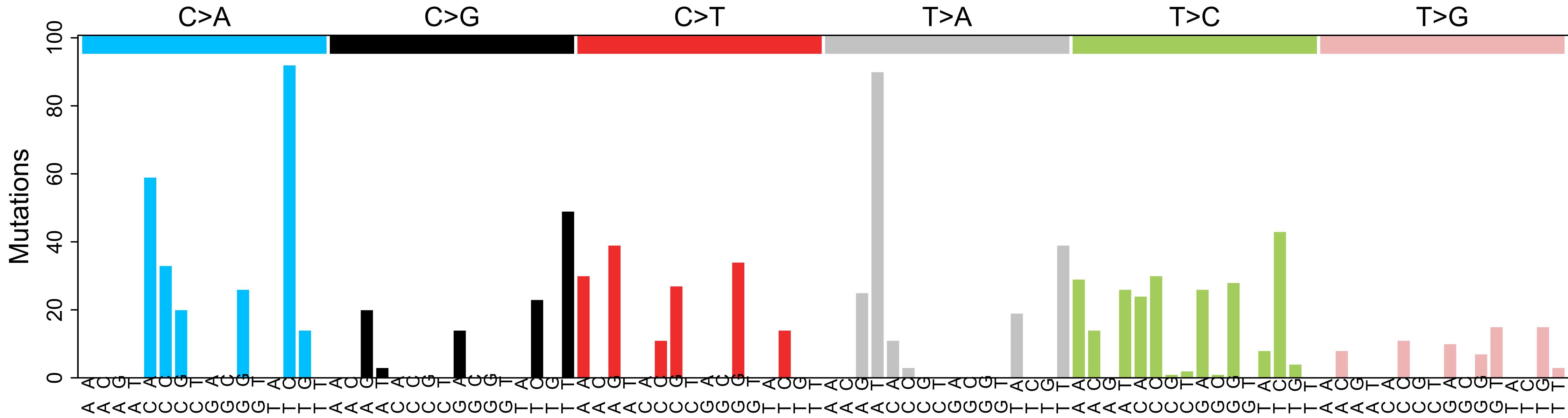
2_nitrofluorene_d908deea4861 (998 mutations)



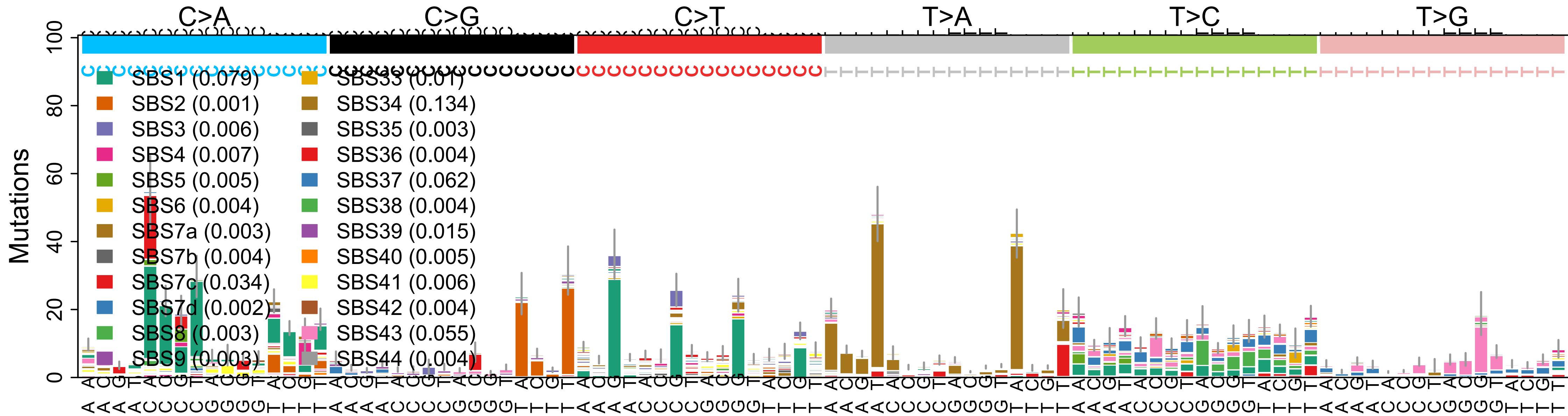
Reconstructed spectrum (cosine similarity = 0.793)



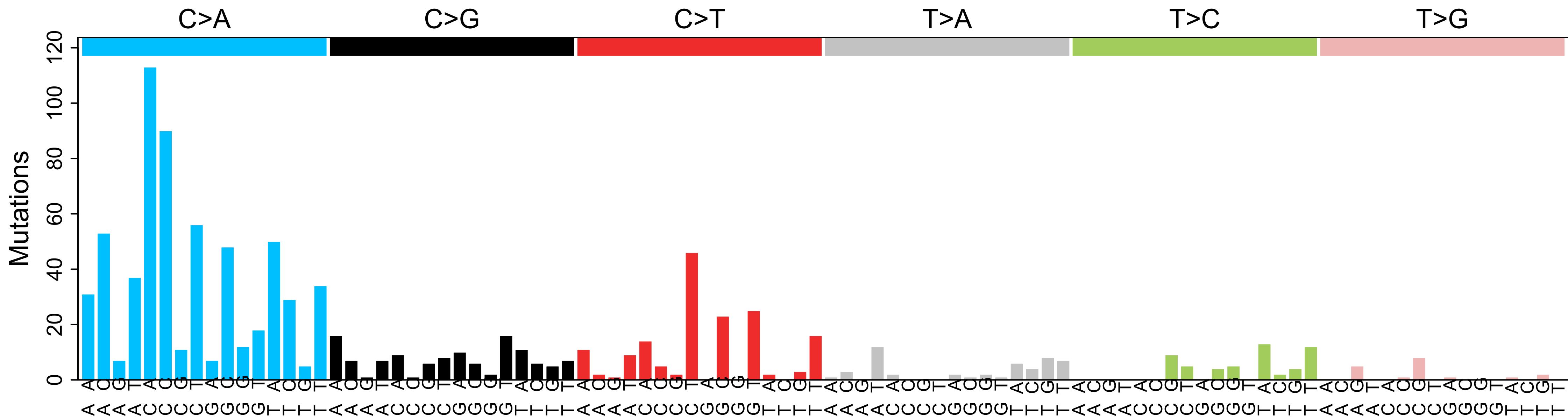
2_nitrotoluene_d1b70070133b (1,000 mutations)



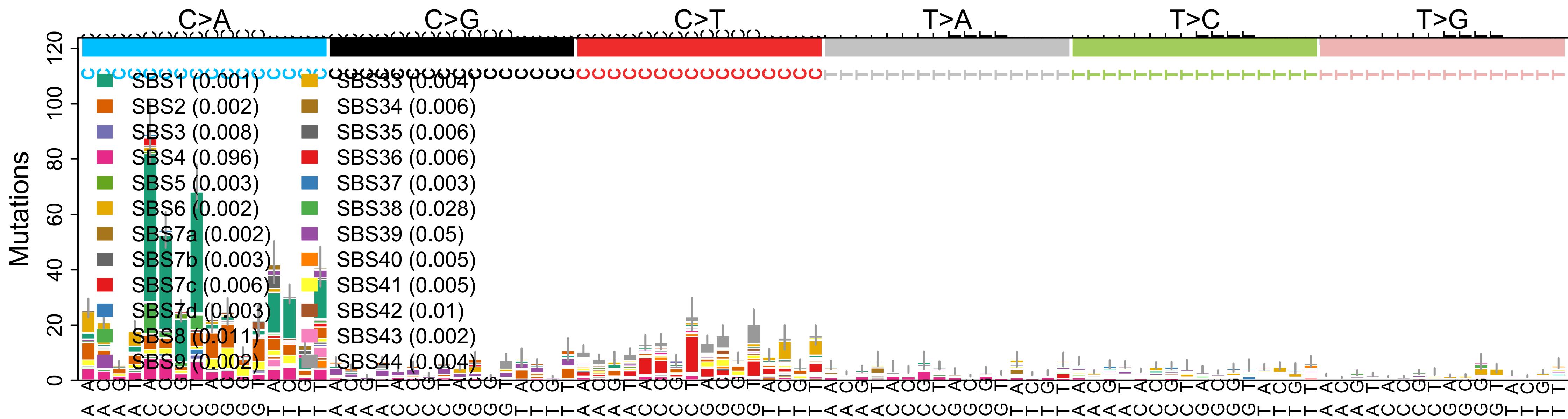
Reconstructed spectrum (cosine similarity = 0.738)



3_chloro_4_dichloromethyl_5_hydroxy_25h_furanone_d6057c2d9433 (999 mutations)



Reconstructed spectrum (cosine similarity = 0.922)



3_chloro_4_dichloromethyl_5_hydroxy_25h_furanone_e40d11eac1ce (1,000 mutations)

C>A

C>G

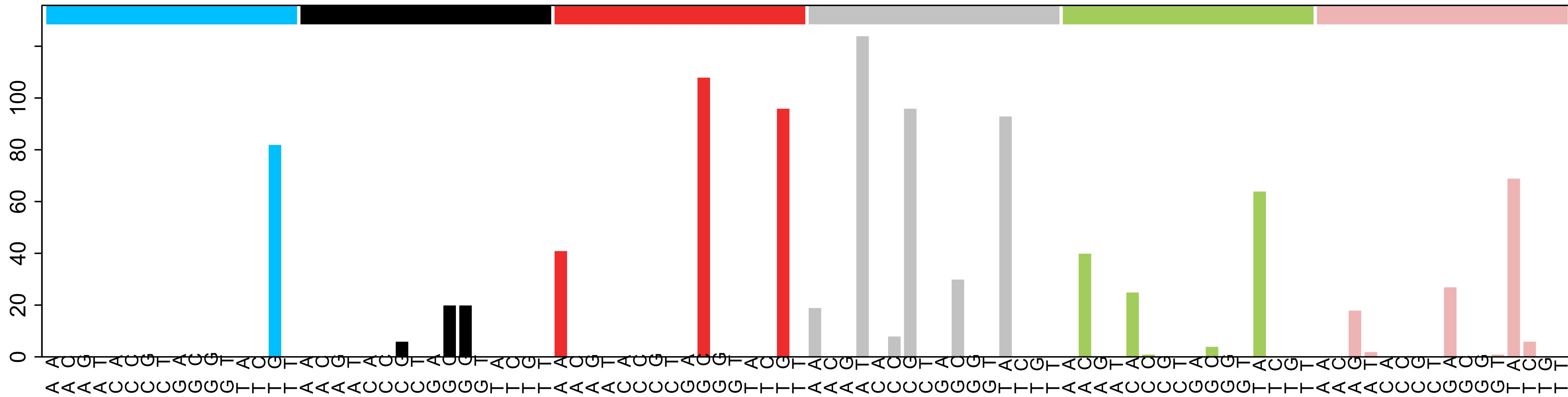
C>T

T>A

T>C

T>G

Mutations



Reconstructed spectrum (cosine similarity = 0.751)

C>A

C>G

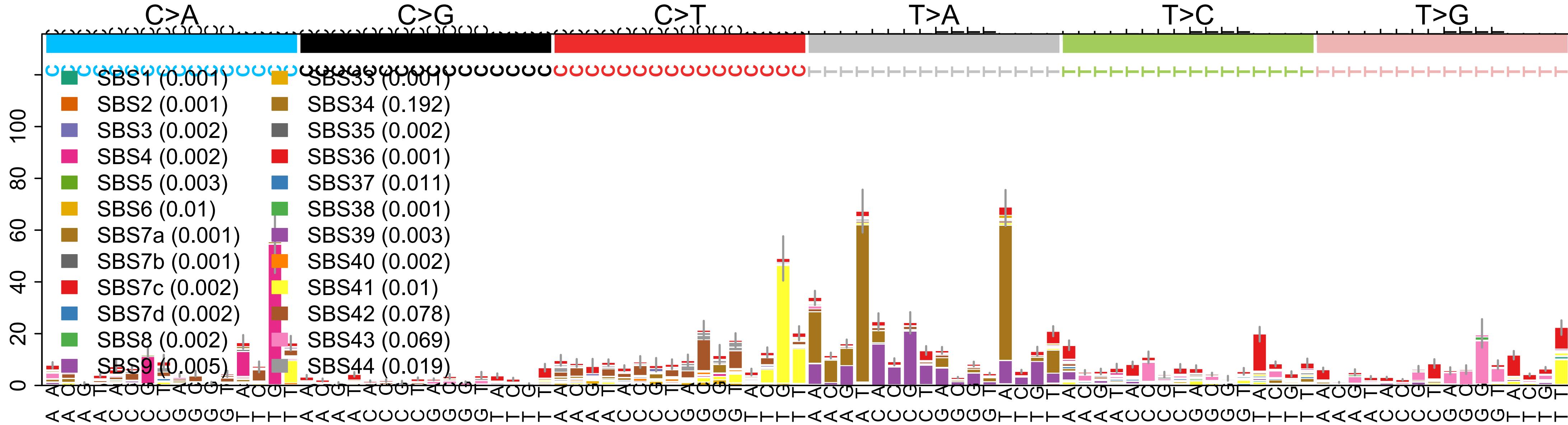
C>T

T>A

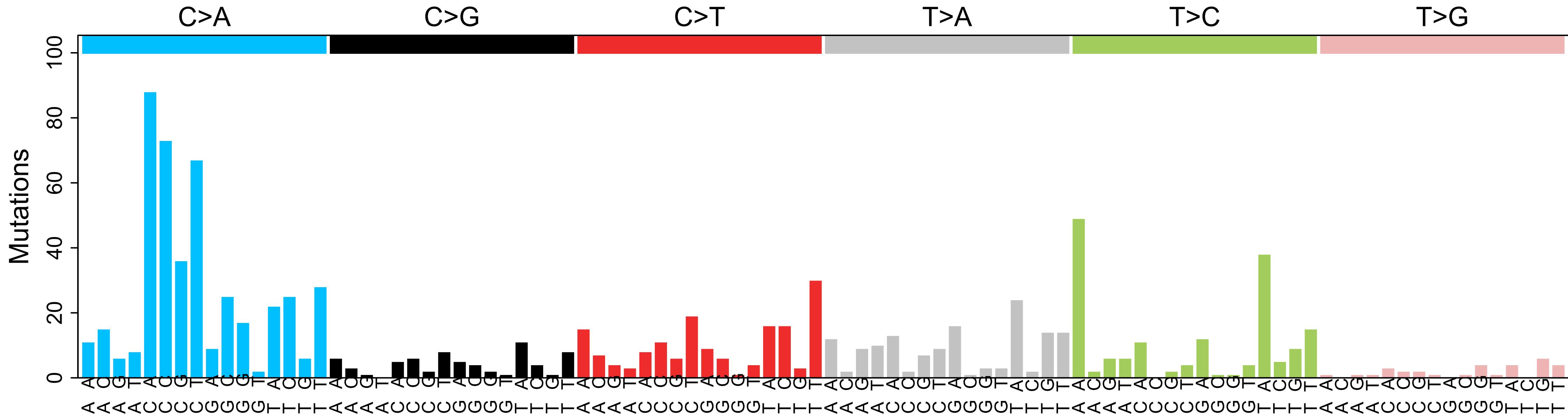
T>C

T>G

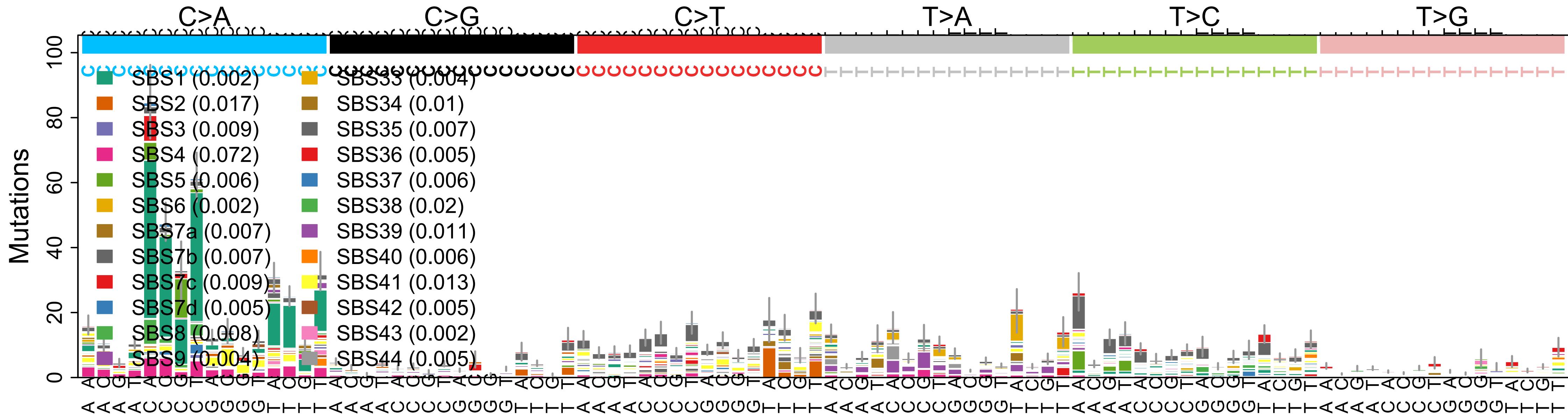
Mutations



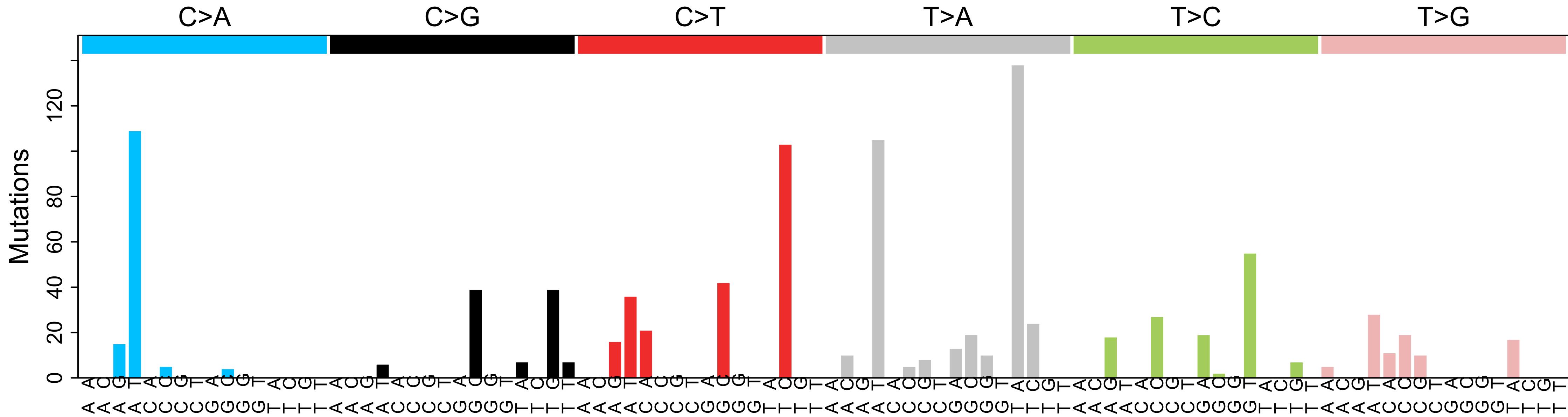
3_nitrobenzanthrone_8bc52f809fe4 (1,000 mutations)



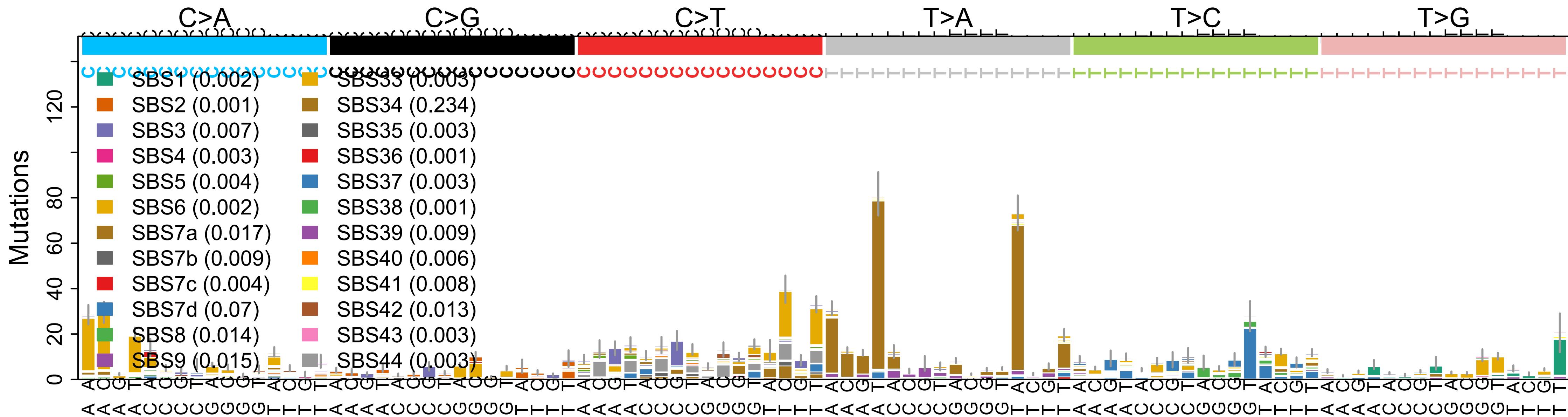
Reconstructed spectrum (cosine similarity = 0.95)



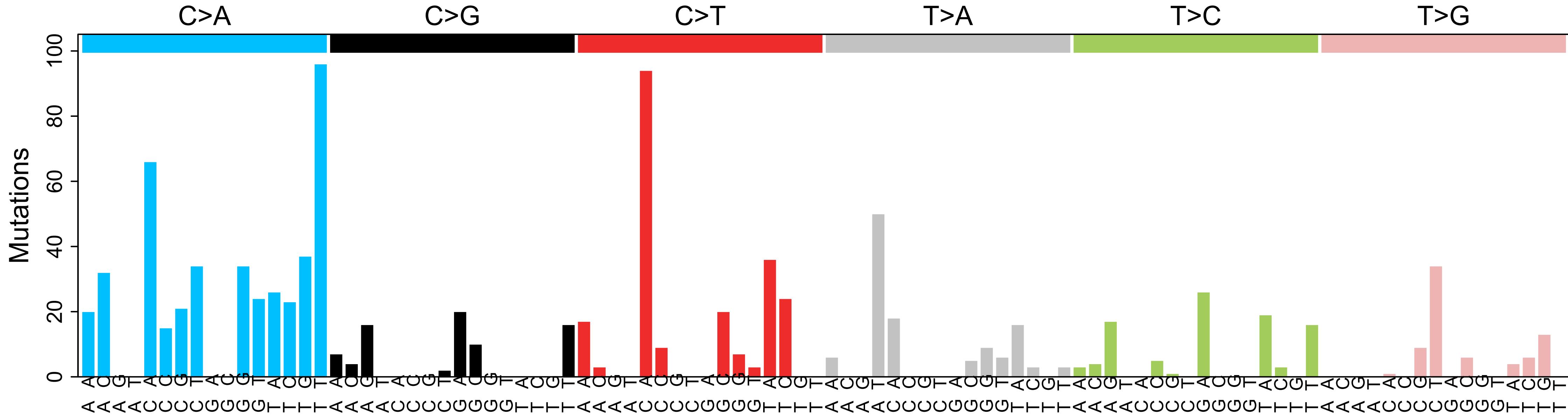
4_4_methylene_bis2_chloroaniline_10dc00a2ca17 (999 mutations)



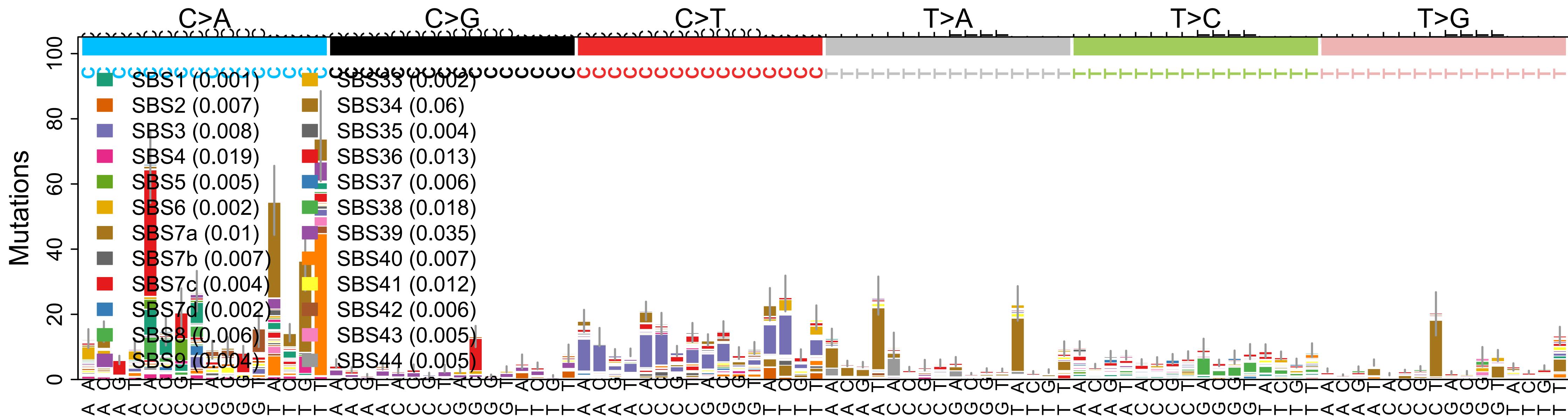
Reconstructed spectrum (cosine similarity = 0.736)



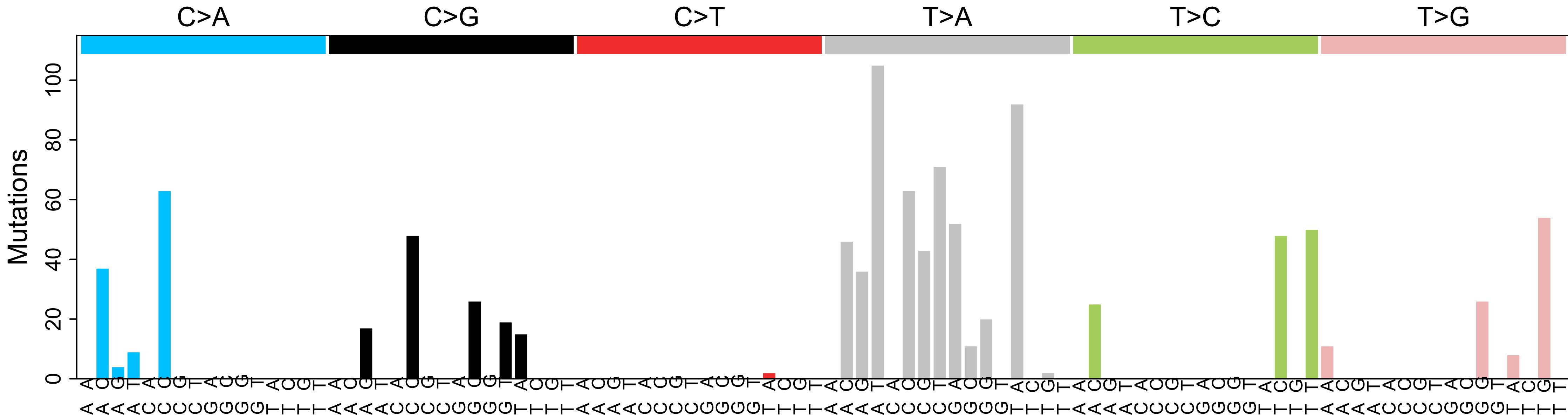
4_4_methylene_bis2_chloroaniline_b43861ea935b (999 mutations)



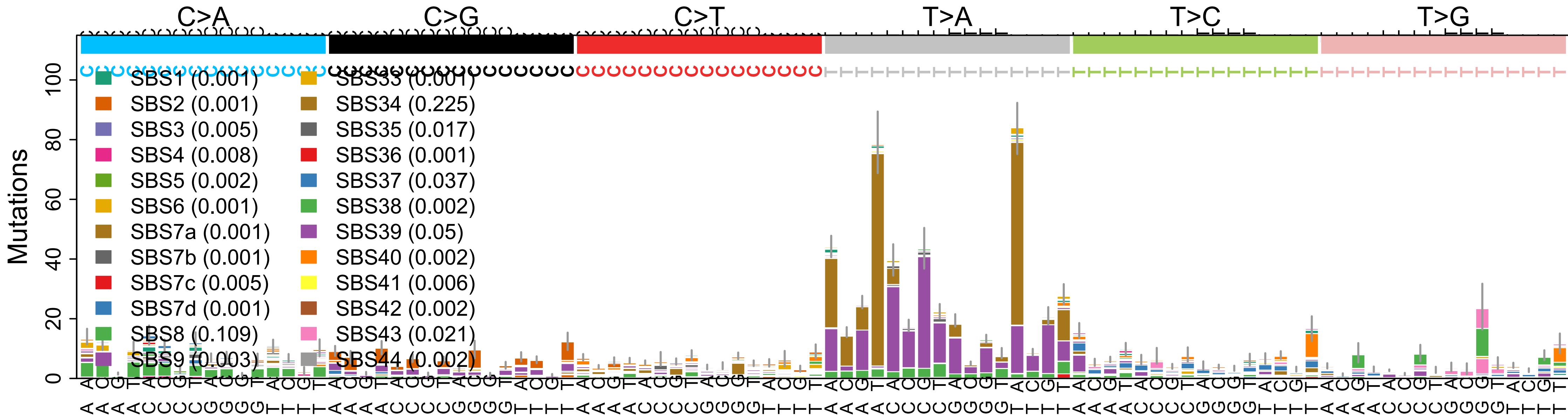
Reconstructed spectrum (cosine similarity = 0.827)



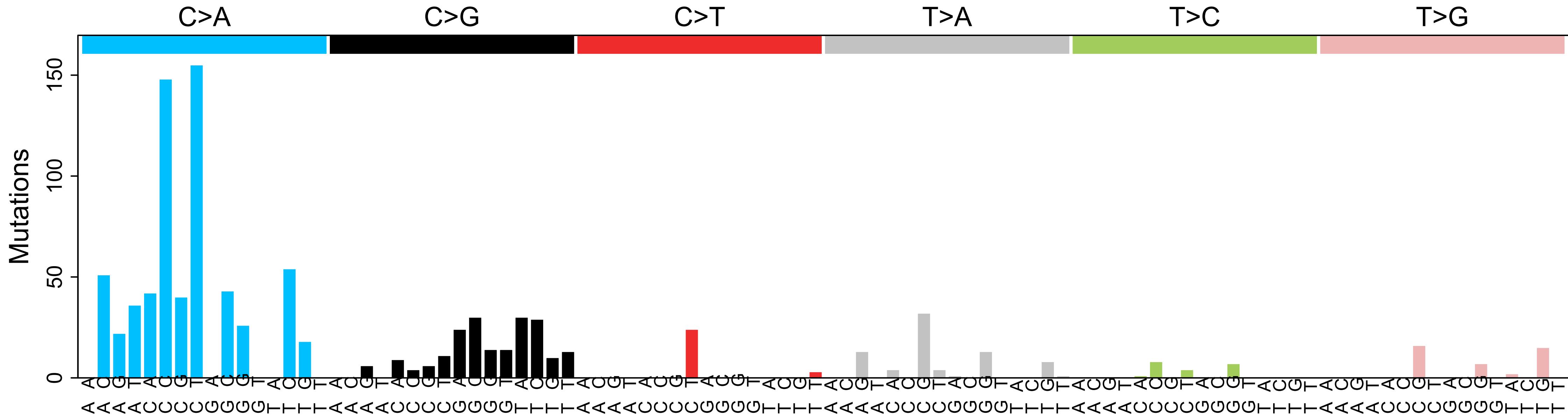
4_aminobiphenyl_dfa9b811bd76 (1,003 mutations)



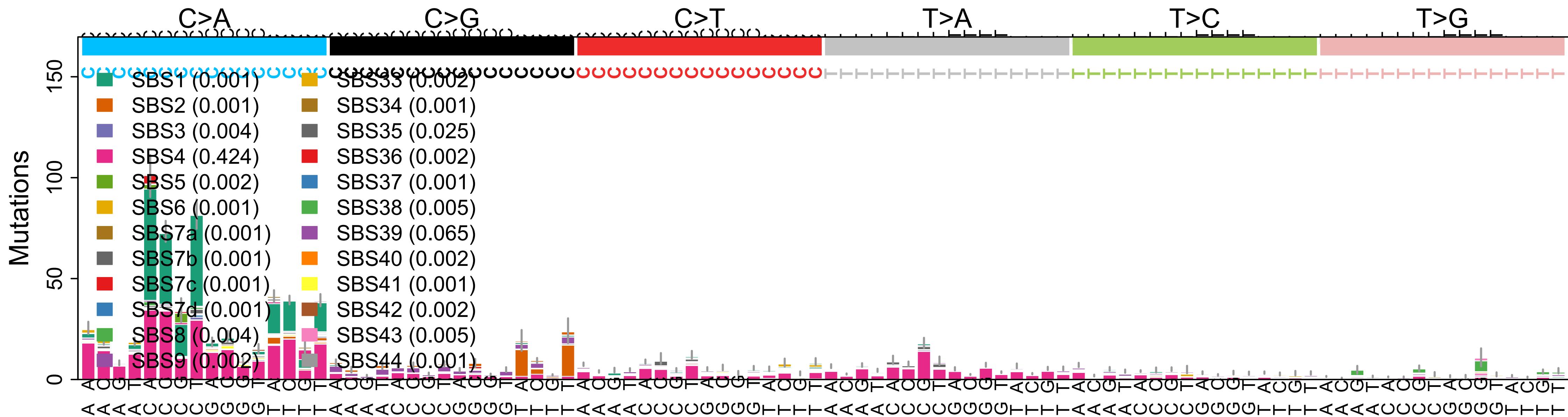
Reconstructed spectrum (cosine similarity = 0.726)



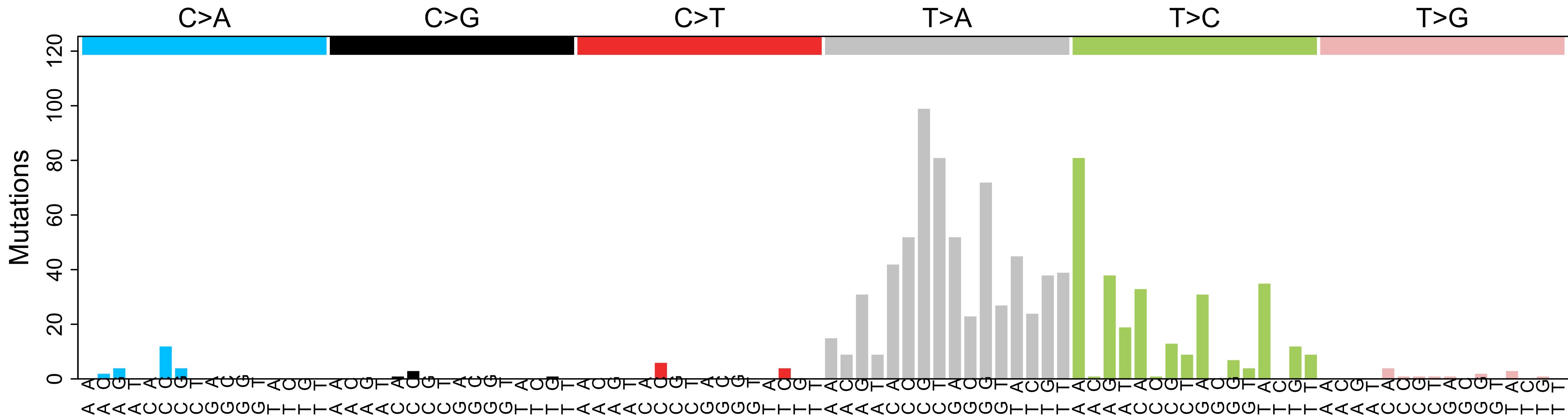
5_methylchrysene_5b2e180a87c7 (998 mutations)



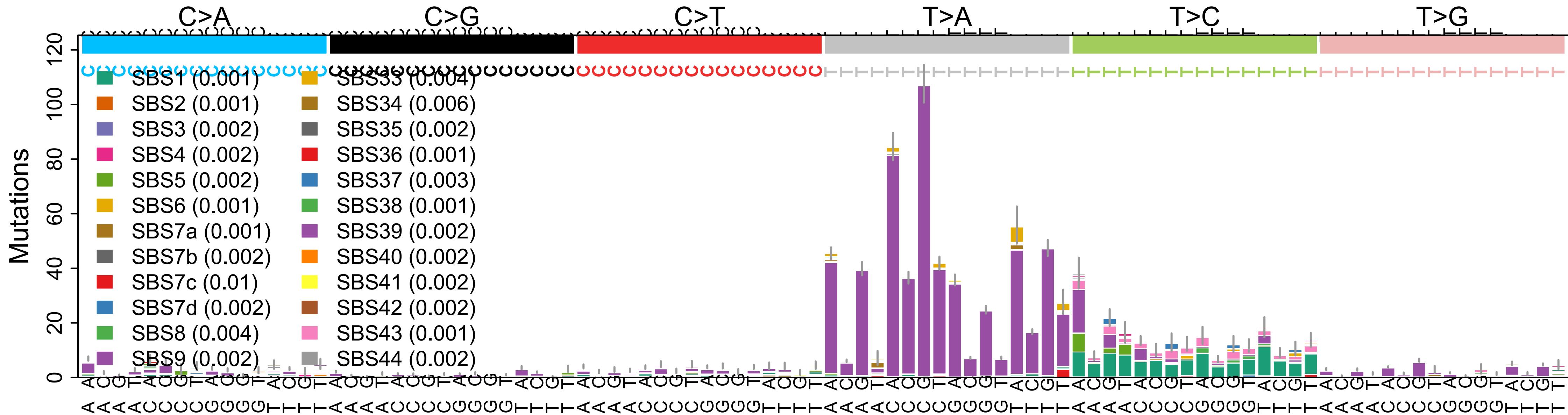
Reconstructed spectrum (cosine similarity = 0.791)



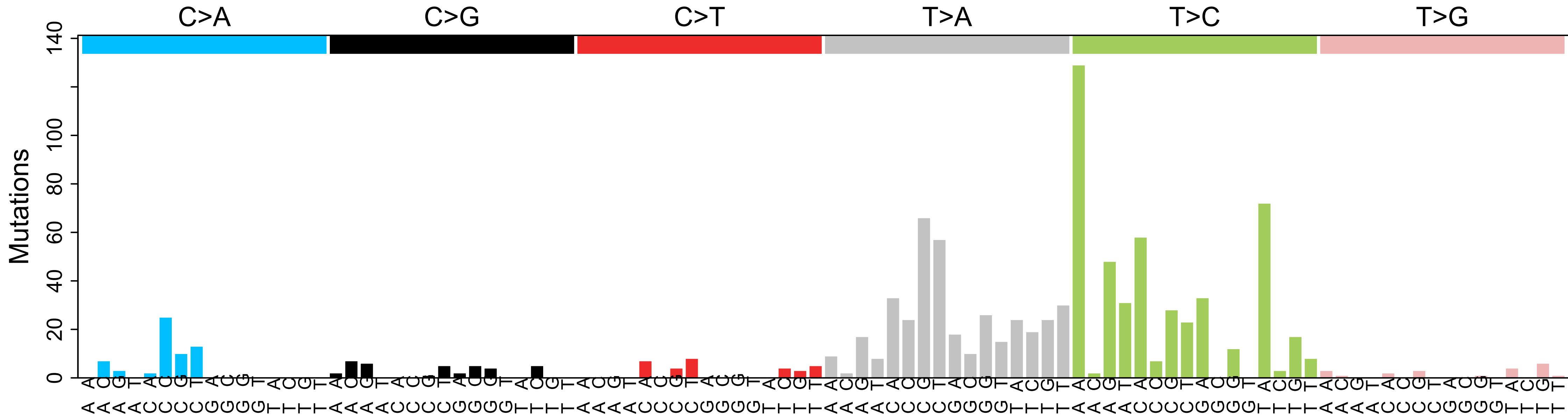
6_nitrochrysene_2a37dfc605b1 (1,002 mutations)



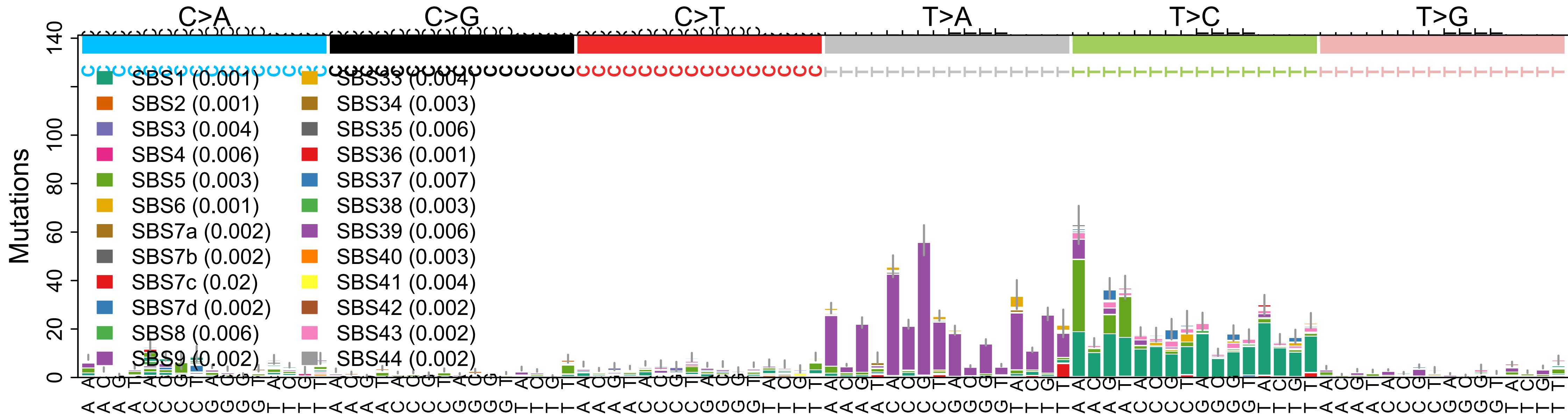
Reconstructed spectrum (cosine similarity = 0.869)



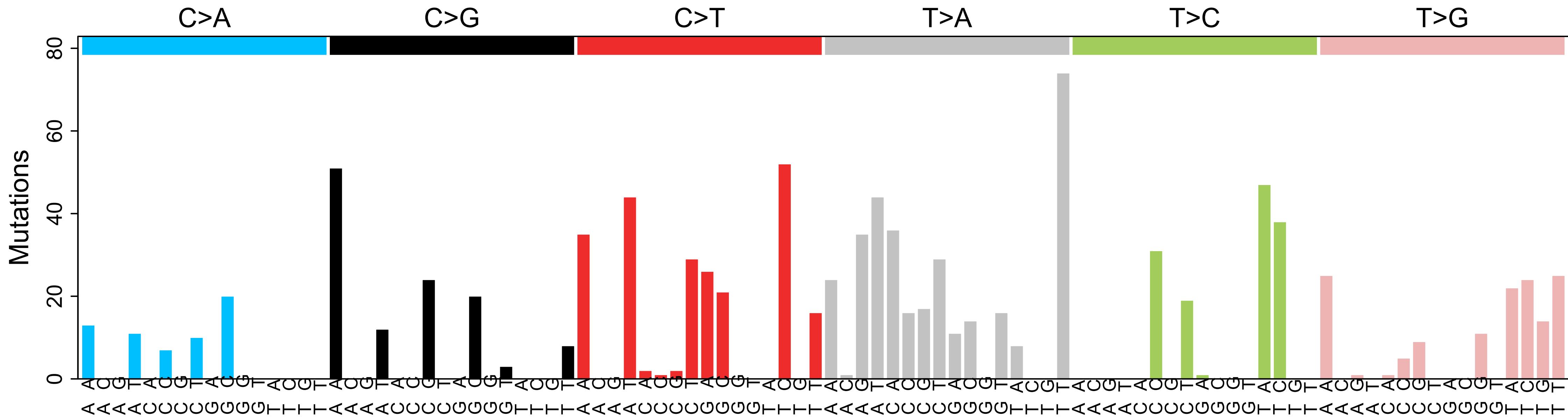
6_nitrochrysene_fd4adb4298d0 (1,002 mutations)



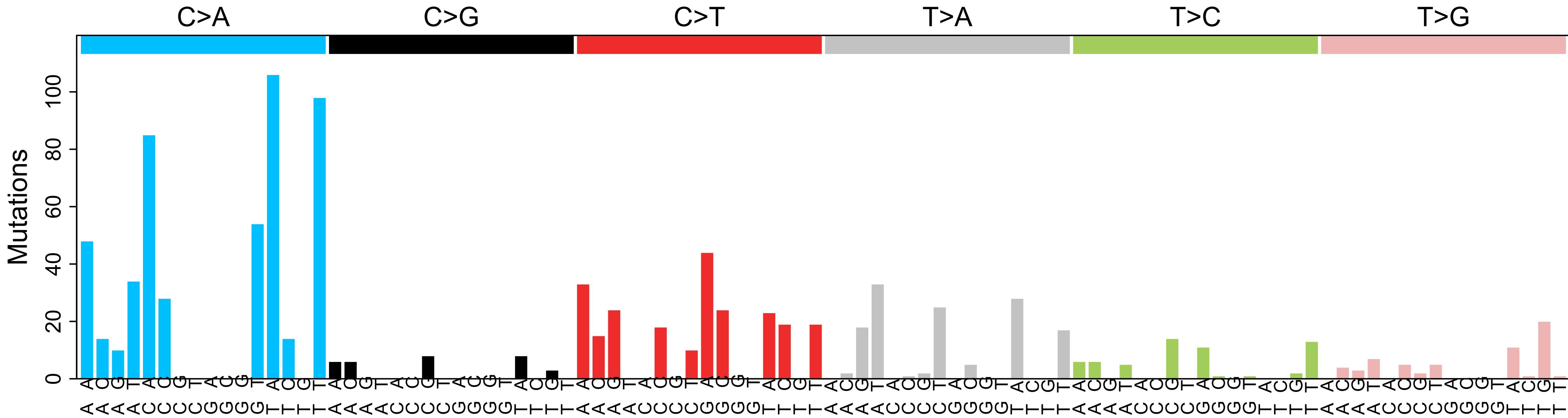
Reconstructed spectrum (cosine similarity = 0.867)



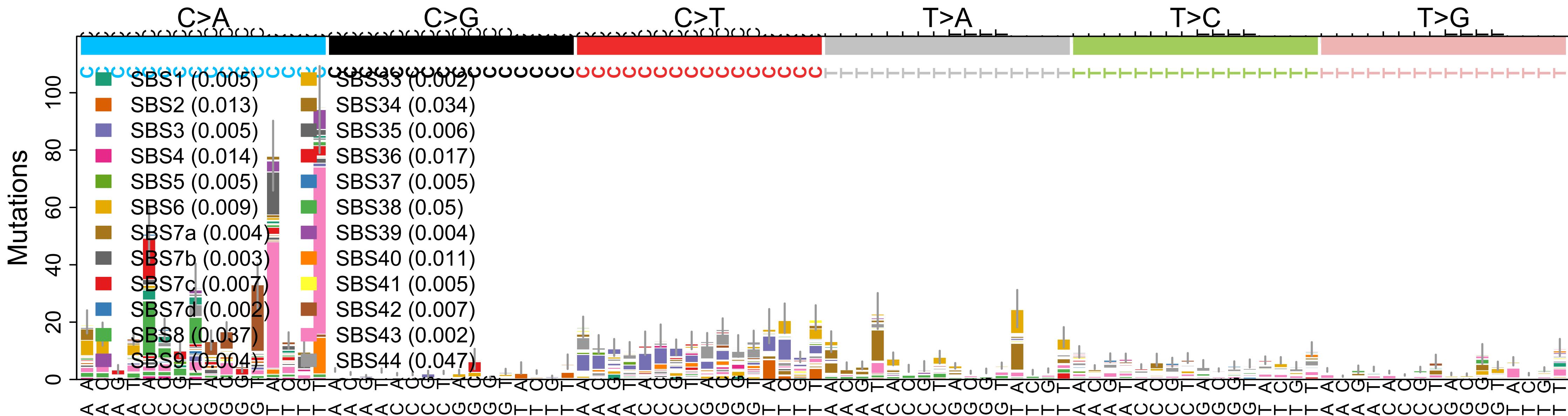
7h_dibenzoc_gcarbazole_af112efa14d2 (1,005 mutations)



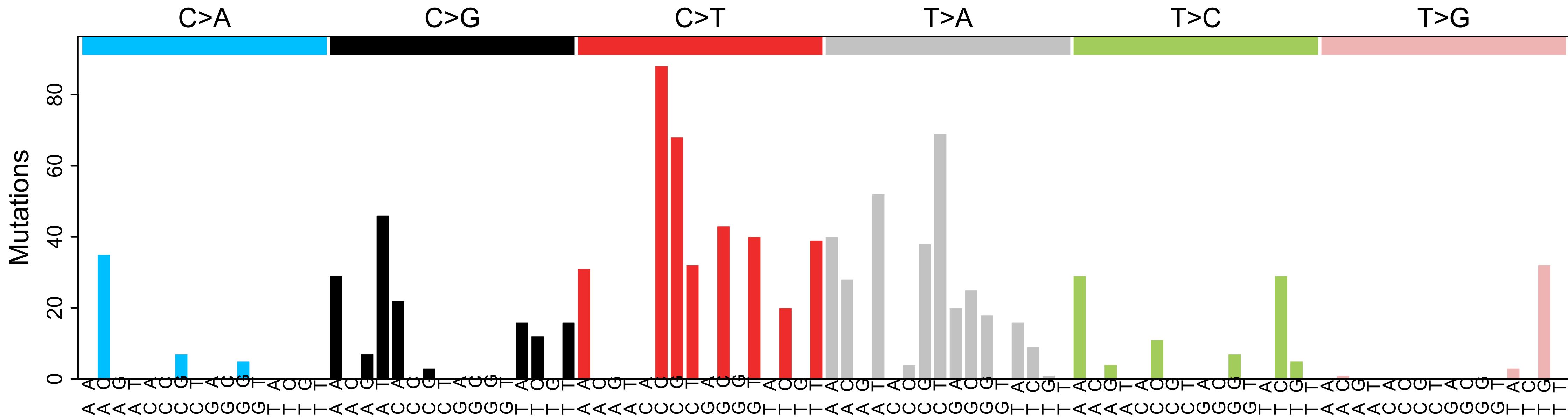
7h_dibenzoc_gcarbazole_b48114ea8899 (1,000 mutations)



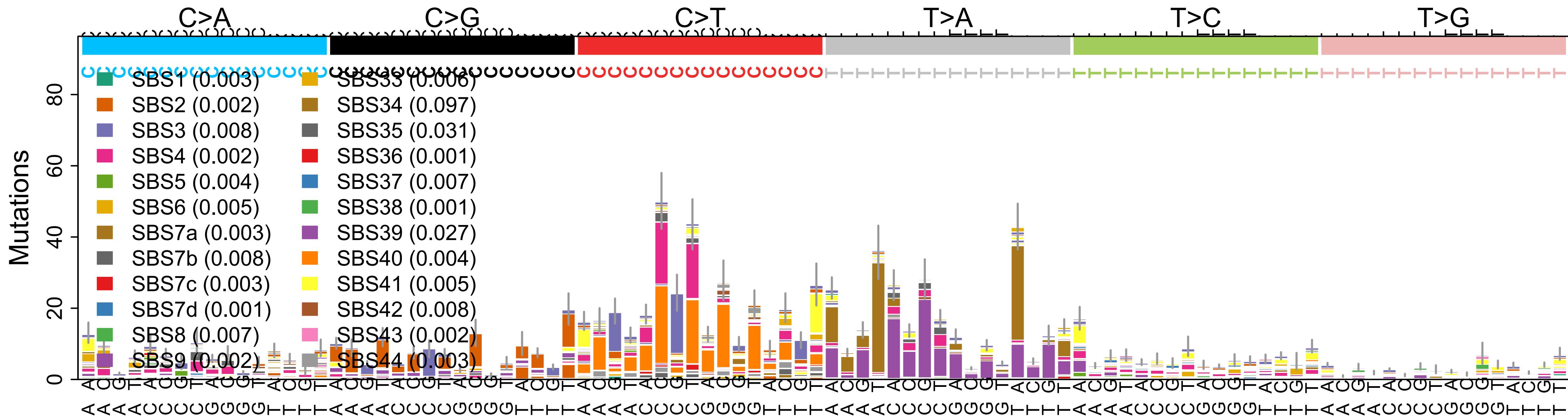
Reconstructed spectrum (cosine similarity = 0.896)



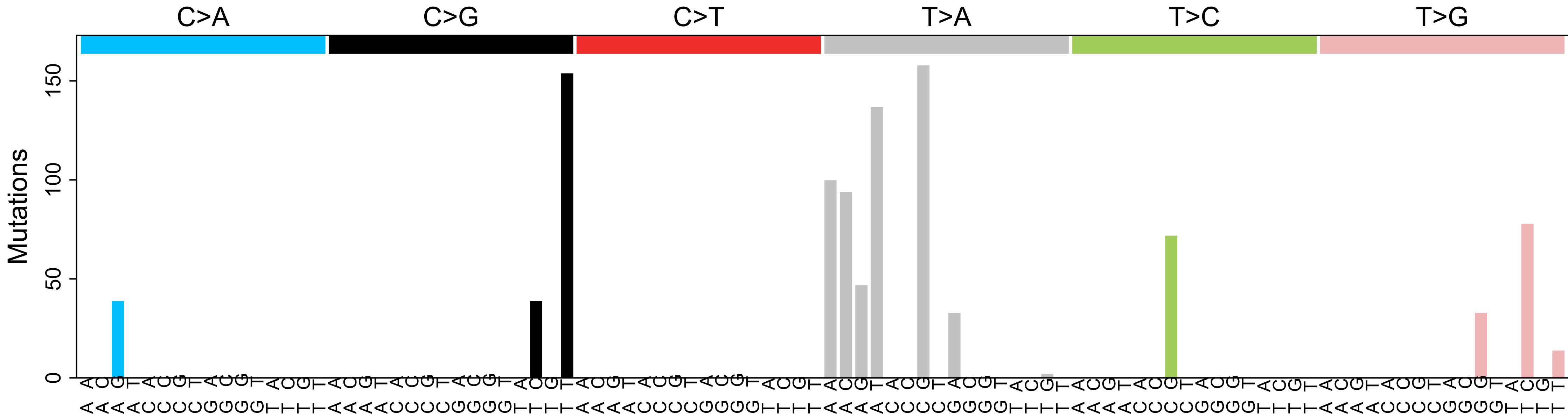
acetaldehyde_9fde73f6e508 (1,000 mutations)



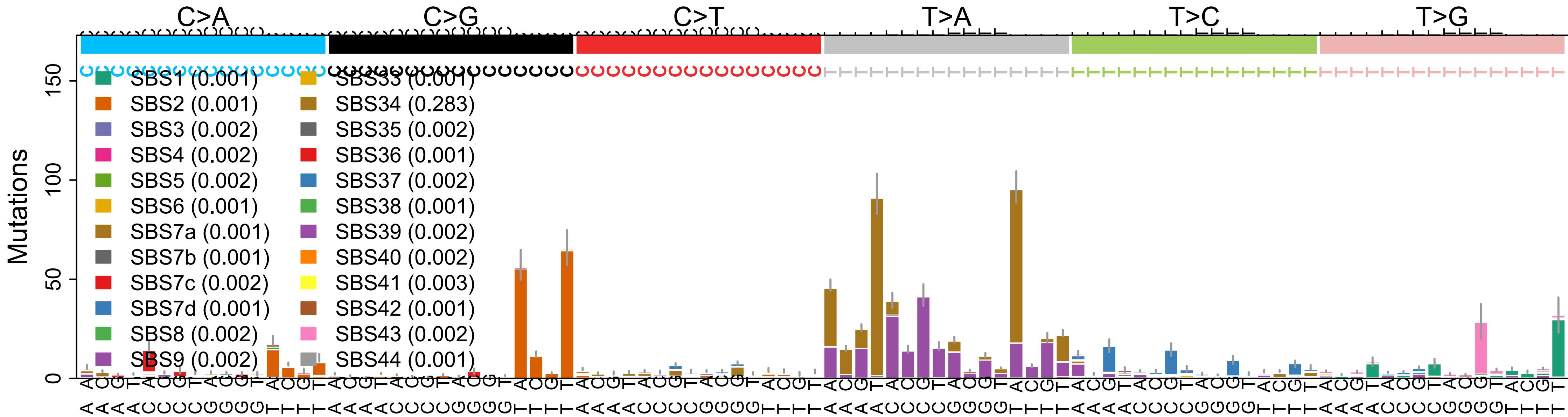
Reconstructed spectrum (cosine similarity = 0.75)



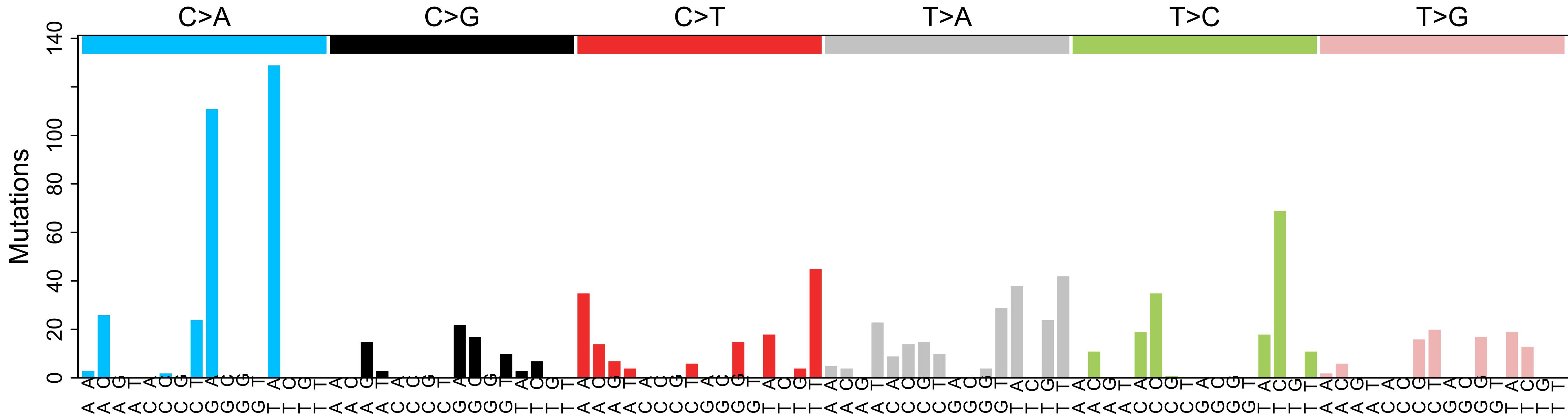
acrolein_7e28b8bb4834 (1,000 mutations)



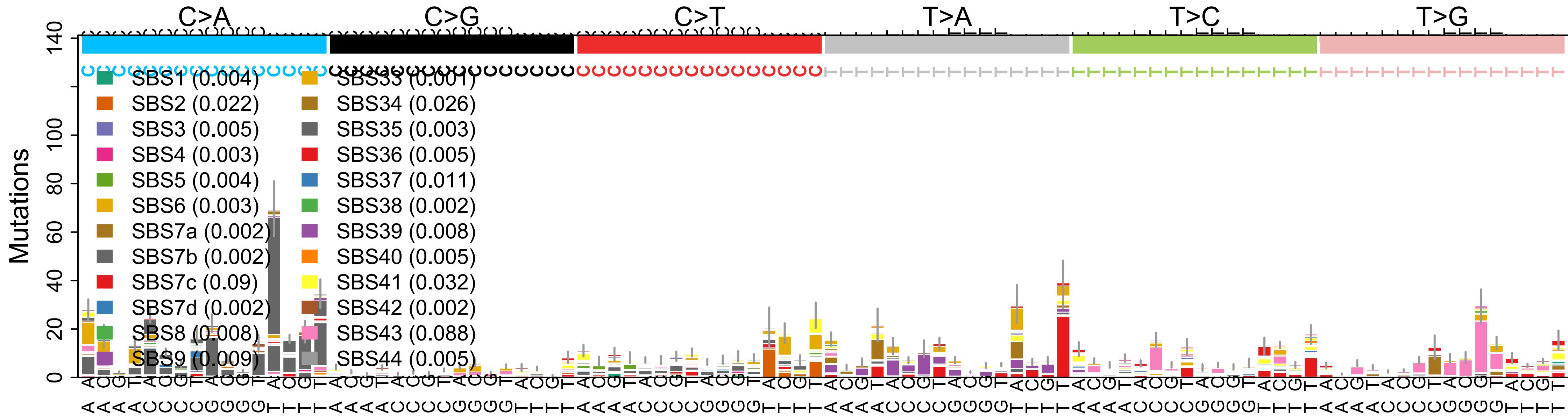
Reconstructed spectrum (cosine similarity = 0.642)



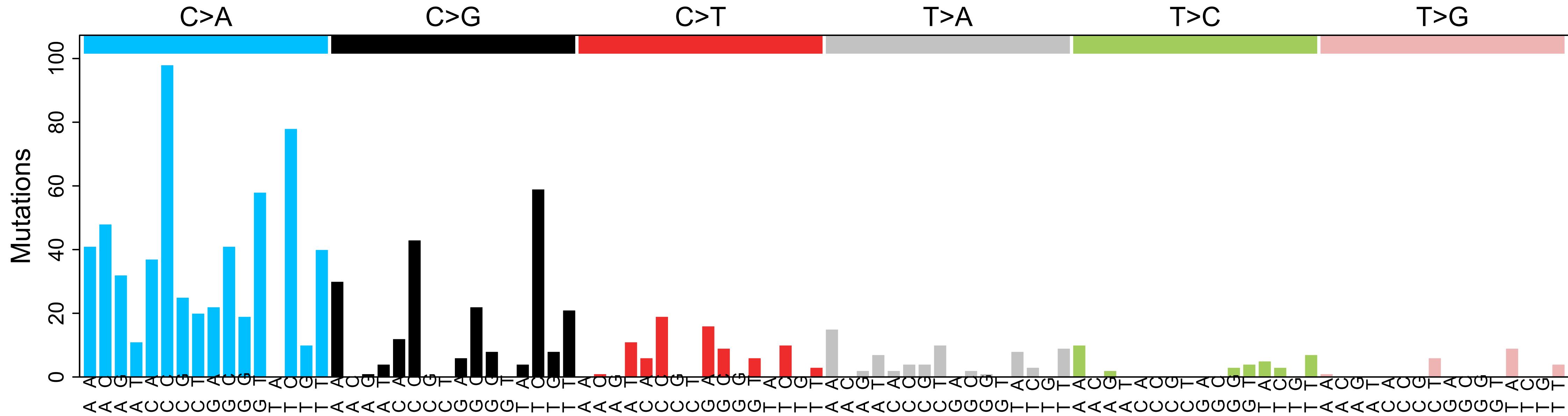
acrylamide_fc03d8ed1dc2 (994 mutations)



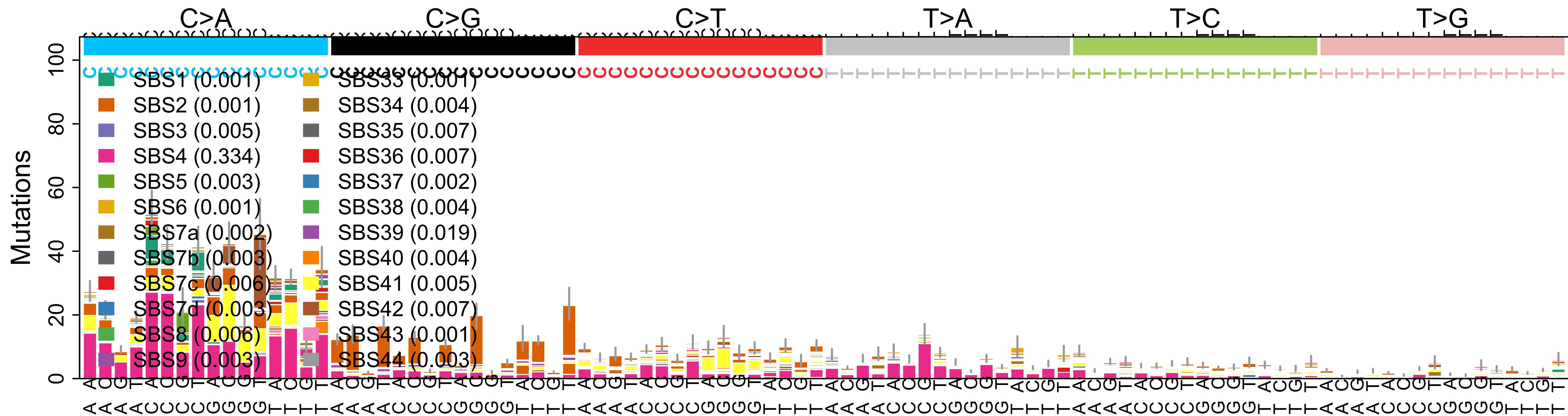
Reconstructed spectrum (cosine similarity = 0.717)



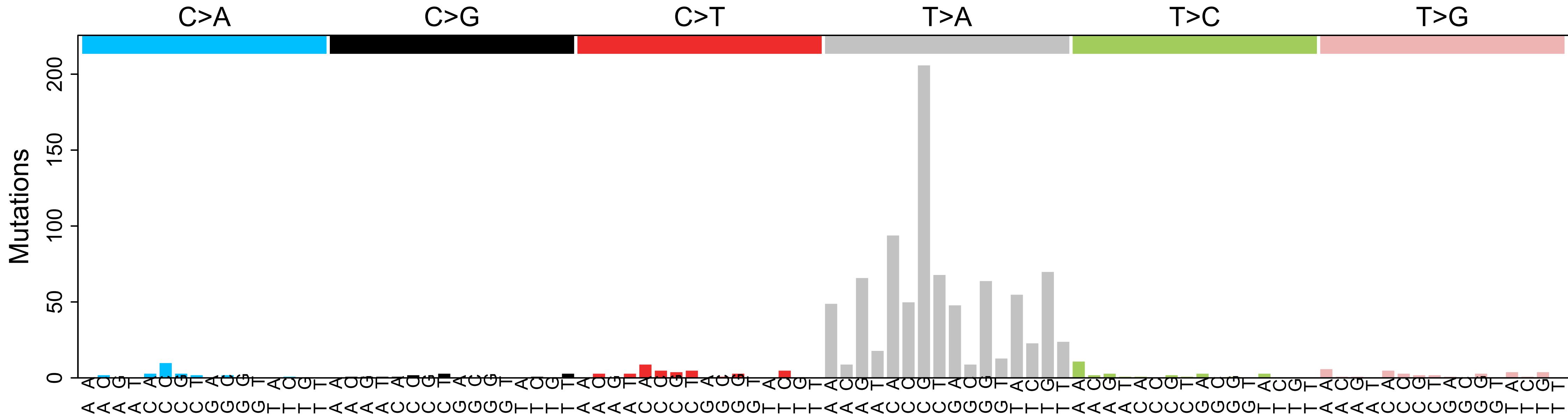
aflatoxin_b1_60c8b83450ec (1,000 mutations)



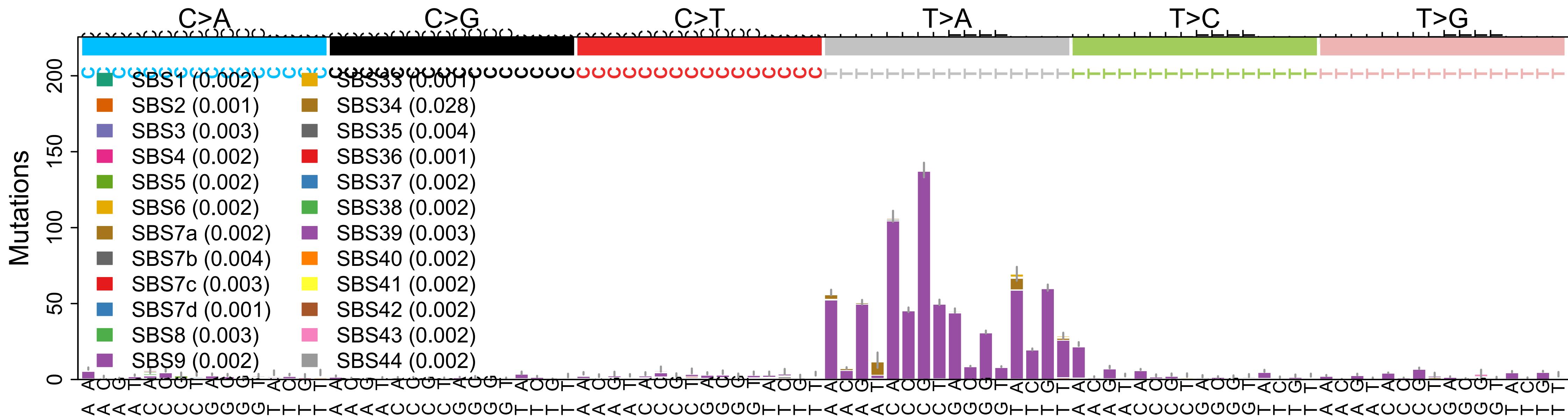
Reconstructed spectrum (cosine similarity = 0.808)



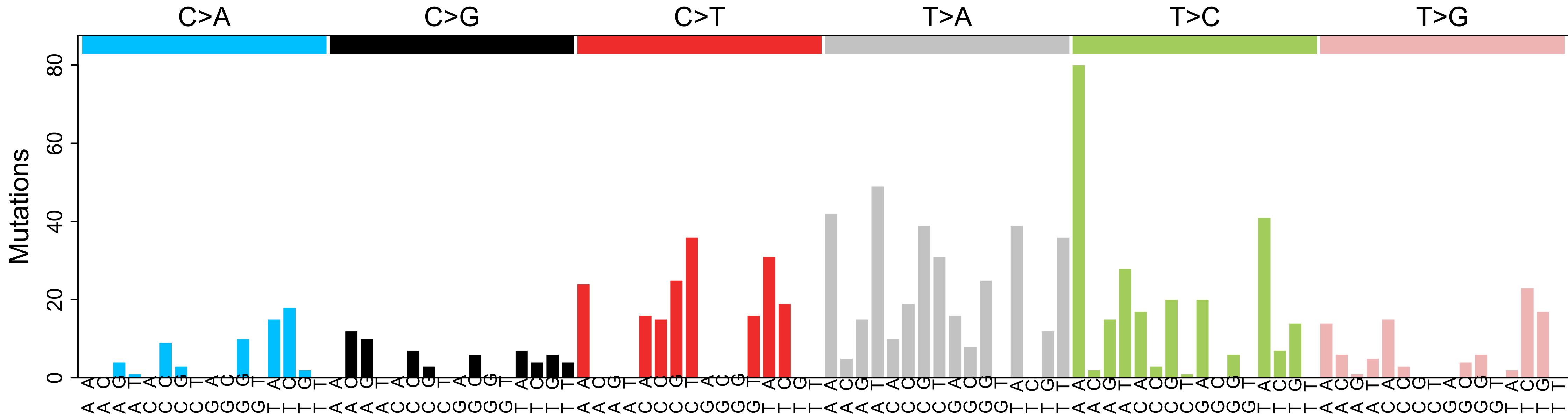
aristolochic_acid_i_b4173d75722f (1,001 mutations)



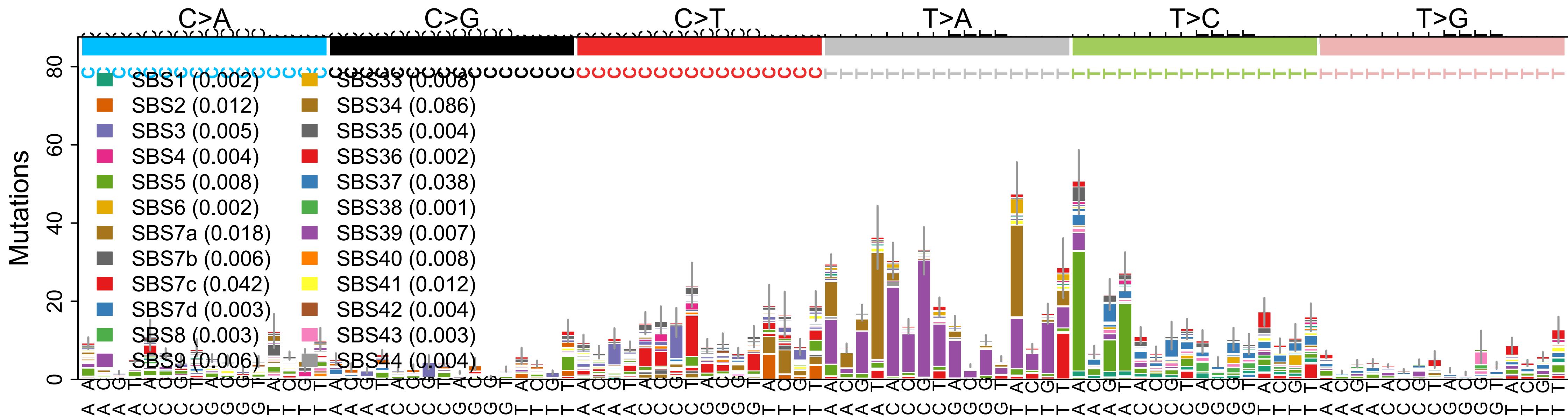
Reconstructed spectrum (cosine similarity = 0.963)



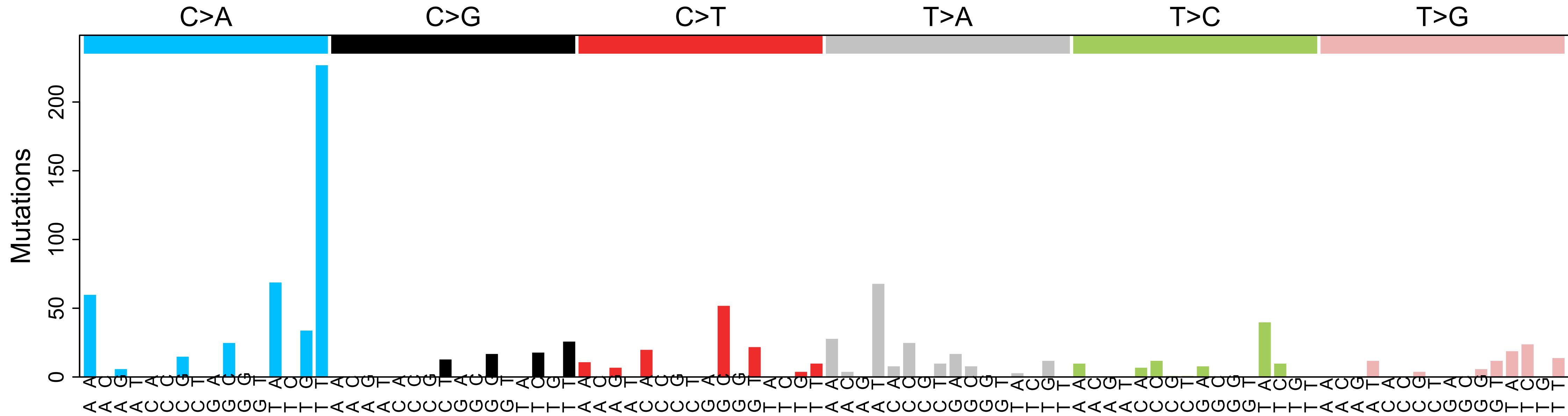
aristolochic_acid_ii_7cfb500c5521 (999 mutations)



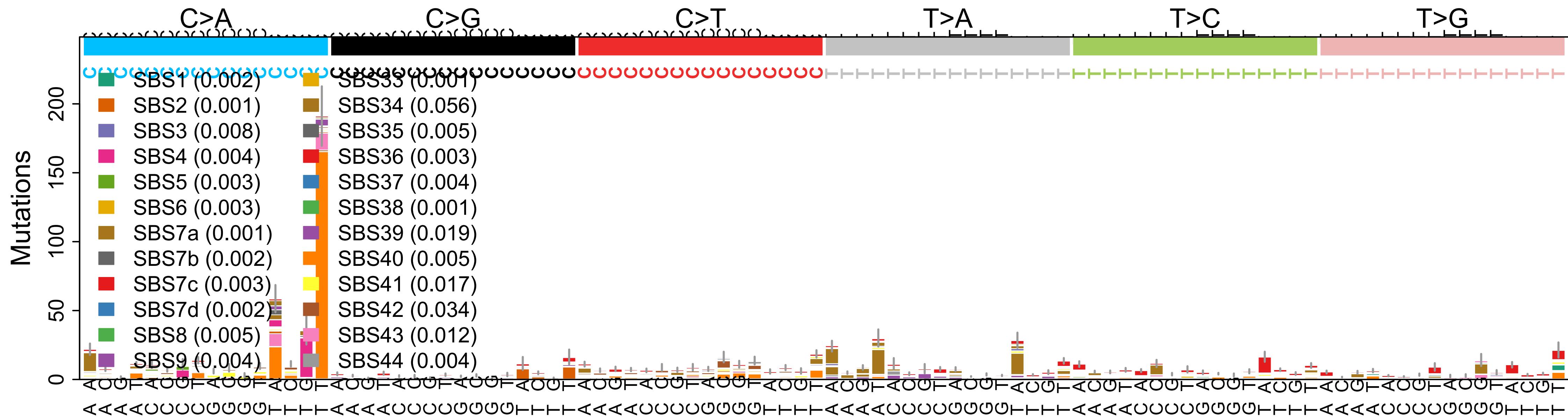
Reconstructed spectrum (cosine similarity = 0.868)



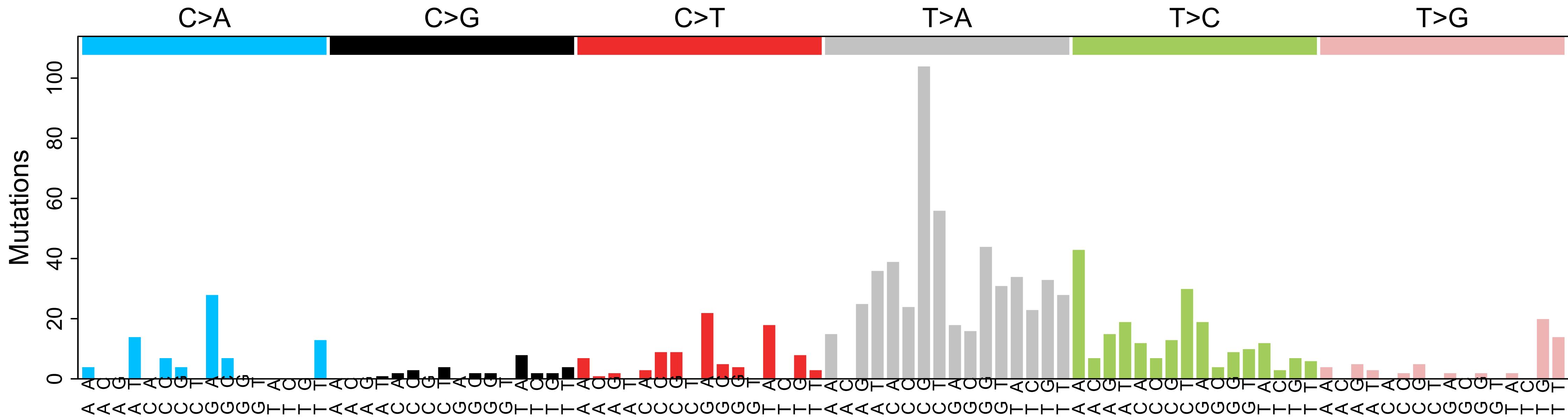
az20_e8f89cf2ec16 (999 mutations)



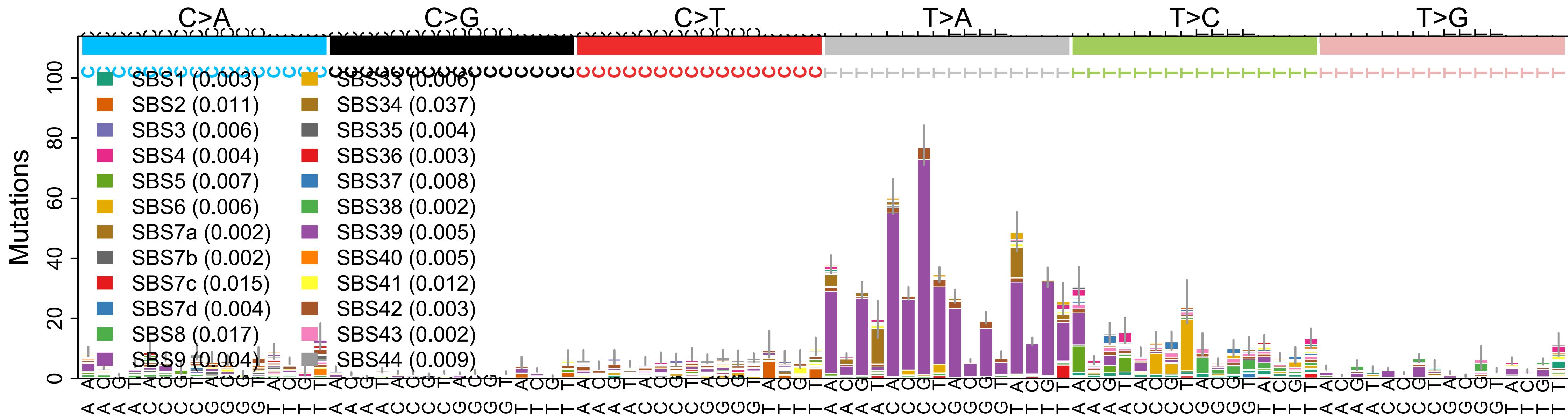
Reconstructed spectrum (cosine similarity = 0.929)



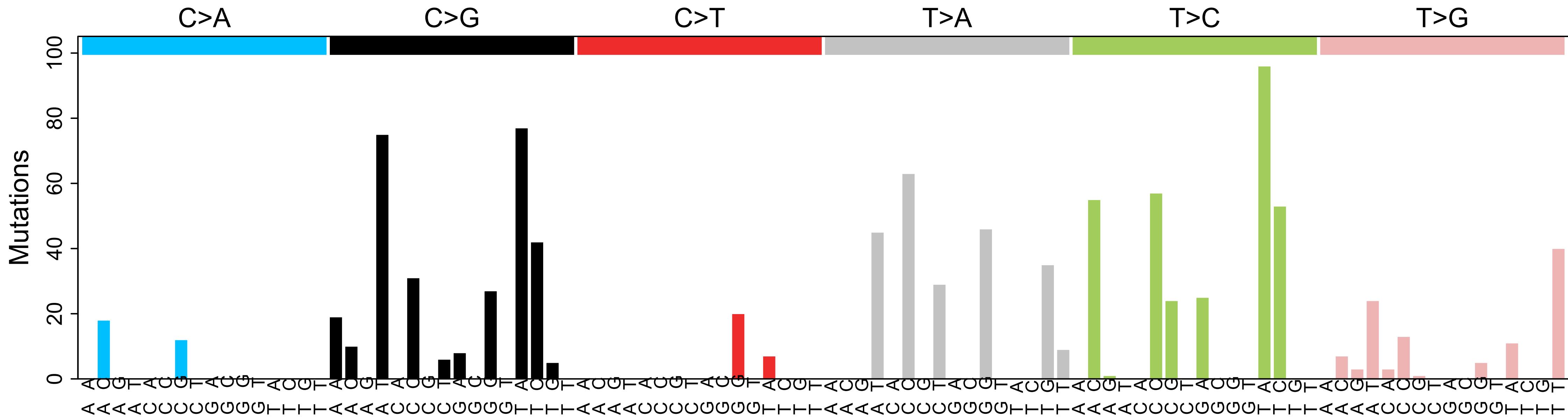
azd7762_c62b92e2486a (999 mutations)



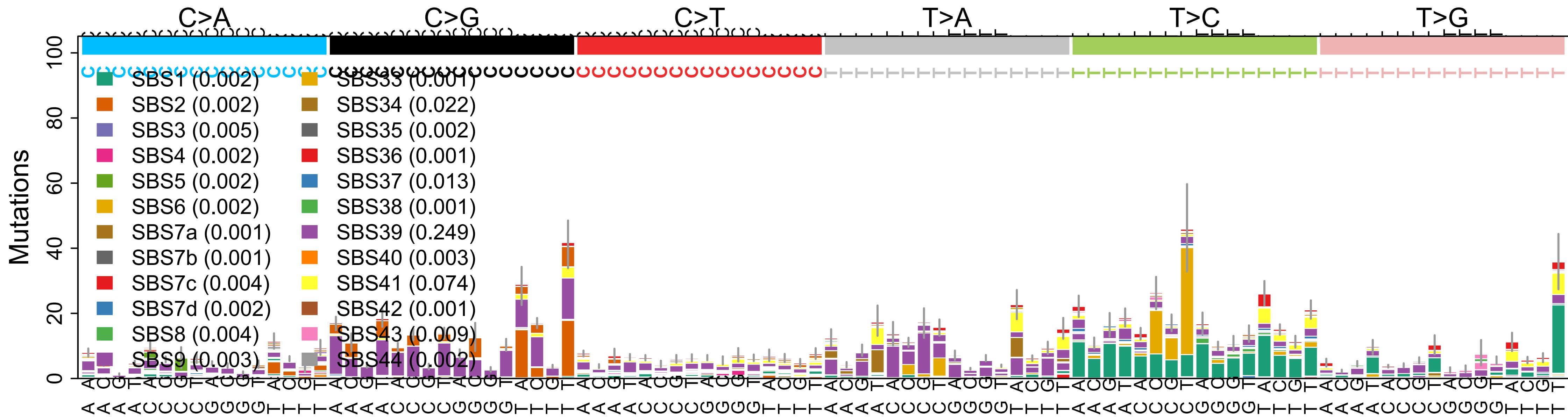
Reconstructed spectrum (cosine similarity = 0.9)



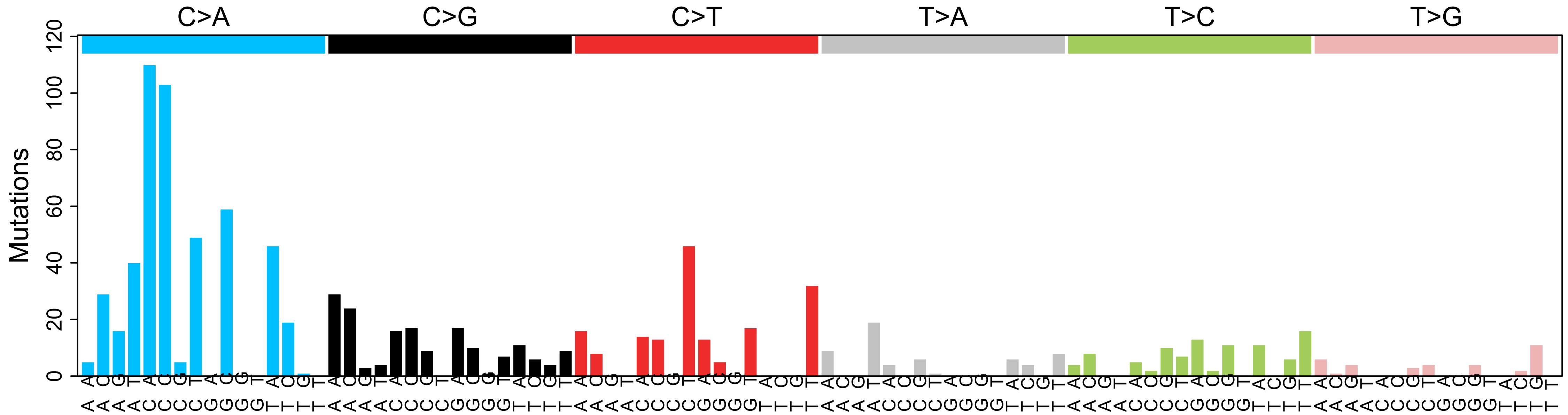
benzidine_5b2123a8cf0e (1,002 mutations)



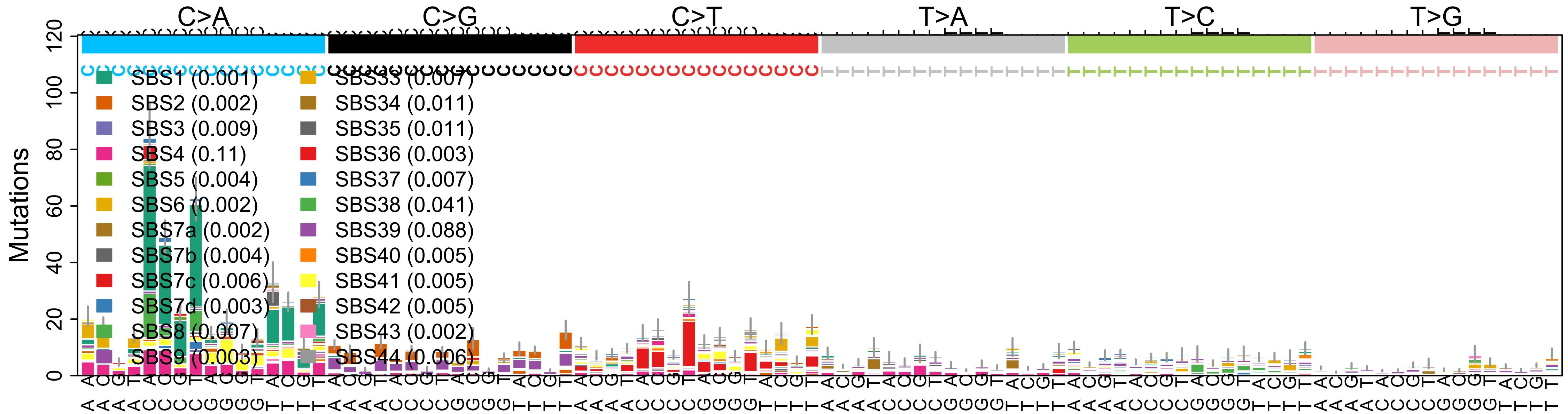
Reconstructed spectrum (cosine similarity = 0.582)



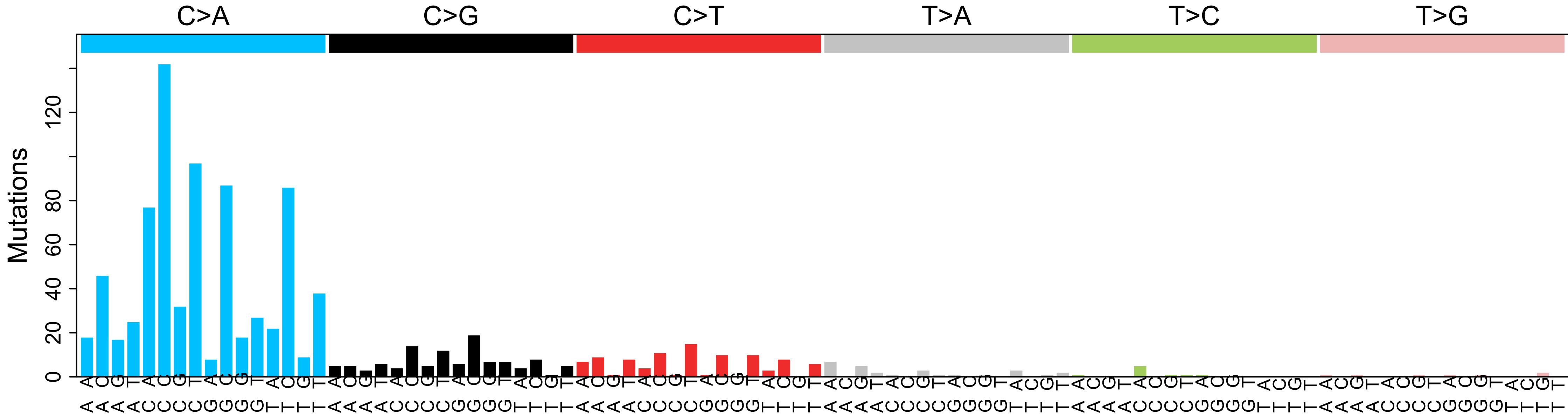
benzidine_6c3042d3a0b5 (1,000 mutations)



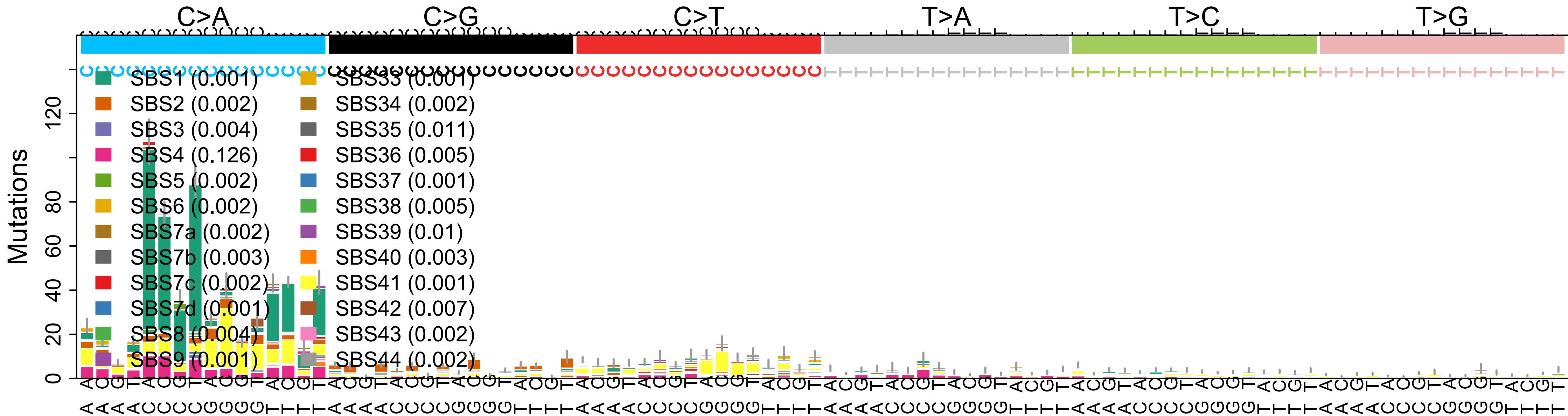
Reconstructed spectrum (cosine similarity = 0.859)



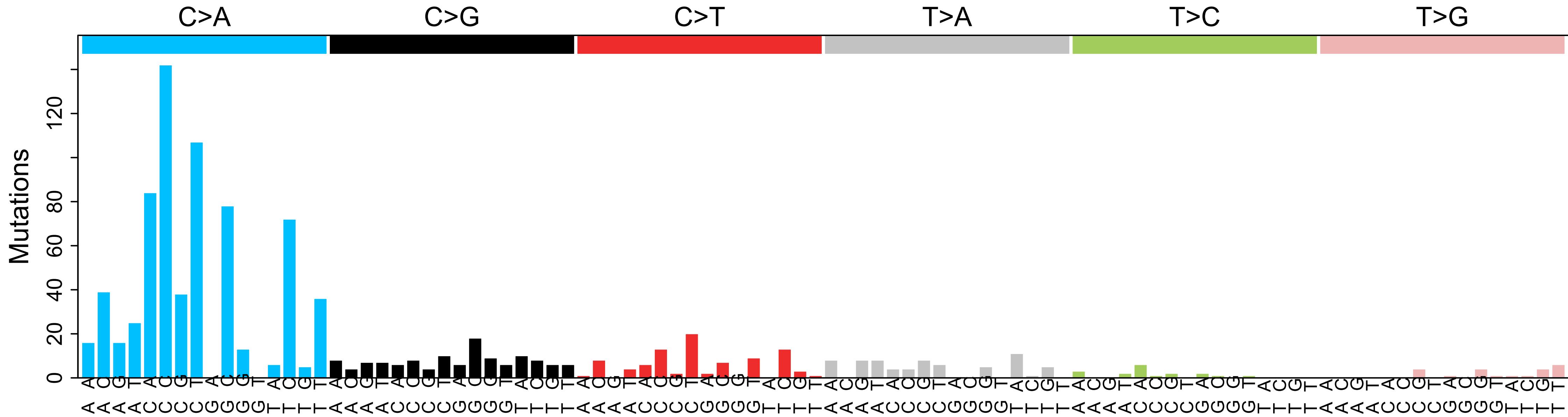
benzoapyrene_7_8_diol_9_10_epoxide_a940ded66b4f (997 mutations)



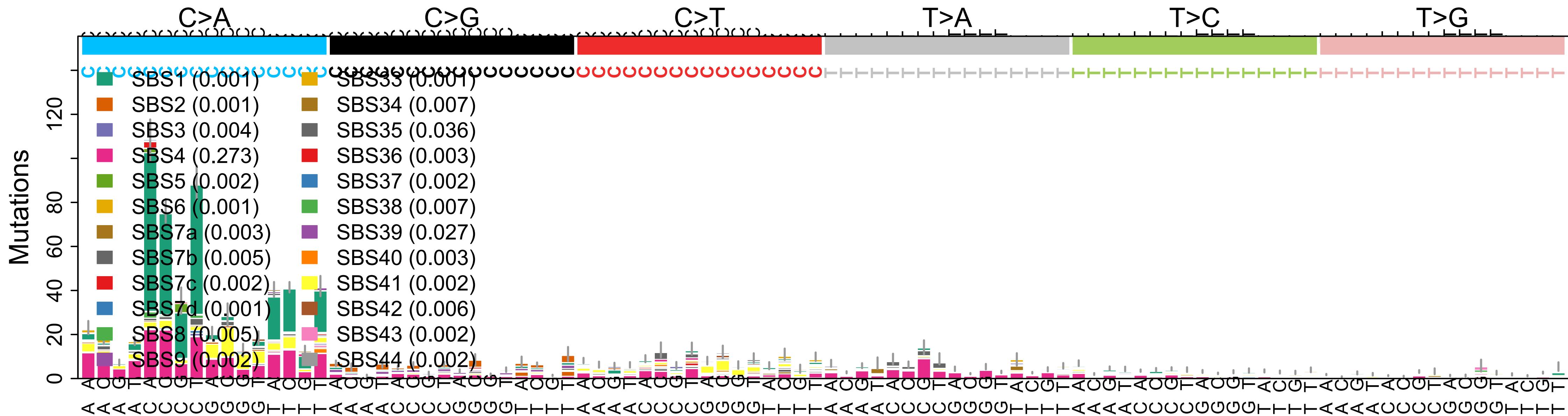
Reconstructed spectrum (cosine similarity = 0.894)



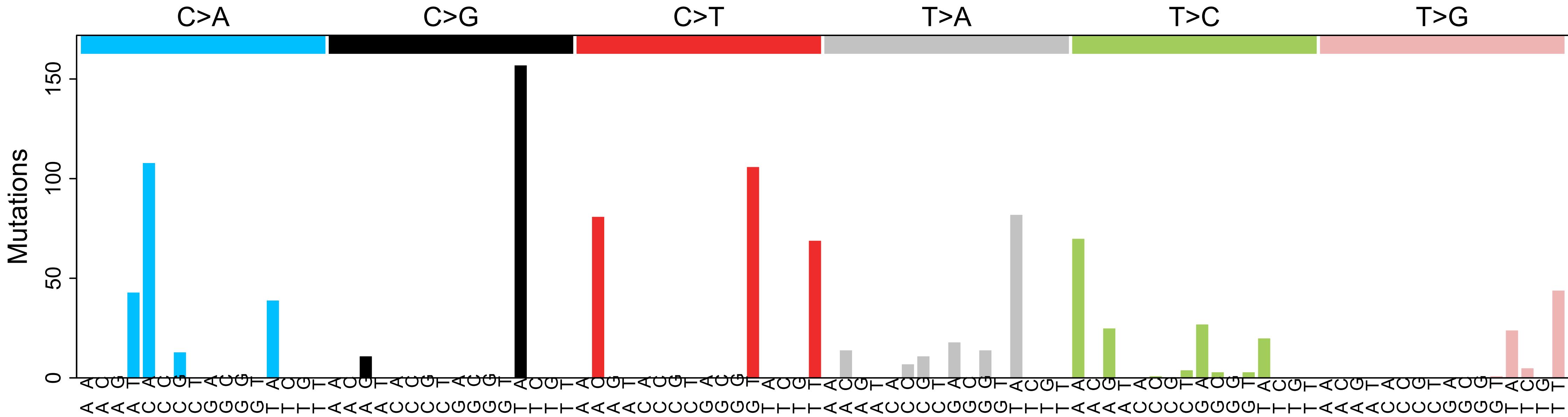
benzoapyrene_b931a8be44c3 (997 mutations)



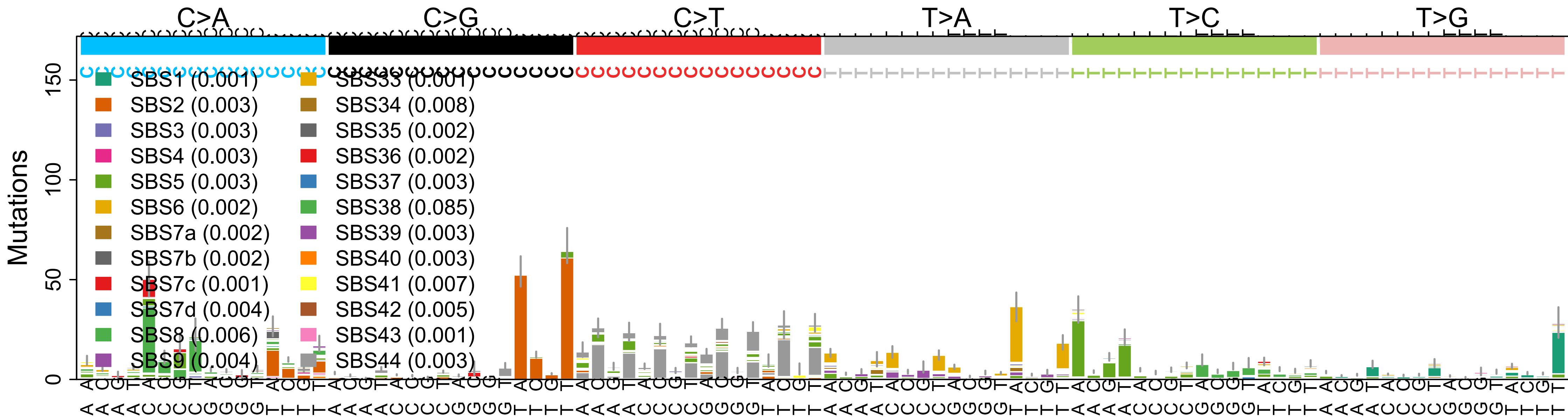
Reconstructed spectrum (cosine similarity = 0.893)



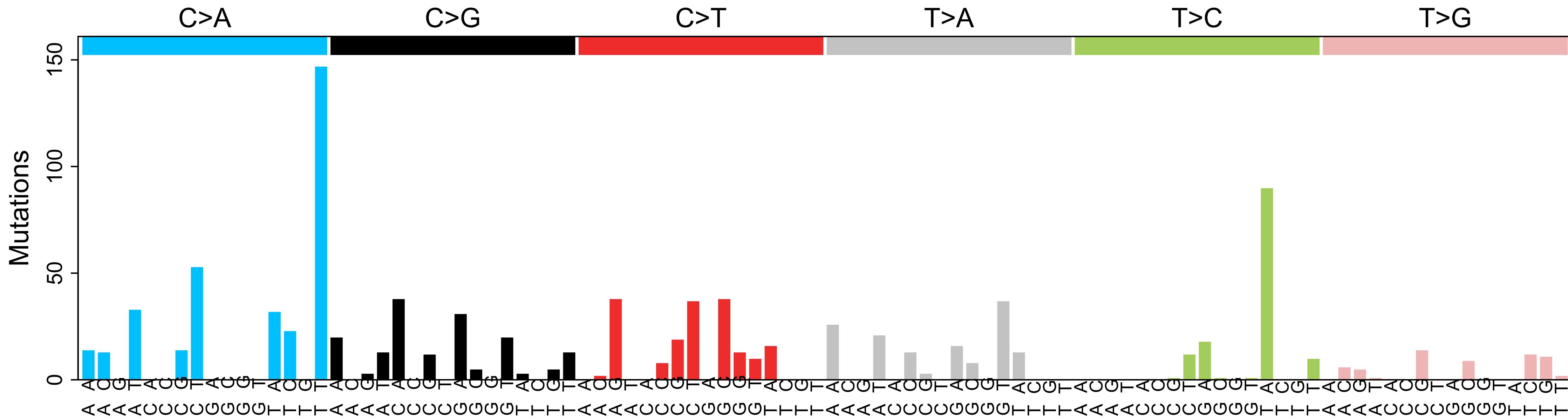
bleomycin_a07bf993a1cf (1,000 mutations)



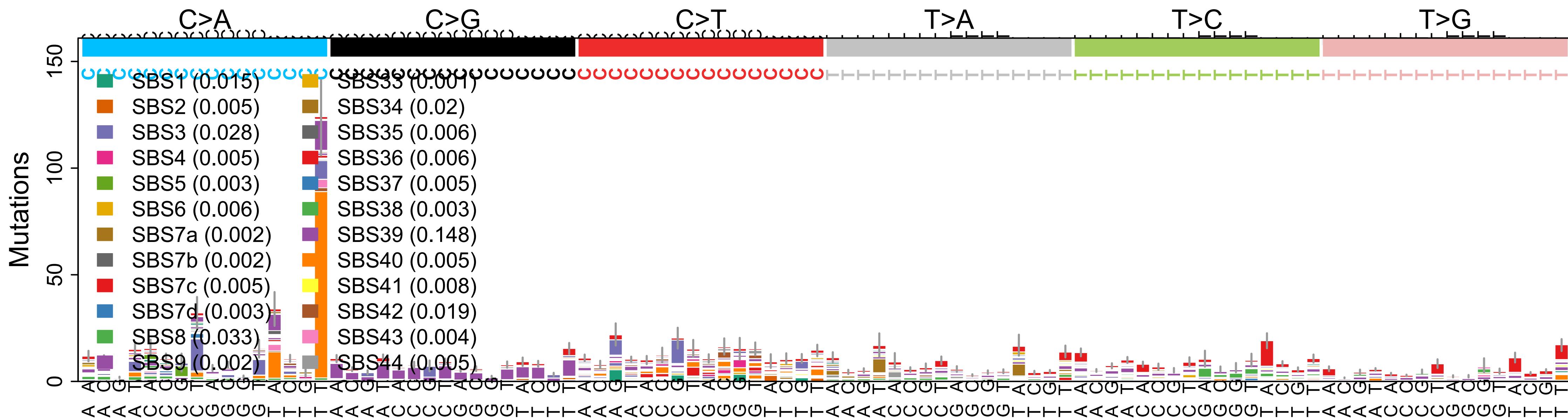
Reconstructed spectrum (cosine similarity = 0.69)



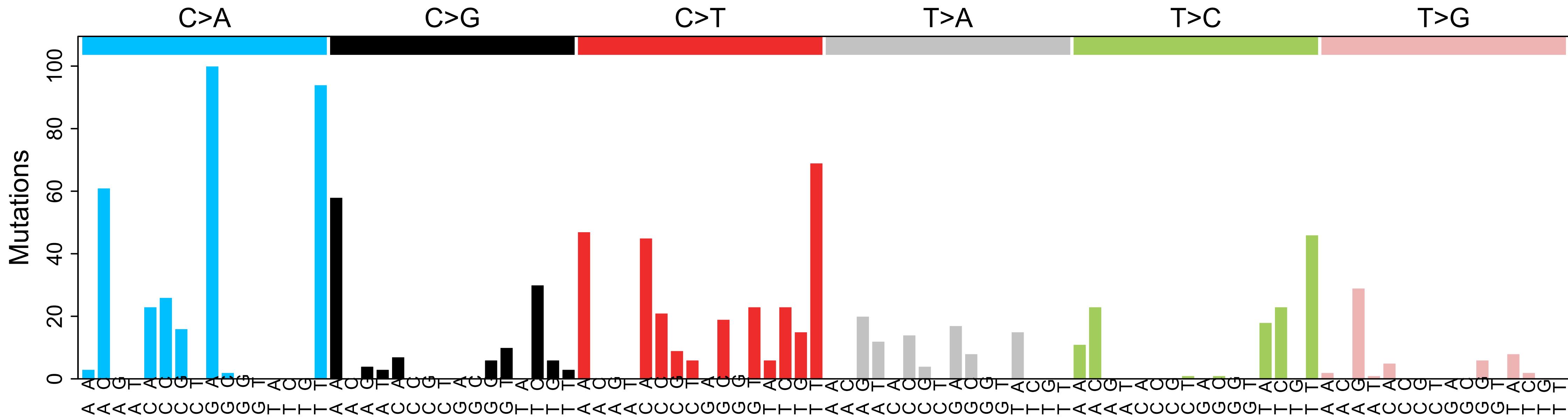
cadmium_chloride_4e155105529e (1,003 mutations)



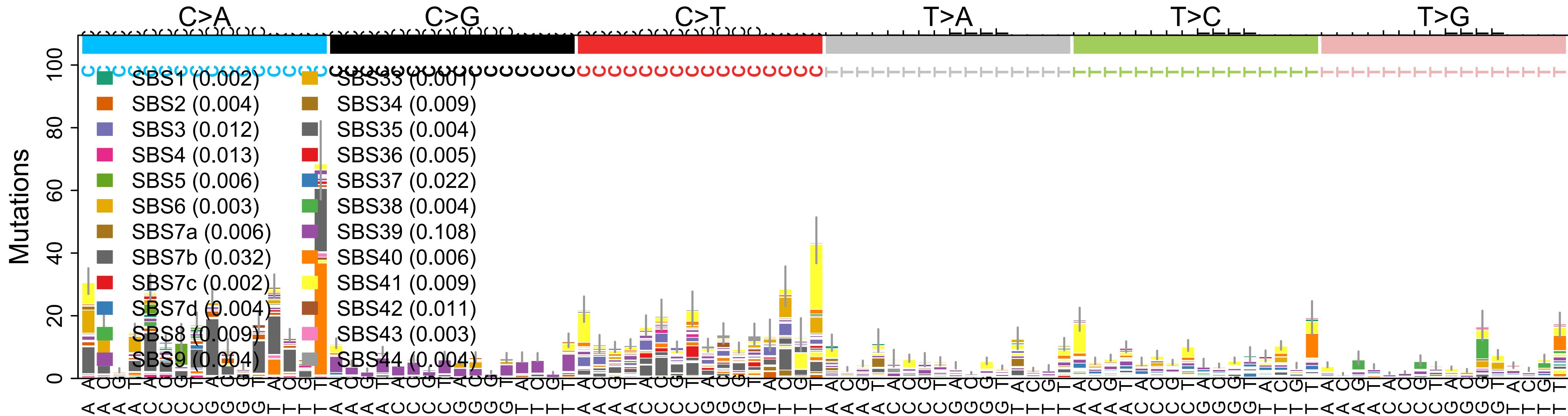
Reconstructed spectrum (cosine similarity = 0.836)



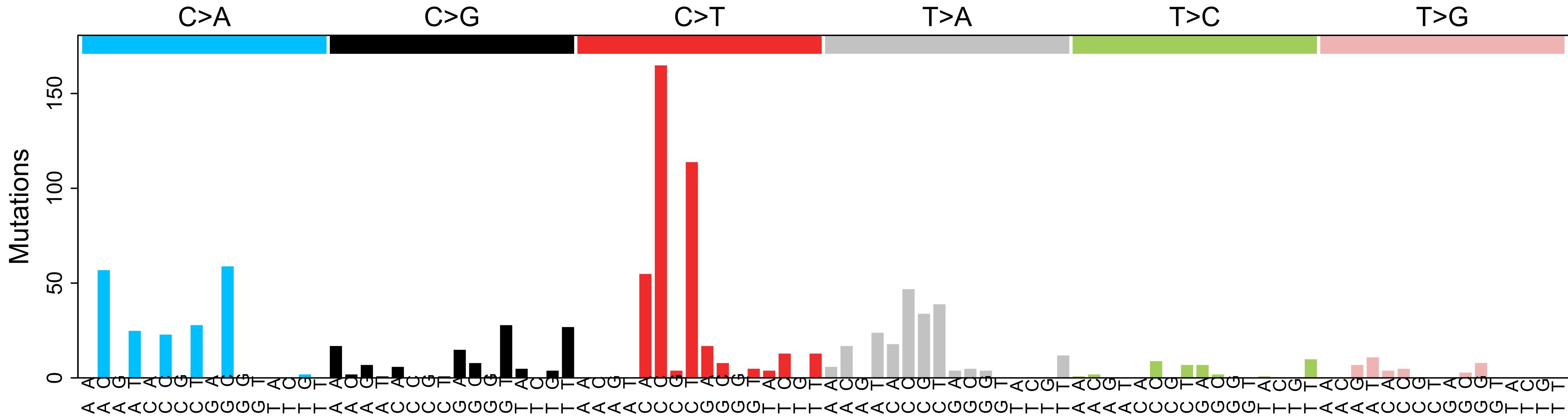
camptothecin_035f5ec44026 (1,001 mutations)



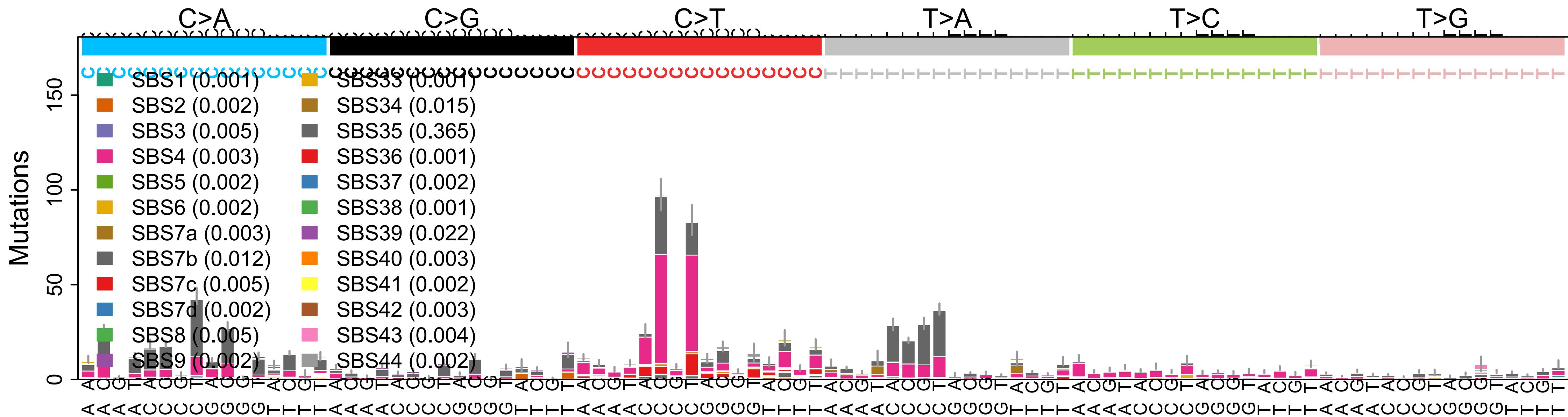
Reconstructed spectrum (cosine similarity = 0.735)



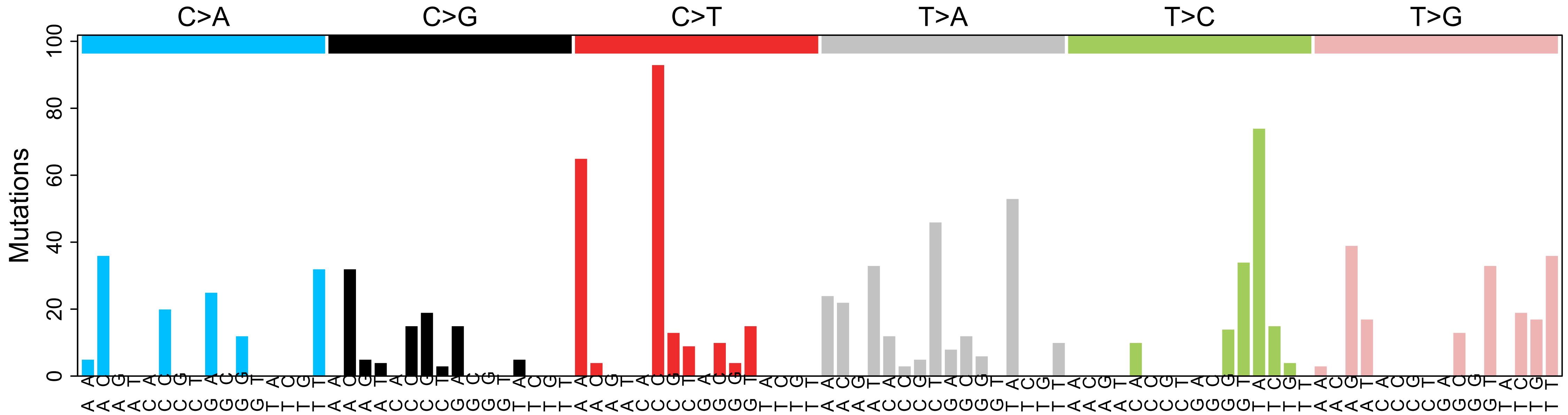
carboplatin_87107e8f10fc (1,001 mutations)



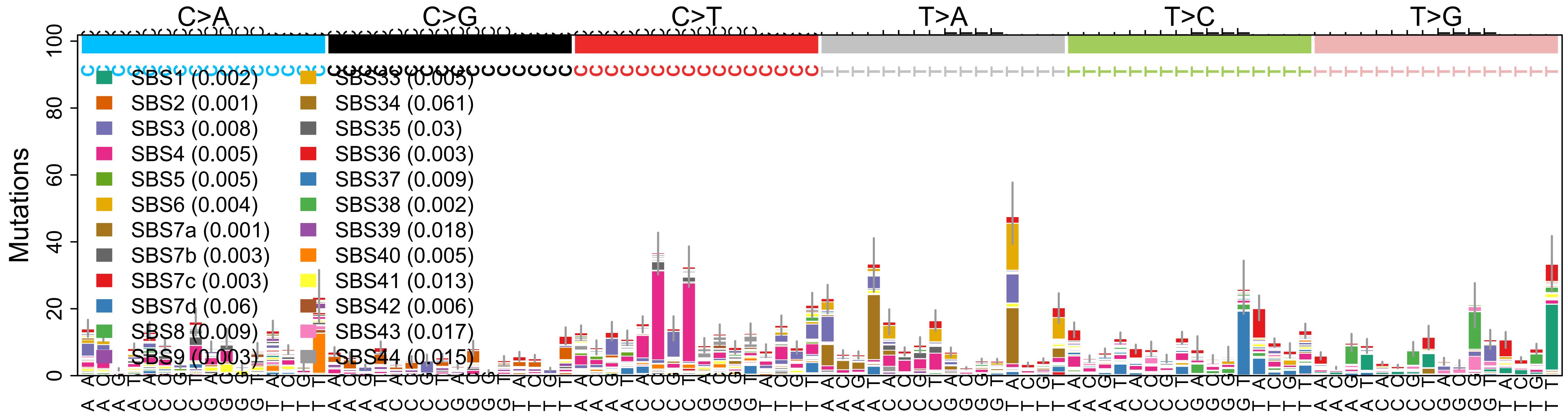
Reconstructed spectrum (cosine similarity = 0.91)



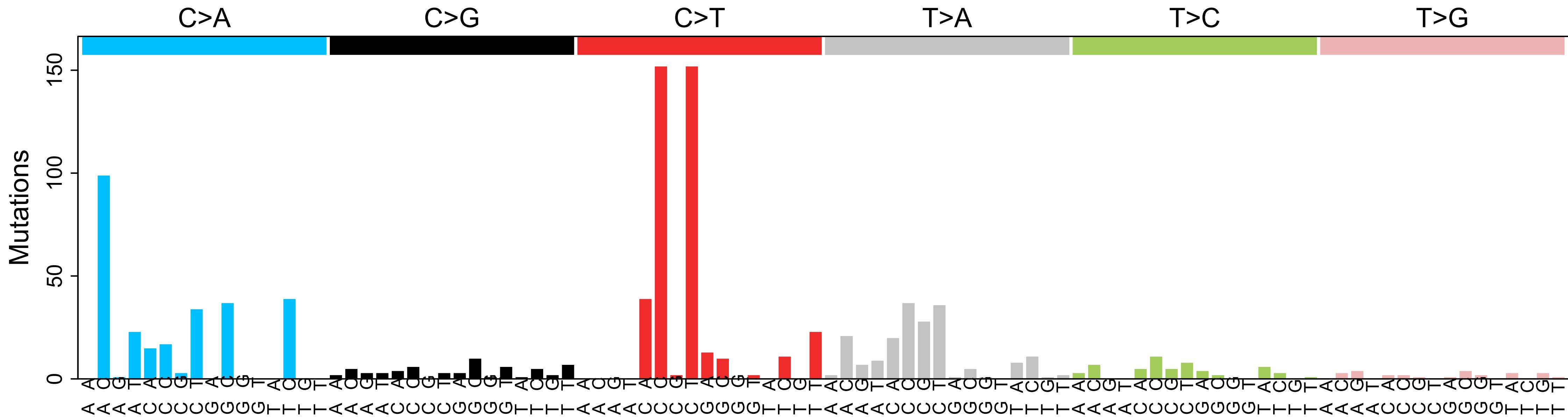
catechol_c6f4cfad7d77 (1,003 mutations)



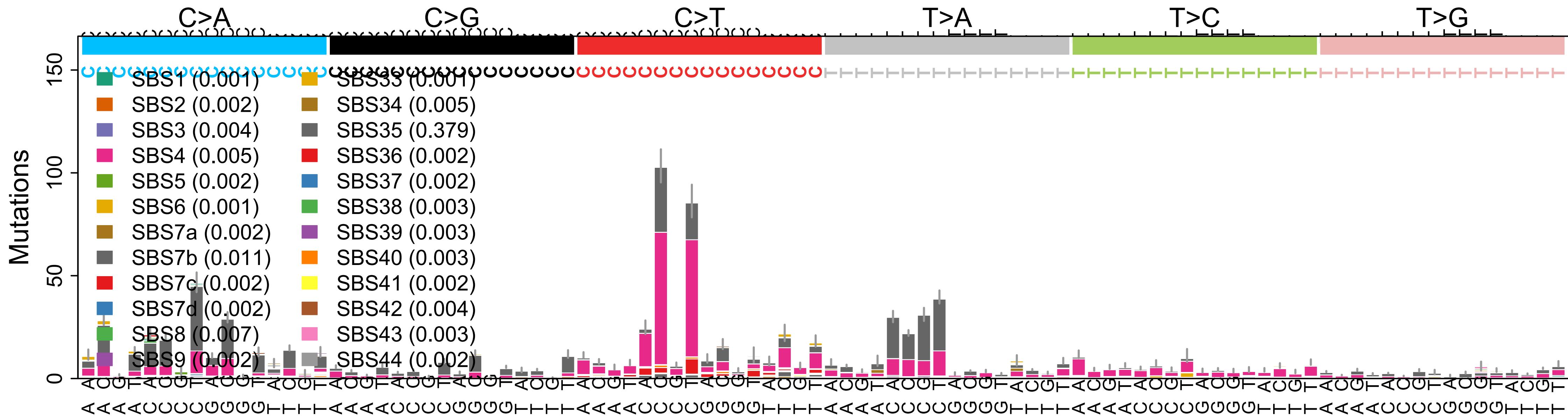
Reconstructed spectrum (cosine similarity = 0.703)



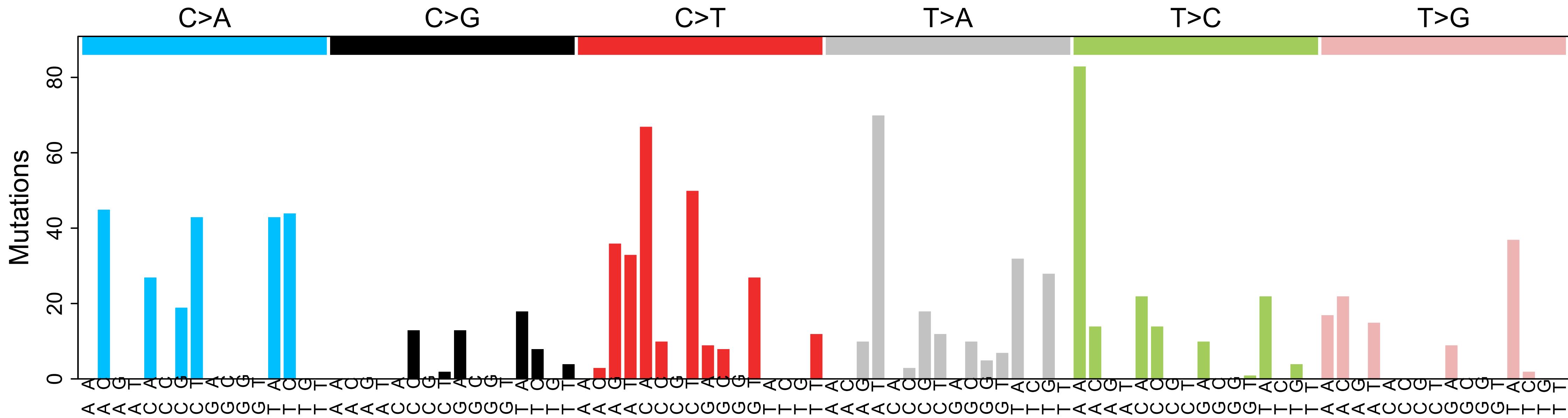
cisplatin_92bd8426ea0e (1,003 mutations)



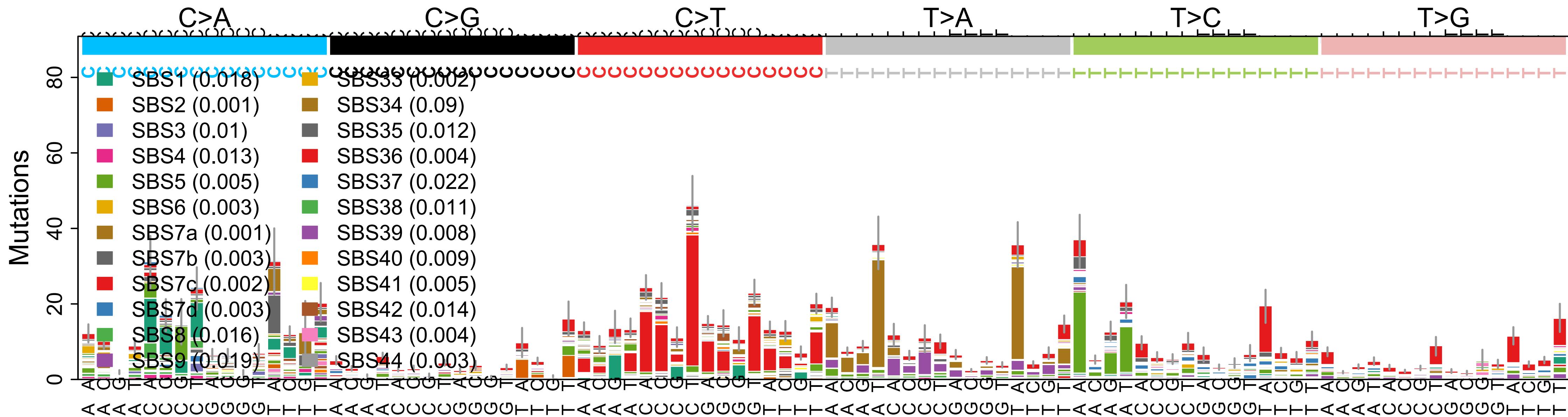
Reconstructed spectrum (cosine similarity = 0.91)



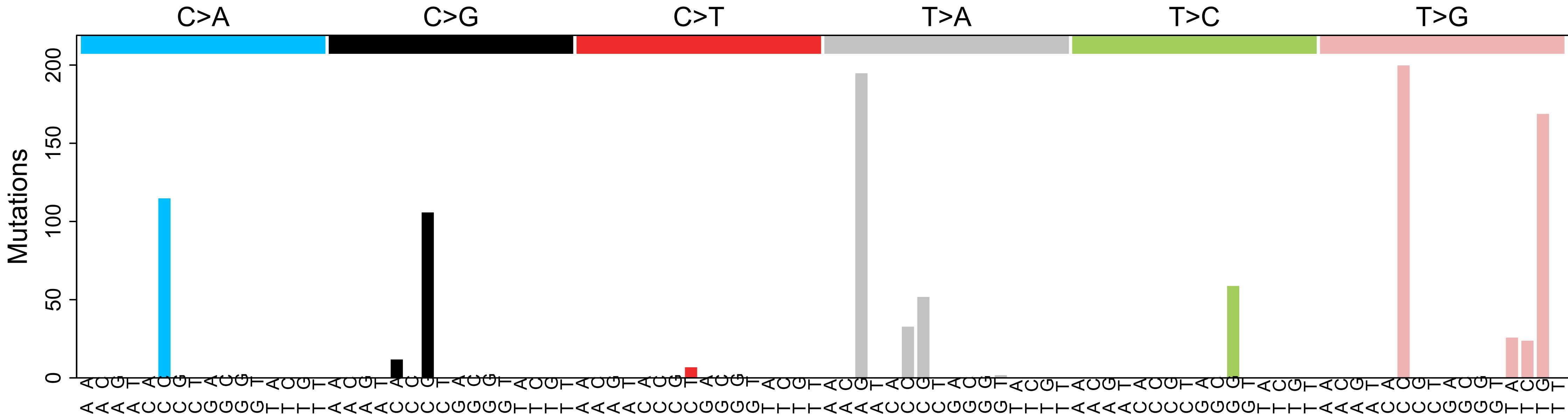
cobalt_chloride_a9e31bc7a88c (1,001 mutations)



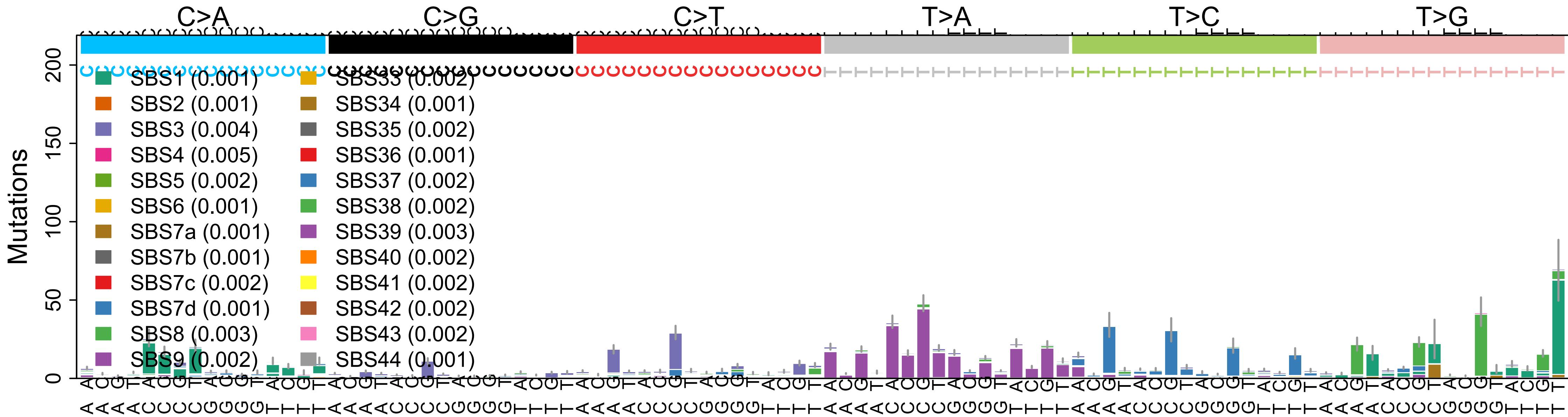
Reconstructed spectrum (cosine similarity = 0.766)



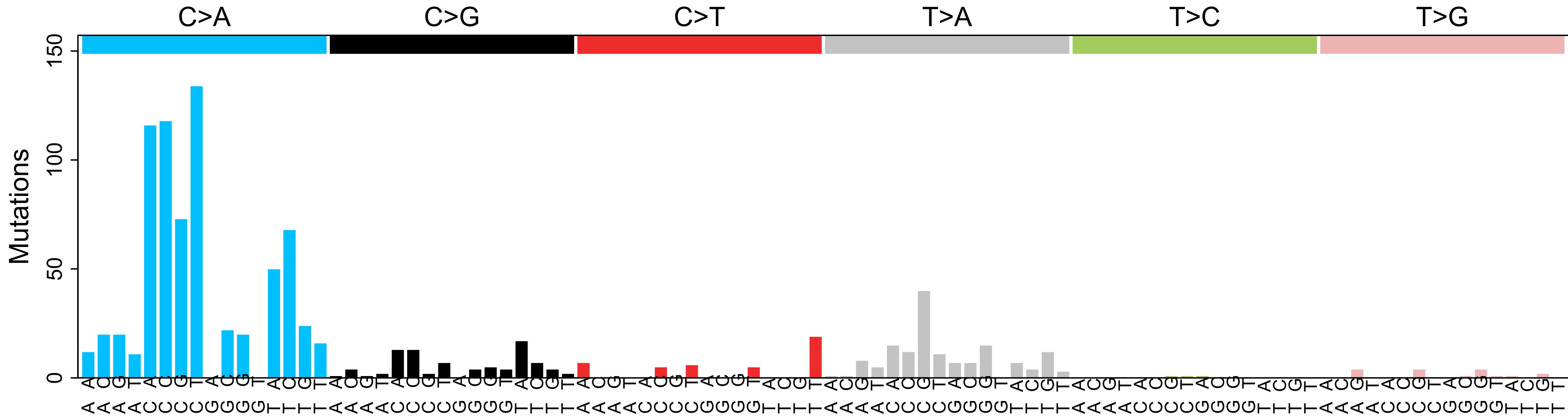
cyclophosphamide_557117b73fe2 (1,000 mutations)



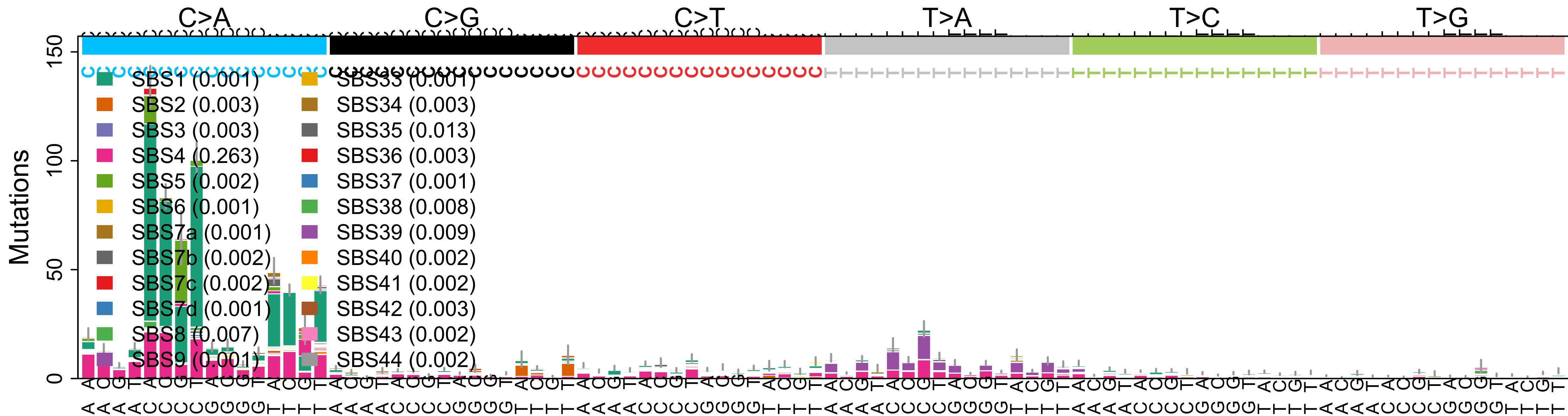
Reconstructed spectrum (cosine similarity = 0.276)



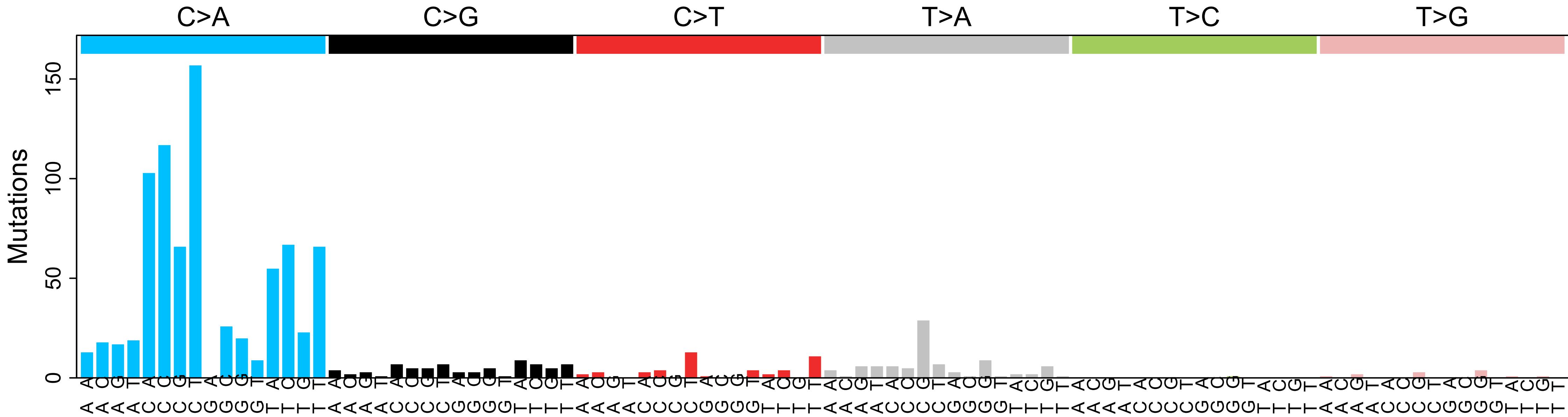
dibenzo_hanthracene_86a56a54eba1 (1,000 mutations)



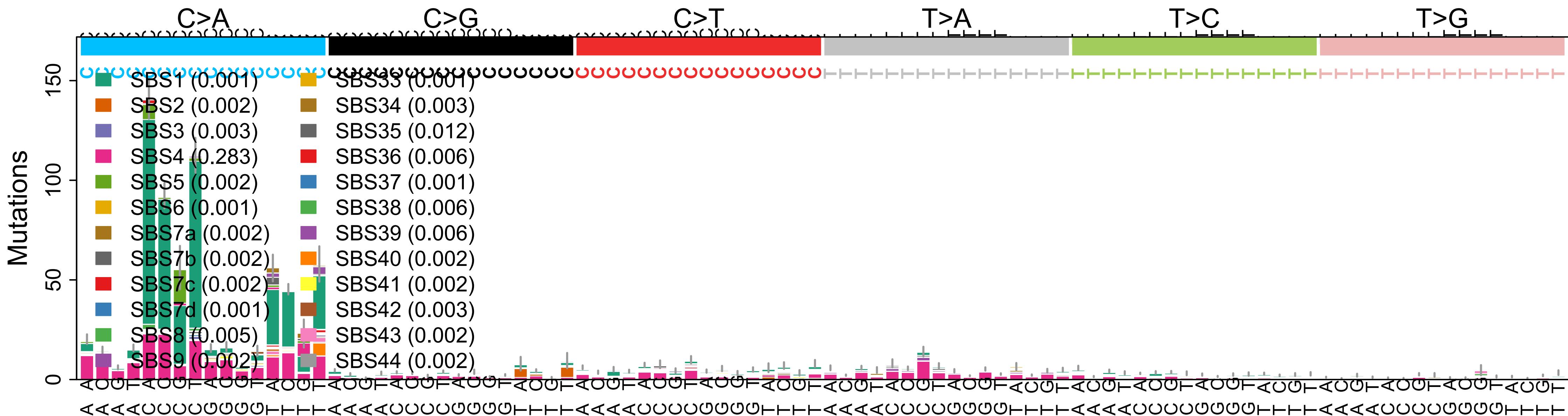
Reconstructed spectrum (cosine similarity = 0.951)



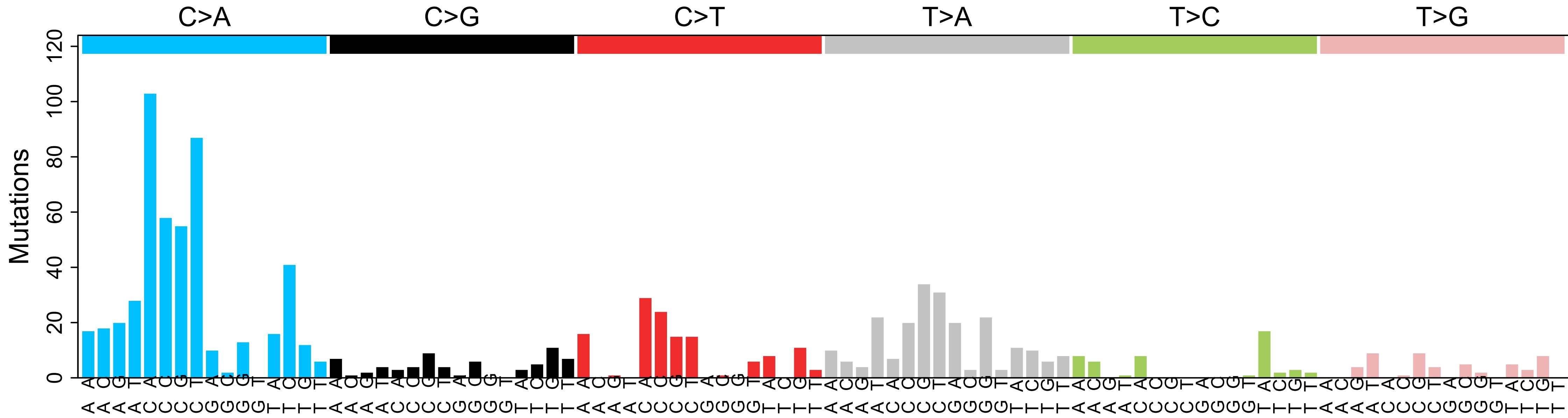
dibenzo_hanthracene_diol_epoxide_d1c39f8181d9 (999 mutations)



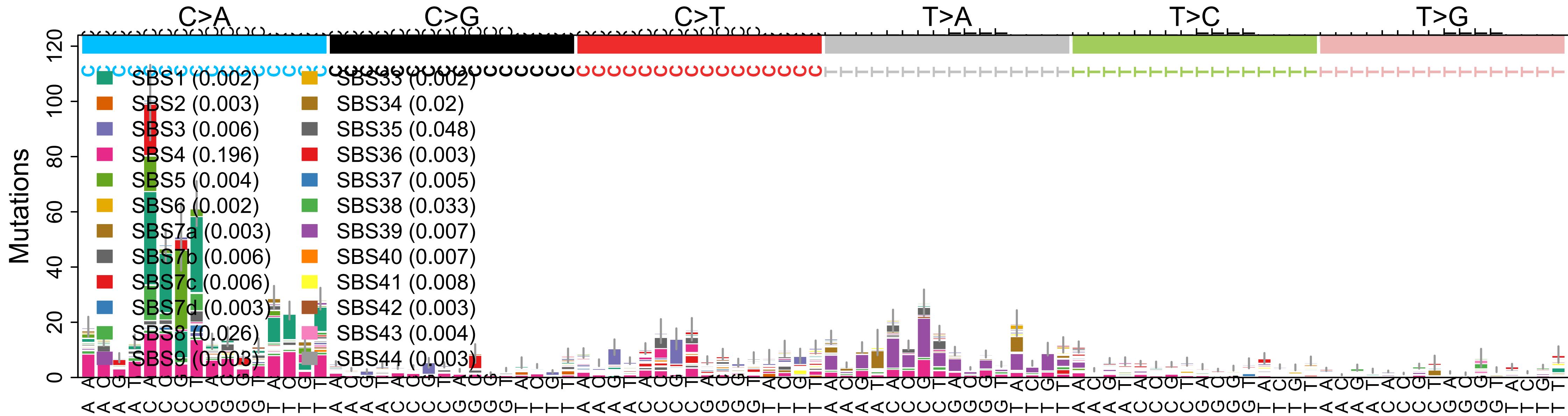
Reconstructed spectrum (cosine similarity = 0.956)



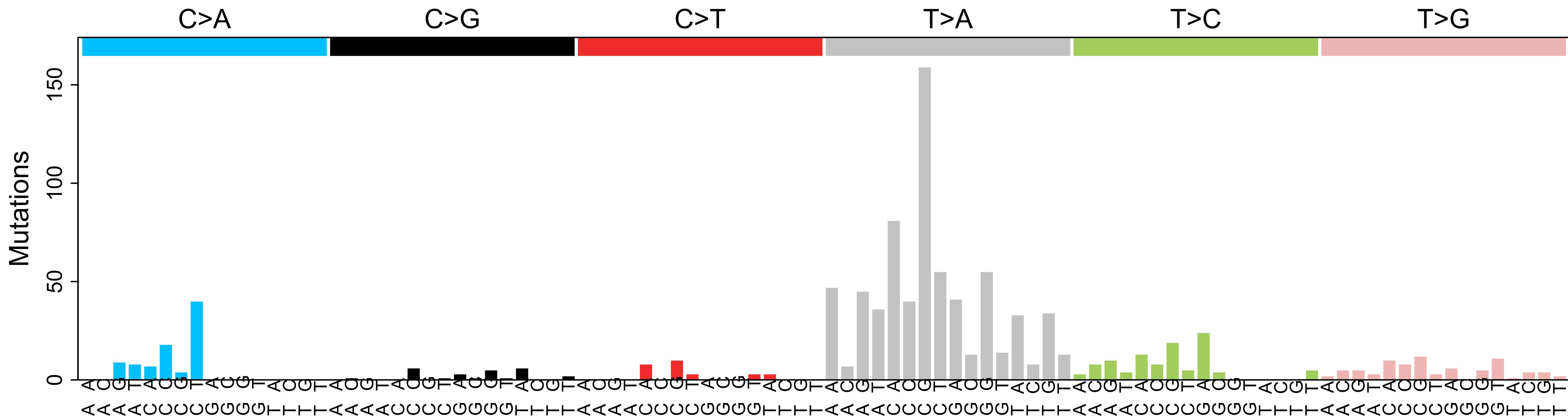
dibenzo_jacridine_ddba8930ac82 (997 mutations)



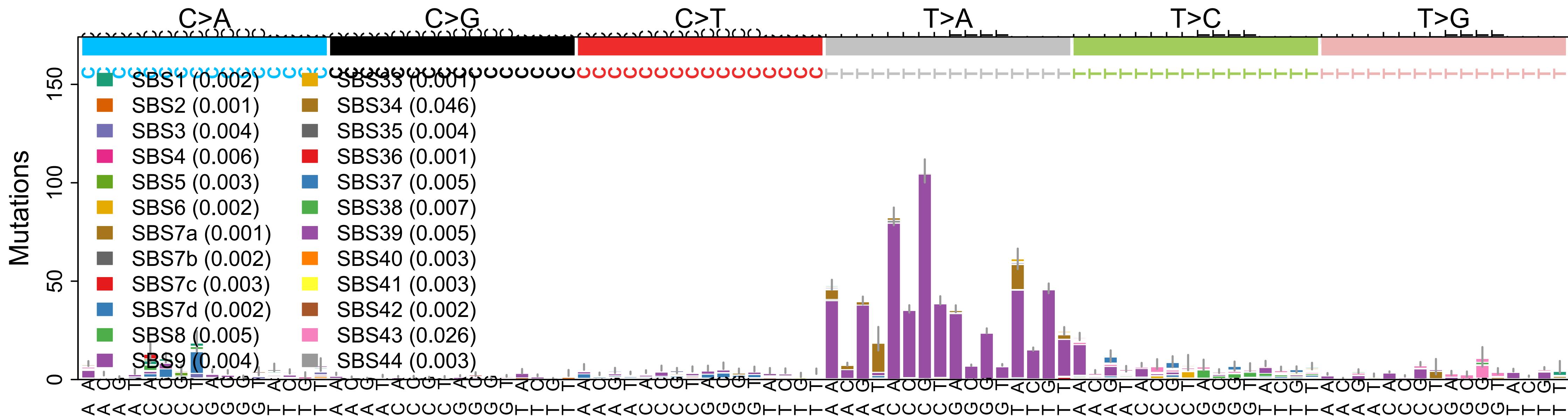
Reconstructed spectrum (cosine similarity = 0.93)



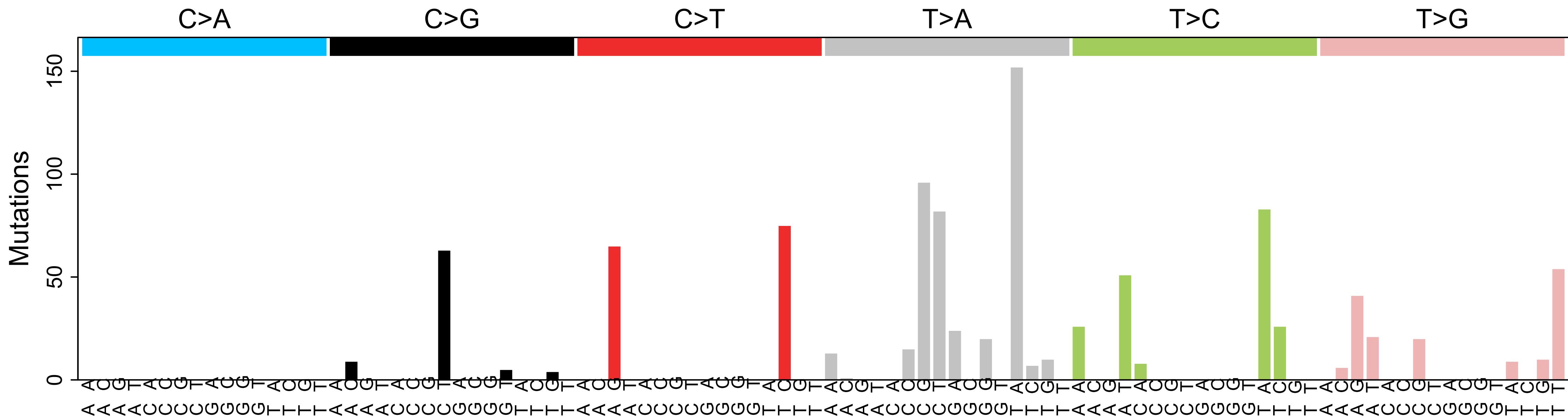
dibenzoa_ipyrene_8d818fe5a7ef (1,004 mutations)



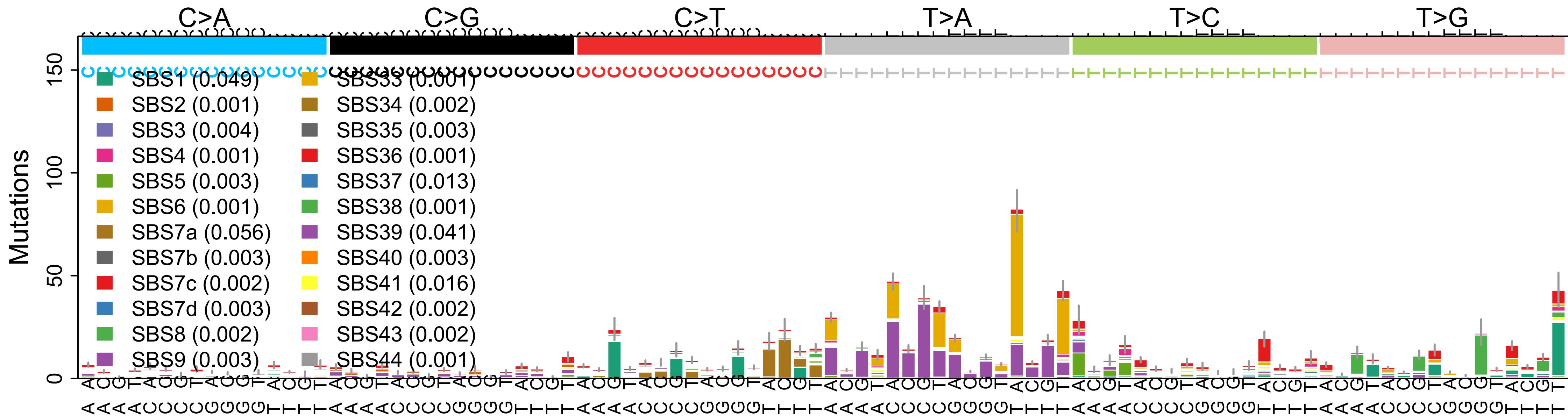
Reconstructed spectrum (cosine similarity = 0.928)



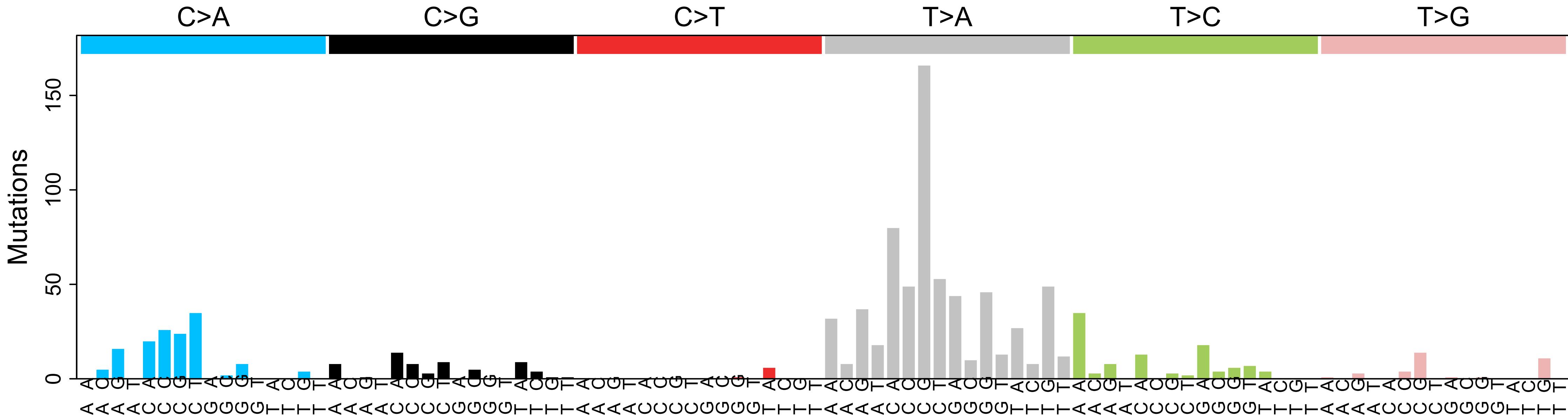
dibenzoa_lpyrene_a8658ca308ee (996 mutations)



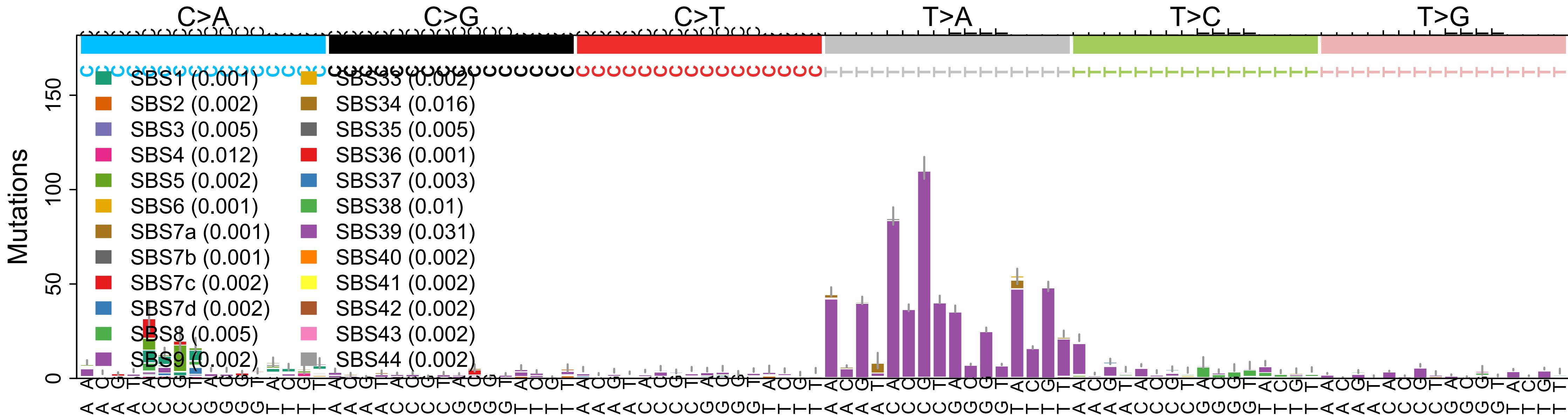
Reconstructed spectrum (cosine similarity = 0.746)



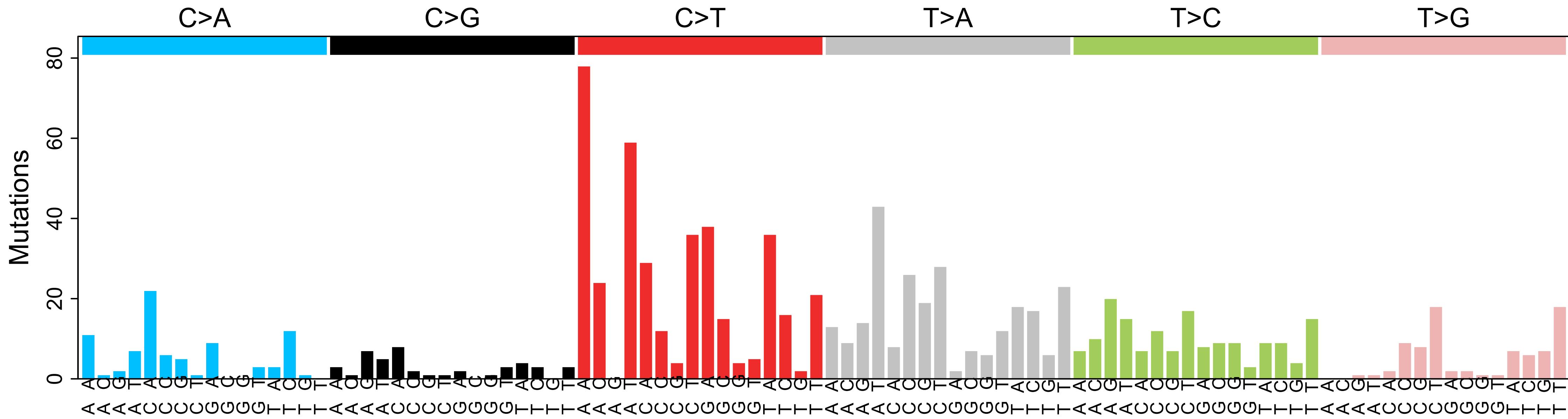
dibenzoa_ipyrene_diol_epoxide_918d83810794 (1,000 mutations)



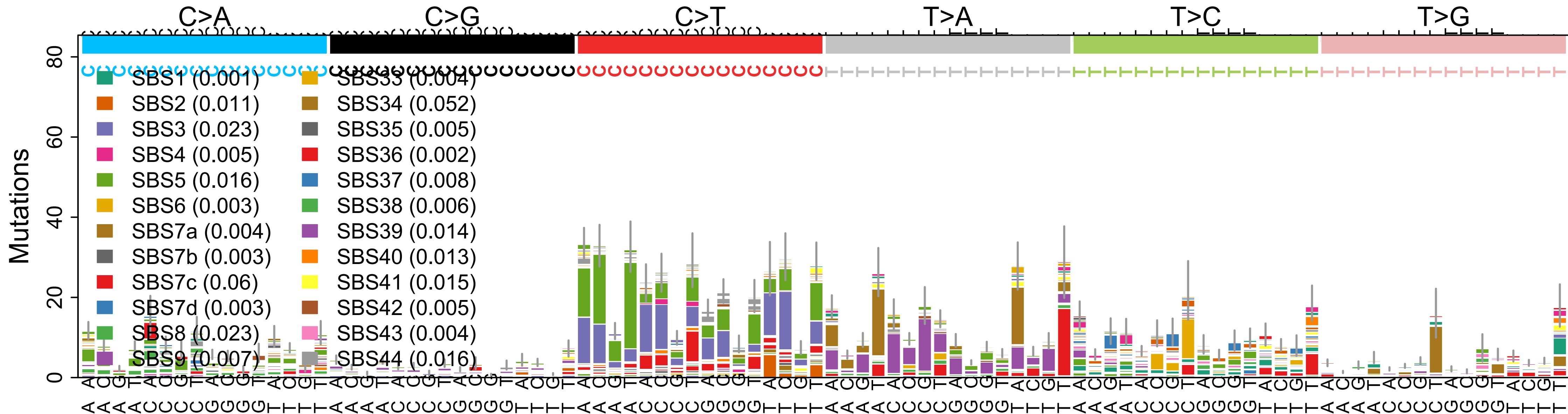
Reconstructed spectrum (cosine similarity = 0.937)



diethyl_sulfate_66c09d32862b (1,001 mutations)



Reconstructed spectrum (cosine similarity = 0.864)



dimethyl_sulfate_31311db64fc6 (1,004 mutations)

C>A

C>G

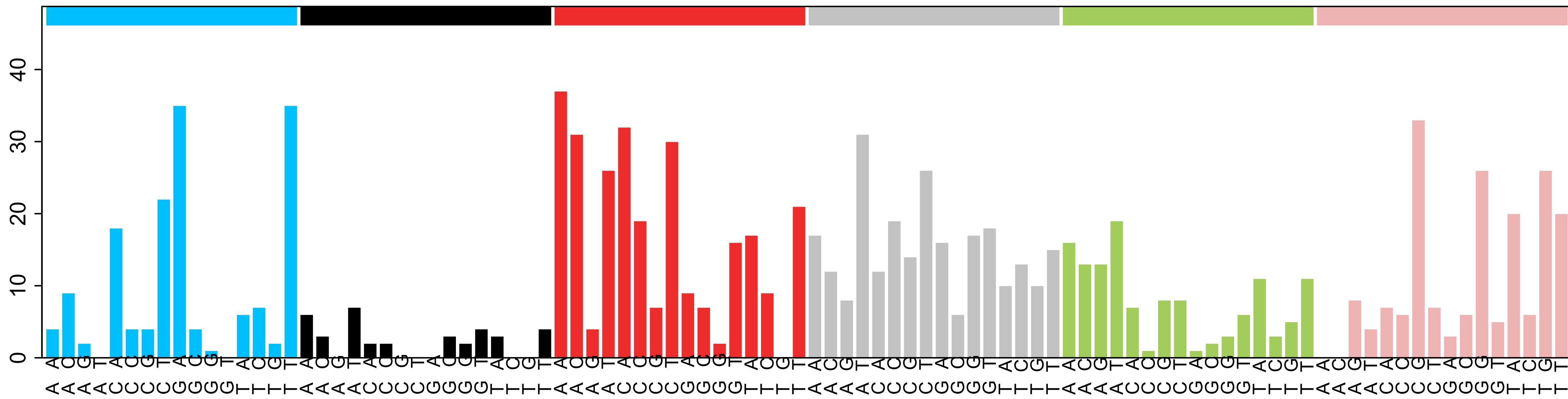
C>T

T>A

T>C

T>G

Mutations



Reconstructed spectrum (cosine similarity = 0.884)

C>A

C>G

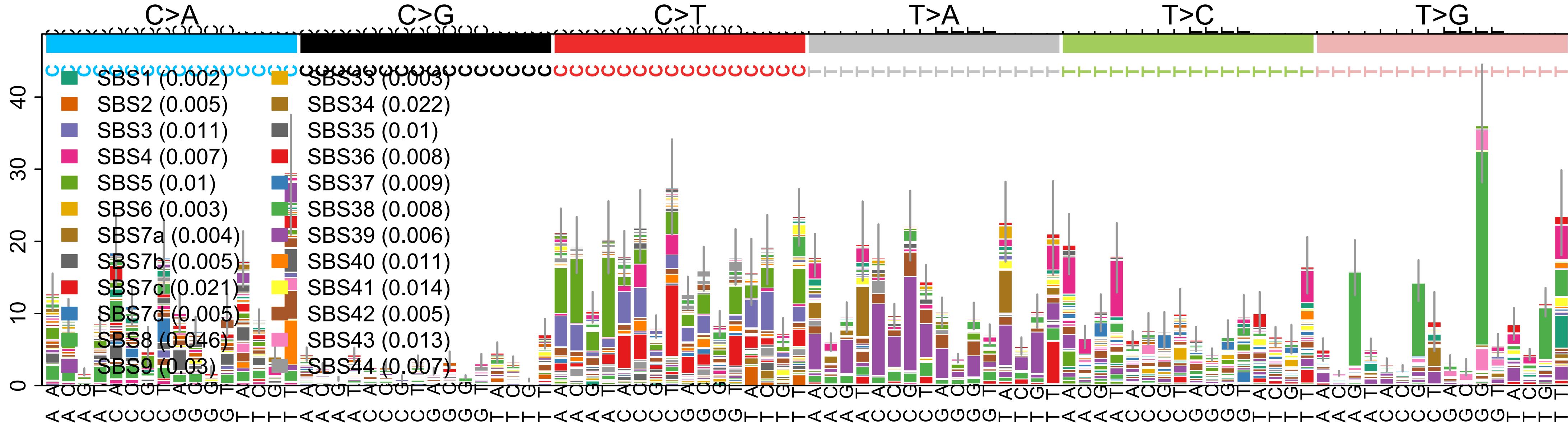
C>T

T>A

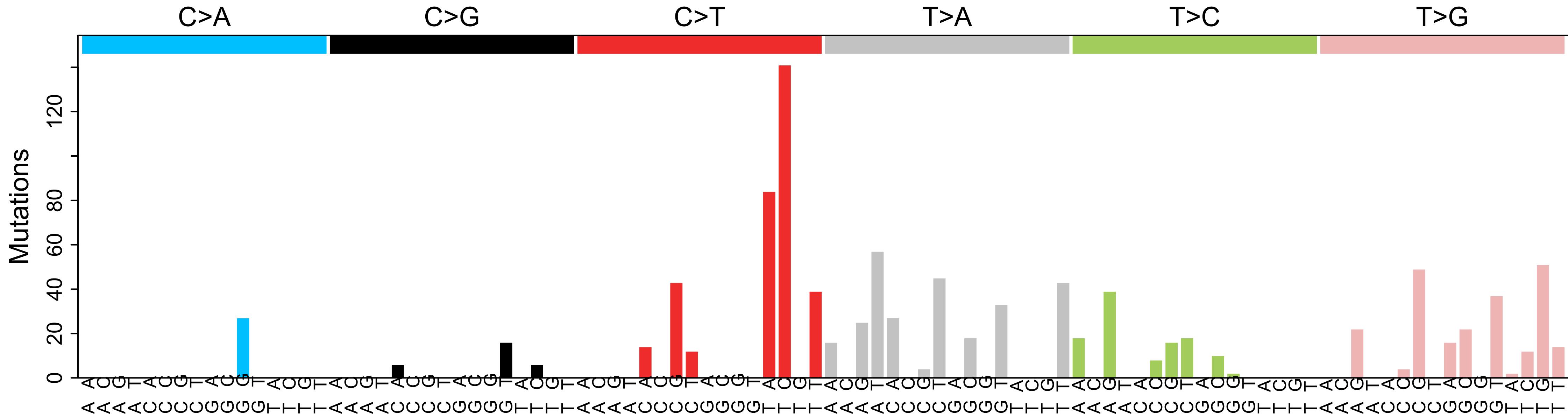
T>C

T>G

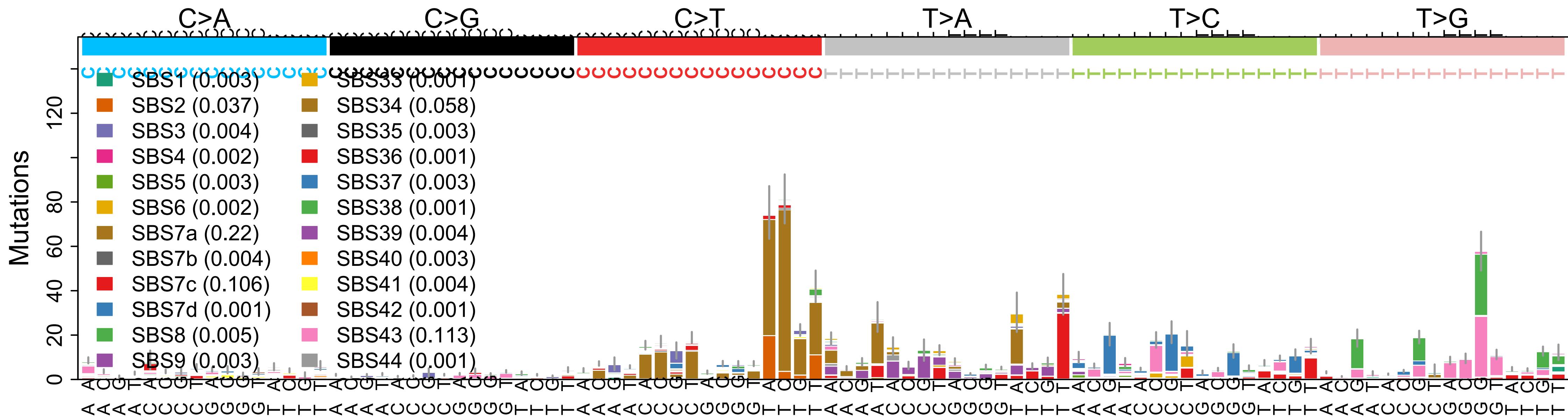
Mutations



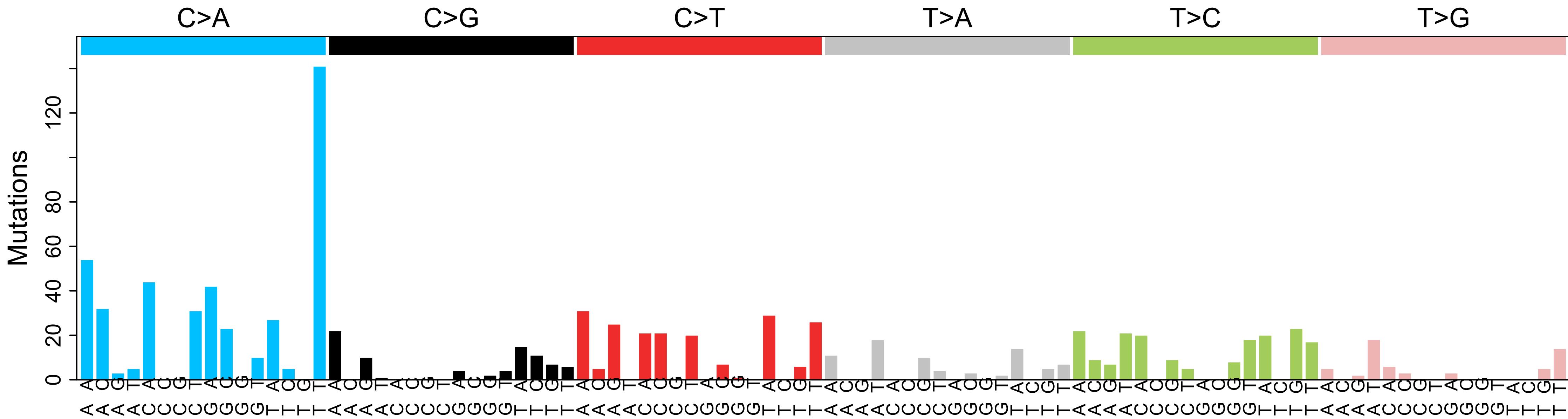
dms0_39bf73141acf (996 mutations)



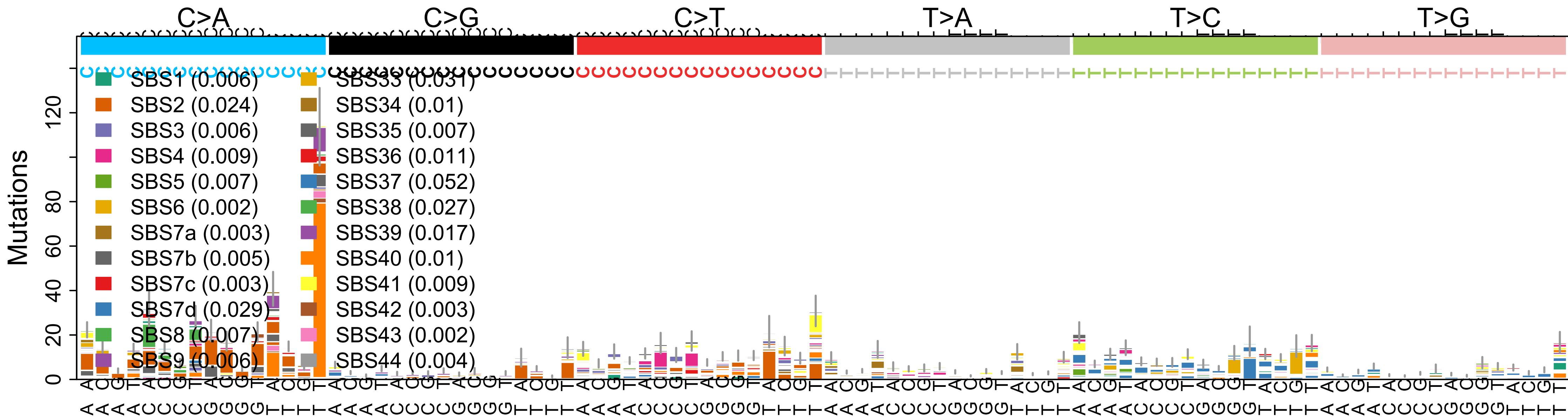
Reconstructed spectrum (cosine similarity = 0.795)



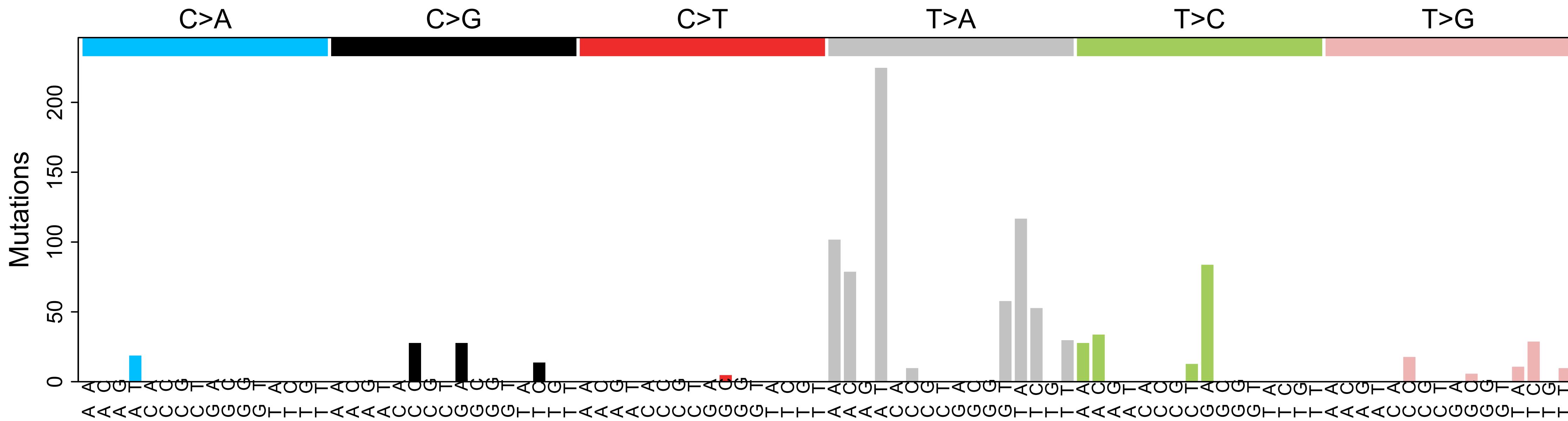
dms0_418f69401d9a (1,000 mutations)



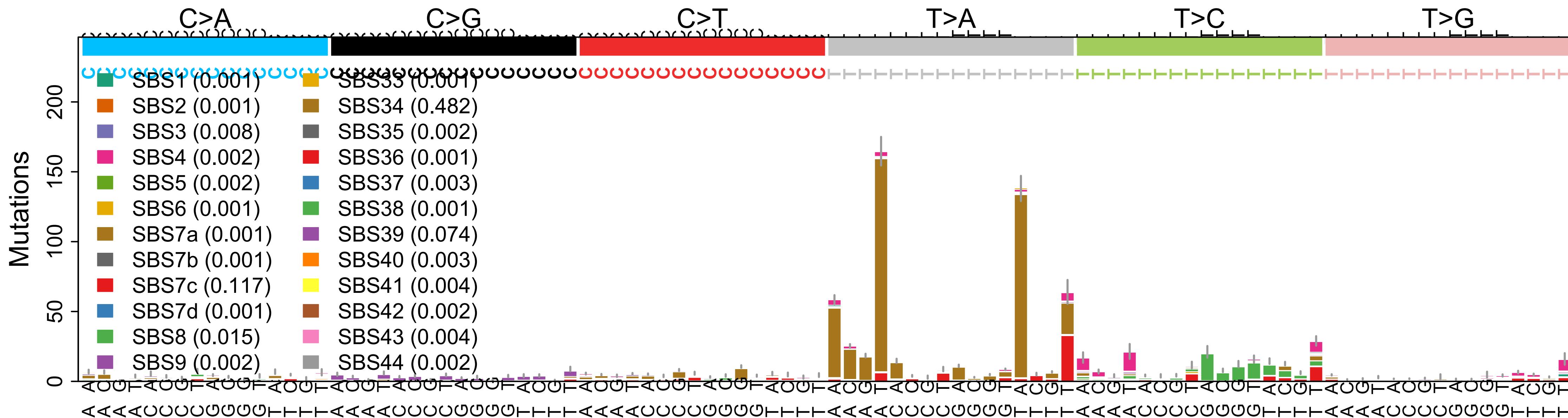
Reconstructed spectrum (cosine similarity = 0.923)



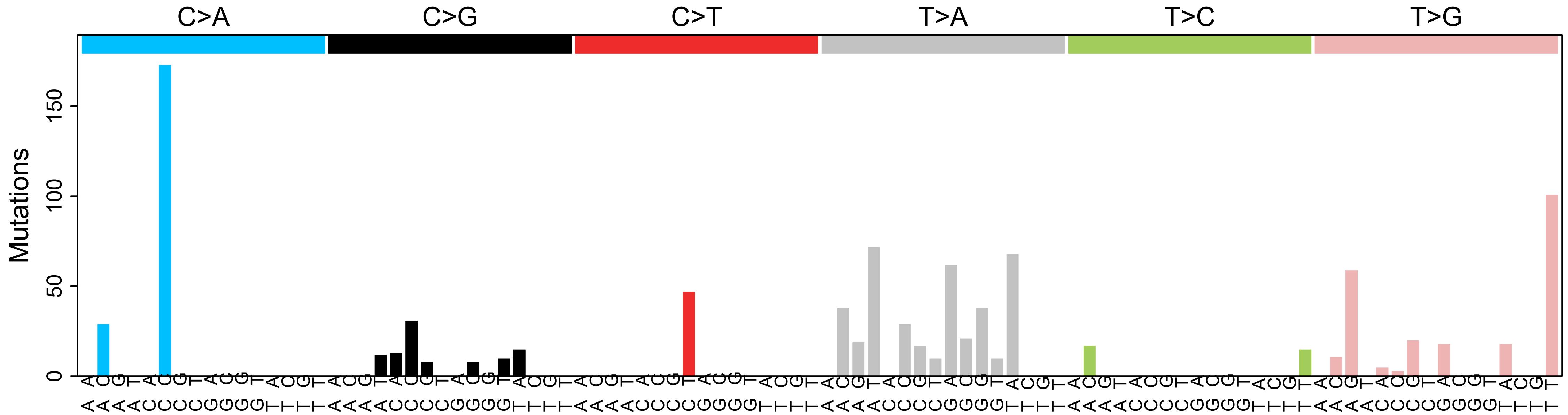
dms0_640c89f54363 (1,001 mutations)



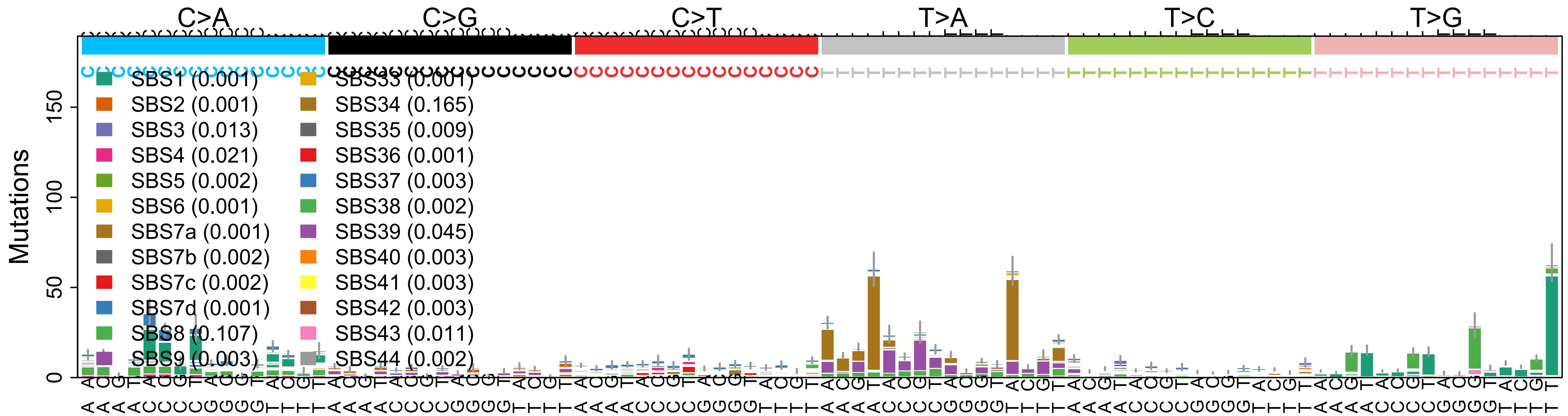
Reconstructed spectrum (cosine similarity = 0.865)



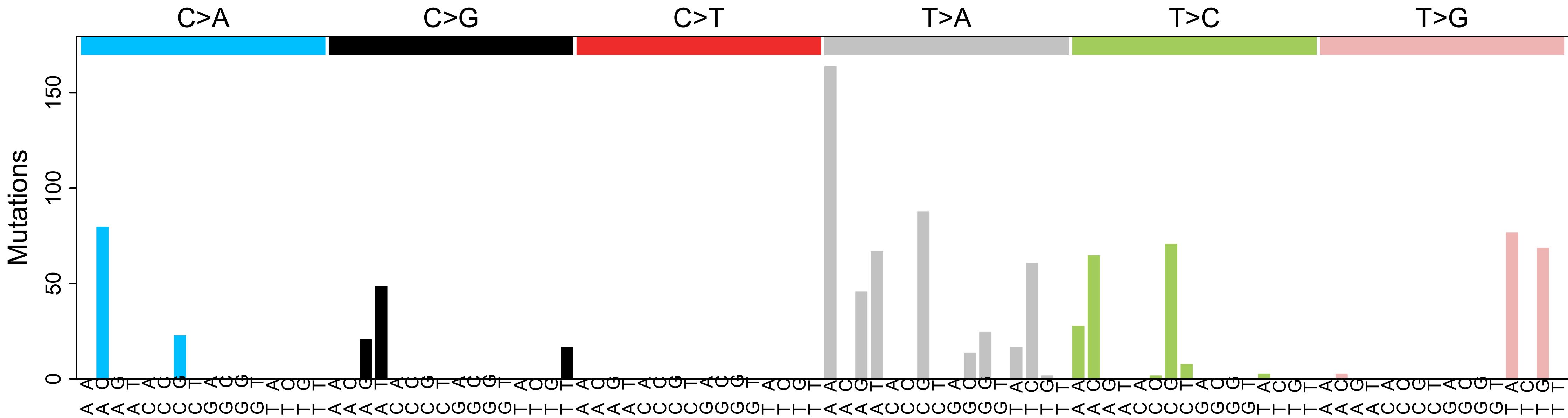
ellipticine_4b8e9b175c6b (997 mutations)



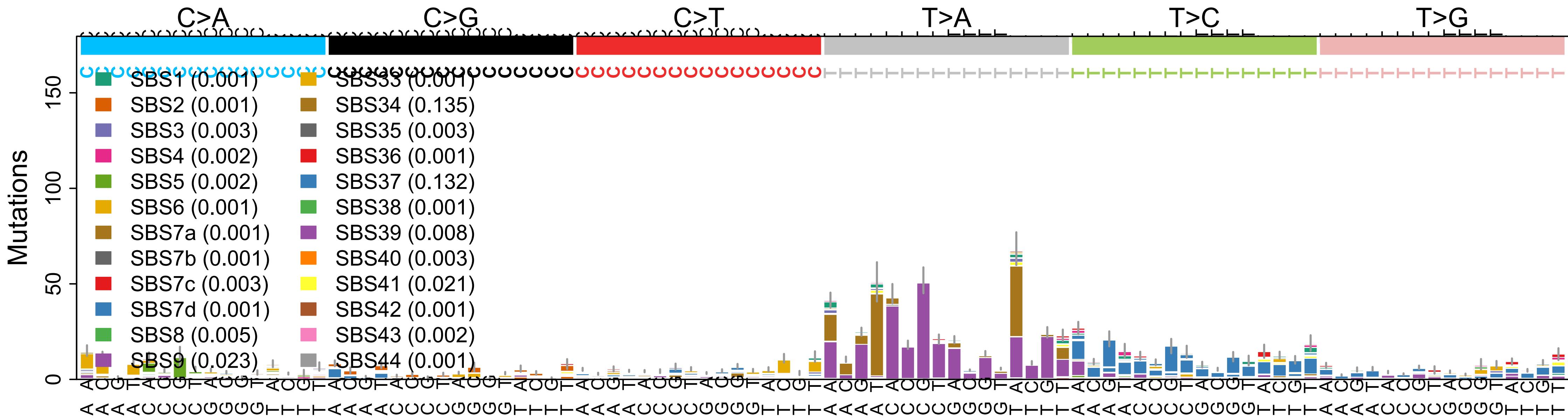
Reconstructed spectrum (cosine similarity = 0.639)



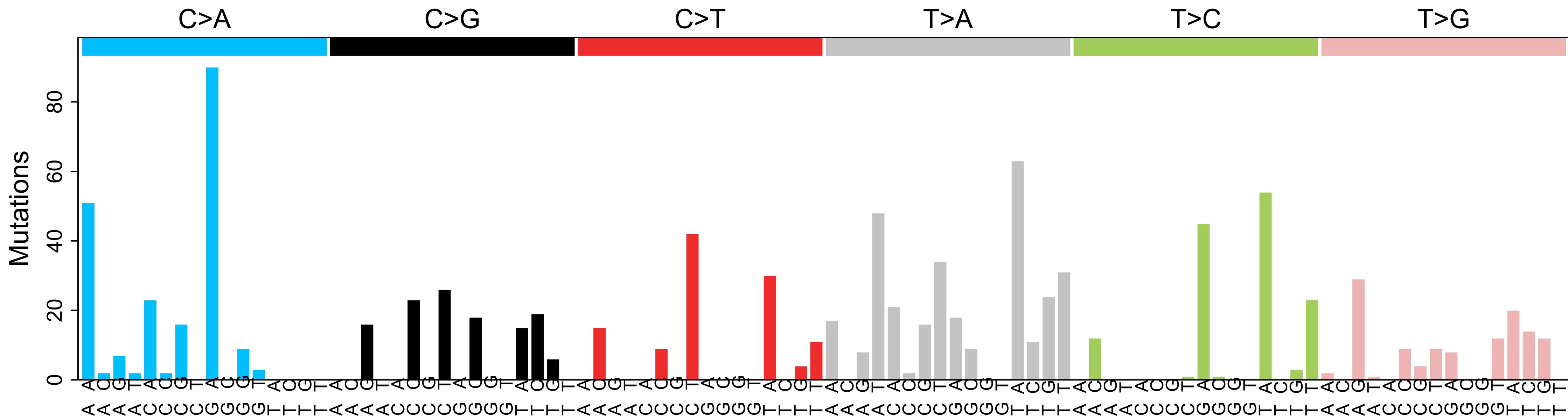
ellipticine_e149a5f58dd0 (1,000 mutations)



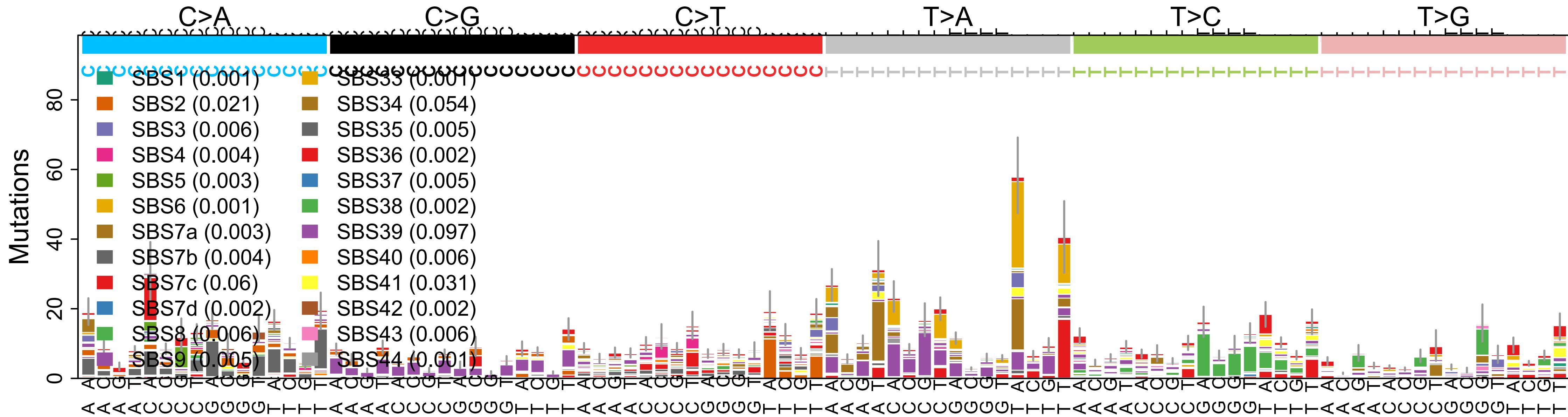
Reconstructed spectrum (cosine similarity = 0.572)



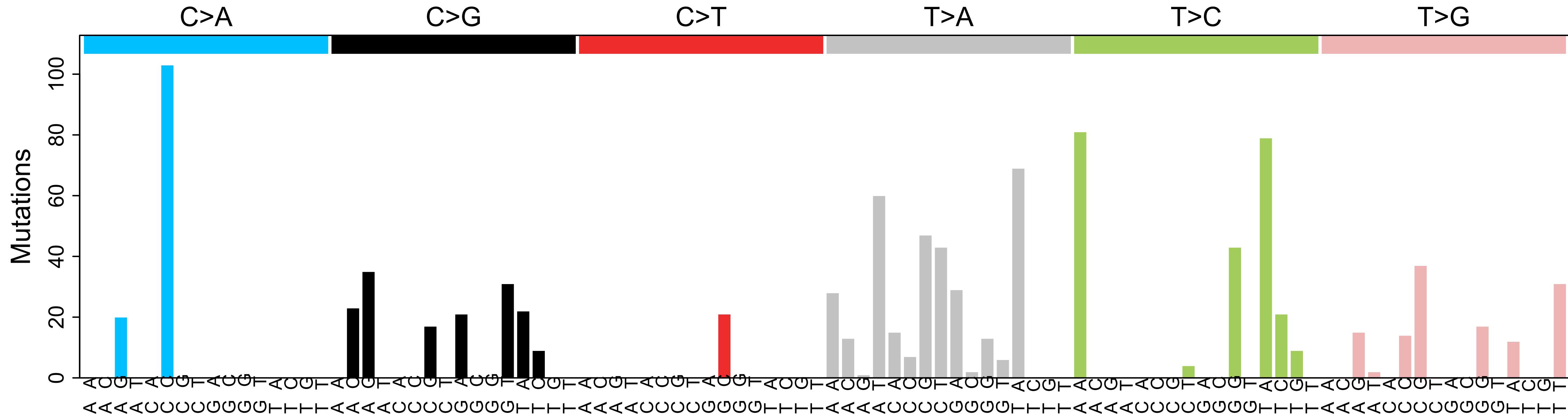
etoposide_d87f22a7e170 (1,000 mutations)



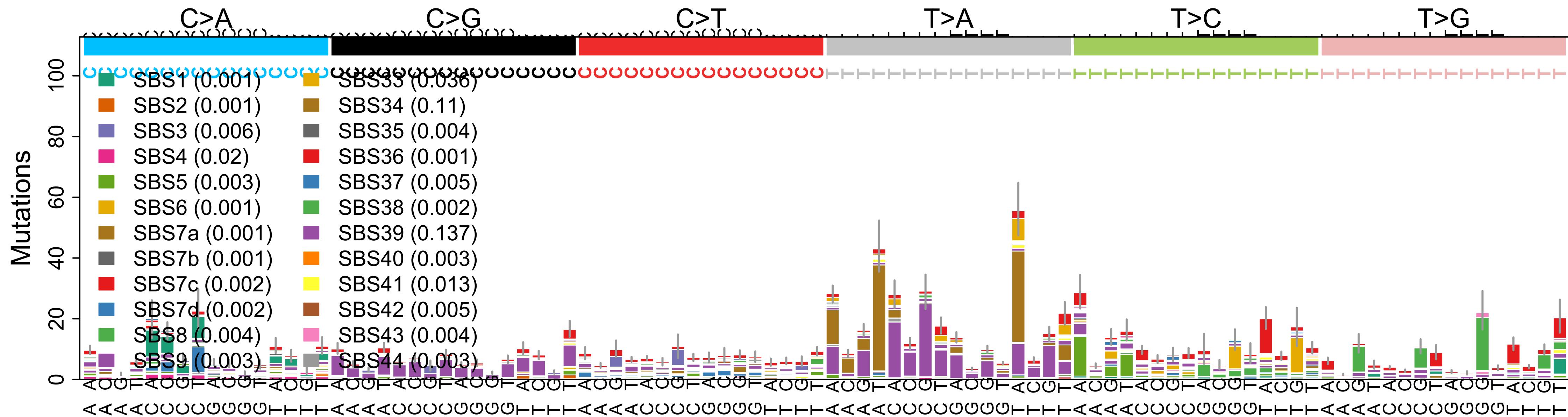
Reconstructed spectrum (cosine similarity = 0.73)



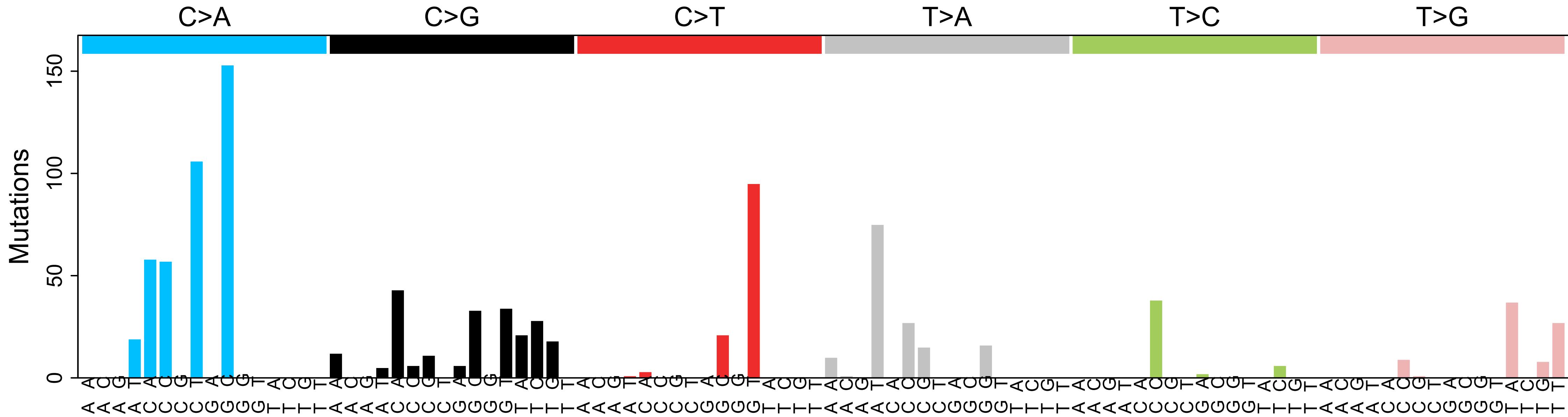
formaldehyde_8c36e95b481c (1,000 mutations)



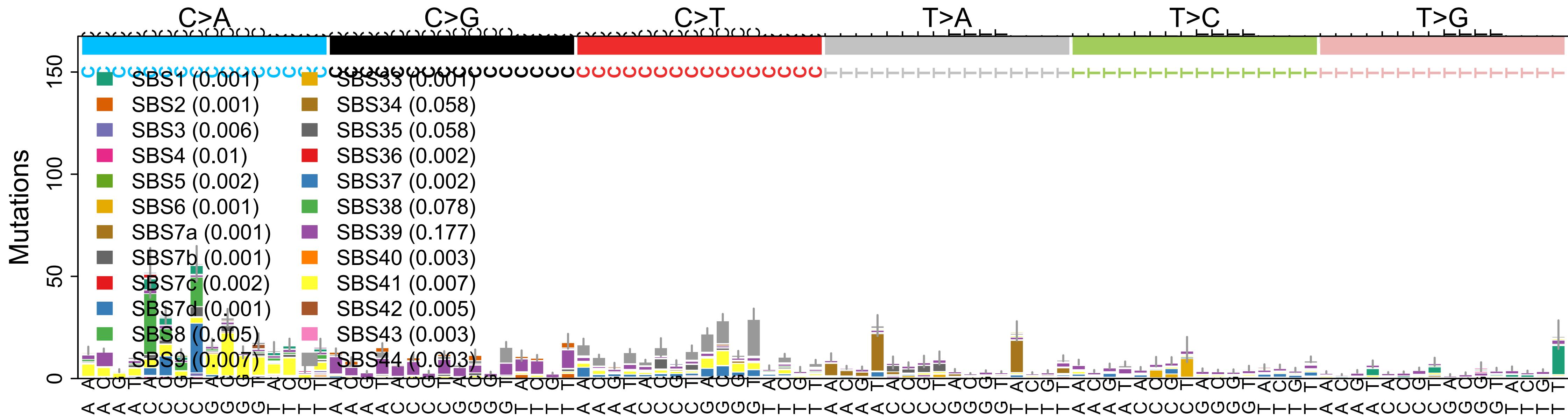
Reconstructed spectrum (cosine similarity = 0.686)



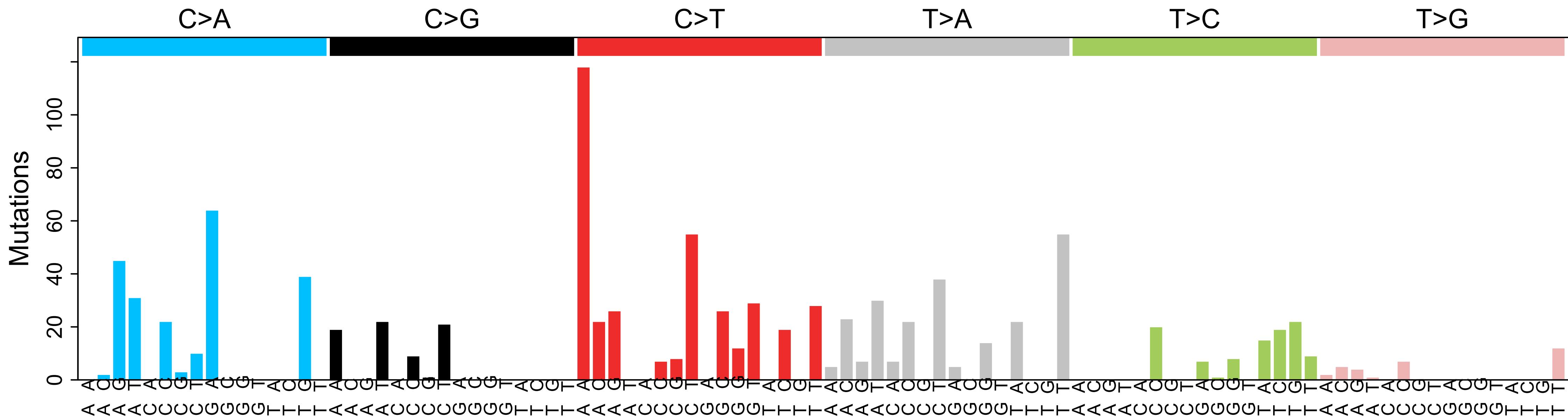
furan_fd4f695c67b1 (1,002 mutations)



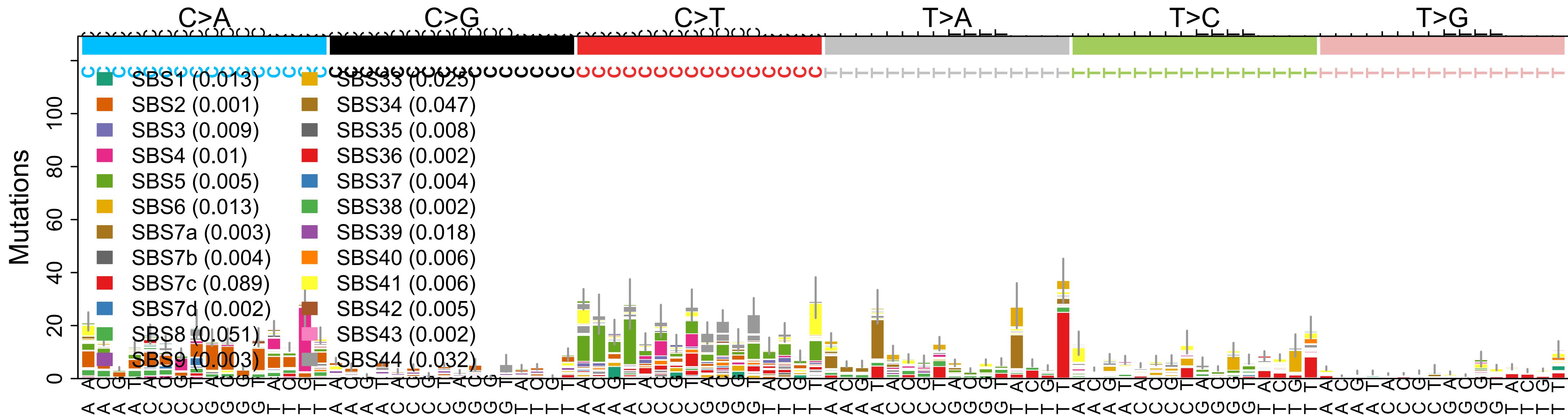
Reconstructed spectrum (cosine similarity = 0.694)



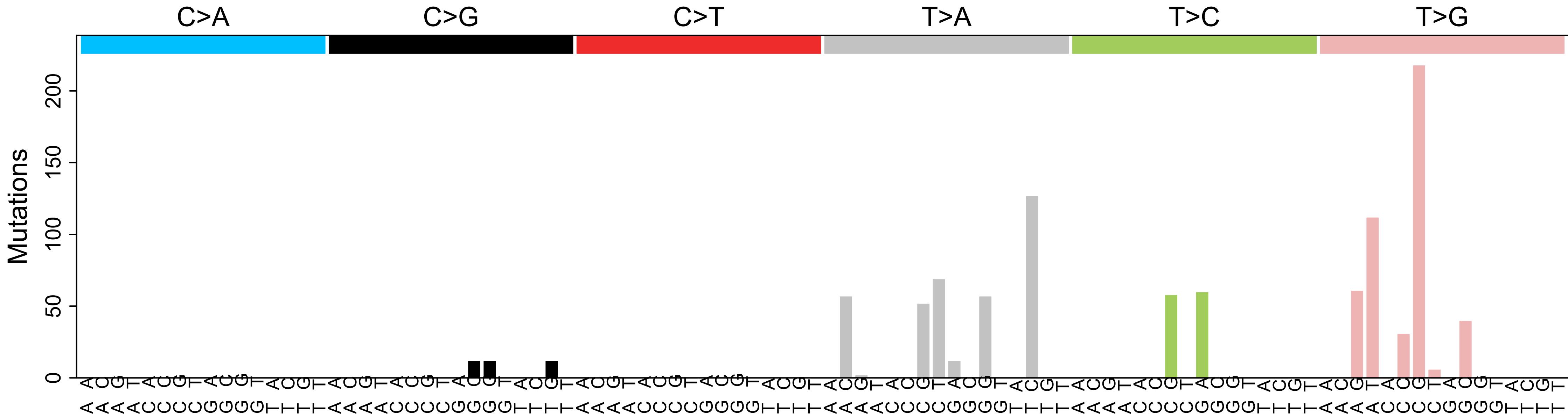
gammaray_8a41562354d7 (998 mutations)



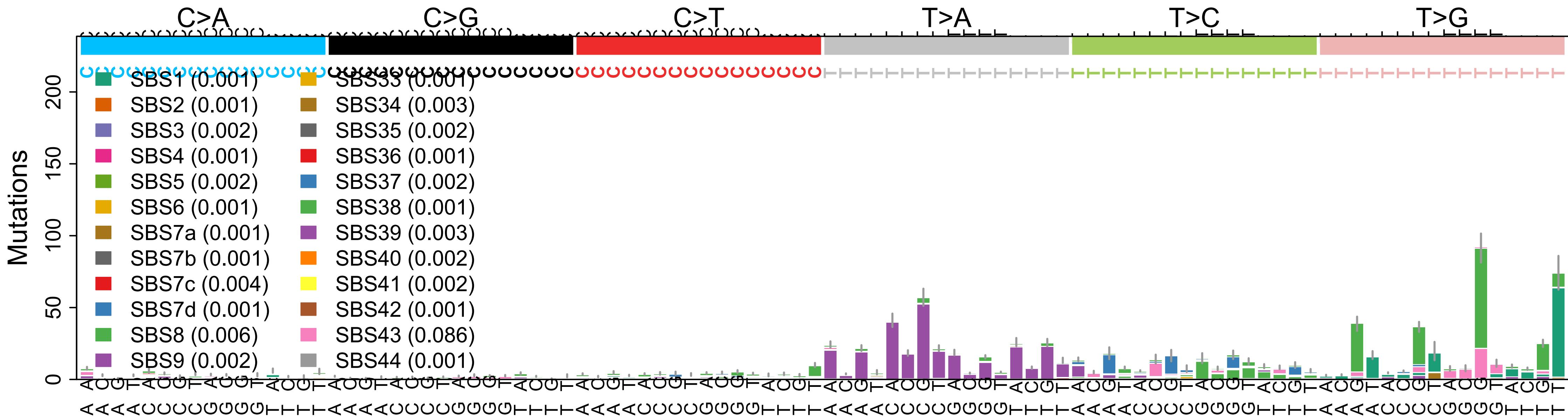
Reconstructed spectrum (cosine similarity = 0.692)



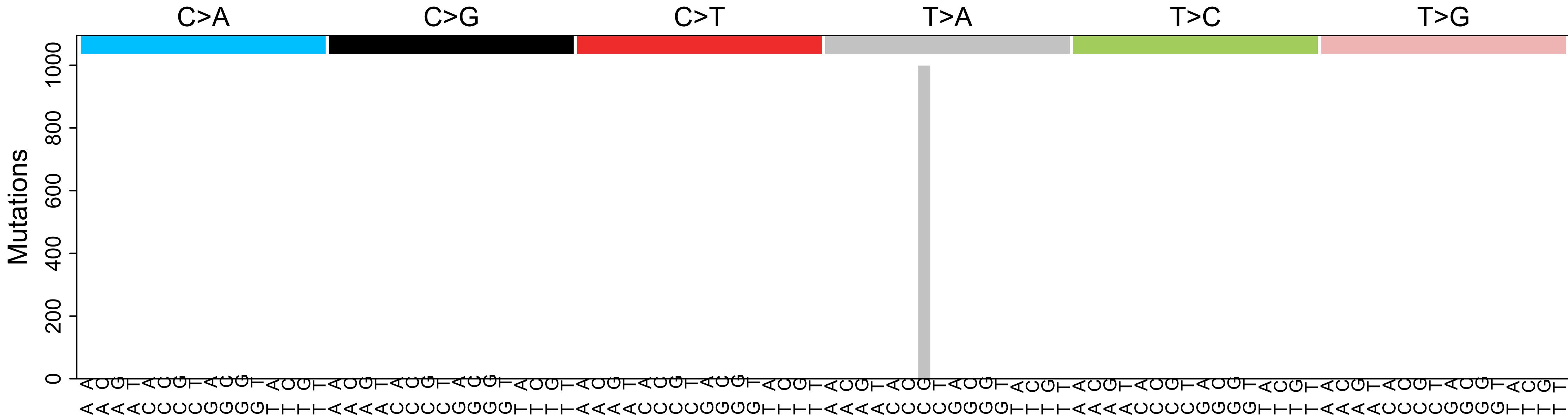
glycidamide_8e1c87cf773d (998 mutations)



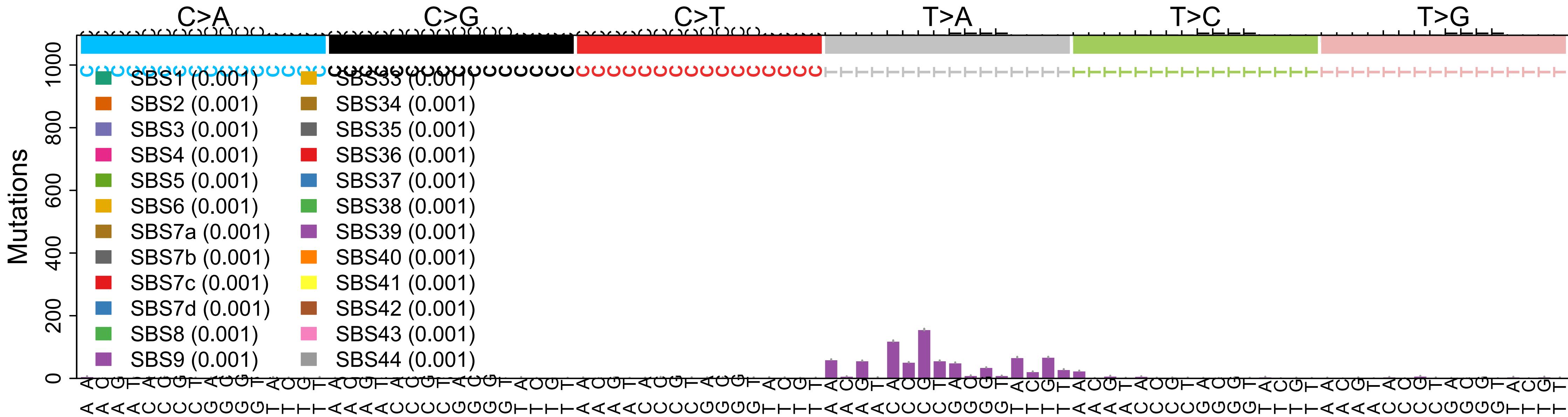
Reconstructed spectrum (cosine similarity = 0.385)



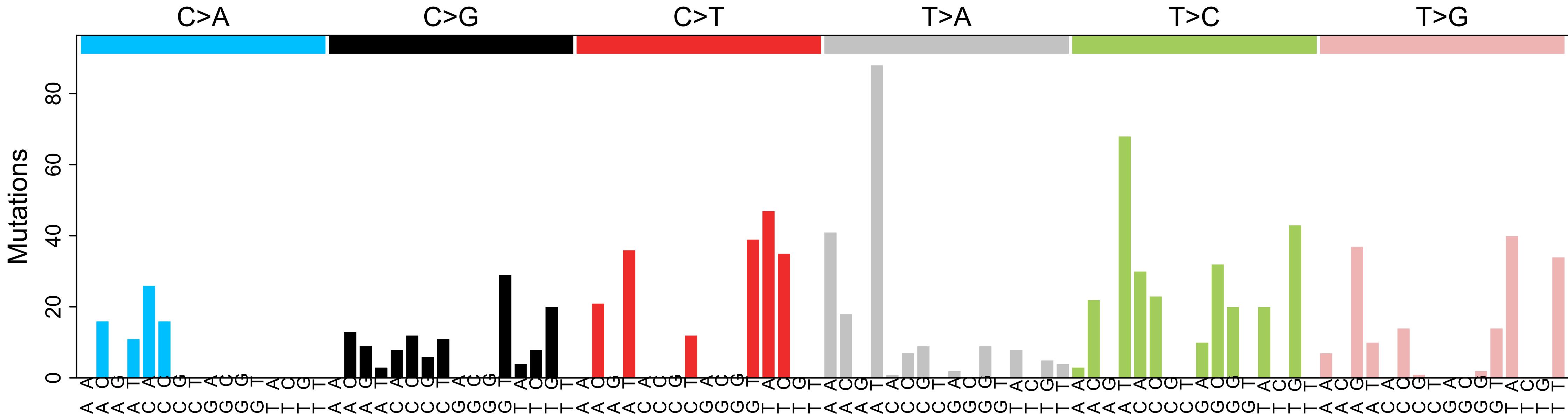
hydrogen_peroxide_ff64f141ad1a (1,000 mutations)



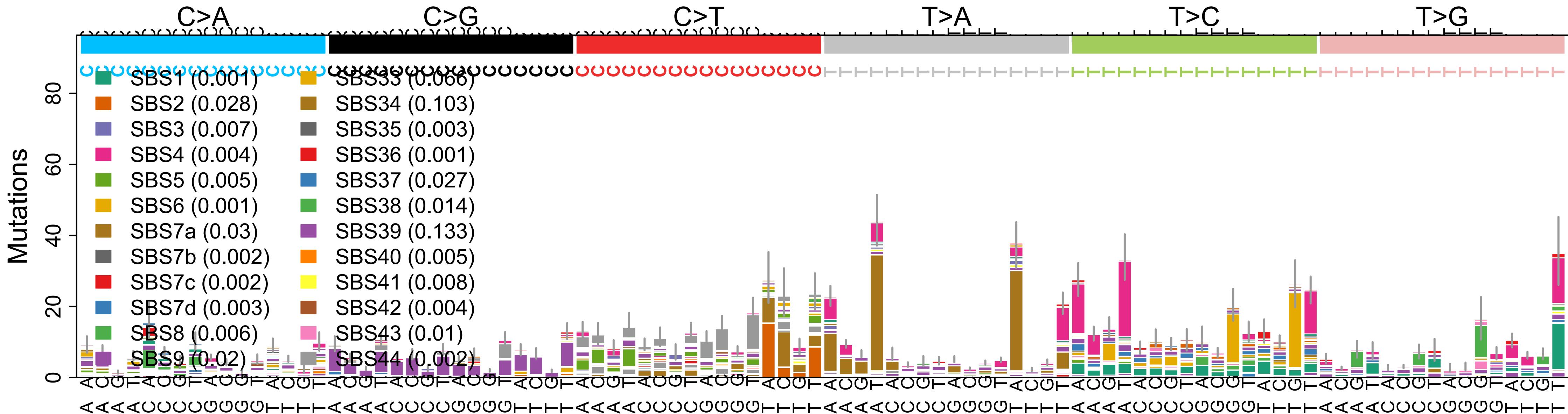
Reconstructed spectrum (cosine similarity = 0.603)



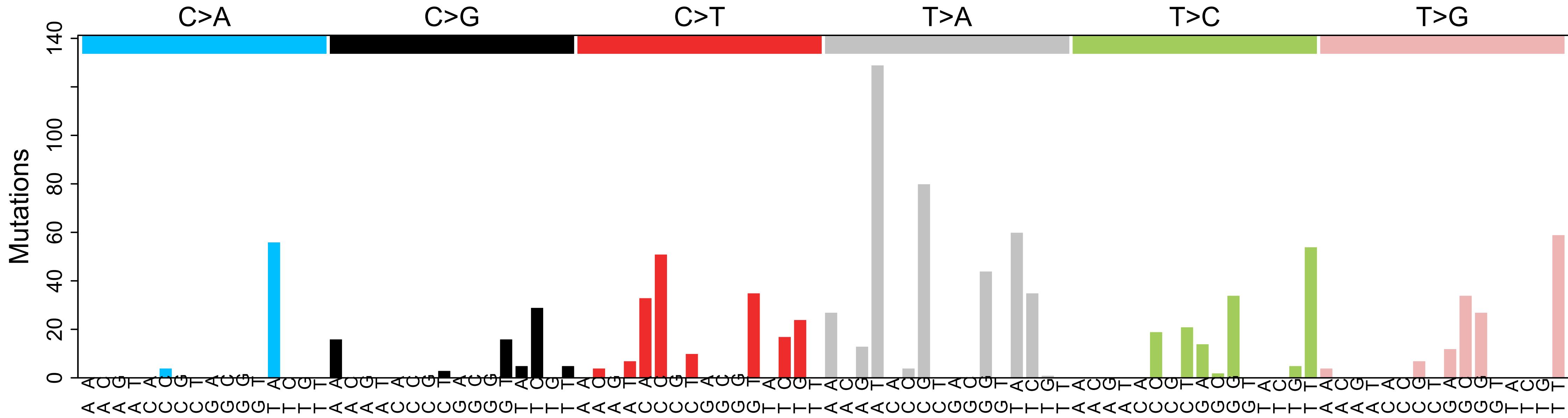
lead_acetate_eb992ae53f06 (1,004 mutations)



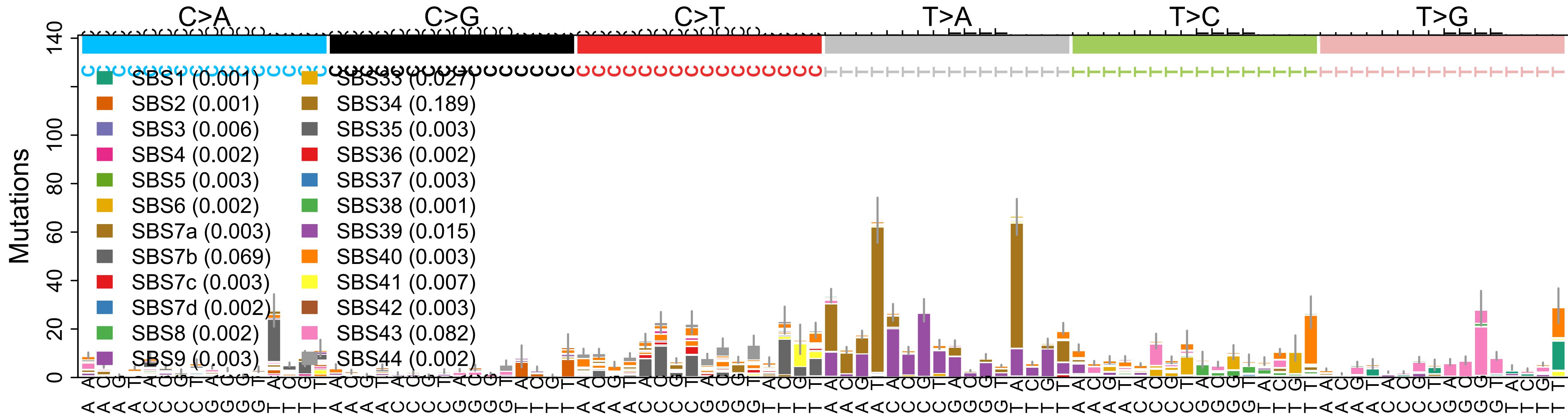
Reconstructed spectrum (cosine similarity = 0.744)



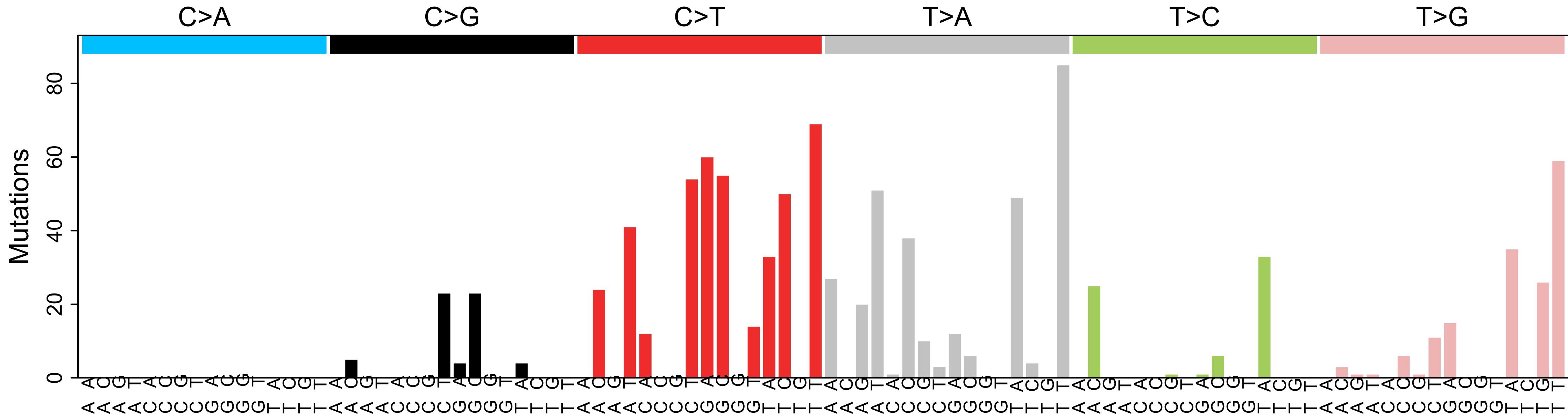
lead_nitrate_3ff280a61a91 (1,000 mutations)



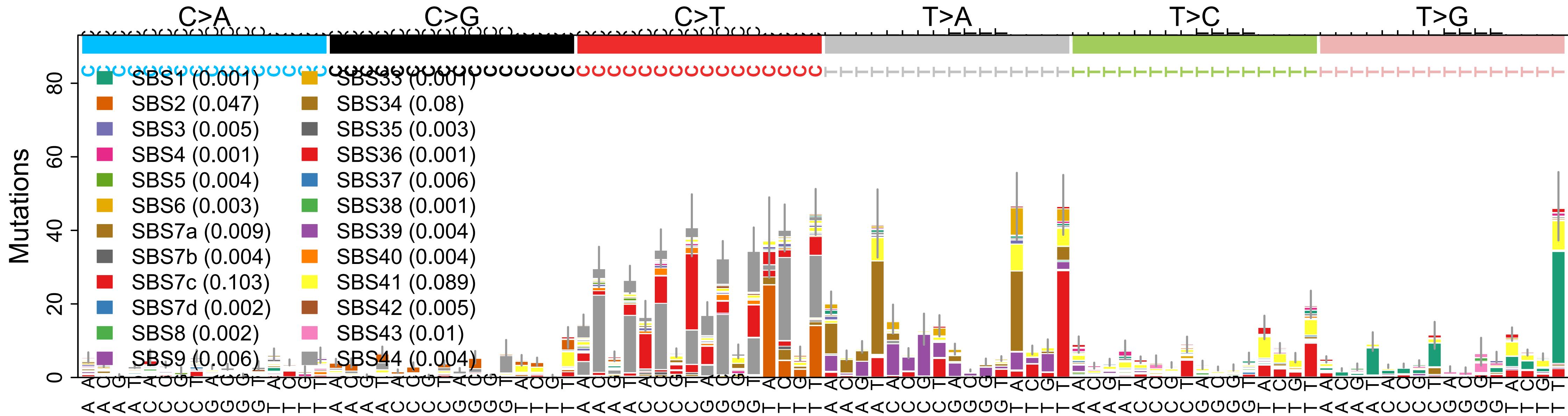
Reconstructed spectrum (cosine similarity = 0.8)



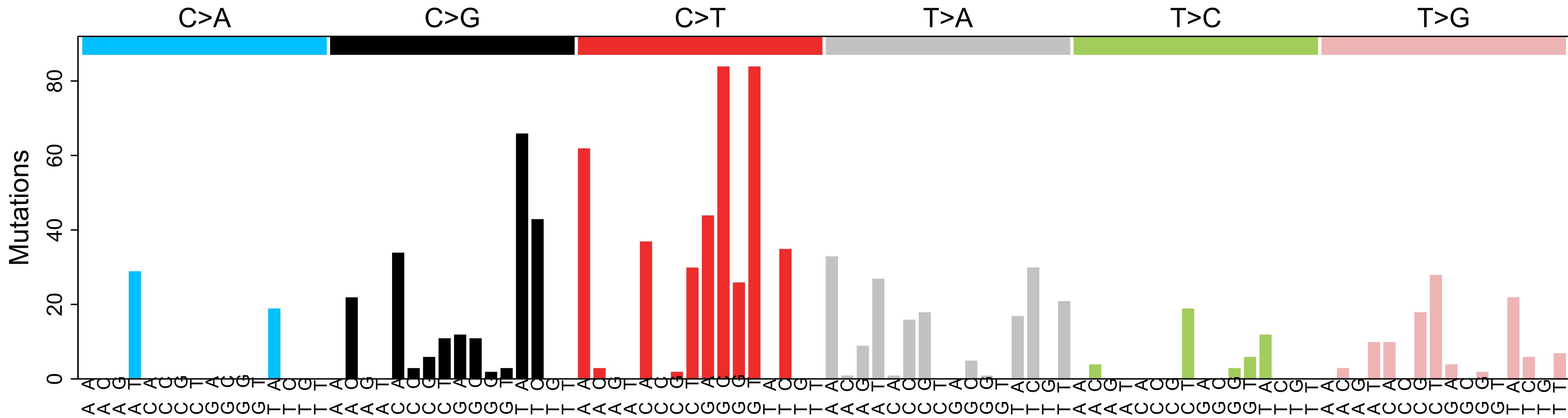
mechllorethamine_48da6be92ec6 (1,001 mutations)



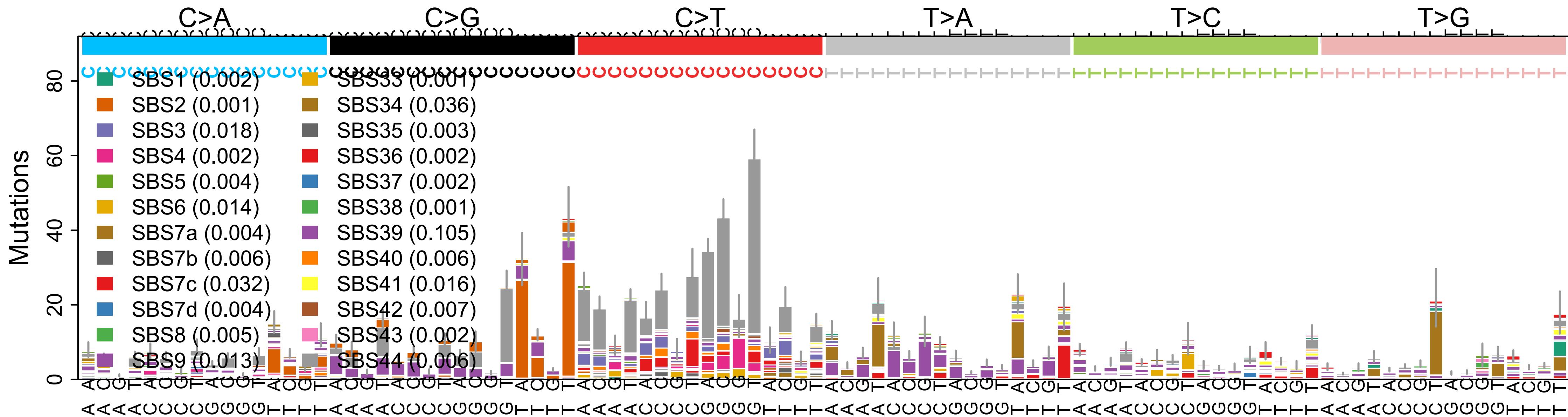
Reconstructed spectrum (cosine similarity = 0.844)



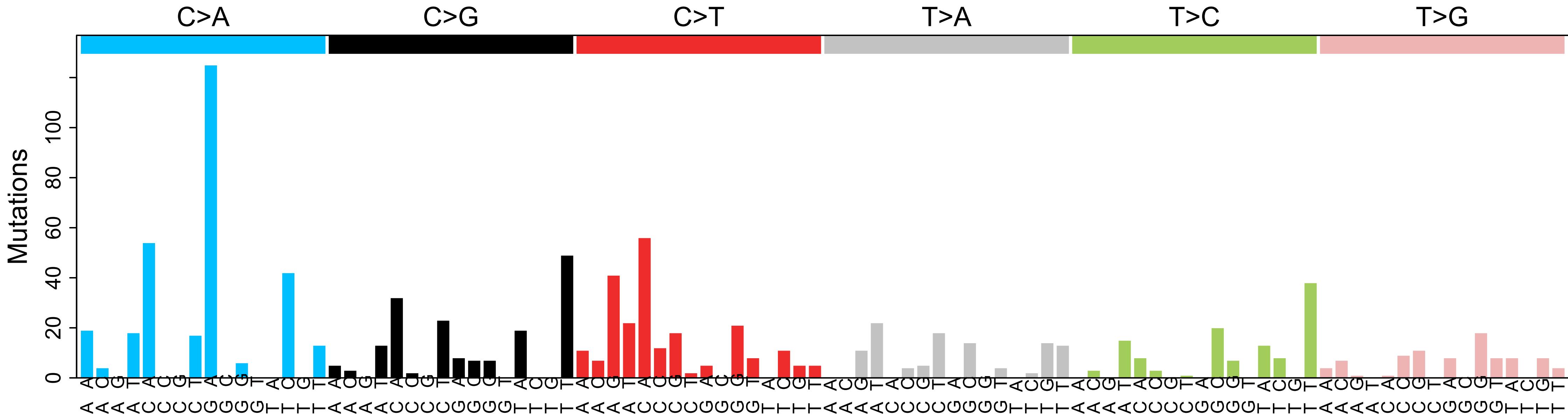
melphalan_dc6d858bb0a4 (1,001 mutations)



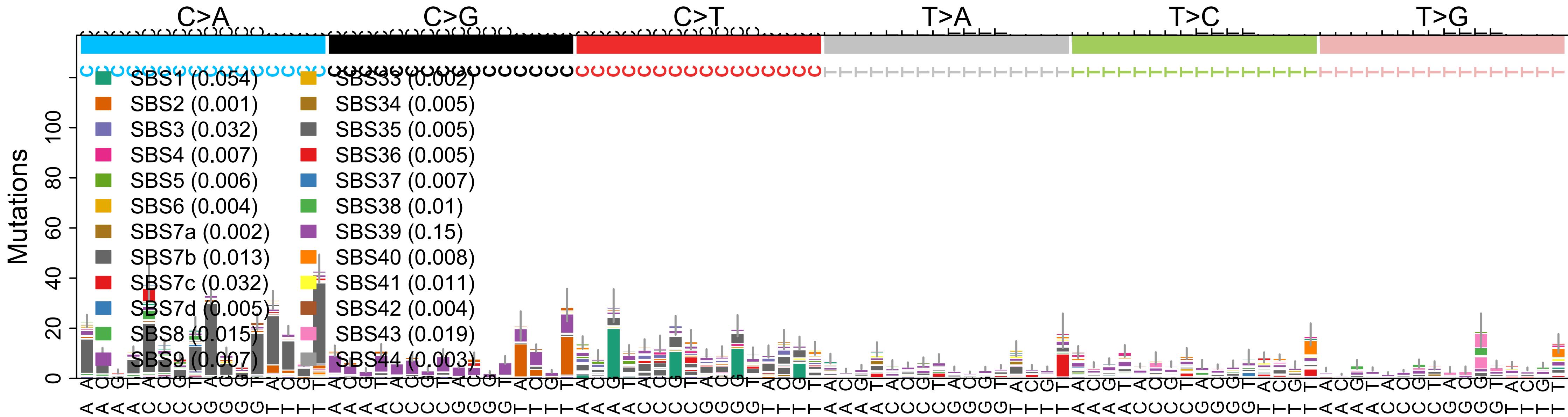
Reconstructed spectrum (cosine similarity = 0.777)



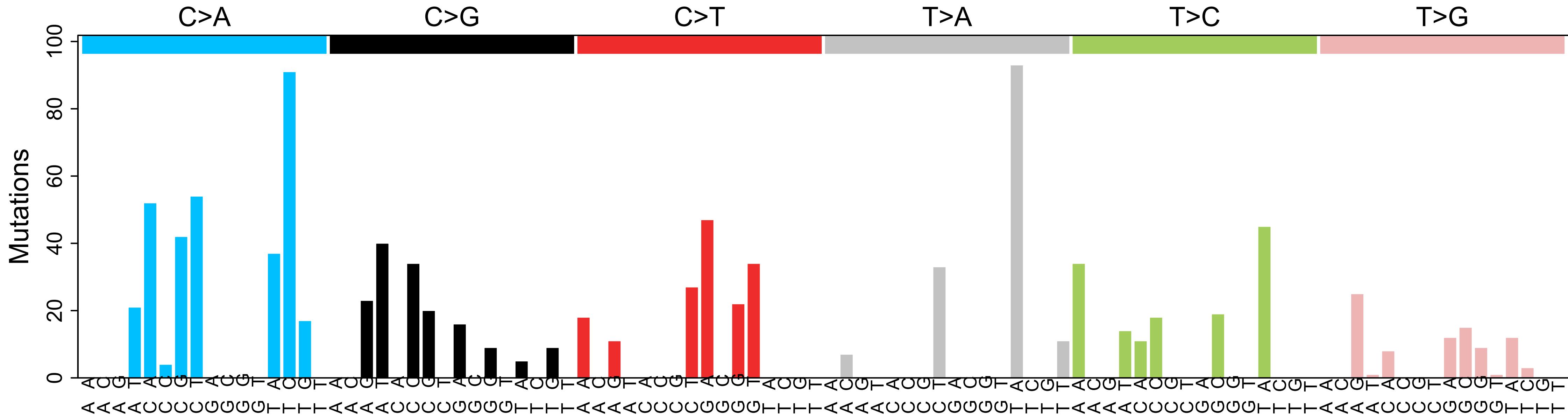
methanol_23bc14314298 (1,000 mutations)



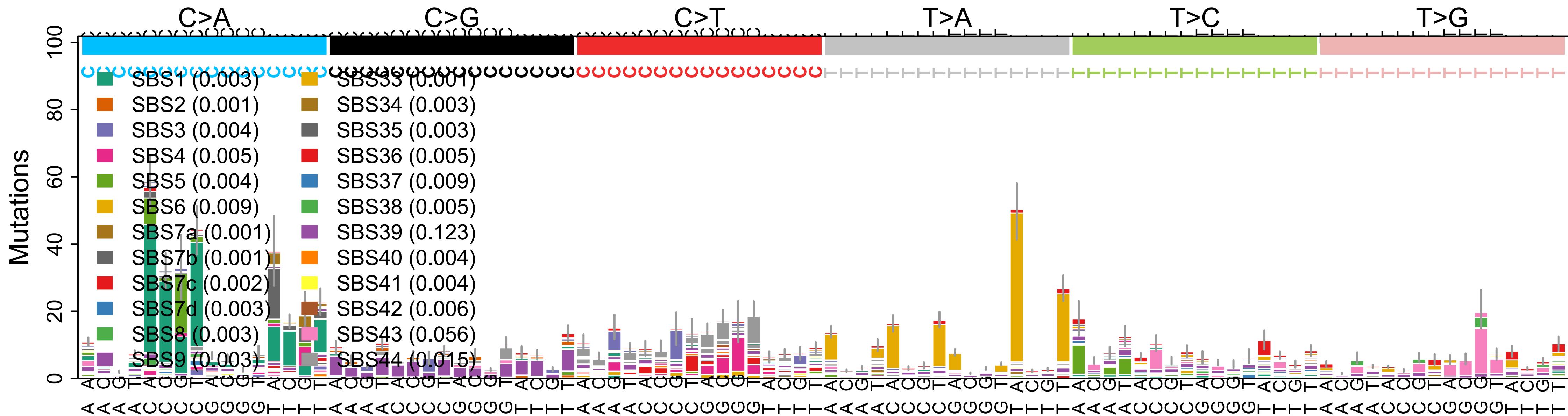
Reconstructed spectrum (cosine similarity = 0.715)



methanol_5f193a12cbbf (1,004 mutations)



Reconstructed spectrum (cosine similarity = 0.743)



methyl_methanesulfonate_f61fcd09adad (1,000 mutations)

C>A

C>G

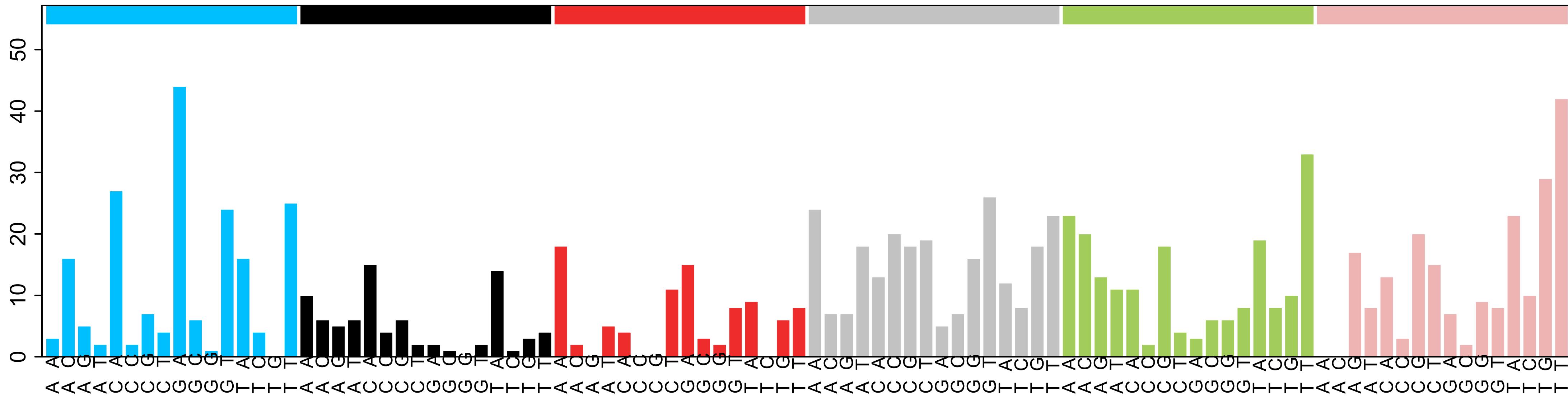
C>T

T>A

T>C

T>G

Mutations



Reconstructed spectrum (cosine similarity = 0.871)

C>A

C>G

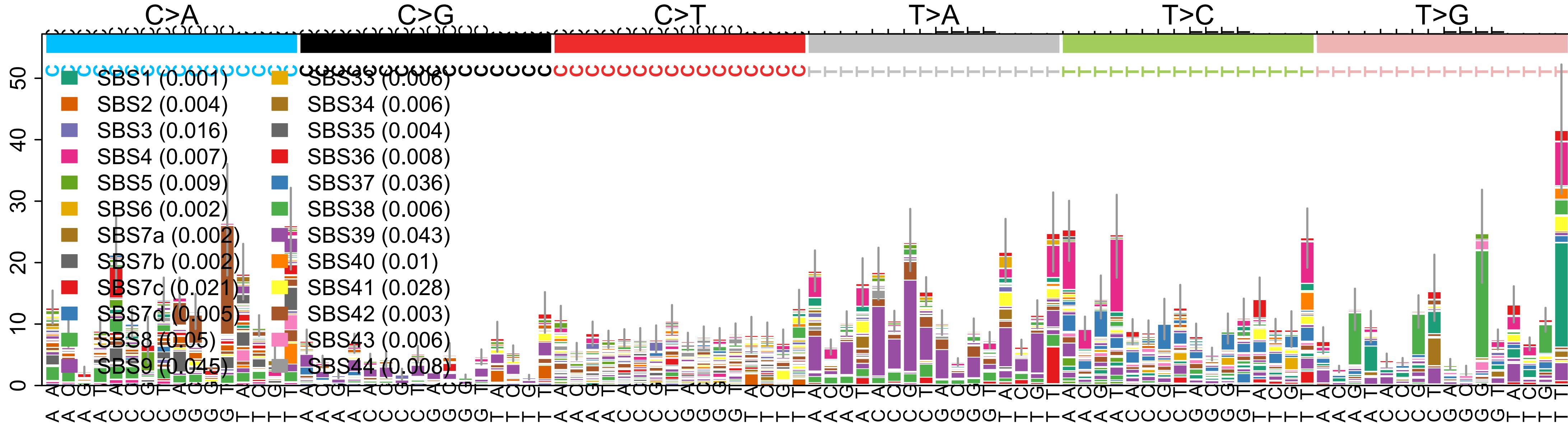
C>T

T>A

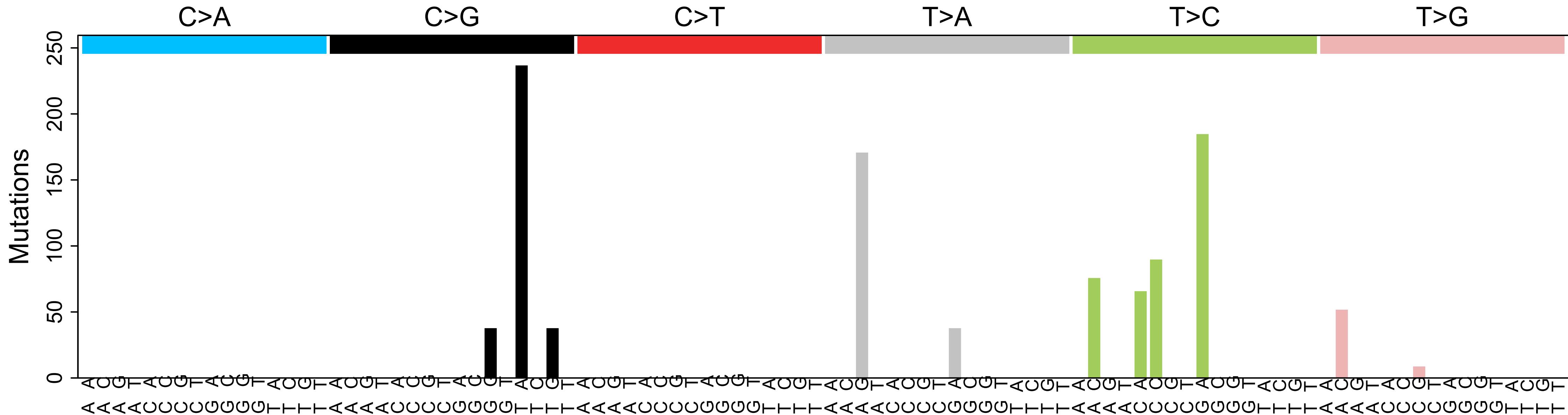
T>C

T>G

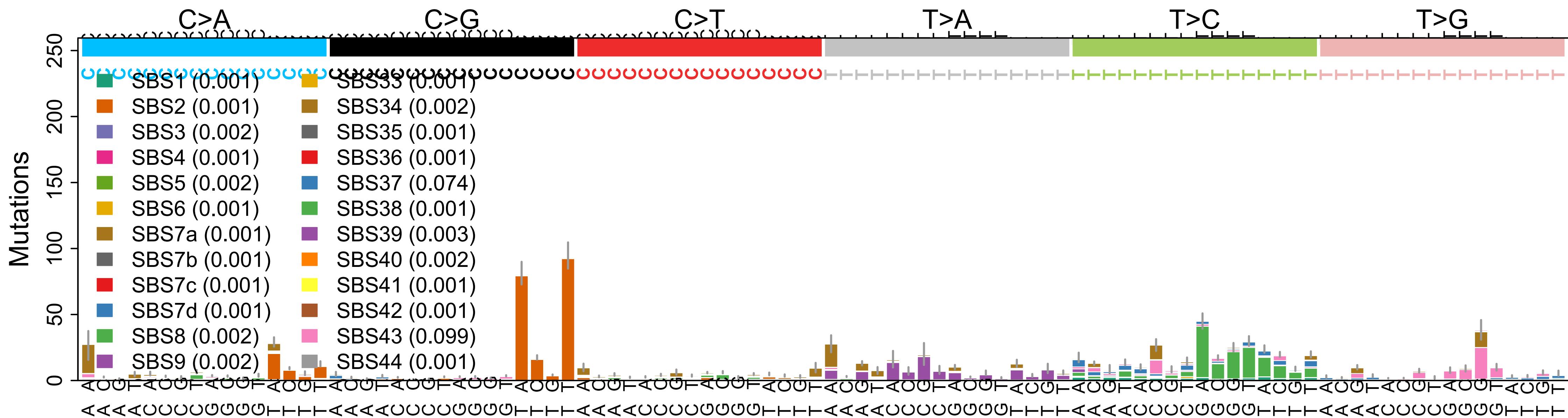
Mutations



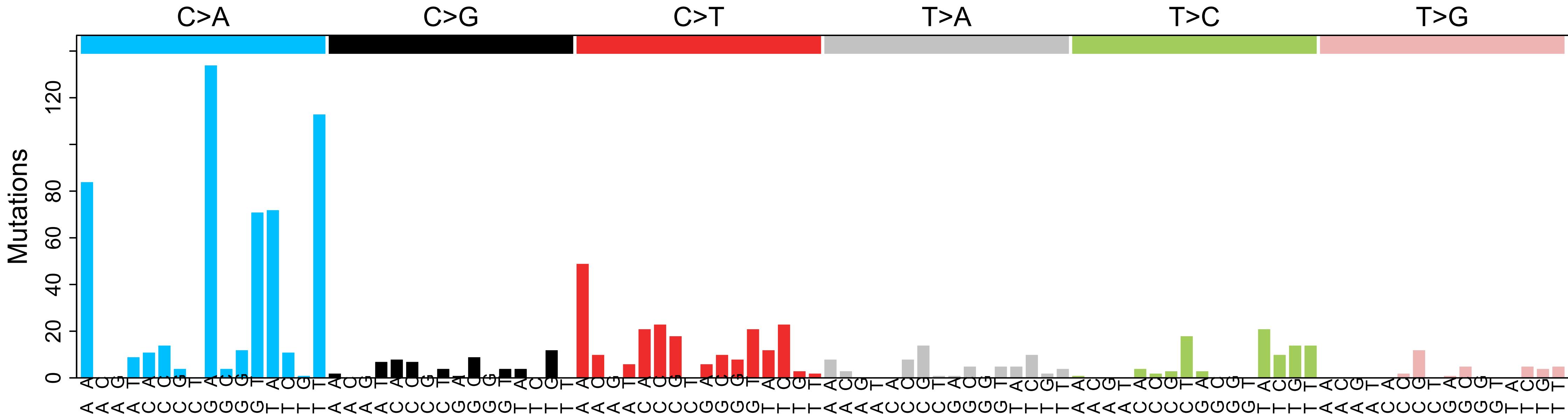
methyleugenol_4048db90dc58 (1,000 mutations)



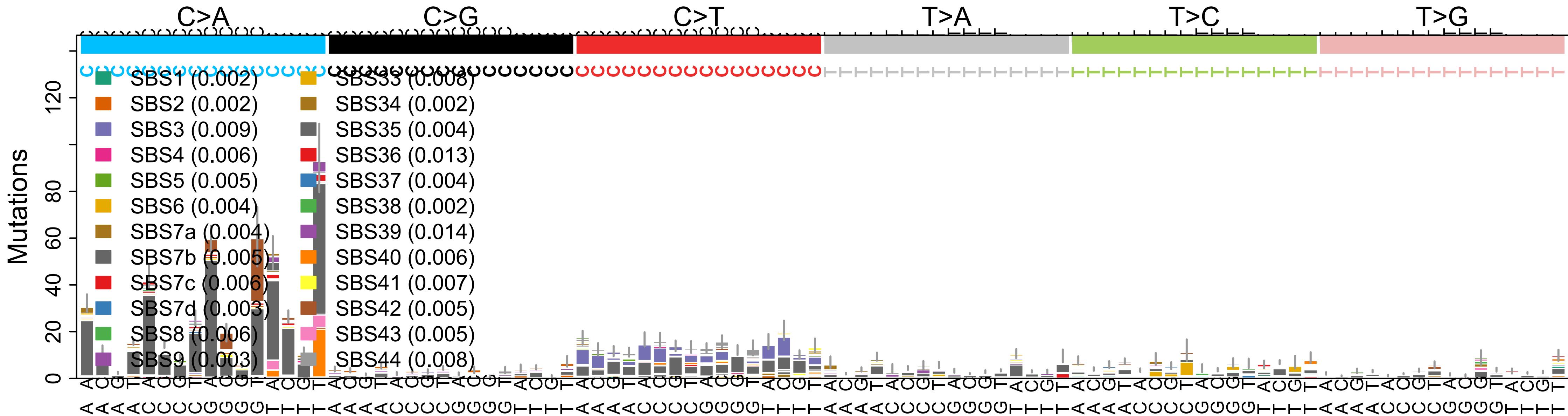
Reconstructed spectrum (cosine similarity = 0.528)



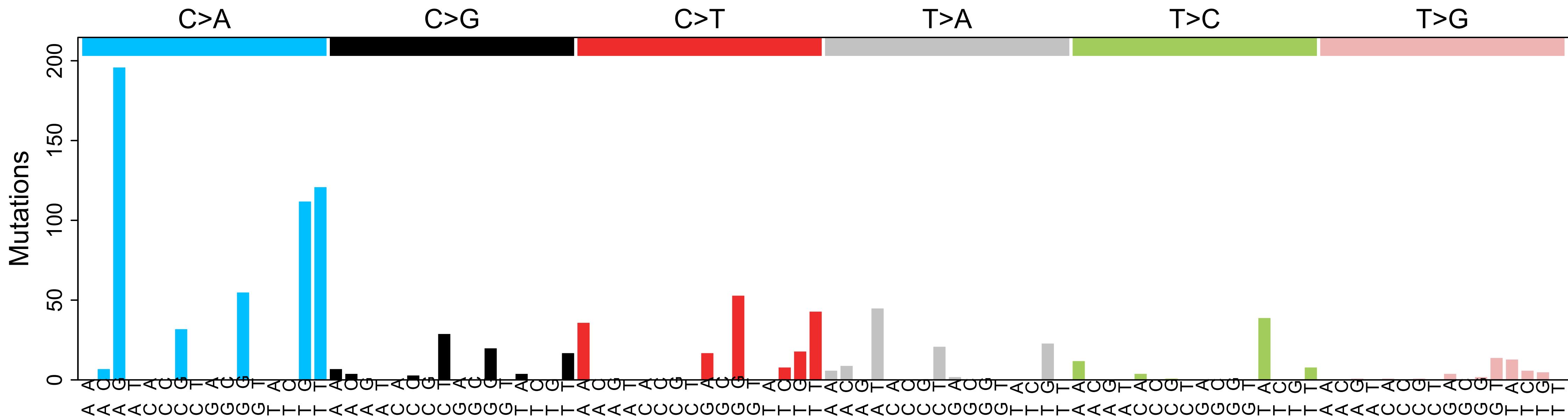
methyleugenol_830517b726f0 (1,000 mutations)



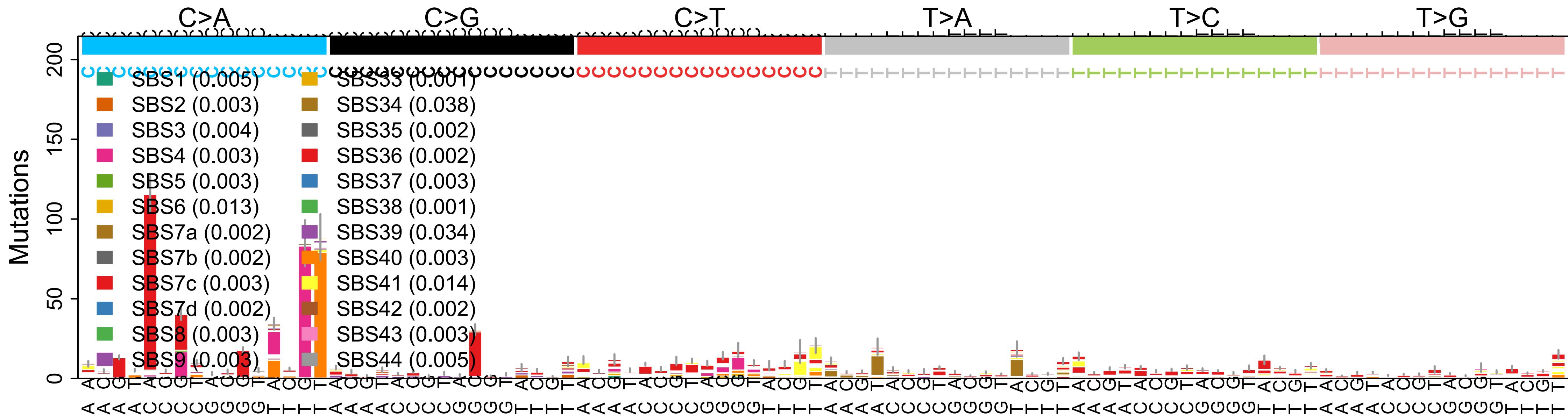
Reconstructed spectrum (cosine similarity = 0.87)



mitomycin_c_1c3f32aa1d84 (999 mutations)



Reconstructed spectrum (cosine similarity = 0.54)



n_ethyl_n_nitrosourea_8164e08a22bc (1,001 mutations)

C>A

C>G

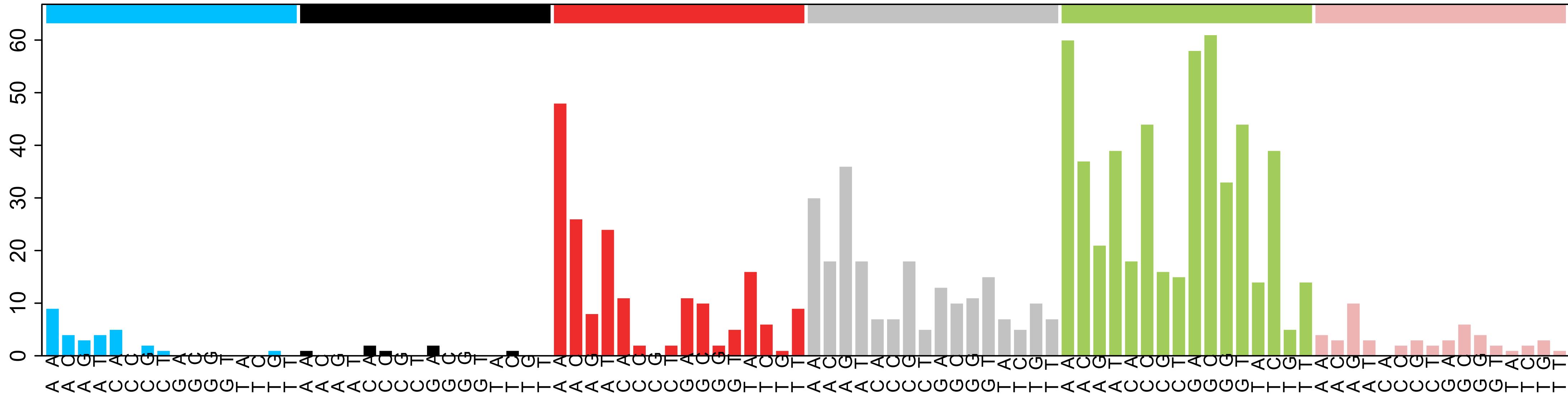
C>T

T>A

T>C

T>G

Mutations



Reconstructed spectrum (cosine similarity = 0.875)

C>A

C>G

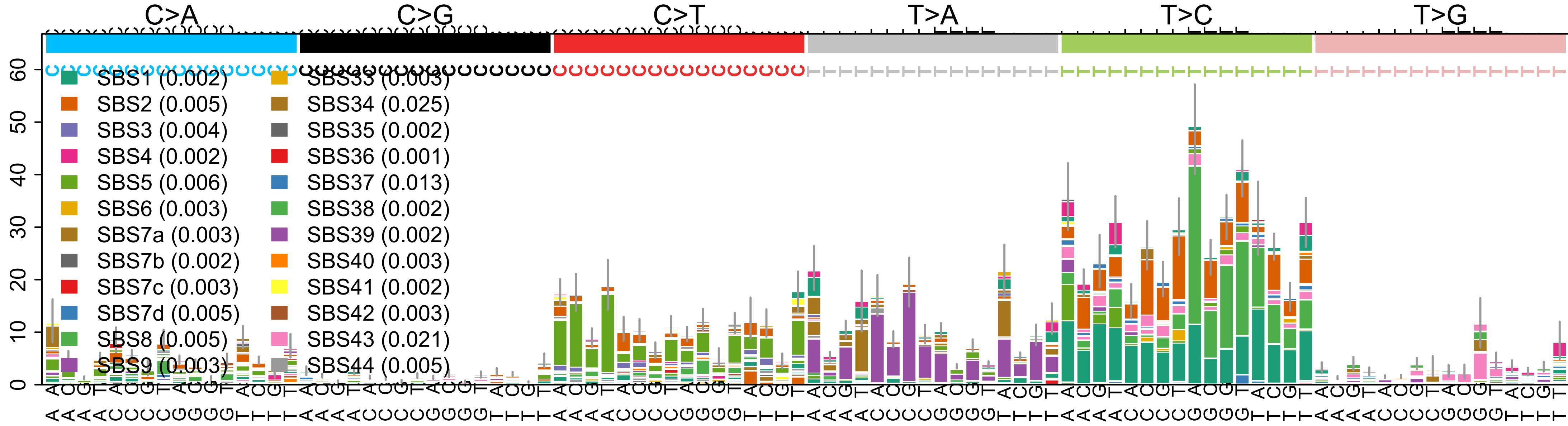
C>T

T>A

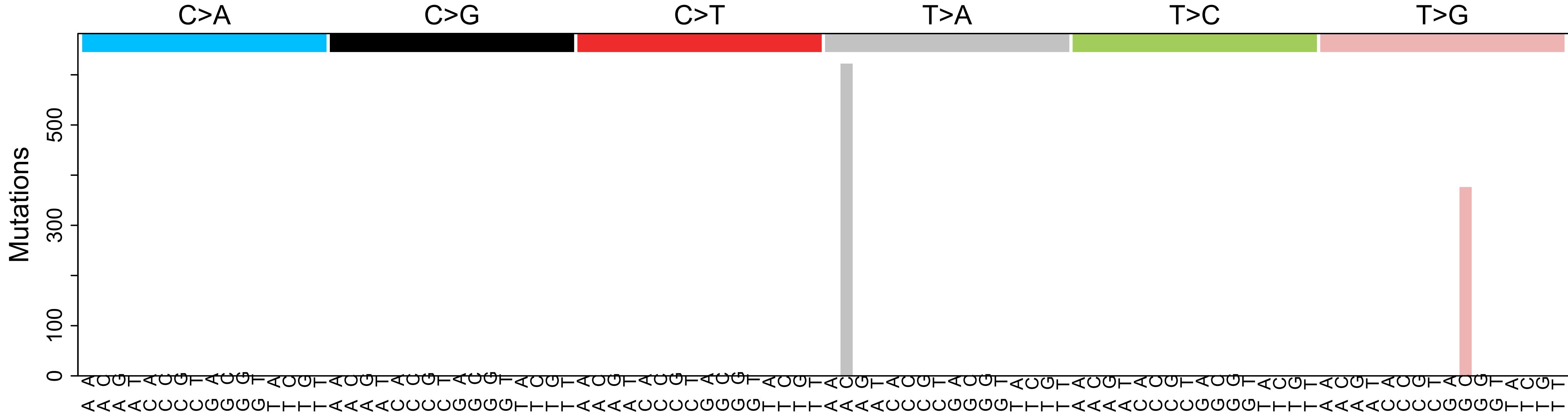
T>C

T>G

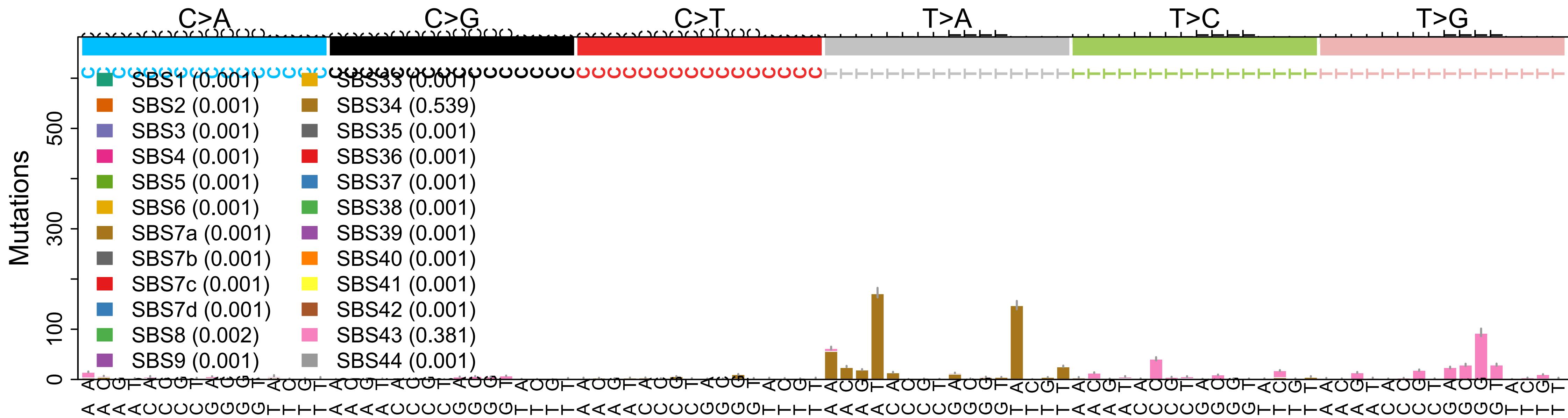
Mutations



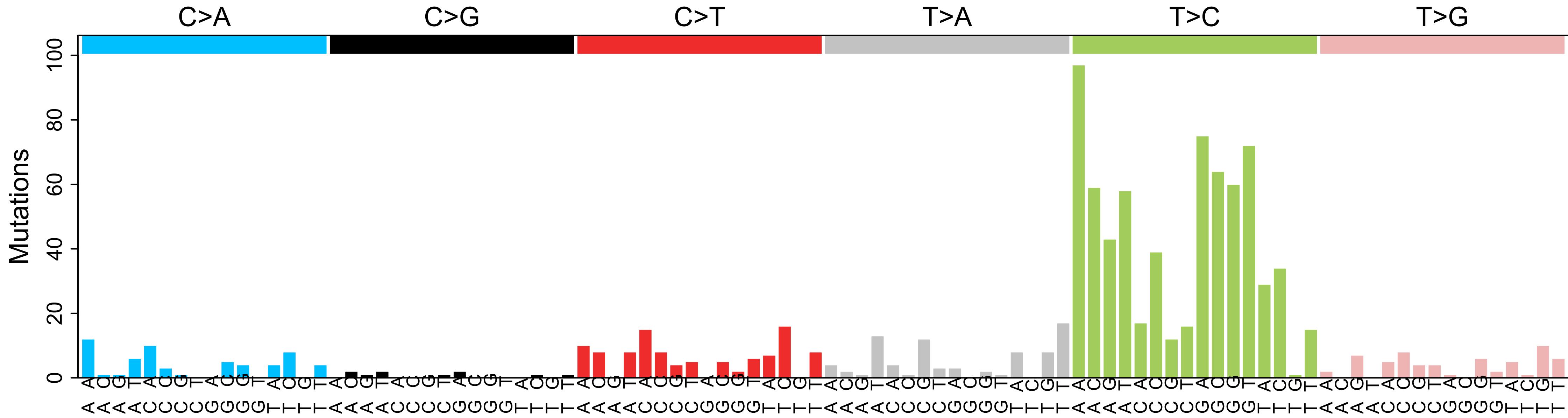
n_methyl_n_nitro_nitrosoguanidine_ca5b1ff8ee0d (1,000 mutations)



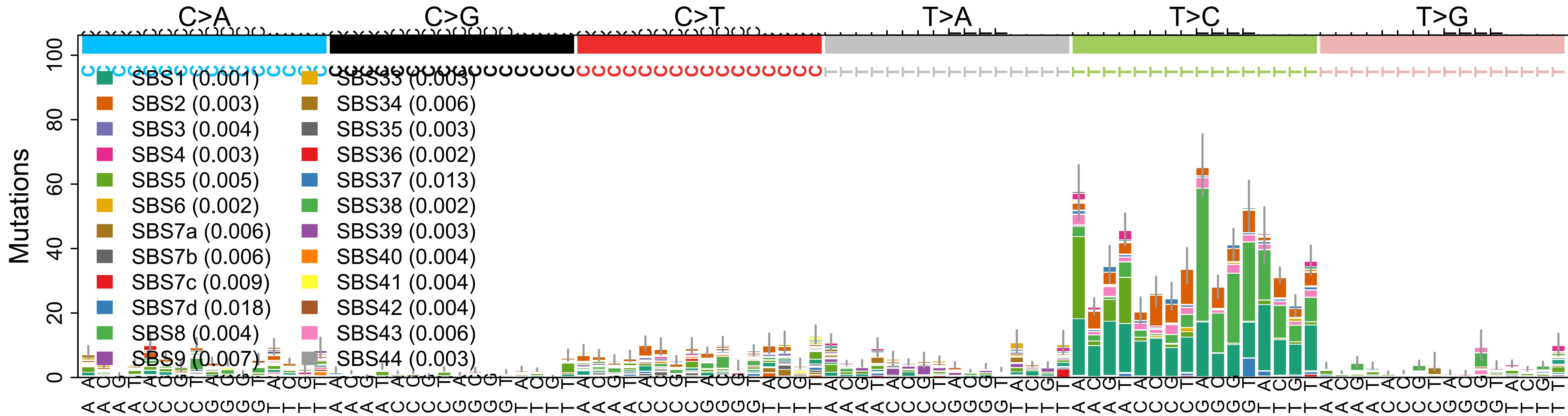
Reconstructed spectrum (cosine similarity = 0.137)



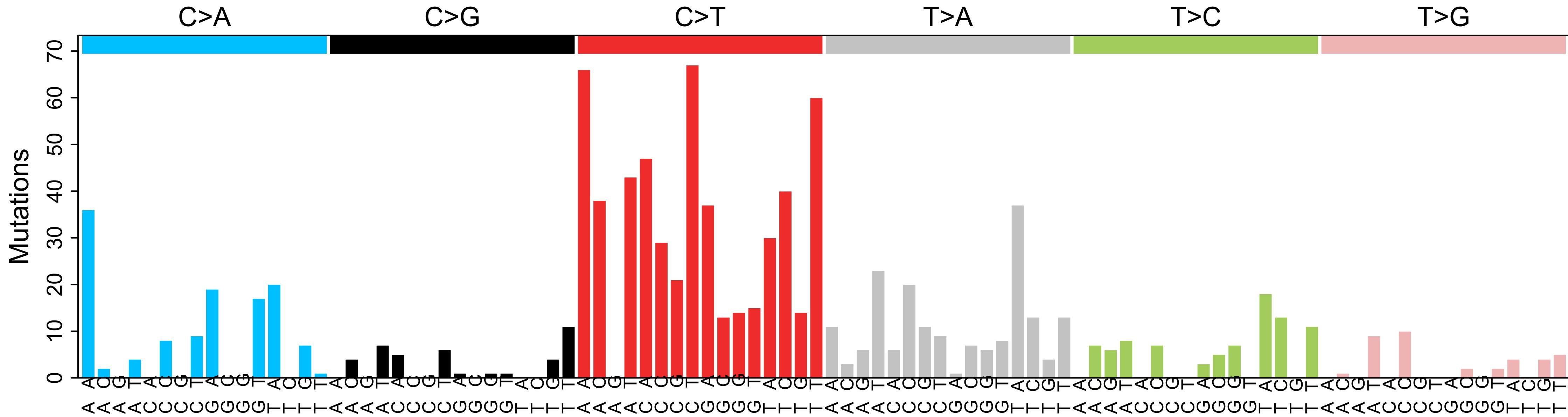
n_methyl_n_nitrosourea_9a944873342f (1,002 mutations)



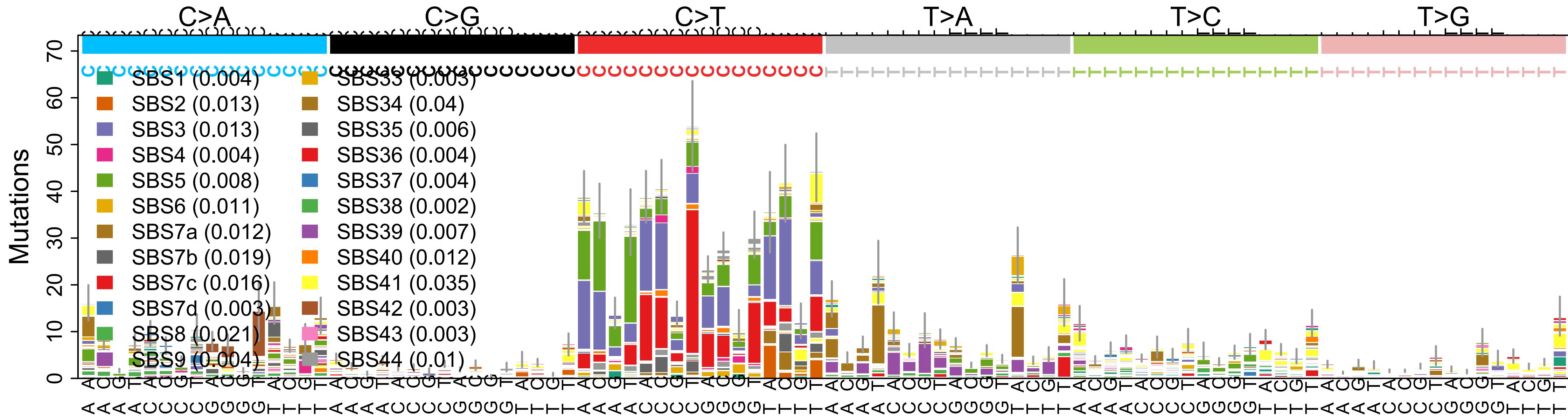
Reconstructed spectrum (cosine similarity = 0.911)



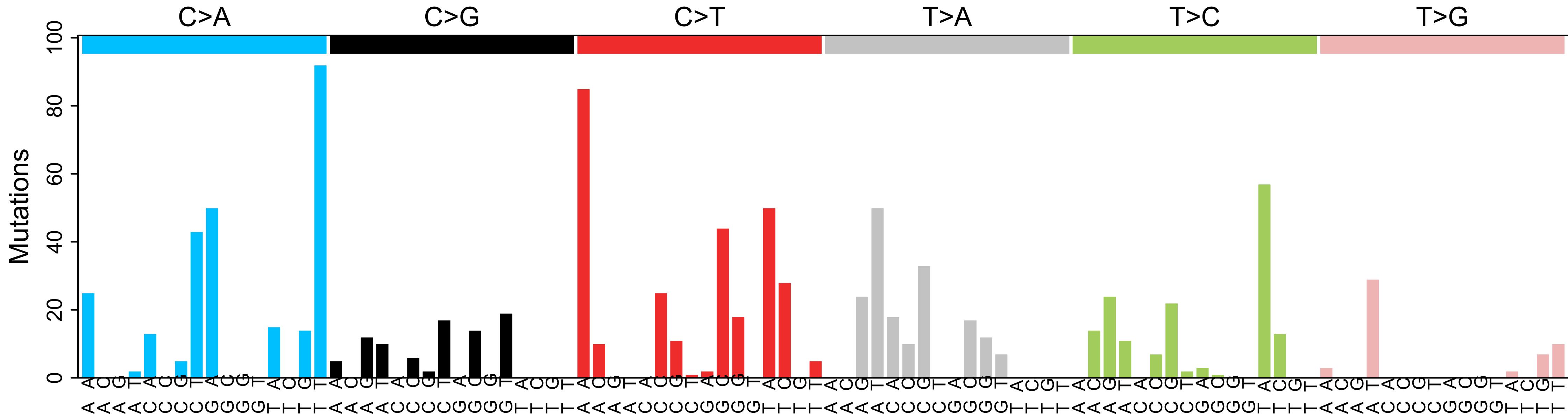
n_nitrosopyrrolidine_ff630a9dde6d (997 mutations)



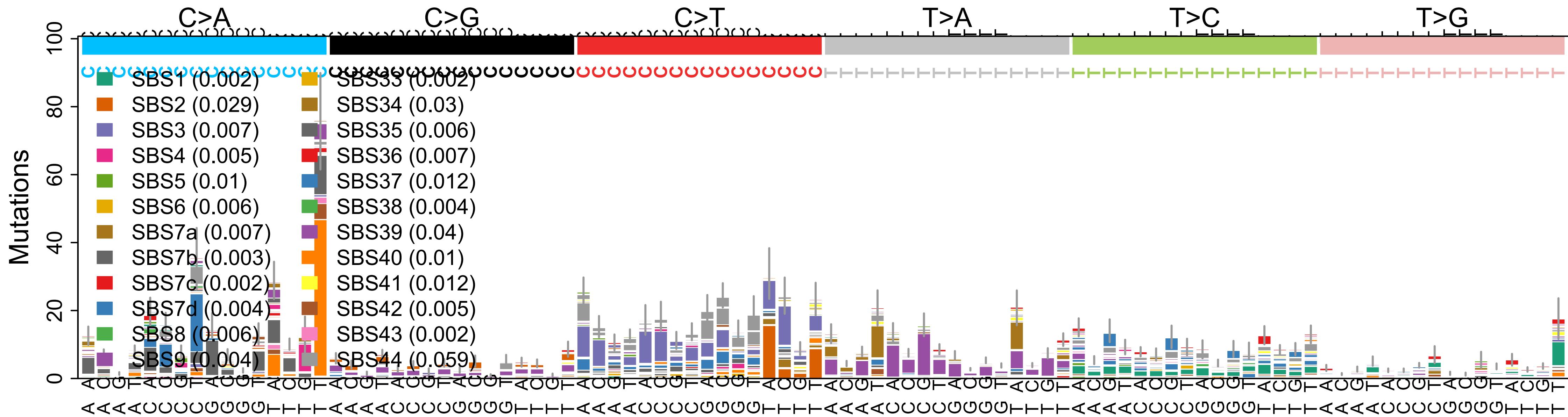
Reconstructed spectrum (cosine similarity = 0.922)



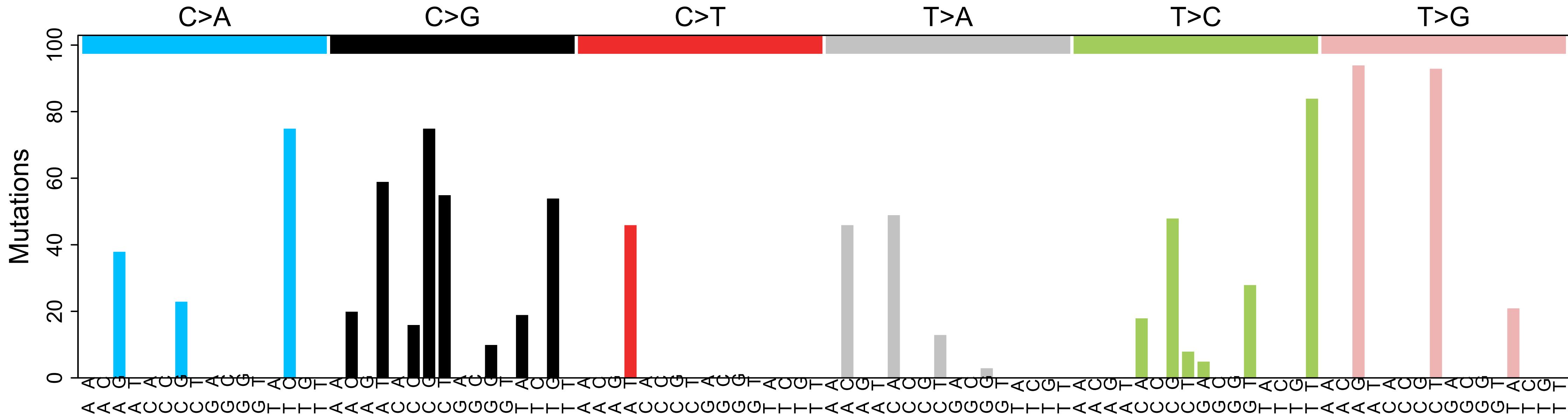
nickel_chloride_70a11a6d19e0 (999 mutations)



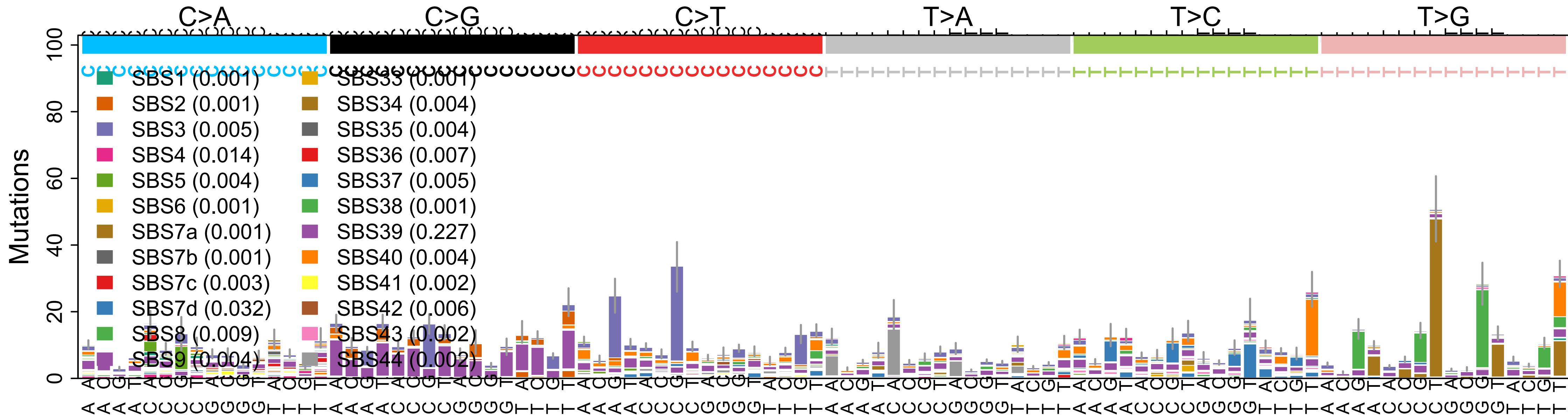
Reconstructed spectrum (cosine similarity = 0.779)



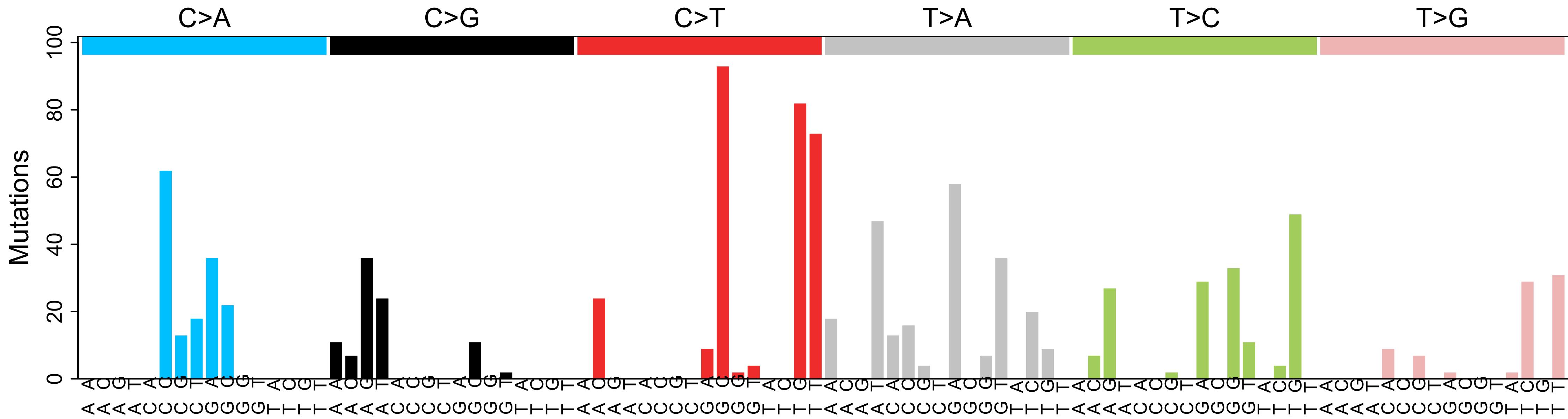
no_treatment_2d9081e4d720 (1,000 mutations)



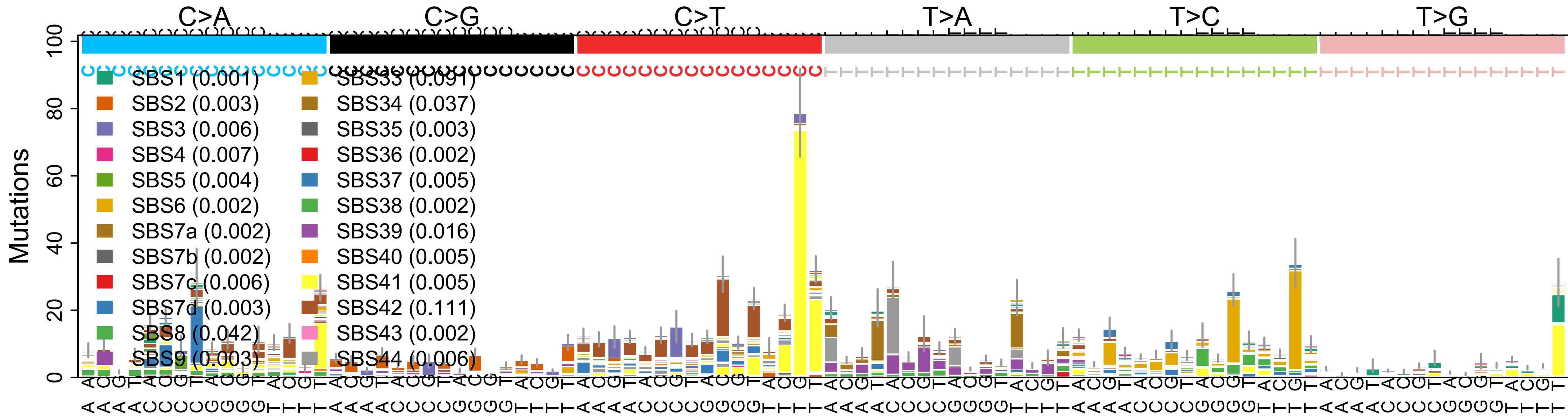
Reconstructed spectrum (cosine similarity = 0.54)



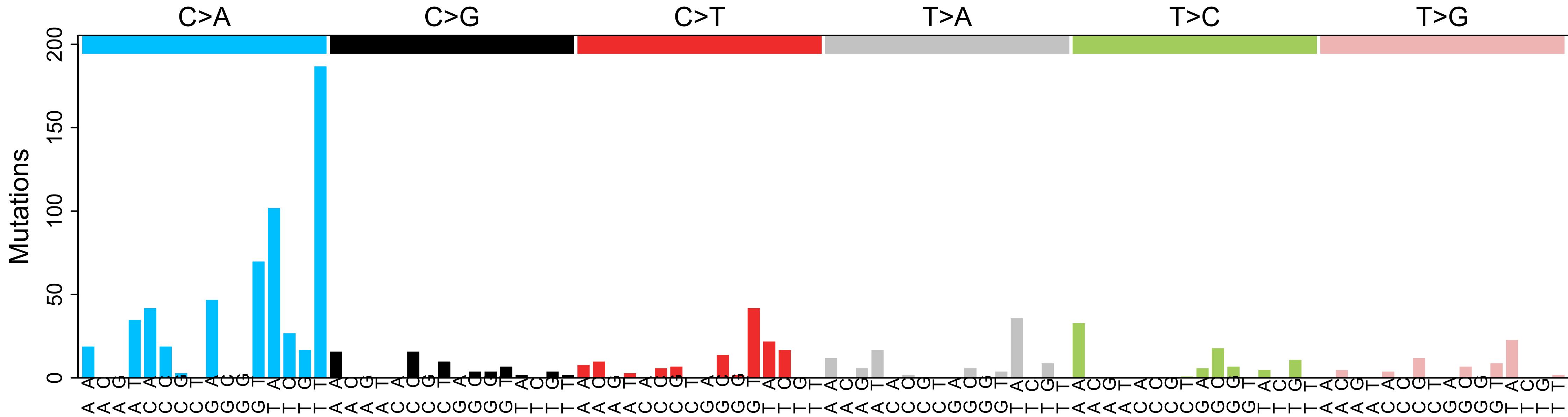
no_treatment_368d8667e685 (999 mutations)



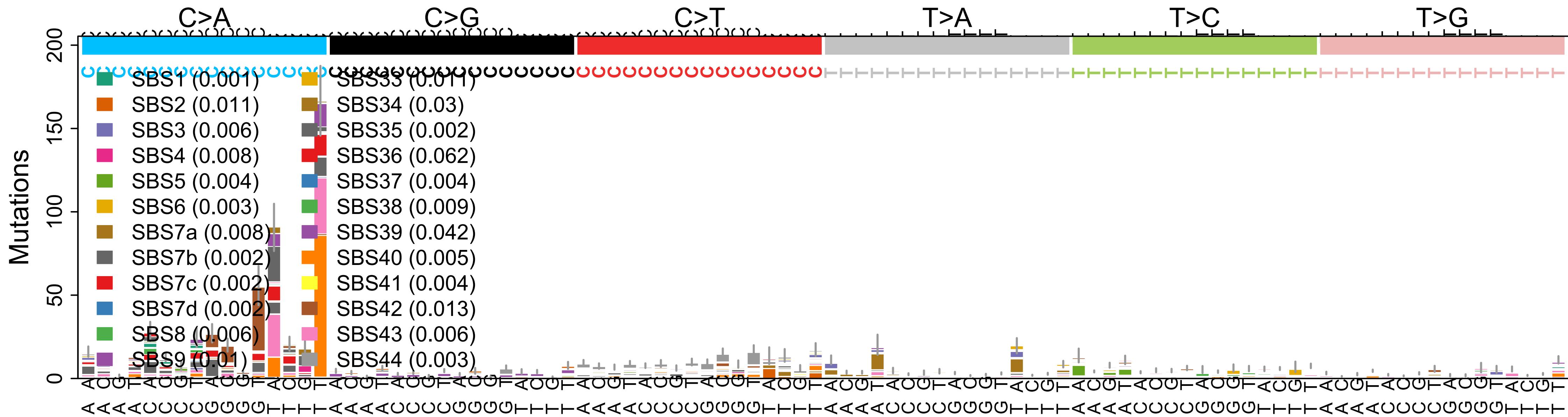
Reconstructed spectrum (cosine similarity = 0.725)



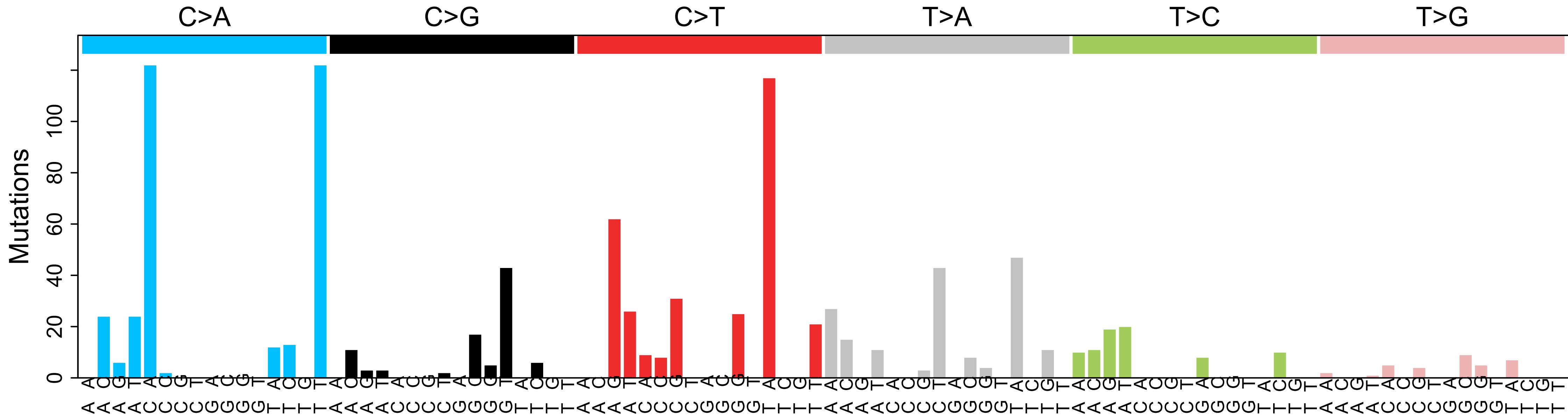
o_anisidine_140b3b7221ca (999 mutations)



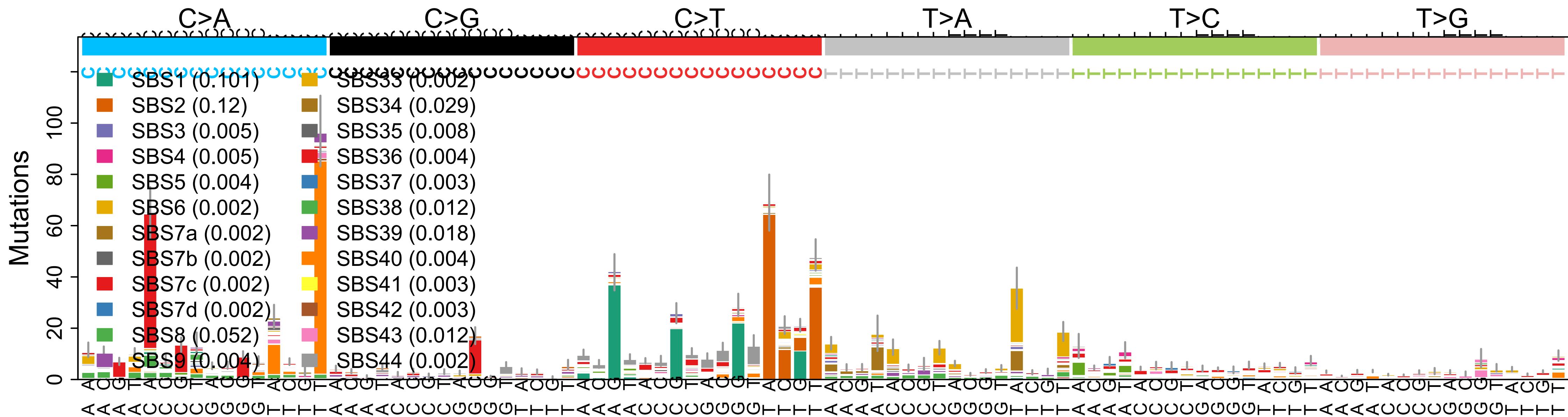
Reconstructed spectrum (cosine similarity = 0.949)



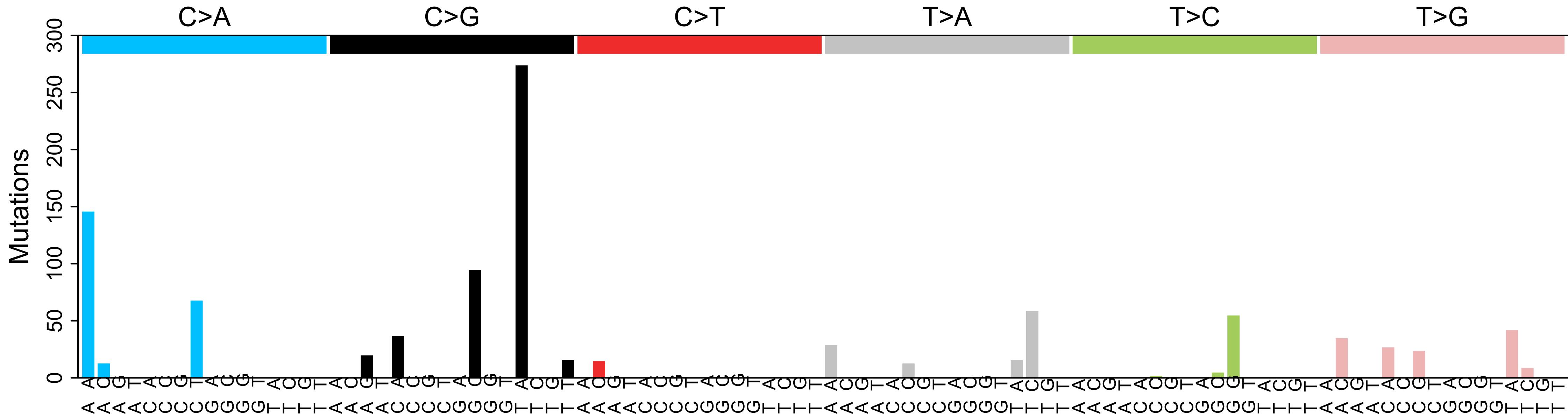
o_anisidine_9552a08d7147 (994 mutations)



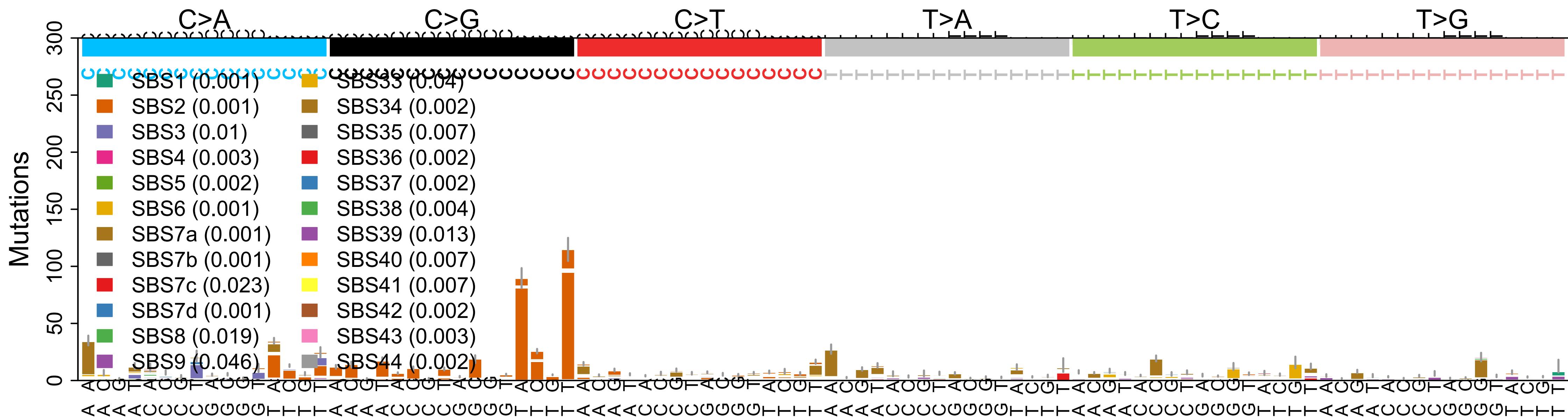
Reconstructed spectrum (cosine similarity = 0.884)



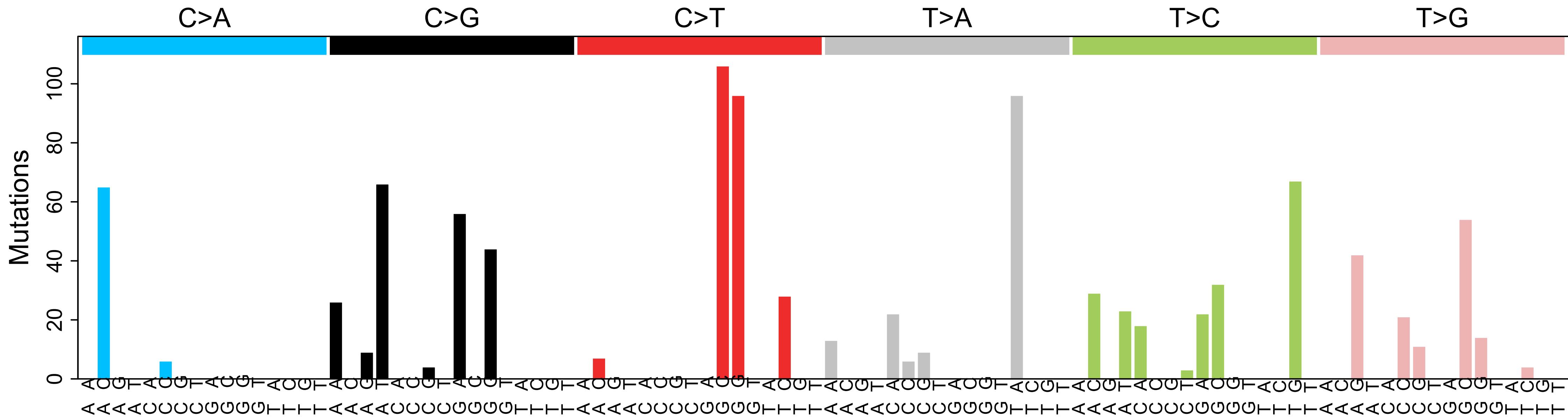
o_toluidine_0d620c5f38d0 (1,000 mutations)



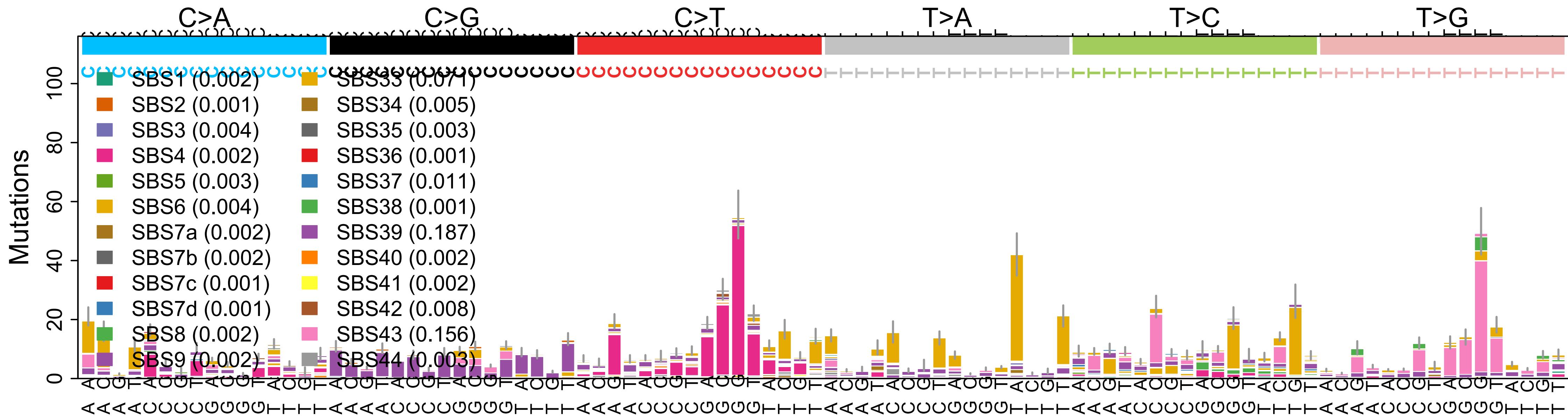
Reconstructed spectrum (cosine similarity = 0.593)



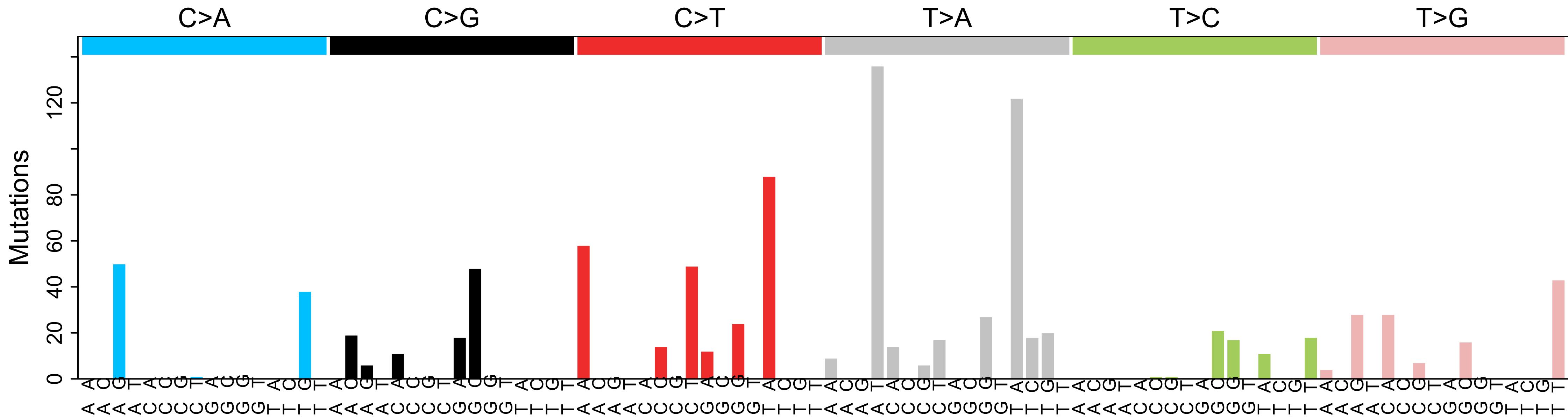
ochratoxin_a_9b5acc8297cd (999 mutations)



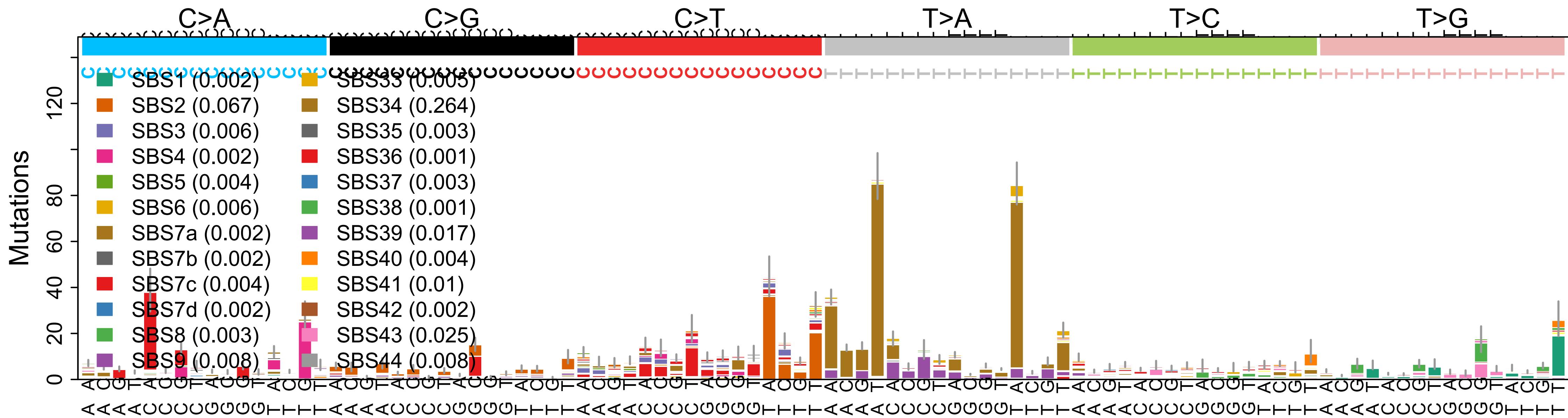
Reconstructed spectrum (cosine similarity = 0.65)



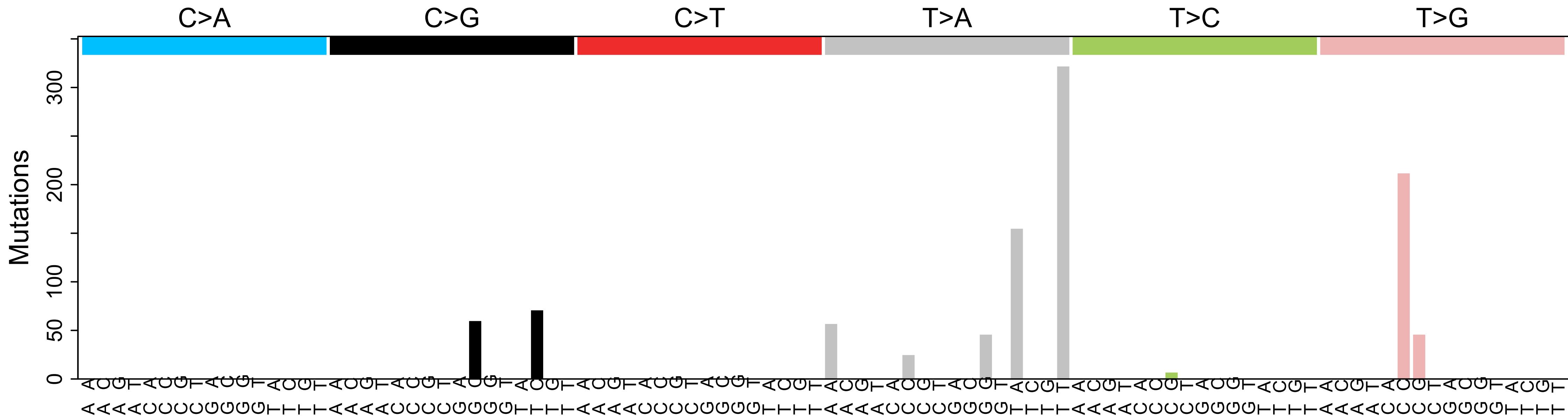
olaparib_43d725f7cc82 (1,000 mutations)



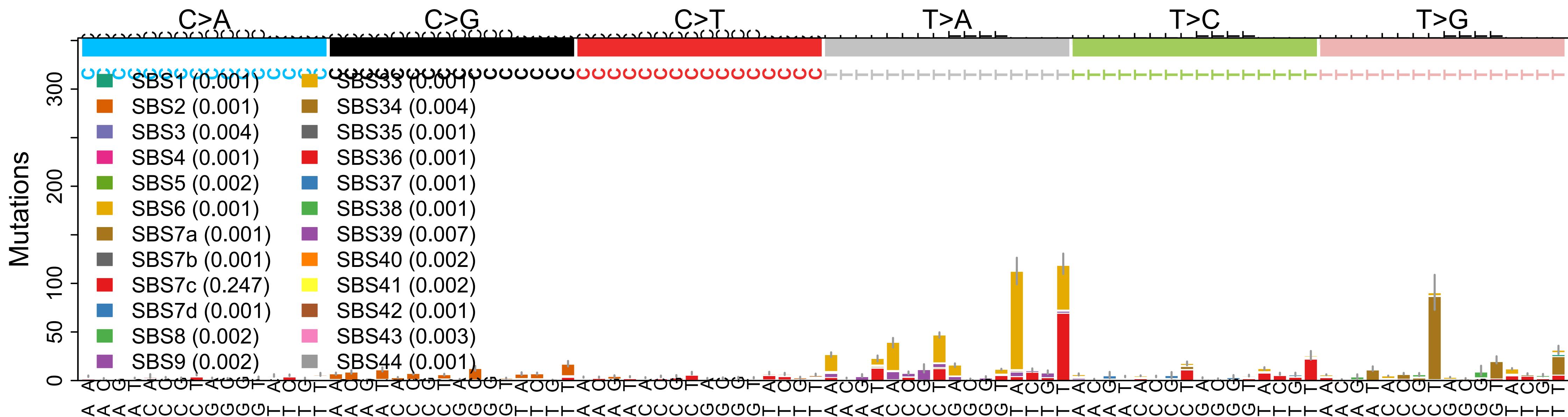
Reconstructed spectrum (cosine similarity = 0.808)



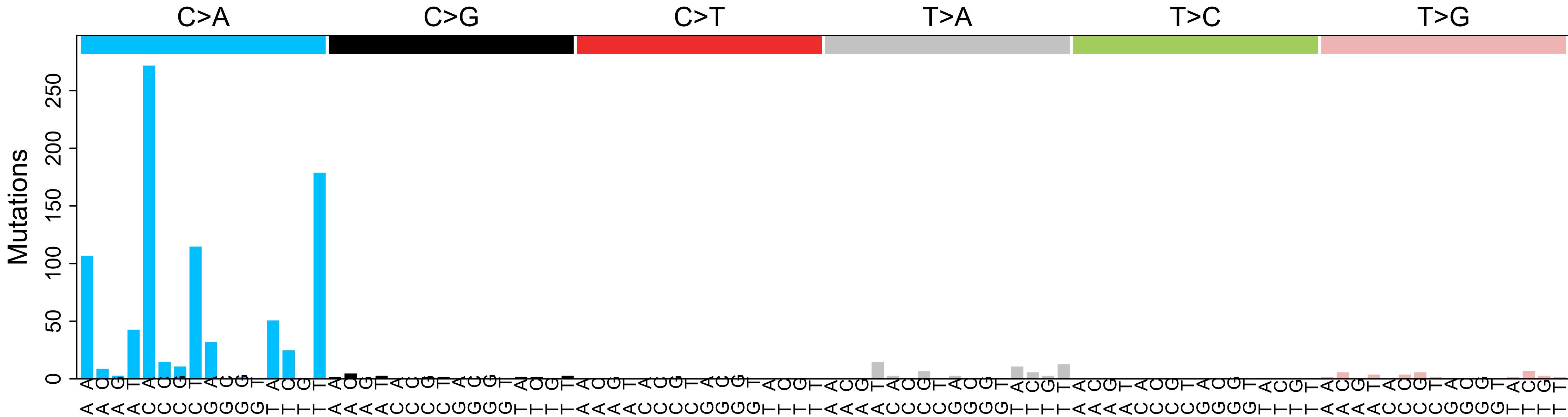
peroxynitrite_7cadeaf3e612 (1,001 mutations)



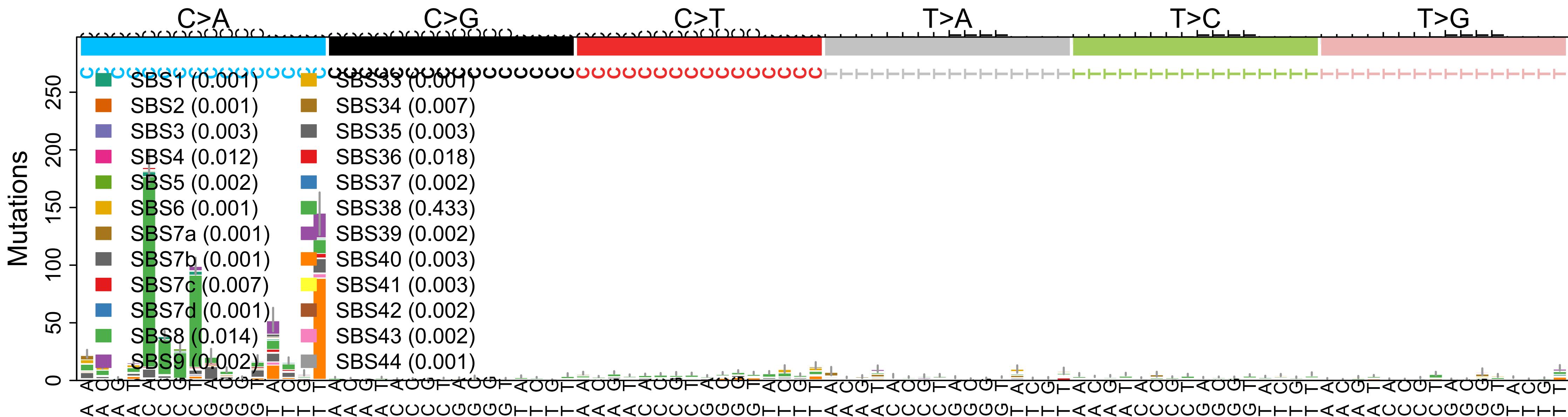
Reconstructed spectrum (cosine similarity = 0.651)



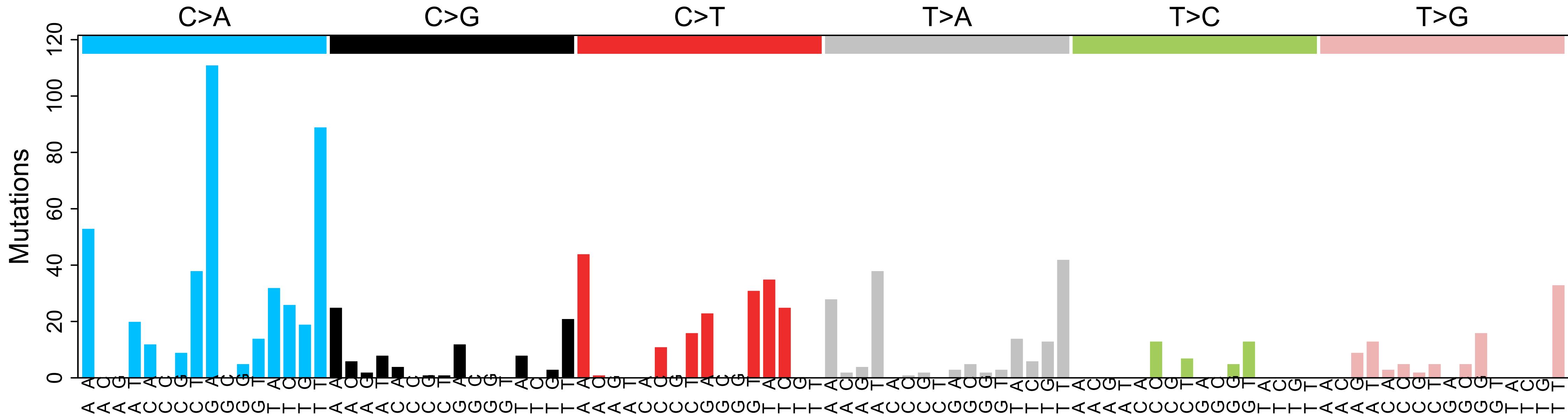
potassium_bromate_69b10ec2b4fd (1,000 mutations)



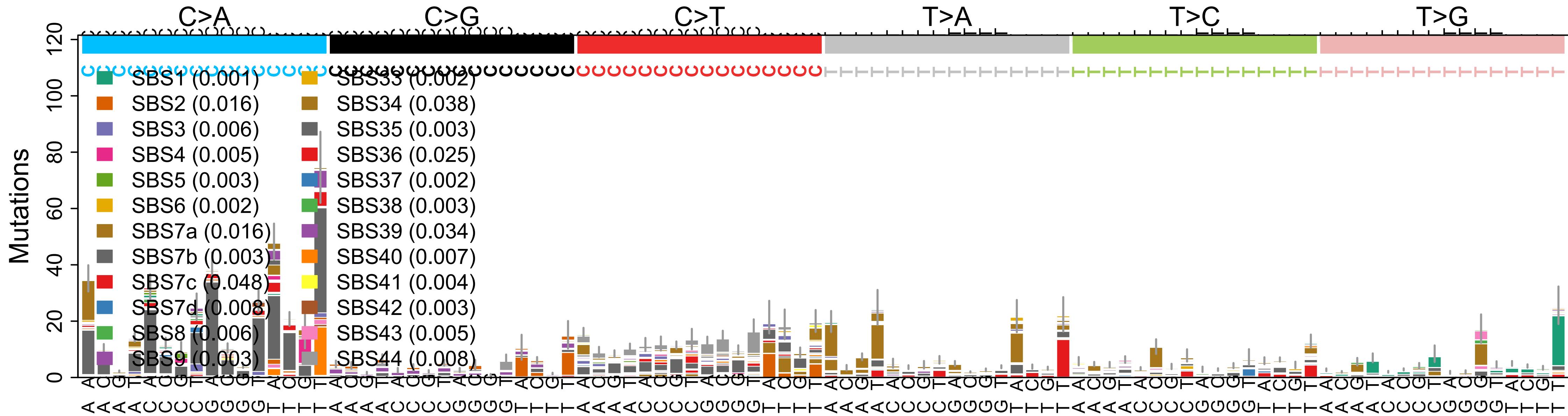
Reconstructed spectrum (cosine similarity = 0.951)



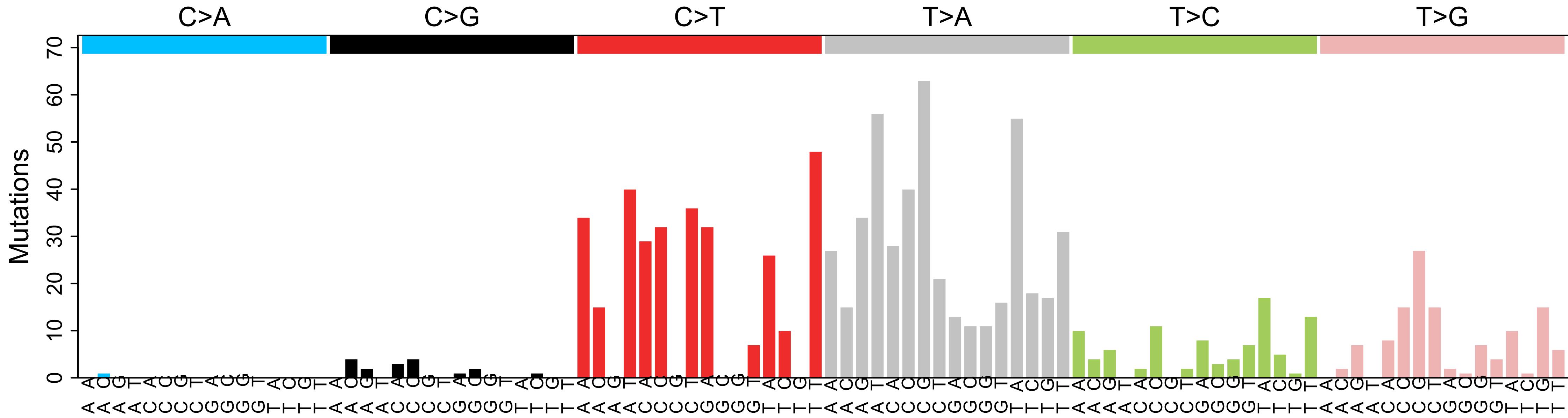
potassium_chromate_0bdc1b5144e0 (997 mutations)



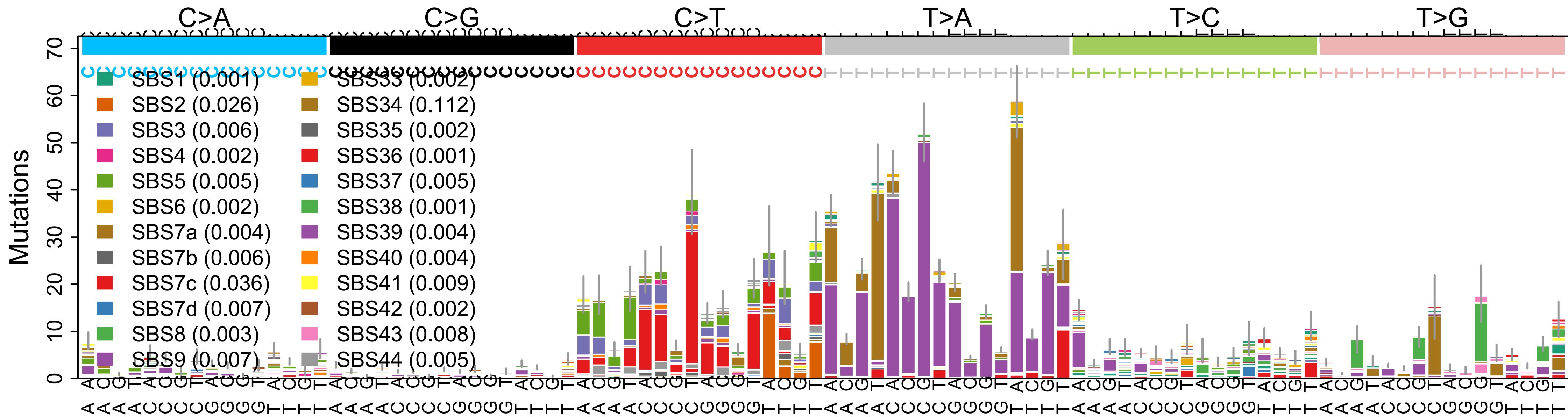
Reconstructed spectrum (cosine similarity = 0.847)



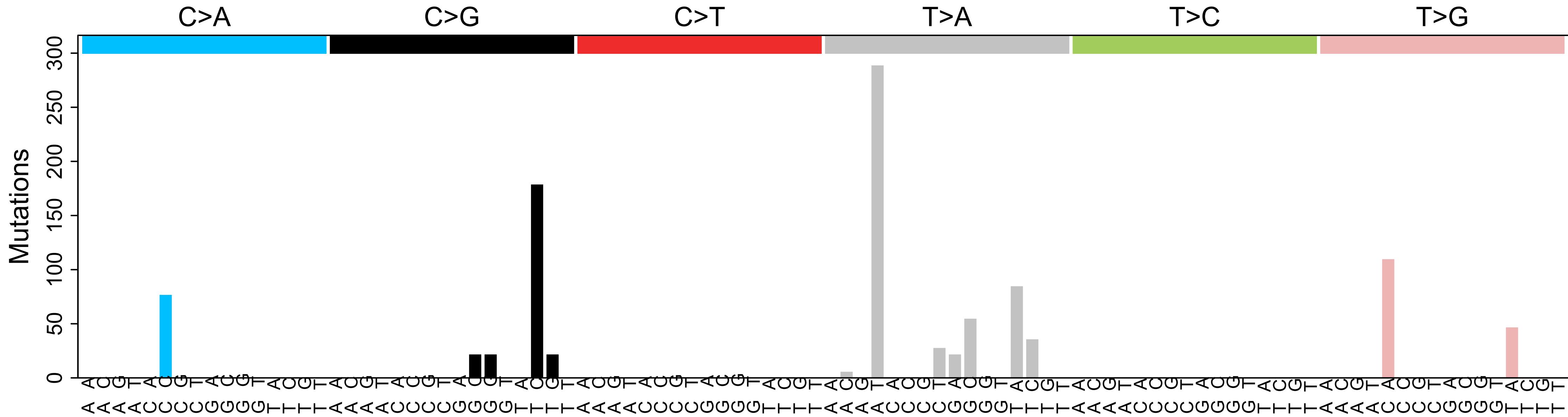
propylene_oxide_7197becf3bd8 (996 mutations)



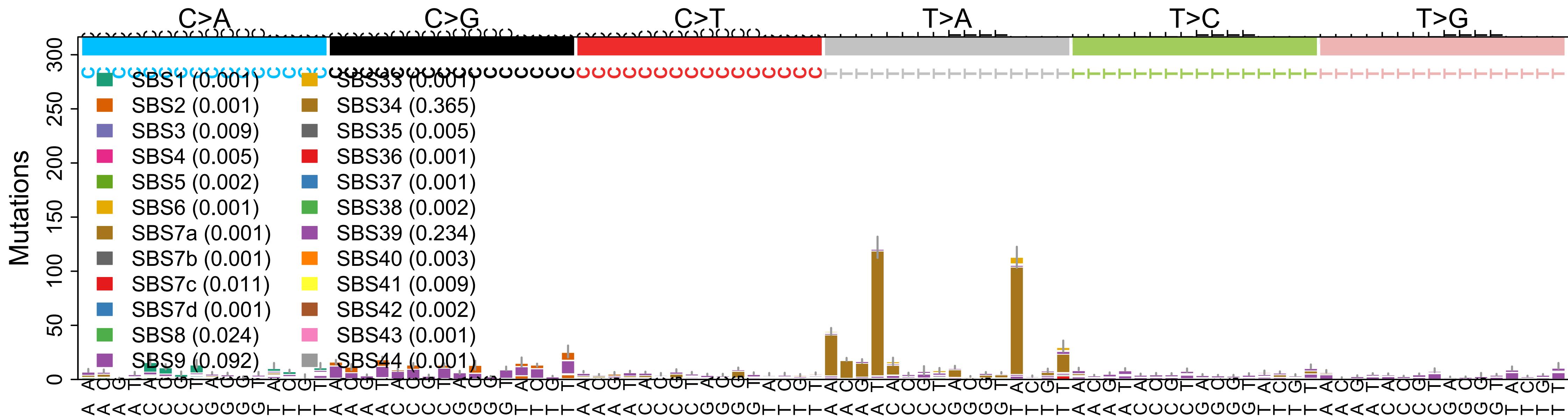
Reconstructed spectrum (cosine similarity = 0.91)



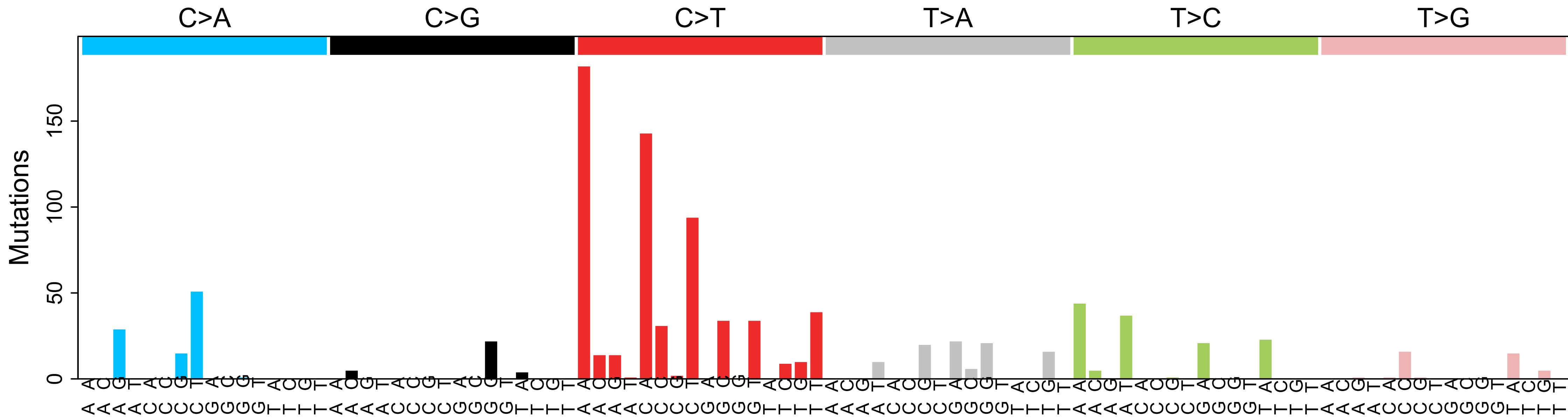
semustine_5a98bdaabcd0 (1,000 mutations)



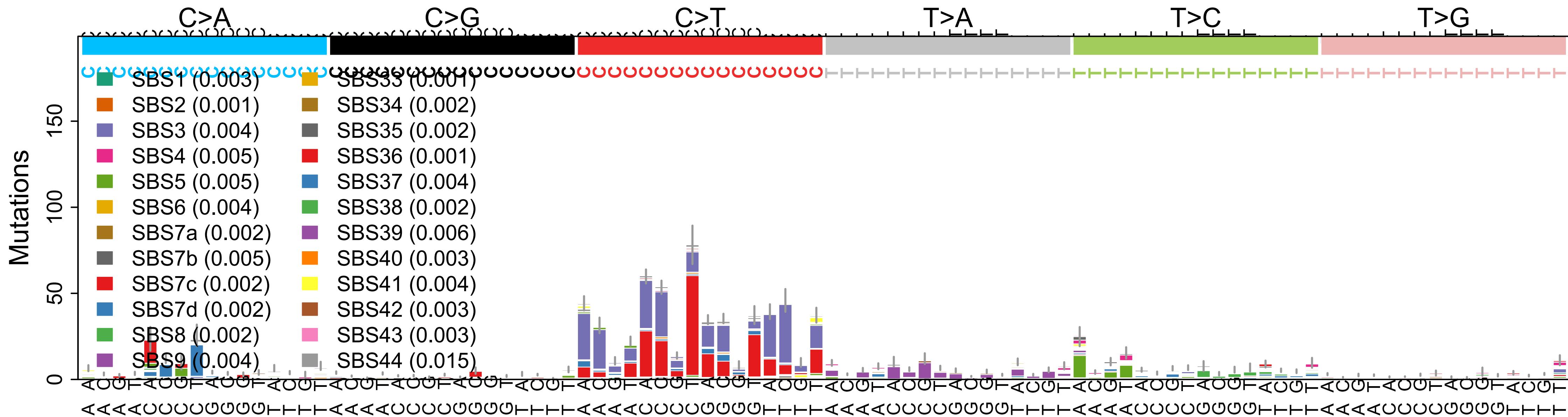
Reconstructed spectrum (cosine similarity = 0.672)



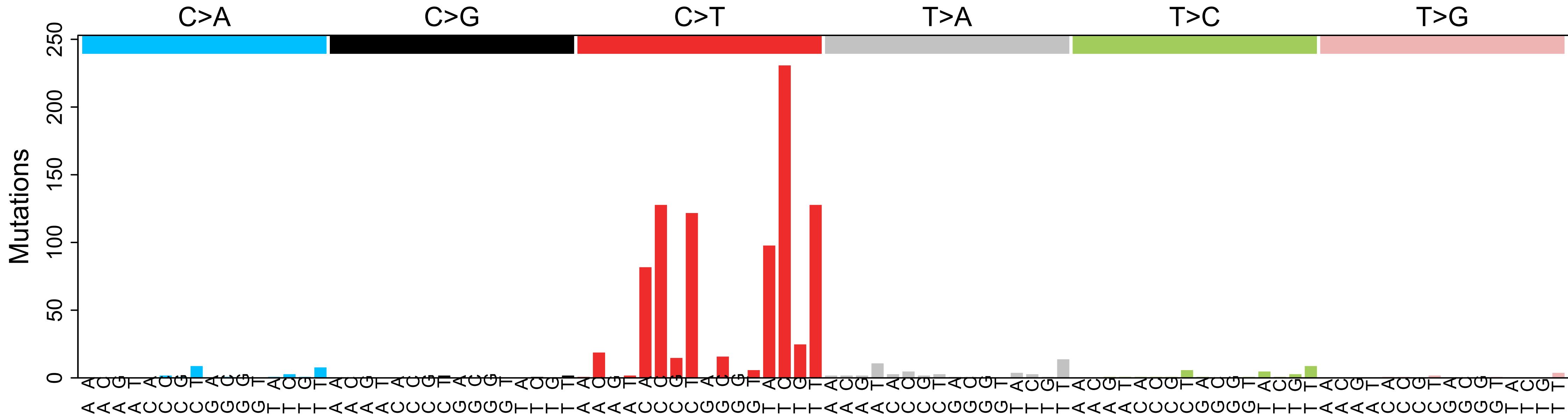
semustine_f81842a4d573 (999 mutations)



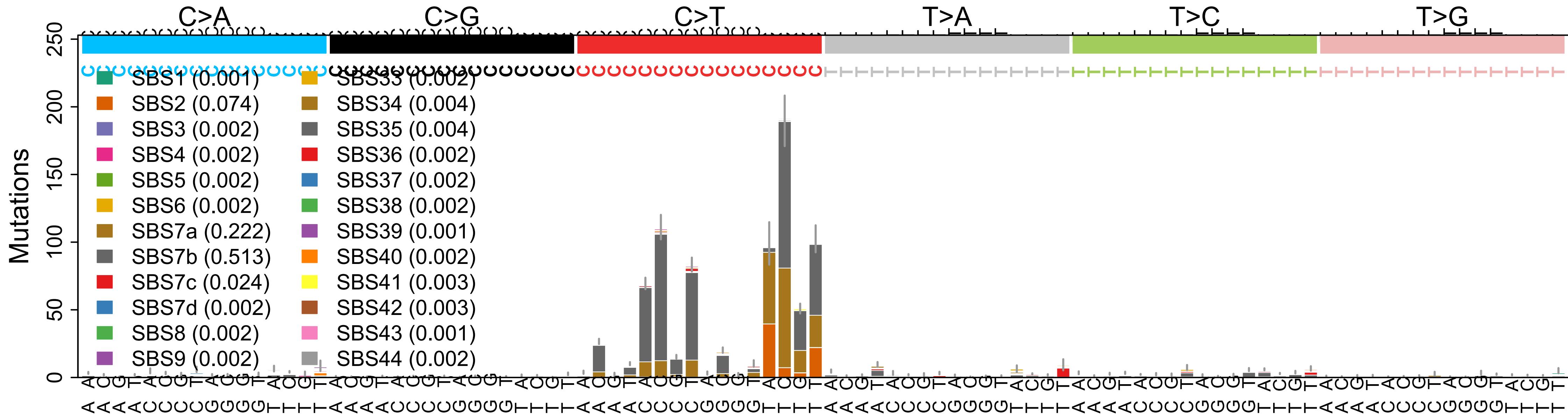
Reconstructed spectrum (cosine similarity = 0.726)



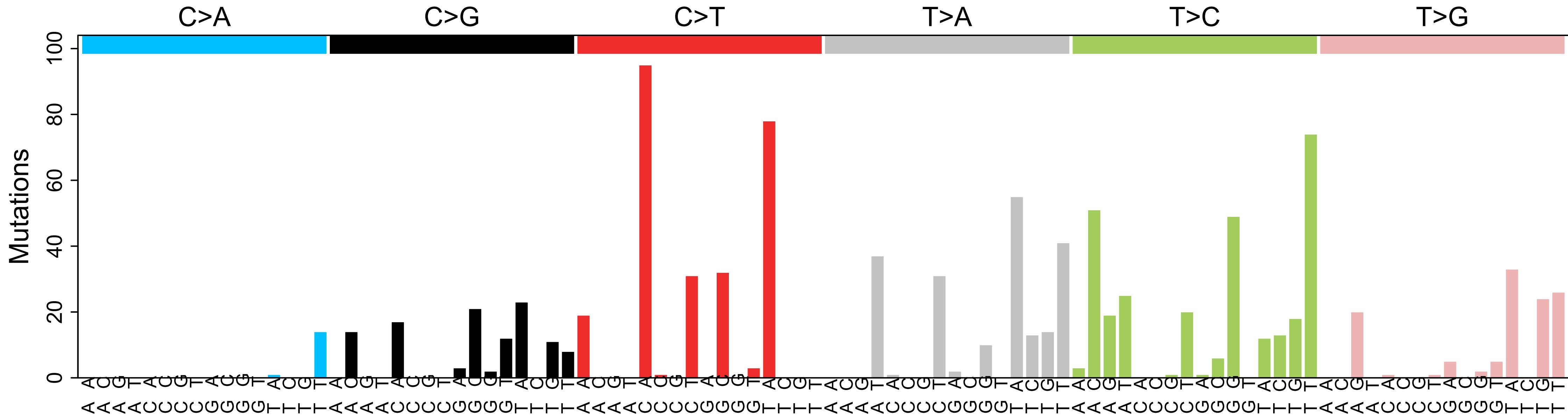
simulated_solar_radiation_04d97e27a495 (998 mutations)



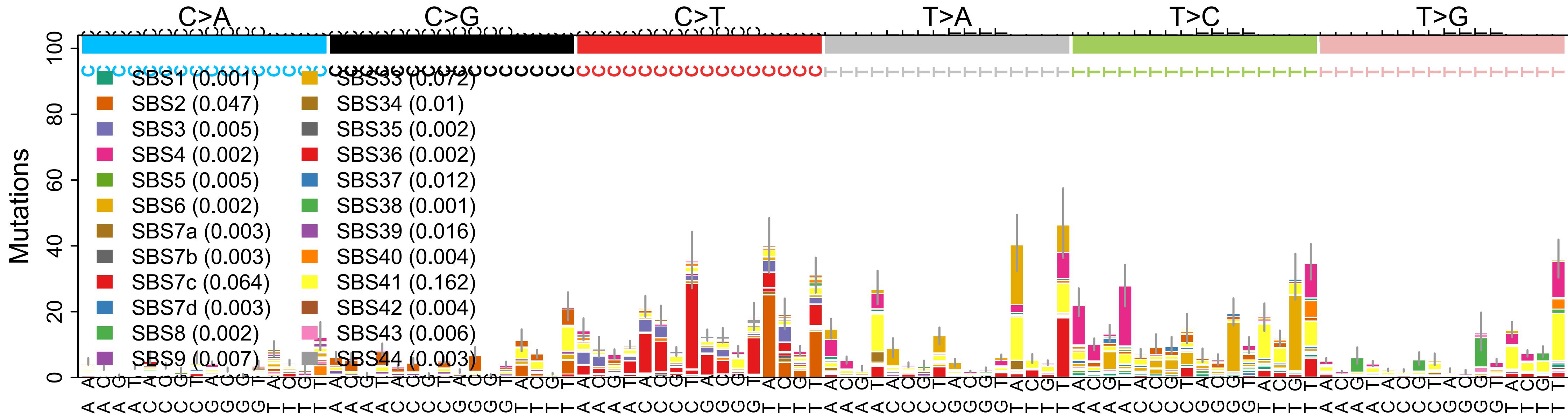
Reconstructed spectrum (cosine similarity = 0.988)



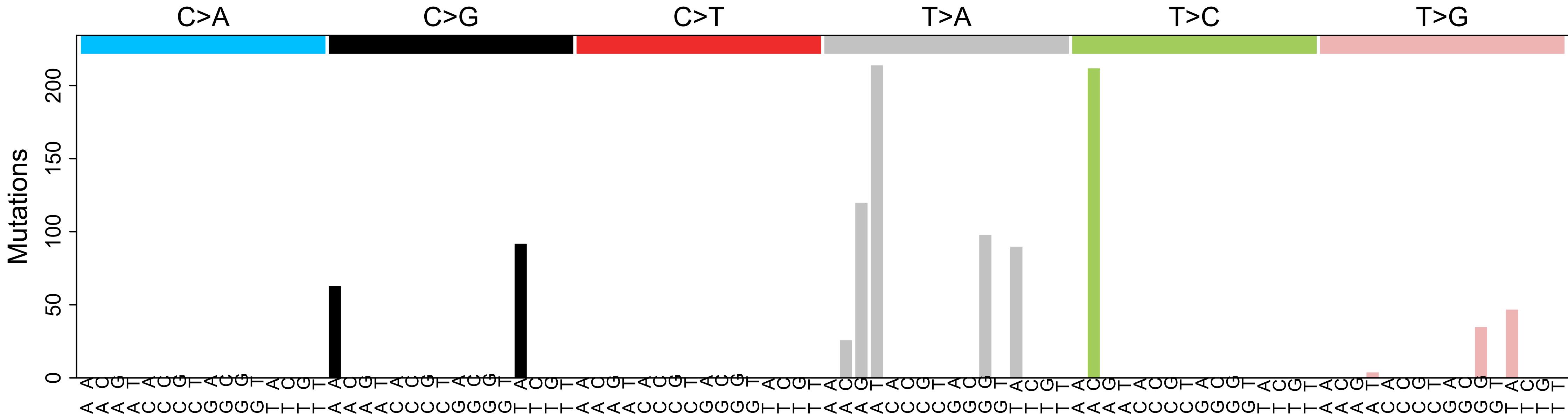
sodium_arsenite_90245b3e0140 (998 mutations)



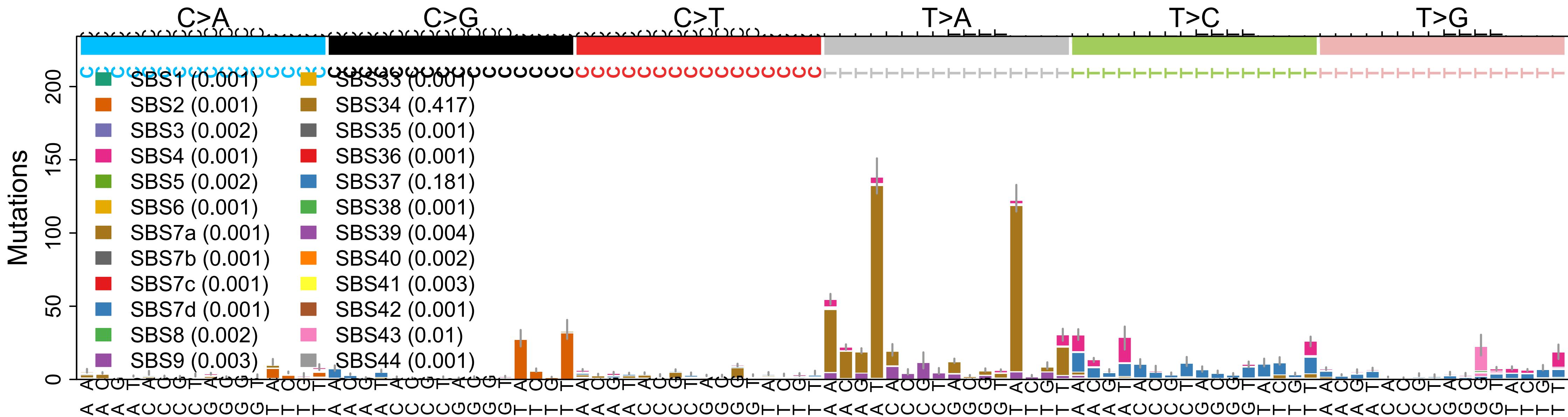
Reconstructed spectrum (cosine similarity = 0.75)



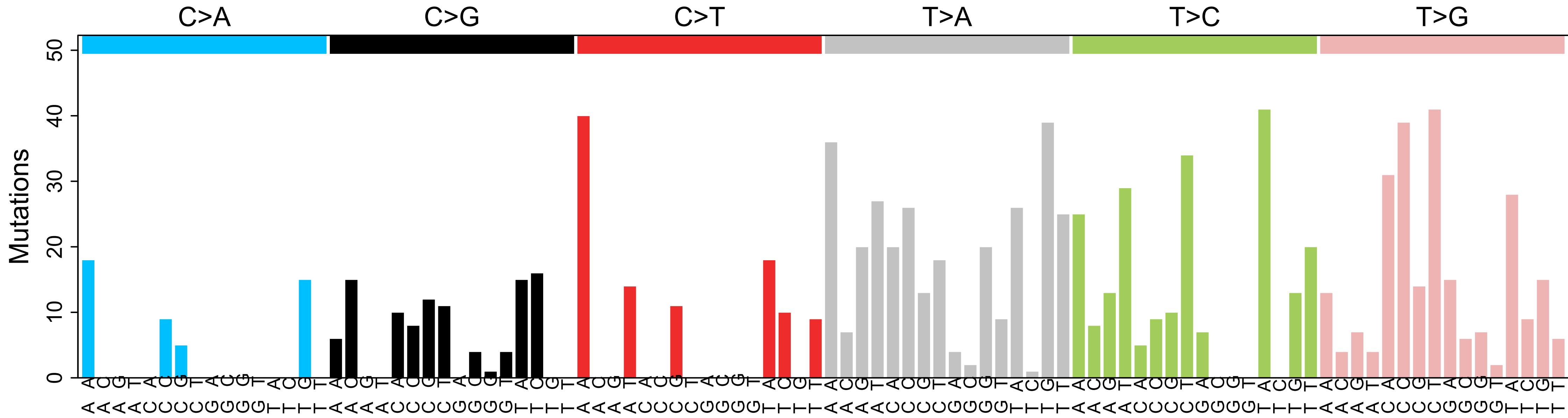
sodium_chloride_02280bd72cf9 (1,001 mutations)



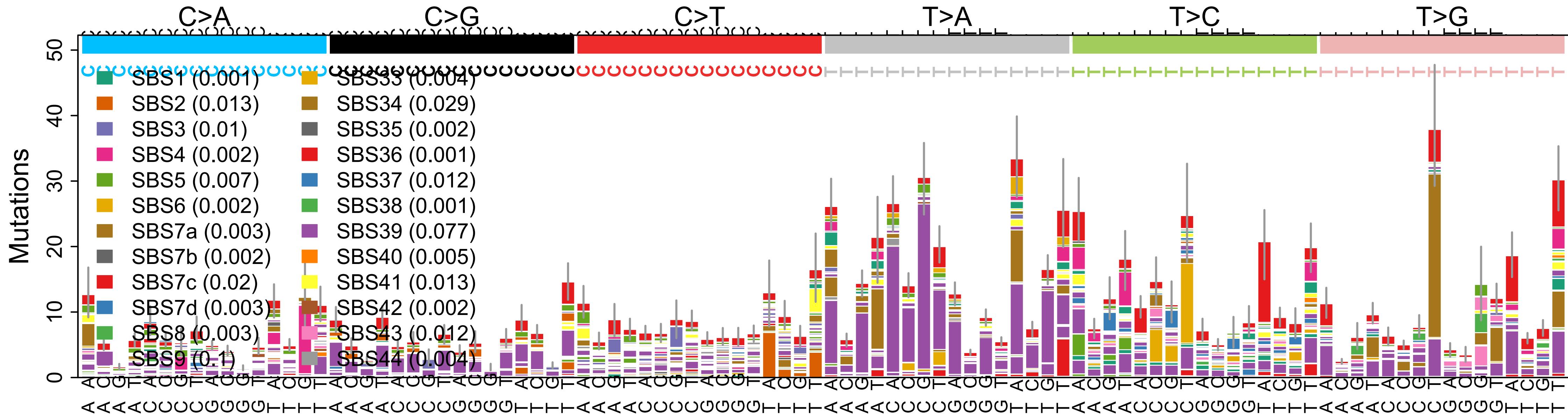
Reconstructed spectrum (cosine similarity = 0.63)



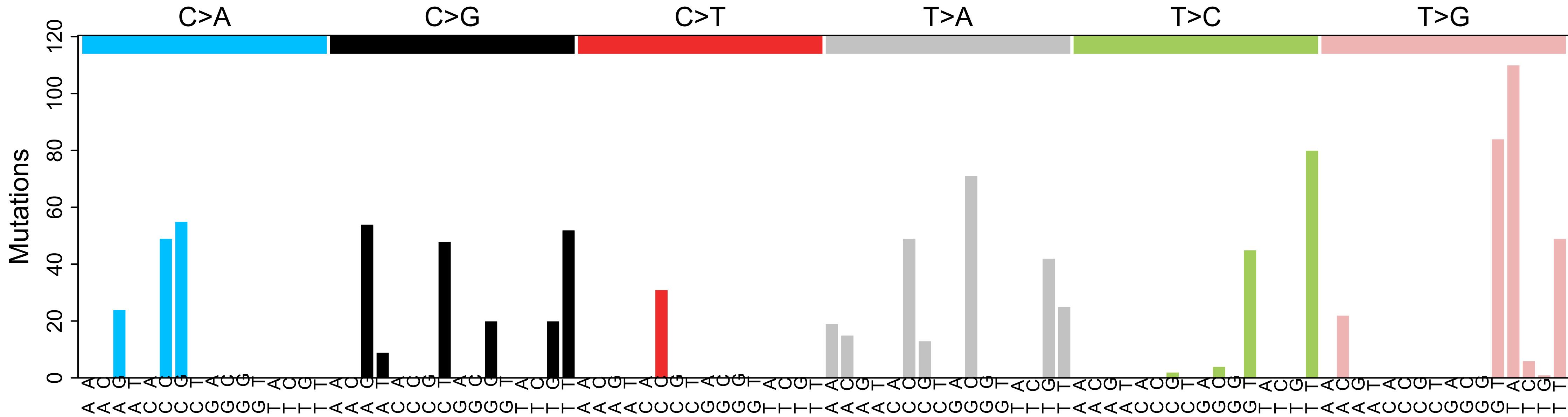
styrene_oxide_2bb934f6fd57 (999 mutations)



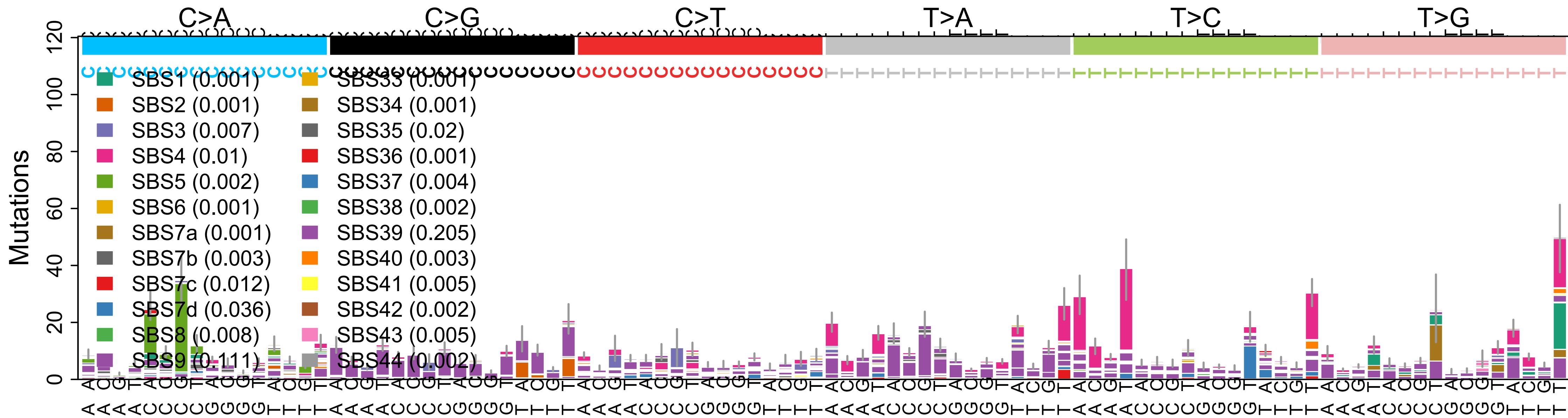
Reconstructed spectrum (cosine similarity = 0.809)



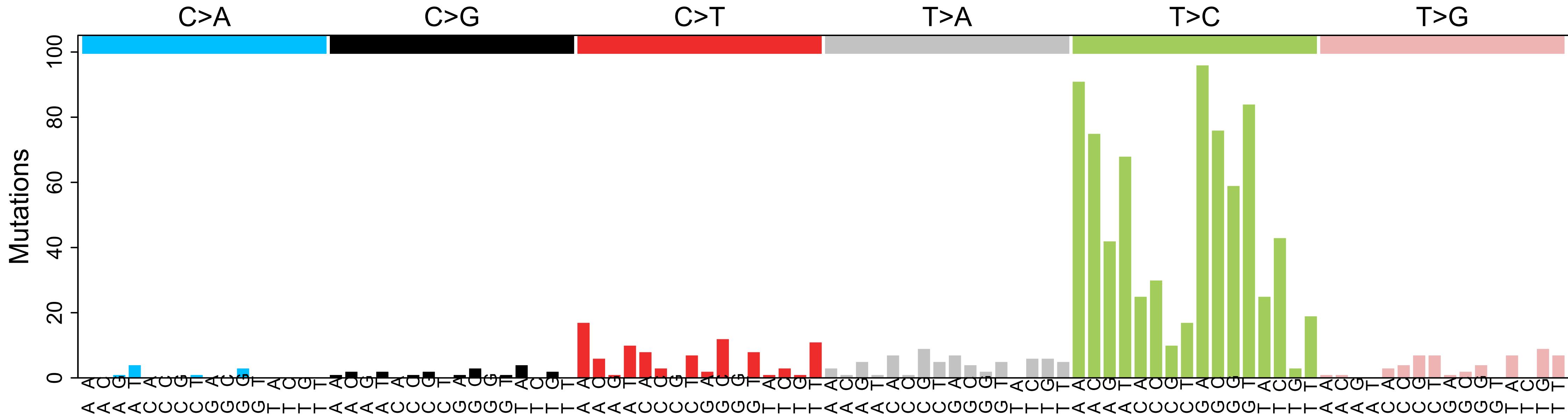
sudan_i_c63d6349b4cb (999 mutations)



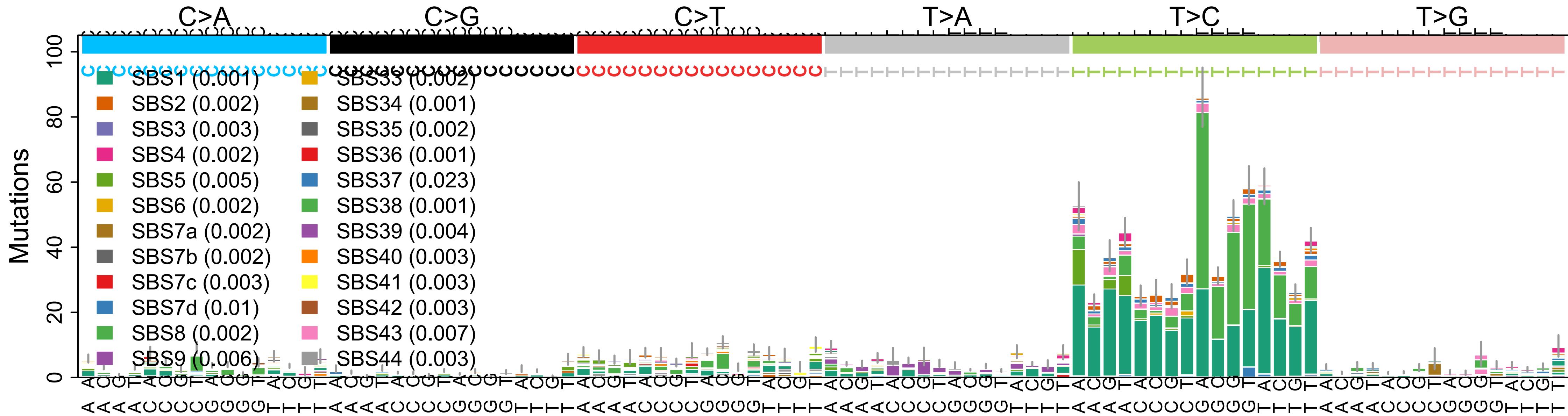
Reconstructed spectrum (cosine similarity = 0.523)



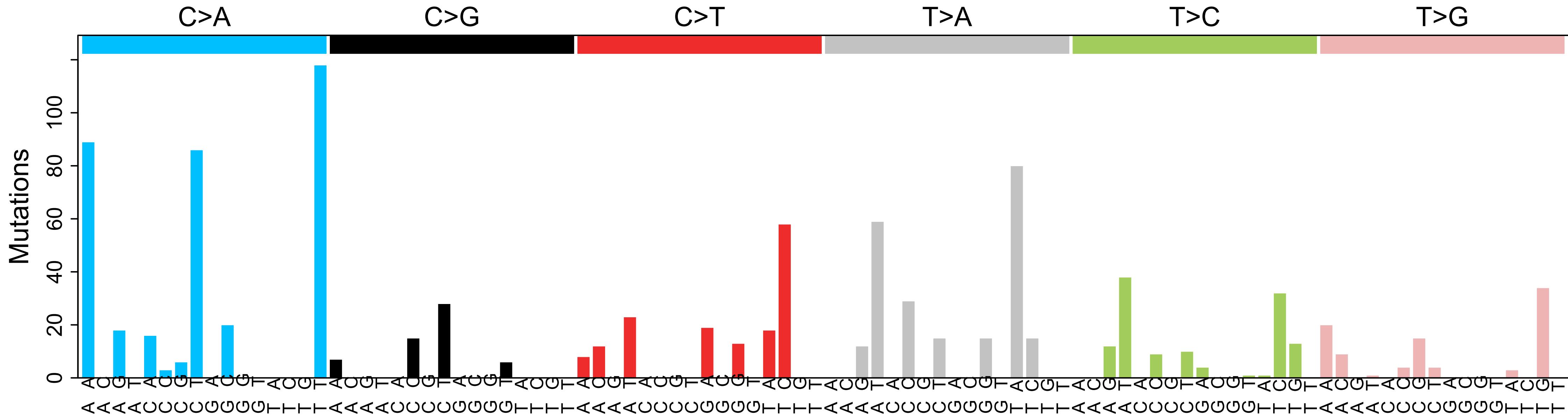
temozolomide_8377cb5da514 (1,001 mutations)



Reconstructed spectrum (cosine similarity = 0.89)



water_5807eebc2535 (998 mutations)



Reconstructed spectrum (cosine similarity = 0.798)

