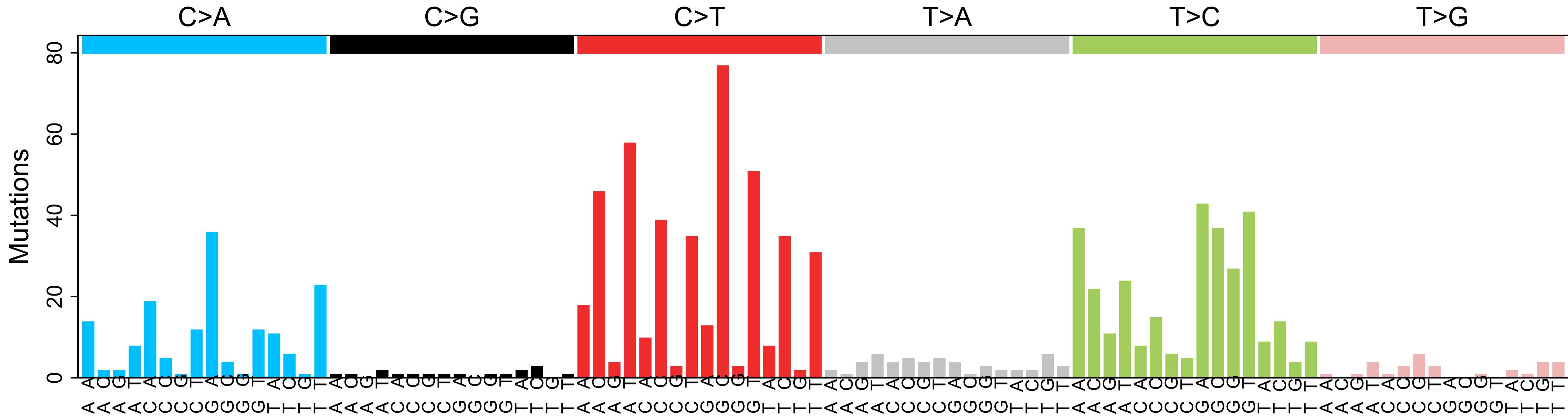
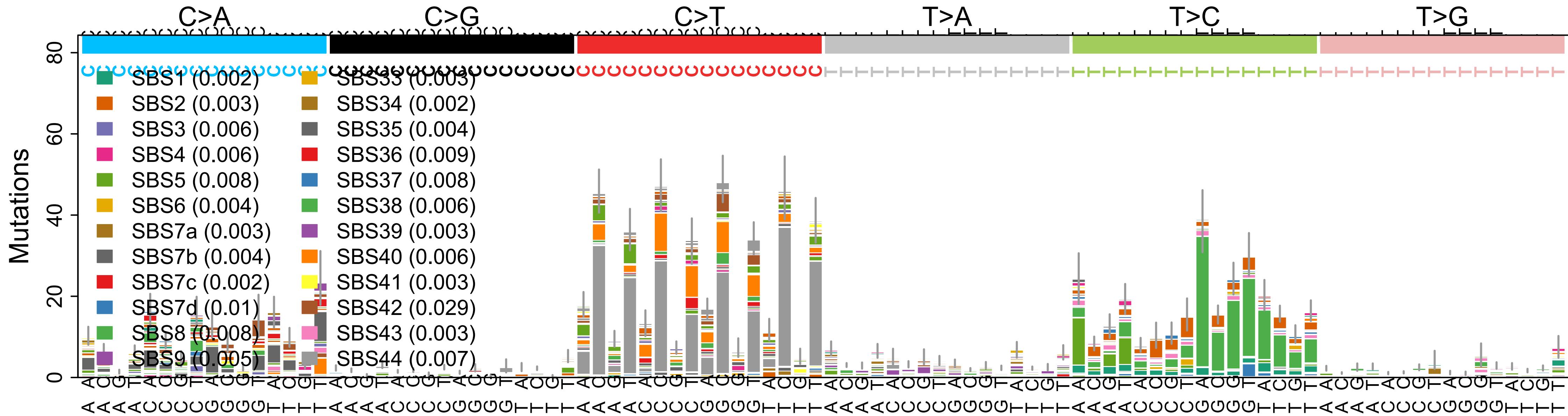


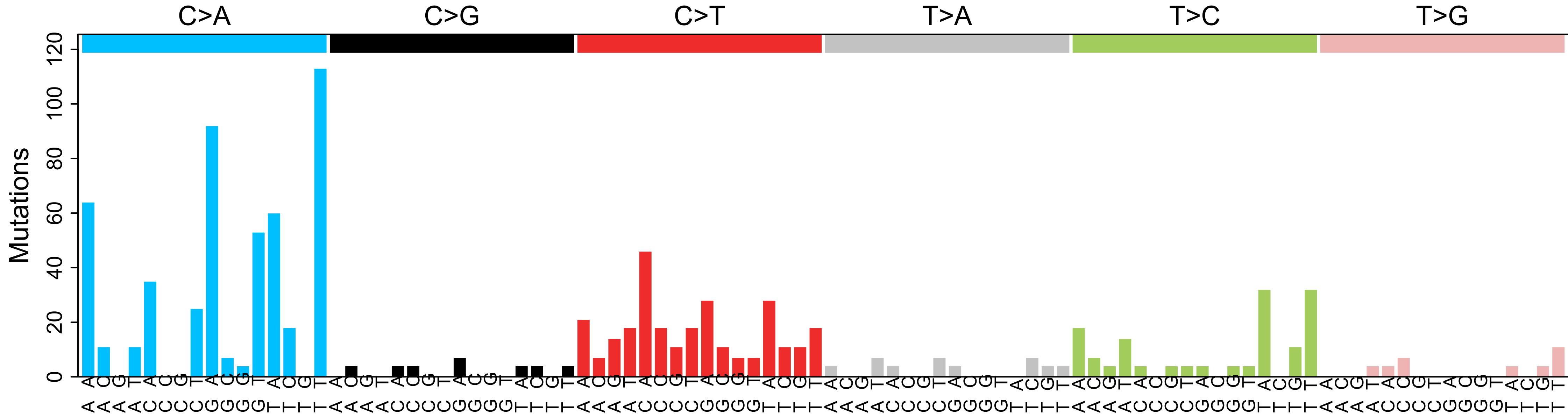
# 1\_2\_dimethylhydrazine\_9cffdc696a32 (1,004 mutations)



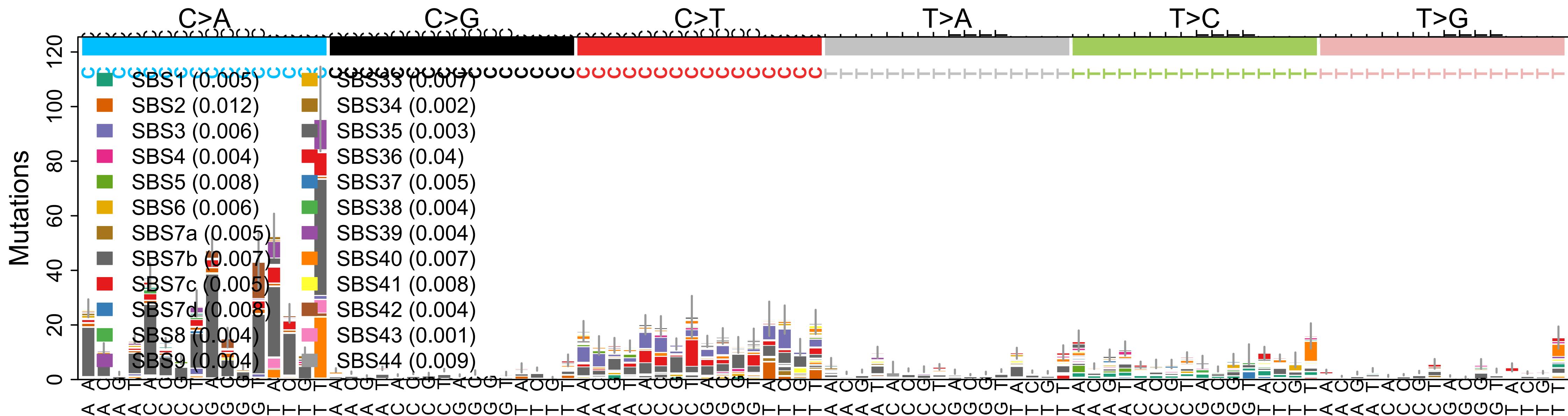
## Reconstructed spectrum (cosine similarity = 0.935)



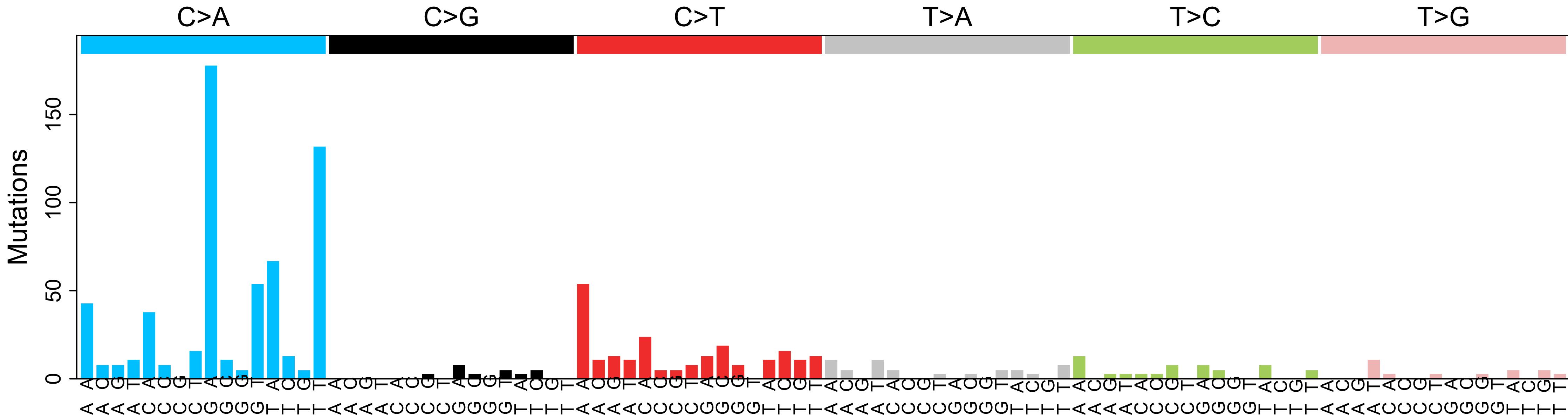
# 1\_2\_dimethylhydrazine\_ef5d55b18c9c (1,015 mutations)



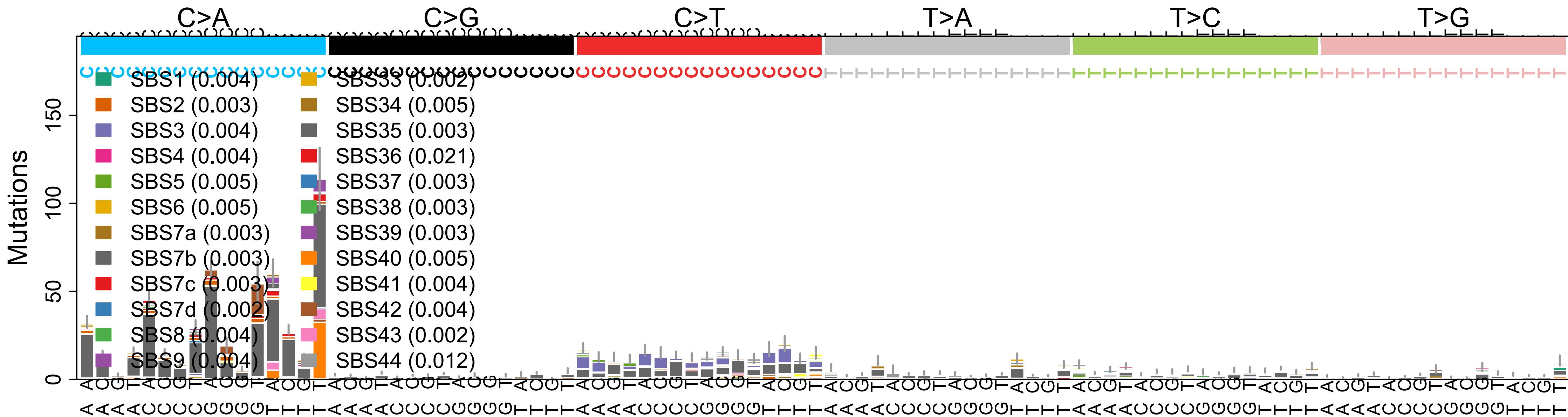
Reconstructed spectrum (cosine similarity = 0.927)



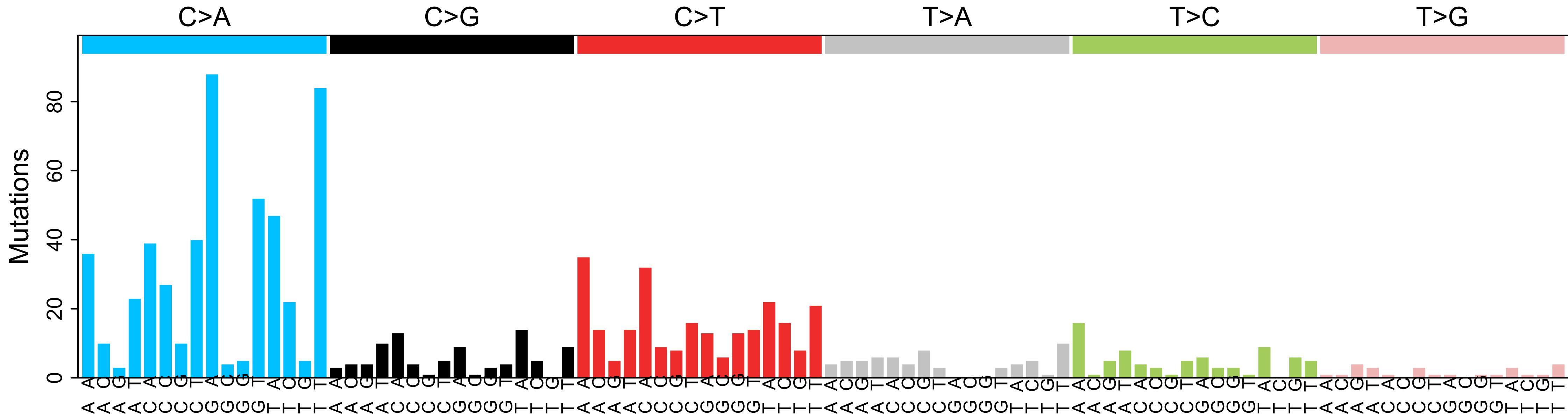
# 1\_4\_benzoquinone\_2d25052e44b1 (997 mutations)



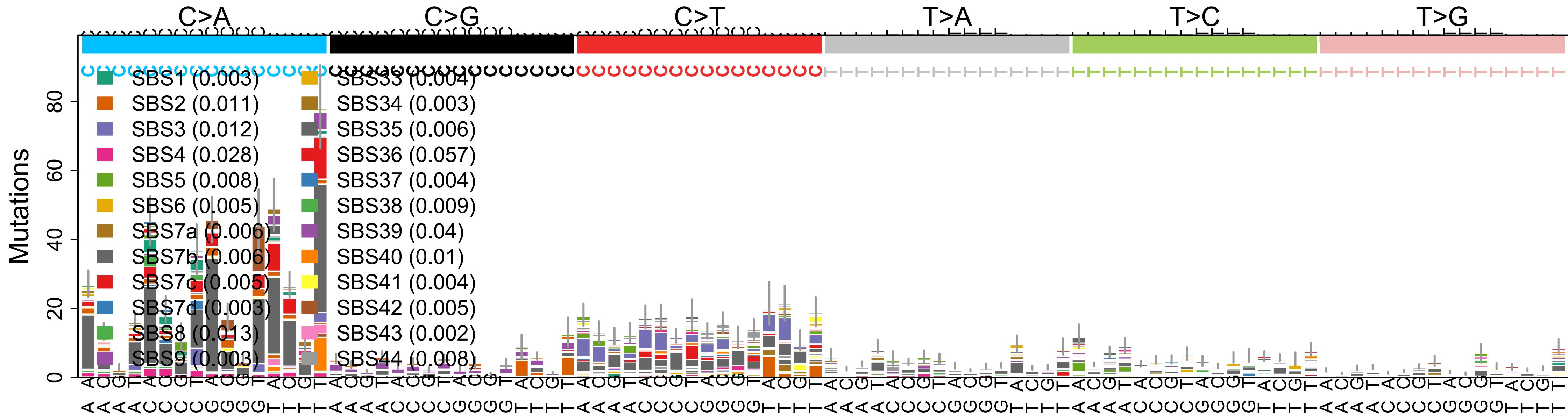
Reconstructed spectrum (cosine similarity = 0.878)



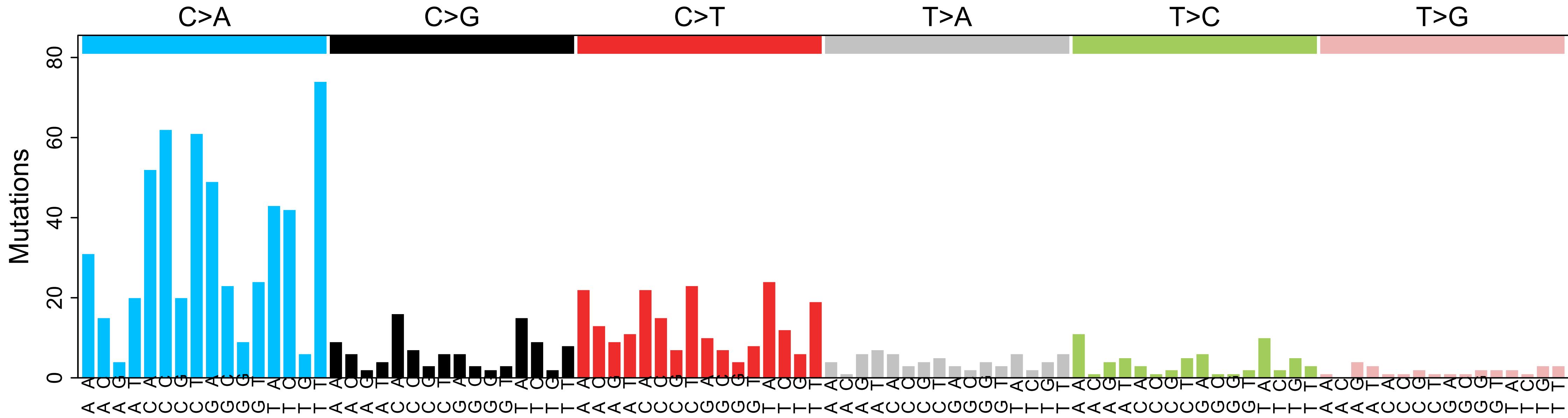
# 1\_6\_dinitropyrene\_77c0ec6159e4 (996 mutations)



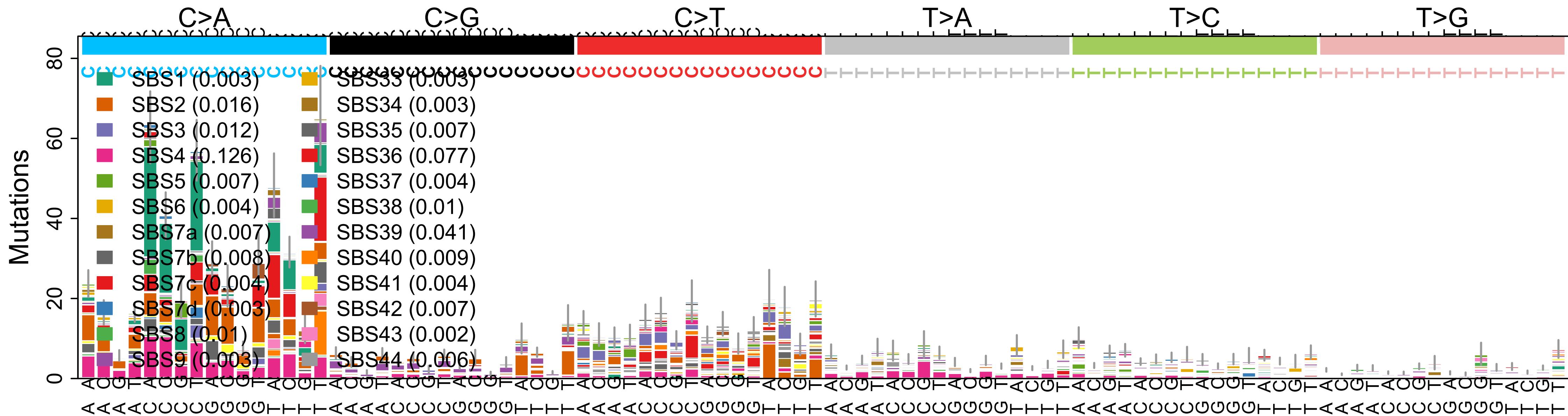
Reconstructed spectrum (cosine similarity = 0.946)



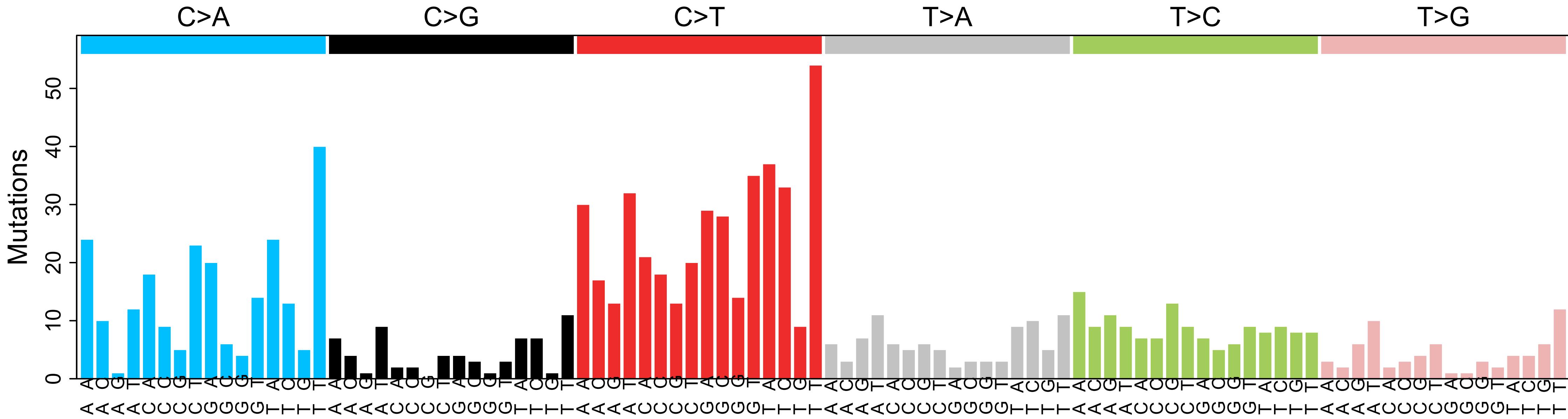
# 1\_8\_dinitropyrene\_da7ddba98e4a (1,004 mutations)



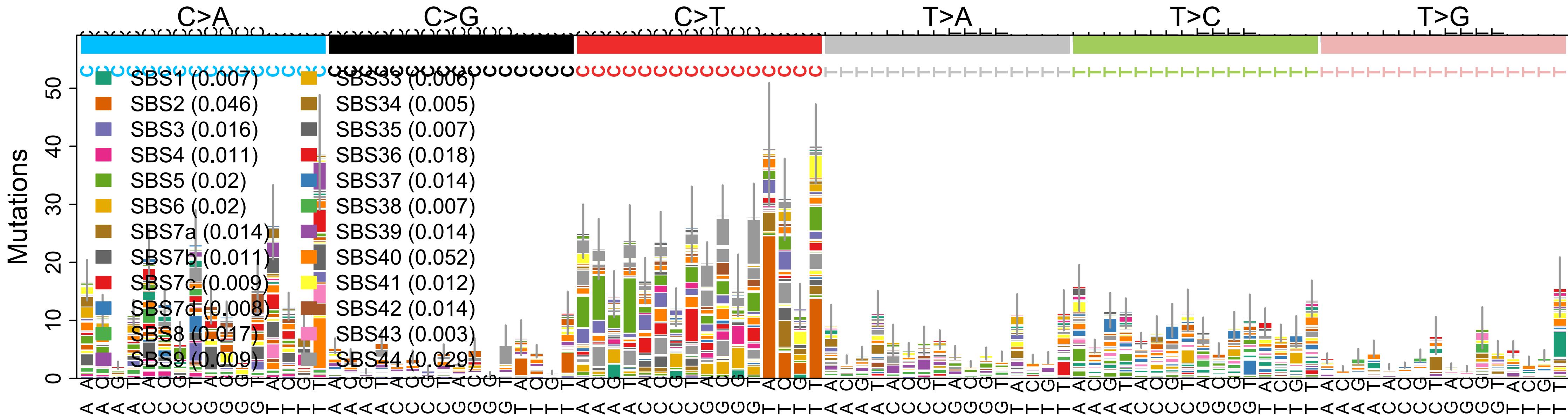
## Reconstructed spectrum (cosine similarity = 0.966)



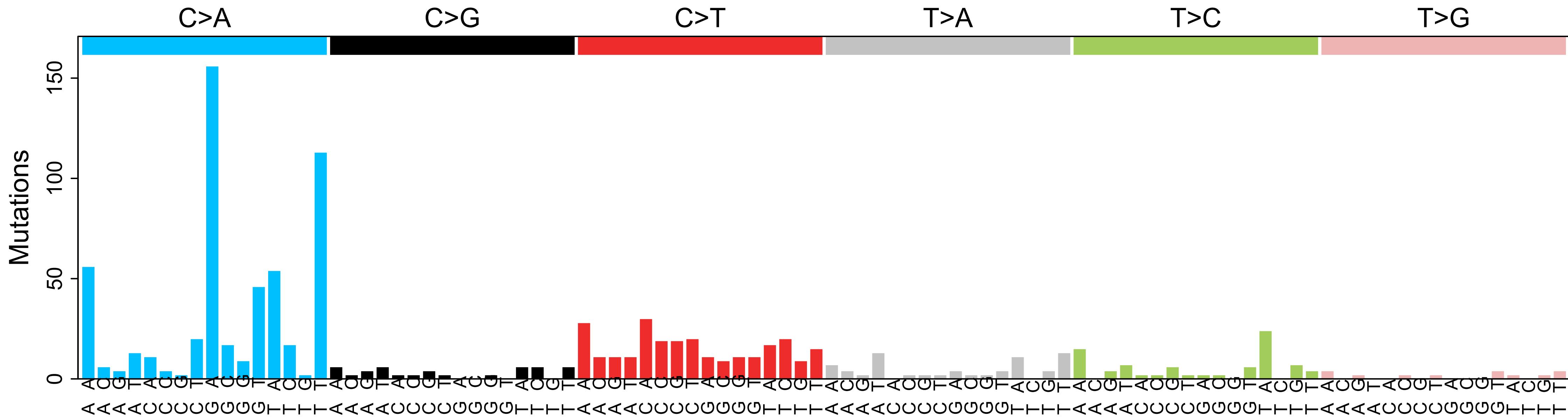
# 1\_naphthylamine\_c07099963bcd (1,001 mutations)



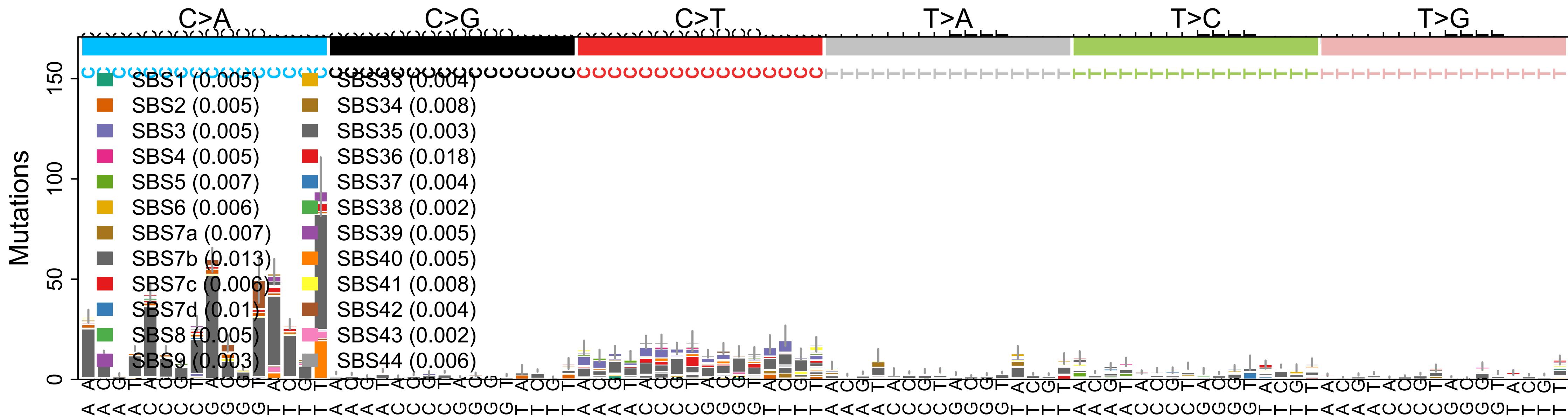
Reconstructed spectrum (cosine similarity = 0.975)



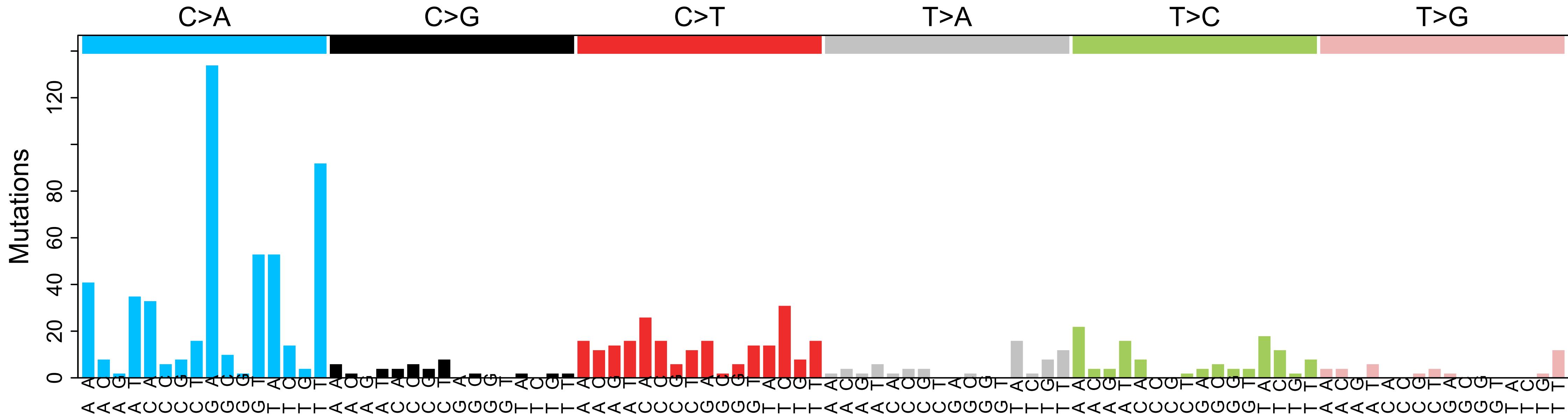
# 1\_nitropyrene\_2c37b07dec5a (1,007 mutations)



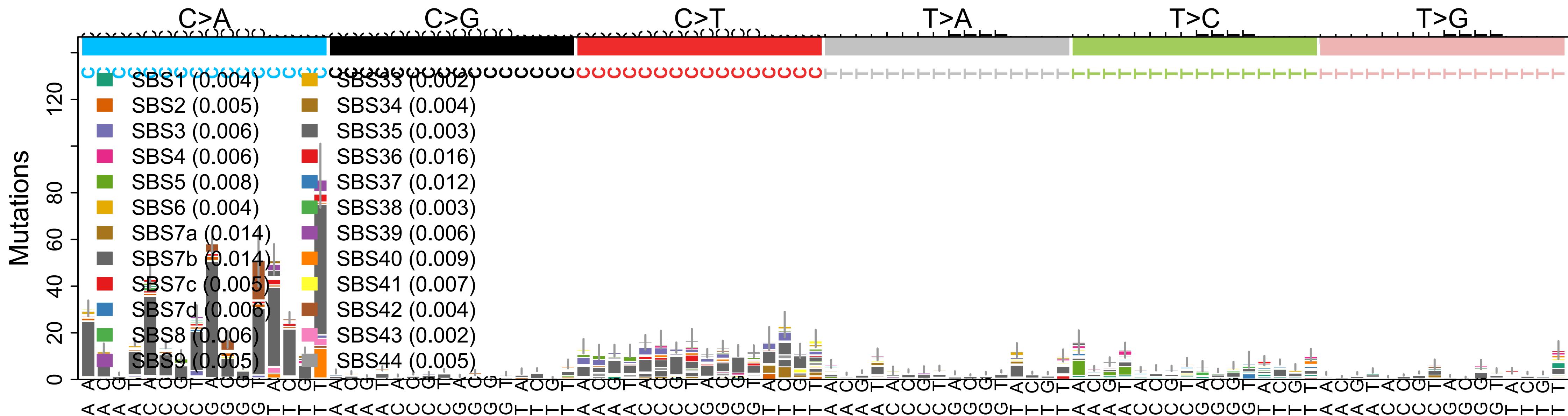
**Reconstructed spectrum (cosine similarity = 0.885)**



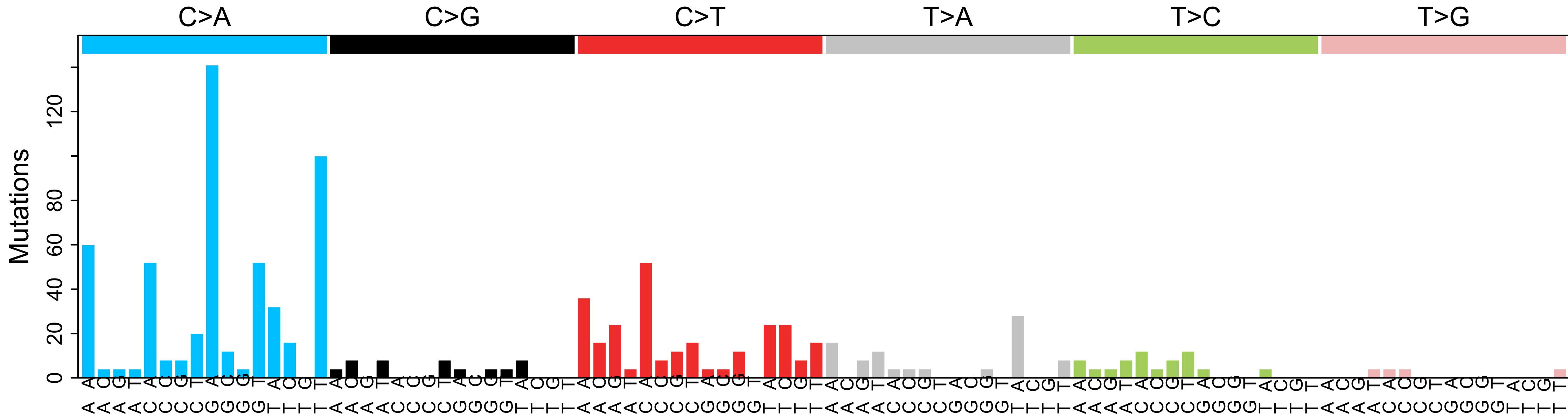
## 2\_6\_dimethylaniline\_3de14f6a14d9 (992 mutations)



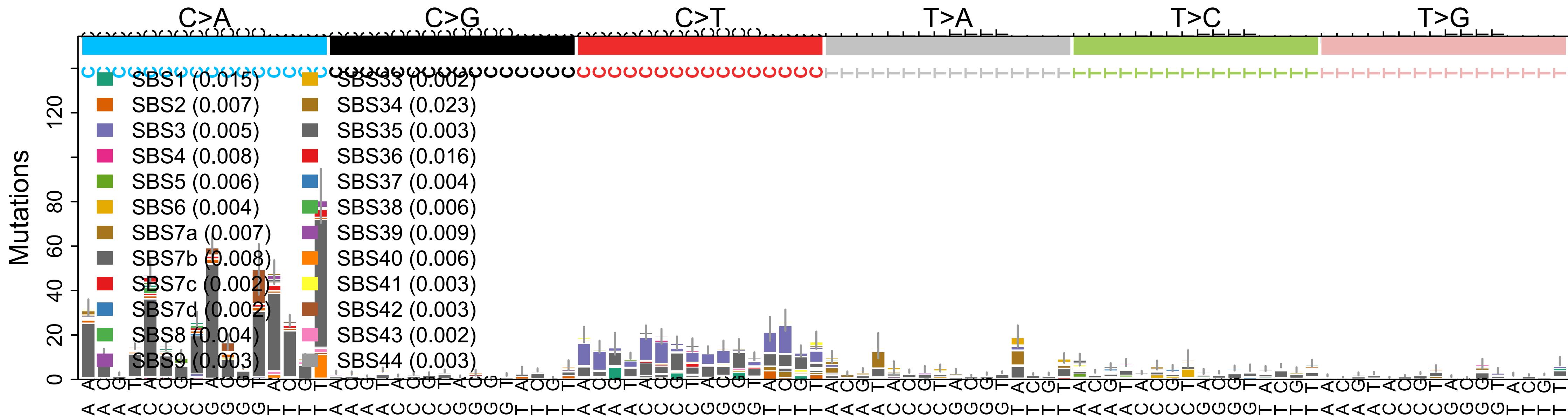
Reconstructed spectrum (cosine similarity = 0.91)



## 2\_6\_dimethylaniline\_42d3abf9de65 (997 mutations)



Reconstructed spectrum (cosine similarity = 0.895)



# 2\_amino\_1\_methyl\_6\_phenylimidazo4\_5\_bpyridine\_d8aa29785596 (998 mutations)

C>A

C>G

C>T

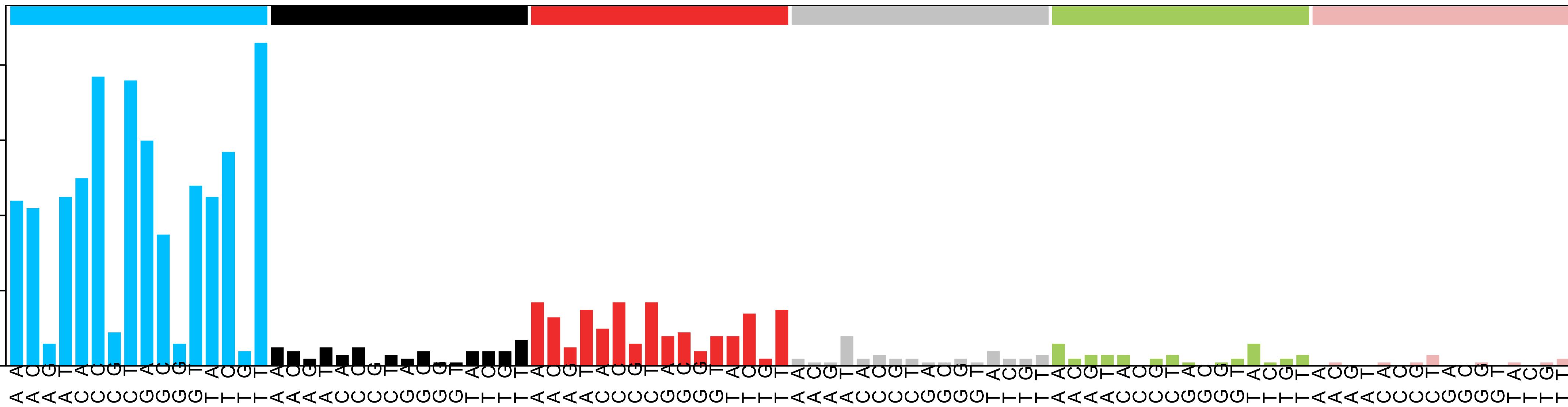
T>A

T>C

T>G

Mutations

80  
60  
40  
20  
0



Reconstructed spectrum (cosine similarity = 0.954)

C>A

C>G

C>T

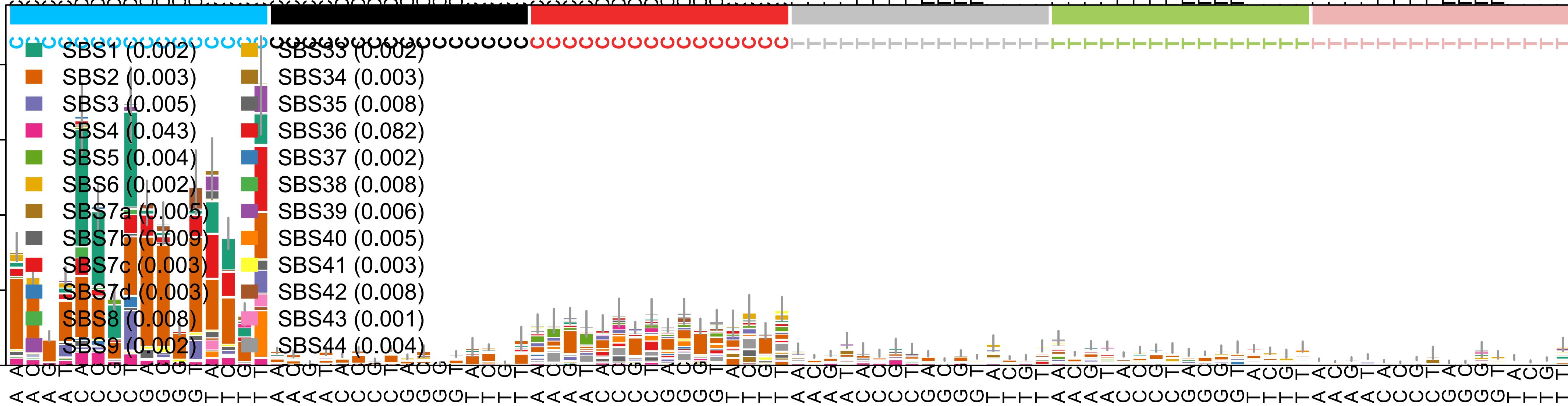
T>A

T>C

T>G

Mutations

80  
60  
40  
20  
0



# 2\_amino\_3\_8\_dimethylimidazo4\_5\_fquinoxaline\_d2762690cb73 (1,003 mutations)

C>A

C>G

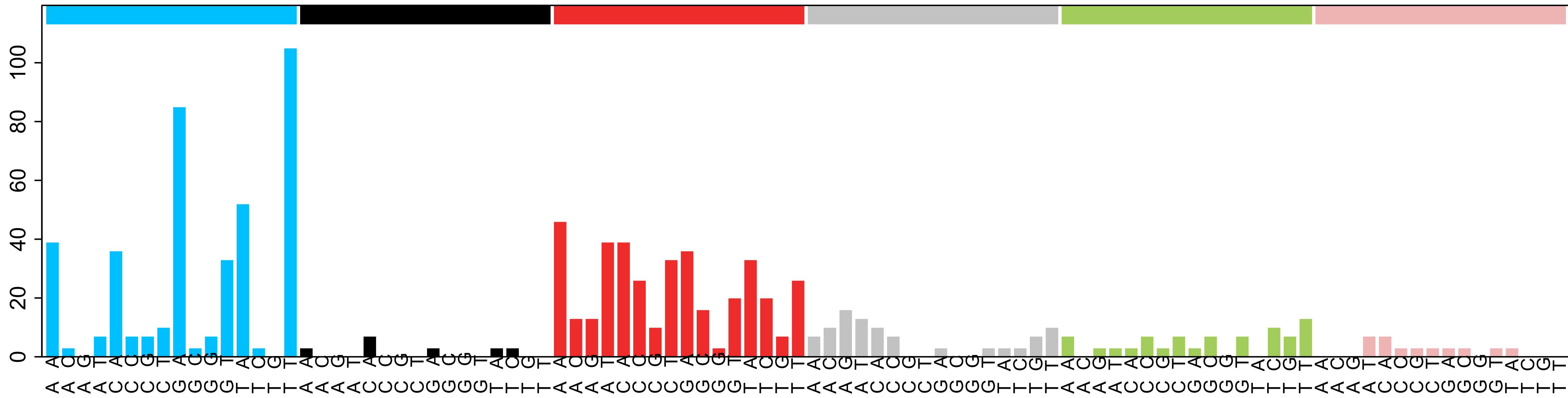
C>T

T>A

T>C

T>G

Mutations



Reconstructed spectrum (cosine similarity = 0.926)

C>A

C>G

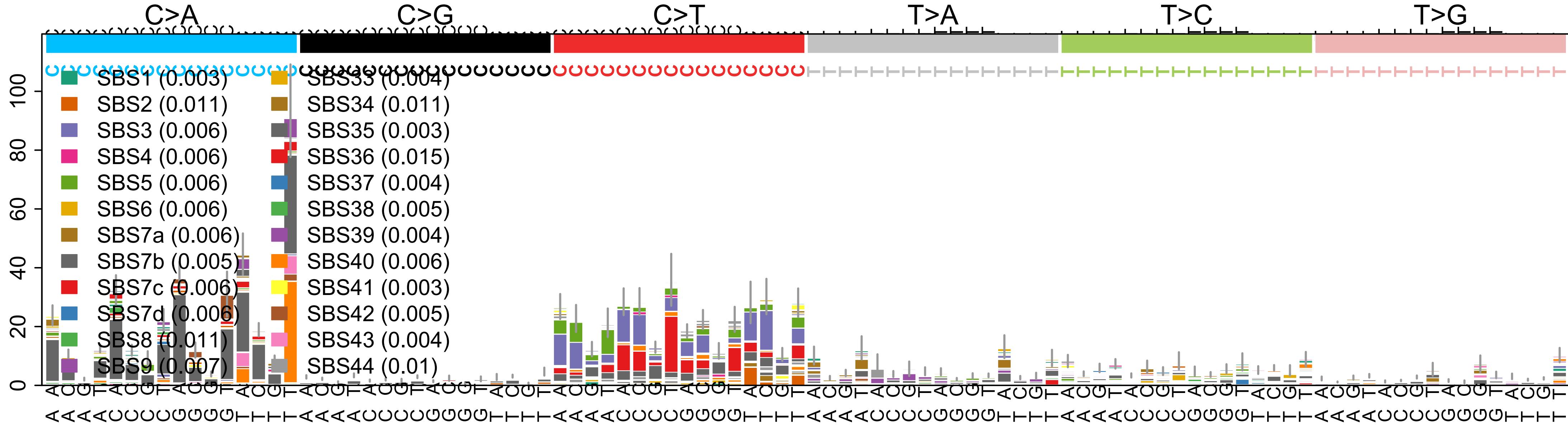
C>T

T>A

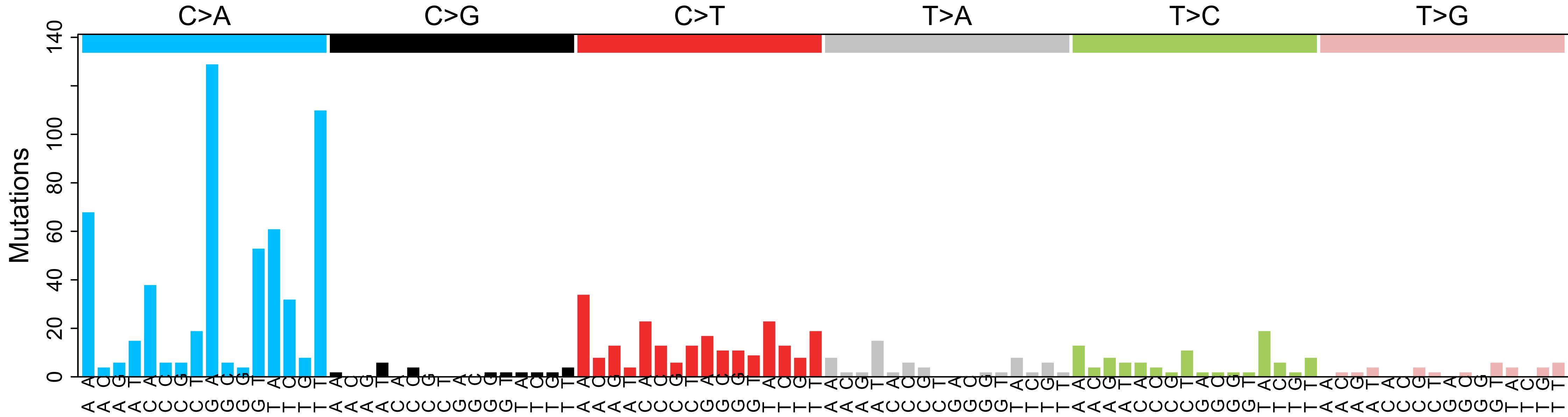
T>C

T>G

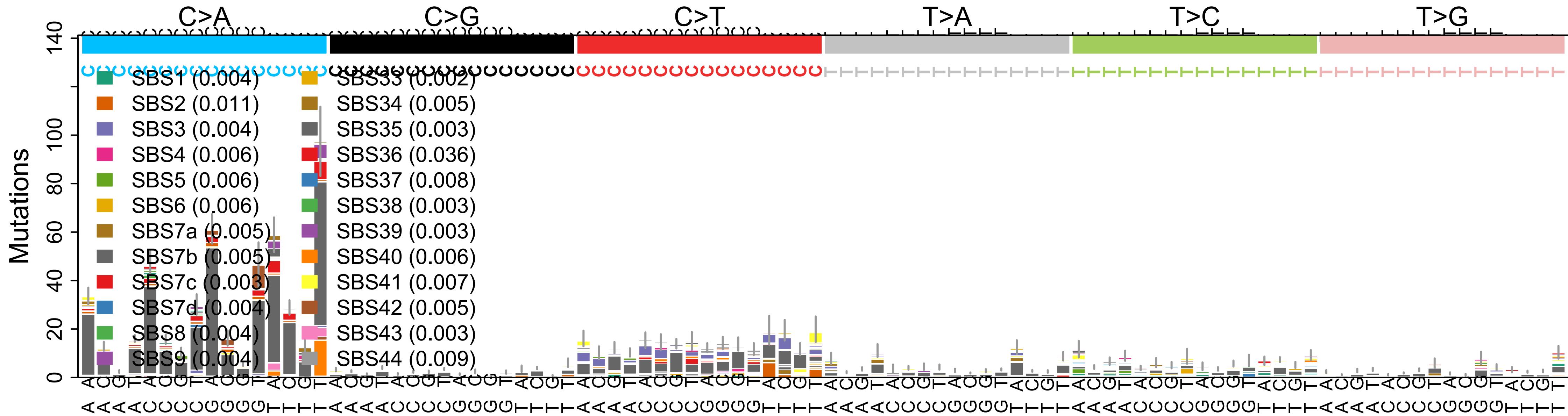
Mutations



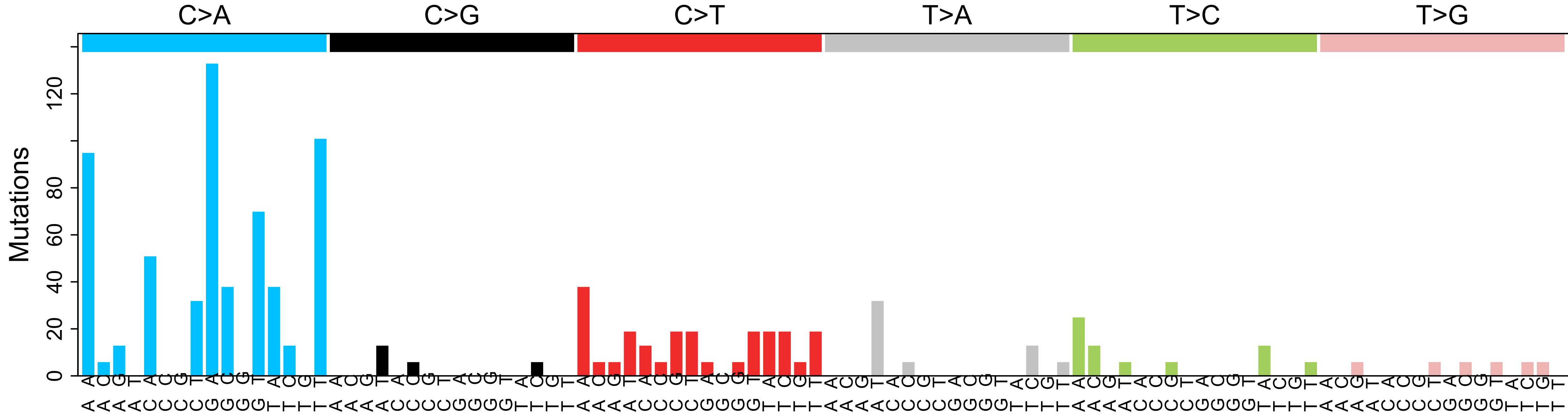
# 2\_amino\_3\_methyl\_9h\_pyrido2\_3\_bindole\_f10529056af1 (1,010 mutations)



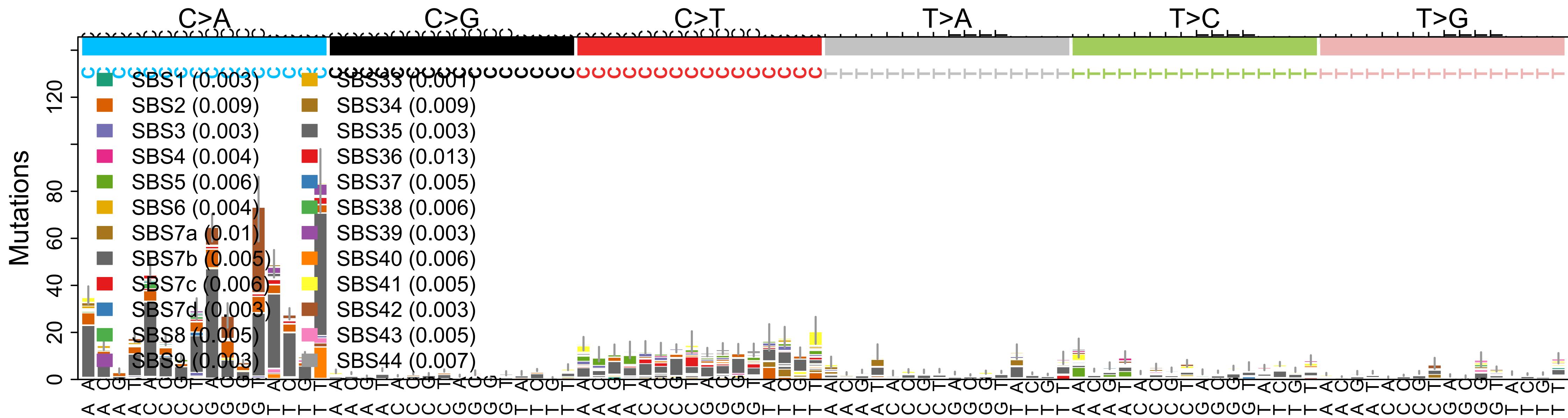
Reconstructed spectrum (cosine similarity = 0.929)



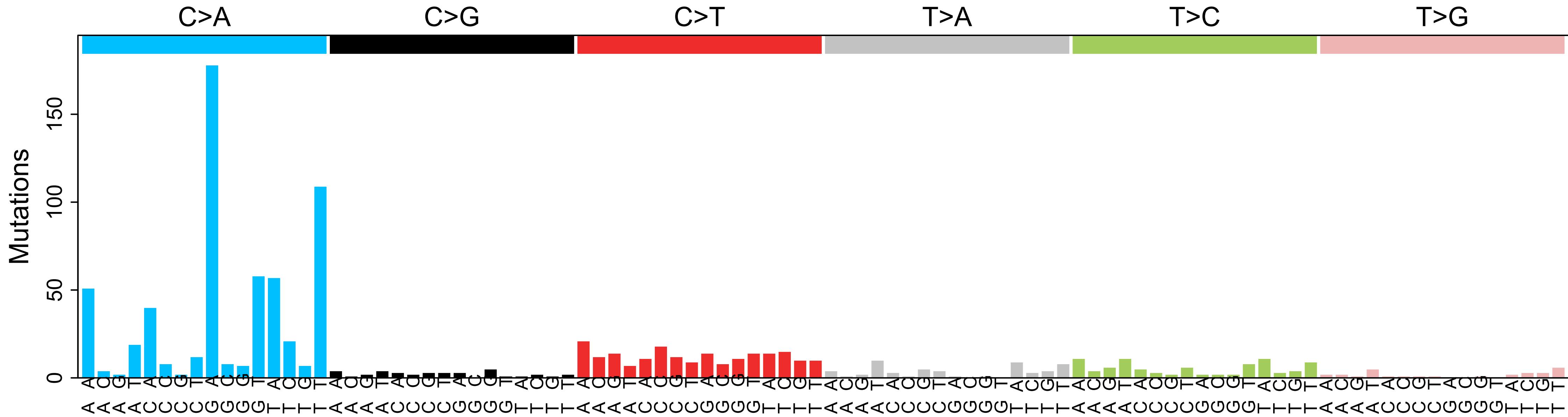
## **2\_amino\_3\_methylimidazo4\_5\_fquinoline\_0e3b1136946a (997 mutations)**



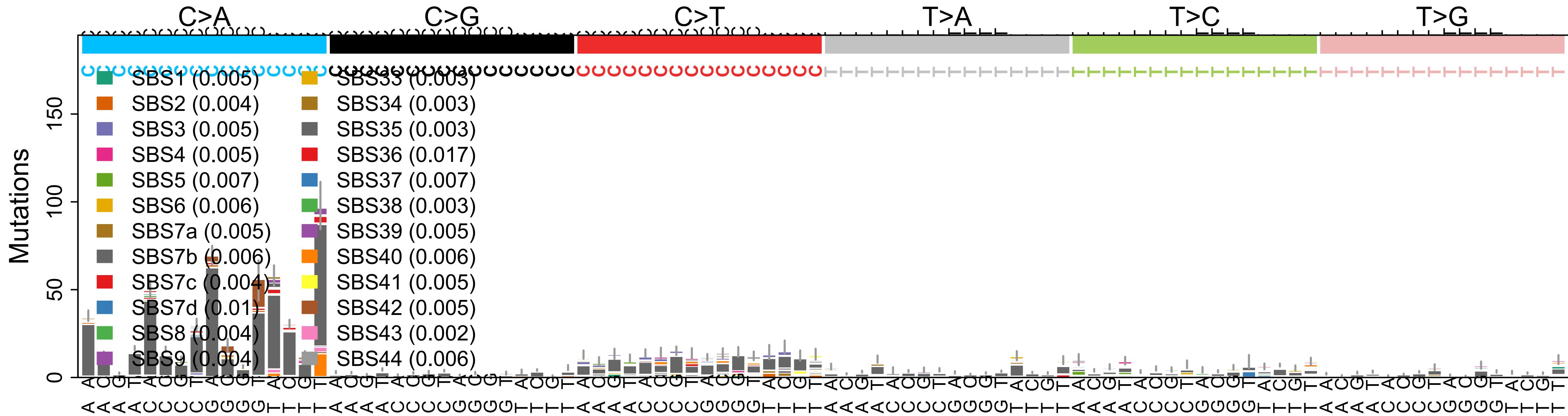
# Reconstructed spectrum (cosine similarity = 0.891)



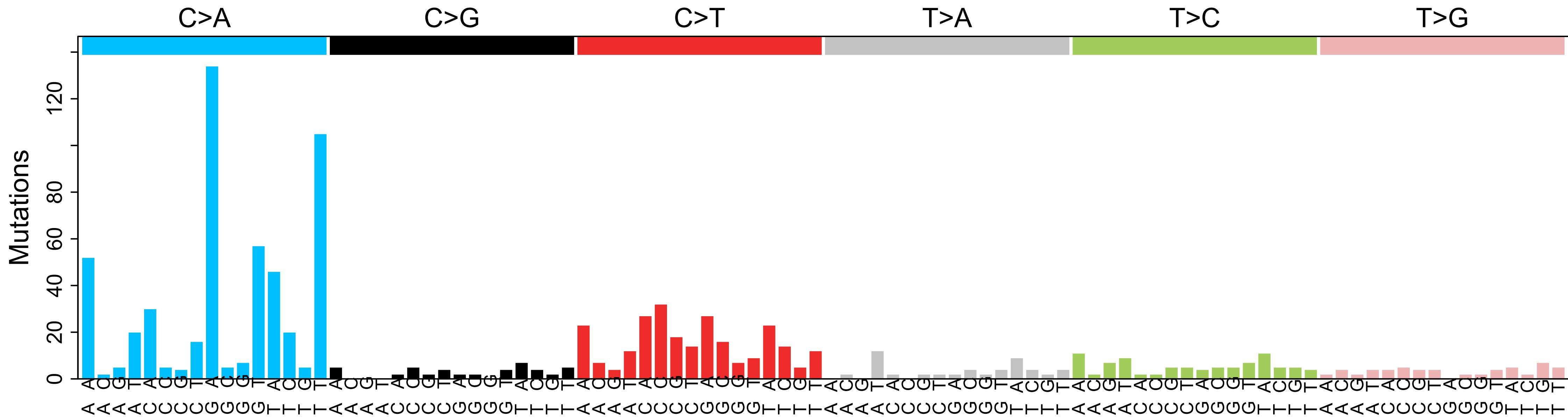
## 2\_naphthylamine\_0678c60a05a6 (994 mutations)



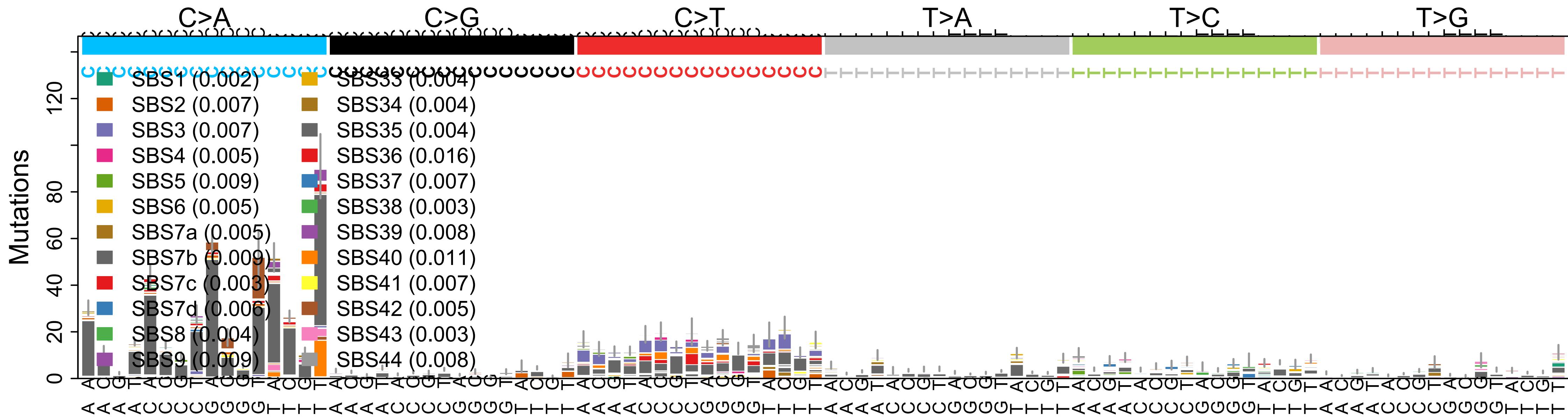
Reconstructed spectrum (cosine similarity = 0.893)



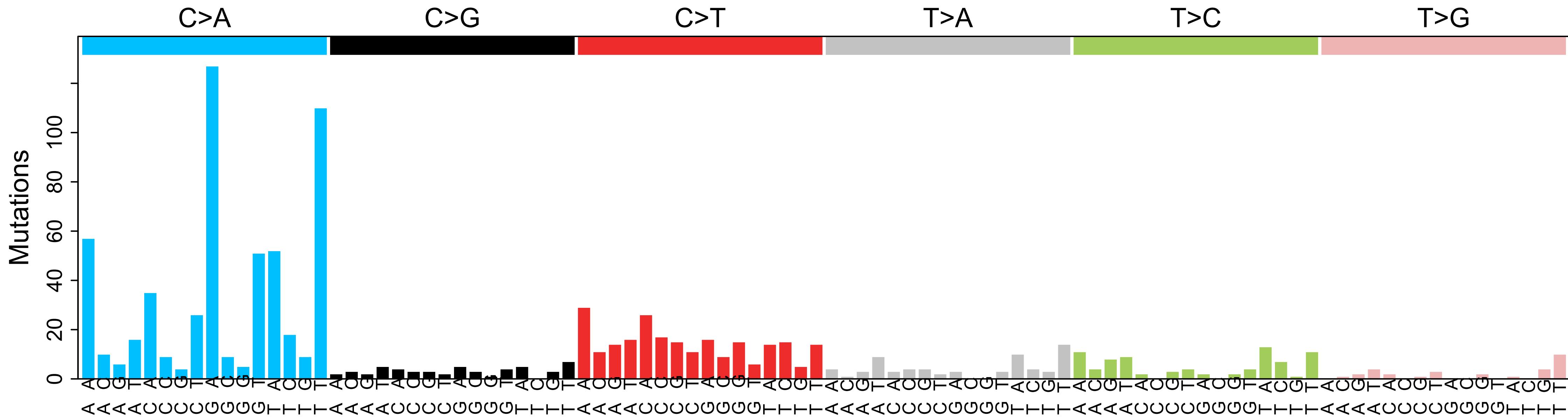
## 2\_naphthylamine\_8d0ae6c5590e (1,003 mutations)



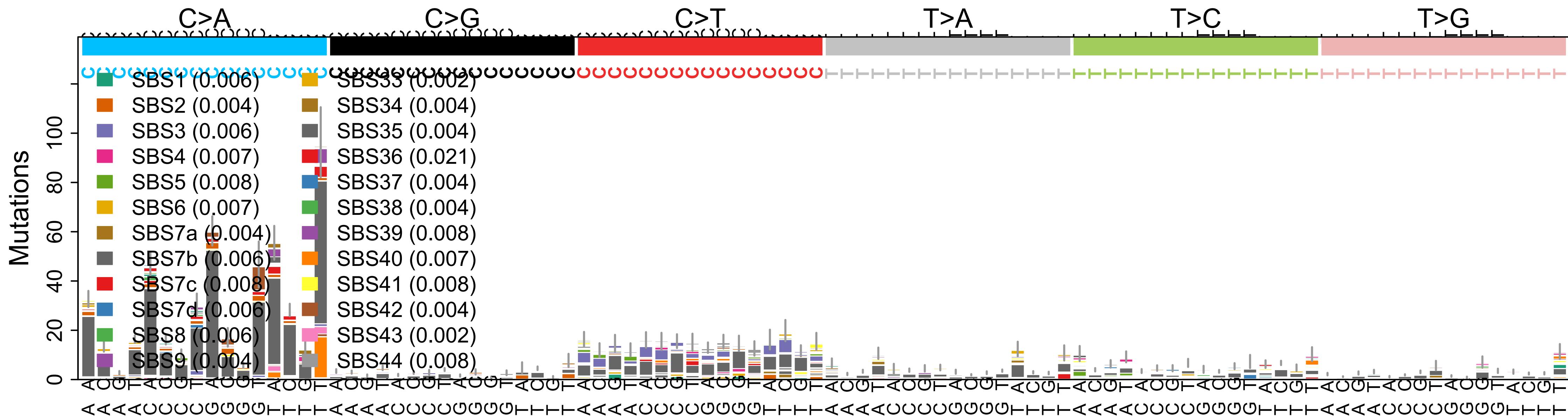
## Reconstructed spectrum (cosine similarity = 0.913)



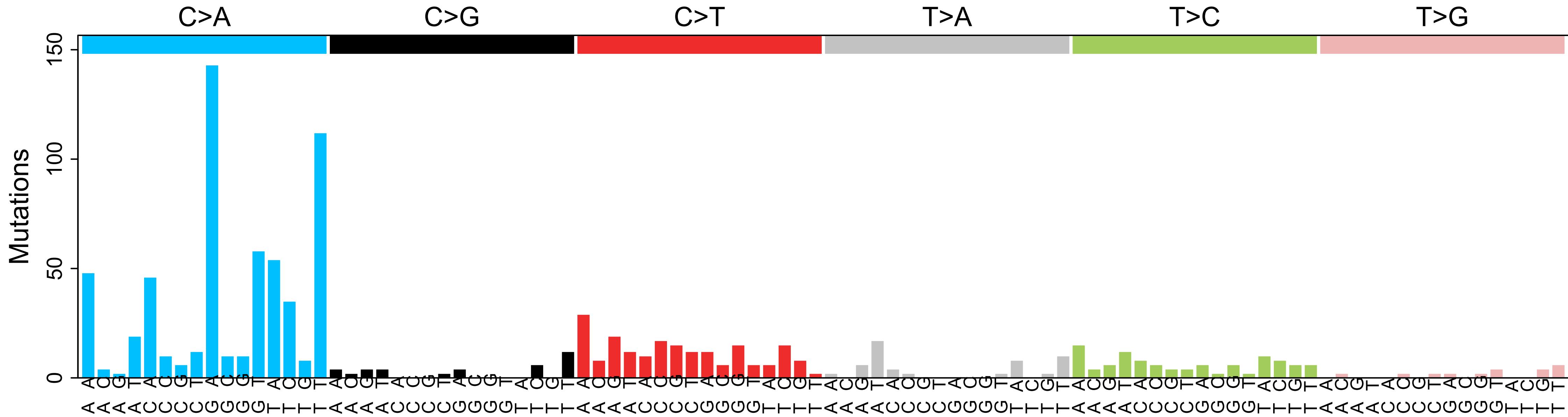
## 2\_nitrofluorene\_d908deea4861 (1,007 mutations)



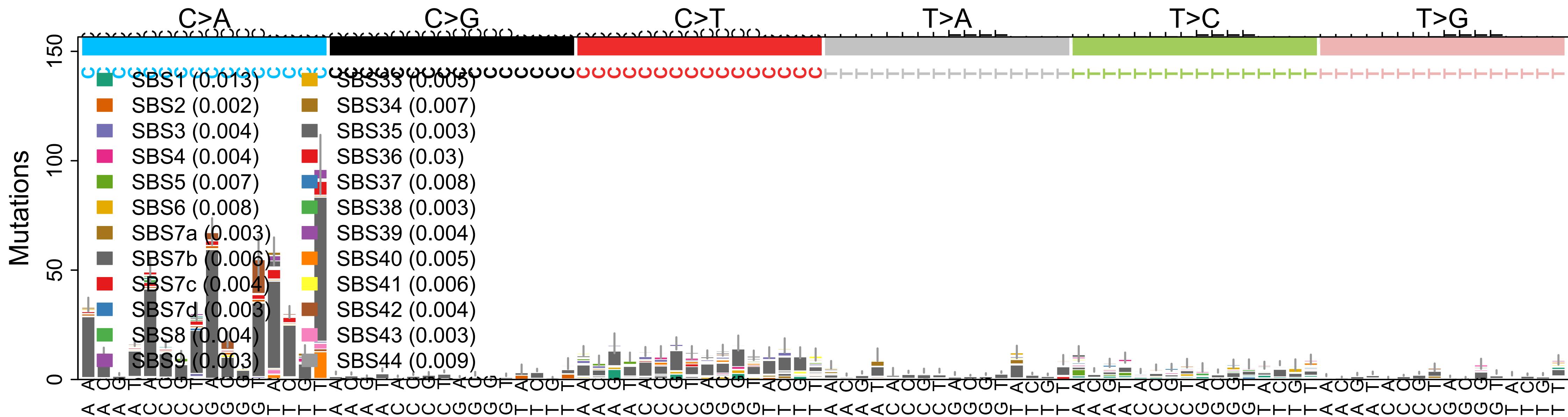
Reconstructed spectrum (cosine similarity = 0.934)



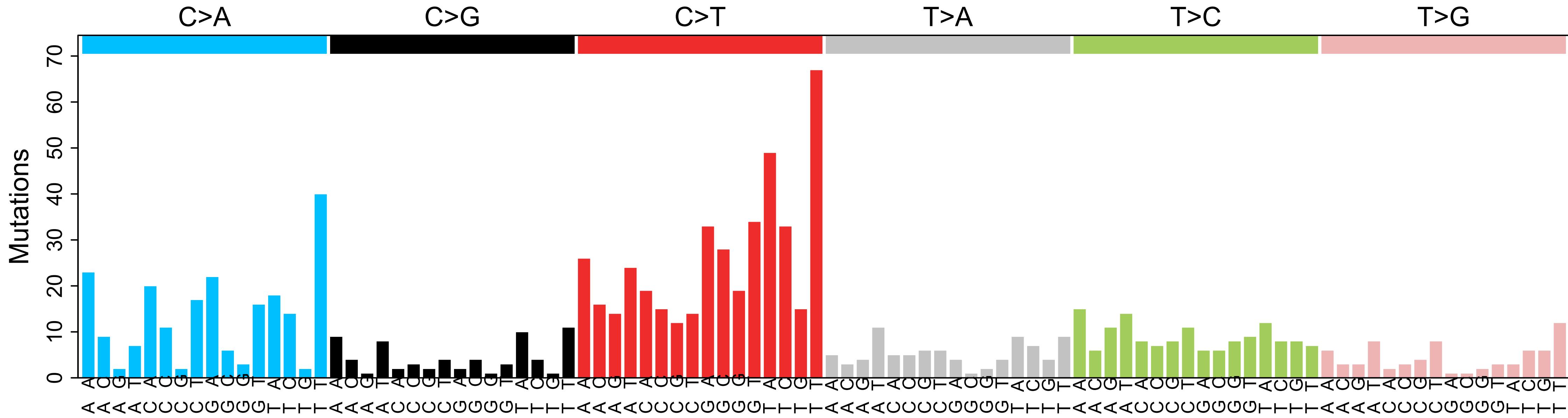
## 2\_nitrotoluene\_d1b70070133b (989 mutations)



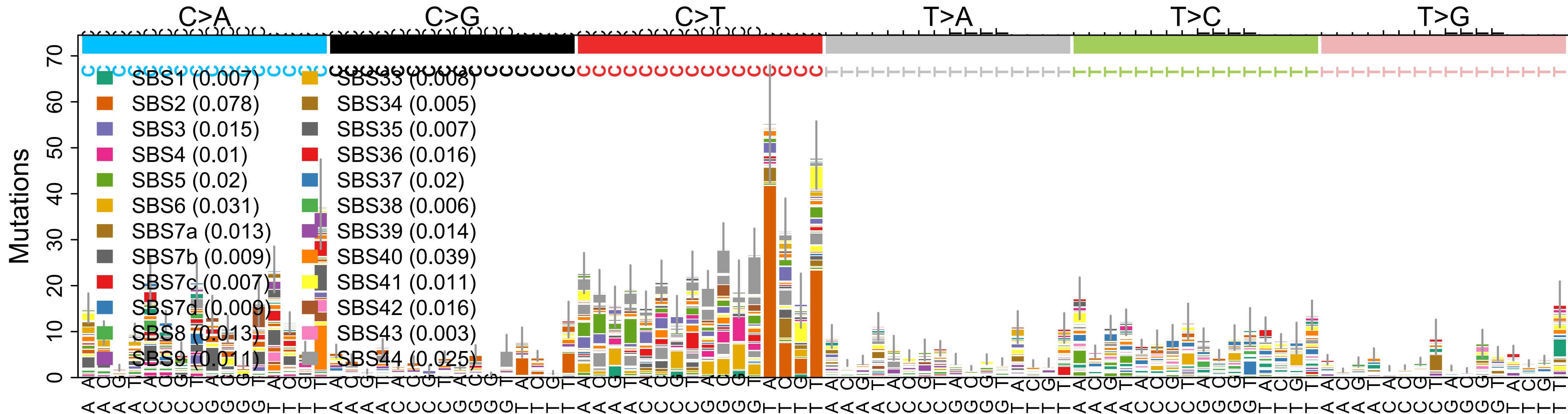
Reconstructed spectrum (cosine similarity = 0.931)



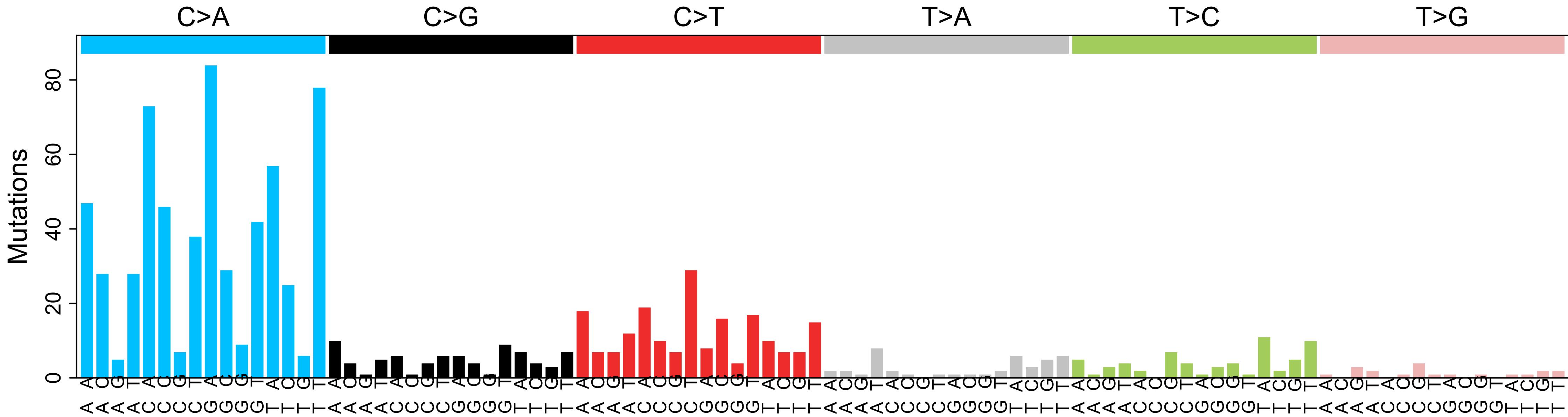
### 3\_aminobiphenyl\_2805765426dd (999 mutations)



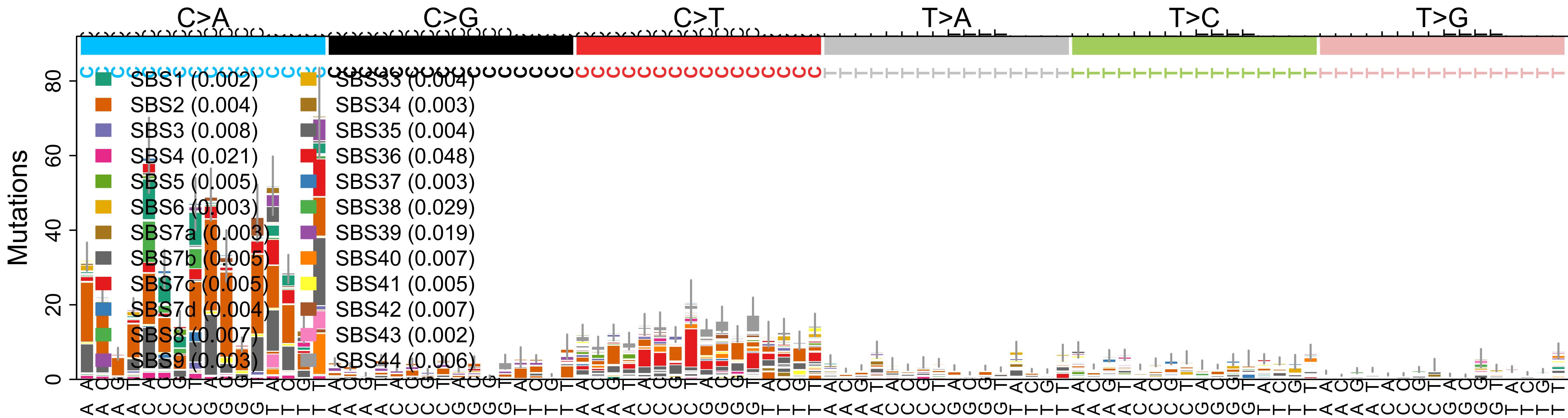
Reconstructed spectrum (cosine similarity = 0.971)



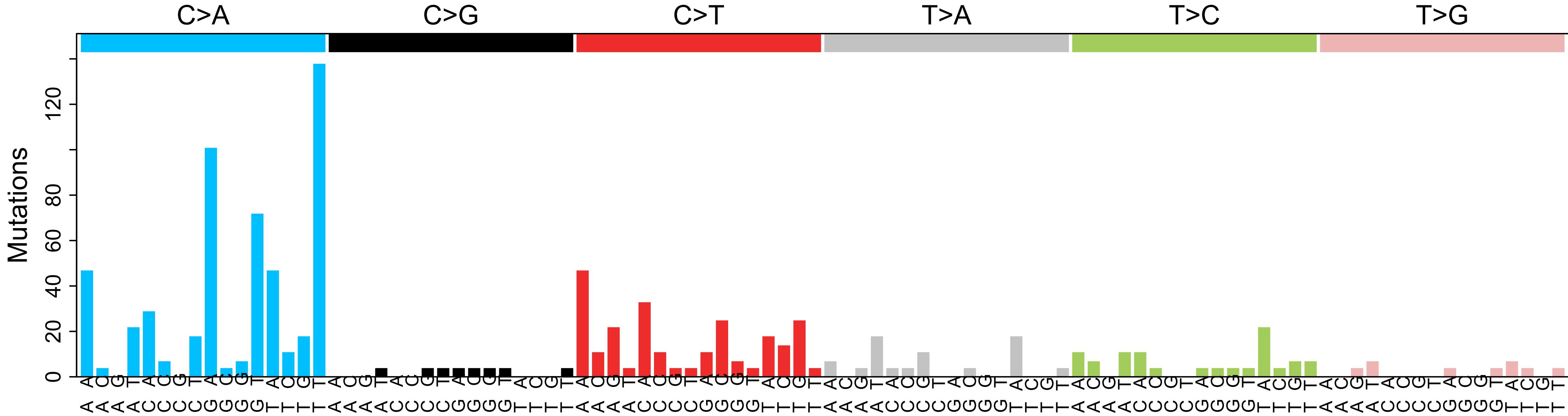
# 3\_chloro\_4\_dichloromethyl\_5\_hydroxy\_25h\_furanone\_d6057c2d9433 (998 mutations)



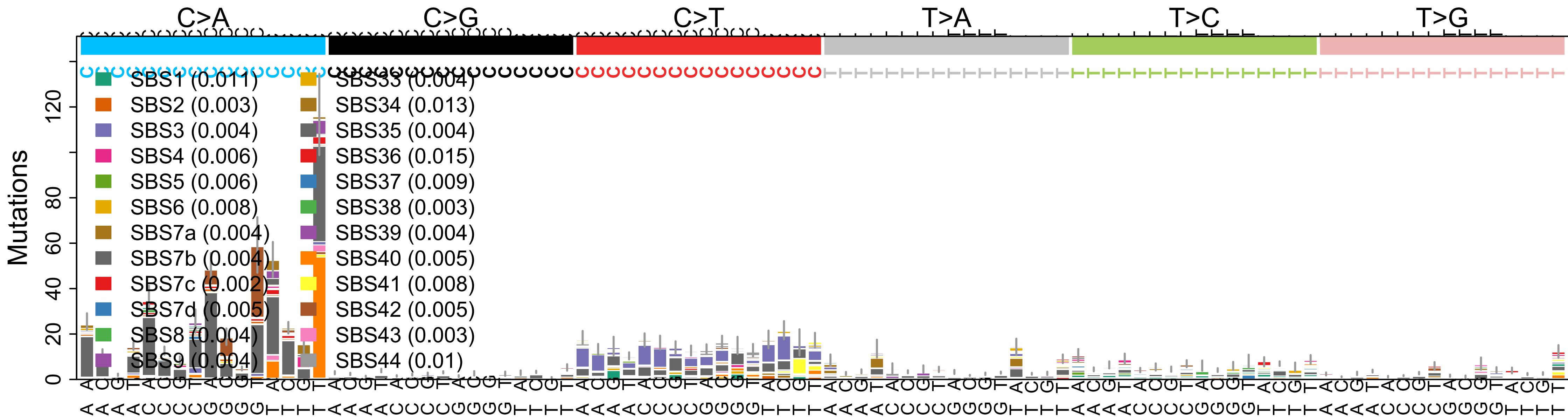
Reconstructed spectrum (cosine similarity = 0.962)



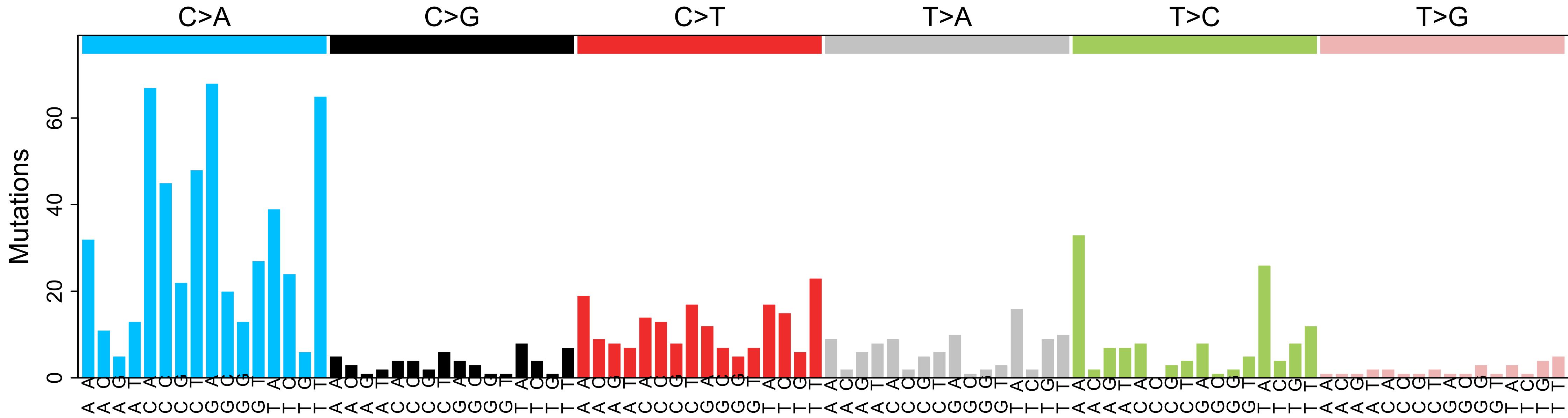
### 3\_chloro\_4\_dichloromethyl\_5\_hydroxy\_25h\_furanone\_e40d11eac1ce (1,009 mutations)



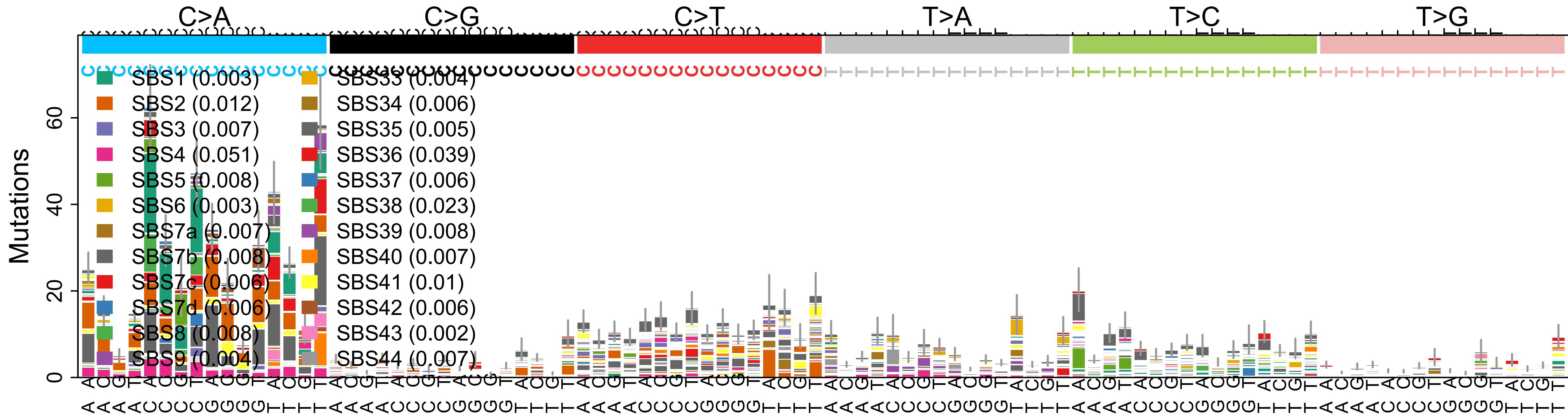
### Reconstructed spectrum (cosine similarity = 0.932)



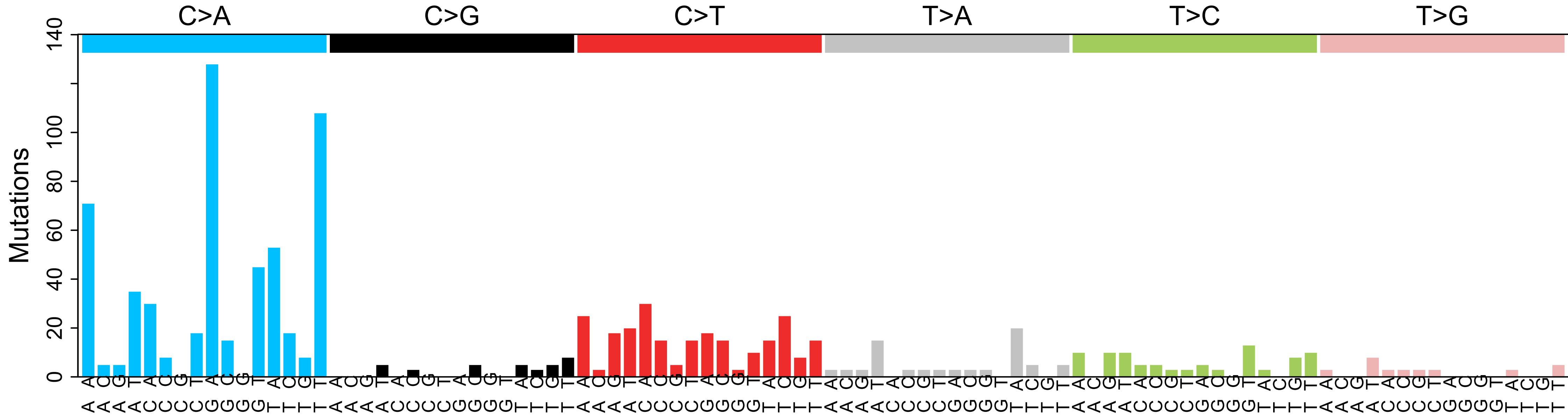
### 3\_nitrobenzanthrone\_8bc52f809fe4 (1,008 mutations)



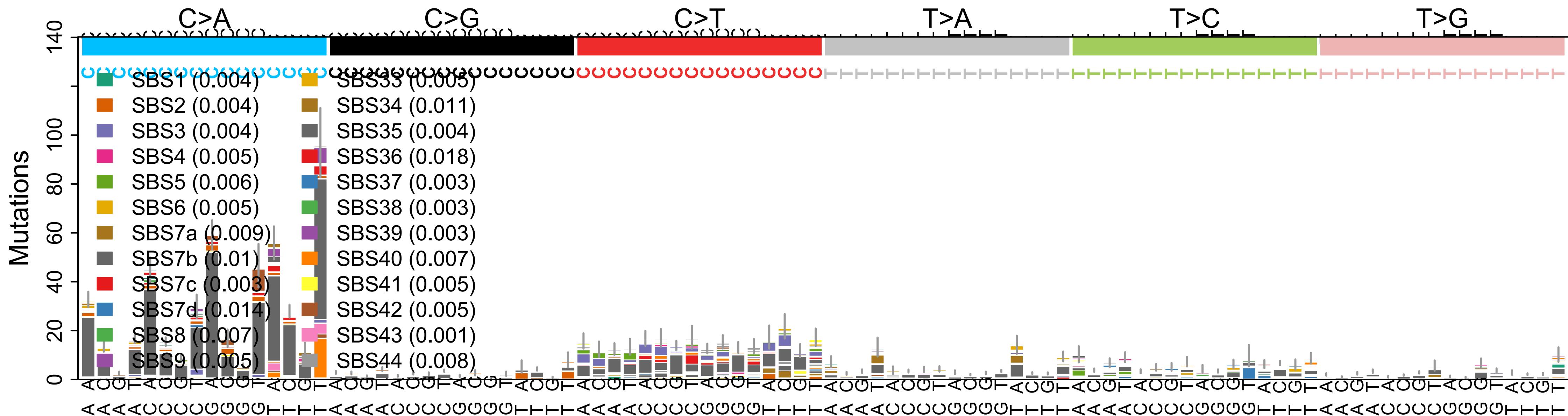
Reconstructed spectrum (cosine similarity = 0.96)



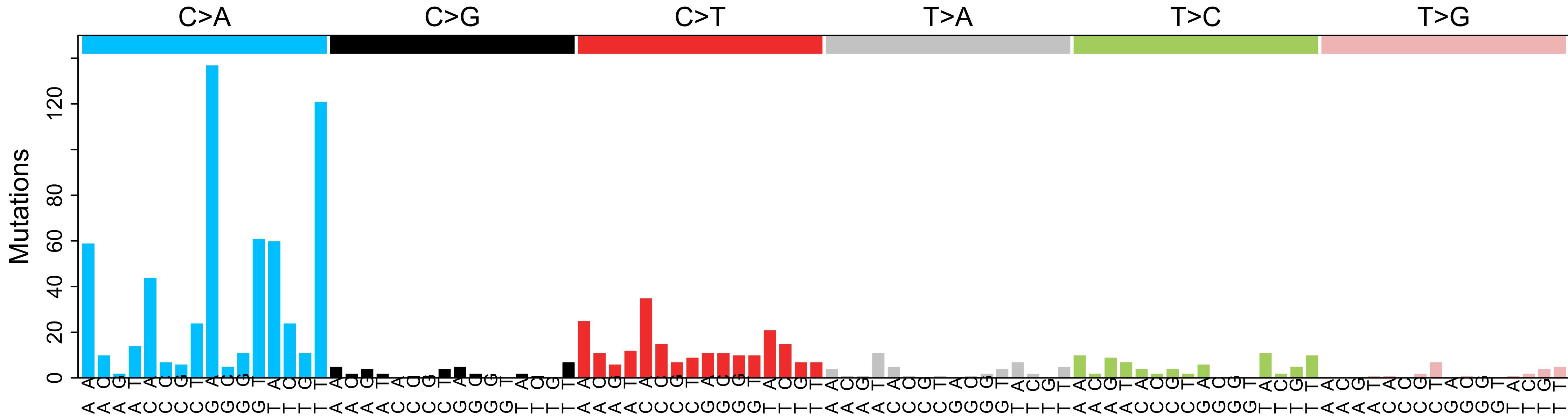
# 4\_4\_methylene\_bis2\_chloroaniline\_10dc00a2ca17 (1,012 mutations)



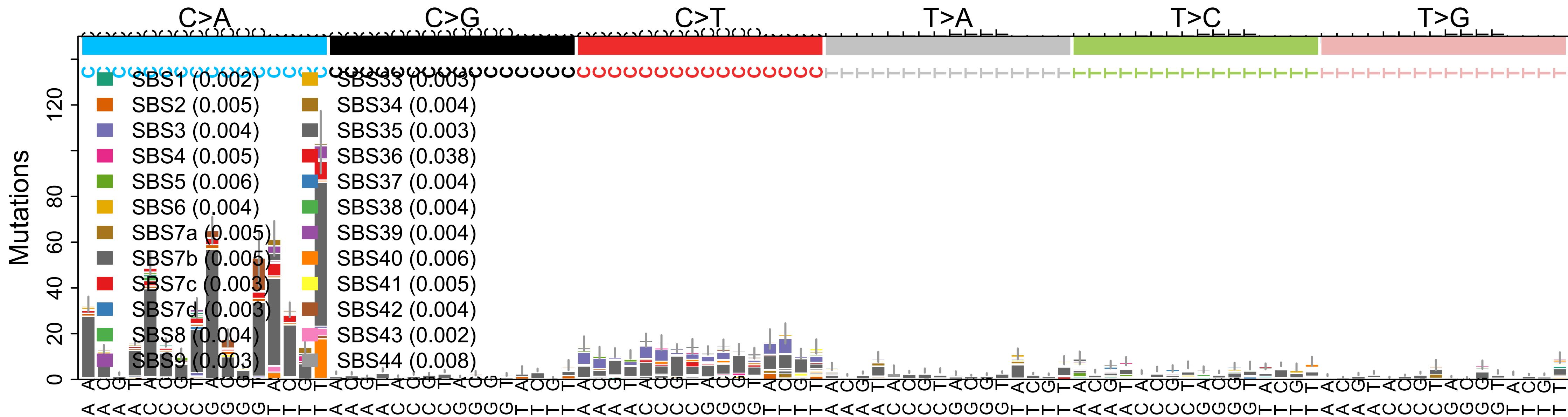
Reconstructed spectrum (cosine similarity = 0.914)



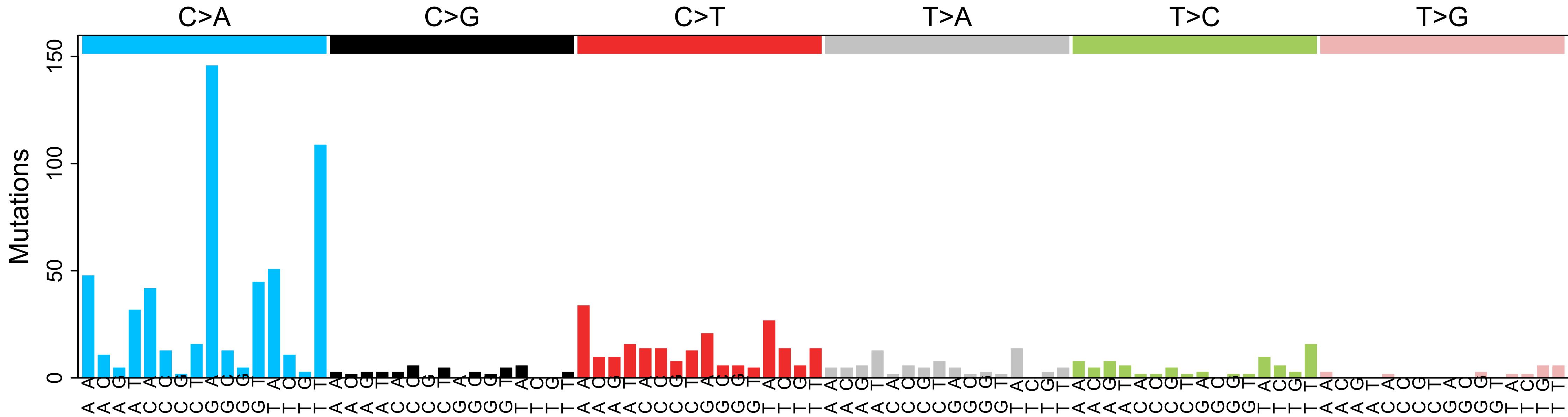
## 4\_4\_methylene\_bis2\_chloroaniline\_b43861ea935b (987 mutations)



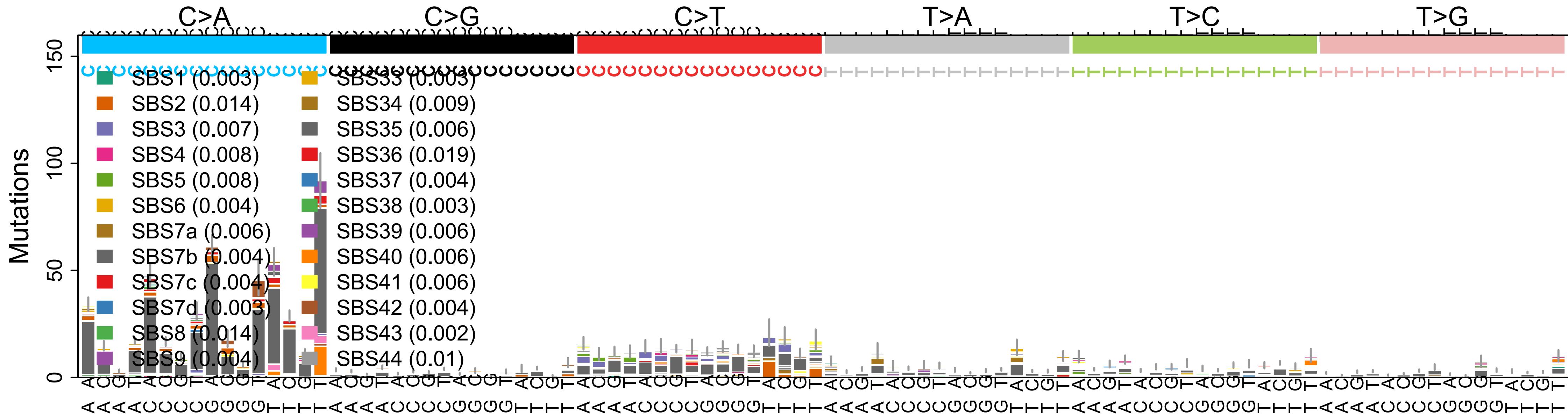
Reconstructed spectrum (cosine similarity = 0.935)



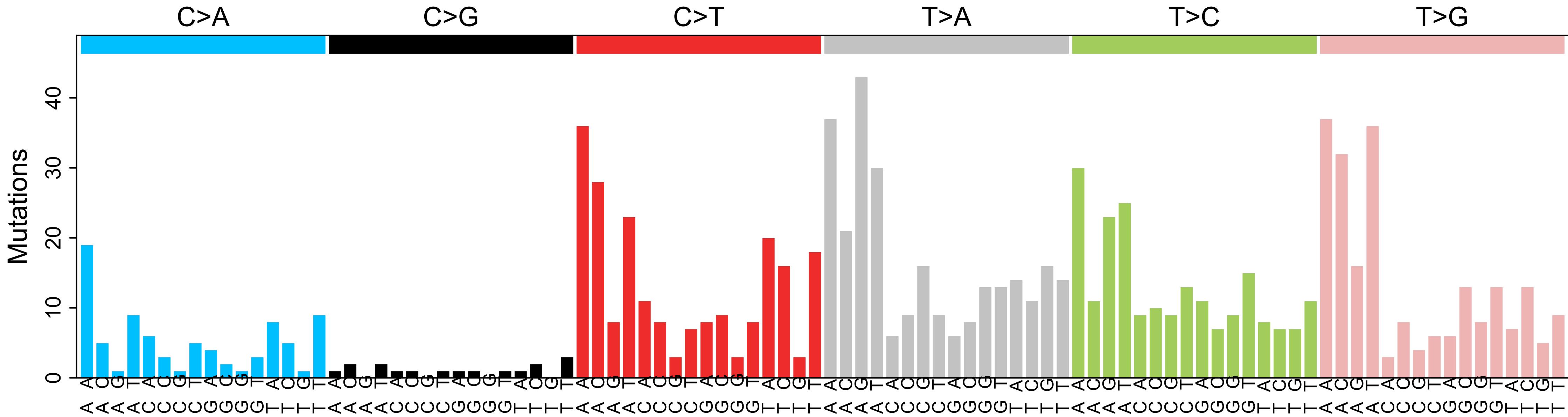
## 4\_aminobiphenyl\_dfa9b811bd76 (1,002 mutations)



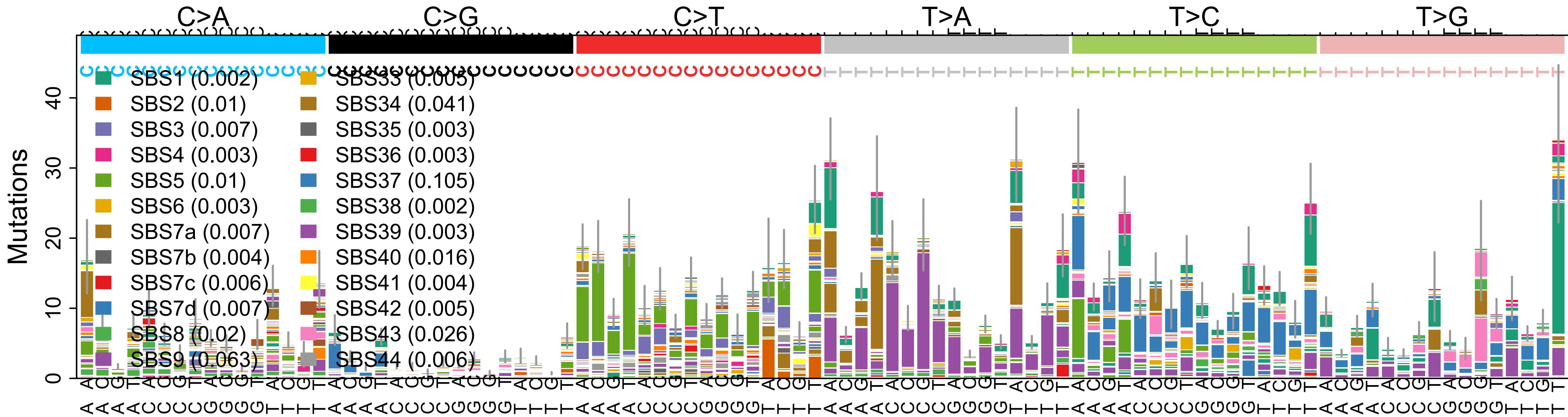
Reconstructed spectrum (cosine similarity = 0.907)



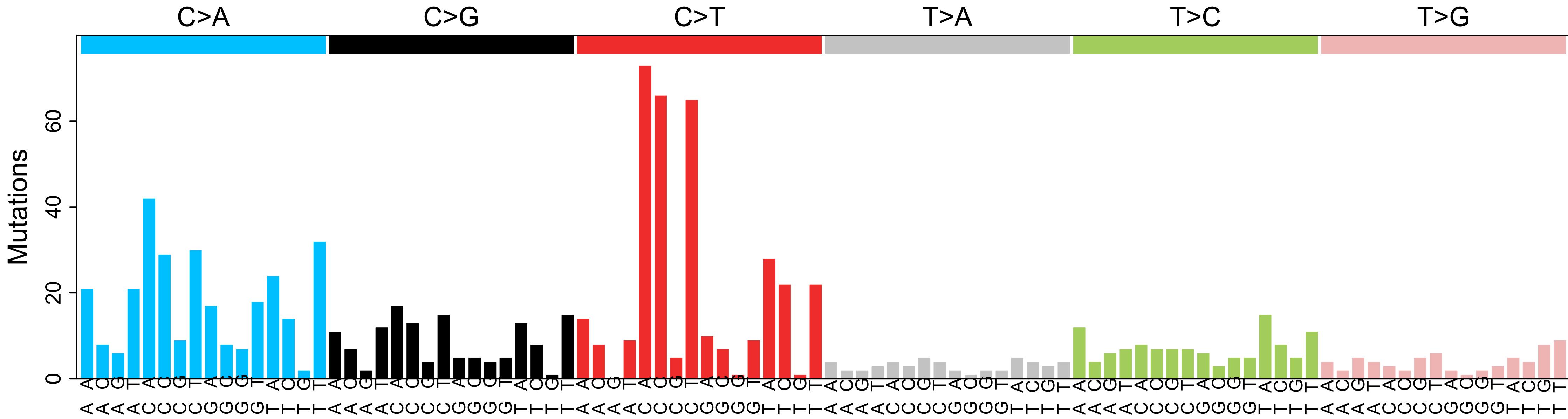
# 4\_methylNitrosamino\_1\_3\_pyridyl\_1\_butanone\_dfb390c0ba8d (995 mutations)



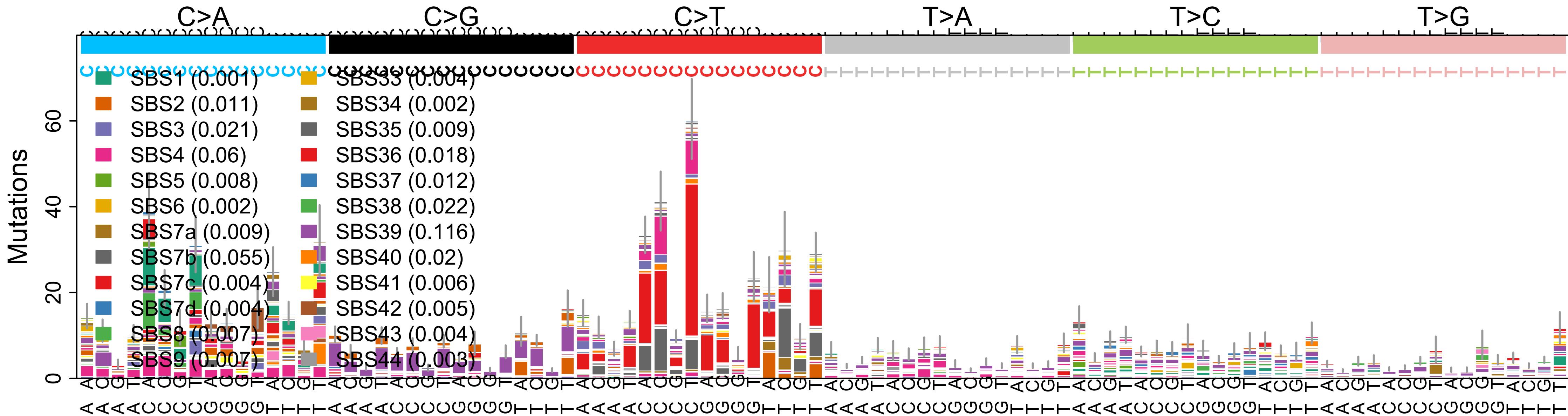
Reconstructed spectrum (cosine similarity = 0.826)



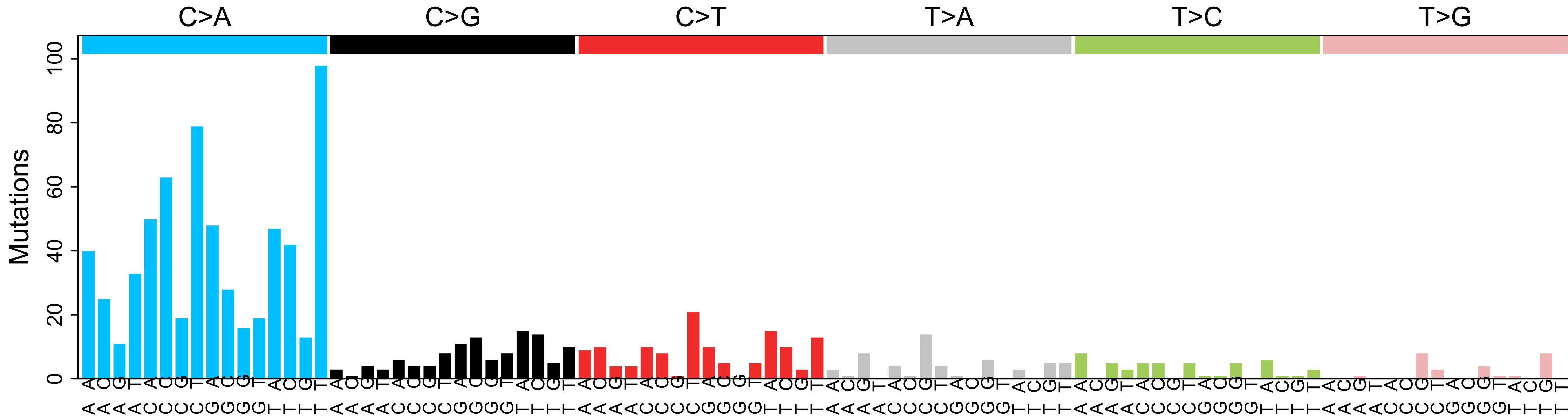
# 4\_nitroquinoline\_n\_oxide\_8799cddc608a (996 mutations)



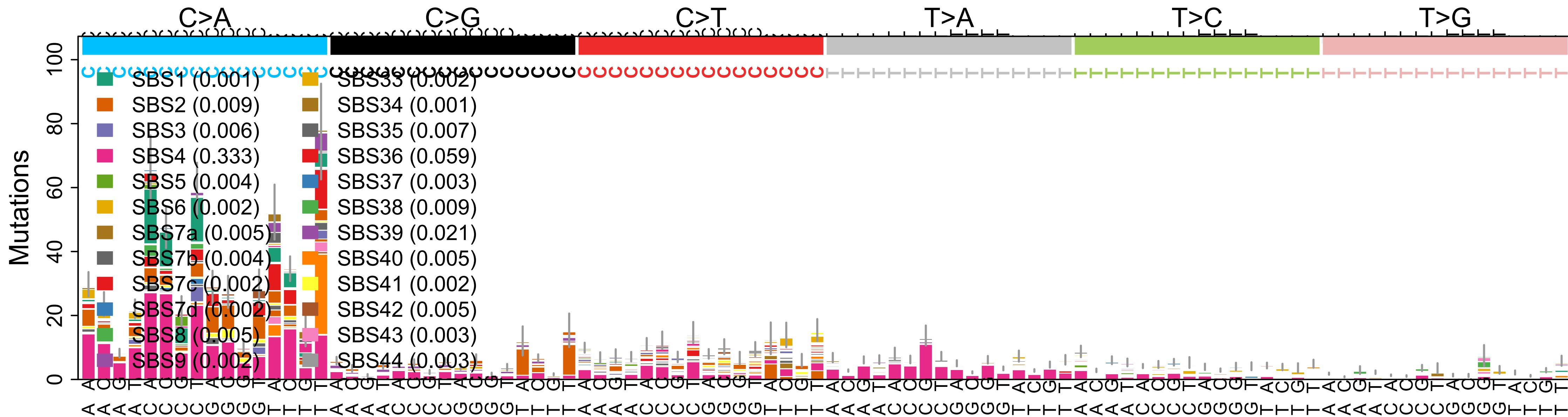
Reconstructed spectrum (cosine similarity = 0.93)



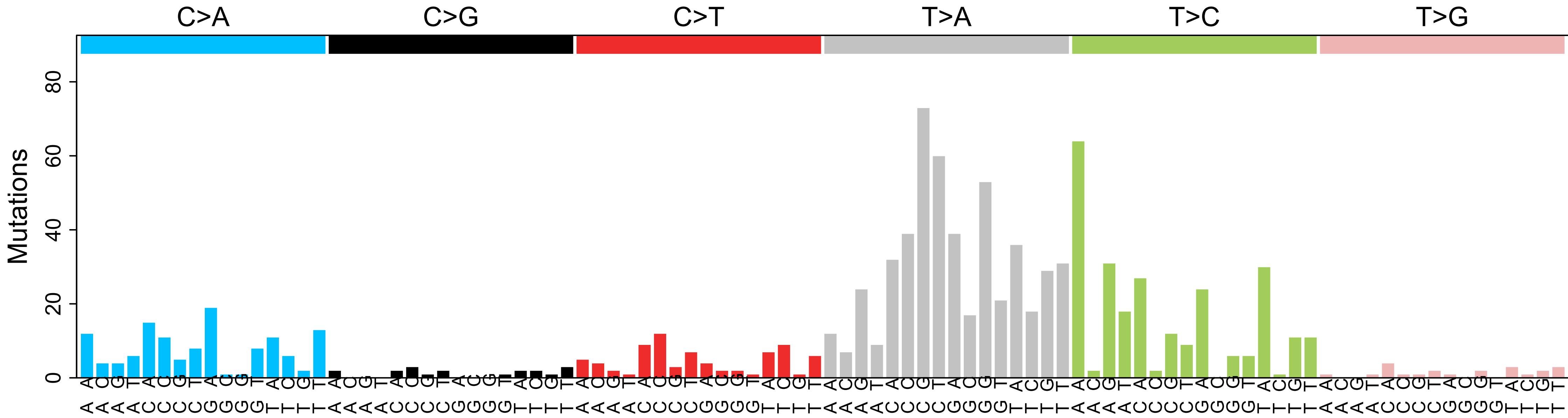
# 5\_methylchrysene\_5b2e180a87c7 (1,004 mutations)



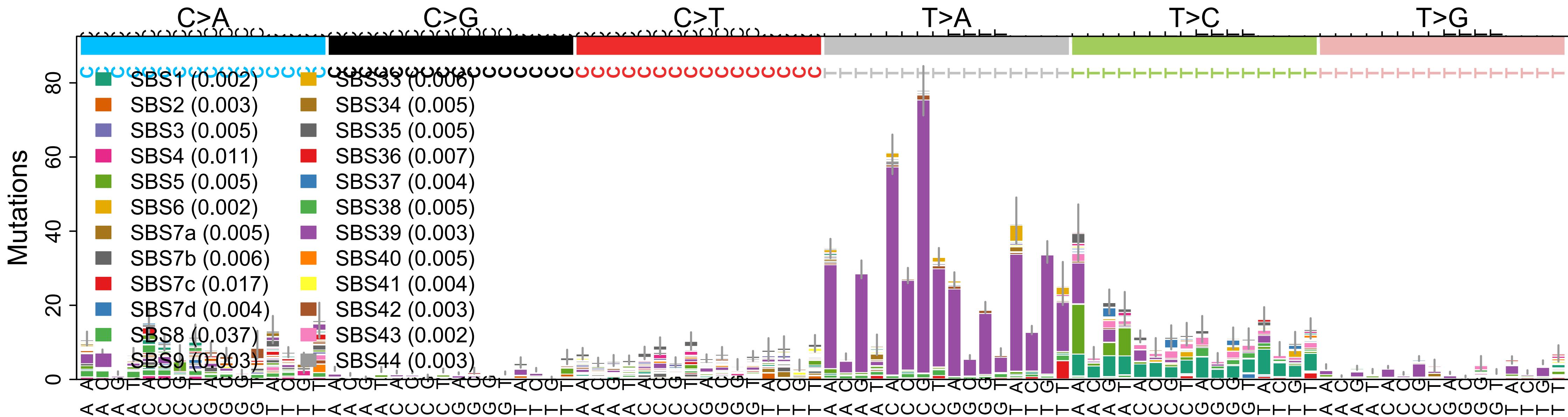
## Reconstructed spectrum (cosine similarity = 0.963)



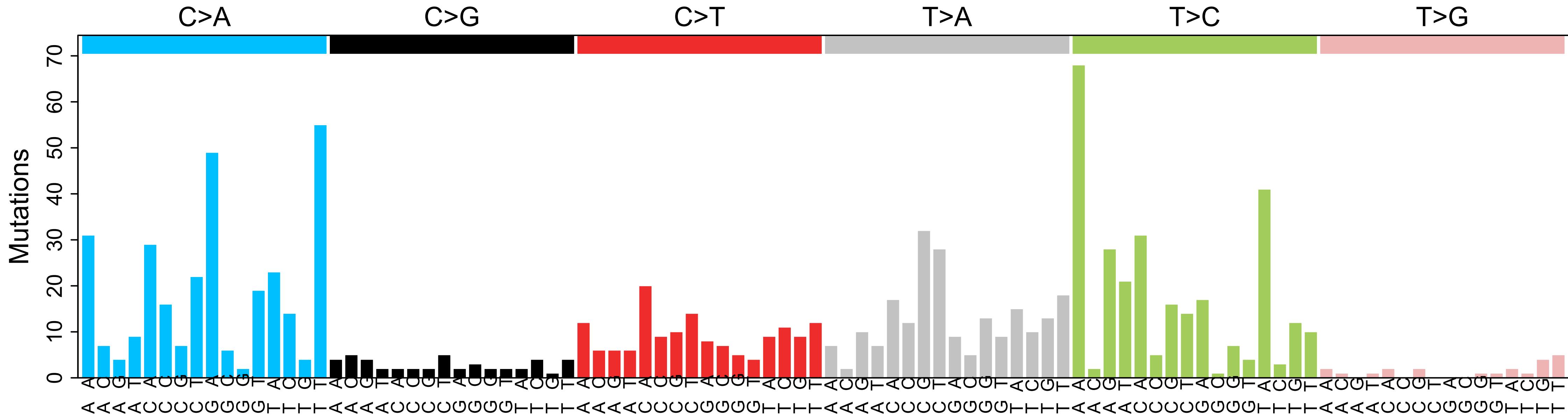
# 6\_nitrochrysene\_2a37dfc605b1 (996 mutations)



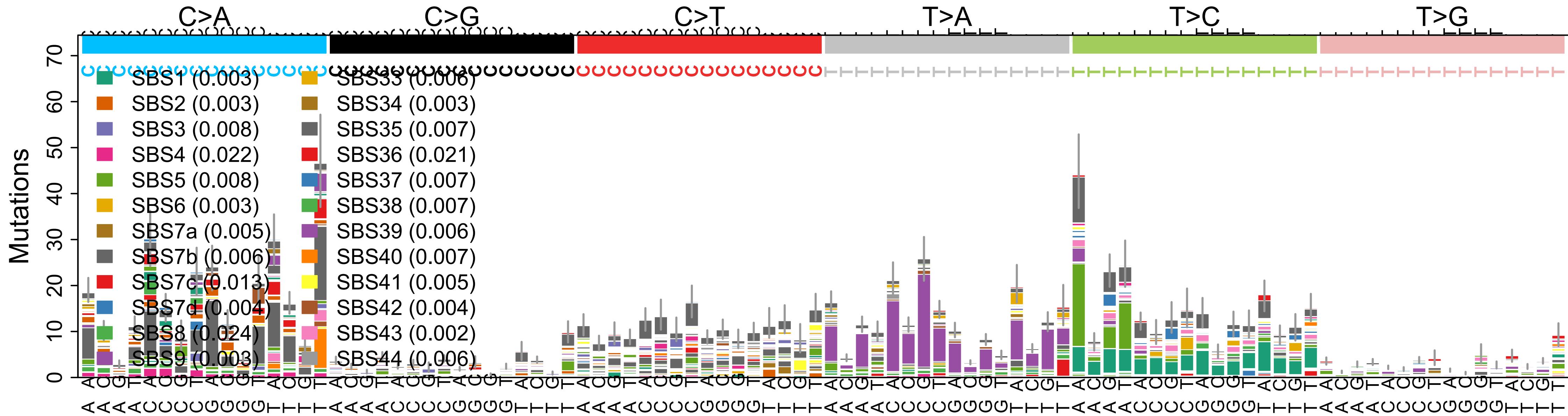
Reconstructed spectrum (cosine similarity = 0.899)



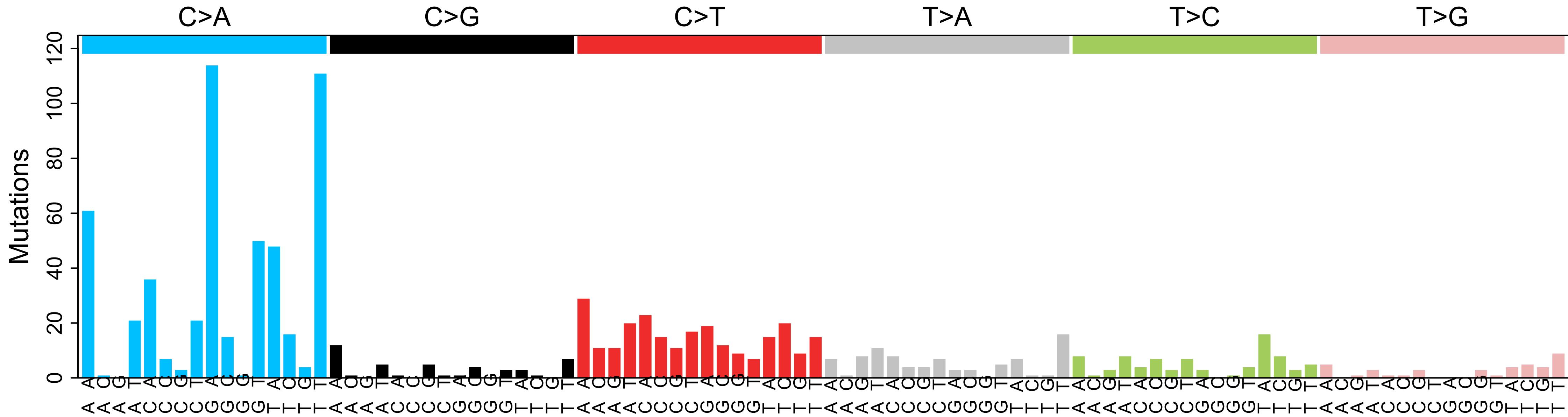
# 6\_nitrochrysene\_fd4adb4298d0 (1,000 mutations)



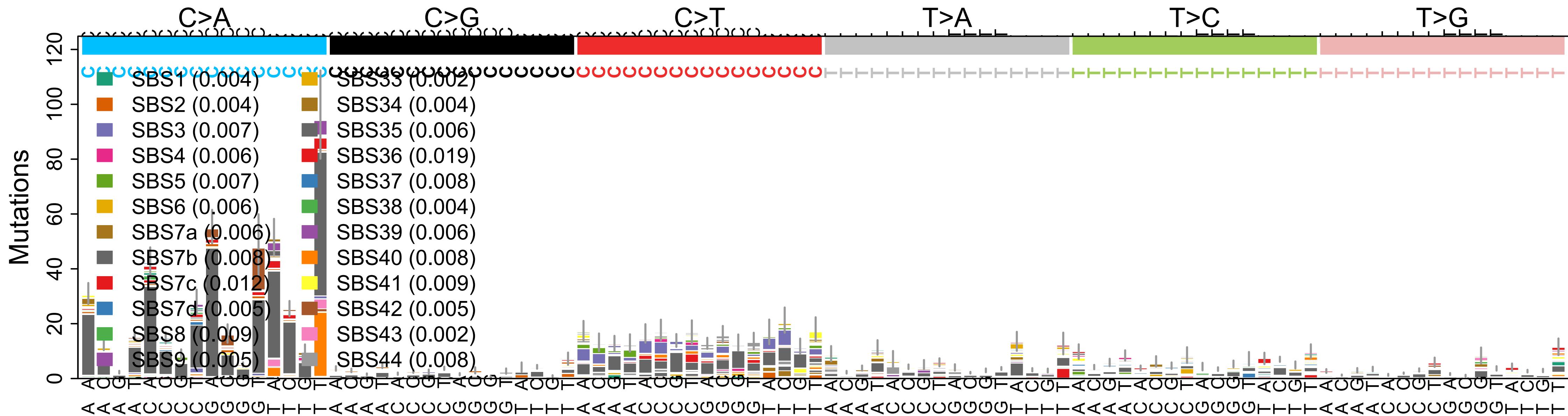
Reconstructed spectrum (cosine similarity = 0.93)



# 7h\_dibenzoc\_gcarbazole\_af112efa14d2 (1,003 mutations)



Reconstructed spectrum (cosine similarity = 0.936)



# 7h\_dibenzoc\_gcarbazole\_b48114ea8899 (1,000 mutations)

C>A

C>G

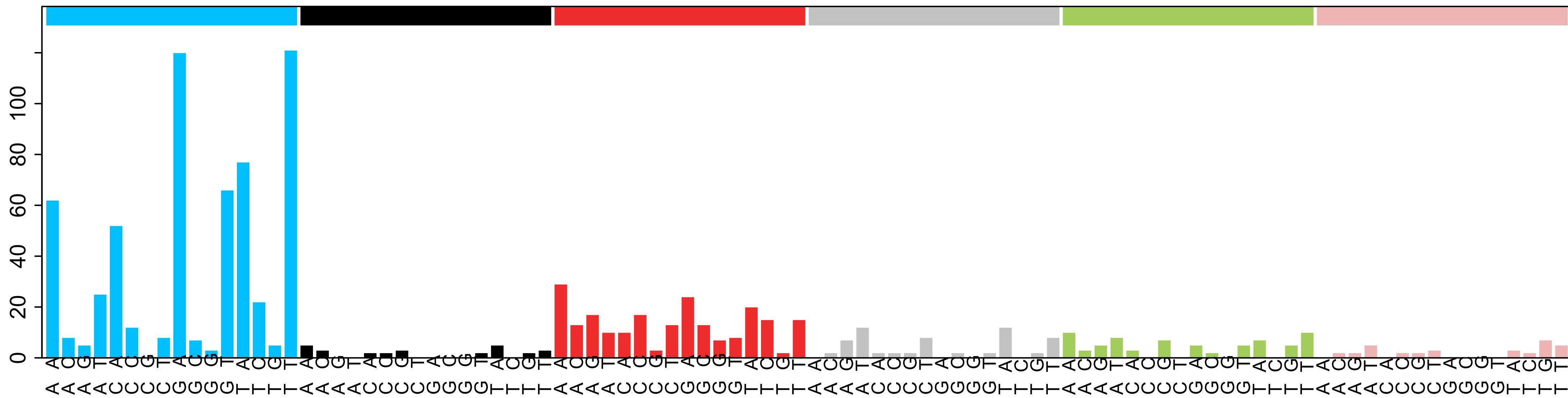
C>T

T>A

T>C

T>G

Mutations



Reconstructed spectrum (cosine similarity = 0.943)

C>A

C>G

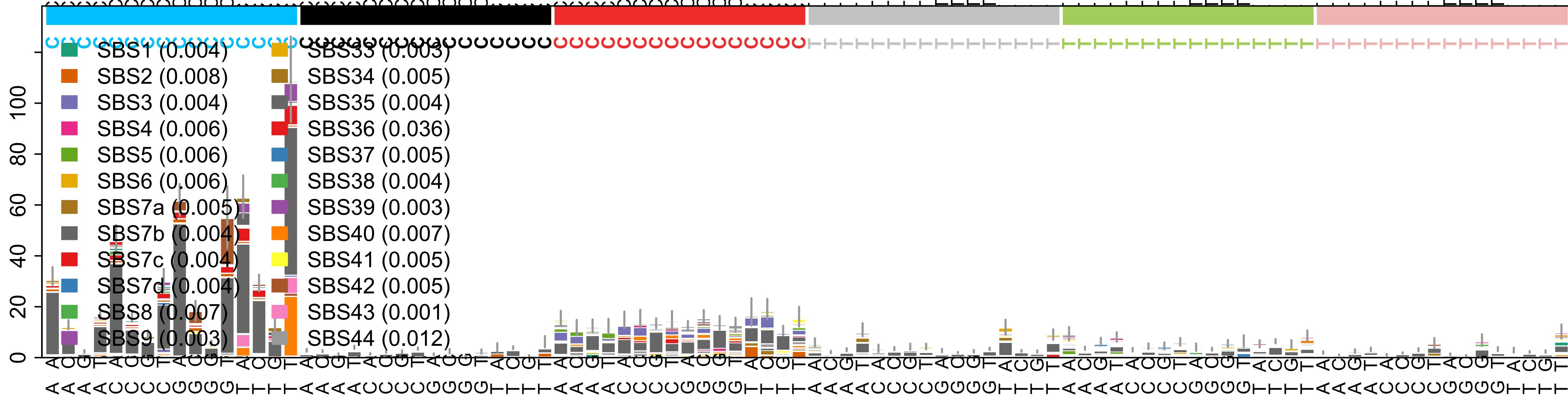
C>T

T>A

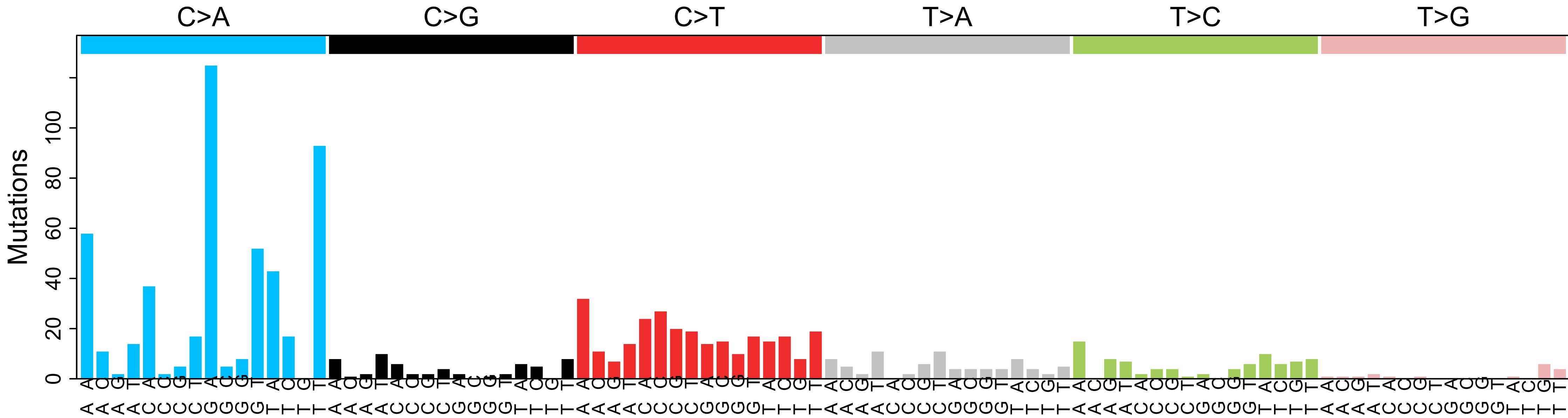
T>C

T>G

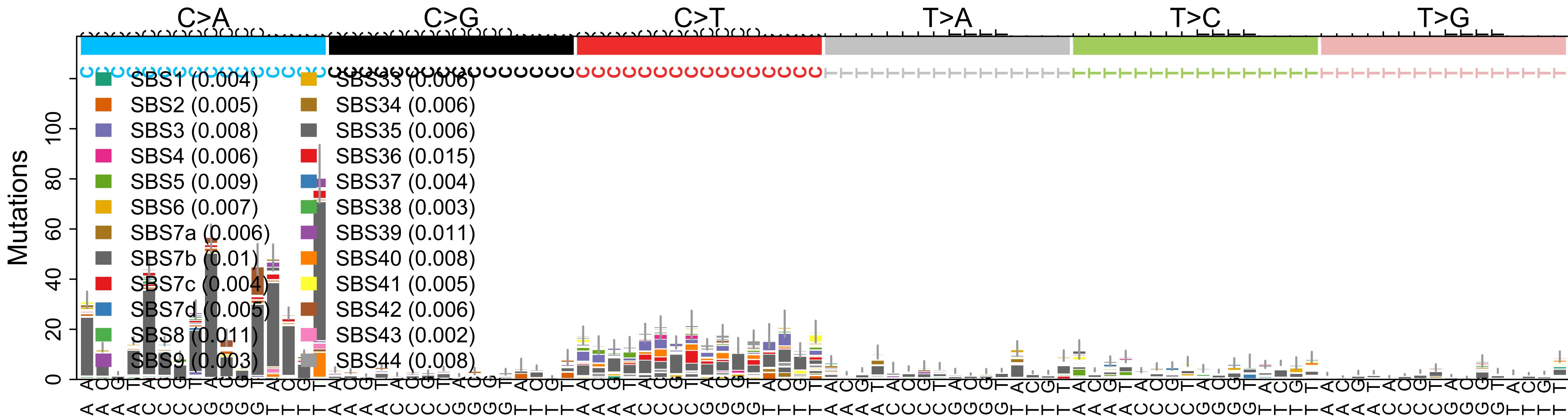
Mutations



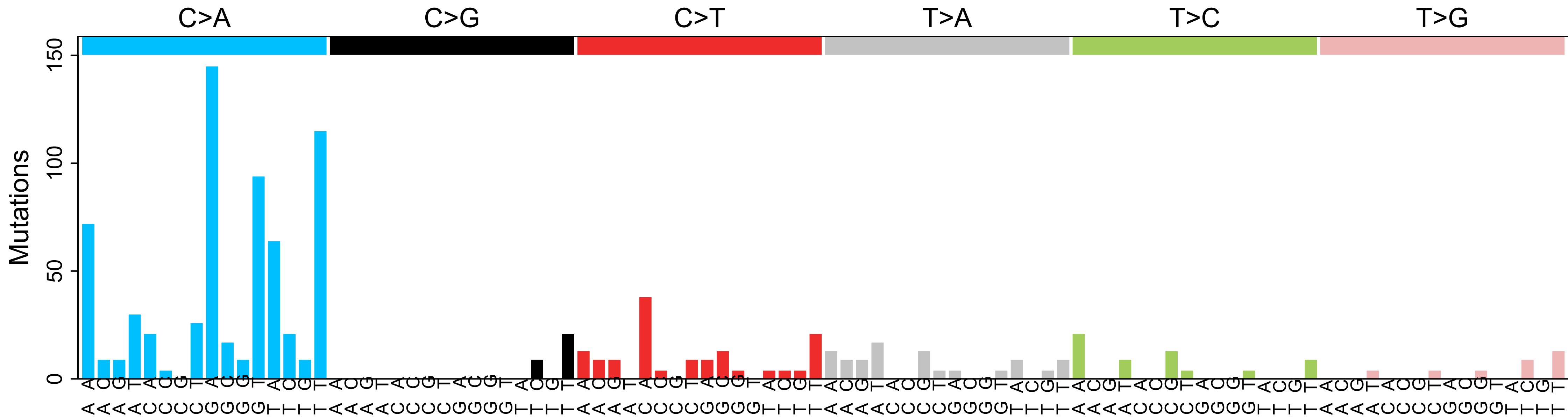
# acetaldehyde\_9fde73f6e508 (999 mutations)



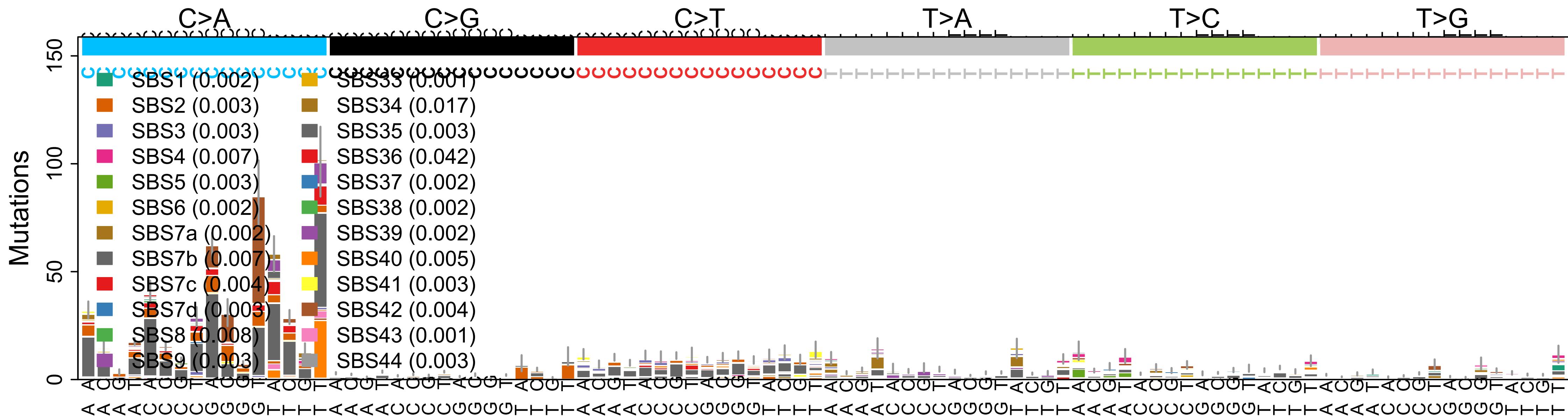
Reconstructed spectrum (cosine similarity = 0.92)



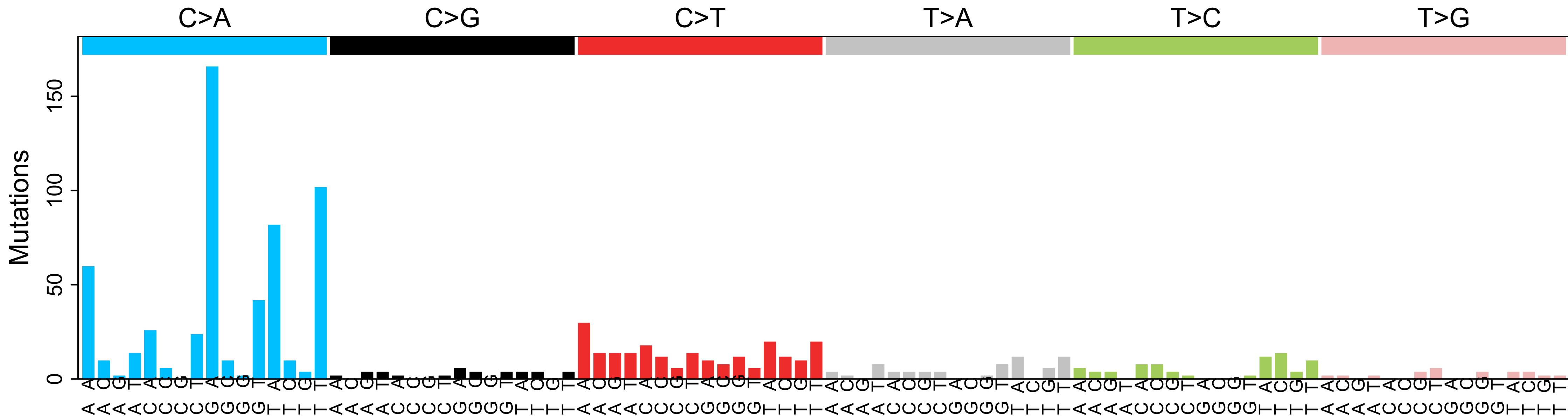
# acrolein\_7e28b8bb4834 (1,005 mutations)



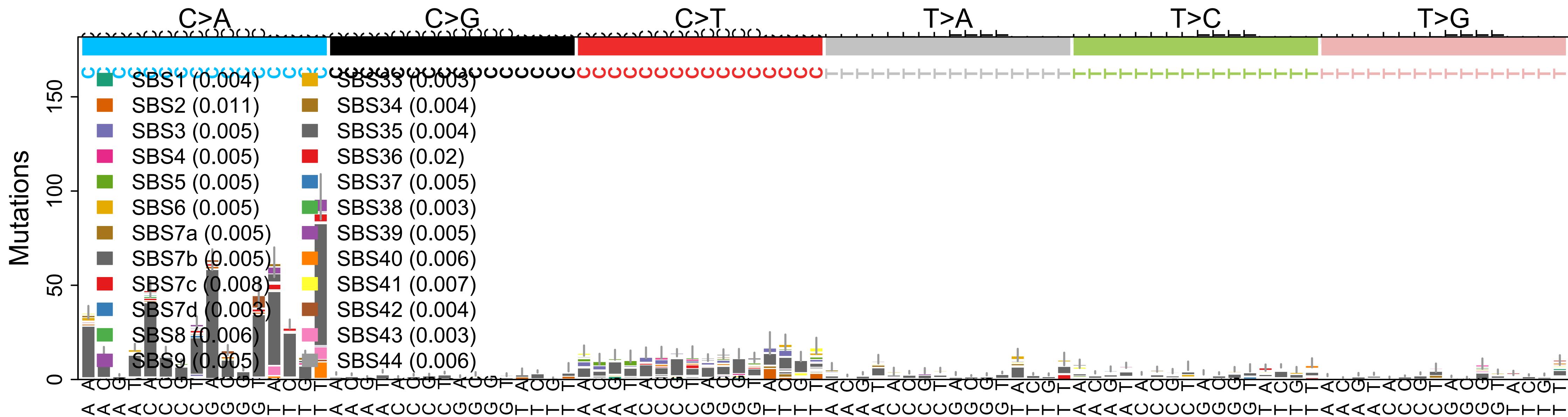
Reconstructed spectrum (cosine similarity = 0.908)



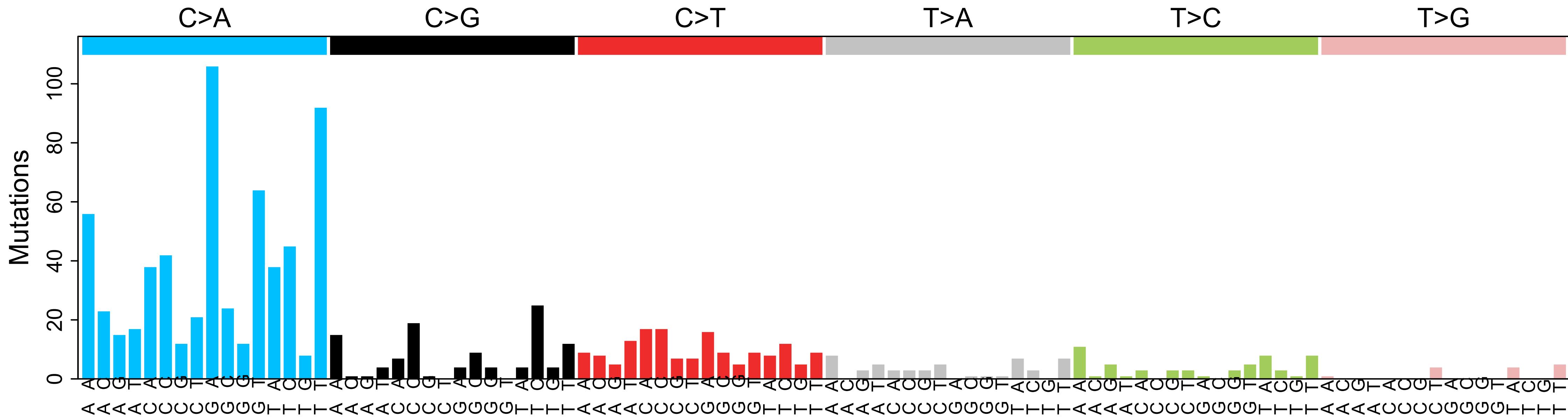
# acrylamide\_fc03d8ed1dc2 (1,000 mutations)



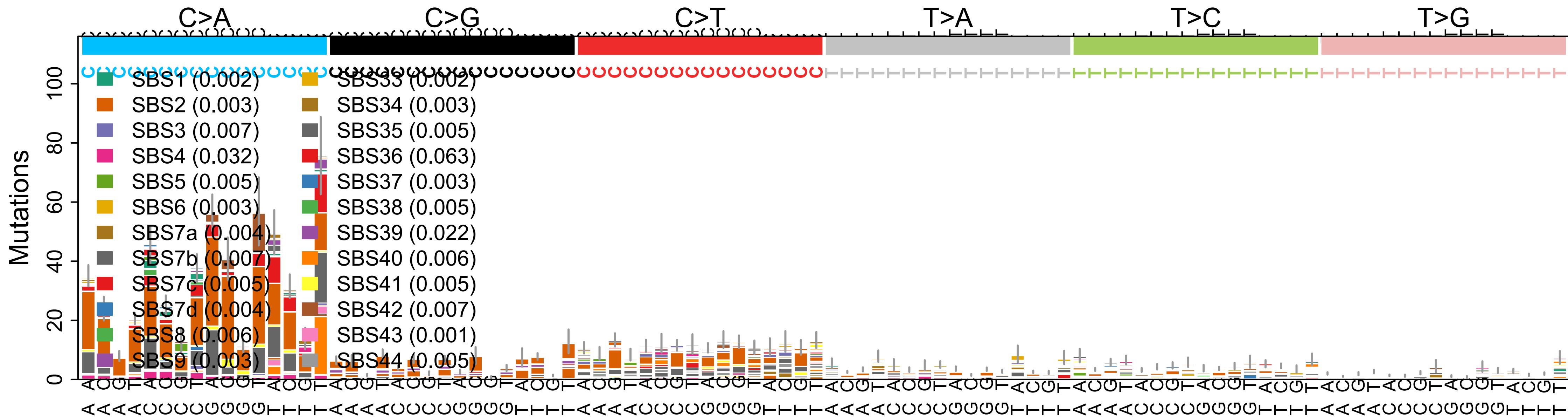
Reconstructed spectrum (cosine similarity = 0.884)



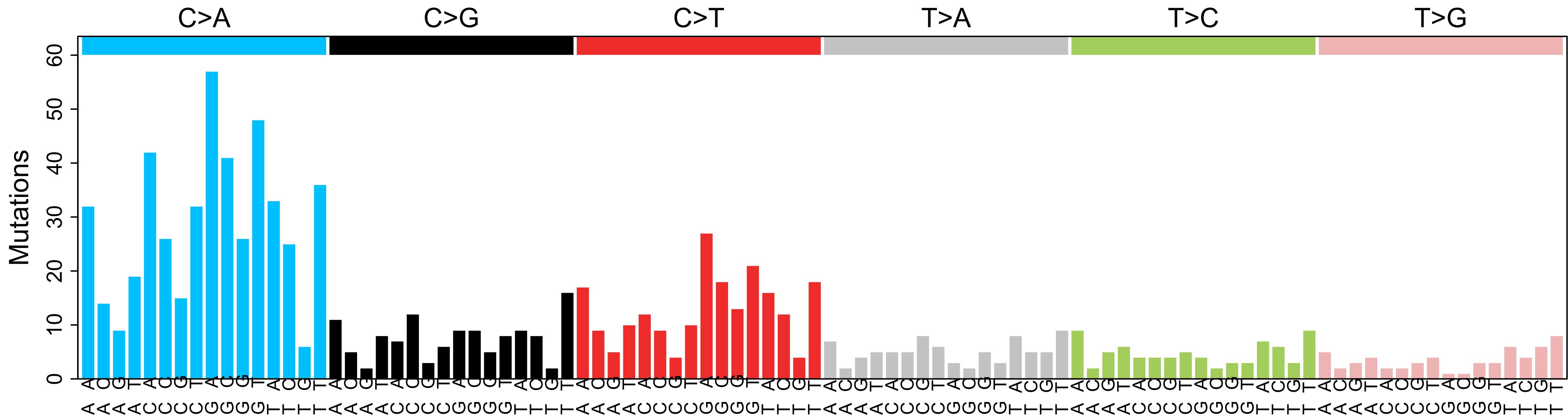
# aflatoxin\_b1\_60c8b83450ec (999 mutations)



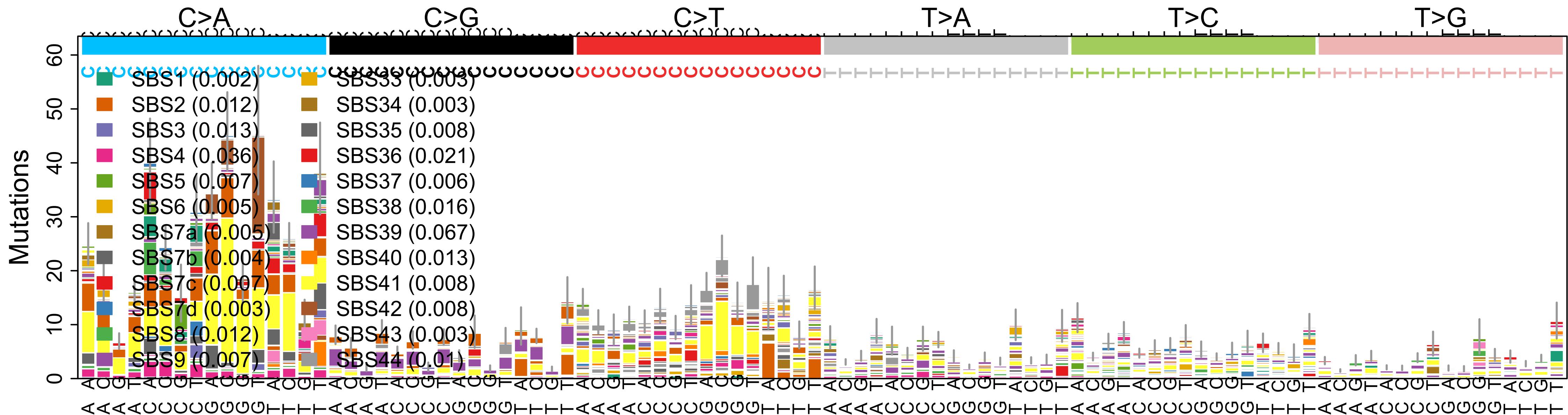
Reconstructed spectrum (cosine similarity = 0.929)



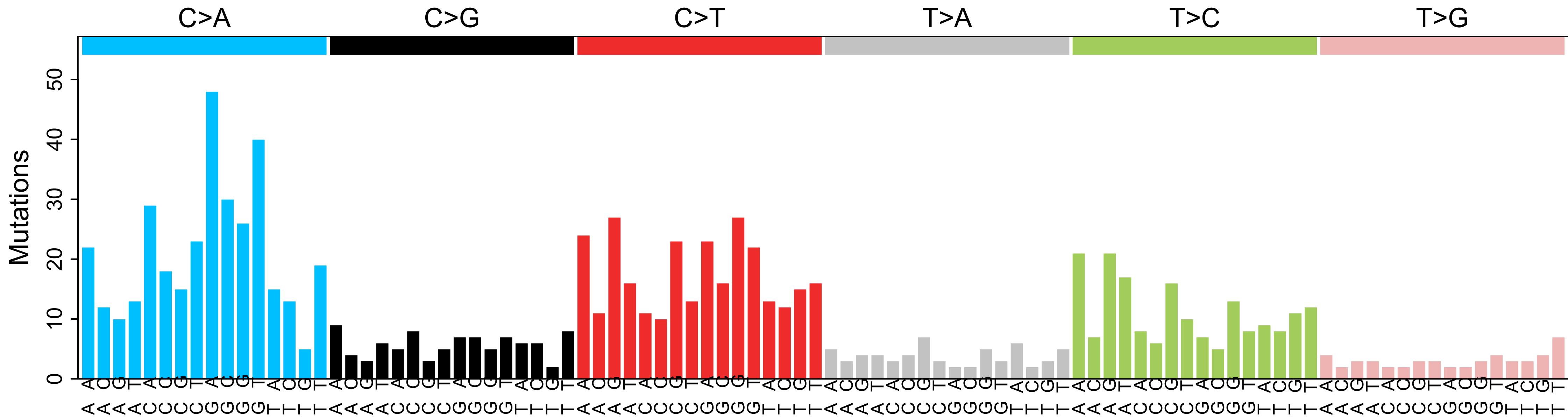
# aflatoxin\_b1\_61dc27c413a9 (1,001 mutations)



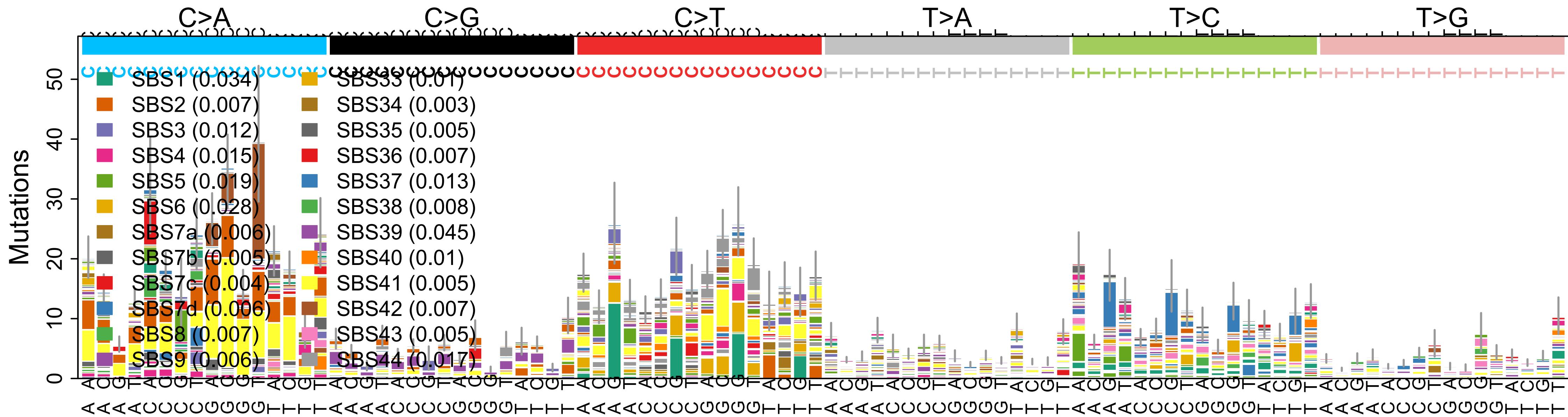
Reconstructed spectrum (cosine similarity = 0.974)



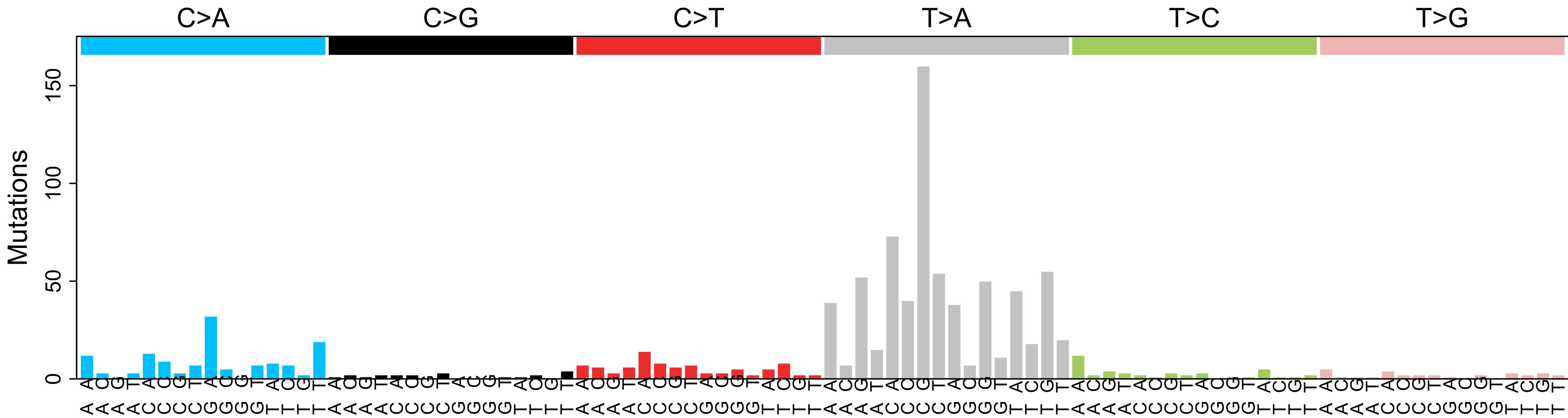
# aflatoxin\_b1\_e6c6aa551e43 (998 mutations)



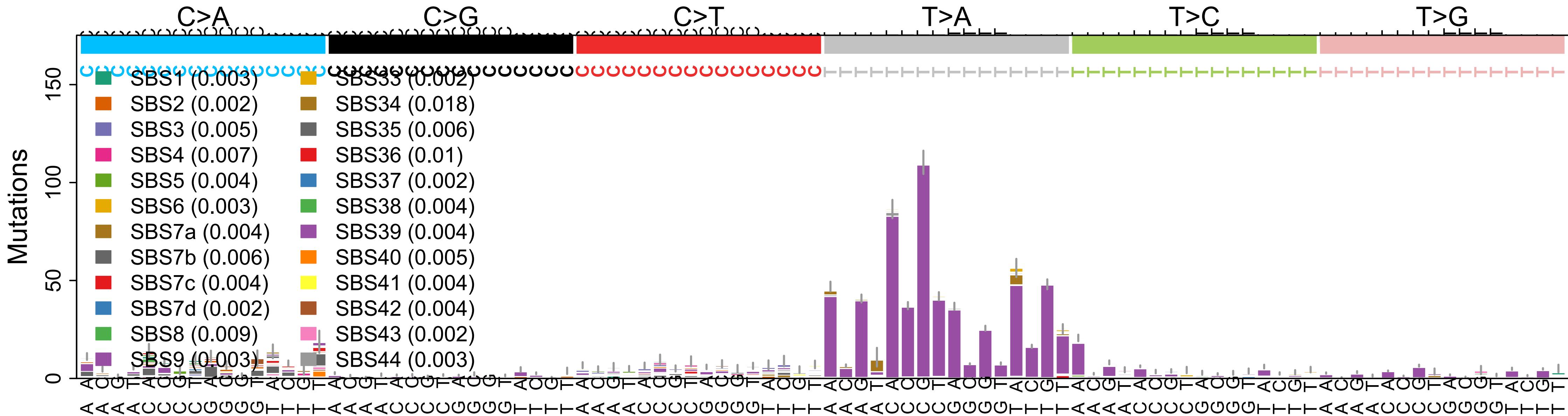
Reconstructed spectrum (cosine similarity = 0.968)



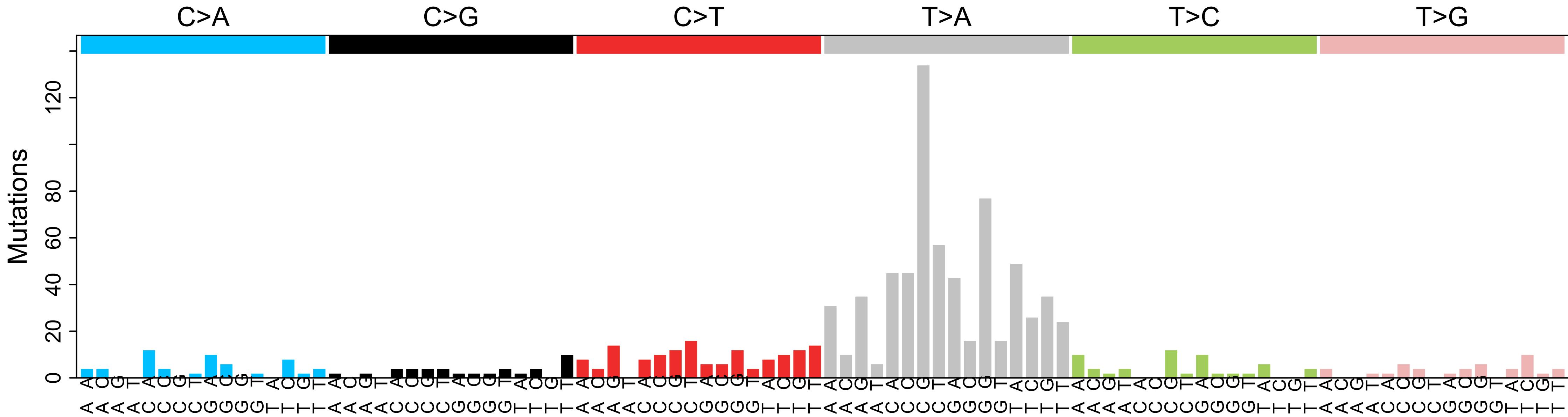
# aristolochic\_acid\_i\_b4173d75722f (997 mutations)



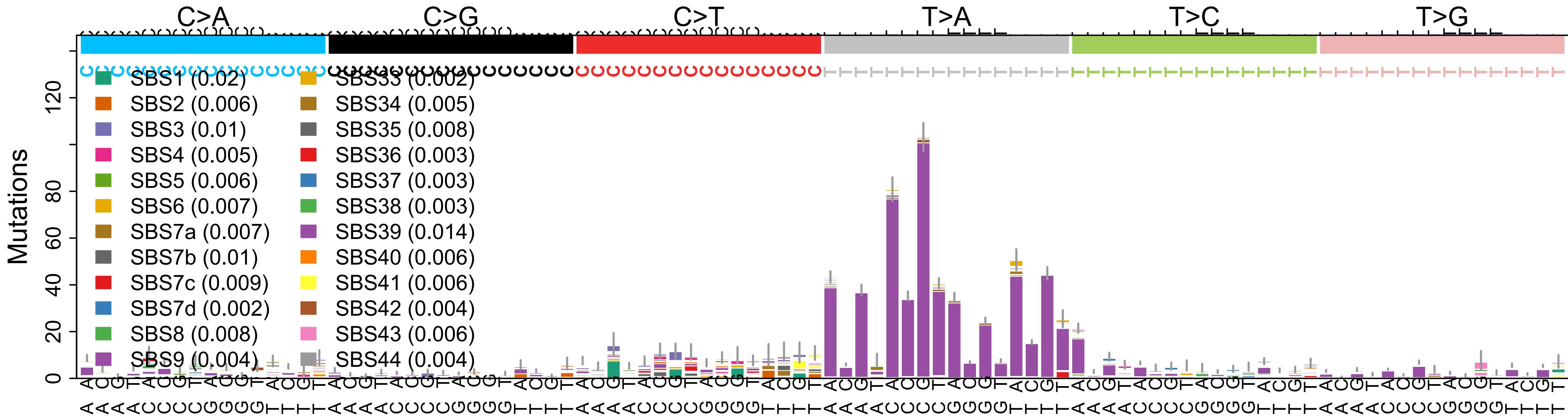
Reconstructed spectrum (cosine similarity = 0.96)



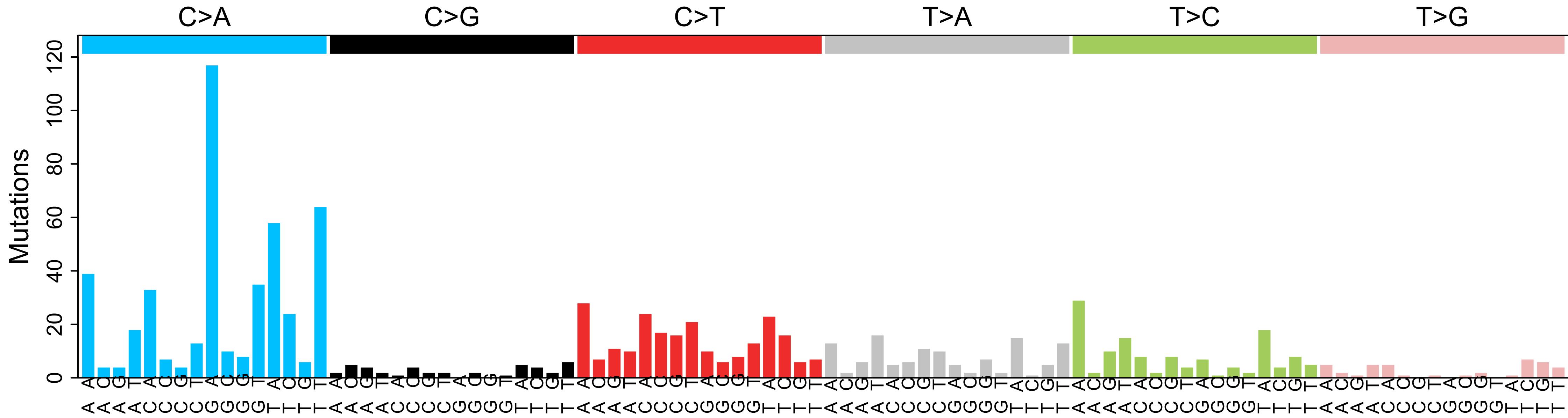
# aristolochic\_acid\_i\_e1077962b83d (1,007 mutations)



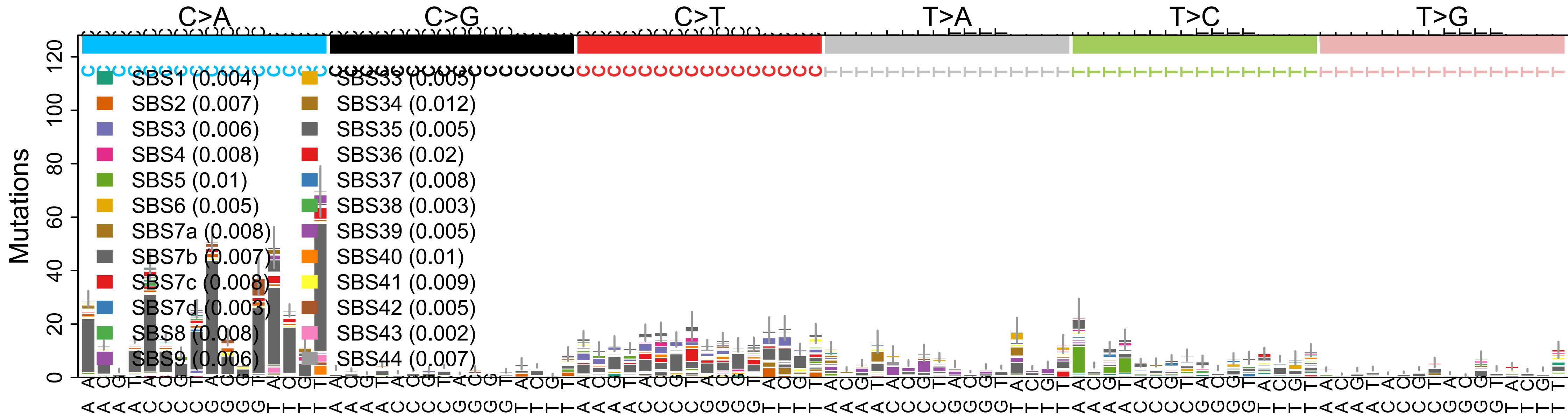
## Reconstructed spectrum (cosine similarity = 0.919)



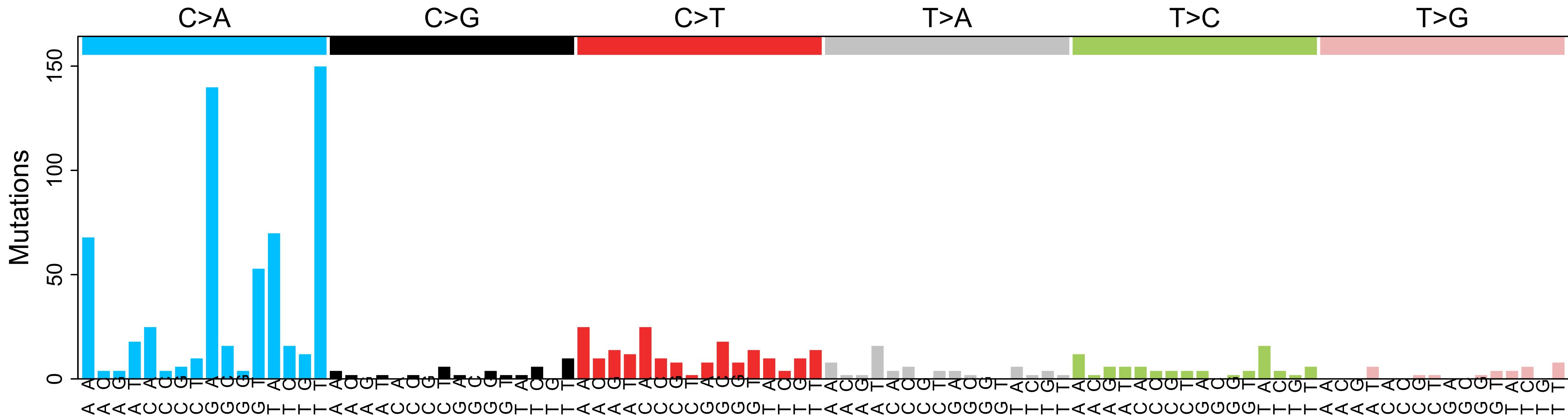
# aristolochic\_acid\_ii\_7cfb500c5521 (996 mutations)



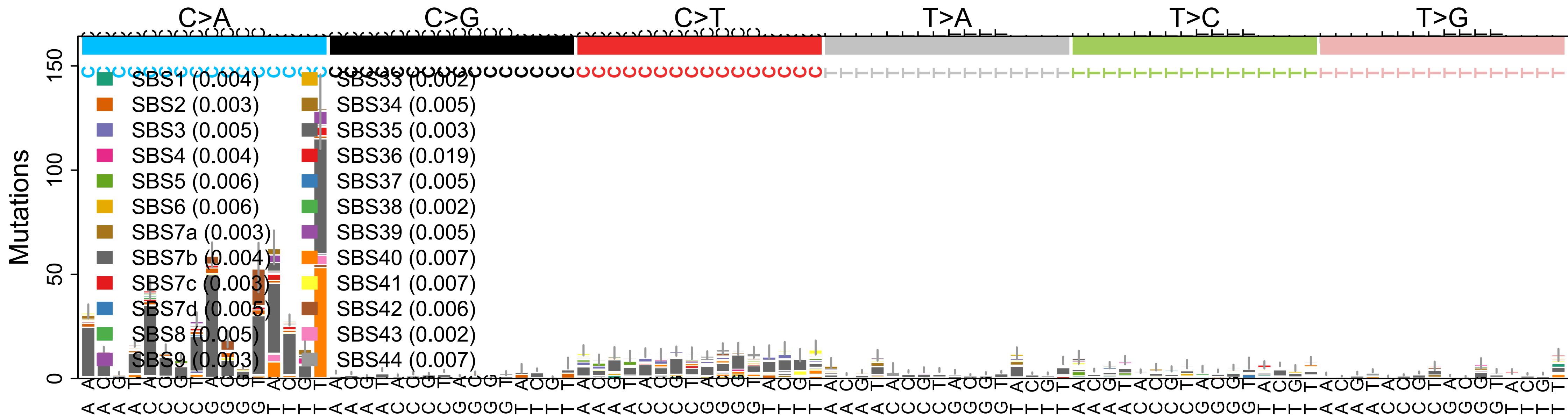
Reconstructed spectrum (cosine similarity = 0.91)



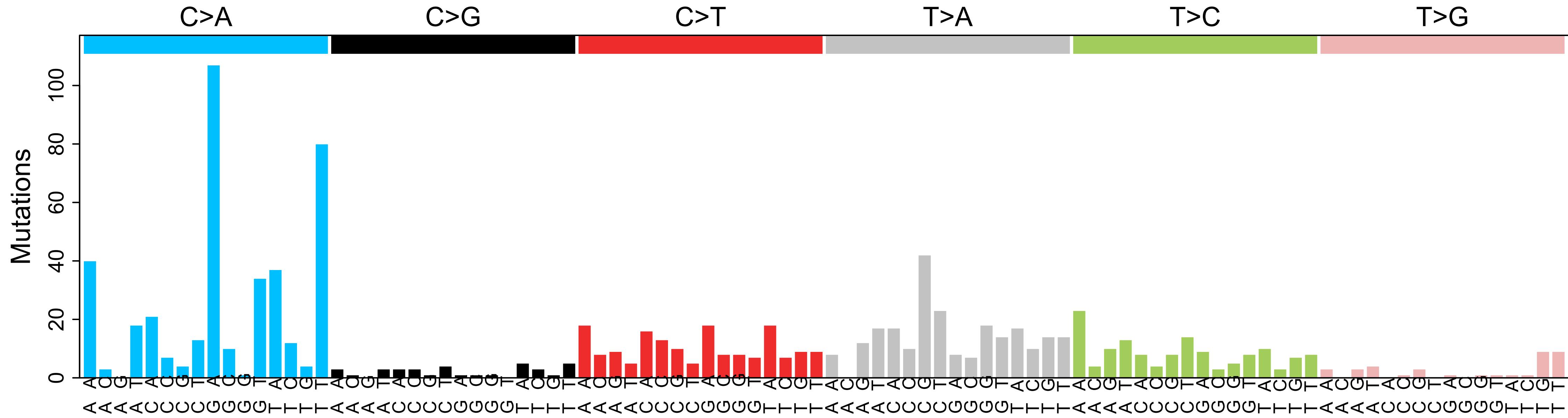
# az20\_e8f89cf2ec16 (1,012 mutations)



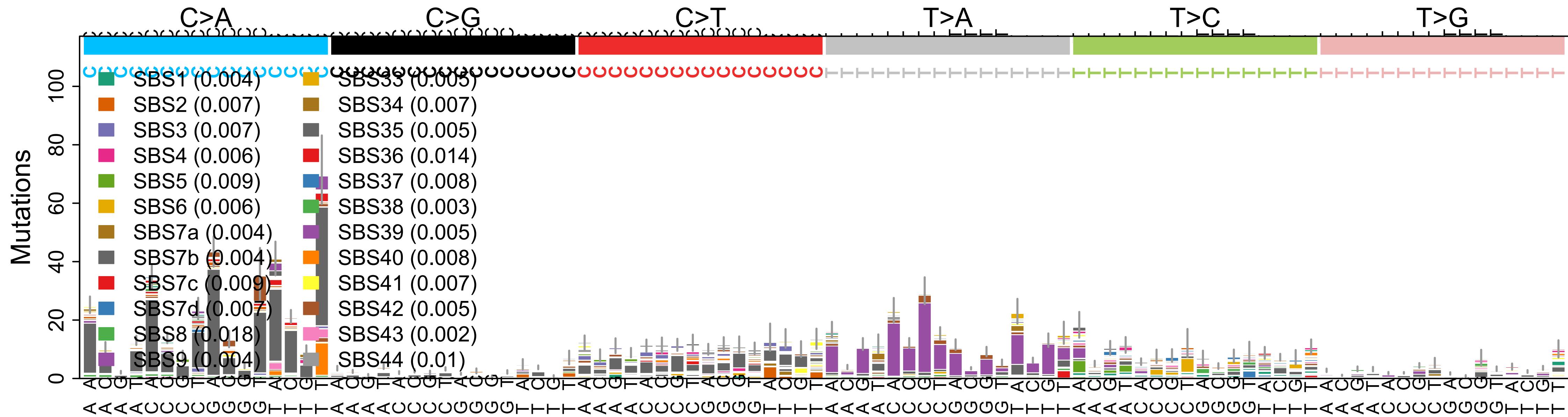
**Reconstructed spectrum (cosine similarity = 0.921)**



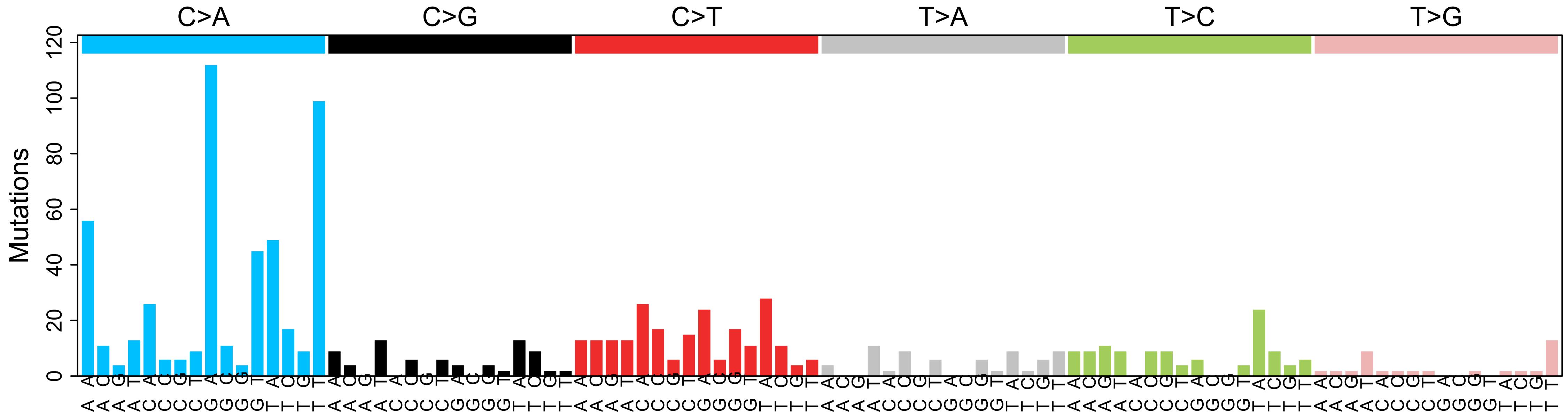
# azd7762\_c62b92e2486a (999 mutations)



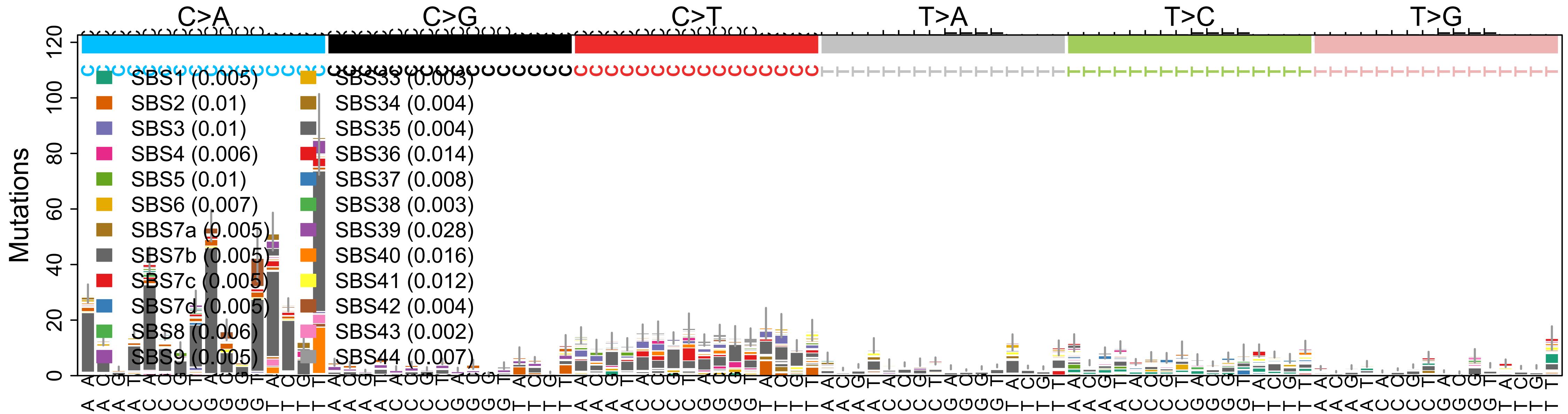
## Reconstructed spectrum (cosine similarity = 0.905)



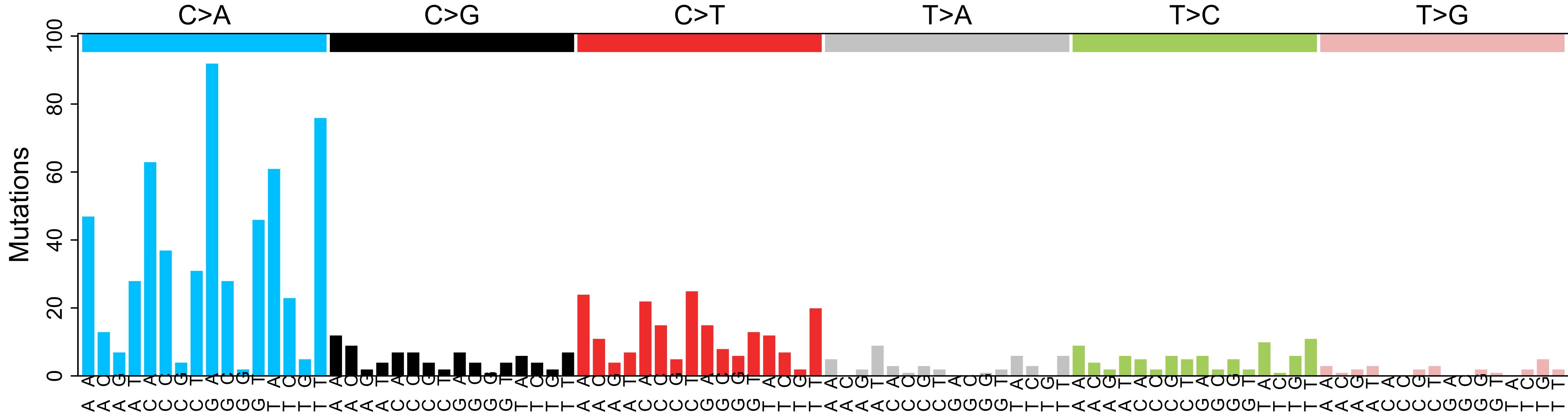
# benzidine\_5b2123a8cf0e (997 mutations)



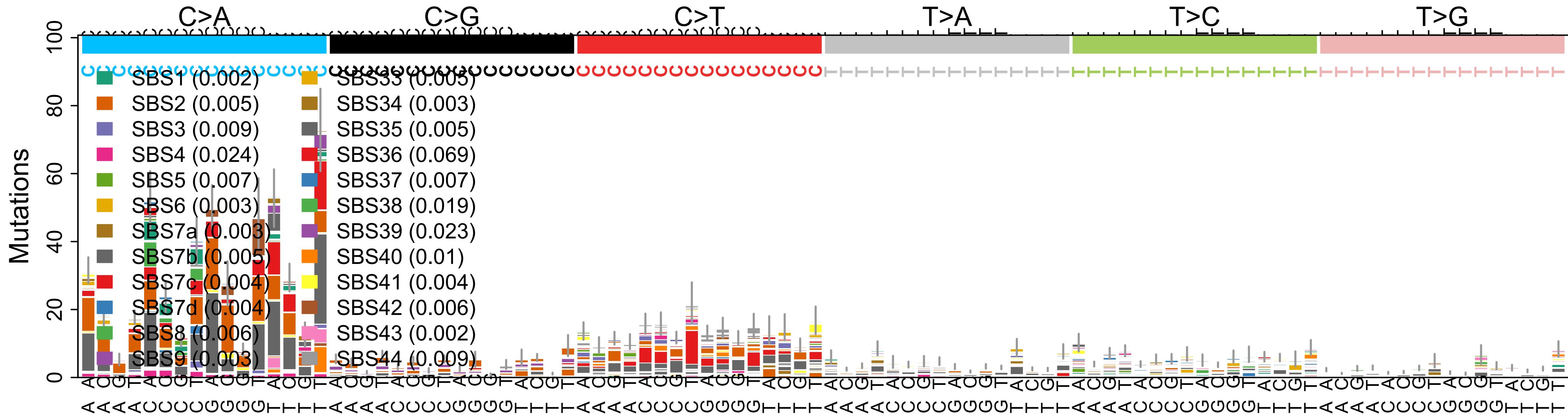
## Reconstructed spectrum (cosine similarity = 0.915)



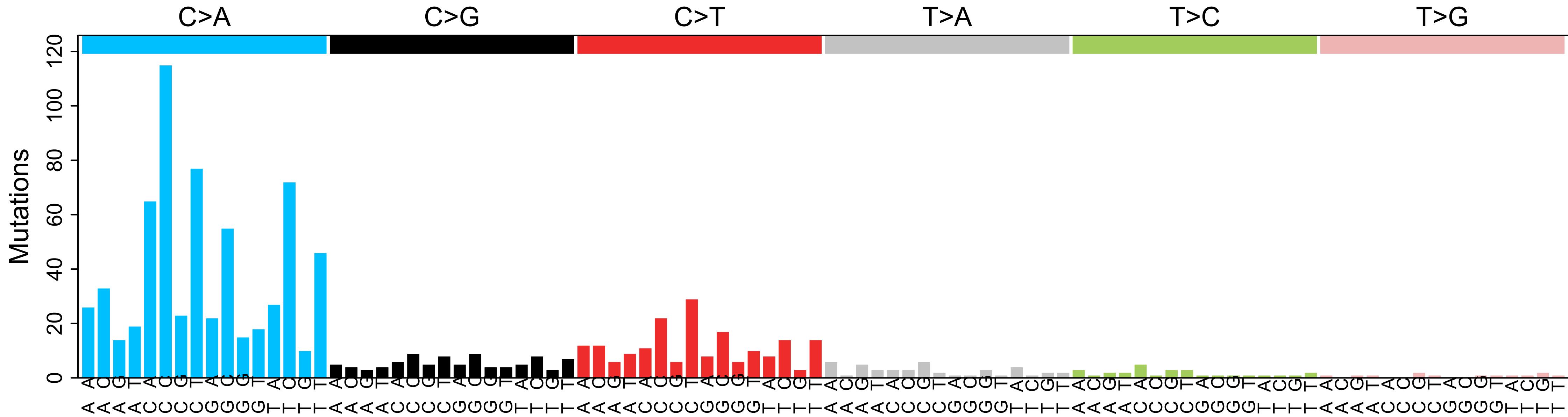
# benzidine\_6c3042d3a0b5 (992 mutations)



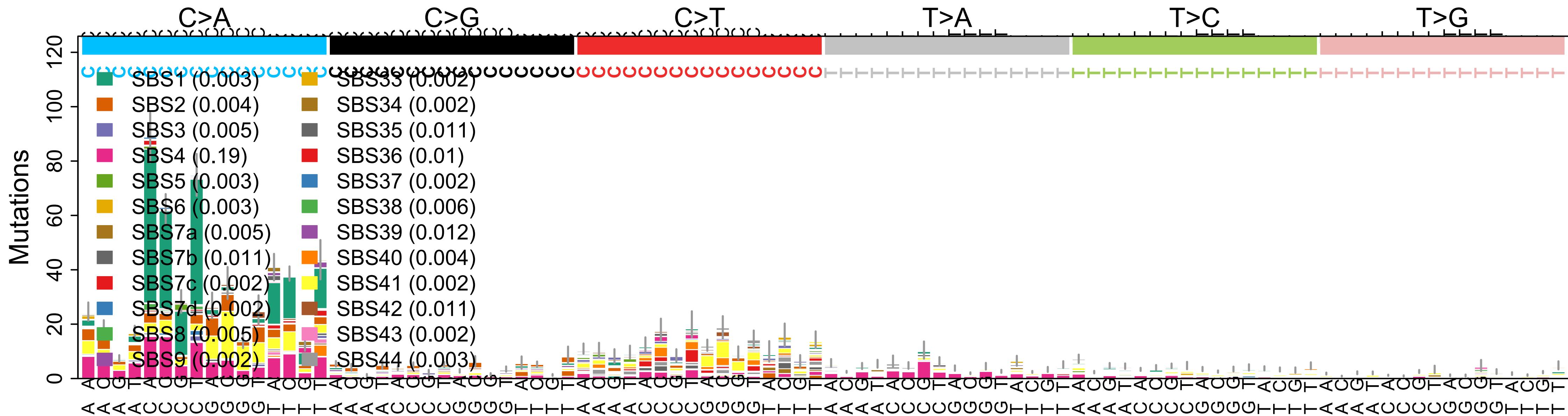
## Reconstructed spectrum (cosine similarity = 0.951)



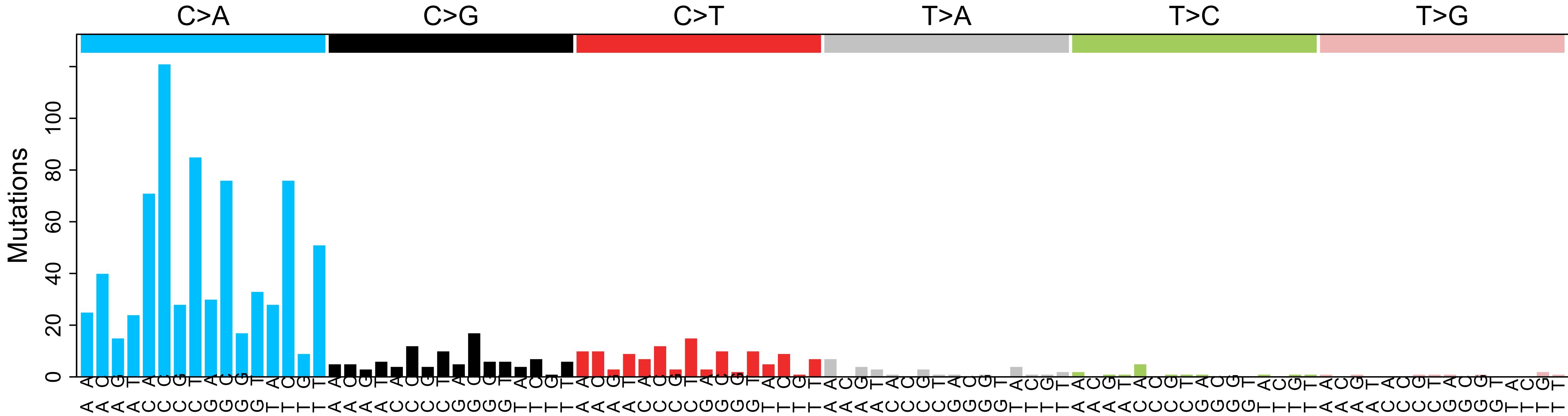
# benzoapyrene\_5157af6fc274 (999 mutations)



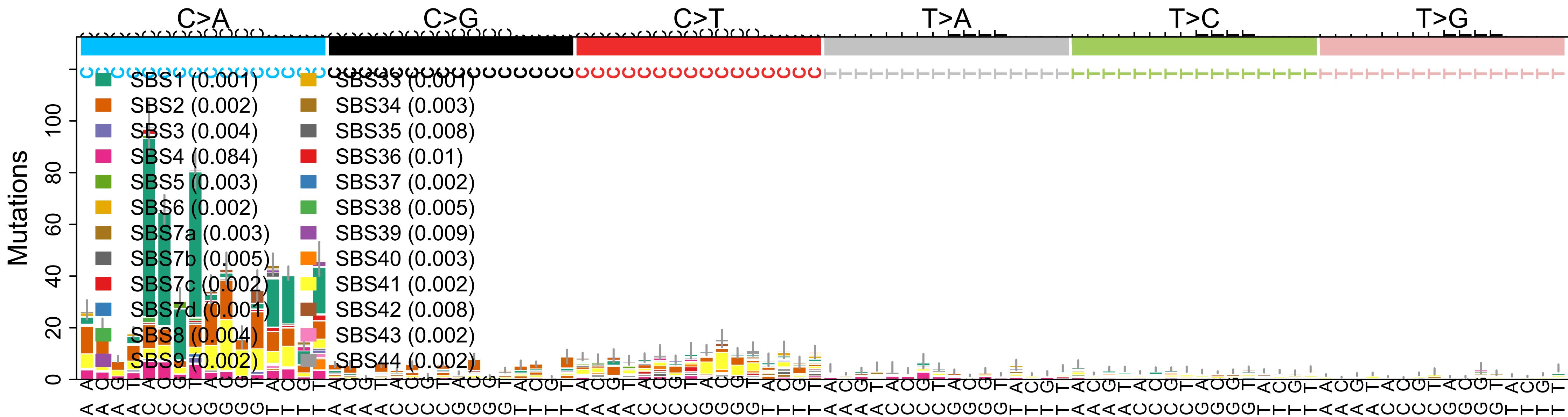
Reconstructed spectrum (cosine similarity = 0.93)



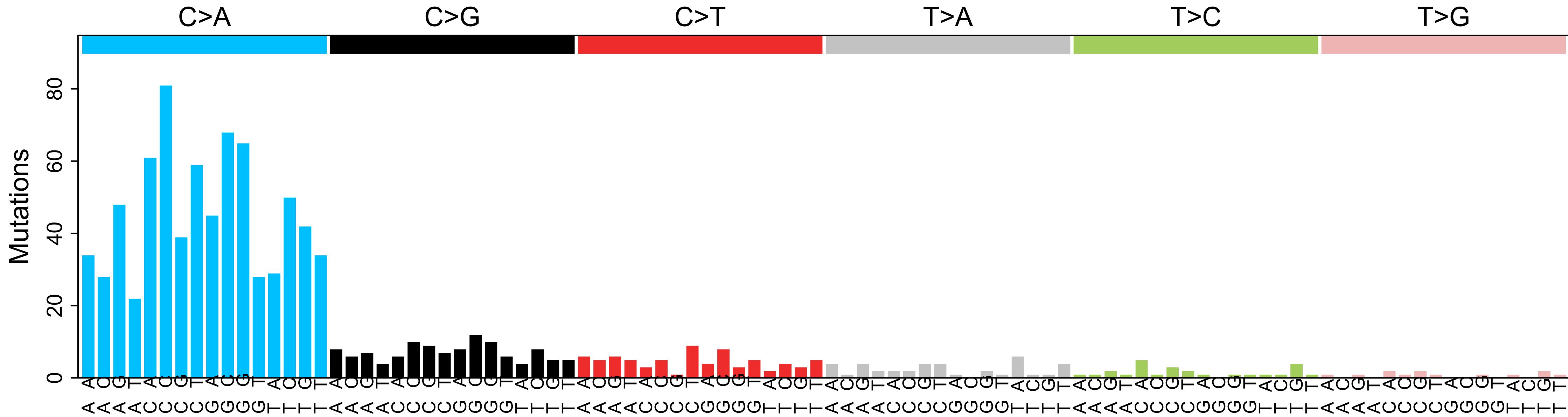
# benzoapyrene\_7\_8\_diol\_9\_10\_epoxide\_a940ded66b4f (999 mutations)



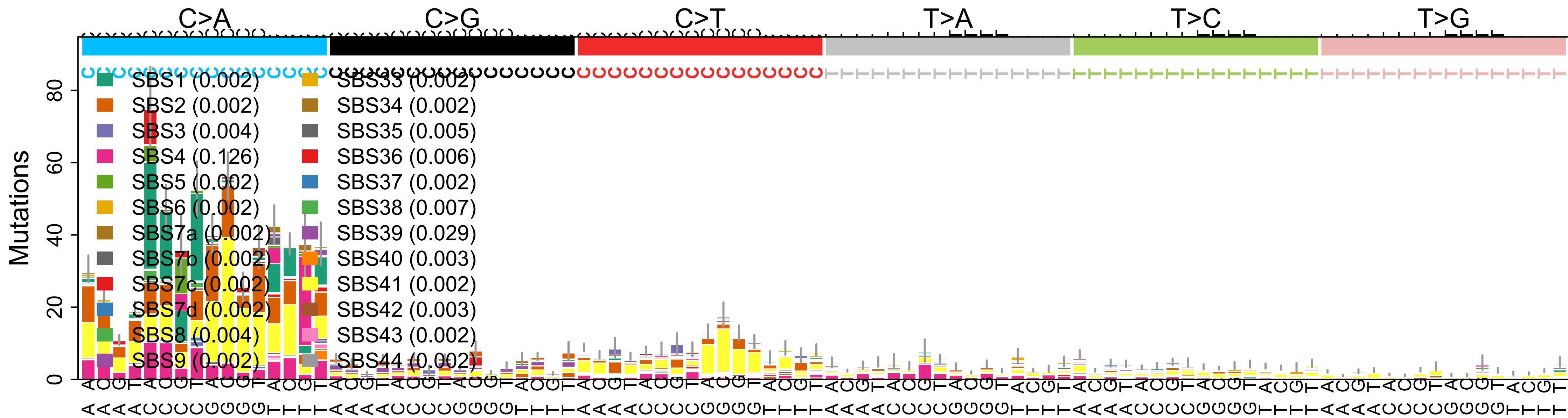
Reconstructed spectrum (cosine similarity = 0.923)



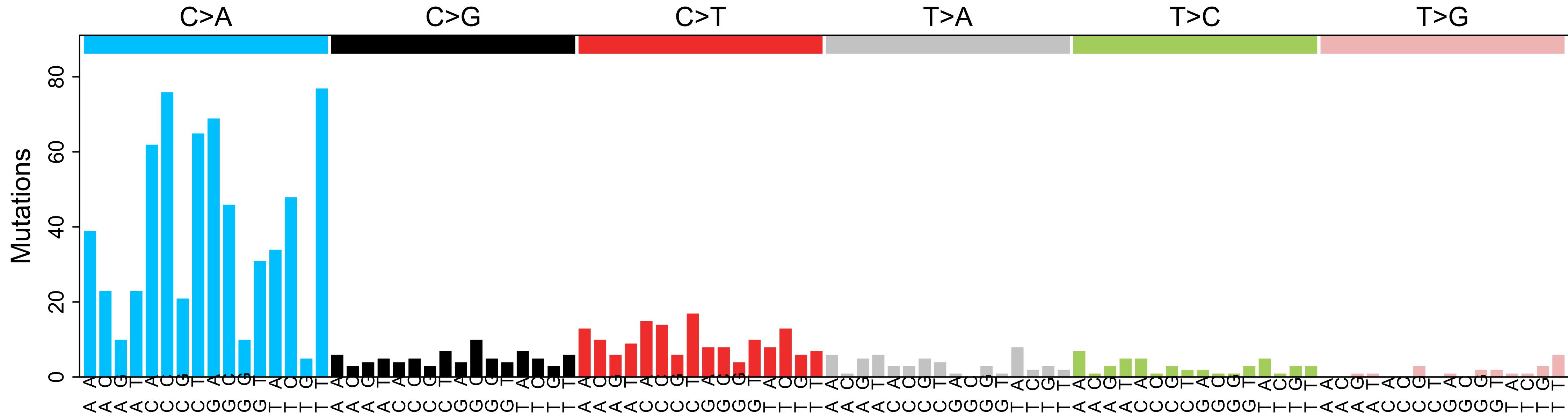
# benzoapyrene\_78ff8416d28d (1,000 mutations)



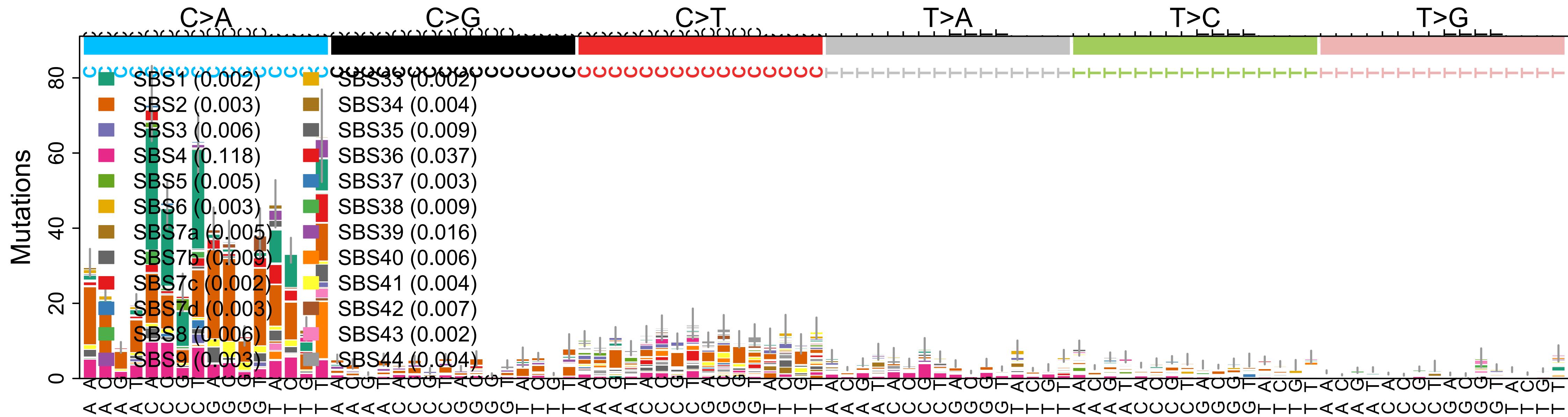
Reconstructed spectrum (cosine similarity = 0.924)



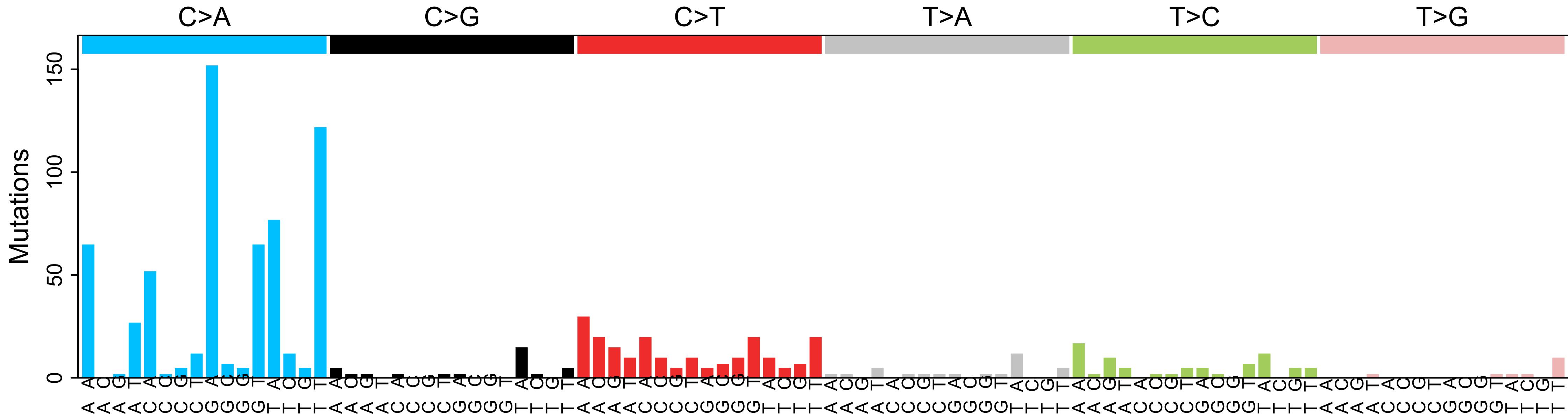
# **benzoapyrene\_b931a8be44c3 (994 mutations)**



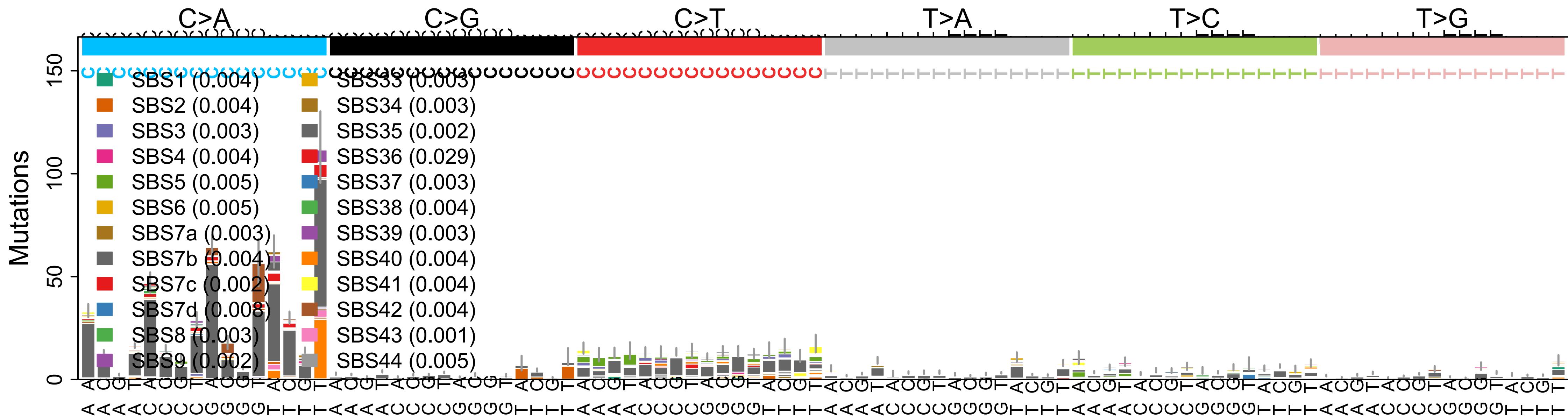
## Reconstructed spectrum (cosine similarity = 0.96)



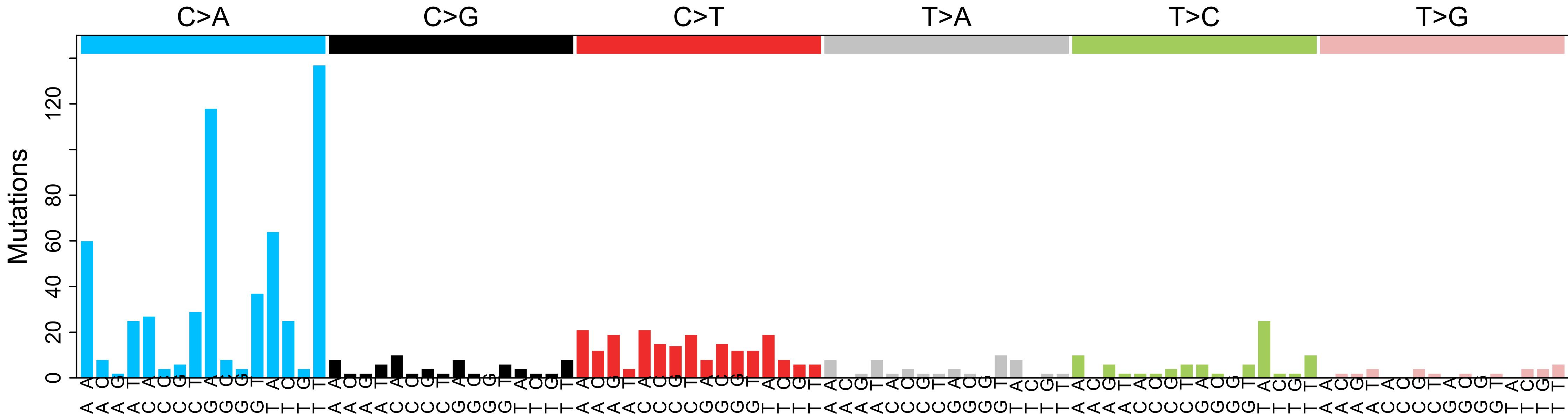
# bleomycin\_a07bf993a1cf (986 mutations)



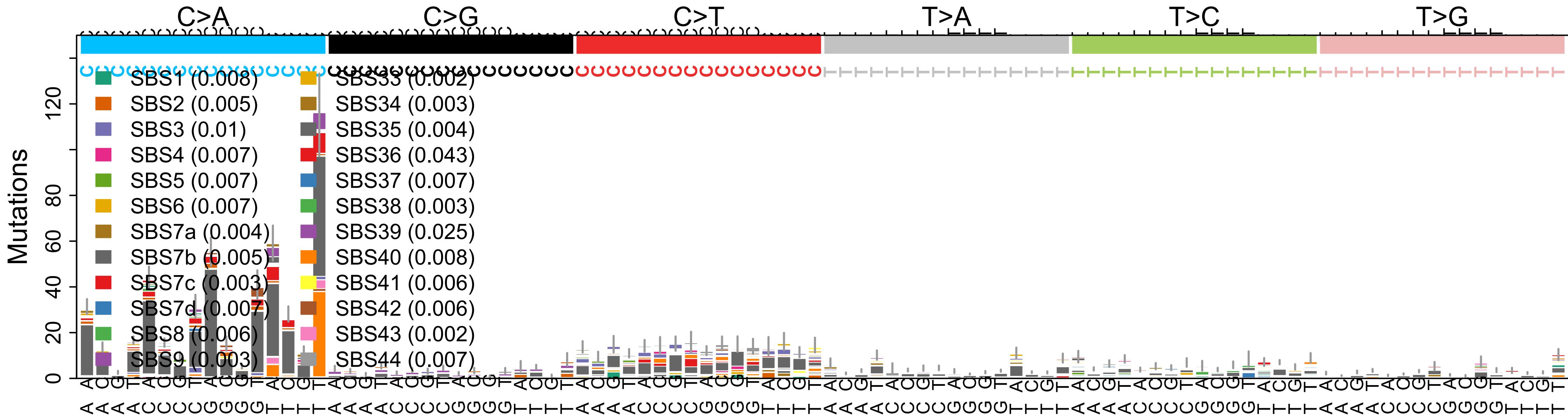
Reconstructed spectrum (cosine similarity = 0.914)



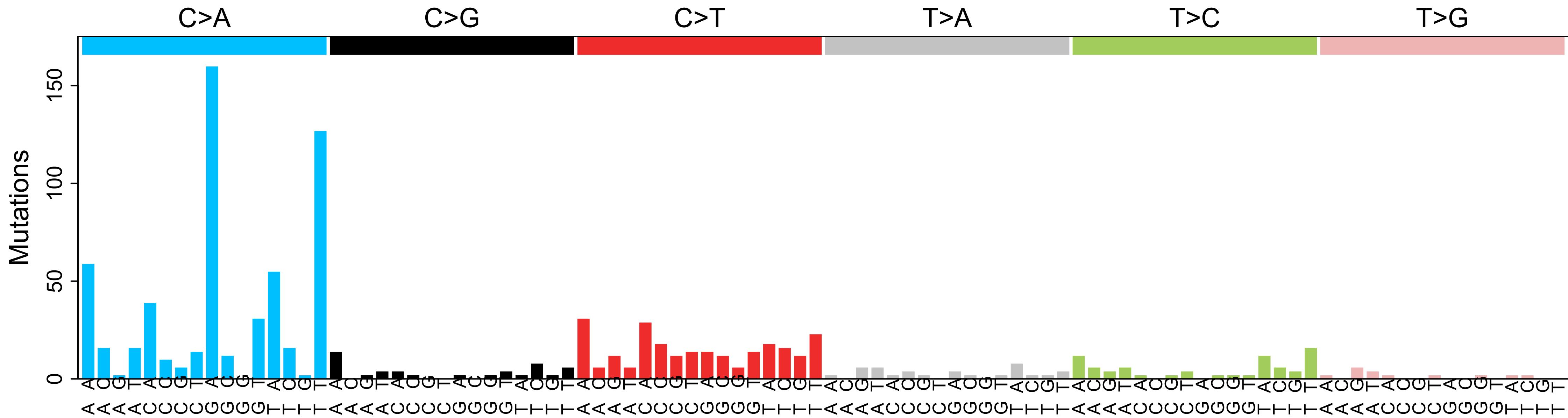
# cadmium\_chloride\_4e155105529e (1,010 mutations)



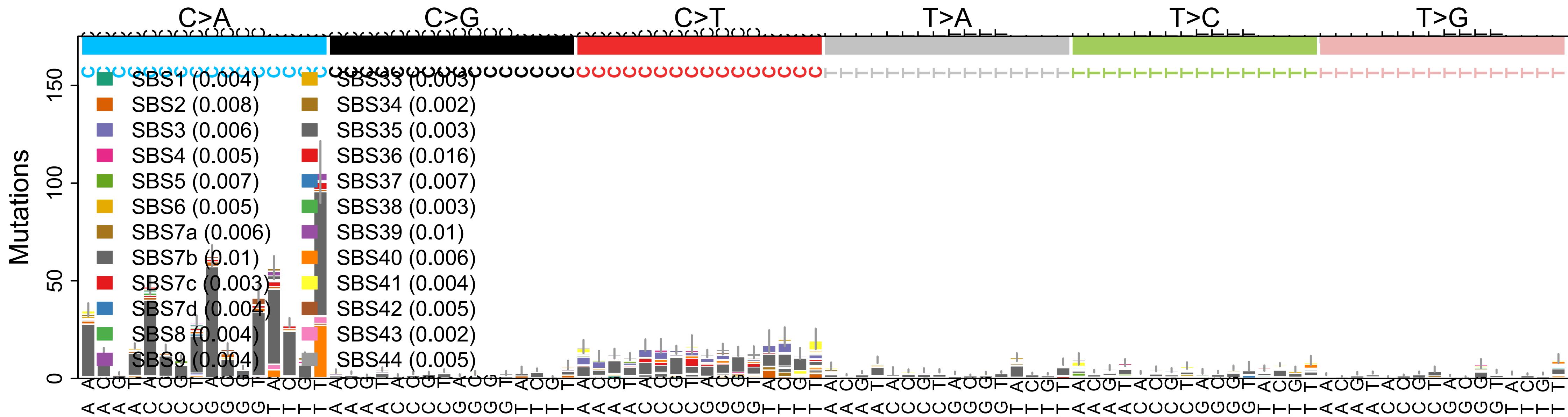
## Reconstructed spectrum (cosine similarity = 0.935)



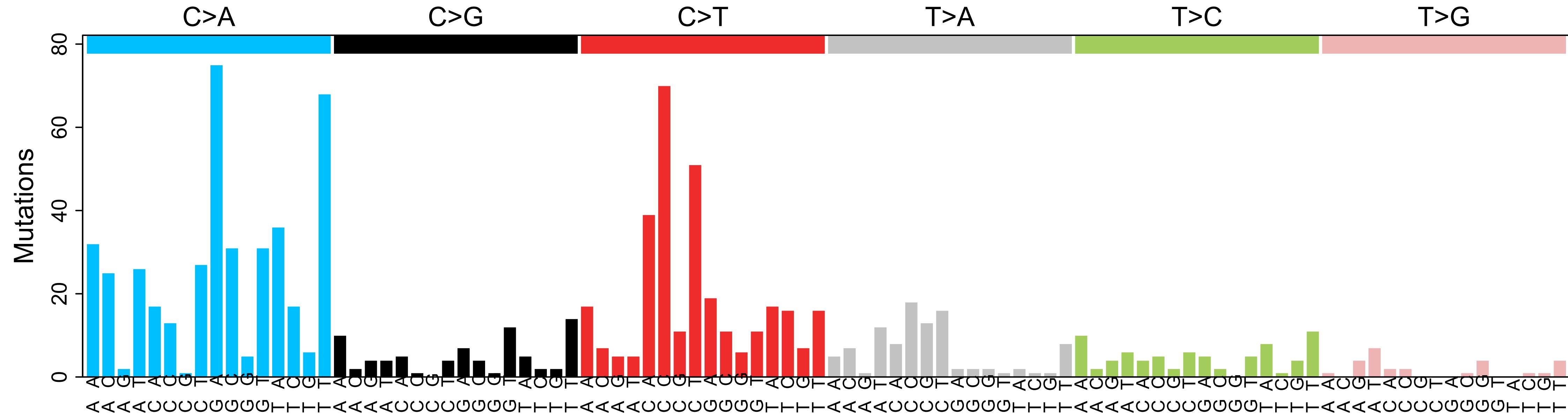
# camptothecin\_035f5ec44026 (1,008 mutations)



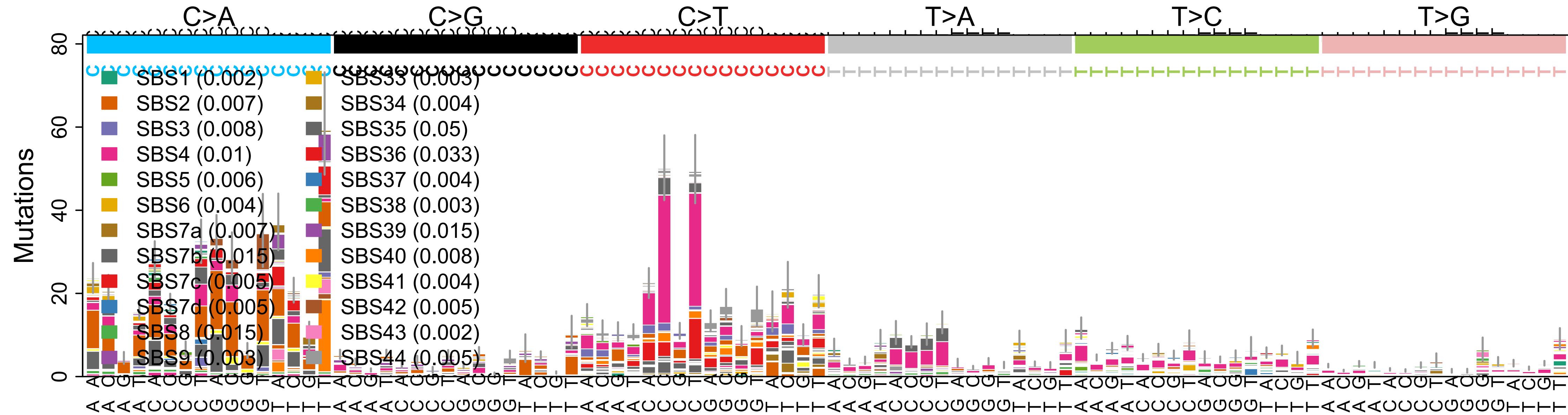
Reconstructed spectrum (cosine similarity = 0.901)



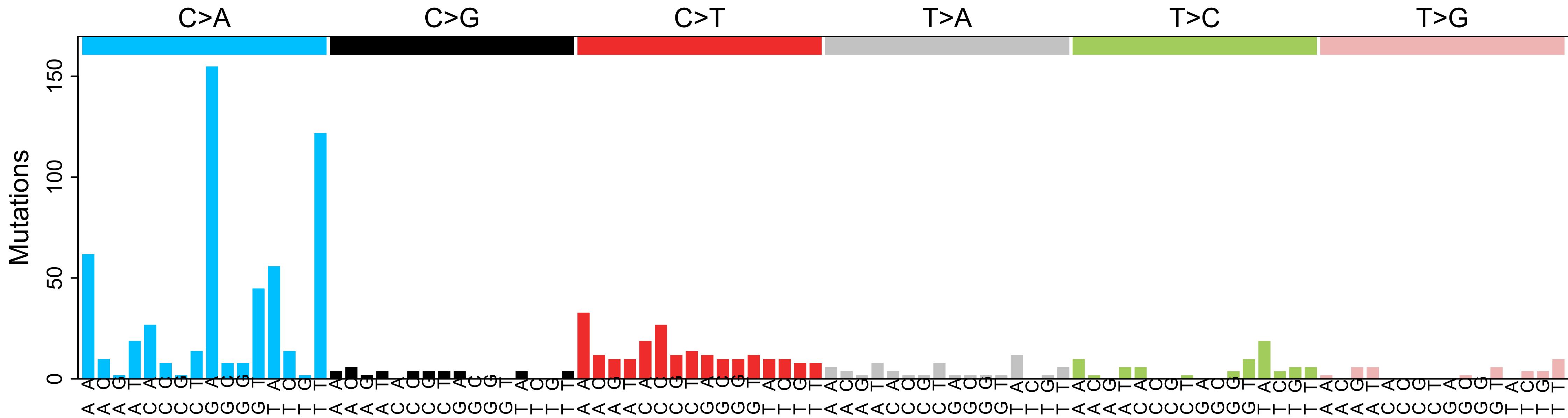
# **carboplatin\_87107e8f10fc (998 mutations)**



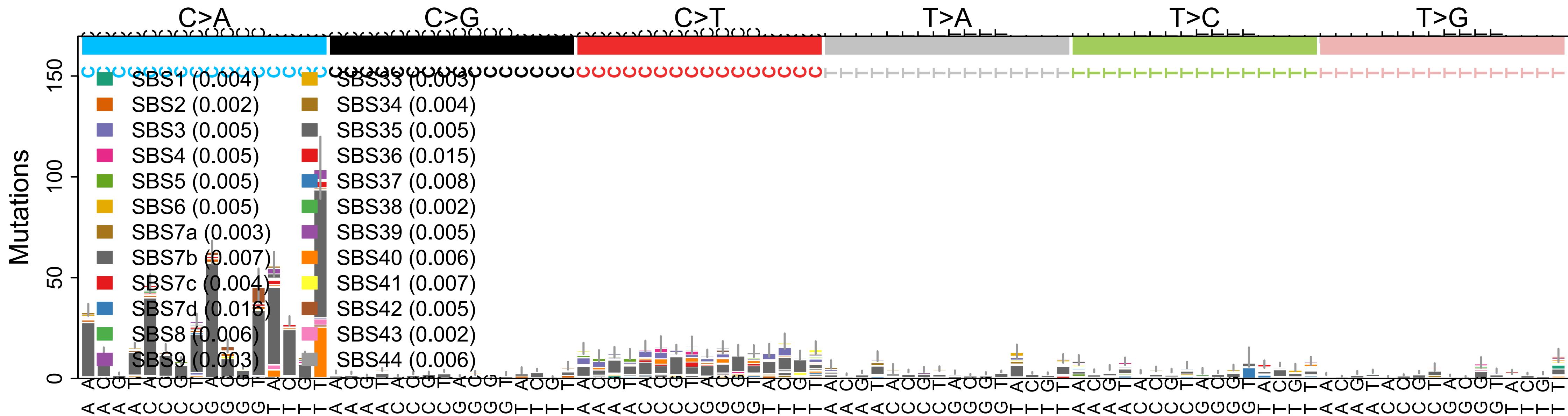
## Reconstructed spectrum (cosine similarity = 0.941)



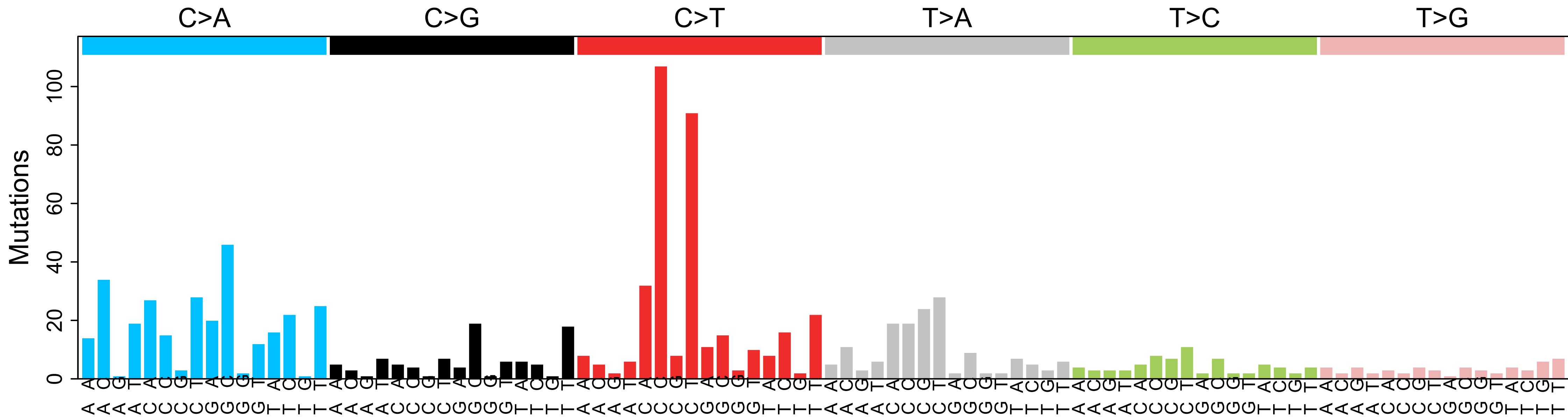
# catechol\_c6f4cfad7d77 (990 mutations)



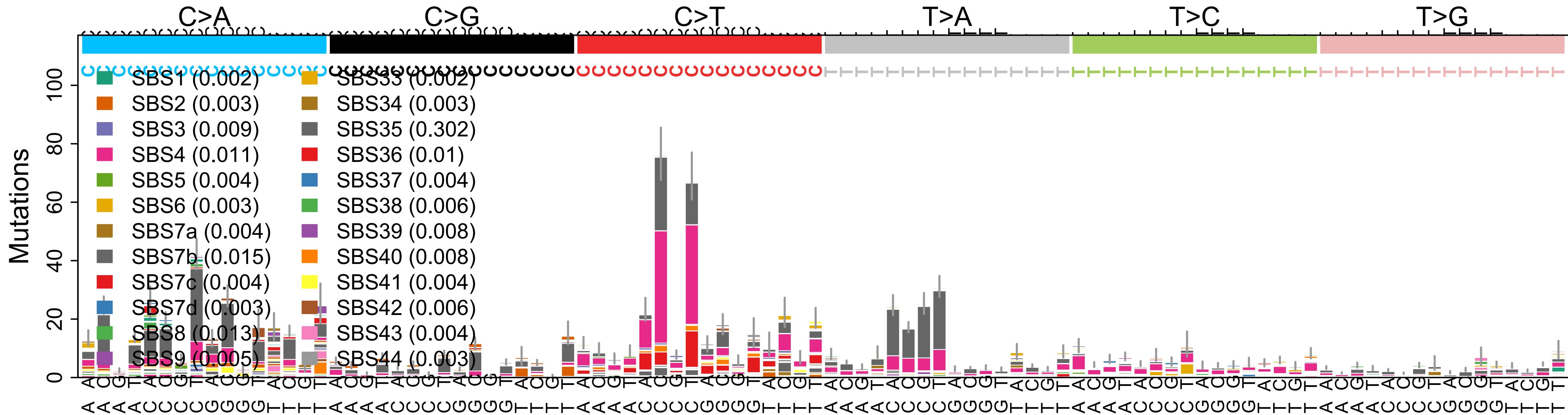
Reconstructed spectrum (cosine similarity = 0.897)



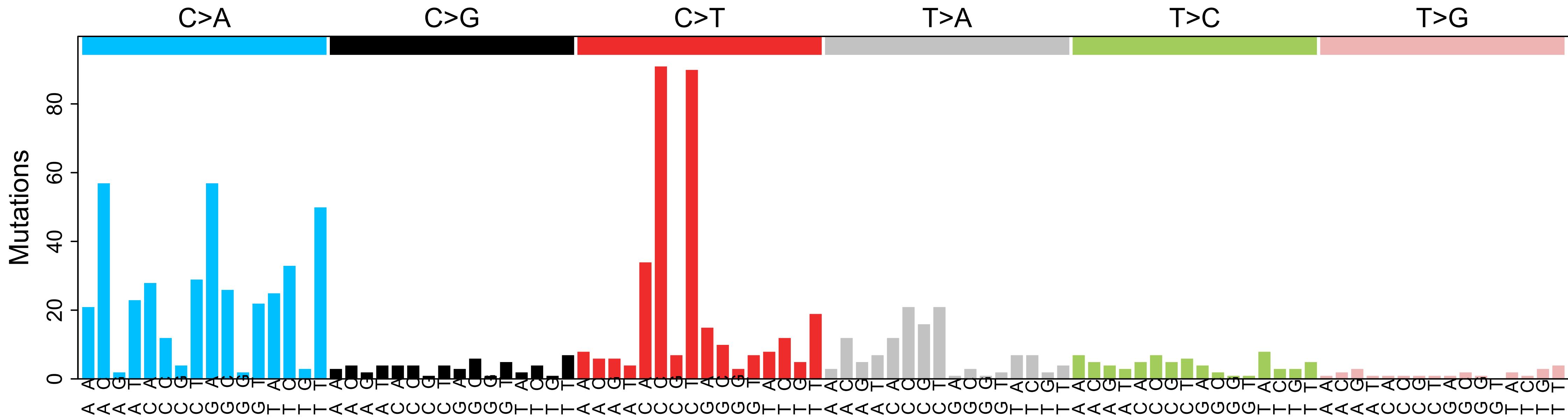
# cisplatin\_244441f785e1 (1,001 mutations)



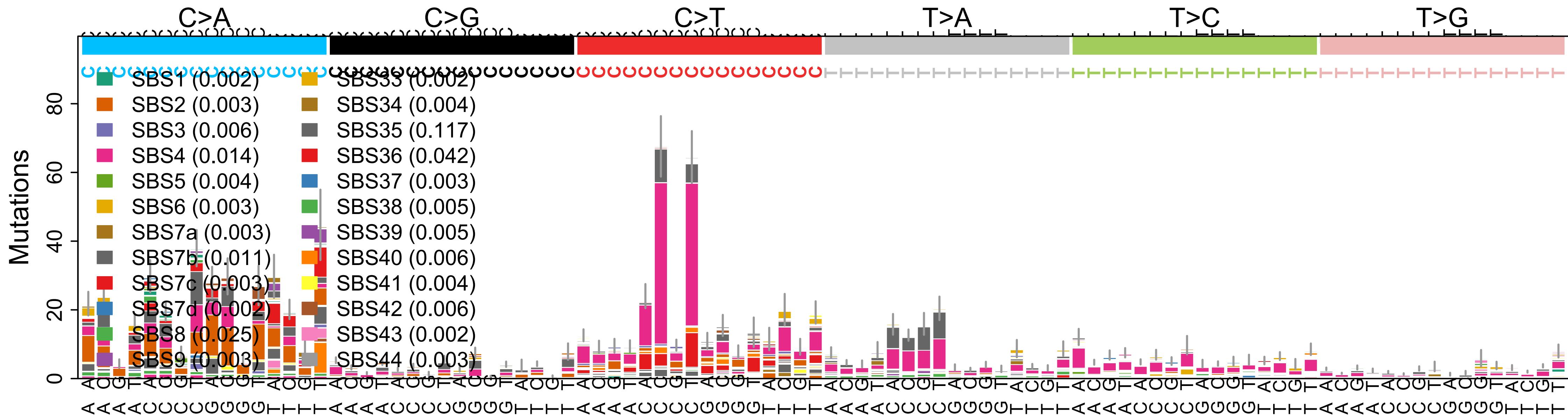
Reconstructed spectrum (cosine similarity = 0.964)



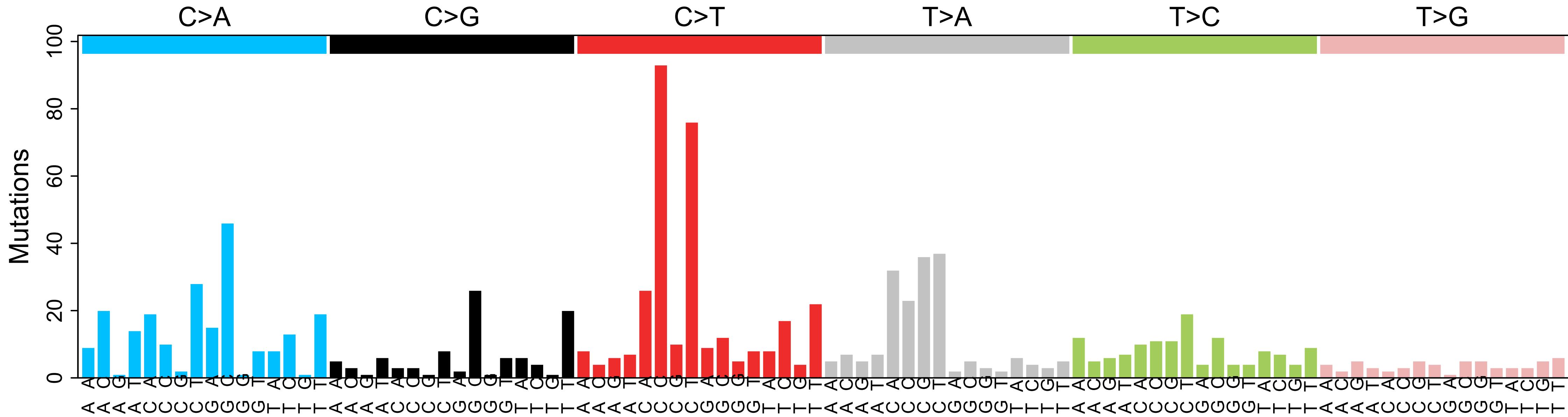
# cisplatin\_92bd8426ea0e (992 mutations)



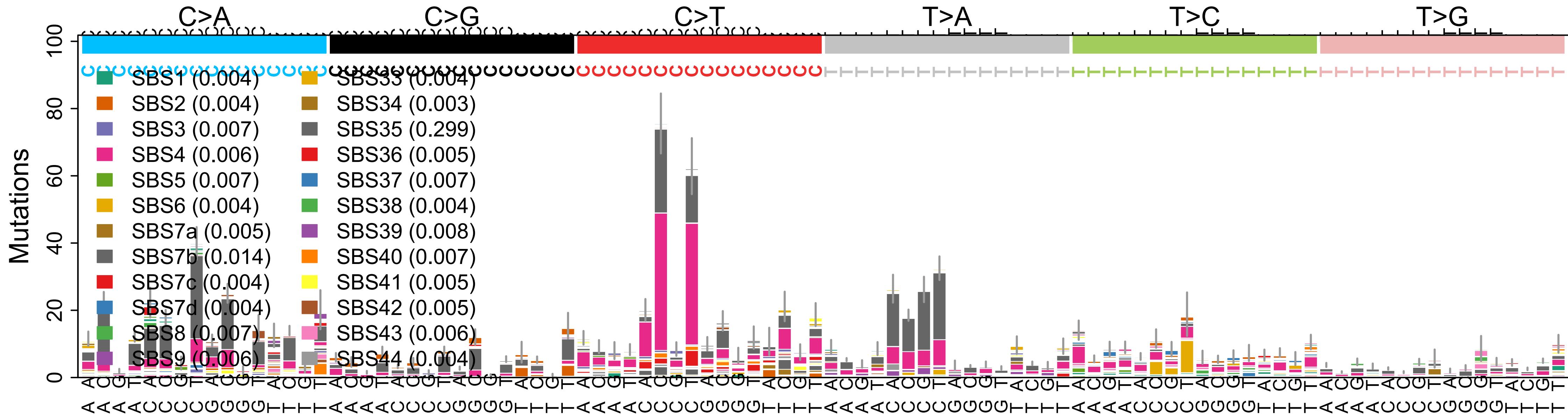
## Reconstructed spectrum (cosine similarity = 0.945)



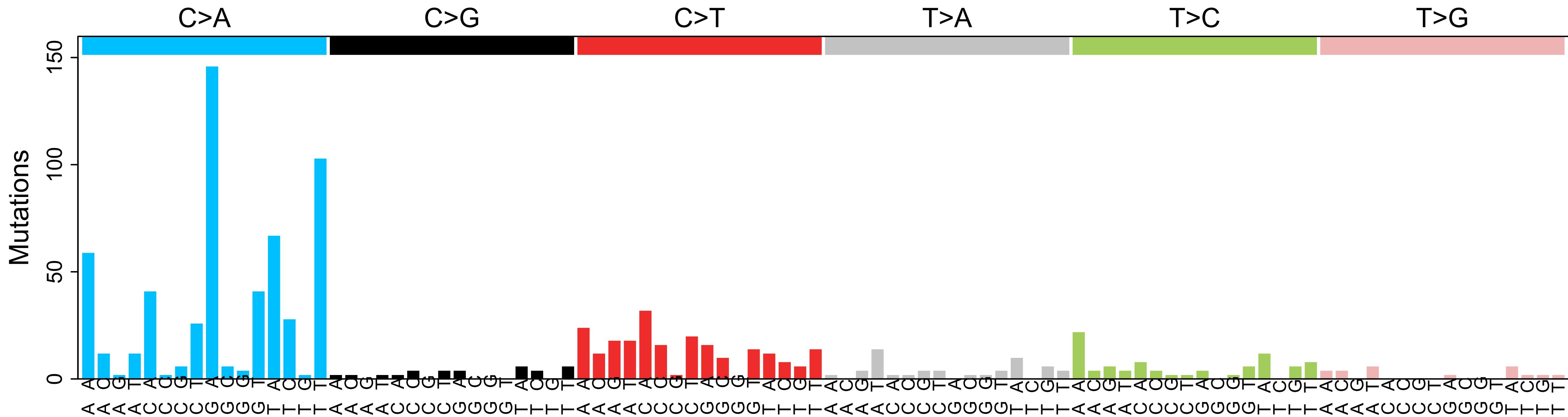
# cisplatin\_93f89a4f687c (999 mutations)



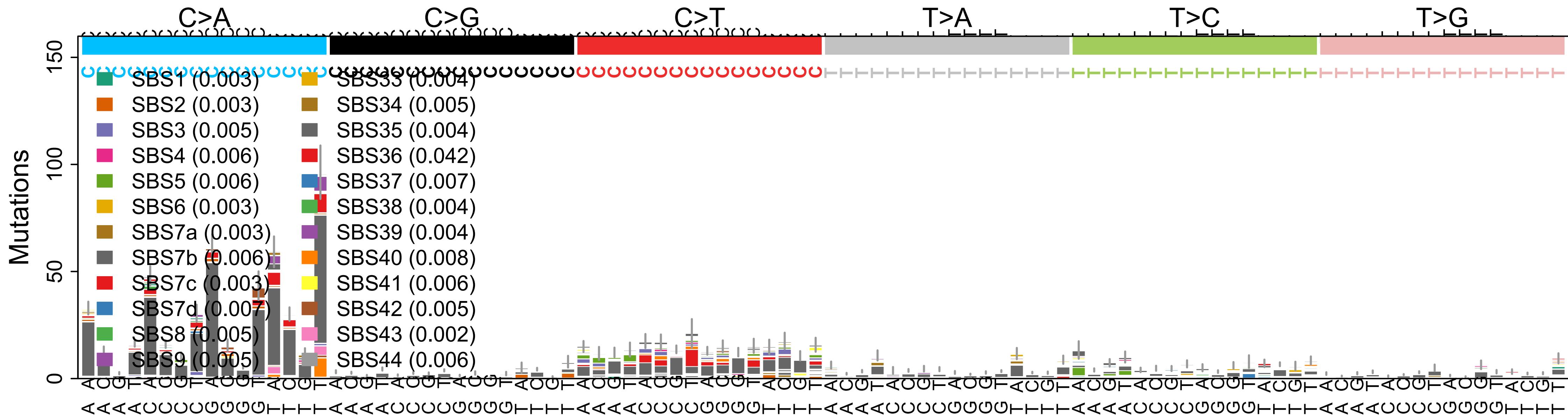
Reconstructed spectrum (cosine similarity = 0.968)



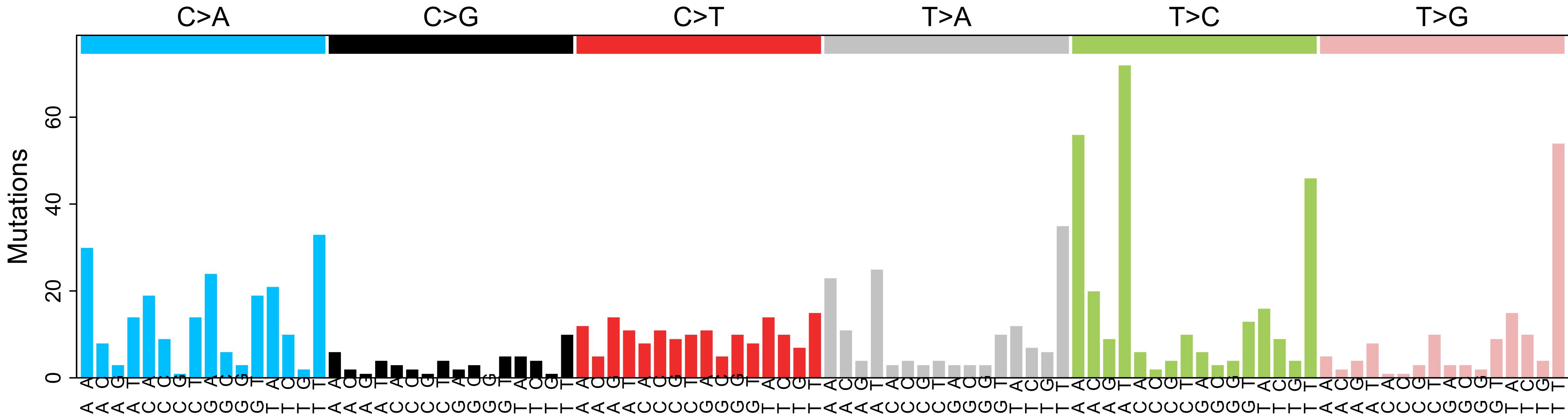
# cobalt\_chloride\_a9e31bc7a88c (993 mutations)



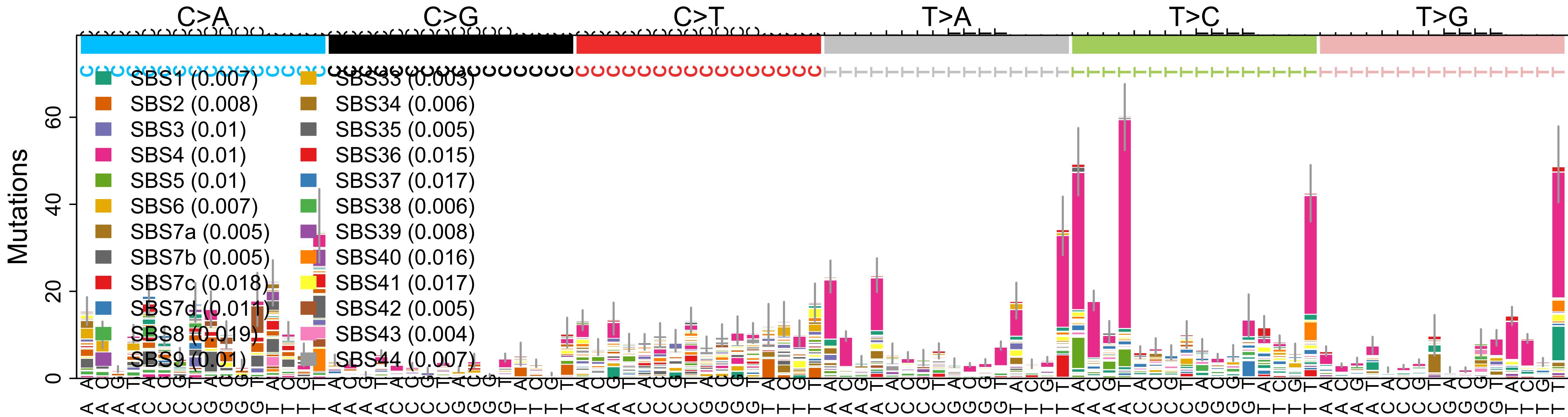
Reconstructed spectrum (cosine similarity = 0.909)



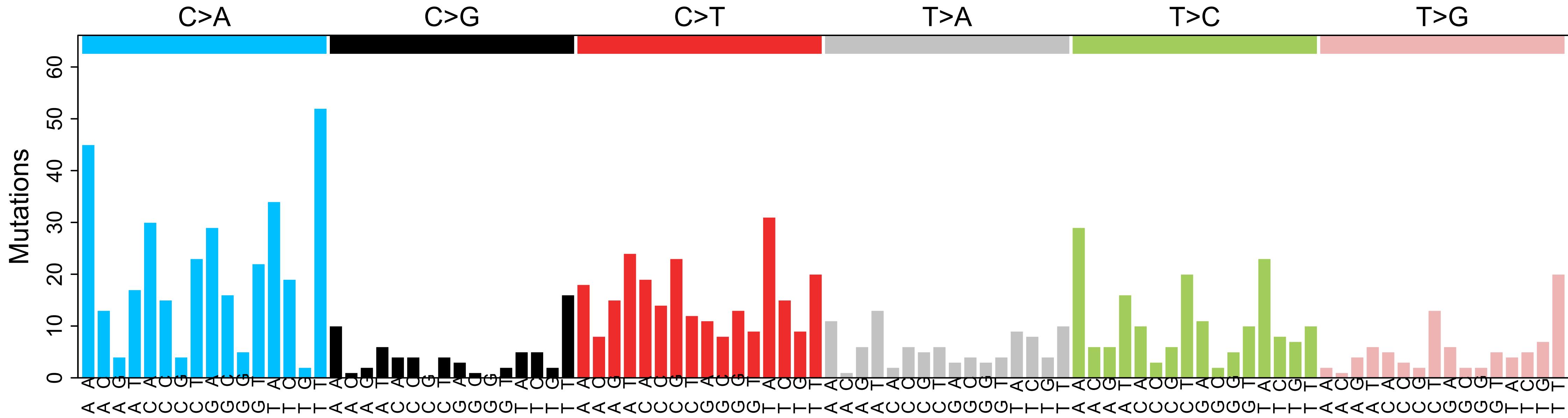
# colibactin\_64a437501c7e (999 mutations)



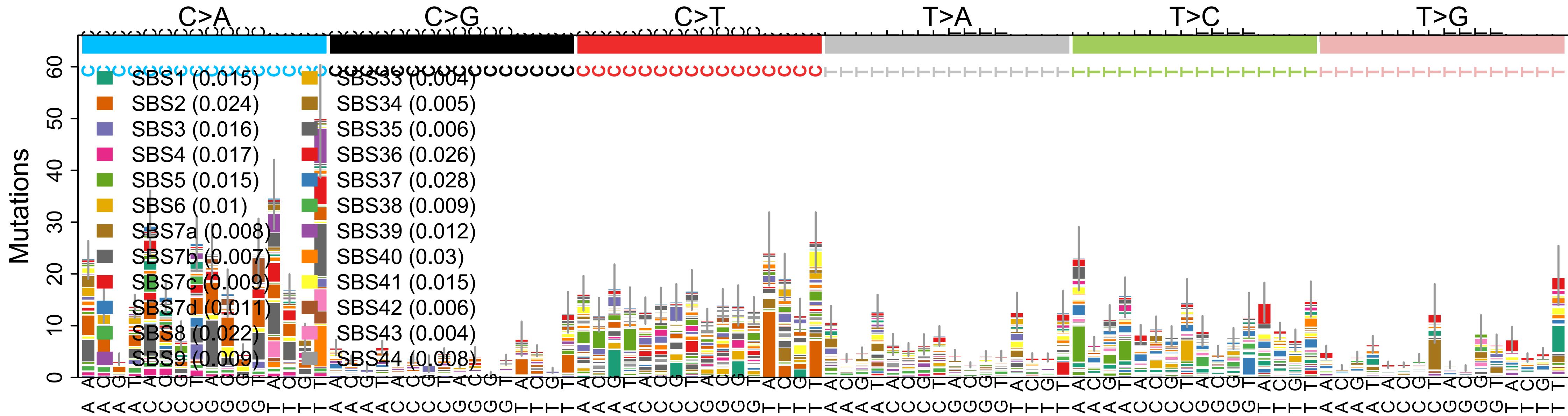
**Reconstructed spectrum (cosine similarity = 0.984)**



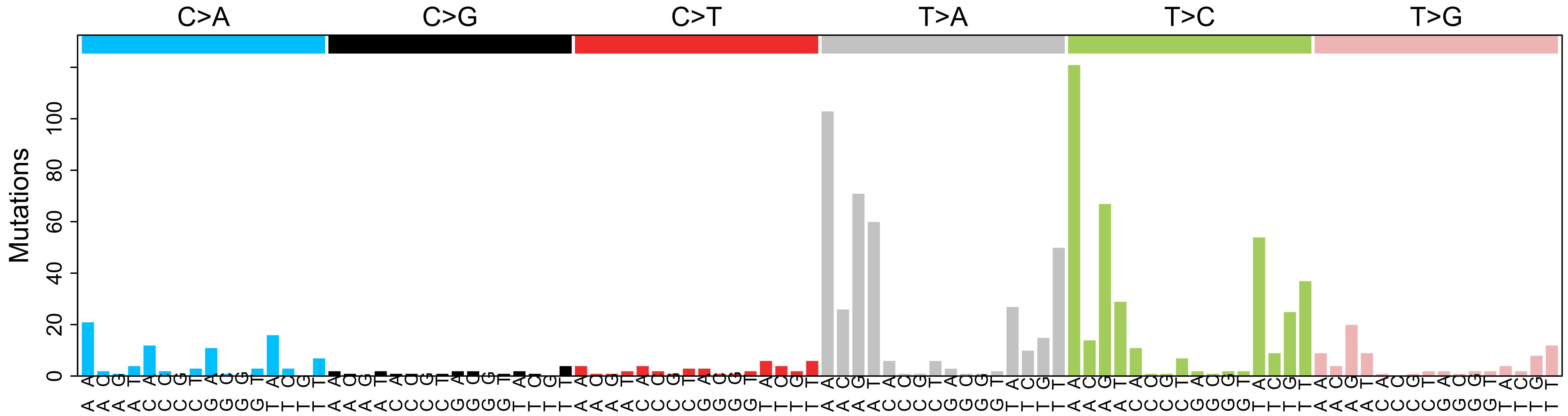
**colibactin\_knockout\_b1ed6d50ae6d (998 mutations)**



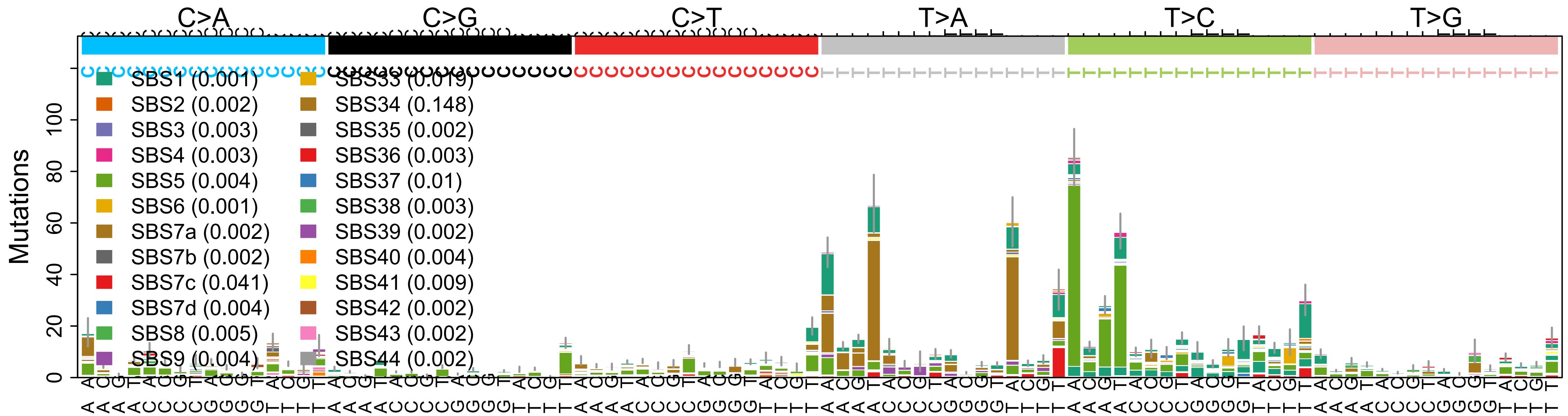
## Reconstructed spectrum (cosine similarity = 0.96)



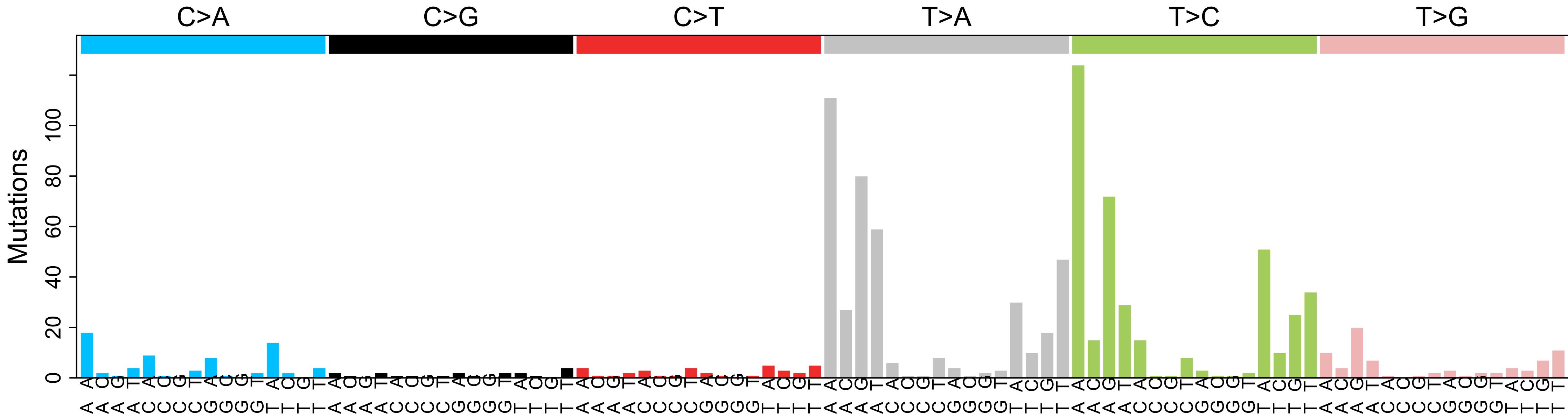
# **cx\_5461\_4b620d37b4ff (994 mutations)**



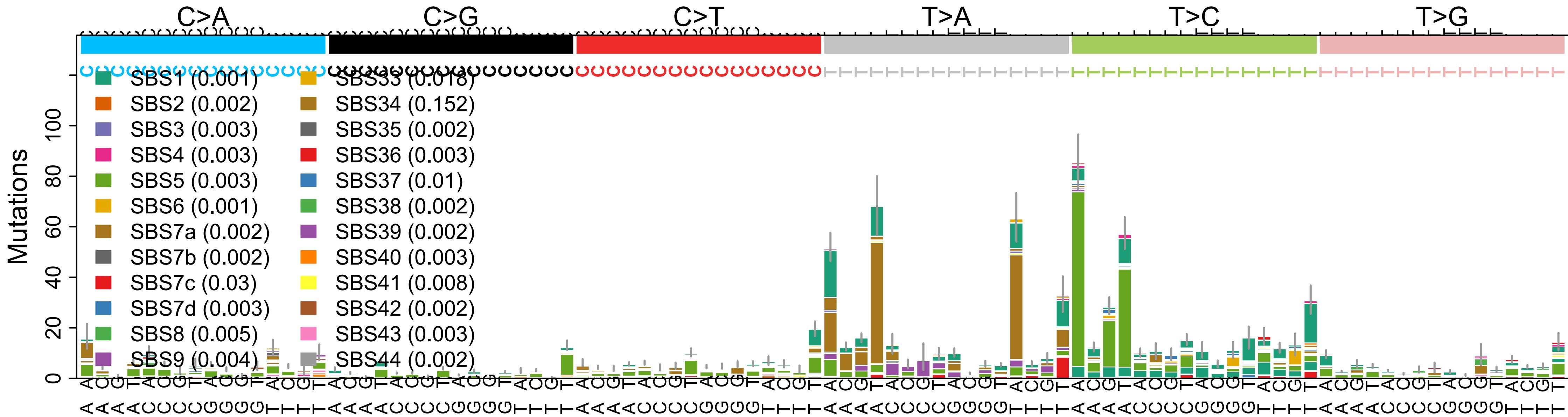
## Reconstructed spectrum (cosine similarity = 0.849)



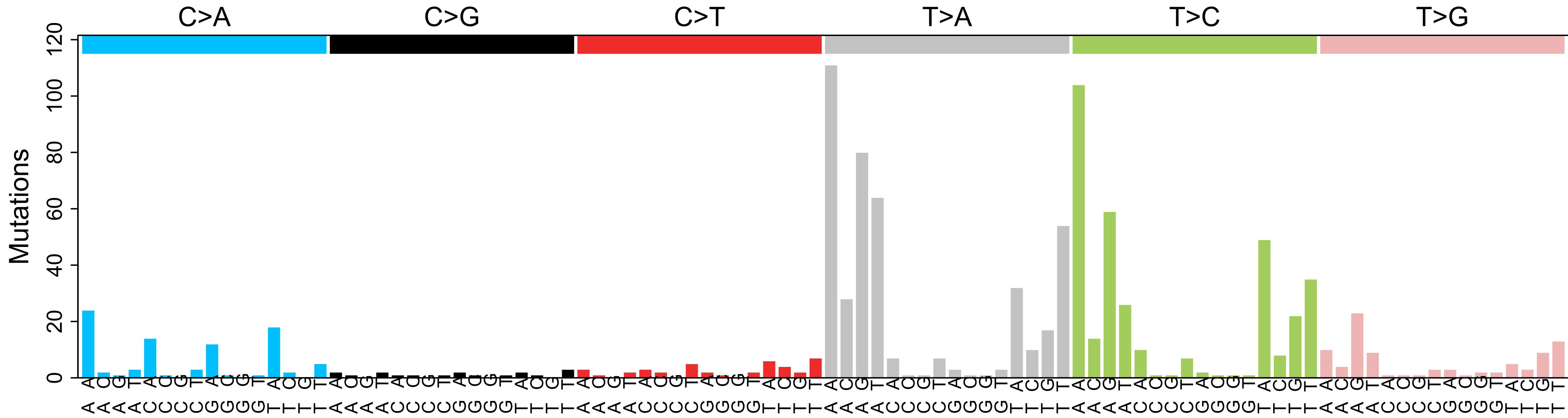
# cx\_5461\_5ea23ae78047 (1,003 mutations)



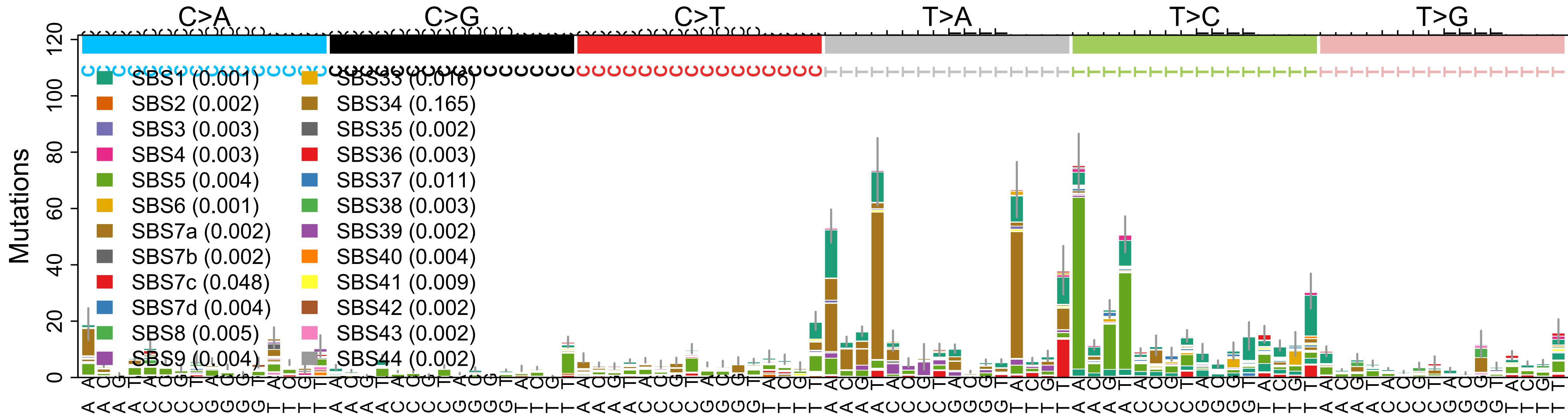
**Reconstructed spectrum (cosine similarity = 0.838)**



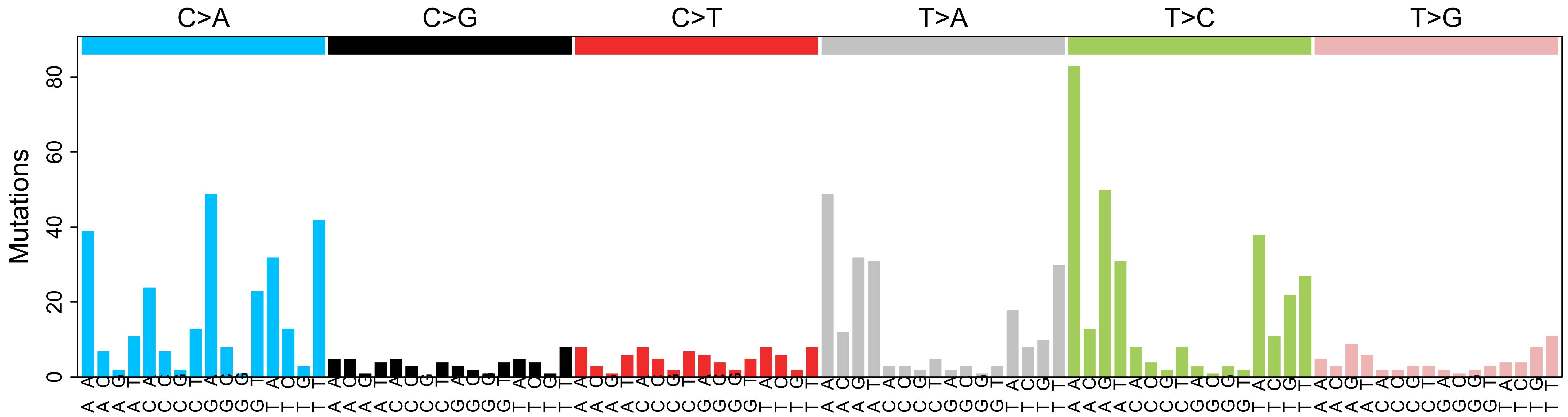
# cx\_5461\_74c9c7216236 (996 mutations)



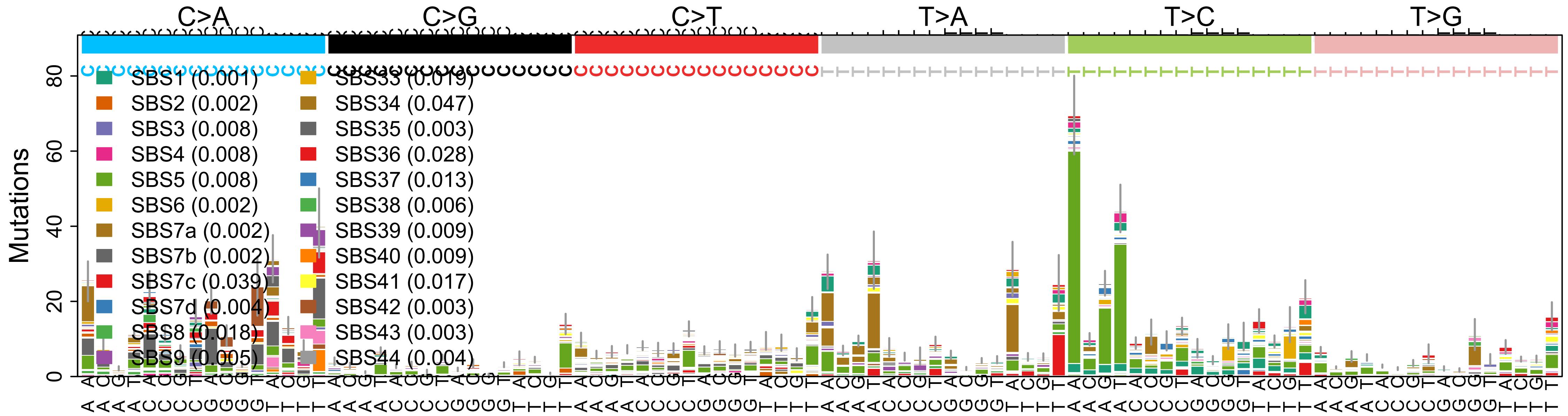
**Reconstructed spectrum (cosine similarity = 0.838)**



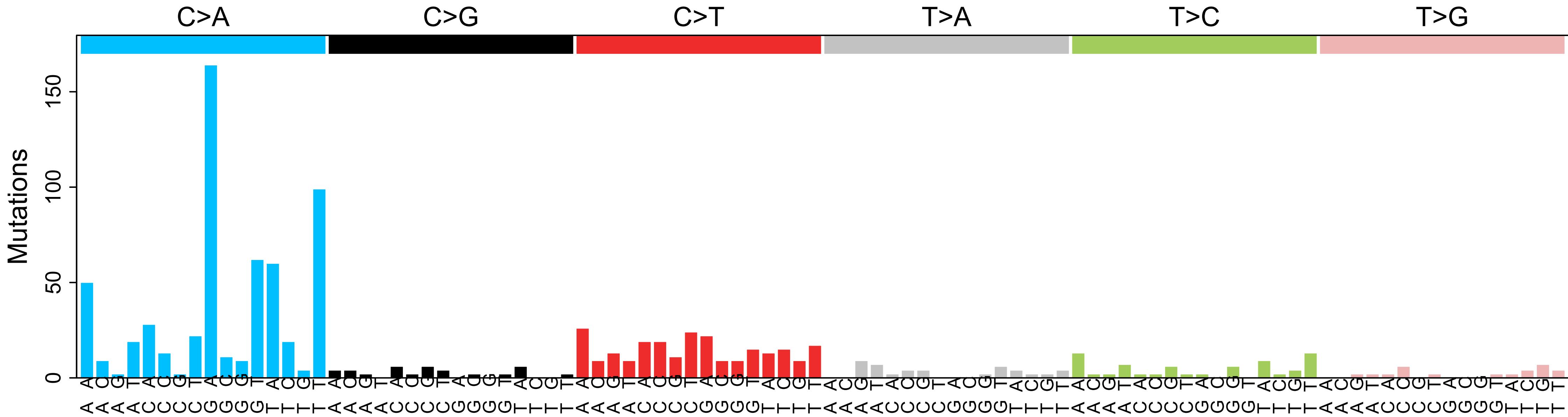
# cx\_5461\_a8d619bd33b3 (998 mutations)



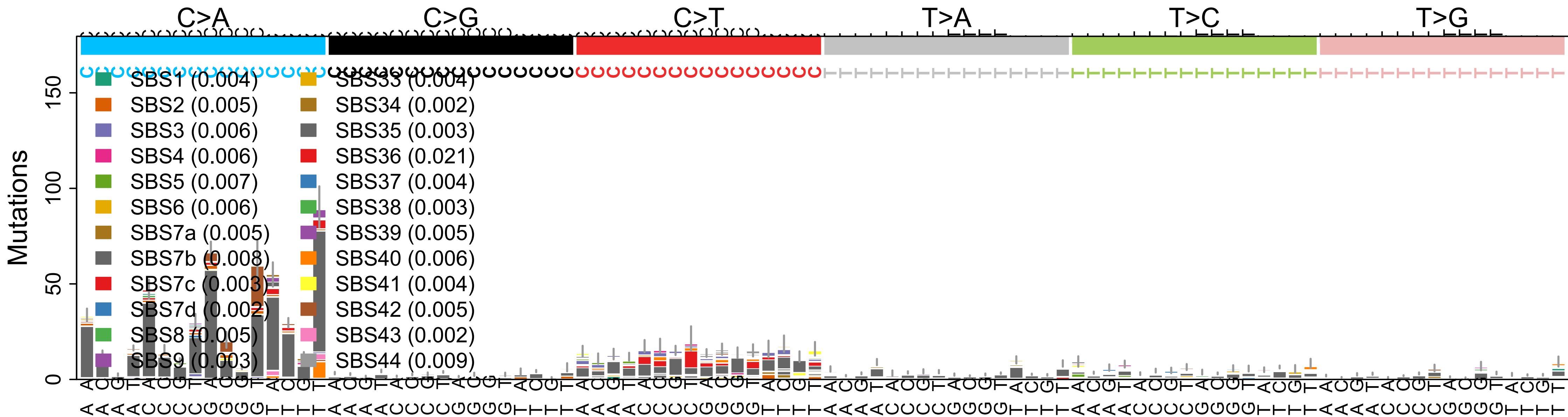
**Reconstructed spectrum (cosine similarity = 0.918)**



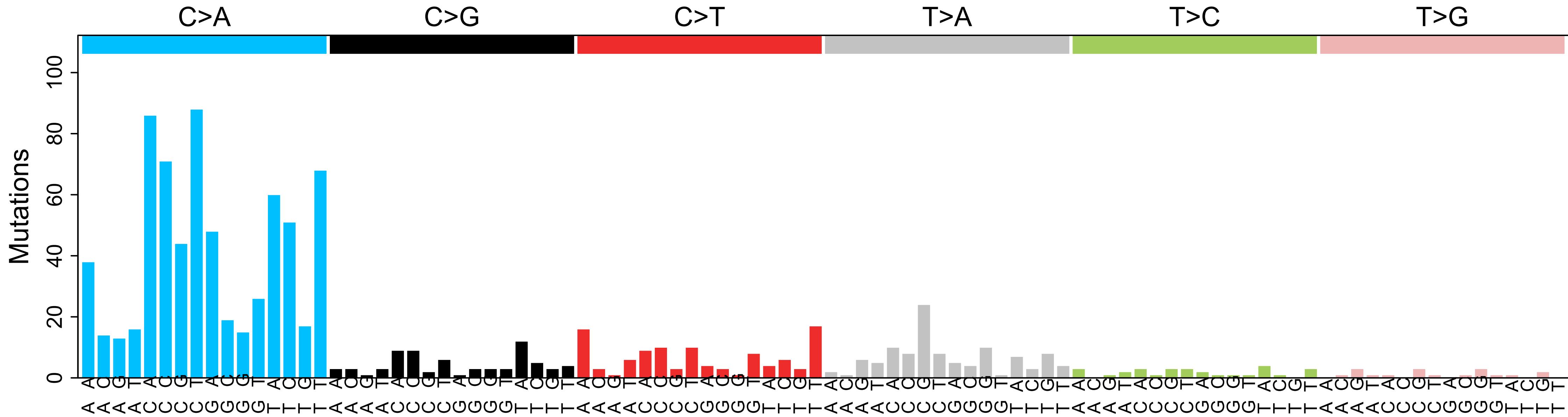
# cyclophosphamide\_557117b73fe2 (1,003 mutations)



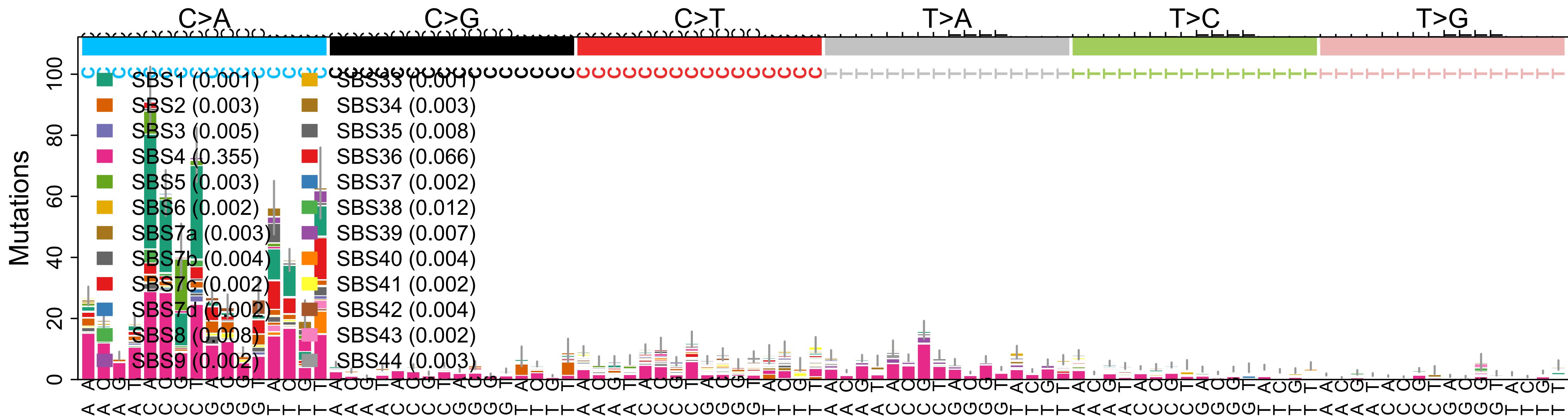
Reconstructed spectrum (cosine similarity = 0.899)



# dibenzo\_hanthracene\_86a56a54eba1 (1,001 mutations)



Reconstructed spectrum (cosine similarity = 0.98)



# dibenzo\_hanthracene\_diol\_epoxide\_d1c39f8181d9 (1,003 mutations)

C>A

C>G

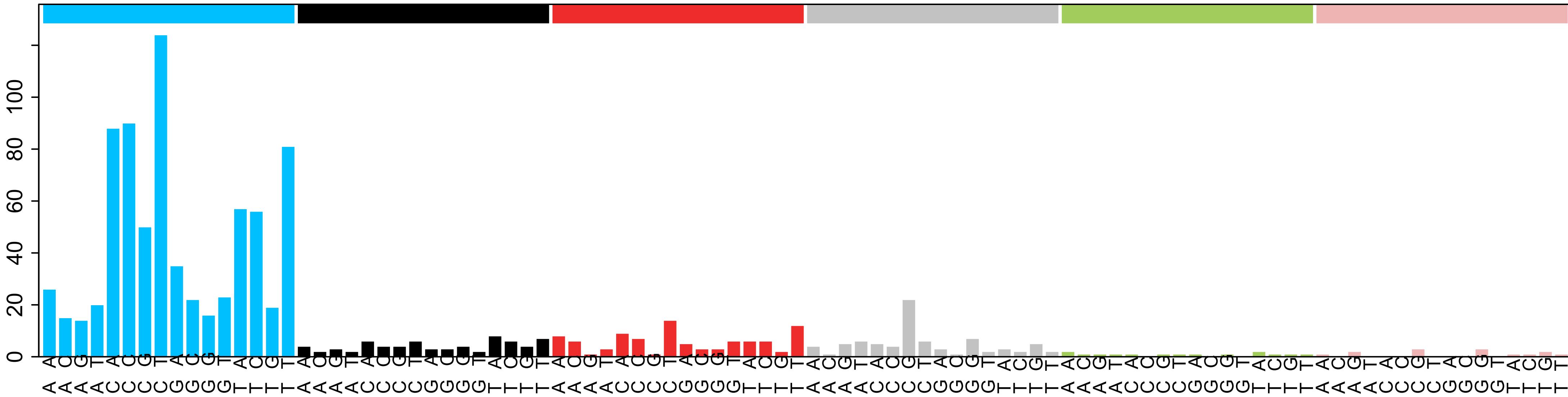
C>T

T>A

T>C

T>G

Mutations



Reconstructed spectrum (cosine similarity = 0.974)

C>A

C>G

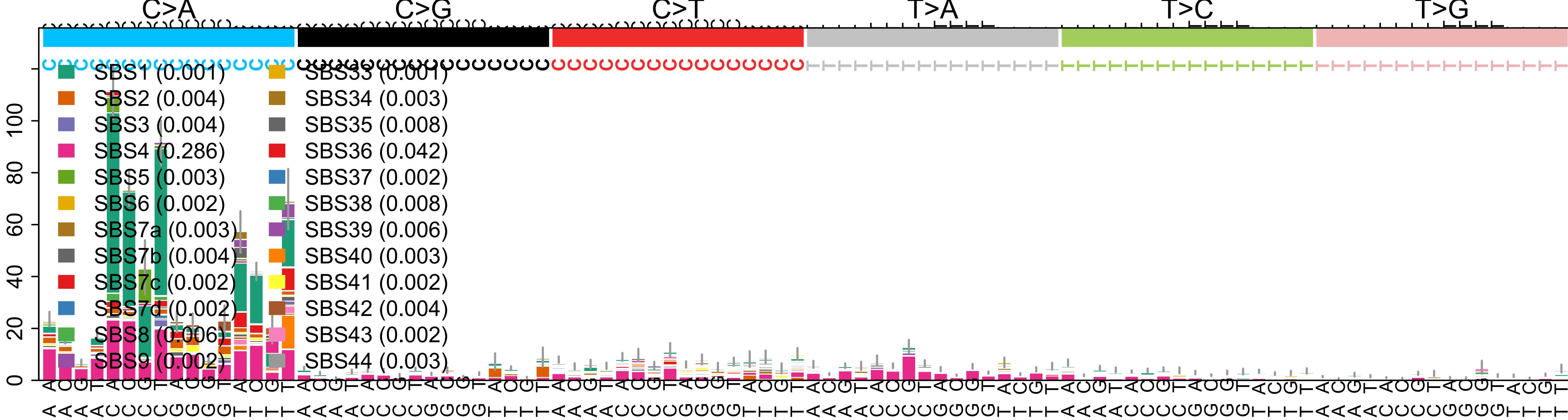
C>T

T>A

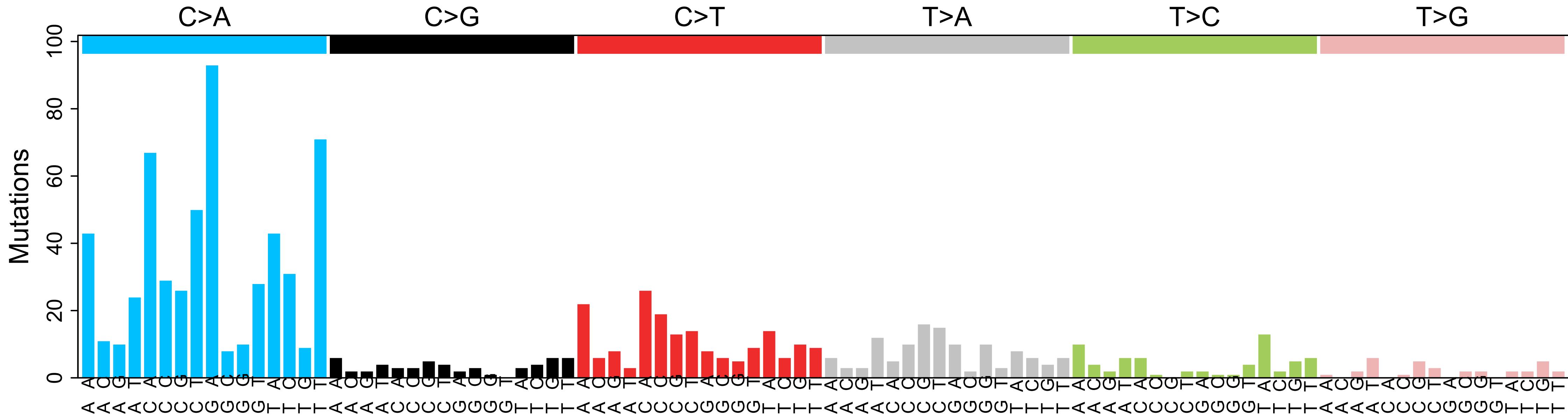
T>C

T>G

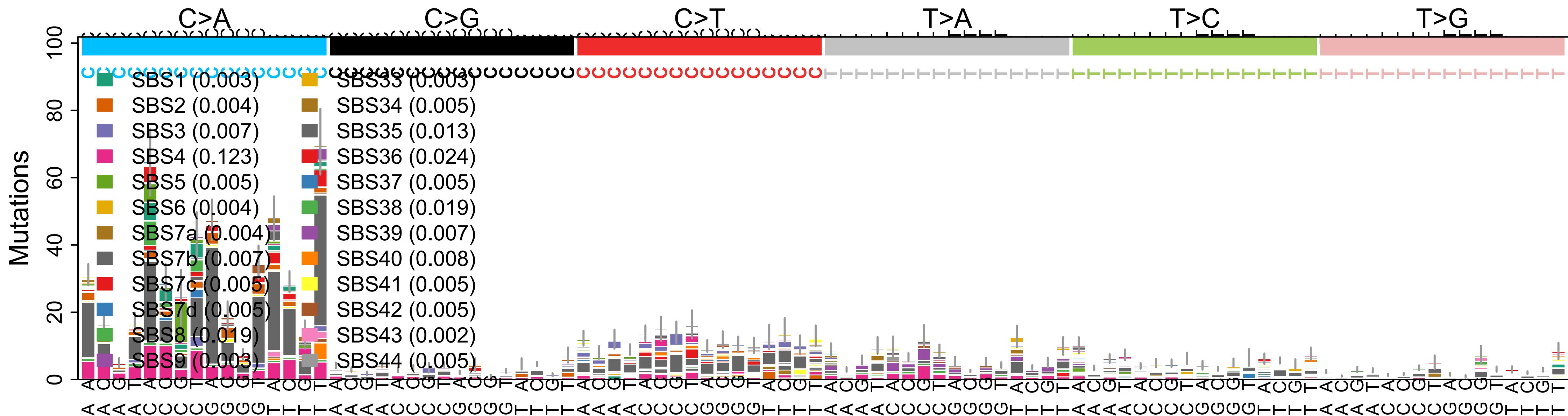
Mutations



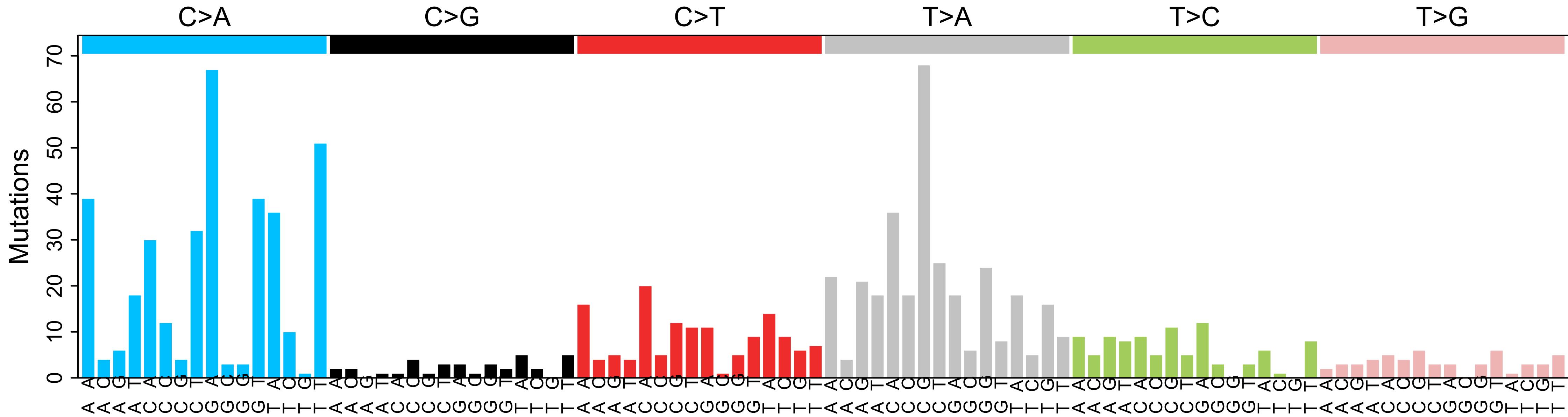
# dibenzo\_jacridine\_ddba8930ac82 (1,002 mutations)



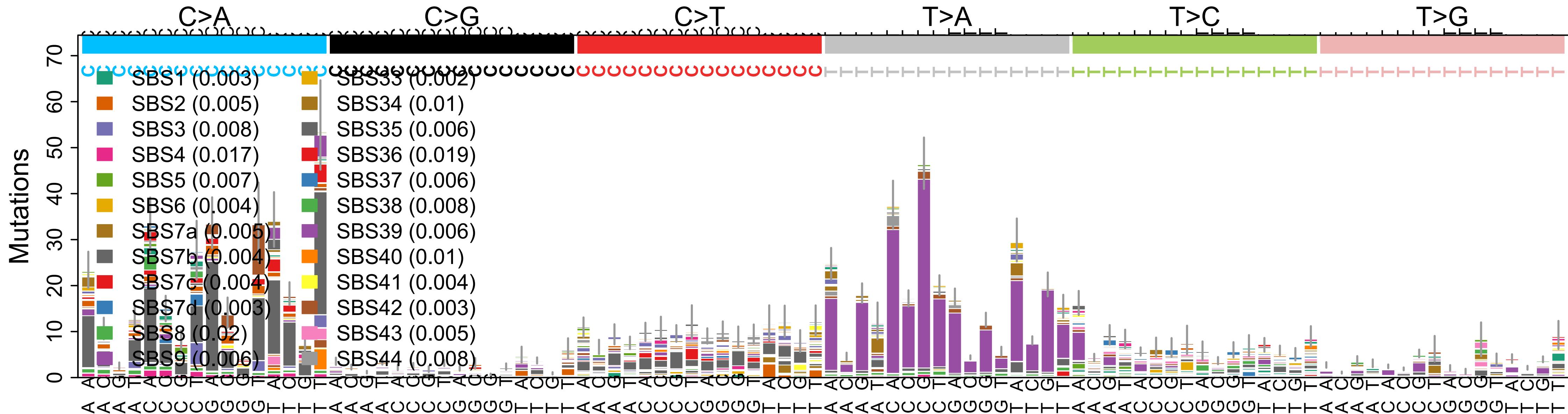
## Reconstructed spectrum (cosine similarity = 0.948)



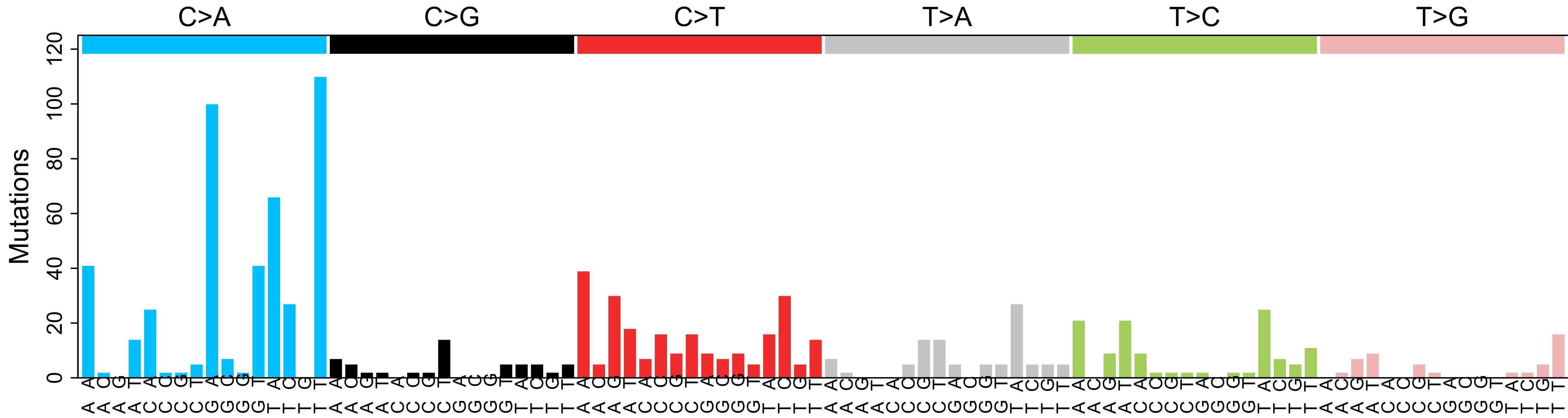
# dibenzoa\_lpyrene\_8d818fe5a7ef (993 mutations)



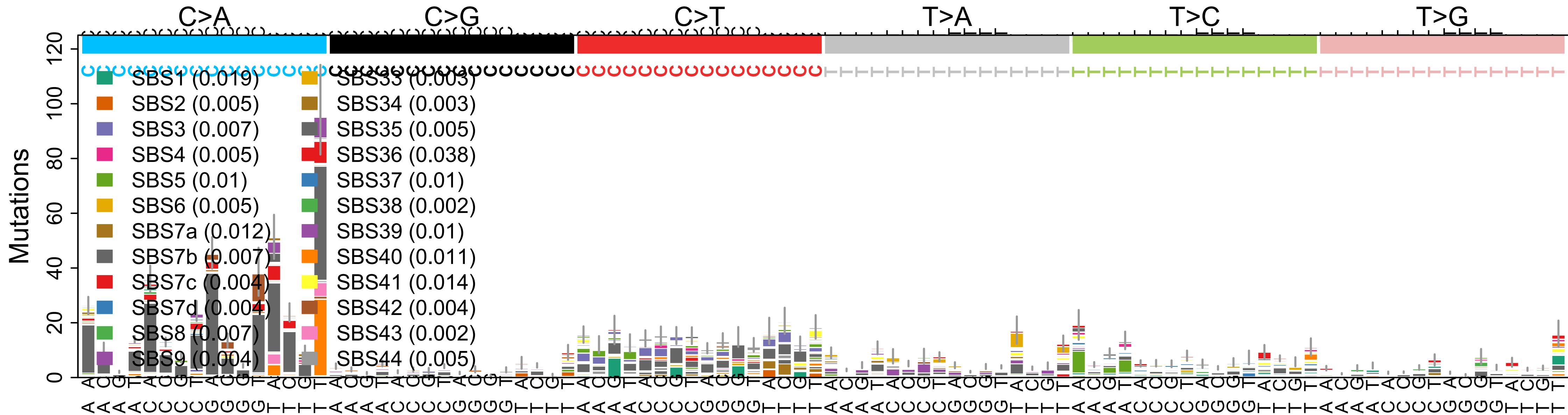
Reconstructed spectrum (cosine similarity = 0.937)



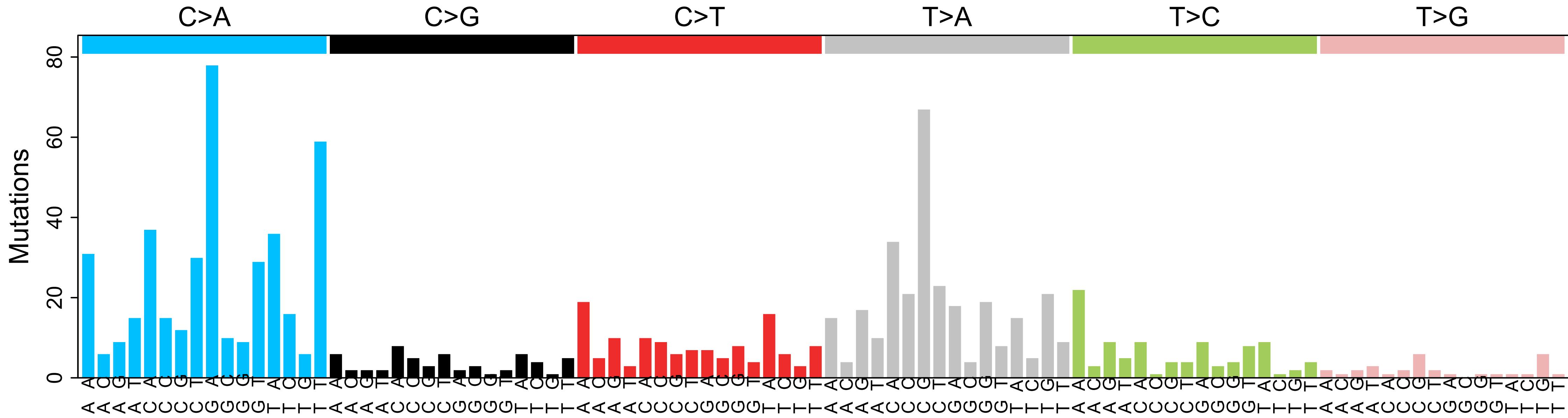
# dibenzoa\_Ipyrene\_a8658ca308ee (1,004 mutations)



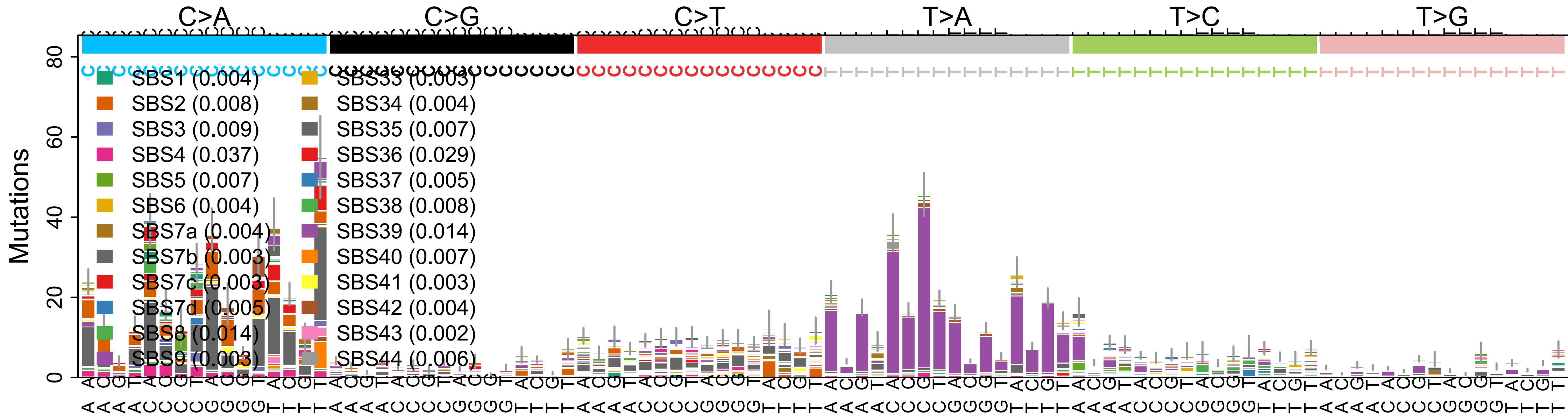
## Reconstructed spectrum (cosine similarity = 0.92)



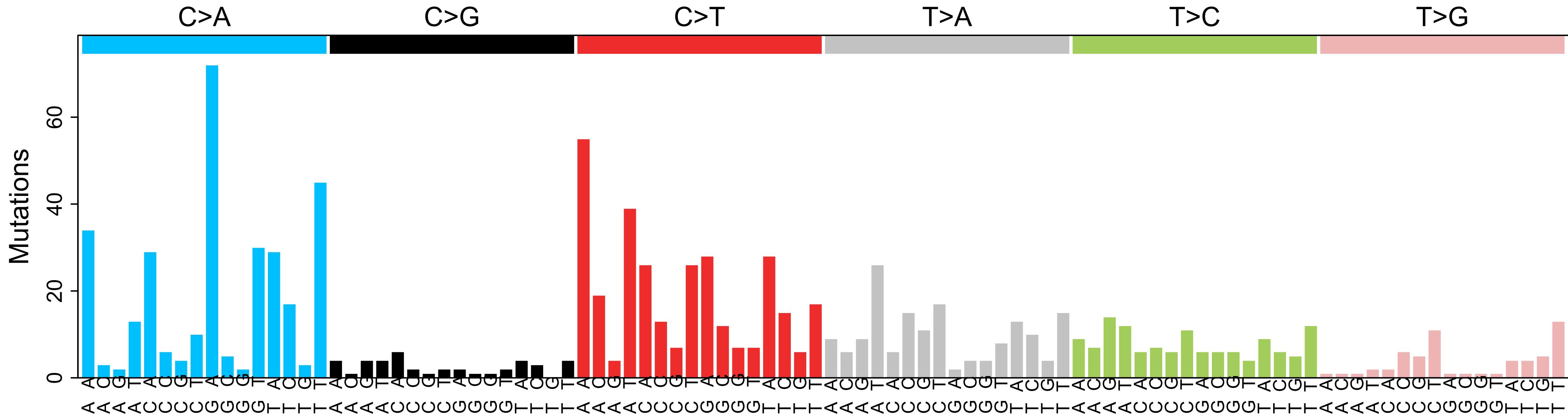
# dibenzoa\_ipyrene\_diol\_epoxide\_918d83810794 (1,000 mutations)



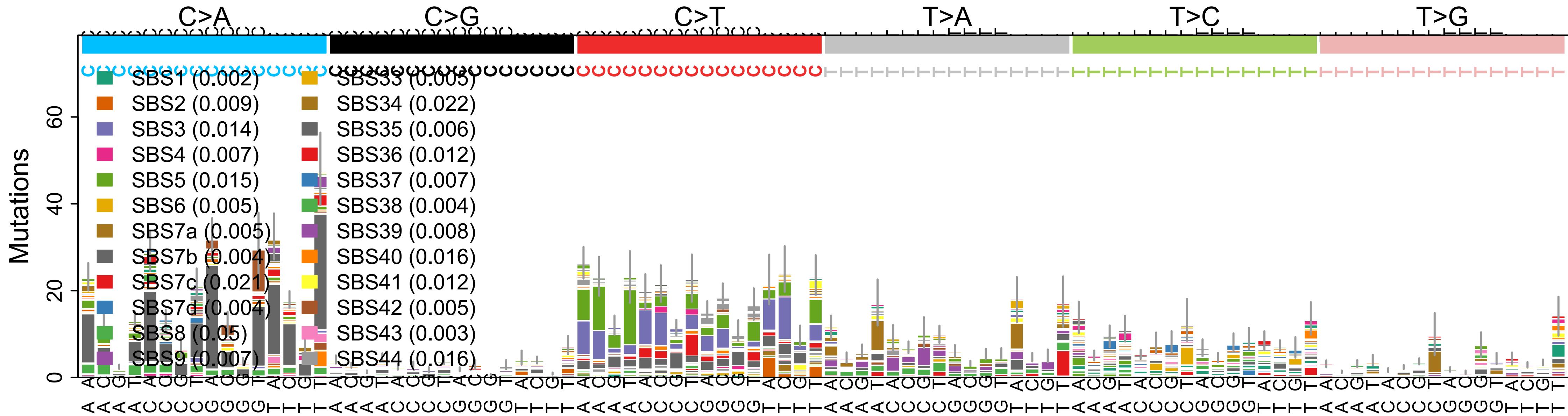
Reconstructed spectrum (cosine similarity = 0.941)



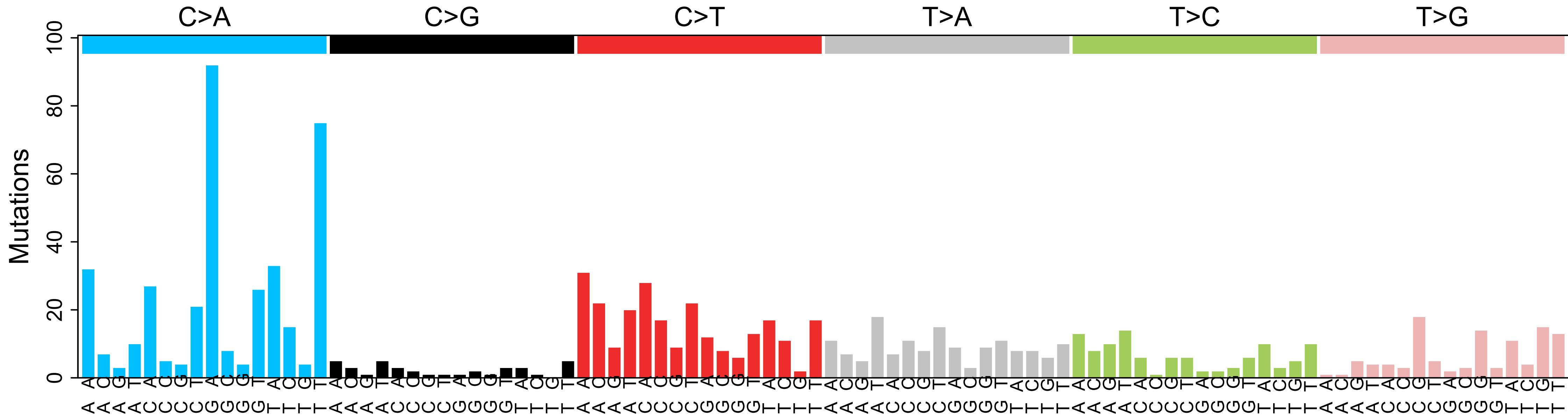
# diethyl\_sulfate\_66c09d32862b (998 mutations)



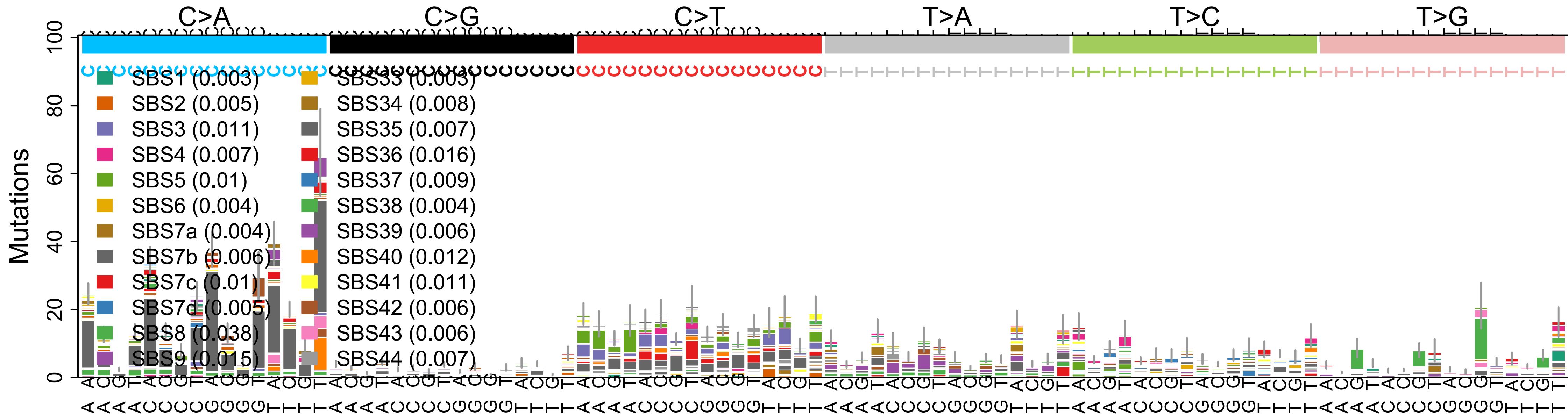
## Reconstructed spectrum (cosine similarity = 0.906)



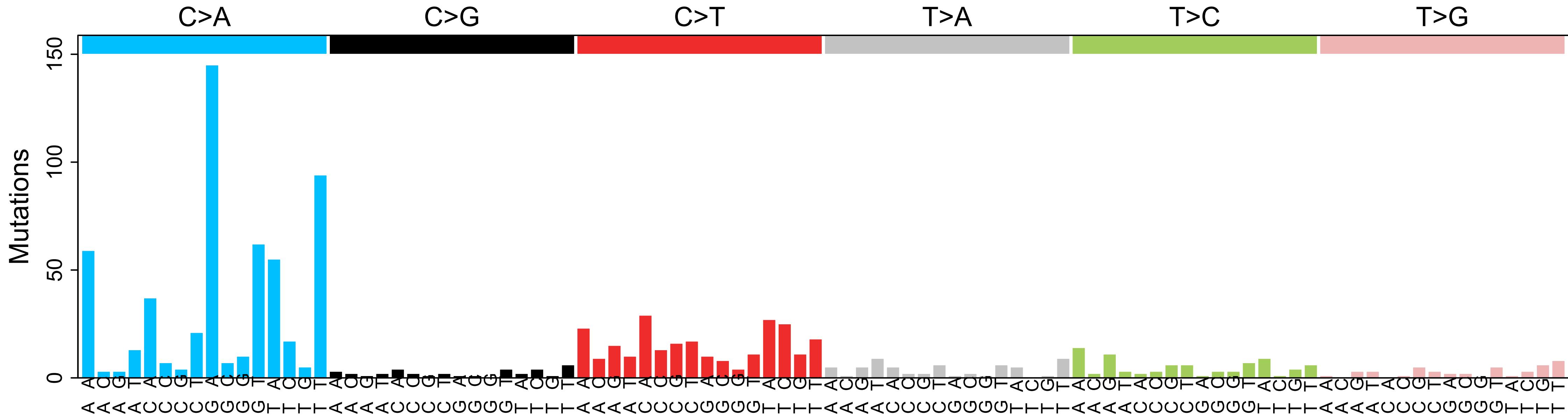
# dimethyl\_sulfate\_31311db64fc6 (1,004 mutations)



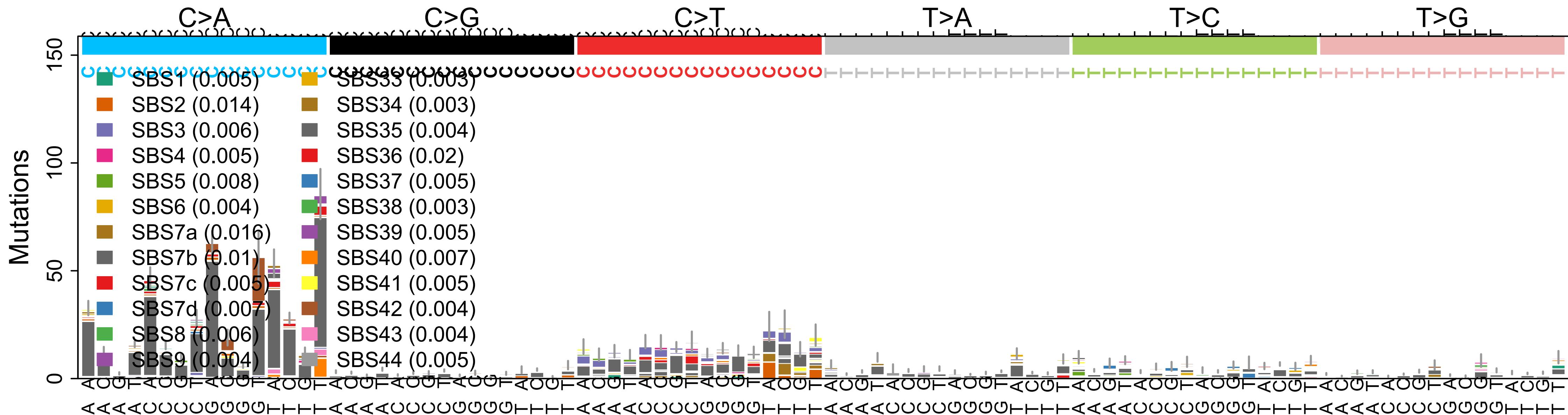
## Reconstructed spectrum (cosine similarity = 0.912)



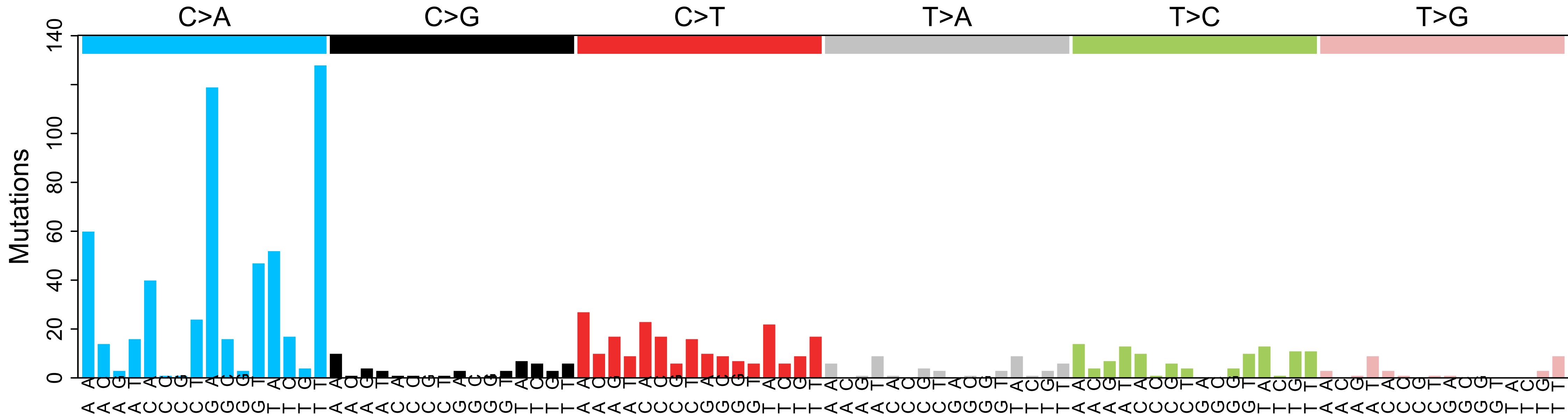
# dmso\_39bf73141acf (1,008 mutations)



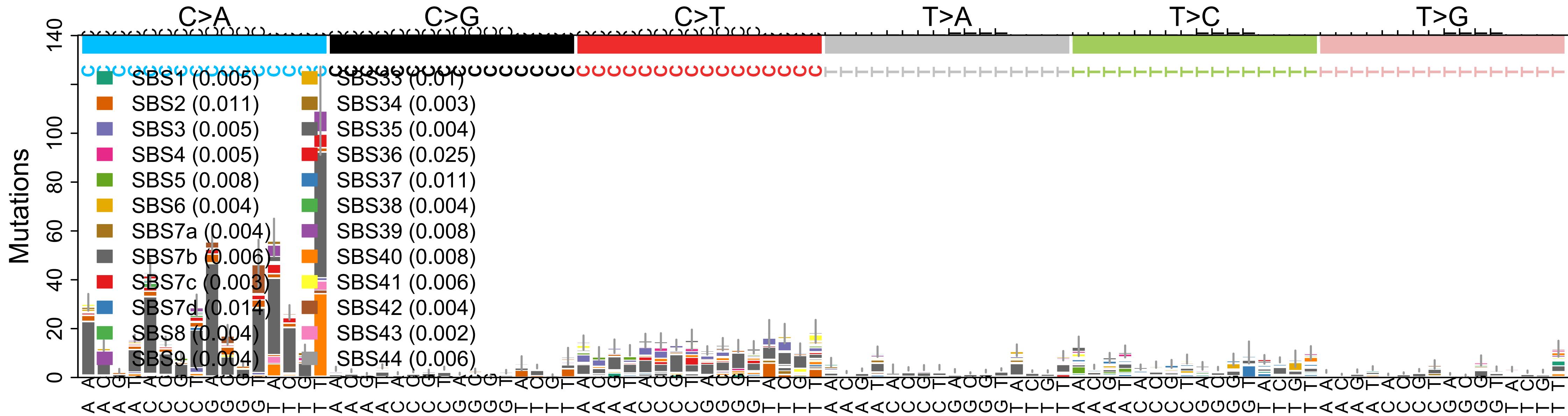
**Reconstructed spectrum (cosine similarity = 0.915)**



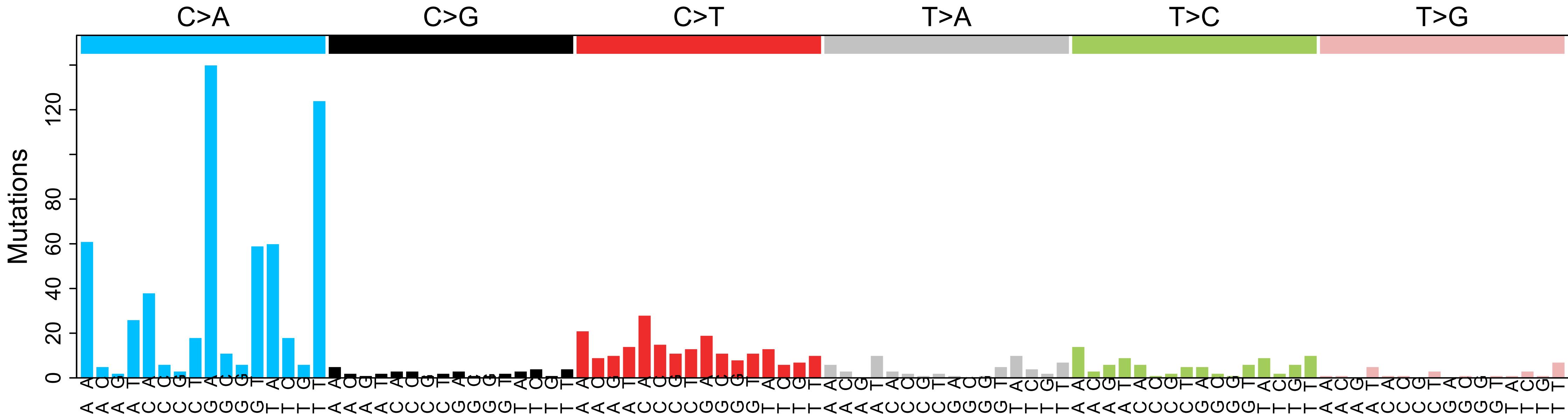
# dms0\_418f69401d9a (993 mutations)



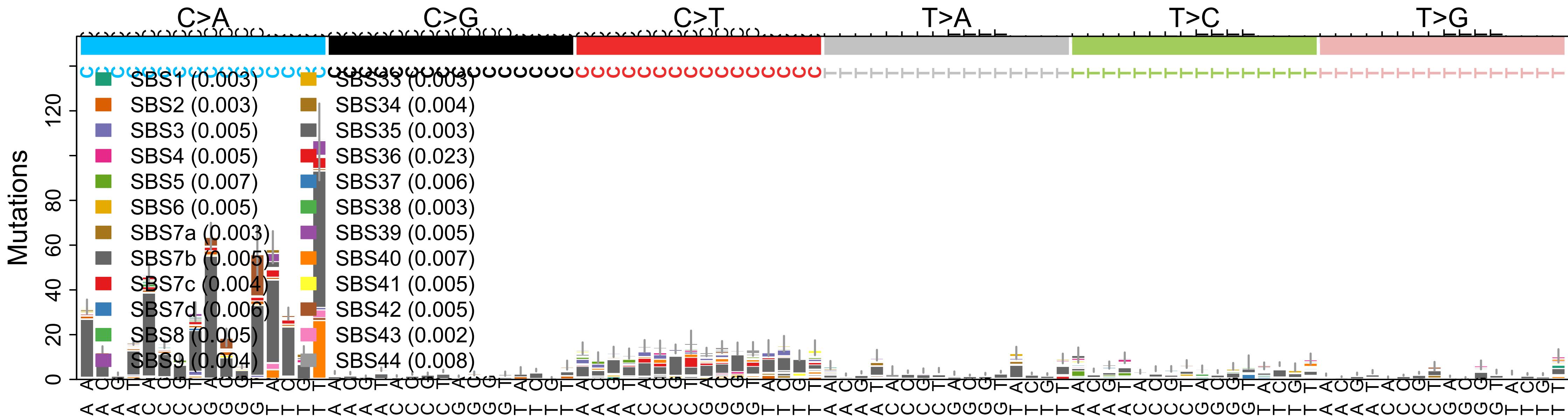
Reconstructed spectrum (cosine similarity = 0.936)



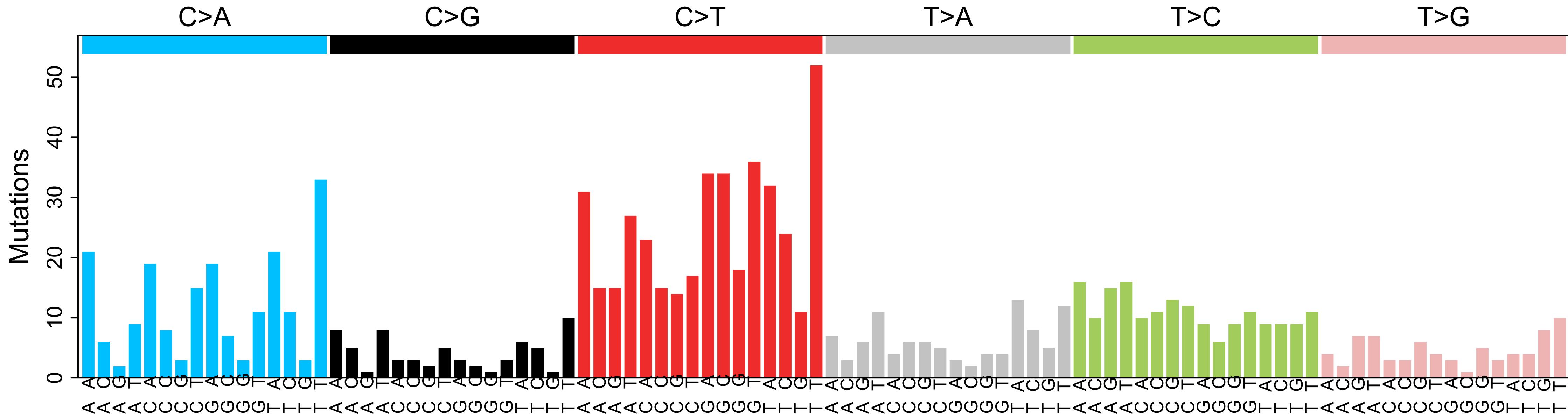
# dms0\_640c89f54363 (997 mutations)



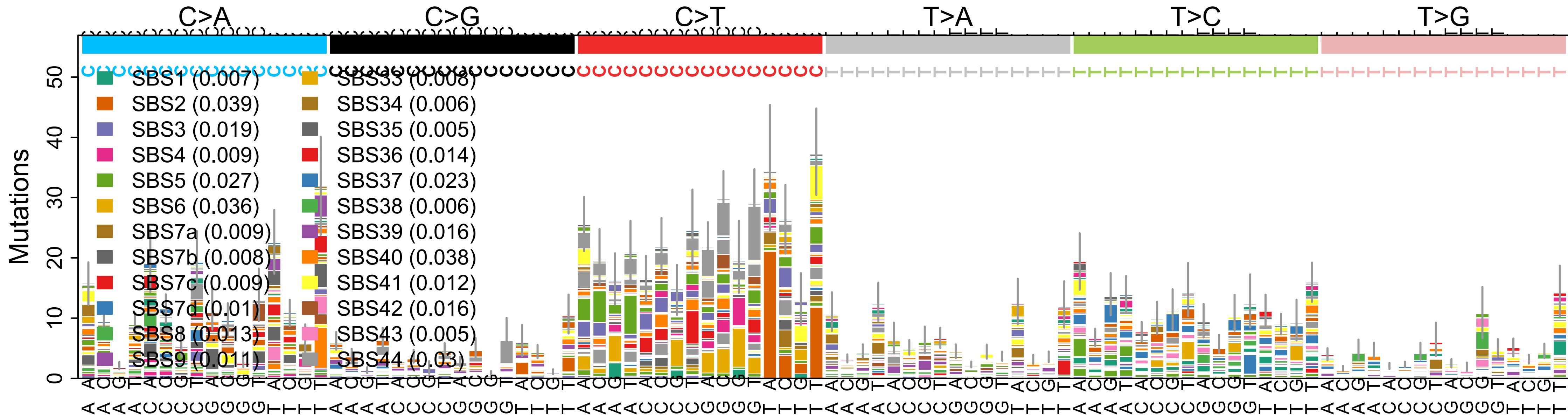
**Reconstructed spectrum (cosine similarity = 0.929)**



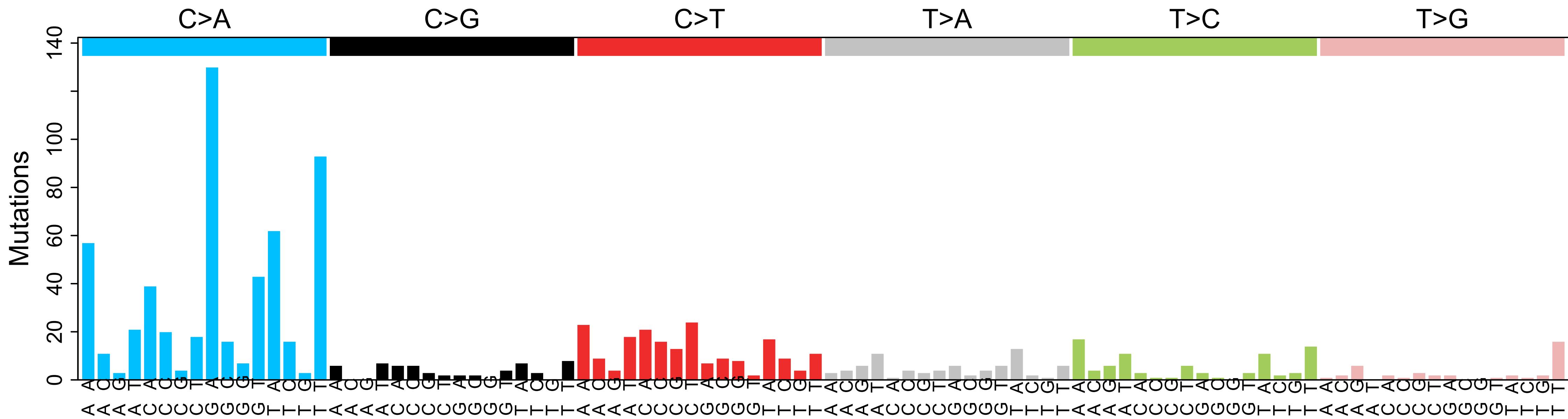
# dms0\_a7c56a3e916e (1,004 mutations)



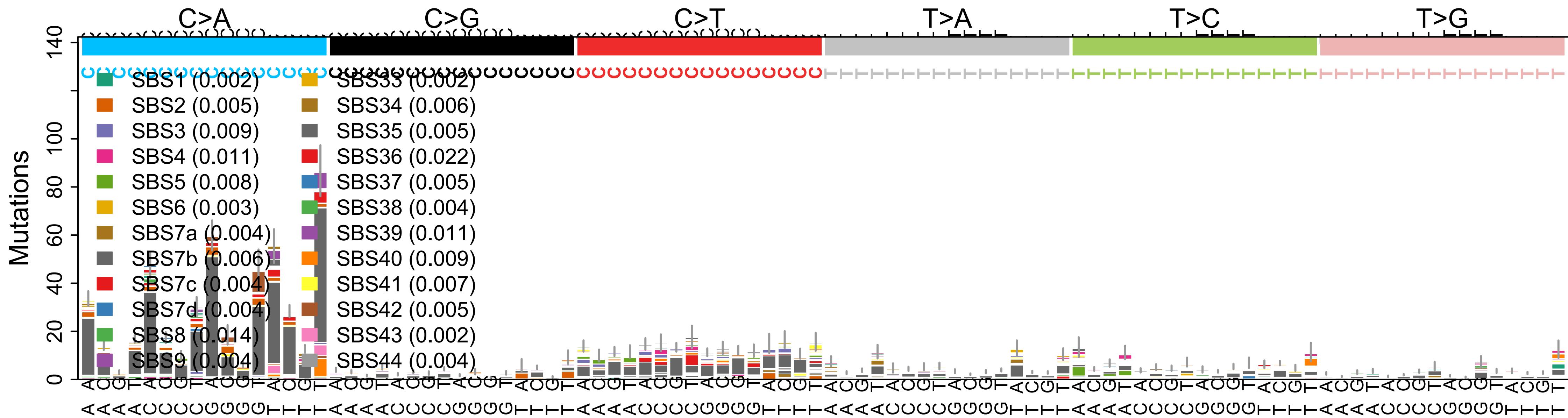
**Reconstructed spectrum (cosine similarity = 0.971)**



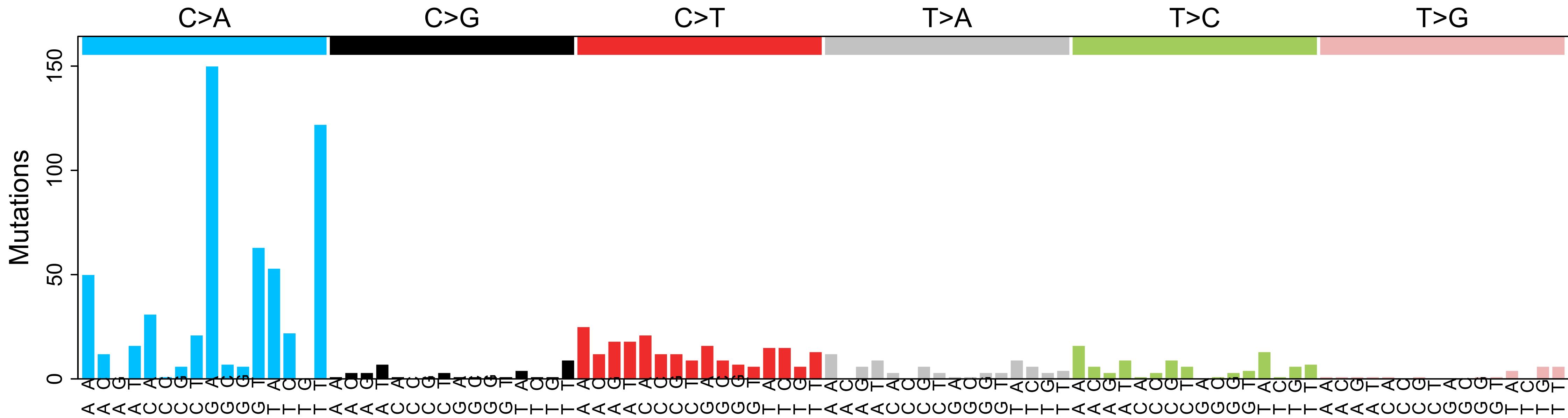
# ellipticine\_4b8e9b175c6b (997 mutations)



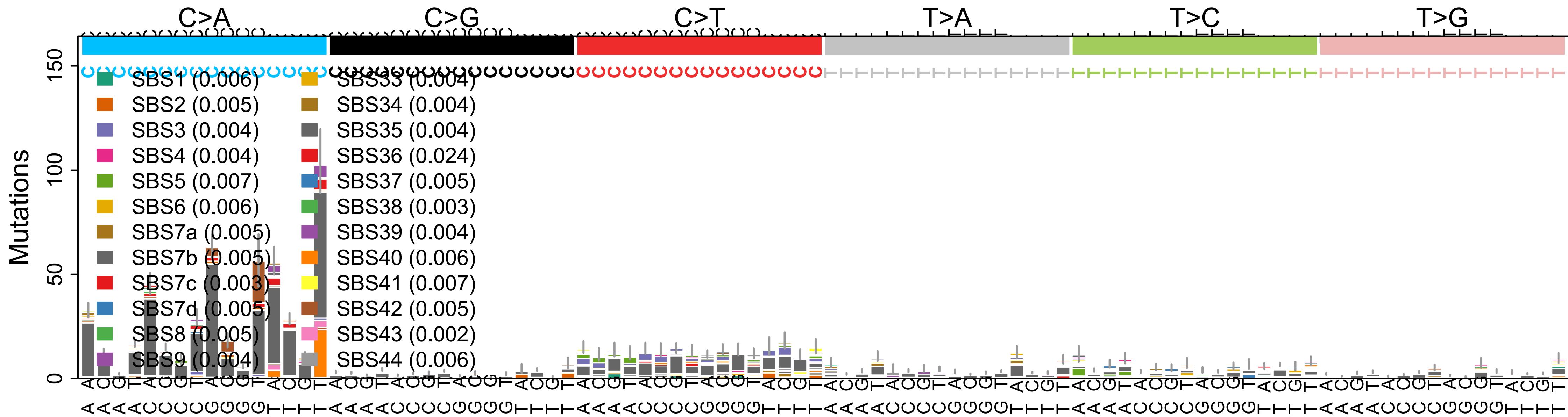
Reconstructed spectrum (cosine similarity = 0.923)



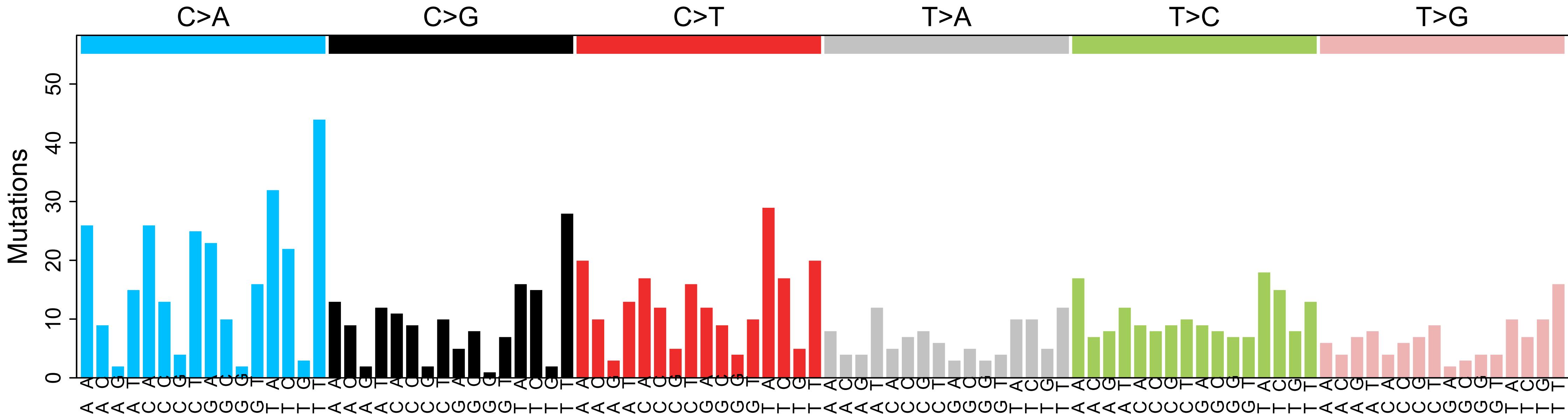
# ellipticine\_e149a5f58dd0 (993 mutations)



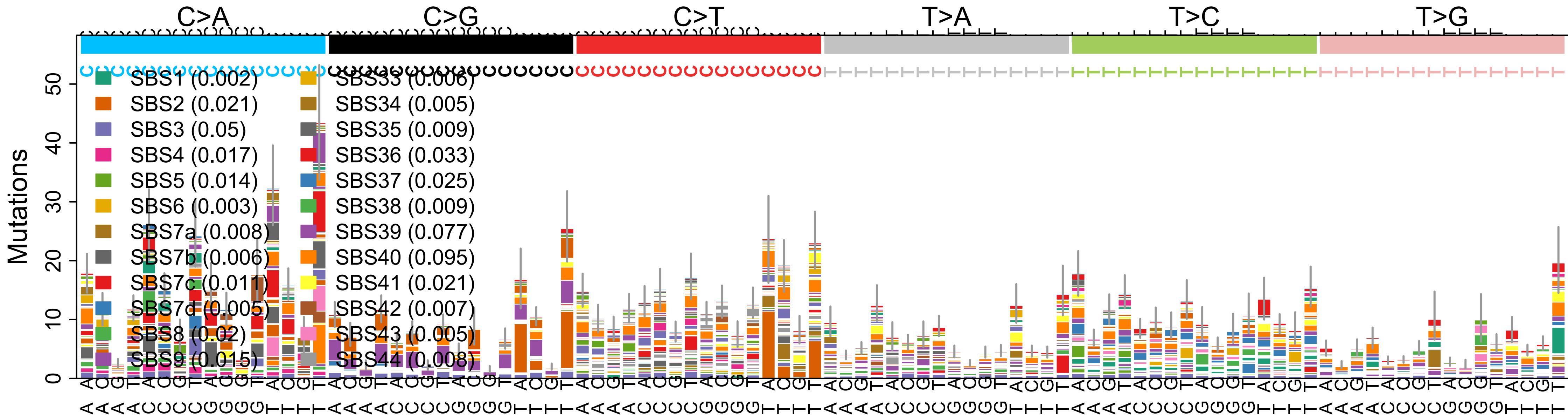
Reconstructed spectrum (cosine similarity = 0.916)



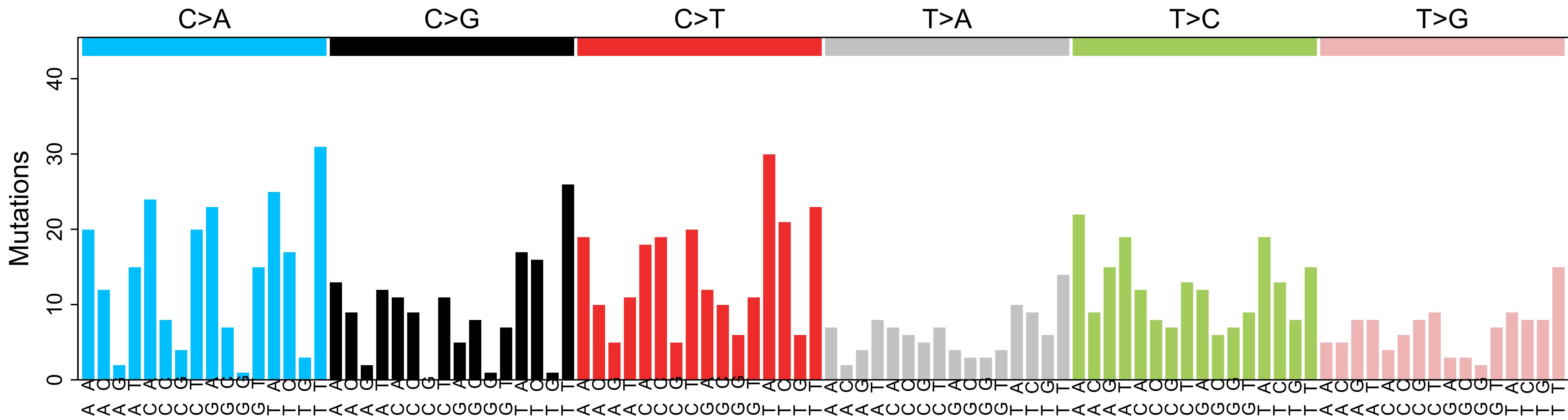
# etoposide\_2fbea1693a7c (1,002 mutations)



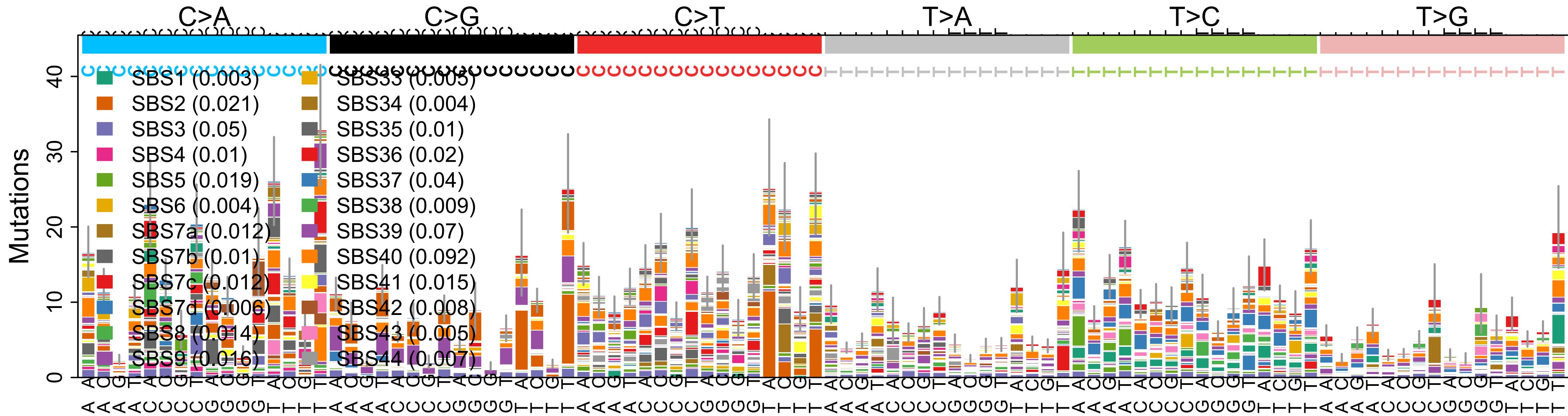
**Reconstructed spectrum (cosine similarity = 0.977)**



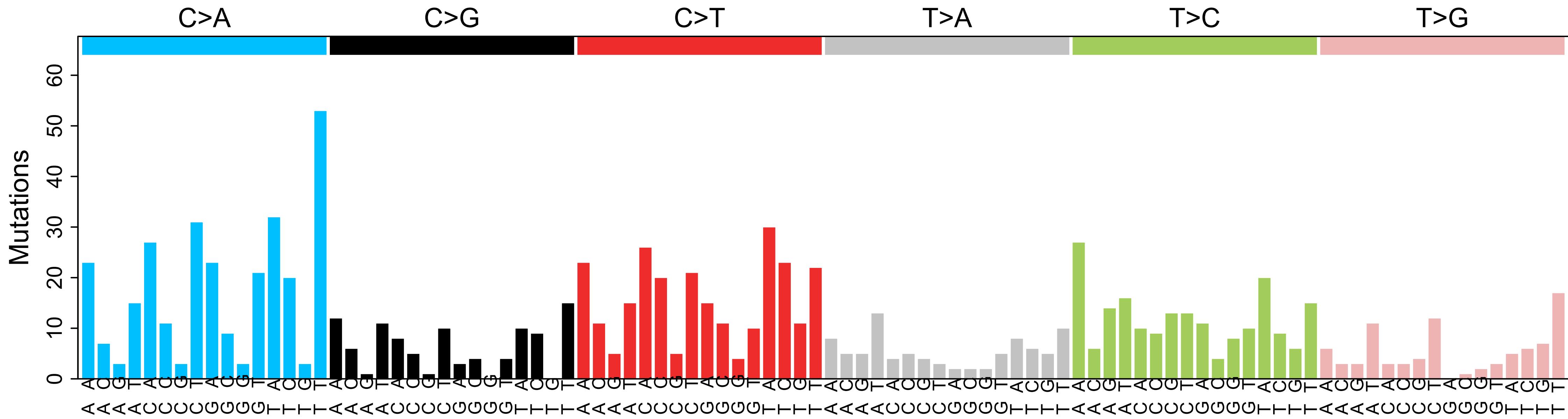
# etoposide\_38326aaa4a4a (1,002 mutations)



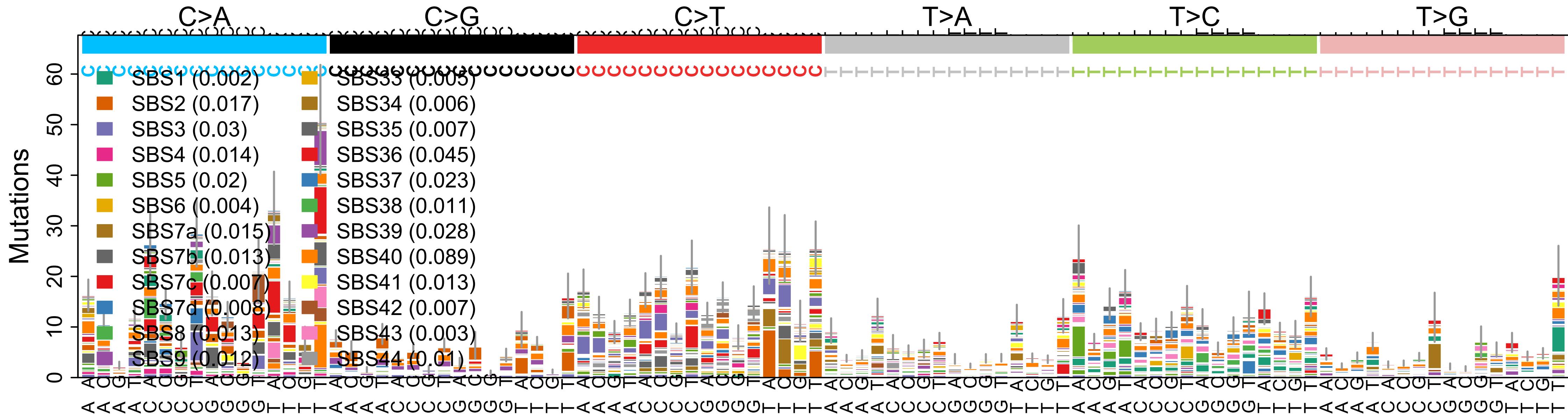
Reconstructed spectrum (cosine similarity = 0.978)



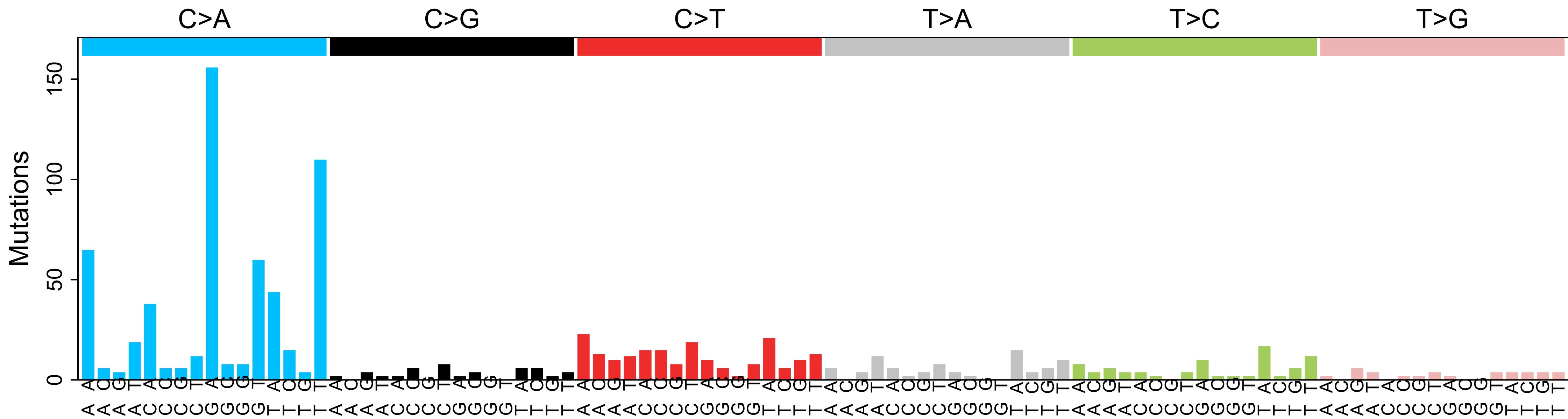
# etoposide\_51f30ea13687 (999 mutations)



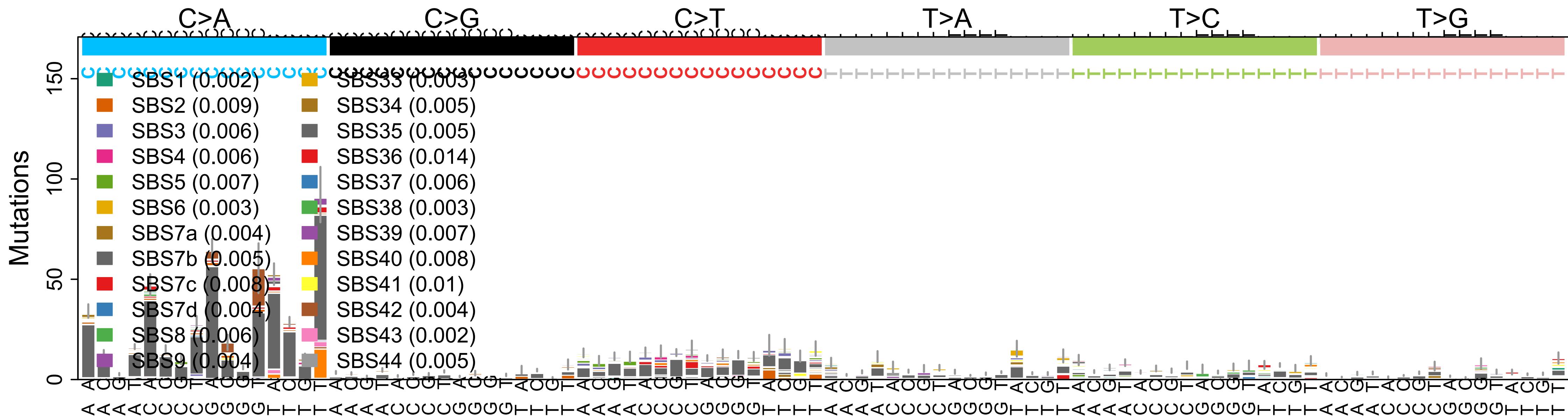
Reconstructed spectrum (cosine similarity = 0.98)



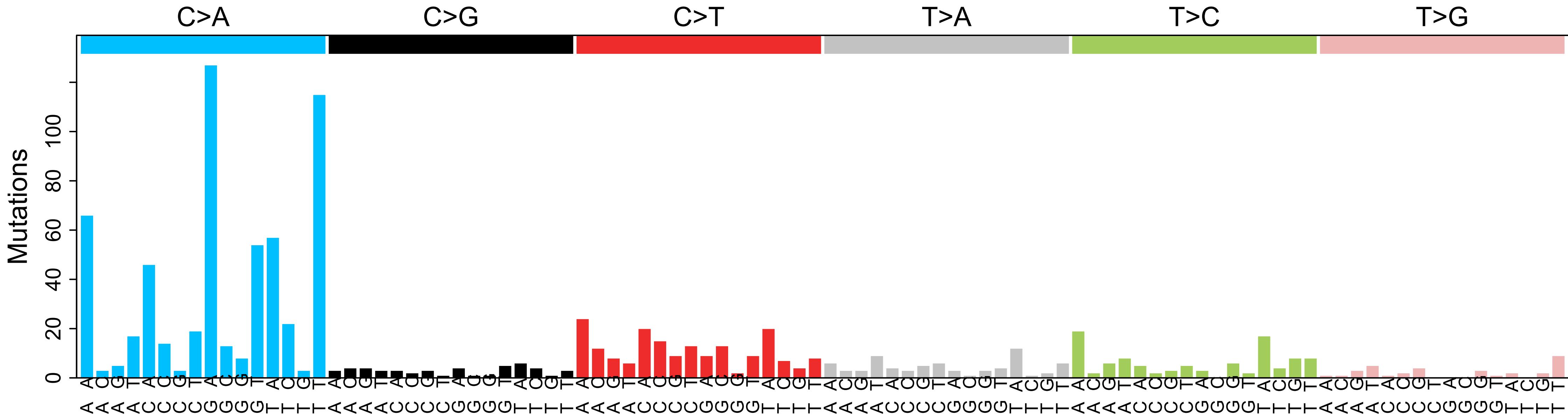
# etoposide\_d87f22a7e170 (1,010 mutations)



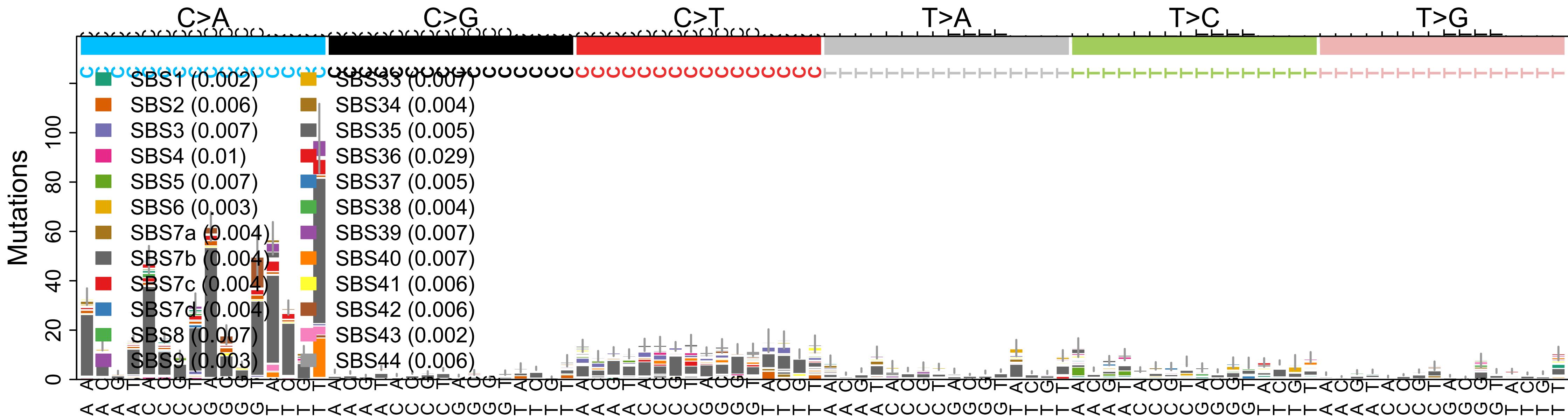
Reconstructed spectrum (cosine similarity = 0.898)



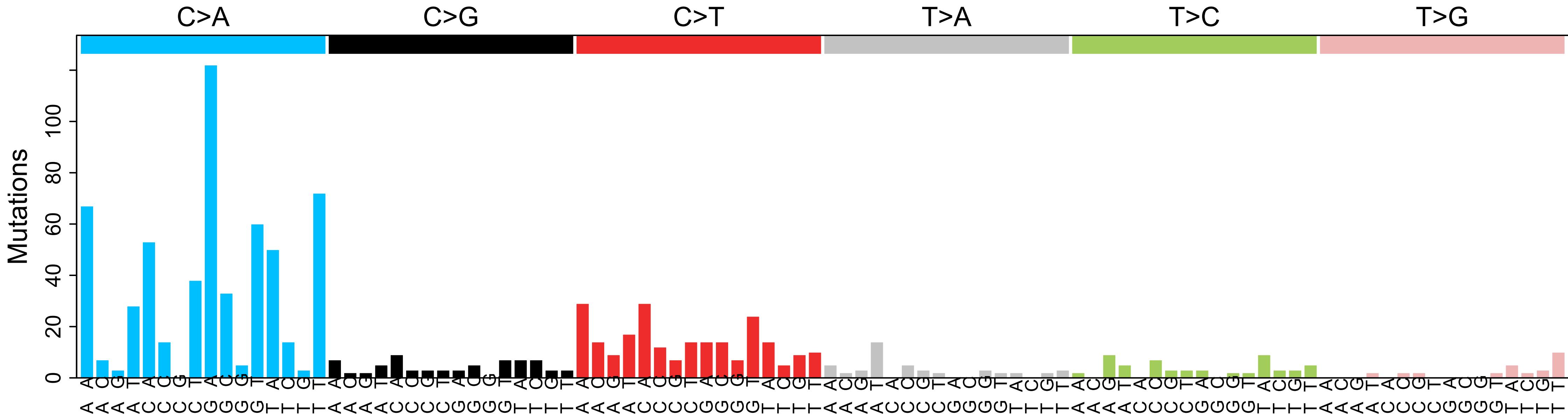
# formaldehyde\_8c36e95b481c (1,002 mutations)



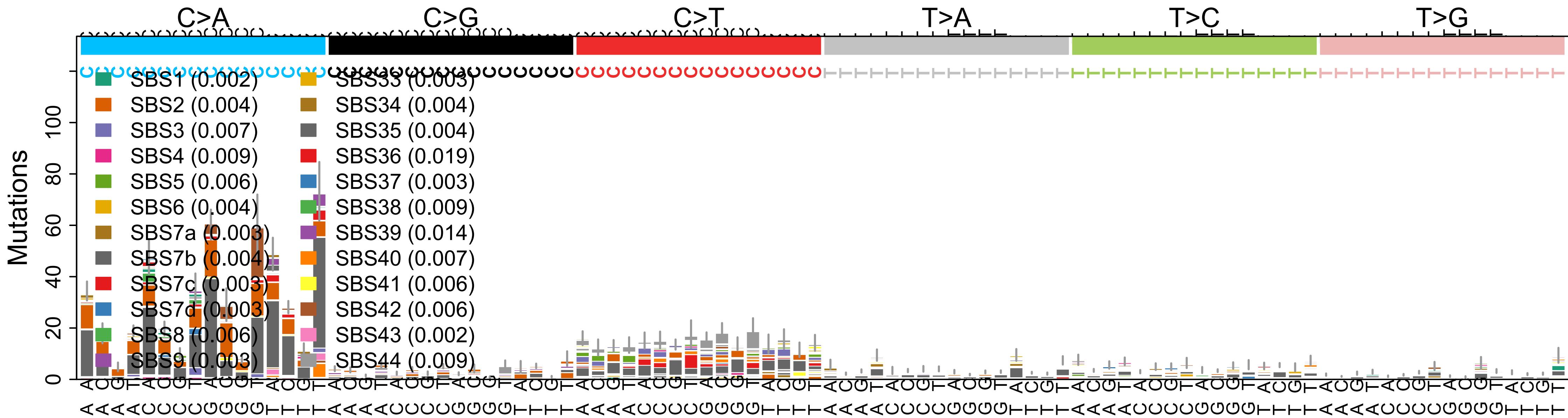
Reconstructed spectrum (cosine similarity = 0.936)



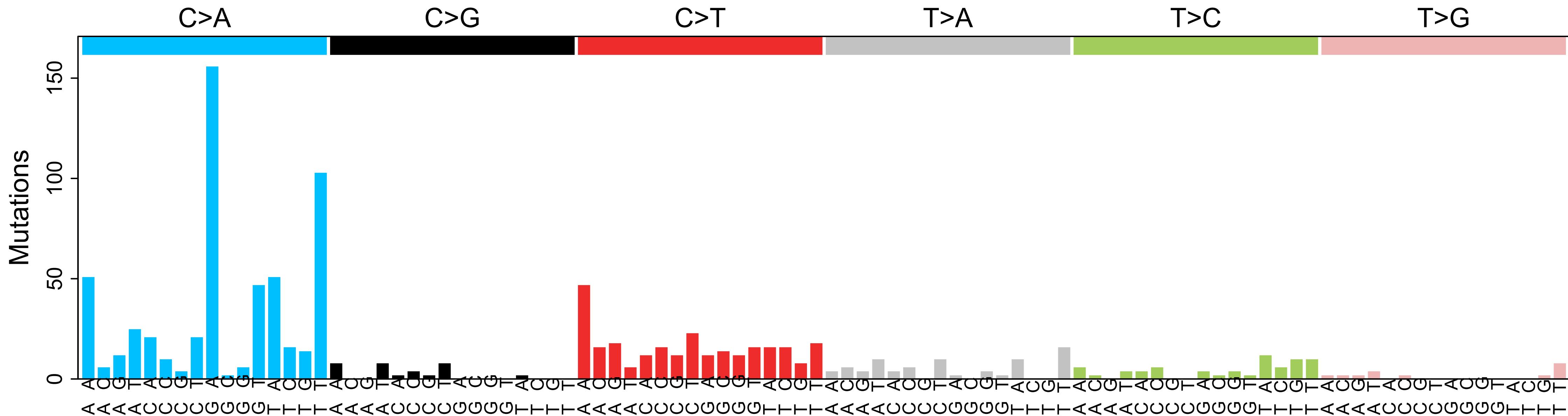
# furan\_fd4f695c67b1 (996 mutations)



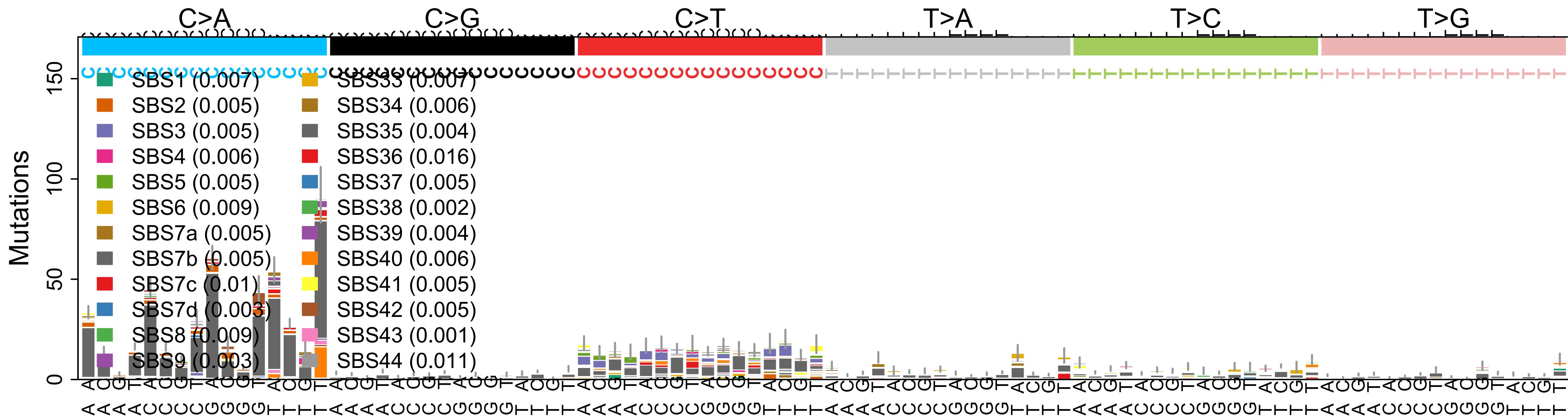
**Reconstructed spectrum (cosine similarity = 0.927)**



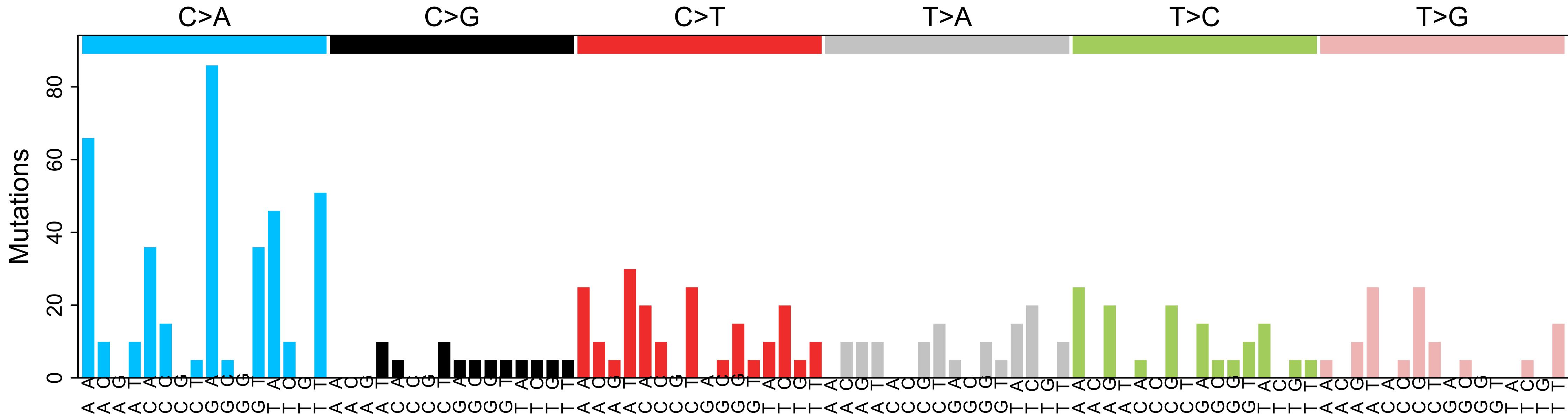
# gammaray\_8a41562354d7 (1,013 mutations)



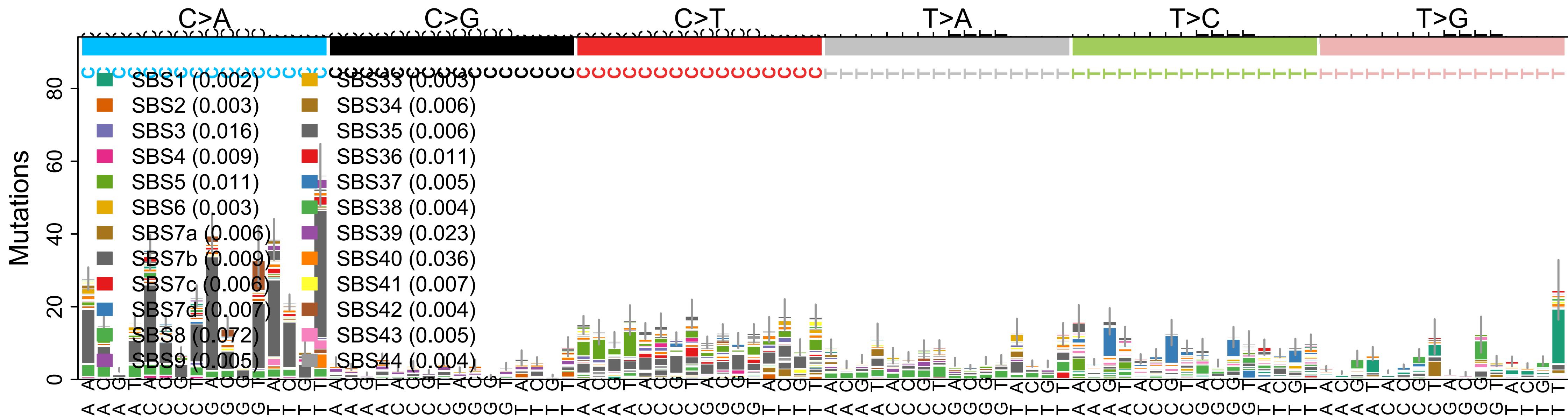
Reconstructed spectrum (cosine similarity = 0.882)



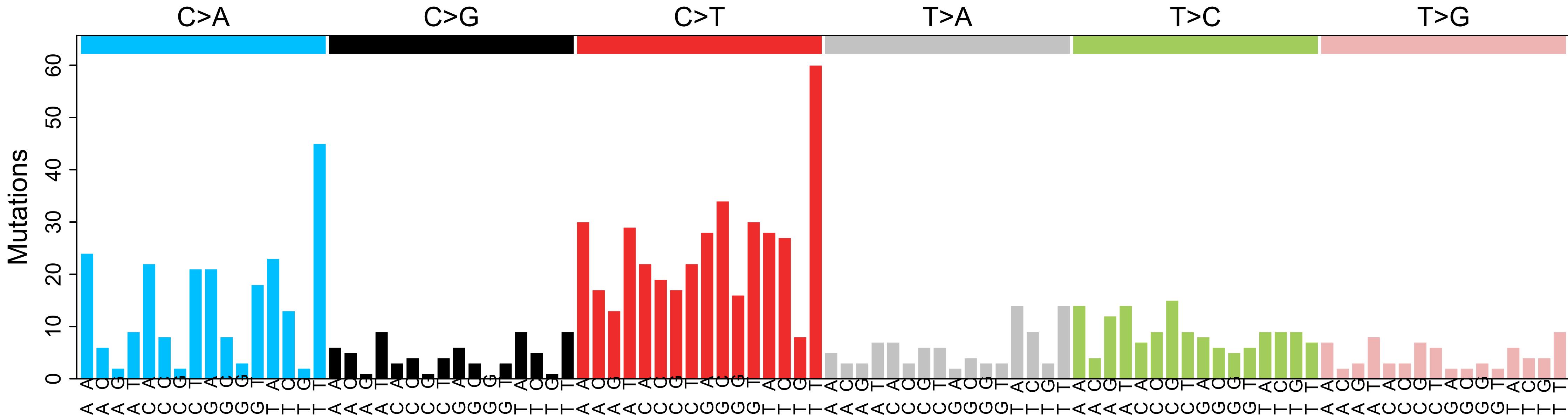
# glycidamide\_8e1c87cf773d (991 mutations)



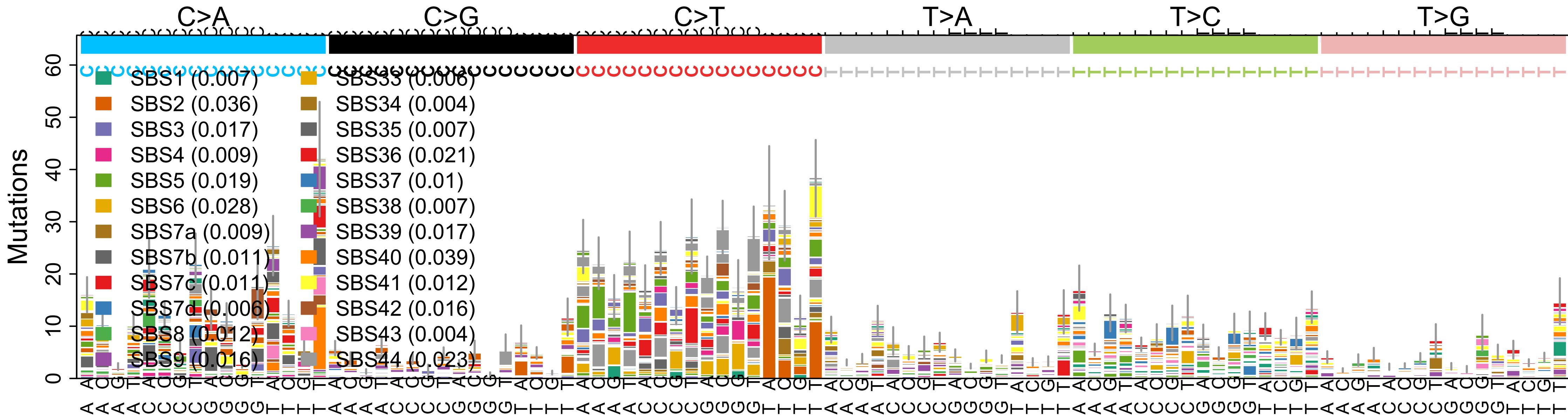
## Reconstructed spectrum (cosine similarity = 0.86)



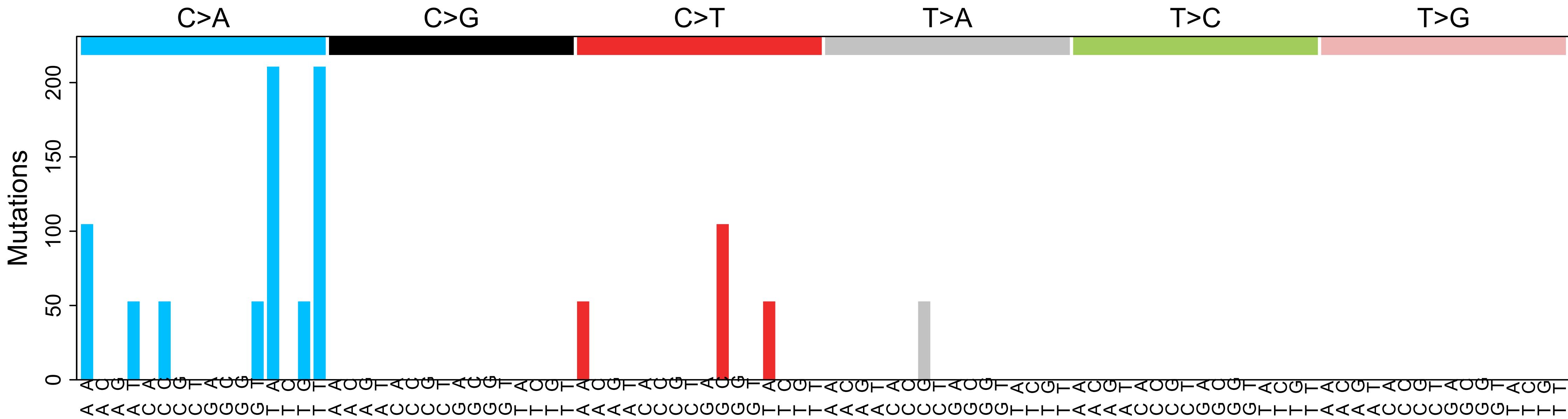
# harmane\_ad913bd008a0 (1,002 mutations)



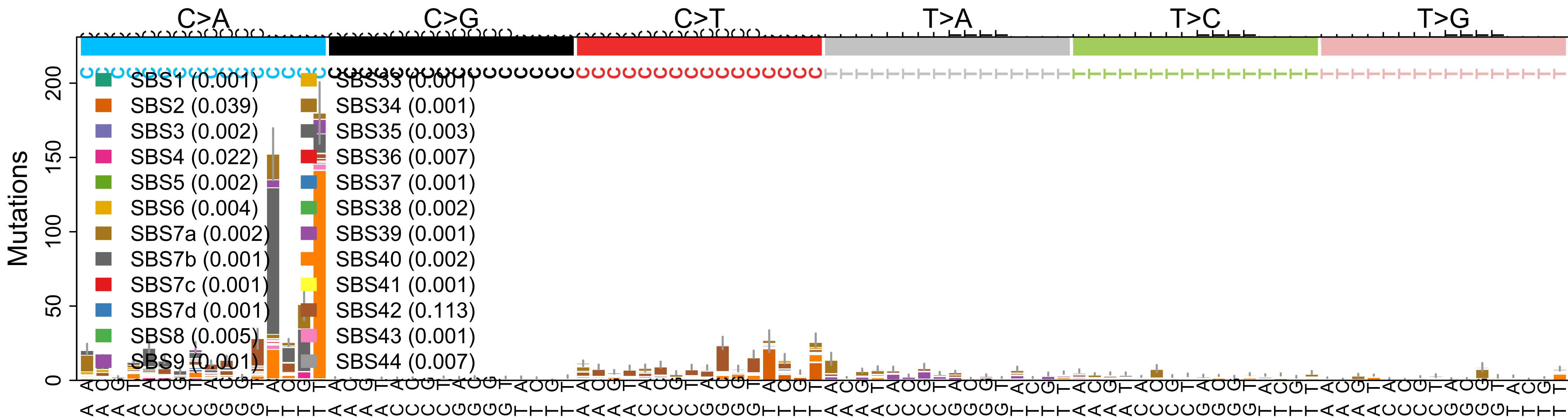
Reconstructed spectrum (cosine similarity = 0.967)



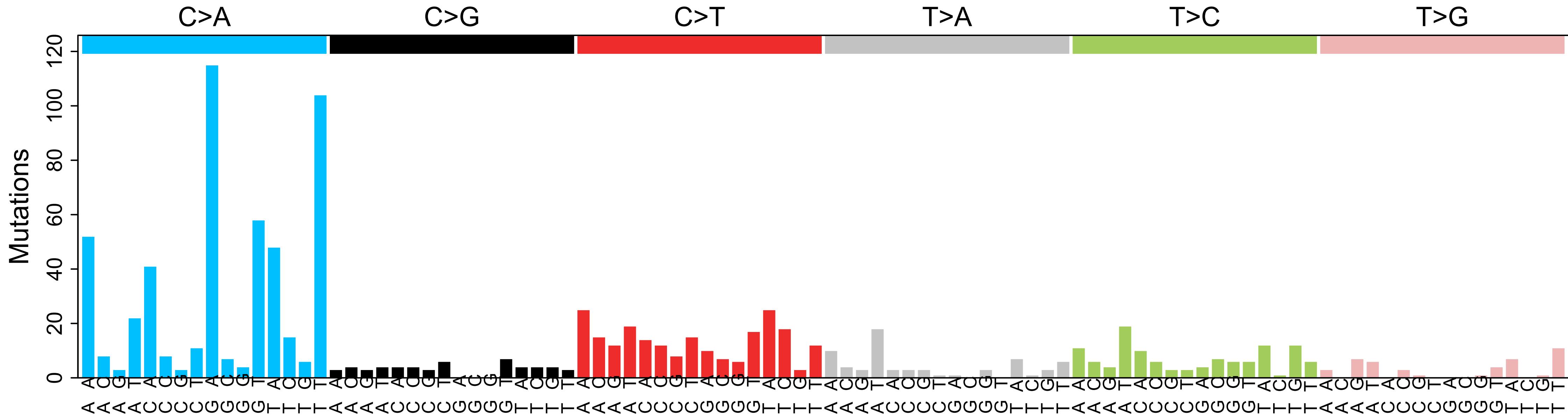
# hydrogen\_peroxide\_ff64f141ad1a (1,003 mutations)



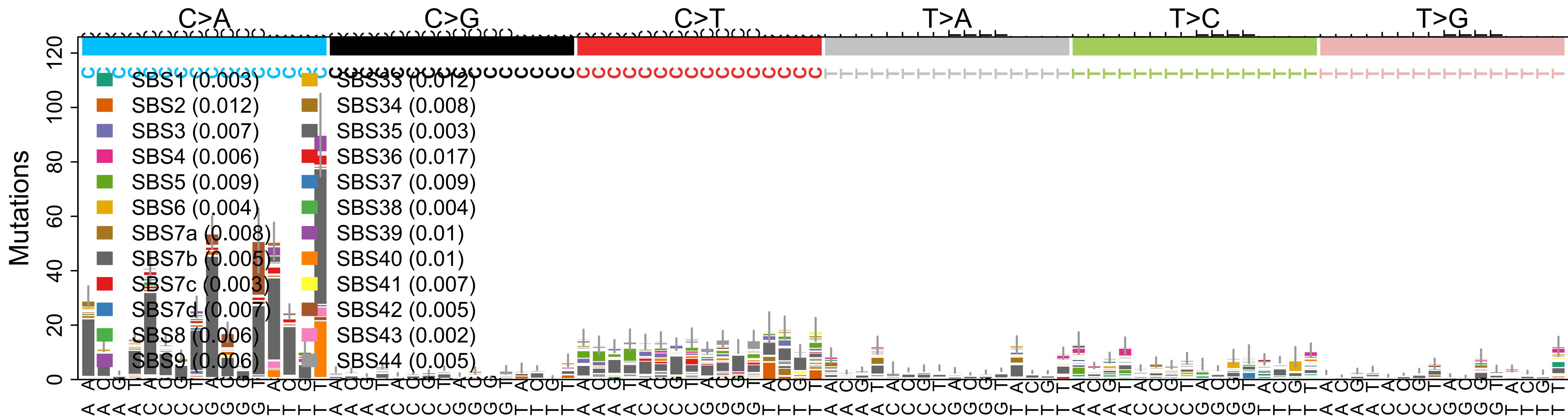
**Reconstructed spectrum (cosine similarity = 0.892)**



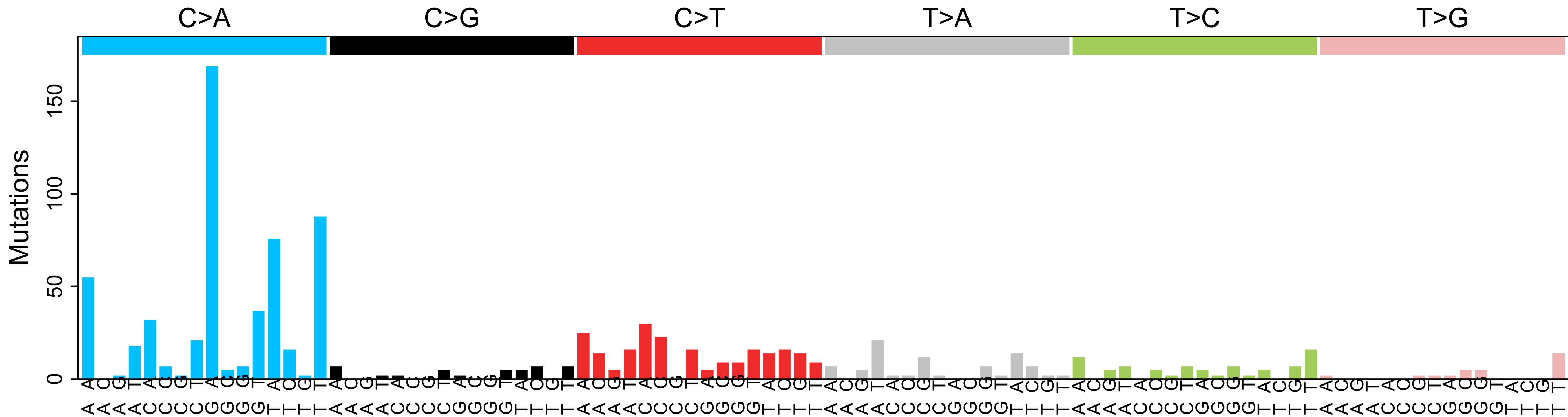
# lead\_acetate\_eb992ae53f06 (1,002 mutations)



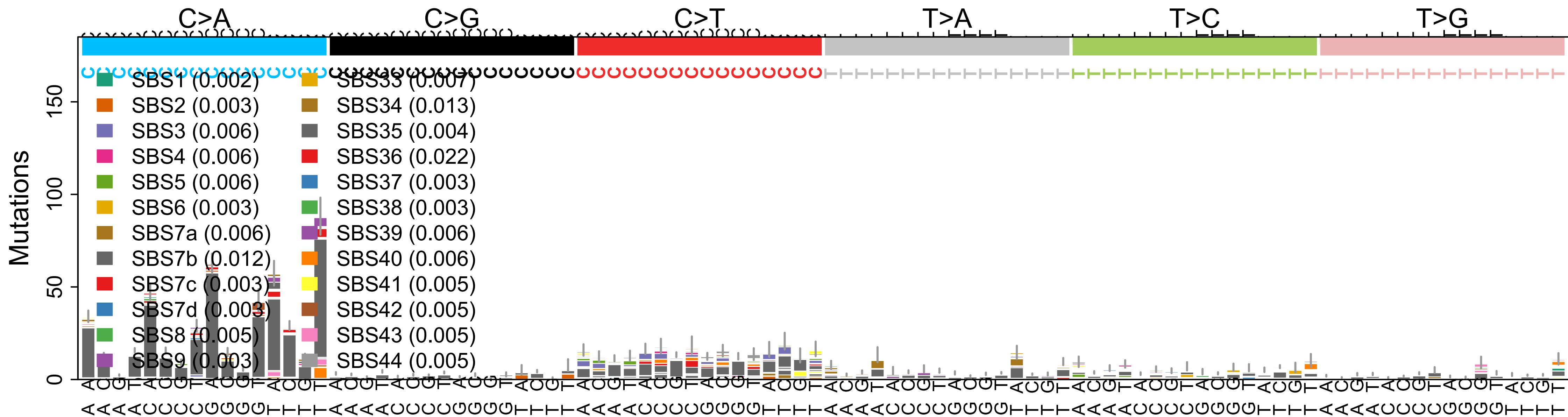
Reconstructed spectrum (cosine similarity = 0.932)



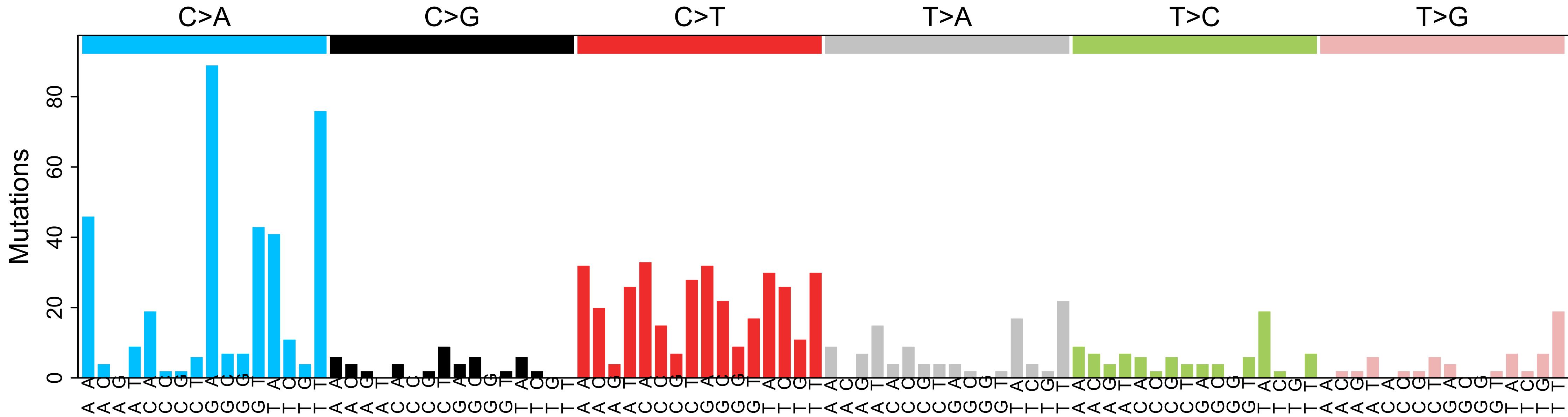
# lead\_nitrate\_3ff280a61a91 (999 mutations)



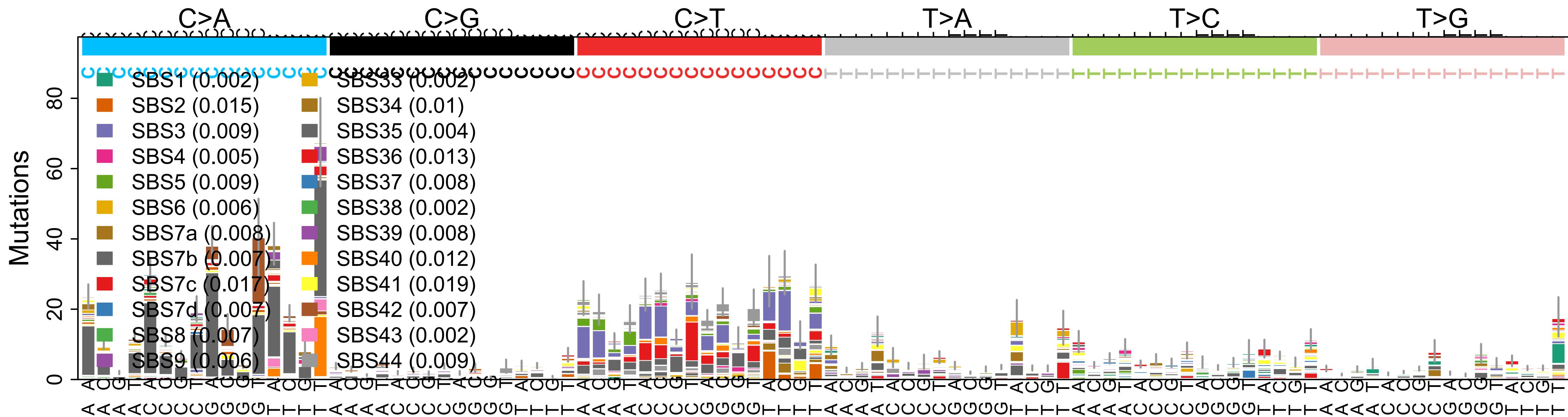
Reconstructed spectrum (cosine similarity = 0.872)



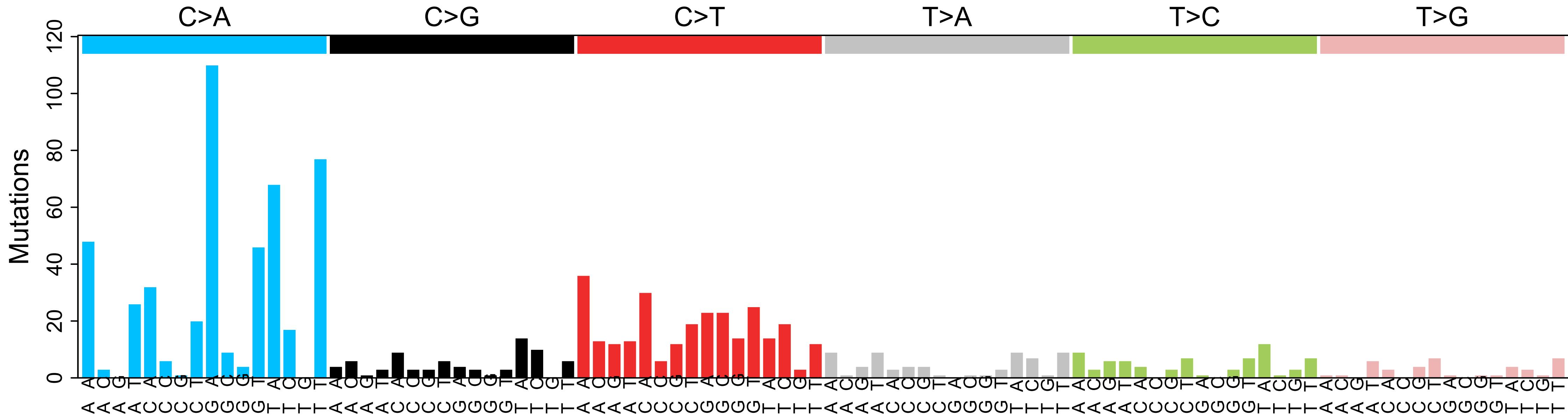
# mechlorethamine\_48da6be92ec6 (1,008 mutations)



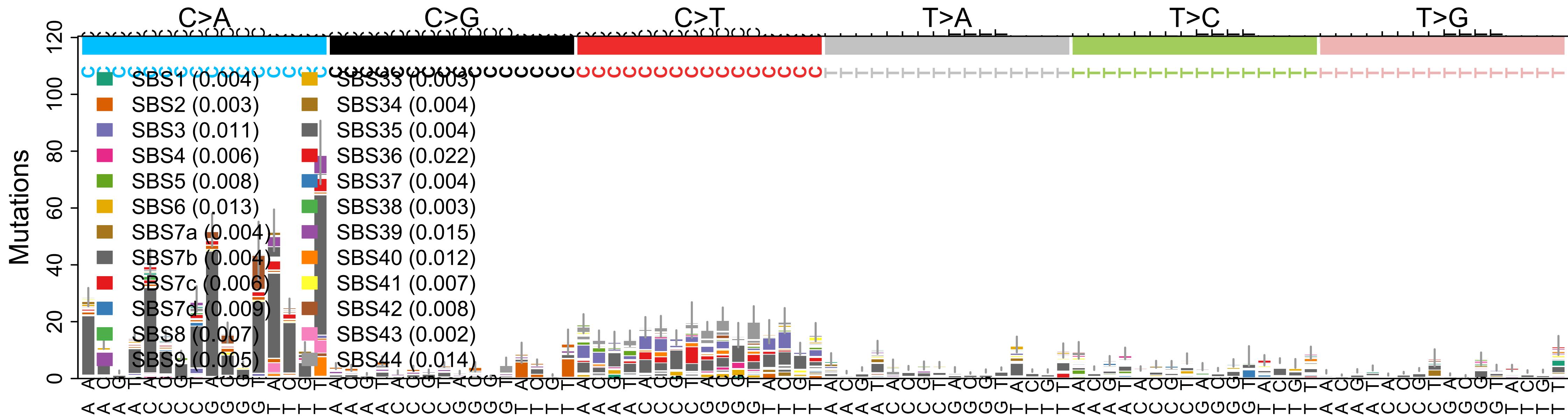
Reconstructed spectrum (cosine similarity = 0.921)



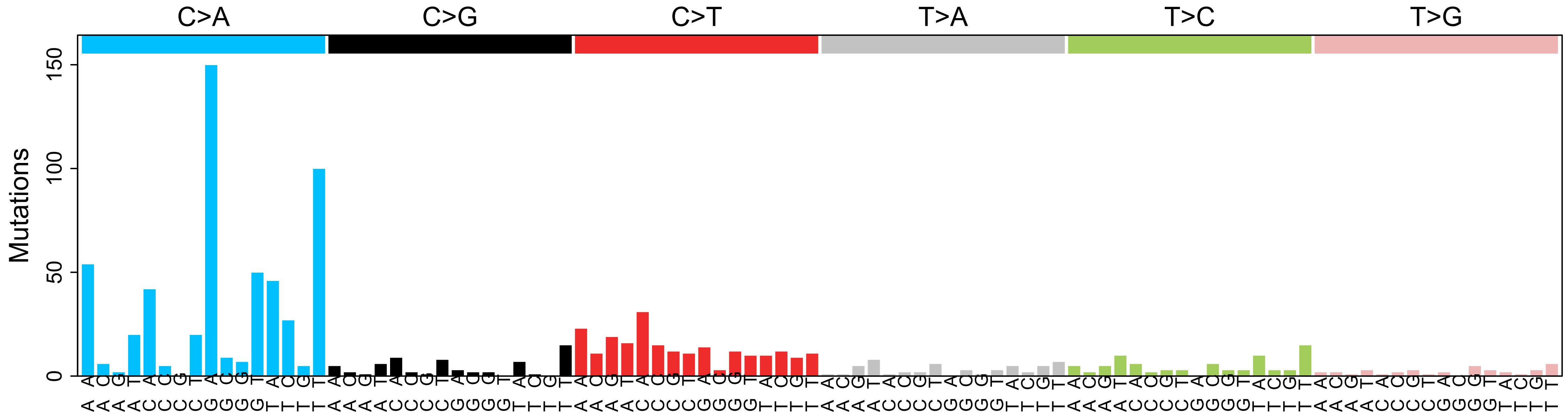
# melphalan\_dc6d858bb0a4 (995 mutations)



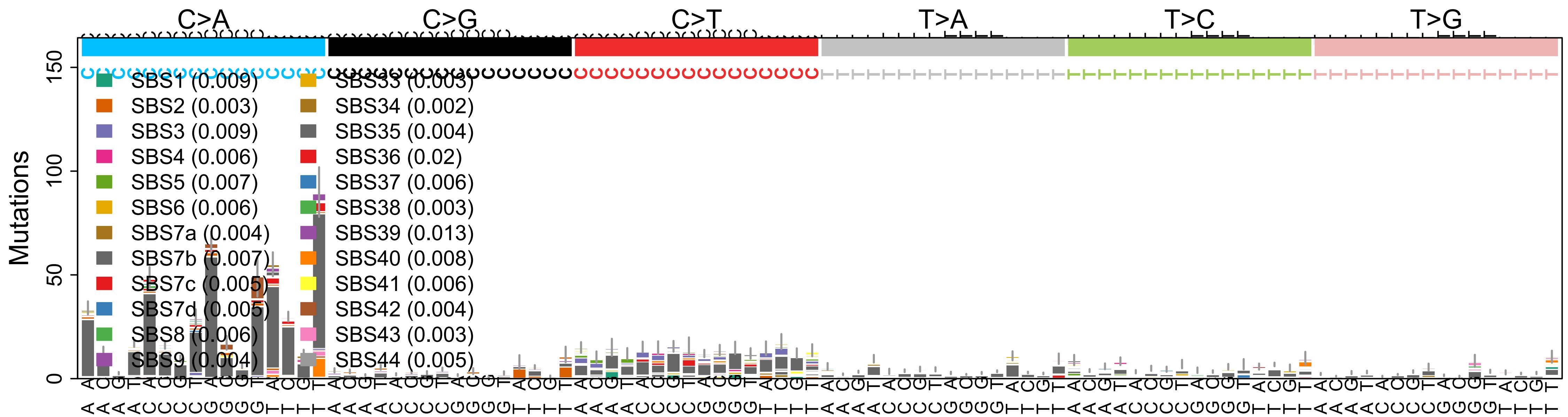
Reconstructed spectrum (cosine similarity = 0.923)



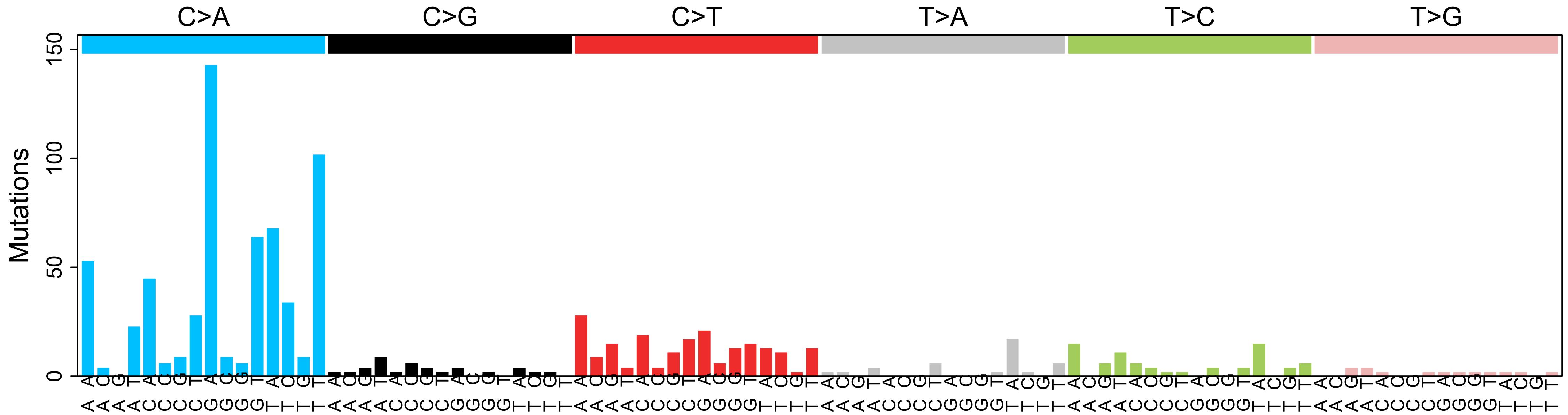
# **methanol\_23bc14314298 (994 mutations)**



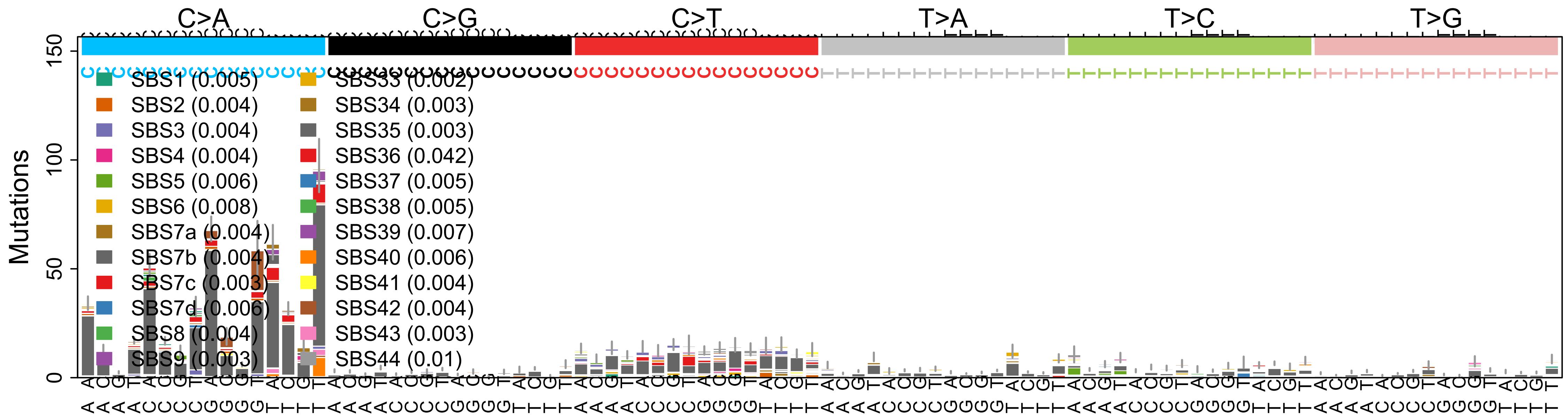
## Reconstructed spectrum (cosine similarity = 0.909)



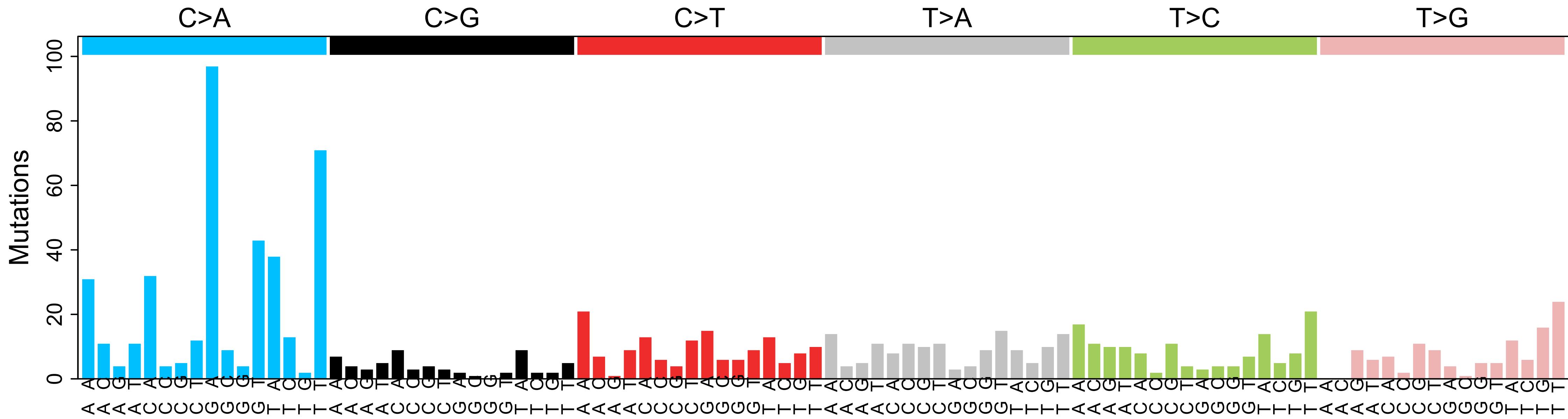
# methanol\_5f193a12cbbf (995 mutations)



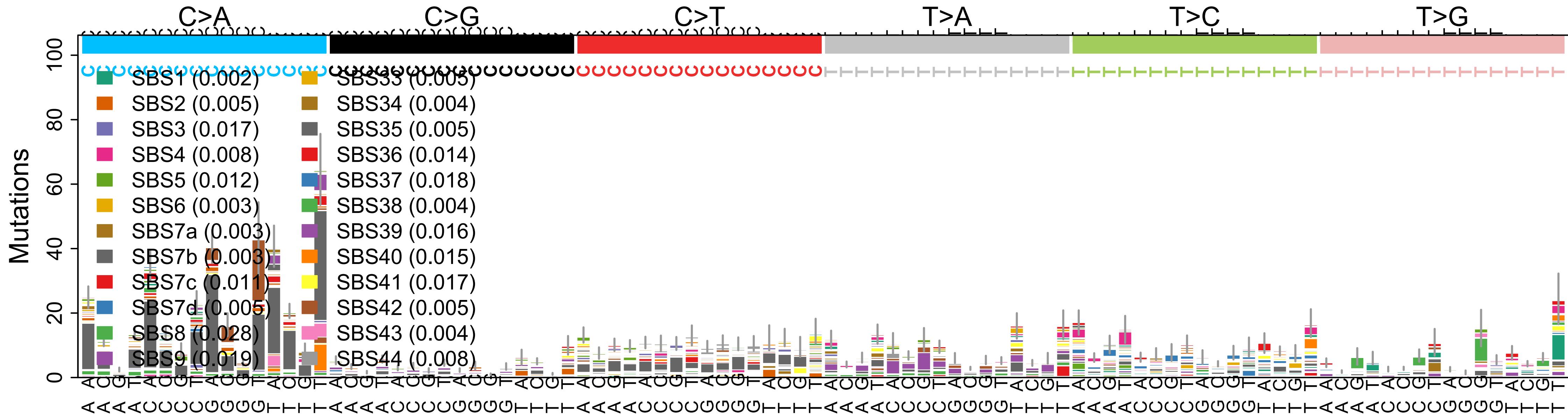
**Reconstructed spectrum (cosine similarity = 0.933)**



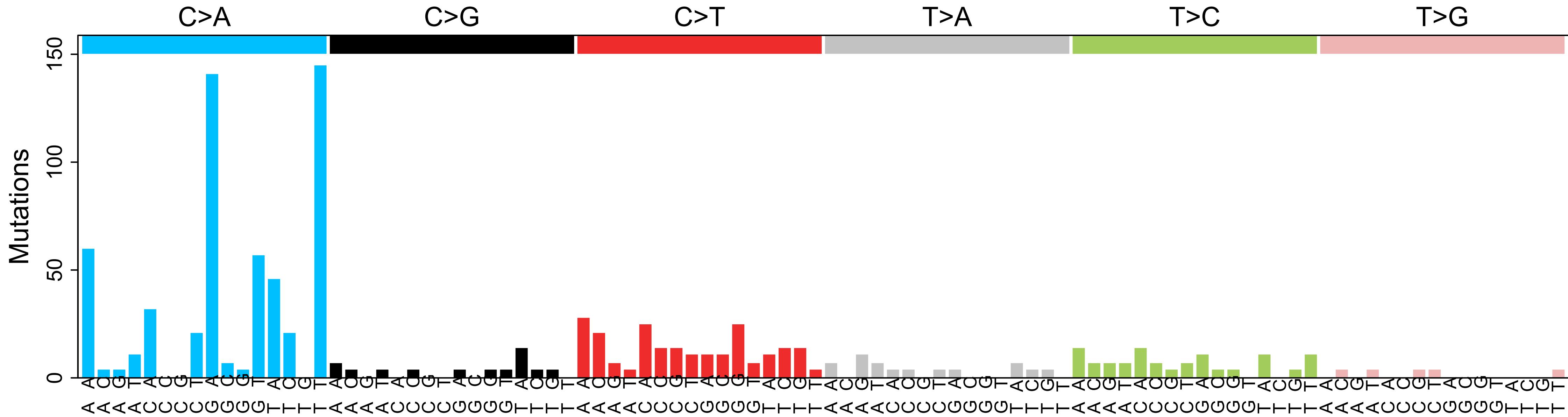
# methyl\_methanesulfonate\_f61fcd09adad (992 mutations)



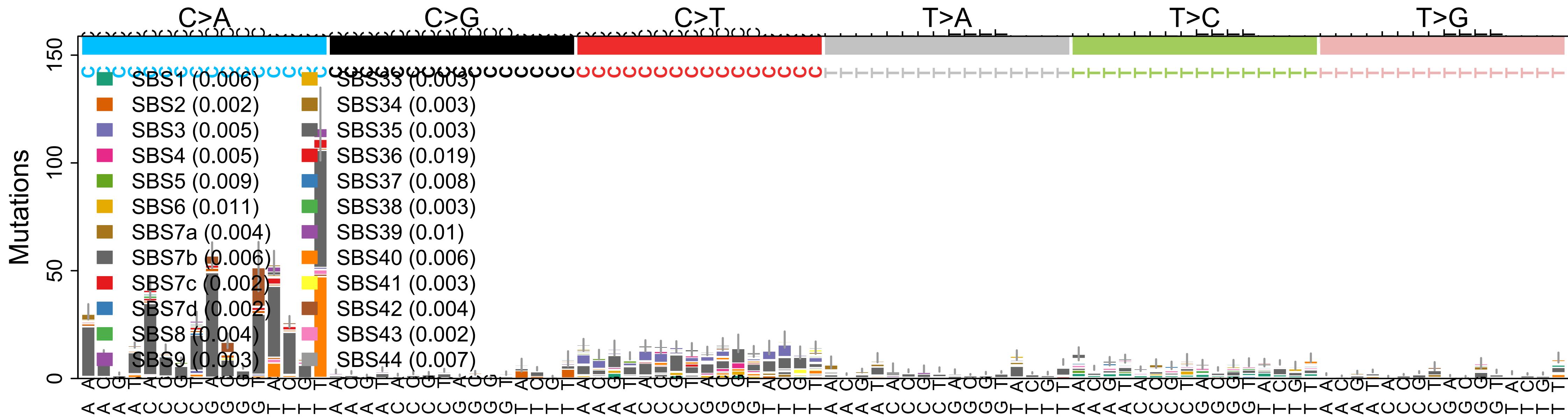
## Reconstructed spectrum (cosine similarity = 0.909)



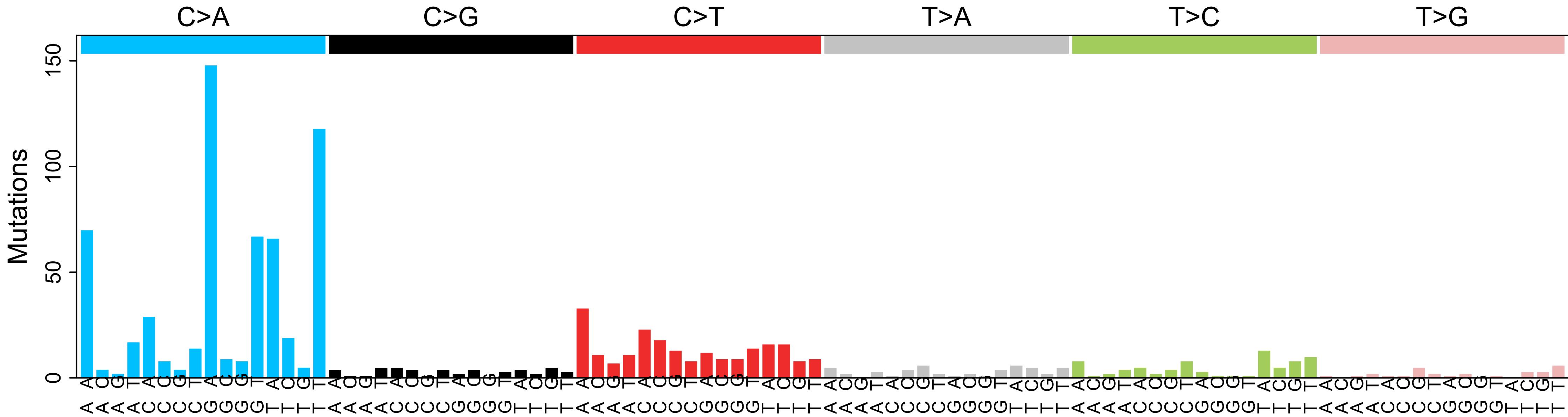
# **methyleugenol\_4048db90dc58 (1,015 mutations)**



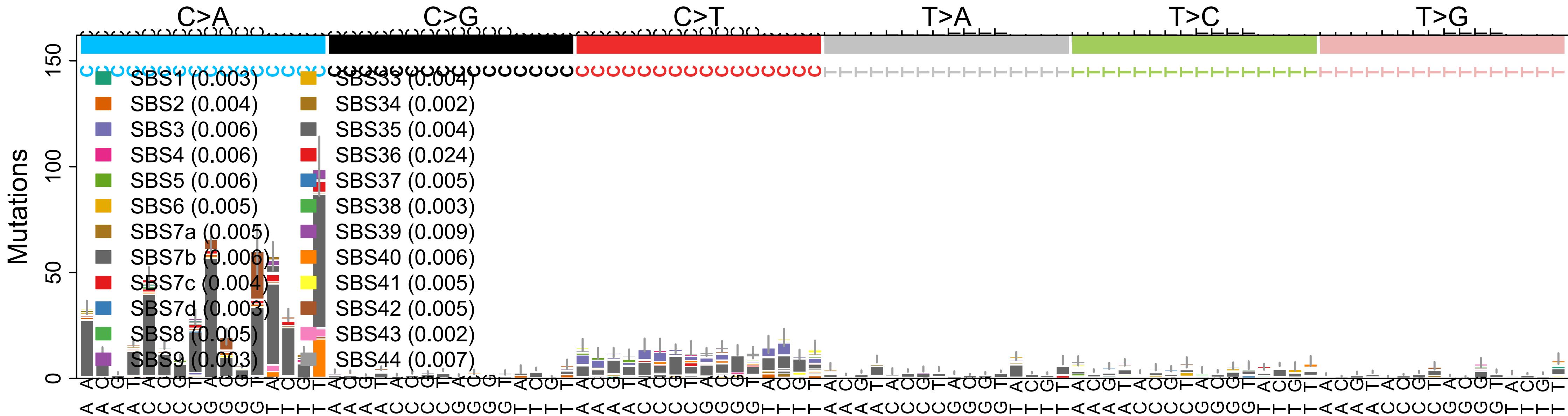
## Reconstructed spectrum (cosine similarity = 0.915)



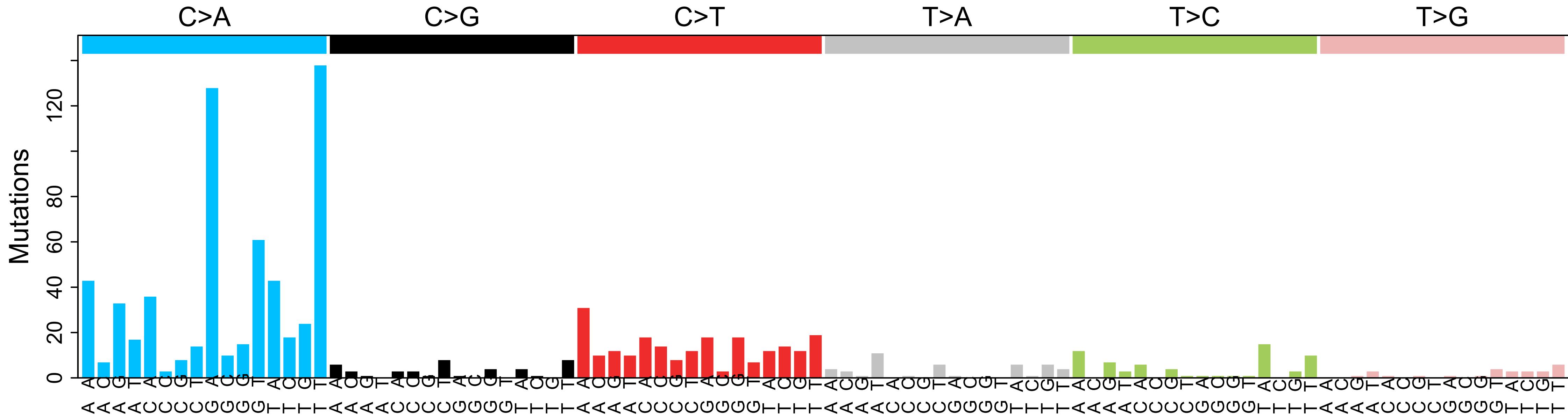
# methyleugenol\_830517b726f0 (1,007 mutations)



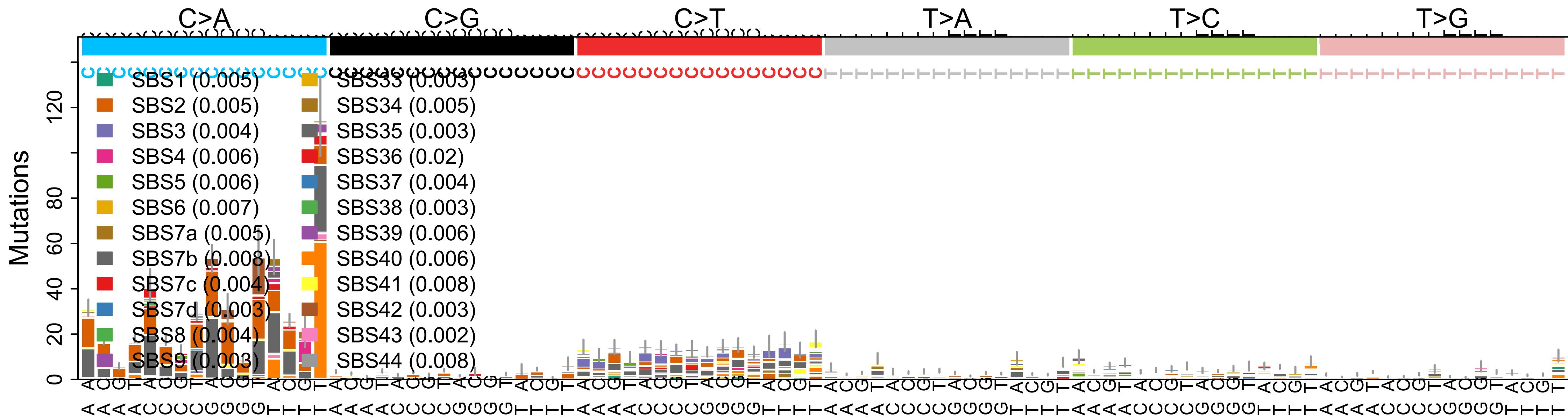
Reconstructed spectrum (cosine similarity = 0.916)



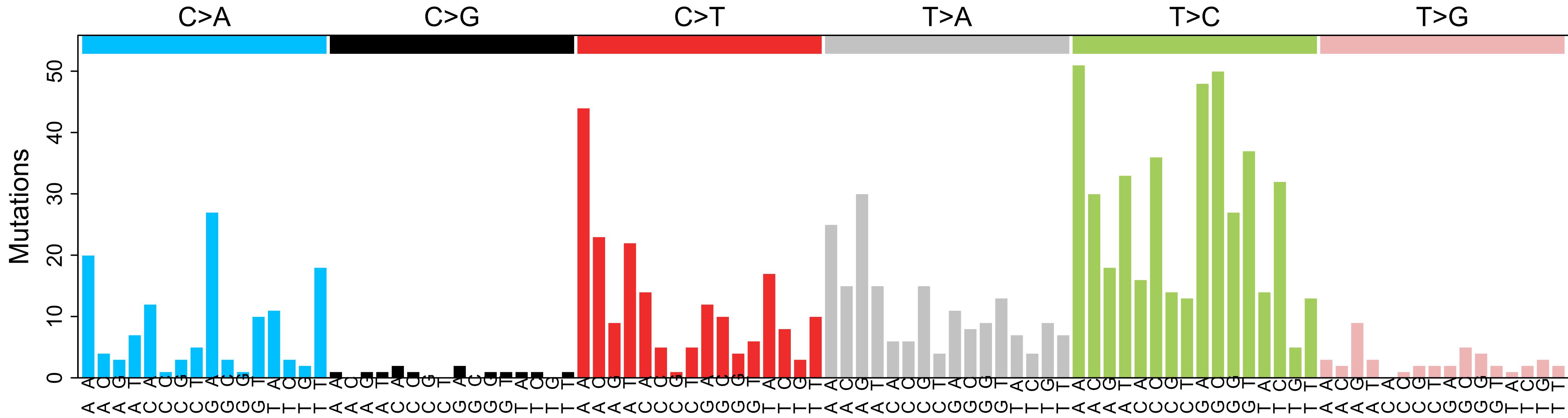
# mitomycin\_c\_1c3f32aa1d84 (995 mutations)



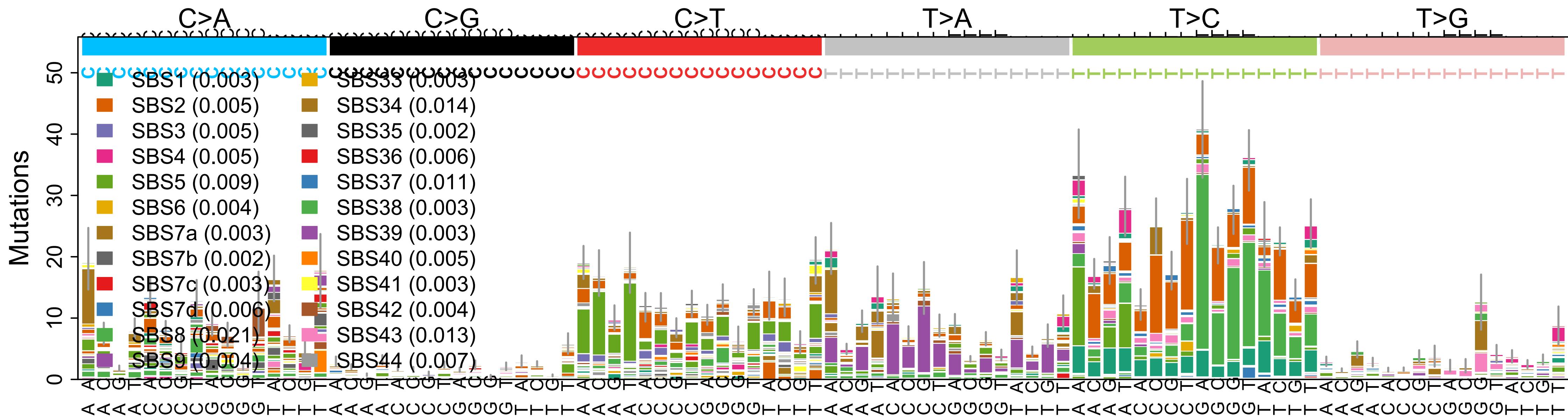
## Reconstructed spectrum (cosine similarity = 0.912)



# n\_ethyl\_n\_nitrosourea\_8164e08a22bc (1,000 mutations)



## Reconstructed spectrum (cosine similarity = 0.899)



# n\_methyl\_n\_nitro\_nitrosoguanidine\_9fbe0253d888 (999 mutations)

C>A

C>G

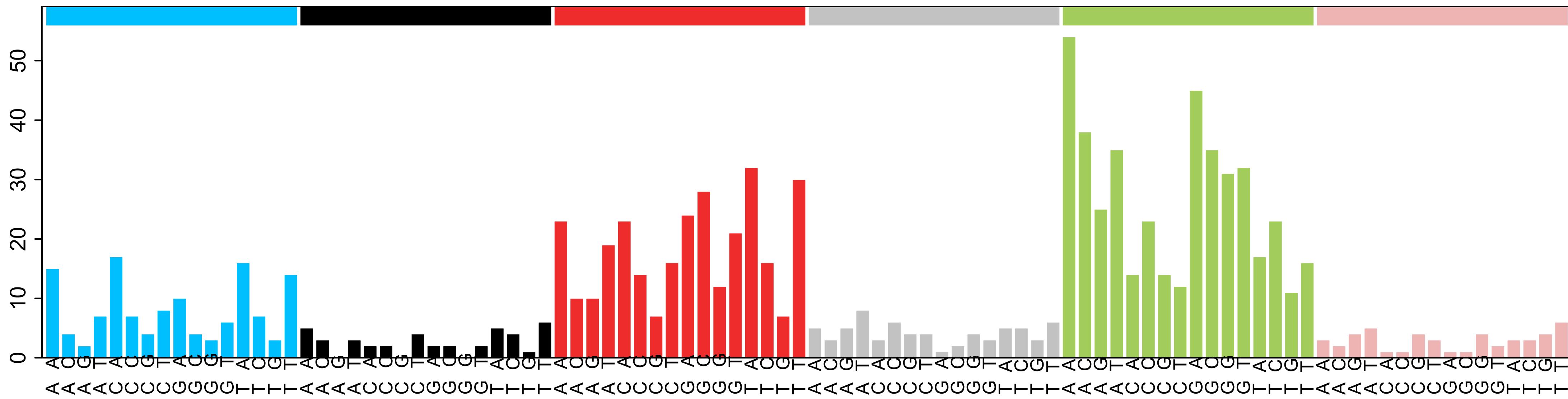
C>T

T>A

T>C

T>G

Mutations



Reconstructed spectrum (cosine similarity = 0.955)

C>A

C>G

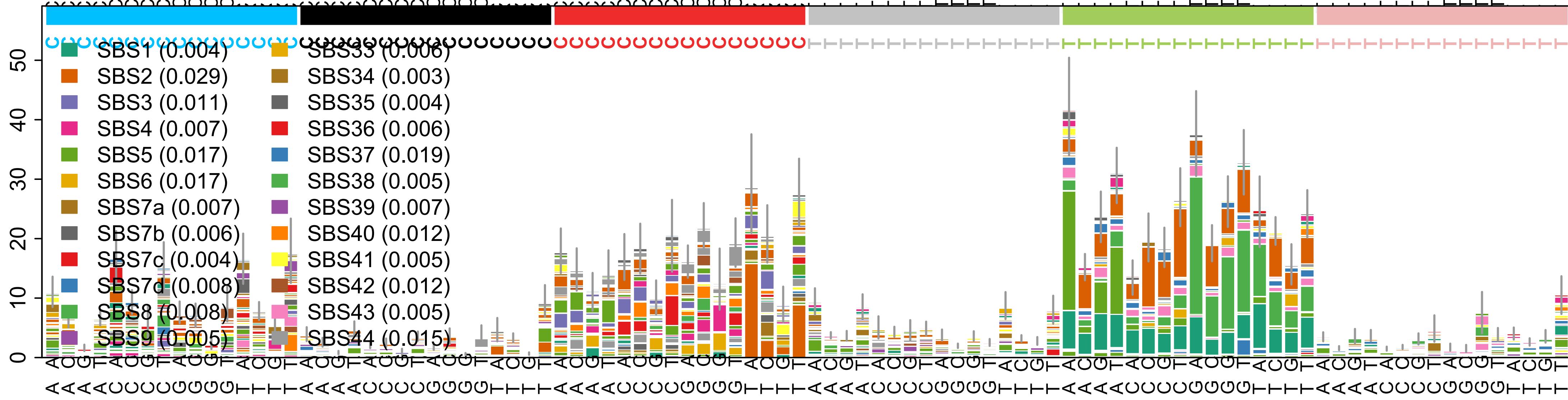
C>T

T>A

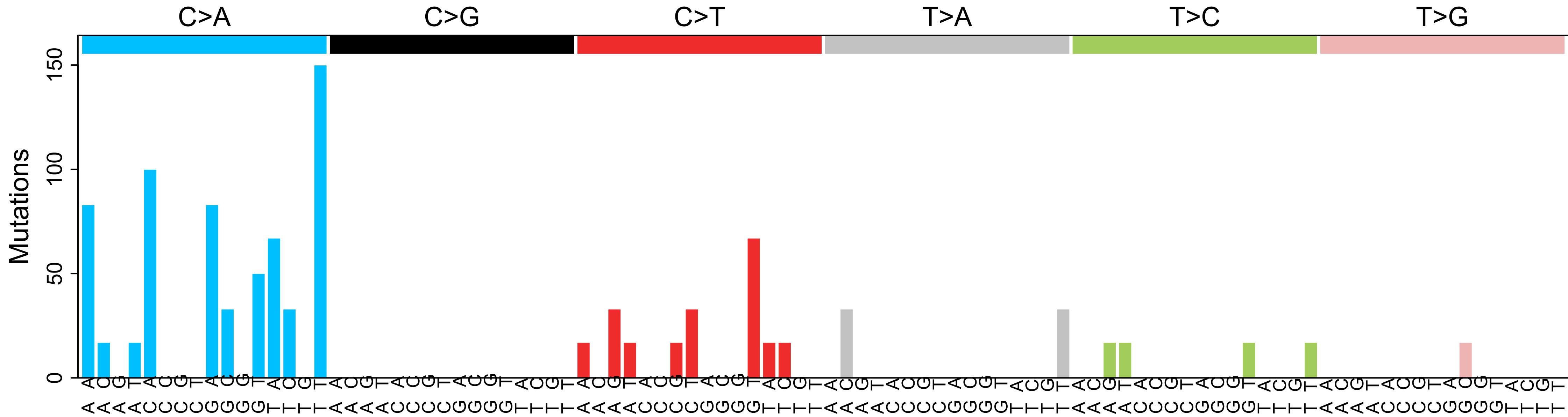
T>C

T>G

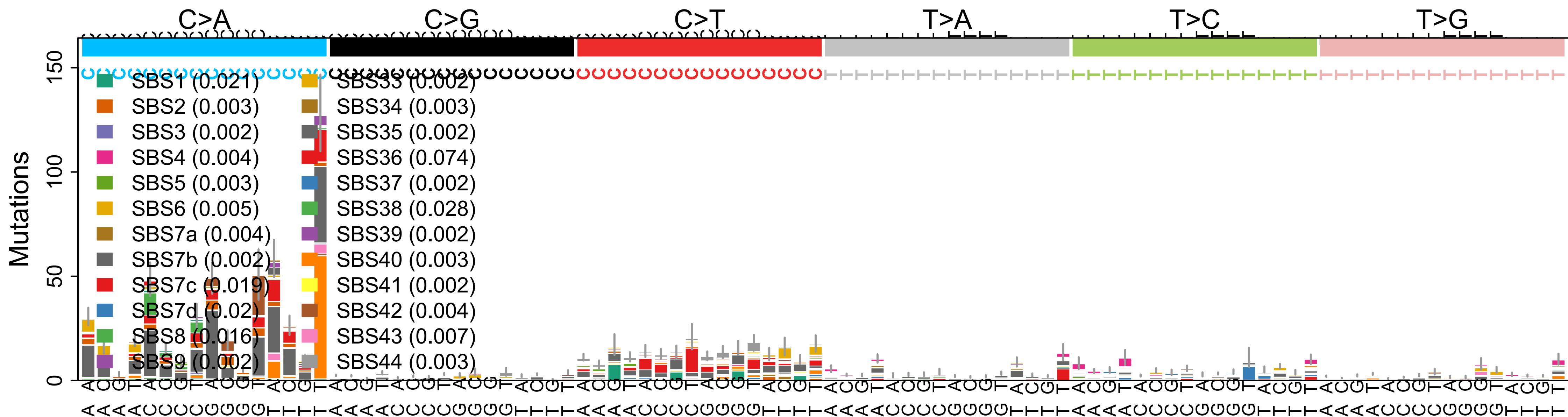
Mutations



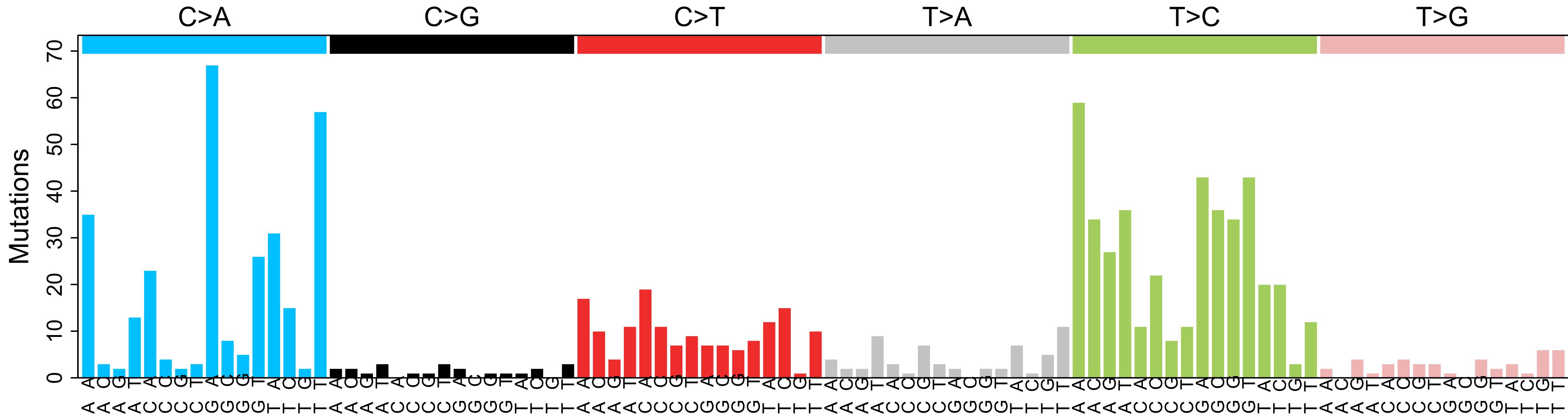
# n\_methyl\_n\_nitro\_nitrosoguanidine\_ca5b1ff8ee0d (1,002 mutations)



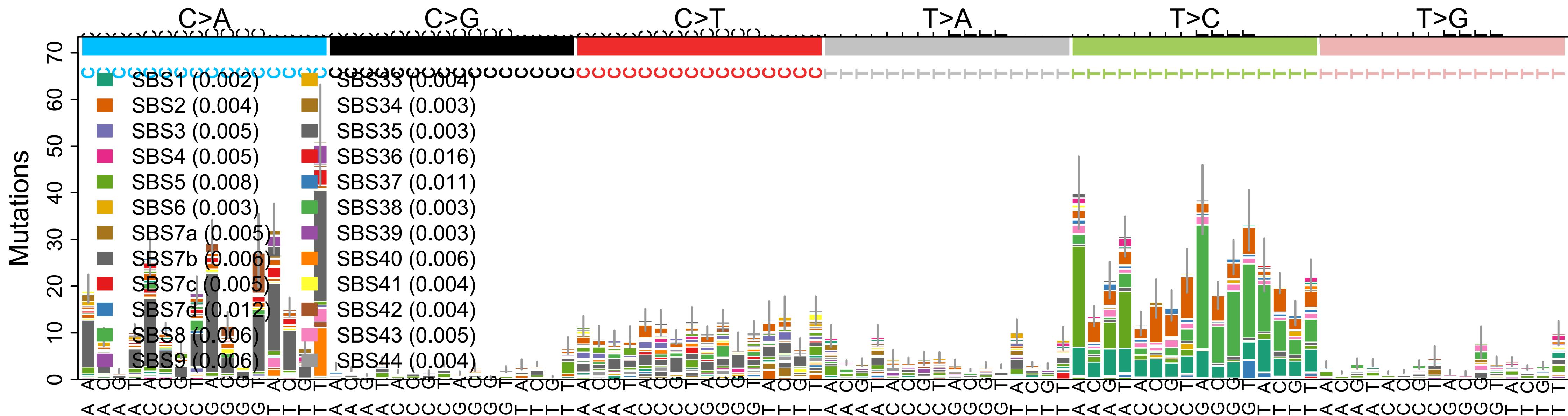
Reconstructed spectrum (cosine similarity = 0.891)



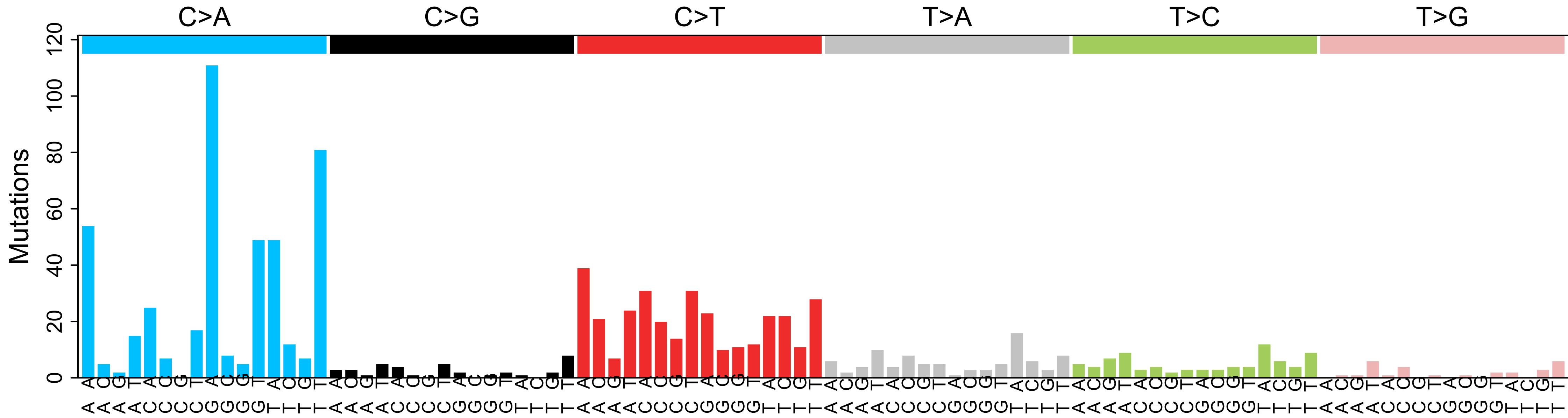
# n\_methyl\_n\_nitrosourea\_9a944873342f (996 mutations)



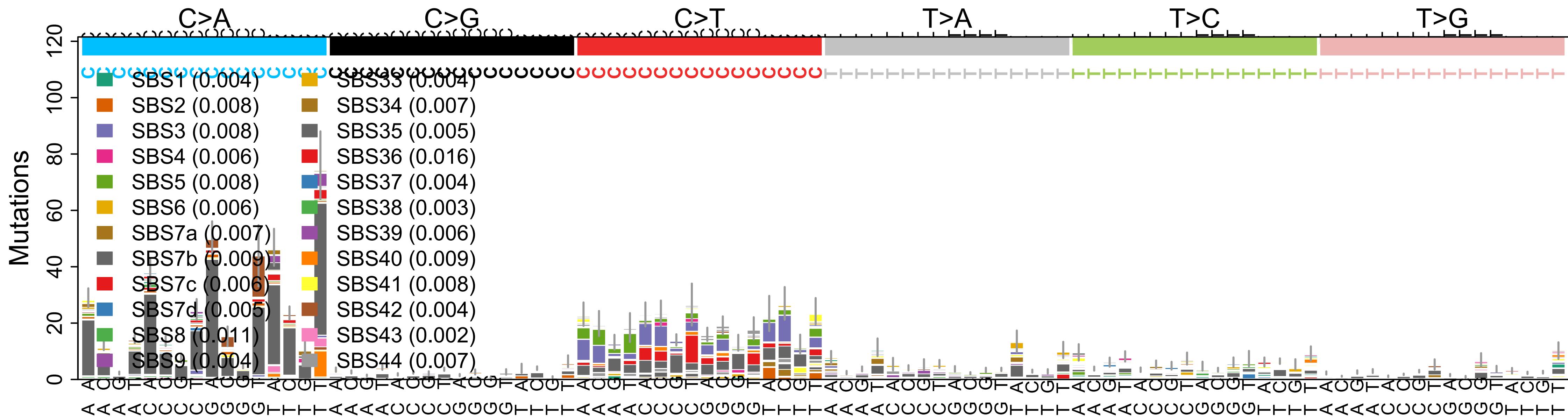
## Reconstructed spectrum (cosine similarity = 0.926)



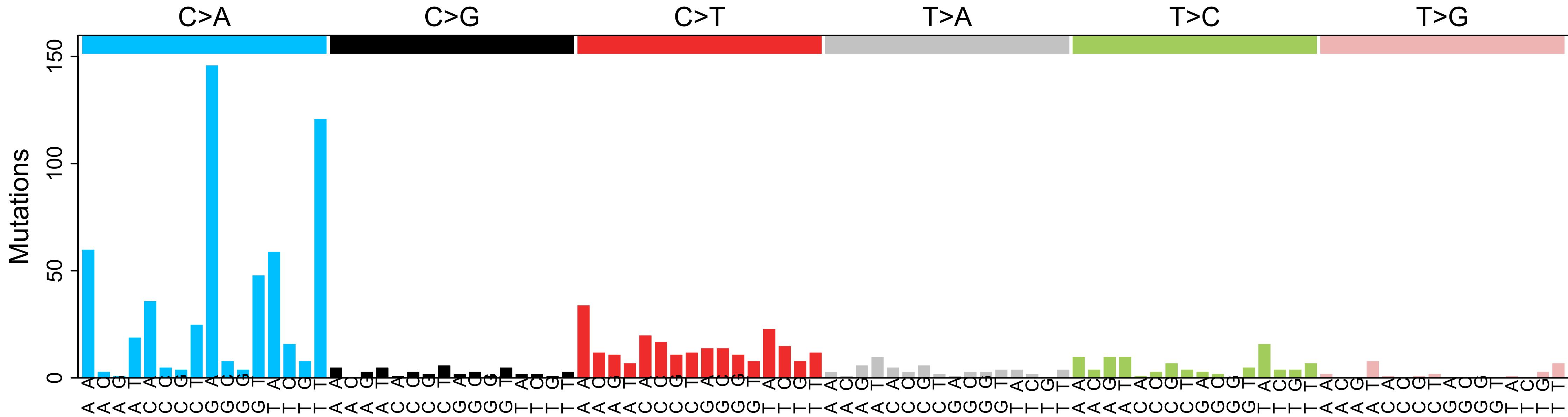
# n\_nitrosopyrrolidine\_ff630a9dde6d (1,010 mutations)



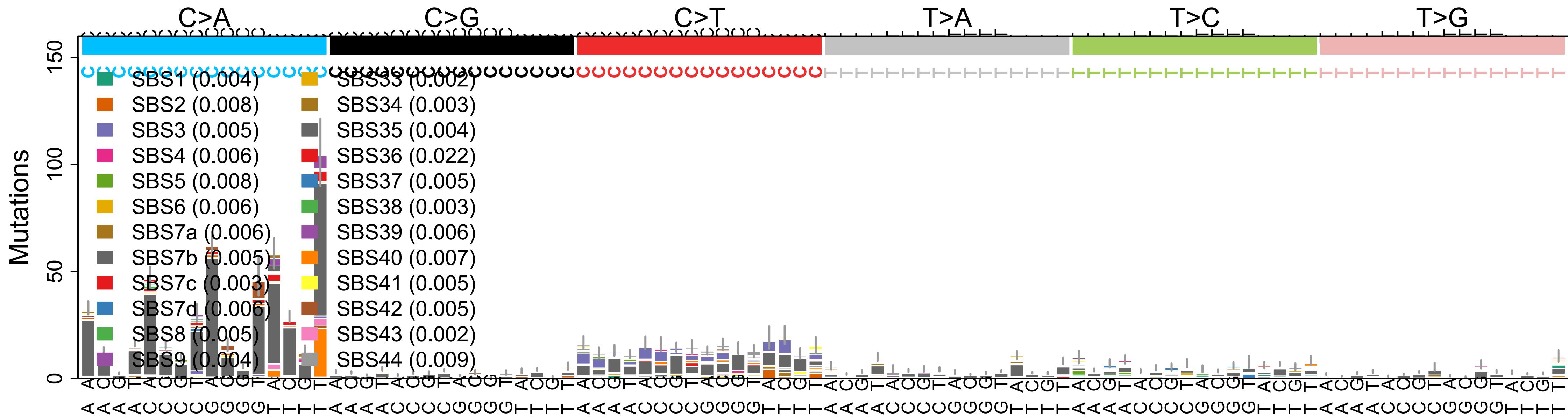
Reconstructed spectrum (cosine similarity = 0.923)



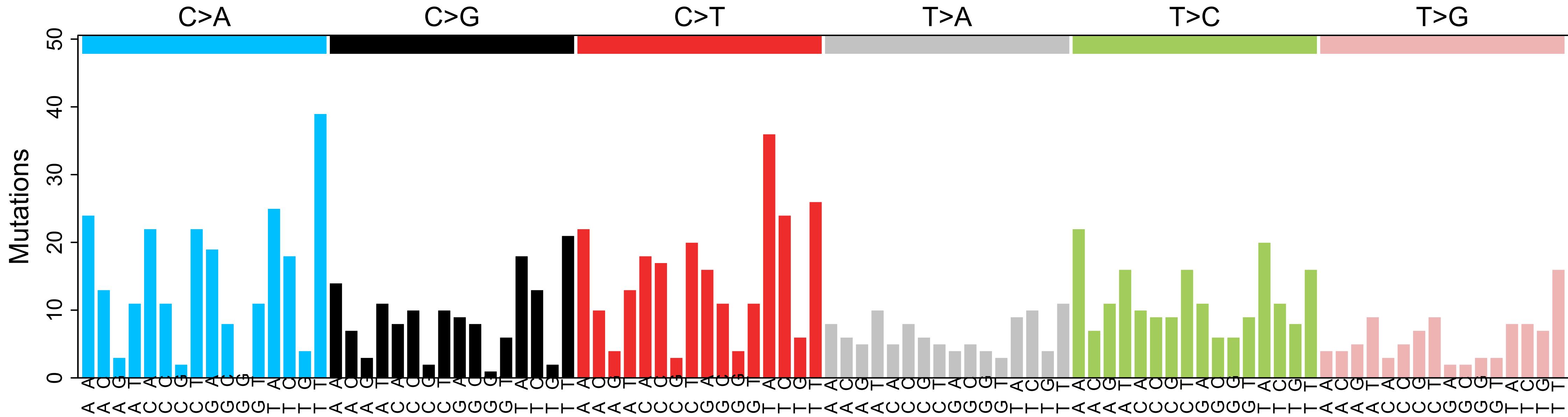
# nickel\_chloride\_70a11a6d19e0 (1,008 mutations)



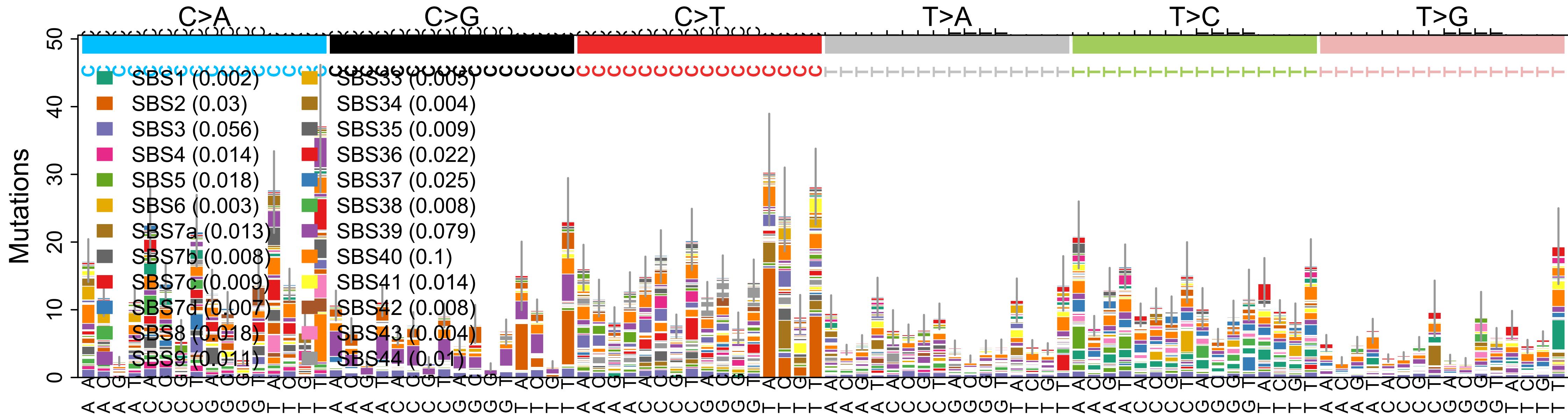
## Reconstructed spectrum (cosine similarity = 0.917)



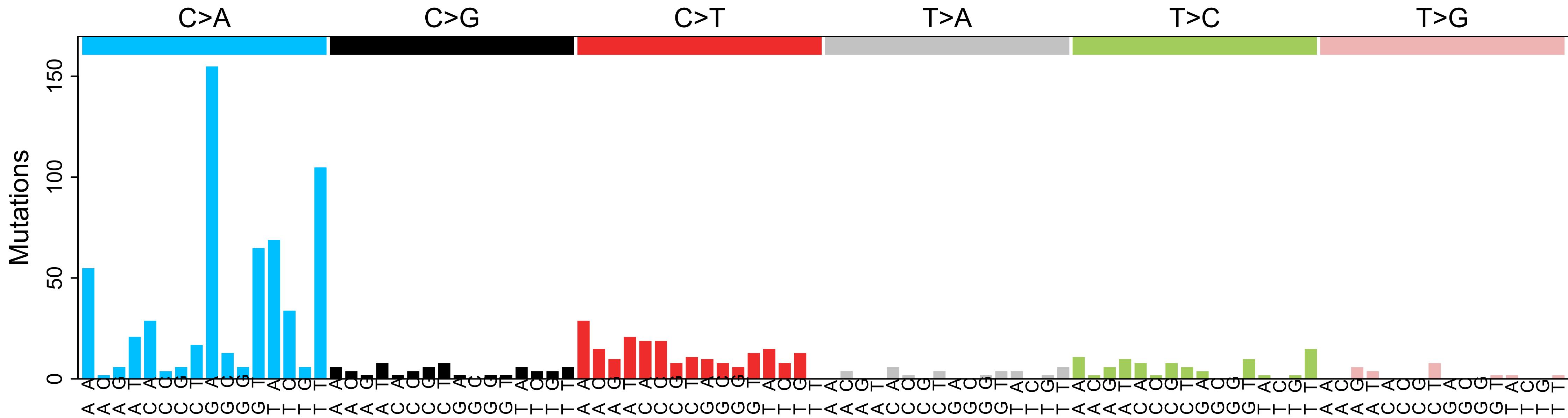
# no\_treatment\_290769de0f7a (1,001 mutations)



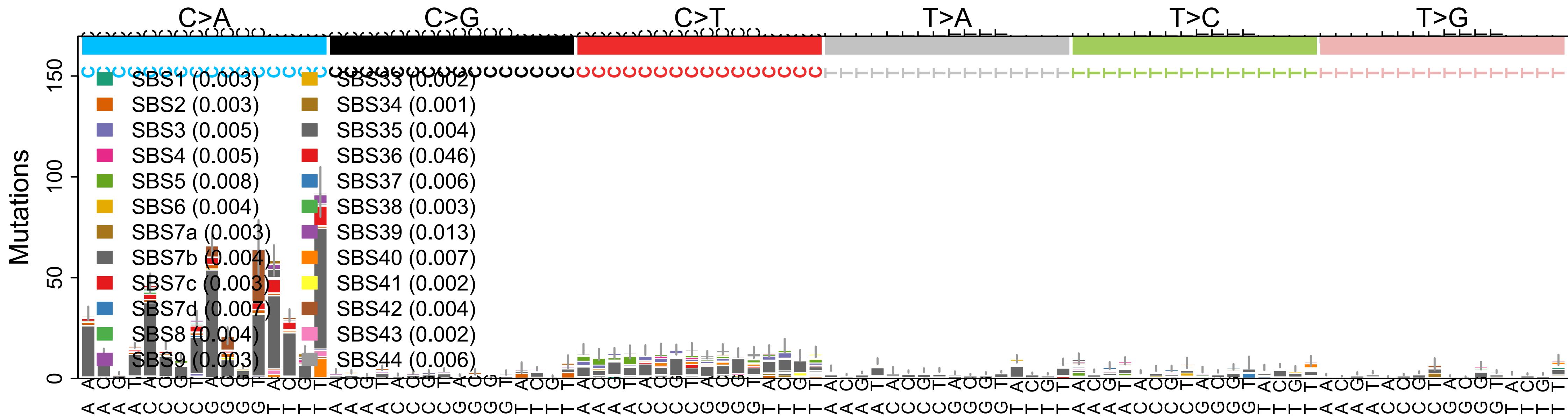
Reconstructed spectrum (cosine similarity = 0.979)



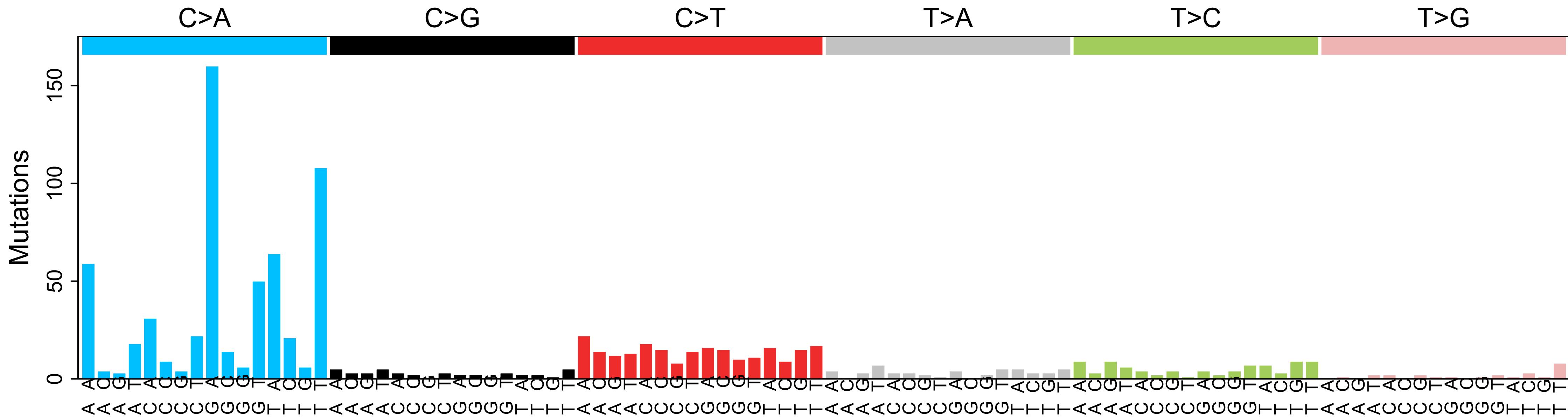
# no\_treatment\_2d9081e4d720 (1,008 mutations)



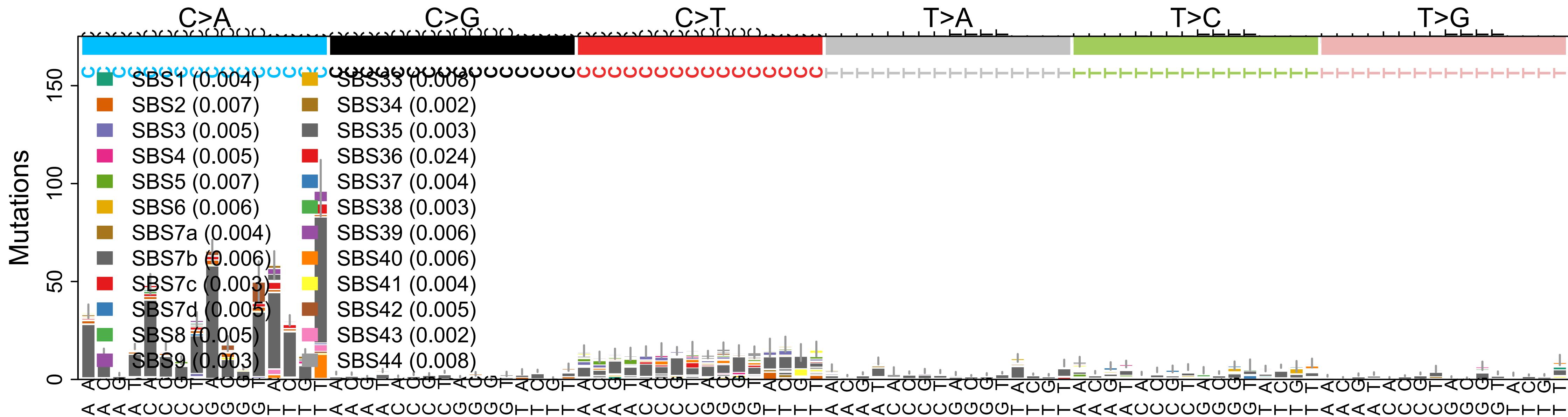
## Reconstructed spectrum (cosine similarity = 0.908)



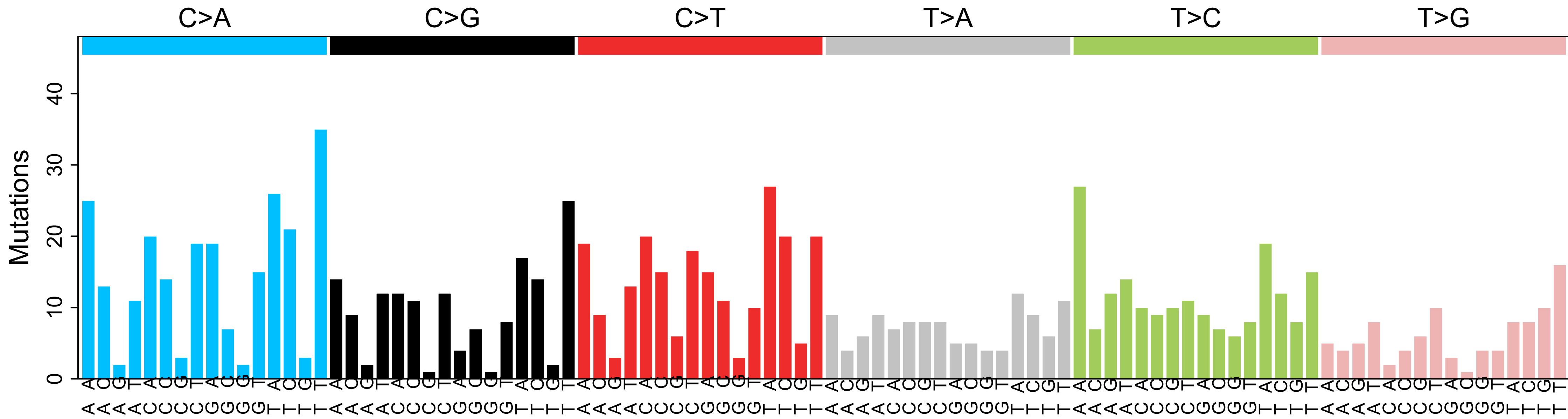
# no\_treatment\_368d8667e685 (1,004 mutations)



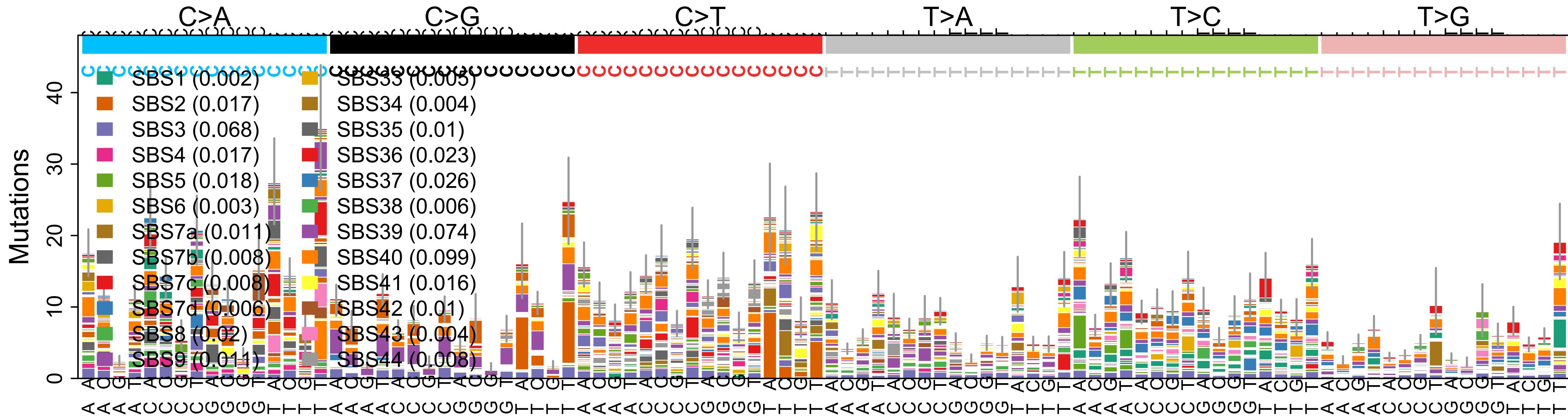
## Reconstructed spectrum (cosine similarity = 0.907)



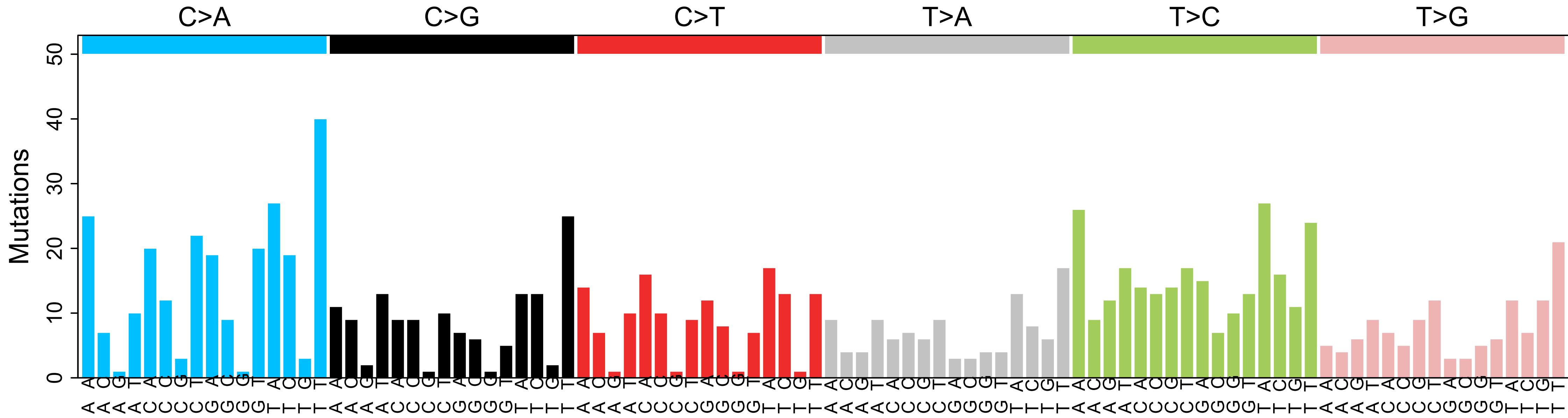
# no\_treatment\_843a6aaaecfd (997 mutations)



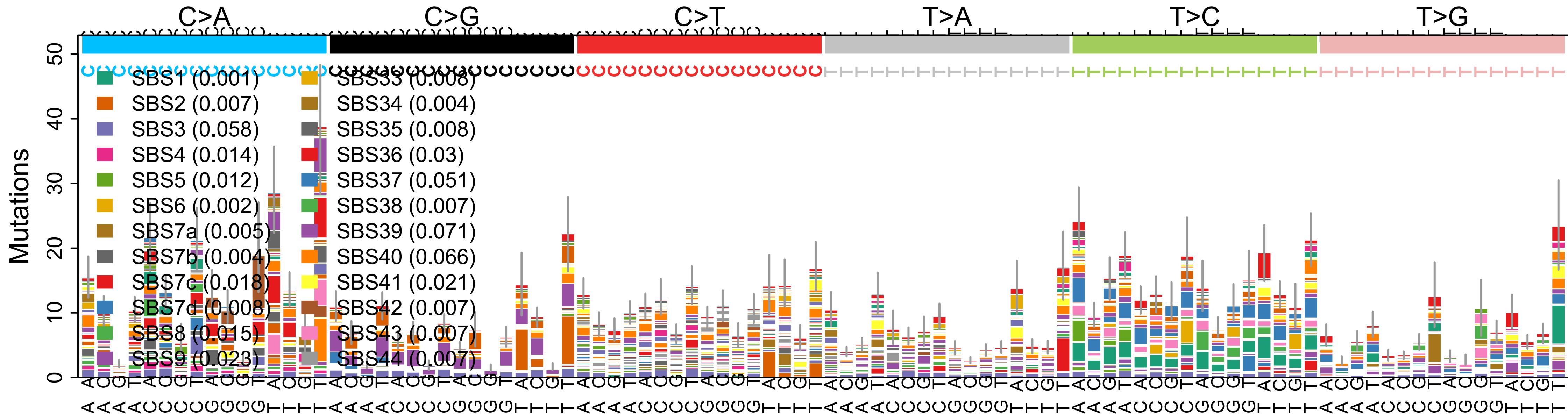
**Reconstructed spectrum (cosine similarity = 0.978)**



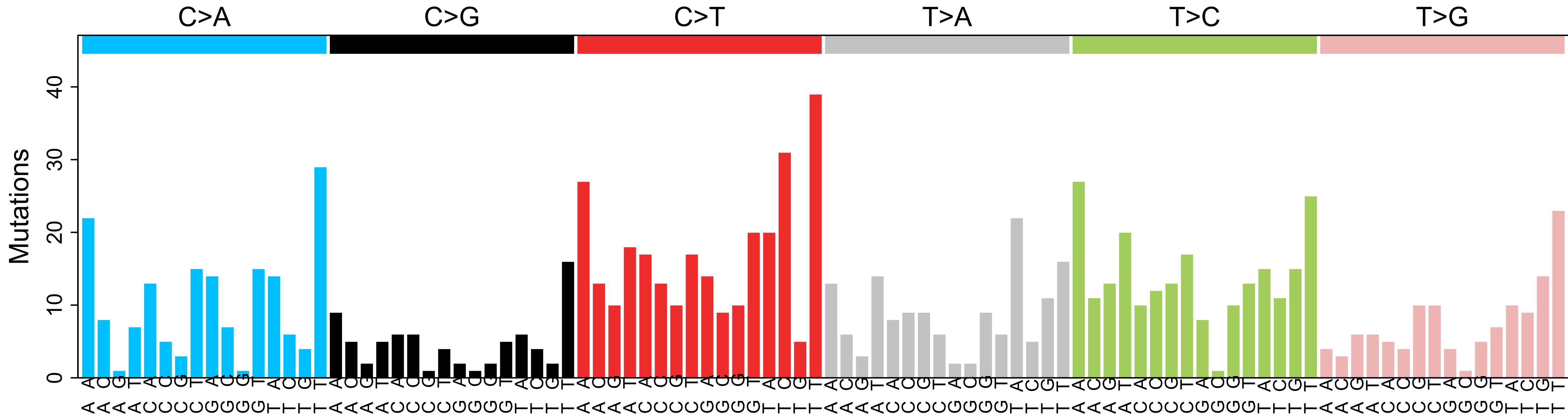
# no\_treatment\_a4b5192aa59c (997 mutations)



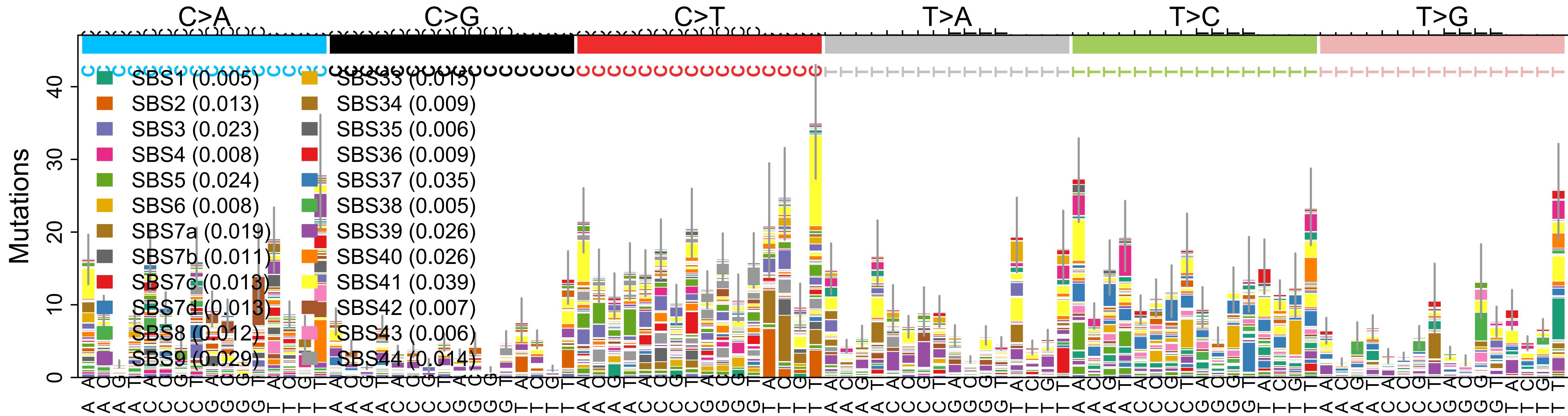
## Reconstructed spectrum (cosine similarity = 0.975)



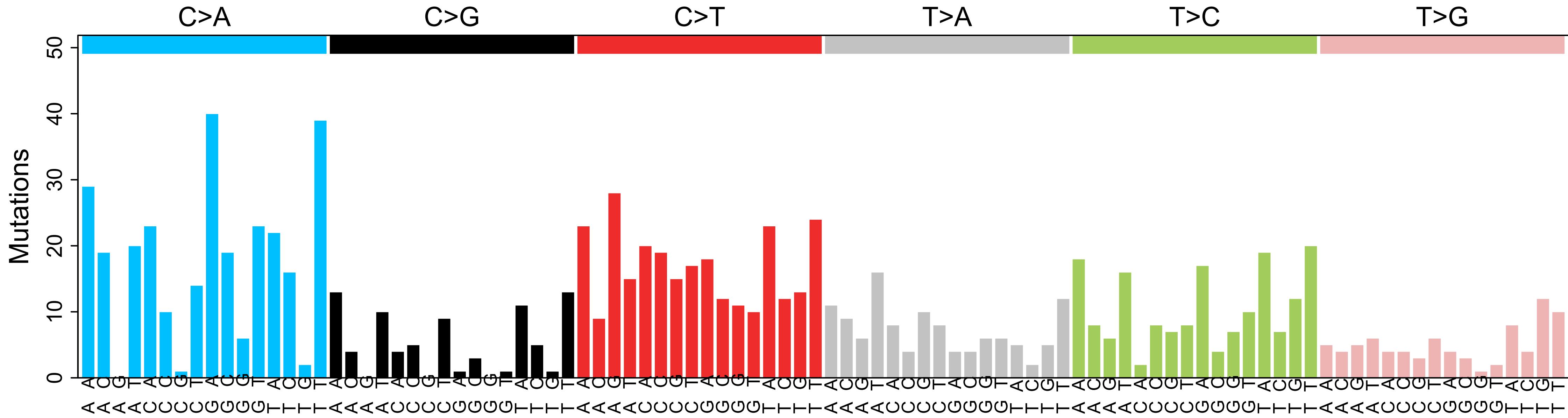
# no\_treatment\_e484b30b812e (996 mutations)



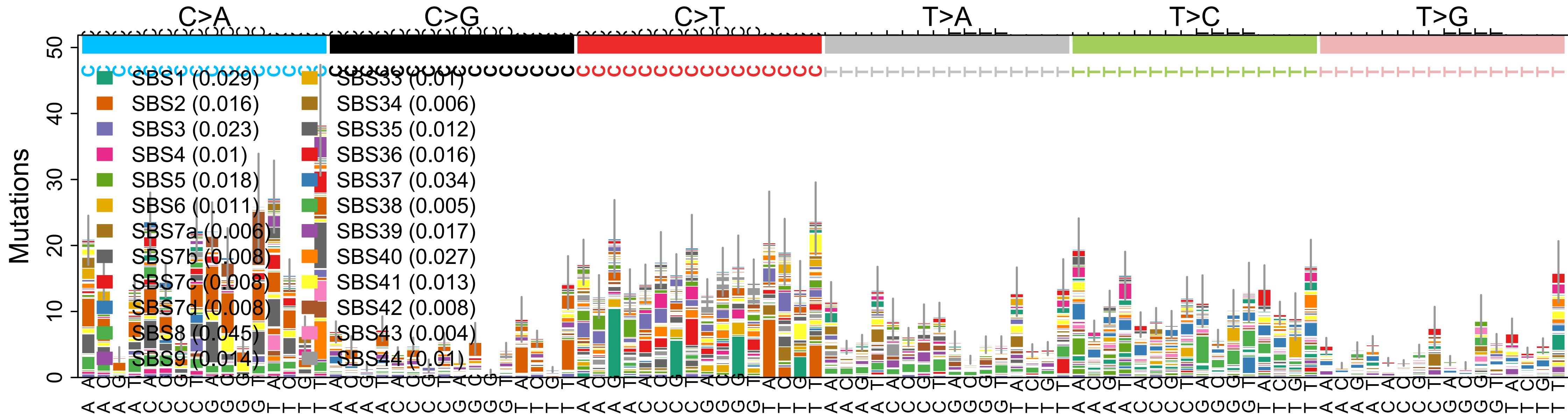
**Reconstructed spectrum (cosine similarity = 0.976)**



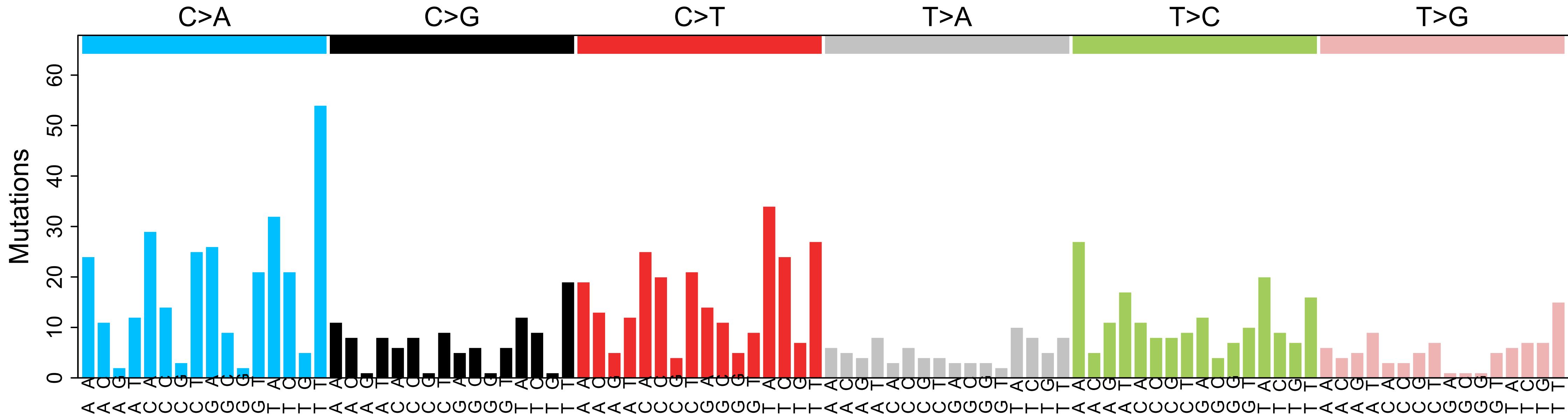
# no\_treatment\_e638523fc587 (998 mutations)



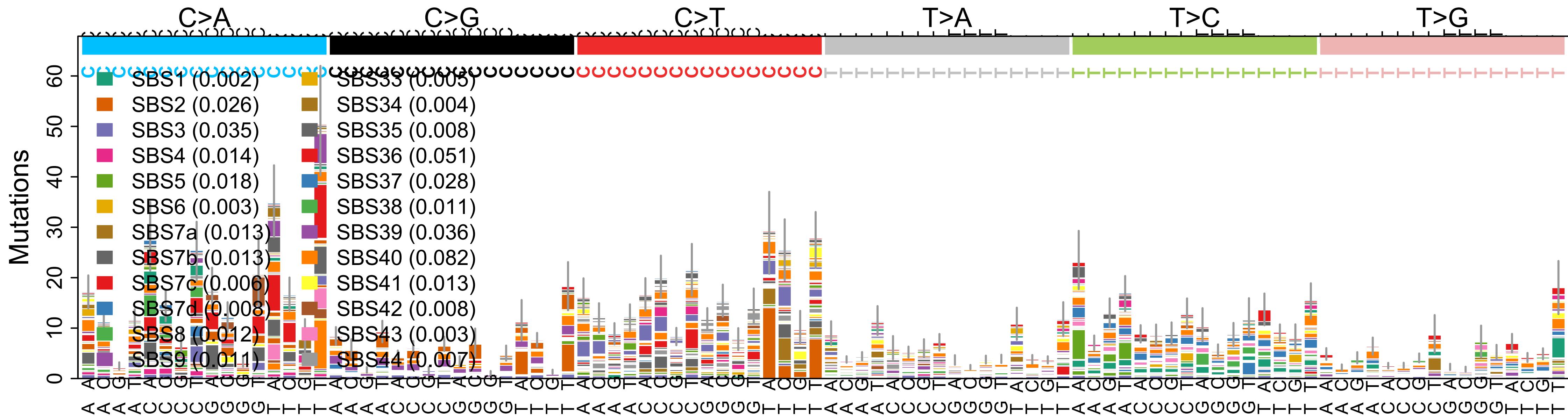
**Reconstructed spectrum (cosine similarity = 0.955)**



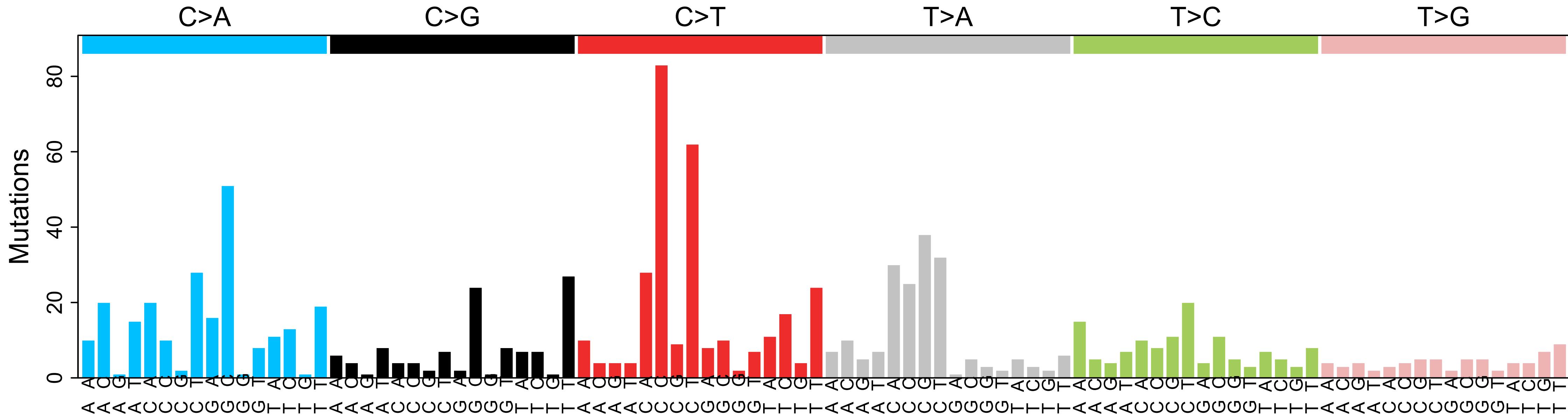
# no\_treatment\_eaf67f5b8560 (999 mutations)



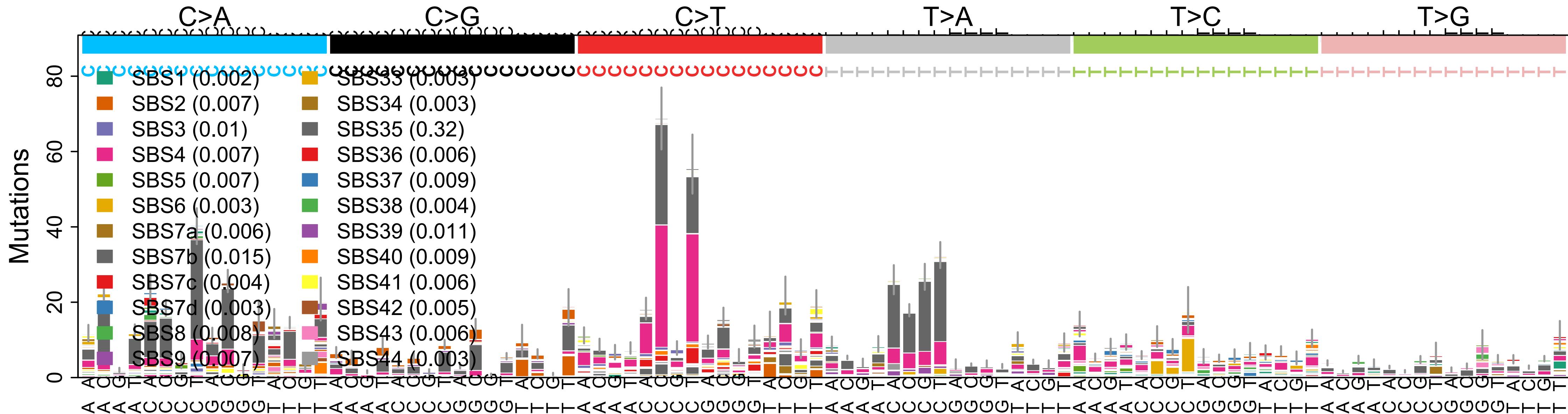
**Reconstructed spectrum (cosine similarity = 0.981)**



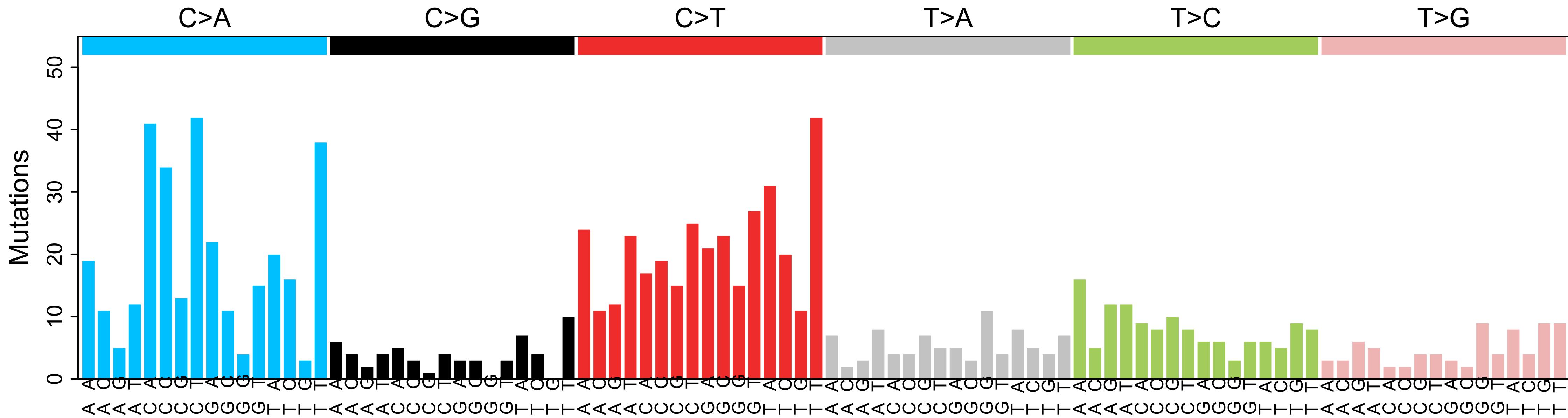
# no\_treatment\_f9c3354b9596 (1,001 mutations)



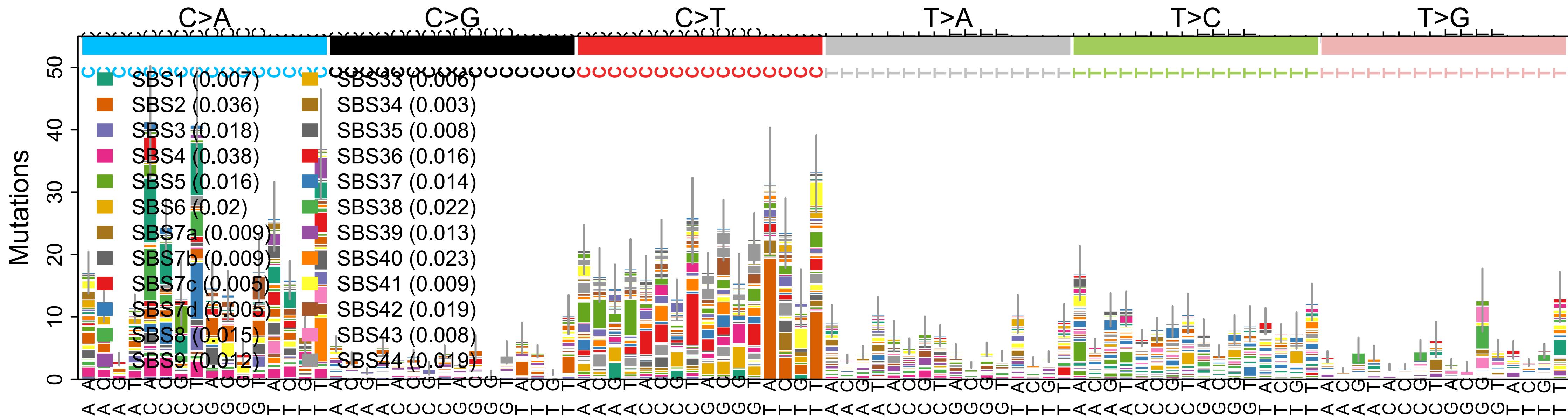
Reconstructed spectrum (cosine similarity = 0.96)



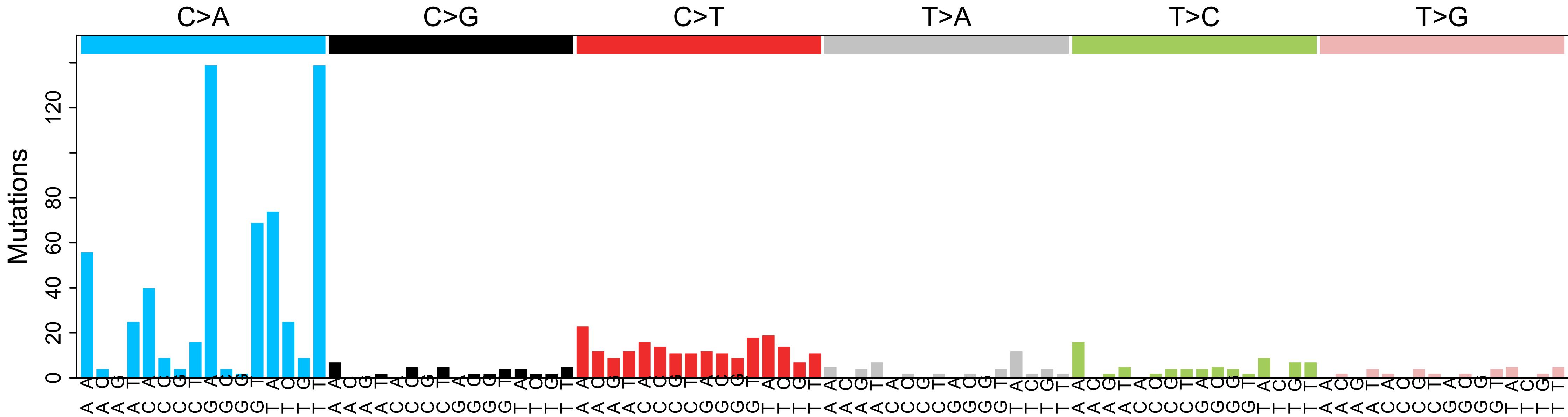
# norharmane\_84d4977cc253 (994 mutations)



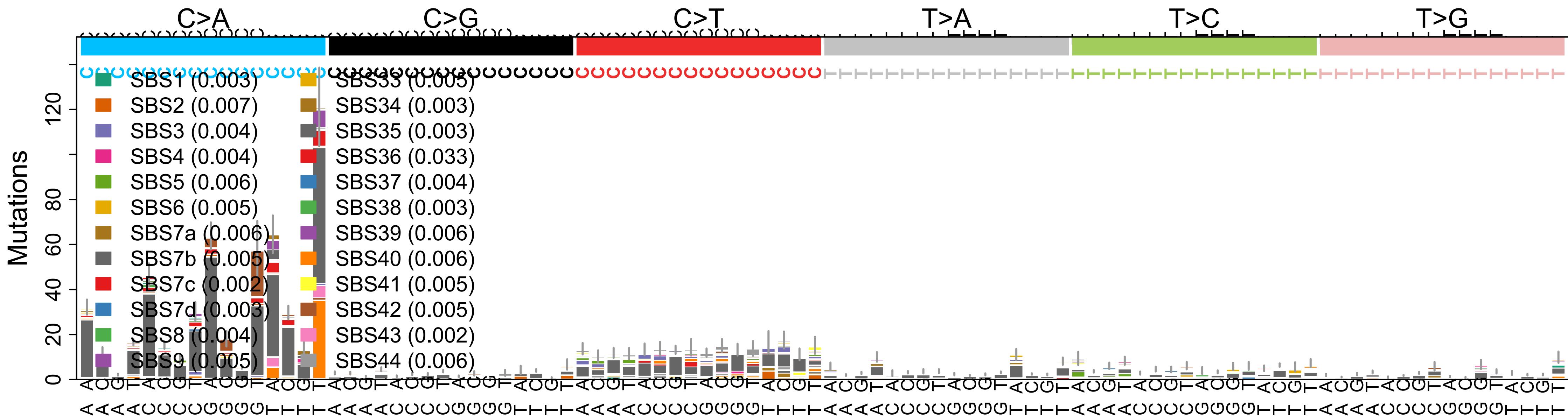
Reconstructed spectrum (cosine similarity = 0.982)



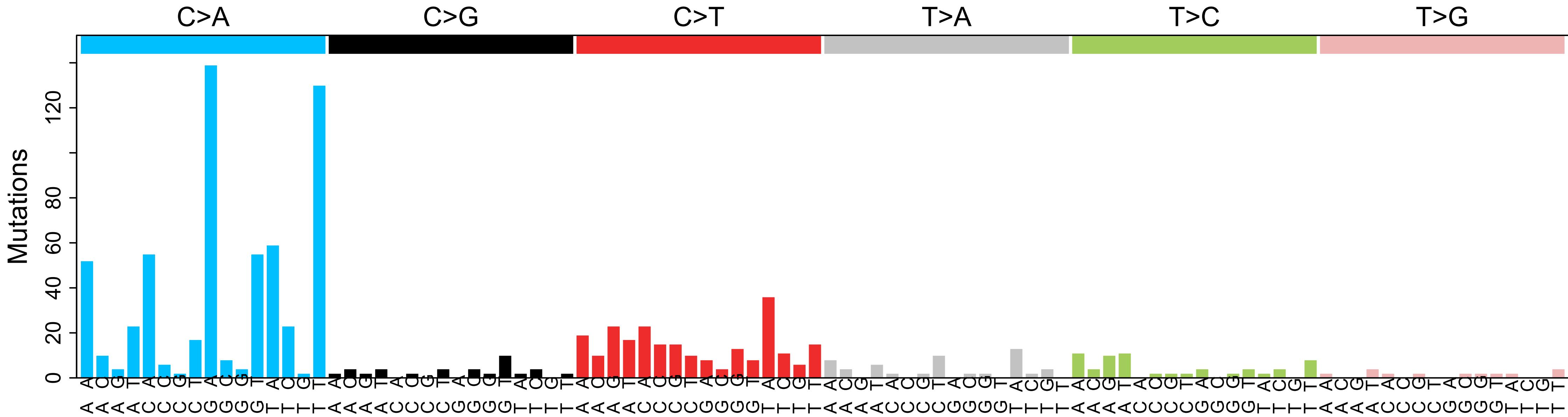
# *o\_anisidine\_140b3b7221ca* (1,013 mutations)



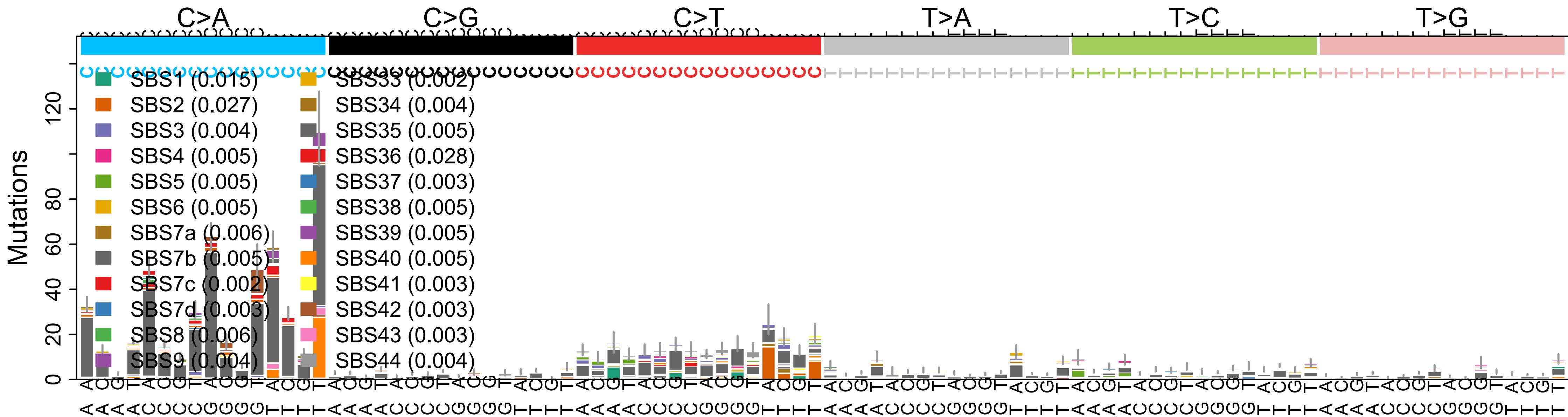
Reconstructed spectrum (cosine similarity = 0.941)



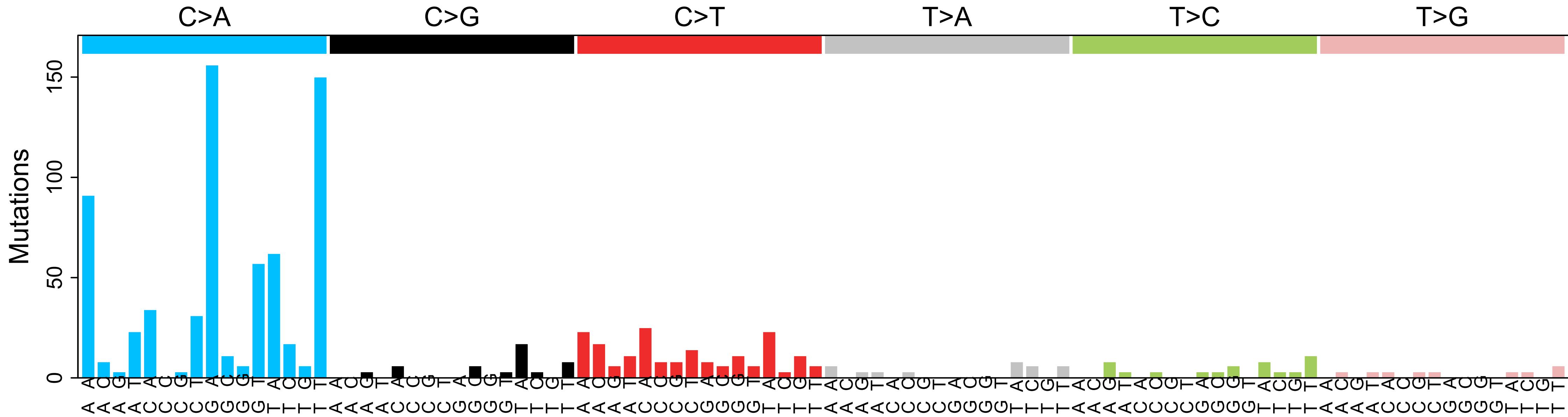
# *o\_anisidine\_9552a08d7147* (1,007 mutations)



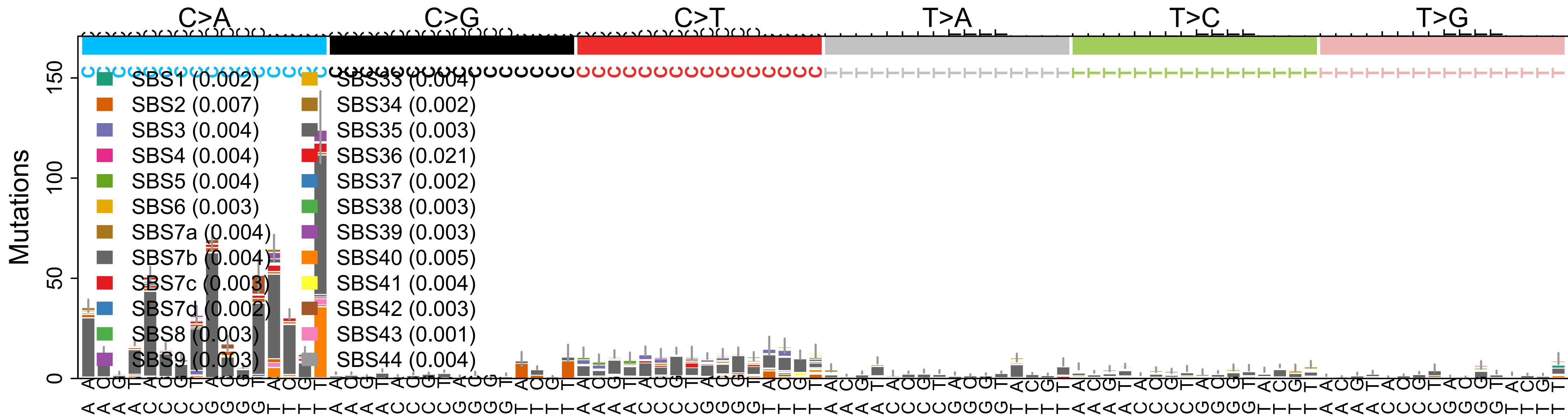
Reconstructed spectrum (cosine similarity = 0.938)



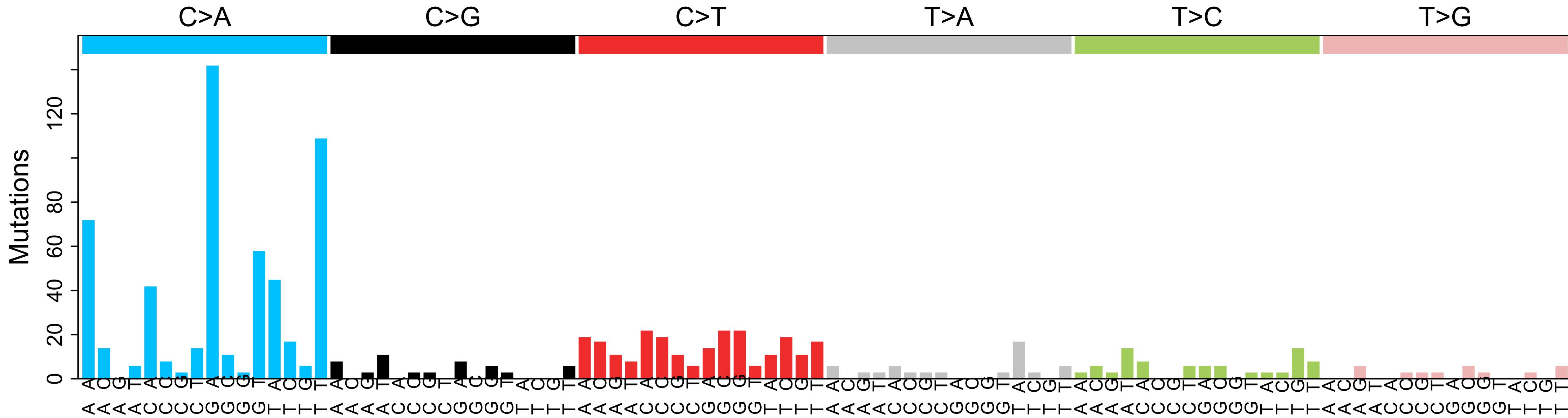
# **o\_toluidine\_0d620c5f38d0 (1,003 mutations)**



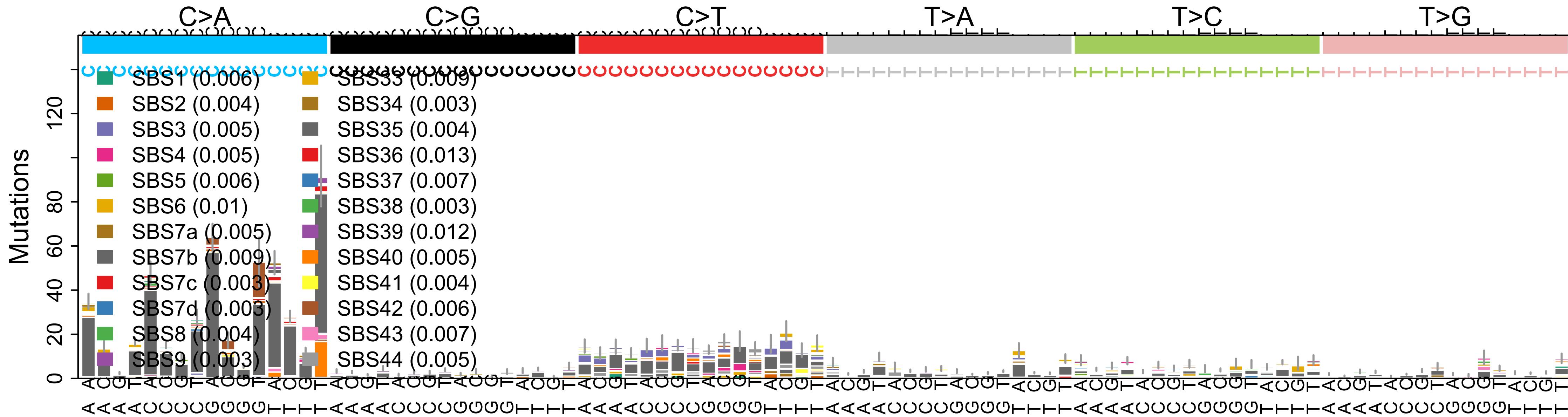
## Reconstructed spectrum (cosine similarity = 0.914)



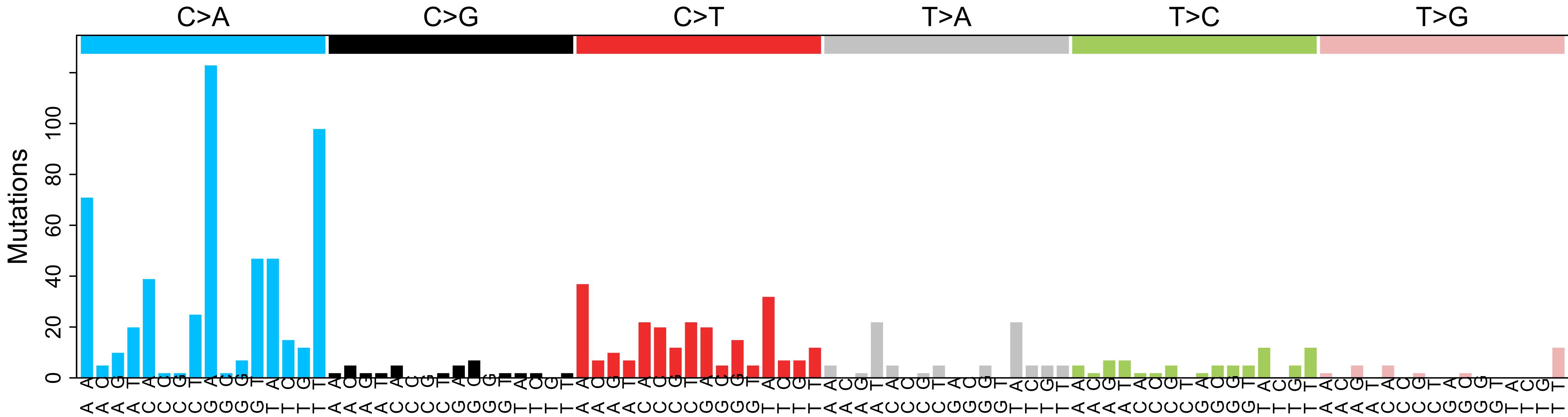
# ochratoxin\_a\_9b5acc8297cd (1,008 mutations)



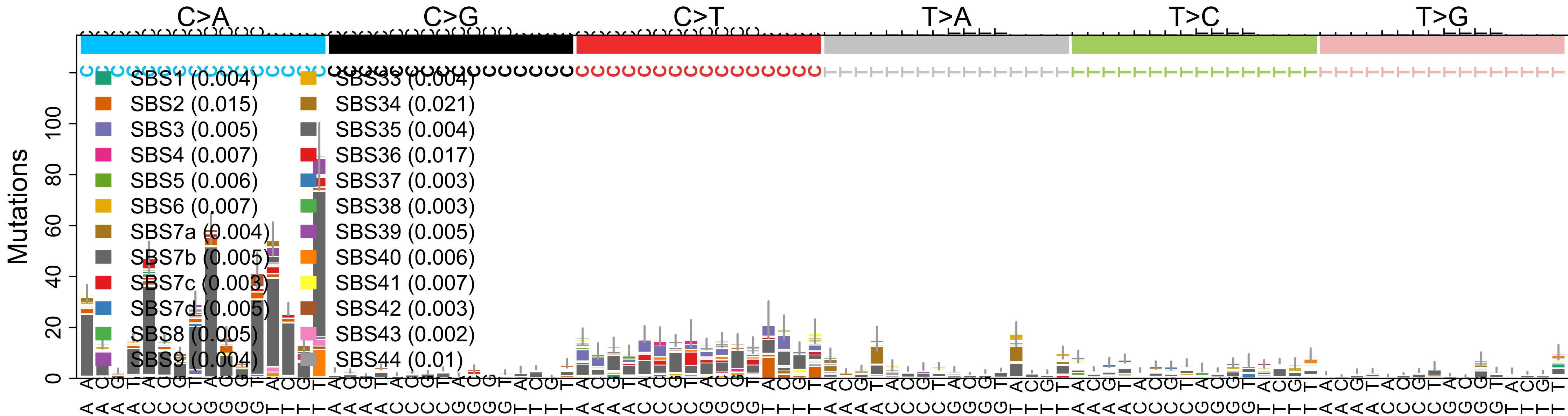
Reconstructed spectrum (cosine similarity = 0.914)



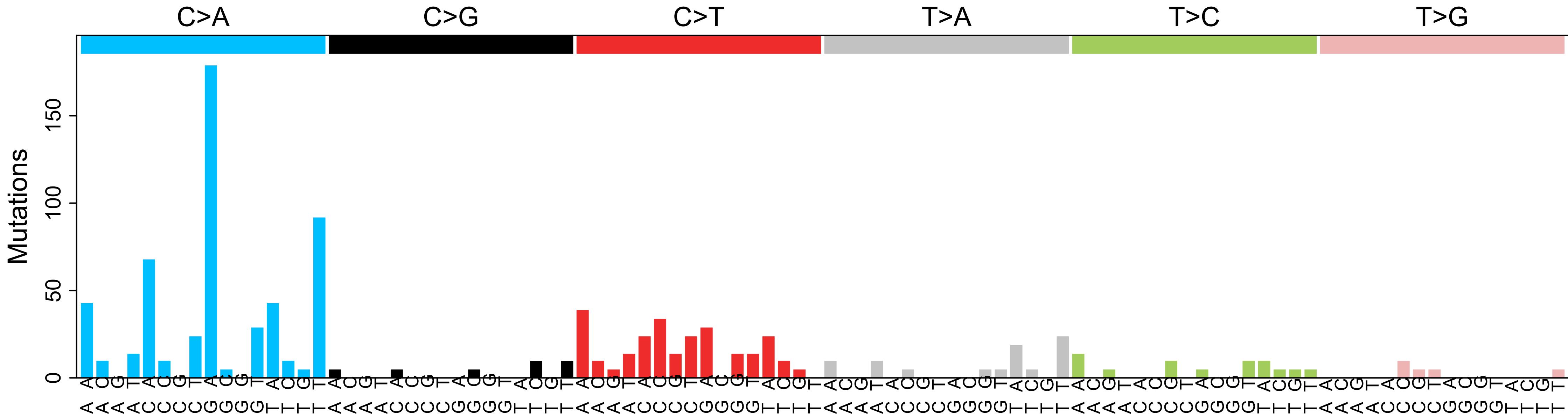
# olaparib\_43d725f7cc82 (990 mutations)



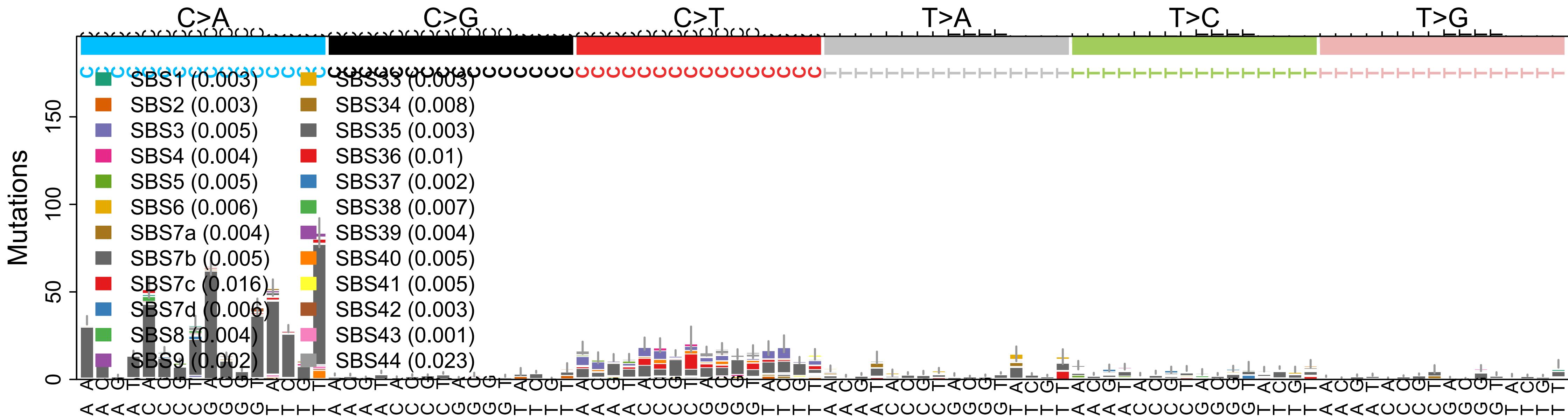
**Reconstructed spectrum (cosine similarity = 0.91)**



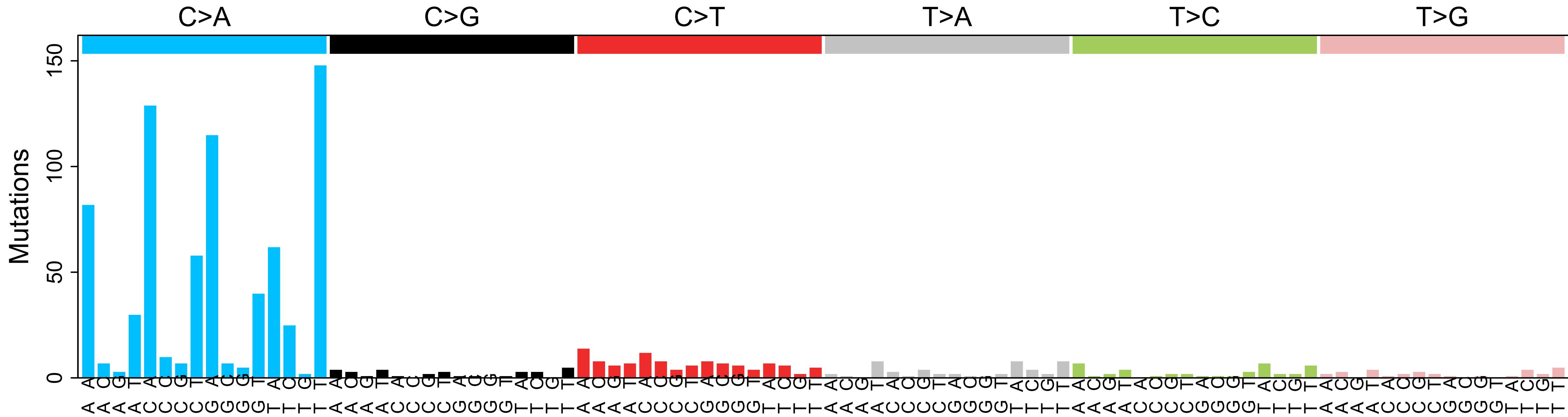
# peroxynitrite\_7cadeaf3e612 (1,004 mutations)



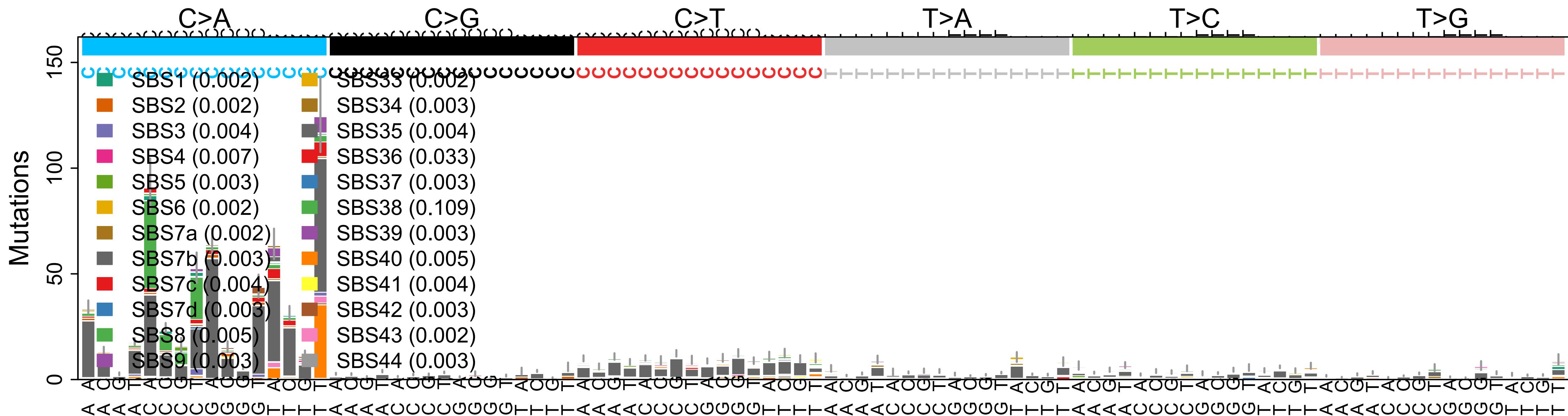
Reconstructed spectrum (cosine similarity = 0.864)



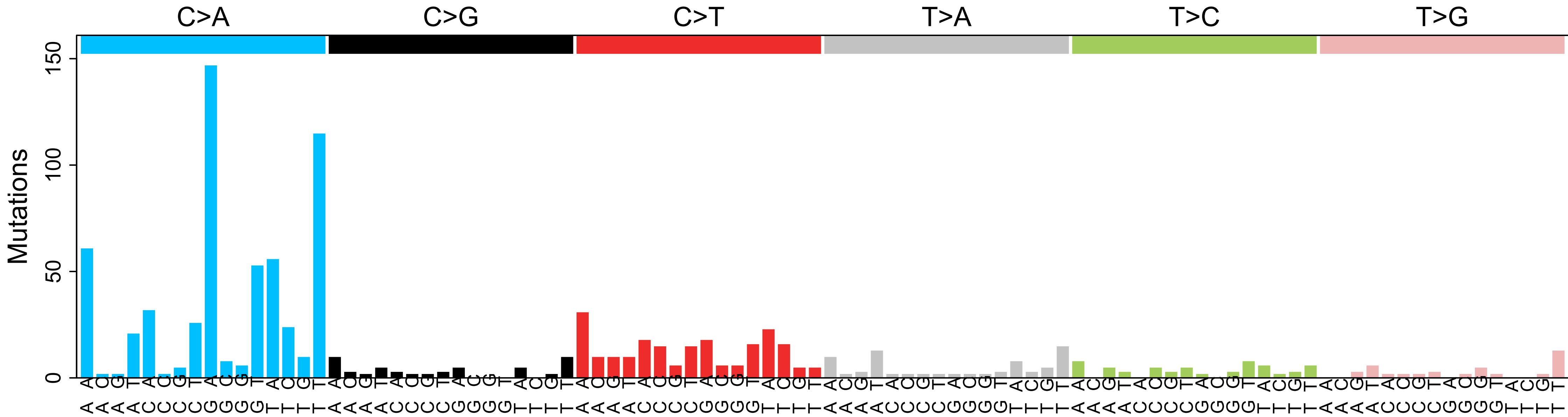
# potassium\_bromate\_69b10ec2b4fd (994 mutations)



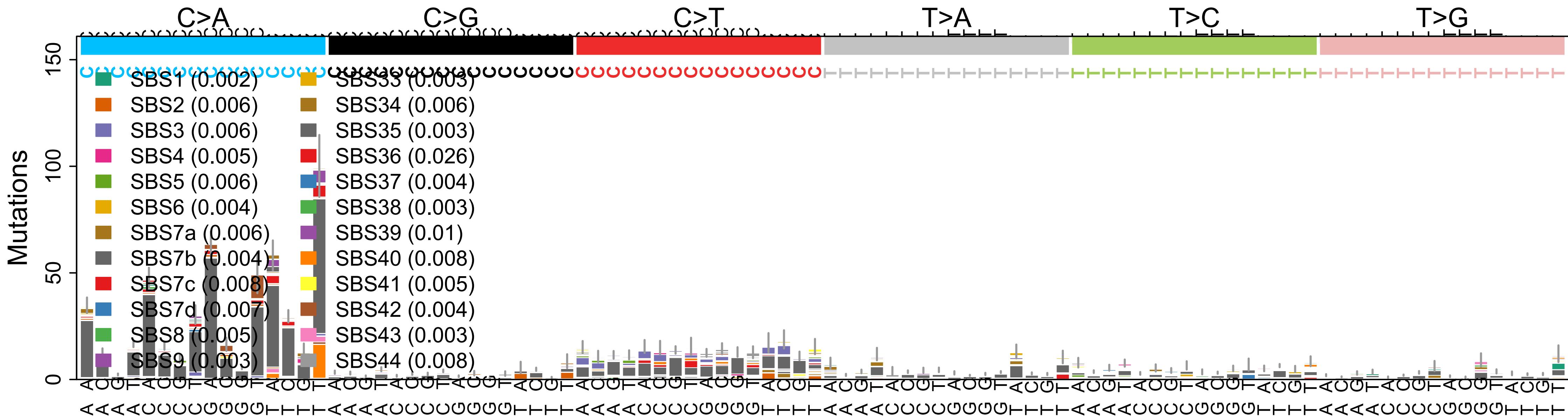
## Reconstructed spectrum (cosine similarity = 0.956)



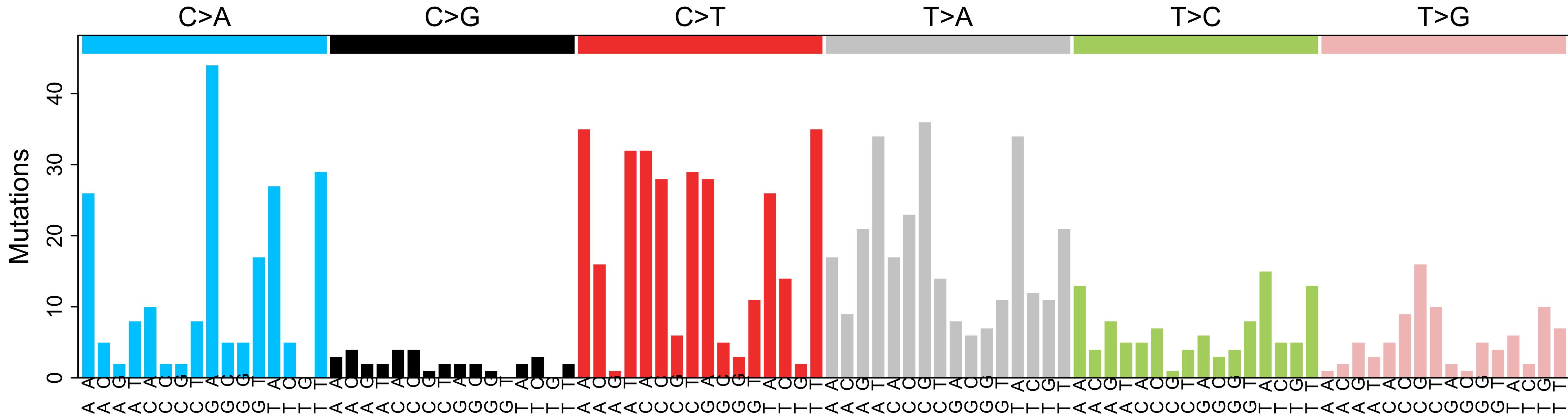
# potassium\_chromate\_0bdc1b5144e0 (1,009 mutations)



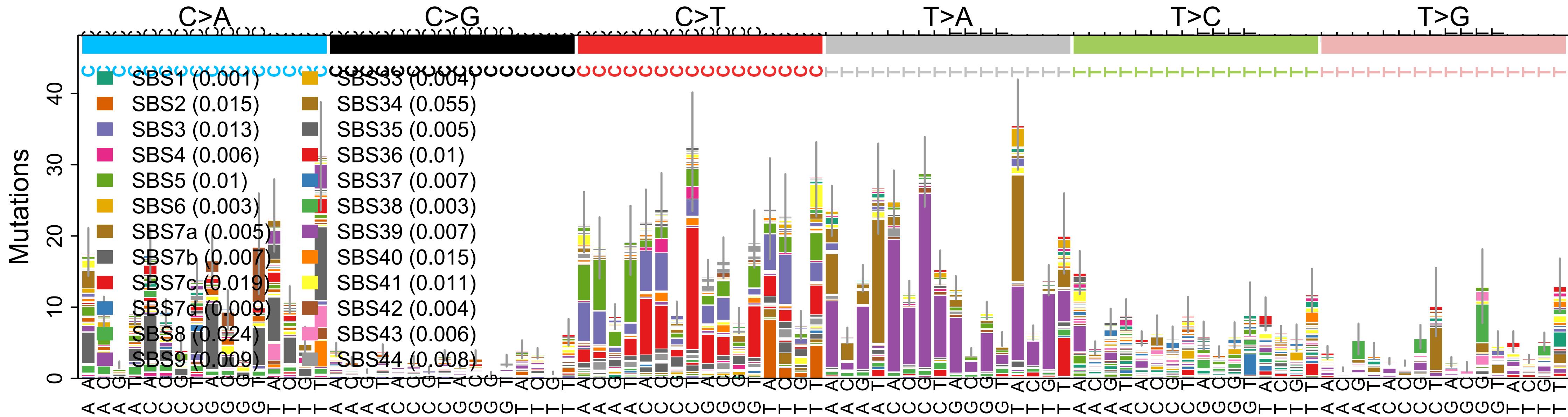
Reconstructed spectrum (cosine similarity = 0.916)



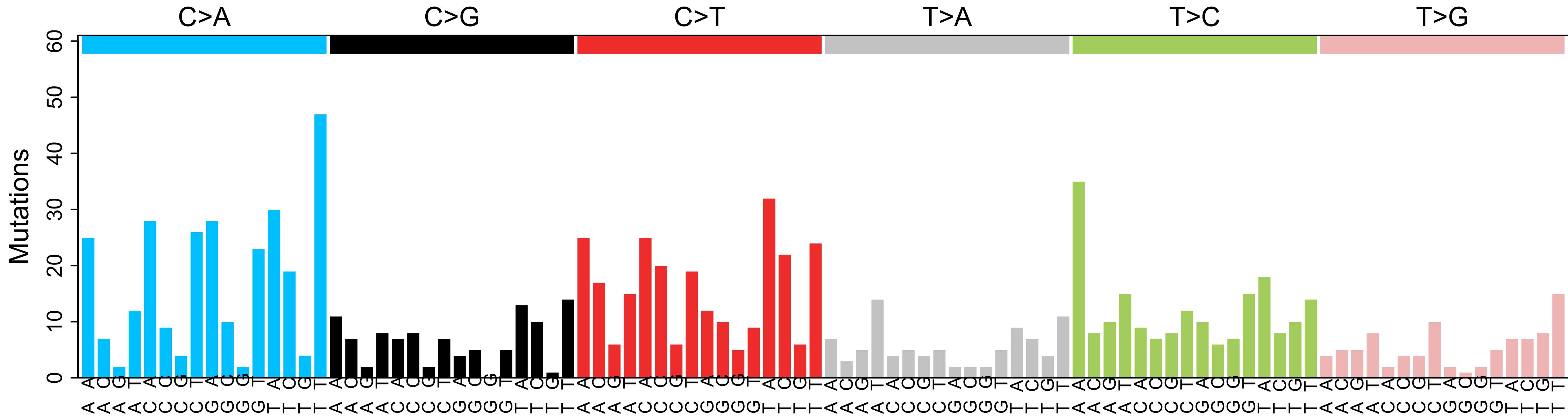
# propylene\_oxide\_7197becf3bd8 (1,007 mutations)



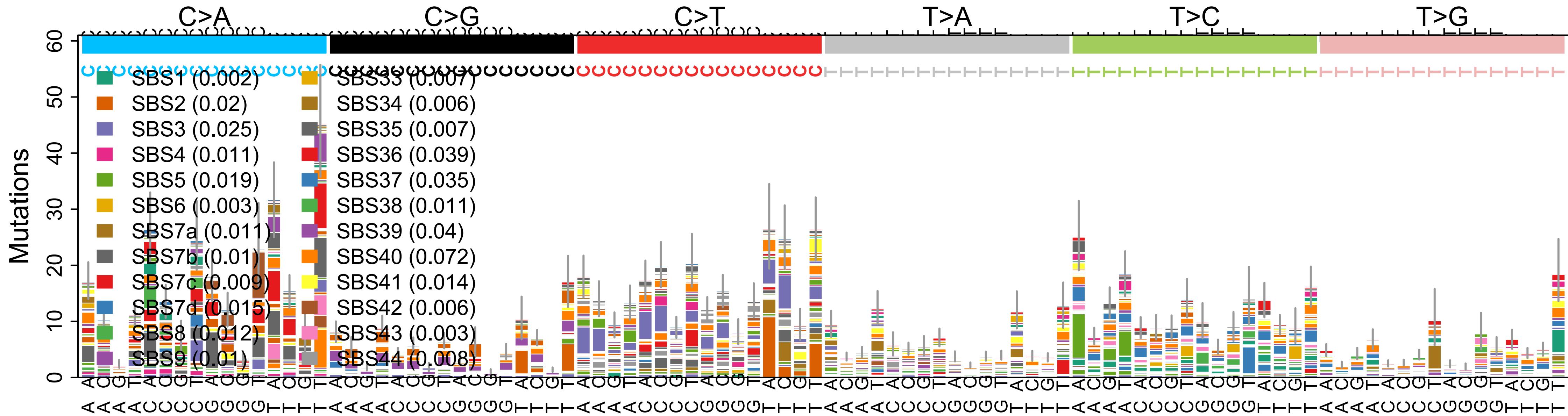
## Reconstructed spectrum (cosine similarity = 0.923)



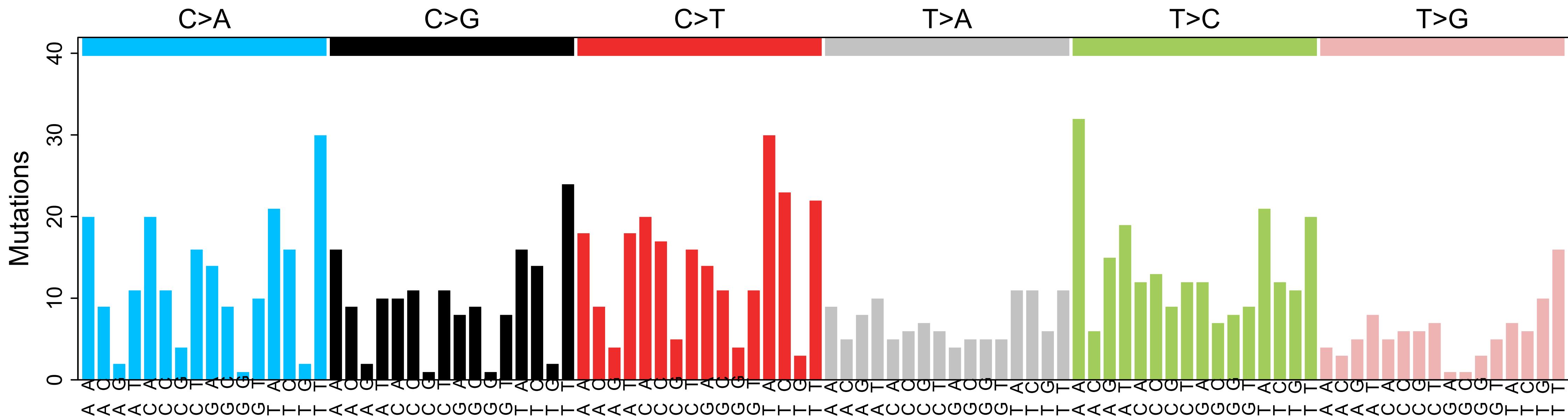
# pyridostatin\_22055eecce72 (1,003 mutations)



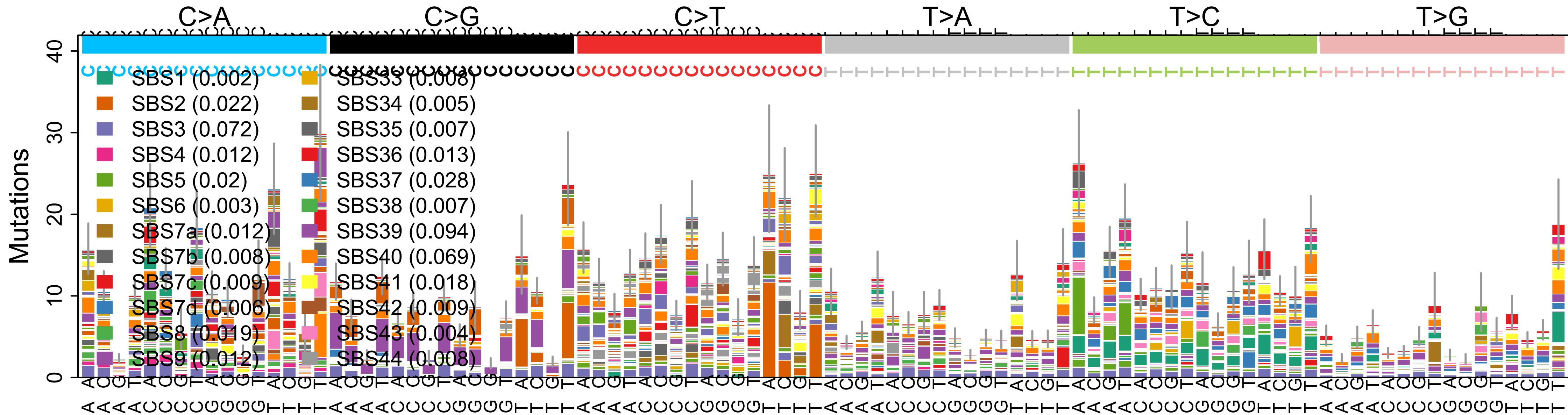
Reconstructed spectrum (cosine similarity = 0.976)



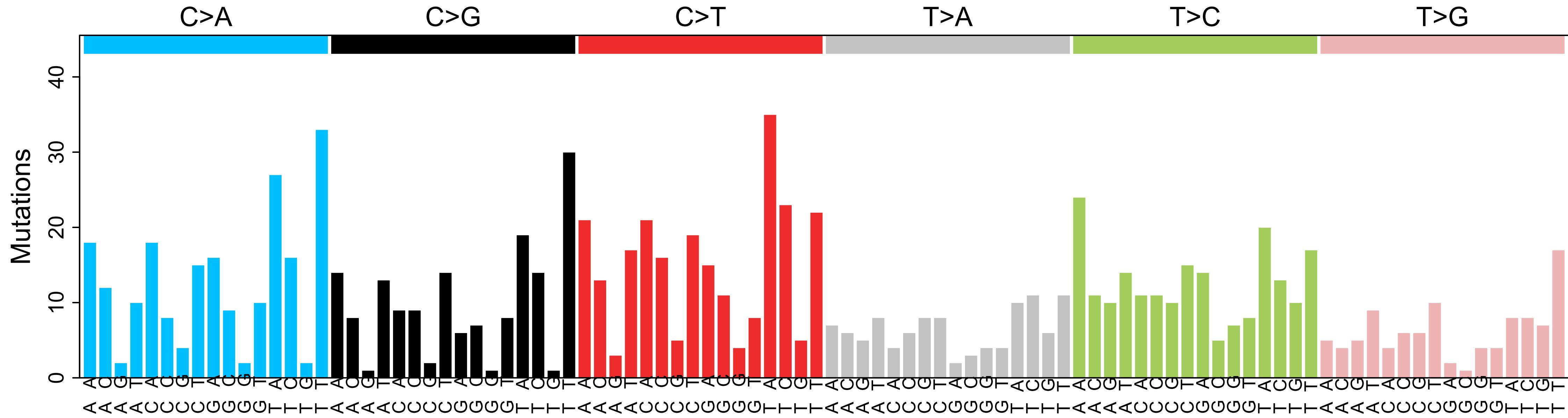
# pyridostatin\_476ee18c3333 (998 mutations)



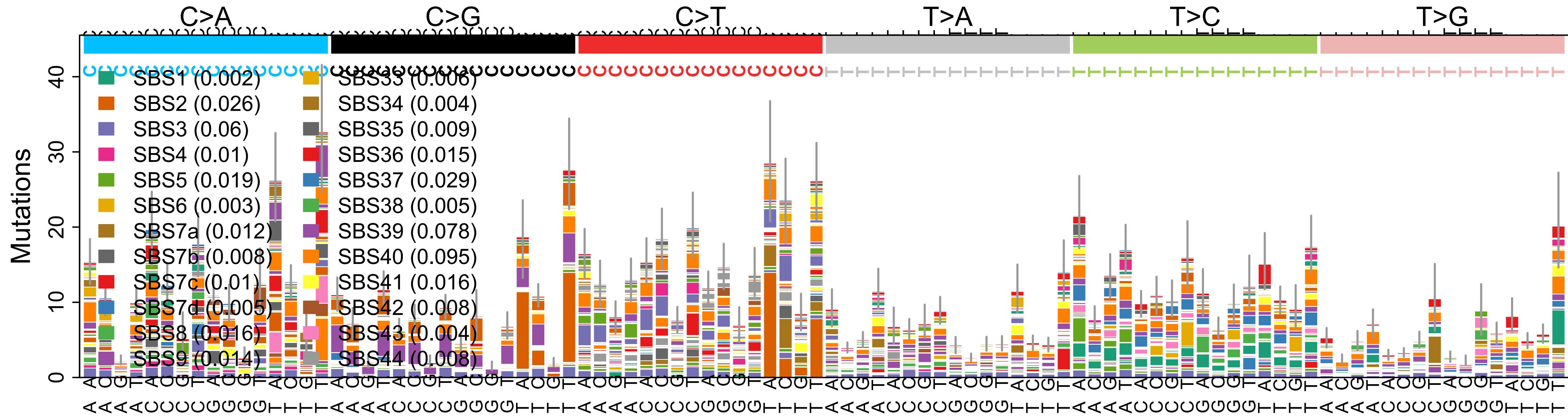
Reconstructed spectrum (cosine similarity = 0.978)



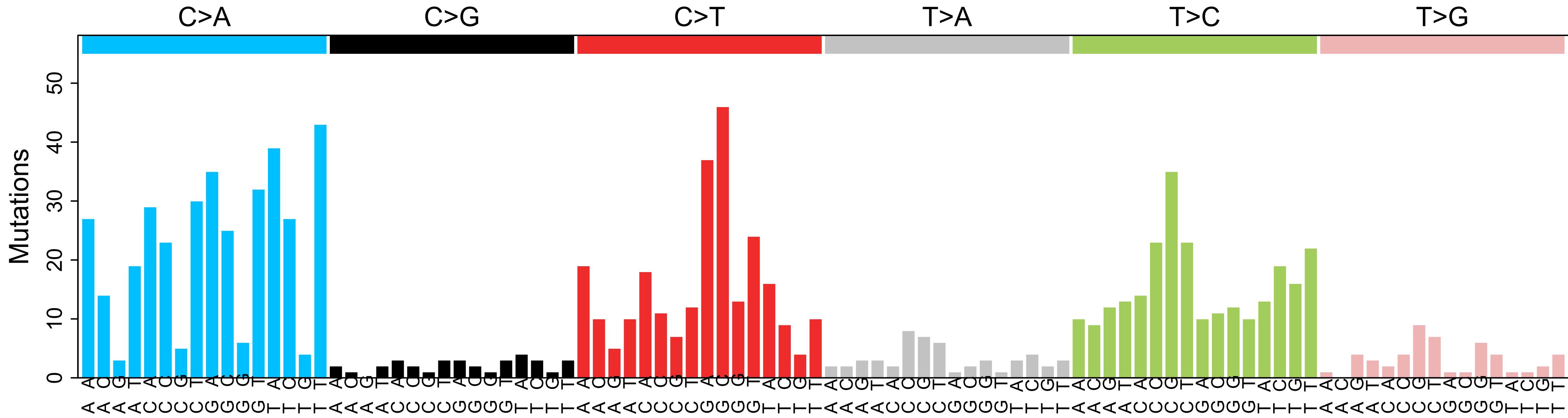
# **pyridostatin\_a7337810aa5e (999 mutations)**



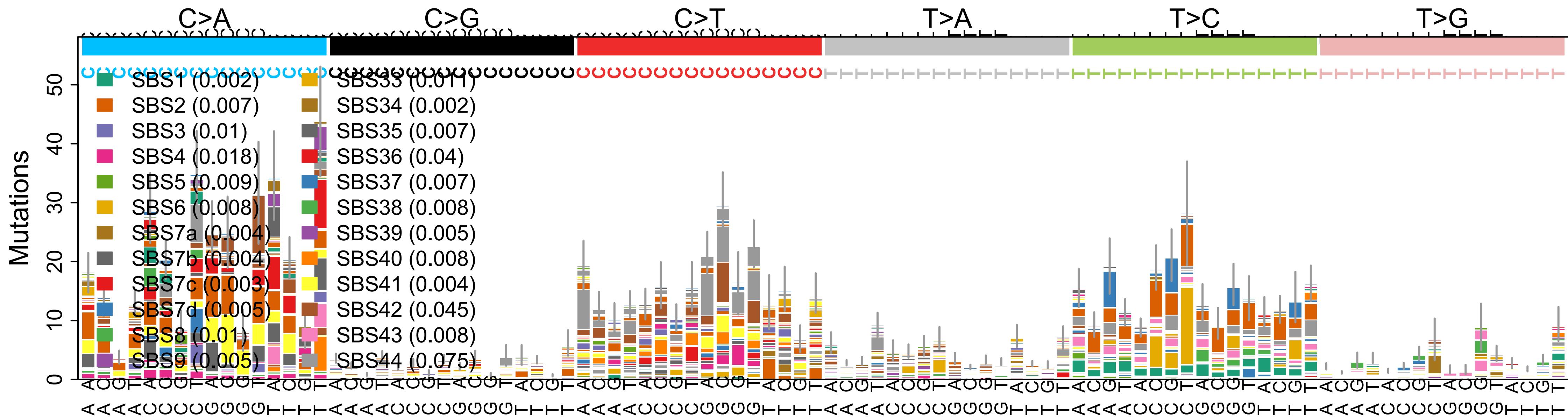
## Reconstructed spectrum (cosine similarity = 0.978)



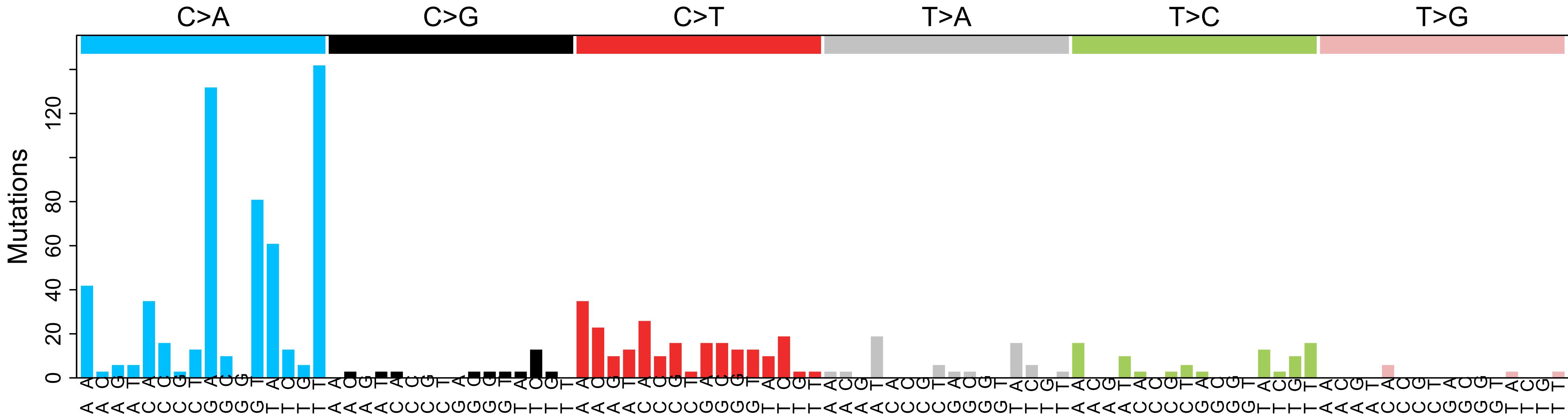
# **pyrrolizidine\_alkaloid\_cebf8492a194 (1,000 mutations)**



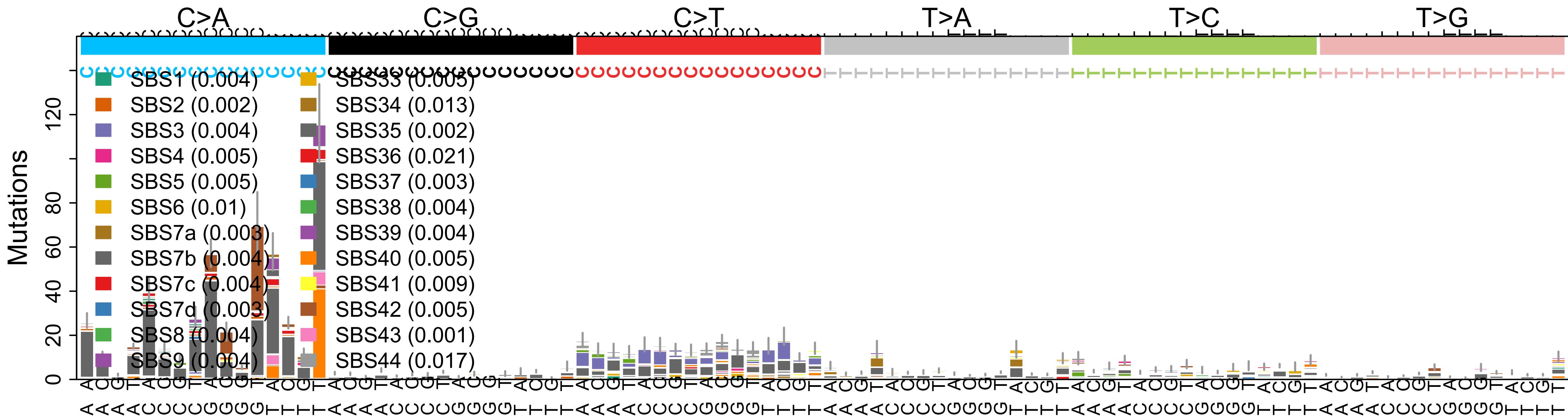
## Reconstructed spectrum (cosine similarity = 0.959)



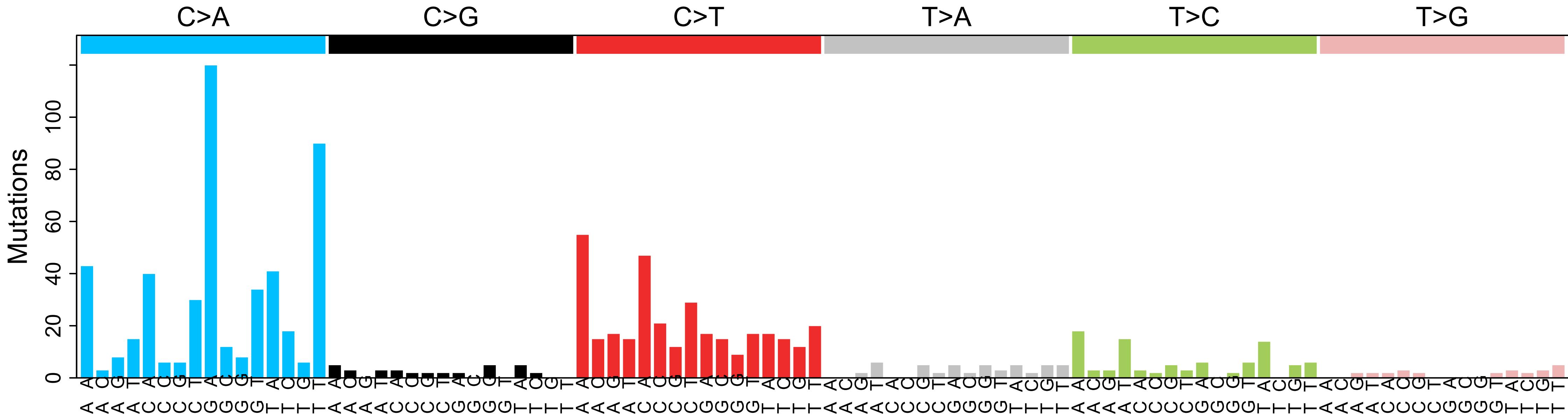
# semustine\_5a98bdaabcd0 (992 mutations)



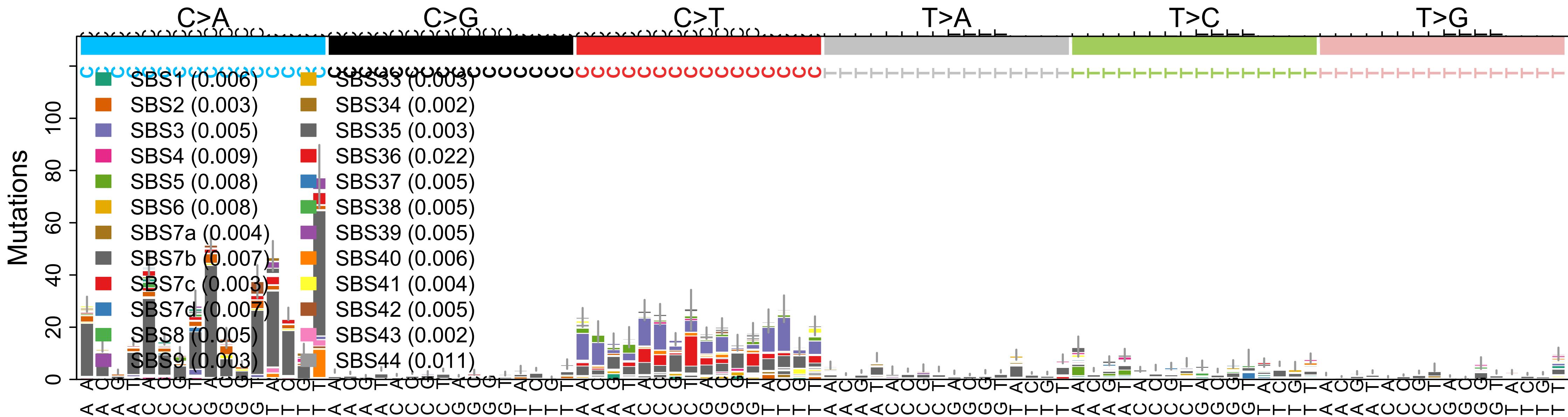
Reconstructed spectrum (cosine similarity = 0.931)



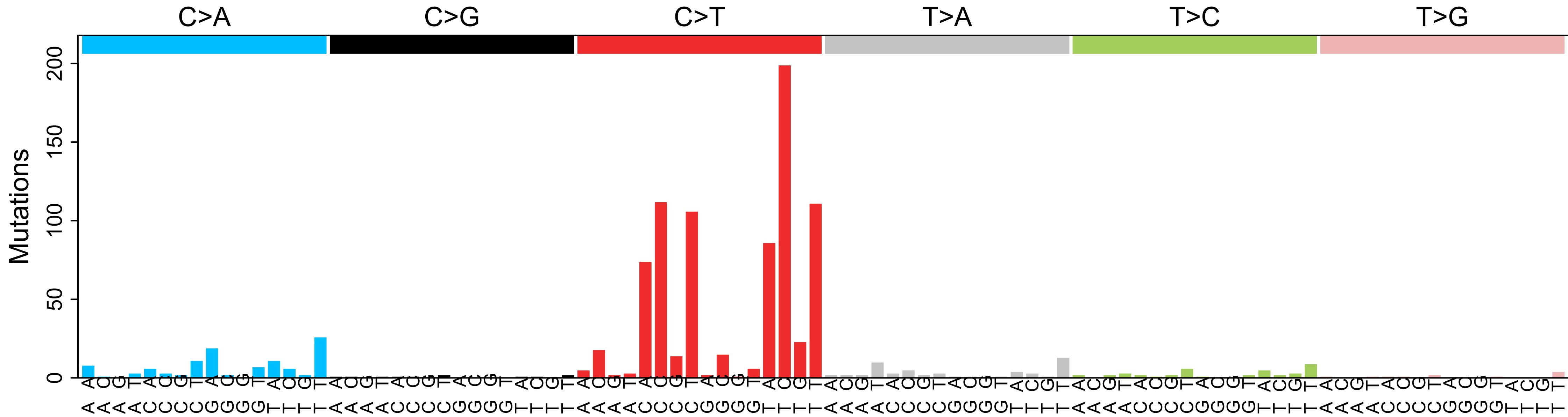
# semustine\_f81842a4d573 (1,011 mutations)



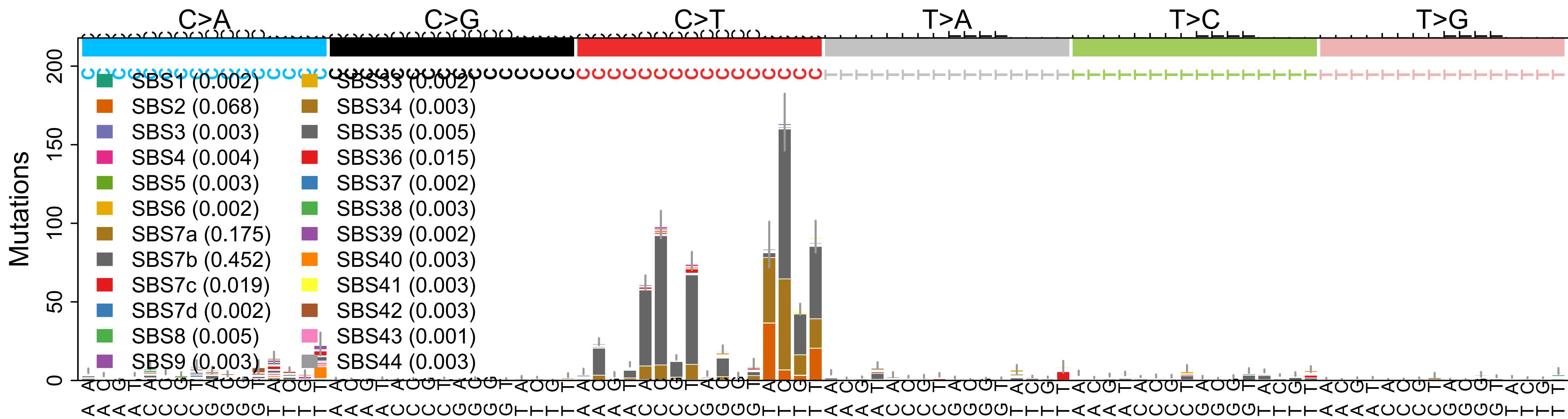
Reconstructed spectrum (cosine similarity = 0.912)



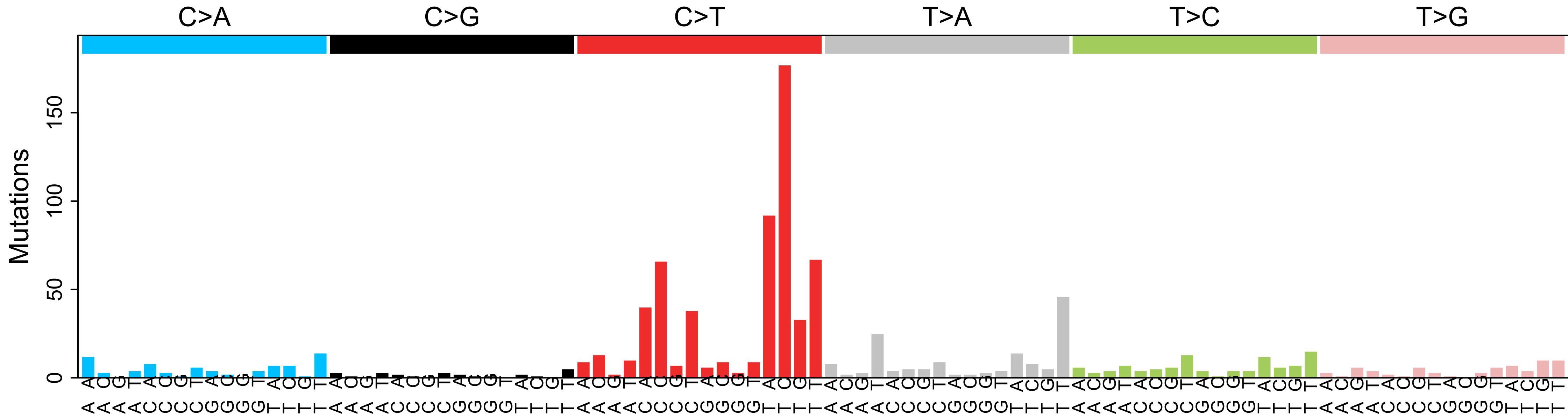
# simulated\_solar\_radiation\_04d97e27a495 (999 mutations)



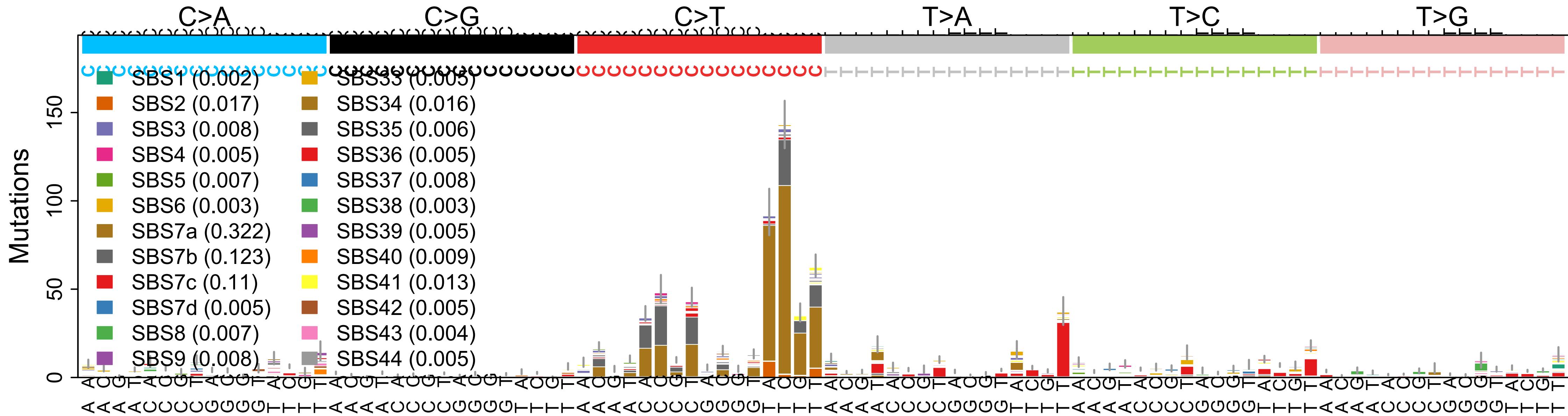
## Reconstructed spectrum (cosine similarity = 0.988)



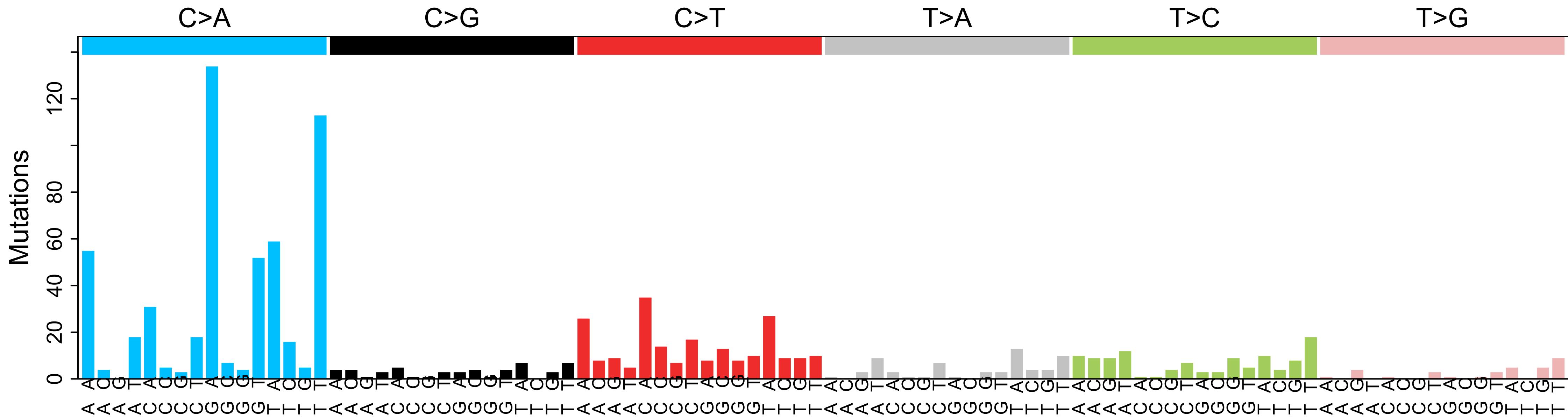
# **simulated\_solar\_radiation\_fa422d8b482e (995 mutations)**



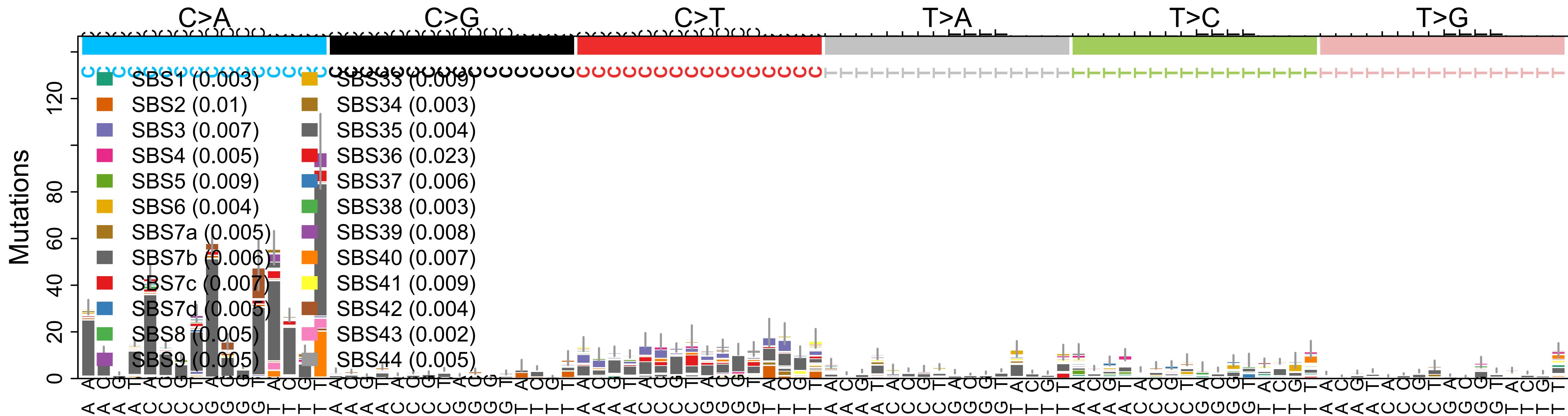
## Reconstructed spectrum (cosine similarity = 0.988)



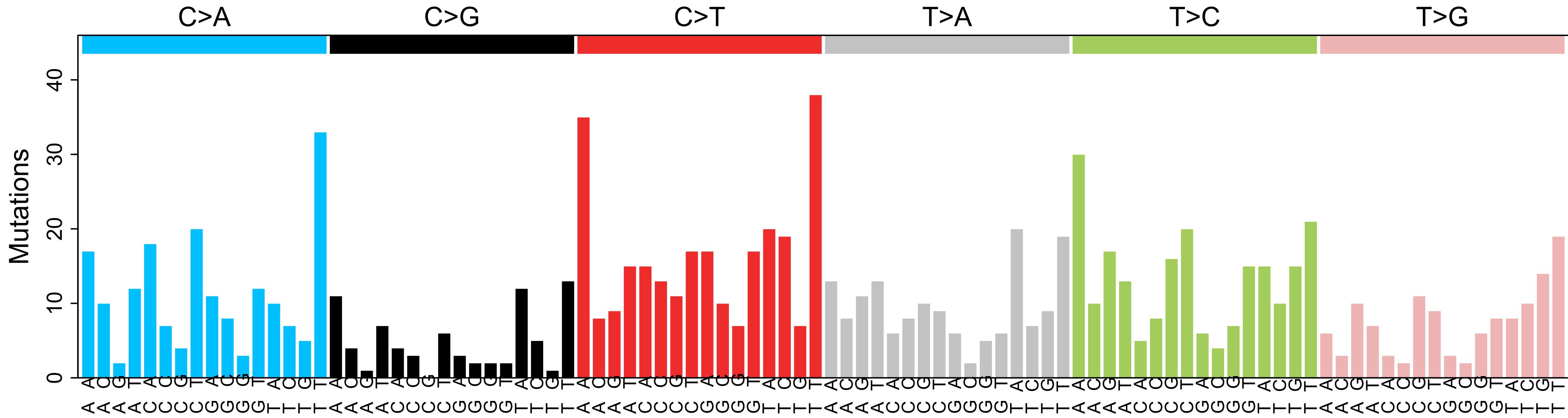
# sodium\_arsenite\_90245b3e0140 (999 mutations)



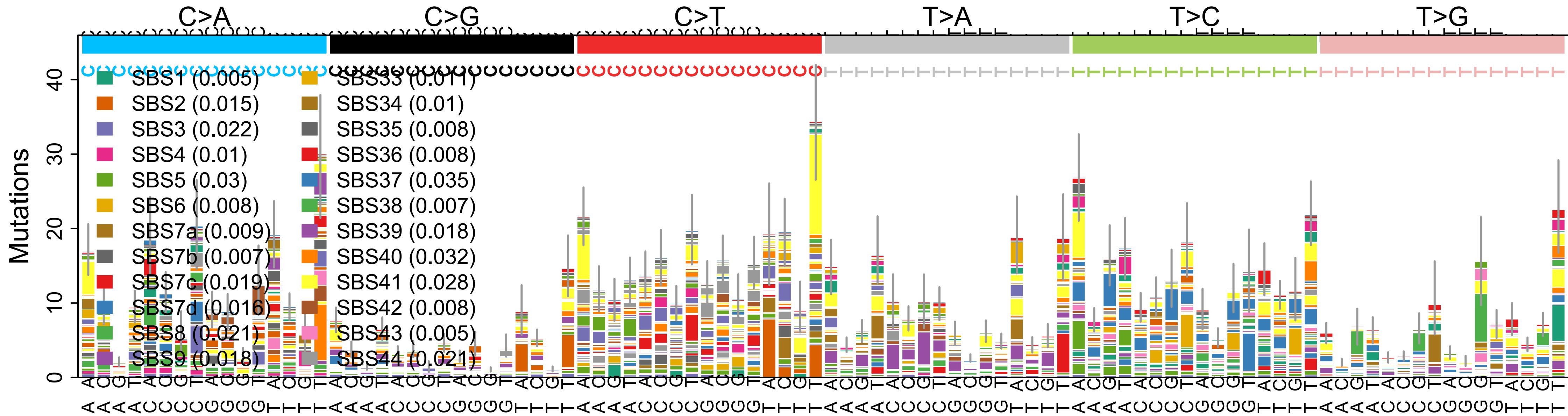
Reconstructed spectrum (cosine similarity = 0.918)



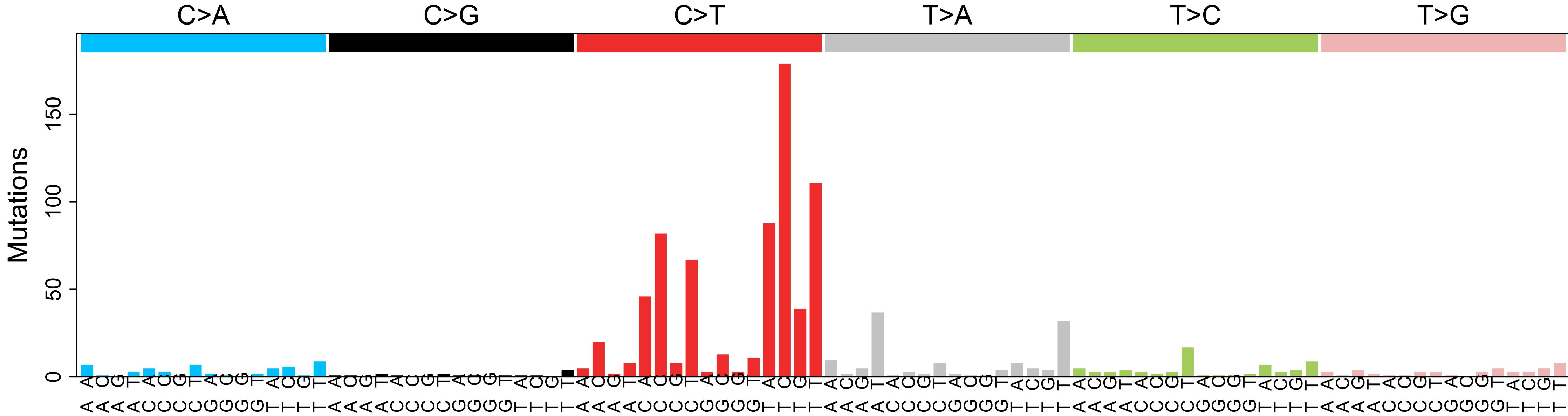
**sodium\_arsenite\_b9afee5488f0 (998 mutations)**



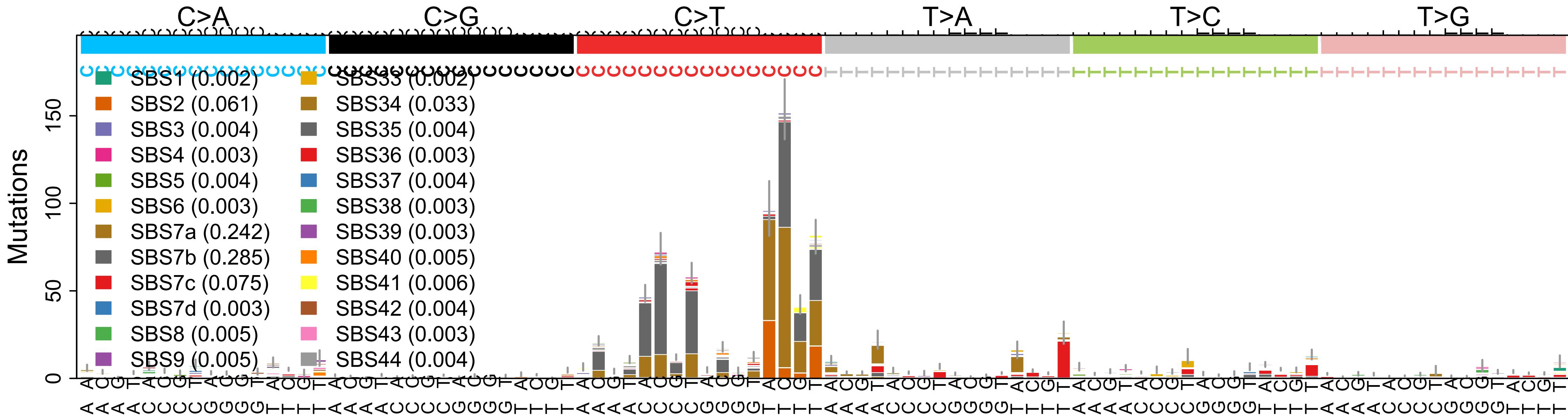
# Reconstructed spectrum (cosine similarity = 0.97)



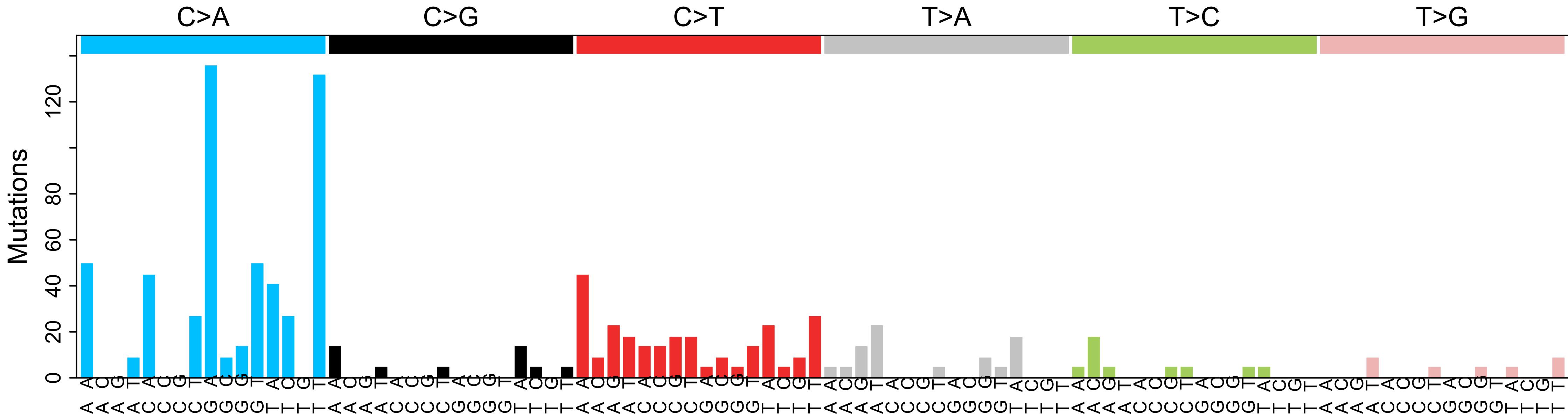
# sodium\_arsenite\_simulated\_solar\_radiation\_63b5316ade6b (993 mutations)



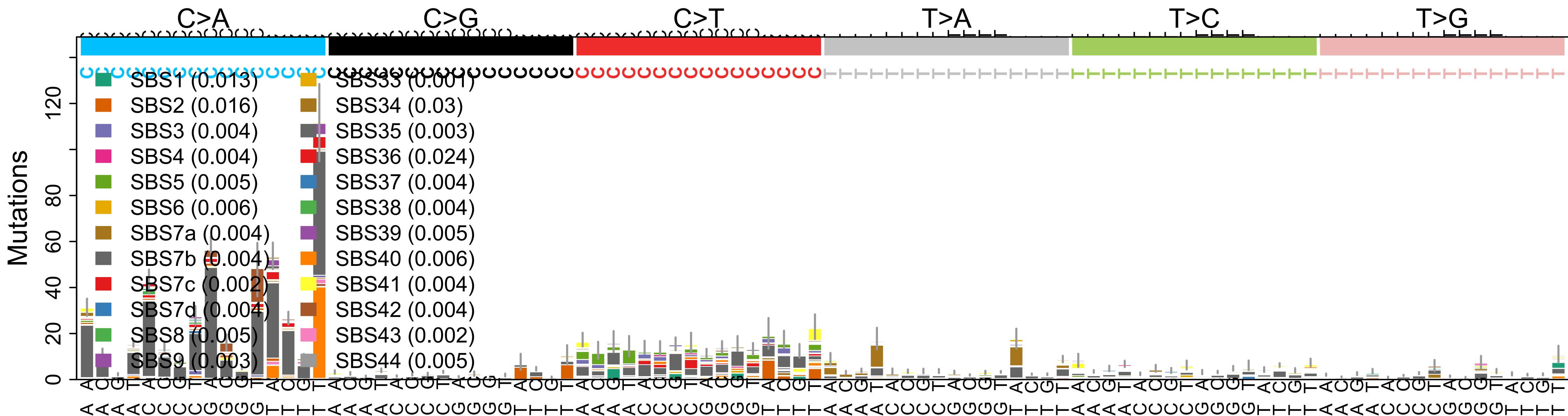
Reconstructed spectrum (cosine similarity = 0.988)



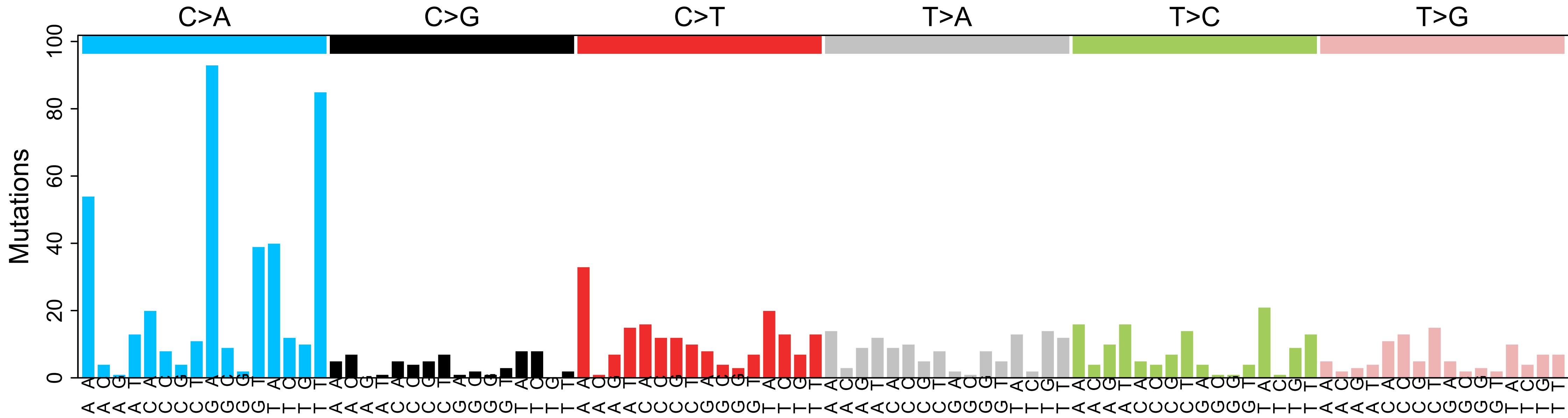
# sodium\_chloride\_02280bd72cf9 (1,009 mutations)



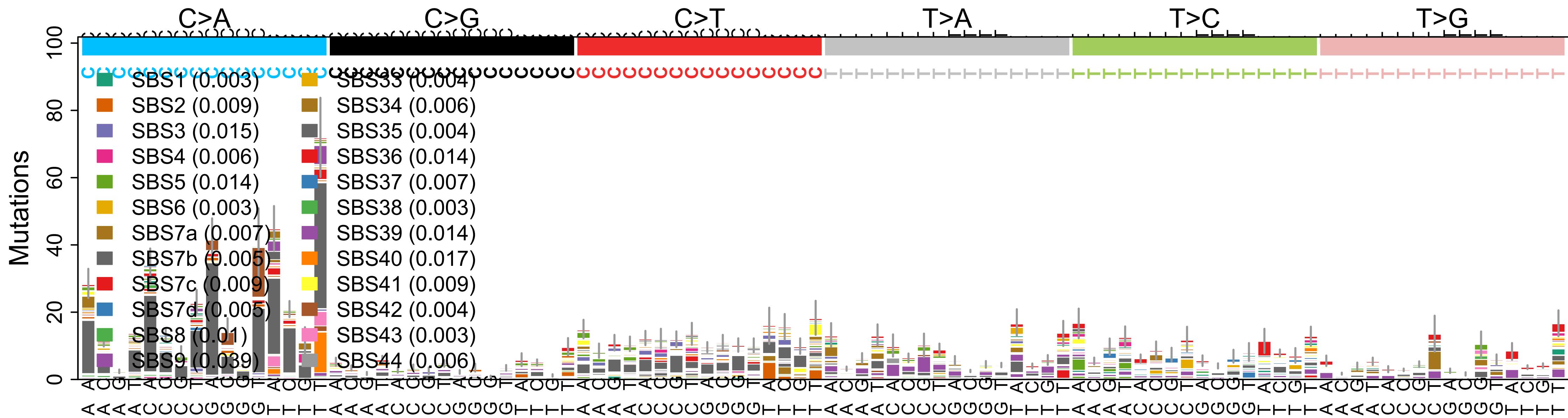
Reconstructed spectrum (cosine similarity = 0.913)



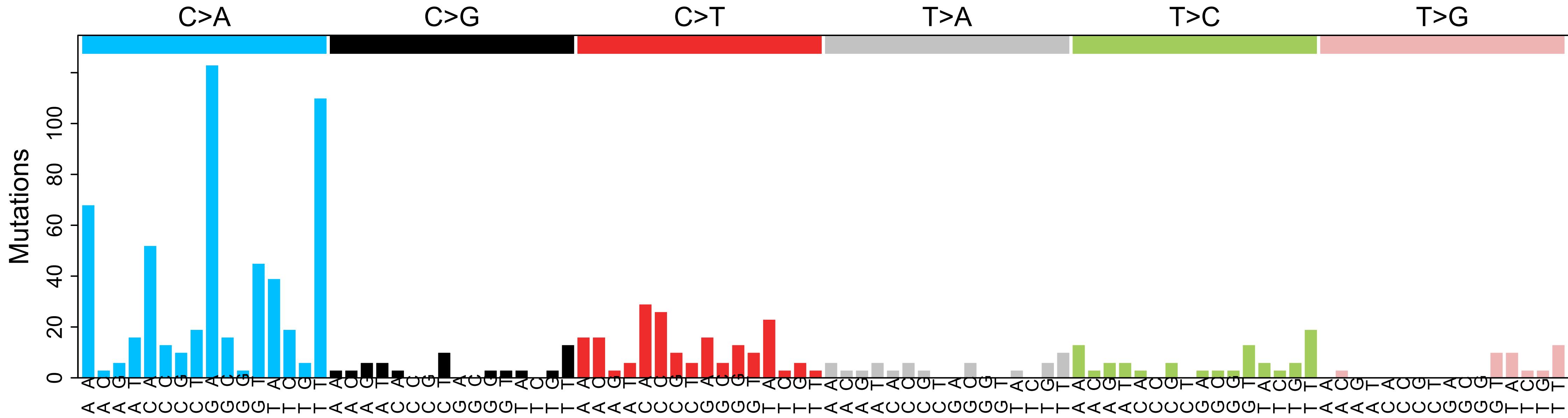
# styrene\_oxide\_2bb934f6fd57 (1,000 mutations)



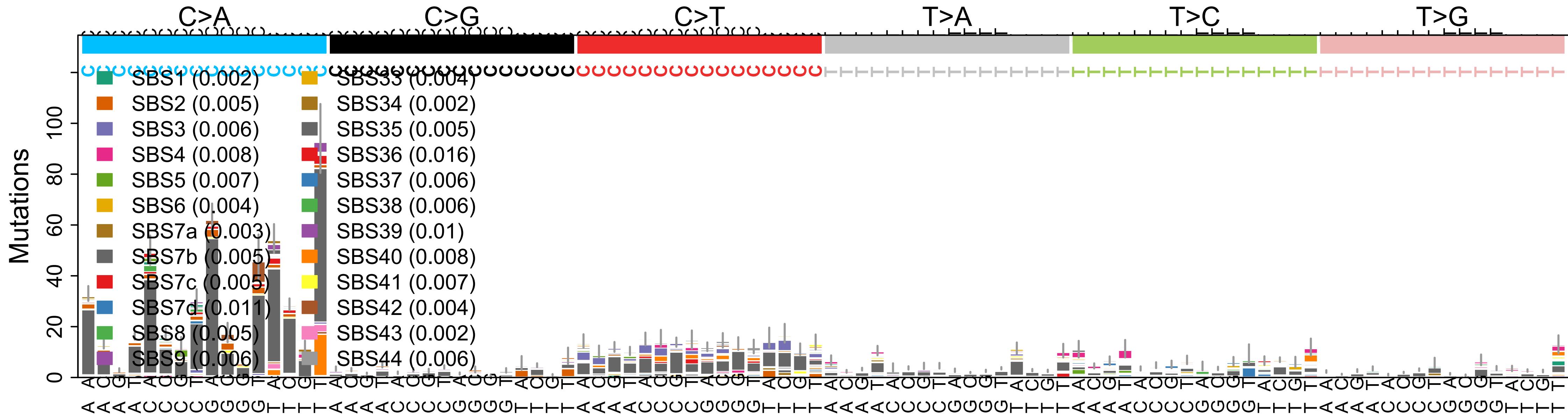
## Reconstructed spectrum (cosine similarity = 0.907)



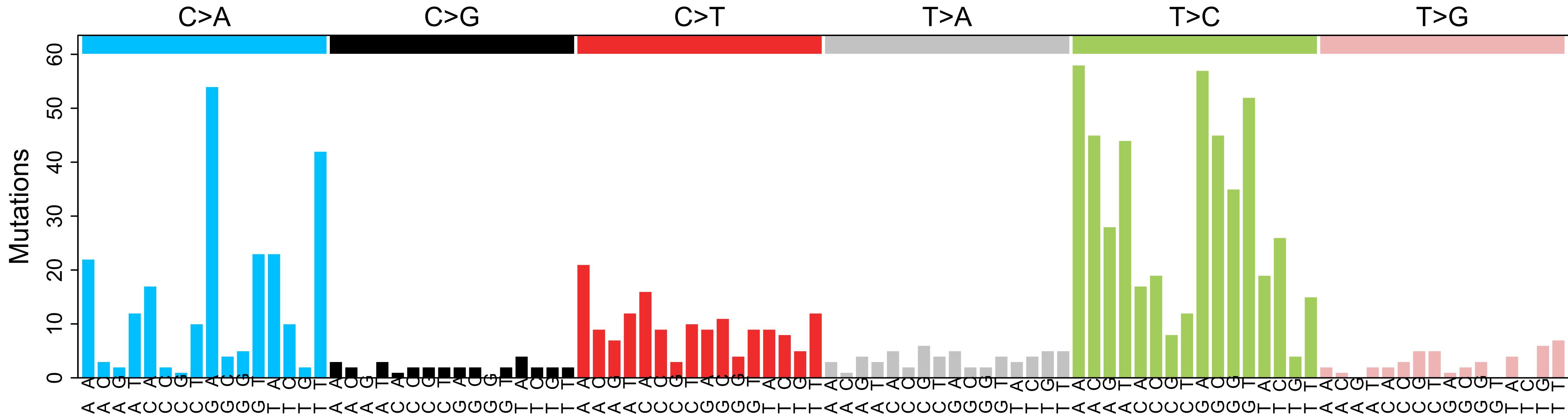
# **sudan\_i\_c63d6349b4cb (986 mutations)**



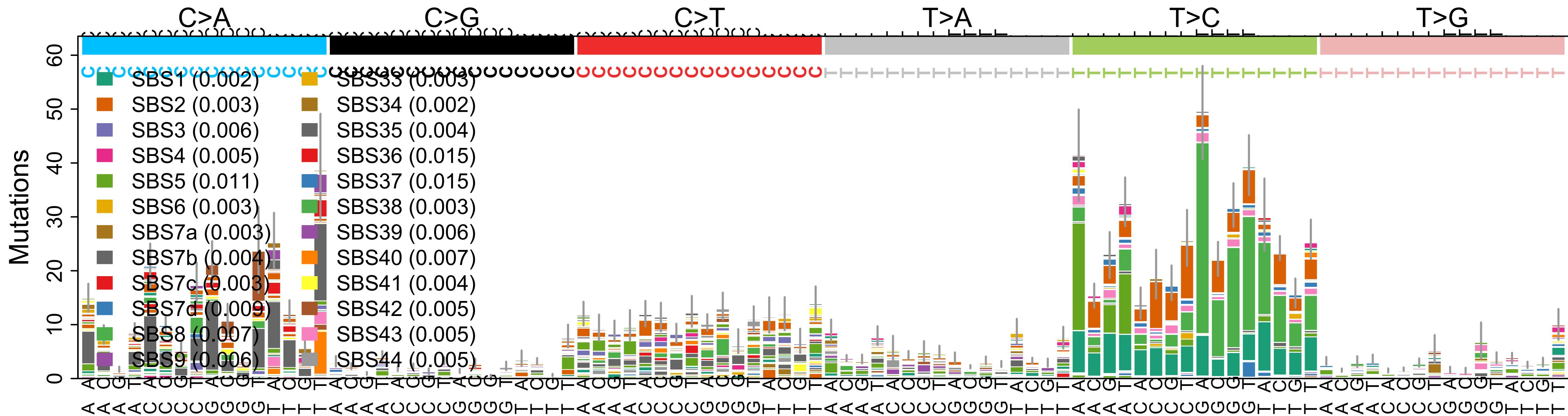
## Reconstructed spectrum (cosine similarity = 0.92)



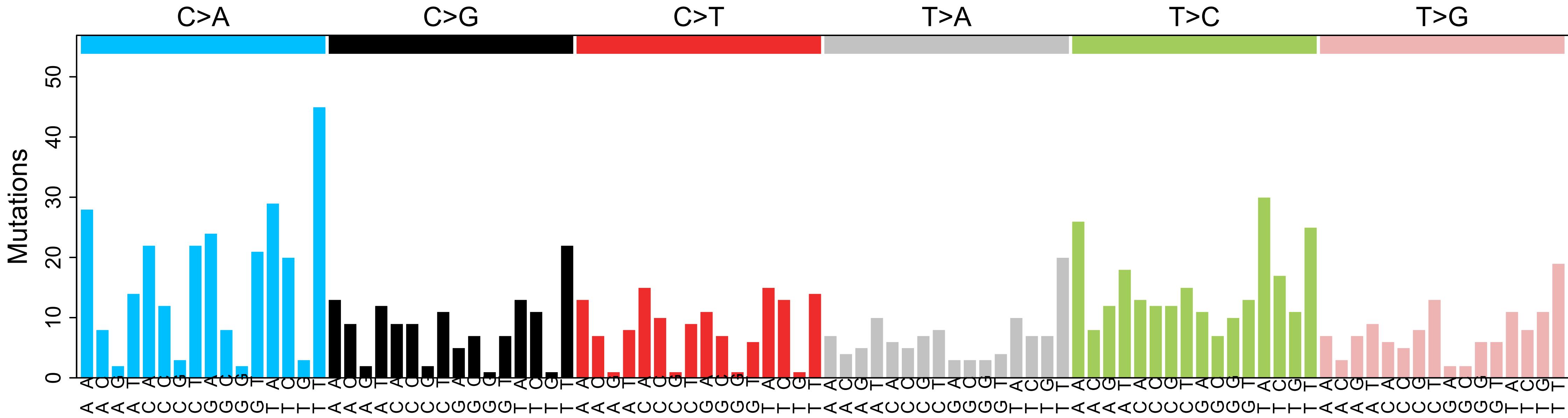
# temozolomide\_8377cb5da514 (1,002 mutations)



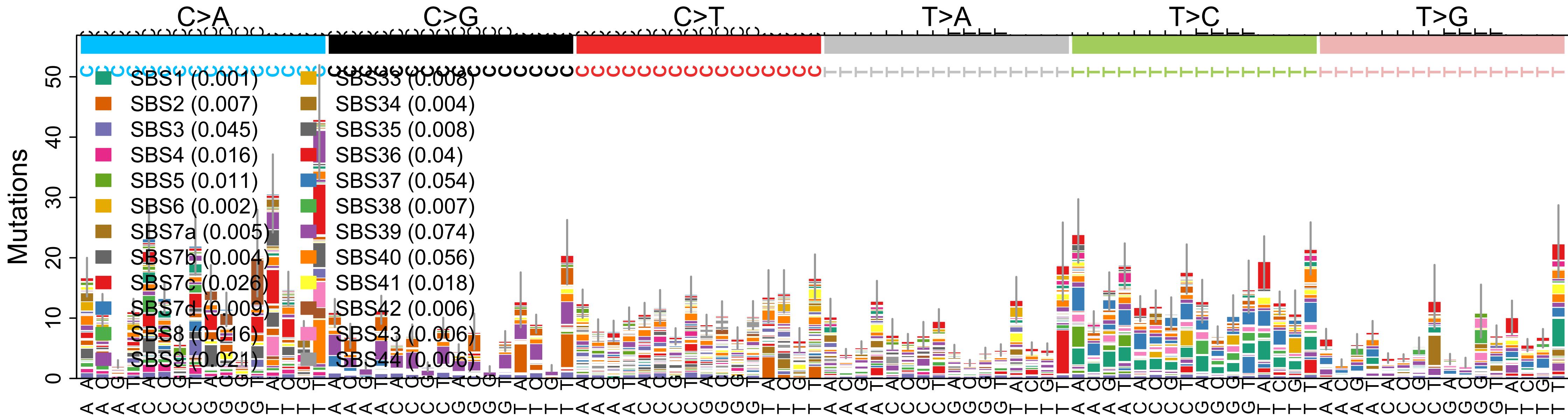
Reconstructed spectrum (cosine similarity = 0.921)



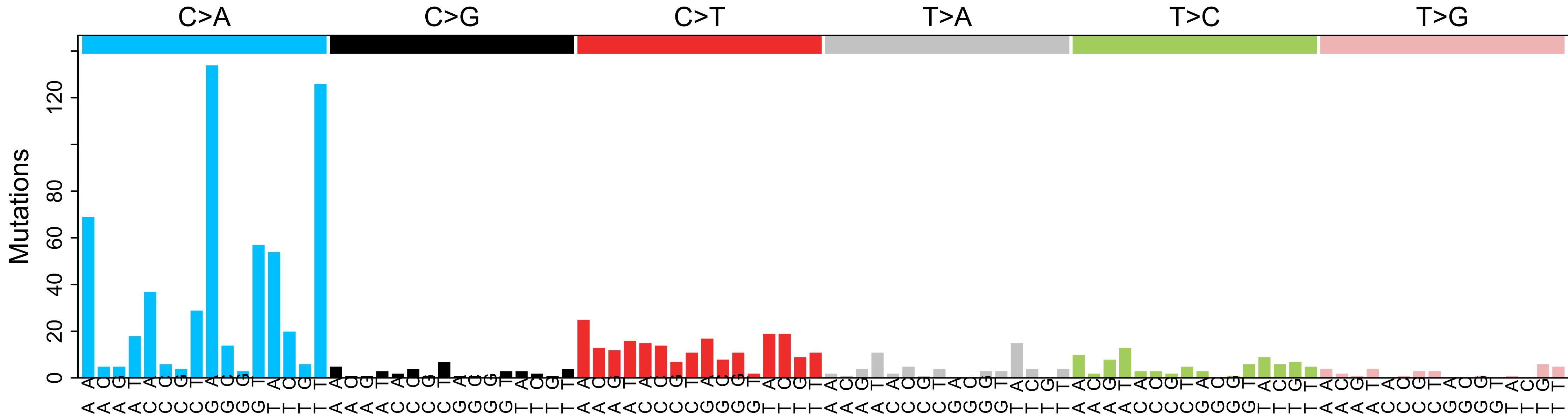
# uva\_7a9189894303 (1,001 mutations)



**Reconstructed spectrum (cosine similarity = 0.973)**



# water\_5807eebc2535 (1,008 mutations)



Reconstructed spectrum (cosine similarity = 0.936)

