```
1 import Pkg, Revise; Pkg.activate(Base.current_project())
    Activating project at `/DATA/cossio/SAM/2024/SamApp2024.jl`
1 import CairoMakie
1 import CSV
1 import FASTX
1 import HDF5
1 import Infernal
1 import KernelDensity
1 import Makie
1 import RestrictedBoltzmannMachines as RBMs
1 import Rfam
1 import SamApp2024
1 import StatsBase
1 import ViennaRNA
1 import ViennaRNA_jll
1 using BioSequences: LongRNA
1 using DataFrames: DataFrame
1 using Distributions: Gamma
1 using Distributions: logpdf
1 using Distributions: pdf
1 using Distributions: Poisson
1 using LinearAlgebra: Diagonal
1 using LinearAlgebra: eigen
1 using Makie: @L_str
```

```
1 using NaNStatistics: nanmean, nansum
1 using Random: bitrand
1 using RestrictedBoltzmannMachines: free_energy
1 using Statistics: cor
1 using Statistics: mean
1 using Statistics: middle
1 using StatsBase: countmap
1 using Unitful: ustrip
  @show Rfam.get_rfam_directory();
  Rfam.get_rfam_directory() = "/DATA/cossio/data/Rfam"
  @show Rfam.get_rfam_version();
  Rfam.get_rfam_version() = "14.7"
1 # load SHAPE data
  shape_data_045 = SamApp2024.load_shapemapper_data_pierre_demux_20230920(; demux=true);
1 # split rep0 from rep4+5
2 shape_data_rep0 = SamApp2024.select_conditions_20231002(shape_data_045,
  filter(endswith("_rep0"), shape_data_045.conditions));
1 # split rep0 from rep4+5
2 shape_data_rep45 = SamApp2024.select_conditions_20231002(shape_data_045,
  filter(endswith("_rep45"), shape_data_045.conditions));
  conds_sam_rep0 = identity.(indexin(["SAMAP_1M7_0-1SAM_5Mg_T30C_rep0", "SAMAP_1M7_0-
  5SAM_5Mg_T30C_rep0", "SAMAP_1M7_1SAM_5Mg_T30C_rep0"], shape_data_rep0.conditions));
  conds_mg_rep0 = identity.(indexin(["SAMAP_1M7_noSAM_5Mg_T30C_rep0"],
  shape_data_rep0.conditions));
  conds_30C_rep0 = identity.(indexin(["SAMAP_1M7_noSAM_noMg_T30C_rep0"],
  shape_data_rep0.conditions));
  conds_sam_rep45 = identity.(indexin(["SAMAP_1M7_0-1SAM_5Mg_T30C_rep45",
  "SAMAP_1M7_1SAM_5Mg_T30C_rep45"], <a href="mailto:shape_data_rep45">shape_data_rep45</a>.conditions));
  conds_mg_rep45 = identity.(indexin(["SAMAP_1M7_noSAM_5Mg_T30C_rep45"],
  shape_data_rep45.conditions));
  conds_30C_rep45 = identity.(indexin(["SAMAP_1M7_noSAM_noMg_T30C_rep45"],
  shape_data_rep45.conditions));
```

```
@show conds_sam_rep0 conds_mg_rep0 conds_30C_rep0;
2
    conds_sam_rep0 = [1, 2, 3]
    conds_mg_rep0 = [4]
    conds_30C_rep0 = [5]
    @show conds_sam_rep45 conds_mg_rep45 conds_30C_rep45;
>_
    conds_sam_rep45 = [1, 2]
    conds_mg_rep45 = [4]
    conds_30C_rep45 = [6]
\triangleright (bps = [1, 2, 3, 4, 5, 6, 7, 8, 13, ... more ,108], nps = [9, 10, 11, 12, 18, 19, 20, 24, 32, ... more
 1 (; bps, nps, pks) = SamApp2024.RF00162_sites_paired()
rbm_seqs =
▶ [207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 22
 1 rbm_seqs = findall(shape_data_045.aptamer_origin .== "RF00162_syn_rbm")
inf_seqs = ▶ [258, 260, 262, 264, 266, 268, 270, 272, 274, 276, 278, 280, 282, 284, 286, 291]
 1 inf_seqs = findall(shape_data_045.aptamer_origin .== "RF00162_syn_inf")
full_seqs =
\triangleright [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, \cdots more ,46, 47, 48, 49, 50,
 1 full_seqs = findall(shape_data_045.aptamer_origin .== "RF00162_full30")
seed_seqs =
▶ [56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, ··· more ,197, 198,
 1 seed_seqs = findall(shape_data_045.aptamer_origin .== "RF00162_seed70")
 1 nat_seqs = full_seqs ∪ seed_seqs;
    bps_reactivities_rep0 = shape_data_rep0.shape_reactivities[bps, nat_seqs,
    conds_sam_rep0];
    nps_reactivities_rep0 = shape_data_rep0.shape_reactivities[nps, nat_seqs,
    conds_sam_rep0];
 1 all_reactivities_rep0 = shape_data_rep0.shape_reactivities[:, nat_seqs, conds_sam_rep0];
    shape_stats_rep0 = SamApp2024.shape_basepair_log_odds_v4(;
        shape_data = shape_data_rep0,
        paired_reactivities = bps_reactivities_rep0,
        unpaired_reactivities = nps_reactivities_rep0,
        all_reactivities = all_reactivities_rep0,
        only_hq_profile = true, p_thresh = 1e-3, nsamples = 1000
 7);
_thresh = 1.6094379124341003
 1 _{\text{thresh}} = \log(5)
```

```
1 _sites = SamApp2024.hallmark_sites_20230507;
x_mg_rep0 =
▶ [-4.86644, -12.1404, -14.8342, -2.11477, 0.0, 0.0, -14.6983, 0.0, -4.65234, 0.0, -12.9099, -9.7€
 1 x_mg_rep0 = nansum(shape_stats_rep0.shape_log_odds[_sites, :, conds_mg_rep0]; dim=(1,3))
x_sam_rep0 =
▶ [15.7896, 4.08177, -18.098, 17.7391, 0.0, 0.0, 7.75366, 0.0, 13.8029, 0.0, -27.6326, 3.38205, 20
 1 x_sam_rep0 = nansum(shape_stats_rep0.shape_log_odds[_sites, :, conds_sam_rep0]; dim=
   (1,3))
 1 _responds_sam_yes_rep0 = (x_mg_rep0 .< -_thresh) .& (x_sam_rep0 .> +_thresh);
 1 _responds_sam_nop_rep0 = (x_mg_rep0 .> +_thresh) . | (x_sam_rep0 .< -_thresh);</pre>
 1 _inconclusive_rep0 = ((!).(_responds_sam_yes_rep0)) .& ((!).(_responds_sam_nop_rep0));
 1 _conclusive_rep0 = _responds_sam_yes_rep0 . | _responds_sam_nop_rep0;
 1 aptamer_rbm_energies = [
       ismissing(seq) ? missing :
       free_energy(SamApp2024.rbm2022(), SamApp2024.onehot(LongRNA{4}(seq)))
       for seq in shape_data_045.aligned_sequences
 5];
wuss =
1 wuss = SamApp2024.rfam_ss("RF00162"; inserts=false)
1 ss = SamApp2024.clean_wuss(wuss)
 1 p1_pos = SamApp2024.RF00162_sites_annotated_secondary_structure().p1;
 1 p2_pos = SamApp2024.RF00162_sites_annotated_secondary_structure().p2;
 1 p3_pos = SamApp2024.RF00162_sites_annotated_secondary_structure().p3;
 1 p4_pos = SamApp2024.RF00162_sites_annotated_secondary_structure().p4;
   pk_pos = SamApp2024.RF00162_sites_annotated_secondary_structure().pk;
 1 ss_without_P1 = join([i ∈ p1_pos ? '.' : c for (i,c) in enumerate(ss)]);
 1 ss_without_P2 = join([i \in p2_pos ? '.' : c for (i,c) in enumerate(ss)]);
 1 ss_without_P3 = join([i \in p3\_pos ? '.' : c for (i,c) in enumerate(ss)]);
 1 ss_without_P4 = join([i \in p4_pos ? '.' : c for (i,c) in enumerate(ss)]);
```

```
ss_pk_only =
 1 ss_pk_only = replace(wuss, r"\(|\)|\[|\]|\{|\}|\<|\>|\-|\_|\," => '.', 'A' => '(', 'a')
 1 sampled_v = SamApp2024.rbm2022samples();
 1 Vienna_energies_fold = [ismissing(seq) ? missing : ustrip(ViennaRNA.energy(string(seq),
   ss)) for seg = shape_data_rep0.aligned_sequences];
 1 Vienna_energies_P1 = [ismissing(seq) ? missing : ustrip(ViennaRNA.energy(string(seq),
   ss)) - ustrip(ViennaRNA.energy(string(seq), ss_without_P1)) for seq =
   shape_data_rep0.aligned_sequences];
 1 Vienna_energies_P2 = [ismissing(seq) ? missing : ustrip(ViennaRNA.energy(string(seq),
   ss)) - ustrip(ViennaRNA.energy(string(seq), ss_without_P2)) for seq =
   shape_data_rep0.aligned_sequences];
 1 Vienna_energies_P3 = [ismissing(seq) ? missing : ustrip(ViennaRNA.energy(string(seq),
   ss)) - ustrip(ViennaRNA.energy(string(seq), ss_without_P3)) for seq =
   shape_data_rep0.aligned_sequences];
 1 Vienna_energies_P4 = [ismissing(seq) ? missing : ustrip(ViennaRNA.energy(string(seq),
   ss)) - ustrip(ViennaRNA.energy(string(seq), ss_without_P4)) for seq =
   shape_data_rep0.aligned_sequences];
   Vienna_energies_Pk = [ismissing(seq) ? missing : ustrip(ViennaRNA.energy(string(seq),
   ss_pk_only)) for seq = shape_data_rep0.aligned_sequences];
 1 @time Vienna_energies_P1_RBM_samples = [
       ustrip(ViennaRNA.energy(string(seq), ss)) - ustrip(ViennaRNA.energy(string(seq),
   ss_without_P1))
      for seq = SamApp2024.rnaseq(sampled_v)
 4 ];
      1.930079 seconds (2.18 M allocations: 129.627 MiB, 1.66% gc time, 49.02% compi
   lation time)
   Vienna_energies_Pk_RBM_samples = [ustrip(ViennaRNA.energy(string(seq), ss_pk_only)) for
```

seq = SamApp2024.rnaseq(sampled_v)];

```
Vienna_energies_Pk_RNAeval =
▶ [-6.6, -7.5, -6.0, -5.5, -8.1, NaN, -6.3, -5.1, -6.0, 2.9, -4.2, -5.5, -7.9, NaN, -7.5, 3.9, -6.3
   1 Vienna_energies_Pk_RNAeval = [ismissing(seq) ? NaN :
          SamApp2024.vienna_pk_binding_energy_rnaeval(seq) for seq =
          shape_data_rep0.aligned_sequences]
           WARNING: bases 25 and 80 (UU) can't pair!
                                                                                                                                                                                                                                                       ?
           WARNING: bases 25 and 80 (AA) can't pair!
           WARNING: bases 27 and 78 (UC) can't pair!
          WARNING: bases 28 and 77
                                                                                  (GA) can't pair!
          WARNING: bases 25 and 80 (AG) can't pair!
          WARNING: bases 28 and 77 (AC) can't pair!
WARNING: bases 25 and 80 (C-) can't pair!
          WARNING: bases 26 and 79 (U-) can't pair!
         WARNING: bases 26 and 79 (U-) can't pair! WARNING: bases 27 and 78 (G-) can't pair! WARNING: bases 28 and 77 (G-) can't pair! WARNING: bases 26 and 79 (GA) can't pair! WARNING: bases 27 and 78 (GA) can't pair! WARNING: bases 25 and 80 (UU) can't pair! WARNING: bases 26 and 79 (AA) can't pair! WARNING: bases 25 and 80 (CU) can't pair! WARNING: bases 25 and 80 (CU) can't pair! WARNING: bases 25 and 80 (AA) can't pair! WARNING: bases 25 and 80 (AG) can't pair! WARNING: bases 26 and 79 (AA) can't pair! WARNING: bases 27 and 78 (AA) can't pair! WARNING: bases 25 and 80 (AG) can't pair! WARNING: bases 25 and 80 (AG) can't pair! WARNING: bases 27 and 78 (GA) can't pair! WARNING: bases 27 and 78 (GA) can't pair! WARNING: bases 27 and 78 (GA) can't pair! WARNING: bases 25 and 80 (AA) can't pair! WARNING: bases 25 and 80 (AA) can't pair! WARNING: bases 25 and 80 (AG) can't pair! WARNING: bases 25 and 80 (CA) can't pair! WARNING: bases 26 and 79 (UU) can't pair! WARNING: bases 25 and 80 (AG) can't pair! WARNING: bases 25 and 80 (AG) can't pair! WARNING: bases 25 and 80 (UU) can't pair! WARNING: bases 25 and 80 (UU) can't pair! WARNING: bases 25 and 80 (UU) can't pair!
          WARNING: bases 27 and 78 (G-) can't pair!
           WARNING: bases 25 and 80 (UU) can't pair!
           WARNING: bases 26 and 79 (AA)
                                                                                               can't pair!
```

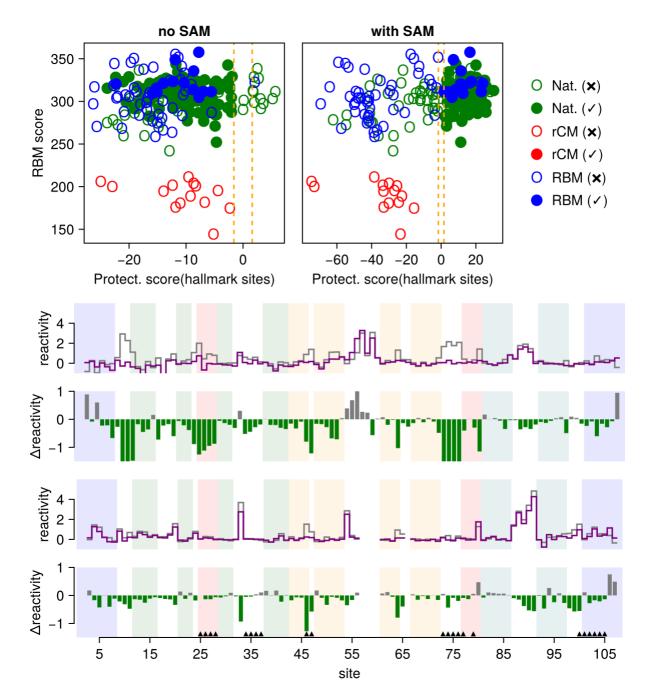
WARNING: bases 28 and 77 (AC) can't pair!

```
1 Vienna_energies_Pk_RBM_samples_RNAeval =
    [SamApp2024.vienna_pk_binding_energy_rnaeval(string(seq)) for seq =
    SamApp2024.rnaseq(sampled_v)];
    WARNING: bases 26 and 79 (UU) can't pair! WARNING: bases 26 and 79 (UU) can't pair! WARNING: bases 27 and 78 (GA) can't pair! WARNING: bases 26 and 79 (U-) can't pair! WARNING: bases 25 and 80 (AG) can't pair! WARNING: bases 25 and 80 (AA) can't pair! WARNING: bases 25 and 80 (CA) can't pair! WARNING: bases 28 and 77 (GG) can't pair! WARNING: bases 25 and 80 (UU) can't pair! WARNING: bases 25 and 80 (UU) can't pair! WARNING: bases 25 and 80 (AG) can't pair!
                                                                                                              3
    WARNING: bases 25 and 80 (AG) can't pair!
    WARNING: bases 25 and 80 (AG) can't pair!
    WARNING: bases 25 and 80 (CA) can't pair!
    WARNING: bases 26 and 79 (UU) can't pair!
    WARNING: bases 28 and 77 (AC) can't pair!
    WARNING: bases 26 and 79 (UU) can't pair!
     WARNING: bases 28 and 77 (AC) can't pair!
     WARNING: bases 25 and 80 (AG) can't pair!
     WARNING: bases 25 and 80 (--) can't pair!
     WARNING: bases 27 and 78 (-C) can't pair!
    WARNING: bases 28 and 77 (-U) can't pair!
    WARNING: bases 25 and 80 (AG) can't pair!
    WARNING: bases 27 and 78 (GA) can't pair!
     WARNING: bases 25 and 80 (AG) can't pair!
     WARNING: bases 27 and 78 (AC) can't pair!
     WARNING: bases 25 and 80 (AA) can't pair!
     WARNING: bases 26 and 79 (UU) can't pair!
     WARNING: bases 25 and 80 (GA) can't pair!
     WARNING: bases 26 and 79
                                    (CU) can't pair!
     WARNING: bases 25 and 80 (AA) can't pair!
     WARNING: bases 25 and 80 (CA)
                                          can't pair!
     WARNING: bases 28 and 77 (AC) can't pair!
 1 # All merged data, for the reactivity profiles plots
 2 shape_data_all_merged =
    SamApp2024.load_shapemapper_data_pierre_demux_20231027_repls_merged();
      Downloading artifact: SAMAP_ALL-REP-MERGED-2023-10-27
                                                                                                              3
      Failure artifact: SAMAP_ALL-REP-MERGED-2023-10-27
Downloading artifact: SAMAP_ALL-REP-MERGED-2023-10-27
    conds_SAM_all_merged = map(identity, indexin(["SAMAP_1M7_0-1SAM_5Mg_T30C_allrep",
    "SAMAP_1M7_1SAM_5Mg_T30C_allrep"], shape_data_all_merged.conditions));
 1 conds_Mg_all_merged = map(identity, indexin(["SAMAP_1M7_noSAM_5Mg_T30C_allrep"],
    shape_data_all_merged.conditions));
▶ ([1, 2], [3])
```

conds_SAM_all_merged, conds_Mg_all_merged

Multiple expressions in one cell. How would you like to fix it? • Split this cell into 4 cells, or • Wrap all code in a begin ... end block.

```
1 # structural motifs
   struct_bands = [
       (; x0=0.5, xf=8.5, color="blue", alpha=0.1), # P1
       (; x0=100.5, xf=108.5, color="blue", alpha=0.1), # P1
       (; x0=11.5, xf=16.5, color="green", alpha=0.1), # P2
       (; x0=20.5, xf=23.5, color="green", alpha=0.1), # P2
       (; x0=28.5, xf=31.5, color="green", alpha=0.1), # P2
       (; x0=37.5, xf=42.5, color="green", alpha=0.1), # P2
       (; x0=42.5, xf=46.5, color="orange", alpha=0.1), # P3
       (; x0=47.5, xf=53.5, color="orange", alpha=0.1), # P3
       (; x0=60.5, xf=64.5, color="orange", alpha=0.1), # P3
       (; x0=66.5, xf=72.5, color="orange", alpha=0.1), # P3
       (; x0=80.5, xf=86.5, color="teal", alpha=0.1), # P4
       (; x0=91.5, xf=97.5, color="teal", alpha=0.1), # P4
       (; x0=24.5, xf=28.5, color="red", alpha=0.1), # Pk
       (; x0=76.5, xf=80.5, color="red", alpha=0.1), # Pk
17 ];
```



```
let fig = Makie.Figure(; halign = :left)
    ax = Makie.Axis(fig[1,1][1,1]; halign=:left, width=200, height=200, xlabel="Protect.
    score(hallmark sites)", ylabel="RBM score", title="no SAM", xgridvisible=false,
    ygridvisible=false)
    #Makie.scatter!(ax, x_mg_rep0, -aptamer_rbm_energies, markersize=10, color=(:silver,
    0.3), label="All probed")
    Makie.scatter!(ax, x_mg_rep0[findall(_responds_sam_nop_rep0) ∩ nat_seqs], -
    aptamer_rbm_energies[findall(_responds_sam_nop_rep0) ∩ nat_seqs], markersize=15,
    color=:green, marker='0')
    Makie.scatter!(ax, x_mg_rep0[findall(_responds_sam_yes_rep0) ∩ nat_seqs], -
    aptamer_rbm_energies[findall(_responds_sam_yes_rep0) ∩ nat_seqs], markersize=15,
    color=:green, marker='●')
    Makie.scatter!(ax, x_mg_rep0[findall(_responds_sam_nop_rep0) ∩ inf_seqs], -
    aptamer_rbm_energies[findall(_responds_sam_nop_rep0) ∩ inf_seqs], markersize=15,
    color=:red, marker='0')
    Makie.scatter!(ax, x_mg_rep0[findall(_responds_sam_yes_rep0) ∩ inf_seqs], -
    aptamer_rbm_energies[findall(_responds_sam_yes_rep0) ∩ inf_seqs], markersize=15,
    color=:red, marker='•')
    Makie.scatter!(ax, x_mg_rep0[findall(_responds_sam_nop_rep0) ∩ rbm_seqs], -
    aptamer_rbm_energies[findall(_responds_sam_nop_rep0) ∩ rbm_seqs], markersize=15,
    color=:blue, marker='0')
```

```
Makie.scatter!(ax, x_mg_rep0[findall(_responds_sam_yes_rep0) ∩ rbm_seqs], -
aptamer_rbm_energies[findall(_responds_sam_yes_rep0) ∩ rbm_seqs], markersize=15,
color=:blue, marker='•')
Makie.vlines!(ax, [-_thresh, _thresh], linestyle=:dash, color=:orange)
ax = Makie.Axis(fig[1,1][1,2]; halign=:left, width=200, height=200, xlabel="Protect.
score(hallmark sites)", ylabel="RBM score", title="with SAM", xgridvisible=false,
ygridvisible=false)
#Makie.scatter!(ax, x_sam_rep0, -aptamer_rbm_energies, markersize=10, color=(:gray,
0.5), label="All probed")
plt1 = Makie.scatter!(ax, x_sam_rep0[findall(_responds_sam_nop_rep0) ∩ nat_seqs], -
aptamer_rbm_energies[findall(_responds_sam_nop_rep0) ∩ nat_seqs], markersize=15,
color=:green, marker='0', label="Nat. (*)")
plt2 = Makie.scatter!(ax, x_sam_rep0[findall(_responds_sam_yes_rep0) ∩ nat_seqs], -
aptamer_rbm_energies[findall(_responds_sam_yes_rep0) ∩ nat_seqs], markersize=15,
color=:green, marker='•', label="Nat. (√)")
plt3 = Makie.scatter!(ax, x_sam_rep0[findall(_responds_sam_nop_rep0) ∩ inf_seqs], -
aptamer_rbm_energies[findall(_responds_sam_nop_rep0) ∩ inf_seqs], markersize=15,
color=:red, marker='0', label="CM (*)")
plt4 = Makie.scatter!(ax, x_sam_rep0[findall(_responds_sam_yes_rep0) ∩ inf_seqs], -
aptamer_rbm_energies[findall(_responds_sam_yes_rep0) ∩ inf_seqs], markersize=15,
color=:red, marker='•', label="CM (√)")
plt5 = Makie.scatter!(ax, x_sam_rep0[findall(_responds_sam_nop_rep0) ∩ rbm_seqs], -
aptamer_rbm_energies[findall(_responds_sam_nop_rep0) ∩ rbm_seqs], markersize=15,
color=:blue, marker='0', label="RBM (*)")
plt6 = Makie.scatter!(ax, x_sam_rep0[findall(_responds_sam_yes_rep0) ∩ rbm_seqs], -
aptamer_rbm_energies[findall(_responds_sam_yes_rep0) ∩ rbm_seqs], markersize=15,
color=:blue, marker='•', label="RBM (√)")
Makie.vlines!(ax, [-_thresh, _thresh], linestyle=:dash, color=:orange)
#Makie.xlims!(ax, -78, 35)
Makie.hideydecorations!(ax)
#Makie.axislegend(ax, position=:rt, framevisible=false)
Makie.Legend(fig[1,1][1,3],
    [plt1, plt2, plt3, plt4, plt5, plt6],
    ["Nat. (*)", "Nat. (\checkmark)", "rCM (*)", "rCM (\checkmark)", "RBM (*)", "RBM (\checkmark)"],
    framevisible=false
)
\# _dummy_ax = Makie.Axis(fig[1,2], width=400, height=300, xgridvisible=false,
ygridvisible=false) # placeholder for the table
# Makie.hidexdecorations!(_dummy_ax)
# Makie.hideydecorations!(_dummy_ax)
# Makie.hidespines!(_dummy_ax, :t, :b, :1, :r)
n_ex_rbm = 299 # rbm example, switcher
#n_ex_nat = 112 # natural example, responsive but not switcher
n_ex_nat = 101 # natural example, responsive but not switcher
_{\text{width}} = 550
_{height} = 70
_R_sam = shape_data_all_merged.shape_reactivities[:, n_ex_rbm,
conds_SAM_all_merged[1]]
_R_mg = shape_data_all_merged.shape_reactivities[:, n_ex_rbm,
only(conds_Mg_all_merged)]
ax_react_1 = Makie.Axis(fig[2,1][1,1], width=_width, height=_height,
xticks=5:10:108, ylabel="reactivity", xgridvisible=false, ygridvisible=false,
yticks=0:2:5, ytrimspine=true)
for (x0, xf, color, alpha) = struct_bands
```

```
Makie.vspan!(ax_react_1, x0, xf; color=(color, alpha))
end
Makie.stairs!(ax_react_1, 1:108, _R_mg, color=:gray, step=:center)
Makie.stairs!(ax_react_1, 1:108, _R_sam, color=:purple, step=:center)
Makie.xlims!(ax_react_1, 0.5, 108.5)
Makie.ylims!(ax_react_1, -1, 4)
Makie.hidespines!(ax_react_1, :t, :r, :b)
Makie.hidexdecorations!(ax_react_1)
ax_diff_1 = Makie.Axis(fig[2,1][2,1]; width=_width, height=_height, xticks=5:10:108,
xlabel="site", ylabel="∆reactivity", xgridvisible=false, ygridvisible=false,
xtrimspine=true, ytrimspine=true, yticks=-2:2)
for (x0, xf, color, alpha) = struct_bands
    Makie.vspan!(ax_diff_1, x0, xf; color=(color, alpha))
end
Makie.barplot!(ax_diff_1, 1:108, _R_sam - _R_mg, color=ifelse.(_R_sam - _R_mg .< 0,</pre>
:green, :gray))
Makie.xlims!(ax_diff_1, 0.5, 108.5)
Makie.ylims!(ax_diff_1, -1.5, 1.5)
Makie.hidespines!(ax_diff_1, :t, :b, :r)
Makie.hidexdecorations!(ax_diff_1)
_R_sam = shape_data_all_merged.shape_reactivities[:, n_ex_nat,
conds_SAM_all_merged[1]]
_R_mg = shape_data_all_merged.shape_reactivities[:, n_ex_nat,
only(conds_Mg_all_merged)]
ax_react_2 = Makie.Axis(fig[2,1][3,1], width=_width, height=_height,
xticks=10:10:108, ylabel="reactivity", xgridvisible=false, ygridvisible=false,
yticks=0:2:5, ytrimspine=true)
for (x0, xf, color, alpha) = struct_bands
    Makie.vspan!(ax_react_2, x0, xf; color=(color, alpha))
end
Makie.stairs!(ax_react_2, 1:108, _R_mg, color=:gray, step=:center)
Makie.stairs!(ax_react_2, 1:108, _R_sam, color=:purple, step=:center)
Makie.xlims!(ax_react_2, 0.5, 108.5)
Makie.ylims!(ax_react_2, -1, 6)
Makie.hidespines!(ax_react_2, :t, :r, :b)
Makie.hidexdecorations!(ax_react_2)
#Makie.hideydecorations!(ax_react_2)
ax_diff_2 = Makie.Axis(fig[2,1][4,1]; width=_width, height=_height, xticks=5:10:108,
xlabel="site", ylabel="∆reactivity", xgridvisible=false, ygridvisible=false,
xtrimspine=true, ytrimspine=true, yticks=-2:2)
for (x0, xf, color, alpha) = struct_bands
    Makie.vspan!(ax_diff_2, x0, xf; color=(color, alpha))
end
Makie.barplot!(ax_diff_2, 1:108, _R_sam - _R_mg, color=ifelse.(_R_sam - _R_mg .< 0,
:green, :gray))
Makie.scatter!(ax_diff_2, _sites, -1.4one.(_sites), markersize=7, color=:black,
marker=:utriangle)
Makie.xlims!(ax_diff_2, 0, 109)
Makie.ylims!(ax_diff_2, -1.5, 1)
Makie.hidespines!(ax_diff_2, :t, :r)
#Makie.hideydecorations!(ax_diff_2)
# Makie.scatter!(ax_diff_1, _sites, one.(_sites), color=:blue, markersize=5)
# Makie.scatter!(ax_diff_2, _sites, one.(_sites), color=:blue, markersize=5)
Makie.linkxaxes!(ax_react_1, ax_diff_1)
```

```
Makie.linkxaxes!(ax_react_2, ax_diff_2)

Makie.linkyaxes!(ax_react_1, ax_react_2)

Makie.linkyaxes!(ax_diff_1, ax_diff_2)

Makie.resize_to_layout!(fig)

#Makie.save("Figures/SAM response Replo v2.pdf", fig)
```