Generamos esqueletos con RFDifussion

In [21]:
```python
def run_rfdiffusion(output_name):
    """
    Ejecuta RFdiffusion con parámetros personalizados
    """
    import subprocess
    cmd = [
    "python", "../scripts/run_inference.py",
    "contigmap.contigs=[150-200]",                      # Longitud del contig 150-200 que suelen tener análogos de insulina
    f"inference.output_prefix=outputs/{output_name}",   #Nombre de carpeta de salida donde estarán los pdb
    "inference.num_designs=10",                         #Número de candidatos 10
    "diffuser.T=50",                                    #Temperatura del difussor, permite diversidad sin sacrificar estabilidad
    # Simetría
    #"inference.symmetry=C2",
    # Escribir trayectorias
    "inference.write_trajectory=True",
    # Parametros de reciclo para entrenamiento
    "denoiser.noise_scale_ca=1.0",
    "denoiser.noise_scale_frame=1.0",
    # Potenciales para mejorar plegamiento
    "potentials.guiding_potentials=['type:monomer_ROG']",
    "potentials.guide_scale=2.0"
]

    # Ejecutar
    result = subprocess.run(" ".join(cmd), shell=True, capture_output=True, text=True)
    print(result.stdout)
    print(result.stderr)

    return f"outputs/{output_name}_0.pdb"
```

In [22]:
```python
pdb_file = run_rfdiffusion(output_name='diabetes_therapeutic')
print(f"✅ RF Difussion ejecutado correctament. Generado: {pdb_file}")
```

```
[2025-10-05 14:40:49,207][__main__][INFO] - Found GPU with device_name NVIDIA GeForce GTX 1650. Will run RFdiffusion on NVIDIA GeForce GTX 165
0
Reading models from /home/kevinwsl/RFdiffusion/rfdiffusion/inference/../../models
[2025-10-05 14:40:49,208][rfdiffusion.inference.model_runners][INFO] - Reading checkpoint from /home/kevinwsl/RFdiffusion/rfdiffusion/inferenc
e/../../models/Base_ckpt.pt
This is inf_conf.ckpt_path
/home/kevinwsl/RFdiffusion/rfdiffusion/inference/../../models/Base_ckpt.pt
Assembling -model, -diffuser and -preprocess configs from checkpoint
USING MODEL CONFIG: self._conf[model][n_extra_block] = 4
USING MODEL CONFIG: self._conf[model][n_main_block] = 32
USING MODEL CONFIG: self._conf[model][n_ref_block] = 4
USING MODEL CONFIG: self._conf[model][d_msa] = 256
USING MODEL CONFIG: self._conf[model][d_msa_full] = 64
USING MODEL CONFIG: self._conf[model][d_pair] = 128
USING MODEL CONFIG: self._conf[model][d_templ] = 64
USING MODEL CONFIG: self._conf[model][n_head_msa] = 8
USING MODEL CONFIG: self._conf[model][n_head_pair] = 4
USING MODEL CONFIG: self._conf[model][n_head_templ] = 4
USING MODEL CONFIG: self._conf[model][d_hidden] = 32
USING MODEL CONFIG: self._conf[model][d_hidden_templ] = 32
USING MODEL CONFIG: self._conf[model][p_drop] = 0.15
USING MODEL CONFIG: self._conf[model][SE3_param_full] = {'num_layers': 1, 'num_channels': 32, 'num_degrees': 2, 'n_heads': 4, 'div': 4, 'l0_in
_features': 8, 'l0_out_features': 8, 'l1_in_features': 3, 'l1_out_features': 2, 'num_edge_features': 32}
USING MODEL CONFIG: self._conf[model][SE3_param_topk] = {'num_layers': 1, 'num_channels': 32, 'num_degrees': 2, 'n_heads': 4, 'div': 4, 'l0_in
_features': 64, 'l0_out_features': 64, 'l1_in_features': 3, 'l1_out_features': 2, 'num_edge_features': 64}
USING MODEL CONFIG: self._conf[model][freeze_track_motif] = False
USING MODEL CONFIG: self._conf[model][use_motif_timestep] = True
USING MODEL CONFIG: self._conf[diffuser][T] = 50
USING MODEL CONFIG: self._conf[diffuser][b_0] = 0.01
USING MODEL CONFIG: self._conf[diffuser][b_T] = 0.07
USING MODEL CONFIG: self._conf[diffuser][schedule_type] = linear
USING MODEL CONFIG: self._conf[diffuser][so3_type] = igso3
USING MODEL CONFIG: self._conf[diffuser][crd_scale] = 0.25
USING MODEL CONFIG: self._conf[diffuser][so3_schedule_type] = linear
USING MODEL CONFIG: self._conf[diffuser][min_b] = 1.5
USING MODEL CONFIG: self._conf[diffuser][max_b] = 2.5
USING MODEL CONFIG: self._conf[diffuser][min_sigma] = 0.02
USING MODEL CONFIG: self._conf[diffuser][max_sigma] = 1.5
USING MODEL CONFIG: self._conf[preprocess][sidechain_input] = False
USING MODEL CONFIG: self._conf[preprocess][motif_sidechain_input] = True
USING MODEL CONFIG: self._conf[preprocess][d_t1d] = 22
USING MODEL CONFIG: self._conf[preprocess][d_t2d] = 44
USING MODEL CONFIG: self._conf[preprocess][prob_self_cond] = 0.5
USING MODEL CONFIG: self._conf[preprocess][str_self_cond] = True
USING MODEL CONFIG: self._conf[preprocess][predict_previous] = False
WARNING: You are changing diffuser.T from the value this model was trained with. Are you sure you know what you are doing?
[2025-10-05 14:40:54,806][rfdiffusion.inference.model_runners][INFO] - Loading checkpoint.
[2025-10-05 14:40:55,014][rfdiffusion.diffusion][INFO] - Using cached IGSO3.
Successful diffuser __init__
[2025-10-05 14:40:55,024][__main__][INFO] - Making design outputs/diabetes_therapeutic_0
[2025-10-05 14:40:55,027][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 14:40:55,063][rfdiffusion.inference.model_runners][INFO] - Sequence init:
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[2025-10-05 14:41:01,698][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:
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[2025-10-05 14:41:05,446][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:
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[2025-10-05 14:41:09,158][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:
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[2025-10-05 14:41:12,922][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:
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[2025-10-05 14:41:16,688][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:
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[2025-10-05 14:41:20,436][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:
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[2025-10-05 14:41:24,163][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:
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[2025-10-05 14:41:27,857][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:
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[2025-10-05 14:41:31,666][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:
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[2025-10-05 14:41:35,456][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:
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[2025-10-05 14:41:39,413][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:
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[2025-10-05 14:41:43,292][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:
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[2025-10-05 14:41:47,073][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:
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[2025-10-05 14:41:50,949][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:
[2025-10-05 14:41:54,888][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:
[2025-10-05 14:41:58,753][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:
[2025-10-05 14:42:02,636][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:
[2025-10-05 14:42:06,530][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:
[2025-10-05 14:42:10,397][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:
[2025-10-05 14:42:14,238][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:
[2025-10-05 14:42:18,064][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:
[2025-10-05 14:42:21,954][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:
[2025-10-05 14:42:25,879][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:
[2025-10-05 14:42:29,877][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:
[2025-10-05 14:42:33,695][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:
[2025-10-05 14:42:37,553][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:
[2025-10-05 14:42:41,383][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:
[2025-10-05 14:42:45,315][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:
[2025-10-05 14:42:49,138][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:
[2025-10-05 14:42:52,931][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:
[2025-10-05 14:42:56,767][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:
[2025-10-05 14:43:00,588][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:
[2025-10-05 14:43:04,313][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:
[2025-10-05 14:43:08,017][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:
[2025-10-05 14:43:11,820][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:
[2025-10-05 14:43:15,631][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:
[2025-10-05 14:43:19,470][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:
[2025-10-05 14:43:23,371][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:
[2025-10-05 14:43:27,190][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:
[2025-10-05 14:43:31,042][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:
[2025-10-05 14:43:34,907][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:
[2025-10-05 14:43:38,700][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:
[2025-10-05 14:43:42,524][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:
[2025-10-05 14:43:46,584][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:
[2025-10-05 14:43:50,471][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:
[2025-10-05 14:43:54,385][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:
[2025-10-05 14:43:58,273][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:
[2025-10-05 14:44:02,237][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:
[2025-10-05 14:44:06,073][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:
[2025-10-05 14:44:12,049][__main__][INFO] - Finished design in 3.28 minutes
[2025-10-05 14:44:12,049][__main__][INFO] - Making design outputs/diabetes_therapeutic_1
[2025-10-05 14:44:12,053][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 14:44:12,073][rfdiffusion.inference.model_runners][INFO] - Sequence init:
[2025-10-05 14:44:15,962][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:
[2025-10-05 14:44:19,615][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:
[2025-10-05 14:44:23,158][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:
[2025-10-05 14:44:26,767][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:
[2025-10-05 14:44:30,364][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:
[2025-10-05 14:44:34,031][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:
[2025-10-05 14:44:37,760][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:
[2025-10-05 14:44:41,320][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:
[2025-10-05 14:44:44,815][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:
[2025-10-05 14:44:48,363][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:
[2025-10-05 14:44:51,886][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:
[2025-10-05 14:44:55,432][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:
[2025-10-05 14:44:58,987][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:
[2025-10-05 14:45:02,522][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:
[2025-10-05 14:45:06,127][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:
[2025-10-05 14:45:09,675][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:
[2025-10-05 14:45:13,103][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:
[2025-10-05 14:45:16,588][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:
[2025-10-05 14:45:20,122][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:
[2025-10-05 14:45:23,717][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:
[2025-10-05 14:45:27,251][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:
[2025-10-05 14:45:30,825][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:
[2025-10-05 14:45:34,358][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:

[2025-10-05 14:45:37,924][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:
[2025-10-05 14:45:41,503][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:
[2025-10-05 14:45:44,940][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:
[2025-10-05 14:45:48,410][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:
[2025-10-05 14:45:51,913][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:
[2025-10-05 14:45:55,384][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:
[2025-10-05 14:45:58,938][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:
[2025-10-05 14:46:02,472][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:
[2025-10-05 14:46:06,007][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:
[2025-10-05 14:46:09,554][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:
[2025-10-05 14:46:13,057][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:
[2025-10-05 14:46:16,547][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:
[2025-10-05 14:46:19,962][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:
[2025-10-05 14:46:23,441][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:
[2025-10-05 14:46:26,930][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:
[2025-10-05 14:46:30,566][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:
[2025-10-05 14:46:34,125][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:
[2025-10-05 14:46:37,726][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:
[2025-10-05 14:46:41,314][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:
[2025-10-05 14:46:44,926][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:
[2025-10-05 14:46:48,438][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:
[2025-10-05 14:46:51,911][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:
[2025-10-05 14:46:55,389][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:
[2025-10-05 14:46:58,910][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:
[2025-10-05 14:47:02,463][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:
[2025-10-05 14:47:06,044][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:
[2025-10-05 14:47:12,061][__main__][INFO] - Finished design in 3.00 minutes
[2025-10-05 14:47:12,061][__main__][INFO] - Making design outputs/diabetes_therapeutic_2
[2025-10-05 14:47:12,066][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 14:47:12,094][rfdiffusion.inference.model_runners][INFO] - Sequence init:
[2025-10-05 14:47:16,312][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:
[2025-10-05 14:47:20,324][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:
[2025-10-05 14:47:24,285][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:
[2025-10-05 14:47:28,423][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:
[2025-10-05 14:47:32,562][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:
[2025-10-05 14:47:36,754][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:
[2025-10-05 14:47:41,012][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:
[2025-10-05 14:47:45,271][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:
[2025-10-05 14:47:49,486][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:
[2025-10-05 14:47:53,549][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:
[2025-10-05 14:47:57,597][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:
[2025-10-05 14:48:01,697][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:
[2025-10-05 14:48:05,873][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:
[2025-10-05 14:48:10,041][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:
[2025-10-05 14:48:14,215][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:
[2025-10-05 14:48:18,366][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:
[2025-10-05 14:48:22,598][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:
[2025-10-05 14:48:26,661][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:
[2025-10-05 14:48:30,730][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:
[2025-10-05 14:48:34,835][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:
[2025-10-05 14:48:38,967][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:
[2025-10-05 14:48:43,081][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:
[2025-10-05 14:48:47,188][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:
[2025-10-05 14:48:51,338][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:
[2025-10-05 14:48:55,515][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:
[2025-10-05 14:48:59,569][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:
[2025-10-05 14:49:03,620][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:
[2025-10-05 14:49:07,718][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:
[2025-10-05 14:49:11,862][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:
[2025-10-05 14:49:16,051][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:
[2025-10-05 14:49:20,186][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:
[2025-10-05 14:49:24,472][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:
[2025-10-05 14:49:28,654][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:

[2025-10-05 14:49:32,702][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:
[2025-10-05 14:49:36,765][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:
[2025-10-05 14:49:40,895][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:
[2025-10-05 14:49:45,055][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:
[2025-10-05 14:49:49,238][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:
[2025-10-05 14:49:53,398][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:
[2025-10-05 14:49:57,533][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:
[2025-10-05 14:50:01,681][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:
[2025-10-05 14:50:05,750][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:
[2025-10-05 14:50:09,817][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:
[2025-10-05 14:50:13,947][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:
[2025-10-05 14:50:18,073][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:
[2025-10-05 14:50:22,249][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:
[2025-10-05 14:50:26,418][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:
[2025-10-05 14:50:30,598][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:
[2025-10-05 14:50:34,717][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:
[2025-10-05 14:50:40,960][__main__][INFO] - Finished design in 3.48 minutes
[2025-10-05 14:50:40,960][__main__][INFO] - Making design outputs/diabetes_therapeutic_3
[2025-10-05 14:50:40,963][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 14:50:40,988][rfdiffusion.inference.model_runners][INFO] - Sequence init:
[2025-10-05 14:50:45,729][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:
[2025-10-05 14:50:50,381][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:
[2025-10-05 14:50:54,992][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:
[2025-10-05 14:50:59,614][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:
[2025-10-05 14:51:04,342][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:
[2025-10-05 14:51:08,820][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:
[2025-10-05 14:51:13,287][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:
[2025-10-05 14:51:17,832][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:
[2025-10-05 14:51:22,408][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:
[2025-10-05 14:51:27,011][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:
[2025-10-05 14:51:31,593][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:
[2025-10-05 14:51:36,182][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:
[2025-10-05 14:51:40,702][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:
[2025-10-05 14:51:45,217][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:
[2025-10-05 14:51:49,764][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:
[2025-10-05 14:51:54,343][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:
[2025-10-05 14:51:59,525][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:
[2025-10-05 14:52:04,755][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:
[2025-10-05 14:52:10,003][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:
[2025-10-05 14:52:15,064][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:
[2025-10-05 14:52:20,279][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:
[2025-10-05 14:52:25,556][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:
[2025-10-05 14:52:30,876][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:
[2025-10-05 14:52:36,170][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:
[2025-10-05 14:52:41,398][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:
[2025-10-05 14:52:46,584][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:
[2025-10-05 14:52:51,783][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:
[2025-10-05 14:52:57,221][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:
[2025-10-05 14:53:02,455][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:
[2025-10-05 14:53:07,772][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:
[2025-10-05 14:53:13,022][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:
[2025-10-05 14:53:18,346][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:
[2025-10-05 14:53:23,527][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:
[2025-10-05 14:53:28,730][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:
[2025-10-05 14:53:34,000][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:
[2025-10-05 14:53:39,236][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:
[2025-10-05 14:53:44,535][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:
[2025-10-05 14:53:49,719][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:
[2025-10-05 14:53:54,890][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:
[2025-10-05 14:54:00,106][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:
[2025-10-05 14:54:05,321][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:
[2025-10-05 14:54:10,602][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:
[2025-10-05 14:54:15,918][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:

[2025-10-05 14:54:21,100][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:

[2025-10-05 14:54:26,235][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:

[2025-10-05 14:54:31,448][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:

[2025-10-05 14:54:36,728][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:

[2025-10-05 14:54:41,967][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:

[2025-10-05 14:54:47,264][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:

[2025-10-05 14:54:54,905][__main__][INFO] - Finished design in 4.23 minutes
[2025-10-05 14:54:54,905][__main__][INFO] - Making design outputs/diabetes_therapeutic_4
[2025-10-05 14:54:54,909][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 14:54:54,928][rfdiffusion.inference.model_runners][INFO] - Sequence init:

[2025-10-05 14:54:58,784][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:

[2025-10-05 14:55:02,630][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:

[2025-10-05 14:55:06,423][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:

[2025-10-05 14:55:10,277][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:

[2025-10-05 14:55:14,090][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:

[2025-10-05 14:55:17,915][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:

[2025-10-05 14:55:21,918][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:

[2025-10-05 14:55:25,738][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:

[2025-10-05 14:55:29,476][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:

[2025-10-05 14:55:33,289][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:

[2025-10-05 14:55:37,090][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:

[2025-10-05 14:55:40,953][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:

[2025-10-05 14:55:44,753][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:

[2025-10-05 14:55:48,559][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:

[2025-10-05 14:55:52,445][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:

[2025-10-05 14:55:56,272][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:

[2025-10-05 14:55:59,997][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:

[2025-10-05 14:56:03,834][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:

[2025-10-05 14:56:07,568][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:

[2025-10-05 14:56:11,314][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:

[2025-10-05 14:56:15,051][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:

[2025-10-05 14:56:18,815][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:

[2025-10-05 14:56:22,679][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:

[2025-10-05 14:56:26,643][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:

[2025-10-05 14:56:30,419][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:

[2025-10-05 14:56:34,177][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:

[2025-10-05 14:56:37,945][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:

[2025-10-05 14:56:41,824][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:

[2025-10-05 14:56:45,607][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:

[2025-10-05 14:56:49,417][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:

[2025-10-05 14:56:53,152][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:

[2025-10-05 14:56:56,914][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:

[2025-10-05 14:57:00,698][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:

[2025-10-05 14:57:04,392][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:

[2025-10-05 14:57:08,108][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:

[2025-10-05 14:57:11,830][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:

[2025-10-05 14:57:15,618][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:

[2025-10-05 14:57:19,440][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:

[2025-10-05 14:57:23,249][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:

[2025-10-05 14:57:27,073][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:

[2025-10-05 14:57:30,863][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:

[2025-10-05 14:57:34,533][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:

[2025-10-05 14:57:38,407][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:

[2025-10-05 14:57:42,184][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:

[2025-10-05 14:57:45,991][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:

[2025-10-05 14:57:49,871][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:

[2025-10-05 14:57:53,860][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:

[2025-10-05 14:57:57,741][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:

[2025-10-05 14:58:01,585][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:

[2025-10-05 14:58:07,537][__main__][INFO] - Finished design in 3.21 minutes
[2025-10-05 14:58:07,537][__main__][INFO] - Making design outputs/diabetes_therapeutic_5
[2025-10-05 14:58:07,542][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 14:58:07,568][rfdiffusion.inference.model_runners][INFO] - Sequence init:

[2025-10-05 14:58:11,378][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:

[2025-10-05 14:58:15,100][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:

[2025-10-05 14:58:18,946][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:

[2025-10-05 14:58:22,762][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:

[2025-10-05 14:58:26,655][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:

[2025-10-05 14:58:30,468][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:

[2025-10-05 14:58:34,310][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:

[2025-10-05 14:58:38,085][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:

[2025-10-05 14:58:41,786][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:

[2025-10-05 14:58:45,442][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:

[2025-10-05 14:58:49,233][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:

[2025-10-05 14:58:53,147][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:

[2025-10-05 14:58:56,965][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:

[2025-10-05 14:59:00,736][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:

[2025-10-05 14:59:04,594][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:

[2025-10-05 14:59:08,419][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:

[2025-10-05 14:59:12,205][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:

[2025-10-05 14:59:16,011][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:

[2025-10-05 14:59:19,871][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:

[2025-10-05 14:59:23,728][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:

[2025-10-05 14:59:27,632][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:

[2025-10-05 14:59:31,501][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:

[2025-10-05 14:59:35,446][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:

[2025-10-05 14:59:39,260][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:

[2025-10-05 14:59:43,022][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:

[2025-10-05 14:59:46,862][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:

[2025-10-05 14:59:50,620][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:

[2025-10-05 14:59:54,511][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:

[2025-10-05 14:59:58,641][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:

[2025-10-05 15:00:02,582][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:

[2025-10-05 15:00:06,401][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:

[2025-10-05 15:00:10,145][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:

[2025-10-05 15:00:13,934][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:

[2025-10-05 15:00:17,587][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:

[2025-10-05 15:00:21,319][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:

[2025-10-05 15:00:25,084][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:

[2025-10-05 15:00:28,988][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:

[2025-10-05 15:00:32,944][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:

[2025-10-05 15:00:36,843][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:

[2025-10-05 15:00:40,624][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:

[2025-10-05 15:00:44,451][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:

[2025-10-05 15:00:48,247][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:

[2025-10-05 15:00:52,133][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:

[2025-10-05 15:00:55,883][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:

[2025-10-05 15:00:59,663][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:

[2025-10-05 15:01:03,414][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:

[2025-10-05 15:01:07,175][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:

[2025-10-05 15:01:10,991][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:

[2025-10-05 15:01:14,834][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:

[2025-10-05 15:01:20,785][__main__][INFO] - Finished design in 3.22 minutes
[2025-10-05 15:01:20,785][__main__][INFO] - Making design outputs/diabetes_therapeutic_6
[2025-10-05 15:01:20,788][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 15:01:20,807][rfdiffusion.inference.model_runners][INFO] - Sequence init:

[2025-10-05 15:01:24,955][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:

[2025-10-05 15:01:29,164][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:

[2025-10-05 15:01:33,472][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:

[2025-10-05 15:01:37,866][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:

[2025-10-05 15:01:42,134][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:

[2025-10-05 15:01:46,691][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:

[2025-10-05 15:01:50,946][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:

[2025-10-05 15:01:55,153][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:

[2025-10-05 15:01:59,330][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:

[2025-10-05 15:02:03,484][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:

[2025-10-05 15:02:07,681][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:

[2025-10-05 15:02:11,949][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:

[2025-10-05 15:02:16,276][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:

[2025-10-05 15:02:20,638][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:

[2025-10-05 15:02:24,928][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:

[2025-10-05 15:02:29,190][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:

[2025-10-05 15:02:33,367][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:

[2025-10-05 15:02:37,722][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:

[2025-10-05 15:02:42,170][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:

[2025-10-05 15:02:46,592][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:

[2025-10-05 15:02:51,007][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:

[2025-10-05 15:02:55,350][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:

[2025-10-05 15:02:59,528][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:

[2025-10-05 15:03:03,761][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:

[2025-10-05 15:03:08,093][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:

[2025-10-05 15:03:12,411][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:

[2025-10-05 15:03:16,718][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:

[2025-10-05 15:03:20,919][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:

[2025-10-05 15:03:25,256][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:

[2025-10-05 15:03:29,374][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:

[2025-10-05 15:03:33,530][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:

[2025-10-05 15:03:37,651][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:

[2025-10-05 15:03:42,018][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:

[2025-10-05 15:03:46,203][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:

[2025-10-05 15:03:50,358][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:

[2025-10-05 15:03:54,390][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:

[2025-10-05 15:03:57,754][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:

[2025-10-05 15:04:01,027][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:

[2025-10-05 15:04:04,286][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:

[2025-10-05 15:04:07,591][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:

[2025-10-05 15:04:10,924][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:

[2025-10-05 15:04:14,249][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:

[2025-10-05 15:04:17,710][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:

[2025-10-05 15:04:21,118][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:

[2025-10-05 15:04:24,498][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:

[2025-10-05 15:04:27,879][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:

[2025-10-05 15:04:31,246][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:

[2025-10-05 15:04:34,529][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:

[2025-10-05 15:04:37,801][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:

[2025-10-05 15:04:42,969][__main__][INFO] - Finished design in 3.37 minutes
[2025-10-05 15:04:42,970][__main__][INFO] - Making design outputs/diabetes_therapeutic_7
[2025-10-05 15:04:42,974][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 15:04:42,995][rfdiffusion.inference.model_runners][INFO] - Sequence init:

[2025-10-05 15:04:46,069][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:

[2025-10-05 15:04:48,854][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:

[2025-10-05 15:04:51,751][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:

[2025-10-05 15:04:54,573][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:

[2025-10-05 15:04:57,391][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:

[2025-10-05 15:05:00,222][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:

[2025-10-05 15:05:03,049][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:

[2025-10-05 15:05:05,838][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:

[2025-10-05 15:05:08,560][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:

[2025-10-05 15:05:11,354][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:

[2025-10-05 15:05:14,110][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:

[2025-10-05 15:05:17,023][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:

[2025-10-05 15:05:19,959][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:

[2025-10-05 15:05:22,936][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:

[2025-10-05 15:05:25,822][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:

[2025-10-05 15:05:28,687][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:

[2025-10-05 15:05:31,615][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:

[2025-10-05 15:05:34,473][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:

[2025-10-05 15:05:37,406][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:

[2025-10-05 15:05:40,257][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:

[2025-10-05 15:05:43,120][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:

[2025-10-05 15:05:45,993][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:

[2025-10-05 15:05:48,754][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:

[2025-10-05 15:05:51,544][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:

[2025-10-05 15:05:54,487][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:

[2025-10-05 15:05:57,299][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:

[2025-10-05 15:06:00,102][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:

[2025-10-05 15:06:02,910][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:

[2025-10-05 15:06:05,733][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:

[2025-10-05 15:06:08,505][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:

[2025-10-05 15:06:11,255][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:

[2025-10-05 15:06:13,951][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:

[2025-10-05 15:06:16,835][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:

[2025-10-05 15:06:19,720][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:

[2025-10-05 15:06:22,763][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:

[2025-10-05 15:06:25,810][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:

[2025-10-05 15:06:28,716][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:

[2025-10-05 15:06:31,665][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:

[2025-10-05 15:06:34,514][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:

[2025-10-05 15:06:37,336][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:

[2025-10-05 15:06:40,134][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:

[2025-10-05 15:06:42,875][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:

[2025-10-05 15:06:45,626][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:

[2025-10-05 15:06:48,369][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:

[2025-10-05 15:06:51,205][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:

[2025-10-05 15:06:54,027][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:

[2025-10-05 15:06:56,870][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:

[2025-10-05 15:06:59,657][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:

[2025-10-05 15:07:02,470][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:

[2025-10-05 15:07:06,971][__main__][INFO] - Finished design in 2.40 minutes
[2025-10-05 15:07:06,971][__main__][INFO] - Making design outputs/diabetes_therapeutic_8
[2025-10-05 15:07:06,975][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 15:07:06,994][rfdiffusion.inference.model_runners][INFO] - Sequence init:

[2025-10-05 15:07:10,685][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:

[2025-10-05 15:07:14,260][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:

[2025-10-05 15:07:17,847][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:

[2025-10-05 15:07:21,464][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:

[2025-10-05 15:07:25,105][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:

[2025-10-05 15:07:28,762][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:

[2025-10-05 15:07:32,422][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:

[2025-10-05 15:07:36,082][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:

[2025-10-05 15:07:39,841][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:

[2025-10-05 15:07:43,591][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:

[2025-10-05 15:07:47,243][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:

[2025-10-05 15:07:50,872][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:

[2025-10-05 15:07:54,542][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:

[2025-10-05 15:07:58,251][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:

[2025-10-05 15:08:02,262][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:

[2025-10-05 15:08:05,994][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:

[2025-10-05 15:08:09,817][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:

[2025-10-05 15:08:13,566][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:

[2025-10-05 15:08:17,273][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:

[2025-10-05 15:08:20,829][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:

[2025-10-05 15:08:25,032][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:

[2025-10-05 15:08:28,868][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:

[2025-10-05 15:08:32,729][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:

[2025-10-05 15:08:36,509][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:

[2025-10-05 15:08:40,331][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:

[2025-10-05 15:08:44,024][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:

[2025-10-05 15:08:47,866][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:

[2025-10-05 15:08:51,533][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:

[2025-10-05 15:08:55,251][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:

[2025-10-05 15:08:58,940][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:

[2025-10-05 15:09:03,293][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:

[2025-10-05 15:09:07,838][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:

[2025-10-05 15:09:12,149][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:

[2025-10-05 15:09:16,567][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:

[2025-10-05 15:09:20,961][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:

[2025-10-05 15:09:25,232][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:

[2025-10-05 15:09:29,525][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:

[2025-10-05 15:09:33,809][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:

[2025-10-05 15:09:38,265][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:

[2025-10-05 15:09:42,603][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:

[2025-10-05 15:09:46,975][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:

[2025-10-05 15:09:51,302][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:

[2025-10-05 15:09:55,507][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:

[2025-10-05 15:09:59,709][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:

[2025-10-05 15:10:04,093][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:

[2025-10-05 15:10:08,414][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:

[2025-10-05 15:10:13,053][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:

[2025-10-05 15:10:17,625][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:

[2025-10-05 15:10:22,375][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:

[2025-10-05 15:10:28,928][__main__][INFO] - Finished design in 3.37 minutes
[2025-10-05 15:10:28,929][__main__][INFO] - Making design outputs/diabetes_therapeutic_9
[2025-10-05 15:10:28,932][rfdiffusion.inference.model_runners][INFO] - Using contig: ['150-200']
With this beta schedule (linear schedule, beta_0 = 0.04, beta_T = 0.28), alpha_bar_T = 0.00013696050154976547
[2025-10-05 15:10:28,950][rfdiffusion.inference.model_runners][INFO] - Sequence init:

[2025-10-05 15:10:31,984][rfdiffusion.inference.model_runners][INFO] - Timestep 50, input to next step:

[2025-10-05 15:10:34,802][rfdiffusion.inference.model_runners][INFO] - Timestep 49, input to next step:

[2025-10-05 15:10:37,504][rfdiffusion.inference.model_runners][INFO] - Timestep 48, input to next step:

[2025-10-05 15:10:40,404][rfdiffusion.inference.model_runners][INFO] - Timestep 47, input to next step:

[2025-10-05 15:10:43,275][rfdiffusion.inference.model_runners][INFO] - Timestep 46, input to next step:

[2025-10-05 15:10:46,482][rfdiffusion.inference.model_runners][INFO] - Timestep 45, input to next step:

[2025-10-05 15:10:49,497][rfdiffusion.inference.model_runners][INFO] - Timestep 44, input to next step:

[2025-10-05 15:10:52,227][rfdiffusion.inference.model_runners][INFO] - Timestep 43, input to next step:

[2025-10-05 15:10:54,947][rfdiffusion.inference.model_runners][INFO] - Timestep 42, input to next step:

[2025-10-05 15:10:57,701][rfdiffusion.inference.model_runners][INFO] - Timestep 41, input to next step:

[2025-10-05 15:11:00,417][rfdiffusion.inference.model_runners][INFO] - Timestep 40, input to next step:

[2025-10-05 15:11:03,116][rfdiffusion.inference.model_runners][INFO] - Timestep 39, input to next step:

[2025-10-05 15:11:05,789][rfdiffusion.inference.model_runners][INFO] - Timestep 38, input to next step:

[2025-10-05 15:11:08,500][rfdiffusion.inference.model_runners][INFO] - Timestep 37, input to next step:

[2025-10-05 15:11:11,190][rfdiffusion.inference.model_runners][INFO] - Timestep 36, input to next step:

[2025-10-05 15:11:13,946][rfdiffusion.inference.model_runners][INFO] - Timestep 35, input to next step:

[2025-10-05 15:11:16,673][rfdiffusion.inference.model_runners][INFO] - Timestep 34, input to next step:

[2025-10-05 15:11:19,364][rfdiffusion.inference.model_runners][INFO] - Timestep 33, input to next step:

[2025-10-05 15:11:22,138][rfdiffusion.inference.model_runners][INFO] - Timestep 32, input to next step:

[2025-10-05 15:11:24,880][rfdiffusion.inference.model_runners][INFO] - Timestep 31, input to next step:

[2025-10-05 15:11:27,625][rfdiffusion.inference.model_runners][INFO] - Timestep 30, input to next step:

[2025-10-05 15:11:30,412][rfdiffusion.inference.model_runners][INFO] - Timestep 29, input to next step:

[2025-10-05 15:11:33,098][rfdiffusion.inference.model_runners][INFO] - Timestep 28, input to next step:

[2025-10-05 15:11:35,823][rfdiffusion.inference.model_runners][INFO] - Timestep 27, input to next step:

[2025-10-05 15:11:38,491][rfdiffusion.inference.model_runners][INFO] - Timestep 26, input to next step:

[2025-10-05 15:11:41,260][rfdiffusion.inference.model_runners][INFO] - Timestep 25, input to next step:

[2025-10-05 15:11:44,123][rfdiffusion.inference.model_runners][INFO] - Timestep 24, input to next step:

[2025-10-05 15:11:46,932][rfdiffusion.inference.model_runners][INFO] - Timestep 23, input to next step:

[2025-10-05 15:11:49,707][rfdiffusion.inference.model_runners][INFO] - Timestep 22, input to next step:

[2025-10-05 15:11:52,505][rfdiffusion.inference.model_runners][INFO] - Timestep 21, input to next step:

[2025-10-05 15:11:55,257][rfdiffusion.inference.model_runners][INFO] - Timestep 20, input to next step:

[2025-10-05 15:11:57,946][rfdiffusion.inference.model_runners][INFO] - Timestep 19, input to next step:

[2025-10-05 15:12:00,676][rfdiffusion.inference.model_runners][INFO] - Timestep 18, input to next step:

[2025-10-05 15:12:03,407][rfdiffusion.inference.model_runners][INFO] - Timestep 17, input to next step:

[2025-10-05 15:12:06,010][rfdiffusion.inference.model_runners][INFO] - Timestep 16, input to next step:

[2025-10-05 15:12:08,645][rfdiffusion.inference.model_runners][INFO] - Timestep 15, input to next step:

[2025-10-05 15:12:11,352][rfdiffusion.inference.model_runners][INFO] - Timestep 14, input to next step:

[2025-10-05 15:12:14,028][rfdiffusion.inference.model_runners][INFO] - Timestep 13, input to next step:

[2025-10-05 15:12:16,733][rfdiffusion.inference.model_runners][INFO] - Timestep 12, input to next step:

[2025-10-05 15:12:19,407][rfdiffusion.inference.model_runners][INFO] - Timestep 11, input to next step:

[2025-10-05 15:12:22,102][rfdiffusion.inference.model_runners][INFO] - Timestep 10, input to next step:

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[2025-10-05 15:12:24,814][rfdiffusion.inference.model_runners][INFO] - Timestep 9, input to next step:
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[2025-10-05 15:12:27,496][rfdiffusion.inference.model_runners][INFO] - Timestep 8, input to next step:
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[2025-10-05 15:12:30,195][rfdiffusion.inference.model_runners][INFO] - Timestep 7, input to next step:
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[2025-10-05 15:12:32,915][rfdiffusion.inference.model_runners][INFO] - Timestep 6, input to next step:
--------------------------------------------------------------------------------------------------------------------------------------------------------------
[2025-10-05 15:12:35,623][rfdiffusion.inference.model_runners][INFO] - Timestep 5, input to next step:
--------------------------------------------------------------------------------------------------------------------------------------------------------------
[2025-10-05 15:12:38,224][rfdiffusion.inference.model_runners][INFO] - Timestep 4, input to next step:
--------------------------------------------------------------------------------------------------------------------------------------------------------------
[2025-10-05 15:12:40,827][rfdiffusion.inference.model_runners][INFO] - Timestep 3, input to next step:
--------------------------------------------------------------------------------------------------------------------------------------------------------------
[2025-10-05 15:12:43,912][rfdiffusion.inference.model_runners][INFO] - Timestep 2, input to next step:
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[2025-10-05 15:12:48,190][__main__][INFO] - Finished design in 2.32 minutes

/home/kevinwsl/RFdiffusion/rfdiffusion/util.py:253: UserWarning: Using torch.cross without specifying the dim arg is deprecated.
Please either pass the dim explicitly or simply use torch.linalg.cross.
The default value of dim will change to agree with that of linalg.cross in a future release. (Triggered internally at /opt/conda/conda-bld/pyt
orch_1729647327249/work/aten/src/ATen/native/Cross.cpp:62.)
  Z = torch.cross(Xn, Yn)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:104: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:128: FutureWarning: `torch.cuda.amp.custom_bwd
(args...)` is deprecated. Please use `torch.amp.custom_bwd(args..., device_type='cuda')` instead.
  def backward(ctx, dZ):
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:177: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:207: FutureWarning: `torch.cuda.amp.custom_bwd
(args...)` is deprecated. Please use `torch.amp.custom_bwd(args..., device_type='cuda')` instead.
  def backward(ctx, *dZ):
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:287: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:304: FutureWarning: `torch.cuda.amp.custom_bwd
(args...)` is deprecated. Please use `torch.amp.custom_bwd(args..., device_type='cuda')` instead.
  def backward(ctx, dZ):
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:352: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:371: FutureWarning: `torch.cuda.amp.custom_bwd
(args...)` is deprecated. Please use `torch.amp.custom_bwd(args..., device_type='cuda')` instead.
  def backward(ctx, *dZ):
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:431: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:467: FutureWarning: `torch.cuda.amp.custom_bwd
(args...)` is deprecated. Please use `torch.amp.custom_bwd(args..., device_type='cuda')` instead.
  def backward(ctx, grad_out):
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:498: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:535: FutureWarning: `torch.cuda.amp.custom_bwd
(args...)` is deprecated. Please use `torch.amp.custom_bwd(args..., device_type='cuda')` instead.
  def backward(ctx, *grad_out):
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:566: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:575: FutureWarning: `torch.cuda.amp.custom_bwd
(args...)` is deprecated. Please use `torch.amp.custom_bwd(args..., device_type='cuda')` instead.
  def backward(ctx, dy):
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:595: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:603: FutureWarning: `torch.cuda.amp.custom_bwd
(args...)` is deprecated. Please use `torch.amp.custom_bwd(args..., device_type='cuda')` instead.
  def backward(ctx, dy):
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:666: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/sparse.py:692: FutureWarning: `torch.cuda.amp.custom_fwd
(args...)` is deprecated. Please use `torch.amp.custom_fwd(args..., device_type='cuda')` instead.
  @custom_fwd(cast_inputs=th.float16)
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/e3nn/o3/_wigner.py:10: FutureWarning: You are using `torch.load` with `weight
s_only=False` (the current default value), which uses the default pickle module implicitly. It is possible to construct malicious pickle data
which will execute arbitrary code during unpickling (See https://github.com/pytorch/pytorch/blob/main/SECURITY.md#untrusted-models for more de
tails). In a future release, the default value for `weights_only` will be flipped to `True`. This limits the functions that could be executed
during unpickling. Arbitrary objects will no longer be allowed to be loaded via this mode unless they are explicitly allowlisted by the user v
ia `torch.serialization.add_safe_globals`. We recommend you start setting `weights_only=True` for any use case where you don't have full contr
ol of the loaded file. Please open an issue on GitHub for any issues related to this experimental feature.
  _Jd, _W3j_flat, _W3j_indices = torch.load(os.path.join(os.path.dirname(__file__), 'constants.pt'))
/home/kevinwsl/RFdiffusion/rfdiffusion/Track_module.py:236: FutureWarning: `torch.cuda.amp.autocast(args...)` is deprecated. Please use `torc
h.amp.autocast('cuda', args...)` instead.
  @torch.cuda.amp.autocast(enabled=False)
/home/kevinwsl/RFdiffusion/rfdiffusion/inference/model_runners.py:183: FutureWarning: You are using `torch.load` with `weights_only=False` (th
e current default value), which uses the default pickle module implicitly. It is possible to construct malicious pickle data which will execut
e arbitrary code during unpickling (See https://github.com/pytorch/pytorch/blob/main/SECURITY.md#untrusted-models for more details). In a futu
re release, the default value for `weights_only` will be flipped to `True`. This limits the functions that could be executed during unpickling
. Arbitrary objects will no longer be allowed to be loaded via this mode unless they are explicitly allowlisted by the user via `torch.seriali
zation.add_safe_globals`. We recommend you start setting `weights_only=True` for any use case where you don't have full control of the loaded
file. Please open an issue on GitHub for any issues related to this experimental feature.
  self.ckpt  = torch.load(
/home/kevinwsl/miniconda3/envs/SE3nv/lib/python3.9/site-packages/dgl/backend/pytorch/tensor.py:352: UserWarning: TypedStorage is deprecated. I
t will be removed in the future and UntypedStorage will be the only storage class. This should only matter to you if you are using storages di
rectly.  To access UntypedStorage directly, use tensor.untyped_storage() instead of tensor.storage()
  assert input.numel() == input.storage().size(), "Cannot convert view " \

✅ RF Difussion ejecutado correctament. Generado: outputs/diabetes_therapeutic_0.pdb
```

In [ ]: