

# buffers

May 16, 2025

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[1]: import pandas as pd
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[2]: Tris_con = 121.14 # g/mol
NaCl_con = 58.44 # g/mol
Imidazole_con = 68.08 # g/mol
TCEP_con = 286.65 # g/mol
HEPES_con = 238.31 # g/mol
KCl_con = 74.55 # g/mol

Tris_mol = {
    "Lysis_buffer" : 20/1000,
    "Elute buffer" : 20/1000,
    "Low-salt buffer" : 20/1000,
    "High-salt buffer" : 20/1000,
    "Dilute buffer" : 20/1000,
    "SEC buffer" : 0
}

NaCl_mol = {
    "Lysis_buffer" : 500/1000,
    "Elute buffer" : 500/1000,
    "Low-salt buffer" : 100/1000,
    "High-salt buffer" : 1000/1000,
    "Dilute buffer" : 0,
    "SEC buffer" : 0
}

Imidazole_mol = {
    "Lysis_buffer" : 20/1000,
    "Elute buffer" : 400/1000,
    "Low-salt buffer" : 0/1000,
    "High-salt buffer" : 0/1000,
    "Dilute buffer" : 0,
    "SEC buffer" : 0
}

glycerol = {
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    "Lysis_buffer" : 5/100,
    "Elute buffer" : 5/100,
    "Low-salt buffer" : 5/100,
    "High-salt buffer" : 5/100,
    "Dilute buffer" : 5/100,
    "SEC buffer" : 0
}

TCEP_mol = {
    "Lysis_buffer" : 1/1000,
    "Elute buffer" : 1/1000,
    "Low-salt buffer" : 1/1000,
    "High-salt buffer" : 1/1000,
    "Dilute buffer" : 1/1000,
    "SEC buffer" : 1/1000
}

HEPES_mol = {
    "Lysis_buffer" : 0/1000,
    "Elute buffer" : 0/1000,
    "Low-salt buffer" : 0/1000,
    "High-salt buffer" : 0/1000,
    "Dilute buffer" : 0,
    "SEC buffer" : 20/1000
}

KCl_mol = {
    "Lysis_buffer" : 0/1000,
    "Elute buffer" : 0/1000,
    "Low-salt buffer" : 0/1000,
    "High-salt buffer" : 0/1000,
    "Dilute buffer" : 0,
    "SEC buffer" : 250/1000
}

Volume = {
    "Lysis_buffer" : 1,
    "Elute buffer" : 0.5,
    "Low-salt buffer" : 1,
    "High-salt buffer" : 0.5,
    "Dilute buffer" : 0.5,
    "SEC buffer" : 1
}

concentration = {
    "Tris" : Tris_con,
    "NaCl" : NaCl_con,

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    "Imidazole" : Imidazole_con,
    "TCEP" : TCEP_con,
    "HEPES" : HEPES_con,
    "KCl" : KCl_con
}

buffer_list = ["Lysis buffer", "Elute buffer", "Low-salt buffer", "High-salt_
↪buffer", "Dilute buffer", "SEC buffer"]
## other way around is more effective: a dictionary for every buffer

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[3]: # Molar masses (g/mol)
concentration = {
    "Tris": 121.14,
    "NaCl": 58.44,
    "Imidazole": 68.08,
    "TCEP": 286.65,
    "HEPES": 238.31,
    "KCl": 74.55
}

# Buffers with molar concentrations (mol/L) and glycerol in %
buffers = {
    "Lysis buffer": {
        "Tris": 20/1000,
        "NaCl": 500/1000,
        "Imidazole": 20/1000,
        "TCEP": 1/1000,
        "HEPES": 0,
        "KCl": 0,
        "Glycerol": 5/100,
        "Volume": 1
    },
    "Elute buffer": {
        "Tris": 20/1000,
        "NaCl": 500/1000,
        "Imidazole": 400/1000,
        "TCEP": 1/1000,
        "HEPES": 0,
        "KCl": 0,
        "Glycerol": 5/100,
        "Volume": 0.5
    },
    "Low-salt buffer": {
        "Tris": 20/1000,
        "NaCl": 100/1000,
        "Imidazole": 0,
        "TCEP": 1/1000,

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        "HEPES": 0,
        "KCl": 0,
        "Glycerol": 5/100,
        "Volume": 1
    },
    "High-salt buffer": {
        "Tris": 20/1000,
        "NaCl": 1000/1000,
        "Imidazole": 0,
        "TCEP": 1/1000,
        "HEPES": 0,
        "KCl": 0,
        "Glycerol": 5/100,
        "Volume": 0.5
    },
    "Dilute buffer": {
        "Tris": 20/1000,
        "NaCl": 0,
        "Imidazole": 0,
        "TCEP": 1/1000,
        "HEPES": 0,
        "KCl": 0,
        "Glycerol": 5/100,
        "Volume": 0.5
    },
    "SEC buffer": {
        "Tris": 0,
        "NaCl": 0,
        "Imidazole": 0,
        "TCEP": 1/1000,
        "HEPES": 20/1000,
        "KCl": 250/1000,
        "Glycerol": 0,
        "Volume": 1
    }
}

```

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[4]: mass_data = []

for buffer_name, components in buffers.items():
    volume = components["Volume"] # in liters
    row = {"Buffer": buffer_name}
    for compound in concentration:
        mol_conc = components.get(compound, 0)
        mass = mol_conc * concentration[compound] * volume # g = mol/L * g/mol *
        ↪ * L
        row[compound] = mass

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    # Glycerol as % v/v, approximated as g/mL ~ mL (density 1.26 g/mL, but
    ↪ assuming ~1 g/mL here)
    glycerol_percent = components.get("Glycerol", 0)
    glycerol_mass = glycerol_percent * volume * 1000 # convert L to mL
    row["Glycerol"] = glycerol_mass
    mass_data.append(row)

# Create DataFrame
df_mass = pd.DataFrame(mass_data)
df_mass.set_index("Buffer", inplace=True)
df_mass.columns = [f"{col} [g]" for col in df_mass.columns]
df_mass.round(3) # Round for display

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[4]:
      Tris [g]  NaCl [g]  Imidazole [g]  TCEP [g]  HEPES [g]  \
Buffer
Lysis buffer    2.423    29.220         1.362    0.287    0.000
Elute buffer     1.211    14.610        13.616    0.143    0.000
Low-salt buffer   2.423     5.844         0.000    0.287    0.000
High-salt buffer  1.211    29.220         0.000    0.143    0.000
Dilute buffer    1.211     0.000         0.000    0.143    0.000
SEC buffer       0.000     0.000         0.000    0.287    4.766

      KCl [g]  Glycerol [g]
Buffer
Lysis buffer    0.000      50.0
Elute buffer     0.000      25.0
Low-salt buffer   0.000      50.0
High-salt buffer  0.000      25.0
Dilute buffer    0.000      25.0
SEC buffer      18.638       0.0

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[5]: # Molar masses (g/mol)
concentration = {
    "Tris": 121.14,
    "NaCl": 58.44,
    "Imidazole": 68.08,
    "TCEP": 286.65,
    "HEPES": 238.31,
    "KCl": 74.55
}

# Stock concentrations (mol/L or %)
stock_concentrations = {
    "Tris": 1.0,
    "NaCl": 5.0,
    "Imidazole": 1.0,
    "TCEP": 0.5,

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    "HEPES": 1.0,
    "KCl": 3.0,
    "Glycerol": 100.0 # % v/v
}

# Volume of stock to prepare in liters
volume_L = 0.1 # 100 mL

# Calculate mass
for compound, stock_conc in stock_concentrations.items():
    if compound == "Glycerol":
        print(f"{compound}: 100 mL of pure glycerol (used as 100%)")
    else:
        molar_mass = concentration[compound]
        moles = stock_conc * volume_L
        mass = molar_mass * moles
        print(f"{compound}: {mass:.2f} g in 100 mL for a {stock_conc} M ↪
↪solution")

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Tris: 12.11 g in 100 mL for a 1.0 M solution  
 NaCl: 29.22 g in 100 mL for a 5.0 M solution  
 Imidazole: 6.81 g in 100 mL for a 1.0 M solution  
 TCEP: 14.33 g in 100 mL for a 0.5 M solution  
 HEPES: 23.83 g in 100 mL for a 1.0 M solution  
 KCl: 22.37 g in 100 mL for a 3.0 M solution  
 Glycerol: 100 mL of pure glycerol (used as 100%)

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[6]: # Define standard stock concentrations in mol/L or % for glycerol
stock_concentrations = {
    "Tris": 1.0, # M
    "NaCl": 5.0, # M
    "Imidazole": 1.0, # M
    "TCEP": 0.5, # M
    "HEPES": 1.0, # M
    "KCl": 3.0, # M
    "Glycerol": 100.0 # %
}

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# Calculate stock volumes needed for each buffer (in mL)
stock_volumes_data = []

for buffer_name, components in buffers.items():
    volume = components["Volume"] # L
    row = {"Buffer": buffer_name}
    for compound, stock_conc in stock_concentrations.items():
        final_conc = components.get(compound, 0)

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    if compound == "Glycerol":
        # For glycerol: use % directly
        stock_volume_ml = (final_conc / stock_conc) * volume * 1000 #
    ↪convert to mL
    else:
        # For molar compounds
        stock_volume_ml = (final_conc * volume) / stock_conc * 1000 #
    ↪convert to mL
    row[f"{compound} stock [mL]"] = stock_volume_ml
    stock_volumes_data.append(row)

# Create DataFrame
df_stock_volumes = pd.DataFrame(stock_volumes_data)
df_stock_volumes.set_index("Buffer", inplace=True)
df_stock_volumes.loc["Total"] = df_stock_volumes.sum()
df_stock_volumes.round(2)

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[6]:
      Tris stock [mL]  NaCl stock [mL]  Imidazole stock [mL]  \
Buffer
Lysis buffer          20.0           100.0                20.0
Elute buffer          10.0            50.0               200.0
Low-salt buffer       20.0            20.0                0.0
High-salt buffer      10.0           100.0                0.0
Dilute buffer         10.0             0.0                0.0
SEC buffer            0.0             0.0                0.0
Total                70.0           270.0               220.0

      TCEP stock [mL]  HEPES stock [mL]  KCl stock [mL]  \
Buffer
Lysis buffer          2.0             0.0             0.00
Elute buffer          1.0             0.0             0.00
Low-salt buffer       2.0             0.0             0.00
High-salt buffer      1.0             0.0             0.00
Dilute buffer         1.0             0.0             0.00
SEC buffer            2.0            20.0            83.33
Total                 9.0            20.0            83.33

      Glycerol stock [mL]
Buffer
Lysis buffer          0.50
Elute buffer          0.25
Low-salt buffer       0.50
High-salt buffer      0.25
Dilute buffer         0.25
SEC buffer            0.00
Total                 1.75

```