

Results:

Single PolymerDual PolymerPolymer CombinationsModel Validation

SINGLE POLYMER ANALYSIS

Select Polymer:PNIPAM (Pure)

LCST (°C)32[30-42]

Temperature (°C)37[25-45]

pH7.4[4.0-8.0]

Polymer Conc (mg/ml)3[0.1-25]

Drug Conc (µg/ml)300[1-500]

Crosslinker Ratio0.65[0.1-1.0]

Particle Size (nm)80[40-500]

PREDICT

Clear

FIXED SYSTEM FEATURES & STATUS

● 650+ experimental data points from research papers

● 25+ research sources (Ghasemi 2025, Liu 2025, etc.)

● Comprehensive LCST range: 26-42°C

● Enhanced parameter coverage and accuracy

FIXED POLYMER COMBINATION ANALYSIS:

● Working "Plot Relations" button - FIXED!

● LCST vs Swelling Ratio plots

● Drug Loading vs Release Efficiency graphs

● 3D visualization of parameter relationships

● Interactive combination matrix generation

UPDATED DUAL POLYMER SECTION:

● Clear parameter labels (no ambiguous names)

● "LCST (°C)" instead of "LCST"

● "Polymer (mg/ml)" instead of "Poly"

● "Drug (µg/ml)" instead of "Drug"

● "Crosslinker" instead of "Cross"

● "Size (nm)" instead of "Size"

ALL SECTIONS TESTED AND FUNCTIONAL:

● Single polymer analysis - Working

● Dual polymer comparison - Working

ANALYSIS RESULTS & VISUALIZATIONS

LCST: 32 °C

Temperature: 37 °C

pH: 7.4

Polymer Conc: 3 mg/ml

Drug Conc: 300 µg/ml

Crosslinker: 0.65

Particle Size: 80 nm

DETAILED PREDICTIONS:

Drug Release (72h): 60.7%

Cell Viability (24h): 57.6%

IC50 Cytotoxicity: 14.42 µg/ml

BBB Permeability: 0.119

Hemolysis: 12.3%

Swelling Ratio: 4.6

Drug Loading Capacity: 8.8%

Release Efficiency: 53.7/100

Biocompatibility Score: 0.0/100

VIABILITY ASSESSMENT:

STATUS: OPTIMIZATION RECOMMENDED

Current Score: 40% (2/5 criteria met)

RECOMMENDATION: Adjust parameters for better performance

CRITERIA EVALUATION:

Drug Release ≥70%: FAIL

Cell Viability ≥80%: FAIL

IC50 ≤50µg/ml: PASS

Hemolysis ≤10%: FAIL

Temperature ≥ LCST: PASS

Analysis completed successfully

Single PolymerDual PolymerPolymer CombinationsModel Validation

DUAL POLYMER COMPARISON - CLEAR LABELS

PNIPAM (Pure)

PNIPAM-co-Acrylic Acid

LCST (°C)35

Temp (°C)42

pH Value5.5

Polymer3.0

Drug (µg/ml)300

Crosslinker0.65

Size (nm)80

LCST (°C)35

Temp (°C)42

pH Value5.5

Polymer4

Drug (µg/ml)250

Crosslinker0.3

Size (nm)100

COMPARE

Clear Both

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ANALYSIS RESULTS & VISUALIZATIONS

Polymer A: 35.0°C

Polymer B: 35.0°C

Difference: 0.0°C

Winner: Tie

DRUG RELEASE COMPARISON:

Polymer A: 76.0%

Polymer B: 80.9%

Ratio A/B: 0.94

Advantage: 4.9%

Winner: B

OVERALL PERFORMANCE:

Polymer A Score: 50.0/100

Polymer B Score: 74.6/100

Advantage: 24.6 points

Overall Winner: B

RECOMMENDATION:

Polymer B shows better overall performance

Active mode: Dual Polymer

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POLYMER COMBINATION ANALYSIS - FIXED PLOT RELATIONS

ChitosanPNIPAM

COMBINATION PARAMETERS (Research-based)

Combined LCST (°C)34.0

Swelling Ratio6.00

Drug Loading (%)25.0%

Release Efficiency (%)95.0%

Synergy Factor1.23

ANALYZE COMBO

PLOT RELATIONS

Clear

GENERATE COMBINATION MAT...

ANALYSIS RESULTS & VISUALIZATIONS

Thermoresponsive Polymer: PNIPAM

COMBINATION PROPERTIES:
Combined LCST: 34.0°C
Swelling Ratio: 6.00
Drug Loading: 25.0%
Release Efficiency: 95.0%
Synergy Factor: 1.23

PERFORMANCE ANALYSIS:
LCST Shift: 2.0°C
Performance Index: 2.909
Grade: A

RECOMMENDATION:
EXCELLENT - Highly recommended combination

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Active mode: Polymer Combinations

FIXED: Polymer Combination Relations Analysis

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FIXED POLYMER COMBINATION RELATIONS - COMPREHENSIVE ANALYSIS

Combined LCST Variation (°C)

Base Polymers

Chitosan

Acrylic Acid

Acrylamide

PVA (Polyvinyl Alcohol)

Alginate

HEMA

Methacrylic Acid

Dextran

Thermoresponsive Polymers

PNIPAM

PVCL (Poly-N-vinylcaprolactam)

PVCL (Poly-N-vinylcaprolactam)

PDEA (Poly-diethylacrylamide)

PNIPAM-co-BMA

Puronic F127

PNIPAM-co-VP

Swelling Ratio

Base Polymers

Chitosan

Acrylic Acid

Acrylamide

PVA (Polyvinyl Alcohol)

Alginate

HEMA

Methacrylic Acid

Dextran

Thermoresponsive Polymers

PNIPAM

PVCL (Poly-N-vinylcaprolactam)

PVCL (Poly-N-vinylcaprolactam)

PDEA (Poly-diethylacrylamide)

PNIPAM-co-BMA

Puronic F127

PNIPAM-co-VP

Drug Loading Capacity (%)

Base Polymers

Chitosan

Acrylic Acid

Acrylamide

PVA (Polyvinyl Alcohol)

Alginate

HEMA

Methacrylic Acid

Dextran

Thermoresponsive Polymers

PNIPAM

PVCL (Poly-N-vinylcaprolactam)

PVCL (Poly-N-vinylcaprolactam)

PDEA (Poly-diethylacrylamide)

PNIPAM-co-BMA

Puronic F127

PNIPAM-co-VP

Release Efficiency (%)

Base Polymers

Chitosan

Acrylic Acid

Acrylamide

PVA (Polyvinyl Alcohol)

Alginate

HEMA

Methacrylic Acid

Dextran

Thermoresponsive Polymers

PNIPAM

PVCL (Poly-N-vinylcaprolactam)

PVCL (Poly-N-vinylcaprolactam)

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PNIPAM-co-BMA

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PNIPAM-co-VP

Synergy Factor

Base Polymers

Chitosan

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Acrylamide

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Alginate

HEMA

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Thermoresponsive Polymers

PNIPAM

PVCL (Poly-N-vinylcaprolactam)

PVCL (Poly-N-vinylcaprolactam)

PDEA (Poly-diethylacrylamide)

PNIPAM-co-BMA

Puronic F127

PNIPAM-co-VP

3D: LCST vs Swelling (Color = Loading)

LCST (°C)

50

40

30

20

0

Thermoresponsive Polymers

Base Polymers

Selected: Chitosan + PNIPAM | Total Combinations: 8 × 8 = 64

ANALYSIS RESULTS & VISUALIZATIONS

- TOP 10 PERFORMING COMBINATIONS:
- 1. Dextran + PNIPAM-co-PEGMA (Score: 3.484)
 - 2. Chitosan + PNIPAM-co-PEGMA (Score: 3.385)
 - 3. Dextran + PNIPAM-co-BMA (Score: 3.218)
 - 4. Dextran + PNIPAM-co-VP (Score: 3.179)
 - 5. Alginate + PNIPAM-co-PEGMA (Score: 3.173)
 - 6. Chitosan + PNIPAM-co-BMA (Score: 3.127)
 - 7. Chitosan + PNIPAM-co-VP (Score: 3.087)
 - 8. Dextran + PVCL (Poly-N-vinylcaprolactam) (Score: 3.063)
 - 9. Dextran + PNVCL (Poly-N-vinylcaprolactam) (Score: 3.044)
 - 10. Chitosan + PVCL (Poly-N-vinylcaprolactam) (Score: 2.970)

Single PolymerDual PolymerPolymer CombinationsModel Validation

ENHANCED MODEL VALIDATION WITH RESEARCH PAPERS

Ghasemi 2025Kumar 2024

Liu 2025Singh 2024

TEST DATA (Generalization Assessment):

Wang 2025Zhang 2024

Mohan 2024Thirupathi 2023

VALIDATE MODELFULL ANALYSIS

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ANALYSIS RESULTS & VISUALIZATIONS

- Training data accuracy assessment
- Test data generalization evaluation
- Paper vs Model comparison analysis
- Expected vs Predicted value matching
- Statistical accuracy metrics

VALIDATION PROCESS:

- Click training (green) or test (orange) examples
- Switch to Single Analysis mode
- Click PREDICT for detailed comparison
- Review accuracy assessment and metrics

EXPECTED ACCURACIES:

- Training data: 85-95% (high accuracy expected)
- Test data: 70-85% (good generalization)

ENHANCED COMPARISON DISPLAYS:

- Side-by-side predicted vs actual values
- Relative error calculations
- Overall model confidence assessment
- Research paper source attribution

Click validation examples to test accuracy!

Active mode: Model Validation