

Supplemental Figures

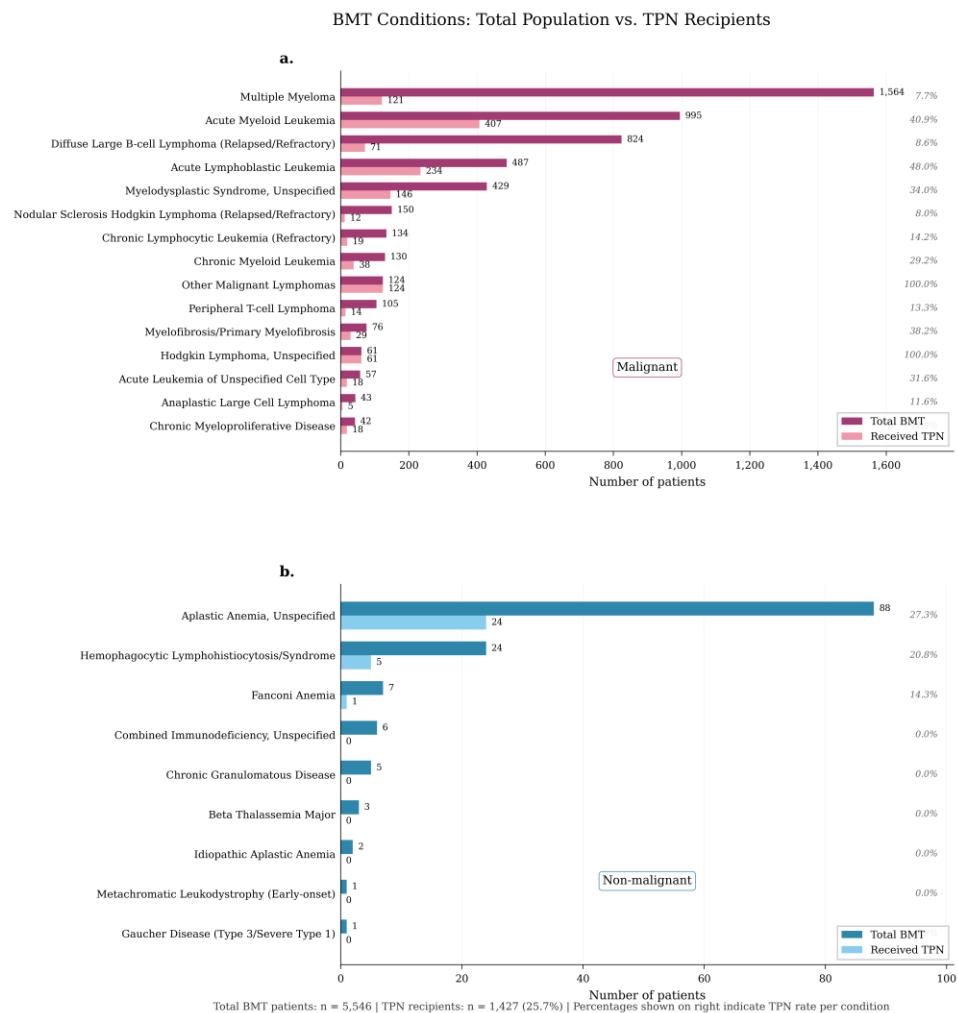


Figure S1: Distribution of conditions that required Hematopoietic stem cell transplantation at Stanford Healthcare. Primary Diagnoses across the Total BMT Population and the Subgroup Treated with TPN

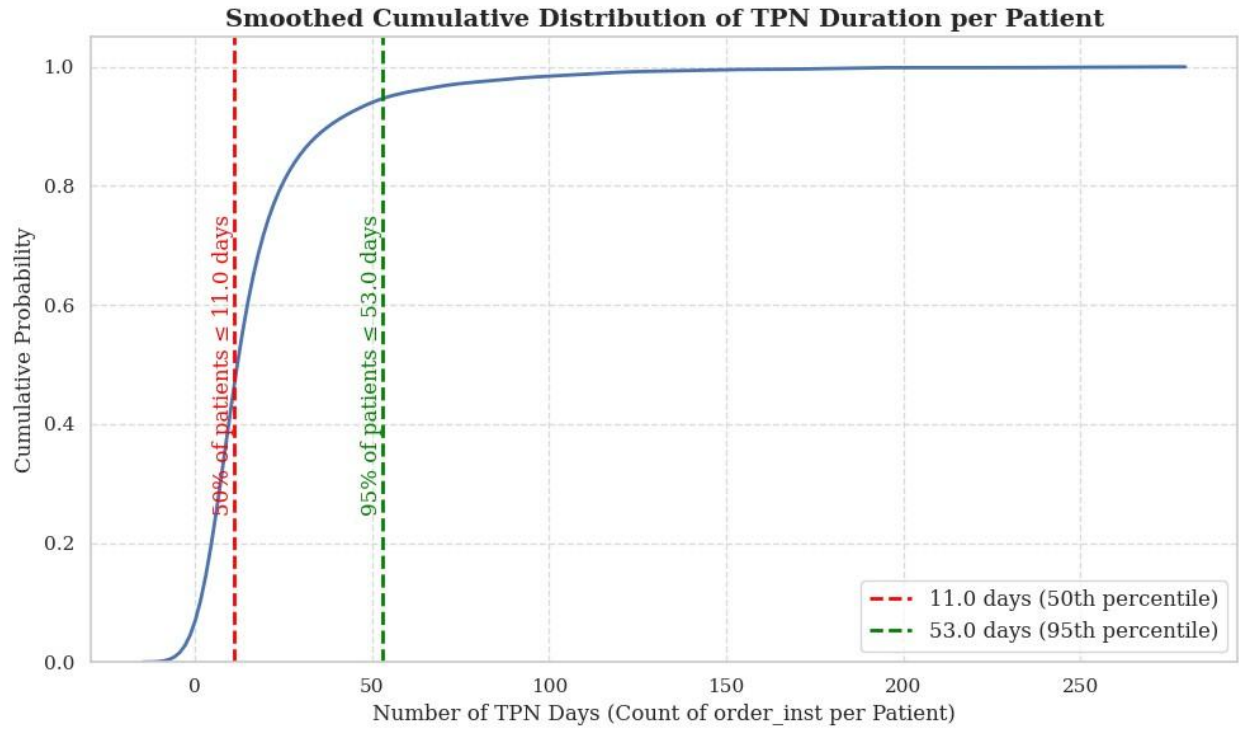


Figure S2: Cumulative Distribution of Total TPN Therapy Days per Patient

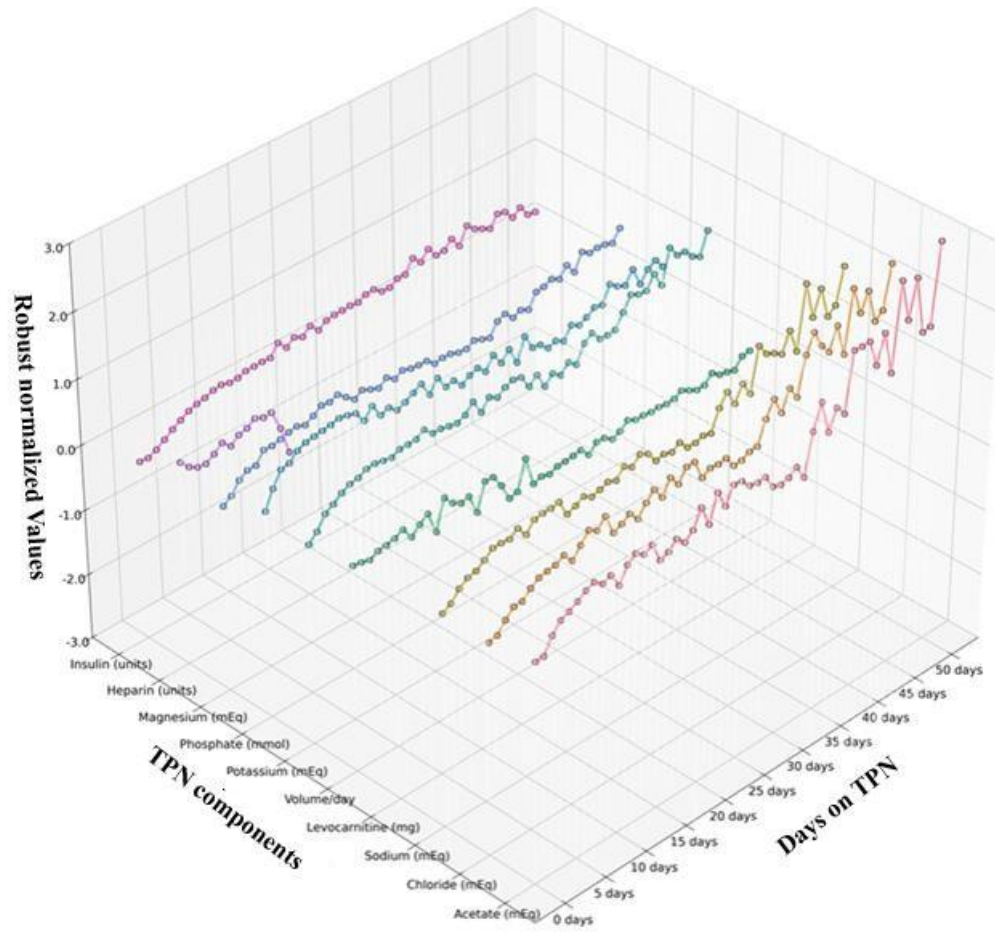


Figure S3: Dynamic of TPN components over time.

Temporal Trajectories of the 10 Most Variable TPN Components Across 50 Days of Therapy.

TPN component ¹	Unit	Typical adult range*
Parenteral amino acids	g	40 – 120 g (protein equivalents)
Acetate	mEq	Adjusts anion gap / acid–base balance
Calcium	mEq	10 – 20 mEq (as CaCl ₂ or Ca-gluconate)
Chloride	mEq	Coupled to Na ⁺ /K ⁺ salts; gap-filler
Chromium	µg	10 – 20 µg trace element
Copper	mg	0.3 – 1.5 mg trace element
Dextrose	g	150 – 400 g ($\approx 3\text{--}5 \text{ mg kg}^{-1} \text{ min}^{-1}$)
Famotidine	mg	Stress-ulcer prophylaxis (5 – 20 mg)
Folic acid	mg	0.2 – 1 mg (vitamin B ₉ supplement)
Heparin	units	500 – 5 000 U (line patency)
Insulin	units	0 – 80 U (inline glucose control)
Levocarnitine	mg	2 – 4 mg kg ⁻¹ (long-term TPN)
Magnesium	mEq	8 – 16 mEq (as MgSO ₄)
Manganese	mg	0.15 – 0.8 mg trace element
Multivitamins (parenteral) “units”†		Standard adult MVI = 1 vial
Phosphate	mmol	15 – 45 mmol (Na/K phos)
Potassium	mEq	40 – 120 mEq
Selenium	µg	40 – 80 µg trace element
Sodium	mEq	70 – 150 mEq
Thiamine	mg	6 – 12 mg (vitamin B ₁)
Pyridoxine	mg	4 – 6 mg (vitamin B ₆)
Ascorbic acid (Vitamin C)	mg	100 – 200 mg
Phytonadione (Vitamin K ₁)	mg	0.1 – 0.4 mg
Zinc	mg	2.5 – 12 mg
Lipids (20 % emulsion)	g	20 – 100 g ($\leq 1 \text{ g kg}^{-1} \text{ d}^{-1}$)**

* Ranges drawn from ASPEN/ESPEN adult-TPN guidelines and Stanford Pharmacy formulary; institutional protocols may vary.

† “1 unit” indicates the standard adult multivitamin vial supplied by pharmacy (Solvit®, Cernevit®, or equivalent).

** Restrict in patients with severe cholestasis or hypertriglyceridemia.

¹ Recommended daily parenteral doses derive from the ASPEN Parenteral Nutrition Handbook (3rd ed., 2020) and the 2019 ESPEN ICU guideline.

Table S1: List of the 25 continuous variables that form a TPN prescription¹. TPN doses were divided into the following individual components to create our dataset.

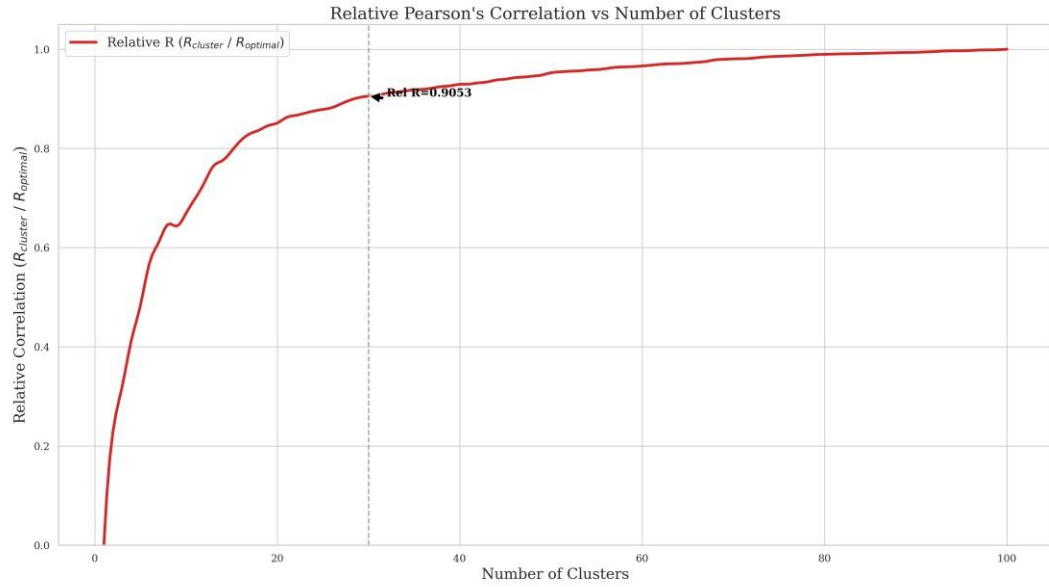


Figure S4: Optimal Cluster Number Identification via Relative Pearson Correlation. The red curve shows the correlation achieved by a clustered model at each K, expressed relative to a high-capacity reference ($R_{cluster}/R_{optimal}$; y-axis). Accuracy rises steeply from K=1 to ~10, then more gradually, with clear diminishing returns beyond $K \approx 30$ (dashed line). At K=30, the model attains ~0.905 of the reference performance, with only marginal gains (<0.5 absolute) up to K=100. This supports $K \approx 30$ as a parsimonious choice balancing fidelity and complexity.

Seq2Seq Transformer: Actual vs. Predicted Values for Each Target

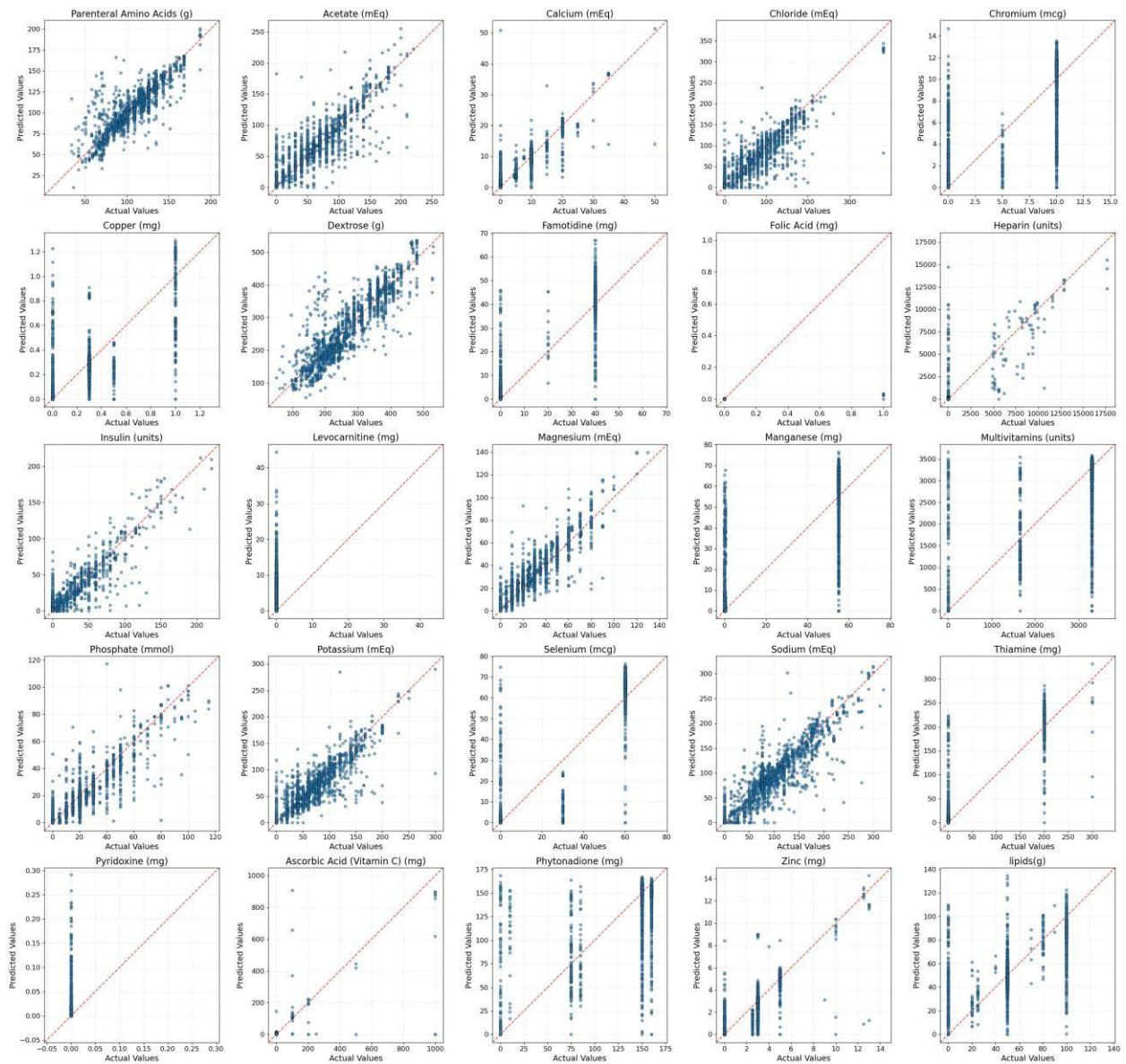


Figure S5: Transformer Dose Predictions: Predicted vs. Actual Scatter. Predicted versus clinician-prescribed TPN doses for each nutrient in the test set. Performance is strong for frequently ordered macronutrients and electrolytes—parenteral amino acids, dextrose, insulin, sodium, and potassium. At higher doses, the model modestly underestimates phosphate, magnesium, and chloride. Panels for medications and vitamins given in fixed vial sizes (famotidine, multivitamins, folate, phytonadione) show vertical striations that reflect formulary step sizes rather than error.

Laboratory test¹	Normal range (adults)	Unit
Potassium [moles/volume] in Serum/Plasma	3.5 – 5.2	mmol L ⁻¹
Sodium [moles/volume] in Serum/Plasma	135 – 145	mmol L ⁻¹
Chloride [moles/volume] in Serum/Plasma	96 – 106	mmol L ⁻¹
Bicarbonate (total CO ₂) [moles/volume] in Specimen	23 – 29	mmol L ⁻¹
Calcium [mass/volume] in Serum/Plasma	8.6 – 10.3	mg dL ⁻¹
Phosphate [mass/volume] in Serum/Plasma	2.5 – 4.5	mg dL ⁻¹
Magnesium [mass/volume] in Serum/Plasma	1.7 – 2.2	mg dL ⁻¹
Glucometer blood glucose (random/non-fasting)	70 – 140	mg dL ⁻¹
Albumin [mass/volume] in Serum/Plasma	3.5 – 5.5	g dL ⁻¹
Protein [mass/volume] in Serum/Plasma (total)	6.0 – 8.3	g dL ⁻¹
Urea nitrogen [mass/volume] in Serum/Plasma (BUN)	7 – 20	mg dL ⁻¹

¹ Adult normal intervals were taken from Tietz Textbook of Clinical Chemistry and Henry's Clinical Diagnosis and Management by Laboratory Methods

Table S2: Normal Lab values. Intervals correspond to typical adult reference values used at Stanford Health Care during the study period. Minor inter-laboratory variation is common; values are rounded to one decimal place where appropriate.

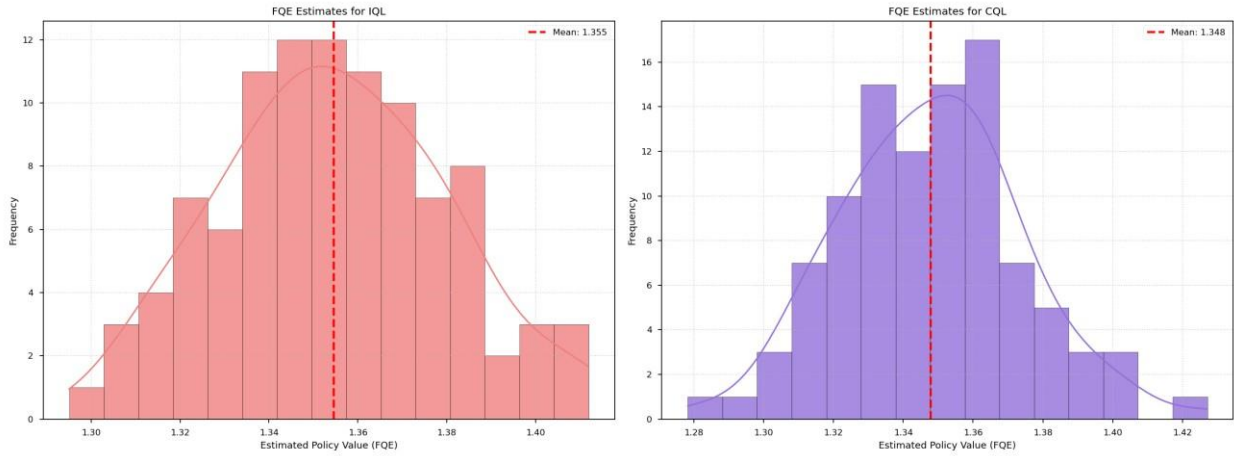


Figure S6: Distribution of Estimated Policy Values for IQL and CQL.

Histograms that visualize the distribution of estimated policy values for the IQL (left) and CQL (right) agents, as determined by Fitted Q Evaluation (FQE). Each distribution is generated through a bootstrap process, where the policy's performance is repeatedly re-calculated on random samples of the data to assess the stability and confidence of the final value. The vertical dashed line in each plot indicates the mean estimated value (1.355 for IQL and 1.348 for CQL), while the spread of the histogram provides a sense of uncertainty in this estimate

Action Distribution Comparison on Test Set: Clinical vs IQL Policy

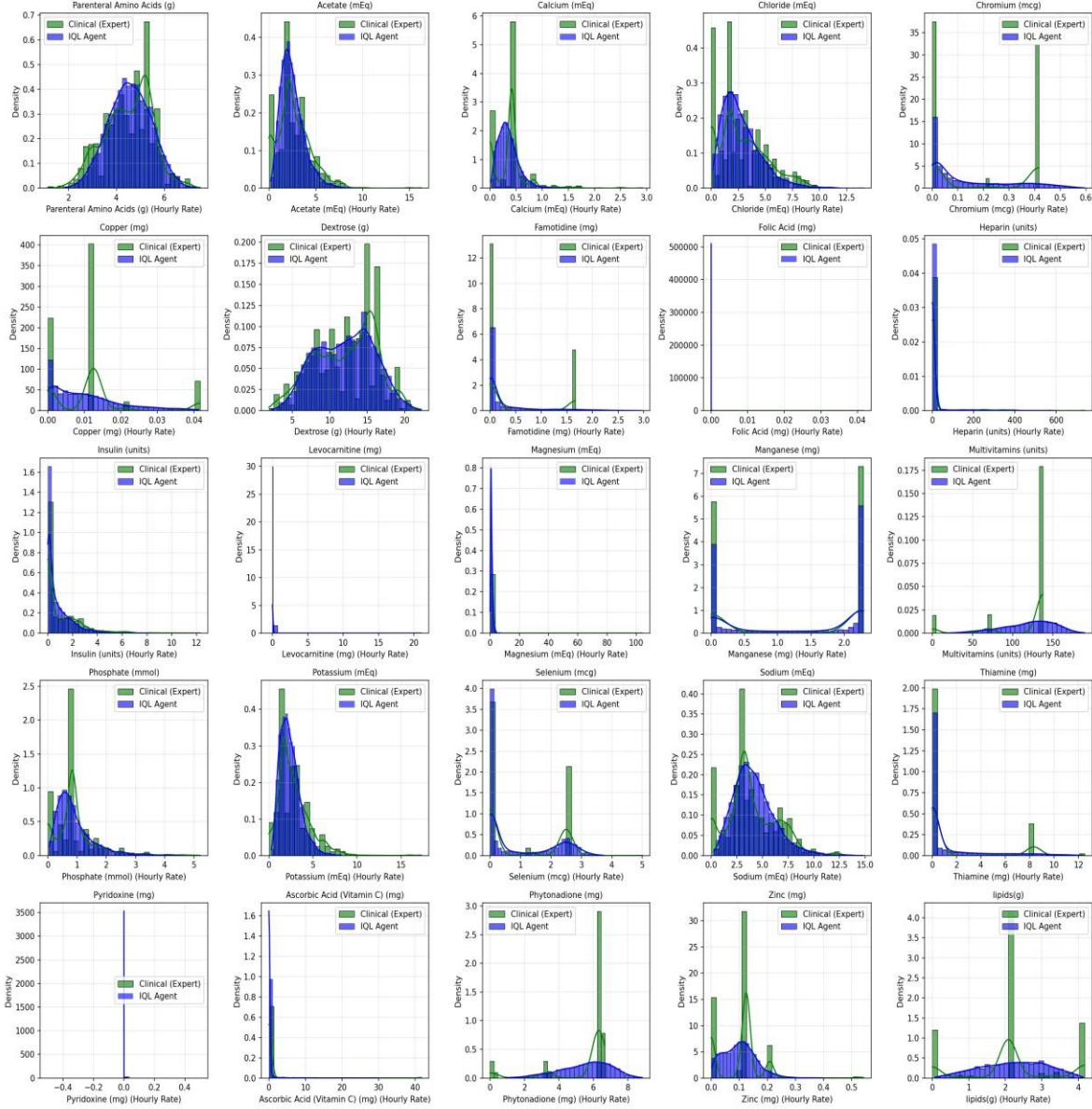


Figure S7: Action Distribution Comparison on Test Set: Clinical vs IQL Policy. For each component, we overlay clinical order distributions (green) with IQL actions (blue). The policy largely mirrors practice for across the different components.