

MENTORIA

Clasificación de Tumoresferas

GRUPO 1 - 2023

PRESENTACIÓN FINAL

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OBJETIVO GENERAL

Analizar los datos obtenidos por procesamiento de imágenes de cultivos de células tumorales y de estructuras celulares denominadas TUMORESFERAS.

Desarrollar un modelo computacional que permita clasificar las mismas como tal y así apoyar en la toma de decisión final del personal calificado.

ALCANCE Y CONTENIDO

- 1. BREVE RESUMEN PREVIO**
- 2. EXPLORACIÓN DE DATOS**
- 3. MODELOS DE APRENDIZAJE**
- 4. CONCLUSIONES Y OBSERVACIONES**



The background features abstract, organic shapes in various colors: blue, orange, yellow, and white. These shapes are irregular and fluid, resembling cells or stylized leaves. Some shapes contain smaller, rounded forms, possibly representing nuclei or organelles.

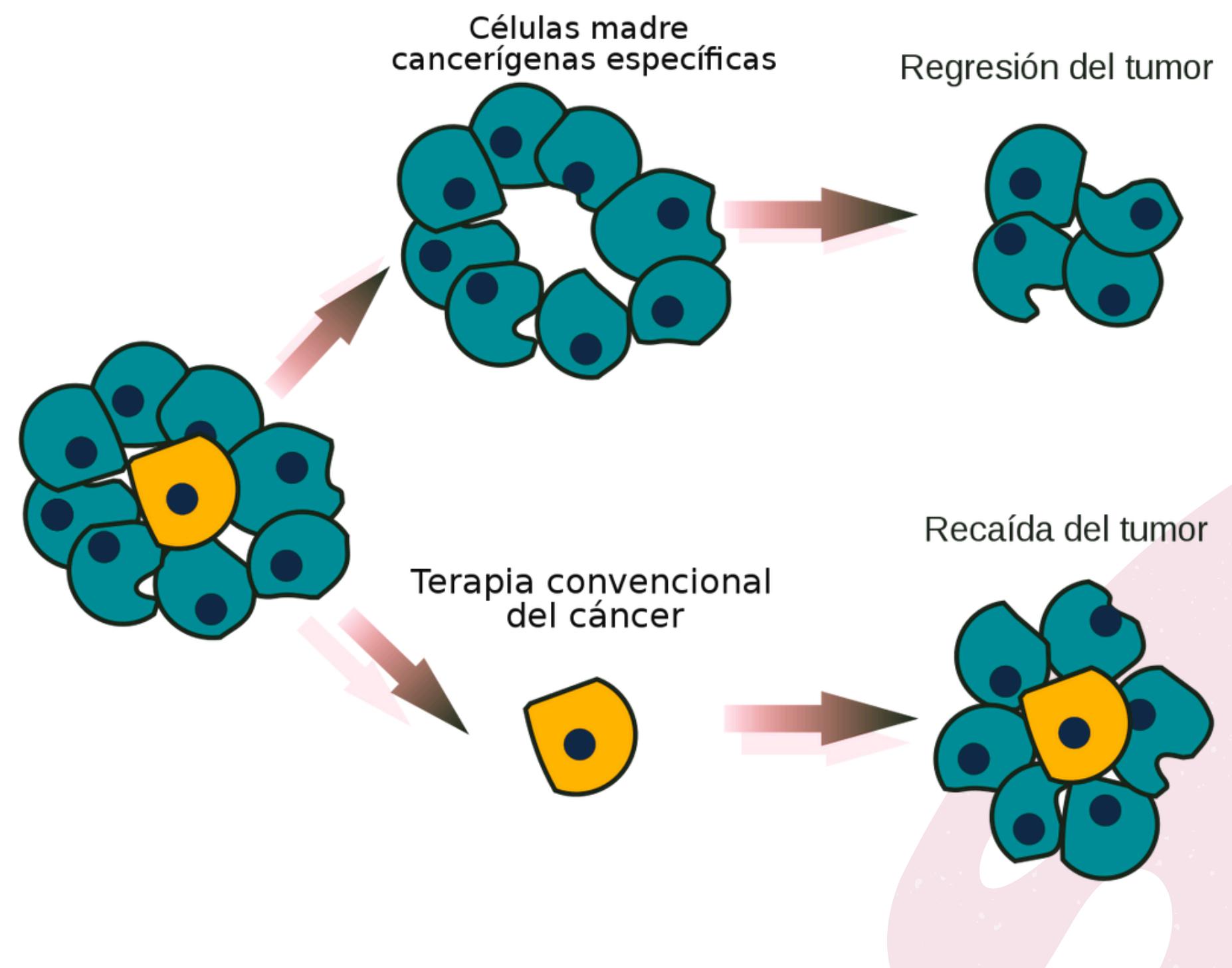
RECORDAMOS!

¿Qué es una Tumoresfera?

Una Tumoresfera es una estructura celular esferoidal originada a partir de una única célula madre cancerosa (CMC) y que crece en suspensión en cultivos celulares in vitro de células cancerosas.

¿Cuál es la importancia de su estudio?

Analizar las tumoresferas podría ayudar a plantear mejoras o alternativas para que los tratamientos anticancerígenos sean más eficientes.

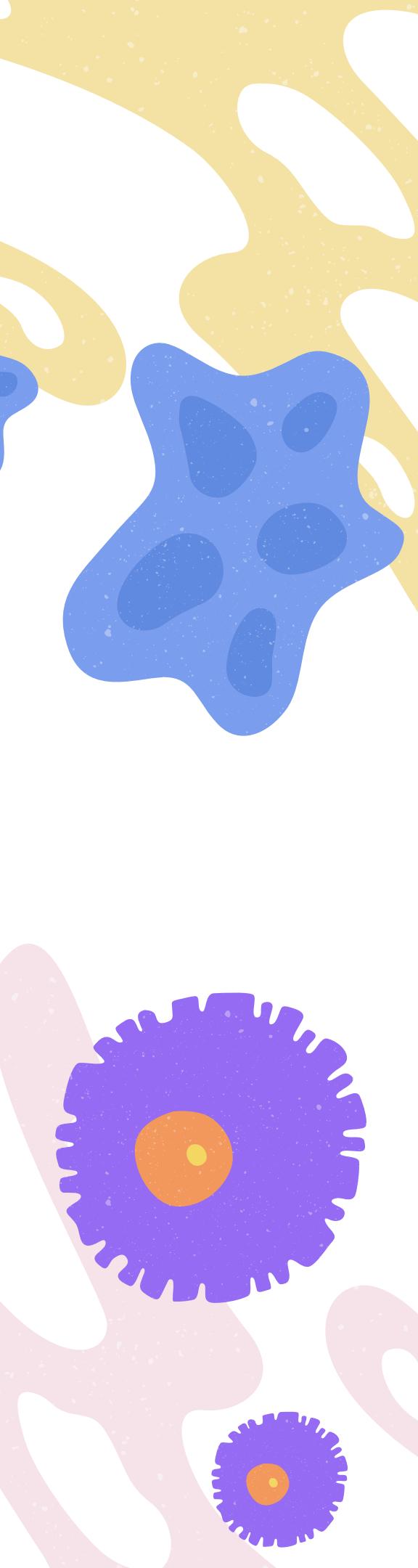
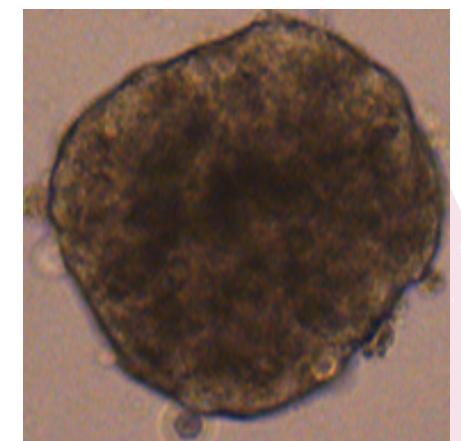
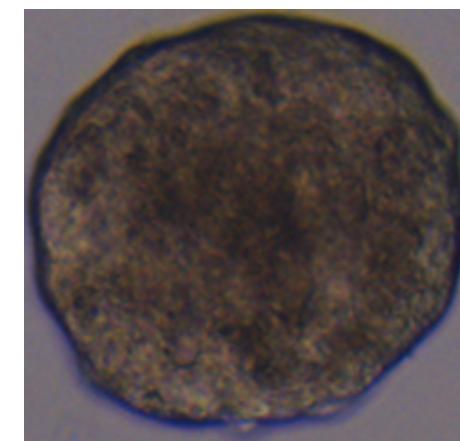
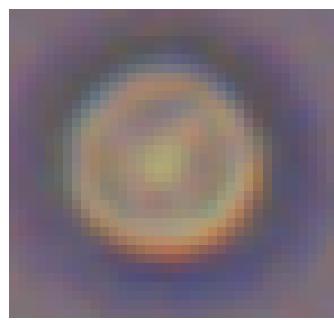
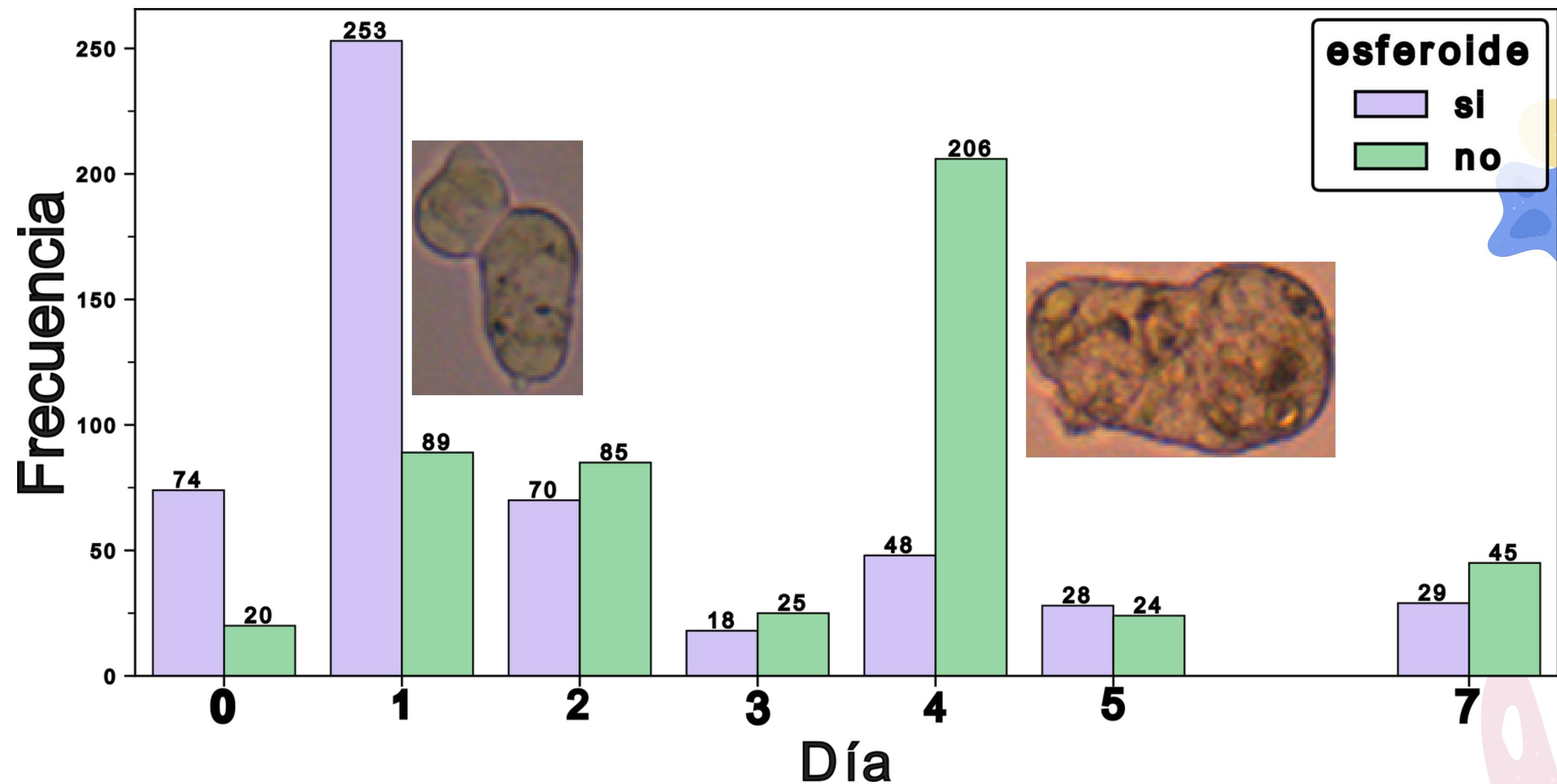


Alcance de 1º práctico

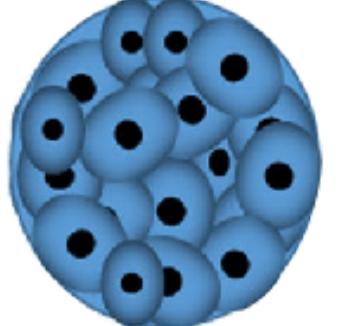
- INTRODUCCIÓN BASE DE DATOS
- ANÁLISIS EXPLORATORIO Y CURACIÓN
- ANÁLISIS DE CORRELACIÓN
- EXPLORACIÓN DE MUESTRAS POR DÍA
- CONCLUSIONES Y OBSERVACIONES



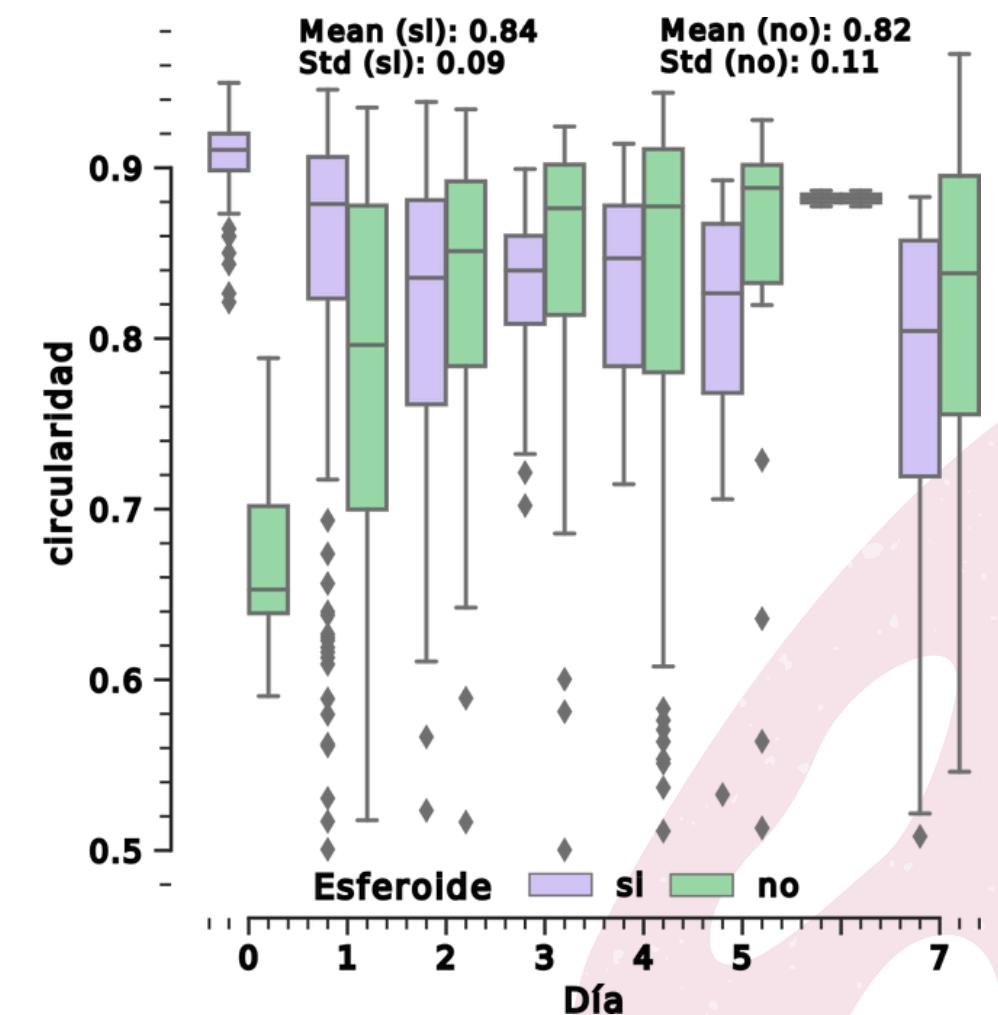
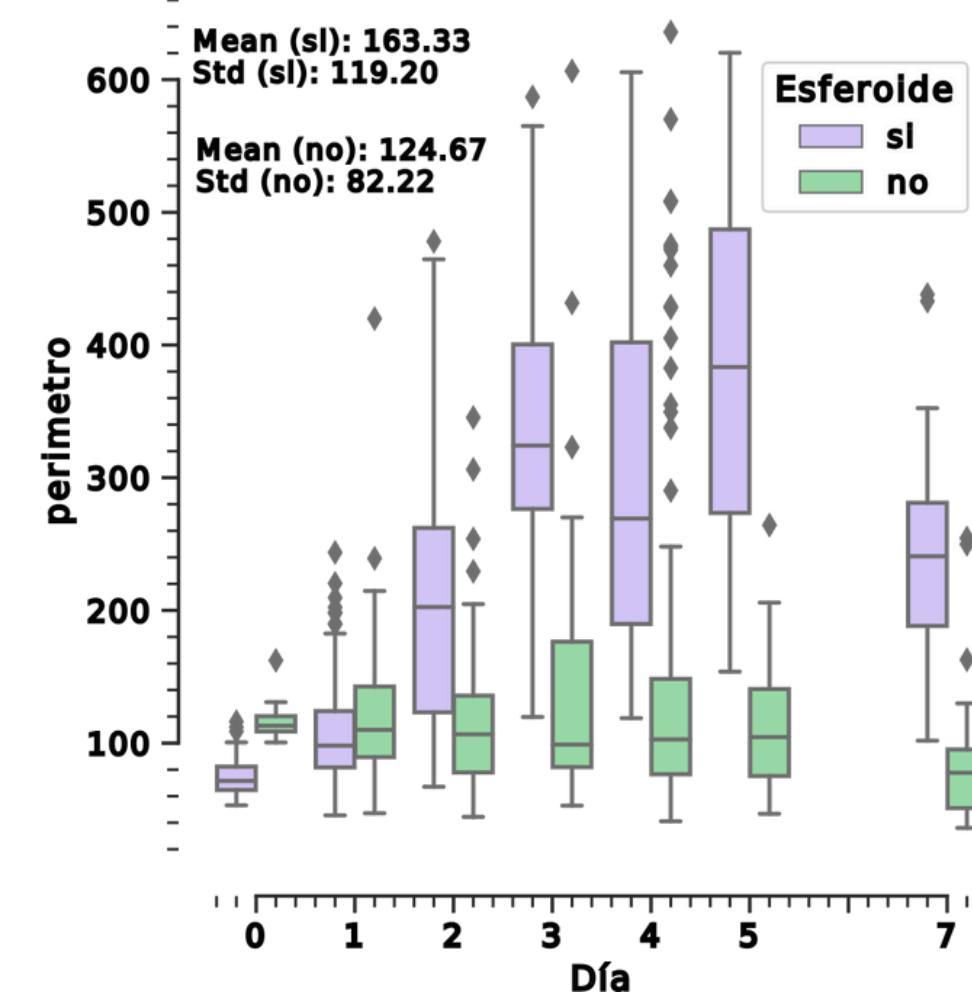
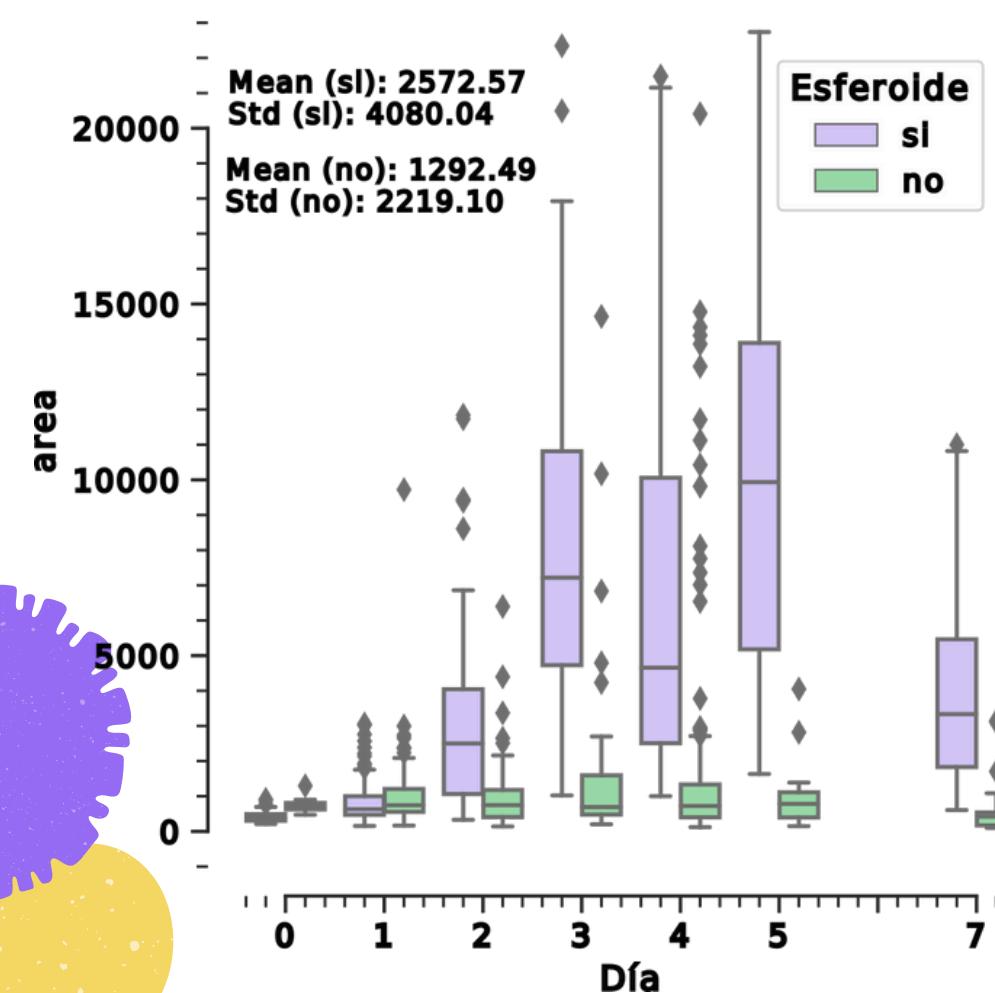
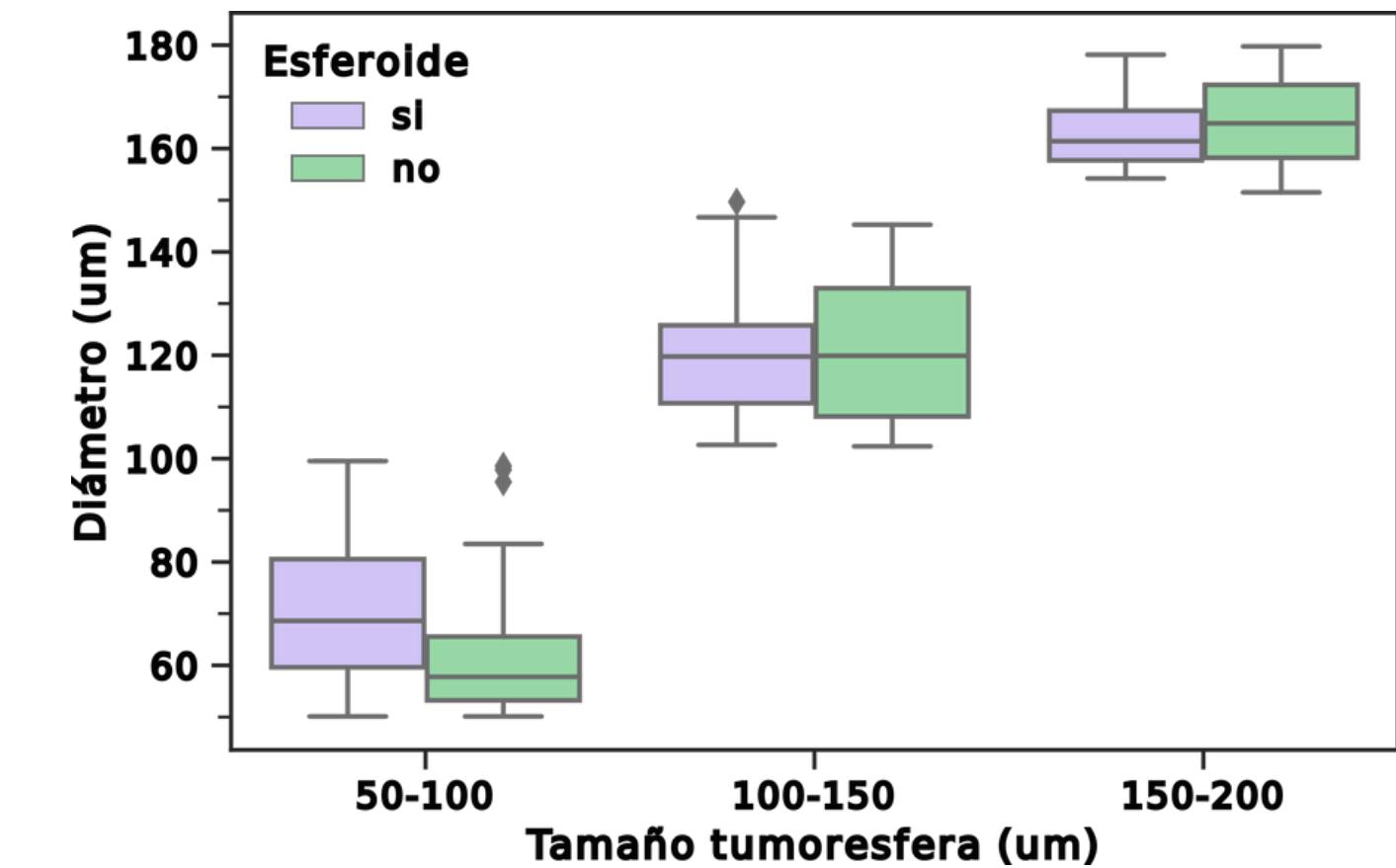
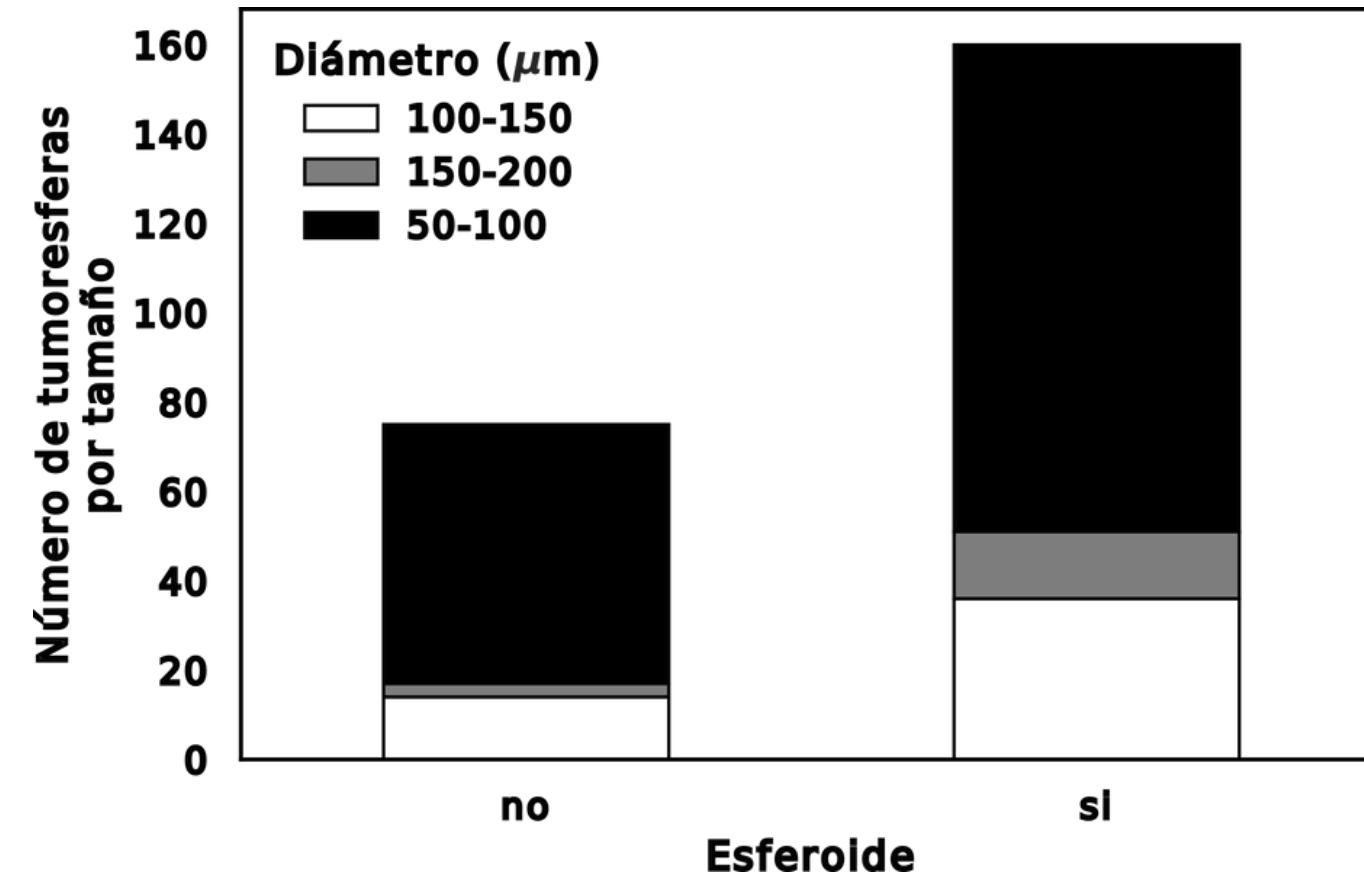
EXPLORACIÓN DE DATOS



circularidad >0.3
A>100 μm^2



50-250 μm



Pocos datos!!



SDV

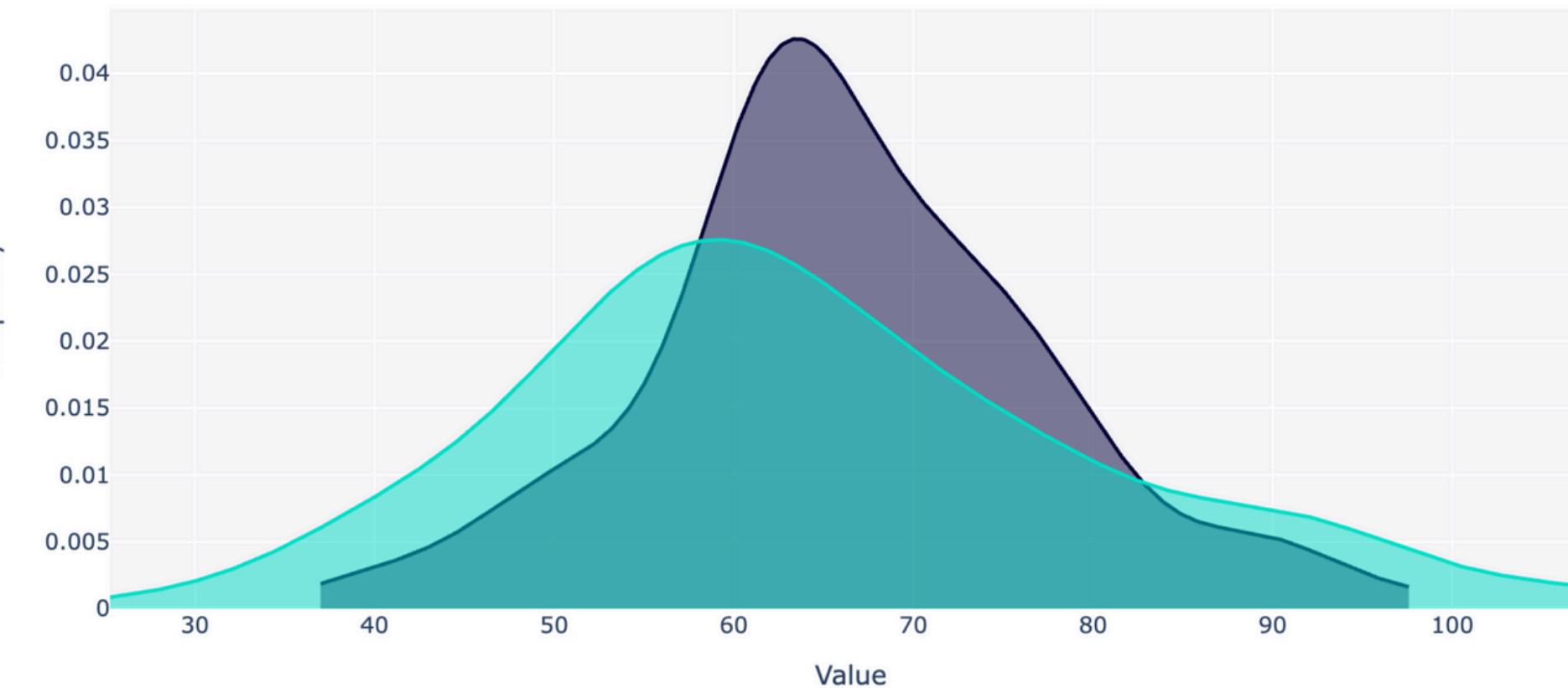
The Synthetic Data Vault



 dataacebo
Copulas

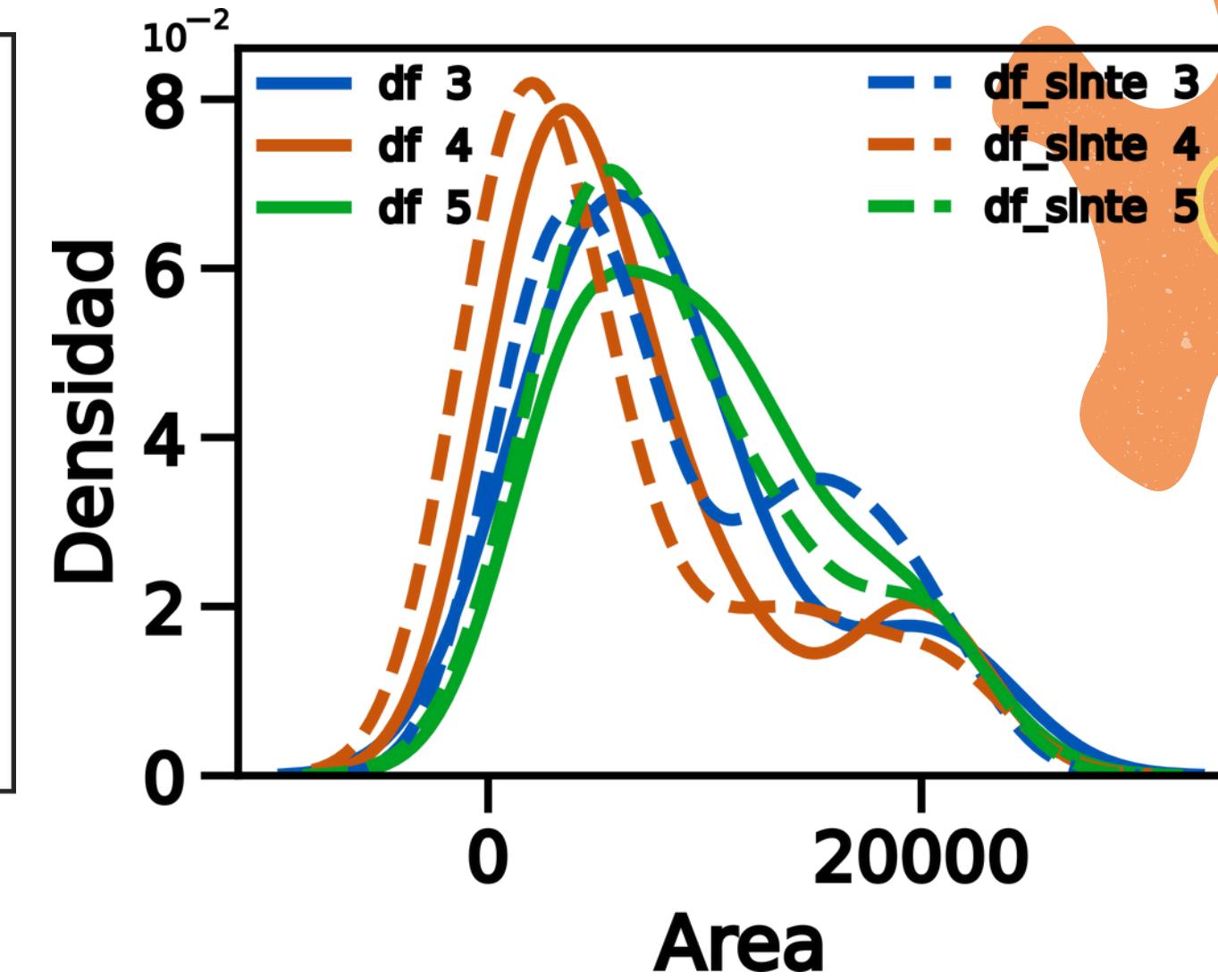
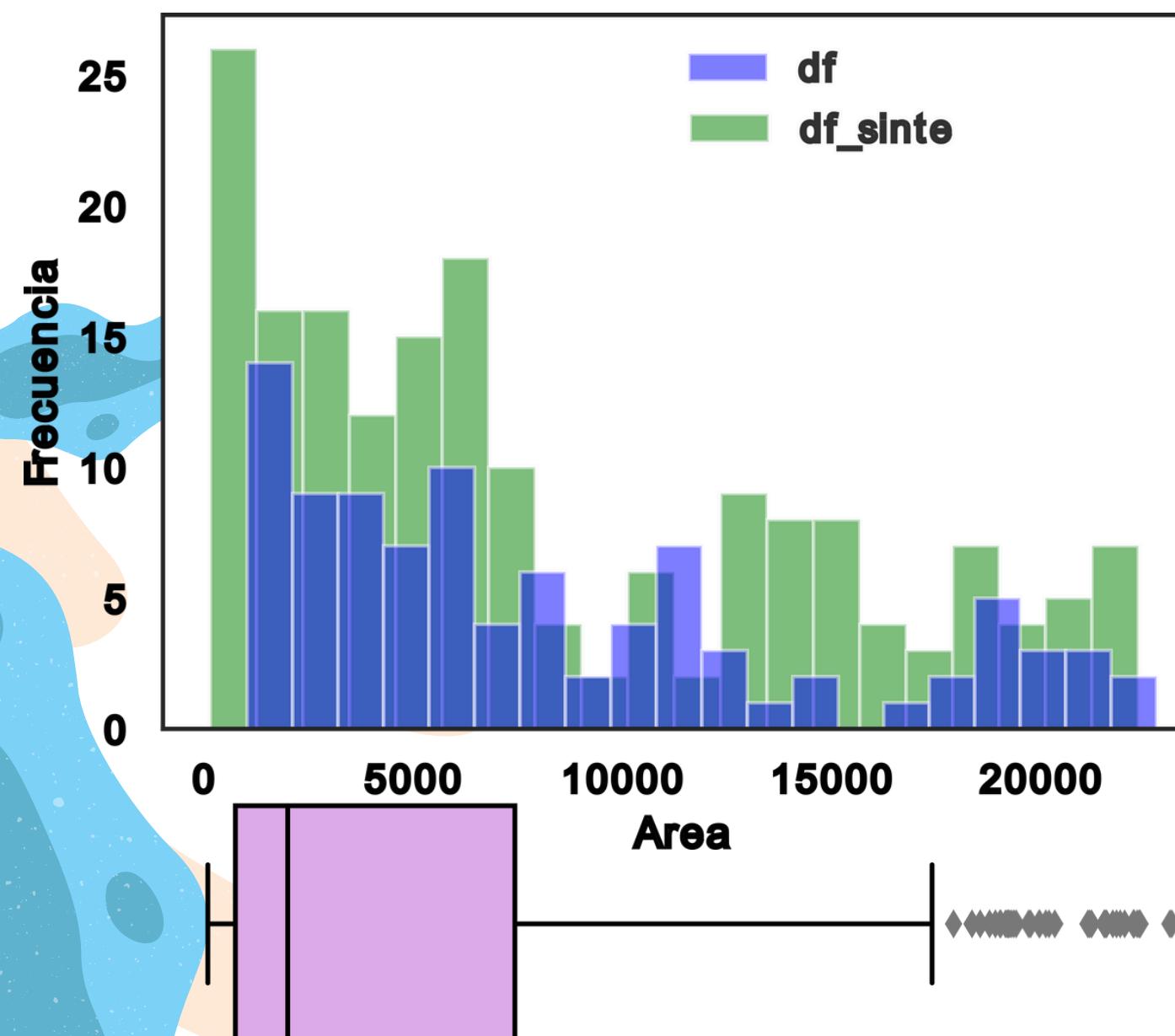
 dataacebo

Real vs. Synthetic Data for column



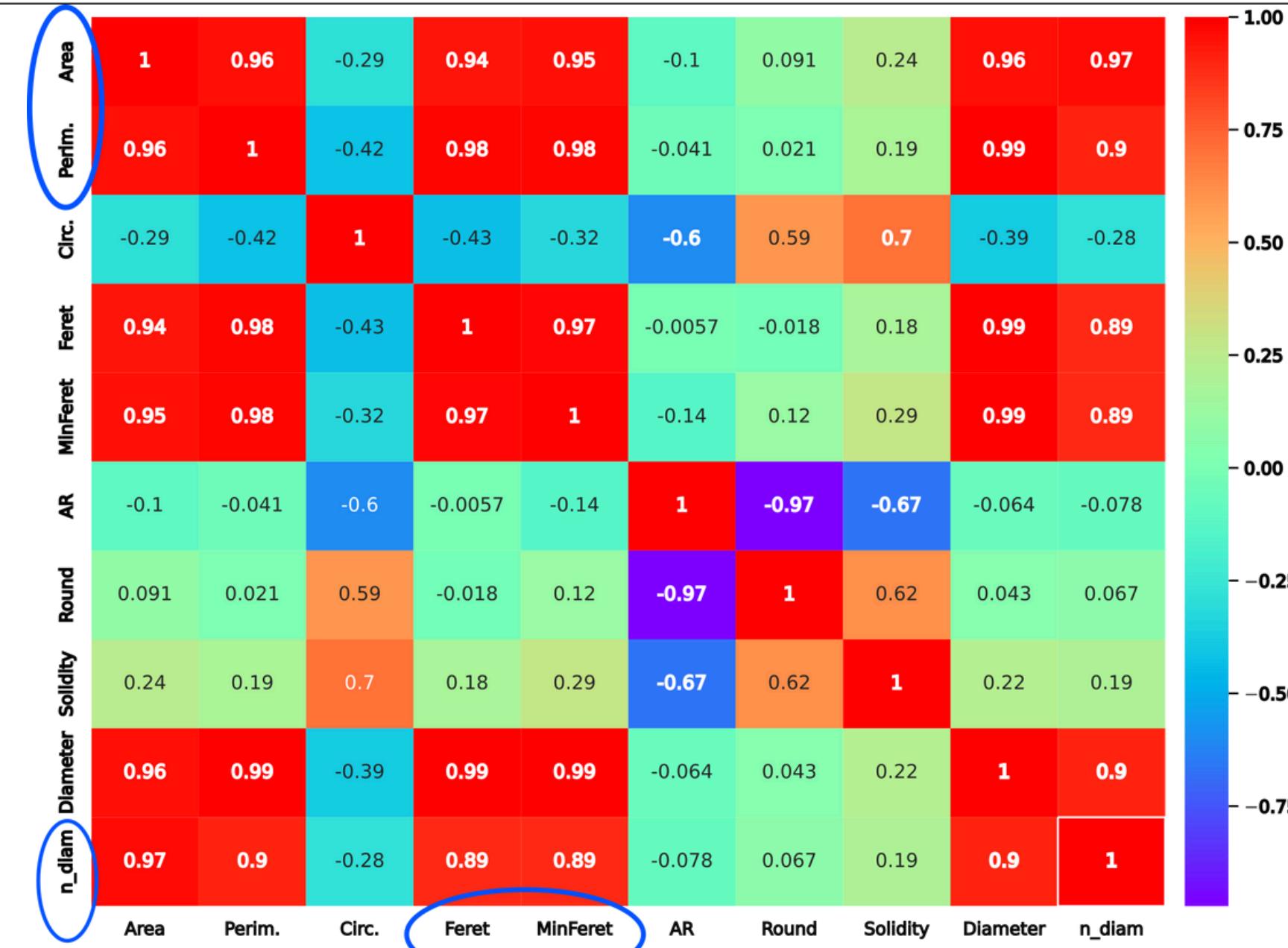
Pocos datos!!

| | labels | Area | Perim. | Circ. | Feret | MinFeret | AR | Round | Solidity | Esferoide | dia | Diameter | n_diam | |
|---|--------|---------|---------|----------|---------|----------|---------|----------|----------|-----------|-----|----------|---------|---------|
| 0 | 0001u | 2108.86 | 158.552 | 0.853148 | 52.0548 | 39.89 | 1.25244 | 0.801927 | 0.9574 | | si | 3 | 44.78 | 11.1182 |
| 1 | 0001v | 5494.72 | 267.744 | 0.765975 | 108.689 | 78.1359 | 1.3679 | 0.729508 | 0.9424 | | si | 5 | 94.0452 | 55.3549 |
| 2 | 0001w | 4604.33 | 208.633 | 0.835749 | 79.215 | 78.5711 | 1.0075 | 0.992155 | 0.9544 | | si | 3 | 74.802 | 24.8861 |
| 3 | 0001x | 3293.43 | 184.969 | 0.888199 | 59.5354 | 55.6766 | 1.03924 | 0.955215 | 0.9792 | | si | 3 | 57.8797 | 19.4266 |
| 4 | 000a0 | 12597.4 | 393.549 | 0.74141 | 115.415 | 98.4842 | 1.12671 | 0.888984 | 0.9568 | | si | 3 | 108.588 | 412.67 |



df_clean y correlación de variables

| labels | | Esferoide | Area | Circ. | AR | Round | Solidity | Diameter | n_diam |
|---|---|-----------|------|-------|-----|-------|----------|----------|--------|
| Esferas_BT474_dia_5_well_1_100X_3_blob_8 | 0 | 1388.7 | 0.9 | 1.1 | 0.9 | 1.0 | 43.0 | 12.9 | |
| 0000v | 1 | 4576.0 | 0.9 | 1.1 | 0.9 | 1.0 | 103.5 | 96.8 | |
| Esferas_BT474_dia_4_well_1_100X_11_blob_8 | 0 | 1061.0 | 0.8 | 1.3 | 0.8 | 1.0 | 38.8 | 9.5 | |
| 000tq | 1 | 1003.1 | 0.9 | 1.1 | 0.9 | 1.0 | 37.8 | 8.3 | |
| Esferas_BT474_dia_4_well_2_100X_1_blob_11 | 0 | 3779.8 | 0.6 | 1.2 | 0.8 | 0.9 | 76.5 | 72.6 | |
| 000rk | 1 | 6178.7 | 0.8 | 1.5 | 0.7 | 1.0 | 81.5 | 165.6 | |
| Esferas_BT474_dia_4_well_2_100X_1_blob_24 | 0 | 388.6 | 0.9 | 1.1 | 0.9 | 1.0 | 23.1 | 2.0 | |
| Esferas_BT474_dia_4_well_2_100X_2_blob_1 | 1 | 2653.2 | 0.9 | 1.1 | 0.9 | 1.0 | 58.7 | 32.8 | |
| Esferas_BT474_dia_5_well_2_100X_1_blob_4 | 0 | 150.5 | 0.9 | 1.1 | 0.9 | 0.9 | 14.3 | 0.5 | |
| 000cd | 1 | 7261.1 | 0.8 | 1.0 | 1.0 | 1.0 | 95.5 | 156.5 | |



MODELOS DE APRENDIZAJE

Modelos:

- Regresión Logística
- Árbol de Decisión
- Random Forest
- XGboost

Datos:

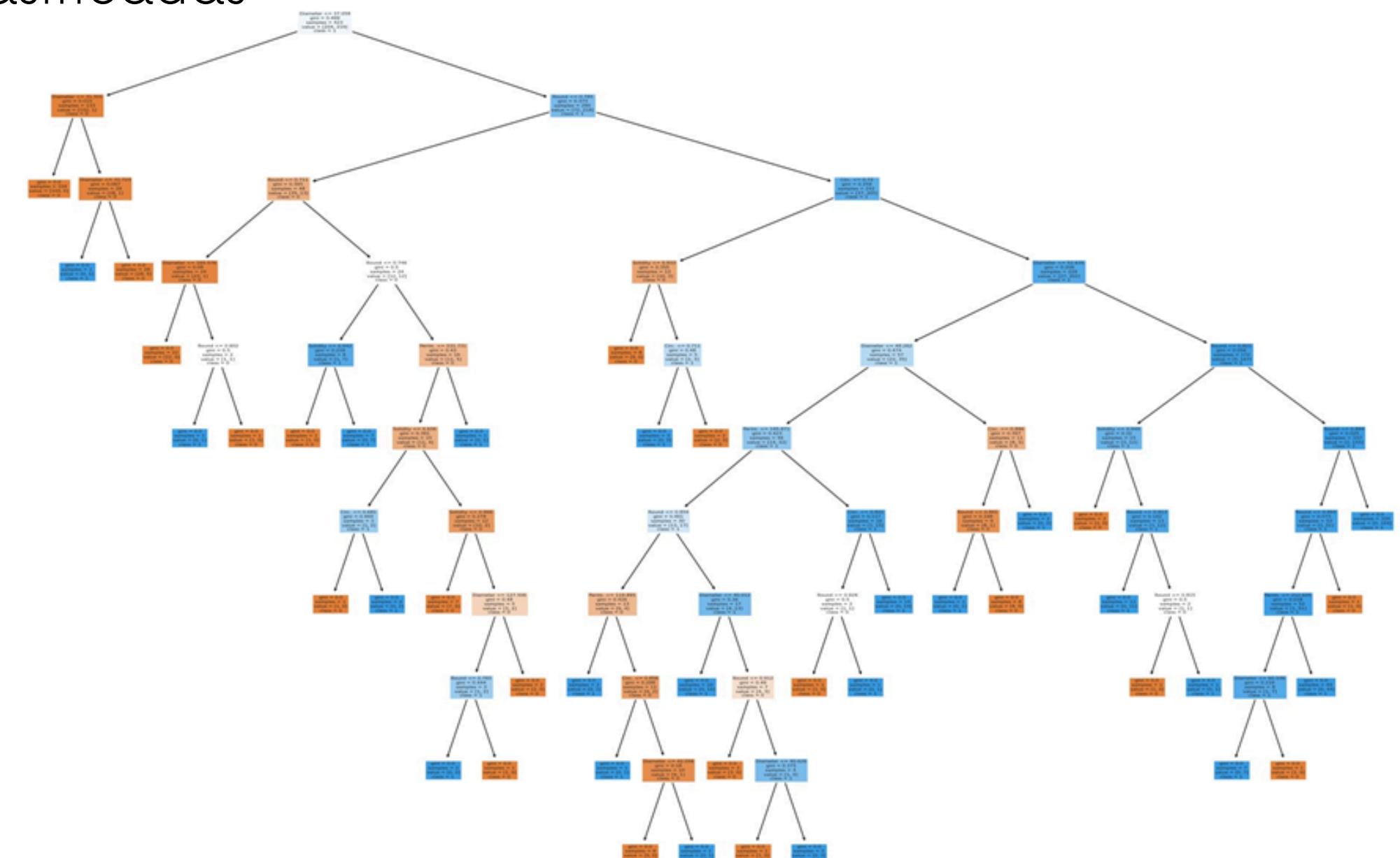
- 80% entrenamiento
- 20% testeo
- 3-4-5 días

Variables:

- Diámetro
- Round
- Perim.
- Circ.
- Solidity

Árbol de Decisión Base

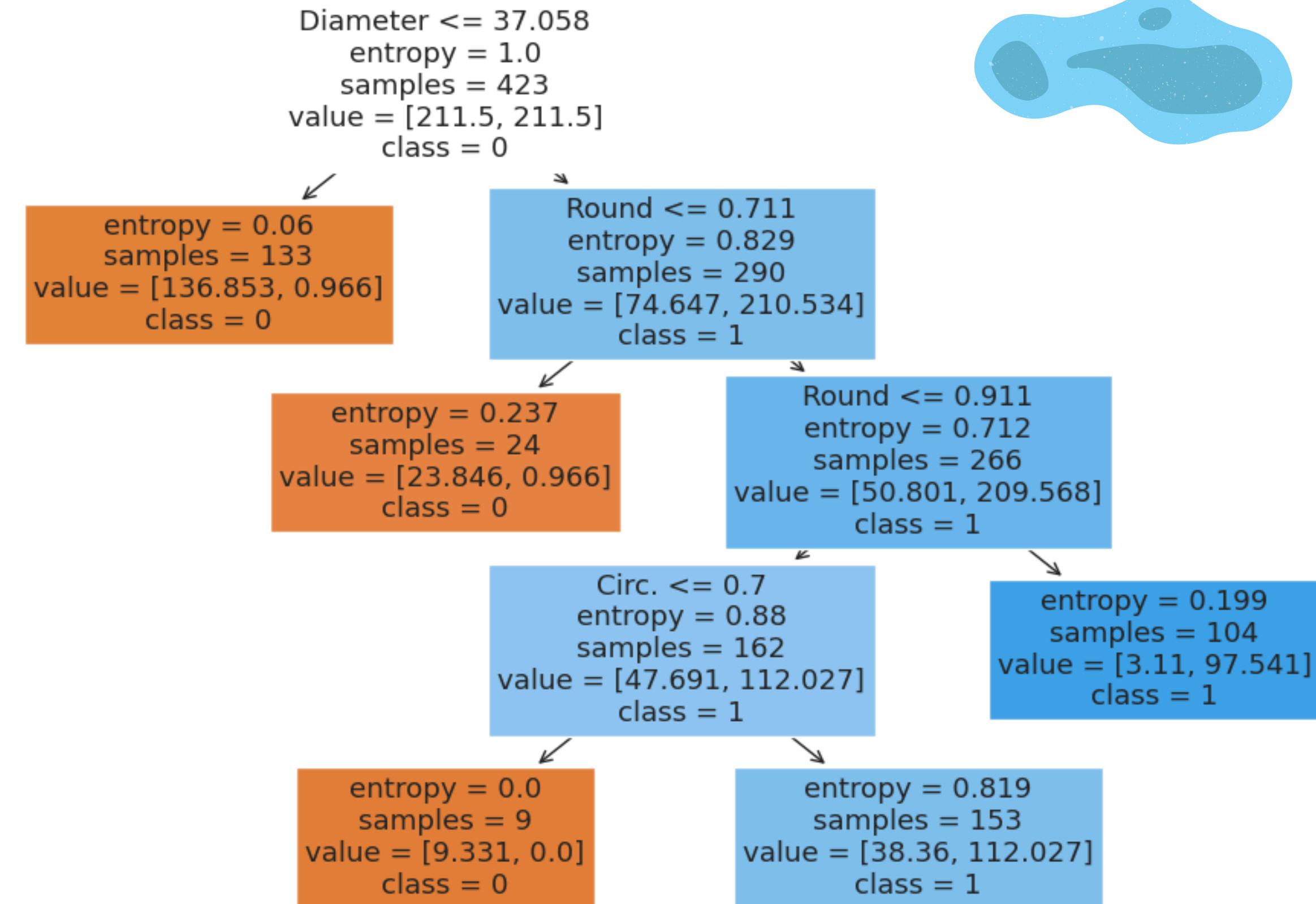
Se observó algunas variables como: diámetro, redondez y circularidad, tiene mayor probabilidad de ser clasificadas como tumoresferas.



Árbol de Decisión Ajustado

Se observó que las células con un diámetro mayor a 37.058, una redondez superior a 0.711 y una circunferencia mayor a 0.7 tienen una mayor probabilidad de ser clasificadas como Tumoresferas.

Estos datos son valiosos para identificar características específicas que podrían indicar la presencia de Tumoresferas en futuras observaciones.



Regresión Logística Base

Informe de Clasificación:

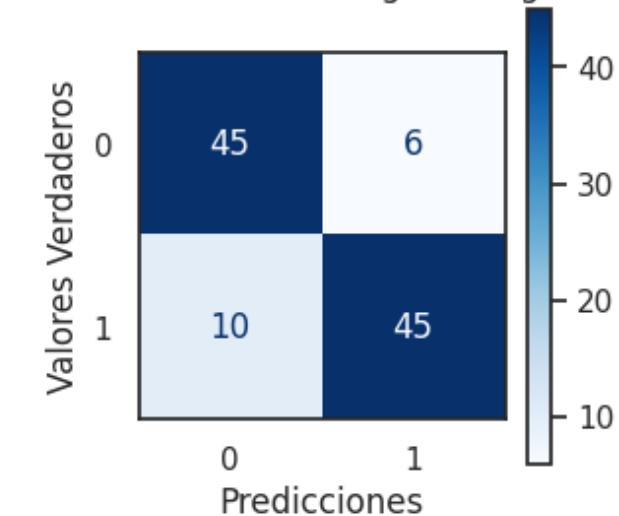
| | precision | recall | f1-score | support |
|--------------|-----------|--------|----------|---------|
| 0 | 0.82 | 0.88 | 0.85 | 51 |
| 1 | 0.88 | 0.82 | 0.85 | 55 |
| accuracy | | | 0.85 | 106 |
| macro avg | 0.85 | 0.85 | 0.85 | 106 |
| weighted avg | 0.85 | 0.85 | 0.85 | 106 |

Accuracy Score (Puntuación de Exactitud): 0.85

Precision Score (Puntuación de Precisión): 0.88

F1 Score: 0.85

Matriz de Confusión - Logistic Regression



Regresión Logística Ajustada

Informe de Clasificación:

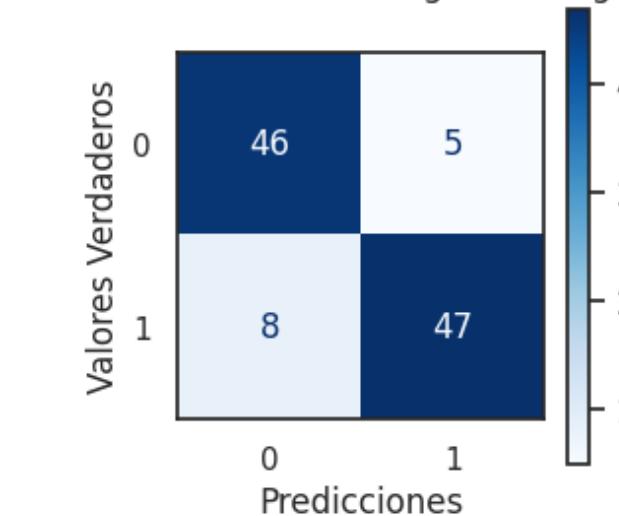
| | precision | recall | f1-score | support |
|--------------|-----------|--------|----------|---------|
| 0 | 0.85 | 0.90 | 0.88 | 51 |
| 1 | 0.90 | 0.85 | 0.88 | 55 |
| accuracy | | | 0.88 | 106 |
| macro avg | 0.88 | 0.88 | 0.88 | 106 |
| weighted avg | 0.88 | 0.88 | 0.88 | 106 |

Accuracy Score (Puntuación de Exactitud): 0.88

Precision Score (Puntuación de Precisión): 0.9

F1 Score: 0.88

Matriz de Confusión - Regresión Logistica



RandomForest Base

Random Forest Sin Ajustar:

Informe de Clasificación:

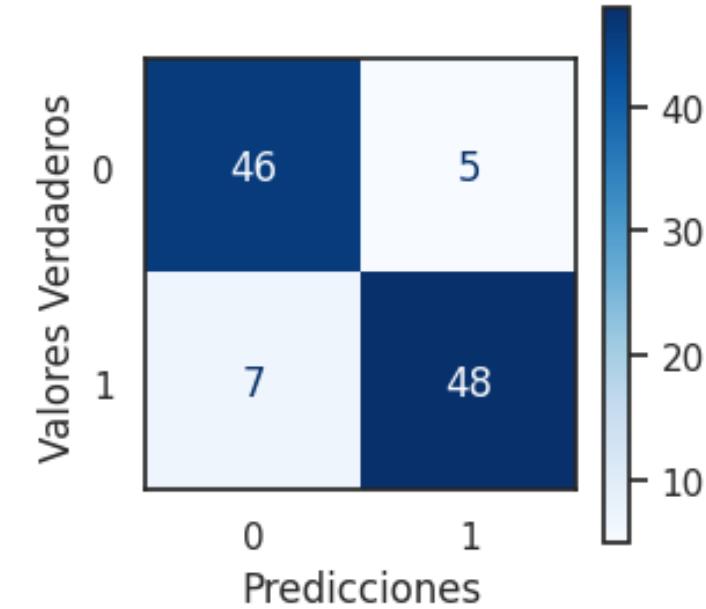
| | precision | recall | f1-score | support |
|--------------|-----------|--------|----------|---------|
| 0 | 0.88 | 0.90 | 0.89 | 51 |
| 1 | 0.91 | 0.89 | 0.90 | 55 |
| accuracy | | | 0.90 | 106 |
| macro avg | 0.90 | 0.90 | 0.90 | 106 |
| weighted avg | 0.90 | 0.90 | 0.90 | 106 |

Accuracy Score (Puntuación de Exactitud): 0.9

Precision Score (Puntuación de Precisión): 0.91

F1 Score: 0.9

Matriz de Confusión - Random Forest



RandomForest Ajustada

Random Forest Ajustado:

Informe de Clasificación:

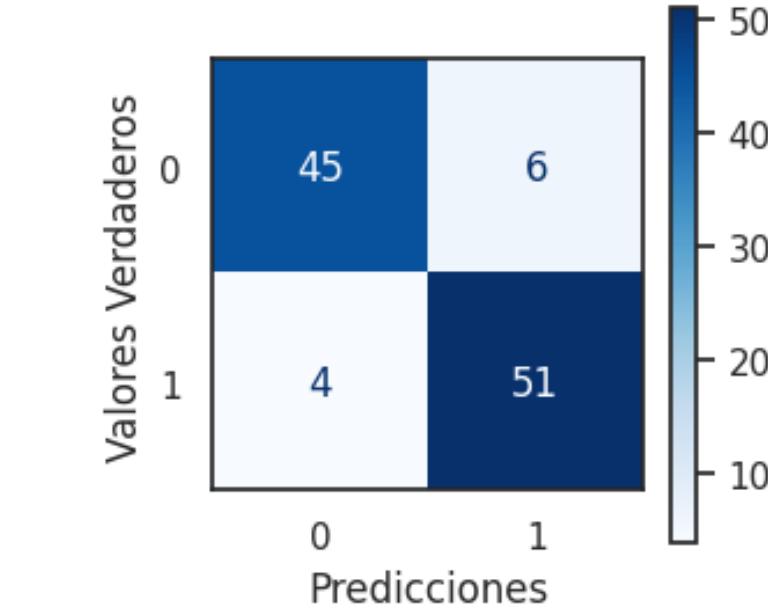
| | precision | recall | f1-score | support |
|--------------|-----------|--------|----------|---------|
| 0 | 0.92 | 0.88 | 0.90 | 51 |
| 1 | 0.89 | 0.93 | 0.91 | 55 |
| accuracy | | | 0.91 | 106 |
| macro avg | 0.91 | 0.90 | 0.91 | 106 |
| weighted avg | 0.91 | 0.91 | 0.91 | 106 |

Accuracy Score (Puntuación de Exactitud): 0.91

Precision Score (Puntuación de Precisión): 0.89

F1 Score: 0.91

Matriz de Confusión - Random Forest

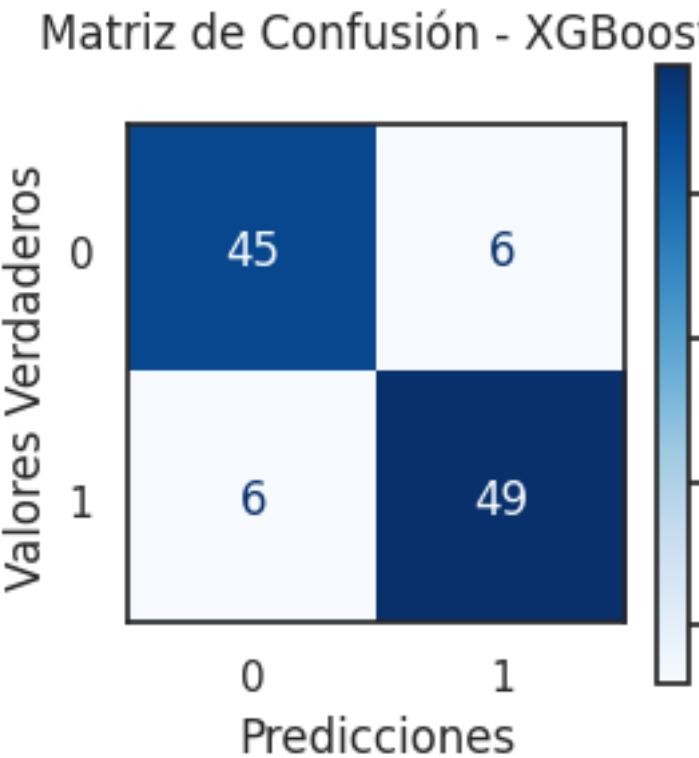


XGboost Base

XGboost Sin Ajustar:

| Informe de Clasificación: | | | | |
|---------------------------|-----------|--------|----------|---------|
| | precision | recall | f1-score | support |
| 0 | 0.88 | 0.88 | 0.88 | 51 |
| 1 | 0.89 | 0.89 | 0.89 | 55 |
| accuracy | | | 0.89 | 106 |
| macro avg | 0.89 | 0.89 | 0.89 | 106 |
| weighted avg | 0.89 | 0.89 | 0.89 | 106 |

Accuracy Score (Puntuación de Exactitud): 0.89
Precision Score (Puntuación de Precisión): 0.89
F1 Score: 0.89

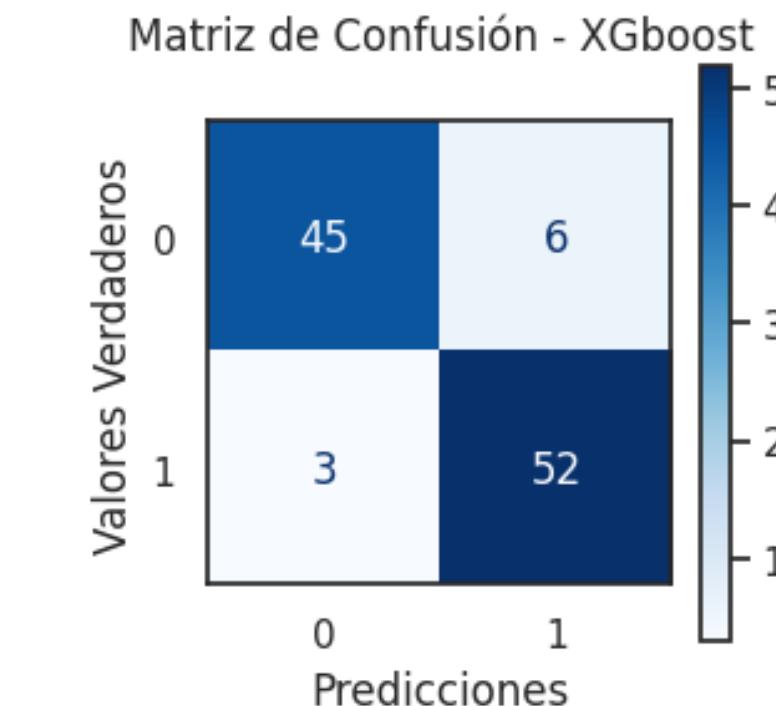


XGboost Ajustada

Informe de Clasificación:

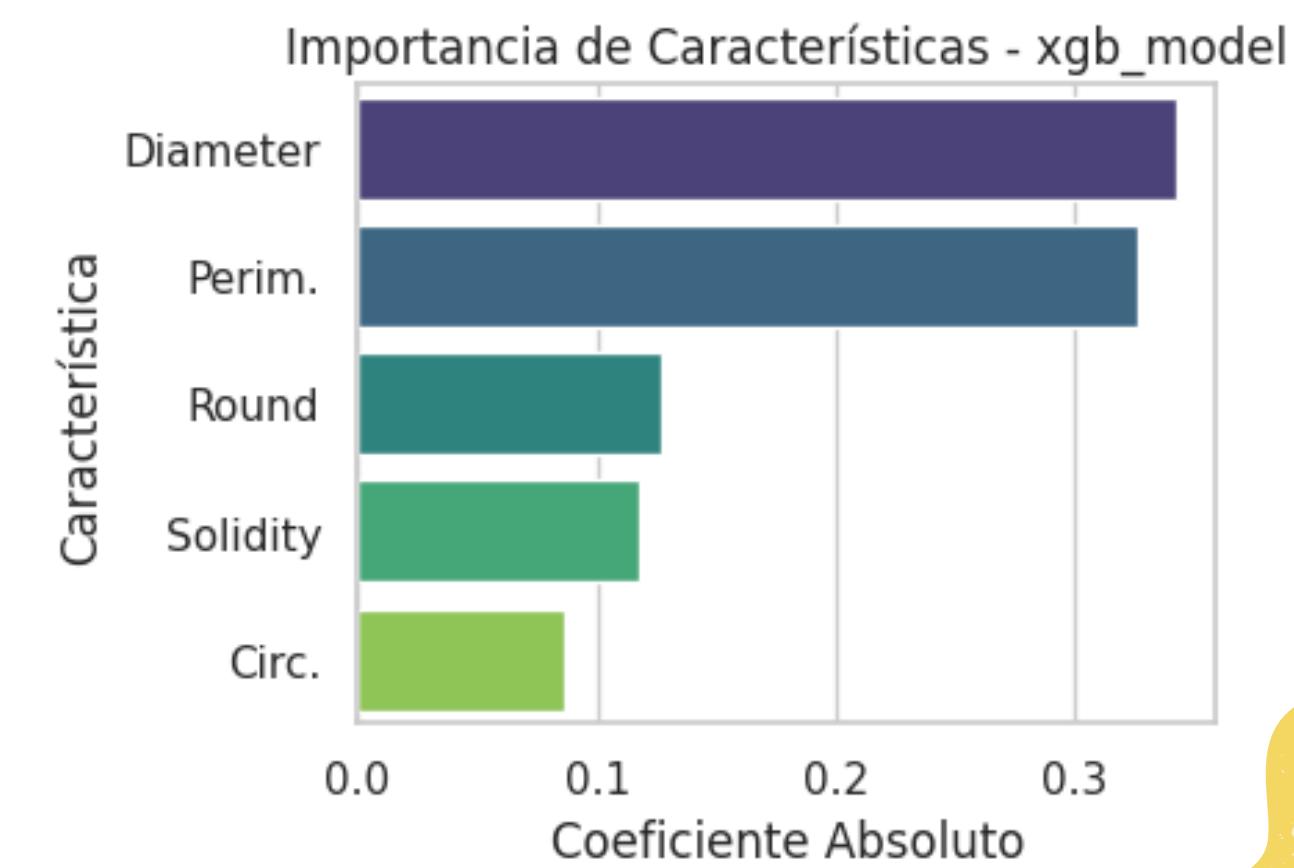
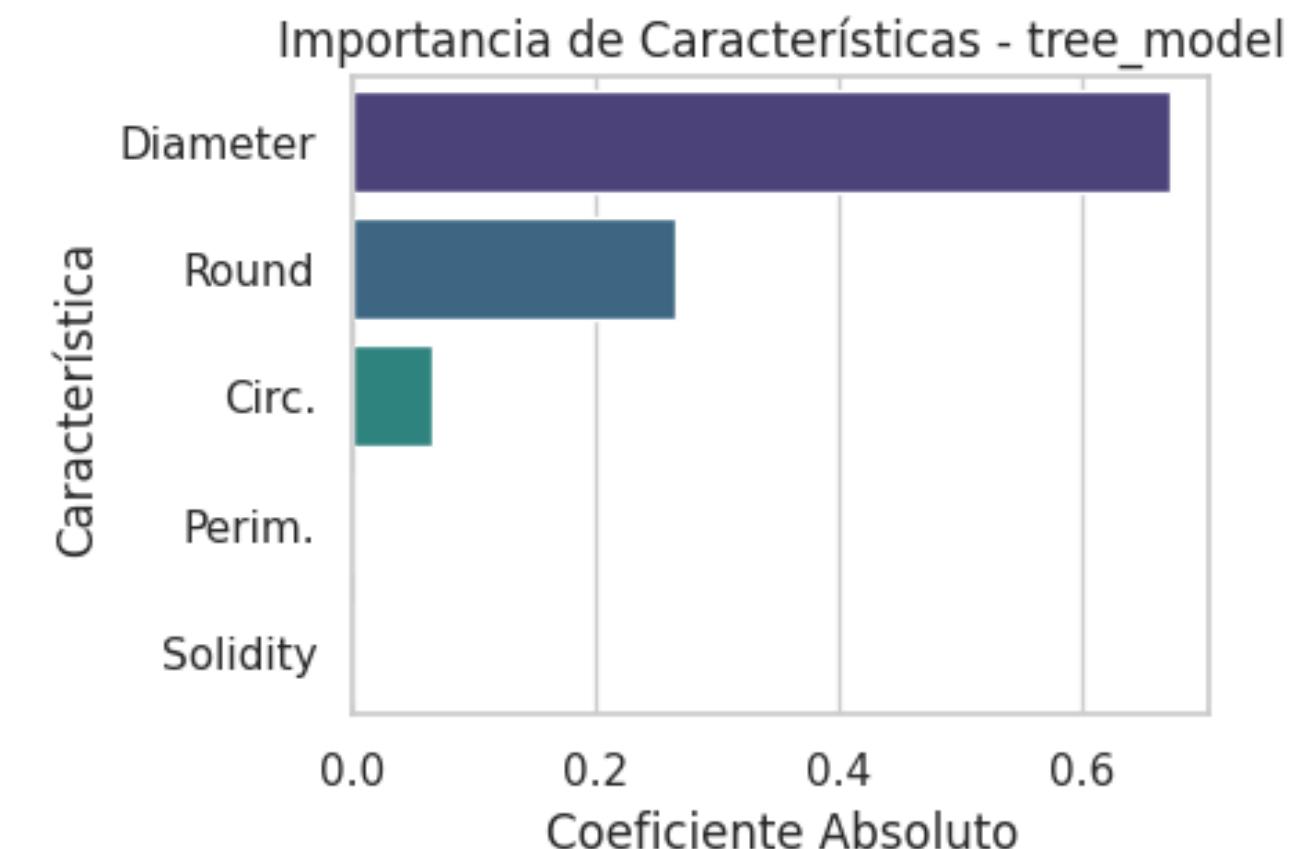
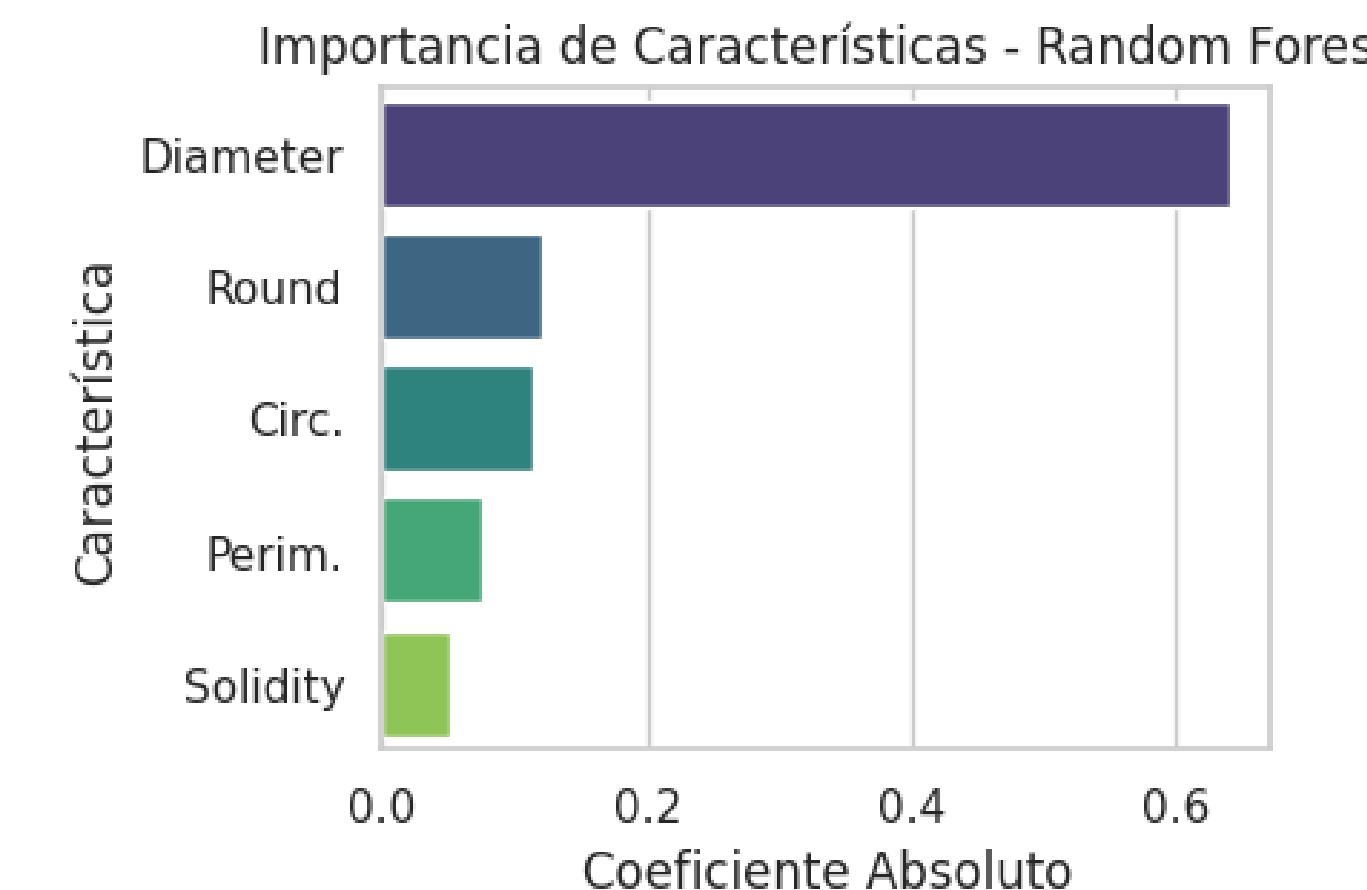
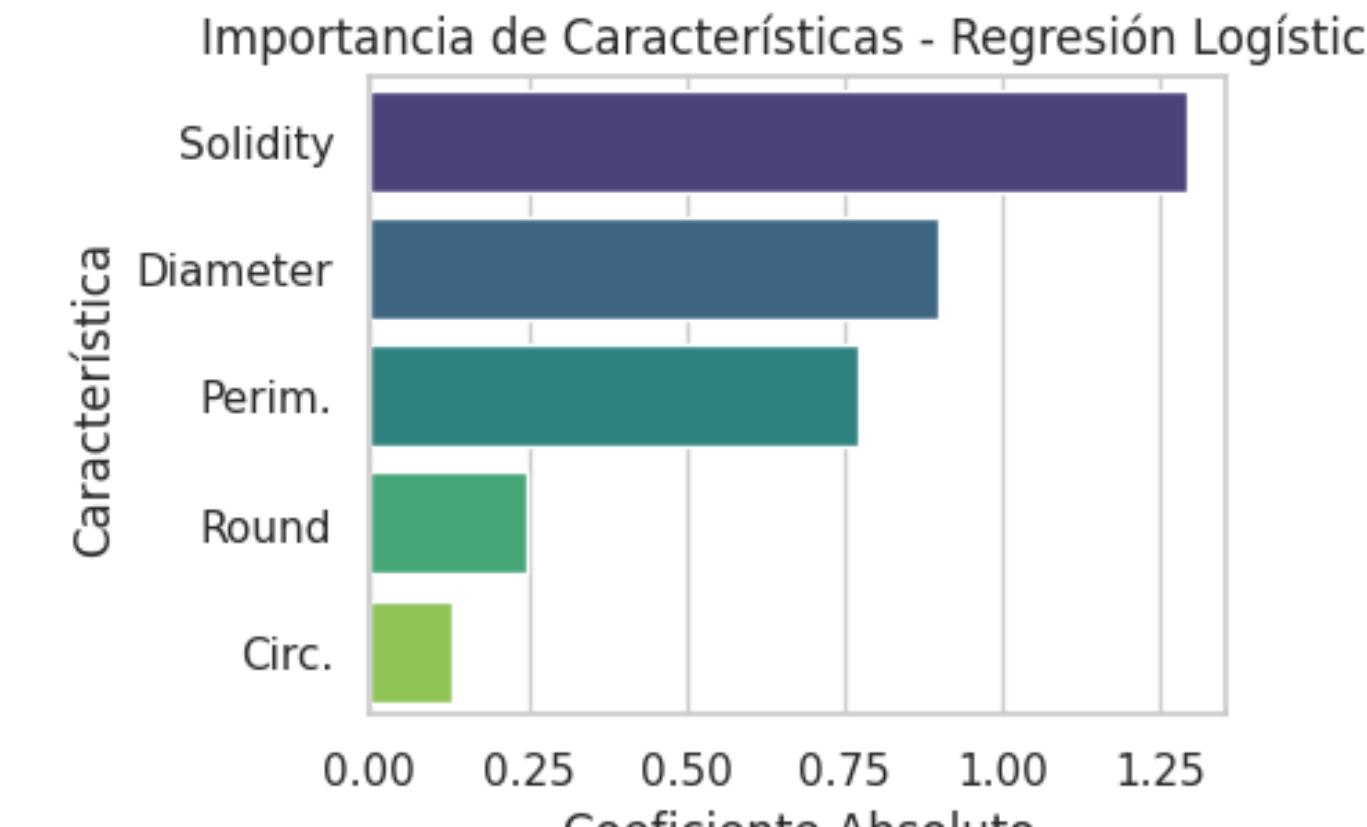
| | precision | recall | f1-score | support |
|--------------|-----------|--------|----------|---------|
| 0 | 0.94 | 0.88 | 0.91 | 51 |
| 1 | 0.90 | 0.95 | 0.92 | 55 |
| accuracy | | | 0.92 | 106 |
| macro avg | 0.92 | 0.91 | 0.91 | 106 |
| weighted avg | 0.92 | 0.92 | 0.91 | 106 |

Accuracy Score (Puntuación de Exactitud): 0.92
Precision Score (Puntuación de Precisión): 0.9
F1 Score: 0.92



Características importantes para los modelos

En términos generales, para los cuatro modelos, se puede destacar la relevancia de la variable a diámetro al momento de ajuste del modelo y denota la posible importancia que esta variable podría tener en la clasificación de las tumoresferas y no tumoresferas.



CONCLUSIONES Y OBSERVACIONES

Modelos Base VS. Modelos Ajustados

En general, los modelos ajustados con hiperparámetros superan en términos de Accuracy y F1-score a los modelos de base, lo que indica que el ajuste puede mejorar significativamente el rendimiento de los modelos.

Modelos Base

| Model | Accuracy | Precision | Recall | F1 Score |
|-------|----------|-----------|--------|----------|
|-------|----------|-----------|--------|----------|

| | | | | |
|---------------------|----------|----------|----------|----------|
| Logistic Regression | 0.849057 | 0.882353 | 0.818182 | 0.849057 |
| Decision Tree | 0.839623 | 0.895833 | 0.781818 | 0.834951 |
| Random Forest | 0.896226 | 0.907407 | 0.890909 | 0.899083 |
| XGBoost | 0.886792 | 0.890909 | 0.890909 | 0.890909 |

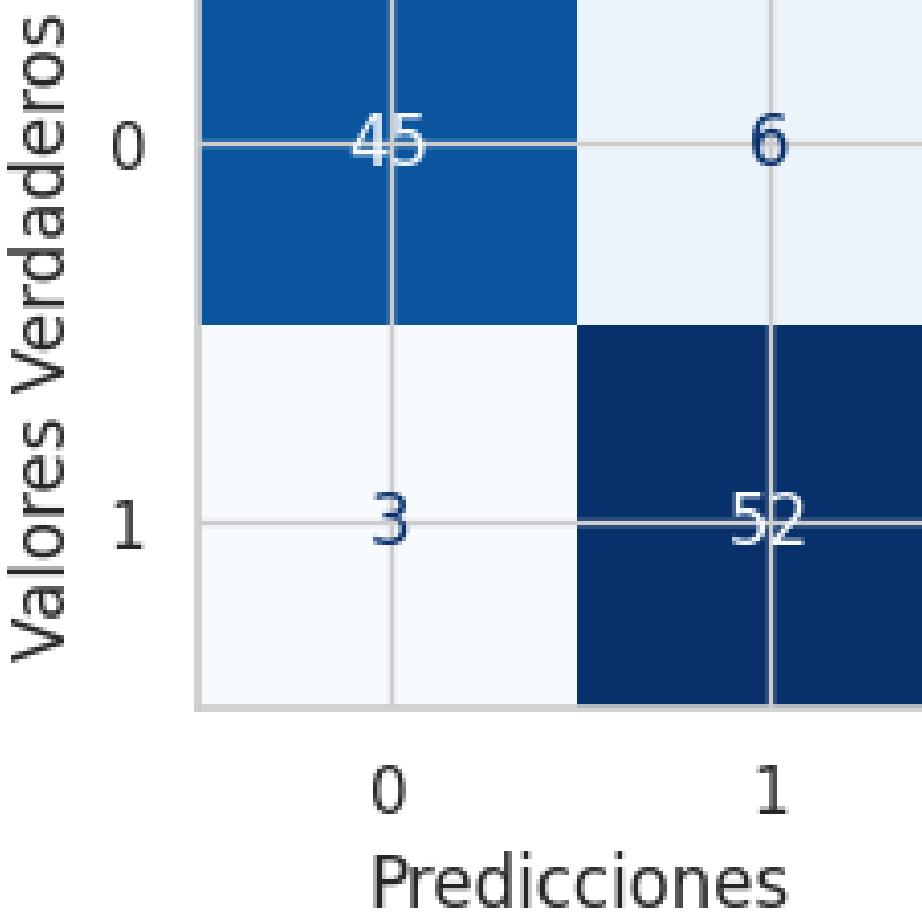
Modelos Ajustados

| Model | Accuracy | Precision | Recall | F1 Score |
|-------|----------|-----------|--------|----------|
|-------|----------|-----------|--------|----------|

| | | | | |
|------------------------|----------|----------|----------|----------|
| LogisticRegression | 0.877358 | 0.903846 | 0.854545 | 0.878505 |
| DecisionTreeClassifier | 0.915094 | 0.896552 | 0.945455 | 0.920354 |
| Random Forest | 0.905660 | 0.894737 | 0.927273 | 0.910714 |
| XGBoost | 0.915094 | 0.896552 | 0.945455 | 0.920354 |

XGboost – D.Tree

Informe de Clasificación:



| | precision | recall | f1-score | support |
|--------------|-----------|--------|----------|---------|
| 0 | 0.94 | 0.88 | 0.91 | 51 |
| 1 | 0.90 | 0.95 | 0.92 | 55 |
| accuracy | | | 0.92 | 106 |
| macro avg | 0.92 | 0.91 | 0.91 | 106 |
| weighted avg | 0.92 | 0.92 | 0.91 | 106 |

Accuracy Score (Puntuación de Exactitud): 0.92
Precision Score (Puntuación de Precisión): 0.9
F1 Score: 0.92

- **Accuracy (Exactitud)**

El 92% de las predicciones son correctas.

- **Precision (Precisión)**

El 90% de las predicciones de tumoresferas fueron correctas

- **Recall (Recuperación o Sensibilidad)**

El modelo detectó correctamente el 95% de las tumoresferas reales.

- **F1-Score**

Un valor de 92% indica un buen equilibrio entre la precisión y la capacidad del modelo para detectar tumoresferas.



Experiencia

Gracias!!