



SIMULTANEOUS SEPARATION METHOD OPTIMIZATION OF ANTIHYPERTENSIVE DRUGS USING HPLC-ASSISTED QSRR COMPUTATIONAL MODELING

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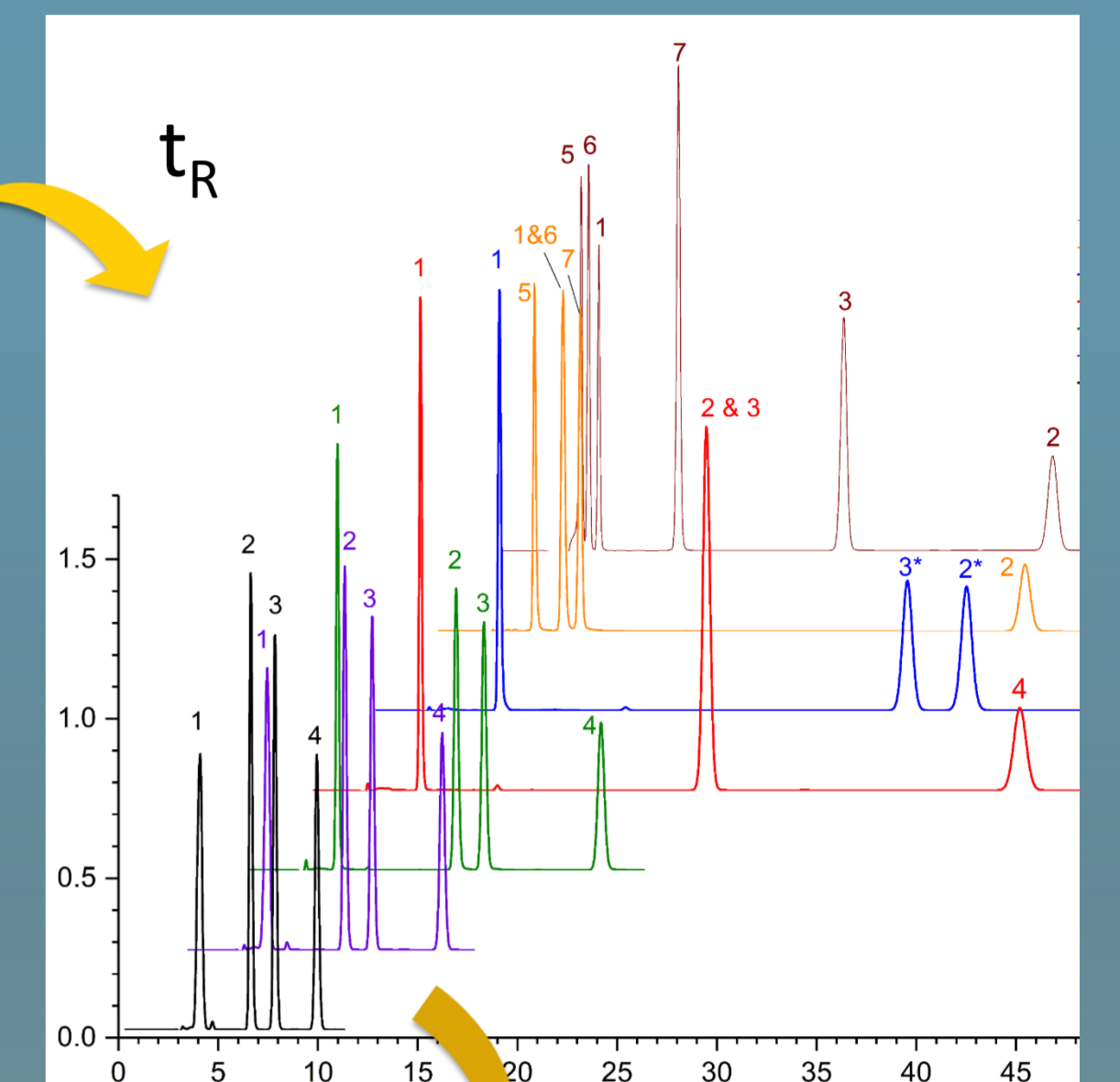
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Abstract

Separating multi compounds of drug mixtures can be challenging and often laborious to find the best conditions. HPLC is one of the prominent separation techniques in performing simultaneous separation. Nowadays, computational approaches assist in shortening the time in method optimization through retention time prediction. This study applied Quantitative Structure Retention Relationships (QSRR) computational modeling to evaluate the separation profiles of antihypertensive drugs from the Sartan group. Separation factors of mobile phase compositions, pH buffer, and the flow rate were optimized in reversed-phase mode. The agreement of QSRR prediction with the observed migration time profiles was analyzed.

Methods

HPLC Waters® Alliance 2695e, UV detector 2489	
Mobile phase	MeCN : 0.5 % v/v phosphate buffer
Stationary phase	Sunfire Waters® 150 x 4.6 mm id, 5 µm
Flow rate	0.5 mL/minute

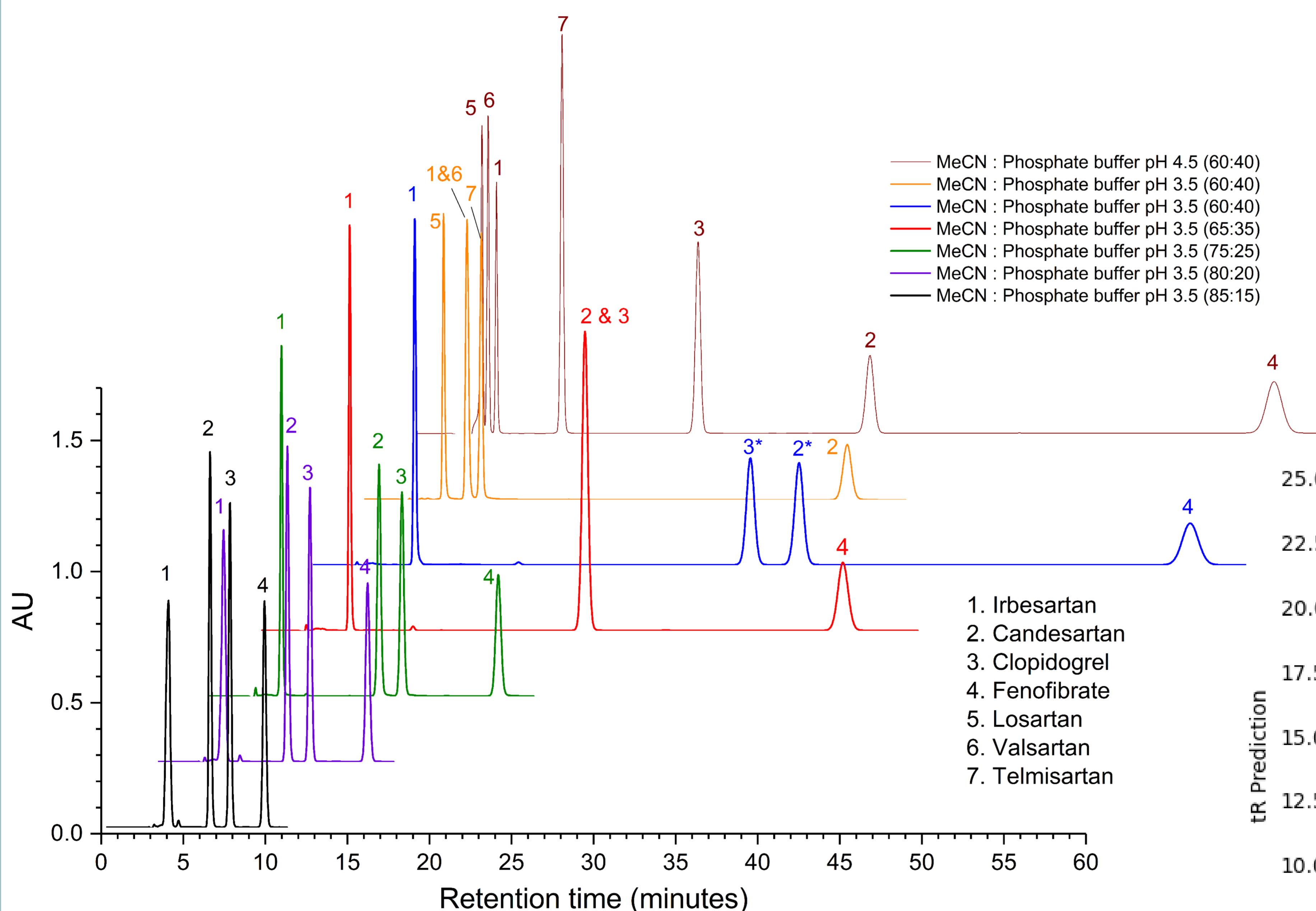


K-Nearest Neighbour (KNN)

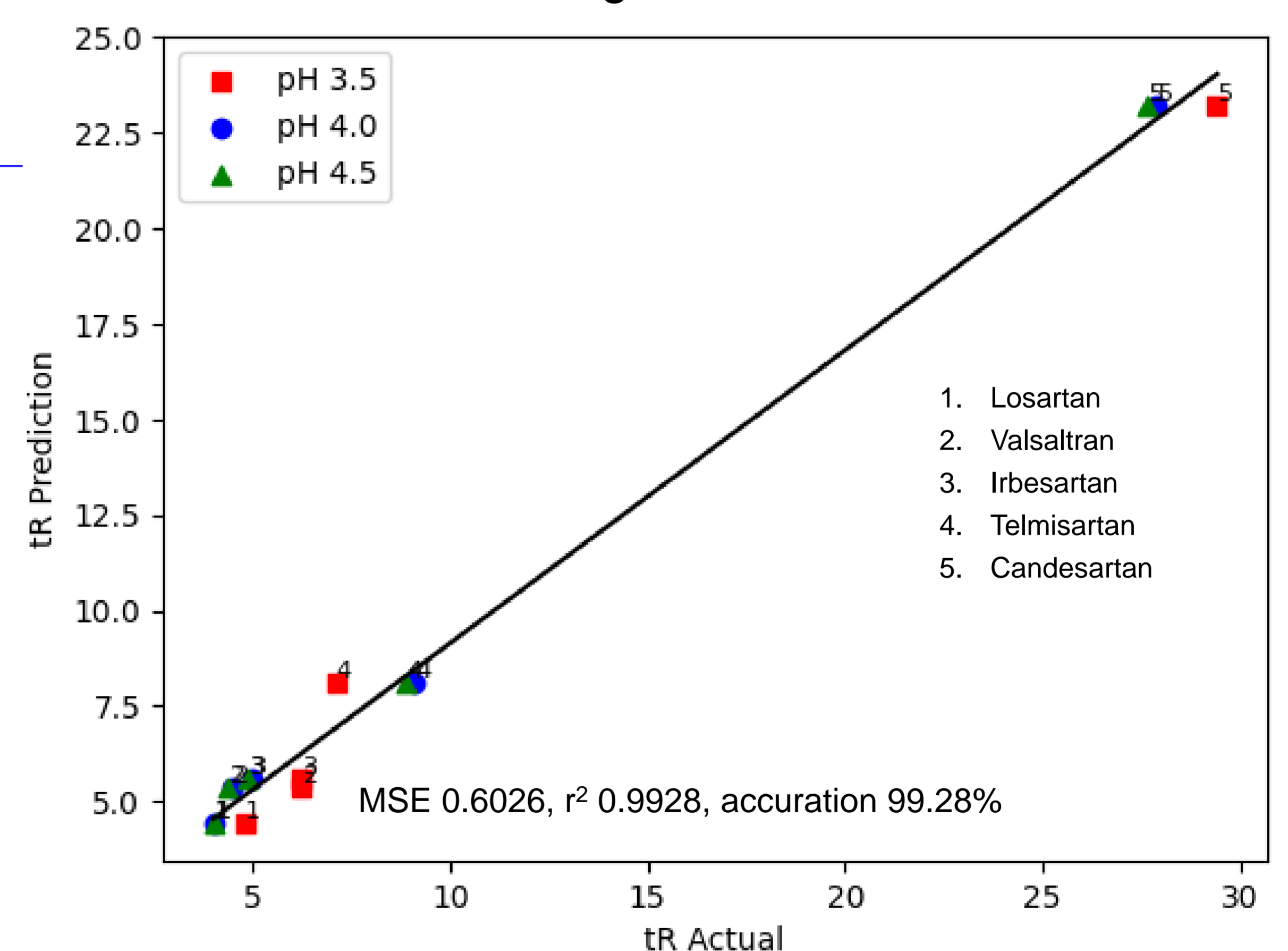
$$d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

d = Euclidean distance; x = Location x; y = Location y

Results



K-Nearest Neighbour Model Evaluation



Conclusion

A statistical approach using the KNN method showed feasibility to perform initial prediction of the retention time of the Sartan group and other compounds involving the proximity of the fingerprint matrix of the compound structure. Close agreement prediction t_R with the lab results was achieved with Mean Square Error 0.6026, r^2 0.9928, and the accuracy of 99.28%.

References

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CERTIFICATE OF ATTENDANCE

This is to officially certify that

Ratih Ratih

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participated in the

HPLC 2023

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and presented a poster with the title

**Simultaneous Separation Method Optimization of Antihypertensive
Drugs using HPLC-assisted QSRR Computational Modeling**



Prof. Dr. Michael Lämmerhofer and Prof. Dr. Oliver J. Schmitz
Chairmen of HPLC 2023