



Degradation Plot

Prediction of degradation products and pathways

Retention Time Report

Client:
Alttox

Username:
alany@alttox.com.br

Study Number:
RetentionTime_Alttox_Metamizole_DegradationPlot_20230918171835

Date:
2023/09/18 - 17:22:13

Program Version:
1.3.3

Molecular Query

Name:
Metamizole

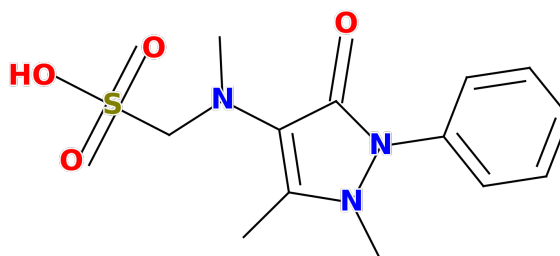
CAS:
50567-35-6

Exact Mass:
311.09397721

Common Name:
Metamizole

Iupac Name:
[(1,5-dimethyl-3-oxo-2-phenylpyrazol-4-yl)-methylamino]methanesulfonic acid

CID:
3111



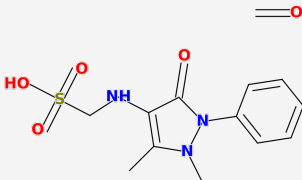
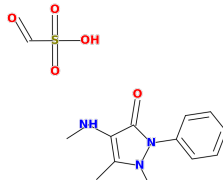
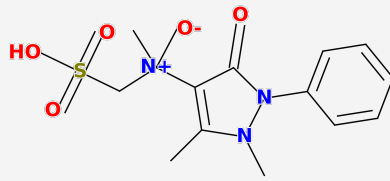
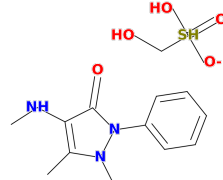
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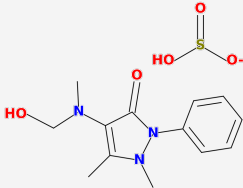
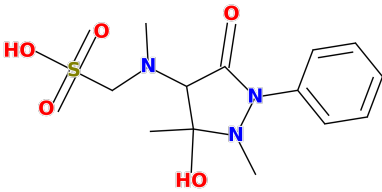
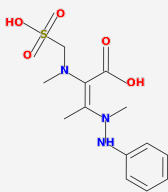
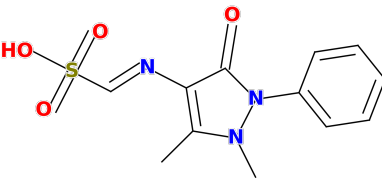
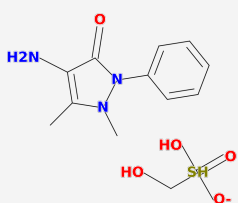
Model Summary

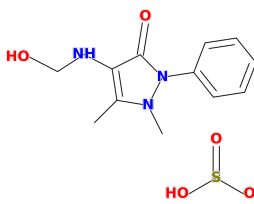
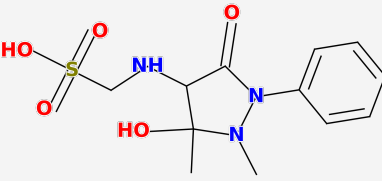
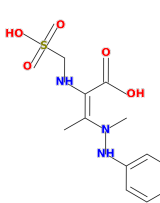
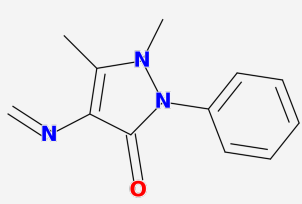
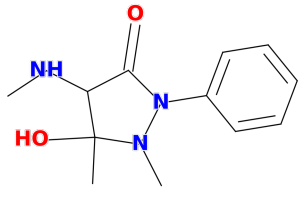
This report presents a prediction of the retention time using neural network and deep learning algorithms. The software Degradation Plot generates the prediction by analyzing a vast amount of historical data and training the neural network to identify patterns and relationships between molecular fragments and the retention time. This approach enables the software to make highly accurate predictions based on real-world data and provides a valuable tool for optimizing and predicting the performance of chromatographic processes. The prediction of retention time will assist in monitoring the degradation of APIs in a more effective and efficient manner. More than 70,000 molecules and their respective retention times were used to train the models, this database was built based on the data set published by Xavier Domingo-Almenara and collaborators¹. This prediction corresponds specifically to a method with the following characteristics: HPLC on an Agilent 1100/1200 series liquid chromatography, Zorbax Extend-C18 reverse-phase column (2.1 x 50 mm, 1.8 μm). The composition for the mobile phases A and B of water + 0.1% formic acid and acetonitrile + 0.1% formic acid, respectively. The gradient consists of 5% B for 3 min, 50% B over 2 min, 85% B over 15 min and held at 85% B for 3 min, with a flow rate of 100 μL/min. All analyzes were performed in positive and negative ionization mode. Dead and dwell volume were 40 μL and 900 μL.

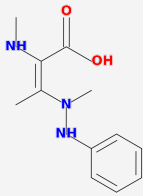
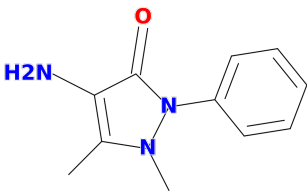
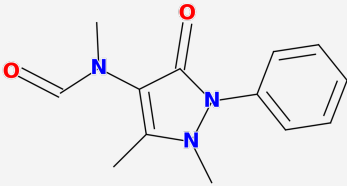
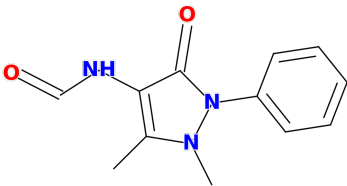
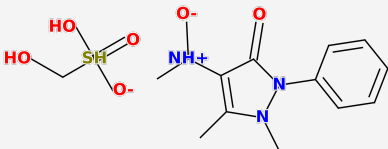
Retention Time Prediction

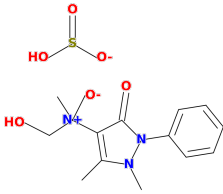
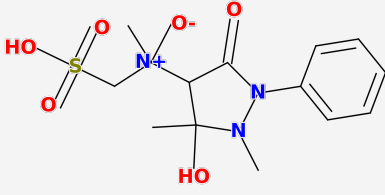
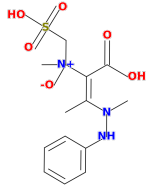
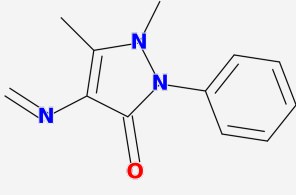
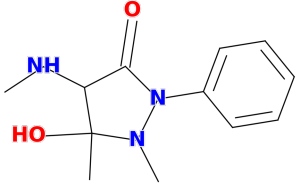
The table below brings the retention time values (in minutes) for degradation products predicted by the degradation plot, as well as the label, chemical formula and exact mass.

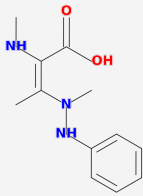
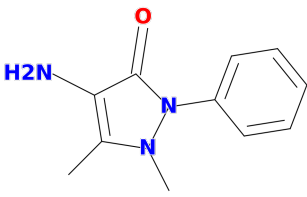
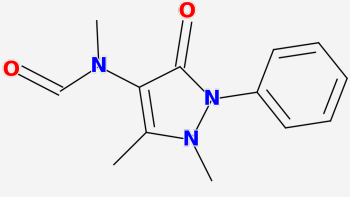
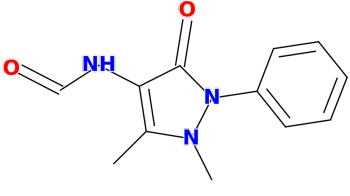
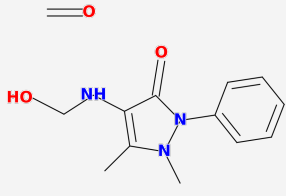
Product	Label	Formula	Mass	Predicted retention time (minutes)
	DP-1-1	CH_2O $\text{C}_{12}\text{H}_{15}\text{N}_3\text{O}_4\text{S}$	30.01056 297.07833	10.9 11.5
	DP-1-2	$\text{C}_{12}\text{H}_{15}\text{N}_3\text{O}$ $\text{CH}_2\text{O}_4\text{S}$	217.12151 109.96738	10.1 12.1
	DP-1-3	$\text{C}_{13}\text{H}_{17}\text{N}_3\text{O}_5\text{S}$	327.08889	13.0
	DP-1-4	$\text{C}_{12}\text{H}_{15}\text{N}_3\text{O}$ $\text{CH}_5\text{O}_4\text{S}^-$	217.12151 112.9914	10.1 10.4

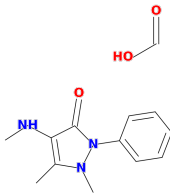
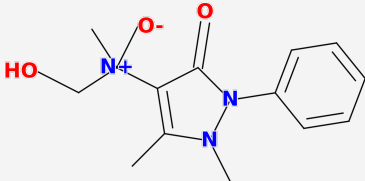
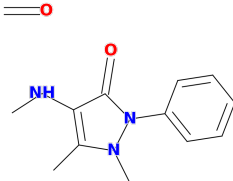
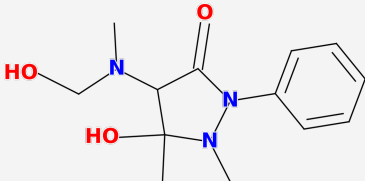
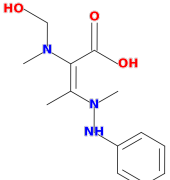
Product	Label	Formula	Mass	Predicted retention time (minutes)
	DP-1-5	$C_{13}H_{17}N_3O_2$ HO_3S^-	247.13208 80.96519	9.5 10.6
	DP-1-6	$C_{13}H_{19}N_3O_5S$	329.10454	11.1
	DP-1-7	$C_{13}H_{19}N_3O_5S$	329.10454	12.5
	DP-2-1	$C_{12}H_{13}N_3O_4S$	295.06268	12.1
	DP-2-2	$C_{11}H_{13}N_3O$ $CH_5O_4S^-$	203.10586 112.9914	10.4 10.4

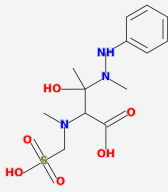
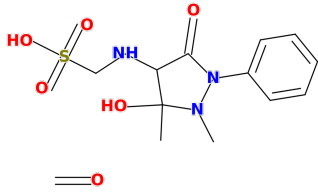
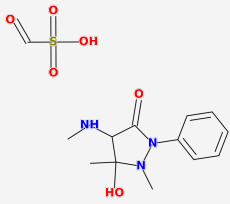
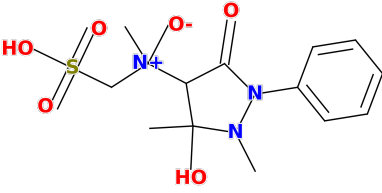
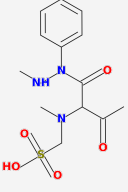
Product	Label	Formula	Mass	Predicted retention time (minutes)
	DP-2-3	$C_{12}H_{15}N_3O_2$ HO_3S^-	233.11643 80.96519	9.9 10.6
	DP-2-4	$C_{12}H_{17}N_3O_5S$	315.08889	12.1
	DP-2-5	$C_{12}H_{17}N_3O_5S$	315.08889	10.7
	DP-2-6	$C_{12}H_{13}N_3O$	215.10586	10.9
	DP-2-7	$C_{12}H_{17}N_3O_2$	235.13208	11.0

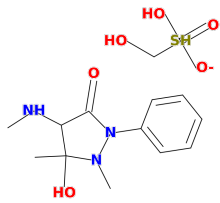
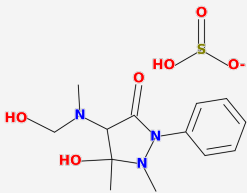
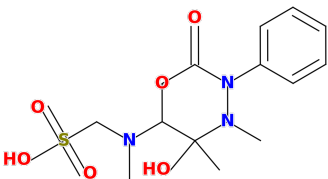
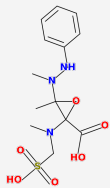
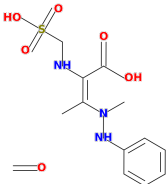
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	DP-2-8	C ₁₂ H ₁₇ N ₃ O ₂	235.13208	9.6
	DP-2-9	C ₁₁ H ₁₃ N ₃ O	203.10586	10.4
	DP-2-10	C ₁₃ H ₁₅ N ₃ O ₂	245.11643	11.8
	DP-2-11	C ₁₂ H ₁₃ N ₃ O ₂	231.10078	10.6
	DP-2-12	C ₁₂ H ₁₅ N ₃ O ₂ CH ₅ O ₄ S ⁻	233.11643 112.9914	10.1 10.4

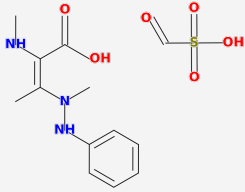
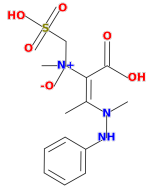
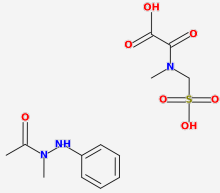
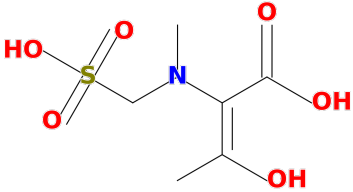
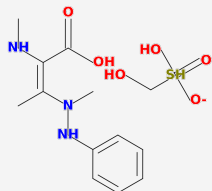
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	DP-2-13	$C_{13}H_{17}N_3O_3$ HO_3S^-	263.12699 80.96519	9.9 10.6
	DP-2-14	$C_{13}H_{19}N_3O_6S$	345.09946	11.6
	DP-2-15	$C_{13}H_{19}N_3O_6S$	345.09946	11.5
	DP-2-16	$C_{12}H_{13}N_3O$	215.10586	10.9
	DP-2-17	$C_{12}H_{17}N_3O_2$	235.13208	11.0

Product	Label	Formula	Mass	Predicted retention time (minutes)
	DP-2-18	C ₁₂ H ₁₇ N ₃ O ₂	235.13208	9.6
	DP-2-19	C ₁₁ H ₁₃ N ₃ O	203.10586	10.4
	DP-2-20	C ₁₃ H ₁₅ N ₃ O ₂	245.11643	11.8
	DP-2-21	C ₁₂ H ₁₃ N ₃ O ₂	231.10078	10.6
	DP-2-22	CH ₂ O C ₁₂ H ₁₅ N ₃ O ₂	30.01056 233.11643	10.9 9.9

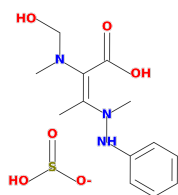
Product	Label	Formula	Mass	Predicted retention time (minutes)
	DP-2-23	$C_{12}H_{15}N_3O$ CH_2O_2	217.12151 46.00548	10.1 11.2
	DP-2-24	$C_{13}H_{17}N_3O_3$	263.12699	9.9
	DP-2-25	CH_2O $C_{12}H_{15}N_3O$	30.01056 217.12151	10.9 10.1
	DP-2-26	$C_{13}H_{19}N_3O_3$	265.14264	9.7
	DP-2-27	$C_{13}H_{19}N_3O_3$	265.14264	10.6

Product	Label	Formula	Mass	Predicted retention time (minutes)
	DP-2-28	$C_{13}H_{21}N_3O_6S$	347.11511	11.7
	DP-2-29	CH_2O $C_{12}H_{17}N_3O_5S$	30.01056 315.08889	10.9 12.1
	DP-2-30	$C_{12}H_{17}N_3O_2$ CH_2O_4S	235.13208 109.96738	11.0 12.1
	DP-2-31	$C_{13}H_{19}N_3O_6S$	345.09946	11.6
	DP-2-32	$C_{13}H_{19}N_3O_5S$	329.10454	11.0

Product	Label	Formula	Mass	Predicted retention time (minutes)
	DP-2-33	$C_{12}H_{17}N_3O_2$ $CH_5O_4S^-$	235.13208 112.9914	11.0 10.4
	DP-2-34	$C_{13}H_{19}N_3O_3$ HO_3S^-	265.14264 80.96519	9.7 10.6
	DP-2-35	$C_{13}H_{19}N_3O_6S$	345.09946	12.9
	DP-2-36	$C_{13}H_{19}N_3O_6S$	345.09946	11.9
	DP-2-37	CH_2O $C_{12}H_{17}N_3O_5S$	30.01056 315.08889	10.9 10.7

Product	Label	Formula	Mass	Predicted retention time (minutes)
	DP-2-38	$C_{12}H_{17}N_3O_2$ CH_2O_4S	235.13208 109.96738	9.6 12.1
	DP-2-39	$C_{13}H_{19}N_3O_6S$	345.09946	11.5
	DP-2-40	$C_9H_{12}N_2O$ $C_4H_7NO_6S$	164.09496 196.99941	10.5 9.9
	DP-2-41	$C_6H_{11}NO_6S$	225.03071	10.0
	DP-2-42	$C_{12}H_{17}N_3O_2$ $CH_5O_4S^-$	235.13208 112.9914	9.6 10.4

Product	Label	Formula	Mass	Predicted retention time (minutes)
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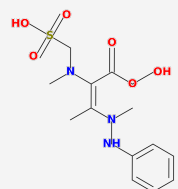


DP-2-43

$C_{13}H_{19}N_3O_3$
 HO_3S^-

265.14264
80.96519

10.6
10.6

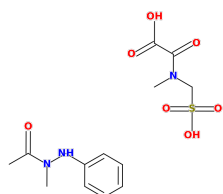


DP-2-44

$C_{13}H_{19}N_3O_6S$

345.09946

13.7



DP-2-45

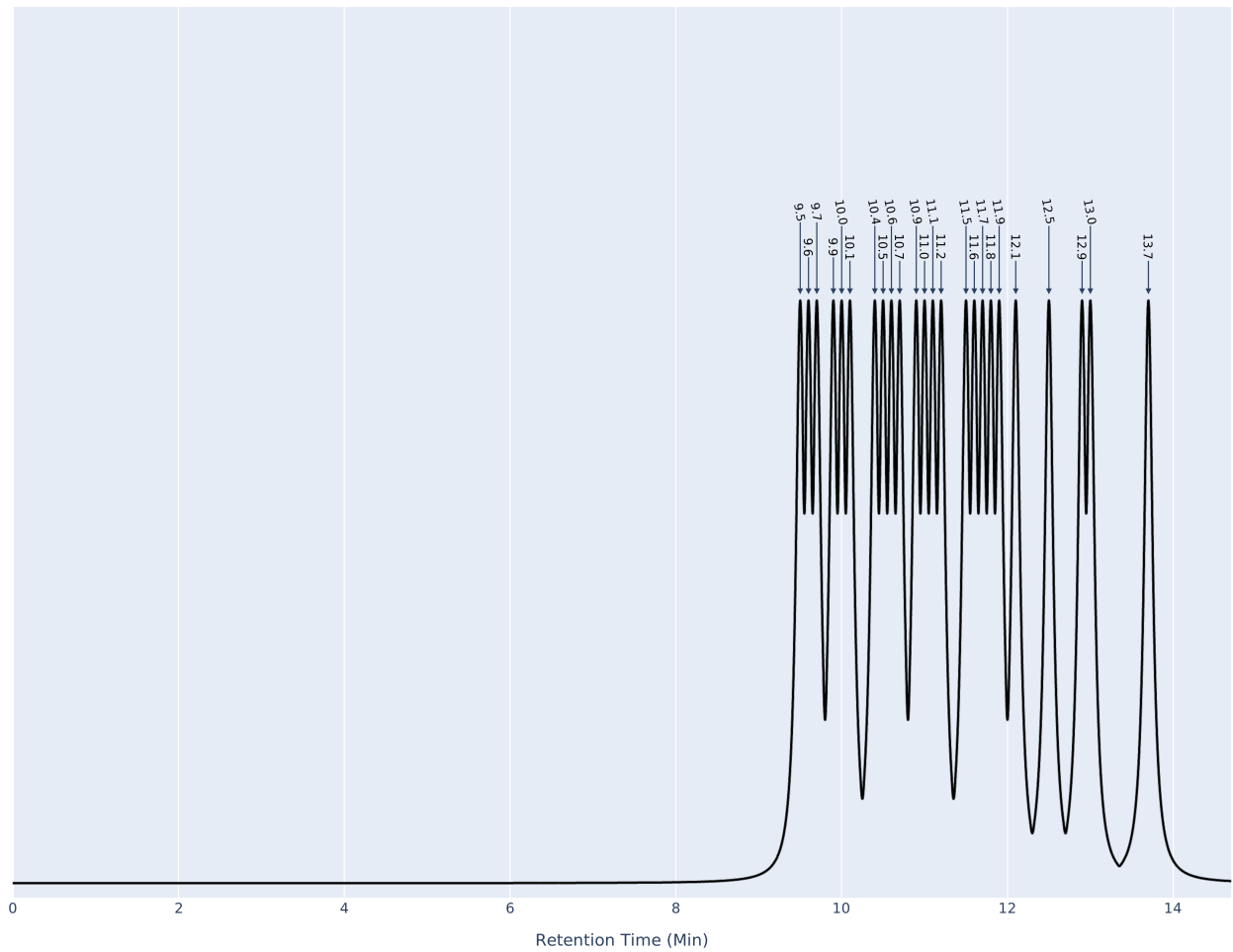
$C_9H_{12}N_2O$
 $C_4H_7NO_6S$

164.09496
196.99941

10.5
9.9

Theoretical Chromatogram

The chart presented below represents a theoretical model generated by applying the Lorentz transformation solely to retention times, disregarding intensities.



References

1. DOMINGO-ALMENARA, Xavier et al. The METLIN small molecule dataset for machine learning-based retention time prediction. *Nature communications*, v. 10, n. 1, p. 5811, 2019.