

Rubemamine and Rubescenamine, Two Naturally Occurring *N*-Cinnamoyl Phenethylamines with Umami Taste Modulating Properties

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**Supplementary Material**

**Table S.1:** References for Spectral Data of Synthesized Compounds

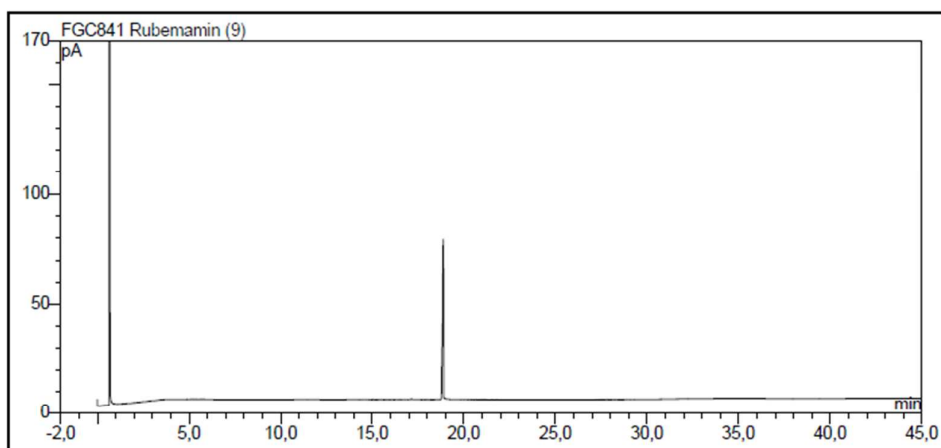
Cpd. No.	Name	Reference
1	<i>N-E</i> -Coumaroyltyramine	Achanta, S.; Liautard, V.; Paugh, R.; Organ, M. G., The Development of a General Strategy for the Synthesis of Tyramine-Based Natural Products by Using Continuous Flow Techniques. <i>Chemistry – A European Journal</i> <b>2010</b> , 16, 12797-12800
2	<i>N-(E)</i> -Coumaryldopamine	El-Gamal, A. A.; Takeya, K.; Itokawa, H.; Halim, A. F.; Amer, M. M.; Saad, H. E. A.; Awad, S. A., Studies on the chemical constituents of <i>Atraphaxis spinosa</i> L., var. <i>sinaica</i> Boiss. <i>Nat. Med.</i> <b>1994</b> , 48, 304-306.
3	<i>N-(E)</i> -Caffeoyltyramine	Chen, T.; He, J.; Zhang, J.; Li, X.; Zhang, H.; Hao, J.; Li, L., The isolation and identification of two compounds with predominant radical scavenging activity in hempseed (seed of <i>Cannabis sativa</i> L.). <i>Food Chem.</i> <b>2012</b> , 134, 1030-1037.
4	<i>N-(E)</i> -Feruloyltyramine	See cpd. 1
5	<i>N-(E)</i> -Feruloyloctopamine	Nesterenko, V.; Putt, K. S.; Hergenrother, P. J., Identification from a Combinatorial Library of a Small Molecule that Selectively Induces Apoptosis in Cancer Cells. <i>J. Am. Chem. Soc.</i> <b>2003</b> , 125, 14672-14677 ((S)-enantiomer)
6	<i>N-(E)</i> -Feruloyldopamine	Wu, Z.; Zheng, L.; Li, Y.; Su, F.; Yue, X.; Tang, W.; Ma, X.; Nie, J.; Li, H., Synthesis and structure–activity relationships and effects of phenylpropanoid amides of octopamine and dopamine on tyrosinase inhibition and antioxidation. <i>Food Chem.</i> <b>2012</b> , 134, 1128-1131.
7	<i>N-(E)</i> -Feruloyl-3-methoxytyramine	Chen, C.-Y.; Chang, F.-R.; Yen, H.-F.; Wu, Y.-C., Amides from stems of <i>Annona cherimola</i> . <i>Phytochemistry</i> <b>1998</b> , 49, 1443-1447.
8	<i>N-(Z)</i> -Feruloyl-3-methoxytyramine	See cpd. 7
9	Rubemamine	Ref. 32
10	Rubescenamine	Ref. 21
11	Armatamide	Kalia, N. K.; Singh, B.; Sood, R. P., A New Amide from <i>Zanthoxylum armatum</i> . <i>J. Nat. Prod.</i> <b>1999</b> , 62, 311-312.
12	Zanthosine	See cpd. 11

13	Zanthosinamide	Adesina, S. K.; Olatunji, O. A.; Bergenthal, D.; Reisch, J., Natural product chemistry. Part 122. Transcinnamoylamides from <i>Zanthoxylum rubescens</i> pericarbs. <i>Pharmazie</i> <b>1988</b> , 43, 517-518.
14	Dioxamine	Adesina, S. K.; Reisch, J., Amides from <i>Zanthoxylum rubescens</i> . <i>Phytochemistry</i> <b>1989</b> , 28, 839-842.
15	Moschamine	Hu, W.; Qin, H.; Cui, Y.; Jia, Y., Total Synthesis of (+)- and (-)-Decursivine and (±)-Serotobenine through a Cascade Witkop Photocyclization/Elimination/Addition Sequence: Scope and Mechanistic Insights. <i>Chemistry – A European Journal</i> <b>2013</b> , 19, 3139-3147.

## NMR and GC data of Rubemamine (9)

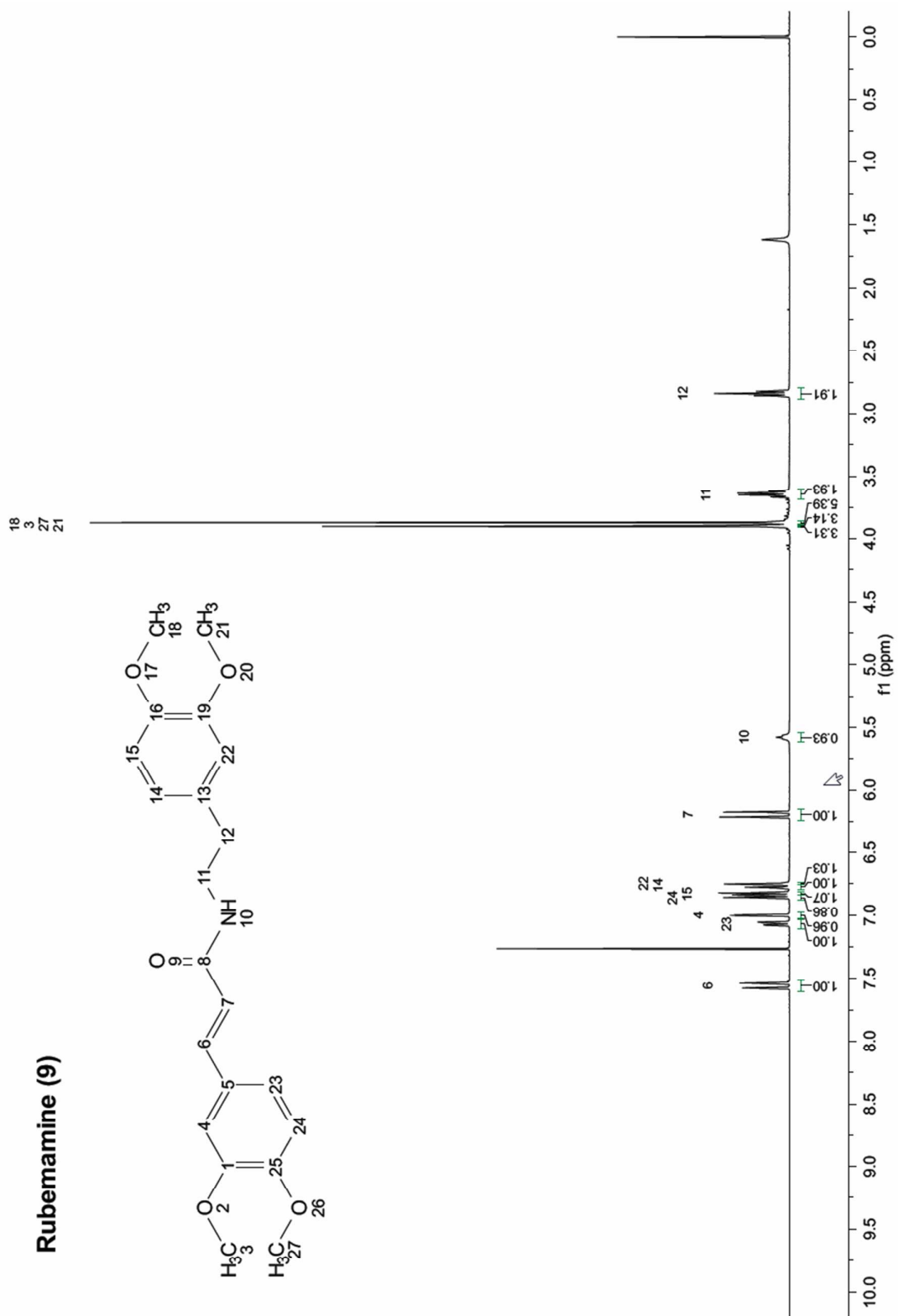
### Rubemamine (9)

Vial Number: 20 Injection Volume: 1,0  
Control Program: FGC841 Sample Type: unknown  
Quantif. Method: FGC841\_Proben Run Time (min): 45,00  
Column Info: 15m MXT-1(HT) 0.1µm df;ID:0.25mm / 60-10-380° KAS



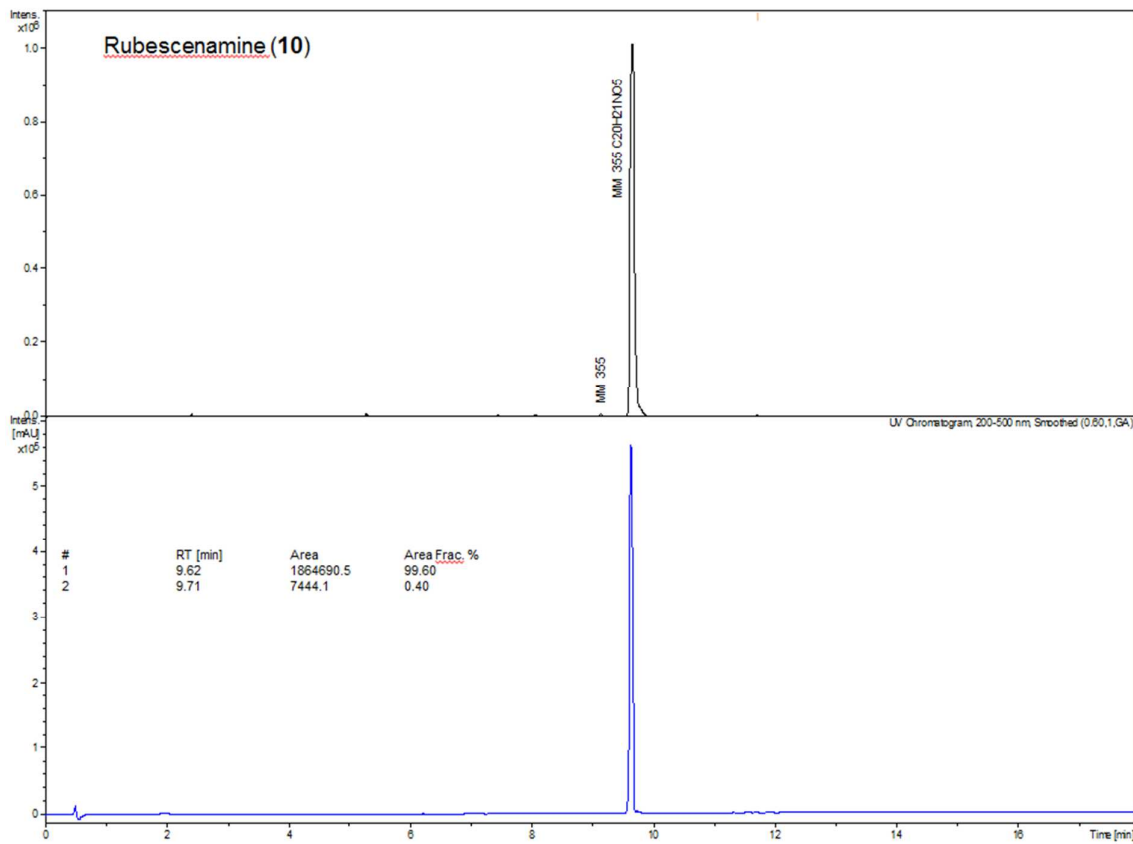
No.	Ret.Time min	Ret.Index	Area pA*min	Type	Rel.Area %	Peak Name
1	17,140	2963,60	0,019	BMB	0,422	n.a.
2	18,877	3257,76	4,527	BMB	99,578	Rubemamine (9)
Total:			4,546		100,000	

Agilent 6890N equipped with a MXT column (length, 15 m; inside diameter, 0.25 mm; film, 0.10 µm); flow rate, 1.0 – 5.0 ml min<sup>-1</sup>; injector, split ratio 1/100, 60°C – 10°/s – 380°C; carrier gas, H<sub>2</sub>; detector, FID, 420°C (Restek, Bad Homburg, Germany).



Varian Unity Innova (400 MHz, CDCl<sub>3</sub>)

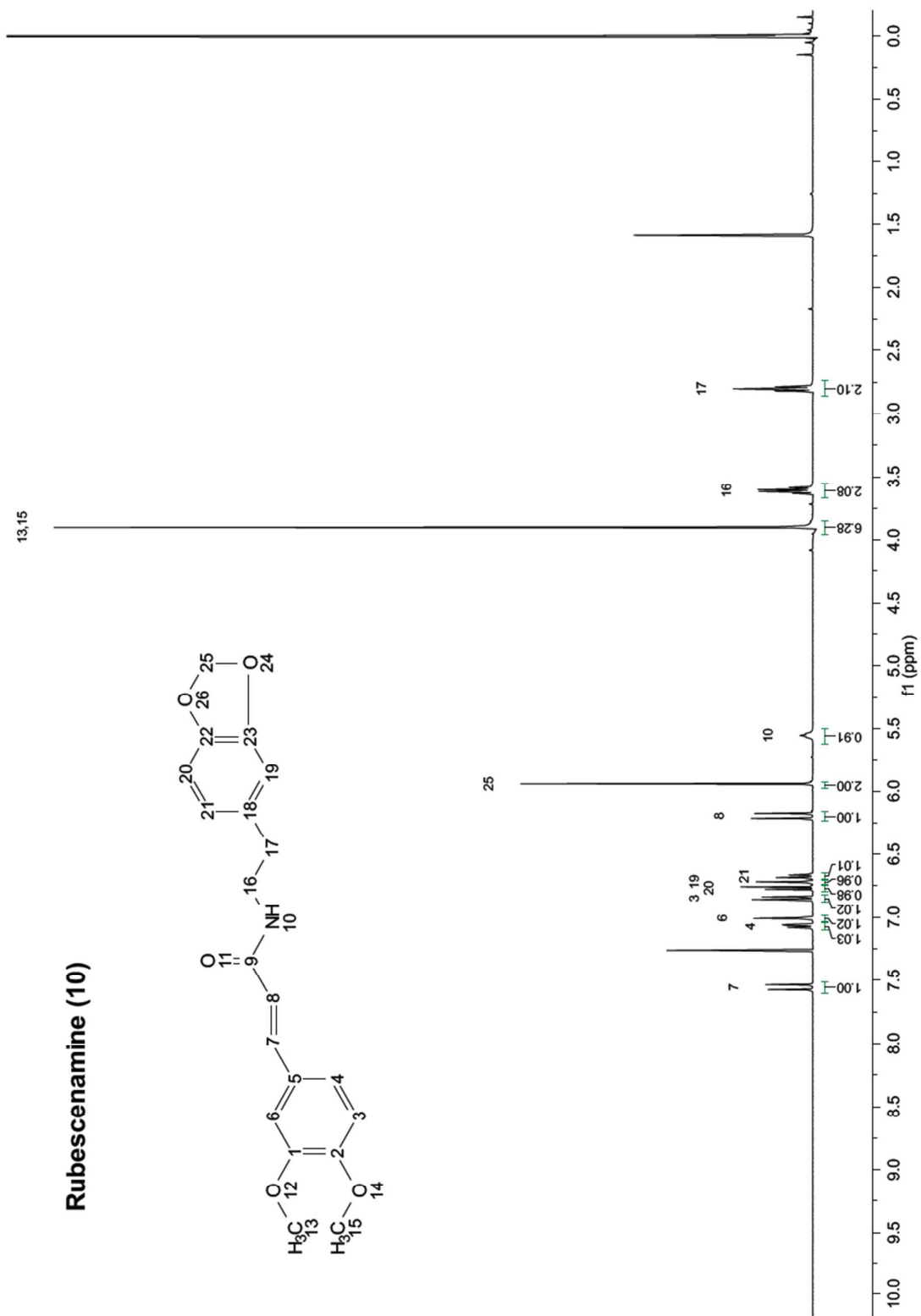
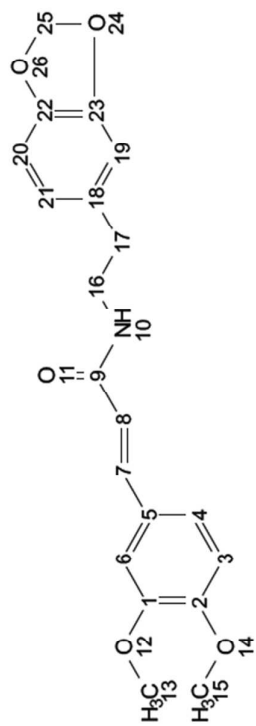
NMR and LC data of Rubescenamine (10)



LC-device: Waters Acquity UPLC  
 MS-device: Bruker micrOTOF Q-II  
 column: Kinetex RP-C18, 1,7 $\mu$ m ( 100 x 2.1mm )  
 mobile phase: A: H<sub>2</sub>O + 0,1% formic acid  
 B: acetonitrile + 0,09% formic acid  
 0.0 min A: 100 % B: 0 %  
 22.0 min A: 5 % B: 95 %  
 27.0 min A: 5 % B: 95 %  
 30.0 min A: 0 % B: 100 %  
 PreRunTime 3 min

flow rate: 0.55 ml / min  
 modus: gradient  
 temperature: 50°C  
 injection volume: 2 $\mu$ l

# Rubescenamine (10)



Varian Mercury Plus (400 MHz, CDCl<sub>3</sub>)