Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supplementary Information

A Novel Approach to Oxazole-Containing Diterpenoid Synthesis from Plant Roots: Salviamines E and F

*Koichi Narita, Narumi Fujisaki, Yuta Sakuma and Tadashi Katoh**

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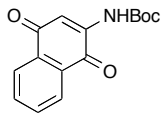
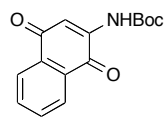
^{1}H NMR of Compound **9**



400 MHz, $CDCl_3$

^{13}C NMR of Compound **9**



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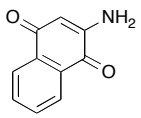
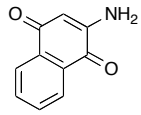
^{1}H NMR of Compound **10**



400 MHz, CD_3OD

^{13}C NMR of Compound **10**



100 MHz, CD_3OD

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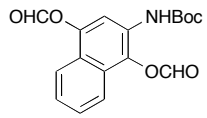
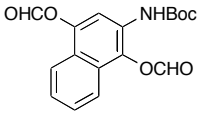


400 MHz, $CDCl_3$

^{13}C NMR of Compound **13**



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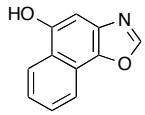

400 MHz, CD_3OD

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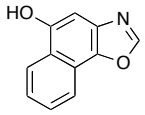

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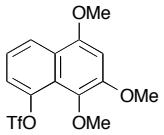

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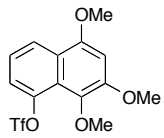

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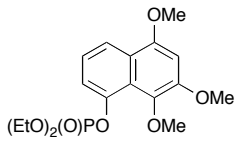

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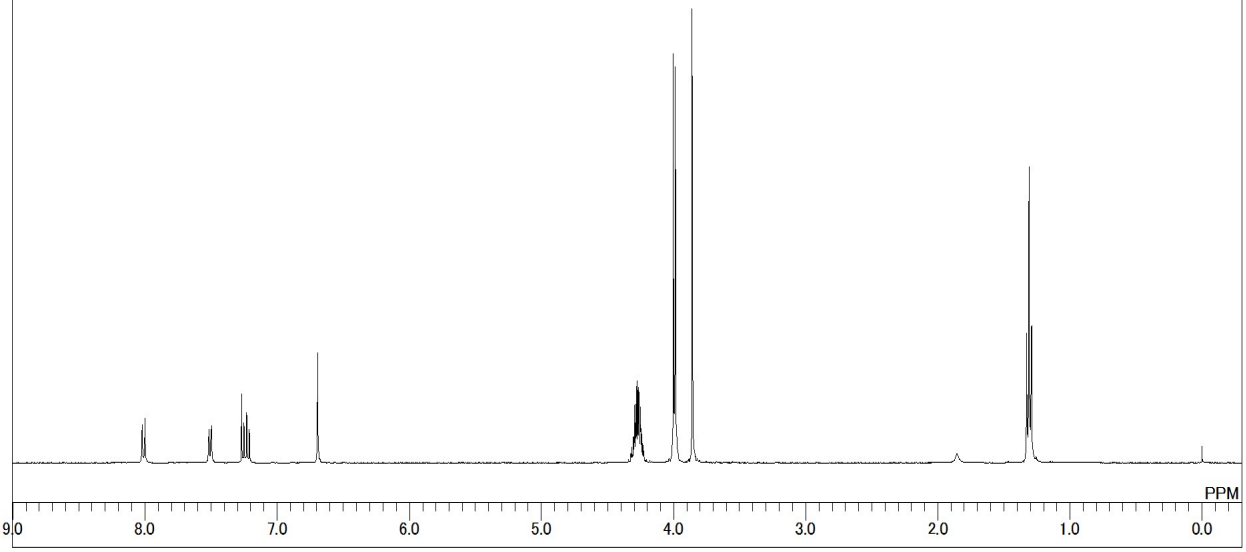

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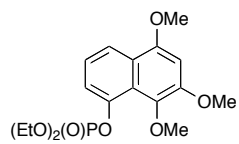

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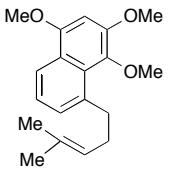

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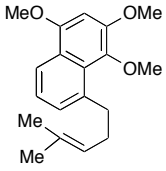
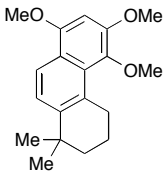
^{13}C NMR of Compound **21**



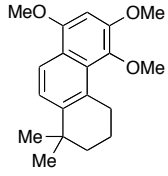
100 MHz, $CDCl_3$

^{1}H NMR of Compound **20**



400 MHz, $CDCl_3$

^{13}C NMR of Compound **20**



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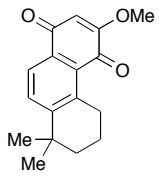

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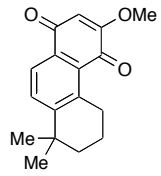
^{13}C NMR of Compound **27**



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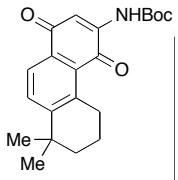

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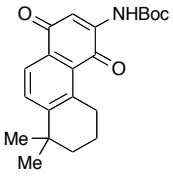
^{13}C NMR of Compound **28**



100 MHz, $CDCl_3$

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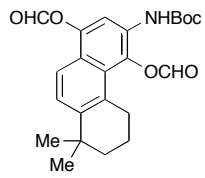
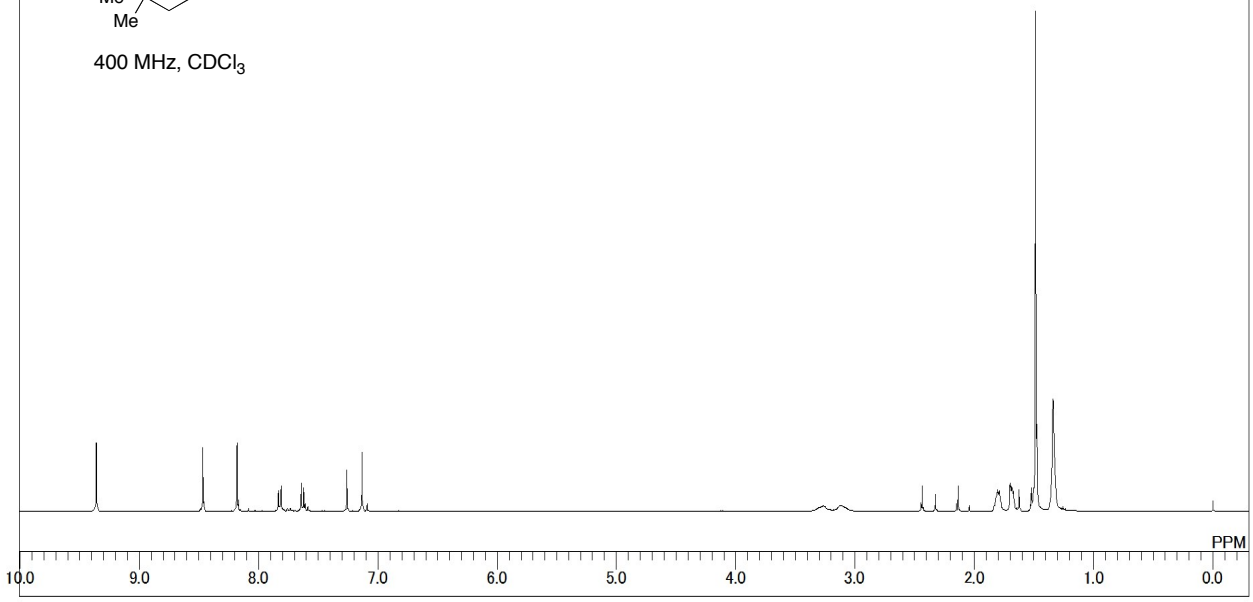


400 MHz, $CDCl_3$



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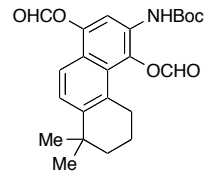
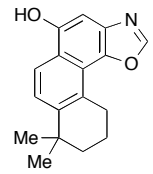


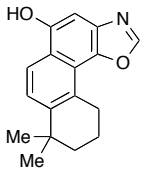
100 MHz, $CDCl_3$

^{1}H NMR of Compound **16**



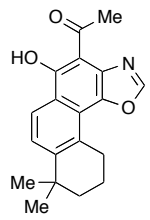
400 MHz, $CDCl_3$

^{13}C NMR of Compound **16**



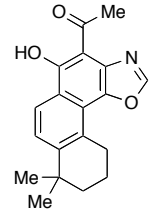
100 MHz, $CDCl_3$

^{1}H NMR of Salviamine F (**6**)
[synthetic]



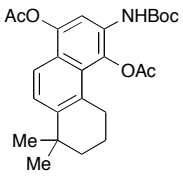
400 MHz, $CDCl_3$

^{13}C NMR of Salviamine F (**6**)
[synthetic]



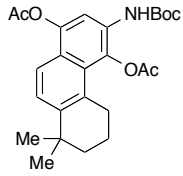
100 MHz, $CDCl_3$

^{1}H NMR of Compound **19**



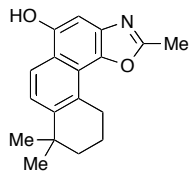
400 MHz, $CDCl_3$

^{13}C NMR of Compound **19**



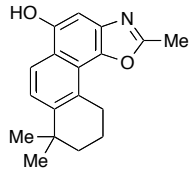
100 MHz, $CDCl_3$

^{1}H NMR of Compound **17**



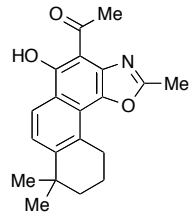
400 MHz, $CDCl_3/CD_3OD$ (10 : 1)

^{13}C NMR of Compound **17**



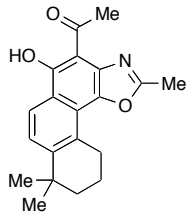
100 MHz, $CDCl_3/CD_3OD$ (10 : 1)

^{1}H NMR of Salviamine E (**5**)
[synthetic]



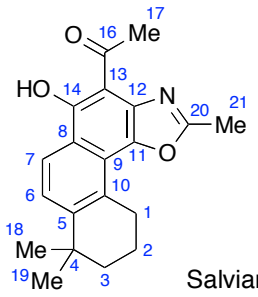
400 MHz, $CDCl_3$

^{13}C NMR of Salviamine E (**5**)
[synthetic]



100 MHz, $CDCl_3$

Comparison of ^{1}H and ^{13}C NMR Data for Natural and Synthetic Salviamine E (**5**) in $CDCl_3$

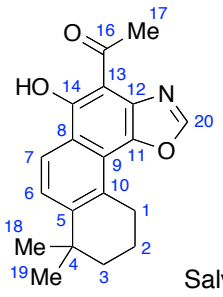


Salviamine E (**5**)

	^{1}H NMR (Hz)		^{13}C NMR (Hz)	
position	Natural (400 MHz)[1]	Synthetic (400 MHz)	Natural (100 MHz)[1]	Synthetic (100 MHz)
1	3.41 (t, *J* = 6.4 Hz, 2H)	3.36 (t, *J* = 6.3 Hz, 2H)	29.4 (t)	29.1 (t)
2	1.98 (m, 2H)	1.94–2.00 (m, 2H)	19.6 (t)	19.4 (t)
3	1.76 (m, 2H)	1.74–1.77 (m, 2H)	38.5 (t)	38.3 (t)
4	———	———	34.9 (s)	34.7 (s)
5	———	———	149.1 (s)	148.8 (s)
6	8.35 (d, *J* = 8.8 Hz, 1H)	8.29 (d, *J* = 8.8 Hz, 1H)	122.9 (d)	122.6 (d)
7	7.55 (d, *J* = 8.8 Hz, 1H)	7.52 (d, *J* = 8.8 Hz, 1H)	124.9 (d)	124.6 (d)
8	———	———	121.9 (s)	121.6 (s)
9	———	———	124.3 (s)	124.0 (s)
10	———	———	129.6 (s)	129.3 (s)
11	———	———	141.2 (s)	140.9 (s)
12	———	———	136.5 (s)	136.3 (s)
13	———	———	106.4 (s)	106.2 (s)
14	———	———	161.8 (s)	161.6 (s)
14-OH	14.62 (s, 1H)	14.57 (s, 1H)	———	———
16	———	———	204.4 (C=O)	204.1 (C=O)
17	3.06 (s, 3H)	3.02 (s, 3H)	31.5 (q)	31.2 (q)
18	1.39 (s, 3H)	1.38 (s, 3H)	31.7 (q)	31.5 (q)
19	1.39 (s, 3H)	1.38 (s, 3H)	31.7 (q)	31.5 (q)
20	———	———	162.1 (s)	161.8 (s)
21	2.73 (s, 3H)	2.70 (s, 3H)	14.9 (q)	14.7 (q)

[1] F.-W. Lin, A. G. Damu, T.-S. Wu, *J. Nat. Prod.*, 2006, **69**, 93–96.

Comparison of ^{1}H and ^{13}C NMR Data for Natural and Synthetic Salviamine F (**6**) in $CDCl_3$



Salviamine F (**6**)

	^{1}H NMR (Hz)		^{13}C NMR (Hz)	
position	Natural (400 MHz)[1]	Synthetic (400 MHz)	Natural (100 MHz)[1]	Synthetic (100 MHz)
1	3.45 (t, *J* = 6.4 Hz, 2H)	3.40 (t, *J* = 6.3 Hz, 2H)	29.3 (t)	29.1 (t)
2	1.98 (m, 2H)	1.95–2.01 (m, 2H)	19.5 (t)	19.4 (t)
3	1.78 (m, 2H)	1.75–1.78 (m, 2H)	38.4 (t)	38.2 (t)
4	———	———	34.9 (s)	34.9 (s)
5	———	———	149.5 (s)	149.3 (s)
6	8.39 (d, *J* = 8.8 Hz, 1H)	8.32 (d, *J* = 8.8 Hz, 1H)	123.0 (d)	123.0 (d)
7	7.61 (d, *J* = 8.8 Hz, 1H)	7.58 (d, *J* = 8.8 Hz, 1H)	125.6 (d)	125.4 (d)
8	———	———	122.7 (s)	122.5 (s)
9	———	———	124.3 (s)	124.0 (s)
10	———	———	130.0 (s)	129.7 (s)
11	———	———	140.9 (s)	140.6 (s)
12	———	———	135.2 (s)	134.9 (s)
13	———	———	106.4 (s)	106.1 (s)
14	———	———	164.5 (s)	164.2 (s)
14-OH	14.70 (s, 1H)	14.66 (s, 1H)	———	———
16	———	———	204.1 (C=O)	203.8 (C=O)
17	3.08 (s, 3H)	3.04 (s, 3H)	31.4 (q)	31.2 (q)
18	1.39 (s, 3H)	1.39 (s, 3H)	31.7 (q)	31.5 (q)
19	1.39 (s, 3H)	1.39 (s, 3H)	31.7 (q)	31.5 (q)
20	8.21 (s, 1H)	8.16 (s, 1H)	150.9 (d)	150.7 (d)

[1] F.-W. Lin, A. G. Damu, T.-S. Wu, *J. Nat. Prod.*, 2006, **69**, 93–96.