## Supporting Information

***Rec. Nat. Prod*. 13:6 (2019) 506-511**

# Cephalounei A, a New Cephalotaxus Alkaloid from the Powdered Stems of *Cephalotaxus fortune* Hook. f

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| Table of Contents | Page |
|---|---|


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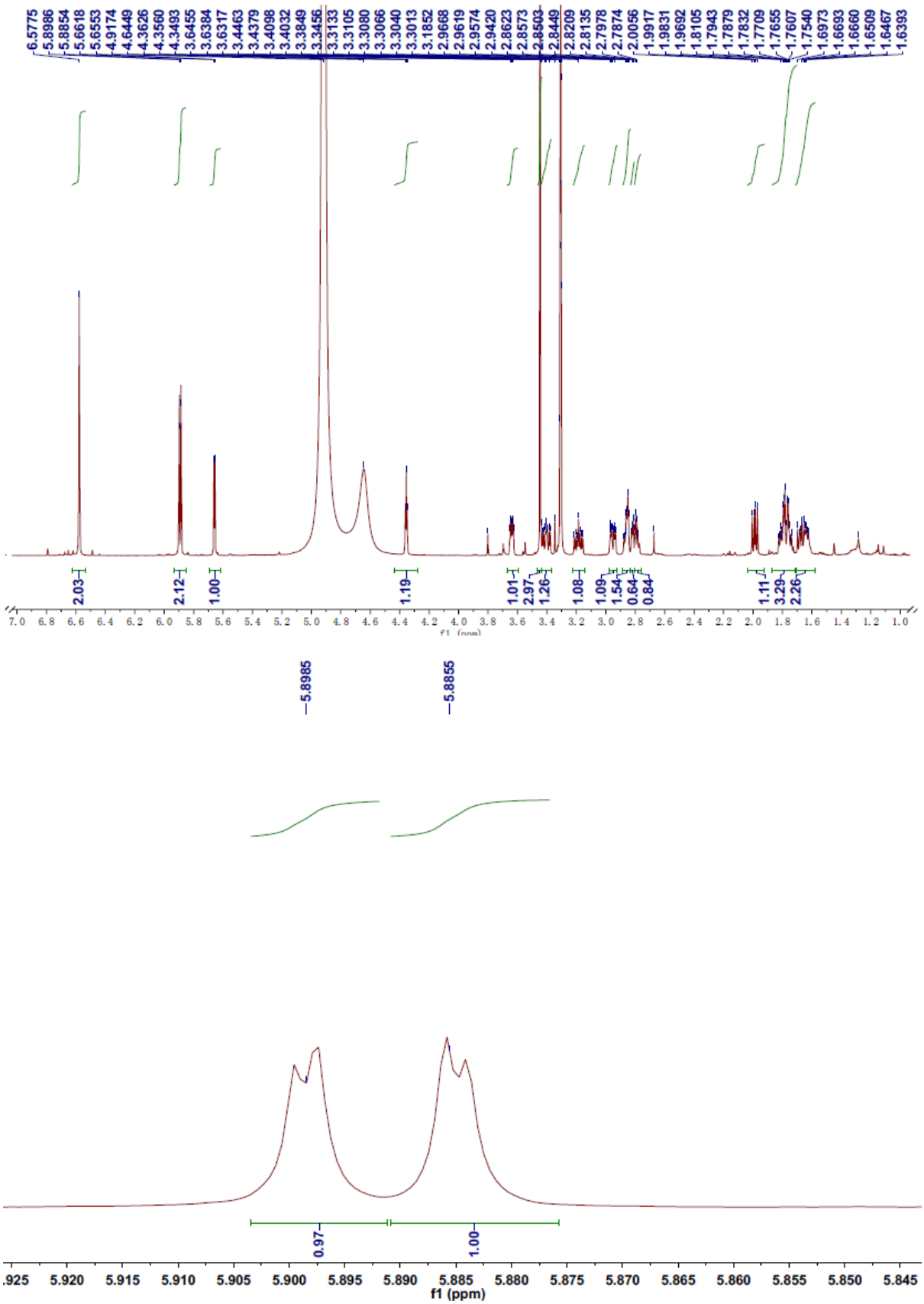



**Figure S1:** [1] H NMR of compound **1** in $CD_3OD$ (600 MHz)

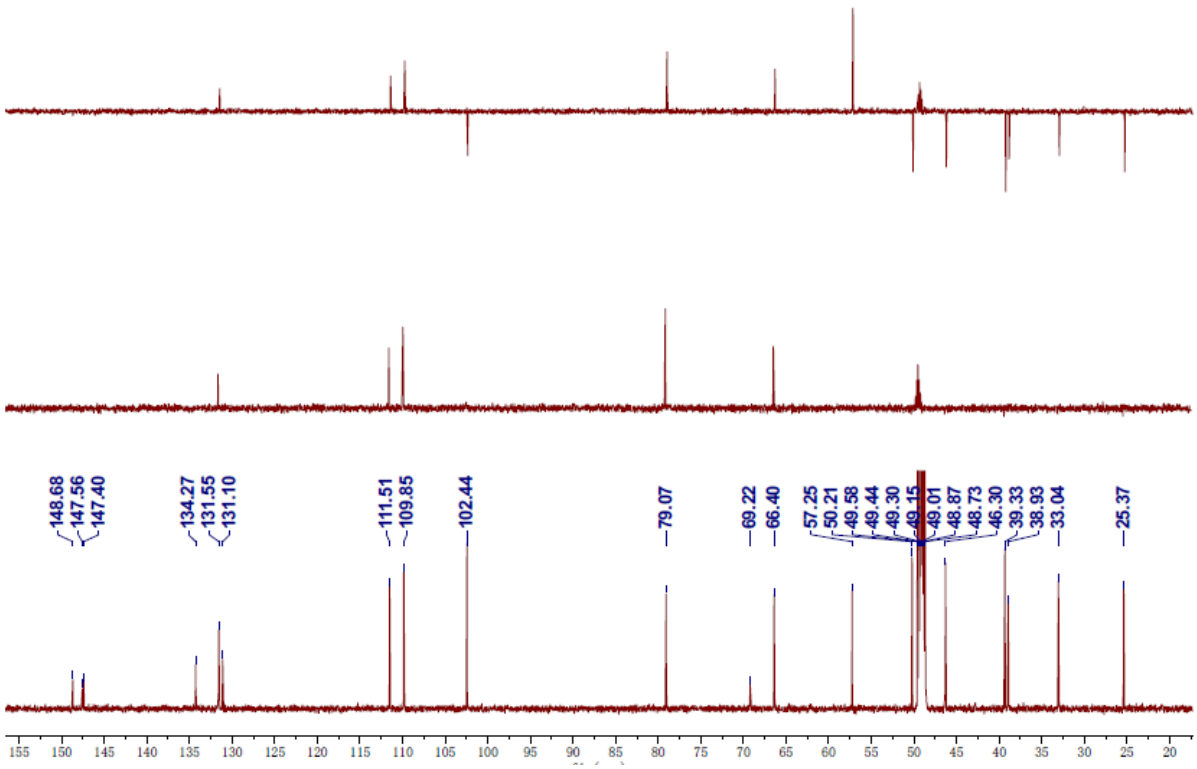



**Figure S2:** $^{13}$C NMR of compound **1** in $CD_3OD$ (150 MHz)

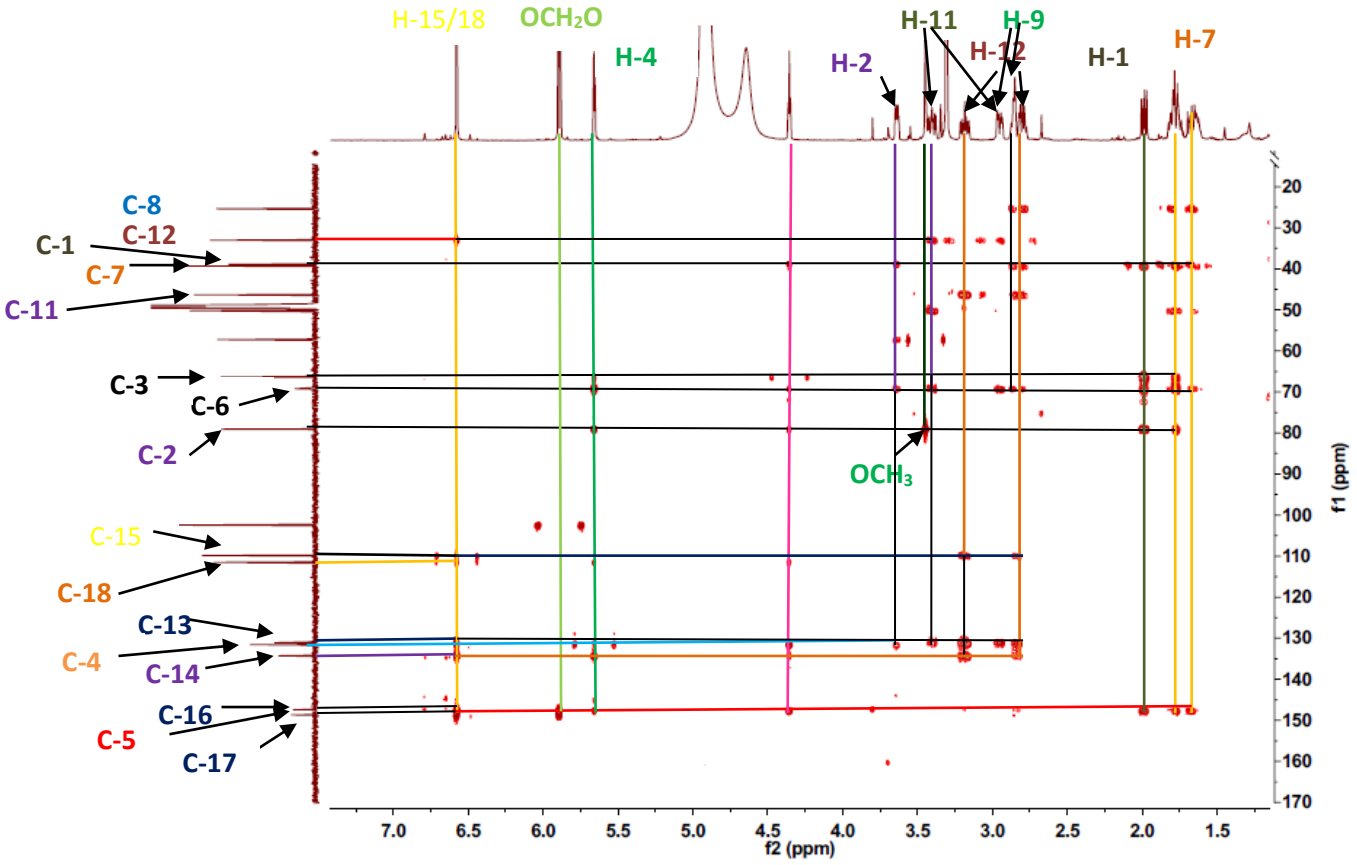



**Figure S3:** HMBC of compound **1** in $CD_3OD$

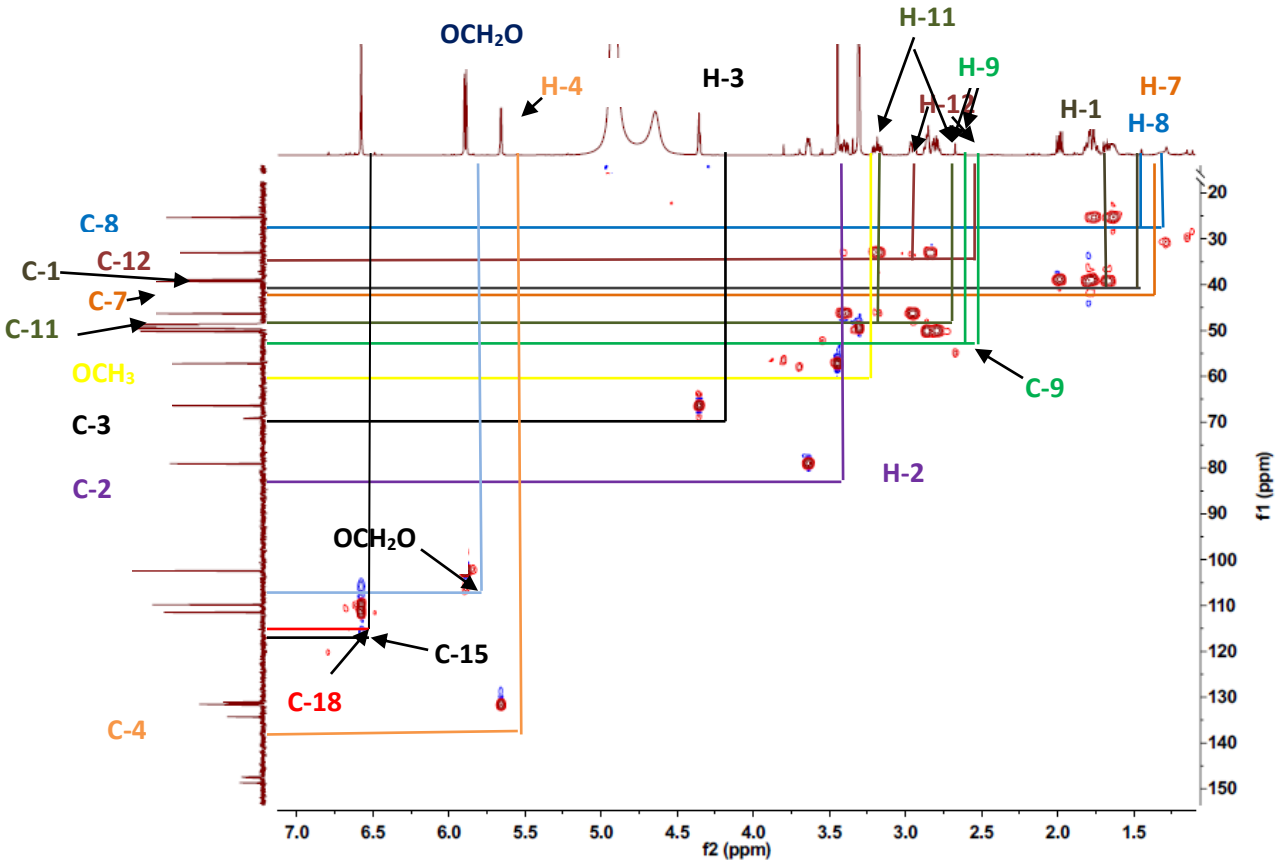



**Figure S4:** HSQC of compound **1** in $CD_3OD$

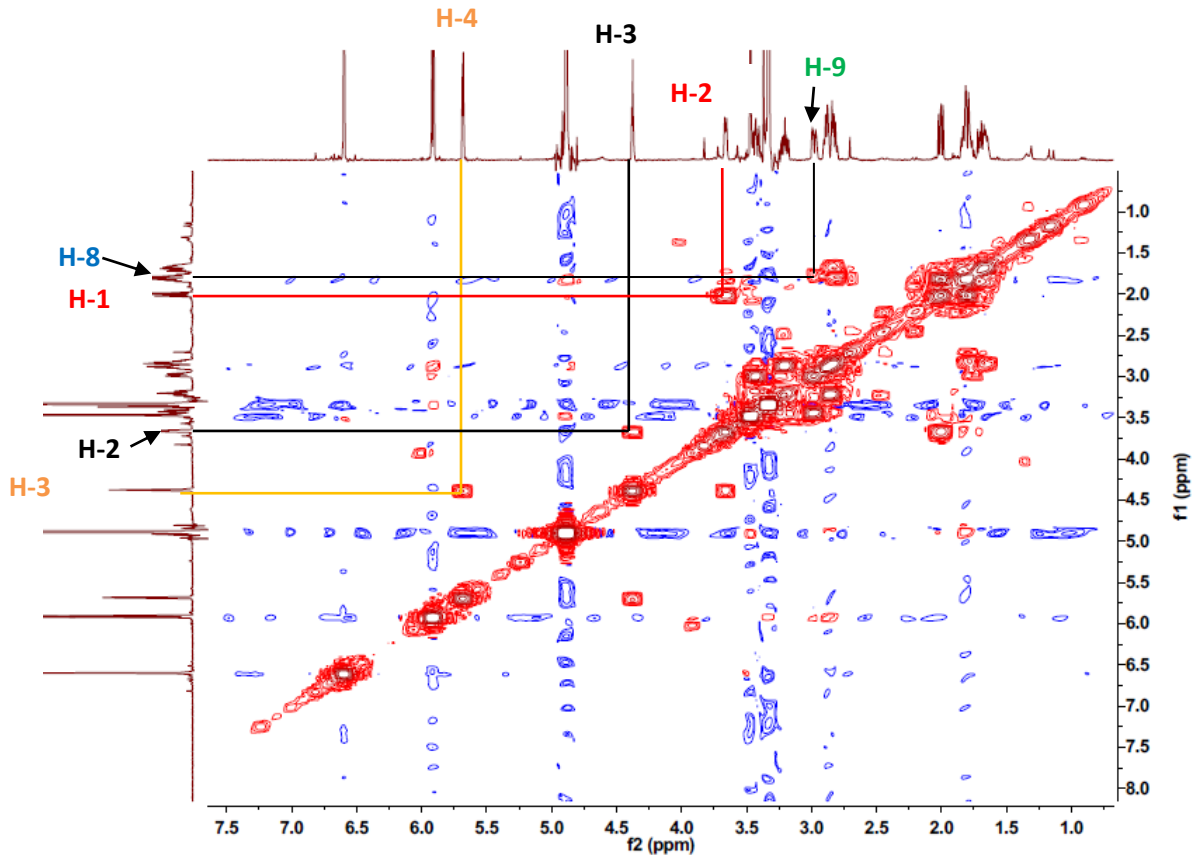



**Figure S5:** $^1H$–$^1H$ COSY of compound **1** in $CD_3OD$

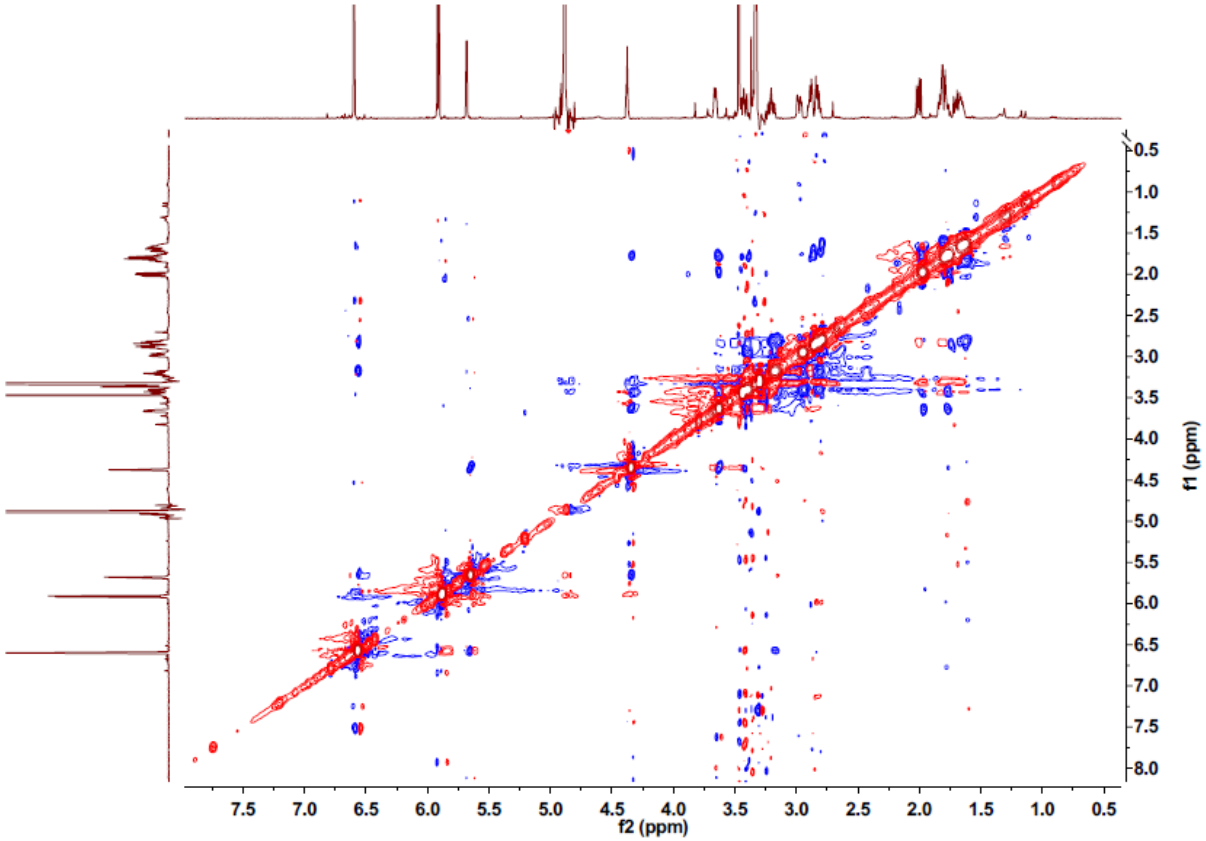



**Figure S6:** $^{1}H$–$^{1}H$ ROESY of compound **1** in $CD_3OD$

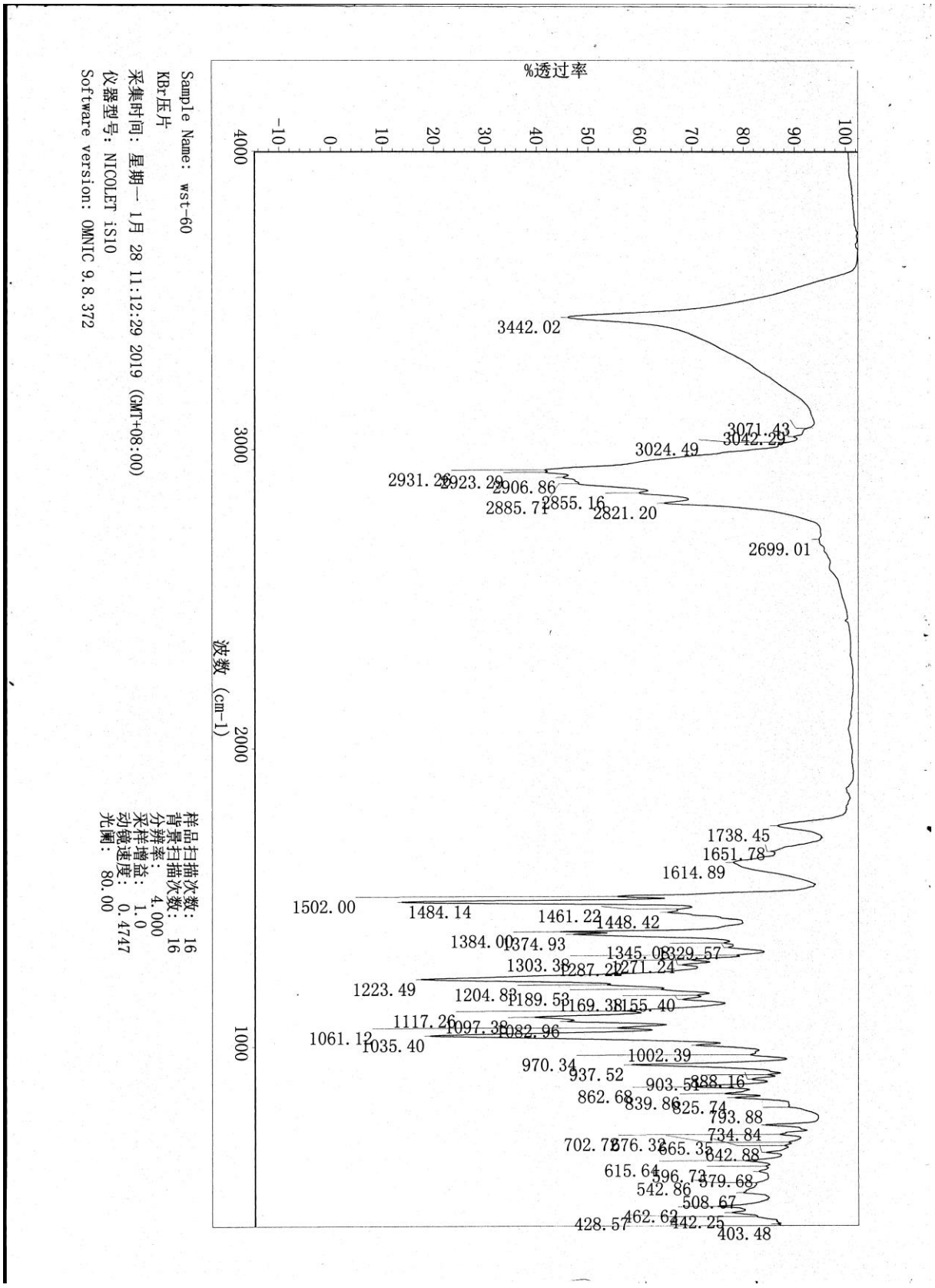



**Figure S7:** IR of compound **1**

Formula Predictor Report - WST-60.lcd

Page 1 of 1

Data File: E:\DATA\2019\0123\WST-60.lcd

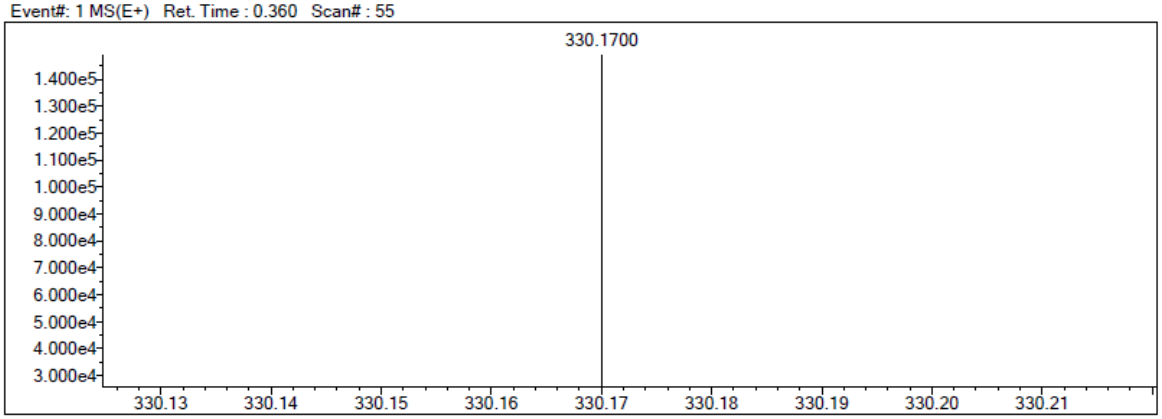
| Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Elmt | Val. | Min | Max | Use Adduct |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H | 1 | 5 | 100 | F | 1 | 0 | 0 | S | 2 | 0 | 0 | Br | 1 | 0 | 5 | H |
| C | 4 | 5 | 50 | Na | 1 | 0 | 0 | Cl | 1 | 0 | 5 | Pd | 2 | 0 | 0 | Na |
| N | 3 | 0 | 10 | Mg | 2 | 0 | 0 | Cu | 2 | 0 | 0 | Ag | 1 | 0 | 0 | |
| O | 2 | 0 | 10 | Si | 4 | 0 | 0 | Se | 2 | 0 | 0 | I | 3 | 0 | 0 | |

Error Margin (ppm): 5
HC Ratio: unlimited
Max Isotopes: all
MSn Iso RI (%): 75.00

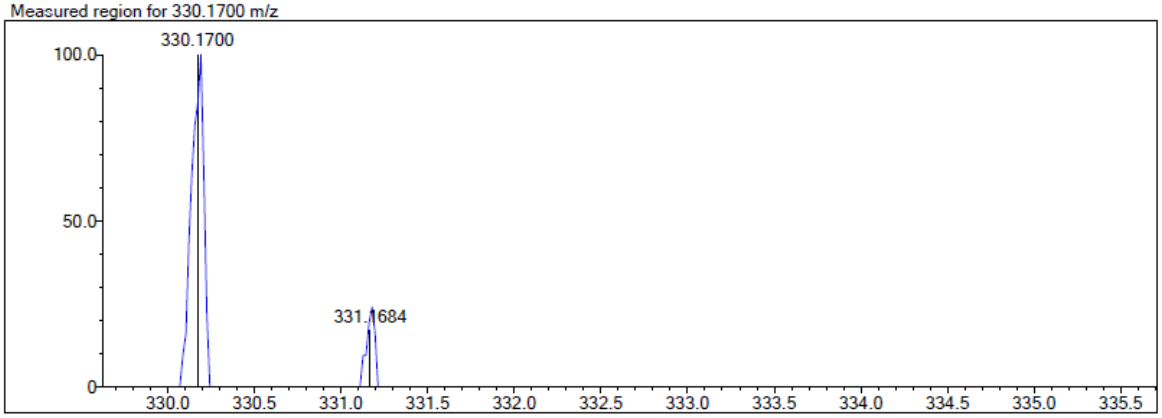
DBE Range: -2.0 - 100.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: OR

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 10

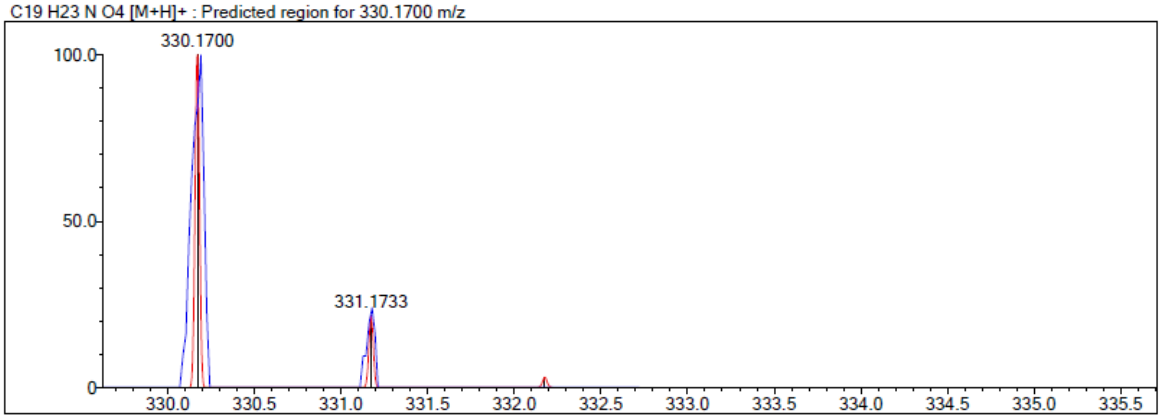
Event#: 1 MS(E+) Ret. Time : 0.360 Scan# : 55




Measured region for 330.1700 m/z

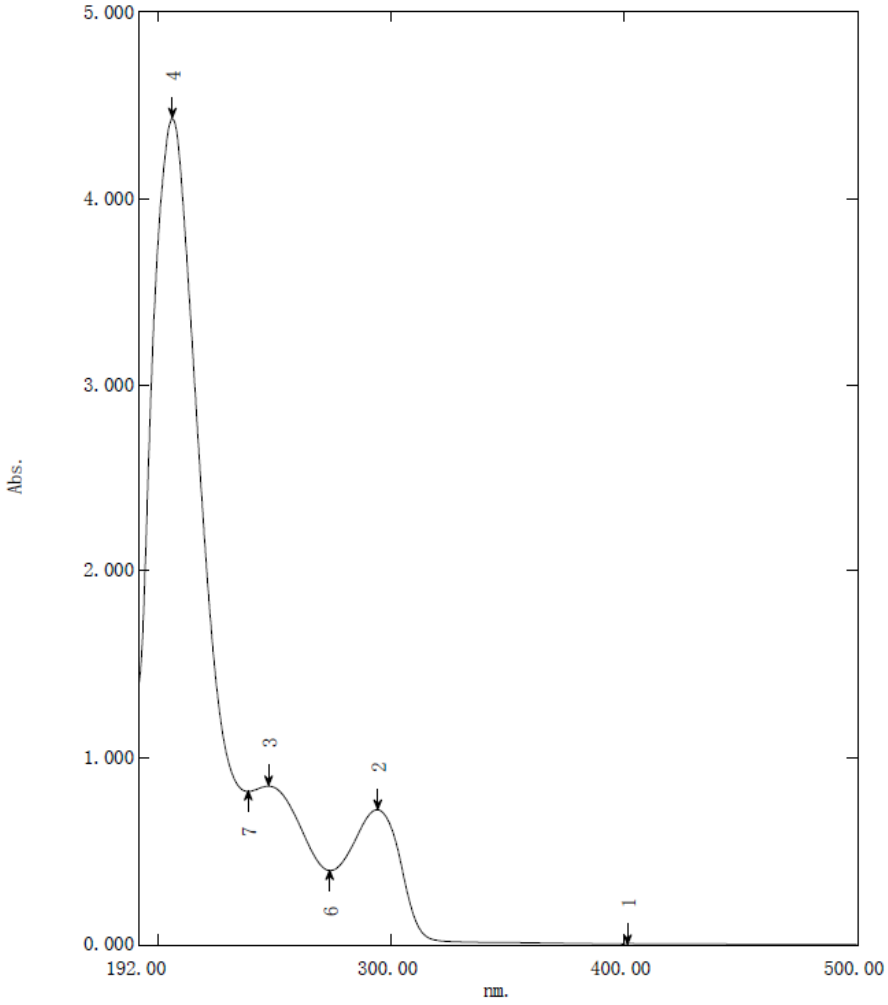



C19 H23 N O4 [M+H]+ : Predicted region for 330.1700 m/z




| Formula (M) | Ion | Meas. m/z | Pred. m/z | Df. (mDa) | Df. (ppm) | DBE |
|---|---|---|---|---|---|---|
| C19 H23 N O4 | [M+H]+ | 330.1700 | 330.1700 | 0.0 | 0.00 | 9.0 |

**Figure S8:** HRESIMS of compound **1**




[测定属性]
波长范围(nm): 192.00 到 500.
扫描速度: 中速
采样间隔: 0.2
自动采样间隔: 启用
扫描模式: 单个

[仪器属性]
仪器类型: UV-2700 系列
测定方式: 吸收值
狭缝宽: 5.0 nm
积分时间: 0.1 秒
光源转换波长: 323.0 nm
检测器单元: 直接
S/R 转换: 标准
阶梯校正: OFF

[附件属性]
附件: 无

[数据处理参数]
阈值: 0.0010000
点: 4
内插: 停用
平均: 停用

[样品准备属性]
重量: 1.2mg
体积: 1ml
稀释: 30倍
光程长: 10mm
附加信息: 2019/01/25 14
wst-60 MeOH

| No. | P/V | 波长(nm) | Abs. | 描述 |
|---|---|---|---|---|
| 1 | ↑ | 401.40 | 0.004 | |
| 2 | ↑ | 294.20 | 0.722 | |
| 3 | ↑ | 247.40 | 0.848 | |
| 4 | ↑ | 206.00 | 4.430 | |
| 5 | ↓ | 398.80 | 0.003 | |
| 6 | ↓ | 274.00 | 0.396 | |
| 7 | ↓ | 238.80 | 0.820 | |

**Figure S9:** UV of compound **1**

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Friday, 25-JAN-2019

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | -3.10 | 0.50 | -16.12 | -2.25 | -3.50 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | wst-60 | 02:42:53 PM | -2.25 | SR | -0.0027 | 589 | 100.00 | 0.120 | 21.6 |
| 2 | wst-60 | 02:43:01 PM | -3.08 | SR | -0.0037 | 589 | 100.00 | 0.120 | 21.6 |
| 3 | wst-60 | 02:43:09 PM | -3.25 | SR | -0.0039 | 589 | 100.00 | 0.120 | 21.6 |
| 4 | wst-60 | 02:43:17 PM | -3.42 | SR | -0.0041 | 589 | 100.00 | 0.120 | 21.6 |
| 5 | wst-60 | 02:43:25 PM | -3.50 | SR | -0.0042 | 589 | 100.00 | 0.120 | 21.6 |

**Figure S10:** Optical Rotation of compound **1**

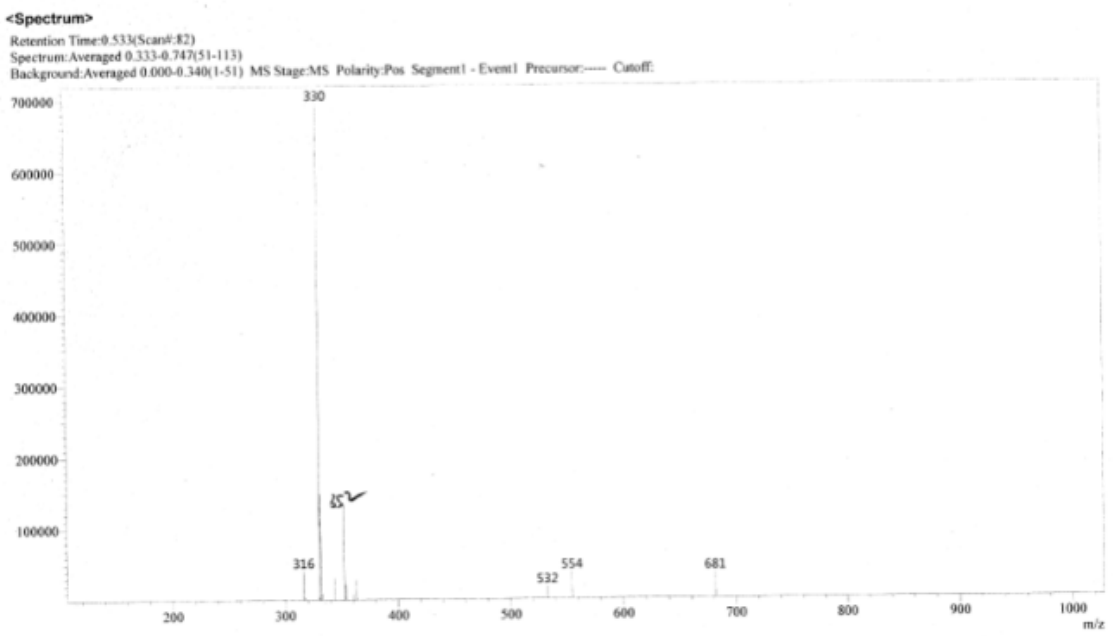
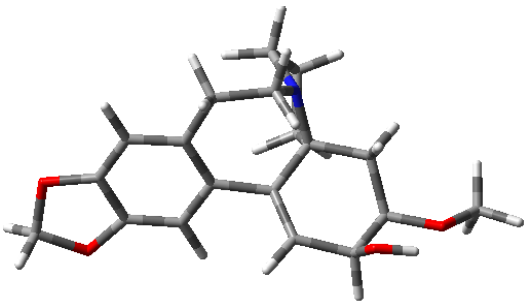



**Figure S11:** low resolution mass spectrometry of compound **1**

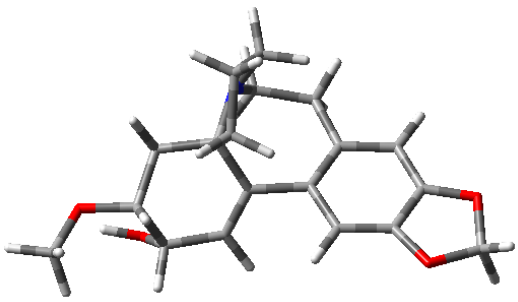
**S12:** ECD computational details of compound **1** (Cephalounei A)

A conformation searches based on molecular mechanics with MMFF94S force fields were performed for compound **1** which gave nine stable conformers [1-2]. Selected six conformers with distributions higher than 1% were further optimized by density functional theory method at the B3LYP/6-31G(d,p) level in Gaussian 09 program package [3], leading to two minimum geometries, which was further checked by frequency calculation and resulted in no imaginary frequencies. The ECD was calculated using TDDFT-B3LYP/6-311G(2d, p) of theory on B3LYP/6-31G(d, p) optimized geometry. The calculated ECD curve for **1** and weighted ECD were all generated using SpecDis 1.64 with σ = 0.3 ev, and UV shift 5 nm [4].

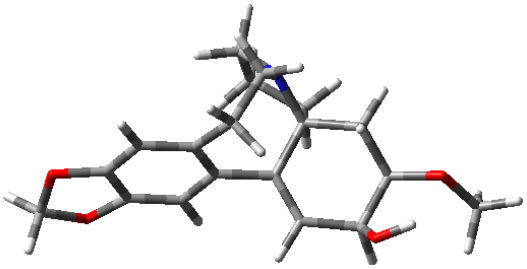
Two optimized conformers of **1**(2*R*, 3*S*, 6*S*)



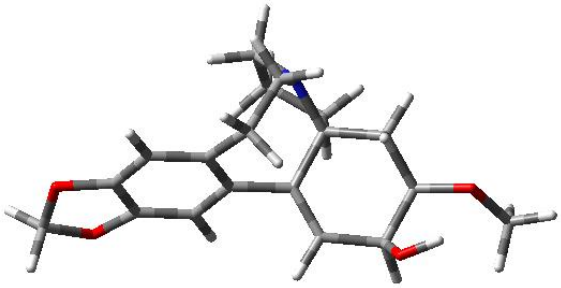
46.28%



37.12%



0.95%



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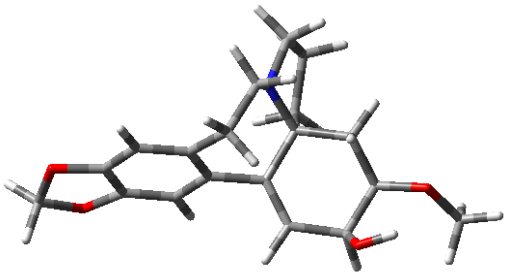
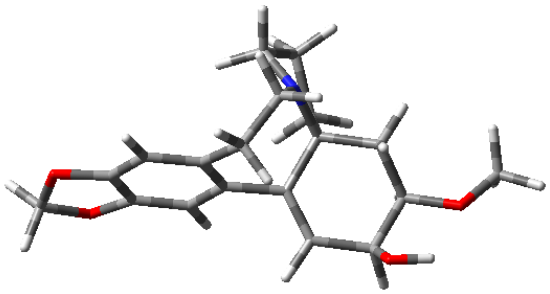


11.33%



3.38%

References:

[1] Goto, H.; Osawa, E.; *J. Am. Chem. Soc.***1989**, *111*, 8950–8951.

[2] Goto, H.; Osawa, E.; *J. Chem. Soc., Perkin Trans. 2*, **1993**, 187–198.

[3] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Jr., Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J.; Gaussian *09*, Revision B.01,Gaussian, Inc., Wallingford CT, 2010.

[4] **SpecDis: Quantifying the Comparison of Calculated and Experimental Electronic Circular Dichroism Spectra**, T. Bruhn, A. Schaumlöffel, Y. Hemberger, G. Bringmann, *Chirality* **2013**, *25*, 243–249.