**Electronic Supplementary Information for**

# Studies on the Asymmetric Synthesis of Pandamarilactonines: An Unexpected *syn*-Selective Vinylogous Mannich Reaction of *N*-*tert*-Butanesulfinimines

Jian-Liang Ye,* Yu-Feng Zhang, Yang Liu, Jin-Yuan Zhang, Yuan-Ping Ruan and Pei-Qiang Huang*

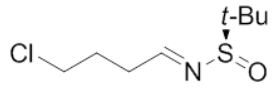
*Department of Chemistry and Fujian Provincial Key Laboratory of Chemical Biology, Collaborative Innovation Centre of Chemistry for Energy Materials, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, Fujian 361005, PR China*

E-mail: pqhuang@xmu.edu.cn; yejl@xmu.edu.cn

**Contents (24 pages):**

$^{1}$H and $^{13}$C NMR spectra of compound **10a**

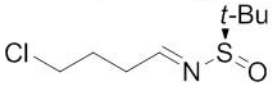
$^{1}$H-NMR ($CDCl_3$, 400 MHz)

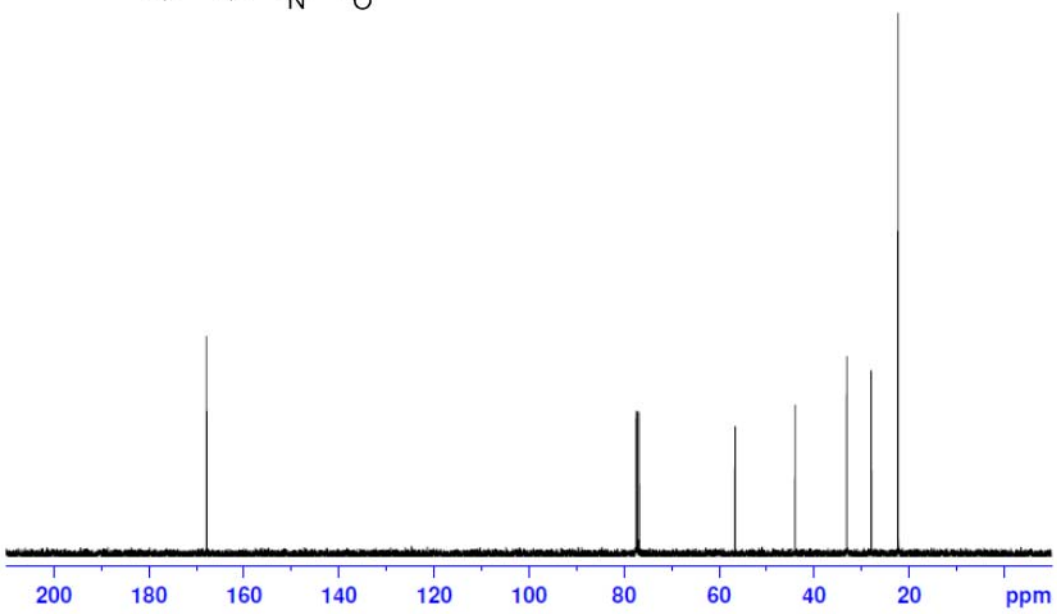




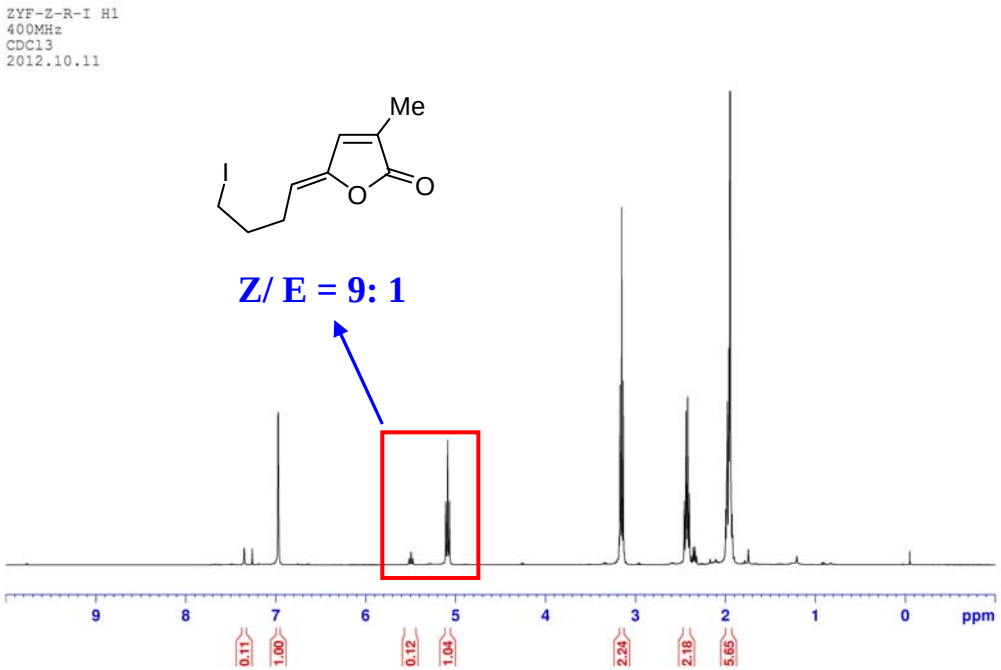


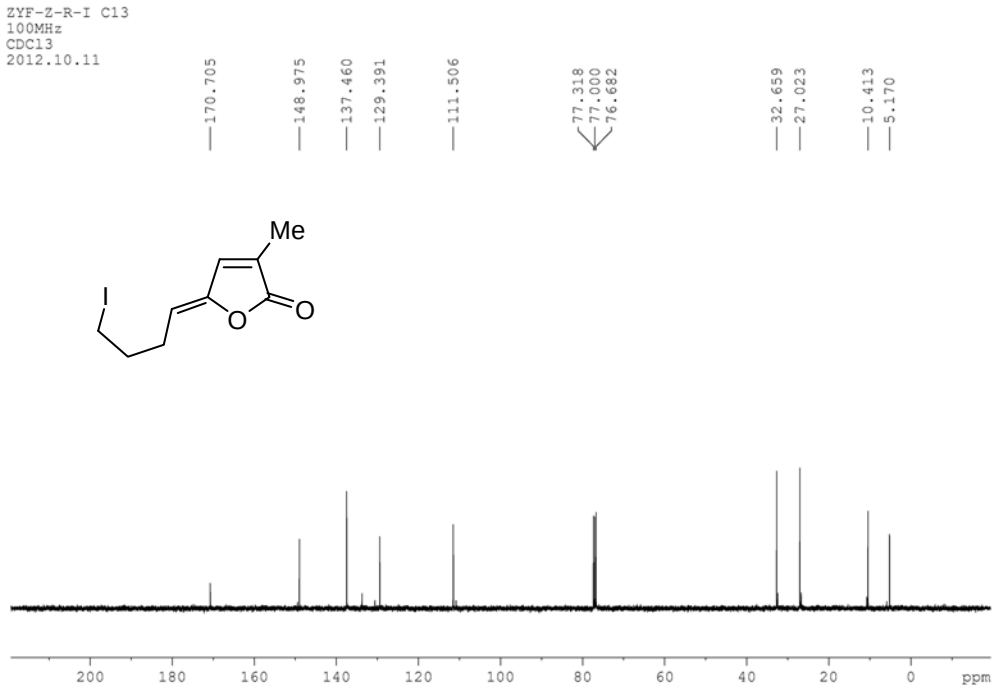

$^{13}$C-NMR ($CDCl_3$, 100 MHz)



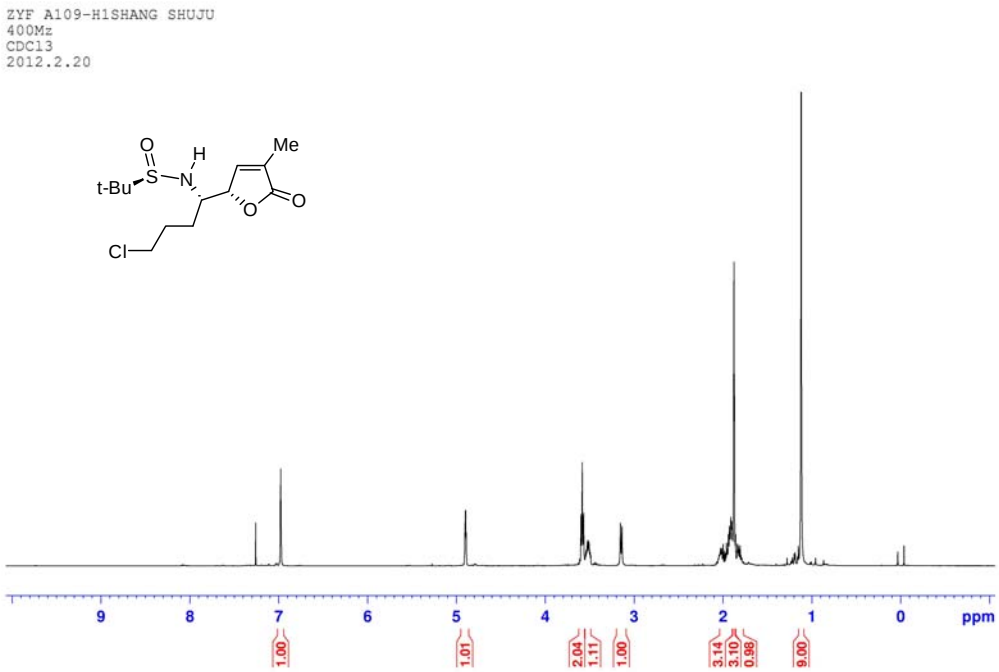



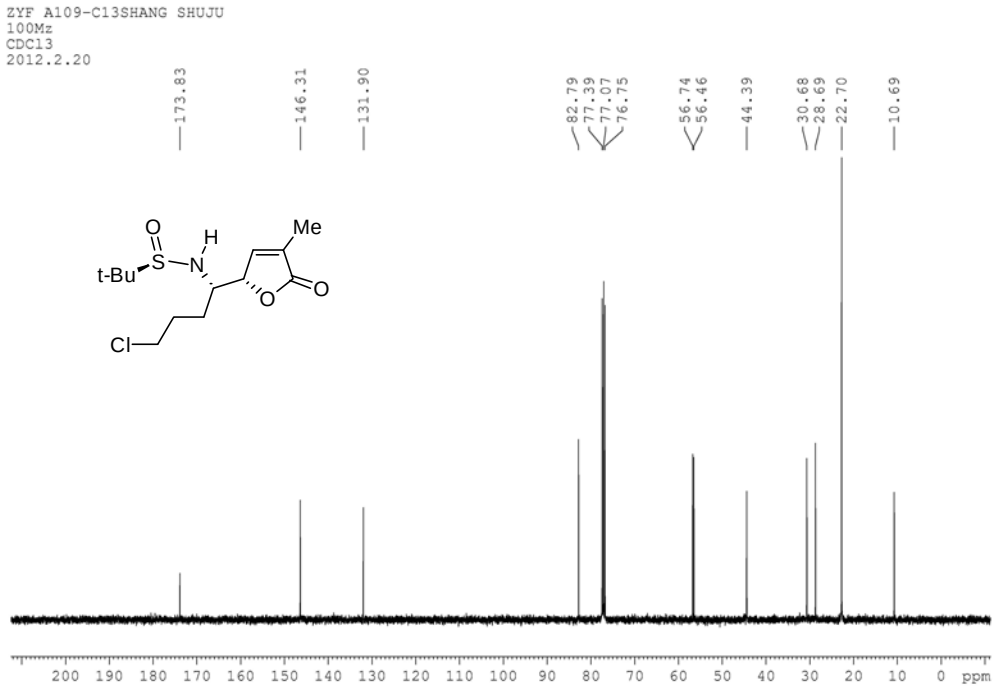
$^{1}$H and $^{13}$C NMR spectra of alkyl iodide **13** with *Z*/ *E* = 9: 1



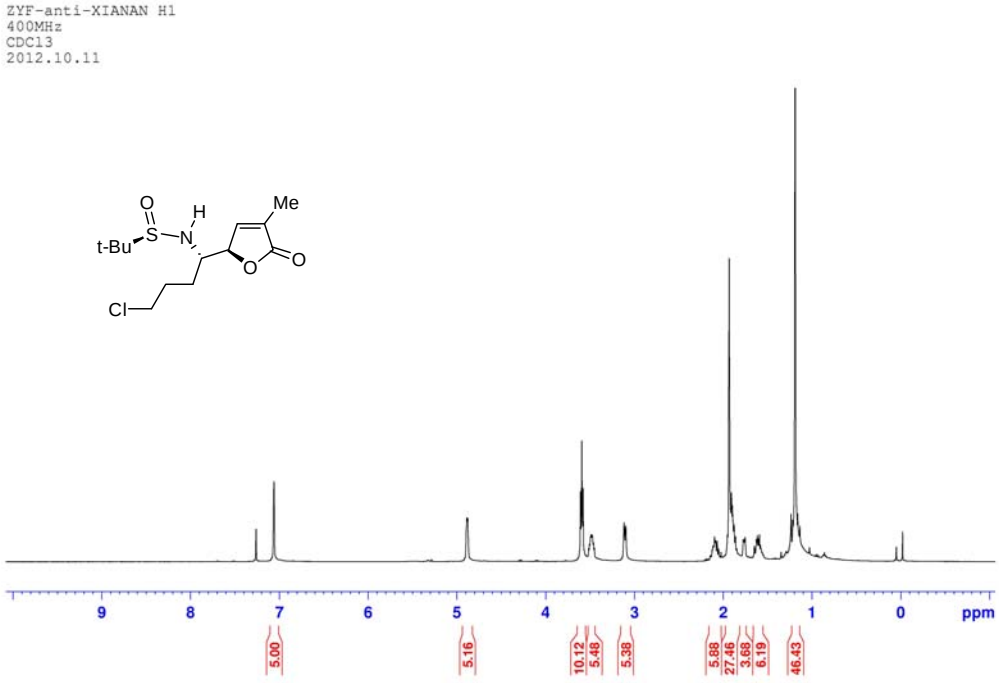



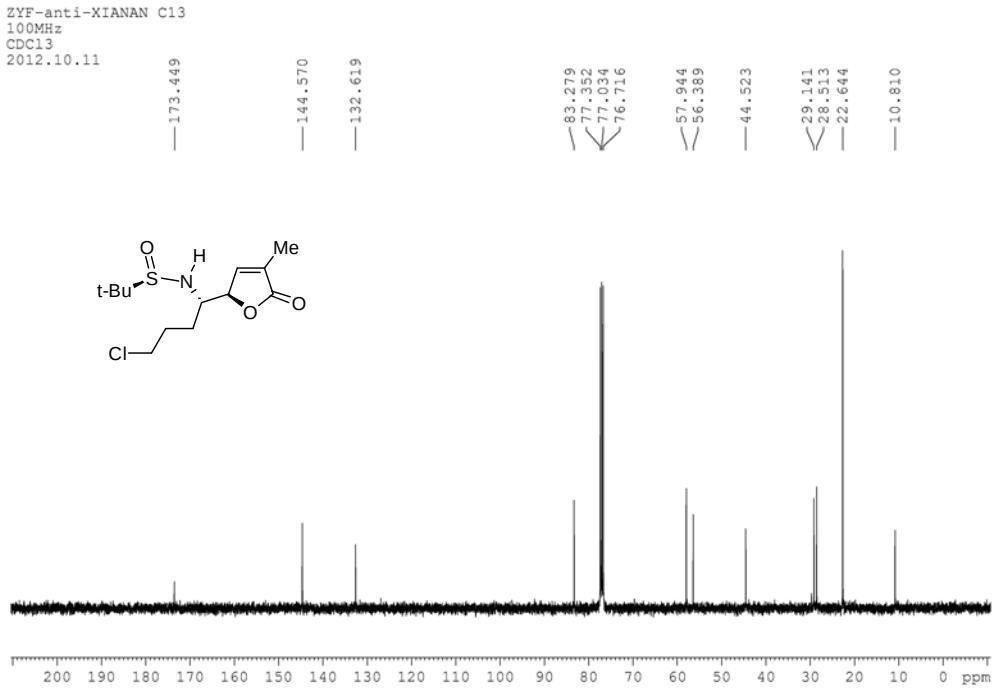
$^{1}$H and $^{13}$C NMR spectra of compound *syn*-**16**



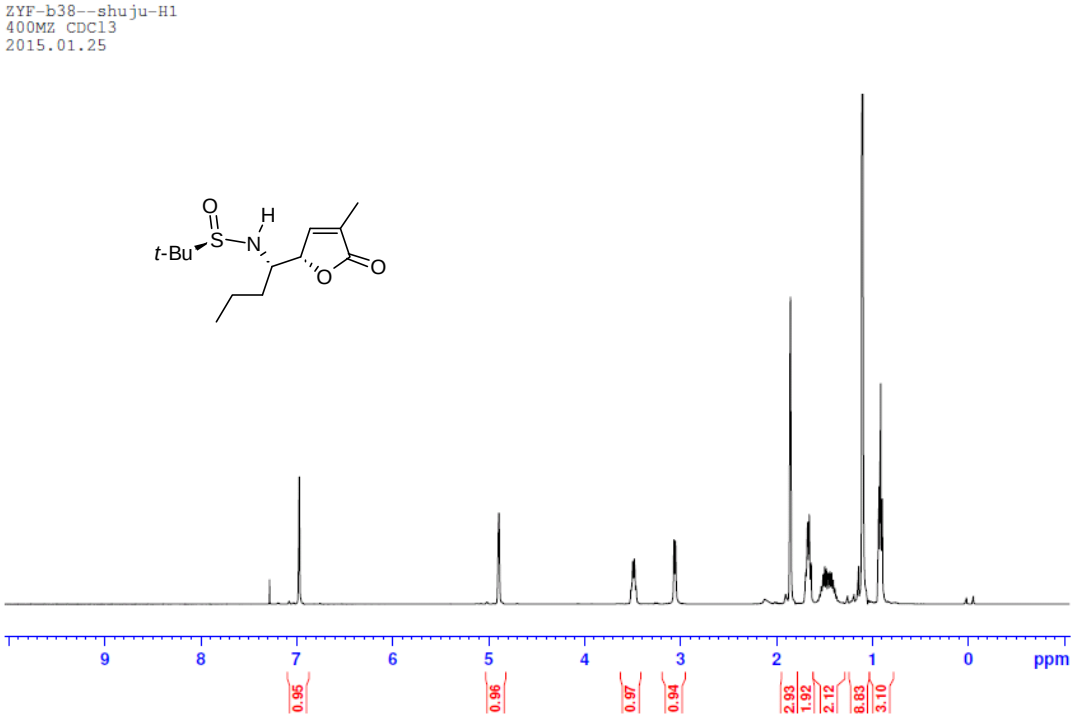



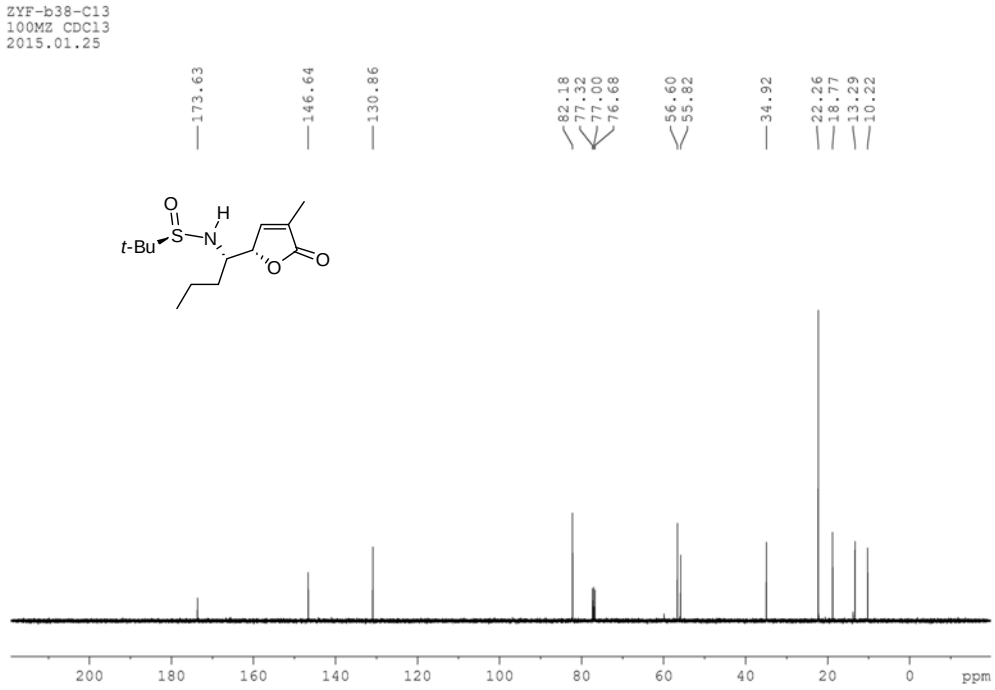
$^{1}H$ and $^{13}C$ NMR spectra of compound *anti*-**16**



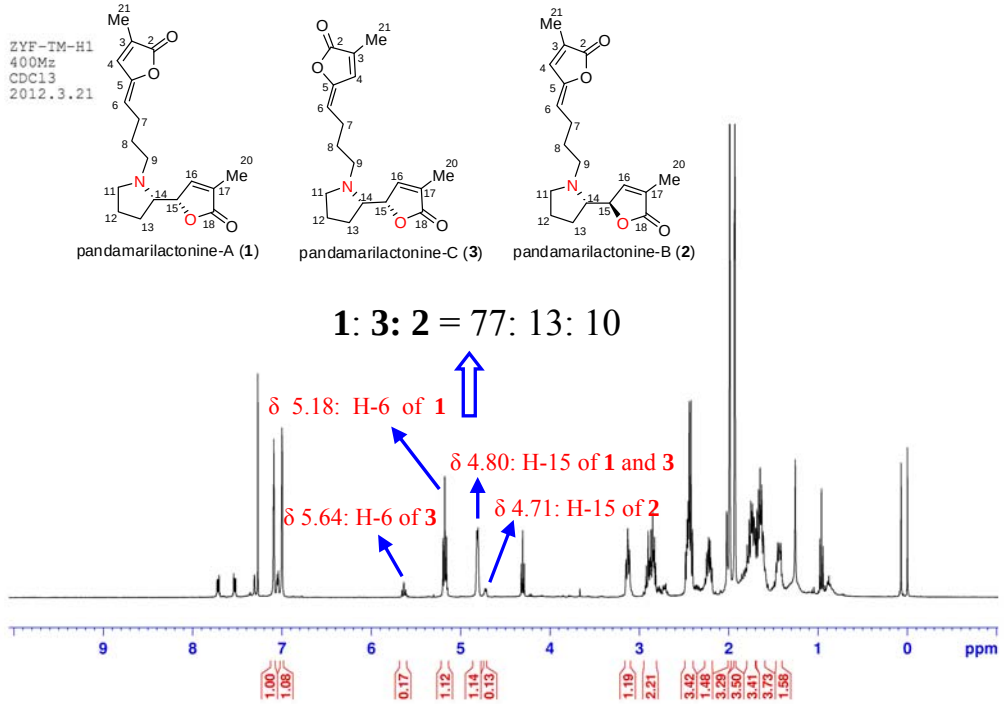



$^{1}$H and $^{13}$C NMR spectra of compound *syn*-**17**



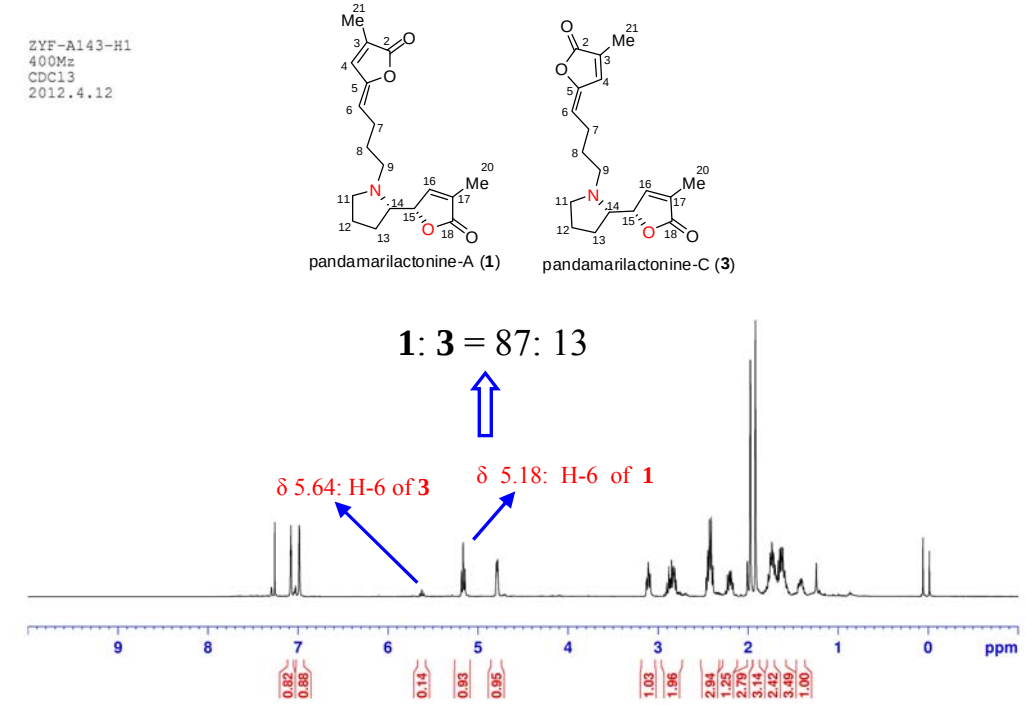
$^{1}$H NMR of crude product of the one-pot desulfinylation, cyclization and coupling reaction of *syn*-**16**

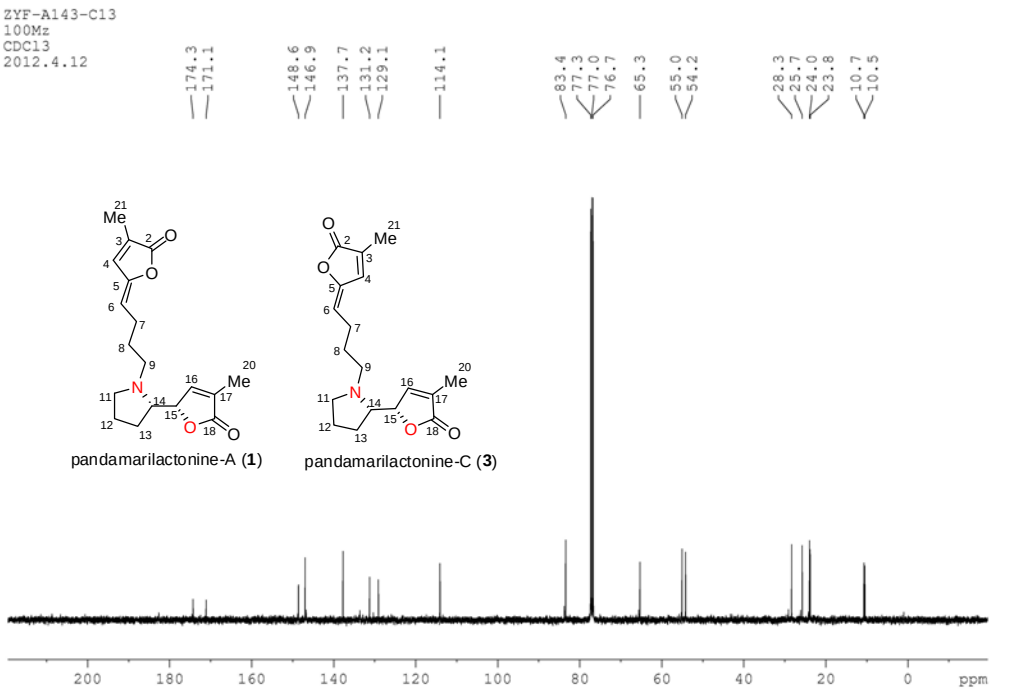



1. H. Takayama, T. Ichikawa, T. Kuwajima, M. Kitajima, H. Seki, N. Aimi and M. G. Nonato, *J. Am. Chem. Soc.*, 2000, **122**, 8635-8639.

2. H. Takayama, T. Ichikawa, M. Kitajima, M. G. Nonato and N. Aimi, *Chem. Pharm. Bull.*, 2002, **50**, 1303-1304.

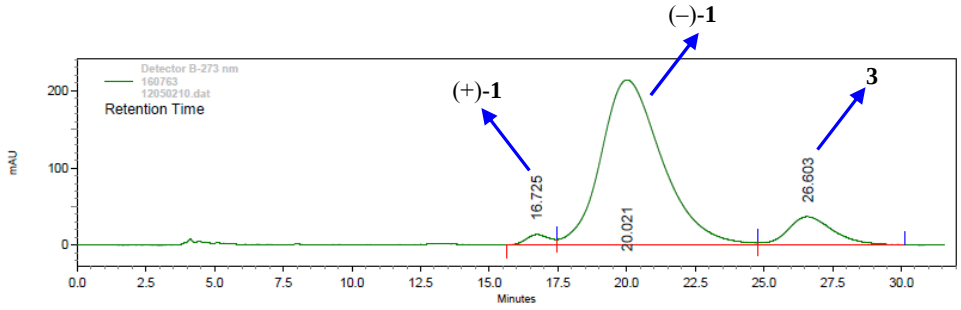
$^{1}$H and $^{13}$C NMR spectra of the mixture of (–)-pandamarilactonines-A [(–)-**1**] and –C (**3**)



Chiral HPLC analysis conditions and results of (–)-pandamarilactonine-A (**1**) and -C (**3**)[1]

**Shimadzu CLASS-VP V6.13 SP2** *Area % Report*
**Method Name: E:\科研数据\121225.met**
**Data Name: E:\科研数据\周洁丹\120502\12050210.dat**
**Column: Chiralcel OB-H**
**Mobile Phase: Hex/IPA = 60/40 (v/v)**
**Flow Rate: 0.80 mL/min**
**CT: 30℃ Sample Name: 160763**




Detector B-273 nm

| Pk # | Retention Time | Area | Area Percent | Resolution |
|---|---|---|---|---|
| 1 | 16.725 | 779631 | 2.05 | 0.00 |
| 2 | 20.021 | 33058892 | 87.03 | 1.07 |
| 3 | 26.603 | 4148431 | 10.92 | 1.69 |
| Totals | | 37986954 | 100.00 | |

**Comparison of the chiral HPLC analysis conditions and results reported by Takayama[1] and this work**

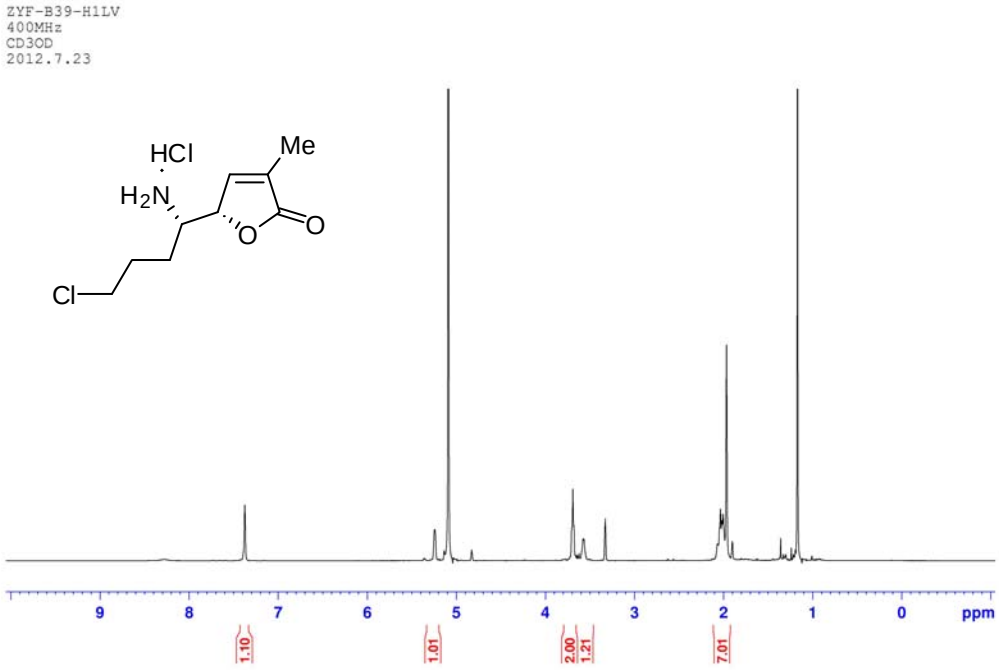
| | Natural (+)-pandamarilactonine-A (**1**)[1] | Our synthetic (–)-pandamarilactonine-A (**1**) |
|---|---|---|
| Column[2] | Chiralcel OB, Daicel Chemical Industries, Ltd. | Chiralcel OB-H, Daicel Chemical Industries, Ltd. |
| column temperature | 30 ºC | 30 ºC |
| Solvent | 40% *i*-PrOH/ *n*-hexane | 40% *i*-PrOH/ *n*-hexane |
| flow rate | 0.3 mL/min | 0.8 mL/min |
| retention time and ratio | 43.2 and 51.9 min (Corresponding retention time 16.2 and 19.5 min with flow rate 0.8 mL/min) in ratios of 63: 37 | 16.7 and 20.0 min in ratio of 2: 87 |

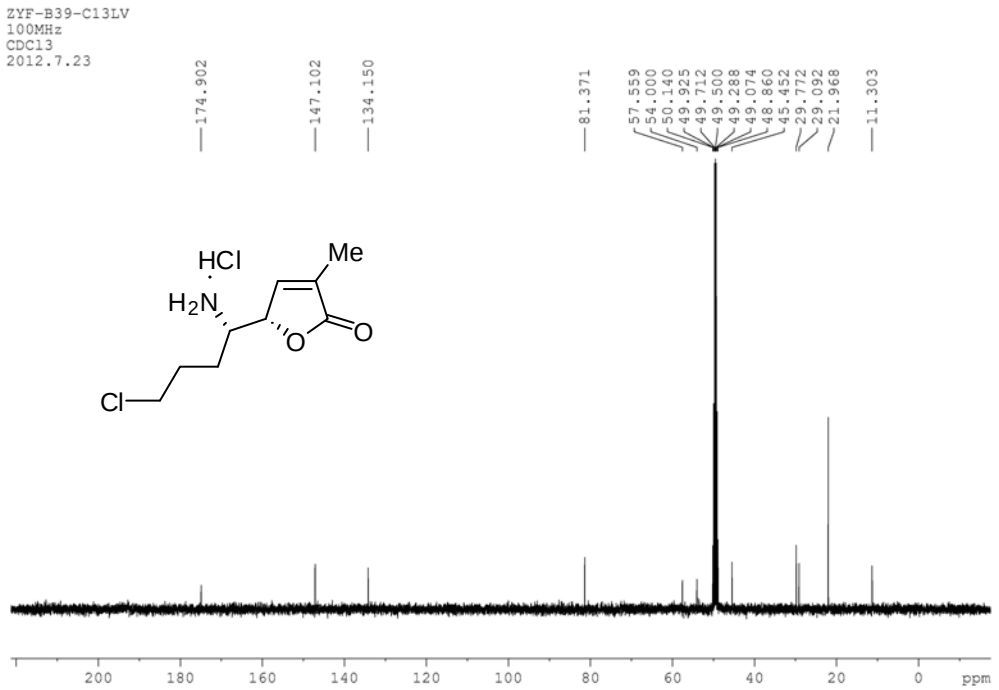
1. Takayama, H.; Nonato, M. G. *J. Am. Chem. Soc.* **2000**, *122*, 8635-8639.
2. The difference between Chiralcel OB and Chiralcel OB-H column resides only in the packing particle size: particle size in Chiralcel OB column: 10 μm, and that in Chiralcel OB-H column: 5μm. Compared with Chiralcel OB column, Chiralcel OB-H column has higher column efficiency and better resolution.

**Comparison of the $^{1}H$ and $^{13}C$ NMR data of our synthetic (–)-pandamarilactonine-A [(–)-1] and those of nature (+)-pandamarilactonine-A (1) reported by Takayama[1]**

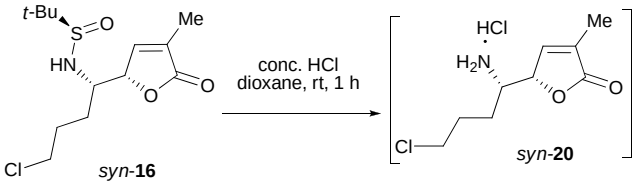
| $^{1}H$ NMR of the nature and synthetic **1** reported by Takayama[1] (500 MHz, $CDCl_3$) δ | $^{1}H$ NMR of the synthetic **1** in this work (400 MHz, $CDCl_3$) δ | $^{13}C$ NMR of the nature and synthetic **1** reported by Takayama[1] (125 MHz, $CDCl_3$) δ | $^{13}C$ NMR of the synthetic **1** in this work (100 MHz, $CDCl_3$) δ |
|---|---|---|---|
| 7.09 (dd, *J* = 1.5 and 1.8 Hz, 1H) | 7.08 (app t, *J* = 1.5 Hz, 1H) | 174.3 | 174.3 |
| 6.99 (d-like, *J* = 1.5 Hz, 1H) | 6.99 (app d, *J* = 1.4 Hz, 1H) | 171.1 | 171.1 |
| 5.18 (dd, *J* = 7.9 and 7.9 Hz, 1H) | 5.17 (t, *J* = 7.9 Hz, 1H) | 148.6 | 148.6 |
| 4.80 (ddd, *J* = 1.8, 1.8 and 5.5 Hz, 1H) | 4.77-4.81 (m, 1H) | 147.0 | 146.9 |
| 3.12 (dd, *J* = 6.7 and 7.6 Hz, 1H) | 3.11 (t, *J* = 7.7 Hz, 1H) | 137.7 | 137.7 |
| 2.88 (ddd, *J* = 4.0, 7.9 and 12.9Hz,1H) | 2.75-2.96 (m, 2H) | 131.2 | 131.2 |
| 2.83 (m, 1H) | | 129.1 | 129.1 |
| 2.45 (m, 1H) | 2.39-2.47 (m, 3H) | 114.1 | 114.1 |
| 2.43 (dd, *J* = 7.3 and 15.0 Hz, 2H) | | 83.4 | 83.4 |
| 2.21 (m, 1H) | 2.16-2.25 (m, 1H) | 65.3 | 65.3 |
| 1.99 (d-like, *J* = 0.9 Hz, 3H) | 1.98 (app dd, *J* = 0.7, 1.2 Hz, 3H) | 55.0 | 55.0 |
| 1.93 (dd, *J* = 1.5 and 1.8 Hz, 3H) | 1.92 (app t, *J* = 1.7 Hz, 3H) | 54.2 | 54.2 |
| 1.70-1.80 (m, 2H) | 1.70-1.79 (m, 2H) | 28.3 | 28.3 |
| 1.59-1.70 (m, 3H) | 1.55-1.69 (m, 3H) | 25.7 | 25.7 |
| | | | |
| 1.42 (m, 1H) | 1.37-1.46 (m, 1H) | 24.0 | 24.0 |
| | | 23.8 | 23.8 |
| | | 10.7 | 10.7 |
| | | 10.5 | 10.5 |

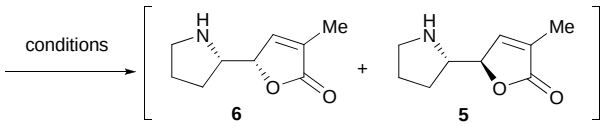
$^{1}H$ and $^{13}C$ NMR of crude product (presumed as *syn*-**20)** obtained after removing the solvent of the desulfinylation reaction of *syn*-**16**



## Investigation of Epimerization of the Desulfinylation Product and the Cyclization Products by $^1$H NMR

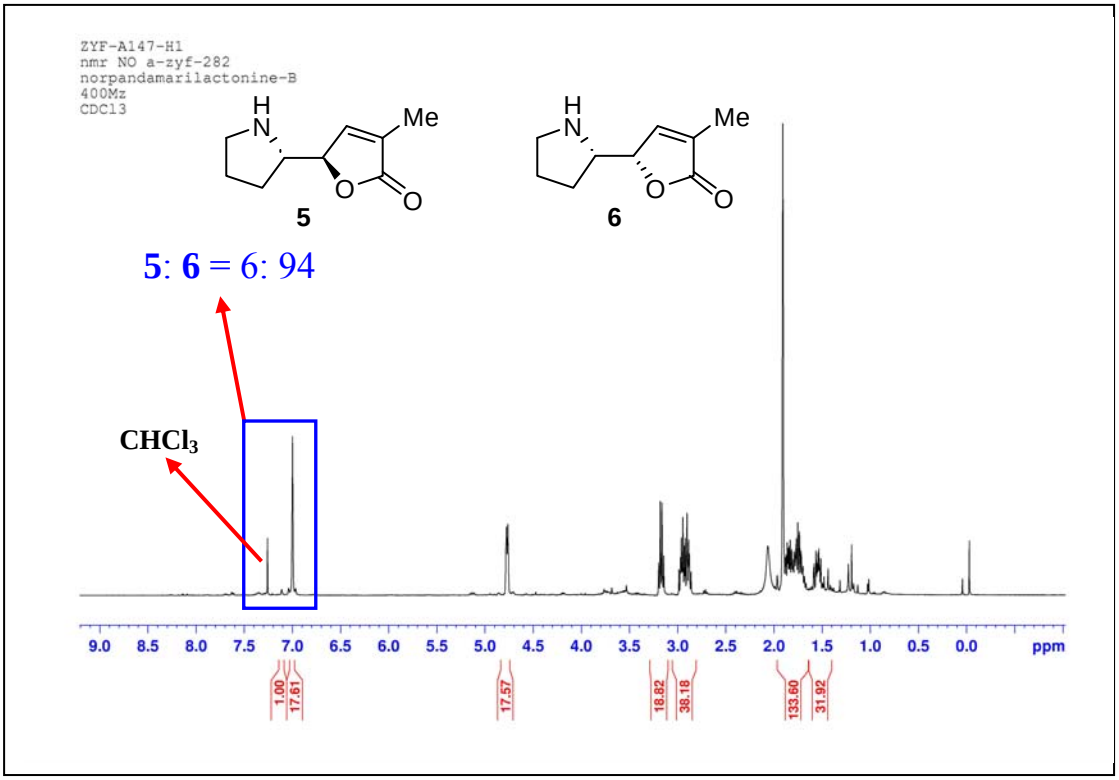


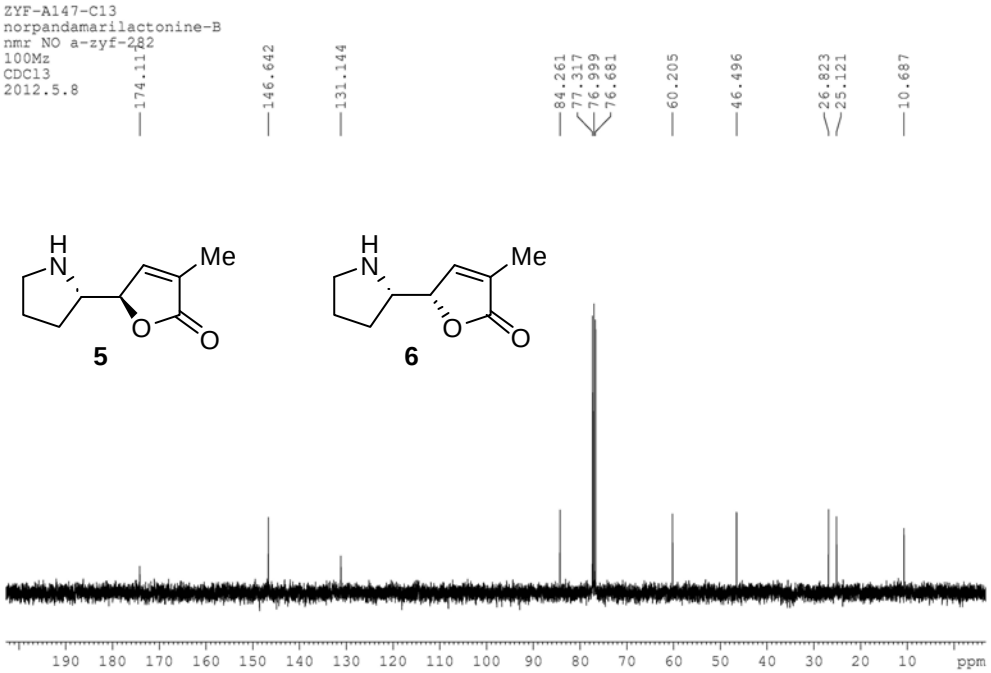




| Entry | Base (eq) | Time (h) | Further treatment | **6**/ **5**[a] |
|---|---|---|---|---|
| 1 | $K_2CO_3$ (4.0) | 12 | no | 94: 6 |
| 2 | $K_2CO_3$ (4.0) | 12 | washed by $NH_3•H_2O$ | 88: 12 |
| 3 | $K_2CO_3$ (4.0) | 12 | added $NH_3•H_2O$ then stayed at rt for 1 day | 62: 38 |
| 4 | $K_2CO_3$ (4.0) & $H_2O$ | 12 | no | 62: 38 |
| 5 | $NH_3•H_2O$ | 2 | no | 67: 33 |

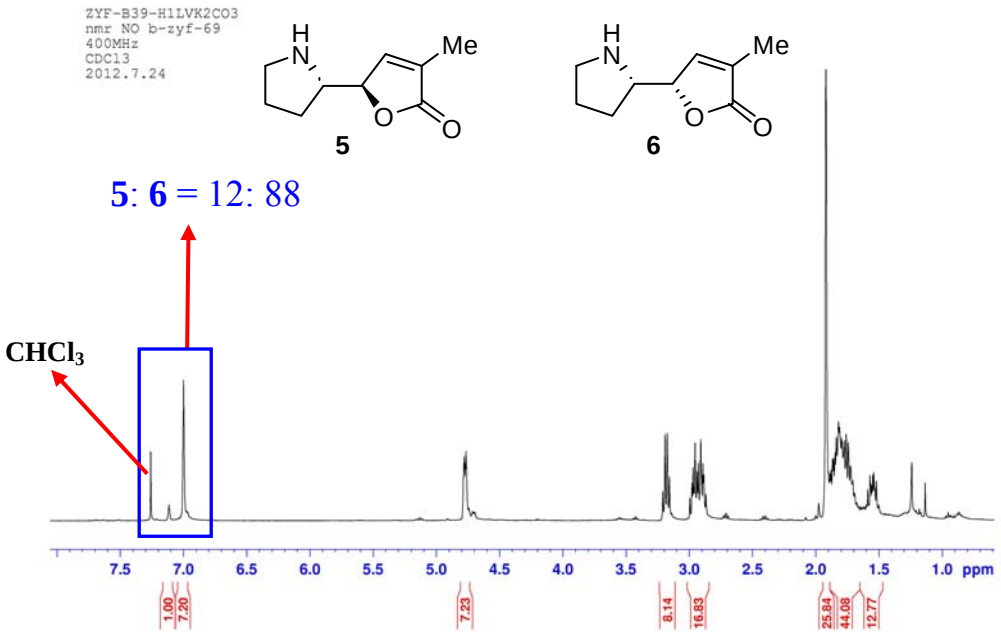
[a] ratios were determined by analysis of 400 MHz $^1$H NMR spectra of unpurified reaction mixtures

$^{1}$H and $^{13}$C NMR of crude product (Table 1 entry 1) from the one-pot desulfinylation and cyclization reactions of *syn*-**16**

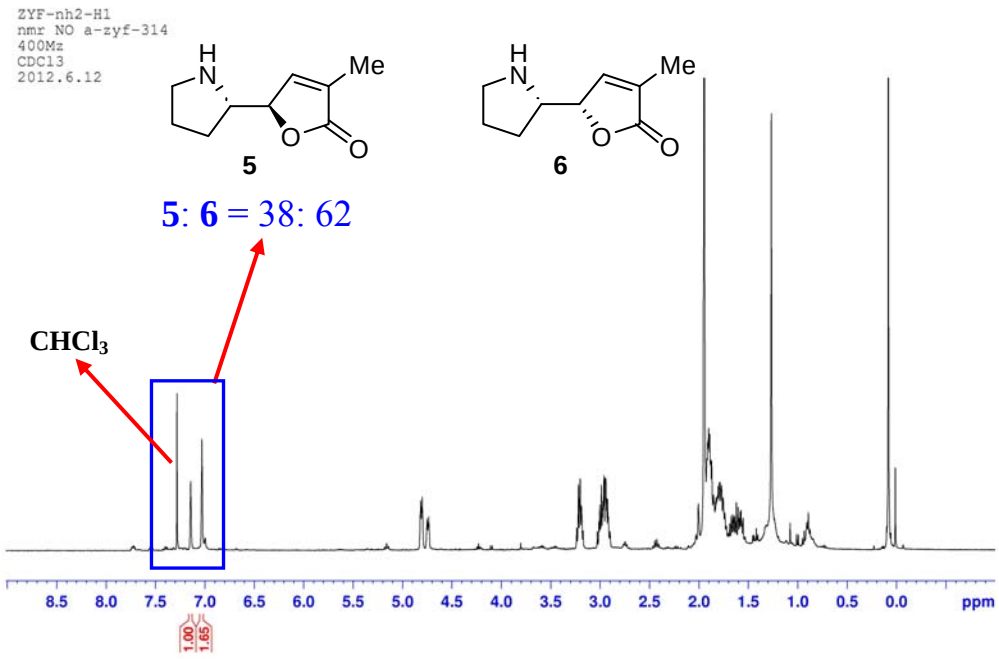


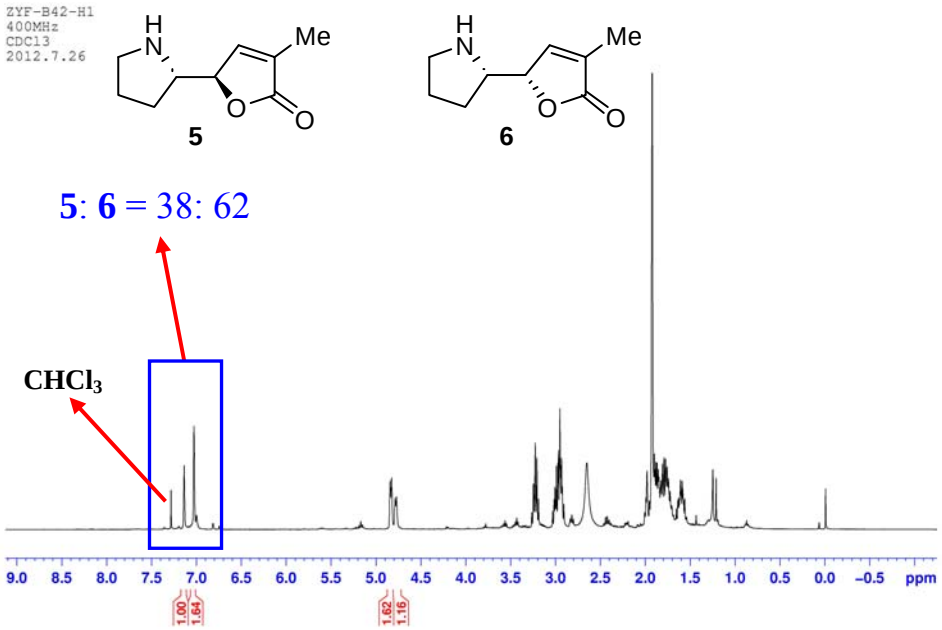
$^1$H NMR of crude product of the one-pot desulfinylation and cyclization reaction of *syn*-**16** (Table 1 entry 2) obtained with following work-up: 1) removed solvent in vacuo; 2) $CH_2Cl_2$ was added in the residue and organic phase was washed with ammonia, concentrated

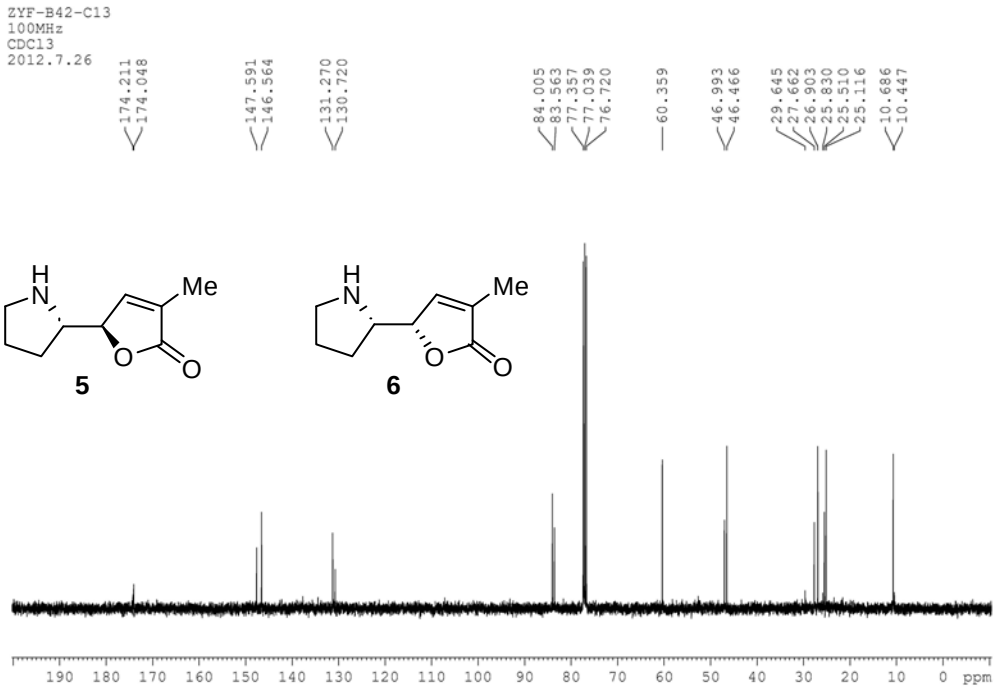



$^1$H NMR of crude product of the one-pot desulfinylation and cyclization reaction of *syn*-**16** (Table 1 entry 3) obtained with following work-up: 1) removed solvent in vacuo; 2) ammonia was added in the residue then stayed 1 day; 3) extracted with $CH_2Cl_2$ and concentrated

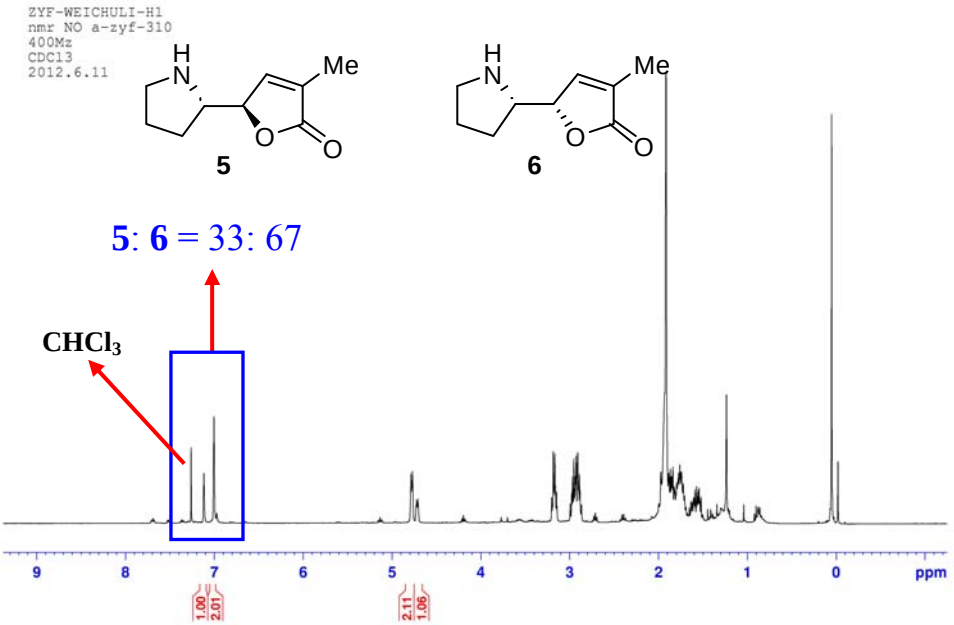


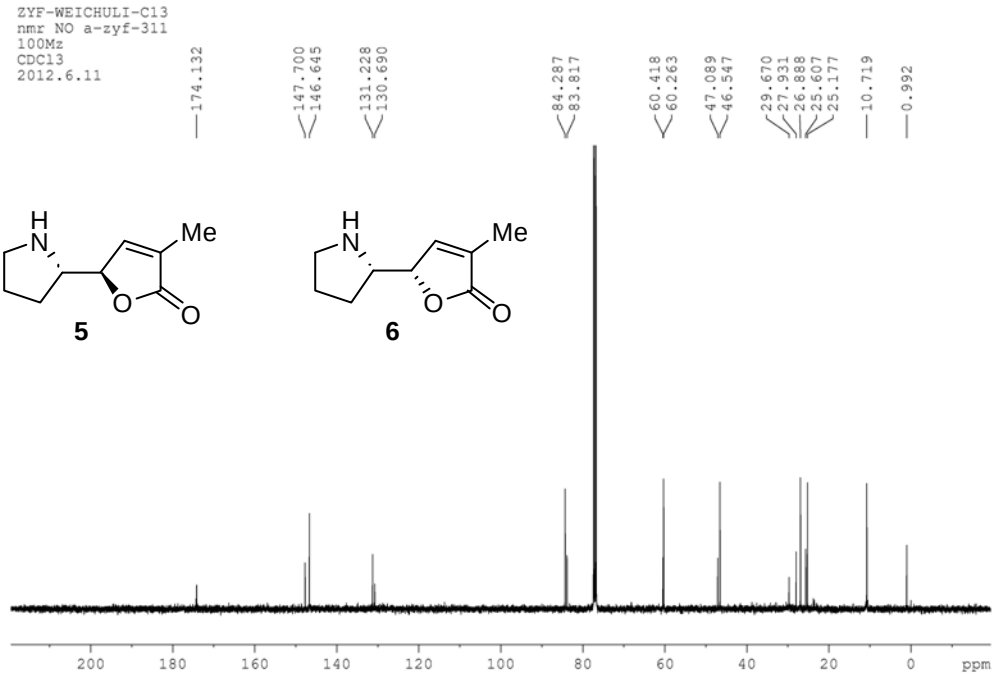
$^{1}H$ and $^{13}C$ NMR of crude product of the one-pot desulfinylation and cyclization reaction of *syn*-**16** (Table 1 entry 4) obtained with following process: 1) removed solvent in vacuo; 2) $K_2CO_3$ and $H_2O$ was added in the mixture and stirred for 12 h; 3) extracted with $CH_2Cl_2$ and concentrated



$^{1}H$ and $^{13}C$ NMR of crude product of the one-pot desulfinylation and cyclization reaction of *syn*-**16** (Table 1 entry 5) obtained with following process: 1) removed solvent of desulfinylation reaction in vacuo; 2) ammonia was added in the residue and stirred for 2 h; 3) extracted with $CH_2Cl_2$ and concentrated



**Comparison of the $^{13}C$ NMR data of our synthetic norpandamarilactonine-A (5) and norpandamarilactonine-B (6) with those of the isolated norpandamarilactonine-A (5) and norpandamarilactonine-B (6) reported by Takayama[2]**

| the synthetic norpandamarilactonine-B (**6**) of Takayama [2] (600 MHz, $CDCl_3$) δ | the crude synthetic norpandamarilactonine-B (**6**) in this work (400 MHz, $CDCl_3$) δ | the synthetic norpandamarilactonine-A (**5**) of Takayama[2] (150 MHz, $CDCl_3$) δ | the crude synthetic norpandamarilactonine-A (**5**) in this work (100 MHz, $CDCl_3$) δ |
|---|---|---|---|
| 174.1 | 174.2 | 174.3 | 174.2 |
| 146.6 | 146.7 | 147.7 | 147.8 |
| 131.2 | 131.2 | 130.7 | 130.7 |
| 84.3 | 84.3 | 83.8 | 83.8 |
| 60.2 | 60.3 | 60.4 | 60.4 |
| 46.5 | 46.5 | 47.1 | 47.1 |
| 26.8 | 26.9 | 27.9 | 27.9 |
| 25.1 | 25.2 | 25.6 | 25.6 |
| 10.7 | 10.7 | 10.7 | 10.7 |

## Crystallographic studies

**Crystal Data [**for *syn*-**17]**. $C_{13}H_{23}NO_3S$ ($M$ =60.76 g/mol): monoclinic, space group $P2_1$ (no.4), $a$ = 10.291(2) Å, $b$ = 5.9808(12) Å, $c$ = 12.068(2) Å, $\beta$ = 103.531 (3)°, $V$ = 722.1(3) Å$^3$, $Z$ = 9, $T$ = 273.15 K, μ(Mo Kα) = 0.225 mm$^{-1}$, *Dcalc* = 1.2573 g/cm$^3$, 4174 reflections measured (3.48° ≤ 2$\theta$≤ 56.5°), 2885 unique ($R_{int}$ = 0.0142, $R_{sigma}$ = 0.0234) which were used in all calculations. The final $R_1$ was 0.0314 (I>=2u(I)) and $wR_2$ was 0.0875 (all data).

**Structure determination** A suitable crystal of *syn*-**17** was selected and measured with Mo$K\alpha$ radiation ($\lambda$ = 0.71073 Å) on a Bruker SMART APEX-CCD diffractometer using a $\psi$-$\omega$ scan mode. The crystal was kept at 273(2) K during data collection. A total of 4174 reflections were collected in the range of 3.48° ≤ 2$\theta$≤ 56.5°, and 2885 were independent ($R_{int}$ = 0.0142, $R_{sigma}$ = 0.0234). Lattice determination and data collection were carried out using Bruker SMART software. Date reduction and absorption corrections were performed with SAINT version 6.28A and SADABS version 2.10, respectively. Using Olex2 [1], the structure was solved with the XS [2] structure solution program using Charge Flipping and refined with the olex2.refine [3] refinement package using Levenberg-Marquardt minimisation. The non-hydrogen atoms were refined anisotropically, and hydrogen atoms were determined with theoretical calculation. A full-matrix least-squares refinement gave the final $R$ = 0.031, $wR$ = 0.088 ($w$ = 1/[$\sigma^2(F_o^2)$ + (0.067$P$)$^2$ + 0.0874$P$] where $P$ = ($F_o^2$ + 2$F_c^2$)/3), $\Delta\rho_{max}$ = 0.39 e Å$^{-3}$ , $\Delta\rho_{min}$ = −0.32 e Å$^{-3}$.

1. Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009), *J. Appl. Cryst.* **42**, 339-341.

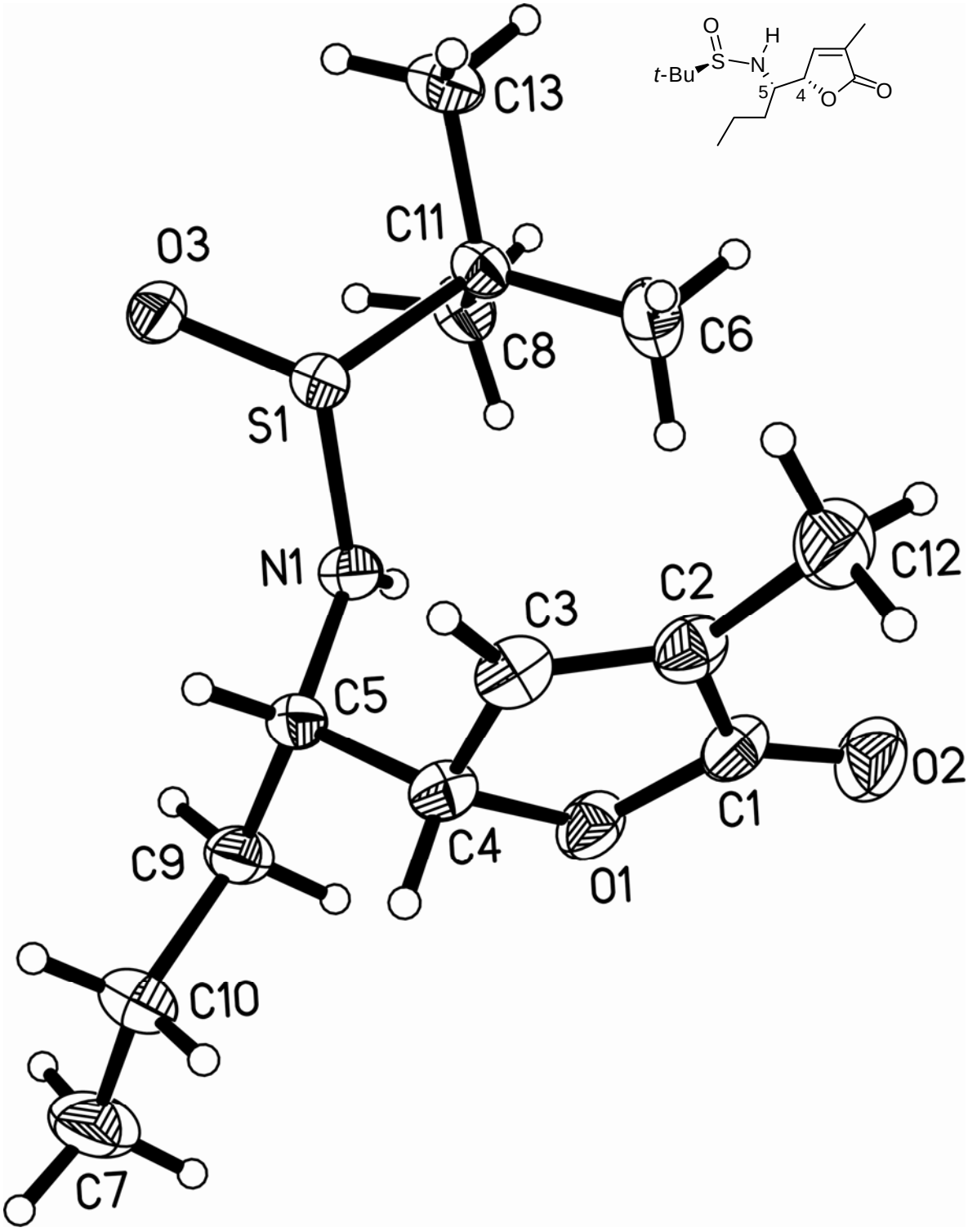
2. Sheldrick, G. M. (2008). *Acta Cryst.* A **64**, 112–122.

3. Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K., Puschmann, H. (2015). *Acta Cryst.* A **71**, 59–71.

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for *syn*-**17**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.

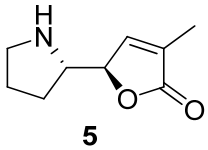
| **Atom** | ***x*** | ***y*** | ***z*** | **U(eq)** |
|---|---|---|---|---|
| S1 | -6193.296(8) | -377.303(8) | -4471.117(8) | 20.68(4) |
| O3 | -5724.803(8) | 80.702(8) | -5538.997(8) | 26.14(5) |
| N1 | -5264.196(8) | 1060.900(8) | -3389.705(8) | 23.68(5) |
| O2 | -6956.398(8) | 385.800(8) | -346.402(8) | 42.67(5) |
| C5 | -4116.499(8) | -147.999(8) | -2661.198(8) | 23.81(5) |
| C6 | -8377.000(8) | 603.100(8) | -3654.203(8) | 34.83(5) |
| C1 | -6278.799(8) | -602.999(8) | -877.402(8) | 28.45(5) |
| C8 | -7557.501(8) | 3713.200(8) | -4730.097(8) | 28.76(5) |
| C9 | -2982.499(8) | 1523.899(8) | -2220.099(8) | 30.03(5) |
| C3 | -5530.704(8) | -3162.299(8) | -1958.197(8) | 28.36(5) |
| C11 | -7776.301(8) | 1209.901(8) | -4654.597(8) | 23.40(5) |
| C4 | -4515.300(8) | -1345.599(8) | -1670.399(8) | 26.02(5) |
| C13 | -8643.401(8) | 324.700(8) | -5776.898(8) | 33.85(5) |
| C2 | -6546.399(8) | -2766.500(8) | -1483.002(8) | 28.03(5) |
| C12 | -7769.298(8) | -4085.698(8) | -1468.803(8) | 41.59(5) |
| C10 | -1638.202(8) | 431.699(8) | -1717.300(8) | 40.40(5) |
| C7 | -560.901(8) | 2167.402(8) | -1254.700(8) | 50.66(5) |
| O1 | -5088.704(8) | 211.700(8) | -1005.599(8) | 31.04(5) |

**ORTEP drawing derived from the single-crystal X-ray analysis of *syn*-17**



## Computational Methods and Details

All calculations were performed with Gaussian 09.[1] Geometries were initially optimized at B3LYP/6-31G* level in gas phase. All structures are characterized by no imaginary frequency. The single point calculations were carried out by B3LYP/6-311++G(2d,p) with SMD solvation model in MeCN on gas phase optimized geometries.

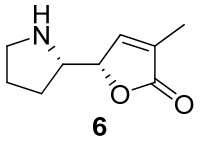


**5**

HF=-556.1706565

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.395346 | 0.214371 | -0.047648 |
| 2 | 6 | 0 | -2.780655 | -0.090899 | 1.342498 |
| 3 | 6 | 0 | -1.392513 | -0.705228 | 1.014452 |
| 4 | 6 | 0 | -1.273924 | -0.582192 | -0.534587 |
| 5 | 7 | 0 | -2.270225 | 0.407823 | -0.973935 |
| 6 | 6 | 0 | 0.114126 | -0.224078 | -1.076784 |
| 7 | 6 | 0 | 1.220418 | -1.168277 | -0.701843 |
| 8 | 6 | 0 | 2.183697 | -0.512040 | -0.044019 |
| 9 | 6 | 0 | 1.766313 | 0.914861 | 0.059246 |
| 10 | 8 | 0 | 0.541106 | 1.048892 | -0.553477 |
| 11 | 8 | 0 | 2.345482 | 1.840316 | 0.572069 |
| 12 | 6 | 0 | 3.479896 | -0.978530 | 0.533793 |
| 13 | 1 | 0 | -1.872898 | 1.333949 | -0.806794 |
| 14 | 1 | 0 | -1.545879 | -1.545221 | -0.992103 |
| 15 | 1 | 0 | 0.030013 | -0.110964 | -2.166394 |
| 16 | 1 | 0 | -3.986303 | -0.642112 | -0.398875 |
| 17 | 1 | 0 | -4.050934 | 1.090302 | -0.055482 |
| 18 | 1 | 0 | -2.661502 | 0.835400 | 1.915376 |
| 19 | 1 | 0 | -3.409065 | -0.761231 | 1.938428 |
| 20 | 1 | 0 | -1.310234 | -1.747917 | 1.338559 |
| 21 | 1 | 0 | -0.592988 | -0.146716 | 1.510233 |
| 22 | 1 | 0 | 1.200597 | -2.223615 | -0.953993 |
| 23 | 1 | 0 | 4.318177 | -0.428728 | 0.089952 |
| 24 | 1 | 0 | 3.514312 | -0.781019 | 1.611666 |
| 25 | 1 | 0 | 3.633507 | -2.048470 | 0.367575 |

---



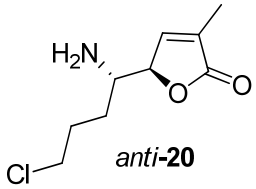
**6**

HF=-556.170233

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.140998 | -0.788101 | -0.378499 |
| 2 | 6 | 0 | -3.499541 | 0.648729 | 0.020430 |
| 3 | 6 | 0 | -2.115362 | 1.305609 | 0.233436 |
| 4 | 6 | 0 | -1.150169 | 0.122704 | 0.537155 |
| 5 | 7 | 0 | -2.010693 | -1.062504 | 0.508352 |
| 6 | 6 | 0 | 0.003809 | 0.062170 | -0.493606 |
| 7 | 6 | 0 | 1.020724 | 1.160473 | -0.374210 |
| 8 | 6 | 0 | 2.222438 | 0.646660 | -0.083246 |
| 9 | 6 | 0 | 2.075388 | -0.834501 | -0.020188 |
| 10 | 8 | 0 | 0.760392 | -1.145035 | -0.279512 |
| 11 | 8 | 0 | 2.913088 | -1.672140 | 0.208191 |
| 12 | 6 | 0 | 3.543997 | 1.300220 | 0.157785 |
| 13 | 1 | 0 | -1.492090 | -1.907630 | 0.284489 |
| 14 | 1 | 0 | -0.685125 | 0.212332 | 1.527326 |
| 15 | 1 | 0 | -0.421222 | 0.004901 | -1.506021 |
| 16 | 1 | 0 | -3.953302 | -1.500257 | -0.195576 |
| 17 | 1 | 0 | -2.894677 | -0.834983 | -1.456694 |
| 18 | 1 | 0 | -4.102942 | 1.165387 | -0.732232 |
| 19 | 1 | 0 | -4.062081 | 0.635641 | 0.959504 |
| 20 | 1 | 0 | -2.122439 | 2.043687 | 1.040350 |
| 21 | 1 | 0 | -1.801668 | 1.831146 | -0.677623 |
| 22 | 1 | 0 | 0.772160 | 2.209588 | -0.495258 |
| 23 | 1 | 0 | 4.289179 | 0.936763 | -0.559640 |
| 24 | 1 | 0 | 3.922693 | 1.045959 | 1.154797 |
| 25 | 1 | 0 | 3.476811 | 2.388620 | 0.074340 |

---



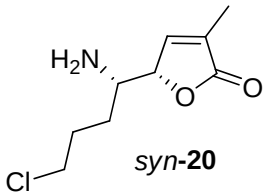
*anti*-**20**

HF=-1017.0213164

---

| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 1.880386 | -1.242837 | -0.141498 |
| 2 | 6 | 0 | 2.773659 | -0.318442 | 0.354716 |
| 3 | 6 | 0 | 2.434962 | 1.012207 | -0.223110 |
| 4 | 6 | 0 | 1.378561 | 0.845716 | -1.028675 |
| 5 | 6 | 0 | 0.959078 | -0.596563 | -1.039642 |
| 6 | 8 | 0 | 3.654308 | -0.612186 | 1.124745 |
| 7 | 6 | 0 | 3.224670 | 2.230021 | 0.130365 |
| 8 | 6 | 0 | -0.500877 | -0.910094 | -0.615563 |
| 9 | 6 | 0 | -0.853202 | -0.302185 | 0.752481 |
| 10 | 6 | 0 | -2.272590 | -0.620476 | 1.244370 |
| 11 | 6 | 0 | -3.400625 | -0.267539 | 0.284670 |
| 12 | 7 | 0 | -0.791484 | -2.346205 | -0.619123 |
| 13 | 17 | 0 | -3.426067 | 1.507181 | -0.159397 |
| 14 | 1 | 0 | -0.129812 | -2.818294 | -0.002466 |
| 15 | 1 | 0 | -0.640838 | -2.736164 | -1.548749 |
| 16 | 1 | 0 | 0.869877 | 1.608879 | -1.608836 |
| 17 | 1 | 0 | 1.117751 | -1.039384 | -2.034990 |
| 18 | 1 | 0 | 4.279165 | 2.095781 | -0.138231 |
| 19 | 1 | 0 | 2.842365 | 3.119166 | -0.378667 |
| 20 | 1 | 0 | 3.198796 | 2.405321 | 1.212284 |
| 21 | 1 | 0 | -1.137783 | -0.446153 | -1.381361 |
| 22 | 1 | 0 | -0.720754 | 0.783739 | 0.699737 |
| 23 | 1 | 0 | -0.139368 | -0.669214 | 1.501002 |
| 24 | 1 | 0 | -2.438637 | -0.112576 | 2.201922 |
| 25 | 1 | 0 | -2.362409 | -1.698615 | 1.425224 |
| 26 | 1 | 0 | -4.376167 | -0.472711 | 0.728642 |
| 27 | 1 | 0 | -3.318036 | -0.814084 | -0.655547 |




*syn*-**20**

HF=-1017.0217

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 2.182438 | 1.076017 | -0.409375 |
| 2 | 6 | 0 | 3.111391 | 0.096763 | -0.145633 |
| 3 | 6 | 0 | 2.392931 | -1.202387 | -0.017646 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | 1.087482 | -0.963222 | -0.191490 |
| 5 | 6 | 0 | 0.858507 | 0.501373 | -0.439116 |
| 6 | 8 | 0 | 4.292251 | 0.324486 | -0.051340 |
| 7 | 6 | 0 | 3.135686 | -2.469148 | 0.255551 |
| 8 | 6 | 0 | -0.005241 | 1.230406 | 0.607181 |
| 9 | 6 | 0 | -1.429198 | 0.655318 | 0.726442 |
| 10 | 6 | 0 | -2.261004 | 0.712101 | -0.562126 |
| 11 | 6 | 0 | -3.715169 | 0.302374 | -0.377346 |
| 12 | 7 | 0 | -0.066716 | 2.644980 | 0.223581 |
| 13 | 17 | 0 | -3.890946 | -1.455663 | 0.088947 |
| 14 | 1 | 0 | -0.497017 | 3.183255 | 0.974191 |
| 15 | 1 | 0 | 0.881989 | 3.000860 | 0.116232 |
| 16 | 1 | 0 | 0.283895 | -1.691465 | -0.171533 |
| 17 | 1 | 0 | 0.450035 | 0.694644 | -1.438966 |
| 18 | 1 | 0 | 3.877696 | -2.656426 | -0.529524 |
| 19 | 1 | 0 | 3.691826 | -2.392969 | 1.197341 |
| 20 | 1 | 0 | 2.460624 | -3.327444 | 0.314132 |
| 21 | 1 | 0 | 0.498071 | 1.066769 | 1.577115 |
| 22 | 1 | 0 | -1.949103 | 1.227956 | 1.508737 |
| 23 | 1 | 0 | -1.376616 | -0.374478 | 1.097050 |
| 24 | 1 | 0 | -1.817667 | 0.082829 | -1.343508 |
| 25 | 1 | 0 | -2.252657 | 1.740782 | -0.944389 |
| 26 | 1 | 0 | -4.285002 | 0.419670 | -1.300723 |
| 27 | 1 | 0 | -4.202809 | 0.871941 | 0.417499 |

---

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