

Anti-inflammatory Endiandric Acid Analogues from the Roots of *Beilschmiedia tsangii*

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[○] Food Industry Research and Development Institute, Hsinchu, Taiwan 300, Republic of China

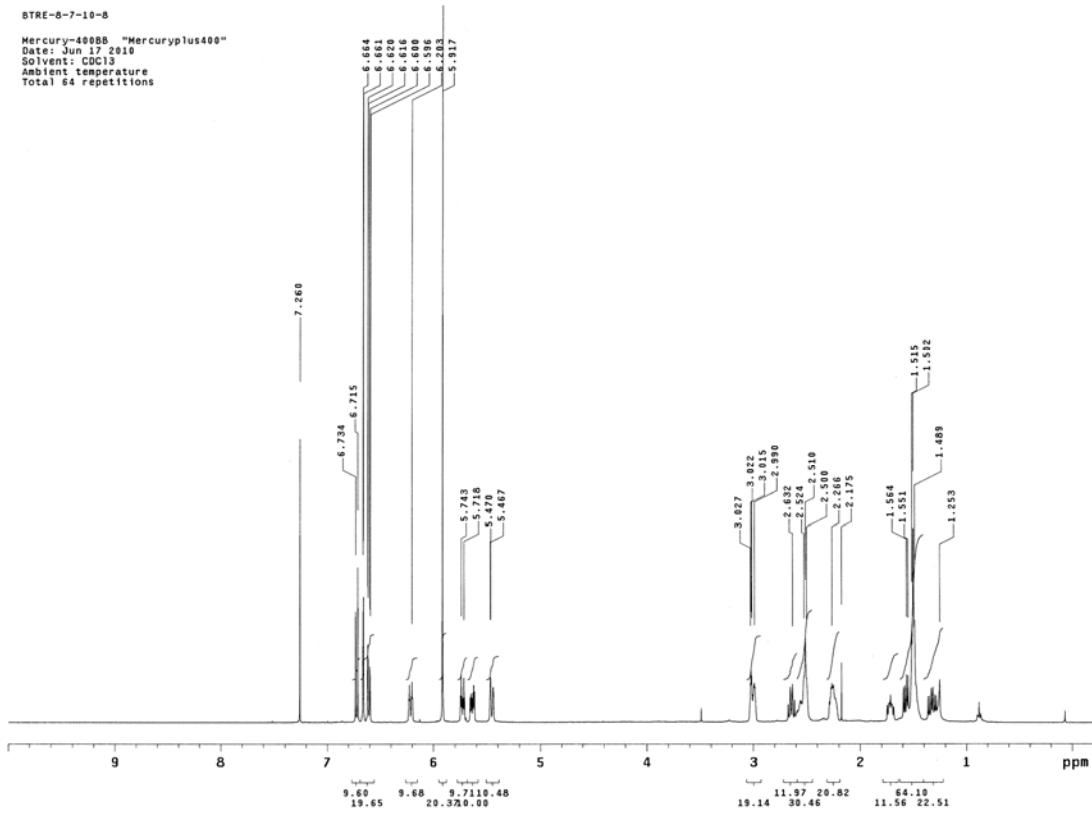
[▽] Department of Medicine, Baylor College of Medicine, Houston, TX 77030, USA

Supporting Information

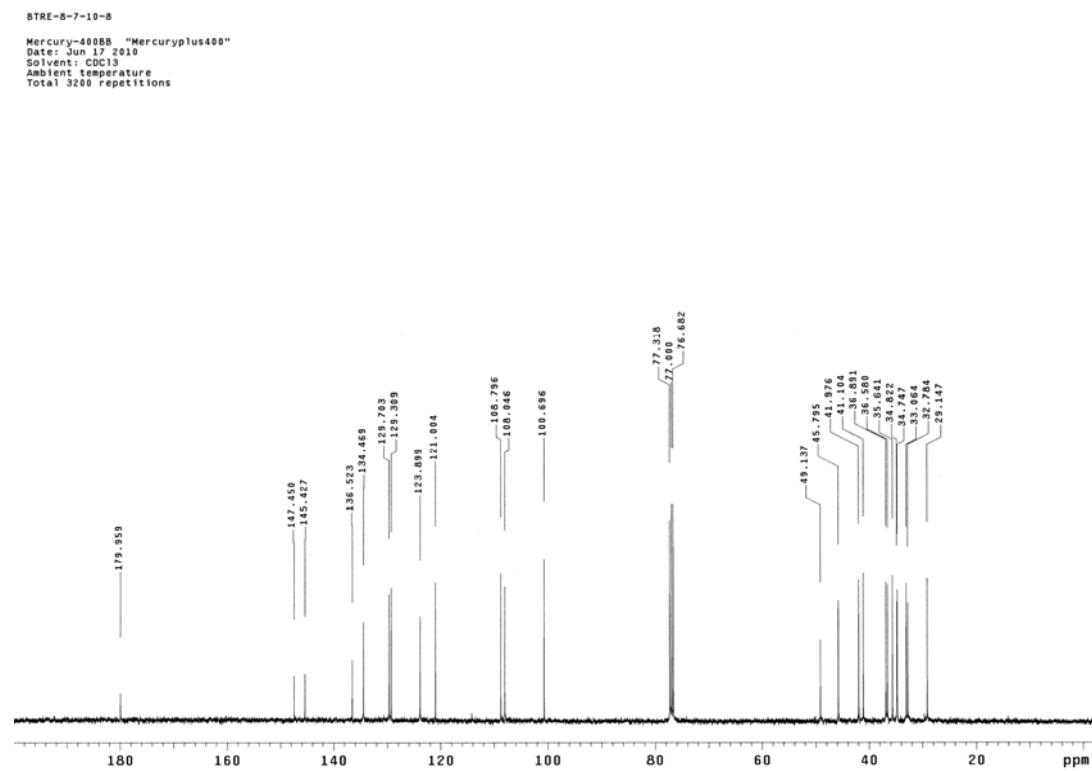
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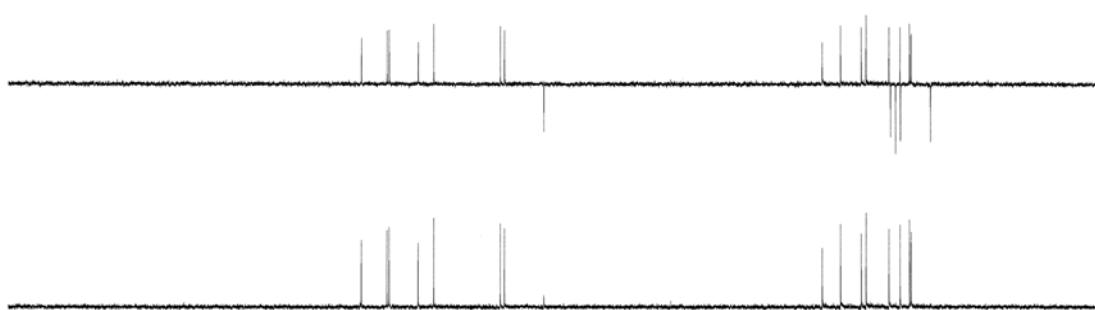
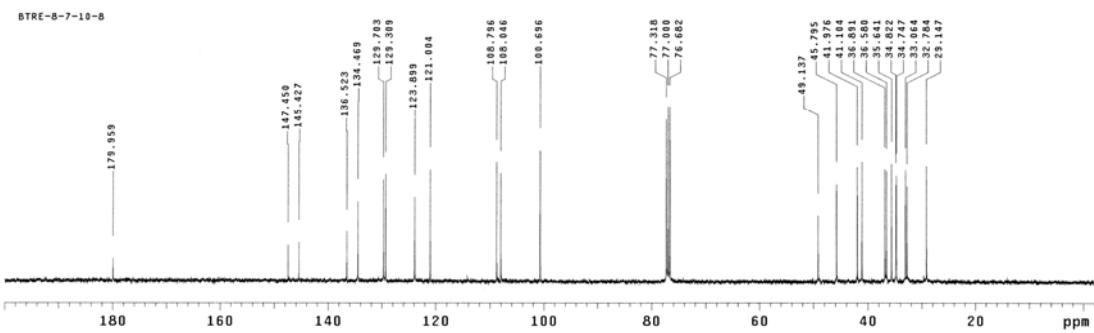
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S58. **Figure 2.** COSY (—) and HMBC (↔) correlations of **1-8**.



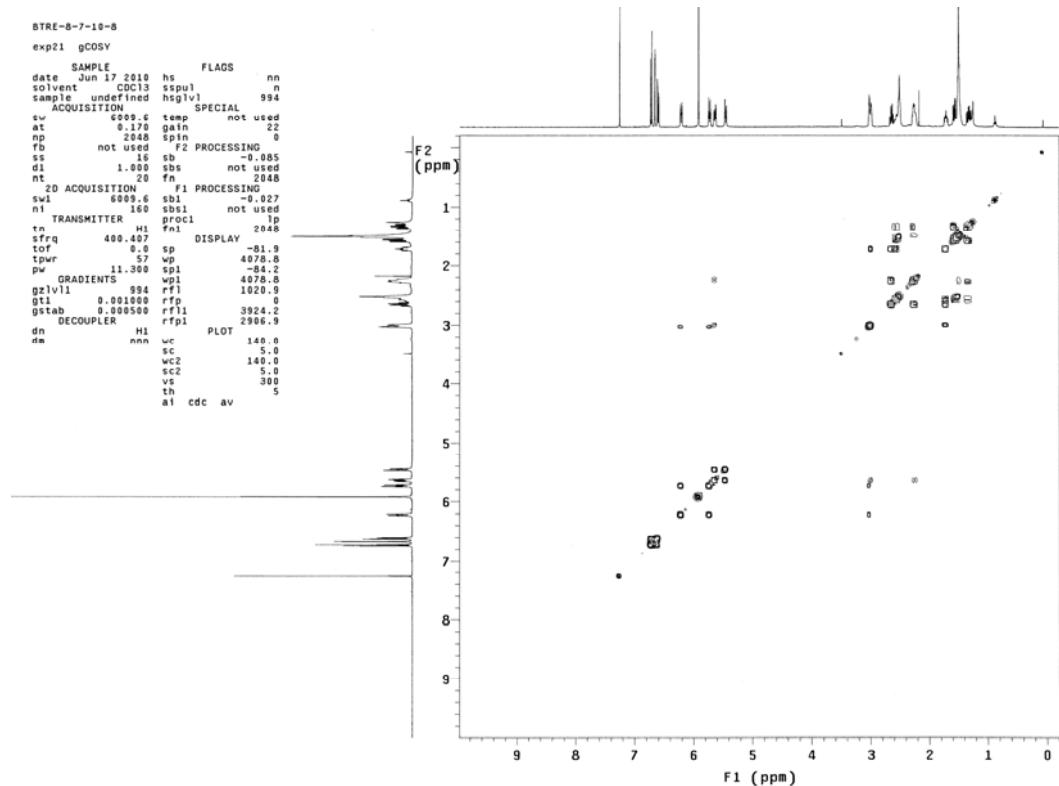
S1. ^1H NMR spectrum of tsangibeilin A (**1**) in CDCl_3 at 400 MHz



S2. ^{13}C NMR spectrum of tsangibeilin A (**1**) in CDCl_3 at 100 MHz

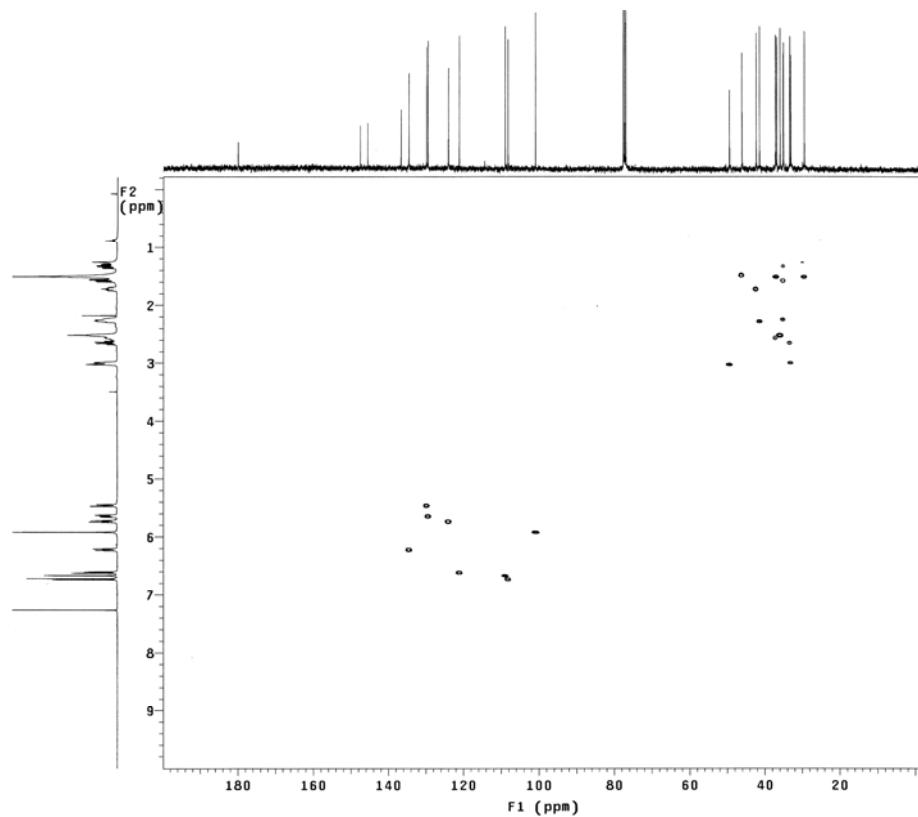


S3. DEPT spectrum of tsangibeilin A (**1**) in CDCl_3



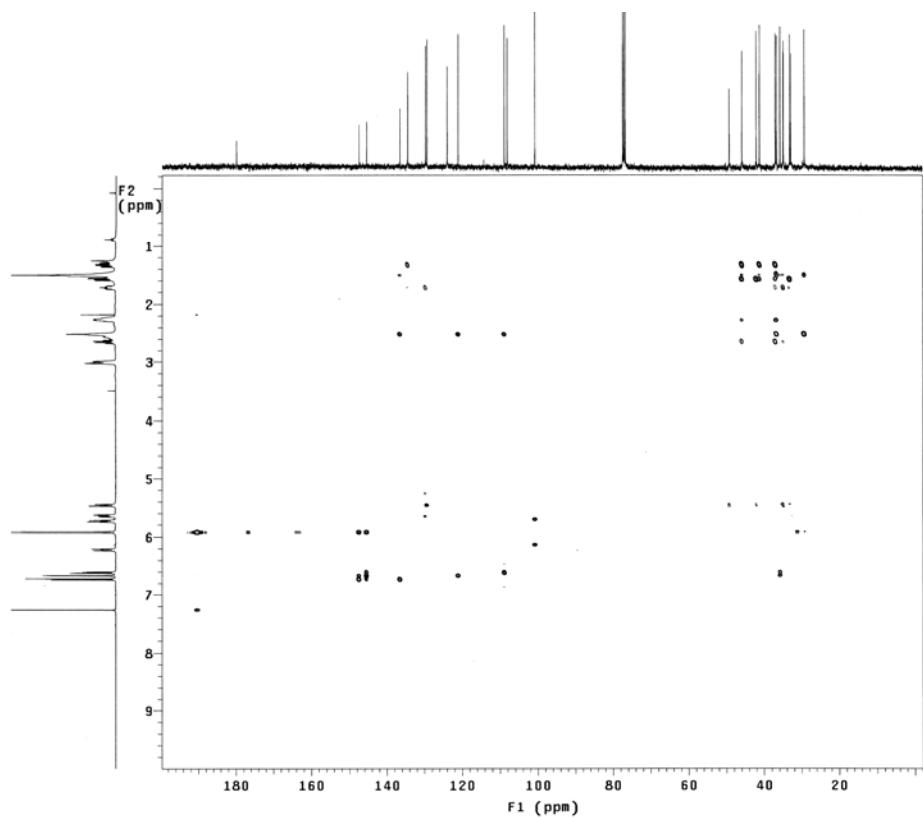
S4. ^1H - ^1H COSY spectrum of tsangibeilin A (**1**) in CDCl_3

BTRE-8-7-10-8

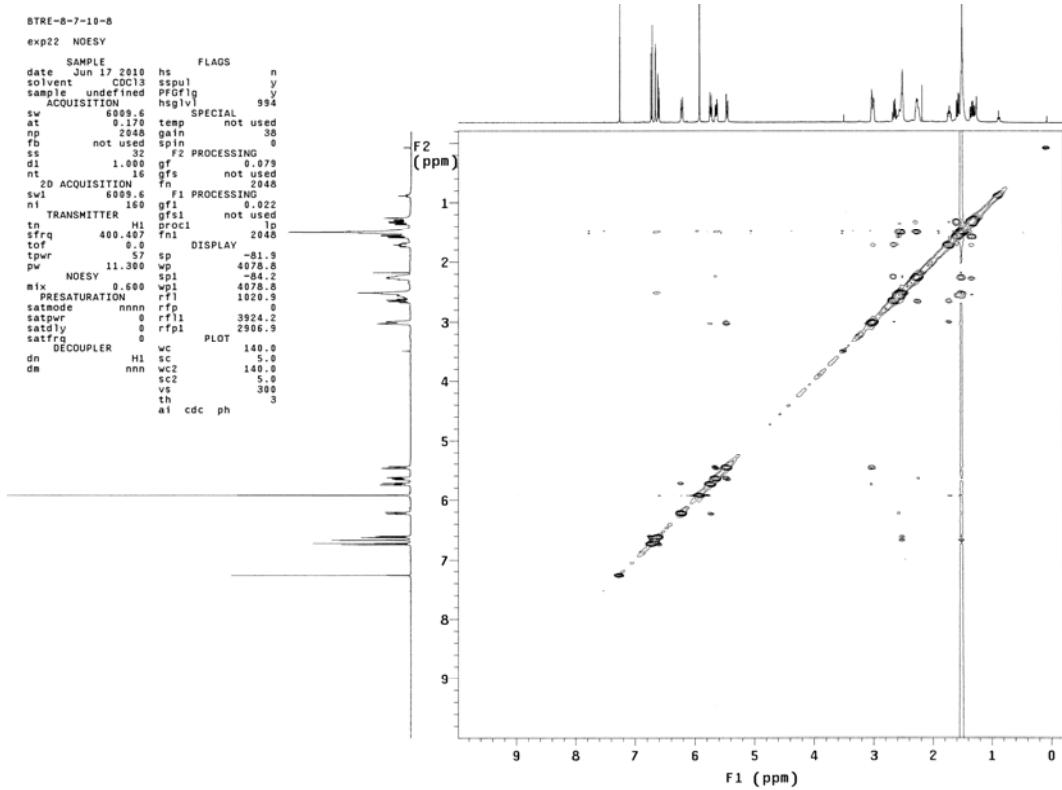


S5. HSQC spectrum of tsangibeilin A (**1**) in CDCl_3

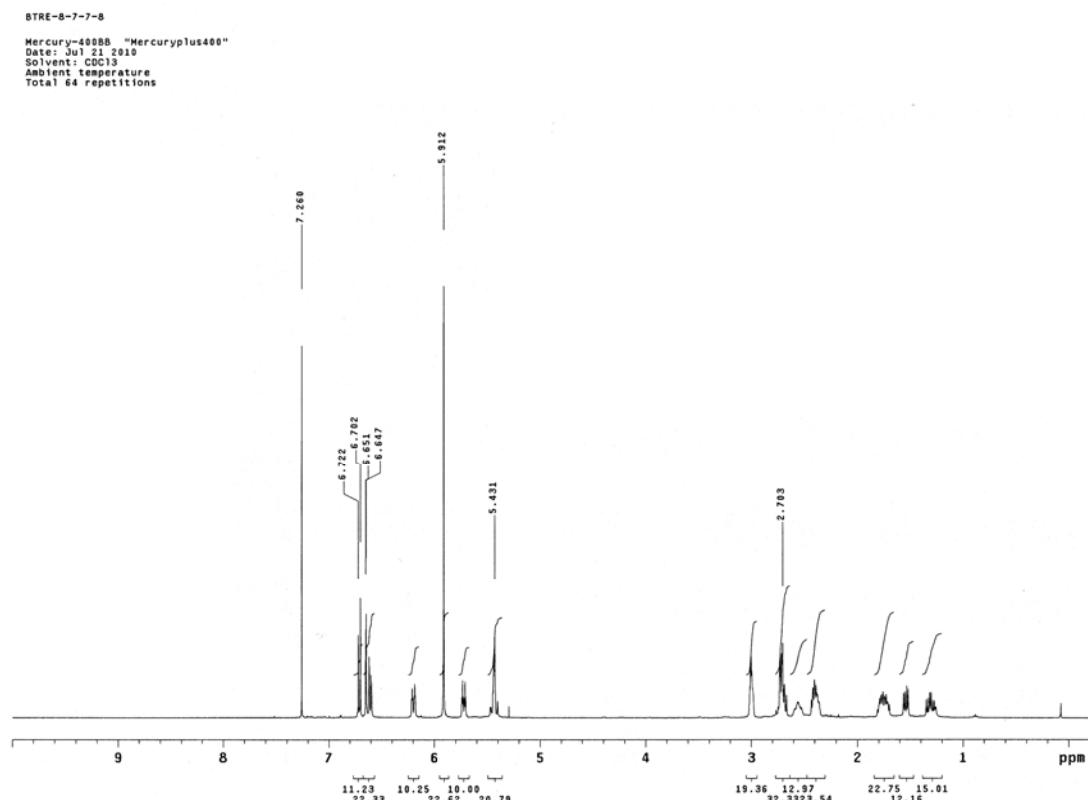
BTRE-8-7-10-8



S6. HMBC spectrum of tsangibeilin A (**1**) in CDCl_3



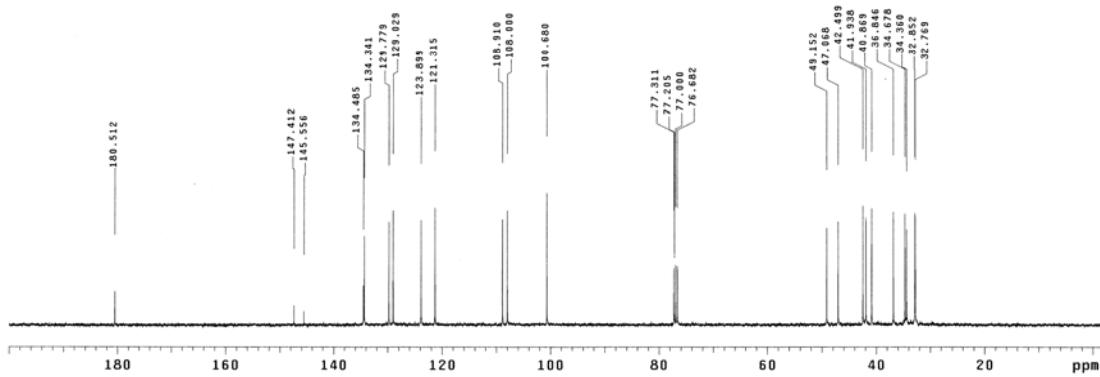
S7. NOESY spectrum of tsangibeilin A (**1**) in CDCl_3



S8. ^1H NMR spectrum of tsangibeilin B (**2**) in CDCl_3 at 400 MHz

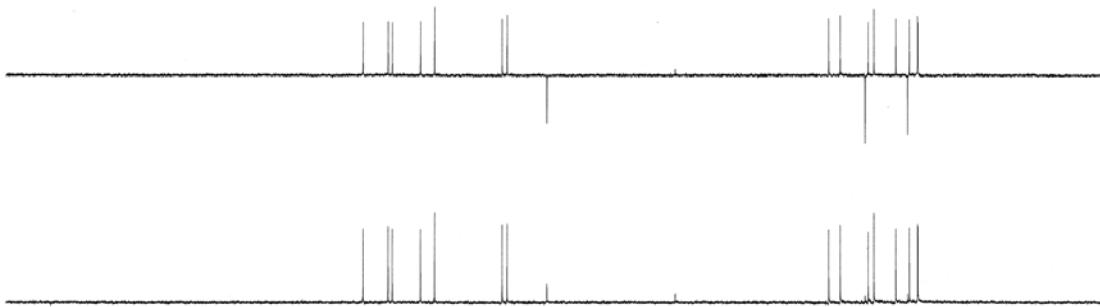
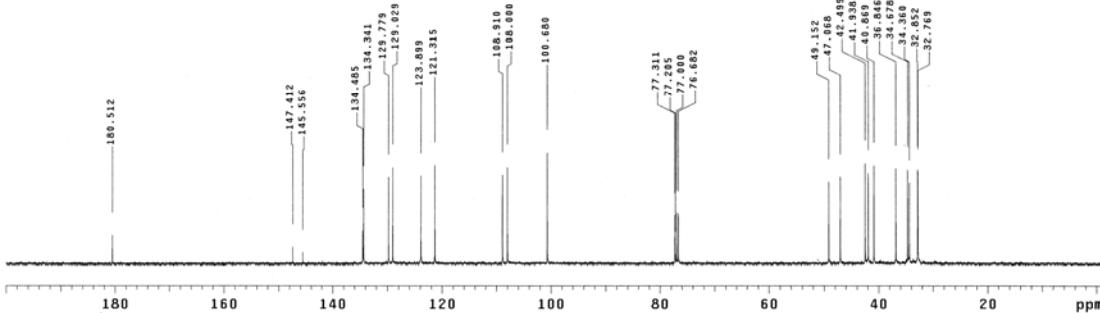
BTRE-8-7-7-8

Mercury-4988B "Mercuryplus400"
Date: Jul 21 2010
Solvent: CDCl₃
Ambient temperature
Total 1328 repetitions

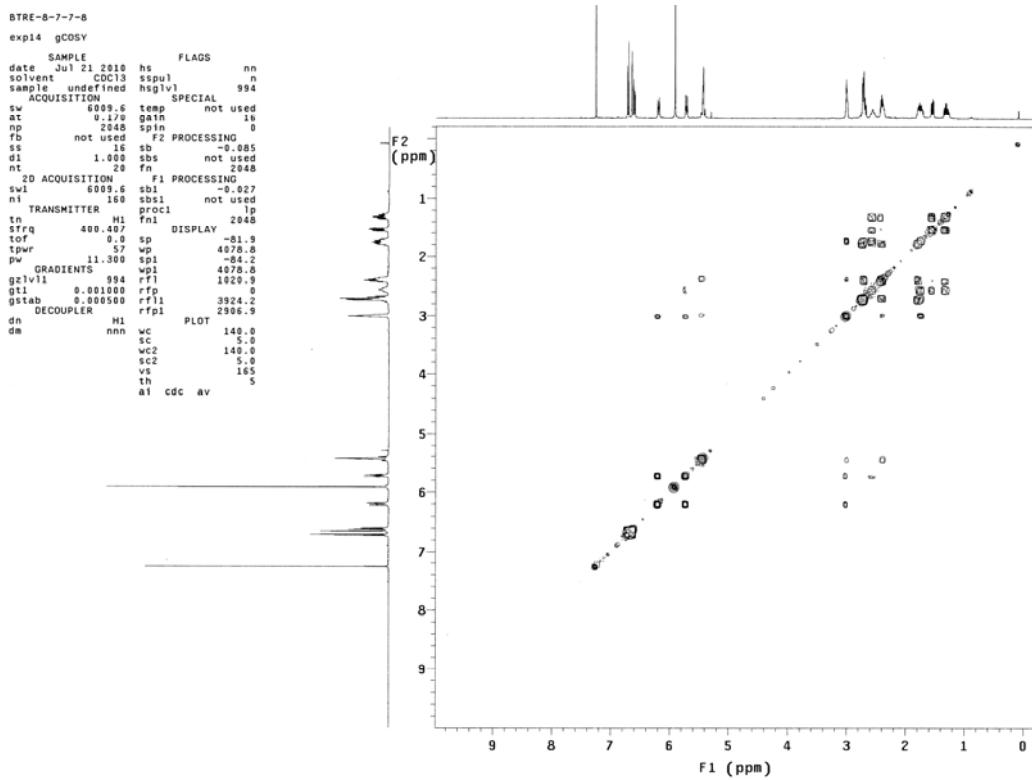


S9. ¹³C NMR spectrum of tsangibeilin B (2) in CDCl₃ at 100 MHz

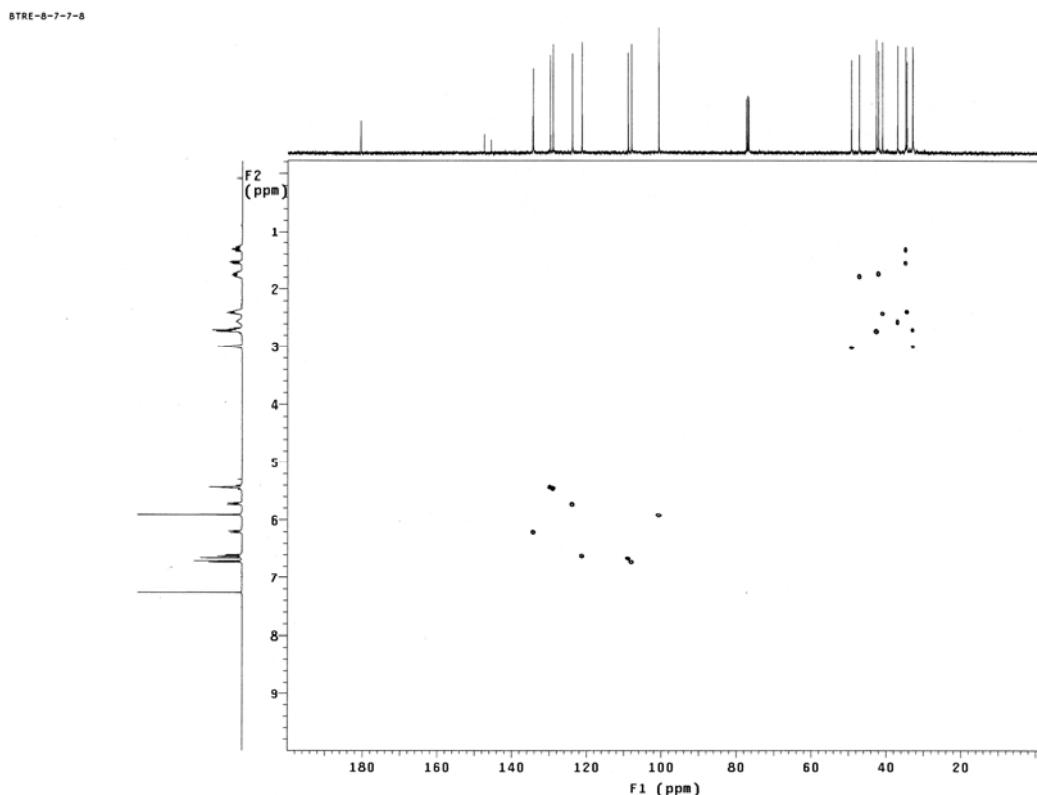
BTRE-8-7-7-8



S10. DEPT spectrum of tsangibeilin B (2) in CDCl₃

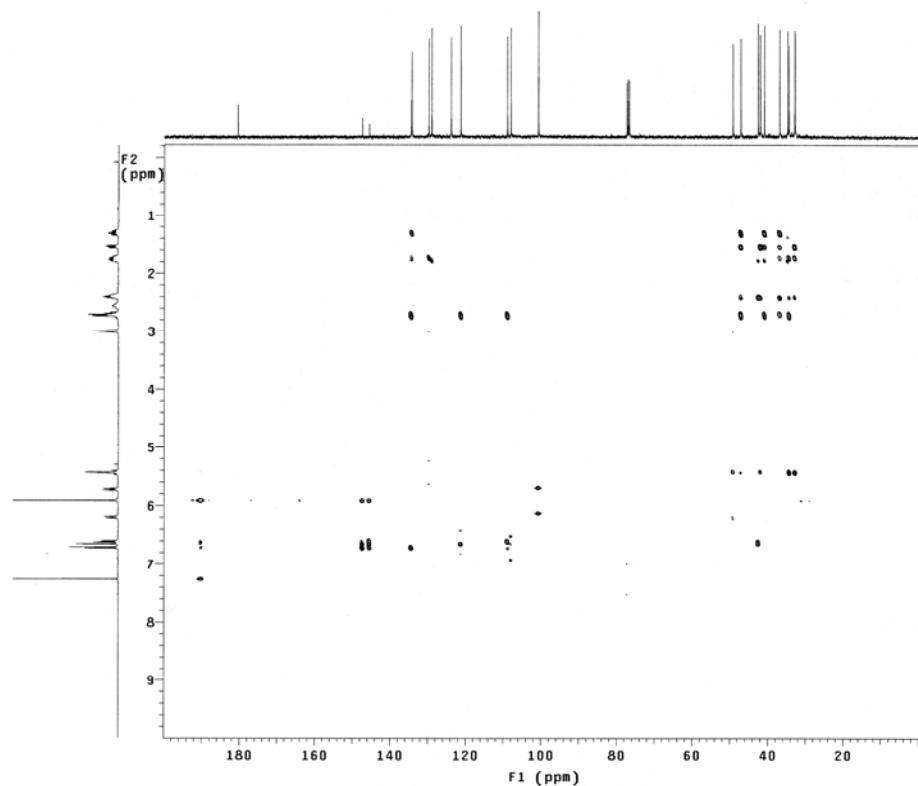


S11. ^1H - ^1H COSY spectrum of tsangibeilin B (**2**) in CDCl_3



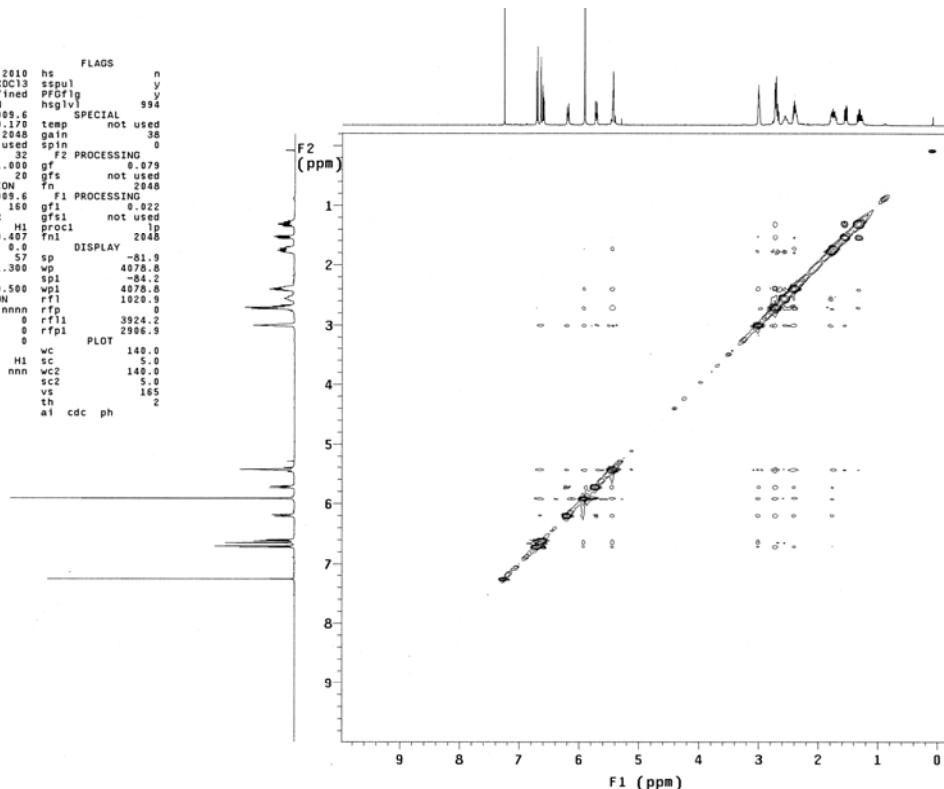
S12. HSQC spectrum of tsangibeilin B (**2**) in CDCl_3

BTRE-8-7-7-8



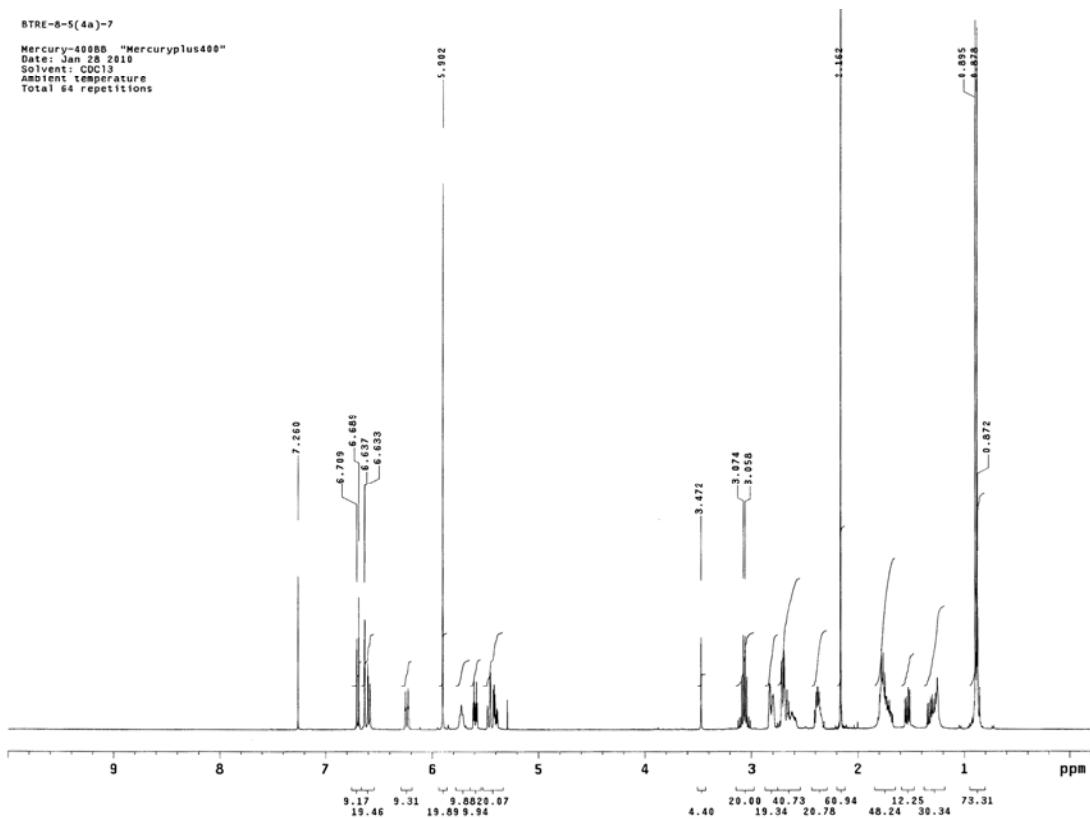
S13. HMBC spectrum of tsangibeilin B (2) in CDCl_3

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sample undefined PGPGDg      y
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at 0.170          ttemp    not used
np 280            gda     38
rb not used       spin    0
ss 32              F2 PROCESSING
di 1.800          gff     0.079
n1 100            fts     not used
t1 2000           fn      2048
sw1 6009.6         F1 PROCESSING
n1 160            gfp1    0.022
tn TRANSMITTER      fts1    not used
t1 H1              proc1   1p
sfrq 400.407        r1      2048
tot 65             w1      DISPLAY
tpwr 57             sp1     -61.9
pw 11.300          wp      4078.8
NOESY 0.500          sp1     -64.2
mix 1000            sp1     4078.8
PRESATURATION      rft1    1029.9
satmode nnnn         rfp    0
satpwr 0             rfp1    3924.2
satby 0             rfp1    2996.9
satfrq 0             PLOT
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dm nnn             sc2    140.0
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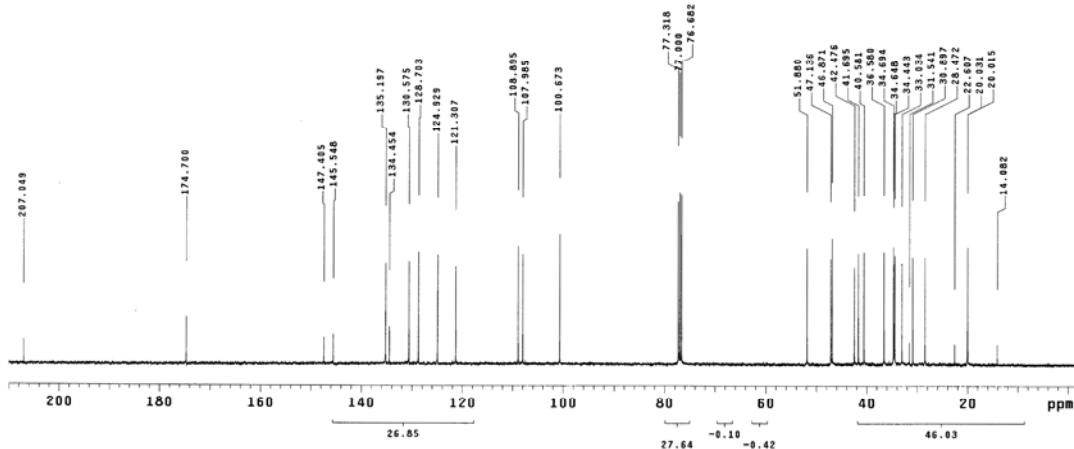
S14. NOESY spectrum of tsangibeilin B (2) in CDCl_3

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 Solvent: CDCl₃
 Ambient temperature
 Total 64 repetitions

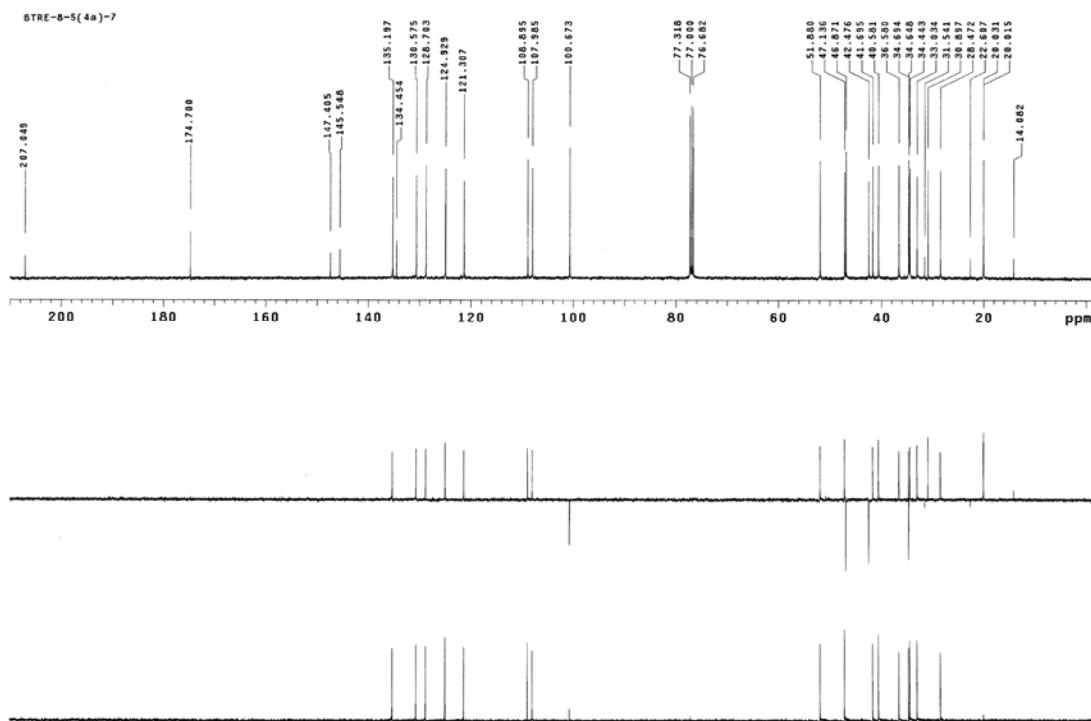


S15. ¹H NMR spectrum of endiandramide A (**3**) in CDCl₃ at 400 MHz

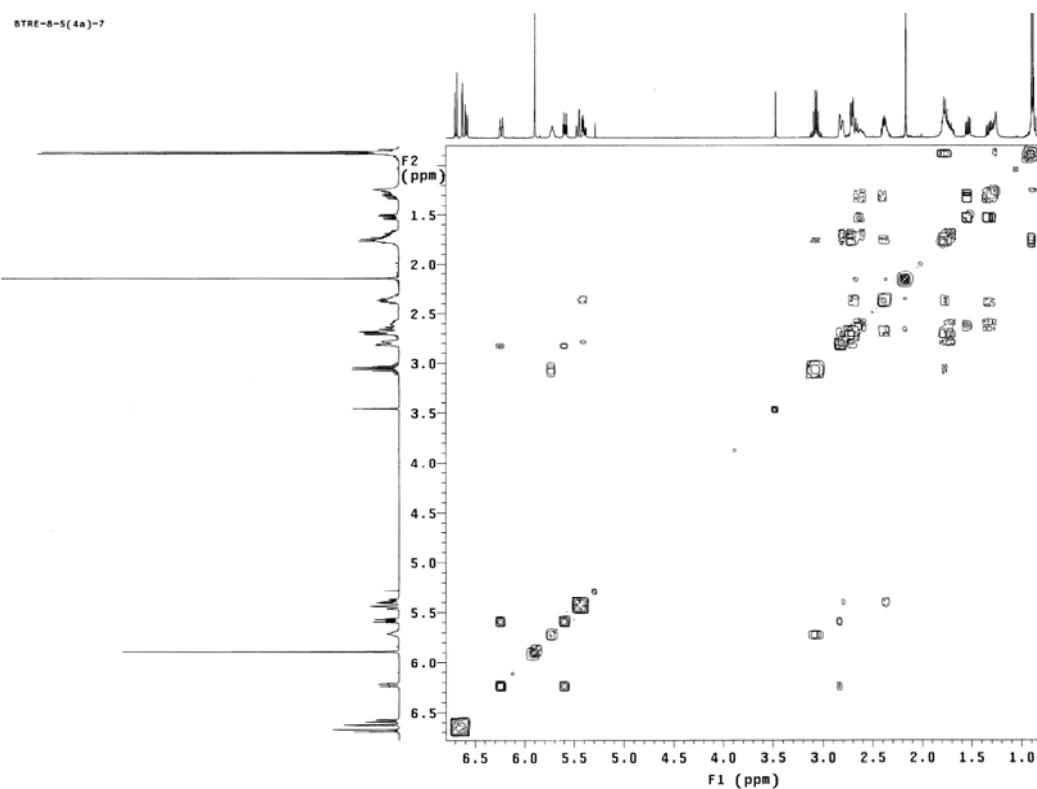
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 Mercury-400BB "Mercuryplus400"
 Date: Jan 28 2010
 Solvent: CDCl₃
 Ambient temperature
 Total 1600 repetitions



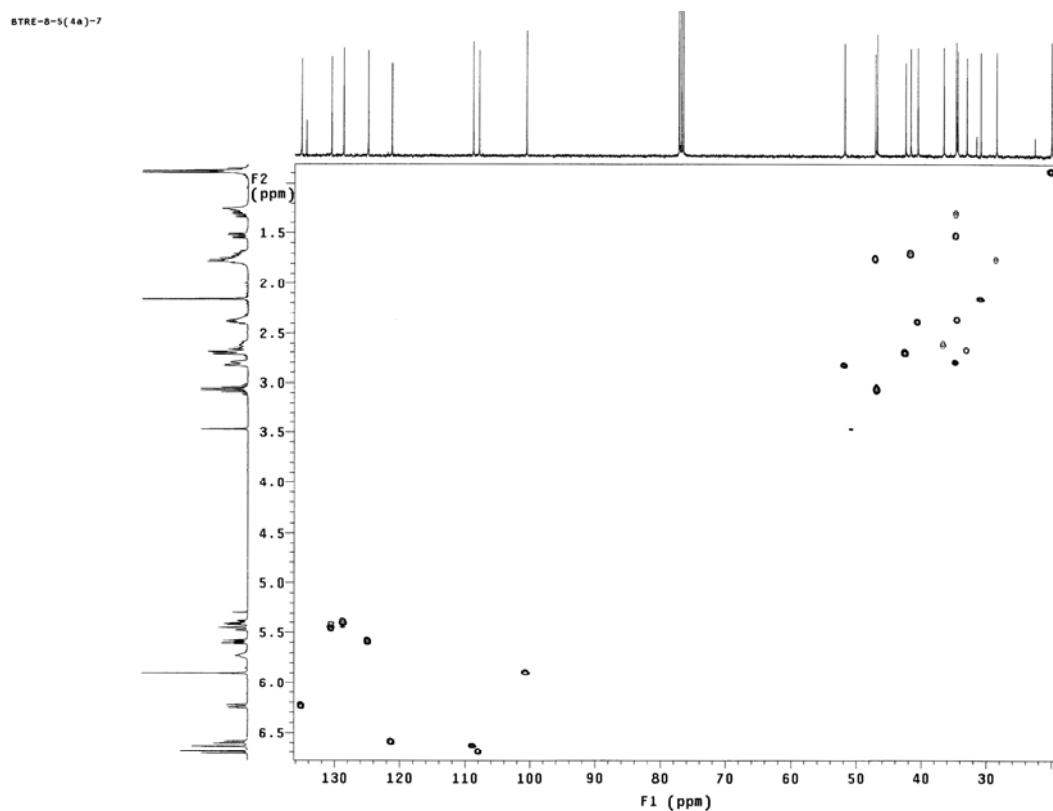
S16. ¹³C NMR spectrum of endiandramide A (**3**) in CDCl₃ at 100 MHz



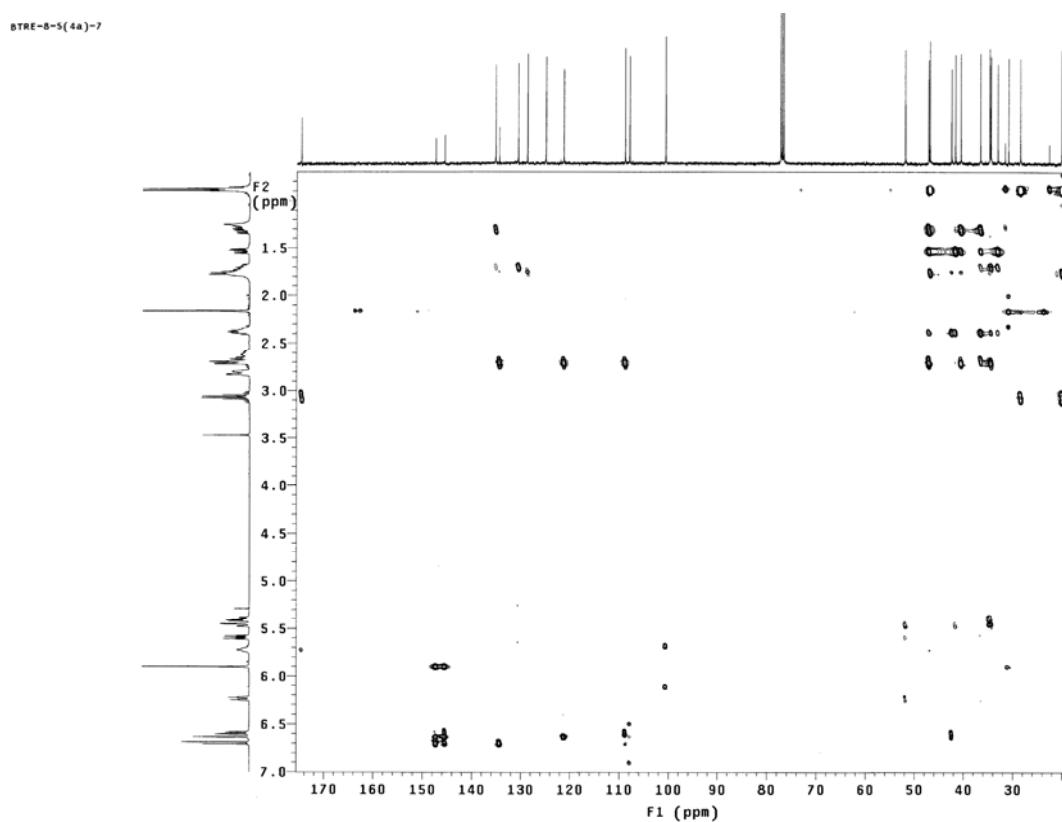
S17. DEPT spectrum of endiandramide A (**3**) in CDCl_3



S18. ^1H - ^1H COSY spectrum of endiandramide A (**3**) in CDCl_3

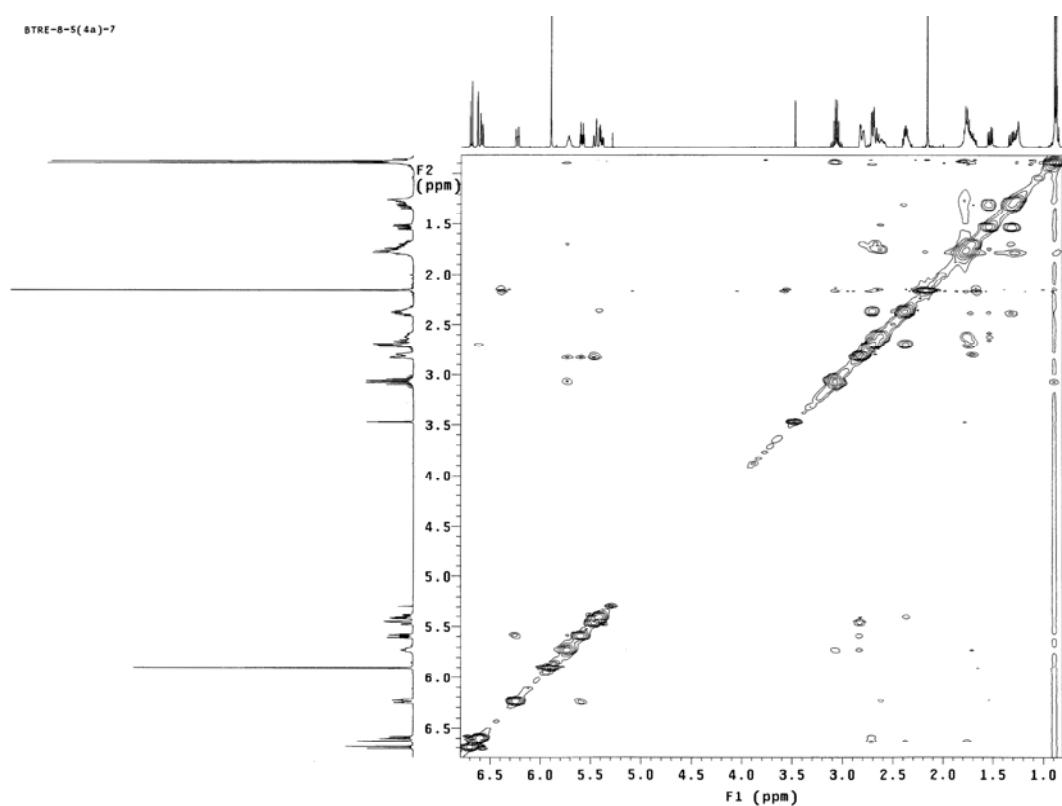


S19. HSQC spectrum of endiandramide A (3) in CDCl_3



S20. HMBC spectrum of endiandramide A (3) in CDCl_3

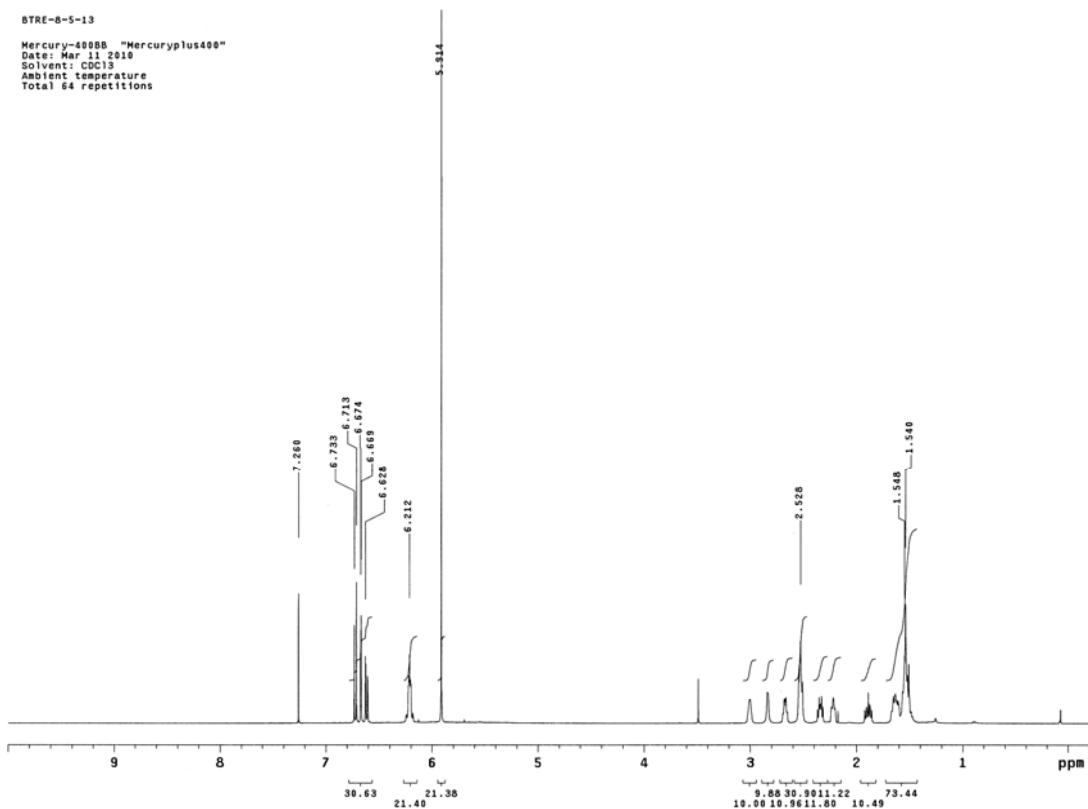
BTRE-8-5(4a)-7



S21. NOESY spectrum of endiandramide A (**3**) in CDCl_3

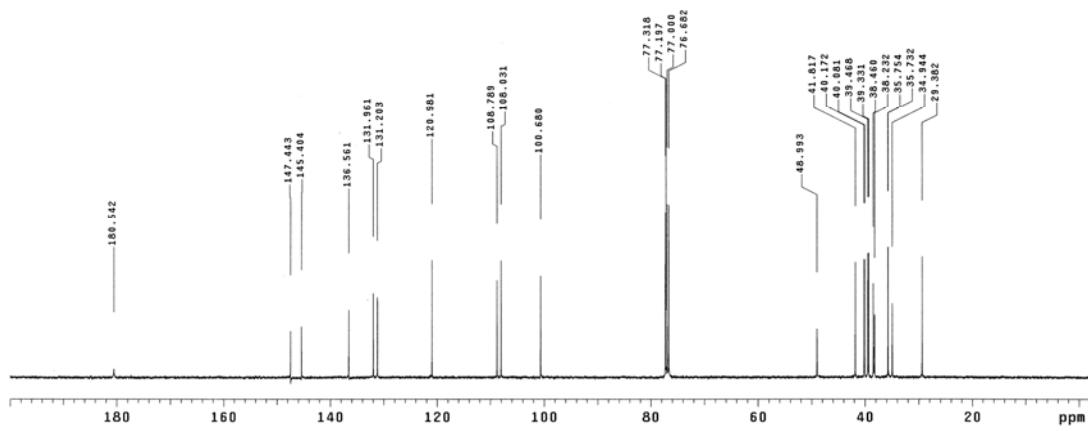
BTRE-8-5-13

Mercury-400BB "Mercuryplus400"
Date: Mar 11 2010
Solvent: CDCl_3
Ambient temperature
Total 64 repetitions

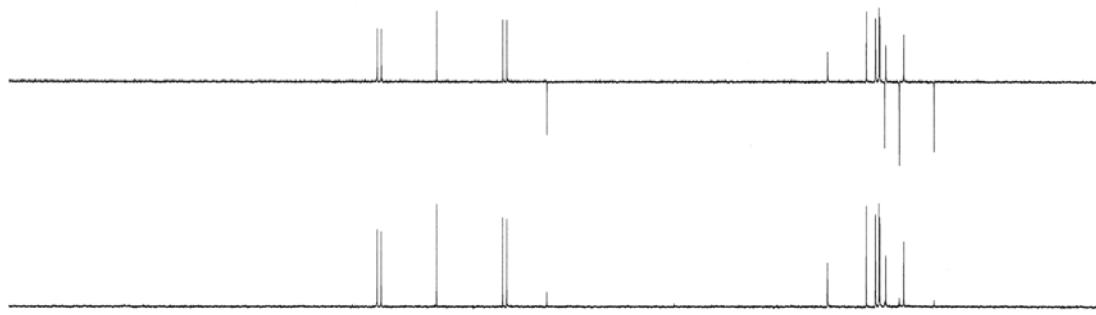
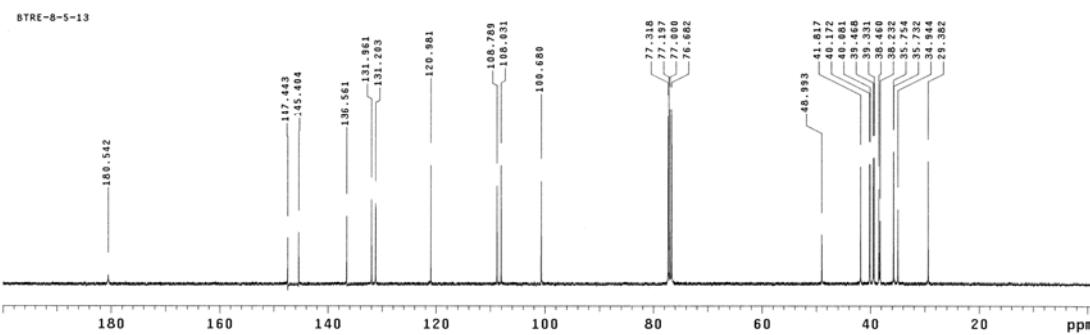


S22. ^1H NMR spectrum of endiandric acid K (**4**) in CDCl_3 at 400 MHz

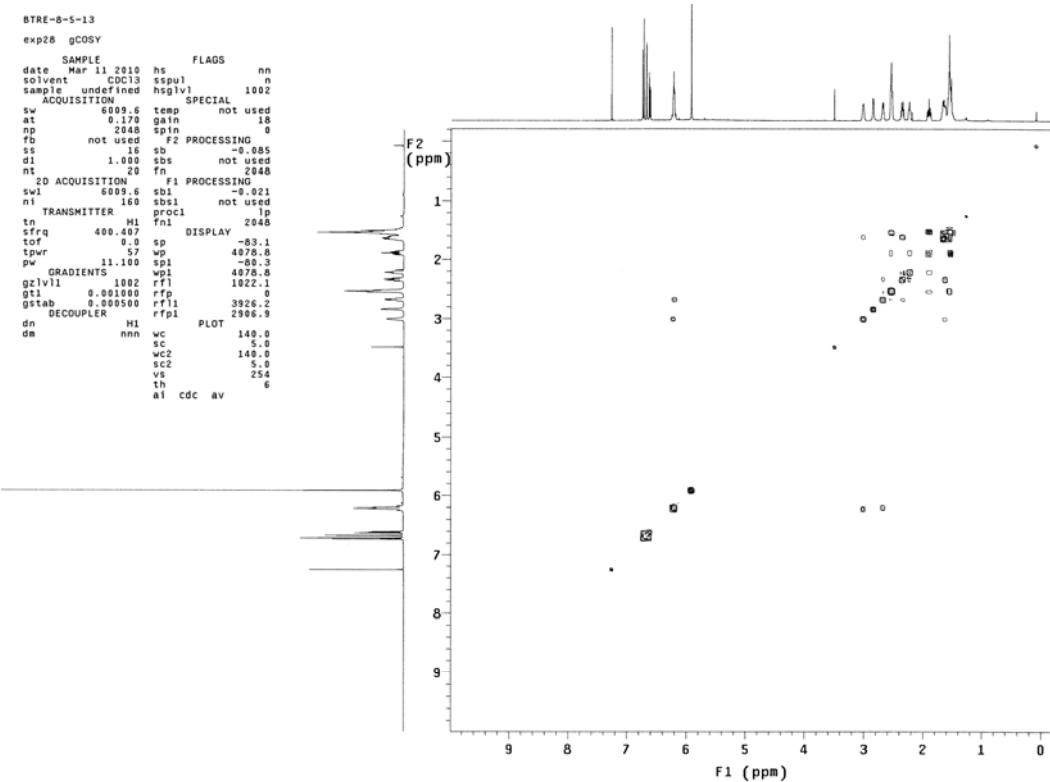
BTRE-8-5-13
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 Date: Mar 11 2010
 Solvent: CDCl₃
 Ambient temperature
 Total 3200 repetitions



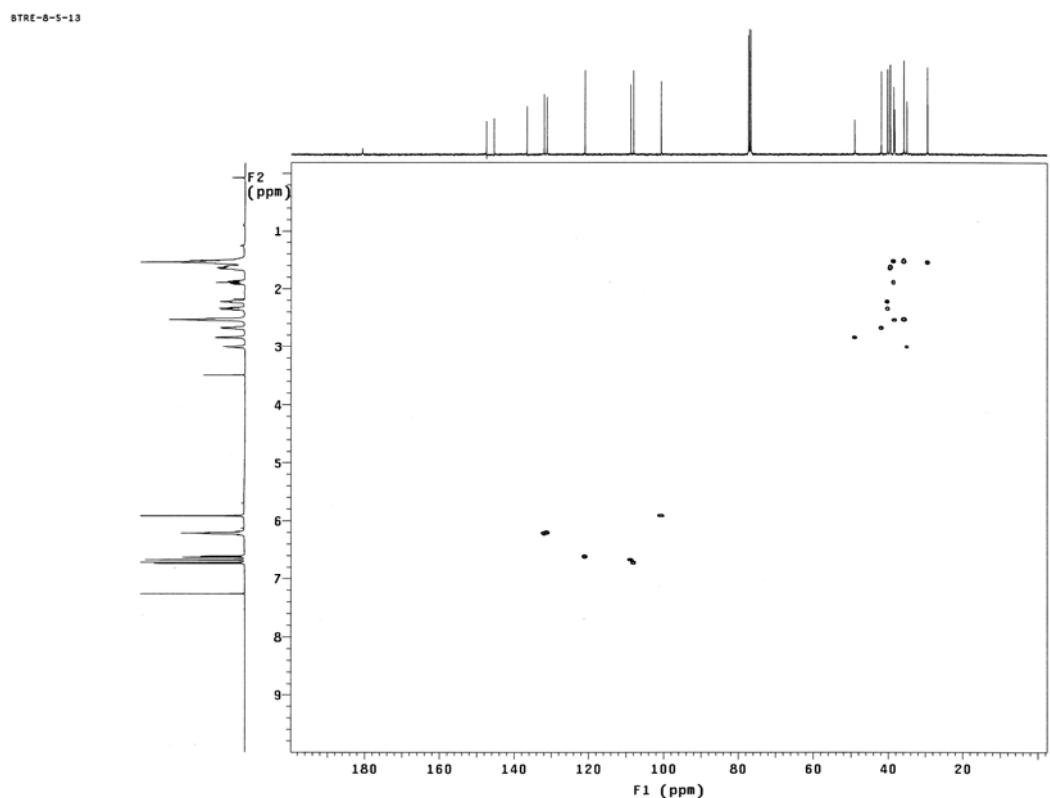
S23. ¹³C NMR spectrum of endiandric acid K (**4**) in CDCl₃ at 100 MHz



S24. DEPT spectrum of endiandric acid K (**4**) in CDCl₃

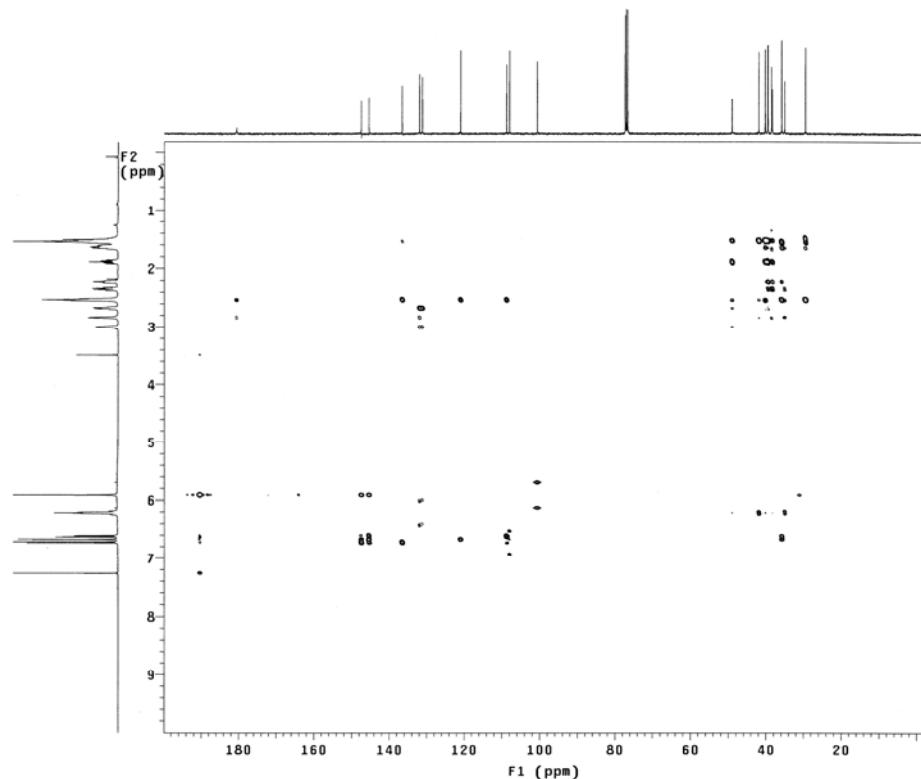


S25. ^1H - ^1H COSY spectrum of endiandric acid K (**4**) in CDCl_3



S26. HSQC spectrum of endiandric acid K (**4**) in CDCl_3

BTRE-8-5-13

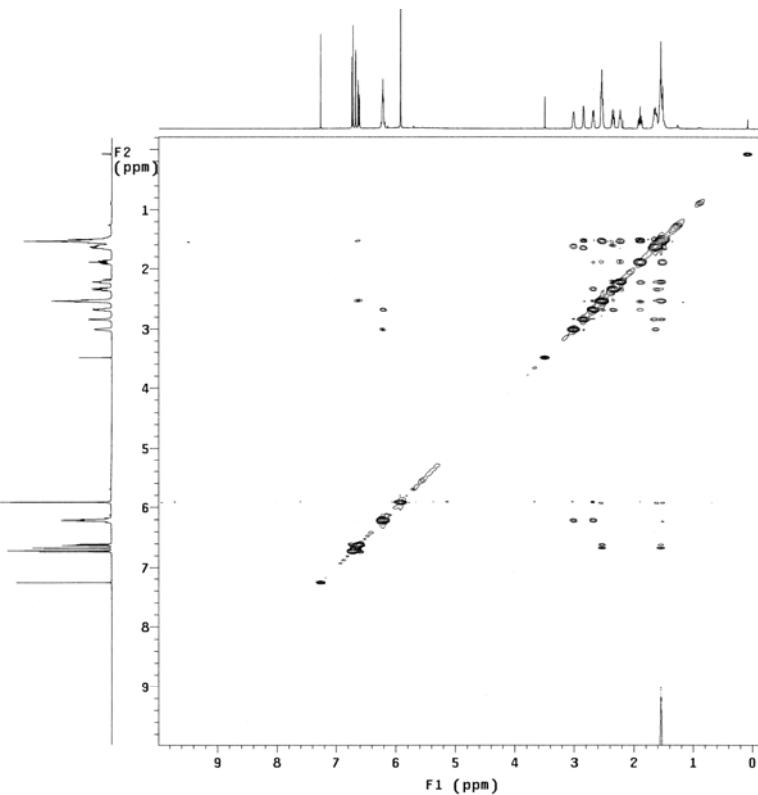


S27. HMBC spectrum of endiandric acid K (4) in CDCl_3

BTRE-8-5-13

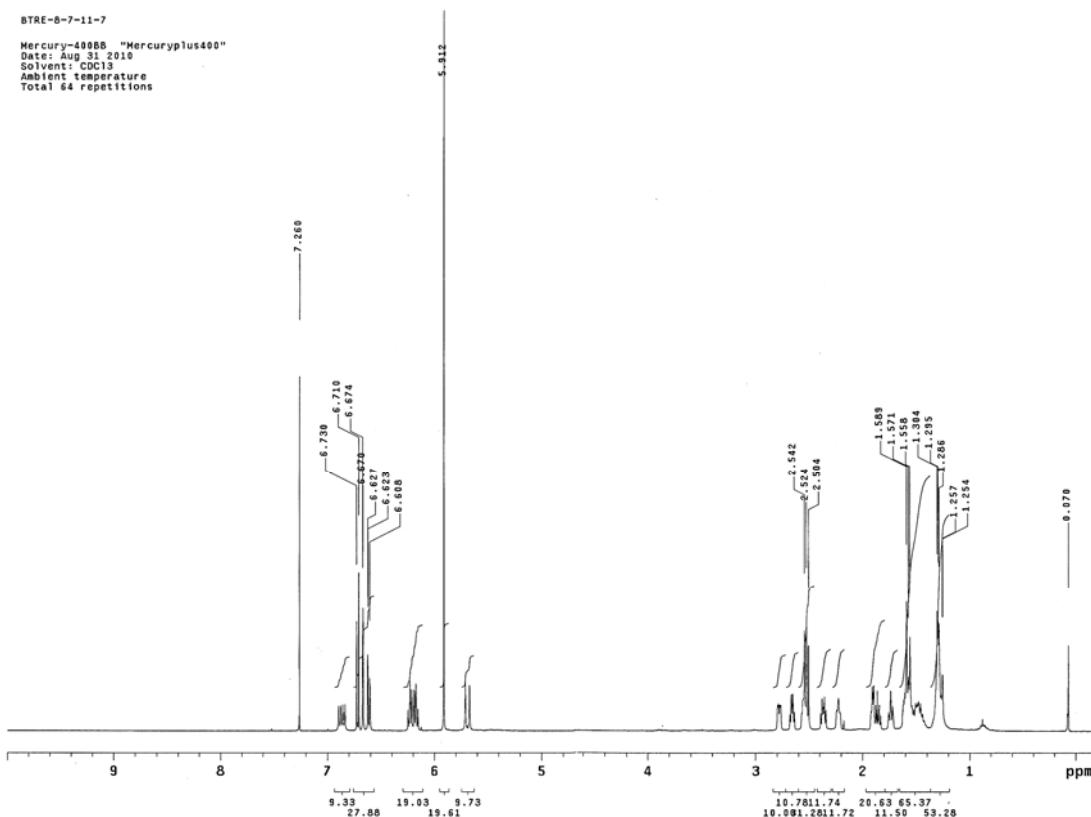
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sample undefined PGF1q   y
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np      2048 gain      18
fb      not used spin    0
ss      32 F2 PROCESSING
d1      1.009 g1      0.079
nt      16 tms      not used
t0f     0.0
td      1.32 sp      DISPLAY -83.2
sw1     6009.6          F1 PROCESSING
ni      160 g1      0.020
tn      TRANSMITTER g1      not used
tn      H1 proc1      1p
sfrq   400.407 f1      2048
tof    0.0
tpwr   0.0
p1     11.100 wp      4078.8
      NOESY   sp1      -80.2
mix    0.600 wpt1      4078.8
      PRESATURATION r11      102.1
satmode nnnn rfp1      0
satpwr 0 rfp1      3926.2
satity 0 rfp1      2906.9
satfrq 0          PLOT
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      at      tdc ph
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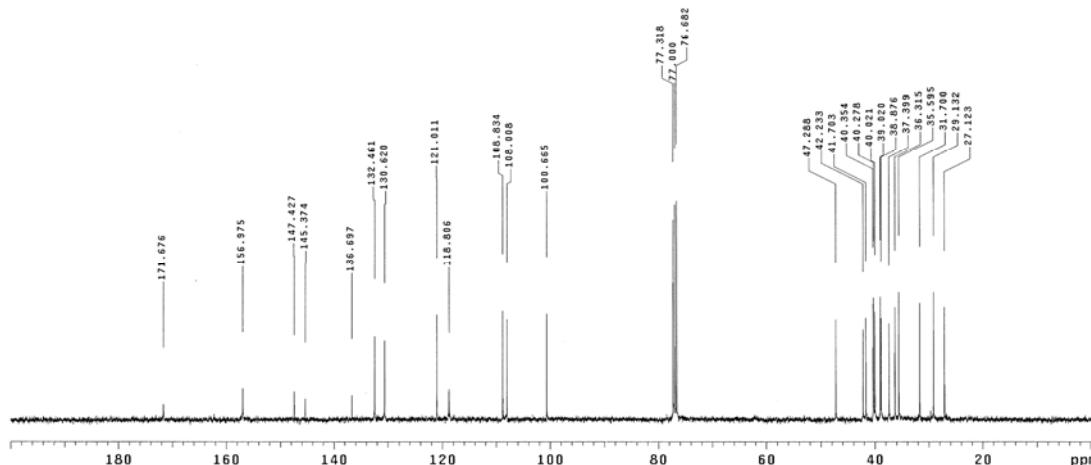
S28. NOESY spectrum of endiandric acid K (4) in CDCl_3

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Date: Aug 31 2010
Solvent: CDCl3
Ambient temperature
Total 64 repetitions

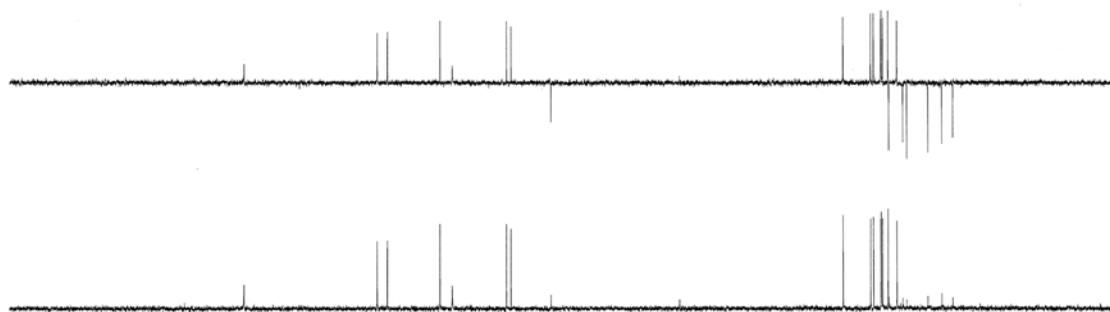
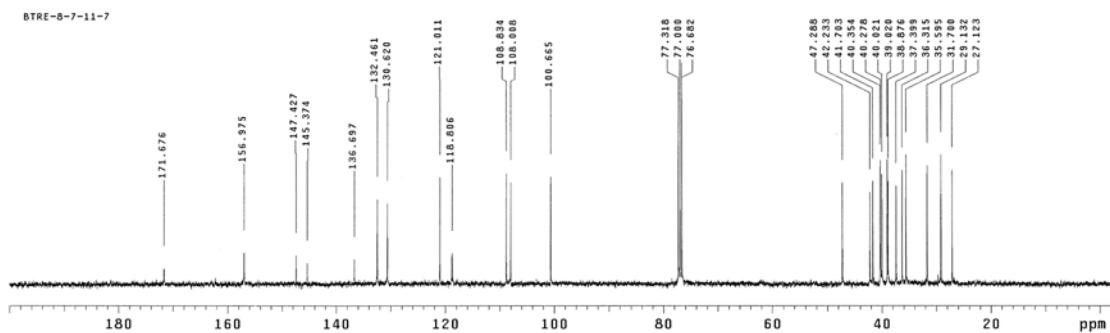


S29. ^1H NMR spectrum of endiandric acid L (**5**) in CDCl_3 at 400 MHz

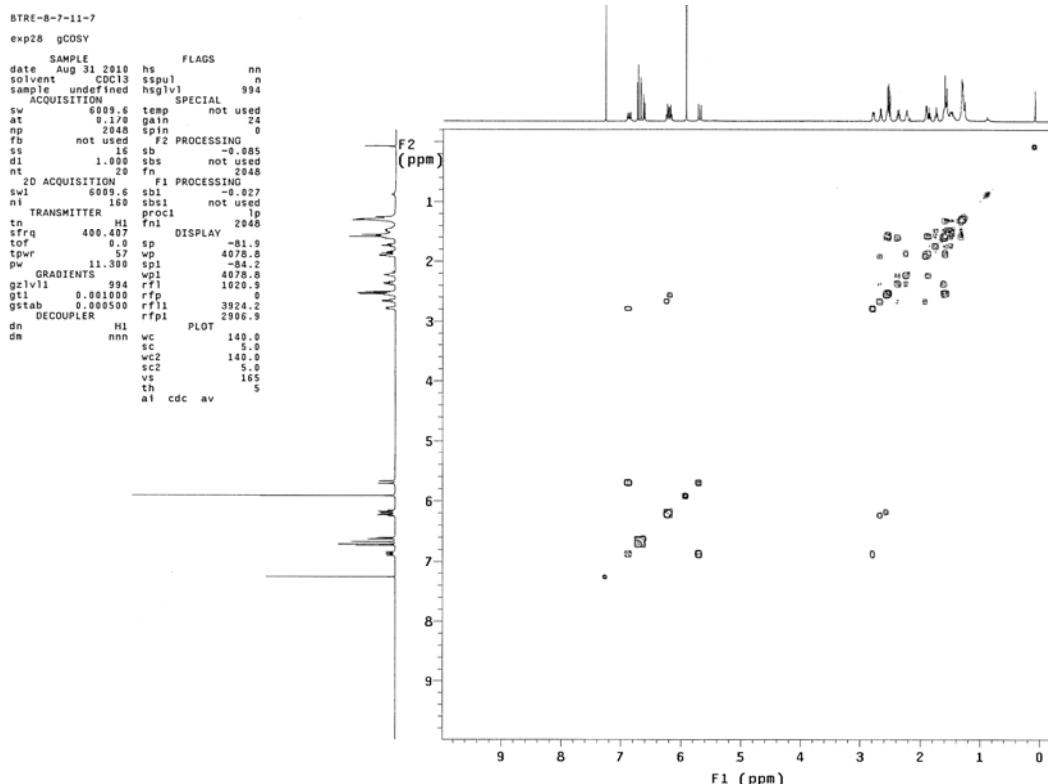
BTRE-8-7-11-7
Mercury-400BB "Mercuryplus400"
Date: Aug 31 2010
Solvent: CDC13
Ambient temperature
Total 4000 repetitions



S30. ^{13}C NMR spectrum of endiandric acid L (**5**) in CDCl_3 at 100 MHz

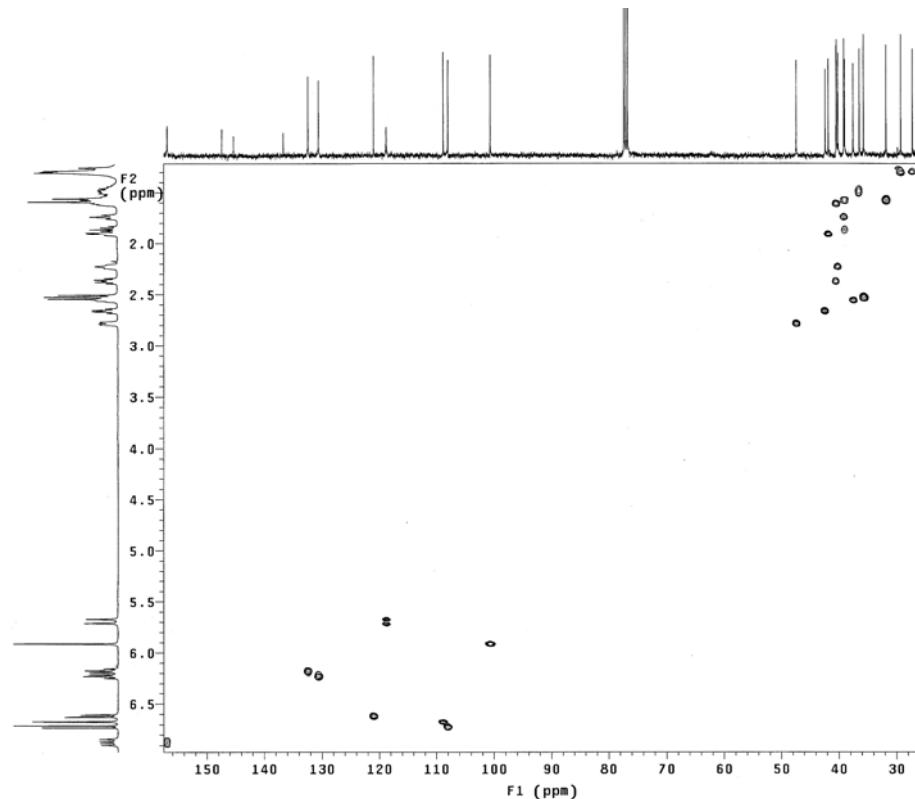


S31. DEPT spectrum of endiandric acid L (5) in CDCl_3



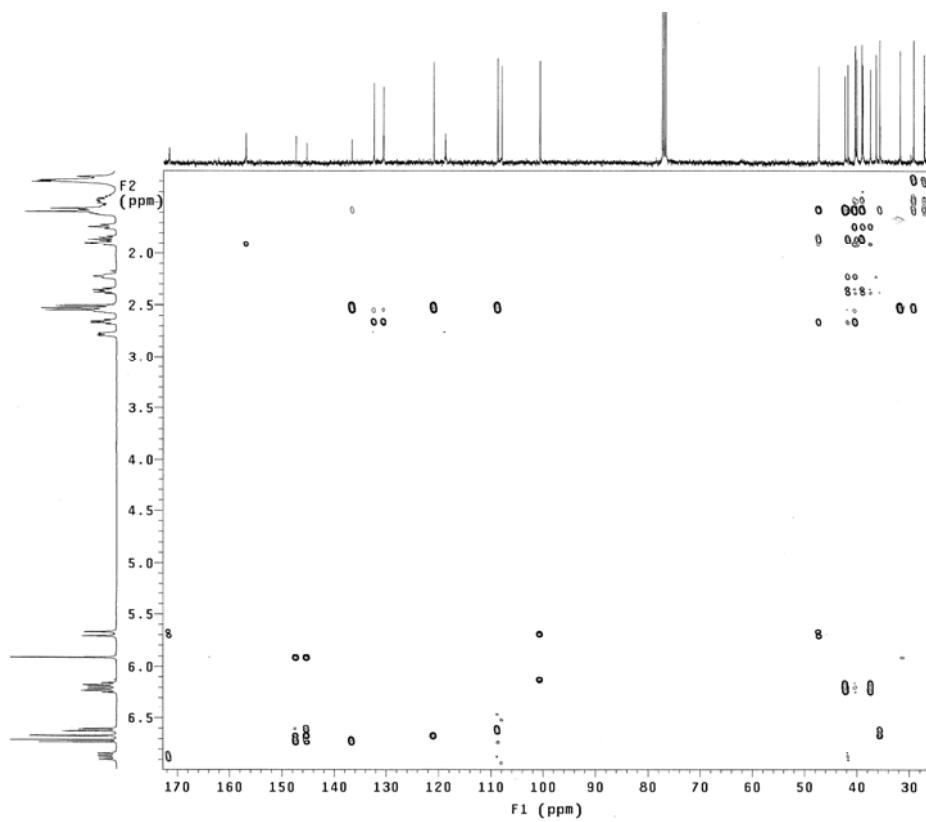
S32. ^1H - ^1H COSY spectrum of endiandric acid L (5) in CDCl_3

BTRE-6-7-11-7

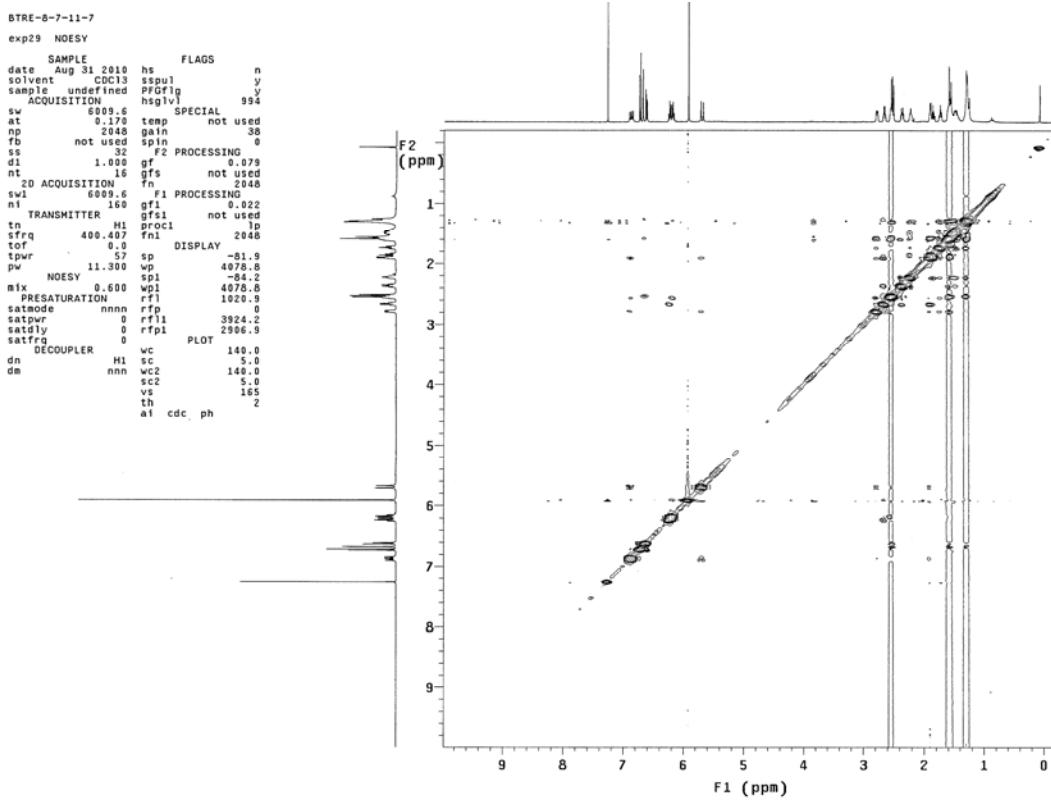


S33. HSQC spectrum of endiandric acid L (**5**) in CDCl_3

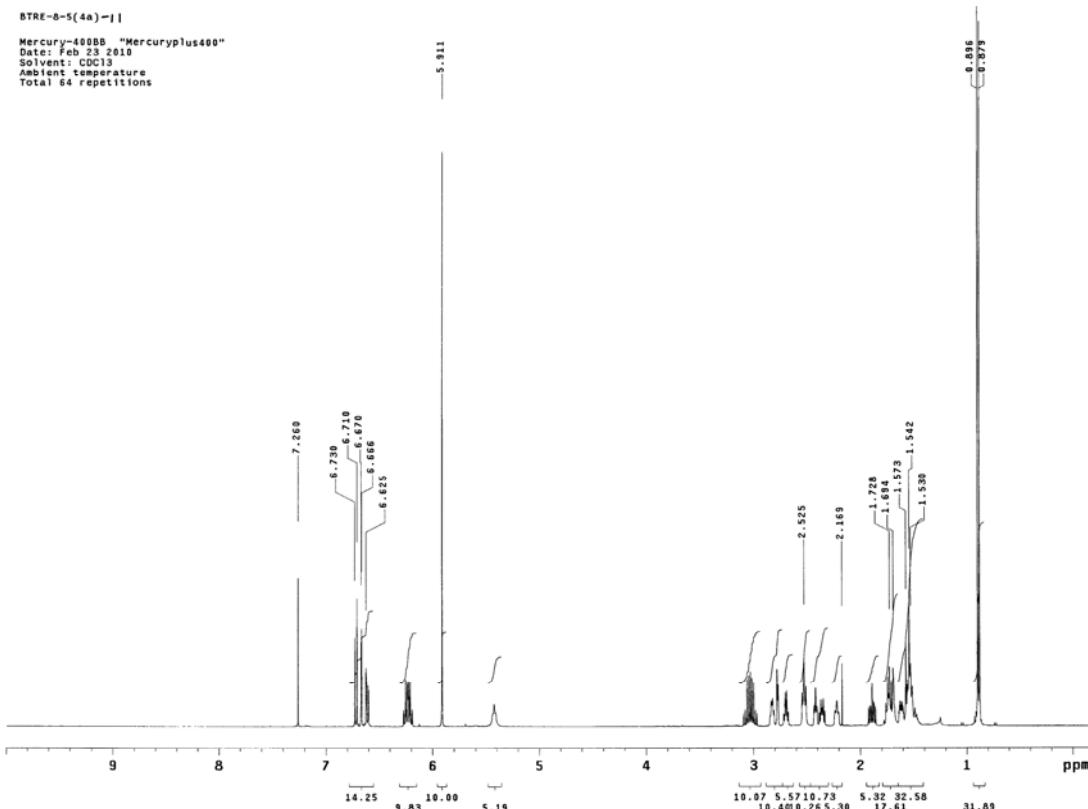
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S34. HMBC spectrum of endiandric acid L (**5**) in CDCl_3

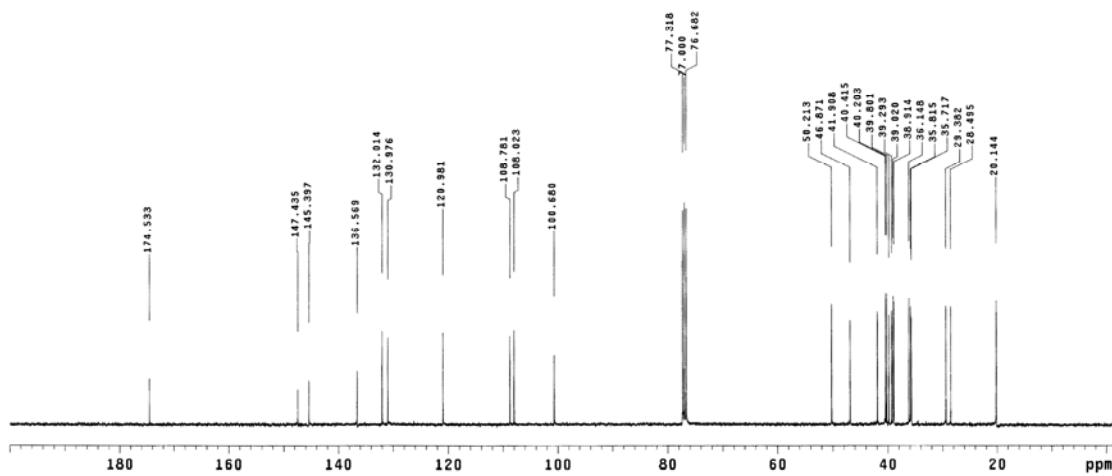


S35. NOESY spectrum of endiandric acid L (5) in CDCl_3



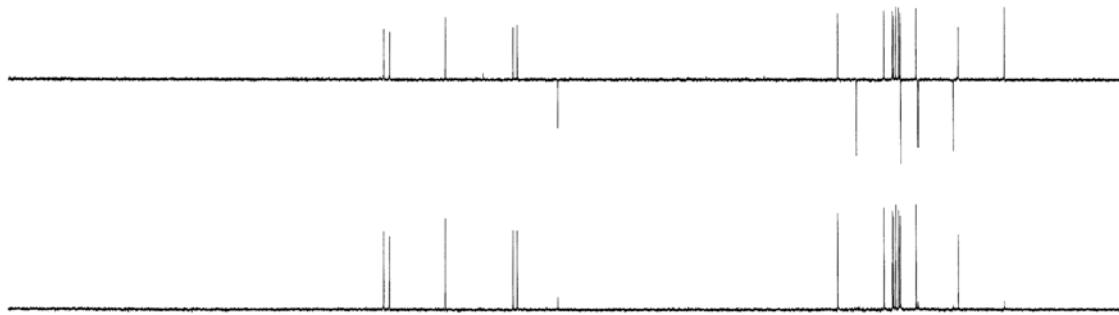
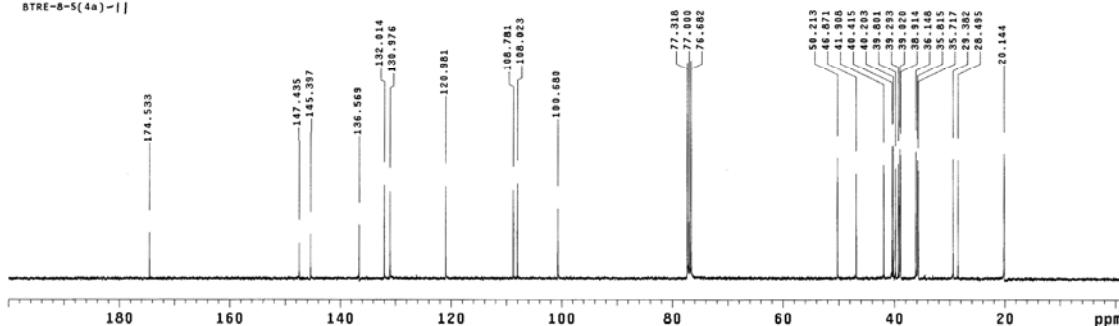
S36. ^1H NMR spectrum of endiandramide B (6) in CDCl_3 at 400 MHz

BTRE-8-5(4a)-1 |
 Mercury-400BB "Mercuryplus400"
 Date: Feb 23 2010
 Solvent: CDCl₃
 Ambient temperature
 Total 3200 repetitions

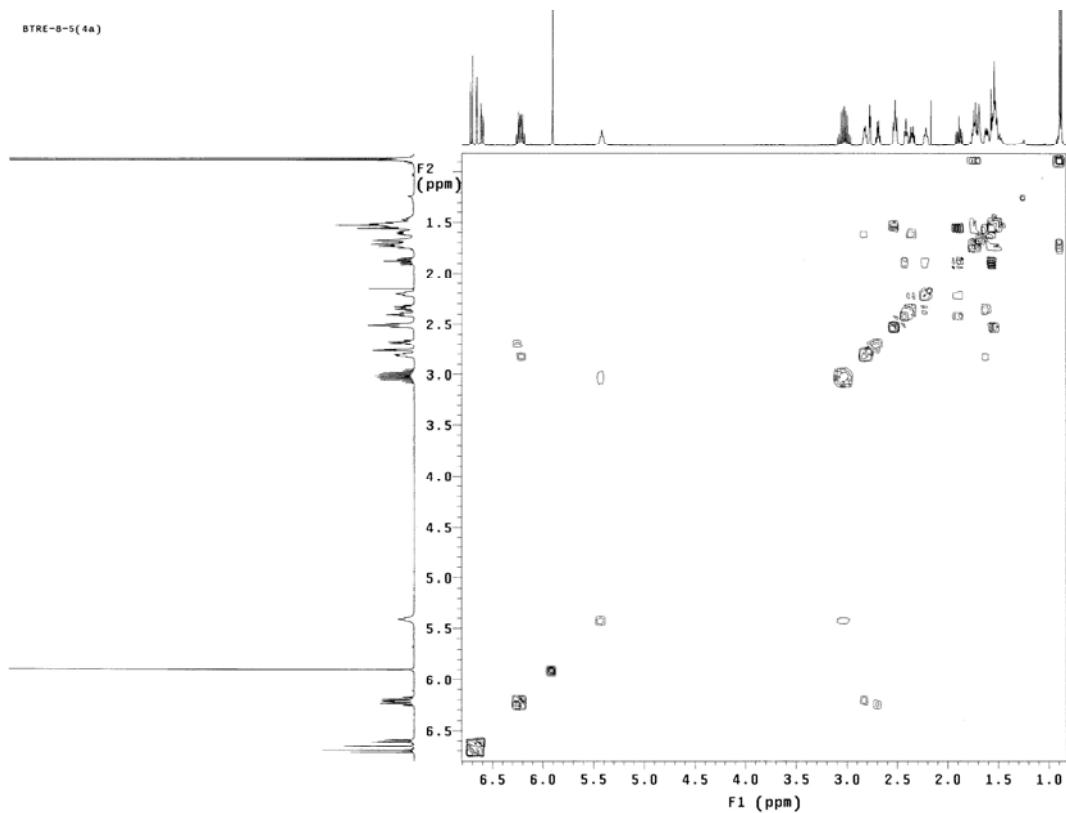


S37. ¹³C NMR spectrum of endiandramide B (6) in CDCl₃ at 100 MHz

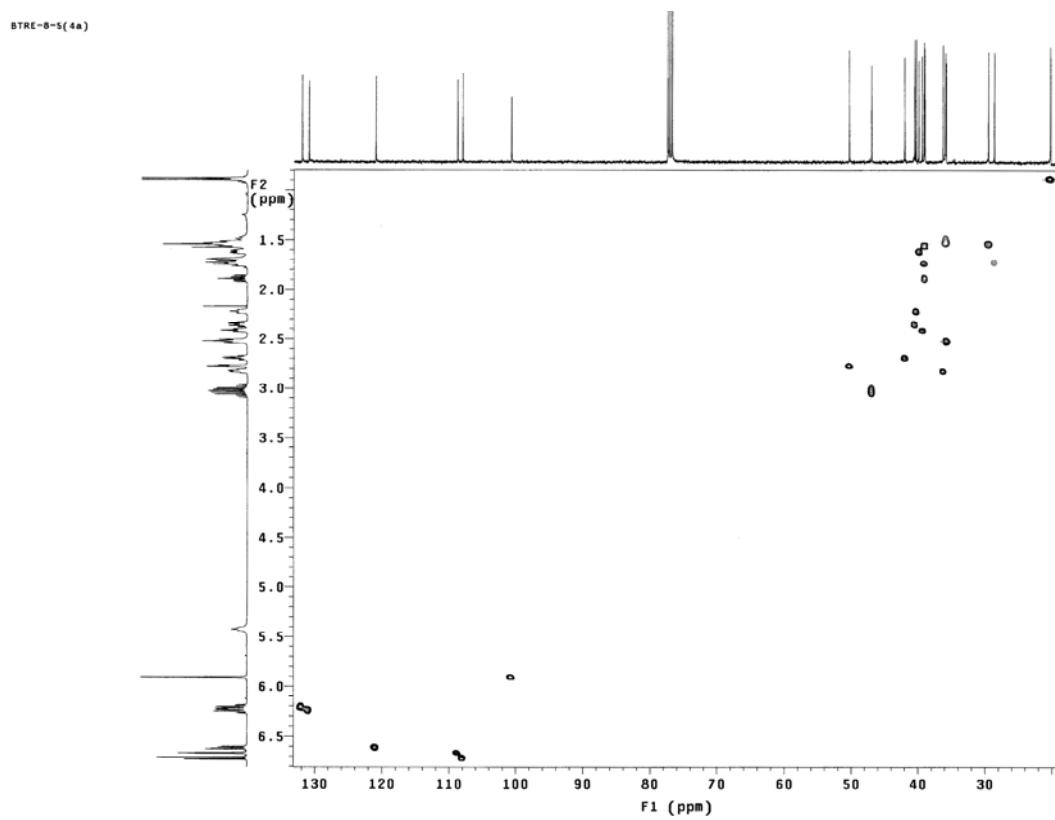
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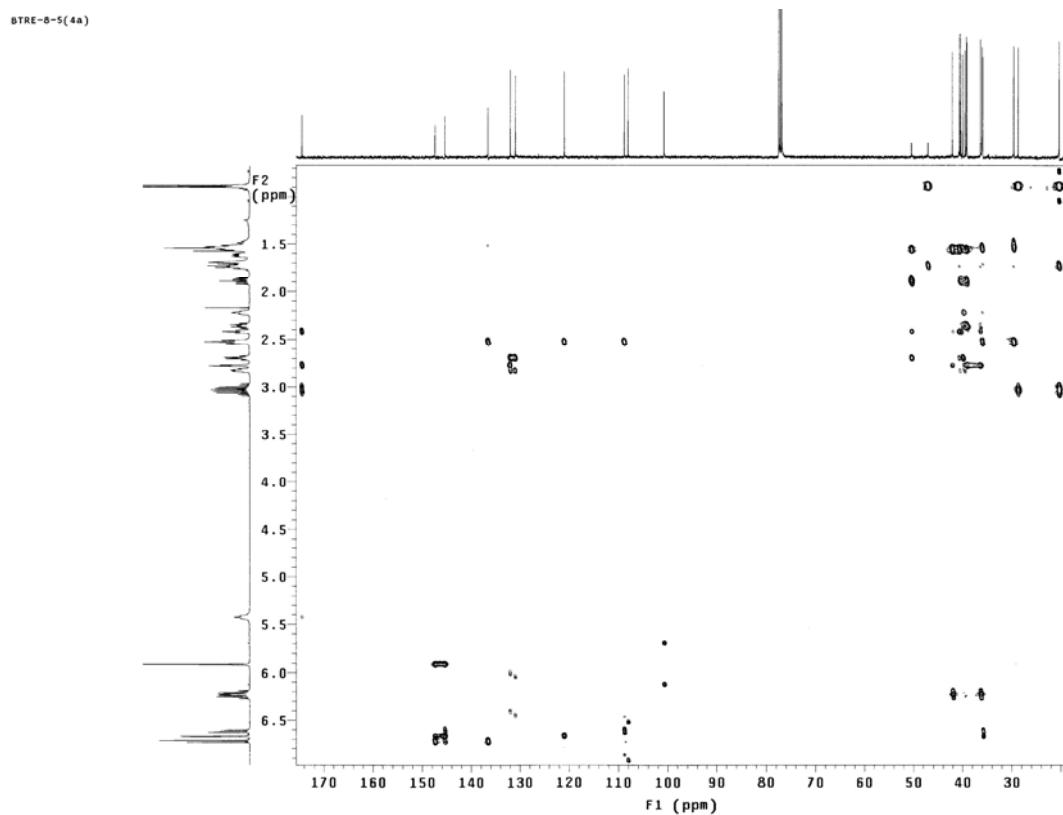
S38. DEPT spectrum of endiandramide B (6) in CDCl₃



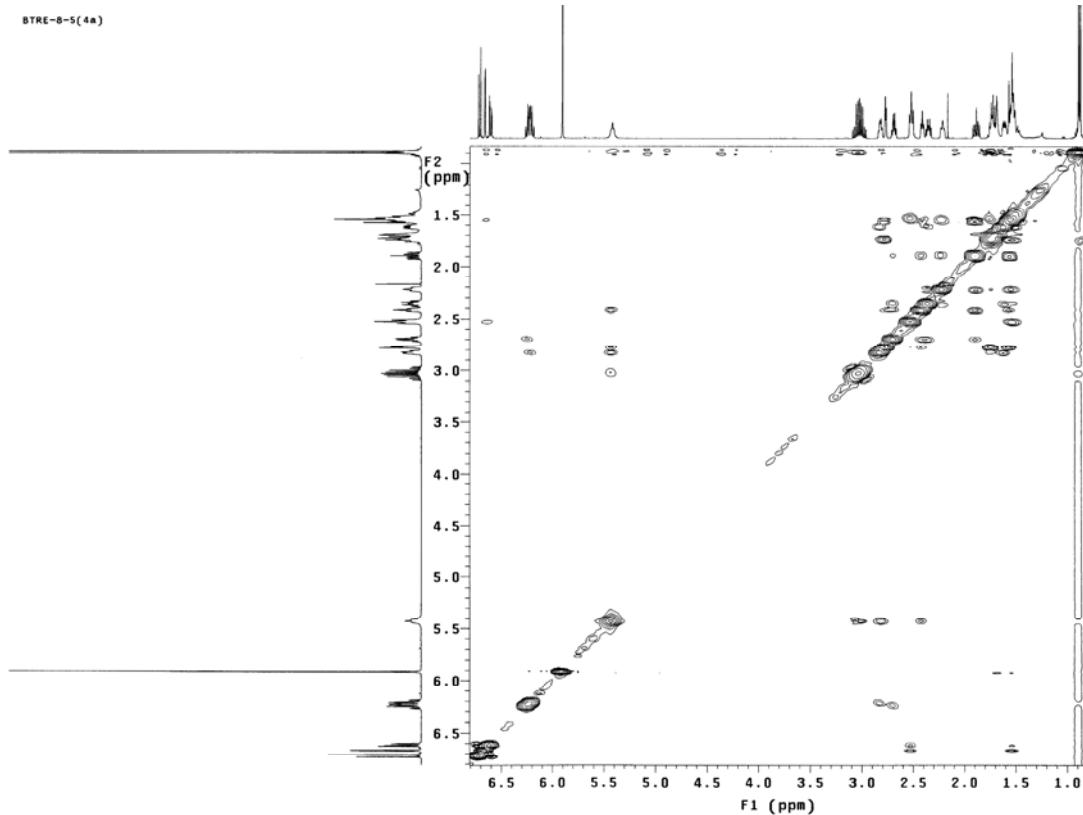
S39. ^1H - ^1H COSY spectrum of endiandramide B (**6**) in CDCl_3



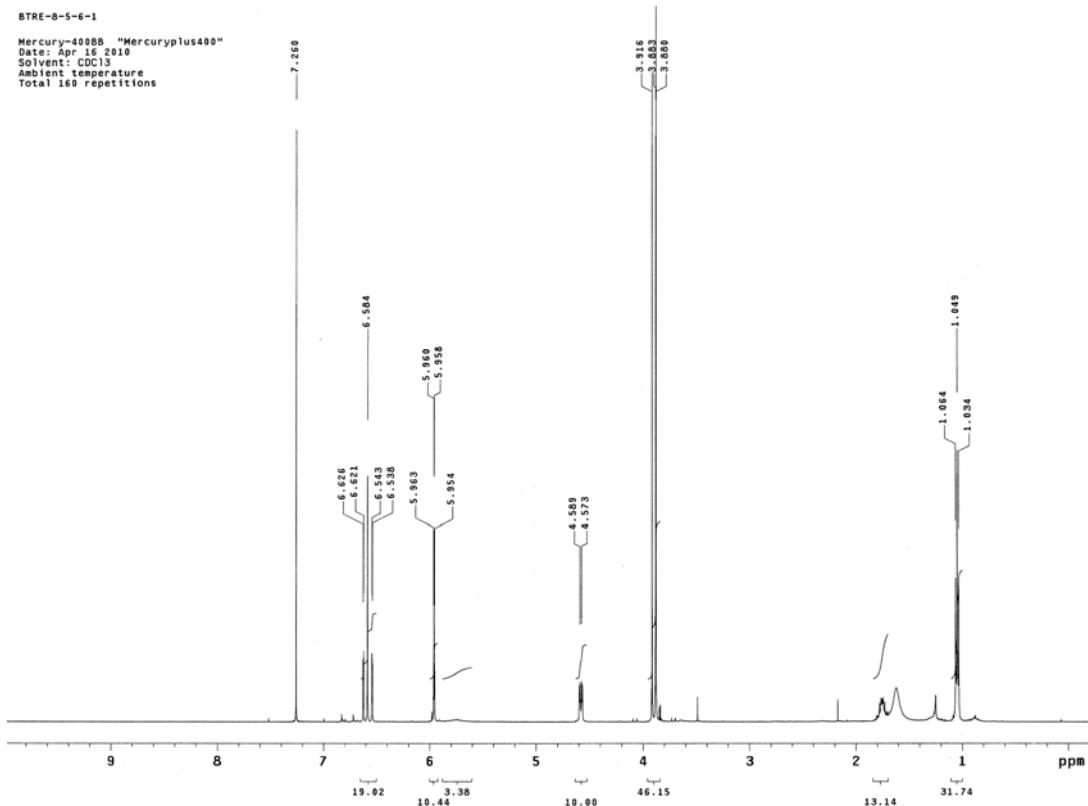
S40. HSQC spectrum of endiandramide B (**6**) in CDCl_3



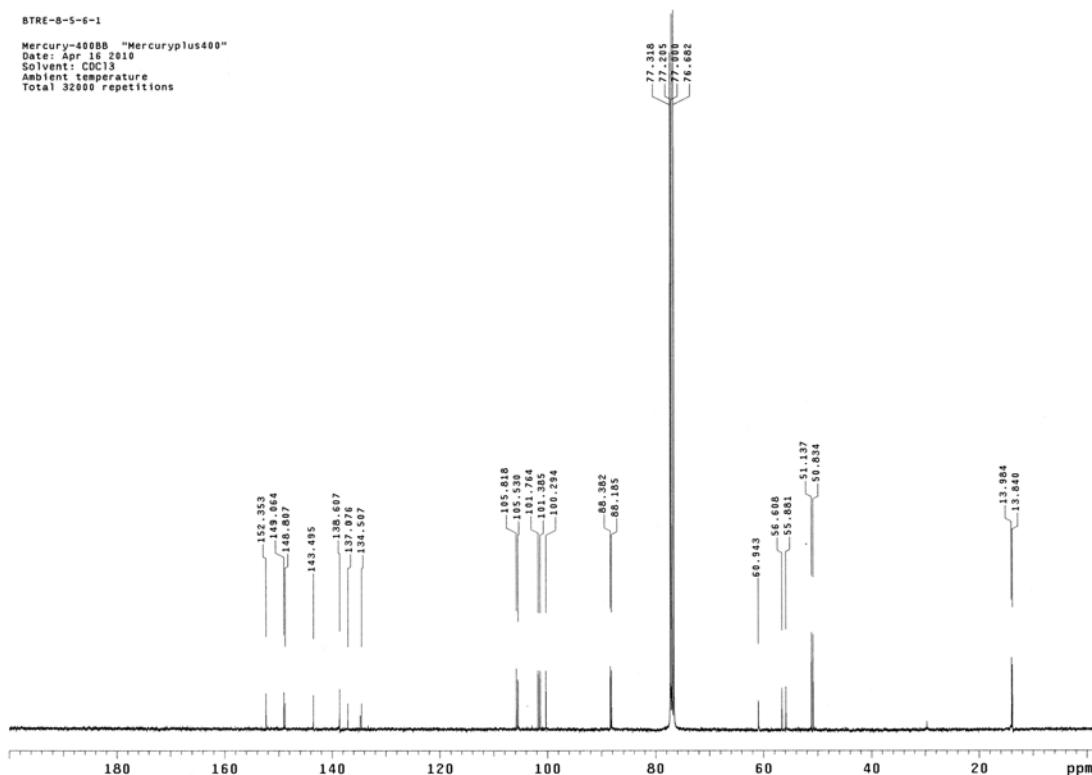
S41. HMBC spectrum of endiandramide B (**6**) in CDCl_3



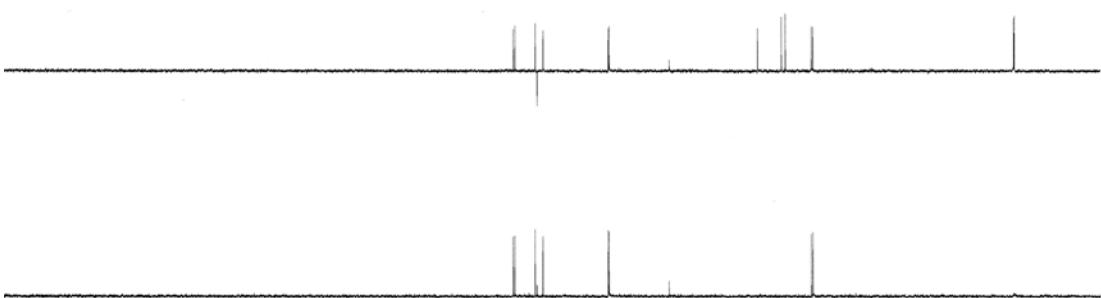
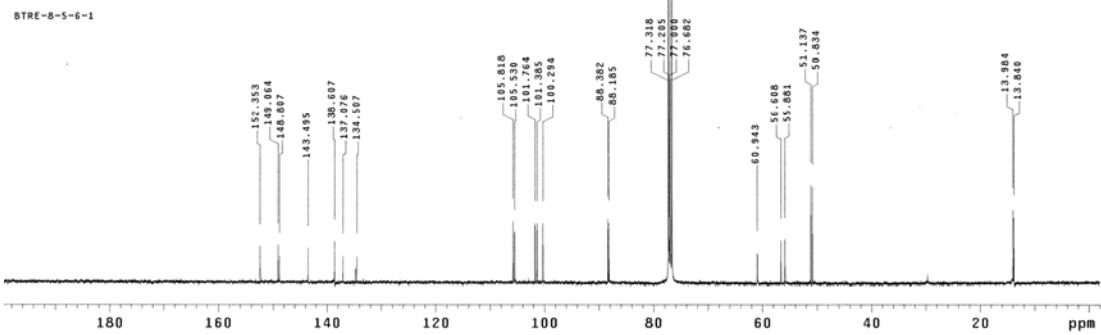
S42. NOESY spectrum of endiandramide B (**6**) in CDCl_3



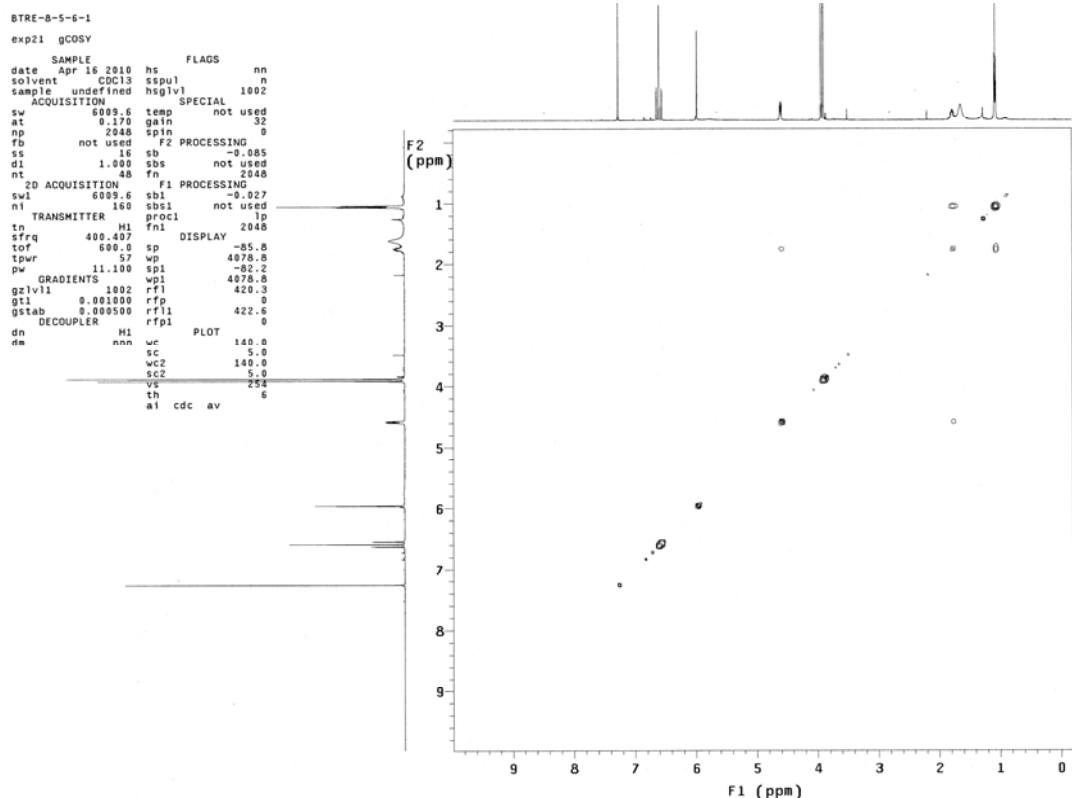
S43. ^1H NMR spectrum of beilschminol A (**7**) in CDCl_3 at 400 MHz



S44. ^{13}C NMR spectrum of beilschminol A (**7**) in CDCl_3 at 100 MHz

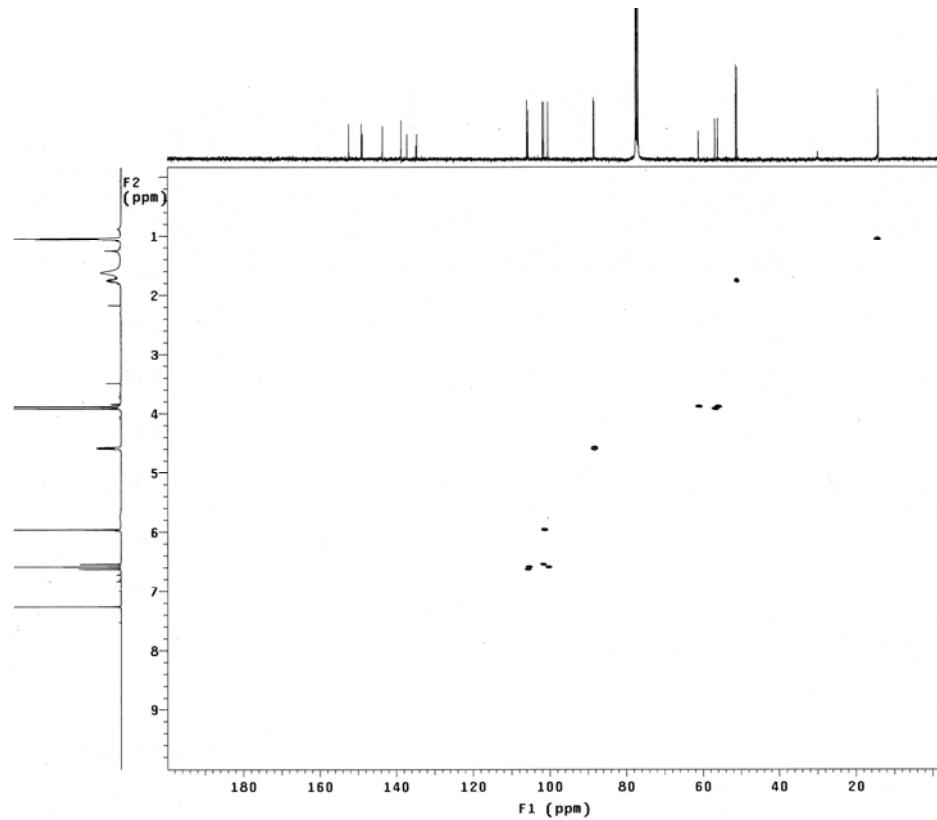


S45. DEPT spectrum of beilschminol A (**7**) in CDCl_3



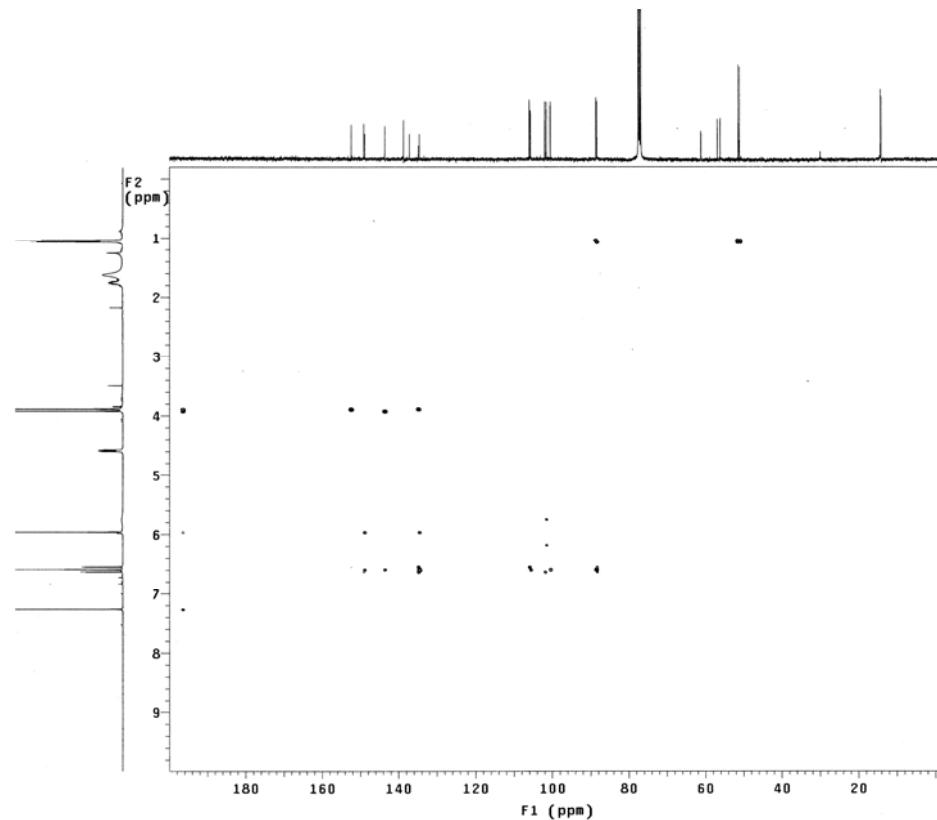
S46. ^1H - ^1H COSY spectrum of beilschminol A (**7**) in CDCl_3

BTRE-8-5-6-1

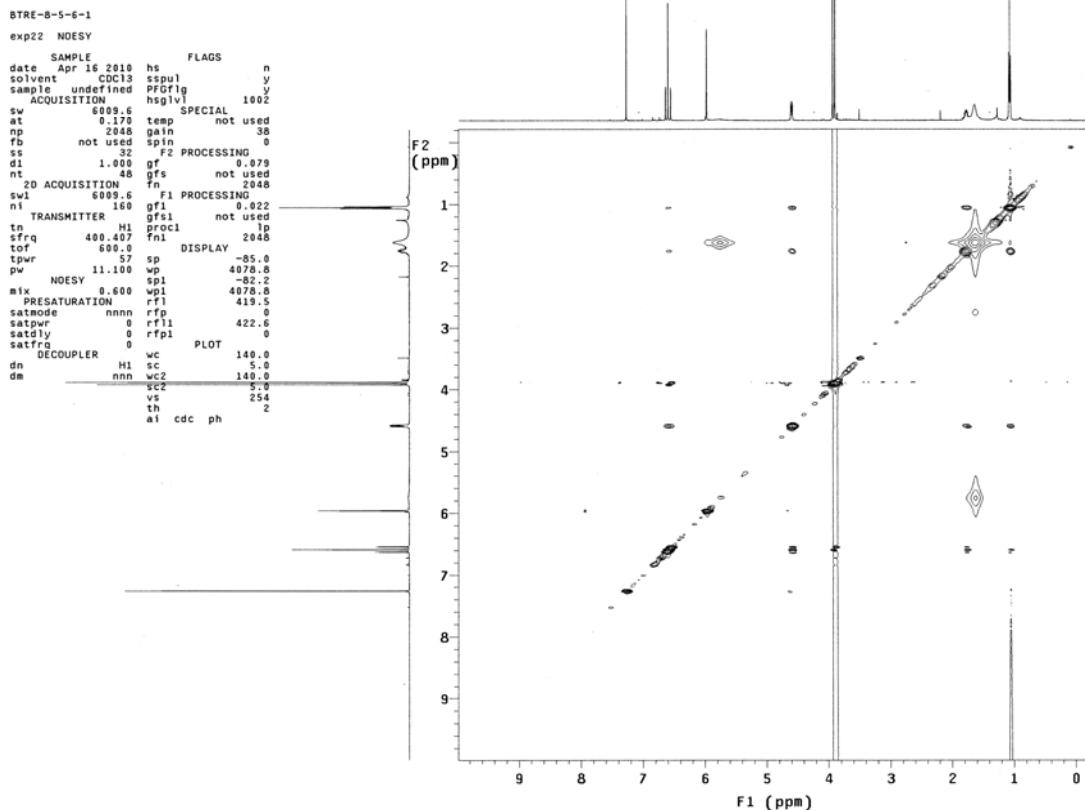


S47. HSQC spectrum of beilschminol A (**7**) in CDCl_3

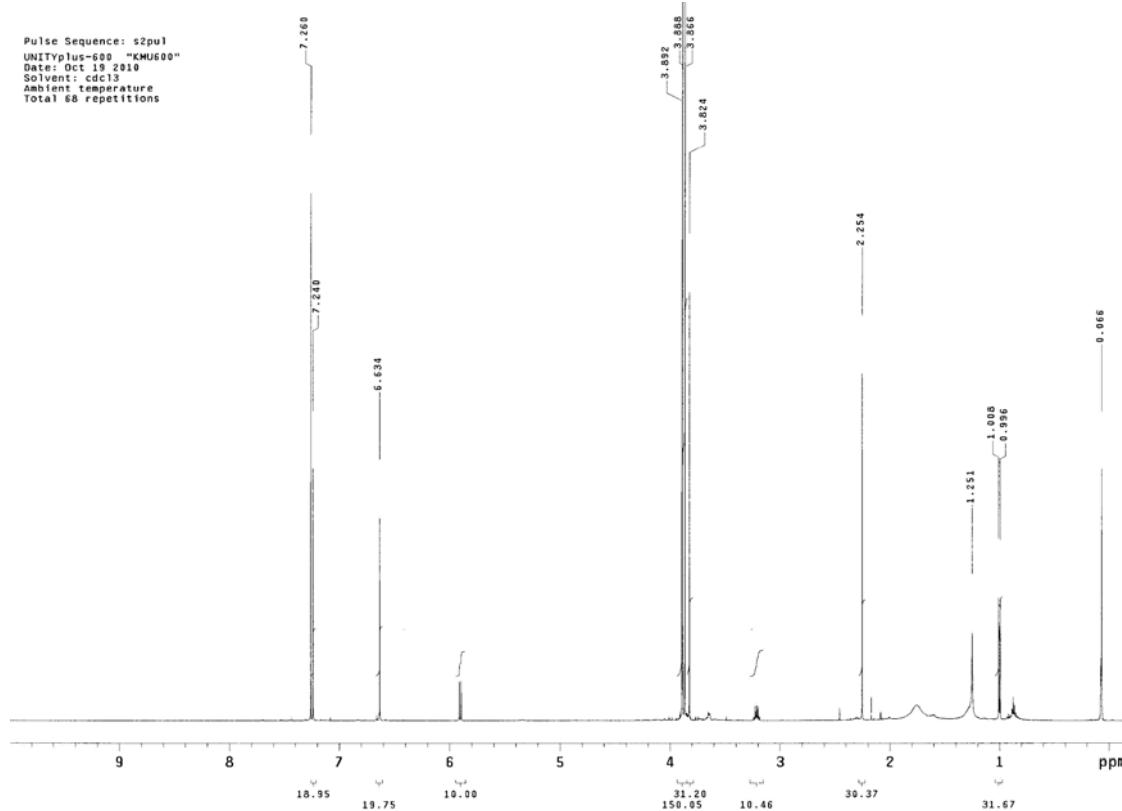
BTRE-8-5-6-1



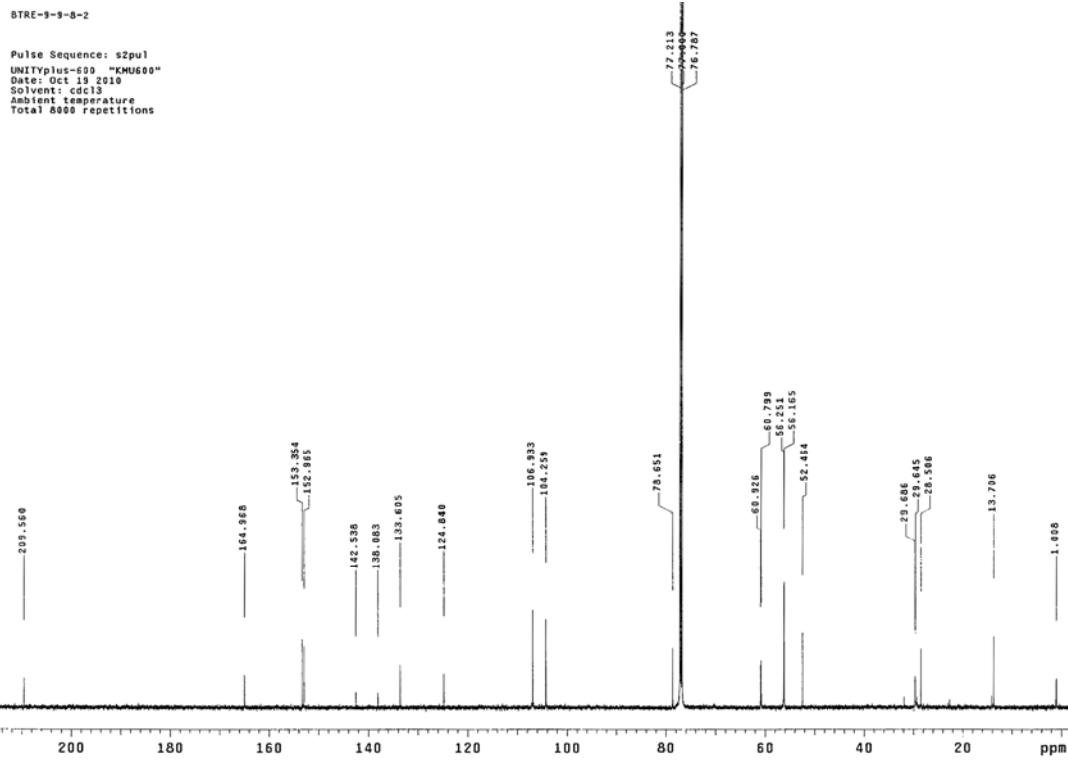
S48. HMBC spectrum of beilschminol A (**7**) in CDCl_3



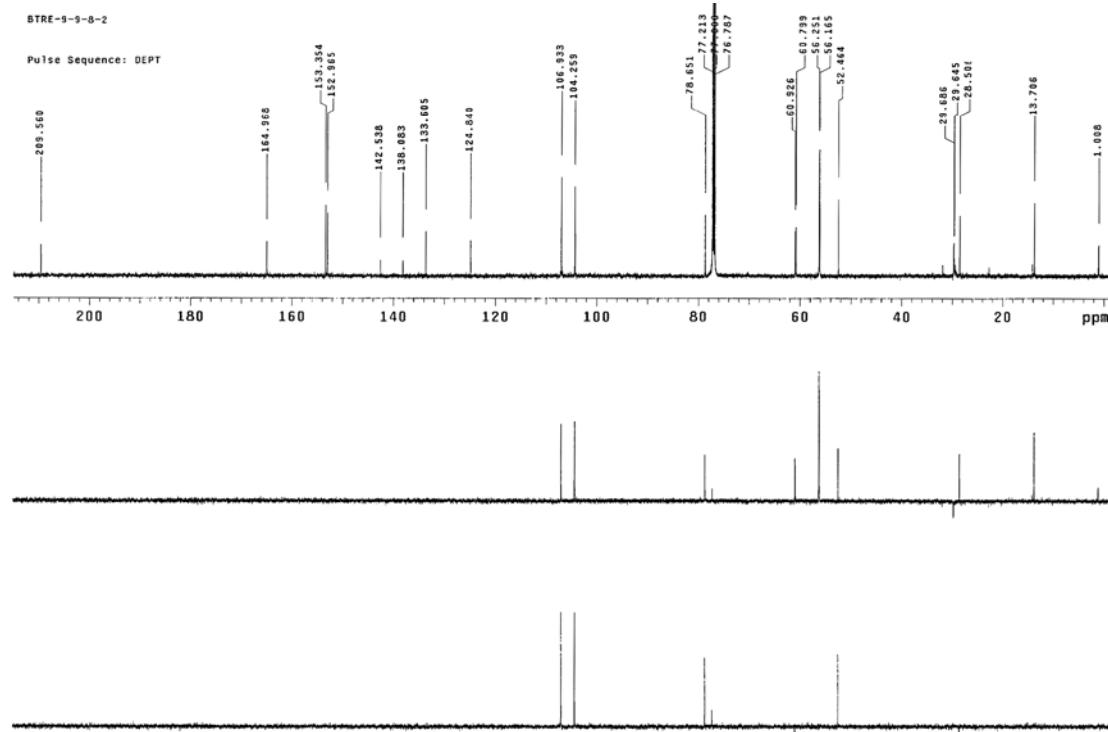
S49. NOESY spectrum of beilschminol A (7) in CDCl_3



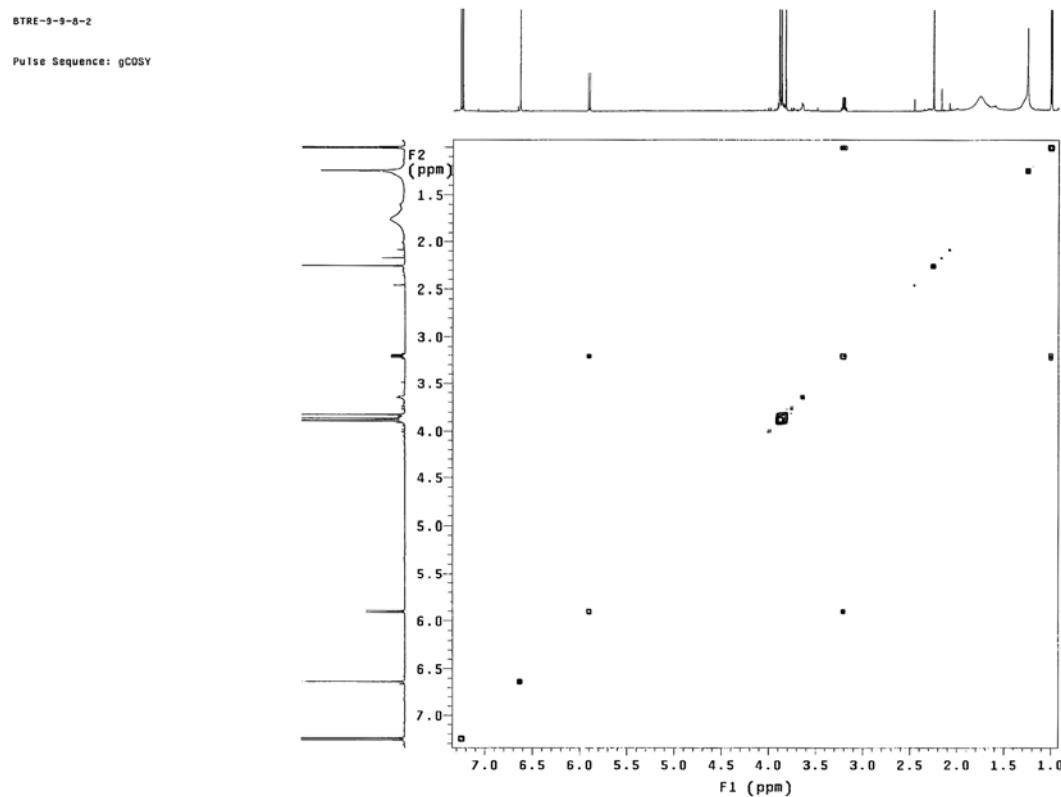
S50. ^1H NMR spectrum of tsangin C (8) in CDCl_3 at 600 MHz



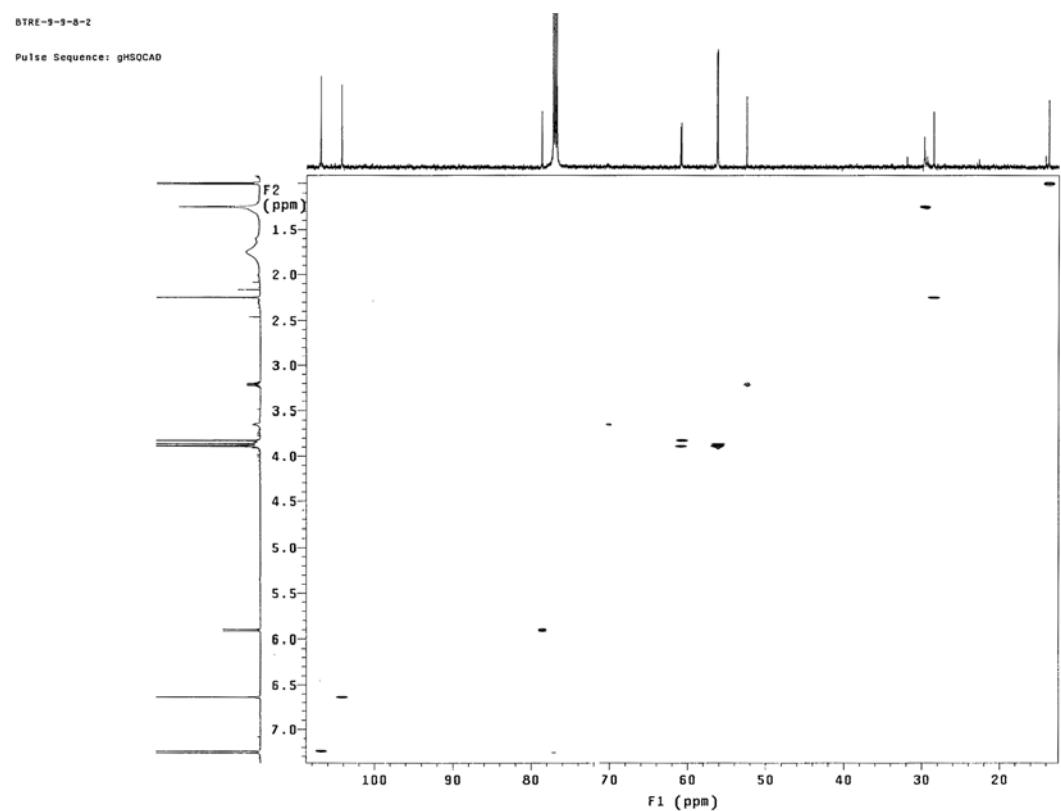
S51. ^{13}C NMR spectrum of tsangin C (**8**) in CDCl_3 at 150 MHz



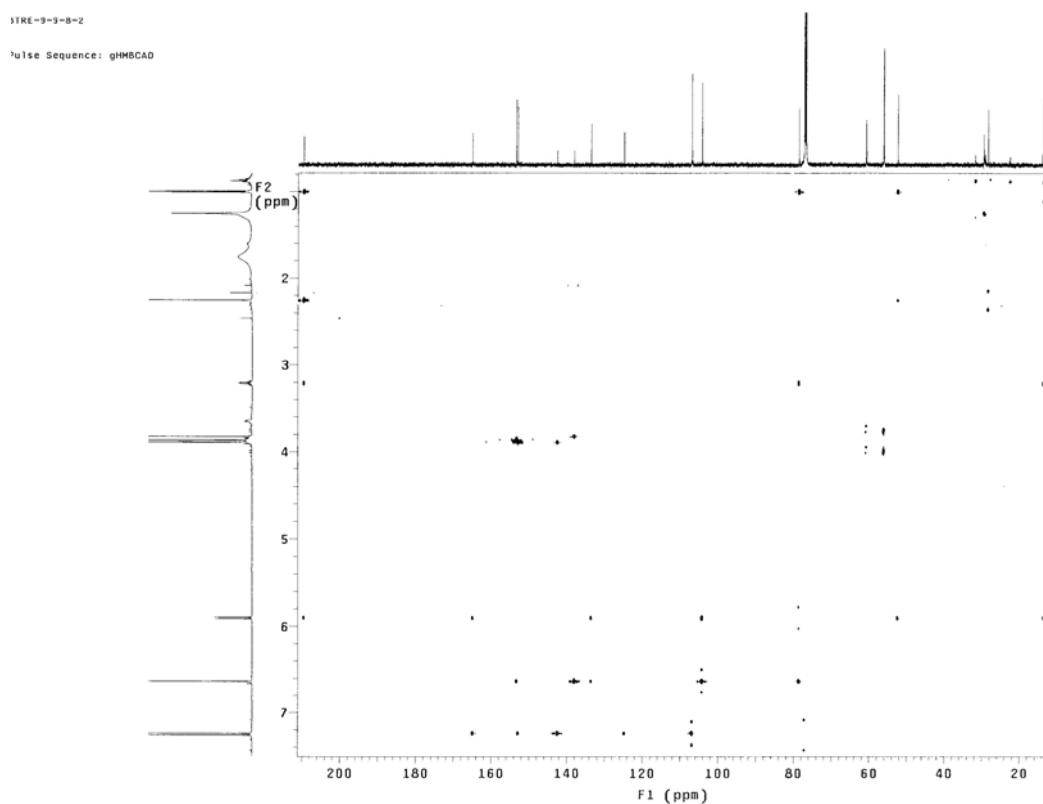
S52. DEPT spectrum of tsangin C (**8**) in CDCl_3



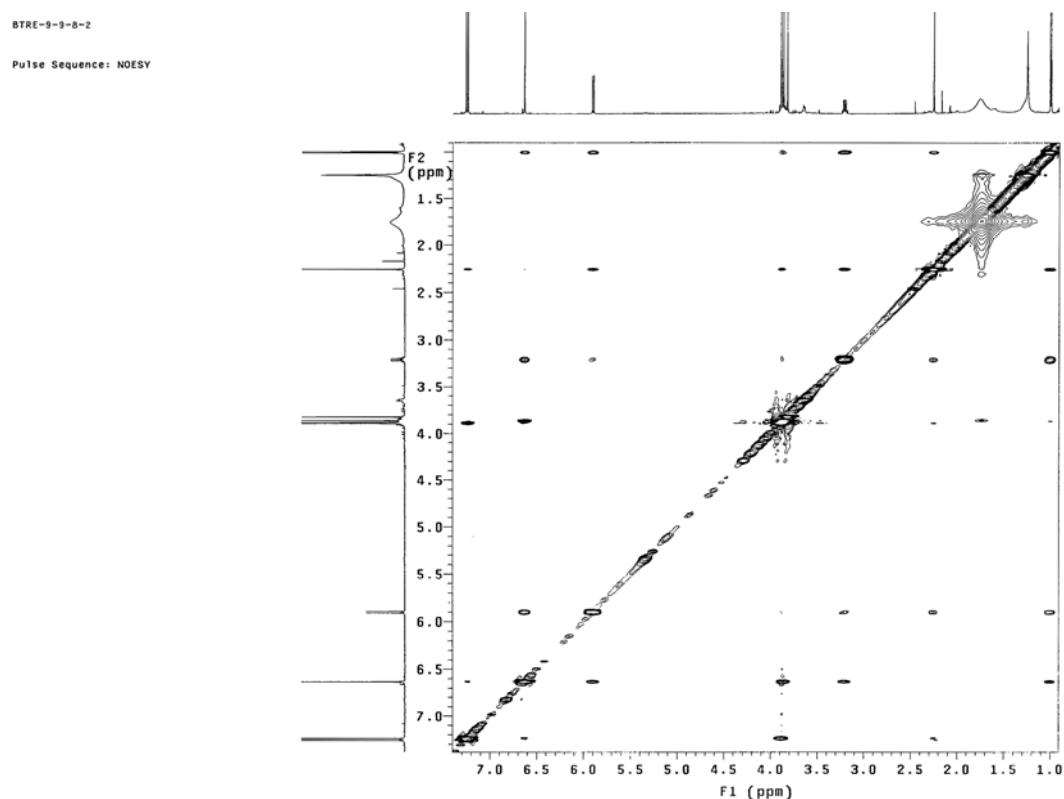
S53. ^1H - ^1H COSY spectrum of tsangin C (**8**) in CDCl_3



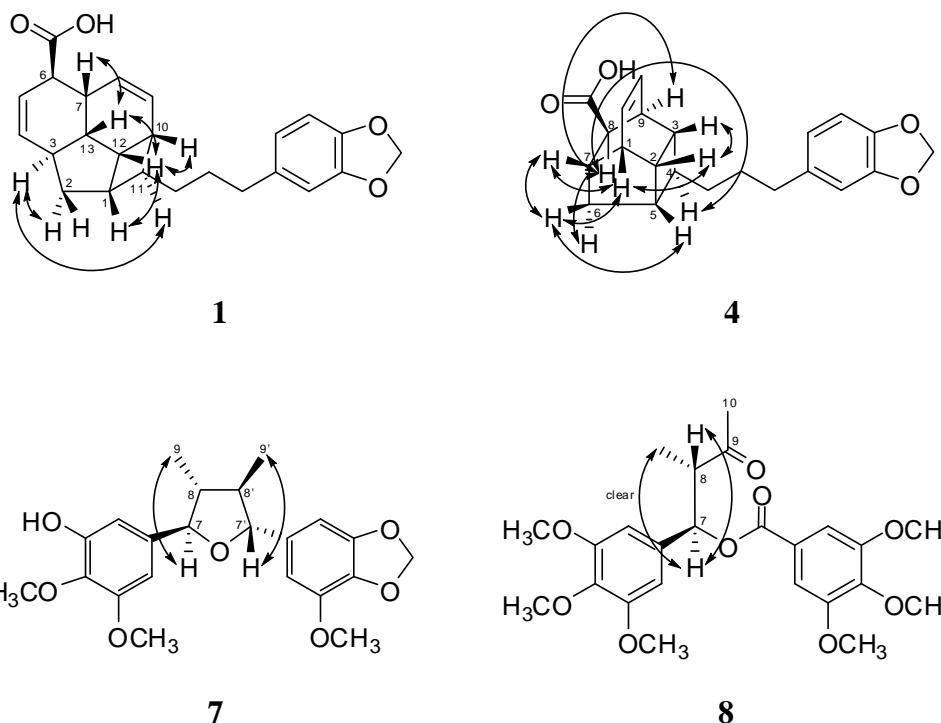
S54. HSQC spectrum of tsangin C (**8**) in CDCl_3



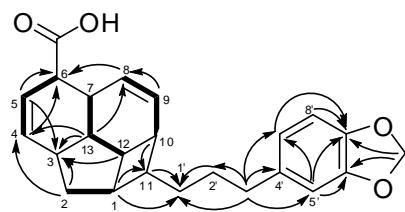
S55. HMBC spectrum of tsangin C (**8**) in CDCl_3



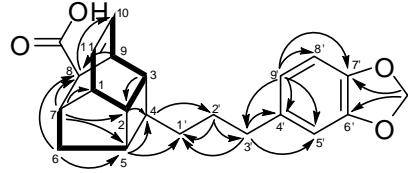
S56. NOESY spectrum of tsangin C (**8**) in CDCl_3



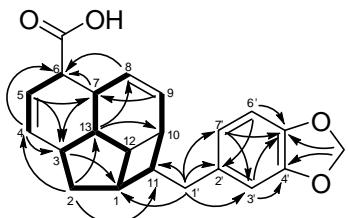
S57. **Figure 1.** NOESY (↘) correlations of **1**, **4**, **7**, and **8**.



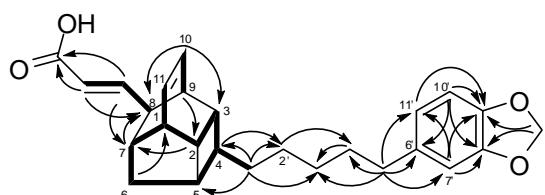
1



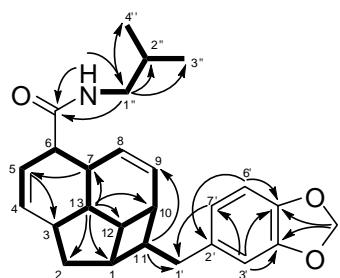
4



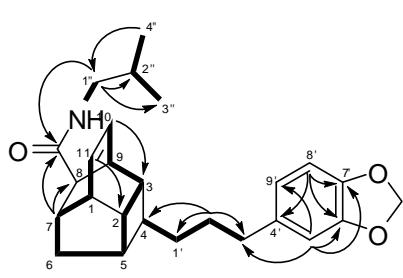
2



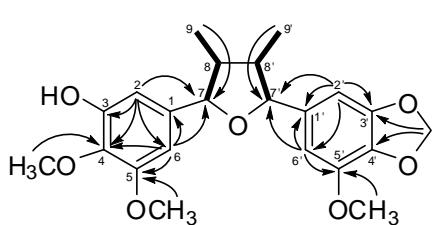
5



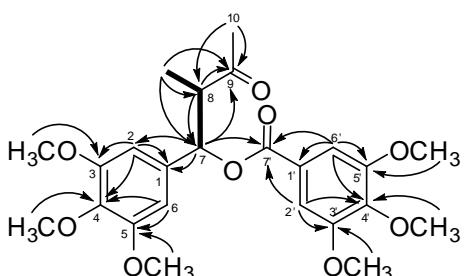
3



6



7



8

S58. Figure 2. COSY (—) and HMBC (↔) correlations of **1-8**.