

Supplementary Materials: Guignardones P–S, New Meroterpenoids from the Endophytic Fungi *Guignardia mangiferae* A348 Derived from the Medicinal Plant *Smilax glabra*

Zhang-Hua Sun, Fa-Liang Liang, Wen Wu, Yu-Chan Chen, Qing-Ling Pan, Hao-Hua Li, Wei Ye,
Hong-Xin Liu, Sai-Ni Li, Guo-Hui Tan and Wei-Min Zhang

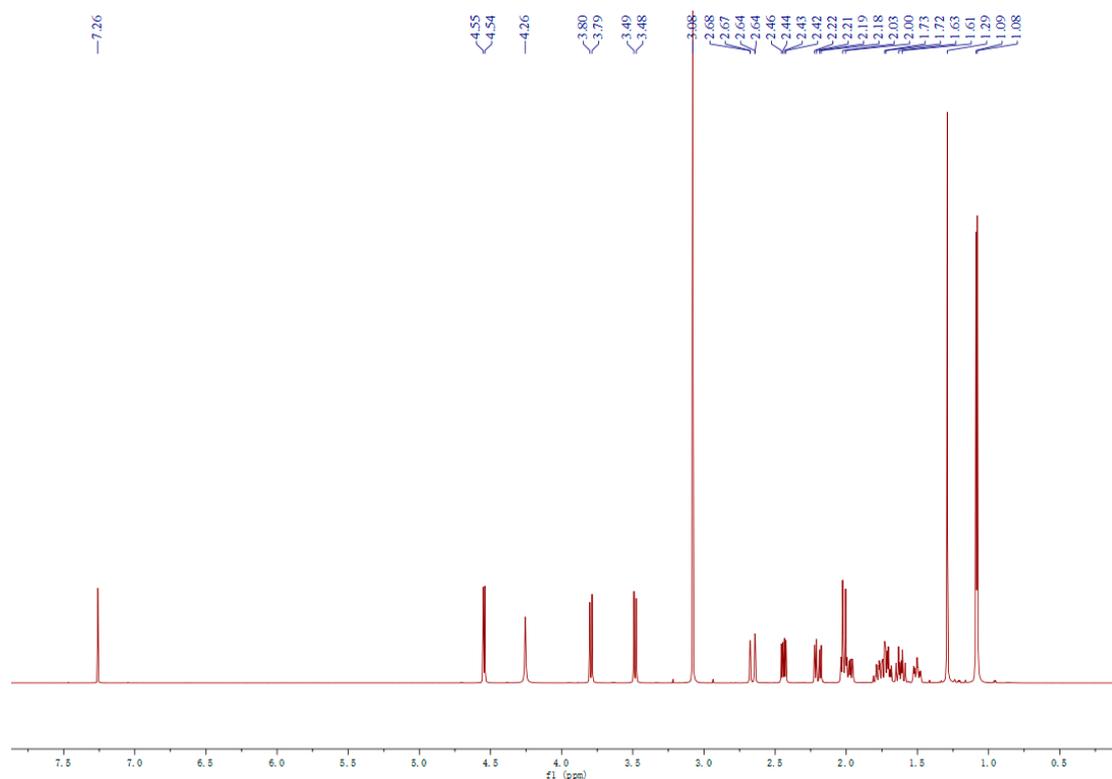


Figure S1. ¹H-NMR spectrum of guignardone P (1) in CDCl₃.

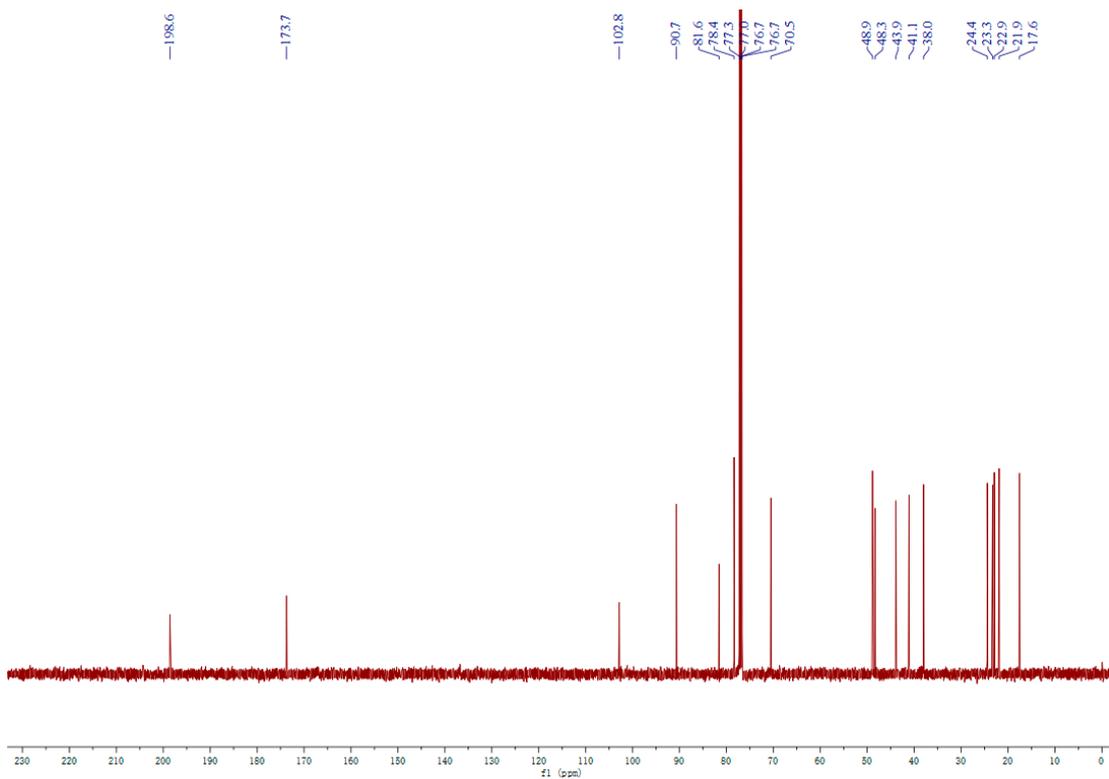


Figure S2. ^{13}C -NMR spectrum of guignardone P (**1**) in CDCl_3 .

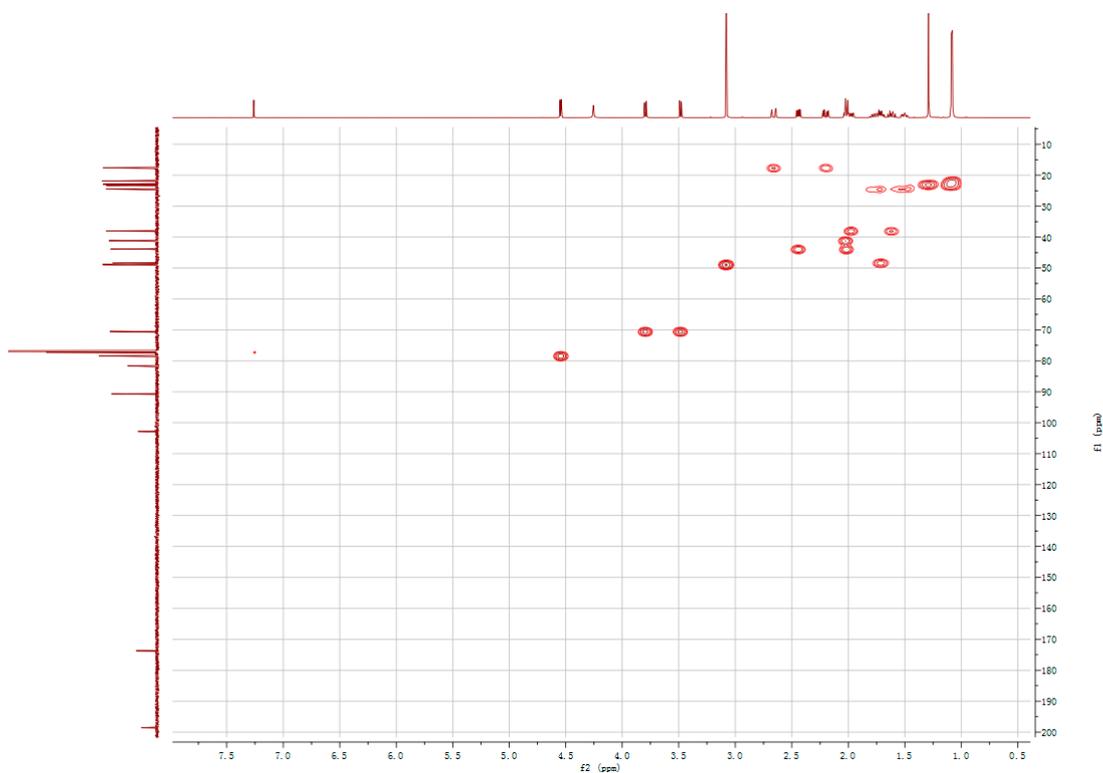


Figure S3. HSQC spectrum of guignardone P (**1**) in CDCl_3 .

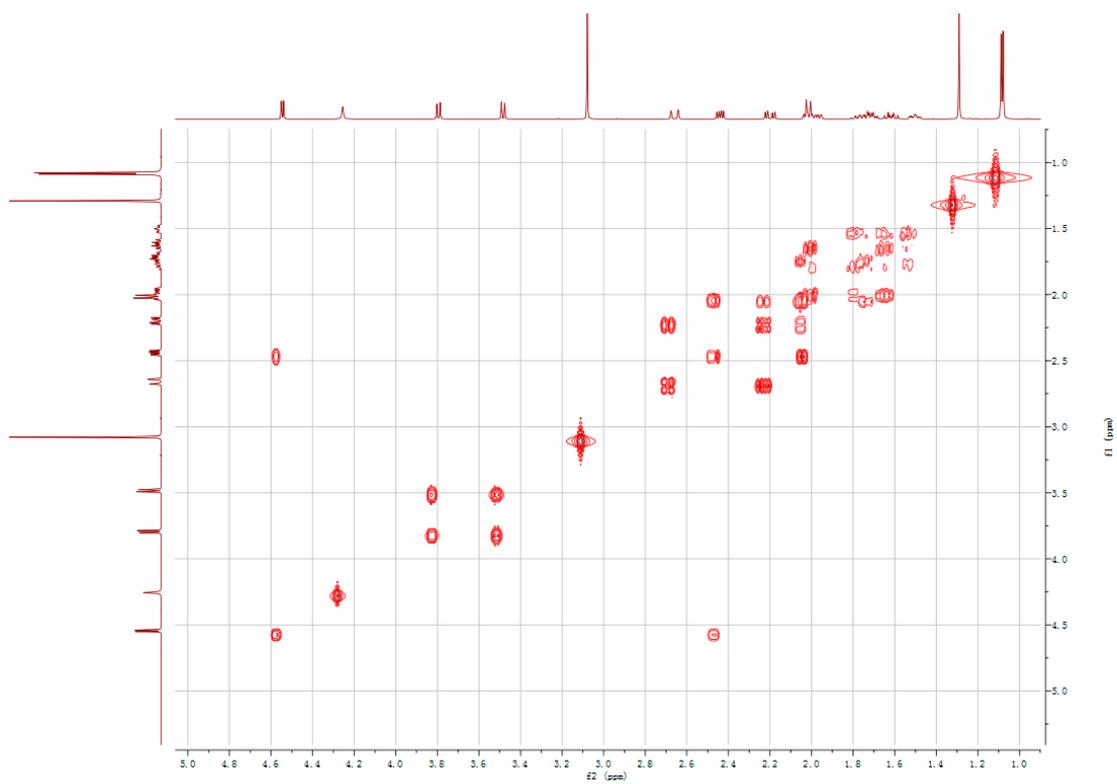


Figure S4. ^1H - ^1H COSY spectrum of guignardone P (1) in CDCl_3 .



Figure S5. HMBC spectrum of guignardone P (1) in CDCl_3 .

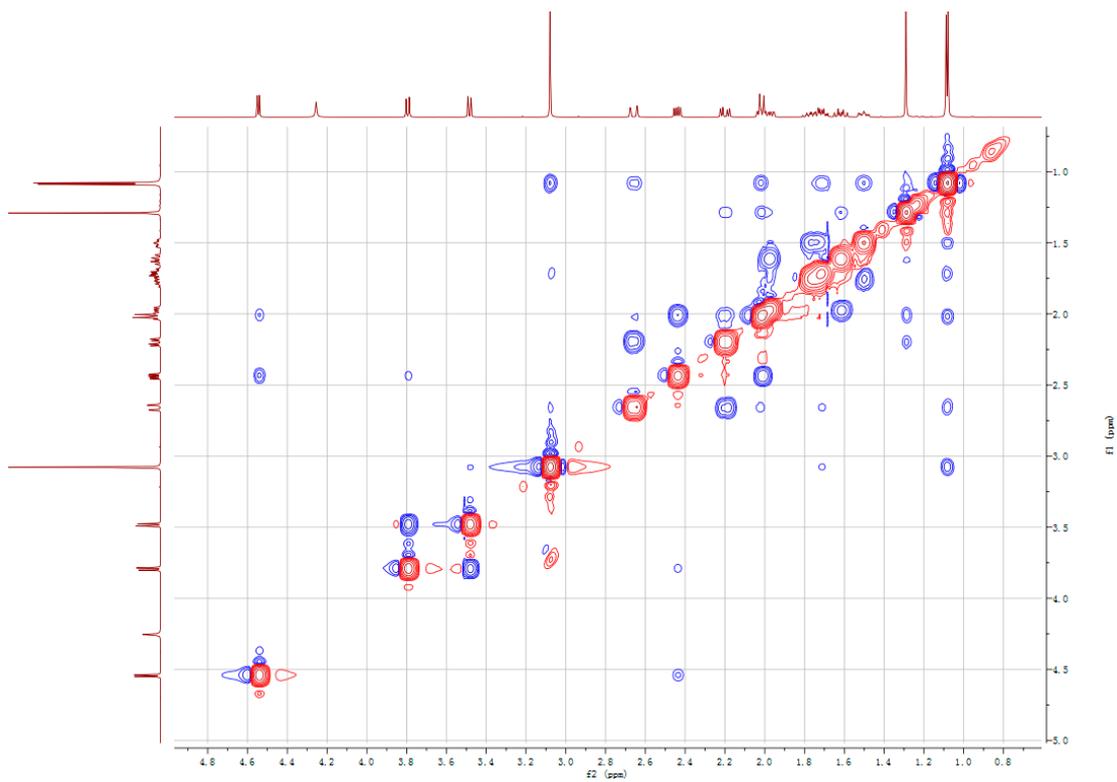


Figure S6. NOESY spectrum of guignardone P (1) in CDCl_3 .

SPECTRUM - MS
 File : D:\DATA-HR\11051704-gy46-c1.RAW
 Full ms [318.100 - 325.500] - Range: 318.100 - 325.500
 Scan No. 30 of 39
 Scan #: 30
 RT: 0.51
 Data points: 1

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
322.1778	100.0	322.1775	0.9	0.3	6.0	$\text{C}_{18}\text{H}_{20}\text{O}_5$

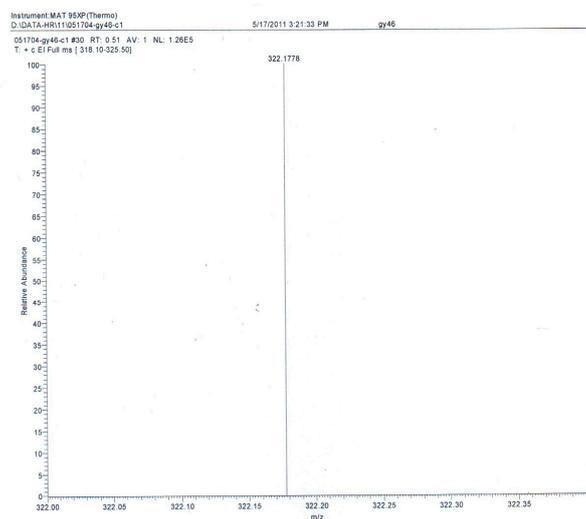


Figure S7. HREIMS spectrum of guignardone P (1).

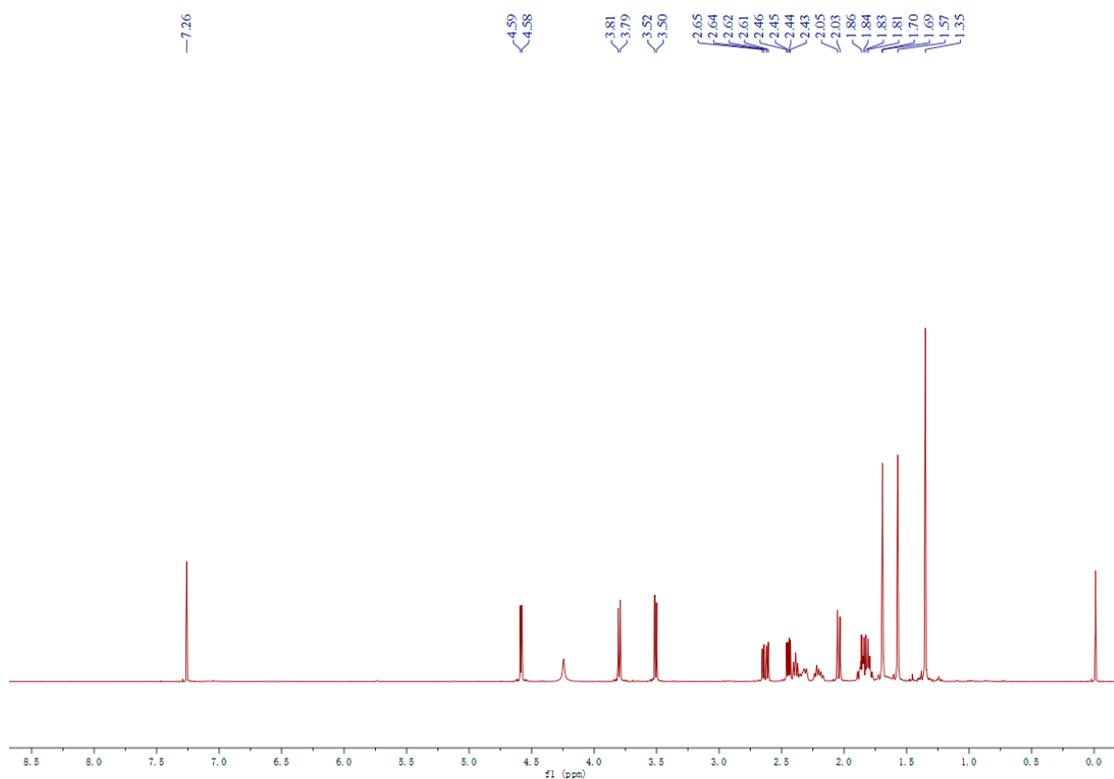


Figure S8. ^1H -NMR spectrum of guignardone Q (**2**) in CDCl_3 .

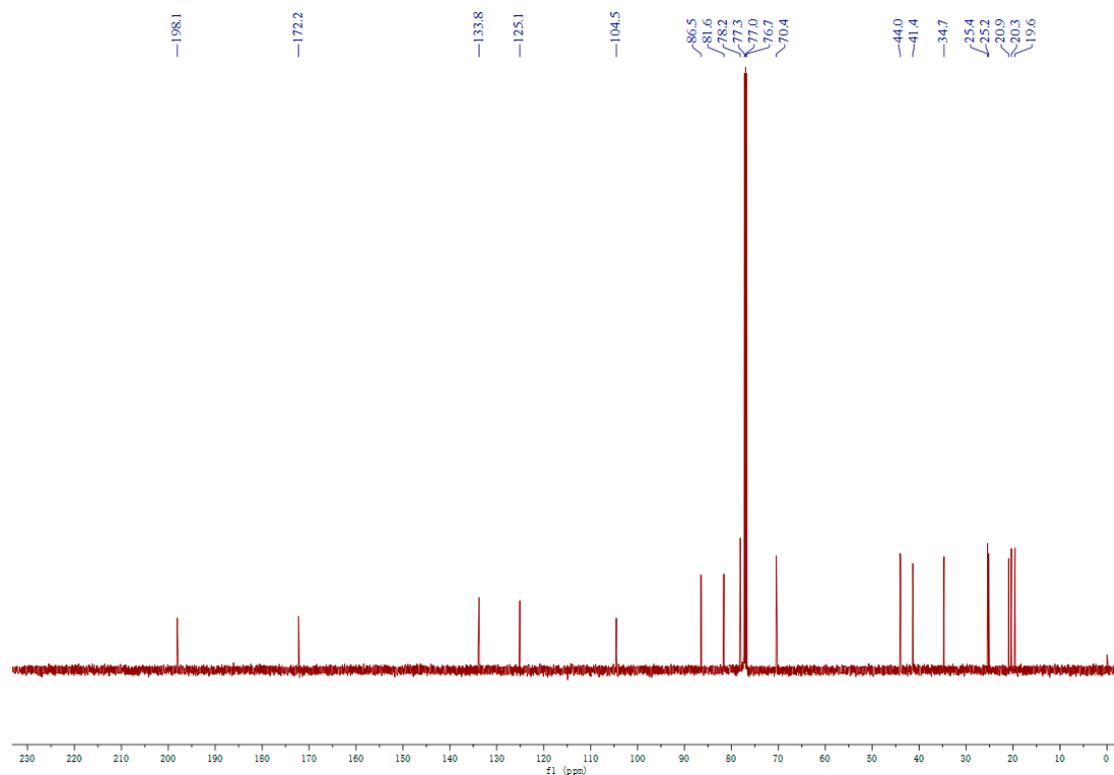


Figure S9. ^{13}C -NMR spectrum of guignardone Q (**2**) in CDCl_3 .

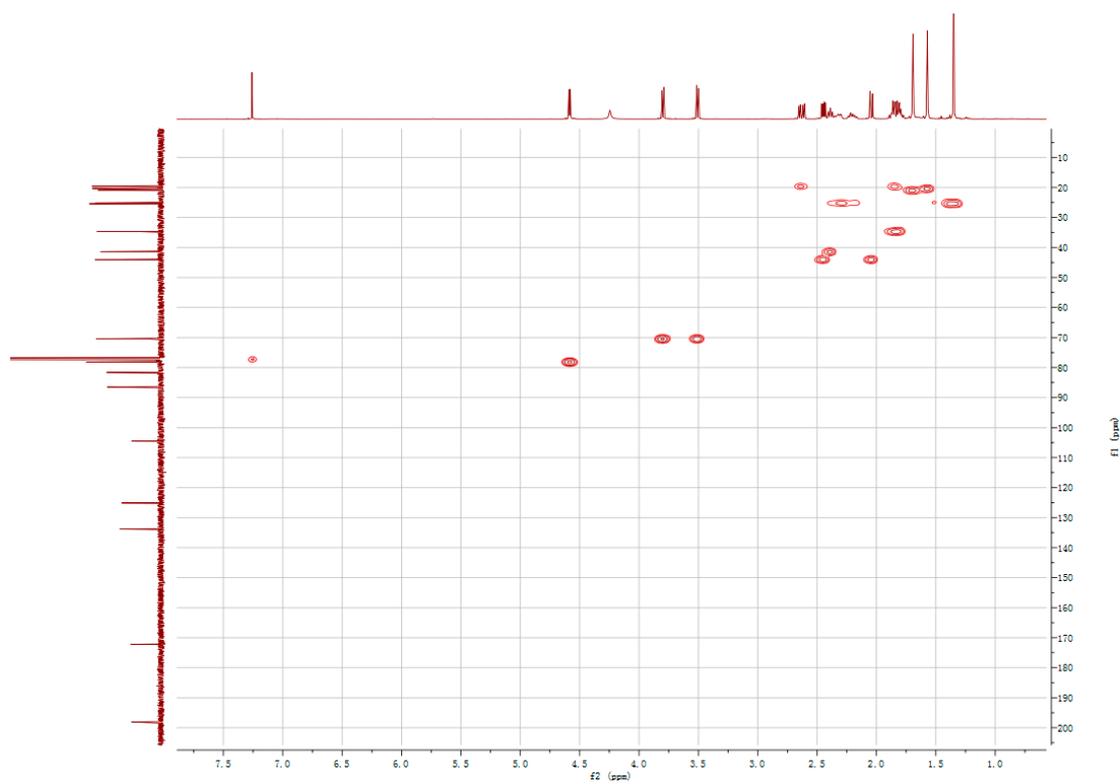


Figure S10. HSQC spectrum of guignardone Q (2) in CDCl₃.

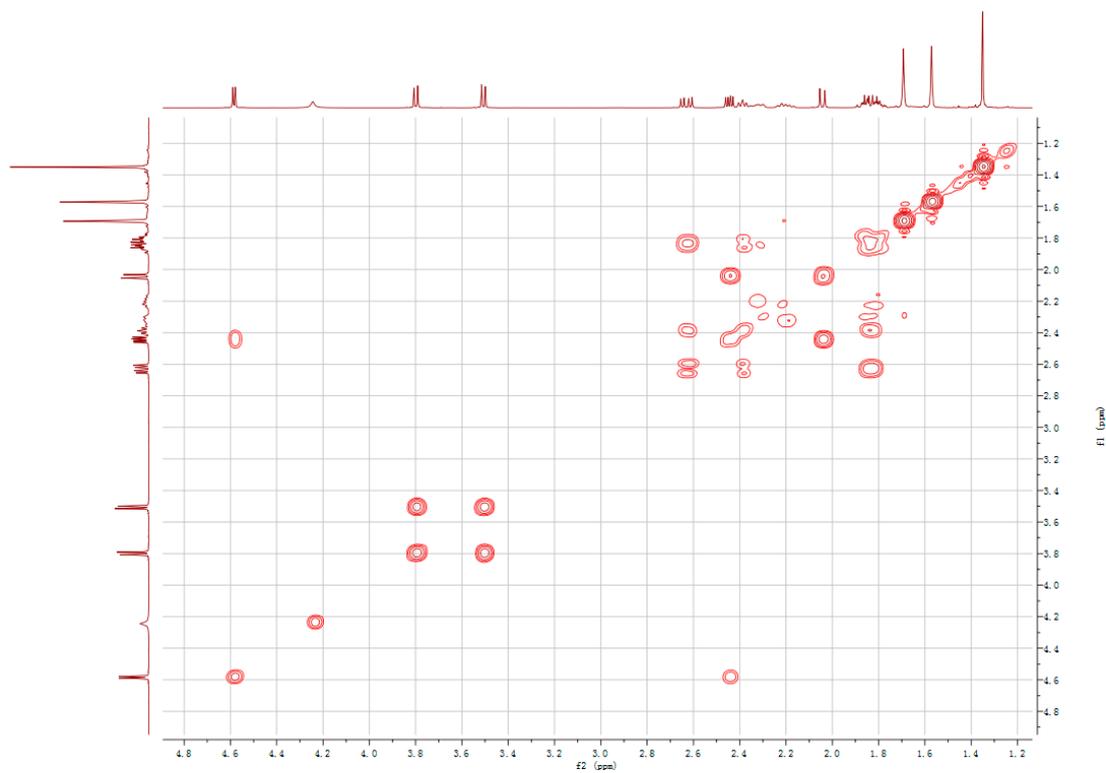


Figure S11. ¹H-¹H COSY spectrum of guignardone Q (2) in CDCl₃.

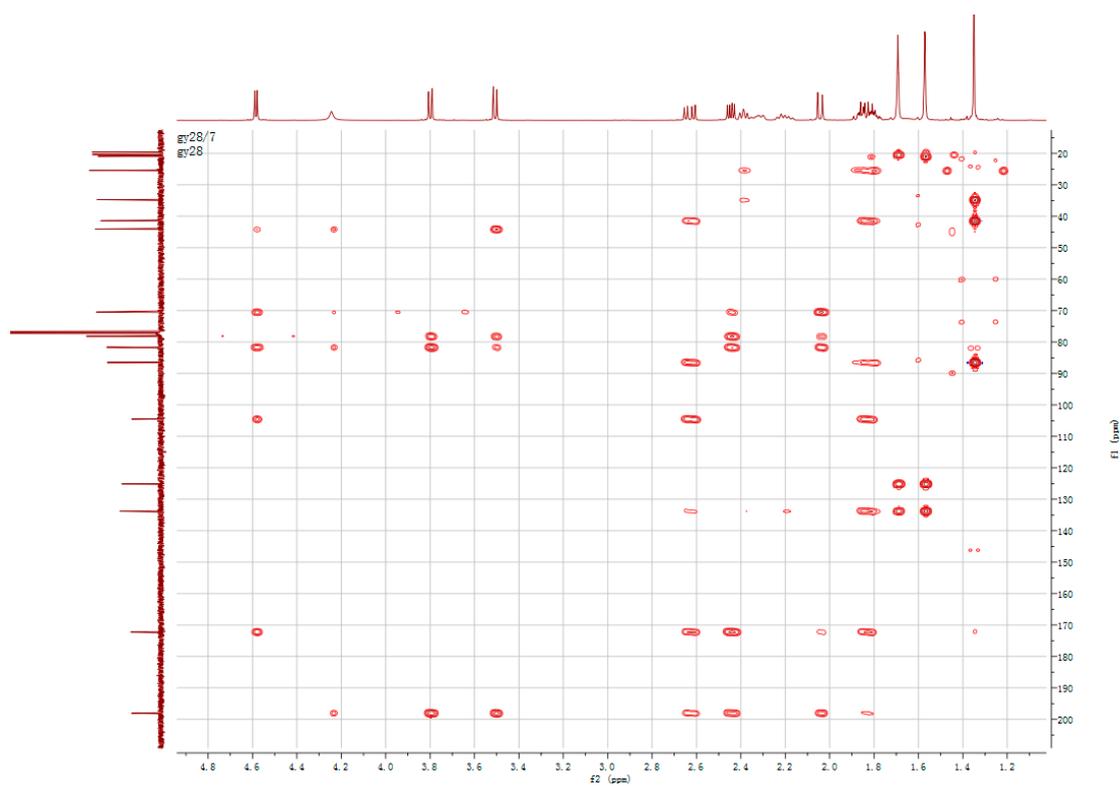


Figure S12. HMBC spectrum of guignardone Q (2) in CDCl₃.

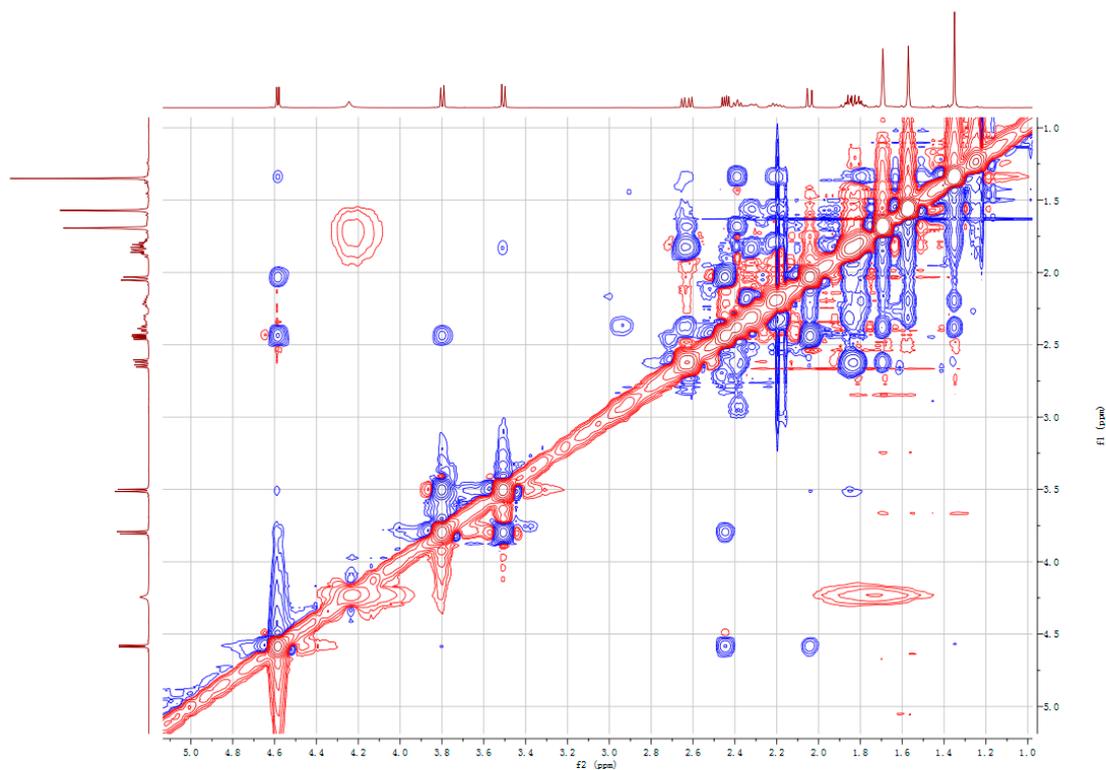


Figure S13. NOESY spectrum of guignardone Q (2) in CDCl₃.

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

106 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

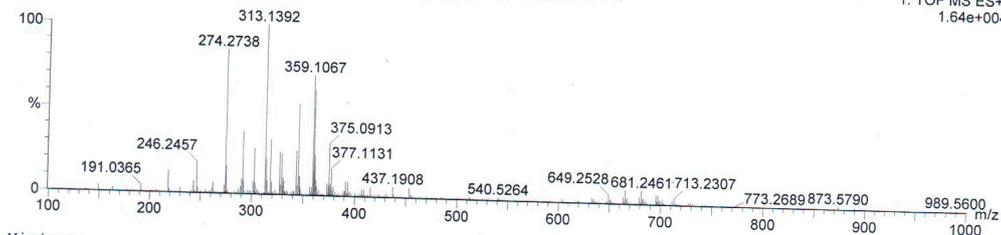
Elements Used:

C: 0-50 H: 0-500 O: 0-20 Na: 0-1

26-Apr-2011 09:55:17

gy28 9 (0.527) AM (Cen,3, 80.00, Ar,5000.0,345.00,0.70,LS 10); Sm (Mn, 2x1.00); Cm (2:14)

1: TOF MS ES+
1.64e+004



Minimum:
Maximum:

10.0 -1.5
10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
313.1392	313.1416	-2.4	-7.7	6.5	325.5	C17 H22 O4 Na
	313.1440	-4.8	-15.3	9.5	295.3	C19 H21 O4

Figure S14. HRESIMS spectrum of guignardone Q (2).

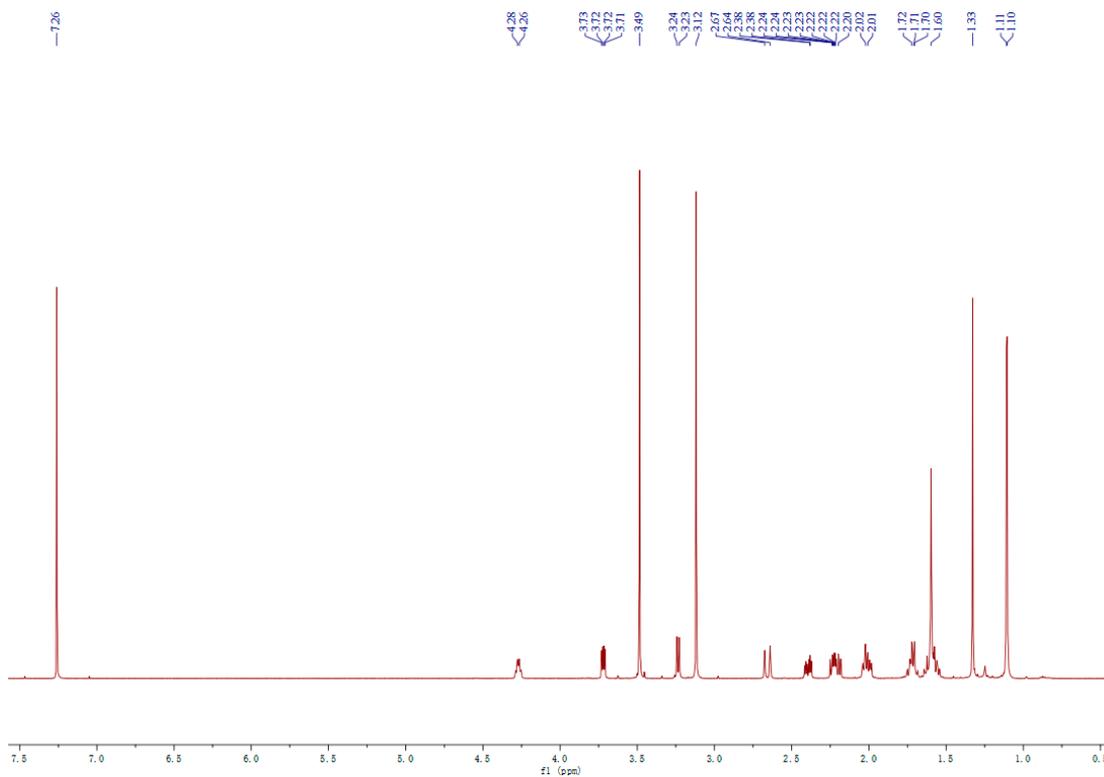


Figure S15. ¹H-NMR spectrum of guignardone R (3) in CDCl₃.

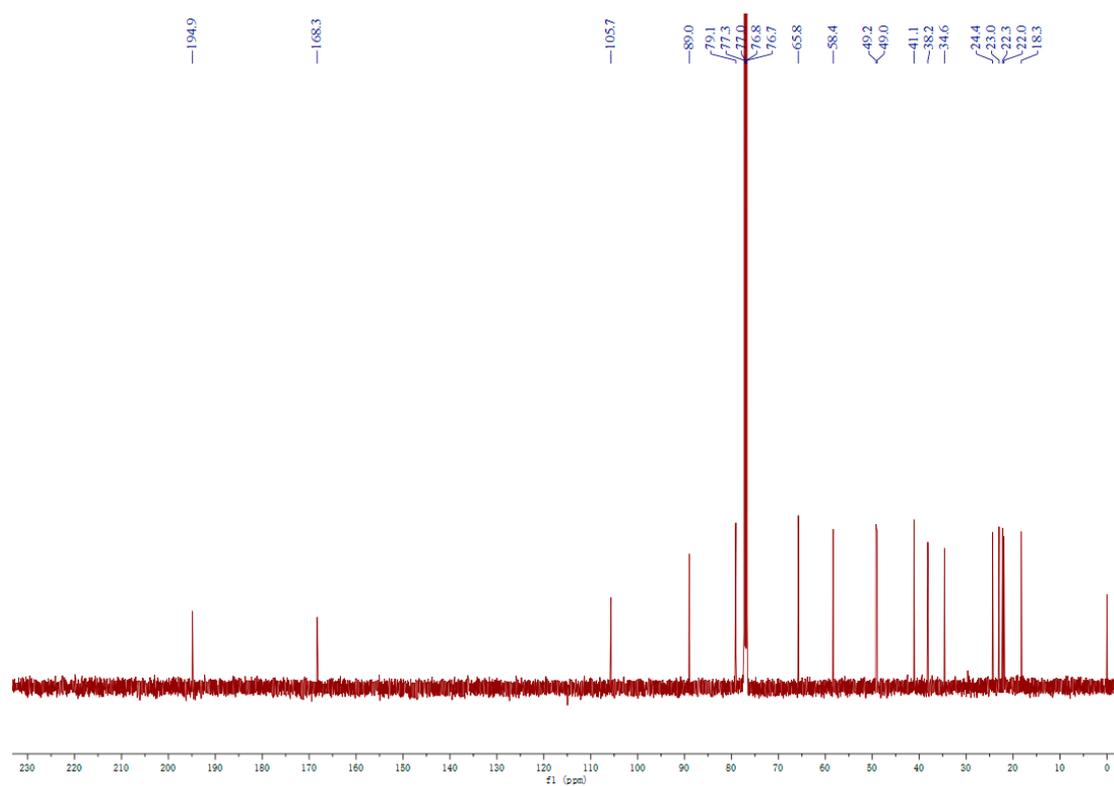


Figure S16. ^{13}C -NMR spectrum of guignardone R (3) in CDCl_3 .

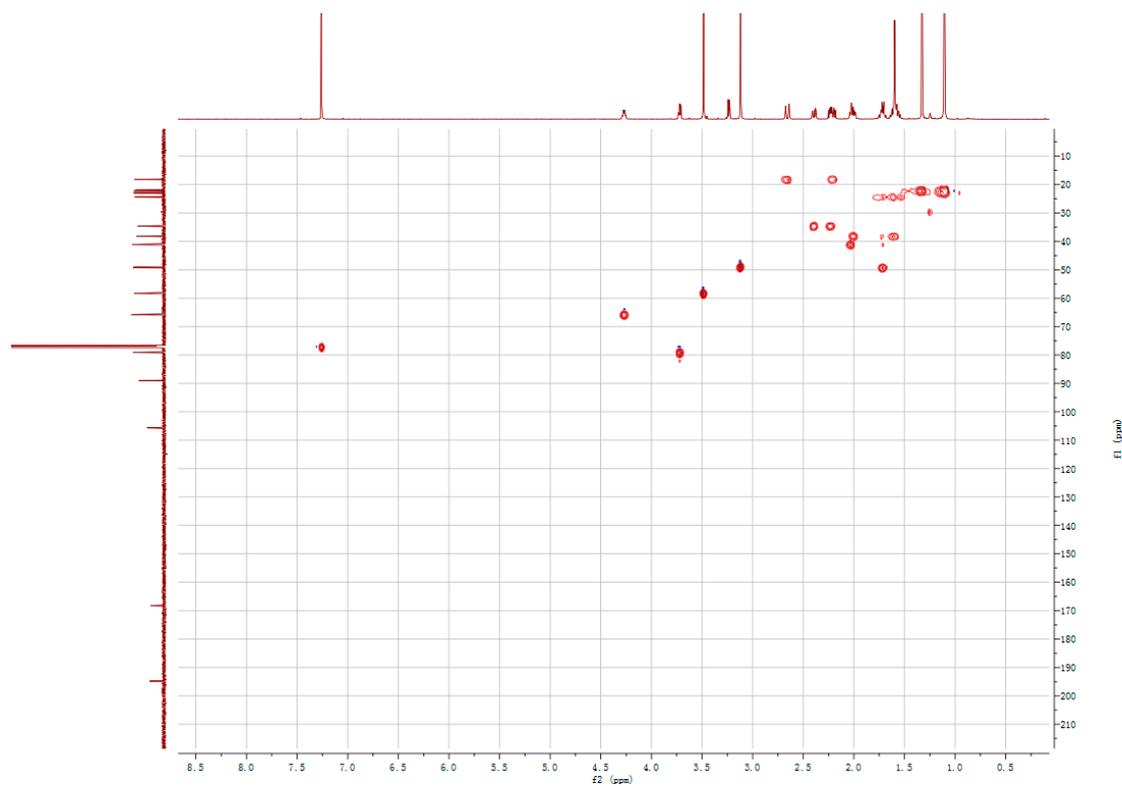


Figure S17. HSQC spectrum of guignardone R (3) in CDCl_3 .

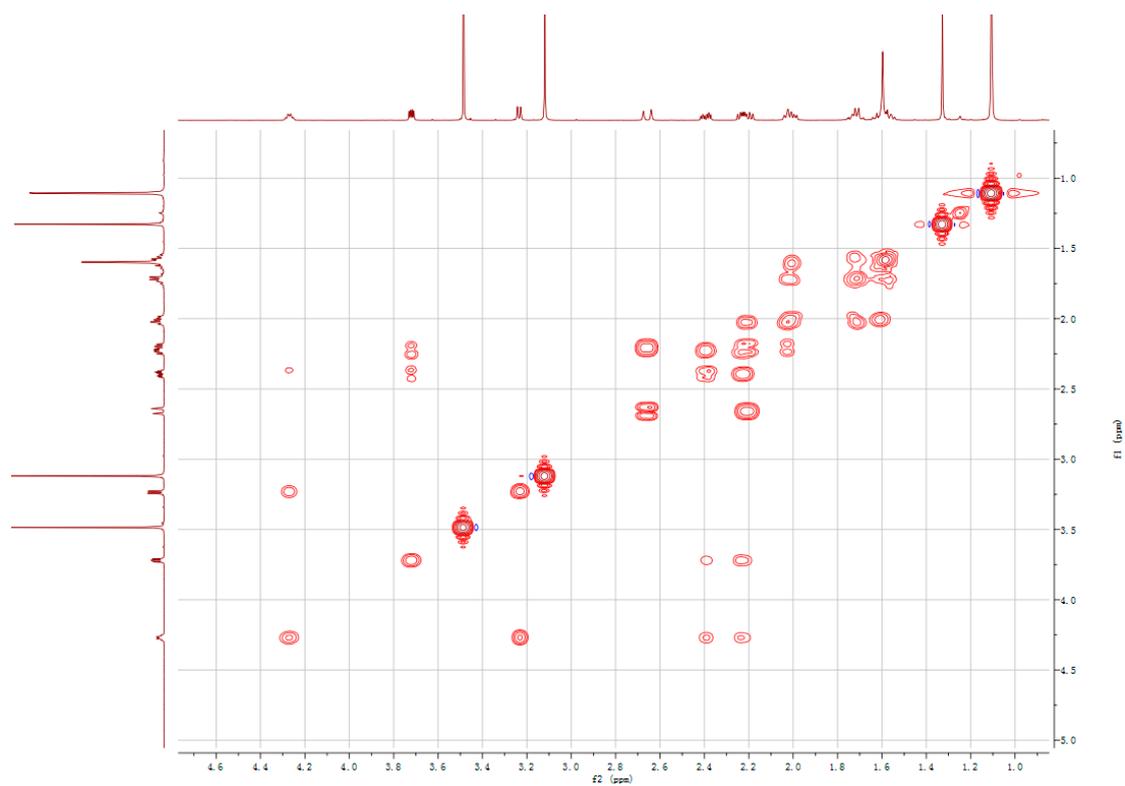


Figure S18. ^1H - ^1H COSY spectrum of guignardone R (**3**) in CDCl_3 .

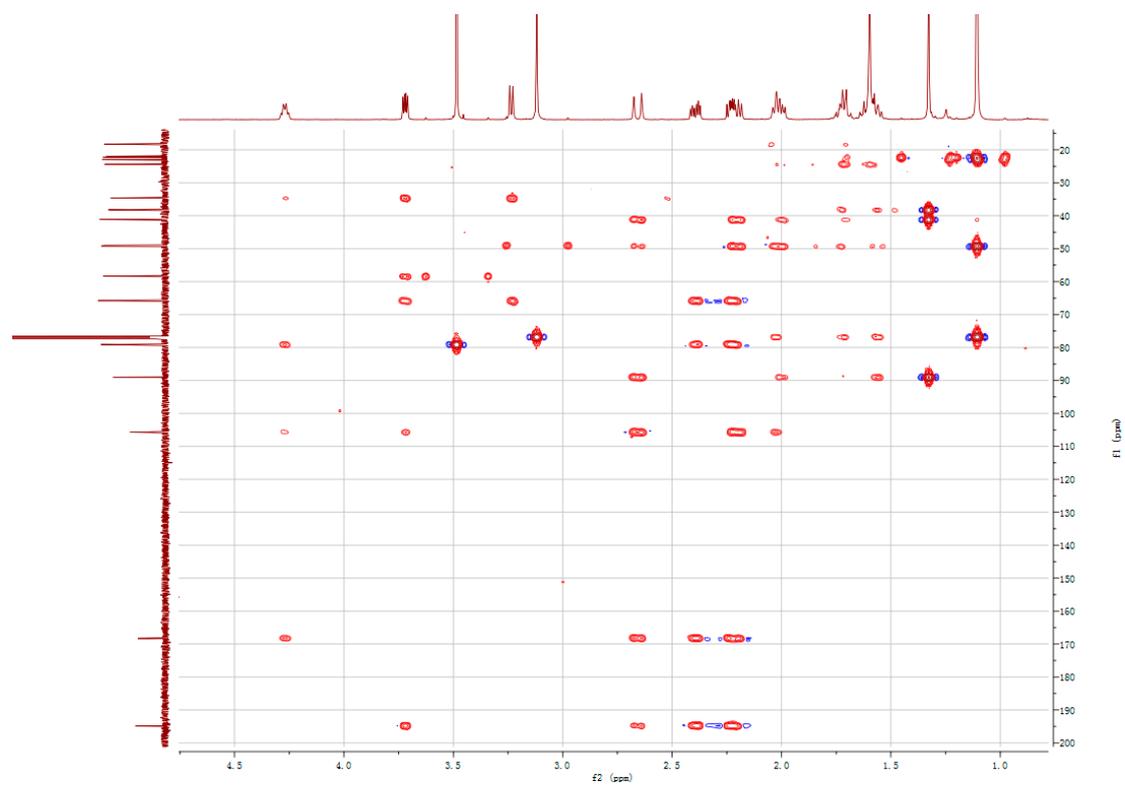


Figure S19. HMBC spectrum of guignardone R (**3**) in CDCl_3 .

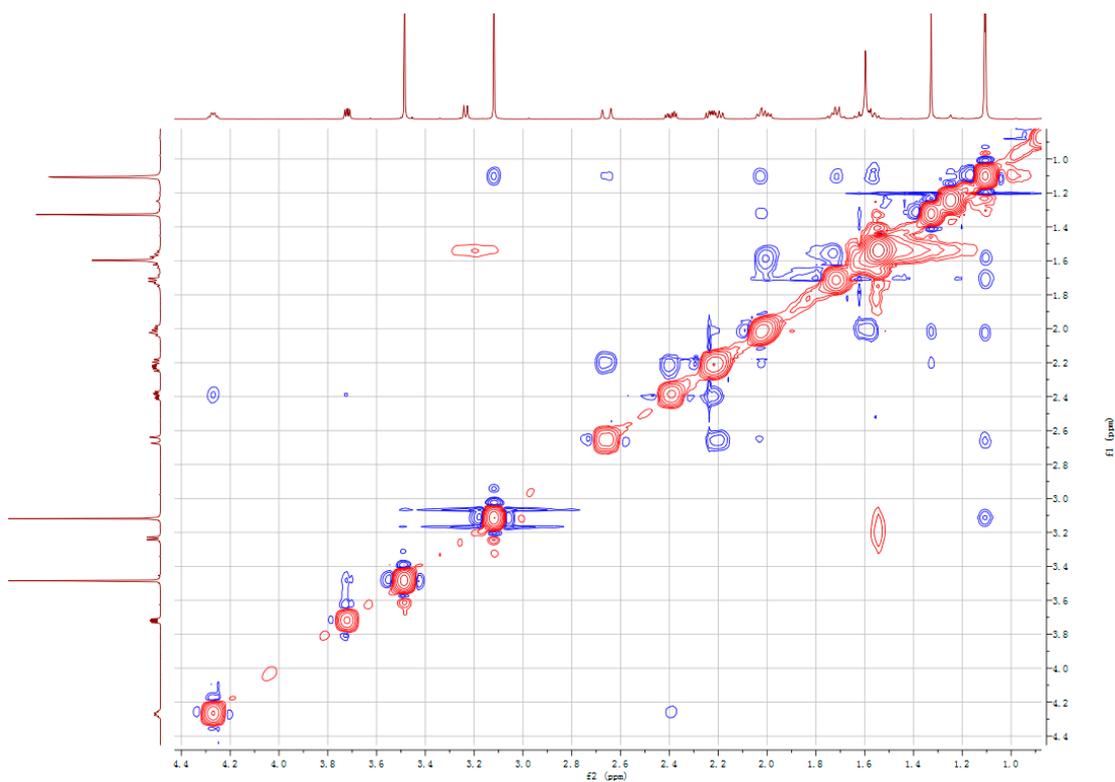


Figure S20. NOESY spectrum of guignardone R (3) in CDCl₃.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

131 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)

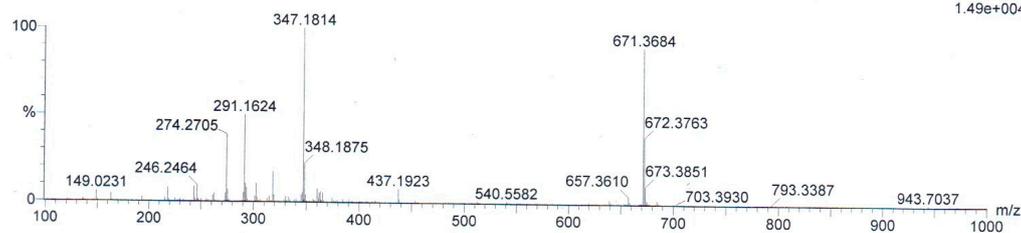
Elements Used:

C: 0-50 H: 0-500 O: 0-20 Na: 0-1

26-Apr-2011 10:23

gy37 5 (0.283) AM (Top,3, Ar,5000.0,345.00,0.70,LS 10); Sm (Mn, 2x1.00); Cm (4:20)

1: TOF MS ES+
1.49e+004



Minimum:
Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
347.1814	347.1800	1.4	4.0	16.5	168.4	C27 H23
	347.1834	-2.0	-5.8	4.5	28.8	C18 H28 O5 Na
	347.1776	3.8	10.9	13.5	107.3	C25 H24 Na
	347.1858	-4.4	-12.7	7.5	18.1	C20 H27 O5

Figure S21. HRESIMS spectrum of guignardone R (3).

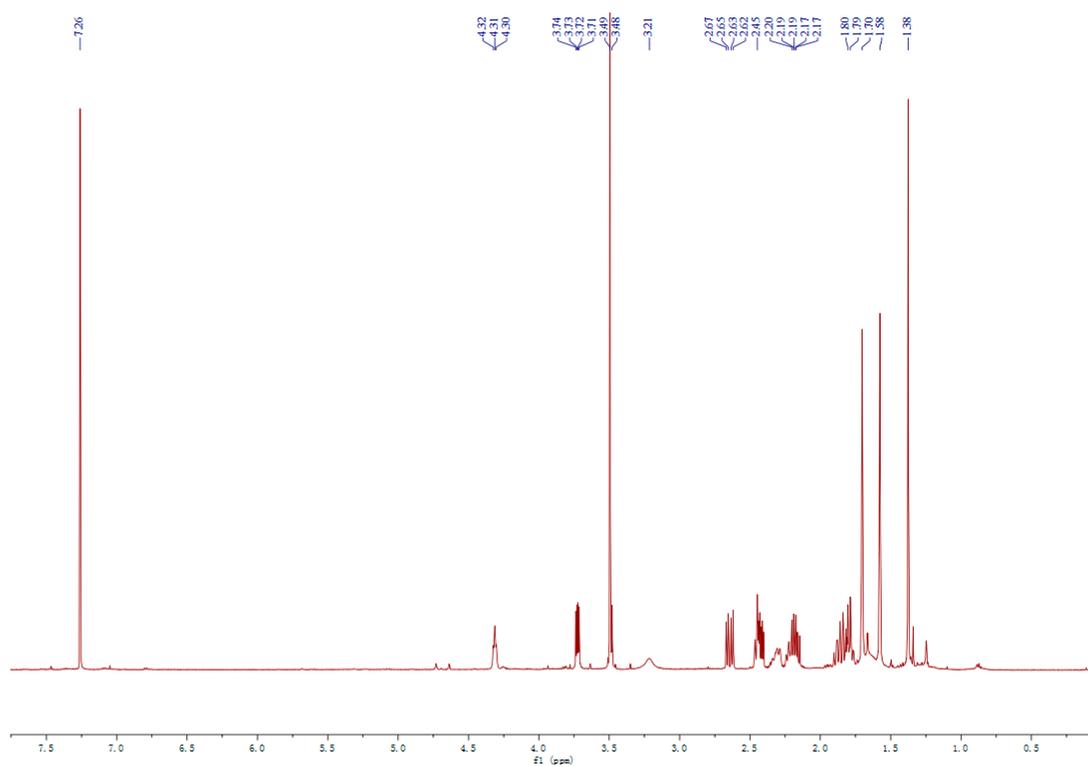


Figure S22. ^1H -NMR spectrum of guignardone S (**4**) in CDCl_3 .

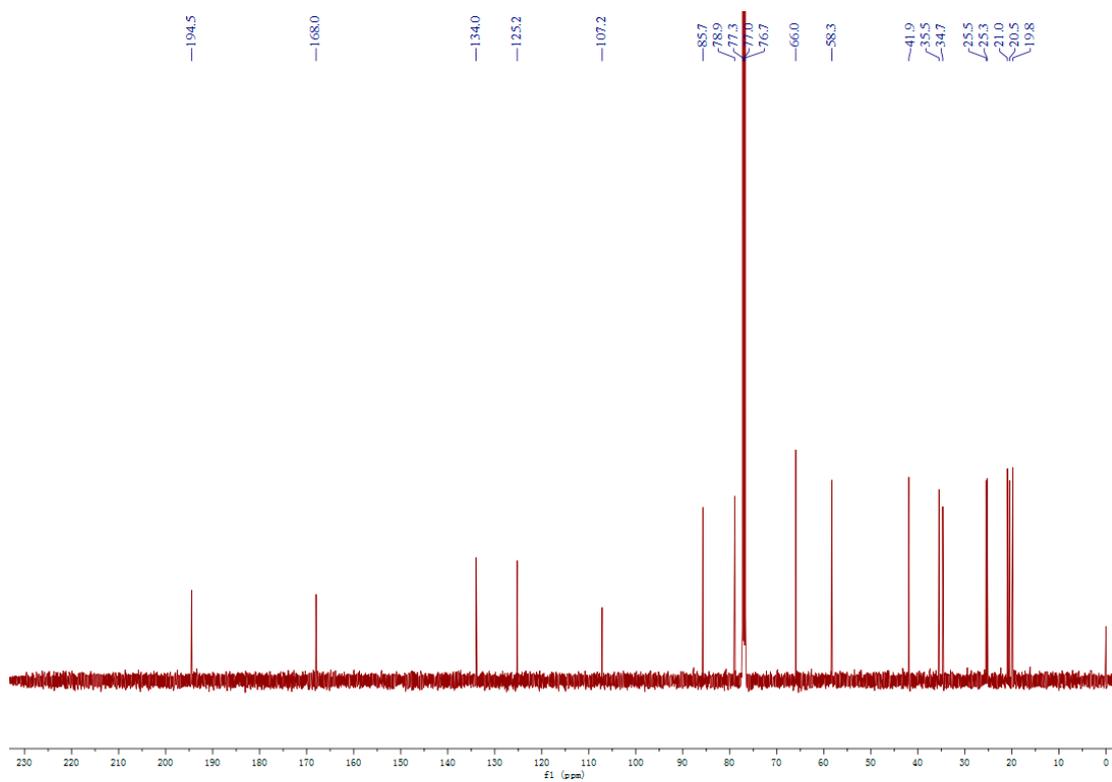


Figure S23. ^{13}C -NMR spectrum of guignardone S (**4**) in CDCl_3 .

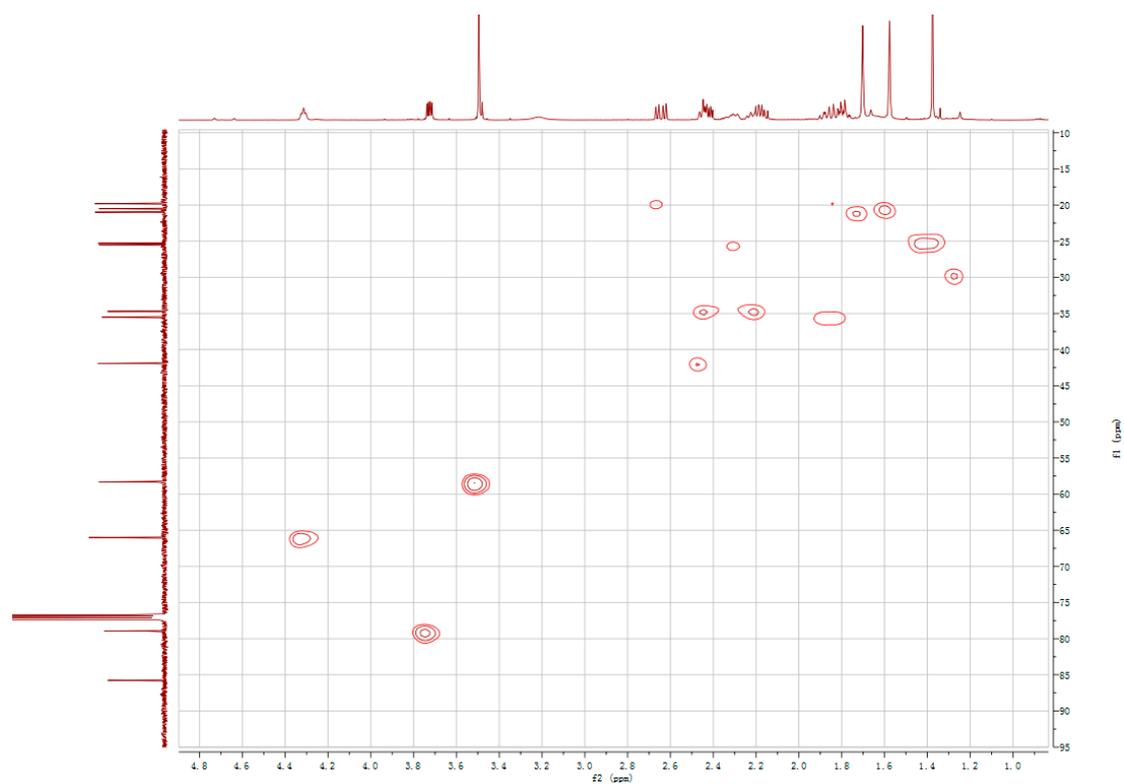


Figure S24. HSQC spectrum of guignardone S (**4**) in CDCl₃.

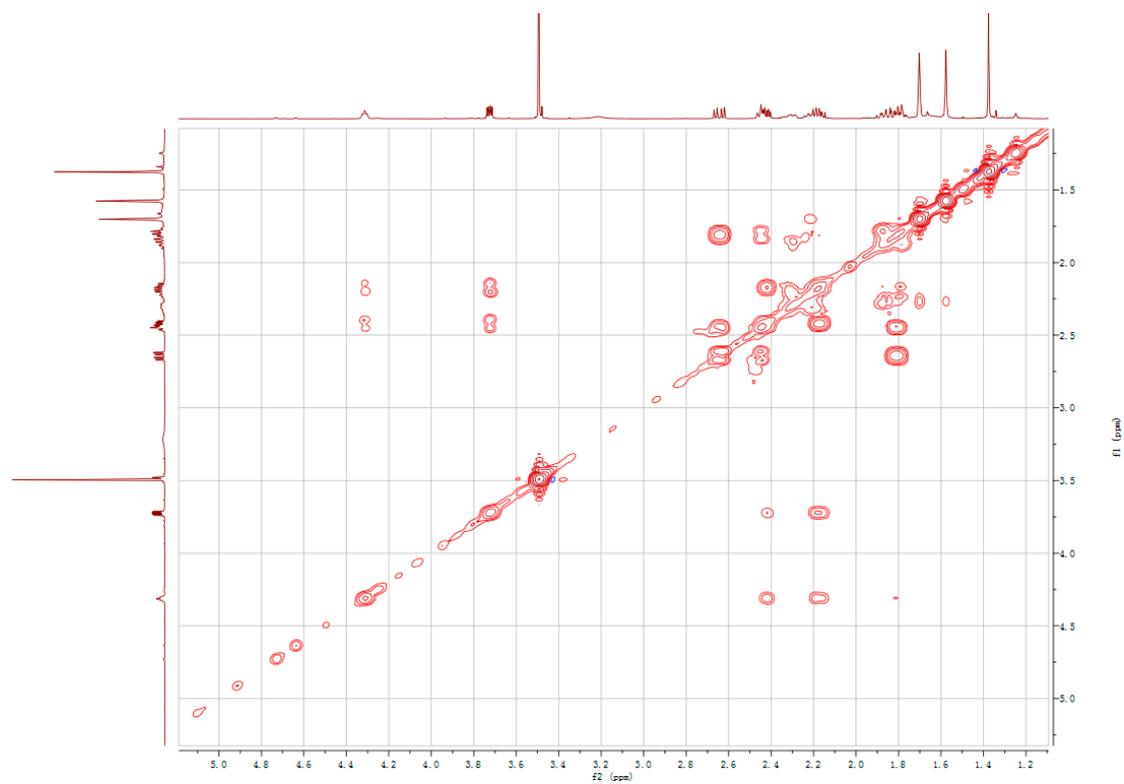


Figure S25. ¹H–¹H COSY spectrum of guignardone S (**4**) in CDCl₃.

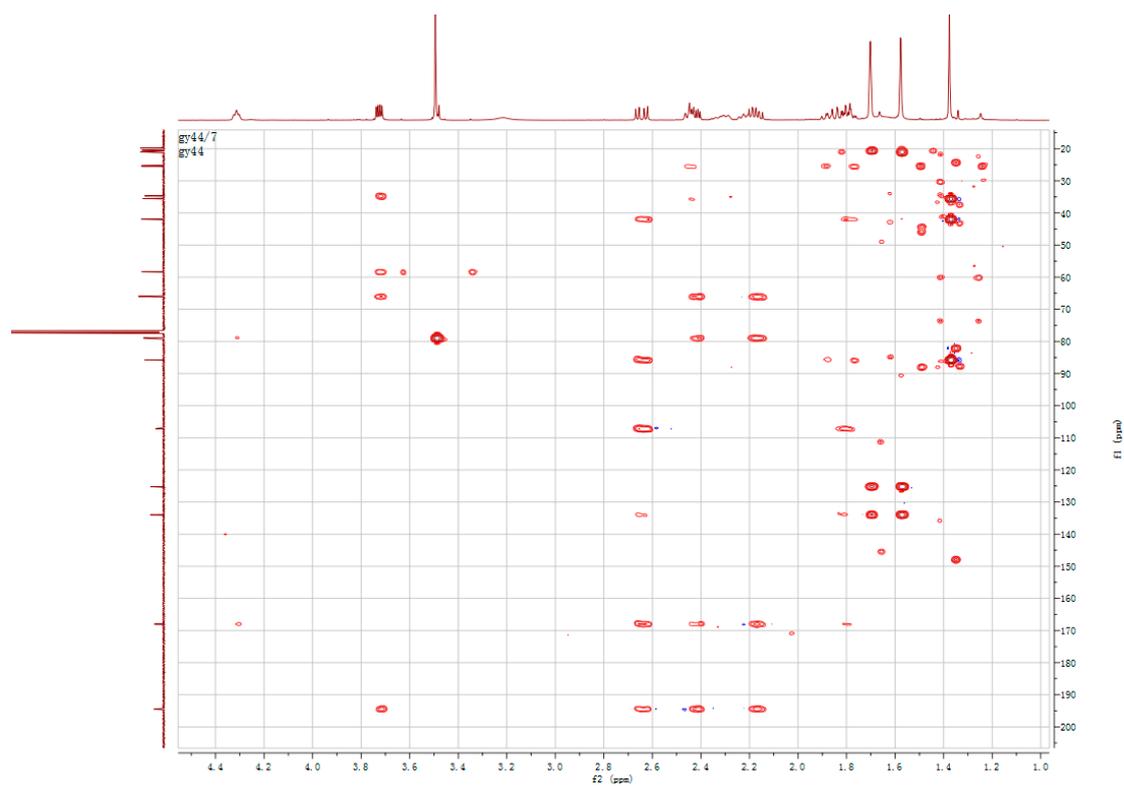


Figure S26. HMBC spectrum of guignardone S (4) in CDCl₃.

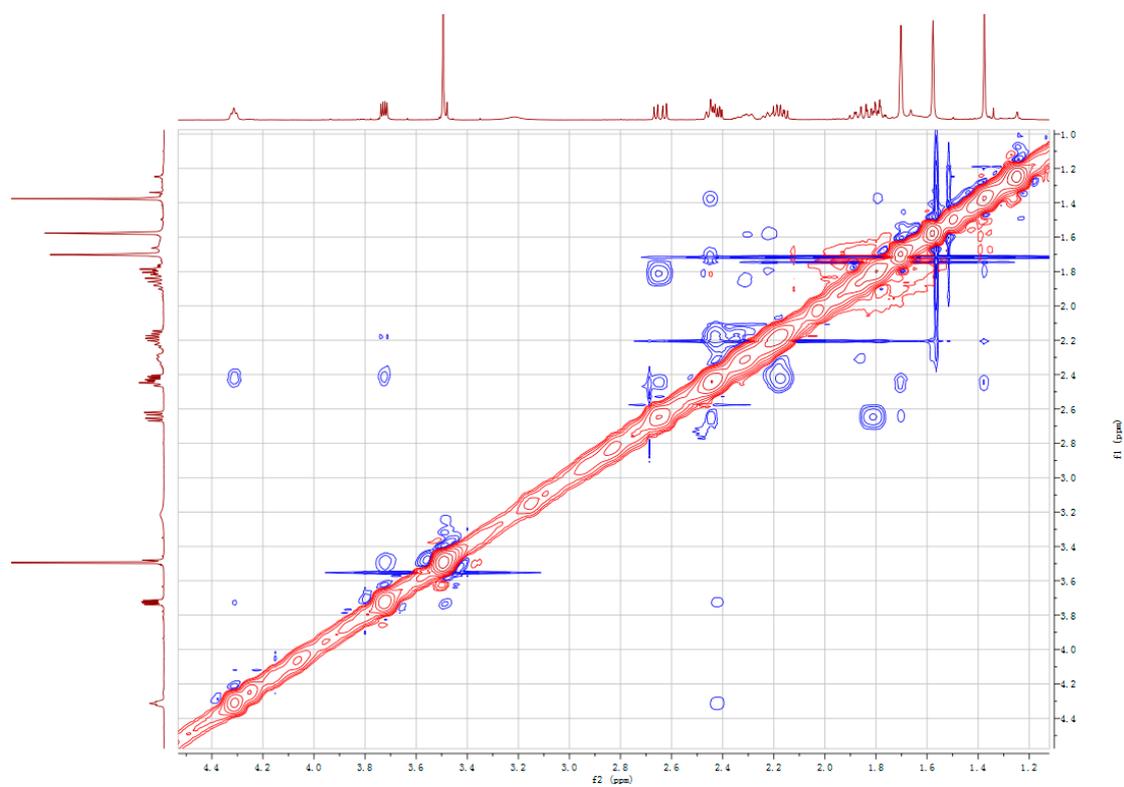


Figure S27. NOESY spectrum of guignardone S (4) in CDCl₃.

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

113 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

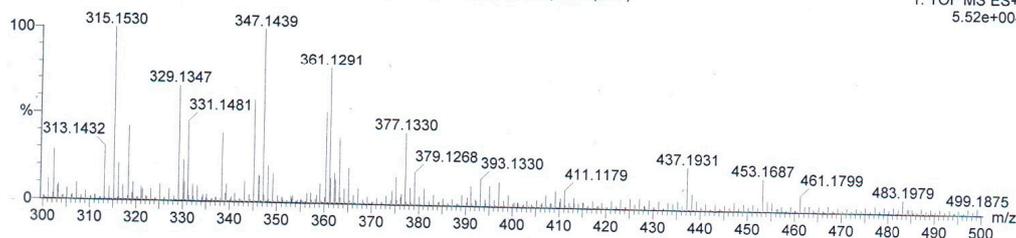
Elements Used:

C: 0-50 H: 0-500 O: 0-20 Na: 0-1

26-Apr-2011 10:49:13

gy44 2 (0.101) AM (Cen,3, 80.00, Ar,5000.0,345.00,0.70,LS 10); Sm (Mn, 2x1.00); Cm (2:31)

1: TOF MS ES+
5.52e+004



Minimum:
Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
315.1530	315.1572	-4.2	-13.3	5.5	1223.6	C17 H24 O4 Na
	315.1596	-6.6	-20.9	8.5	1101.5	C19 H23 O4
	315.1444	8.6	27.3	4.5	1355.9	C15 H23 O7

Figure S28. HRESIMS spectrum of guignardone S (4).

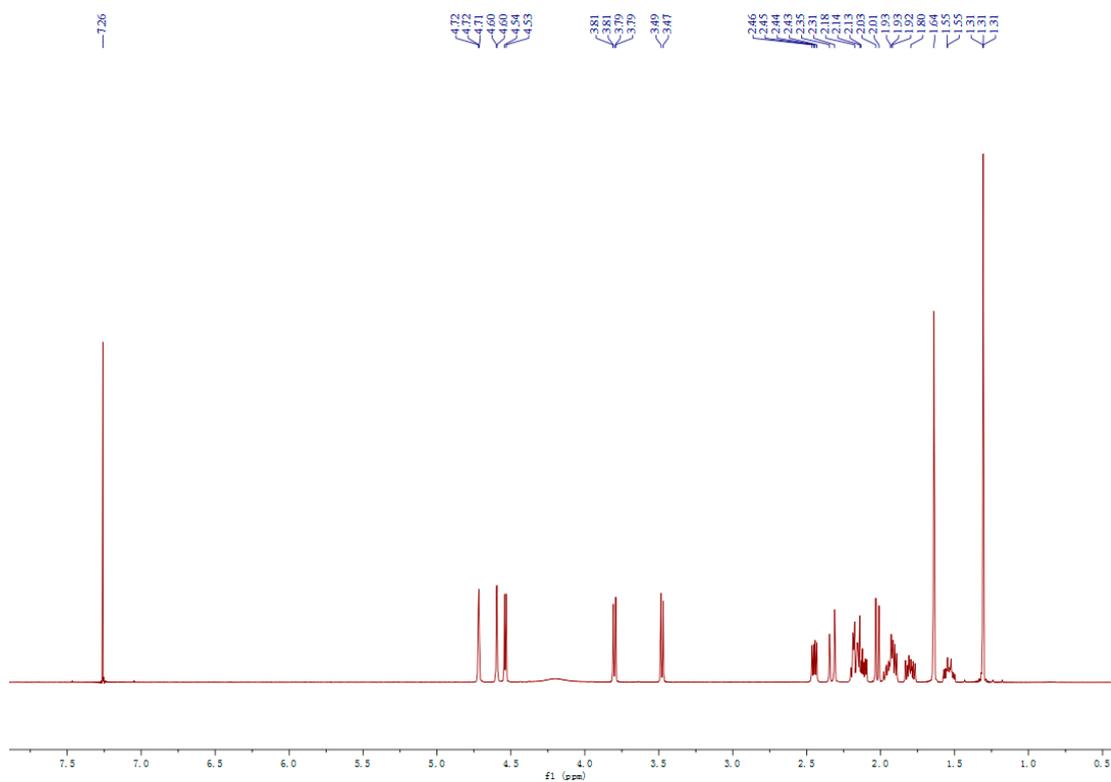


Figure S29. ¹H-NMR spectrum of guignardone A (5) in CDCl₃.

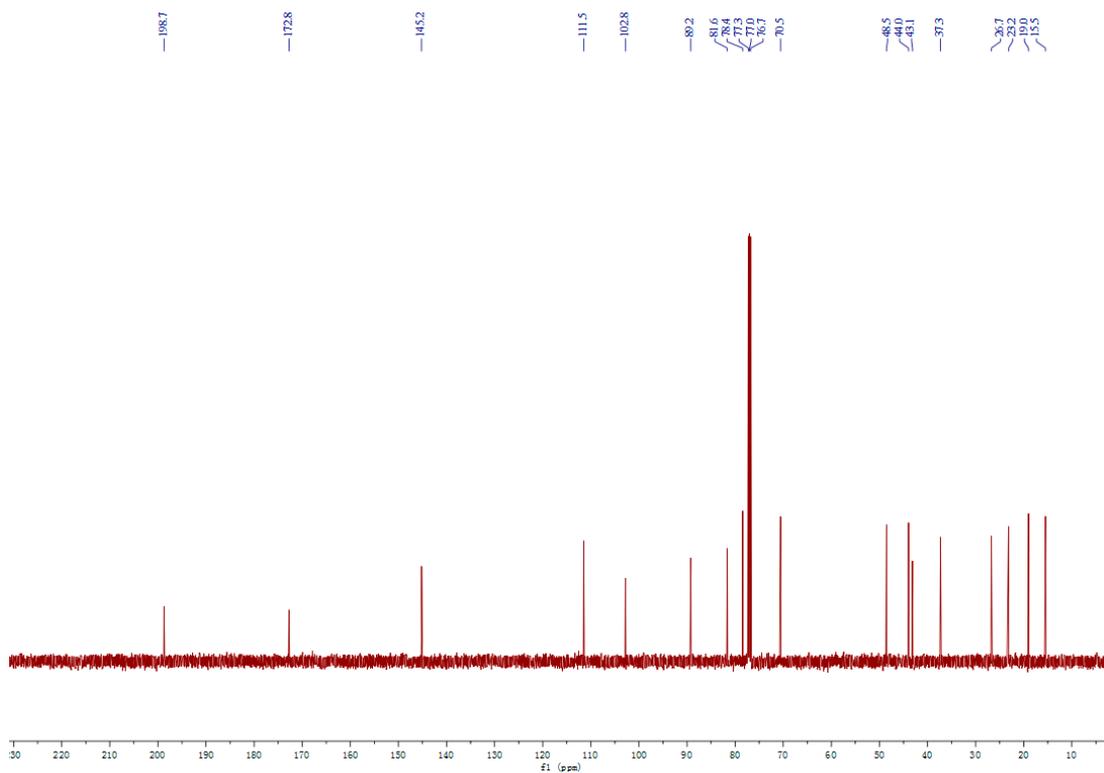


Figure S30. ^{13}C -NMR spectrum of guignardone A (5) in CDCl_3 .

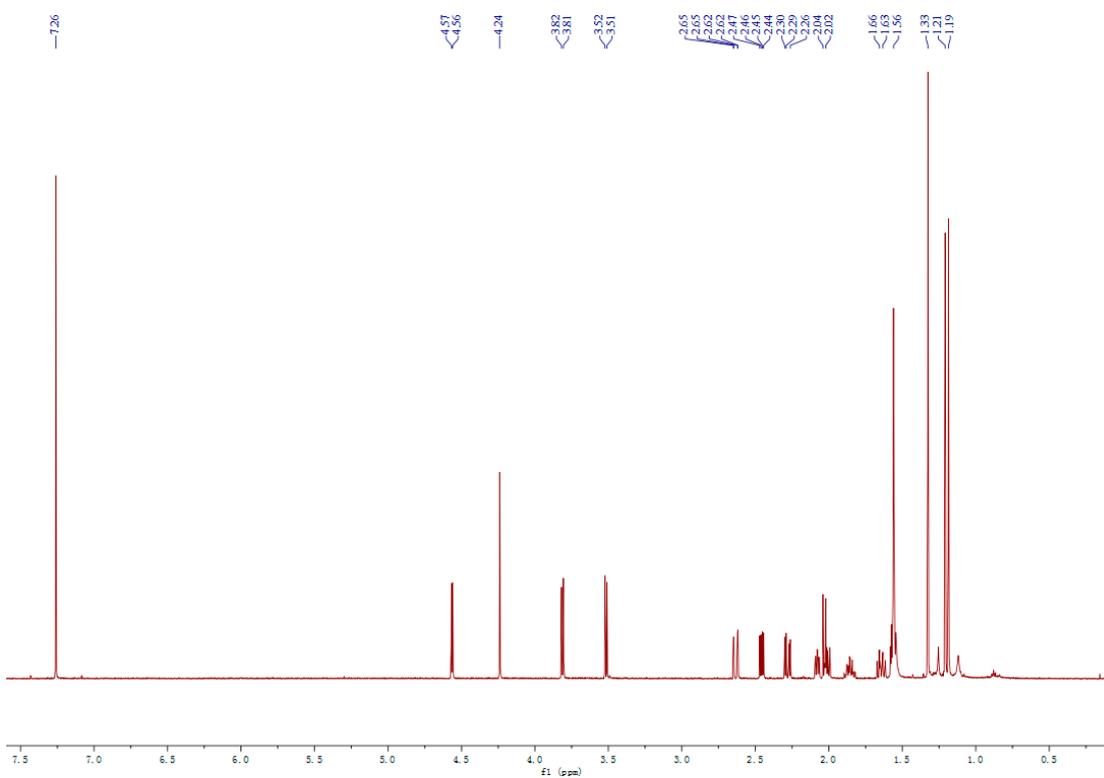


Figure S31. ^1H -NMR spectrum of guignardone B (6) in CDCl_3 .

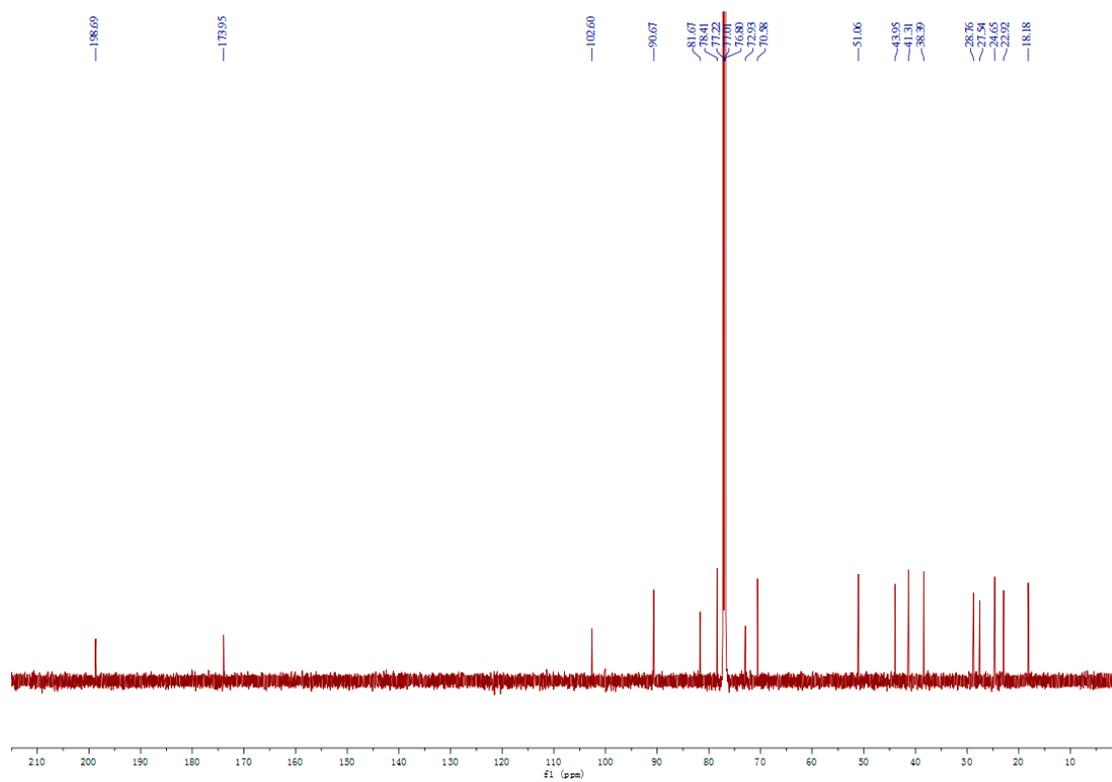


Figure S32. ¹³C-NMR spectrum of guignardone B (6) in CDCl₃.

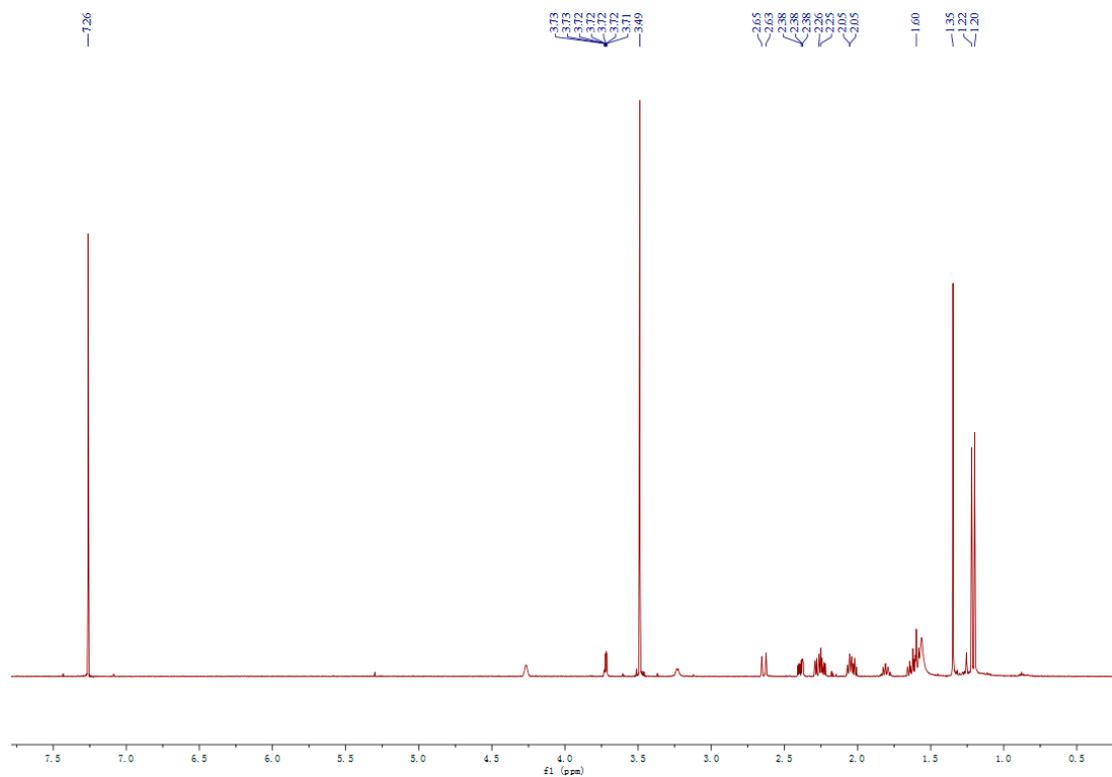


Figure S33 ¹H-NMR spectrum of guignardone I (7) in CDCl₃.

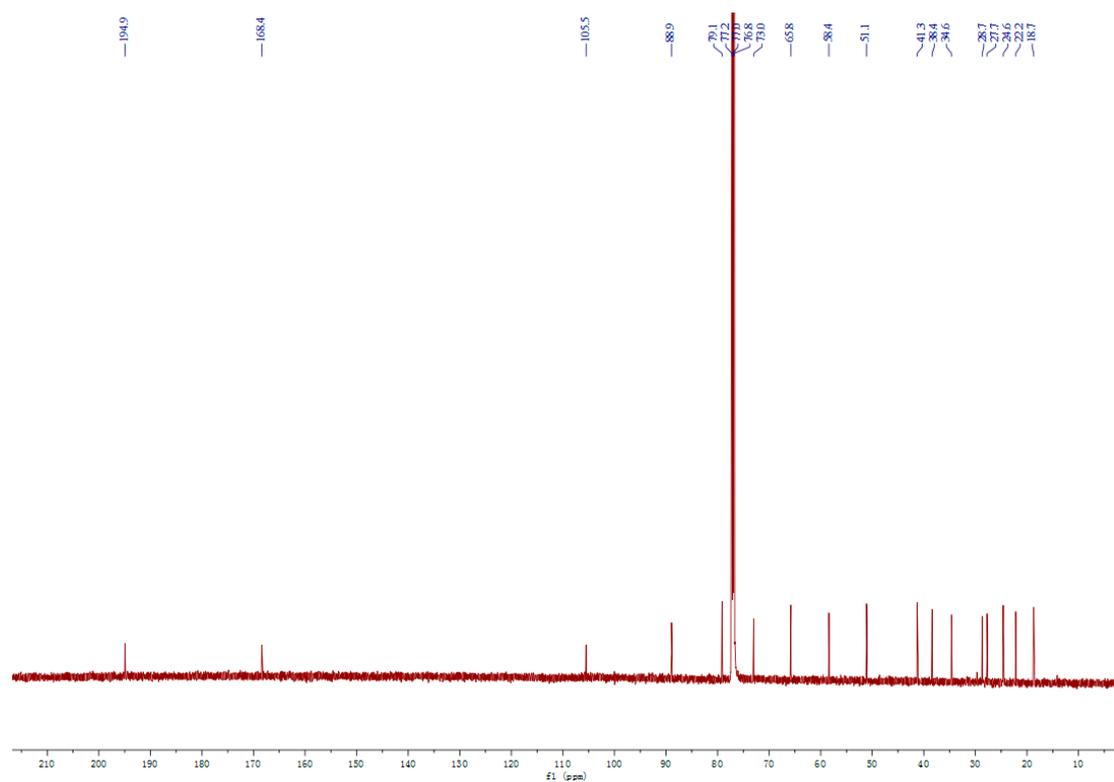


Figure S34. ¹³C-NMR spectrum of guignardone I (7) in CDCl₃.