Supporting Information

Lignans and Neolignans with Antioxidant and Human Cancer Cell Proliferation Inhibitory Activities from *Cinnamomum bejolghota* Confirm its Functional Food Property

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S1. ECD Calculations.

Figure S1. $^{1}H–^{1}H$ COSY (▬), Selected HMBC (H→C) and key ROESY (H↔H) correlations of **2**

Figure S2. $^{1}H–^{1}H$ COSY (▬), Selected HMBC (H→C) and key ROESY (H↔H) correlations of **3**

Figure S3. $^{1}H–^{1}H$ COSY (▬), Selected HMBC (H→C) and key ROESY (H↔H) correlations of **4**

Figure S4. $^{1}H–^{1}H$ COSY (▬), Selected HMBC (H→C) and key ROESY (H↔H) correlations of **10**

For bejolghotin A (1)

Figure S5. ^{1}H NMR spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

Figure S6. ^{13}C NMR spectrum (150 MHz) of bejolghotin A (**1**) in $CDCl_3$

Figure S7. $^{1}H–^{1}H$ COSY spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

Figure S8. HSQC spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

Figure S9. HMBC spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

Figure S10. ROESY spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

Figure S11. HRESIMS spectrum of bejolghotin A (**1**)

Figure S12. UV spectrum of bejolghotin A (**1**)

Figure S13. IR spectrum (KBr disc) of bejolghotin A (**1**)

For bejolghotin B (2)

Figure S14. ^{1}H NMR spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

Figure S15. ^{13}C NMR spectrum (150 MHz) of bejolghotin B (**2**) in $CDCl_3$

Figure S16. $^{1}H–^{1}H$ COSY spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

Figure S17. HSQC spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

Figure S18. HMBC spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

Figure S19. ROESY spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

Figure S20. HRESIMS spectrum of bejolghotin B (**2**)

Figure S21. UV spectrum of bejolghotin B (**2**)

Figure S22. IR spectrum (KBr disc) of bejolghotin B (**2**)

For bejolghotin C (3)

S1. ECD Calculations.

Conformational search was carried out by CONFLEX using the Merck molecular force field (MMFF) with standard parameters.[1] Next, they were subjected to geometry optimization at the B3LYP/6-31G(d) level of DFT calculations. Based on the DFT energies, conformers with a Boltzmann distribution $\geqslant$1% were chosen for ECD calculations. The conformers were imported into Gaussian 09 package.[2] The ECD curves of the conformers were calculated by the TDDFT method at the B3LYP/6-311++G (2d, p) level with the CPCM model in a methanol solution.

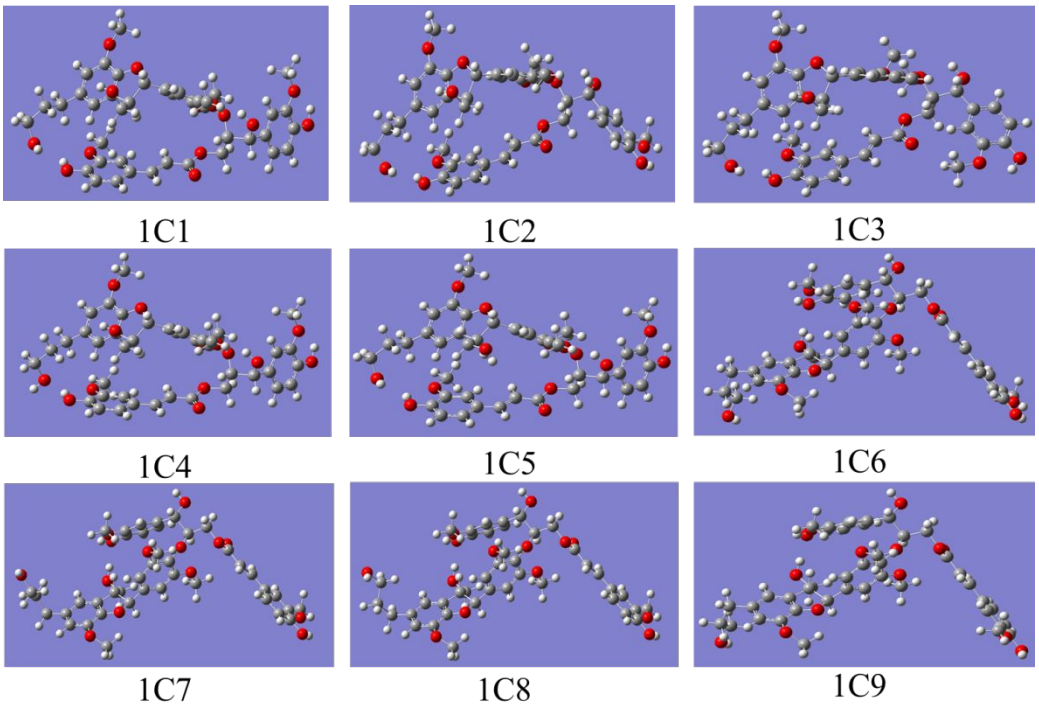


Fig. 1. B3LYP/6-311+G(d,p) optimized lowest energy conformers for compound **1**.

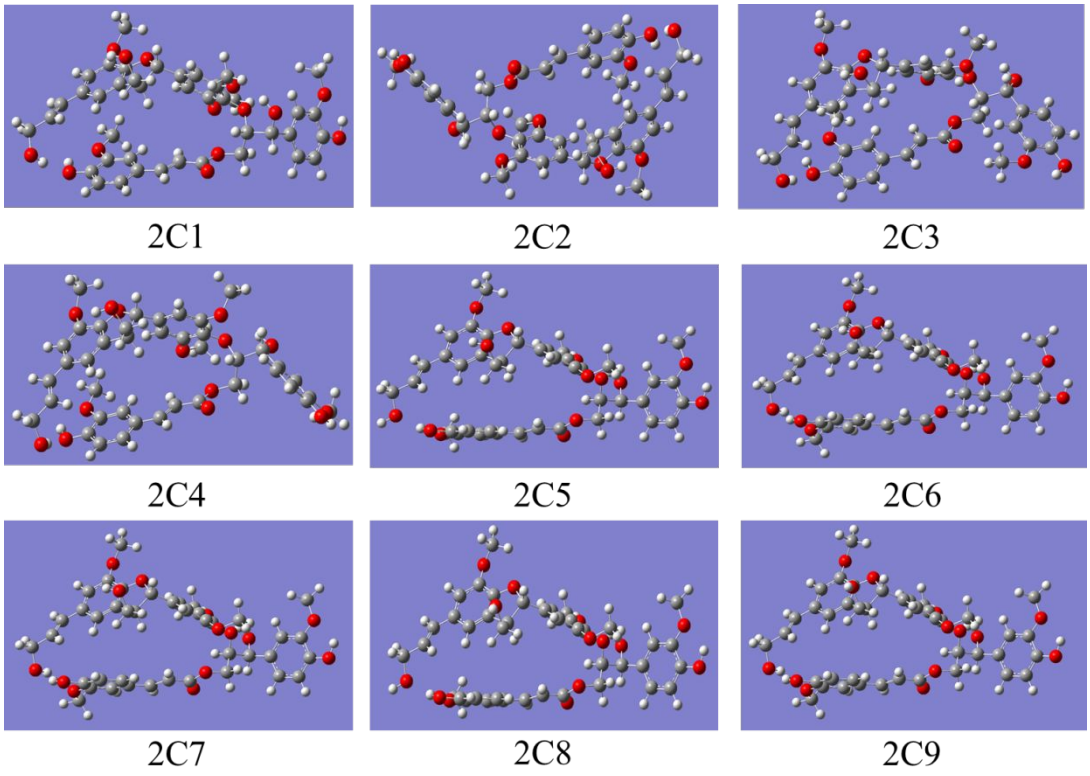


Fig. 2. B3LYP/6-311+G(d,p) optimized lowest energy conformers for compound **2**.

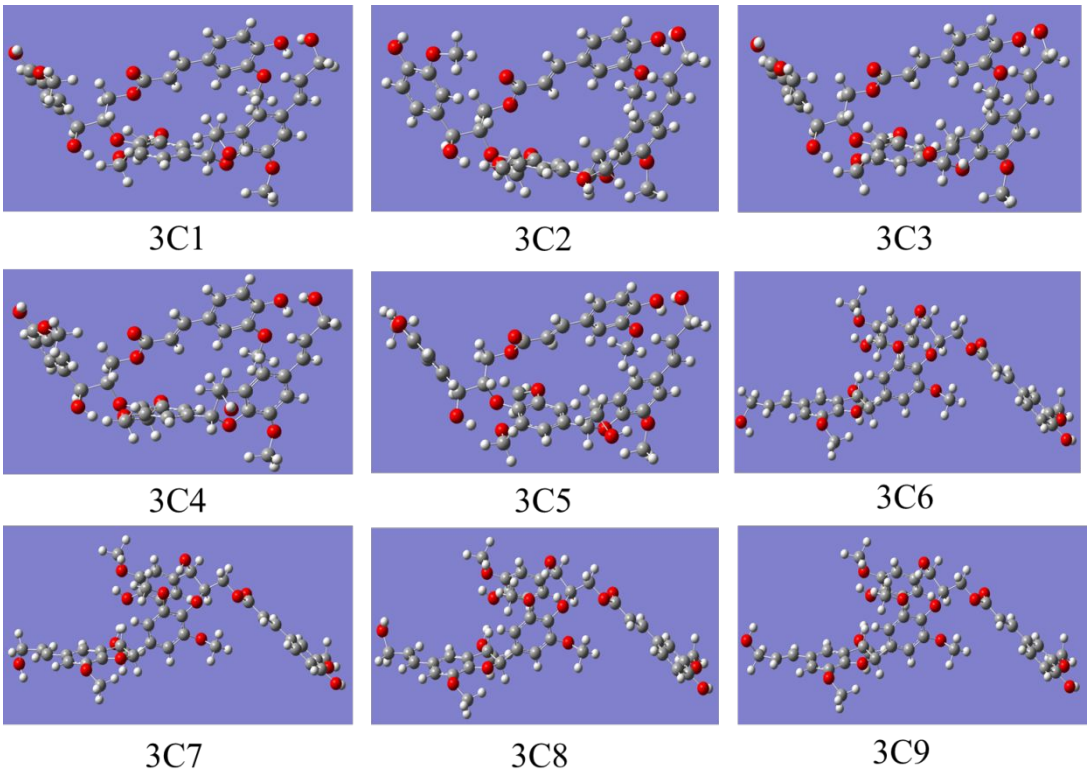


Fig. 3. B3LYP/6-311+G(d,p) optimized lowest energy conformers for compound **3**.

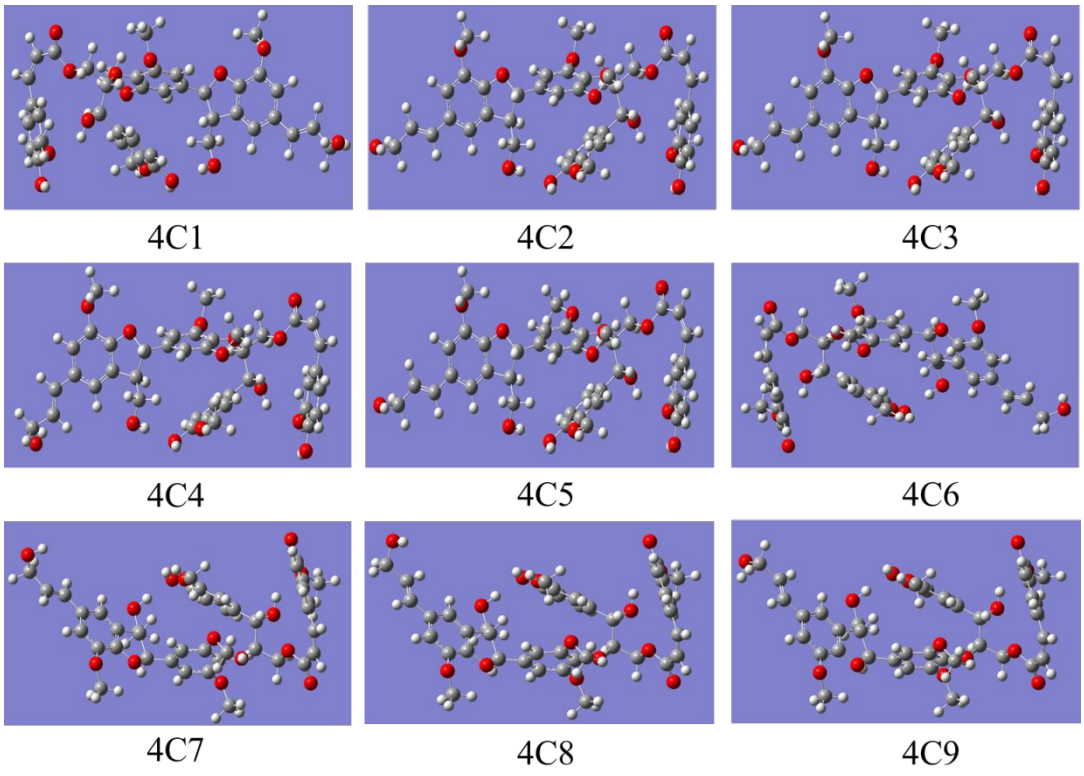


Fig. 4. B3LYP/6-311+G(d,p) optimized lowest energy conformers for compound **4**.

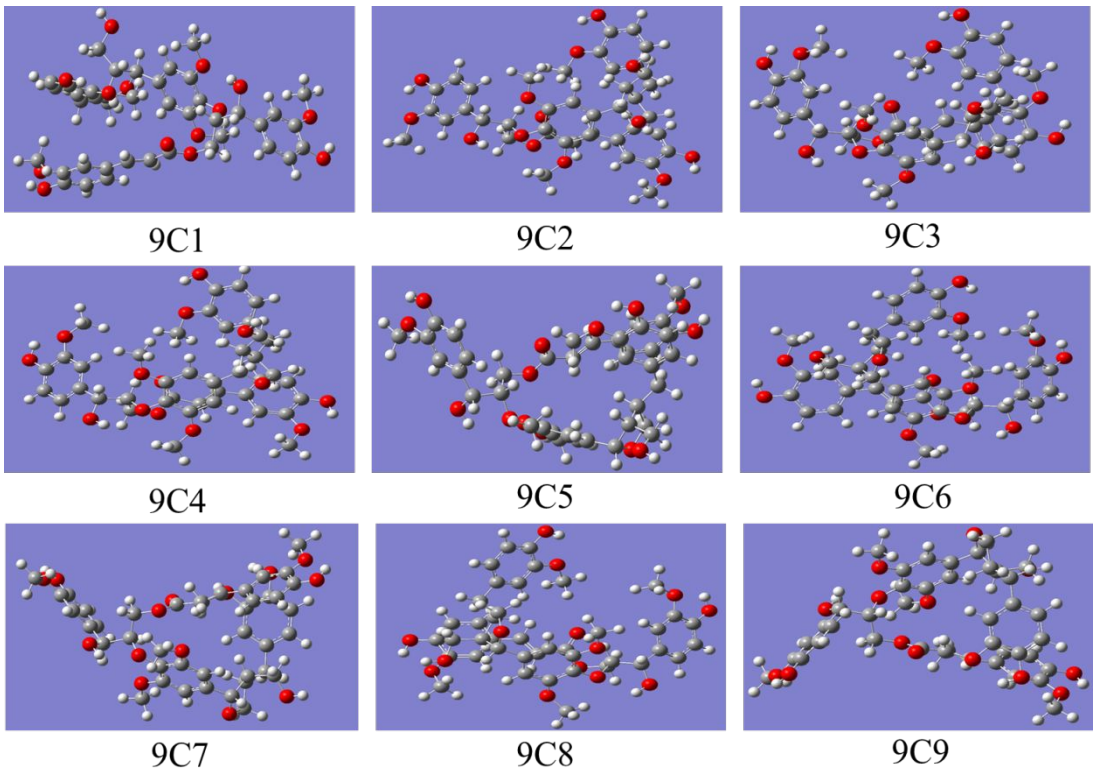


Fig. 5. B3LYP/6-311+G(d,p) optimized lowest energy conformers for compound **9**.

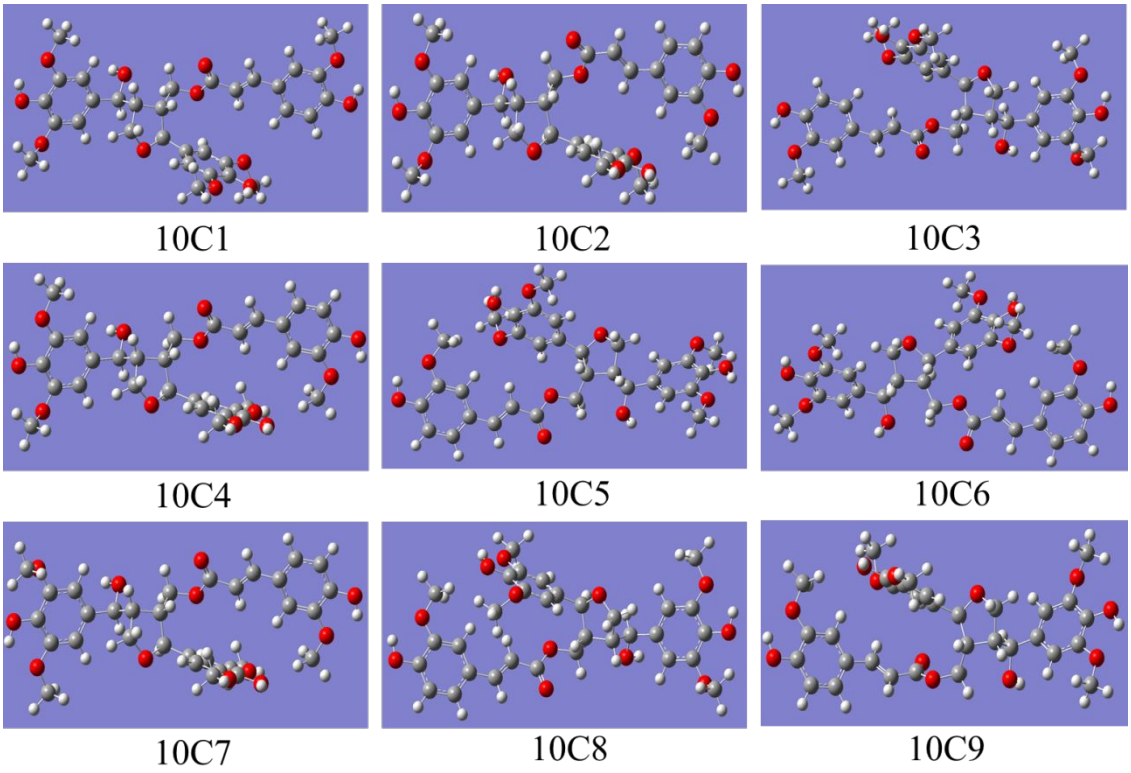


Fig. 6. B3LYP/6-311+G(d,p) optimized lowest energy conformers for compound **10**.

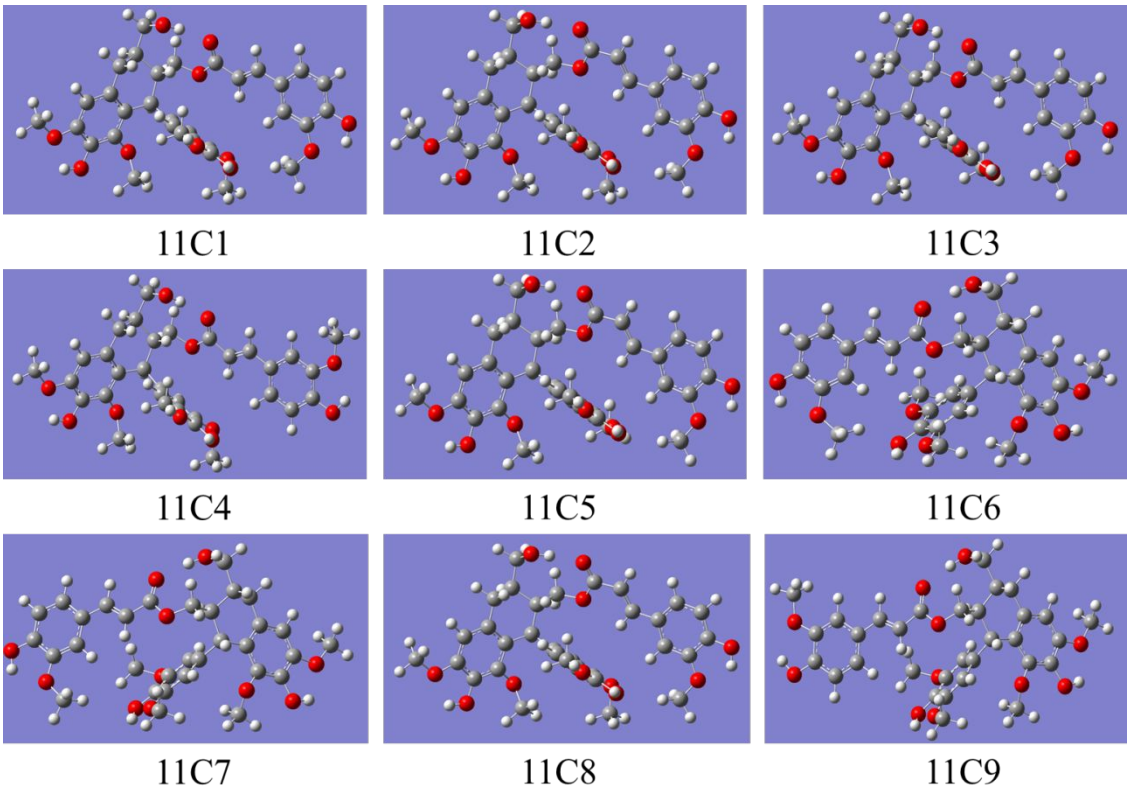


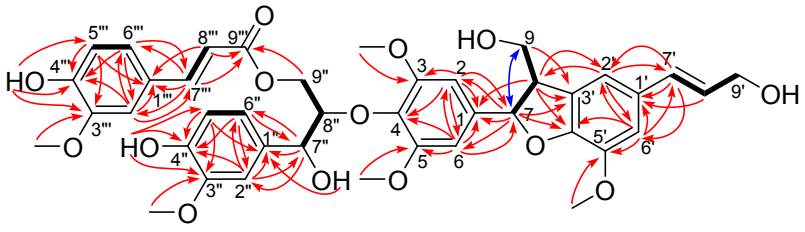
Fig. 7. B3LYP/6-311+G(d,p) optimized lowest energy conformers for compound **11**.

Reference:

(1) Jagannadh, B.; Reddy, S. S.; Thangavelu, R. P. Conformational preferences of 1,4,7-trithiacyclononane: a molecular mechanics and density functional theory study. *J. Mol. Model.* **2004**, *10*, 55−59.

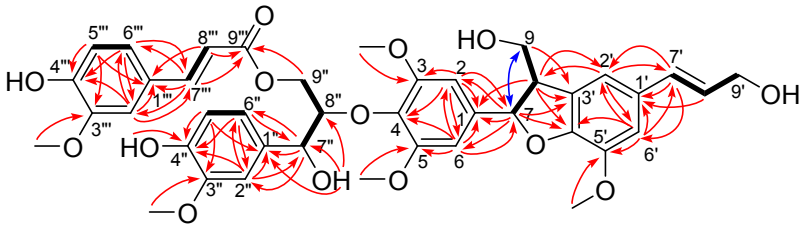
(2) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, Jr., J. A.; 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.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc.: Wallingford CT, 2016.

Figure S1. ^{1}H–^{1}H COSY (▬), Selected HMBC (H→C) and key ROESY (H↔H) correlations of **2**



2

Figure S2. ^{1}H–^{1}H COSY (▬), Selected HMBC (H→C) and key ROESY (H↔H) correlations of **3**



3

Figure S3. ^{1}H–^{1}H COSY (▬), Selected HMBC (H→C) and key ROESY (H↔H) correlations of **4**

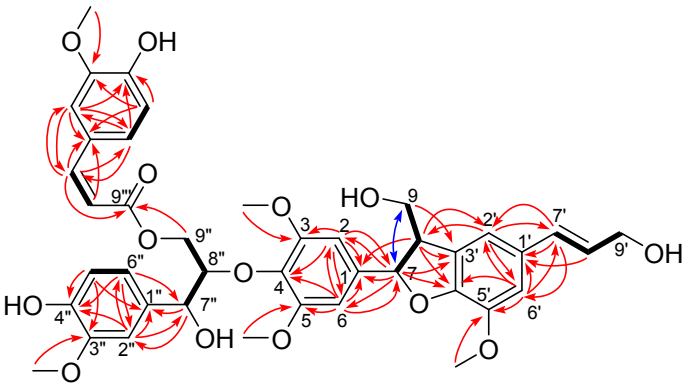


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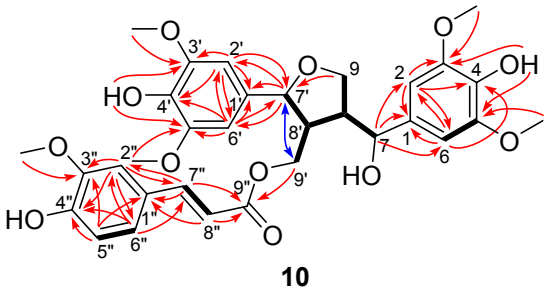
Figure S4. ^{1}H–^{1}H COSY (▬), Selected HMBC (H→C) and key ROESY (H↔H) correlations of **10**



10

Figure S5. ^{1}H NMR spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

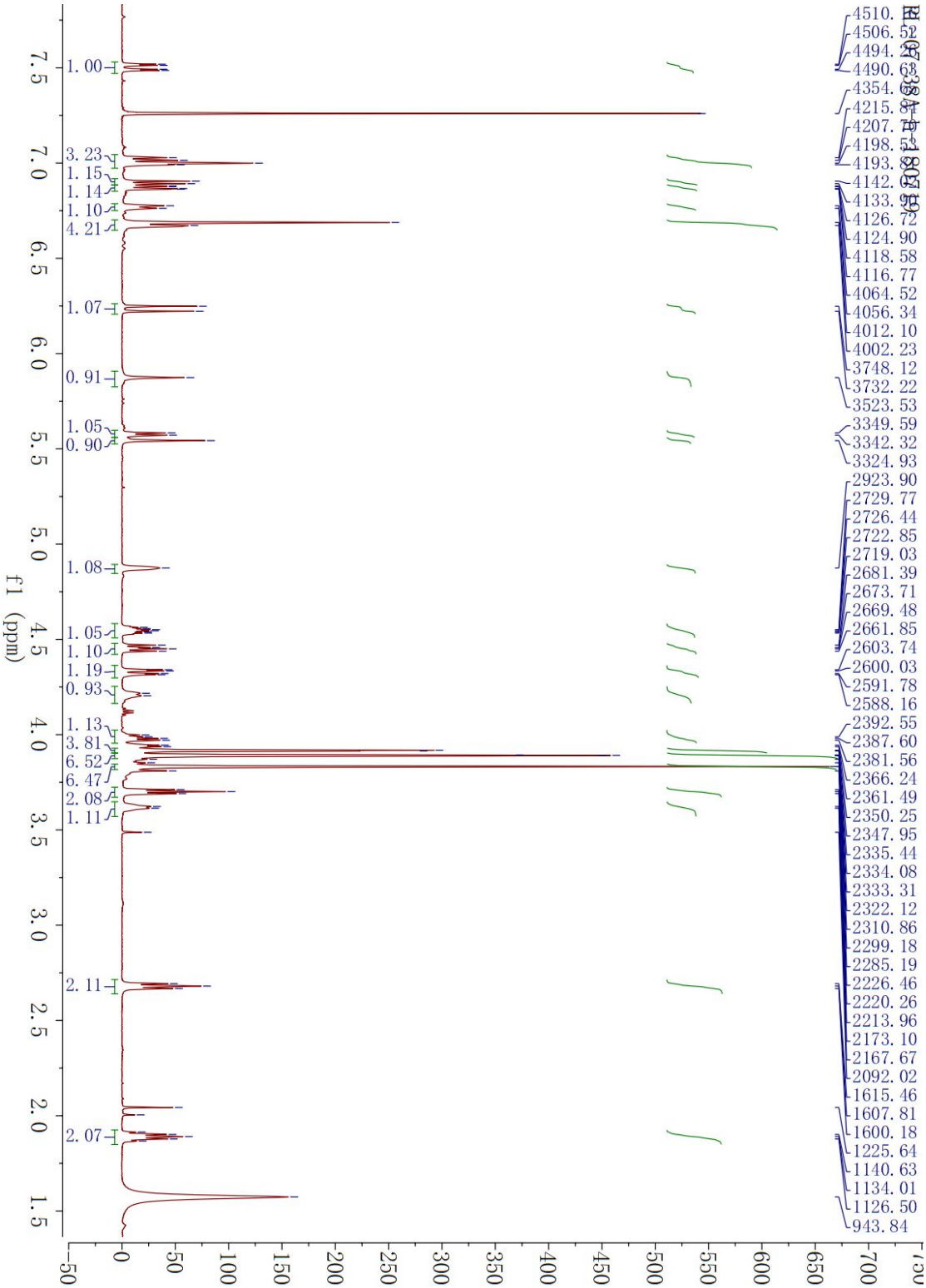


Figure S6. ^{13}C NMR spectrum (150 MHz) of bejolghotin A (**1**) in $CDCl_3$

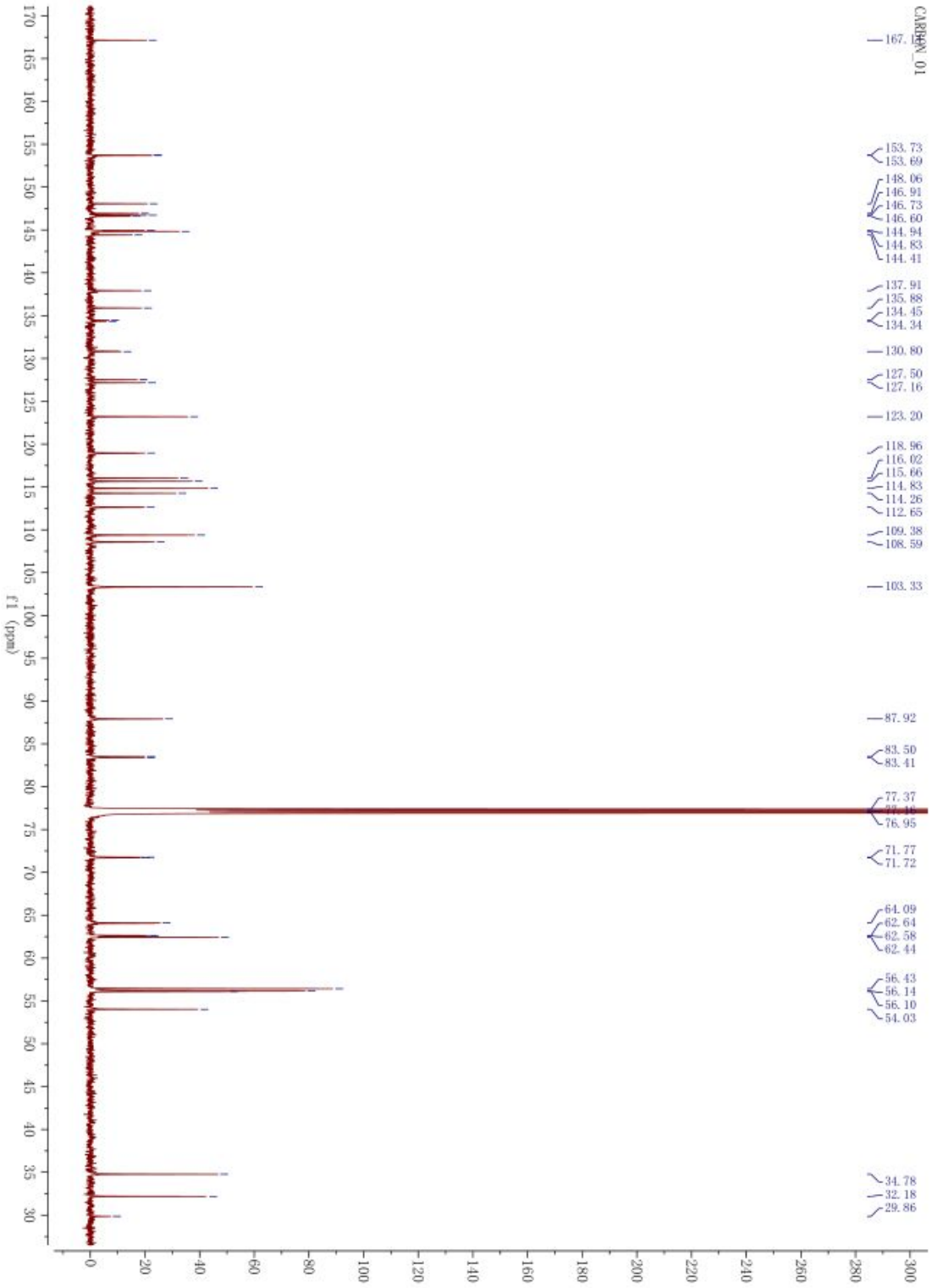


Figure S7. $^{1}H-^{1}H$ COSY spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

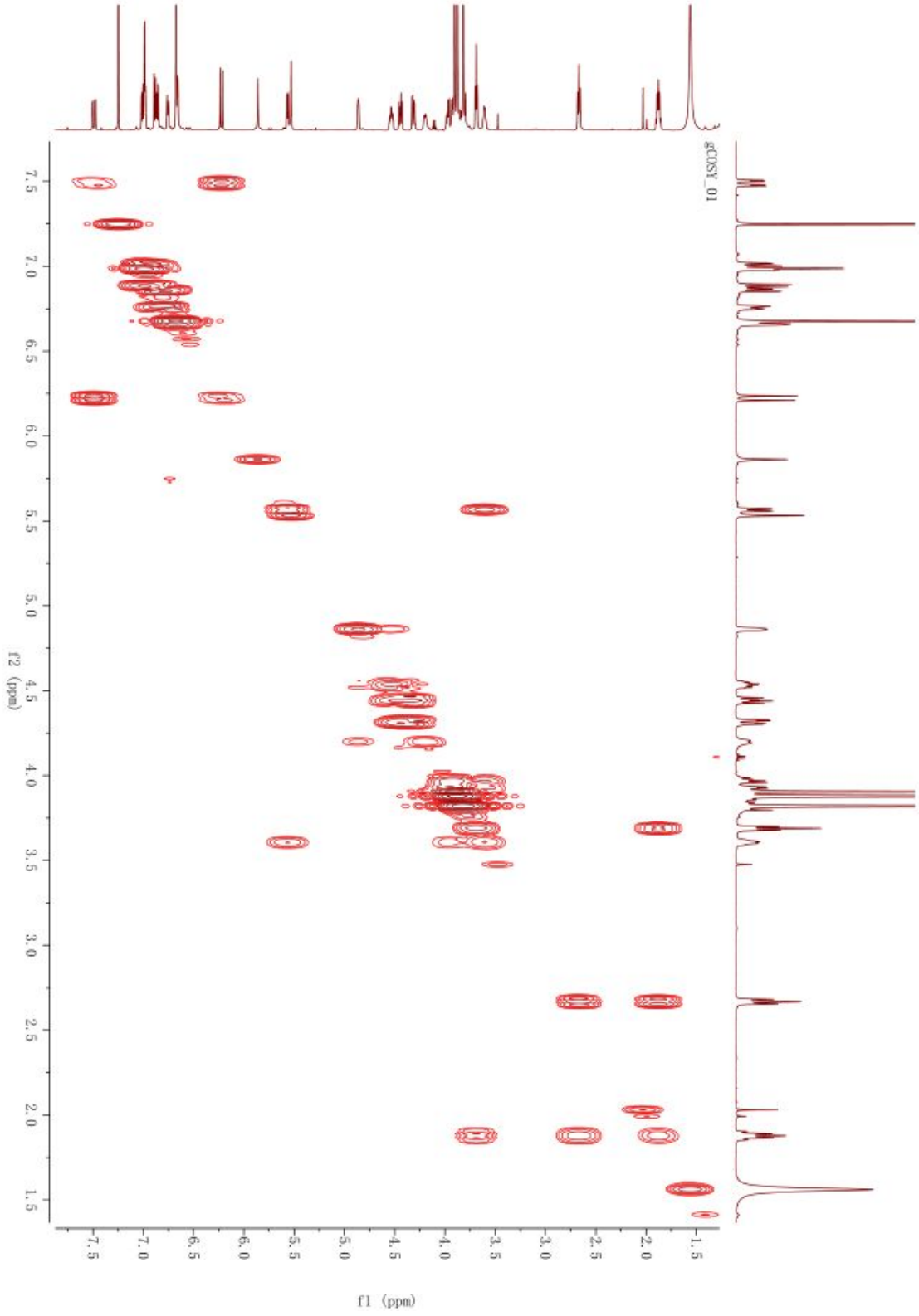


Figure S8. HSQC spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

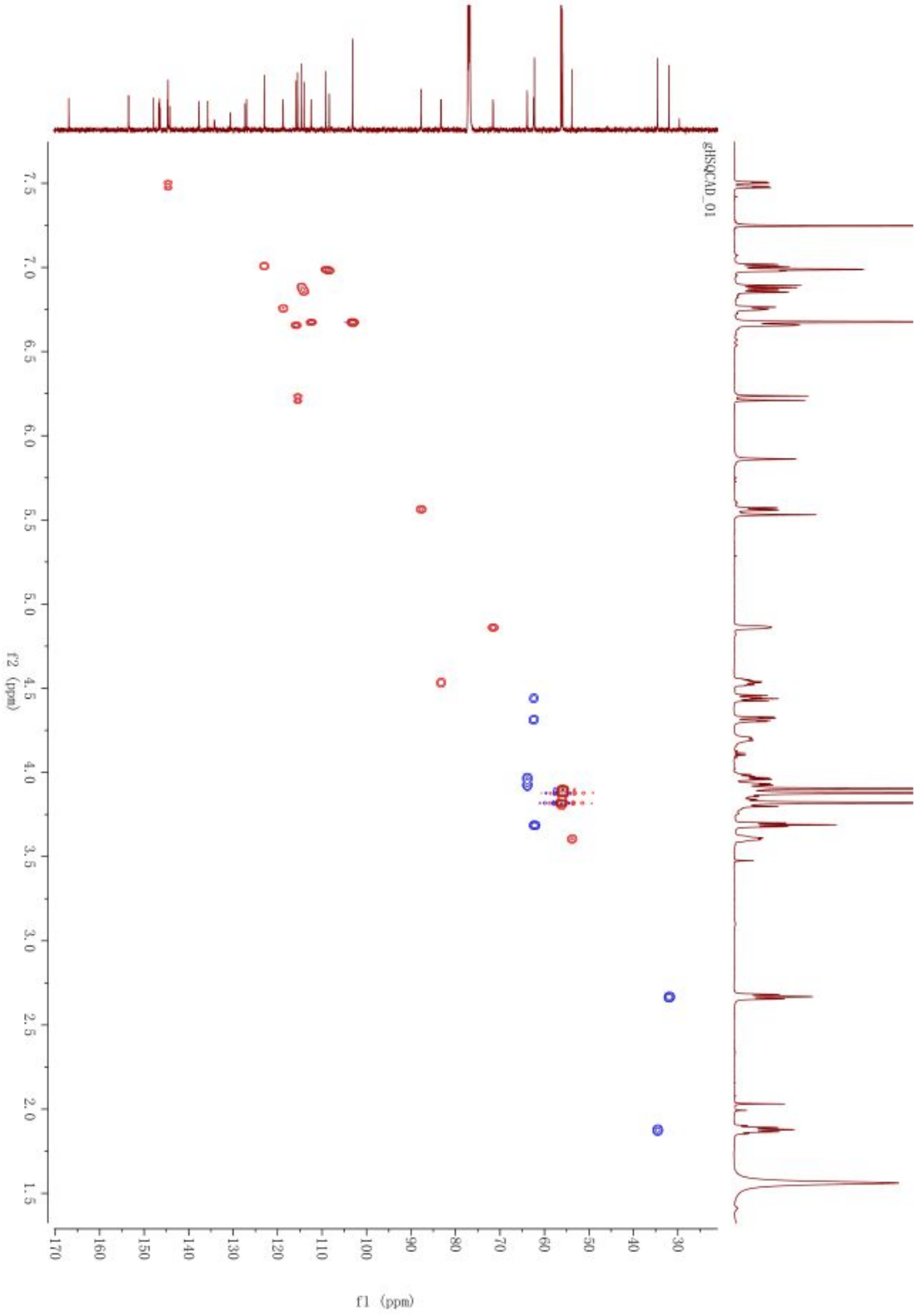


Figure S9. HMBC spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

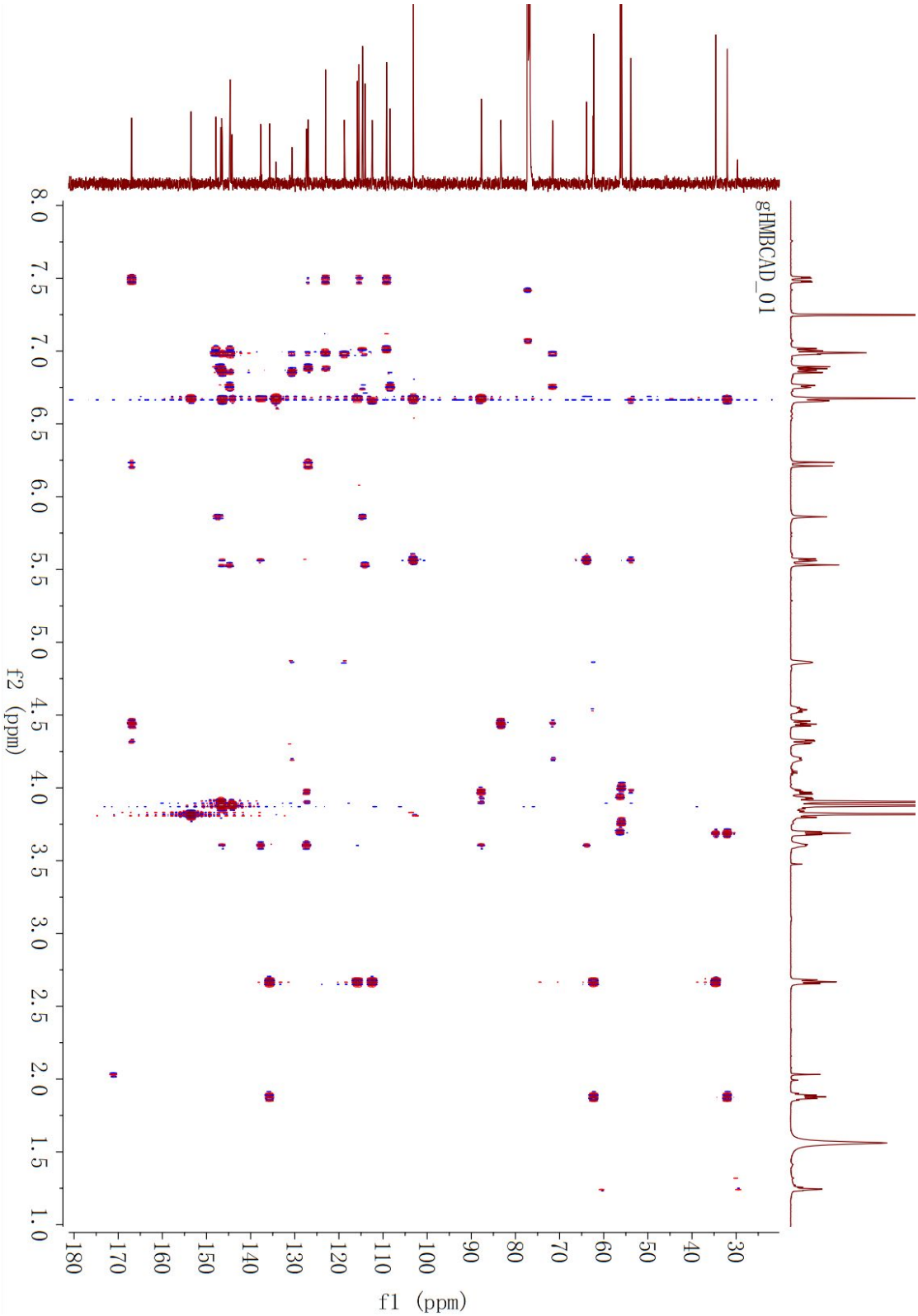


Figure S10. ROESY spectrum (600 MHz) of bejolghotin A (**1**) in $CDCl_3$

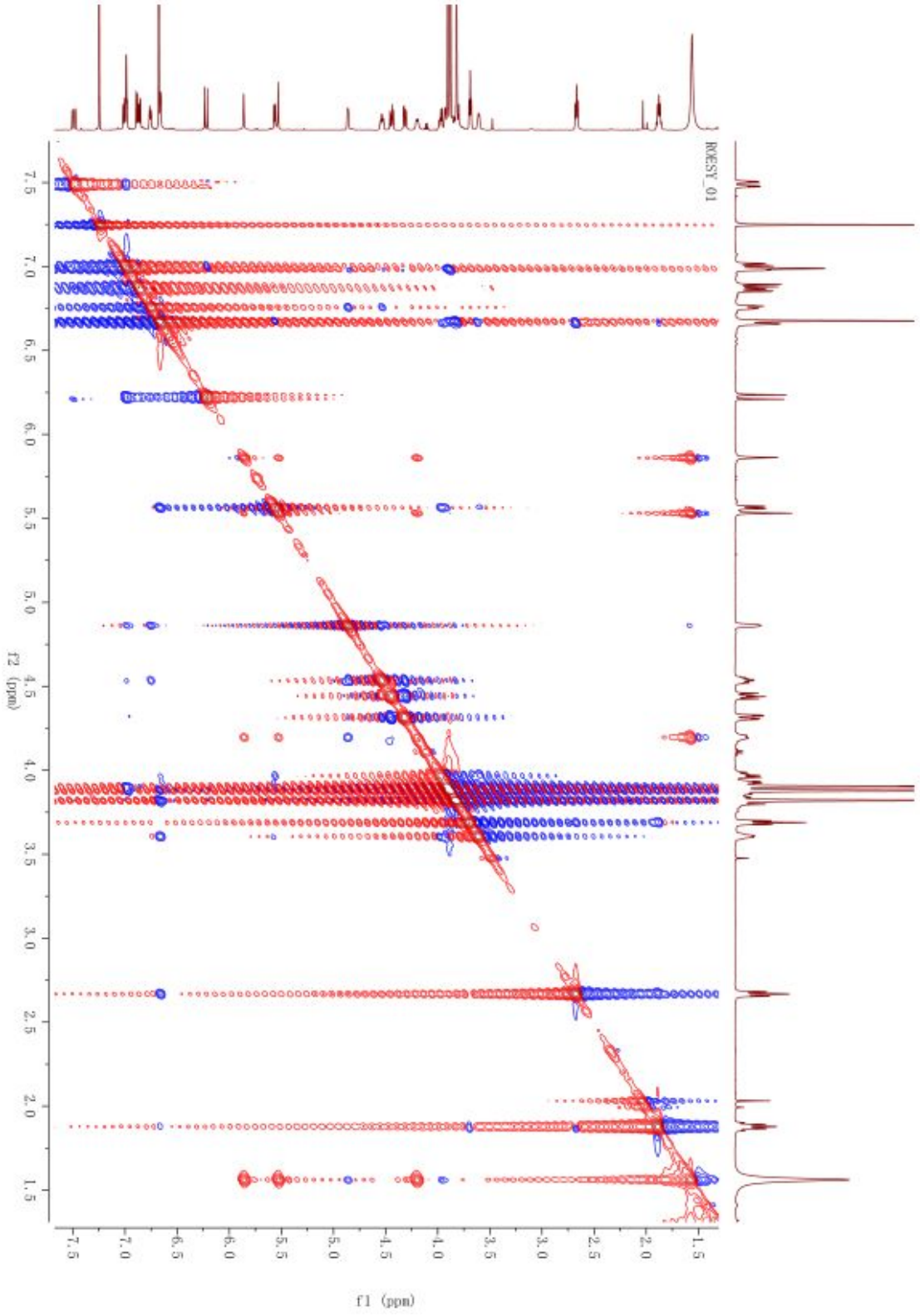


Figure S11. HRESIMS spectrum of bejolghotin A (**1**)

Mass Spectrum SmartFormula Report

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Sample Name	RL0738A	Instrument	solariX
Comment			

Acquisition Parameter

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Broadband High Mass	1100.0 m/z	n/a	n/a	n/a	n/a
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Pulse Program	basic	n/a	n/a	Calibration Date	Sun Apr 8 02:39:02 2018
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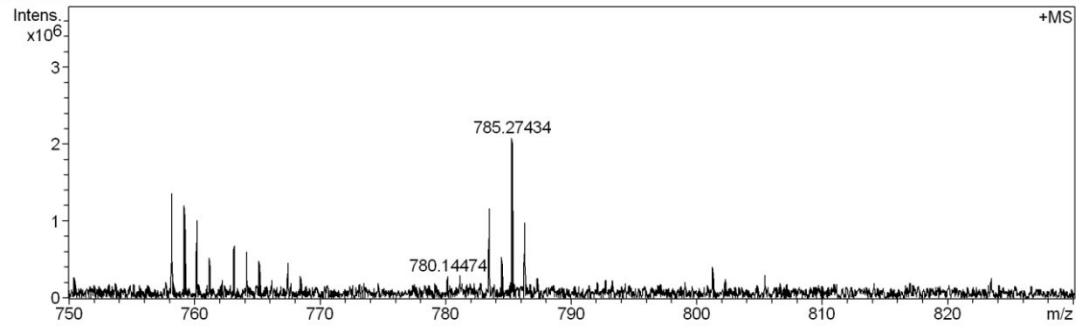

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785.27434	1	C 41 H 46 Na O 14	100.00	785.27798	4.63	3.55	16.0	18.5	even	ok

Figure S12. UV spectrum of bejolghotin A (**1**)

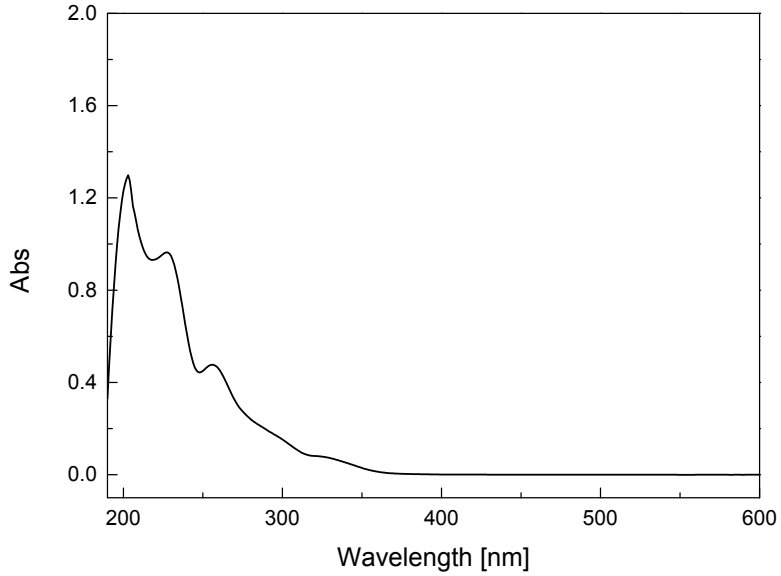


Figure S13. IR spectrum (KBr disc) of bejolghotin A (**1**)

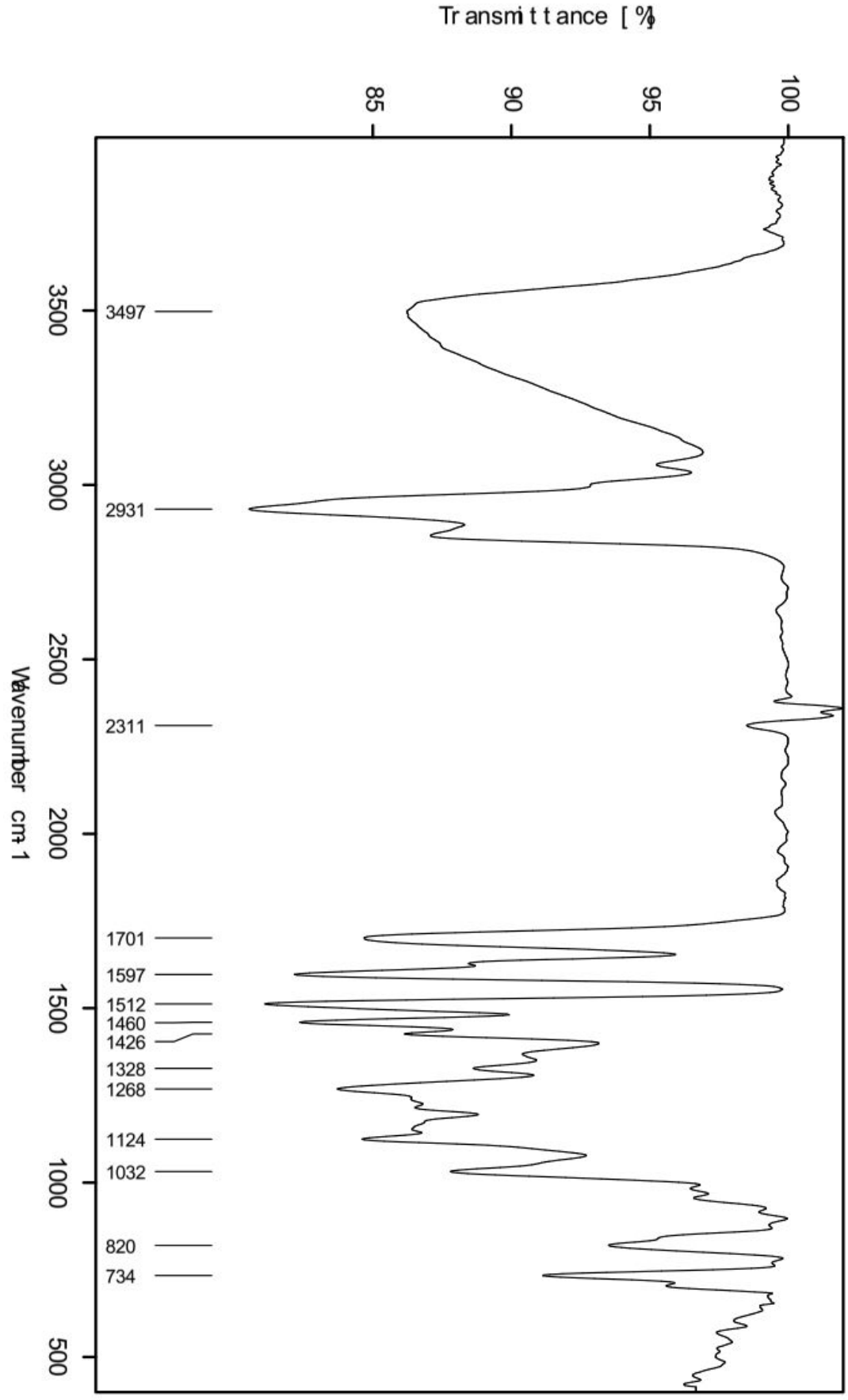


Figure S14. ^{1}H NMR spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

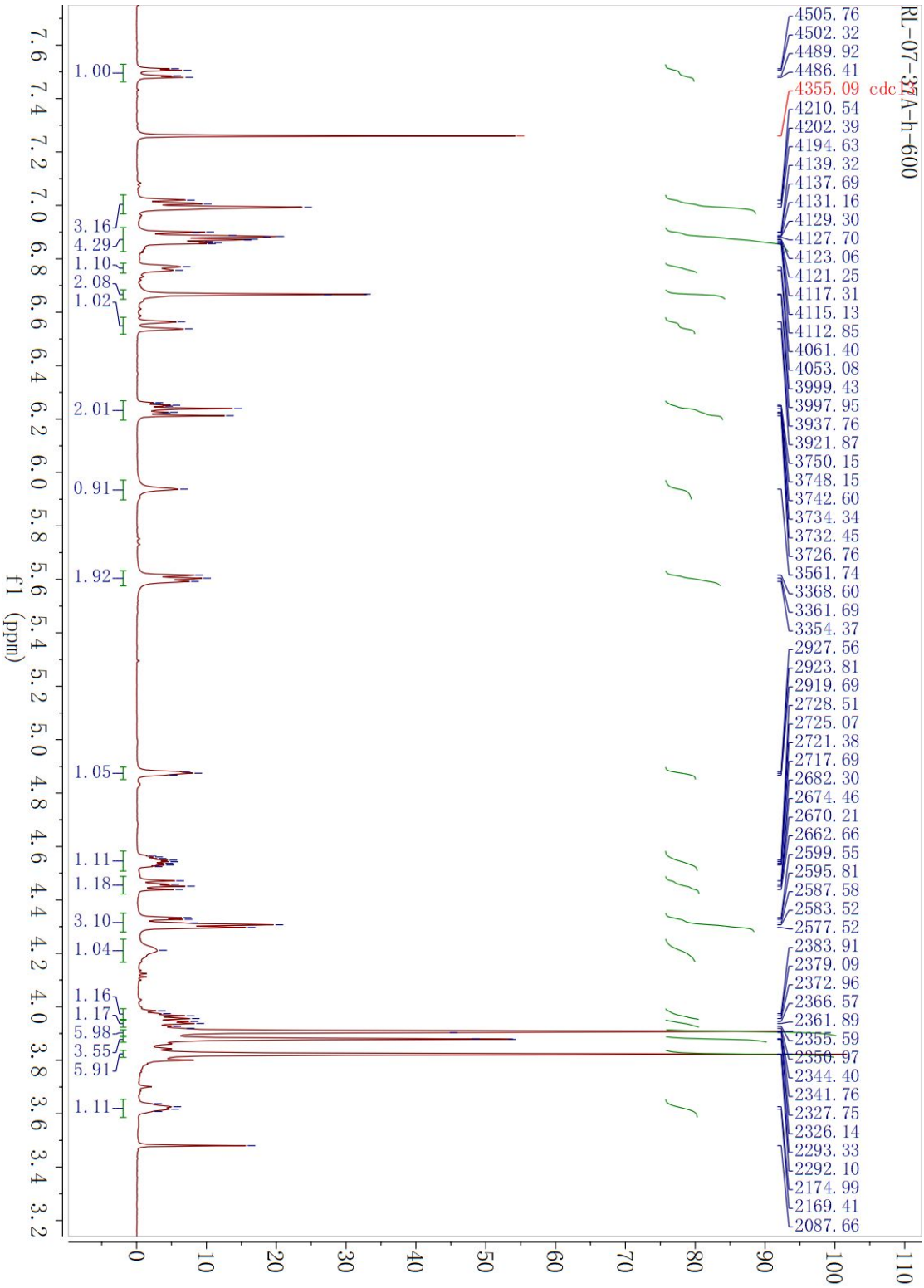


Figure S15. ^{13}C NMR spectrum (150 MHz) of bejolghotin B (**2**) in $CDCl_3$

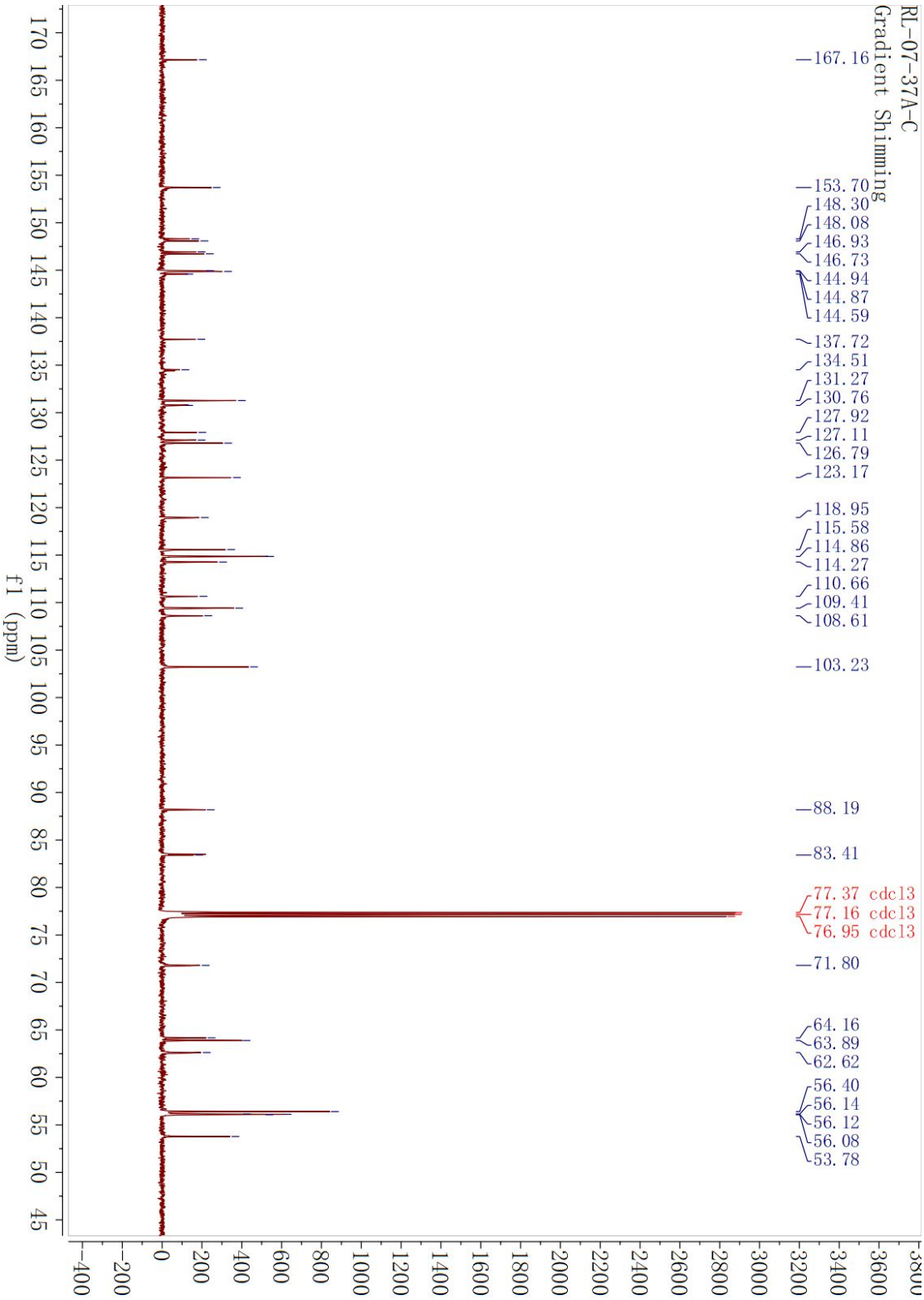


Figure S16. $^{1}H-^{1}H$ COSY spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

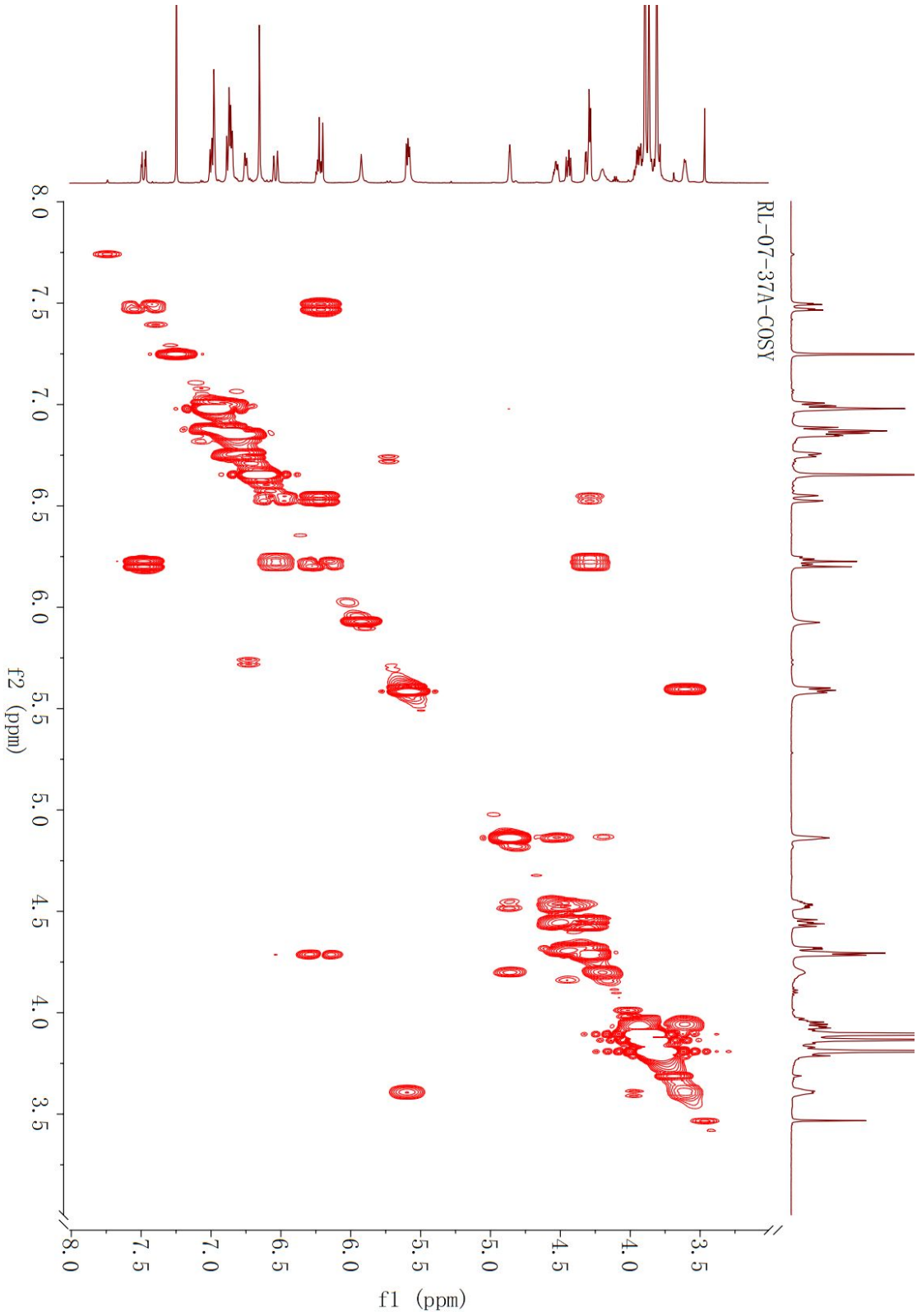


Figure S17. HSQC spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

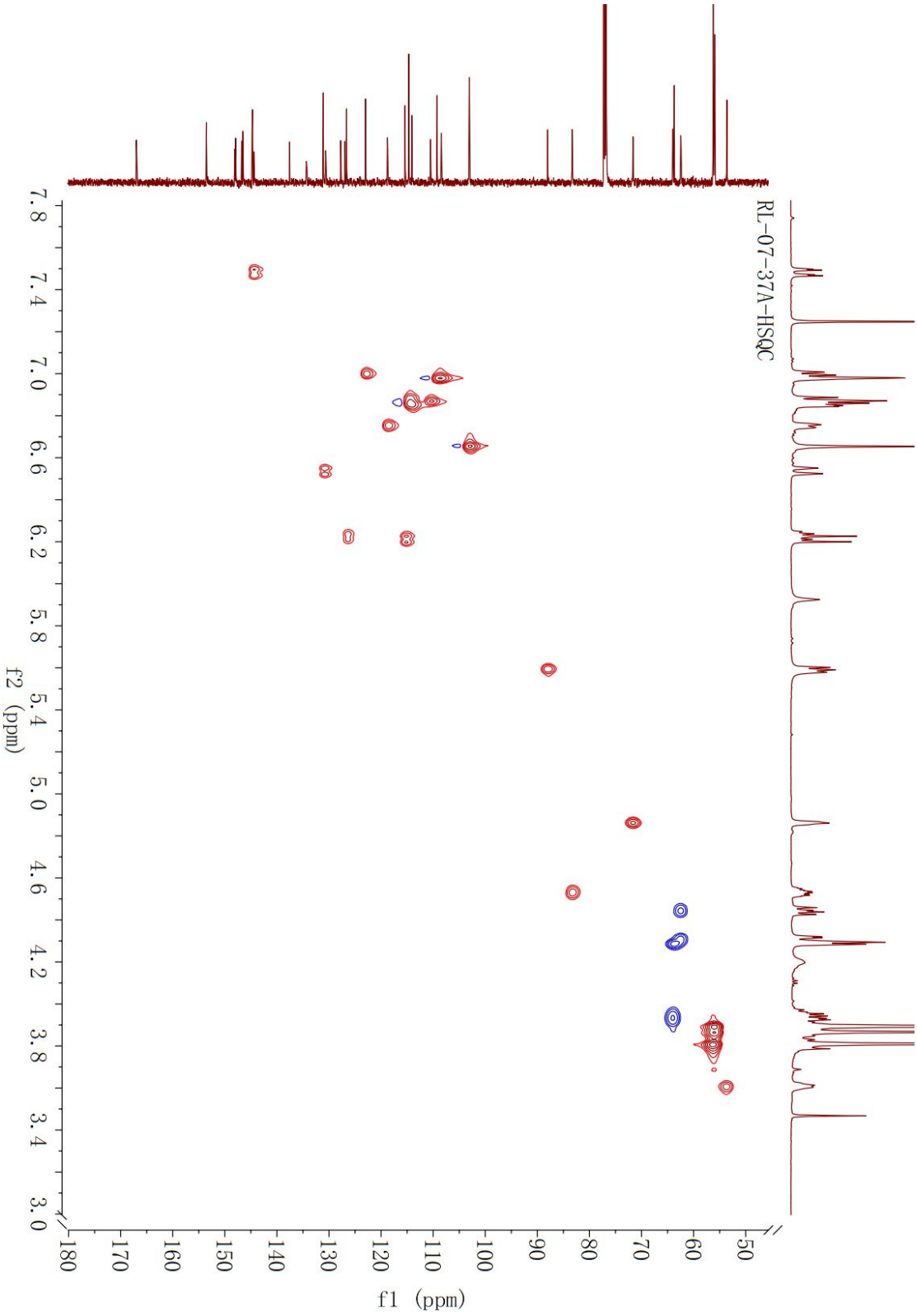


Figure S18. HMBC spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

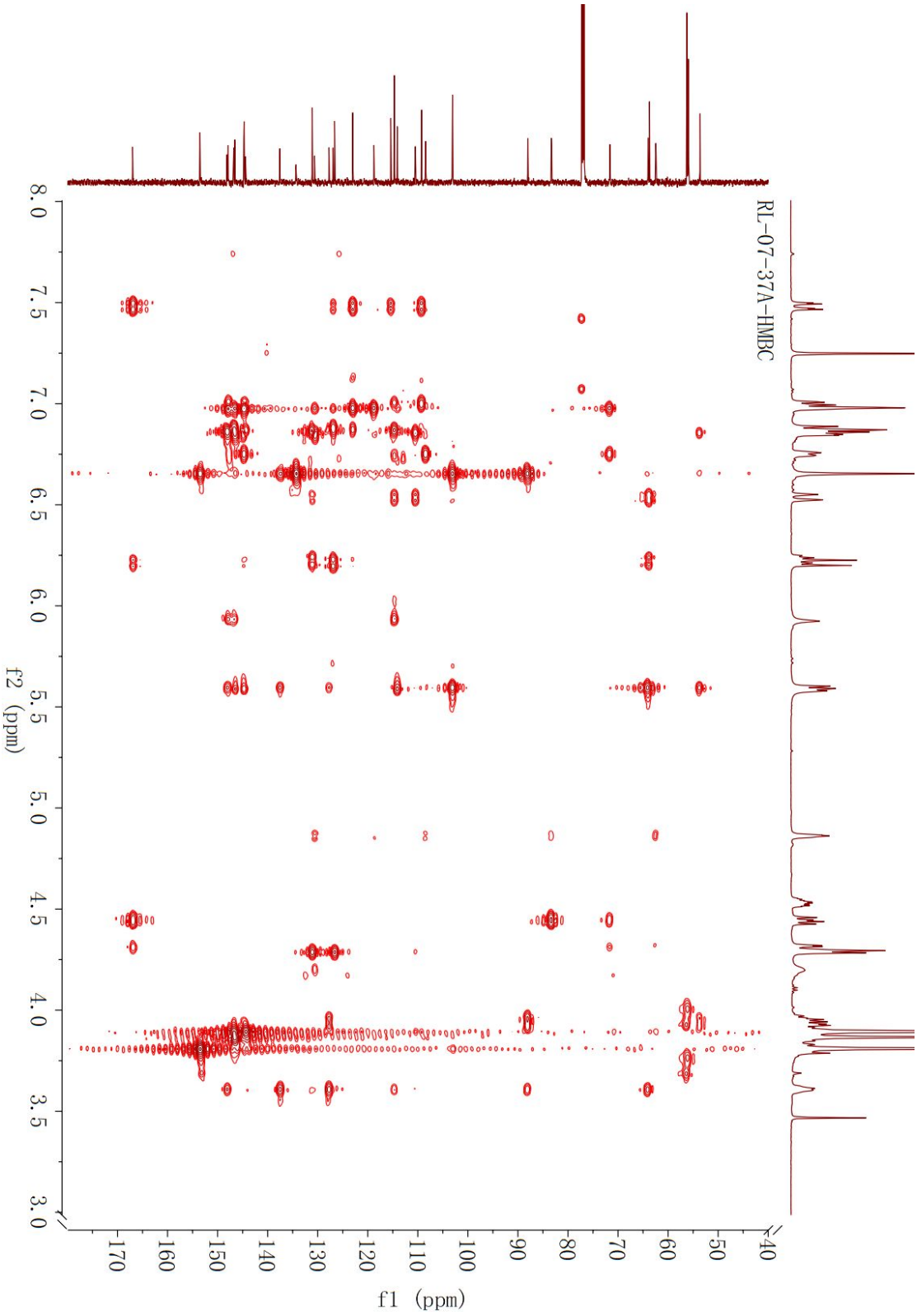


Figure S19. ROESY spectrum (600 MHz) of bejolghotin B (**2**) in $CDCl_3$

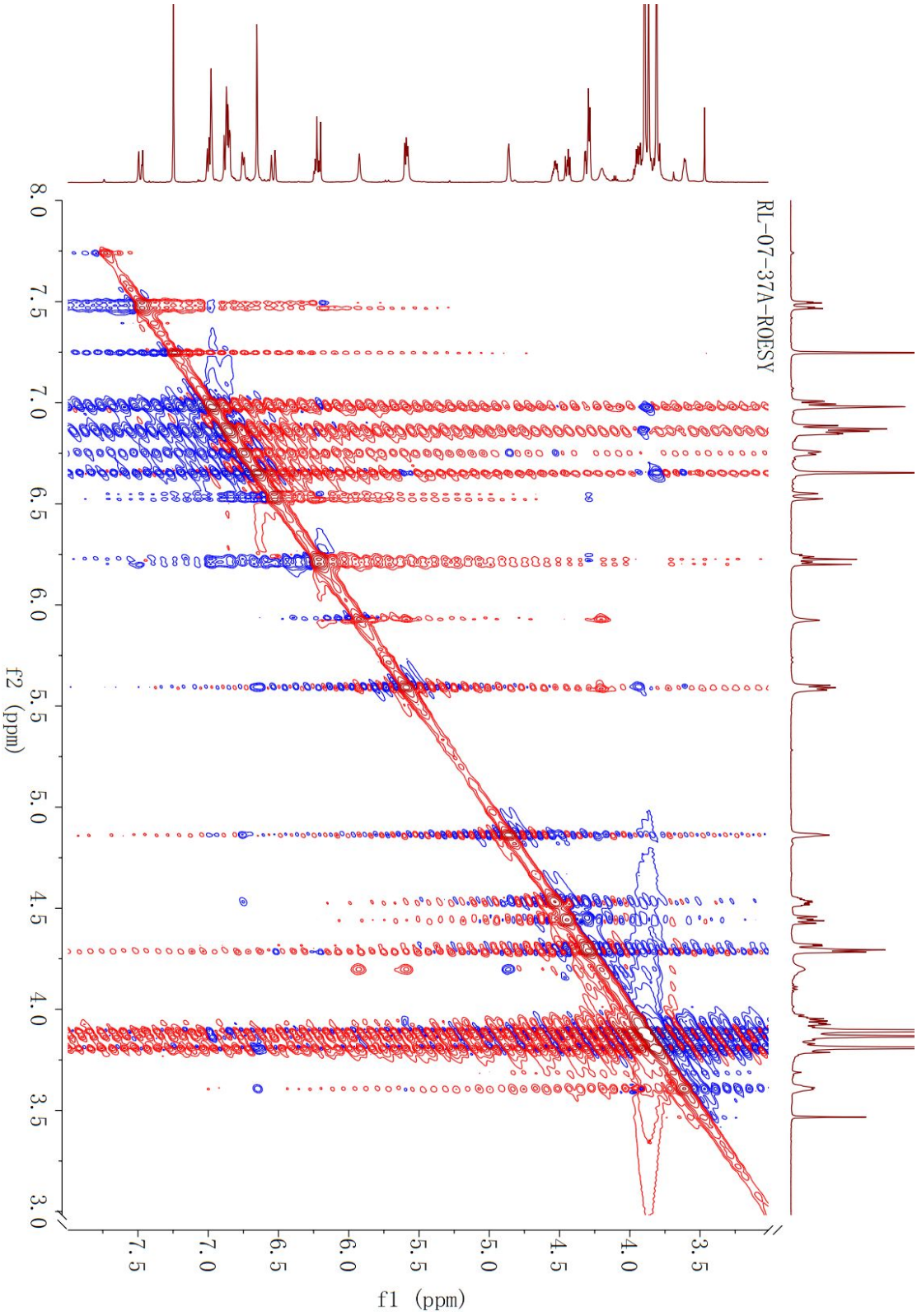
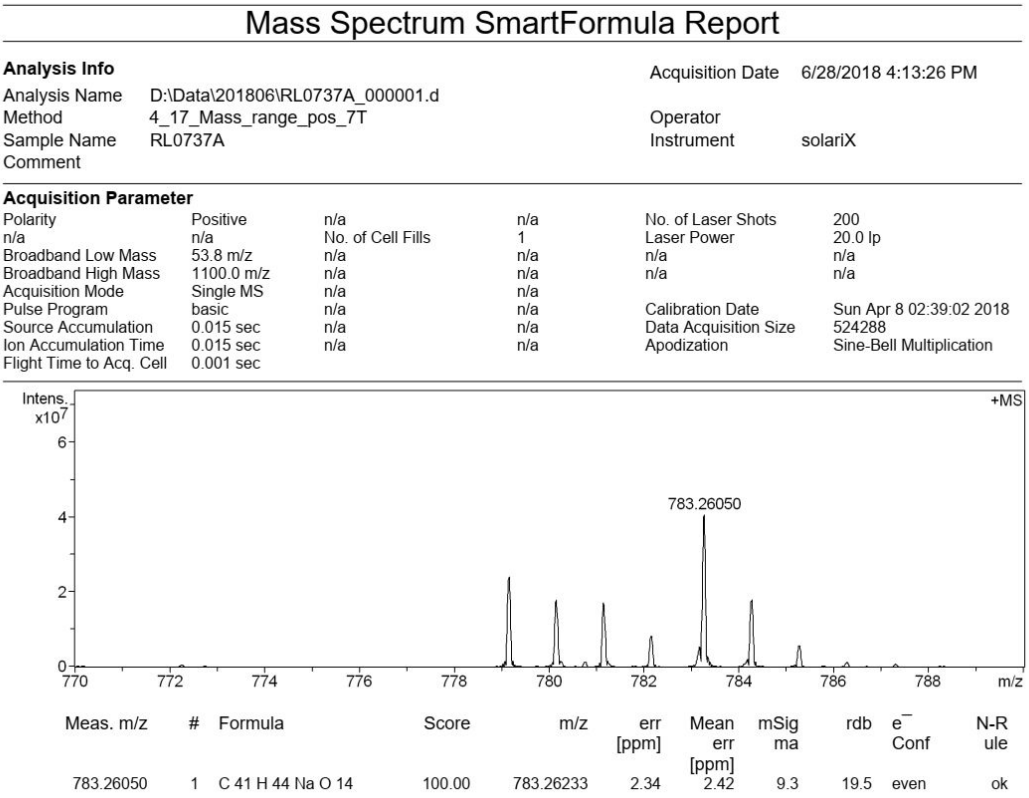


Figure S20. HRESIMS spectrum of bejolghotin B (**2**)



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Comment			

Acquisition Parameter

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n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
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Broadband High Mass	1100.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Sun Apr 8 02:39:02 2018
Source Accumulation	0.015 sec	n/a	n/a	Data Acquisition Size	524288
Ion Accumulation Time	0.015 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e⁻ Conf	N-R ule
783.26050	1	C 41 H 44 Na O 14	100.00	783.26233	2.34	2.42	9.3	19.5	even	ok

Figure S21. UV spectrum of bejolghotin B (**2**)

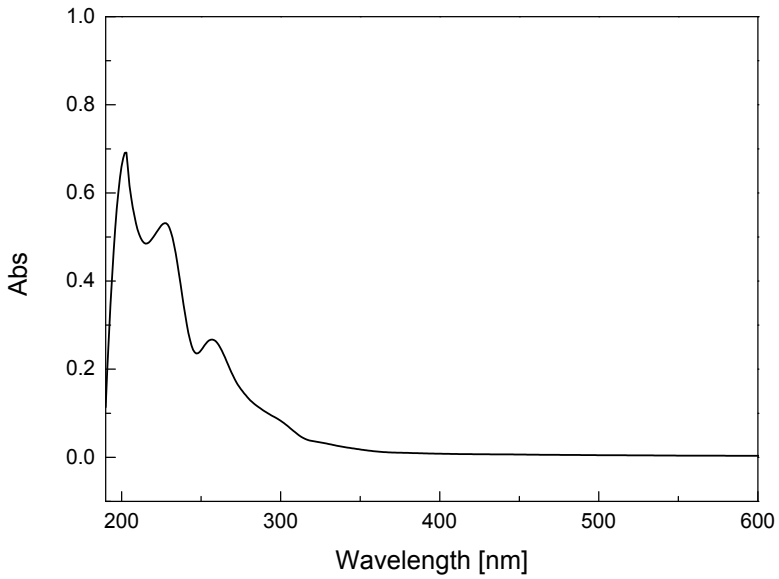


Figure S22. IR spectrum (KBr disc) of bejolghotin B (**2**)

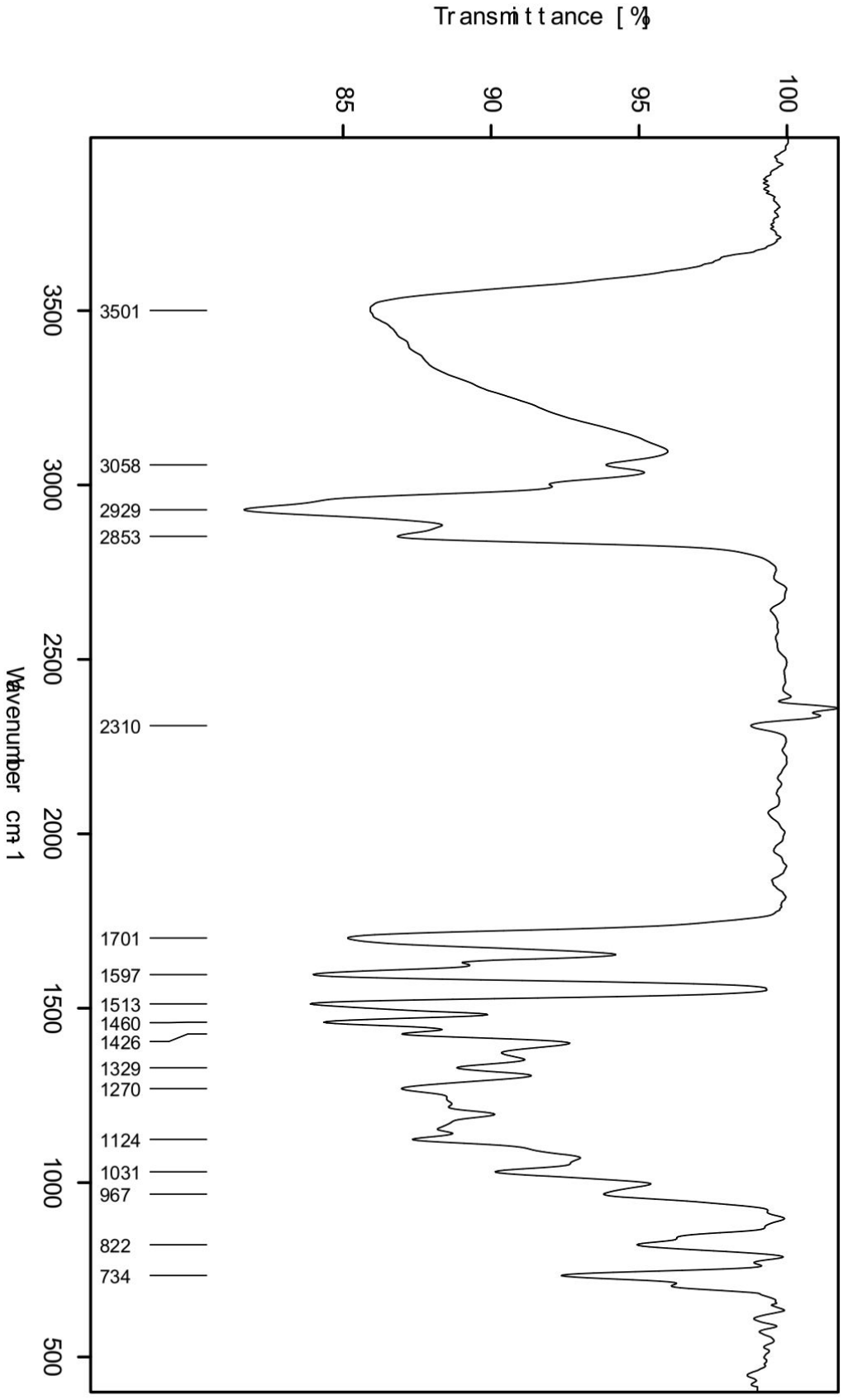


Figure S23. ^{1}H NMR spectrum (600 MHz) of bejolghotin C (**3**) in $CDCl_3$

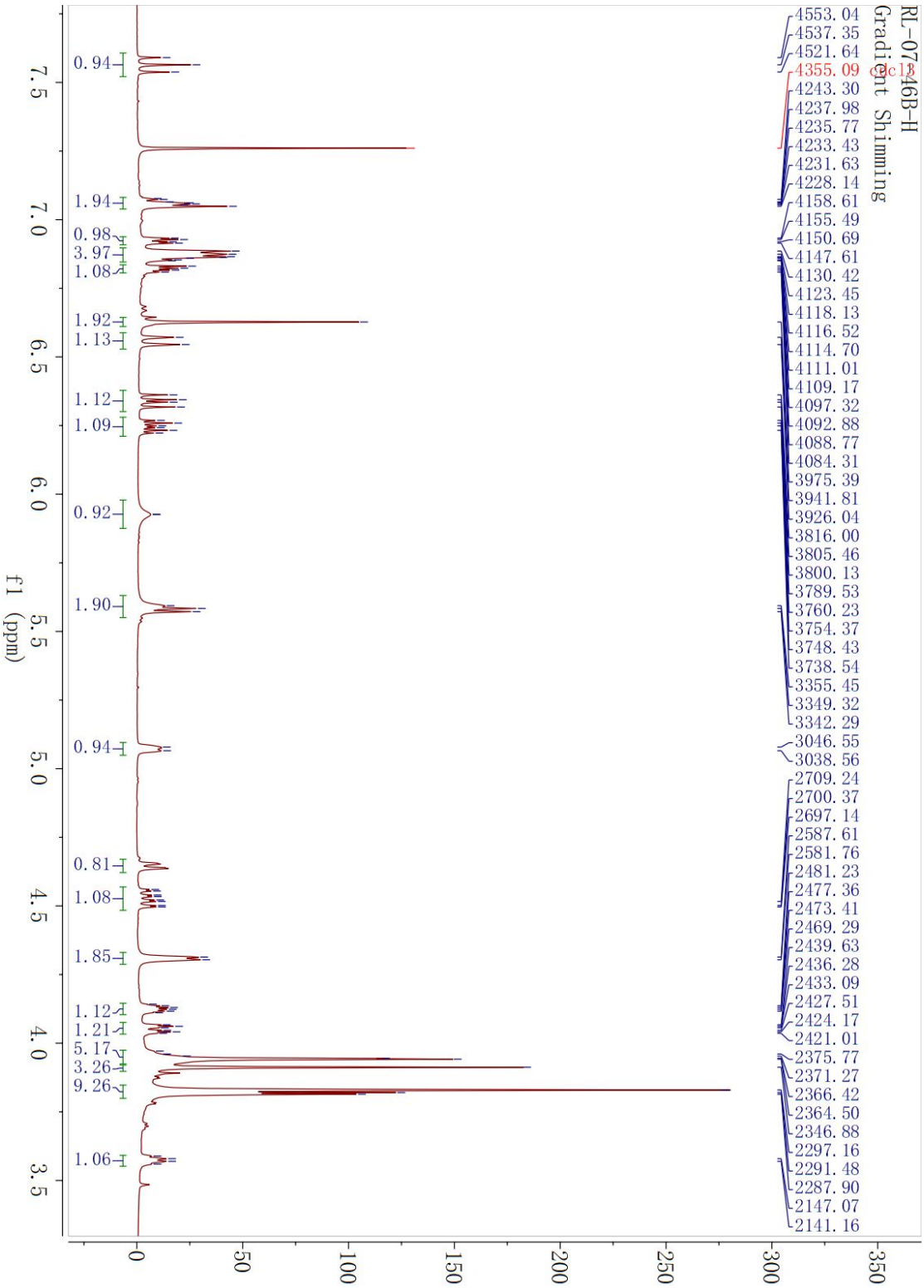


Figure S24. ^{13}C NMR spectrum (150 MHz) of bejolghotin C (**3**) in $CDCl_3$

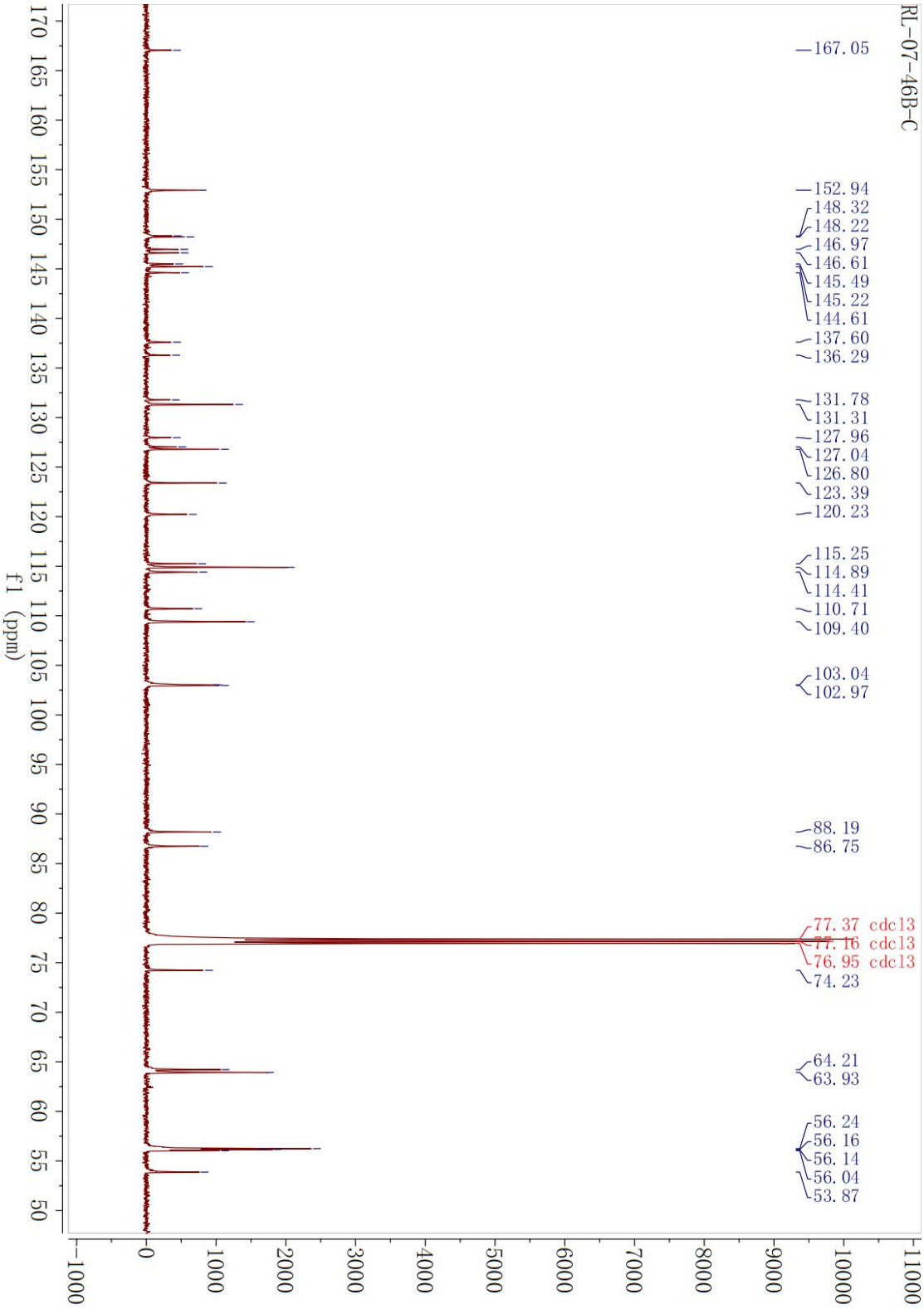


Figure S25. $^{1}H-^{1}H$ COSY spectrum (600 MHz) of bejolghotin C (**3**) in $CDCl_3$

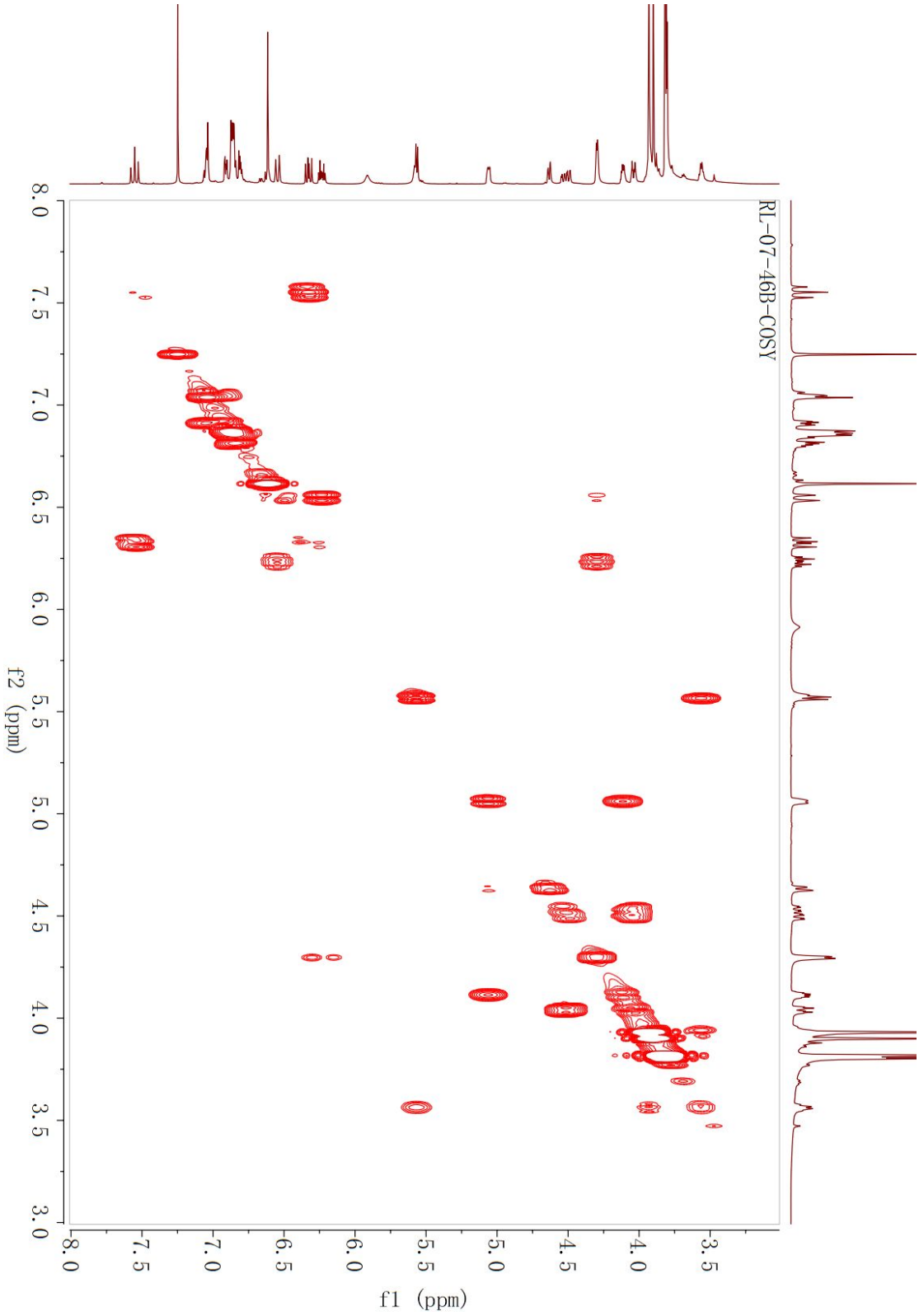


Figure S26. HSQC spectrum (600 MHz) of bejolghotin C (**3**) in $CDCl_3$

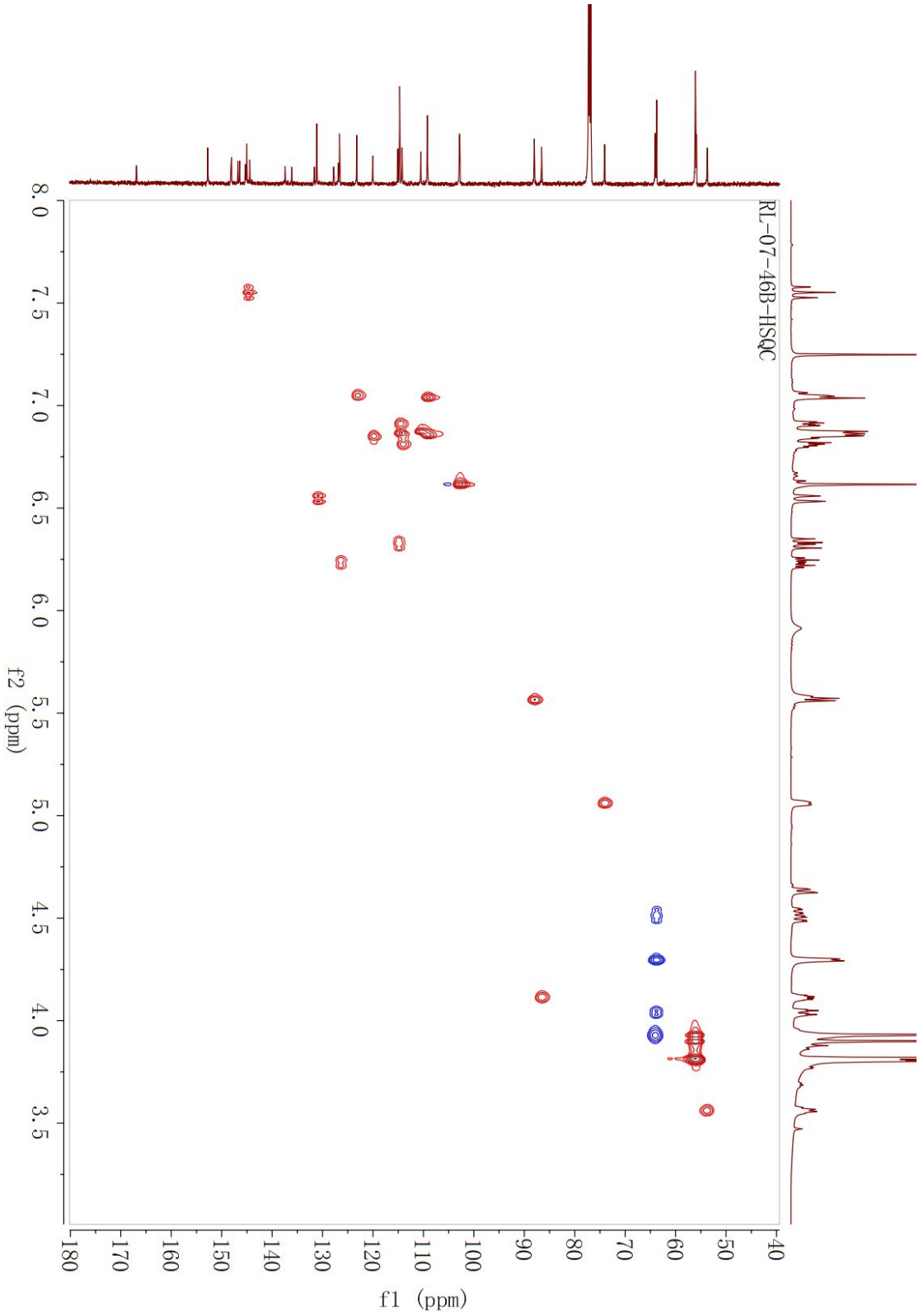


Figure S27. HMBC spectrum (600 MHz) of bejolghotin C (**3**) in $CDCl_3$

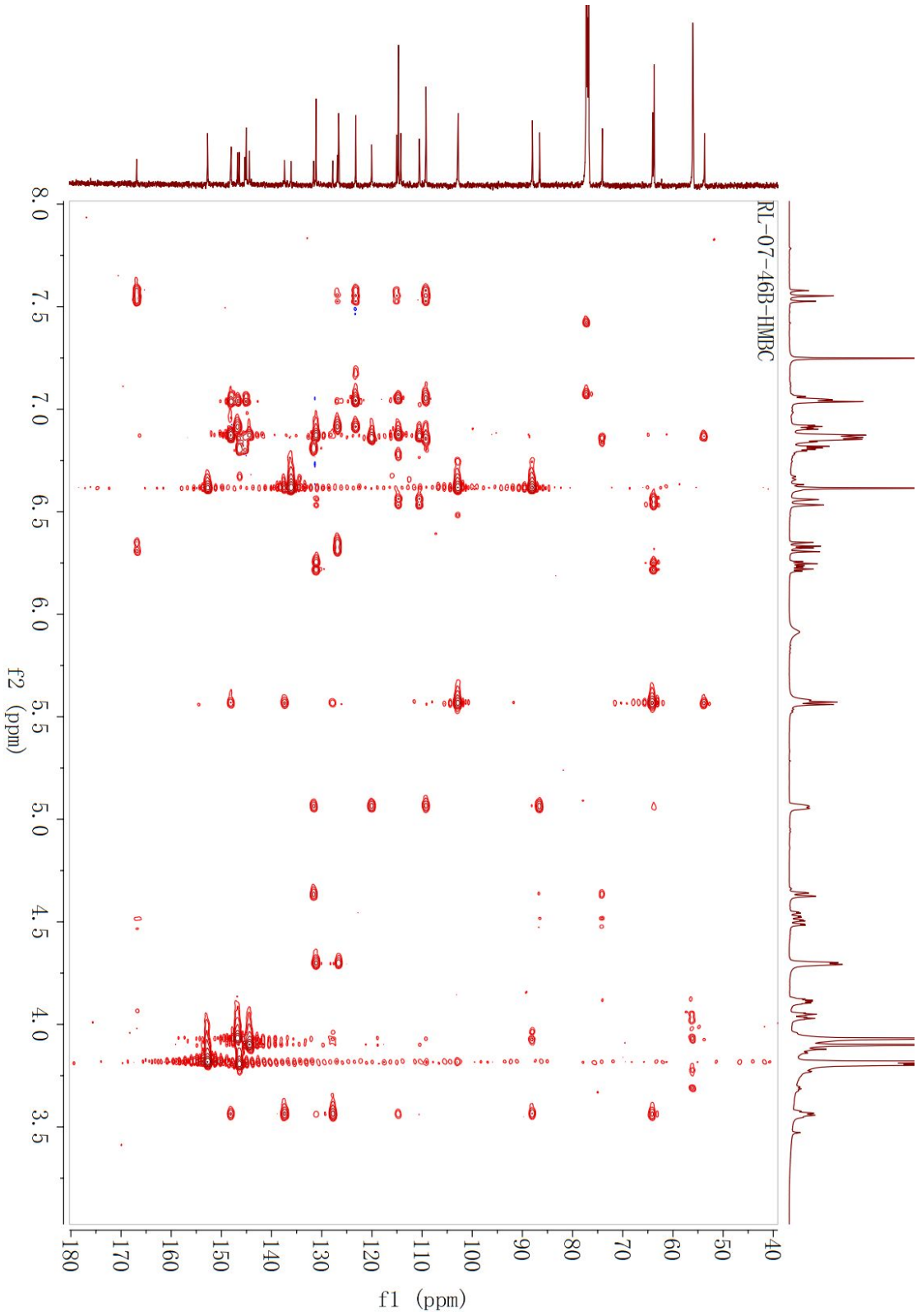


Figure S28. ROESY spectrum (600 MHz) of bejolghotin C (**3**) in $CDCl_3$

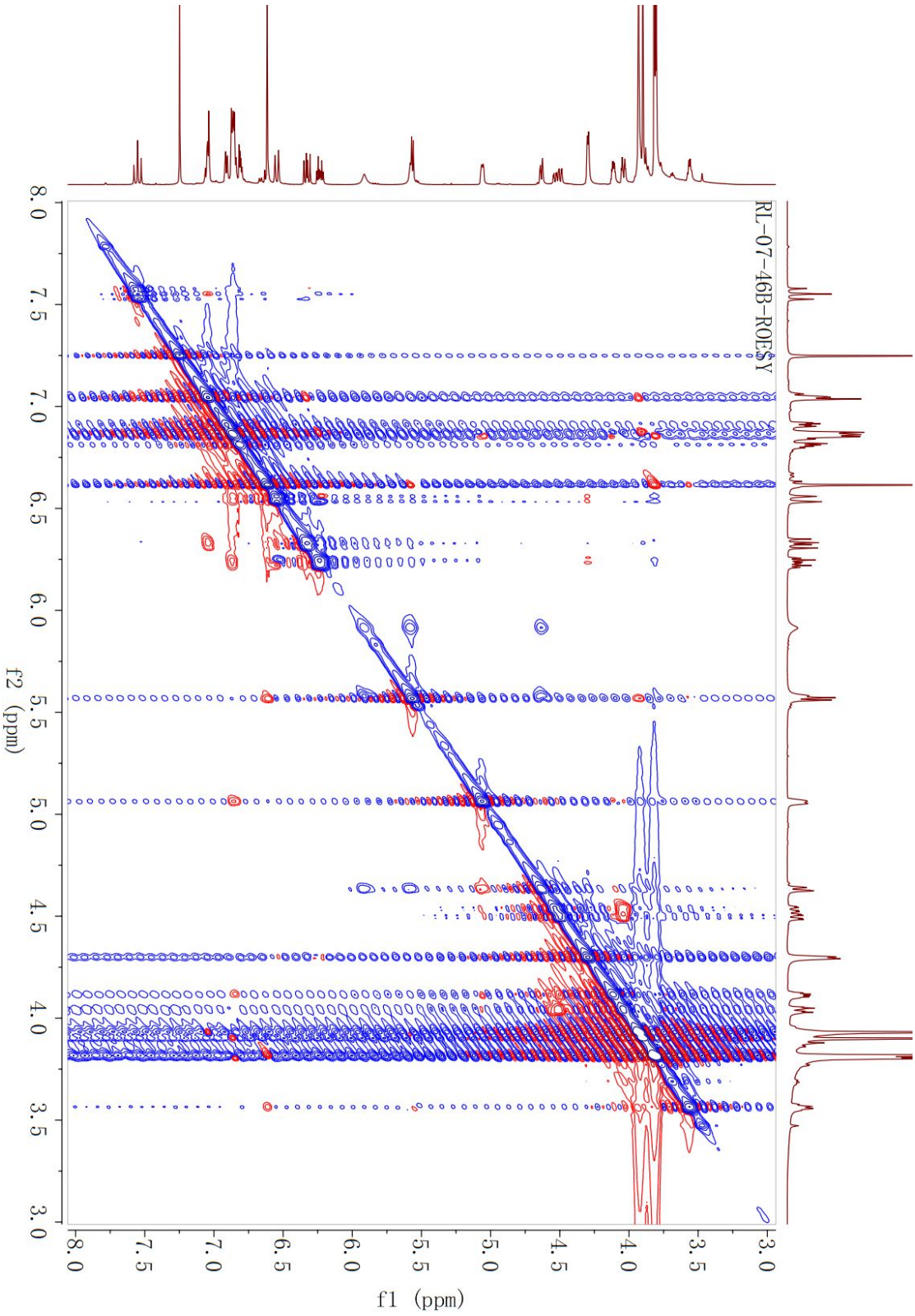


Figure S29. HRESIMS spectrum of bejolghotin C (**3**)

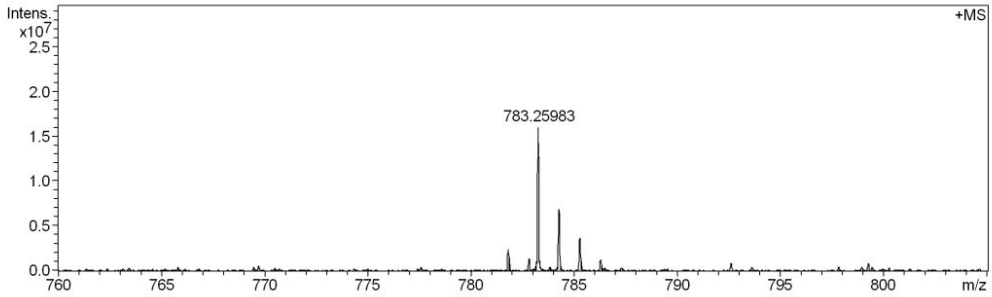
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201810\RL-07-46B_000001.d	Acquisition Date	10/12/2018 10:50:17 AM
Method	4_17_Mass_range_pos_7T	Operator	
Sample Name	RL-07-46B	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	53.8 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1100.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Sun Apr 8 02:39:02 2018
Source Accumulation	0.025 sec	n/a	n/a	Data Acquisition Size	524288
Ion Accumulation Time	0.025 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e⁻ Conf	N-R ule
783.25983	1	C 41 H 44 Na O 14	100.00	783.26233	3.19	2.22	56.7	19.5	even	ok

Figure S30. UV spectrum of bejolghotin C (**3**)

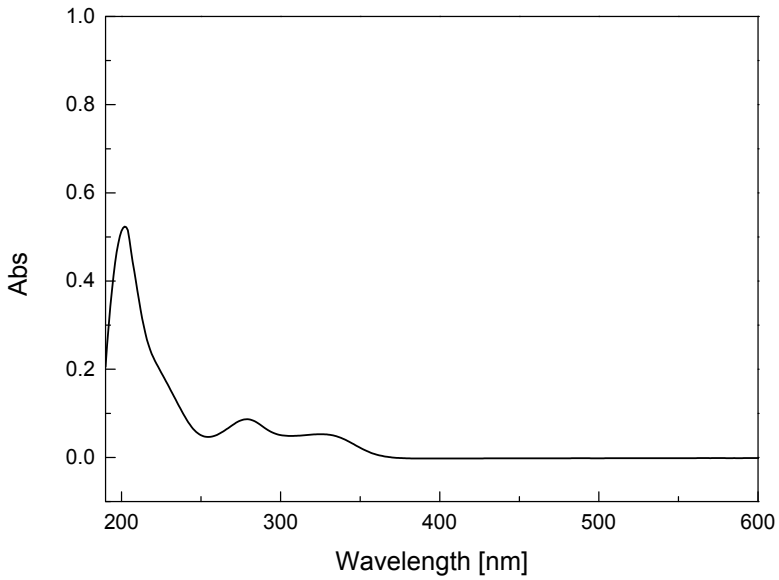


Figure S31. IR spectrum (KBr disc) of bejolghotin C (**3**)

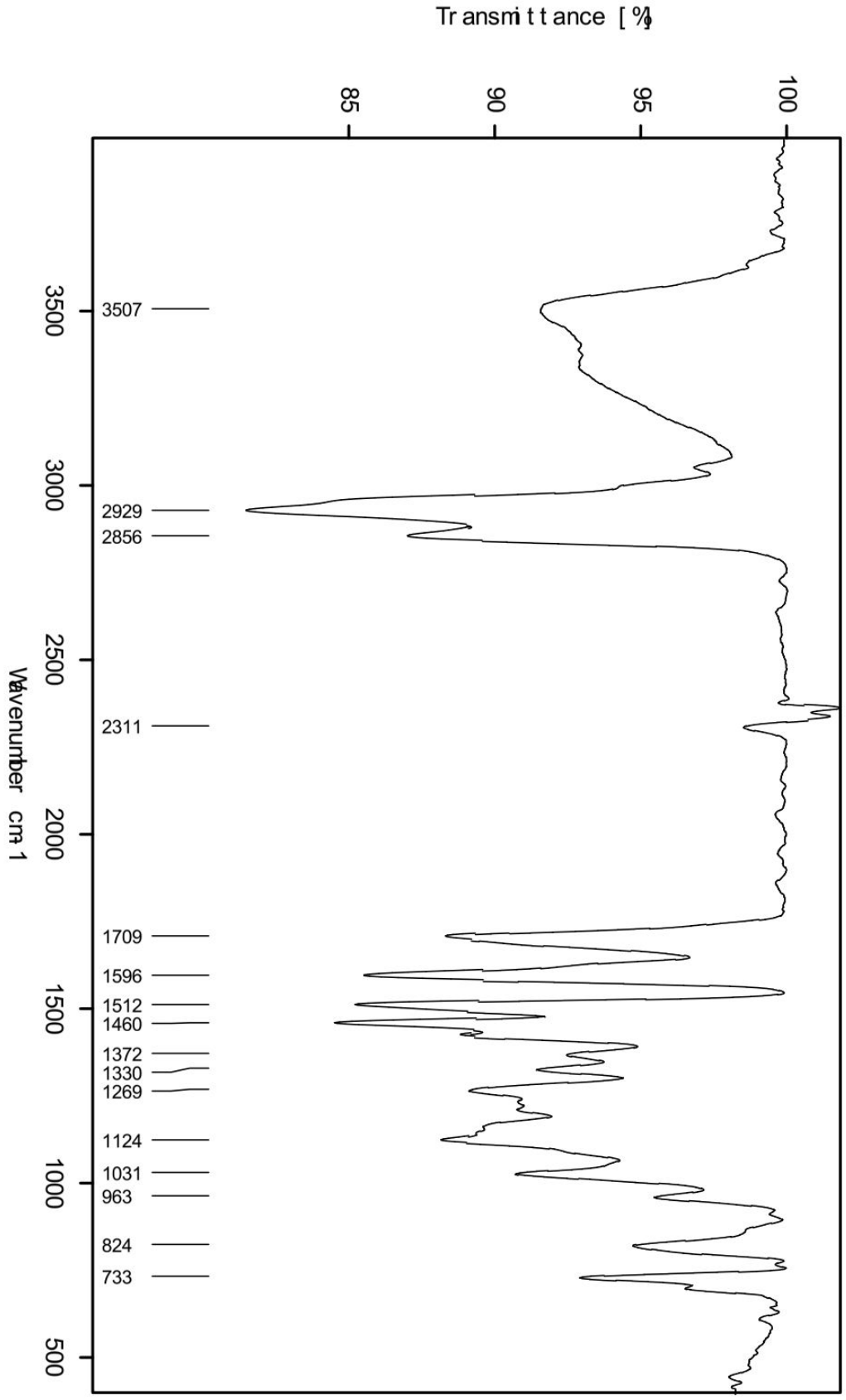


Figure S32. ^{1}H NMR spectrum (600 MHz) of bejolghotin D (**4**) in $CDCl_3$

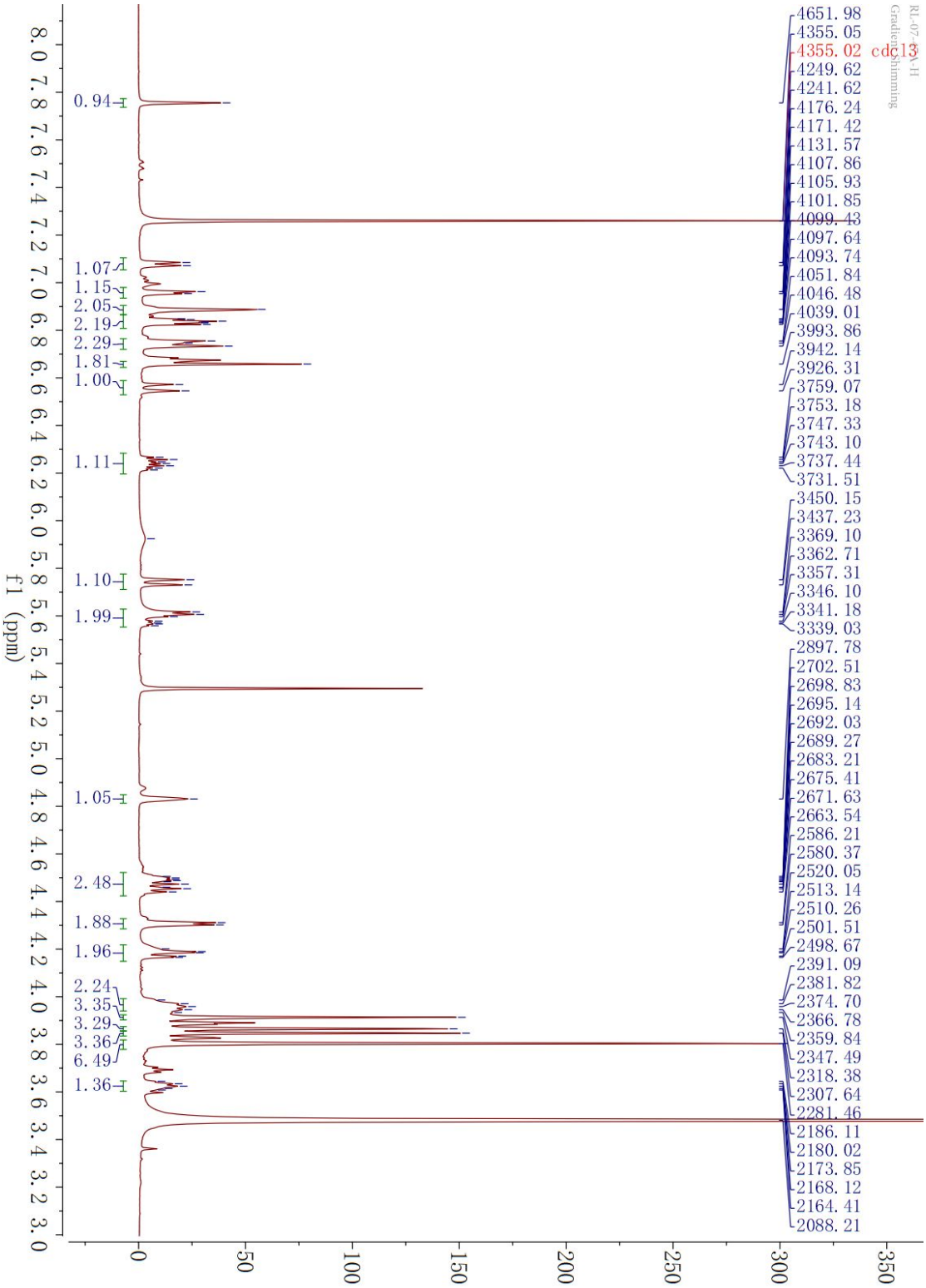


Figure S33. ^{13}C NMR spectrum (150 MHz) of bejolghotin D (**4**) in $CDCl_3$

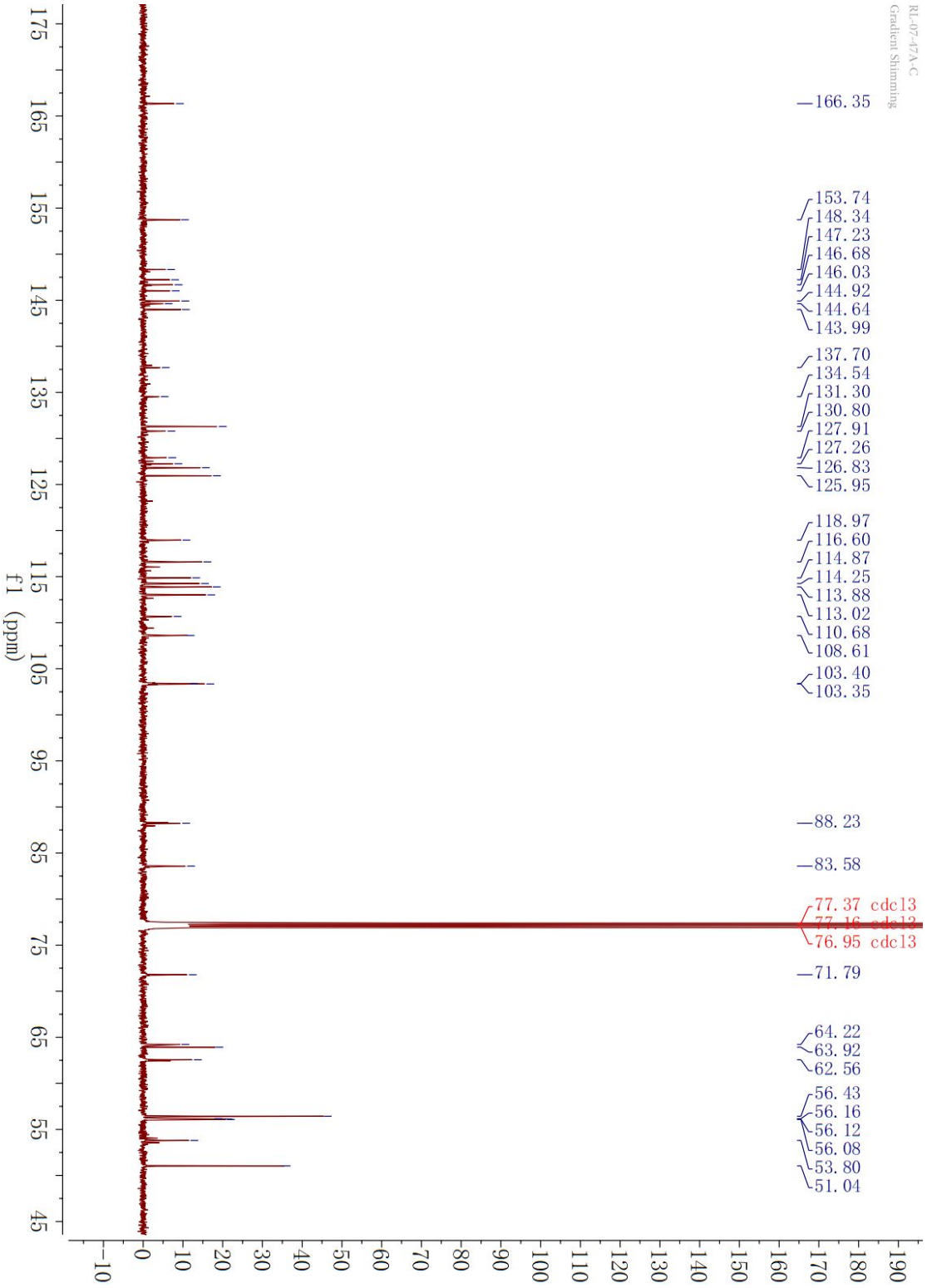


Figure S34. $^{1}H-^{1}H$ COSY spectrum (600 MHz) of bejolghotin D (**4**) in $CDCl_3$

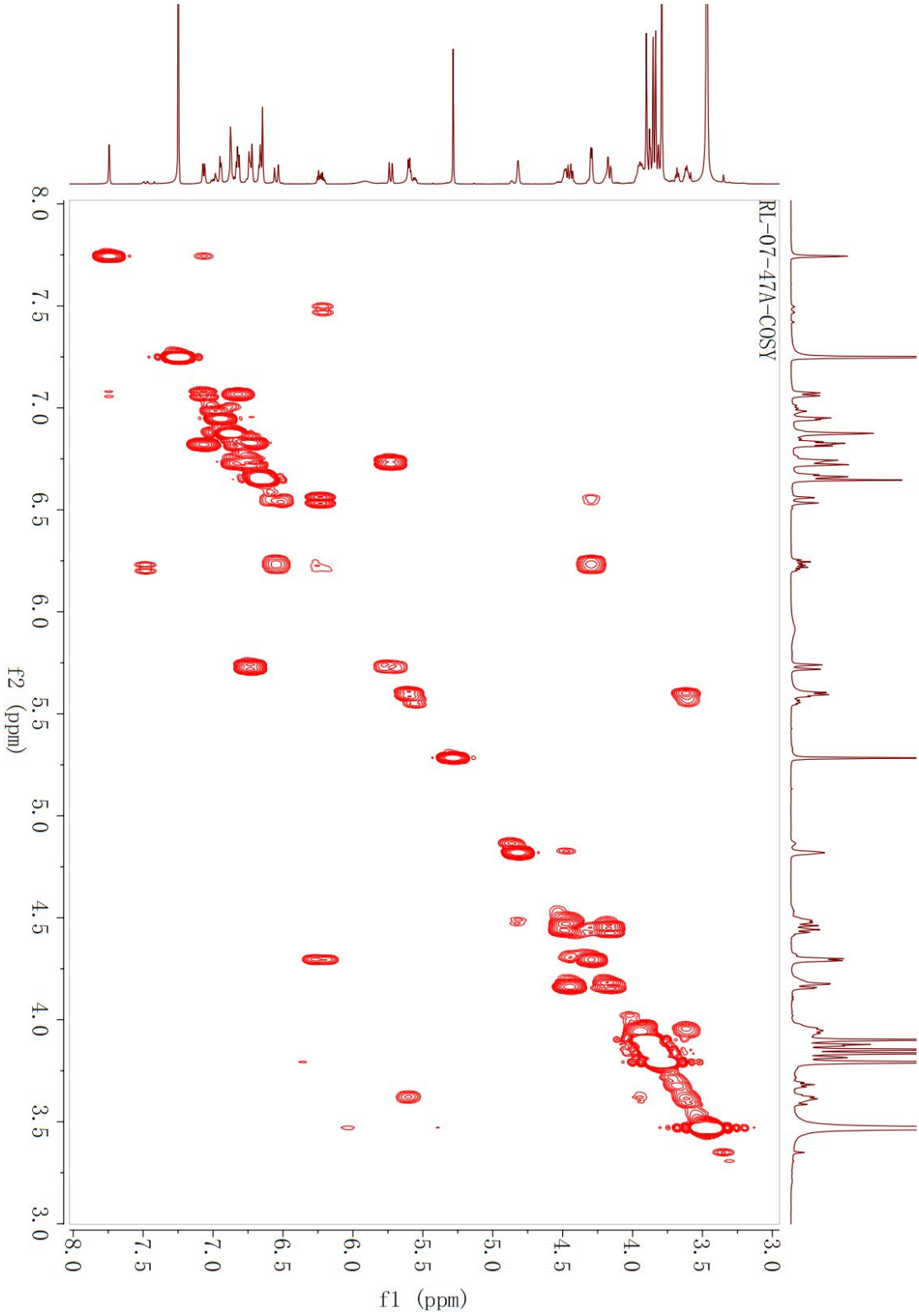


Figure S35. HSQC spectrum (600 MHz) of bejolghotin D (**4**) in $CDCl_3$

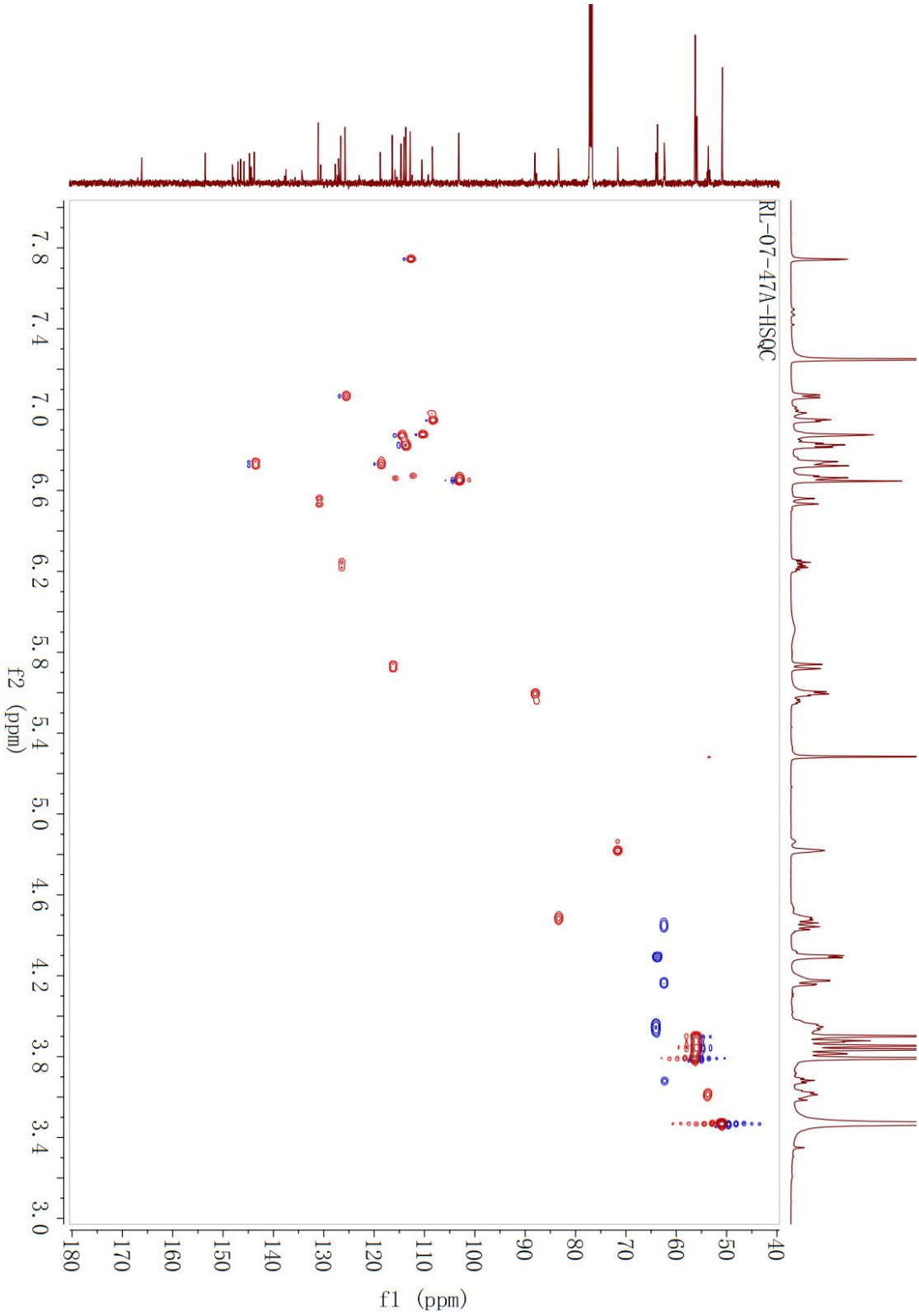


Figure S36. HMBC spectrum (600 MHz) of bejolghotin D (**4**) in $CDCl_3$

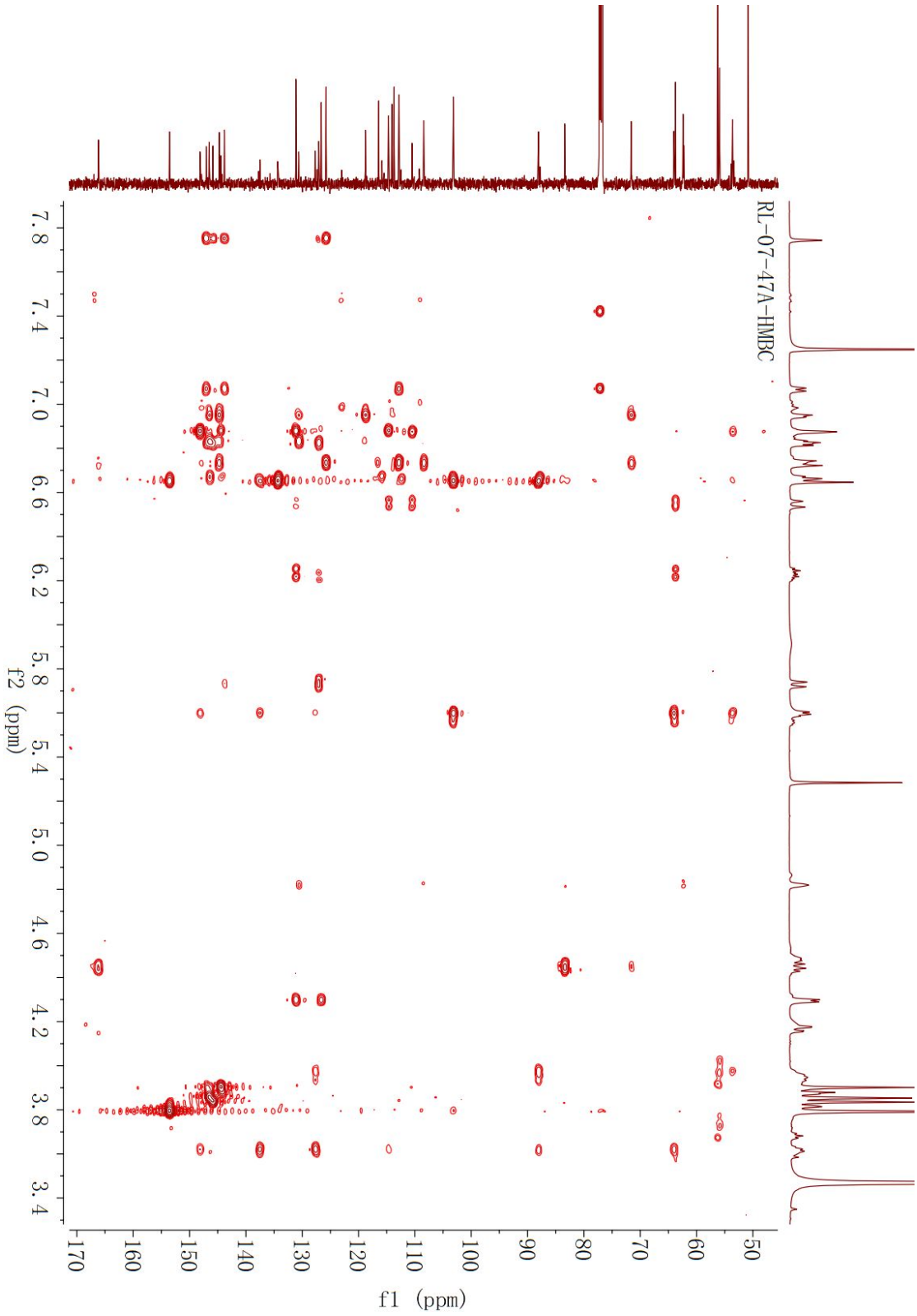


Figure S37. ROESY spectrum (600 MHz) of bejolghotin D (**4**) in $CDCl_3$

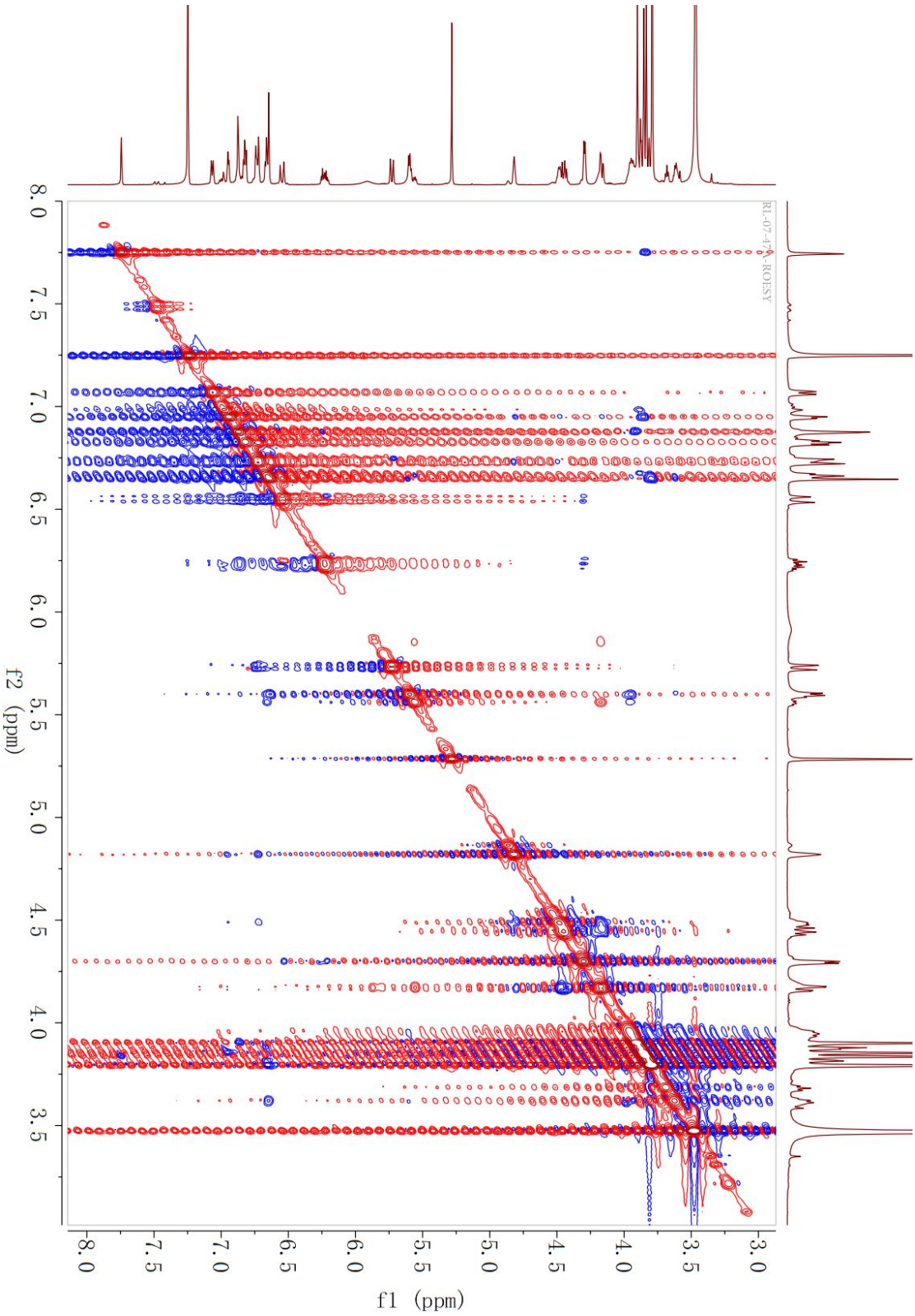
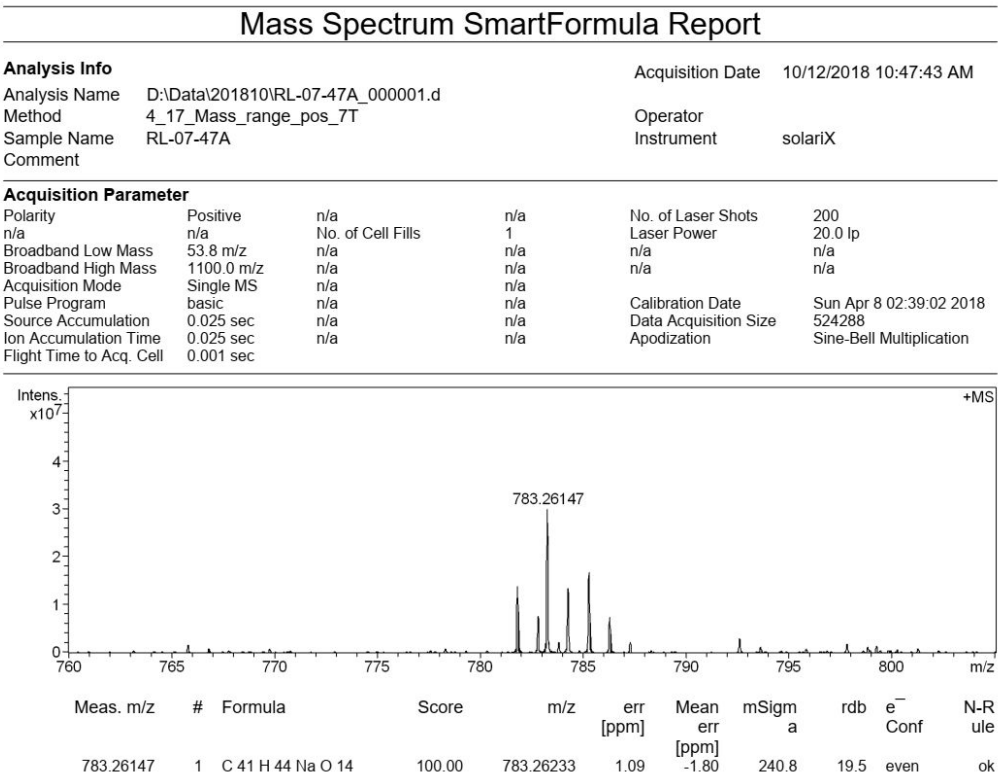


Figure S38. HRESIMS spectrum of bejolghotin D (**4**)



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201810\RL-07-47A_000001.d	Acquisition Date	10/12/2018 10:47:43 AM
Method	4_17_Mass_range_pos_7T	Operator	
Sample Name	RL-07-47A	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	53.8 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1100.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Sun Apr 8 02:39:02 2018
Source Accumulation	0.025 sec	n/a	n/a	Data Acquisition Size	524288
Ion Accumulation Time	0.025 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
783.26147	1	C 41 H 44 Na O 14	100.00	783.26233	1.09	-1.80	240.8	19.5	even	ok

Figure S39. UV spectrum of bejolghotin D (**4**)

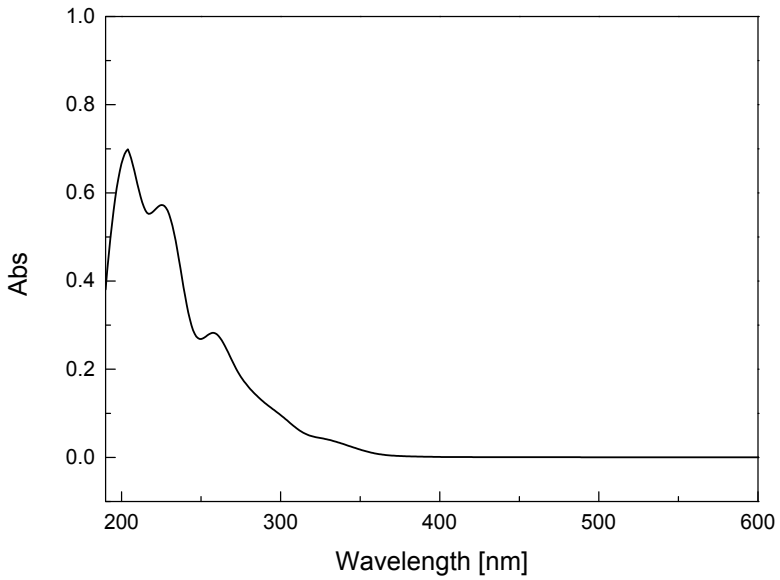


Figure S40. IR spectrum (KBr disc) of bejolghotin D (**4**)

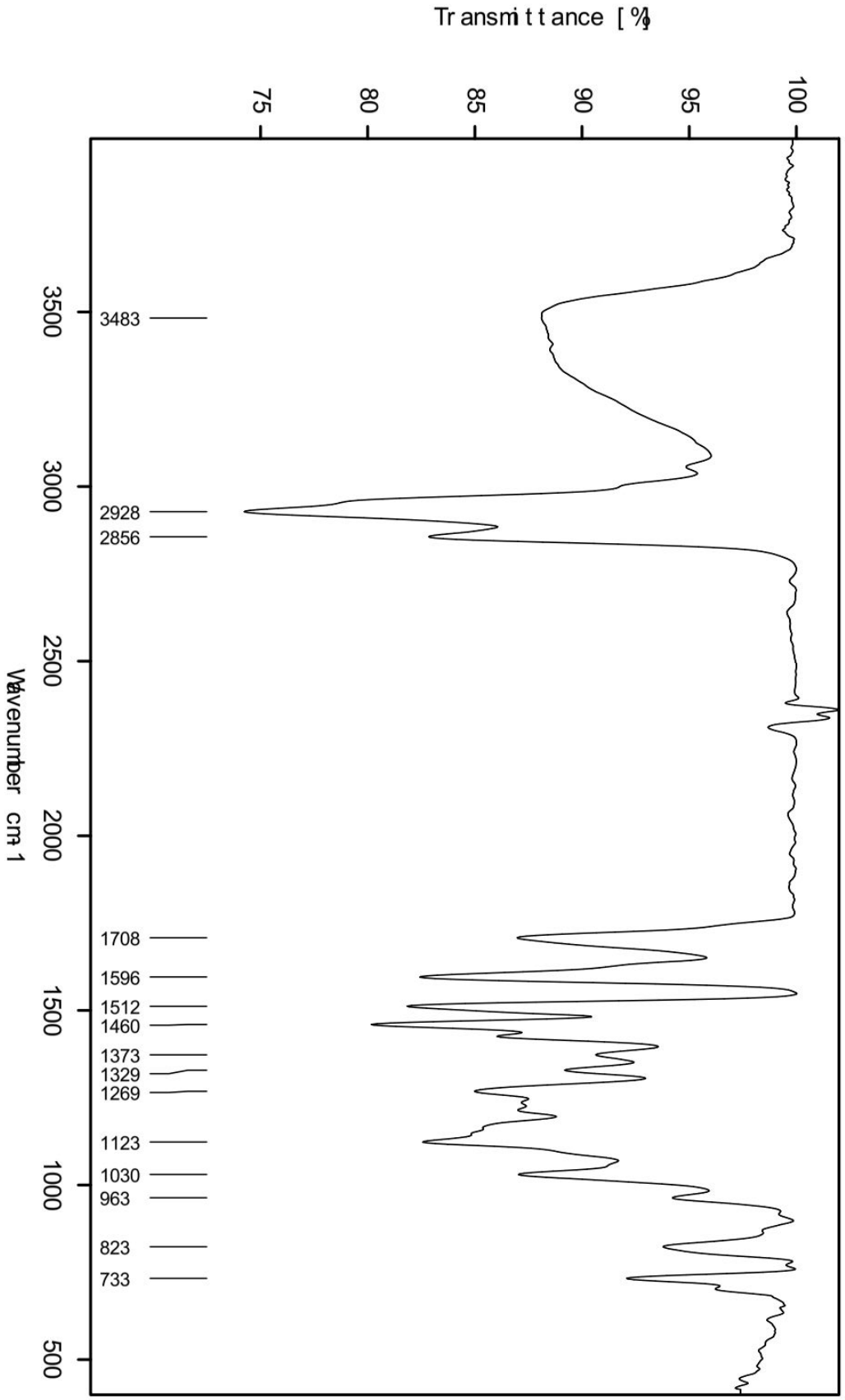


Figure S41. ^{1}H NMR spectrum (600 MHz) of bejolghotin E (**9**) in $CDCl_3$

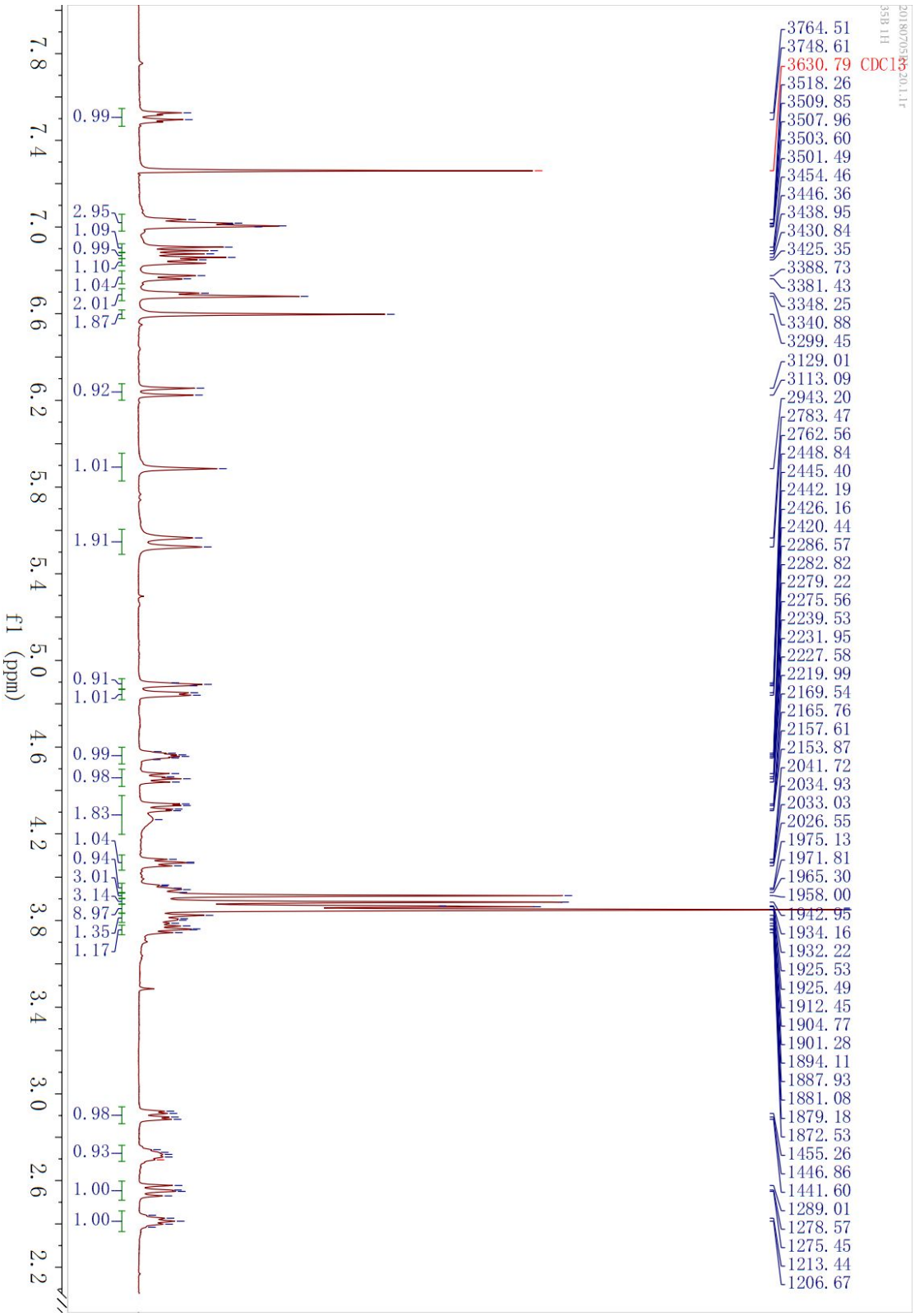


Figure S42. ^{13}C NMR spectrum (150 MHz) of bejolghotin E (**9**) in $CDCl_3$

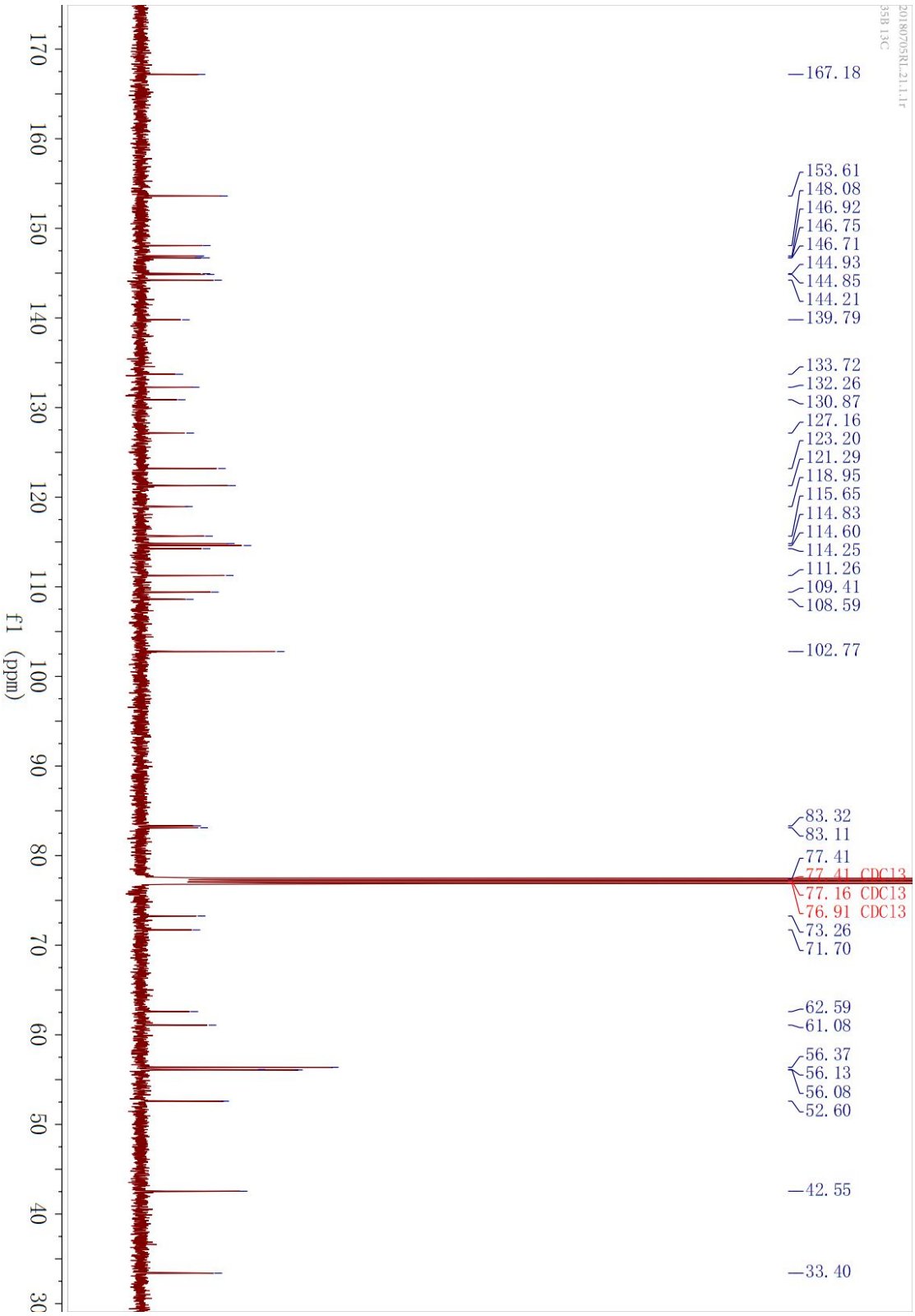


Figure S43. $^{1}H-^{1}H$ COSY spectrum (600 MHz) of bejolghotin E (**9**) in $CDCl_3$

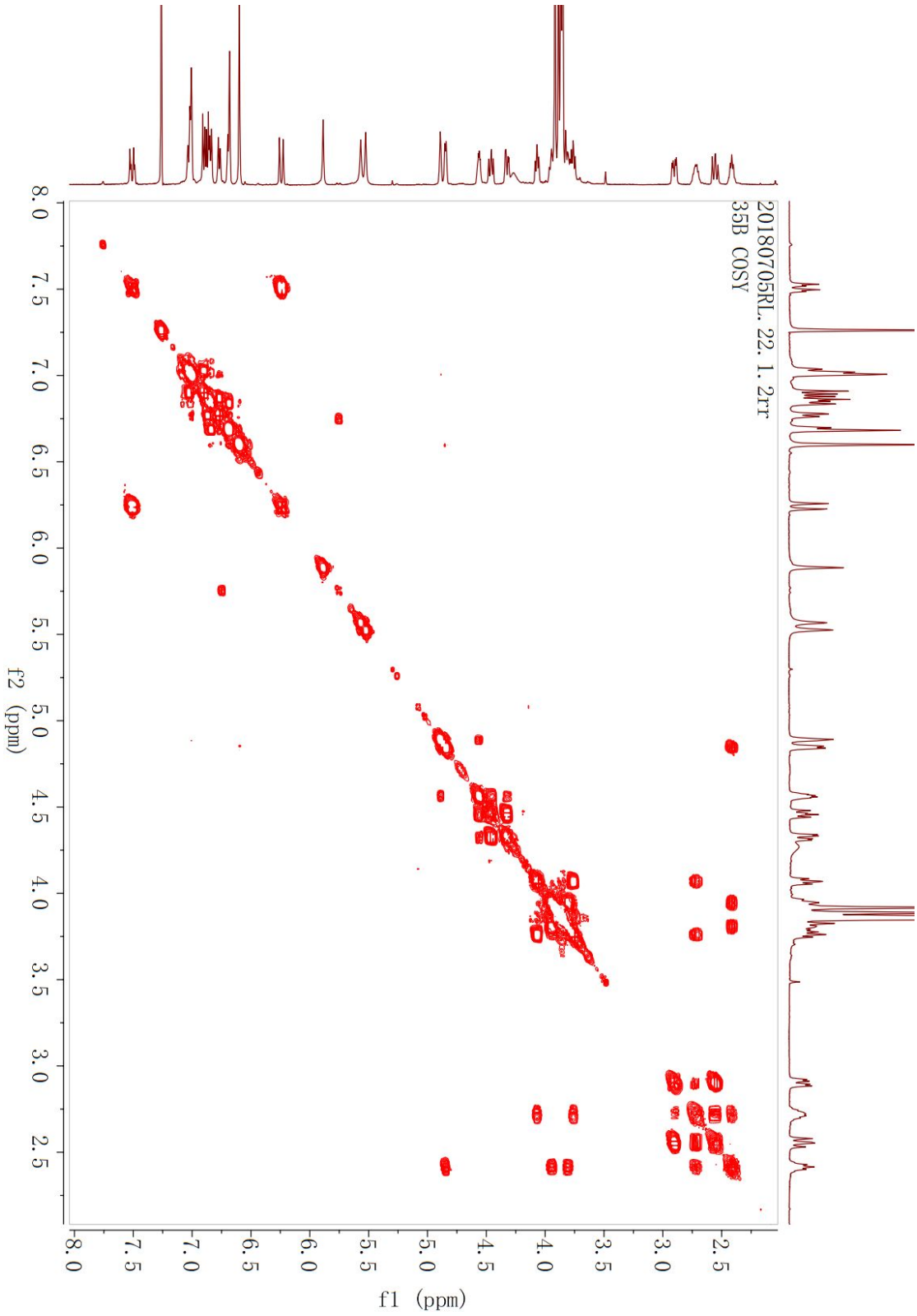


Figure S44. HSQC spectrum (600 MHz) of bejolghotin E (**9**) in $CDCl_3$

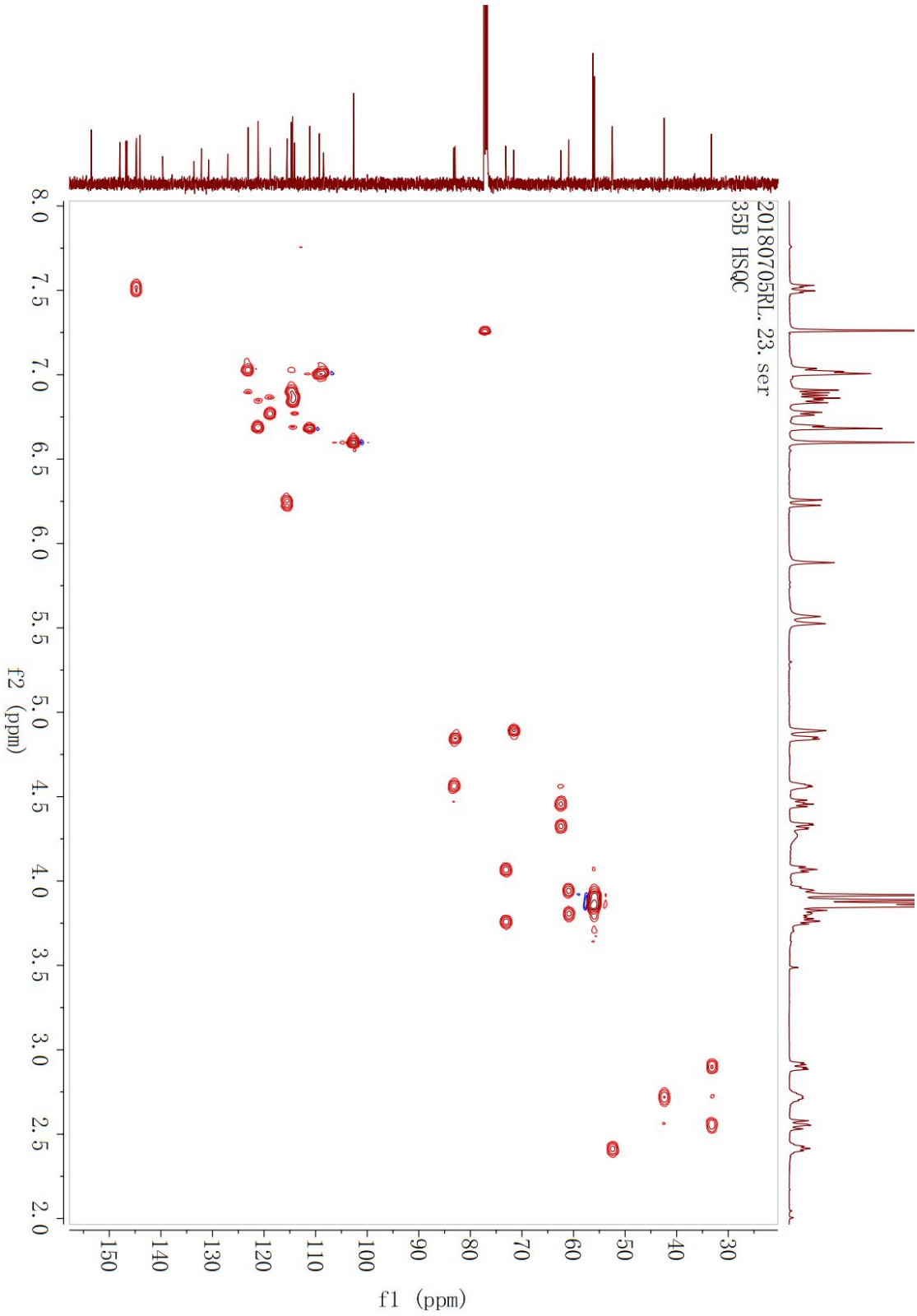


Figure S45. HMBC spectrum (600 MHz) of bejolghotin E (**9**) in $CDCl_3$

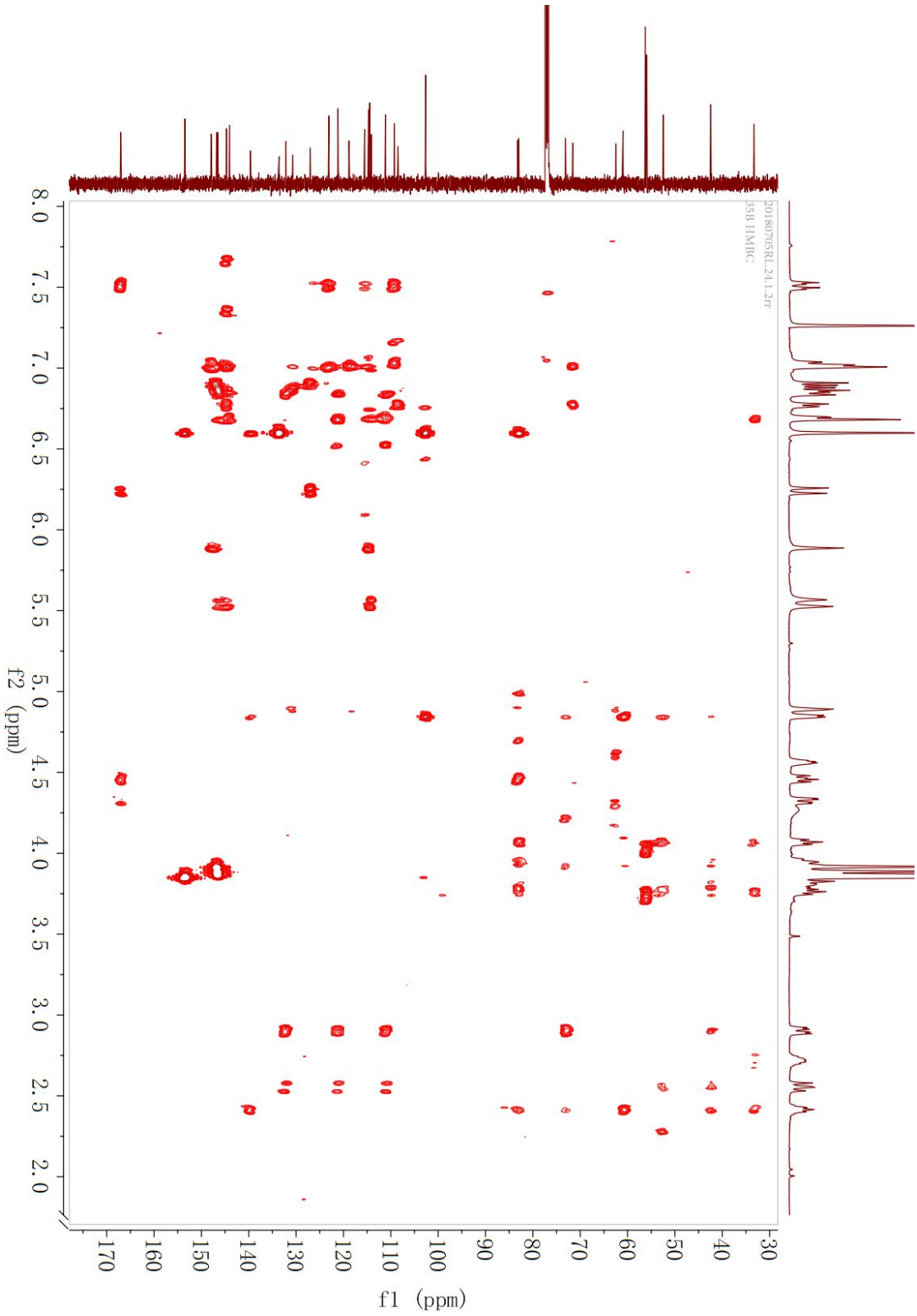


Figure S46. ROESY spectrum (600 MHz) of bejolghotin E (**9**) in $CDCl_3$

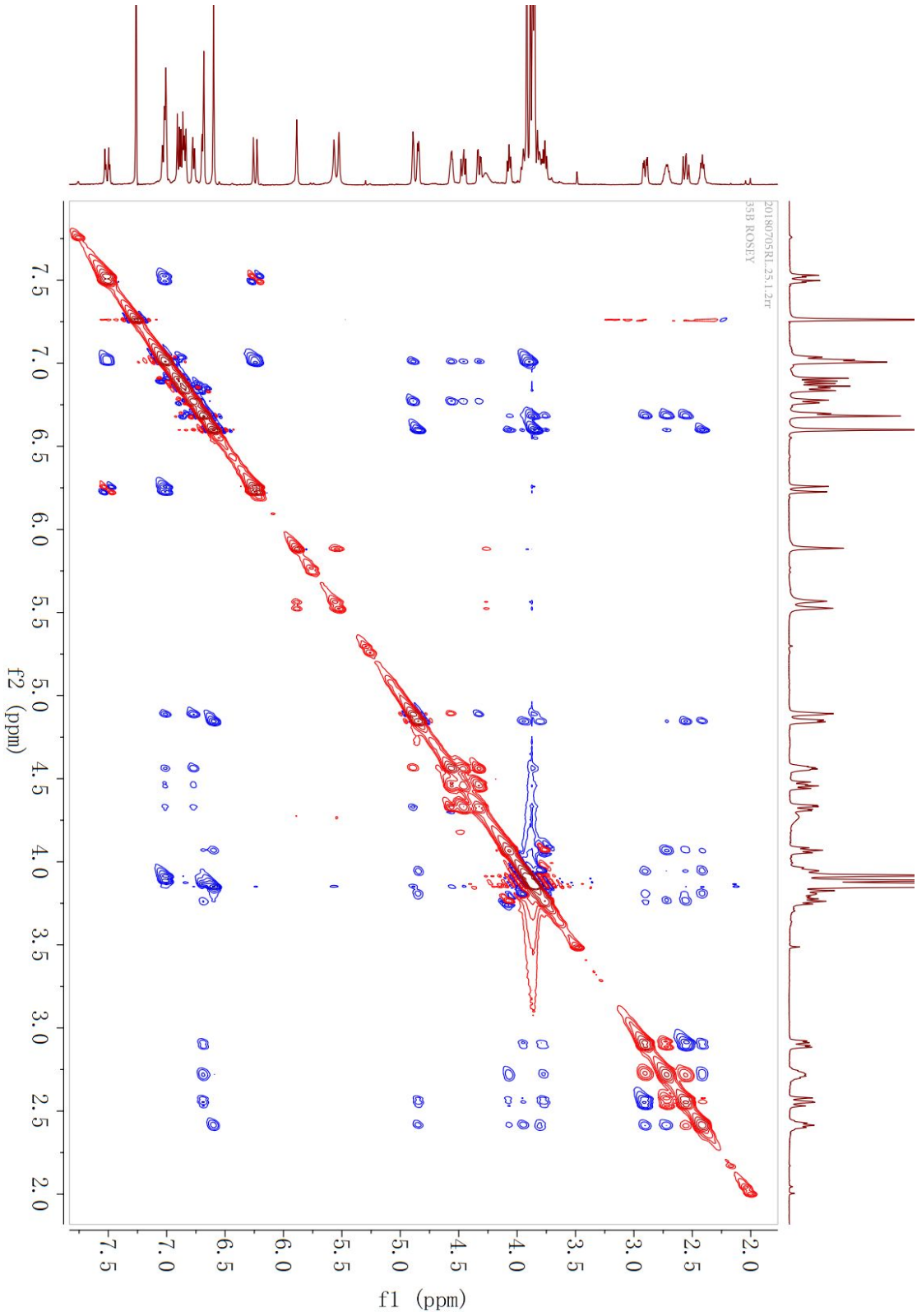
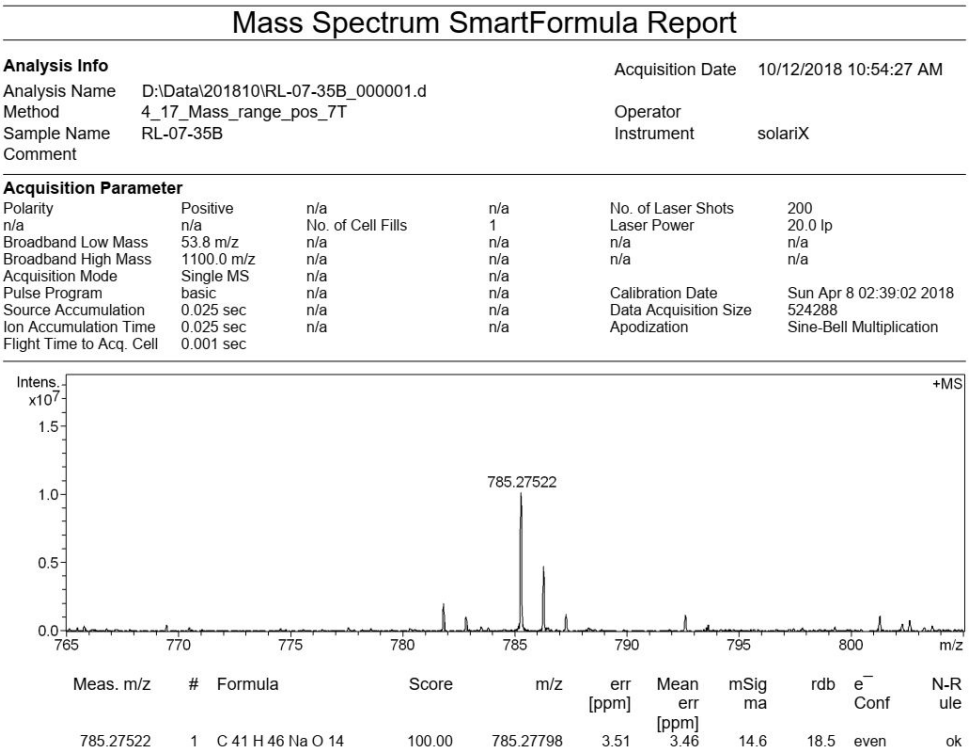


Figure S47. HRESIMS spectrum of bejolghotin E (**9**)



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201810\RL-07-35B_000001.d	Acquisition Date	10/12/2018 10:54:27 AM
Method	4_17_Mass_range_pos_7T	Operator	
Sample Name	RL-07-35B	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	53.8 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1100.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Sun Apr 8 02:39:02 2018
Source Accumulation	0.025 sec	n/a	n/a	Data Acquisition Size	524288
Ion Accumulation Time	0.025 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
785.27522	1	C 41 H 46 Na O 14	100.00	785.27798	3.51	3.46	14.6	18.5	even	ok

Figure S48. UV spectrum of bejolghotin E (**9**)

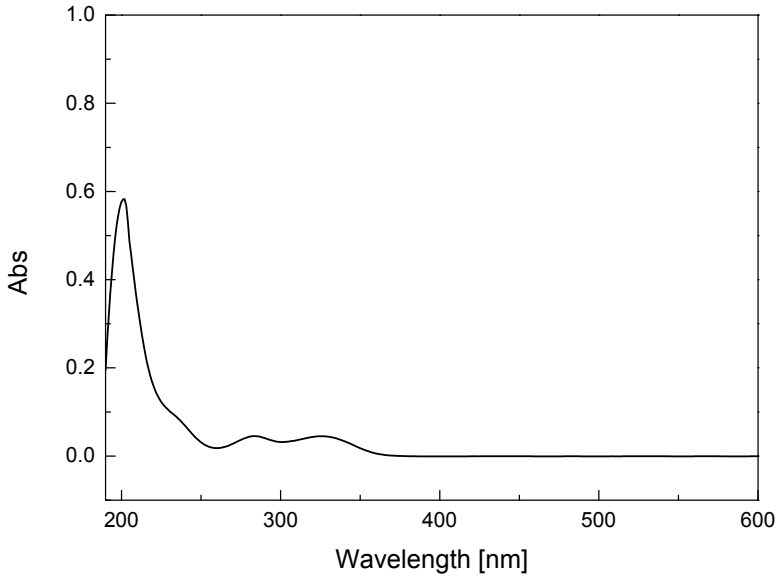


Figure S49. IR spectrum (KBr disc) of bejolghotin E (**9**)

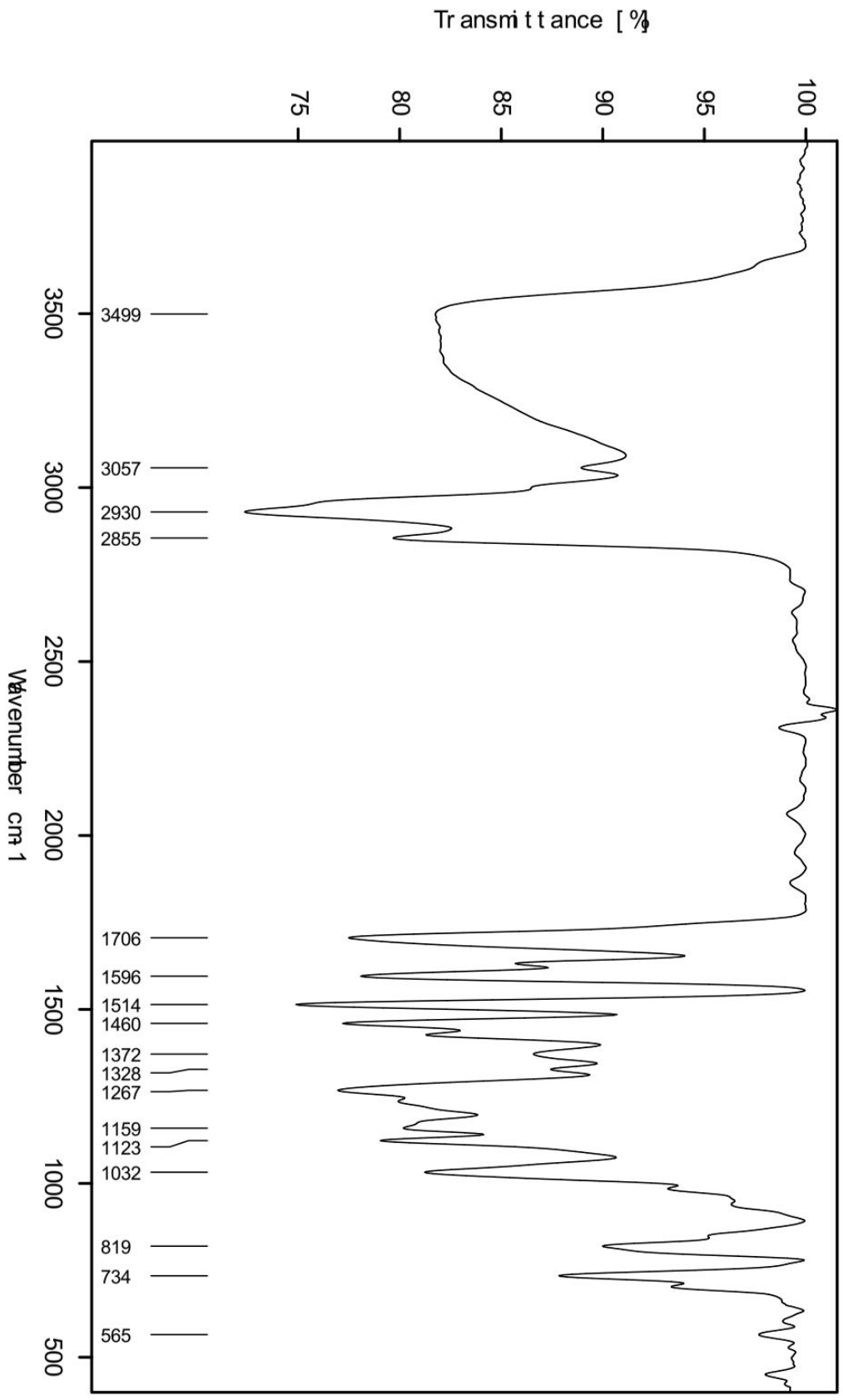


Figure S50. ^{1}H NMR spectrum (600 MHz) of bejolghotin F (**10**) in $CDCl_3$

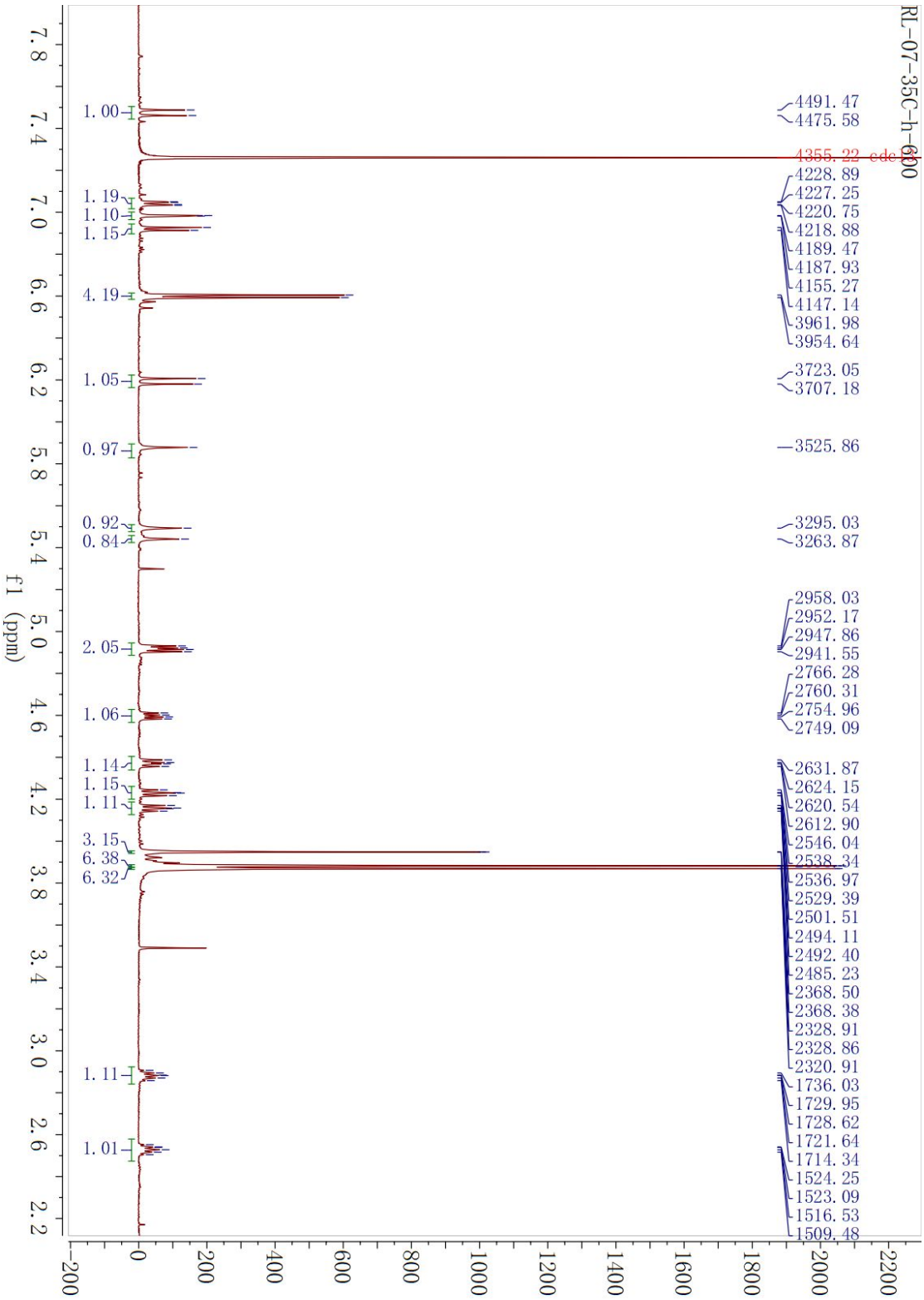


Figure S51. ^{13}C NMR spectrum (150 MHz) of bejolghotin F (**10**) in $CDCl_3$

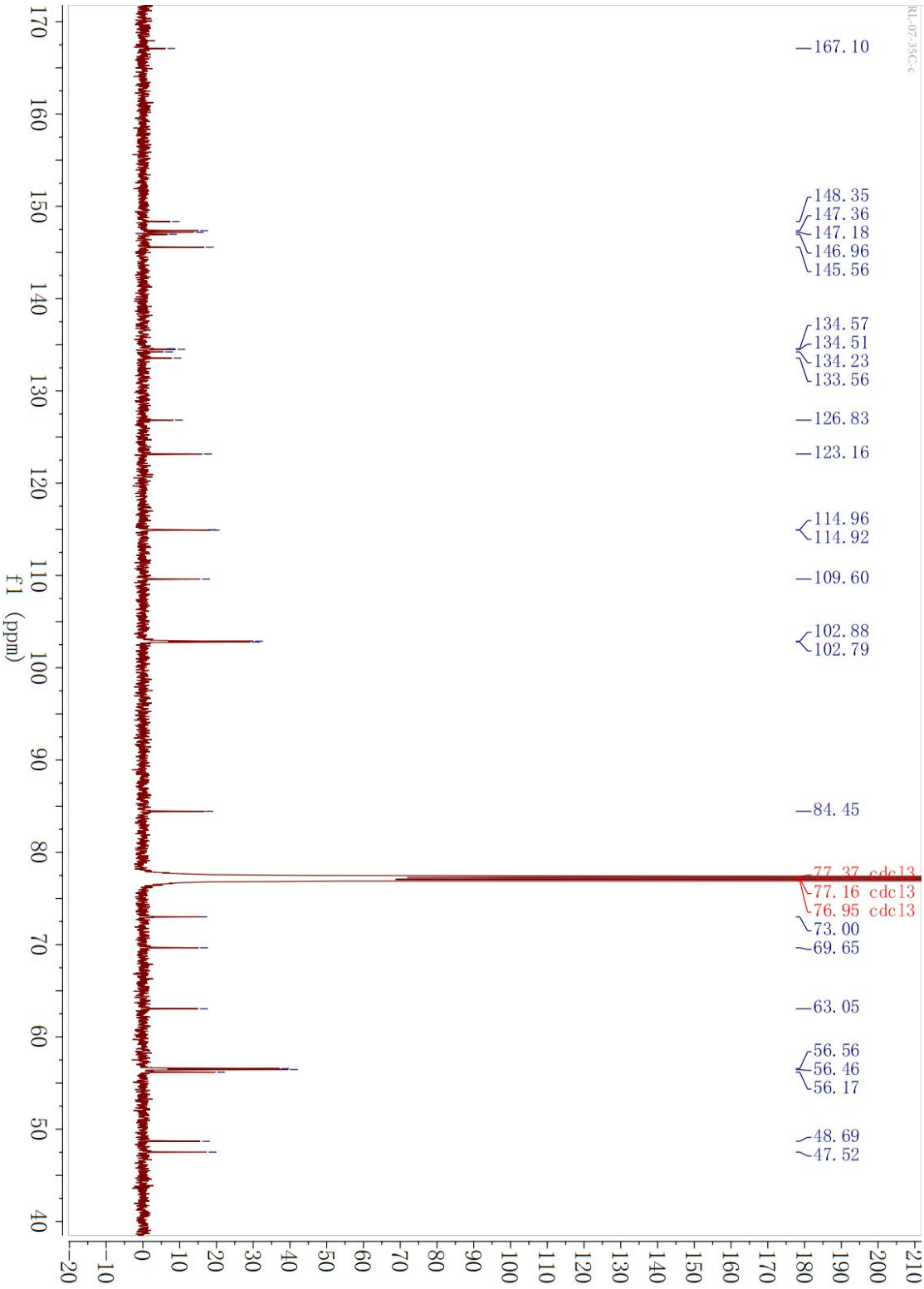


Figure S52. $^{1}H-^{1}H$ COSY spectrum (600 MHz) of bejolghotin F (**10**) in $CDCl_3$

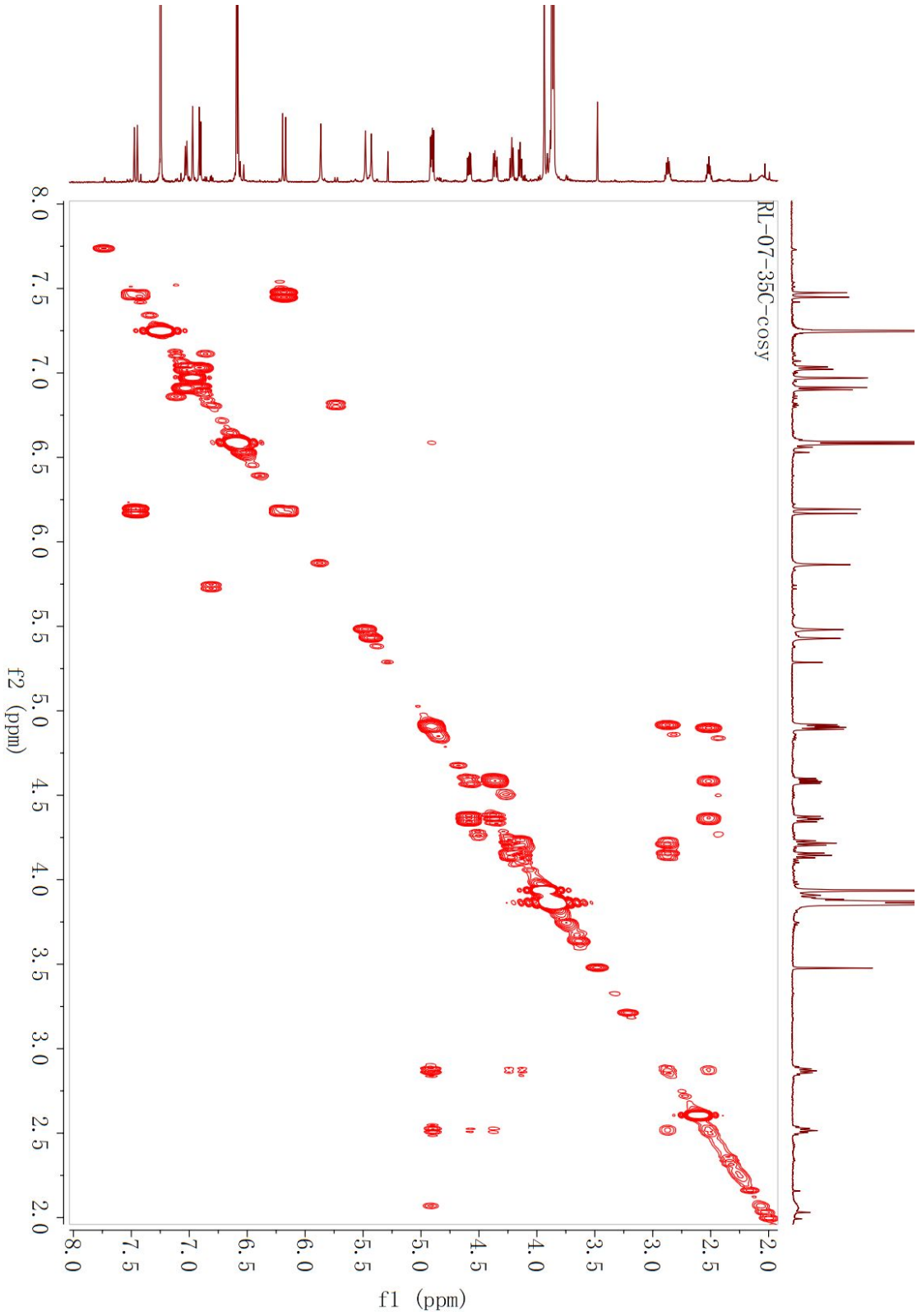


Figure S53. HSQC spectrum (600 MHz) of bejolghotin F (**10**) in $CDCl_3$

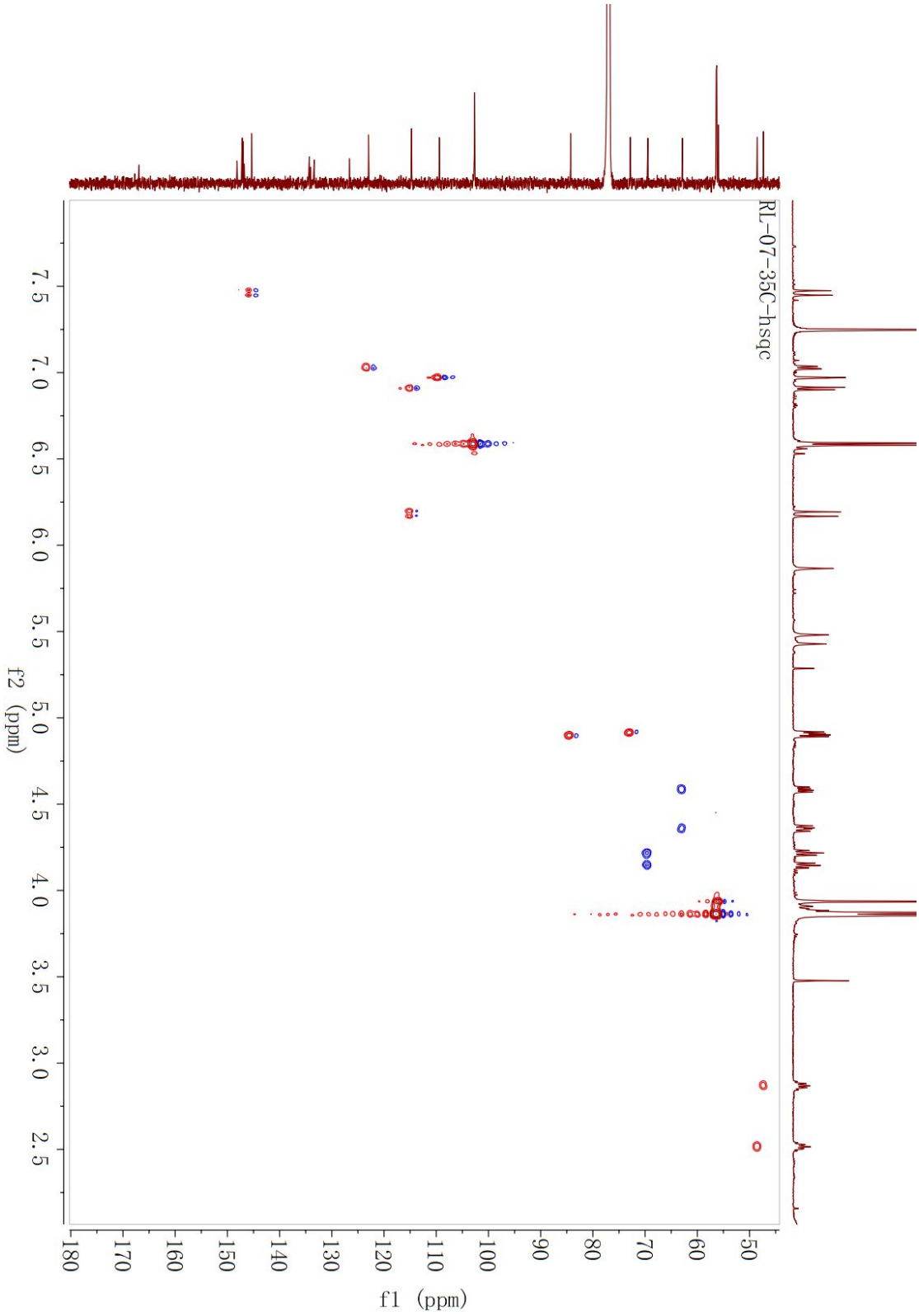


Figure S54. HMBC spectrum (600 MHz) of bejolghotin F (**10**) in $CDCl_3$

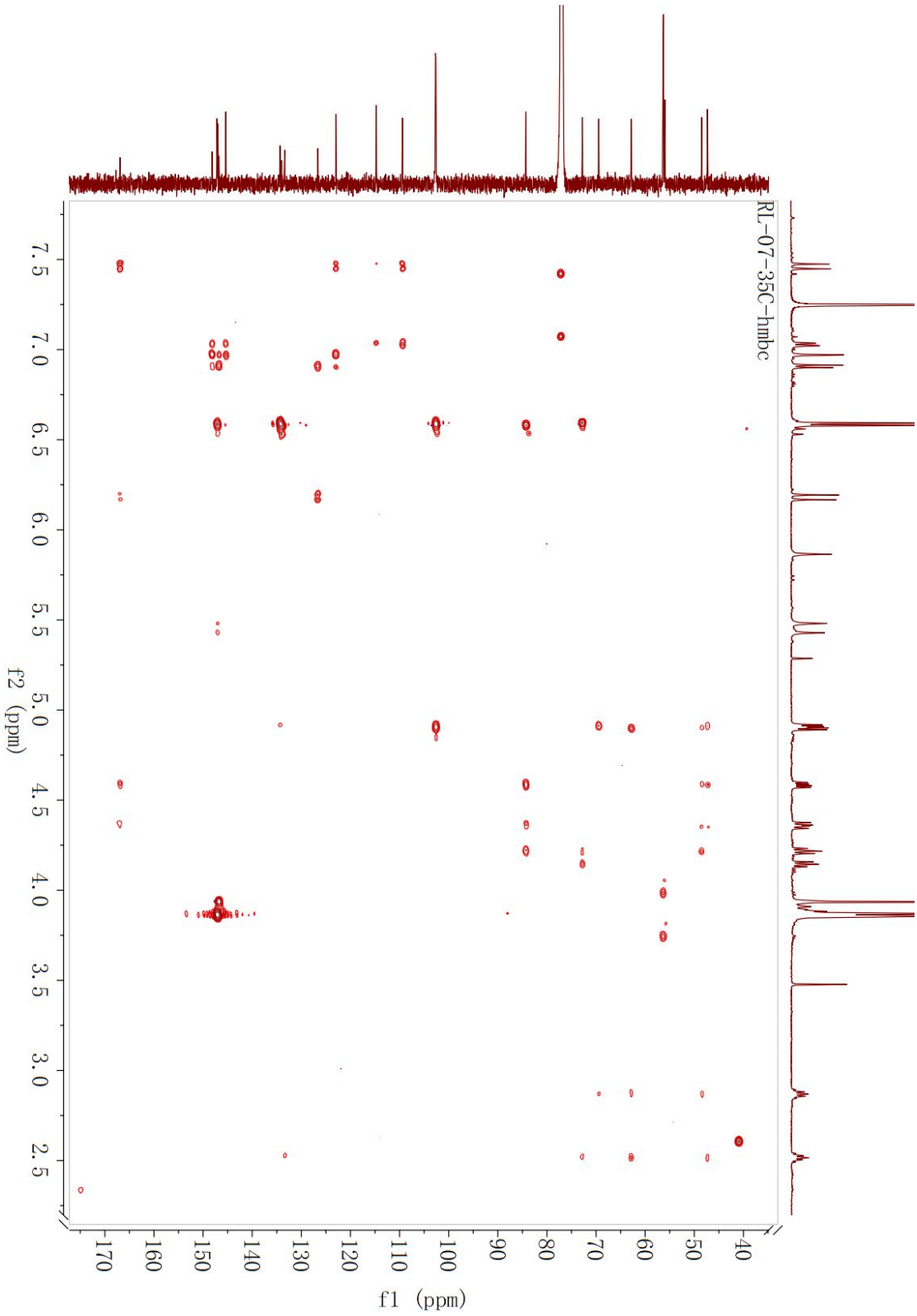


Figure S55. ROESY spectrum (600 MHz) of bejolghotin F (**10**) in $CDCl_3$

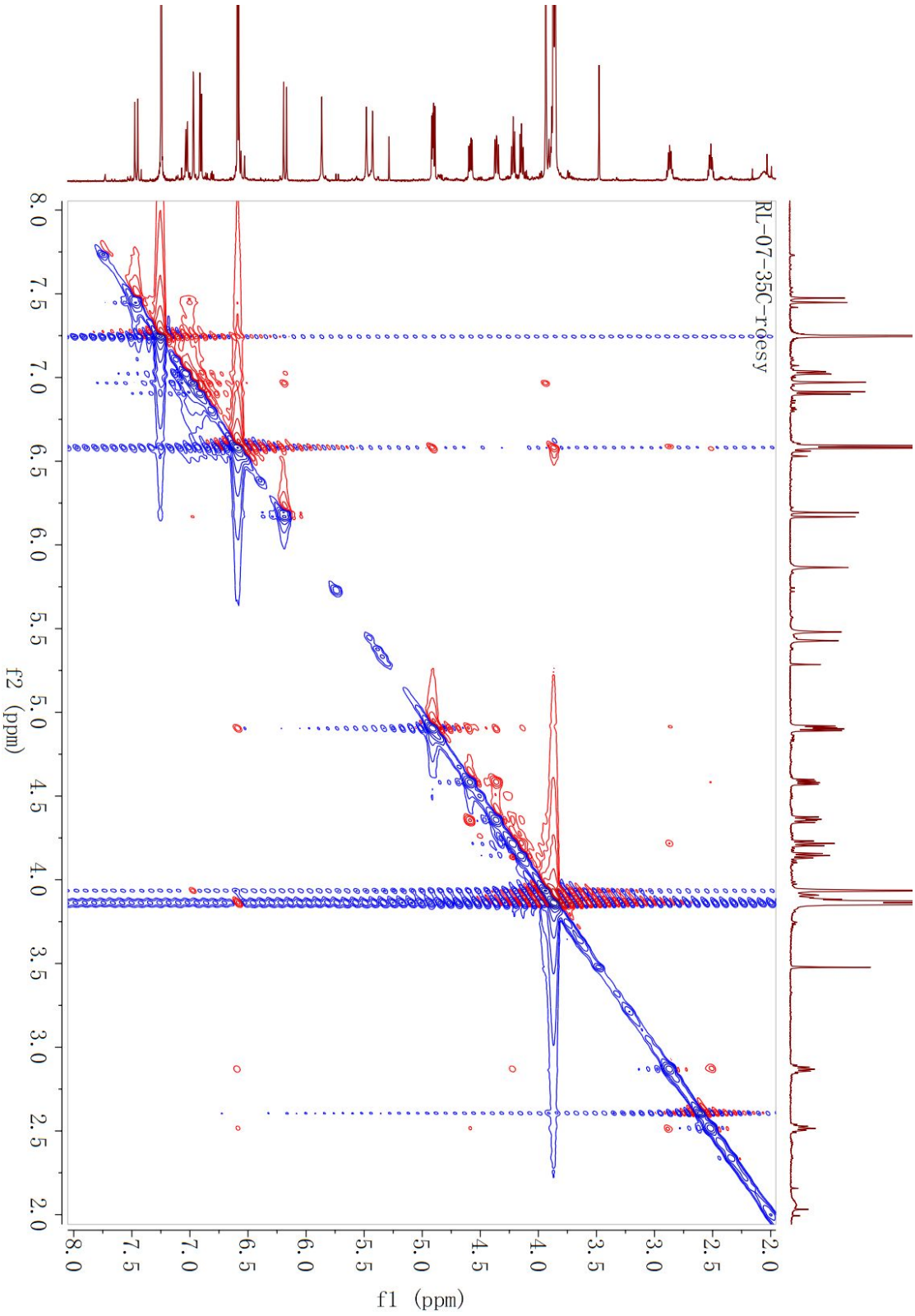
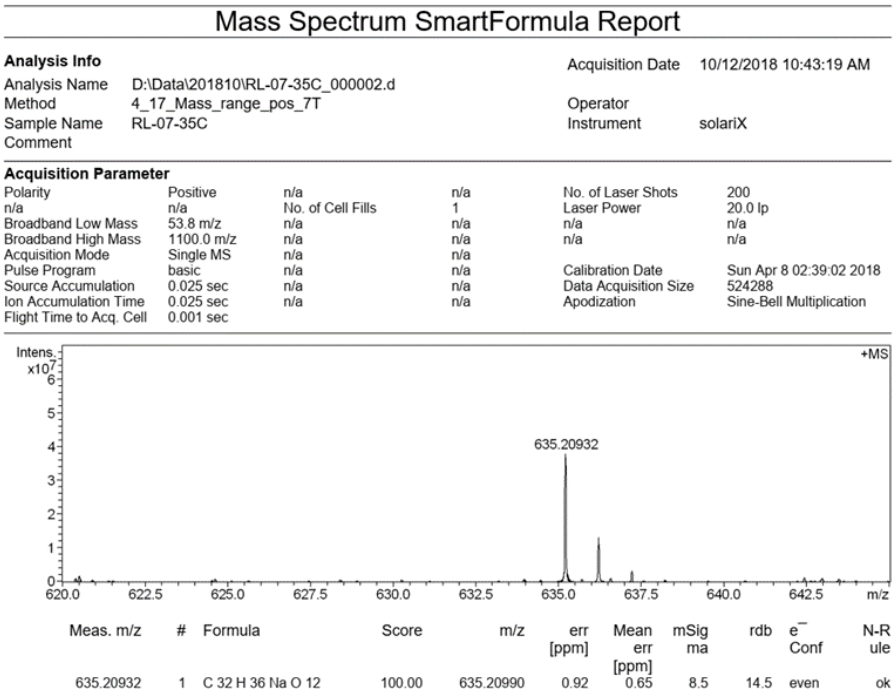


Figure S56. HRESIMS spectrum of bejolghotin F (**10**)



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201810\RL-07-35C_000002.d	Acquisition Date	10/12/2018 10:43:19 AM
Method	4_17_Mass_range_pos_7T	Operator	
Sample Name	RL-07-35C	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	53.8 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1100.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Sun Apr 8 02:39:02 2018
Source Accumulation	0.025 sec	n/a	n/a	Data Acquisition Size	524288
Ion Accumulation Time	0.025 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e⁻ Conf	N-R ule
635.20932	1	C 32 H 36 Na O 12	100.00	635.20990	0.92	0.65	8.5	14.5	even	ok

Figure S57. UV spectrum of bejolghotin F (**10**)

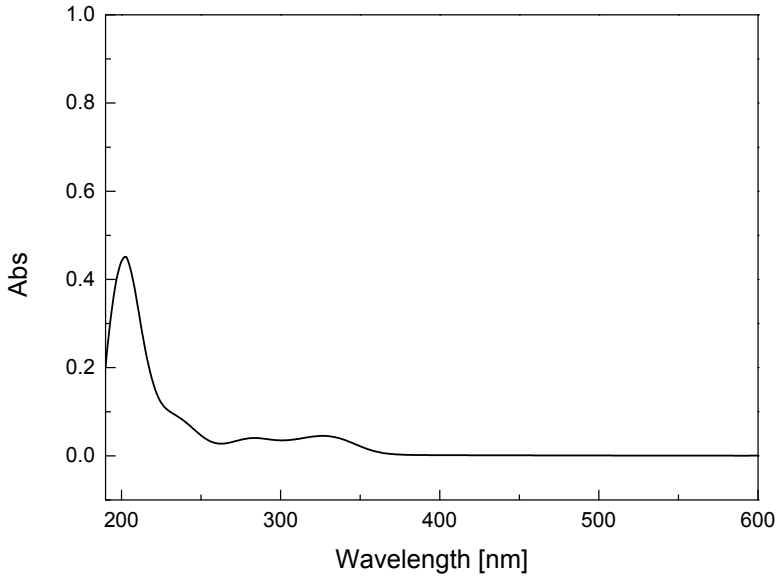


Figure S58. IR spectrum (KBr disc) of bejolghotin F (**10**)

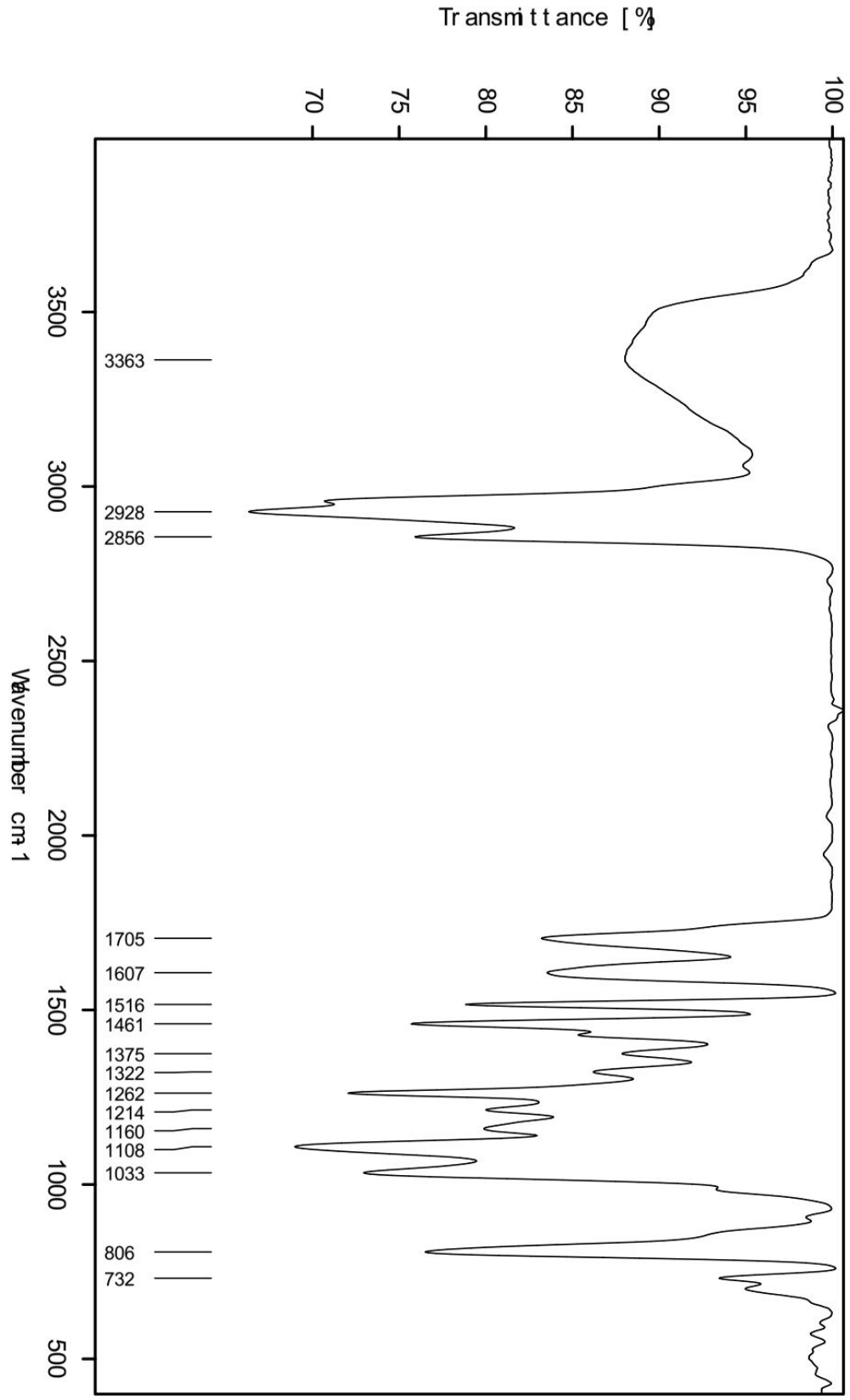


Figure S59. ^{1}H NMR spectrum (600 MHz) of bejolghotin G (**11**) in $CDCl_3$

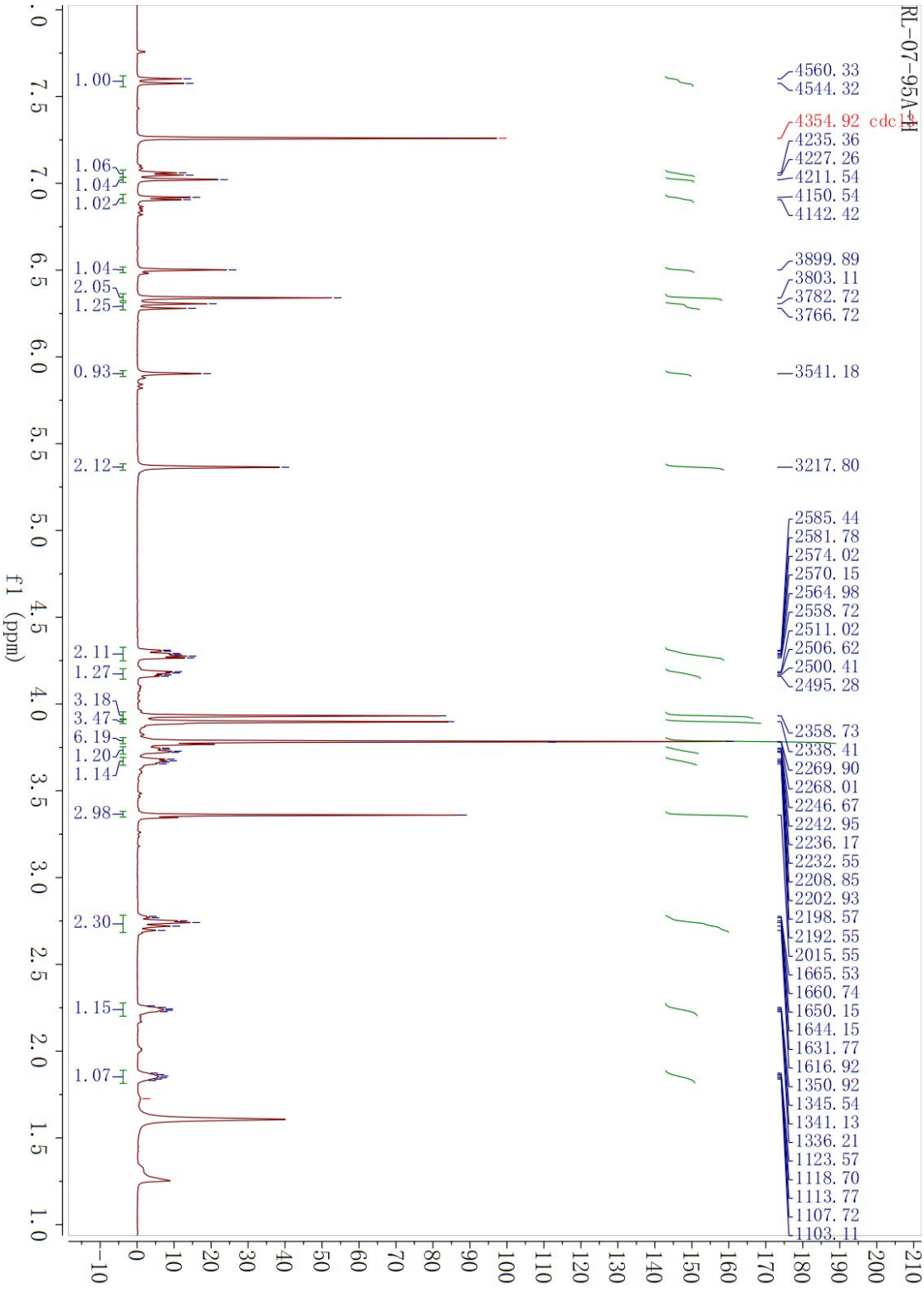


Figure S60. ^{13}C NMR spectrum (150 MHz) of bejolghotin G (**11**) in $CDCl_3$

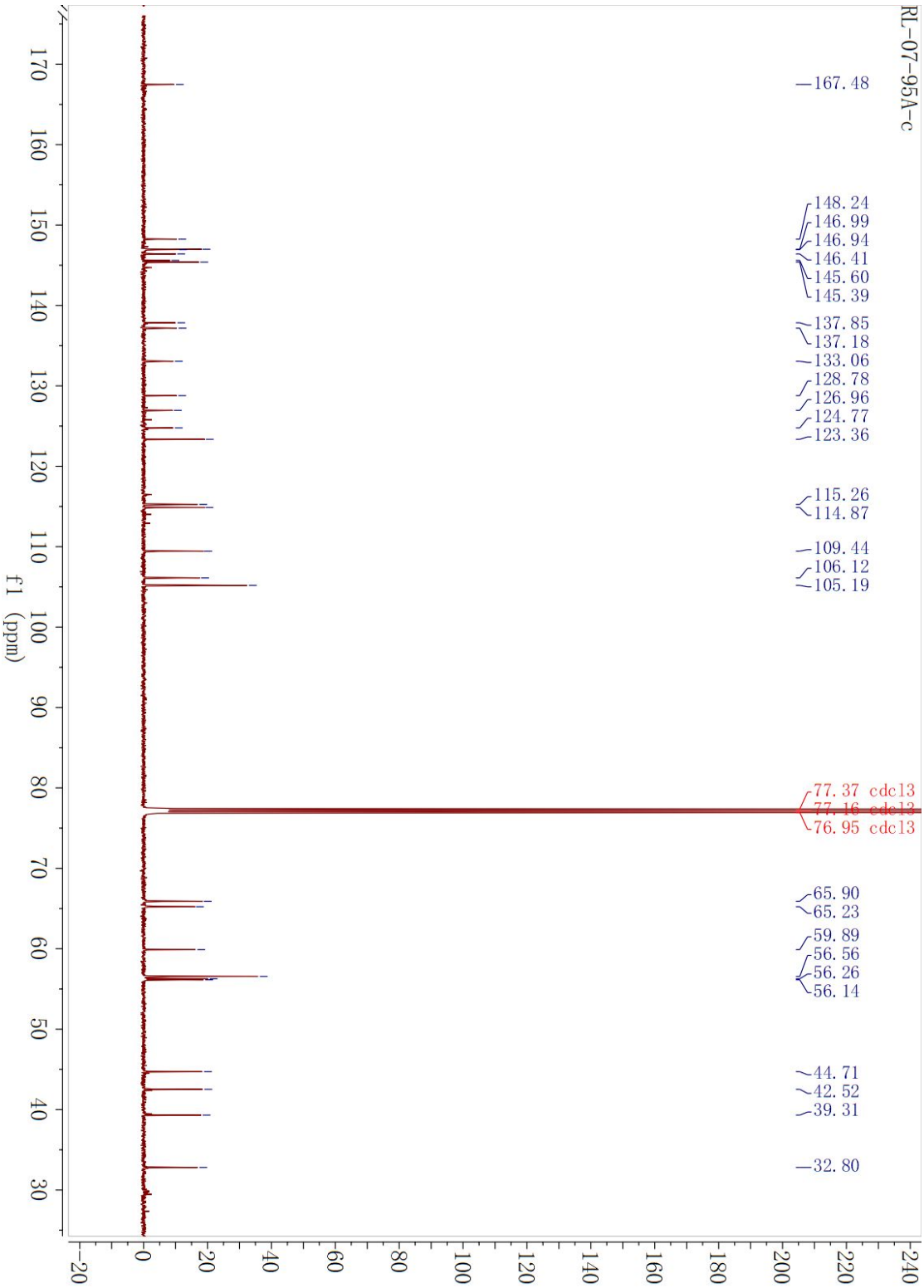


Figure S61. $^{1}H-^{1}H$ COSY spectrum (600 MHz) of bejolghotin G (**11**) in $CDCl_3$

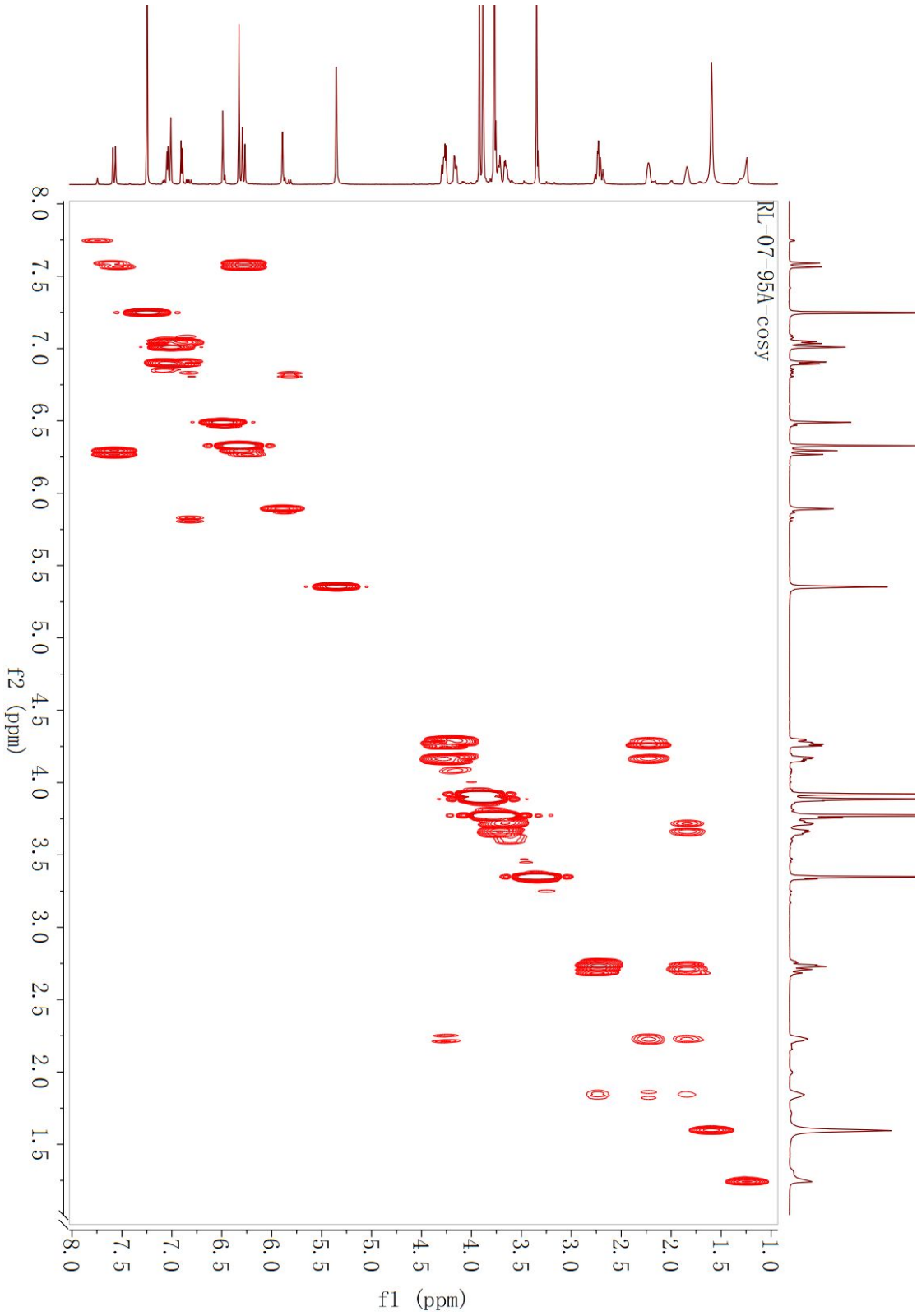


Figure S62. HSQC spectrum (600 MHz) of bejolghotin G (**11**) in $CDCl_3$

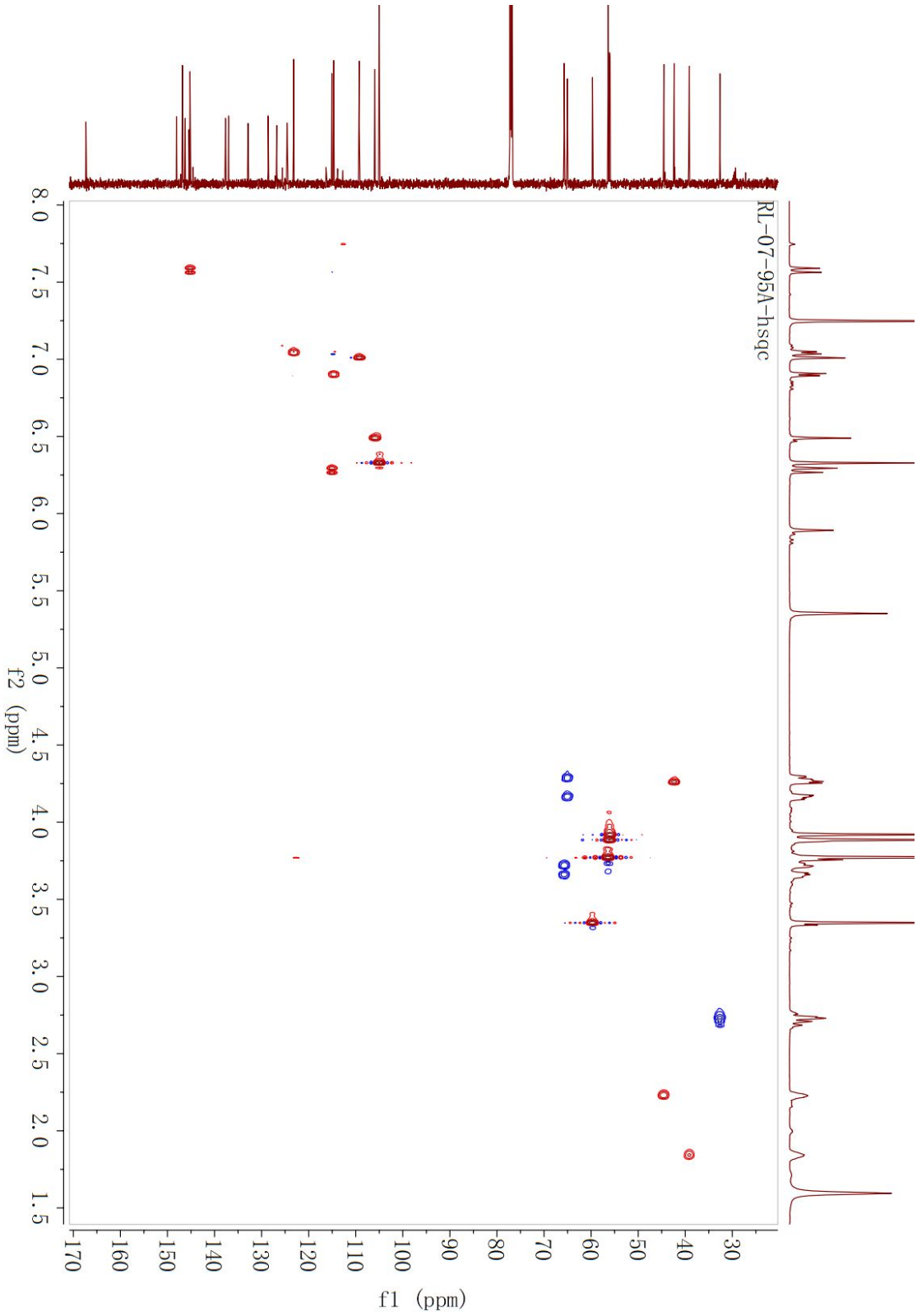


Figure S63. HMBC spectrum (600 MHz) of bejolghotin G (**11**) in $CDCl_3$

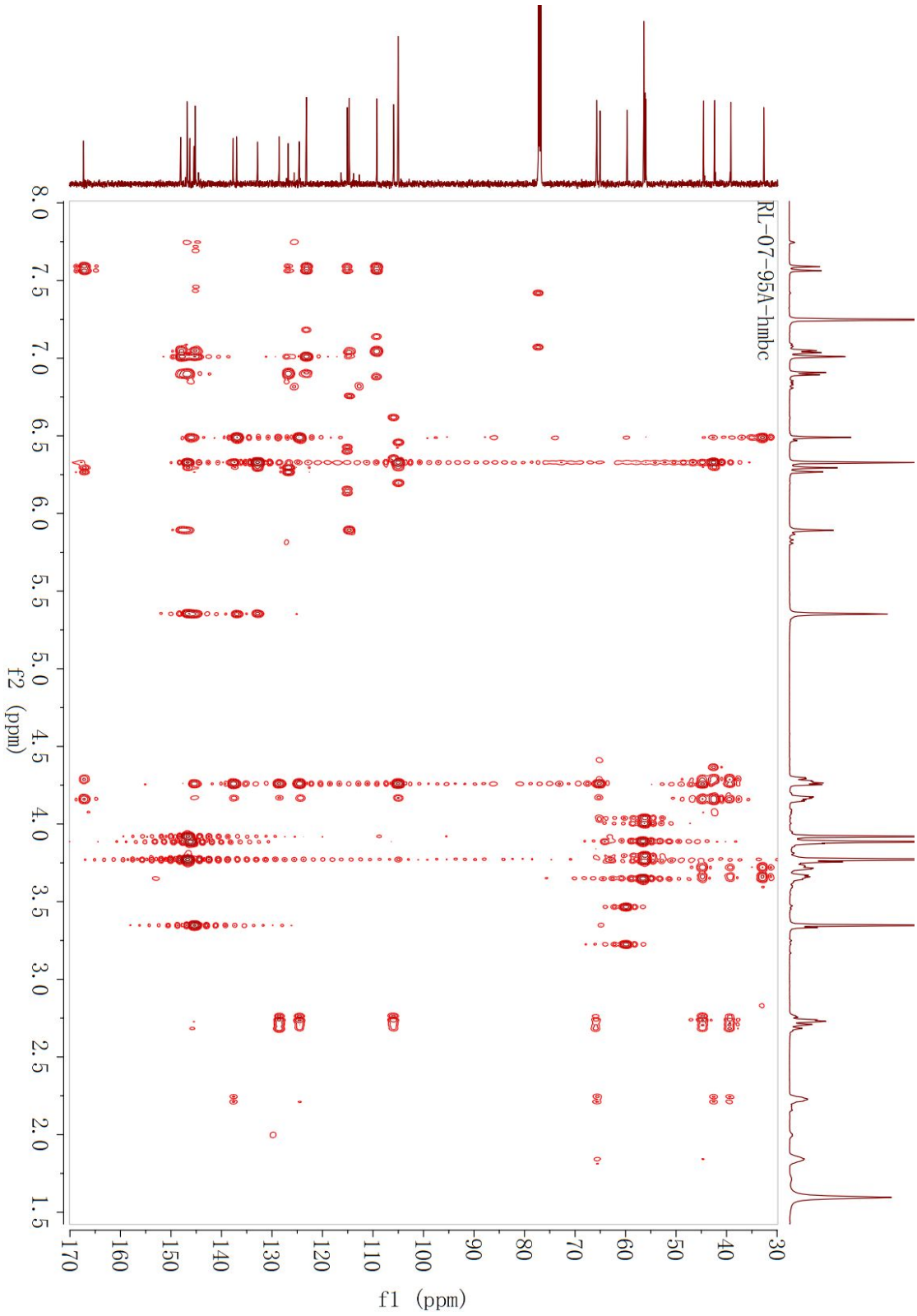


Figure S64. ROESY spectrum (600 MHz) of bejolghotin G (**11**) in $CDCl_3$

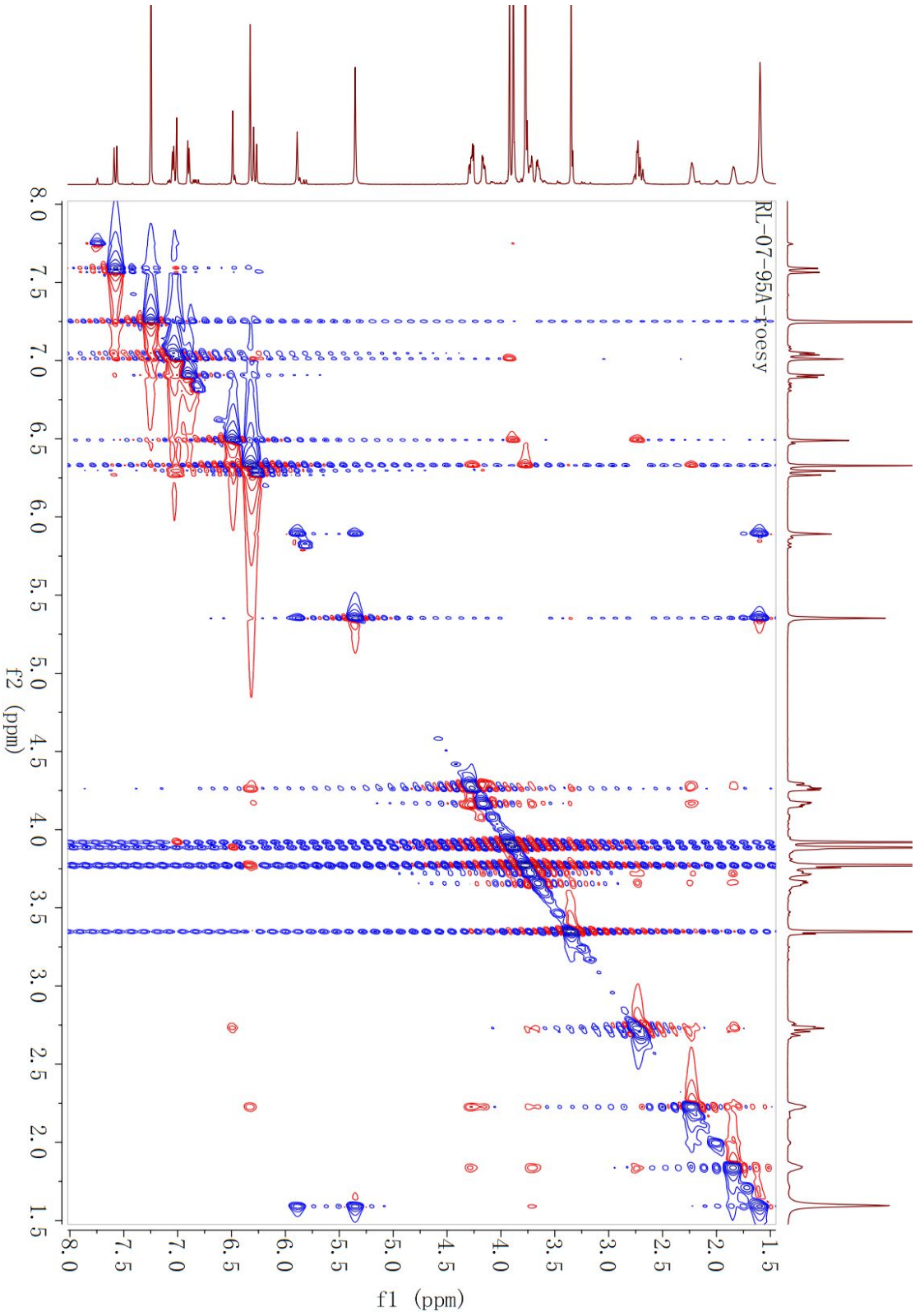
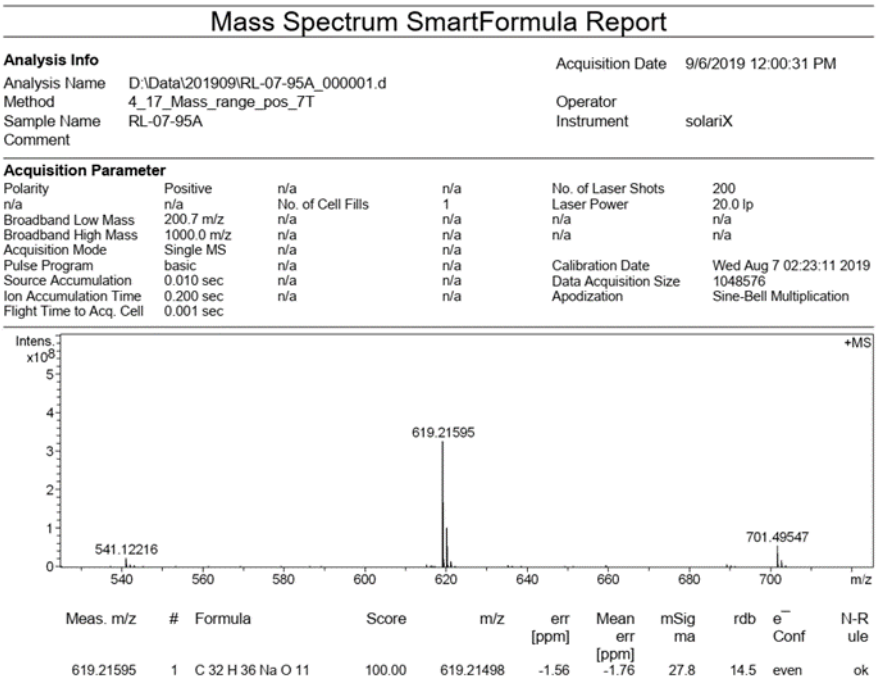


Figure S65. HRESIMS spectrum of bejolghotin G (**11**)



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201909\RL-07-95A_000001.d	Acquisition Date	9/6/2019 12:00:31 PM
Method	4_17_Mass_range_pos_7T	Operator	
Sample Name	RL-07-95A	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Wed Aug 7 02:23:11 2019
Source Accumulation	0.010 sec	n/a	n/a	Data Acquisition Size	1048576
Ion Accumulation Time	0.200 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
619.21595	1	C 32 H 36 Na O 11	100.00	619.21498	-1.56	-1.76	27.8	14.5	even	ok

Figure S66. UV spectrum of bejolghotin G (**11**)

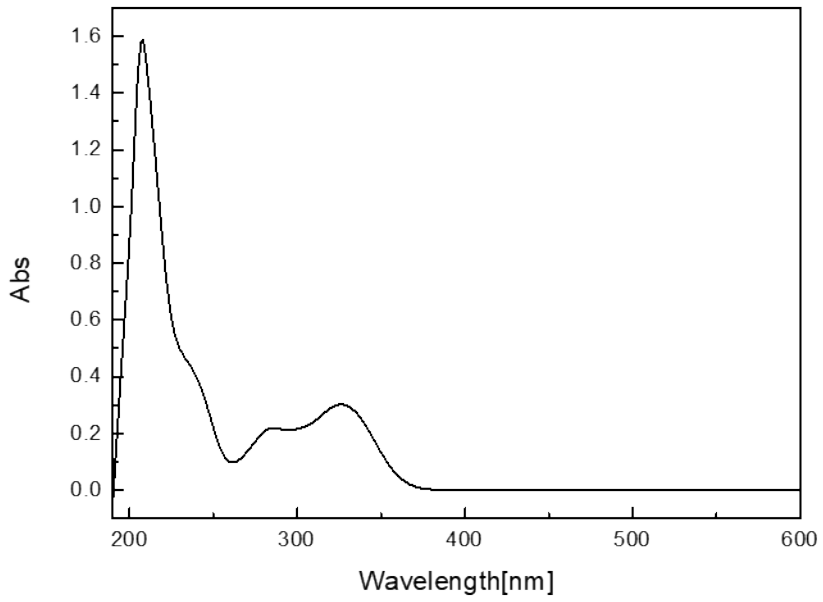


Figure S67. IR spectrum (KBr disc) of bejolghotin G (**11**)