Supporting Information

Labdane-type Diterpenoids from the Fruits of *Vitex trifolia*

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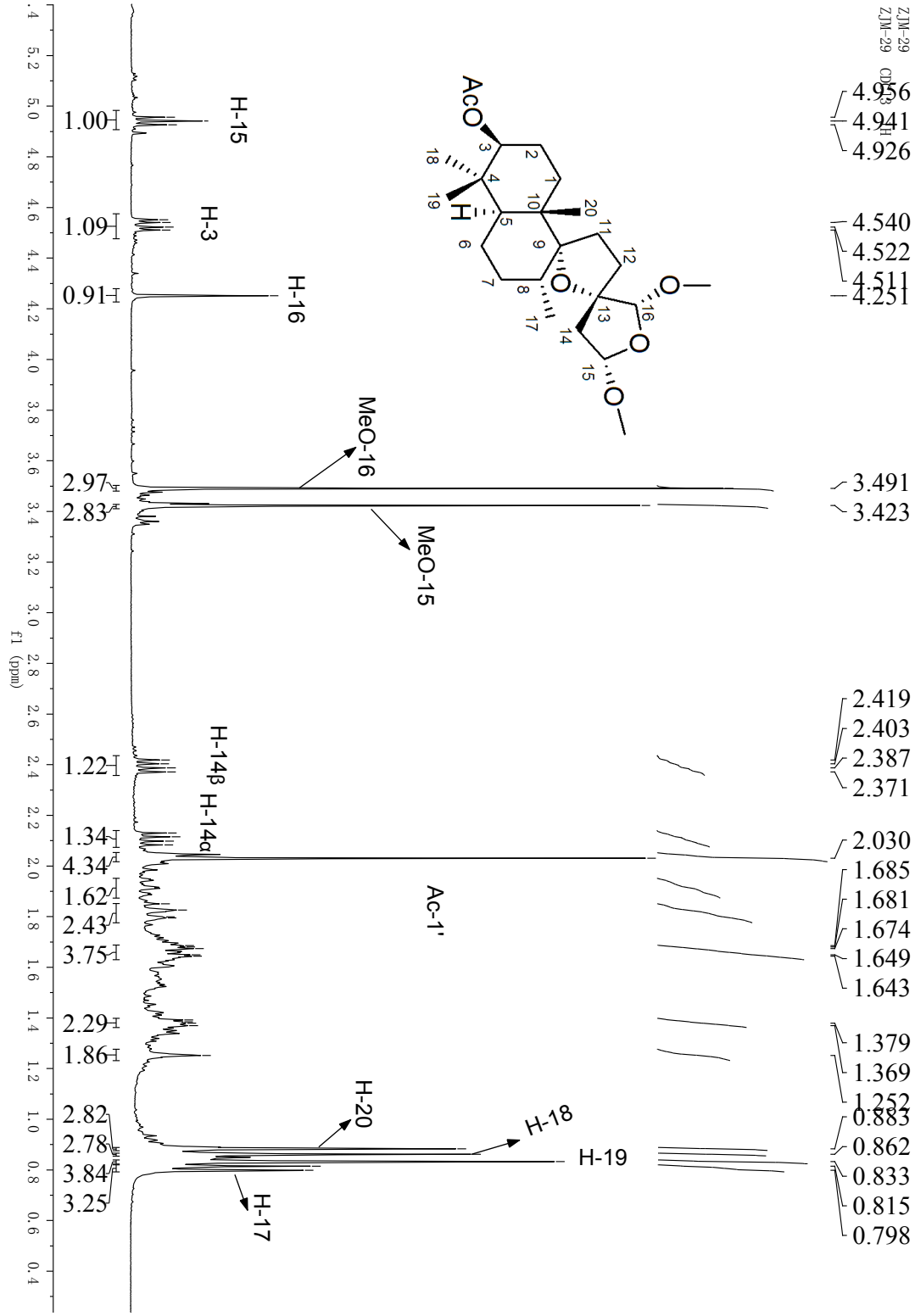
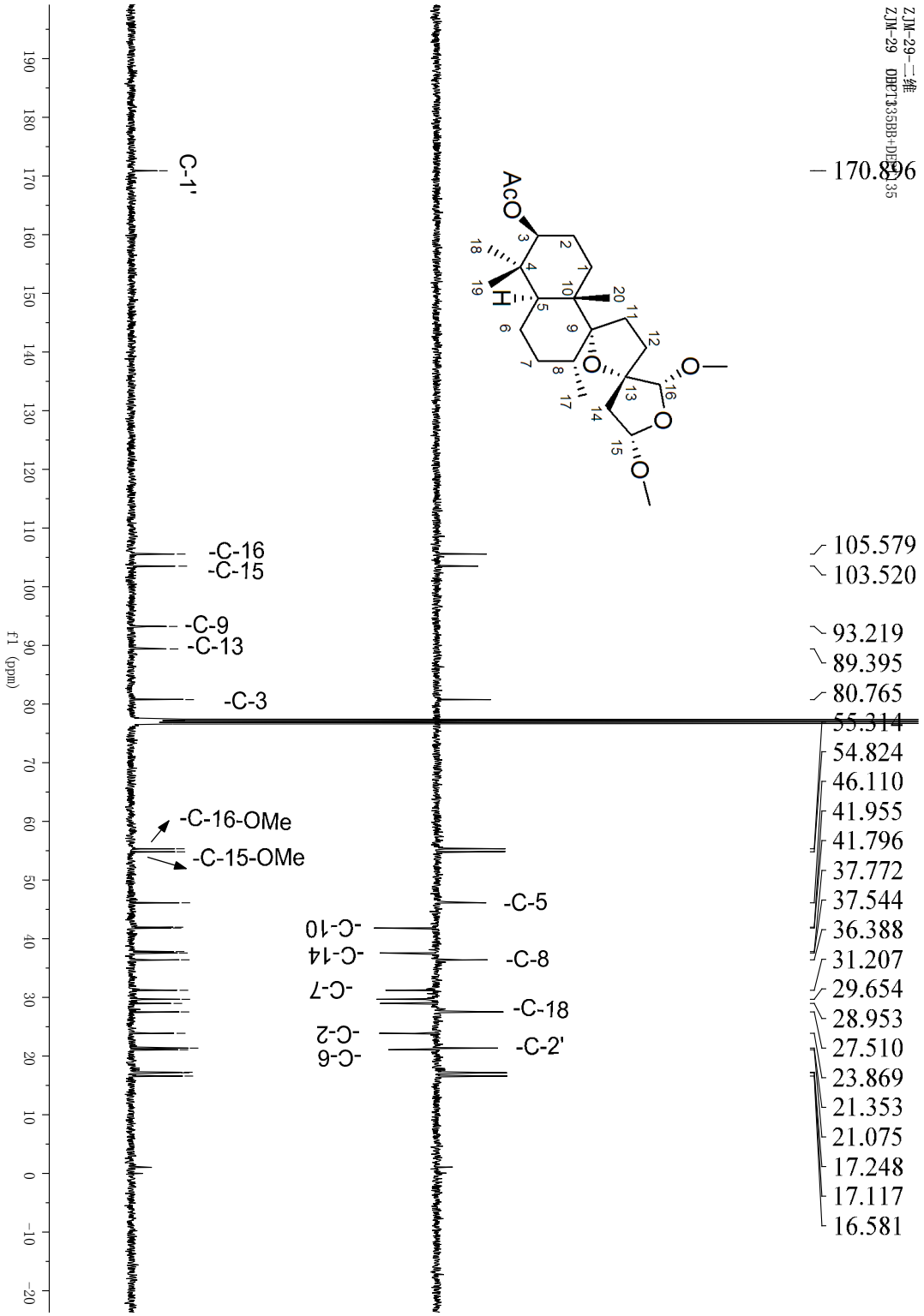
Supporting Information

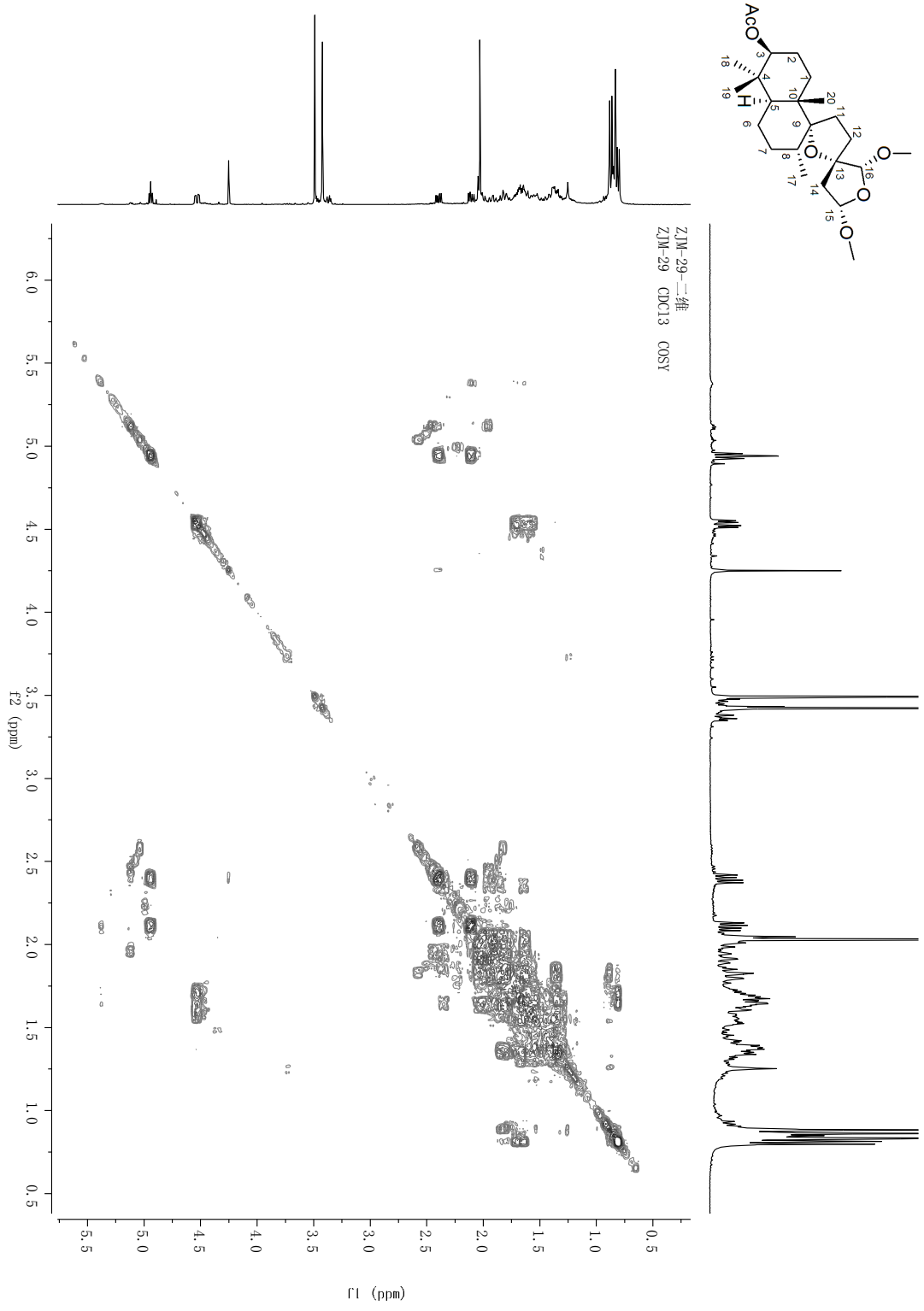
S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of vitextrifolin A (**1**)



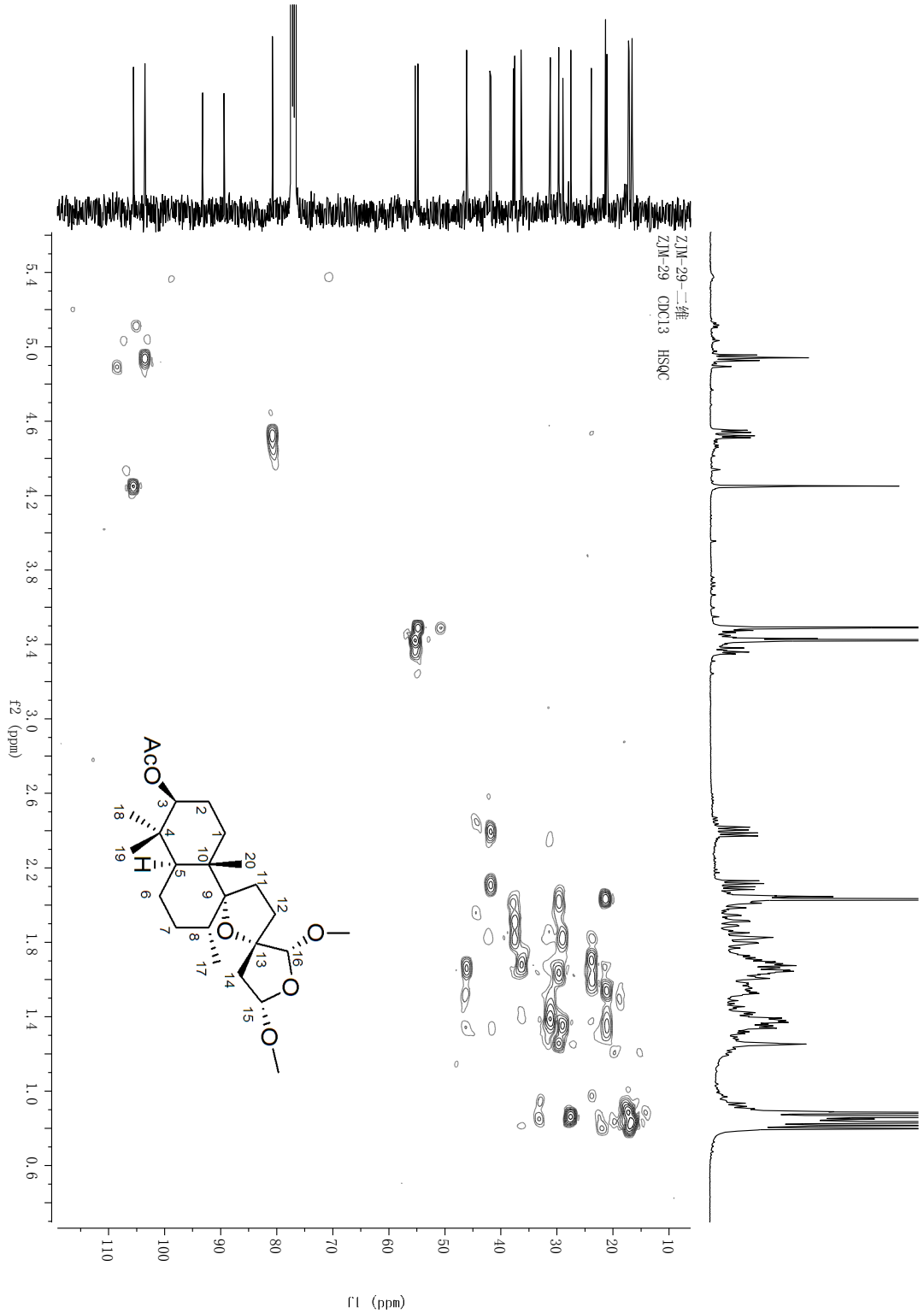
S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of vitextrifolin A (**1**)



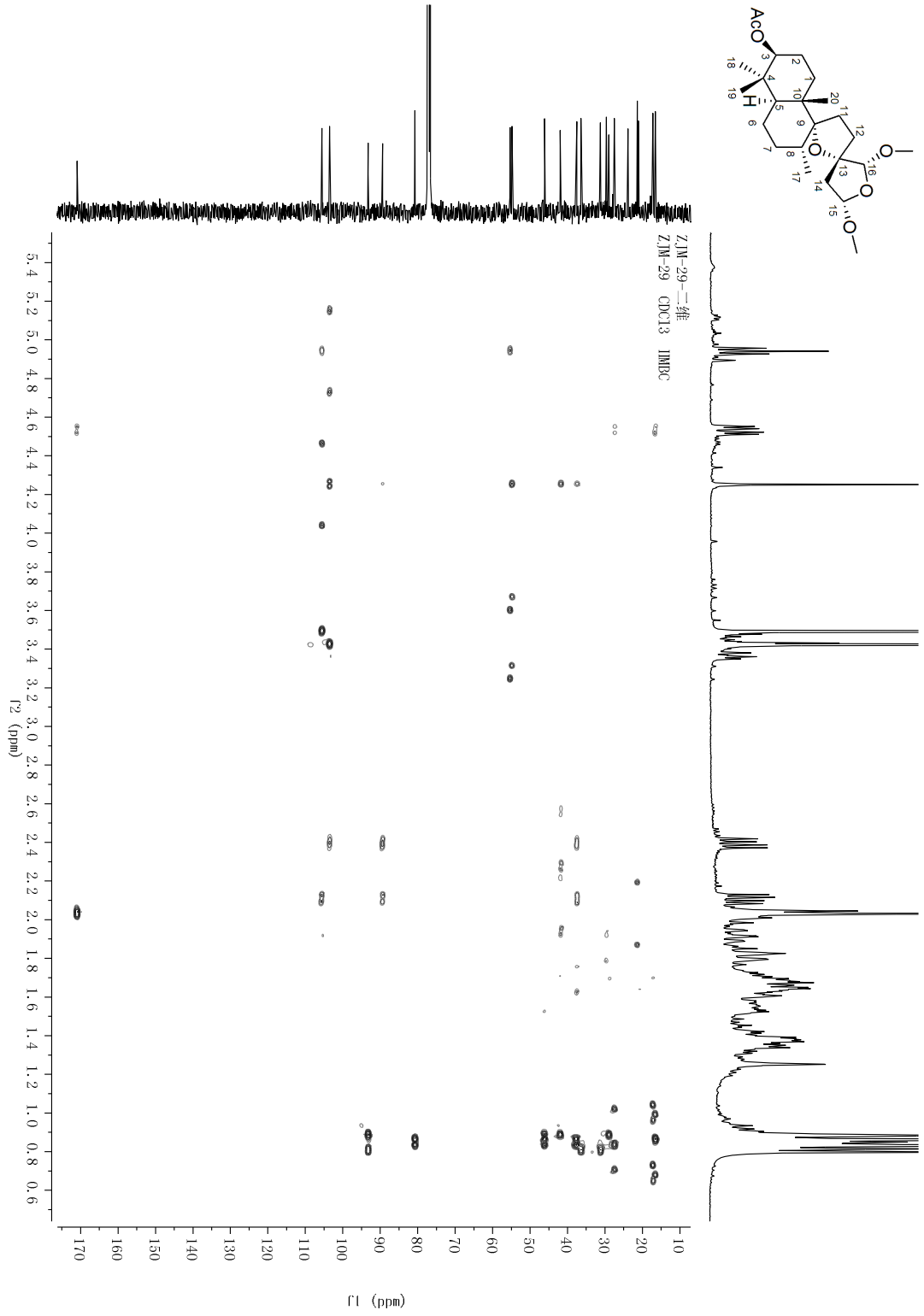
S3. ^{1}H-^{1}H COSY spectrum of vitextrifolin A (**1**) in $CDCl_3$



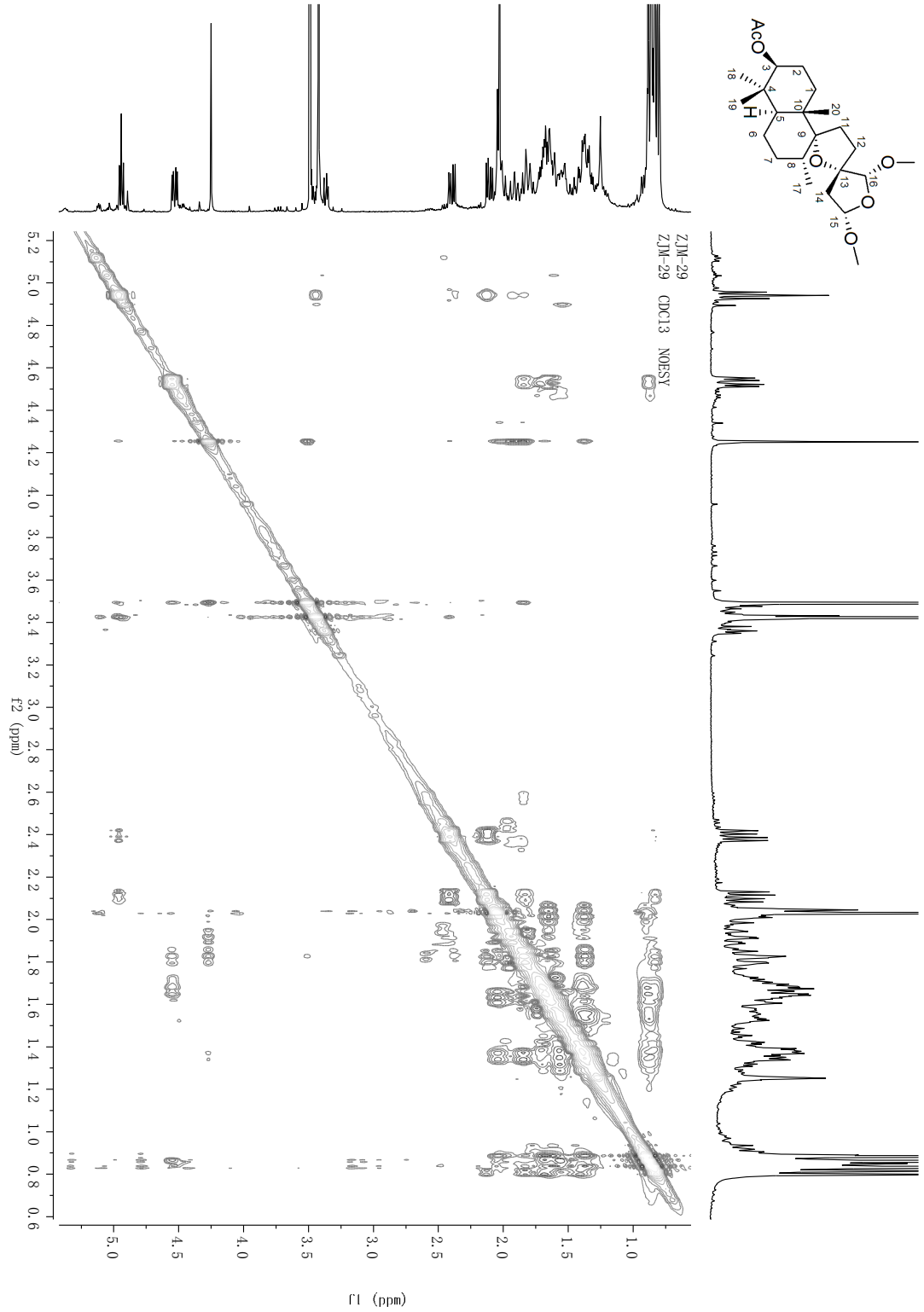
S4. HMQC spectrum of vitextrifolin A (**1**) in $CDCl_3$



S5. HMBC spectrum of vitextrifolin A (**1**) in $CDCl_3$



S6. NOESY spectrum of vitextrifolin A (**1**) in $CDCl_3$



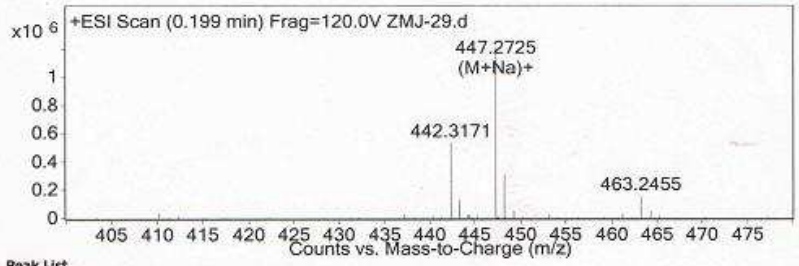
S7. HRESIMS spectrum of vitextrifolin A (**1**)

Qualitative Analysis Report

Data Filename	ZMJ-29.d	**Sample Name**	ZMJ-29
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEST-POS-01.m	**Acquired Time**	1/4/2012 10:04:18 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	Esi



Peak List

m/z	z	Abund	Formula	Ion
274.2743	1	441119		
275.2004		149062		
318.2999		127526		
335.2217		162028		
393.2636		190006		
442.3171	1	531313		
443.3197	1	133580		
447.2725	1	1214601	C24 H40 Na O6	(M+Na)+
448.2754	1	299385	C24 H40 Na O6	(M+Na)+
463.2455		156329		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C24 H40 O6	TRUE	424.2833	424.2825	-1.91	C24 H40 Na O6	97.42

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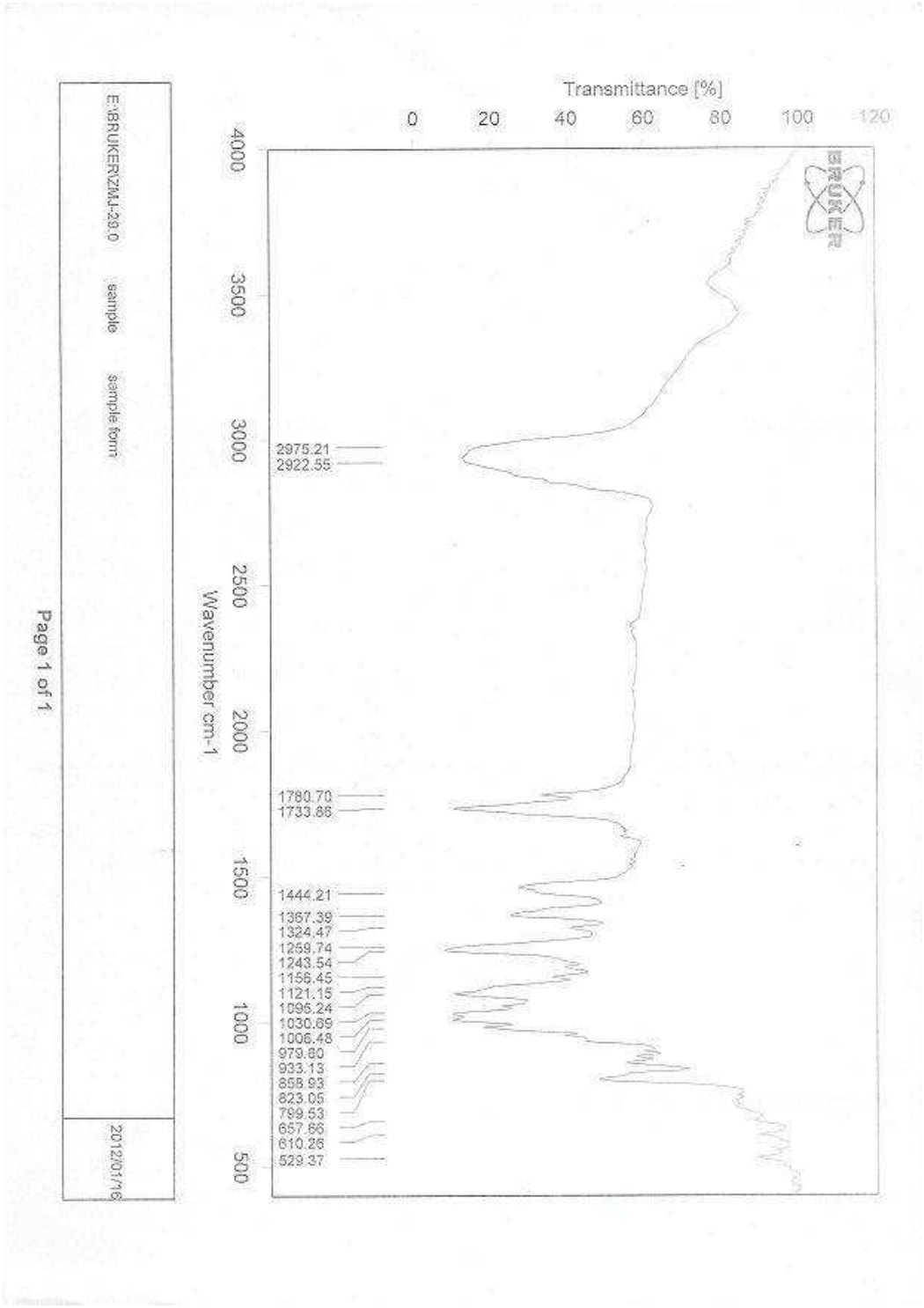
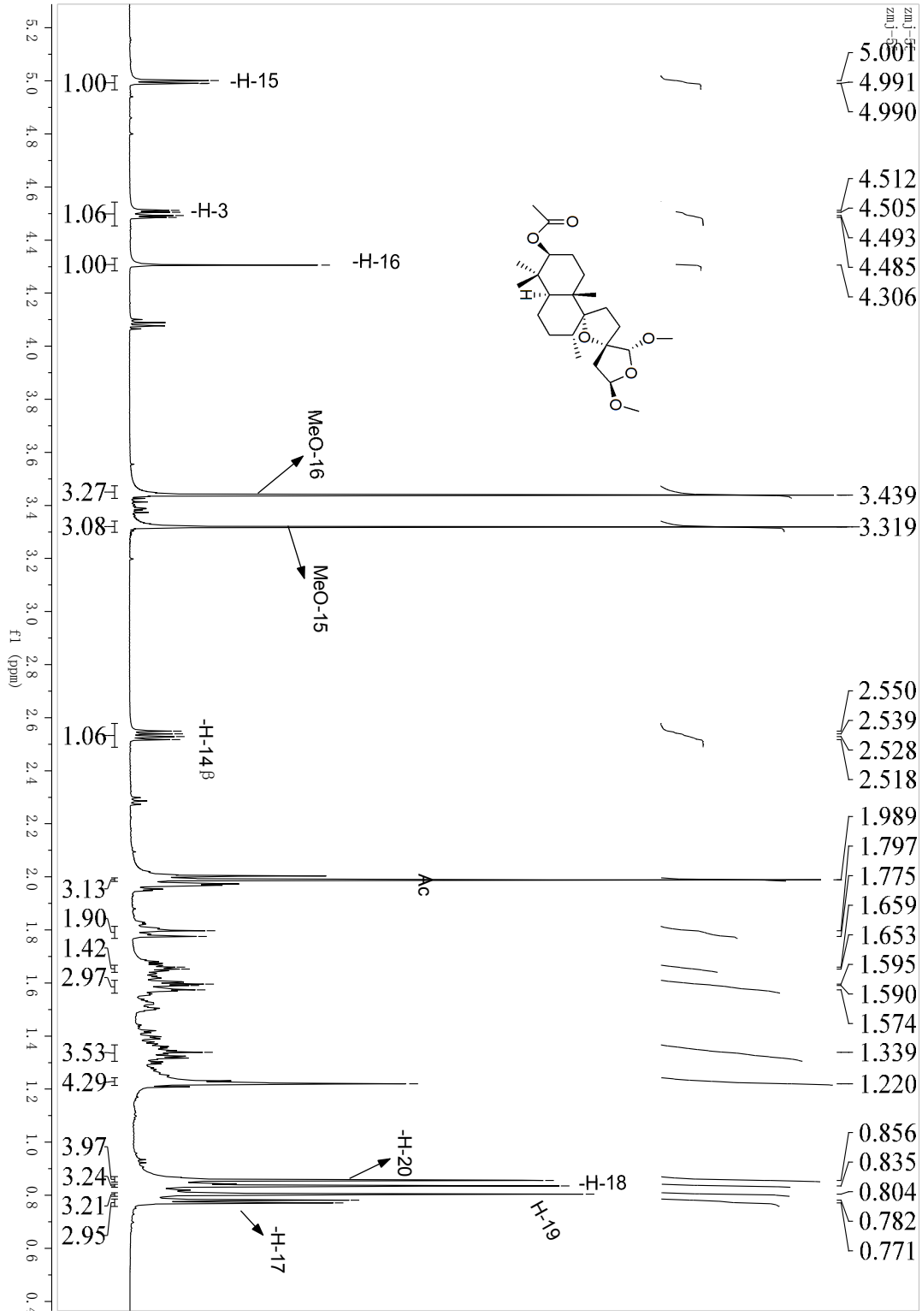
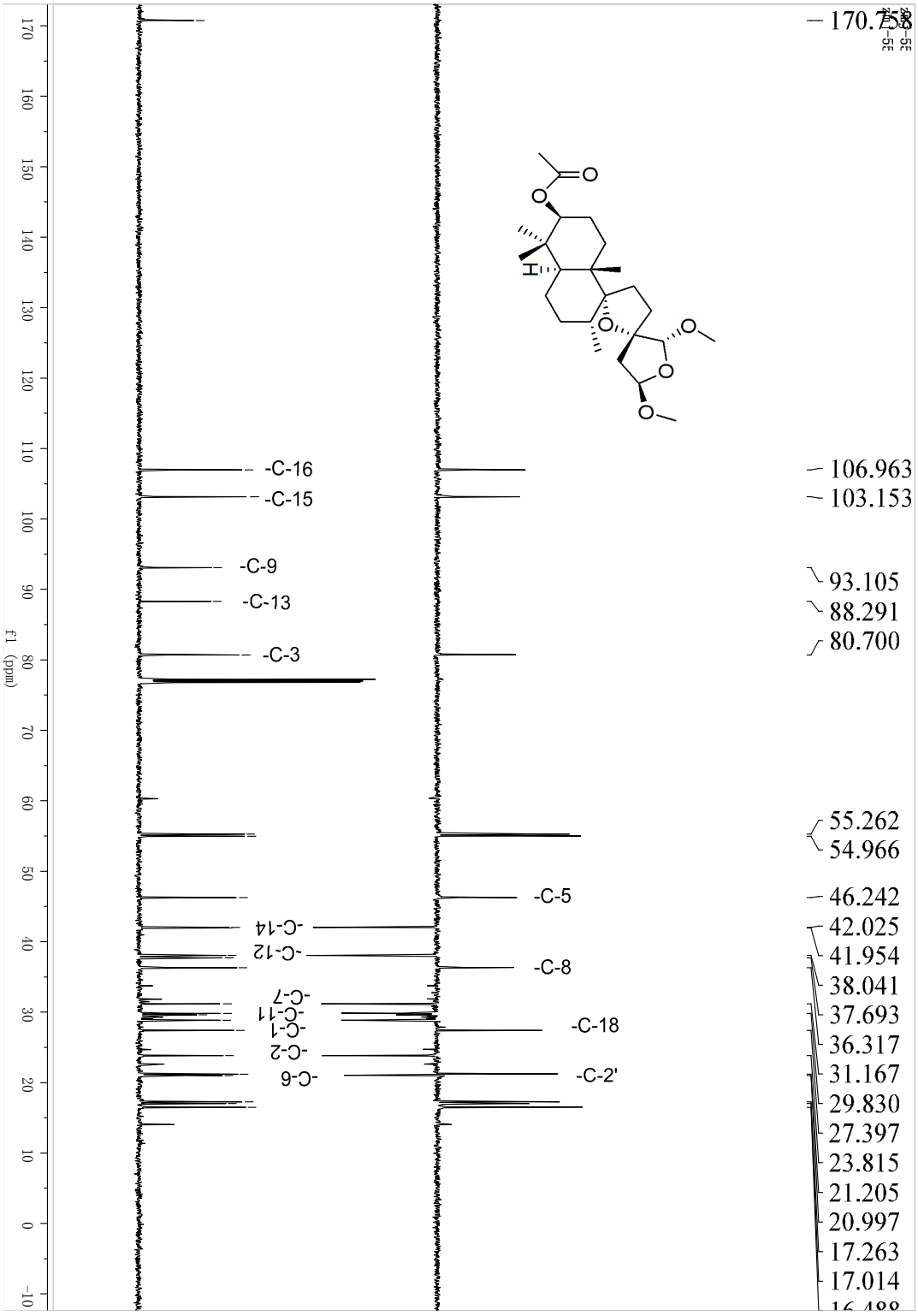
S8. IR (KBr disc) spectrum of vitextrifolin A (**1**)



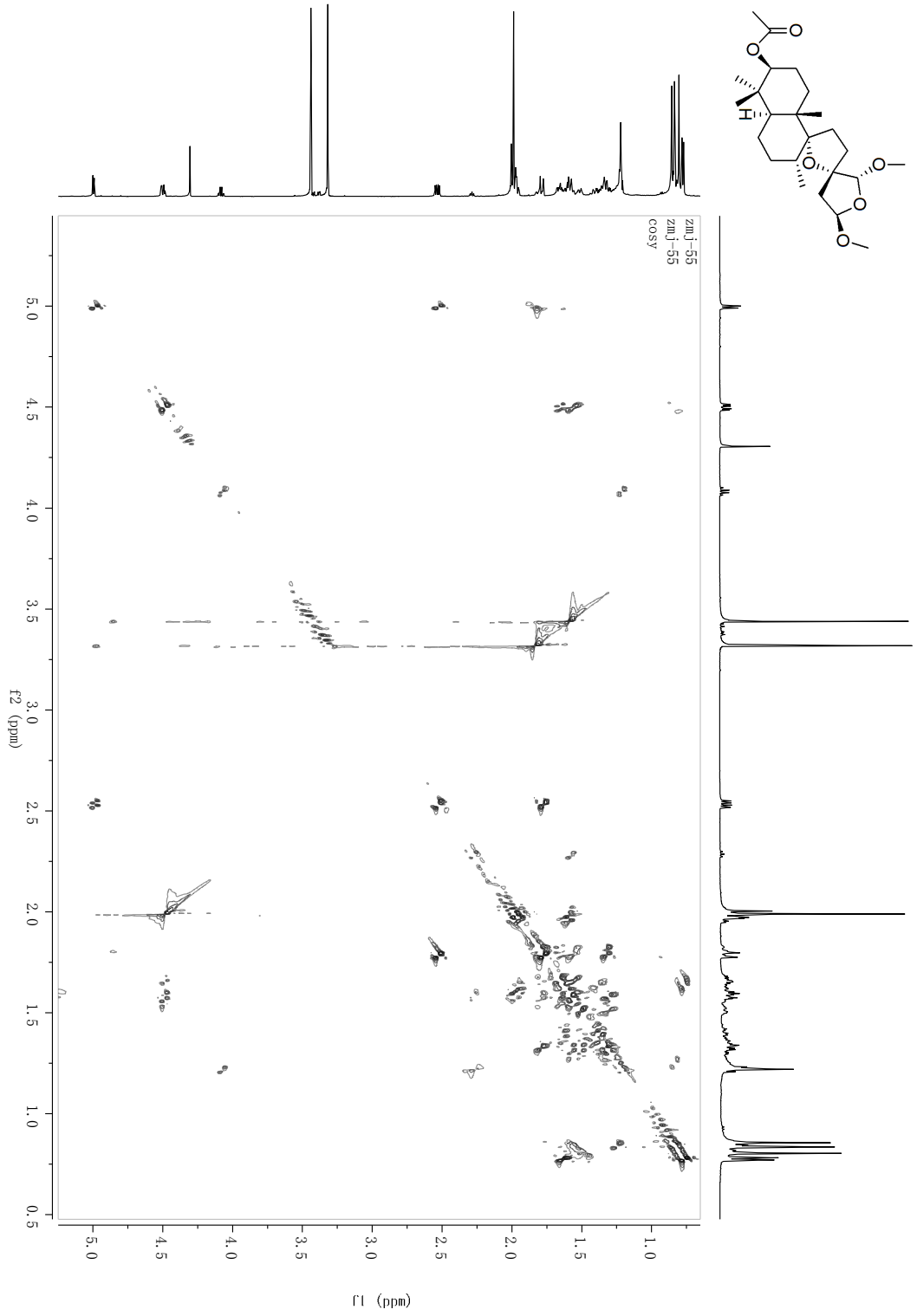
S9. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of vitextrifolin B (**2**)



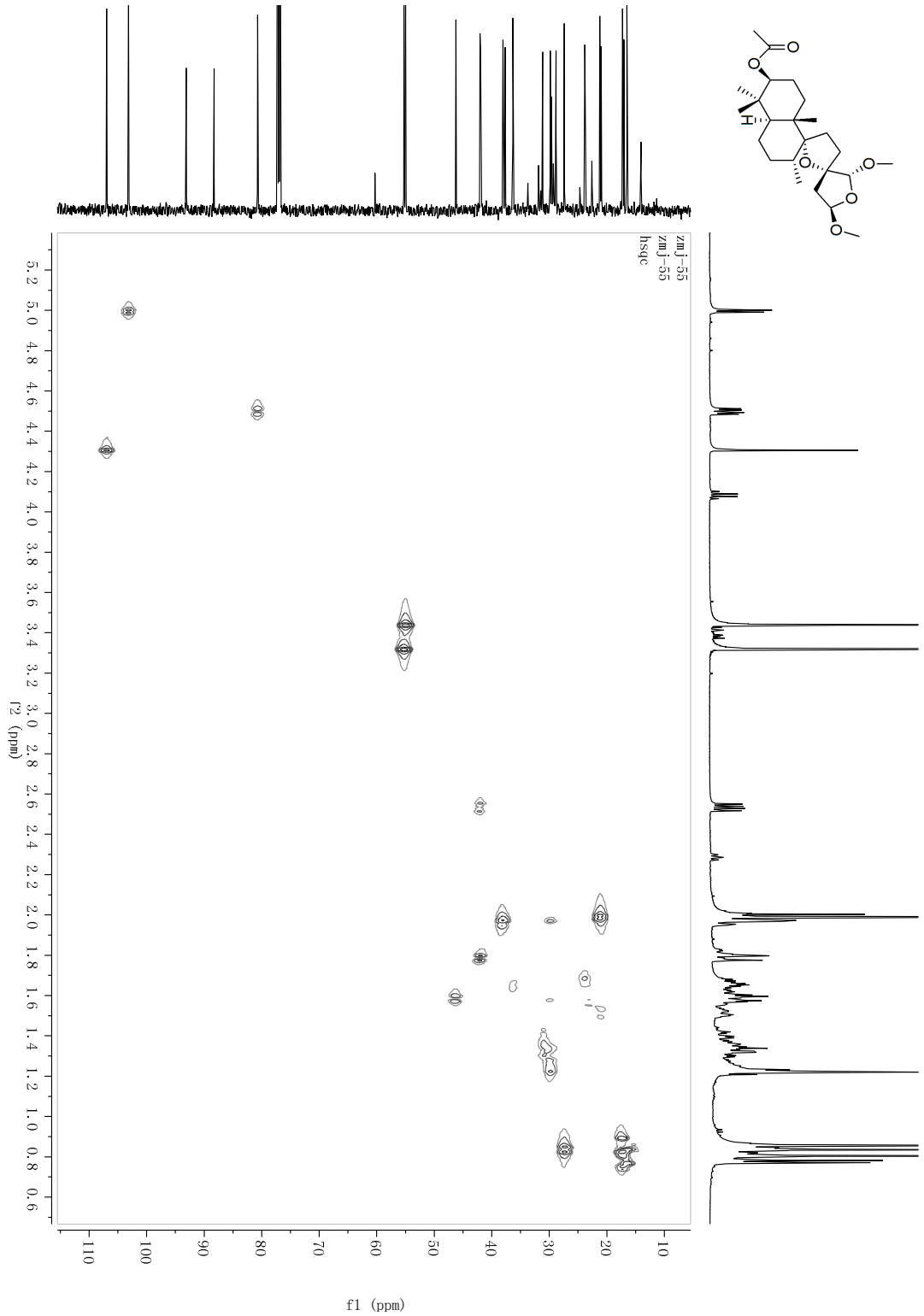
S10. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of vitextrifolin B (**2**)



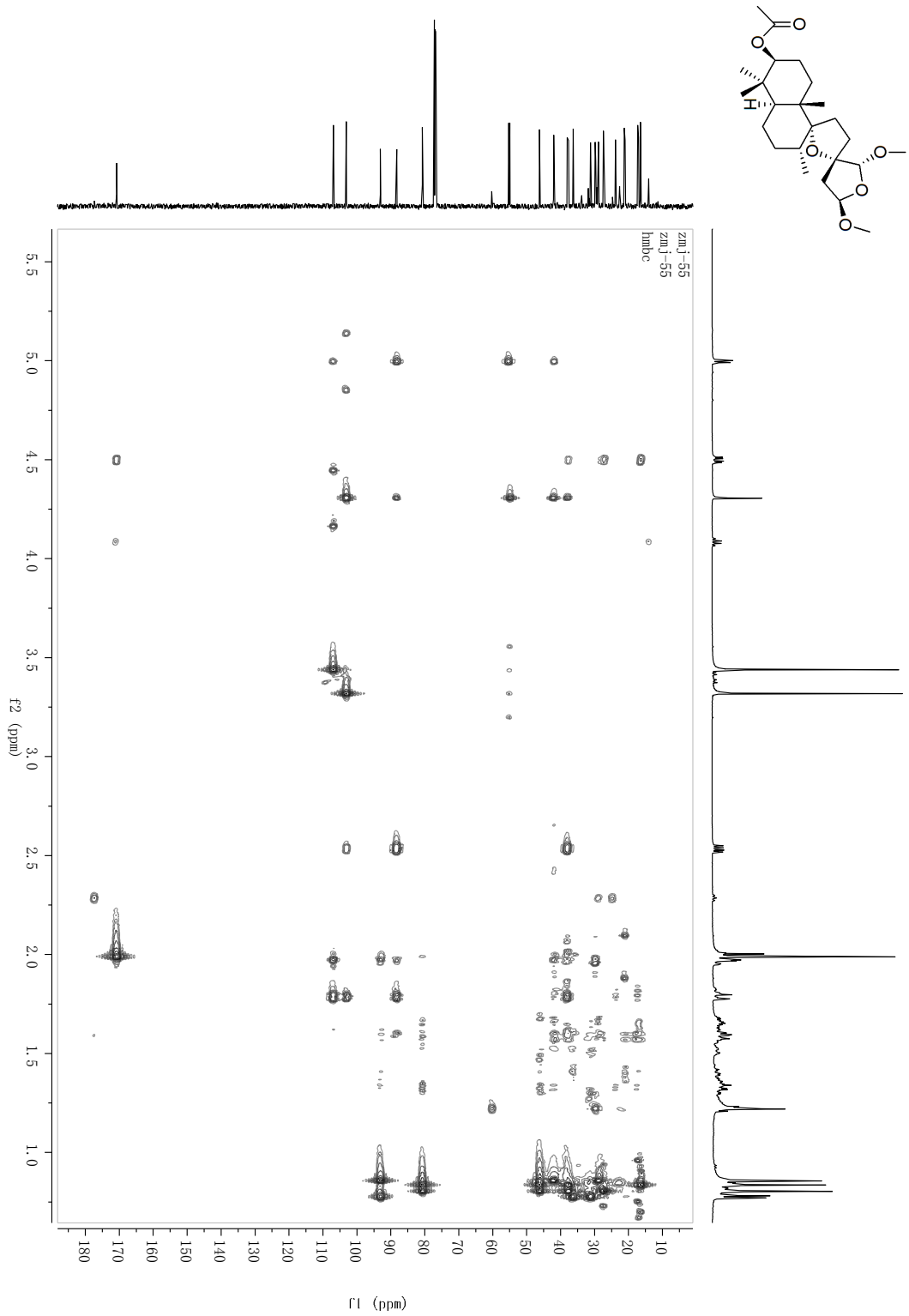
S11. ^{1}H-^{1}H COSY spectrum of vitextrifolin B (**2**) in $CDCl_3$



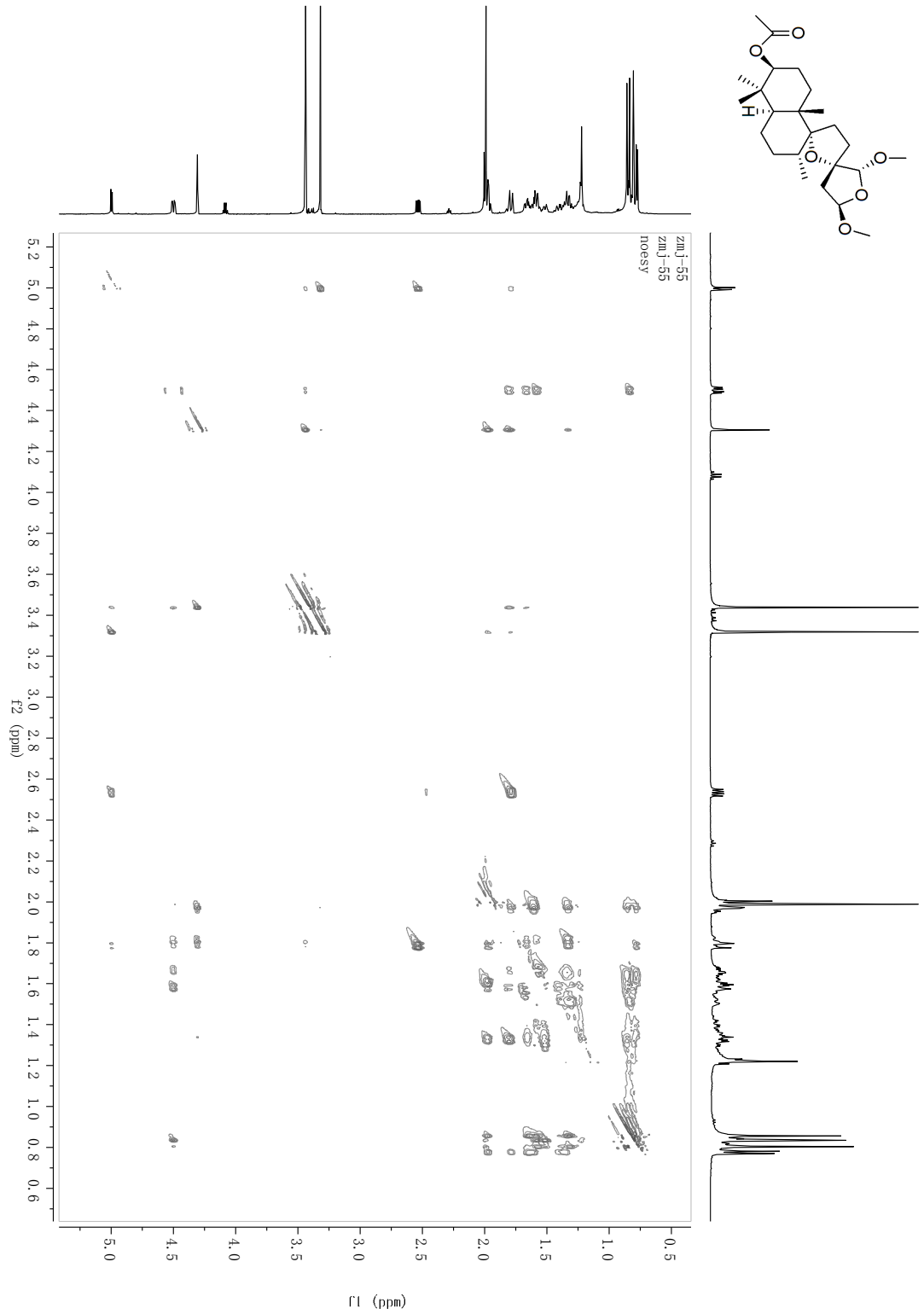
S12. HSQC spectrum of vitextrifolin B (**2**) in $CDCl_3$



S13. HMBC spectrum of vitextrifolin B (**2**) in $CDCl_3$



S14. NOESY spectrum of vitextrifolin B (**2**) in $CDCl_3$



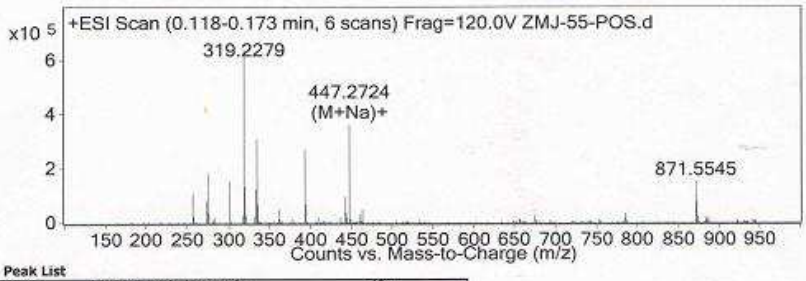
S15. HRESIMS spectrum of vitextrifolin B (**2**)

Qualitative Analysis Report

Data Filename	ZMJ-55-POS.d	**Sample Name**	ZMJ-55
Sample Type	Sample	**Position**	P1-E1
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEST-POS-01.m	**Acquired Time**	3/14/2012 3:03:32 PM
IRM Calibration Status	Some Ions Missed	**DA Method**	ERROR.m
Comment			

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	Esi



Peak List

m/z	z	Abund	Formula	Ion
257.1904		107366		
275.2011	1	187007		
301.2166	1	156722		
319.2279	1	642196		
320.2307	1	135199		
333.2427		123002		
335.2224	1	309105		
393.2641	1	271003		
447.2724	1	362529	C24 H40 Na O6	(M+Na)+
871.5545	1	152564		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	5

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C24 H40 O6	TRUE	424.2832	424.2825	-1.66	C24 H40 Na O6	98.28
C25 H36 N4 O2		424.2832	424.2838	1.48	C25 H36 N4 Na O2	97.33

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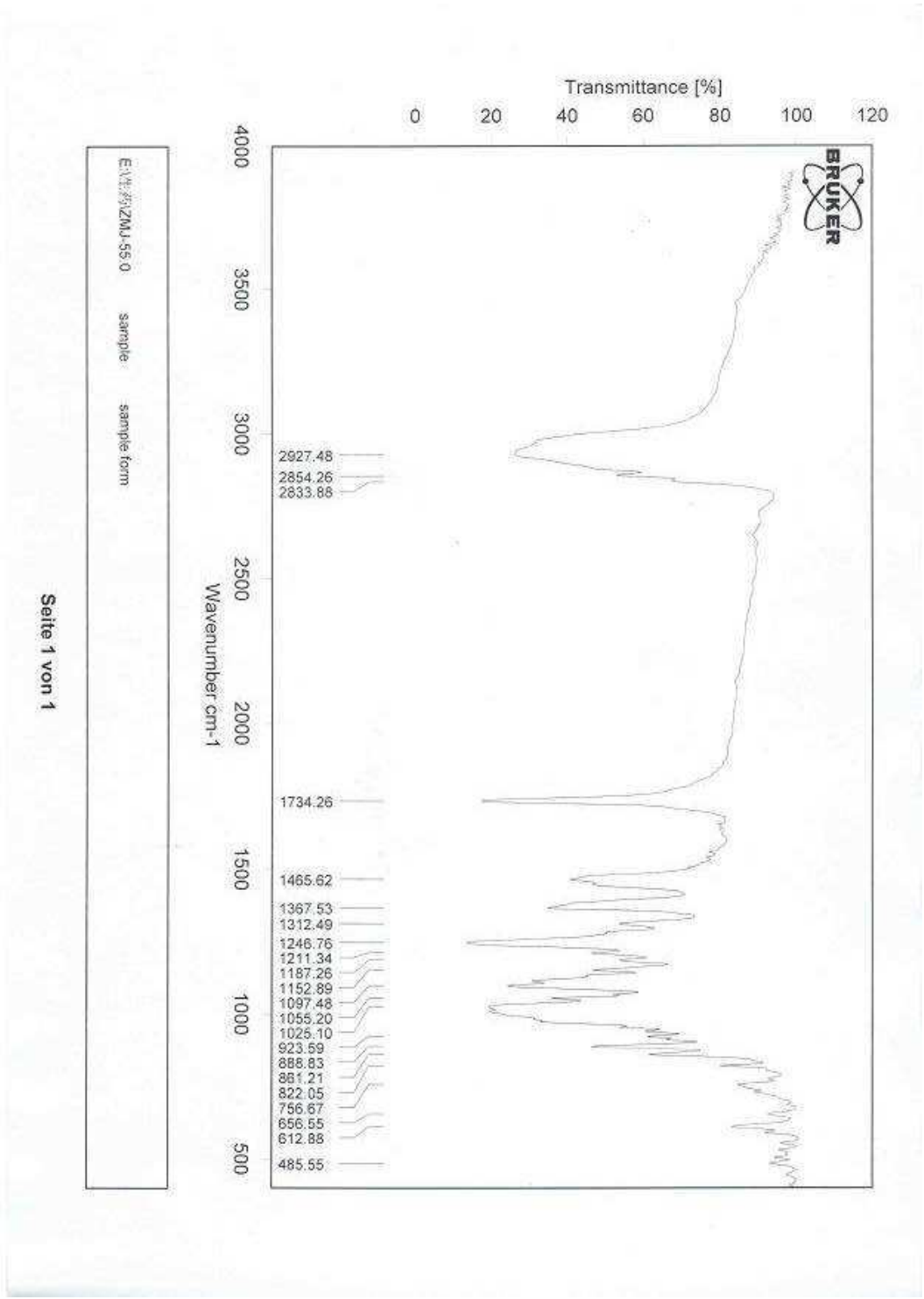
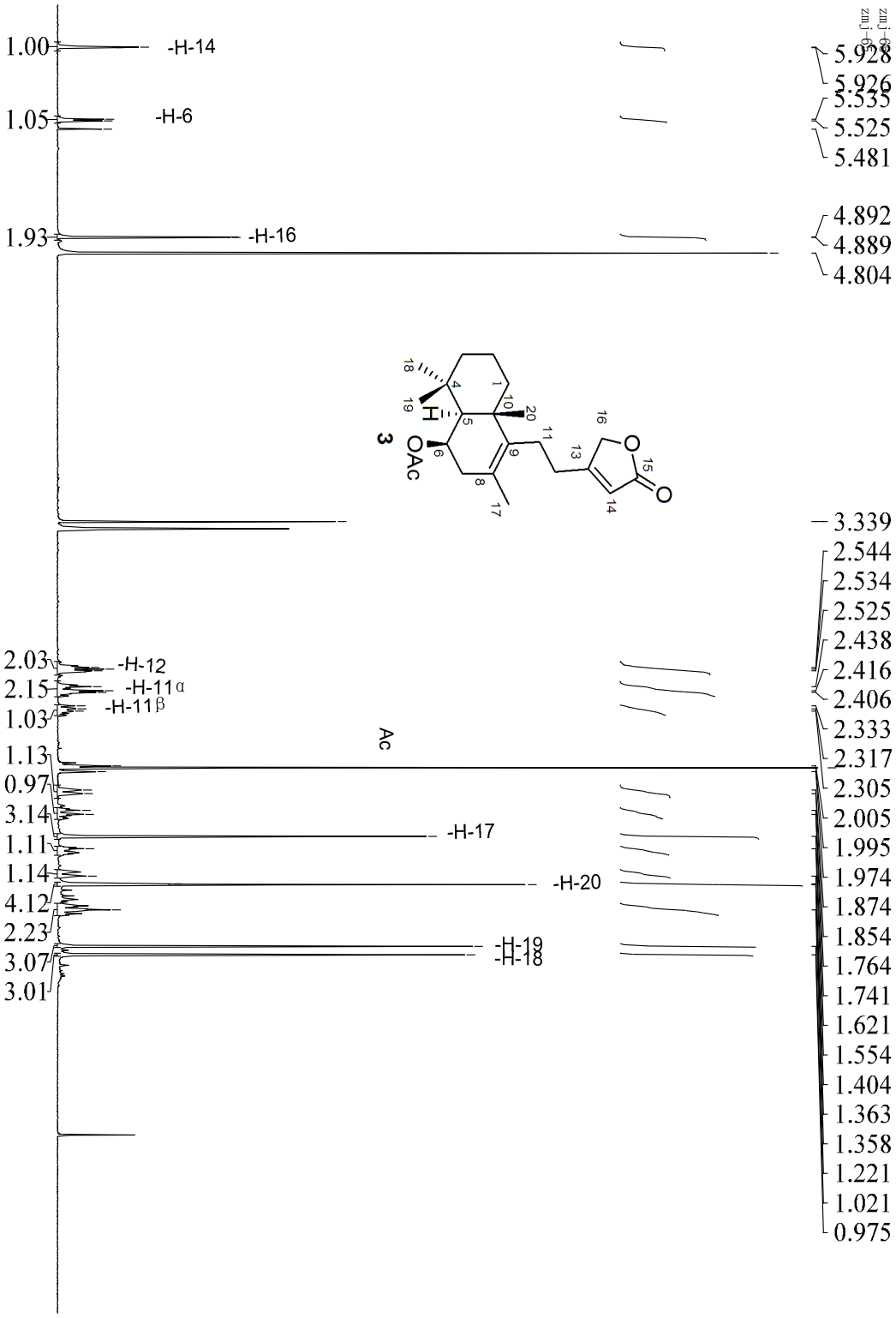
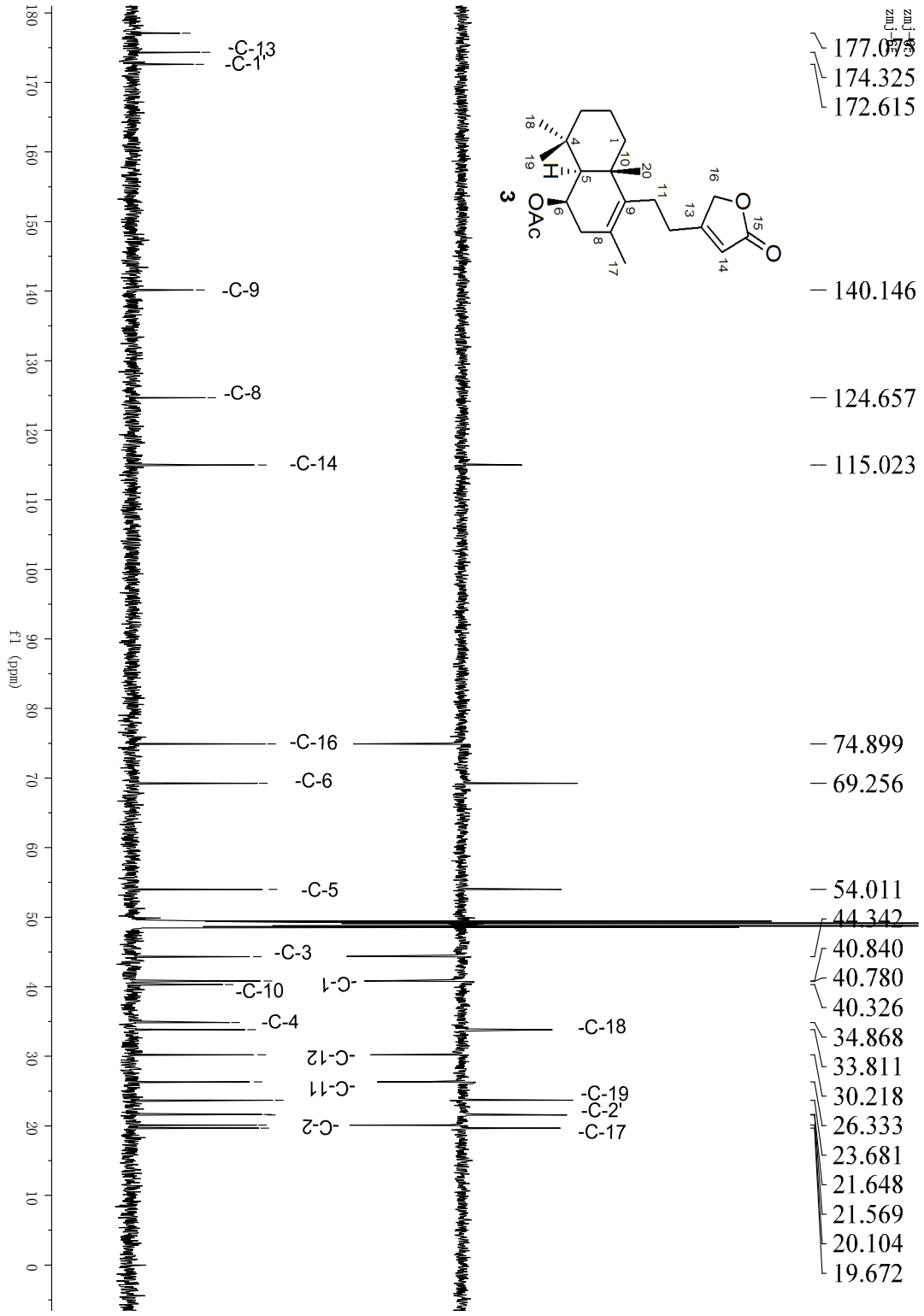
S16. IR (KBr disc) spectrum of vitextrifolin B (**2**)



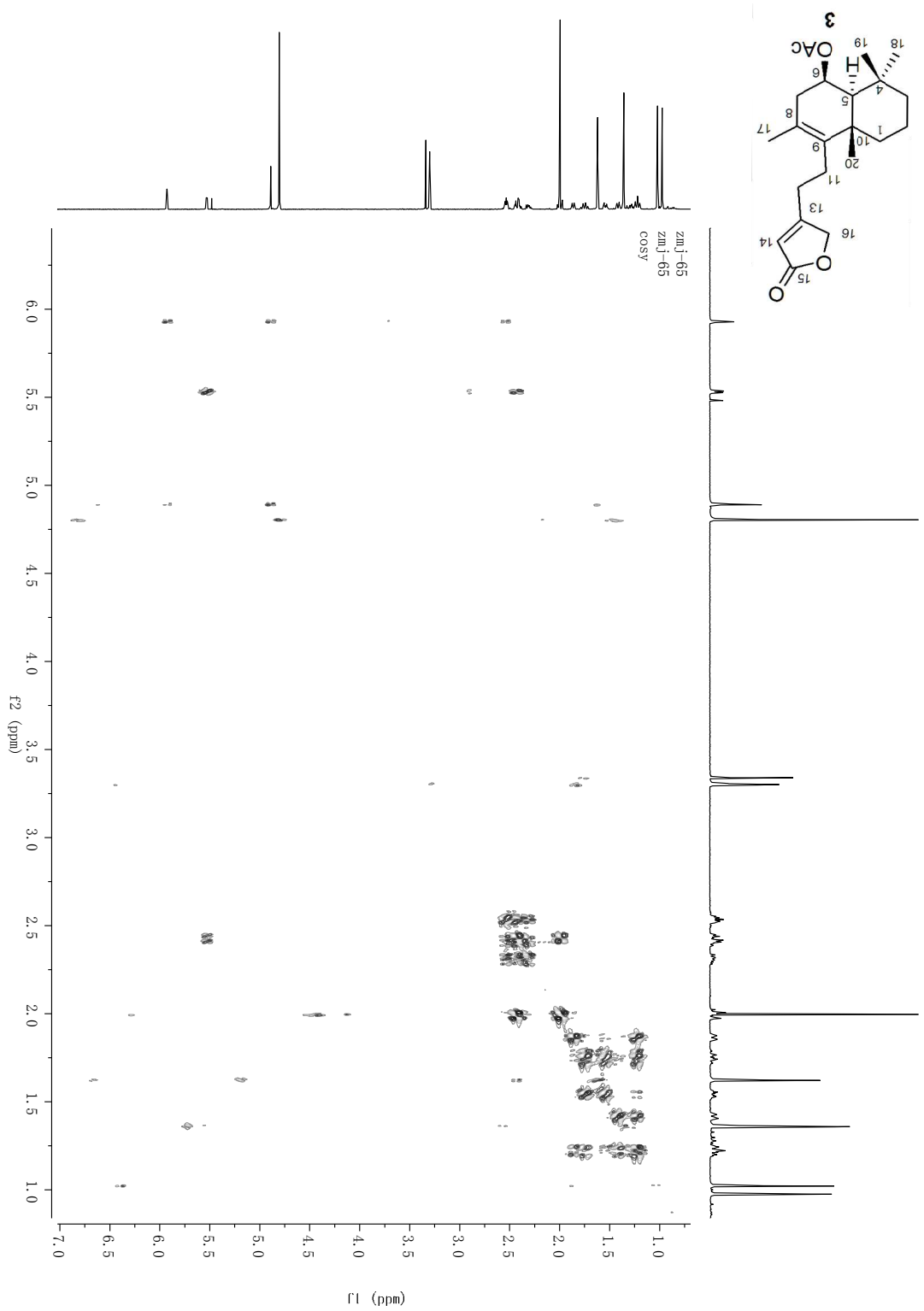
S17. ^{1}H NMR (600 MHz, CD_3OD) spectrum of vitextrifolin C (**3**)



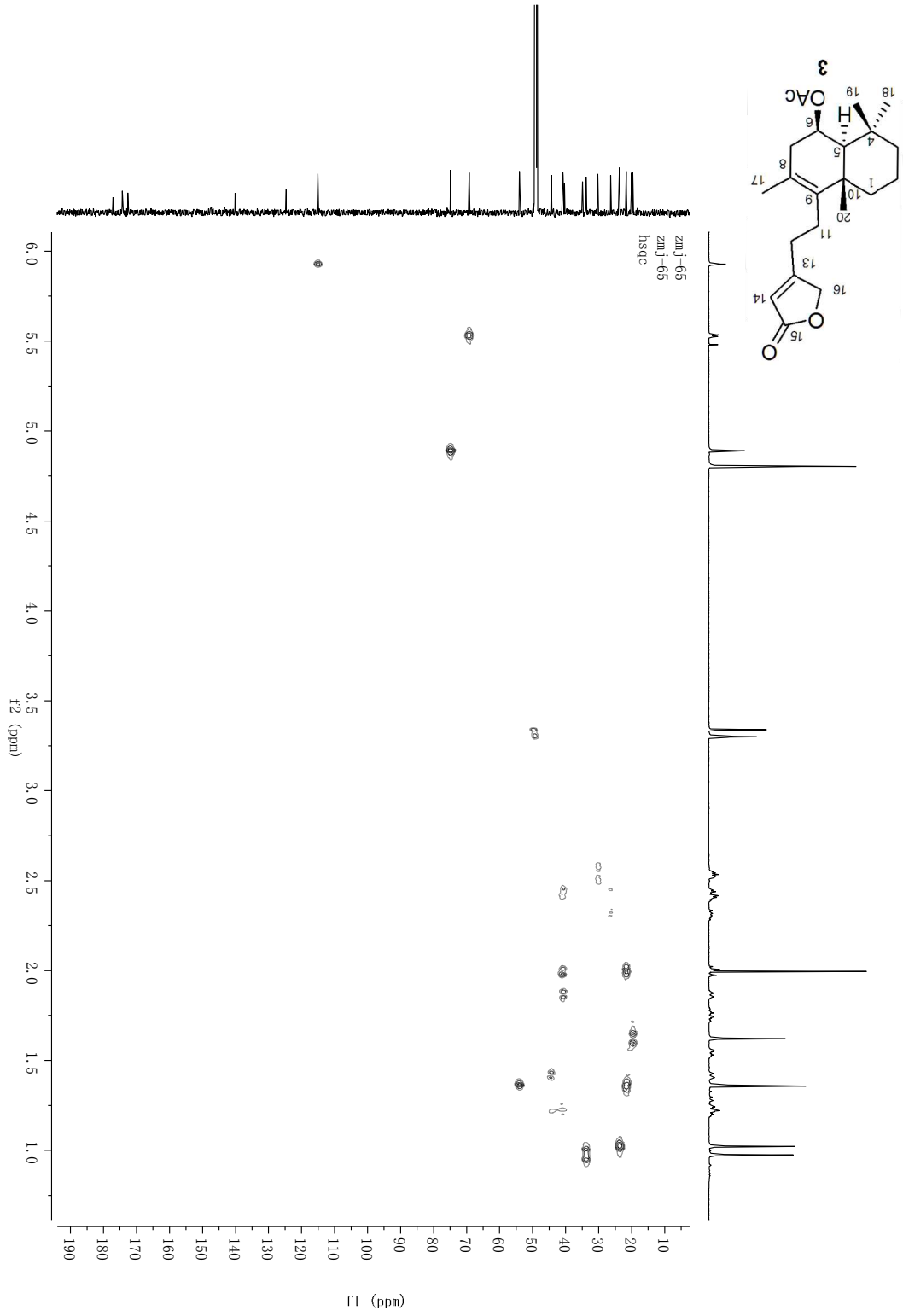
S18. ^{13}C NMR (150 MHz, CD_3OD) spectrum of vitextrifolin C (**3**)



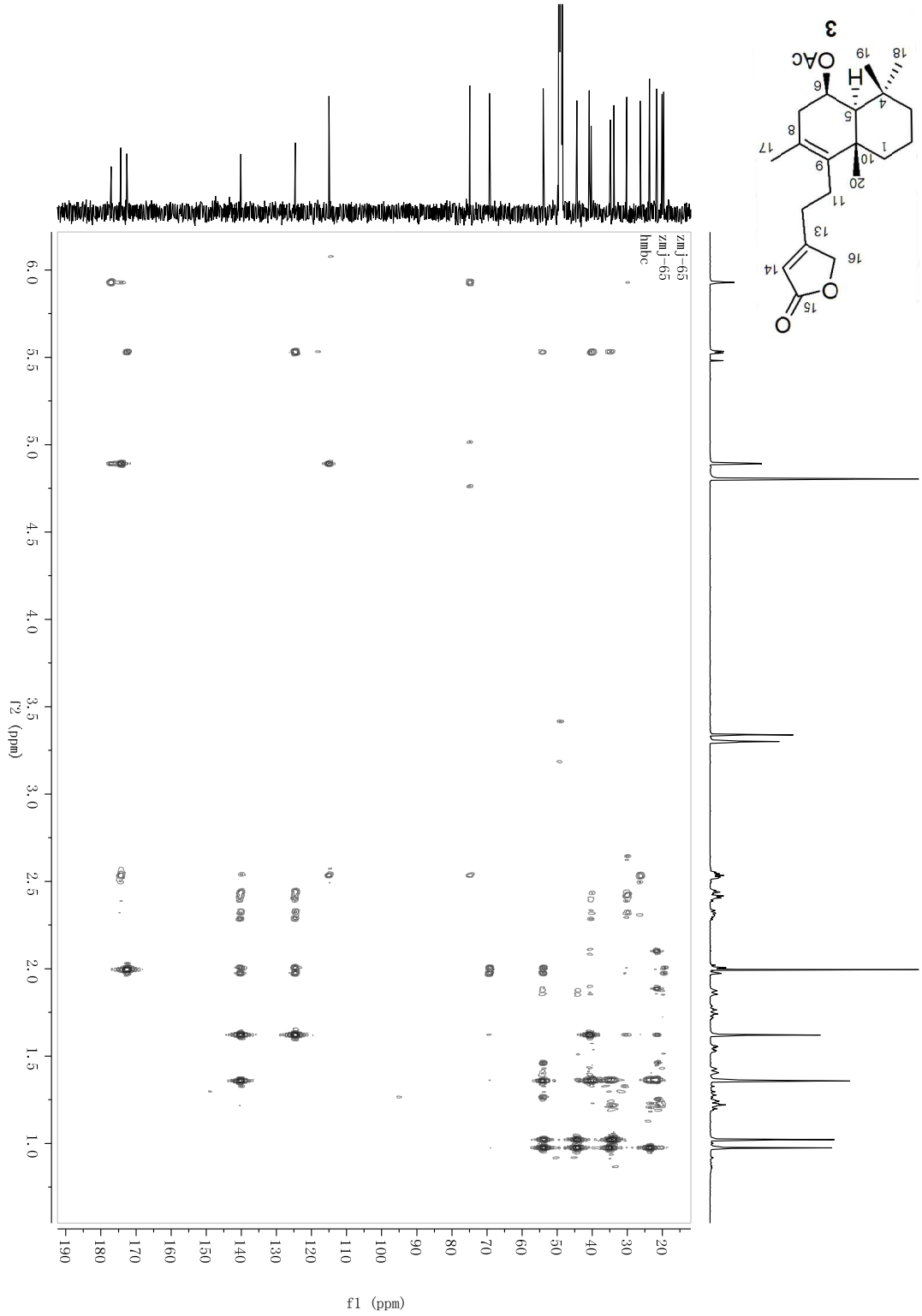
S19. ^{1}H-^{1}H COSY spectrum of vitextrifolin C (**3**) in $CDCl_3$



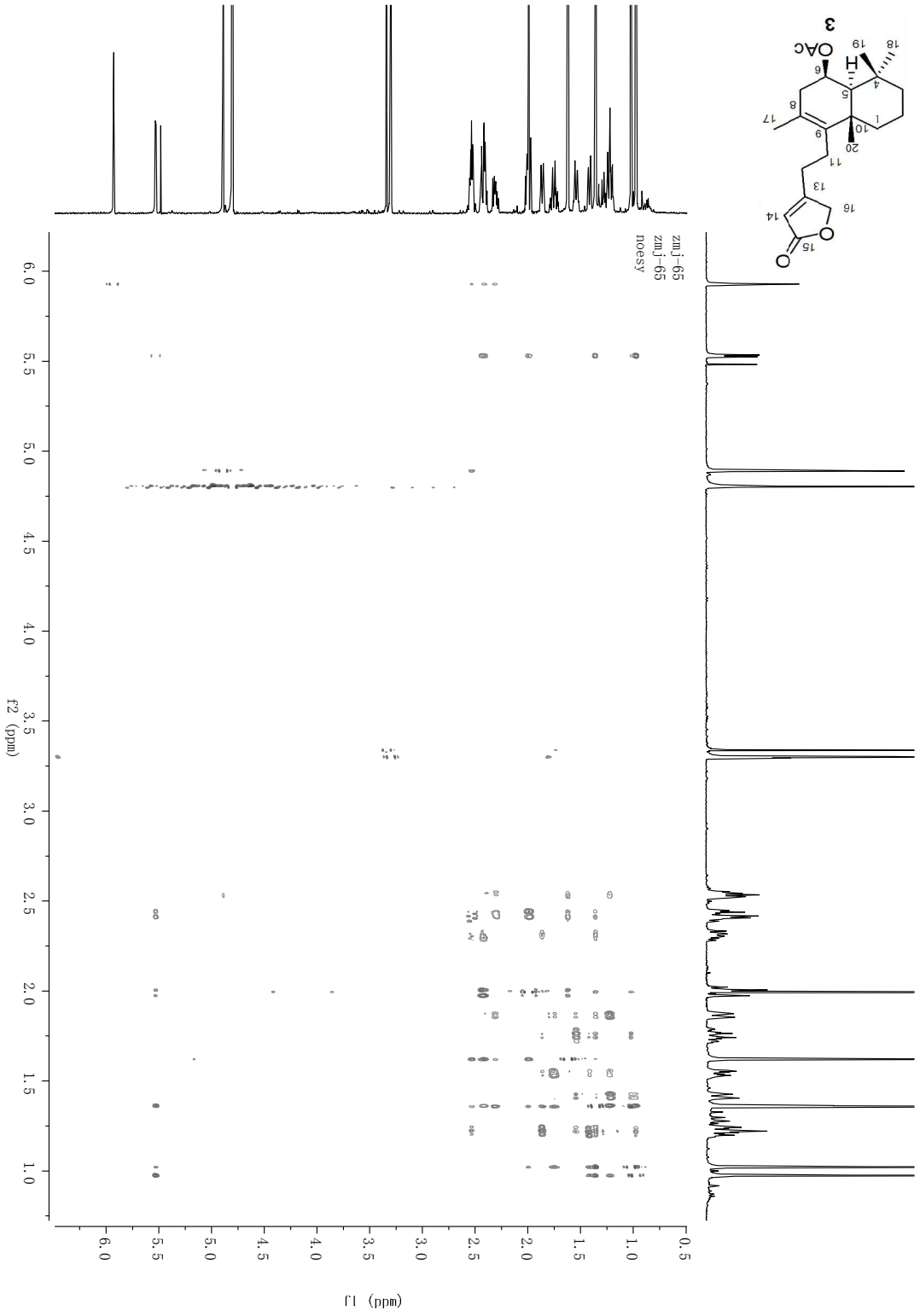
S20. HSQC spectrum of vitextrifolin C (**3**) in $CDCl_3$



S21. HMBC spectrum of vitextrifolin C (**3**) in $CDCl_3$



S22. NOESY spectrum of vitextrifolin C (**3**) in $CDCl_3$



S23. HRESIMS spectrum of vitextrifolin C (**3**)

Qualitative Analysis Report

Data Filename	ZMJ-65-POS.d	**Sample Name**	ZMJ-65
Sample Type	Sample	**Position**	P1-E2
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEST-POS-01.m	**Acquired Time**	3/14/2012 3:05:08 PM
IRM Calibration Status	Some Ions Missed	**DA Method**	ERROR.m
Comment			

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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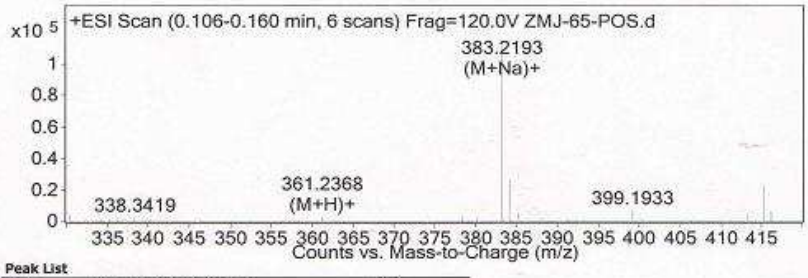

Peak List

m/z	z	Abund	Formula	Ion
217.1219	1	18786		
282.279	1	28861		
301.2161	1	87909		
302.2195	1	18691		
383.2193	1	111351	C22 H32 Na O4	(M+Na)+
384.2226	1	26281	C22 H32 Na O4	(M+Na)+
415.2113	1	23377		
437.1934	1	73284		
438.1964	1	19441		
453.1671	1	35668		

Formula Calculator Element Limits

Element	Min	Max
C	0	40
H	0	120
O	0	10

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C22 H32 O4	TRUE	360.23	360.2301	0.07	C22 H32 Na O4	99.78
C22 H32 O4	TRUE	360.2296	360.2301	1.27	C22 H33 O4	78.02

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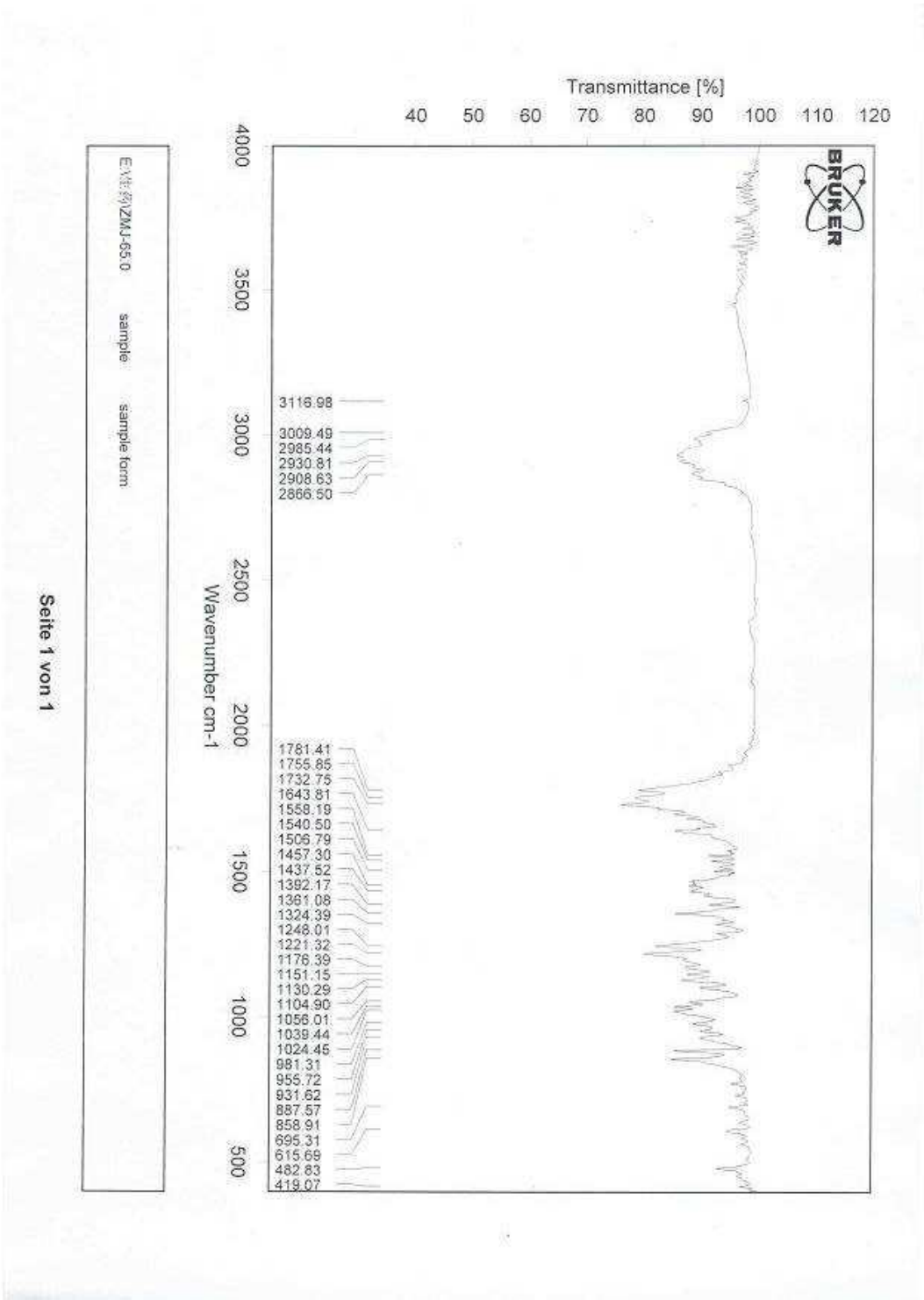
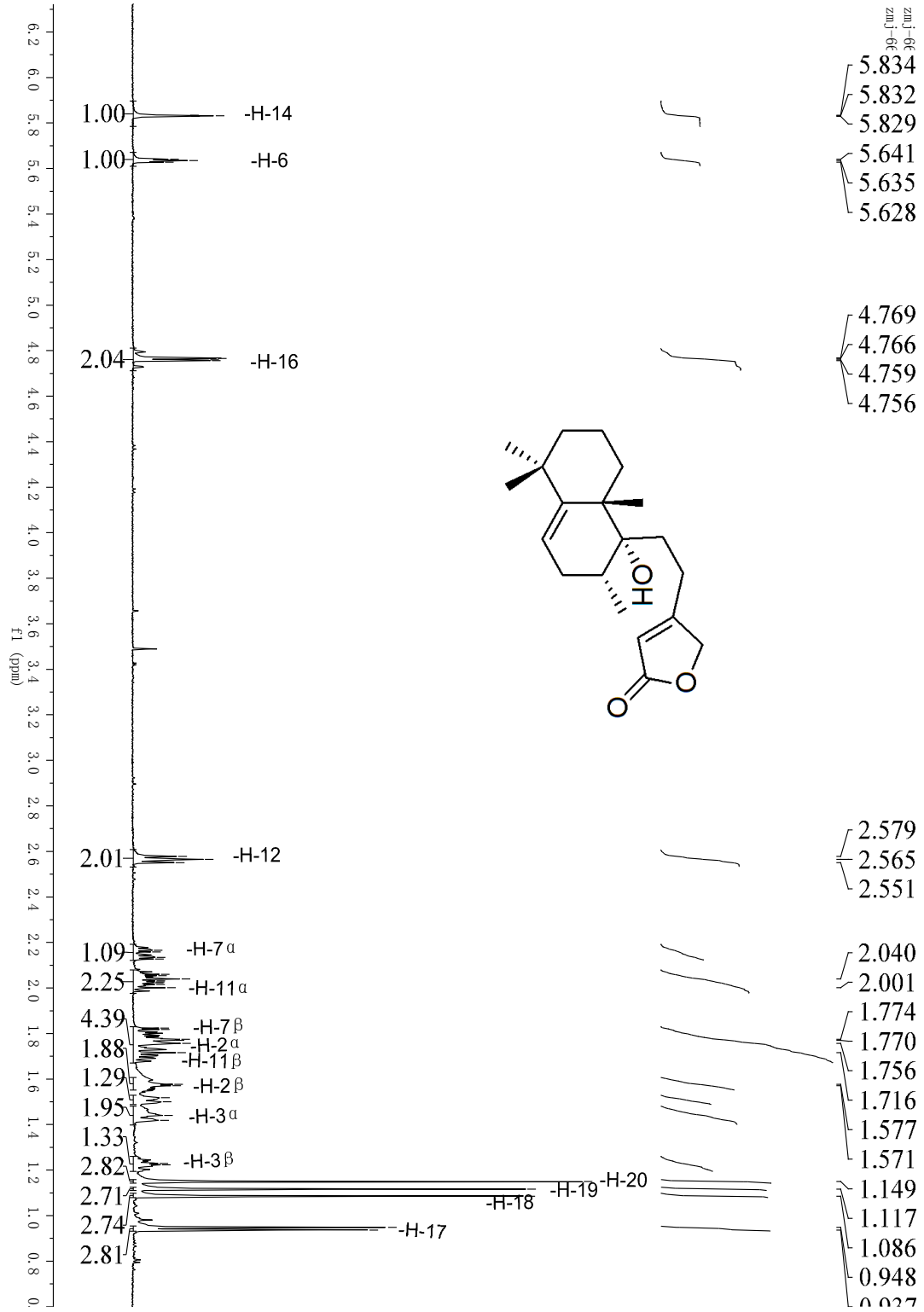
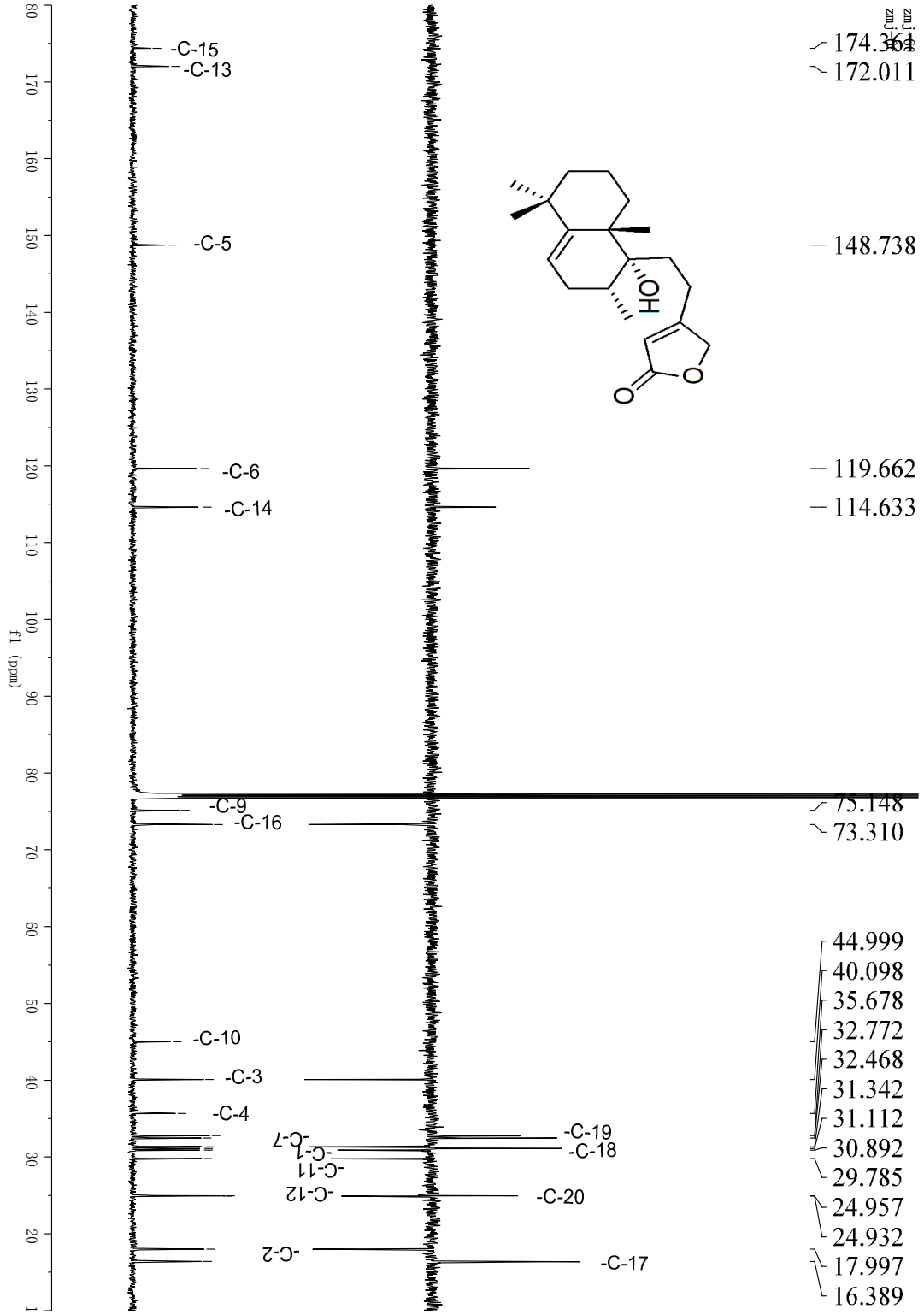
S24. IR (KBr disc) spectrum of vitextrifolin C (**3**)



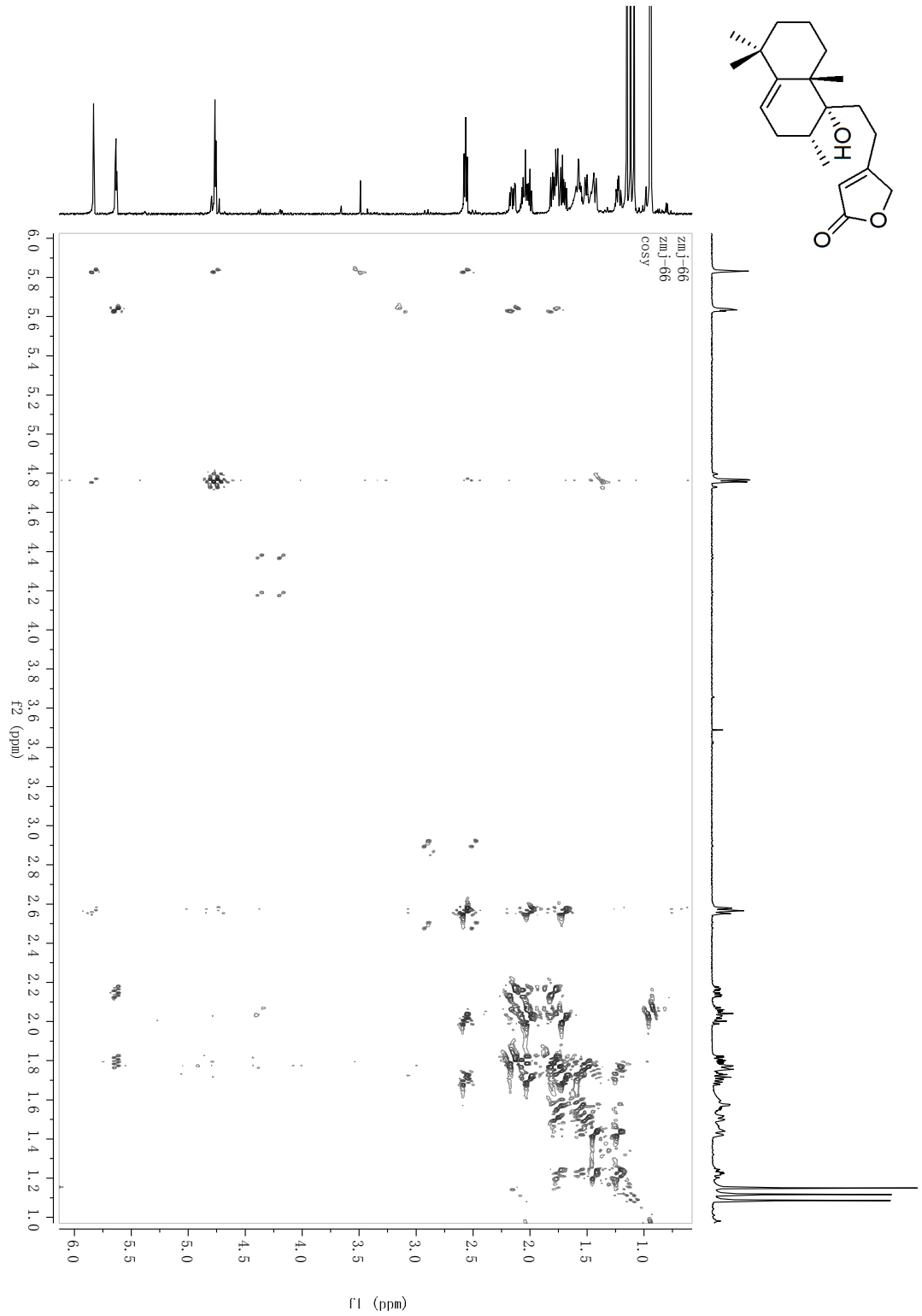
S25. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of vitextrifolin D (**4**)



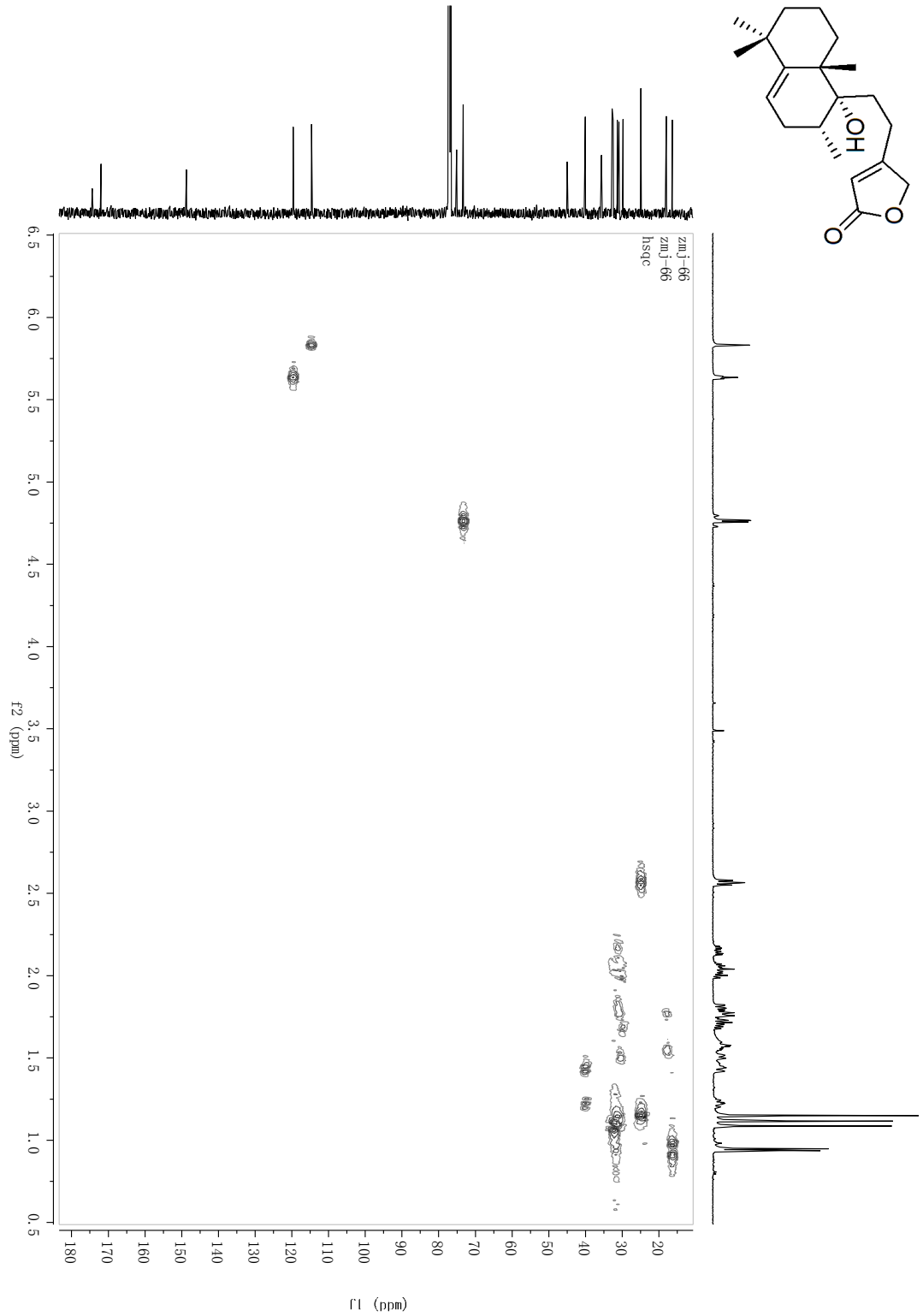
S26. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of vitextrifolin D (**4**)



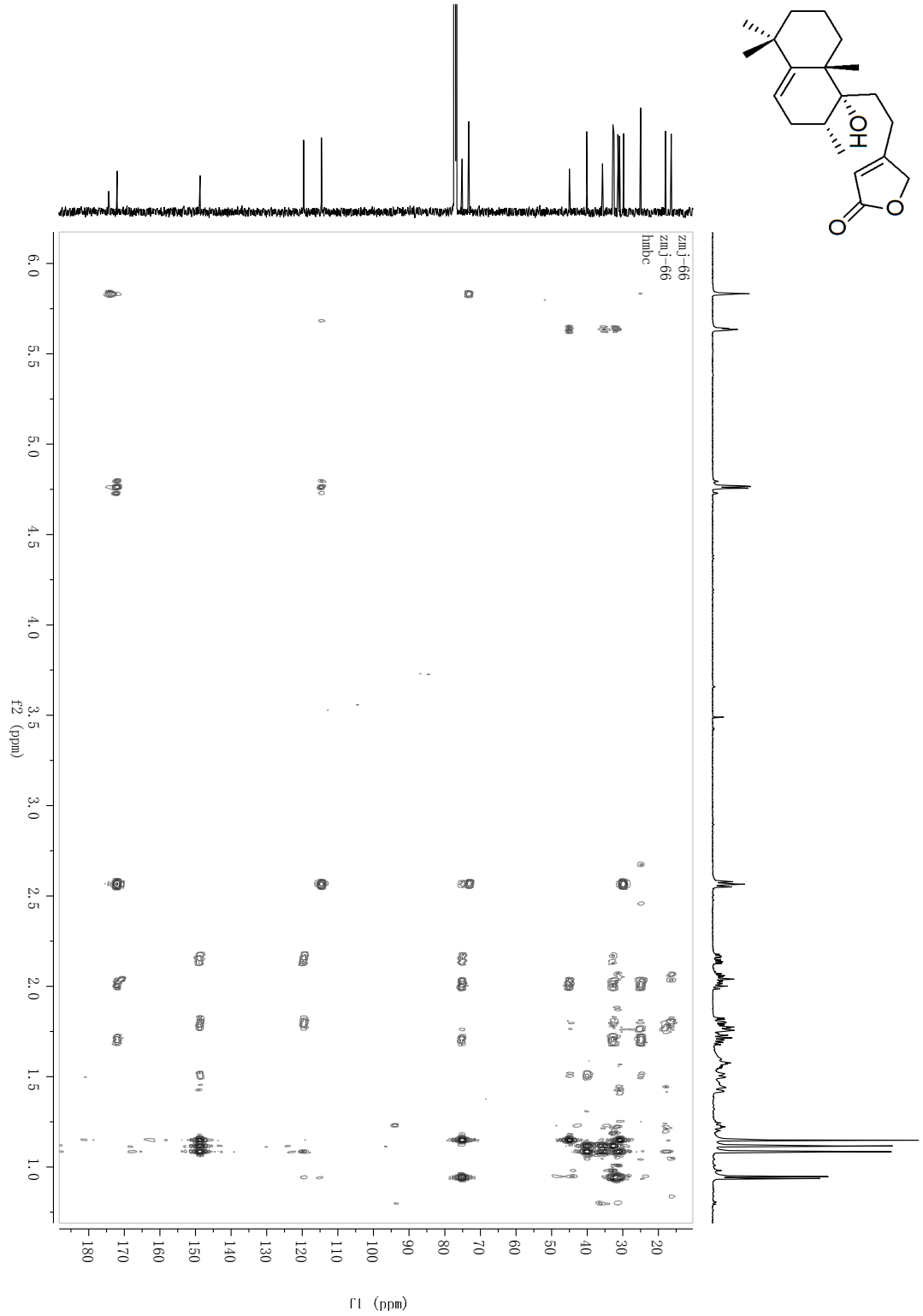
S27. ^{1}H-^{1}H COSY spectrum of vitextrifolin D (**4**) in $CDCl_3$



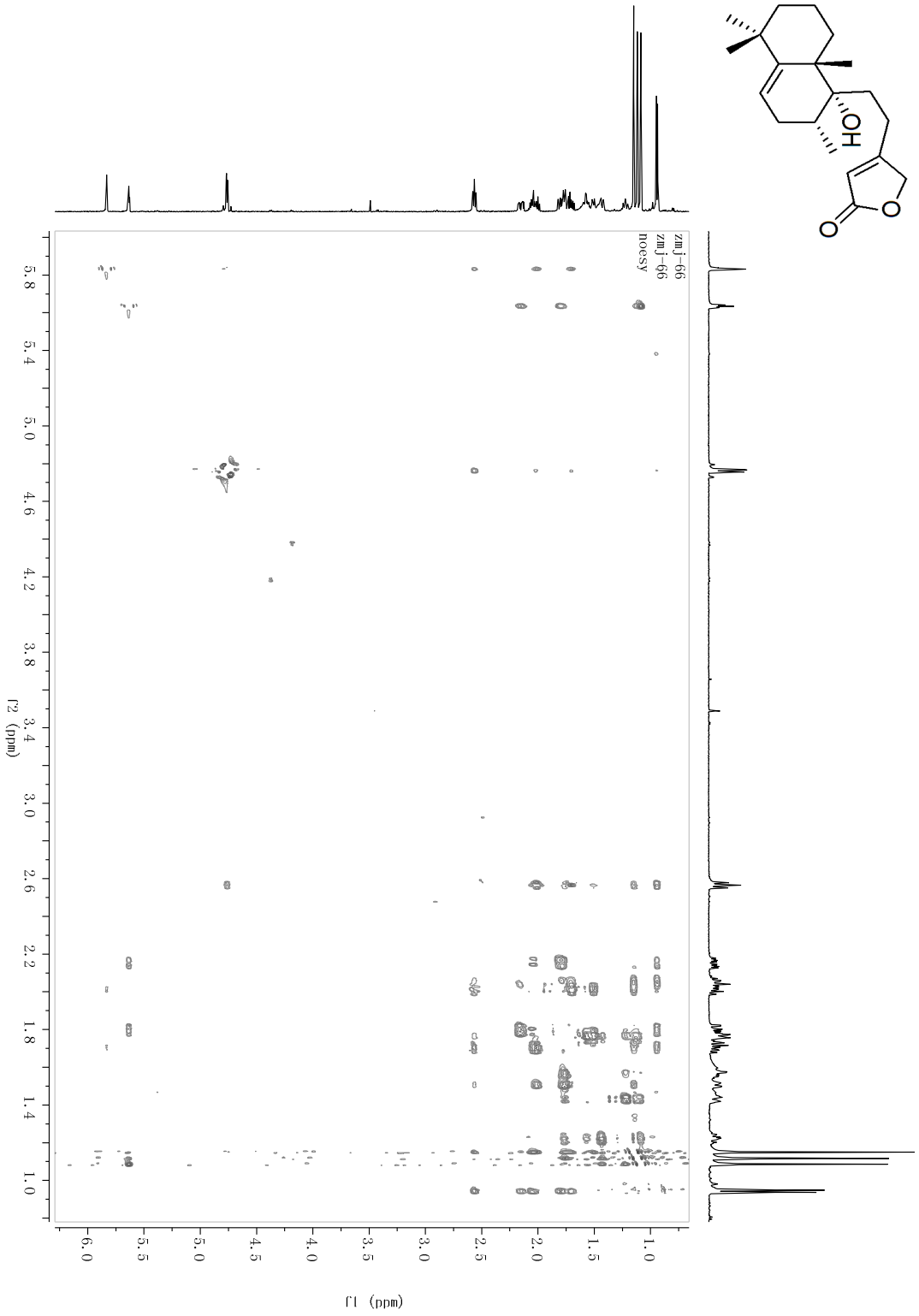
S28. HSQC spectrum of vitextrifolin D (**4**) in $CDCl_3$



S29. HMBC spectrum of vitextrifolin D (**4**) in $CDCl_3$



S30.NOESY spectrum of vitextrifolin D (**4**) in $CDCl_3$



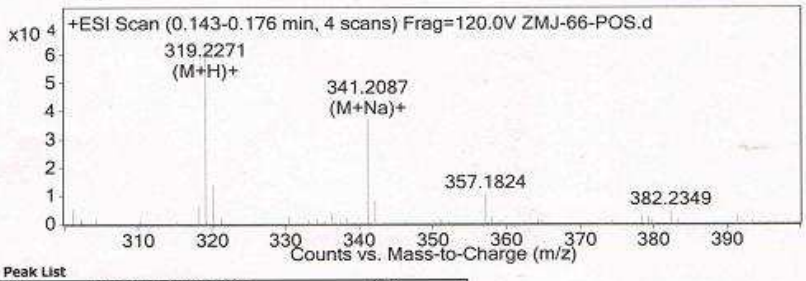
S31. HRESIMS spectrum of vitextrifolin D (**4**)

Qualitative Analysis Report

Data Filename	ZMJ-66-POS.d	**Sample Name**	ZMJ-66
Sample Type	Sample	**Position**	P1-E3
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEST-POS-01.m	**Acquired Time**	3/14/2012 3:06:46 PM
IRM Calibration Status	Some Ions Missed	**DA Method**	ERROR.m
Comment			

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	Esi



Peak List

m/z	z	Abund	Formula	Ion
282.279	1	21927		
319.2271	1	61829	C20 H31 O3	(M+H)+
320.2338	1	13736	C20 H31 O3	(M+H)+
341.2087	1	36770	C20 H30 Na O3	(M+Na)+
357.1824		10252		
437.1932	1	21167		
453.1669	1	21271		
659.4275	1	33928		
660.4306	1	14236		
922.0098		14749		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	5

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C20 H30 O3	TRUE	318.2199	318.2195	-1.28	C20 H31 O3	90.14
C20 H30 O3	TRUE	318.2194	318.2195	0.16	C20 H30 Na O3	99.64

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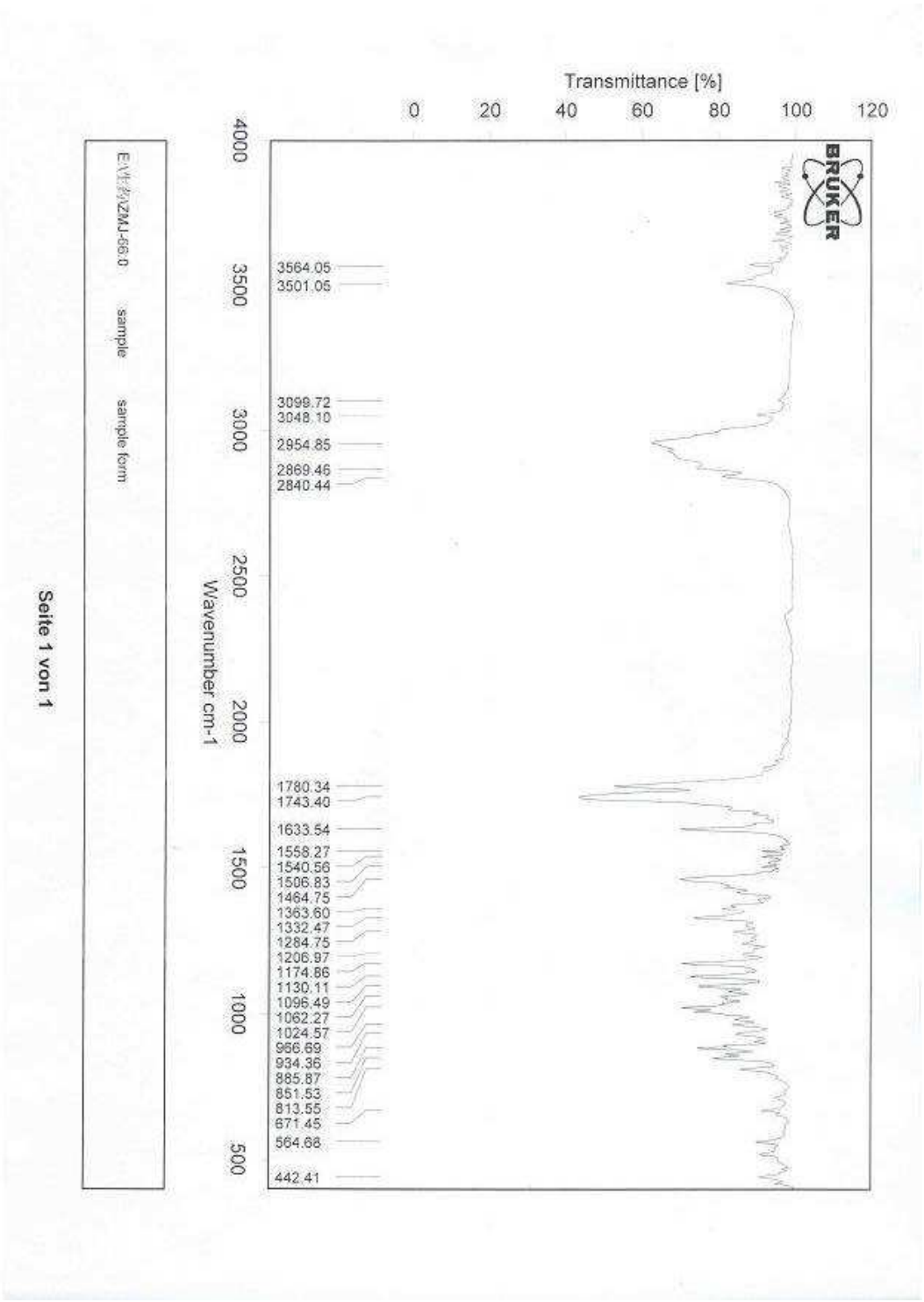
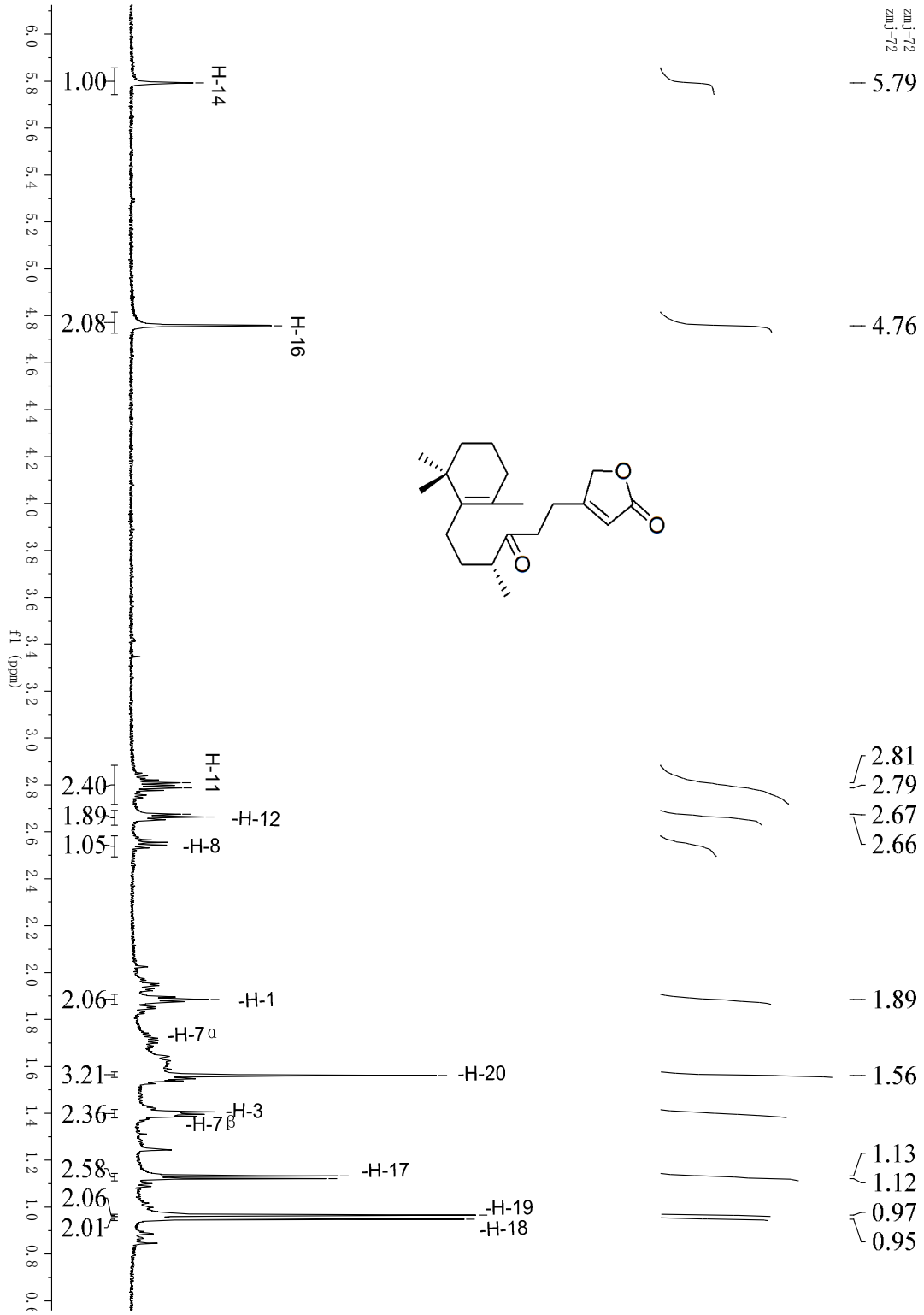
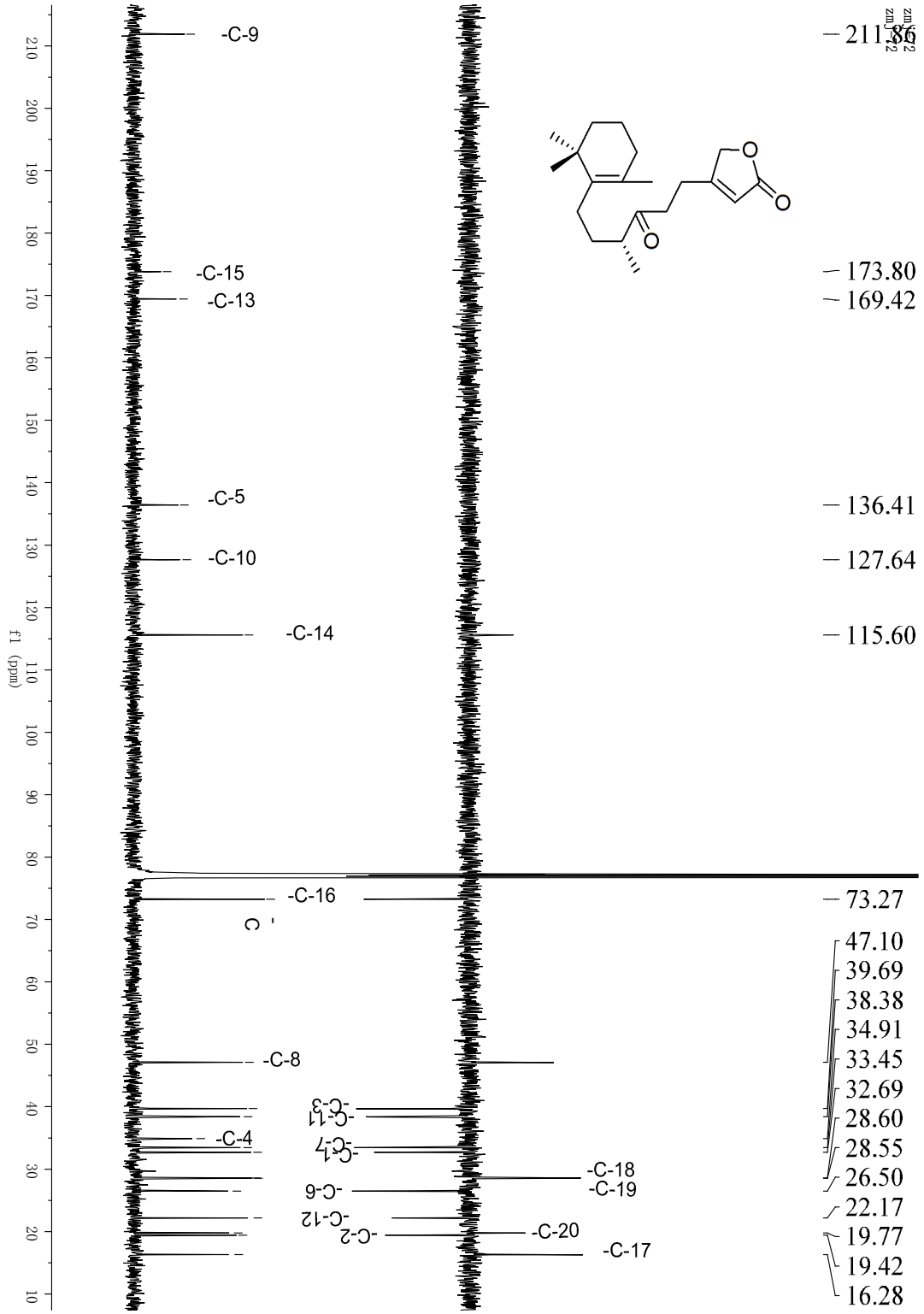
S32. IR (KBr disc) spectrum of vitextrifolin D (**4**)



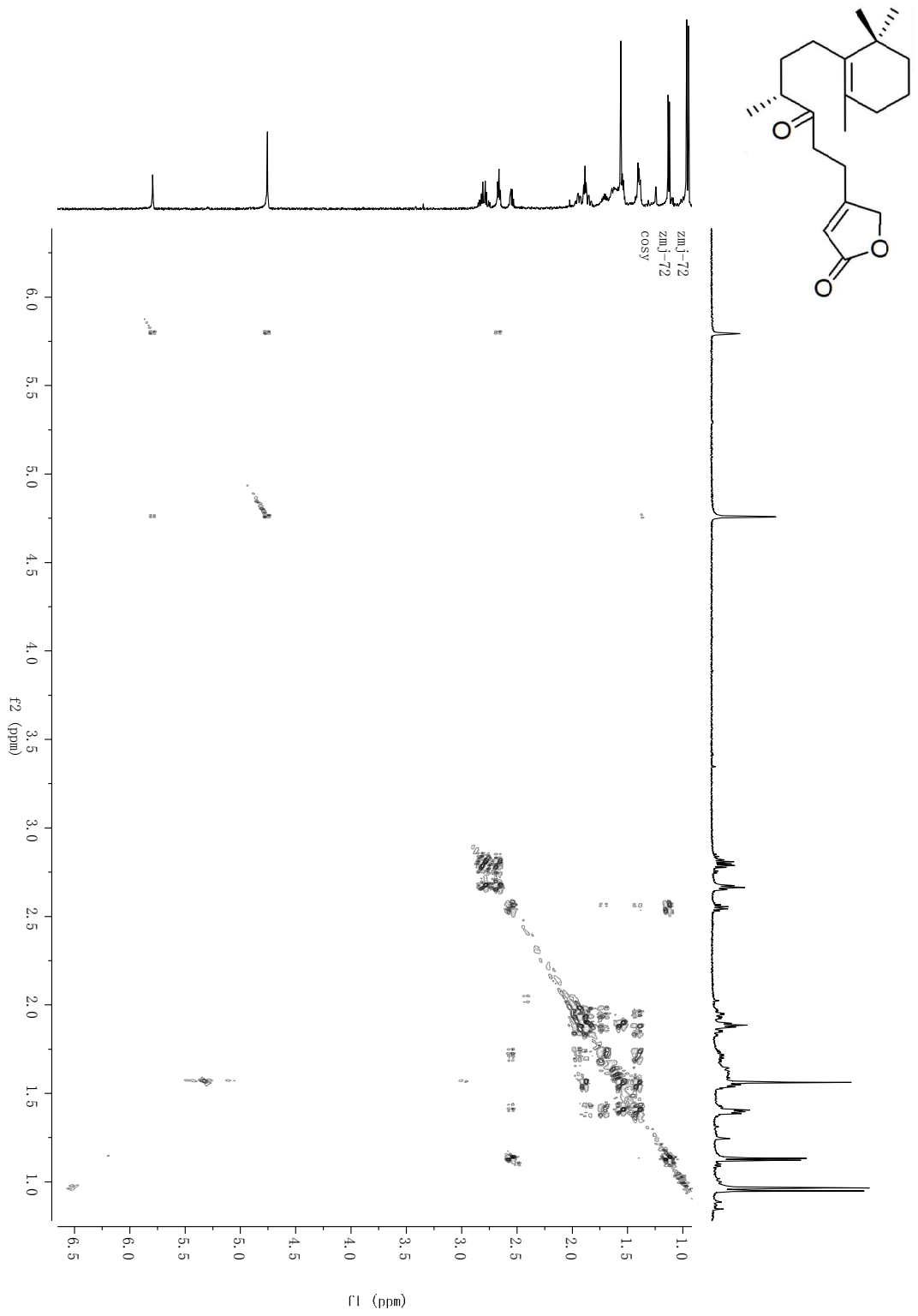
S33.[1]H NMR (600 MHz, $CDCl_3$) spectrum of vitextrifolin E (**5**)



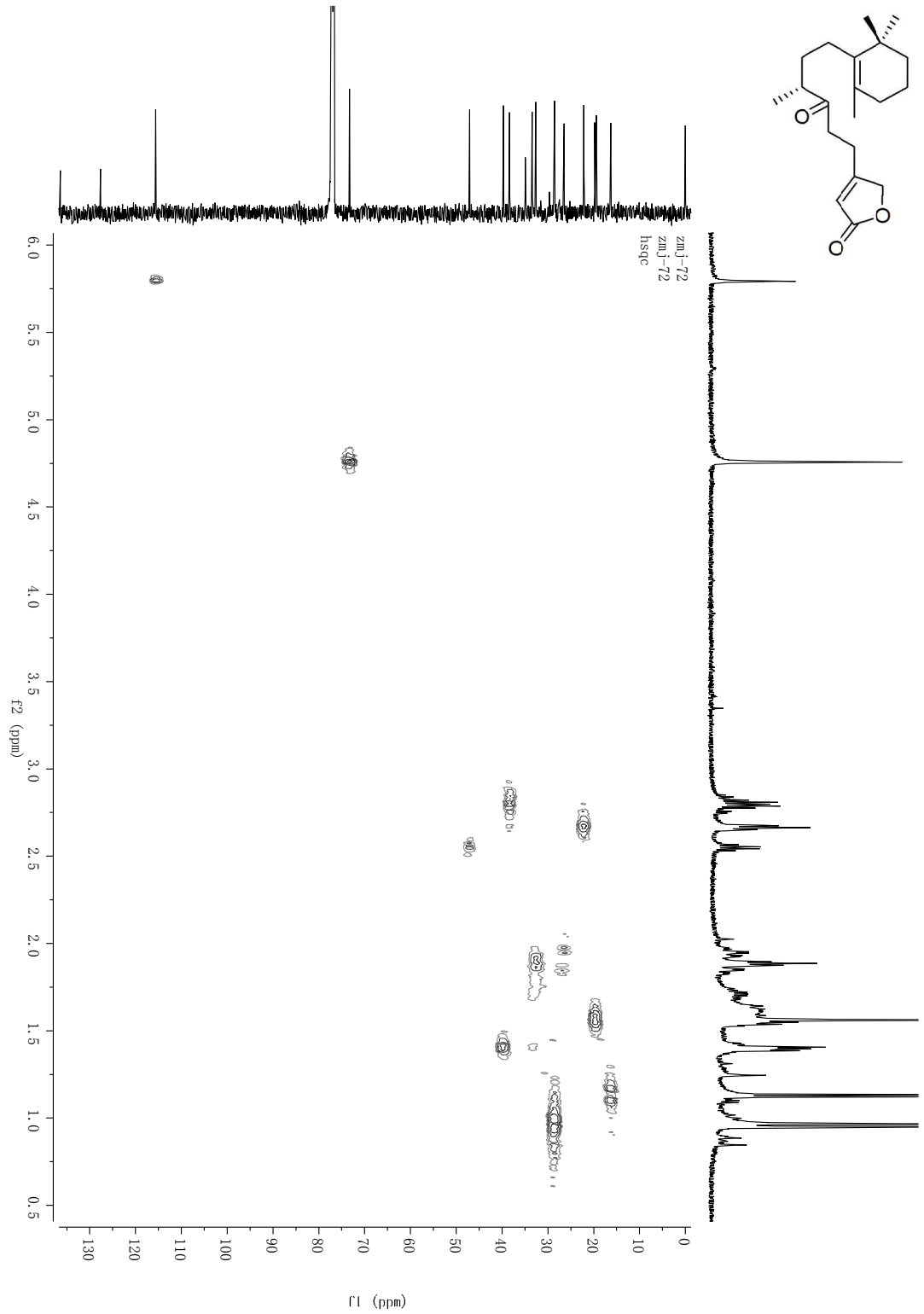
S34. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of vitextrifolin E (**5**)



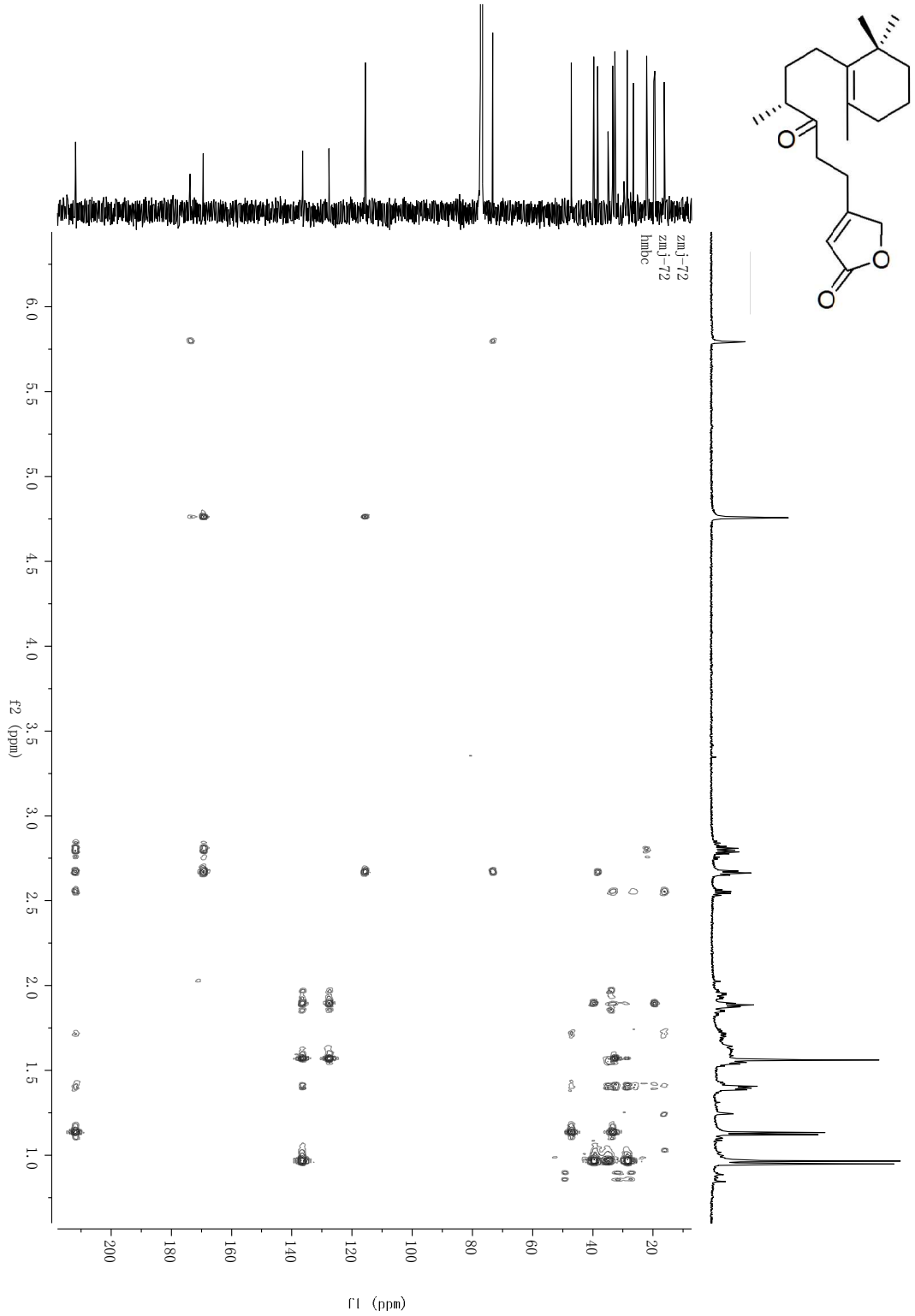
S35. ^{1}H-^{1}H COSY spectrum of vitextrifolin E (**5**) in $CDCl_3$



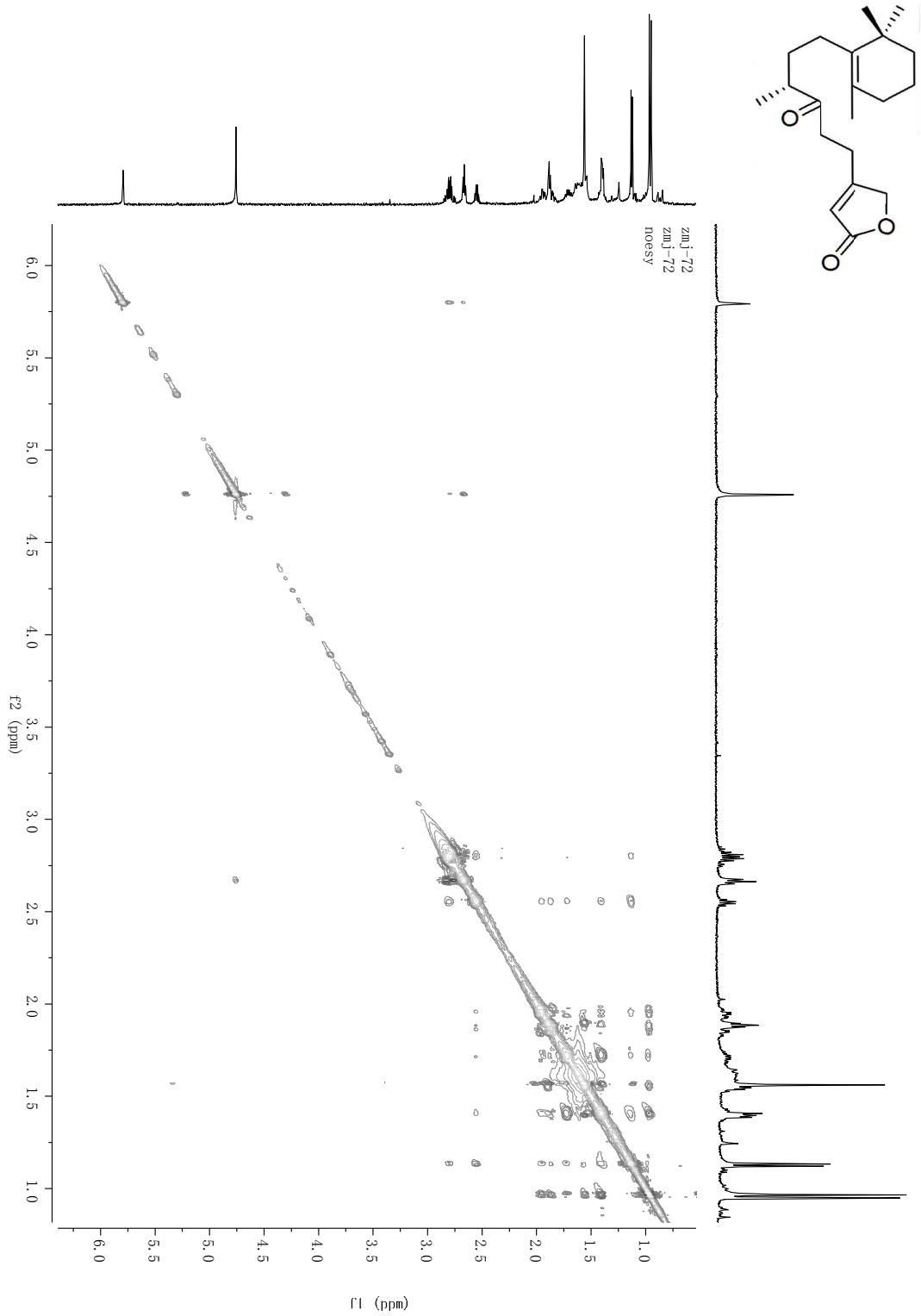
S36. HSQC spectrum of vitextrifolin E (**5**) in $CDCl_3$



S37. HMBC spectrum of vitextrifolin E (**5**) in $CDCl_3$



S38. NOESY spectrum of vitextrifolin E (**5**) in $CDCl_3$



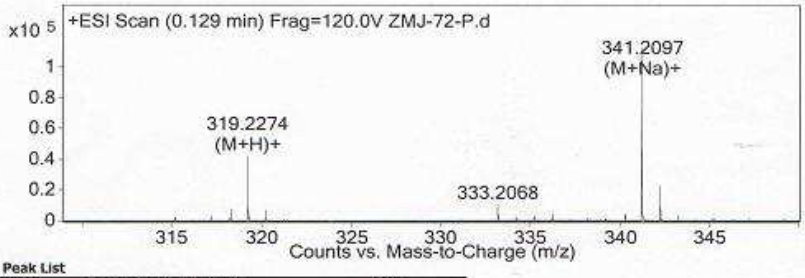
S39. HRESIMS spectrum of vitextrifolin E (**5**)

Qualitative Analysis Report

Data Filename	ZMJ-72-P.d	**Sample Name**	ZMJ-72
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEST-POS-01.m	**Acquired Time**	7/13/2012 12:01:39 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	Esi



Peak List

m/z	z	Abund	Formula	Ion
319.2274	1	43889	C20 H31 O3	(M+H)+
341.2097	1	113540	C20 H30 Na O3	(M+Na)+
342.213	1	23143	C20 H30 Na O3	(M+Na)+
355.1882	1	32233		
357.2003	1	26770		
373.1993	1	103013		
374.2024	1	22699		
389.1744		22940		
437.1942		23077		
453.1676	1	27400		

Formula Calculator Element Limits

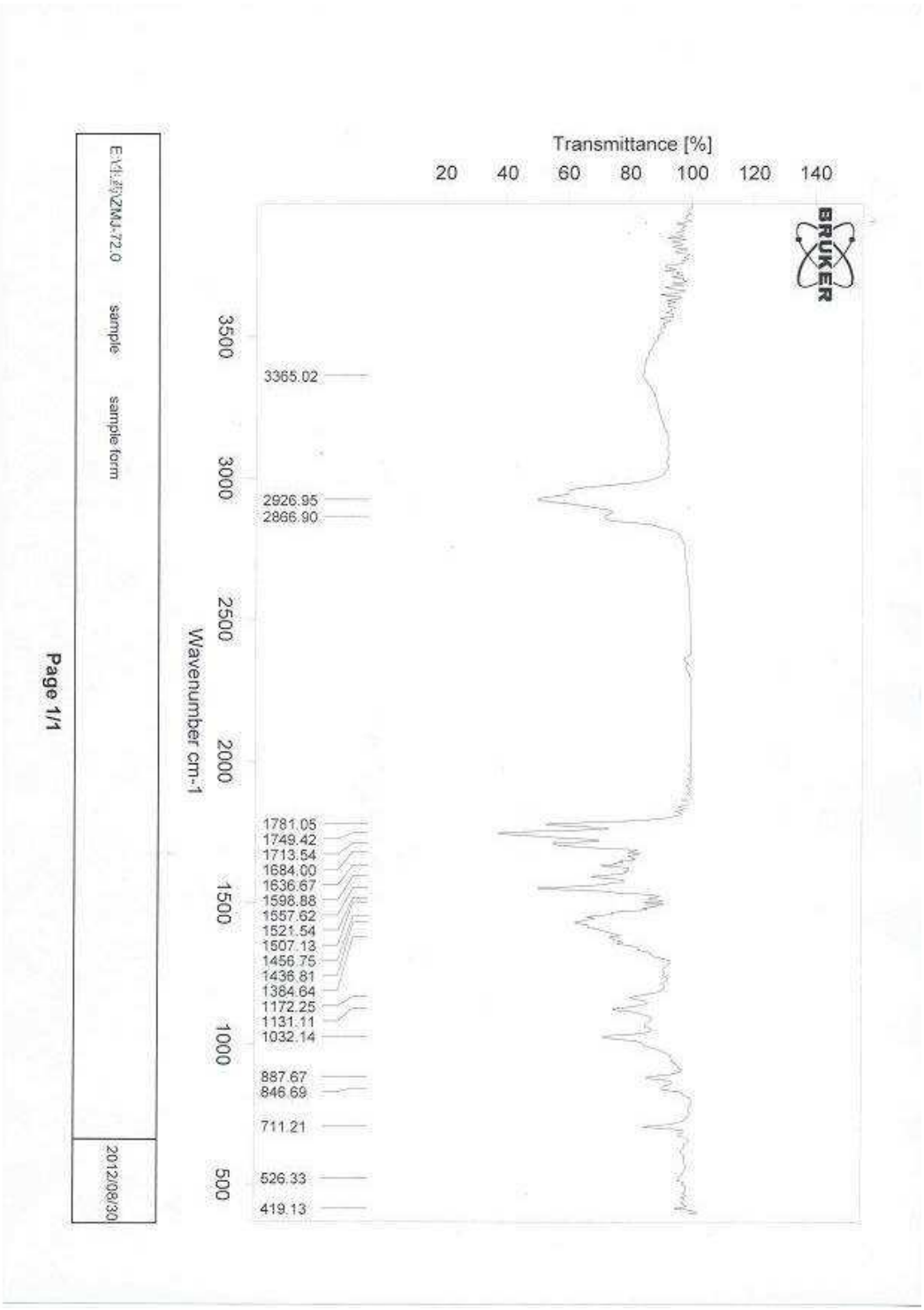
Element	Min	Max
C	2	45
H	2	200
O	0	35

Formula Calculator Results

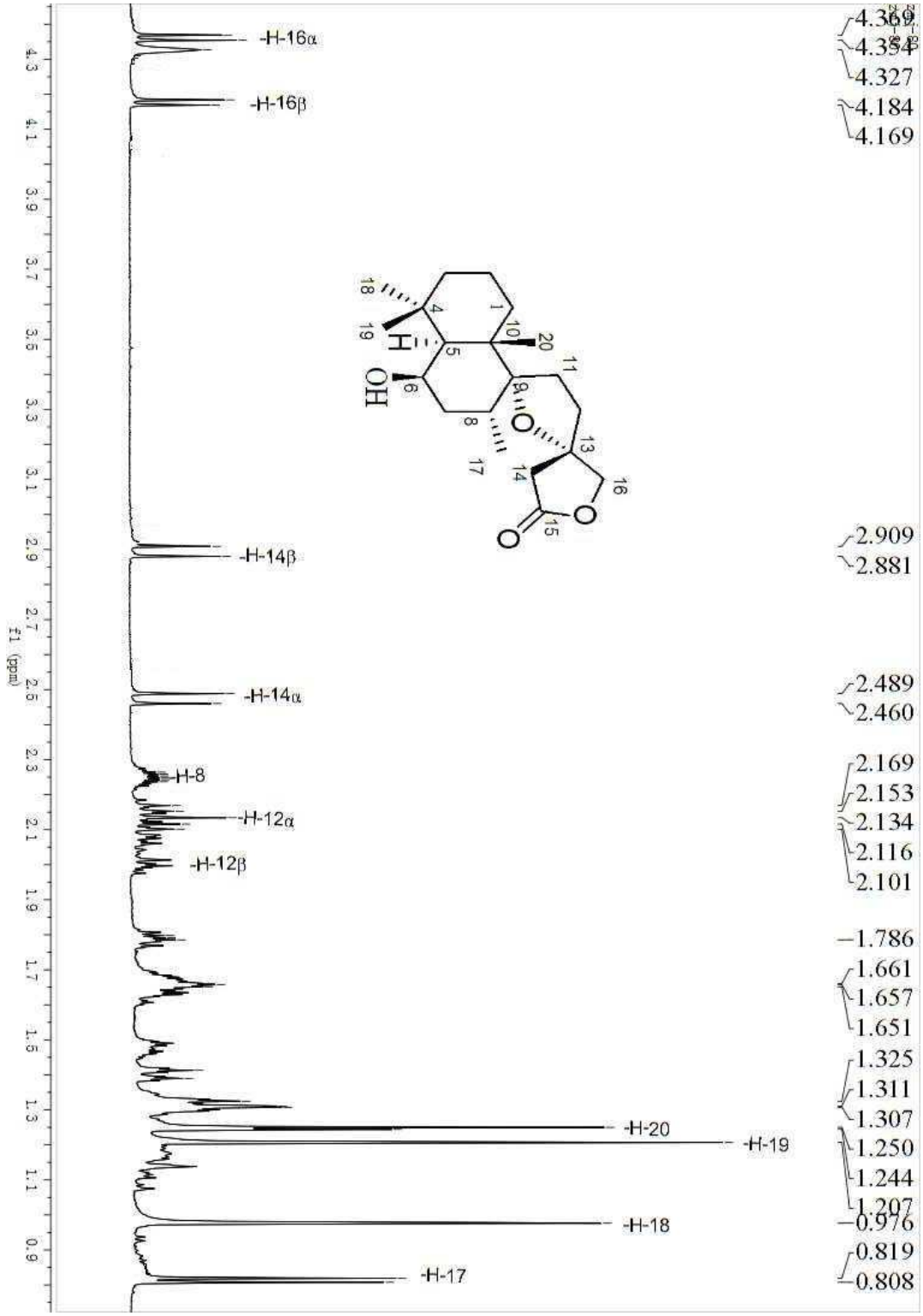
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C20 H30 O3	TRUE	318.2201	318.2195	-2.05	C20 H31 O3	93.11
C20 H30 O3	TRUE	318.2204	318.2195	-2.97	C20 H30 Na O3	96.65

--- End Of Report ---

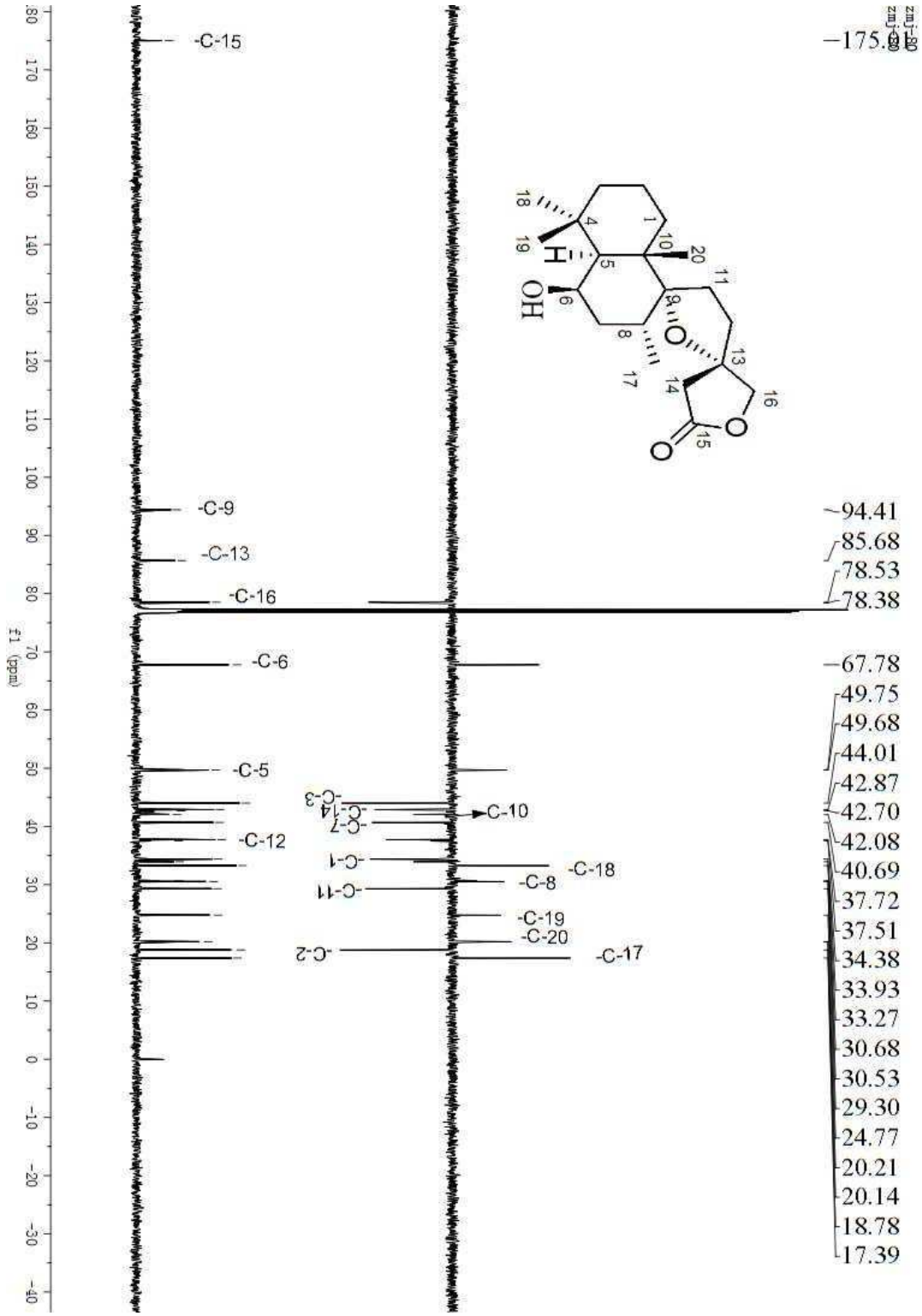
S40. IR (KBr disc) spectrum of vitextrifolin E (**5**)



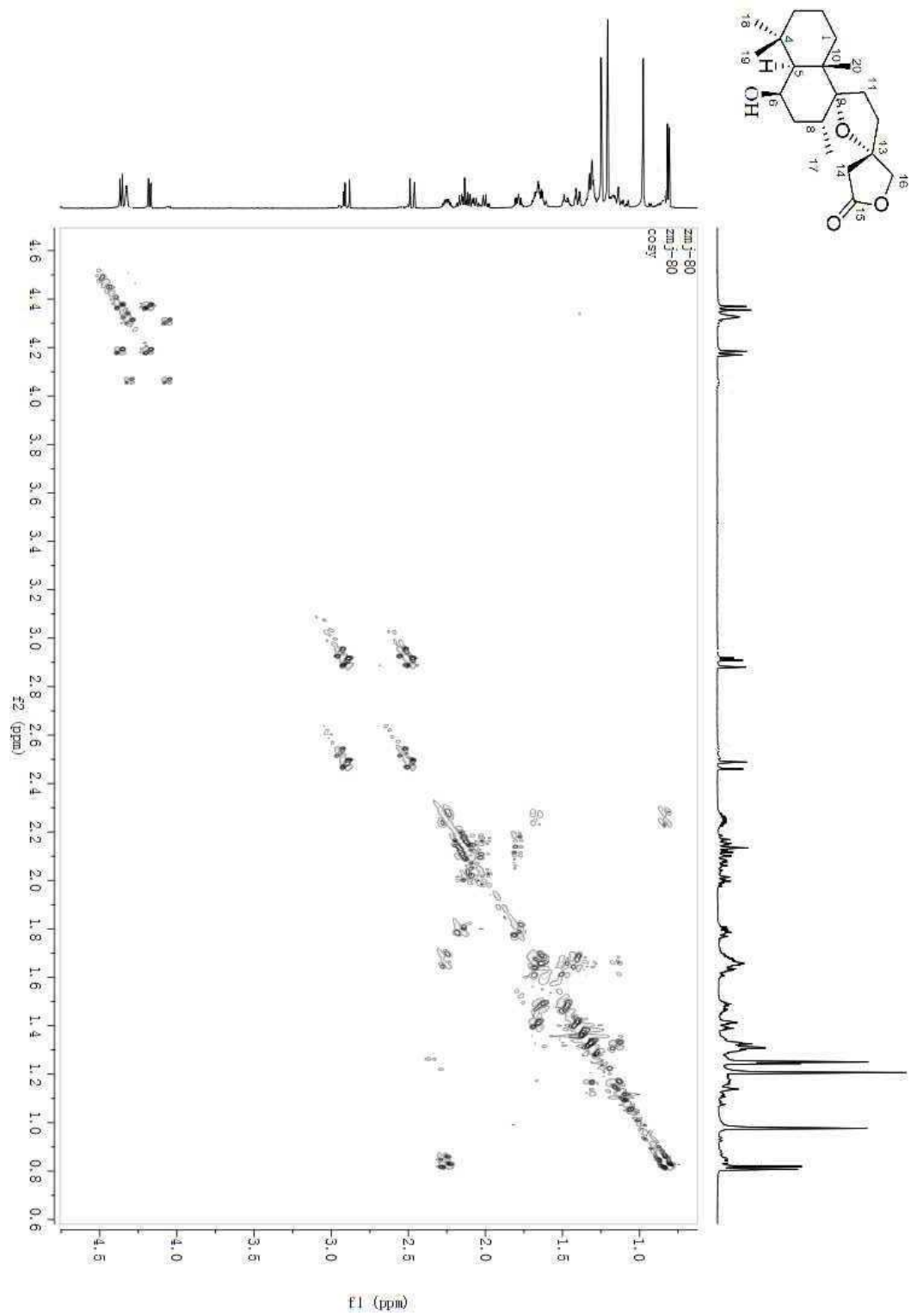
S41. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of vitextrifolin F (**6**)



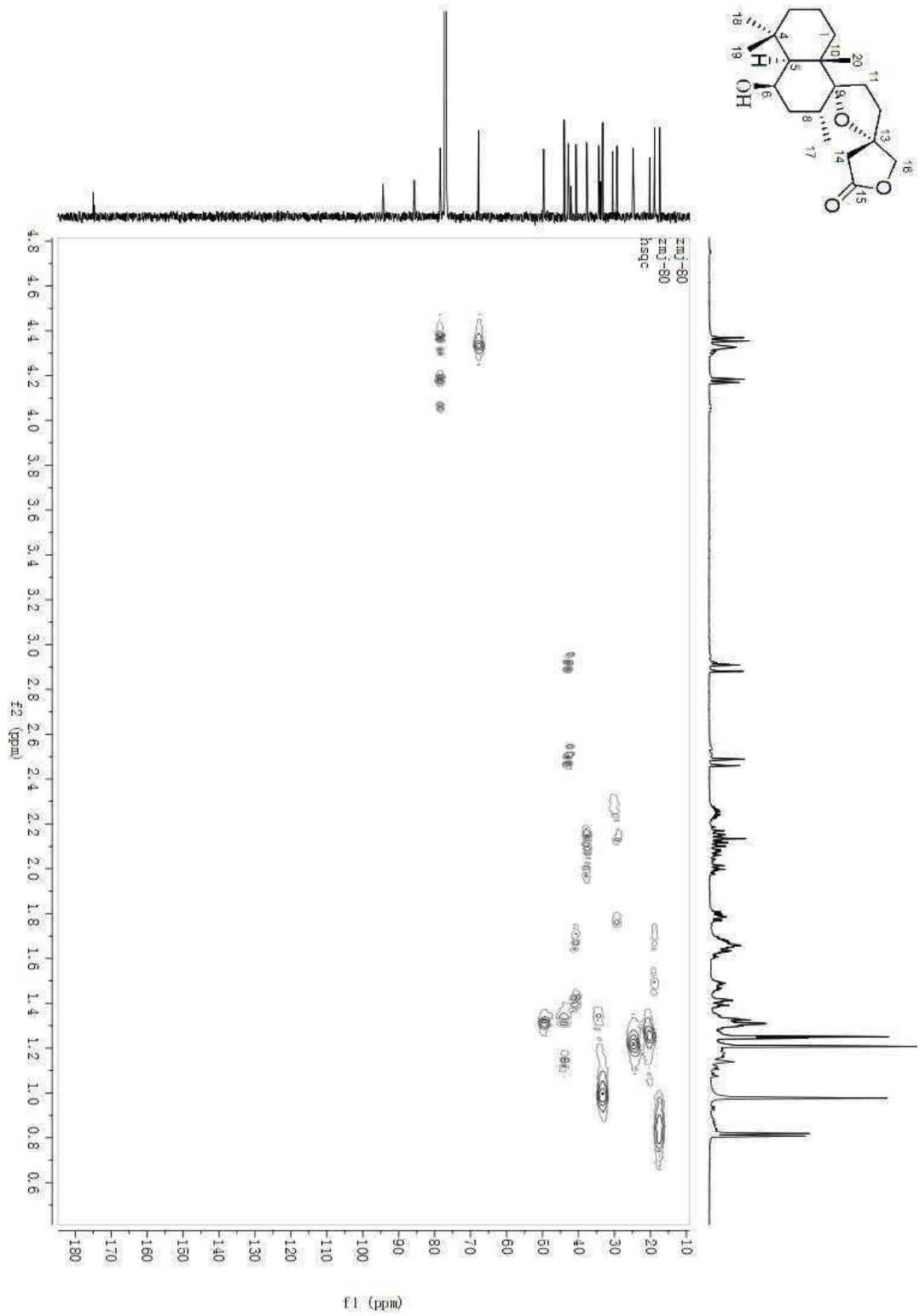
S42. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of vitextrifolin F (**6**)



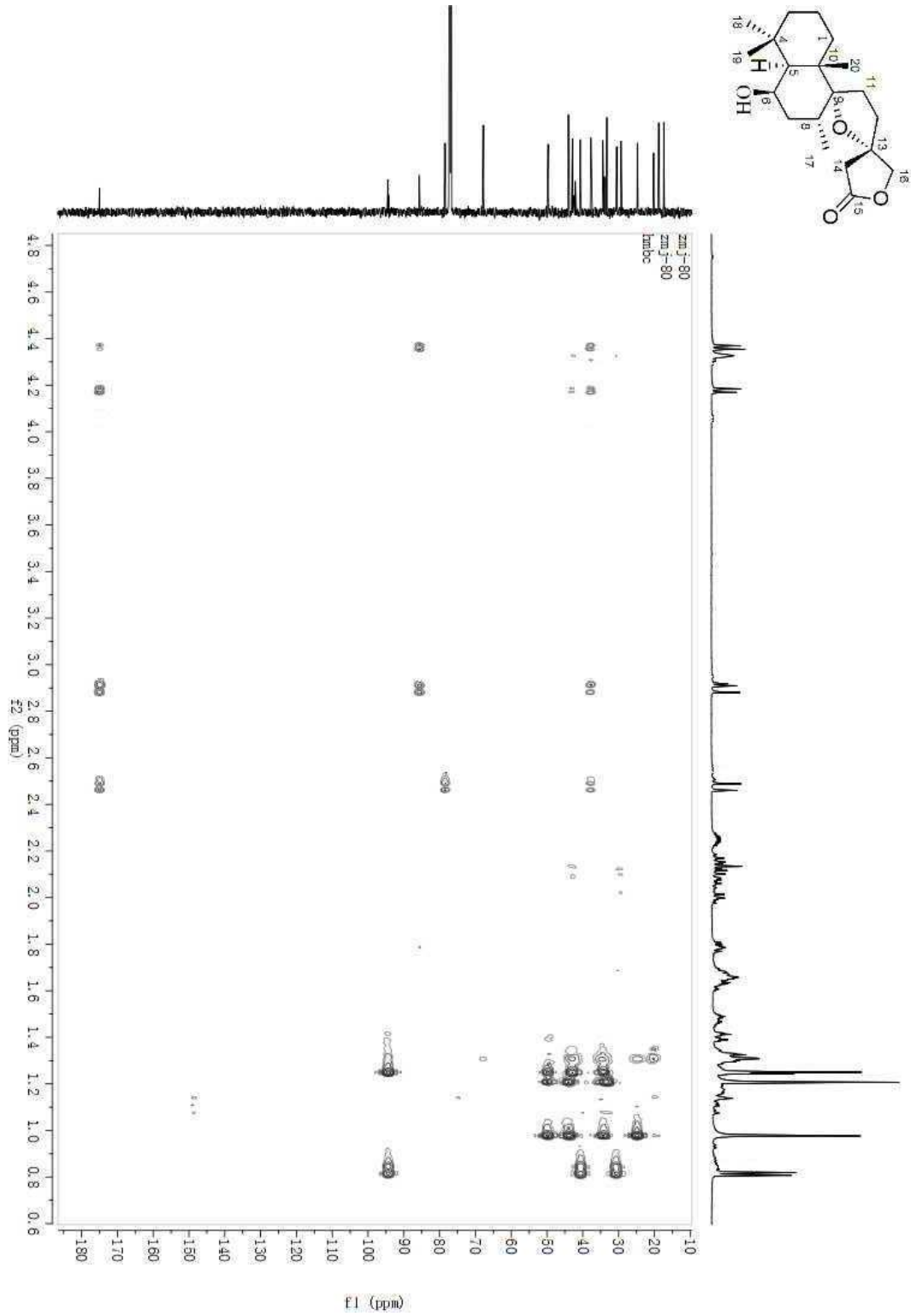
S43. ^{1}H-^{1}H COSY spectrum of vitextrifolin F (**6**) in $CDCl_3$



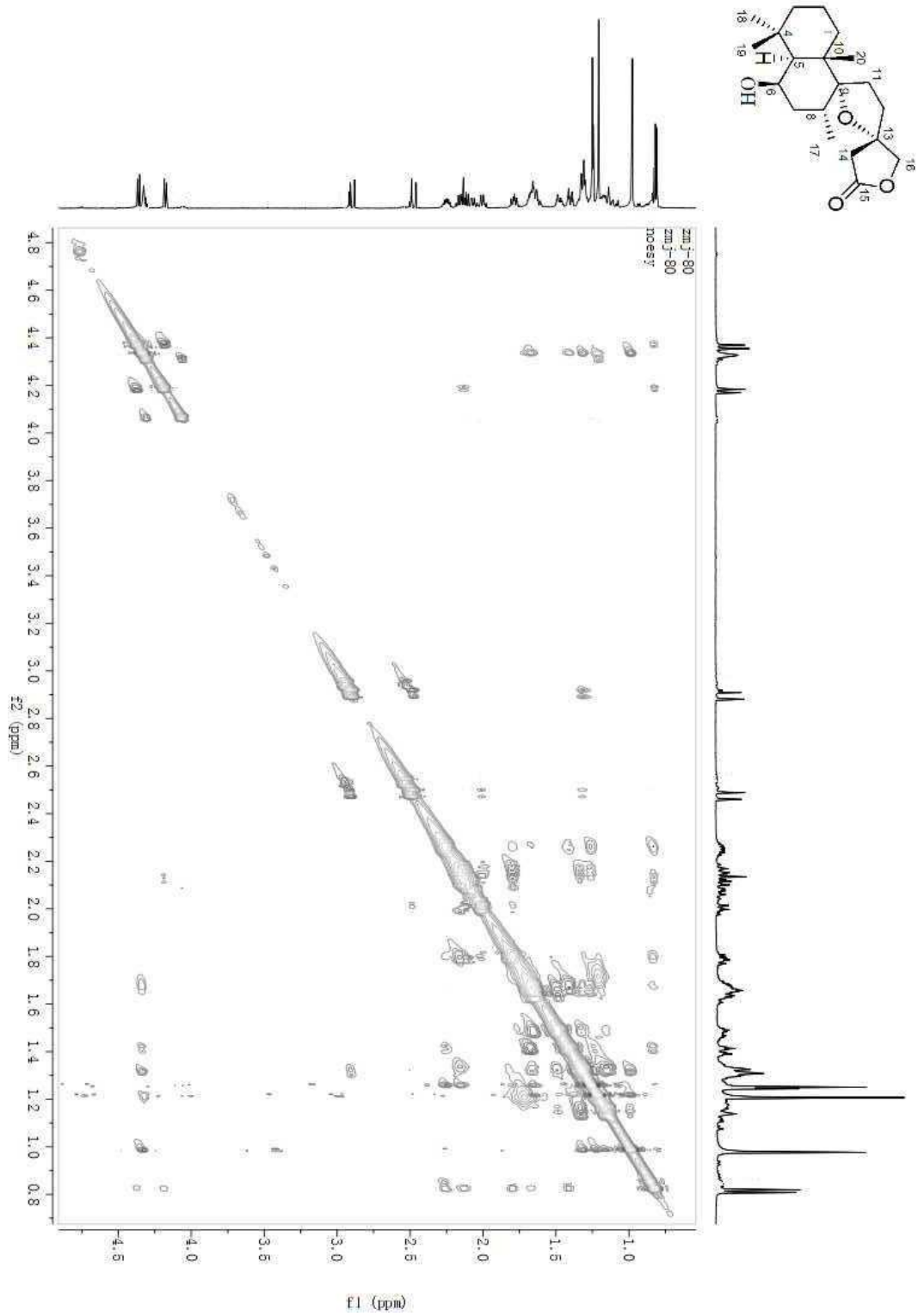
S44. HSQC spectrum of vitextrifolin F (**6**) in $CDCl_3$



S45. HMBC spectrum of vitextrifolin F (**6**) in $CDCl_3$



S46. NOESY spectrum of vitextrifolin F (**6**) in $CDCl_3$



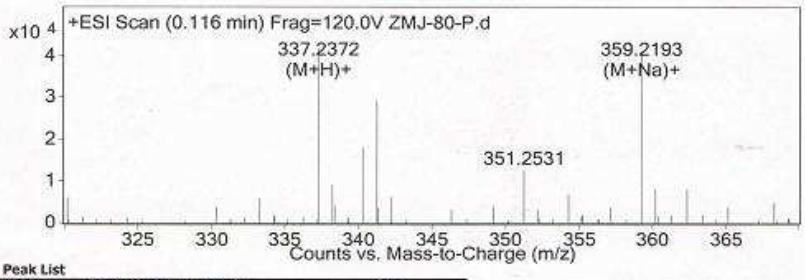
S47. HRESIMS spectrum of vitextrifolin F (**6**)

Qualitative Analysis Report

Data Filename	ZMJ-80-P.d	**Sample Name**	ZMJ-80
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEST-POS-01.m	**Acquired Time**	7/18/2012 10:04:07 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	Esi



Peak List

m/z	z	Abund	Formula	Ion
274.274		33581		
319.227		30665		
337.2372	1	41670	C20 H33 O4	(M+H)+
341.209		29163		
359.2193	1	40879	C20 H32 Na O4	(M+Na)+
391.2458	1	111622		
392.2485	1	25949		
437.1937	1	146413		
438.1971	1	35442		
453.1674	1	93448		

Formula Calculator Element Limits

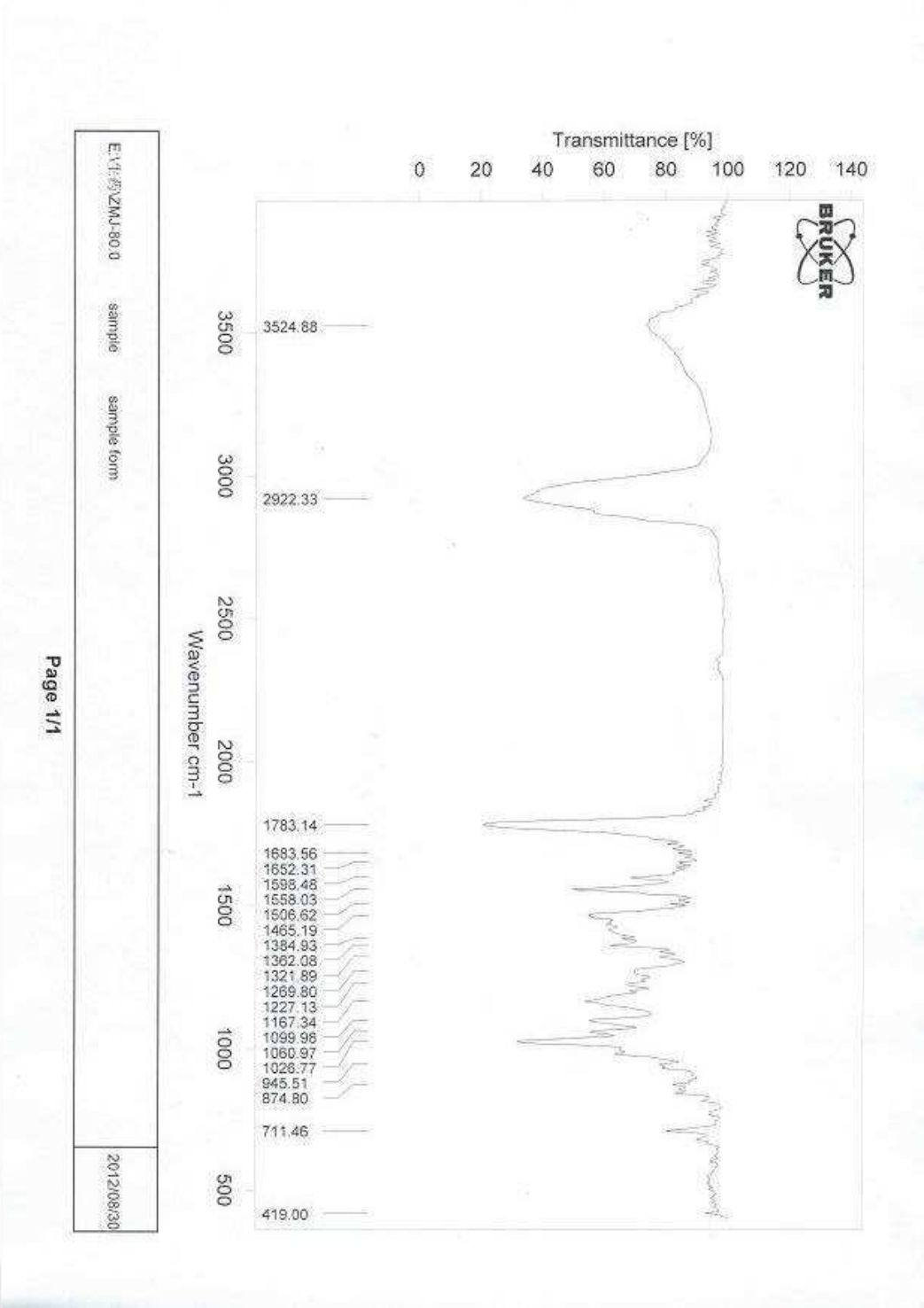
Element	Min	Max
C	2	120
H	2	200
O	0	20

Formula Calculator Results

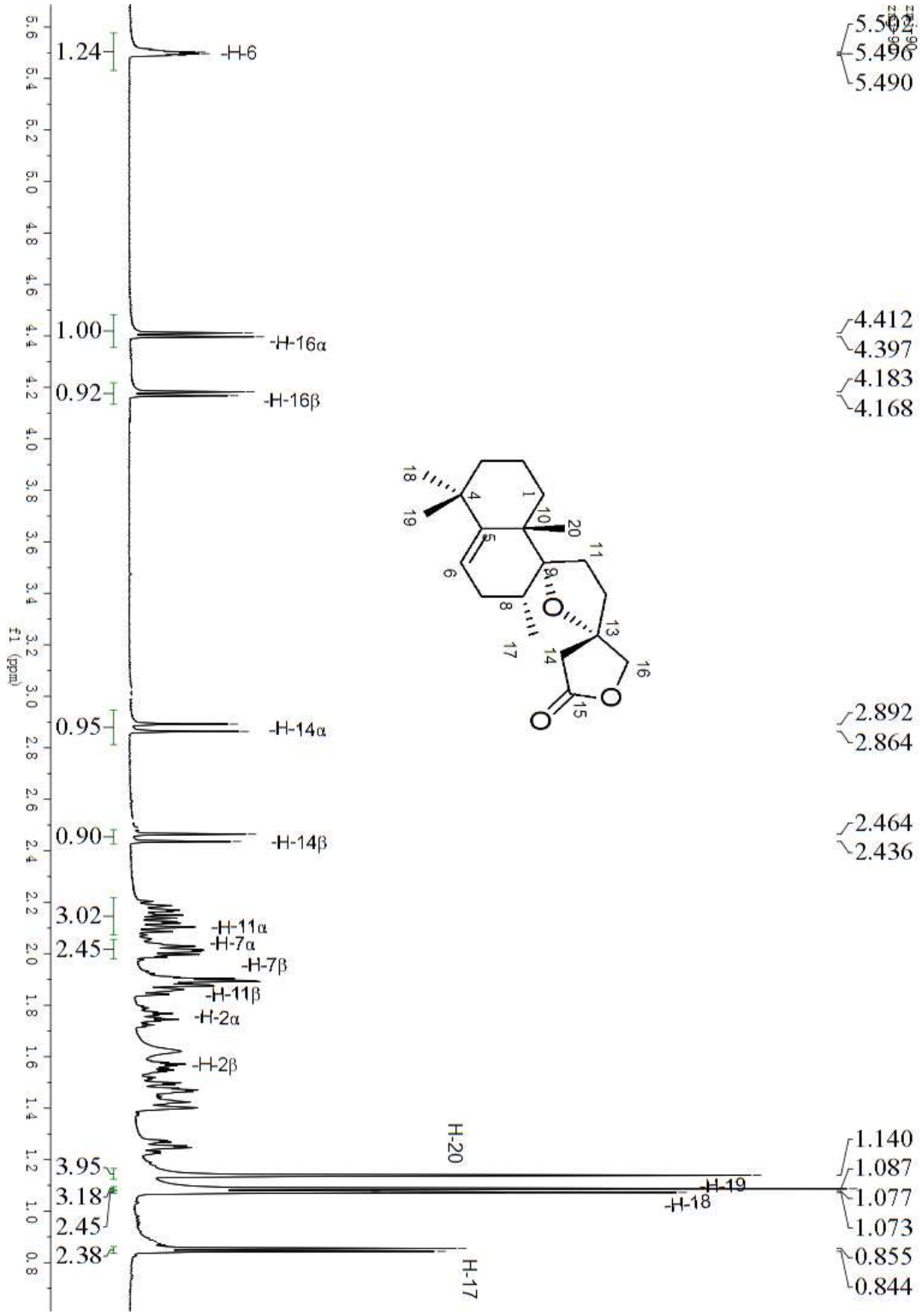
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C20 H32 O4	TRUE	336.2299	336.2301	0.33	C20 H33 O4	99.46
C20 H32 O4	TRUE	336.23	336.2301	0.06	C20 H32 Na O4	96.91

--- End Of Report ---

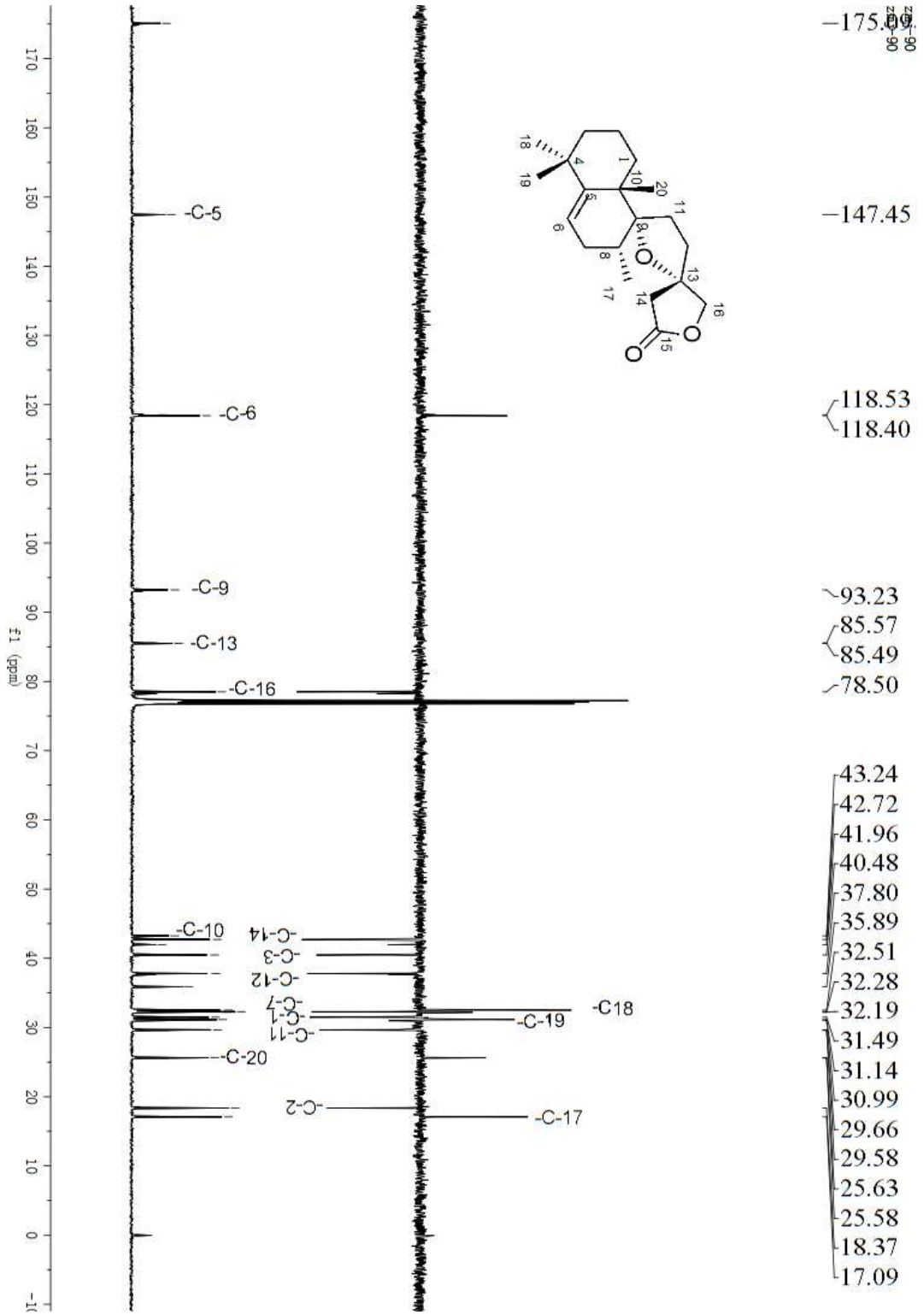
S48. IR (KBr disc) spectrum of vitextrifolin F (**6**)



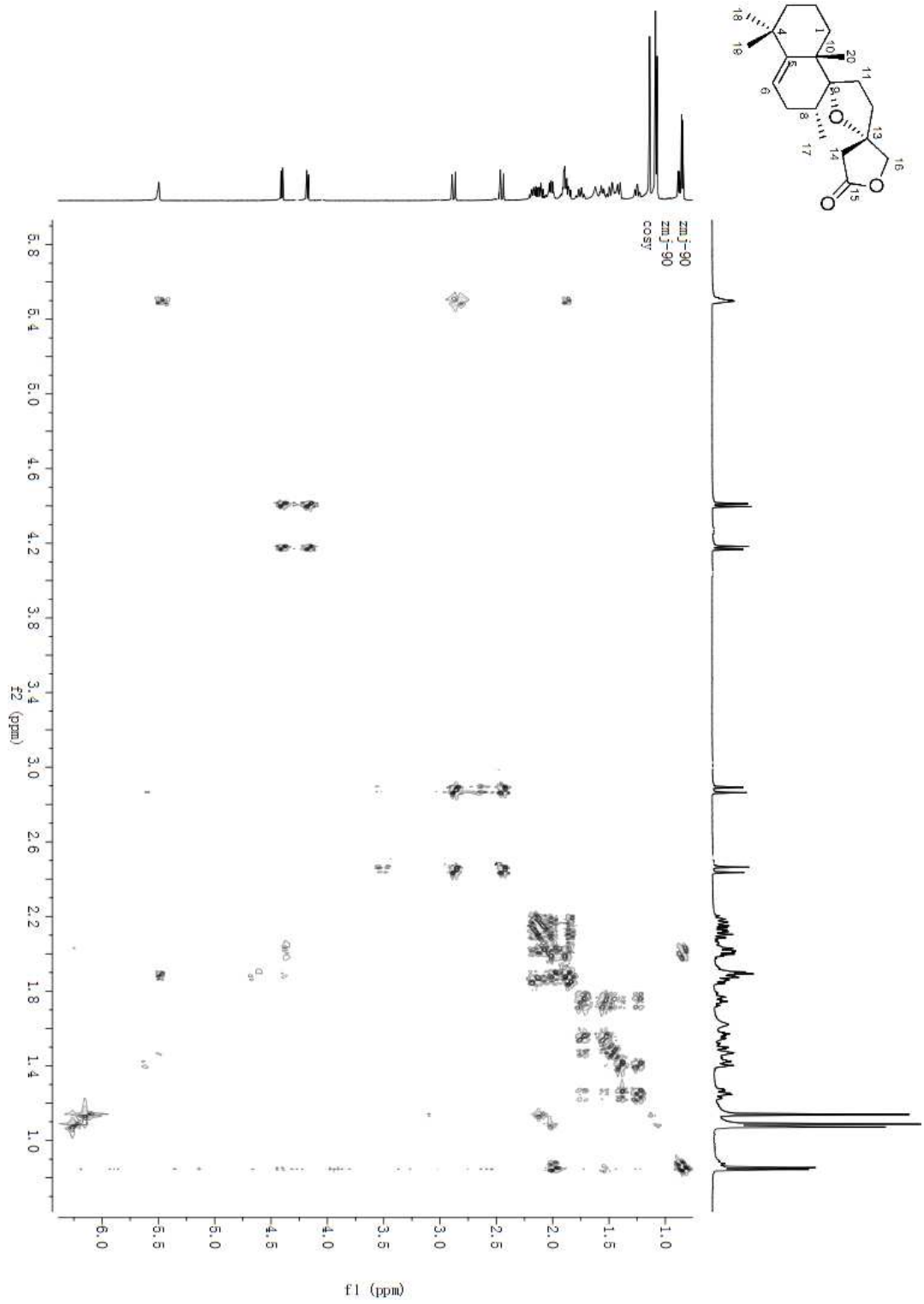
S49. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of vitextrifolin G (**7**)



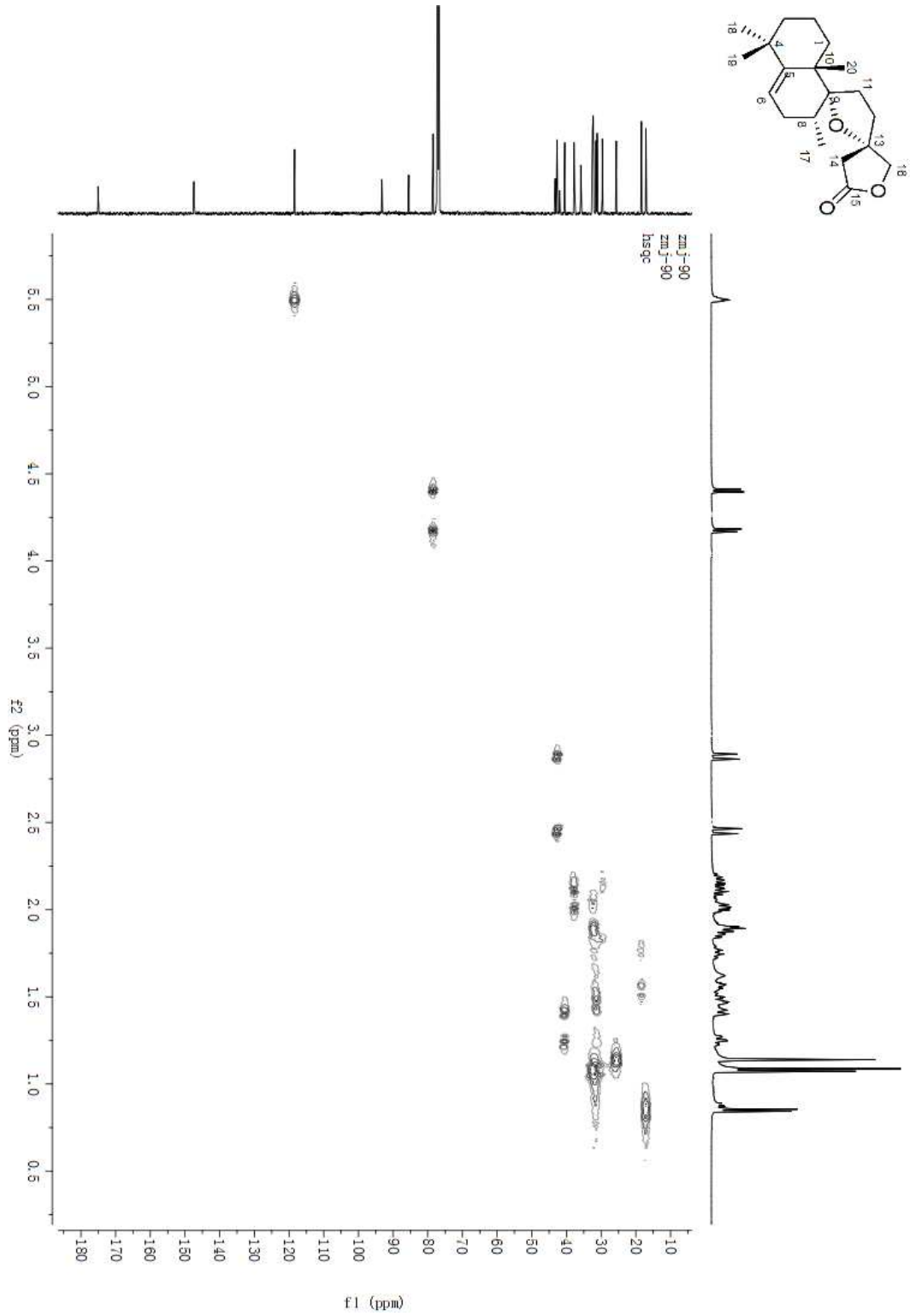
S50. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of vitextrifolin G (**7**)



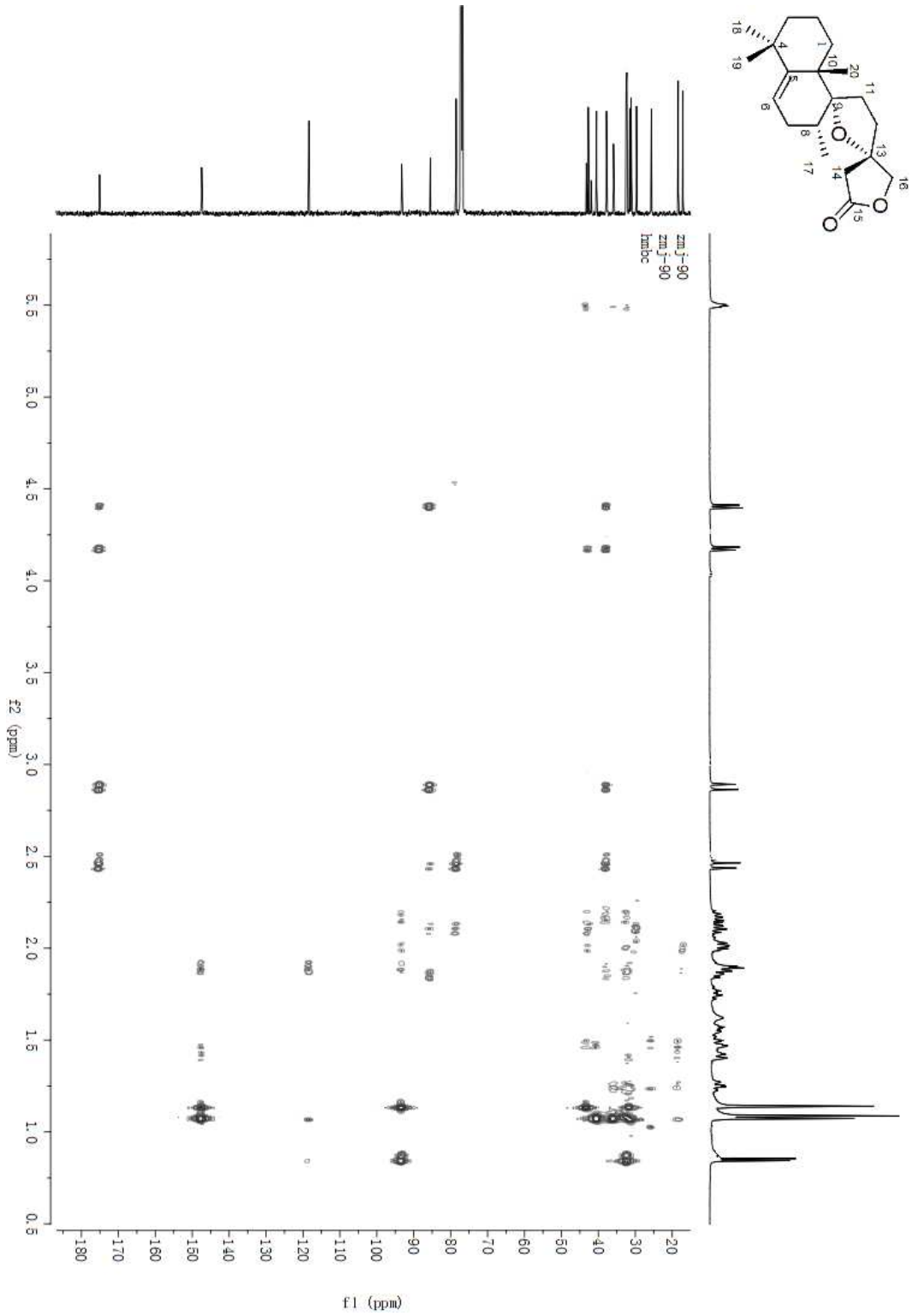
S51. ^{1}H-^{1}H COSY spectrum of vitextrifolin G (**7**) in $CDCl_3$



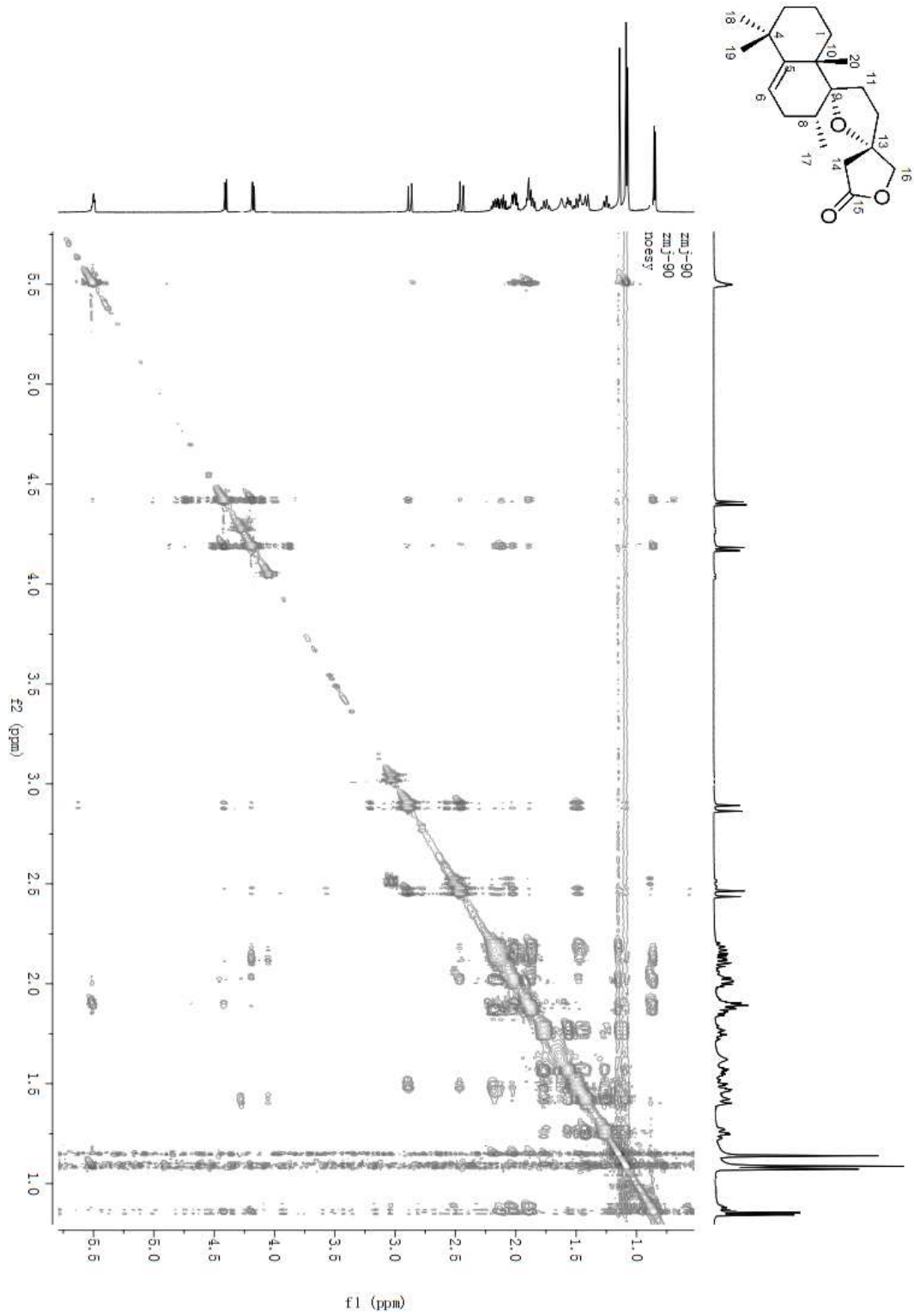
S52. HSQC spectrum of vitextrifolin G (**7**) in $CDCl_3$



S53. HMBC spectrum of vitextrifolin G (**7**) in $CDCl_3$



S54. NOESY spectrum of vitextrifolin G (**7**) in $CDCl_3$



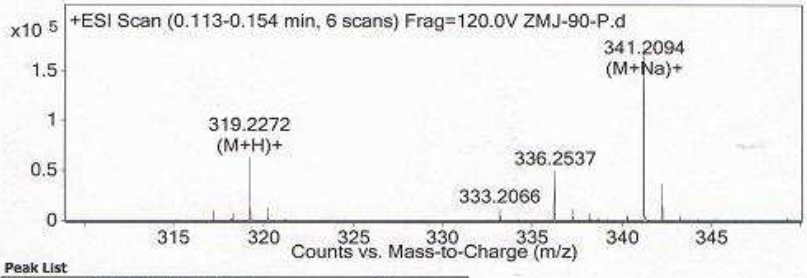
S55. HRESIMS spectrum of vitextrifolin G (**7**)

Qualitative Analysis Report

Data Filename	ZMJ-90-P.d	**Sample Name**	ZMJ-90
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEST-POS-01.m	**Acquired Time**	7/13/2012 12:04:51 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	Esi



Peak List

m/z	z	Abund	Formula	Ion
181.0858		23029		
319.2272	1	67649	C20 H31 O3	(M+H)+
336.2537	1	51213		
341.2094	1	174557	C20 H30 Na O3	(M+Na)+
342.2126	1	36840	C20 H30 Na O3	(M+Na)+
351.2532		34583		
373.2355	1	185198		
374.2386	1	39779		
405.2249		20886		
437.1938	1	36383		

Formula Calculator Element Limits

Element	Min	Max
C	2	45
H	2	200
O	0	35

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C20 H30 O3	TRUE	318.2199	318.2195	-1.22	C20 H31 O3	98.49
C20 H30 O3	TRUE	318.2201	318.2195	-2.04	C20 H30 Na O3	98.45

--- End Of Report ---

S56. IR (KBr disc) spectrum of vitextrifolin G (**7**)