

Electronic Supporting Information

Structure and biosynthesis of scabichelin, a novel *tris*-hydroxamate siderophore of the plant pathogen *Streptomyces scabies* 87.22

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Table S1. Strains, plasmids and oligonucleotide primers used in this study

Strain/plasmid/primer	Properties	Source/reference
<i>S. antibioticus</i> NBRC 13838	Wild type	National Institute of Technology and Evaluation, Japan
<i>S. noursei</i> NBRC 15452	Wild type	National Institute of Technology and Evaluation, Japan
<i>S. virginiae</i> NBRC 12827	Wild type	National Institute of Technology and Evaluation, Japan
<i>S. aureofaciens</i> NBRC12843	Wild type	National Institute of Technology and Evaluation, Japan
<i>S. albus</i> NBRC 13014	Wild type	National Institute of Technology and Evaluation, Japan
<i>S. scabies</i> JCM 7914	Wild type	Riken BioResource Centre, Japan
<i>S. turgidiscabies</i> JCM10429	Wild type	Riken BioResource Centre, Japan
<i>E. coli</i> DH5α	General cloning host	Lab collection
<i>E. coli</i> BW25113/pIJ790	Strain used for λRED-mediated recombination	Gust et al. 2004
<i>E. coli</i> ET12567/pUZ8002	Strain used for <i>E. coli/S. scabies</i> conjugation	Gust et al. 2004
<i>S. scabies</i> 87.22	Wild type	Rose Loria, Cornell University
<i>S. scabies</i> W1000	<i>scab85471::apr</i> mutant of <i>S. scabies</i> 87.22	This study
pIJ773	Source of <i>oriT-apr</i> cassette for gene disruption	Gust et al. 2004
S57	Supercos1 derivative containing <i>scab85251</i> to <i>scab85521</i> genes	Rose Loria, Cornell University
S57:: <i>oriT-apr</i>	<i>scab85471</i> internal fragment replaced with <i>oriT-apr</i> cassette in S57	This study
Replacement_fw (5'-cagggcgccgcacccgtgcgggtggatgaactgctgcggattcc-3')	Used to amplify the <i>oriT-apr</i> cassette from pIJ773	This study
Replcmnt_rv (5'-gttcgagtgaaagaacaggeccctctggagcggggcggatgttaggctggagctgttc-3')	Used to amplify the <i>oriT-apr</i> cassette from pIJ773	This study
Test_fw (5'- cgccatccacccatcc-3')	Used to confirm correct integration of S57:: <i>oriT-apr</i> into the <i>S. scabies</i> 87.22 genome	This study
Test_rv (5'- aaggccccggccagatcac-3')	Used to confirm correct integration of S57:: <i>oriT-apr</i> into the <i>S. scabies</i> 87.22 genome	This study

Table S2. NMR spectroscopic data for Ga-scabichelin in DMSO-*d*₆

	Position	δH (ppm)	δC (ppm)
N-Me hfOrn1	N-CH ₃	2.51 m	31.2
	NH	8.77 br	
	CO		167.4
	α	3.90 br	59.1
	β	1.89 m	25.2
		1.53 m	
	γ	1.62 m	17.2
		1.31 m	
	δ	3.46 m	49.7
		3.40 m	
Ser2	formyl	8.06 s	152.4
	NH	8.99 m	
	CO		160.5
	α	4.73 m	50.4
	β	3.68 m	60.1
		3.63 m	
N-Me hOrn3	OH	5.21 t, J = 5.70 Hz	
	N-CH ₃	2.47 m	31.1
	NH	8.92 br	
	CO		166.5
	α	3.68 m	60.1
	β	1.71 m	26.7
		1.65 m	
	γ	1.68 m	22.5
		1.59 m	
Orn4	δ	4.10 ddd, J = 14.14, 7.25, 6.46	50.1
		3.38 m	
	NH	8.99 m	
	CO		168.5
	α	4.49 ddd, J = 14.50, 7.15, 1.73	51.6
	β	1.68 m	28.9
		1.49 m	
	γ	1.48 m	23.3
Cyclic hOrn5		1.43 m	
	δ	2.77 m	38.3
	NH ₂	7.71 m	
	NH	8.64 d, J = 9.52 Hz	
	CO		159.0
	α	4.73 m	44.4
	β	1.96 m	26.1
		1.59 m	
	γ	2.31 m	17.1
		1.78 m	
	δ	3.51 m	49.4

Table S3. NMR spectroscopic data for Ga-turgichelin in DMSO-*d*₆

	Position	δH (ppm)		δC
N-Me hOrn1	N-CH ₃	2.50	m	31.4
	NH	8.77	br	
	CO			167.6
	α	3.90	m	59.3
	β	1.90	m	25.4
		1.53	m	
	γ	1.63	m	17.4
		1.31	m	
	δ	3.47	m	49.6
		3.40	m	
	formyl	8.07	s	152.5
Ser2	NH	8.99	d, J= 7.60Hz	
	CO			160.7
	α	4.72	m	50.2
	β	3.71	dd, J = 10.93, 5.15 Hz	60.3
		3.60	dd, J = J10.93, 8.37 Hz	
	OH	ND		
N-Me hOrn3	N-CH ₃	2.47	m	31.1
	NH	8.92	br	
	CO			167.1
	α	3.63	m	60.1
	β	1.71	m	26.7
		1.65	m	
	γ	1.68	m	22.5
		1.59	m	
	δ	4.10	td, J = 13.62, 6.59 Hz	50.1
		3.39		
Ser4	NH	8.87	d, J= 8.84Hz	
	CO			168.3
	α	4.50	td, J = 8.54, 5.74 Hz	53.9
	β	3.36	dd, J = 10.30, 5.74 Hz	60.5
		3.59	m	
	OH	ND		
Cyclic hOrn5	NH	8.52	d, J= 8.99Hz	
	CO			159.2
	α	4.73	m	44.7
	β	1.96	m	25.4
		1.60	m	
	γ	2.28	m	17.2
		1.77	m	
	δ	3.50	m	49.4

Fig. S1. ESI-MS spectrum of scabichelin

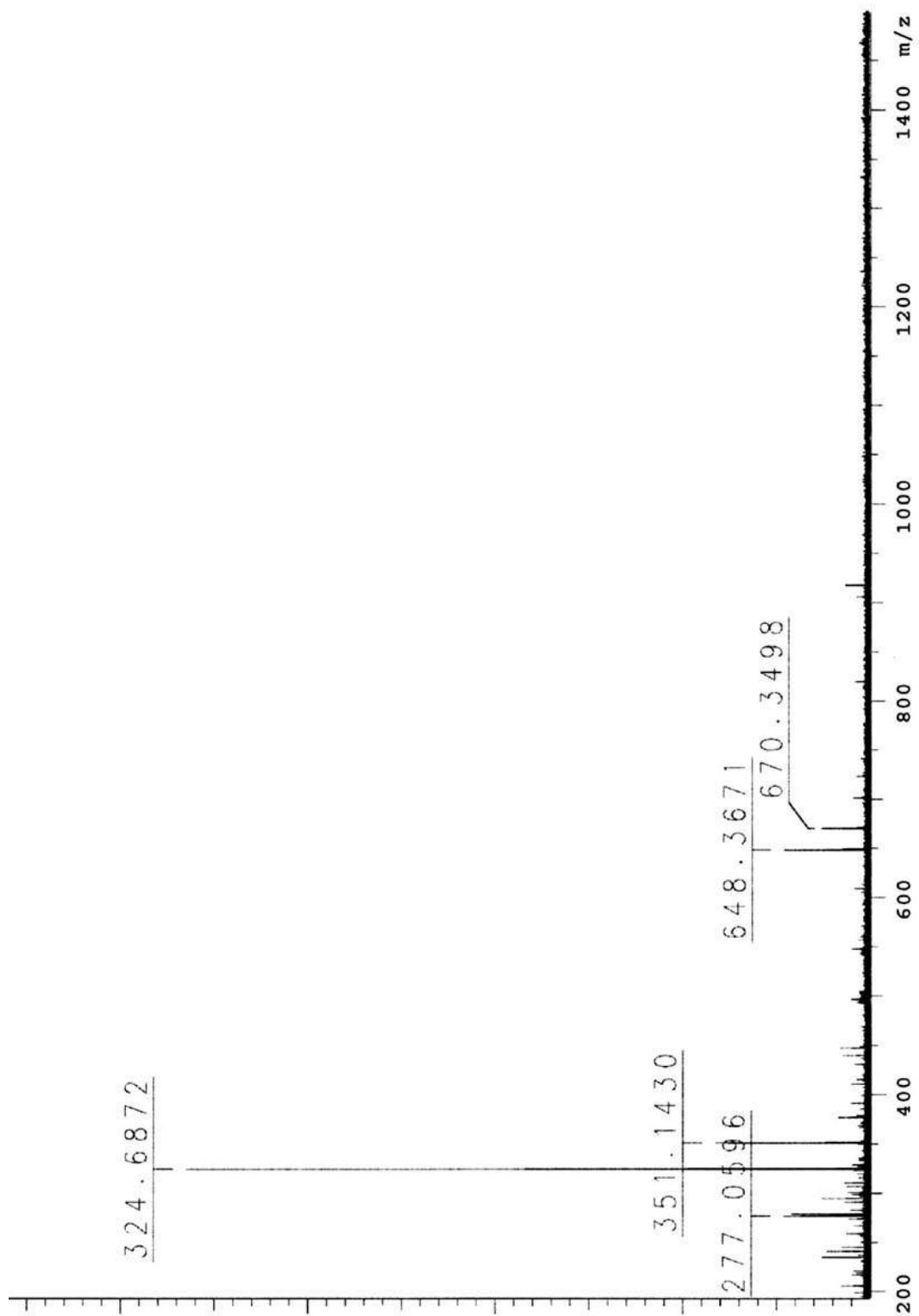


Fig. S2. ESI-MS spectrum of Ga-scabichelin

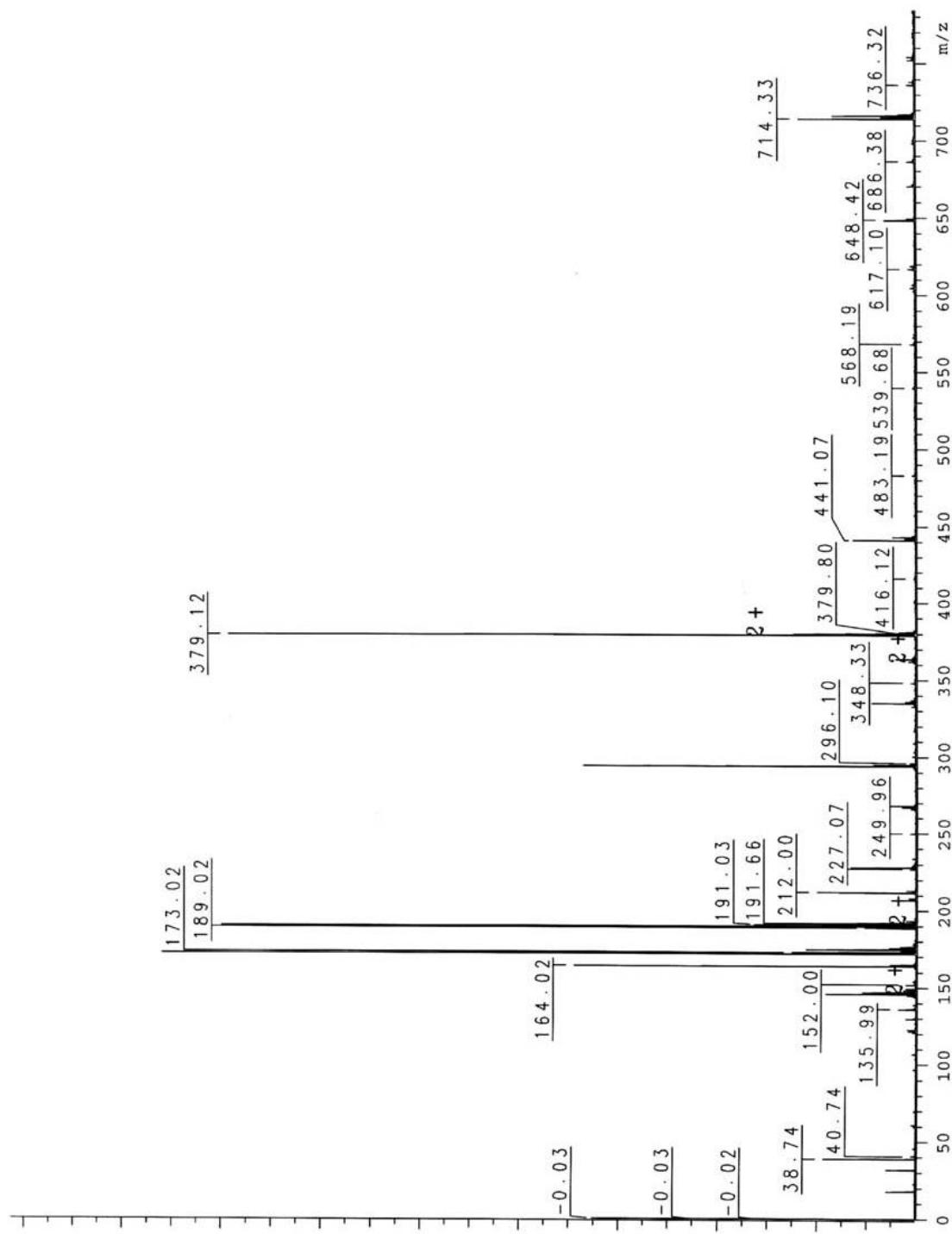


Fig. S3. ESI-MSMS spectrum of scabichelin

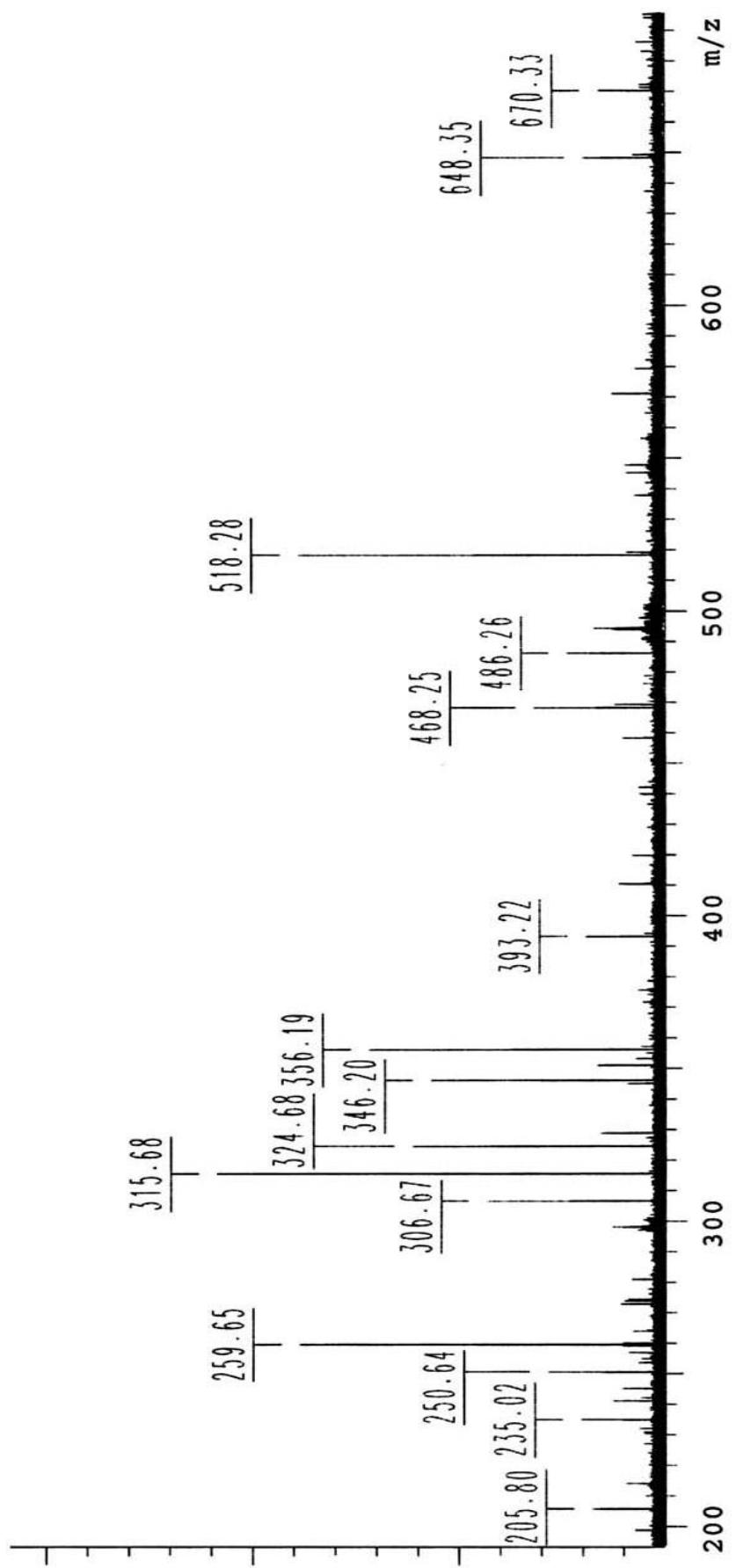


Fig. S4. ^1H NMR spectrum of Ga-scabichelin

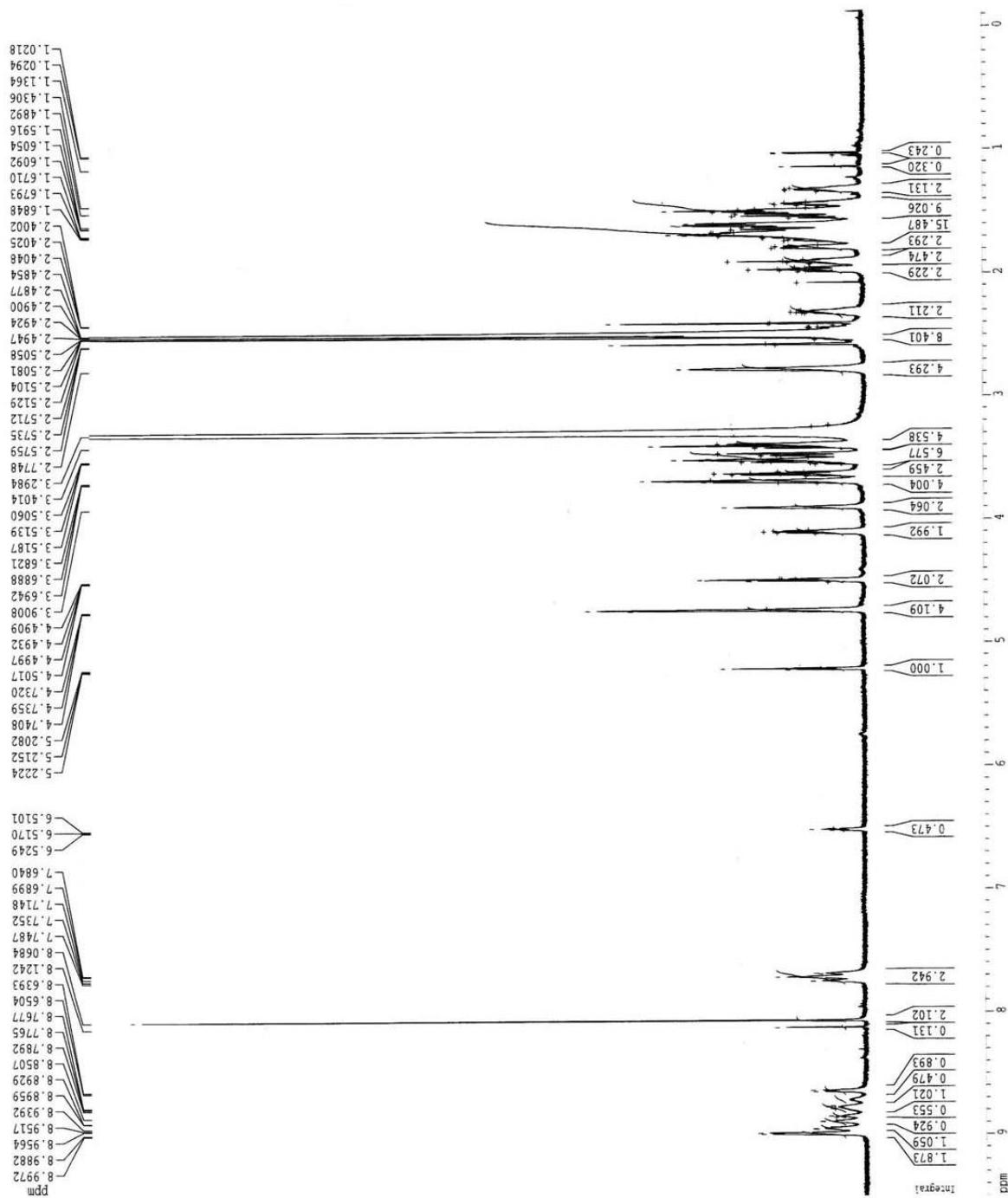


Fig. S5. ^{13}C NMR spectrum of Ga-scabichelin

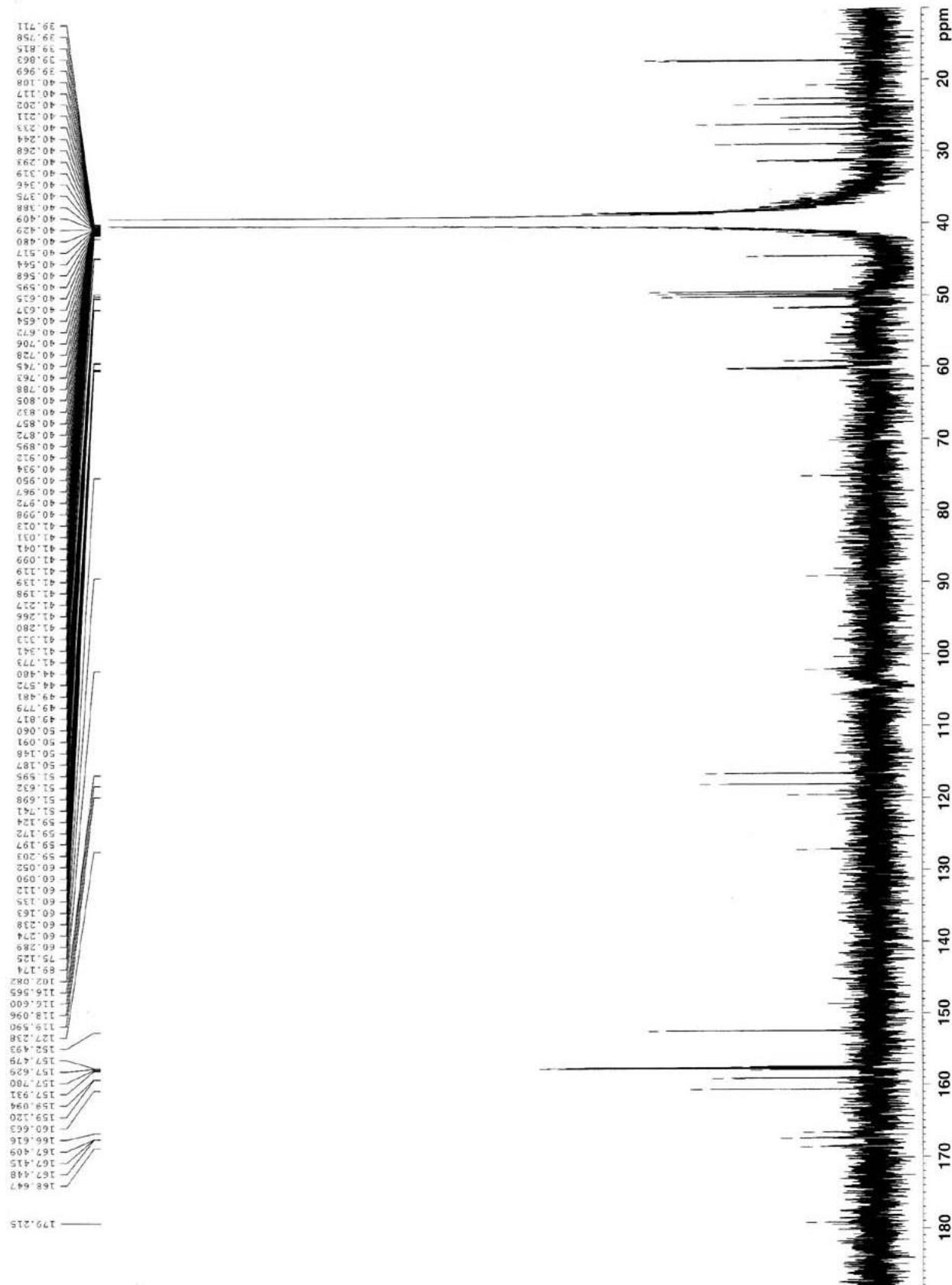


Fig. S6. DQF-COSY spectrum of Ga-scabichelin

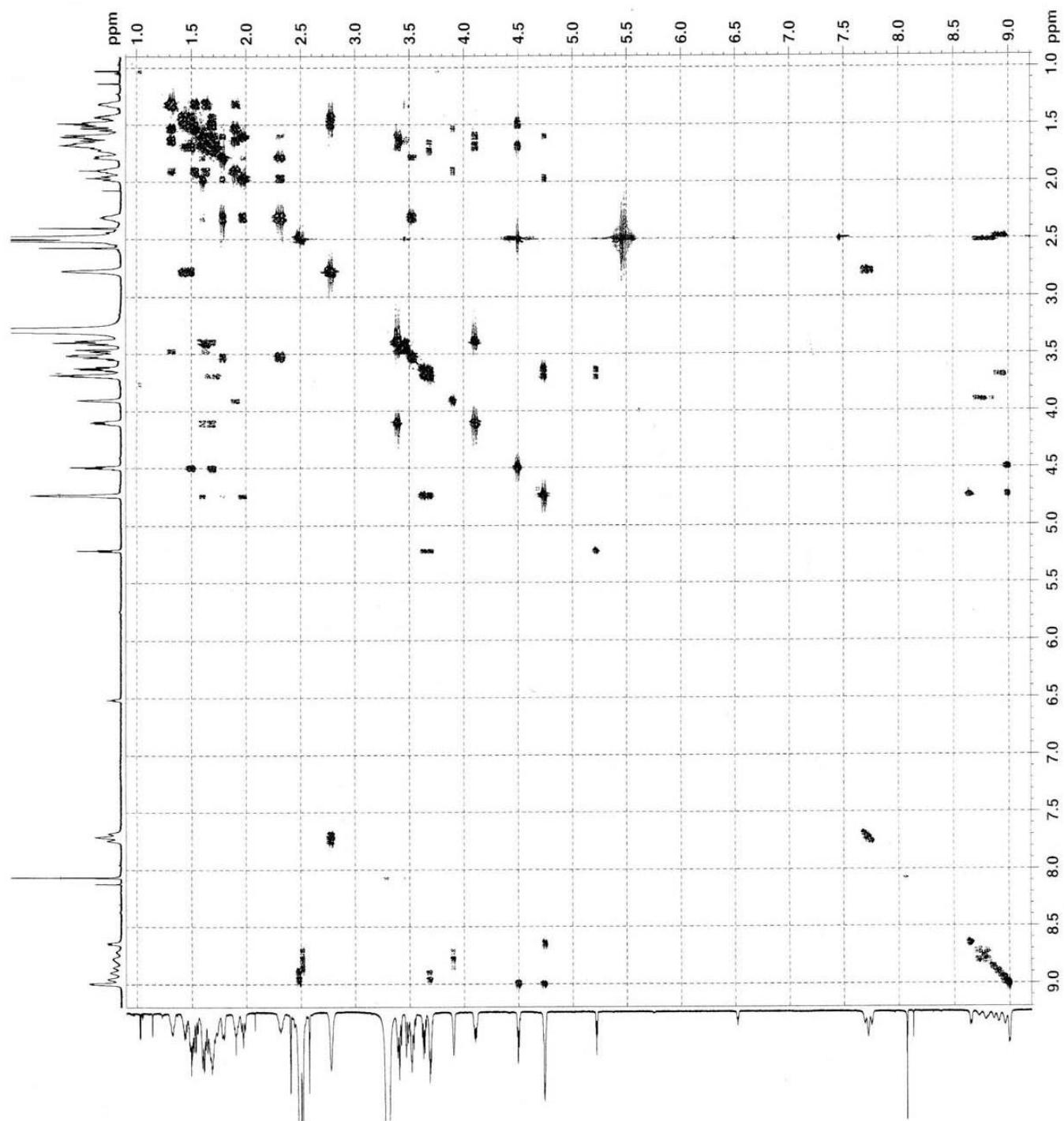


Fig. S7. TOCSY spectrum of Ga-scabichelin

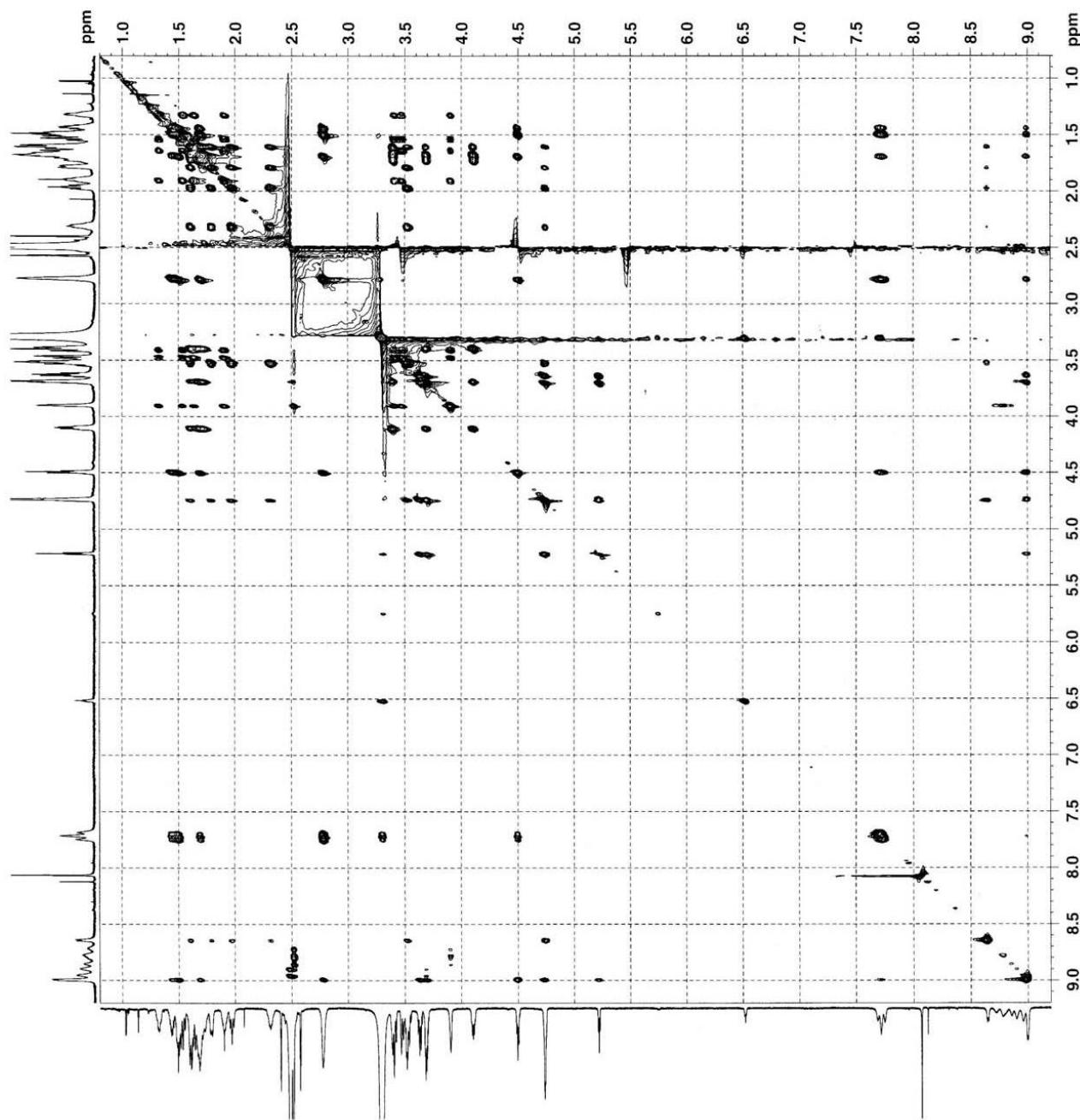


Fig. S8. ROESY spectrum of Ga-scabichelin

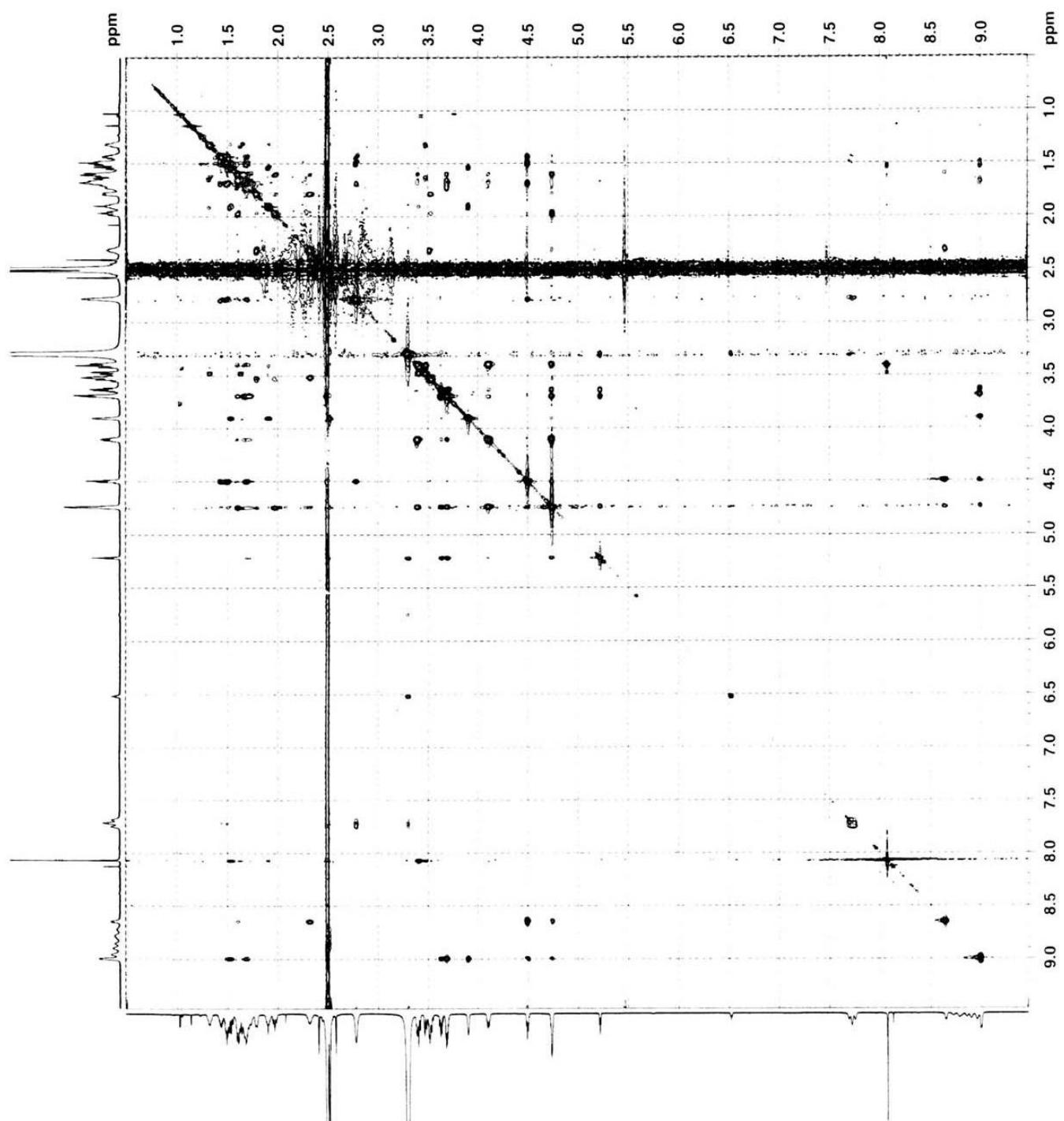


Fig. S9. HSQC spectrum of Ga-scabichelin

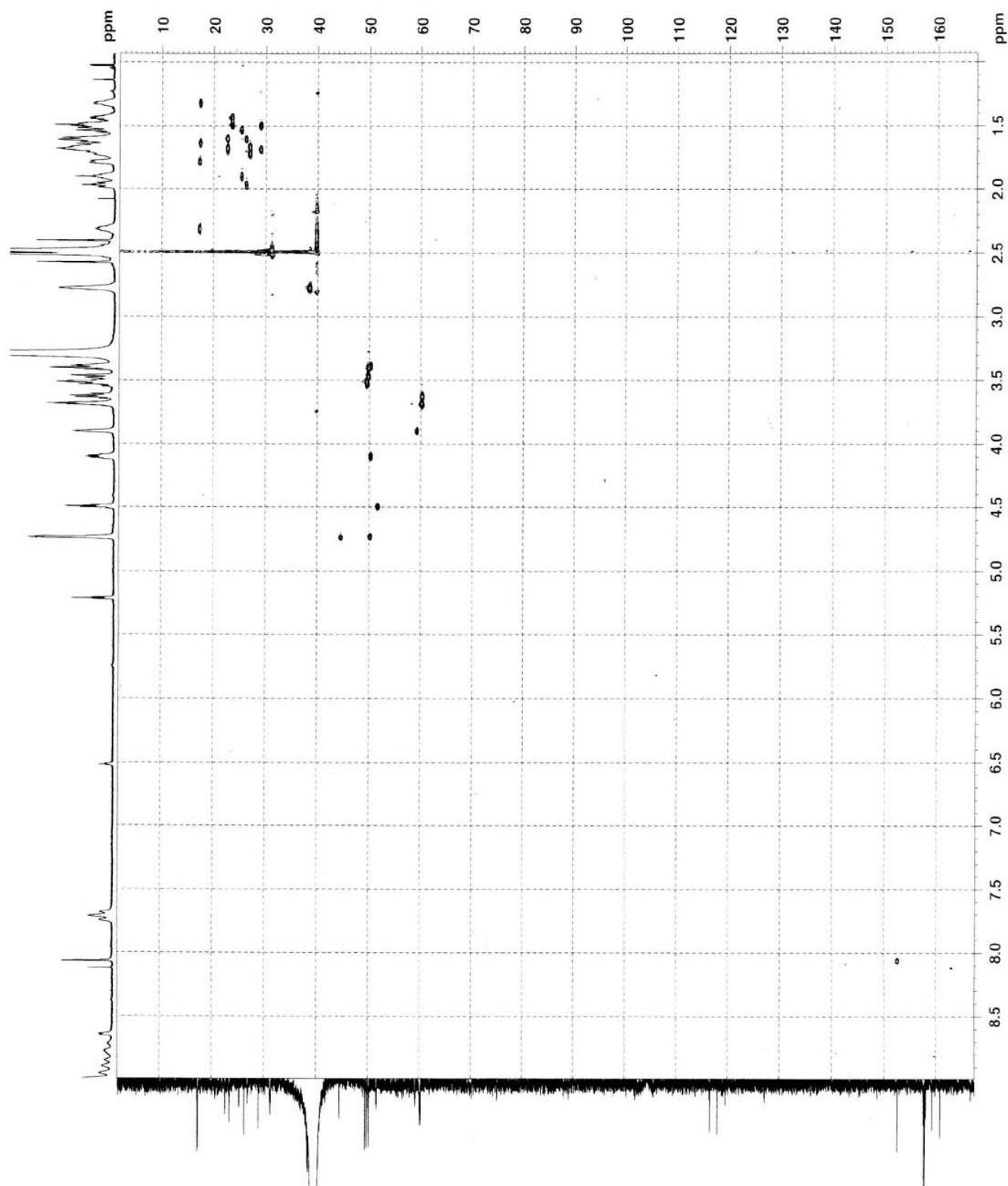


Fig. S10. HMBC spectrum of Ga-scabichelin

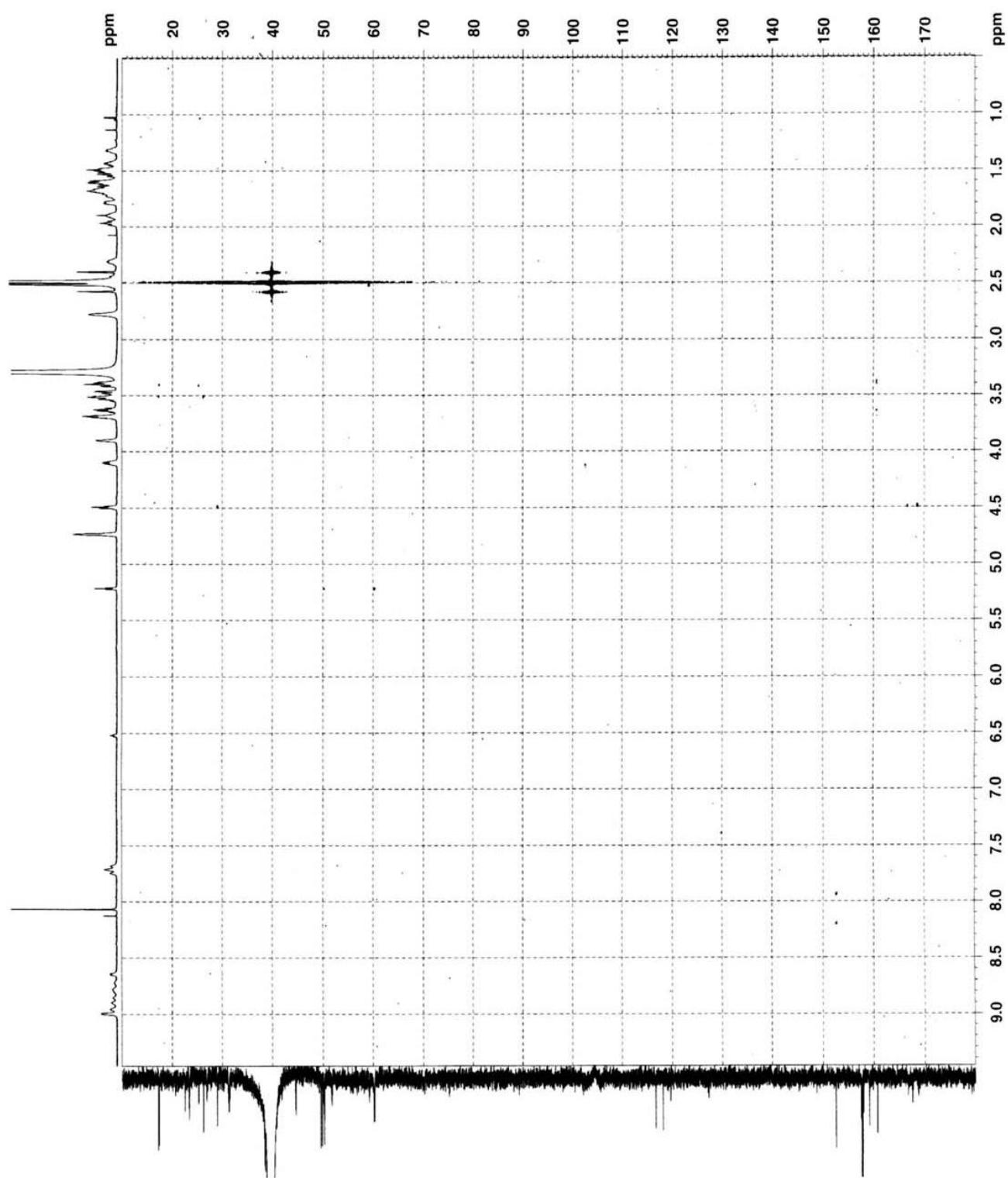


Fig. S11. ESI-MS spectrum of turgichelin

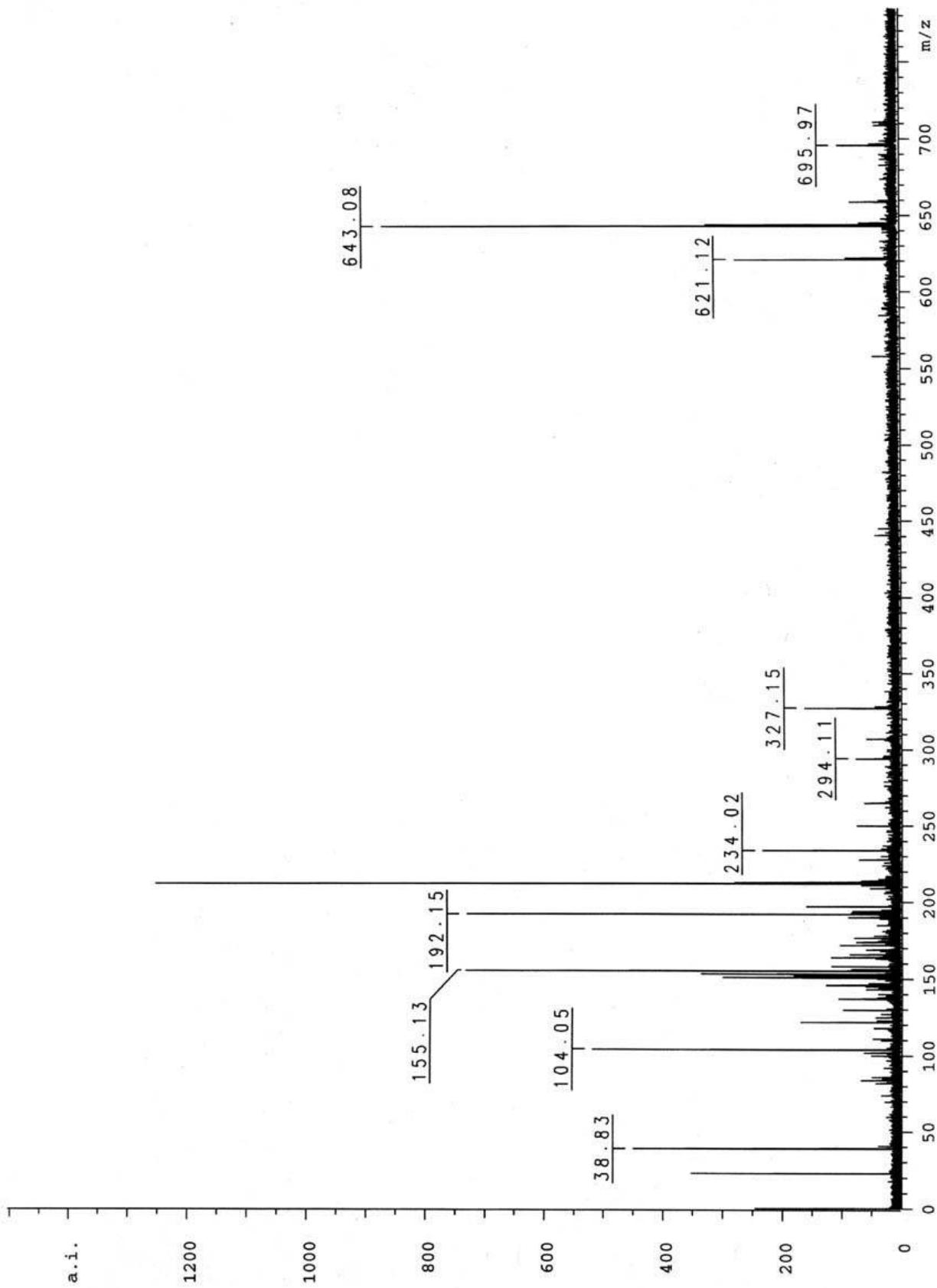


Fig. S12. ESI-MS spectrum of Ga-turgichelin

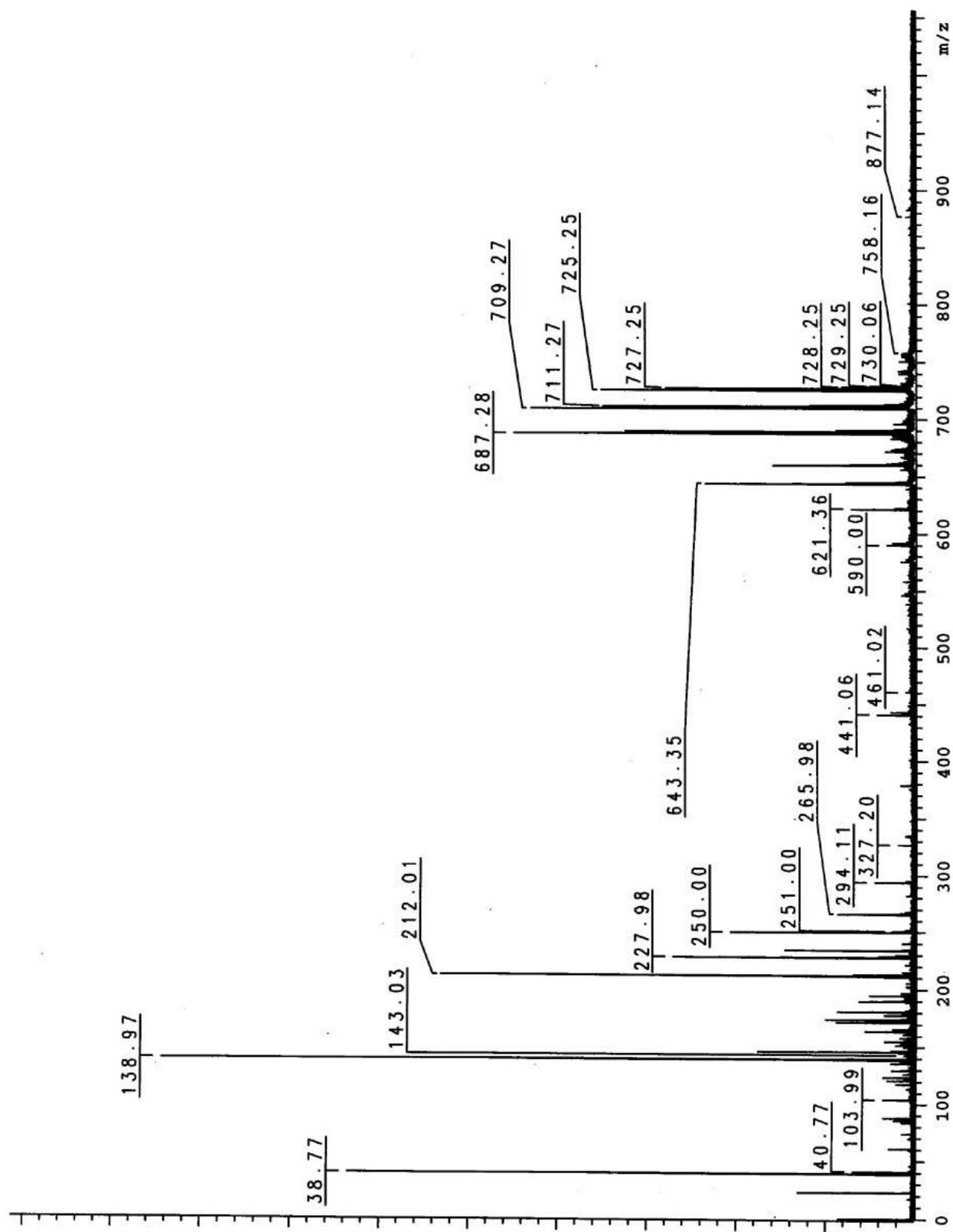


Fig. S13. ESI-MSMS spectrum of turgichelin

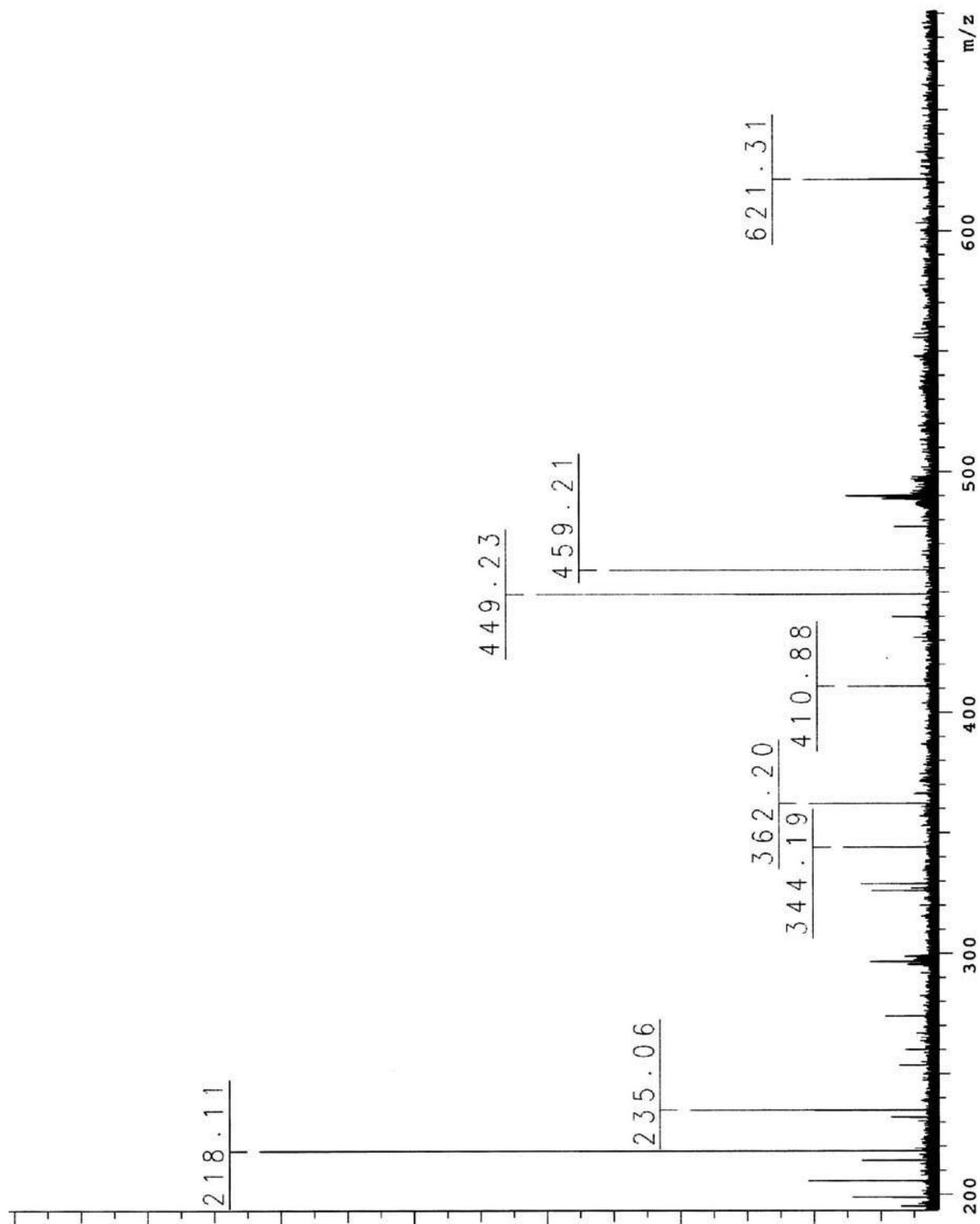


Fig. S14. ^1H NMR spectrum of Ga-turgichelin

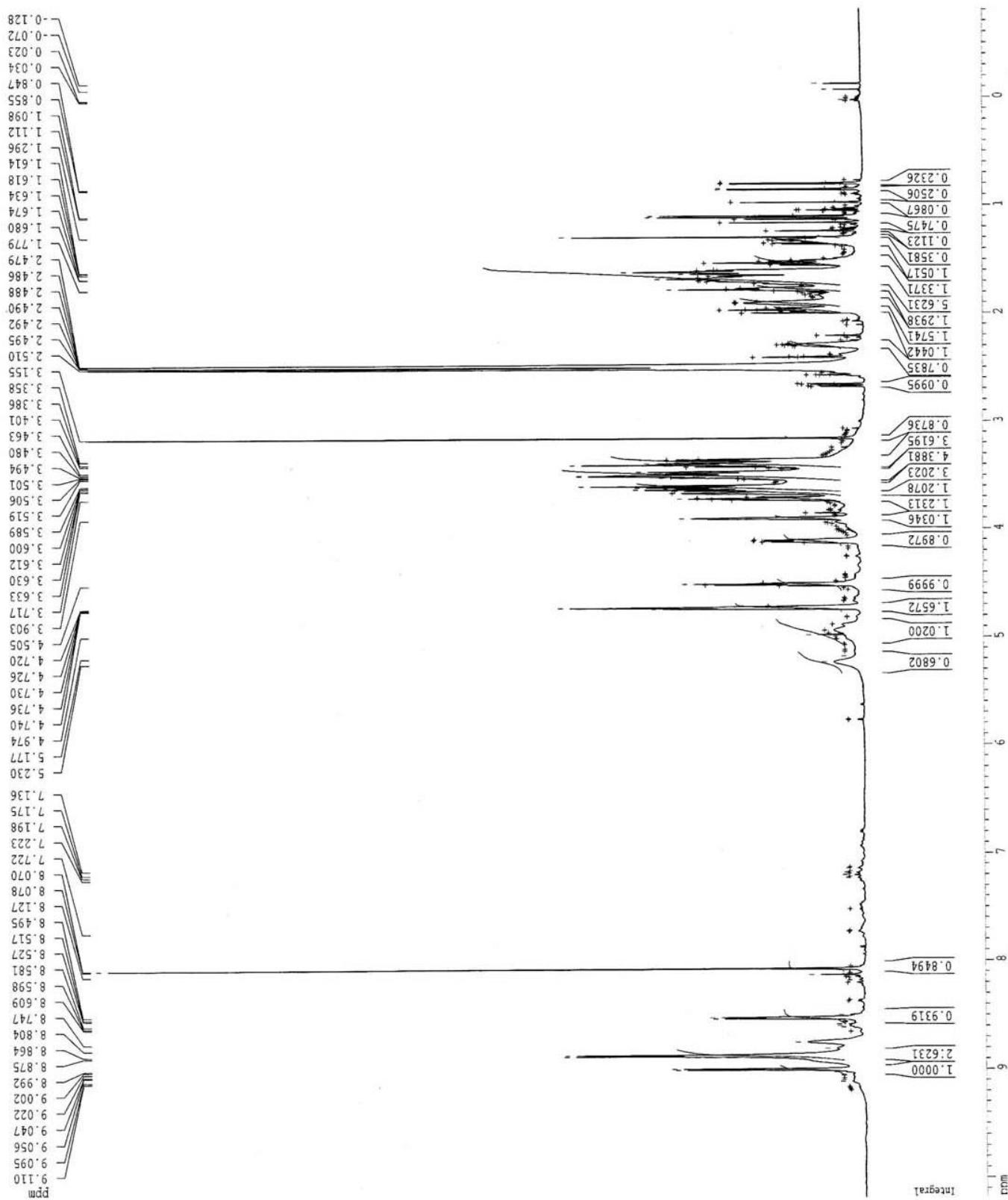


Fig. S15. ^{13}C NMR spectrum of Ga-turgichelin

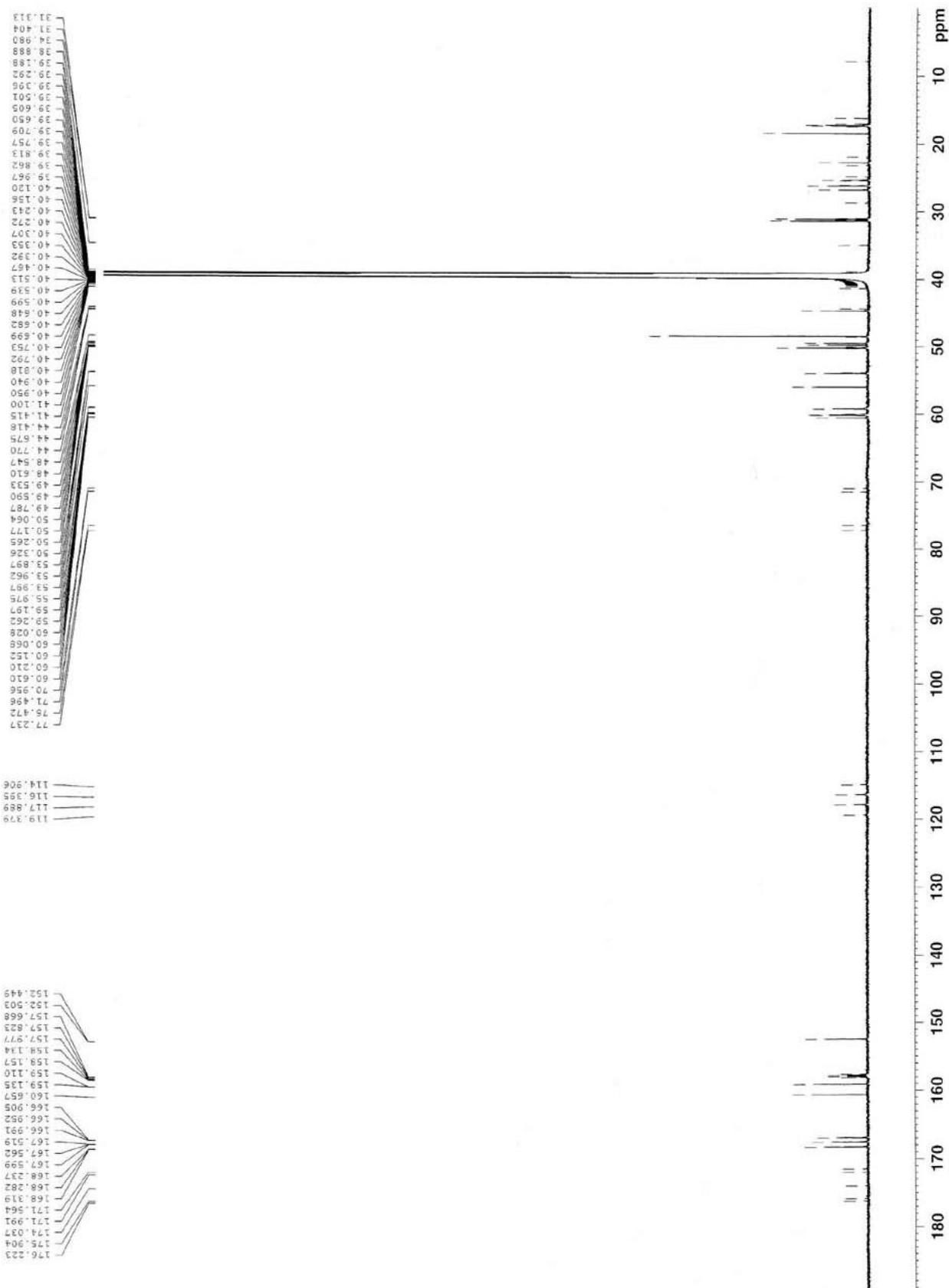


Fig. S16. DQF-COSY spectrum of Ga-turgichelin

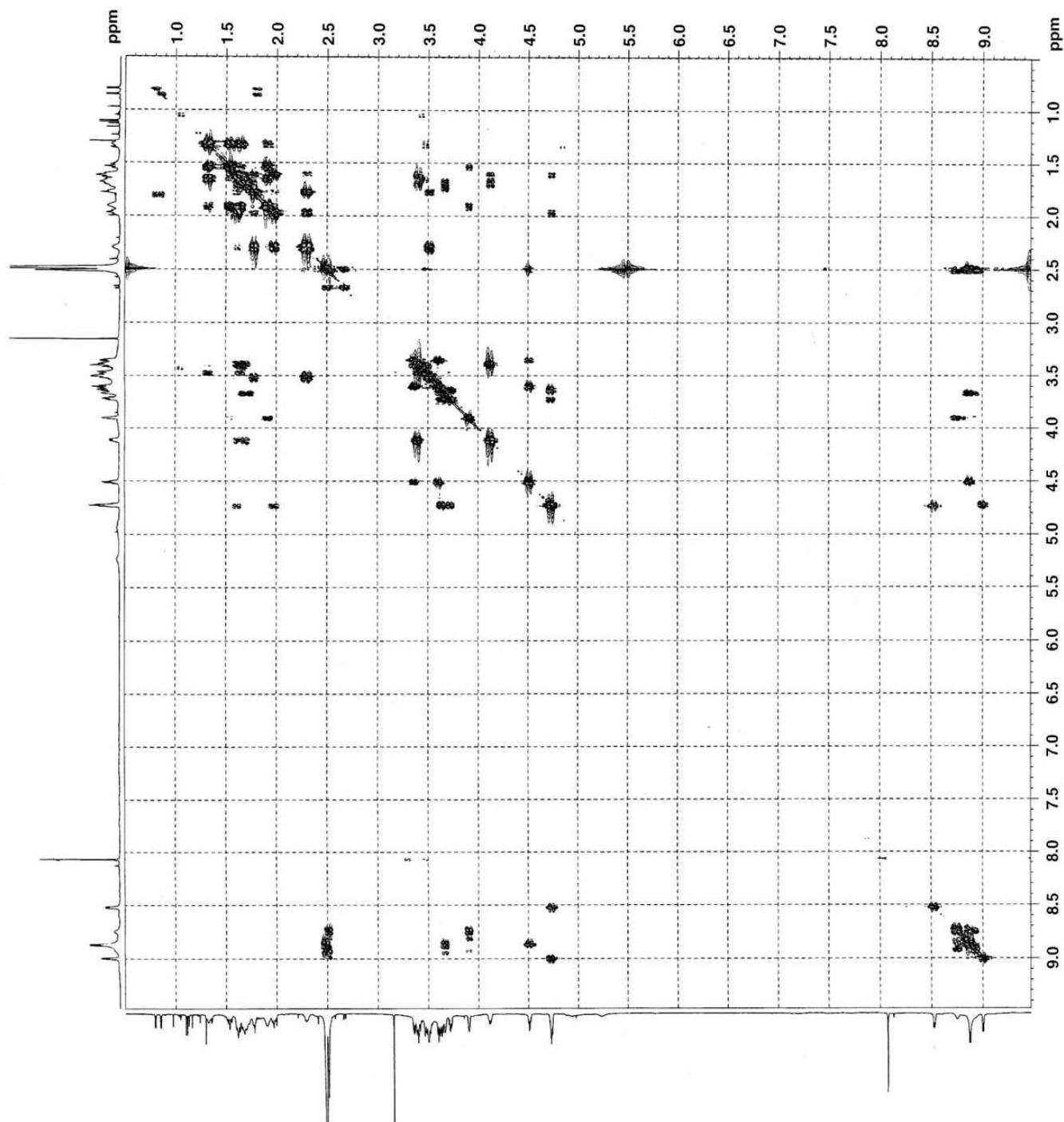


Fig. S17. TOCSY spectrum of Ga-turgichelin

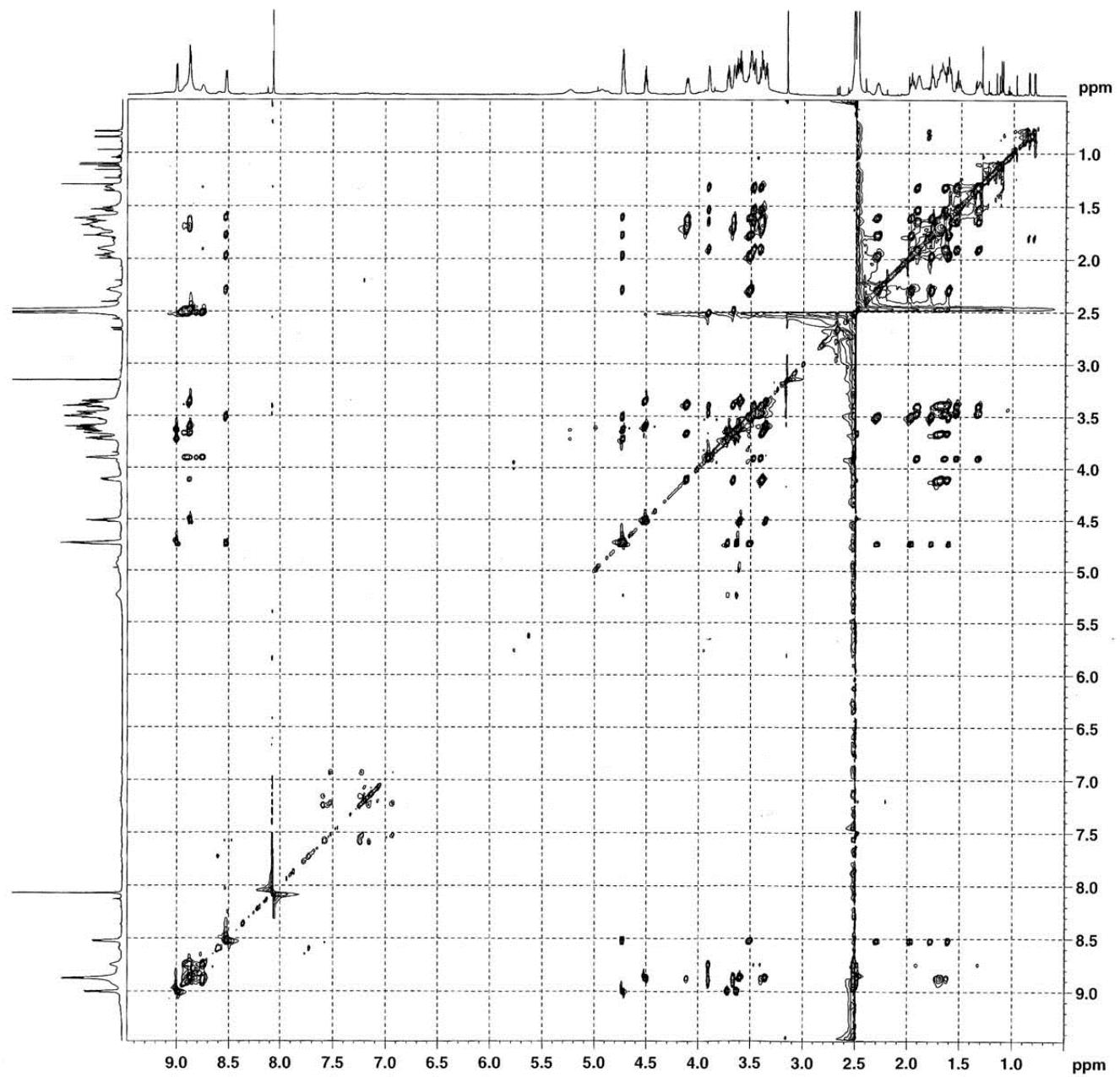


Fig. S18. ROESY spectrum of Ga-turgichelin

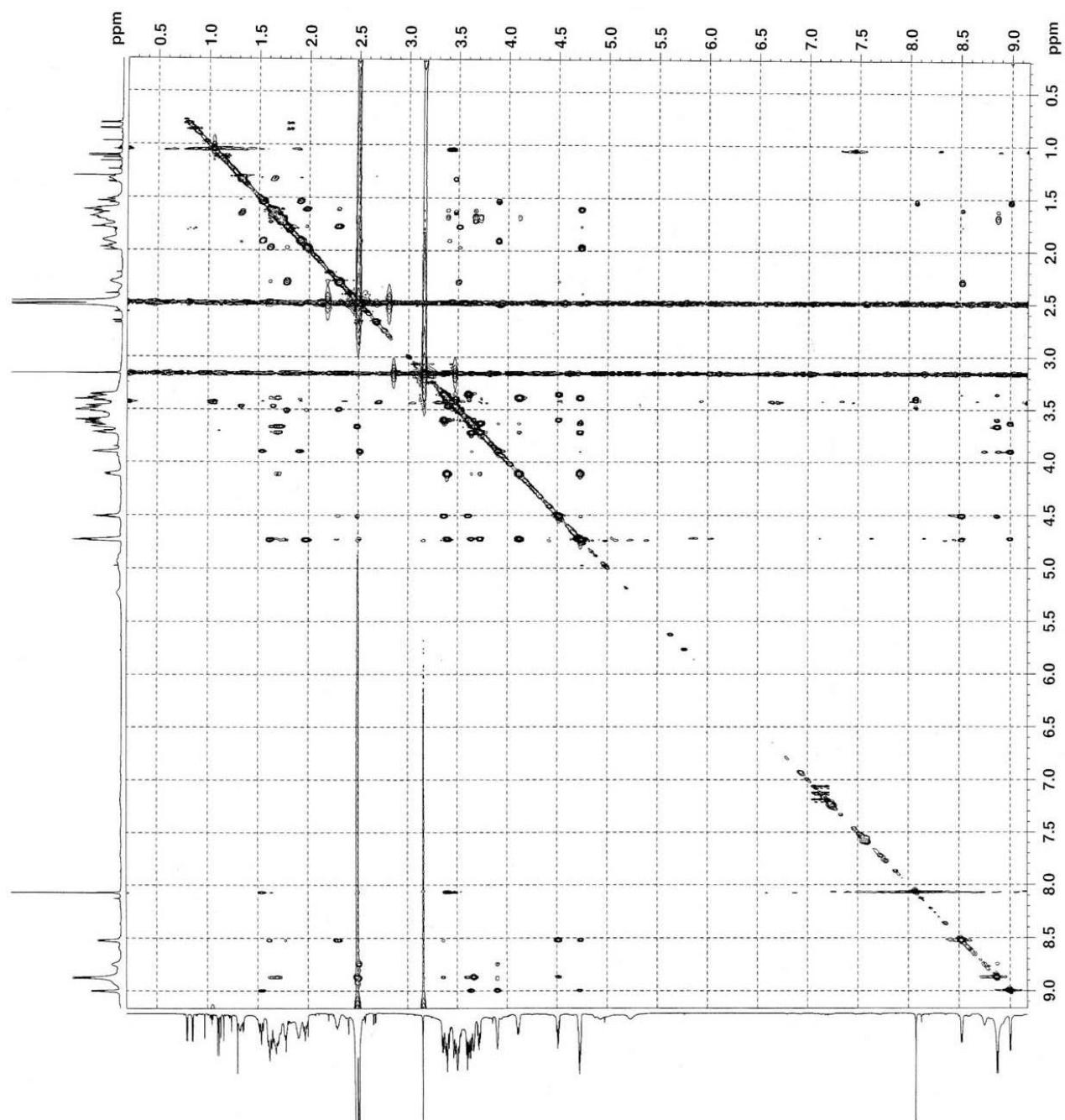


Fig. S19. HSQC spectrum of Ga-turgichelin

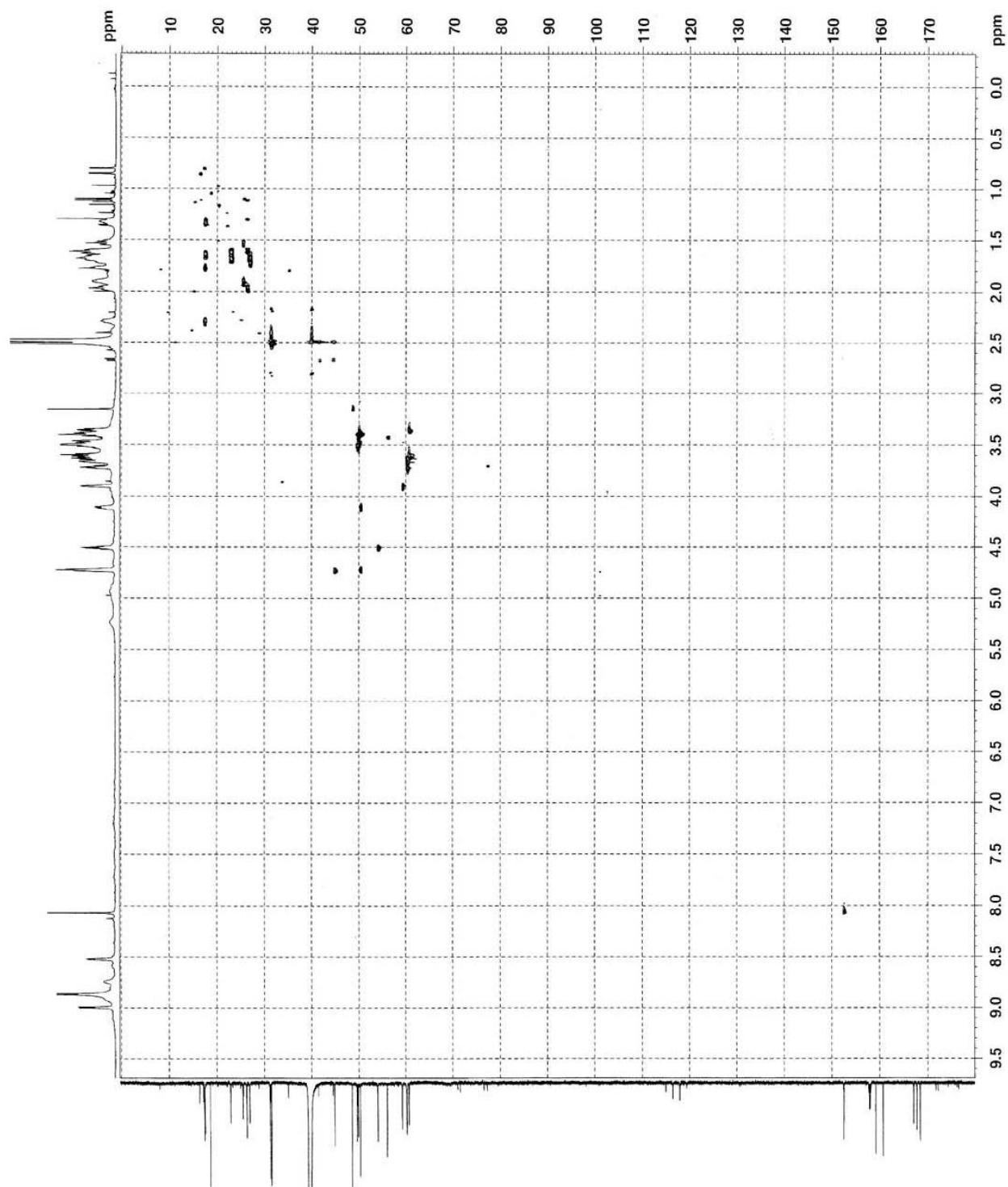


Fig. S20. HMBC spectrum of Ga-turgichelin

