

Supporting Information

Rec. Nat. Prod. 9:2 (2015) 267-270

Antibacterial triterpenoids from *Melia toosendan*

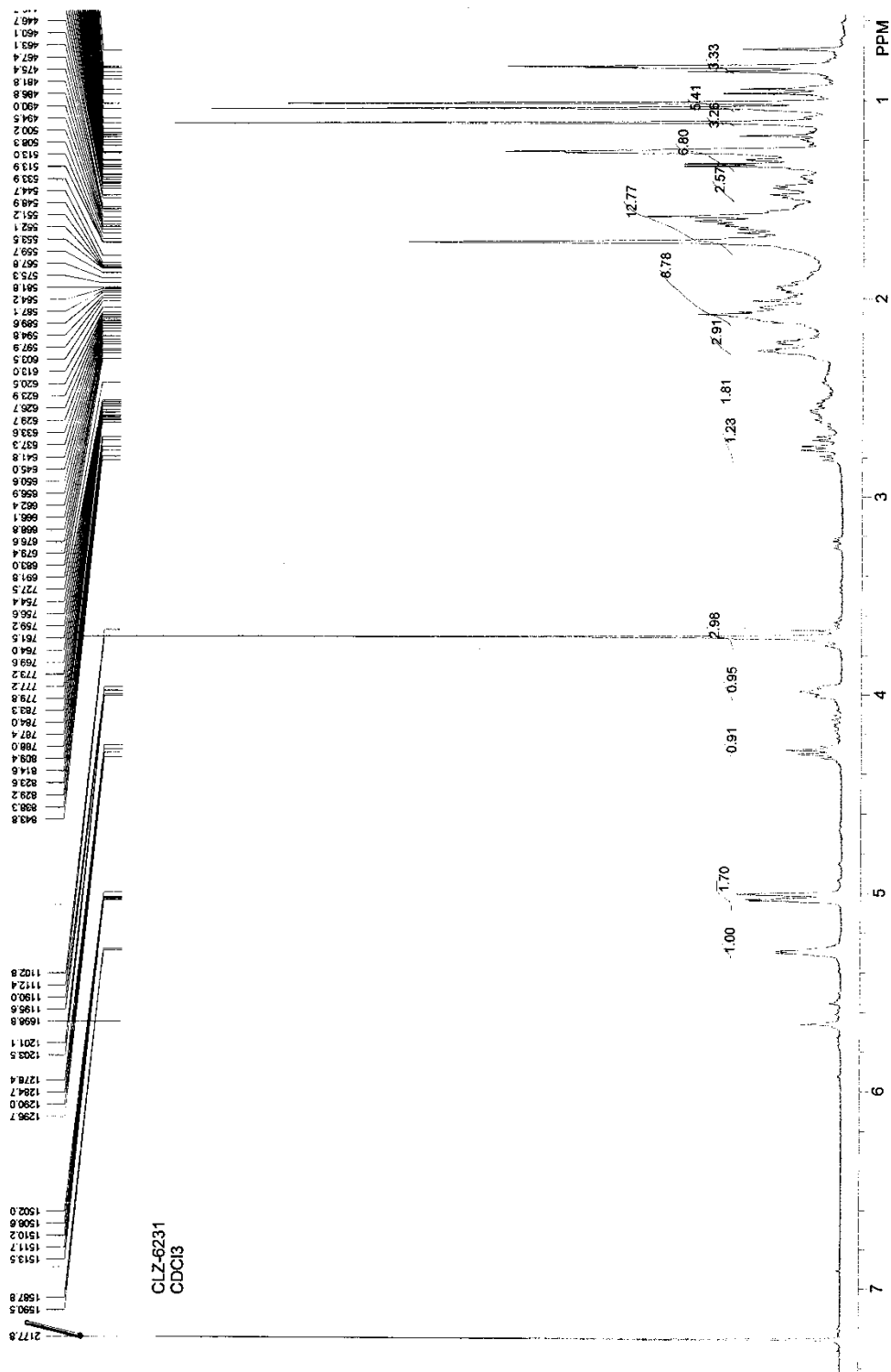
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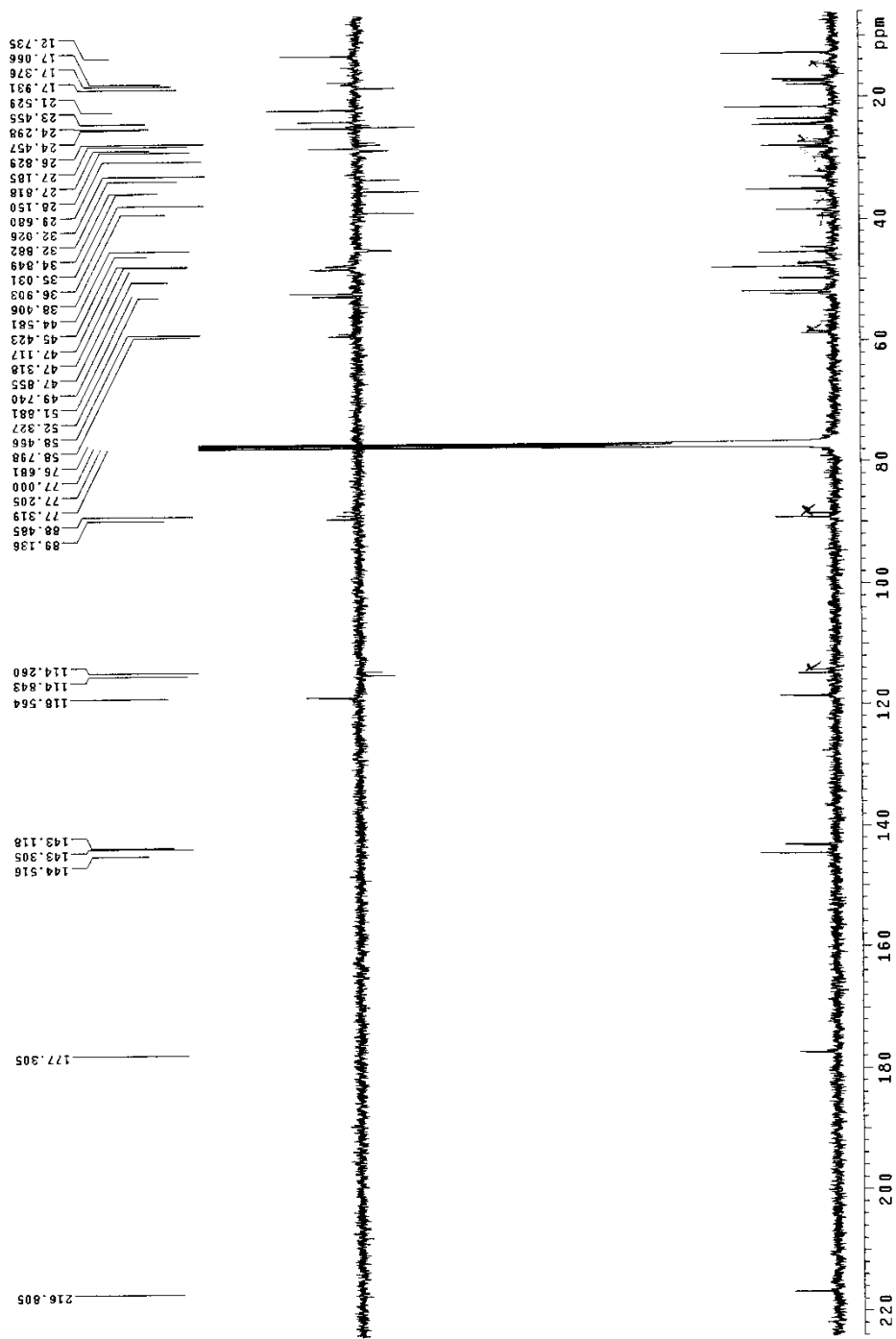
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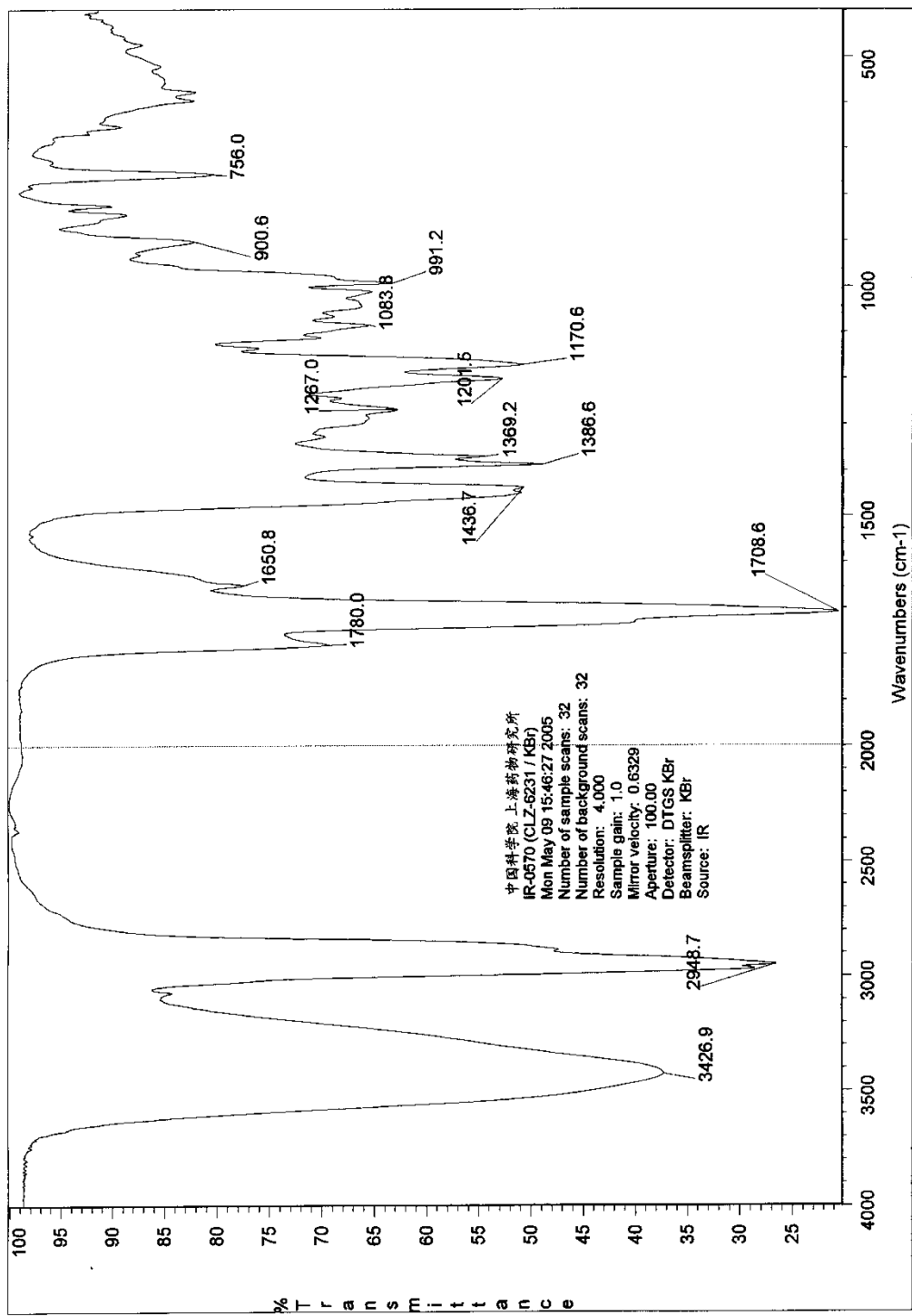


S1: ¹H NMR spectrum of Compound 1: toosendanin A

CL126-2-3-1 CDC13 88+DEPT-135 Apr 19 2005



S2: ^{13}C NMR and DEPT-135 spectra of Compound 1: toosendanin A

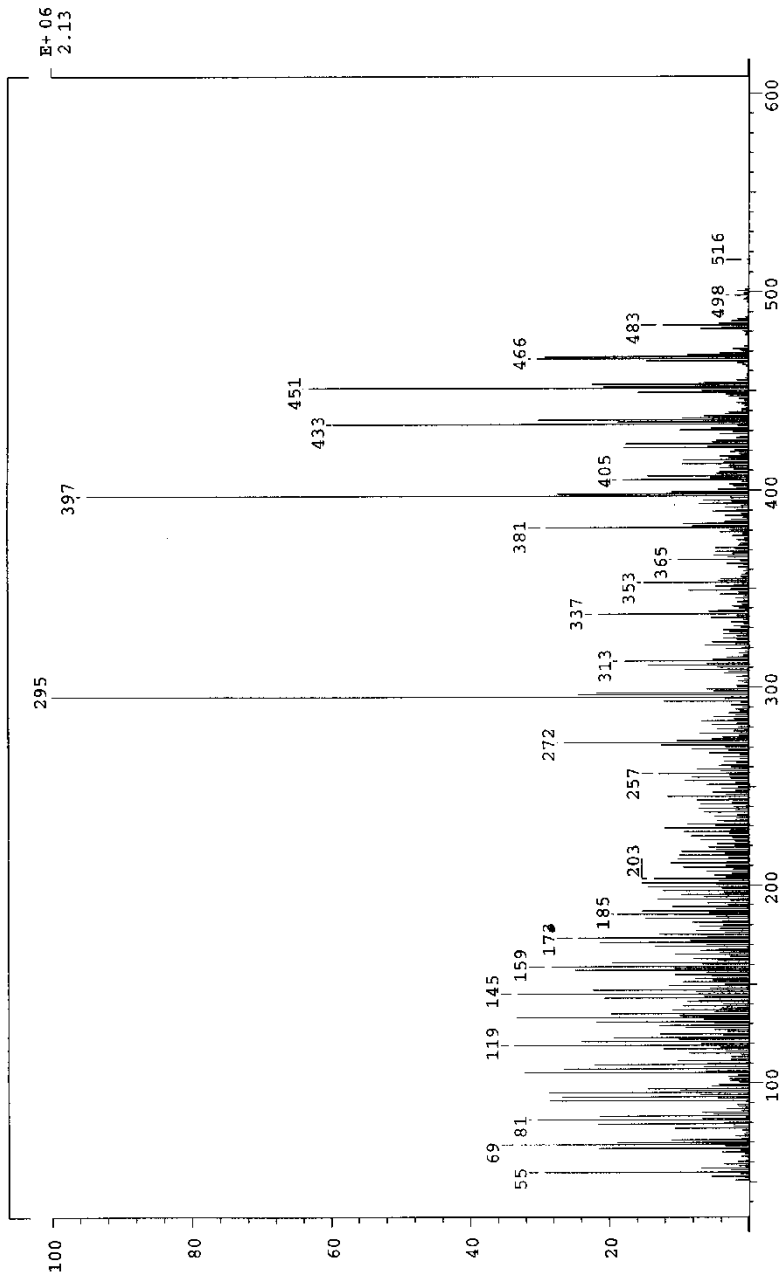


S3: IR spectrum of Compound 1: toosendanin A

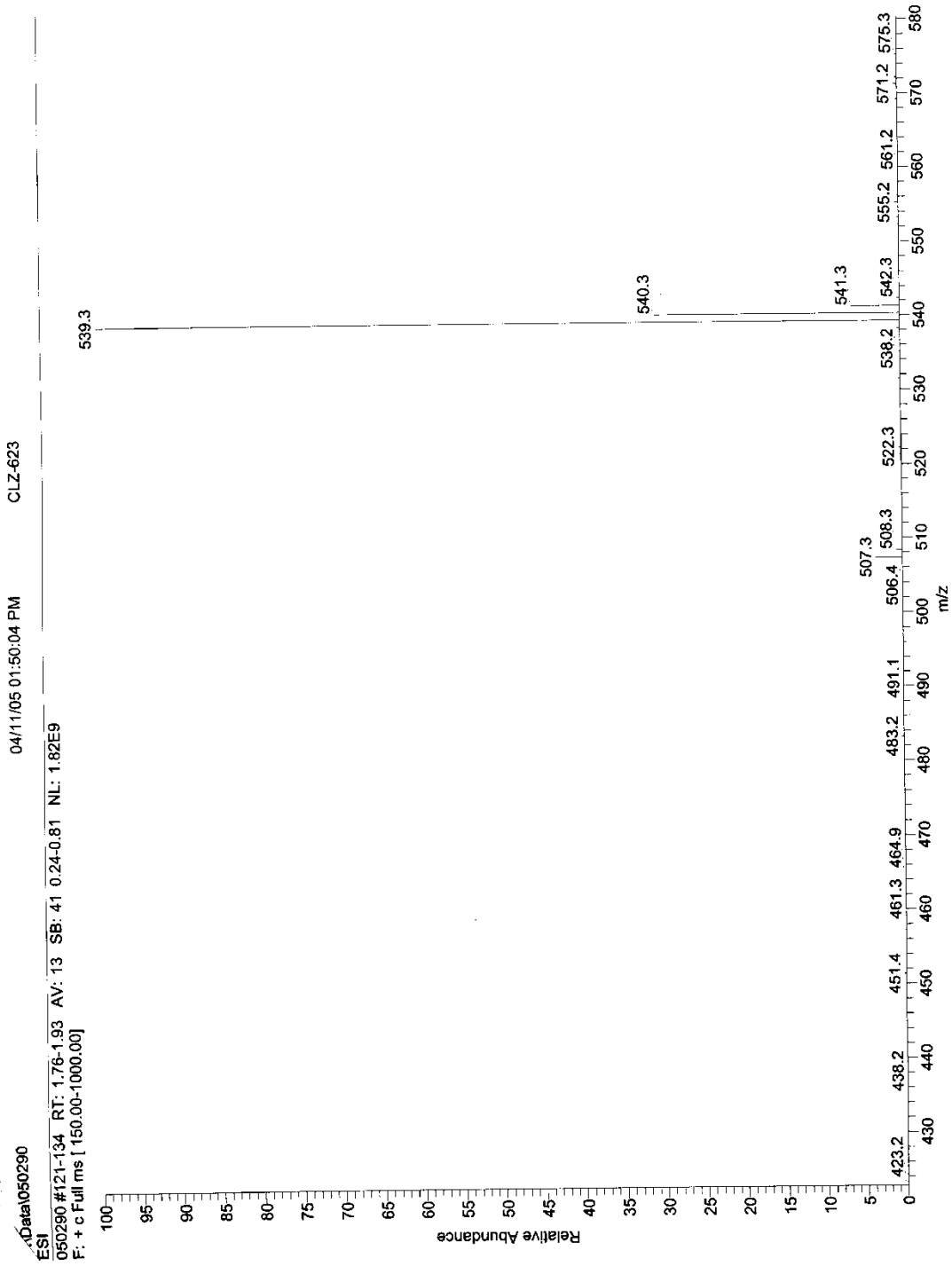
SPEC: 151372
 Samp: CLZ 6-2-3-1
 Comm: Finnigan/MAT95/70eV/Tsou:200c/R:1000
 Mode: EI +VE +LMR BSCAN (EXP) UP LR NRM
 Oper: WANG J.@SINM.CAS Client: S/N:SW01-0001
 Base: 295.2 Inten: 2129139
 Norm: 295.2 RIC : 67266501
 Peak: 1000.00 mmu

19-Apr-05 Elapse: 03:23.5 32
 Start : 16:55:08 33

Inlet :
 Masses: 50 > 750
 #peaks: 637



S4: EIMS spectrum of Compound 1: toosendanin A



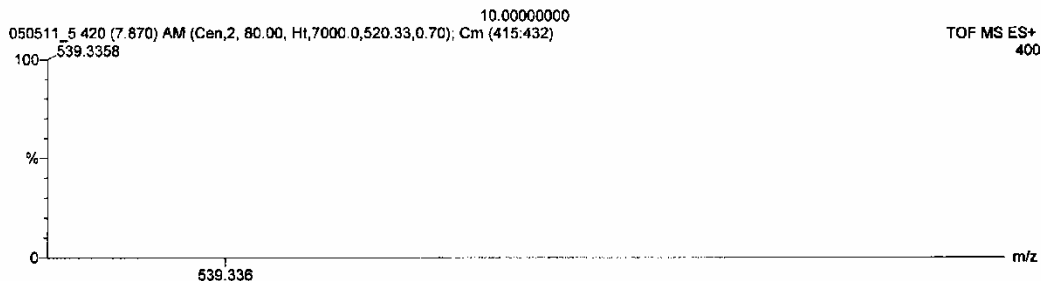
S5: ESIMS spectrum of Compound 1: toosendanin A

Elemental Composition Report

Pa

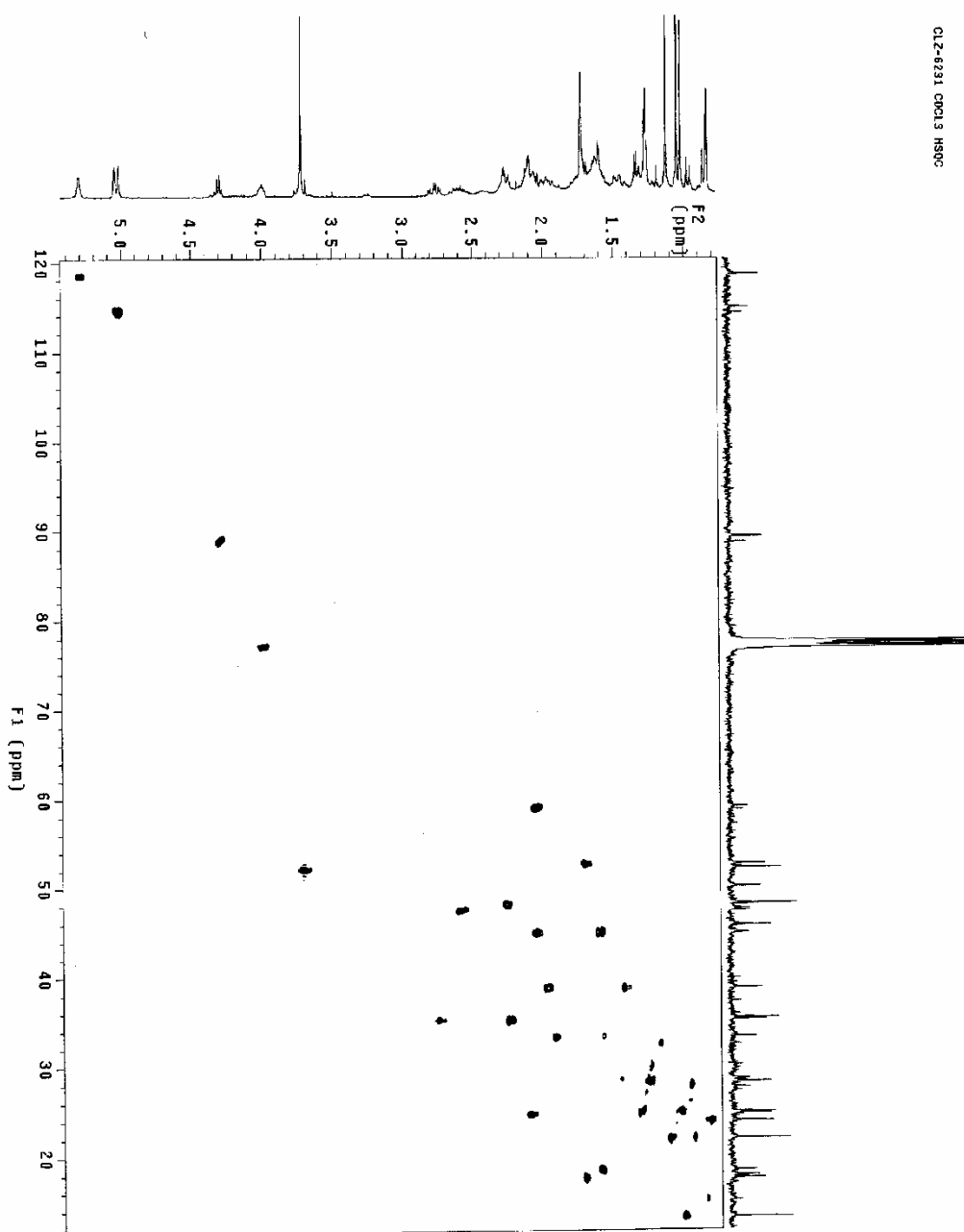
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
 12 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

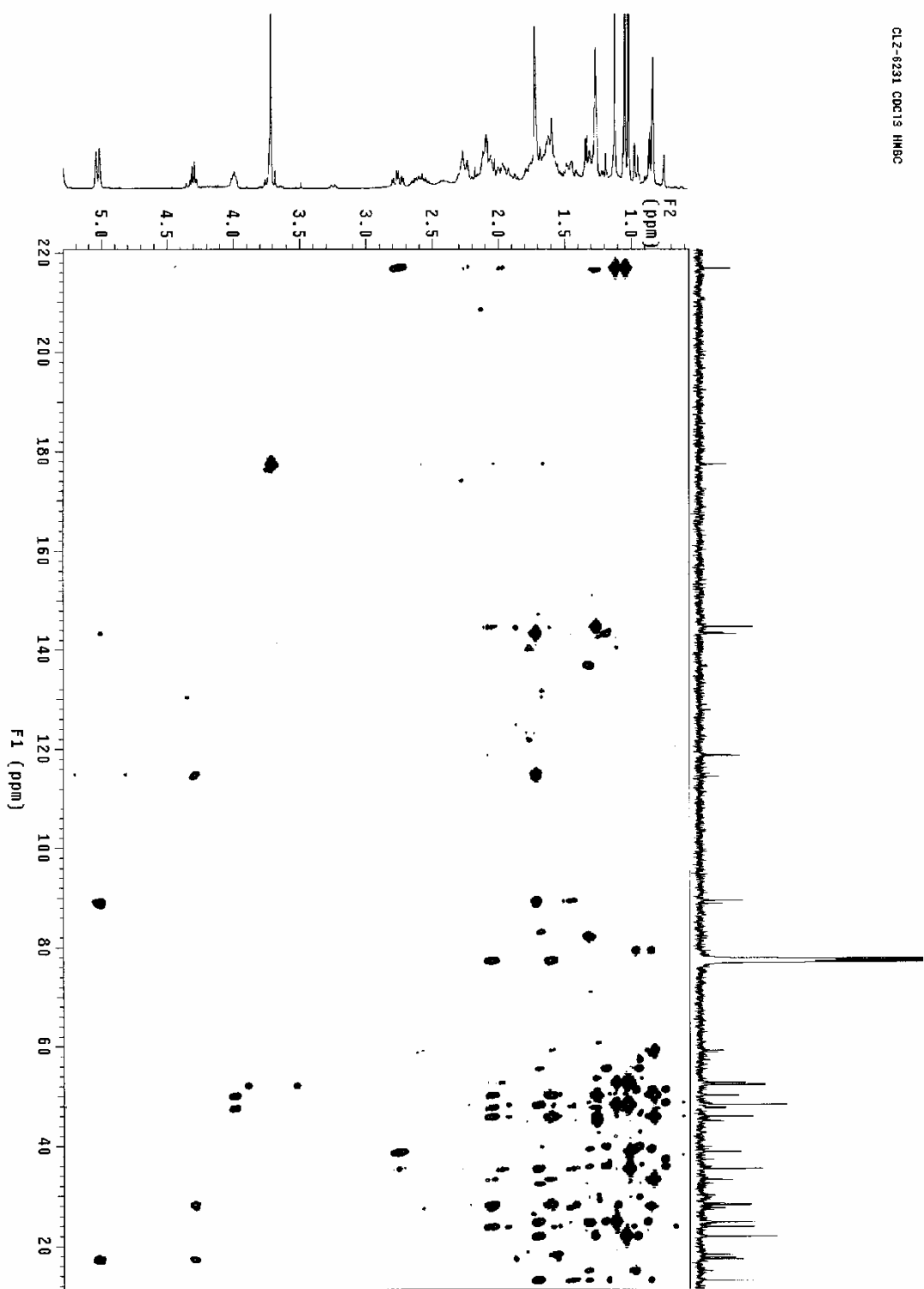


Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
539.3358	539.3349	0.9	1.7	7.5	1	C31 H48 O6 Na

S6: HRESIMS spectrum of Compound 1: toosendanin A



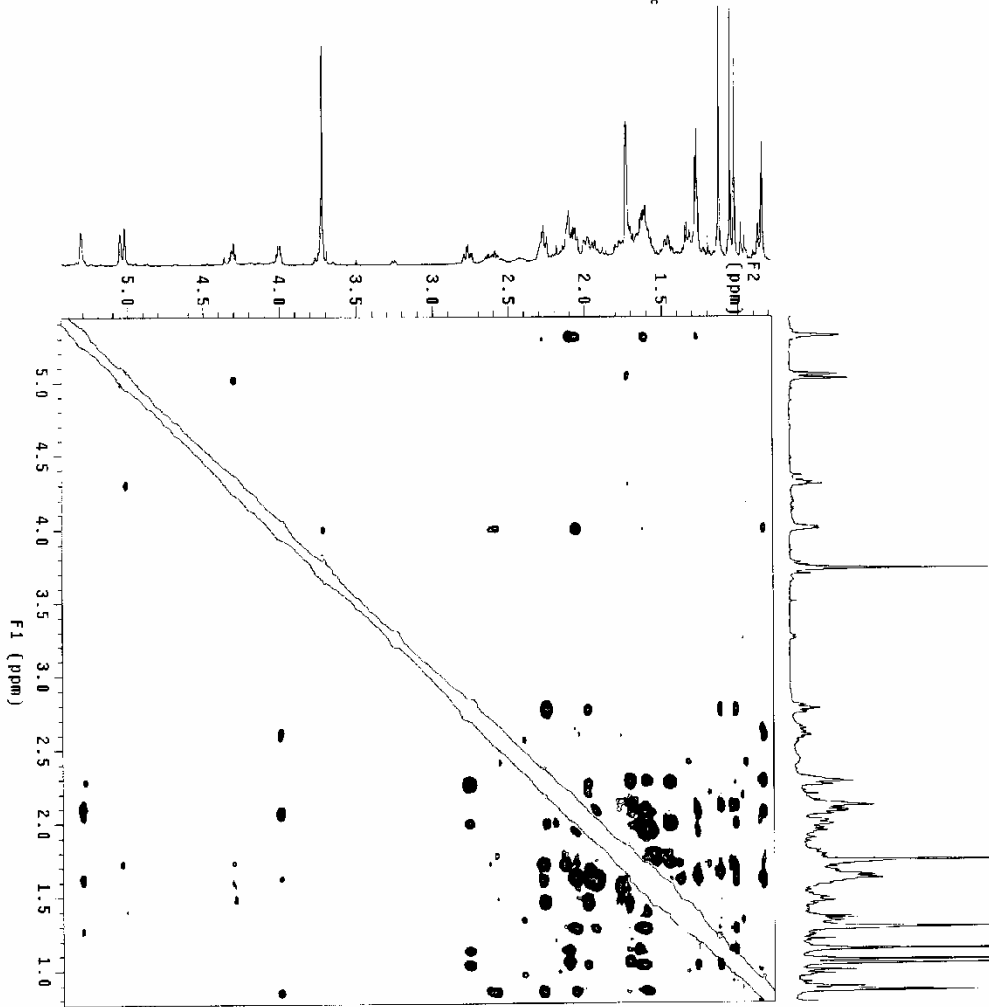
S8: HMBC spectrum of Compound **1**: toosendanin A



S9: HMBC spectrum of Compound 1: toosendanin A

CLZ-9231 CDCl3 ROESY

Solvent: CDCl3
Temperature: 300.2 K
Pulse sequence: zgpg30
F1: 400.136 MHz
F2: 400.136 MHz
Relax. delay: 1.000 sec
Mixing: 0.300 sec
Acq. time: 0.213 sec
Sweep rate: 1.000 Hz
20 Width: 8000.0 Hz
4 repetitions
2 X S12 increments
OBSERVED F1 F2
DESPICED F1 F2
F1 DATA PROCESSING
Gauss apodization: 0.056 sec
F2 apodization: 0.200 sec
Total time: 1 hr, 47 min, 50 sec



S10: ROESY spectrum of Compound 1: toosendanin A

S11: General experimental procedures

Optical rotations were taken on a Perkin-Elmer 341 polarimeter. IR spectra were recorded on Nicolet Magna FT-IR 750 spectrophotometer. ^1H NMR and ^{13}C NMR spectra were recorded on Bruker AM-400 NMR spectrometer. The chemical shift (δ) values are in ppm with TMS as internal standard, and coupling constants (J) are given in Hz. EI-MS spectra were recorded on Finnigan MAT95 spectrometer. ESI-MS and HRESI-MS spectra were recorded on Micromass Q-TOF mass spectrometer (Waters). Silica gel used for flash chromatography was produced by Qingdao Marine Chemical Industrials. TLC was carried out on GF254 pre-coated glass sheets (Yantai Jiangyou Silica Gel Development Co. Ltd.); spots were viewed at UV 254 nm and indicated by 5% sulfuric acid in alcohol containing 10mg/mL Vanillin.