

Supporting Information Available

for

**Insecticidal Cyclodepsipeptides from *Beauveria*
*felina***

*Aude Langenfeld, Alain Blond, Sabelle Gueye, Patrick Herson, Bastien Nay, Joëlle Dupont
and Soizic Prado**

Page S2-ESI-MS/MS spectra of $[M+H]^+$ of iso-isariin B (1)

Page S3- ESI-MS/MS spectra of $[M+H]^+$ of isaridin E (2)

Page S4-Table S1- Noesy diagram for Iso-isariin B (1)

Page S4-Table S2- Main chain angles for Isaridin E (2)

Page S5-Table S3- Distances O.....HN (Å) atoms bonds for Isaridin E (2)

Page S6 –Crystal data for Isaridin E (2)

Page S7 – Intensity Measurements for Isaridin E (2)

Page S8- Isaridin E (2) structure solution and refinement

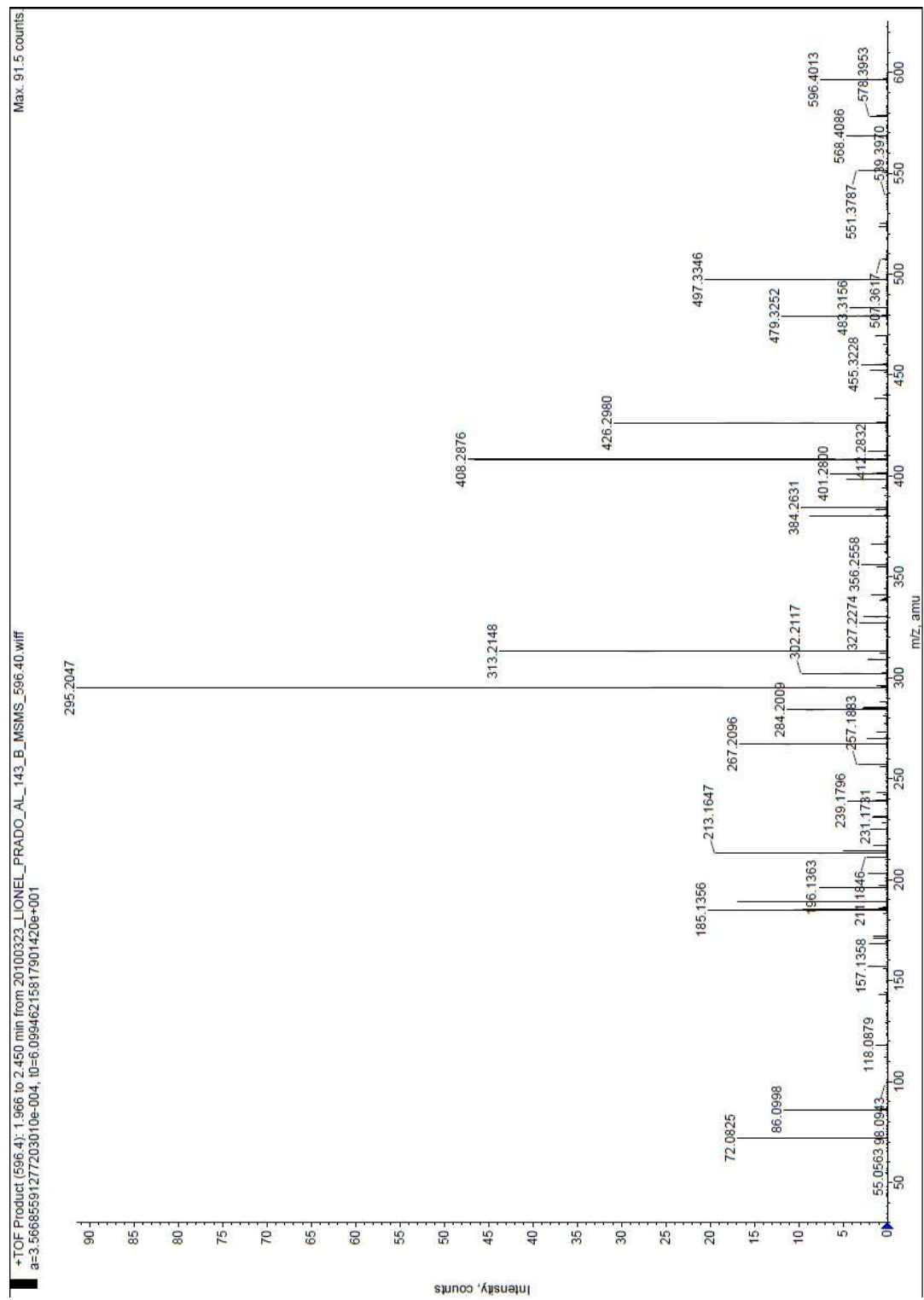
Page S9- ^1H NMR spectrum of Iso-isariin B (DMSO-*d*₆, 298 K, 400.13 MHz)

Page S10- ^{13}C NMR spectrum of Iso-isariin B (DMSO-*d*₆, 298 K, 75.04 MHz)

Page S11- ^1H NMR spectrum of Isaridin E (CDCl₃-*d*₆, 298 K, 400.13 MHz)

Page S12- ^{13}C NMR spectrum of Isaridin E (CDCl₃-*d*₆, 298 K, 75.04 MHz)

ESI-MS/MS spectrum of $[M+H]^+$ of Iso-isarinin B (1)



ESI-MS/MS spectrum of $[M+H]^+$ of Isaridin E (2)

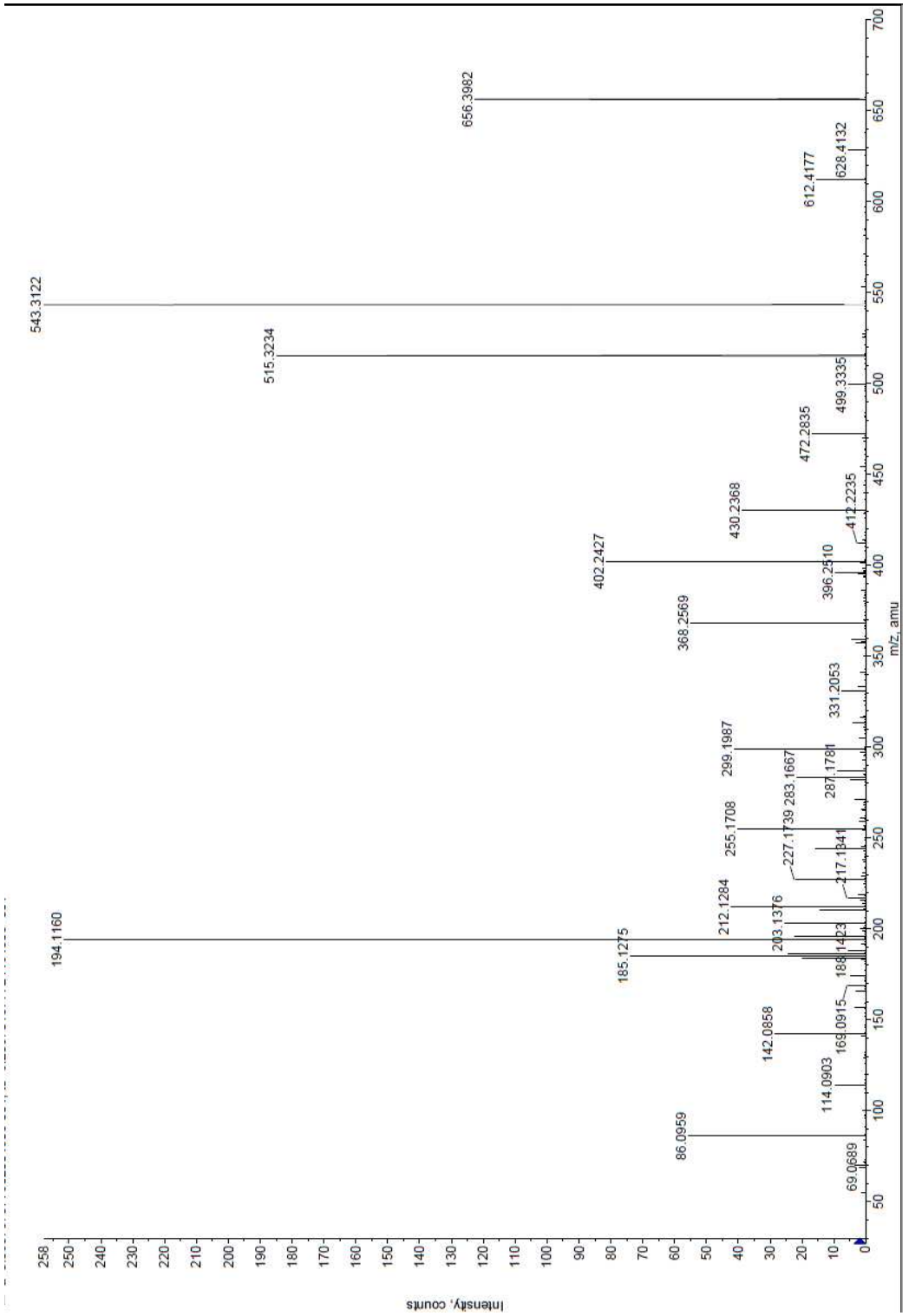


Table S1. Noesy diagram showing the distribution of the NOE correlations (weak and strong) between NH, α H, β H, the temperature coefficient of amide protons ($-\Delta\delta/\Delta T$, ppb K^{-1}) and the coupling constants ($^3J_{NHCH_\alpha}$) for Iso-isariin B (**1**) in DMSO-*d*₆ solution.²

<i>Cyclo</i>	HMA ¹	Gly ²	Val ³	Leu ⁴	Ala ⁵	Val ⁶
$d_{NN(i, i+1)}$		—————		—————	—————	—————
$d_{\alpha N(i, i+1)}$	—————	—————	—————	—————	—————	—————
$d_{\beta N(i, i+1)}$	—————			—————	—————	
$d_{\beta N(i, i+2)}$	—————	—————				
$-\Delta\delta/\Delta T$		4	5.6	6.6	3.4	0.8
$^3J_{NHCH_\alpha}$		3.8 ; 6.7	7.6	6.5	7.9	7.7

Table S2. Main chain angles in degrees for Isaridin E (**2**)

Residue	ϕ (°)	ψ (°)	ω (°)
HyLeu ¹	62.7	-149.8	-4.9
Pro ²	80.8	5.5	-178.2
Phe ³	66.0	-155.4	174.7
NMeVal ⁴	110.2	-99.4	-0.2
NMeVal ⁵	122	-110.7	-173.5
β -Ala ⁶	130.3	58.9	-140.3

Table S3. Distances O.....HN (Å) atoms bonds for Isaridin E (2)

N/O	HyLeu ¹	Pro ²	Phe ³	N-Me-Val ⁴	N-Me-Val ⁵	β-Ala ⁶
HyLeu ¹	-	-	-	-	-	-
Pro ²	2.26	-	4.62	9.10	8.38	3.42
Phe ³	3.50	2.99	-	6.96	6.64	2.19
N-Me-Val ⁴	-	-	-	-	-	-
N-Me-Val ⁵	-	-	-	-	-	-
β-Ala ⁶	5.47	5.21	2.08	4.96	2.99	-

Crystal data for Isaridin E (2)

Formula : $C_{37}H_{56}N_6O_7$

Crystal Class : monoclinic

Space Group : P 21

a = 13.0206(5)

b = 9.8032(7)

c = 15.4303(15)

alpha = 90

beta = 94.550(6)

gamma = 90

Volume = 1963.4(2)

Z value : 2

Intensity Measurements for Isaridin E (2)

Radiation type : Mo K α

Wavelength : 0.710730

ρ = 1.18

μ = 0.082

Mr = 696.89

Temperature (K) : 200

Size : 0.08x 0.11x 0.25

Colour : colourless

Shape : block

Cell from : 109 Reflections

Theta range : 3 to 21

Diffractometer type : KAPPACCD

Scan type : PHIOMEGA

Absorption type : multi-scan

Transmission range : 0.99 0.99

Reflections measured 20570

Independent reflections :6006

Theta max : 30.00

Hmin, Hmax : -18 17

Kmin, Kmax : -13 13

Lmin, Lmax : -21 20

Isaridin E (2) Structure solution and refinement

R[I>2 σ (I)] 0.052

WR2(all) 0.144

Max shift/su 0.0036

Delta Rho min -0.45

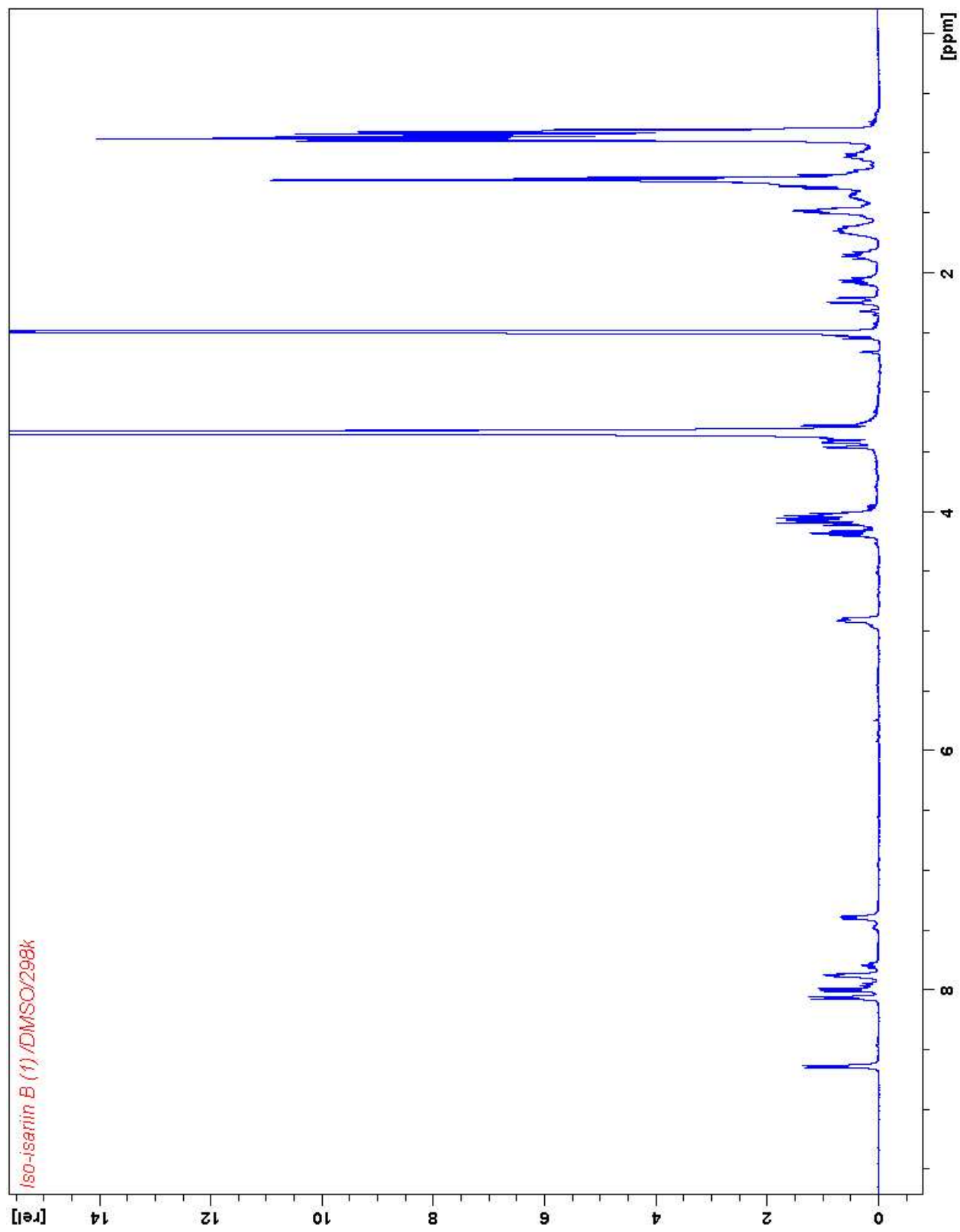
Delta Rho max : 0.47

Reflections used : 6003

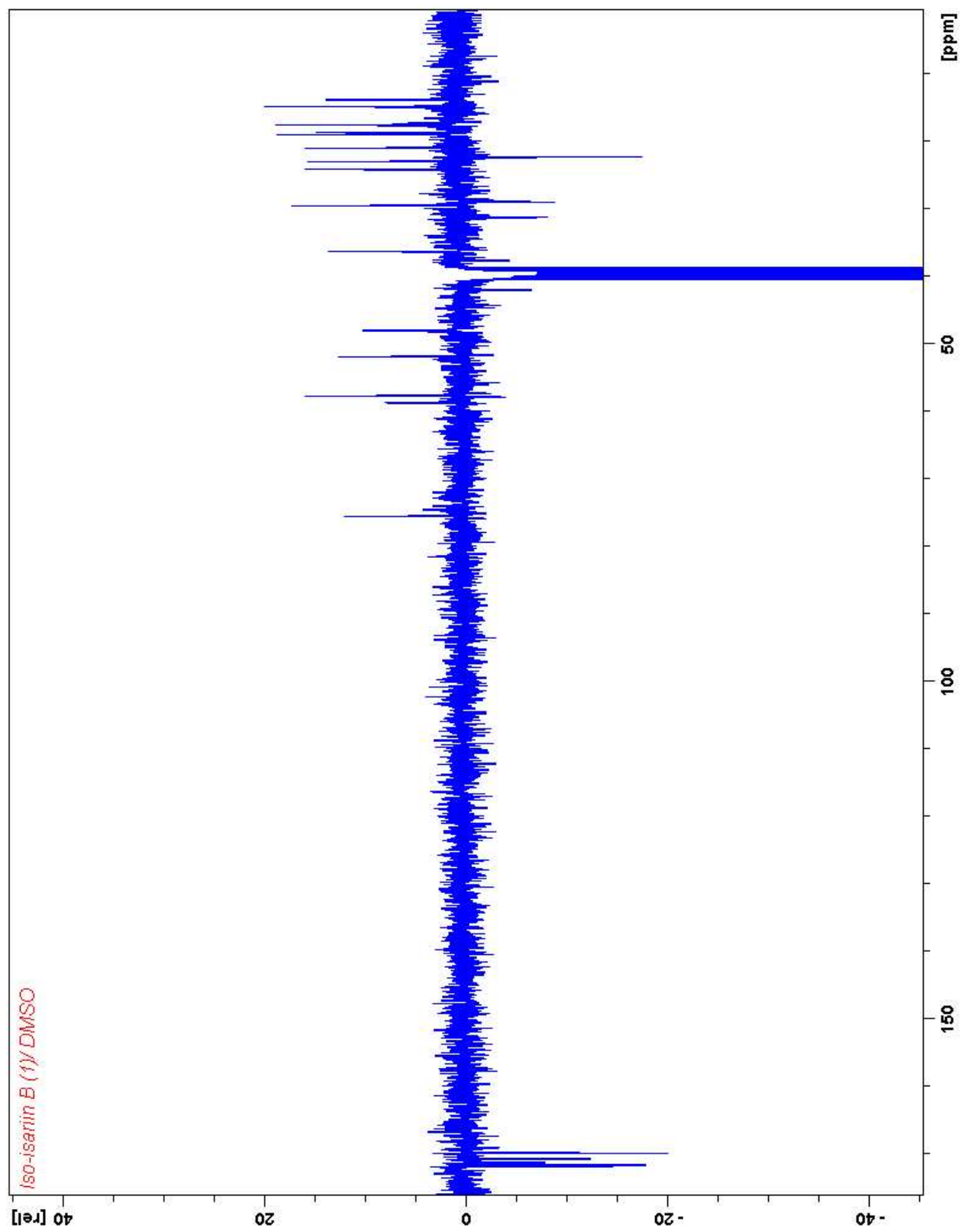
Number of parameters : 452

Goodness of fit : 0.953

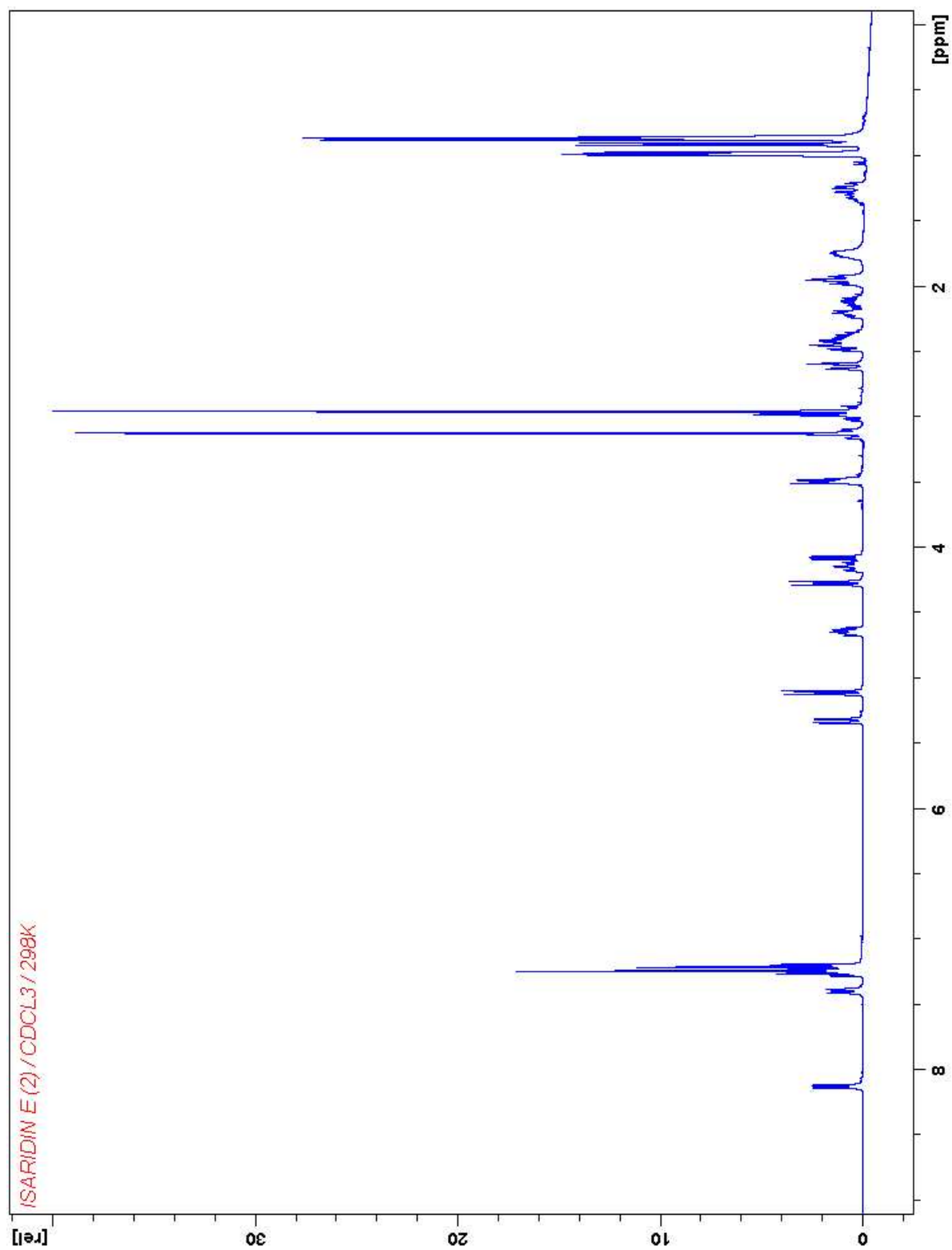
¹H NMR spectrum of Iso-isartirin B (DMSO-*d*₆, 298 K, 400.13 MHz)



^{13}C NMR spectrum of Iso-isariin B (DMSO-*d*₆, 298 K, 75.04 MHz)



¹H NMR spectrum of Isaridin E (DMSO-*d*₆, 298 K, 400.13 MHz)



^{13}C NMR spectrum of Isaridin E (DMSO-*d*₆, 298 K, 75.04 MHz)

