Supporting Information

Agladupols A-E, Triterpenoids from *Aglaia duperreana*

Bo-Jun Xie, Sheng-Ping Yang, Hua-Dong Chen and Jian-Min Yue*

State Key Laboratory of Drug Research, Institute of Materia Medica, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, 555 Zu Chong Zhi Road, Zhangjiang Hi-Tech Park, Shanghai, 201203, P. R. China

Figure S3. Selected HMBC (H→C) and ROESY (↔) correlations for agladupol A (**1**).

Figure S4. Selected HMBC (H→C) and ROESY (↔) correlations for agladupol B (**2**).

Figure S5. Selected HMBC (H→C) and ROESY (↔) correlations for agladupol C (**3**).

Figure S6. Selected HMBC (H→C) and ROESY (↔) correlations for agladupol D (**4**).

Figure S7. Coefficients between agladupol D (**4**) and sapelin A.

Figure S8. ^{1}H NMR spectrum of agladupol A (**1**) in $CDCl_3$.

Figure S9. ^{13}C NMR spectrum of agladupol A (**1**) in $CDCl_3$.

Figure S10. ESIMS spectrum of agladupol A (**1**).

Figure S11. IR spectrum of agladupol A (**1**).

Figure S12. HSQC spectrum of agladupol A (**1**) in $CDCl_3$.

Figure S13. HMBC spectrum of agladupol A (**1**) in $CDCl_3$.

Figure S14. ROESY spectrum of agladupol A (**1**) in $CDCl_3$.

Figure S15. ^{1}H NMR spectrum of agladupol B (**2**) in $CDCl_3$.

Figure S16. ^{13}C NMR spectrum of agladupol B (**2**) in $CDCl_3$.

Figure S17. ESIMS spectrum of agladupol B (**2**).

Figure S18. IR spectrum of agladupol B (**2**).

Figure S19. HSQC spectrum of agladupol B (**2**) in $CDCl_3$.

Figure S20. HMBC spectrum of agladupol B (**2**) in $CDCl_3$.

* Corresponding author. Tel.: +86-21-50806718, Fax: +86-21-50806718, E-mail: jmyue@mail.shcnc.ac.cn

Figure S21. ROESY spectrum of agladupol B (**2**) in $CDCl_3$.

Figure S22. ^{1}H NMR spectrum of agladupol C (**3**) in $CDCl_3$.

Figure S23. ^{13}C NMR spectrum of agladupol C (**3**) in $CDCl_3$.

Figure S24. ESIMS spectrum of agladupol C (**3**).

Figure S25. IR spectrum of agladupol C (**3**).

Figure S26. HSQC spectrum of agladupol C (**3**) in $CDCl_3$.

Figure S27. HMBC spectrum of agladupol C (**3**) in $CDCl_3$.

Figure S28. ROESY spectrum of agladupol C (**3**) in $CDCl_3$.

Figure S29. ^{1}H NMR spectrum of agladupol D (**4**) in $CDCl_3$.

Figure S30. ^{13}C NMR spectrum of agladupol D (**4**) in $CDCl_3$.

Figure S31. EIMS spectrum of agladupol D (**4**).

Figure S32. IR spectrum of agladupol D (**4**).

Figure S33. HSQC spectrum of agladupol D (**4**) in $CDCl_3$.

Figure S34. HMBC spectrum of agladupol D (**4**) in $CDCl_3$.

Figure S35. ROESY spectrum of agladupol D (**4**) in $CDCl_3$.

Figure S36. ^{1}H NMR spectrum of agladupol E (**5**) in $CDCl_3$.

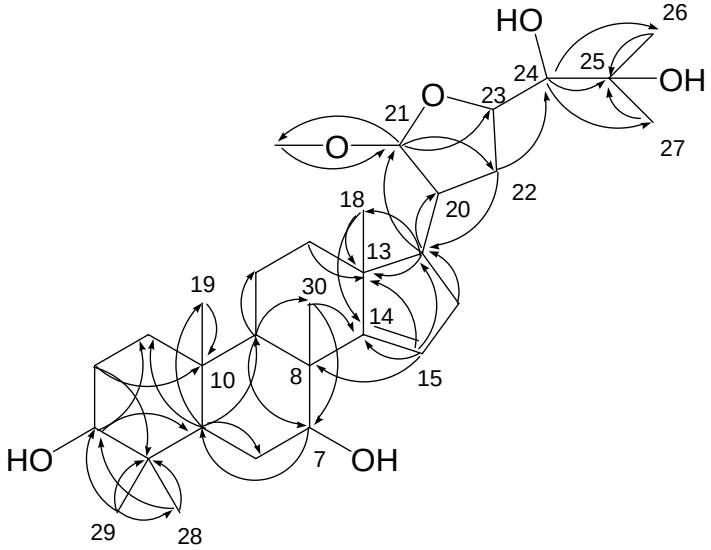
Figure S37. ^{13}C NMR spectrum of agladupol E (**5**) in $CDCl_3$.

Figure S38. EIMS spectrum of agladupol E (**5**).

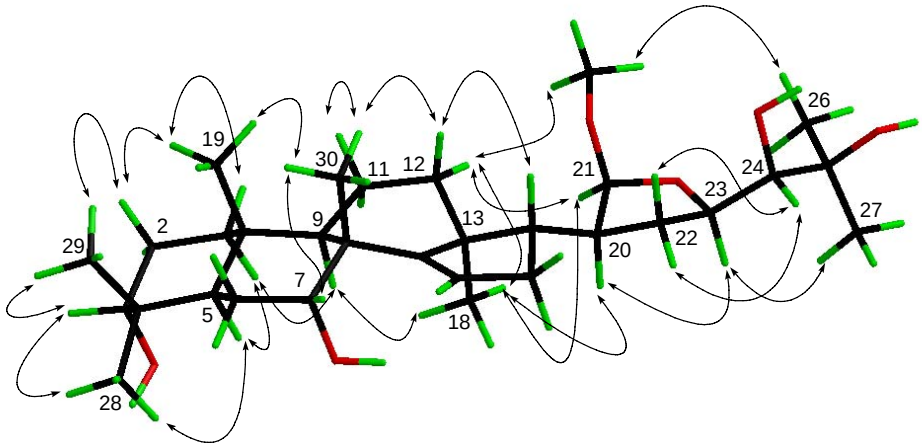
Figure S39. IR spectrum of agladupol E (**5**).

Figure S40. HSQC spectrum of agladupol E (**5**) in $CDCl_3$.

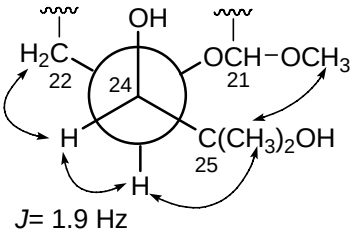
Figure S3. Selected HMBC (H→C) and ROESY (↔) correlations for agladupol A (**1**).



Selected HMBC (H→C) correlations for **1**

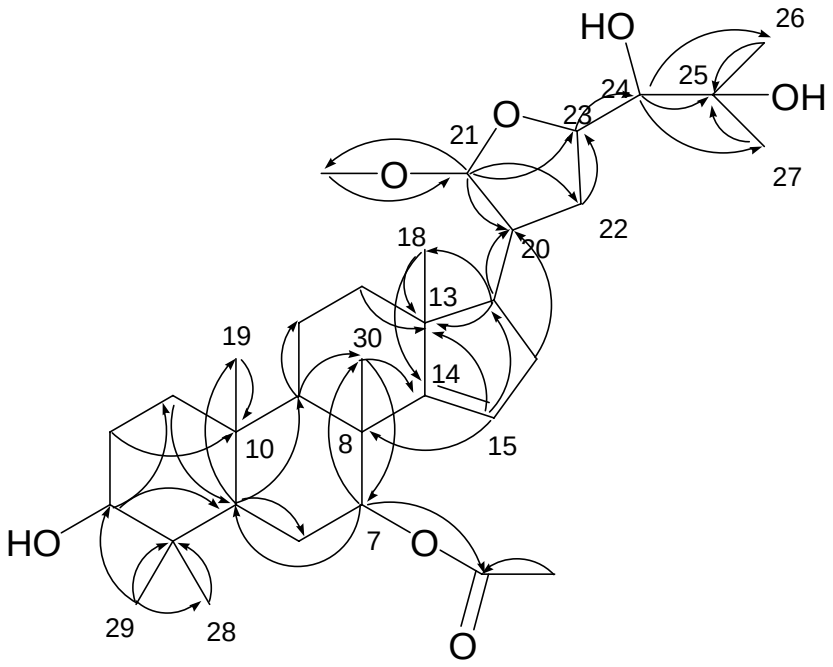


Key ROESY correlations (↔) for **1**

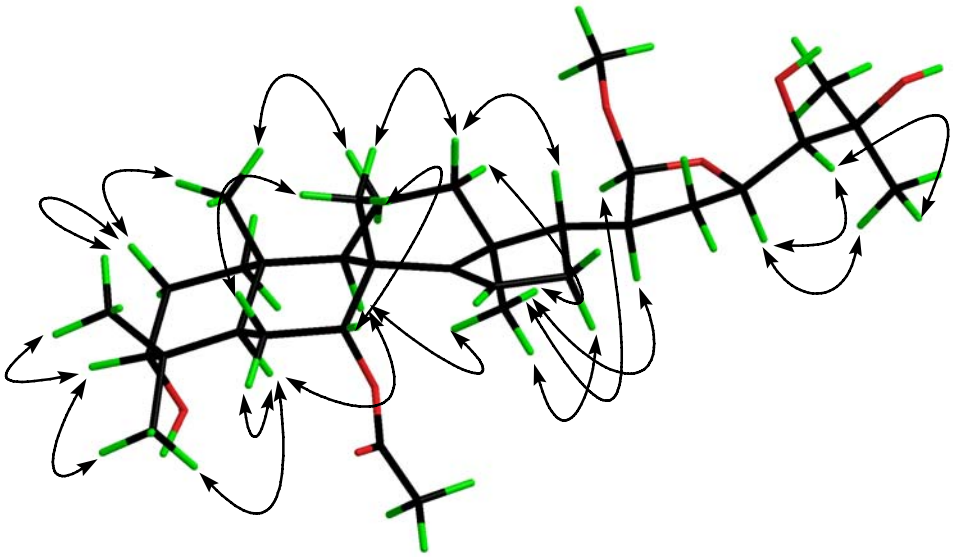


Newman projection around C-24 and C-23 for **1**; ROESY correlations (↔)

Figure S4. Selected HMBC (H→C) and ROESY (↔) correlations for agladupol B (**2**).

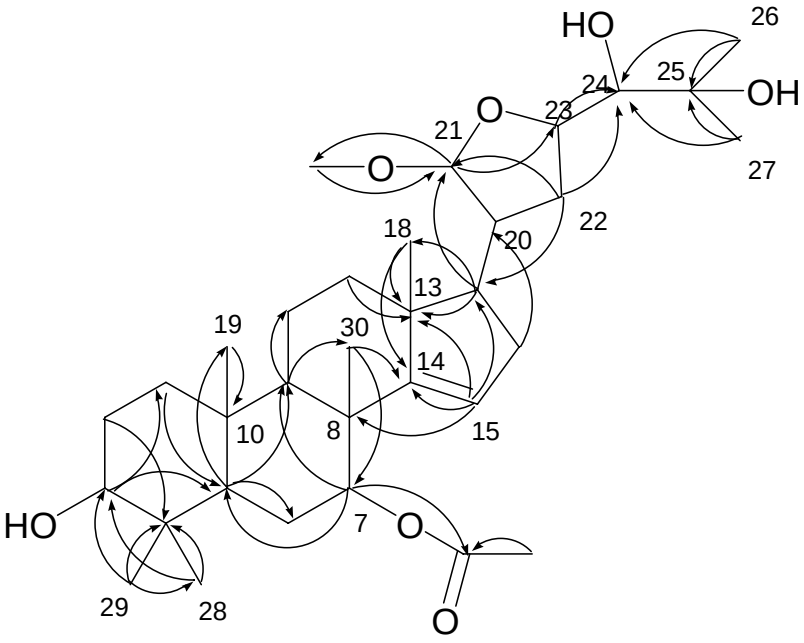


Selected HMBC (H→C) correlations of **2**

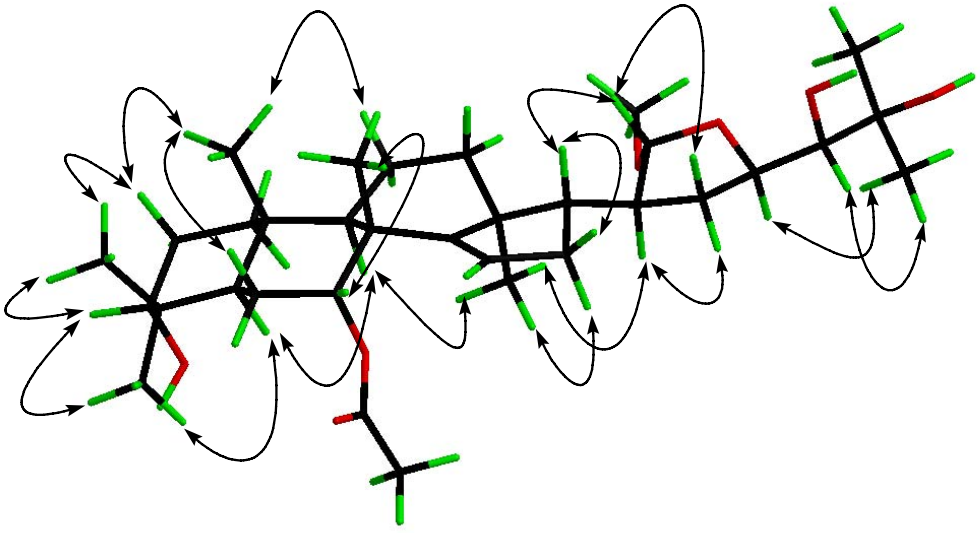


Key ROESY correlations (↔) of **2**

Figure S5. Selected HMBC (H→C) and ROESY (↔) correlations for agladupol C (**3**).

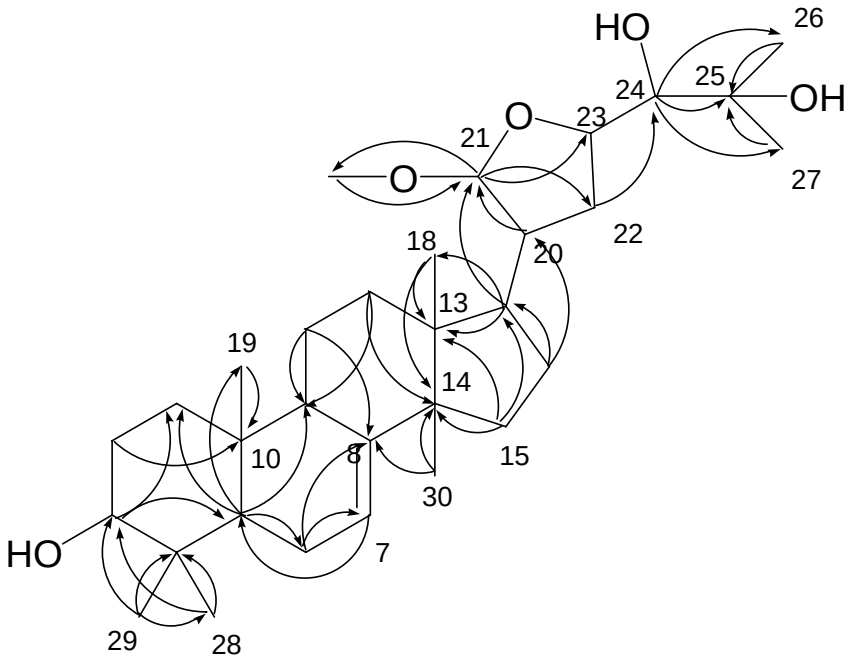


Selected HMBC (H→C) correlations of **3**

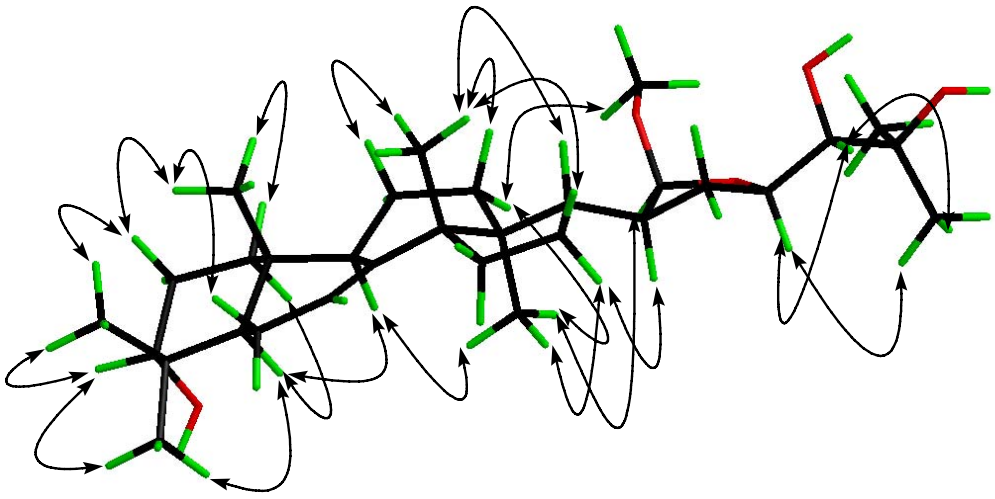


Key ROESY correlations (↔) of **3**

Figure S6. Selected HMBC (H→C) and ROESY (↔) correlations for agladupol D (**4**).

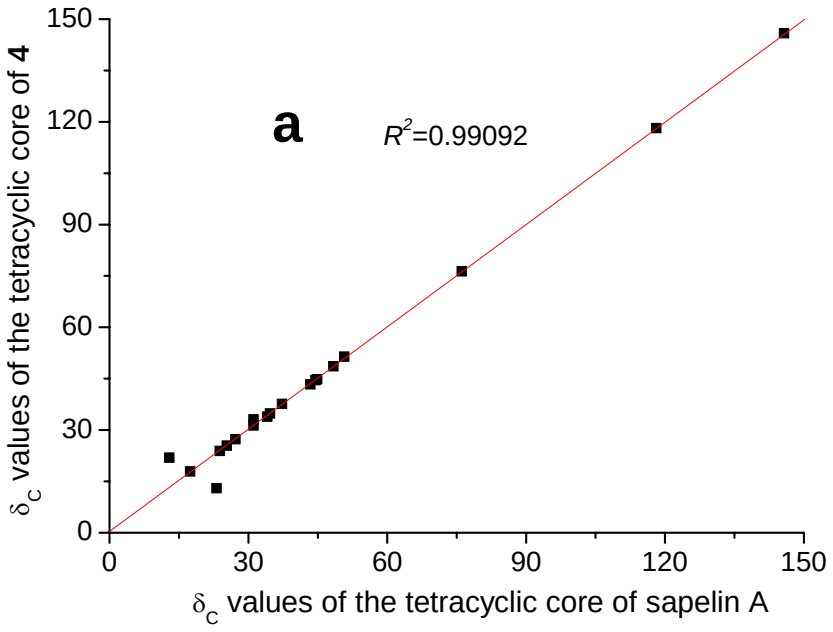


Selected HMBC (H→C) correlations of **4**

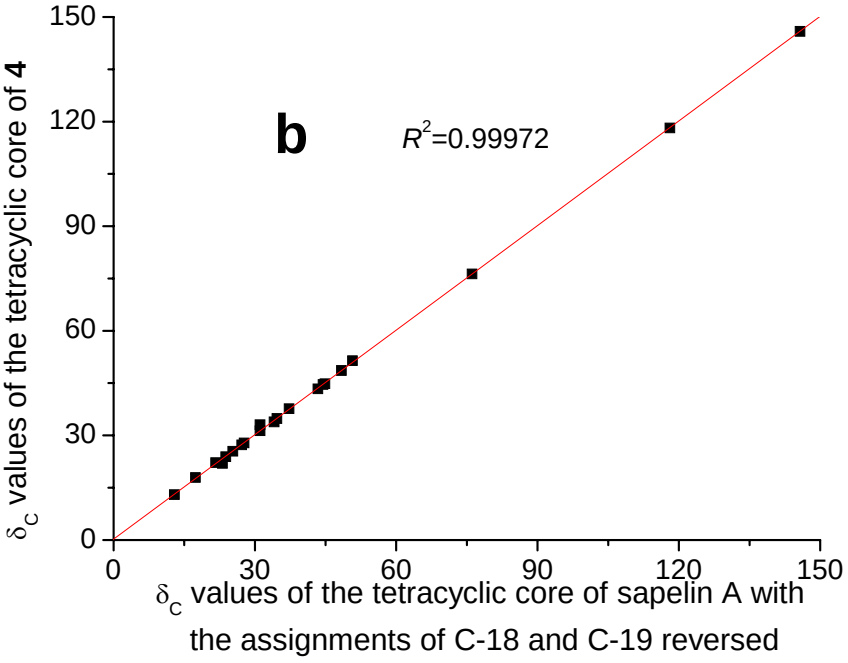


Key ROESY correlations (↔) of **4**

Figure S7. Coefficients between agladupol D (**4**) and sapelin A



a) ^{13}C NMR data of the tetracyclic core of **4** vs those of sapelin A



b) ^{13}C NMR data of the tetracyclic core of **4** vs those of sapelin A with the assignments of C-18 and C-19 reversed

Figure S8. ^{1}H NMR spectrum of agladupol A (**1**) in $CDCl_3$.

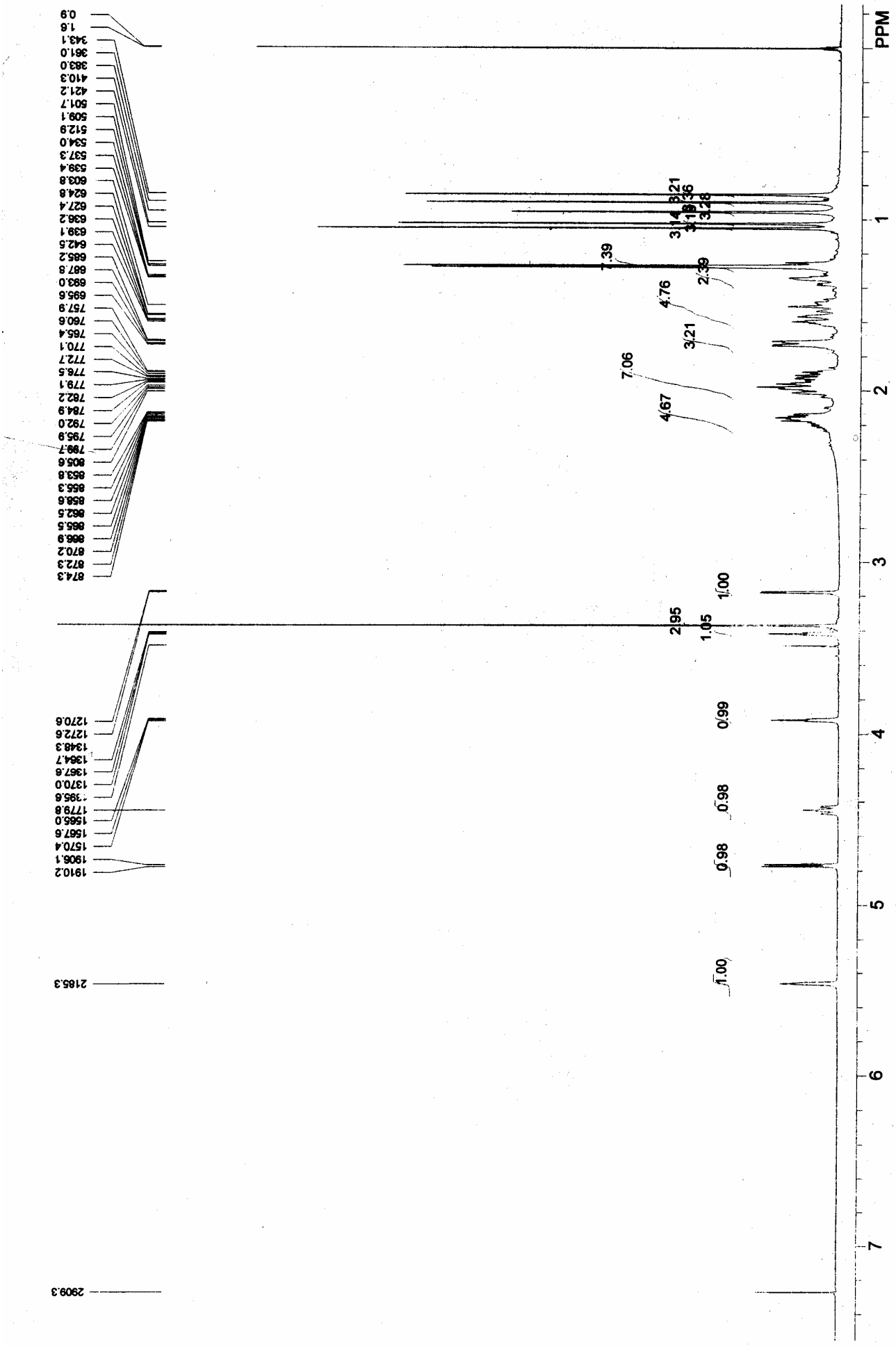


Figure S9. ^{13}C NMR spectrum of agladupol A (**1**) in $CDCl_3$.

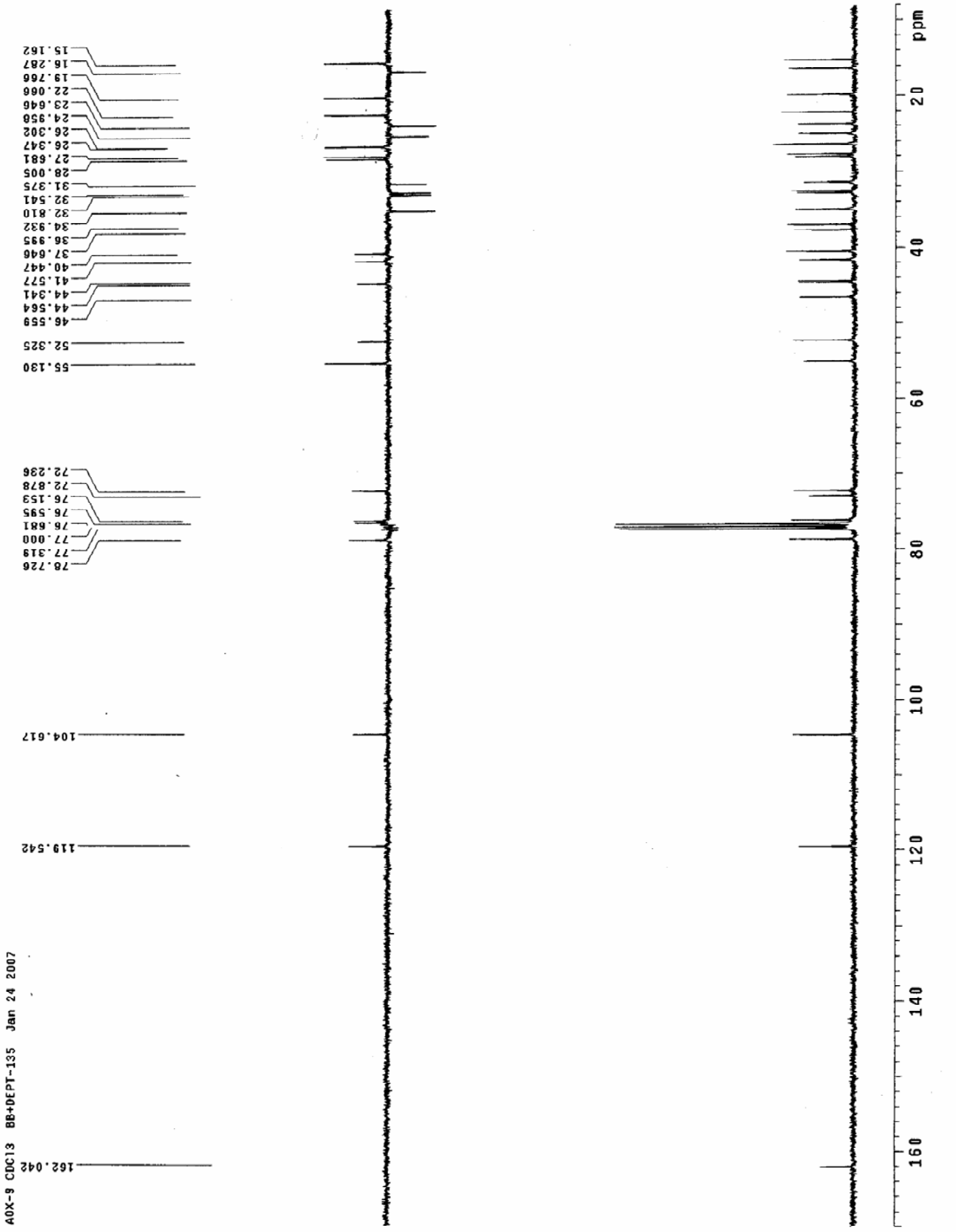


Figure S10. ESIMS spectrum of agladupol A (**1**).

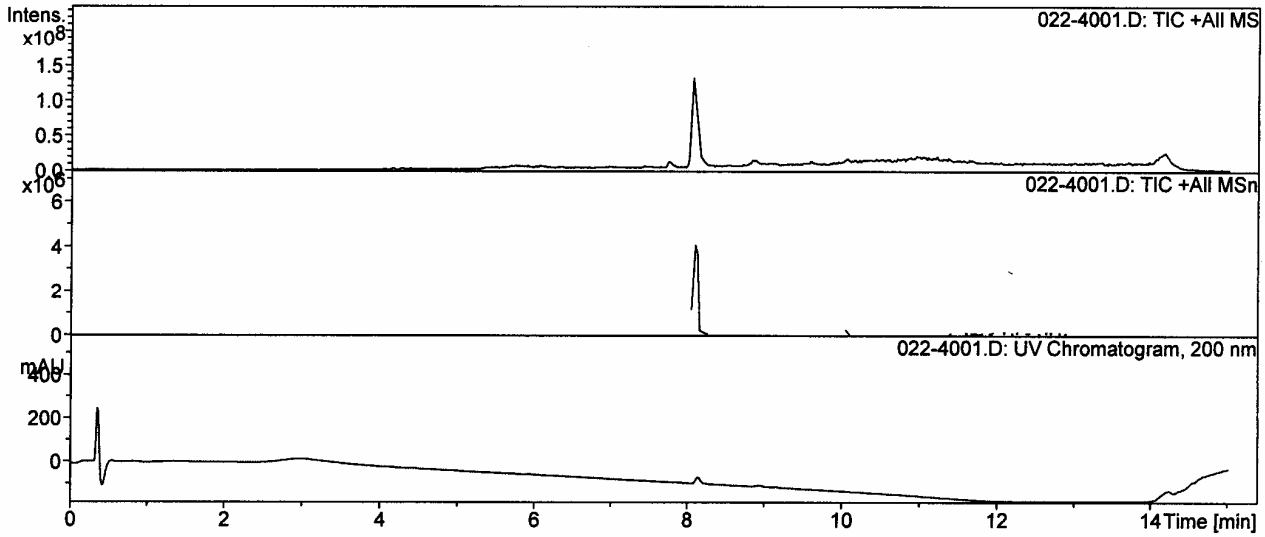
Display Report

Analysis Info

Analysis Name	022-4001.D	Acquisition Date	01/29/07 19:21:30
Method	Copy of SOPMSMSP.M	Operator	Administrator
Sample Name	yjm-AOX-9	Instrument	esquire3000plus
Comment	?		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Std/Normal	Scan Begin	100 m/z	Scan End	1750 m/z
Capillary Exit	158.5 Volt	Skim 1	40.0 Volt	Trap Drive	85.4
Accumulation Time	5414 鑹	Averages	3 Spectra	Auto MS/MS	on



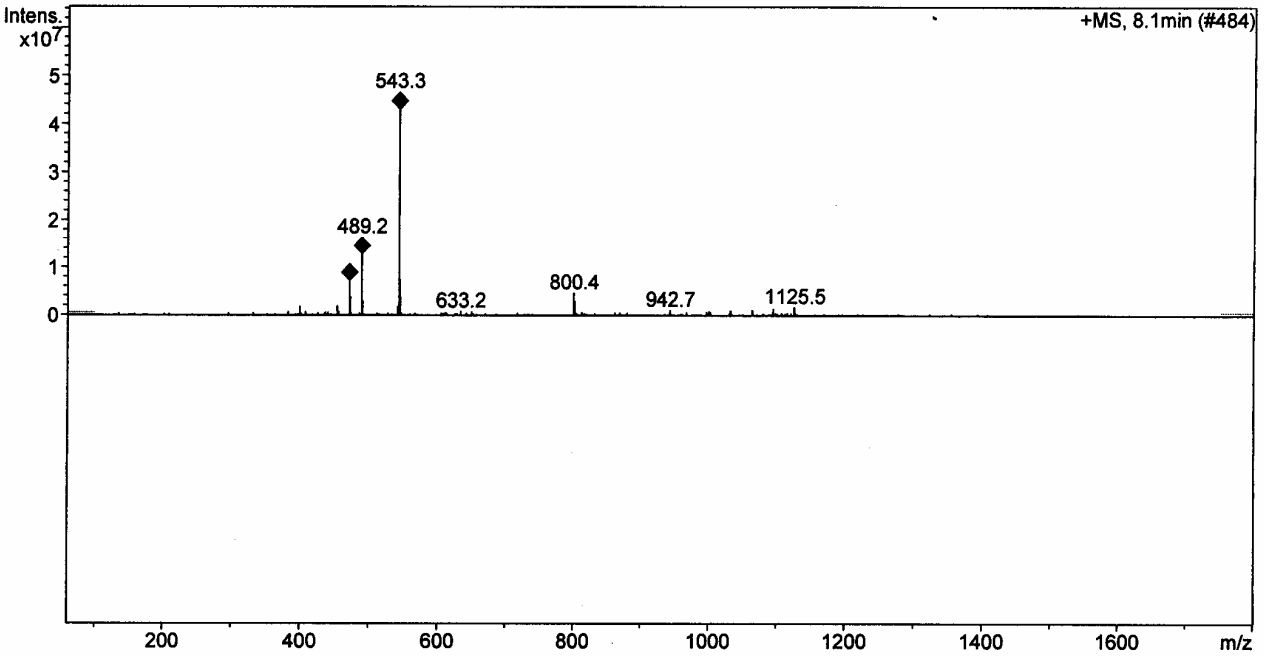


Figure S11. IR spectrum of agladupol A (**1**).

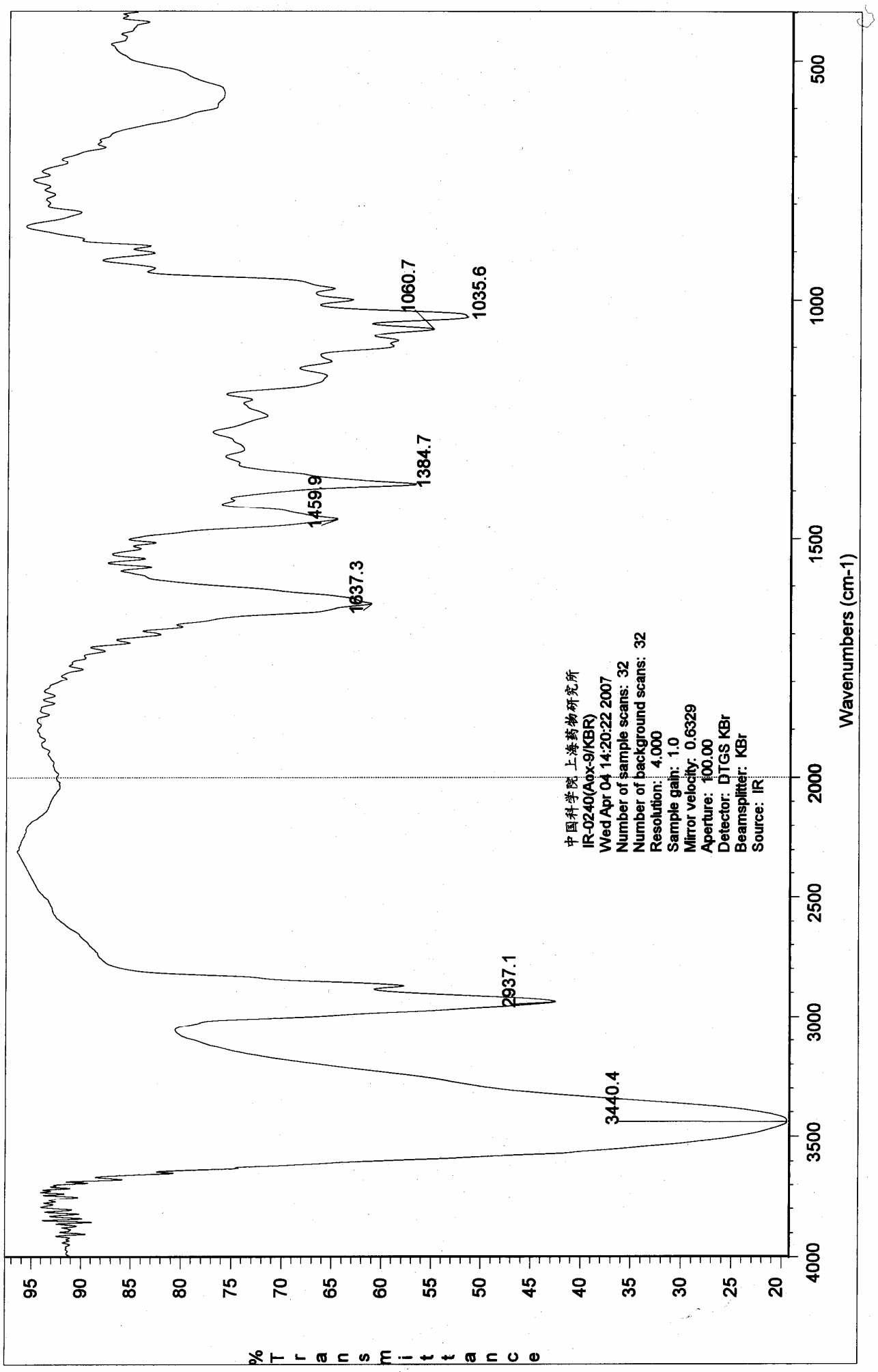


Figure S12. HSQC spectrum of agladupol A (**1**) in $CDCl_3$.

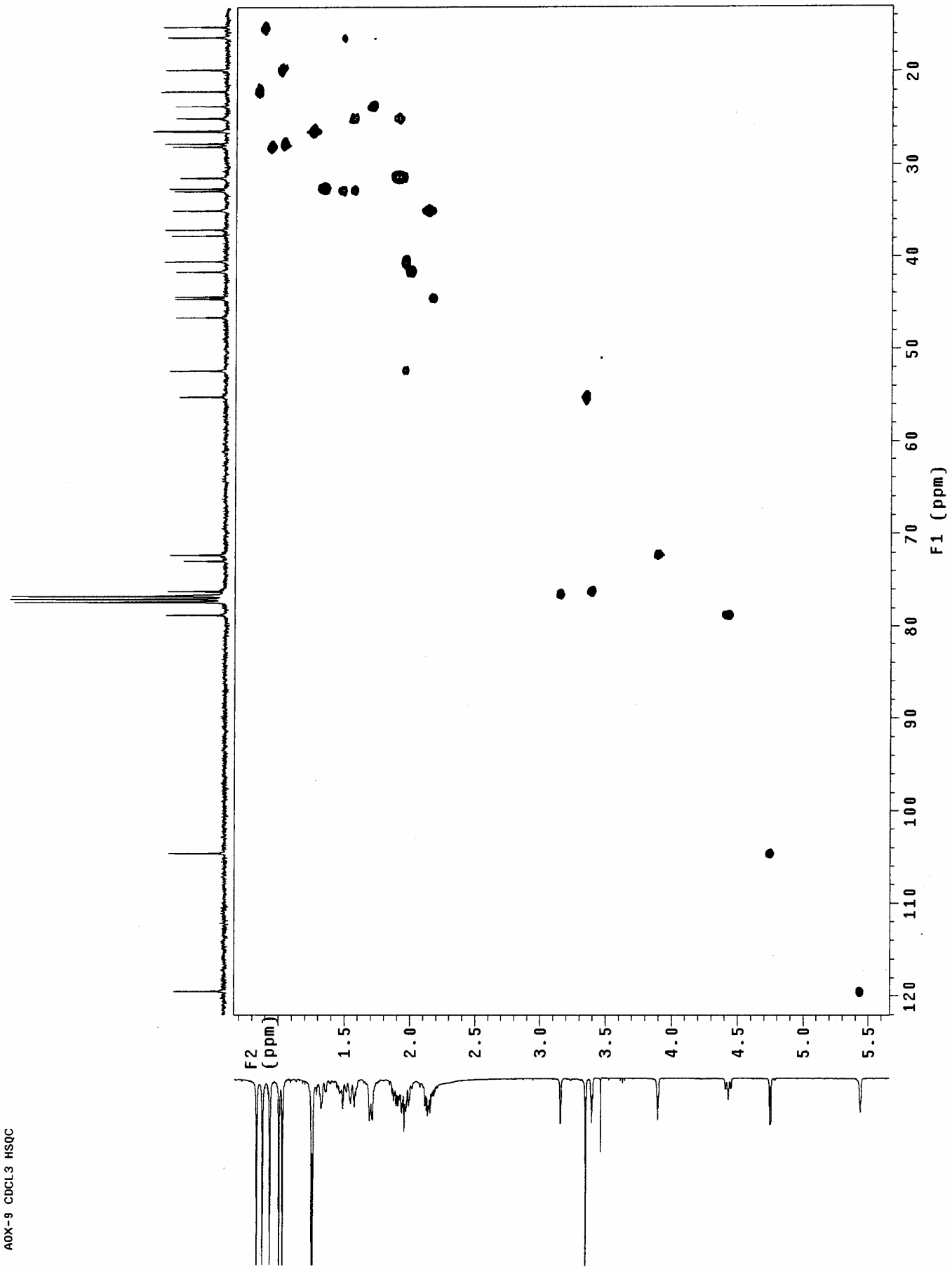


Figure S13. HMBC spectrum of agladupol A (**1**) in $CDCl_3$.

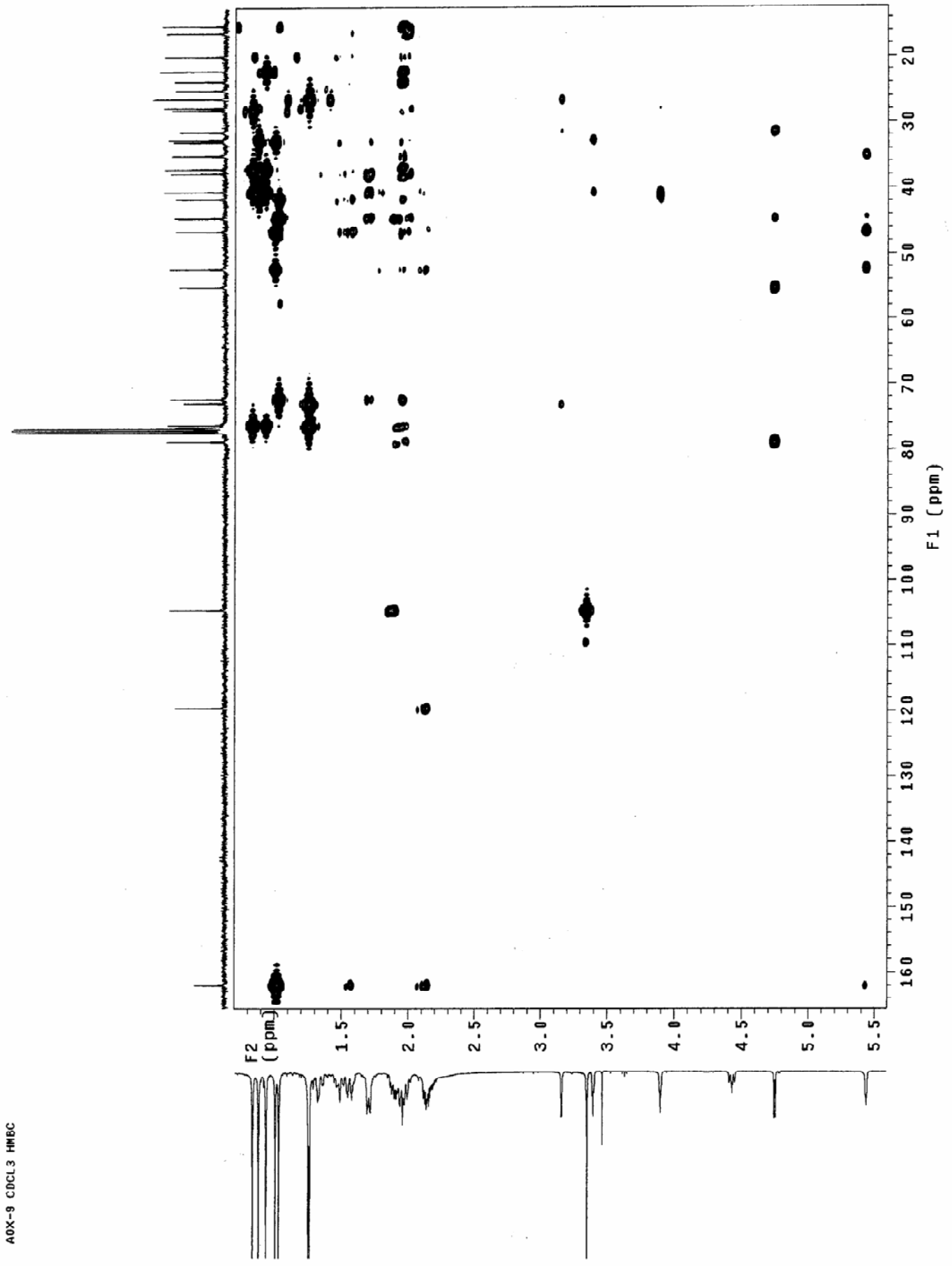


Figure S14. ROESY spectrum of agladupol A (**1**) in $CDCl_3$.

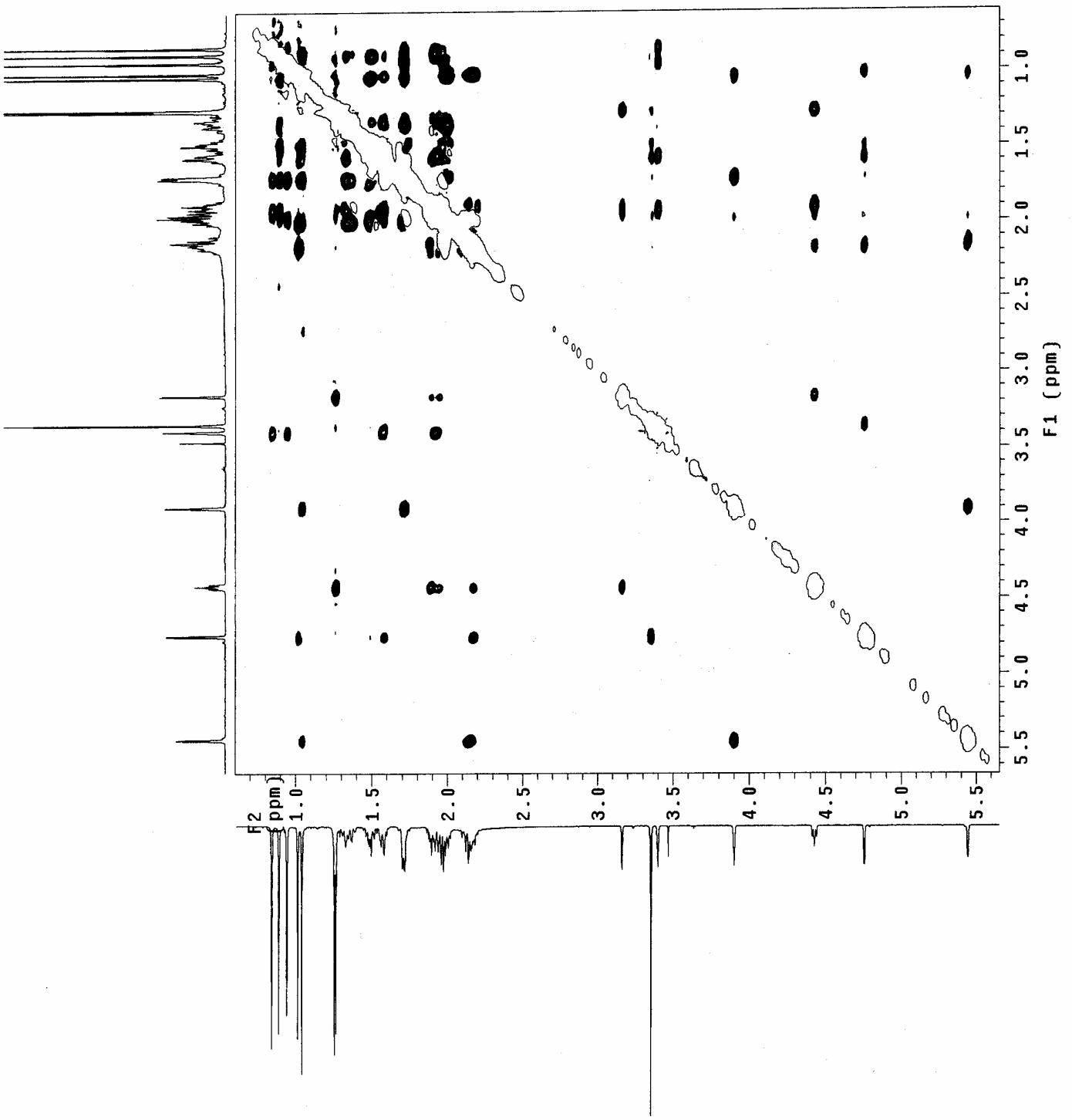


Figure S15. ^{1}H NMR spectrum of agladupol B (**2**) in $CDCl_3$.

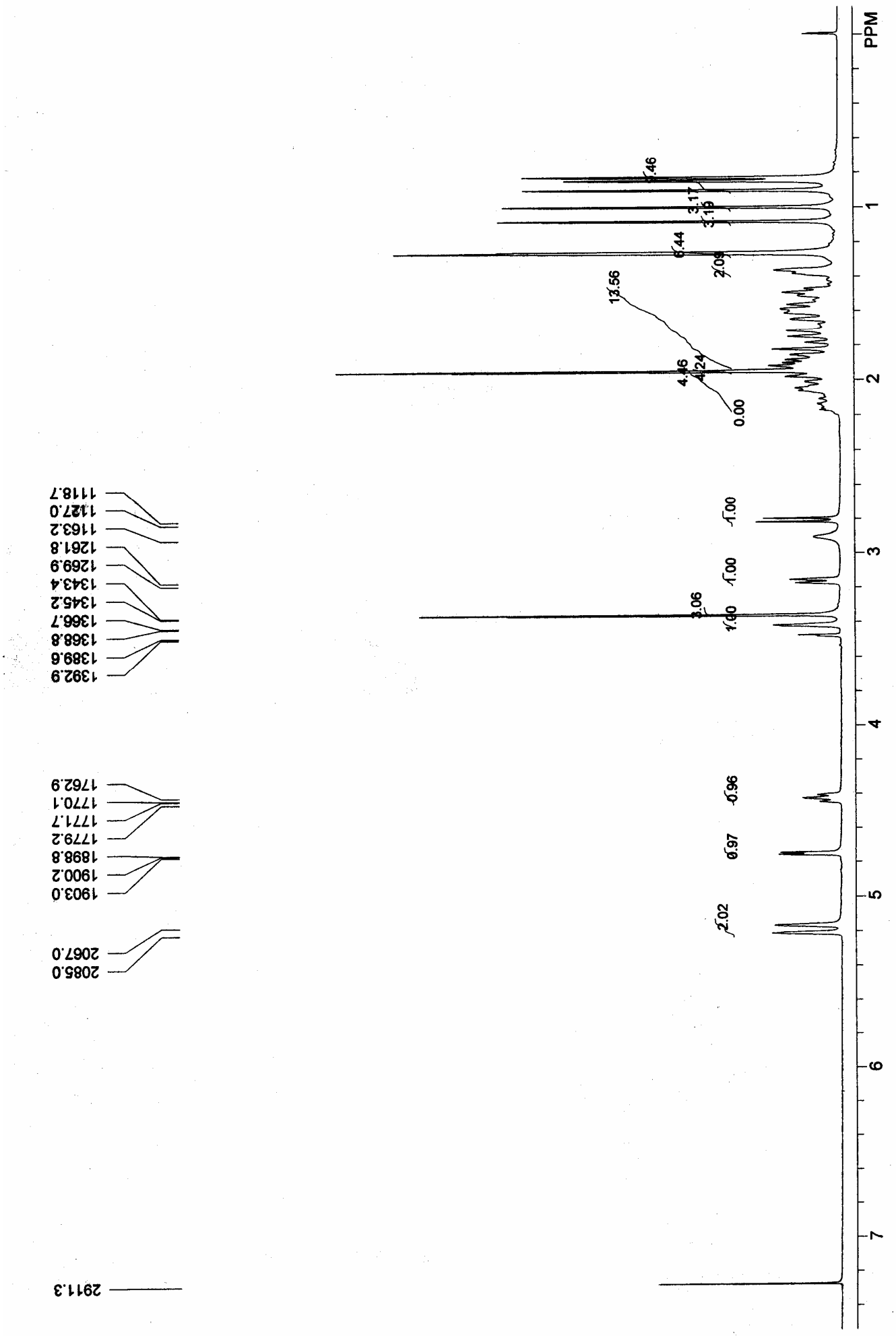


Figure S16. ^{13}C NMR spectrum of agladupol B (**2**) in $CDCl_3$.

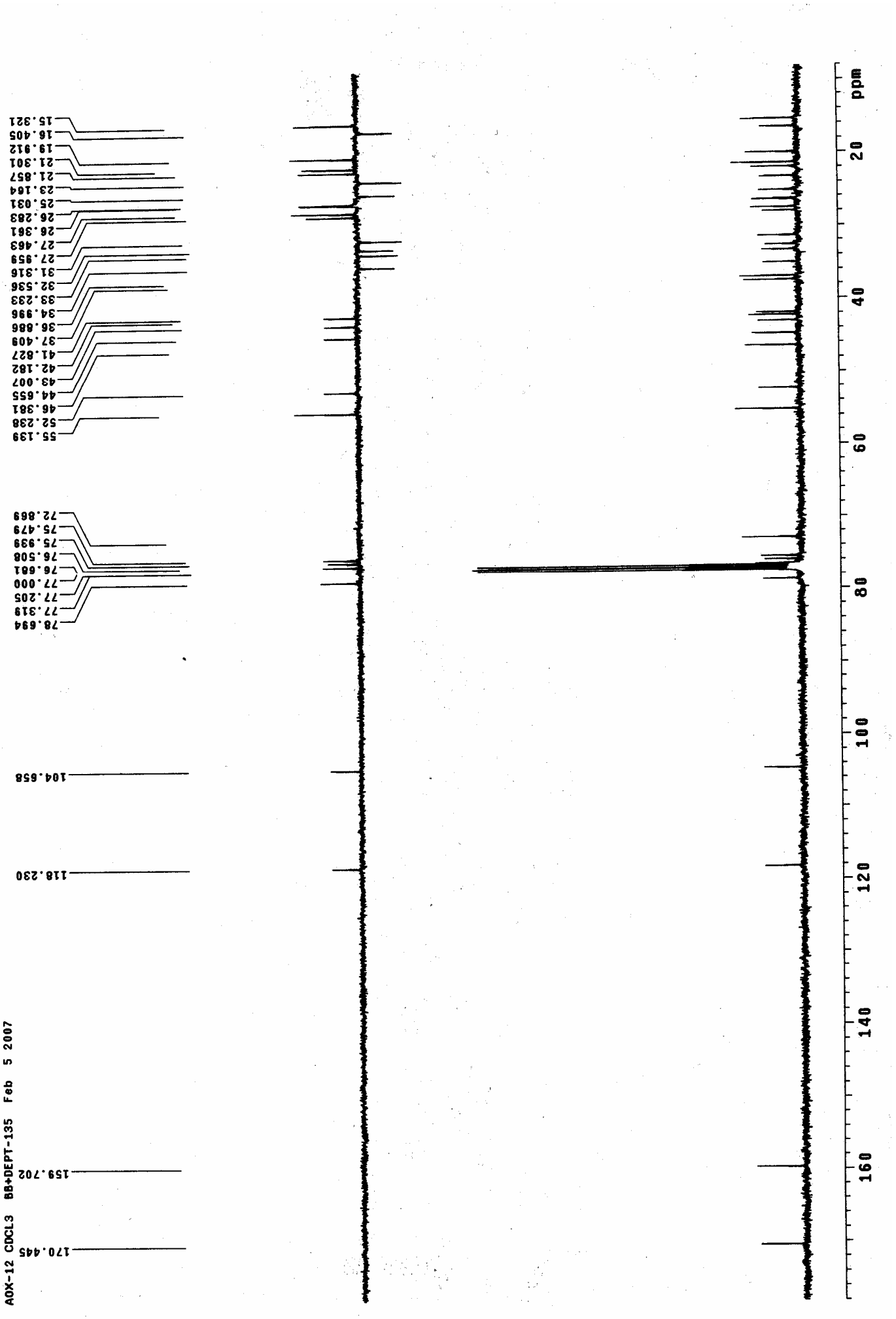


Figure S17. ESIMS spectrum of agladupol B (**2**).

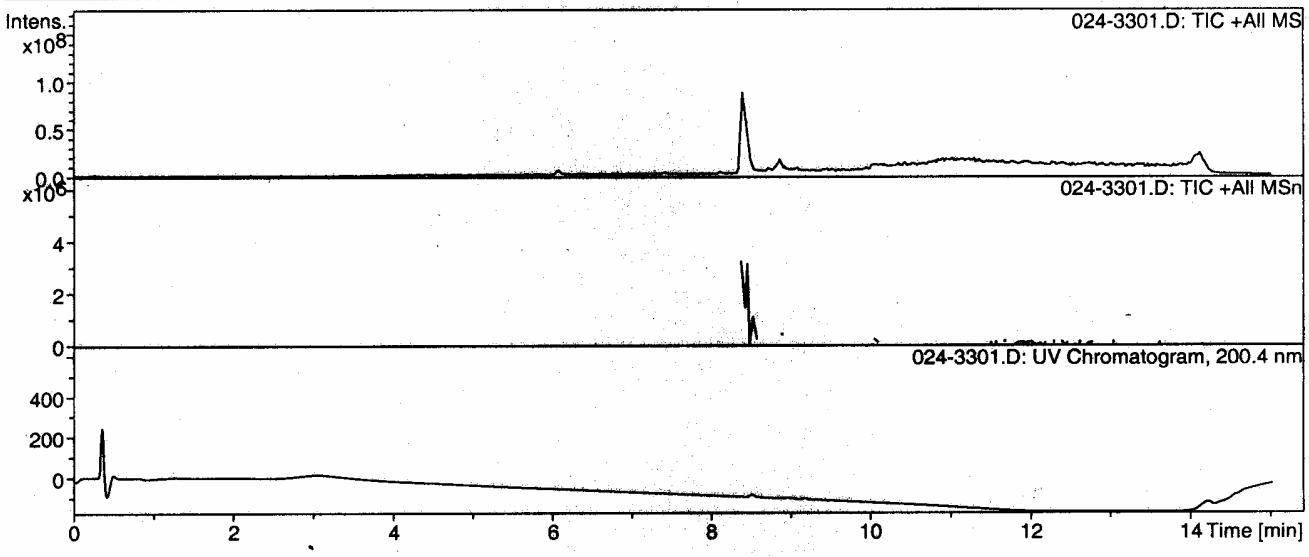
Display Report

Analysis Info

Analysis Name	024-3301.D	Acquisition Date	02/05/07 18:50:12
Method	Copy of SOPMSMSP.M	Operator	Administrator
Sample Name	yjm-Aox-12	Instrument	esquire3000plus_01005
Comment	□=□		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Std/Normal	Scan Begin	100 m/z	Scan End	1750 m/z
Capillary Exit	158.5 Volt	Skim 1	40.0 Volt	Trap Drive	85.4
Accumulation Time	5551 µs	Averages	3 Spectra	Auto MS/MS	on



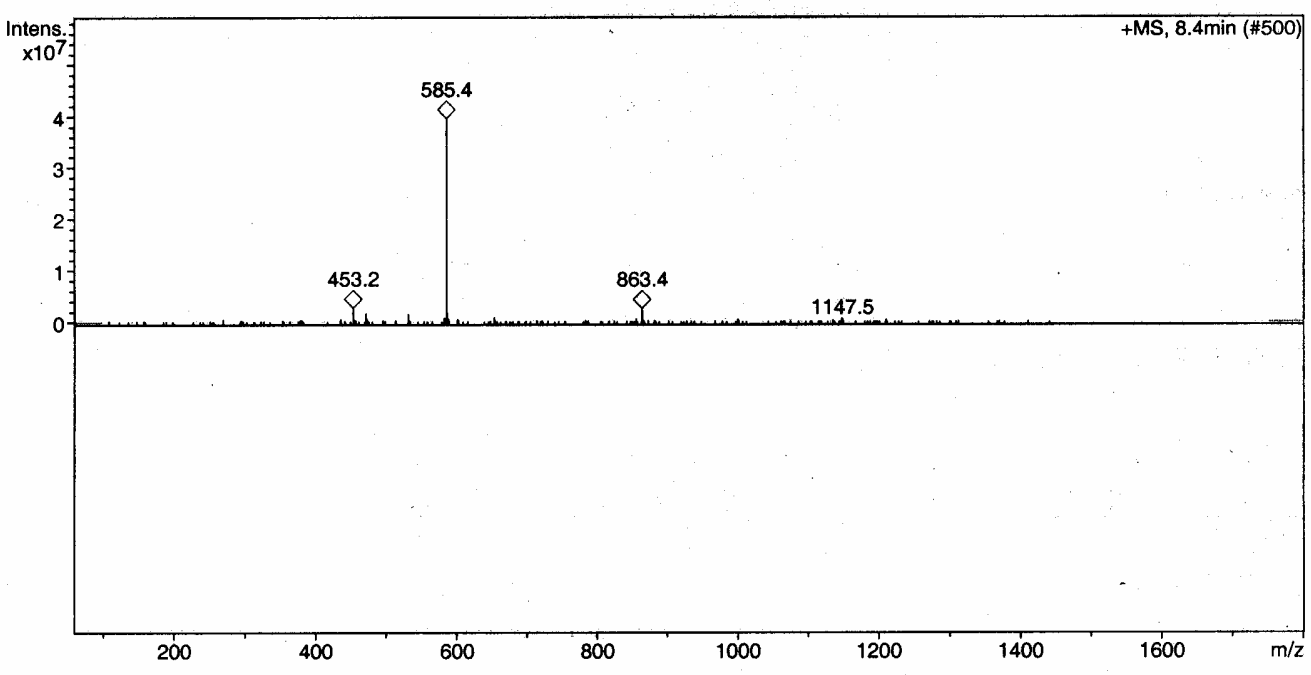


Figure S18. IR spectrum of agladupol B (**2**).

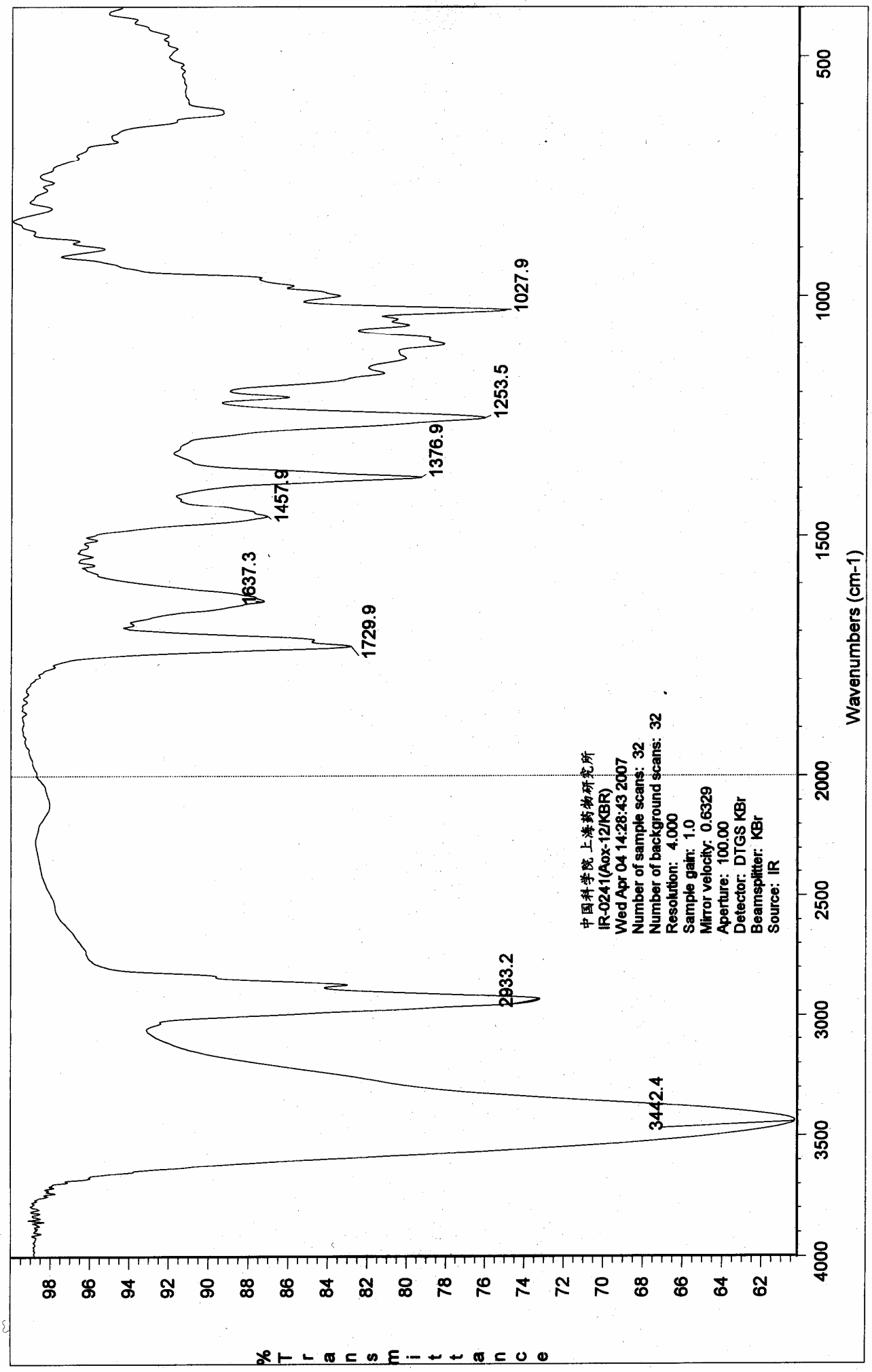


Figure S19. HSQC spectrum of agladupol B (**2**) in $CDCl_3$.

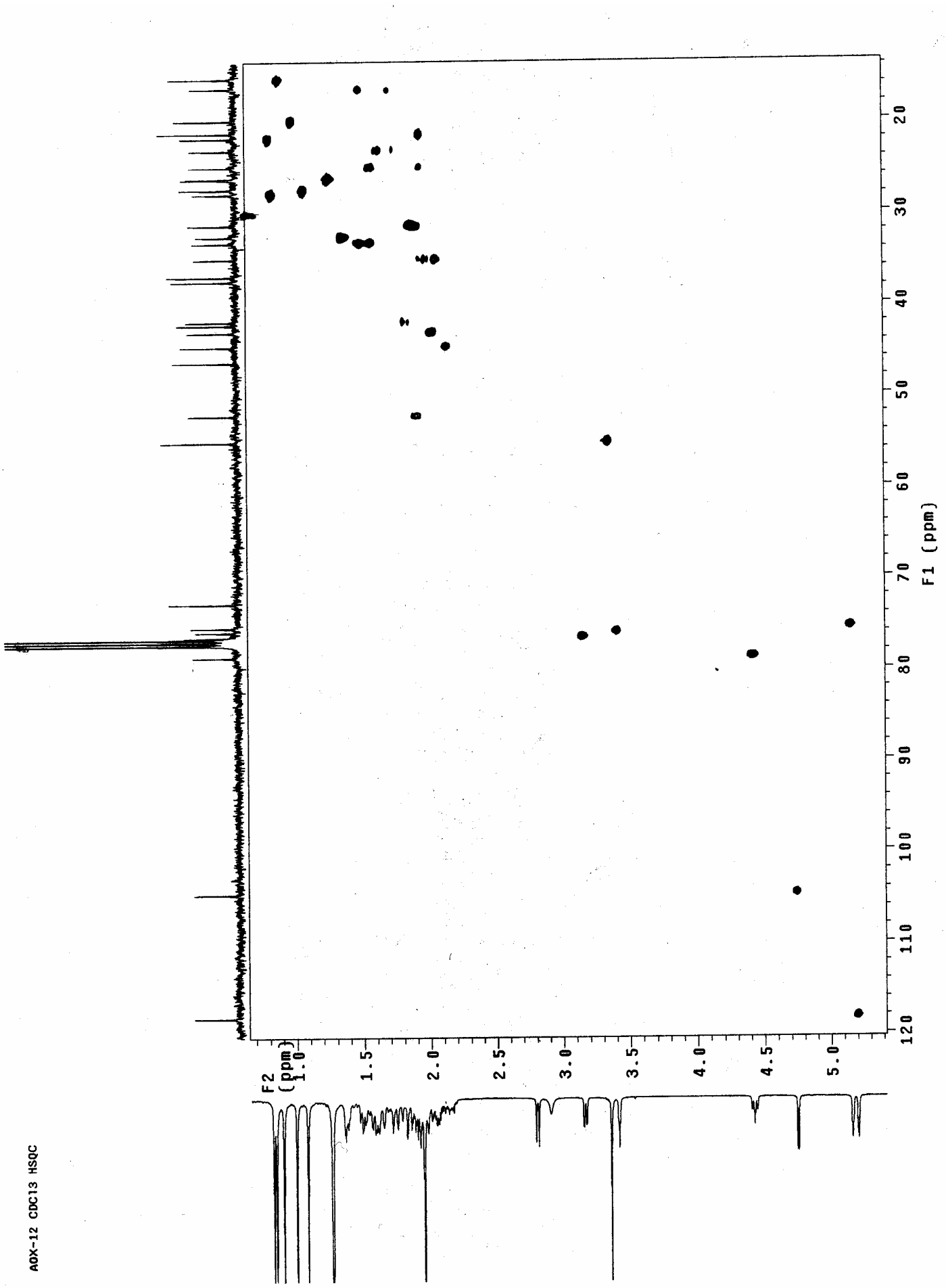


Figure S20. HMBC spectrum of agladupol B (**2**) in $CDCl_3$.

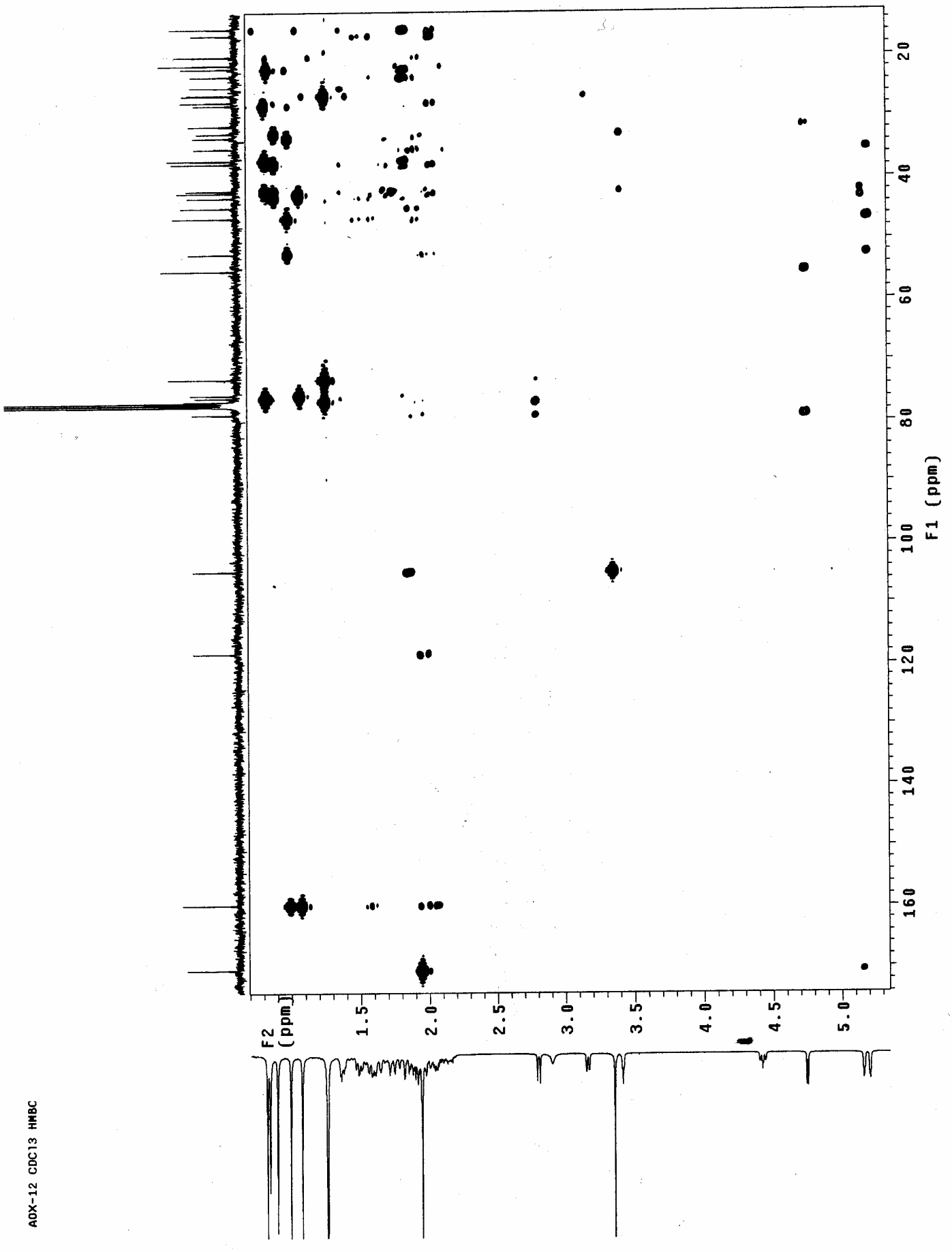


Figure S21. ROESY spectrum of agladupol B (**2**) in $CDCl_3$.

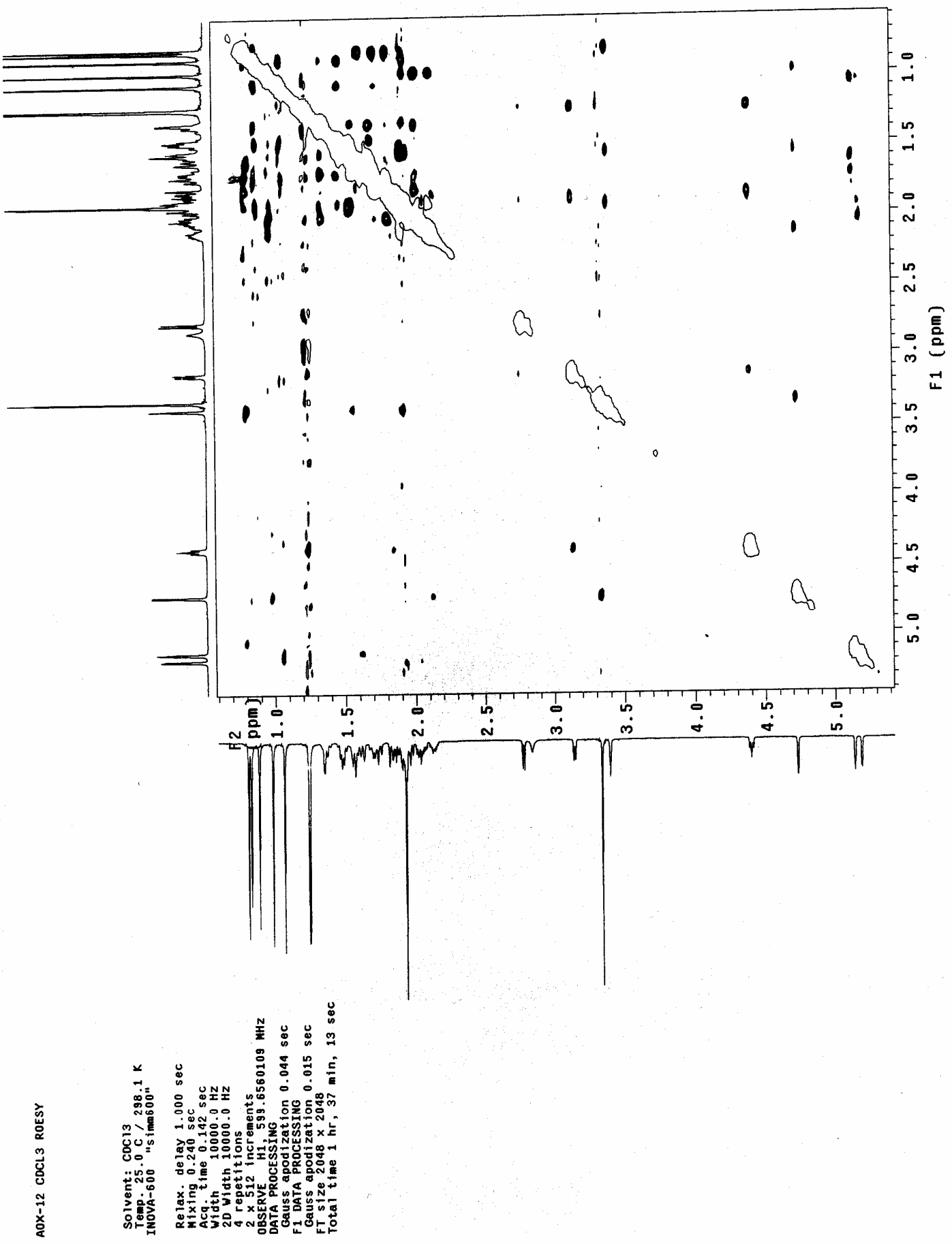


Figure S22. ^{1}H NMR spectrum of agladupol C (**3**) in $CDCl_3$.

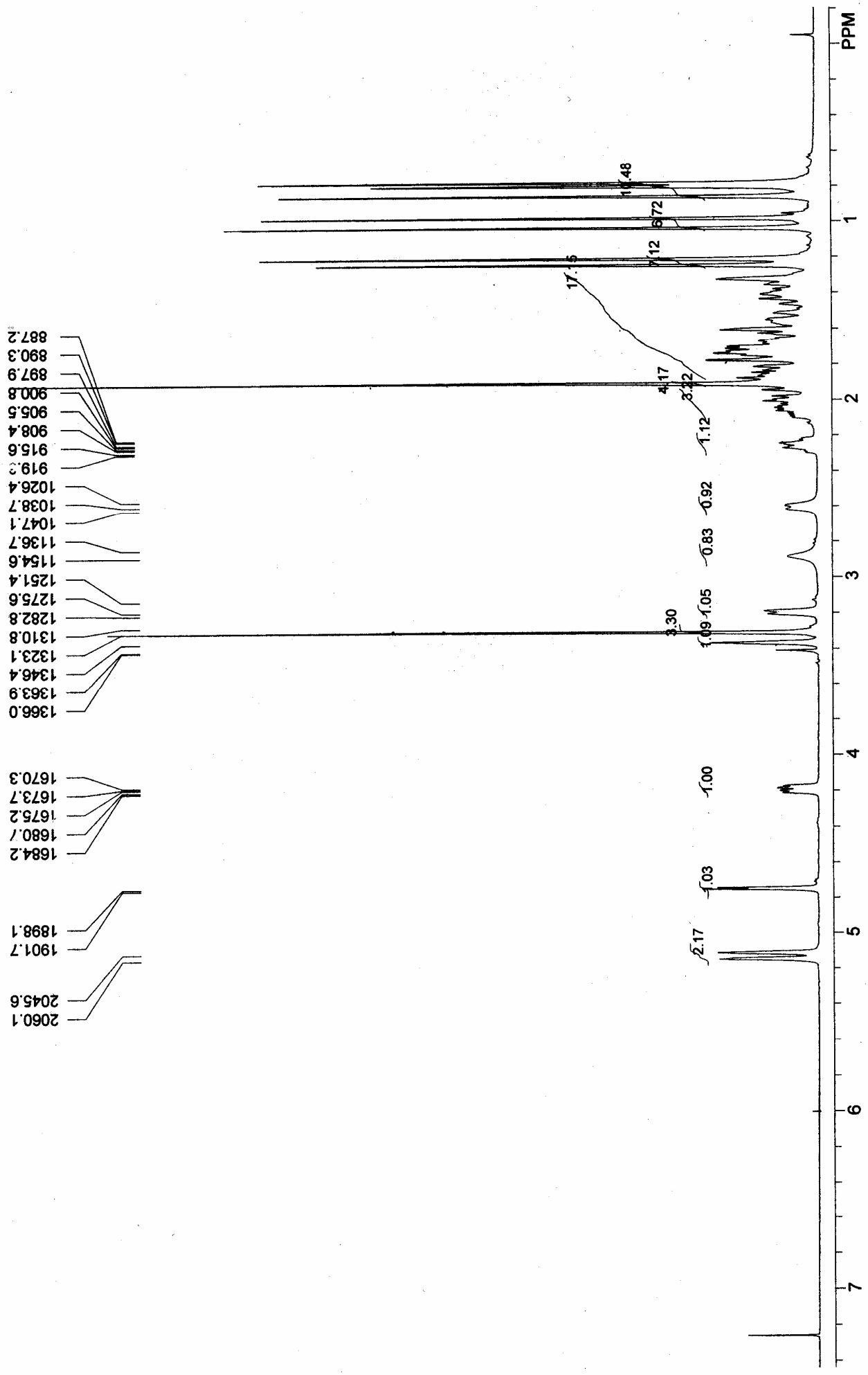


Figure S23. ^{13}C NMR spectrum of agladupol C (**3**) in $CDCl_3$.

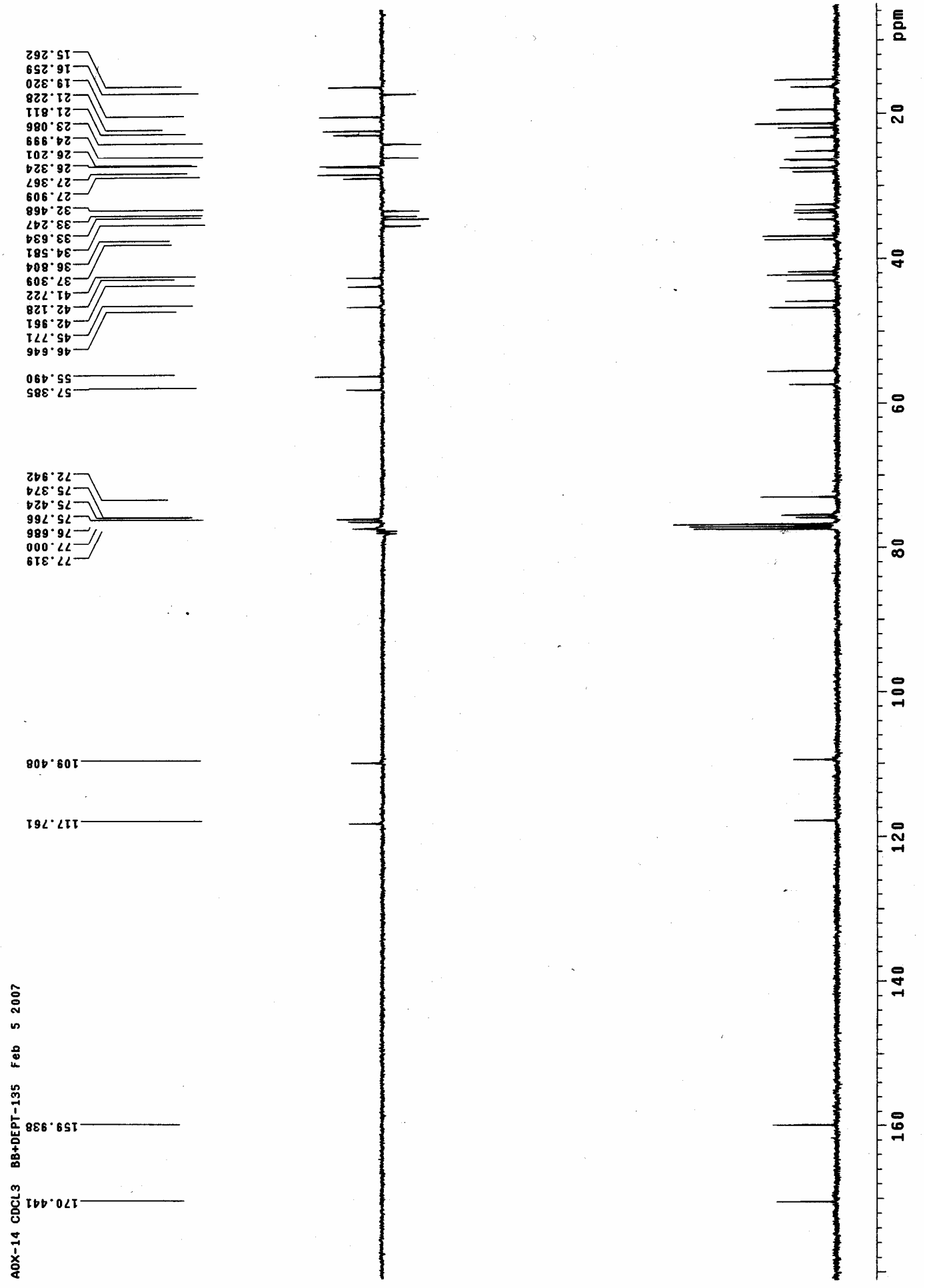


Figure S24. ESIMS spectrum of agladupol C (**3**).

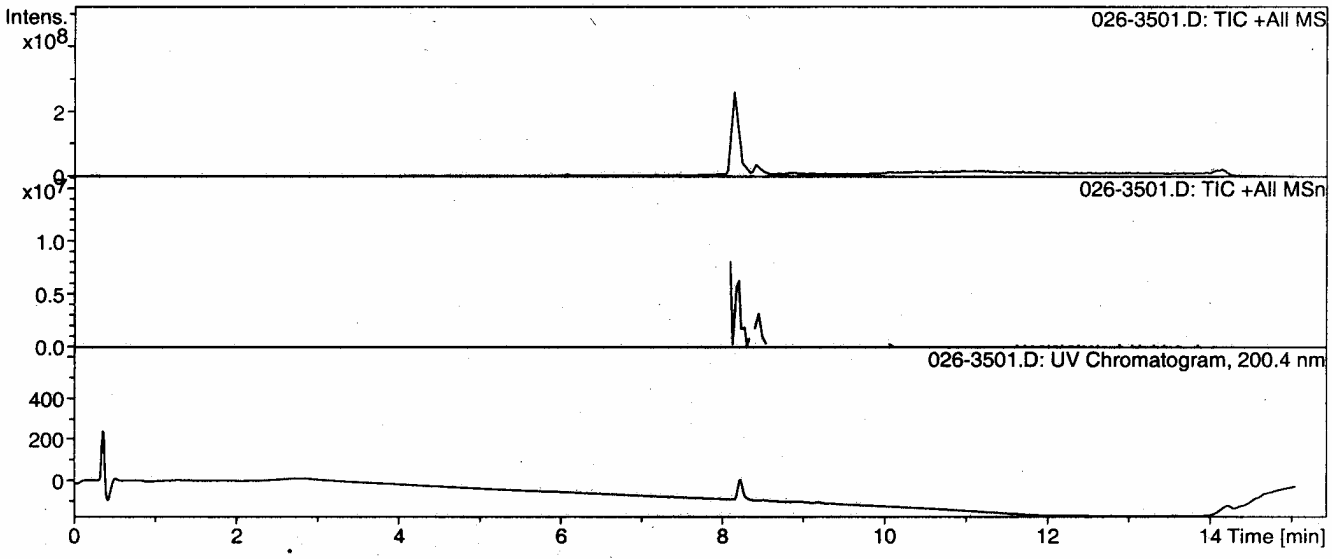
Display Report

Analysis Info

Analysis Name	026-3501.D	Acquisition Date	02/05/07 19:23:29
Method	Copy of SOPMSMSP.M	Operator	Administrator
Sample Name	yjm-Aox-14	Instrument	esquire3000plus_01005
Comment	□=□		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Std/Normal	Scan Begin	100 m/z	Scan End	1750 m/z
Capillary Exit	158.5 Volt	Skim 1	40.0 Volt	Trap Drive	85.4
Accumulation Time	6375 µs	Averages	3 Spectra	Auto MS/MS	on



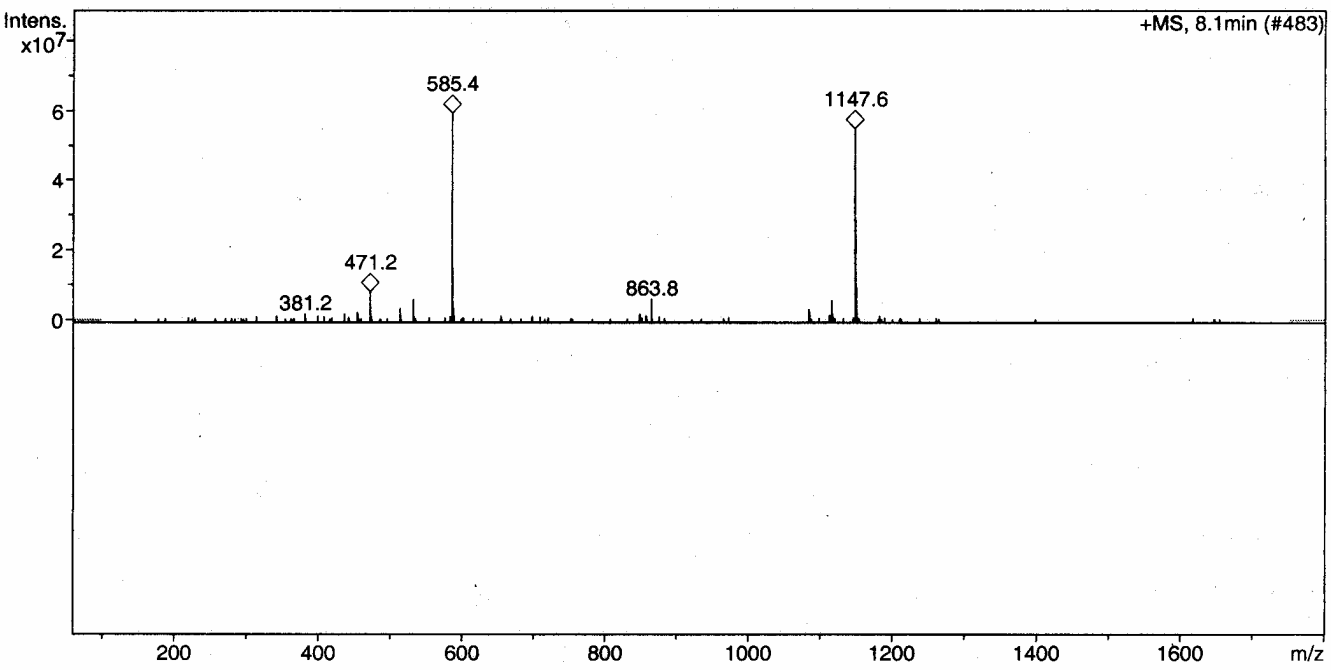


Figure S25. IR spectrum of agladupol C (**3**).

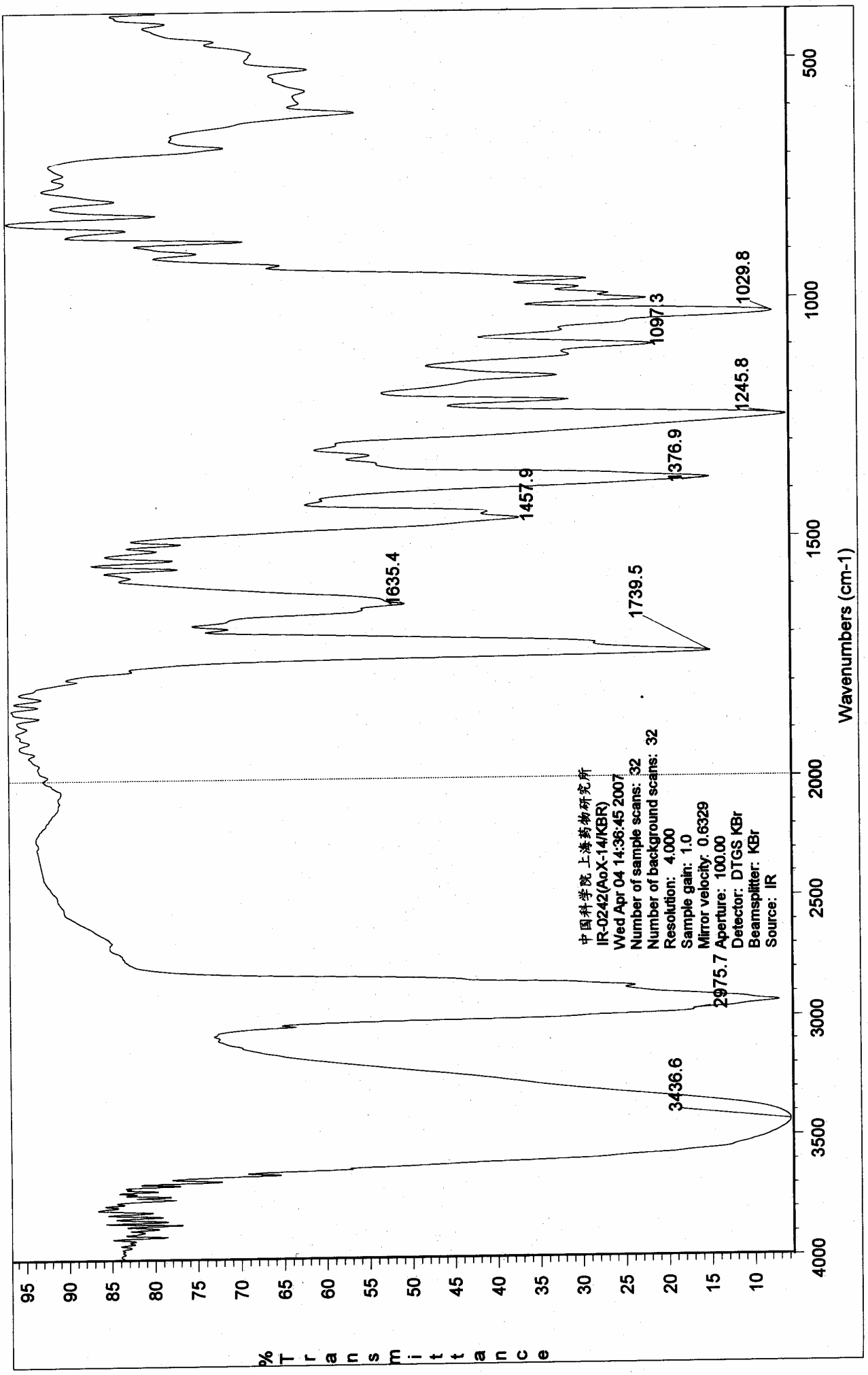


Figure S26. HSQC spectrum of agladupol C (**3**) in $CDCl_3$.

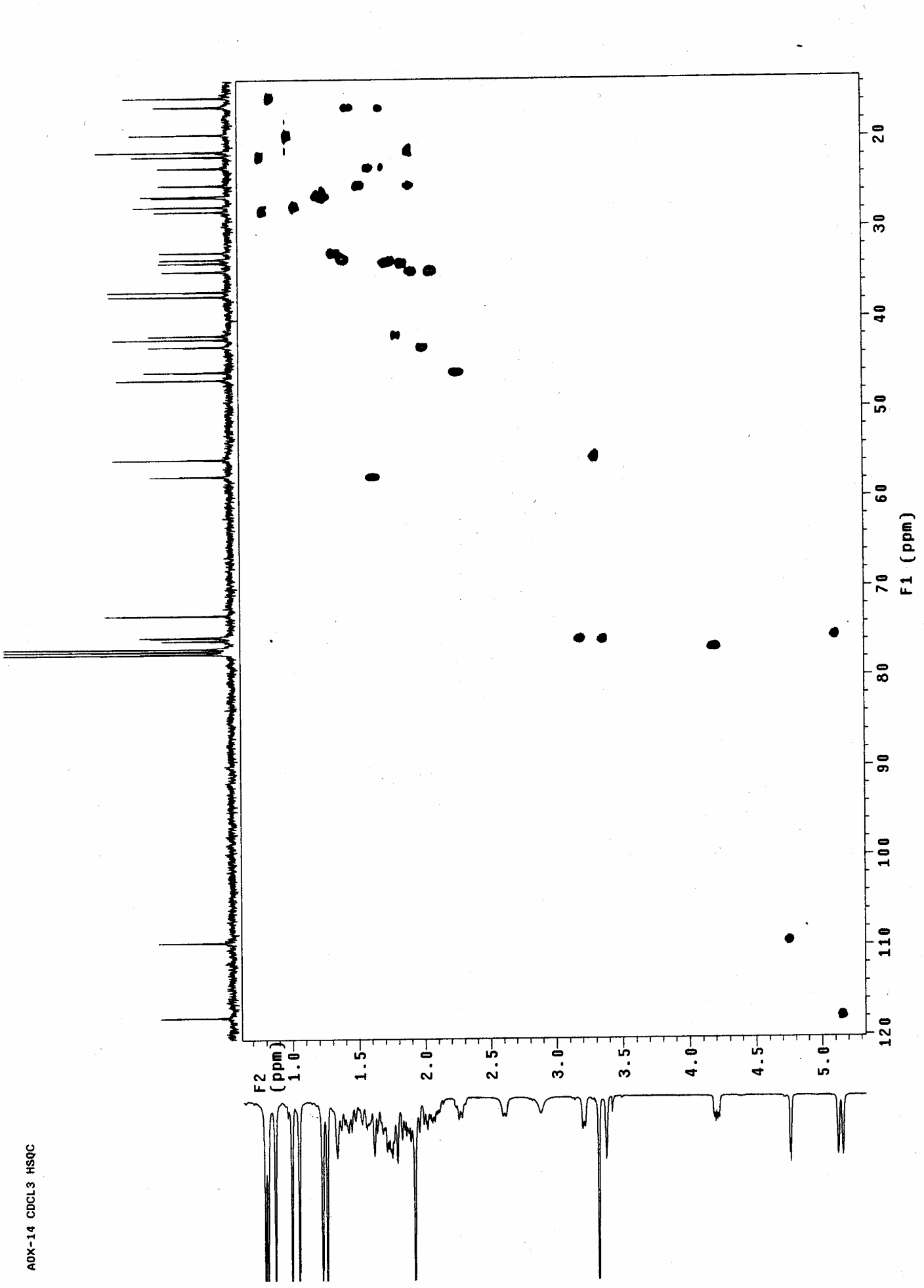


Figure S27. HMBC spectrum of agladupol C (**3**) in $CDCl_3$.

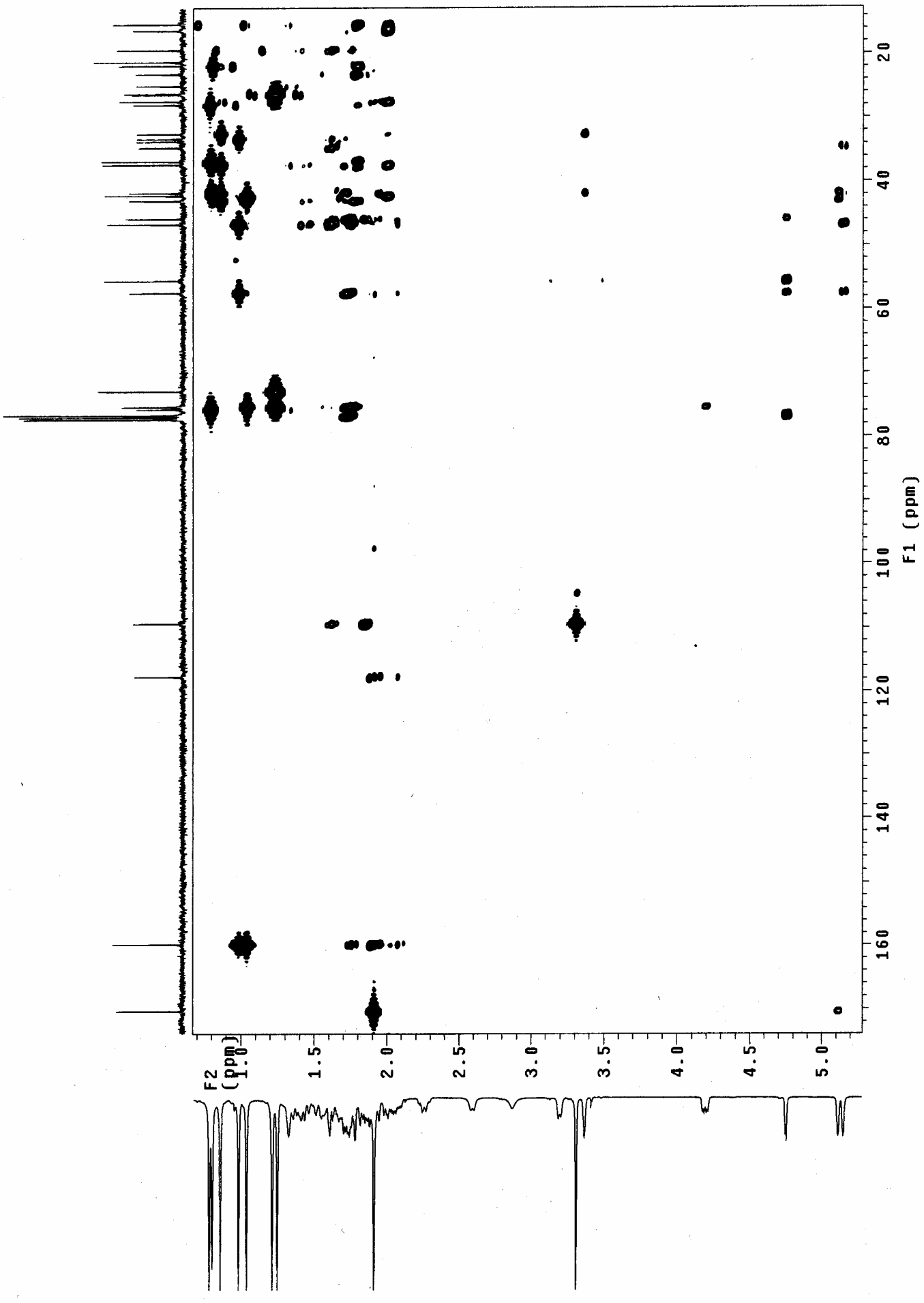


Figure S28. ROESY spectrum of agladupol C (**3**) in $CDCl_3$.

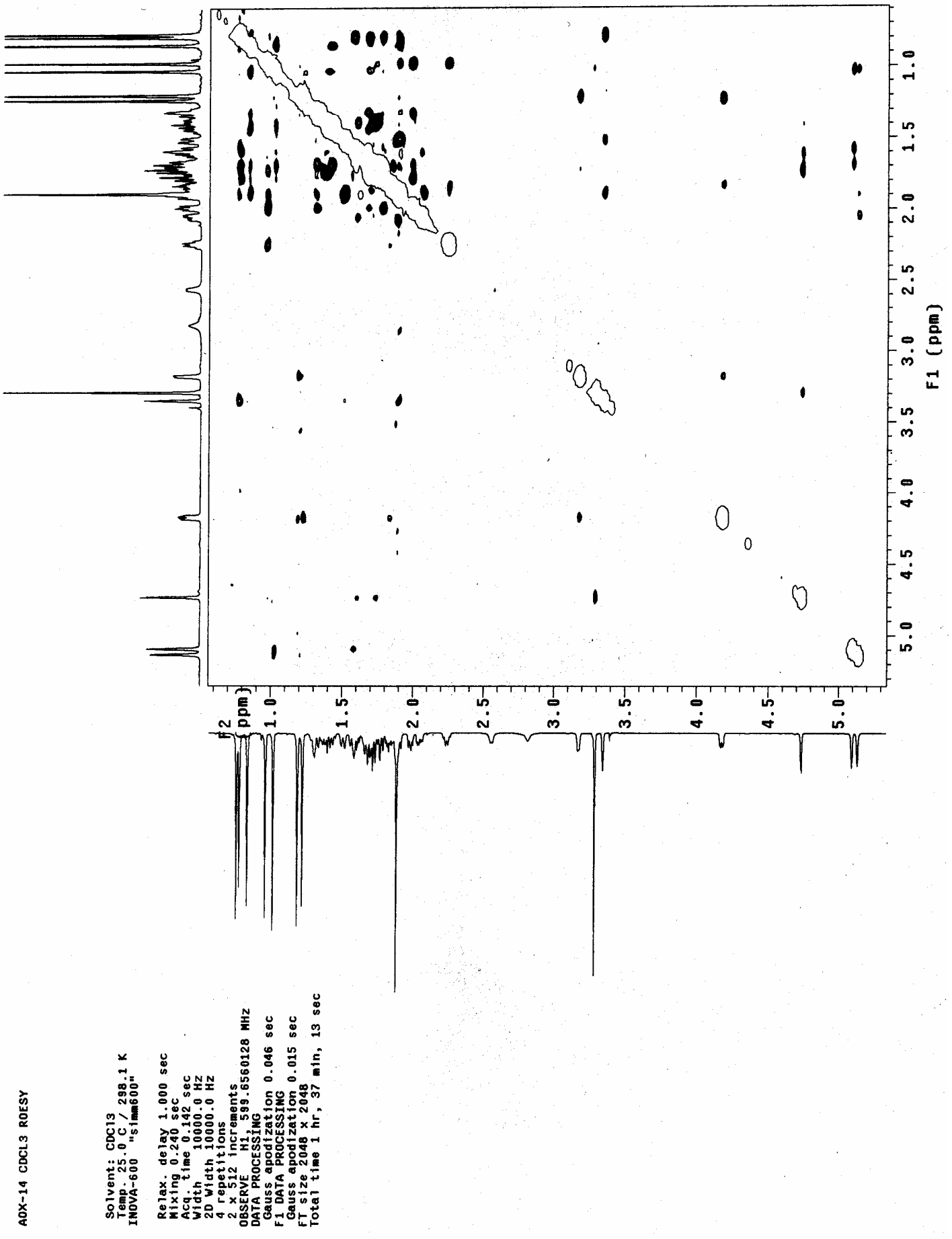


Figure S29. ^{1}H NMR spectrum of agladupol D (**4**) in $CDCl_3$.

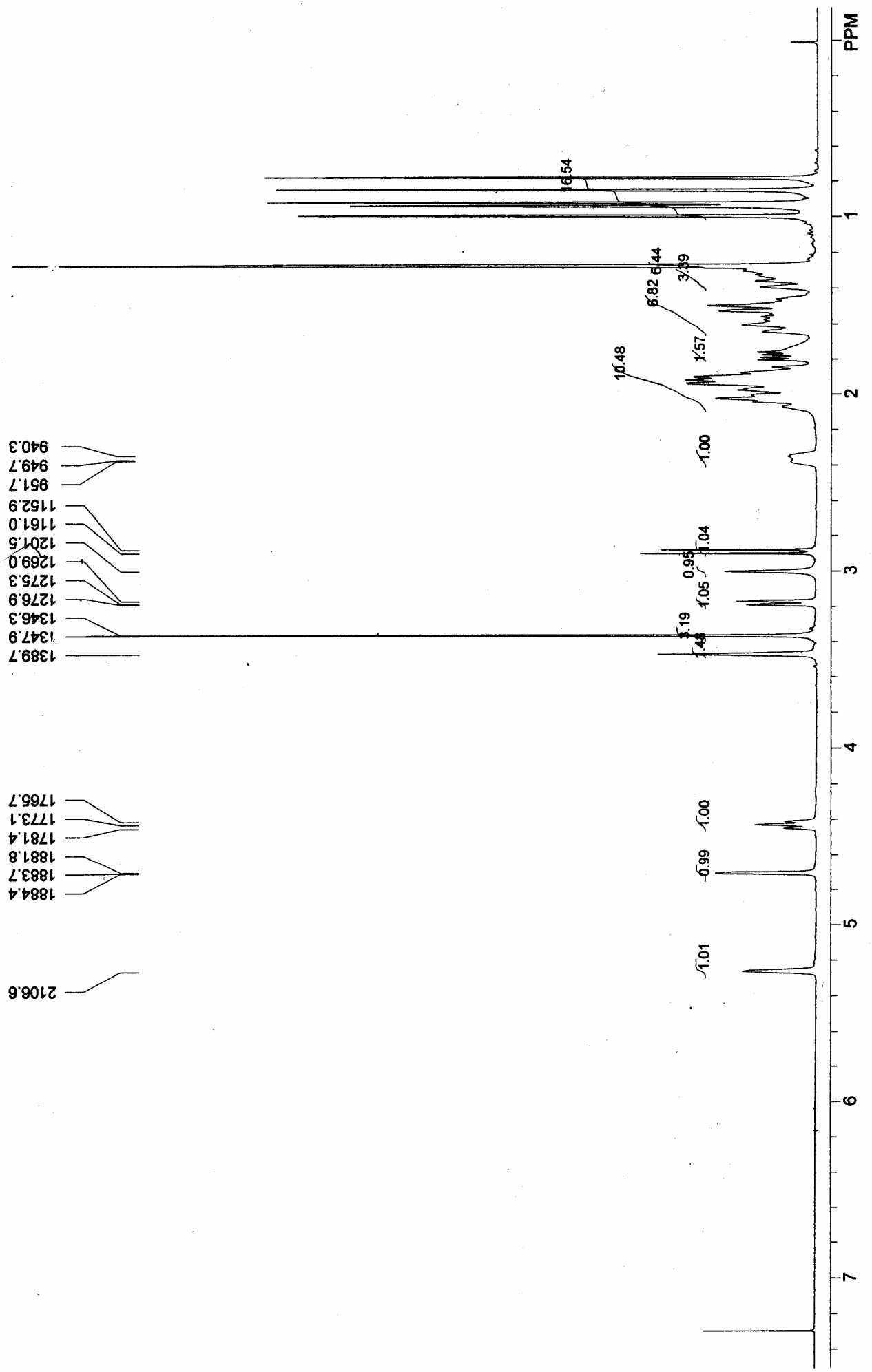


Figure S30. ^{13}C NMR spectrum of agladupol D (**4**) in $CDCl_3$.

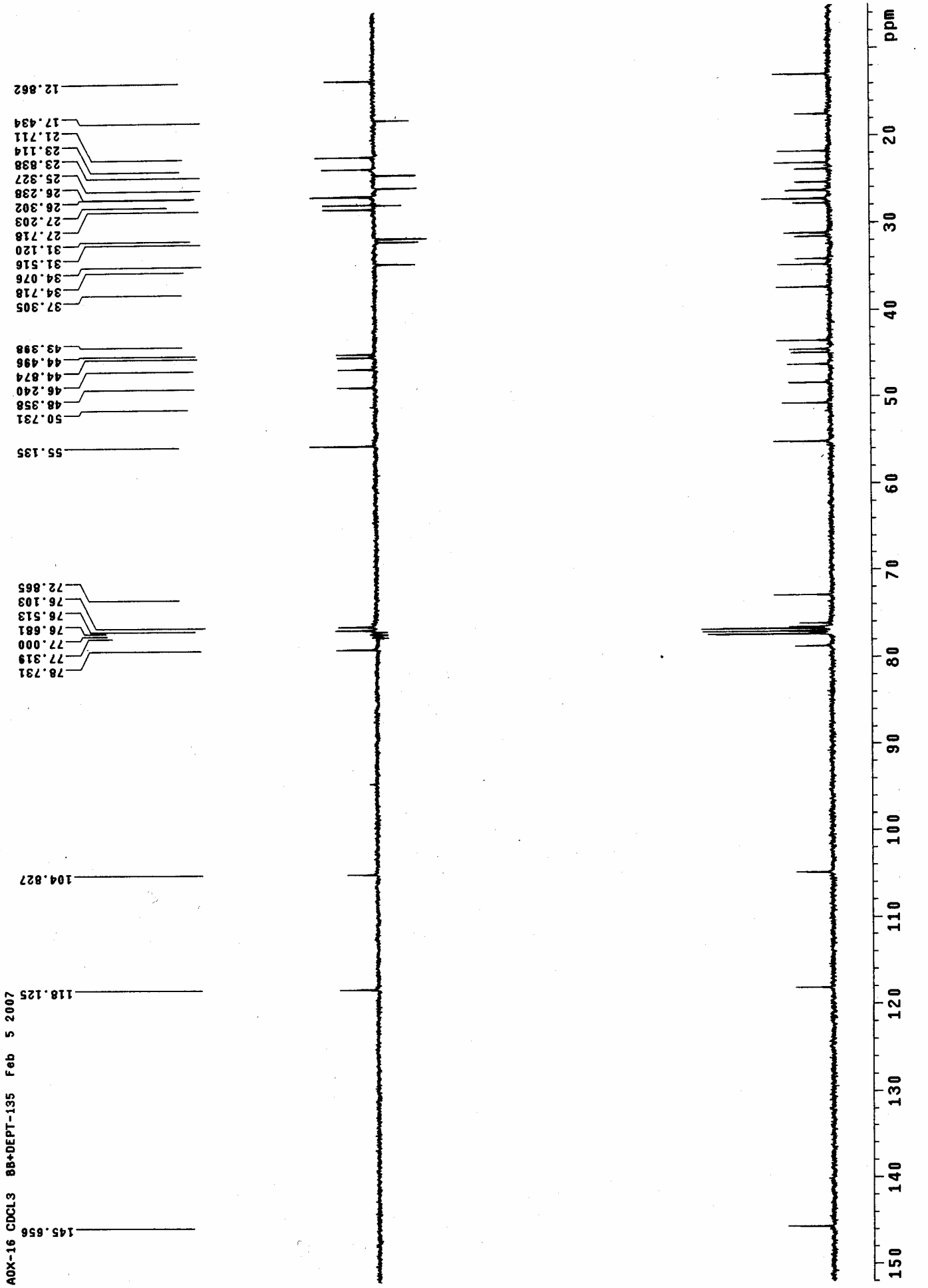


Figure S31. EIMS spectrum of agladupol D (**4**).

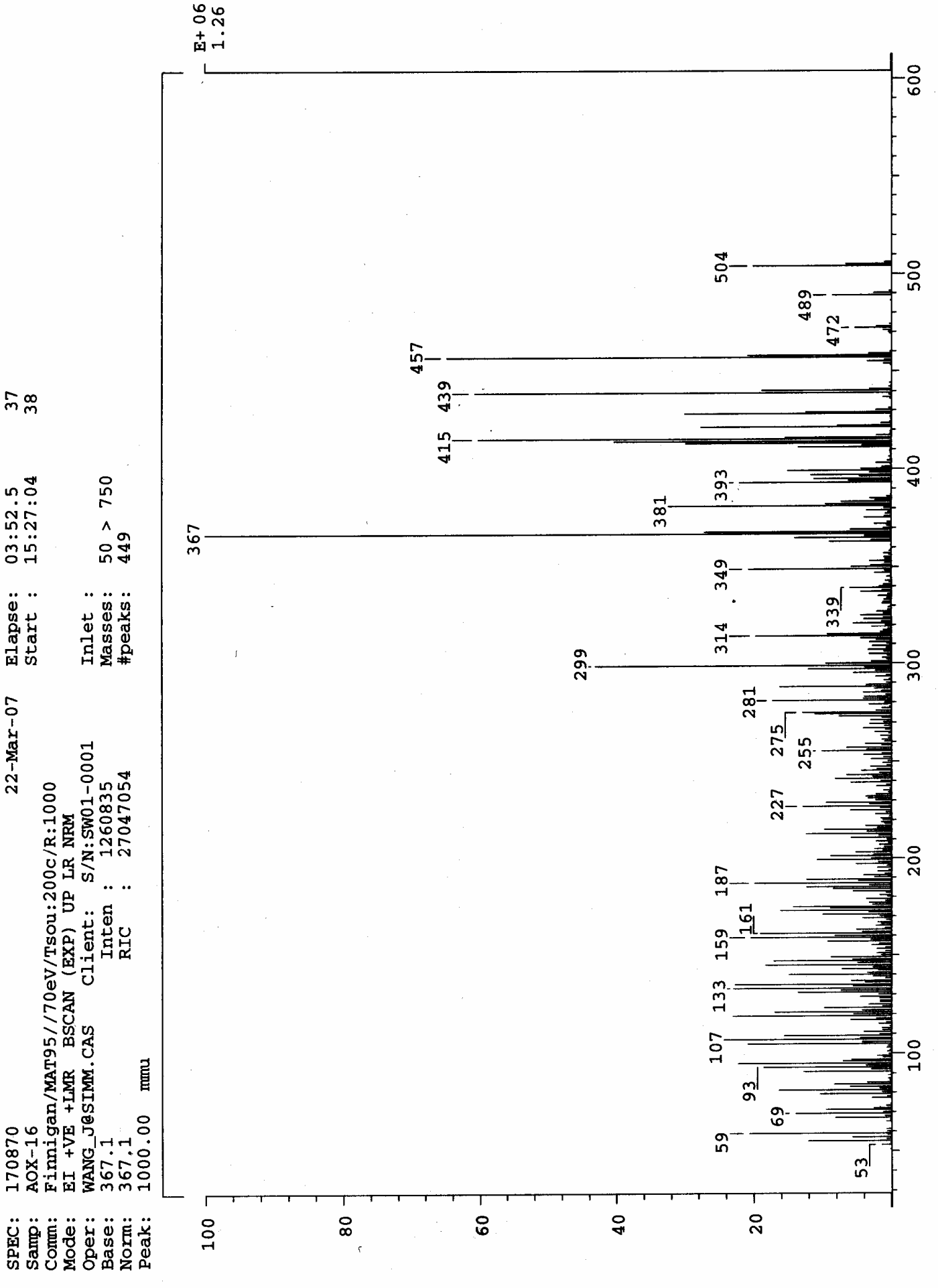


Figure S32. IR spectrum of agladupol D (**4**).

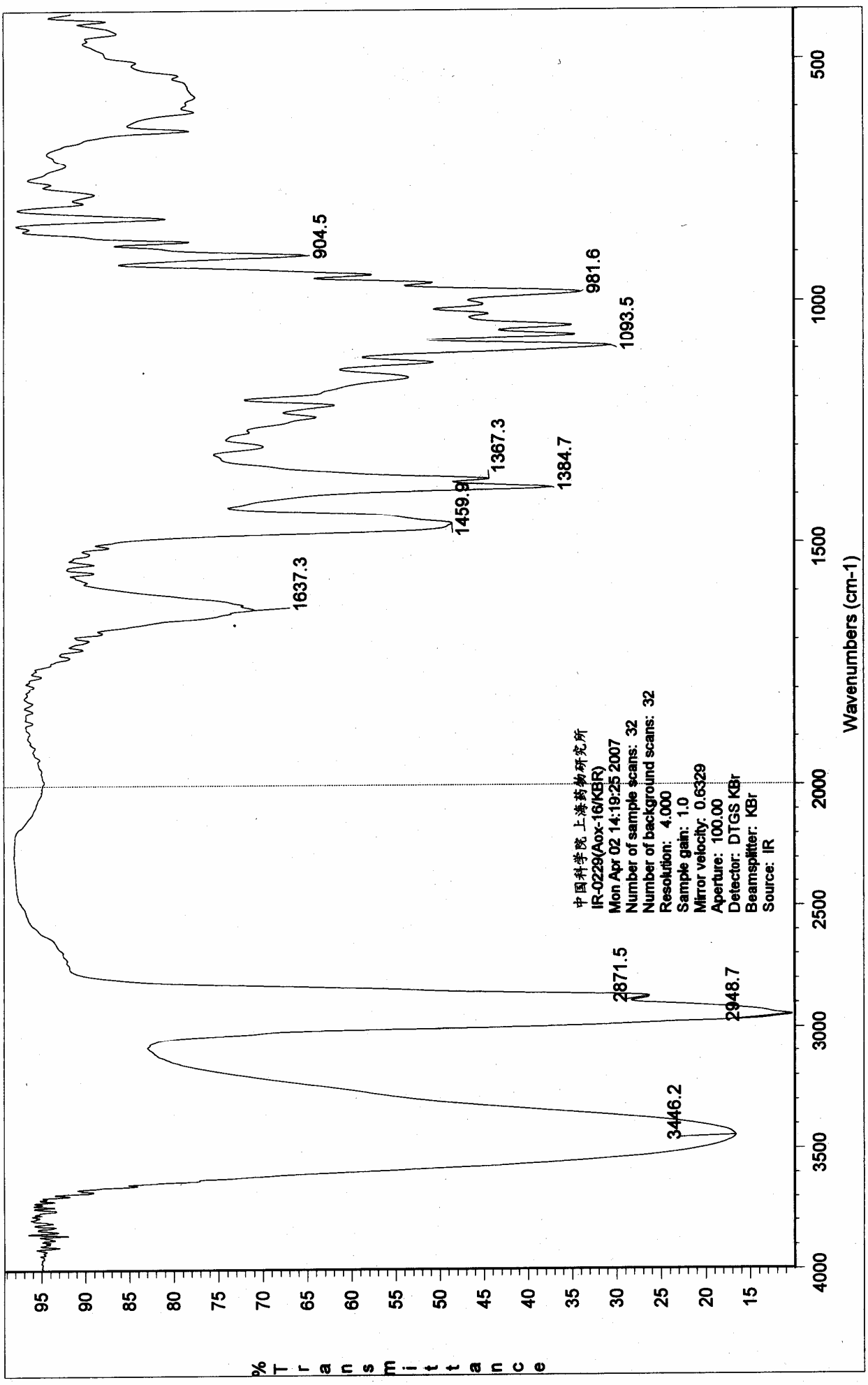


Figure S33. HSQC spectrum of agladupol D (**4**) in $CDCl_3$.

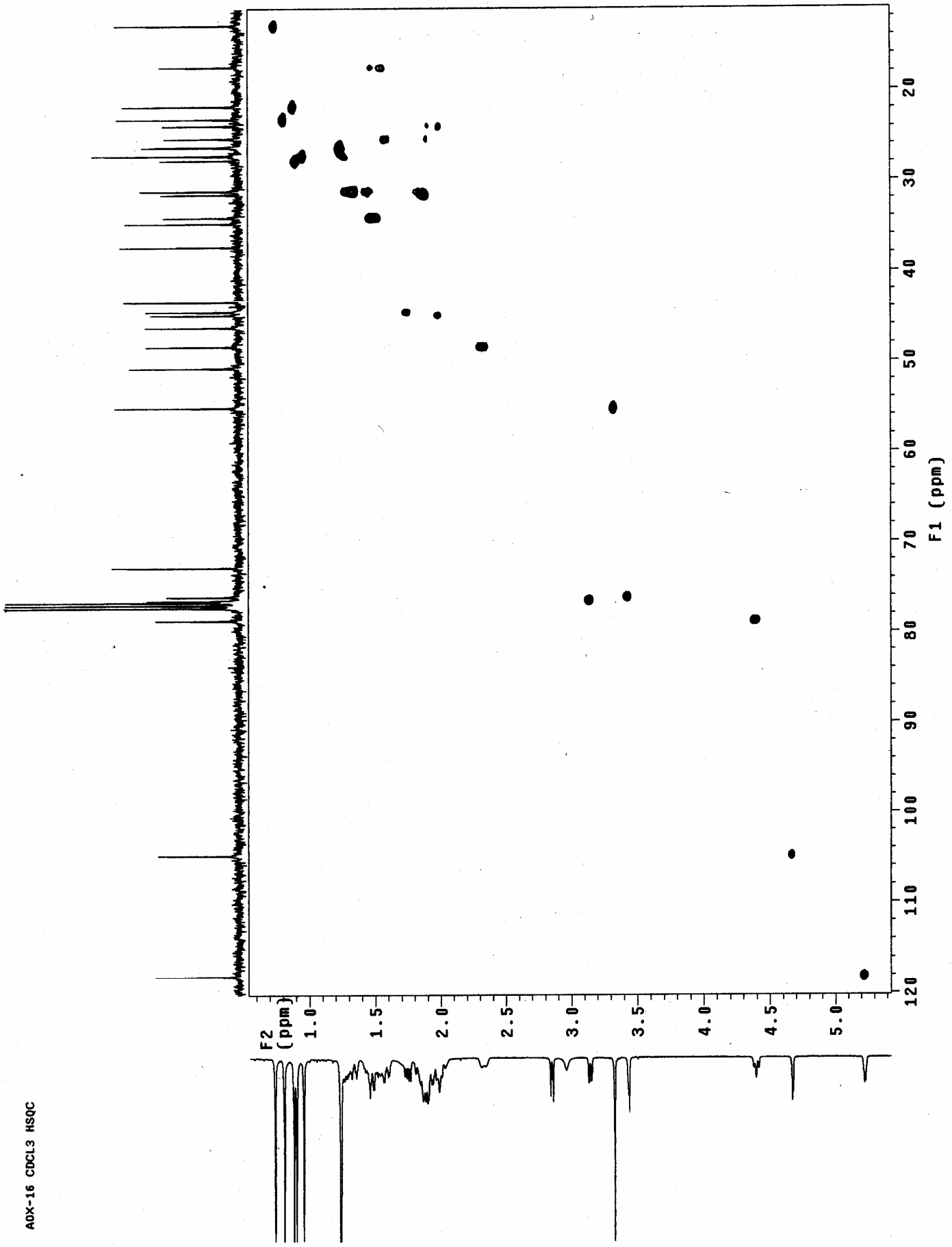


Figure S34. HMBC spectrum of agladupol D (**4**) in $CDCl_3$.

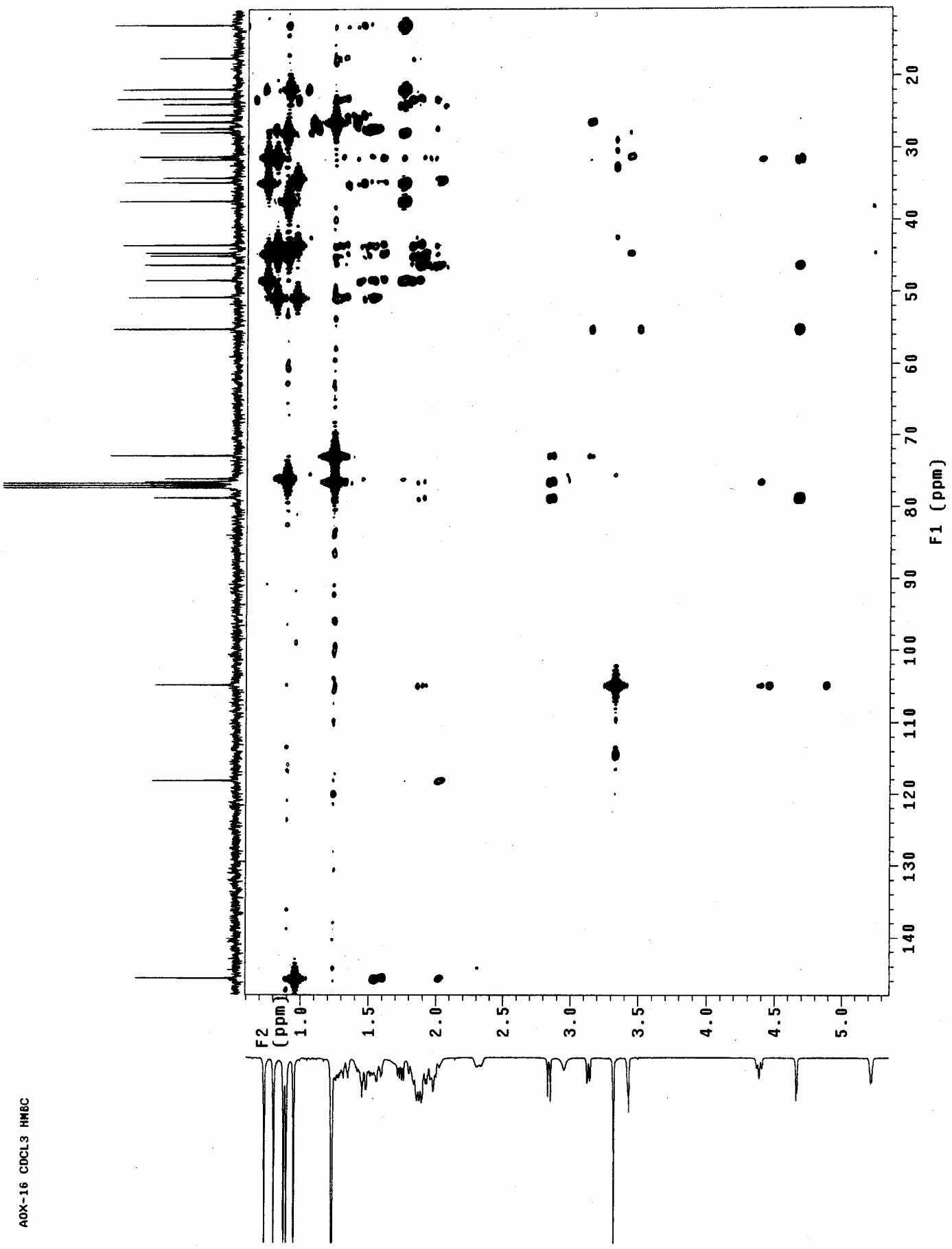


Figure S35. ROESY spectrum of agladupol D (**4**) in $CDCl_3$.

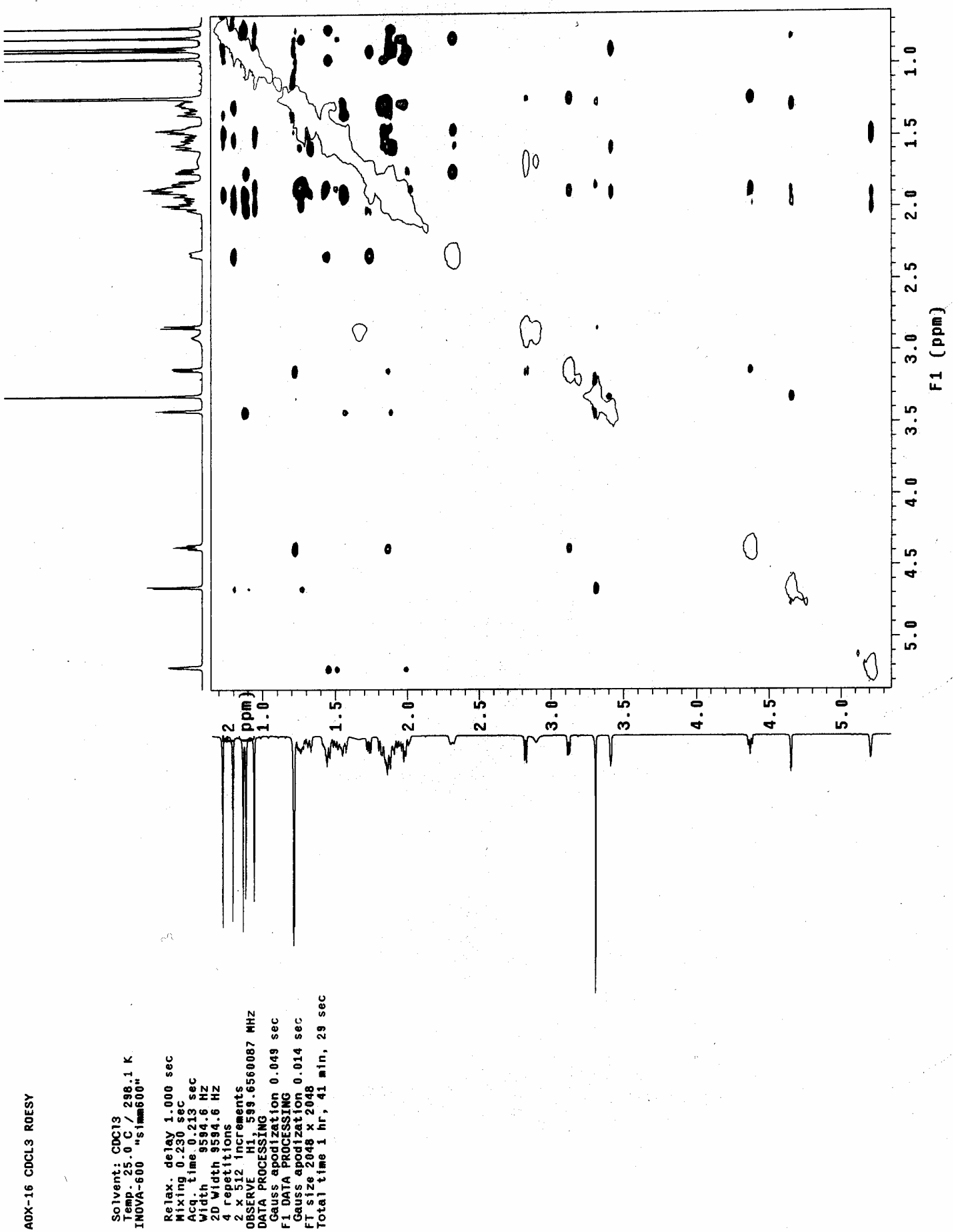


Figure S36. ^{1}H NMR spectrum of agladupol E (**5**) in $CDCl_3$

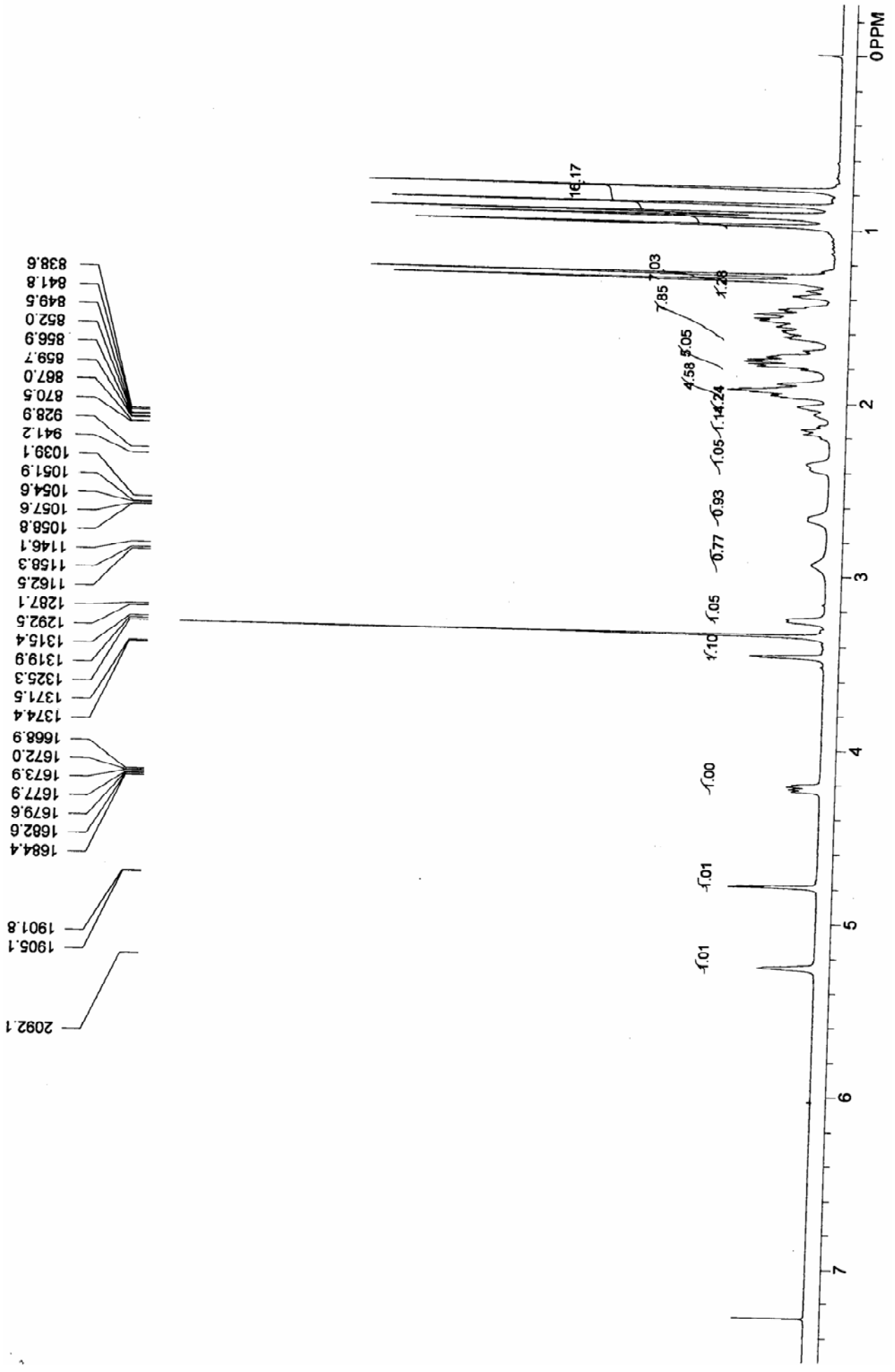


Figure S37. ^{13}C NMR spectrum of agladupol E (**5**) in $CDCl_3$

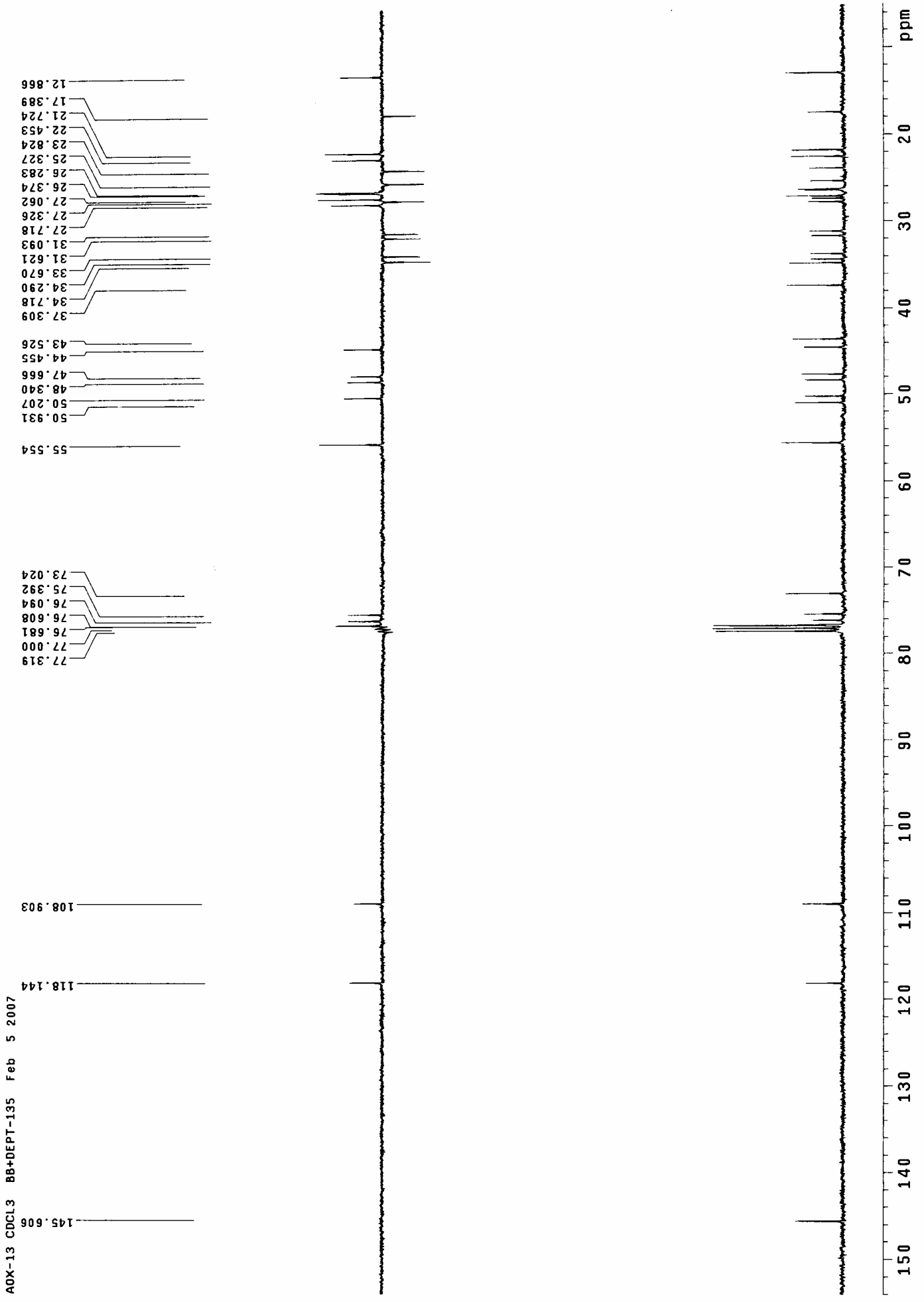


Figure S38. EIMS spectrum of agladupol E (**5**)

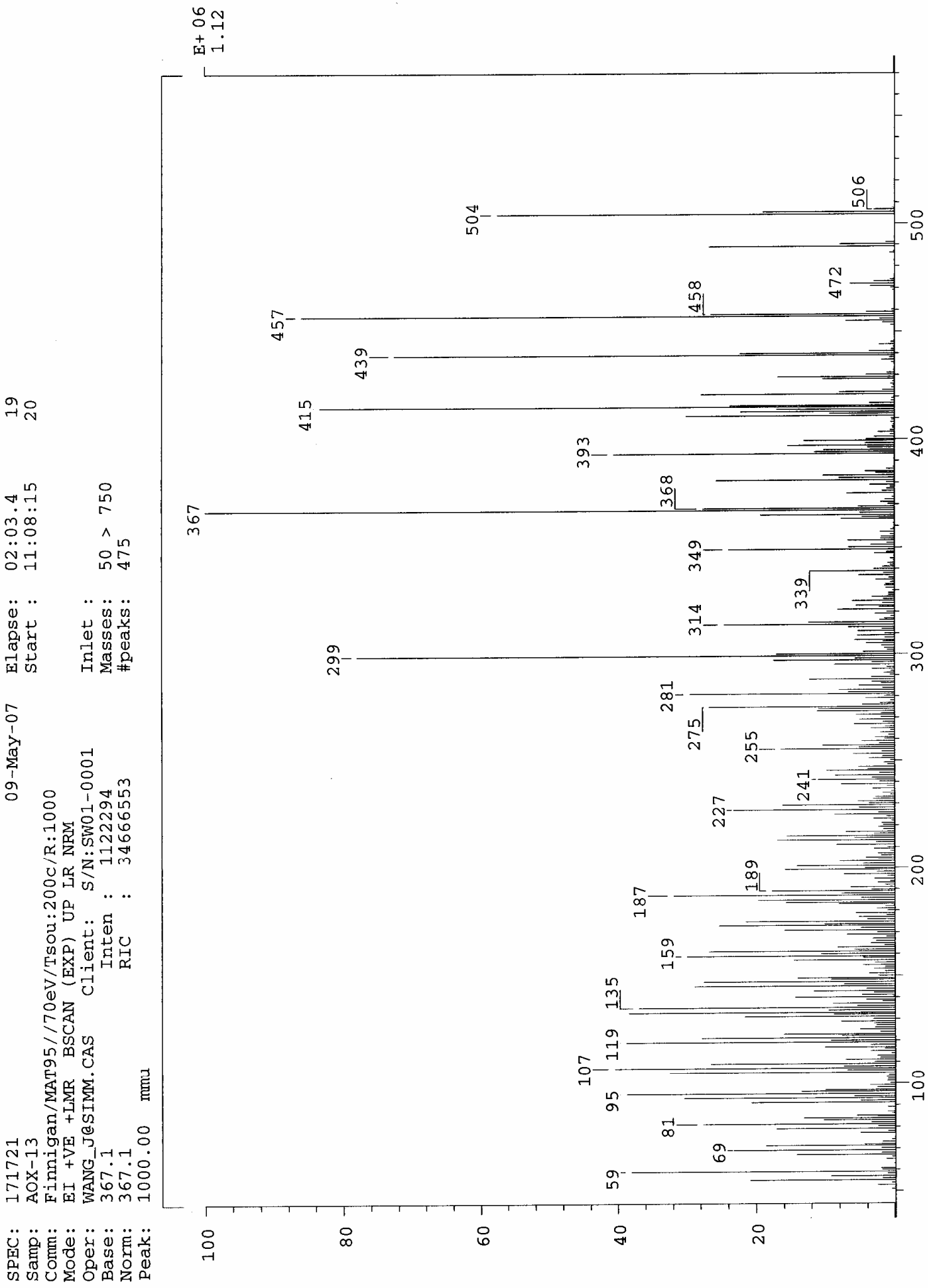


Figure S39. IR spectrum of agladupol E (**5**)

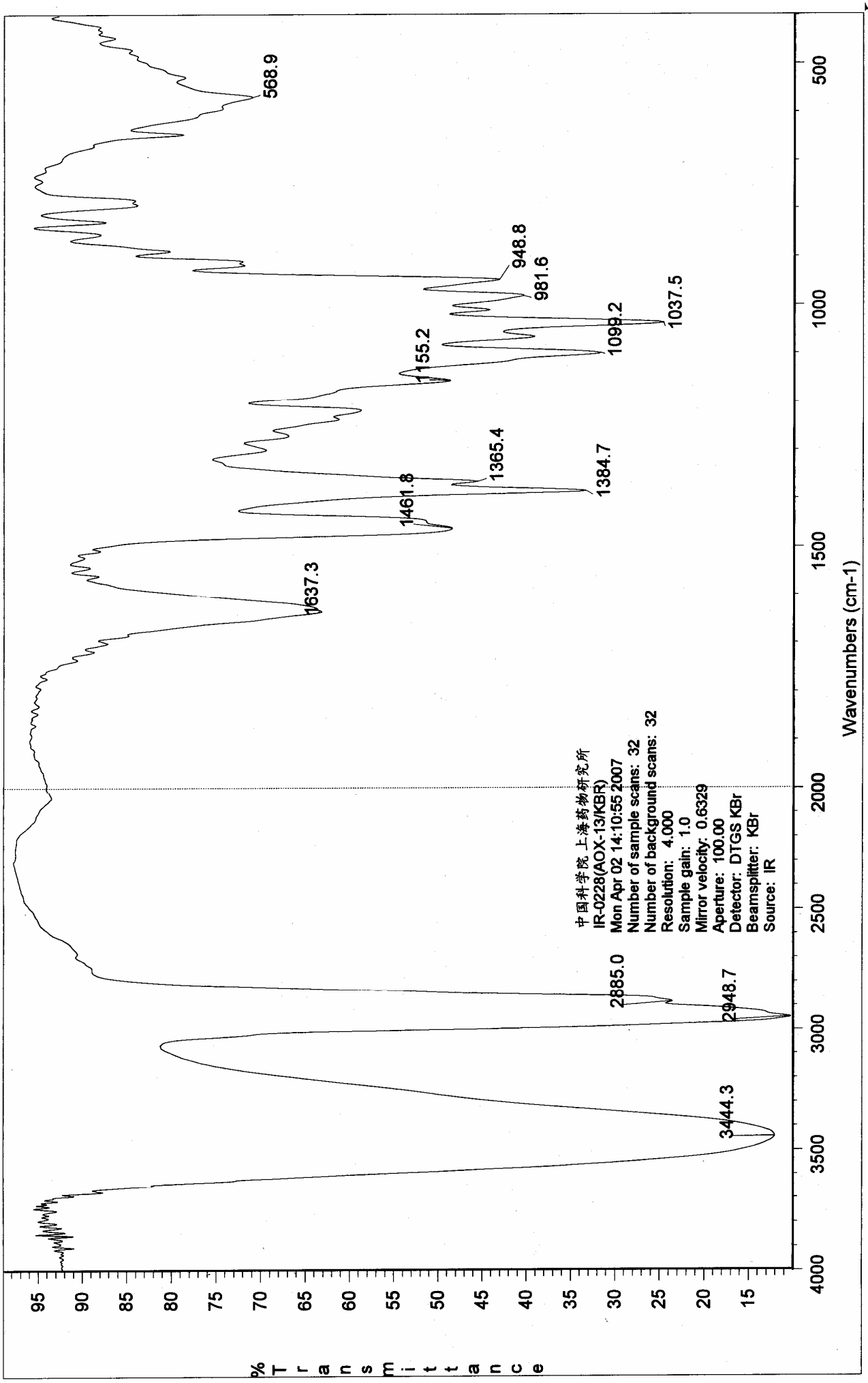
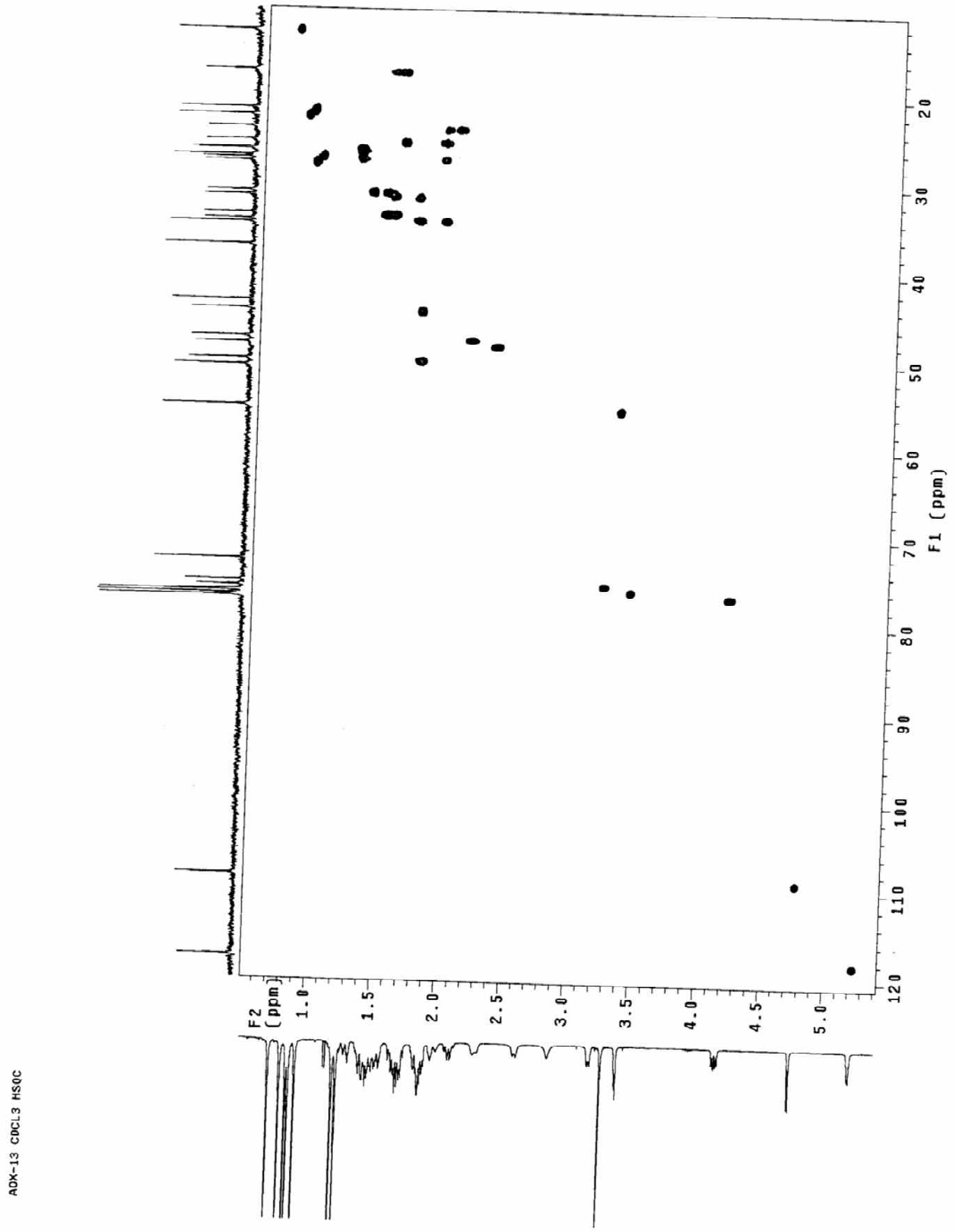



Figure S40. HSQC spectrum of agladupol E (**5**) in $CDCl_3$