

Antioxidant Activity, Molecular Docking, and Modeling Pharmacokinetics Study of Some Benzo[f]quinoline Candidates

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Ψ: The first and second authors are equally contributed to this work.

Spectral data:

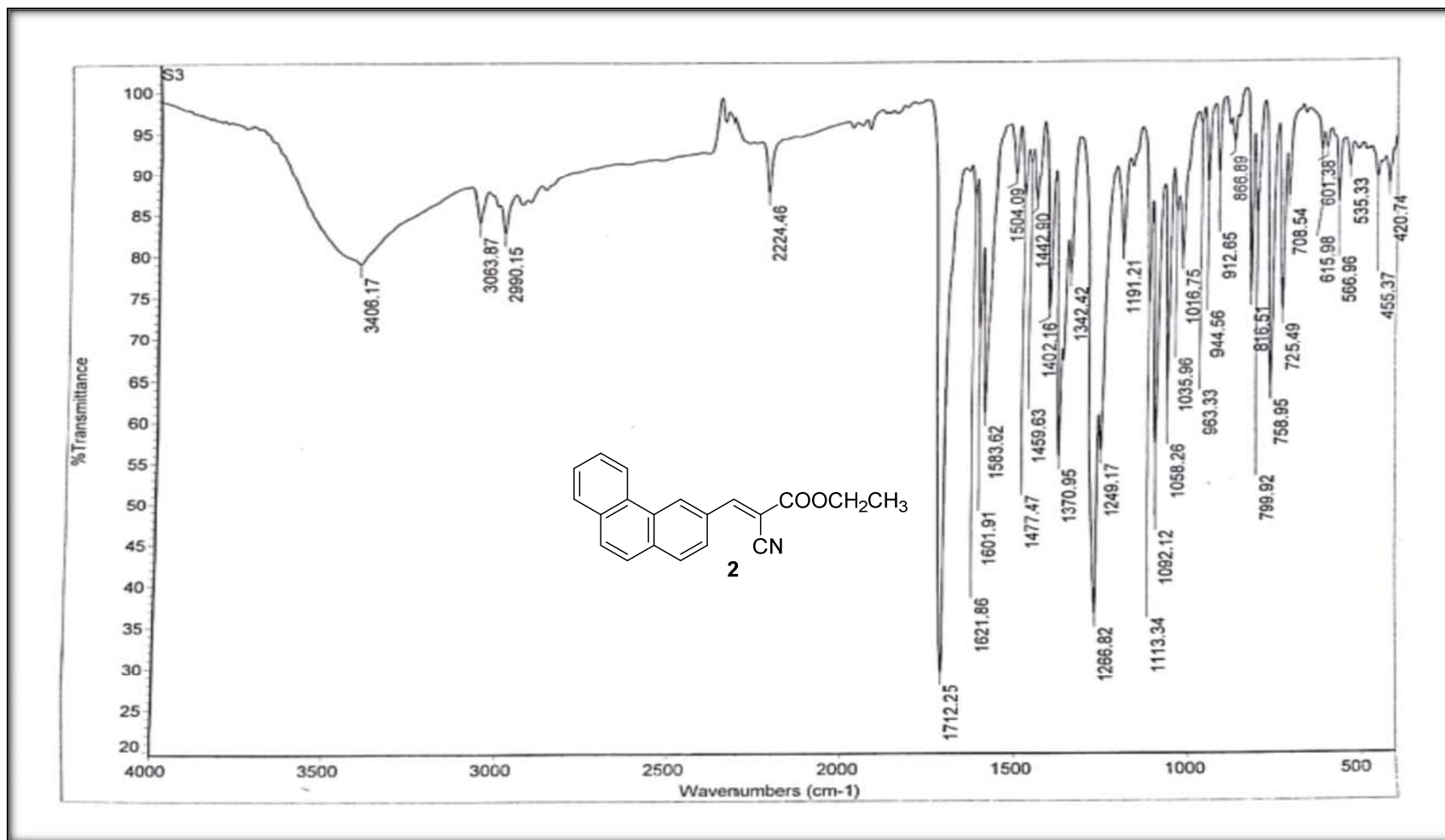


Fig. SD1. IR spectrum of compound 2

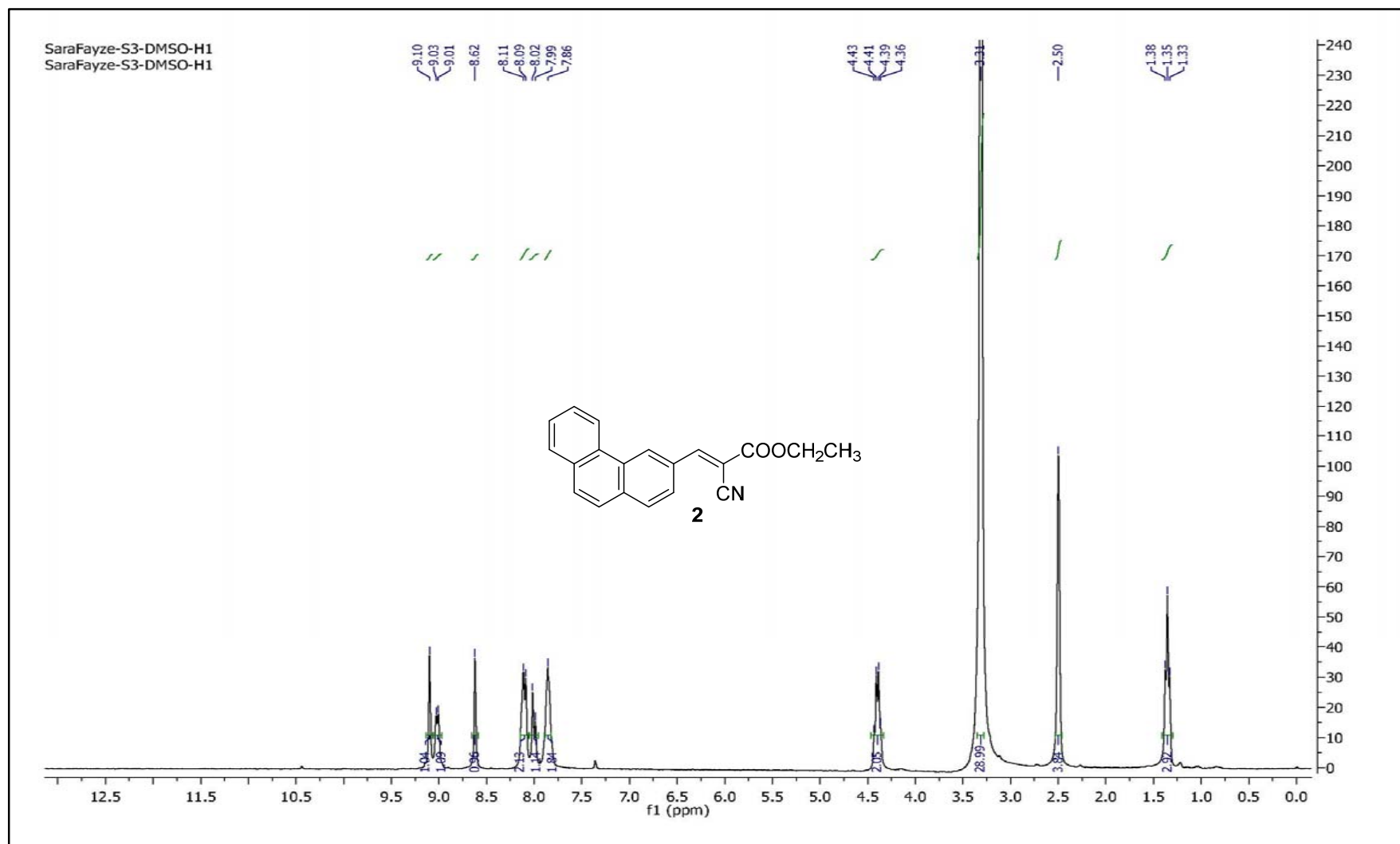
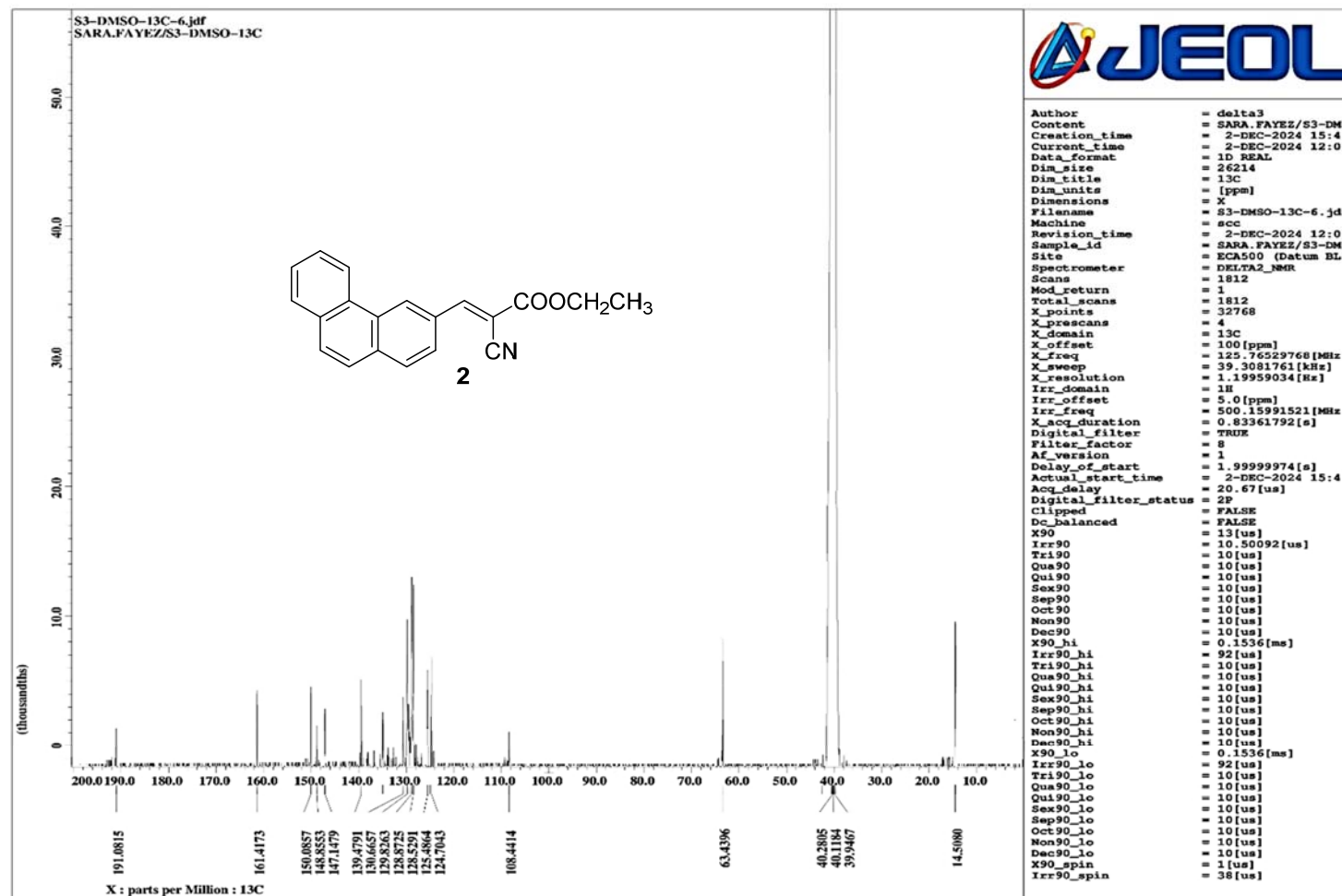


Fig. SD2. ^1H NMR spectrum ($\text{DMSO}-d_6$) of compound **2**



Cont. Fig. SD2. ¹³C NMR spectrum (DMSO-*d*₆) of compound 2

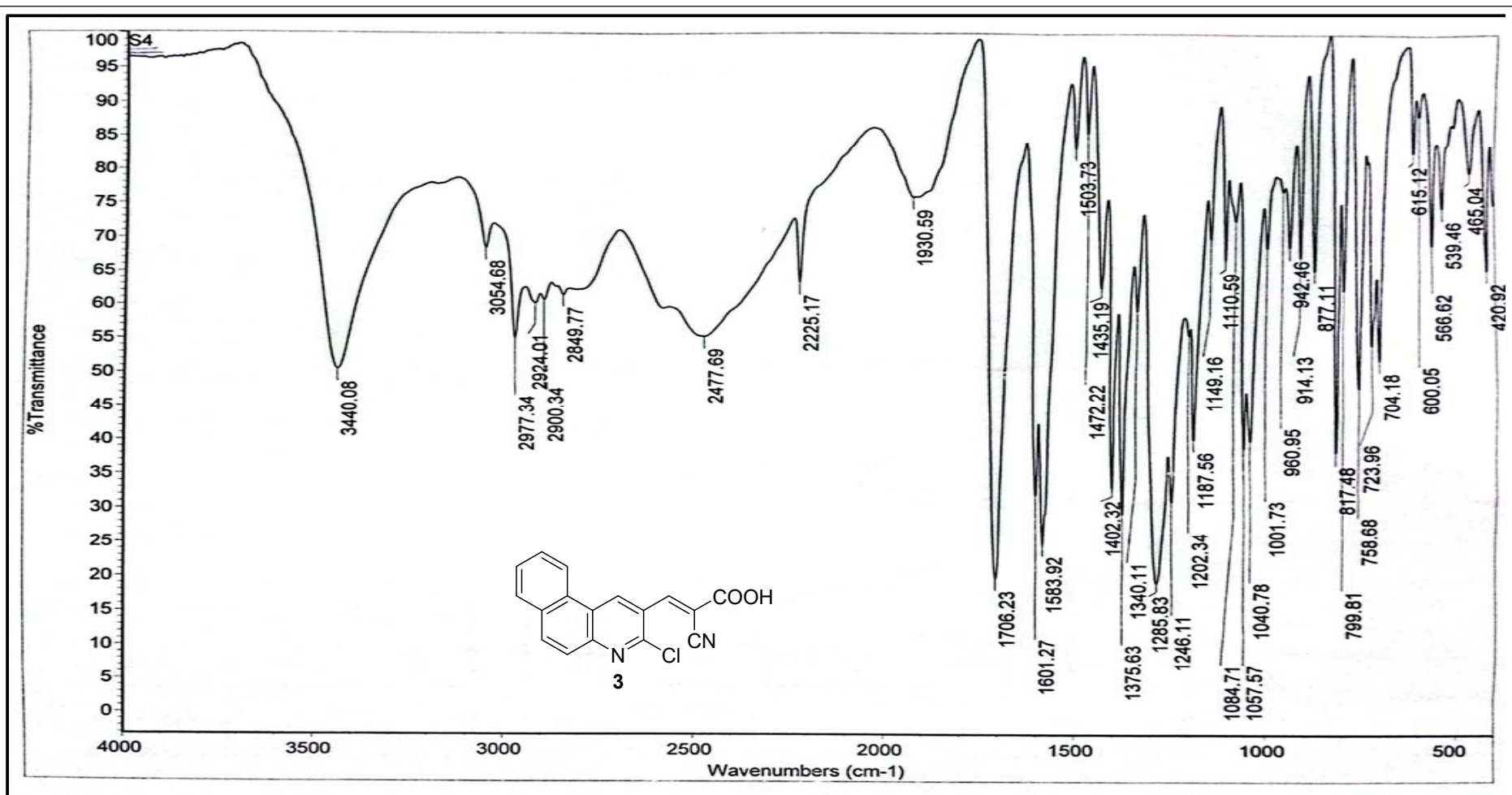


Fig. SD3. IR spectrum of compound 3

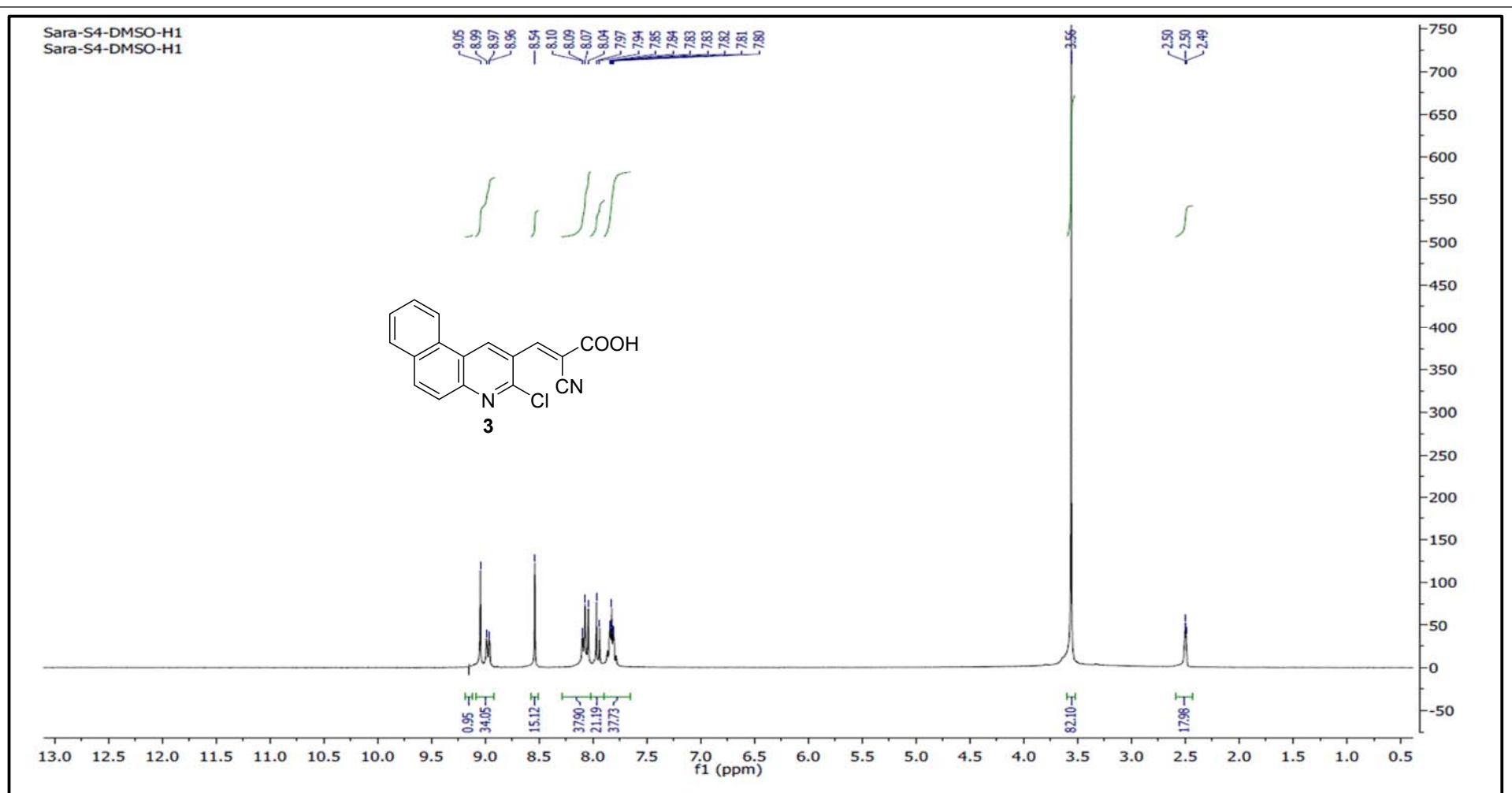


Fig. SD4. ^1H NMR spectrum ($\text{DMSO-}d_6$) of compound **3**

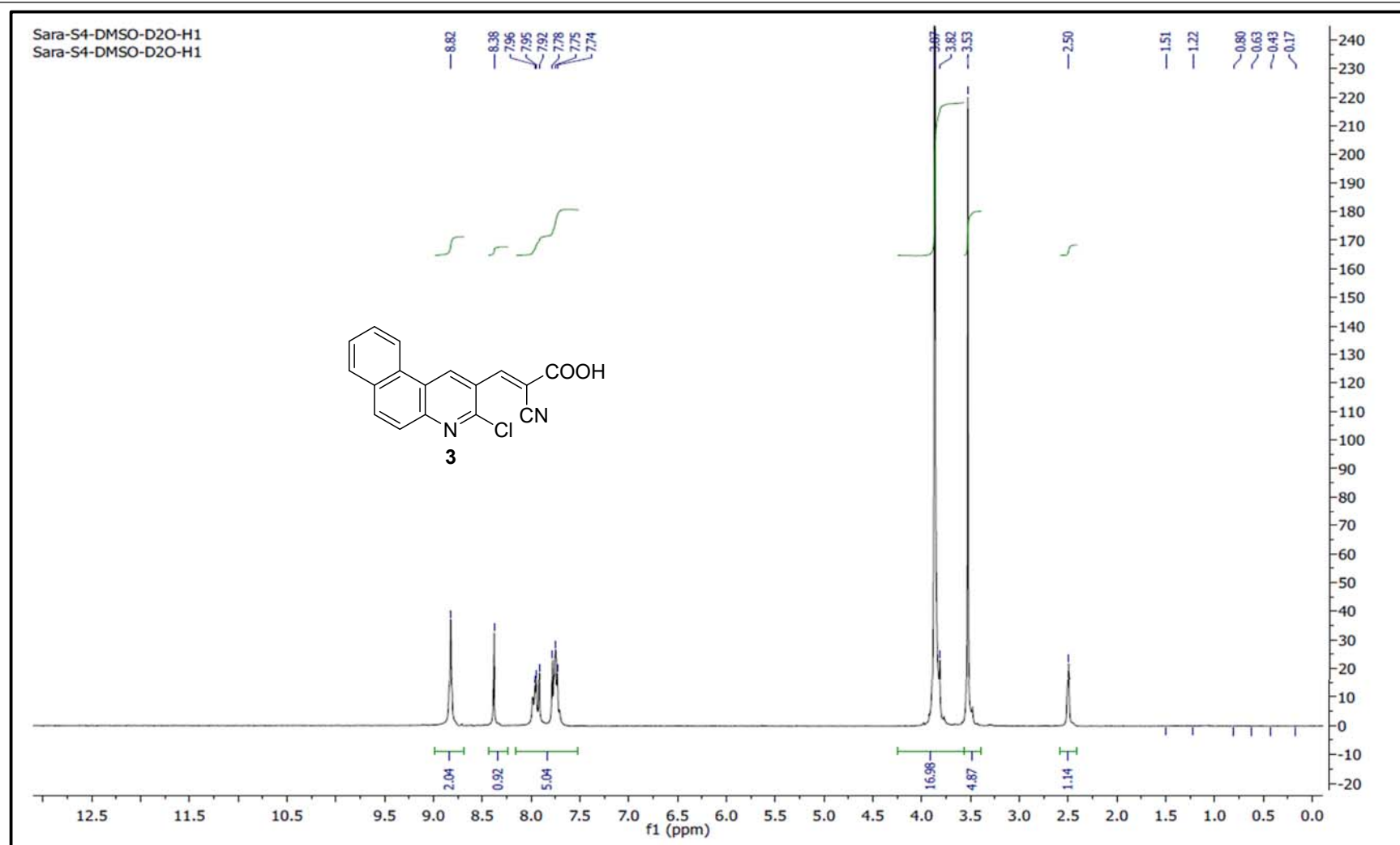


Fig. SD5. ^1H NMR spectrum ($\text{DMSO-}d_6+\text{D}_2\text{O}$) of compound 3

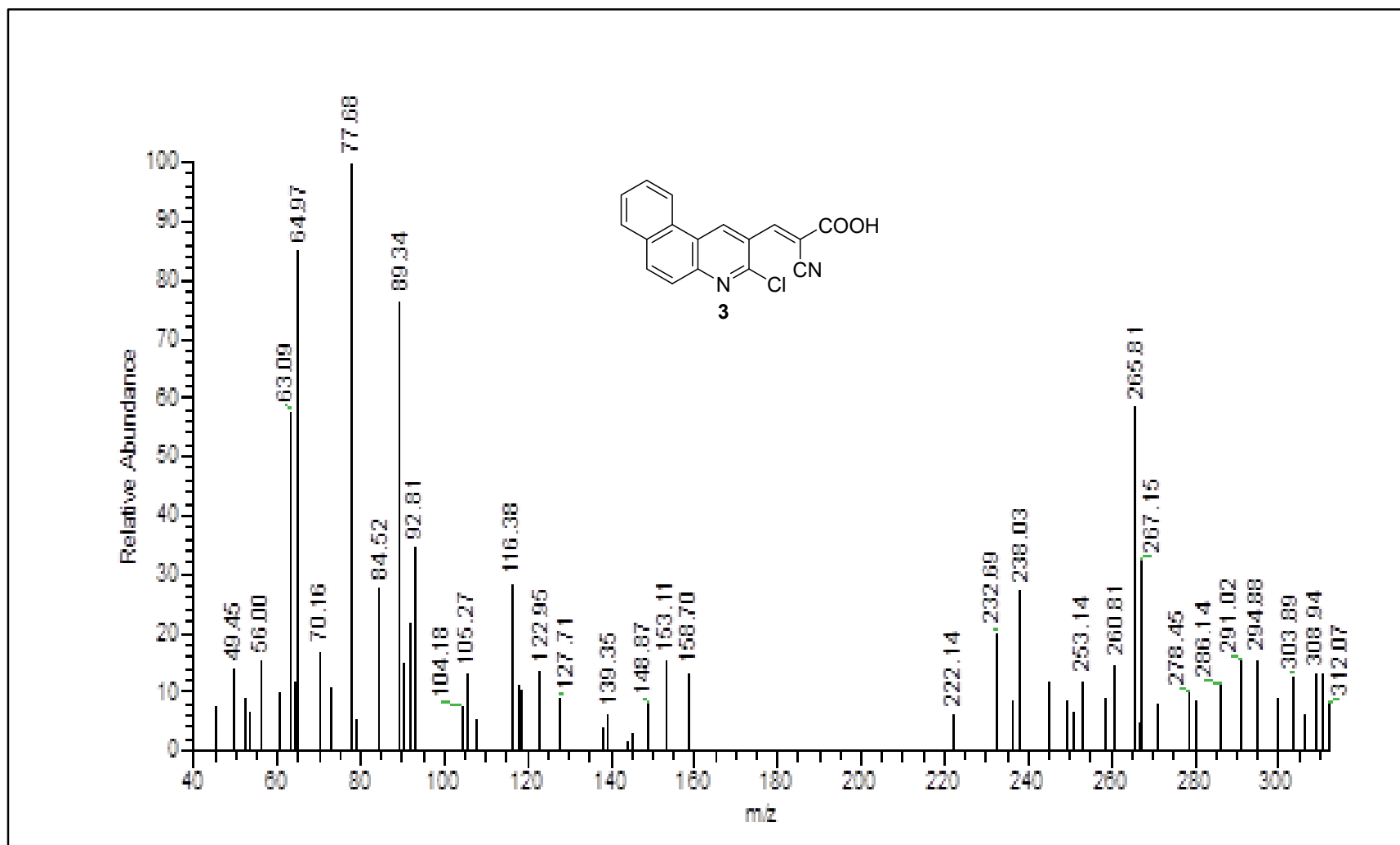


Fig. SD6. Mass spectrum of compound 3

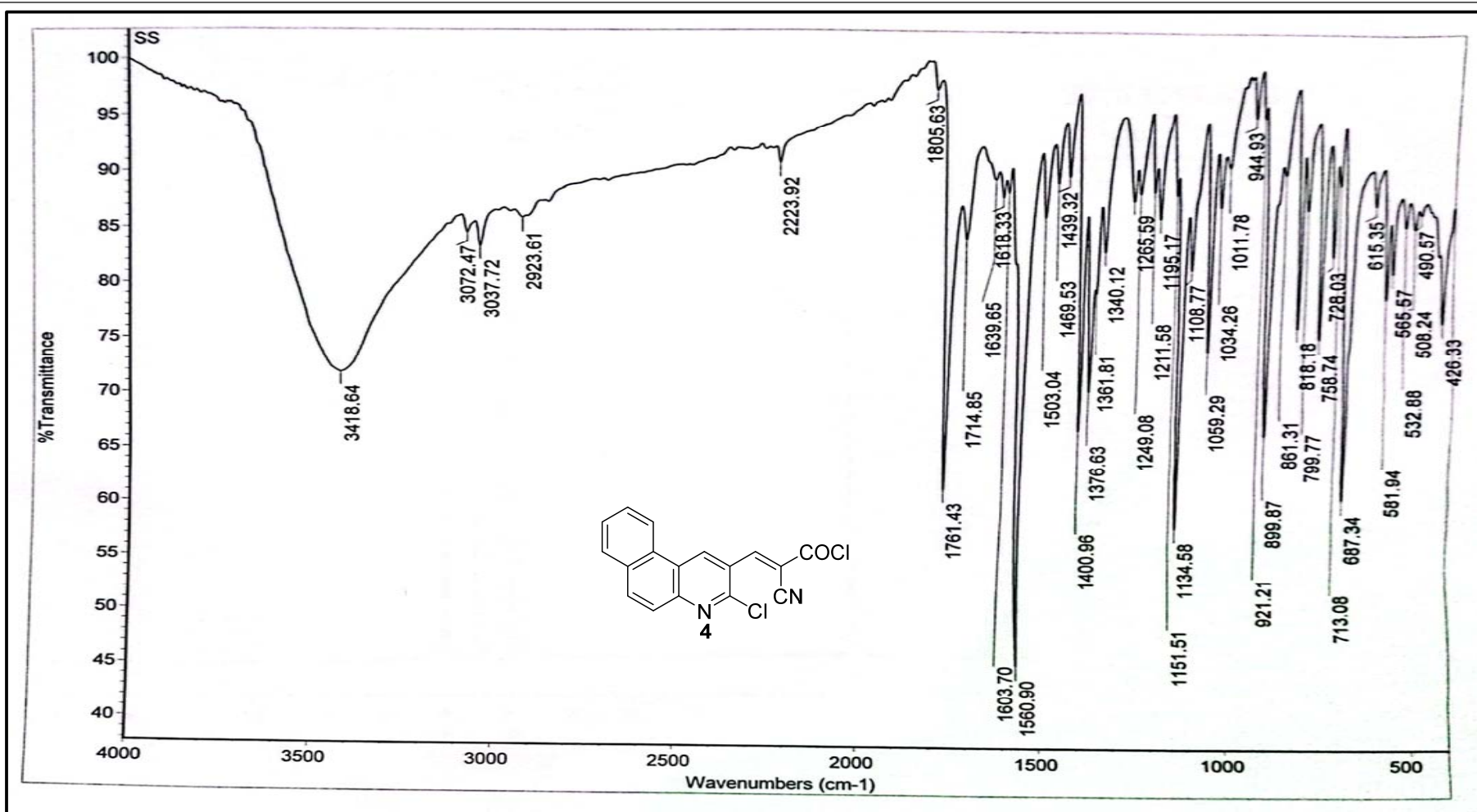


Fig. SD7. IR spectrum of compound 4

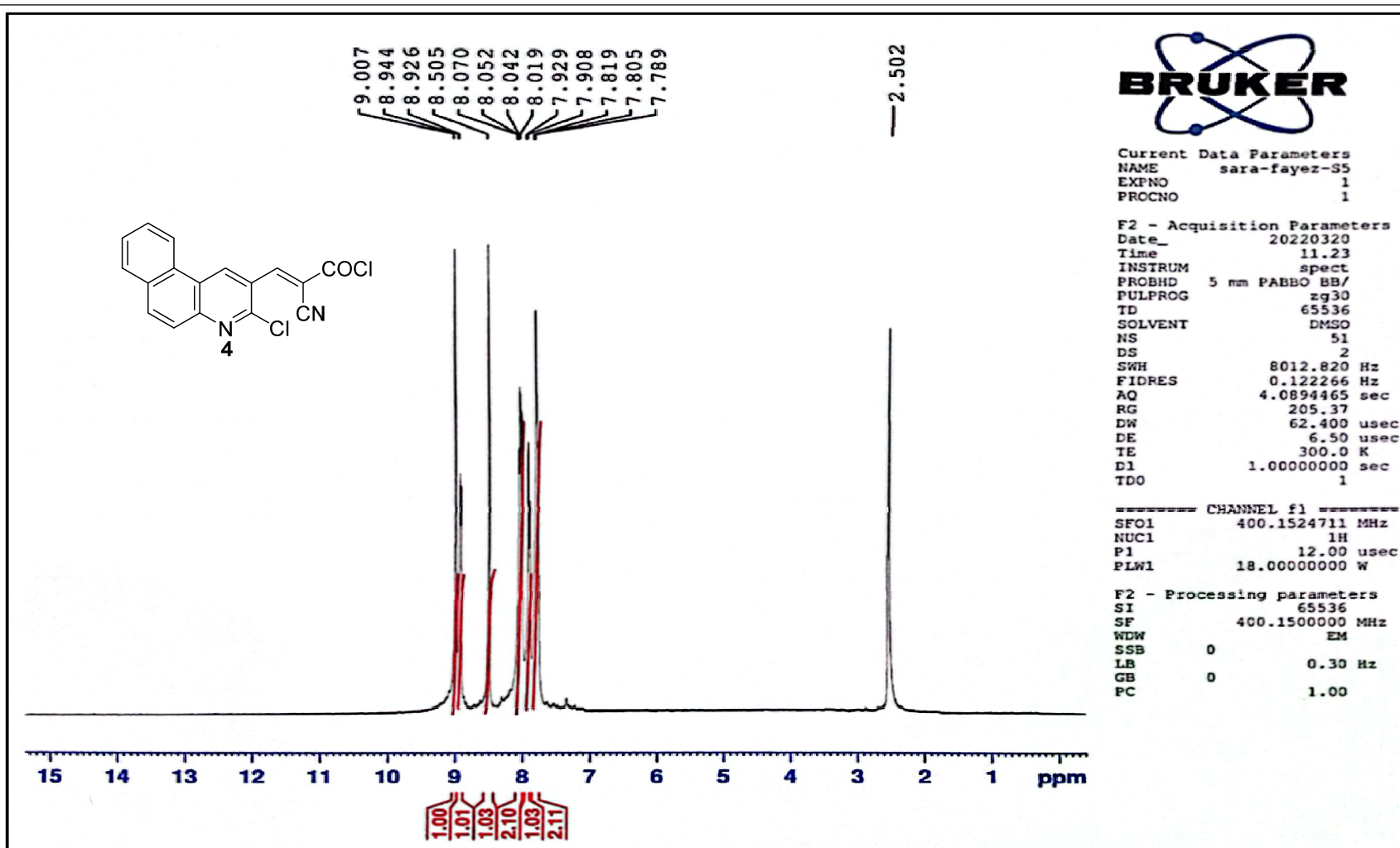
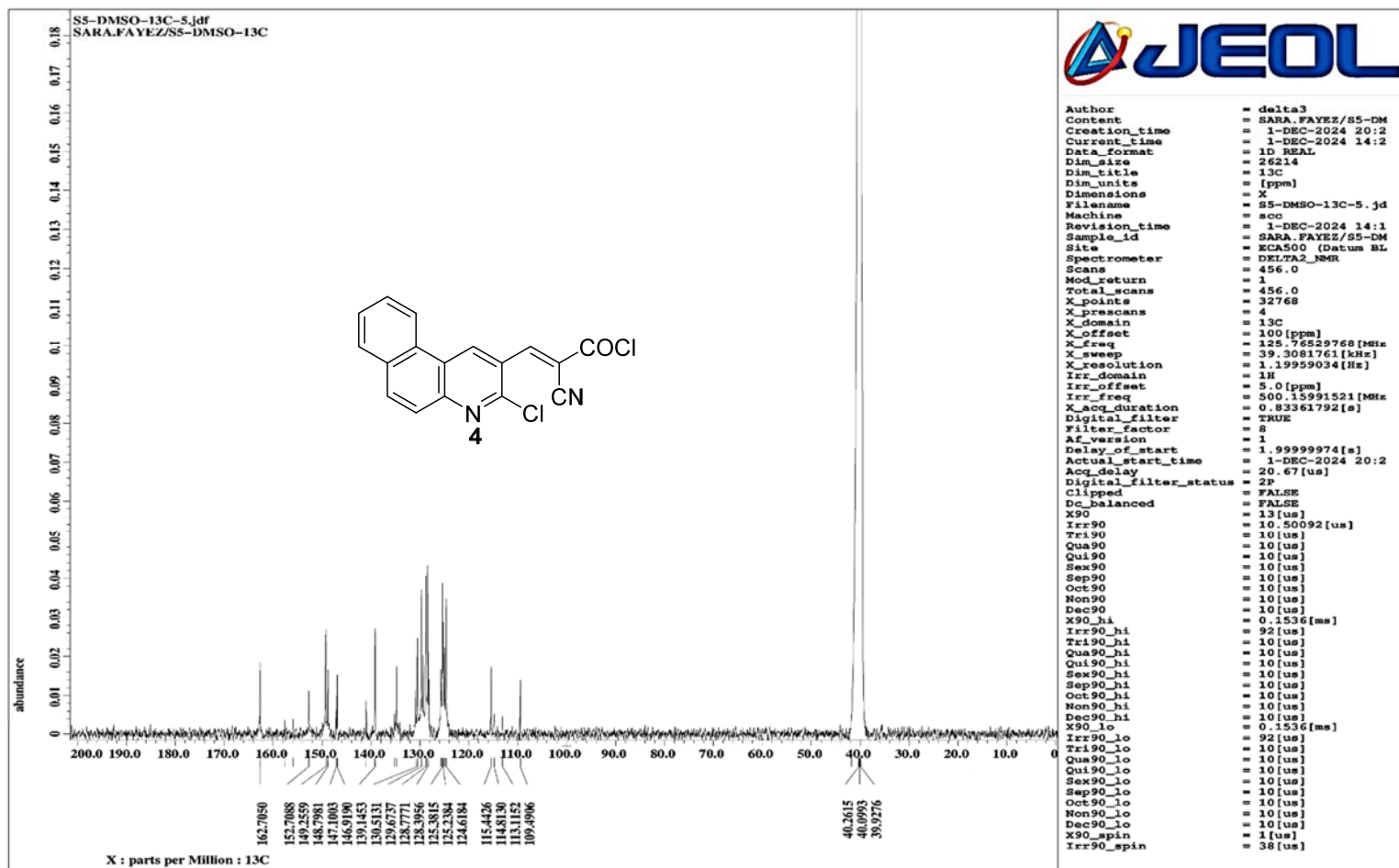


Fig. SD8. ¹H NMR spectrum (DMSO-*d*₆) of compound 4



Cont. Fig. SD8. ^{13}C NMR spectrum ($\text{DMSO-}d_6$) of compound 4

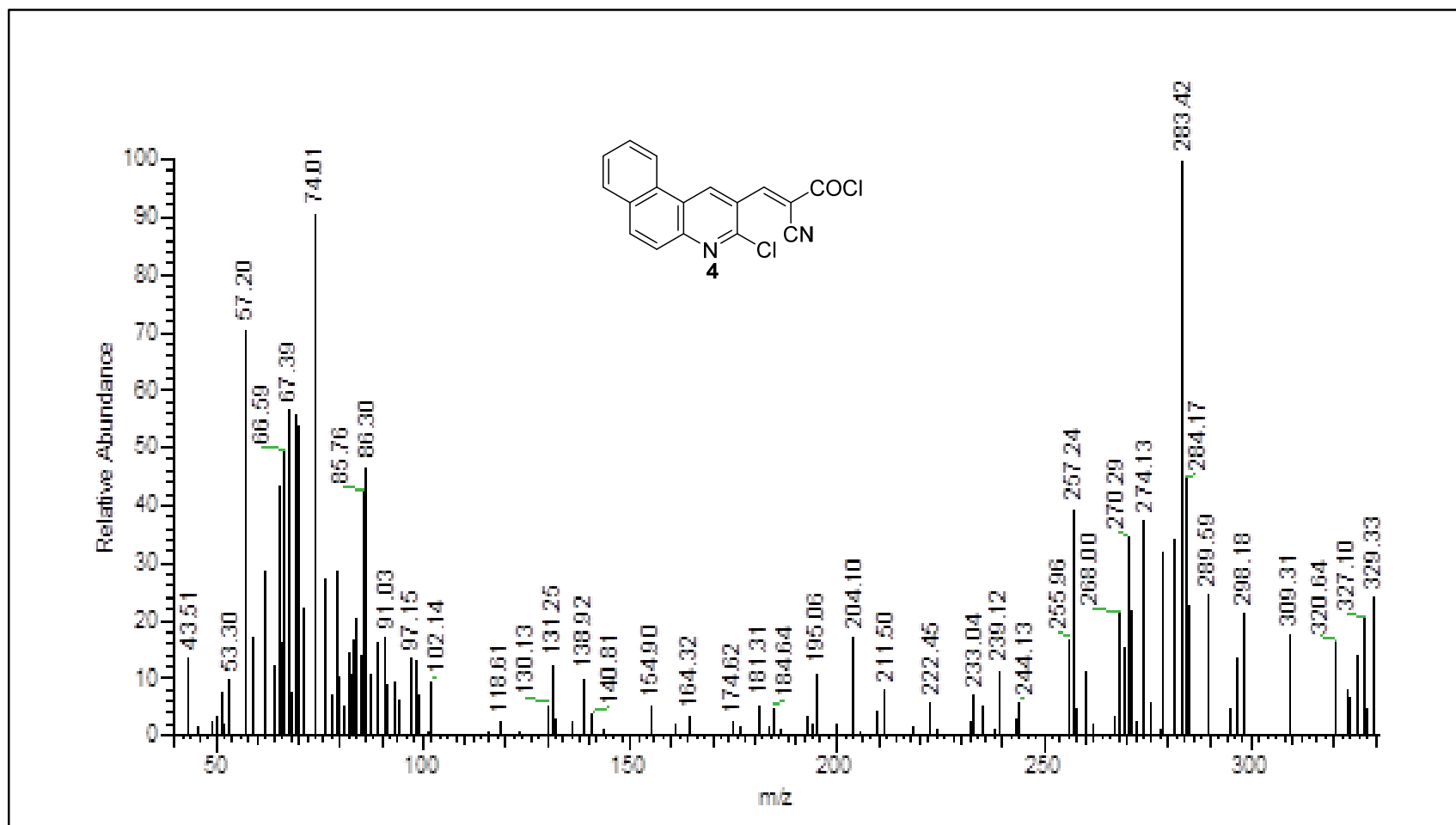


Fig. SD9. Mass spectrum of compound 4

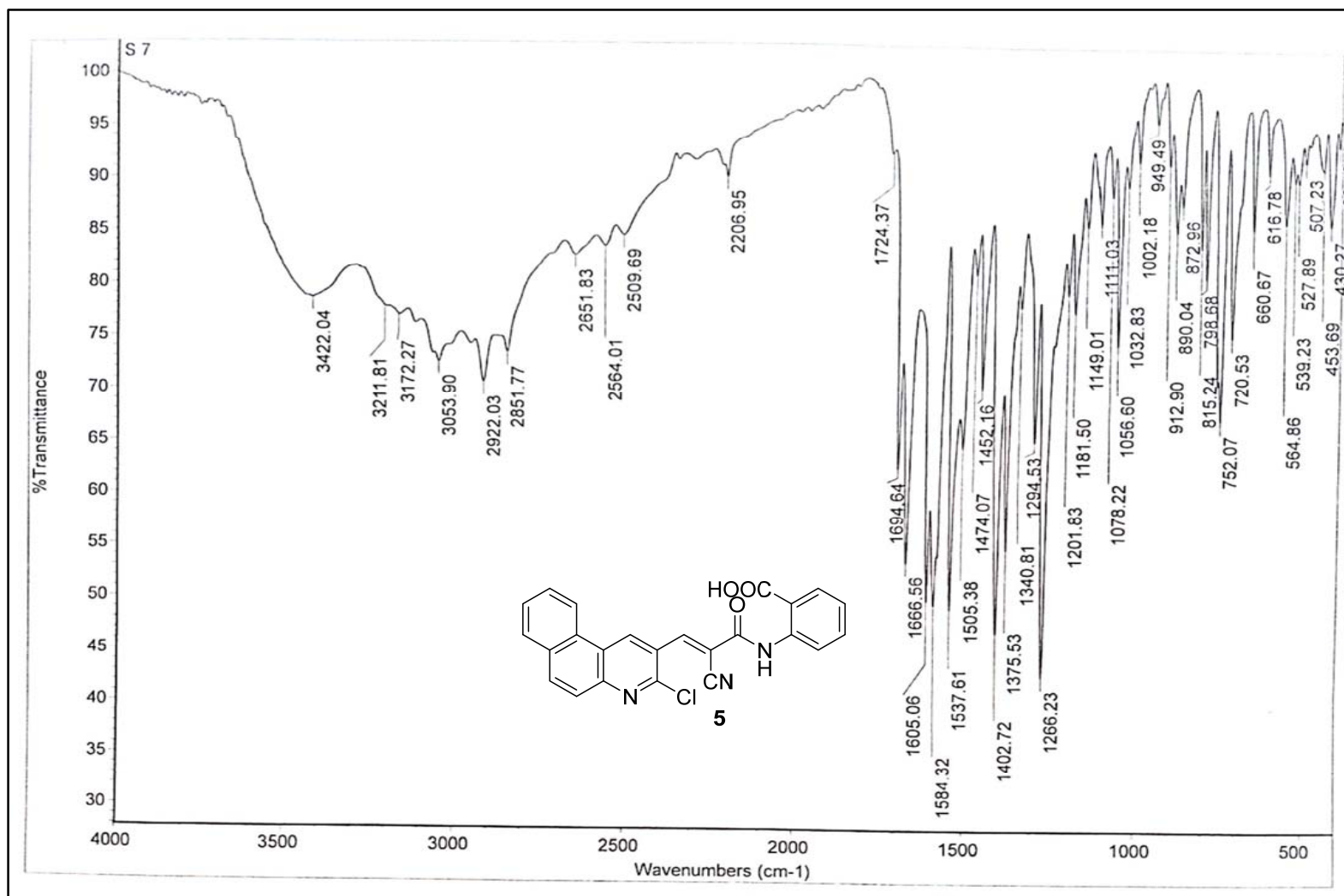


Fig. SD10. IR spectrum of compound 5

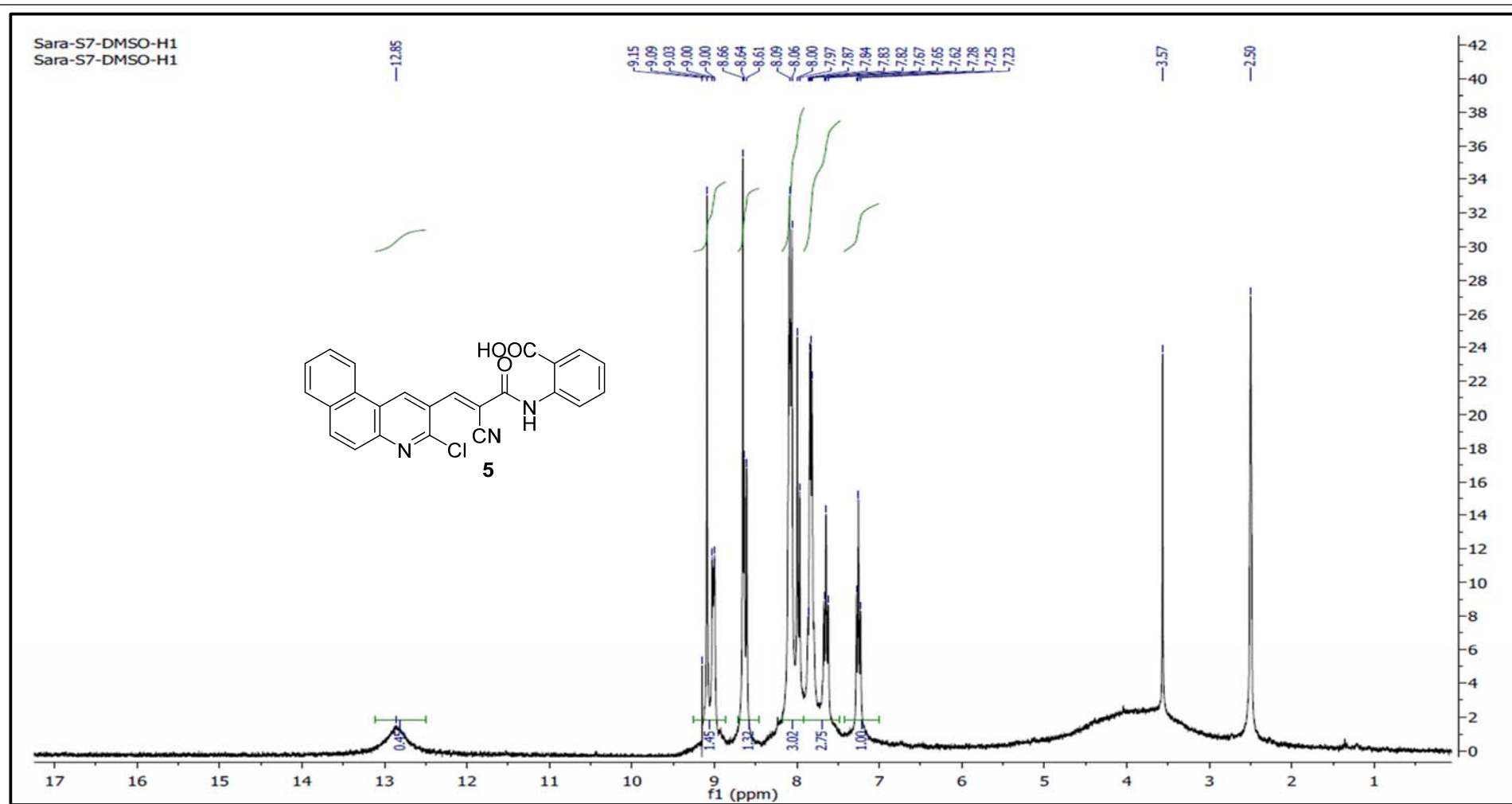


Fig. SD11. ^1H NMR spectrum (DMSO- d_6) of compound **5**

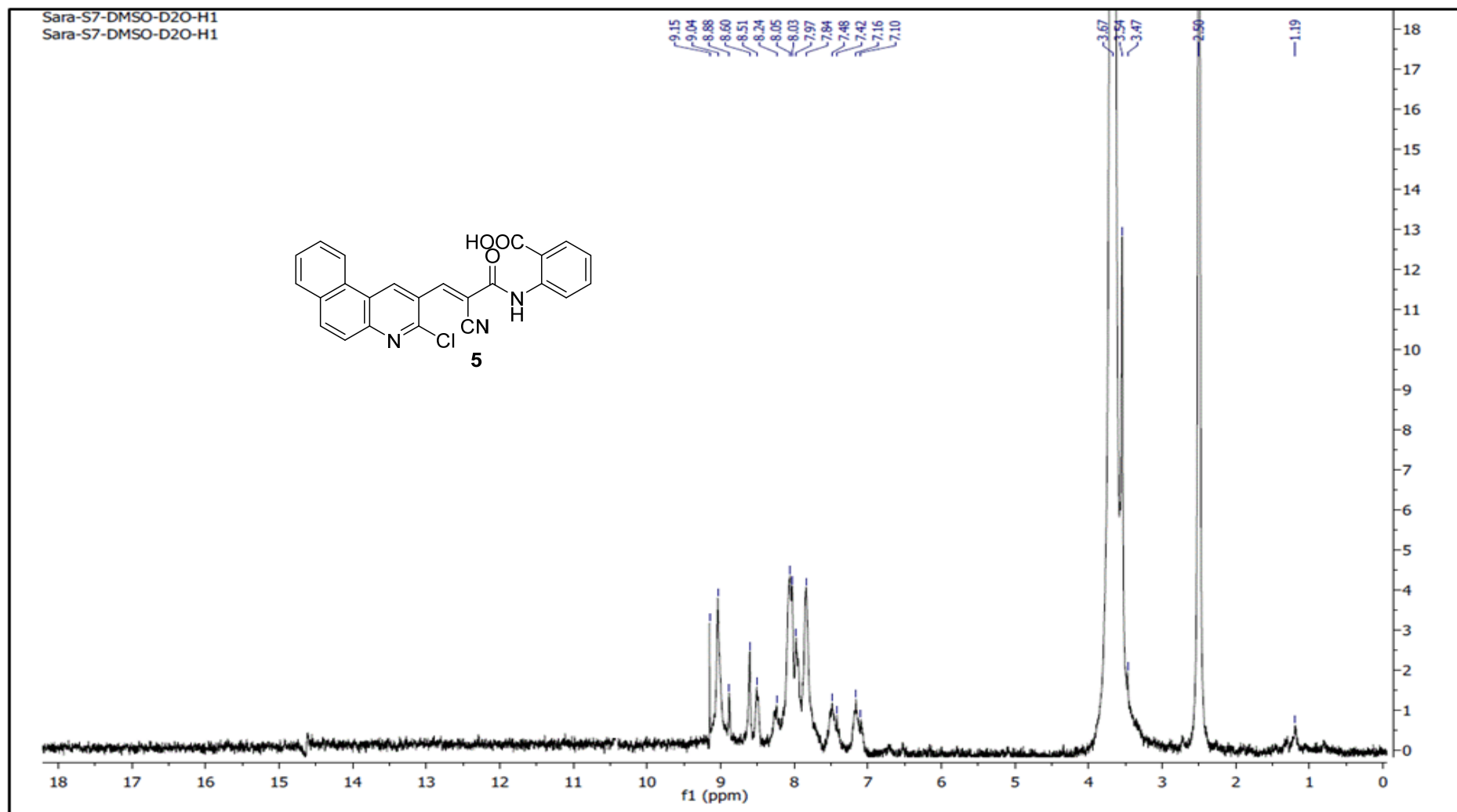


Fig. SD12. ^1H NMR spectrum ($\text{DMSO}-d_6+\text{D}_2\text{O}$) of compound **5**

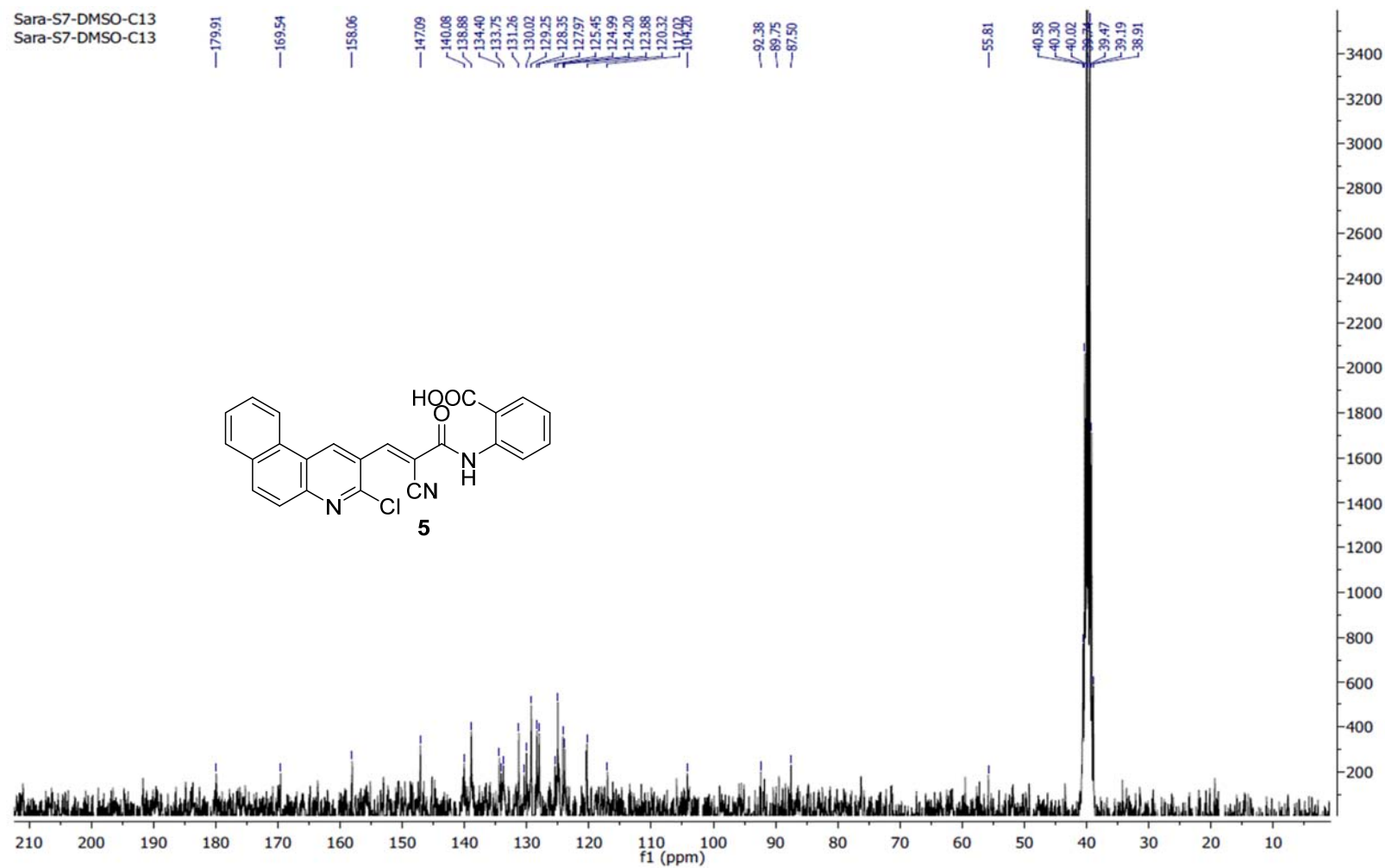


Fig. SD13. ^{13}C NMR spectrum ($\text{DMSO}-d_6$) of compound **5**

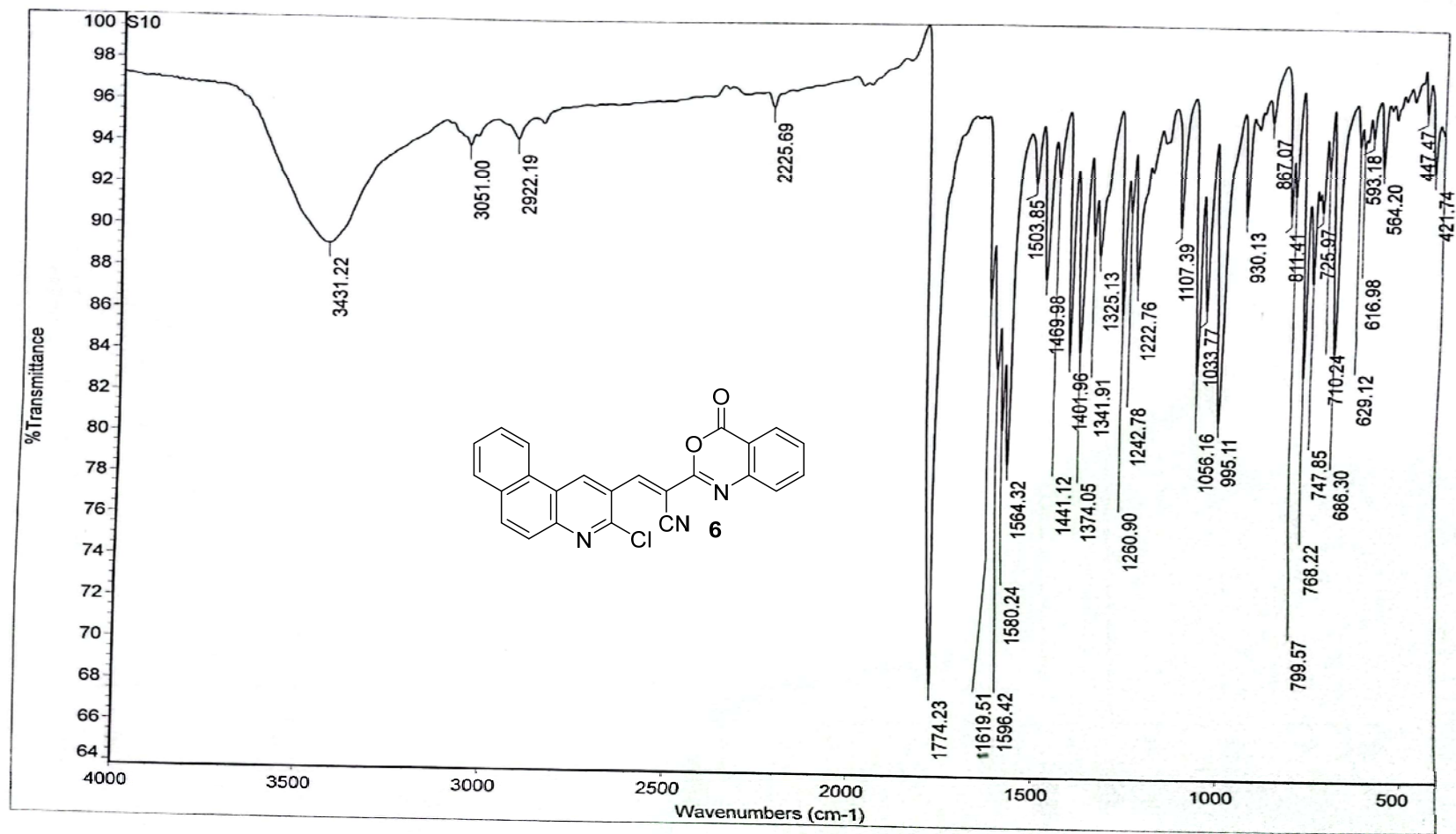


Fig. SD14. IR spectrum of compound 6

Sara Fayed_H_S10

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MAU
Microanalytical Unit
FOPCU
وحدة التحليل الطيفي

20
FACULTY OF PHARMACY
CAIRO UNIVERSITY

BRUKER

Current Data Parameters
NAME: Sara Fayed_H_S10
EXPNO: 10
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20230605
Time: 9.41
INSTRUM: spect
PROBHD: 5 mm PABBO BB/
PULPROG: zg30
TD: 65536
SOLVENT: DMSO
NS: 32
DS: 2
SWH: 8012.820 Hz
FIDRES: 0.122266 Hz
AQ: 4.0894465 sec
RG: 202.37
DW: 62.400 usec
DE: 6.50 usec
TE: 298.0 K
D1: 1.00000000 sec
TDO: 1

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SFOL: 400.192413 MHz
NUC1: 1H
P1: 15.00 usec
PLW1: 10.39999952 W

F2 - Processing parameters
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WDW: EM
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LB: 0.30 Hz
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PC: 1.00

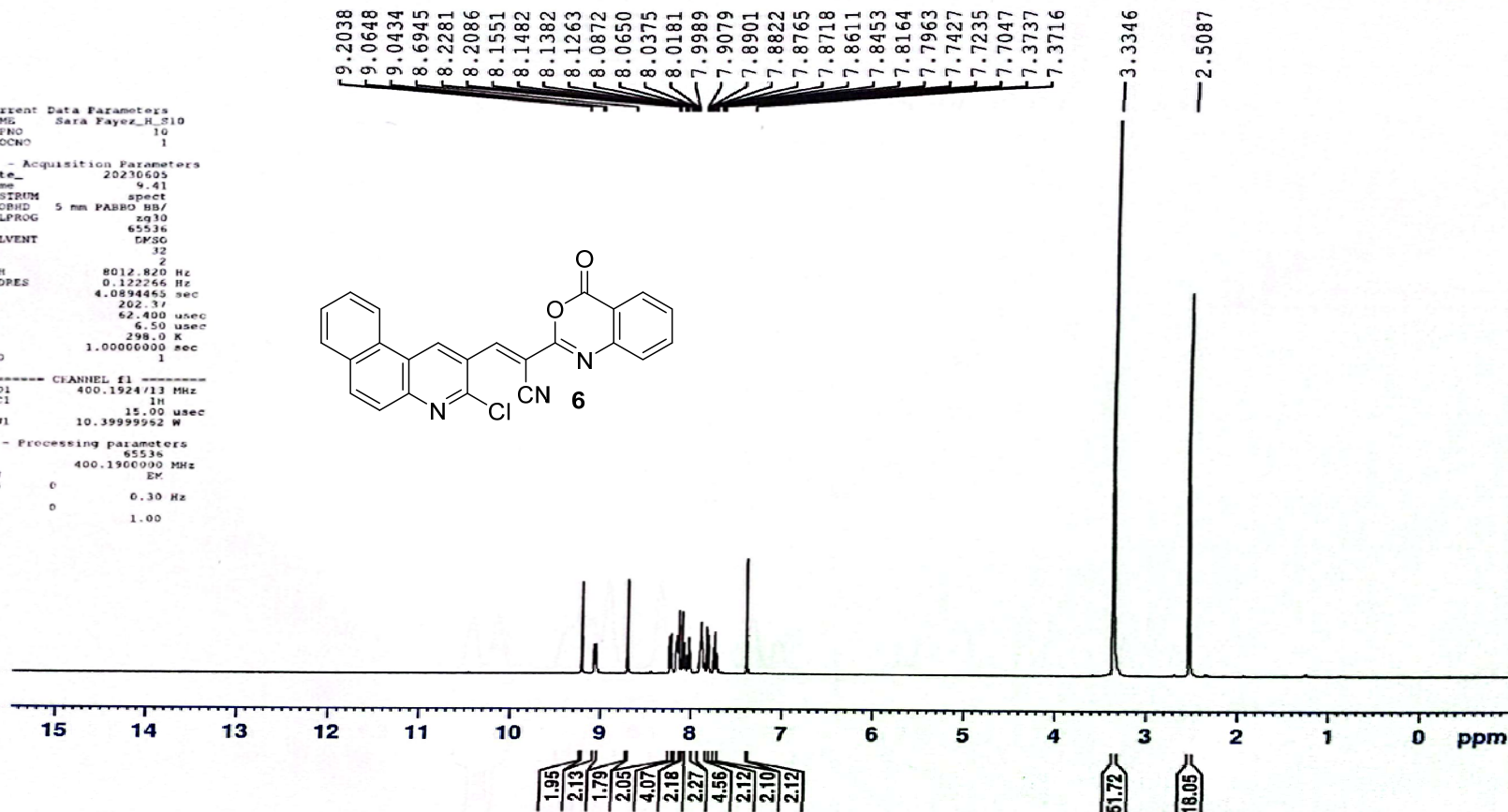
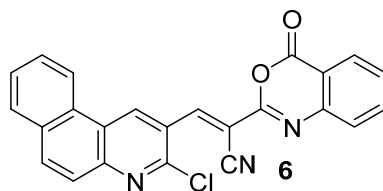
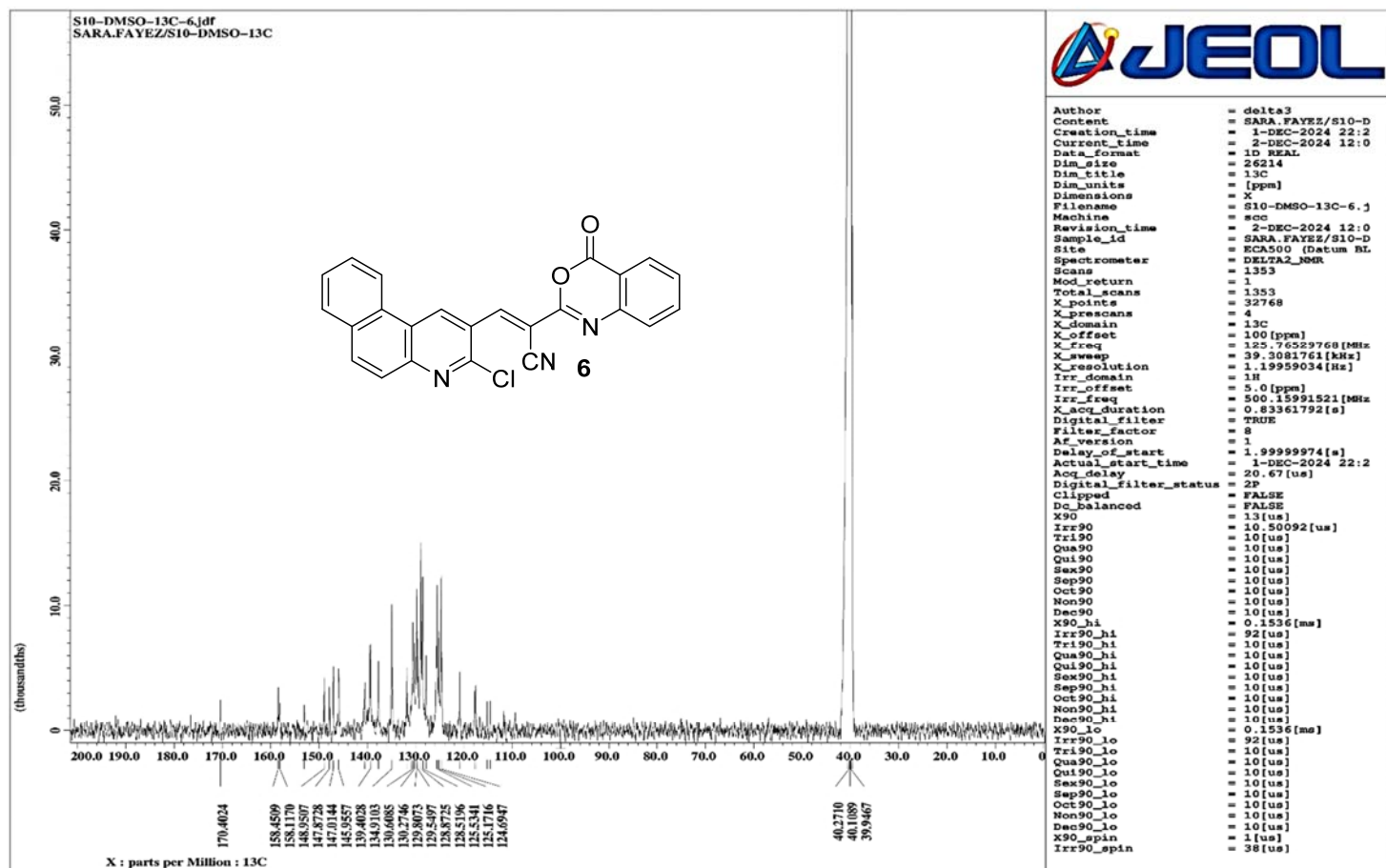


Fig. SD15. ¹H NMR spectrum (DMSO-*d*₆) of compound 6



Cont. Fig. SD15. ^{13}C NMR spectrum (DMSO- d_6) of compound 6

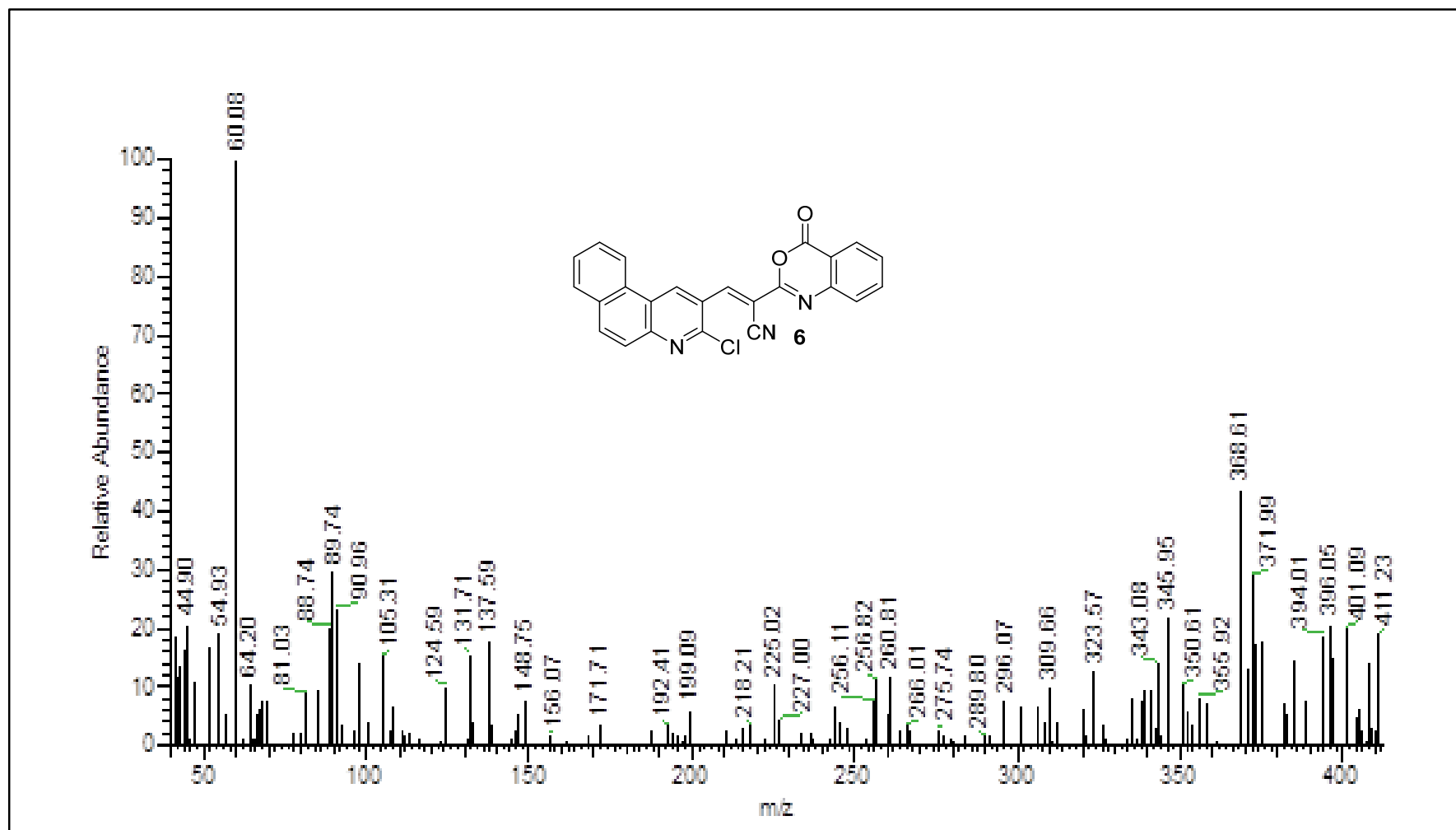


Fig. SD16. Mass spectrum of compound 6

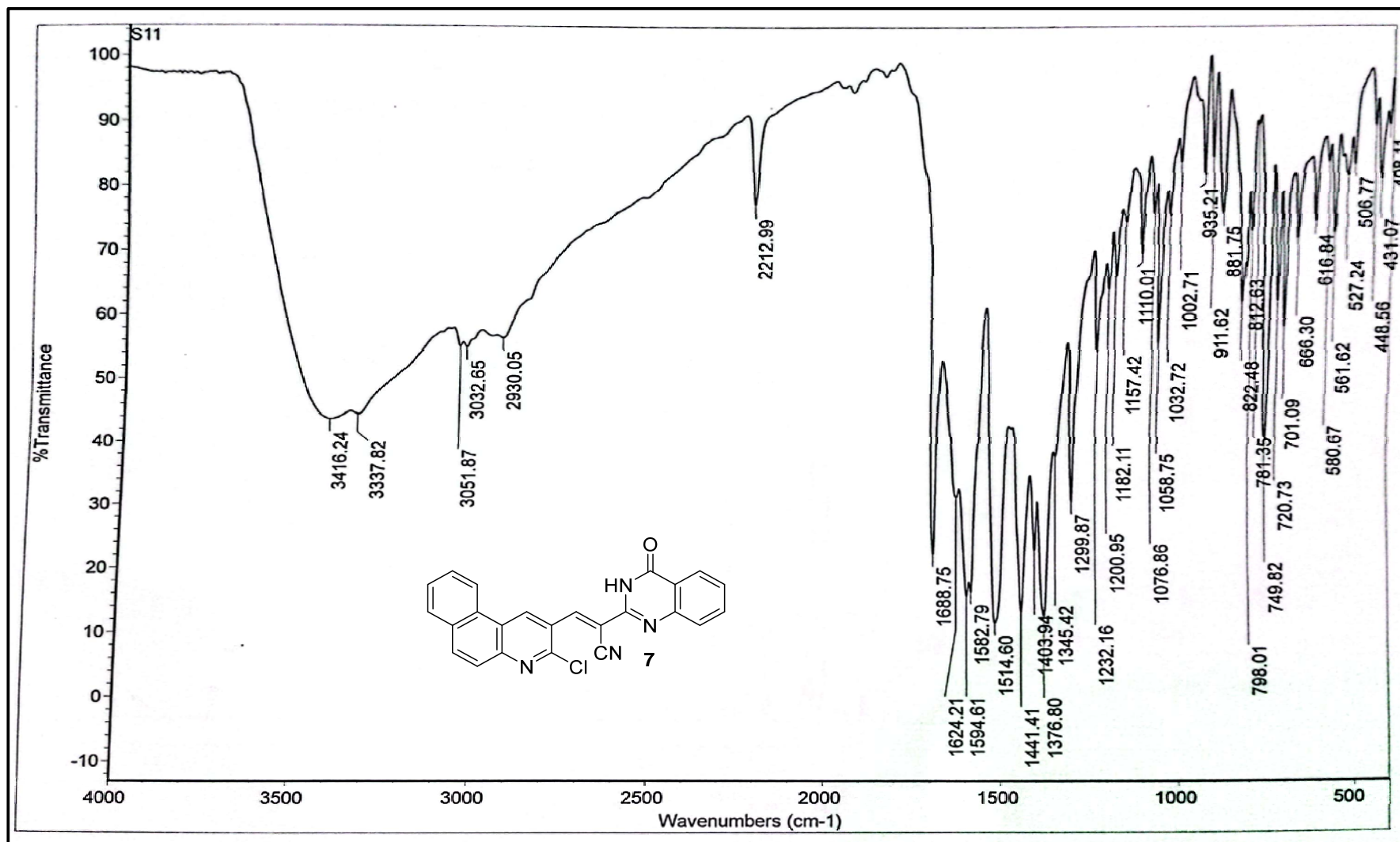


Fig. SD17. IR spectrum of compound 7

Sarahfayez-S11-DMSO-H1

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Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
13 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Mar 26 2023

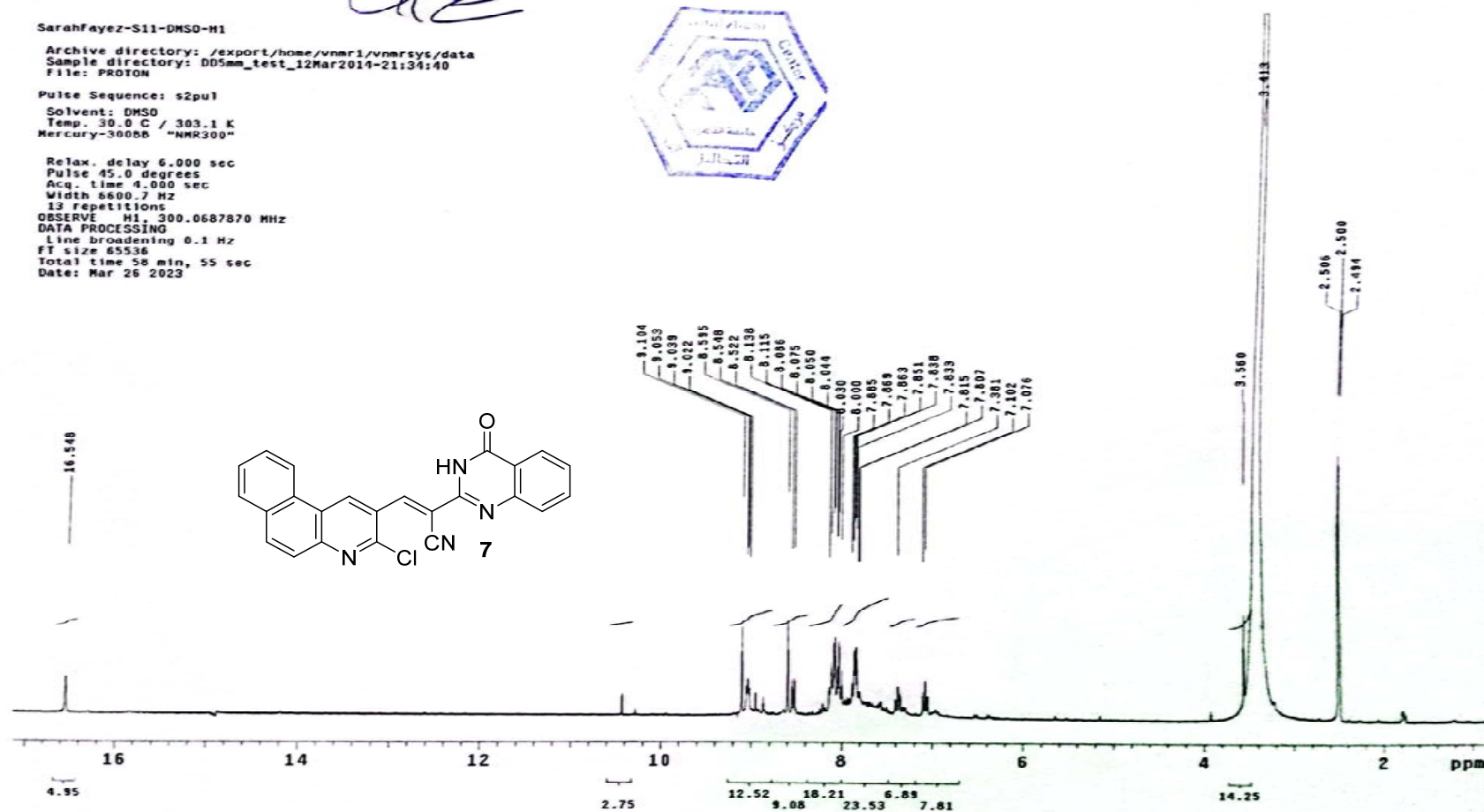


Fig. SD18. ^1H NMR spectrum (DMSO- d_6) of compound 7

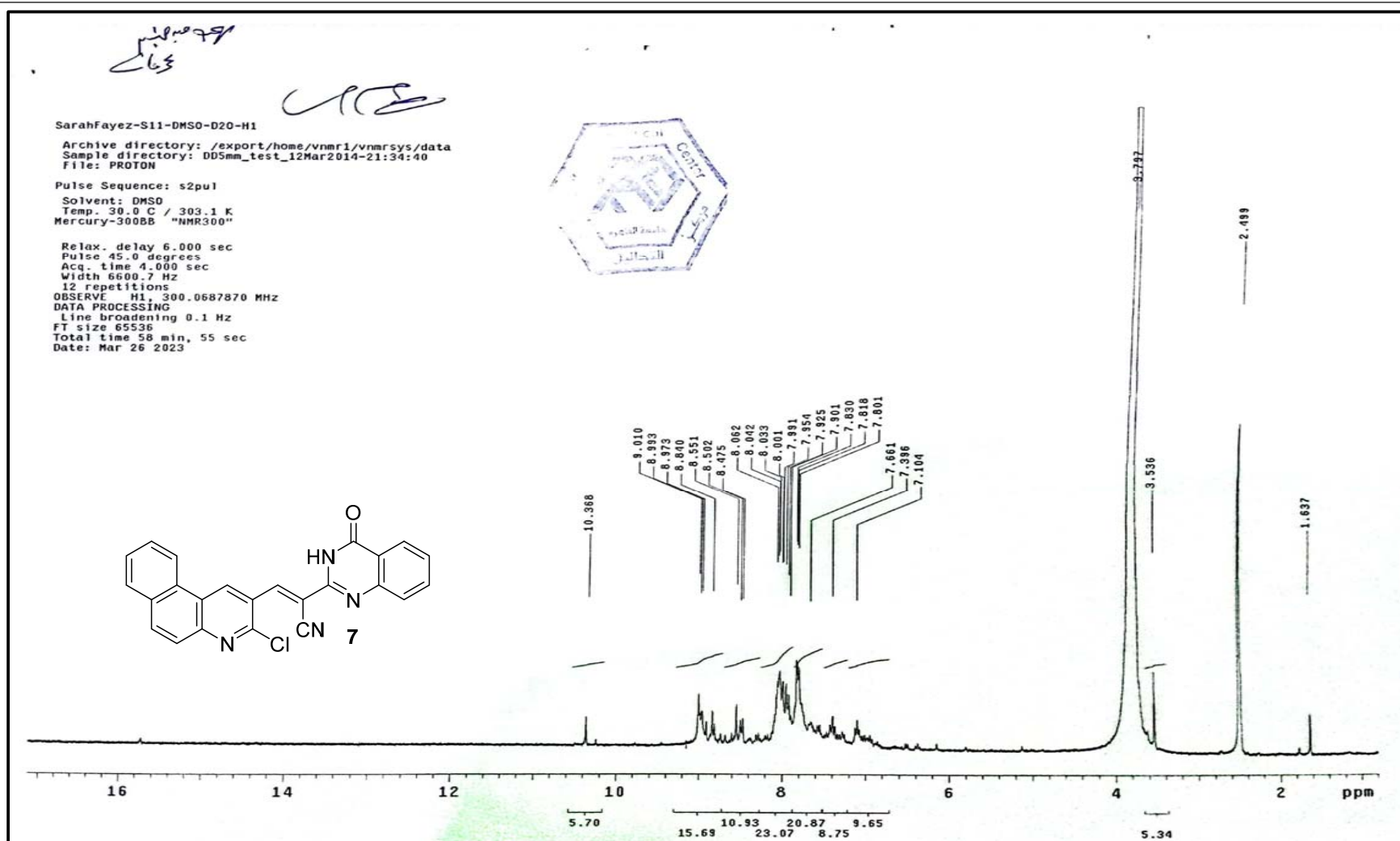


Fig. SD19. ^1H NMR spectrum ($\text{DMSO-}d_6 + \text{D}_2\text{O}$) of compound 7

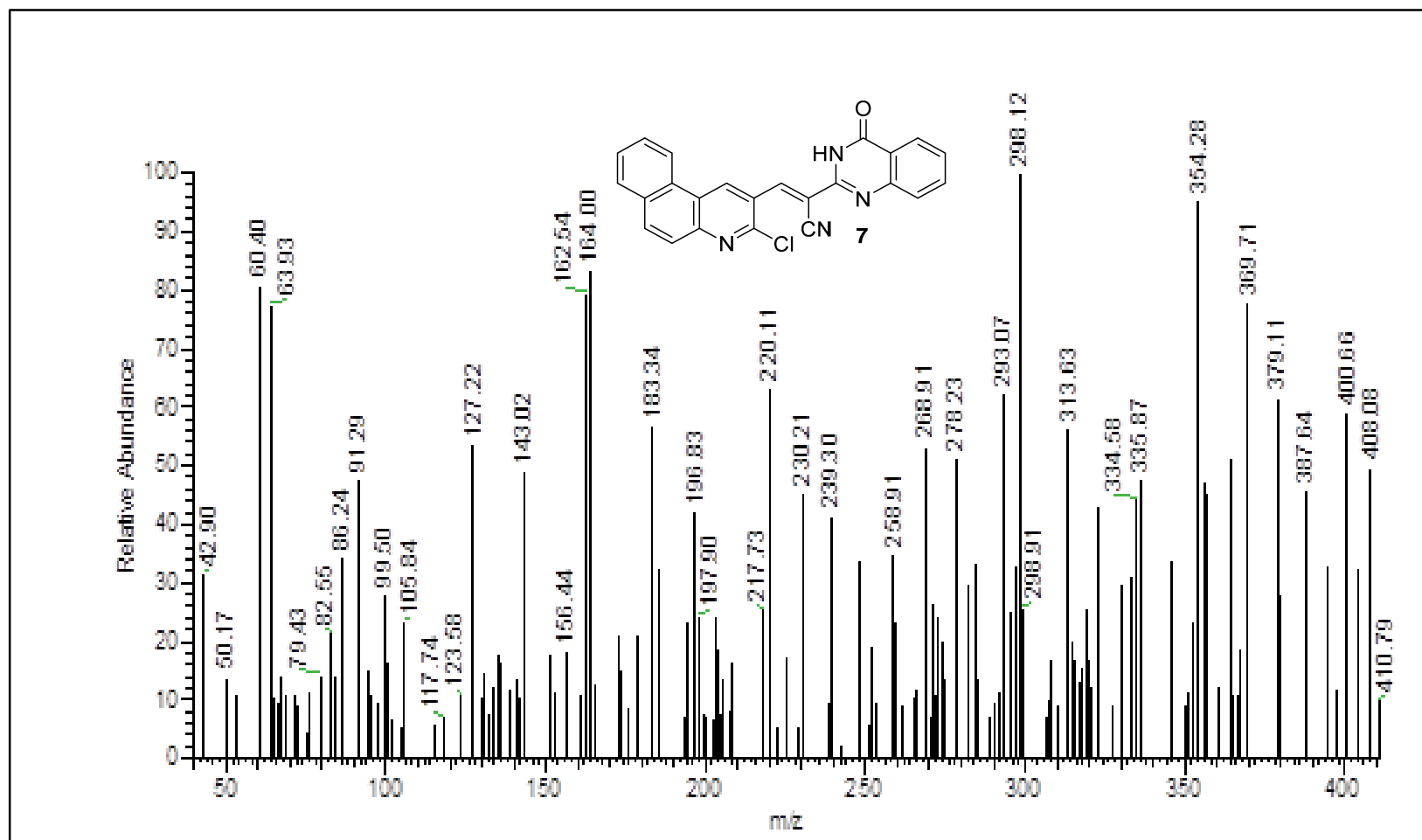


Fig. SD20. Mass spectrum of compound 7

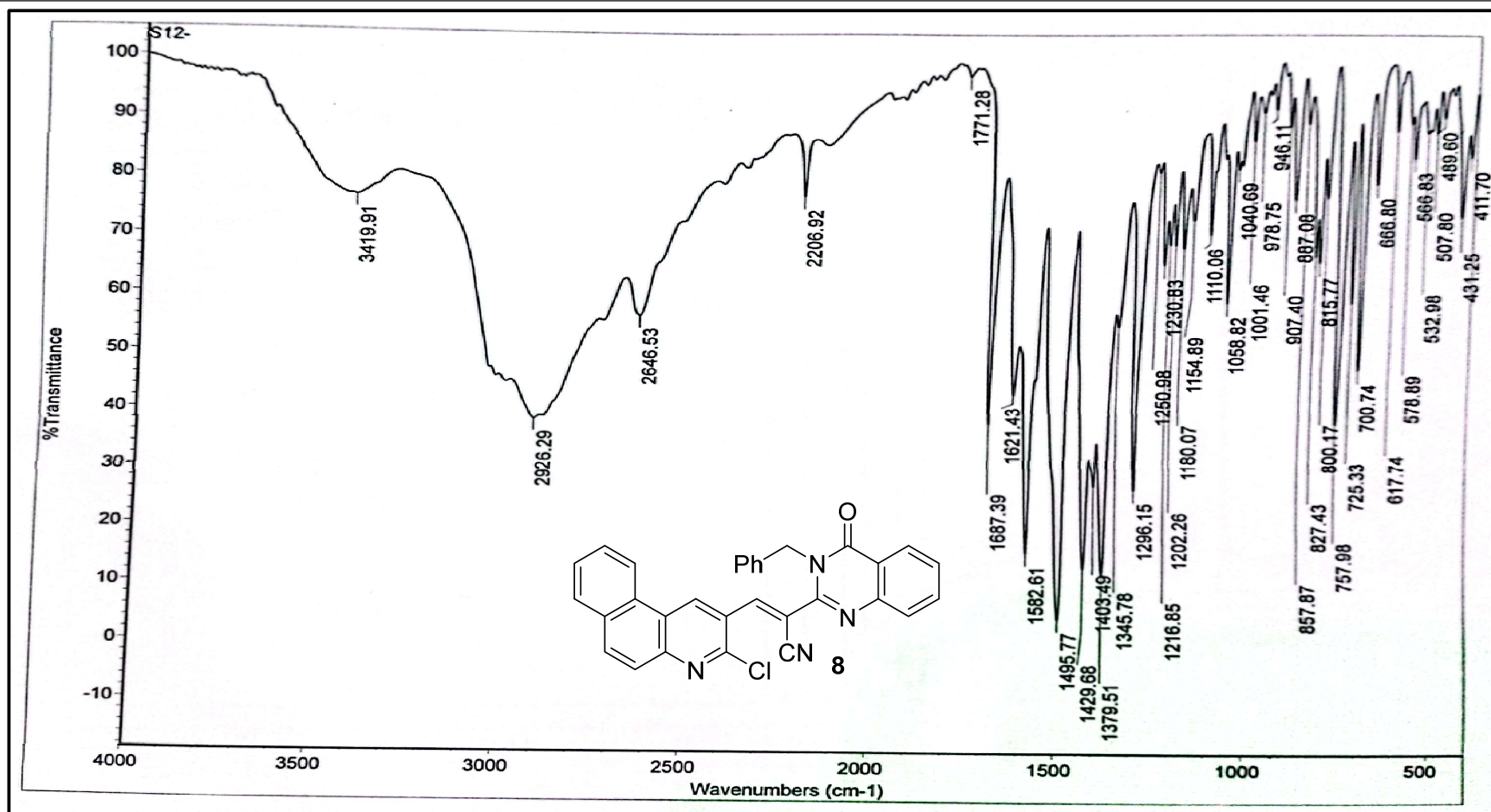


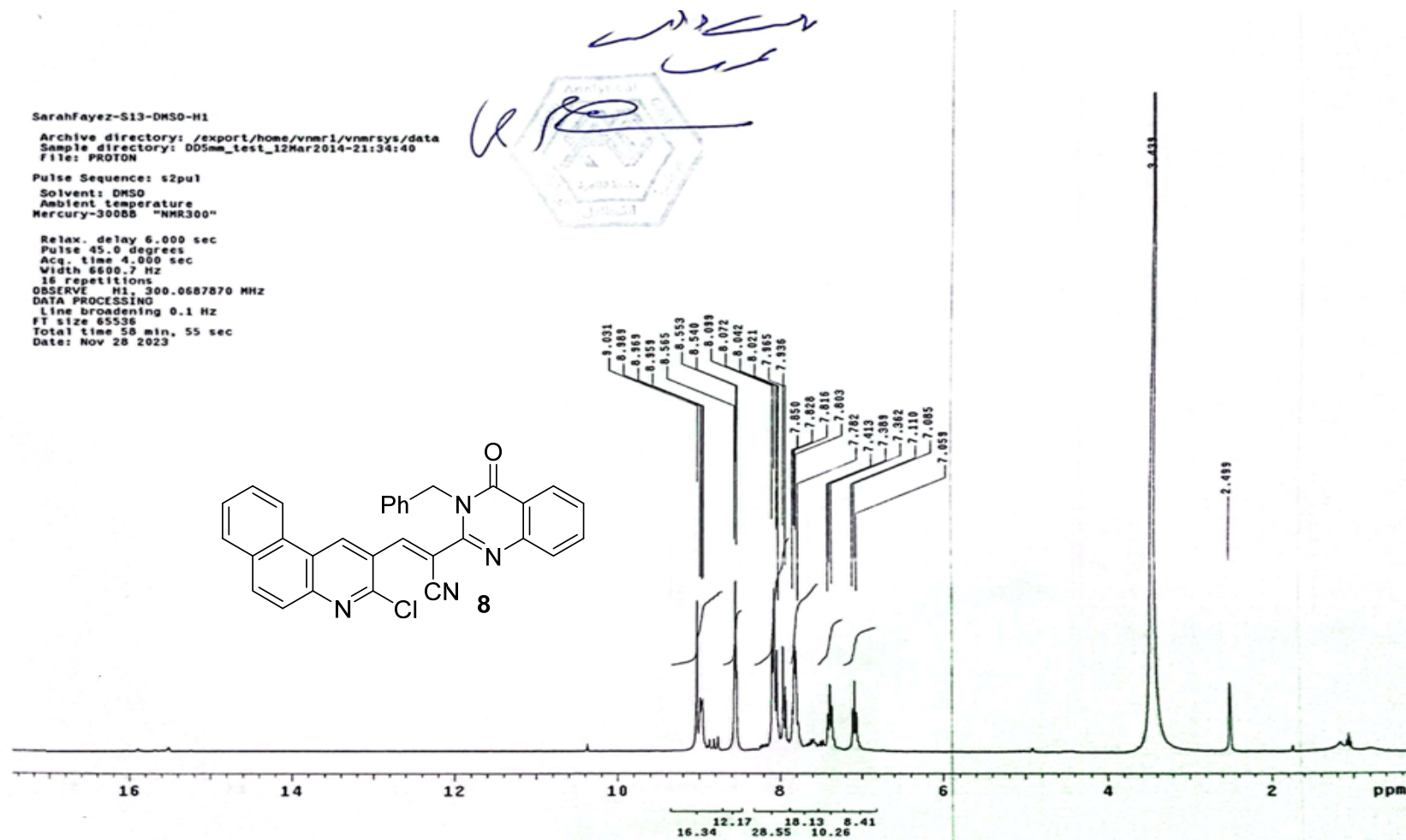
Fig. SD21. IR spectrum of compound 8

SarahFayez-S13-DMSO-H1

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Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

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Solvent: DMSO
Ambient temperature
Mercury-300DB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
16 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Nov 28 2023



SarahFayez-S13-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
4800 repetitions
OBSERVE C13, 75.4523925 MHz
DECOUPLE H1, 300.0702630 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Nov 28 2023

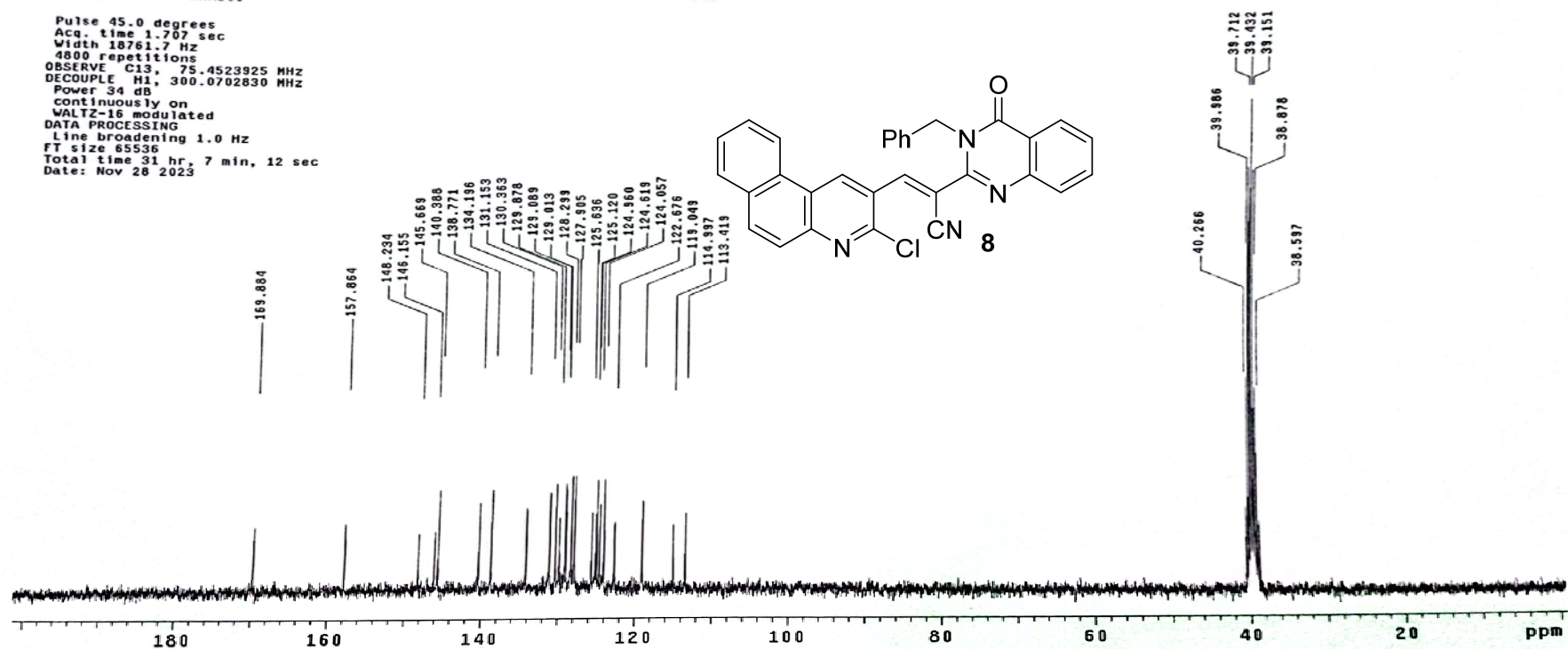


Fig. SD23. ^{13}C NMR spectrum (DMSO- d_6) of compound 8

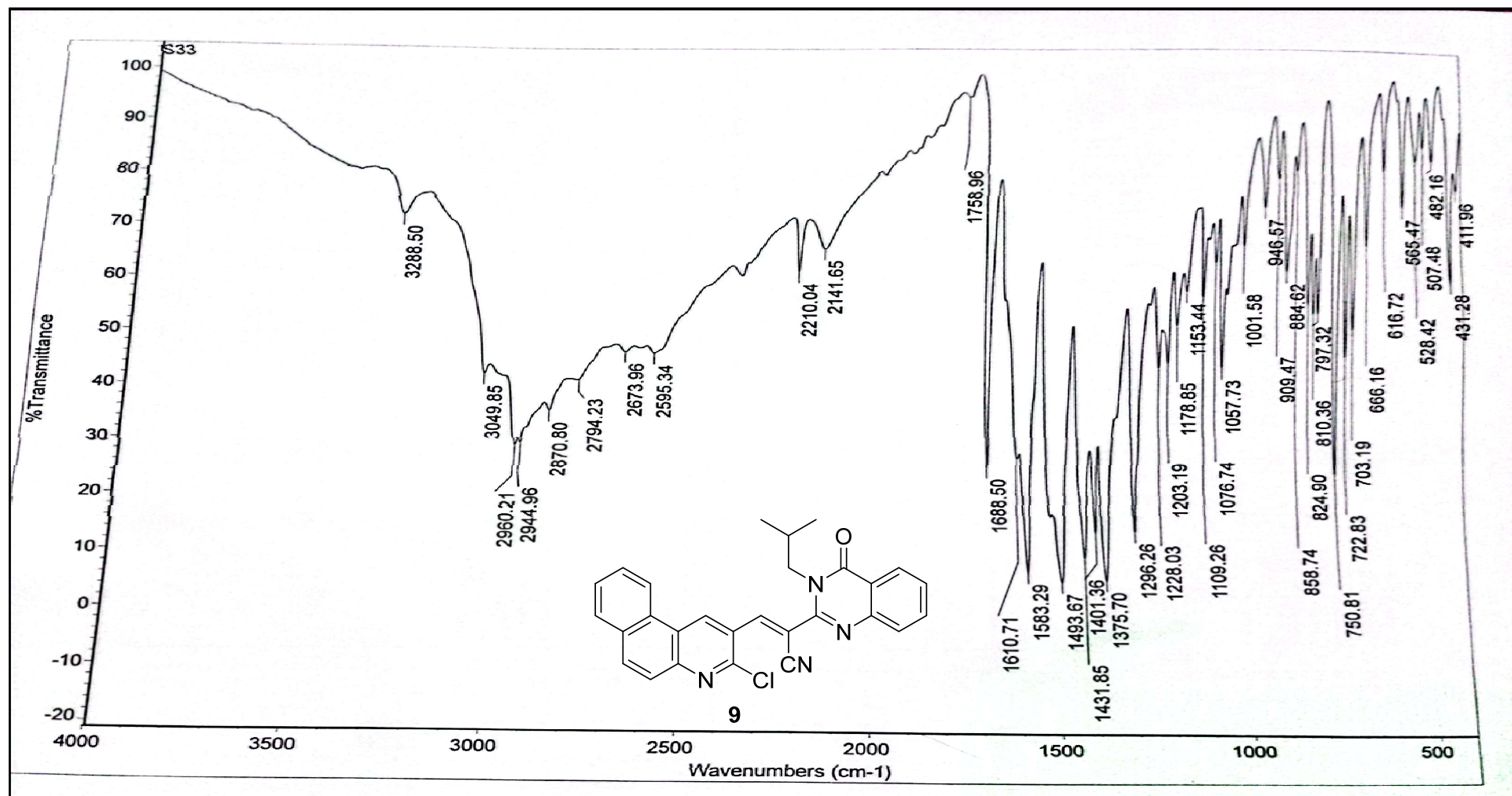


Fig. SD24. IR spectrum of compound 9

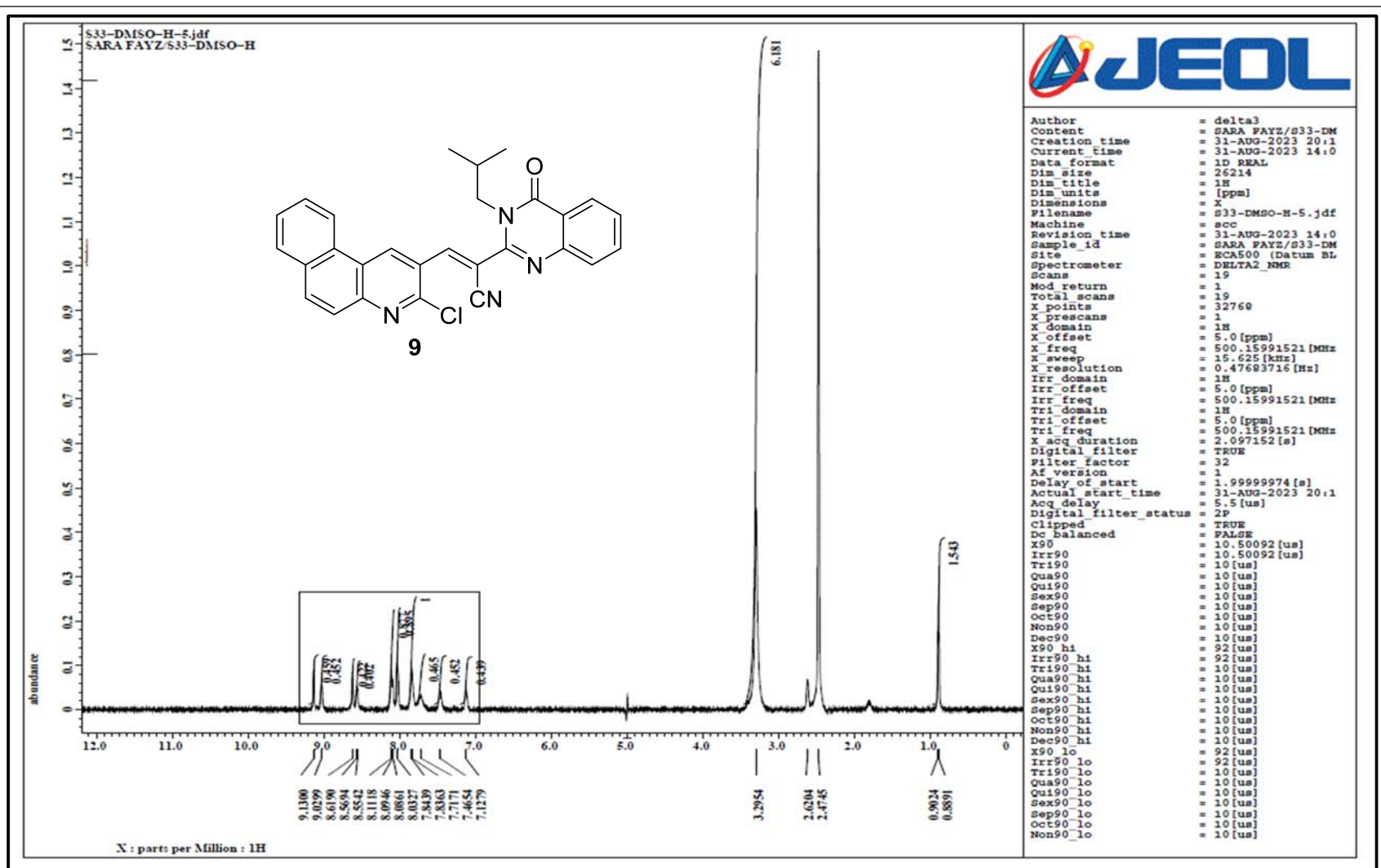


Fig. SD25. ¹H NMR spectrum (DMSO-*d*₆) of compound 9

Sara-S33 #243-247 RT: 4.08-4.15 AV: 5 SB: 2 3.82, 3.53 NL: 1.44E2
T: {0,0} + c EI Full ms [40.00-1000.00]

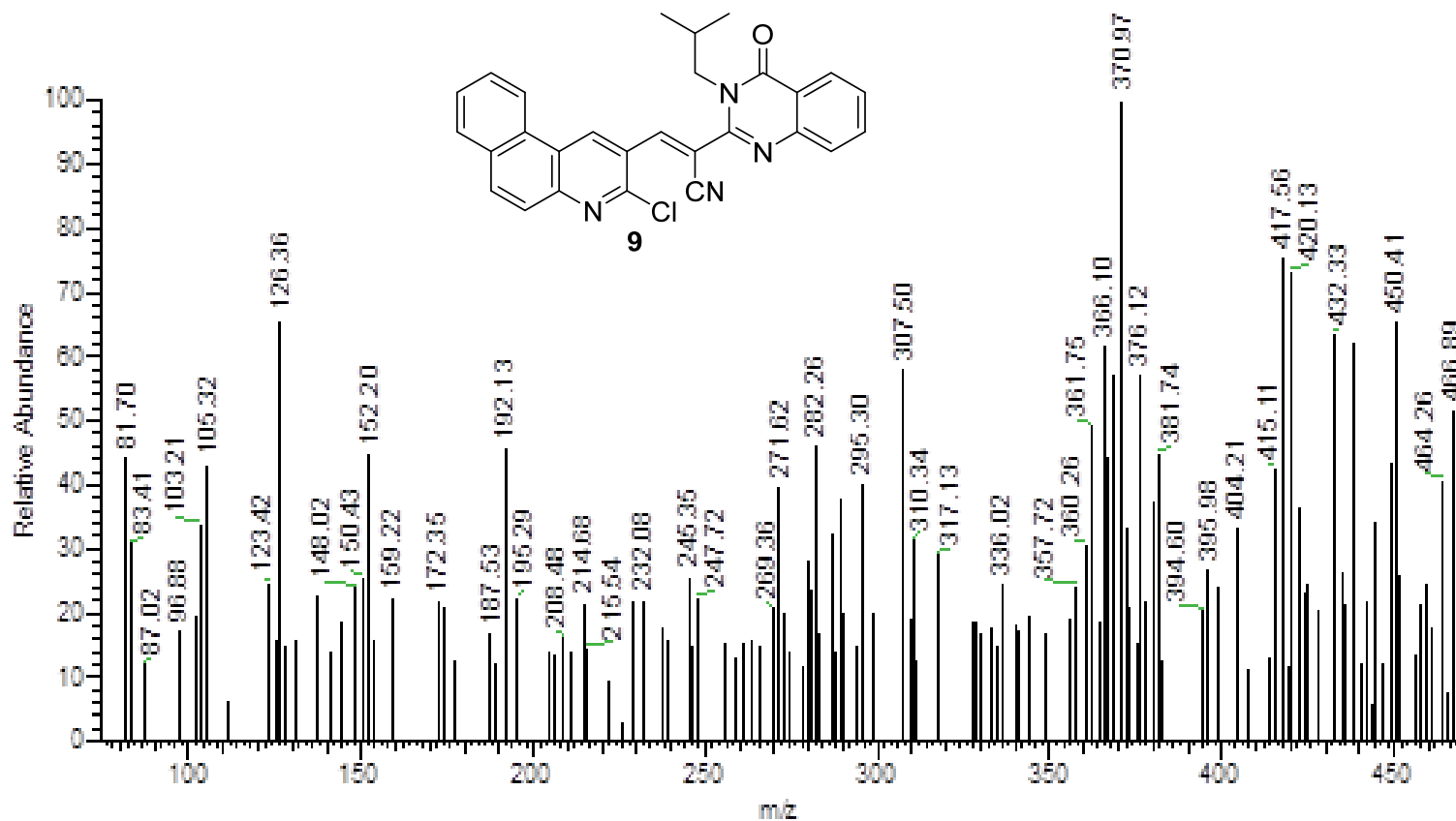


Fig. SD26. Mass spectrum of compound 9

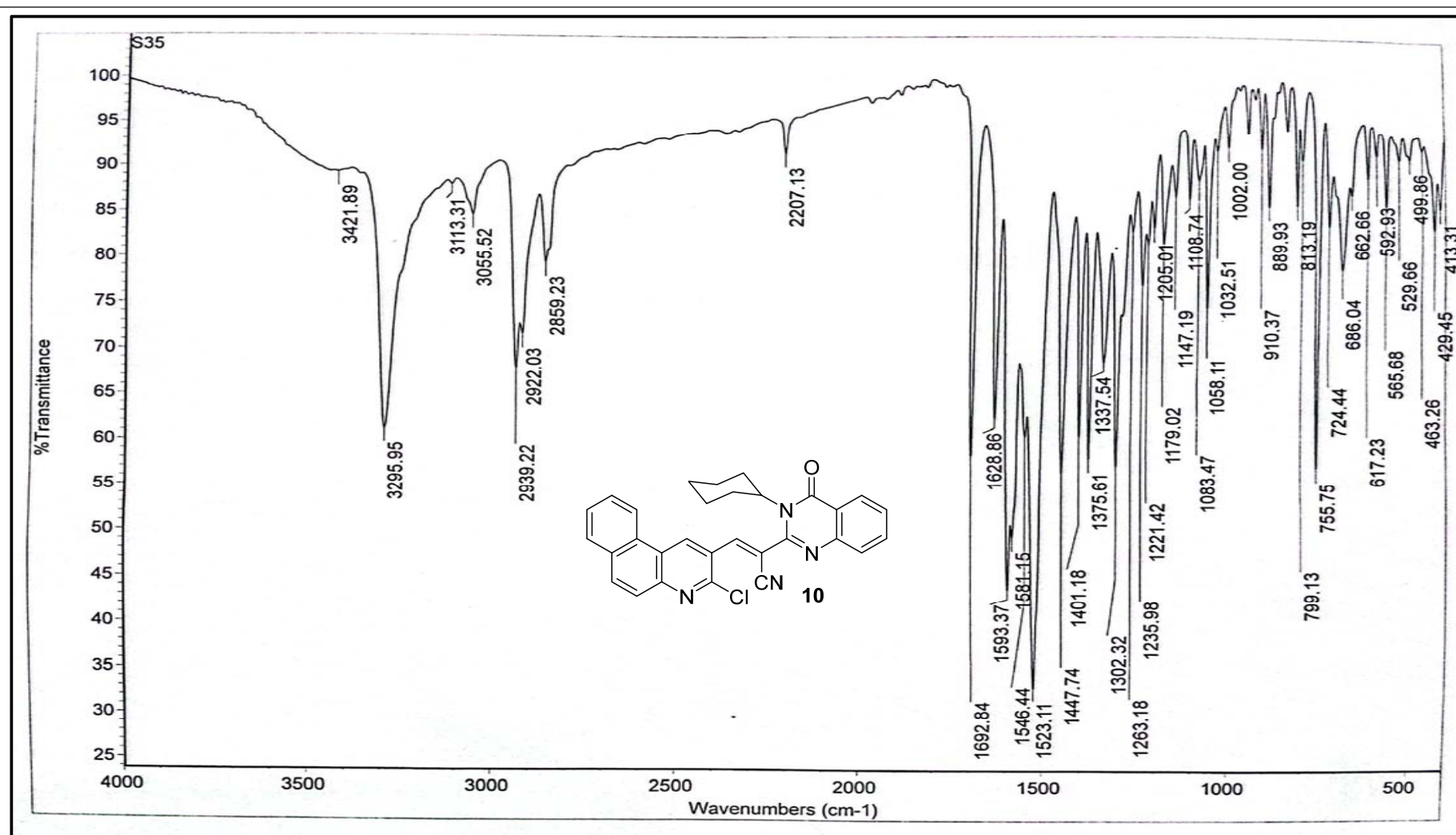


Fig. SD27. IR spectrum of compound 10

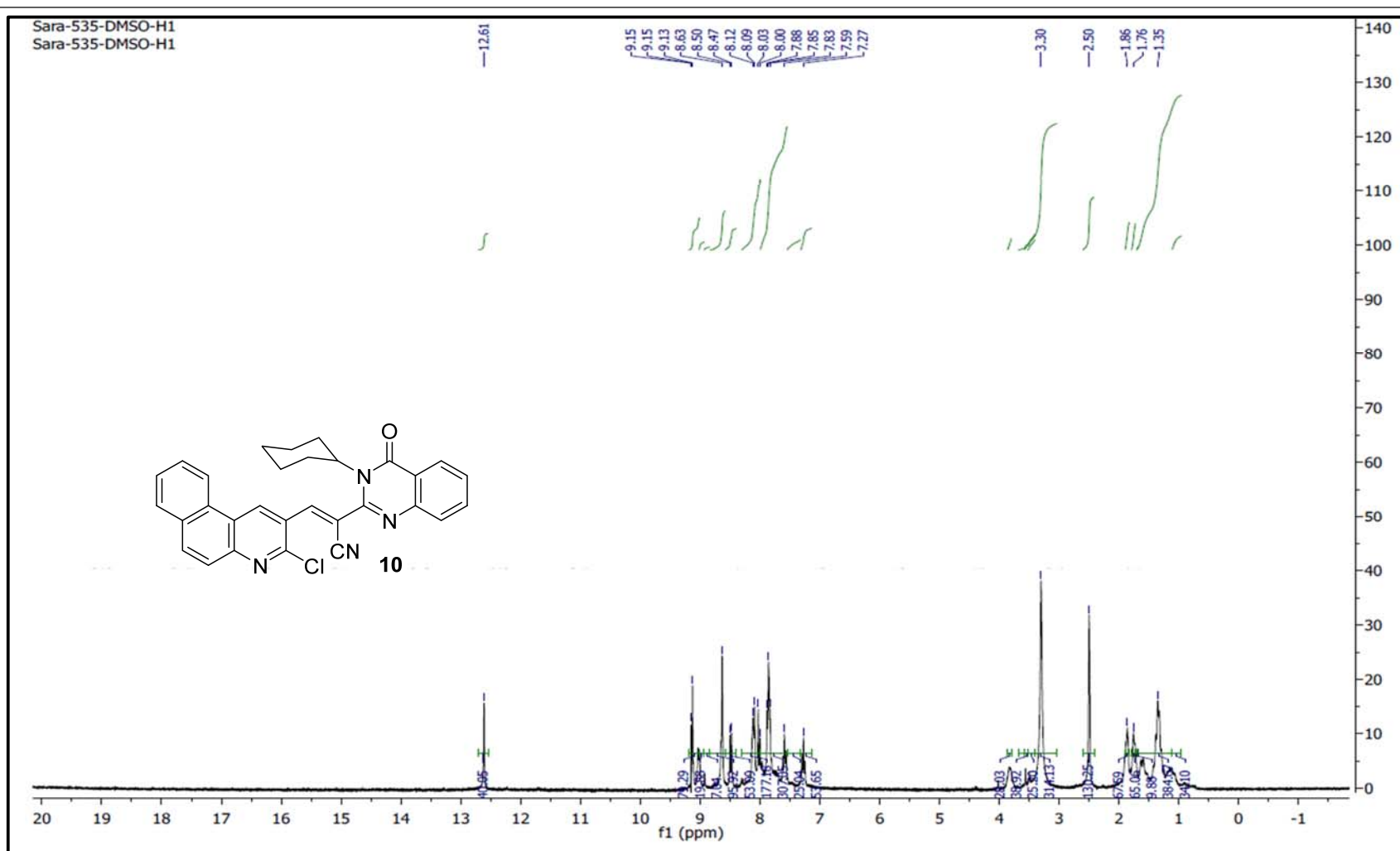
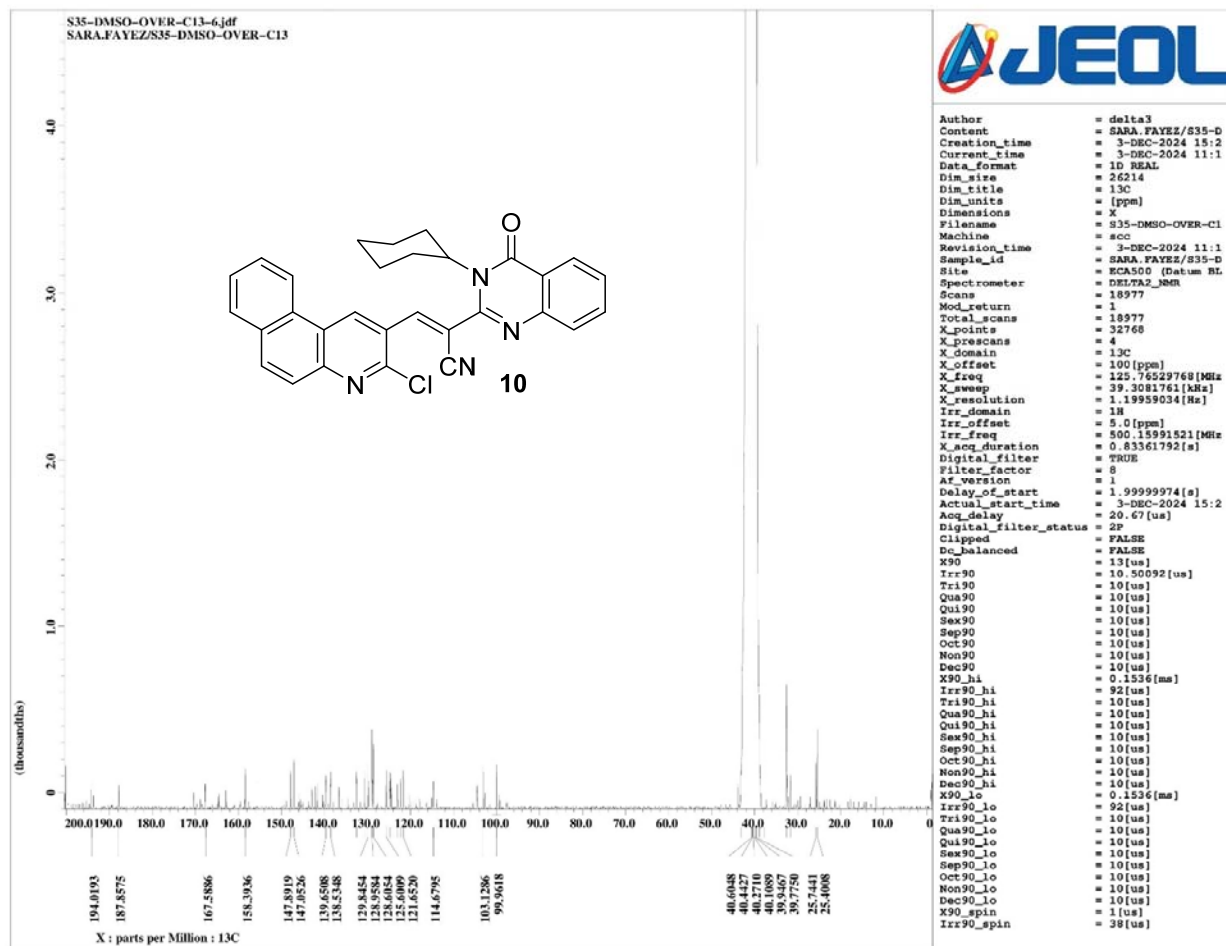


Fig. SD28. ^1H NMR spectrum ($\text{DMSO}-d_6$) of compound **10**



Cont. Fig. SD28. ¹³C NMR spectrum (DMSO-*d*₆) of compound 10

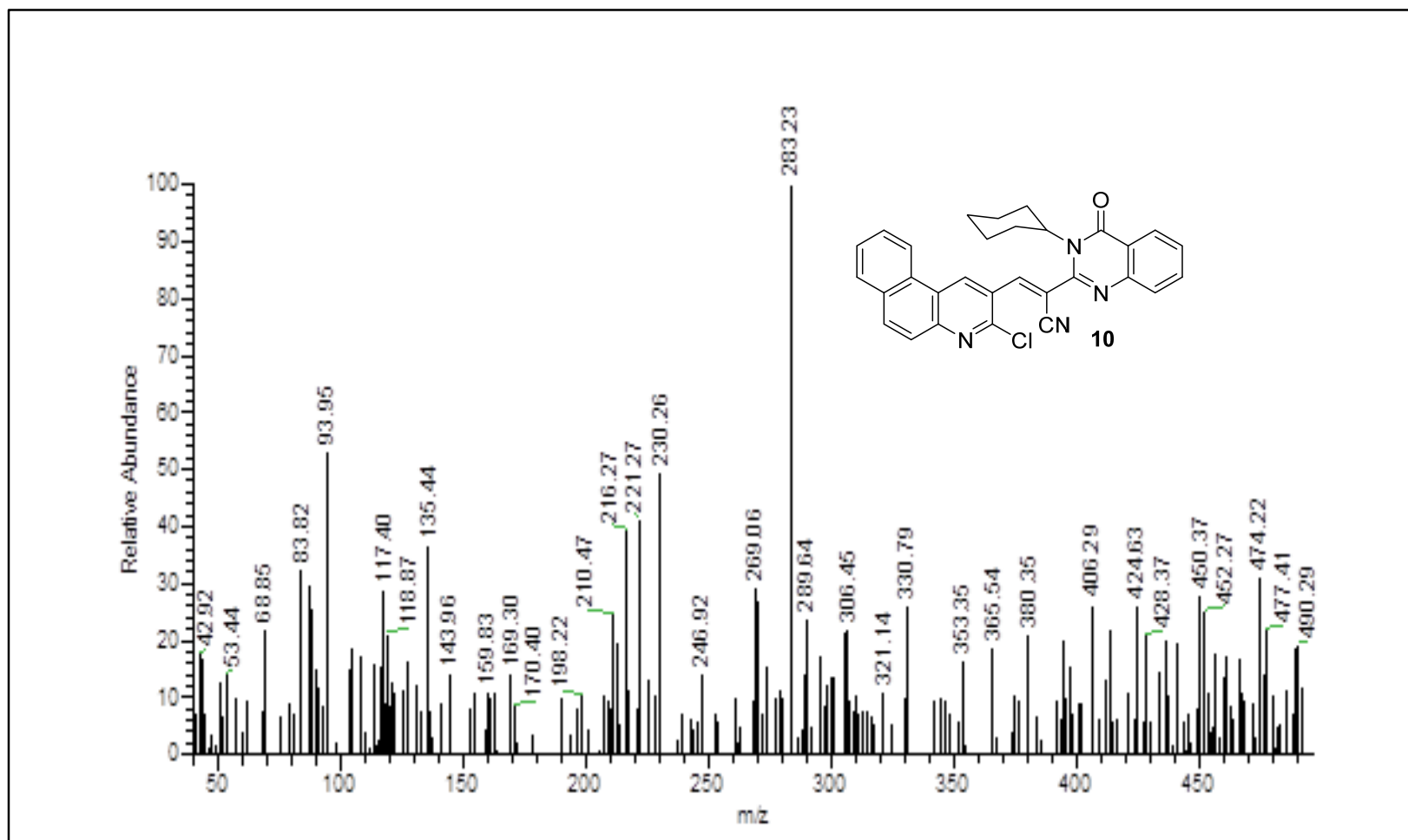


Fig. SD29. Mass spectrum of compound 10

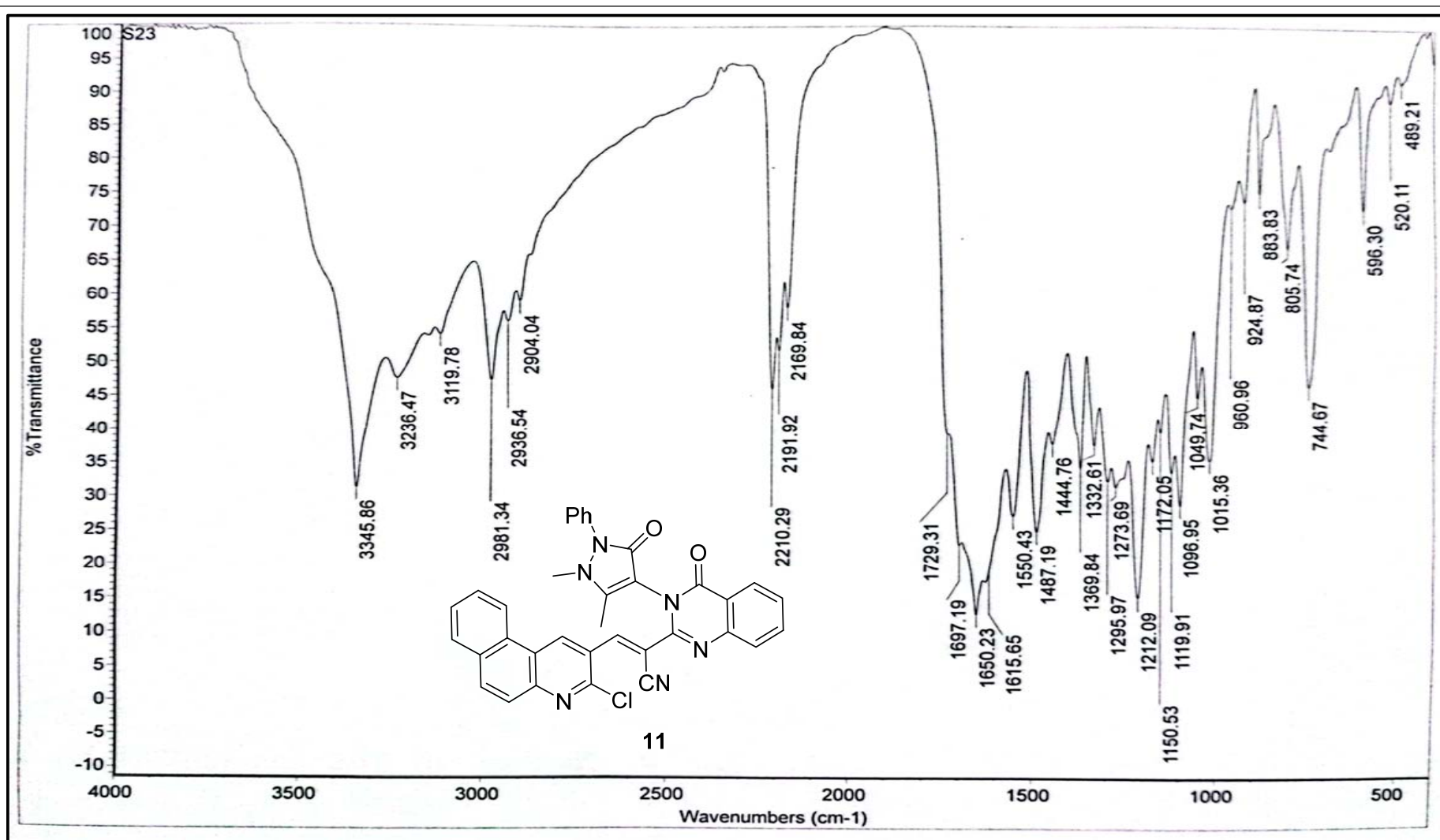


Fig. SD30. IR spectrum of compound 11

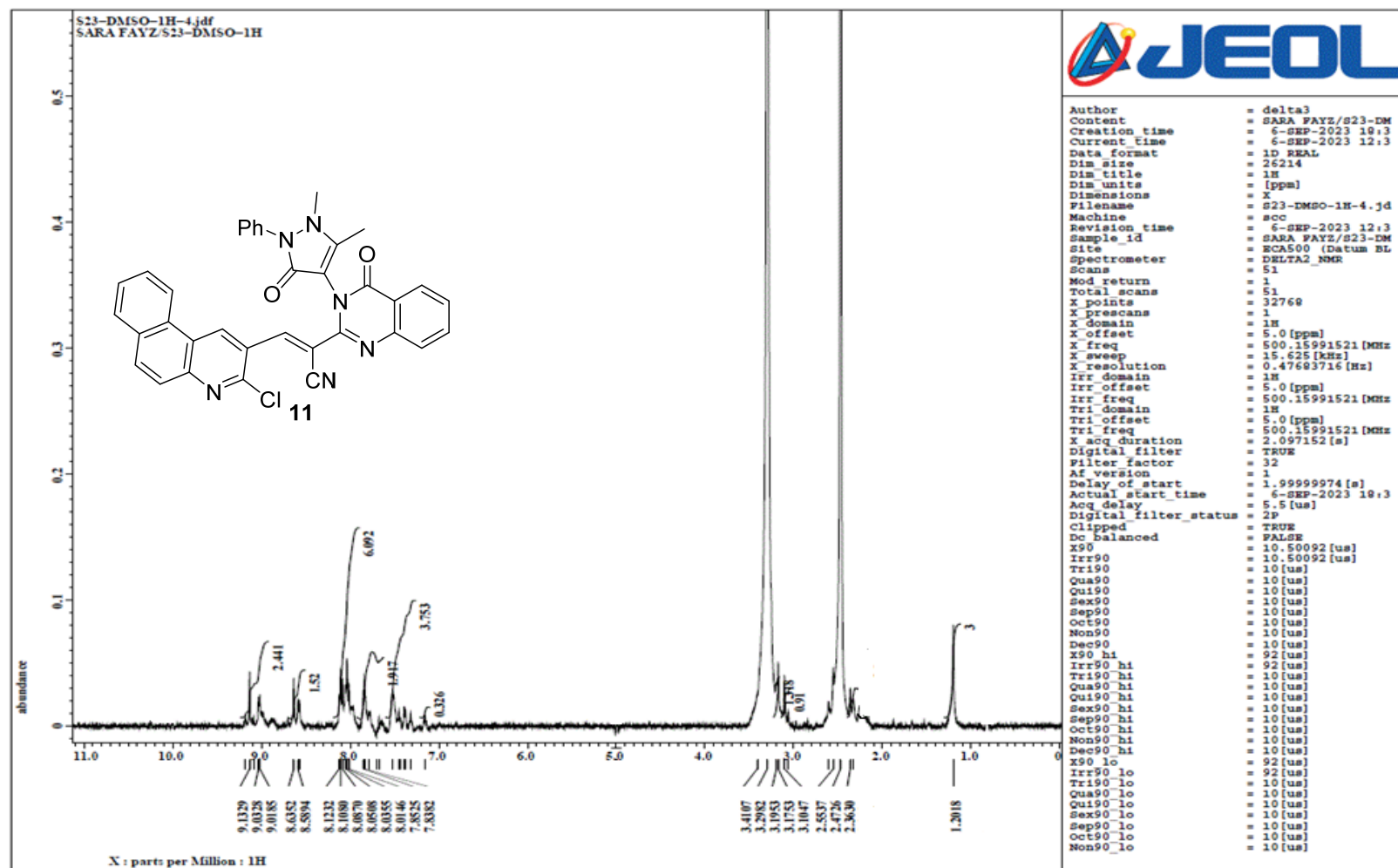


Fig. SD31. ^1H NMR spectrum ($\text{DMSO}-d_6$) of compound 11

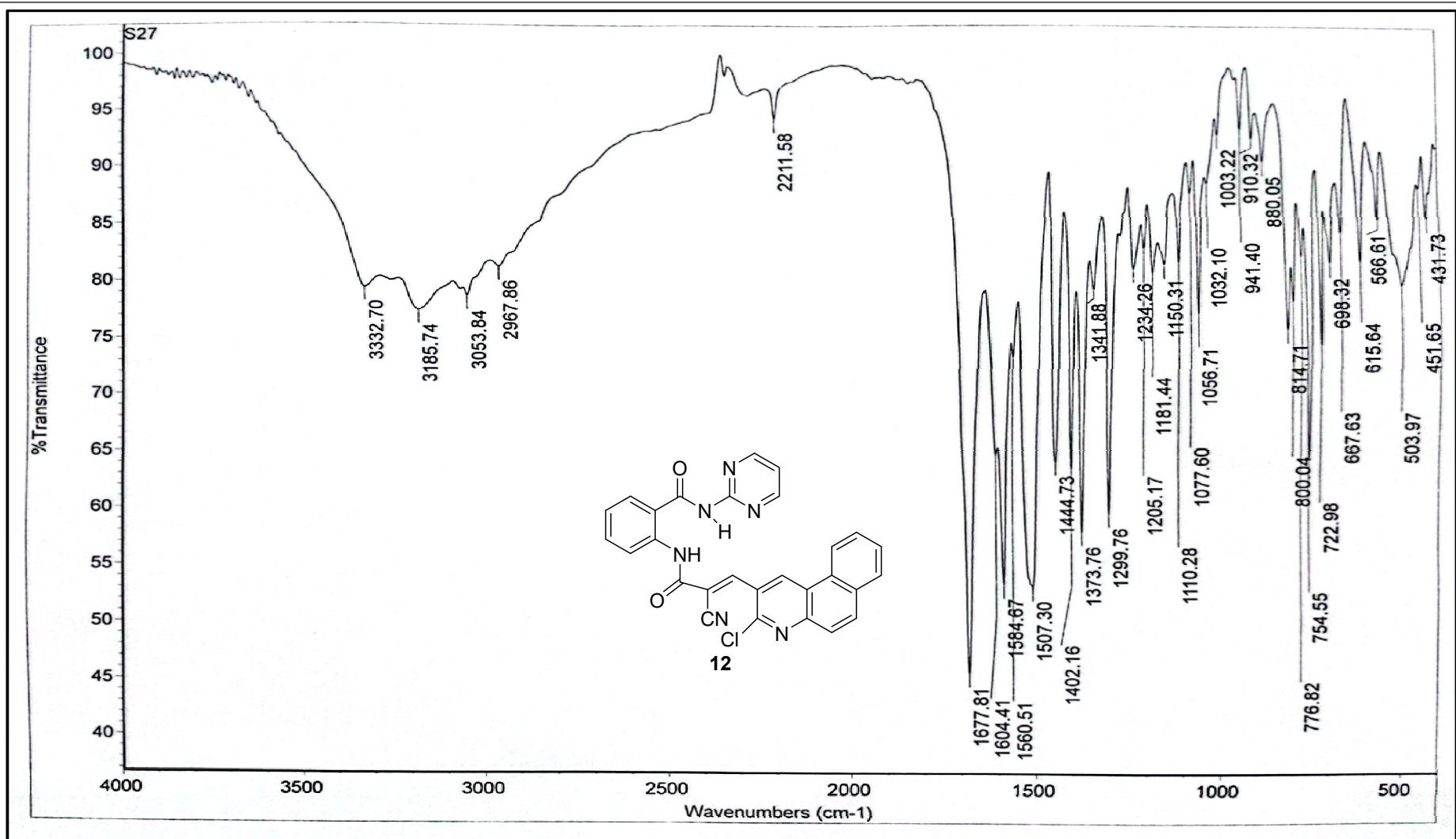


Fig. SD32. IR spectrum of compound 12

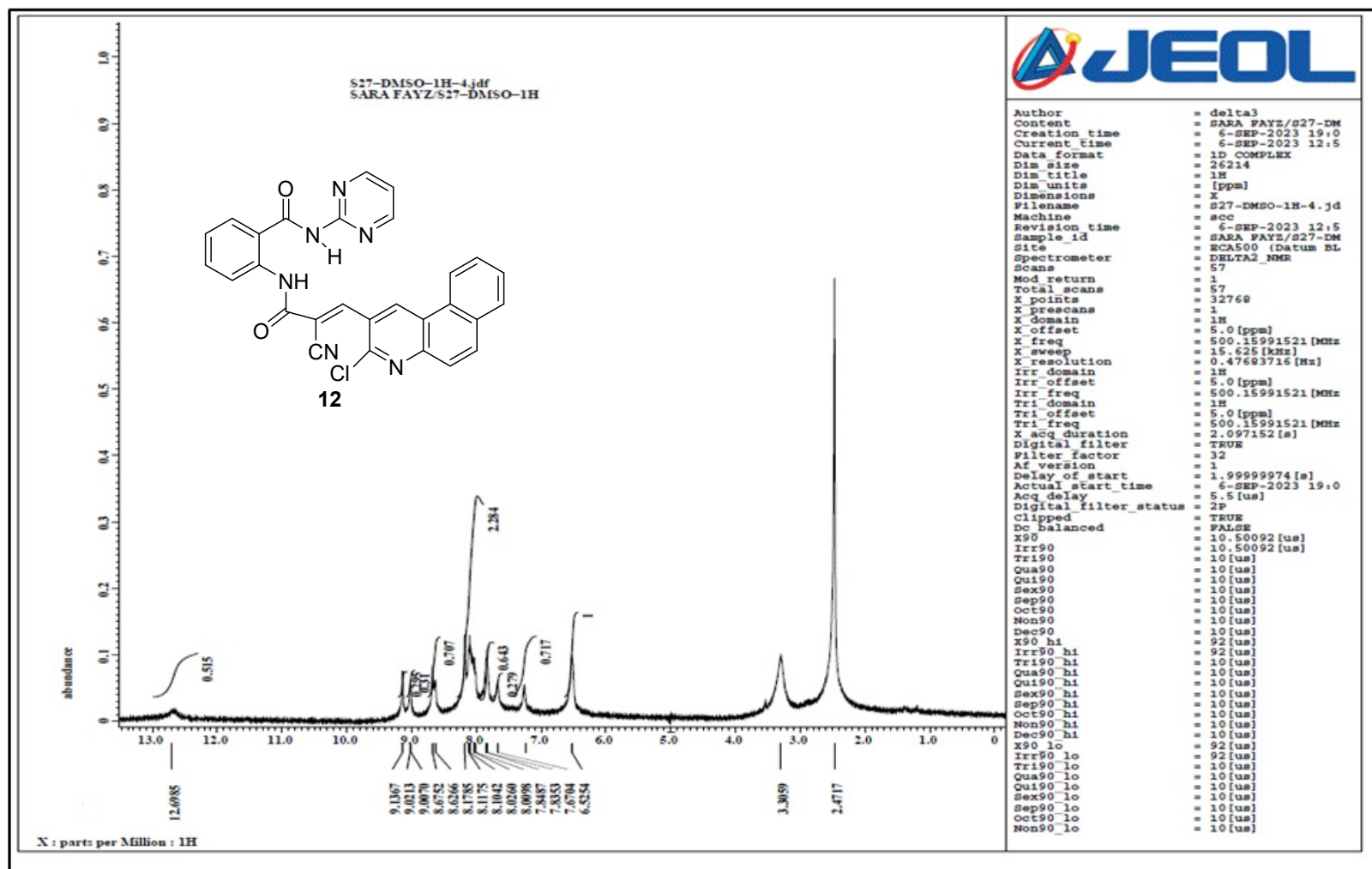


Fig. SD33. ^1H NMR spectrum (DMSO- d_6) of compound 12

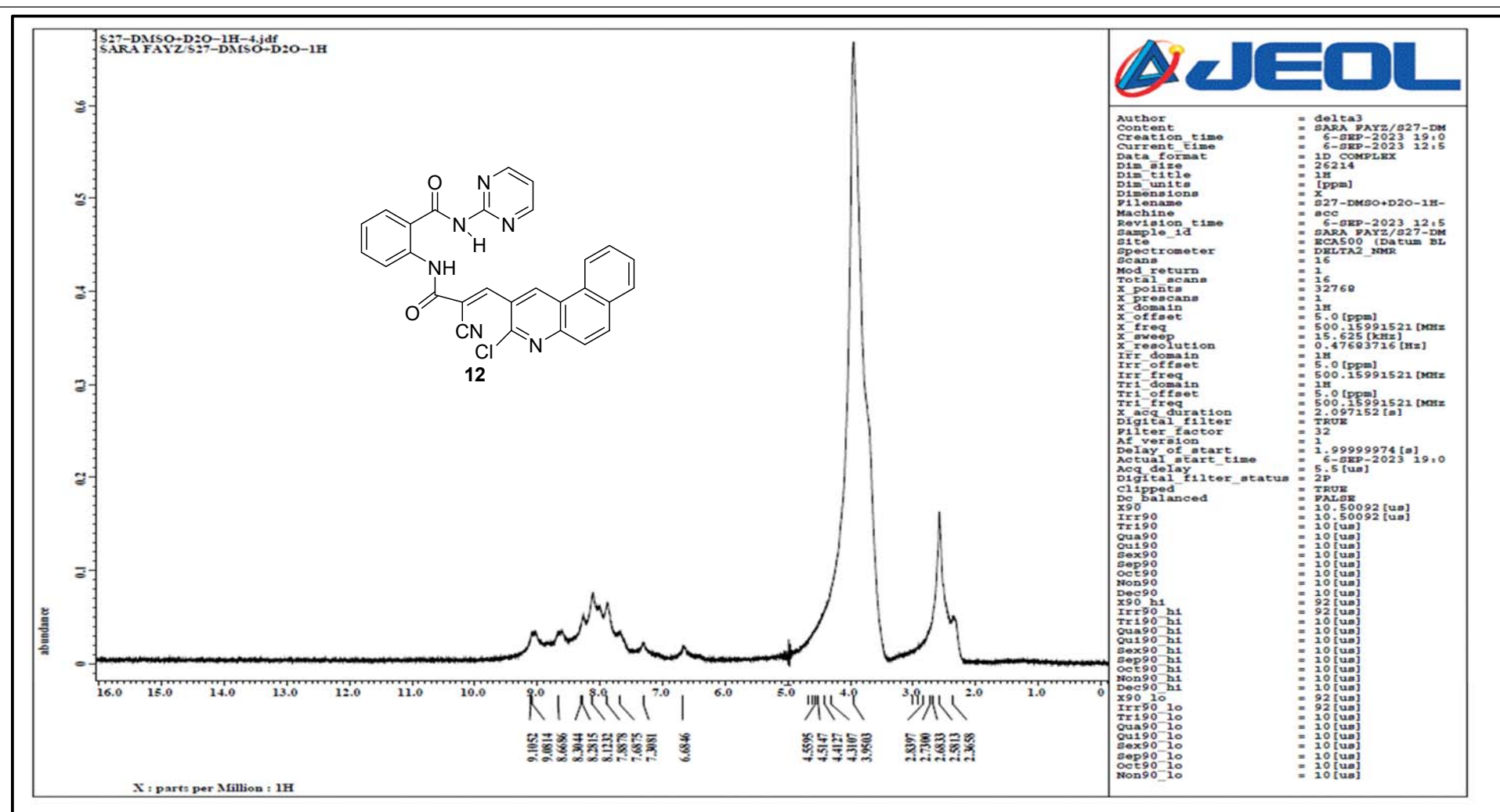


Fig. SD34. ¹H NMR spectrum (DMSO-*d*₆+D₂O) of compound 12

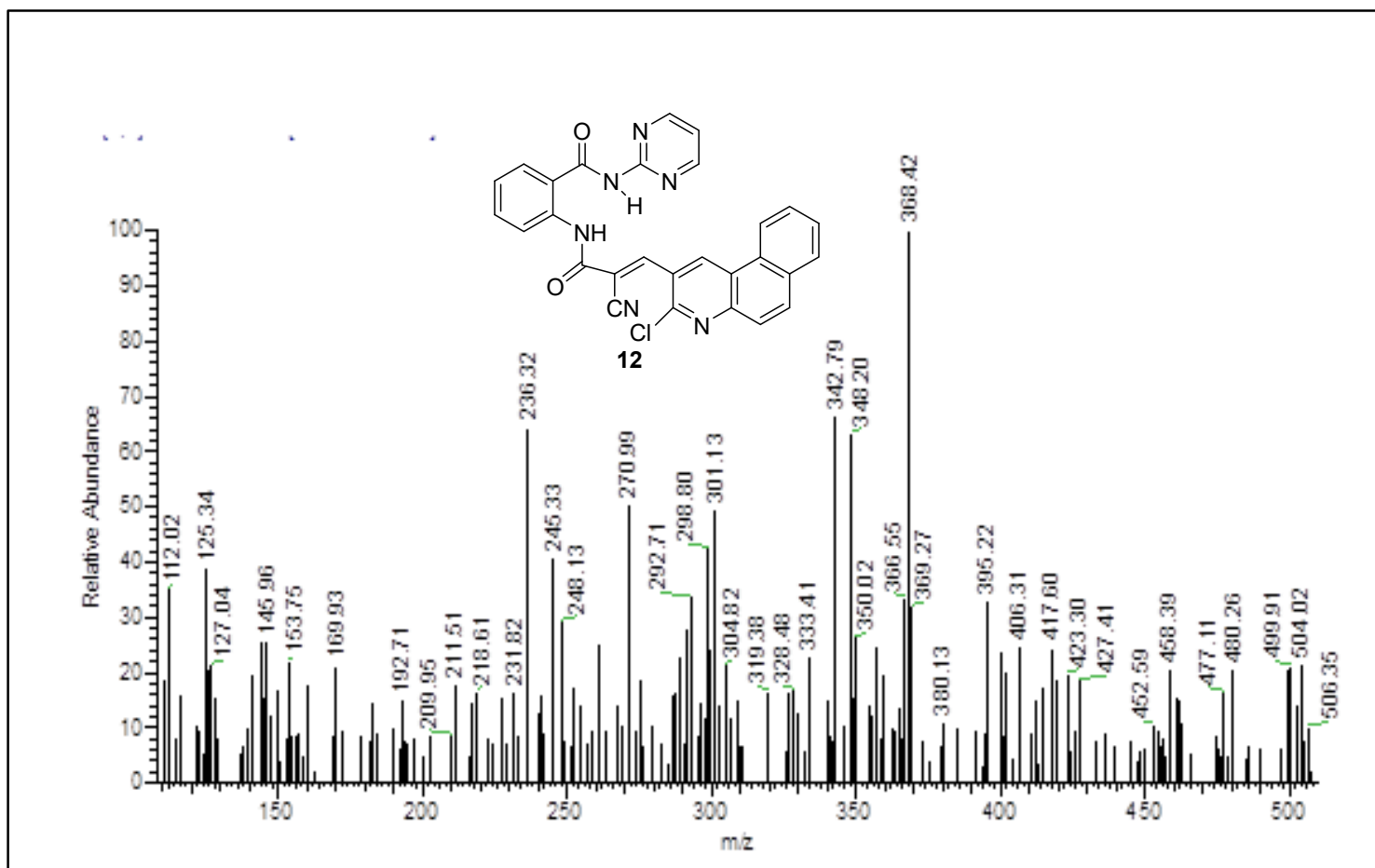


Fig. SD35. Mass spectrum of compound 12

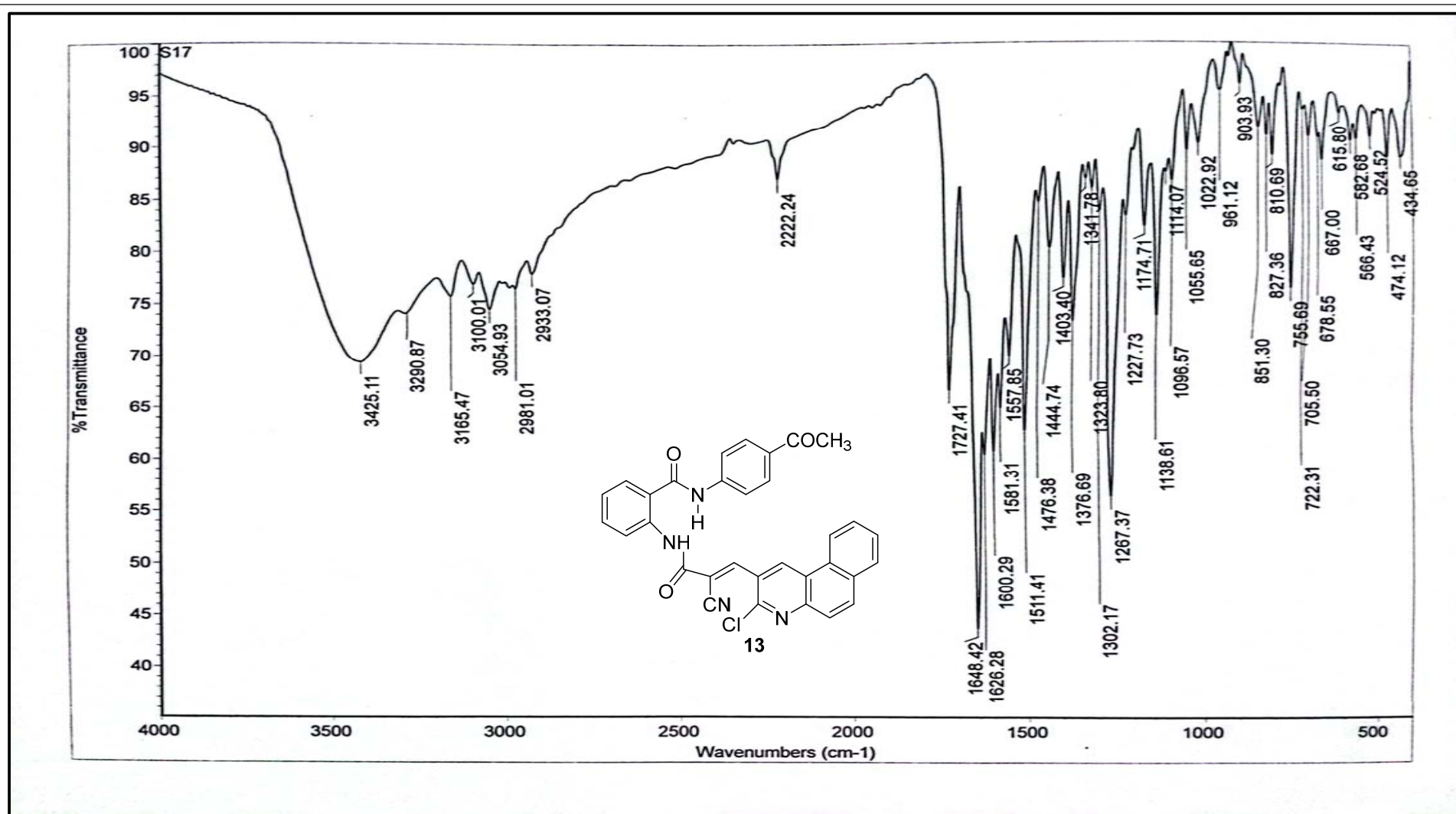


Fig. SD36. IR spectrum of compound 13

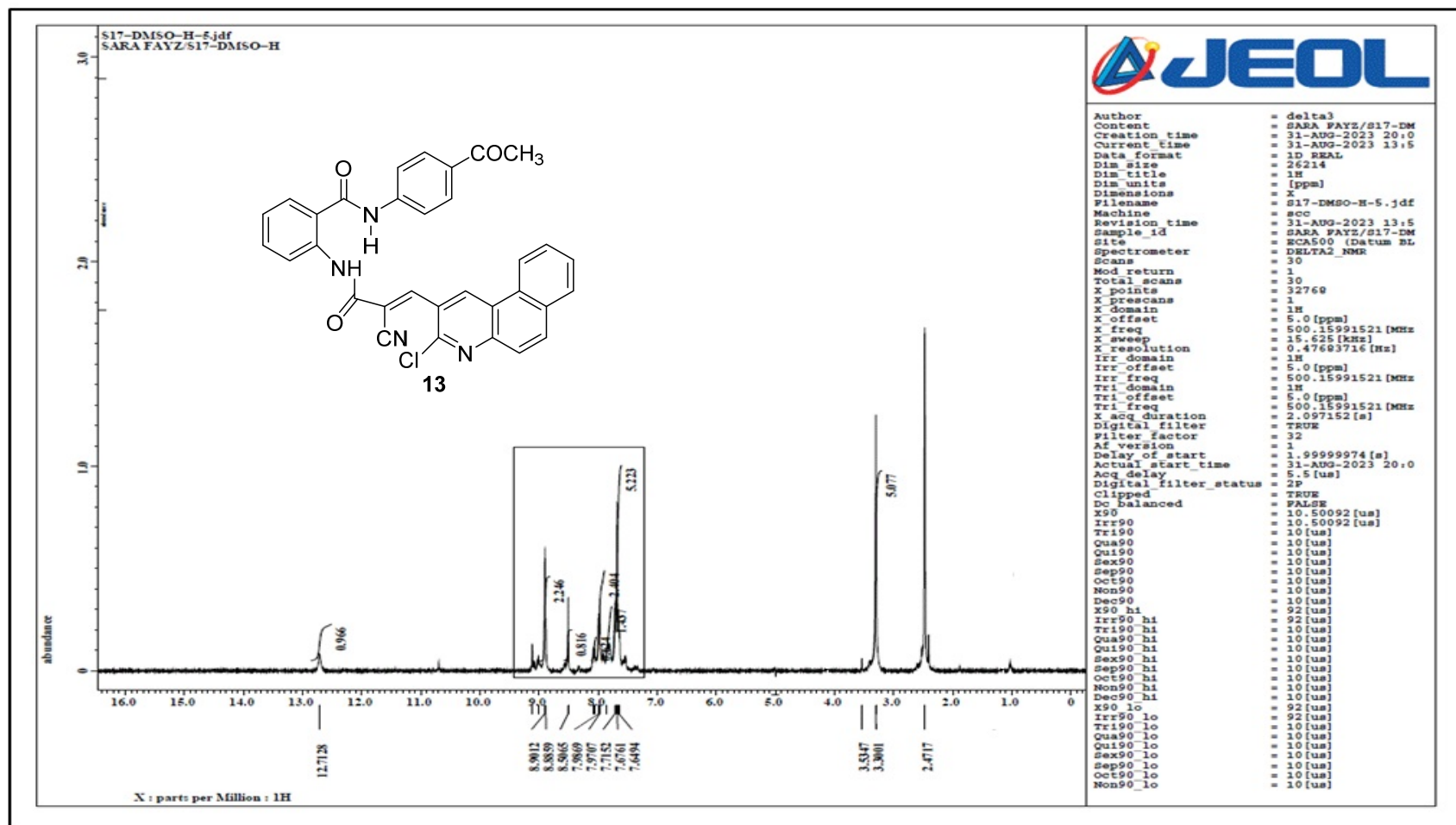


Fig. SD37. ¹H NMR spectrum (DMSO-d₆) of compound 13

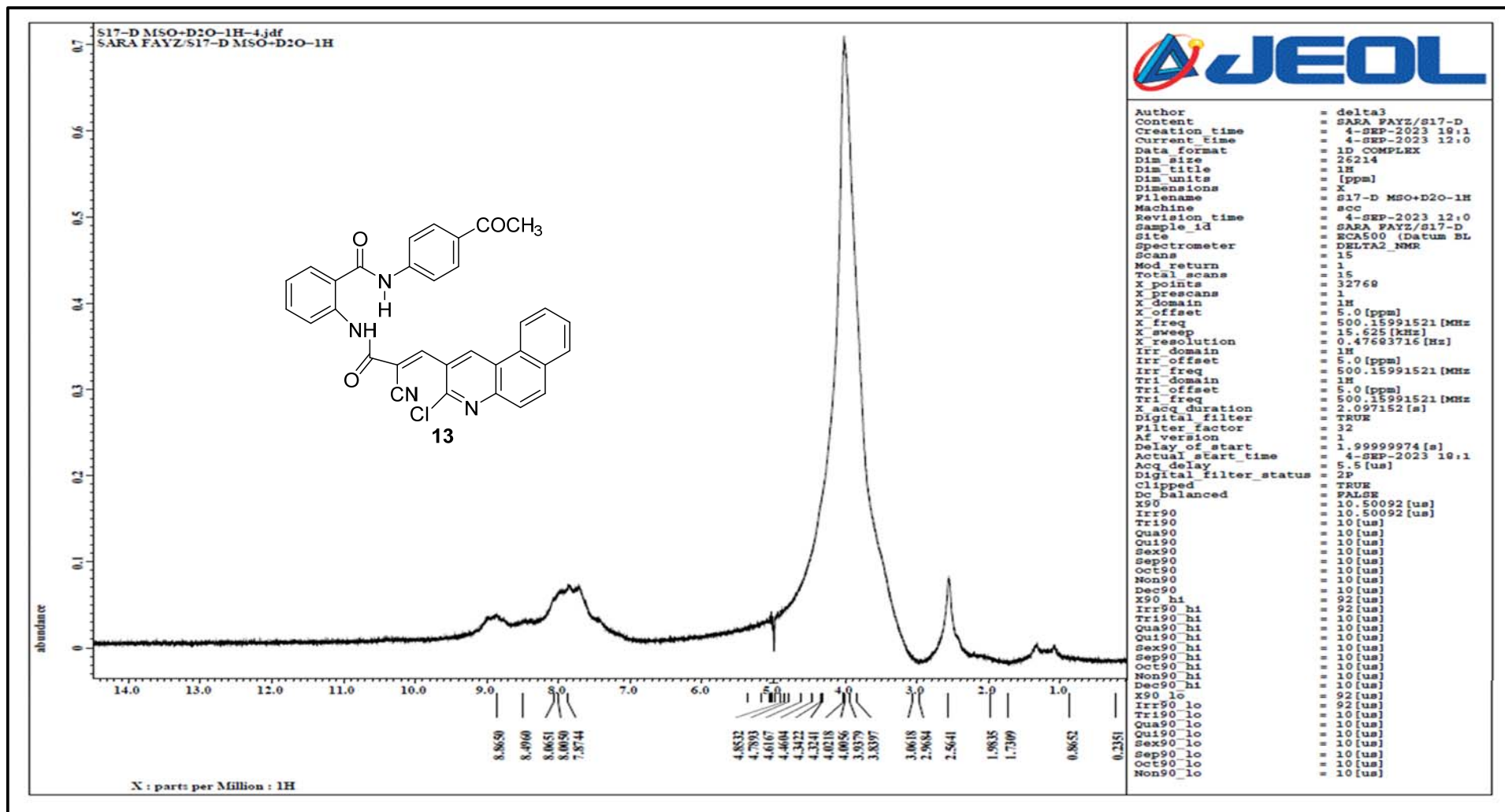


Fig. SD38. ¹H NMR spectrum (DMSO-*d*₆+D₂O) of compound 13

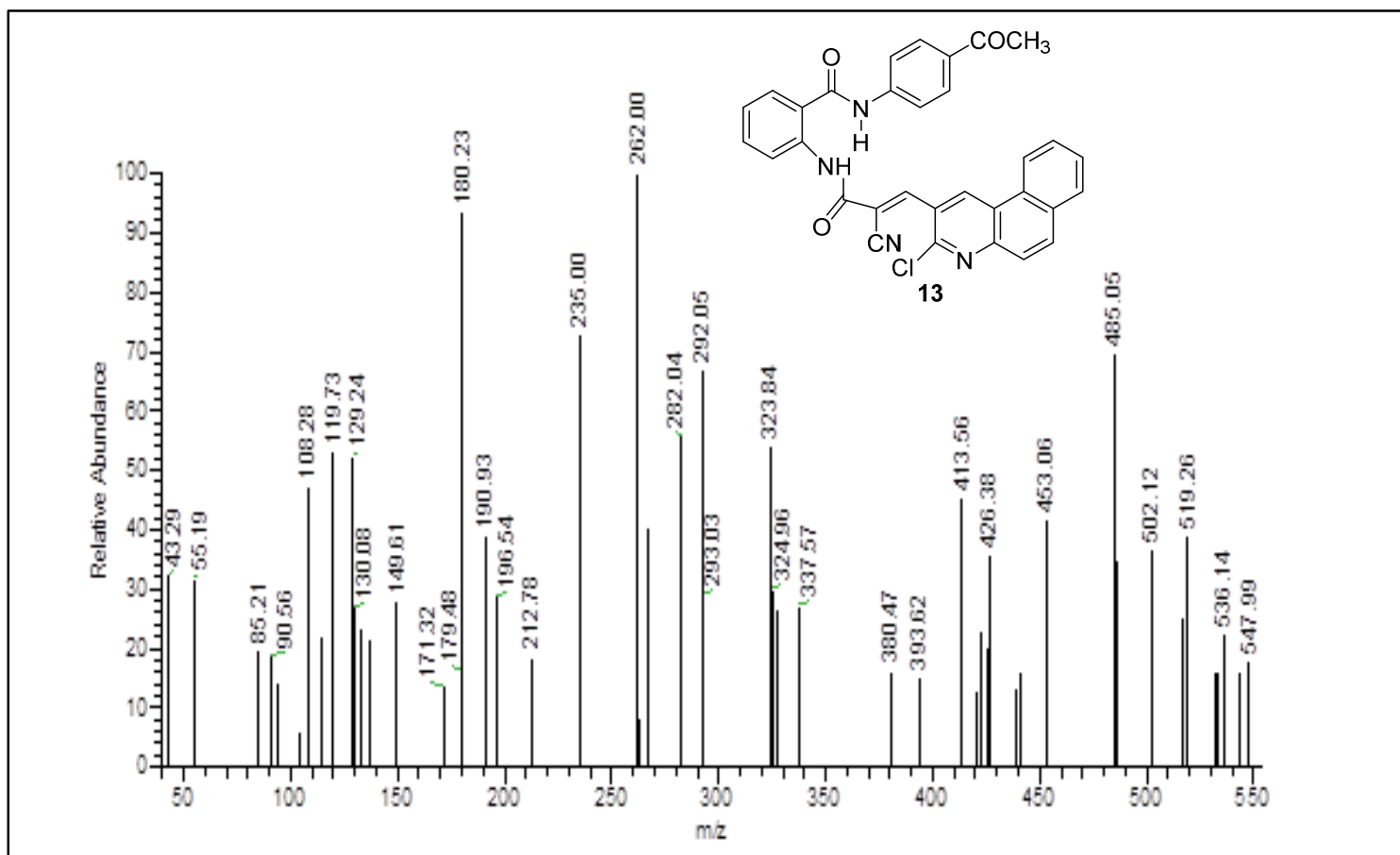


Fig. SD39. Mass spectrum of compound 13

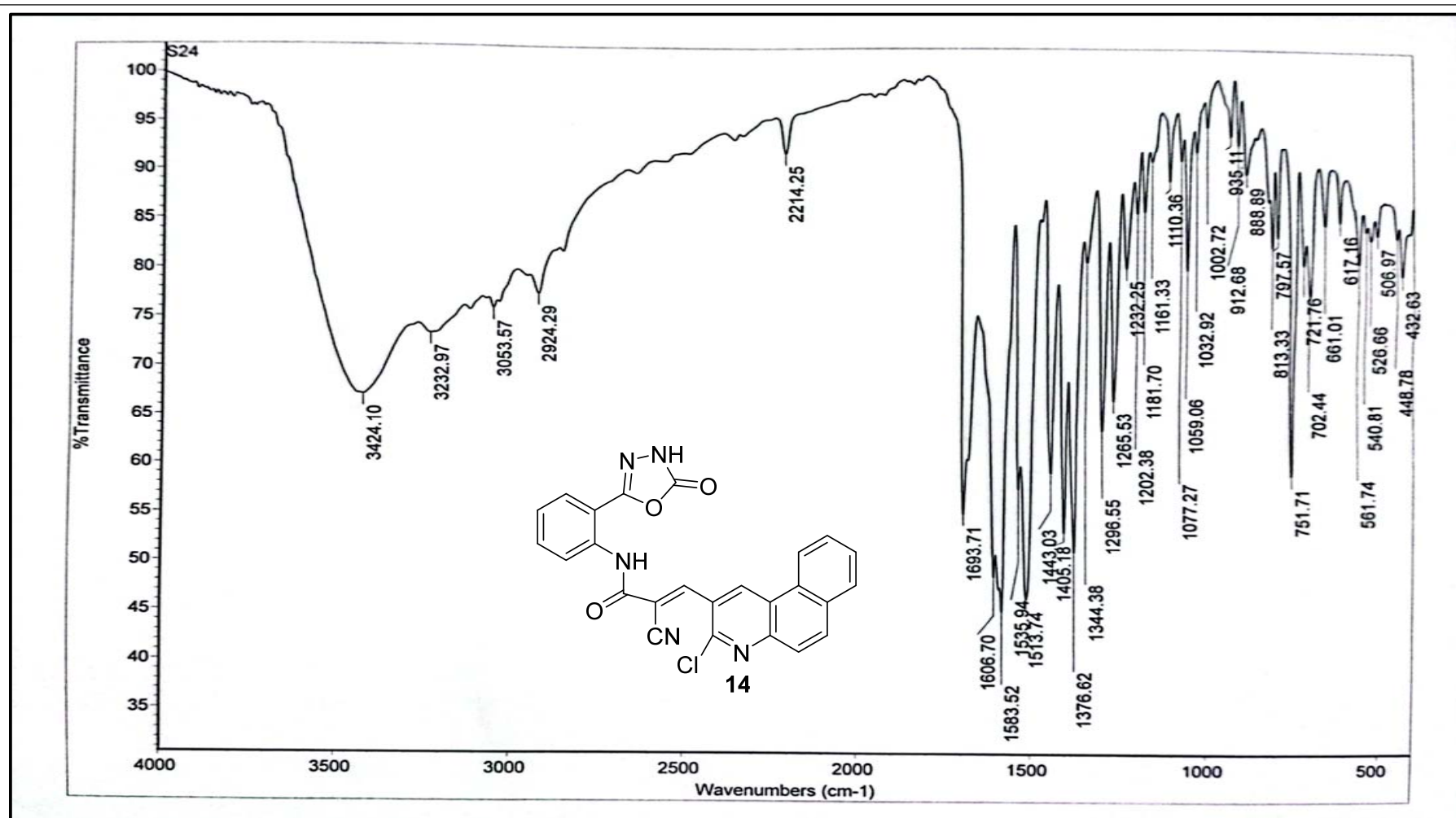


Fig. SD40. IR spectrum of compound 14

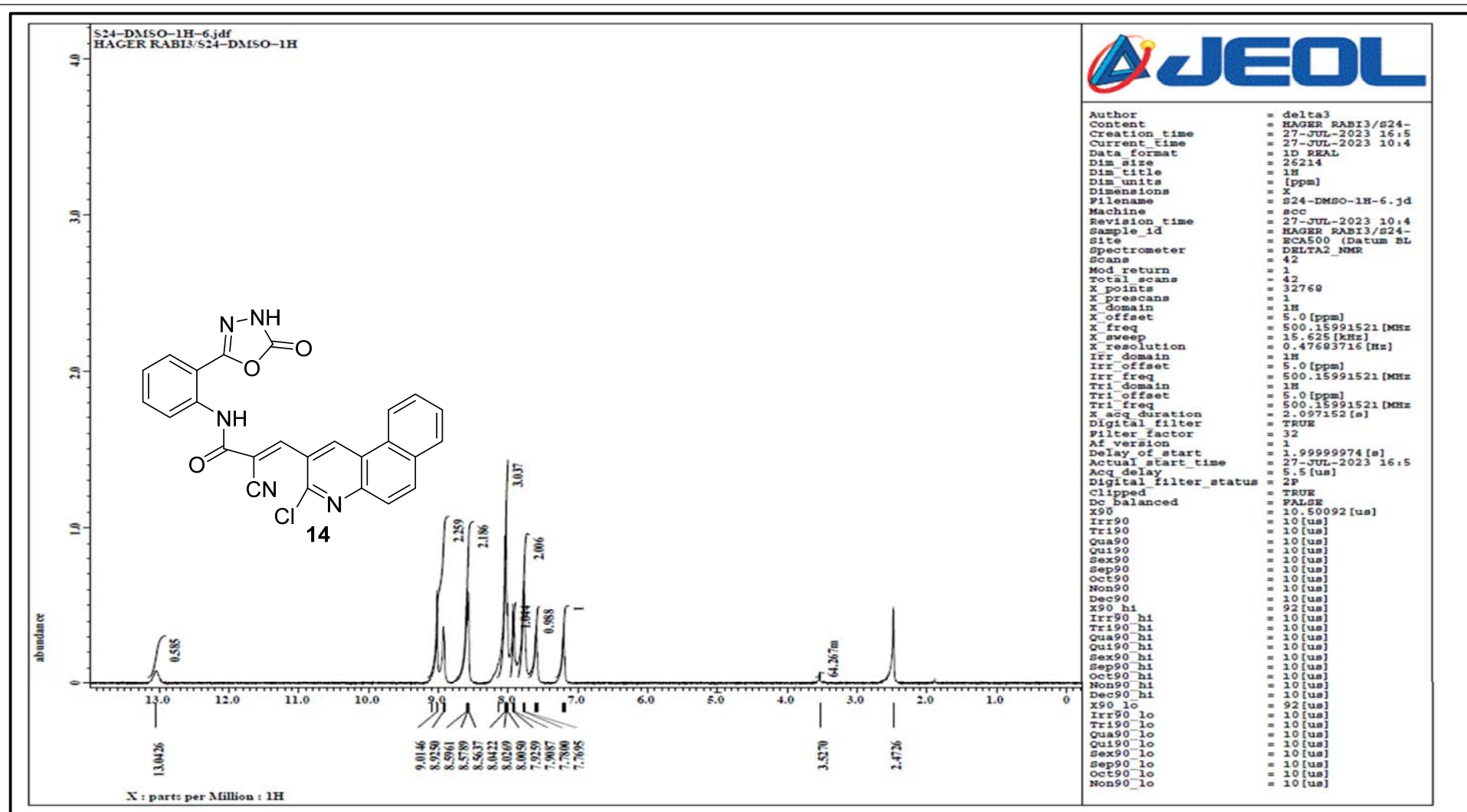


Fig. SD41. ¹H NMR spectrum (DMSO-*d*₆) of compound 14

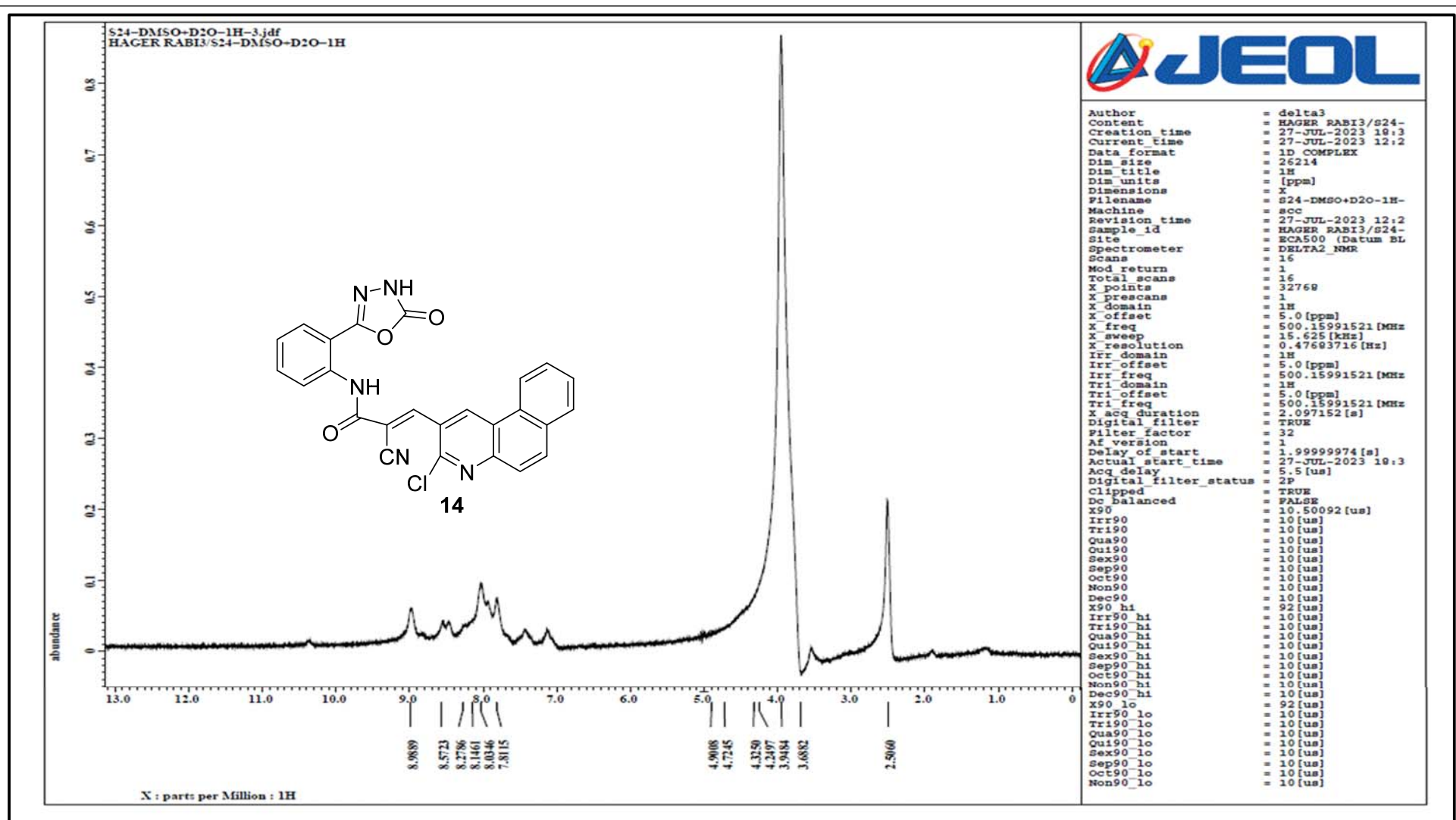


Fig. SD42. ¹H NMR spectrum (DMSO-*d*₆+D₂O) of compound 14

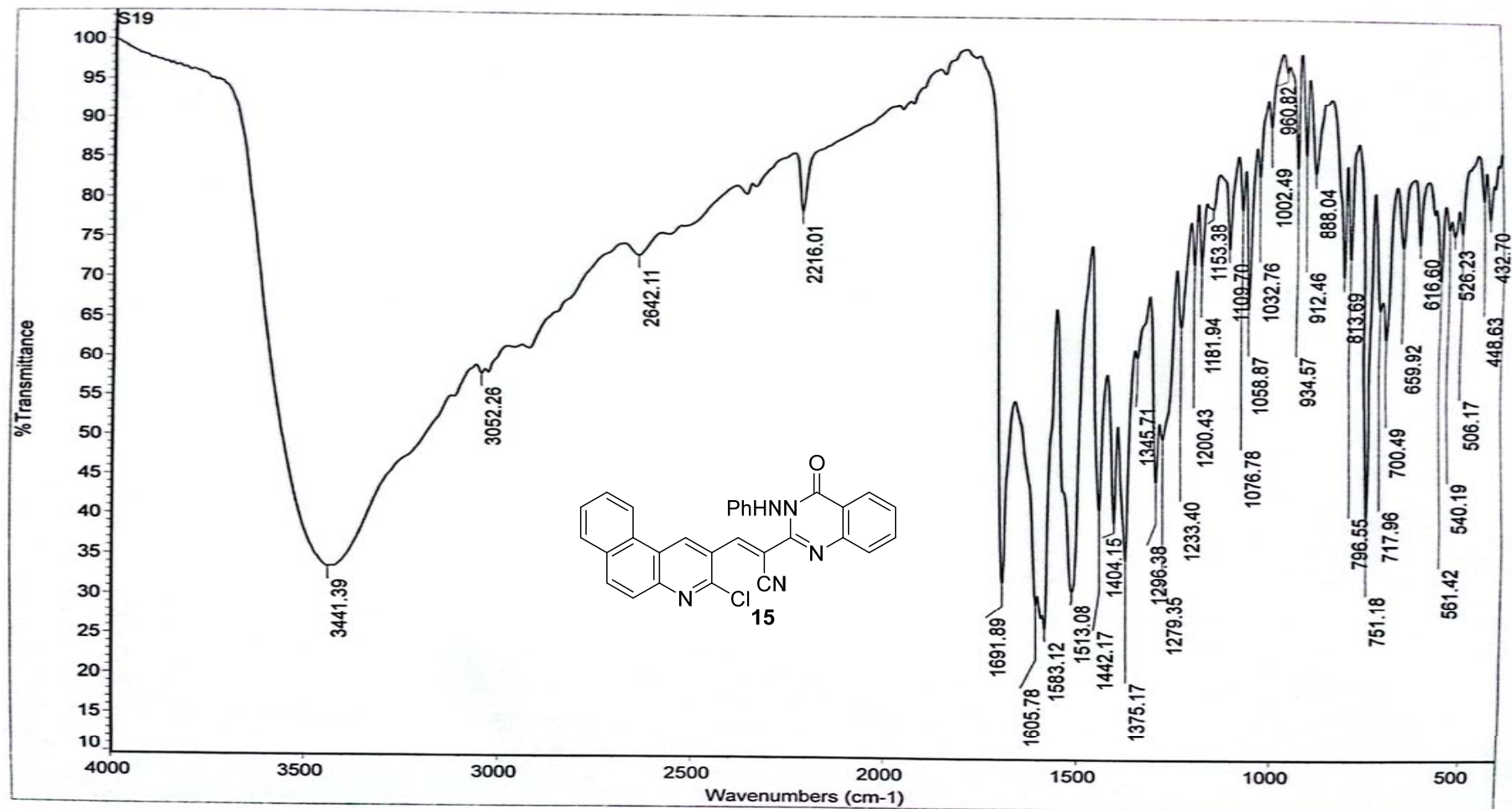
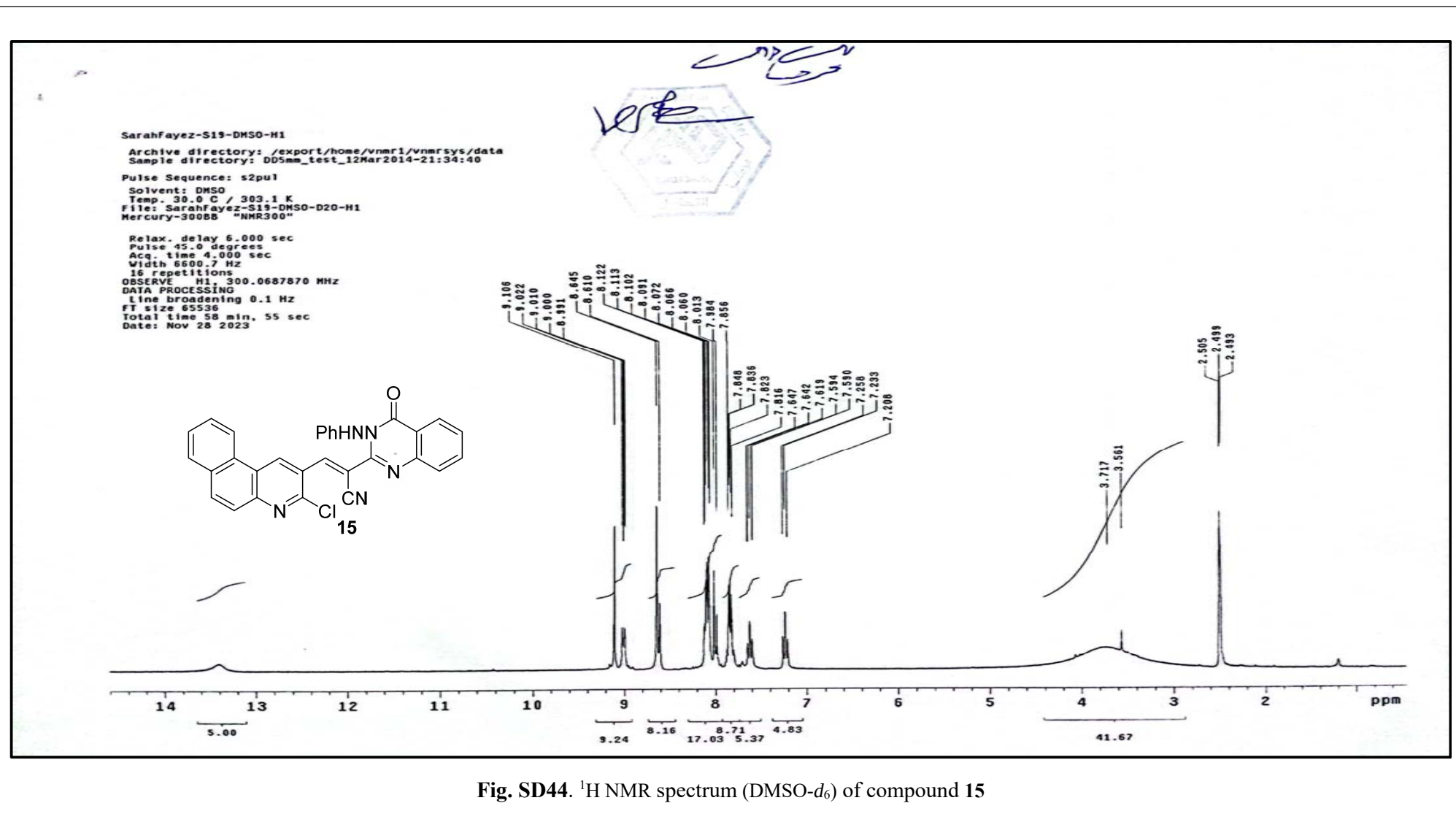


Fig. SD43. IR spectrum of compound 15



Sarahfayez-S19-DMSO-D2O--H1

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Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul1

Solvent: DMSO

Temp. 30.0 C / 303.1 K

Mercury-300DB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
15 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FI size 65536
Total time 50 min, 55 sec
Date: Nov 28 2023

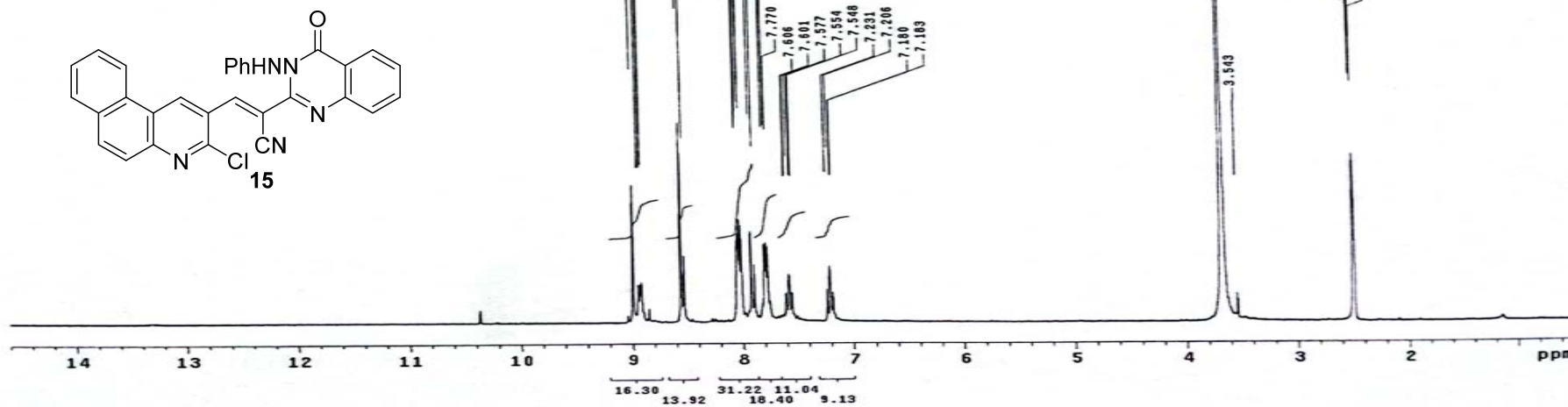


Fig. SD45. ^1H NMR spectrum ($\text{DMSO-}d_6+\text{D}_2\text{O}$) of compound 15

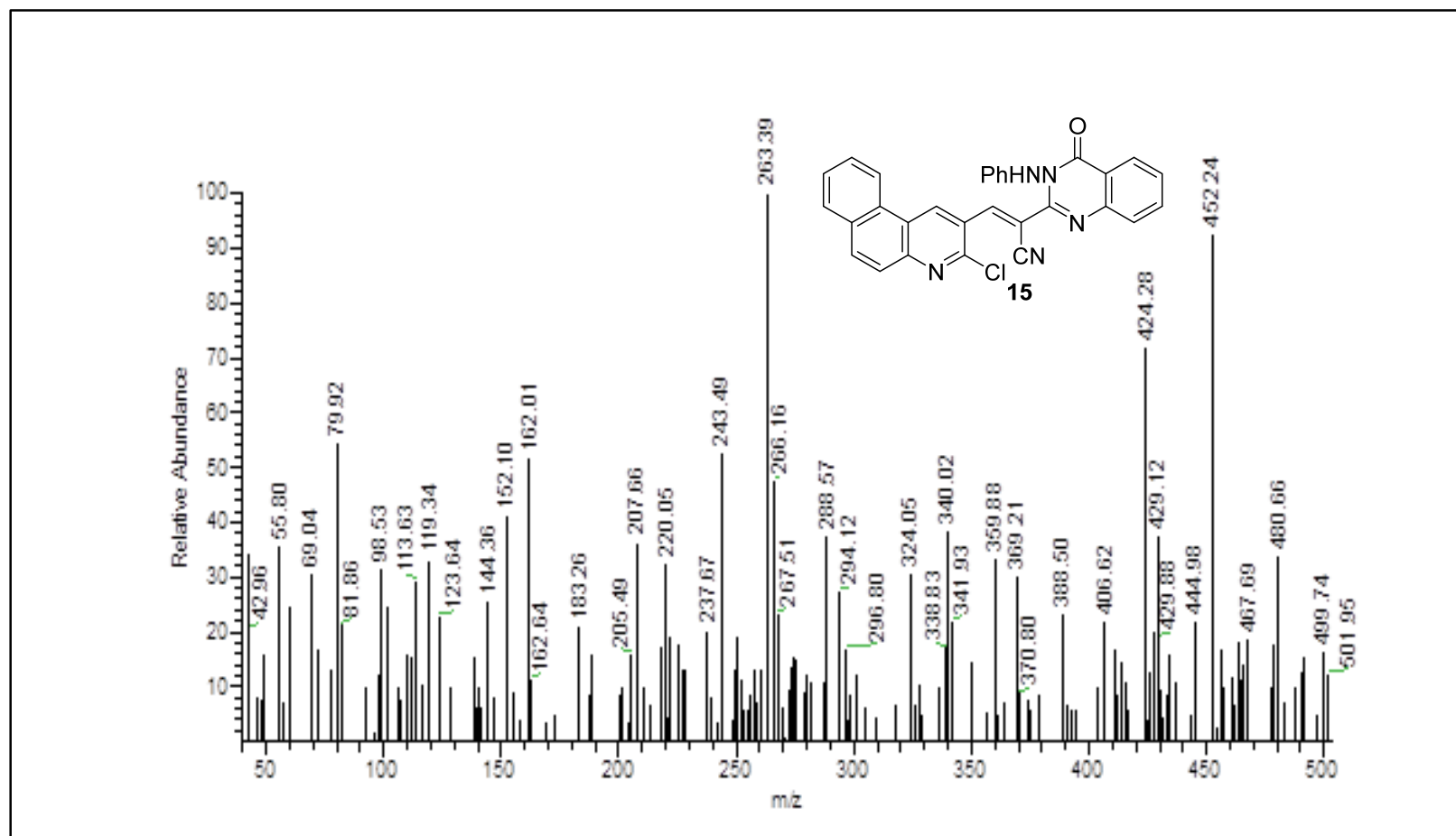
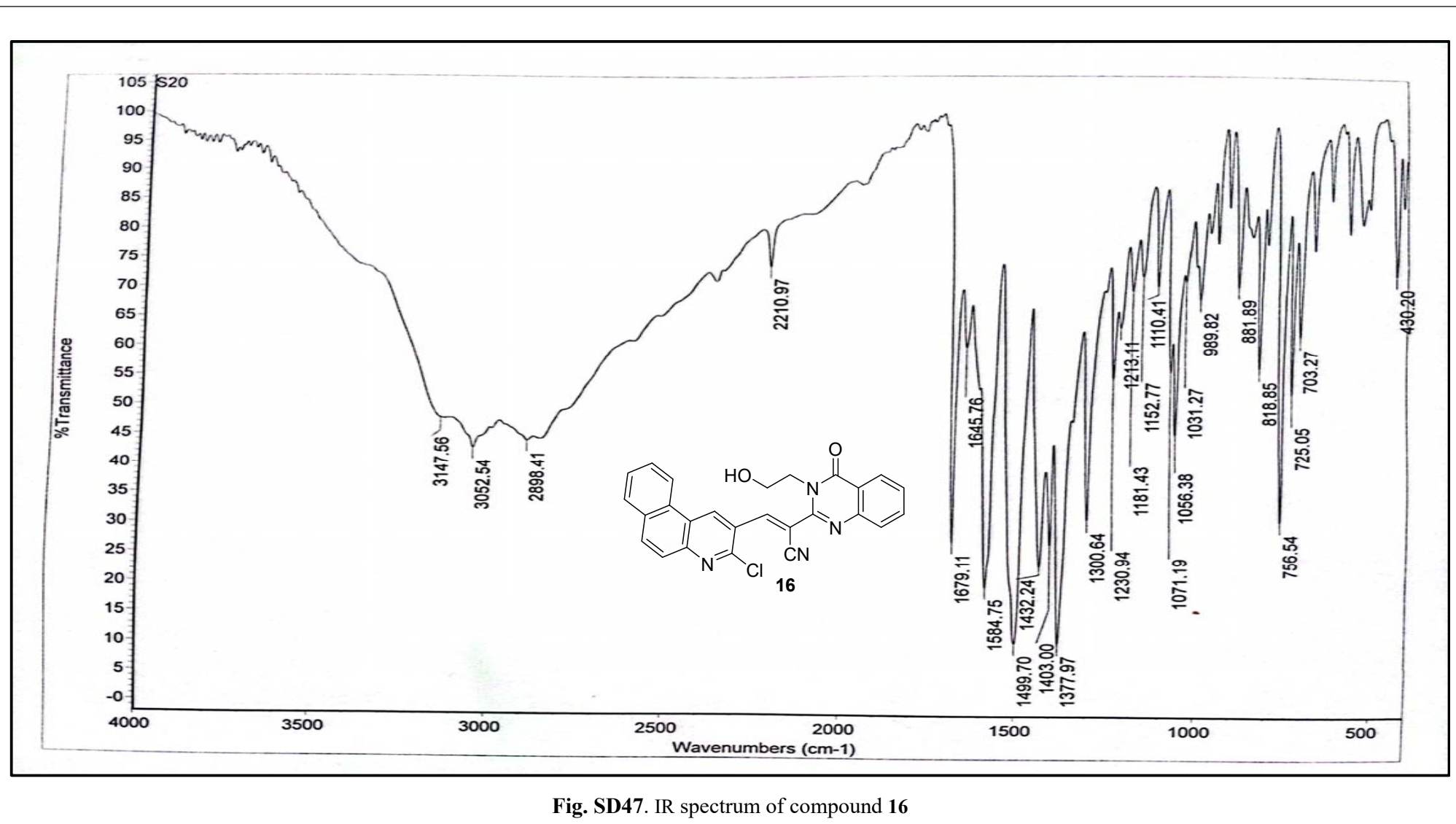


Fig. SD46. Mass spectrum of compound 15



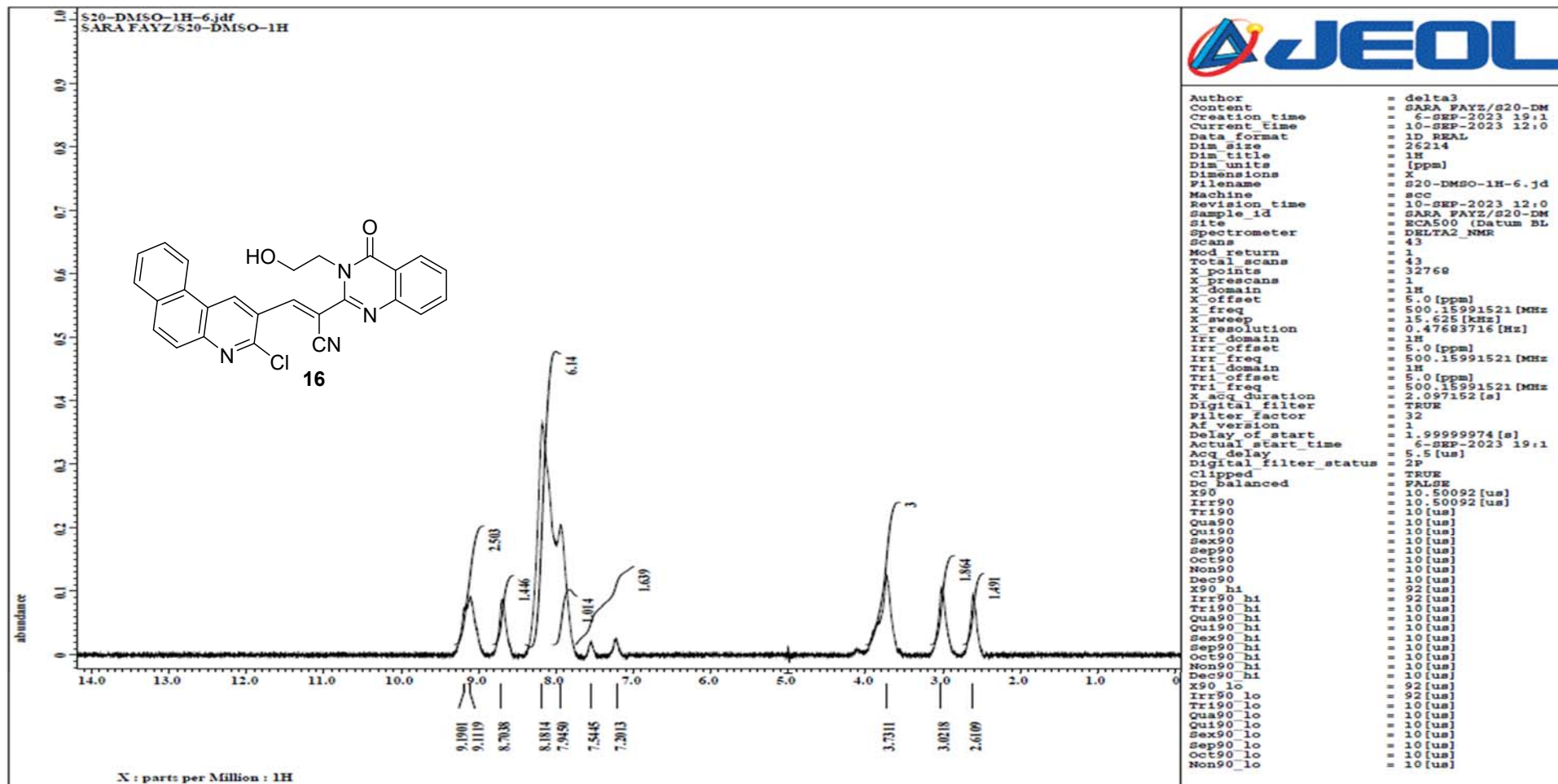


Fig. SD48. ^1H NMR spectrum (DMSO- d_6) of compound 16

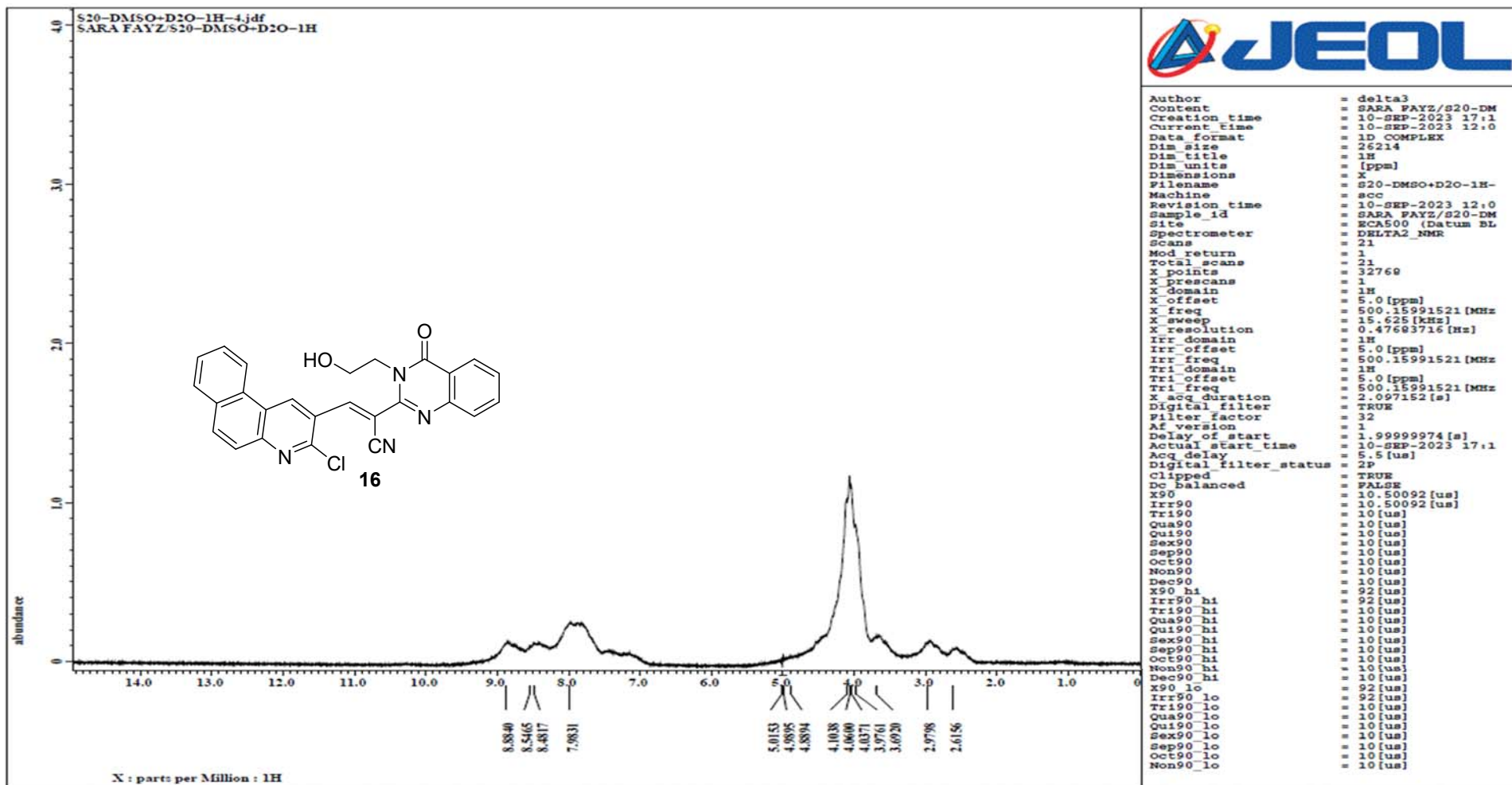


Fig. SD49. ¹H NMR spectrum (DMSO-*d*₆+D₂O) of compound 16

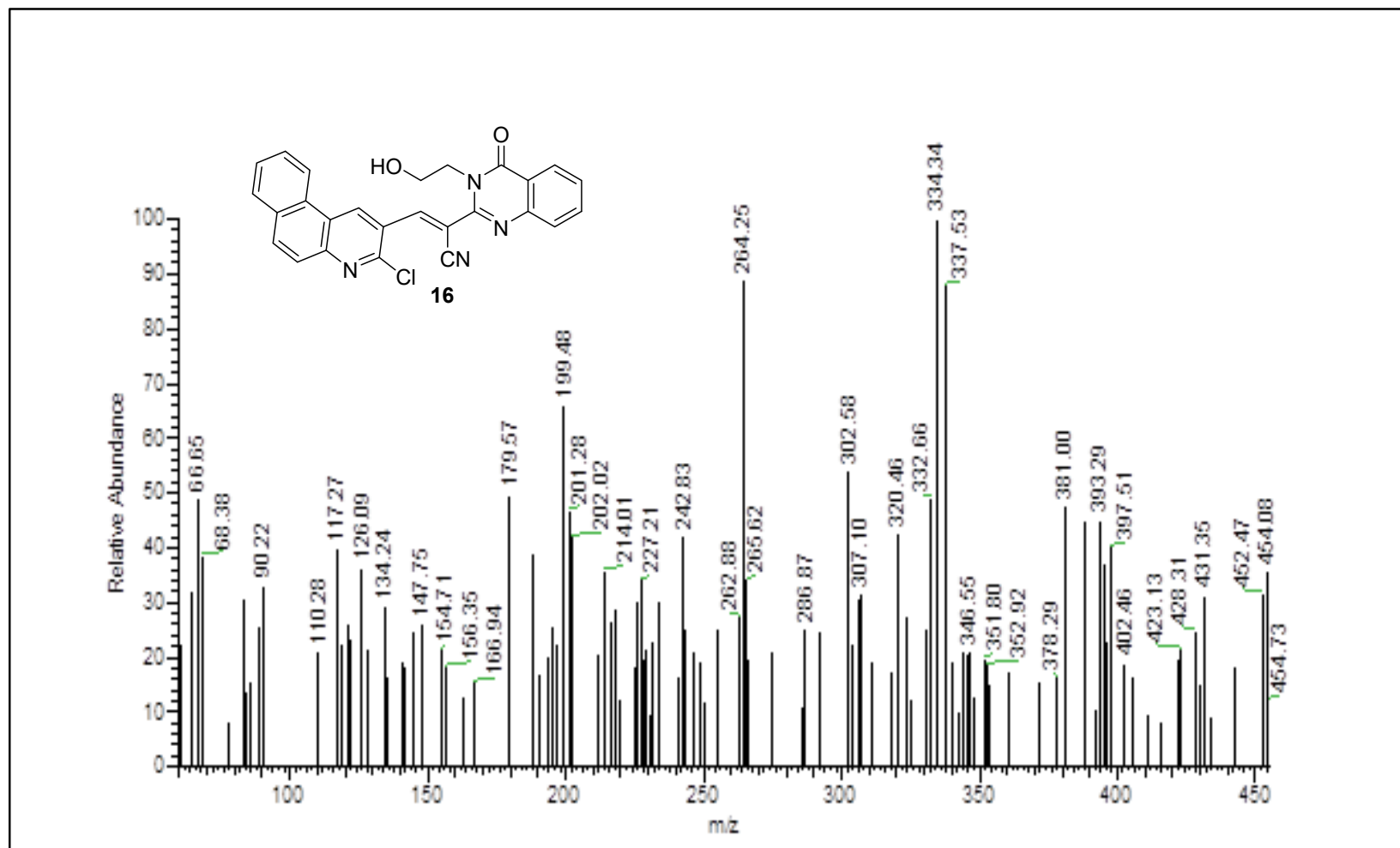


Fig. SD50. Mass spectrum (DMSO- d_6) of compound 16

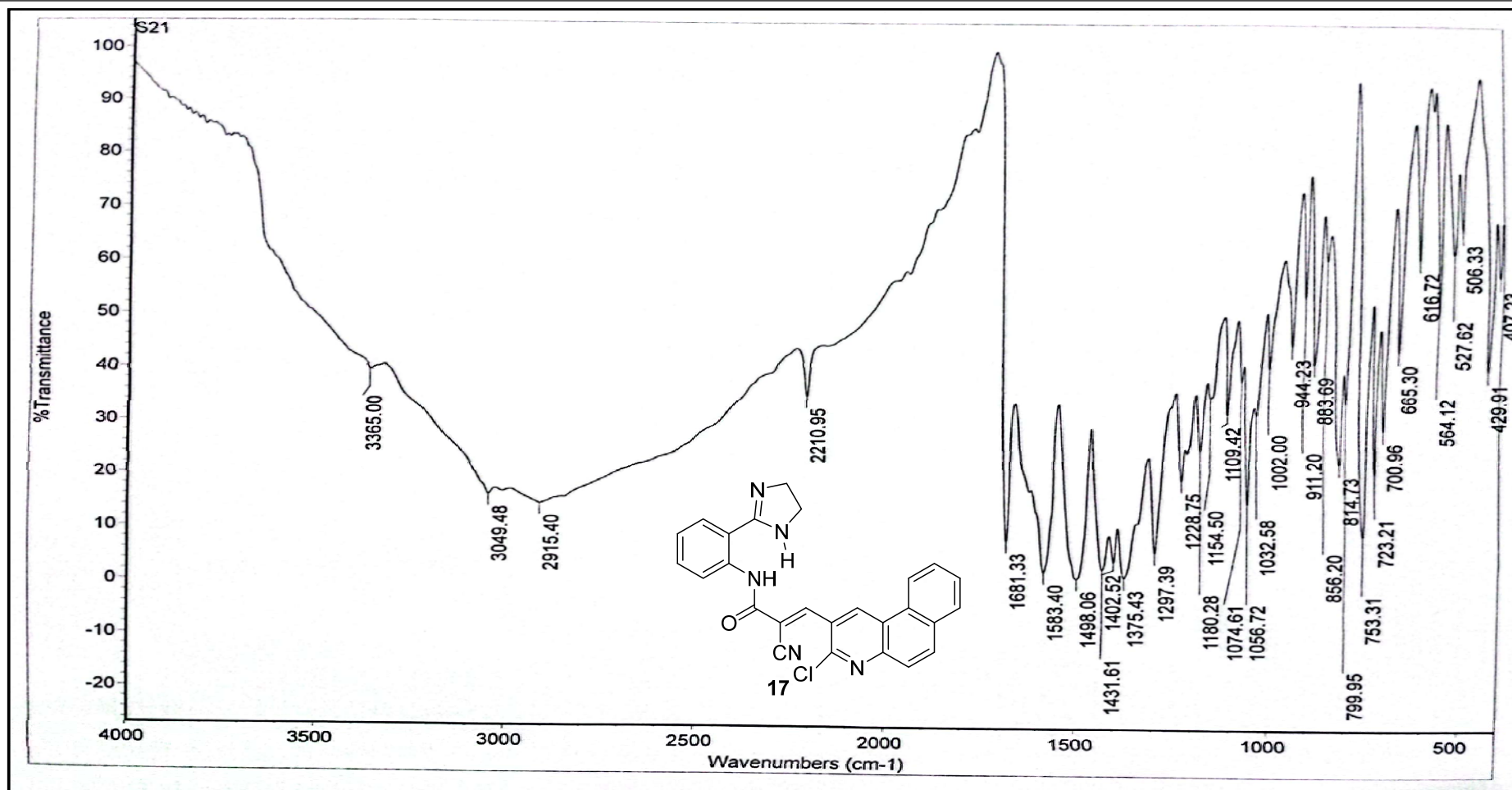


Fig. SD51. IR spectrum of compound 17

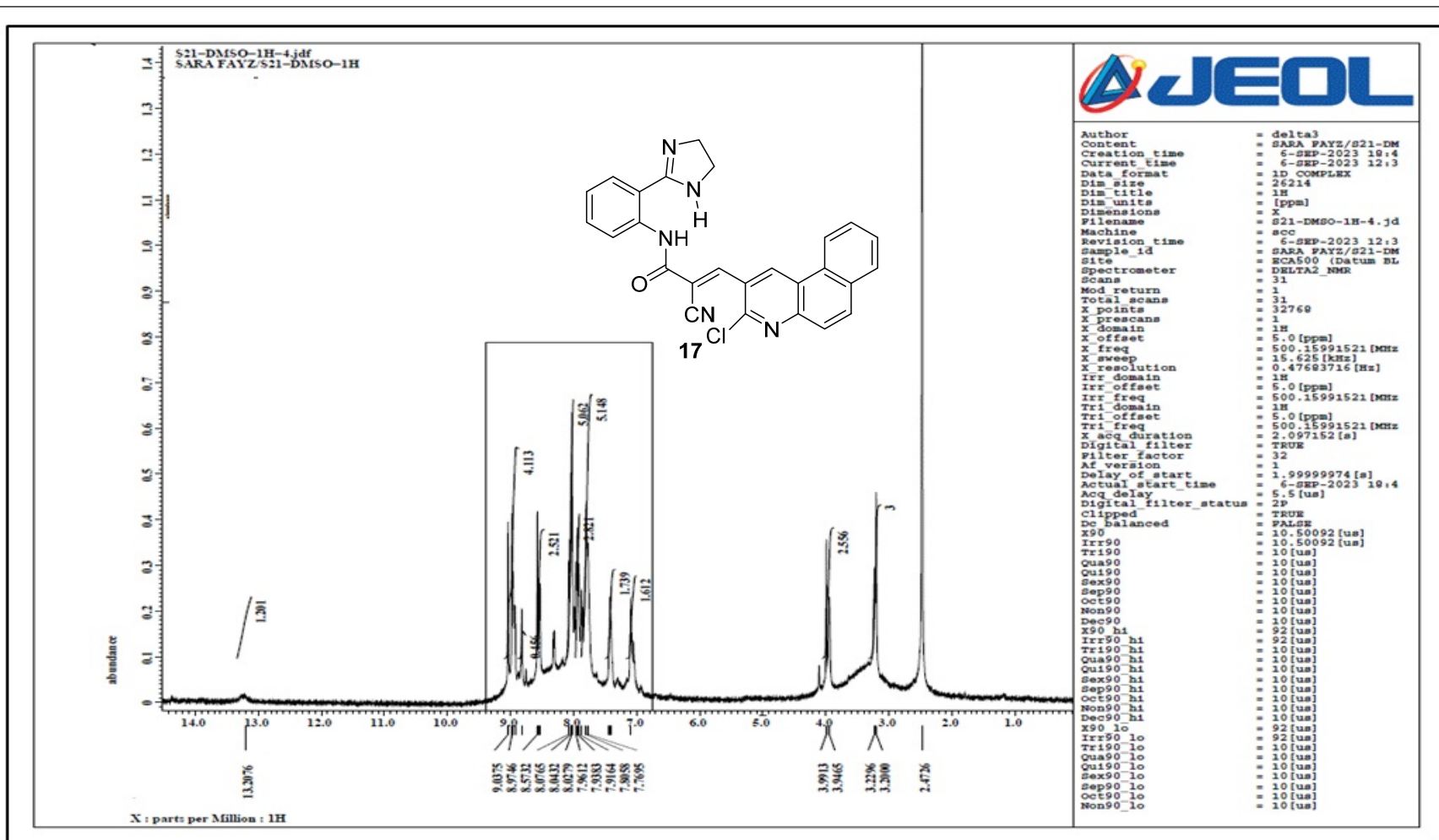


Fig. SD52. ¹H NMR spectrum (DMSO-d₆) of compound 17

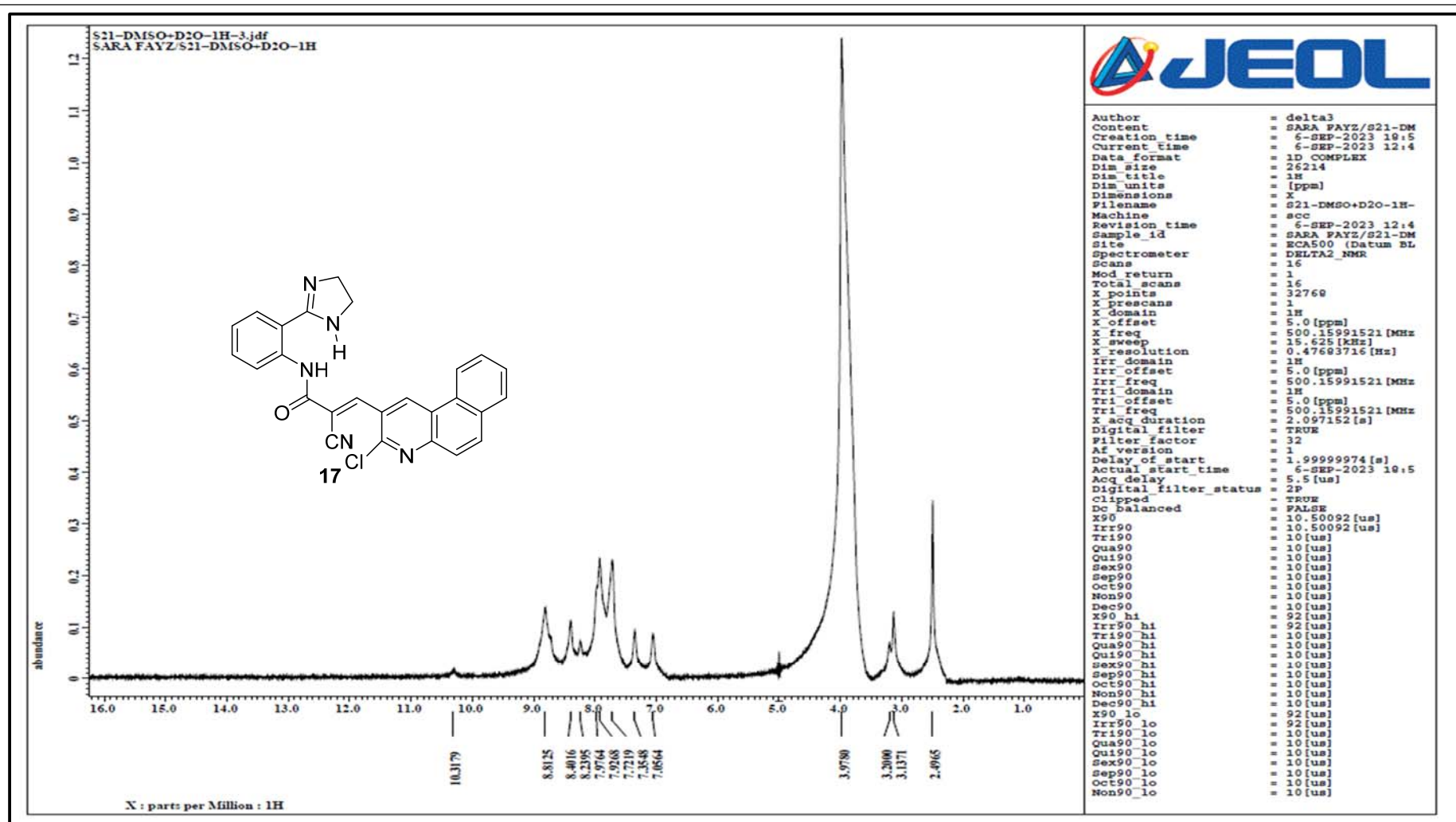


Fig. SD53. ^1H NMR spectrum (DMSO- d_6 +D $_2$ O) of compound 17

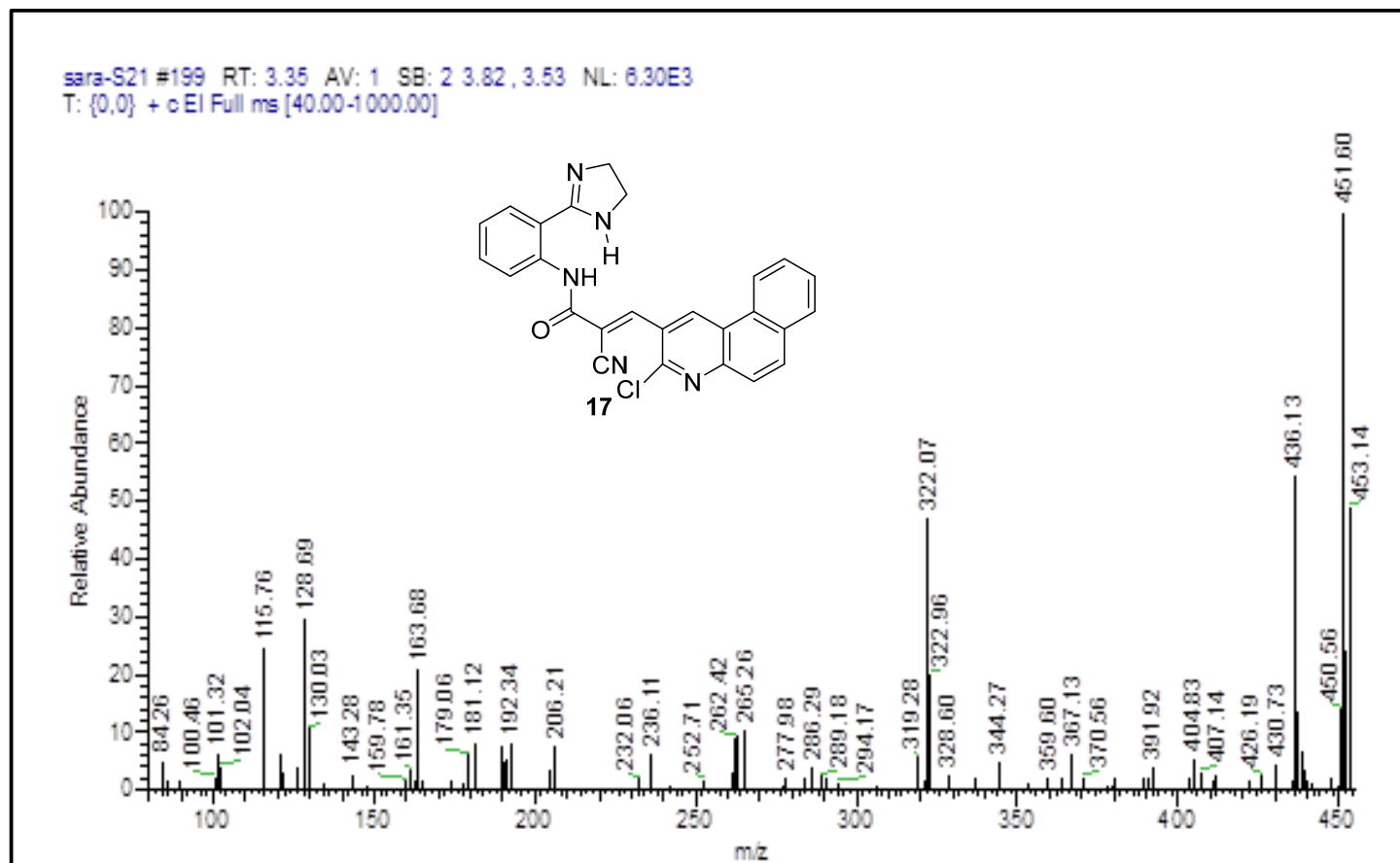


Fig. SD54. Mass spectrum of compound 17

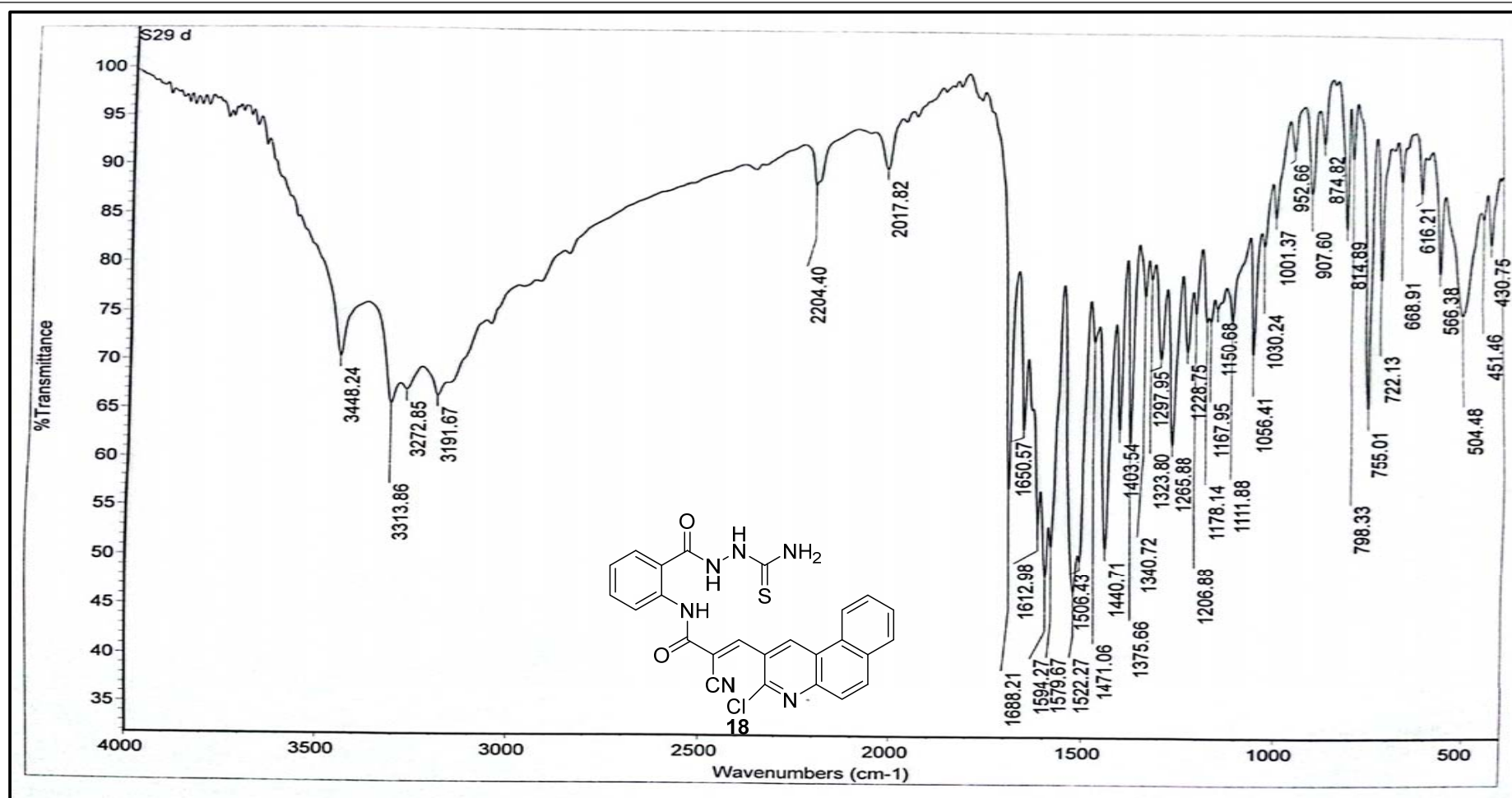


Fig. SD55. IR spectrum of compound 18

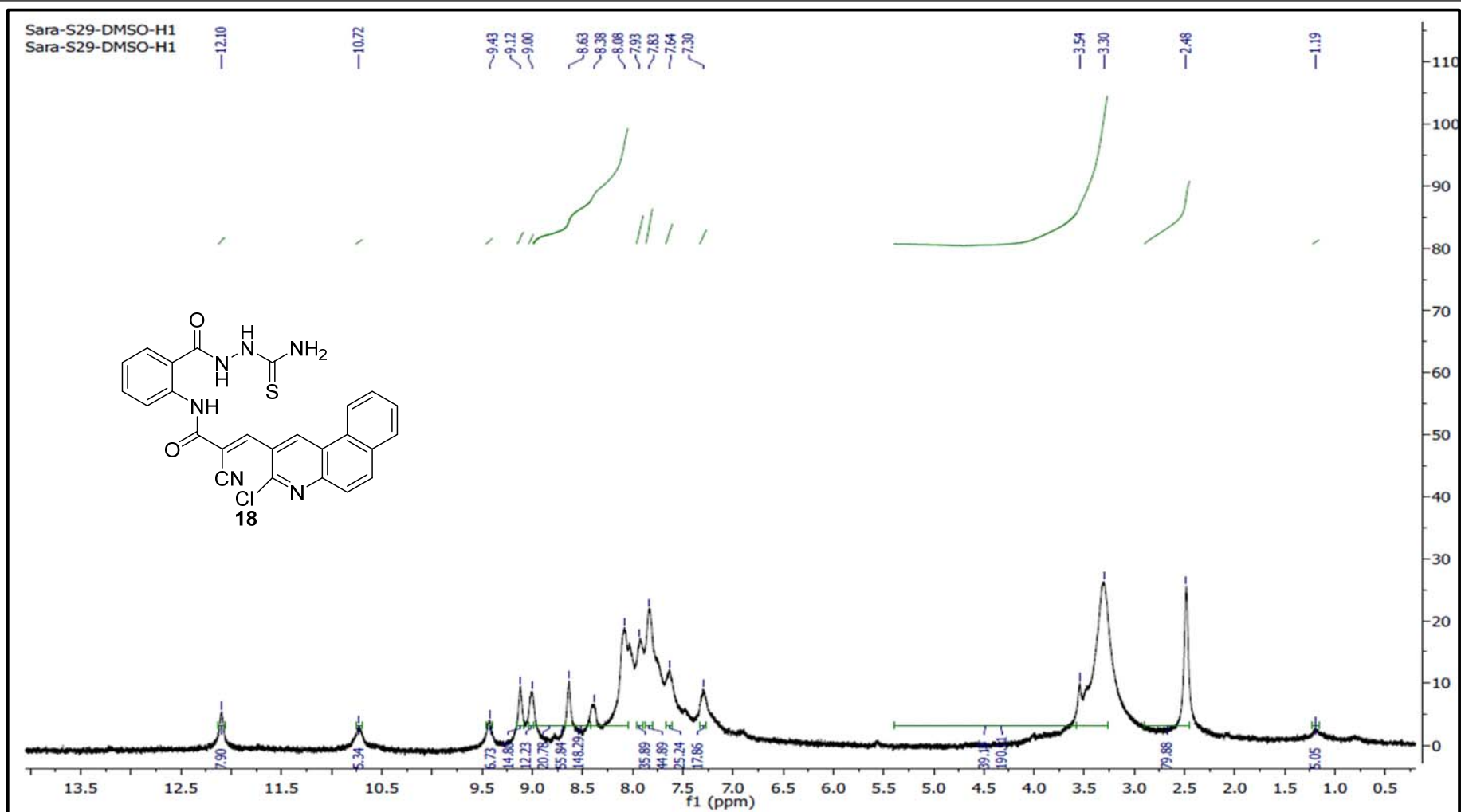


Fig. SD56. ^1H NMR spectrum ($\text{DMSO}-d_6$) of compound 18

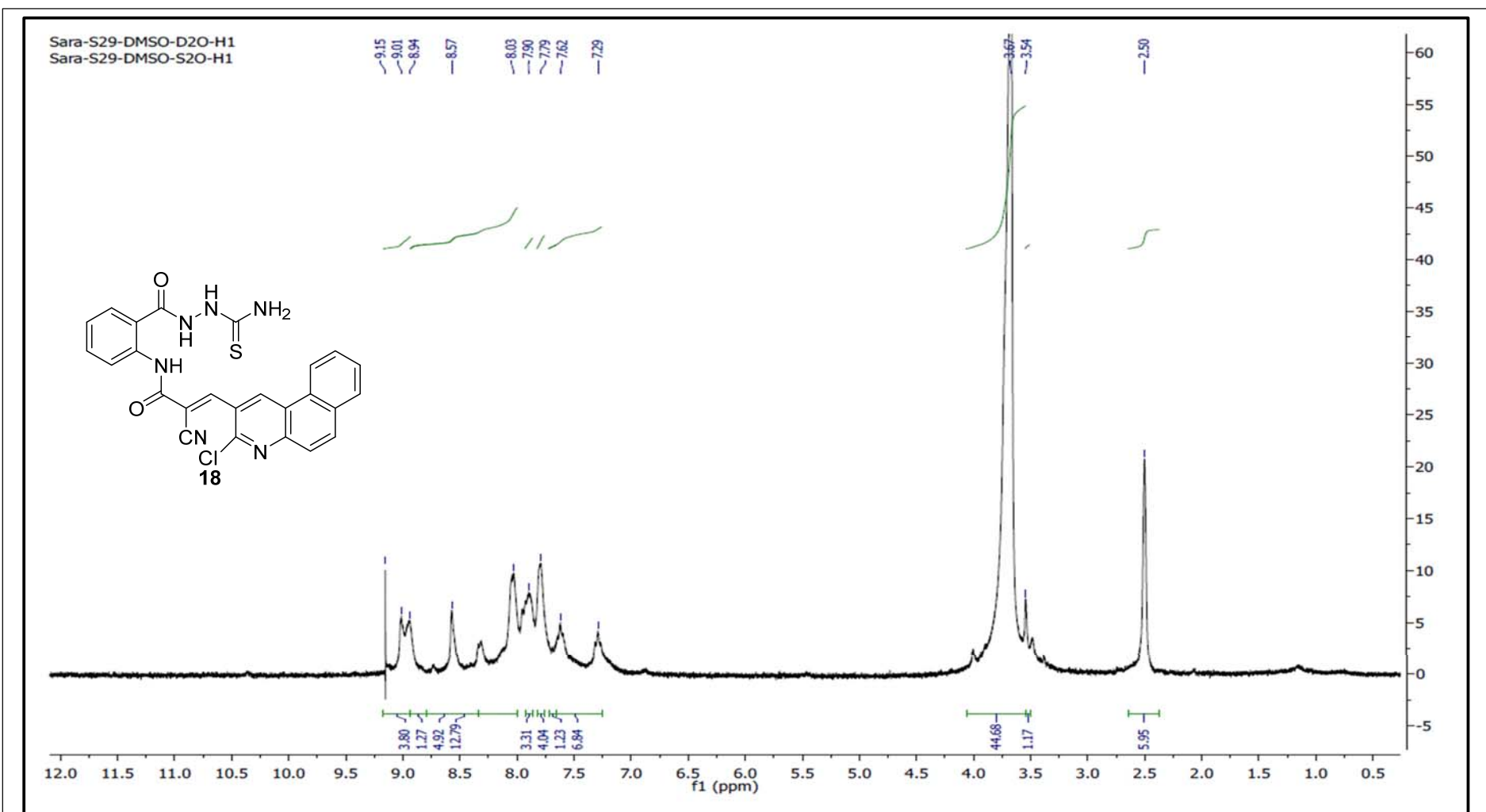


Fig. SD57. ^1H NMR spectrum ($\text{DMSO-}d_6+\text{D}_2\text{O}$) of compound **18**

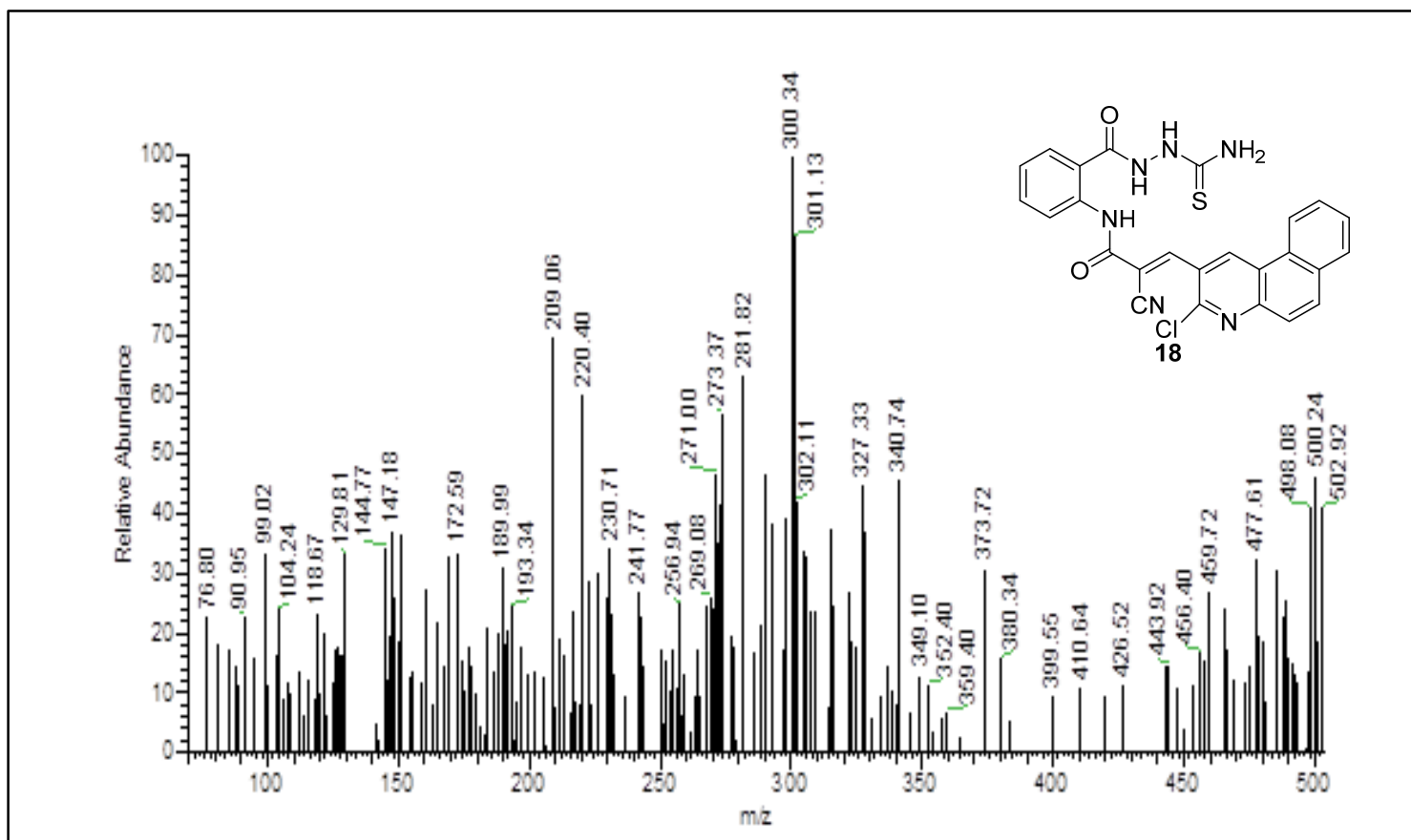


Fig. SD58. Mass spectrum of compound **18**

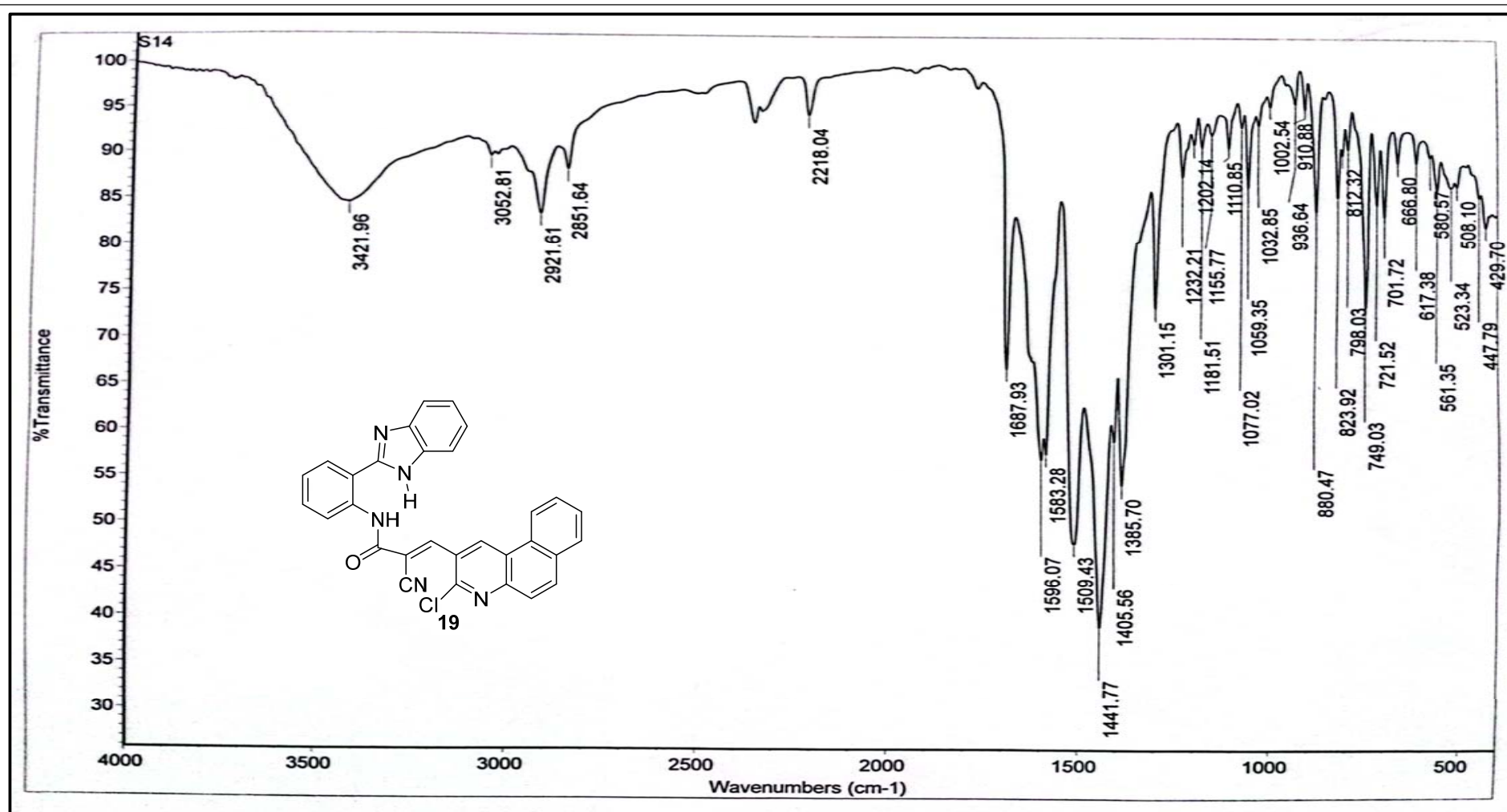


Fig. SD59. IR spectrum of compound 19

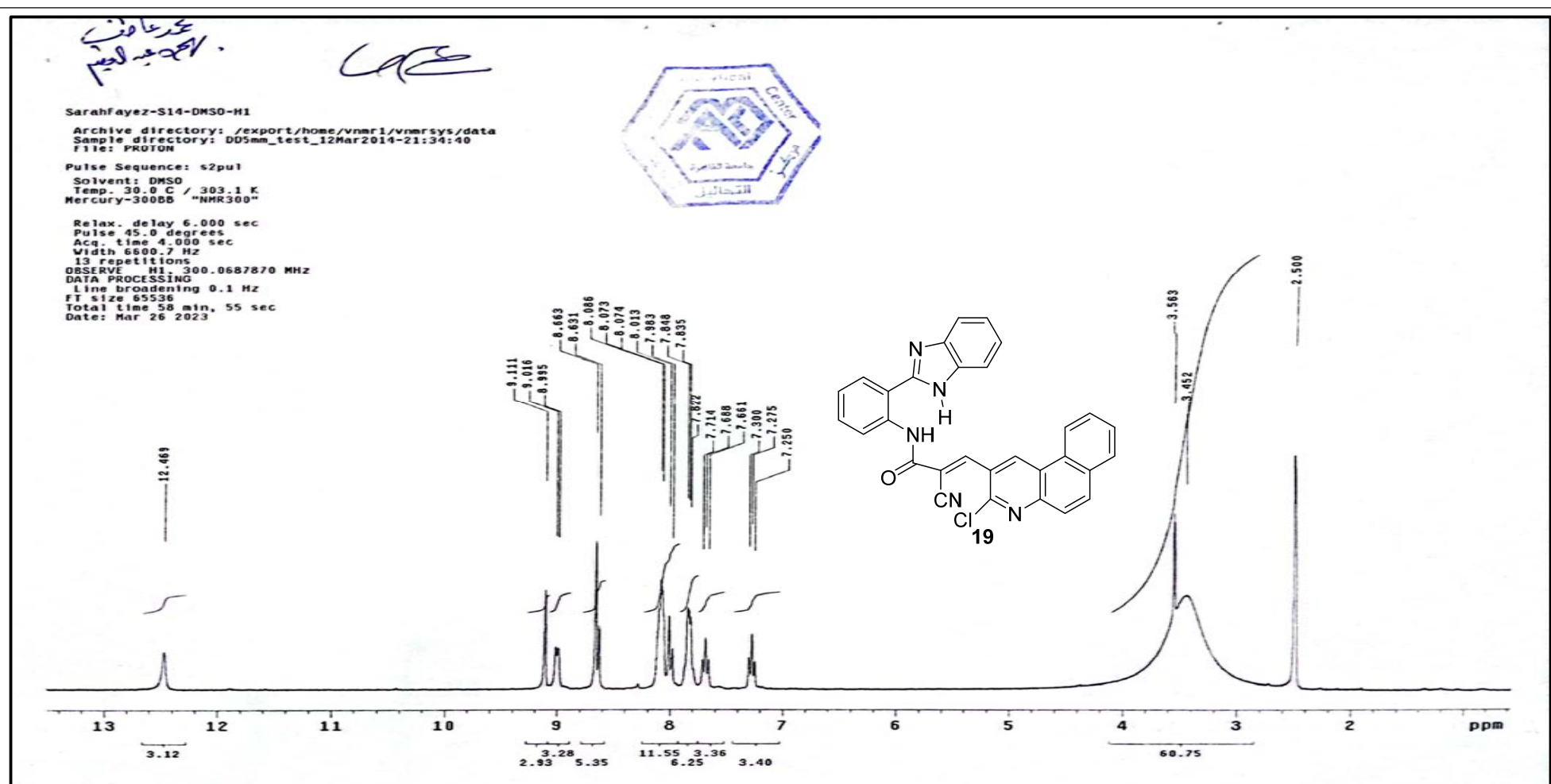


Fig. SD60. ^1H NMR spectrum (DMSO- d_6) of compound 19

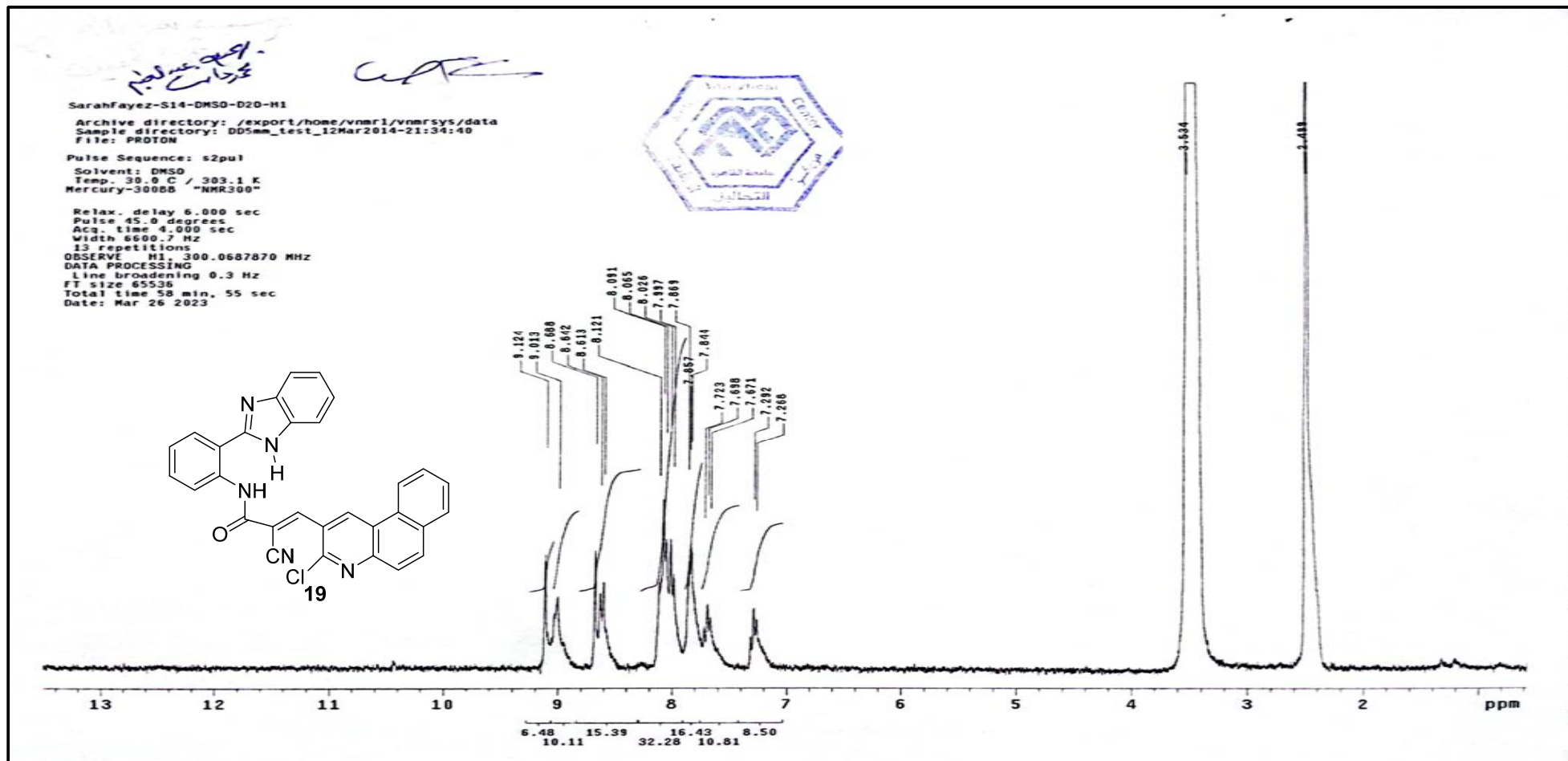


Fig. SD61. ^1H NMR spectrum ($\text{DMSO}-d_6$) of compound 19

