

Supporting information

[3+2] Cycloaddition mediated synthesis of Spirooxindole Pyrrolidine/Piperidine Fused Chromene Aldehyde Derivatives: DFT Studies, Antibacterial Evaluation and Molecular Docking Investigation as DNA gyrase inhibitors

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1. ^1H , ^{13}C NMR and HRMS spectra of synthesized compounds **16(a-k)**, **16'(a-f)** and **17**

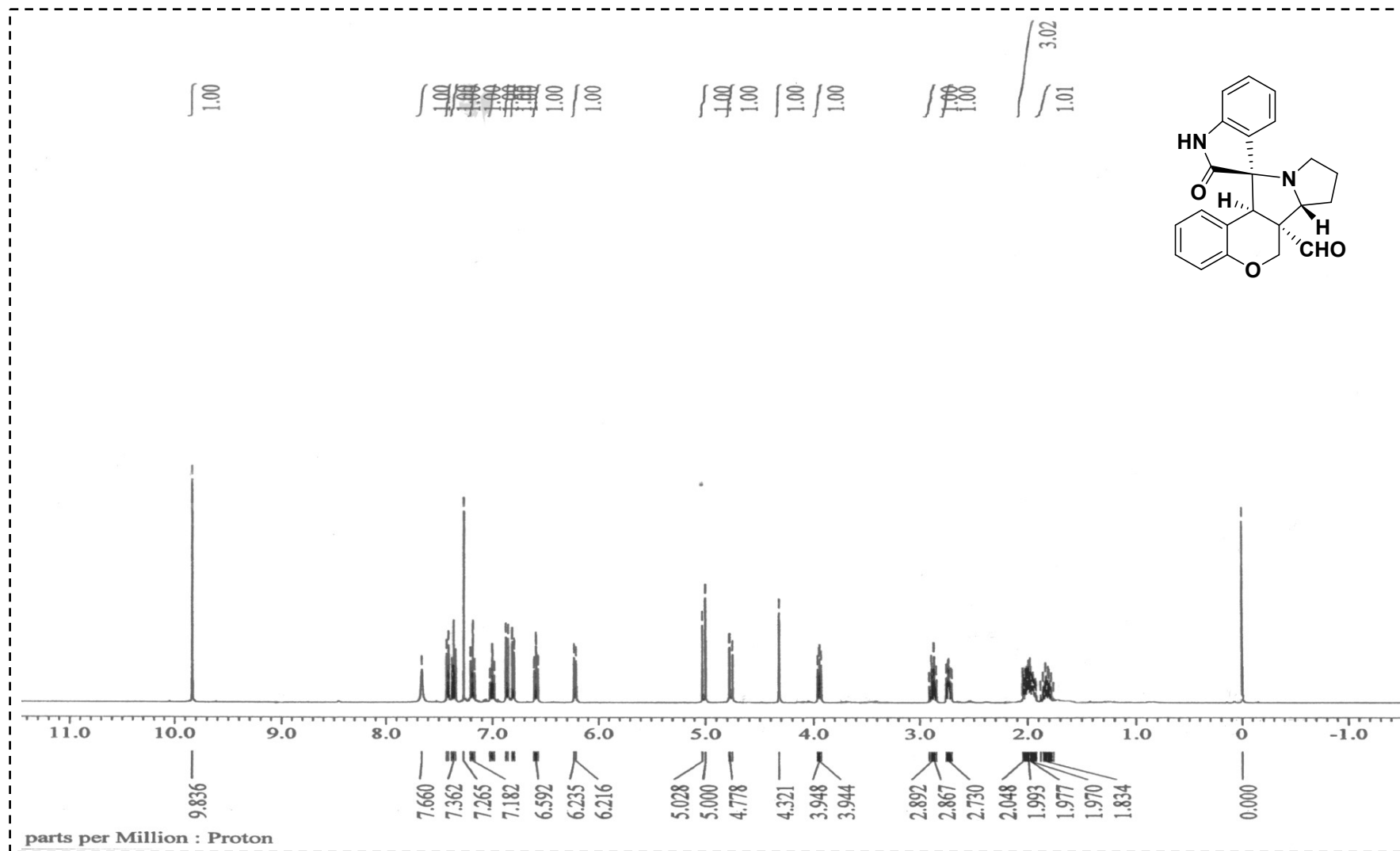


Fig S1. ^1H NMR spectrum of compound **16a** in CDCl_3

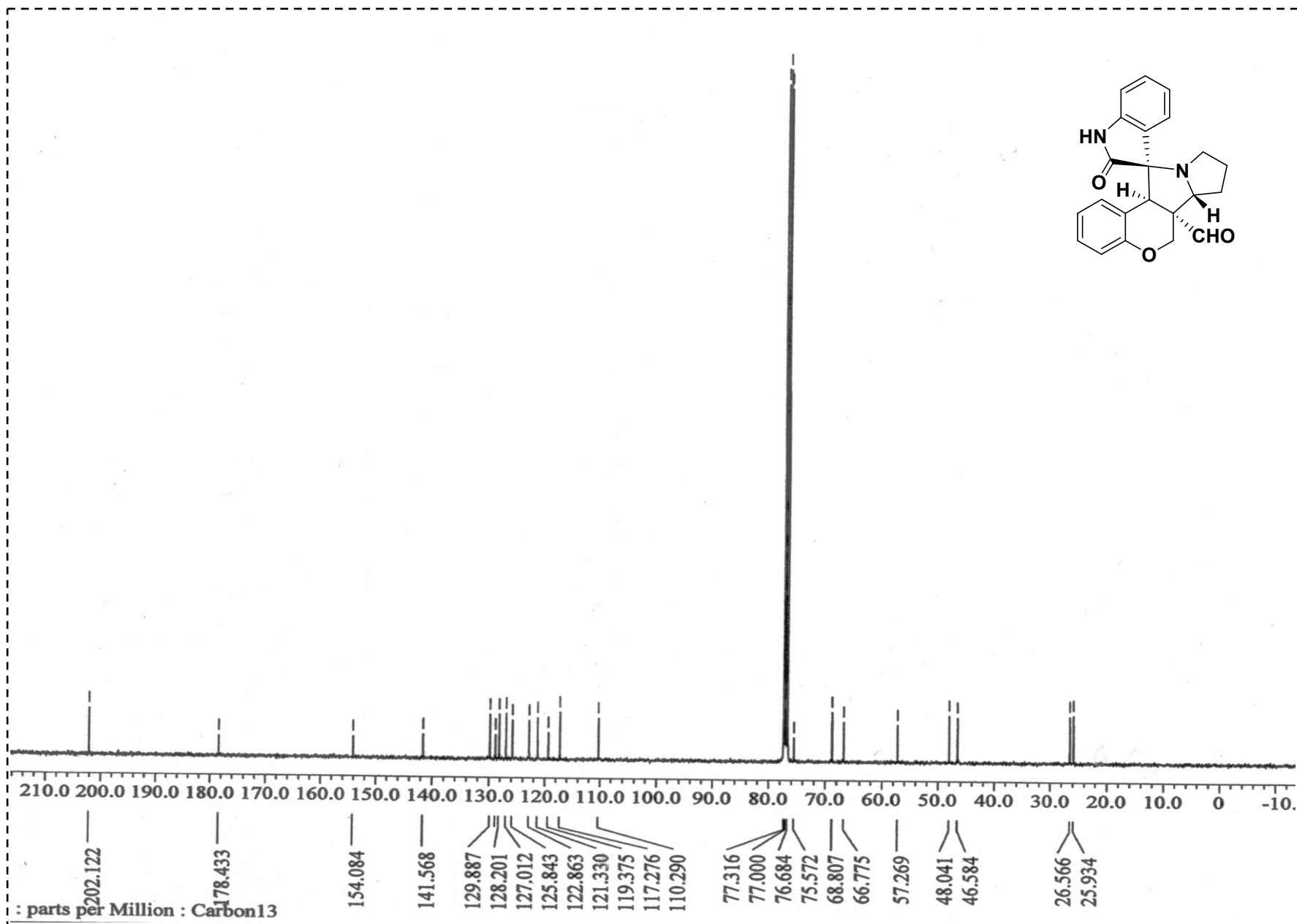


Fig S2. ^{13}C NMR spectrum of compound **16a** in CDCl_3

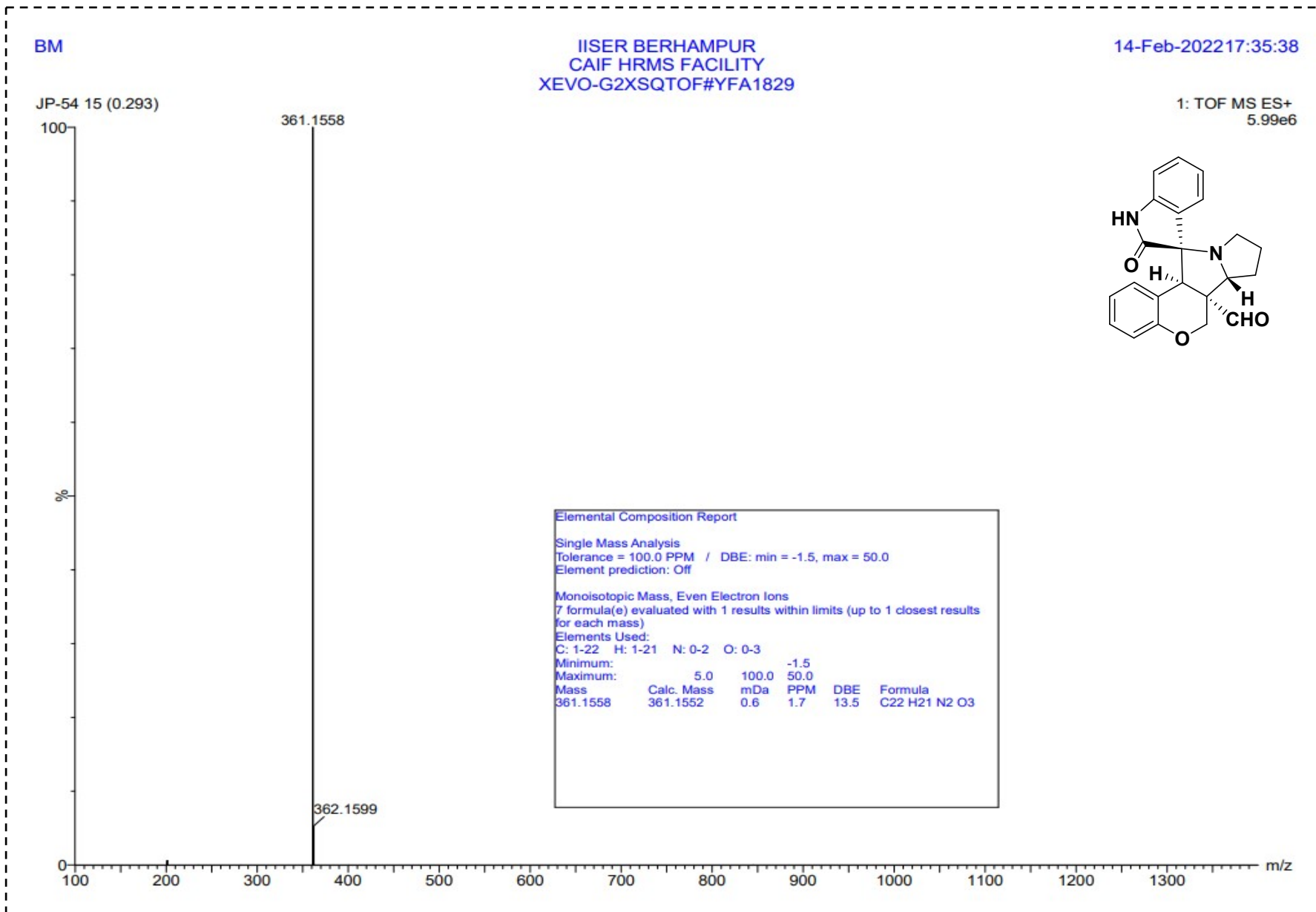


Fig S3. HRMS of compound 16a

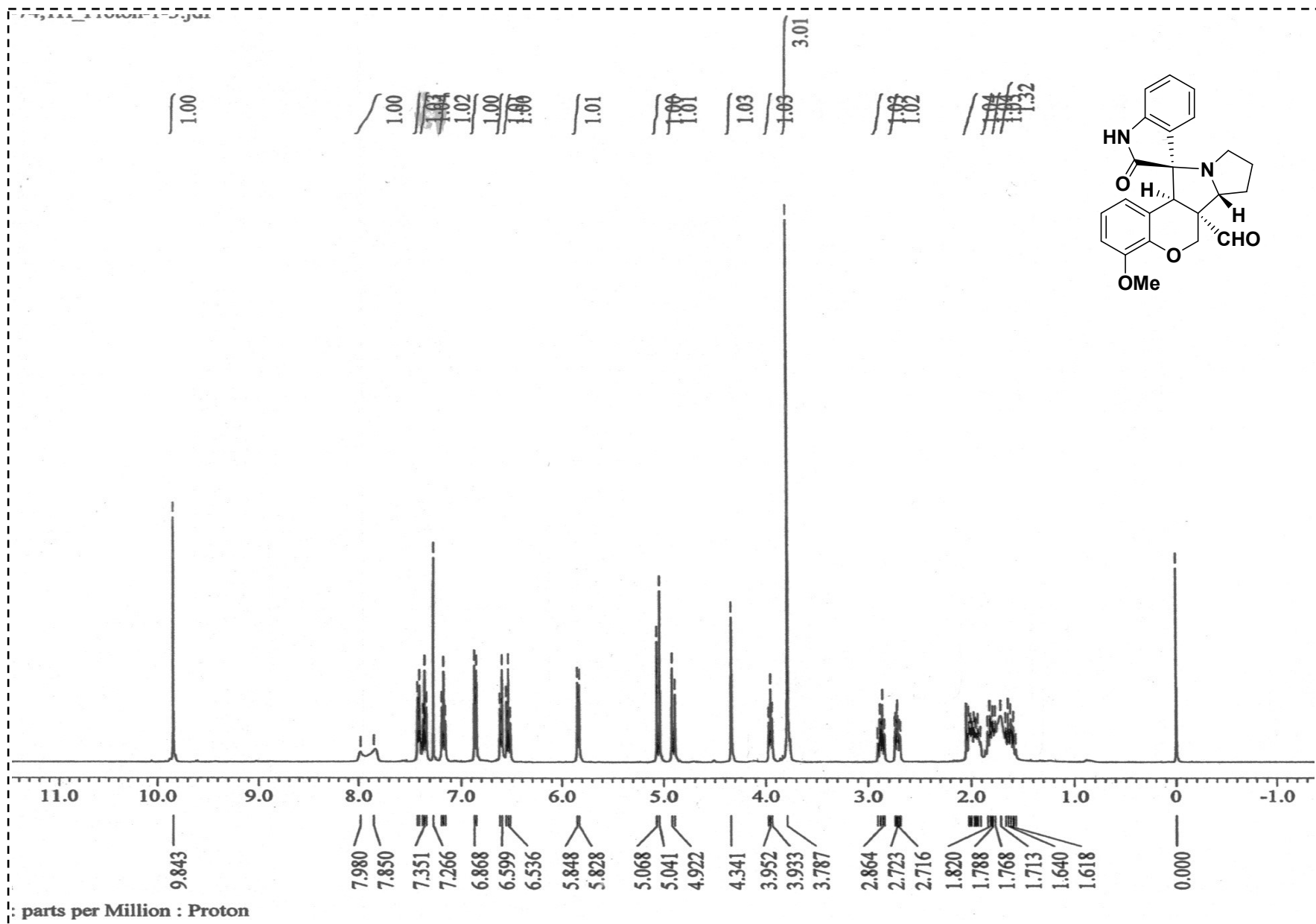


Fig S4. ^1H NMR spectrum of compound **16b** in CDCl_3

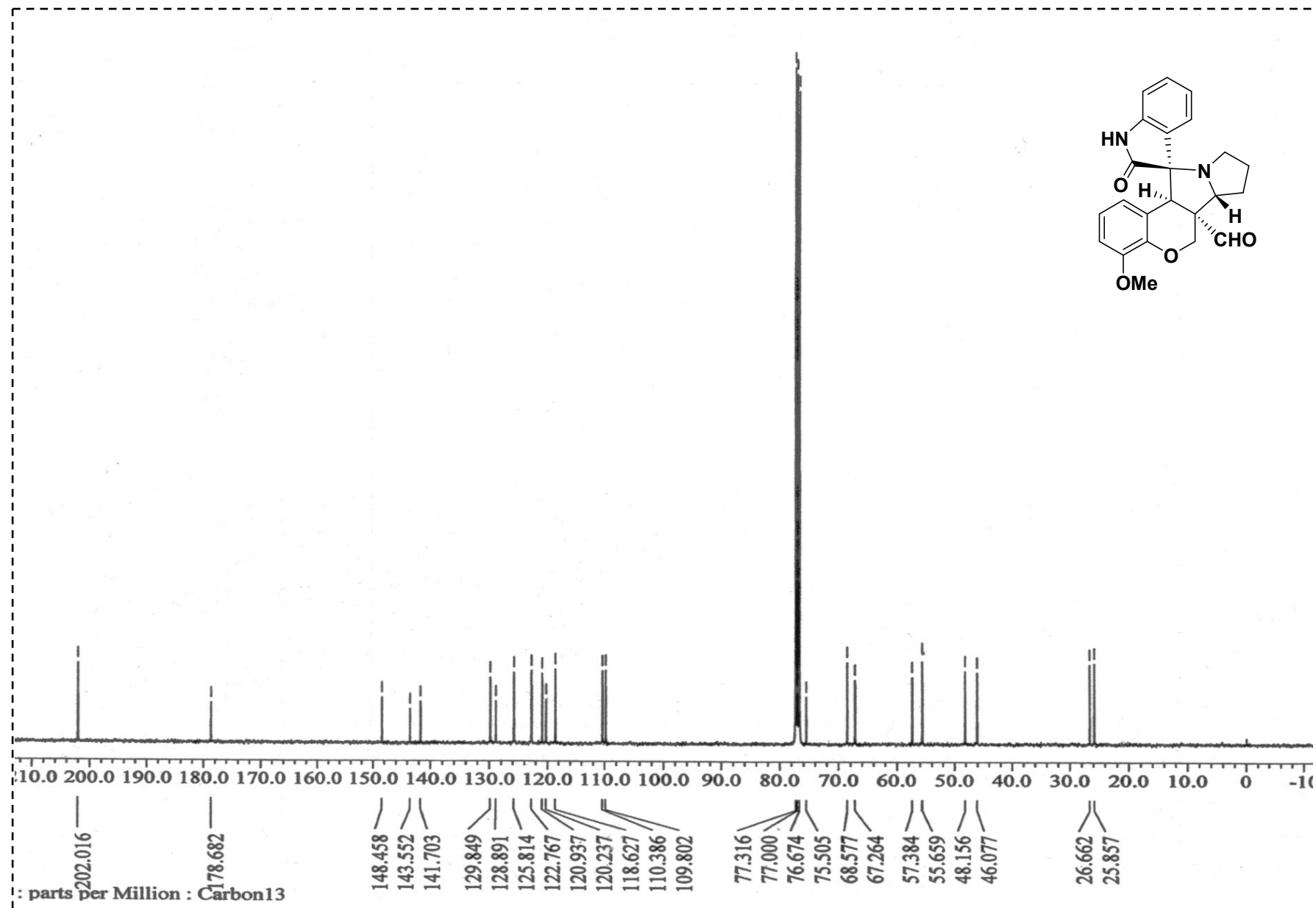


Fig S5. ¹³C NMR spectrum of compound **16b** in CDCl₃

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CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

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JP-74 10 (0.209) Cm (9:10)

1: TOF MS ES+
1.36e7

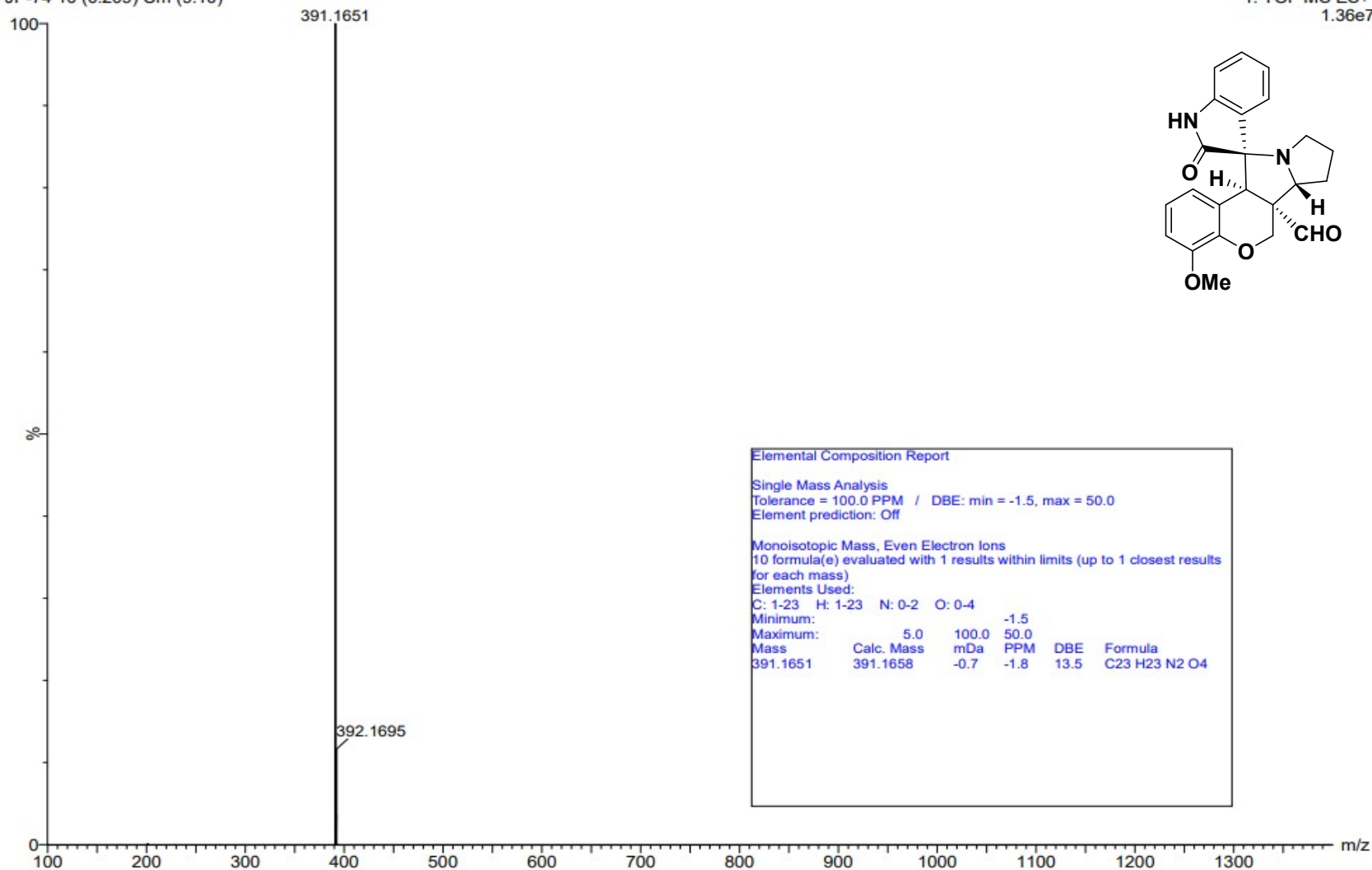


Fig S6. HRMS of compound 16b

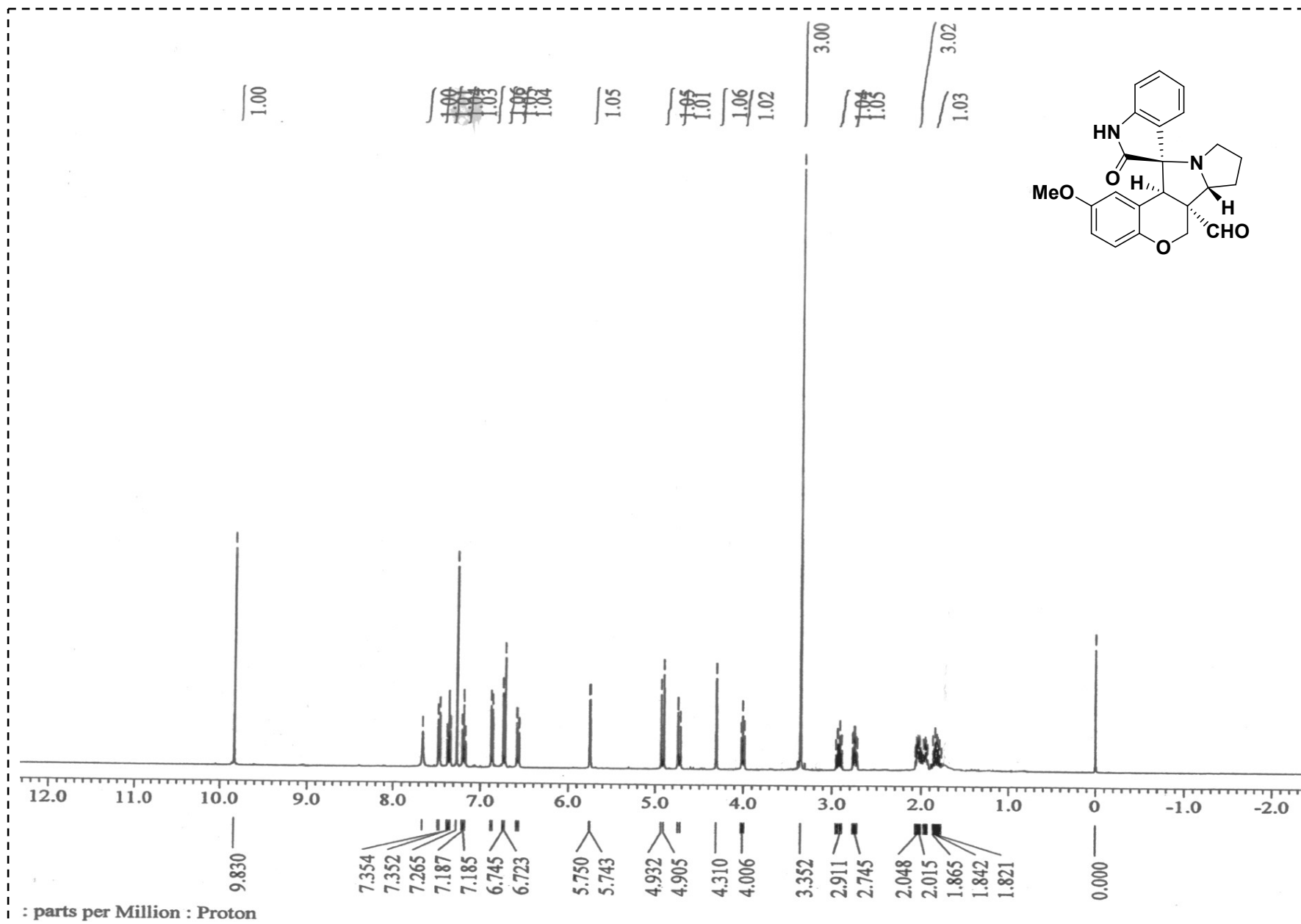


Fig S7. ¹H NMR spectrum of compound 16c in CDCl₃

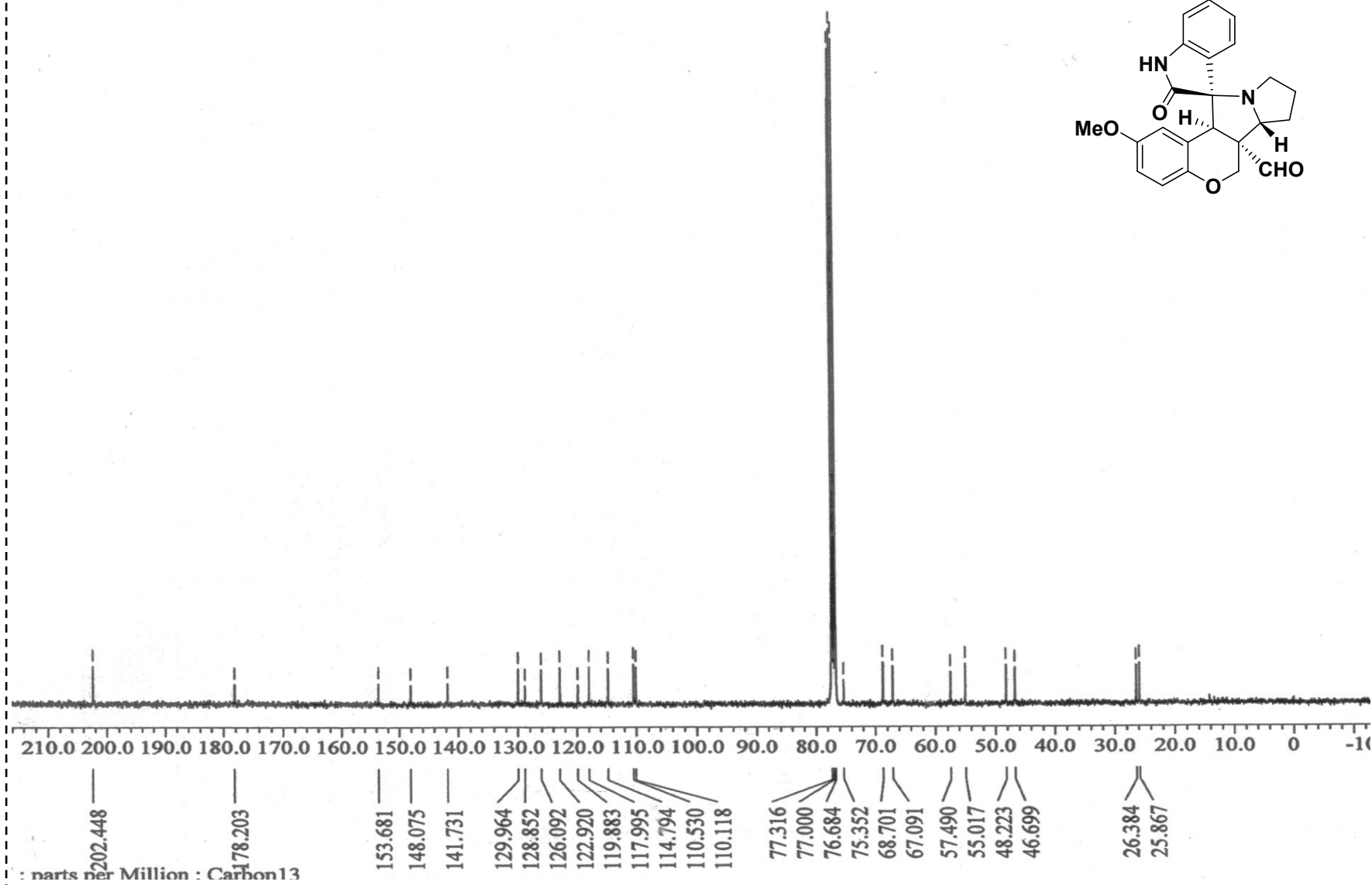
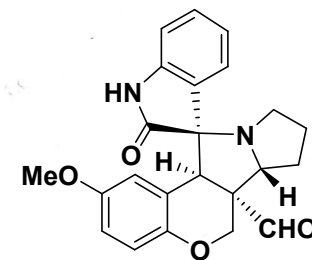


Fig S8. ¹³C NMR spectrum of compound 16c in CDCl₃

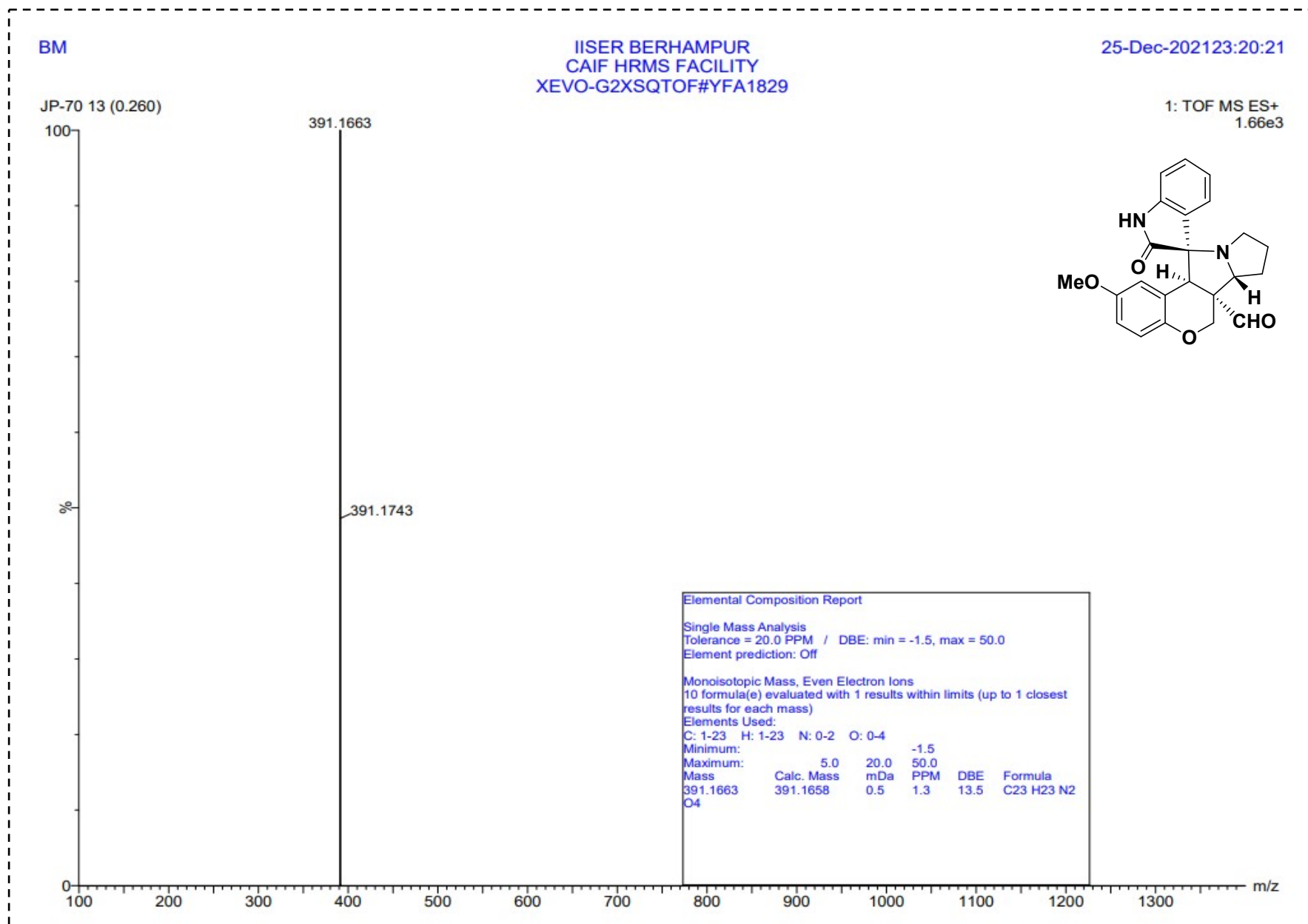


Fig S9. HRMS of compound 16c

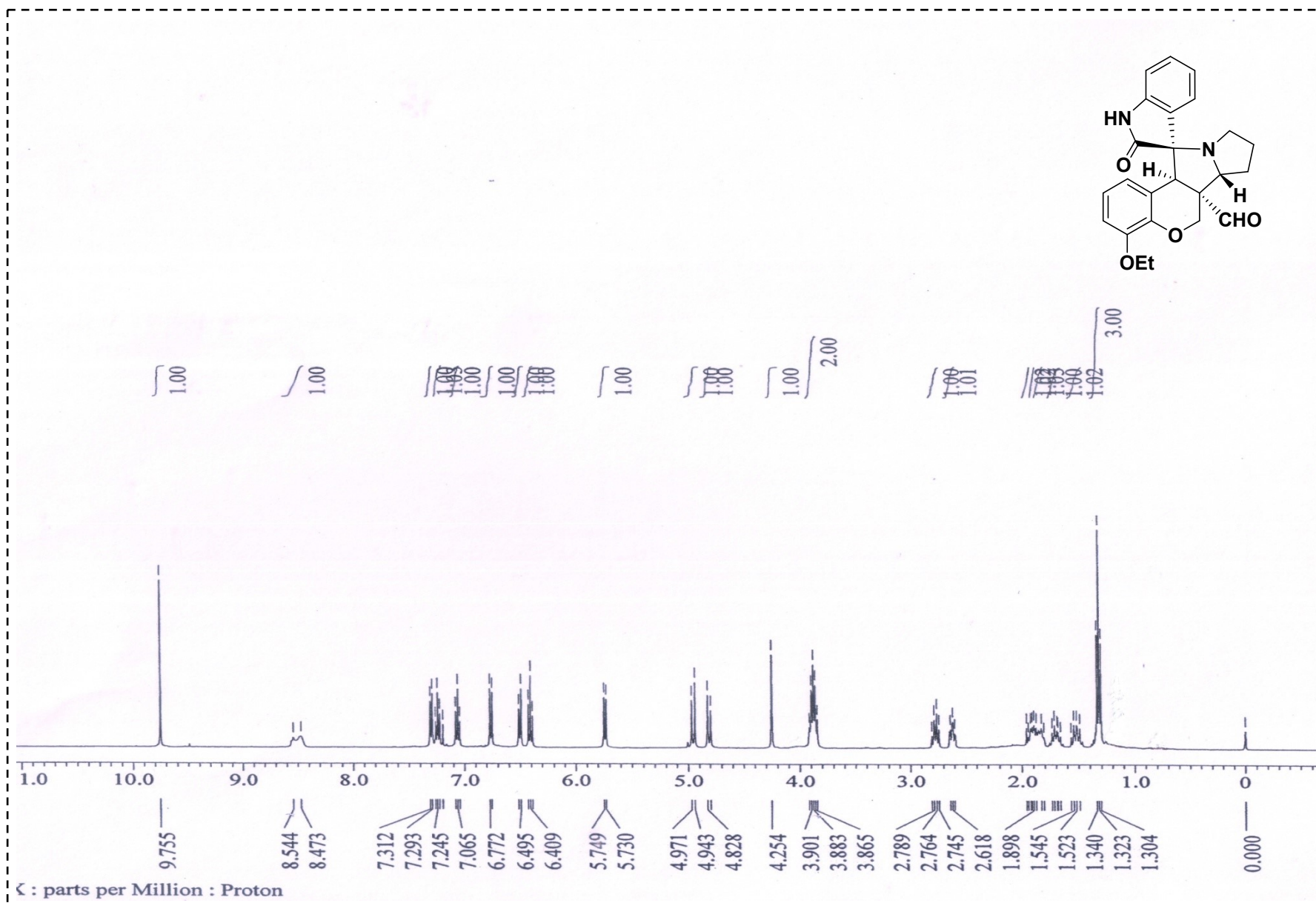


Fig S10. ¹H NMR spectrum of compound **16d** in CDCl₃

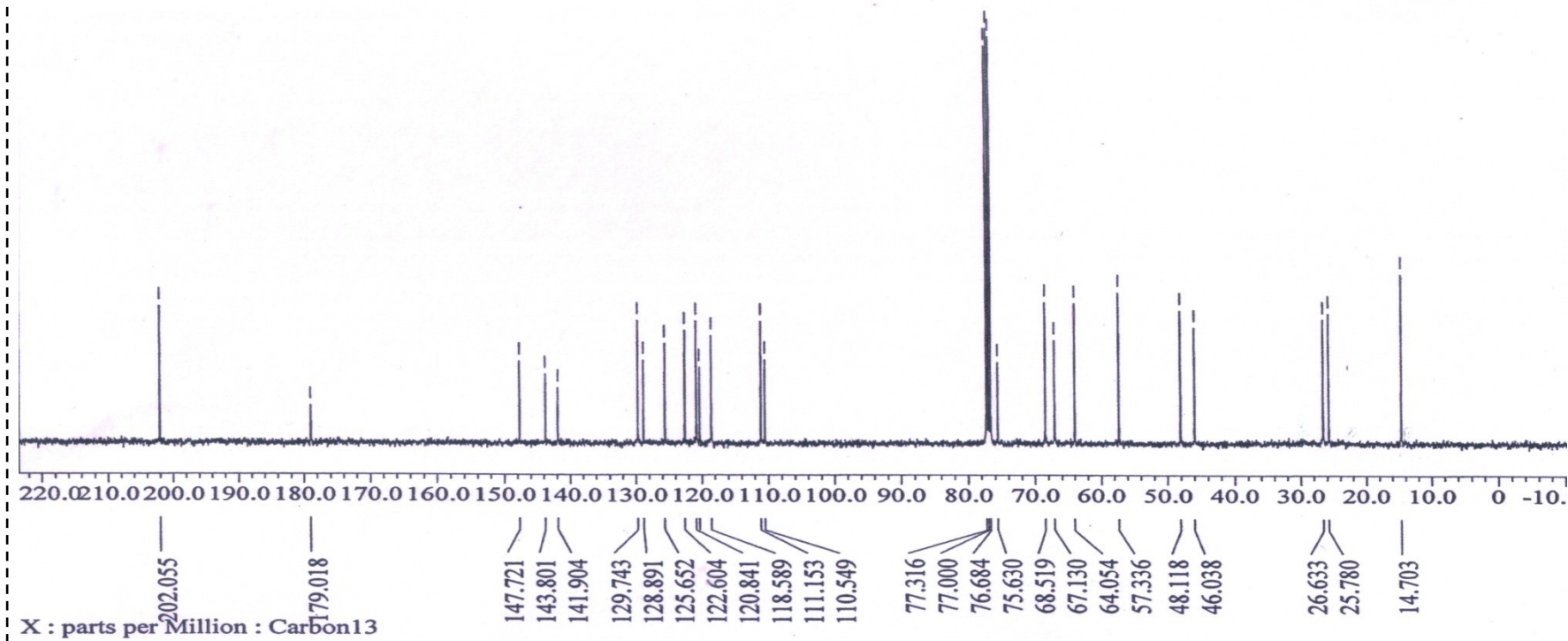
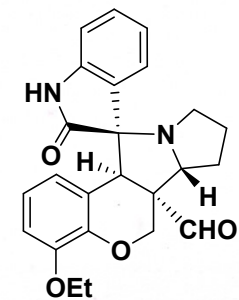


Fig S11. ^{13}C NMR spectrum of compound 16d in CDCl_3

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25-Dec-2021 23:38:41

JP-71 7 (0.147)

1: TOF MS ES+
1.58e4

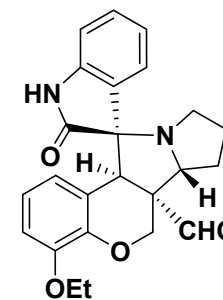
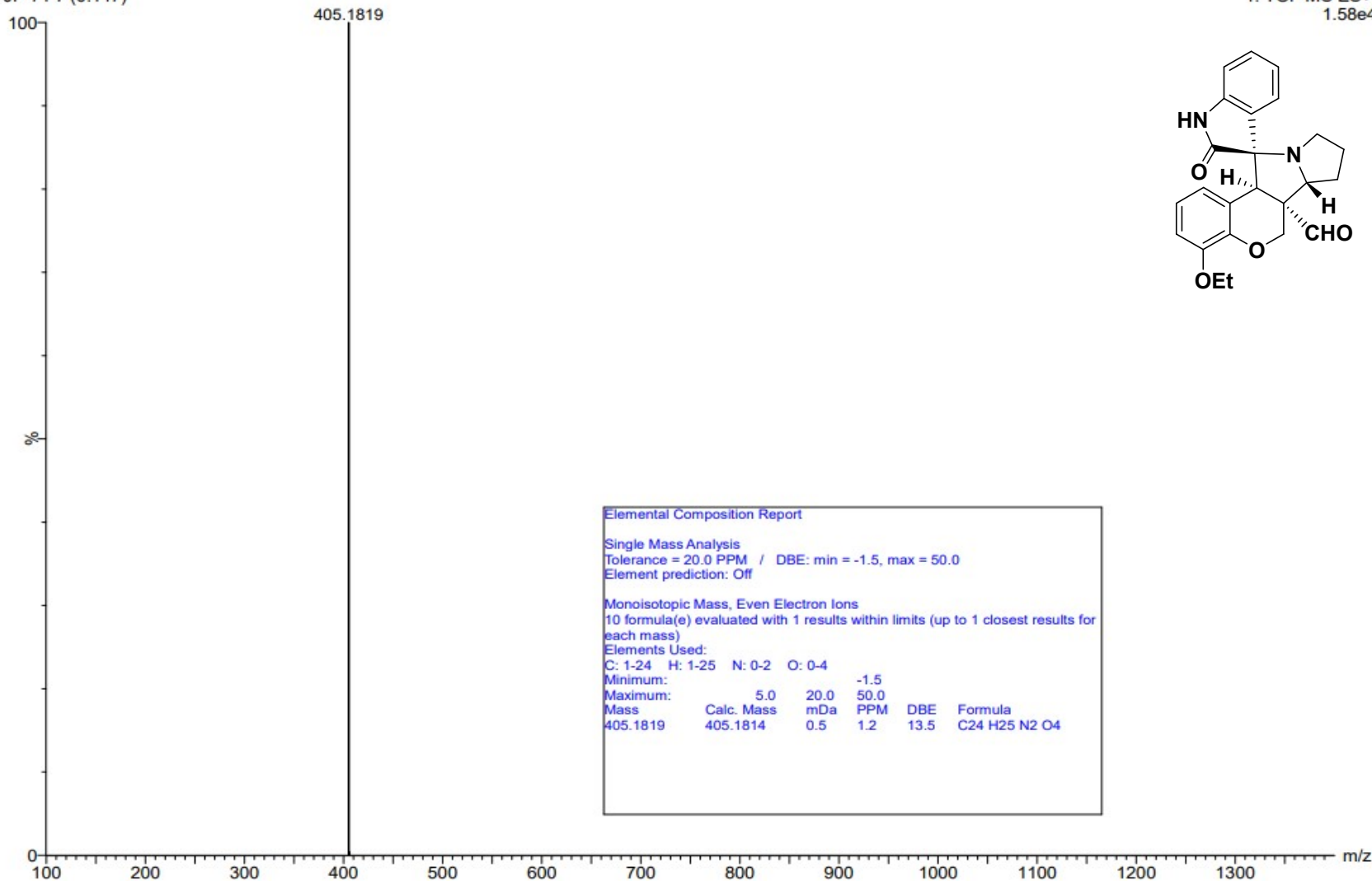


Fig S12. HRMS of compound 16d

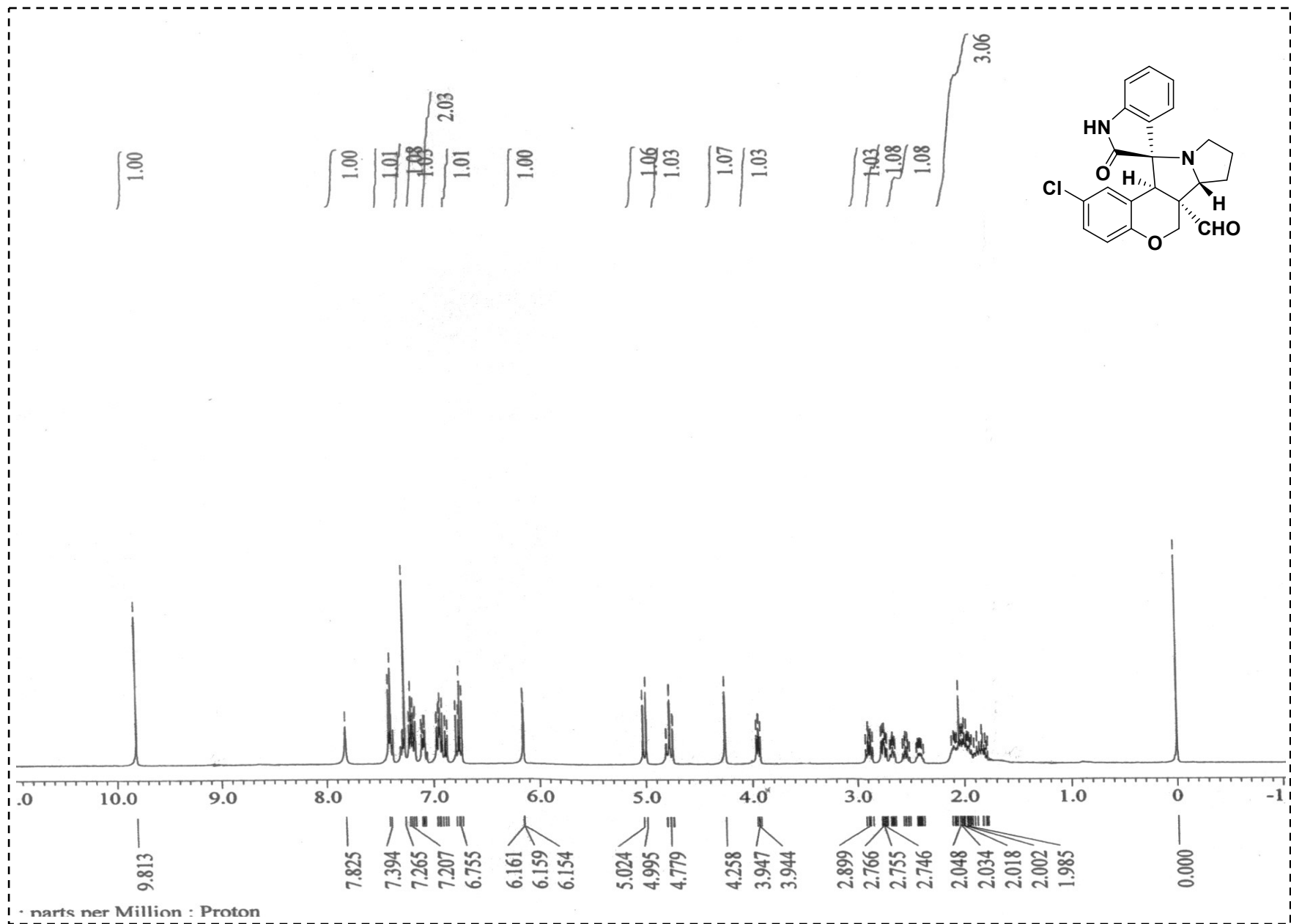


Fig S13. ¹H NMR spectrum of compound **16e** in CDCl₃

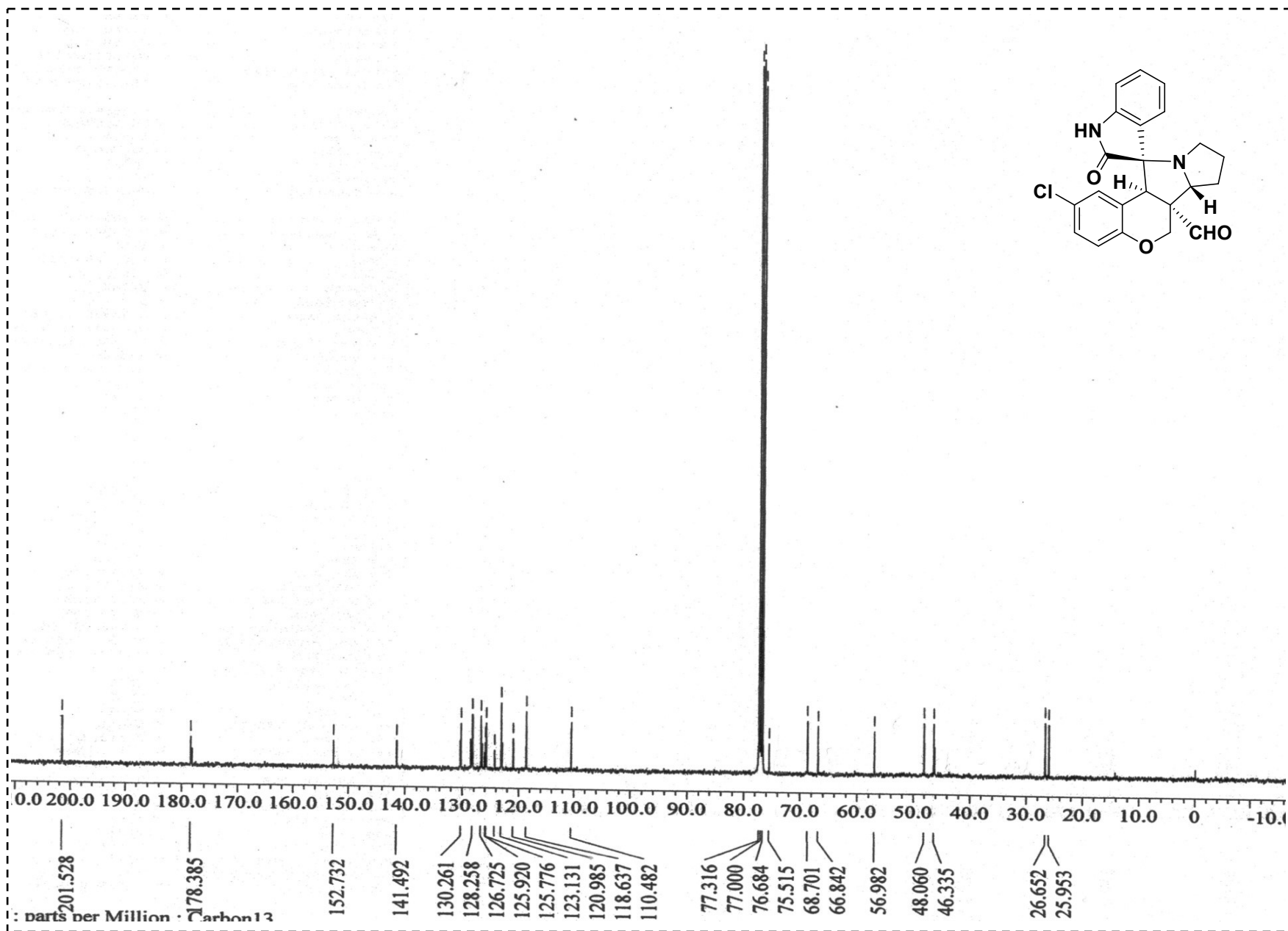
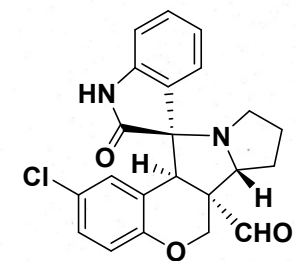


Fig S14. ¹³C NMR spectrum of compound 16e in CDCl₃

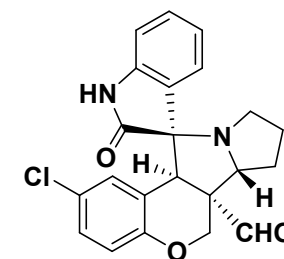
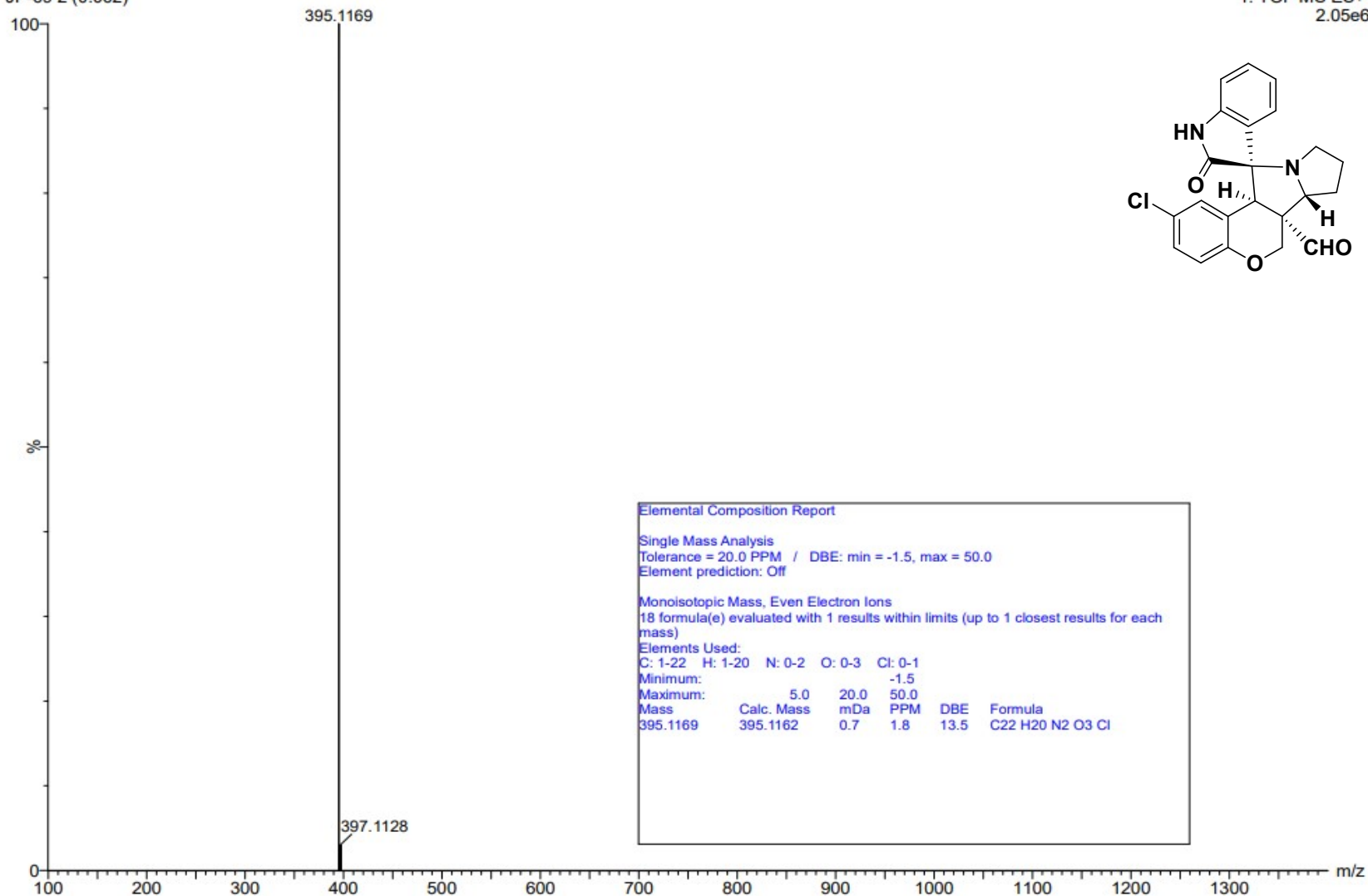
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CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

25-Dec-2021 23:05:08

JP-69 2 (0.062)

1: TOF MS ES+
2.05e6



Elemental Composition Report

Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

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

Elements Used:

C: 1-22 H: 1-20 N: 0-2 O: 0-3 Cl: 0-1

Minimum: 5.0 20.0 50.0 -1.5

Maximum: 5.0 20.0 50.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	Formula
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Fig S15. HRMS of compound 16e

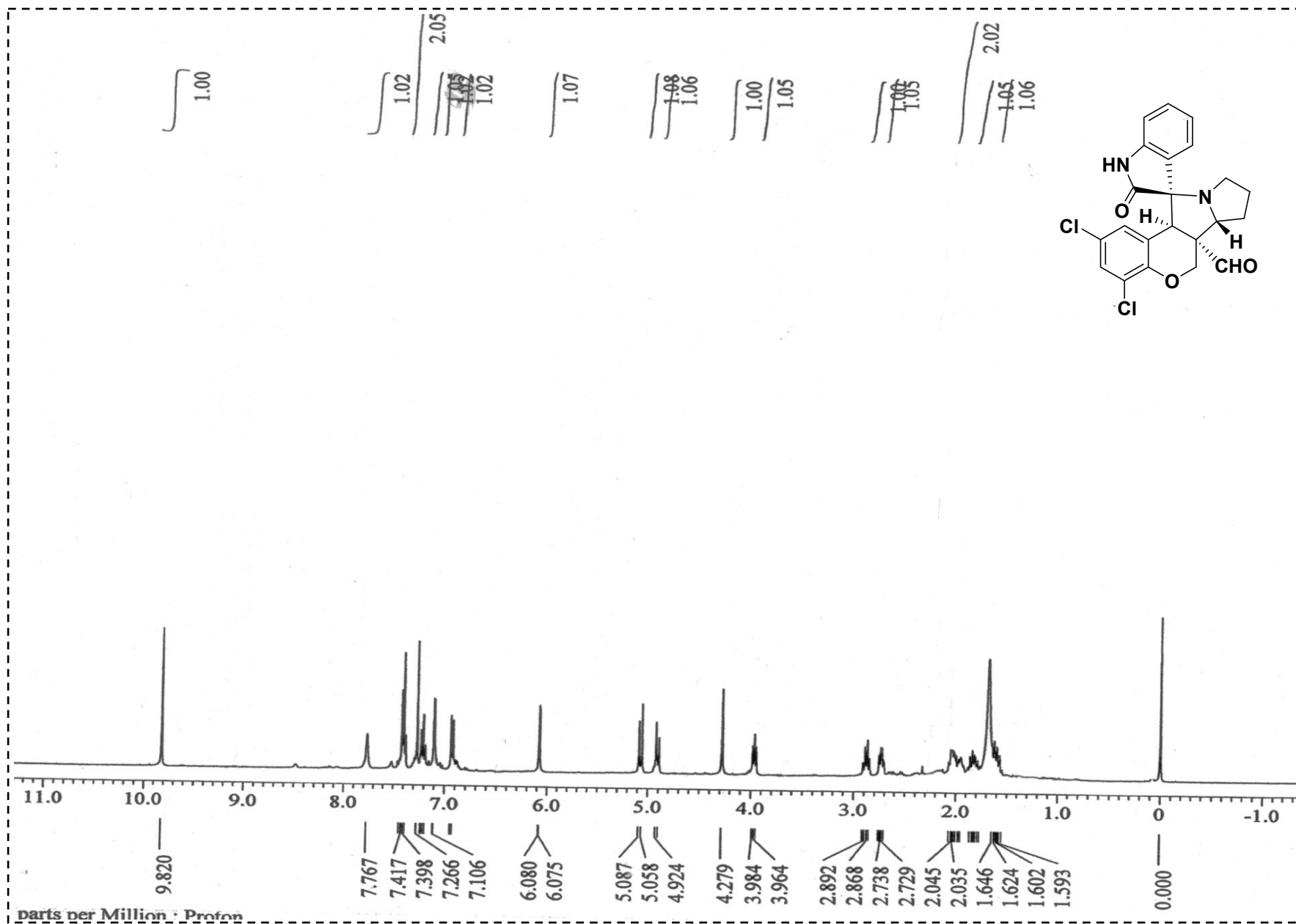


Fig S16. ¹H NMR spectrum of compound 16f in CDCl₃

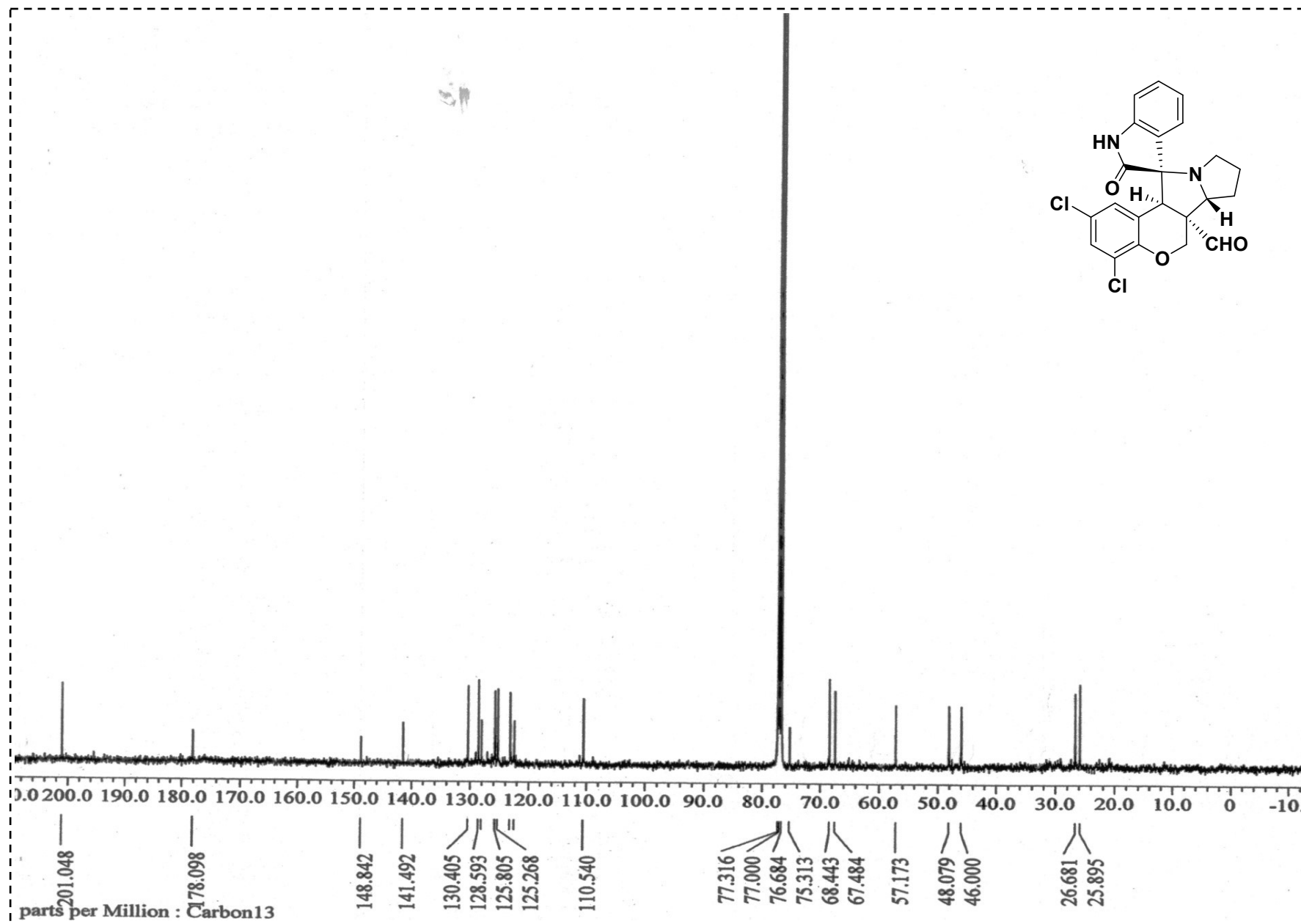


Fig S17. ¹³C NMR spectrum of compound **16f** in CDCl₃

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CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

15-Feb-2022 10:40:31

JP-50 16 (0.310)

1: TOF MS ES+
2.16e4

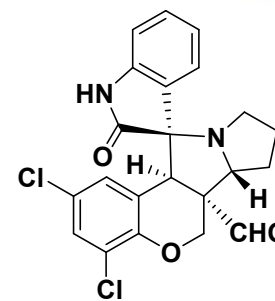
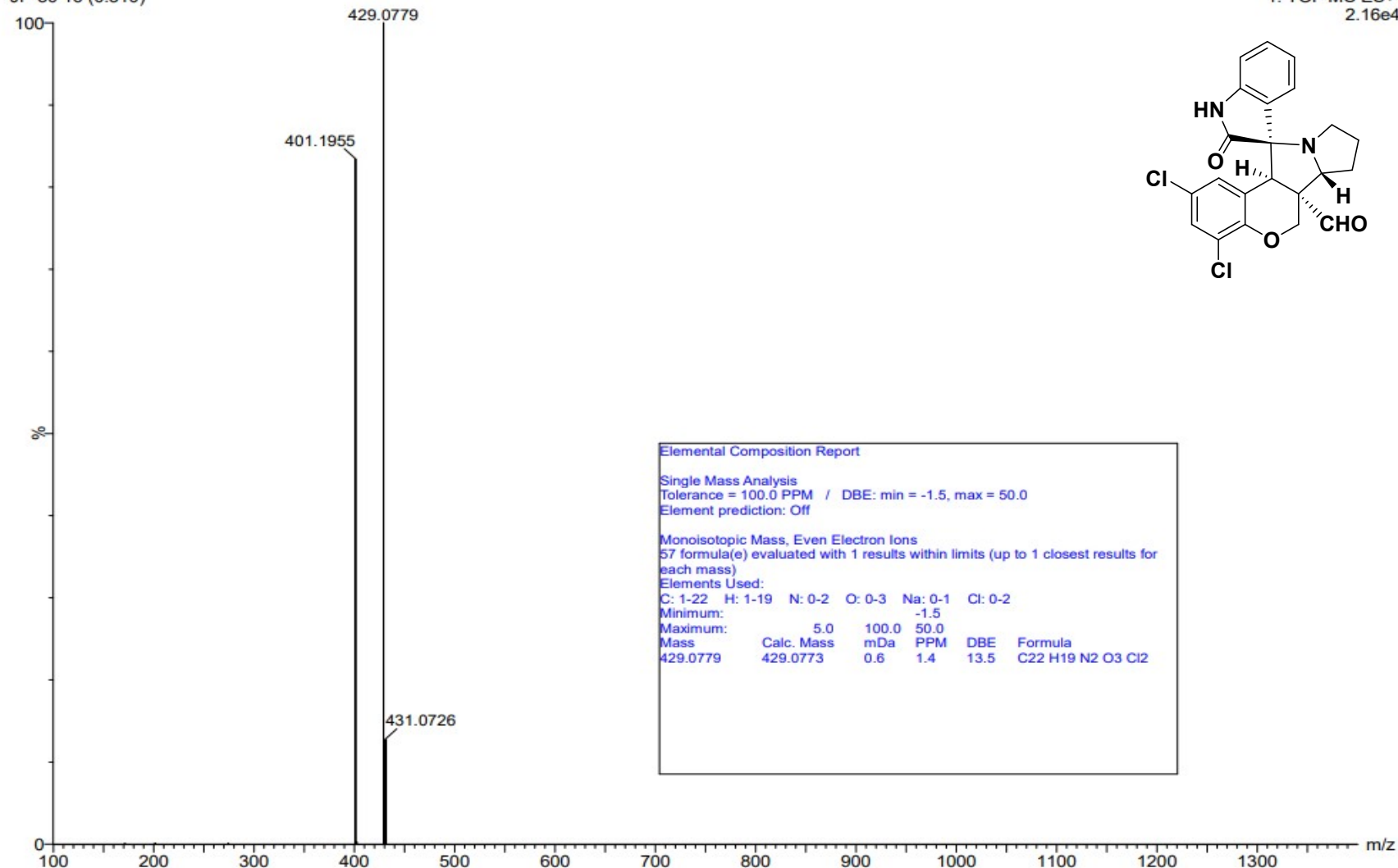


Fig S18. HRMS of compound 16f

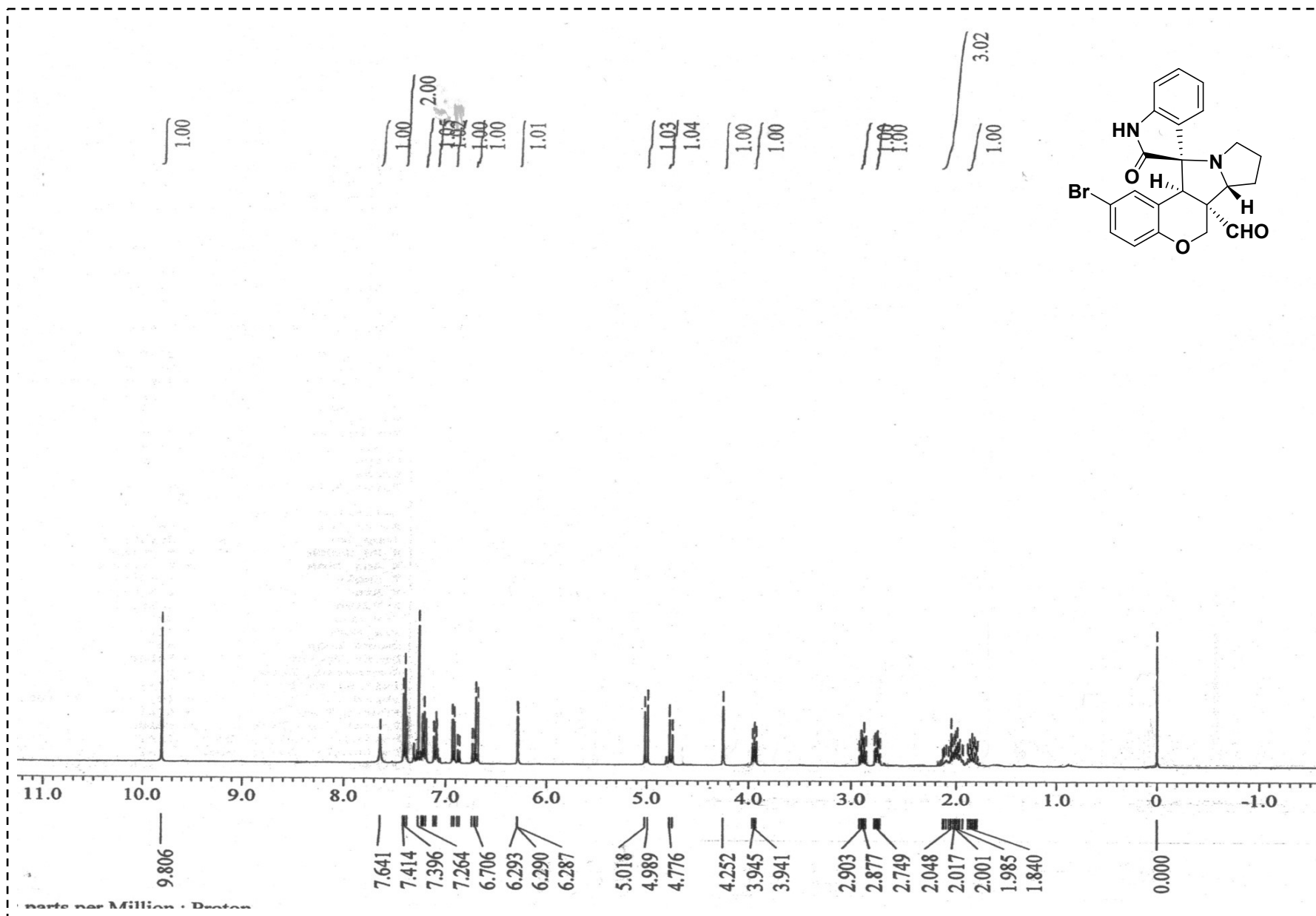


Fig S19. ¹H NMR spectrum of compound 16g in CDCl₃

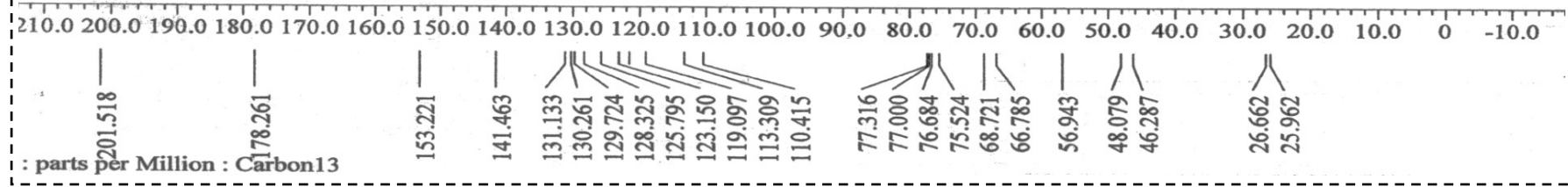
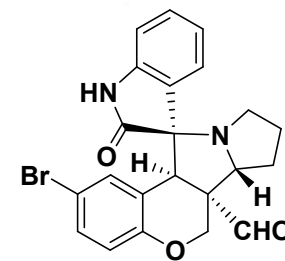


Fig S20. ¹³C NMR spectrum of compound 16g in CDCl₃

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CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

15-Feb-2022 10:51:01

JP-75 5 (0.113)

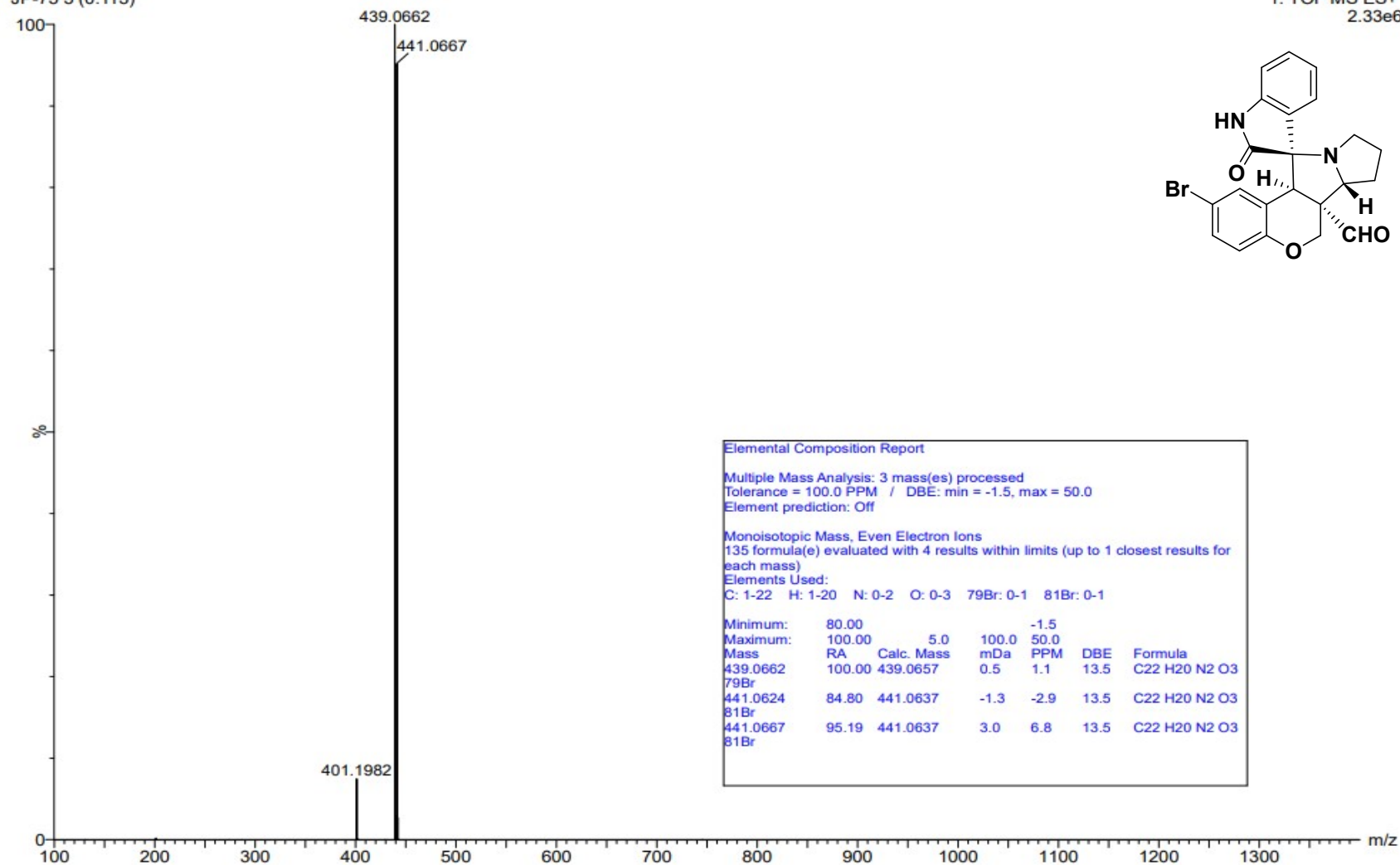
1: TOF MS ES+
2.33e6

Fig S21. HRMS of compound 16g

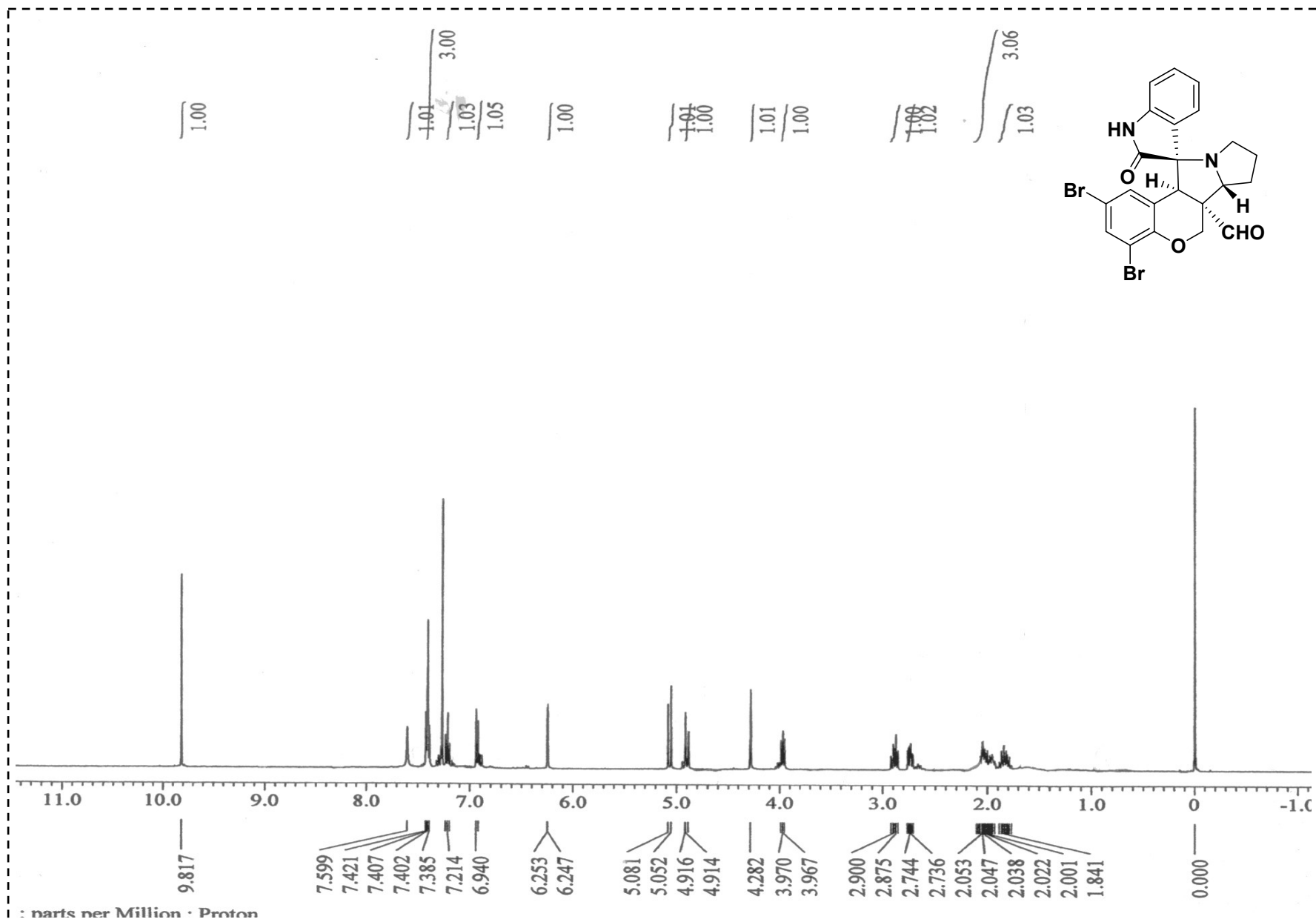


Fig S22. $^1\text{H NMR}$ spectrum of compound **16h** in CDCl_3

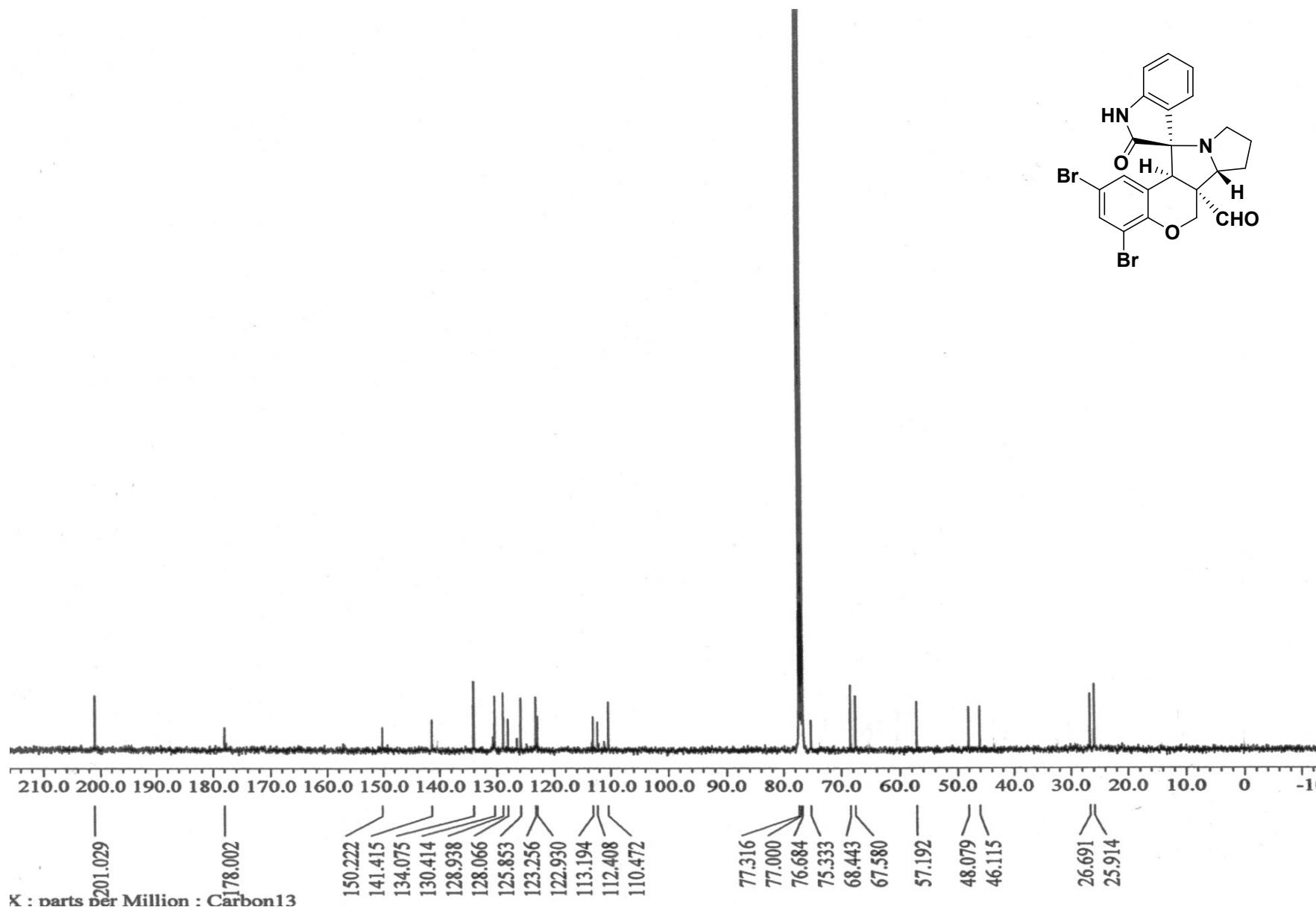
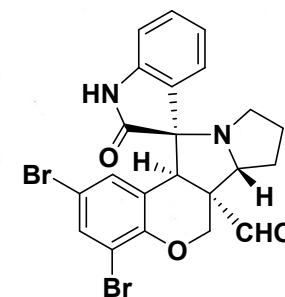


Fig S23. ^{13}C NMR spectrum of compound 16h in CDCl_3

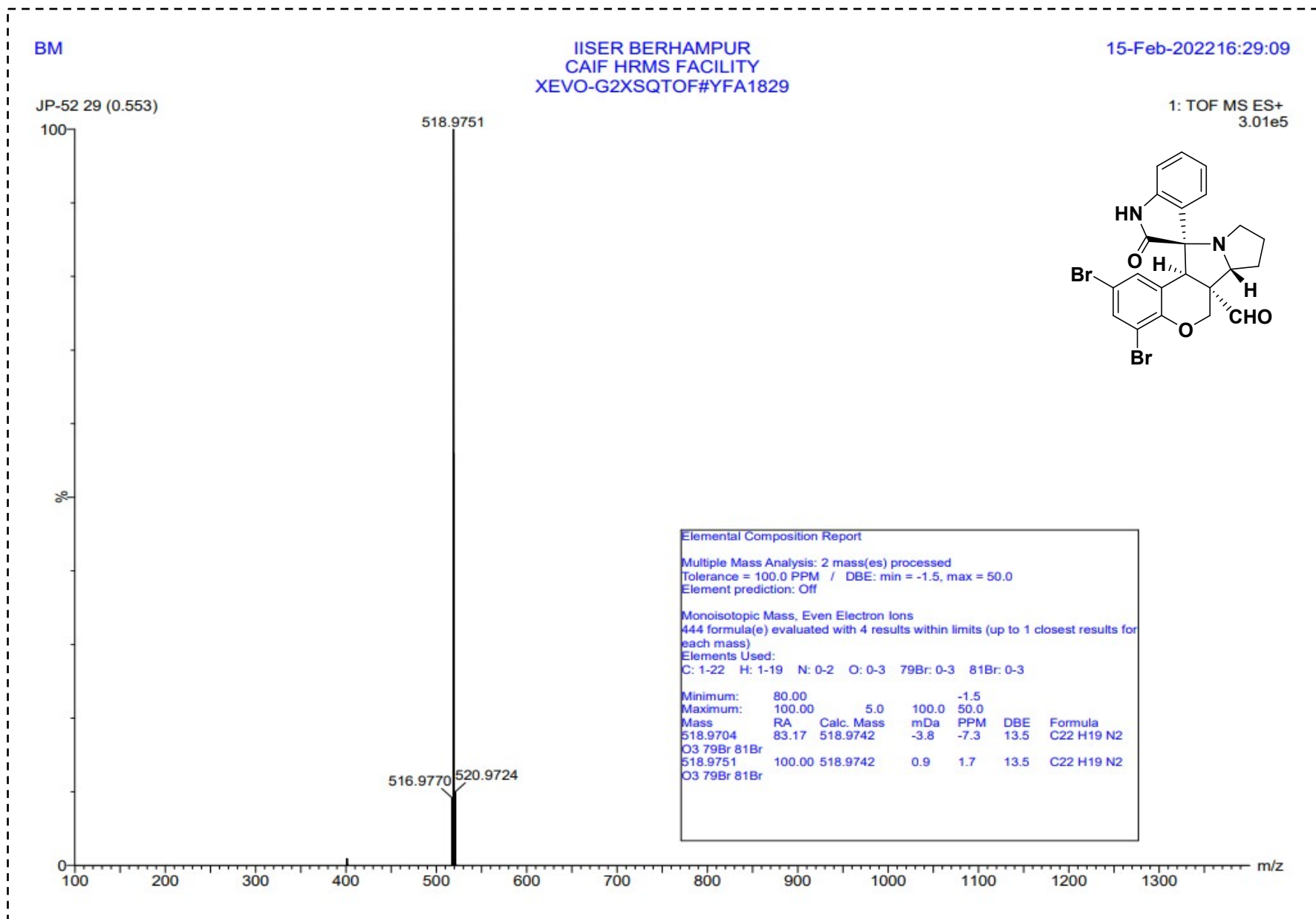


Fig S24. HRMS of compound 16h

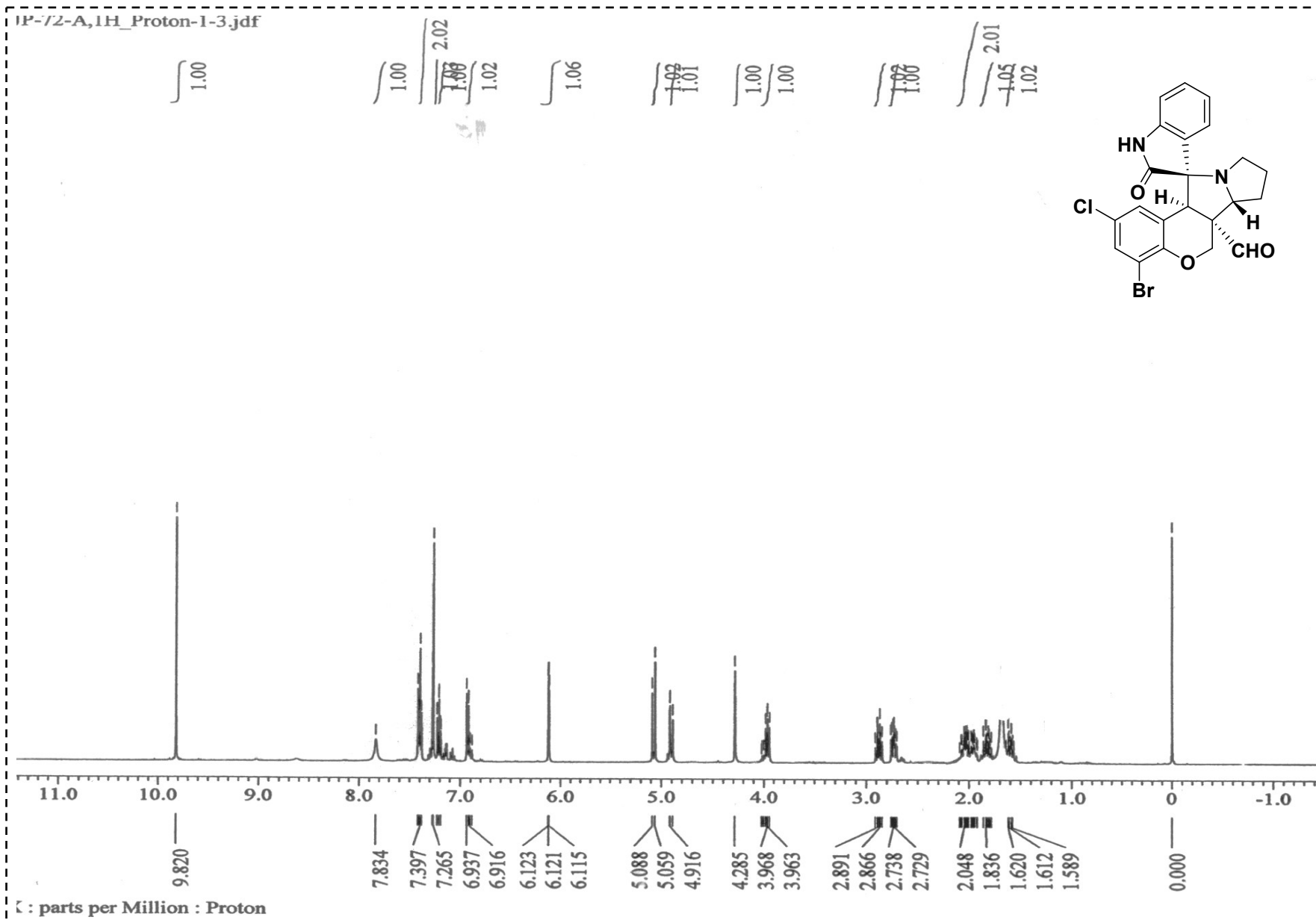


Fig S25. ¹H NMR spectrum of compound 16i in CDCl₃

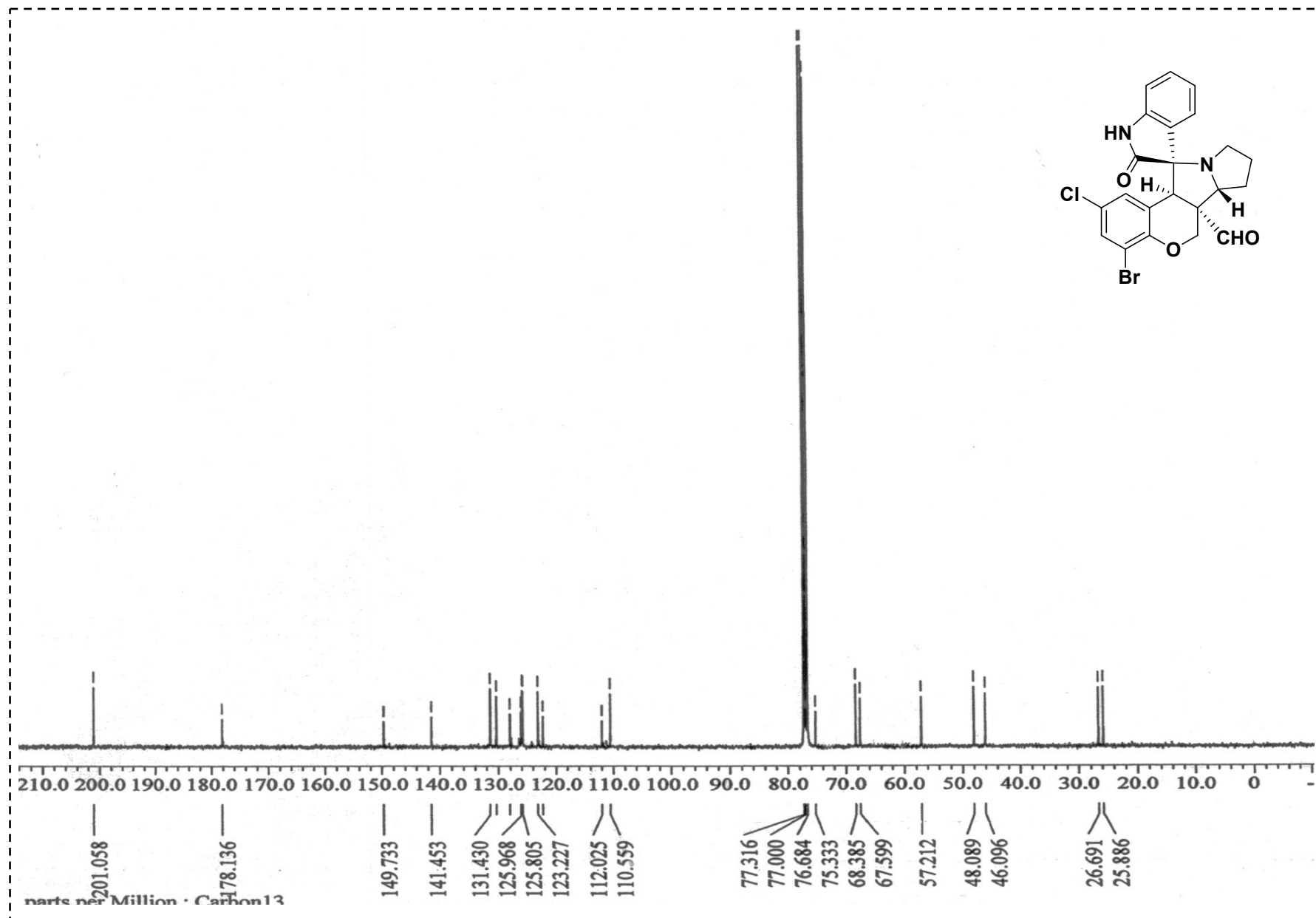


Fig S26. ^{13}C NMR spectrum of compound 16i in CDCl_3

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CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

25-Dec-2021 23:49:10

JP-72 3 (0.079)

1: TOF MS ES+
6.24e6

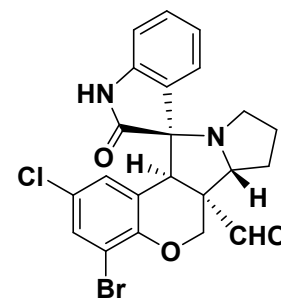
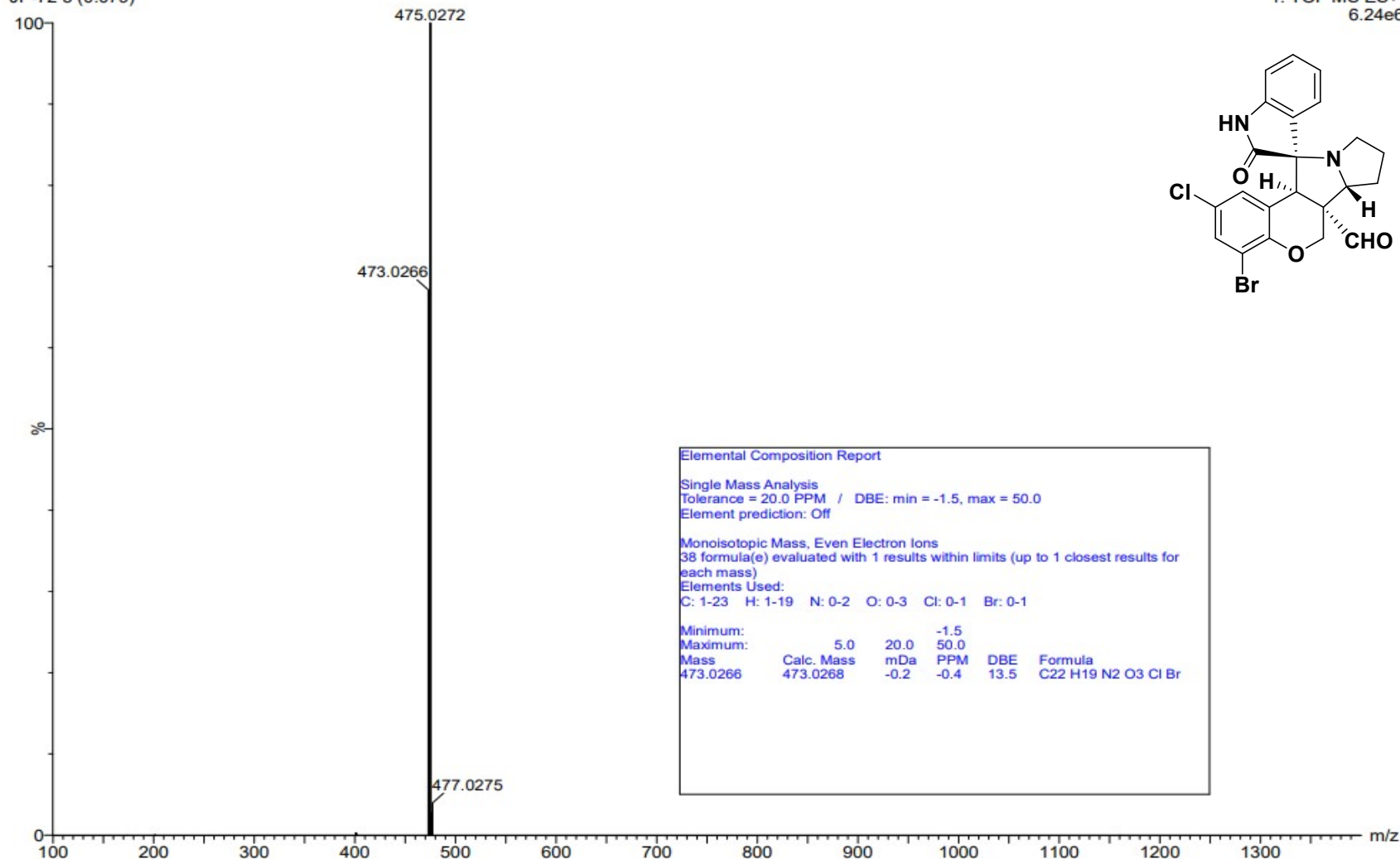


Fig S27. HRMS of compound 16i

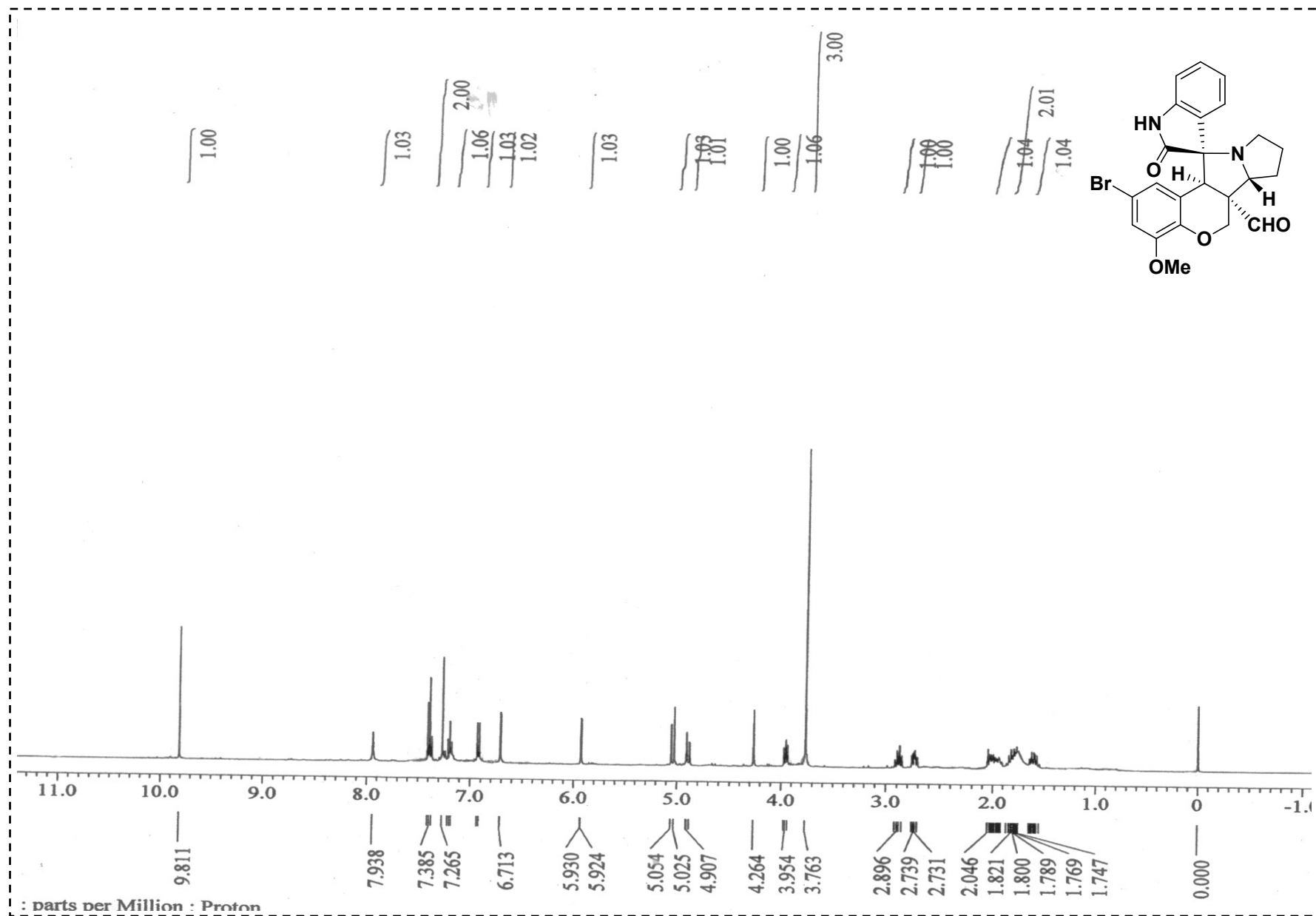


Fig S28. ¹H NMR spectrum of compound 16j in CDCl₃

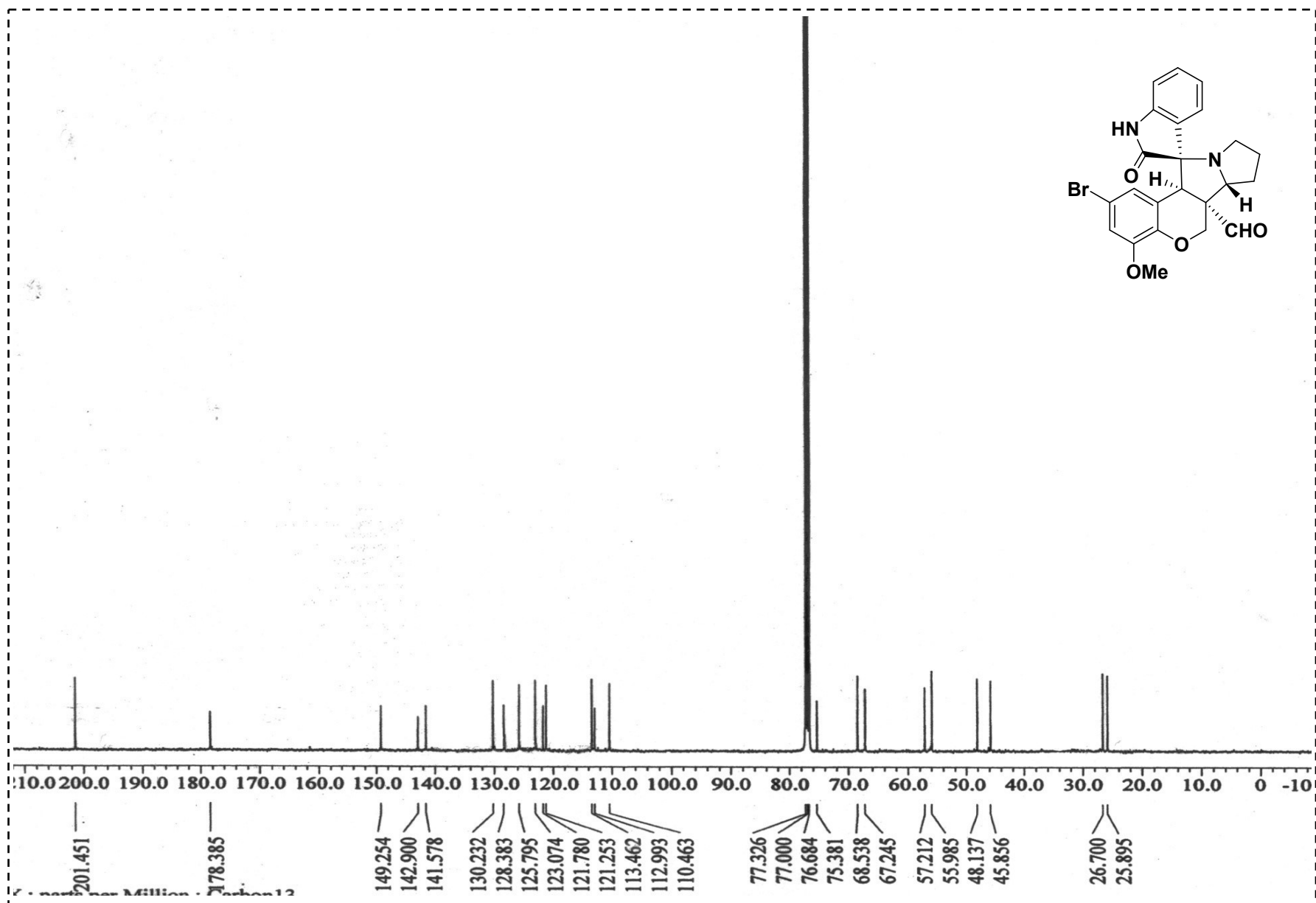
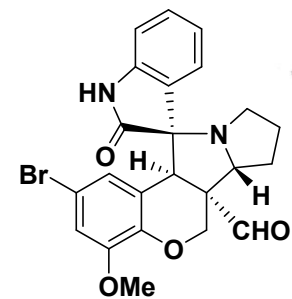


Fig S29. ¹³C NMR spectrum of compound 16j in CDCl₃

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CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

25-Dec-2021 22:43:14

JP-48 29 (0.553)

100

469.0769

%

0

100

200

300

400

500

600

700

800

900

1000

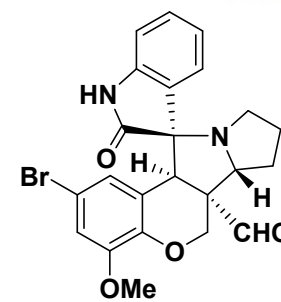
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1200

1300

m/z

1: TOF MS ES+
4.00e5



Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 1-23 H: 1-22 N: 0-2 O: 0-4 Br: 0-1

Minimum:

Maximum: 5.0 20.0 -1.5

Mass Calc. Mass mDa PPM DBE Formula

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Fig 30. HRMS of compound 16j

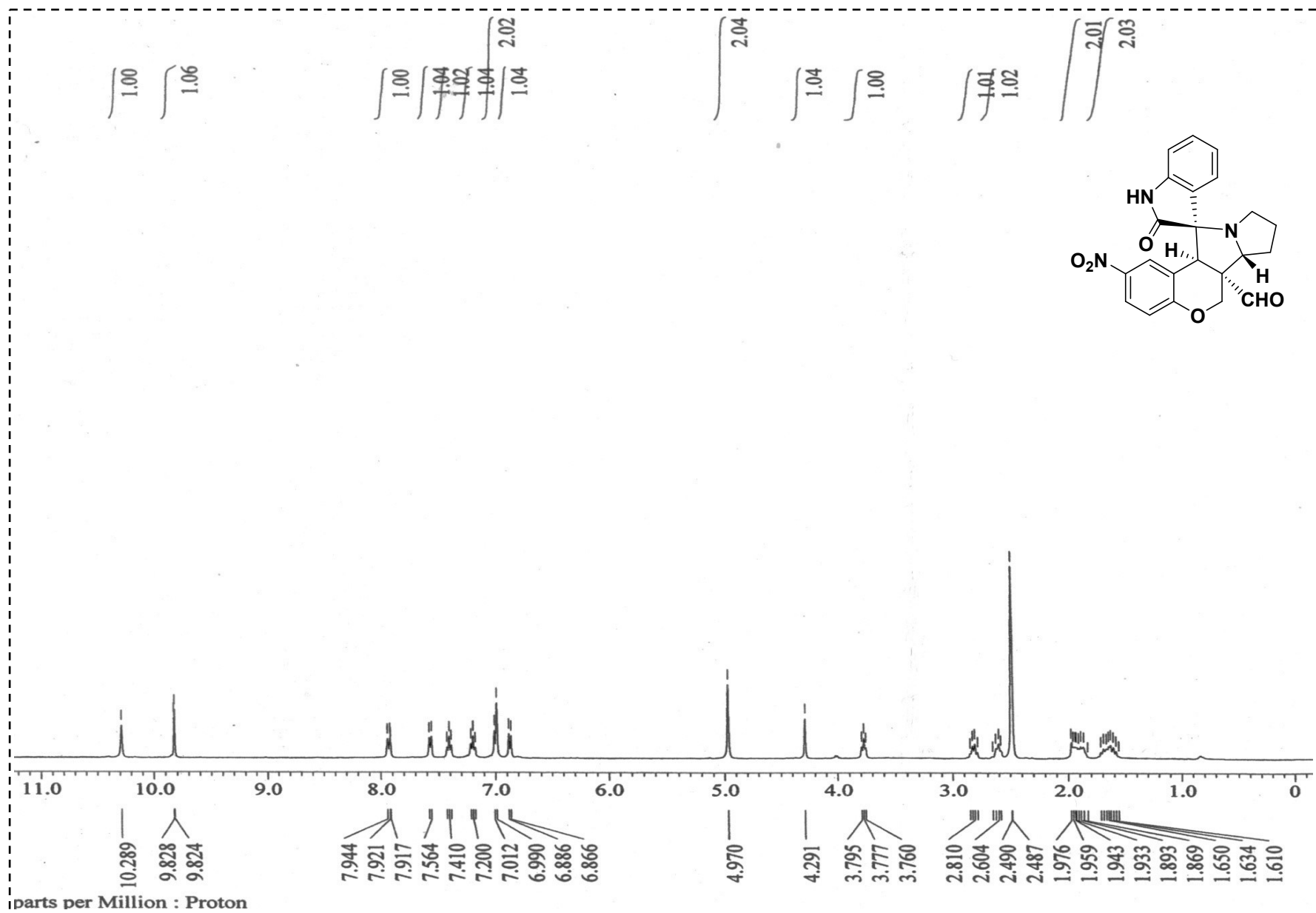


Fig S31. ¹H NMR spectrum of compound 16k in DMSO-d₆

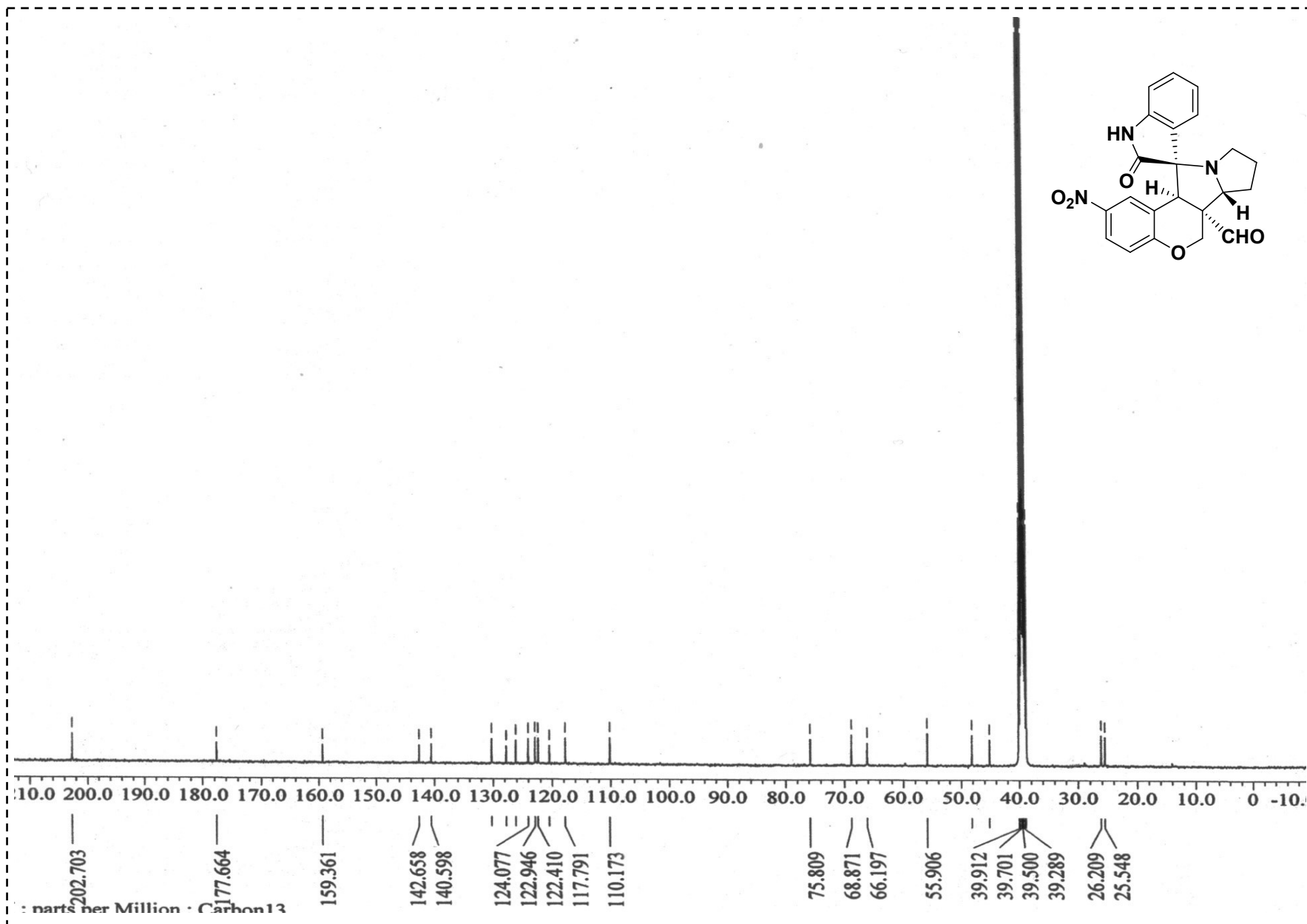


Fig S32. ¹³C NMR spectrum of compound 16k in DMSO-d₆

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IISER BERHAMPUR
CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

16-May-2022 13:03:42

JP-226-1 6 (0.130)

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7.22e5

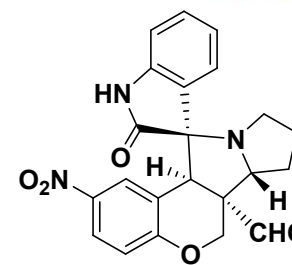
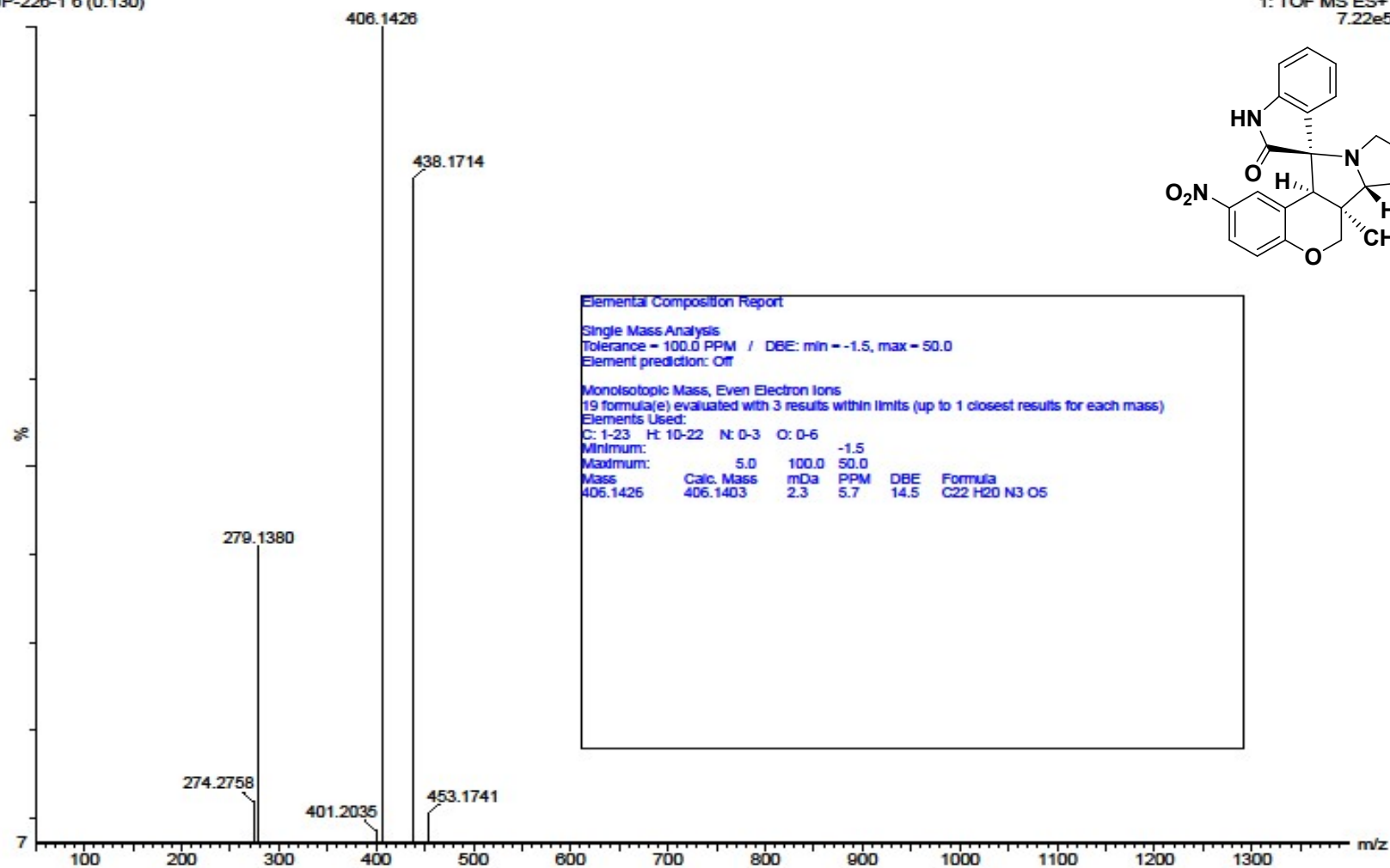


Fig S33. HRMS of compound 16k

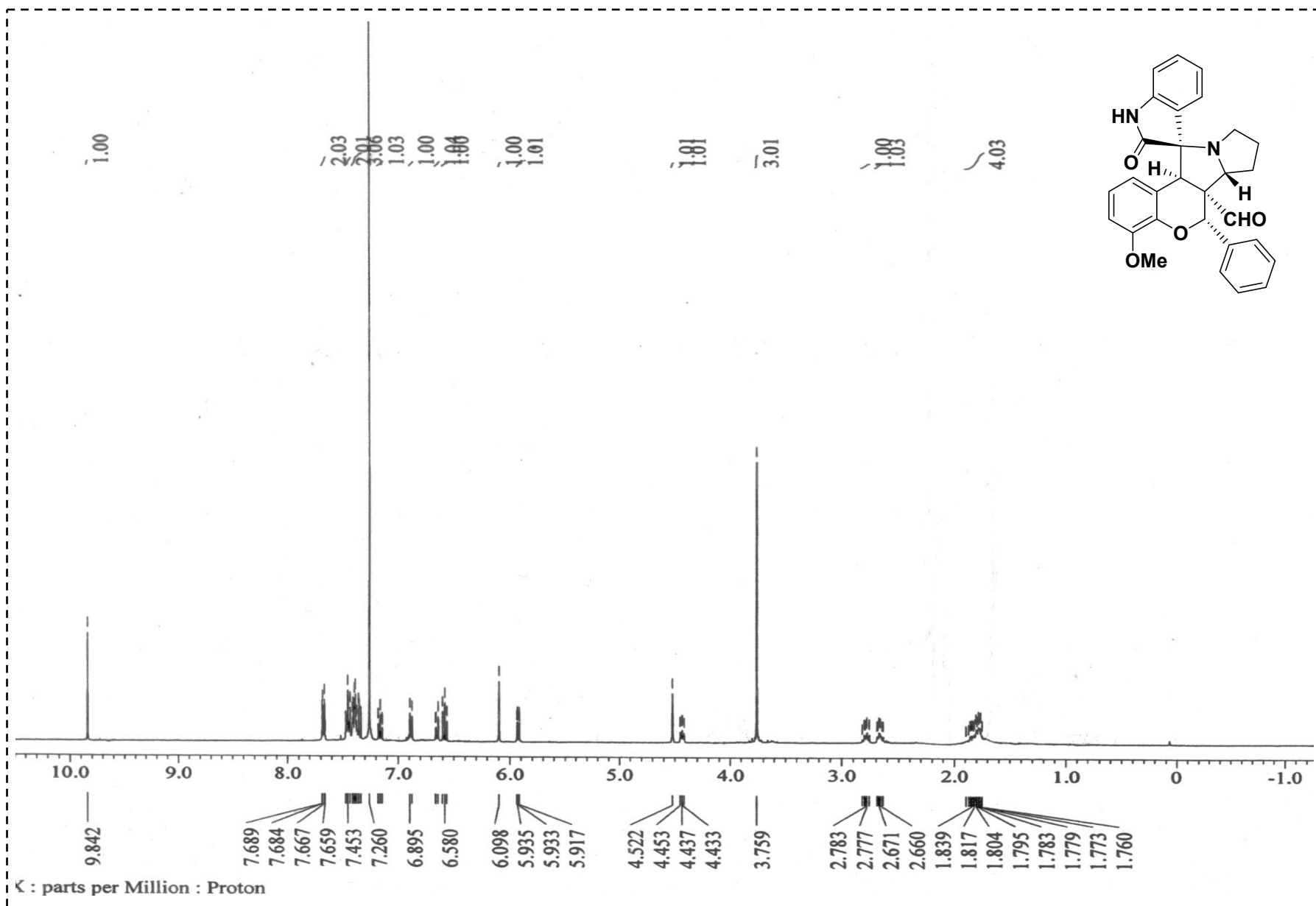


Fig S34. ^1H NMR spectrum of compound **16'a** in CDCl₃

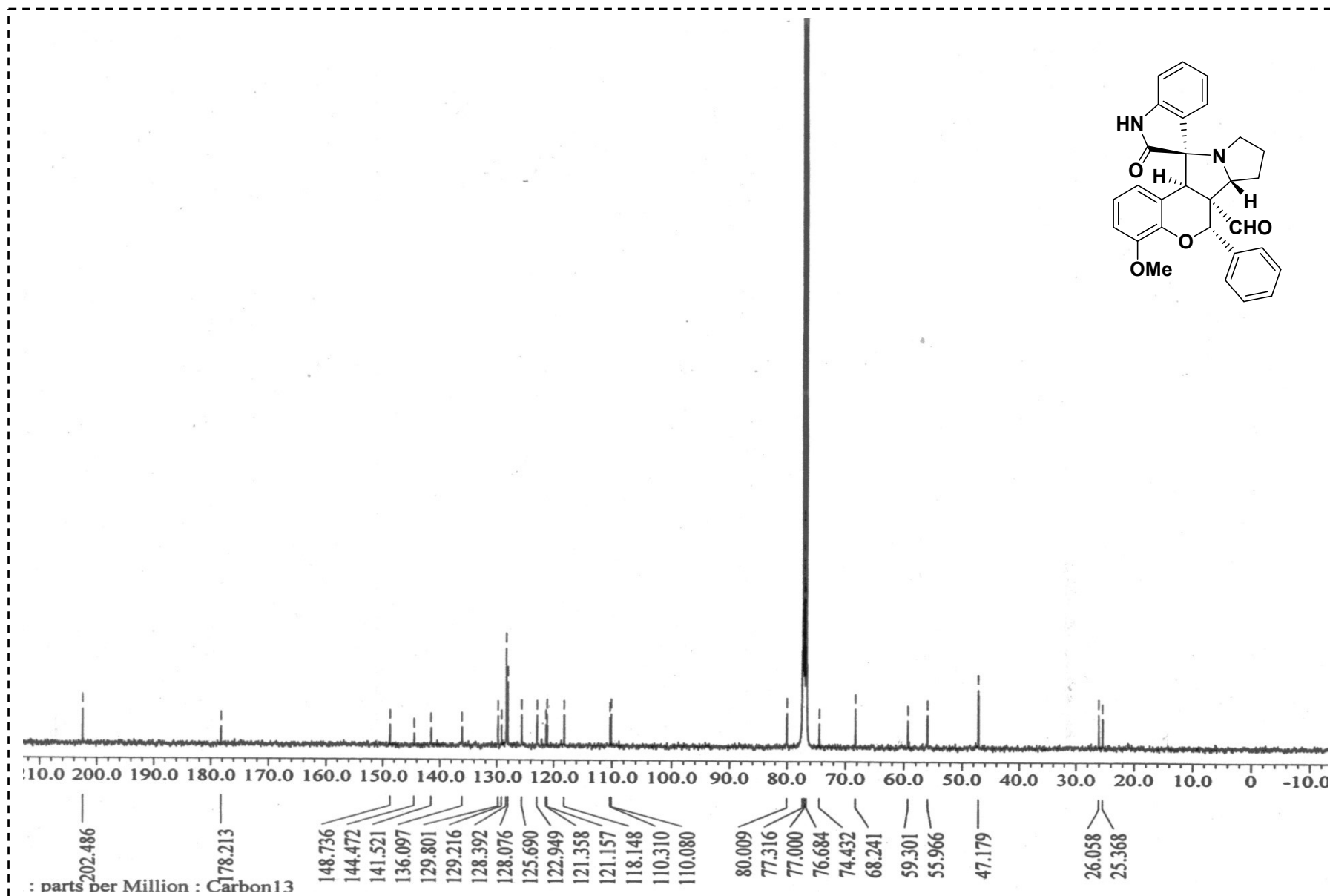


Fig S35. ¹³C NMR spectrum of compound 16'a in CDCl₃

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CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

27-Jun-2022 19:33:19

JP-250 48 (0.897)

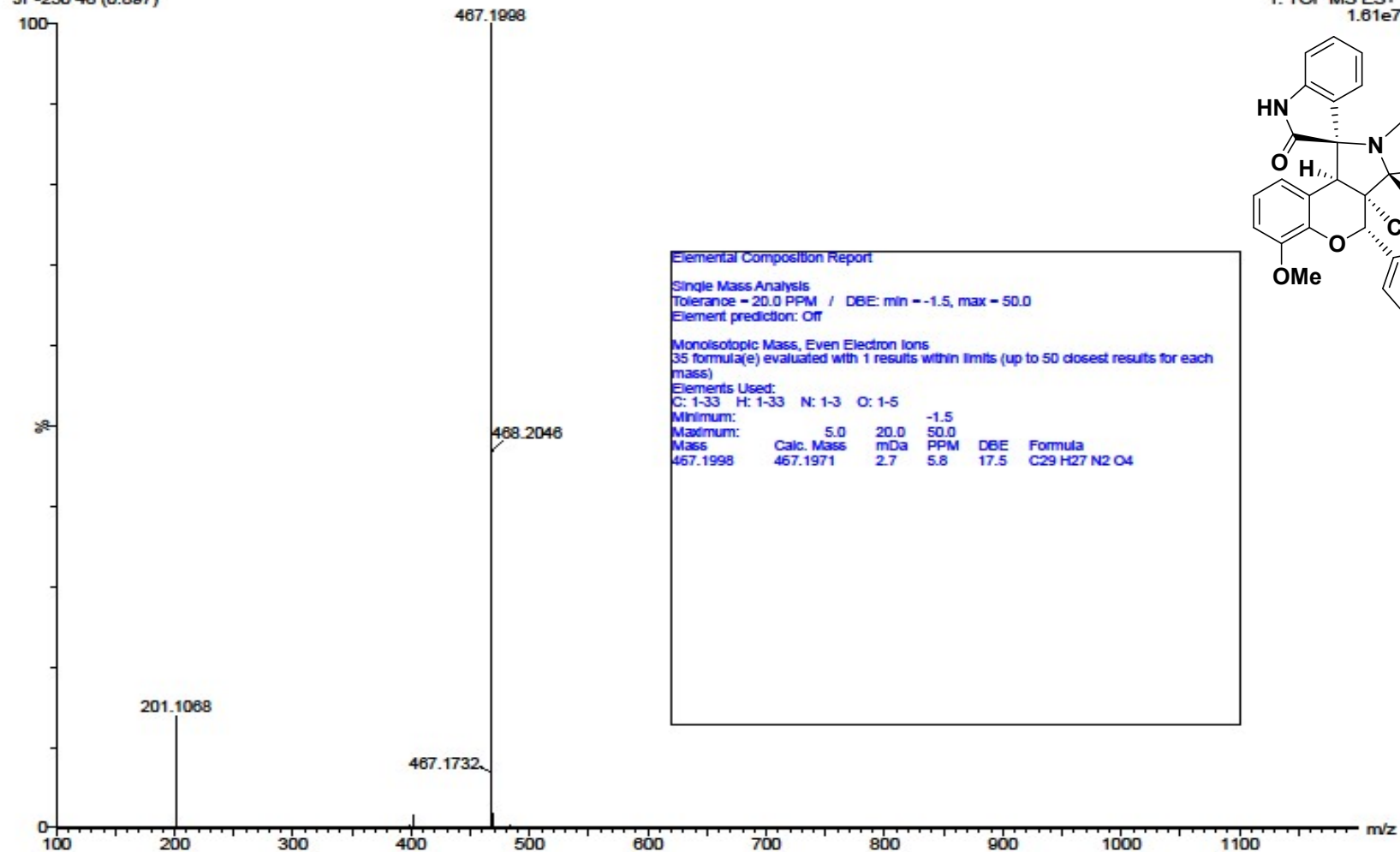


Fig S36. HRMS of compound 16'a

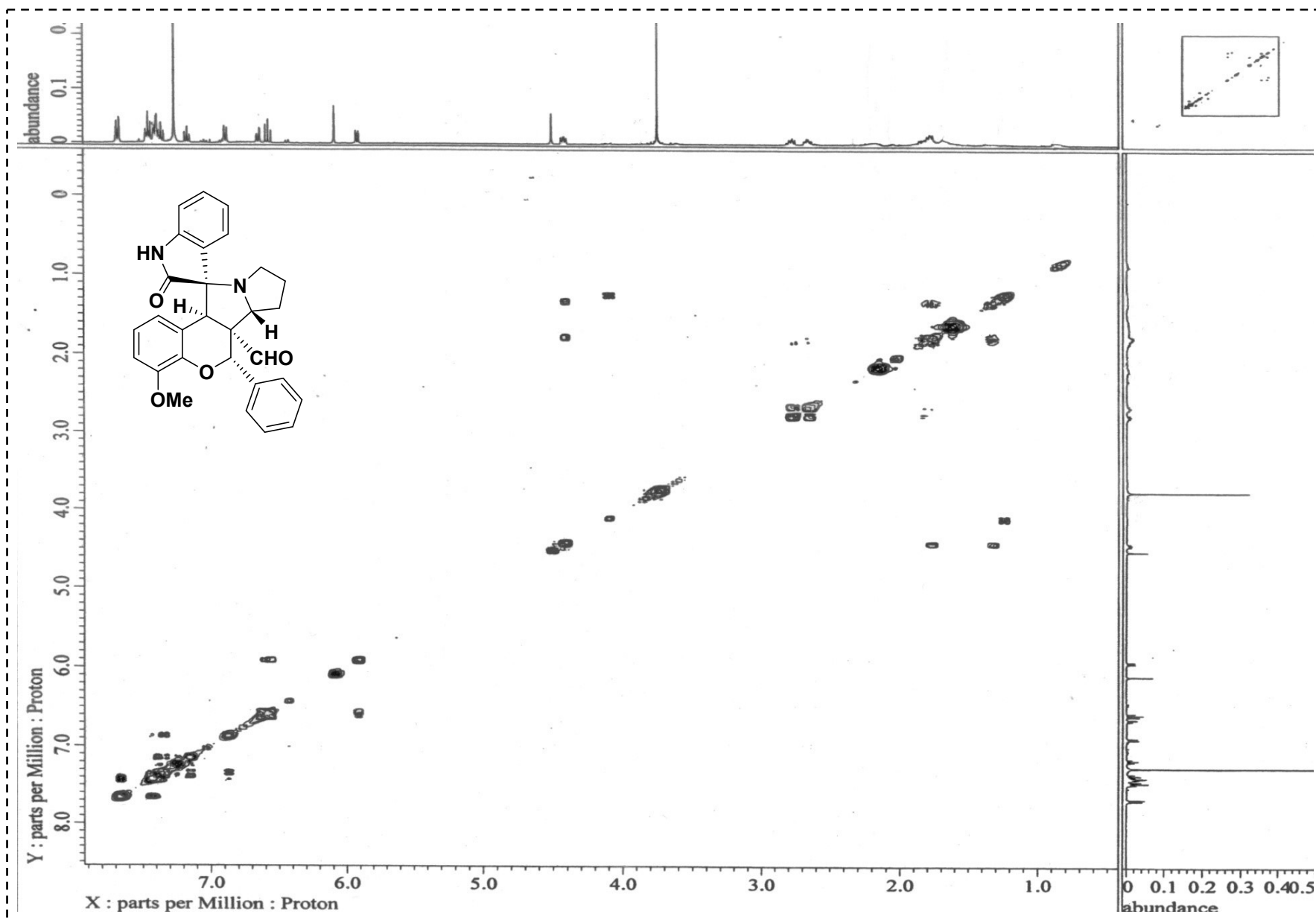


Fig S37. COSY Spectra of compound 16'a

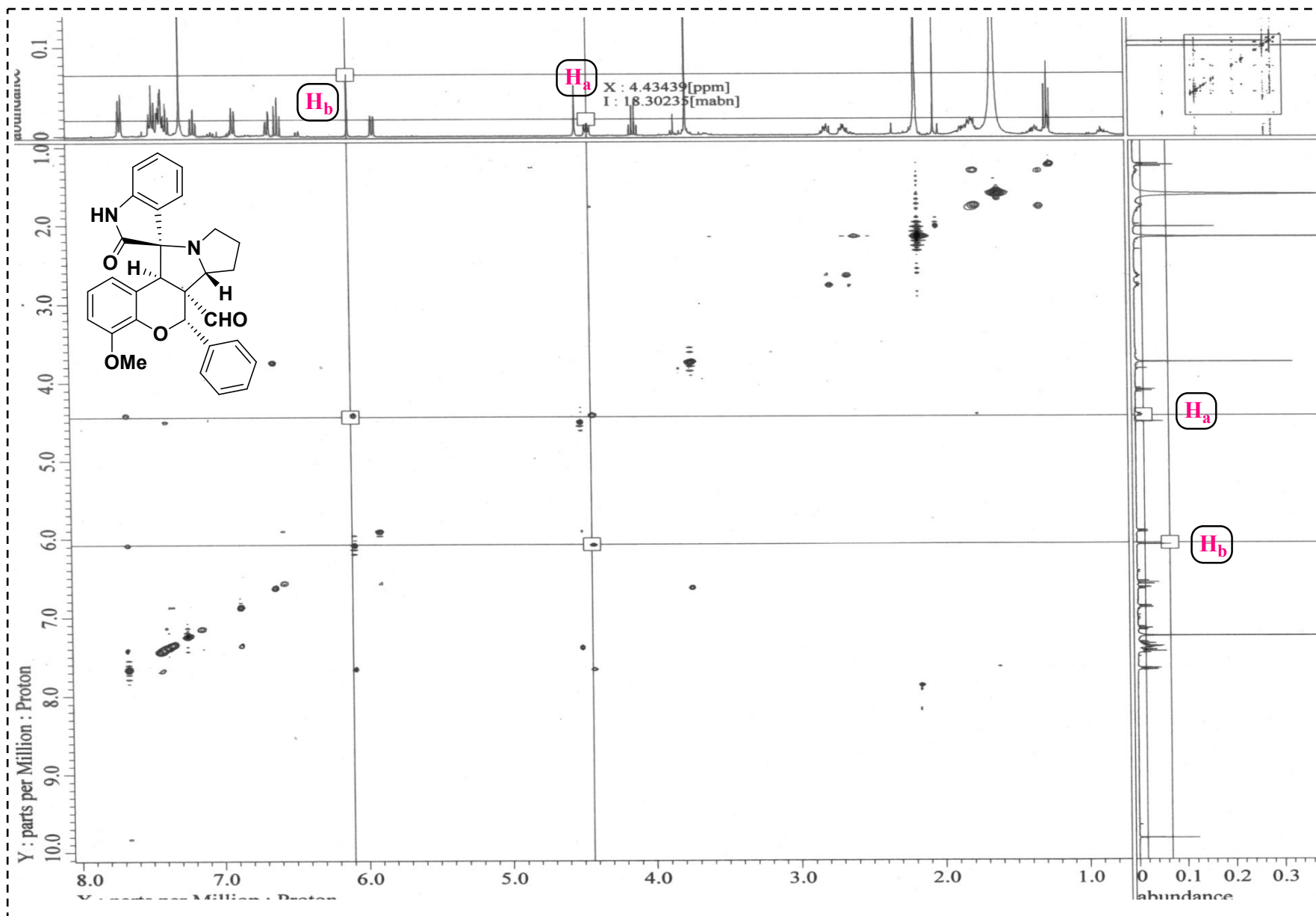


Fig S38. NOESY Spectra of compound 16'a

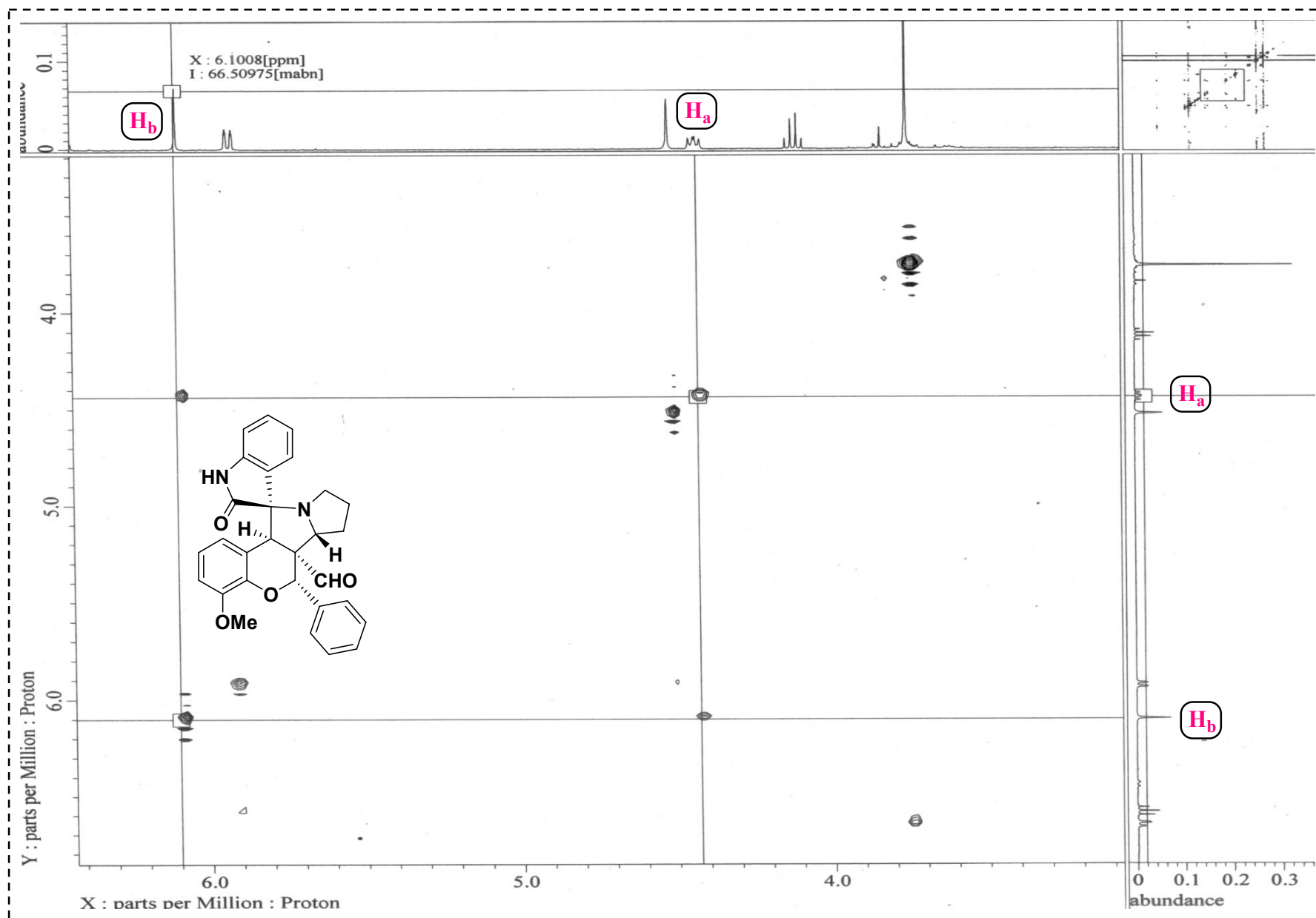


Fig S39. NOESY Expansion Spectra of compound 16'a

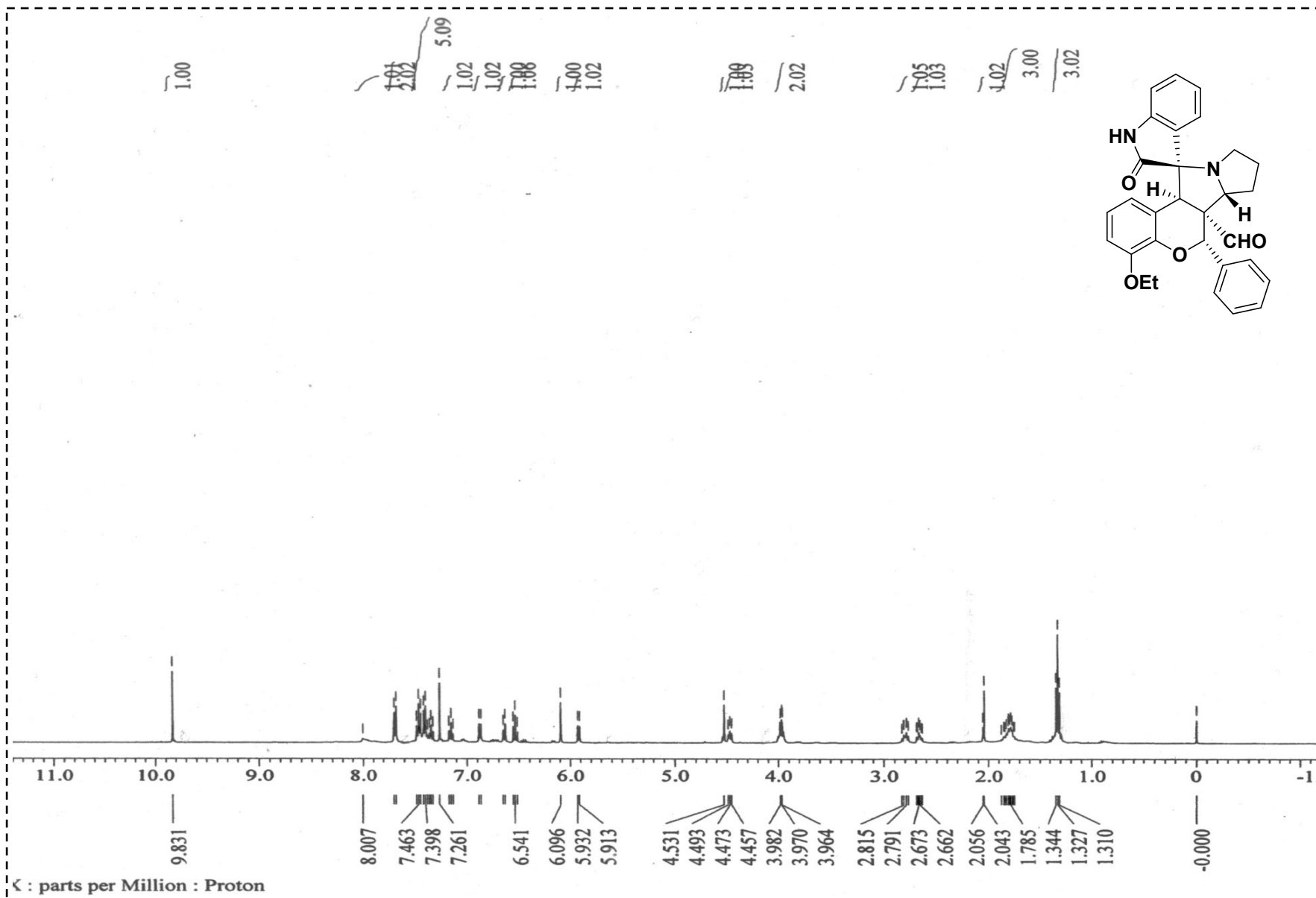


Fig S40. ^1H NMR spectrum of compound **16'b** in CDCl_3

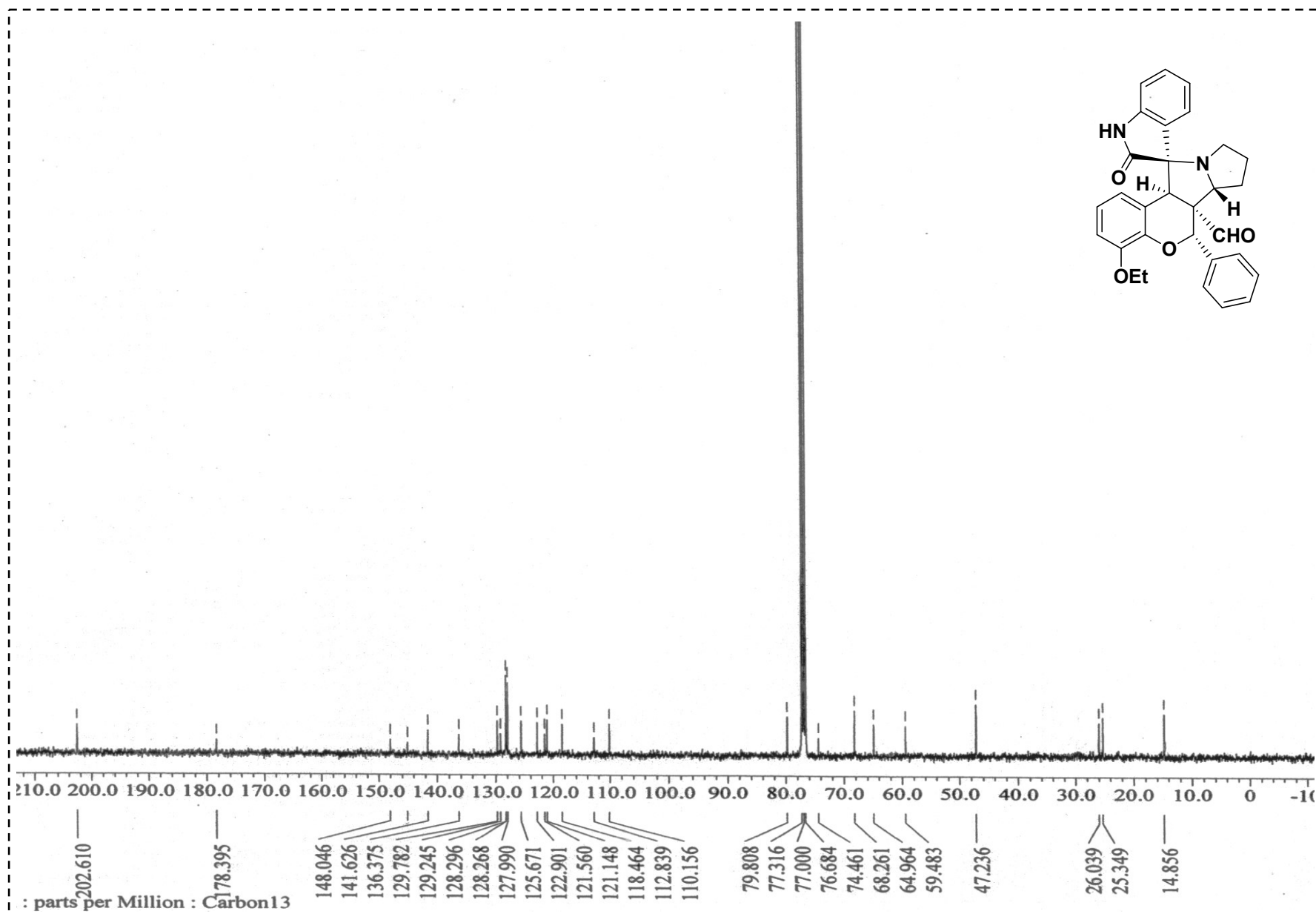


Fig S41. ¹³C NMR spectrum of compound 16'b in CDCl₃

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CAIF HRMS FACILITY
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16-May-2022 15:26:19

JP-220 35 (0.666) Cm (19:37)

1: TOF MS ES+
5.60e7

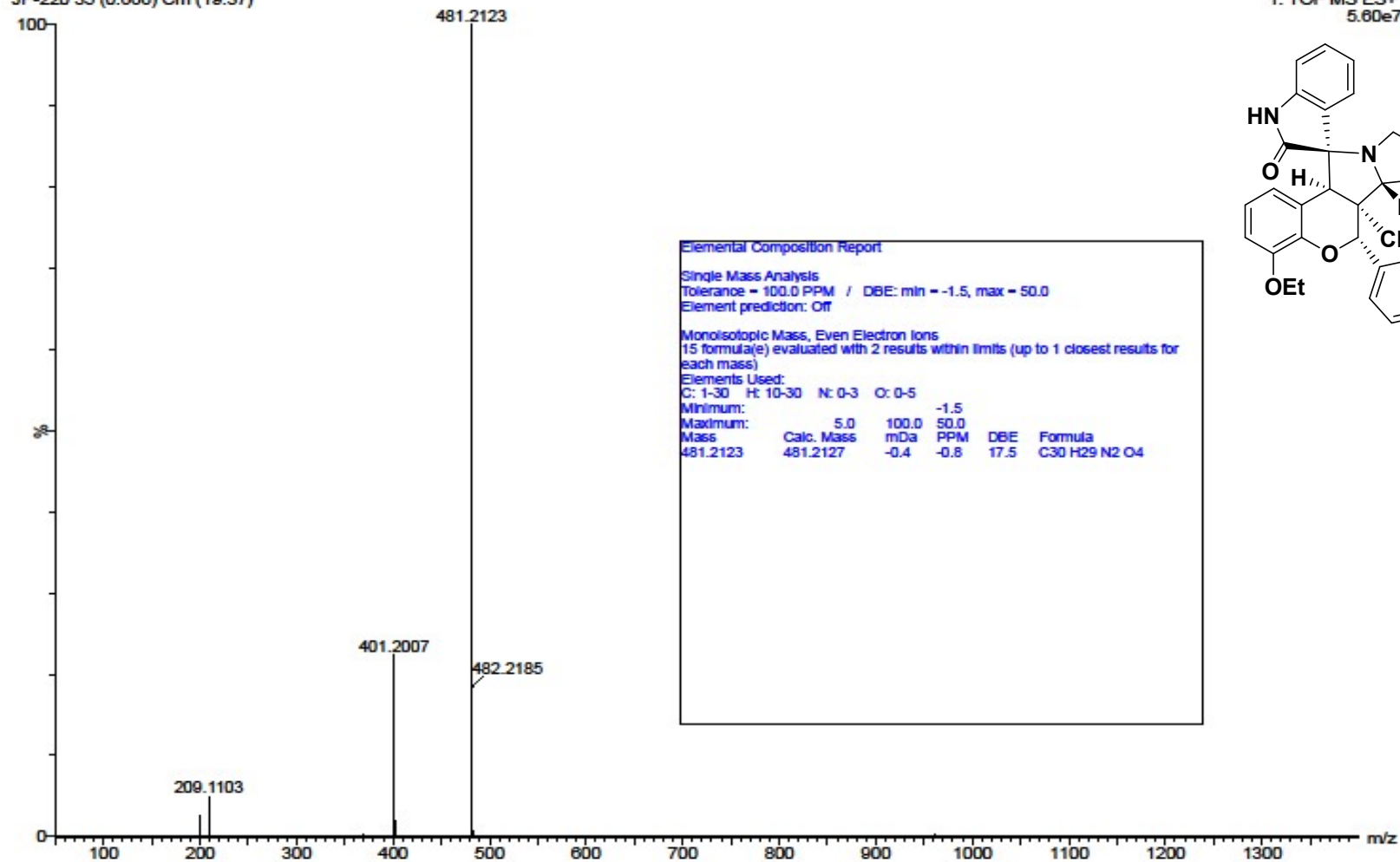


Fig S42. HRMS of compound 16'b

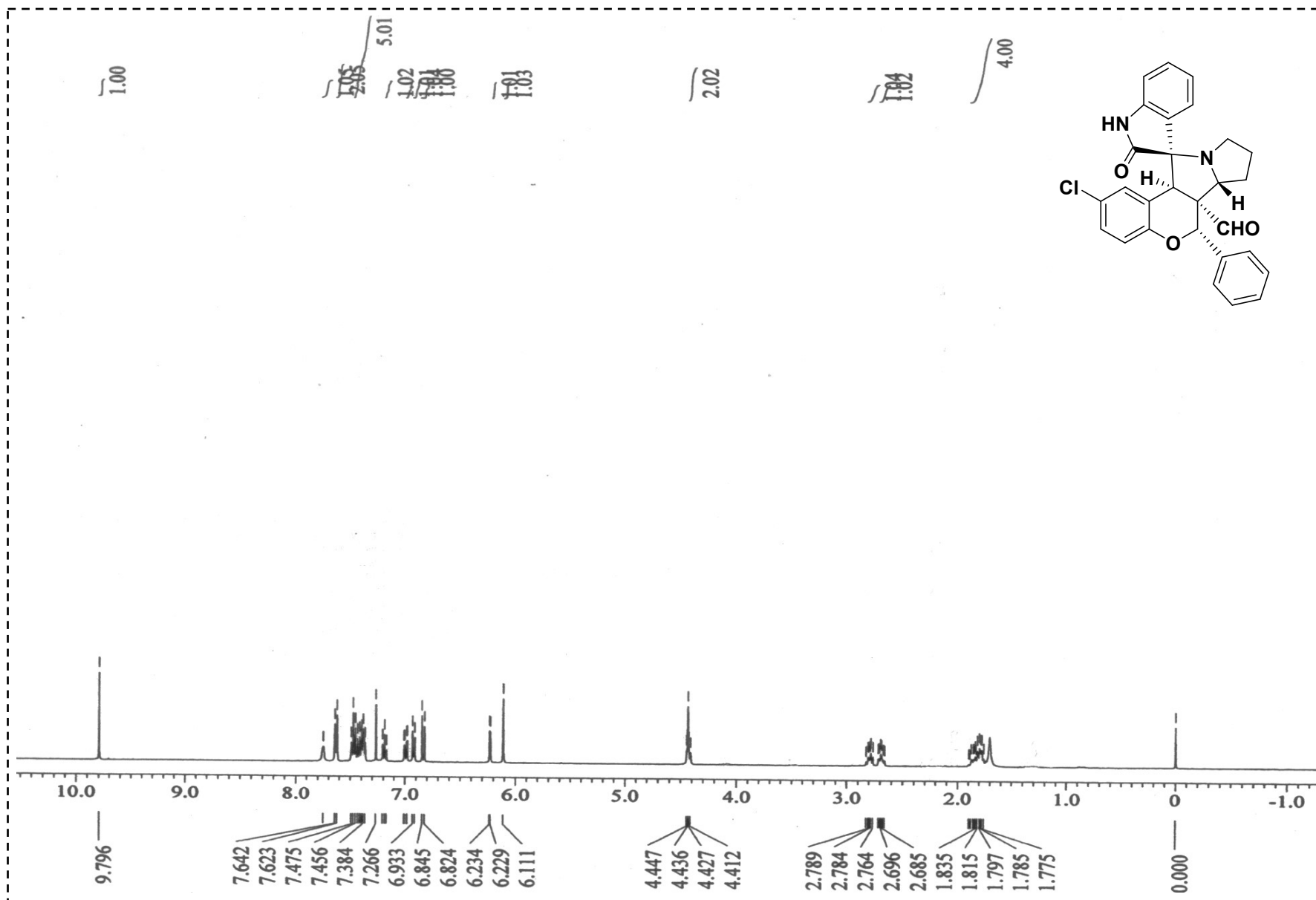


Fig S43. ¹H NMR spectrum of compound 16c in CDCl₃

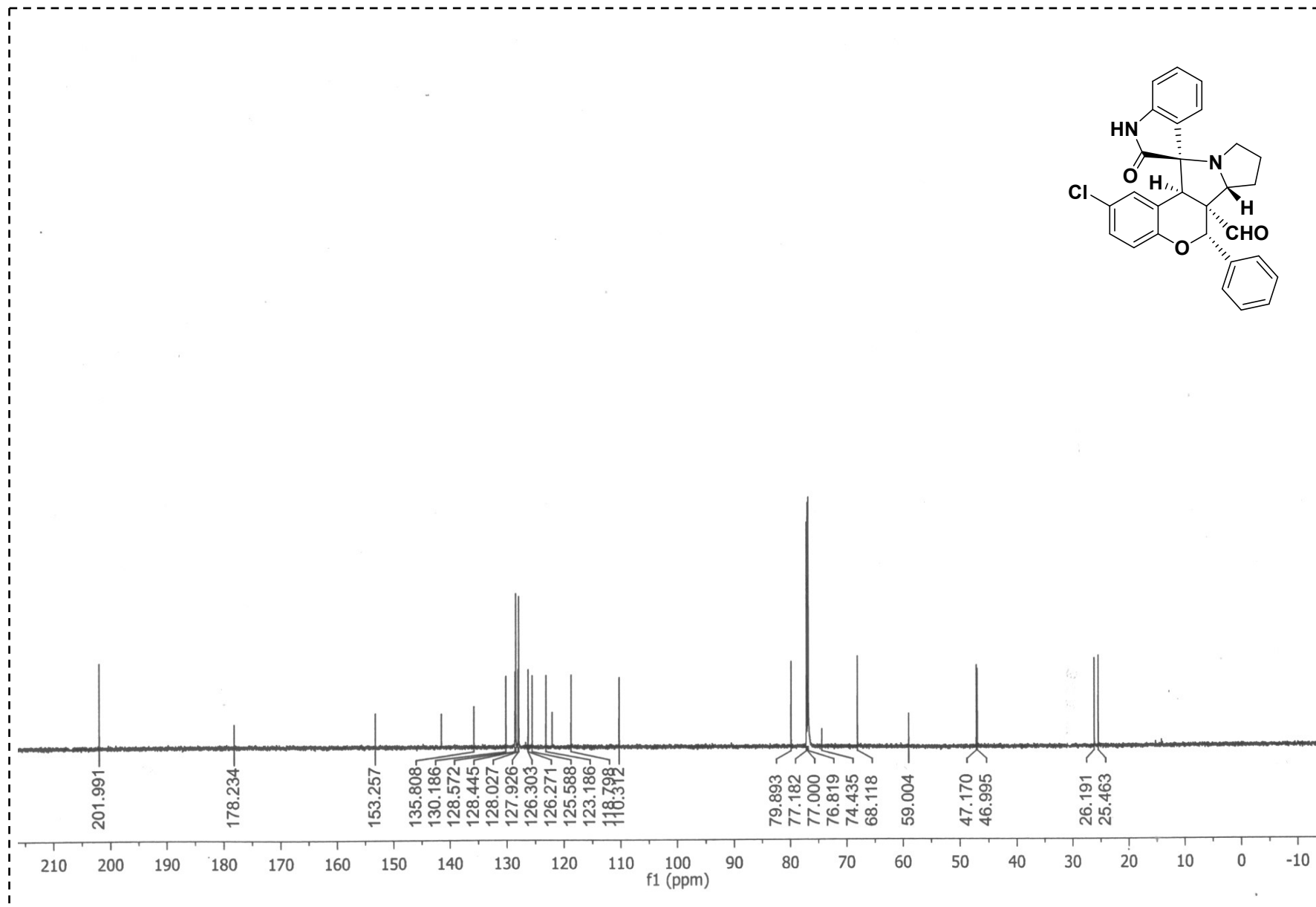


Fig S44. ¹³C NMR spectrum of compound 16c in CDCl₃

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IISER BERHAMPUR
CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

16-May-2022 13:42:39

JP-224-1 10 (0.209) Cm (4:29)

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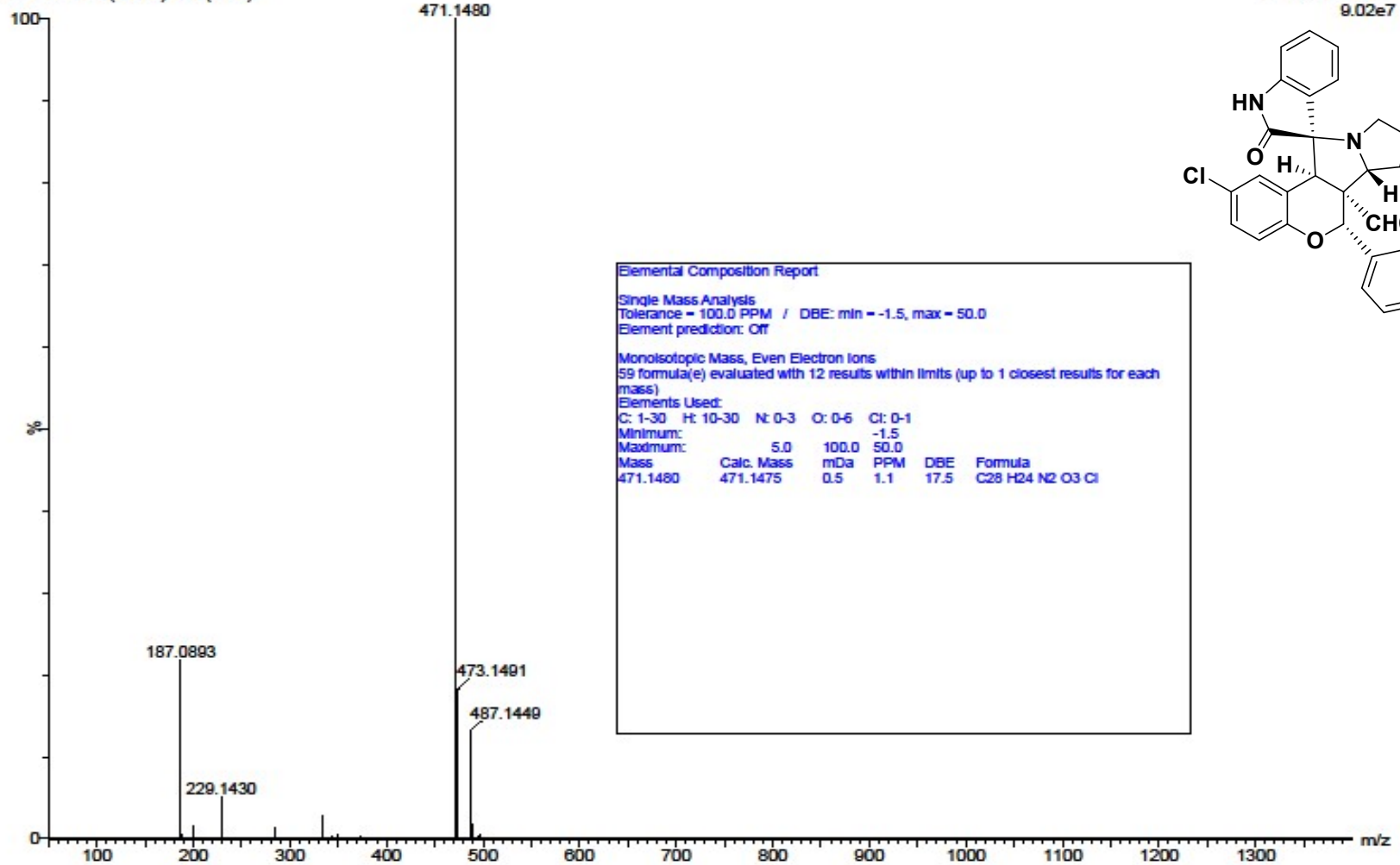


Fig S45. HRMS of compound 16c

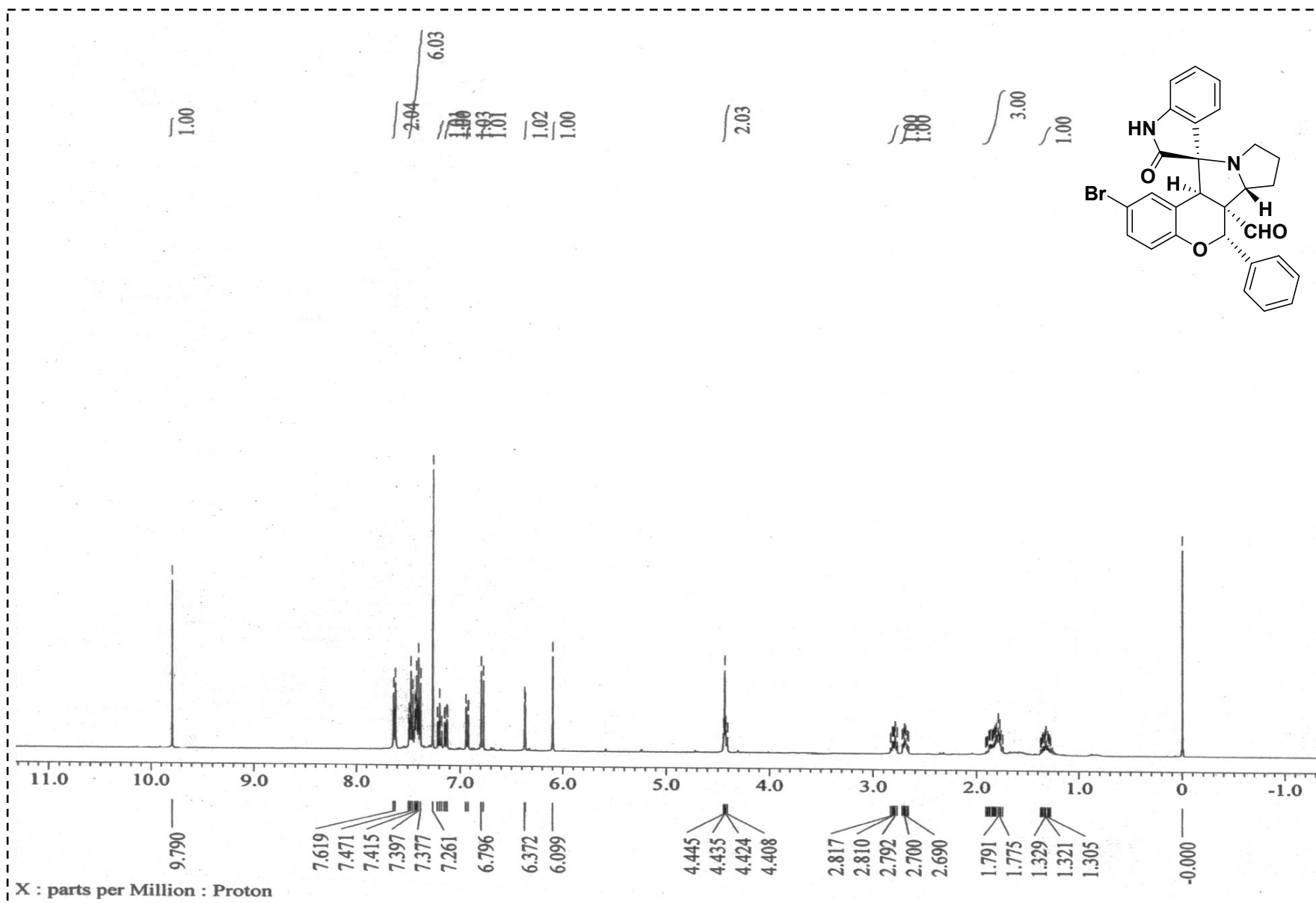


Fig S46. ¹H NMR spectrum of compound 16'd in CDCl₃

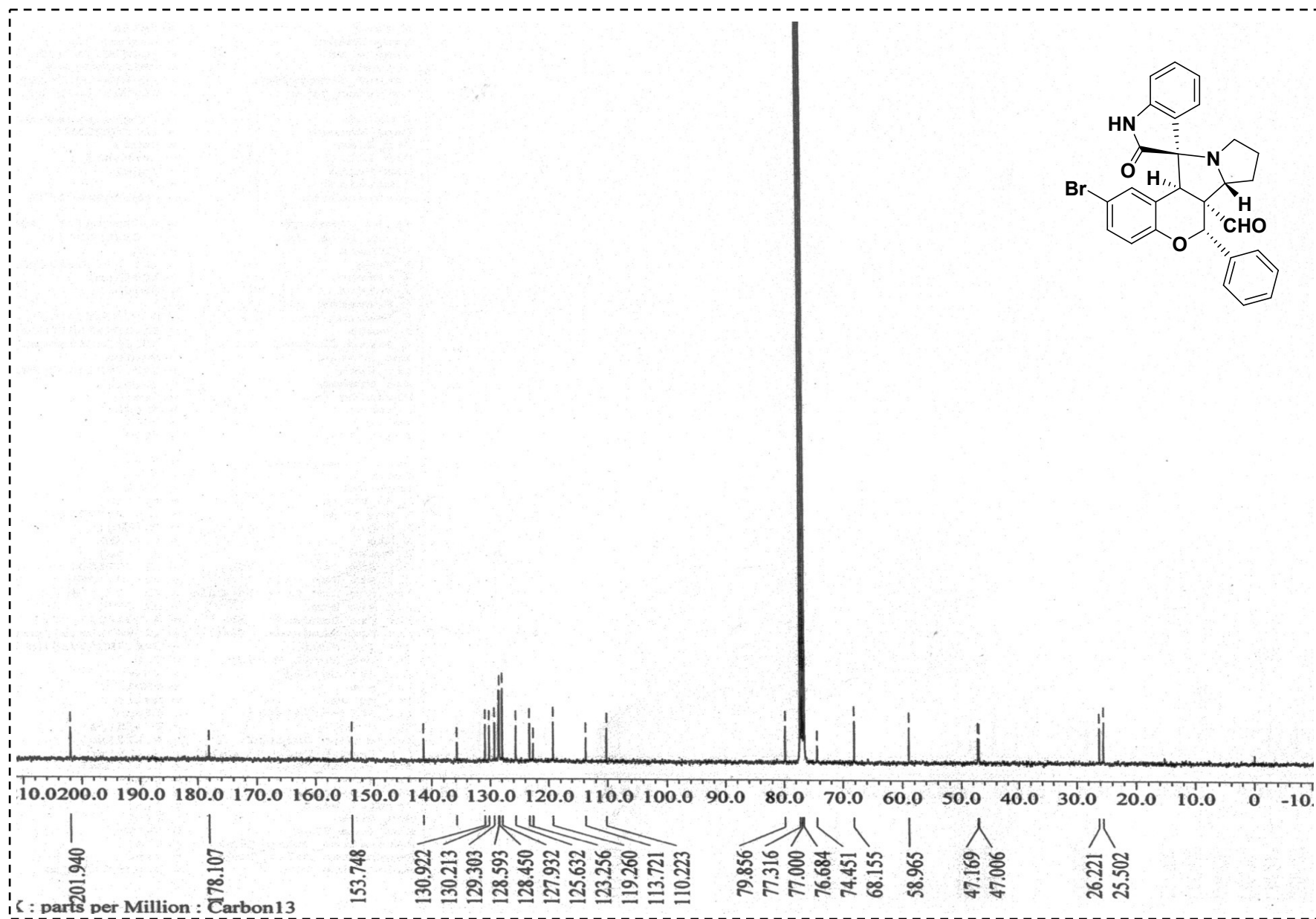


Fig S47. ^{13}C NMR spectrum of compound 16'd in CDCl_3

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IISER BERHAMPUR
CAIF HRMS FACILITY
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16-May-2022 14:47:16

JP-222-4 (0.096)

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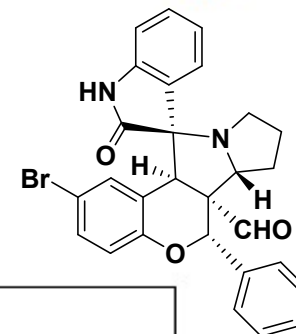
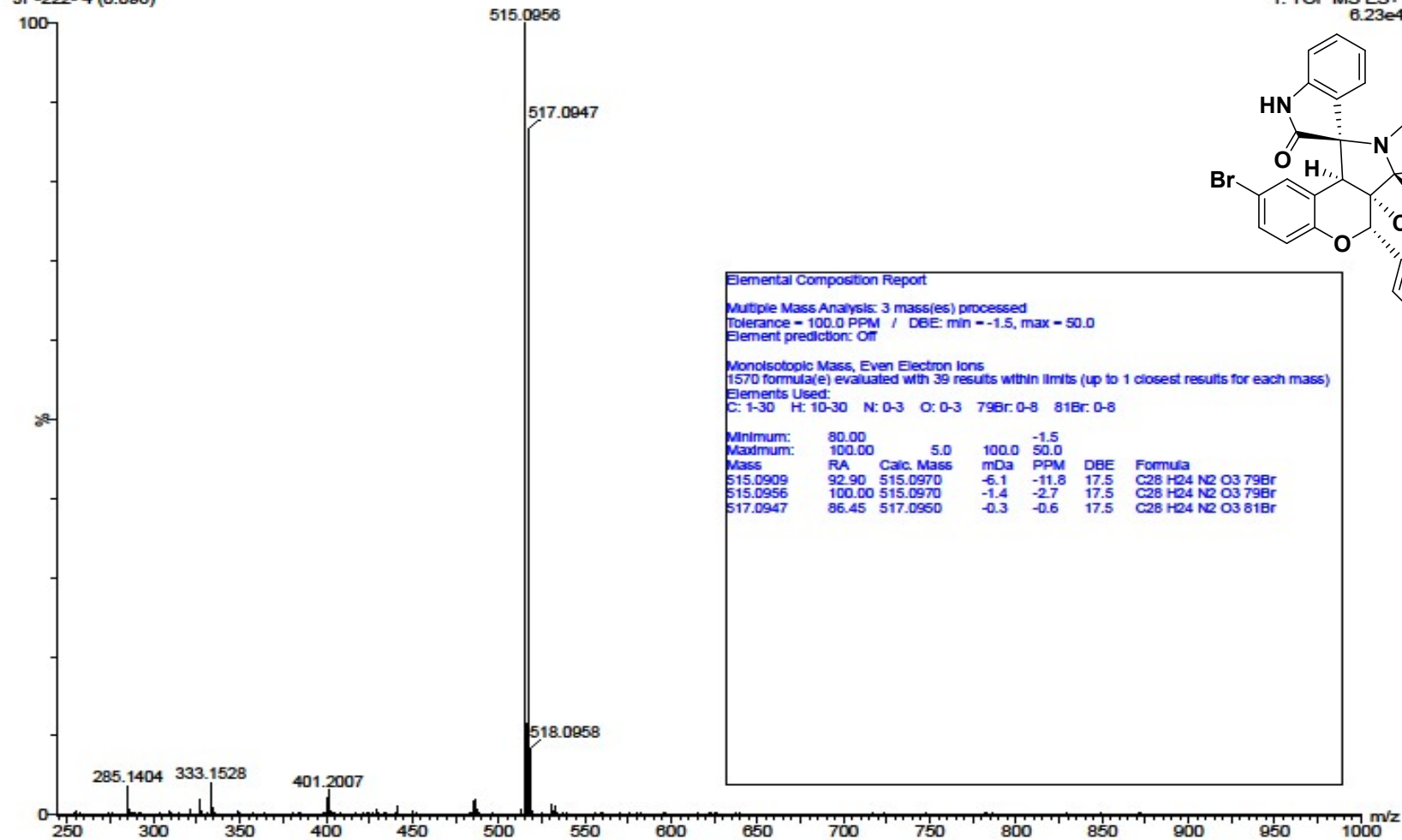


Fig S48. HRMS of compound 16'd

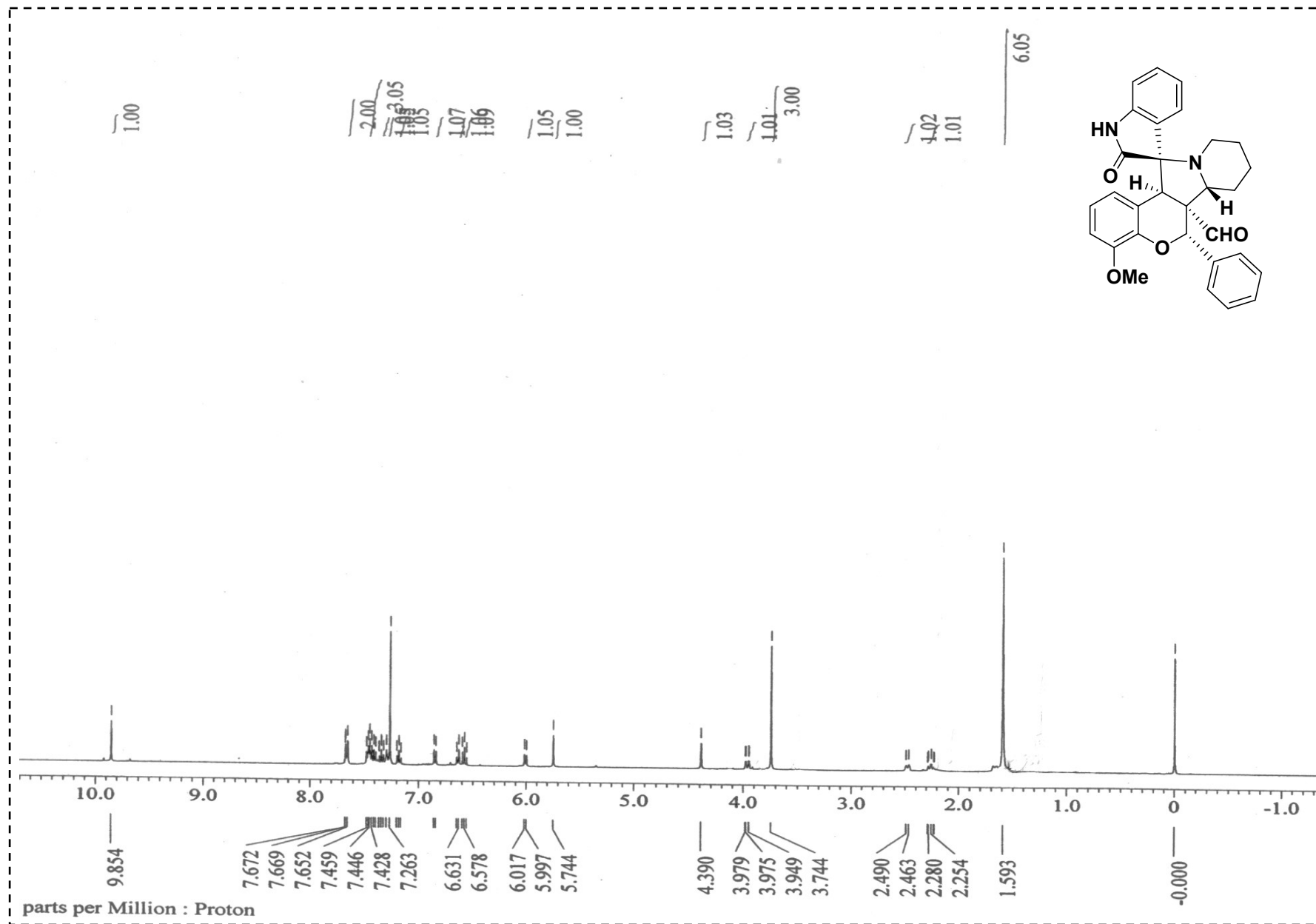


Fig S49. ¹H NMR spectrum of compound **16'e** in CDCl₃

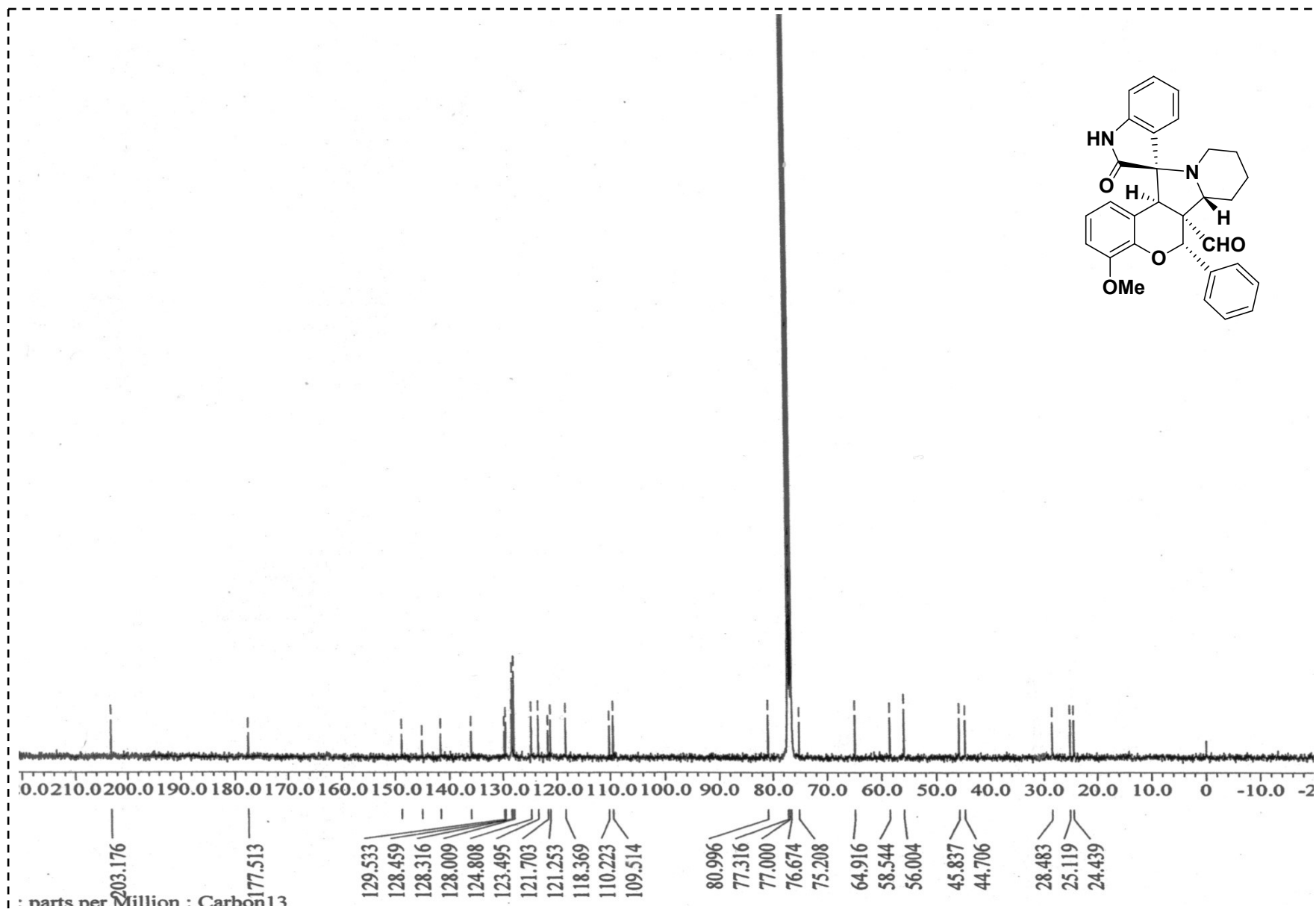


Fig S50. ^{13}C NMR spectrum of compound **16'e** in CDCl_3

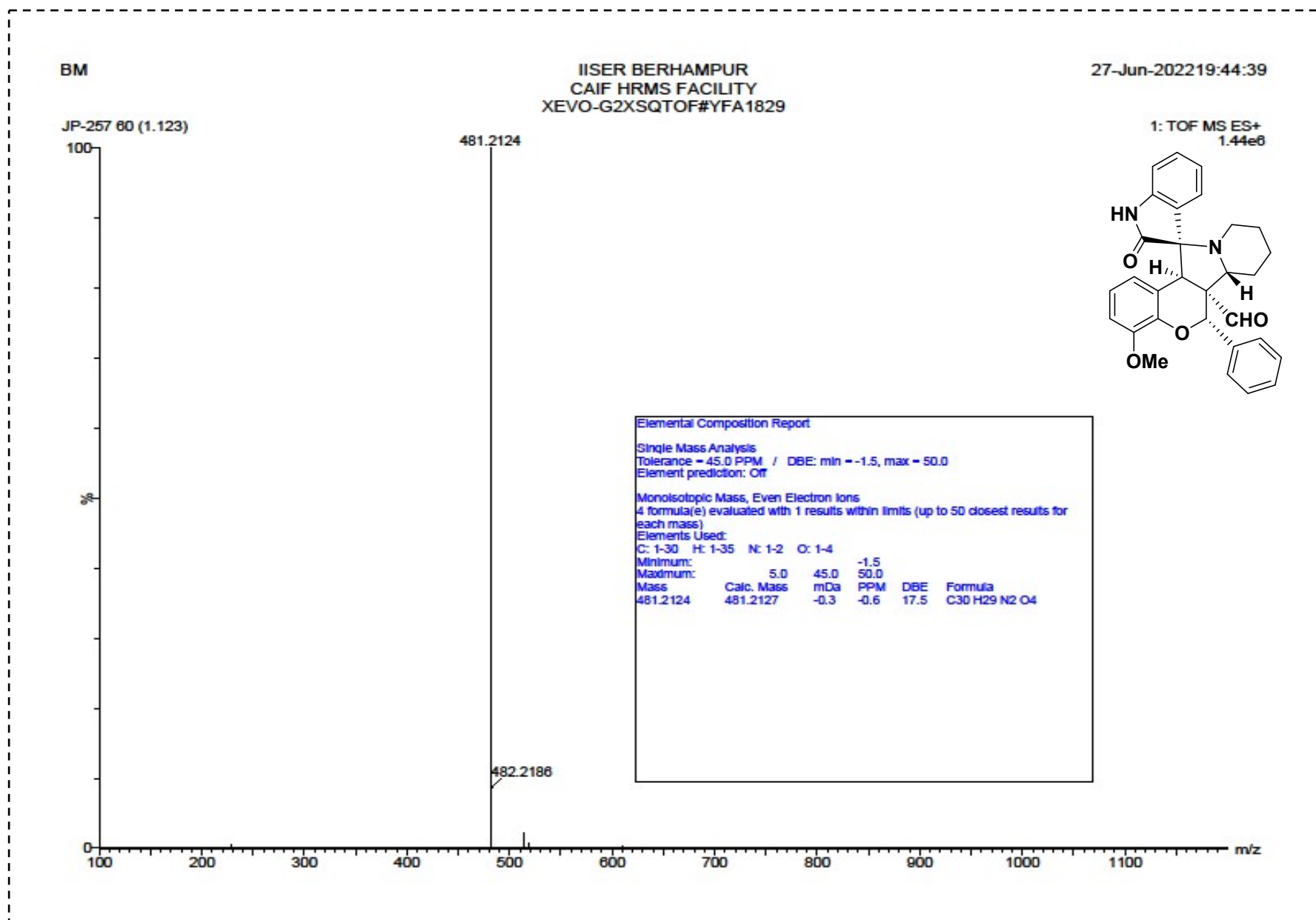


Fig S51. HRMS of compound 16'e

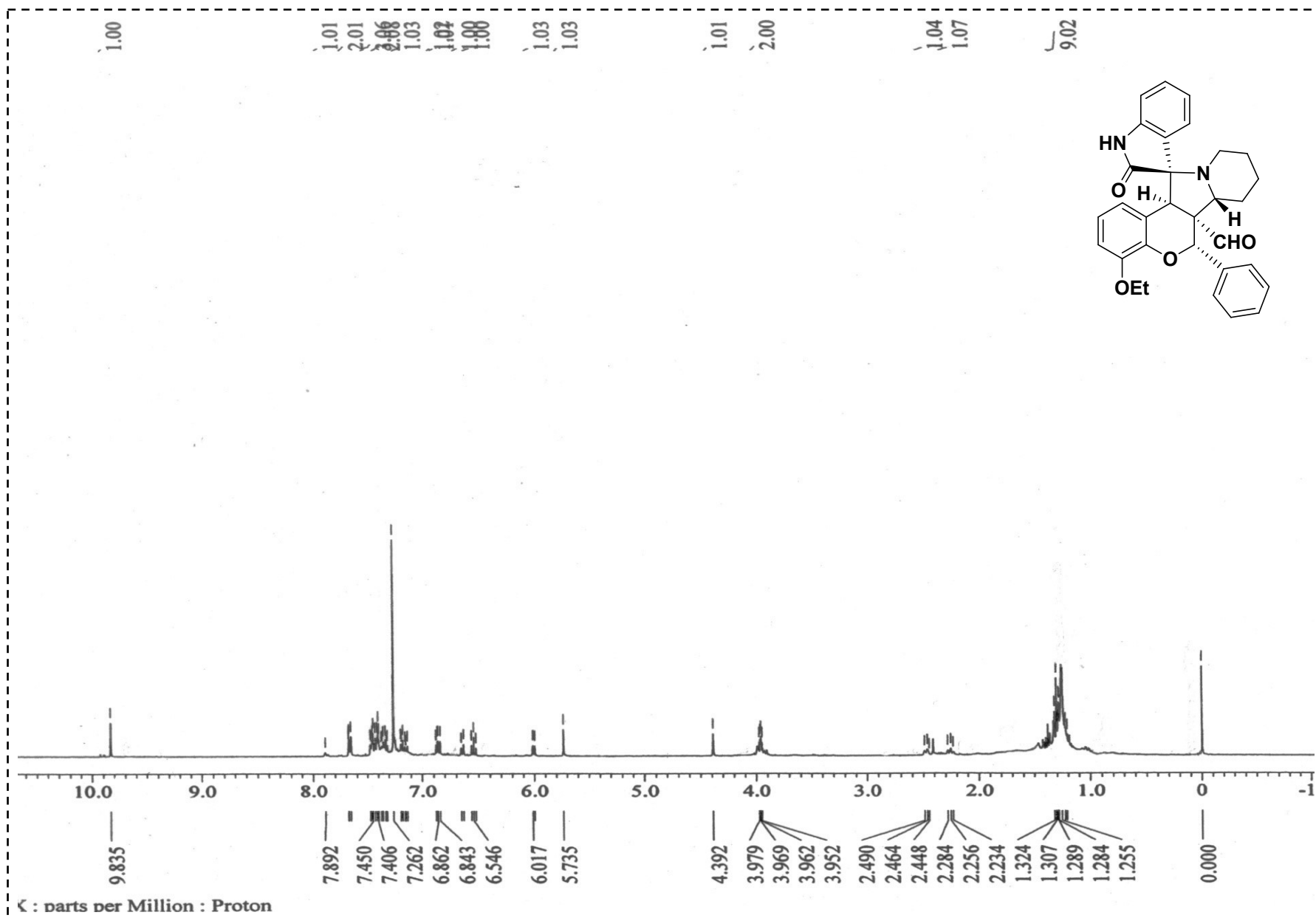


Fig S52. ¹H NMR spectrum of compound 16f in CDCl₃

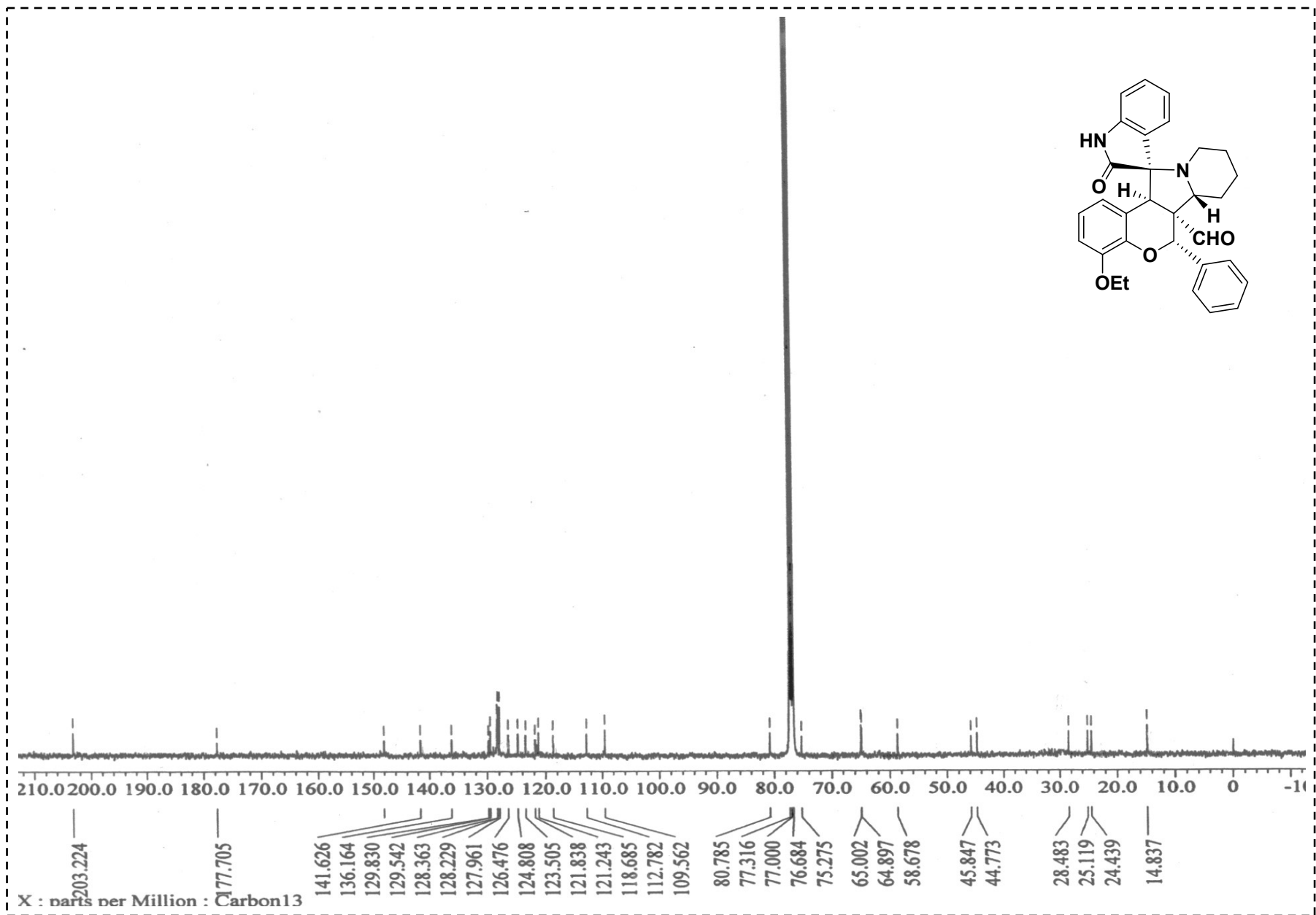


Fig S53. ^{13}C NMR spectrum of compound 16f in CDCl_3

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XEVO-G2XSQTOF#YFA1829

27-Jun-2022 19:50:19

JP-263 84 (1.564) Cm (84:89)

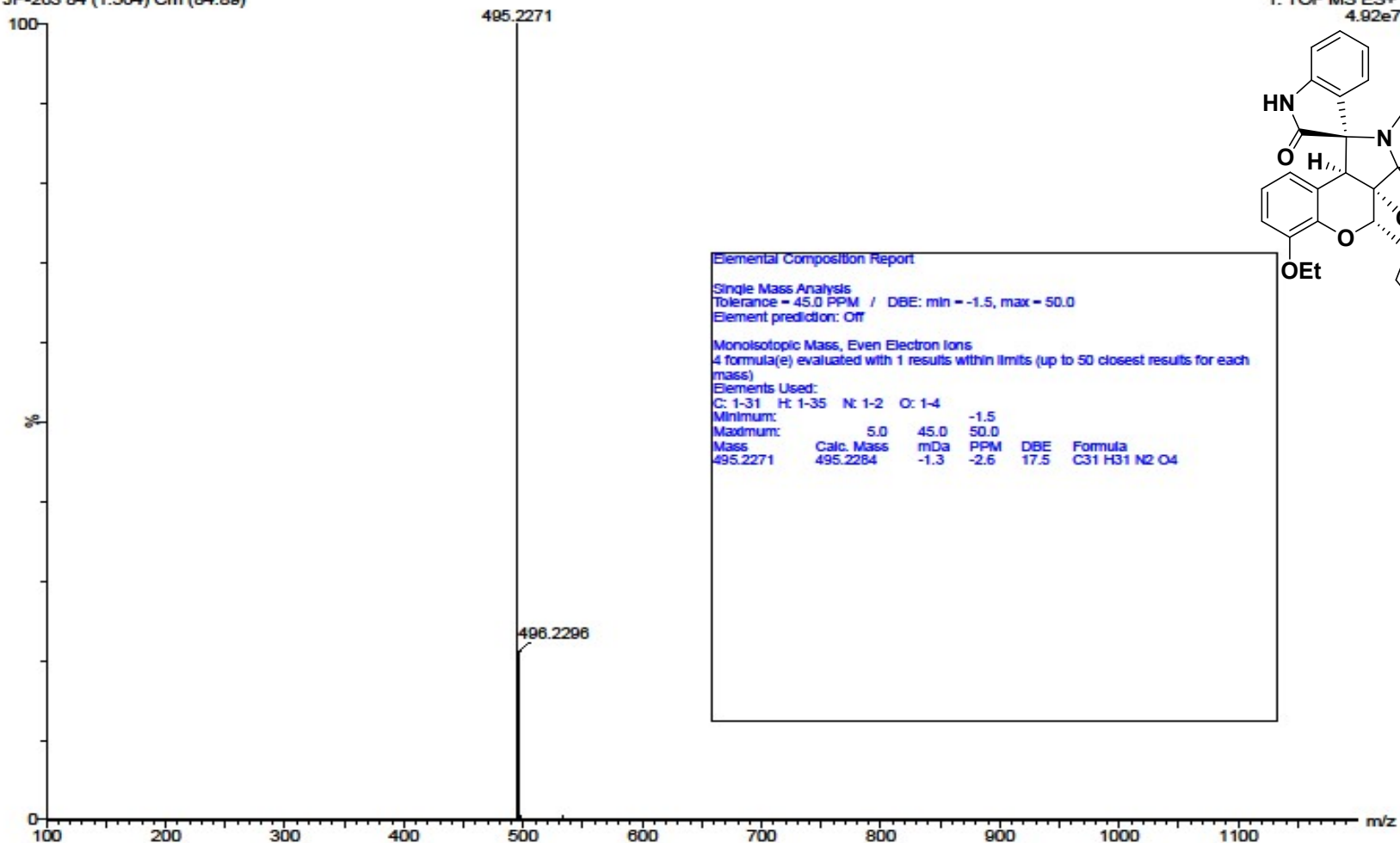


Fig S54. HRMS of compound 16'f

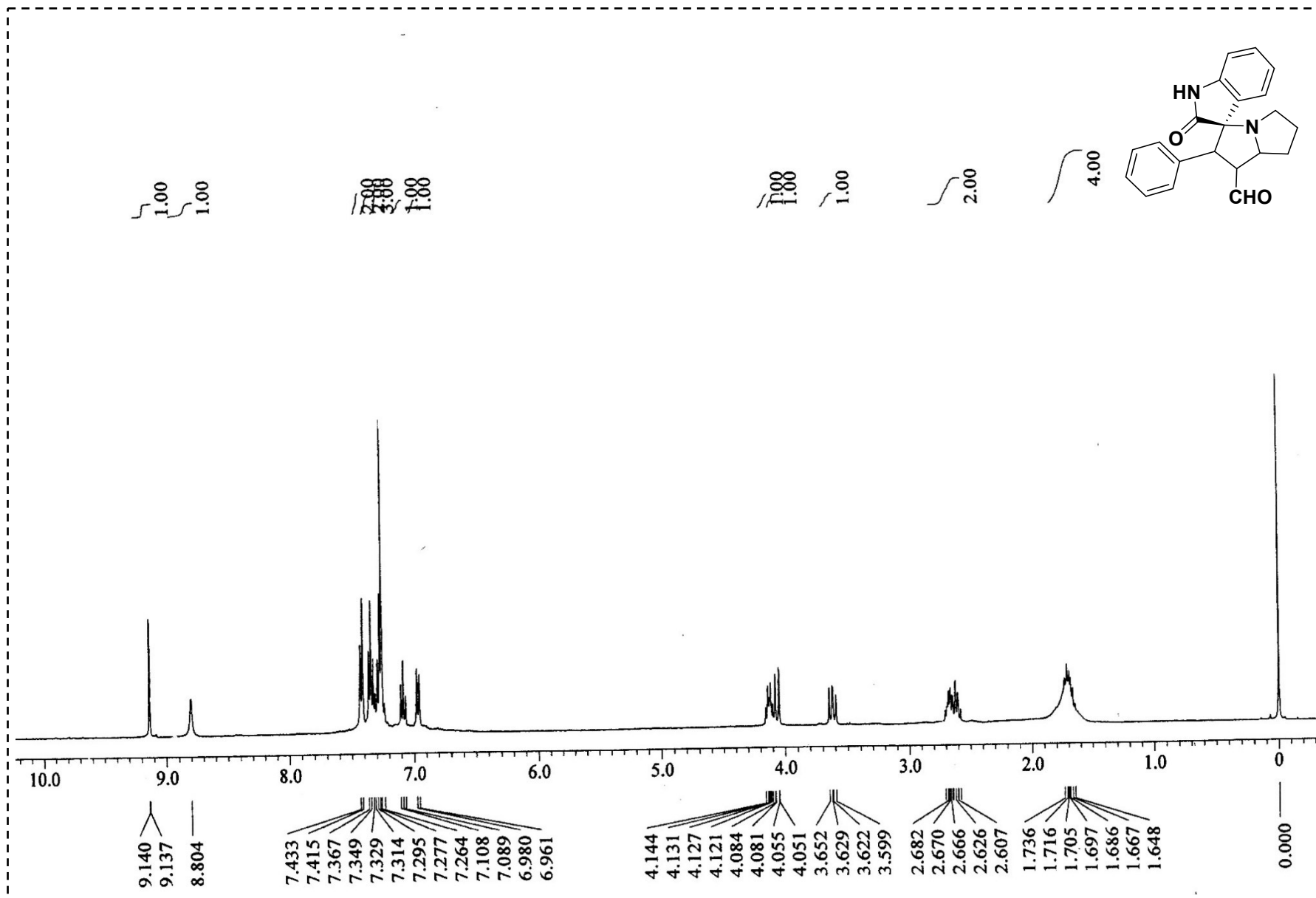


Fig S55. ¹H NMR spectrum of compound 17 in CDCl₃

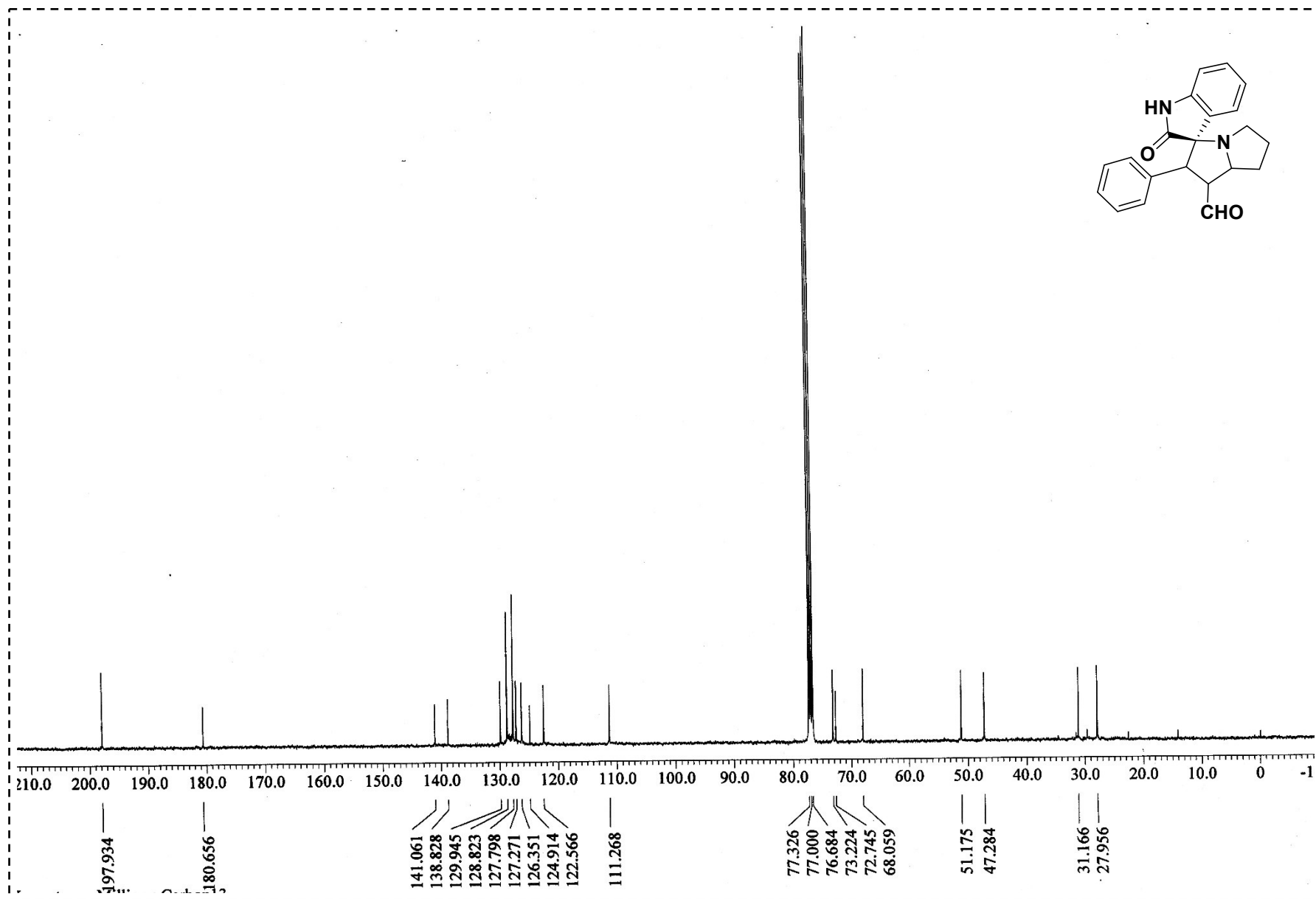


Fig S56. ^{13}C NMR spectrum of compound 17 in CDCl_3

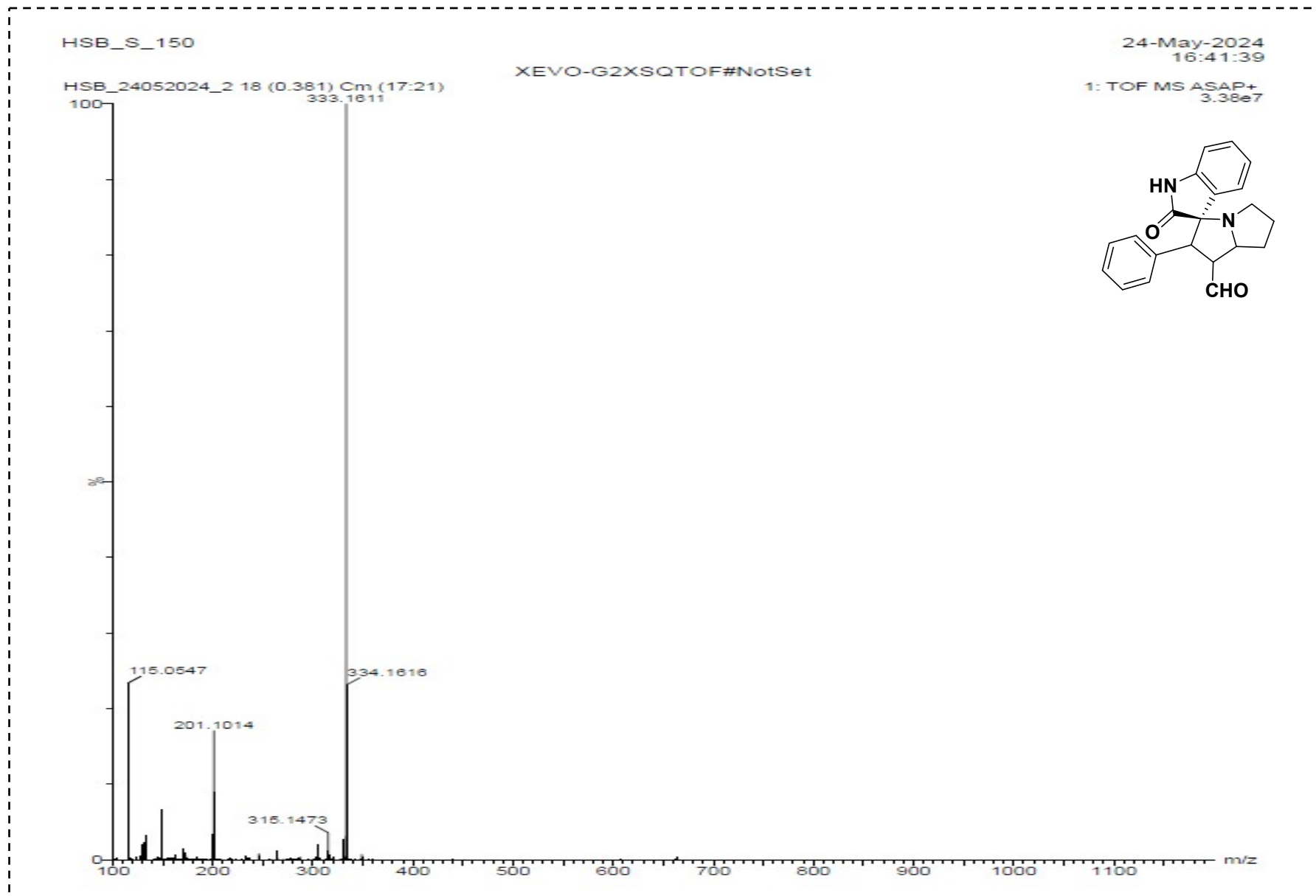


Fig S57. HRMS of compound 17

2. ^1H , ^{13}C NMR and HRMS spectra of synthesized compound **18d**

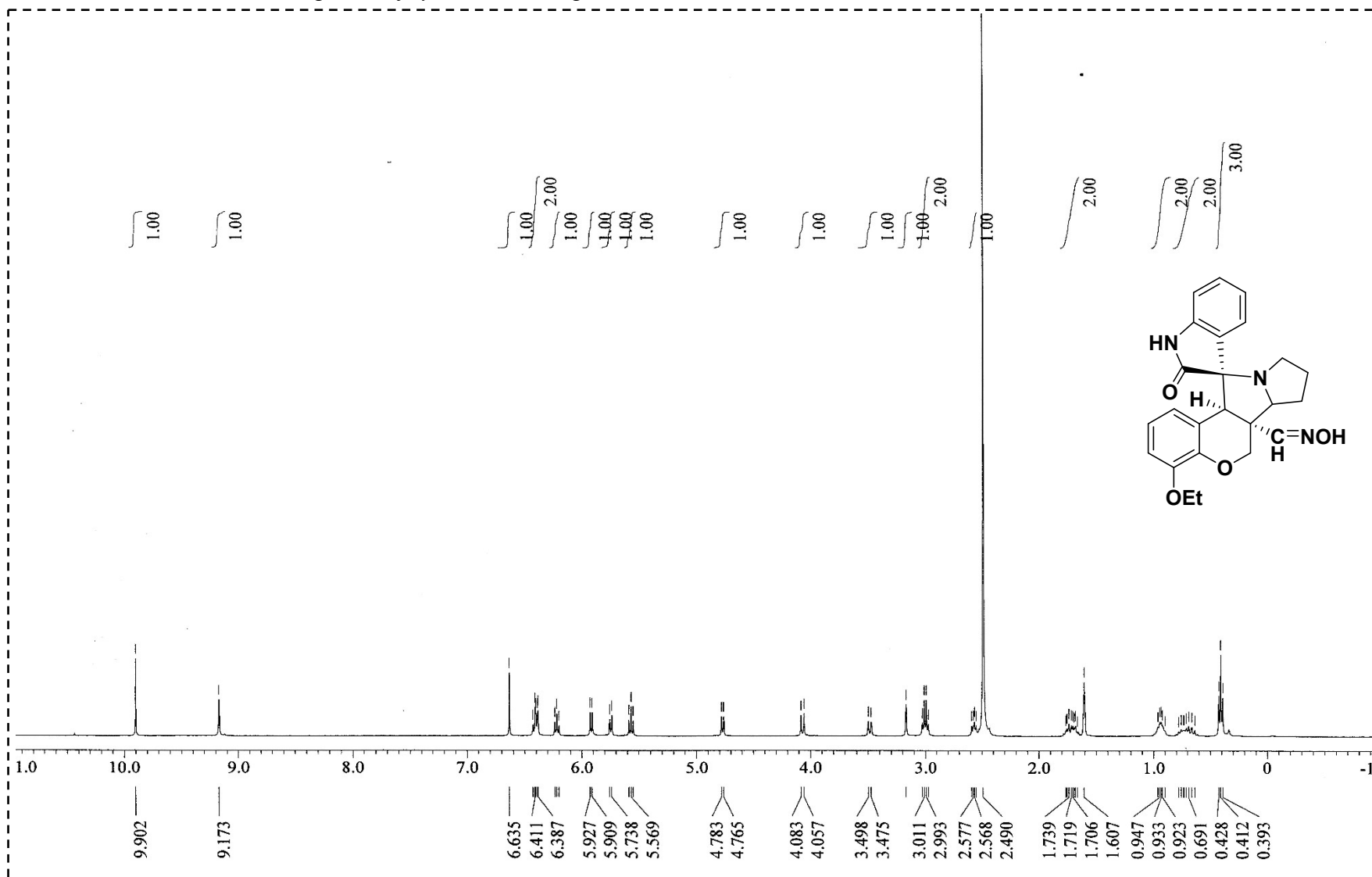


Fig S58. ^1H NMR spectrum of compound **18d** in DMSO- d_6

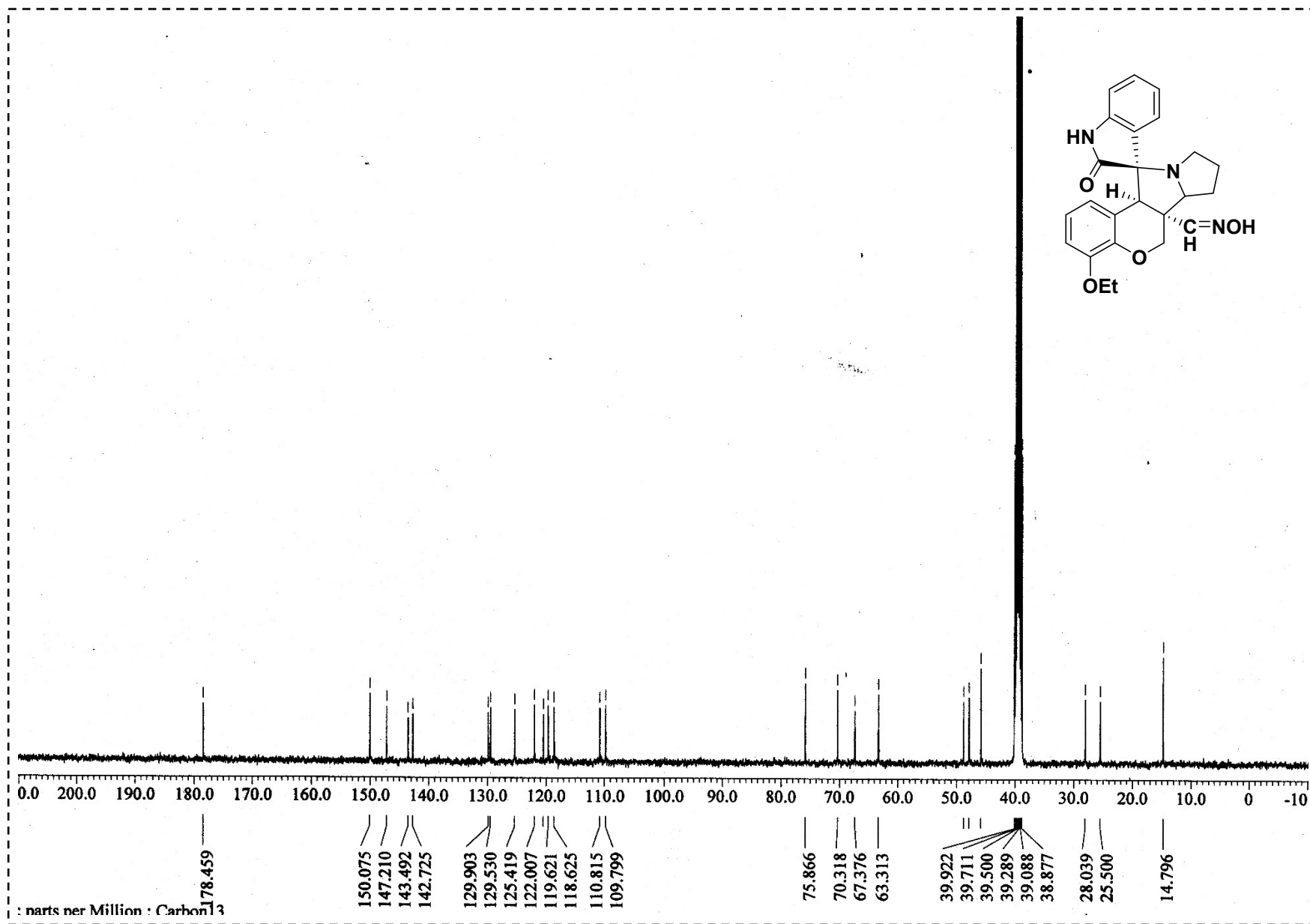


Fig S59. ¹³C NMR spectrum of compound 18d in DMSO-d₆

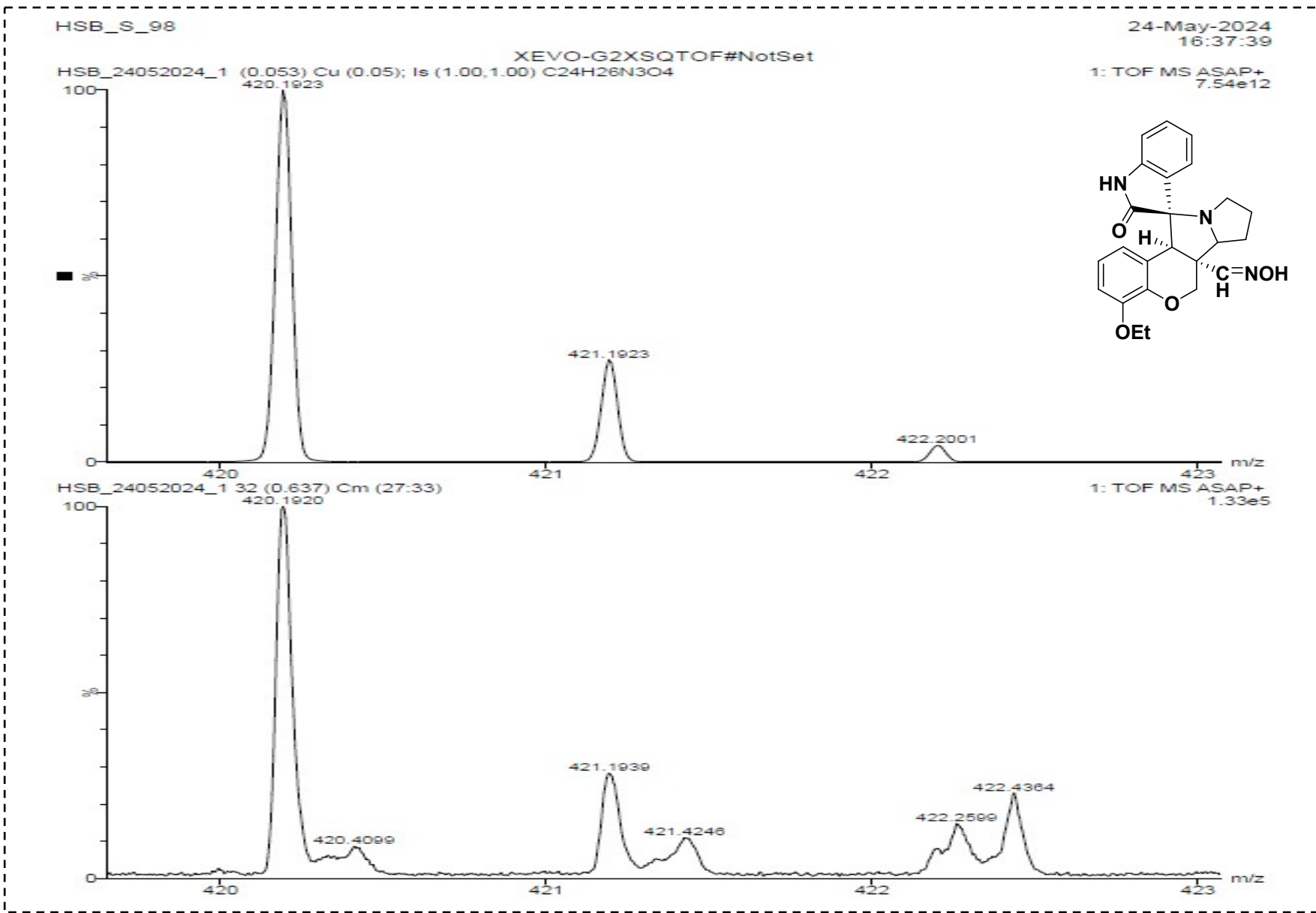


Fig S60. HRMS of compound 18d

3. Co-ordinates of the optimized geometries of all the species:

Reactant 11, EE+ ZPE= -536.097245 a.u				Radical reactant AY, EE+ ZPE= -648.952276 a.u			
C	-2.858506000	-1.272305000	0.093294000	C	2.641357000	0.638897000	-0.141410000
C	-1.511047000	-1.592165000	0.128932000	N	1.547693000	-0.057006000	-0.042567000
C	-0.538242000	-0.592392000	0.038565000	C	0.248581000	0.417879000	-0.024926000
C	-0.947029000	0.745710000	-0.095355000	C	-0.990480000	-0.316225000	-0.023319000
C	-2.297383000	1.068148000	-0.161449000	C	-2.013043000	0.669063000	0.038131000
C	-3.245003000	0.058689000	-0.060886000	C	-3.359440000	0.346729000	0.051436000
H	1.231814000	-1.878309000	-0.204565000	C	-3.717426000	-0.998669000	-0.002064000
H	-3.606483000	-2.051483000	0.172333000	C	-2.735527000	-1.984664000	-0.075218000
H	-1.193658000	-2.625257000	0.222657000	C	-1.381587000	-1.658138000	-0.089744000
C	0.884707000	-0.866069000	-0.023799000	C	-0.033884000	1.820914000	0.021054000
H	-2.586402000	2.104687000	-0.284972000	H	-4.111985000	1.125980000	0.100101000
H	-4.297658000	0.314389000	-0.099284000	H	-0.654213000	-2.456025000	-0.160720000
C	1.762519000	0.142463000	0.090580000	C	1.831985000	-1.511913000	0.030348000
O	-0.037711000	1.741756000	-0.238227000	H	2.573021000	1.713254000	-0.230728000
C	1.226946000	1.517245000	0.389385000	H	1.541915000	-1.953993000	-0.924660000
H	1.884836000	2.299956000	0.012274000	N	-1.419594000	1.915780000	0.068605000
H	1.110484000	1.657340000	1.472987000	H	1.231532000	-1.948623000	0.825538000
C	3.210306000	-0.082264000	-0.039111000	O	0.731432000	2.796506000	0.029714000
				H	-1.904122000	2.796518000	0.105572000
				H	-4.765300000	-1.275682000	0.008178000

O	3.724795000	-1.168391000	-0.194974000	H	-3.026045000	-3.028202000	-0.124954000
H	3.836783000	0.829396000	0.013240000	C	3.335285000	-1.578982000	0.298026000
				C	3.863133000	-0.209459000	-0.160020000
				H	3.800045000	-2.409994000	-0.229437000
				H	3.514496000	-1.708969000	1.366064000
				H	4.272912000	-0.239050000	-1.176690000
				H	4.645866000	0.188727000	0.487983000
Reactant MN-alpha, EE+ ZPE= -767.049273 a.u				Reactant MN-beta, EE+ ZPE= -767.049273 a.u			
C	3.850946000	-0.930333000	0.722434000	C	-3.850897000	-0.930346000	0.722440000
C	3.093084000	0.174229000	1.074598000	C	-3.093079000	0.174268000	1.074558000
C	1.952097000	0.516597000	0.343643000	C	-1.952097000	0.516632000	0.343601000
C	1.583629000	-0.271993000	-0.758229000	C	-1.583608000	-0.272003000	-0.758228000
C	2.350136000	-1.372119000	-1.124296000	C	-2.350041000	-1.372186000	-1.124238000
C	3.477142000	-1.695937000	-0.381785000	C	-3.477050000	-1.696006000	-0.381718000
H	4.730629000	-1.193996000	1.296352000	H	-4.730585000	-1.193996000	1.296355000
H	3.376490000	0.787858000	1.923011000	H	-3.376527000	0.787928000	1.922934000
C	1.137797000	1.679785000	0.631502000	C	-1.137812000	1.679837000	0.631433000
H	2.051031000	-1.959035000	-1.983984000	H	-2.050896000	-1.959145000	-1.983883000
H	4.068412000	-2.559042000	-0.665256000	H	-4.068275000	-2.559158000	-0.665139000
C	-0.052170000	1.829986000	0.029030000	C	0.052156000	1.830025000	0.028974000
O	0.522090000	0.057612000	-1.532420000	O	-0.522042000	0.057610000	-1.532421000
				H	-1.507275000	2.428041000	1.327295000

H	1.507247000	2.427975000	1.327385000	C	0.882938000	3.004138000	0.291281000
C	-0.882944000	3.004099000	0.291320000	O	1.962477000	3.199612000	-0.224601000
O	-1.962444000	3.199612000	-0.224641000	H	0.454301000	3.725911000	1.013095000
H	-0.454369000	3.725832000	1.013210000	C	1.510300000	-0.228166000	-0.246891000
C	-0.566673000	0.765272000	-0.901886000	C	2.483708000	-0.843394000	-1.033736000
H	-1.088654000	1.240824000	-1.732571000	C	1.396336000	-0.588611000	1.094436000
C	-1.510316000	-0.228189000	-0.246906000	C	3.329277000	-1.802707000	-0.492544000
C	-2.483814000	-0.843317000	-1.033735000	H	2.579549000	-0.565948000	-2.078567000
C	-1.396319000	-0.588690000	1.094401000	C	2.239638000	-1.551675000	1.637849000
C	-3.329408000	-1.802590000	-0.492542000	H	0.652458000	-0.113636000	1.723899000
H	-2.579683000	-0.565792000	-2.078541000	C	3.206957000	-2.159891000	0.846589000
C	-2.239642000	-1.551750000	1.637812000	H	4.085622000	-2.268913000	-1.113518000
H	-0.652414000	-0.113762000	1.723868000	H	2.142102000	-1.824001000	2.682521000
C	-3.207027000	-2.159864000	0.846572000	H	3.866982000	-2.906957000	1.272480000
H	-4.085830000	-2.268721000	-1.113480000	C	0.566670000	0.765294000	-0.901923000
H	-2.142054000	-1.824123000	2.682466000	H	1.088690000	1.240852000	-1.732584000
H	-3.867075000	-2.906928000	1.272433000				
TS-ON, imaginary frequency = -428.64 cm ⁻¹ , EE+ ZPE= -1185.051252 a.u				TS-OX, imaginary frequency = -435.92 cm ⁻¹ , EE+ ZPE= -1185.055640 a.u			
C	-0.634180000	1.497034000	-0.889323000	C	-0.892813000	-1.746233000	-0.931920000
N	0.693645000	1.424336000	-0.632305000	N	-0.010596000	-0.797768000	-1.328955000

C	1.404071000	0.284621000	-0.686087000	C	1.187525000	-0.658817000	-0.735879000
C	2.764815000	0.030426000	-0.237634000	C	2.084478000	0.480473000	-0.732950000
C	3.103220000	-1.248494000	-0.729372000	C	3.301324000	0.016931000	-0.190289000
C	4.312007000	-1.858022000	-0.447822000	C	4.371636000	0.858622000	0.052679000
C	5.219956000	-1.163259000	0.347460000	C	4.223106000	2.206208000	-0.265231000
C	4.911929000	0.101142000	0.842401000	C	3.032034000	2.687588000	-0.803674000
C	3.688958000	0.703338000	0.560062000	C	1.956234000	1.835313000	-1.034731000
C	1.006982000	-0.844073000	-1.547185000	C	1.970076000	-1.839825000	-0.294454000
H	4.542070000	-2.842798000	-0.836350000	H	5.293709000	0.478392000	0.475274000
H	3.482168000	1.682981000	0.963991000	H	1.037688000	2.237583000	-1.437471000
C	1.237267000	2.703049000	-0.114669000	C	-0.643179000	0.227503000	-2.180718000
H	-1.030899000	0.784509000	-1.597892000	H	-0.465263000	-2.671506000	-0.576313000
H	1.944905000	3.085159000	-0.854233000	H	-0.031574000	0.350799000	-3.075537000
N	2.048882000	-1.738815000	-1.484879000	N	3.210342000	-1.348790000	0.033696000
H	1.738709000	2.533478000	0.830538000	H	-0.679219000	1.171281000	-1.639187000
O	-0.010922000	-1.004617000	-2.211850000	O	1.647469000	-3.019325000	-0.247060000
H	2.043313000	-2.612171000	-1.985672000	H	3.932981000	-1.924496000	0.433202000
H	6.177488000	-1.614456000	0.579899000	H	5.047534000	2.887204000	-0.088953000
H	5.631471000	0.627226000	1.458293000	H	2.936713000	3.739954000	-1.042727000
C	0.001293000	3.582723000	0.047913000	C	-2.051201000	-0.320503000	-2.463973000
C	-1.033996000	2.948305000	-0.884564000	C	-2.072536000	-1.735442000	-1.856083000
H	0.209545000	4.623794000	-0.193380000	H	-2.260918000	-0.335775000	-3.532545000

H	-0.345680000	3.533166000	1.081621000	H	-2.799626000	0.309549000	-1.983021000
H	-0.956584000	3.344654000	-1.902907000	H	-1.936184000	-2.508017000	-2.618888000
H	-2.054915000	3.114533000	-0.548603000	H	-3.005712000	-1.953405000	-1.336188000
C	-5.105907000	0.406036000	-0.435831000	C	-4.801259000	0.298146000	0.457416000
C	-3.826587000	0.864588000	-0.160253000	C	-3.771921000	-0.592938000	0.734895000
C	-2.823105000	0.009442000	0.301797000	C	-2.448534000	-0.160325000	0.808774000
C	-3.155699000	-1.343131000	0.496374000	C	-2.187006000	1.206102000	0.645646000
C	-4.444709000	-1.806160000	0.242361000	C	-3.206095000	2.103836000	0.361748000
C	-5.414839000	-0.935301000	-0.227742000	C	-4.514030000	1.644725000	0.256821000
H	-1.454966000	1.381048000	1.329099000	H	-5.822894000	-0.057135000	0.395351000
H	-5.861220000	1.093371000	-0.797300000	H	-3.989596000	-1.645716000	0.883708000
H	-3.608579000	1.916858000	-0.288728000	C	-1.306776000	-1.076302000	0.998263000
C	-1.479493000	0.475756000	0.729458000	H	-2.960885000	3.150577000	0.226559000
H	-4.662382000	-2.852880000	0.418421000	H	-5.310755000	2.344537000	0.032889000
H	-6.413118000	-1.304798000	-0.432590000	O	-0.904944000	1.672392000	0.694317000
C	-0.565329000	-0.521179000	1.072084000	C	-0.068827000	0.999703000	1.637096000
O	-2.261848000	-2.235301000	0.990788000	H	0.937080000	1.383917000	1.473025000
C	-0.897144000	-1.922340000	0.671686000	H	-0.379468000	1.288971000	2.652091000
H	-0.287290000	-2.650408000	1.206479000	C	-0.129154000	-0.494989000	1.496530000
H	-0.780928000	-2.076987000	-0.407391000	C	0.826016000	-1.256489000	2.258114000
C	0.550325000	-0.229287000	1.933857000	O	1.727049000	-0.763336000	2.925316000
O	0.820832000	0.880329000	2.382933000	H	0.698093000	-2.355278000	2.211254000

H	1.185697000	-1.099499000	2.192199000	H	-1.551090000	-2.083111000	1.325218000
TS-MN, imaginary frequency = -351.80 cm ⁻¹ , EE+ ZPE= -1185.056677 a.u				TS-MX, imaginary frequency = -357.10 cm ⁻¹ , EE+ ZPE= - 1185.050881.u			
C	-2.603734000	-0.345933000	0.874617000	C	2.280989000	-1.443575000	0.287122000
N	-1.706897000	-1.186646000	0.416193000	N	1.041554000	-1.429322000	0.745112000
C	-0.339549000	-0.936174000	0.458942000	C	-0.040937000	-1.254120000	-0.104746000
C	0.670087000	-1.890813000	-0.026761000	C	-1.431157000	-1.198415000	0.371506000
C	1.777029000	-1.782436000	0.829922000	C	-2.224652000	-1.812602000	-0.610793000
C	2.969392000	-2.439789000	0.587385000	C	-3.605394000	-1.834391000	-0.543143000
C	3.050375000	-3.231267000	-0.555790000	C	-4.208008000	-1.224649000	0.555830000
C	1.970183000	-3.343303000	-1.426991000	C	-3.442974000	-0.603453000	1.537542000
C	0.778699000	-2.665908000	-1.174930000	C	-2.053130000	-0.573008000	1.443724000
C	0.203086000	-0.400329000	1.747158000	C	-0.075039000	-2.103682000	-1.338432000
H	3.813390000	-2.330981000	1.257405000	H	-4.195774000	-2.308236000	-1.317904000
H	-0.037187000	-2.742890000	-1.882170000	H	-1.481365000	-0.046649000	2.196179000
C	-2.313544000	-2.184962000	-0.488379000	C	0.983446000	-1.195298000	2.202072000
H	-2.316805000	0.408699000	1.587787000	H	2.464042000	-1.809380000	-0.708946000
H	-1.853565000	-3.156836000	-0.320480000	H	0.250426000	-1.871124000	2.640961000
N	1.468685000	-0.904911000	1.864344000	N	-1.400214000	-2.320124000	-1.612036000
H	-2.123498000	-1.873082000	-1.519340000	H	0.667021000	-0.169819000	2.396649000
O	-0.341056000	0.336399000	2.554027000	O	0.861017000	-2.512319000	-2.005594000
H	2.088380000	-0.646274000	2.615093000	H	-1.711500000	-2.835955000	-2.419264000

H	3.971769000	-3.759296000	-0.771638000	H	-5.288579000	-1.230642000	0.638990000
H	2.056909000	-3.956163000	-2.316050000	H	-3.930906000	-0.122803000	2.376830000
C	-3.800195000	-2.132335000	-0.128494000	C	2.418967000	-1.467273000	2.667357000
C	-3.991835000	-0.757342000	0.540152000	C	3.282404000	-1.401501000	1.390345000
H	-4.037502000	-2.927967000	0.578398000	H	2.483346000	-2.461665000	3.109089000
H	-4.426181000	-2.261991000	-1.009349000	H	2.732816000	-0.744566000	3.418824000
H	-4.617310000	-0.799133000	1.433577000	H	3.985544000	-2.232463000	1.314589000
H	-4.437082000	-0.009600000	-0.126755000	H	3.872302000	-0.482726000	1.319401000
C	3.465841000	1.450439000	-0.767811000	C	-2.588966000	2.625815000	-0.580754000
C	2.263595000	0.784596000	-0.946248000	C	-1.747528000	1.588587000	-0.947676000
C	1.044919000	1.366762000	-0.583273000	C	-0.394329000	1.581793000	-0.597009000
C	1.056961000	2.679945000	-0.084777000	C	0.108488000	2.682620000	0.113131000
C	2.265031000	3.355441000	0.089320000	C	-0.732745000	3.731346000	0.484592000
C	3.461833000	2.739384000	-0.239871000	C	-2.075977000	3.698307000	0.145465000
H	4.397250000	0.974107000	-1.049412000	H	-3.635259000	2.601440000	-0.860521000
H	2.259159000	-0.205310000	-1.388097000	H	-2.138841000	0.760935000	-1.528878000
C	-0.254854000	0.703675000	-0.821667000	H	-0.308253000	4.567181000	1.028230000
H	2.239375000	4.368142000	0.474006000	H	-2.722533000	4.516330000	0.442506000
H	4.394407000	3.273037000	-0.095010000	O	1.424245000	2.822031000	0.406831000
C	-1.404924000	1.480351000	-0.584287000	C	1.900351000	0.712156000	-0.730367000
O	-0.071547000	3.378211000	0.177306000	C	2.929595000	0.426290000	-1.690477000
H	-0.274196000	0.058211000	-1.697872000	O	4.107243000	0.754723000	-1.605623000

C	-2.570050000	1.318837000	-1.384654000	H	2.580645000	-0.170719000	-2.559503000
O	-3.592802000	2.005741000	-1.355415000	C	0.536875000	0.532666000	-1.062222000
H	-2.507471000	0.467736000	-2.099359000	H	0.335016000	0.181075000	-2.070826000
C	-1.281158000	2.626972000	0.372991000	C	2.203320000	1.618354000	0.424873000
H	-1.281958000	2.294095000	1.415969000	H	3.244971000	1.933073000	0.384187000
H	-2.100285000	3.328717000	0.222872000	H	2.025873000	1.141542000	1.395330000
Product-ON, EE+ ZPE= -1185.097943 a.u				Product-OX, EE+ ZPE= -1185.098913 a.u			
C	-0.772563000	1.534317000	-0.893959000	C	-0.860344000	-1.607639000	-1.021266000
N	0.690153000	1.392035000	-0.879202000	N	0.241510000	-0.706767000	-1.357511000
C	0.999676000	0.052920000	-0.403421000	C	1.023022000	-0.538112000	-0.135622000
C	2.431276000	-0.196474000	0.043560000	C	2.004008000	0.618169000	-0.176849000
C	3.038454000	-1.074079000	-0.857983000	C	3.296045000	0.102436000	-0.313129000
C	4.347744000	-1.498948000	-0.719254000	C	4.415243000	0.908534000	-0.410326000
C	5.070170000	-1.020990000	0.371277000	C	4.222911000	2.288079000	-0.365797000
C	4.488047000	-0.153772000	1.287827000	C	2.949453000	2.825635000	-0.226239000
C	3.165429000	0.259387000	1.128335000	C	1.833569000	1.992493000	-0.132154000
C	0.918177000	-0.839596000	-1.687855000	C	1.991334000	-1.761584000	-0.137415000
H	4.793004000	-2.179757000	-1.434239000	H	5.404866000	0.480976000	-0.514955000
H	2.732666000	0.928350000	1.861525000	H	0.848038000	2.423528000	-0.015901000
C	1.310638000	2.601616000	-0.306925000	C	-0.319265000	0.491532000	-2.013268000
H	-1.181301000	1.156615000	-1.832536000	H	-0.484927000	-2.629214000	-0.968538000
H	1.867280000	3.123600000	-1.092449000	H	0.377742000	0.848329000	-2.774200000

N	2.132739000	-1.429065000	-1.856925000	N	3.251652000	-1.292785000	-0.323695000
H	2.017492000	2.371164000	0.487276000	H	-0.484885000	1.308789000	-1.307717000
O	-0.033390000	-0.962412000	-2.427972000	O	1.675363000	-2.926709000	-0.010389000
H	2.346036000	-2.013317000	-2.650306000	H	4.056929000	-1.897408000	-0.365768000
H	6.098667000	-1.335198000	0.505052000	H	5.081357000	2.945800000	-0.438149000
H	5.060934000	0.205628000	2.133635000	H	2.817362000	3.900144000	-0.188334000
C	0.145703000	3.459752000	0.191363000	C	-1.666215000	0.035277000	-2.609258000
C	-1.008017000	3.035035000	-0.719954000	C	-1.823285000	-1.436160000	-2.187616000
H	0.362700000	4.527338000	0.136624000	H	-1.686889000	0.142323000	-3.694503000
H	-0.080966000	3.210409000	1.231243000	H	-2.477752000	0.641405000	-2.202151000
H	-0.936092000	3.536608000	-1.689178000	H	-1.500813000	-2.100410000	-2.992407000
H	-1.990674000	3.253311000	-0.298237000	H	-2.851151000	-1.697152000	-1.938810000
C	-4.957343000	0.056283000	-0.600573000	C	-4.825122000	0.215427000	0.155781000
C	-3.696678000	0.638408000	-0.547541000	C	-3.773295000	-0.684809000	0.249743000
C	-2.631362000	-0.001534000	0.084034000	C	-2.467683000	-0.254495000	0.489765000
C	-2.863709000	-1.261058000	0.641998000	C	-2.267146000	1.106541000	0.711926000
C	-4.121215000	-1.850975000	0.605394000	C	-3.305334000	2.024933000	0.611786000
C	-5.172198000	-1.184704000	-0.009884000	C	-4.584524000	1.577521000	0.316448000
H	-1.393537000	1.321572000	1.147958000	H	-5.828474000	-0.142479000	-0.042029000
H	-5.770692000	0.573503000	-1.095733000	H	-3.960080000	-1.745976000	0.119641000
H	-3.542850000	1.614185000	-0.995055000	C	-1.307059000	-1.221355000	0.434032000
C	-1.291672000	0.663031000	0.279496000	H	-3.095386000	3.074549000	0.779866000

H	-4.254201000	-2.828995000	1.052613000	H	-5.397845000	2.289443000	0.236898000
H	-6.154063000	-1.642757000	-0.041005000	O	-1.023084000	1.576194000	1.032314000
C	-0.156231000	-0.322894000	0.624125000	C	-0.278902000	0.655654000	1.811900000
O	-1.842282000	-1.951862000	1.238924000	H	0.655252000	1.145768000	2.077624000
C	-0.611900000	-1.781529000	0.542909000	H	-0.838154000	0.450174000	2.732892000
H	0.106131000	-2.452034000	1.018833000	C	-0.007351000	-0.663523000	1.074986000
H	-0.753120000	-2.089144000	-0.494151000	C	0.553294000	-1.581647000	2.156420000
C	0.345001000	-0.095987000	2.046746000	O	1.566271000	-1.322180000	2.754599000
O	0.138433000	0.888970000	2.706948000	H	-0.042744000	-2.480980000	2.400405000
H	0.945679000	-0.928698000	2.459518000	H	-1.613111000	-2.136643000	0.949293000
Product-MN, EE+ ZPE= -1185.107567 a.u				Product-MX, EE+ ZPE= -1185.107741 a.u			
C	-1.324799000	-1.923263000	0.720341000	C	2.477078000	-0.728704000	-0.236418000
N	0.132428000	-1.977417000	0.563709000	N	1.326336000	-1.626607000	-0.126350000
C	0.595506000	-0.607773000	0.364447000	C	0.101969000	-0.982276000	-0.559372000
C	1.989902000	-0.469406000	-0.202518000	C	-1.113169000	-1.136321000	0.334664000
C	2.810903000	0.130863000	0.752261000	C	-2.105961000	-1.814632000	-0.375251000
C	4.137909000	0.430113000	0.502704000	C	-3.351538000	-2.084673000	0.162565000
C	4.642188000	0.114373000	-0.758218000	C	-3.601258000	-1.650397000	1.462872000
C	3.835404000	-0.466693000	-1.730422000	C	-2.632279000	-0.964641000	2.185843000
C	2.497874000	-0.755292000	-1.456767000	C	-1.384736000	-0.701839000	1.620030000
C	0.762707000	0.028409000	1.774796000	C	-0.381958000	-1.667667000	-1.872304000
H	4.758936000	0.900321000	1.255241000	H	-4.107097000	-2.608979000	-0.409727000

H	1.871317000	-1.189960000	-2.226478000	H	-0.651087000	-0.149882000	2.193215000
C	0.399468000	-2.949197000	-0.500526000	C	1.423305000	-2.452842000	1.069632000
H	-1.563182000	-1.707386000	1.762084000	H	2.943459000	-0.854463000	-1.221640000
H	1.445027000	-3.257697000	-0.490329000	H	0.929133000	-3.416189000	0.921822000
N	2.068466000	0.395680000	1.904522000	N	-1.646488000	-2.126455000	-1.659137000
H	0.170847000	-2.553620000	-1.504547000	H	0.979509000	-1.983657000	1.960234000
O	-0.090084000	0.154097000	2.627203000	O	0.258245000	-1.770260000	-2.895086000
H	2.431555000	0.823326000	2.741821000	H	-2.180258000	-2.617740000	-2.358903000
H	5.678758000	0.336495000	-0.983678000	H	-4.568532000	-1.846776000	1.910658000
H	4.244252000	-0.692246000	-2.707724000	H	-2.845986000	-0.626760000	3.192497000
C	-0.569143000	-4.071858000	-0.157134000	C	2.934771000	-2.581152000	1.236254000
C	-1.828781000	-3.326865000	0.324710000	C	3.444825000	-1.179374000	0.868220000
H	-0.154192000	-4.677891000	0.650999000	H	3.322652000	-3.322634000	0.533004000
H	-0.763238000	-4.724407000	-1.008991000	H	3.219464000	-2.881238000	2.245430000
H	-2.290454000	-3.824029000	1.177576000	H	4.480326000	-1.178687000	0.528142000
H	-2.587084000	-3.286064000	-0.458389000	H	3.386899000	-0.529412000	1.743356000
C	0.355130000	3.786770000	-0.684810000	C	-2.599154000	2.635559000	-1.042309000
C	0.460752000	2.404322000	-0.703612000	C	-1.638460000	1.688005000	-1.355302000
C	-0.627253000	1.584075000	-0.393061000	C	-0.479785000	1.547442000	-0.590276000
C	-1.840699000	2.197367000	-0.067983000	C	-0.296391000	2.391338000	0.503592000
C	-1.958411000	3.586557000	-0.058616000	C	-1.251968000	3.357746000	0.819890000
C	-0.864482000	4.378243000	-0.366060000	C	-2.397948000	3.475062000	0.052261000

H	1.215521000	4.398804000	-0.927467000	H	-3.494099000	2.725175000	-1.646012000
H	1.403904000	1.946112000	-0.980057000	H	-1.782251000	1.034301000	-2.210537000
C	-0.525572000	0.079833000	-0.482183000	H	-1.075801000	4.000835000	1.673966000
H	-2.917906000	4.021407000	0.195313000	H	-3.138450000	4.224044000	0.308528000
H	-0.962650000	5.457686000	-0.353300000	O	0.806964000	2.352058000	1.296173000
C	-1.824823000	-0.662311000	-0.101898000	C	1.878307000	0.704927000	-0.189627000
O	-2.961956000	1.483180000	0.216636000	C	2.763943000	1.645352000	-0.980446000
H	-0.282671000	-0.167180000	-1.522720000	O	3.375650000	2.569527000	-0.513276000
C	-2.551231000	-1.077820000	-1.365434000	H	2.840419000	1.401550000	-2.060216000
O	-3.740753000	-1.006157000	-1.532918000	C	0.536037000	0.492411000	-0.912596000
H	-1.897188000	-1.488024000	-2.163797000	H	0.728902000	0.496964000	-1.990968000
C	-2.723637000	0.198132000	0.778761000	C	1.655740000	1.213201000	1.225824000
H	-2.255264000	0.320012000	1.758004000	H	2.596210000	1.539662000	1.666245000
H	-3.703662000	-0.263944000	0.888772000	H	1.242570000	0.415577000	1.850336000
TS-MN-alpha, imaginary frequency = -350.86 cm-1, EE+ ZPE= -1415.999365 a.u				TS-MN-beta, imaginary frequency = -345.57 cm-1, EE+ ZPE= -1416.003571 a.u			
C	-0.582887000	2.236291000	-0.717938000	C	-1.147675000	-1.821561000	0.543862000
N	0.664689000	2.149589000	-0.324441000	N	0.140698000	-2.021974000	0.399738000
C	1.414408000	0.981053000	-0.430319000	C	1.074239000	-0.994777000	0.488802000
C	2.825515000	0.896589000	-0.016479000	C	2.518972000	-1.178677000	0.283885000
C	3.468815000	0.049139000	-0.931711000	C	3.167105000	-0.273761000	1.140118000
C	4.777640000	-0.365242000	-0.765652000	C	4.535392000	-0.074500000	1.108497000

C	5.460977000	0.088878000	0.359857000	C	5.274848000	-0.807011000	0.183191000
C	4.839677000	0.920245000	1.287869000	C	4.652226000	-1.698018000	-0.686552000
C	3.516209000	1.319896000	1.112231000	C	3.270896000	-1.880147000	-0.650727000
C	1.342187000	0.262663000	-1.743009000	C	0.949388000	-0.069797000	1.655313000
H	5.248498000	-1.029089000	-1.480303000	H	5.011133000	0.635602000	1.773869000
H	3.043380000	1.941197000	1.862033000	H	2.805397000	-2.559276000	-1.353692000
C	1.024819000	3.260666000	0.580824000	C	0.422012000	-3.321487000	-0.243104000
H	-0.970917000	1.523552000	-1.425976000	H	-1.504686000	-0.940097000	1.047226000
H	2.035519000	3.597947000	0.359165000	H	1.297719000	-3.774442000	0.218213000
N	2.571149000	-0.302768000	-1.935020000	N	2.219086000	0.358224000	1.936938000
H	0.989768000	2.890404000	1.609069000	H	0.628563000	-3.146487000	-1.302350000
O	0.398598000	0.179568000	-2.513708000	O	-0.057619000	0.254815000	2.261424000
H	2.776710000	-0.899443000	-2.720062000	H	2.416072000	1.046708000	2.644900000
H	6.488438000	-0.217847000	0.516573000	H	6.349267000	-0.673021000	0.136910000
H	5.385889000	1.254657000	2.161542000	H	5.244326000	-2.251958000	-1.405006000
C	-0.055673000	4.308703000	0.302175000	C	-0.873835000	-4.106989000	-0.026595000
C	-1.222566000	3.512142000	-0.312920000	C	-1.949081000	-3.027892000	0.208477000
H	0.316123000	5.041309000	-0.414959000	H	-0.779545000	-4.737867000	0.857981000
H	-0.340145000	4.835603000	1.211028000	H	-1.098263000	-4.746169000	-0.878496000
H	-1.686274000	4.013313000	-1.164143000	H	-2.643251000	-3.280008000	1.011819000
H	-2.020795000	3.292212000	0.407398000	H	-2.552460000	-2.822499000	-0.683591000
C	2.358895000	-3.451645000	0.657524000	C	2.908763000	3.038473000	-0.878744000

C	2.035626000	-2.120788000	0.868144000	C	2.398412000	1.777376000	-1.157200000
C	0.756780000	-1.628483000	0.587332000	C	1.060590000	1.477361000	-0.903284000
C	-0.218007000	-2.530954000	0.139631000	C	0.227213000	2.479293000	-0.398587000
C	0.099301000	-3.873312000	-0.065399000	C	0.730387000	3.743445000	-0.114350000
C	1.385015000	-4.326941000	0.181595000	C	2.073283000	4.015390000	-0.345605000
H	3.358578000	-3.807894000	0.875309000	H	3.951998000	3.256669000	-1.073247000
H	2.780031000	-1.445796000	1.274203000	H	3.042550000	1.004844000	-1.564308000
C	0.354424000	-0.236517000	0.874473000	C	0.475463000	0.147529000	-1.131353000
H	-0.679648000	-4.542986000	-0.410076000	H	0.061149000	4.496873000	0.283733000
H	1.624478000	-5.370877000	0.013709000	H	2.463572000	5.001551000	-0.121015000
C	-1.017701000	0.078246000	0.742164000	C	-0.926523000	0.068536000	-1.270299000
O	-1.510275000	-2.174874000	-0.043654000	O	-1.078521000	2.238510000	-0.122483000
H	0.860835000	0.197524000	1.734374000	H	1.056084000	-0.491445000	-1.792436000
C	-1.562647000	1.048354000	1.638343000	C	-1.436224000	-0.932184000	-2.149715000
O	-2.718273000	1.447221000	1.764607000	O	-2.579427000	-1.044836000	-2.589069000
H	-0.775410000	1.487411000	2.295082000	H	-0.666426000	-1.671962000	-2.463904000
C	-1.790708000	-0.772173000	-0.245597000	C	-3.058230000	0.957615000	-0.126492000
H	-1.441517000	-0.547790000	-1.259432000	C	-4.248838000	0.698173000	-0.801081000
C	-3.290549000	-0.621112000	-0.215655000	C	-3.052591000	0.944887000	1.267268000
C	-3.918602000	0.209243000	-1.137668000	C	-5.409518000	0.402506000	-0.095822000
C	-4.060772000	-1.305463000	0.720678000	H	-4.256594000	0.703486000	-1.883411000
C	-5.298256000	0.380965000	-1.108480000	C	-4.213736000	0.648622000	1.973038000

H	-3.328444000	0.729557000	-1.885452000	H	-2.130747000	1.156991000	1.794309000
C	-5.439199000	-1.144250000	0.745781000	C	-5.395637000	0.373087000	1.294541000
H	-3.573524000	-1.961489000	1.432196000	H	-6.328399000	0.199291000	-0.634664000
C	-6.062183000	-0.294863000	-0.164638000	H	-4.193825000	0.637100000	3.057311000
H	-5.776152000	1.035190000	-1.829049000	H	-6.301238000	0.143484000	1.844926000
H	-6.031223000	-1.679949000	1.479615000	C	-1.789993000	1.266935000	-0.905274000
H	-7.138688000	-0.167764000	-0.142515000	H	-2.090203000	1.756414000	-1.844043000
Product-MN-beta, EE+ ZPE= -1416.052566 a.u				Product-MN-alpha, EE+ ZPE= -1416.050017 a.u			
C	1.002895000	-1.307516000	-0.374285000	C	-0.713476000	-1.602765000	0.400708000
N	-0.355210000	-1.783375000	-0.634625000	N	0.709435000	-1.940277000	0.354846000
C	-1.251171000	-0.677859000	-0.358861000	C	1.427933000	-0.664308000	0.309232000
C	-2.700626000	-0.998141000	-0.084539000	C	2.887829000	-0.775690000	-0.066559000
C	-3.494409000	-0.371209000	-1.045870000	C	3.667765000	-0.424863000	1.035560000
C	-4.876483000	-0.429858000	-1.011897000	C	5.049439000	-0.402925000	0.986011000
C	-5.465901000	-1.143631000	0.030431000	C	5.654843000	-0.742939000	-0.223246000
C	-4.692470000	-1.761692000	1.007074000	C	4.895034000	-1.077868000	-1.338522000
C	-3.300255000	-1.681668000	0.957929000	C	3.501398000	-1.089474000	-1.265419000
C	-1.353629000	0.159752000	-1.669921000	C	1.516618000	-0.134582000	1.769312000
H	-5.478598000	0.065029000	-1.763968000	H	5.638175000	-0.123237000	1.850887000
H	-2.704792000	-2.149959000	1.732951000	H	2.916315000	-1.335378000	-2.143743000
C	-0.522888000	-3.072685000	0.031685000	C	0.855492000	-2.814761000	-0.815951000
H	1.343004000	-0.746430000	-1.242287000	H	-0.962672000	-1.298576000	1.415049000

H	-1.365011000	-3.620588000	-0.393658000	H	1.804692000	-3.349810000	-0.784099000
N	-2.680400000	0.297534000	-1.961072000	N	2.836049000	-0.075770000	2.102091000
H	-0.695748000	-2.988372000	1.115845000	H	0.823761000	-2.249490000	-1.763251000
O	-0.439077000	0.579496000	-2.342153000	O	0.593338000	0.158416000	2.499508000
H	-3.008212000	0.782753000	-2.781305000	H	3.154506000	0.238685000	3.005293000
H	-6.546631000	-1.208452000	0.081312000	H	6.736342000	-0.735087000	-0.293260000
H	-5.171560000	-2.303504000	1.813375000	H	5.385756000	-1.326648000	-2.271500000
C	0.825042000	-3.737550000	-0.237644000	C	-0.365324000	-3.733162000	-0.726790000
C	1.842295000	-2.580081000	-0.154072000	C	-1.431562000	-2.897764000	0.020449000
H	0.823915000	-4.163797000	-1.243052000	H	-0.120668000	-4.633255000	-0.160471000
H	1.037882000	-4.538587000	0.471327000	H	-0.695848000	-4.043518000	-1.718828000
H	2.622257000	-2.666185000	-0.910814000	H	-1.752550000	-3.406440000	0.930300000
H	2.351078000	-2.567331000	0.812423000	H	-2.317166000	-2.703146000	-0.578995000
C	-2.327430000	3.518030000	0.924972000	C	2.037173000	3.758089000	-0.396574000
C	-2.063731000	2.169851000	1.125183000	C	1.935125000	2.376219000	-0.453853000
C	-0.843303000	1.616538000	0.741152000	C	0.692100000	1.738069000	-0.445703000
C	0.122503000	2.447181000	0.177501000	C	-0.451062000	2.535666000	-0.380009000
C	-0.128885000	3.799812000	-0.025640000	C	-0.361482000	3.924389000	-0.335777000
C	-1.358749000	4.329028000	0.339534000	C	0.882324000	4.534377000	-0.346075000
H	-3.282229000	3.934521000	1.222617000	H	3.013247000	4.228196000	-0.401819000
H	-2.816992000	1.526711000	1.569288000	H	2.837054000	1.778581000	-0.526152000
C	-0.589036000	0.140626000	0.818241000	C	0.564025000	0.244430000	-0.616046000

H	0.644396000	4.416437000	-0.467952000	H	-1.276444000	4.502615000	-0.286804000
H	-1.556320000	5.382567000	0.178290000	H	0.950712000	5.615368000	-0.307735000
C	0.914141000	-0.267629000	0.804159000	C	-0.880023000	-0.310191000	-0.499856000
O	1.325283000	1.948275000	-0.211917000	O	-1.701301000	1.991139000	-0.374047000
H	-1.057264000	-0.237972000	1.732431000	H	0.915443000	0.025928000	-1.630833000
C	1.148490000	-0.927698000	2.151290000	C	-1.419970000	-0.554383000	-1.904048000
O	1.931636000	-0.566907000	2.992456000	O	-2.448185000	-1.120153000	-2.170475000
H	0.486892000	-1.792962000	2.353041000	H	-0.789531000	-0.147732000	-2.722156000
C	3.217347000	0.552387000	0.066456000	C	-1.778376000	0.714079000	0.251441000
C	4.209333000	0.036926000	0.898865000	H	-1.346948000	0.801070000	1.254532000
C	3.470867000	0.667551000	-1.299828000	C	-3.234884000	0.338367000	0.371375000
C	5.427279000	-0.375790000	0.371044000	C	-3.660599000	-0.455724000	1.434866000
H	4.021509000	-0.046640000	1.962374000	C	-4.173577000	0.781793000	-0.558445000
C	4.689819000	0.257297000	-1.826242000	C	-4.994534000	-0.829575000	1.549272000
H	2.707353000	1.081119000	-1.946944000	H	-2.951576000	-0.779001000	2.189098000
C	5.670441000	-0.270662000	-0.993662000	C	-5.508662000	0.419810000	-0.438128000
H	6.189409000	-0.775914000	1.030223000	H	-3.855427000	1.414591000	-1.377234000
H	4.872837000	0.350703000	-2.890806000	C	-5.922633000	-0.394315000	0.610942000
H	6.620430000	-0.592316000	-1.405148000	H	-5.309055000	-1.450173000	2.380532000
C	1.870328000	0.940564000	0.637690000	H	-6.228289000	0.772710000	-1.168192000
H	2.018044000	1.381902000	1.628758000	H	-6.964638000	-0.679131000	0.701926000

4. Molecular docking studies of **16(a-k)** and **16'(a-f)** derivatives with *E. coli* DNA gyrase (PDB ID: 1KZN)

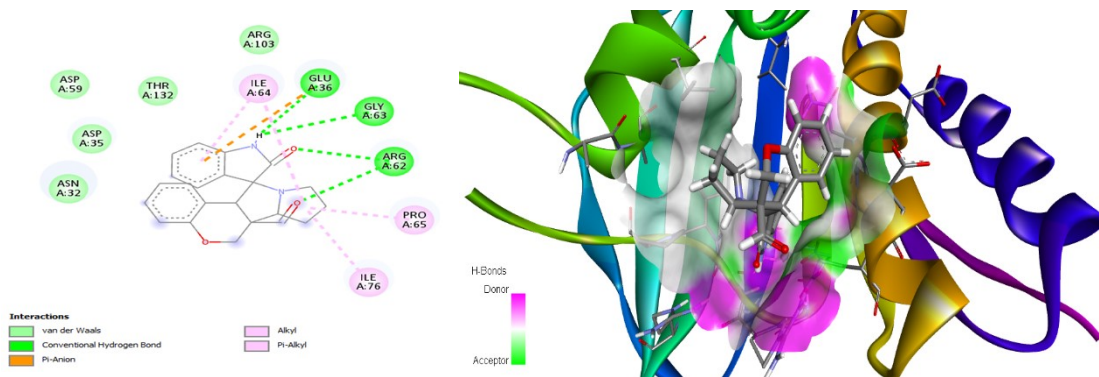


Fig. S61. Docking interaction and 3D binding image of compound **16a** with *E. coli* DNA gyrase (PDB ID: 1KZN)

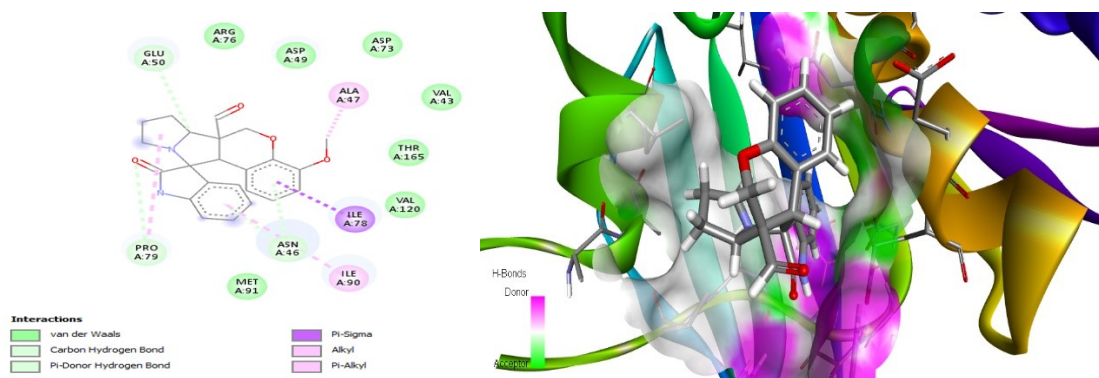


Fig. S62. Docking interaction and 3D binding image of compound **16b** with *E. coli* DNA gyrase (PDB ID: 1KZN)

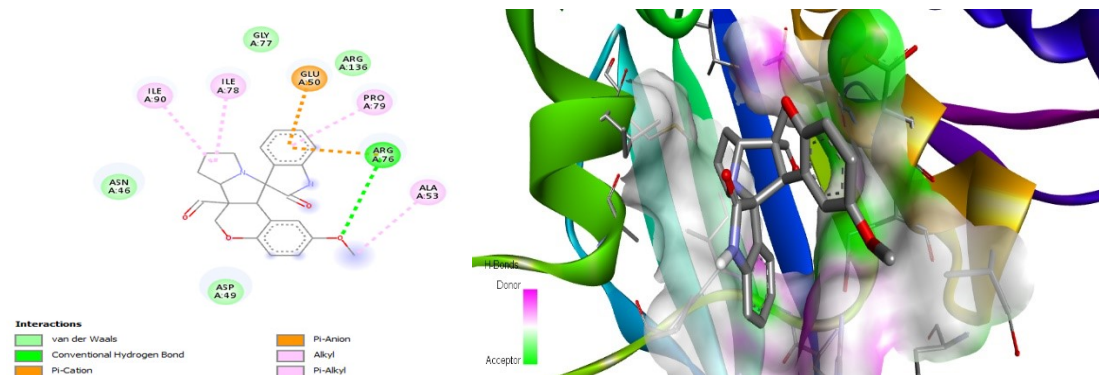


Fig. S63. Docking interaction and 3D binding image of compound 16c with *E. coli* DNA gyrase (PDB ID: 1KZN)

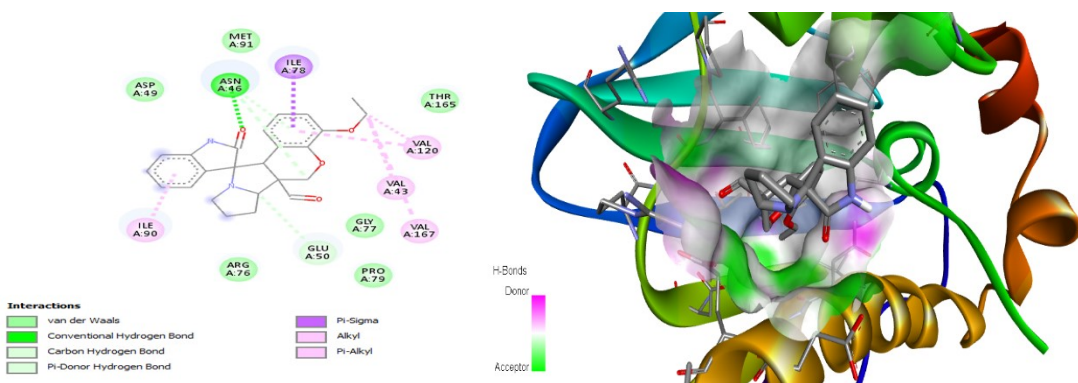


Fig. S64. Docking interaction and 3D binding image of compound 16d with *E. coli* DNA gyrase (PDB ID: 1KZN)

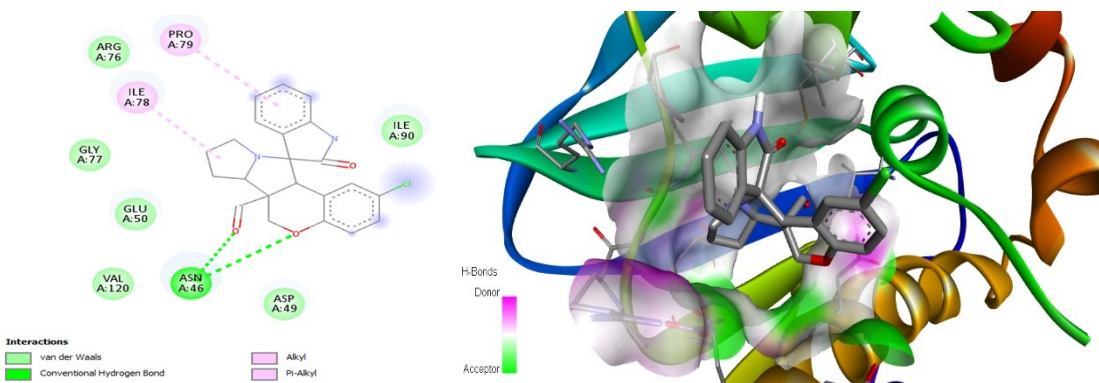


Fig. S65. Docking interaction and 3D binding image of compound **16e** with *E. coli* DNA gyrase (PDB ID: 1KZN)

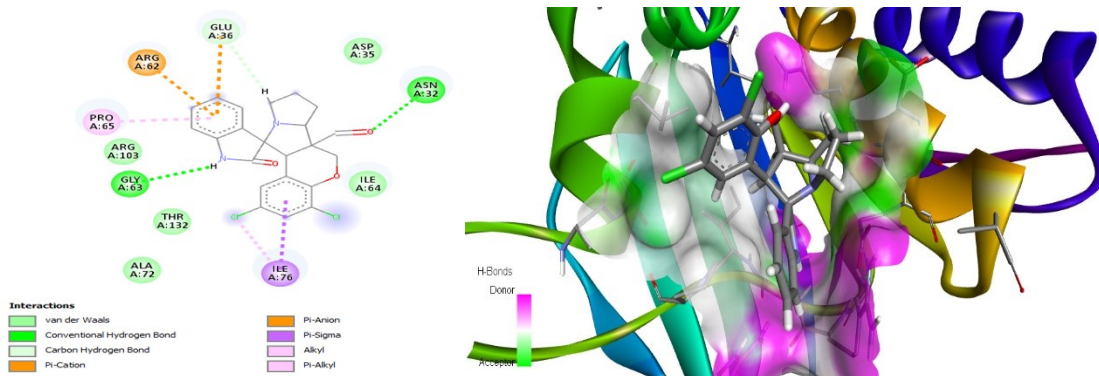


Fig. S66. Docking interaction and 3D binding image of compound **16f** with *E. coli* DNA gyrase (PDB ID: 1KZN)

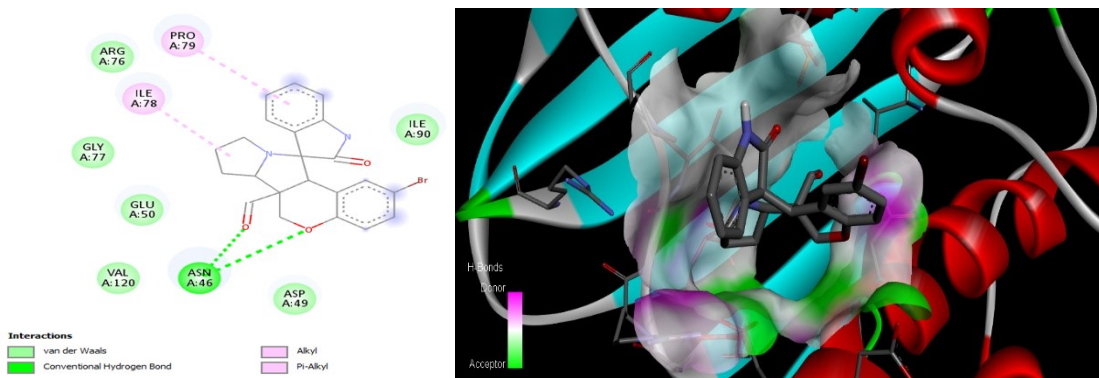


Fig. S67. Docking interaction and 3D binding image of compound **16g** with *E. coli* DNA gyrase (PDB ID: 1KZN)

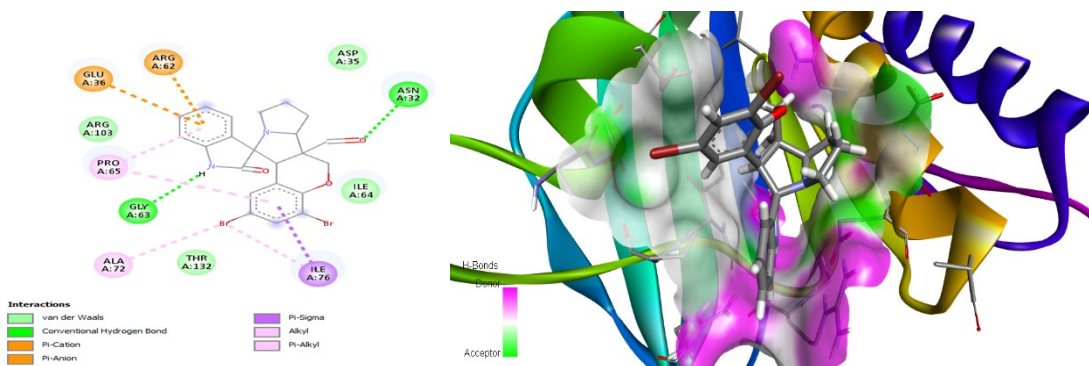


Fig. S68. Docking interaction and 3D binding image of compound **16h** with *E. coli* DNA gyrase (PDB ID: 1KZN)

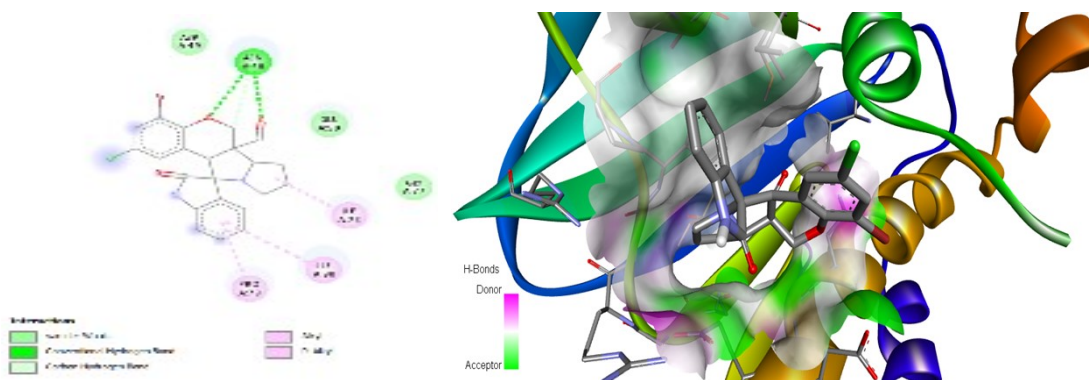


Fig. S69. Docking interaction and 3D binding image of compound **16i** with *E. coli* DNA gyrase (PDB ID: 1KZN)

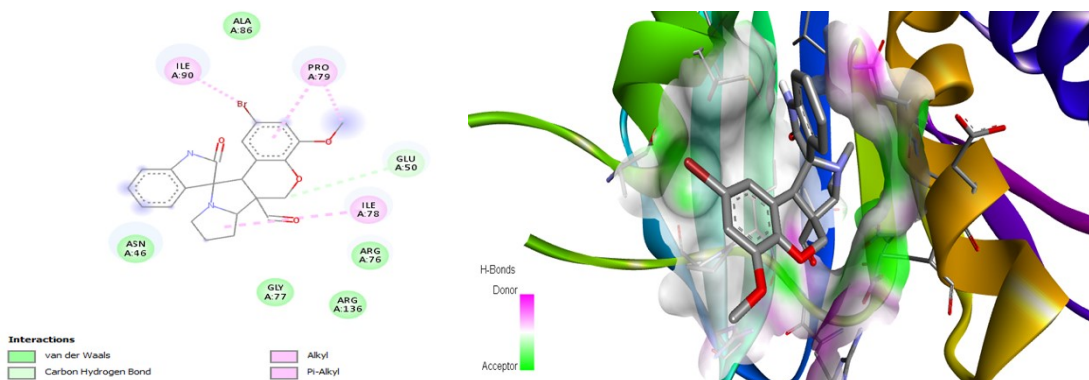


Fig. S70. Docking interaction and 3D binding image of compound **16j** with *E. coli* DNA gyrase (PDB ID: 1KZN)

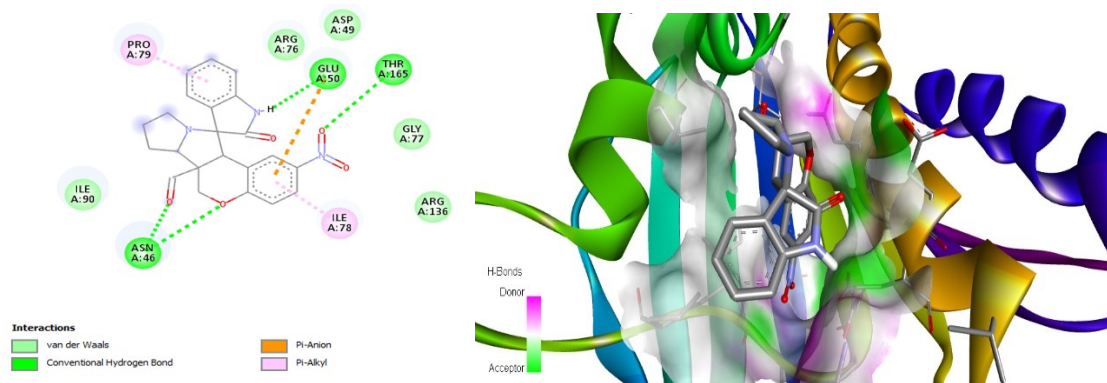


Fig. S71. Docking interaction and 3D binding image of compound **16k** with *E. coli* DNA gyrase (PDB ID: 1KZN)

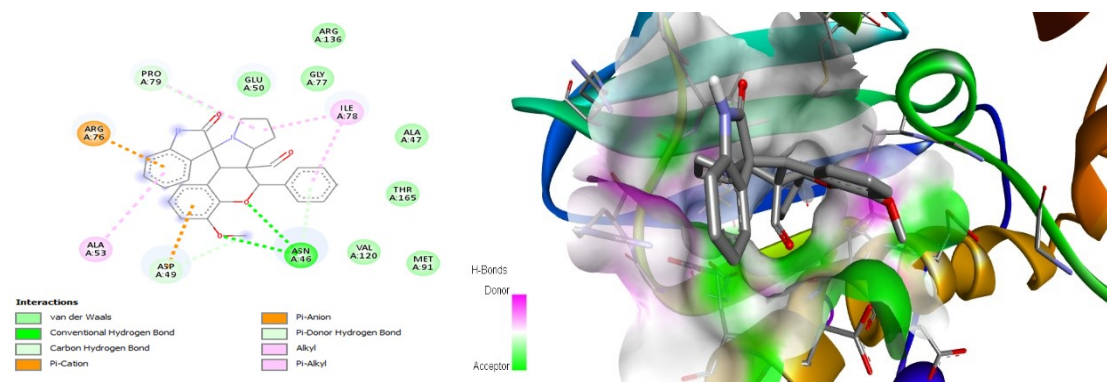


Fig. S72. Docking interaction and 3D binding image of compound **16'a** with *E. coli* DNA gyrase (PDB ID: 1KZN)

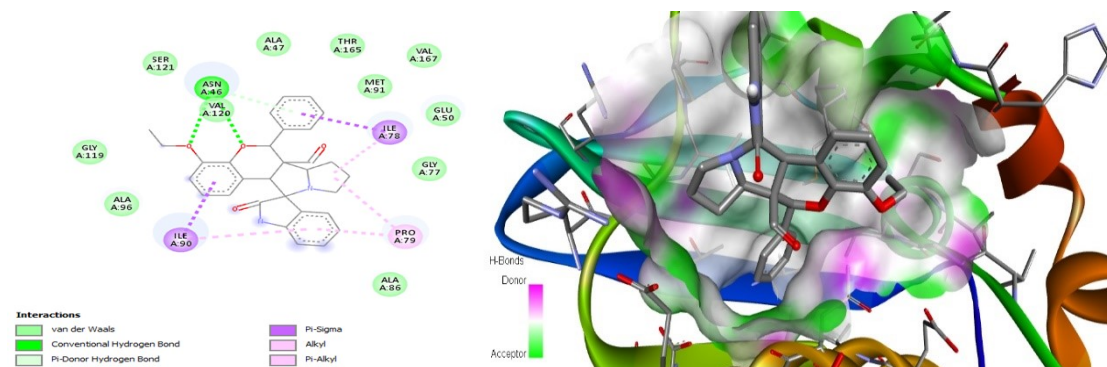


Fig. S73. Docking interaction and 3D binding image of compound **16'b** with *E. coli* DNA gyrase (PDB ID: 1KZN)

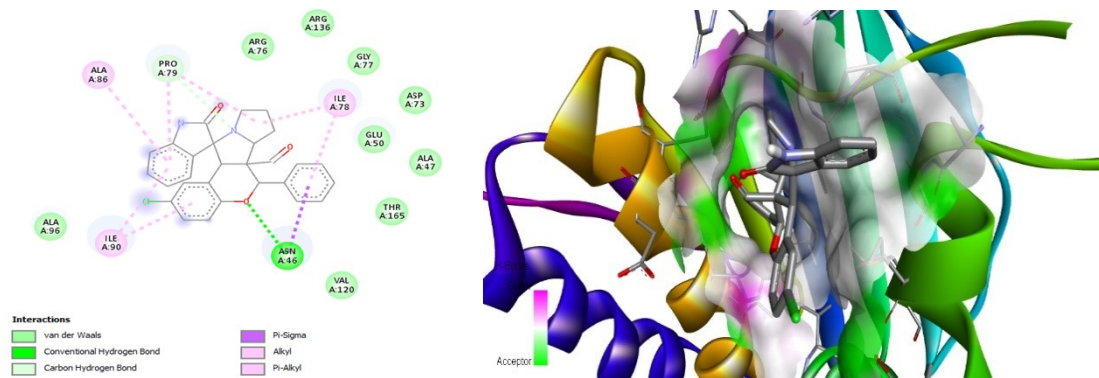


Fig. S74. Docking interaction and 3D binding image of compound **16'c** with *E. coli* DNA gyrase (PDB ID: 1KZN)

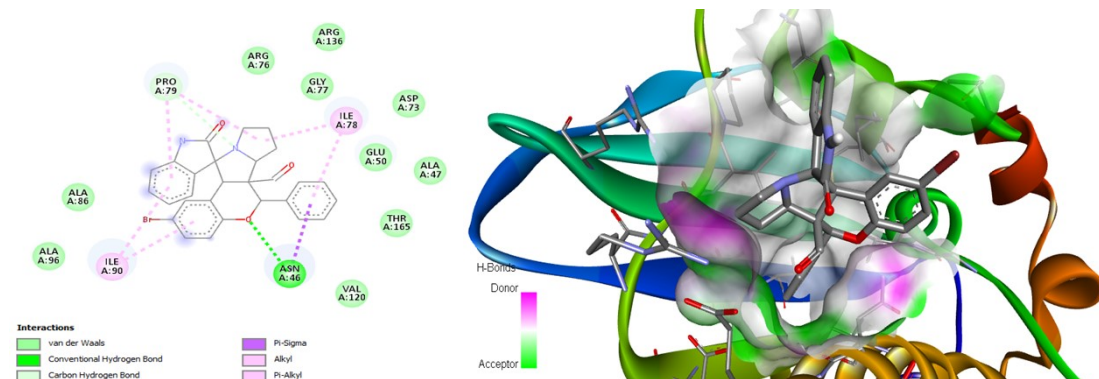


Fig. S75. Docking interaction and 3D binding image of compound **16'd** with *E. coli* DNA gyrase (PDB ID: 1KZN)

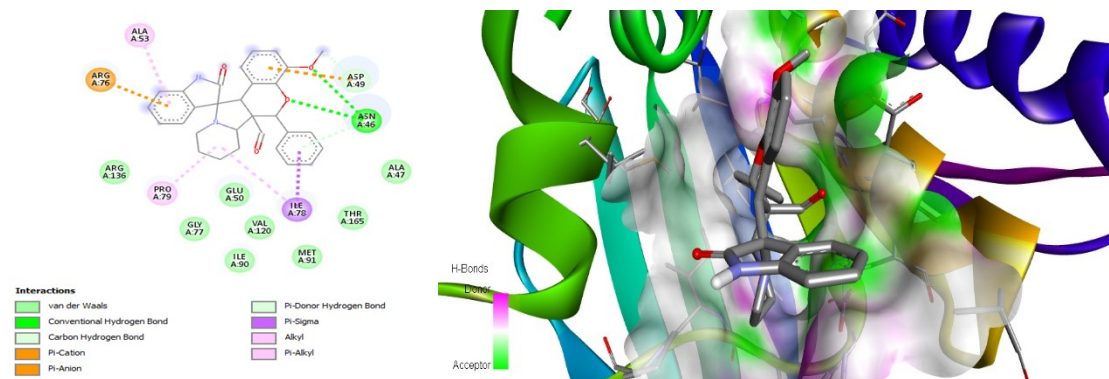


Fig. S76. Docking interaction and 3D binding image of compound **16'e** with *E. coli* DNA gyrase (PDB ID: 1KZN)

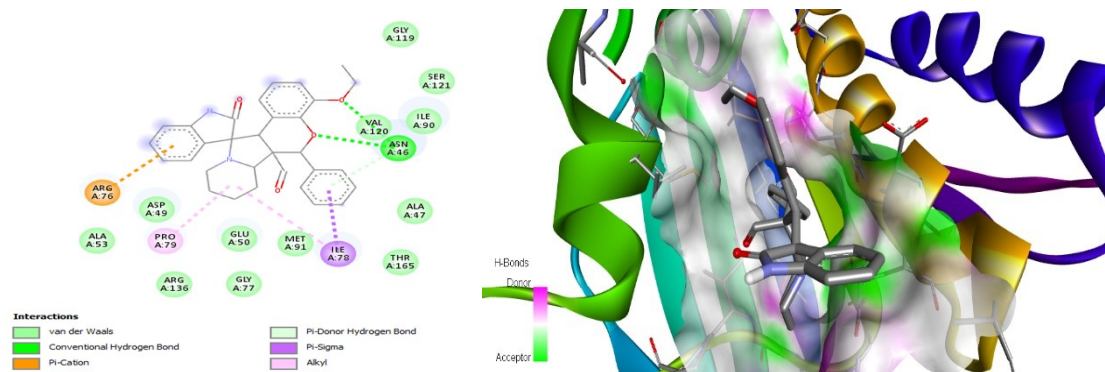


Fig. S77. Docking interaction and 3D binding image of compound **16'f** with *E. coli* DNA gyrase (PDB ID: 1KZN)

5. Molecular docking studies of **16(a-k) and **16'(a-f)** derivatives with *S. aureus* DNA gyrase (PDB ID: 3G7B)**

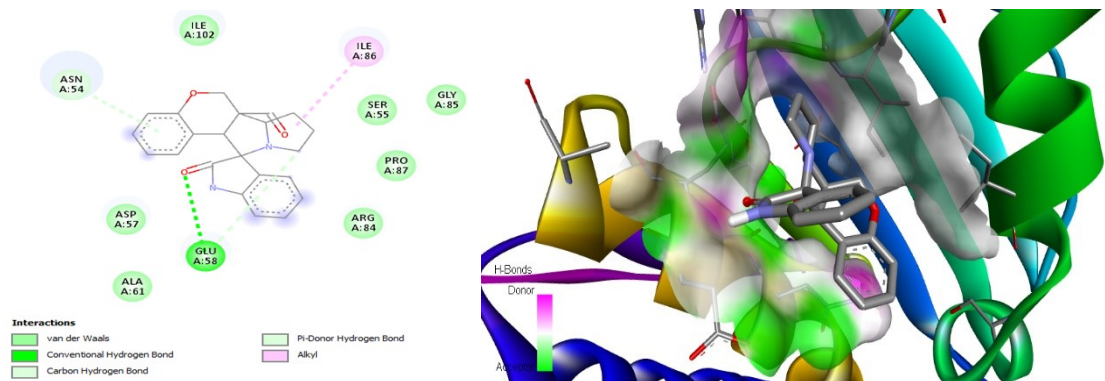


Fig. S78. Docking interaction and 3D binding image of compound **16a** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

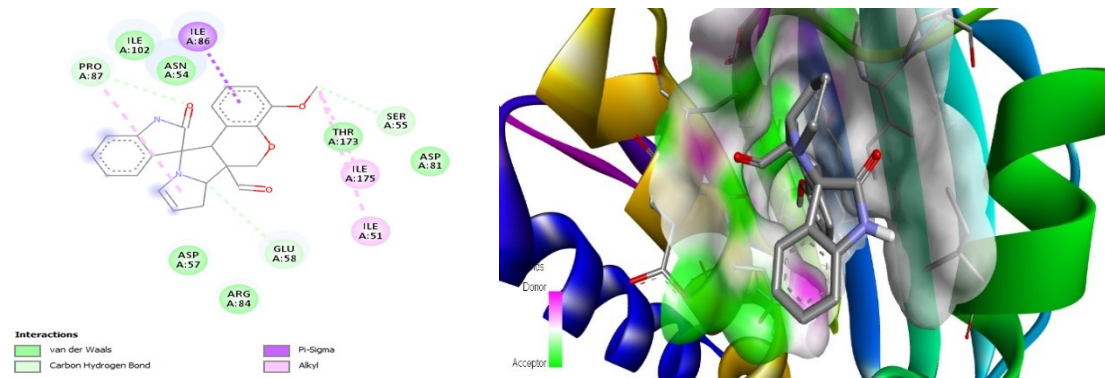


Fig. S79. Docking interaction and 3D binding image of compound **16b** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

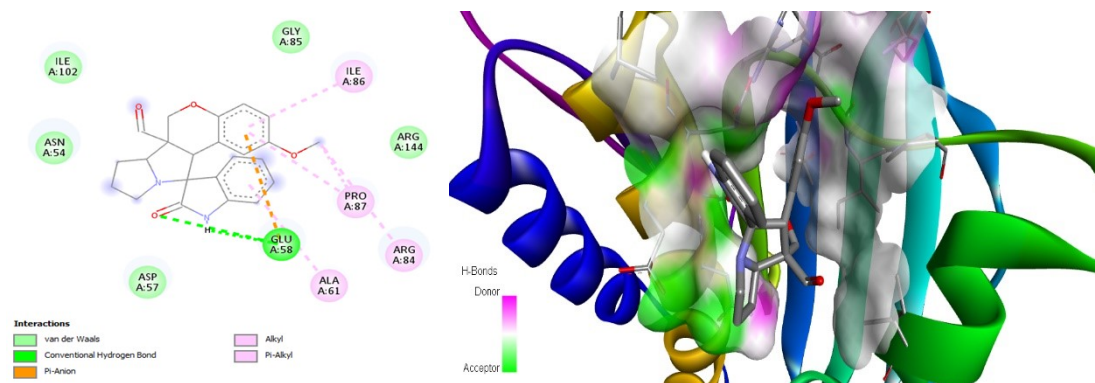


Fig. S80. Docking interaction and 3D binding image of compound **16c** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

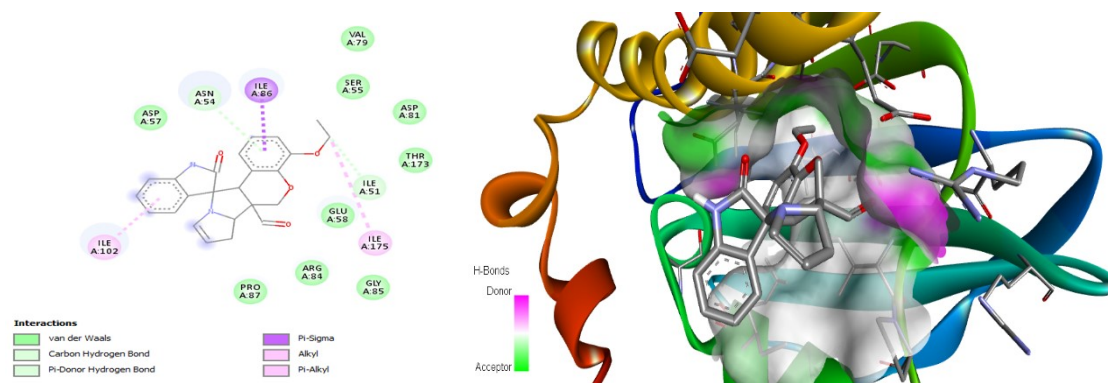


Fig. S81. Docking interaction and 3D binding image of compound **16d** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

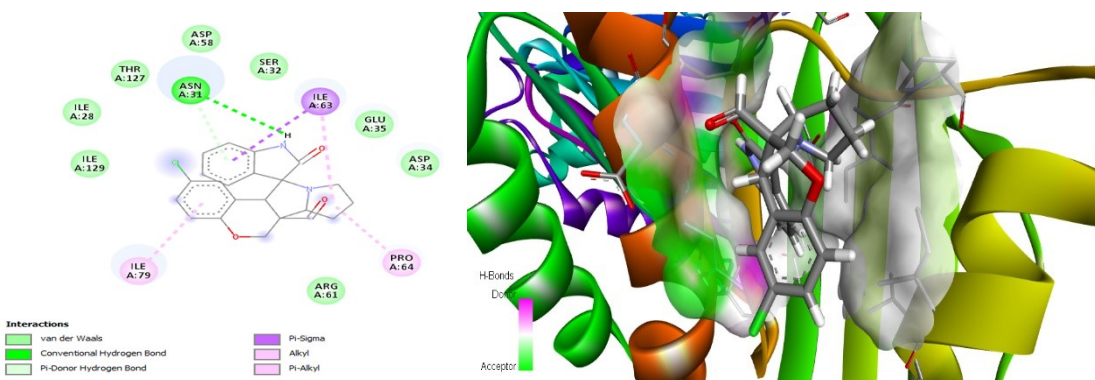


Fig. S82. Docking interaction and 3D binding image of compound **16e** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

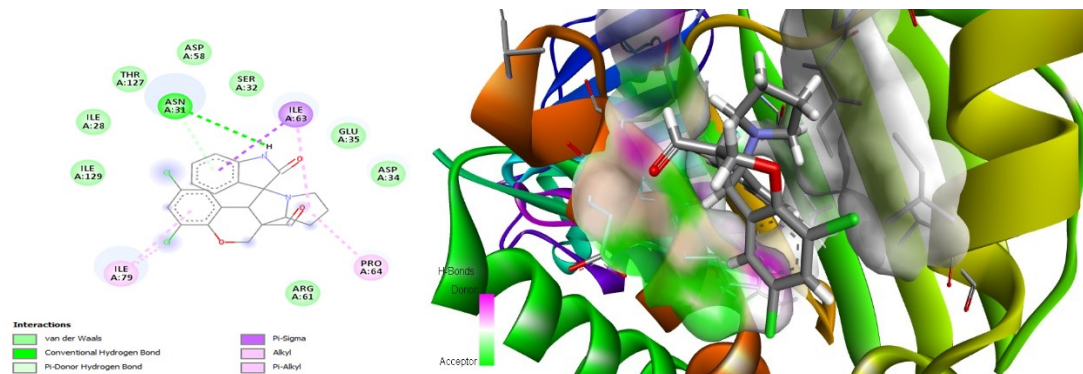


Fig. S83. Docking interaction and 3D binding image of compound **16f** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

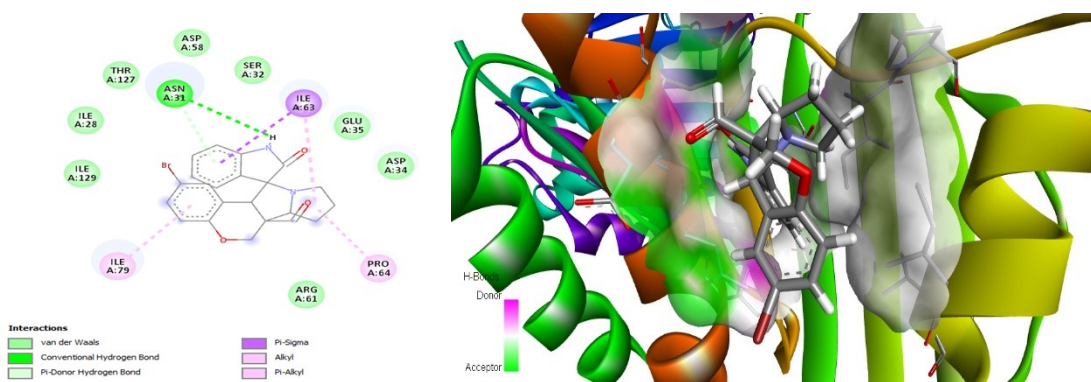


Fig. S84. Docking interaction and 3D binding image of compound **16g** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

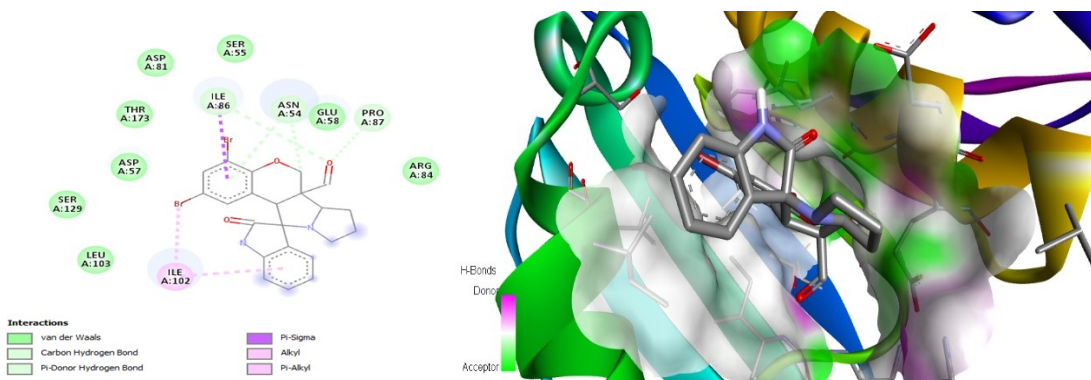


Fig. S85. Docking interaction and 3D binding image of compound **16h** with *S. aureus DNA gyrase* (PDB ID: 3G7B)

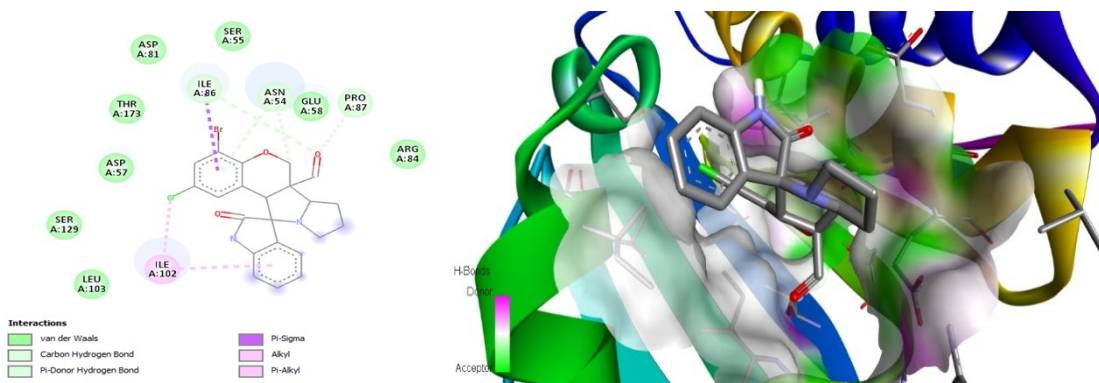


Fig. S86. Docking interaction and 3D binding image of compound **16i** with *S. aureus DNA gyrase* (PDB ID: 3G7B)

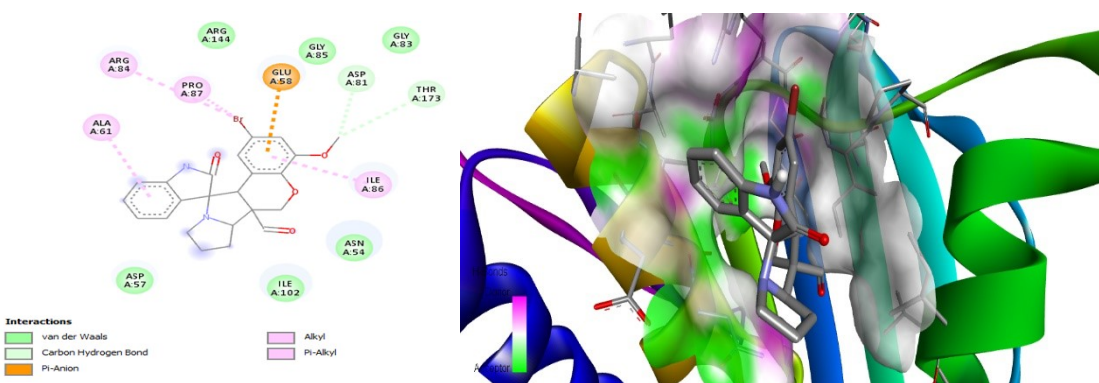


Fig. S87. Docking interaction and 3D binding image of compound **16j** with *S. aureus DNA gyrase* (PDB ID: 3G7B)

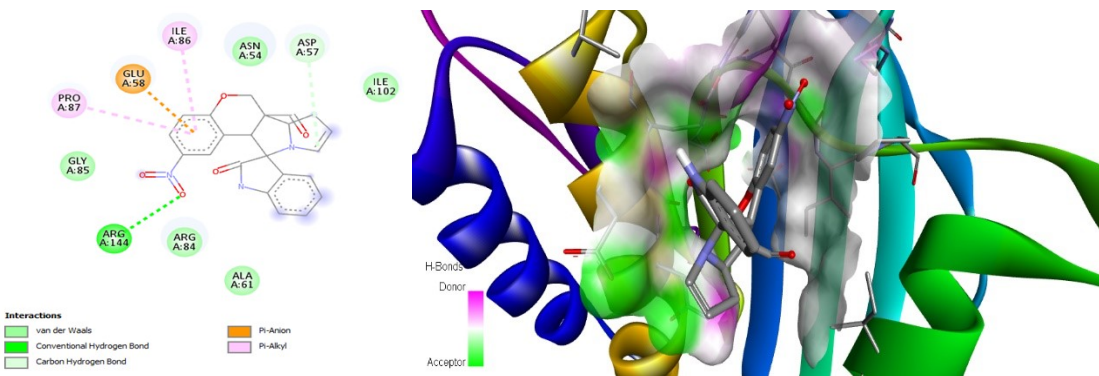


Fig. S88. Docking interaction and 3D binding image of compound **16k** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

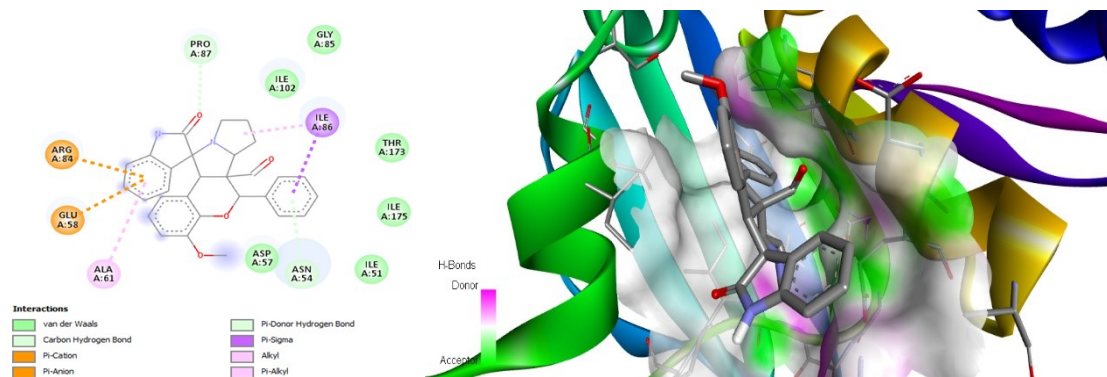


Fig. S89. Docking interaction and 3D binding image of compound **16'a** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

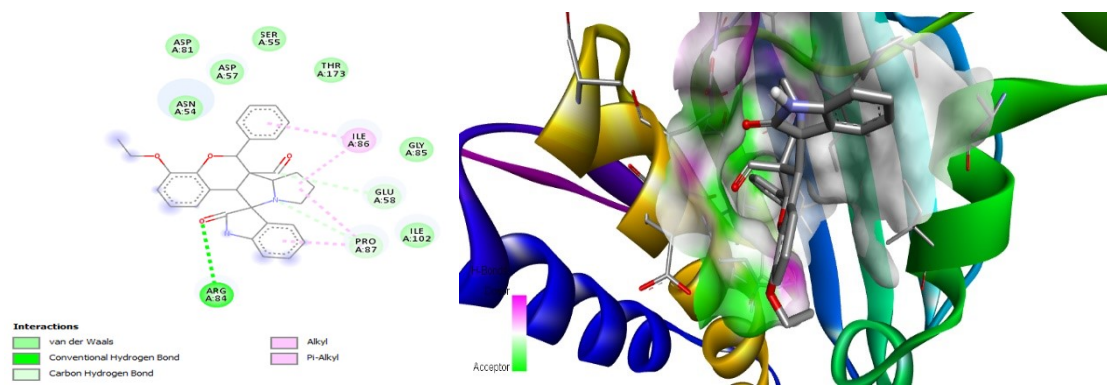


Fig. S90. Docking interaction and 3D binding image of compound **16'b** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

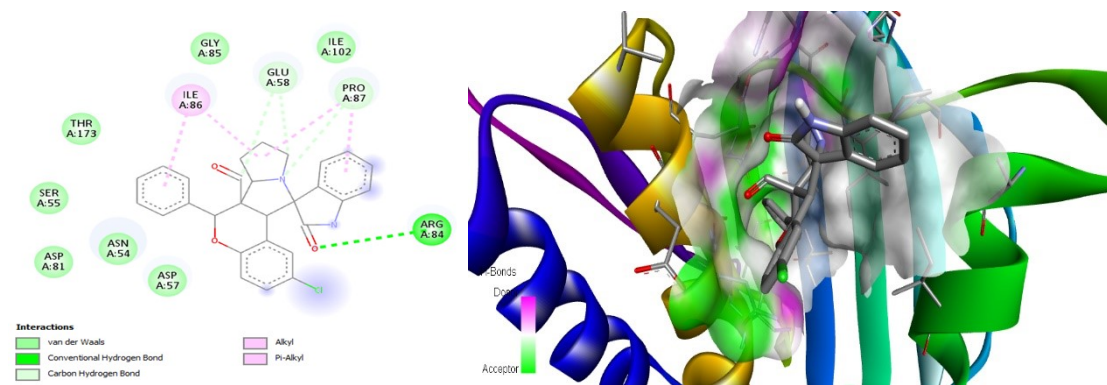


Fig. S91. Docking interaction and 3D binding image of compound **16'c** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

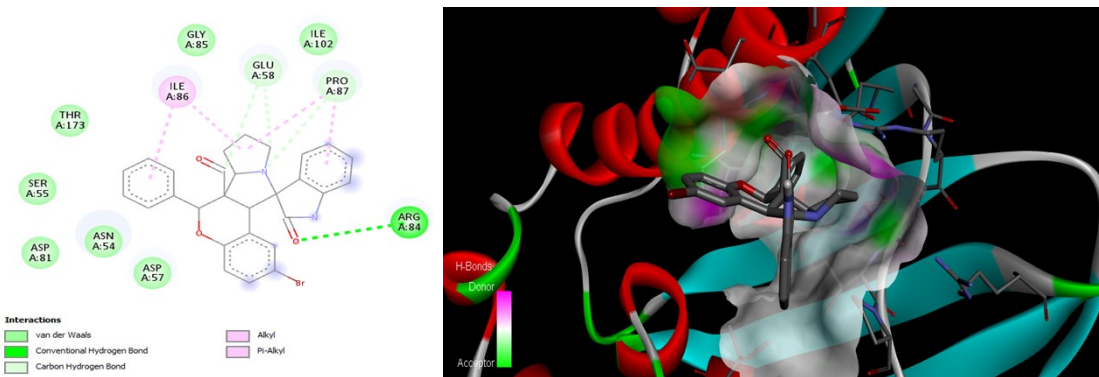


Fig. S92. Docking interaction and 3D binding image of compound **16'd** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

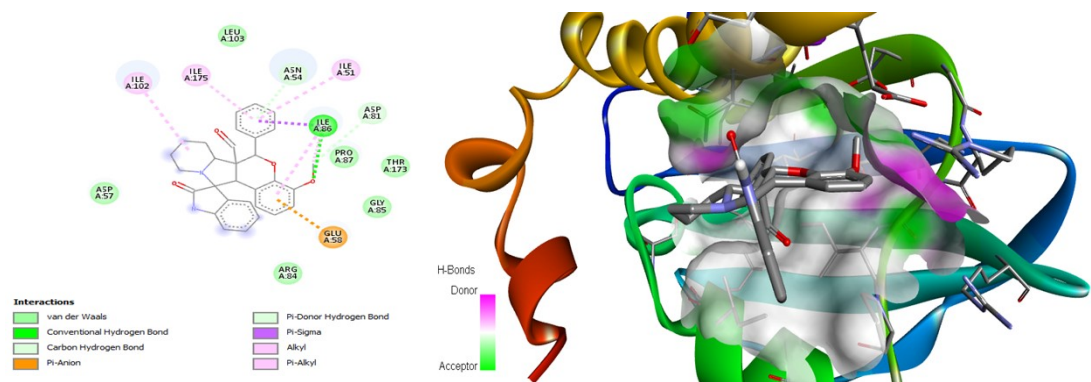


Fig. S93. Docking interaction and 3D binding image of compound **16'e** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

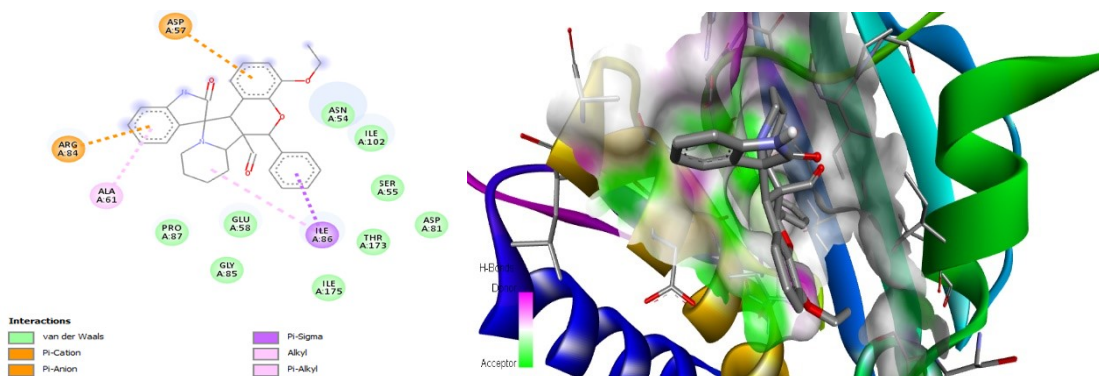


Fig. S94. Docking interaction and 3D binding image of compound **16'f** with *S. aureus* DNA gyrase (PDB ID: 3G7B)

6. Bioavailability radar plots of Ciprofloxacin and **16(a-k)** and **16'(a-f)** derivatives

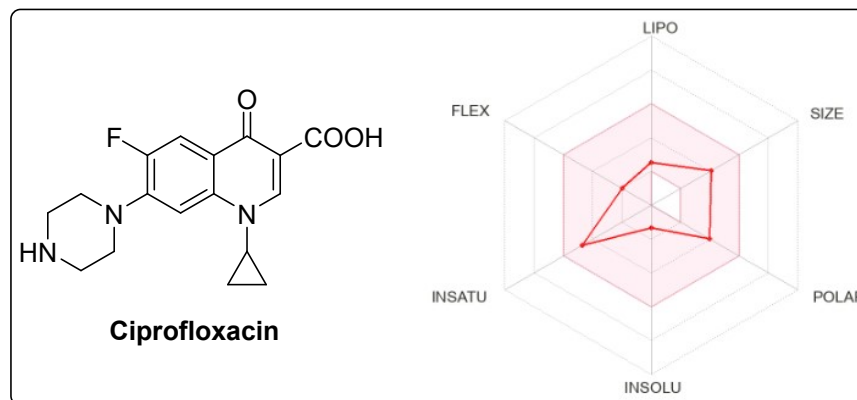


Fig S95. Bioavailability radar plot of Ciprofloxacin

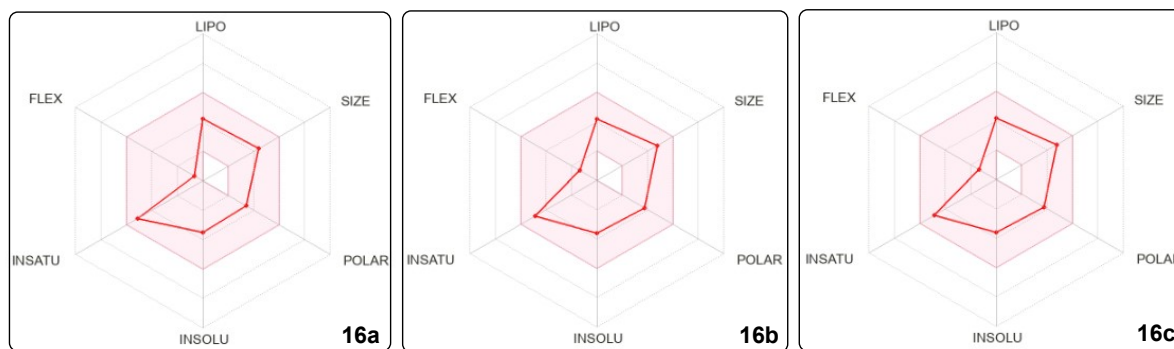


Fig S96. Bioavailability radar plot of **16(a-c)**

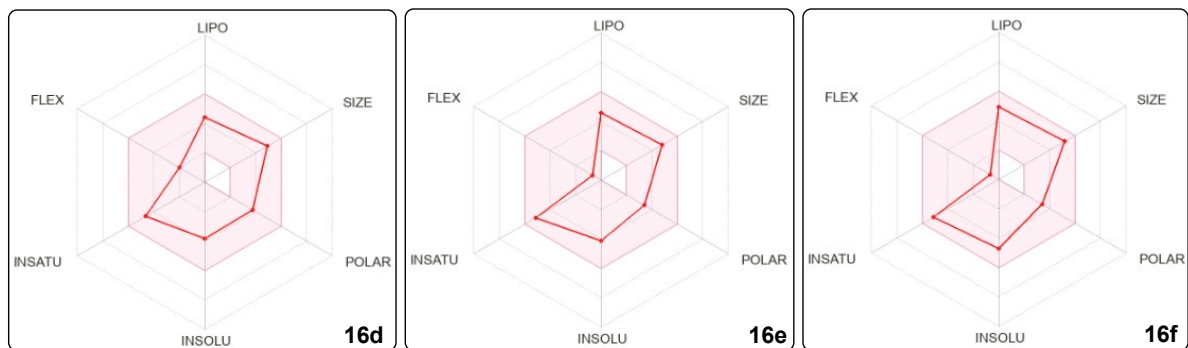


Fig S97. Bioavailability radar plot of **16(d-f)**

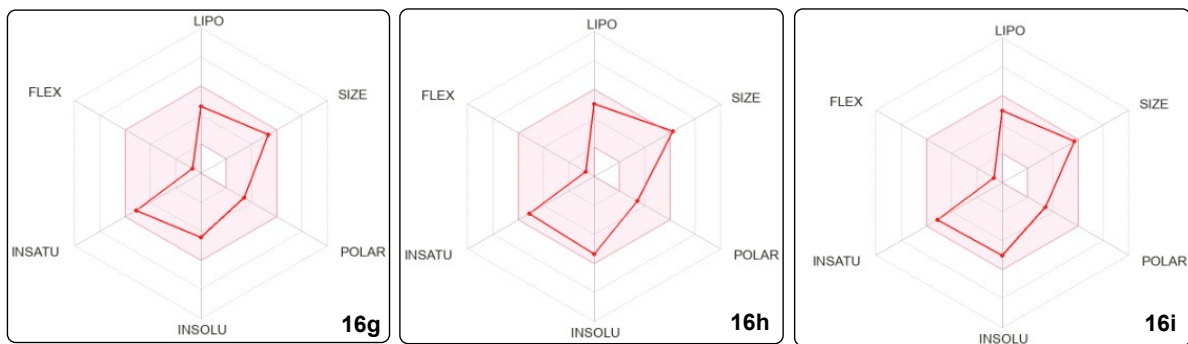


Fig S98. Bioavailability radar plot of **16(g-i)**

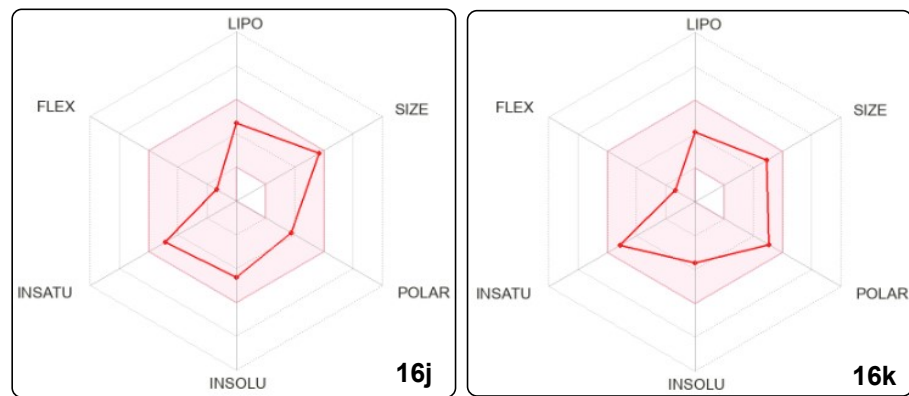


Fig S99. Bioavailability radar plot of **16(j-k)**

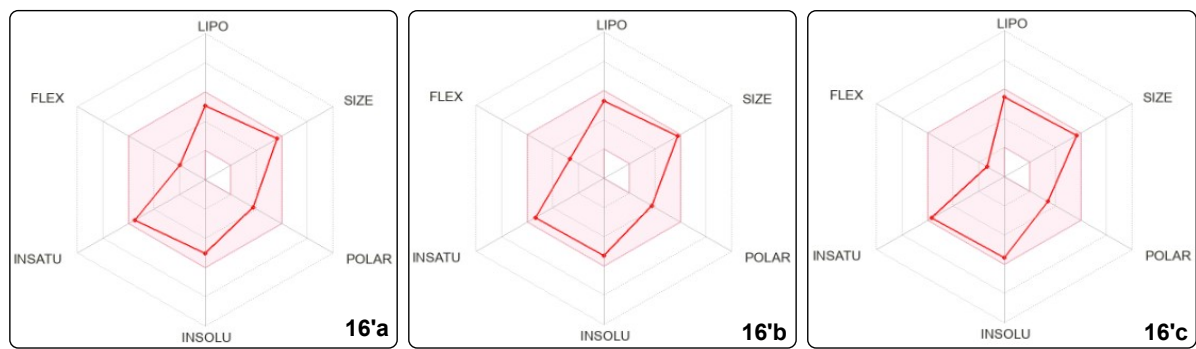


Fig S100. Bioavailability radar plot of **16'(a-c)**

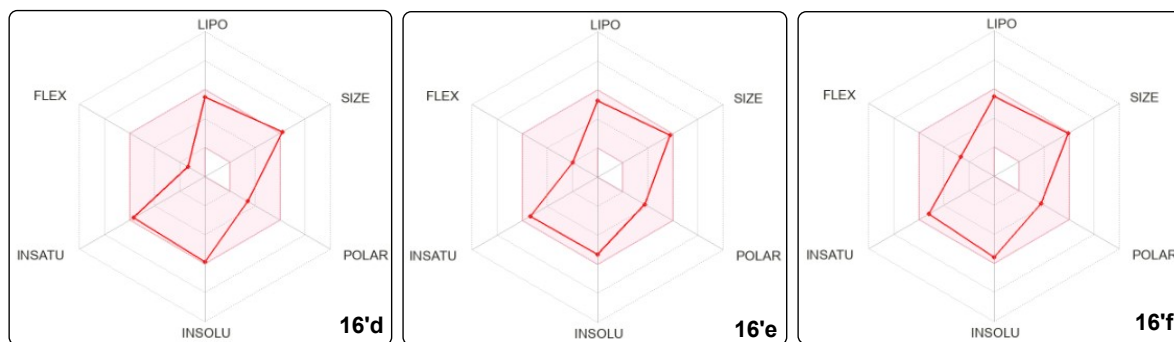


Fig S101. Bioavailability radar plot of 16'(d-f)

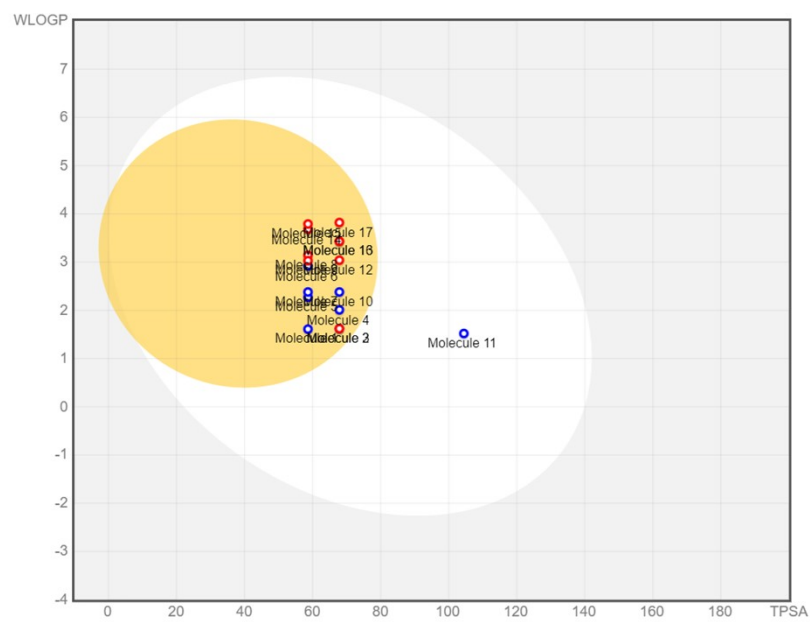


Fig S102. Plot of TPSA with WLOGP

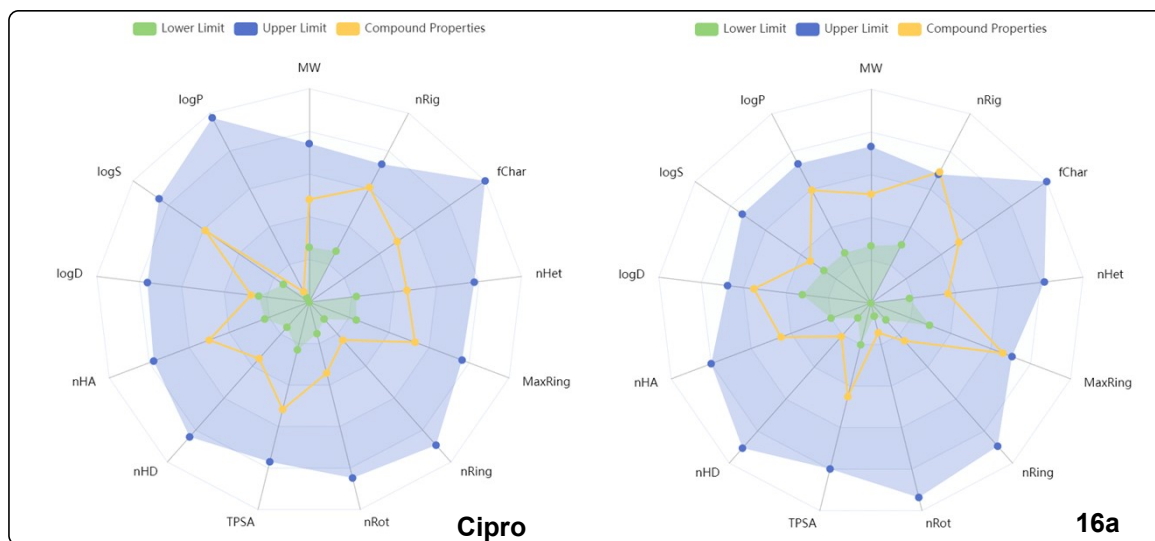


Fig. 103. Radar chart of the physicochemical properties of Ciprofloxacin and **16a** showing the *in-silico* measurements of the descriptors MW, nRig, fChar, nHet, MaxRig, nRing, nRot, TPSA, nHD, nHA, LogD, LogS, LogP.