Electronic Supplementary Material (ESI) for ChemComm.

KO^{t}Bu-Mediated annulation of acetonitrile with aldehyde: synthesis of substituted dihydropyridin-2(1*H*)-ones, pyridin-2(1*H*)-ones, and thiopyridin-2(1*H*)-ones

Abhimanyu Yadav, Ajay Verma, Saket Patel, Amit Kumar, Vandana Rathore, Meenakshi, Shailesh Kumar and Sangit Kumar*

Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal, Indore By-pass Road, Bhauri, Bhopal, Madhya Pradesh, India, Pin: 462 066

*E-mail: *sangitkumar@iiserb.ac.in*

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Figure S1 ^{1}H NMR spectra of **1**

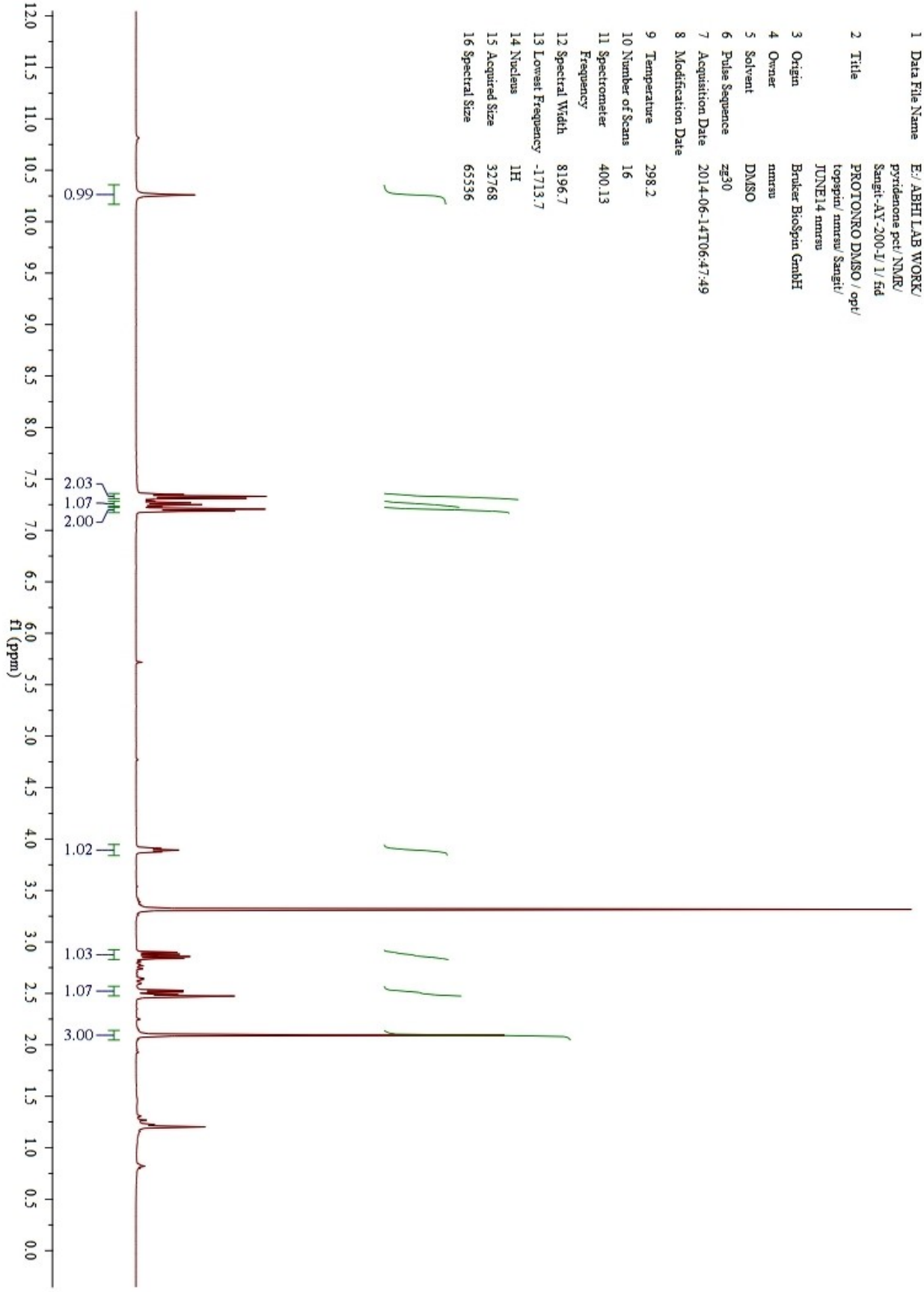


Figure S2 ^{13}C NMR spectra of **1**

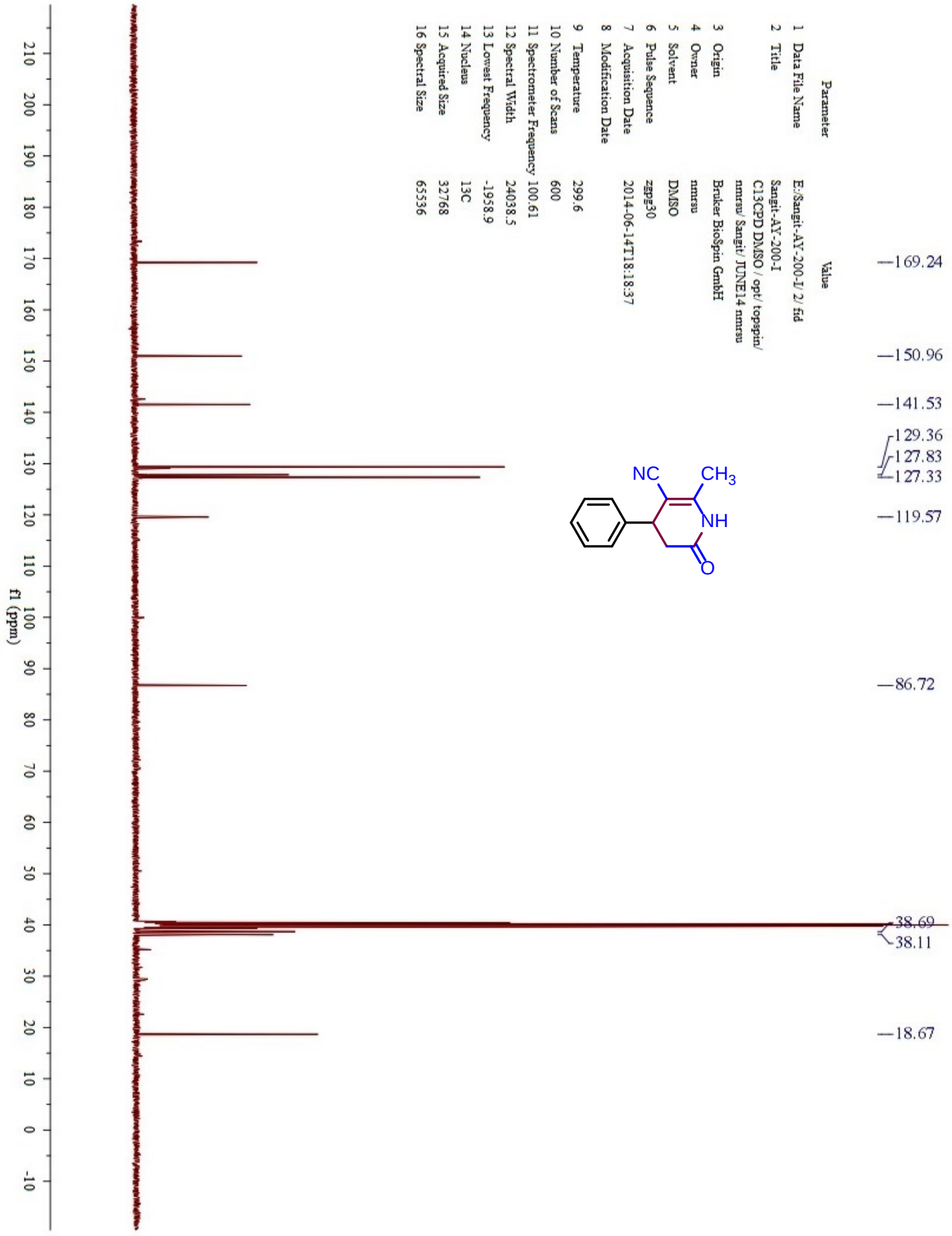


Figure S3 135-DEPT spectra NMR of **1**

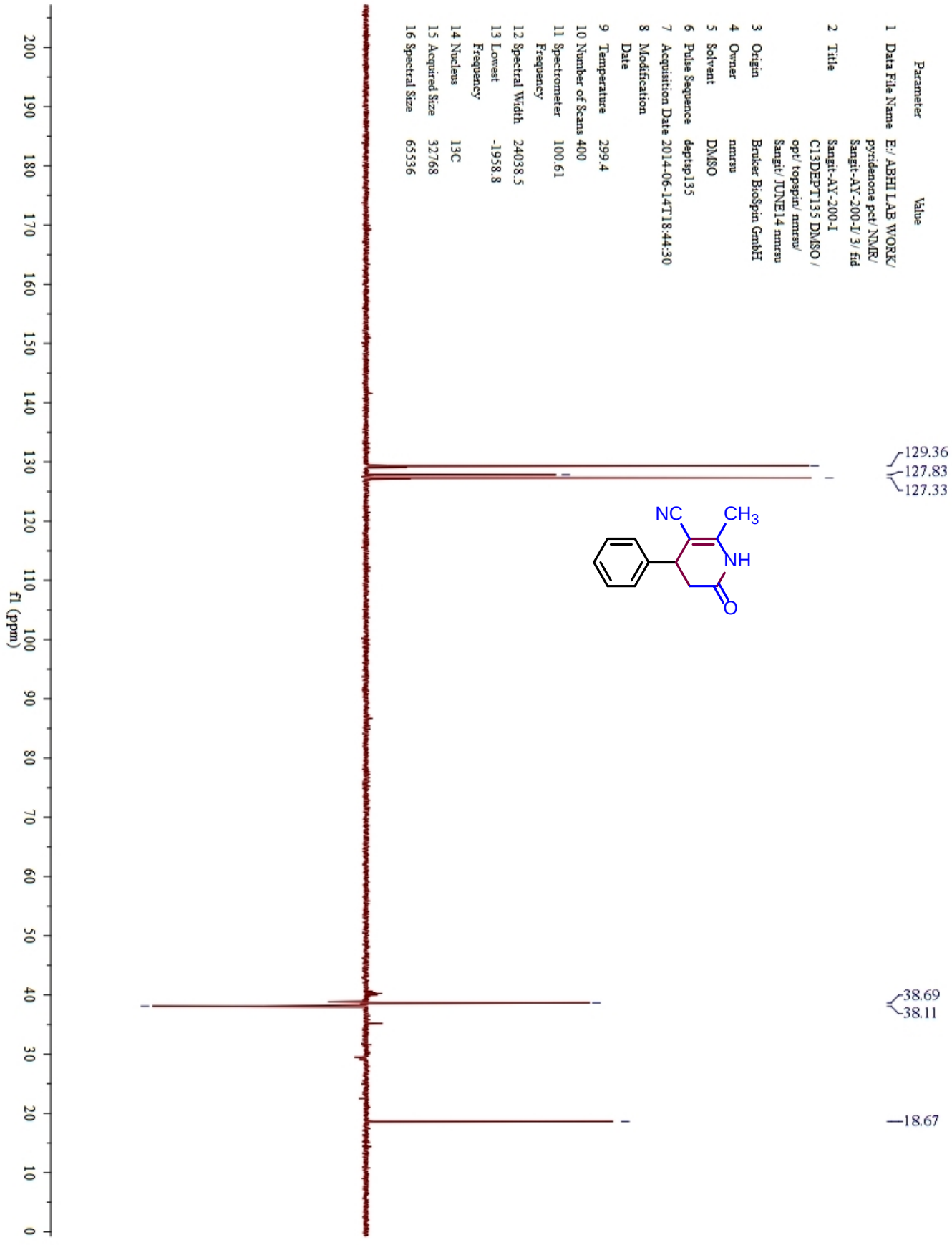


Figure S4 HRMS spectra of **1**

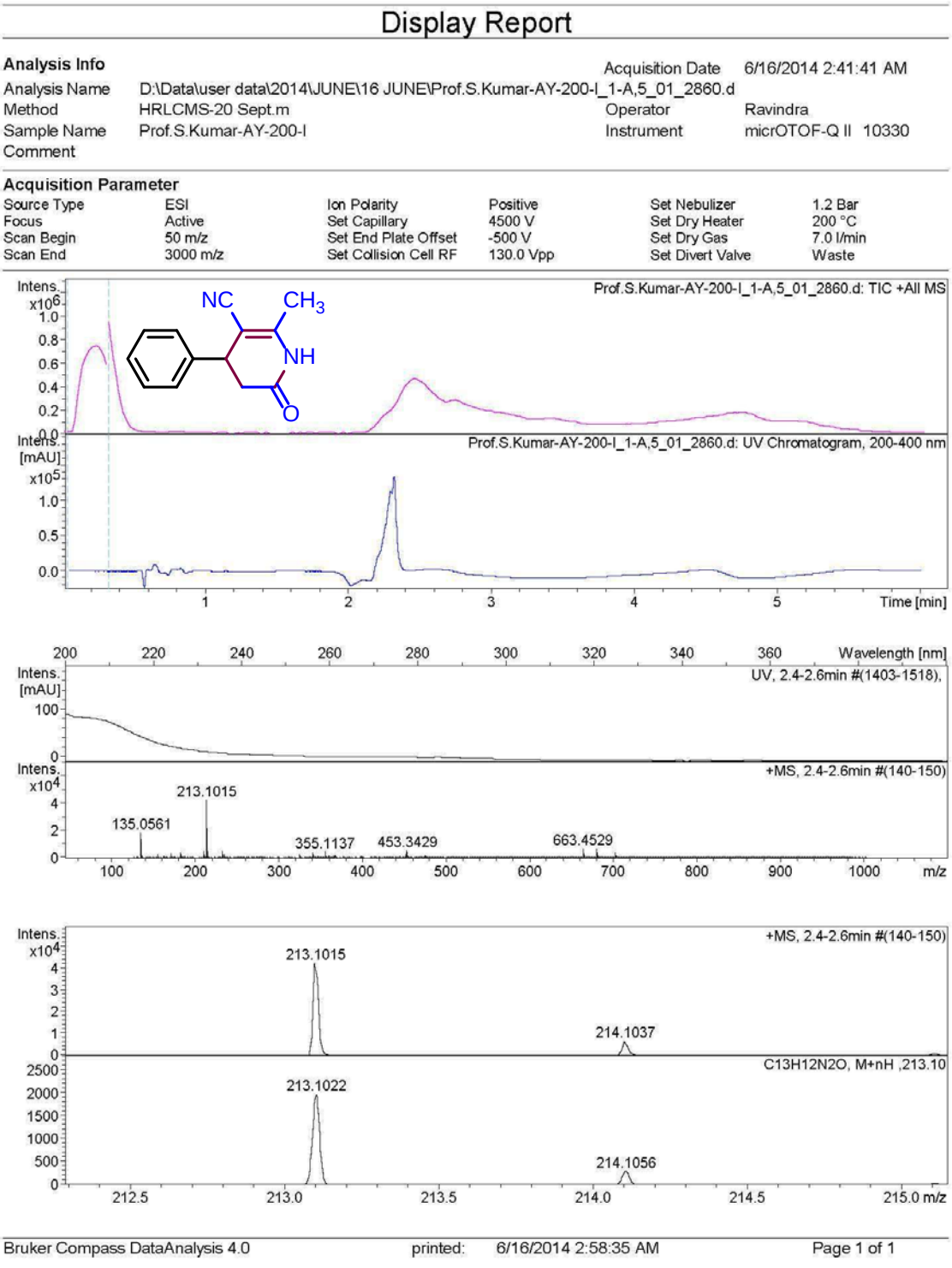
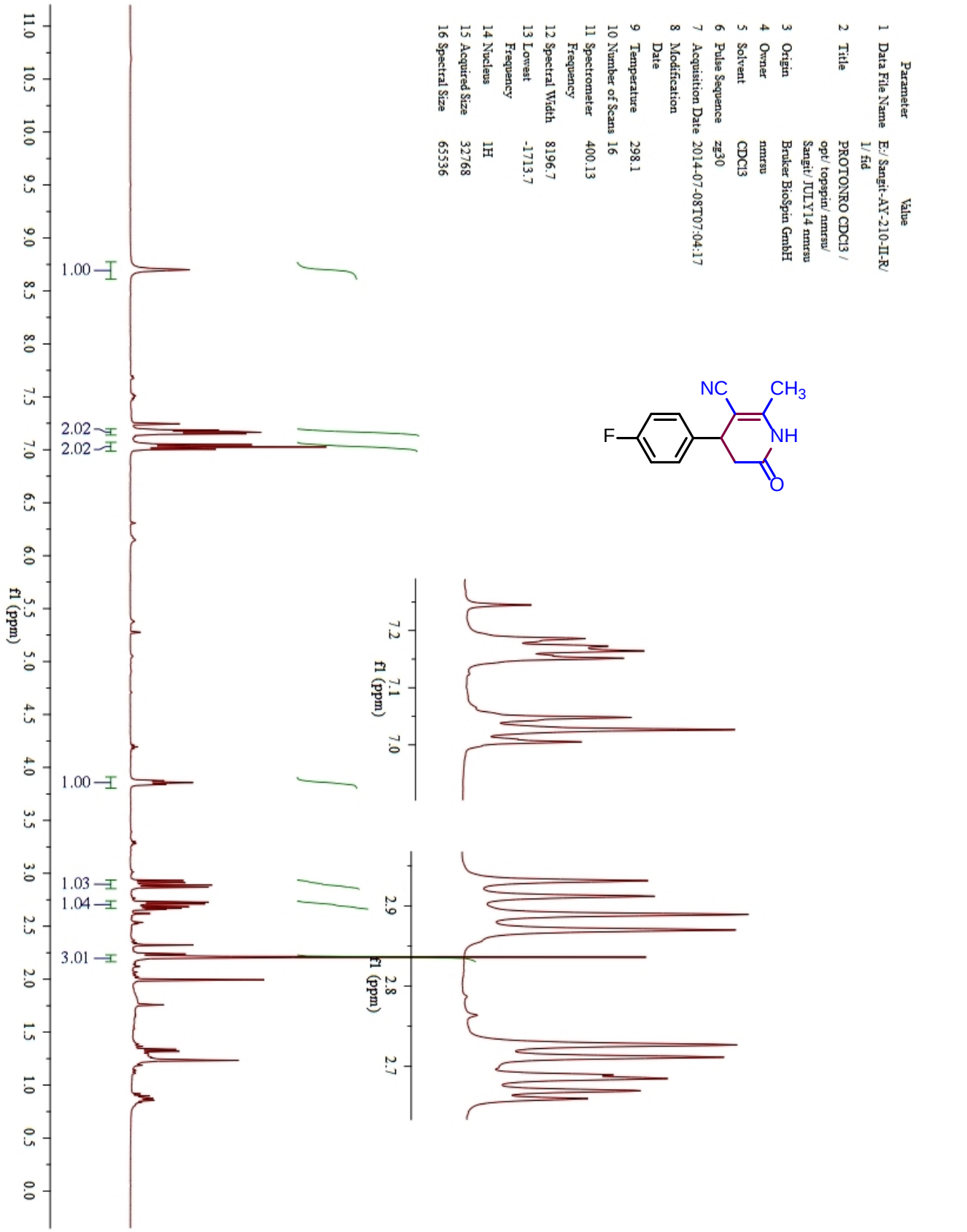


Figure S5 ^{1}H NMR spectra of **3**



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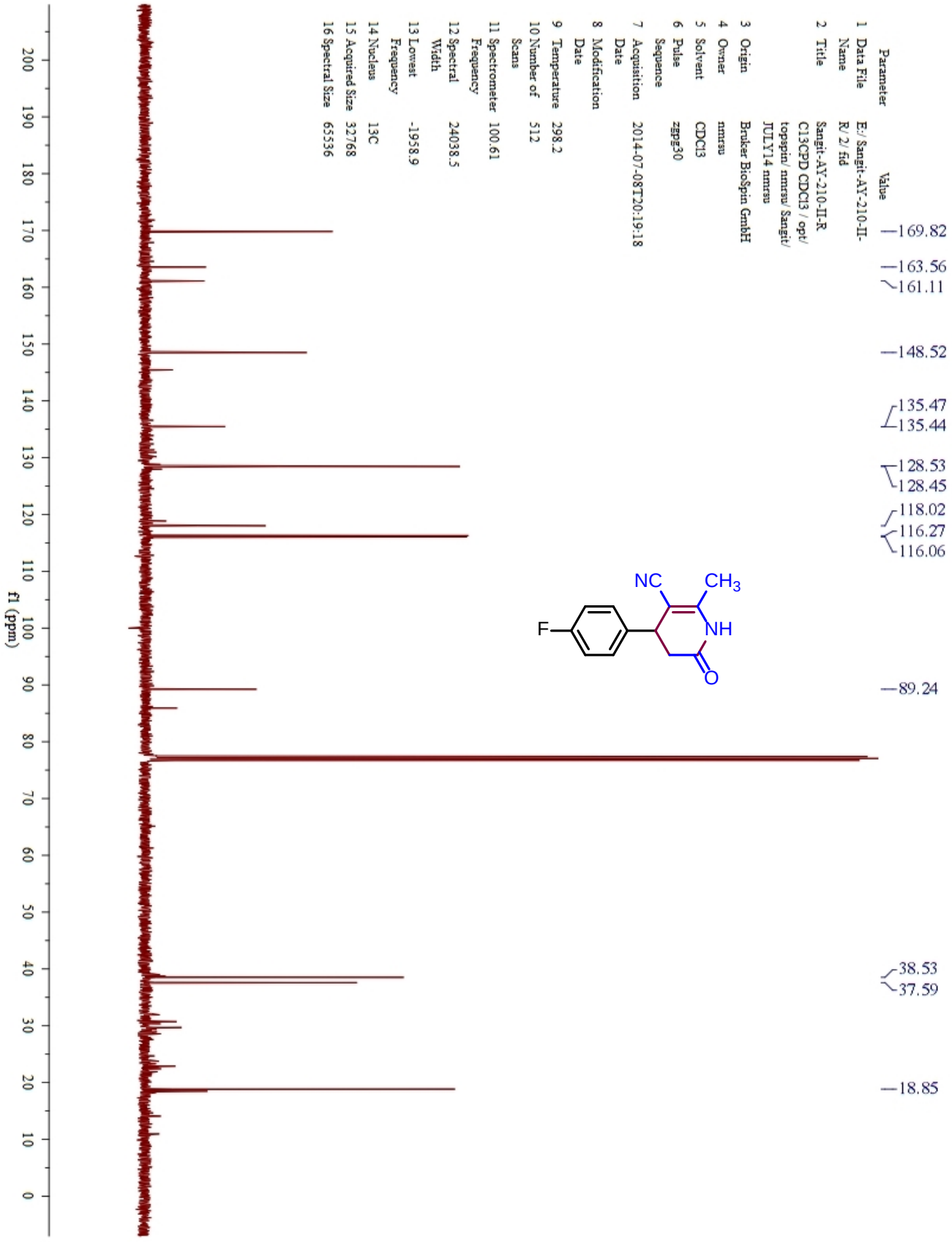


Figure S7 HRMS spectra of **3**

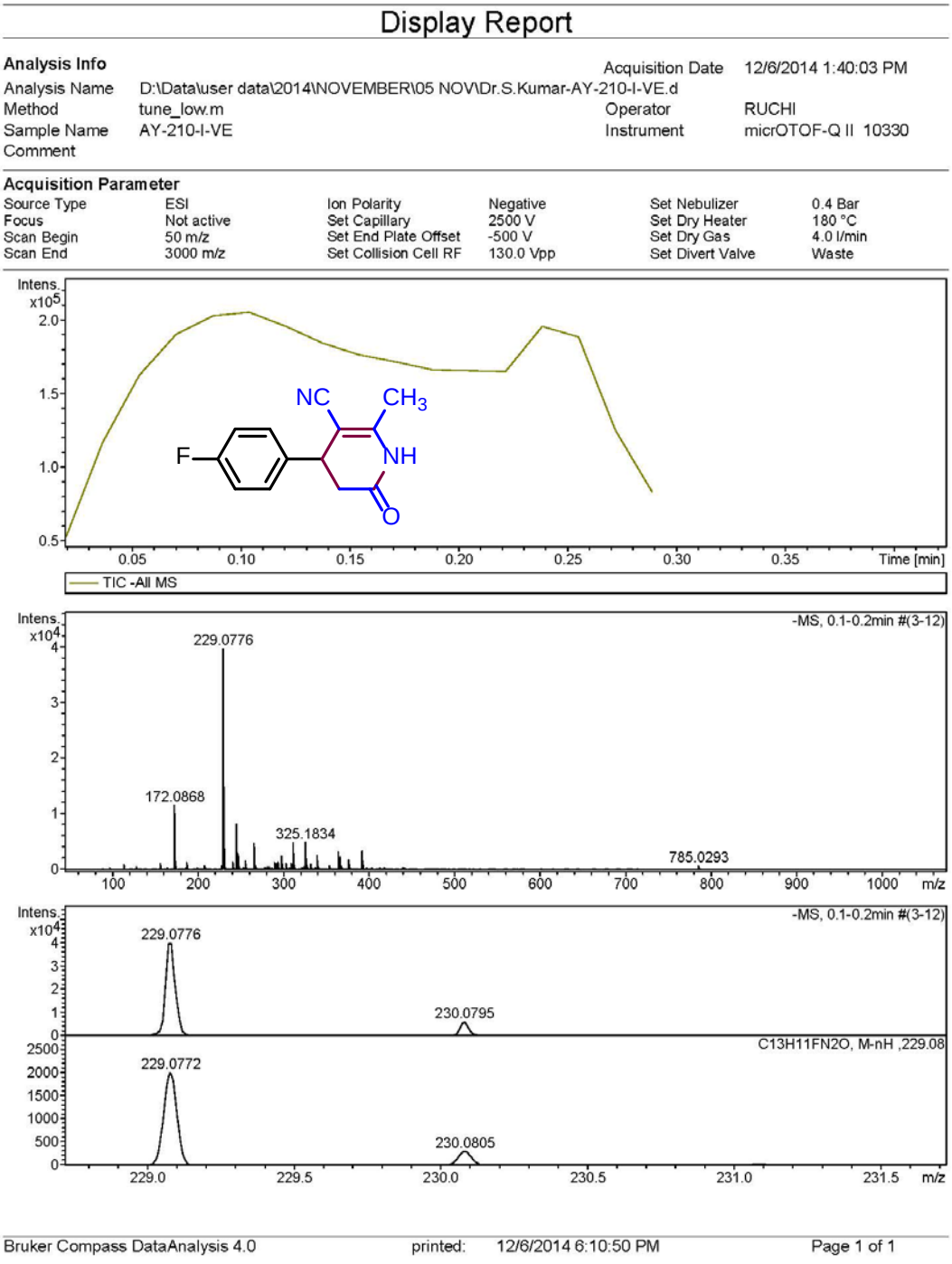
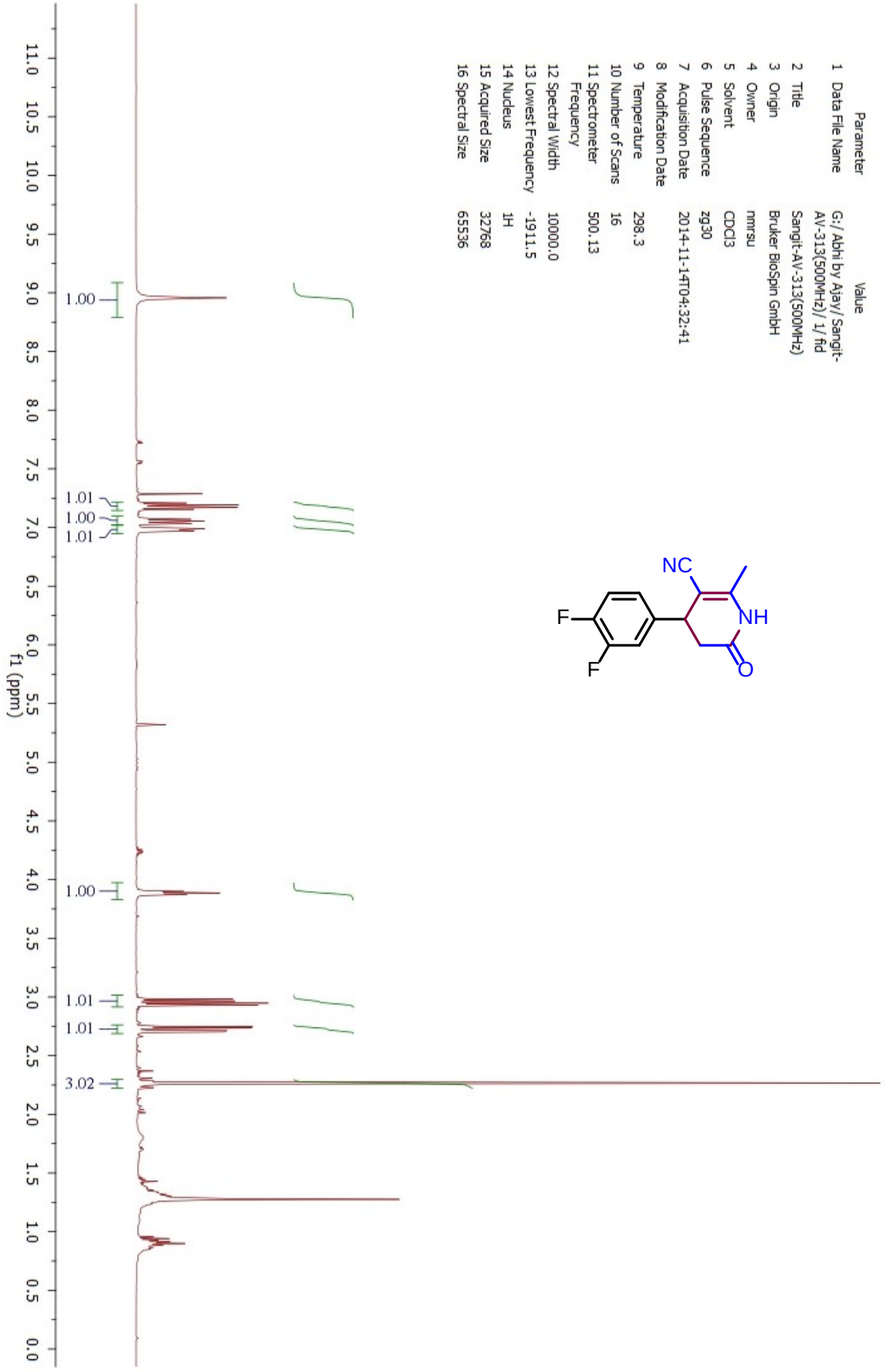


Figure S8 ^{1}H NMR spectra of **4**



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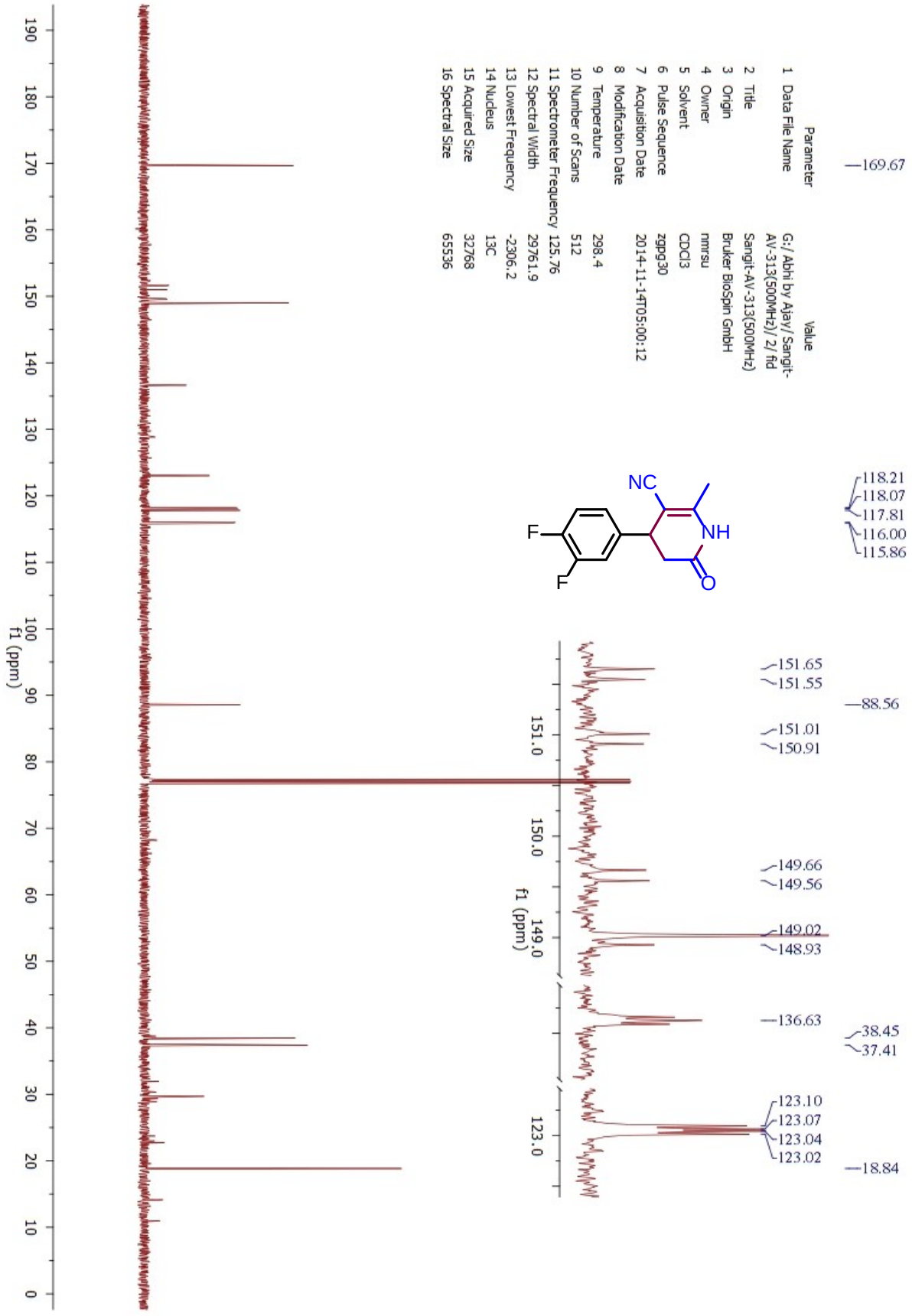

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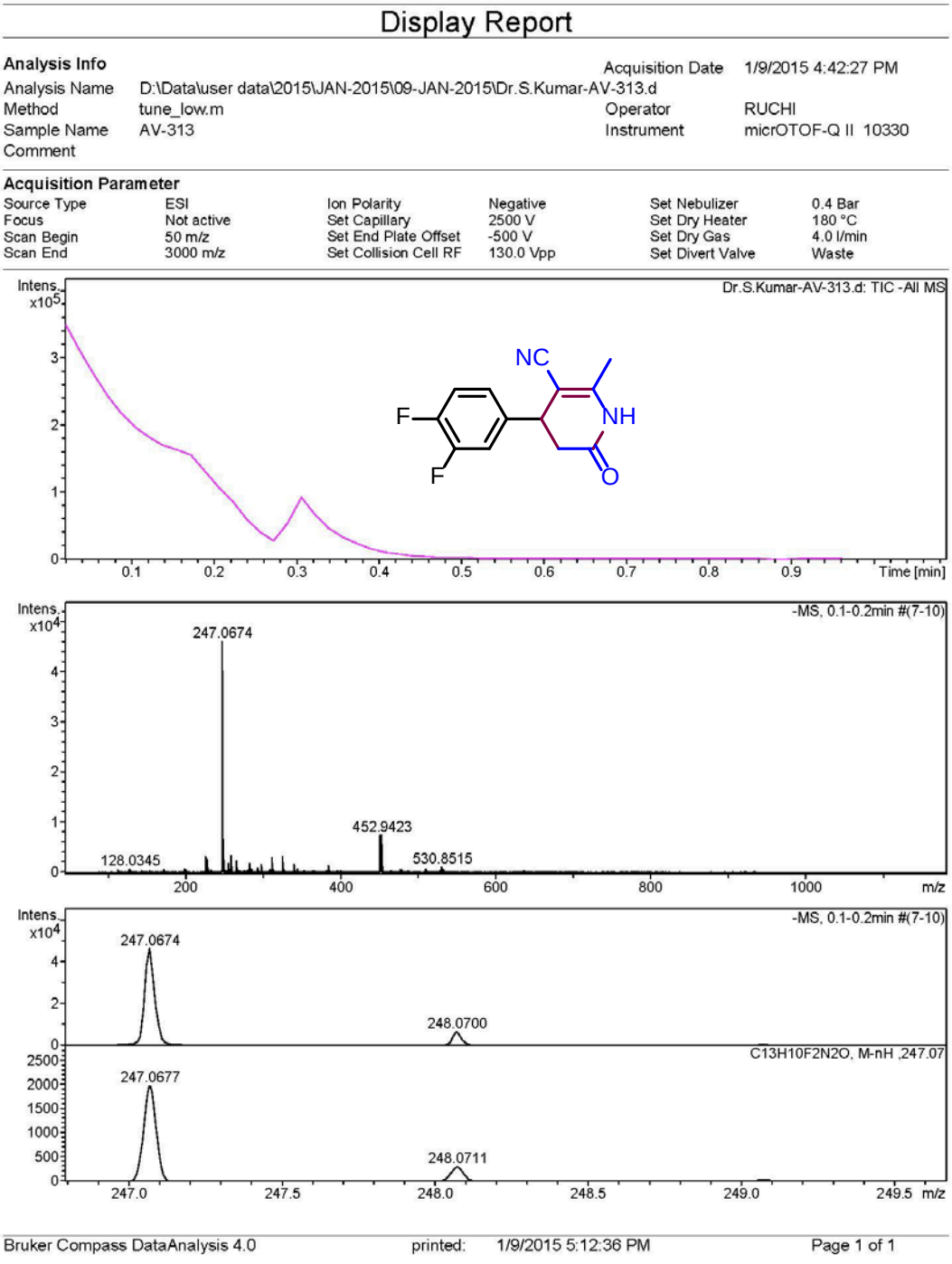

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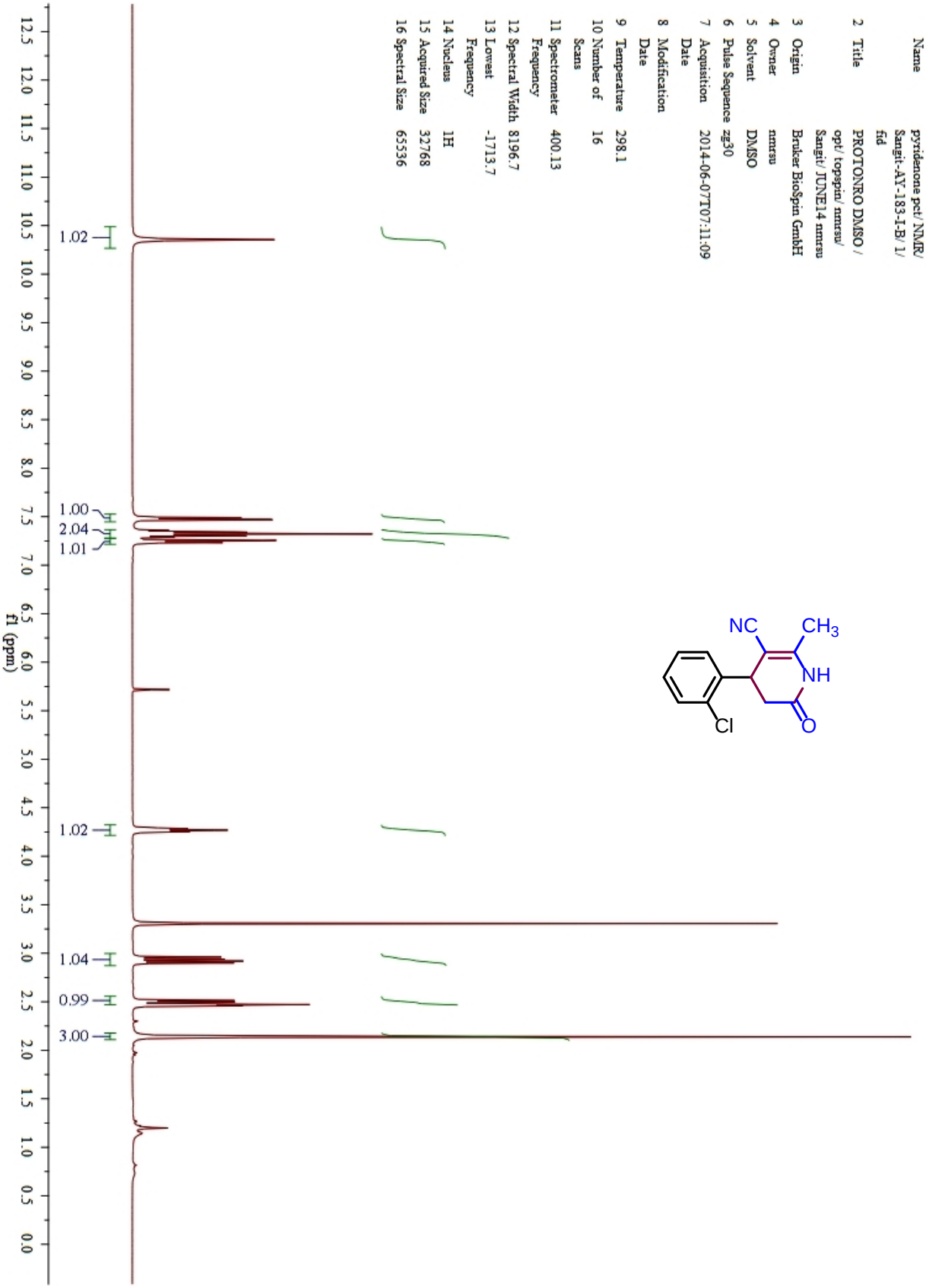


Figure S12 ^{13}C NMR spectra of **5**

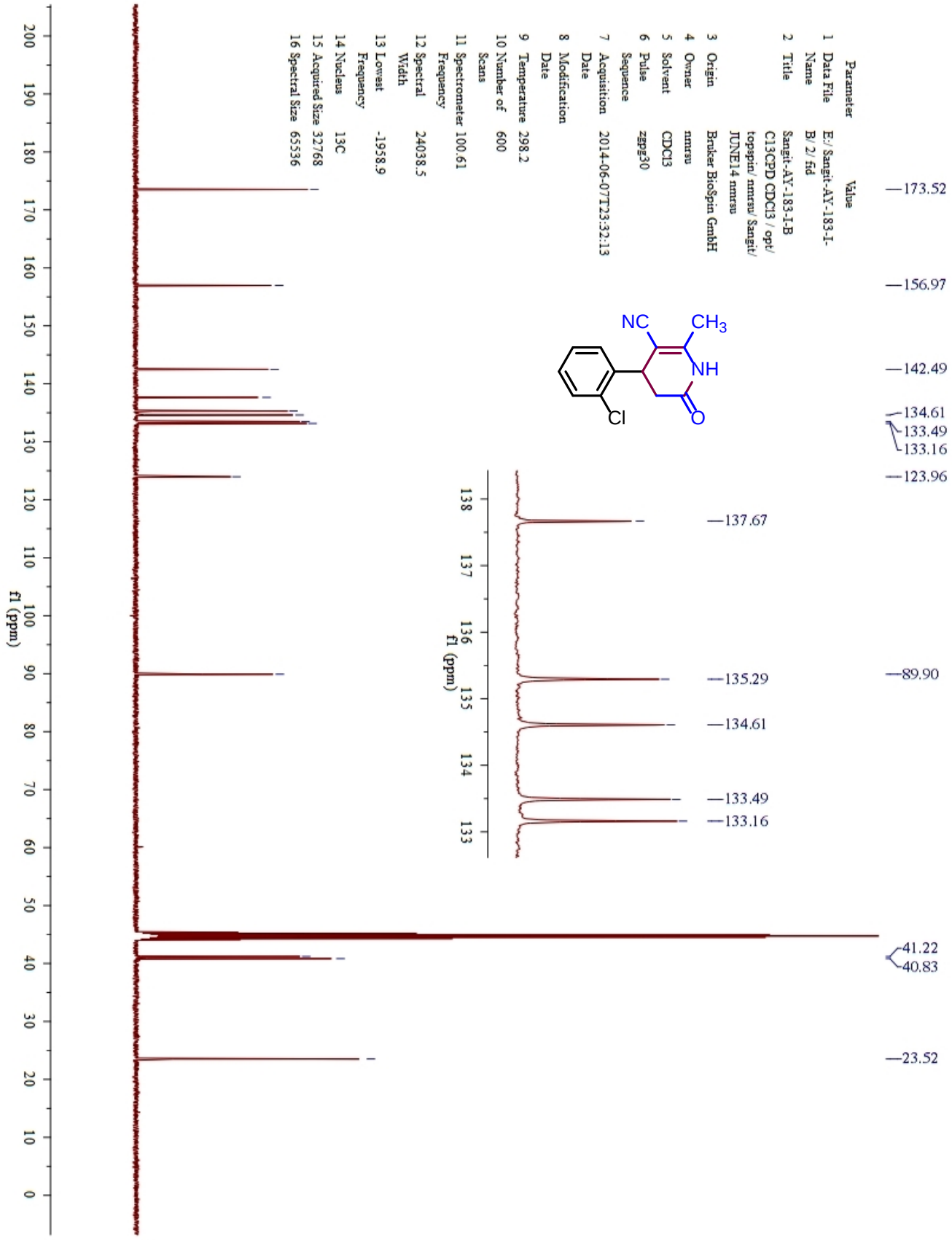
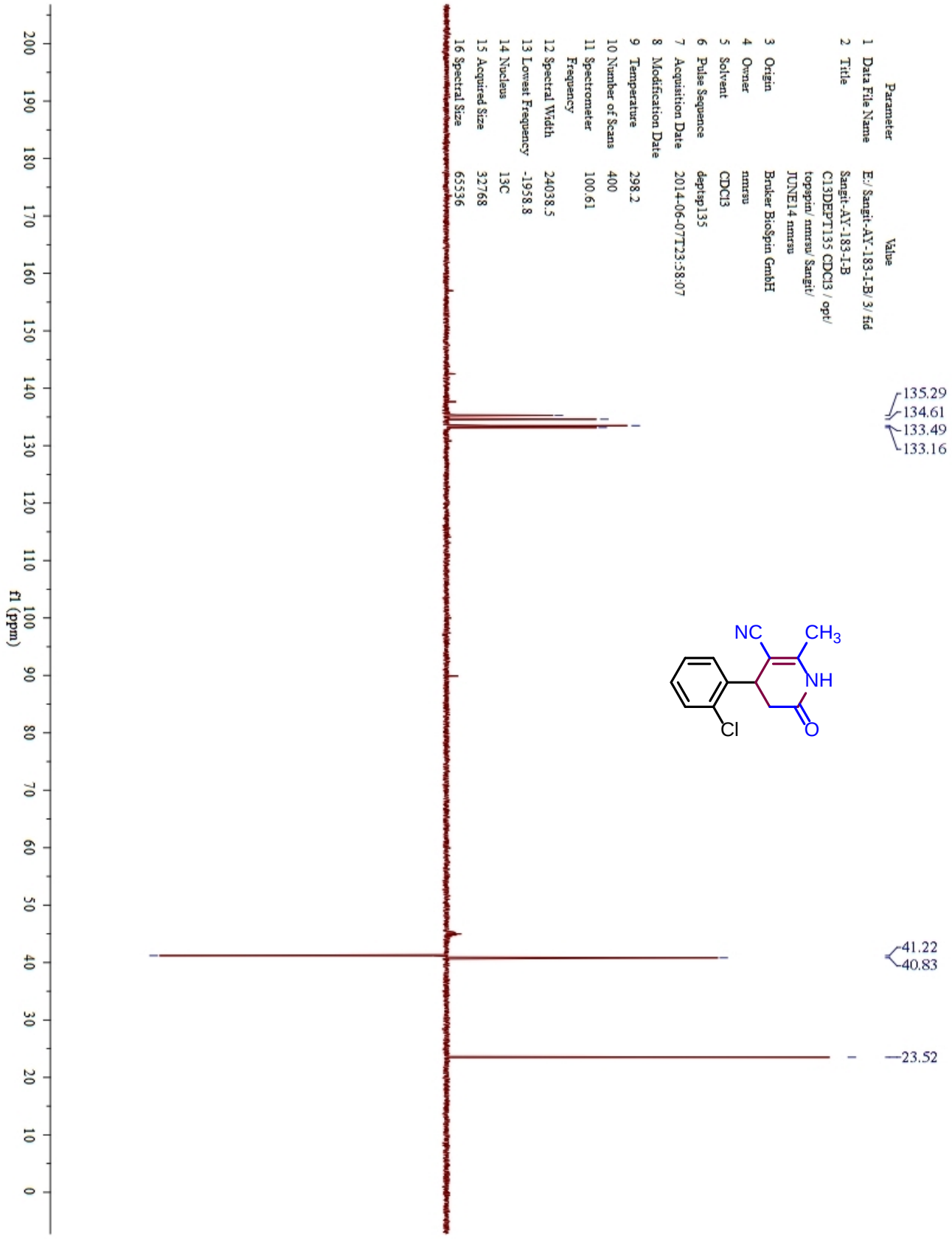


Figure S13 135-DEPT NMR spectra of **5**



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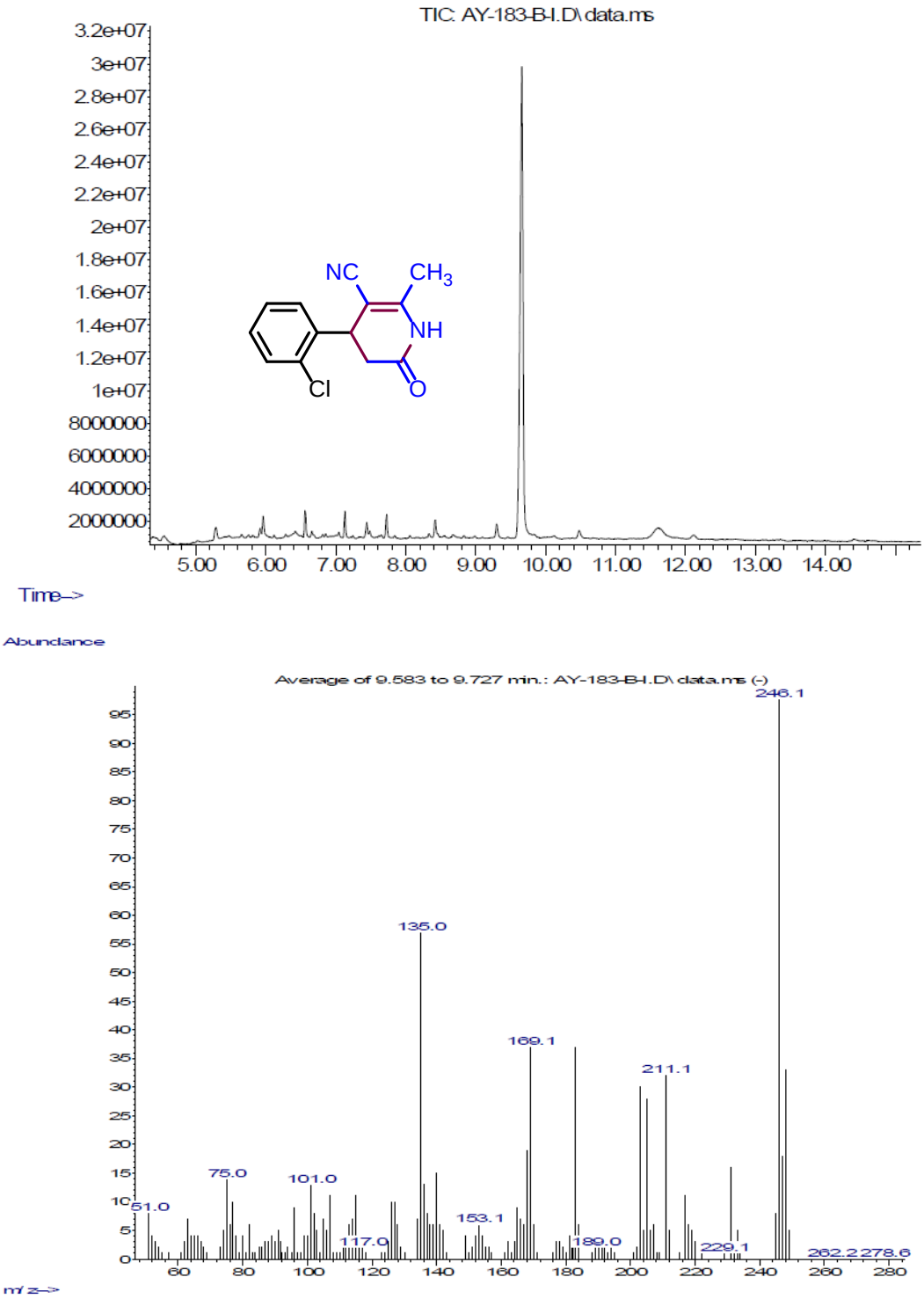

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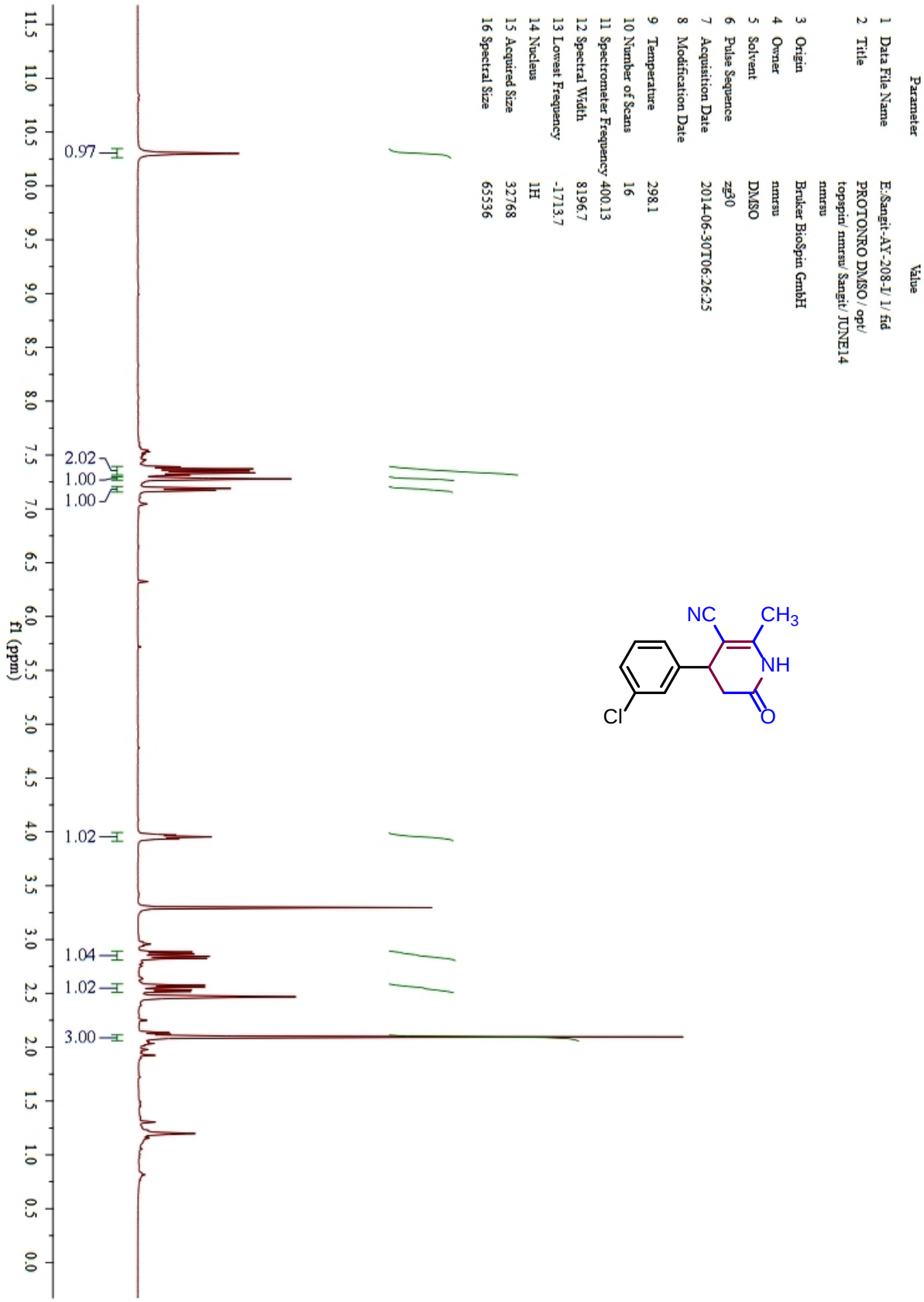

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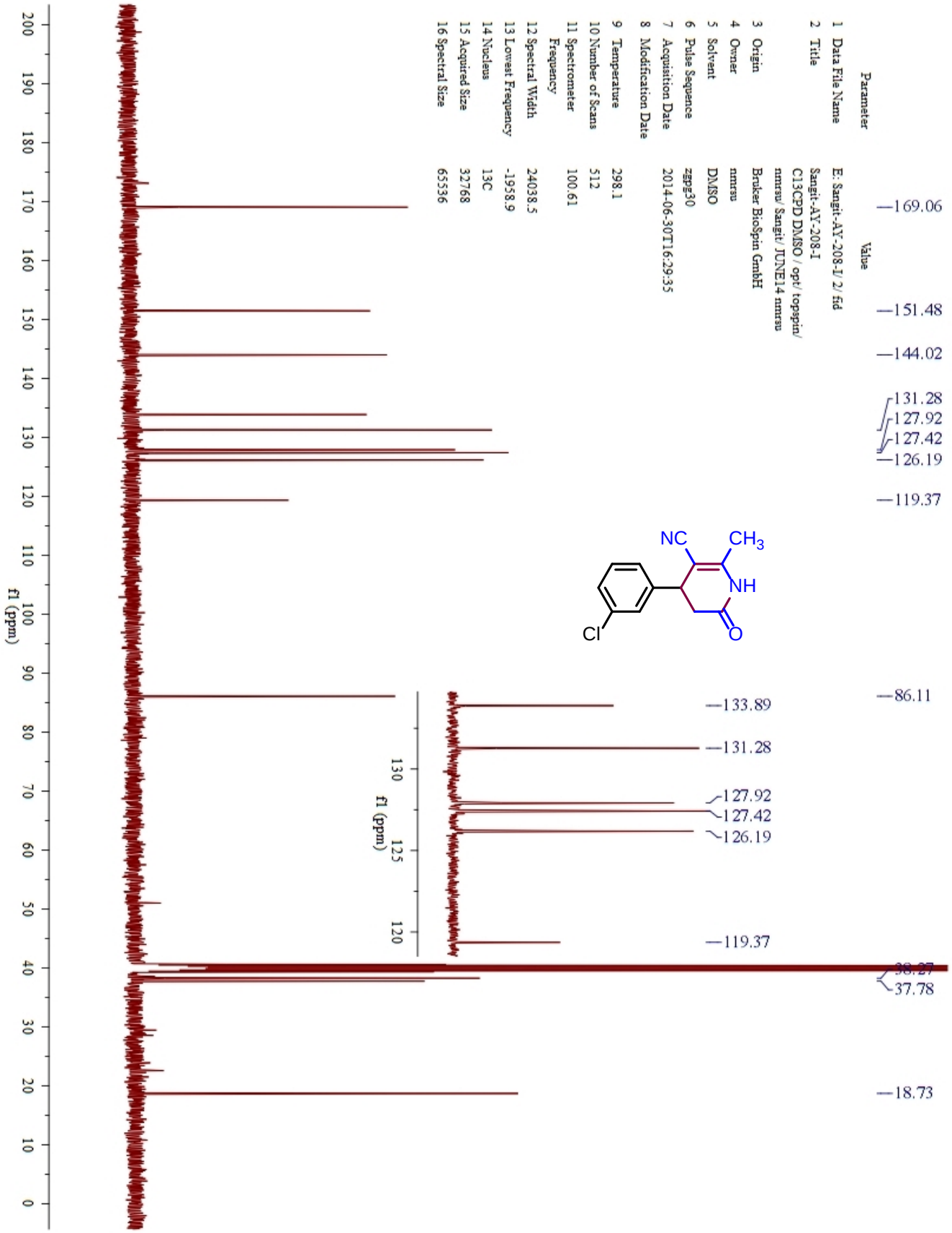

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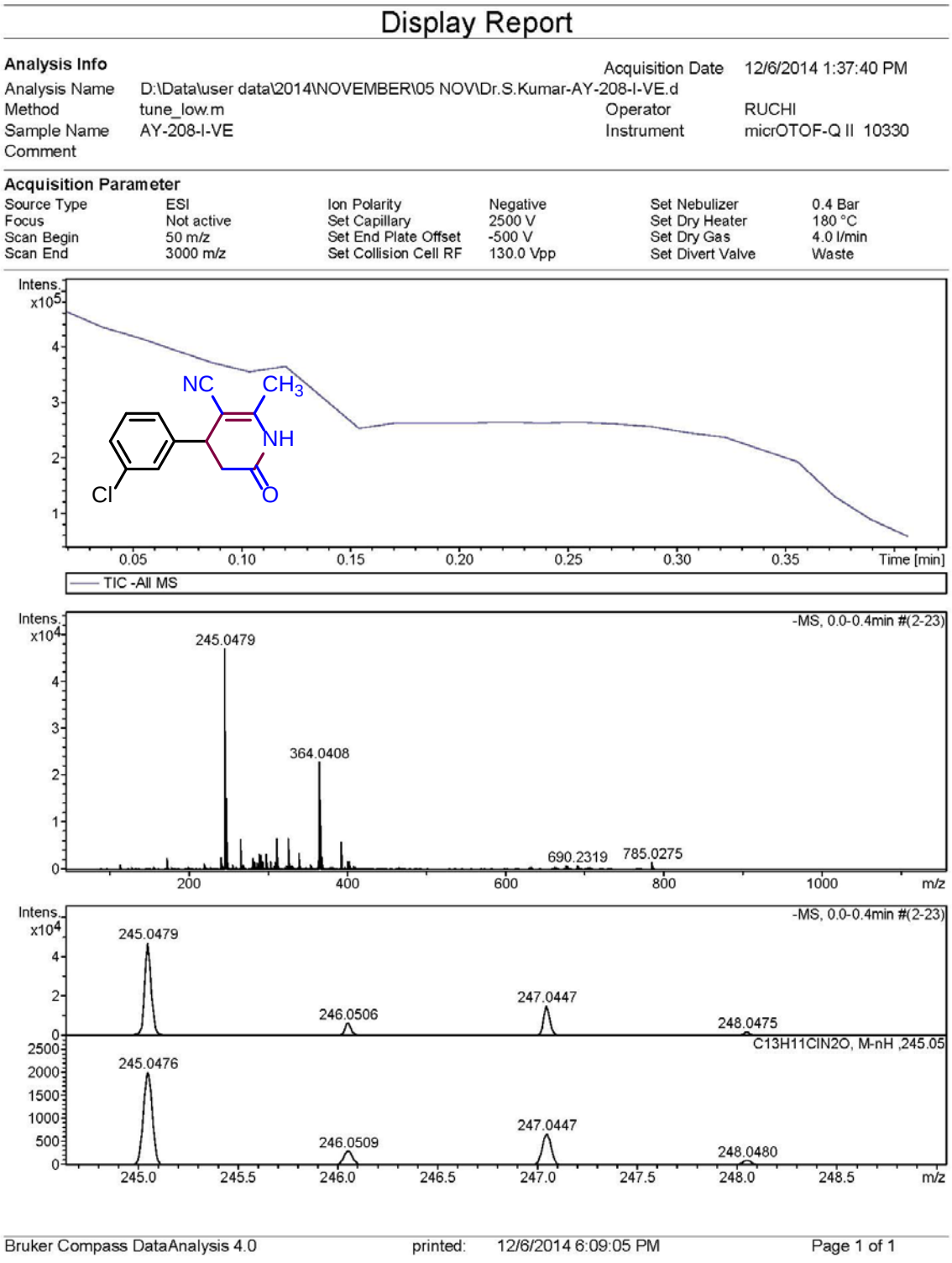

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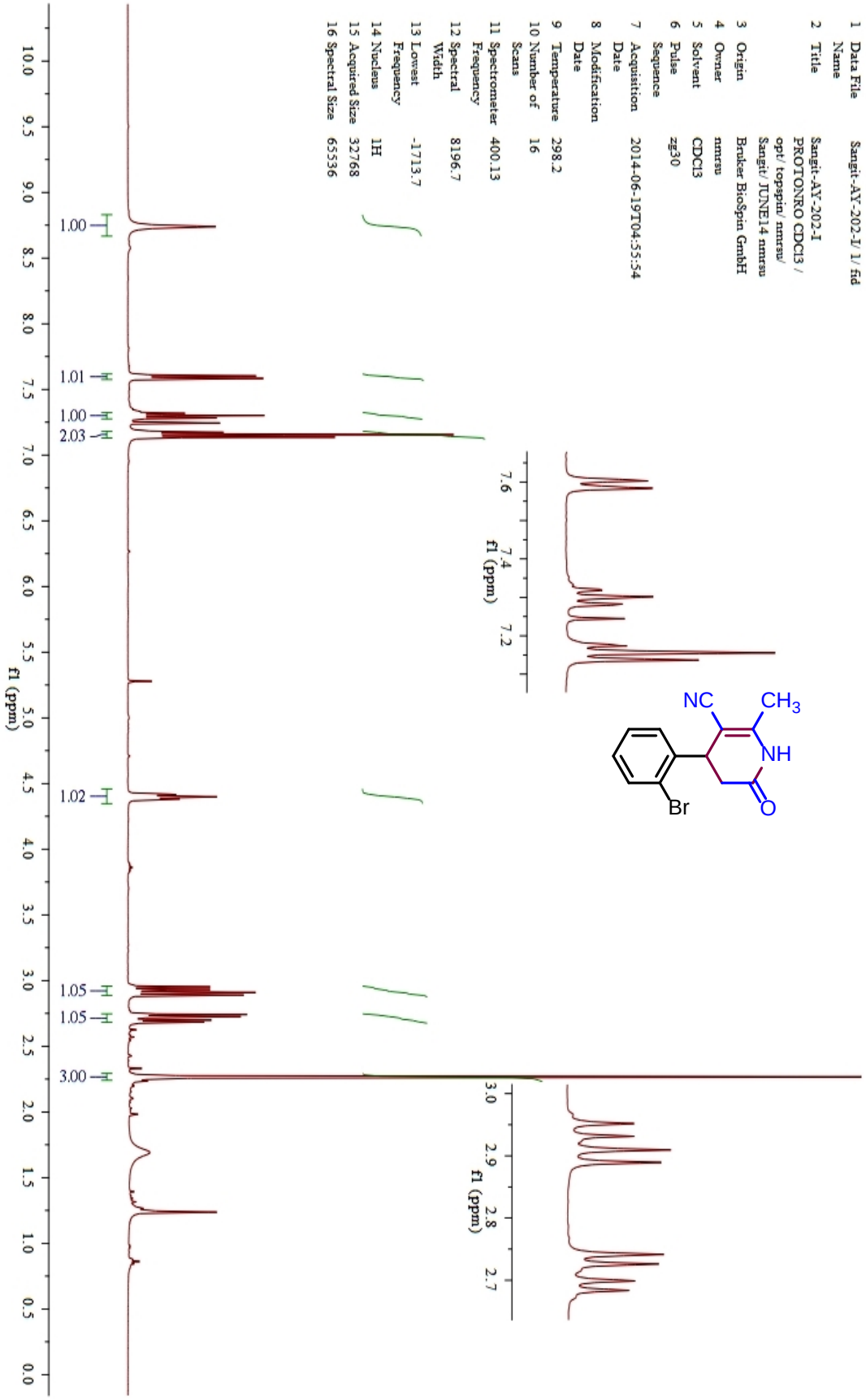

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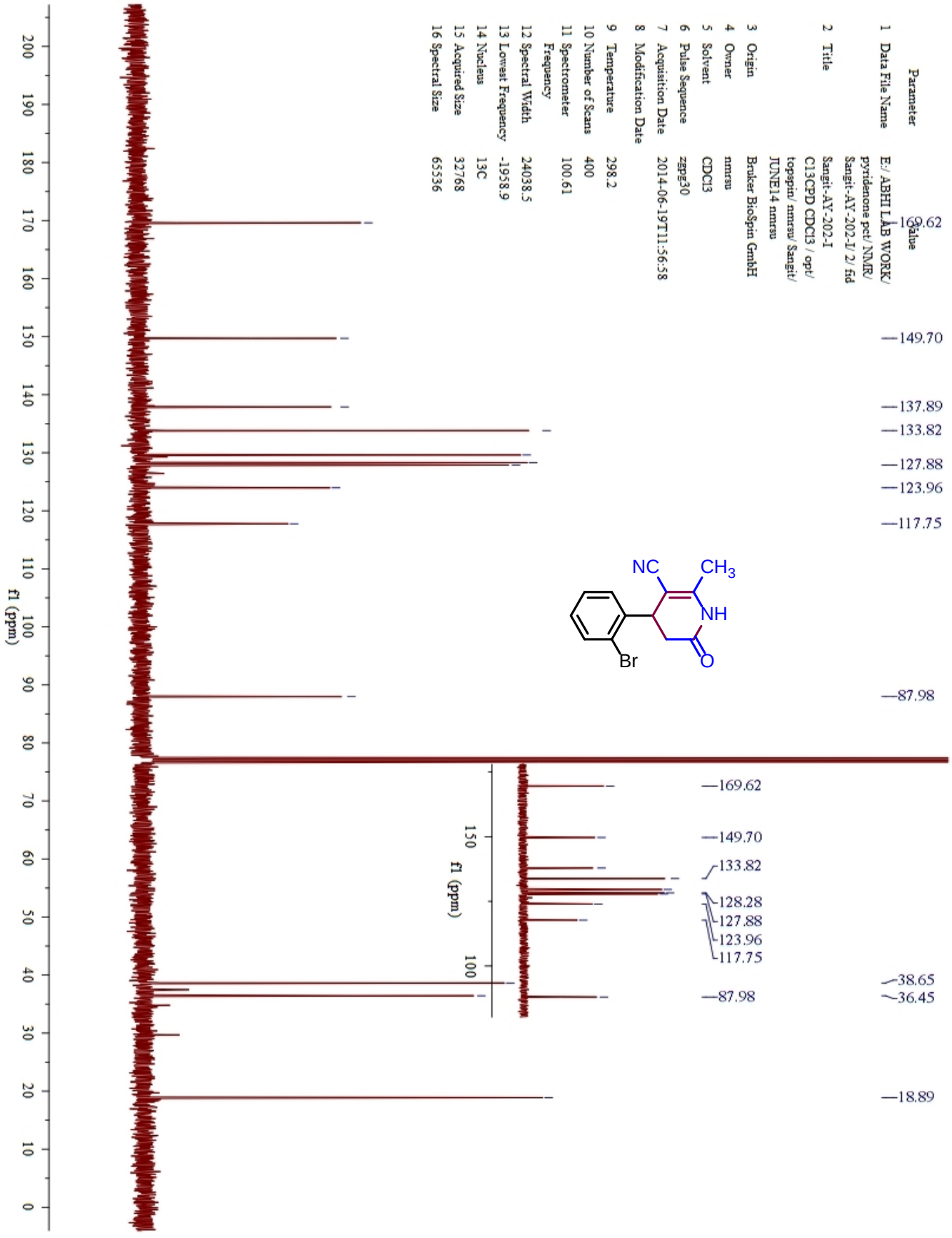

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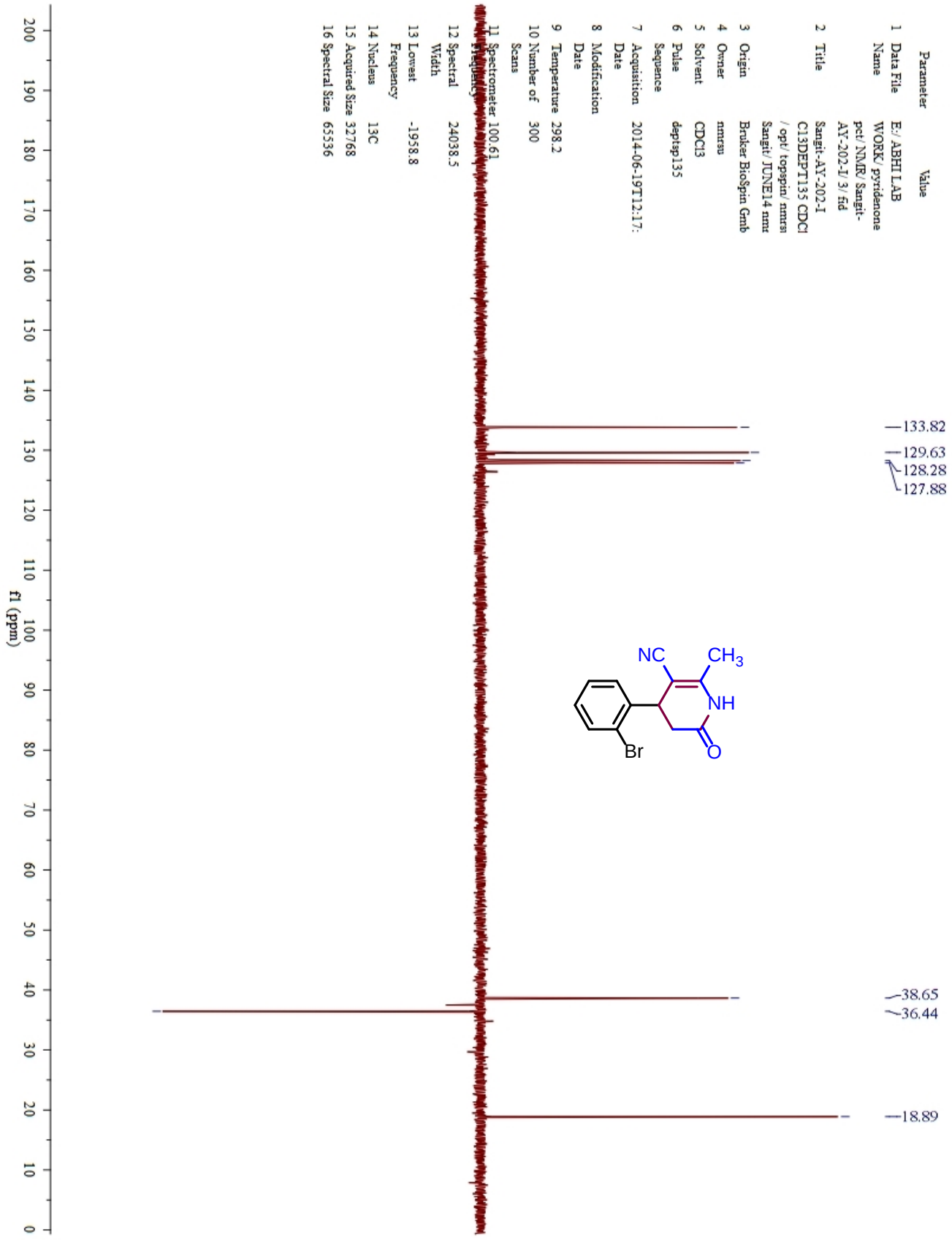

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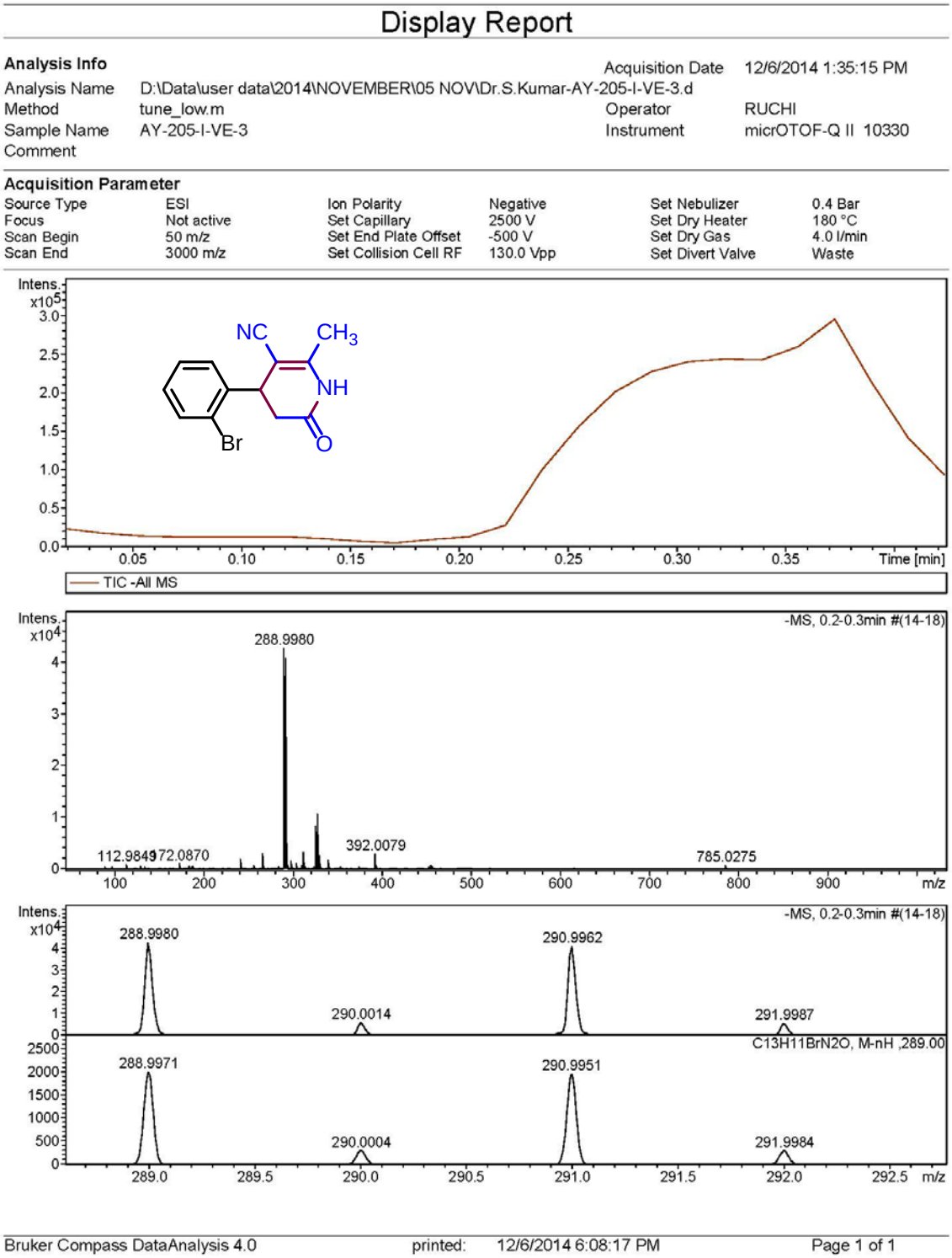


Figure S22 ^{1}H NMR spectra of **8**

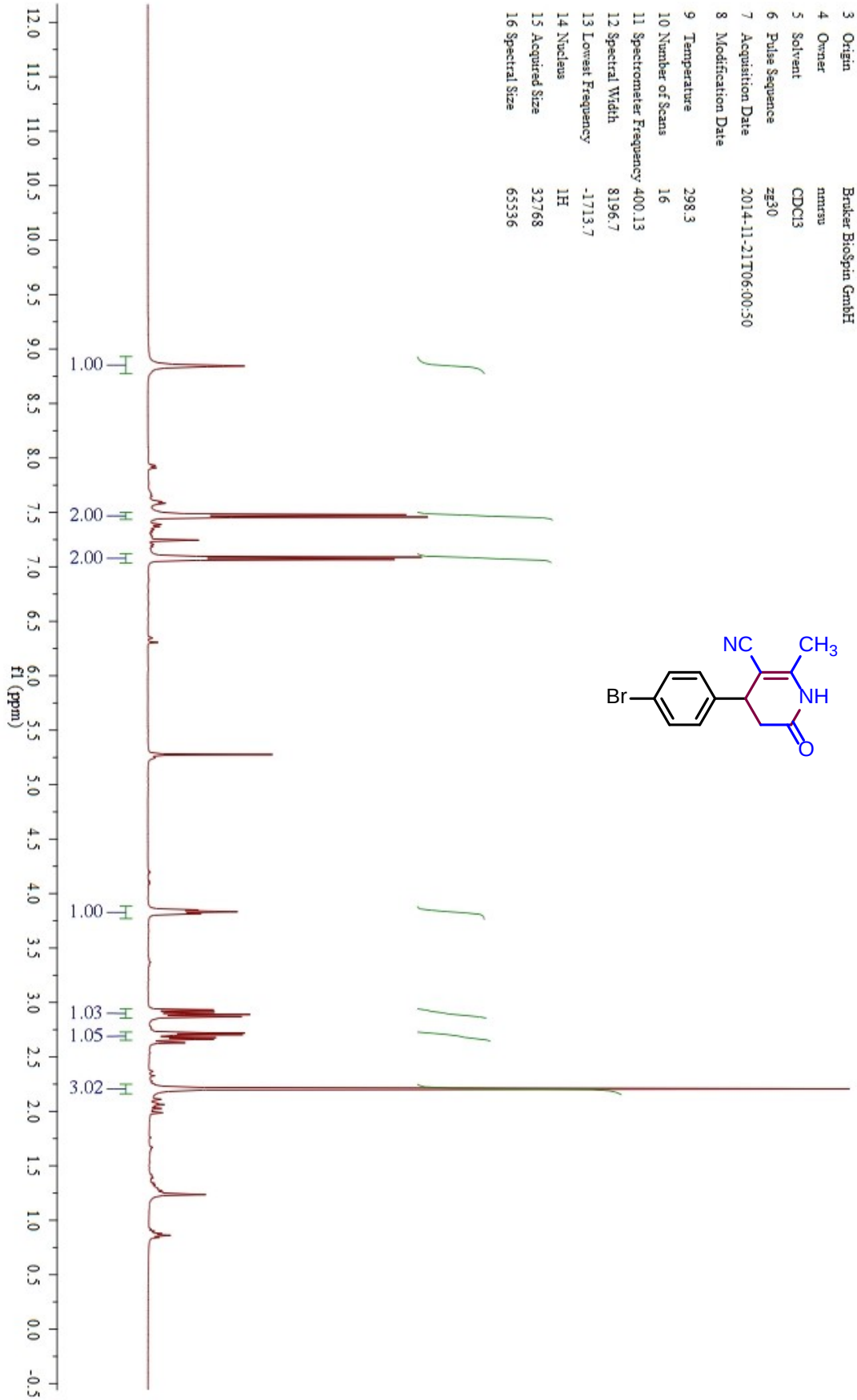


Figure S23 ^{13}C NMR spectra of **8**

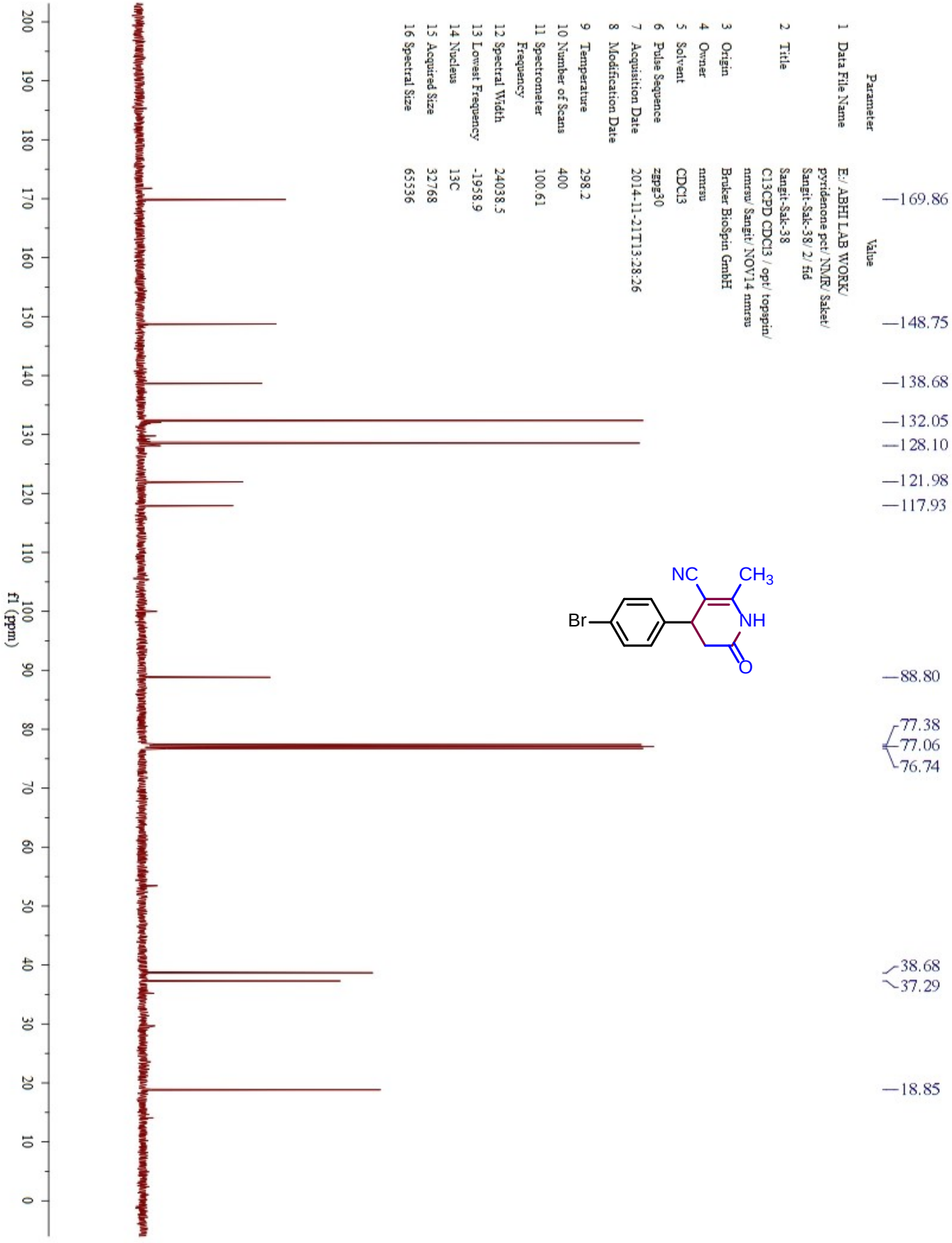
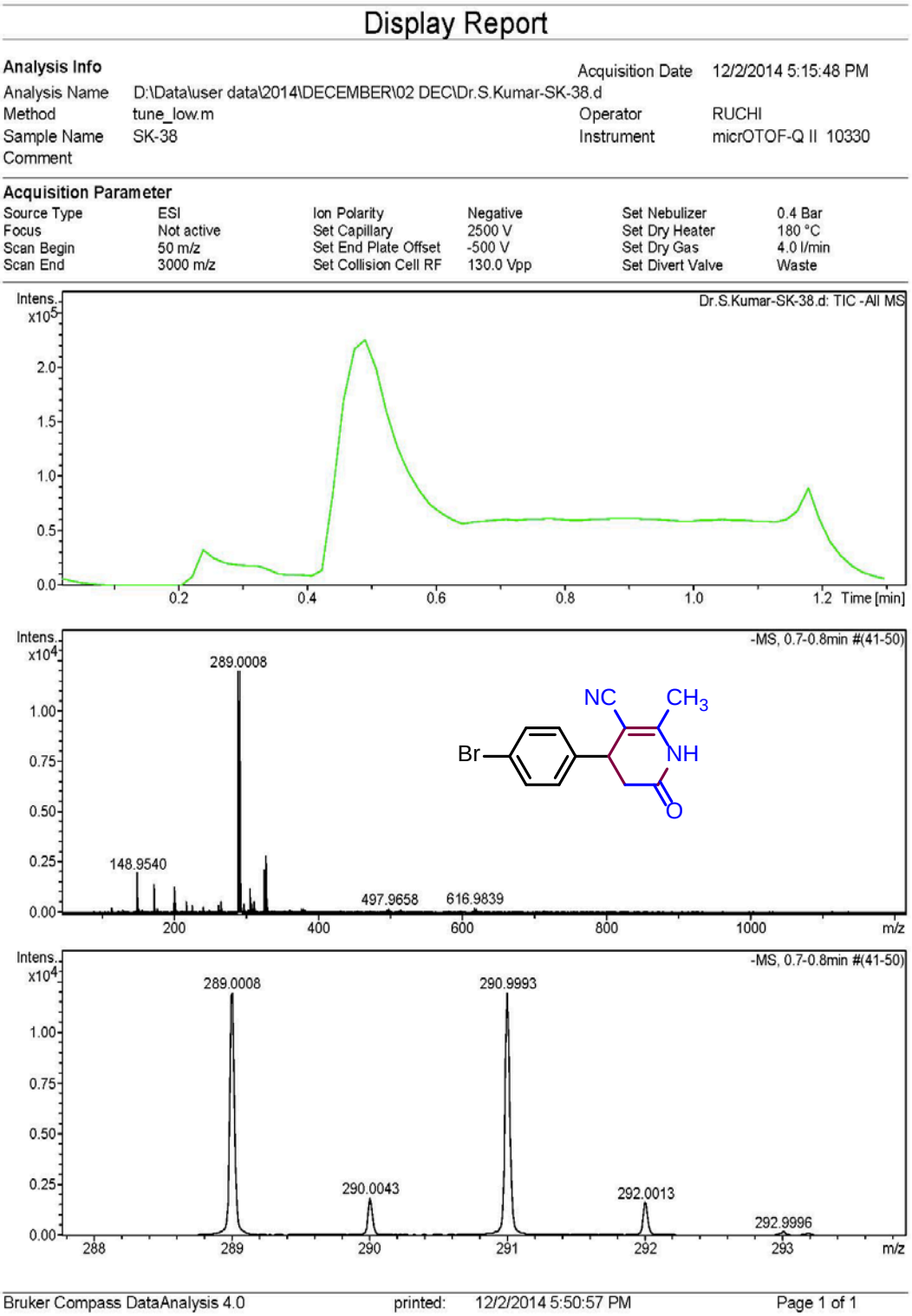


Figure S24 HRMS spectra of **8**



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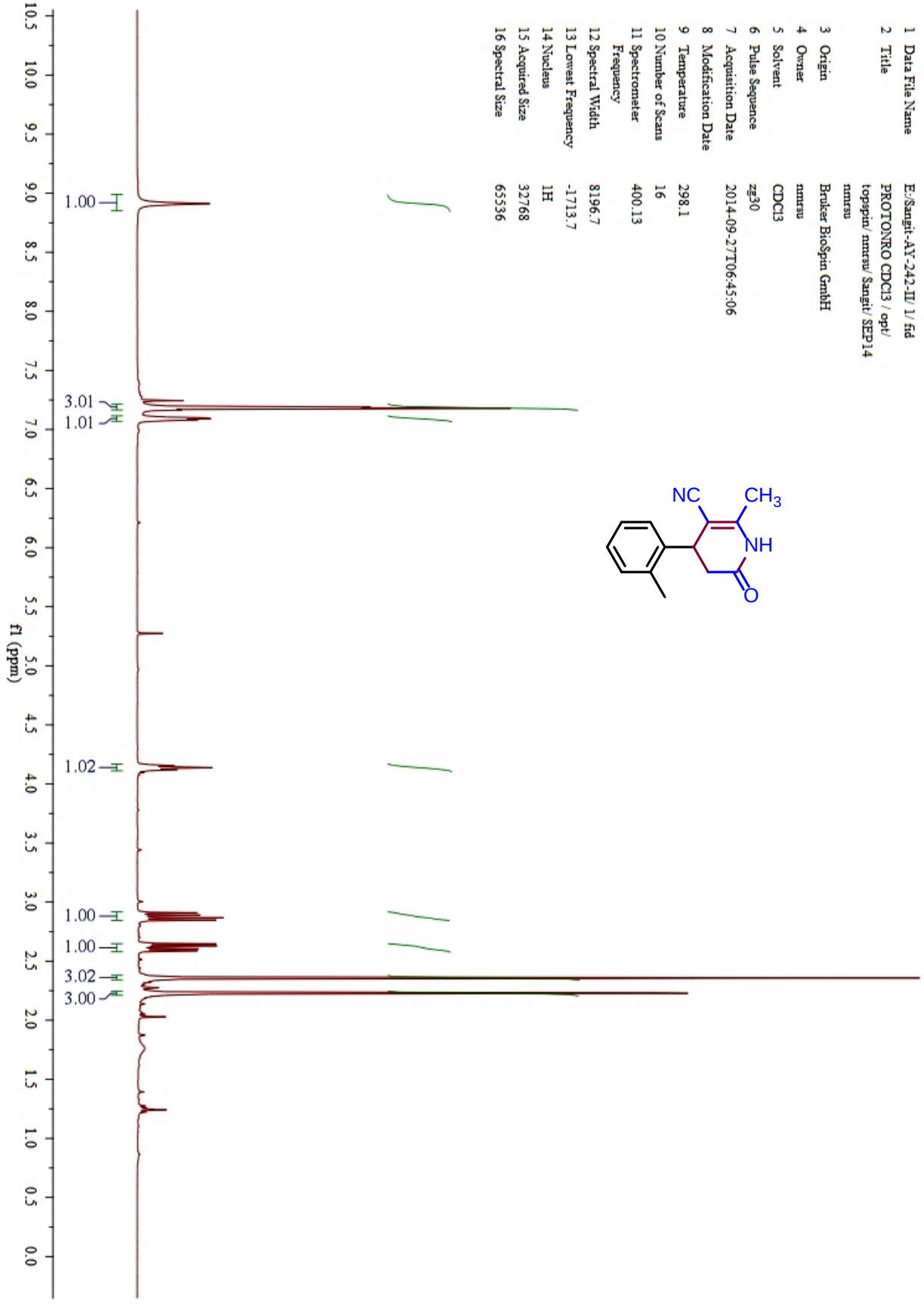

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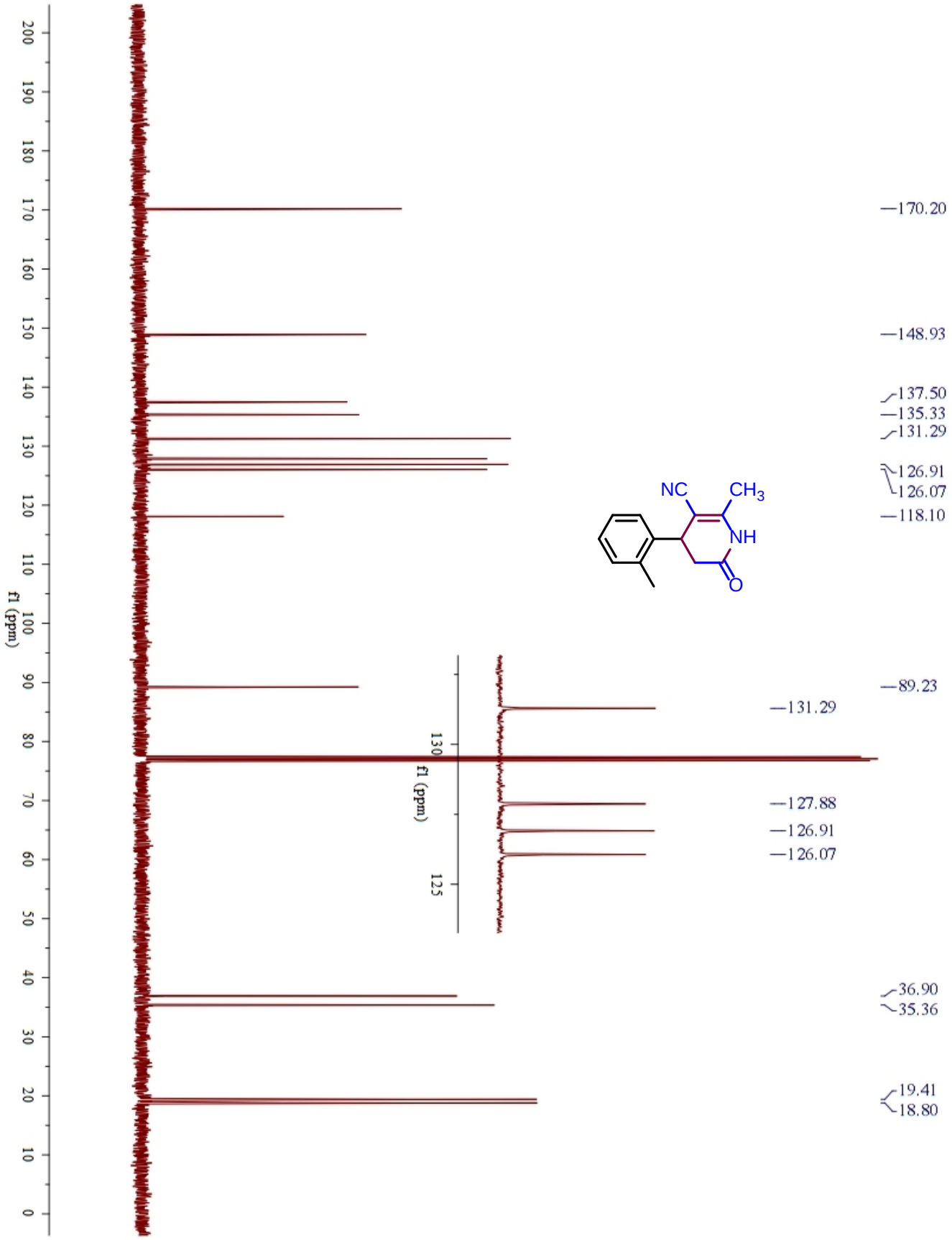

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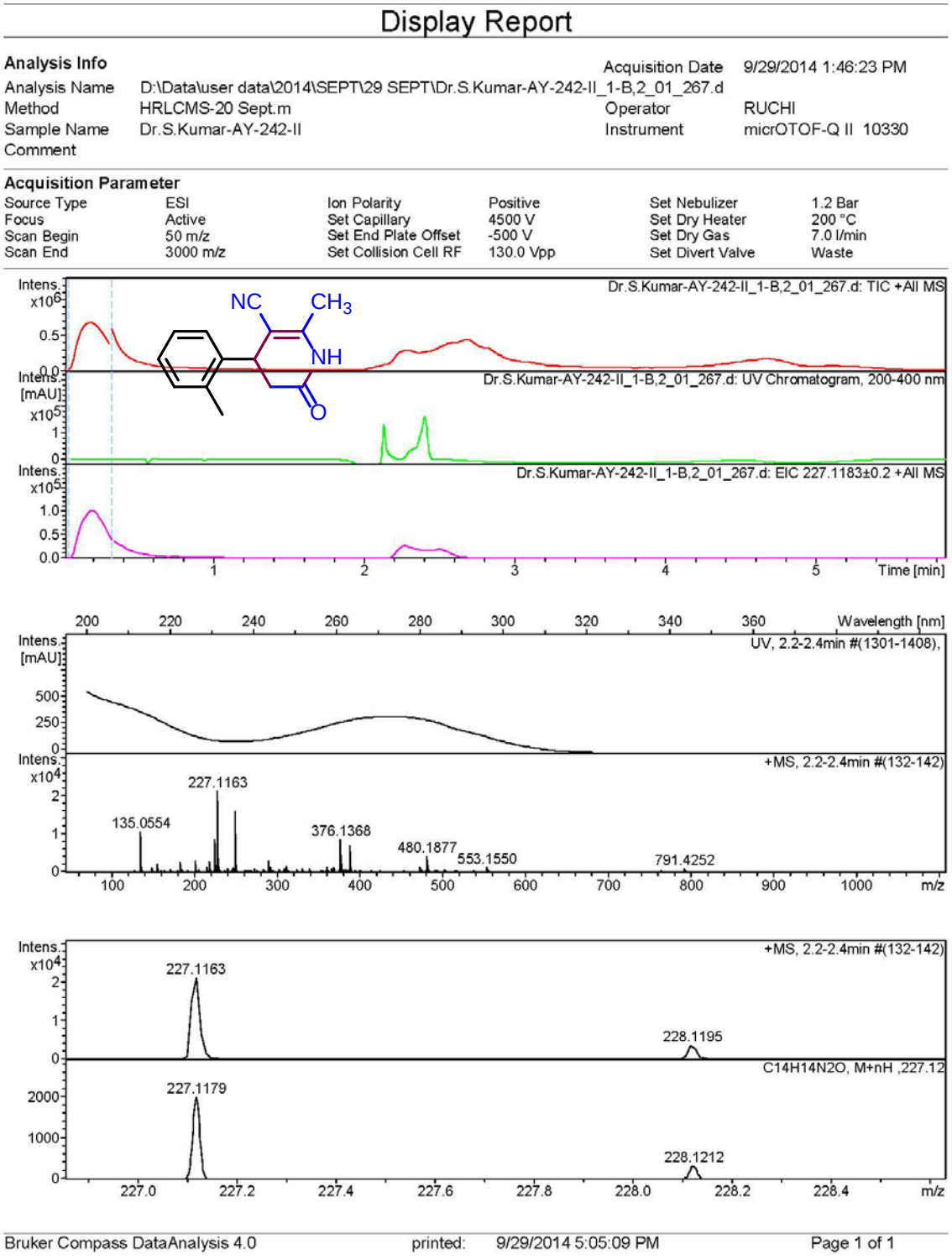

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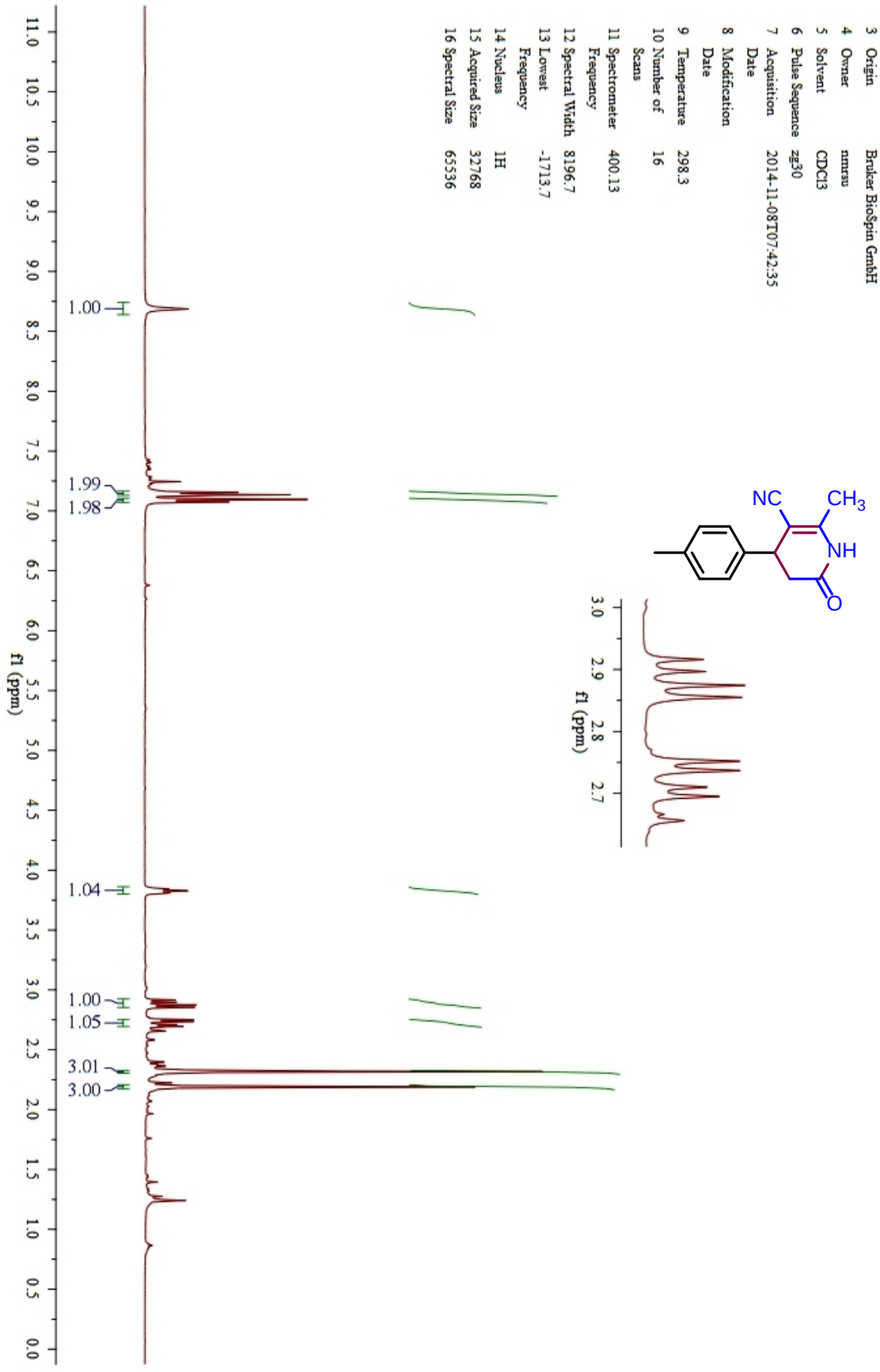


Figure S29 ^{13}C NMR spectra of **10**

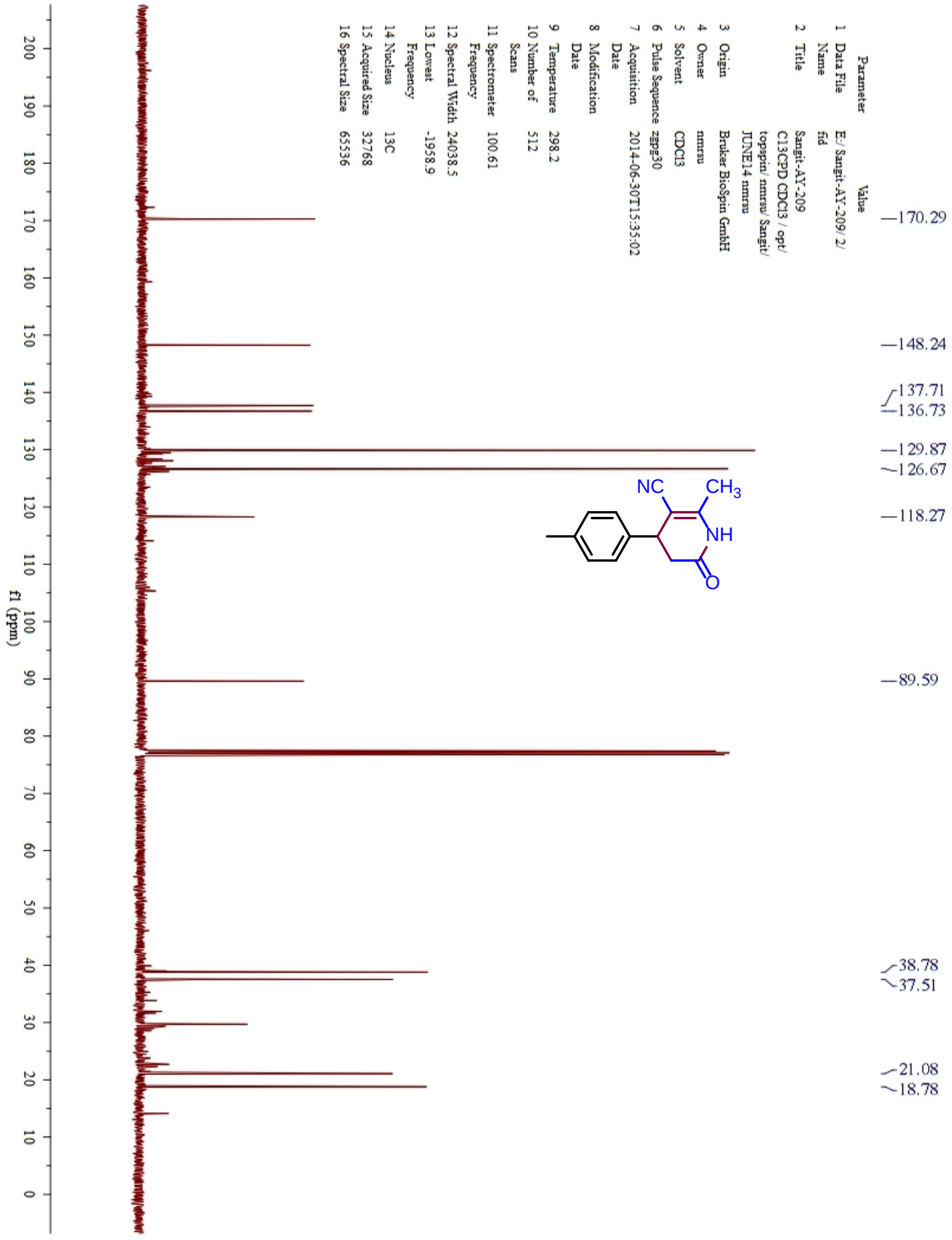
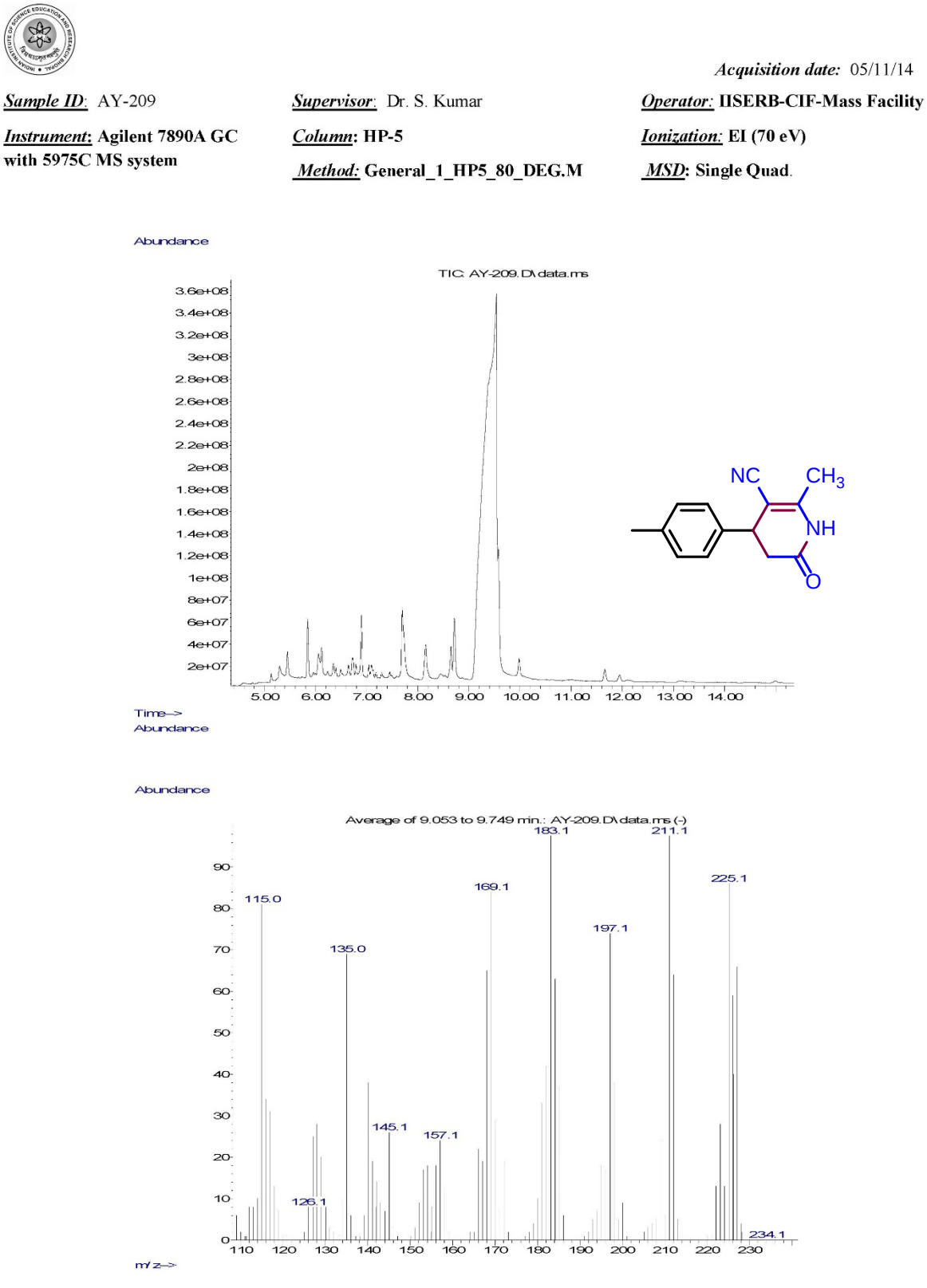


Figure S30 HRMS spectra of **10**



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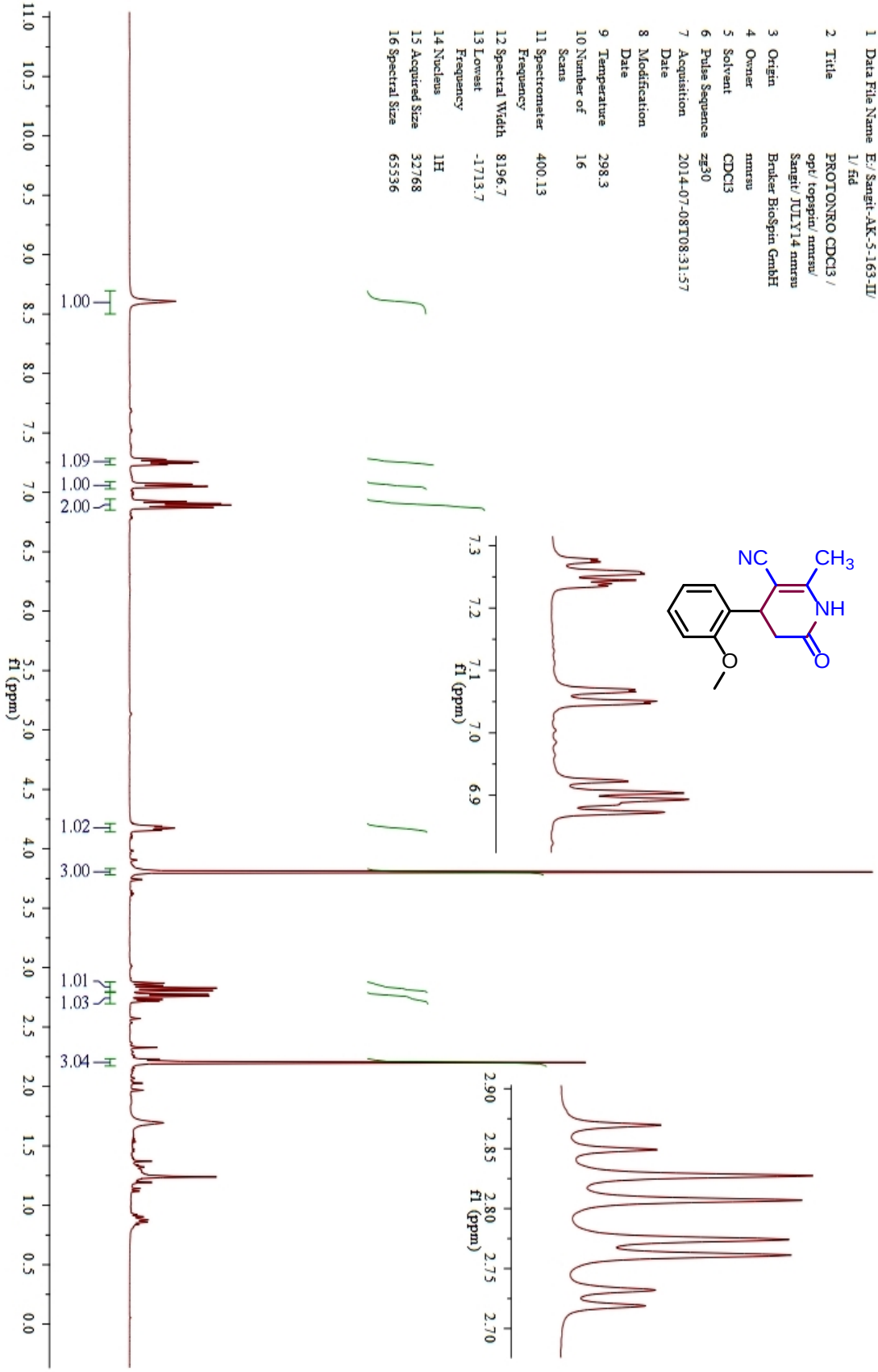

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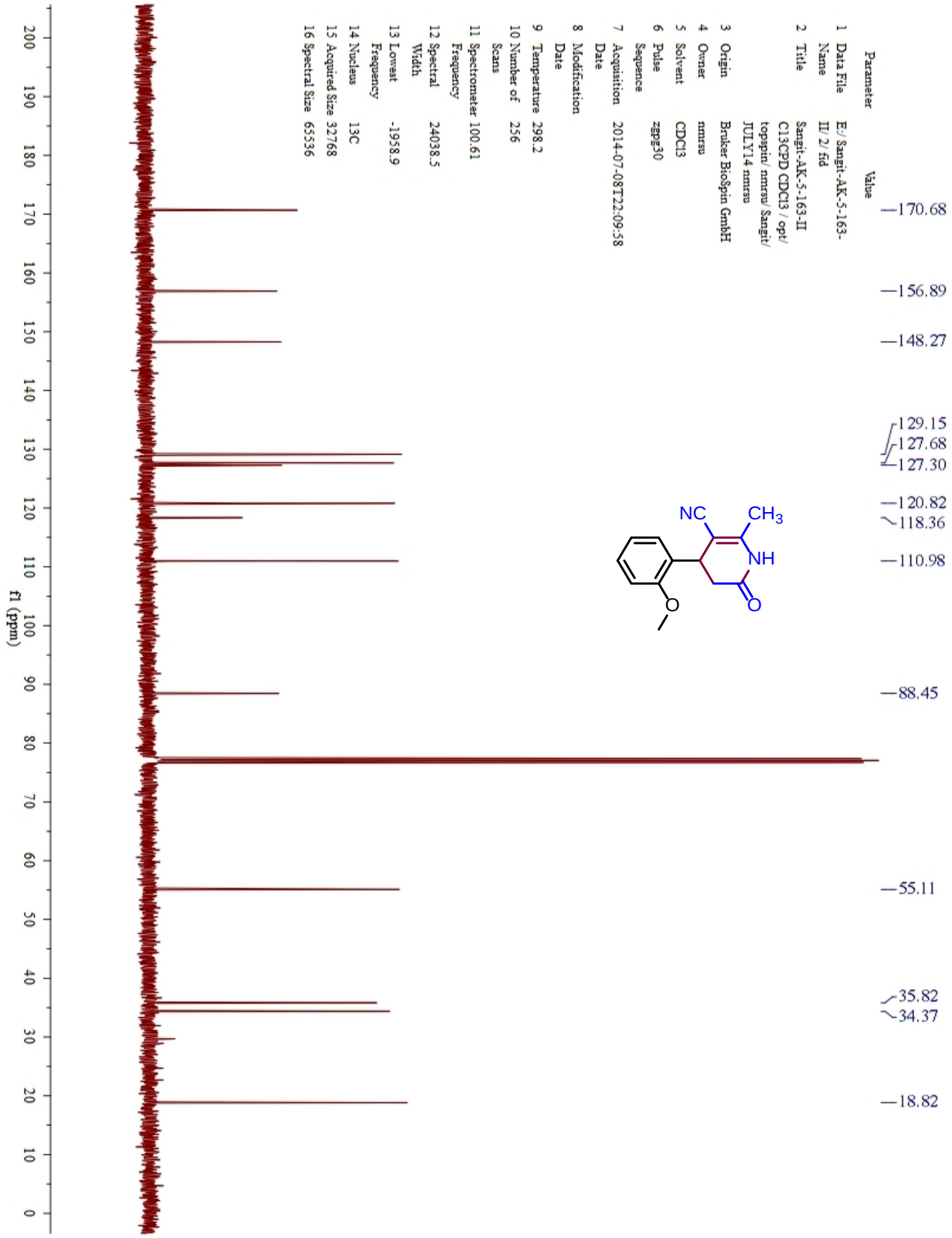

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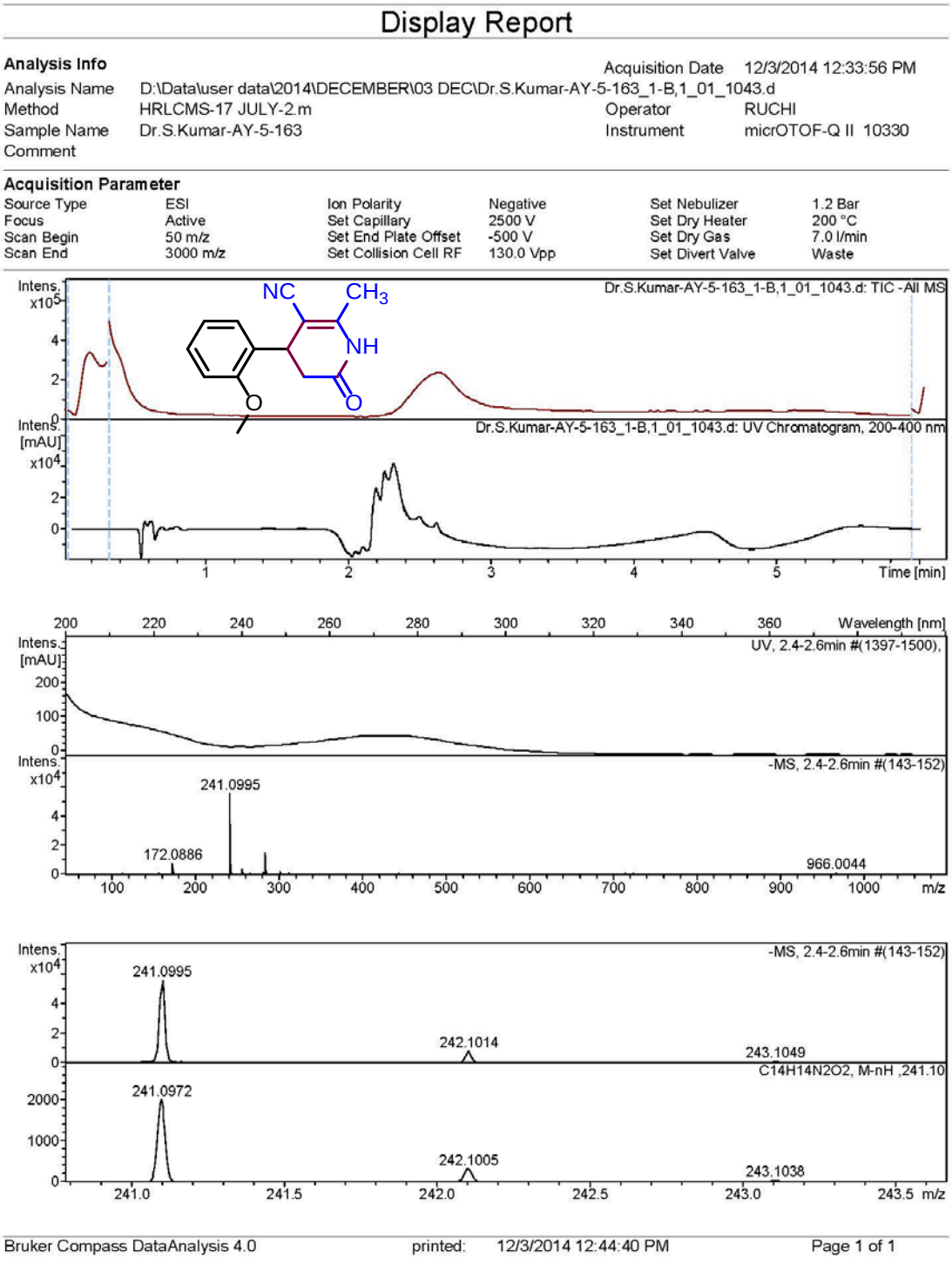
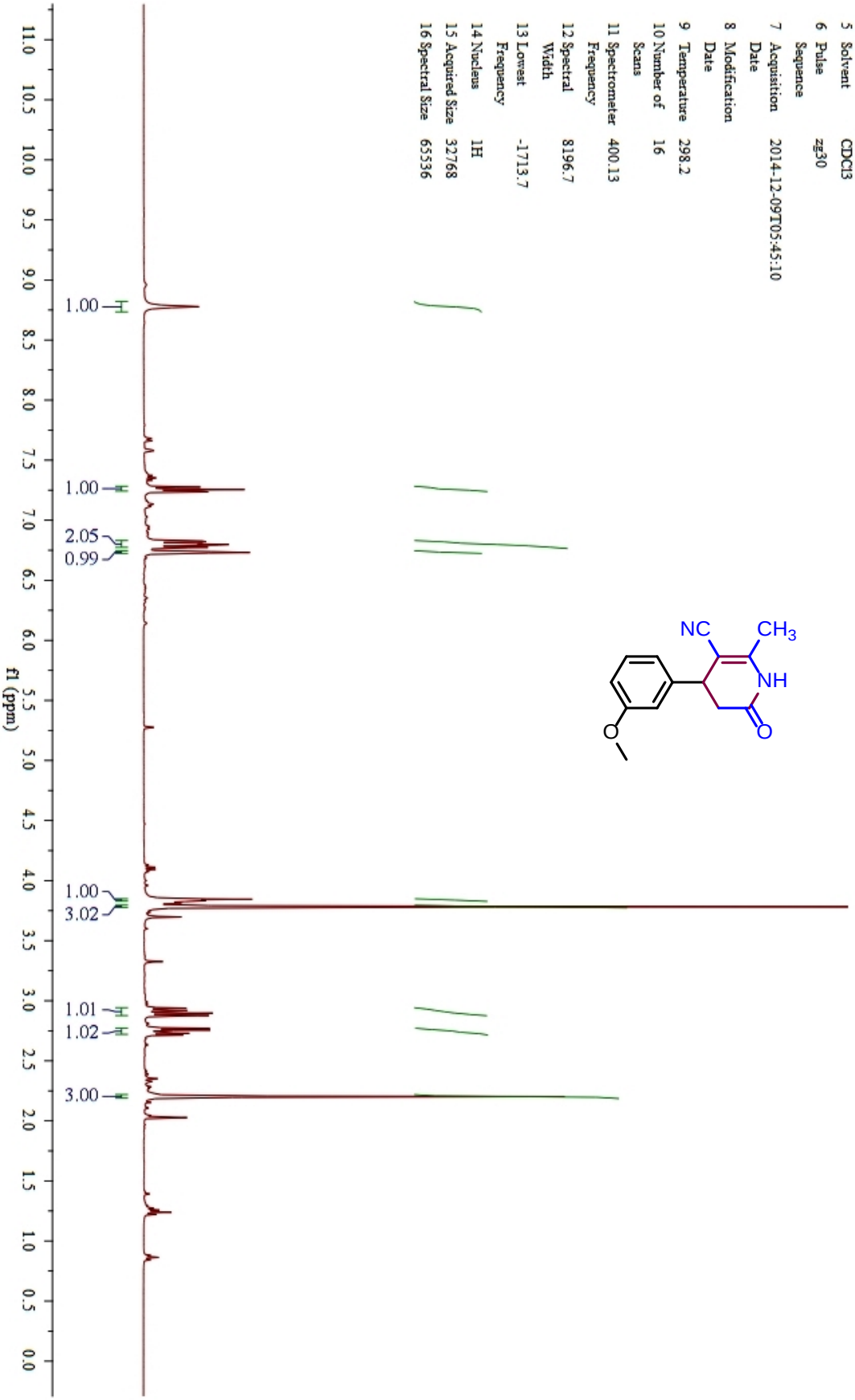


Figure S34 ^{1}H NMR spectra of **12**



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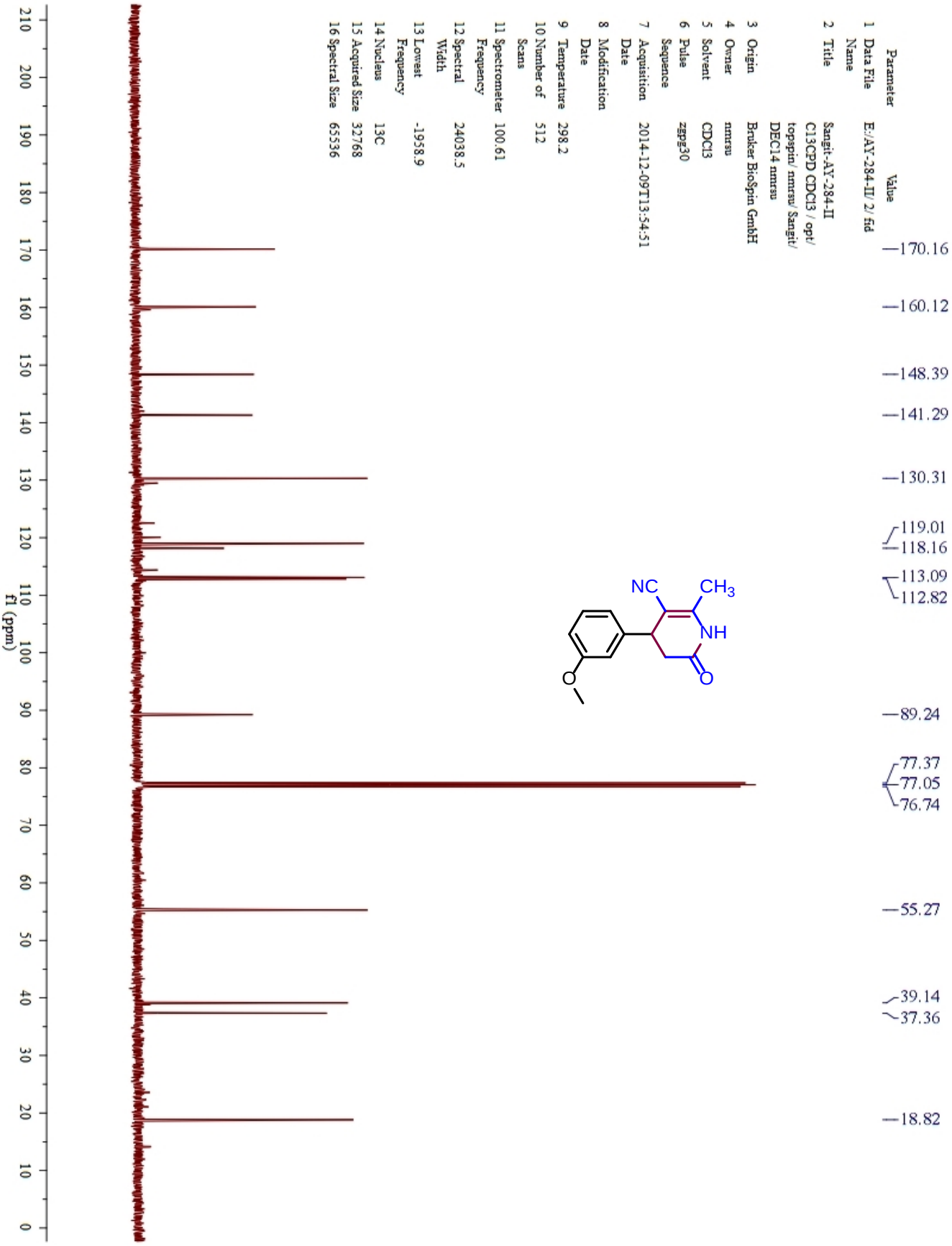

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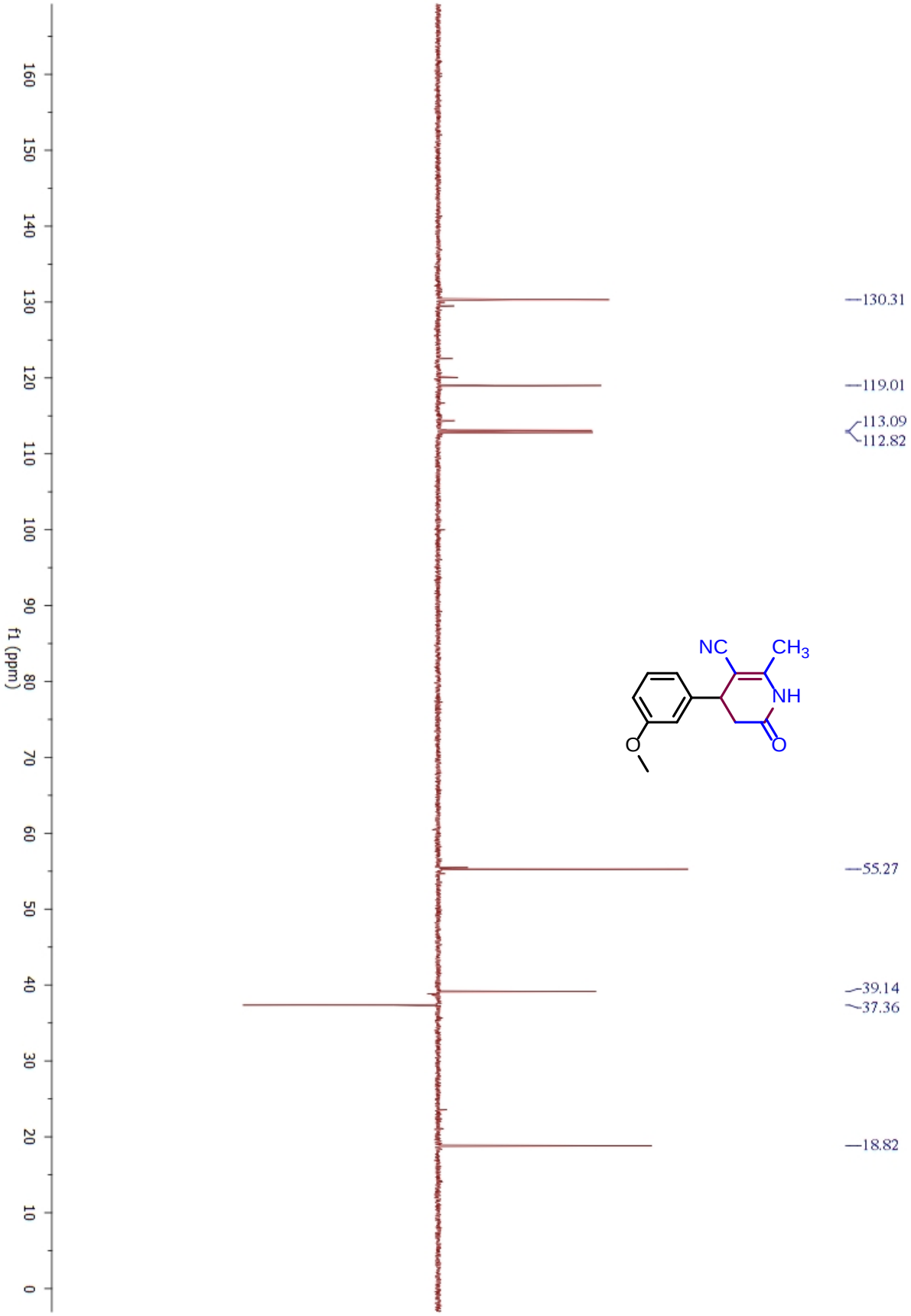

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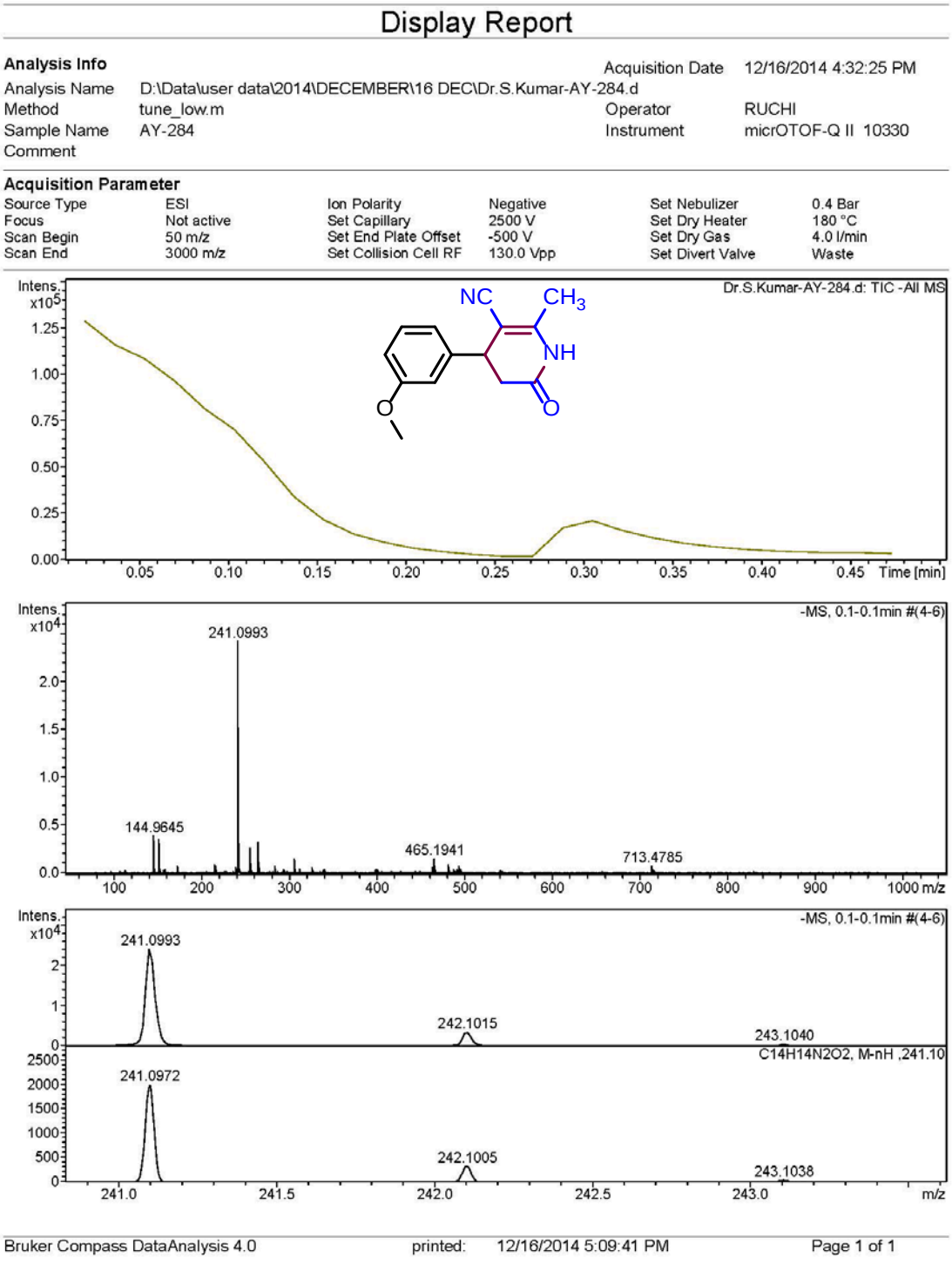

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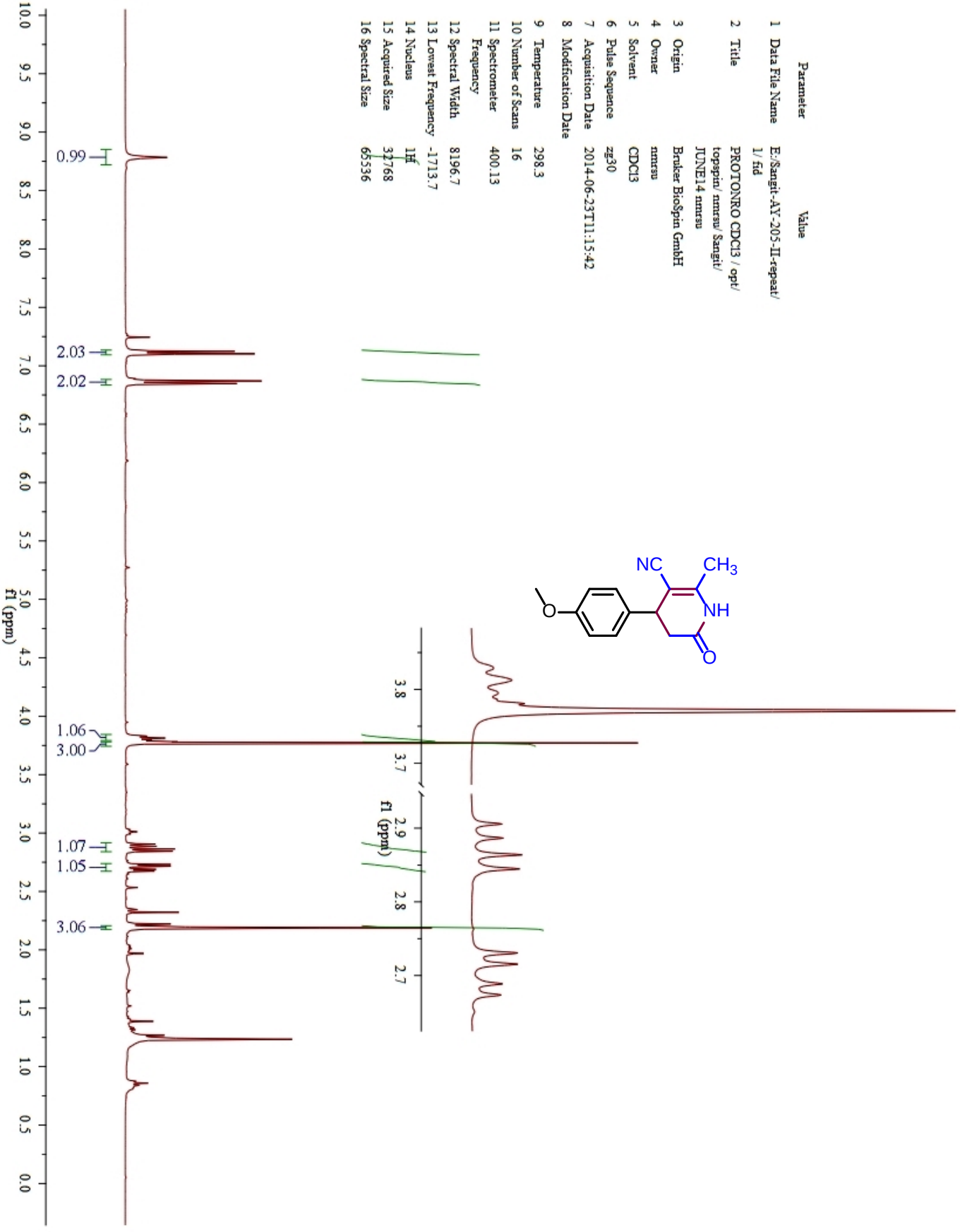

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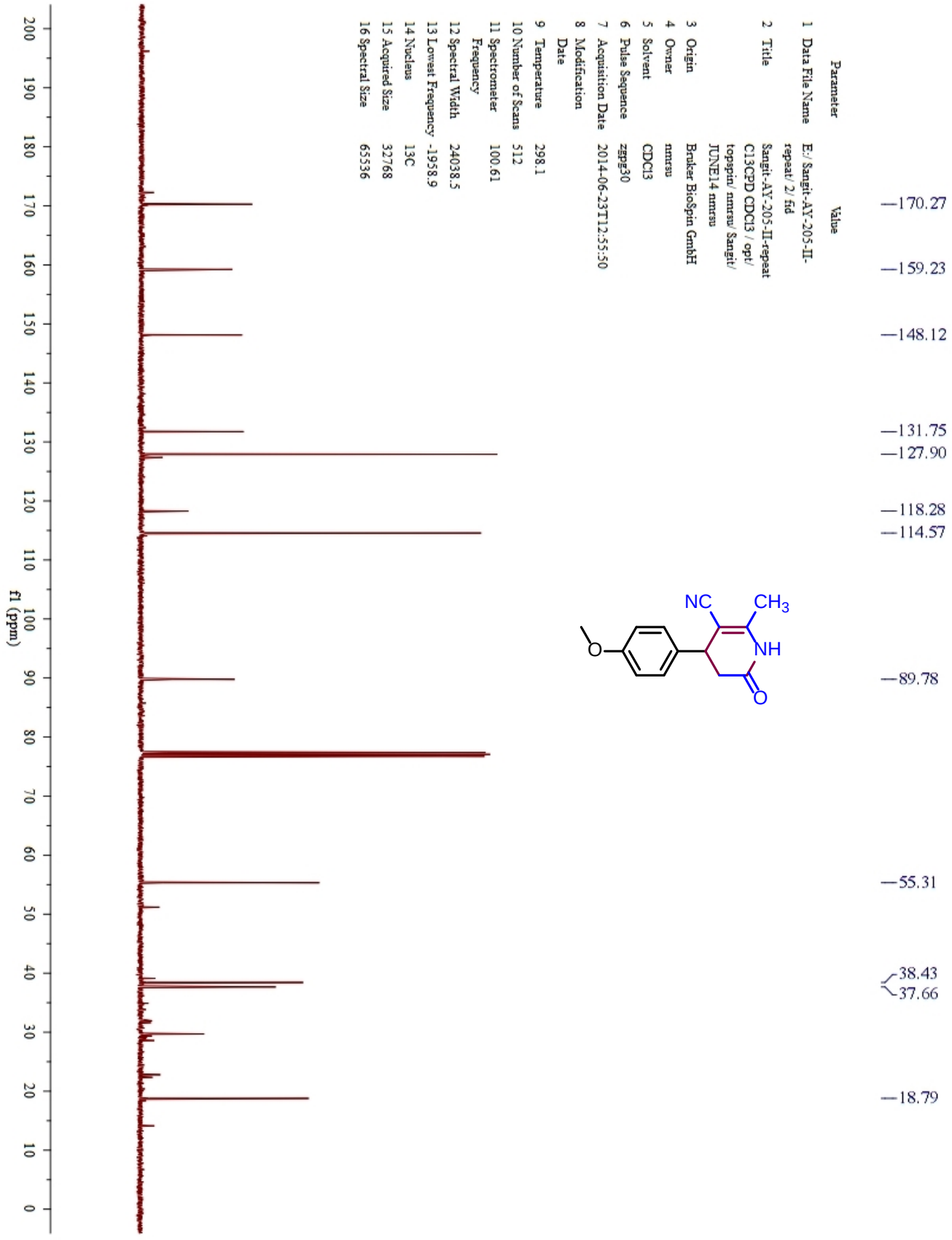

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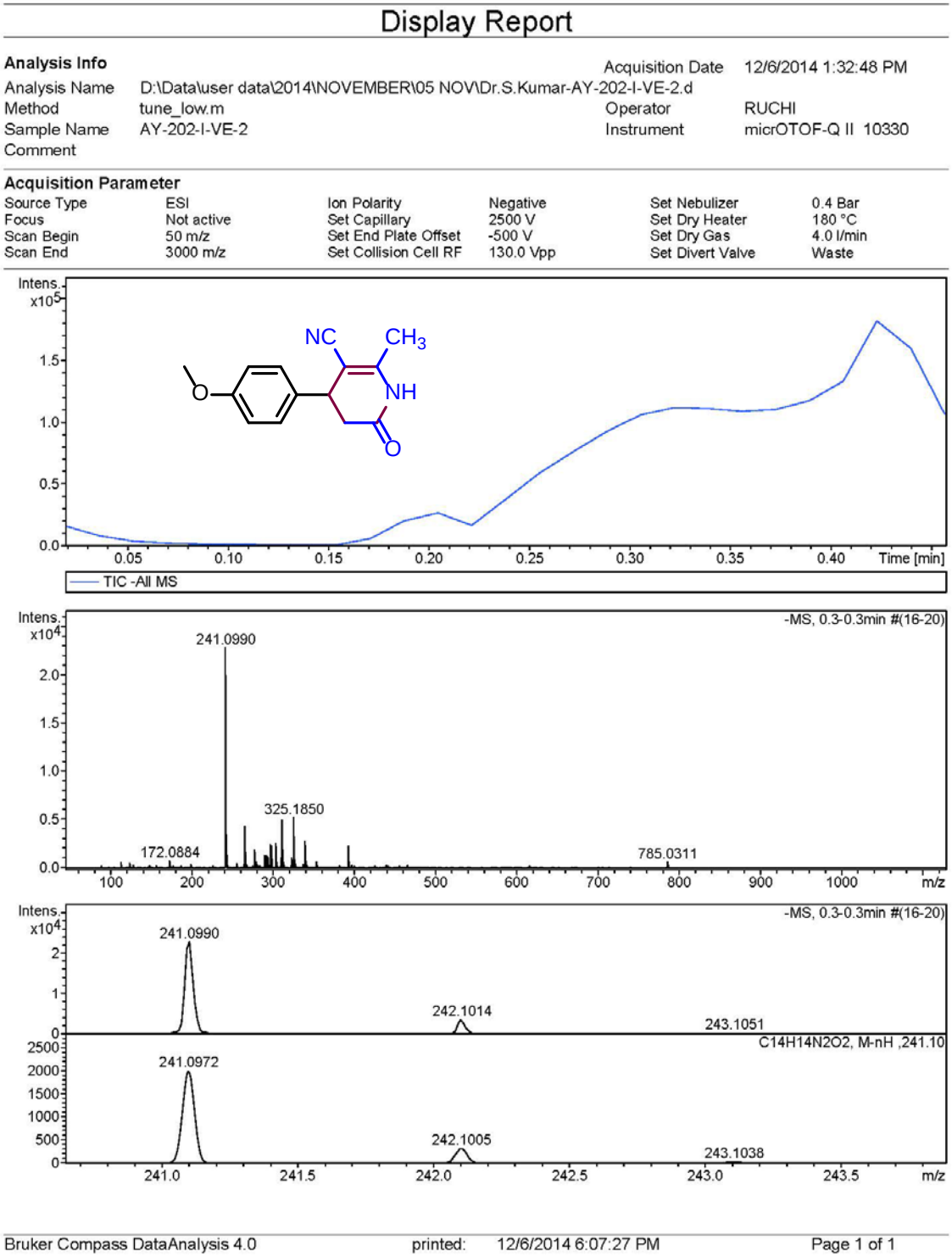

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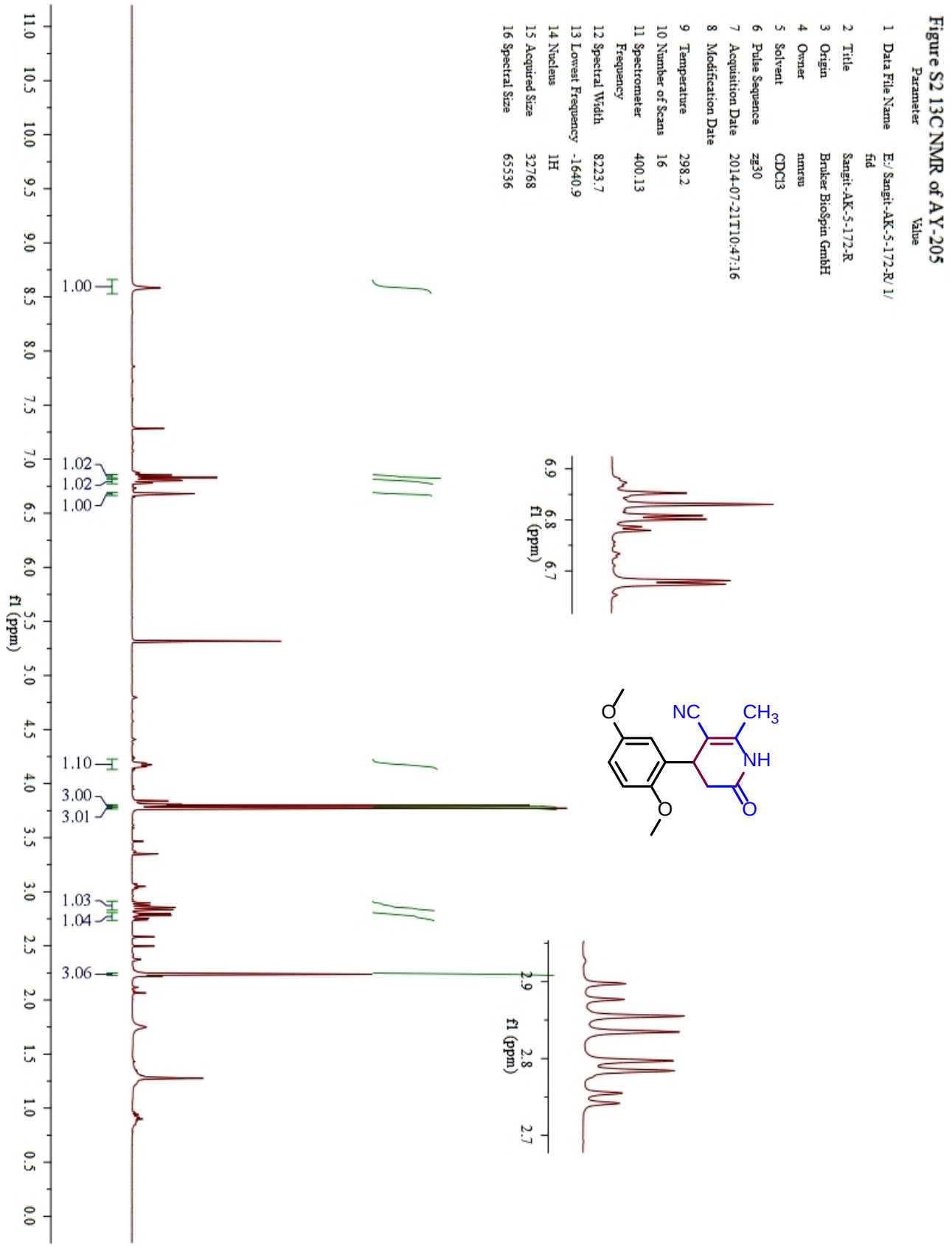

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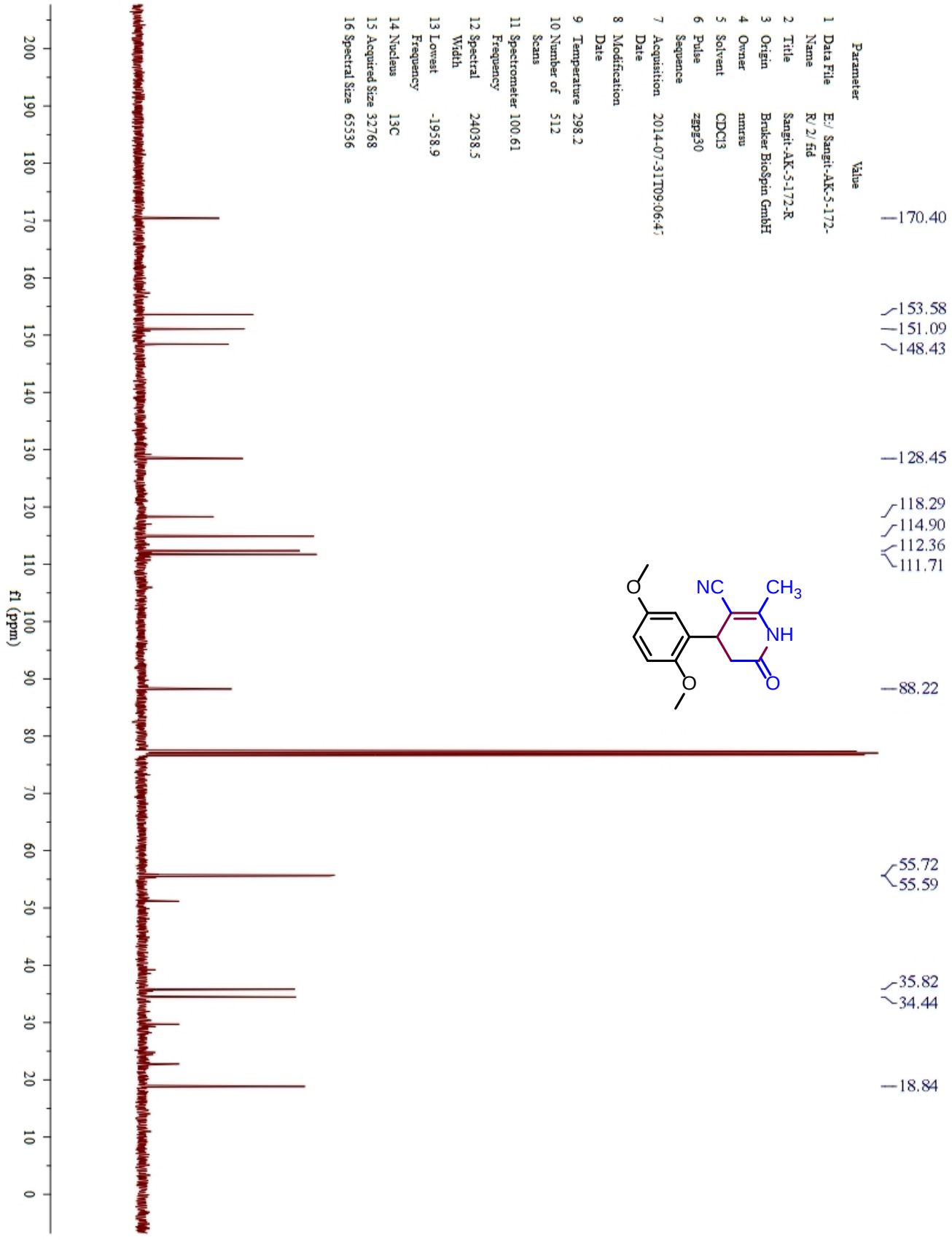

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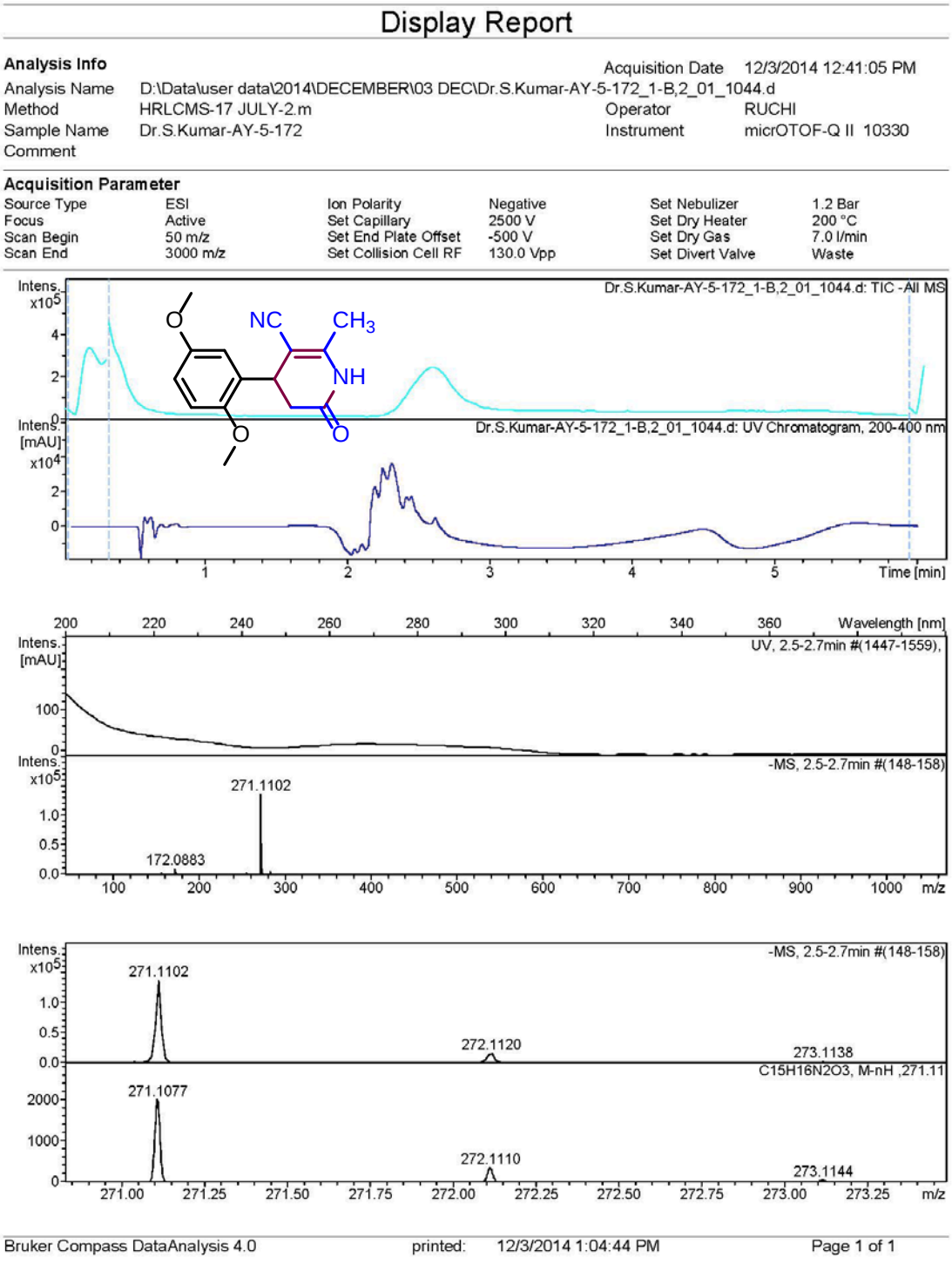

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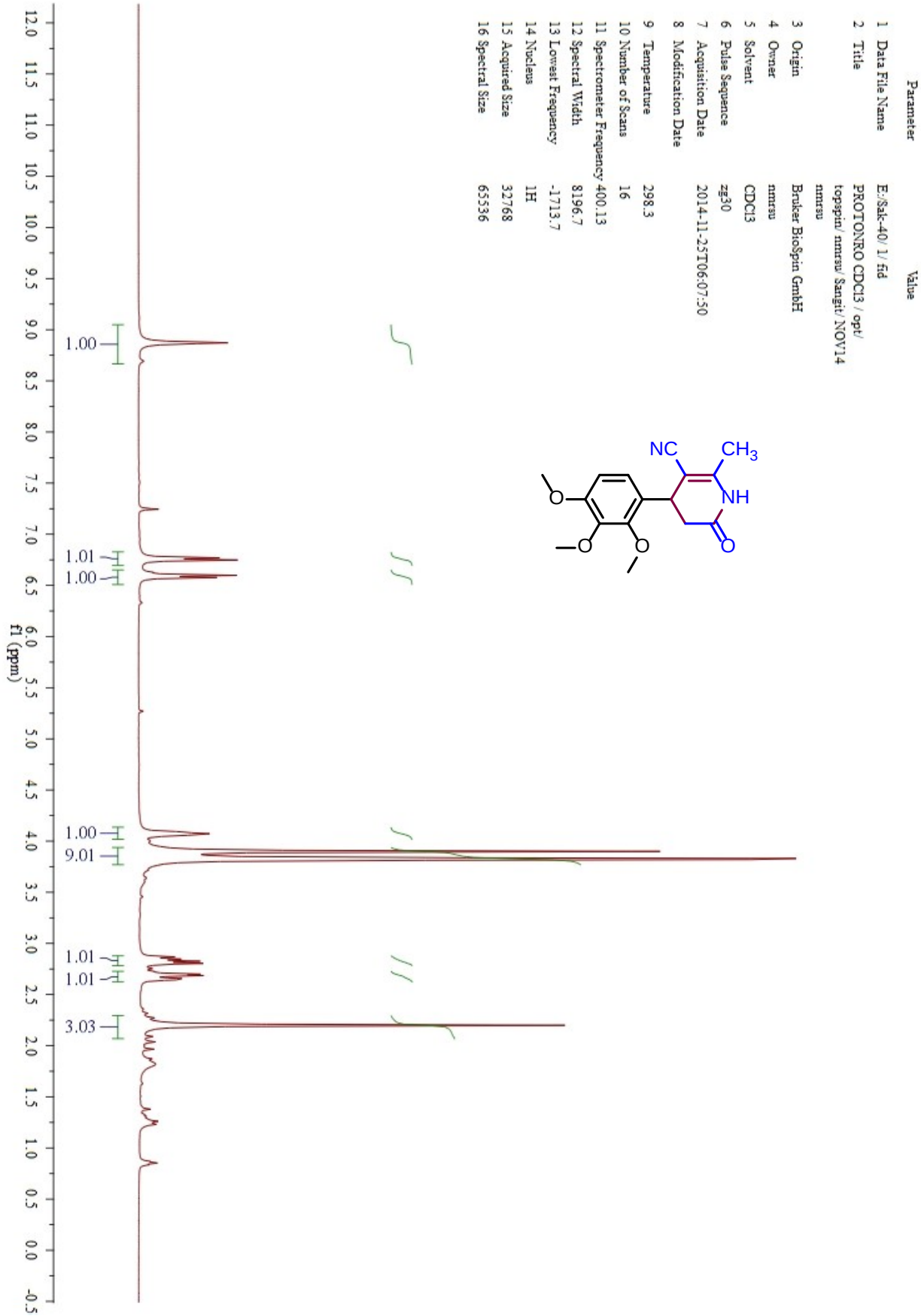
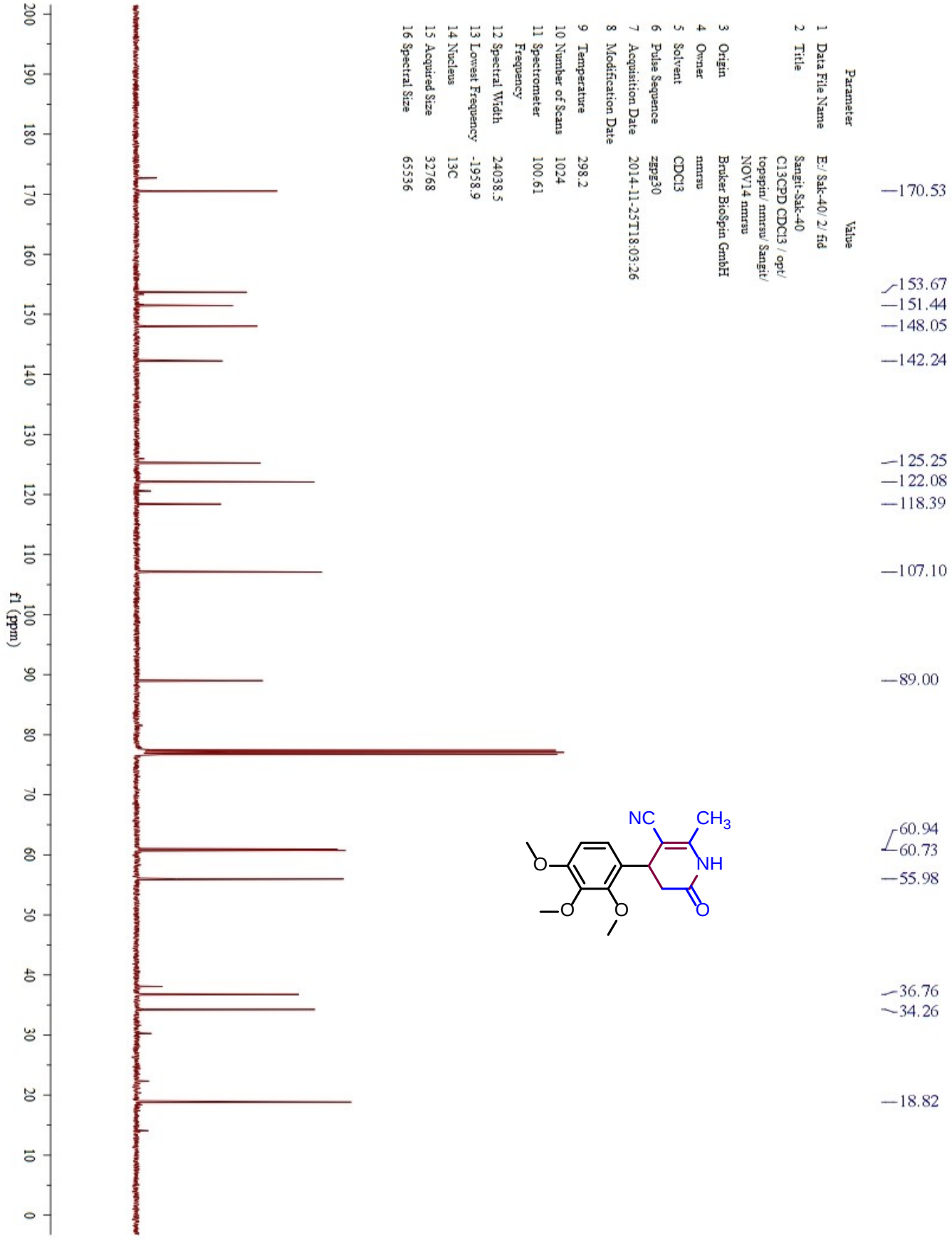


Figure S45 ^{13}C NMR spectra of **15**



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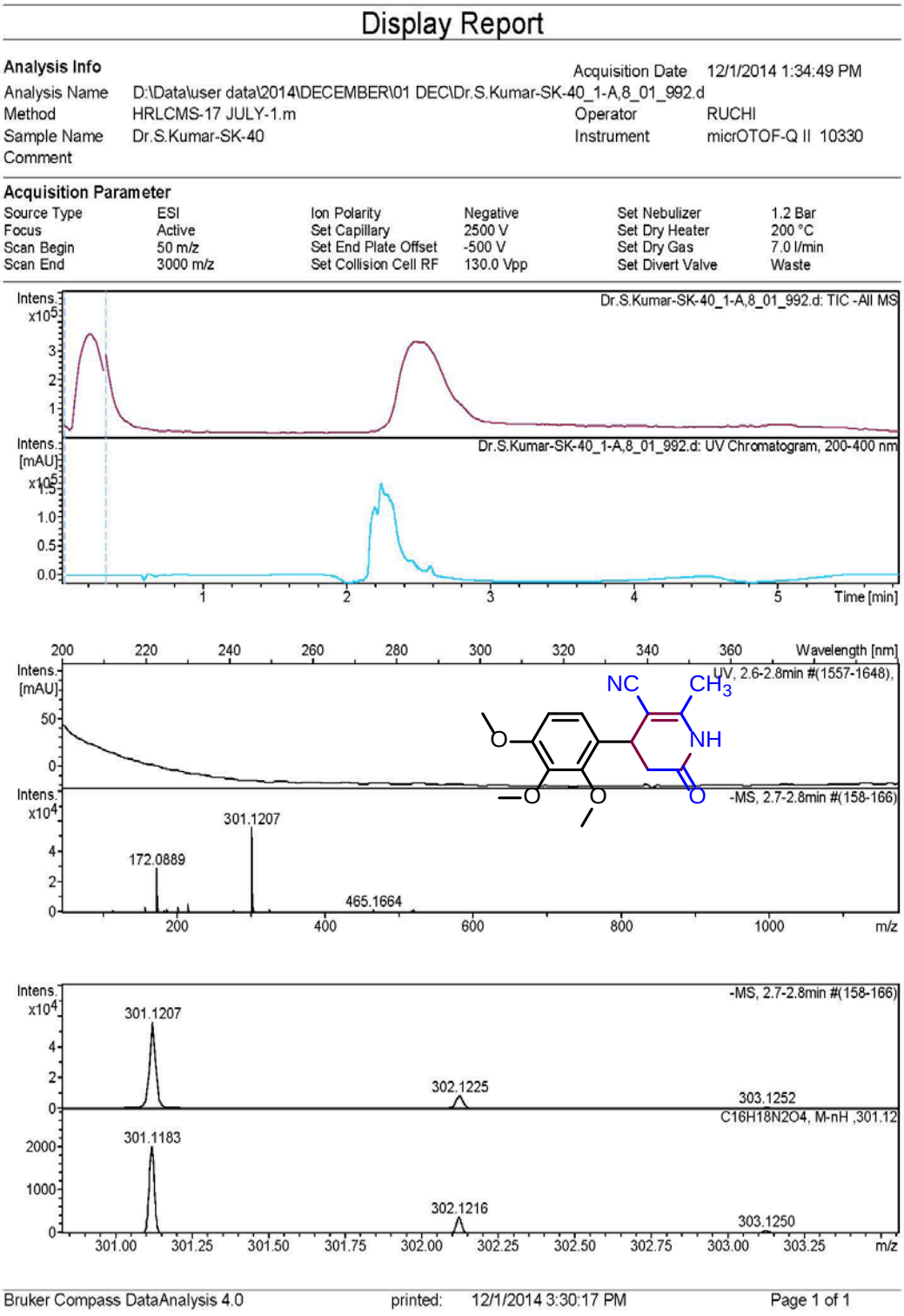
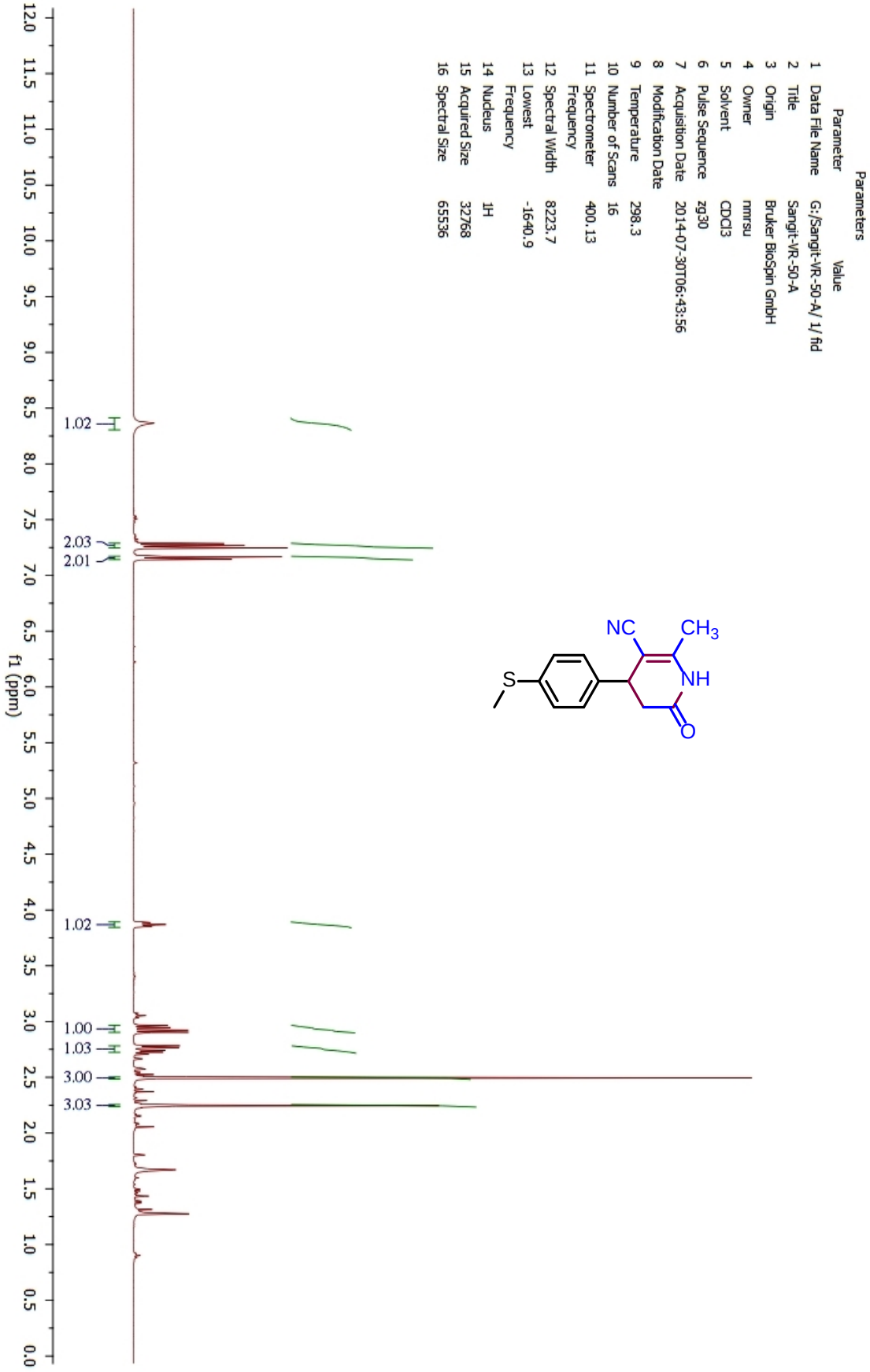


Figure S47 ^{1}H NMR spectra of **16**



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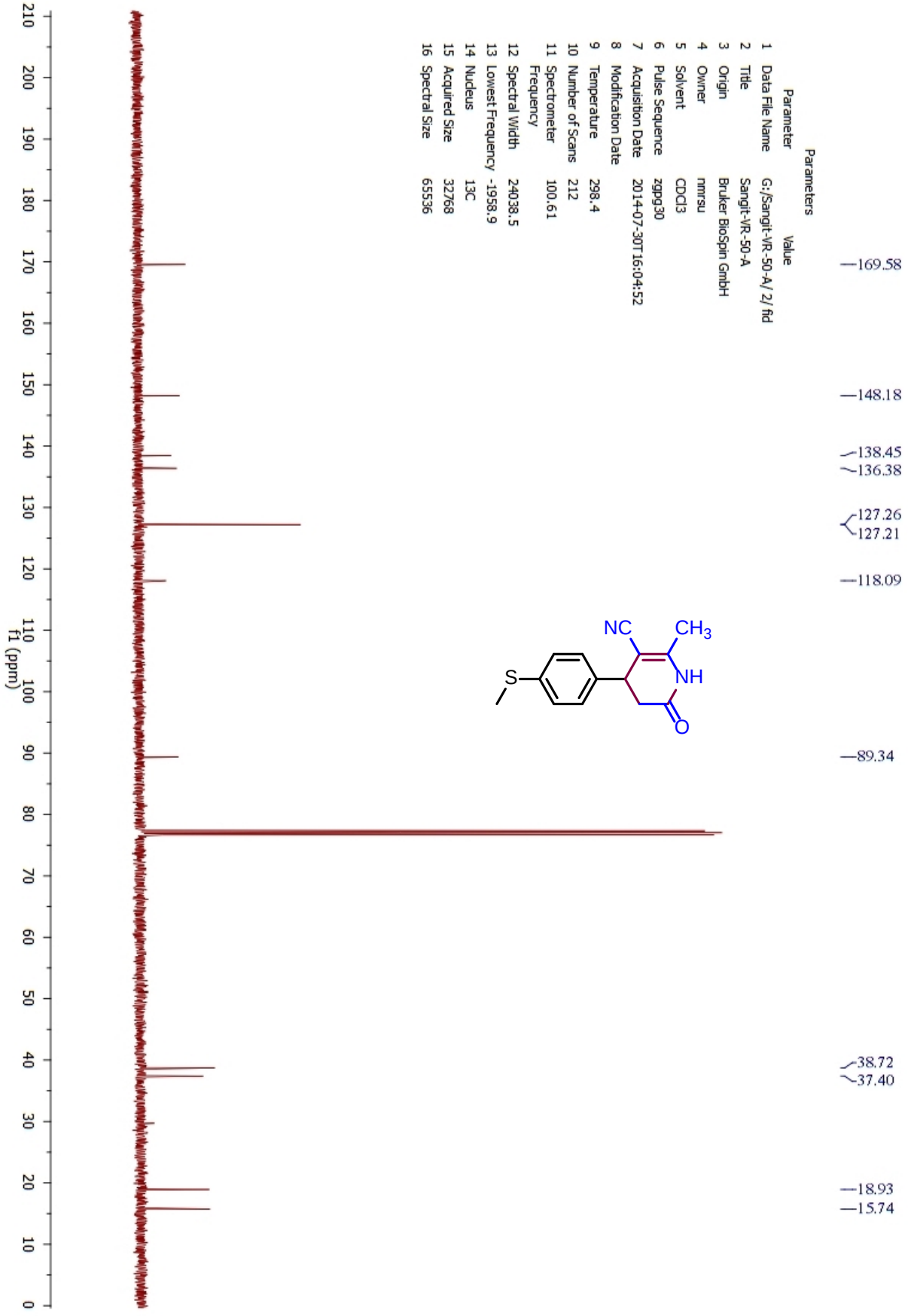

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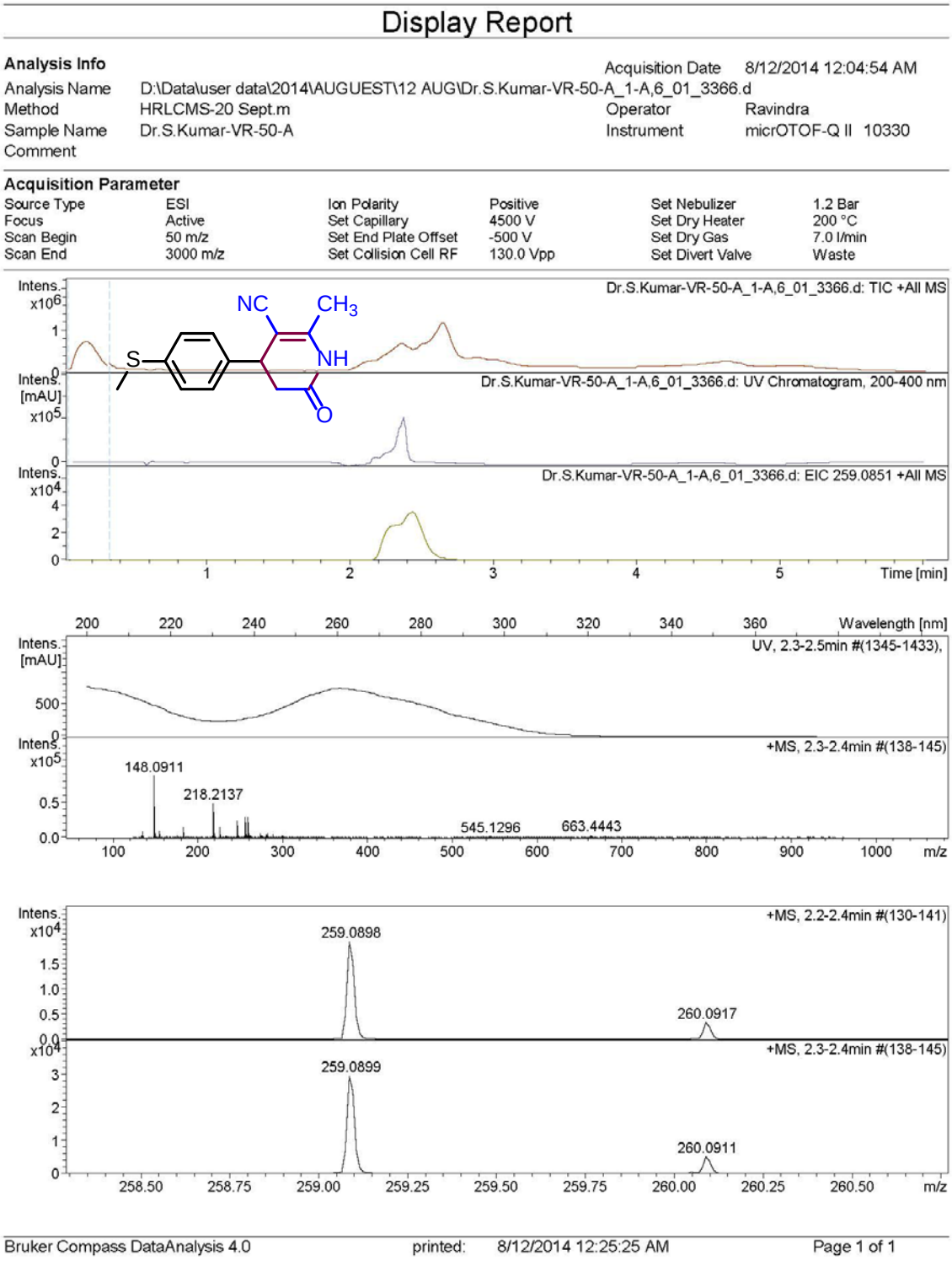

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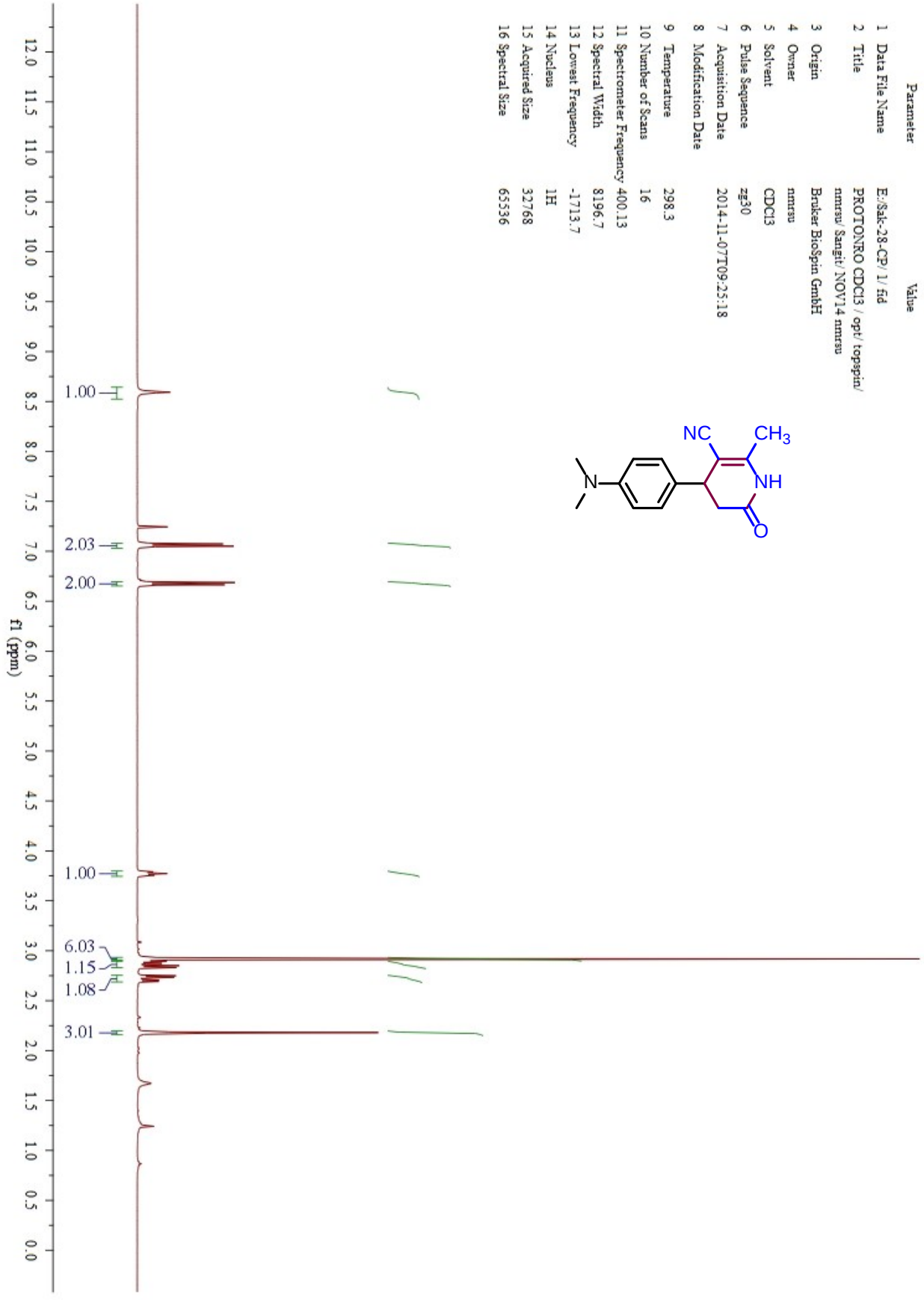

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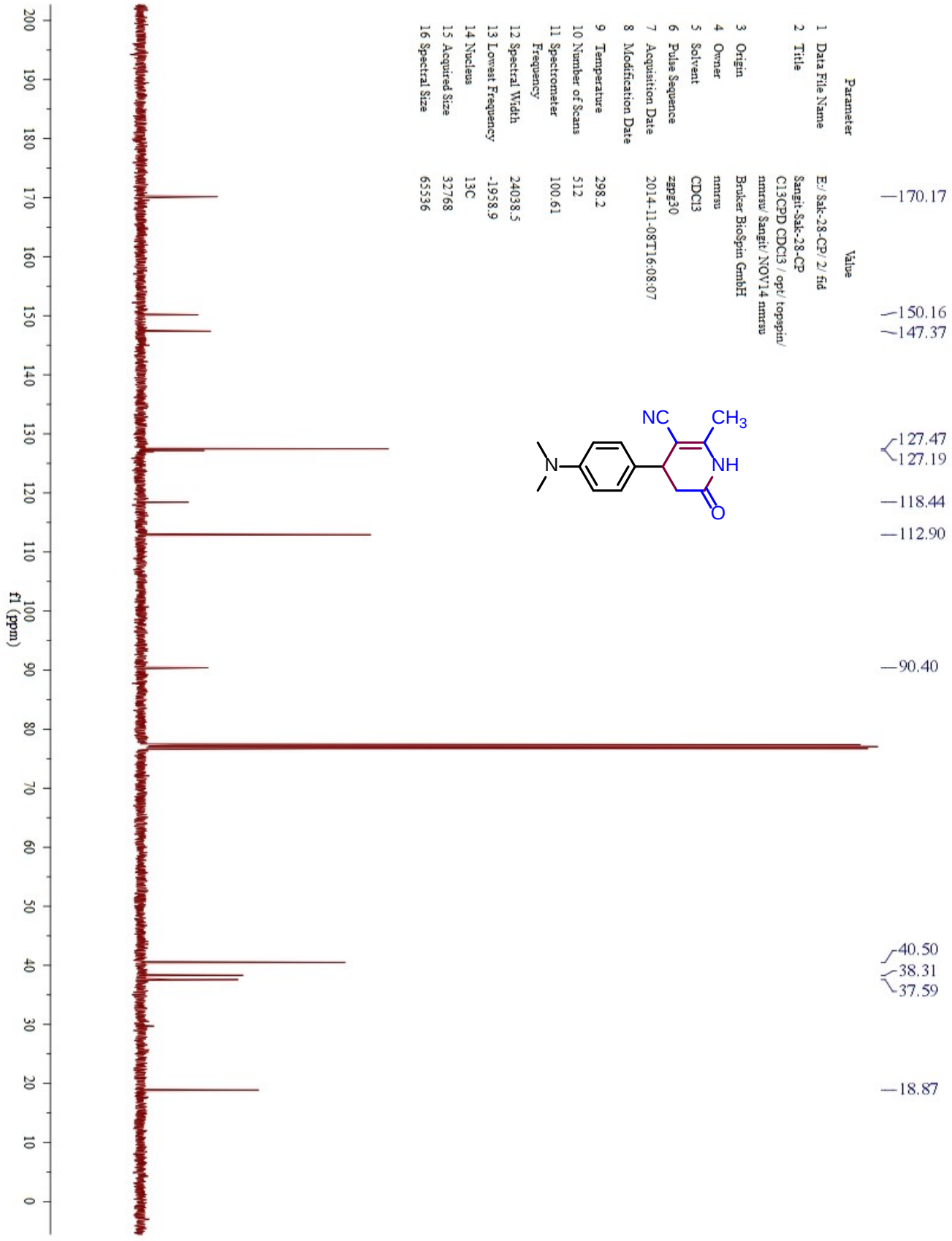

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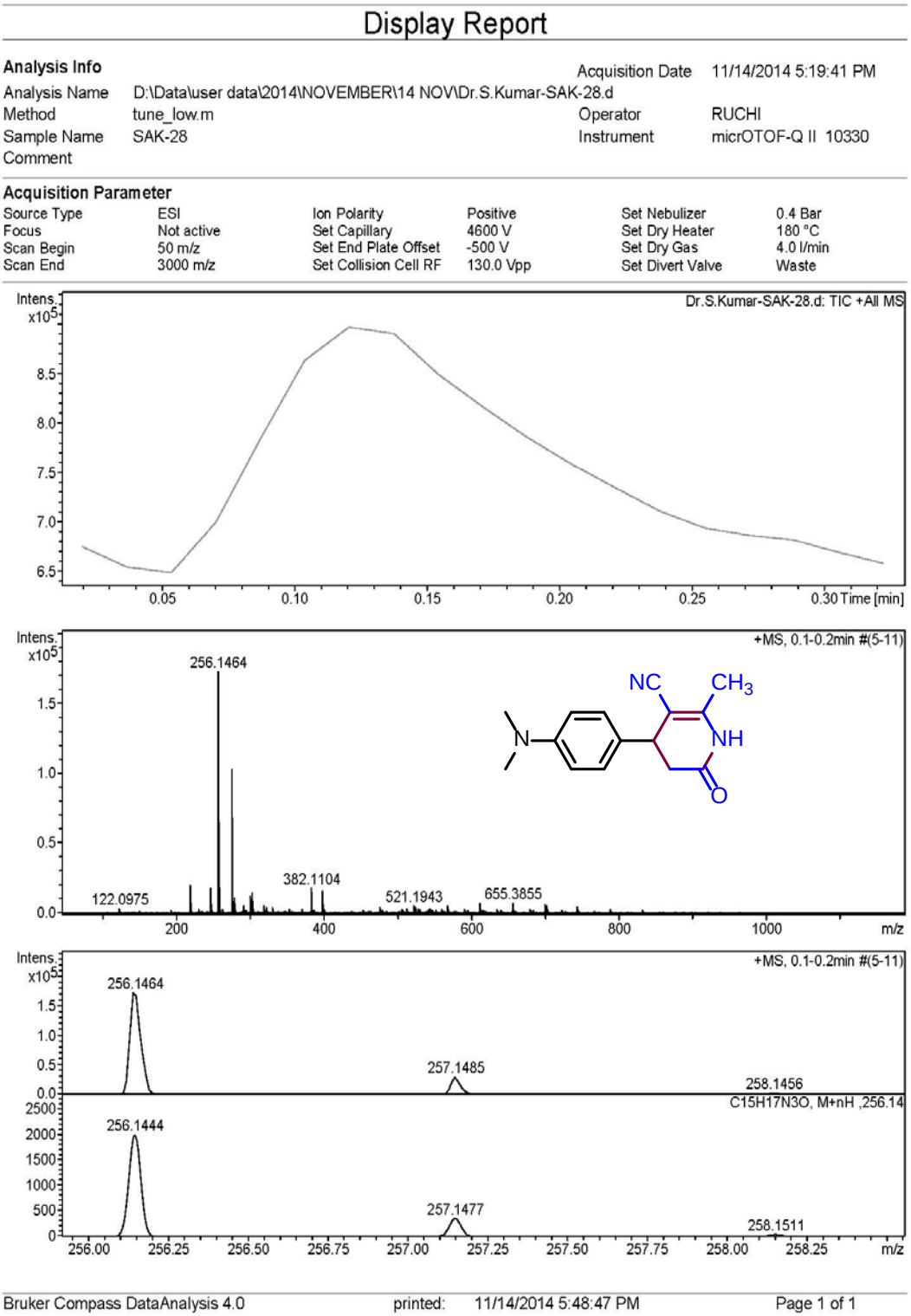

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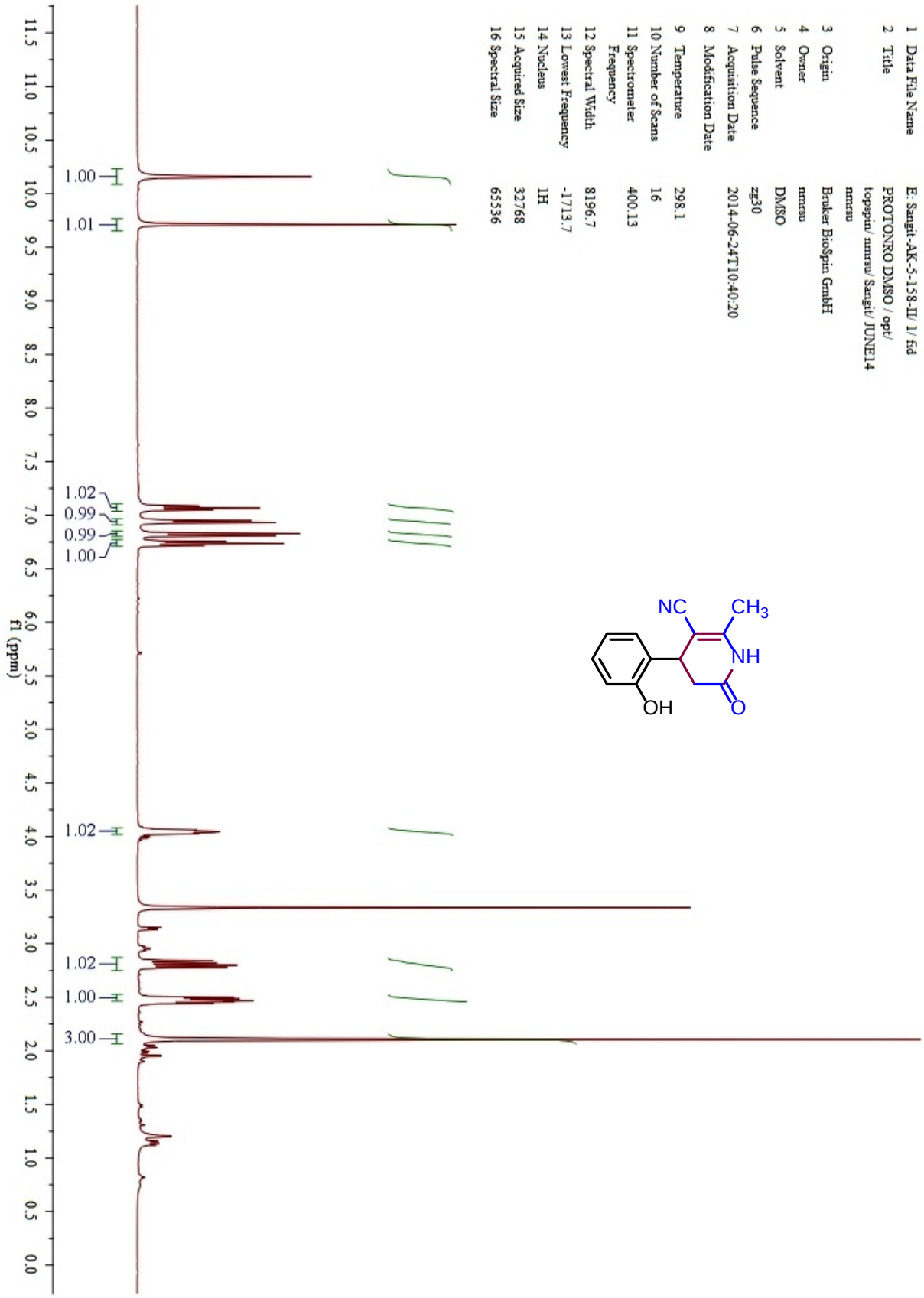


Figure S54 ^{13}C NMR spectra of **18**

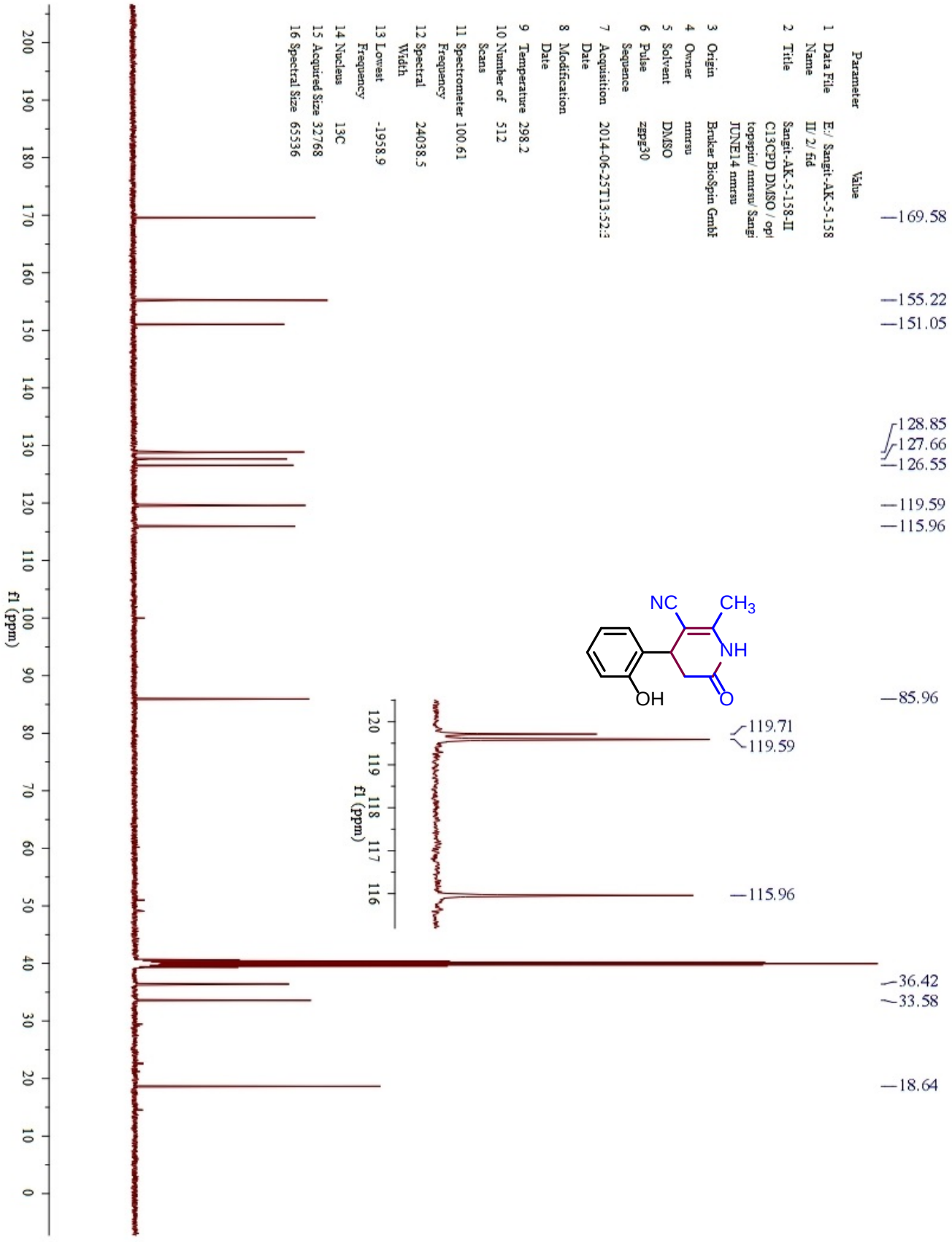


Figure S55 HRMS spectra of **18**

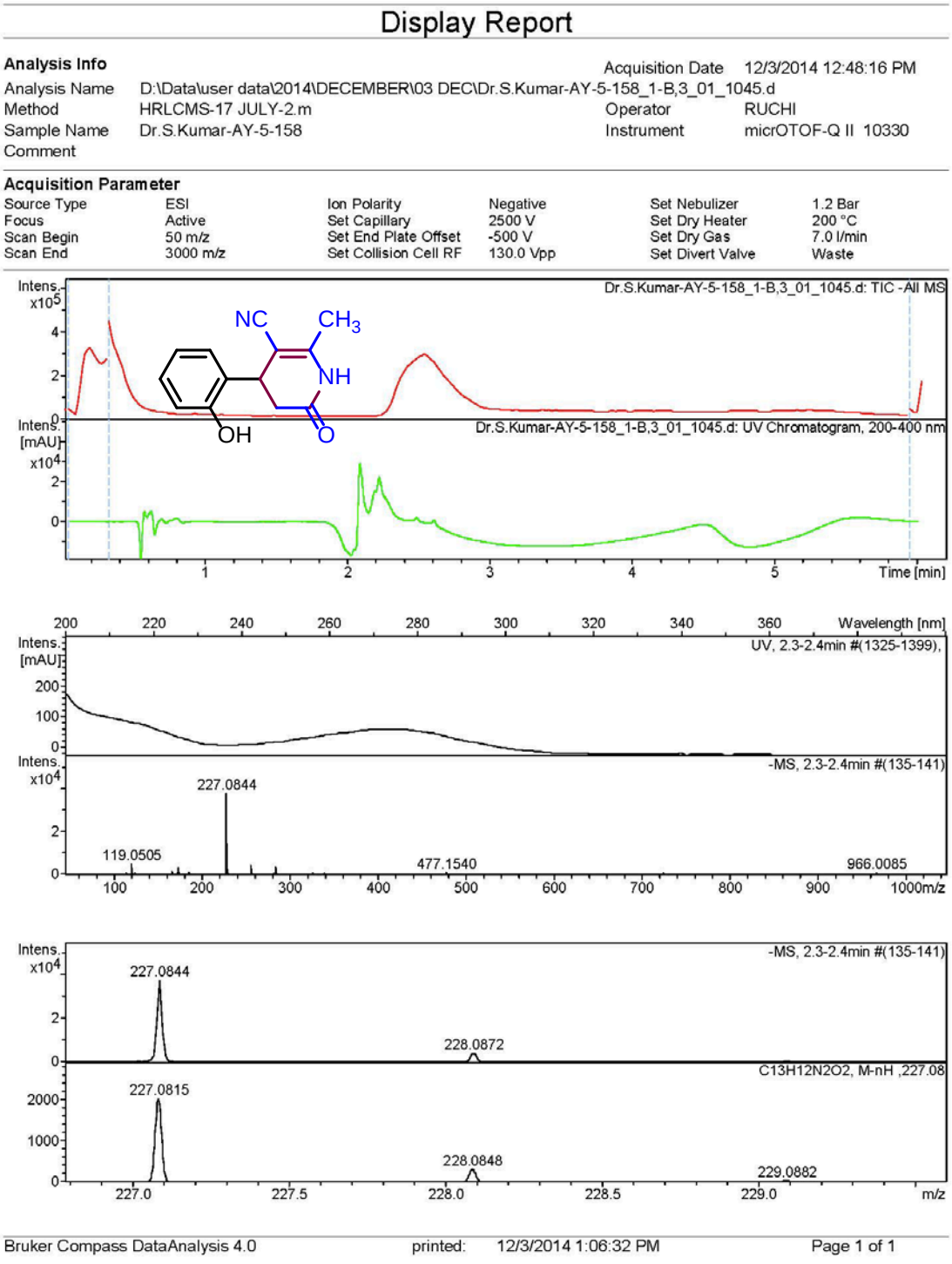


Figure S56 ^{1}H NMR spectra of **19**

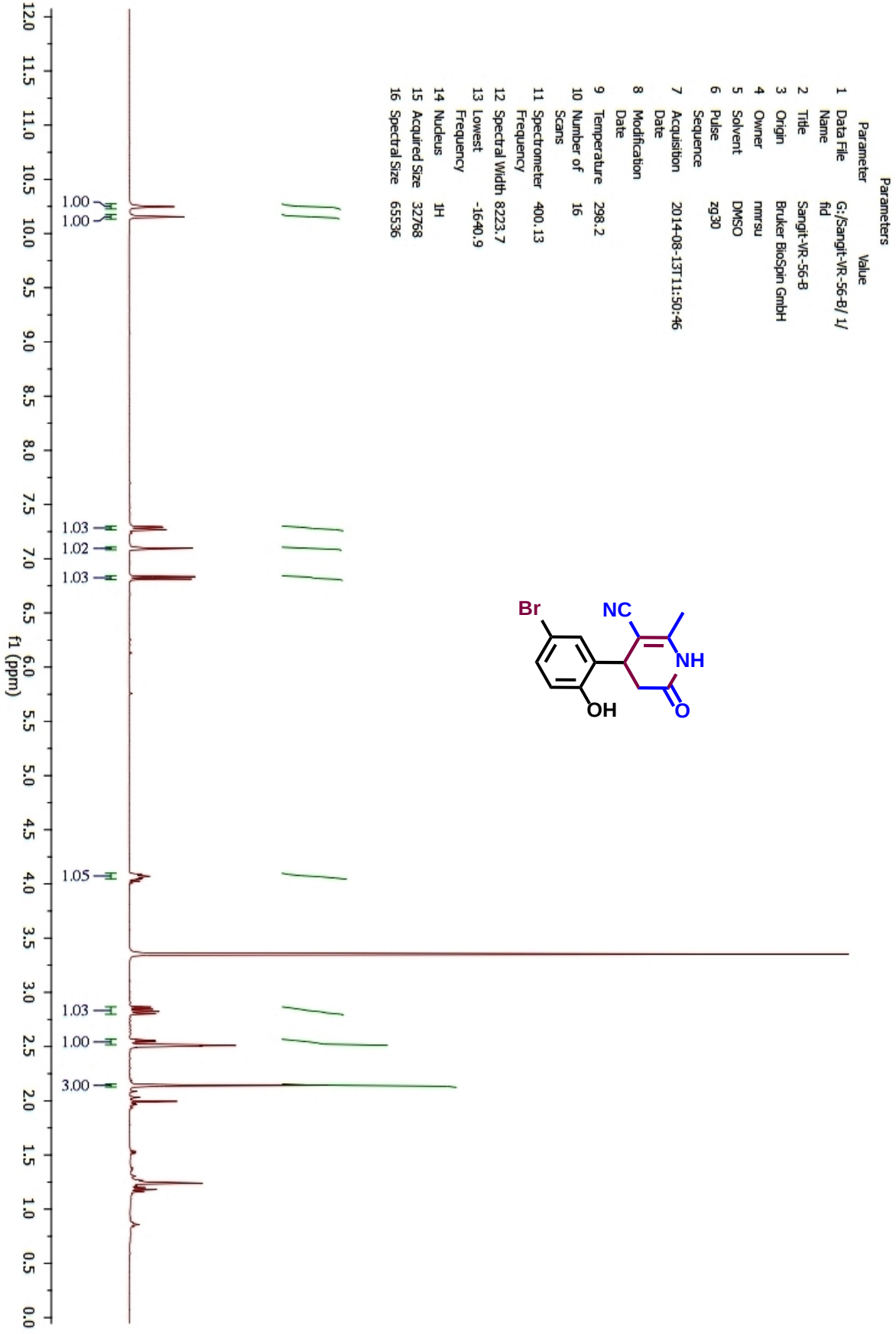


Figure S57 ^{13}C NMR spectra of **19**

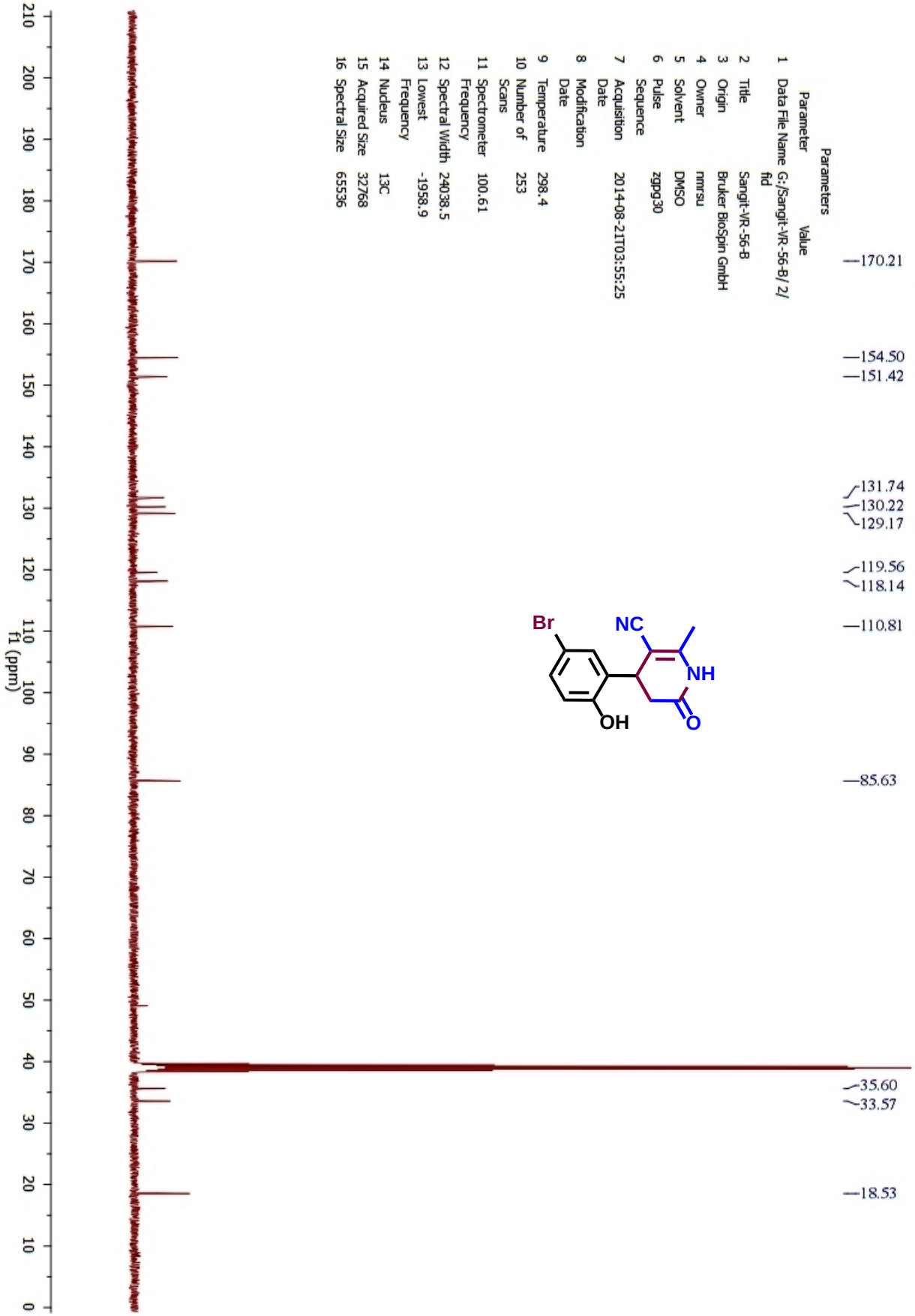


Figure S58 HRMS spectra of **19**

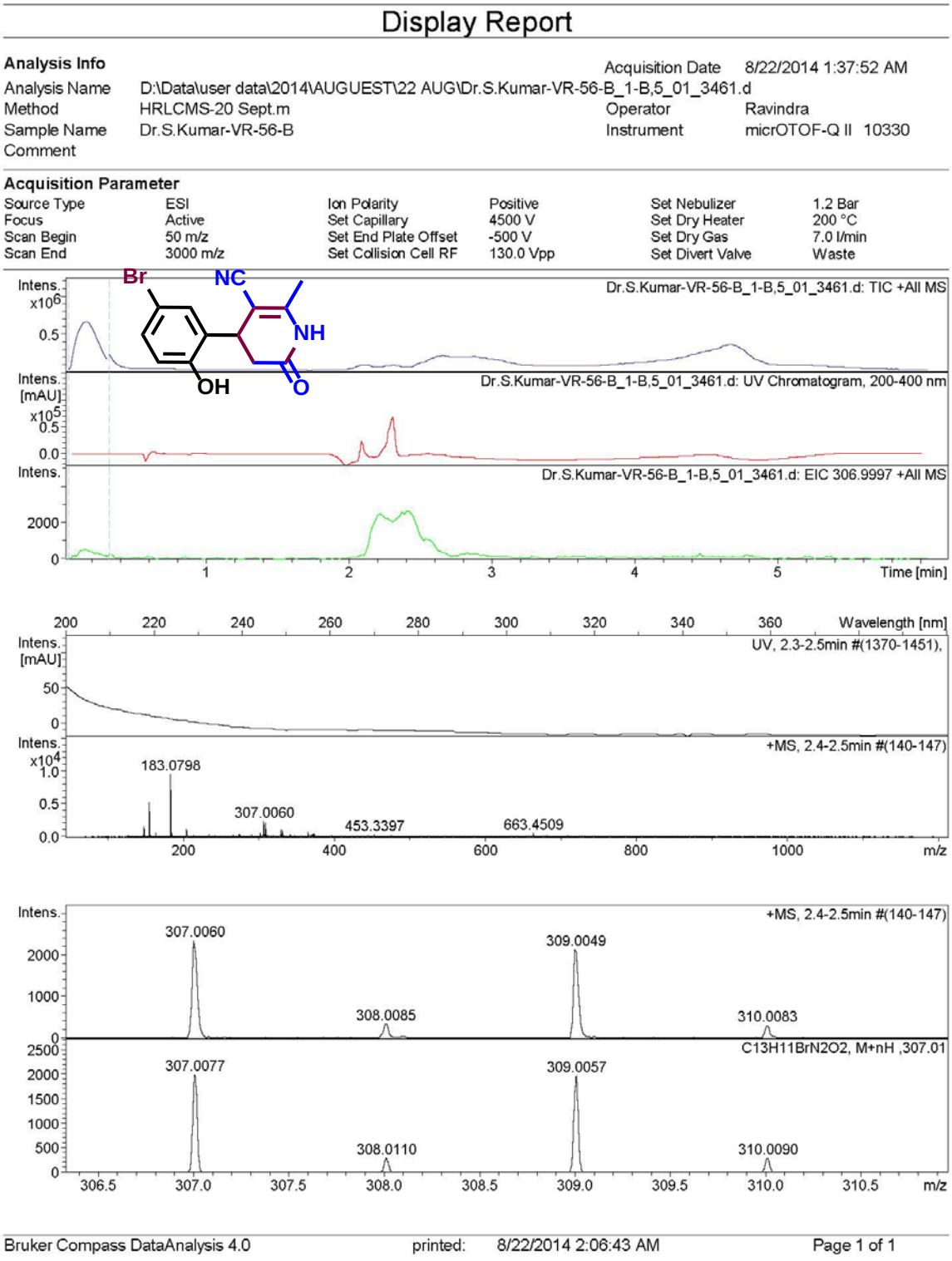


Figure S59 ^{1}H NMR spectra of **20**

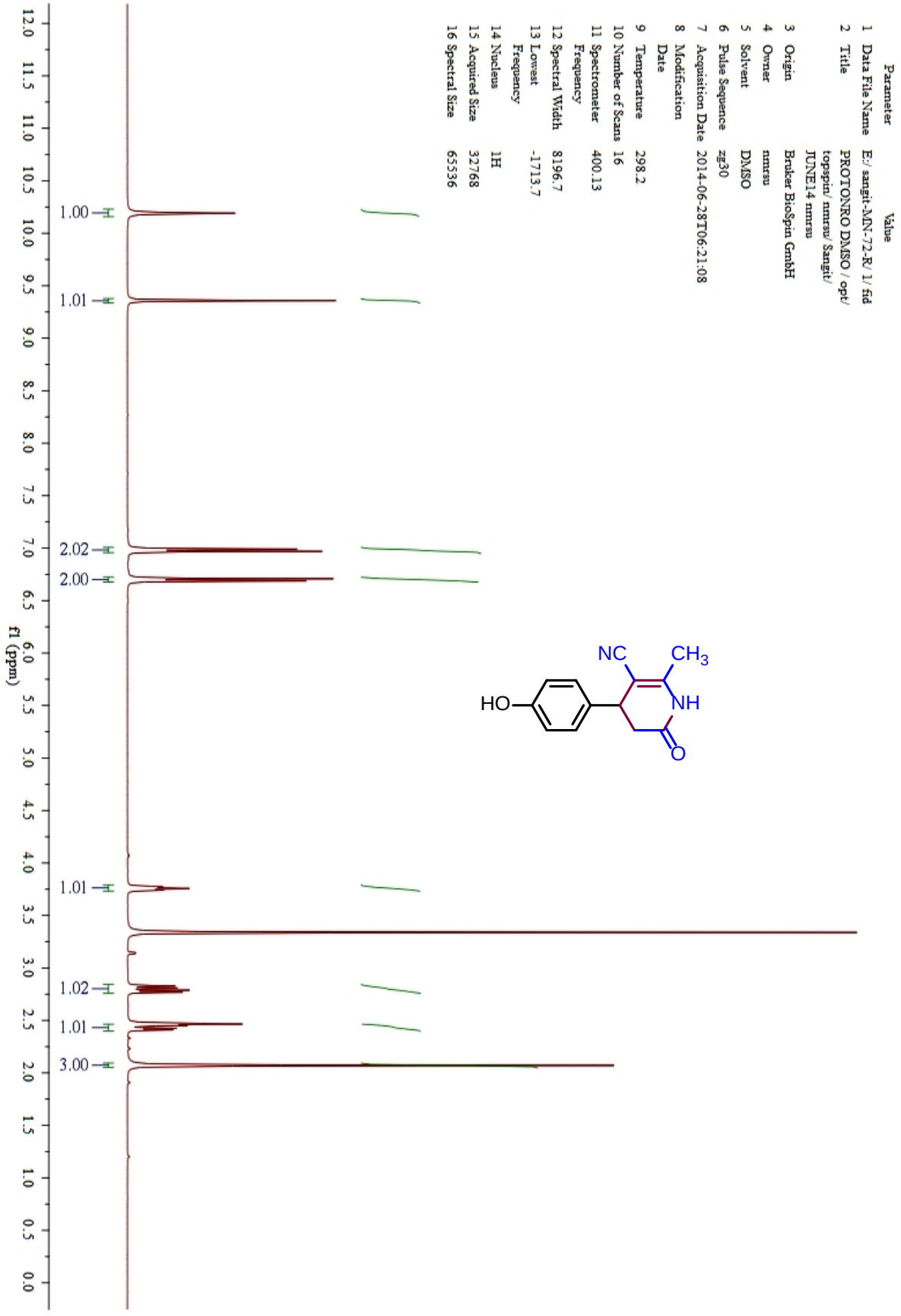


Figure S60 ^{13}C NMR spectra of **20**

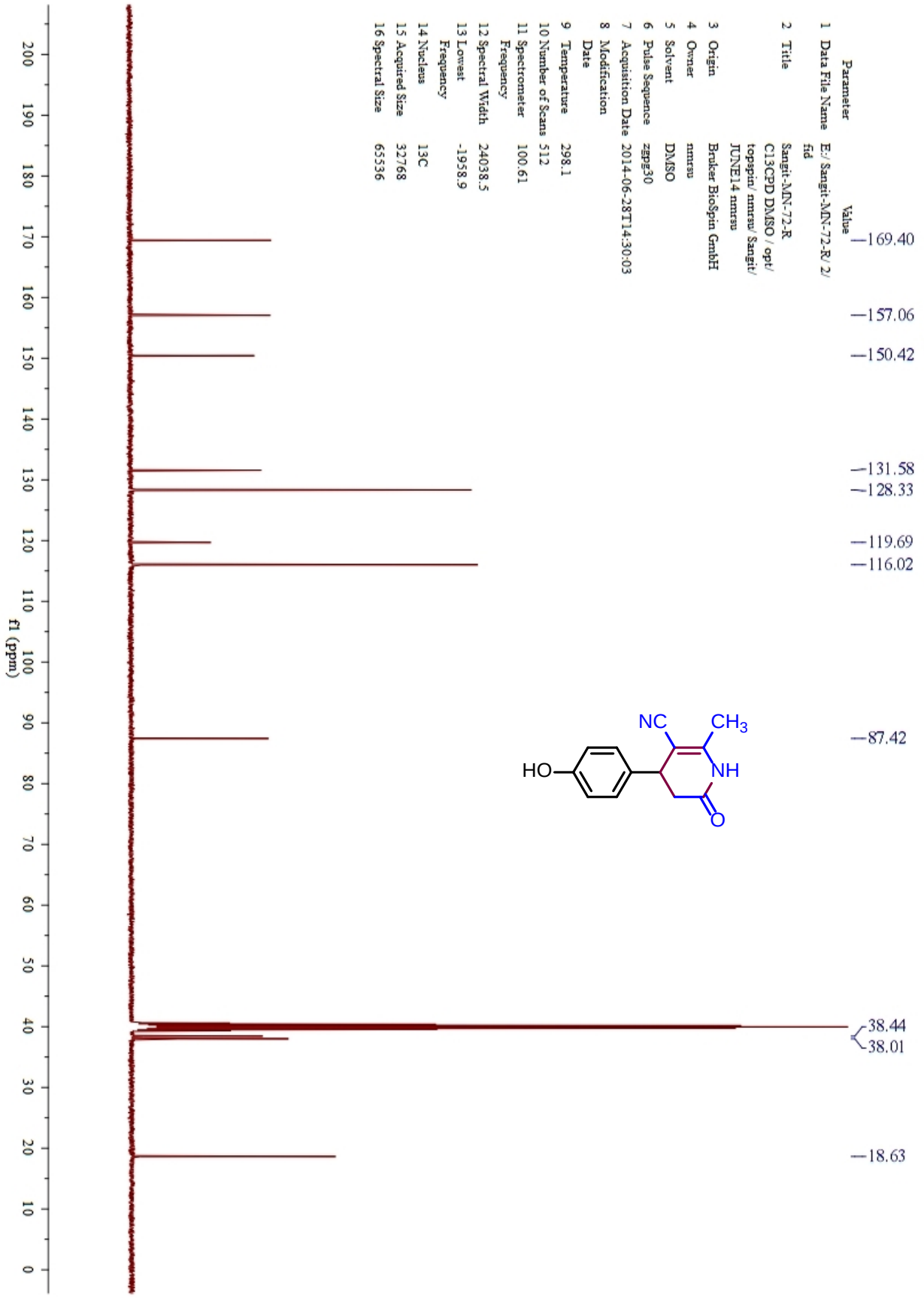


Figure S61 Mass spectra of **20**

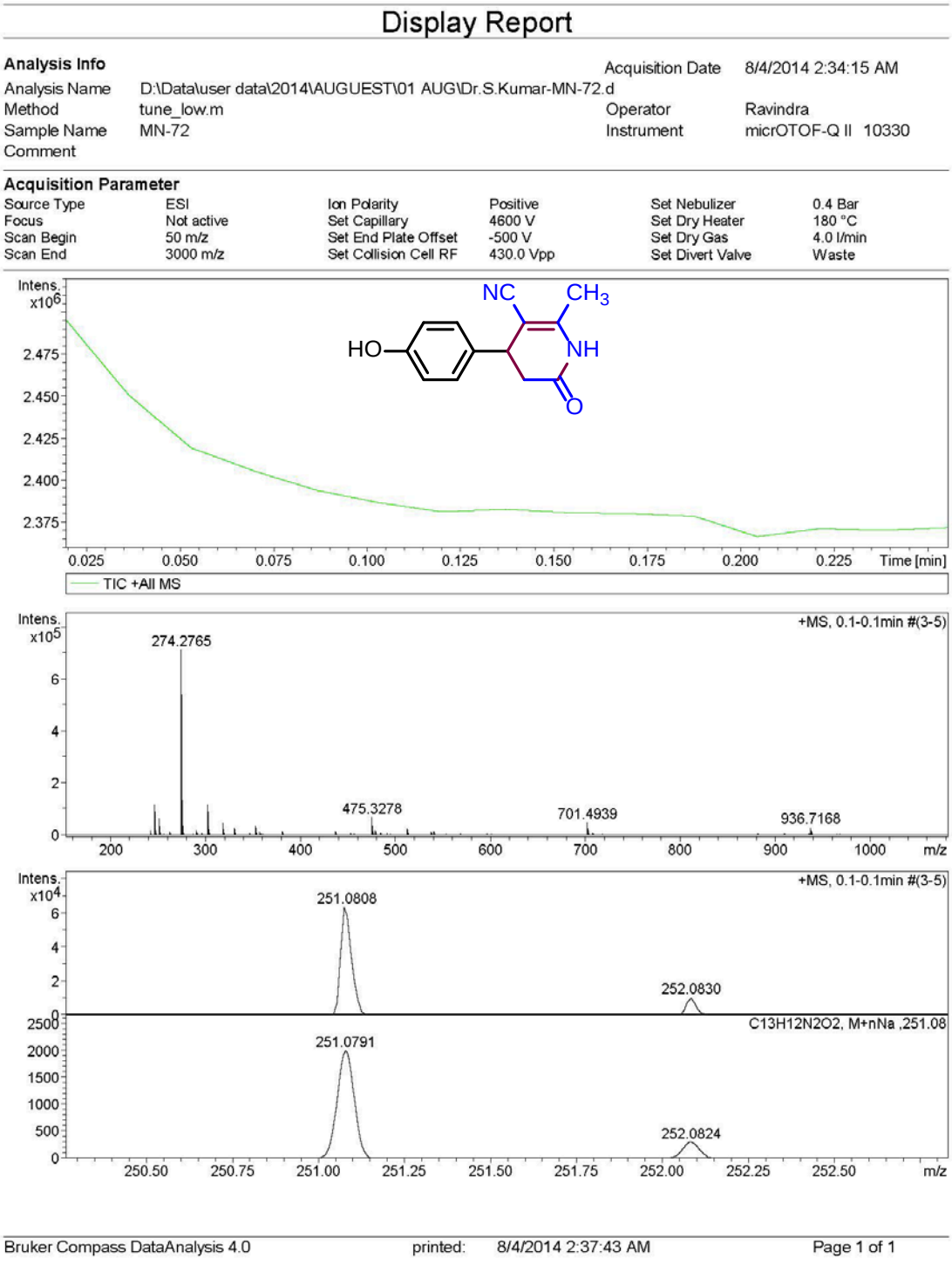


Figure S62 ^{1}H NMR spectra of **21**

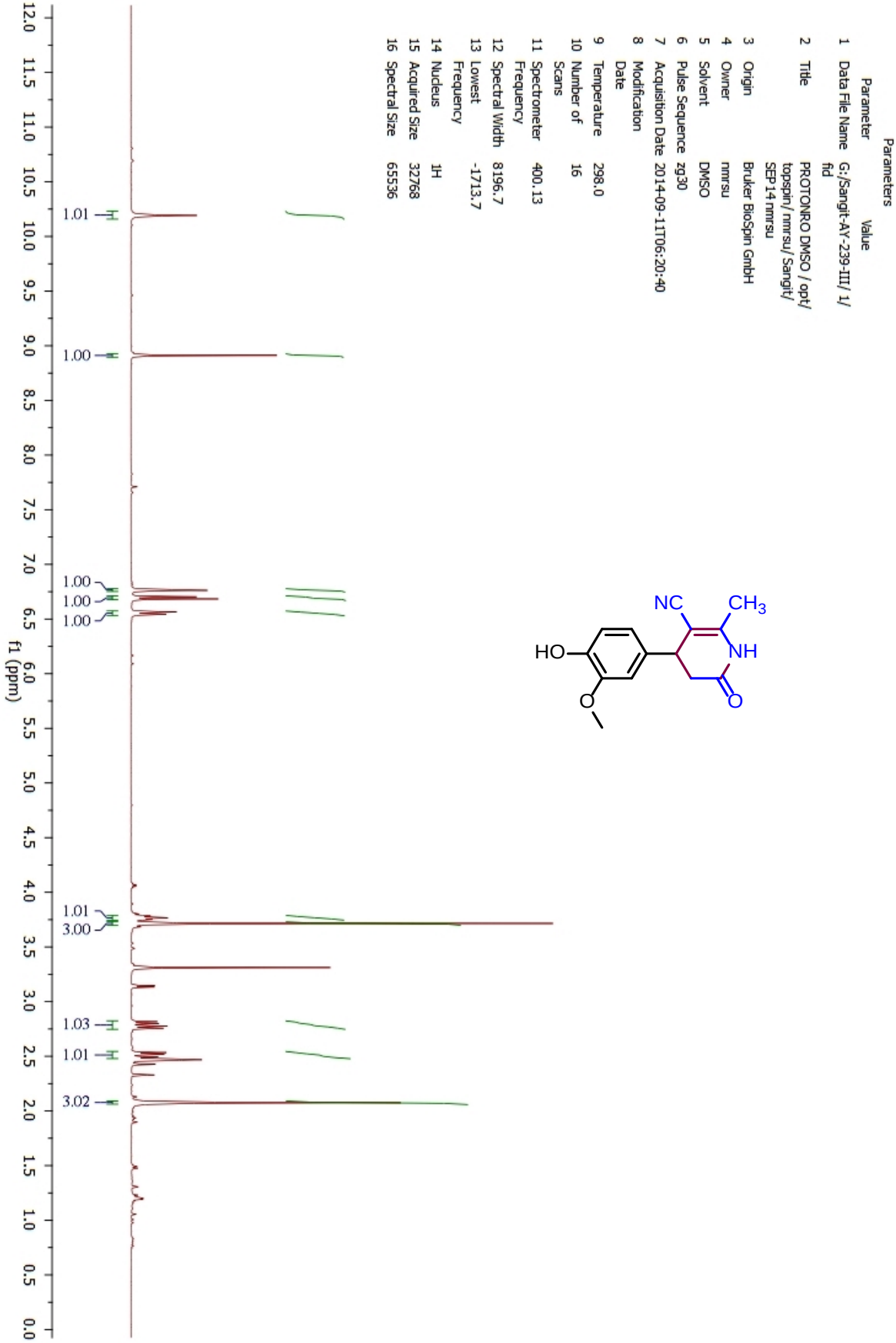


Figure S63 ^{13}C NMR spectra of **21**

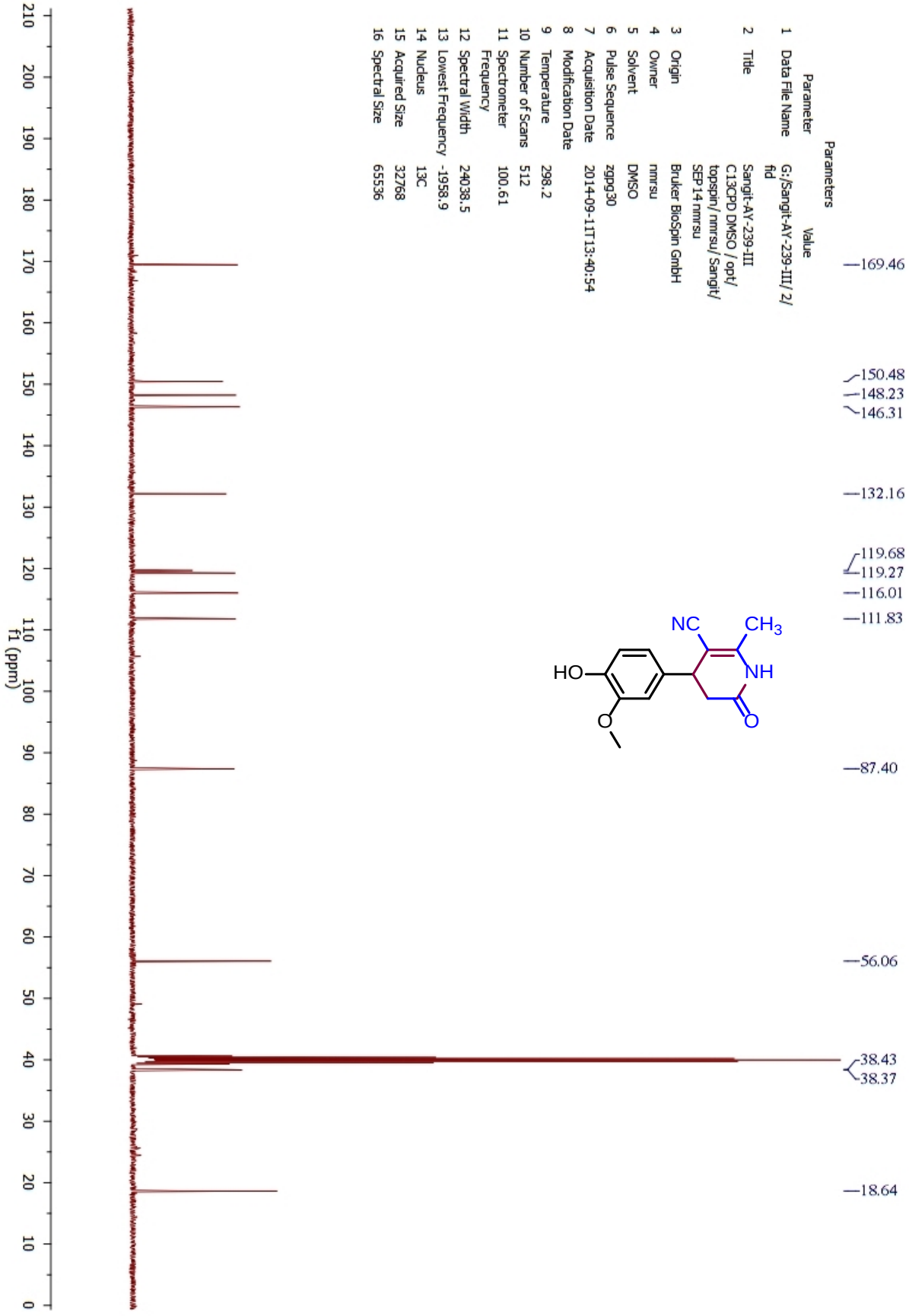


Figure S64 HRMS spectra of **21**

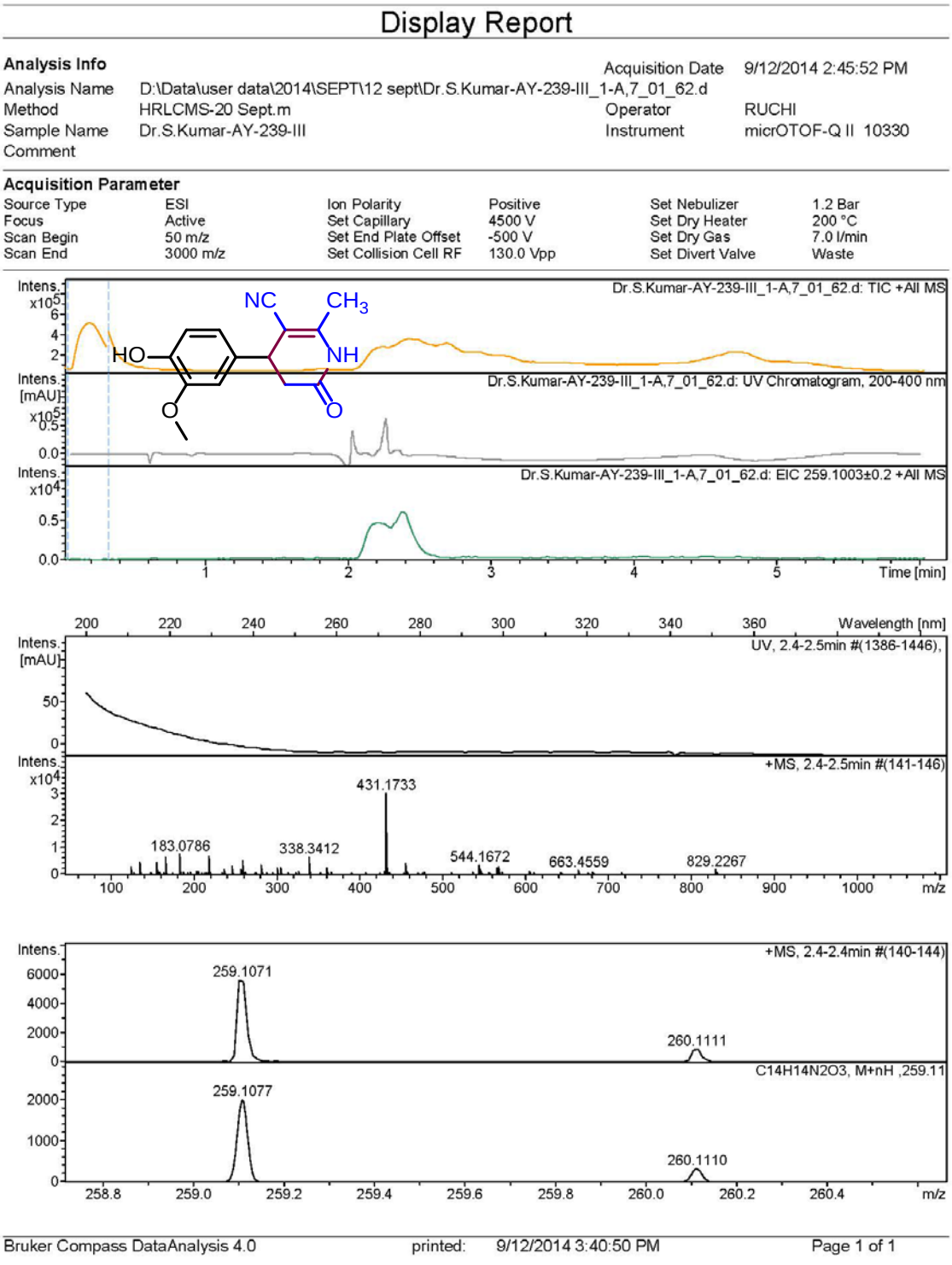


Figure S65 ^{1}H NMR spectra of **22**

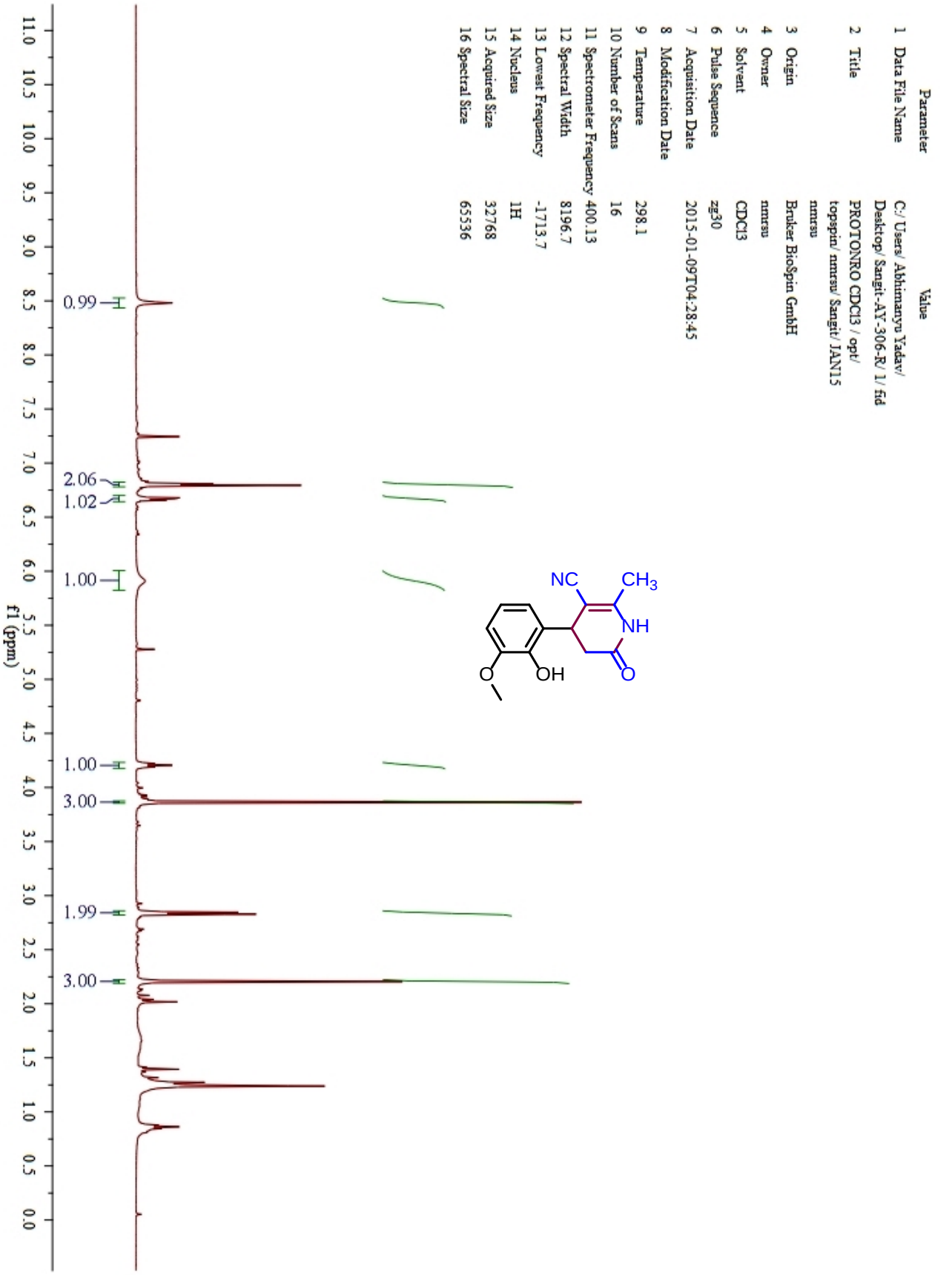


Figure S66 ^{13}C NMR spectra of **22**

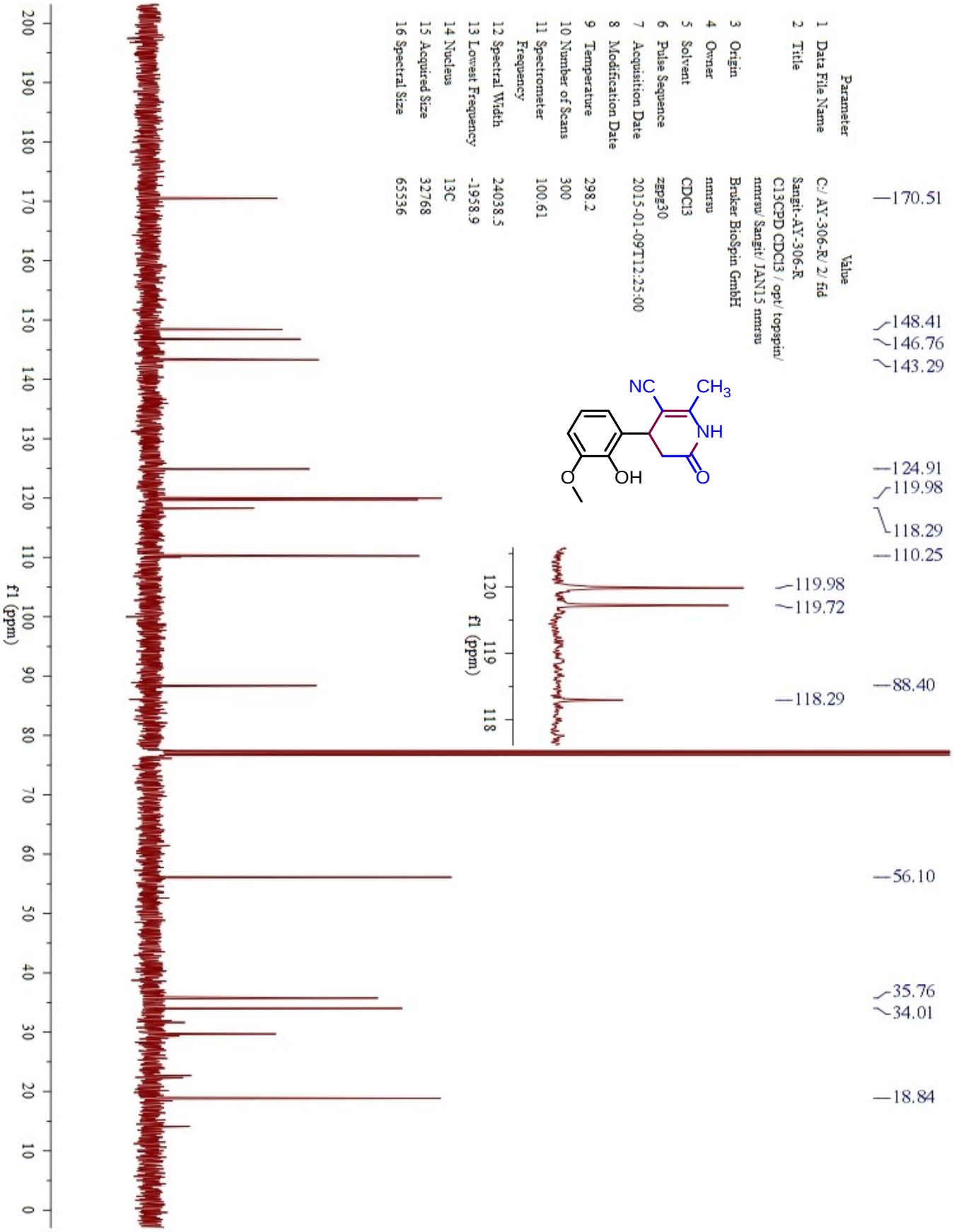


Figure S67 HRMS spectra of **22**

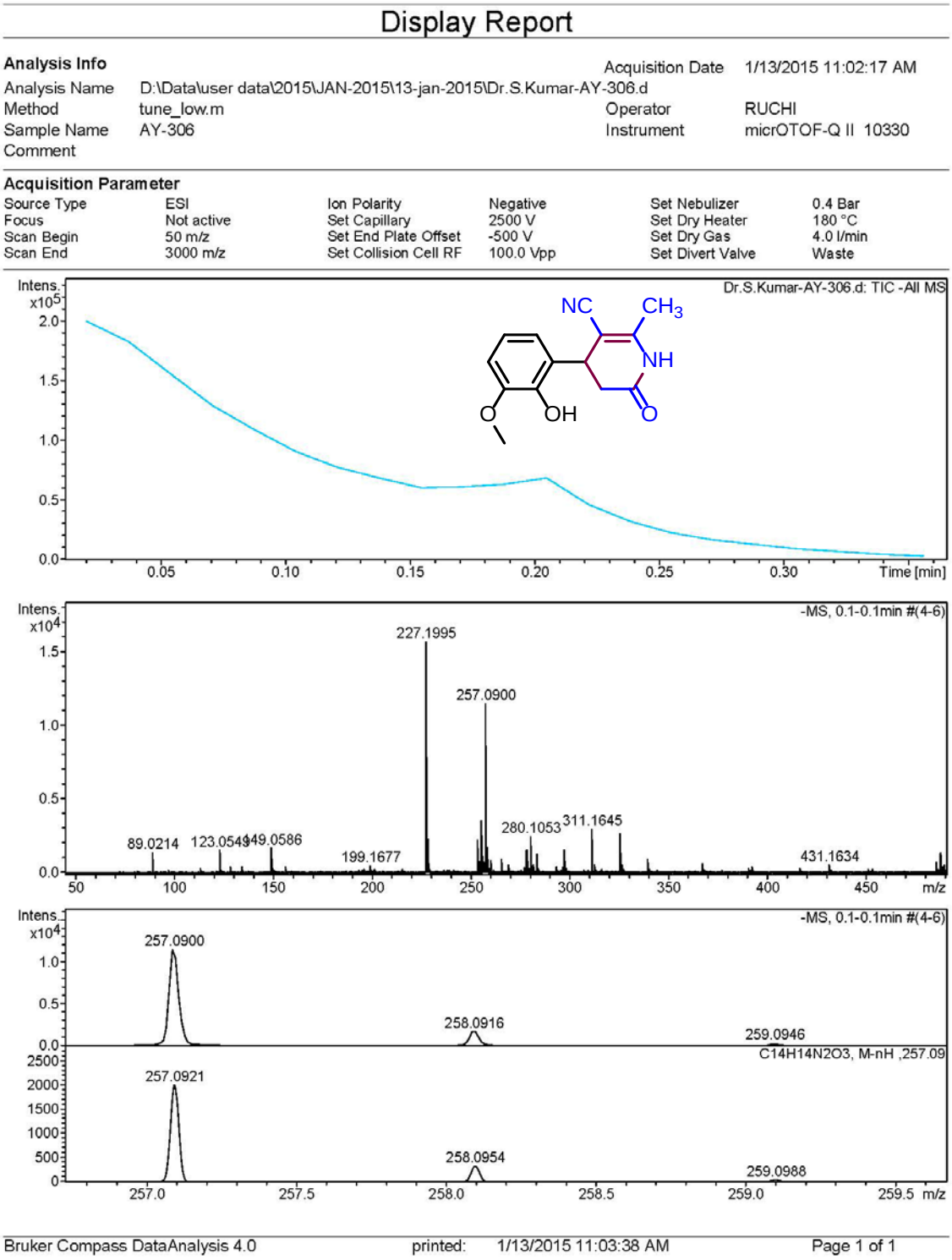


Figure S68 ^{1}H NMR spectra of **23**

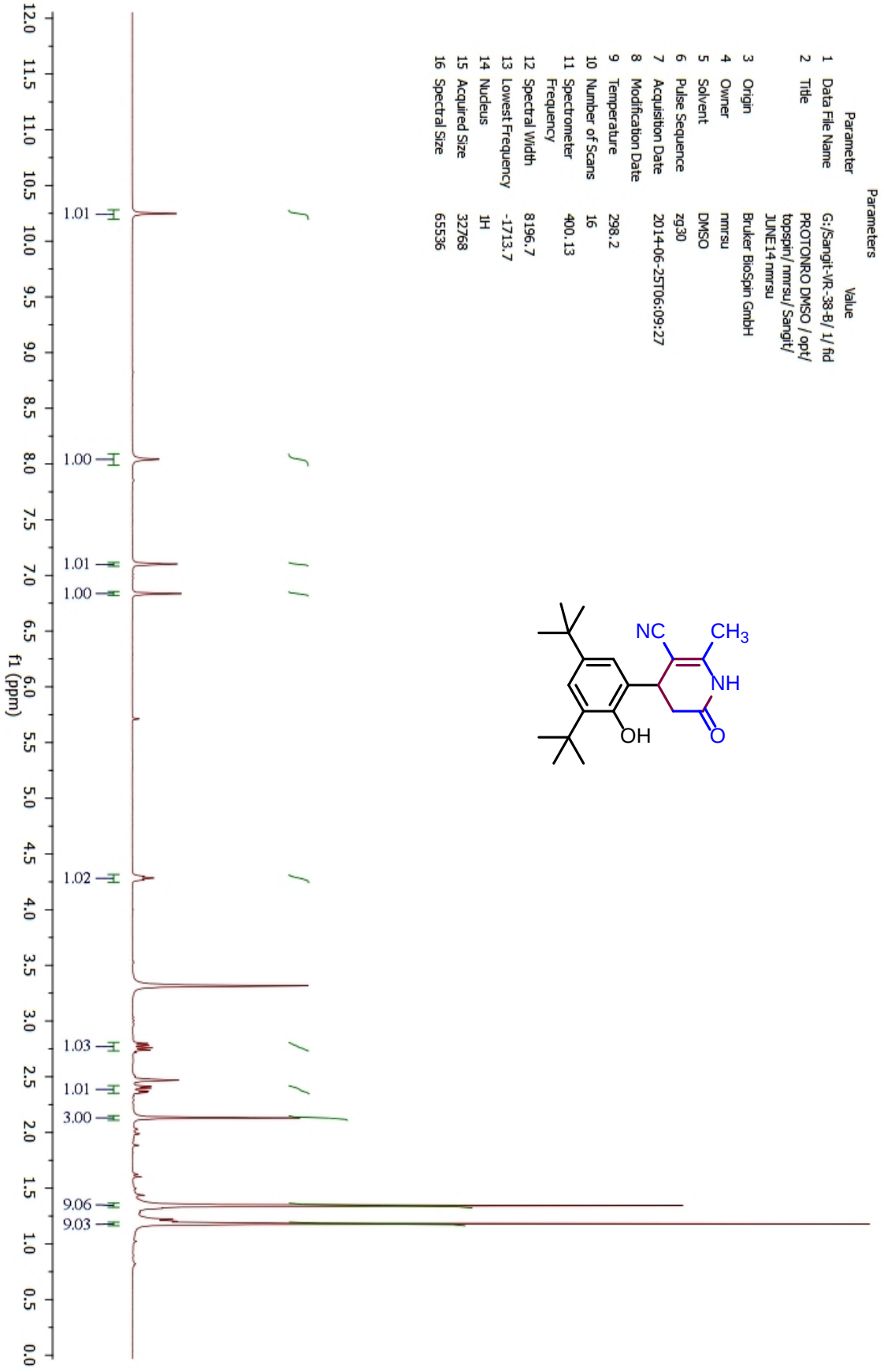


Figure S69 ^{13}C NMR spectra of **23**

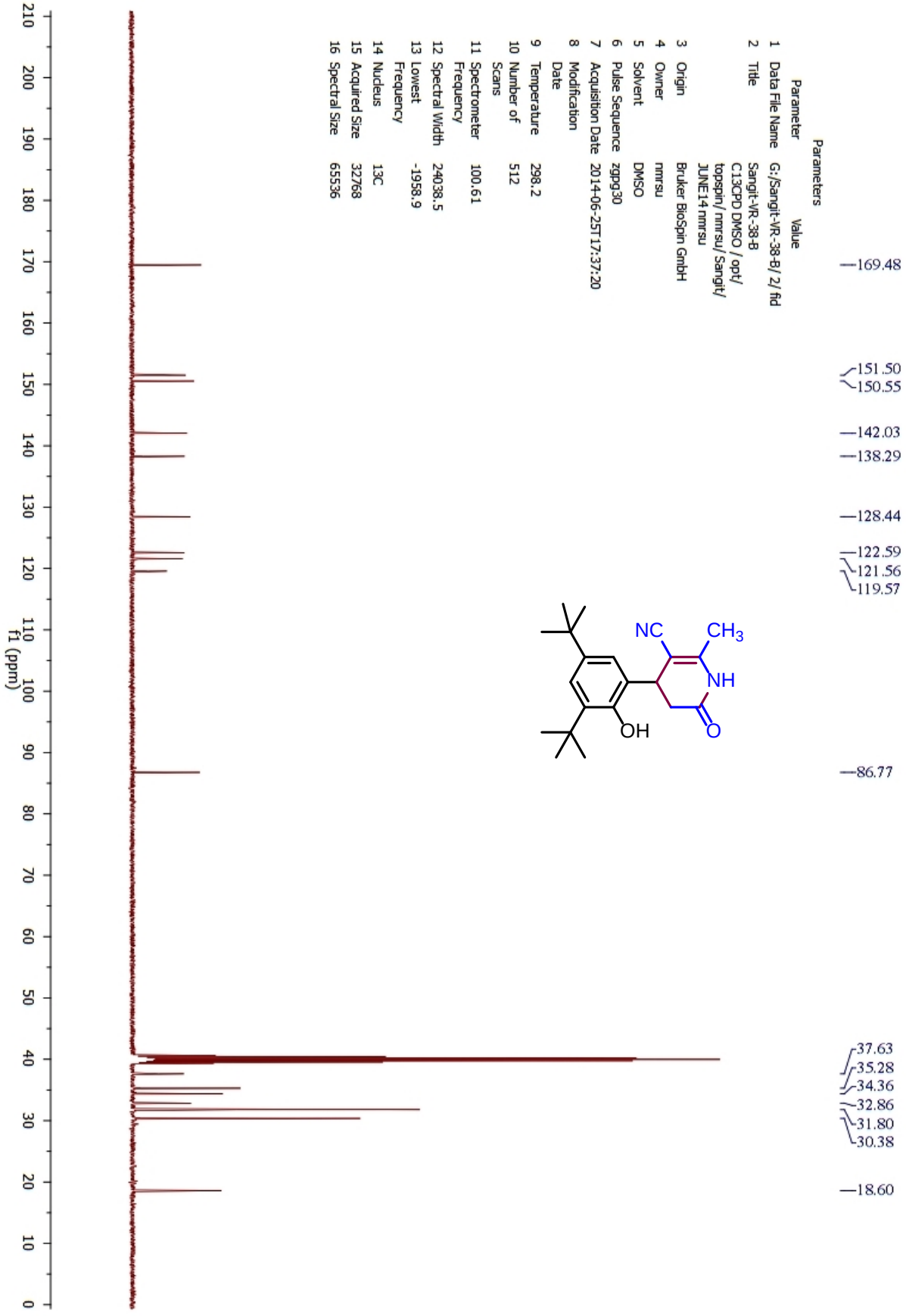


Figure S70 HRMS spectra of **23**

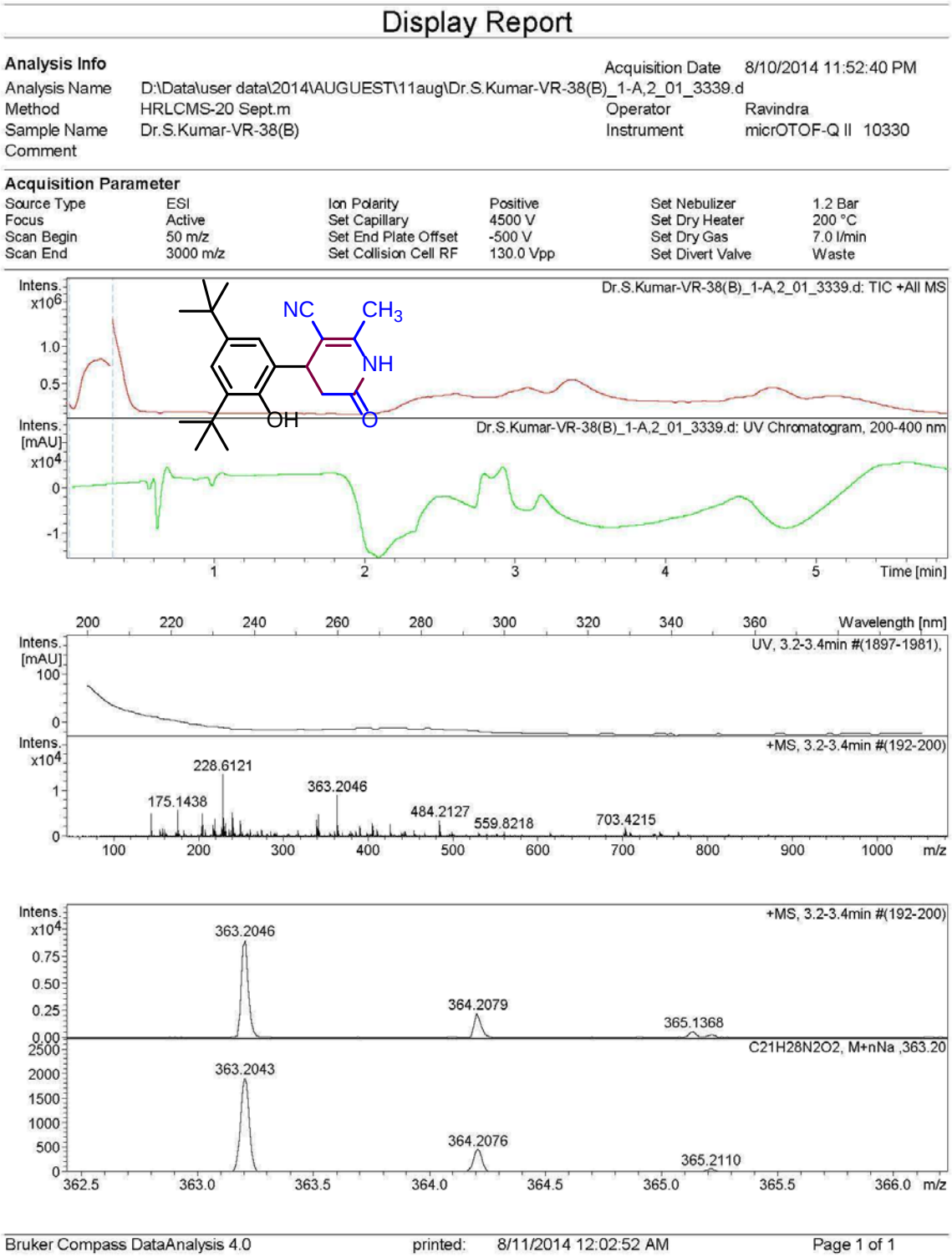


Figure S71 ^{1}H NMR spectra of **24**

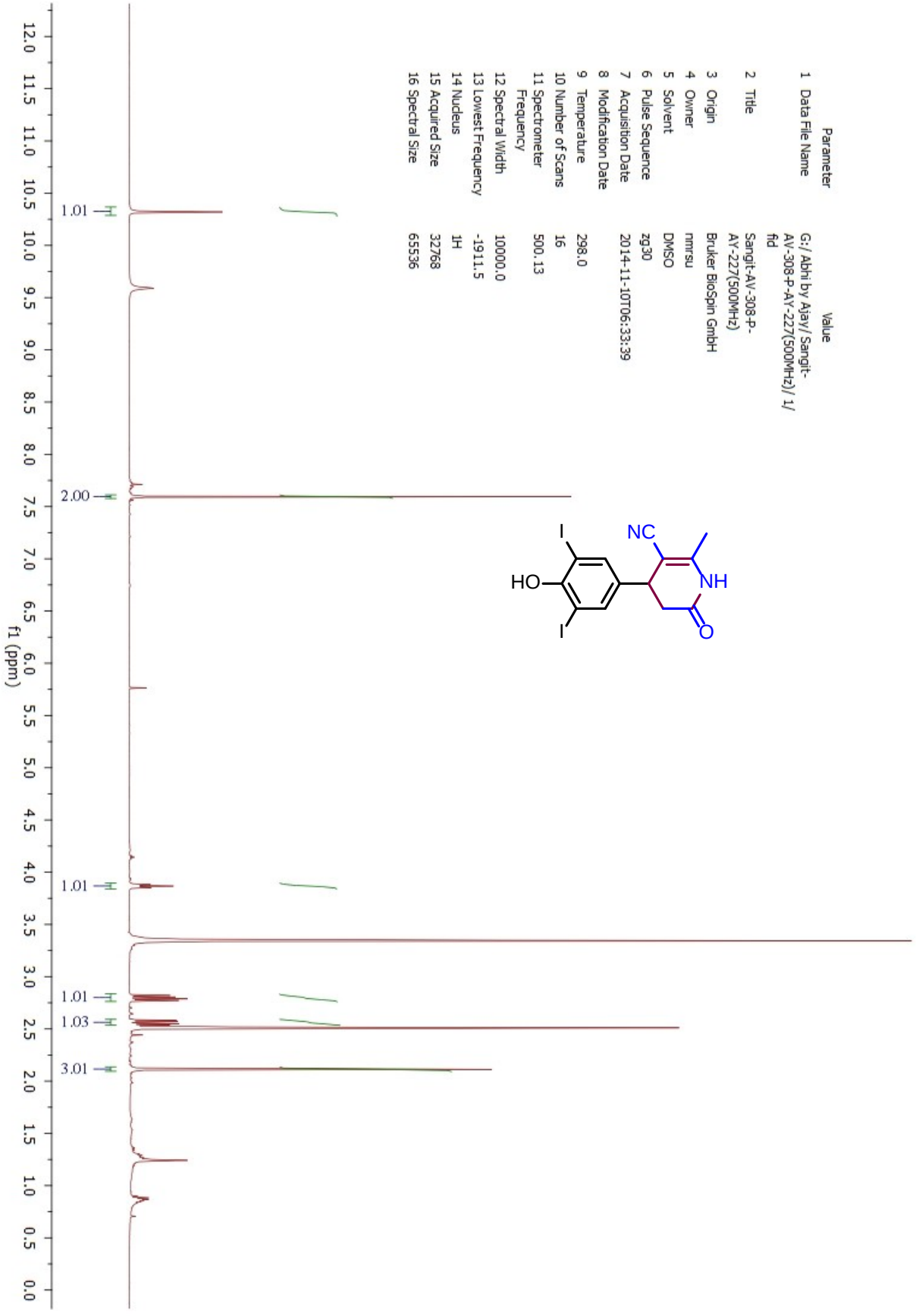


Figure S72 ^{13}C NMR spectra of **24**

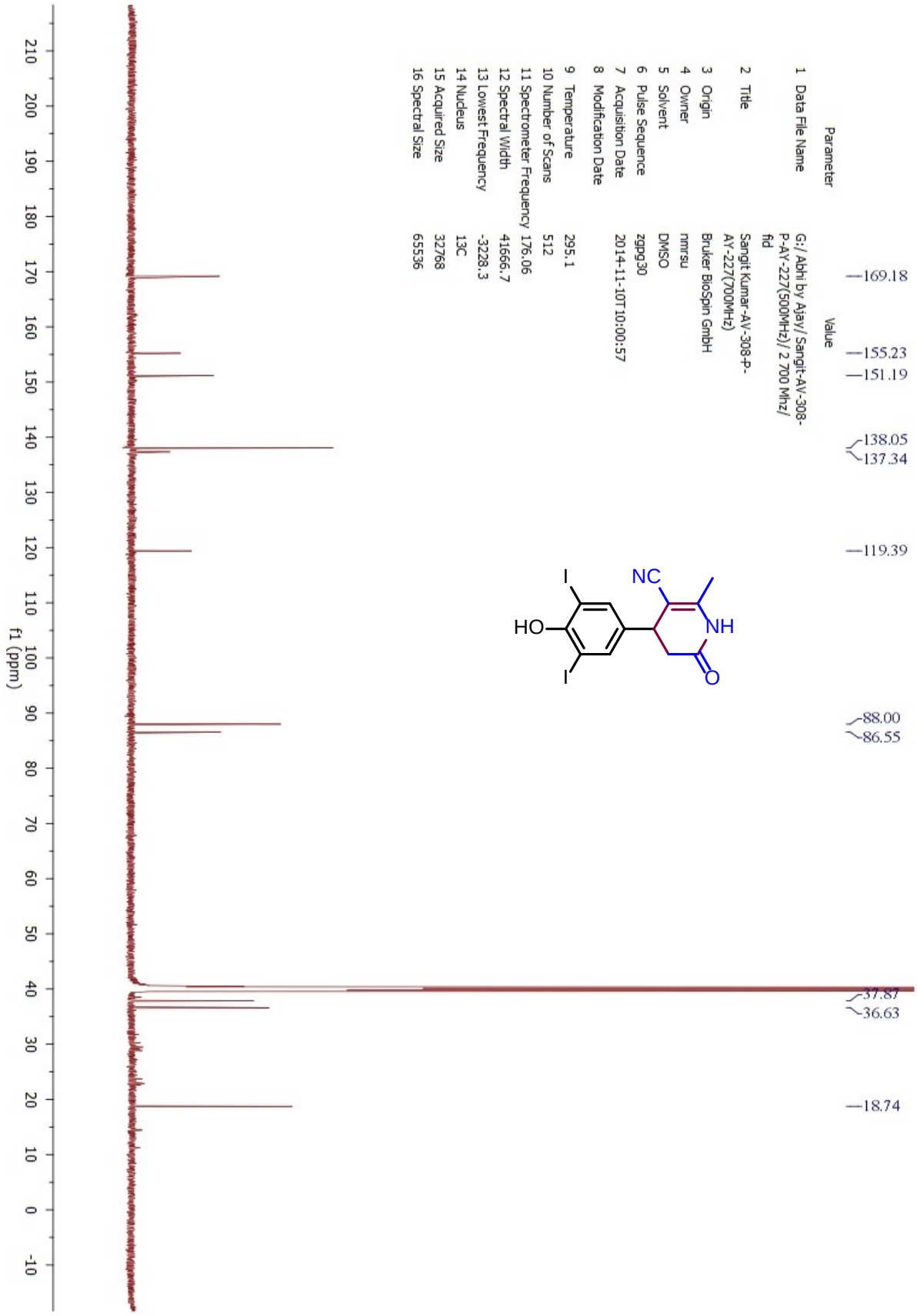


Figure S73 HRMS spectra of **24**

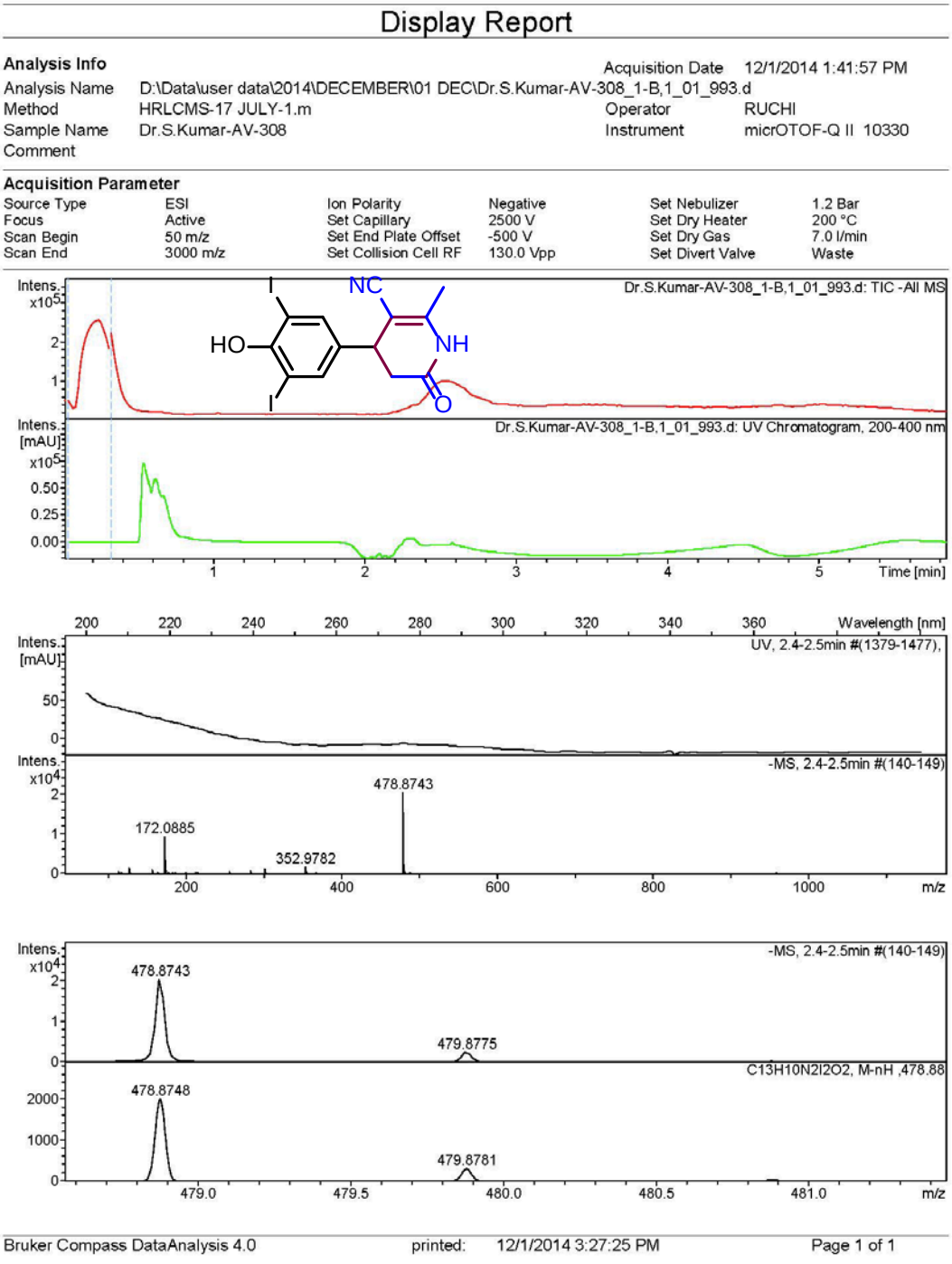


Figure S74 ^{1}H NMR spectra of **25**

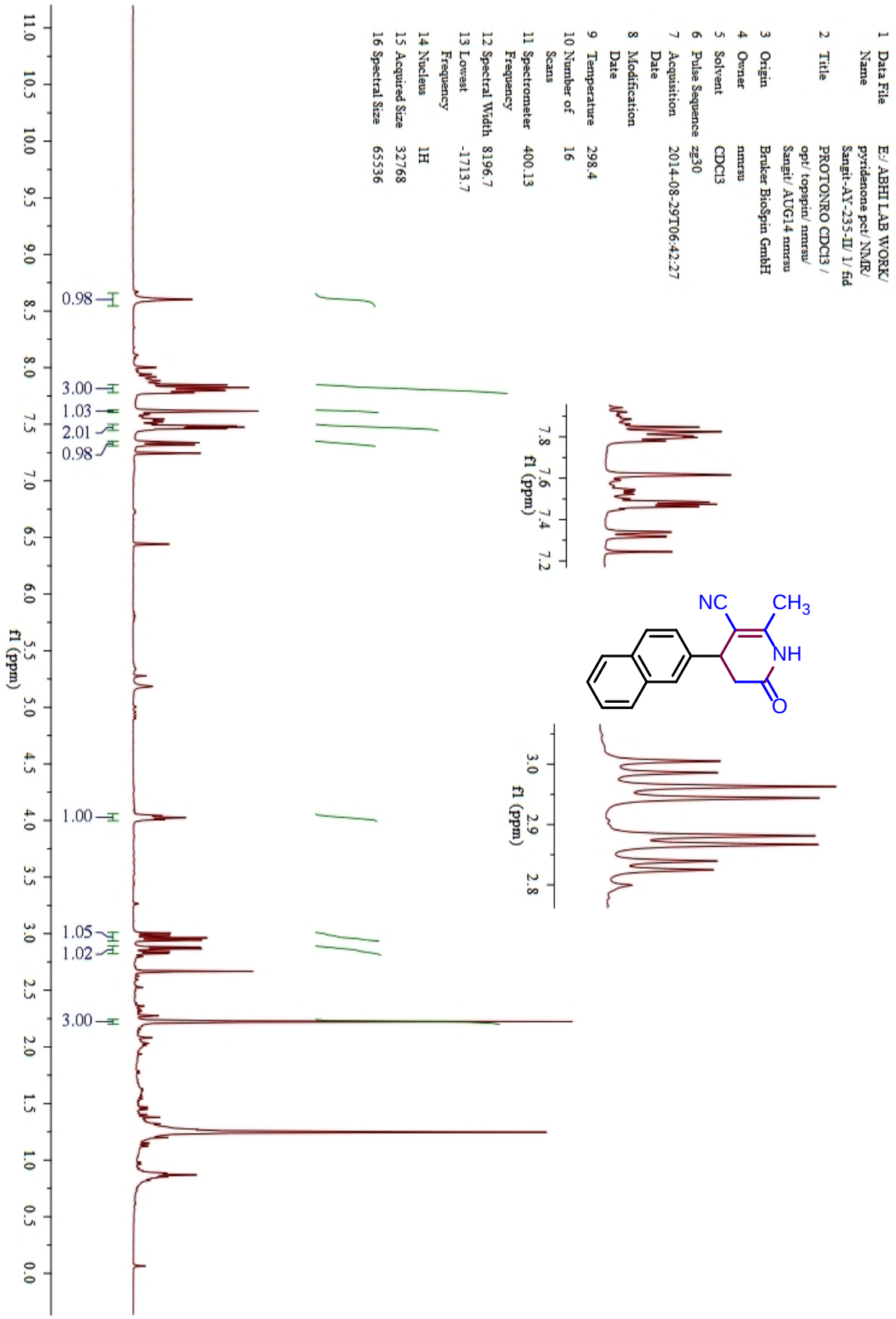


Figure S75 ^{13}C NMR spectra of **25**

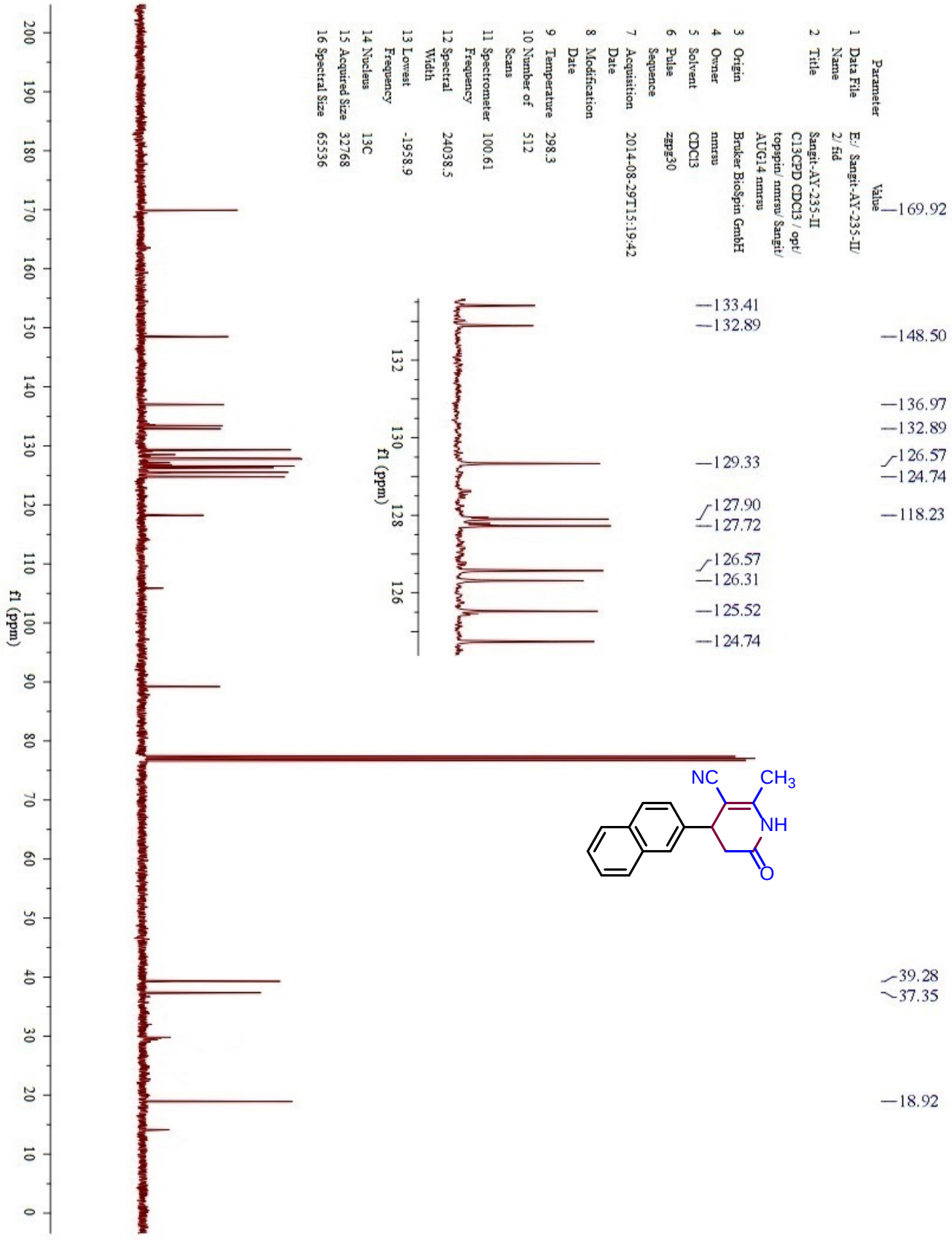
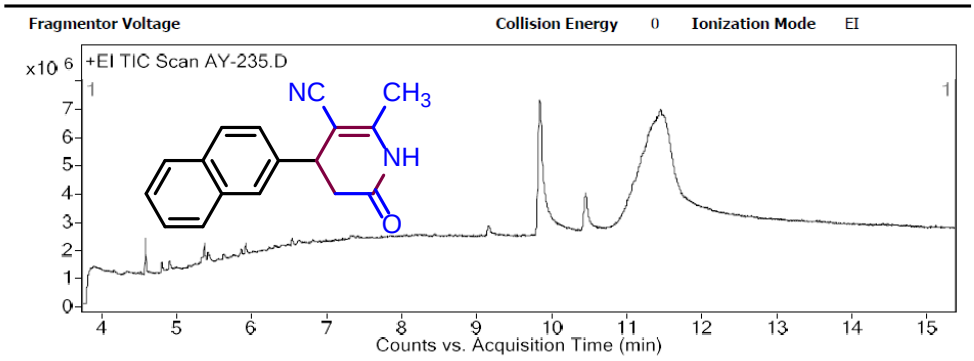


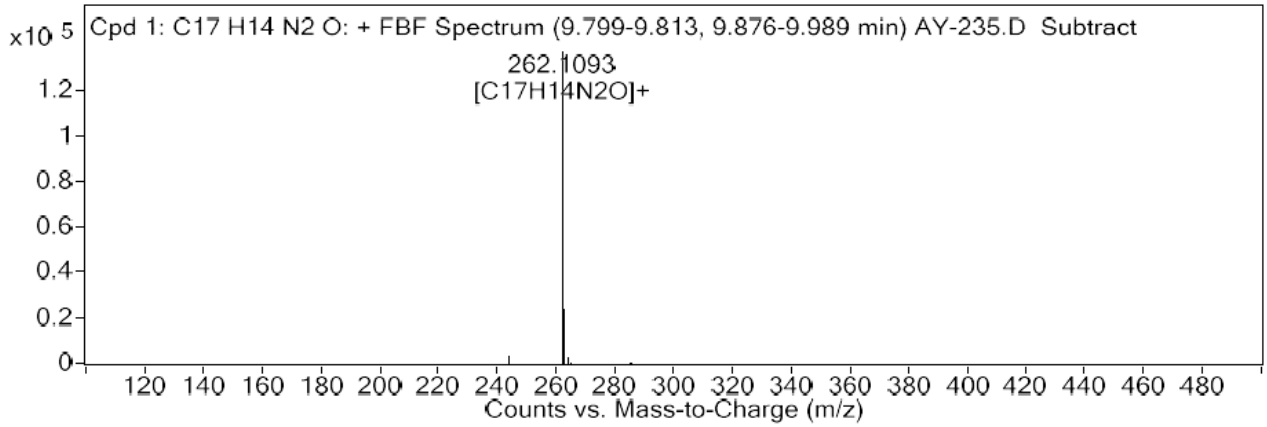
Figure S76 GC HRMS spectra of **25**

Data Filename	AY-235.D	**Sample Name**	AY-235
Sample Type		**Position**	1
Instrument Name	GCQTOF	**User Name**	Agilent-PC\admin
Acq Method	IISER_GENERAL_HP5_80.M	**Acquired Time**	09-Sep-14 3:33:48 PM
IRM Calibration Status	Success	**DA Method**	iiSER13MAY 2013.m
Comment			
Expected Barcode		**Sample Amount**	
Dual Inj Vol	0.1	**TuneName**	Install_tune.ei.tune_1_4_13.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200\	**TuneDateStamp**	41421.21309
MSFirmwareVersion	G.7200.01.09	**OperatorName**	Agilent-PC\admin
RunCompletedFlag	TRUE		

User Chromatograms



Qualitative Analysis Report



--- End Of Report ---

Figure S77 ^{1}H NMR spectra of **26**

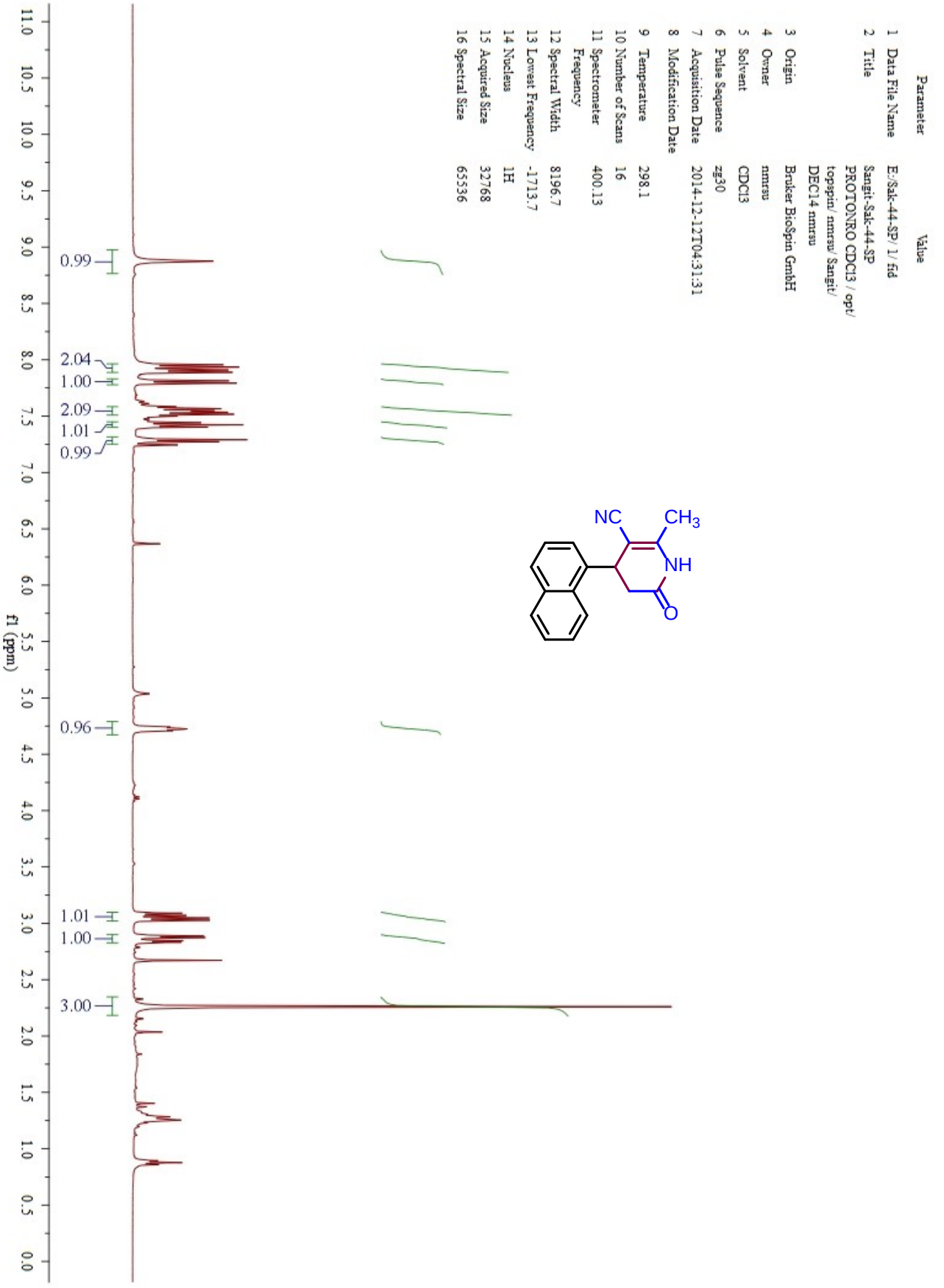


Figure S78 ^{13}C NMR spectra of **26**

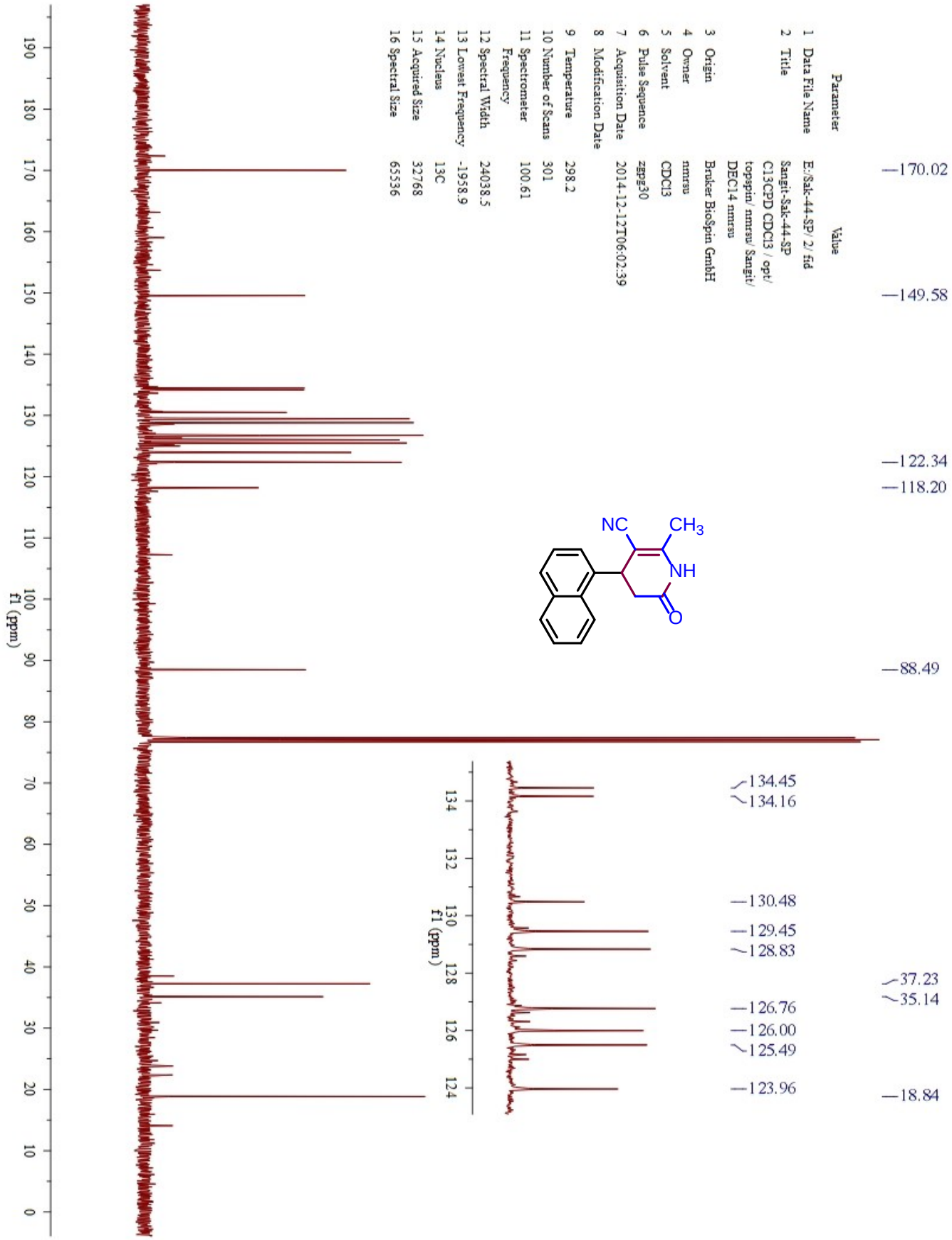


Figure S79 Mass spectra of **26**

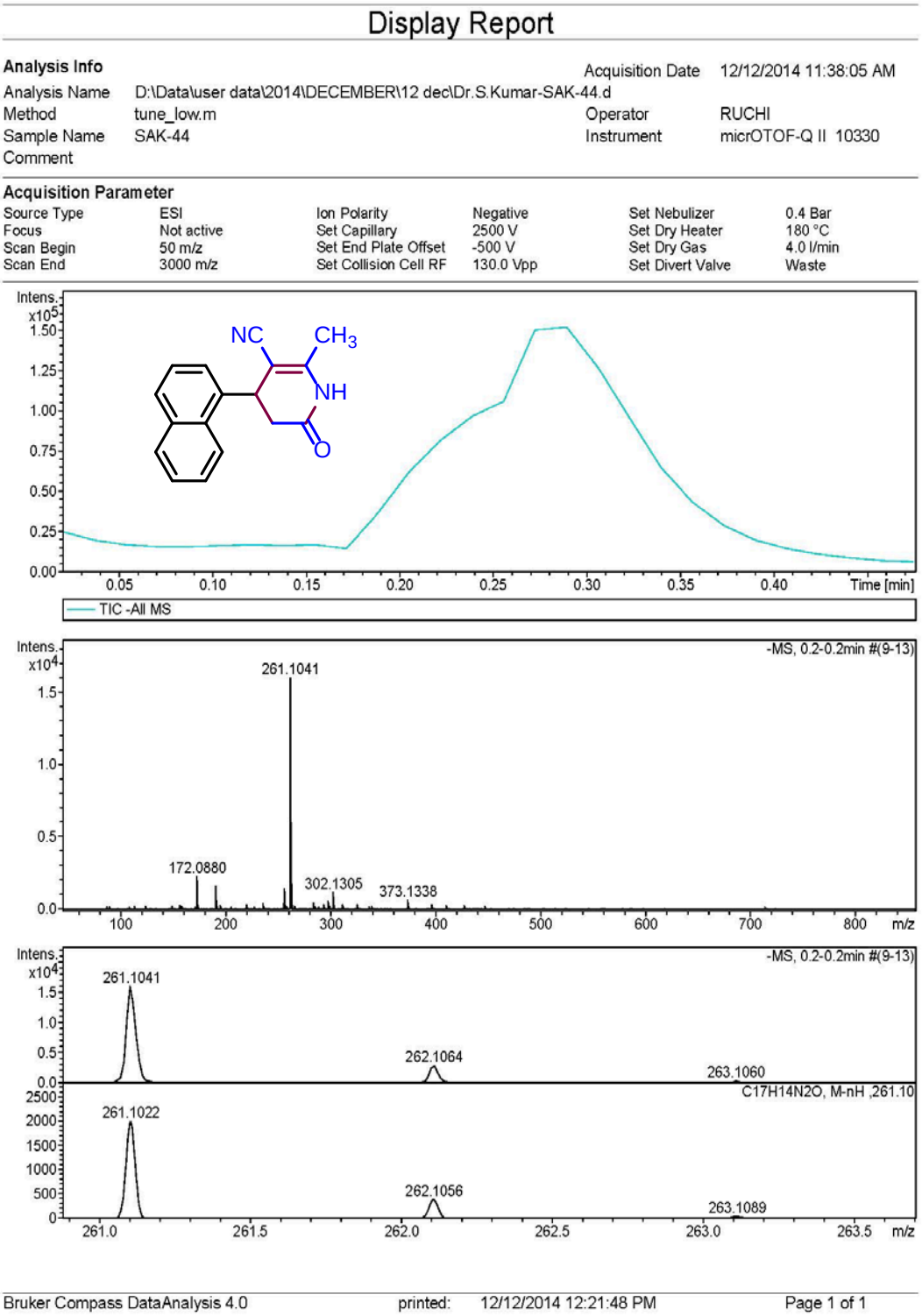


Figure S80 ^{1}H NMR spectra of **27**

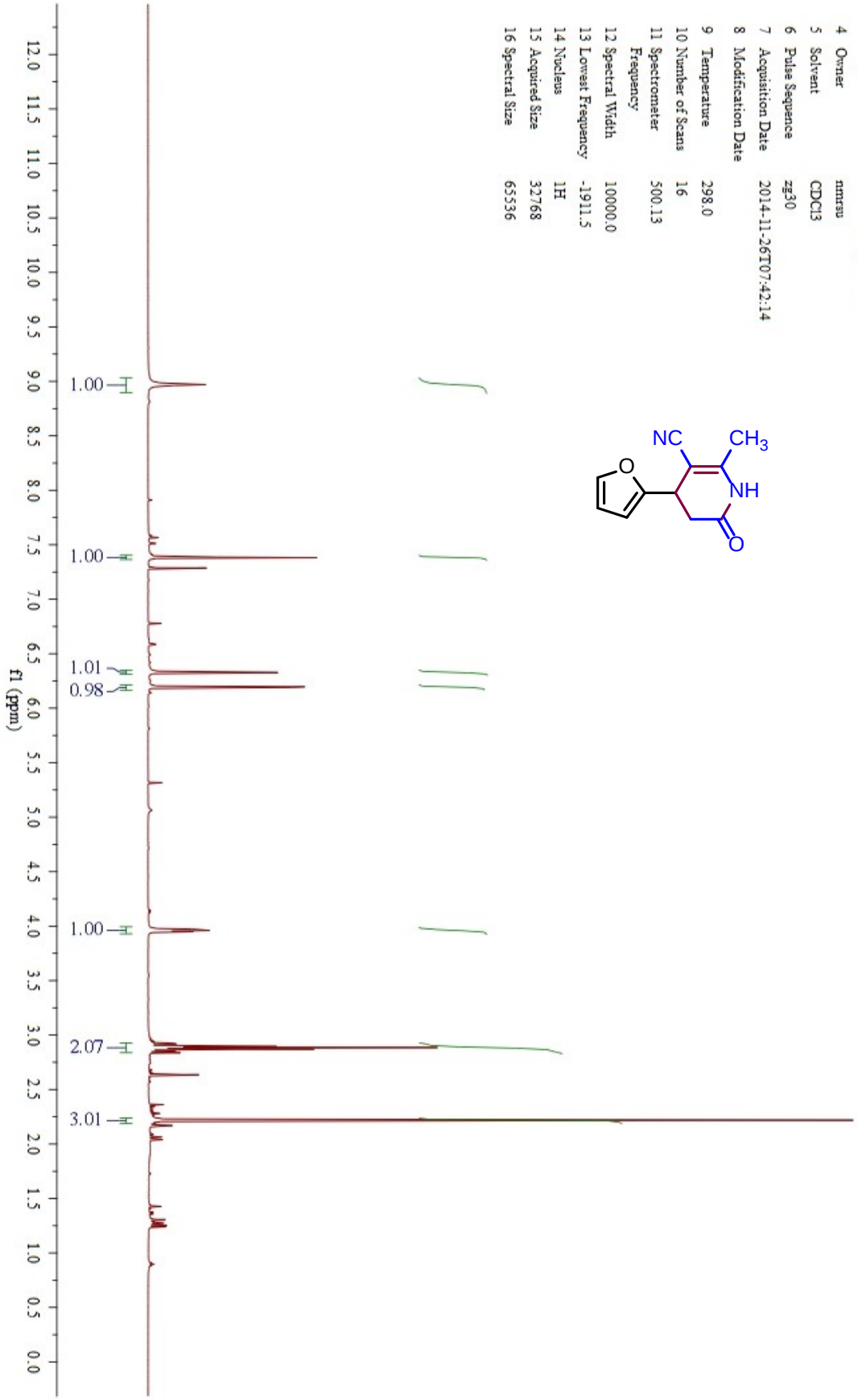


Figure S81 ^{13}C NMR spectra of **27**

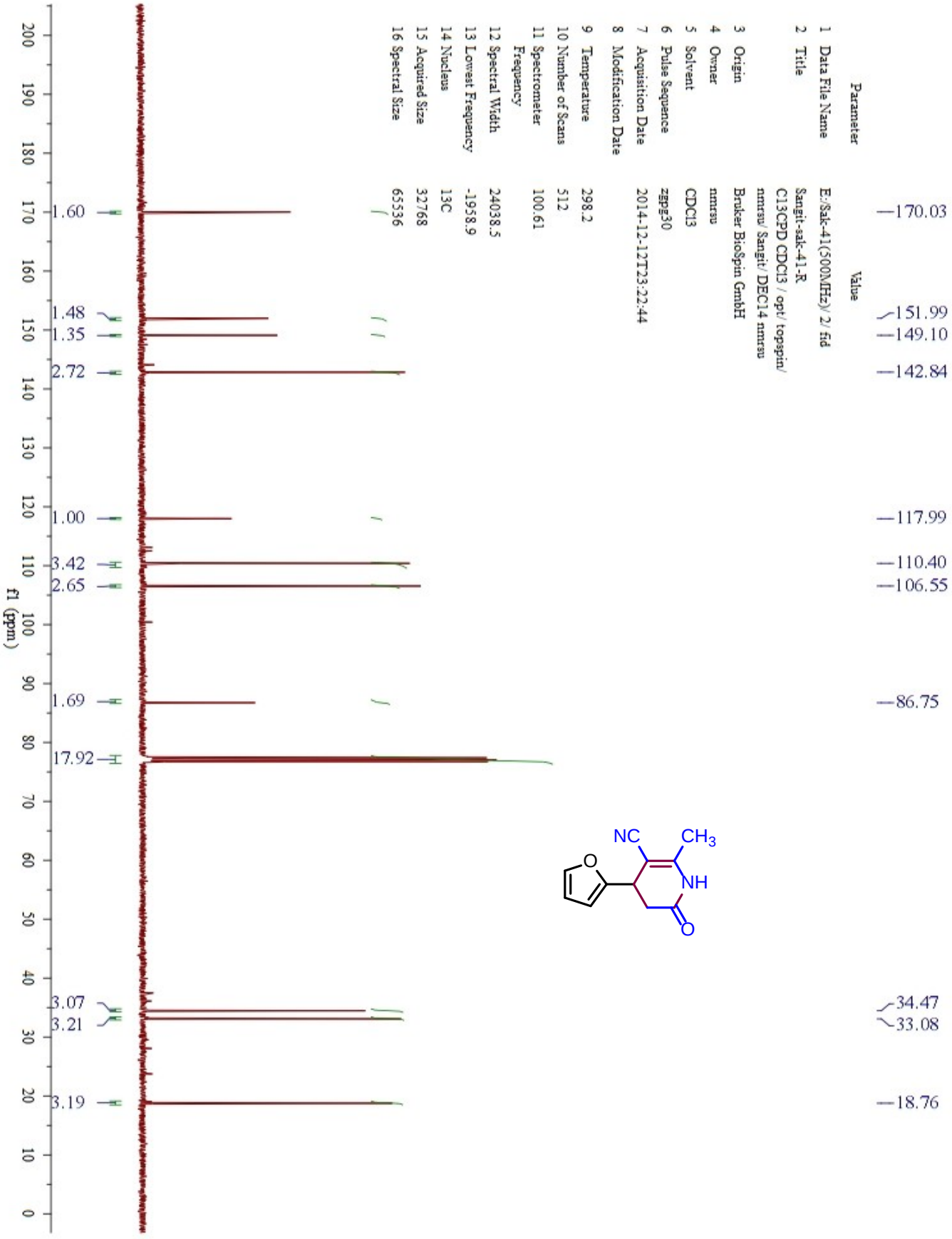


Figure S82 Mass spectra of **27**

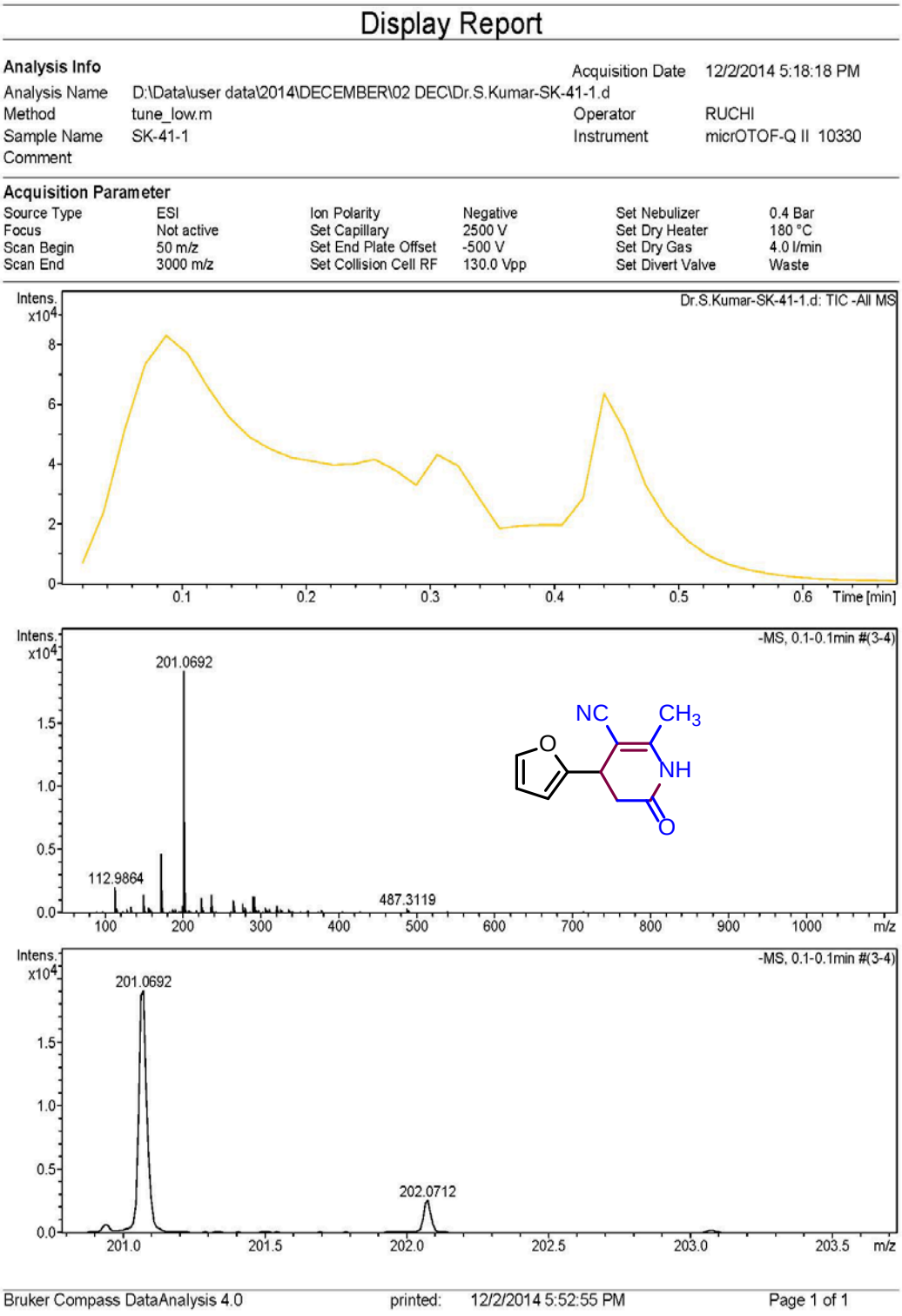


Figure S83 ^{1}H NMR spectra of **28**

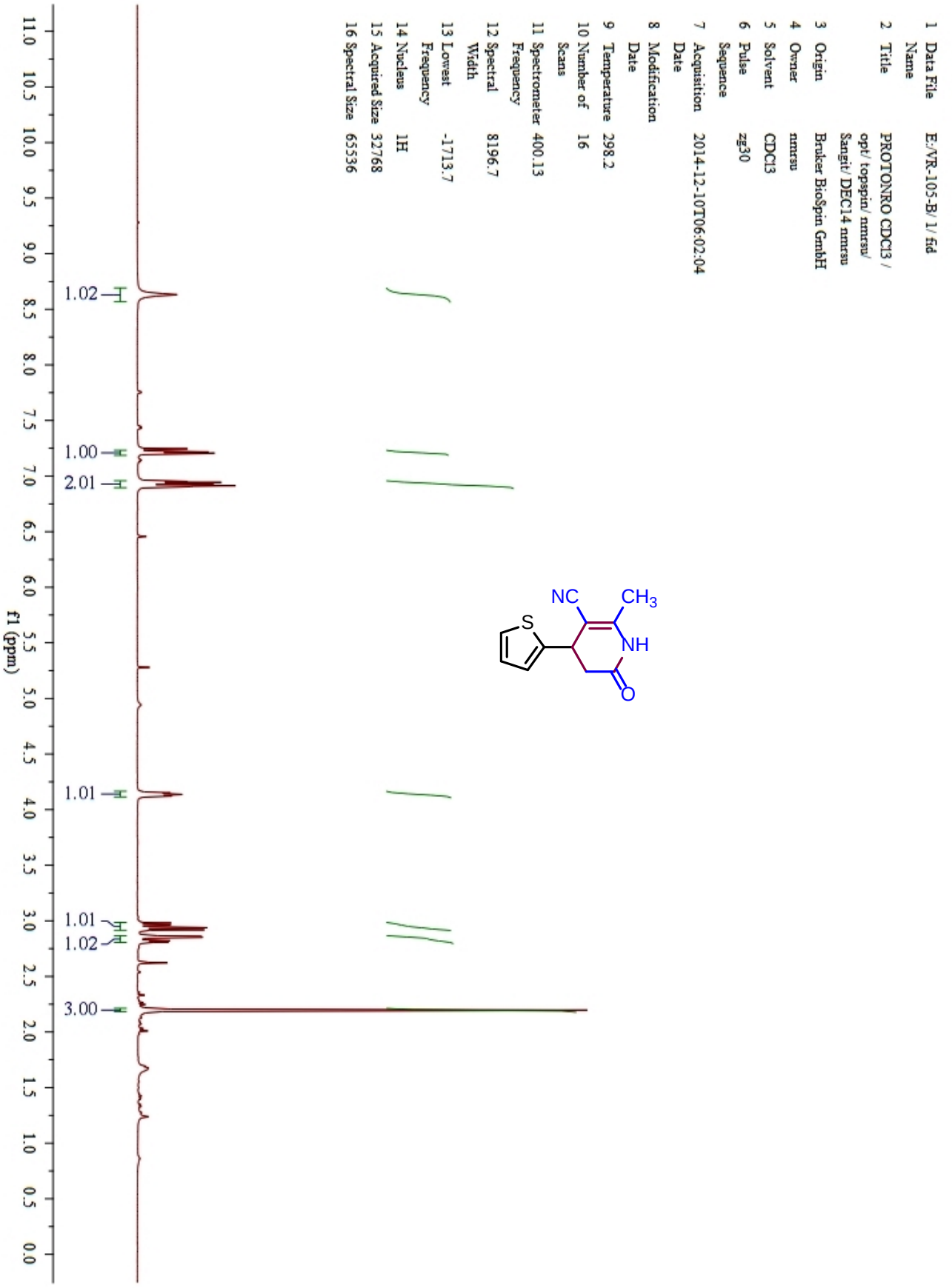


Figure S84 ^{13}C NMR spectra of **28**

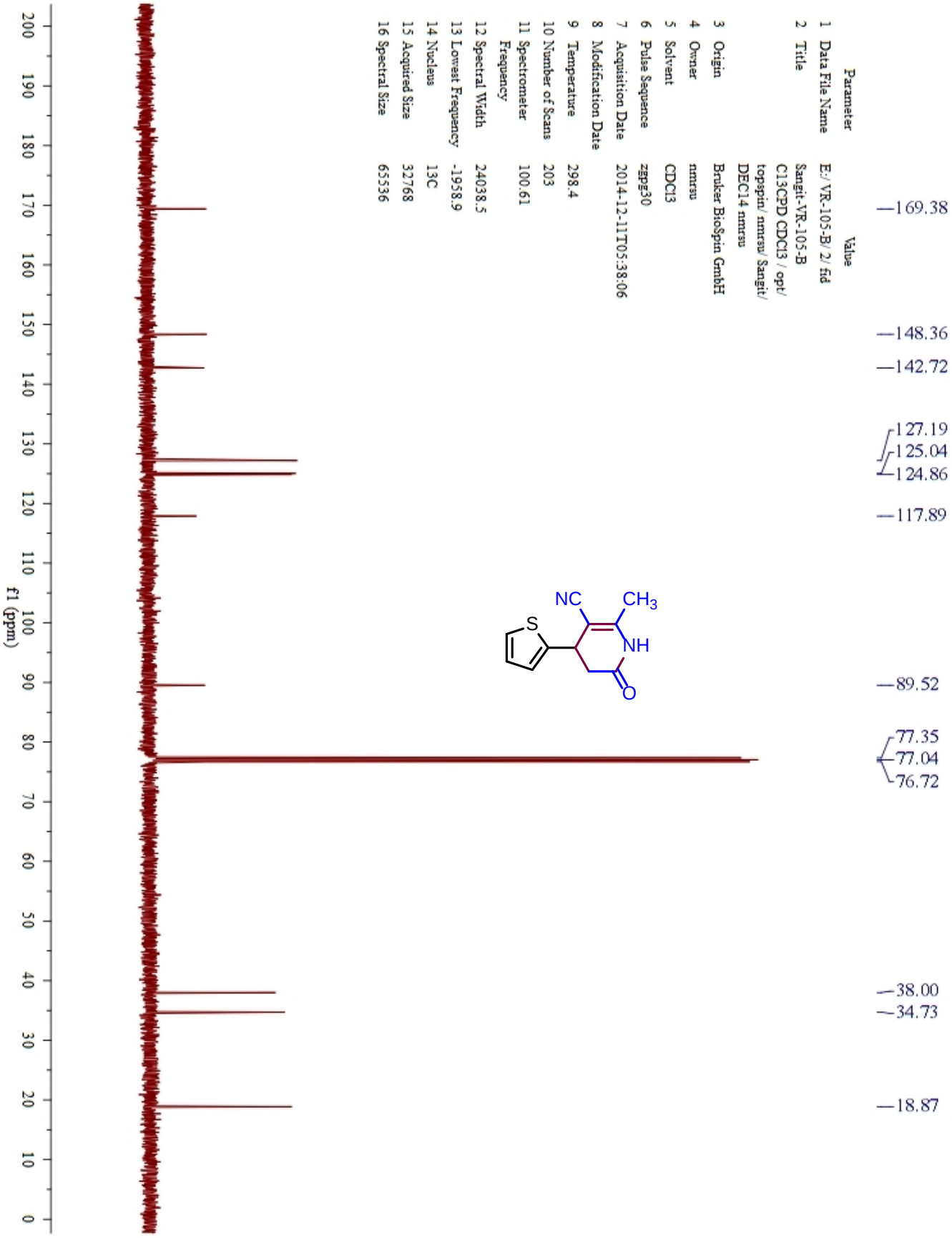


Figure S85 Mass spectra of **28**

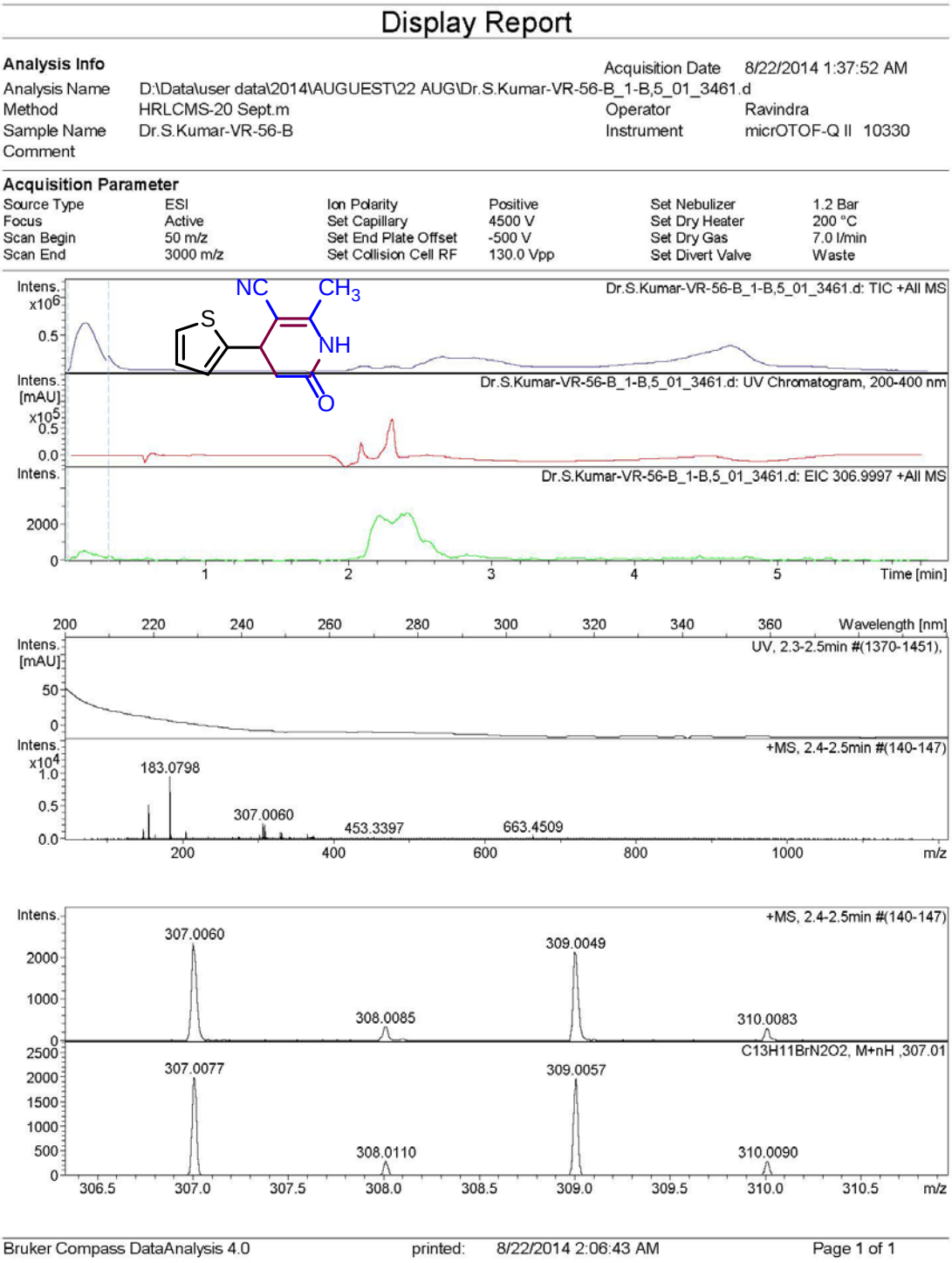


Figure S86 ^{1}H NMR spectra of **29**

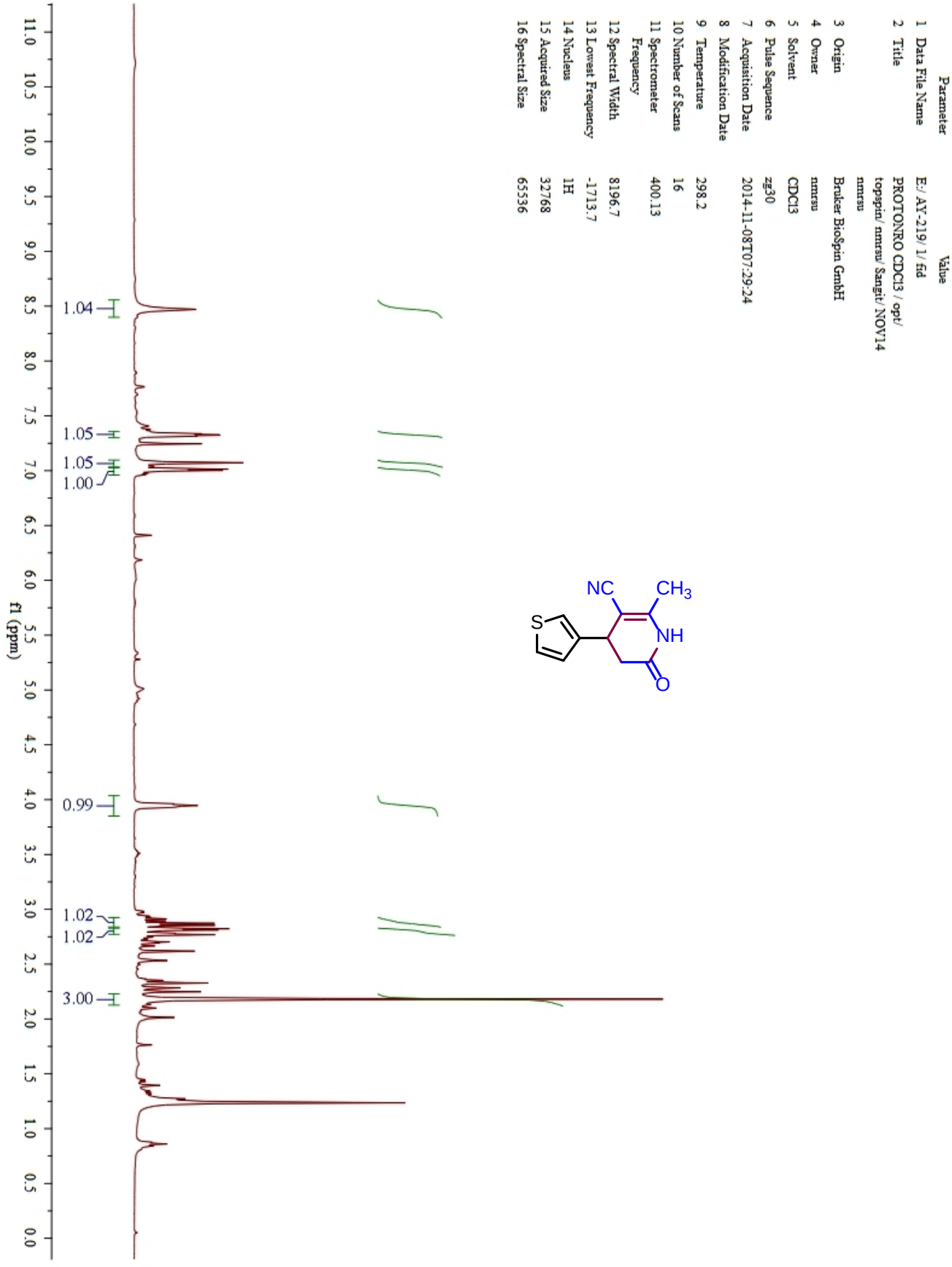


Figure S87 ^{13}C NMR spectra of **29**

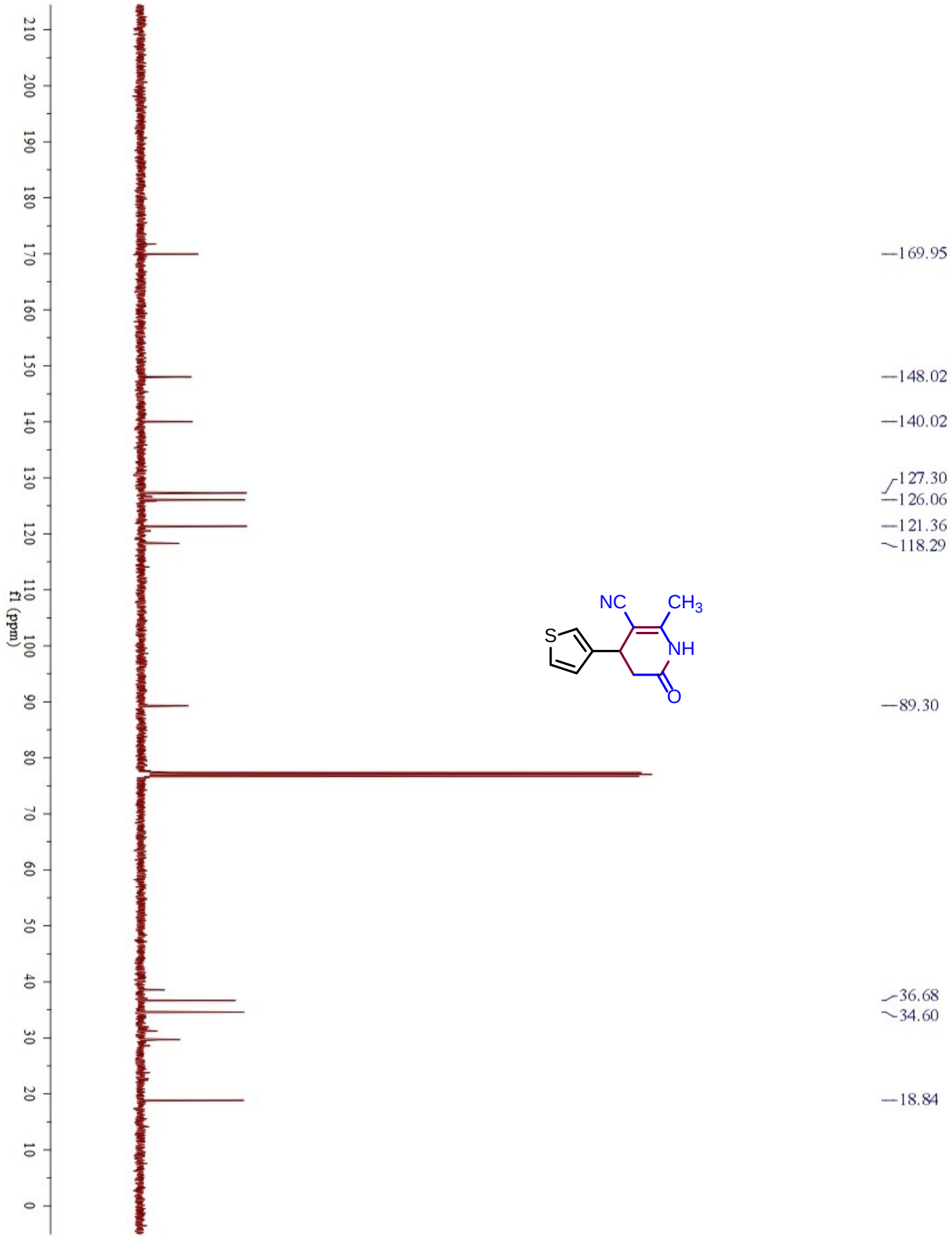


Figure S88 Mass spectra of **29**

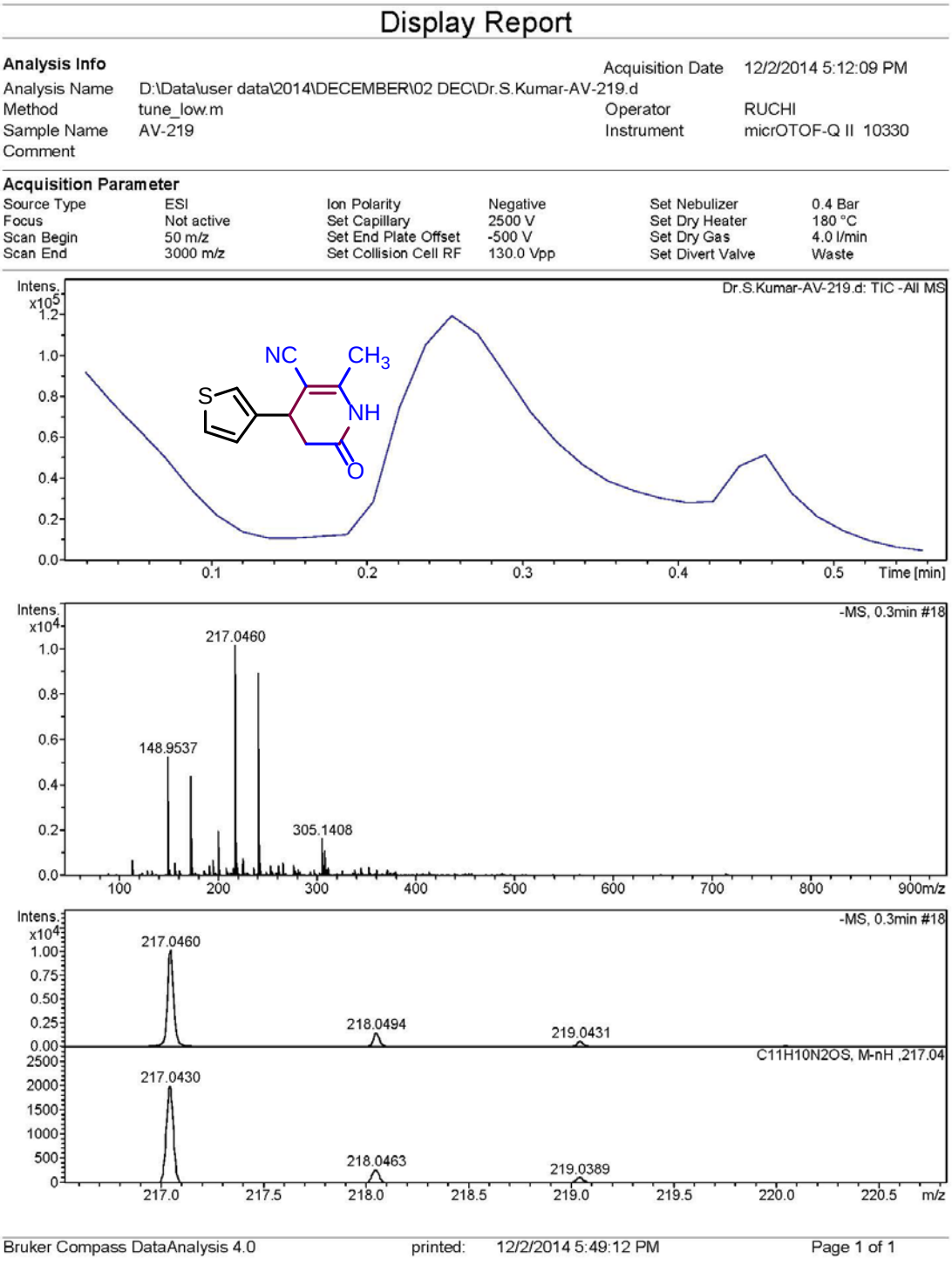


Figure S89 ^{1}H NMR spectra of **30**

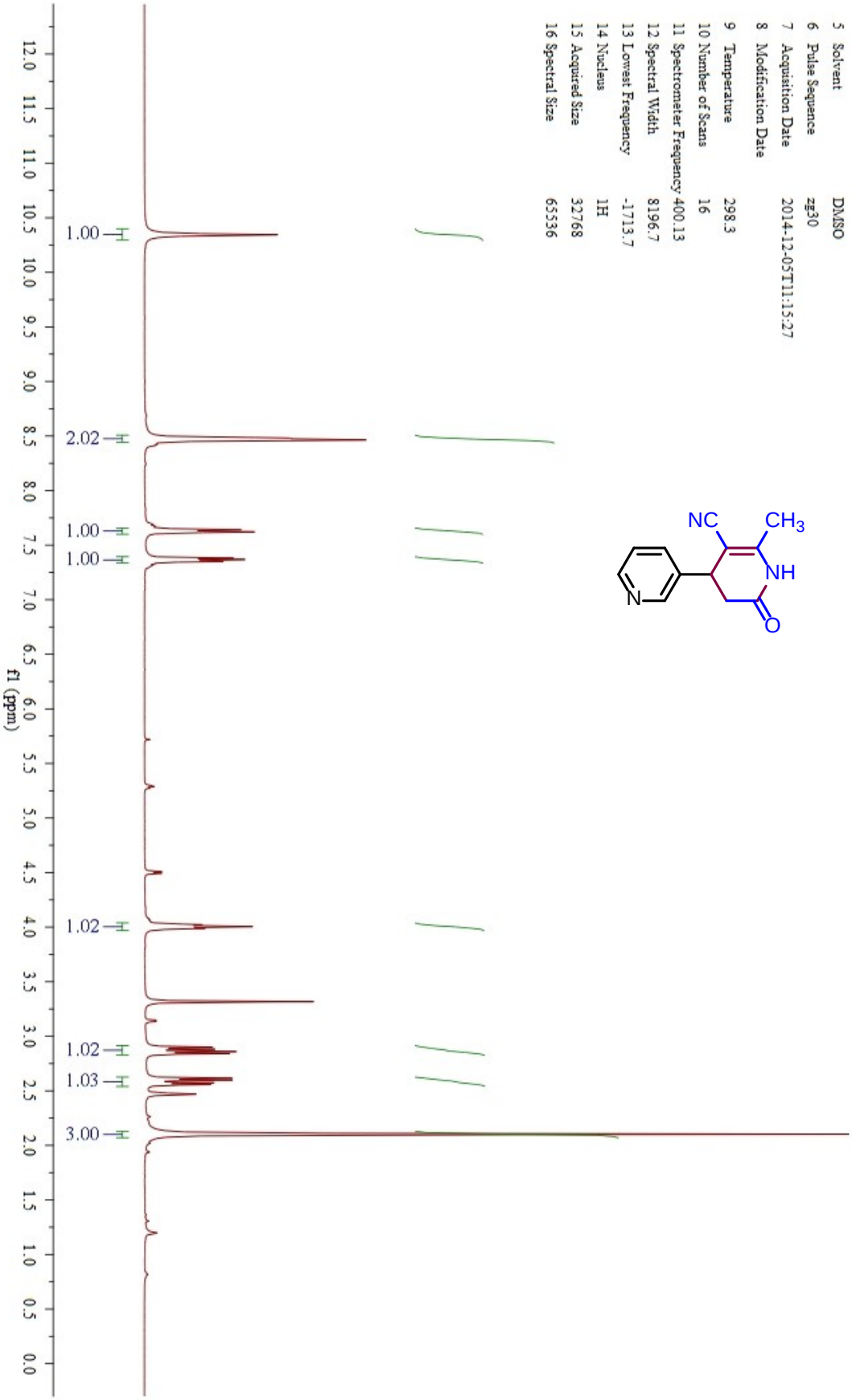


Figure S90 ^{13}C NMR spectra of **30**

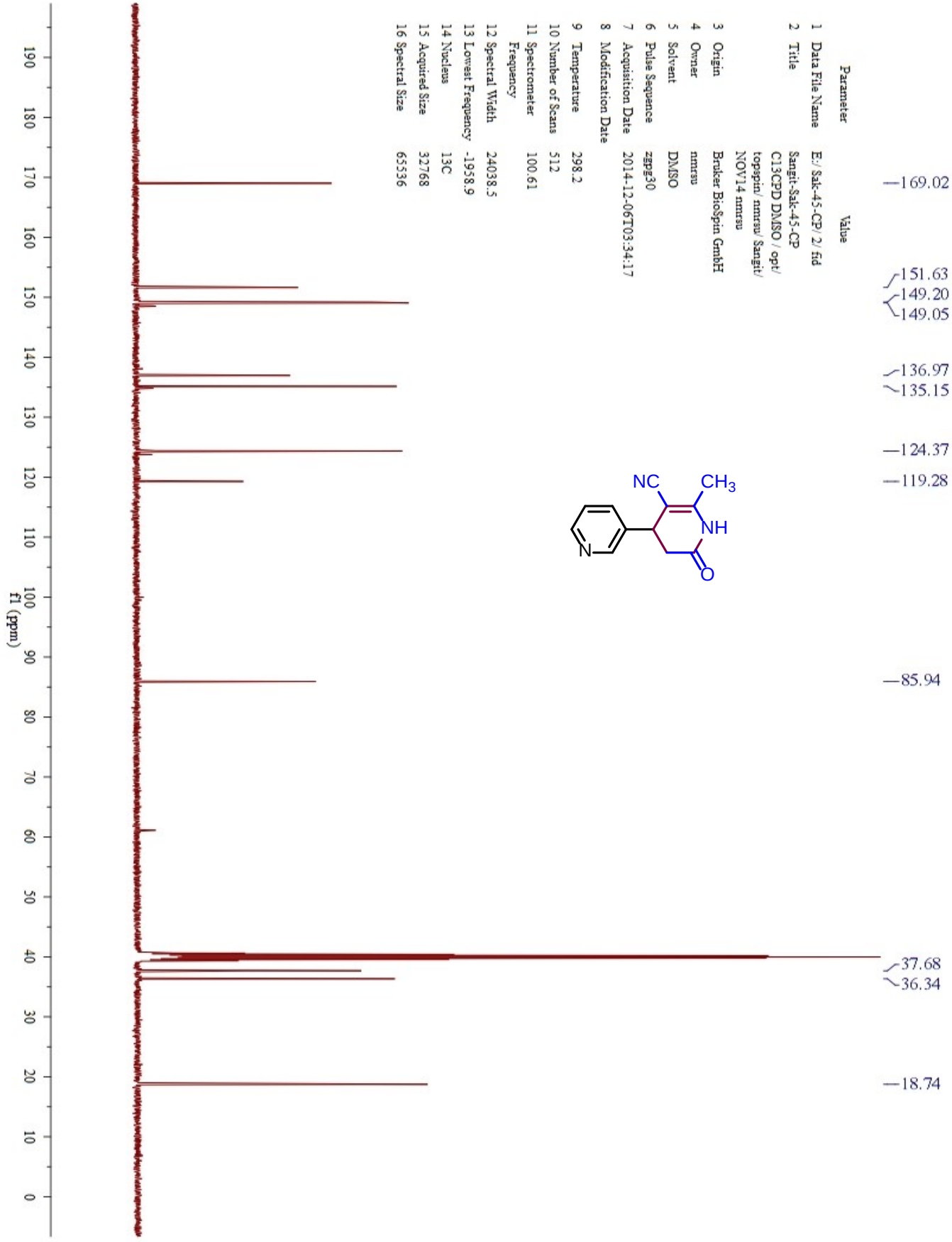


Figure S91 Mass spectra of **30**

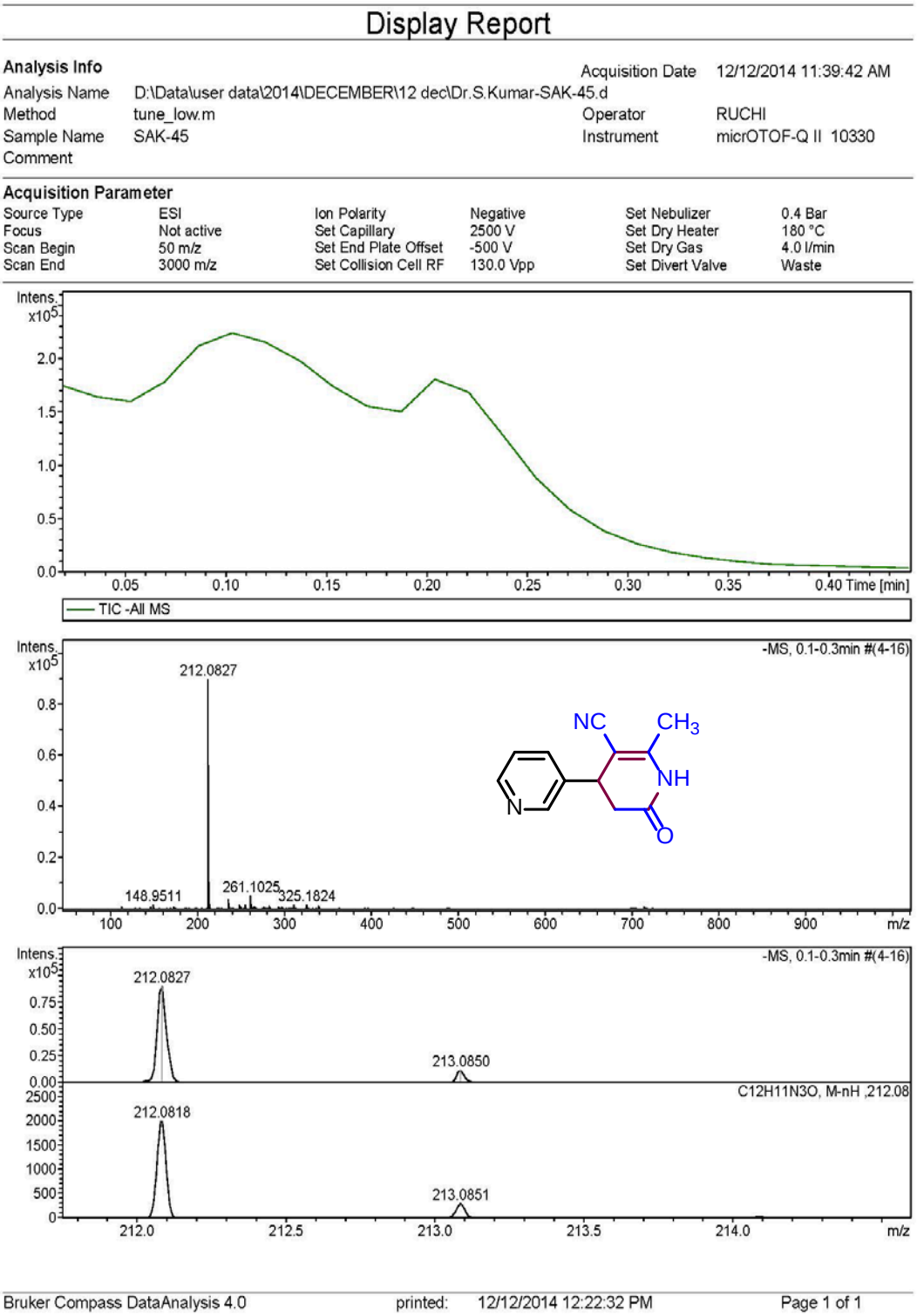


Figure S92 ^{1}H NMR spectra of **31**

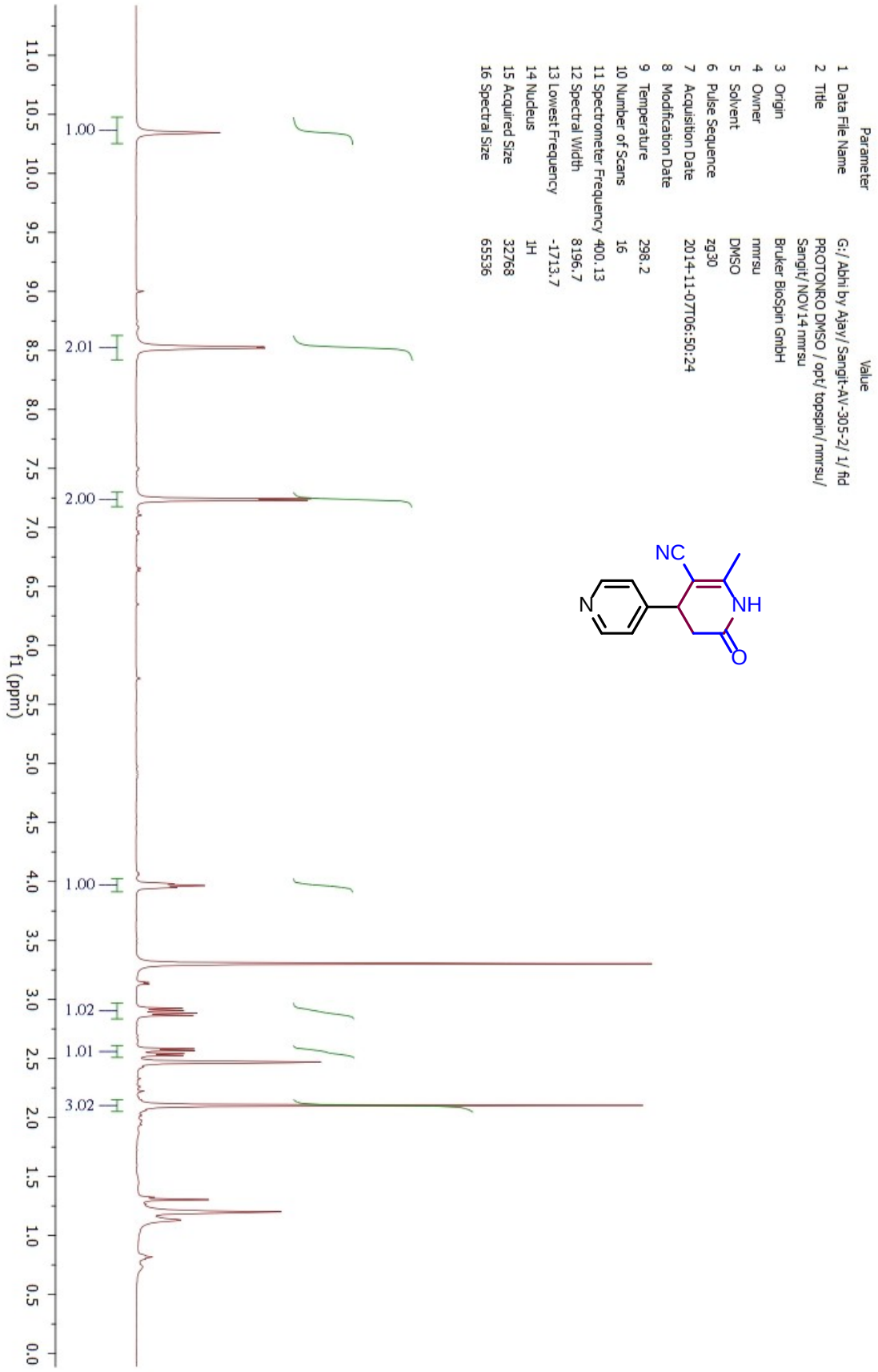


Figure S93 ^{13}C NMR spectra of **31**

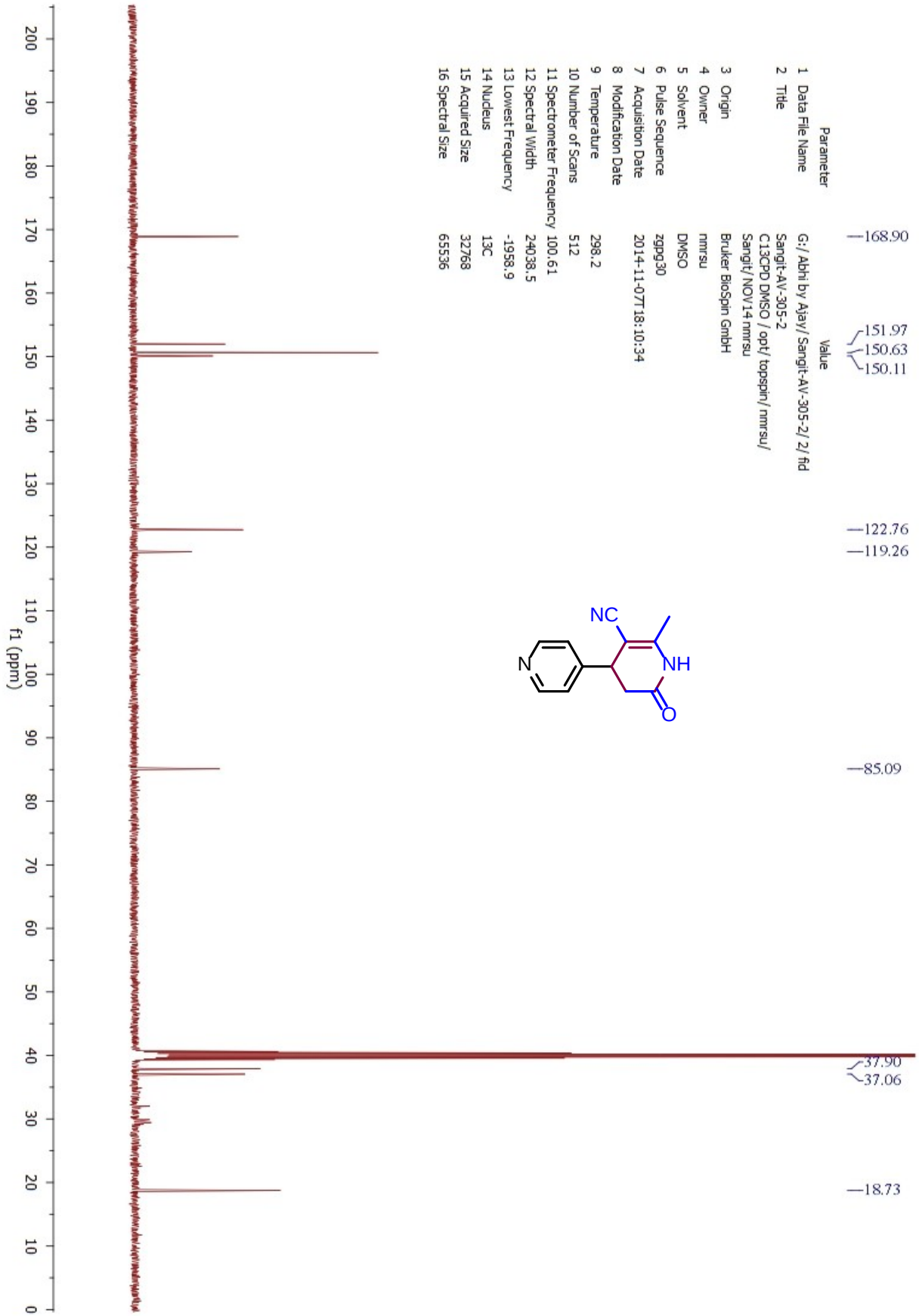


Figure S94 HRMS spectra of **31**

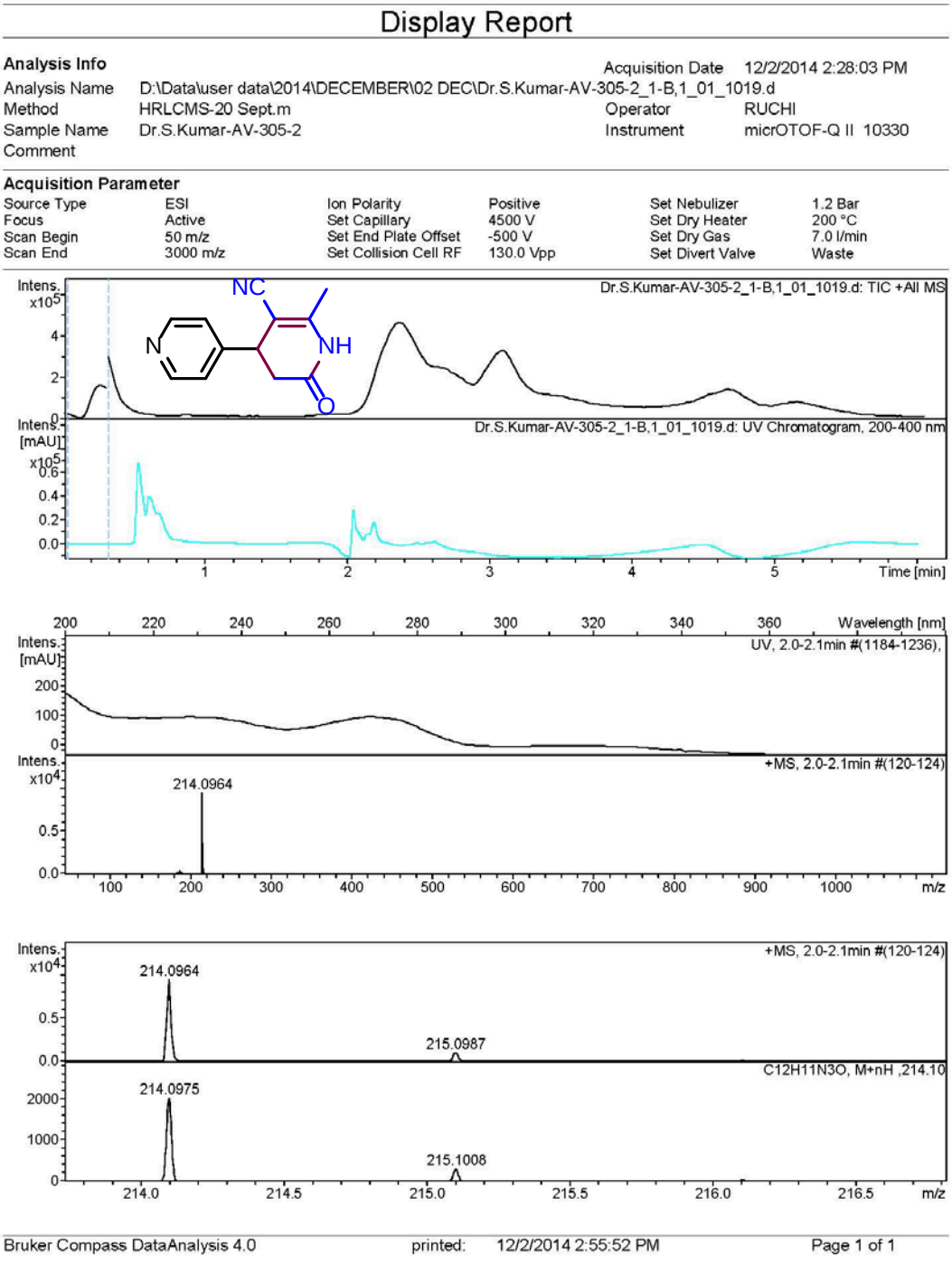


Figure S95 ^{1}H NMR spectra of **32**

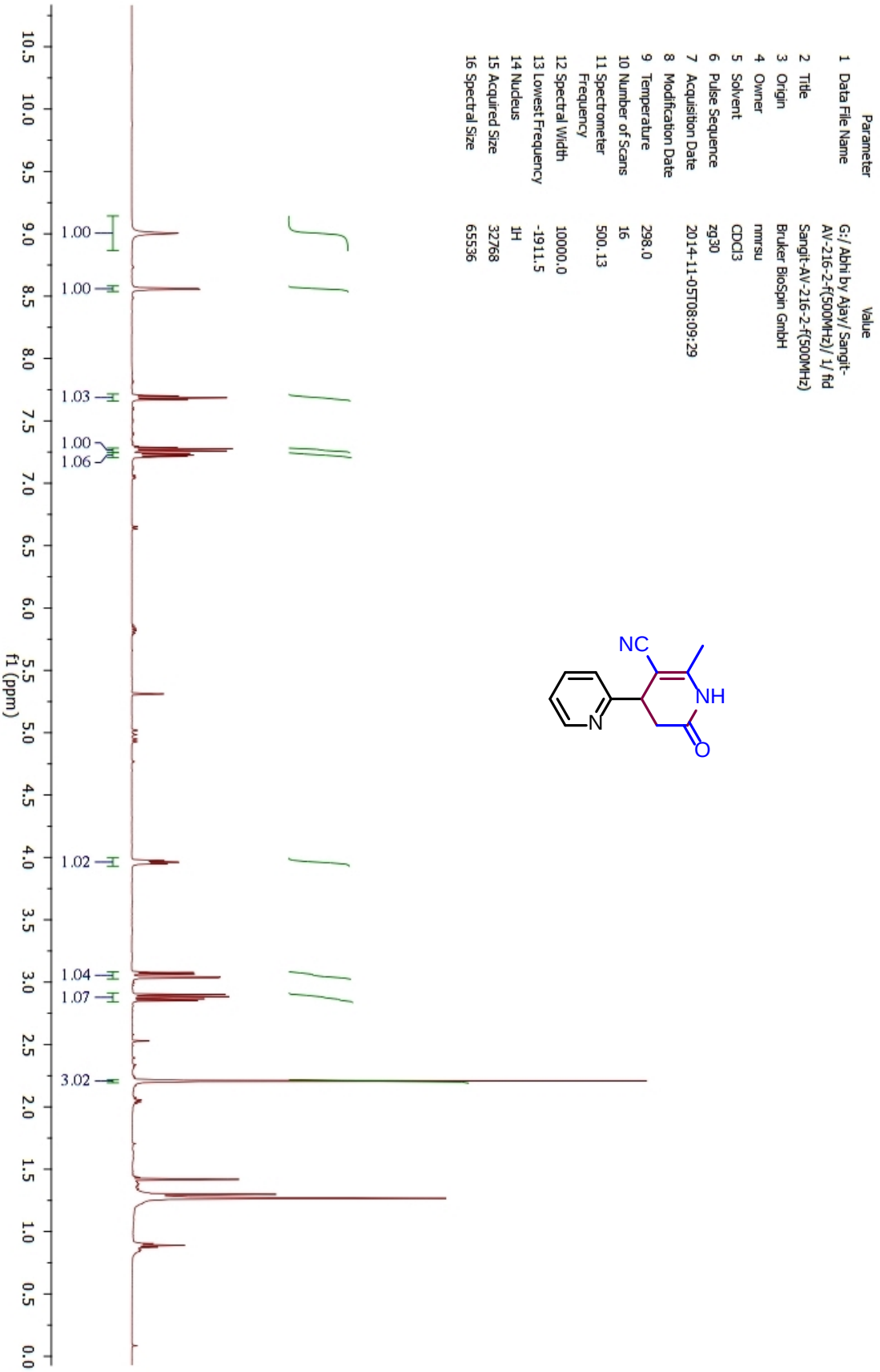


Figure S96 ^{13}C NMR spectra of **32**

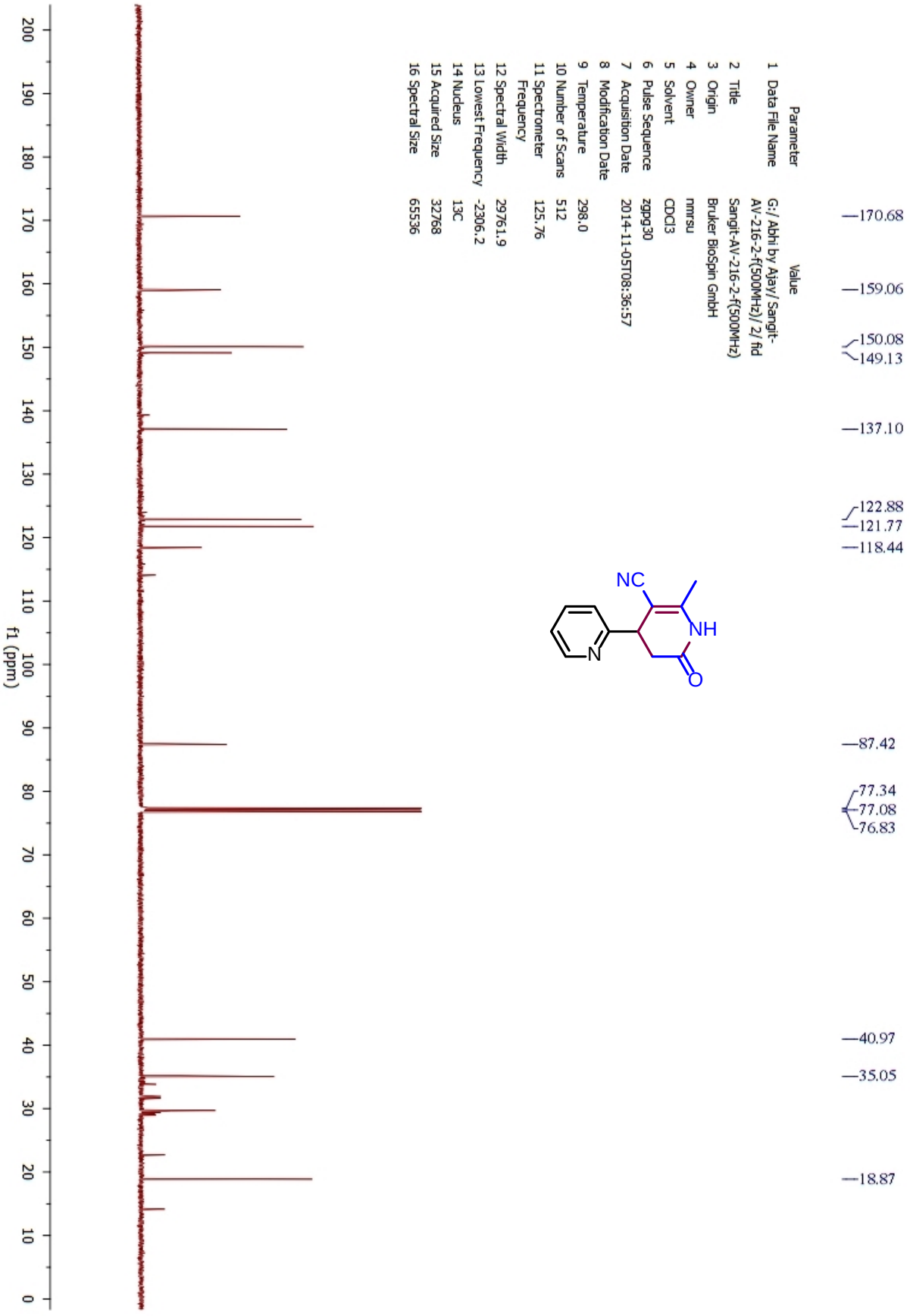


Figure S97 HRMS spectra of **32**

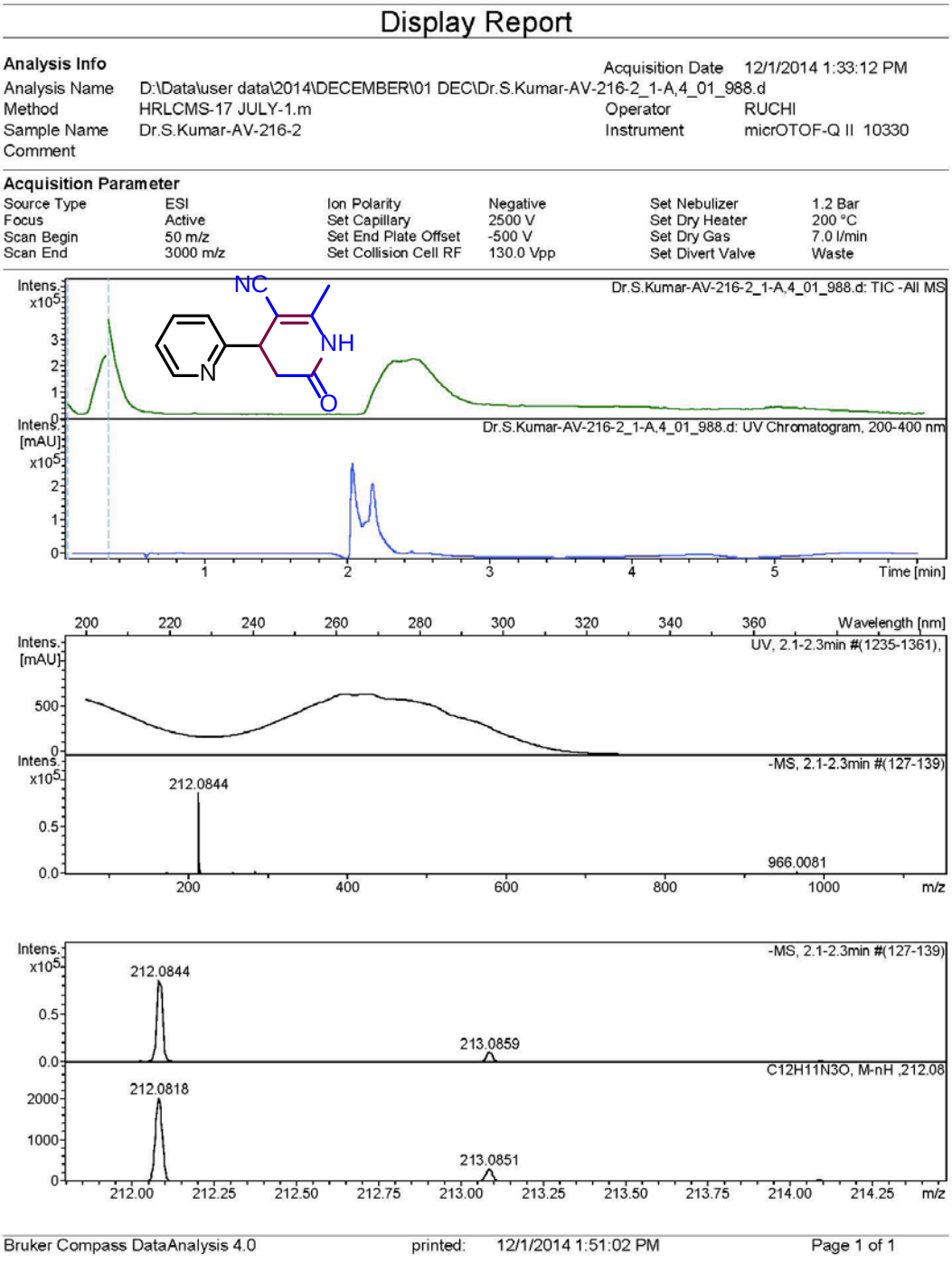


Figure S98 ^{1}H NMR spectra of **33**

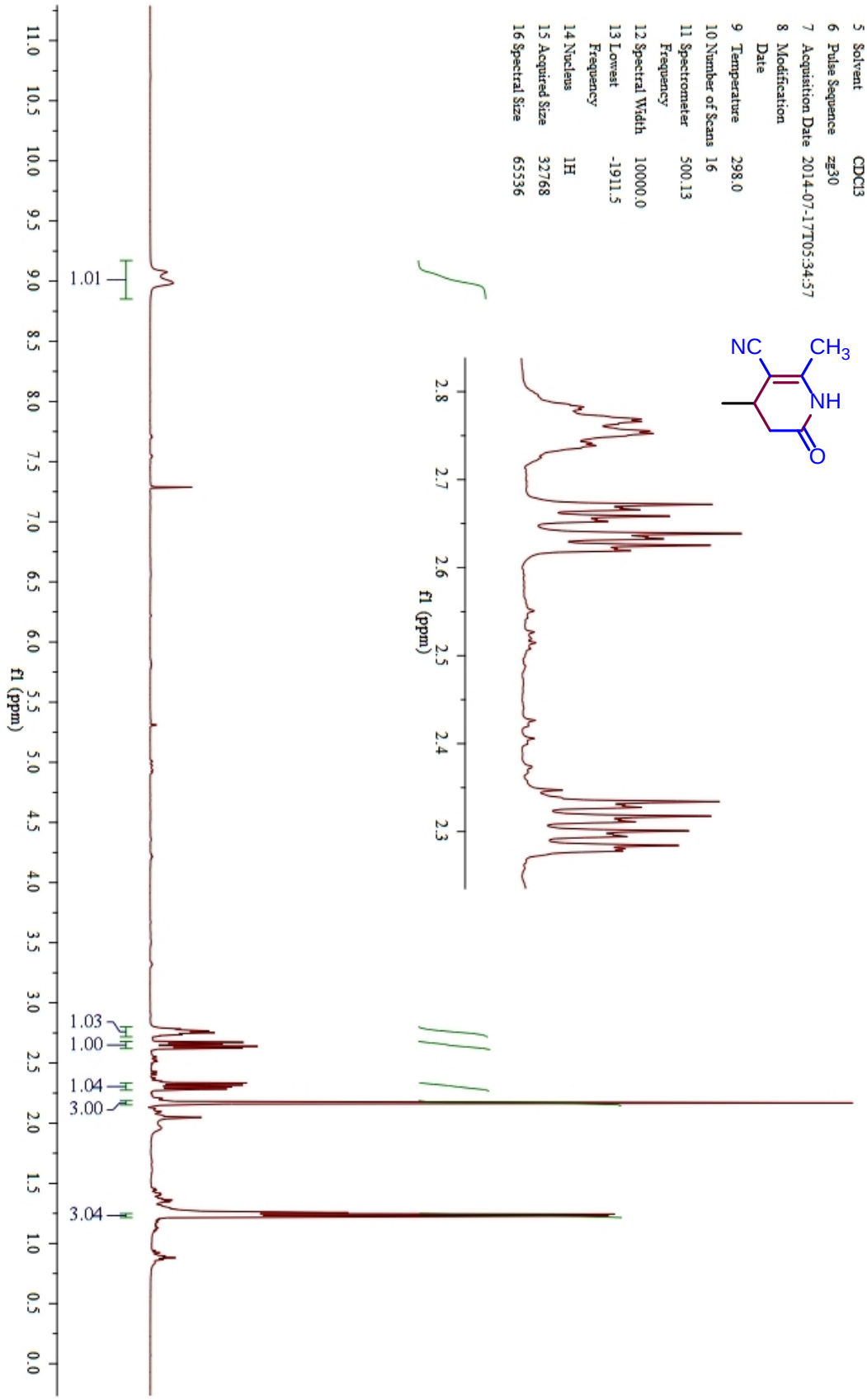


Figure S99 ^{13}C NMR spectra of **33**

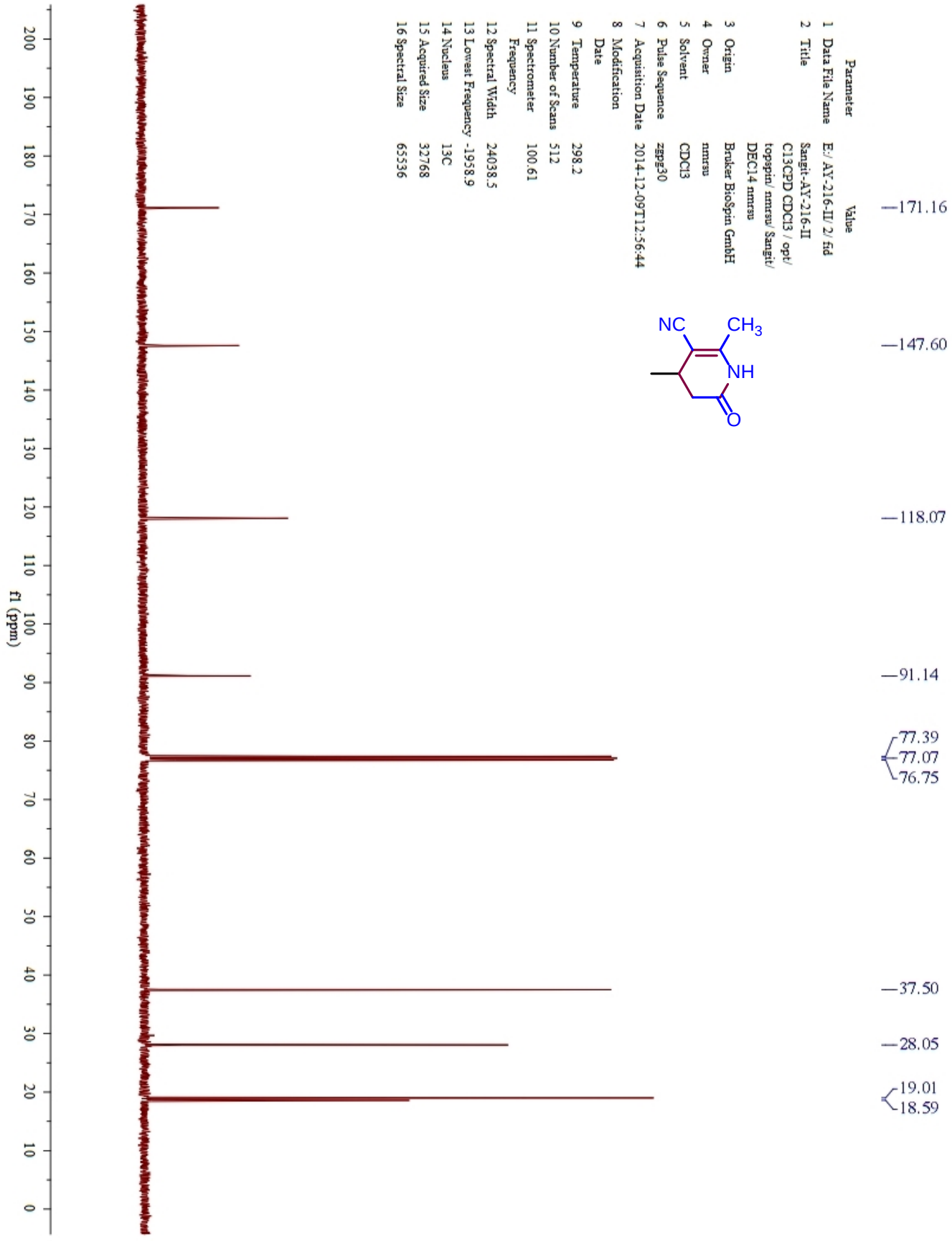


Figure S100 135-DEPT NMR spectra of **33**

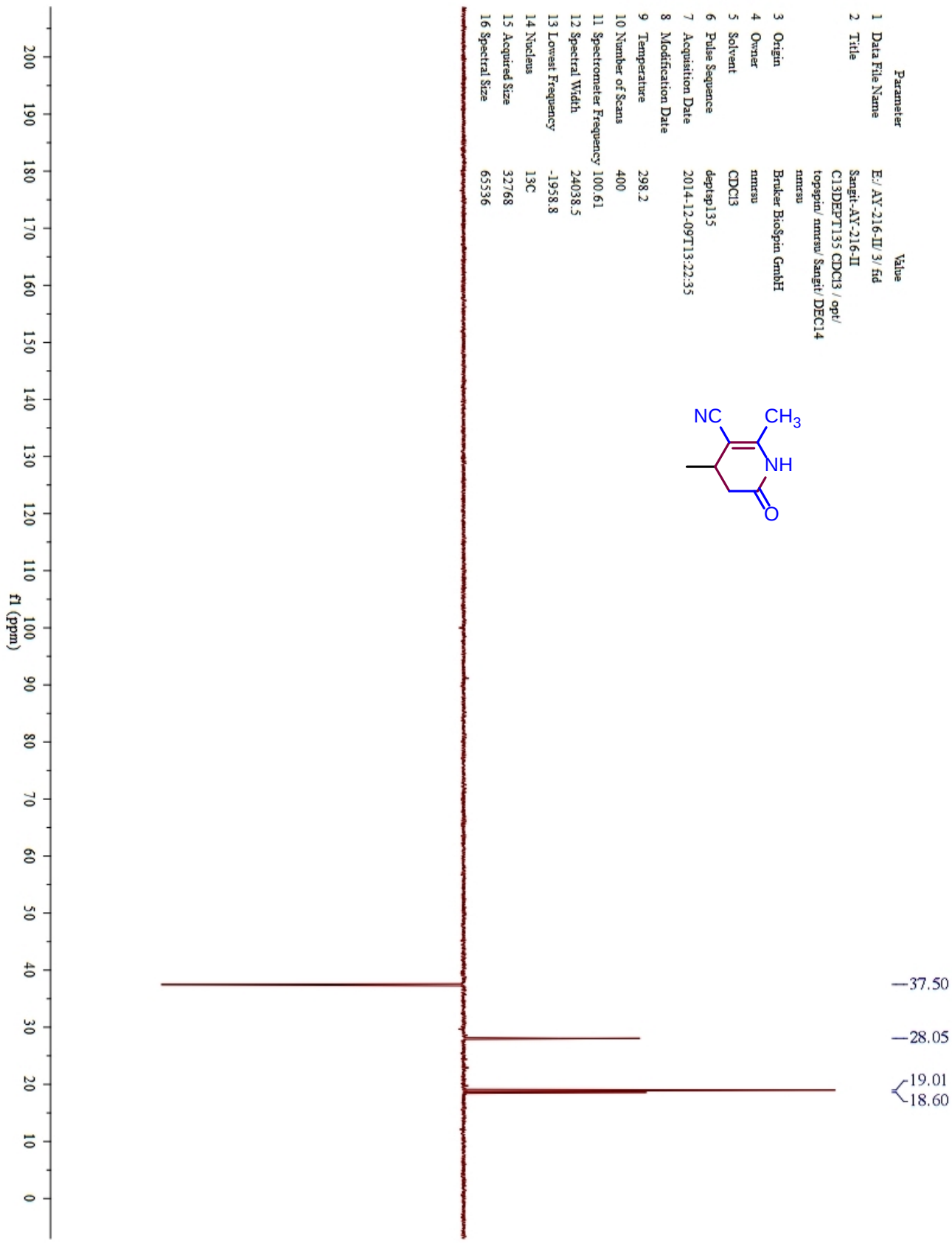


Figure S101 HRMS spectra of **33**

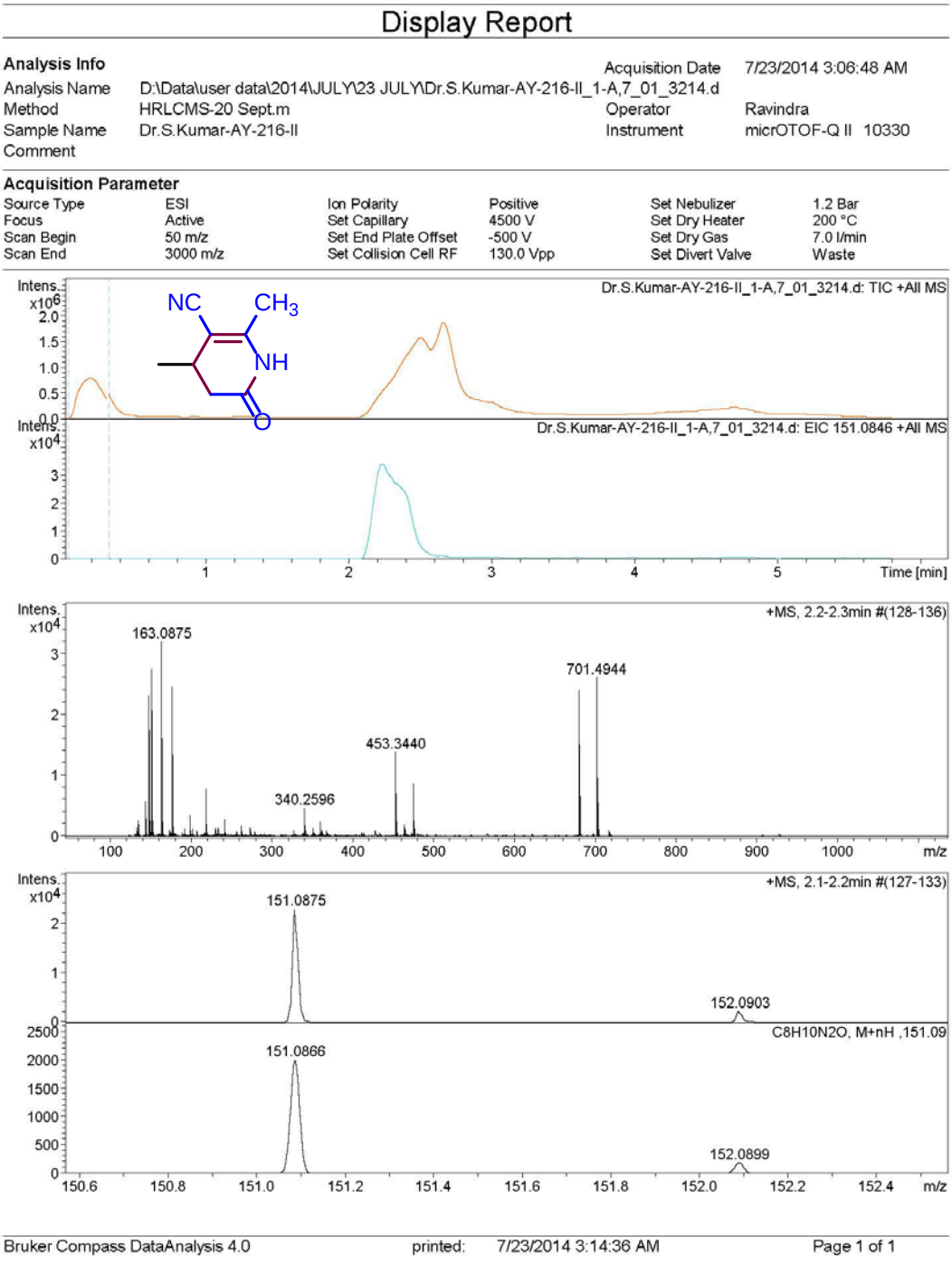


Figure S102 ^{1}H NMR spectra of **34**

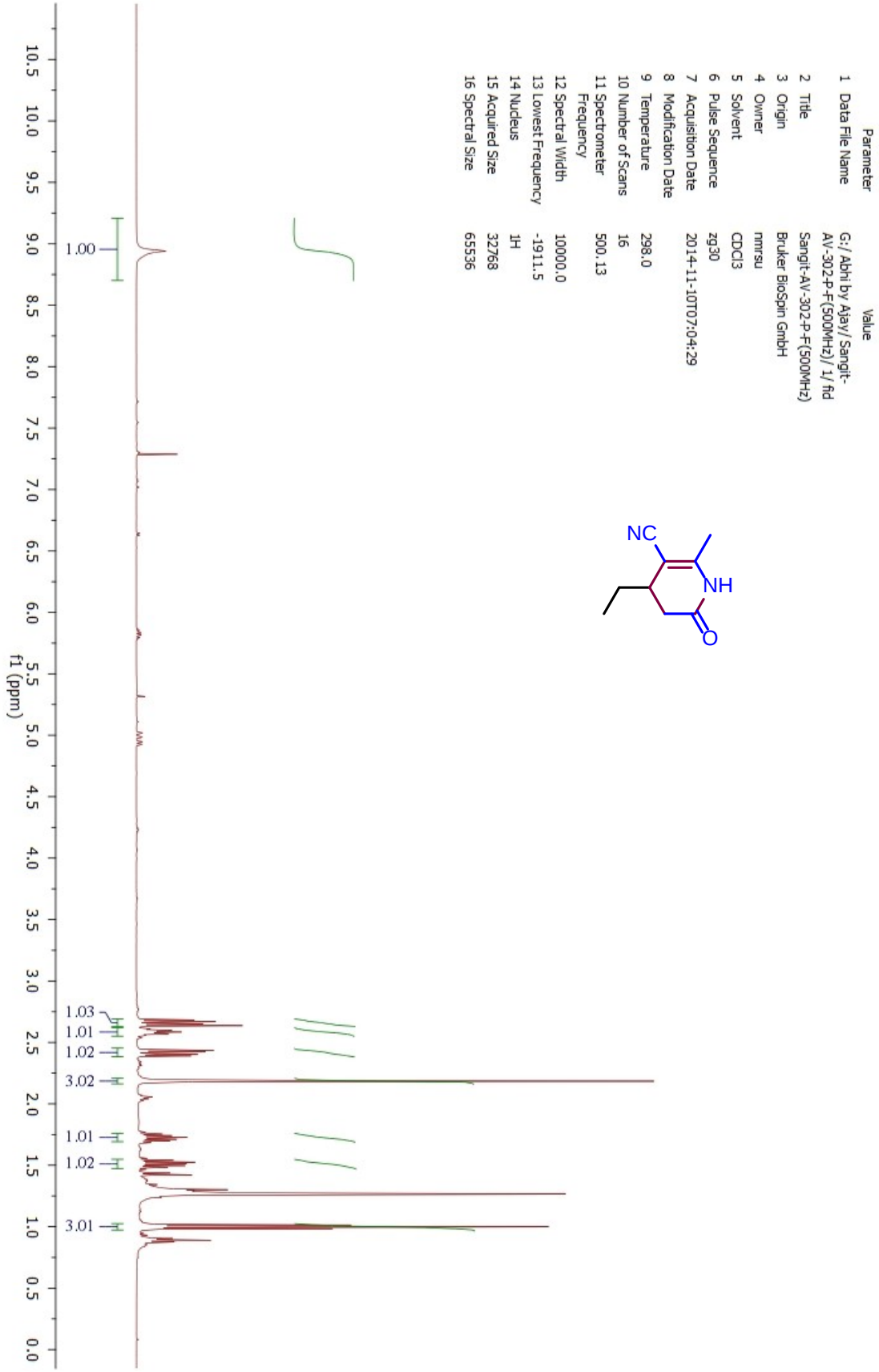


Figure S103 ^{13}C NMR spectra of **34**

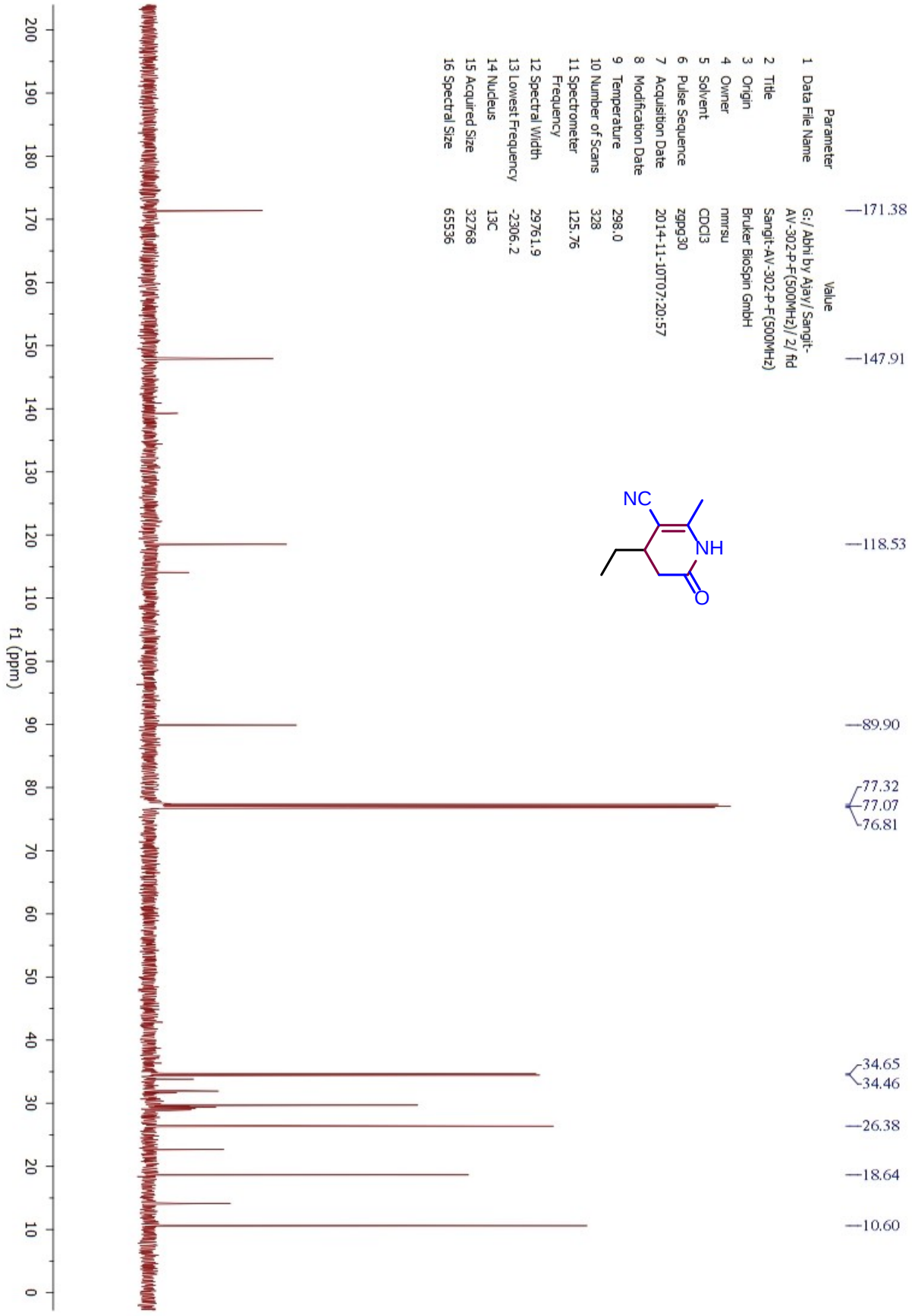


Figure S104 HRMS spectra of **34**

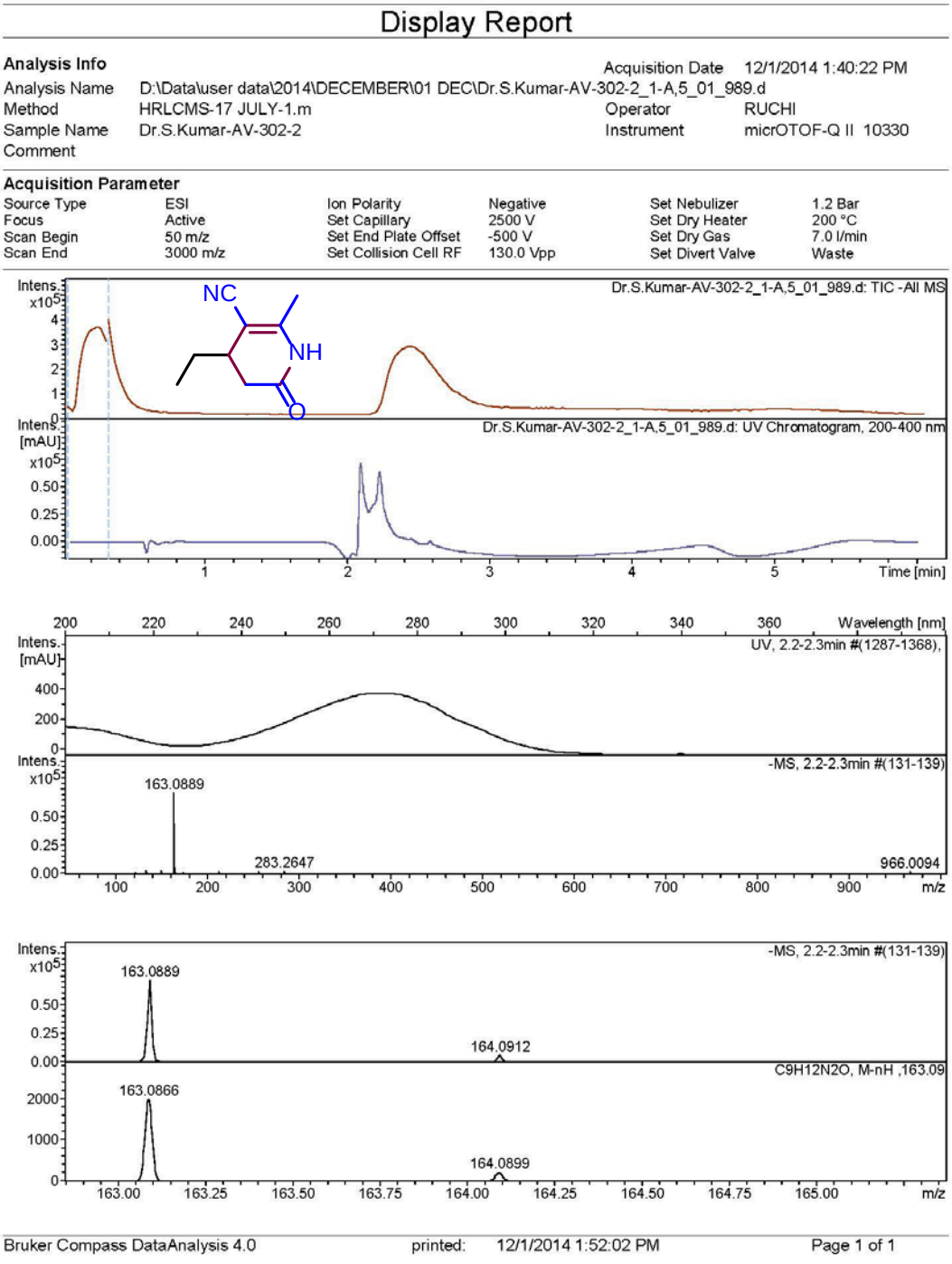


Figure S105 ^{1}H NMR spectra of **35**

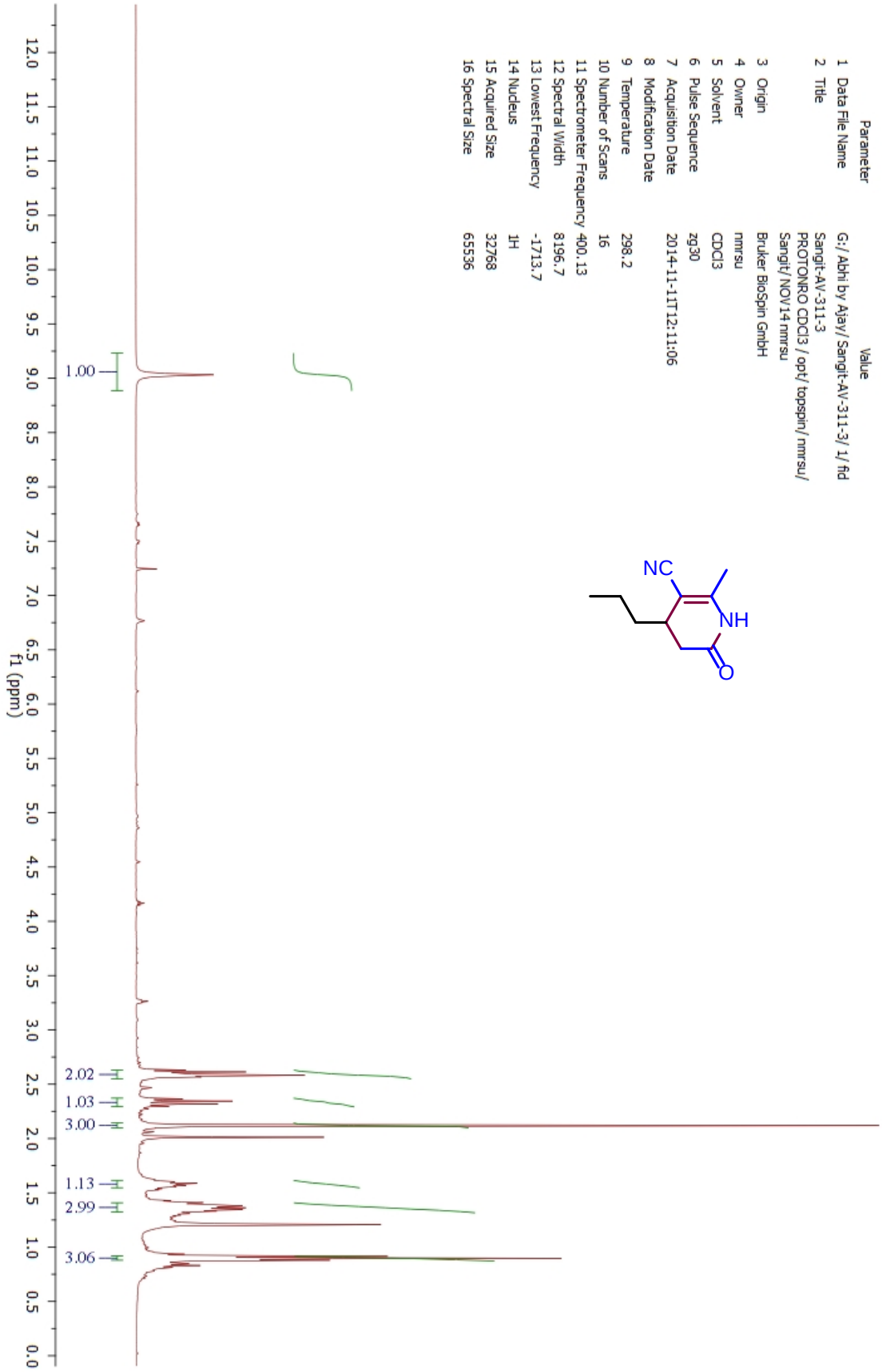


Figure S106 ^{13}C NMR spectra of **35**

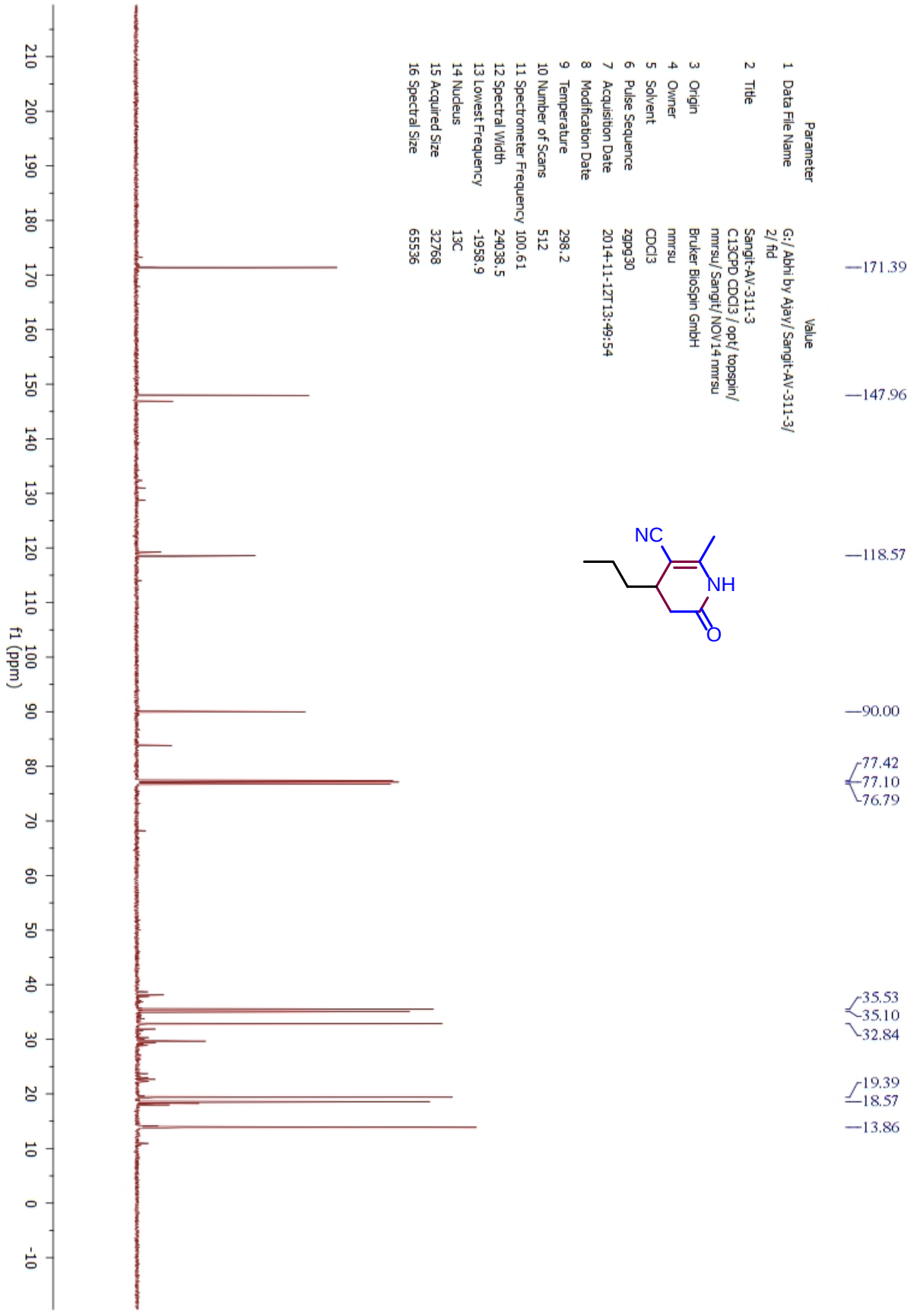


Figure S107 HRMS spectra of **35**

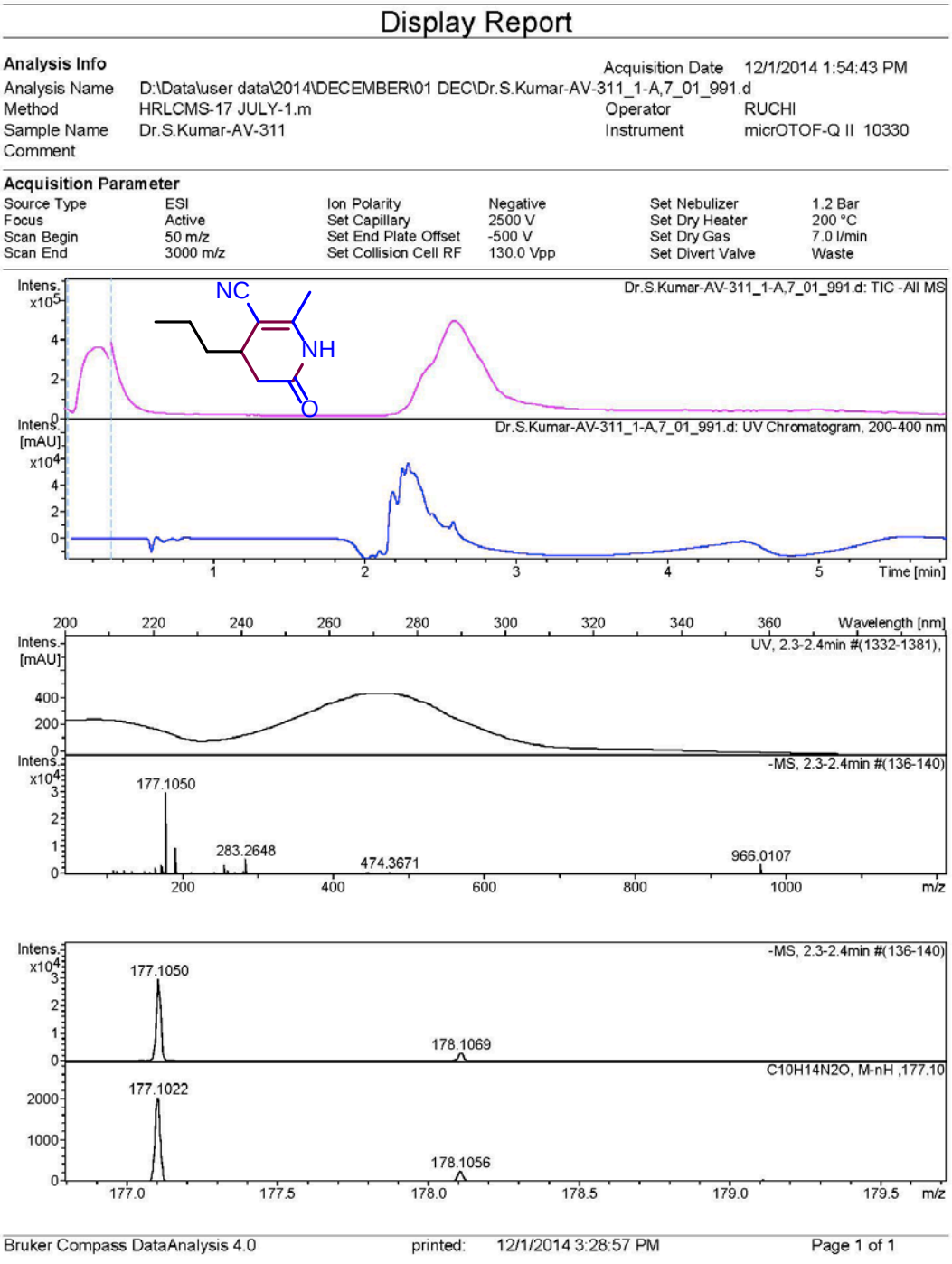


Figure S108 ^{1}H NMR spectra of **36**

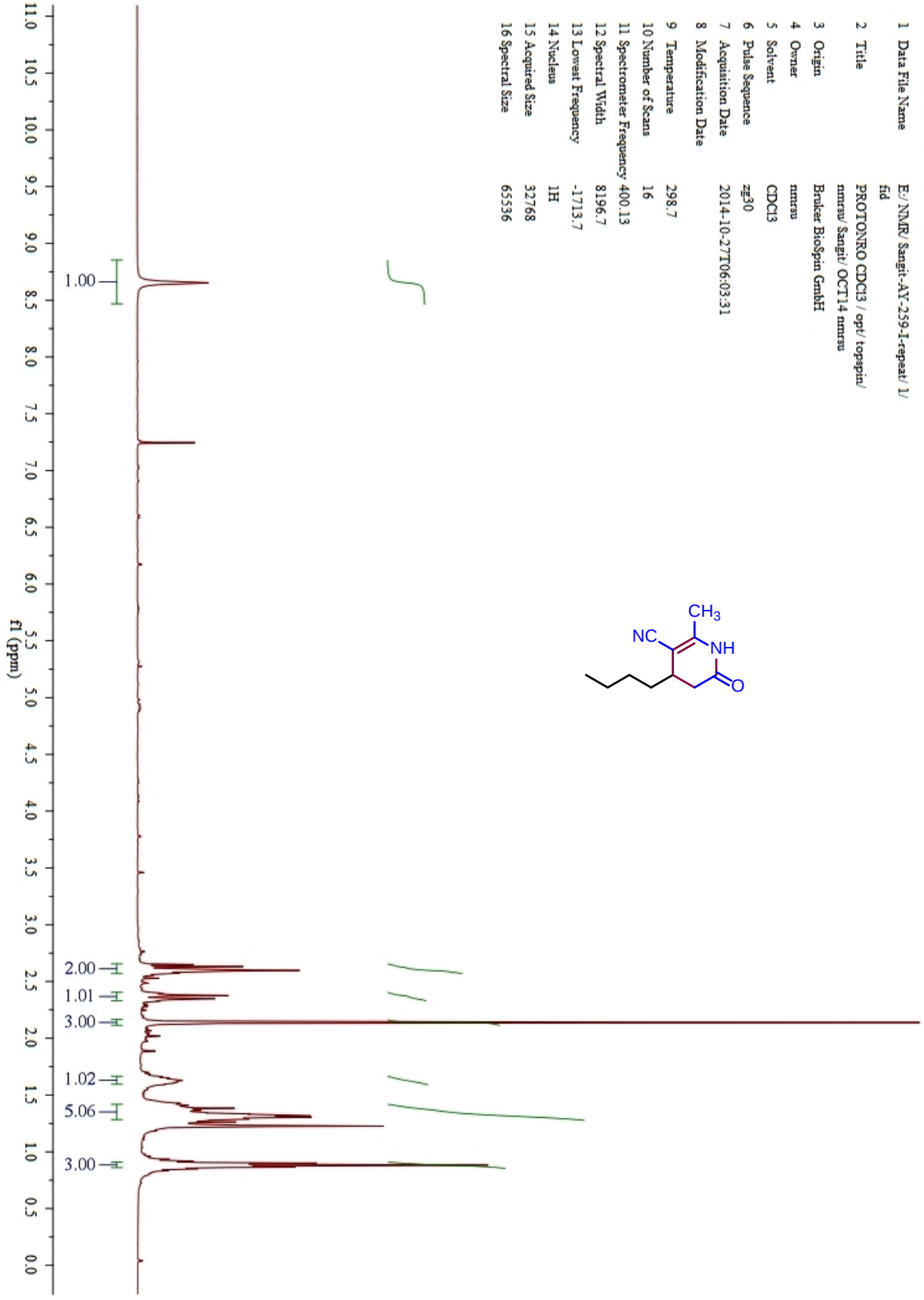


Figure S109 ^{13}C NMR spectra of **36**

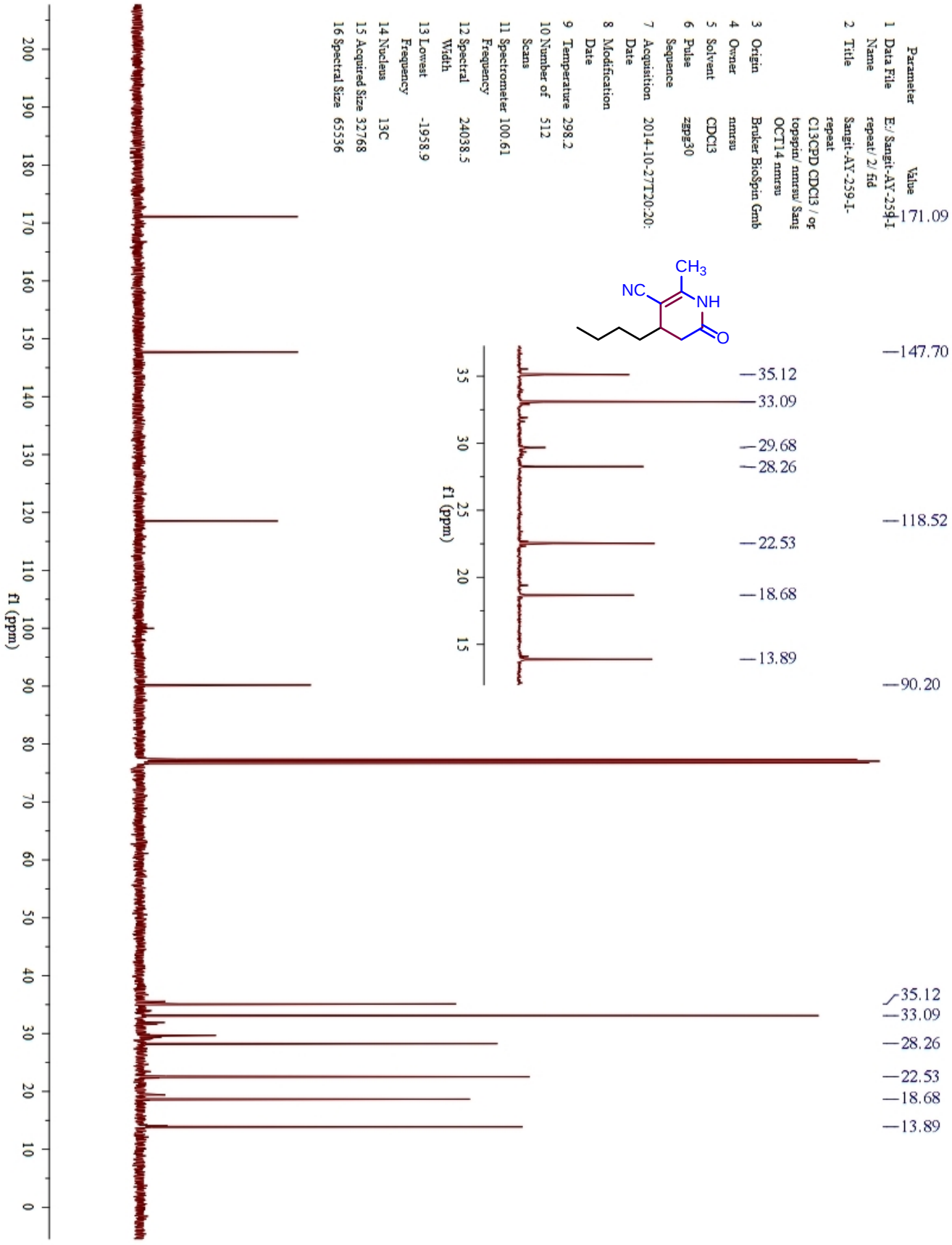


Figure S110 HRMS spectra of **36**

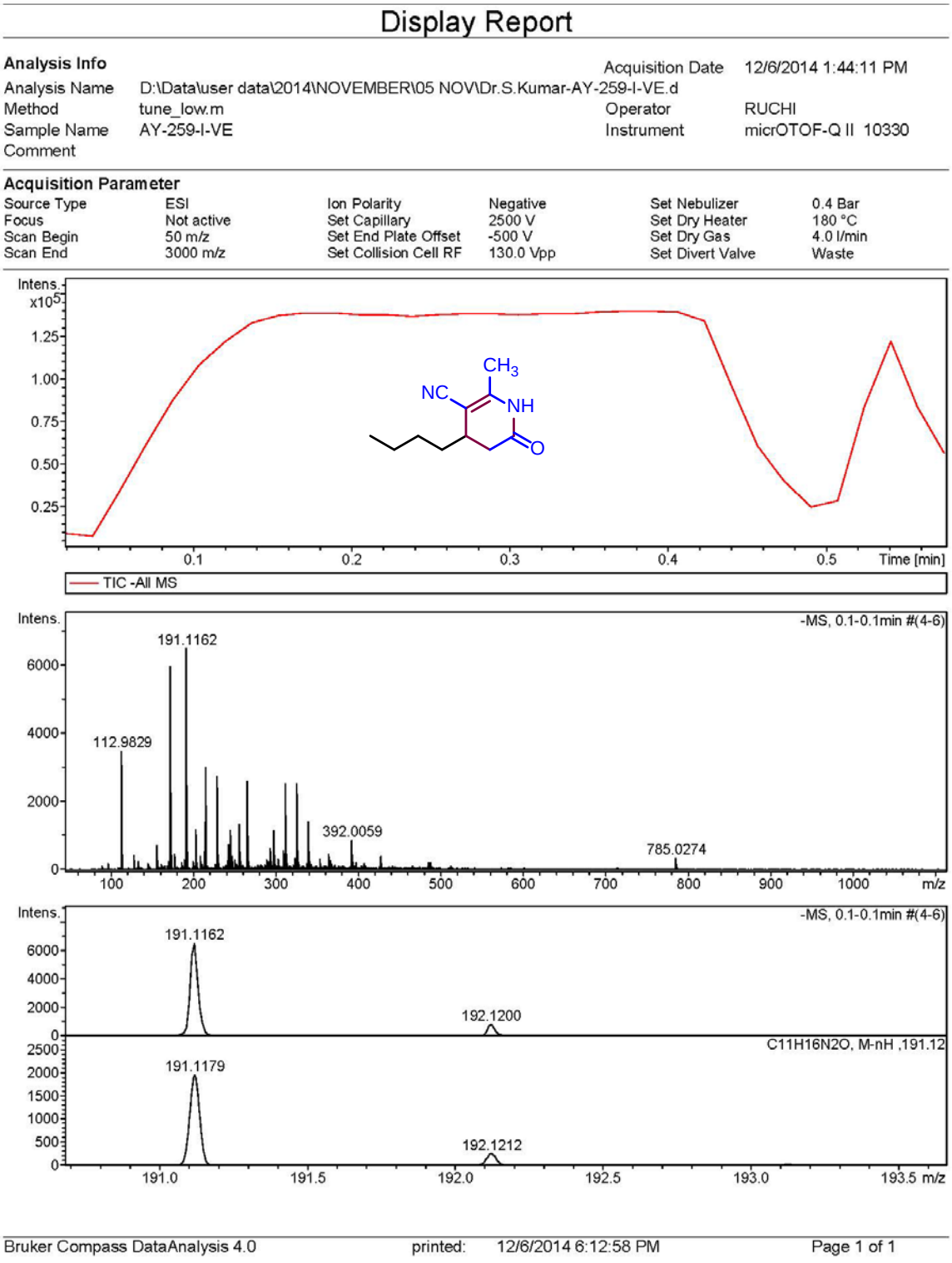


Figure S111 ^{1}H NMR spectra of **37**

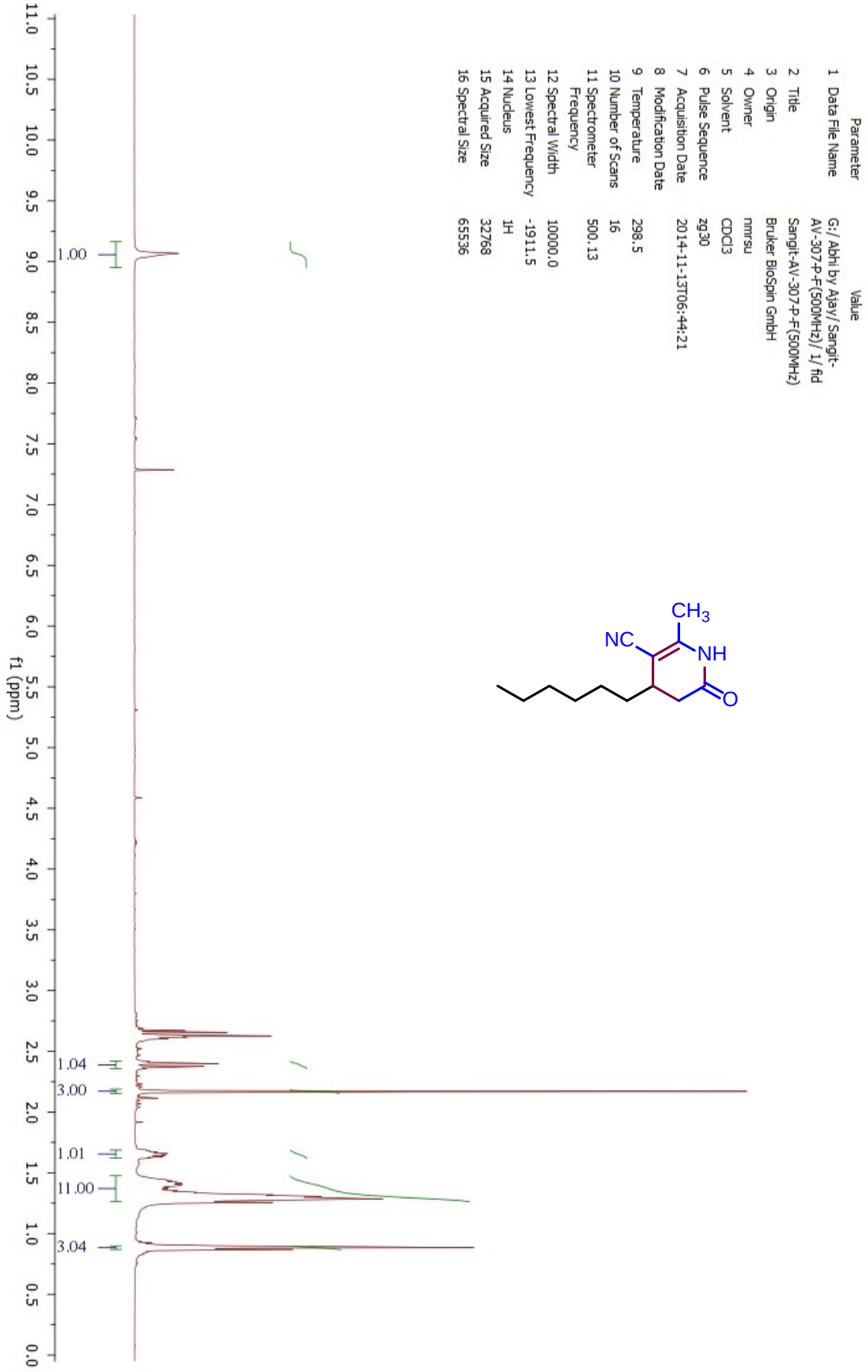


Figure S112 ^{13}C NMR spectra of **37**

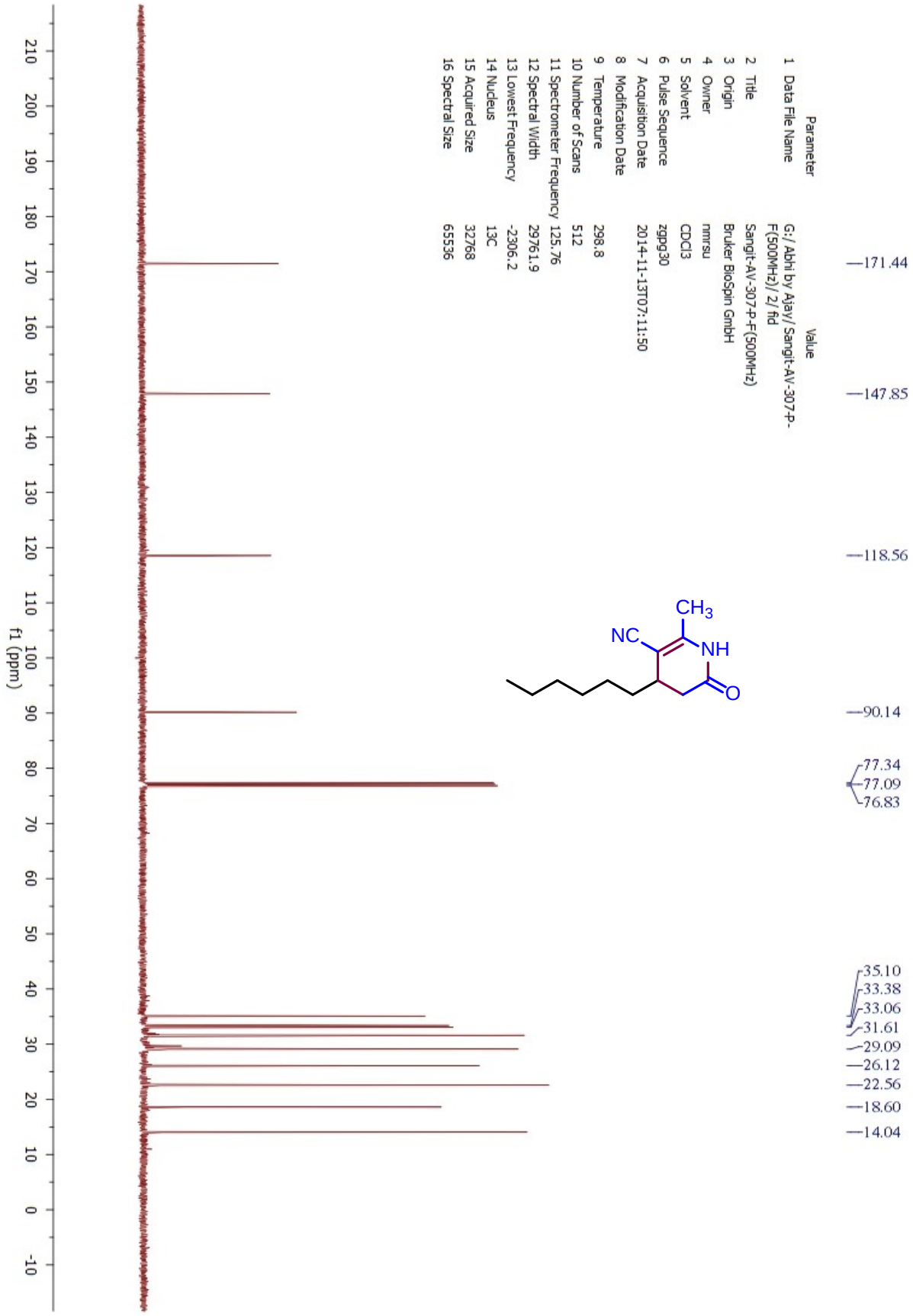


Figure S113 HRMS spectra of **37**

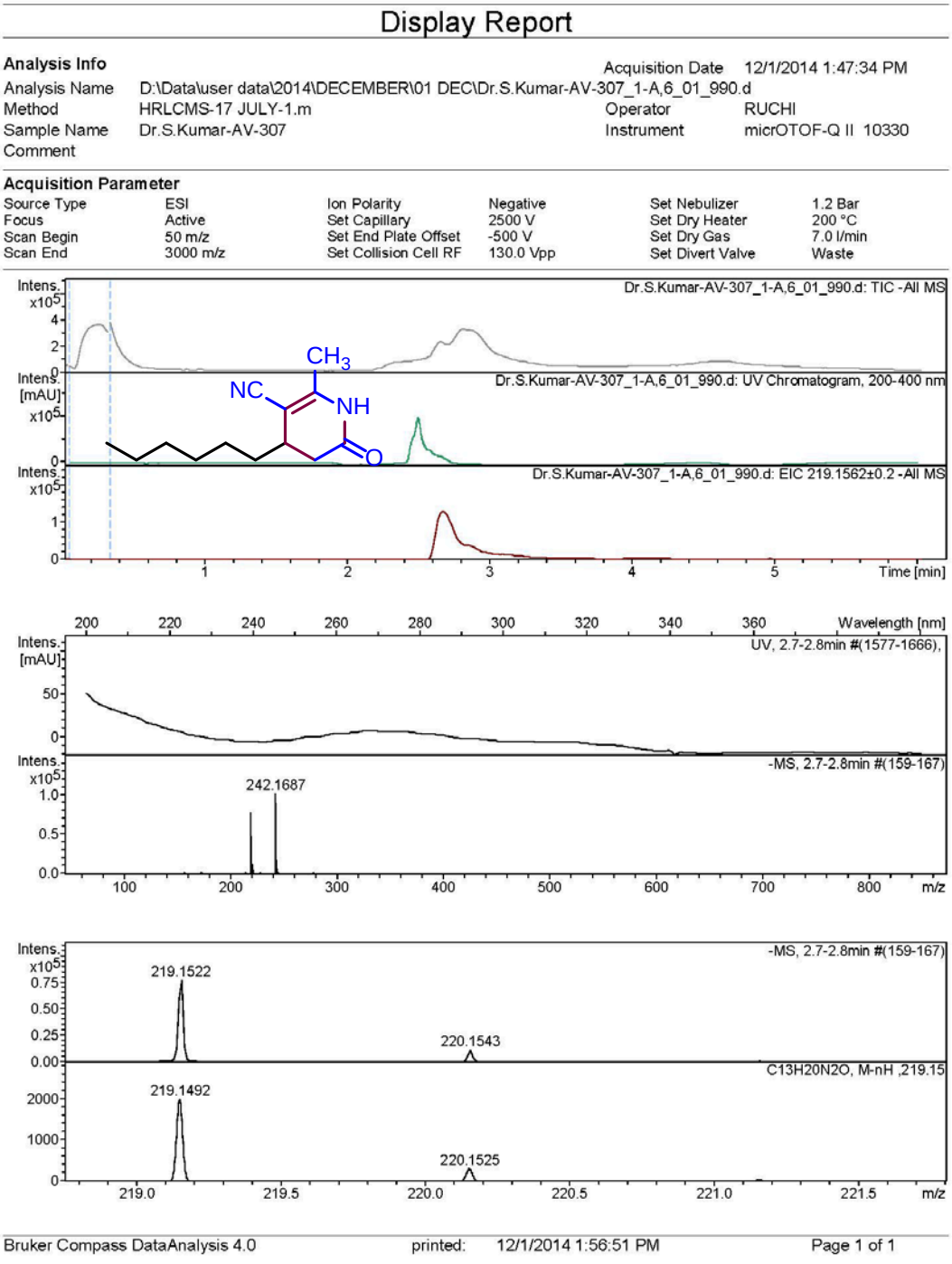


Figure S114 ^{1}H NMR spectra of **38**

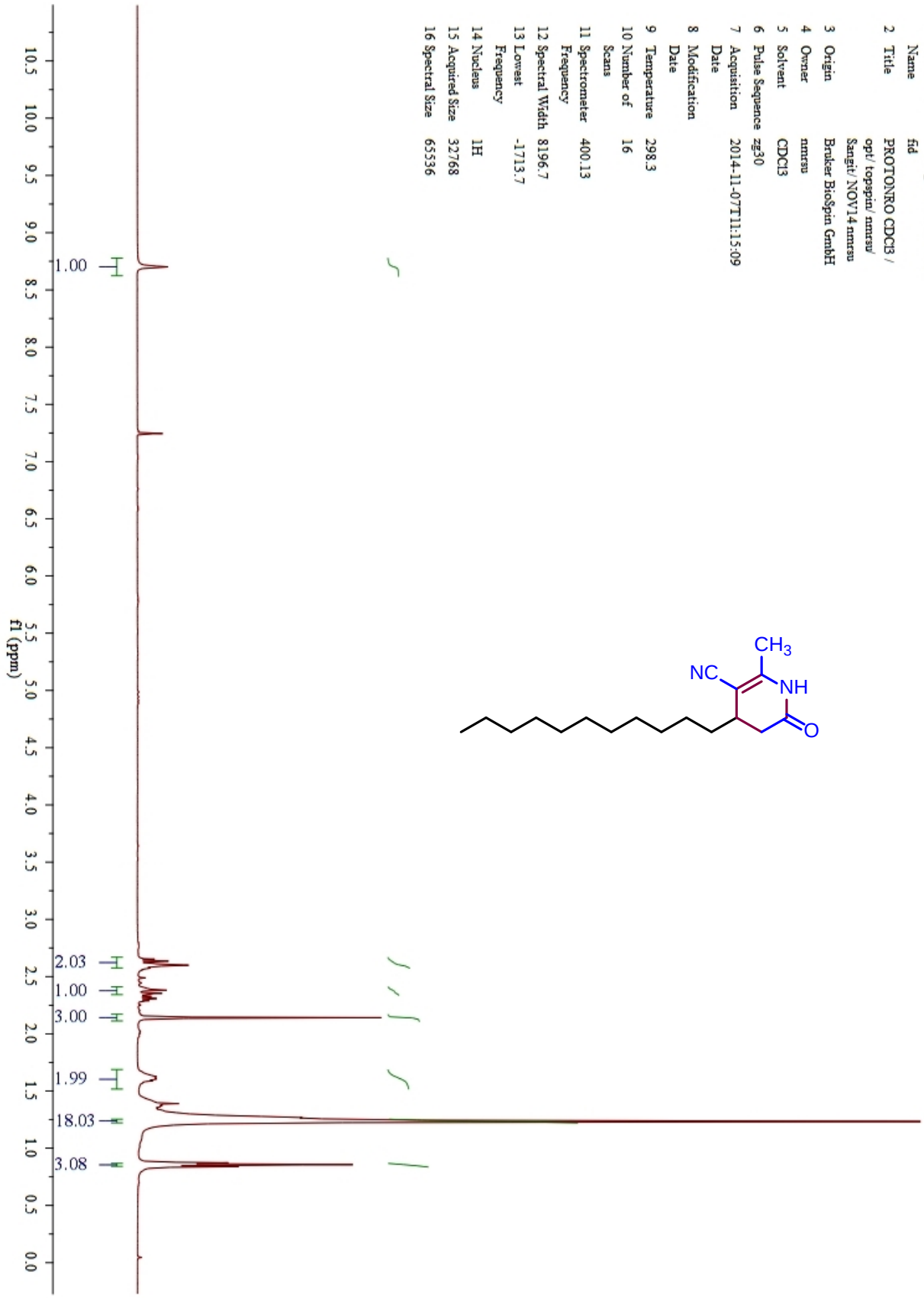


Figure S115 ^{13}C NMR spectra of **38**

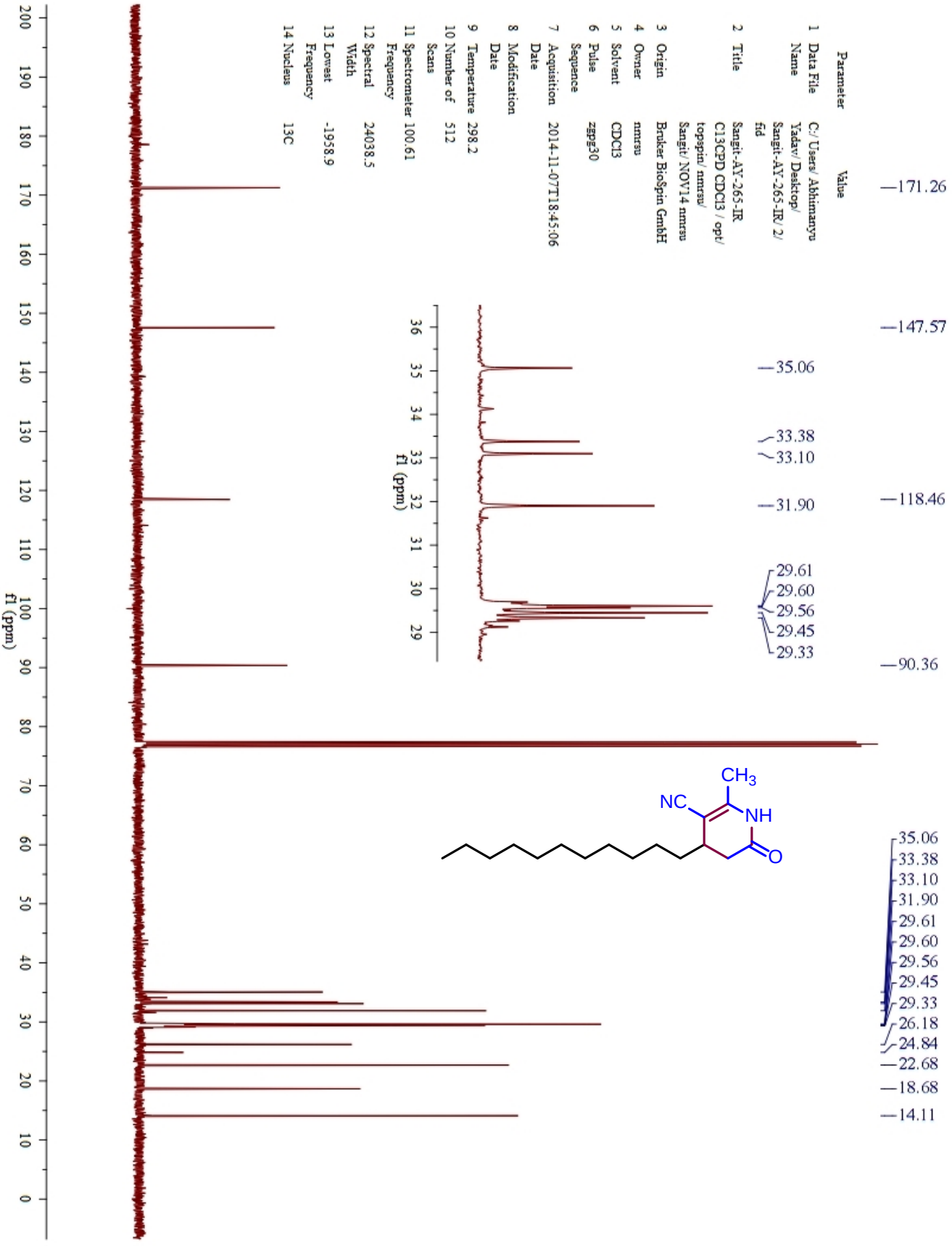


Figure S116 Mass spectra of **38**

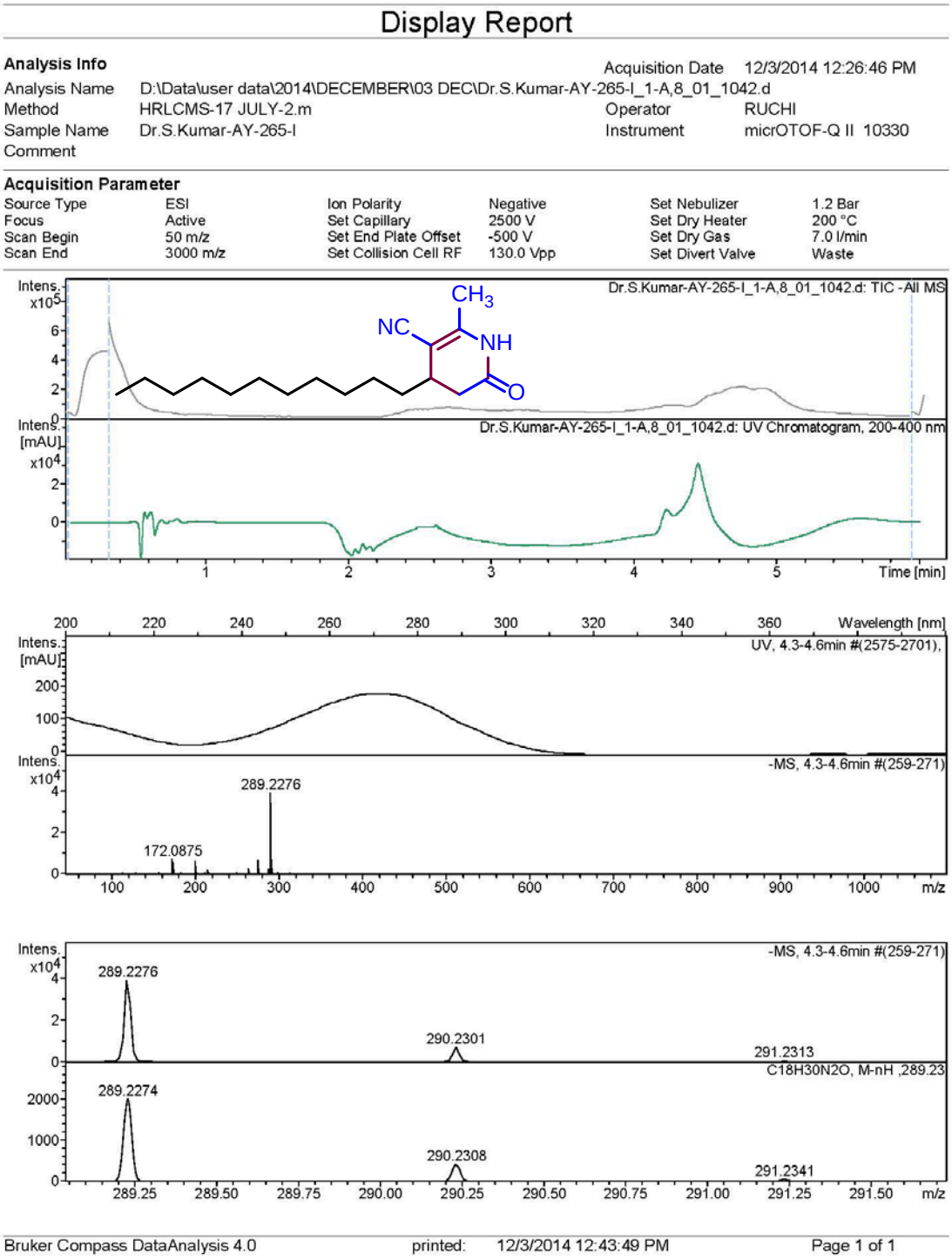


Figure S117 ^{1}H NMR spectra of **39**

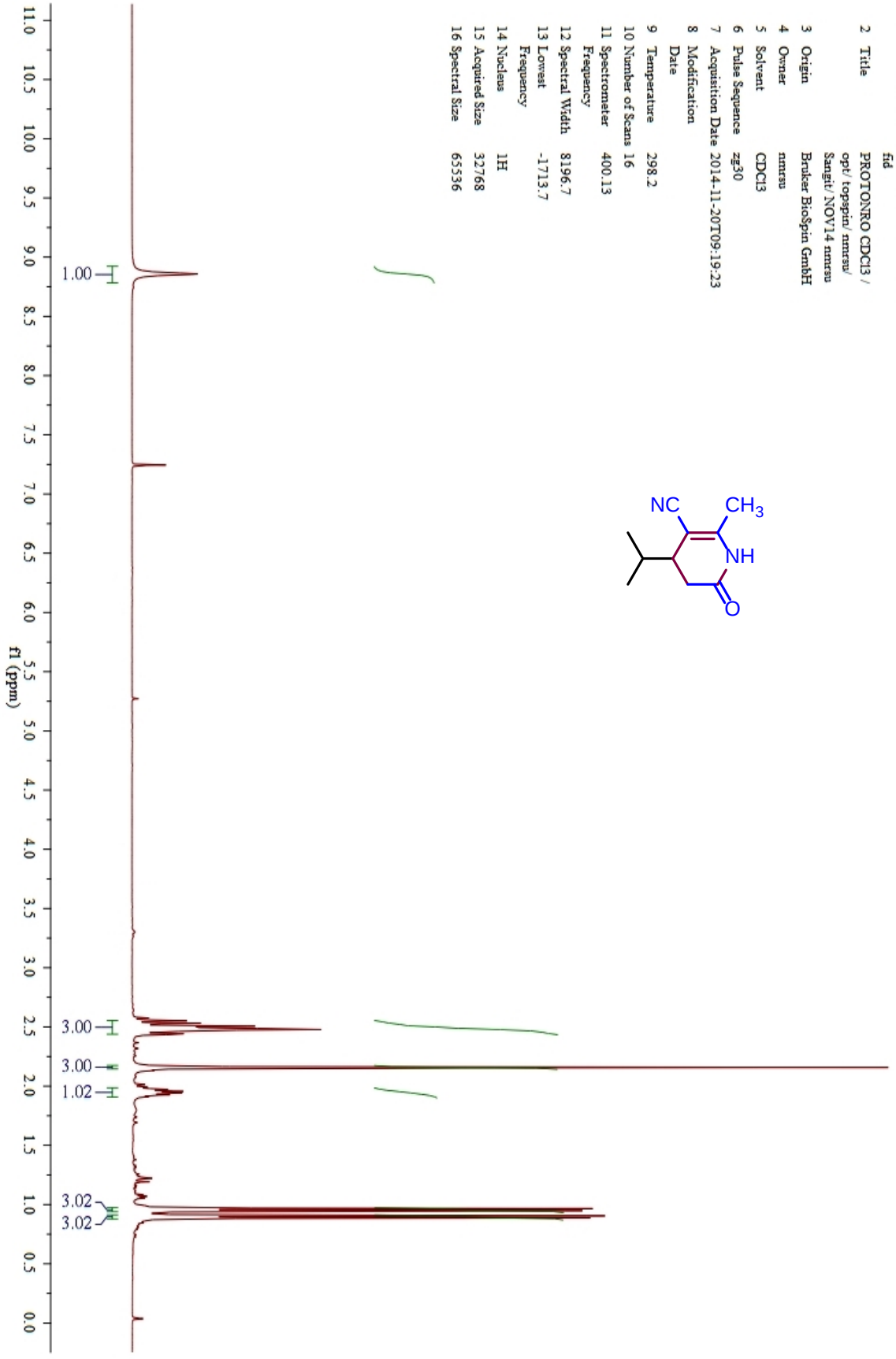


Figure S118 ^{13}C NMR spectra of **39**

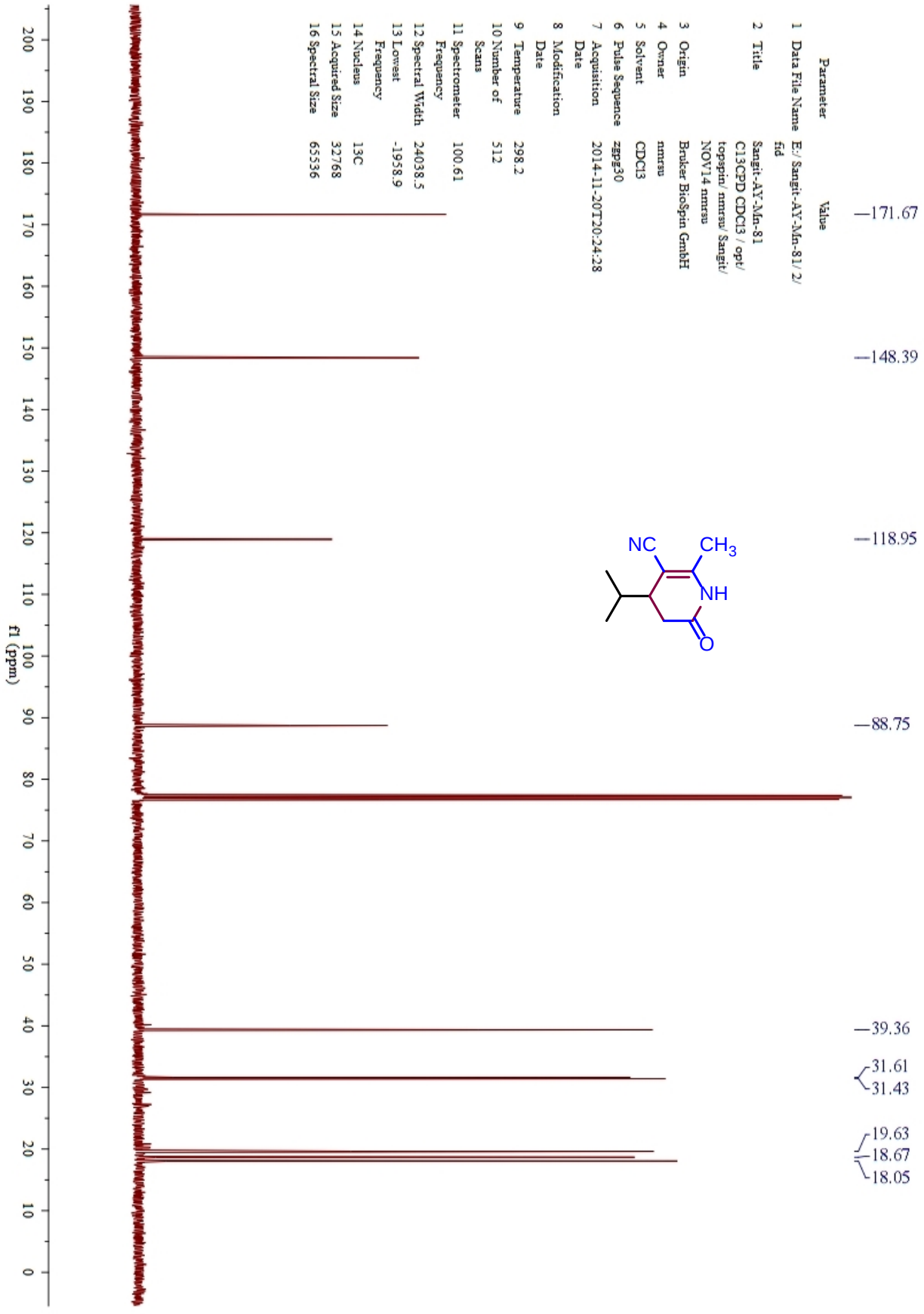


Figure S119 Mass spectra of **39**

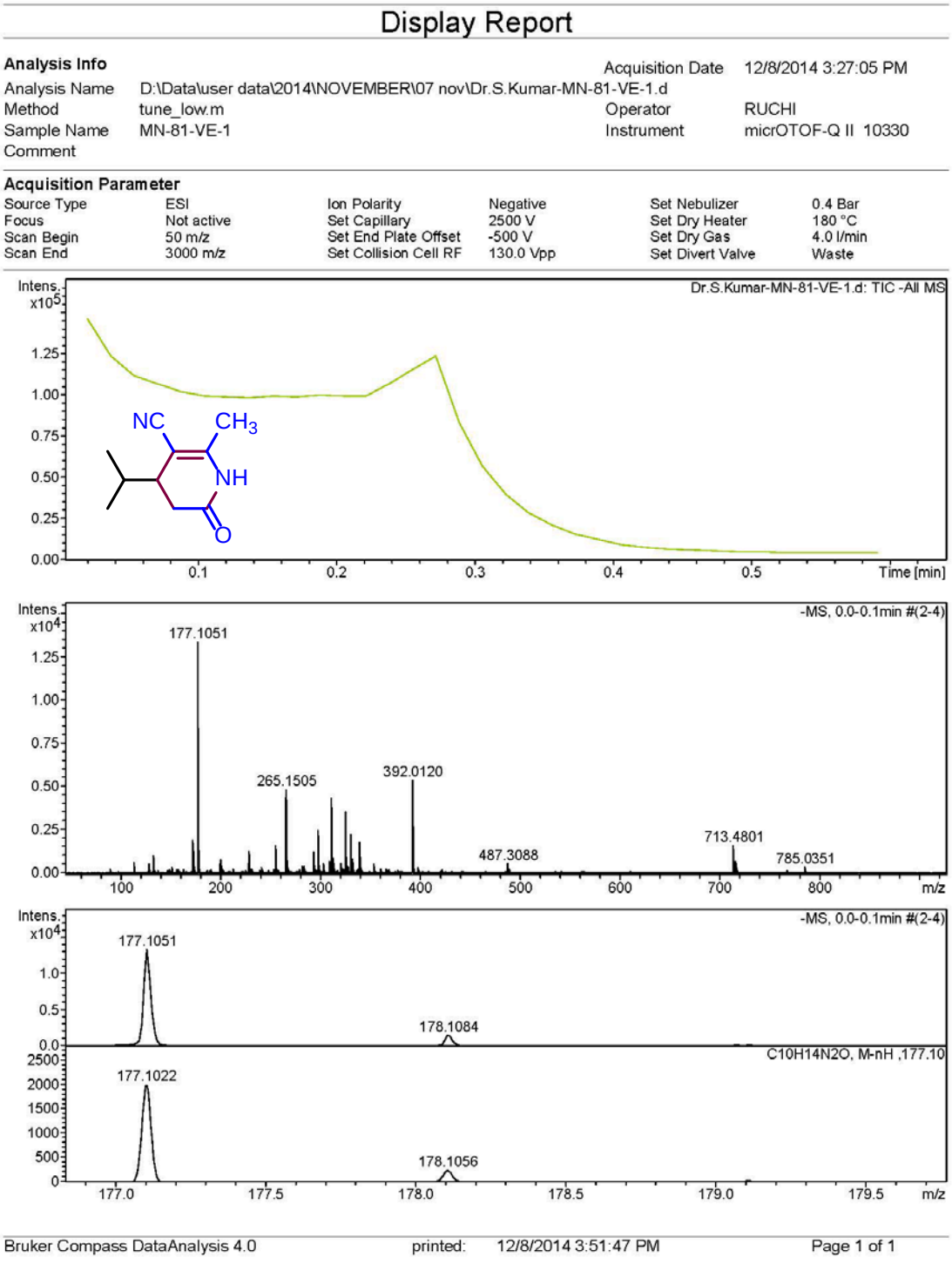


Figure S120 ^{1}H NMR spectra of **40**

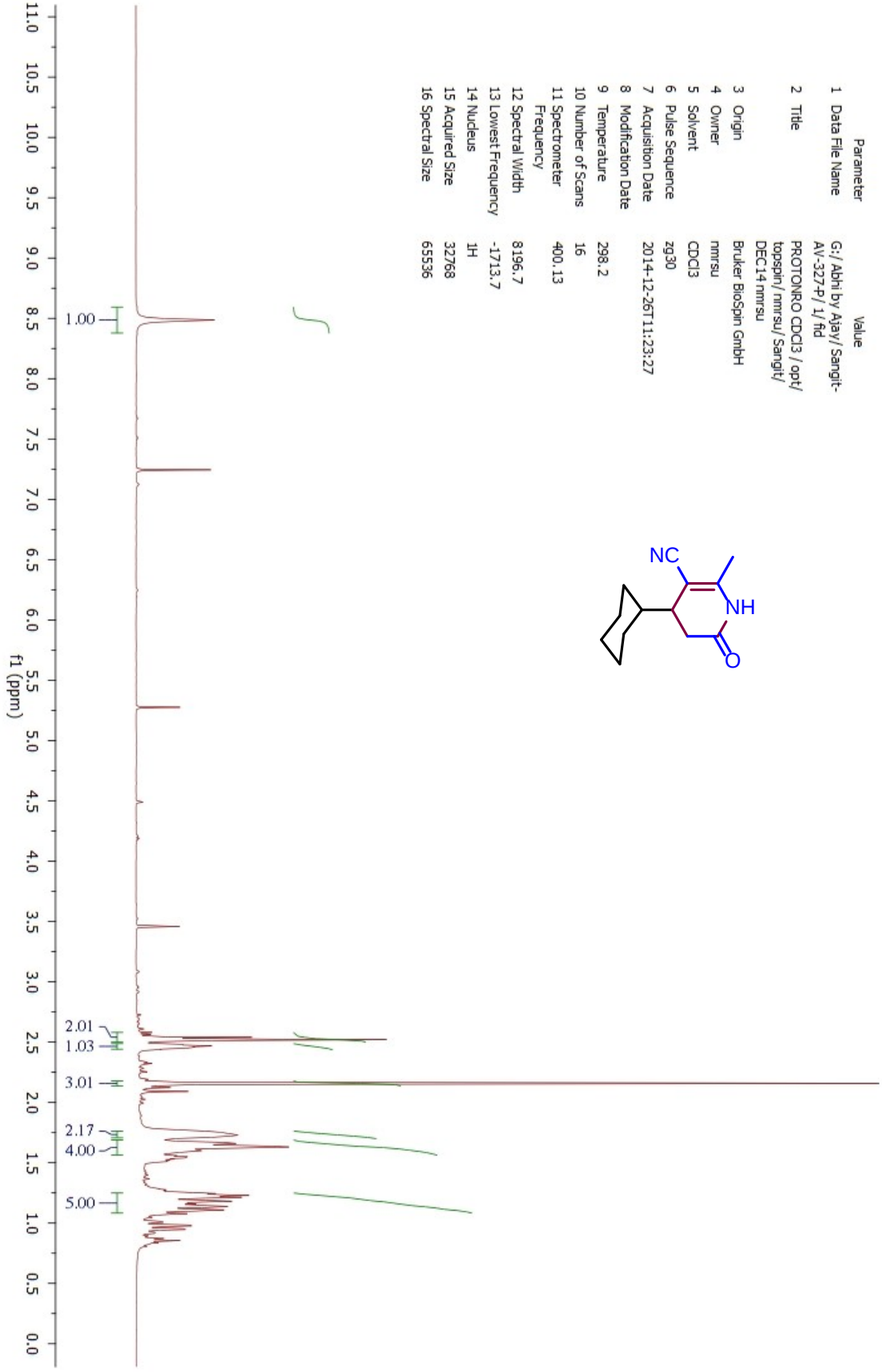


Figure S121 ^{13}C NMR spectra of **40**

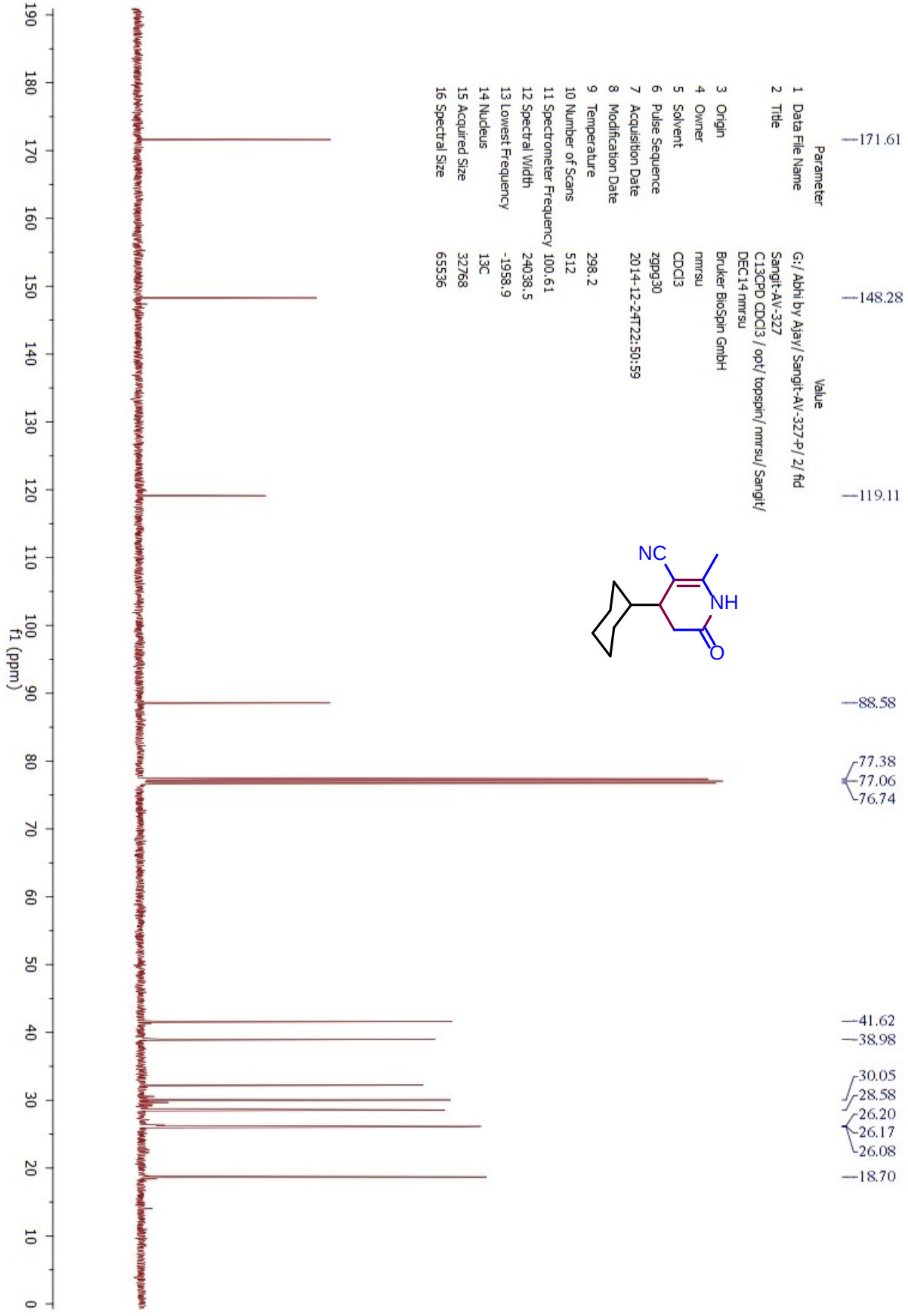


Figure S122 HRMS spectra of **40**

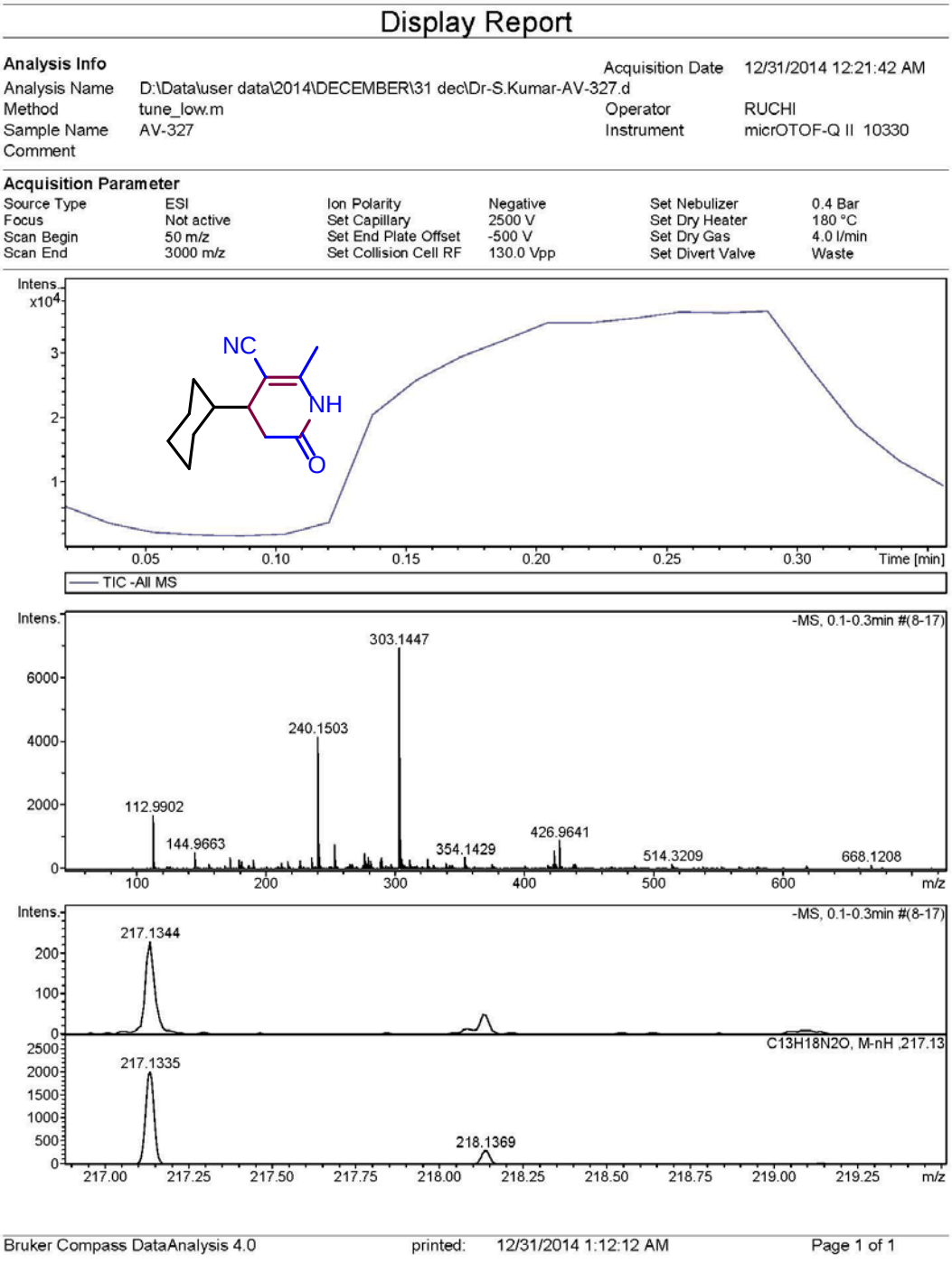


Figure S123 ^{1}H NMR spectra of **41**

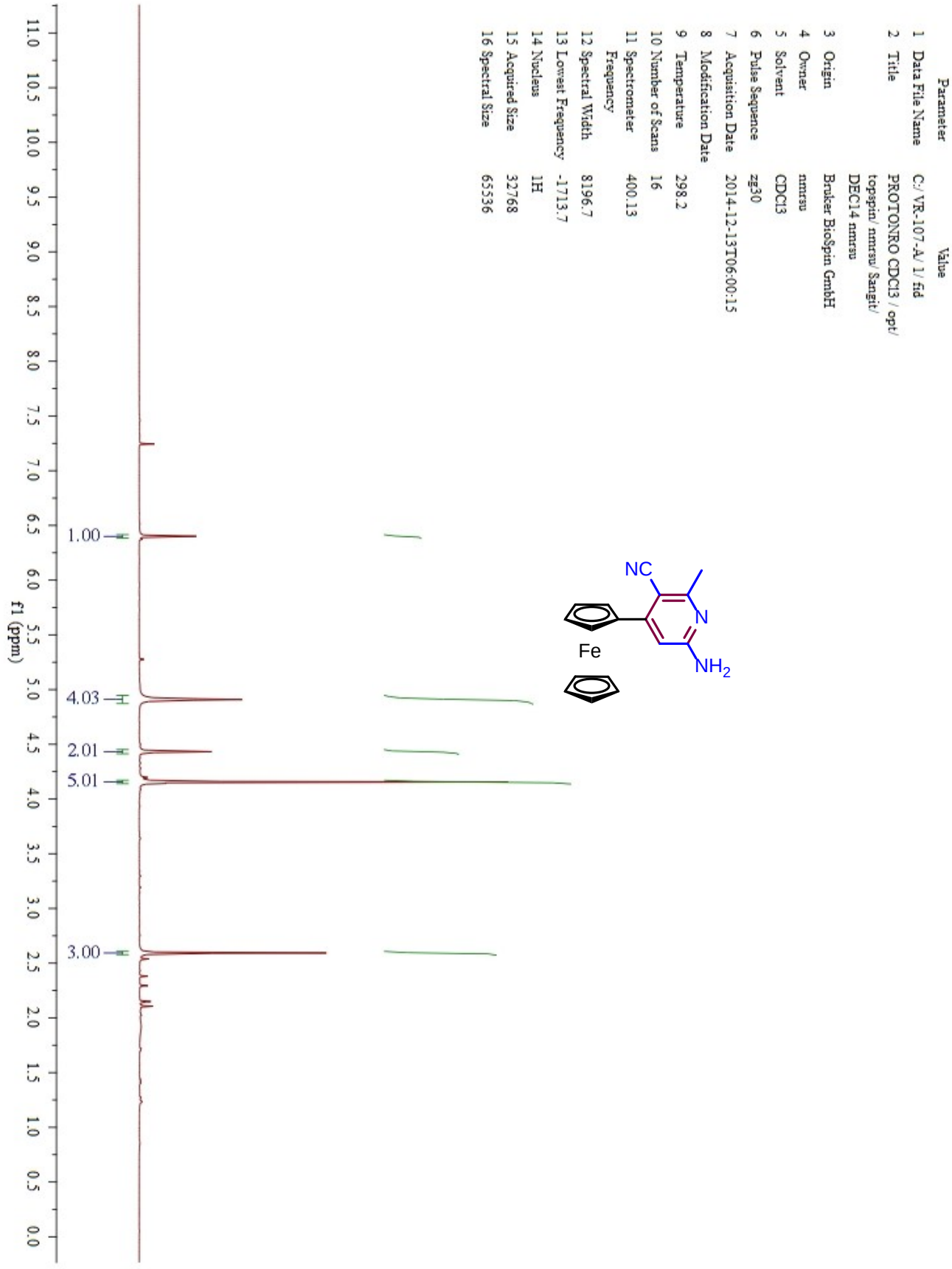


Figure S124 ^{13}C NMR spectra of **41**

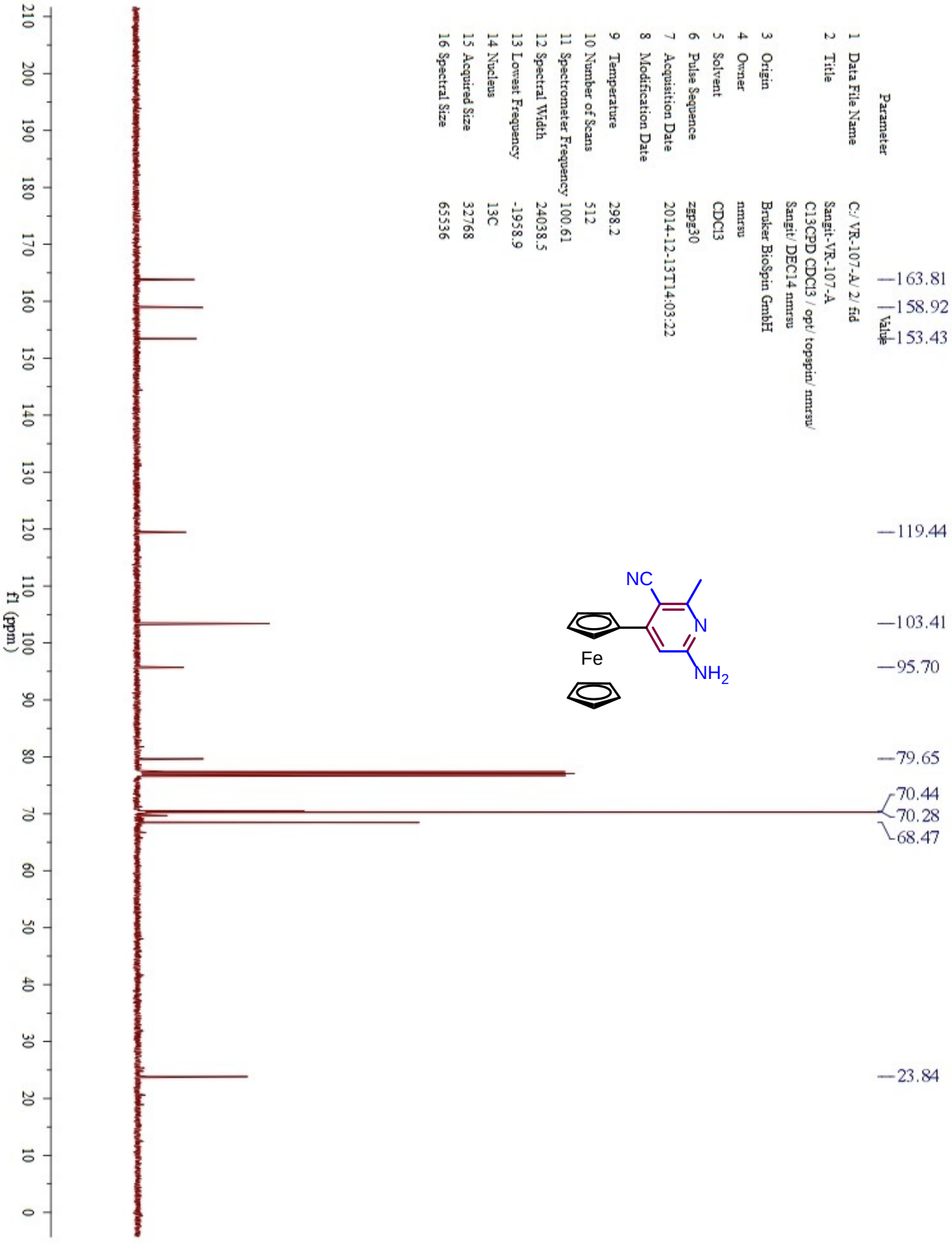


Figure S125 DEPT spectra of **41**

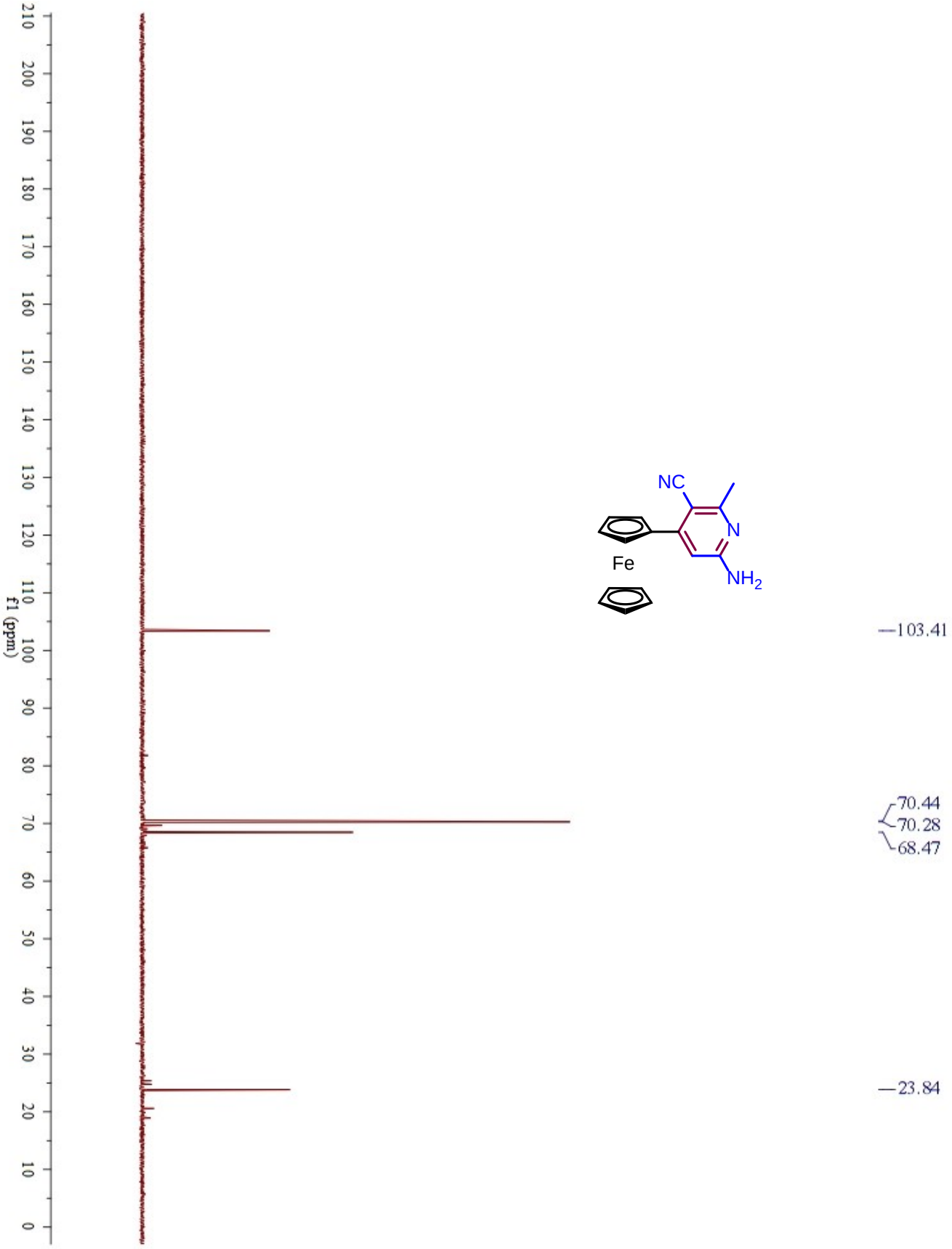


Figure S126 Mass spectra of **41**

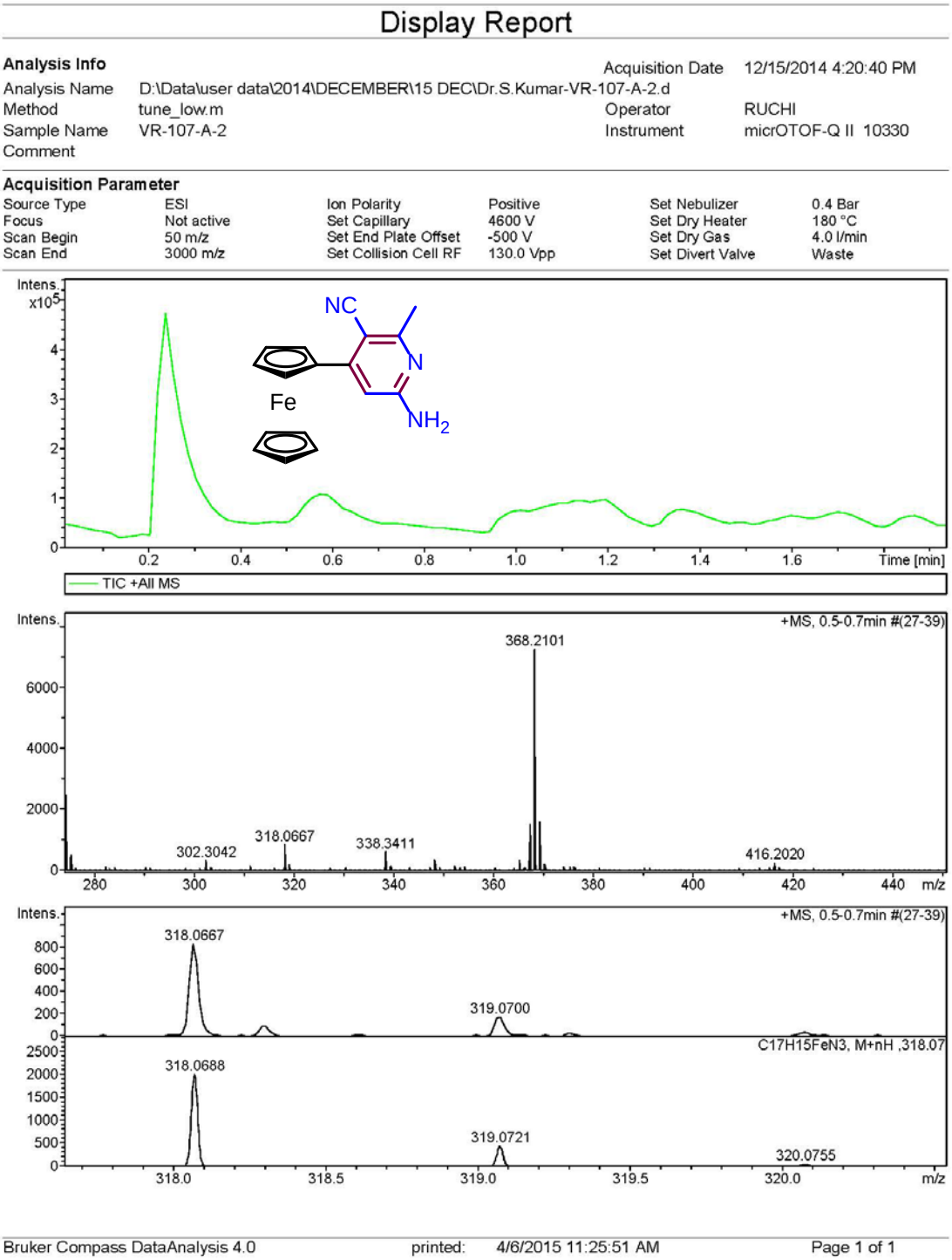


Figure S127 ^{1}H NMR spectra of **42**

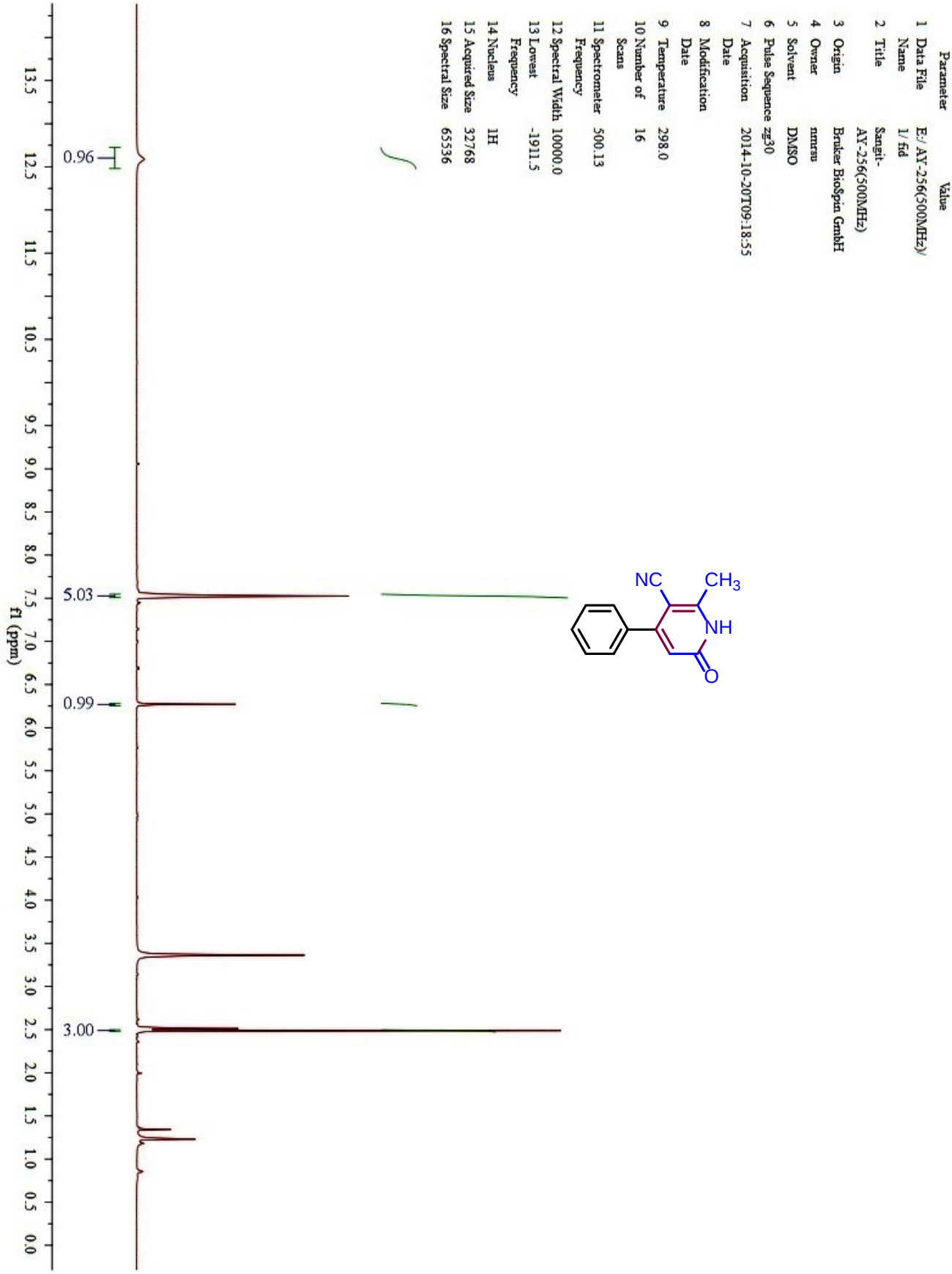


Figure S128 ^{13}C NMR spectra of **42**

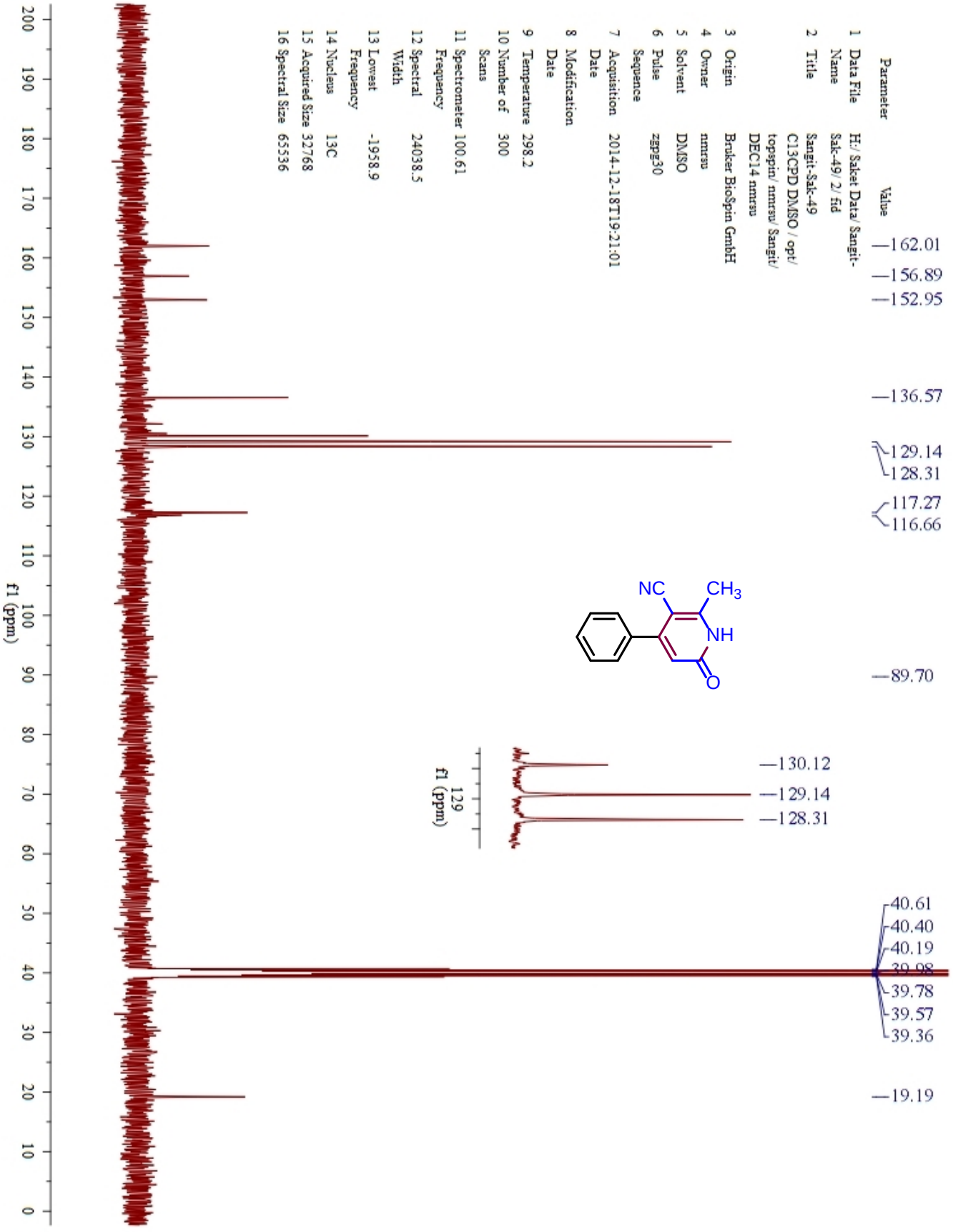


Figure S129 135-DEPT spectra of **42**

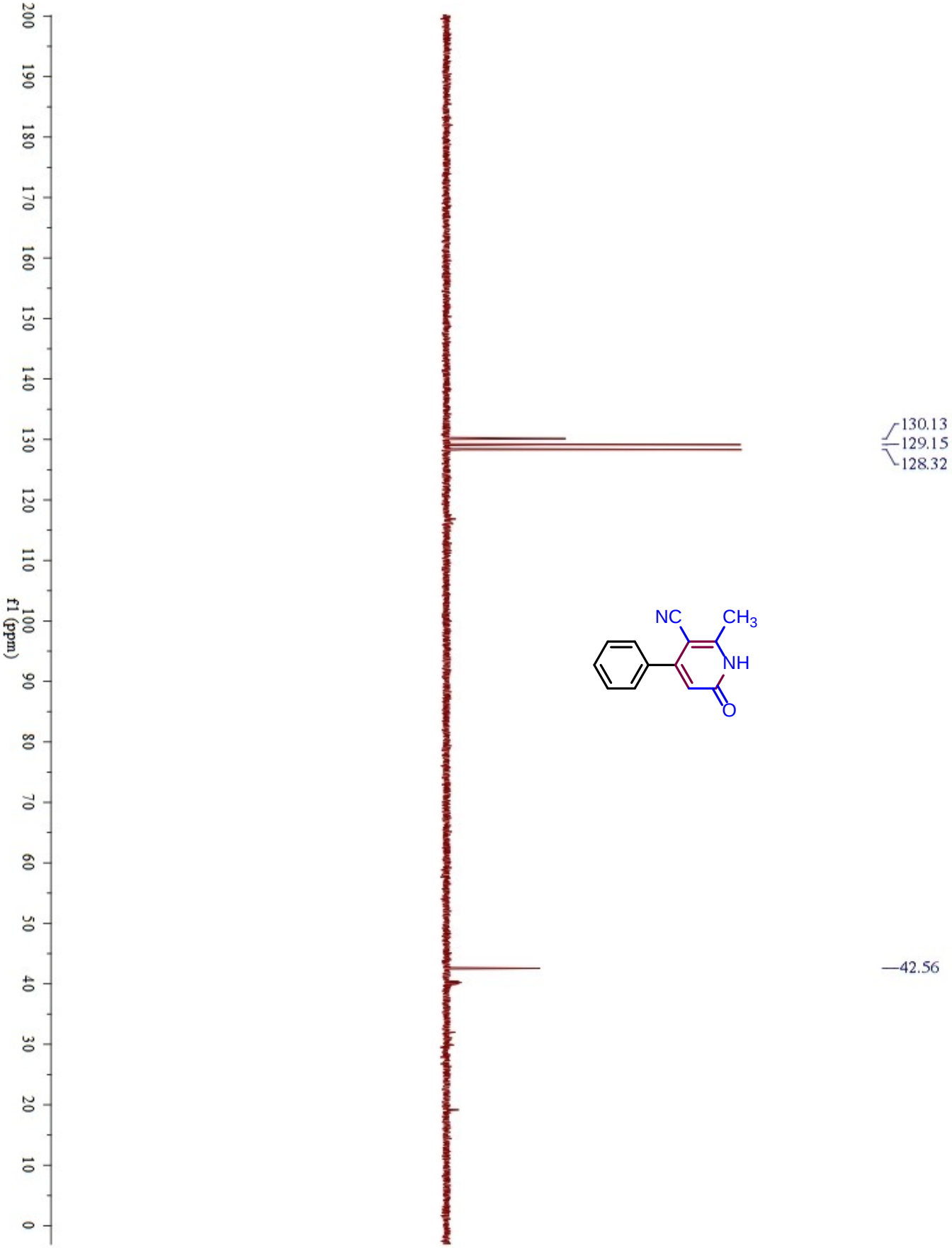


Figure S130 Mass spectra of **42**

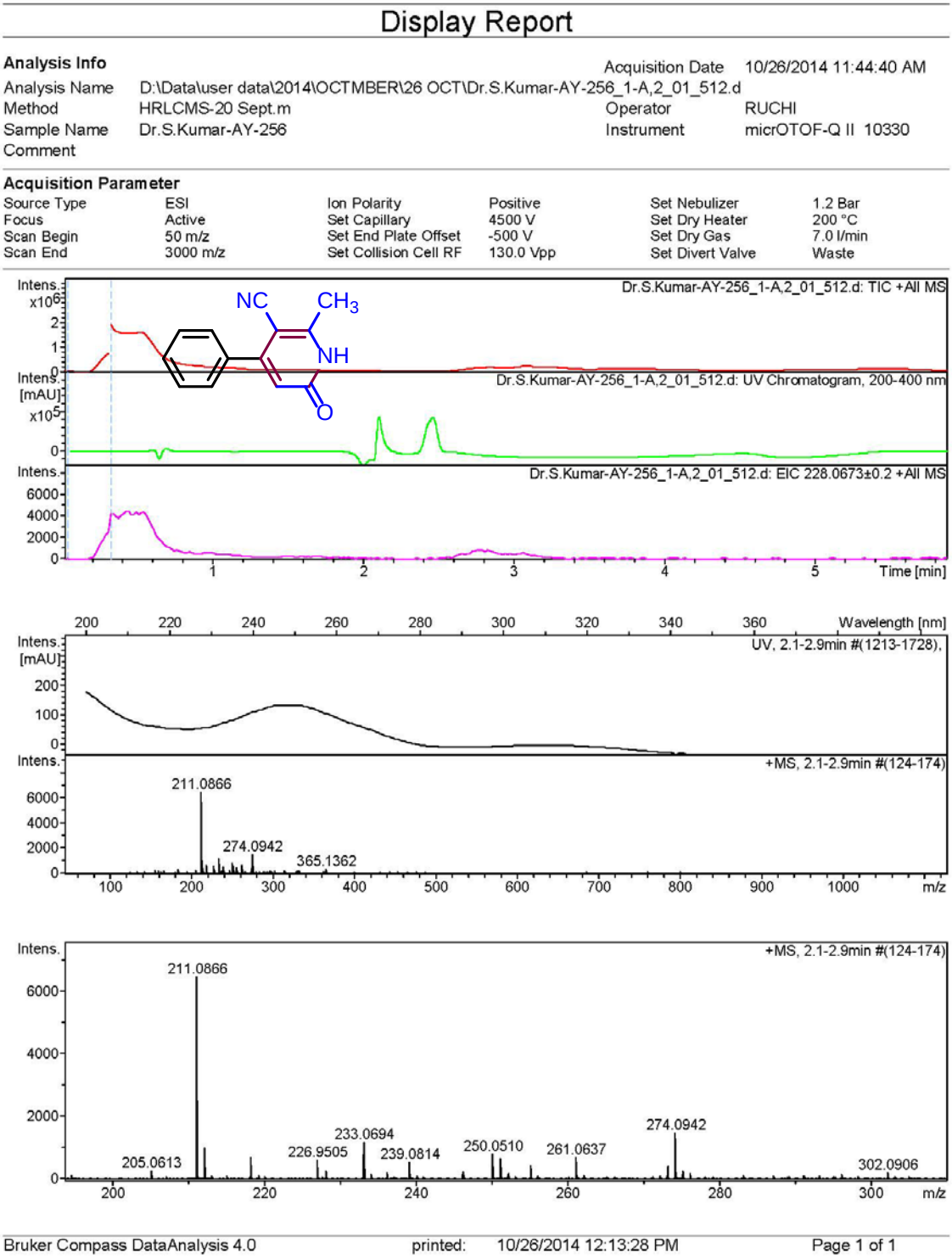


Figure S131 ^{1}H NMR spectra of **43**

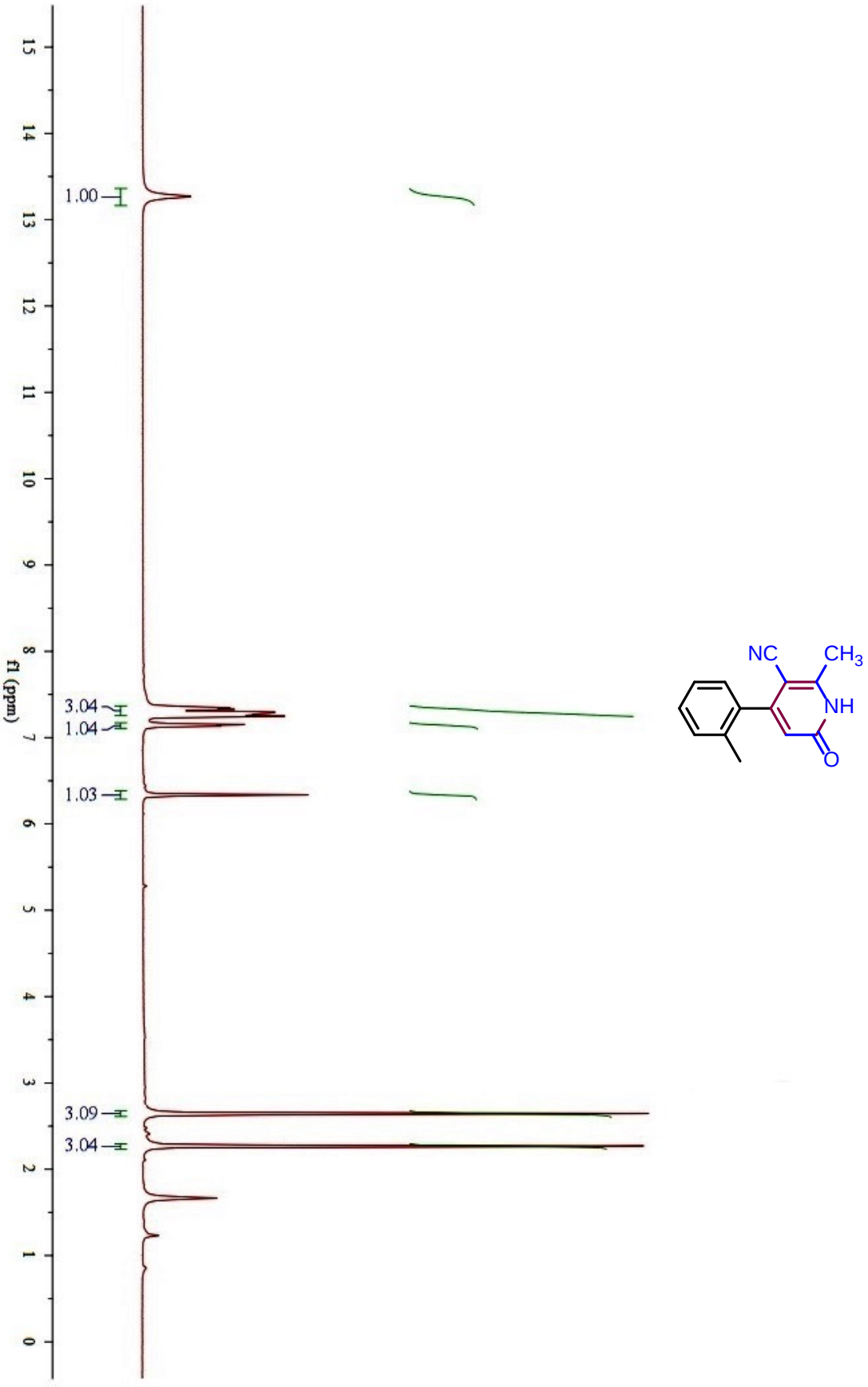


Figure S132 ^{13}C NMR spectra of **43**

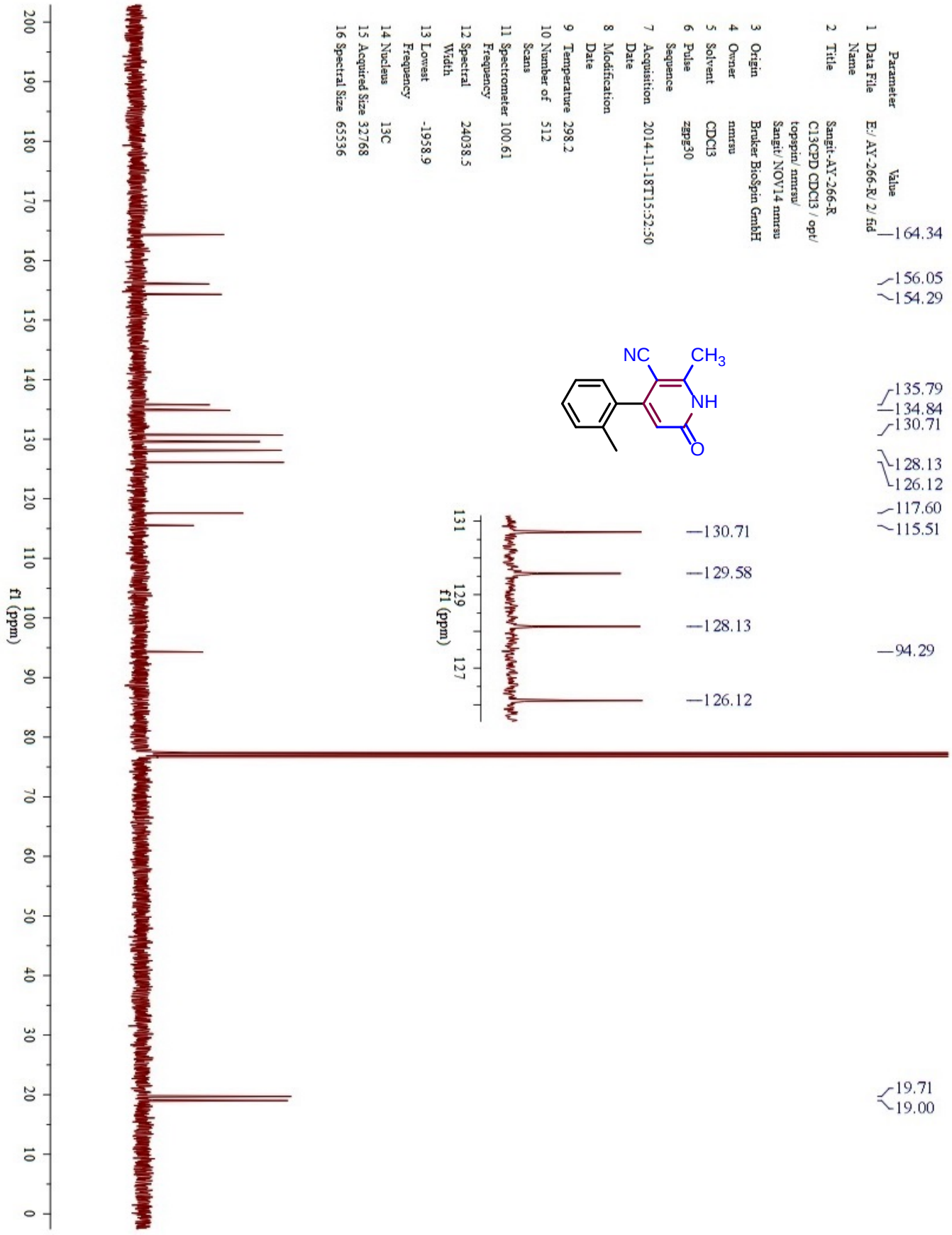


Figure S133 Mass spectra of **43**

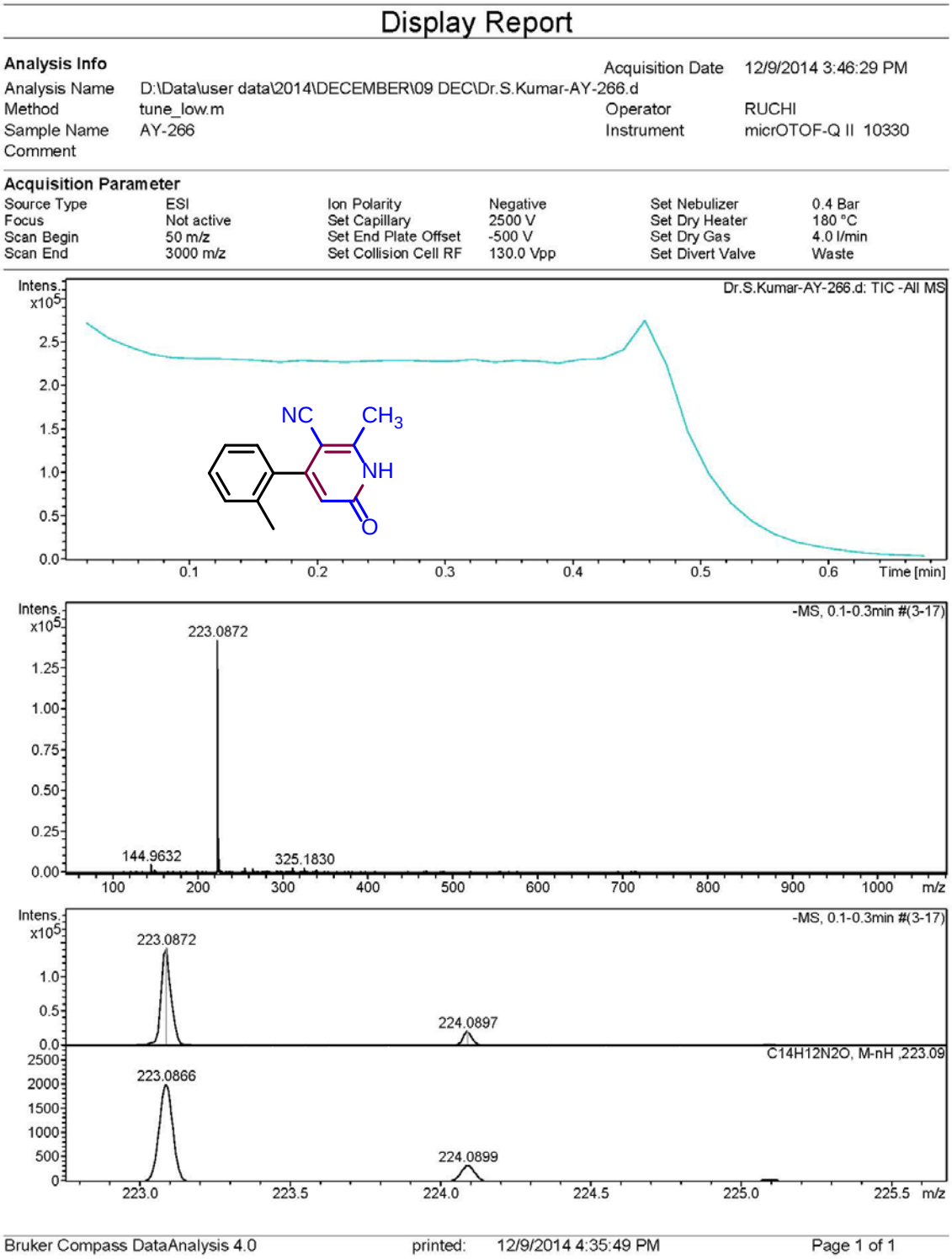


Figure S134 ^{1}H NMR spectra of **44**

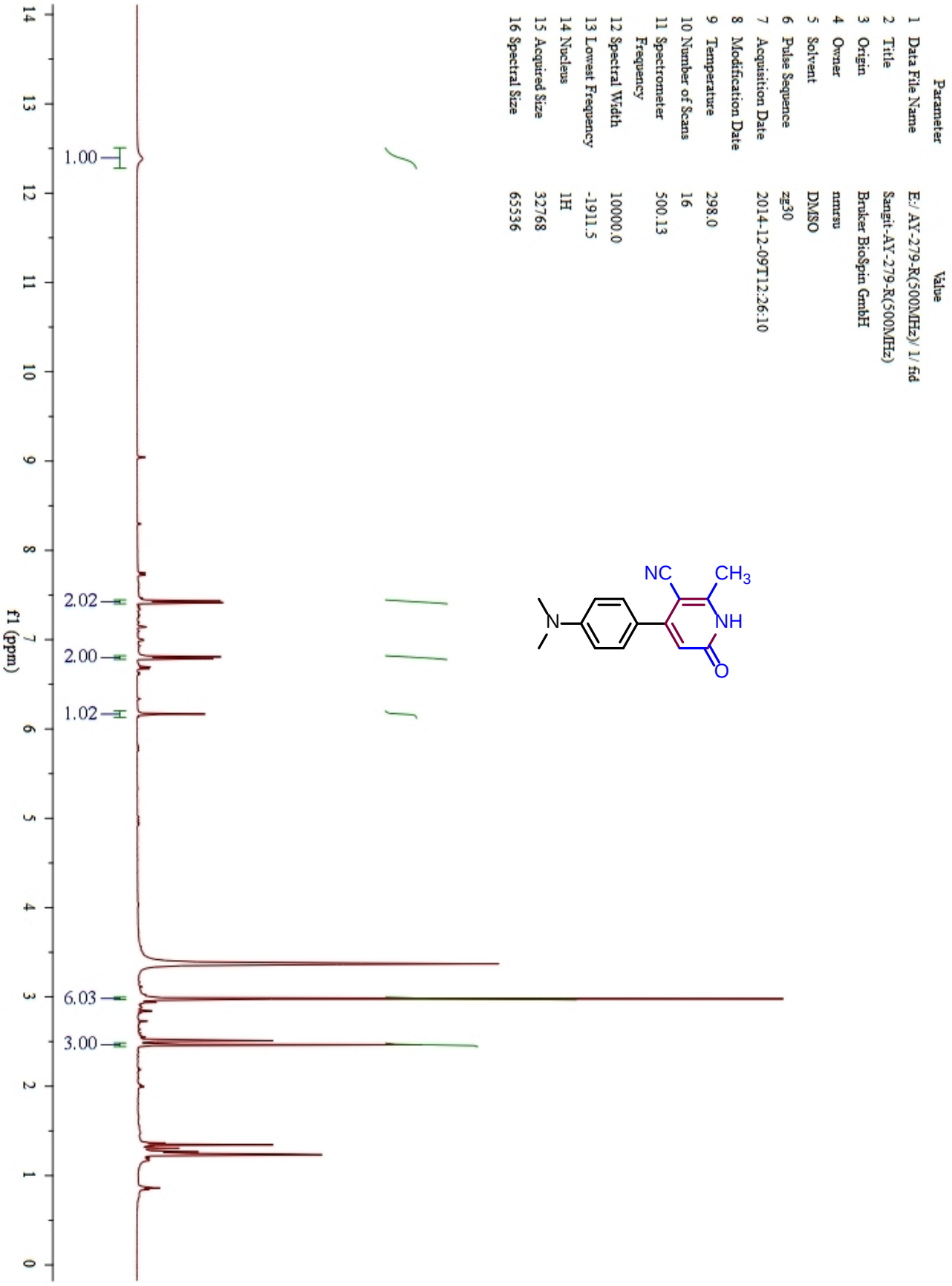


Figure S135 ^{13}C NMR spectra of **44**

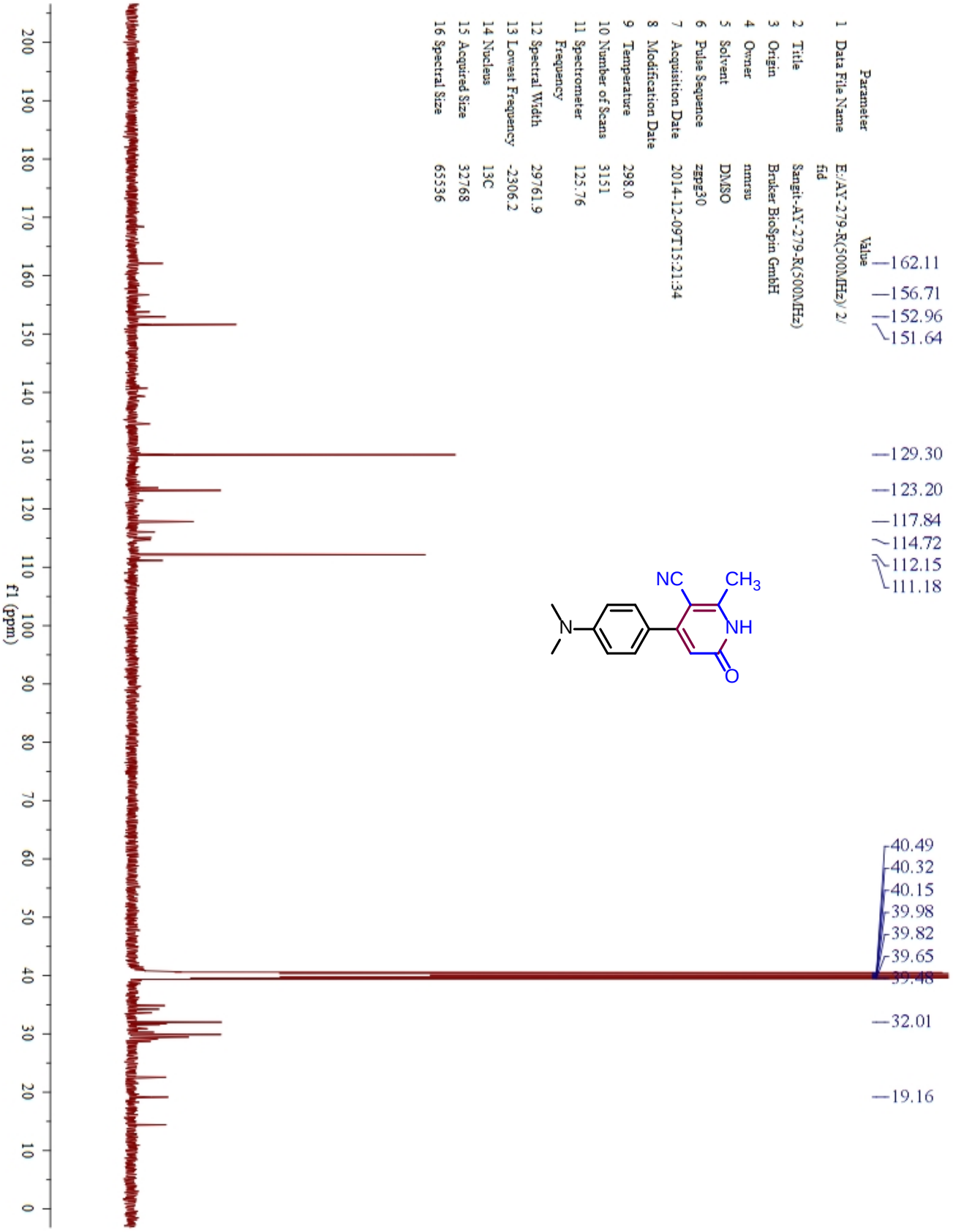


Figure S136 Mass spectra of **44**

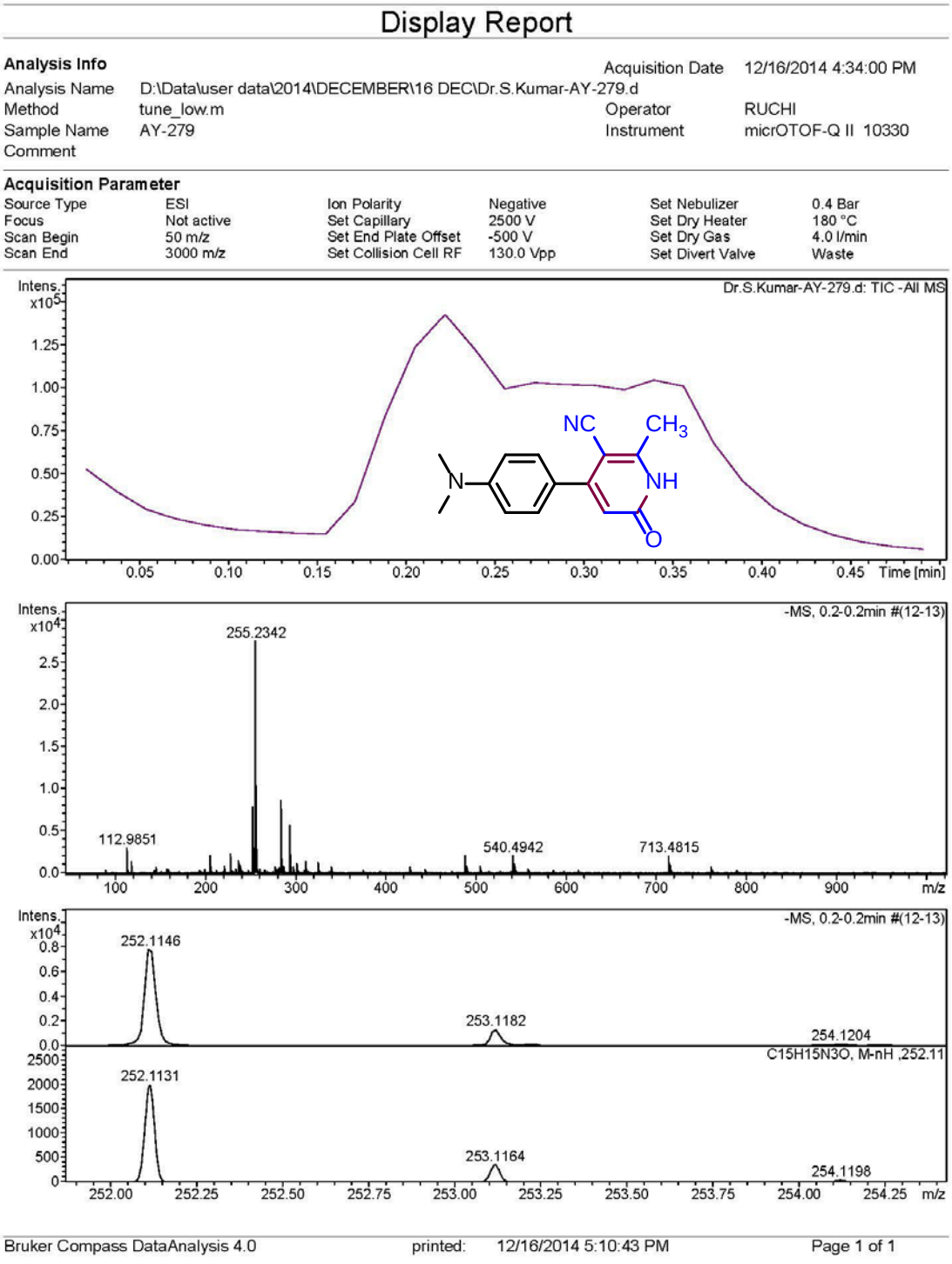


Figure S137 ^{1}H NMR spectra of **45**

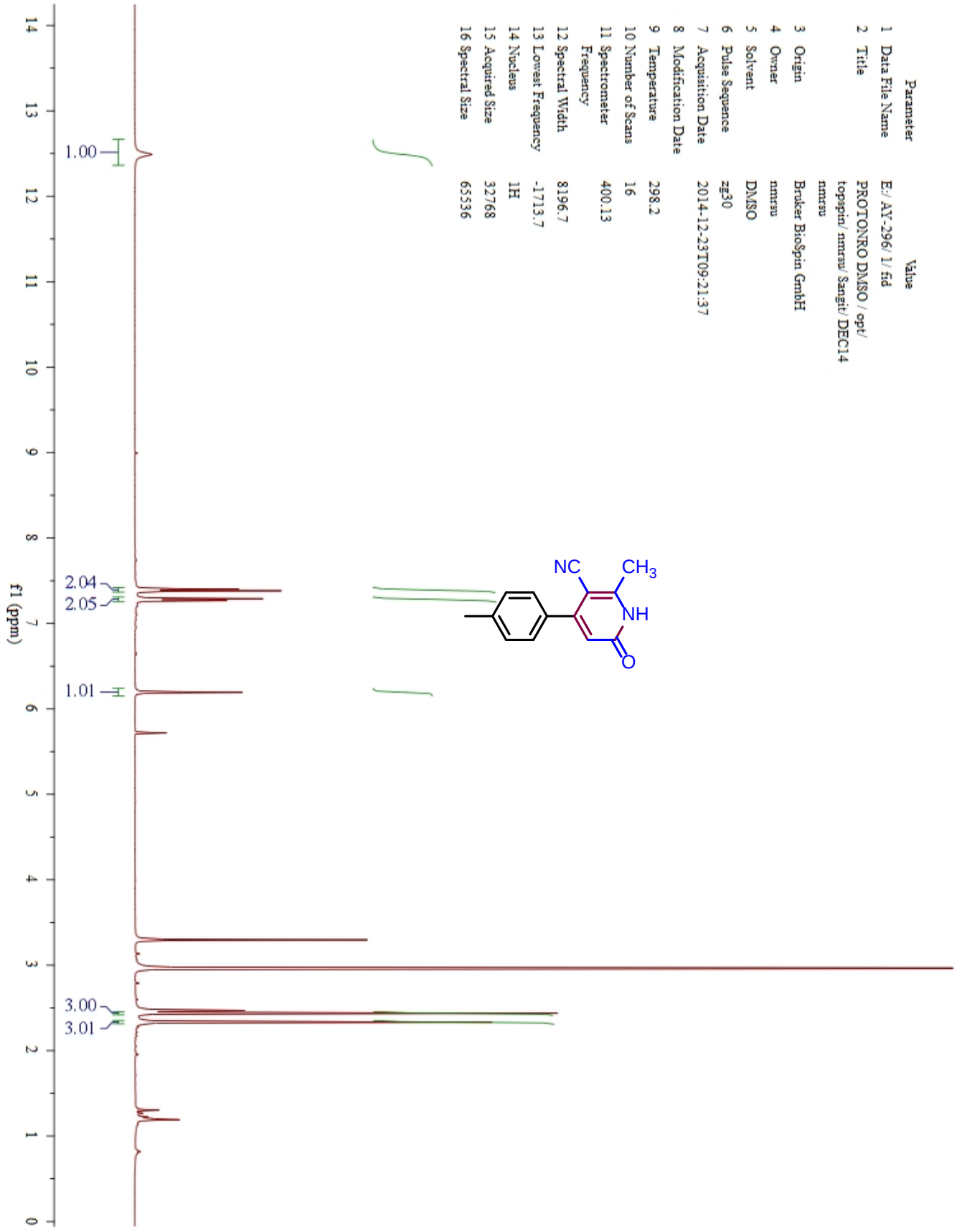


Figure S138 ^{13}C NMR spectra of **45**

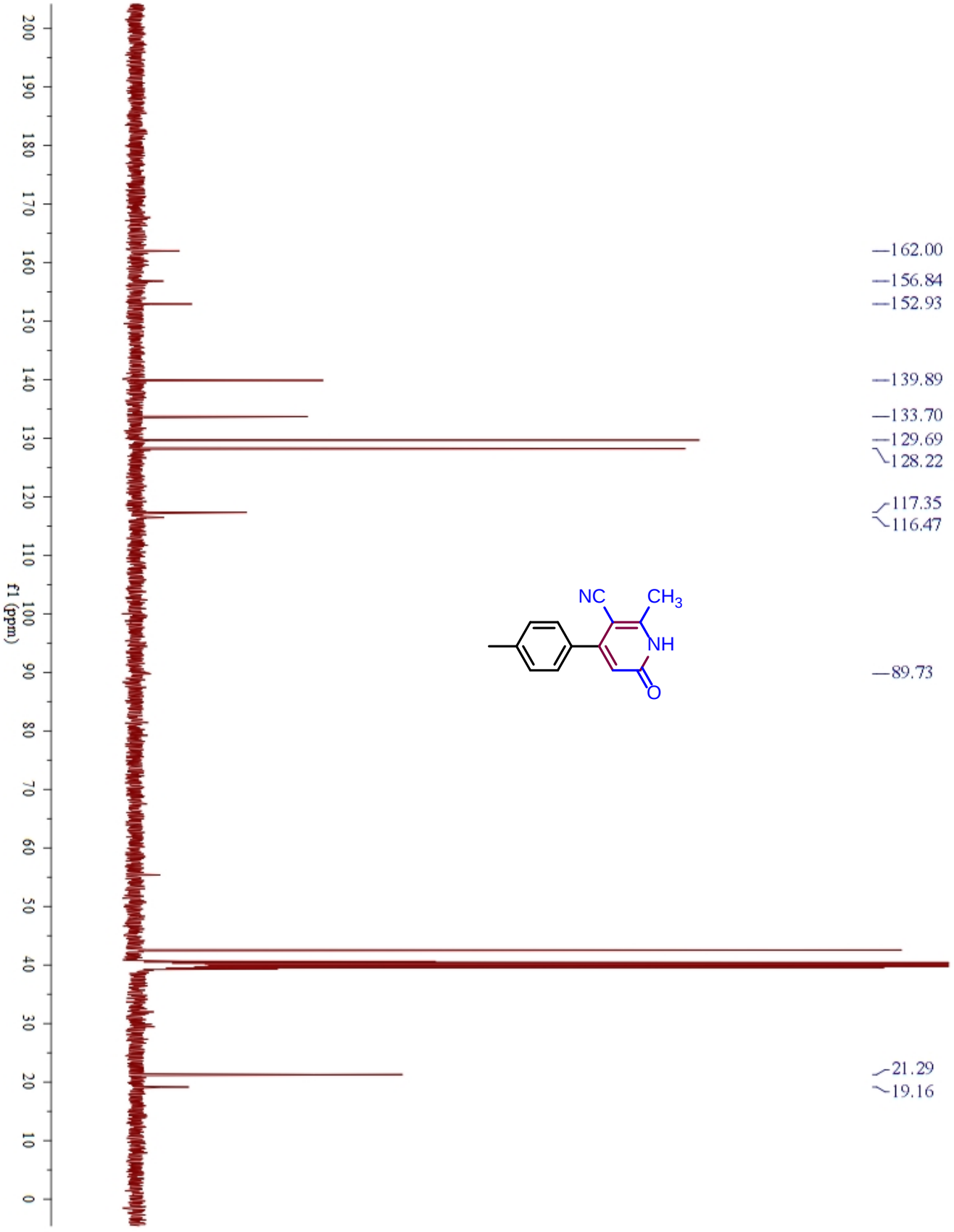


Figure S139 Mass spectra of **45**

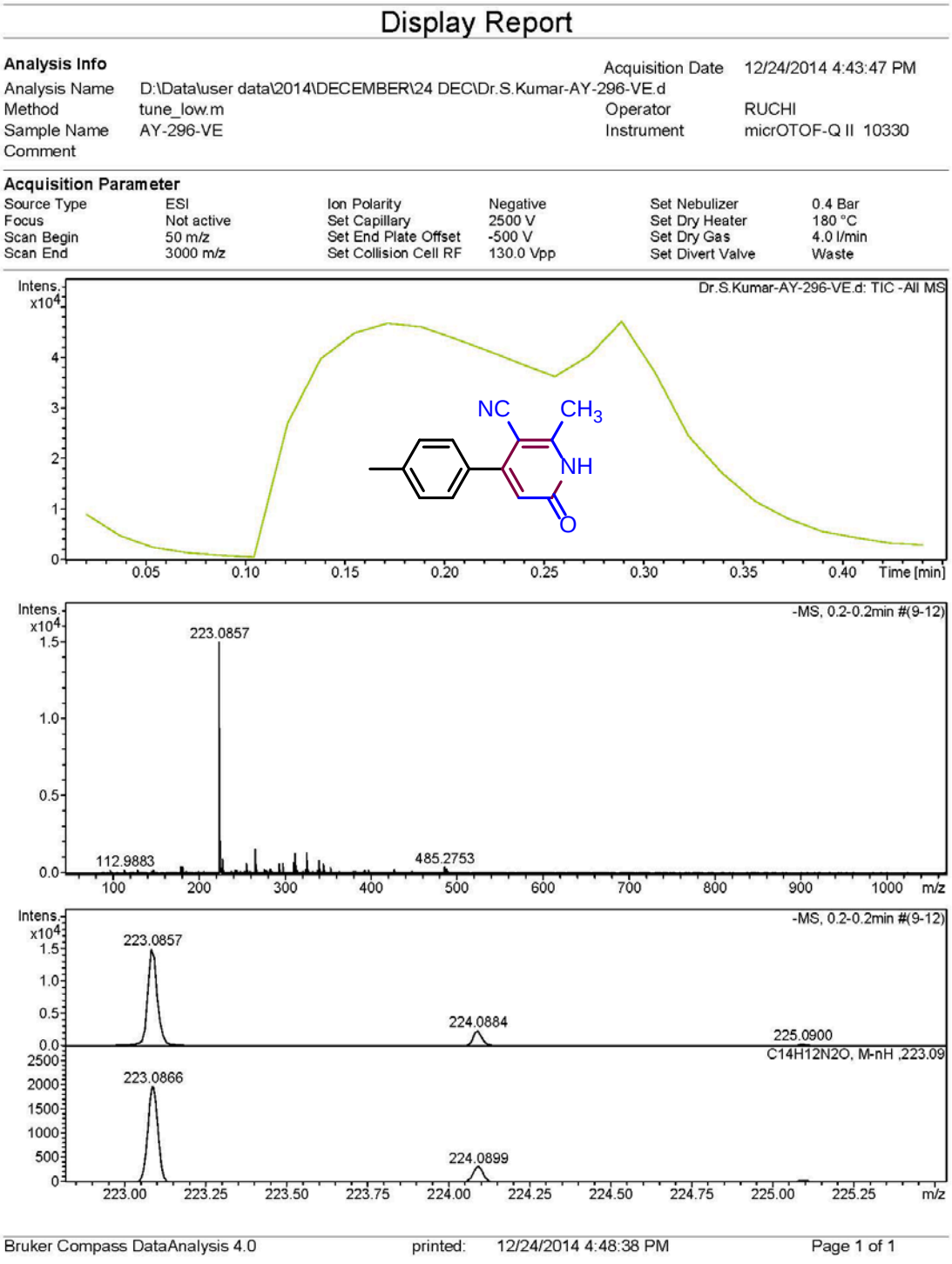


Figure S140 ^{1}H NMR spectra of **46**

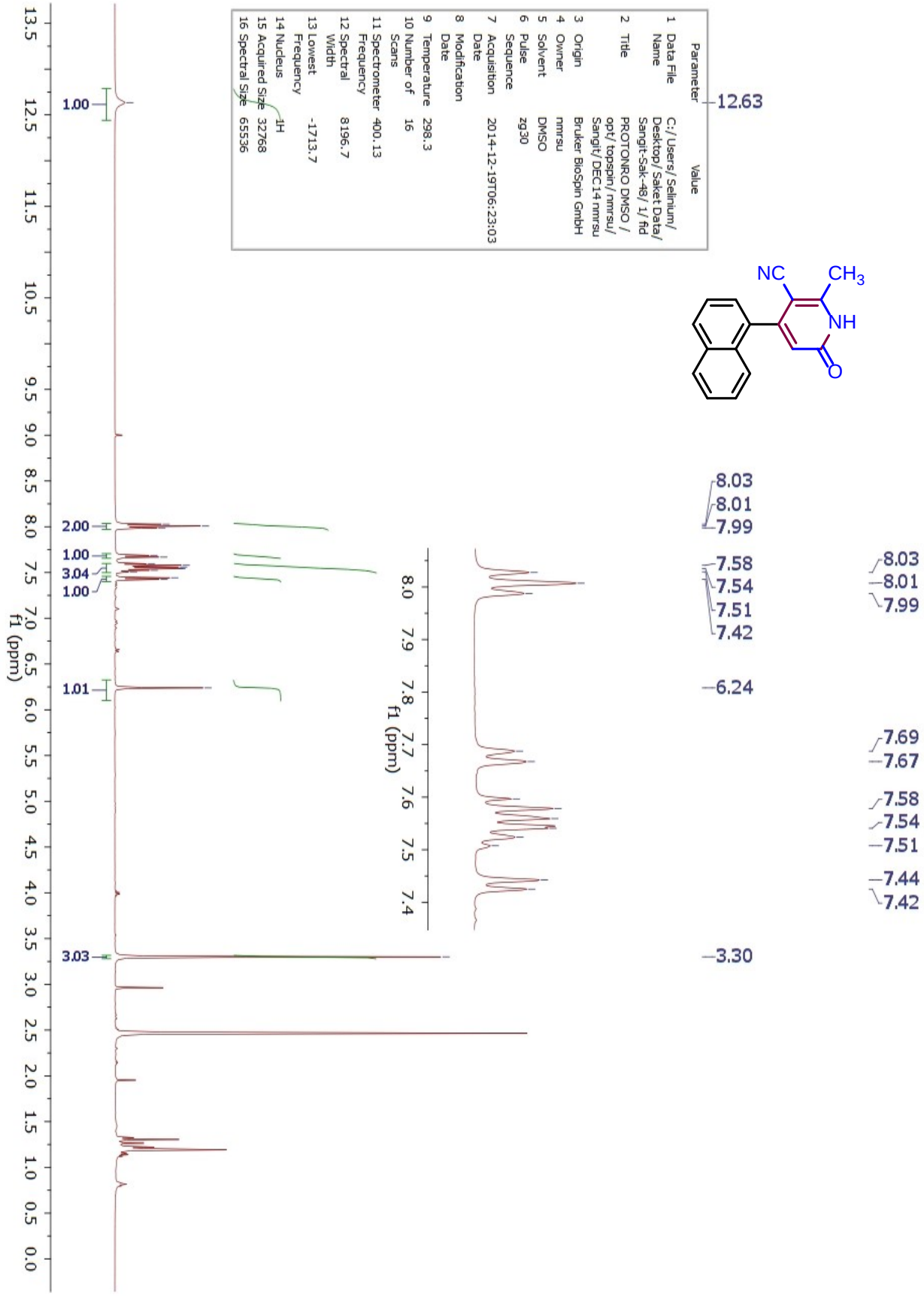


Figure S141 ^{13}C NMR spectra of **46**

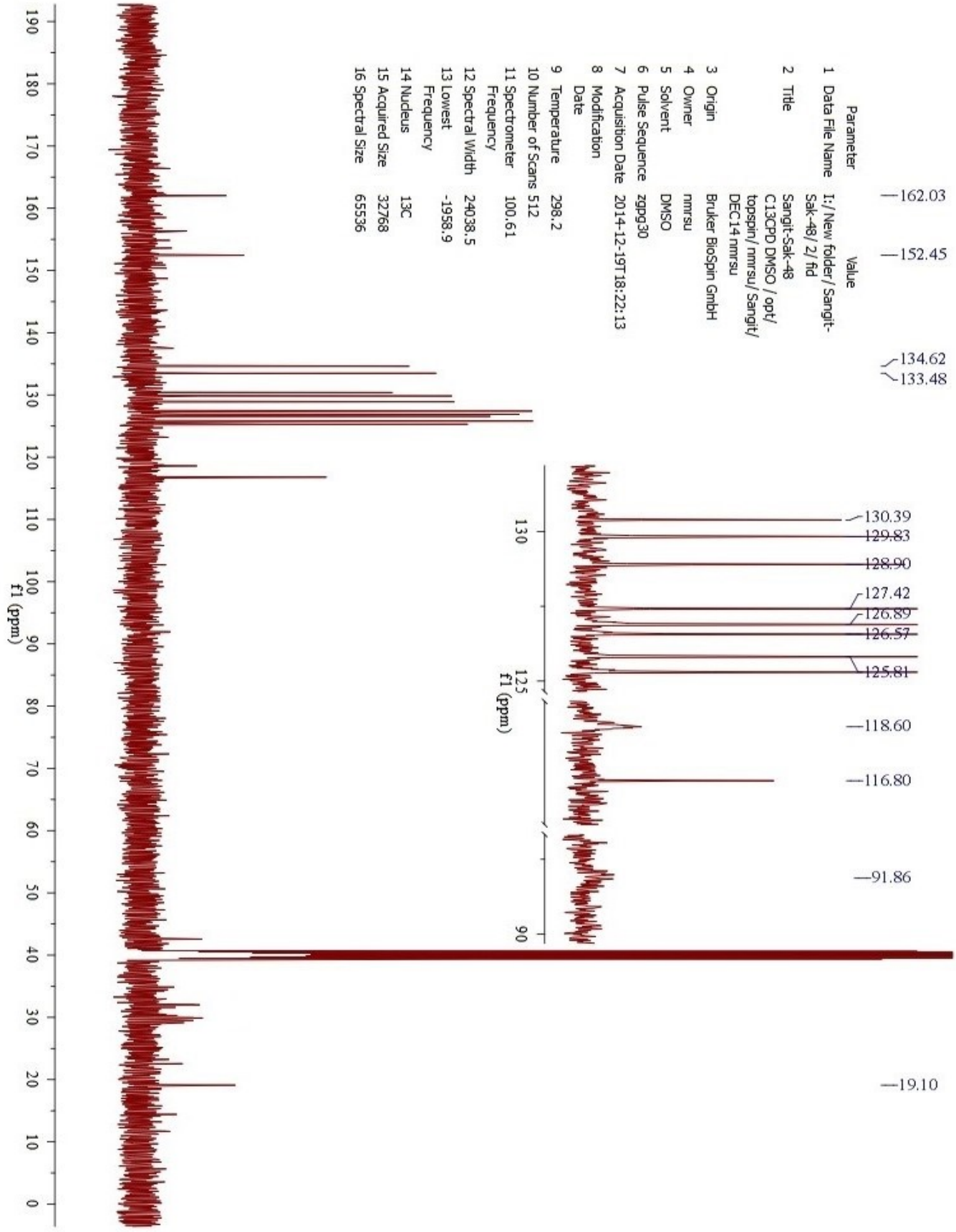


Figure S142 Mass spectra of **46**

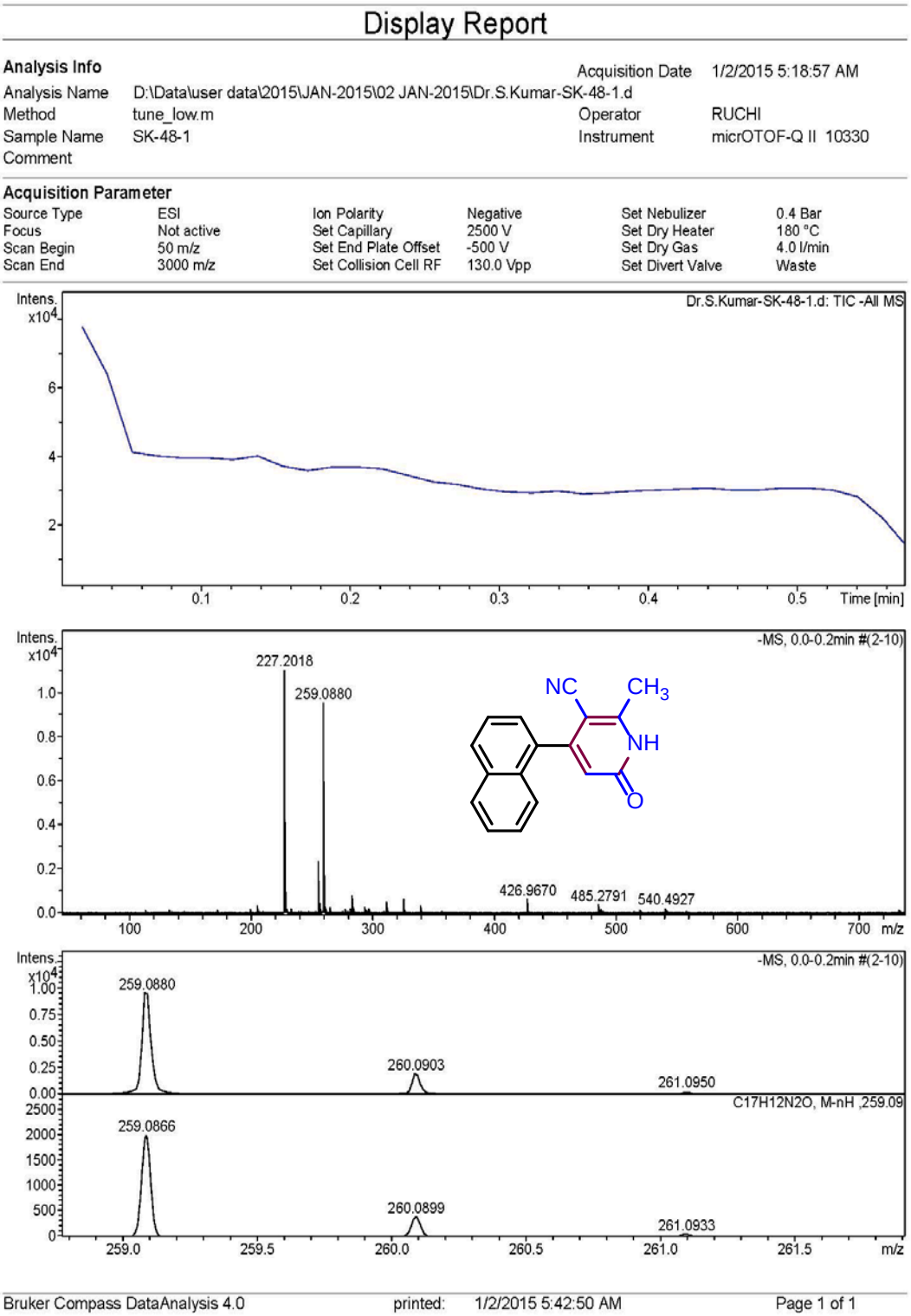


Figure S143 ^{1}H NMR spectra of **47**

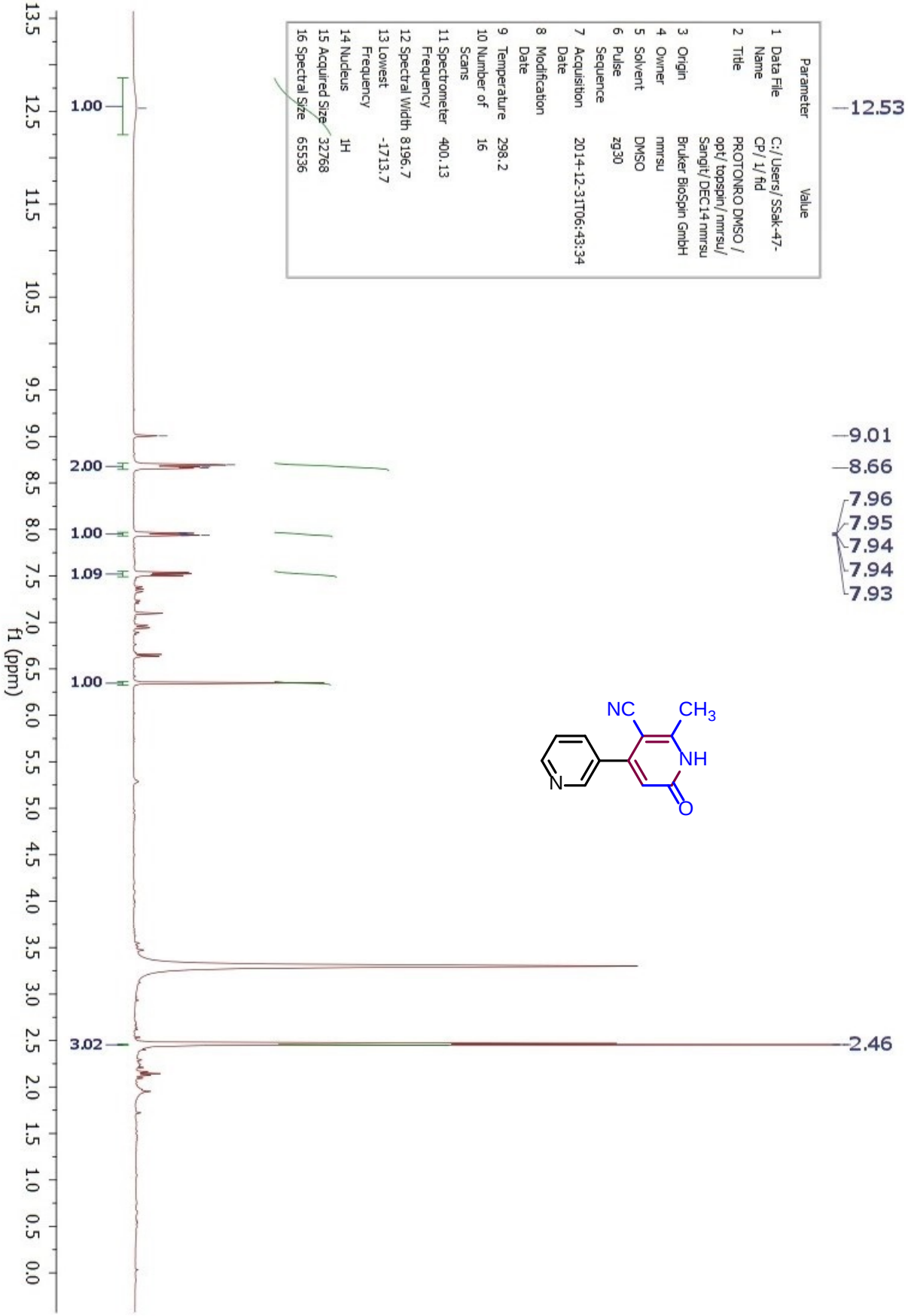


Figure S144 ^{13}C NMR spectra of **47**

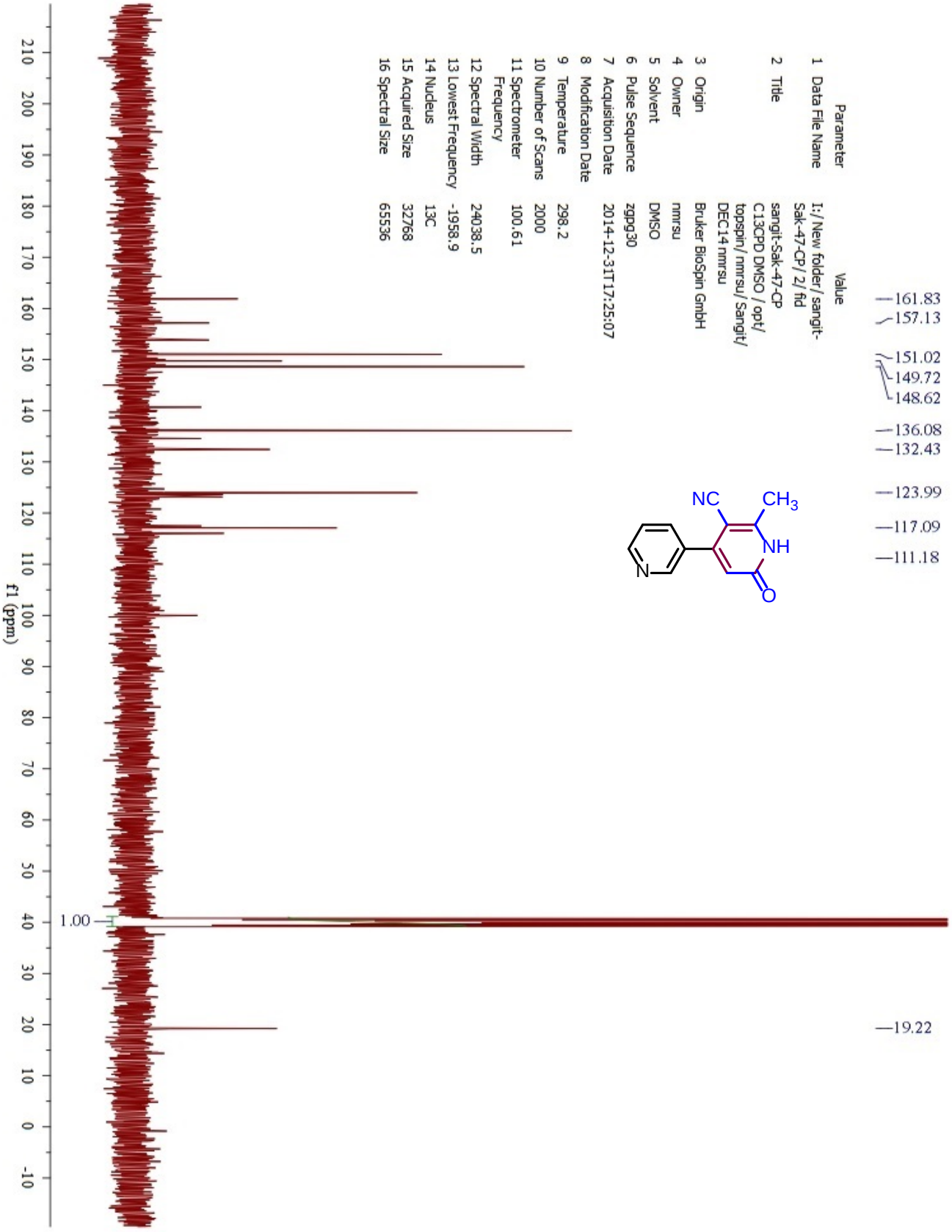


Figure S145 Mass spectra of **47**

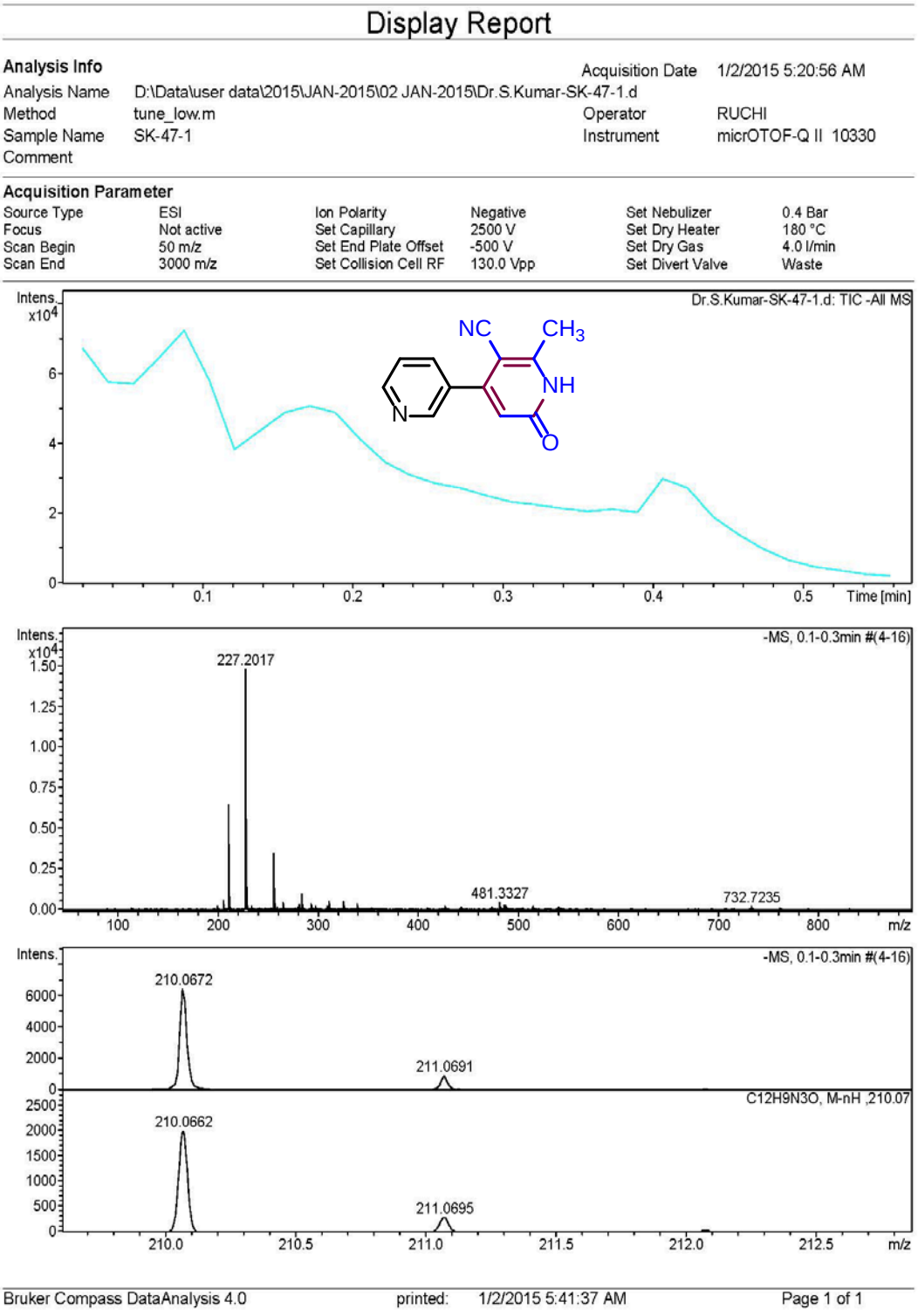


Figure S146 ^{1}H NMR spectra of **48**

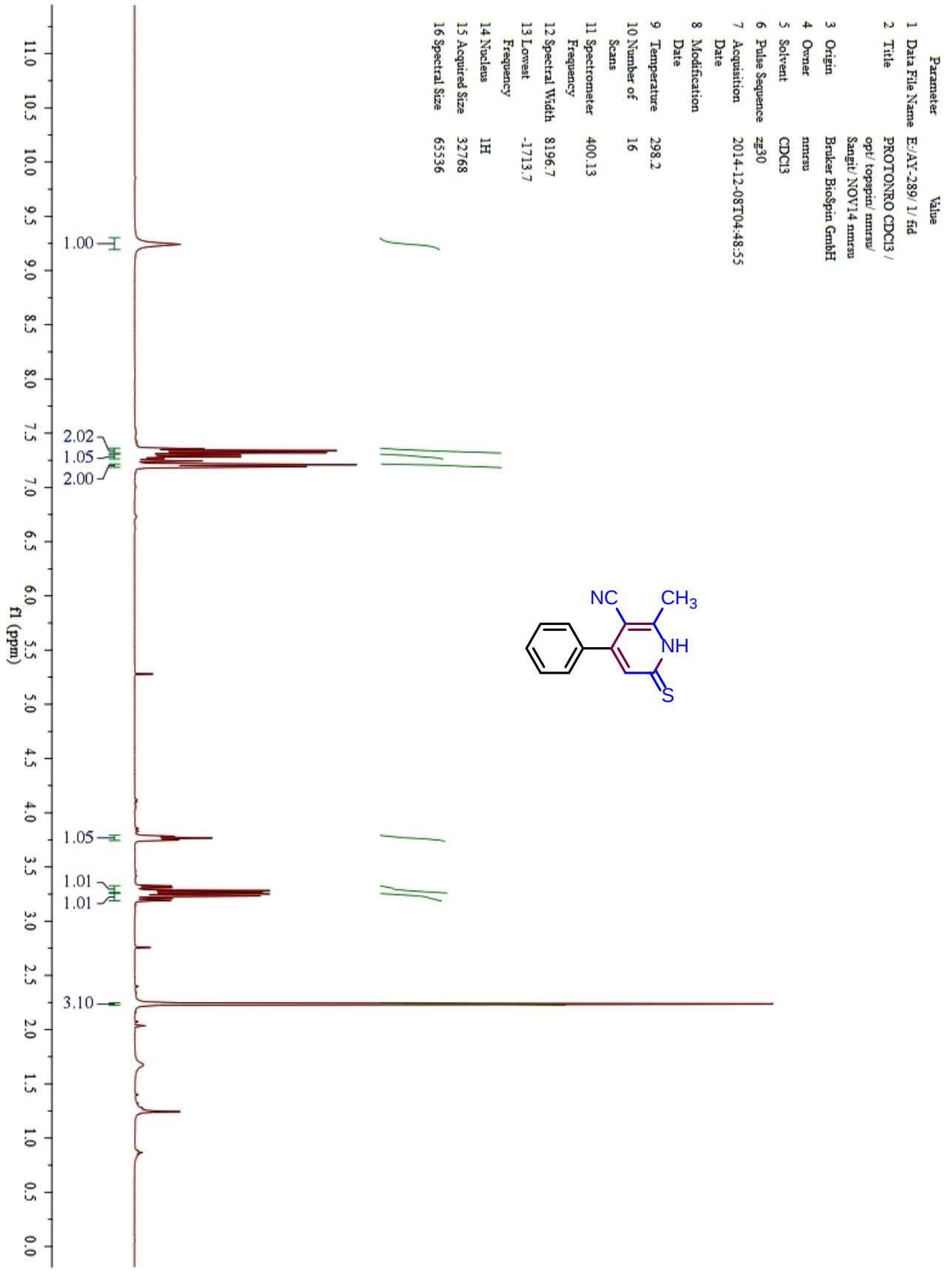


Figure S147 ^{13}C NMR spectra of **48**

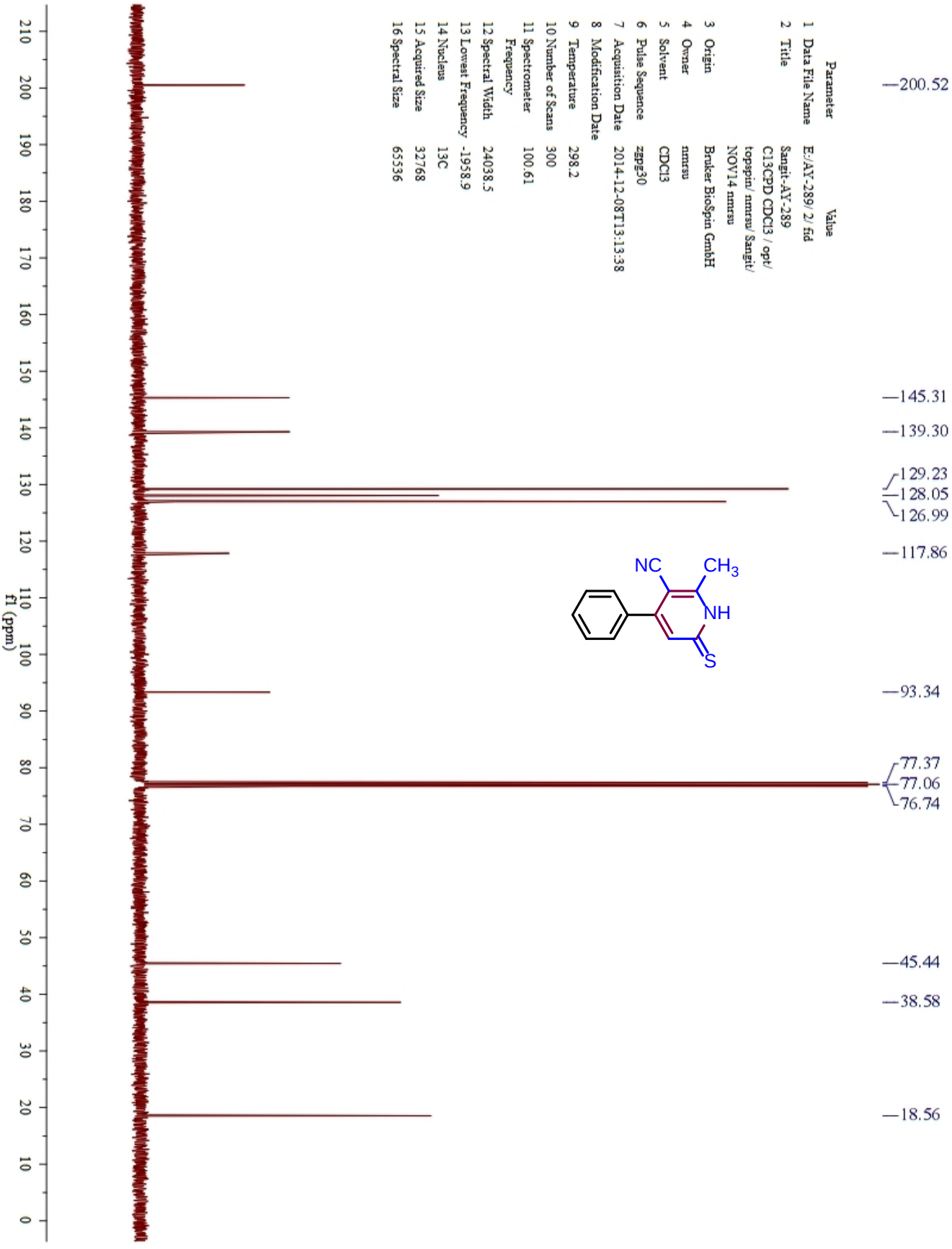


Figure S148 135-DEPT spectra of **48**

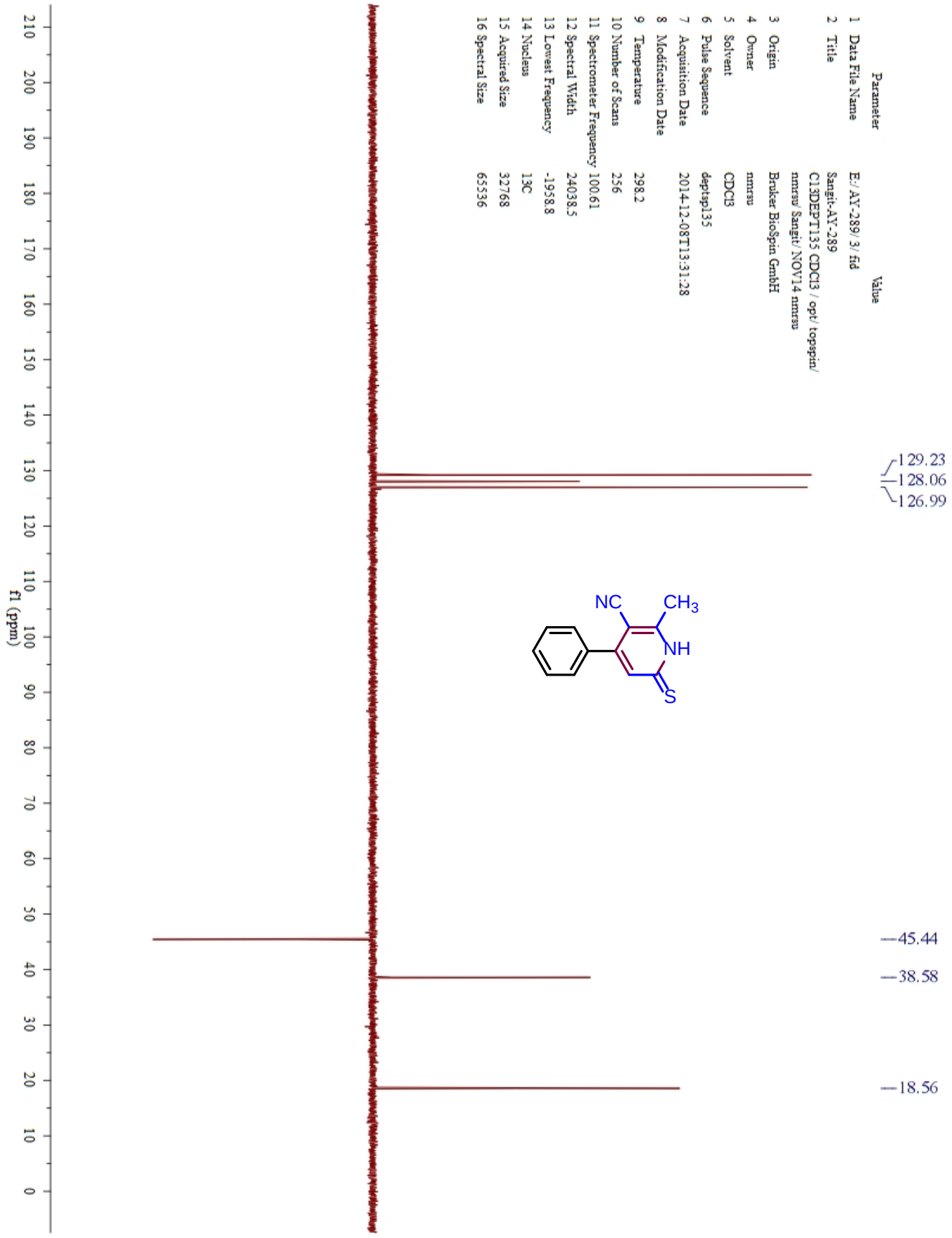


Figure S149 Mass spectra of **48**

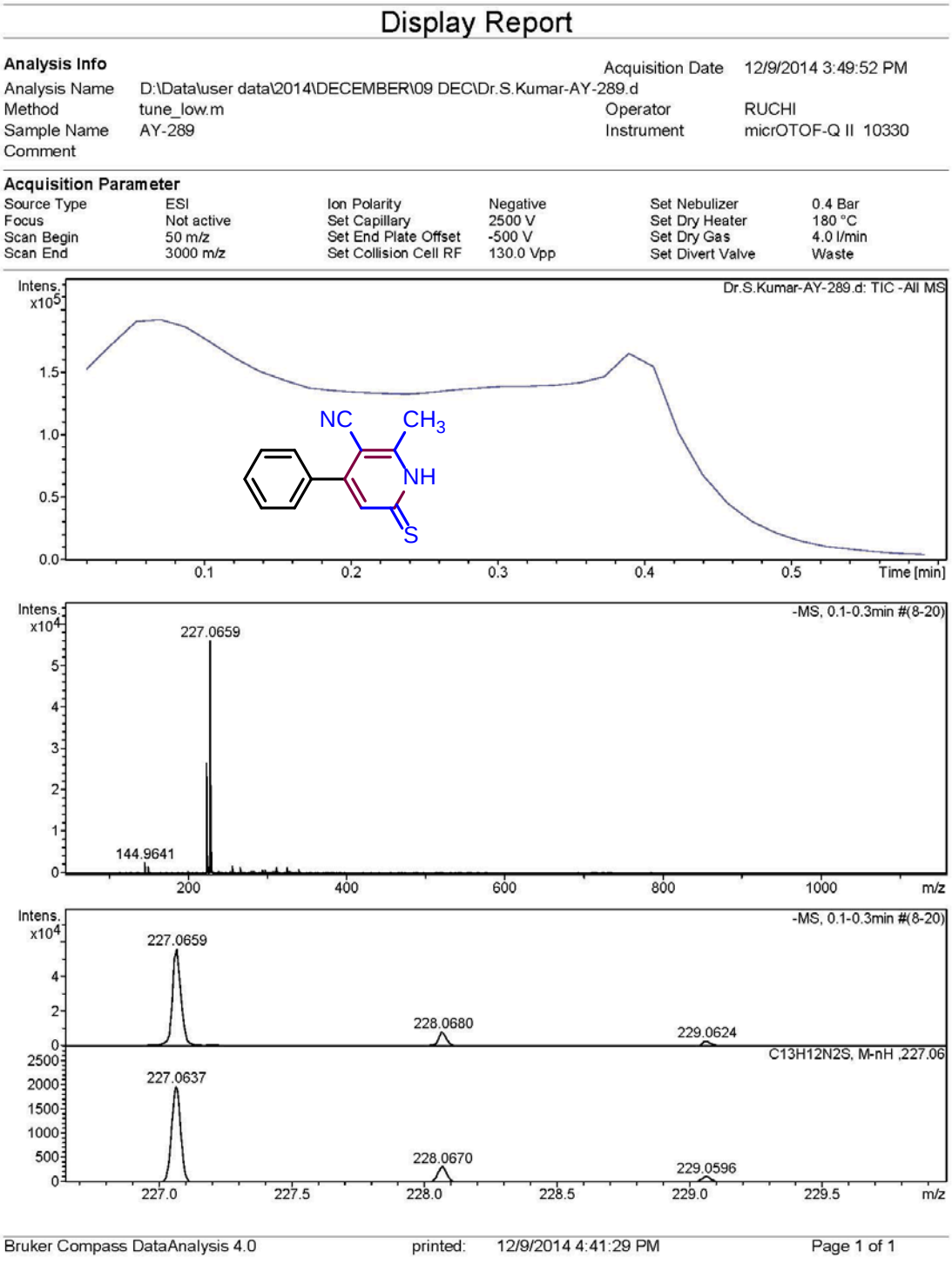


Figure S150 ^{1}H NMR spectra of **49**

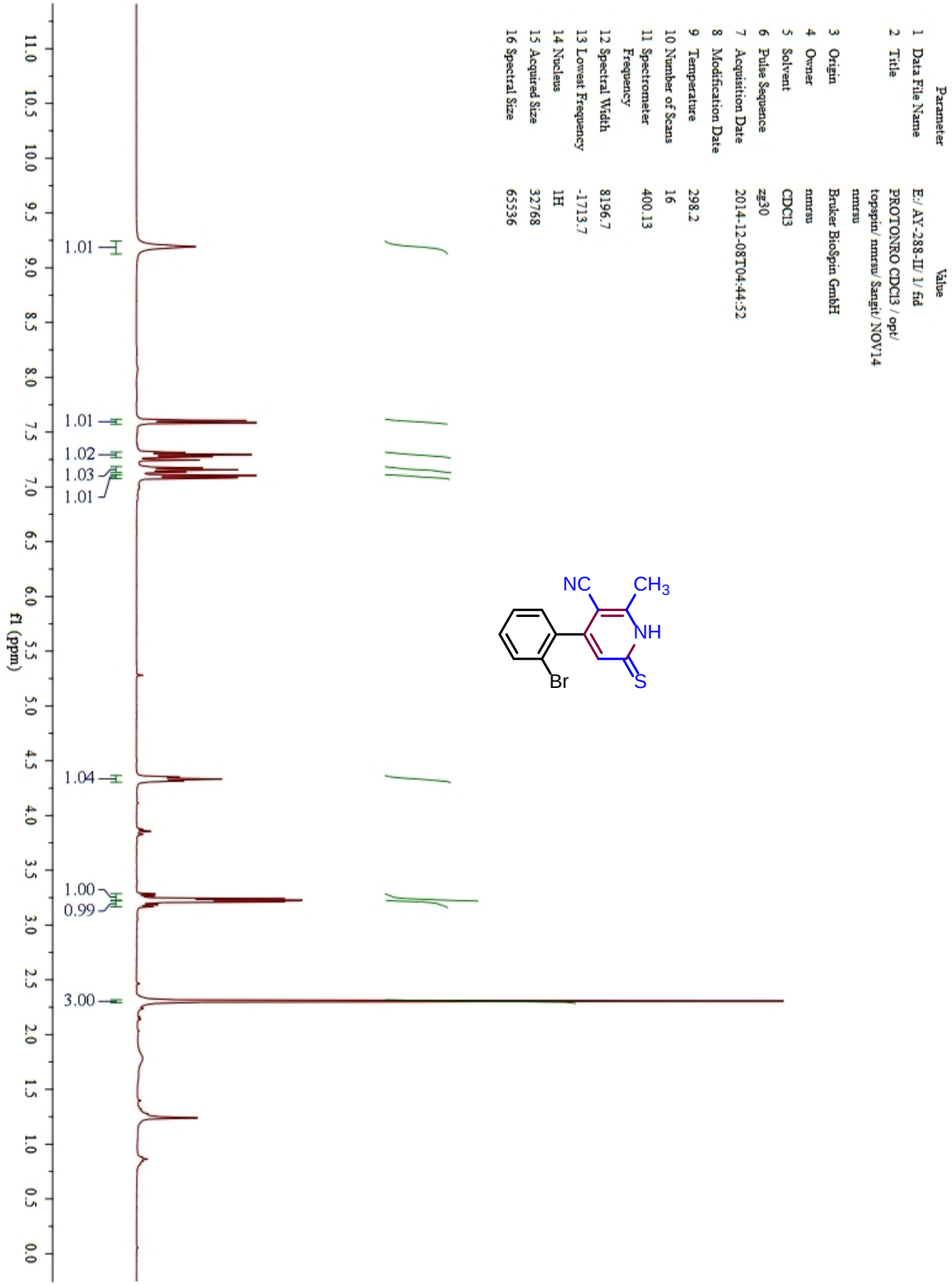


Figure S151 ^{13}C NMR spectra of **49**

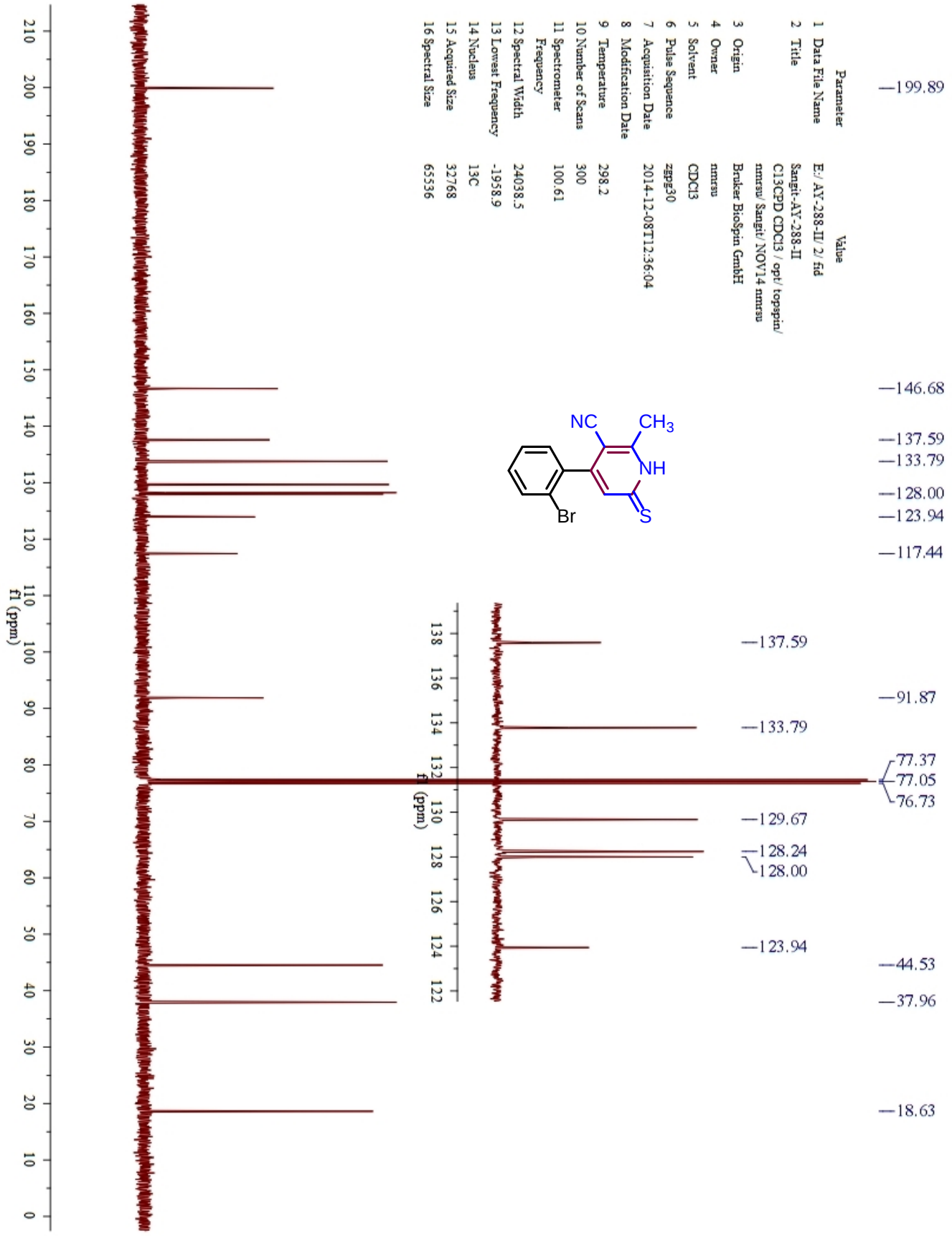


Figure S152 135-DEPT spectra of **49**

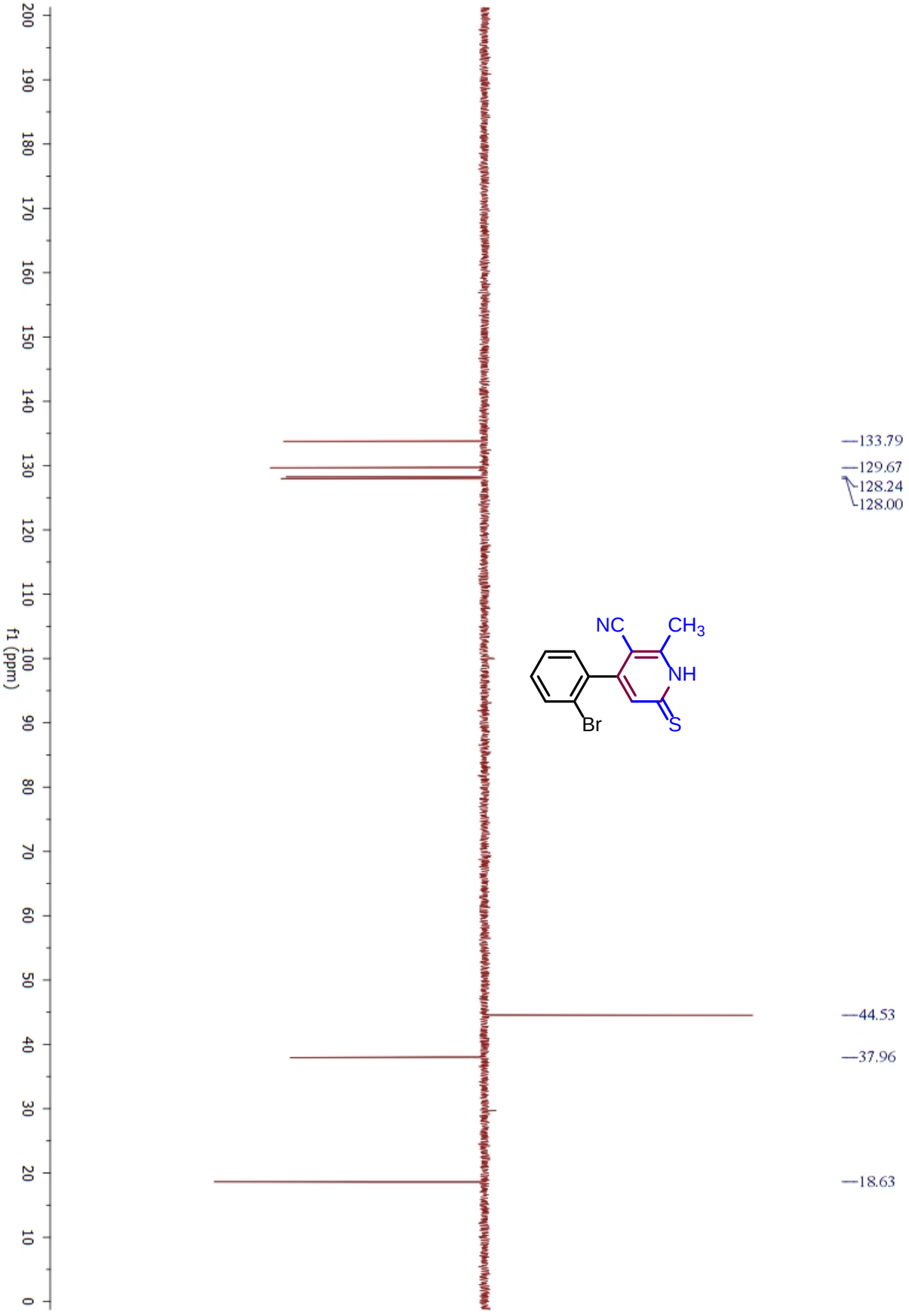


Figure S153 Mass spectra of **49**

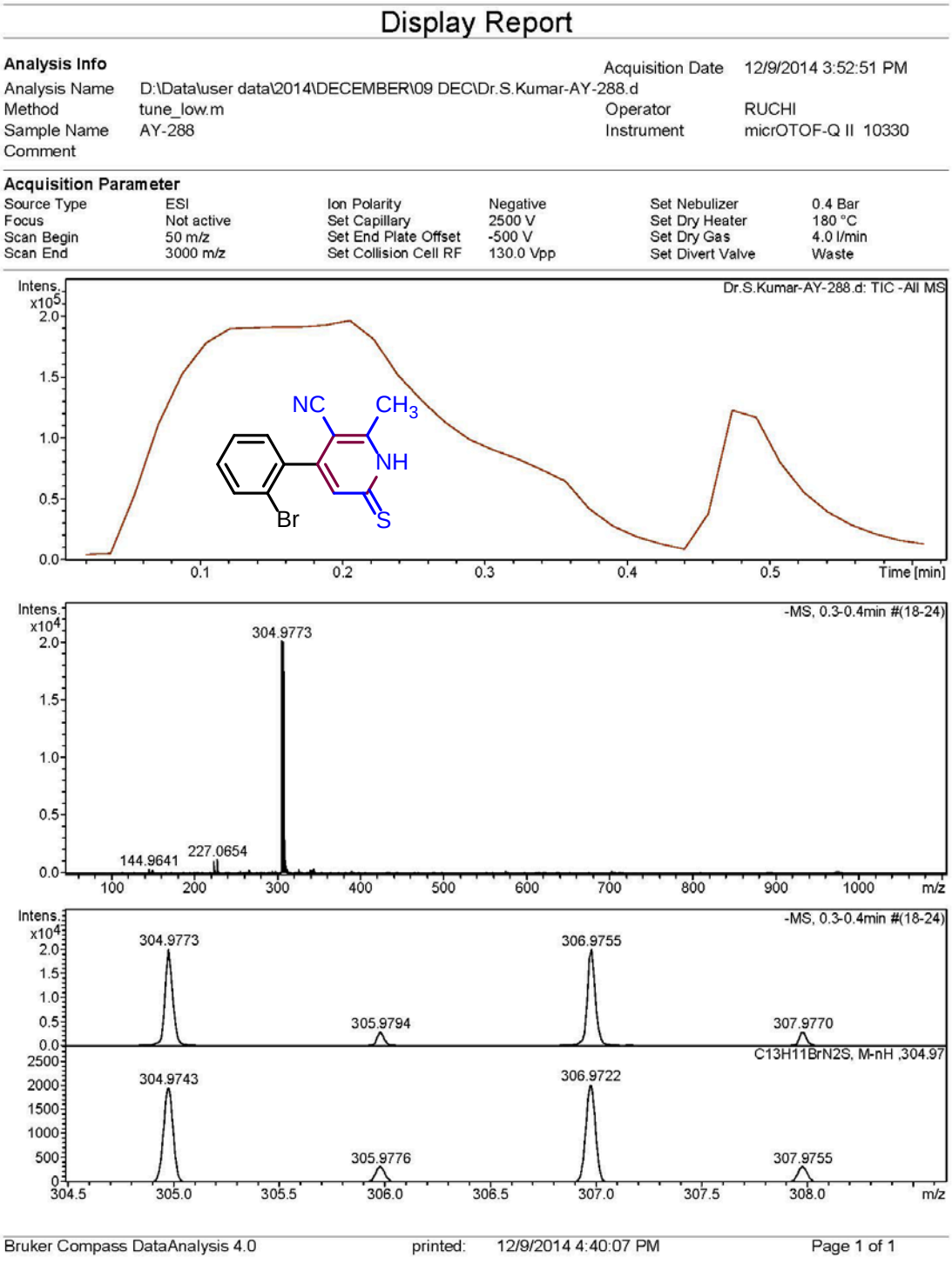


Figure S154 ^{1}H NMR spectra of **50**

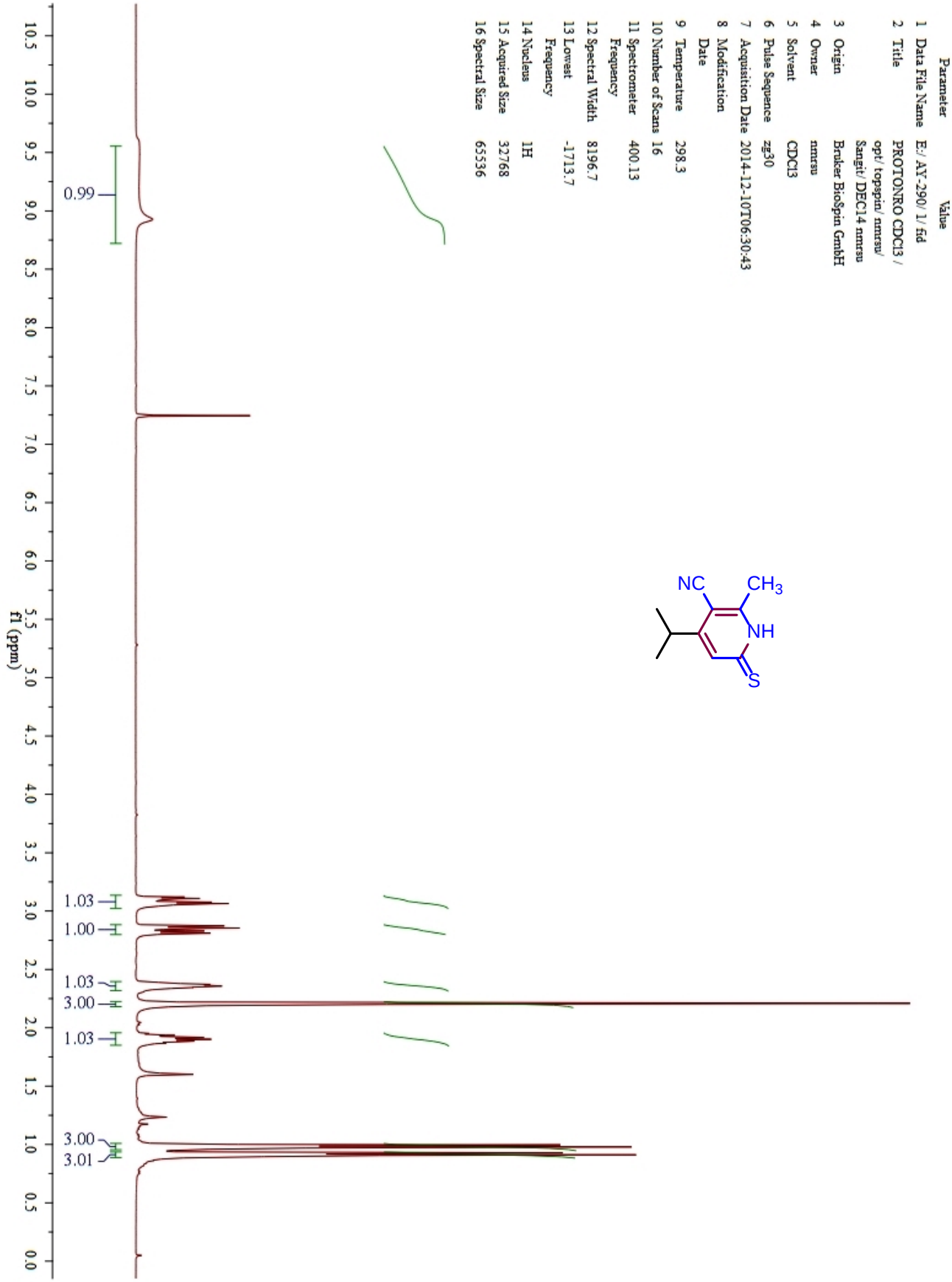


Figure S155 ^{13}C NMR spectra of **50**

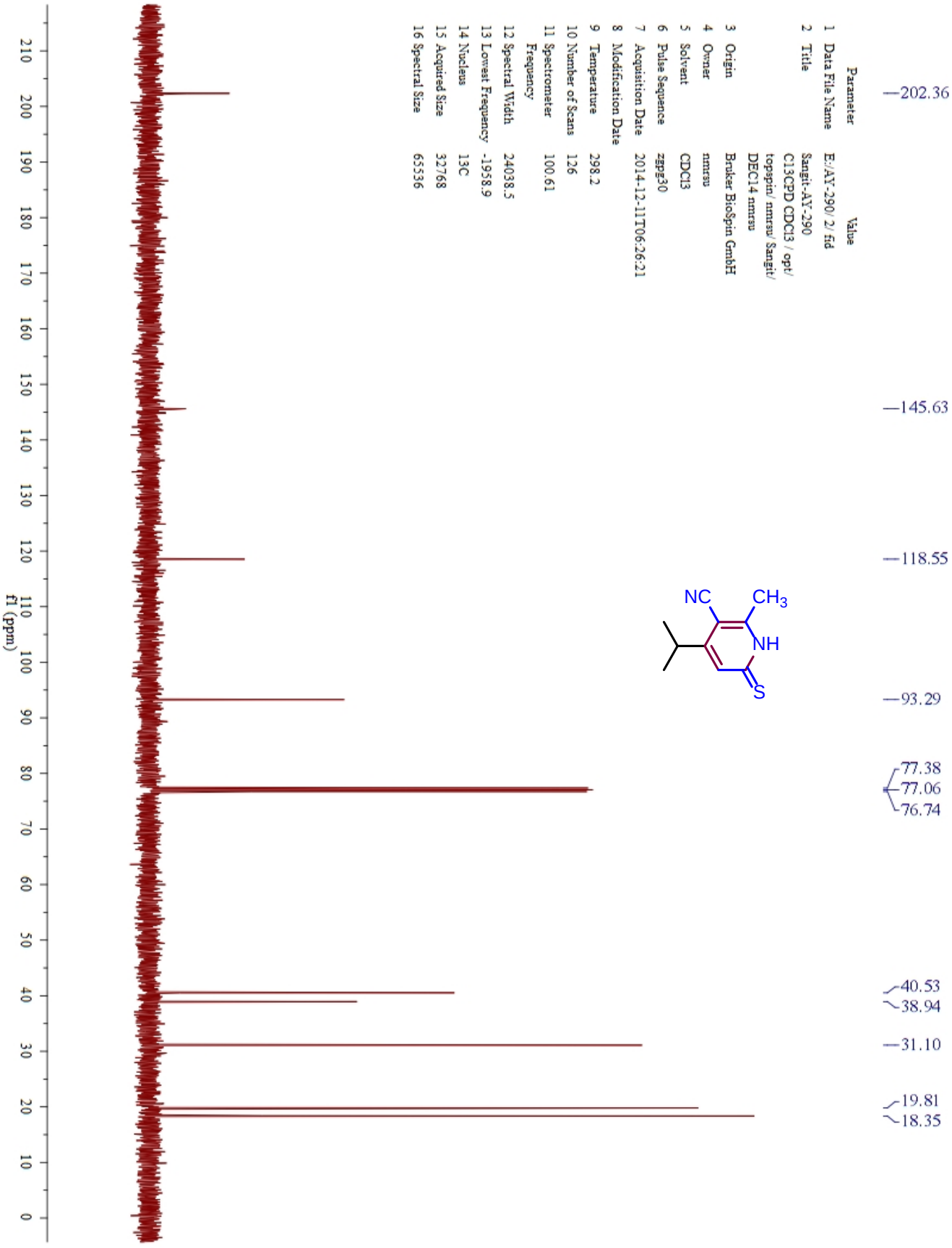
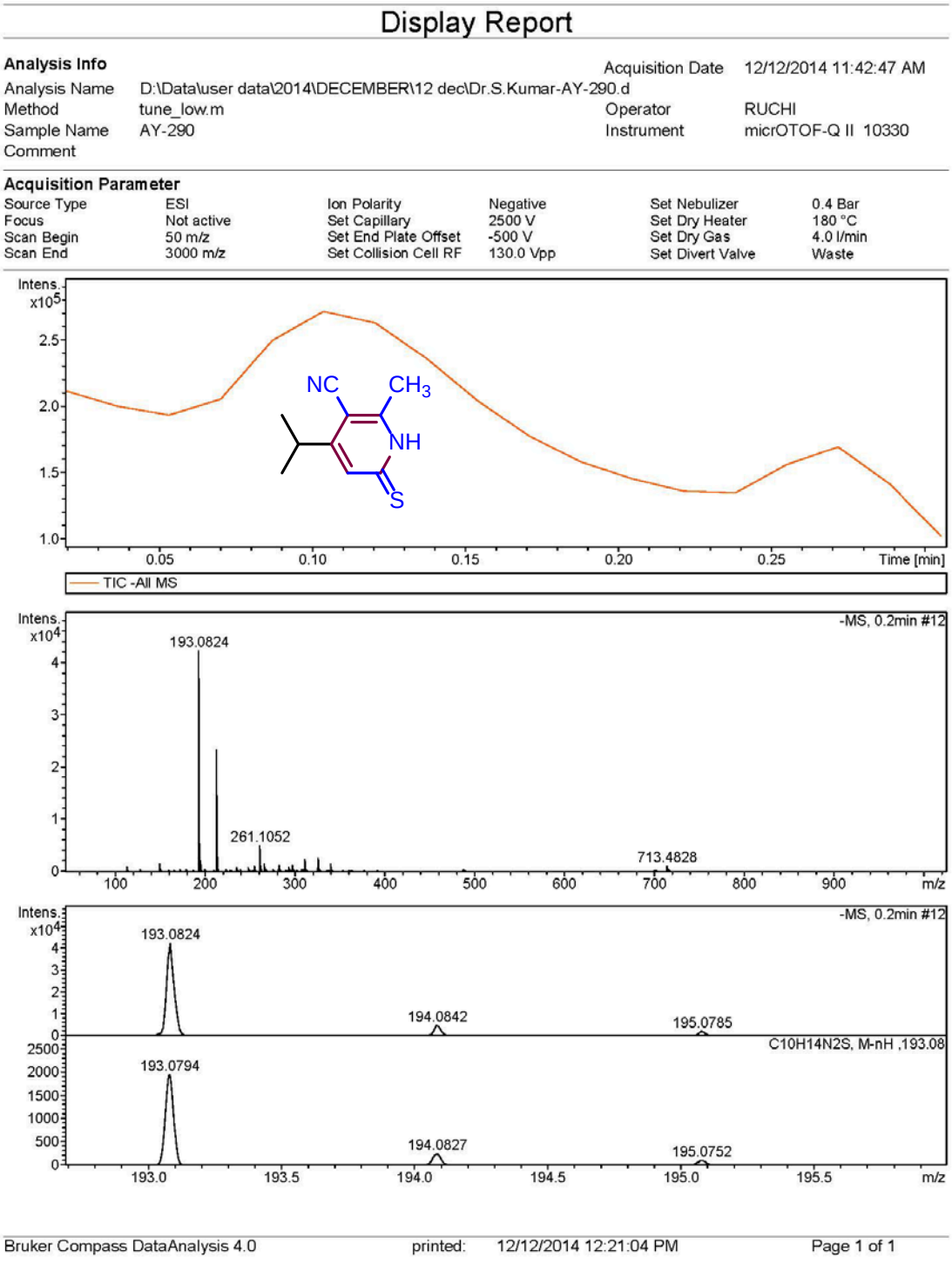
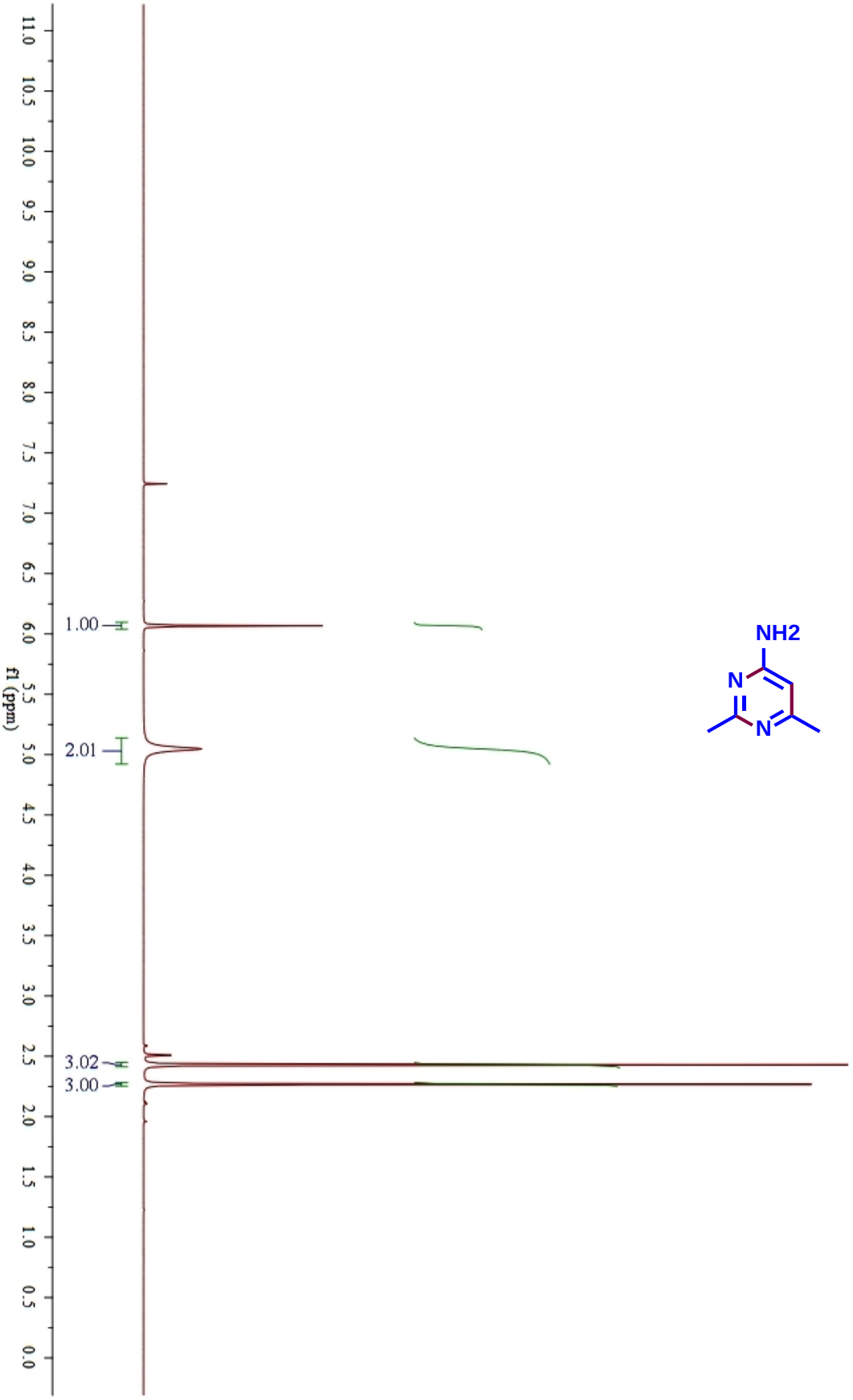


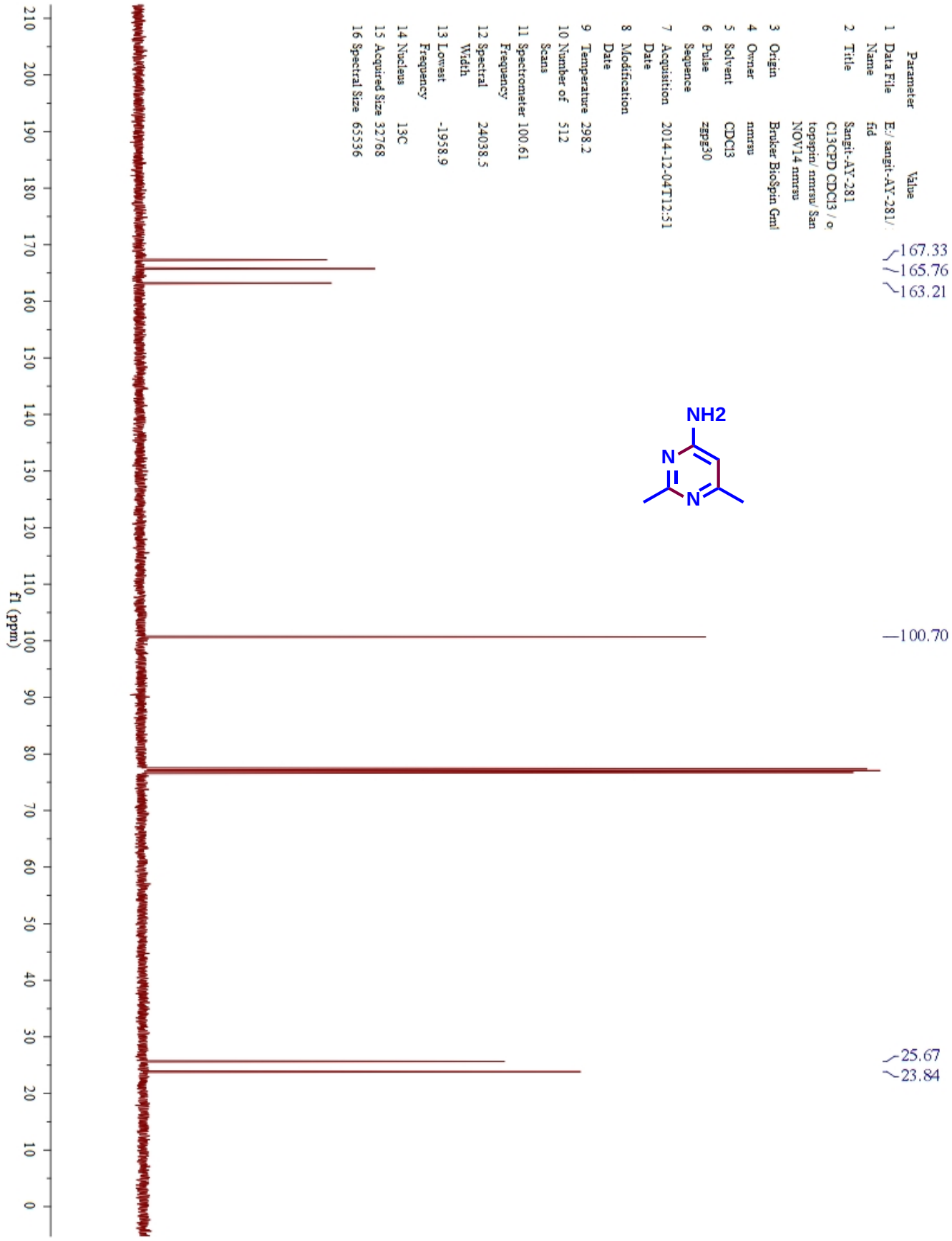
Figure S156 Mass spectra of **50**



^{1}H NMR spectra of **2,6-Dimethylpyrimidin-4-amine**



^{13}C NMR spectra of **2,6-Dimethylpyrimidin-4-amine**



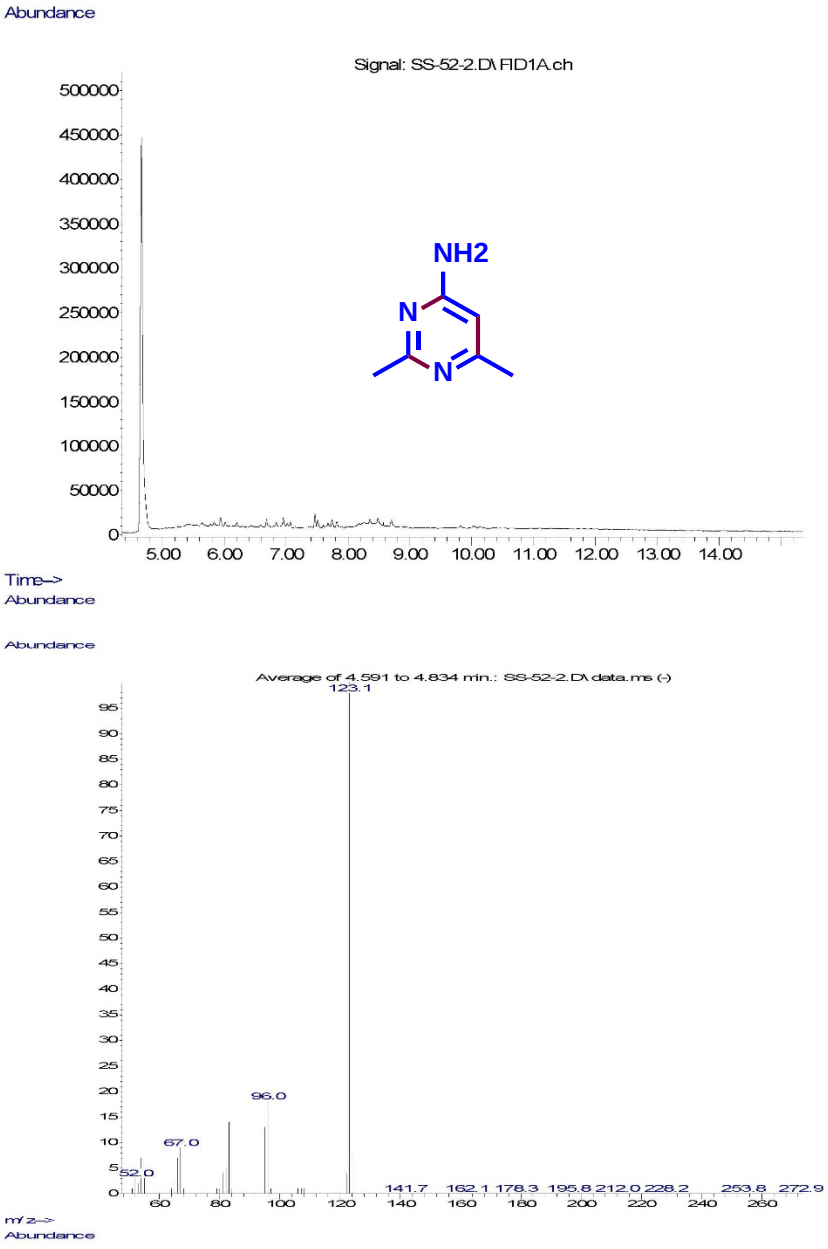
GCMS spectra of **2,6-Dimethylpyrimidin-4-amine**

Acquisition date: 26/02/14

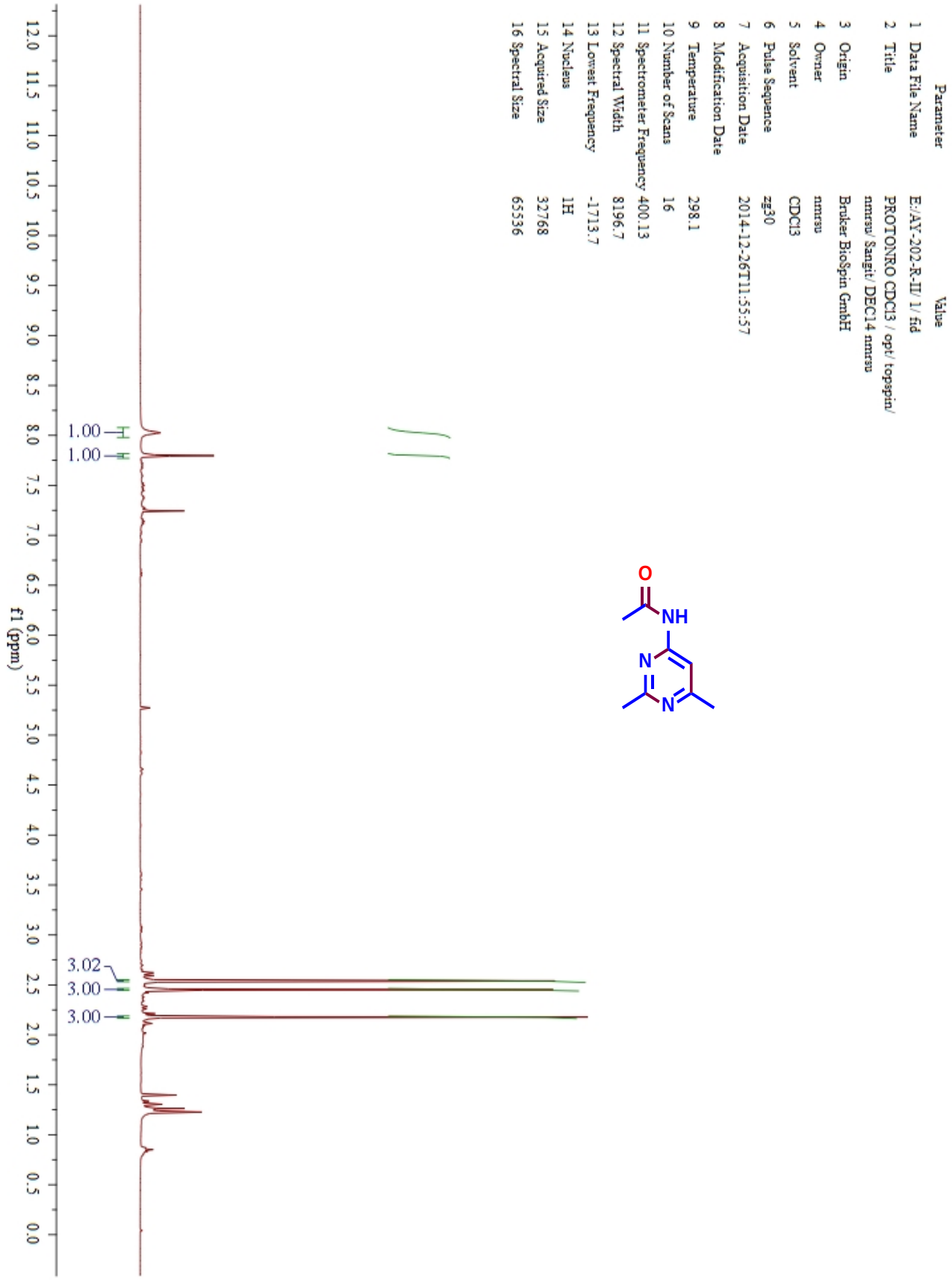
Sample ID: SS-52-2 | ***Supervisor***: Dr. S. Kumar | ***Operator:*** **IISERB-CIF-Mass Facility**

Instrument*: Agilent 7890A GC with 5975C MS system** | ***Column*: HP-5** | ***Ionization: **EI (70 eV)**

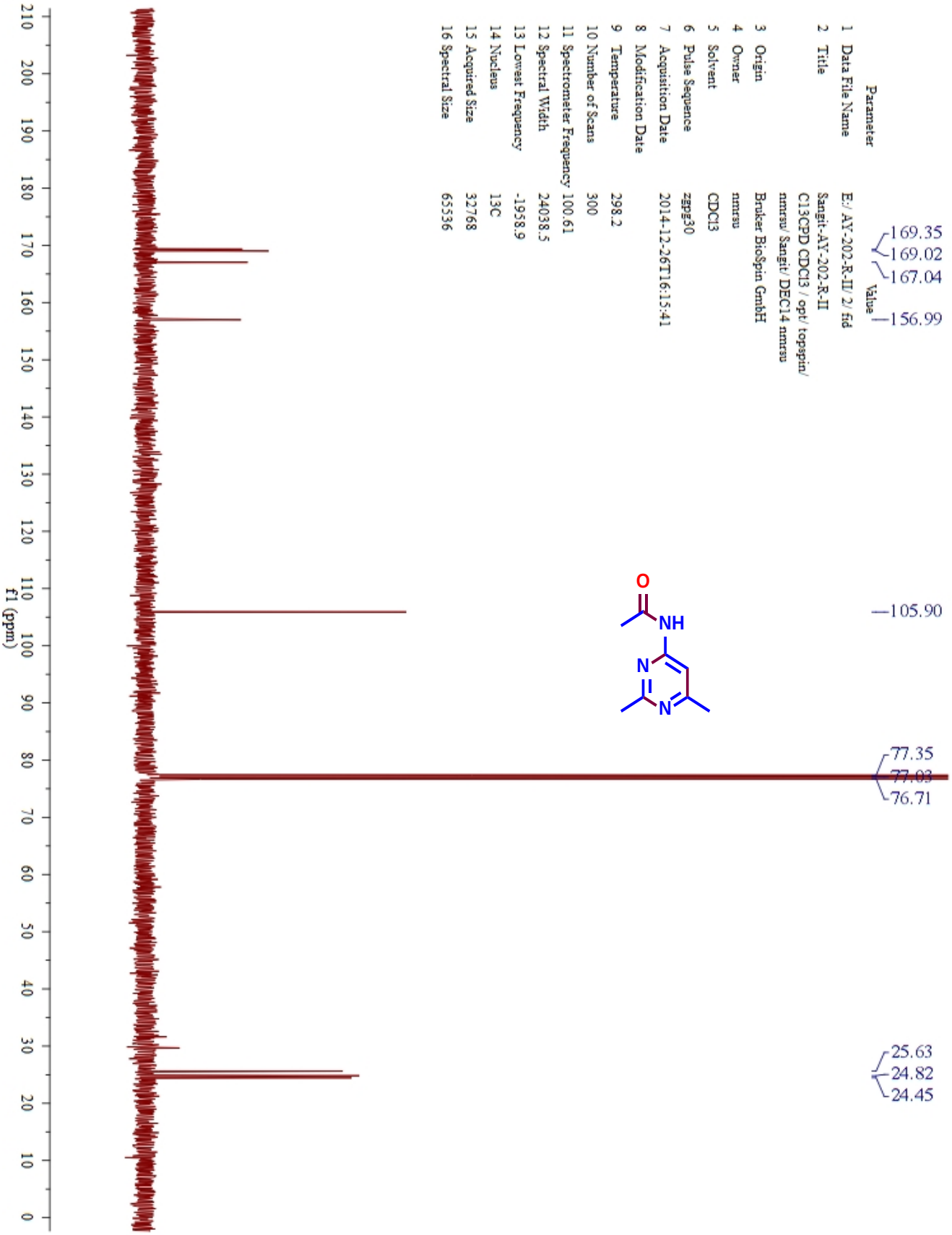
Method: **General_1_HP5_80_DEG.M** | ***MSD*: Single Quad.**



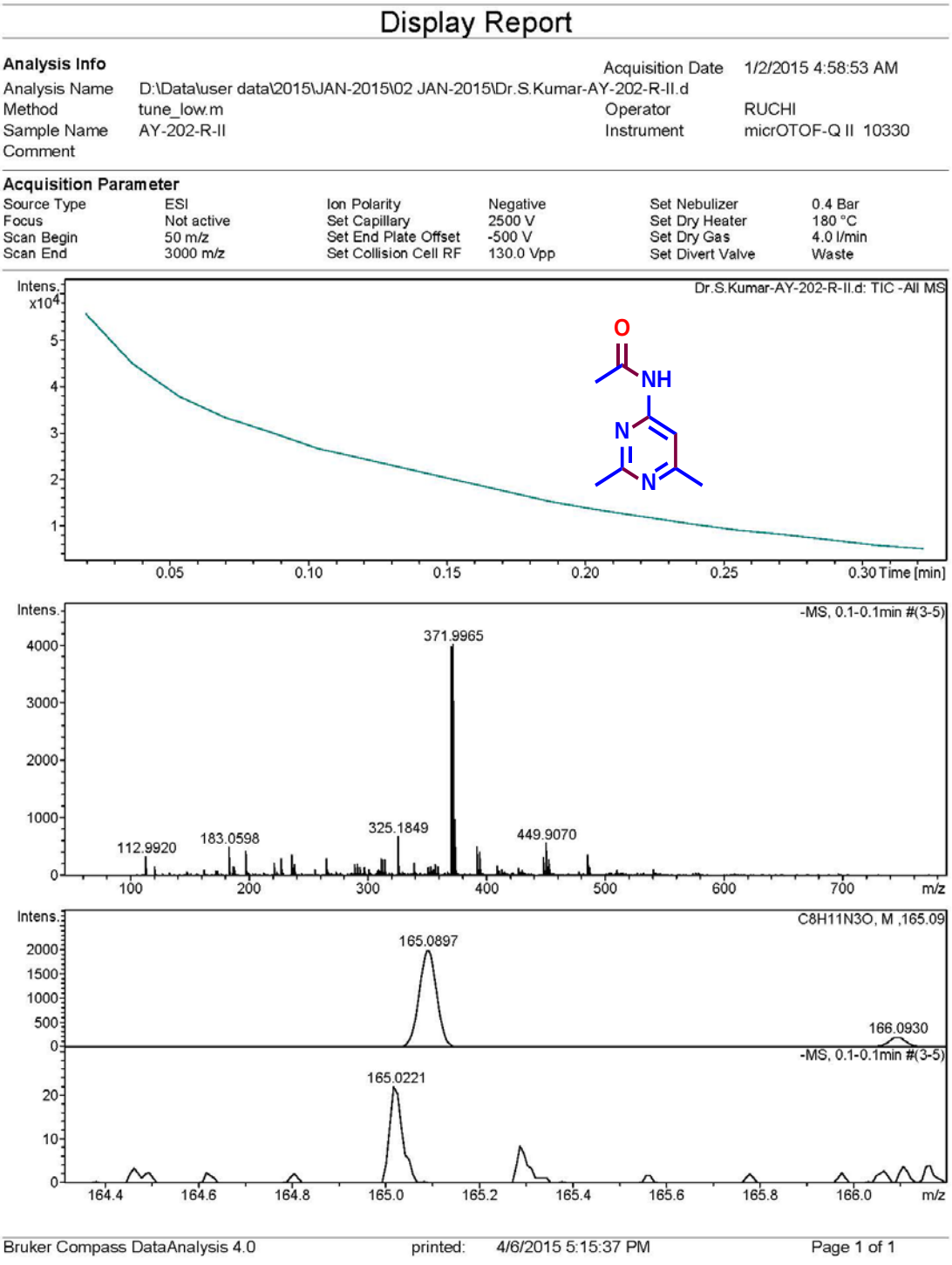
[1]H NMR spectra of ***N*-(2,6-Dimethylpyrimidin-4-yl)acetamide**



^{13}C NMR spectra of ***N*-(2,6-Dimethylpyrimidin-4-yl)acetamide**



LRMS spectra of ***N*-(2,6-Dimethylpyrimidin-4-yl)acetamide**



Mass spectra for optimization of reaction with benzaldehyde, KOH in acetonitrile (see optimization table)

Acquisition date: 27/03/15

Sample ID: AV-381 | ***Supervisor:*** Dr. S. Kumar | ***Operator:*** IISERB-CIF-Mass Facility

Instrument: Agilent 7890A GC with 5975C MS system | ***Column:*** HP-5 | ***Ionization:*** EI (70 eV)

Method: General_1_HP5_80_DEG.M | ***MSD:*** Single Quad.