

Supporting Information

Instant detection of synthetic cannabinoids on physical matrices, implemented on a low-cost, ultra-portable device.

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Movies

Movie S1. Ultra-portable device detection of synthetic cannabinoids on variety of physical matrices. See video file in online supporting information.

Figures

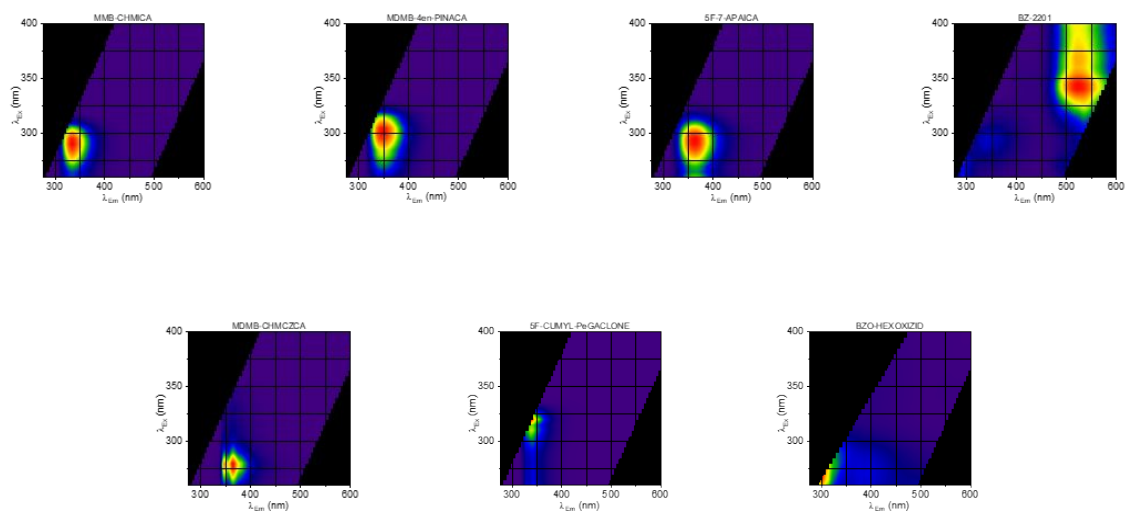


Figure S1. Example FSFs for the range of ‘core’ moieties that give rise to SC fluorescence.

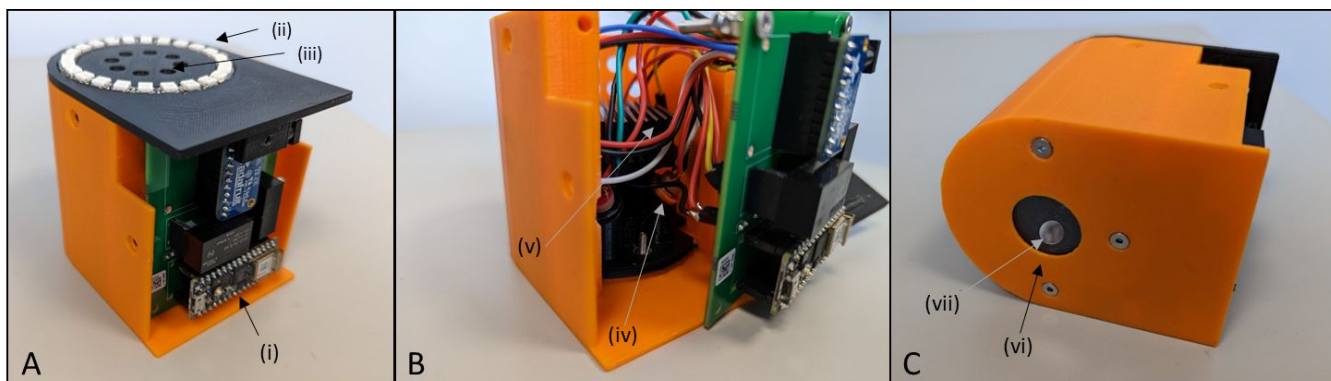


Figure S2. Further details of device design. (i) Custom PCB with power handling and conversion, LED driver, ADC and microcontroller. (ii) LED ring for reporting. (iii) ventilation for heatsink. (iv) Photodiode (one of four). (v) The heatsink. (vi) a sapphire window to protect the bandpass filters. (vii) bandpass filter (one of four).

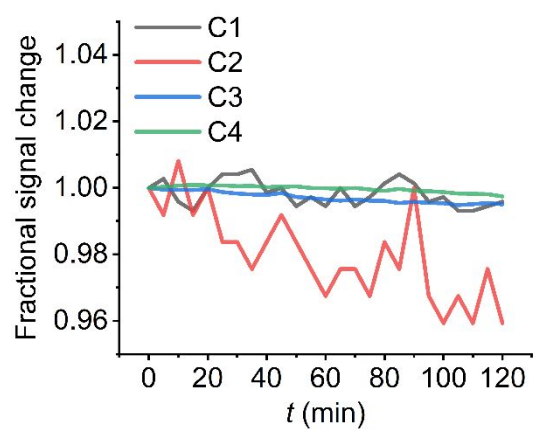


Figure S3. Fluctuation in signal for each recorded change with respect to time.

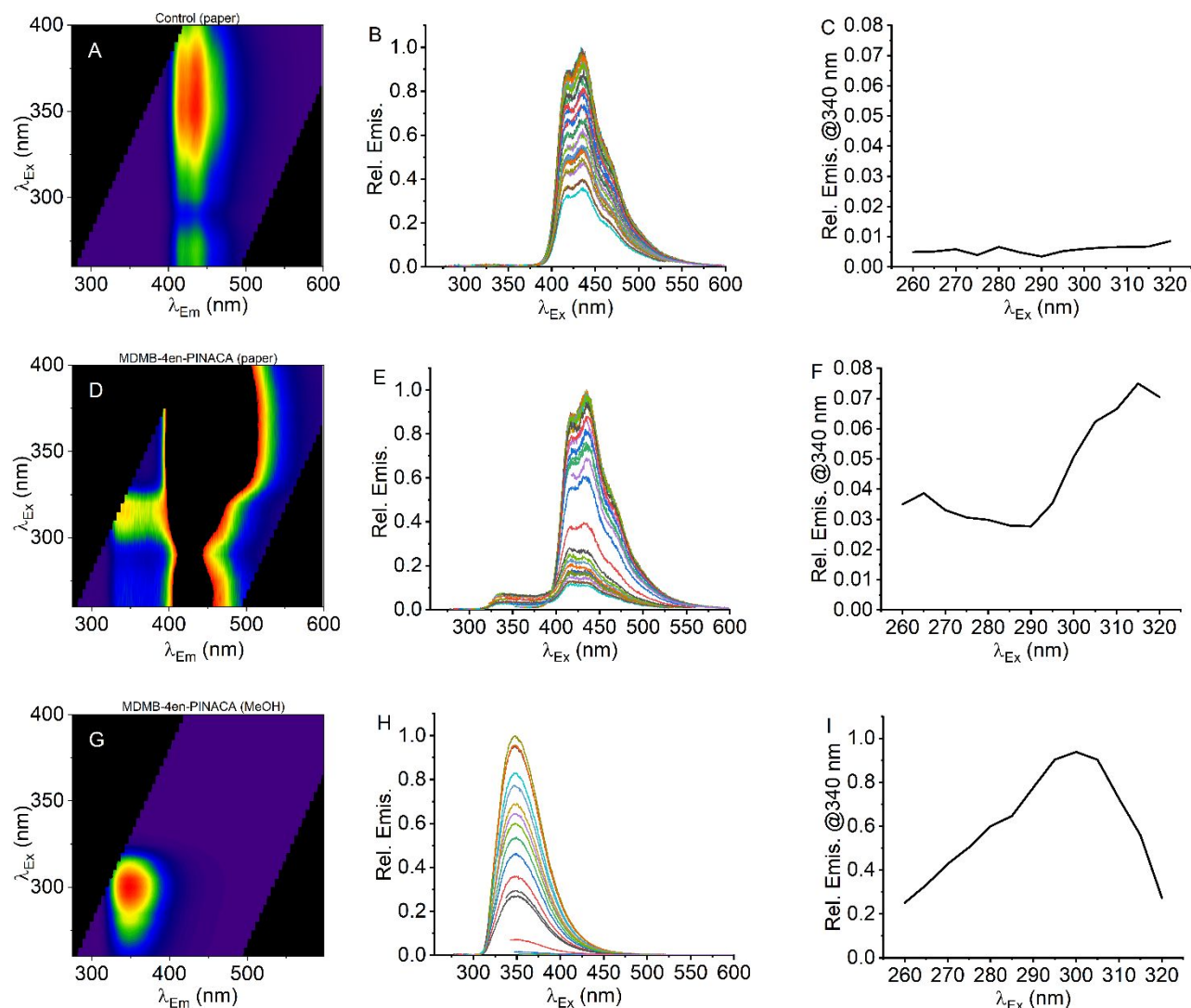


Figure S4. Fluorescence spectral data for an example SC (MDMB-4en-PINACA) on paper and in solution (MeOH). Each row shows the EEM (at left), constituent spectra (middle panel) and excitation spectrum at 340 nm emission (at right) for paper (**A-C**), paper with MDMB-4en-PINACA (**D-F**) and MDMB-4en-PINACA in MeOH (**G-I**).

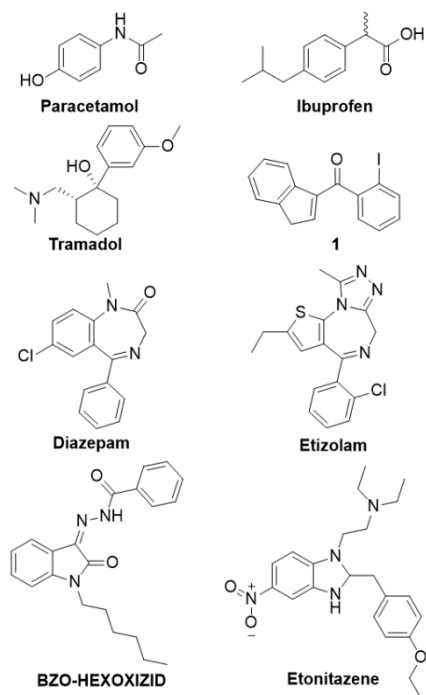
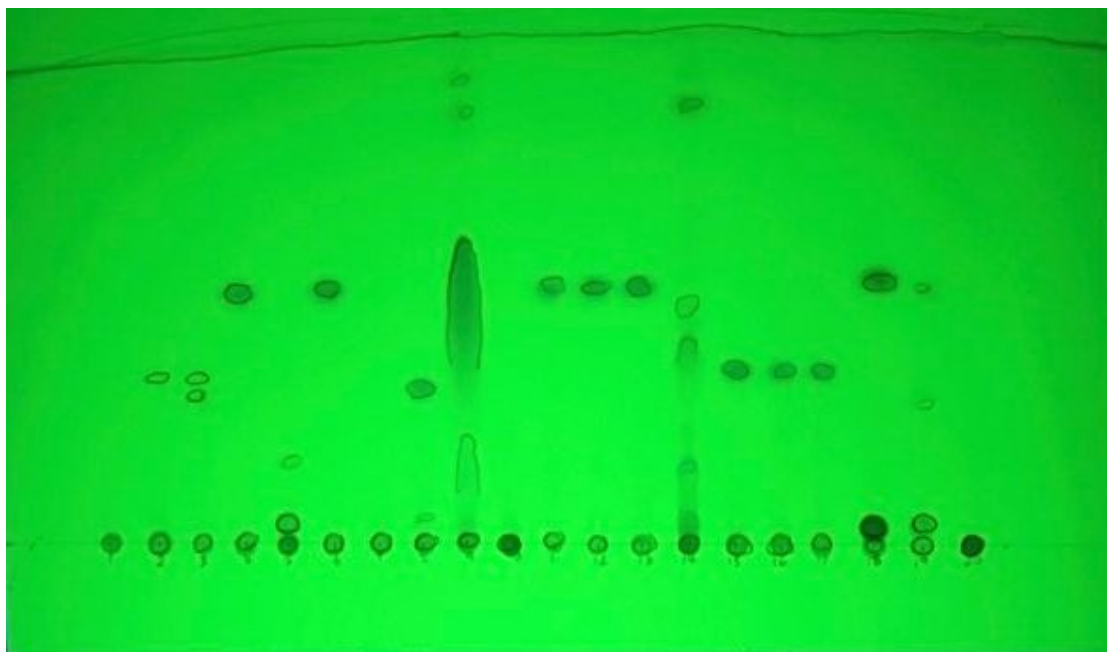
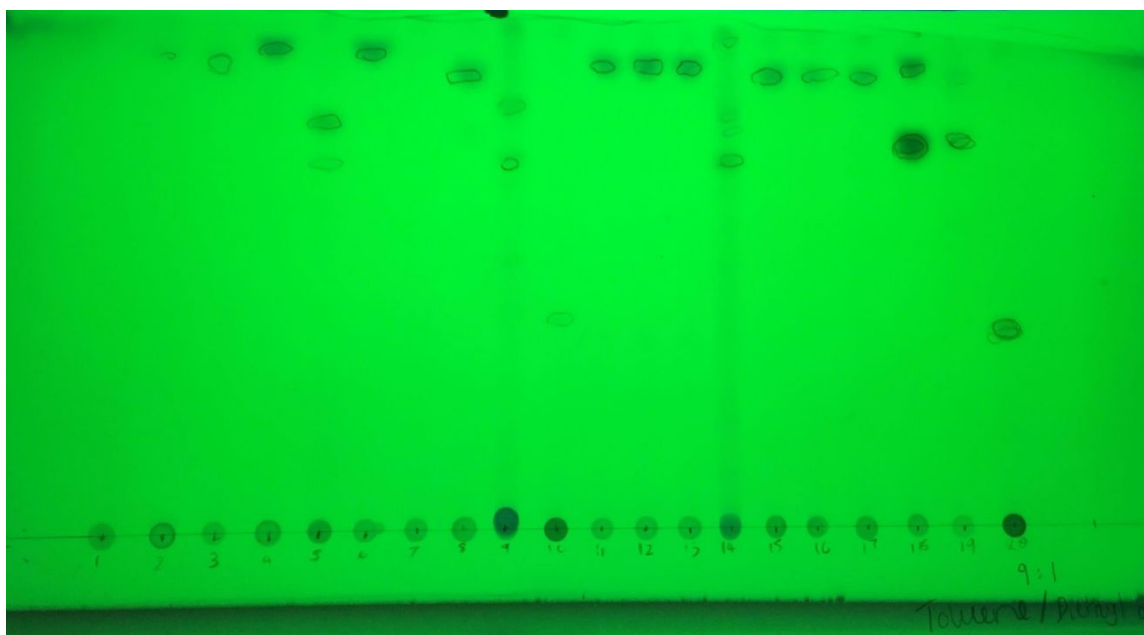


Figure S5. Structures of analytes shown in Figure 5.



Silica TLC plate showing ASP 1-20, run in hexane : diethyl ether, 2 : 1



Silica TLC plate showing ASP 1-20, run in toluene : diethyl amine, 9 : 1

Figure S6. TLC Data of extractions from samples ASP 1-20.

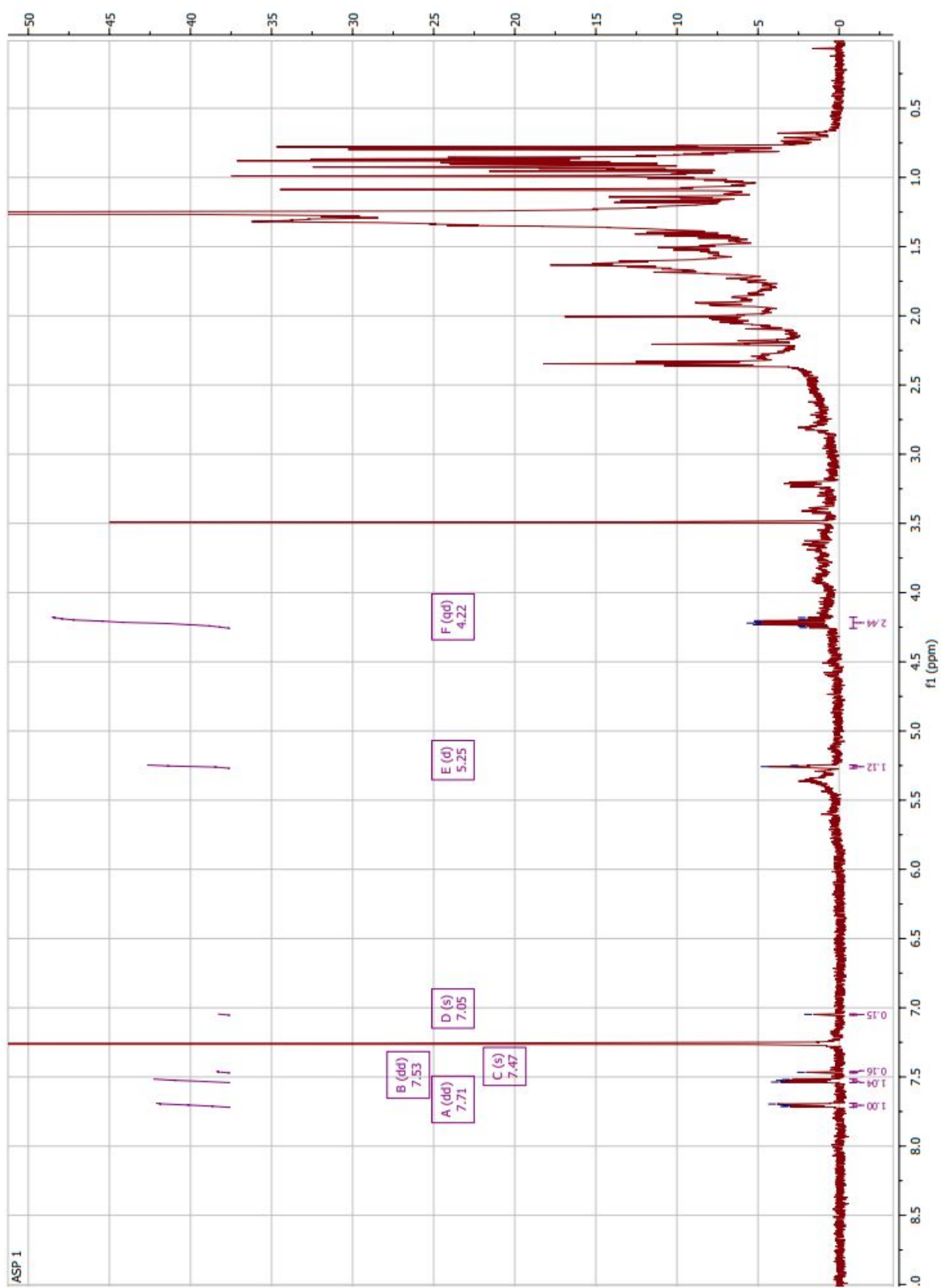


Figure S7. Labelled ^1H NMR of ASP1 in CDCl_3 .

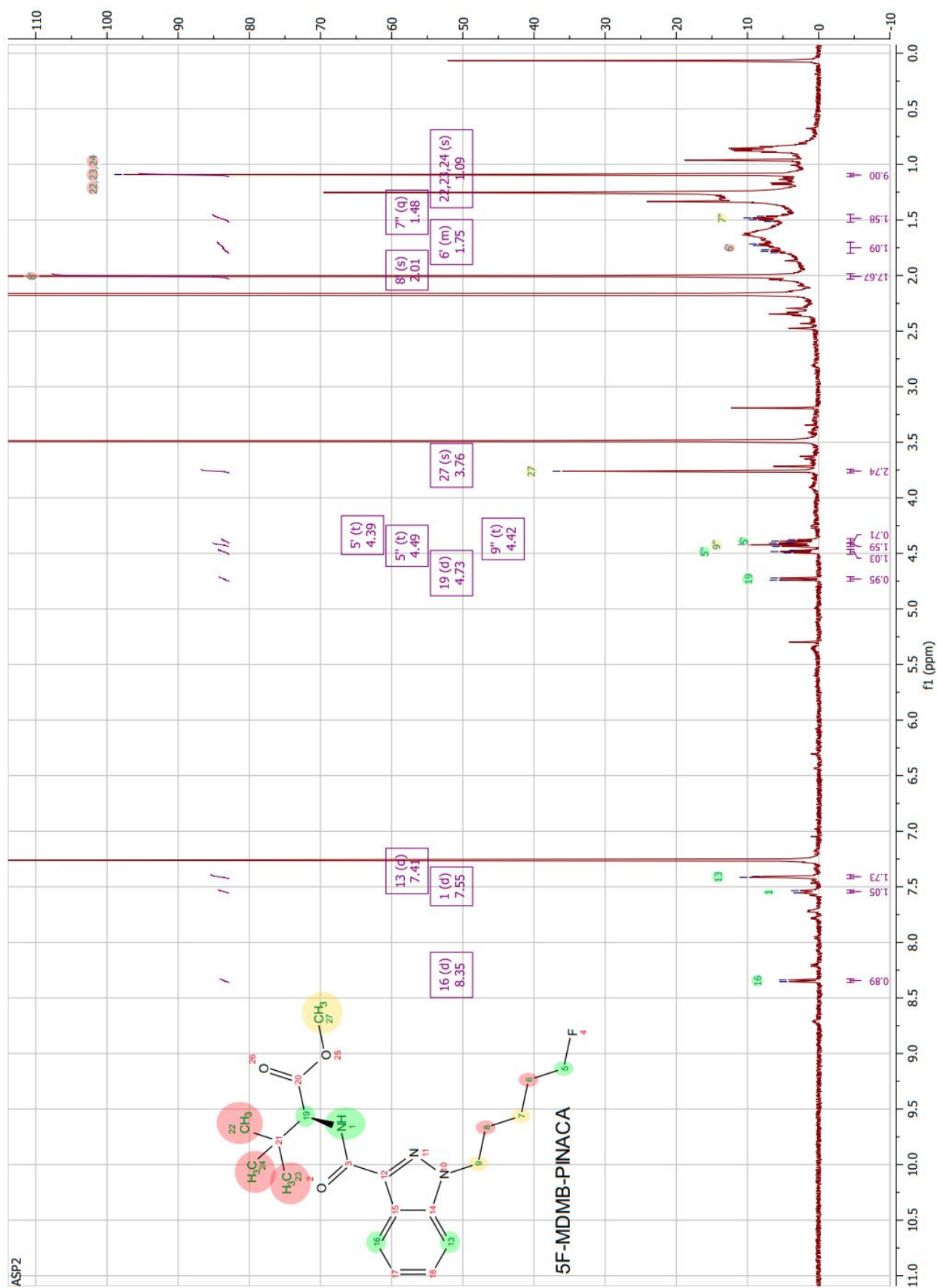


Figure S8. Labelled ^1H NMR of ASP2 in CDCl_3 .

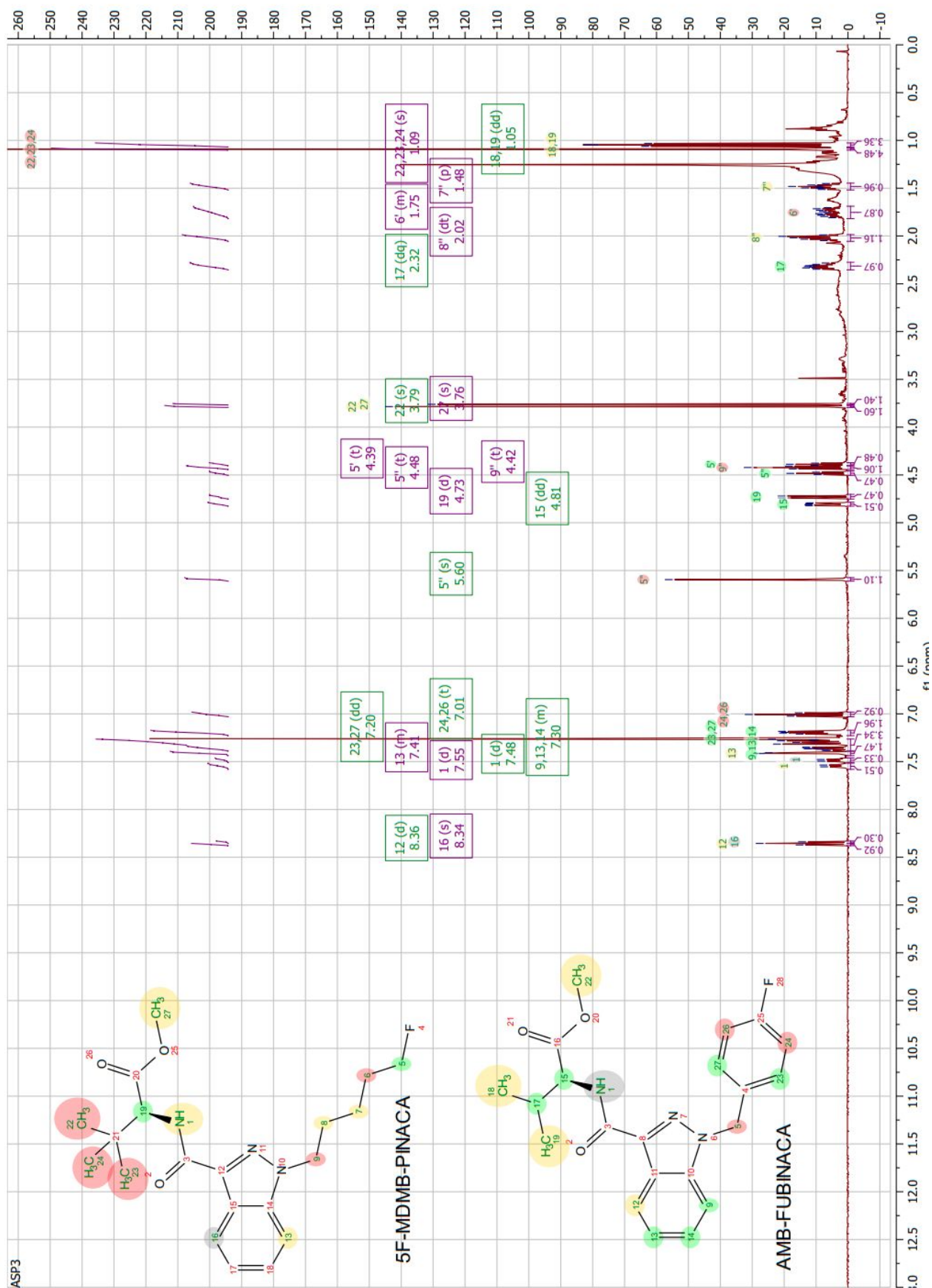


Figure S9. Labelled ^1H NMR of ASP3 in CDCl_3 .

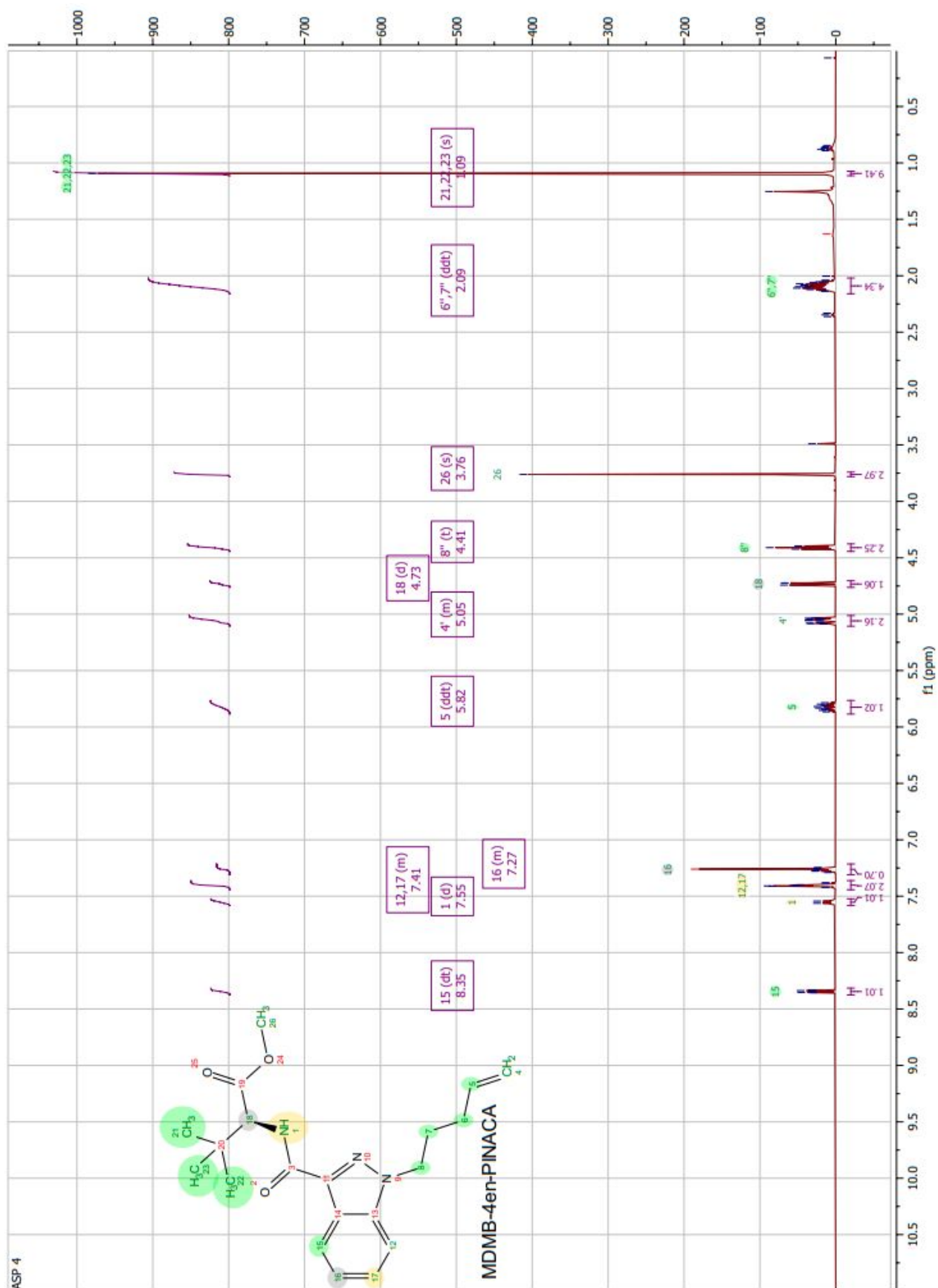


Figure S10. Labelled ^1H NMR of ASP4 in CDCl_3 .

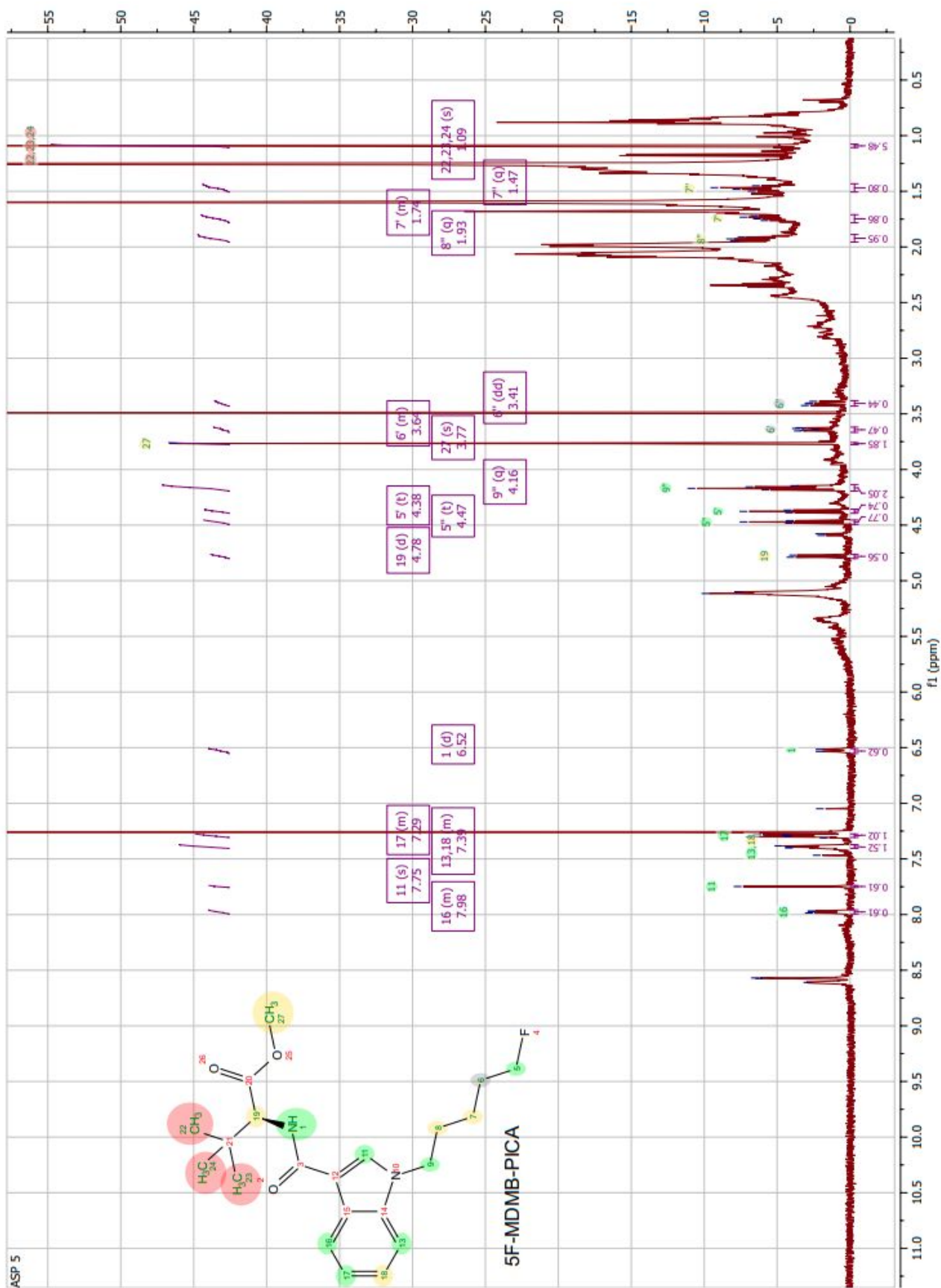
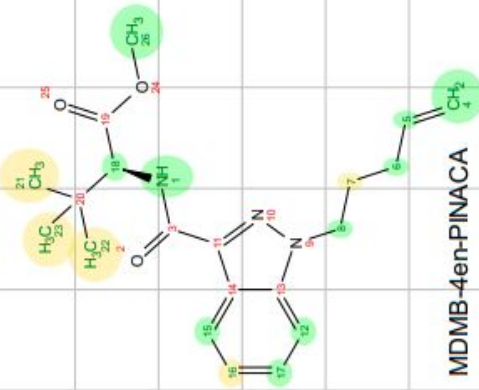


Figure S11. Labelled ^1H NMR of ASP5 in CDCl_3 .



S16

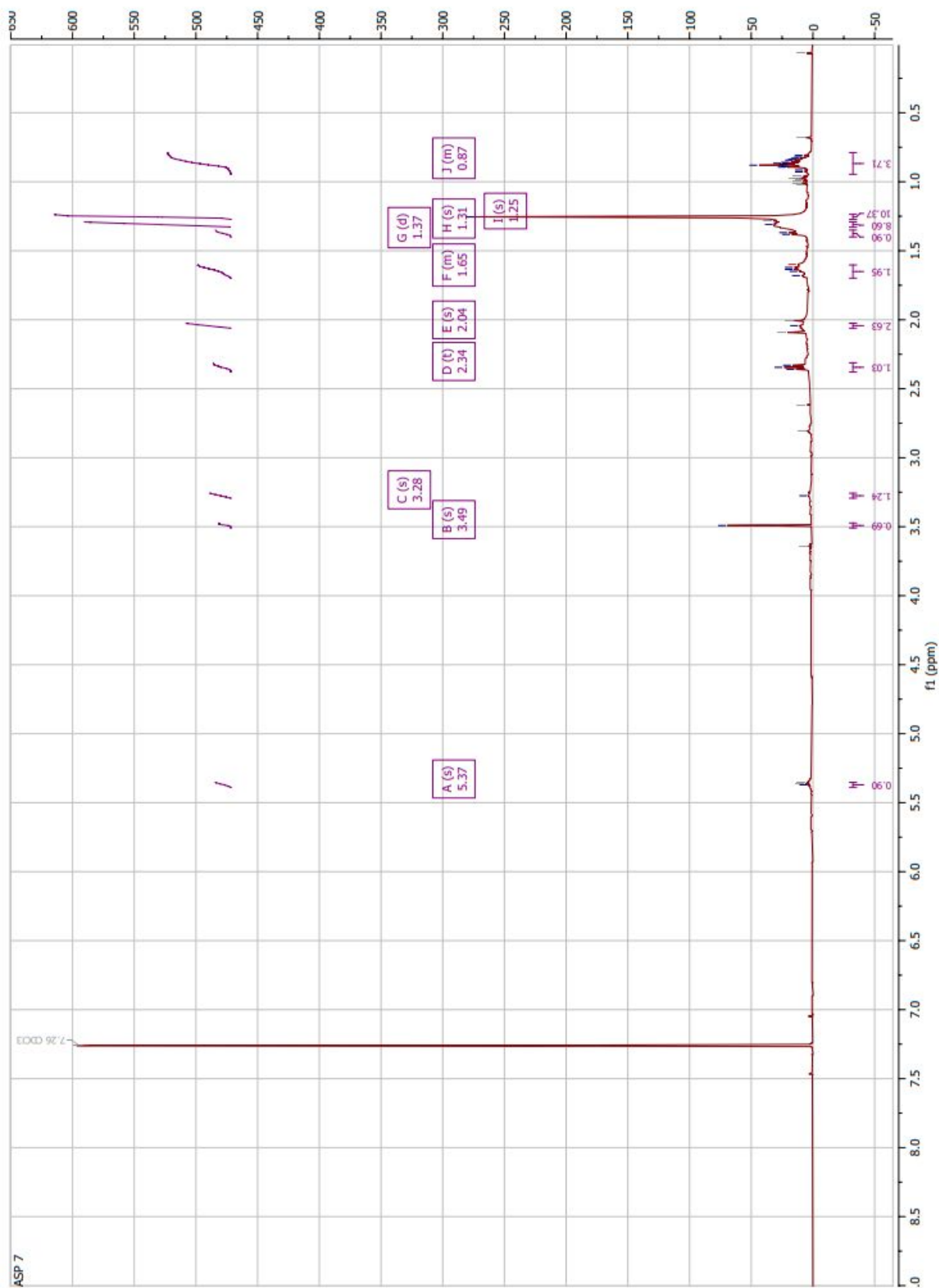
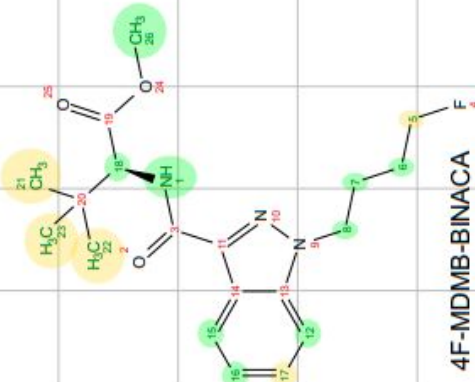


Figure S13. Labelled ^1H NMR of ASP7 in CDCl_3 .



S18

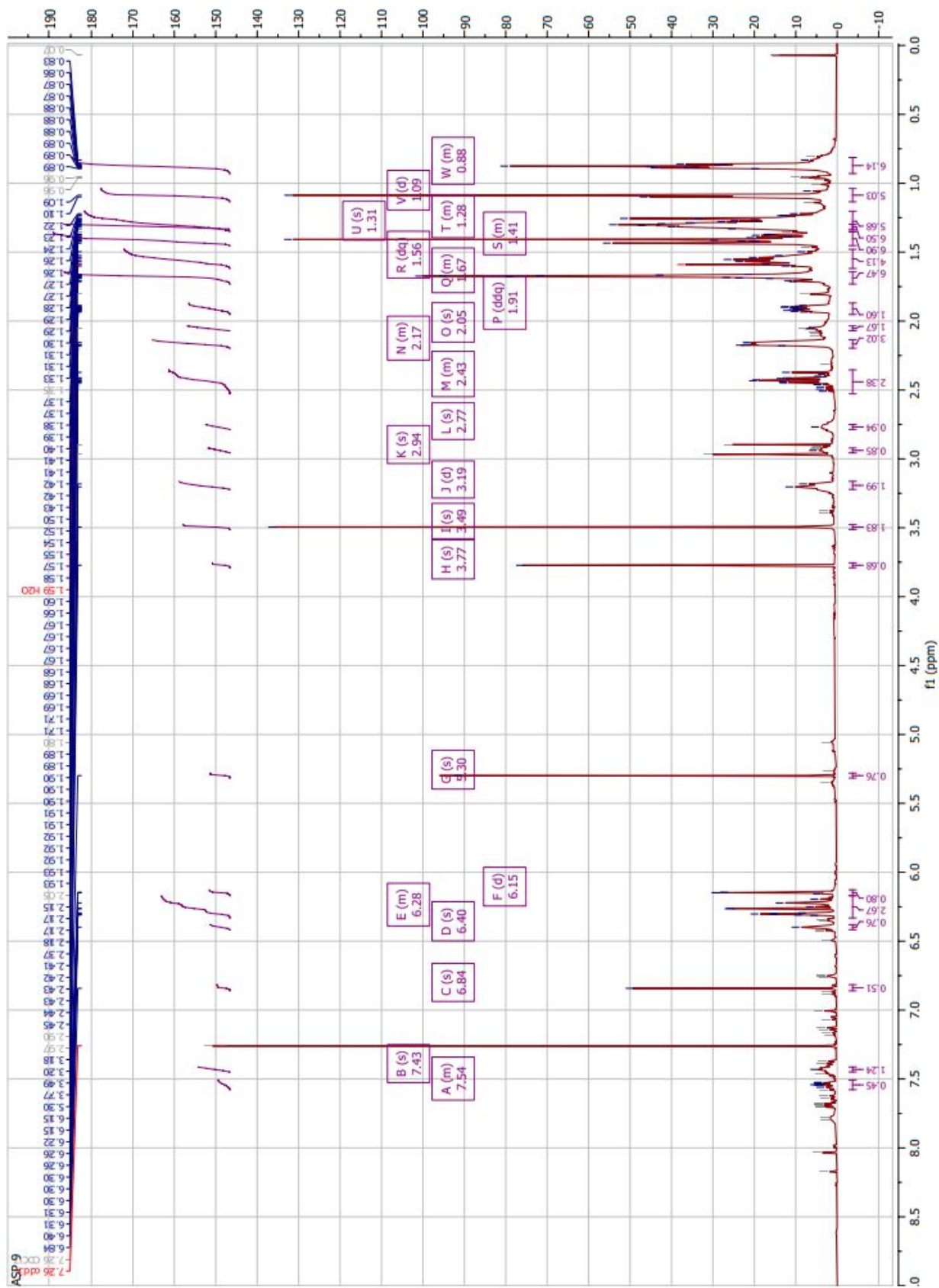


Figure S15. Labelled ^1H NMR of ASP9 in CDCl_3 .

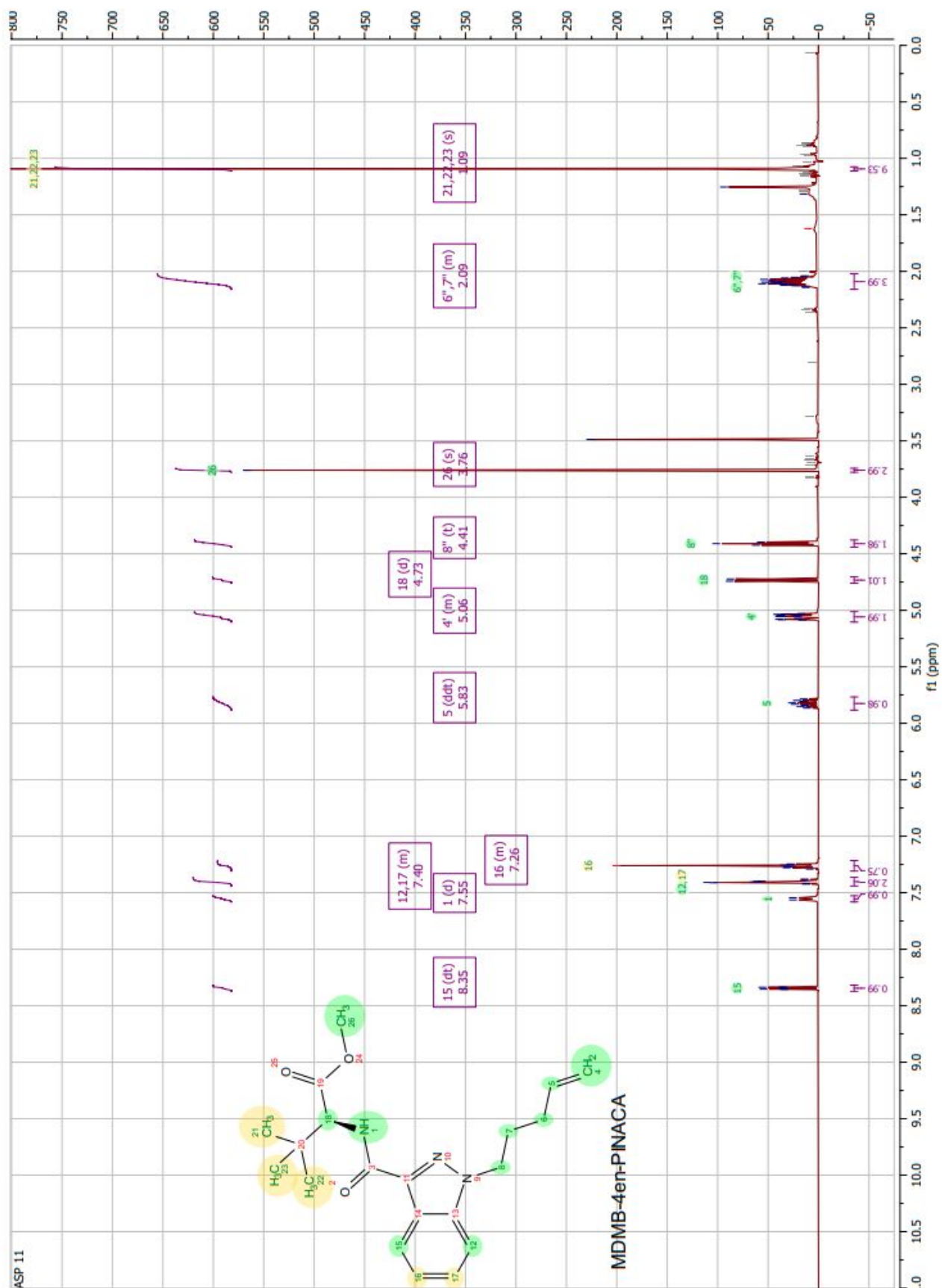


Figure S17. Labelled ^1H NMR of ASP11 in CDCl_3 .

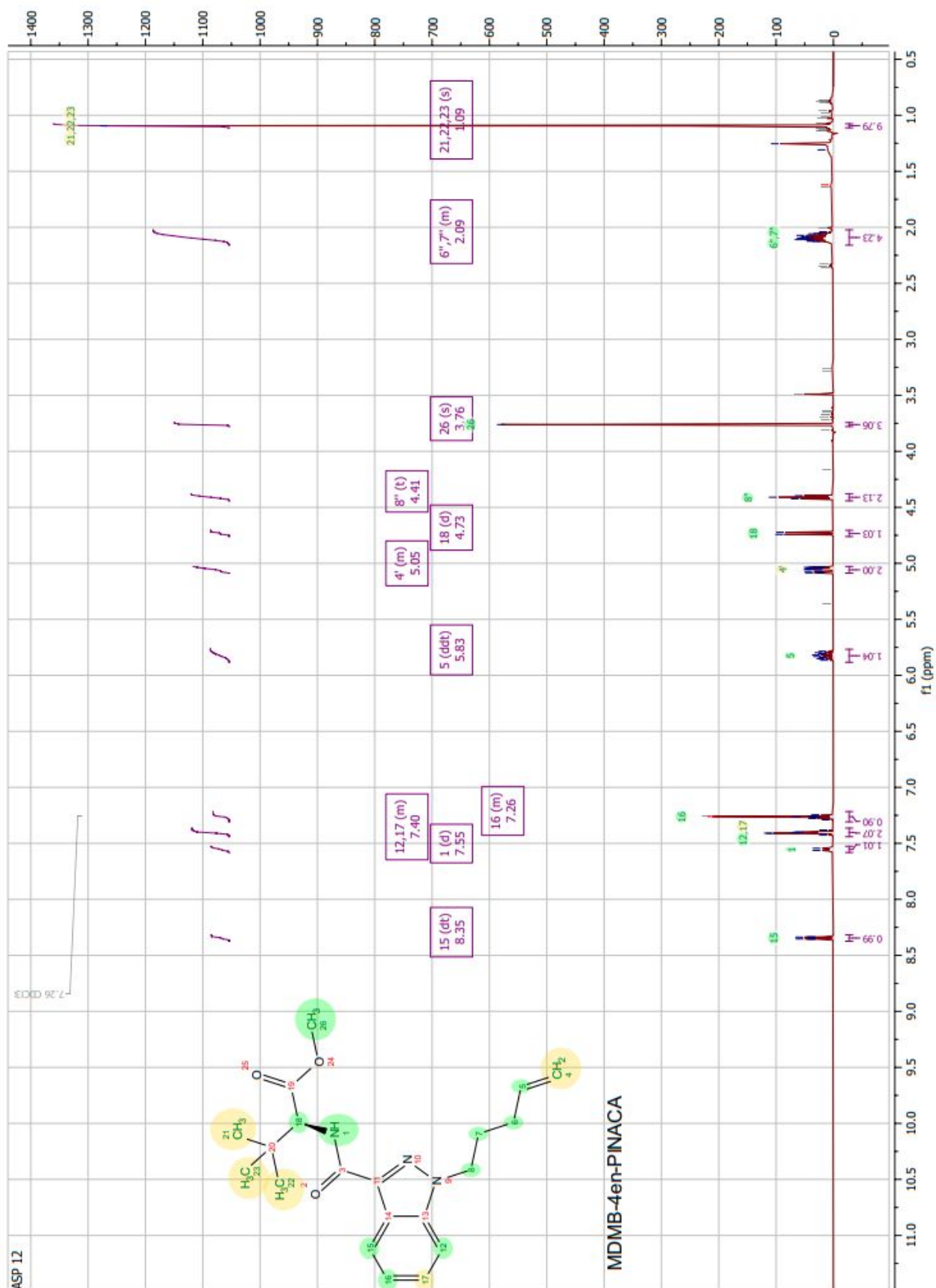


Figure S18. Labelled ^1H NMR of ASP12 in CDCl_3 .

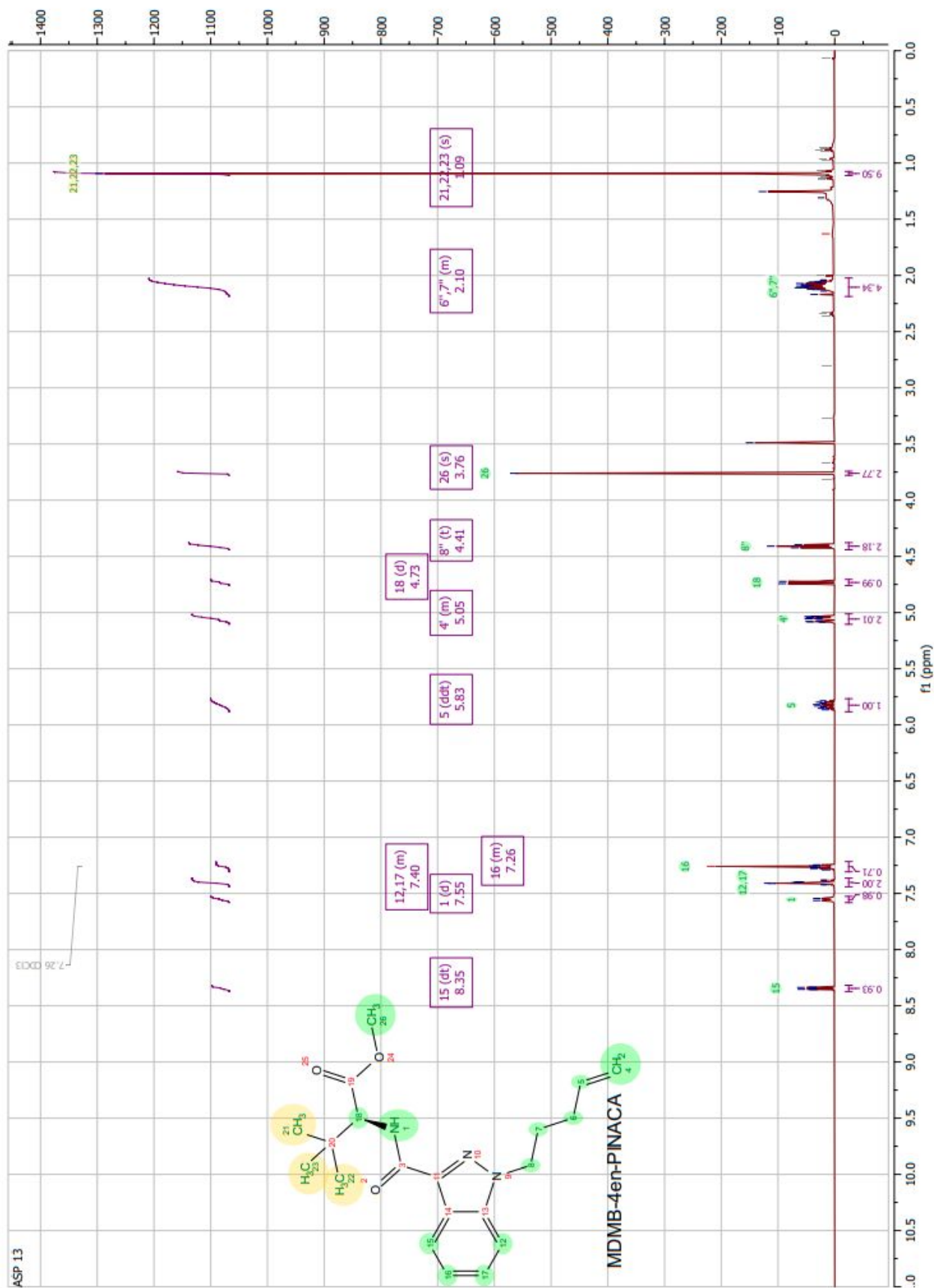


Figure S19. Labelled ¹H NMR of ASP13 in CDCl₃.

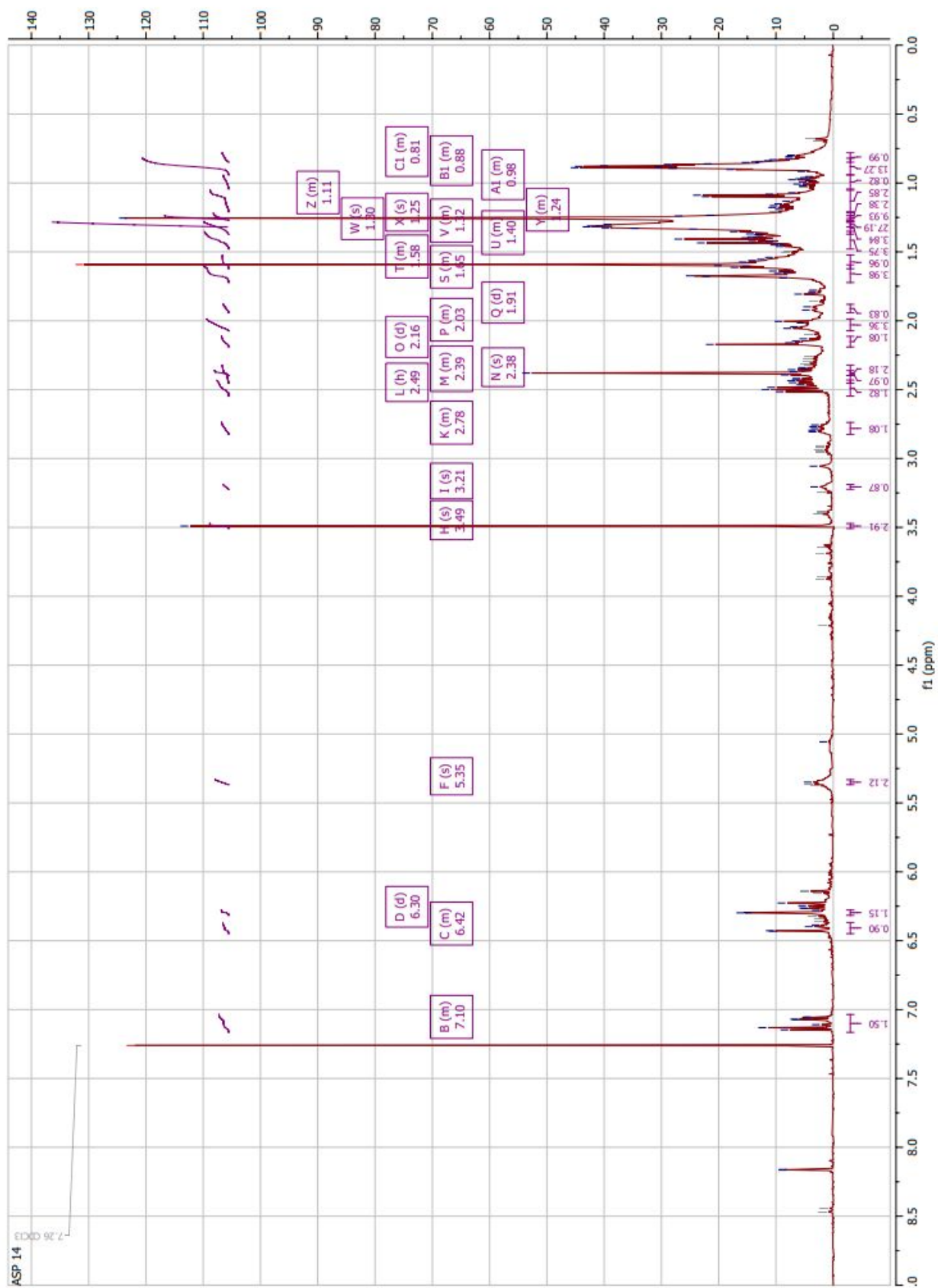


Figure S20. Labelled ¹H NMR of ASP14 in CDCl₃.

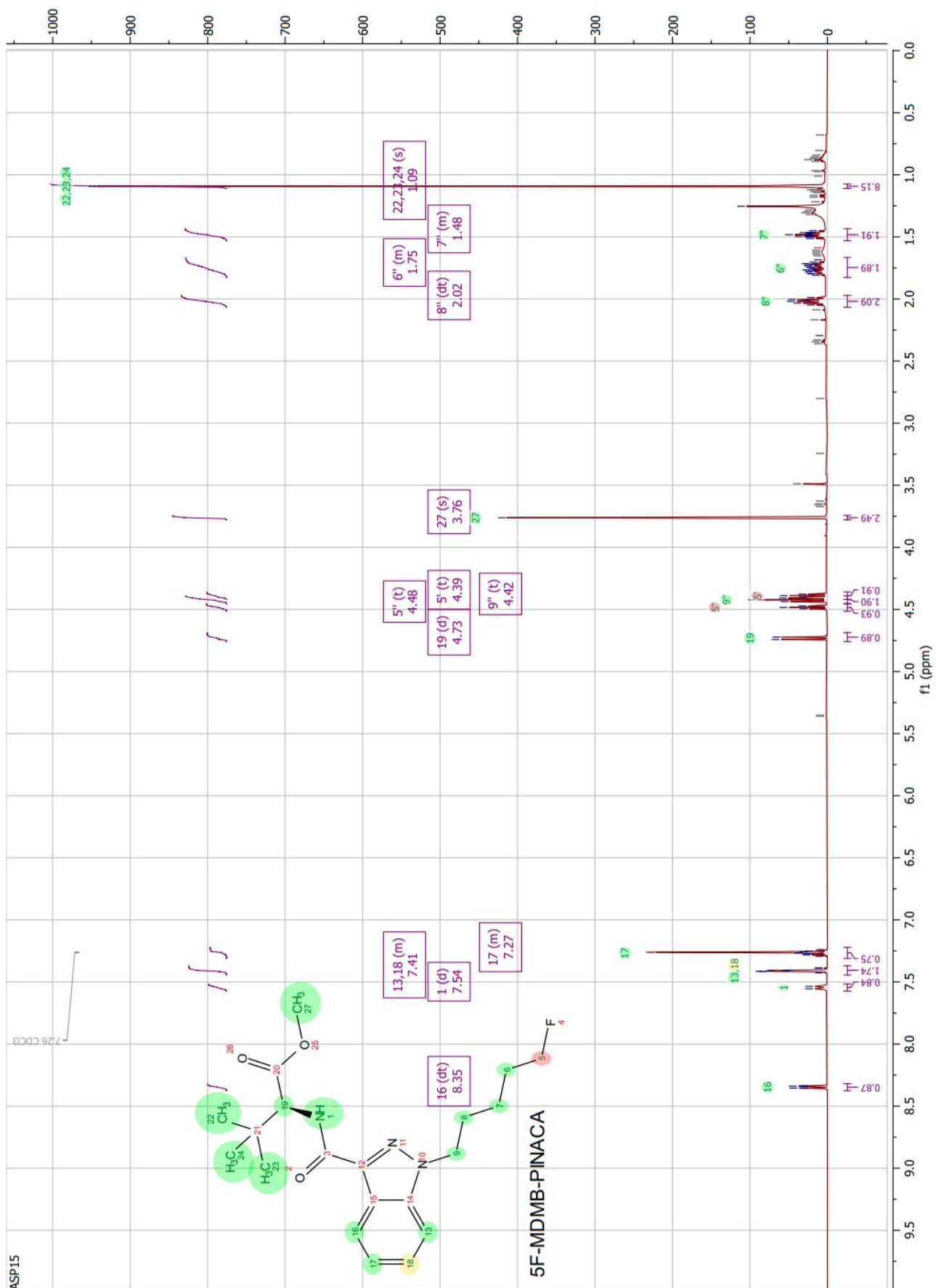


Figure S21. Labelled ¹H NMR of ASP15 in CDCl₃.

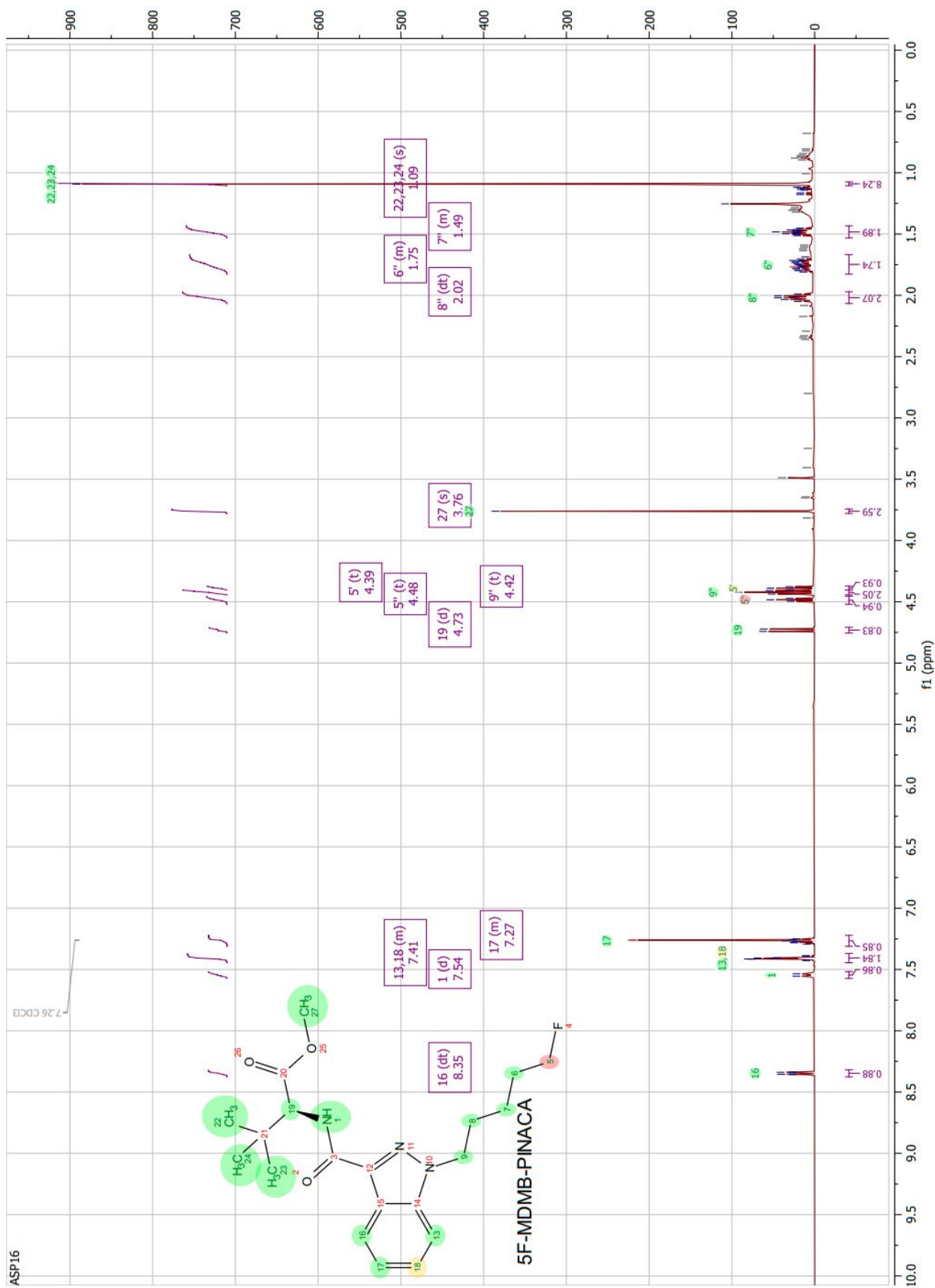


Figure S22. Labelled ¹H NMR of ASP16 in CDCl₃.

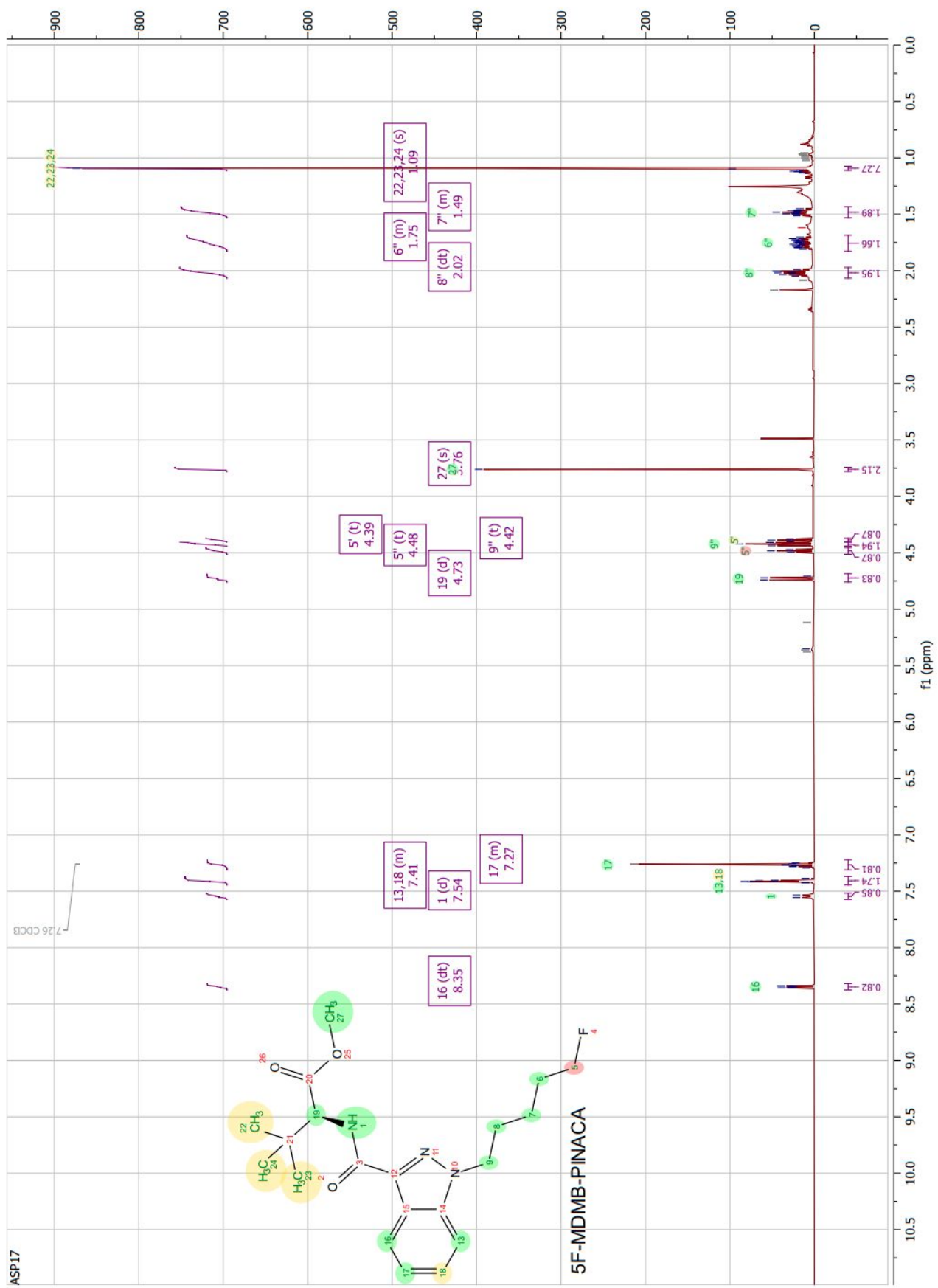


Figure S23. Labelled ¹H NMR of ASP17 in CDCl₃.

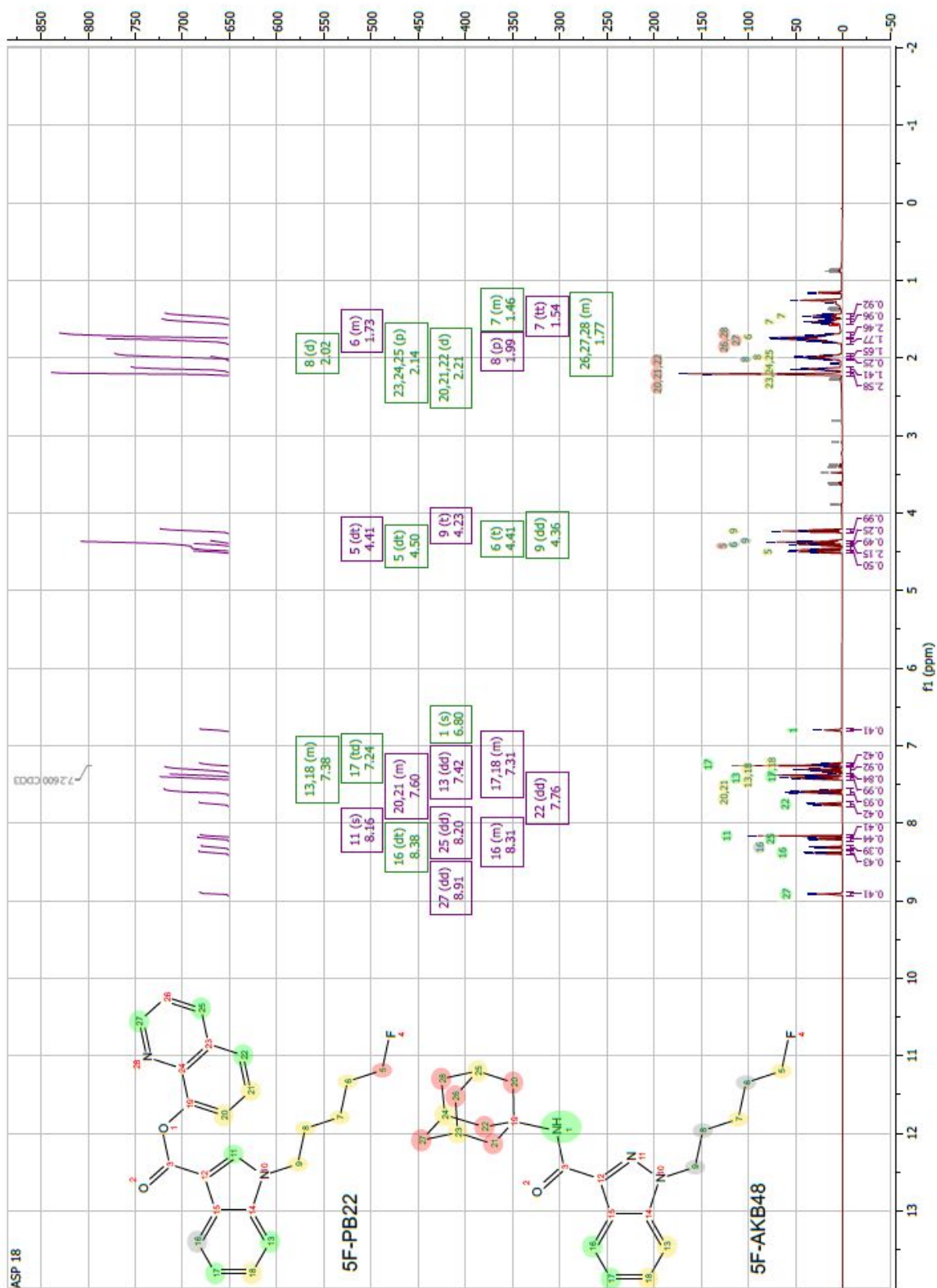


Figure S24. Labelled ¹H NMR of ASP18 in CDCl₃.

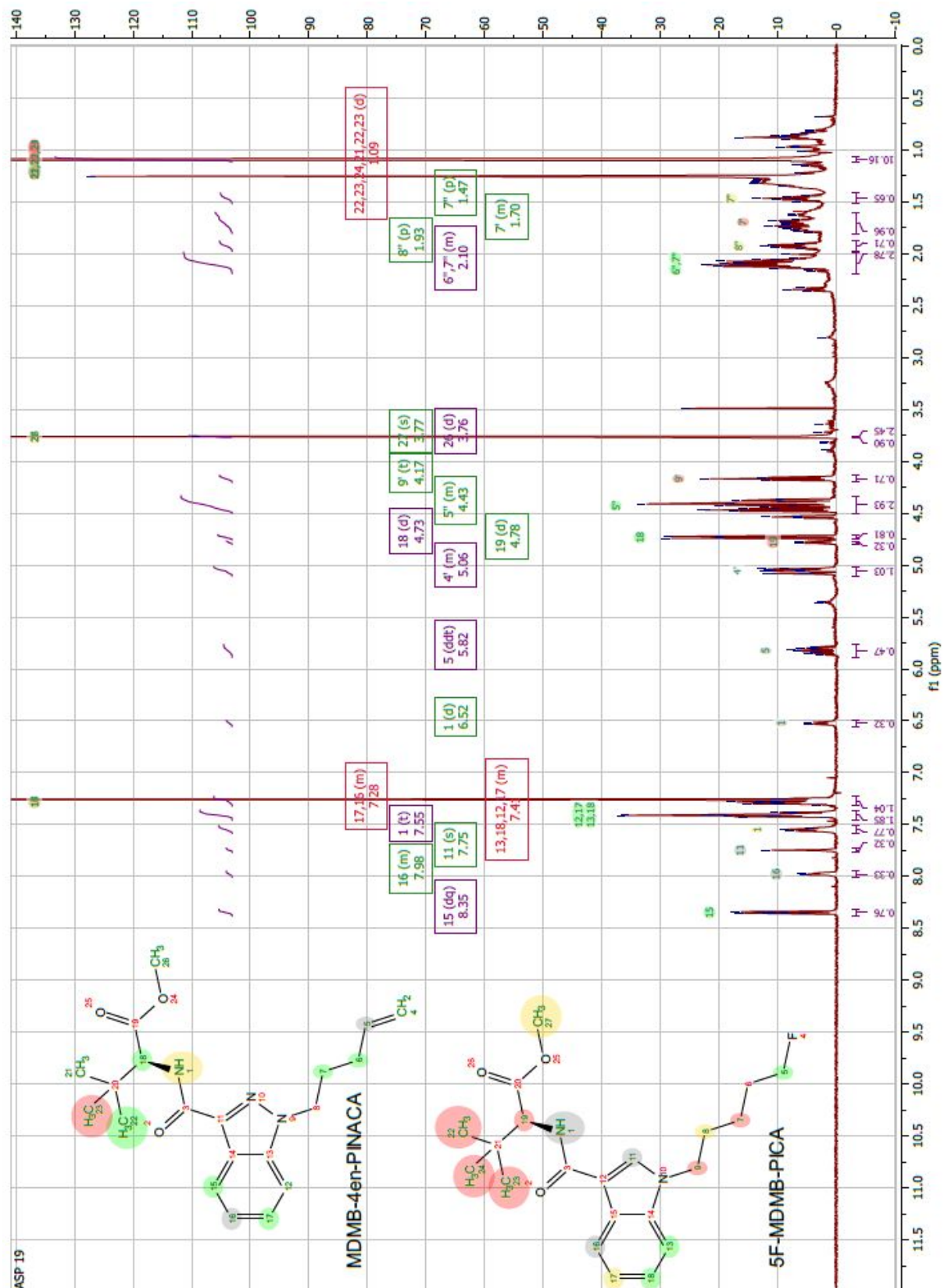


Figure S25. Labelled ^1H NMR of ASP19 in CDCl_3 .

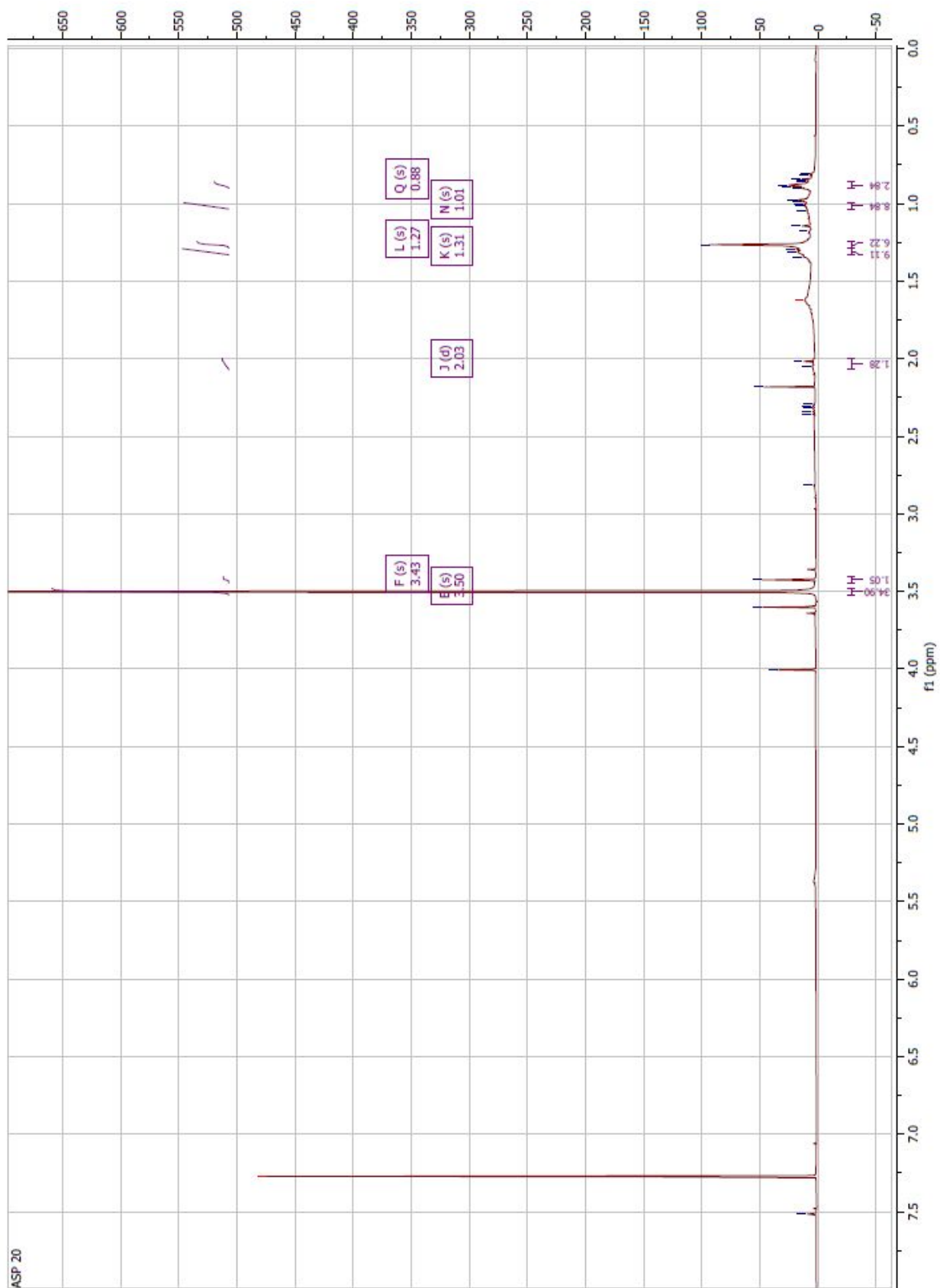


Figure S26. Labelled ^1H NMR of ASP20 in CDCl_3 .

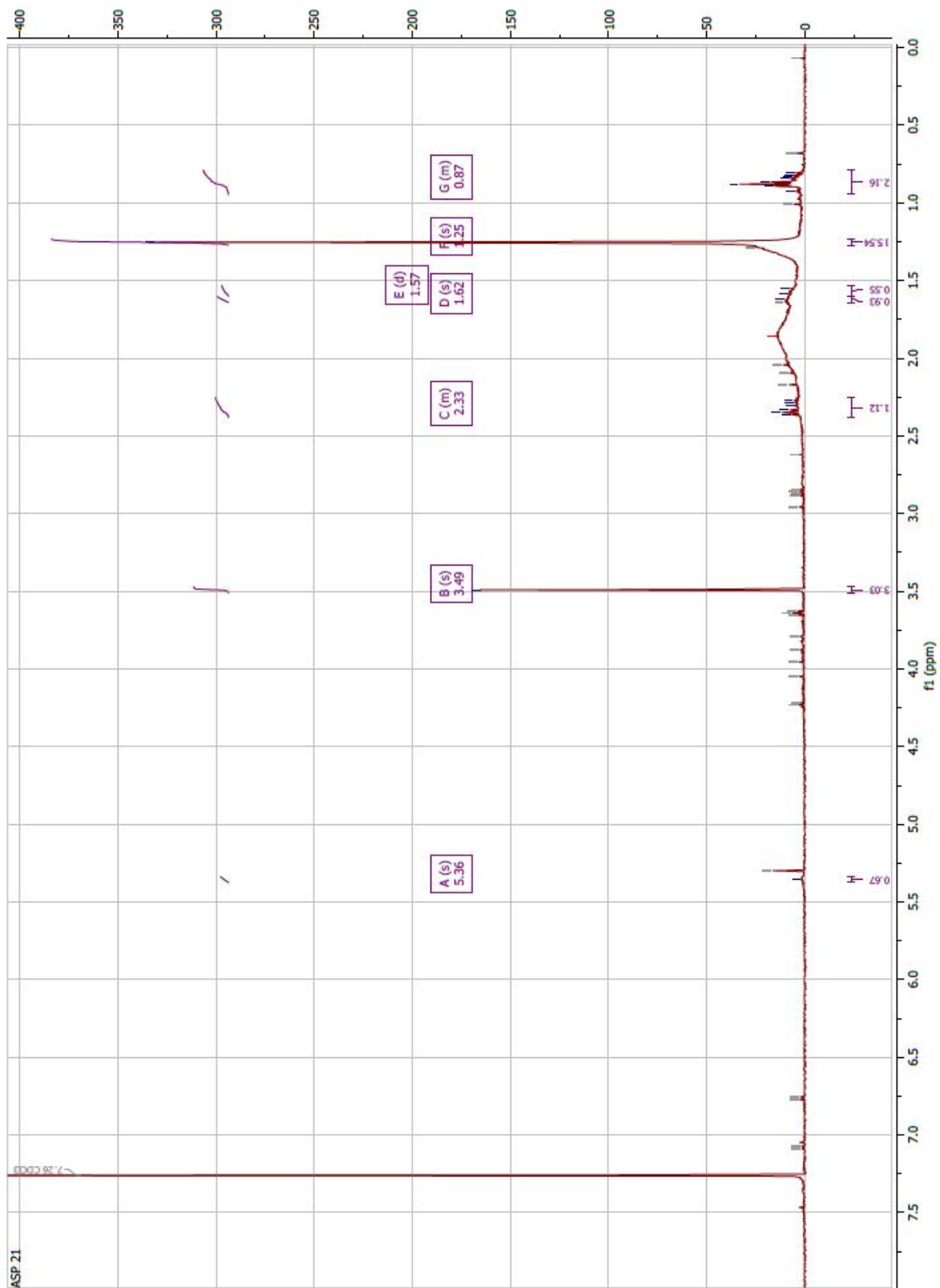


Figure S27. Labelled ¹H NMR of ASP21 in CDCl₃.

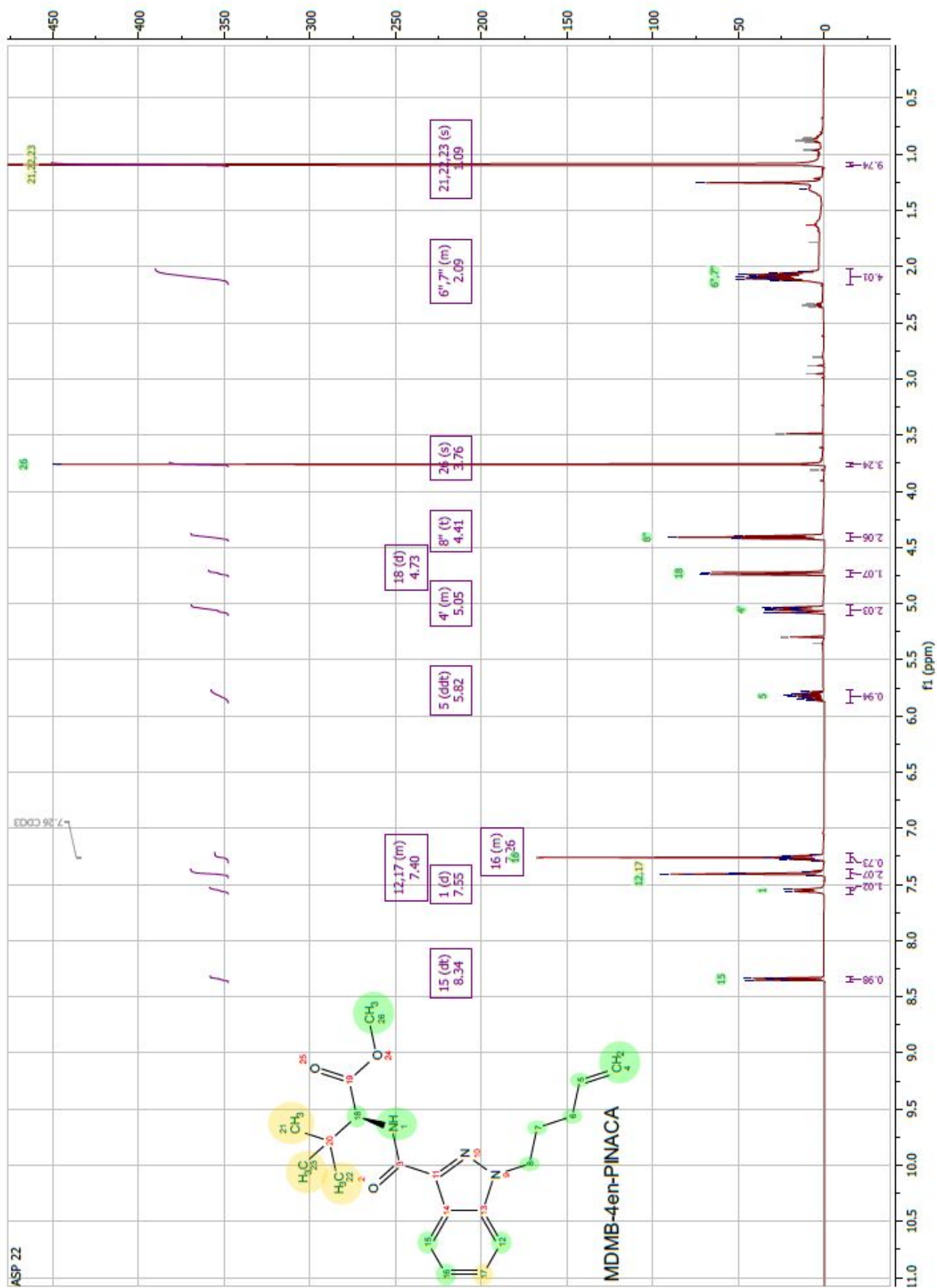


Figure S28. Labelled ^1H NMR of ASP22 in CDCl_3 .

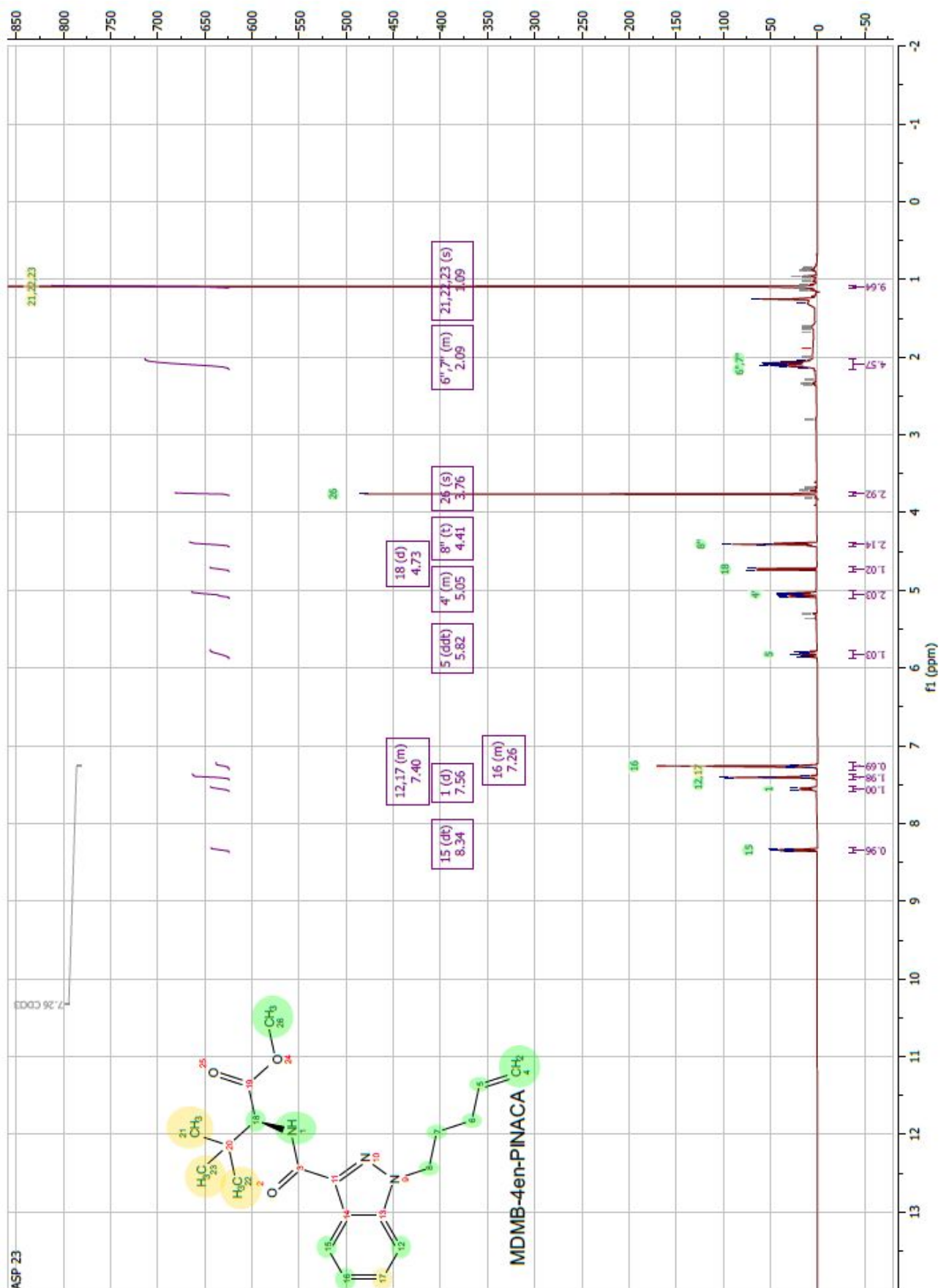


Figure S29. Labelled ¹H NMR of ASP23 in CDCl₃.

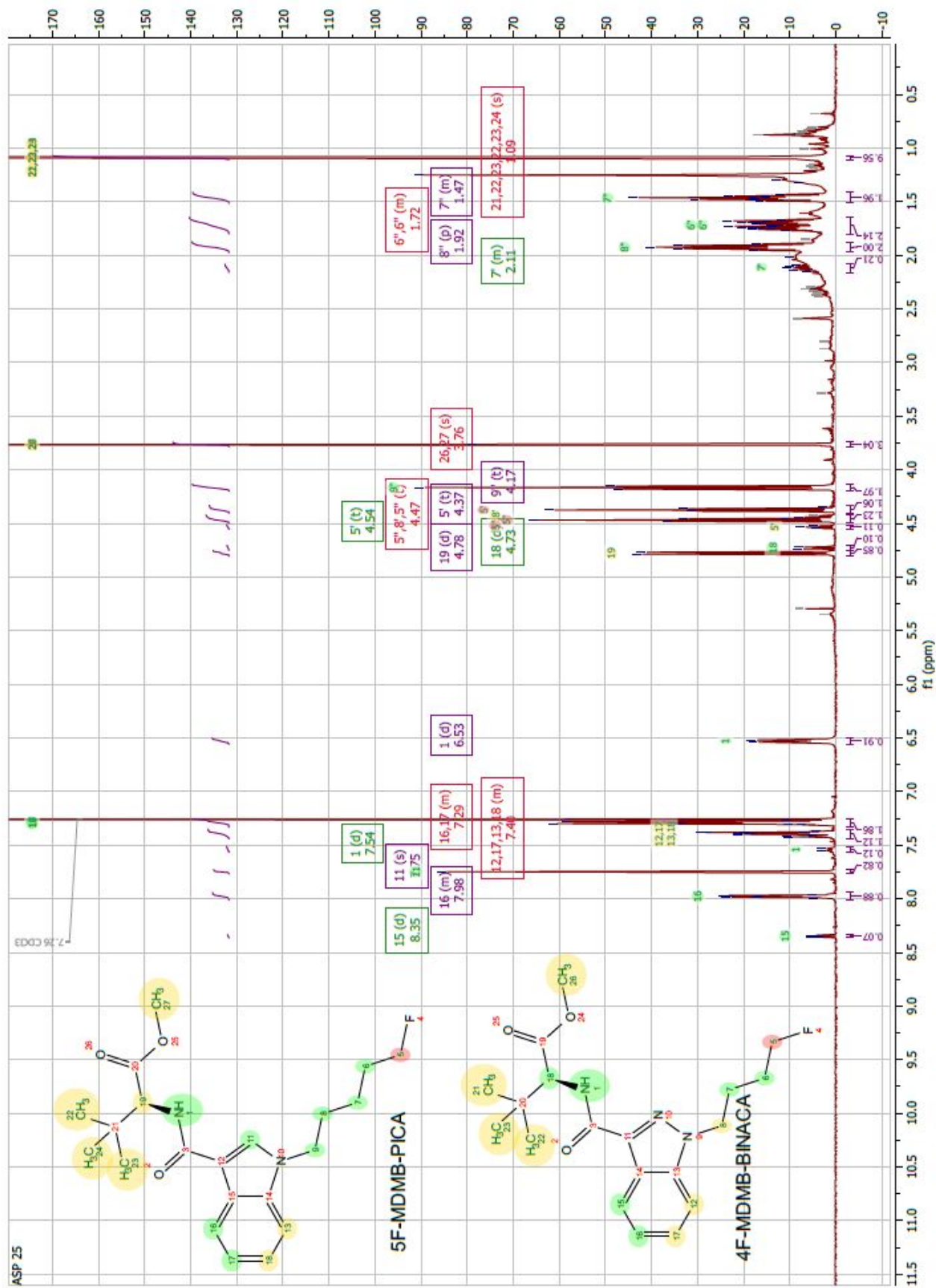


Figure S31. Labelled ¹H NMR of ASP25 in CDCl₃.

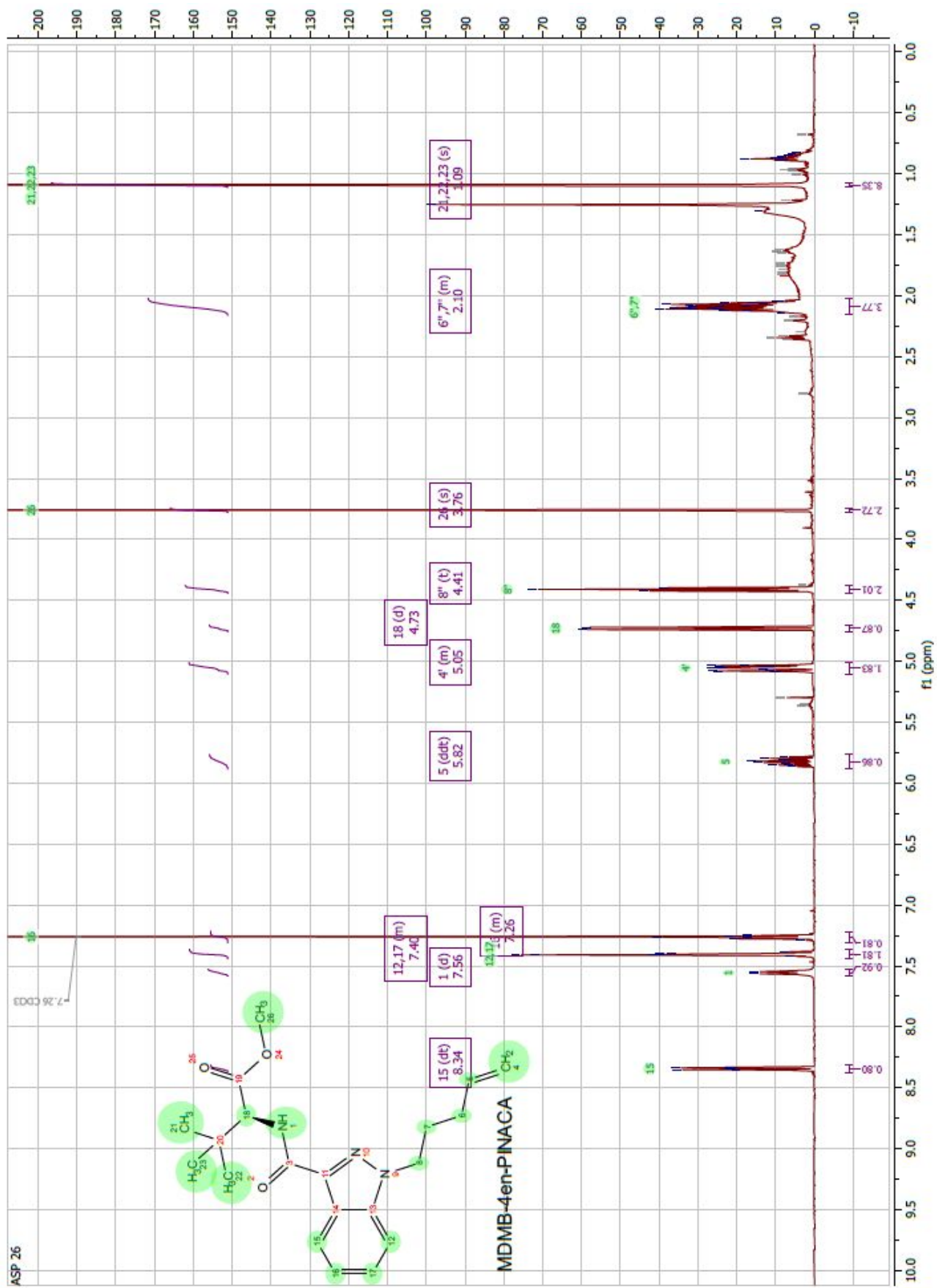
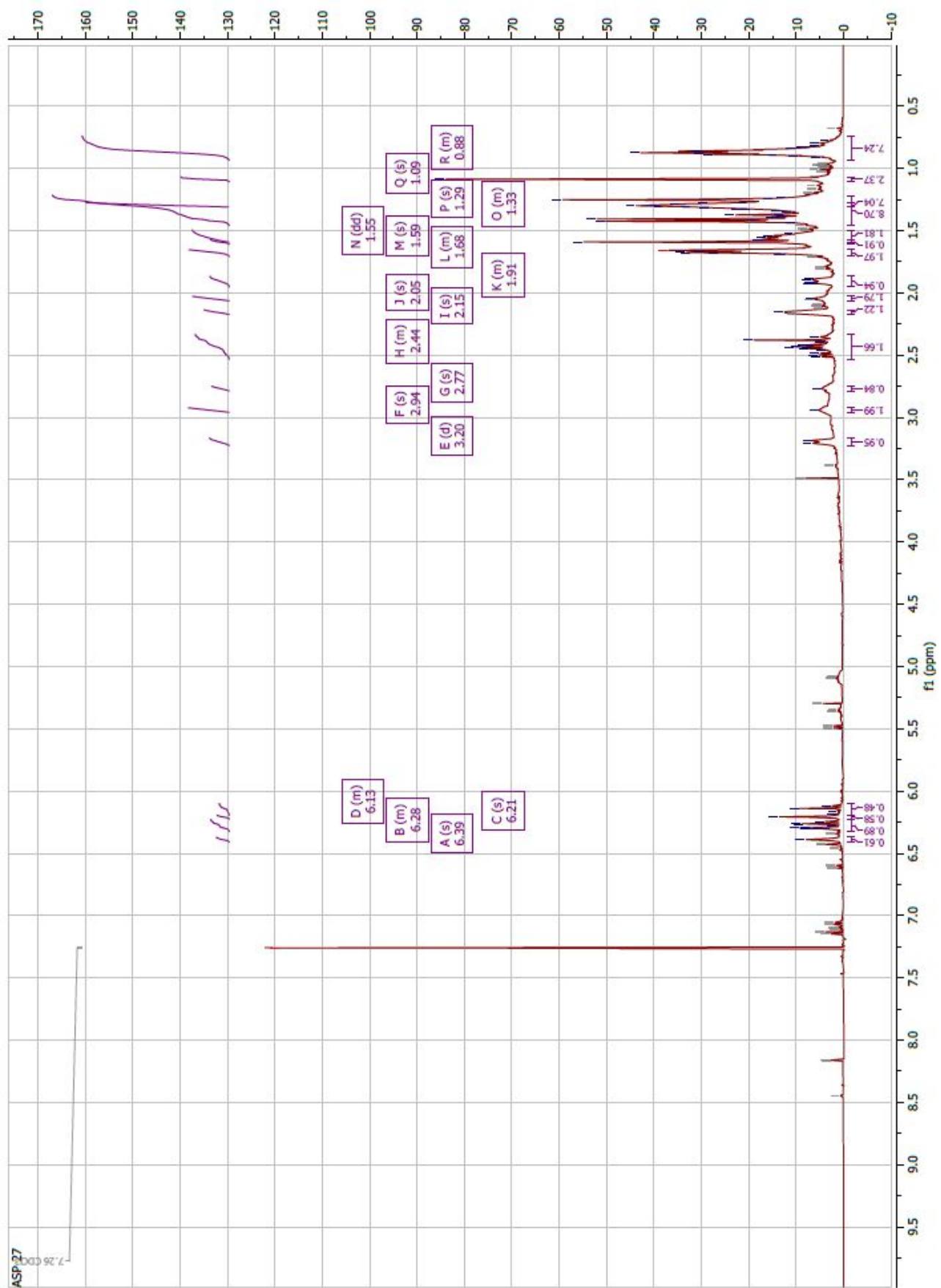


Figure S32. Labelled ¹H NMR of ASP26 in CDCl₃.



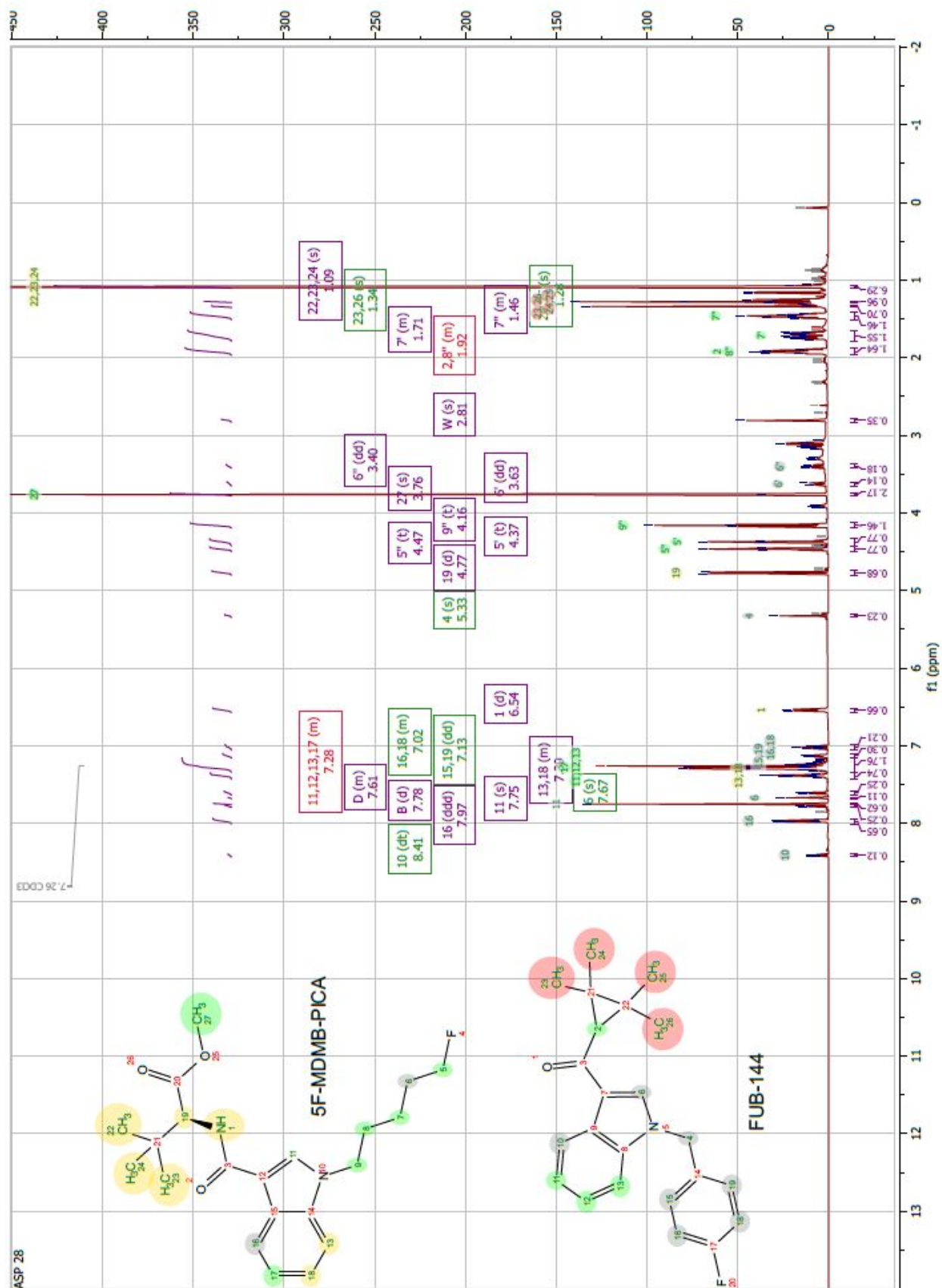


Figure S34. Labelled ¹H NMR of ASP28 in CDCl₃.

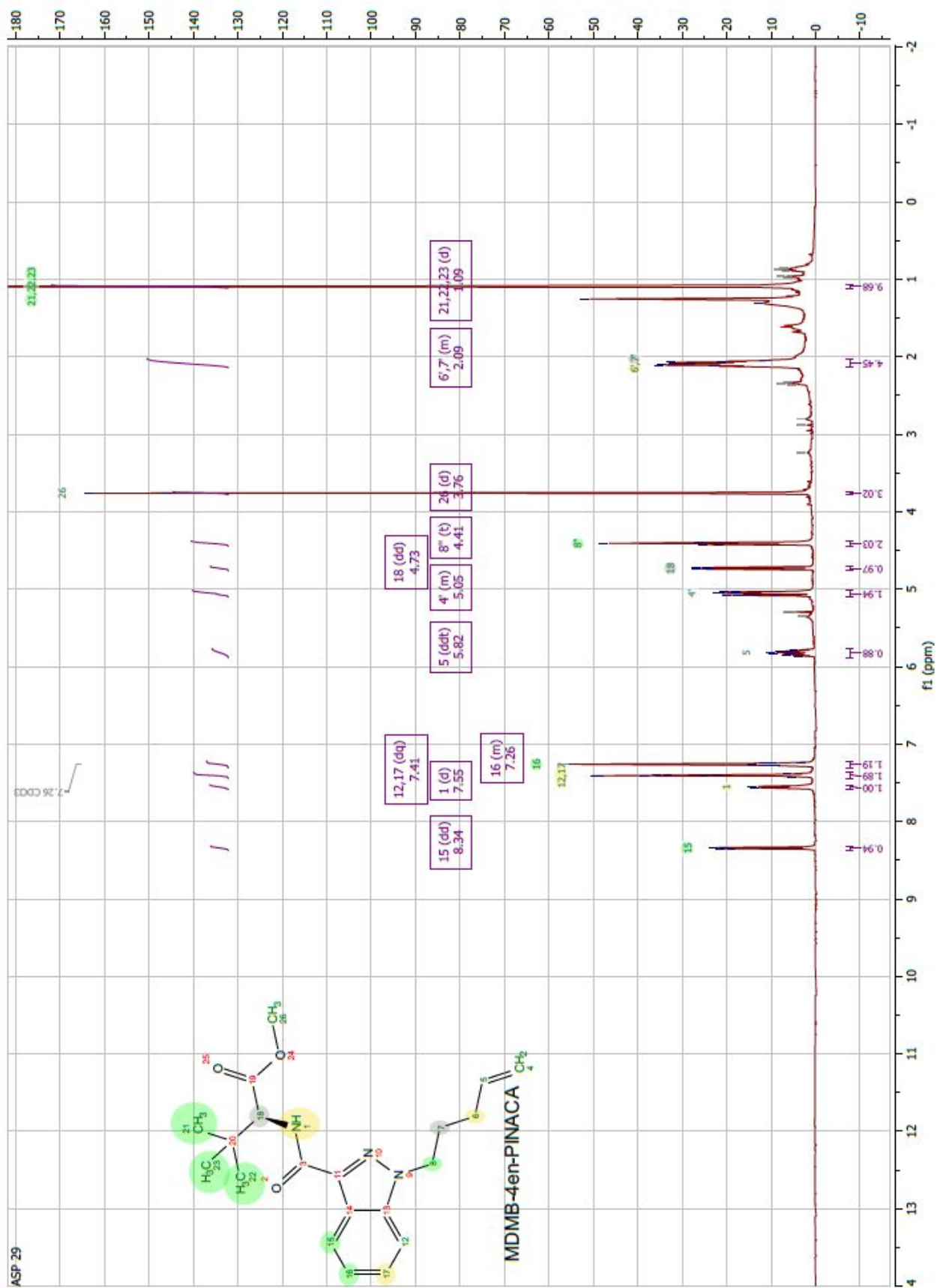


Figure S35. Labelled ^1H NMR of ASP29 in CDCl_3 .

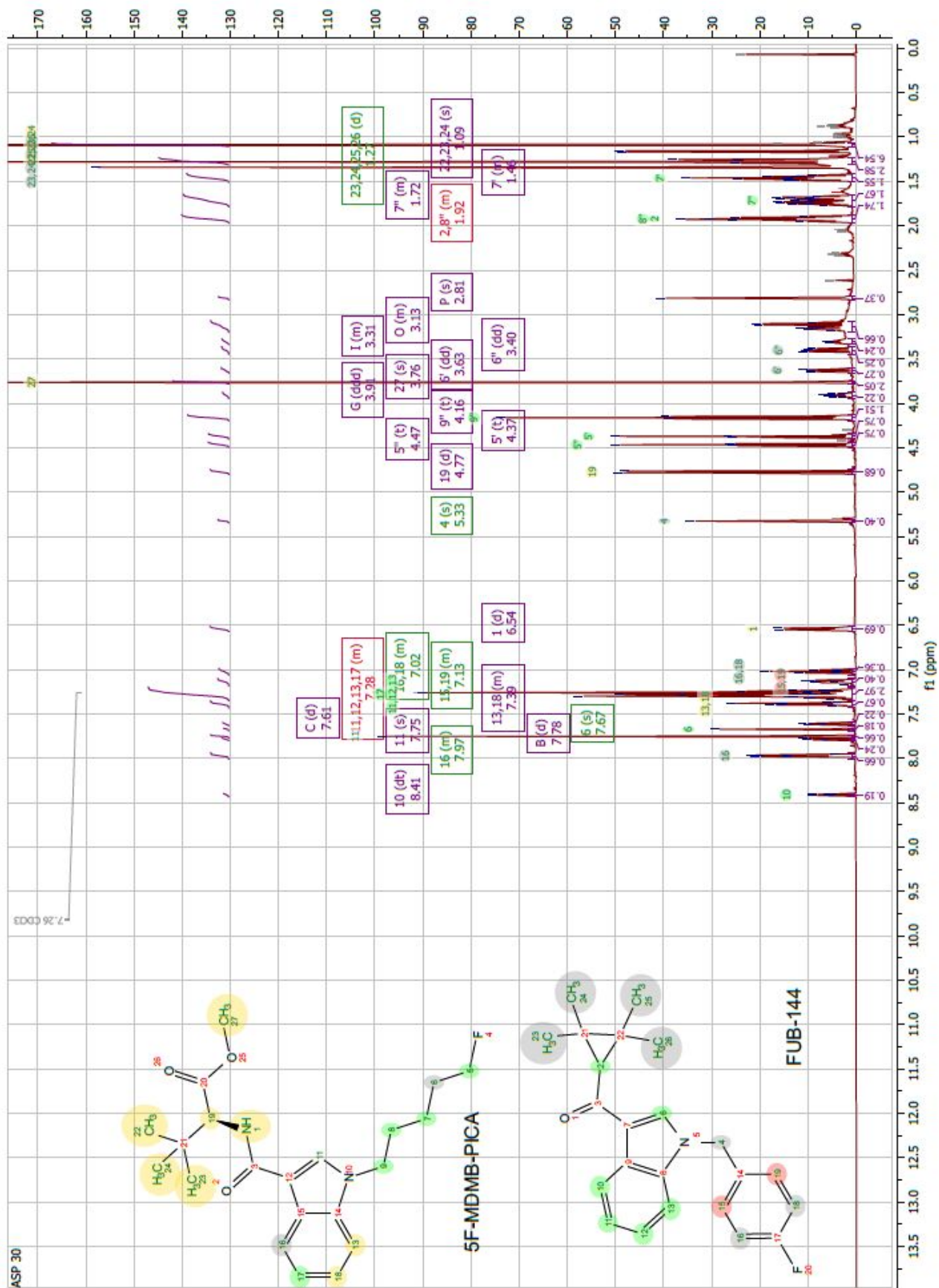


Figure S36. Labelled ¹H NMR of ASP30 in CDCl₃.

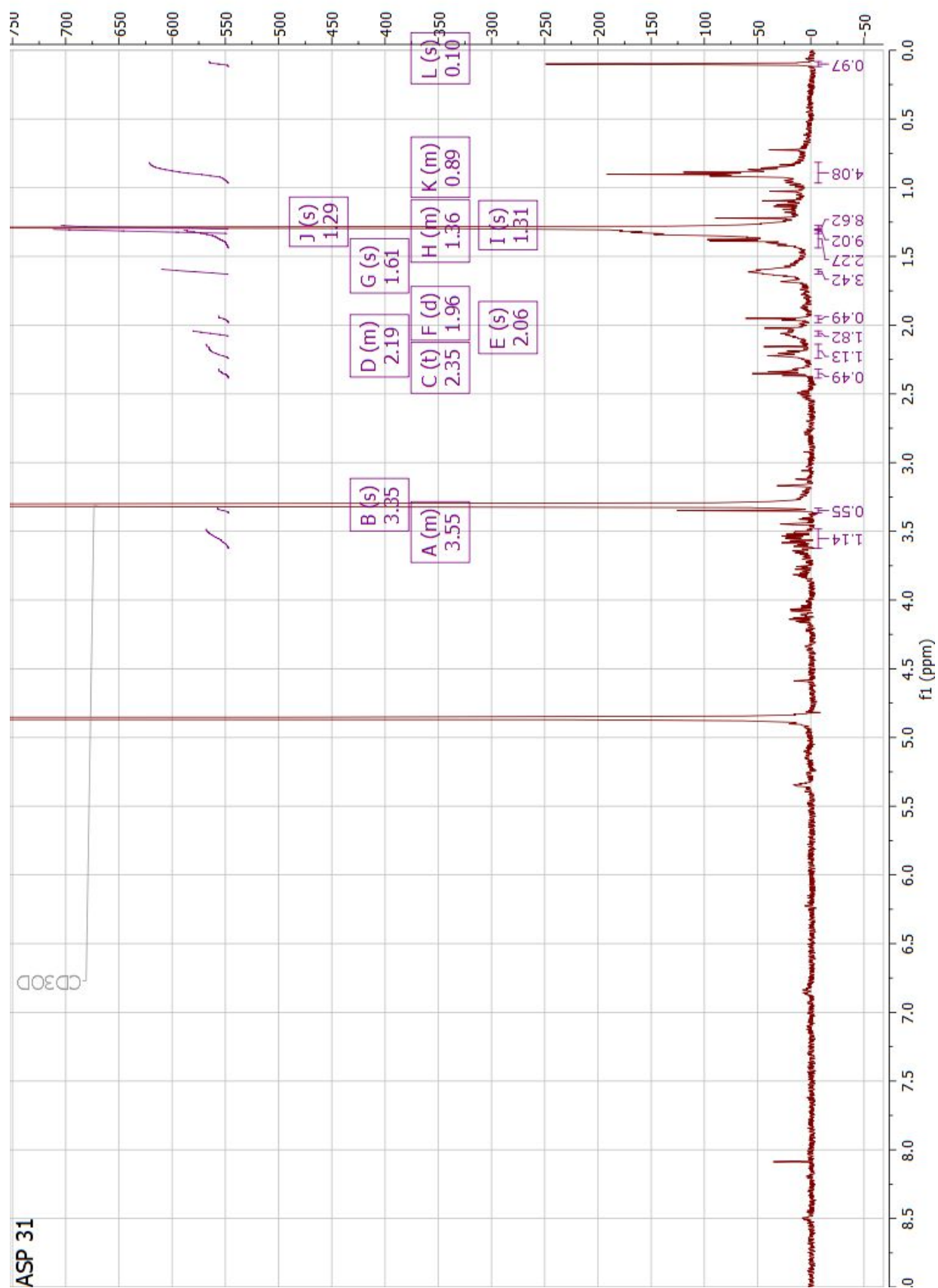


Figure S37. Labelled ¹H NMR of ASP31 in CD₃OD.

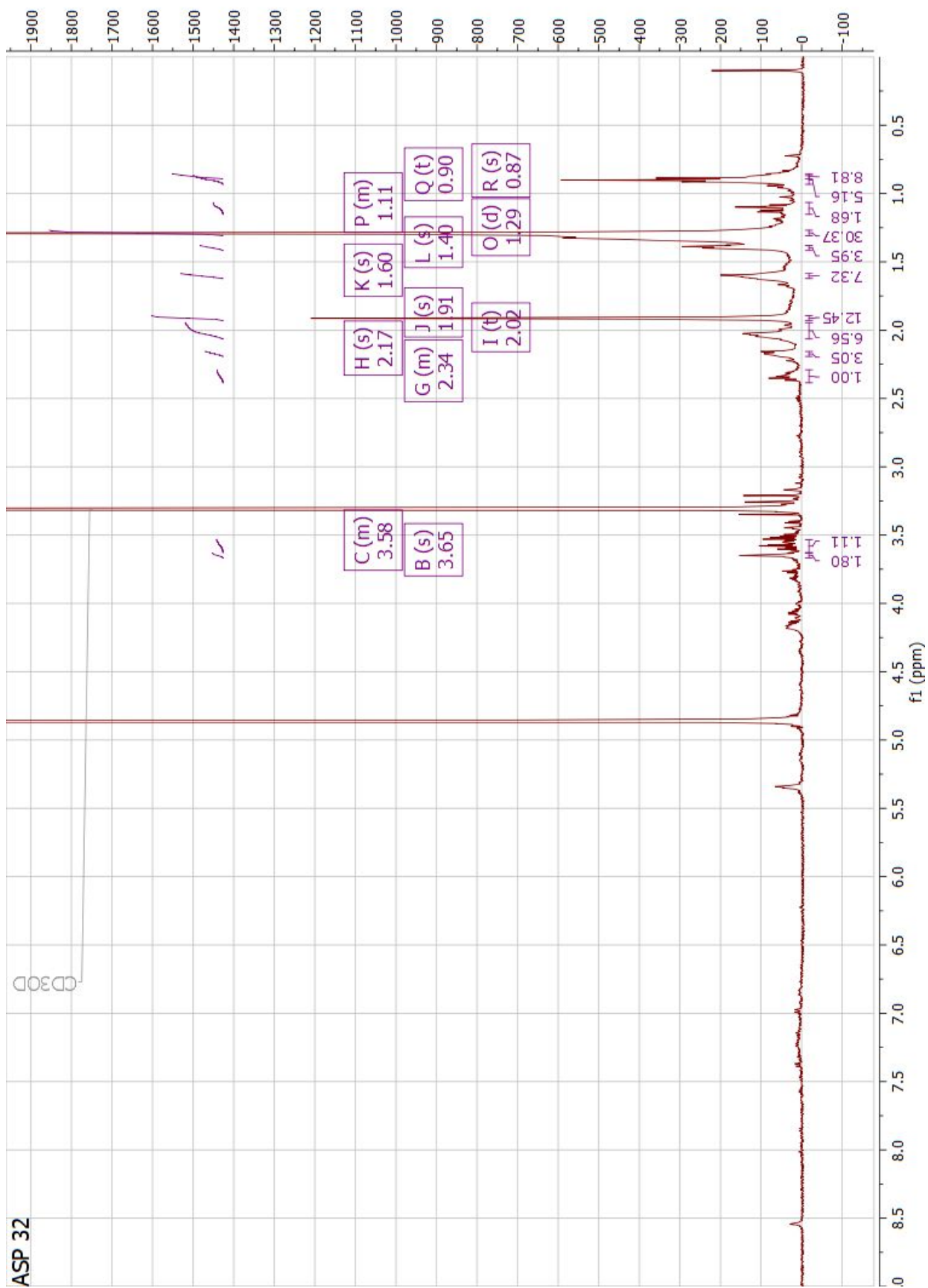


Figure S38. Labelled ^1H NMR of ASP32 in CD_3OD .

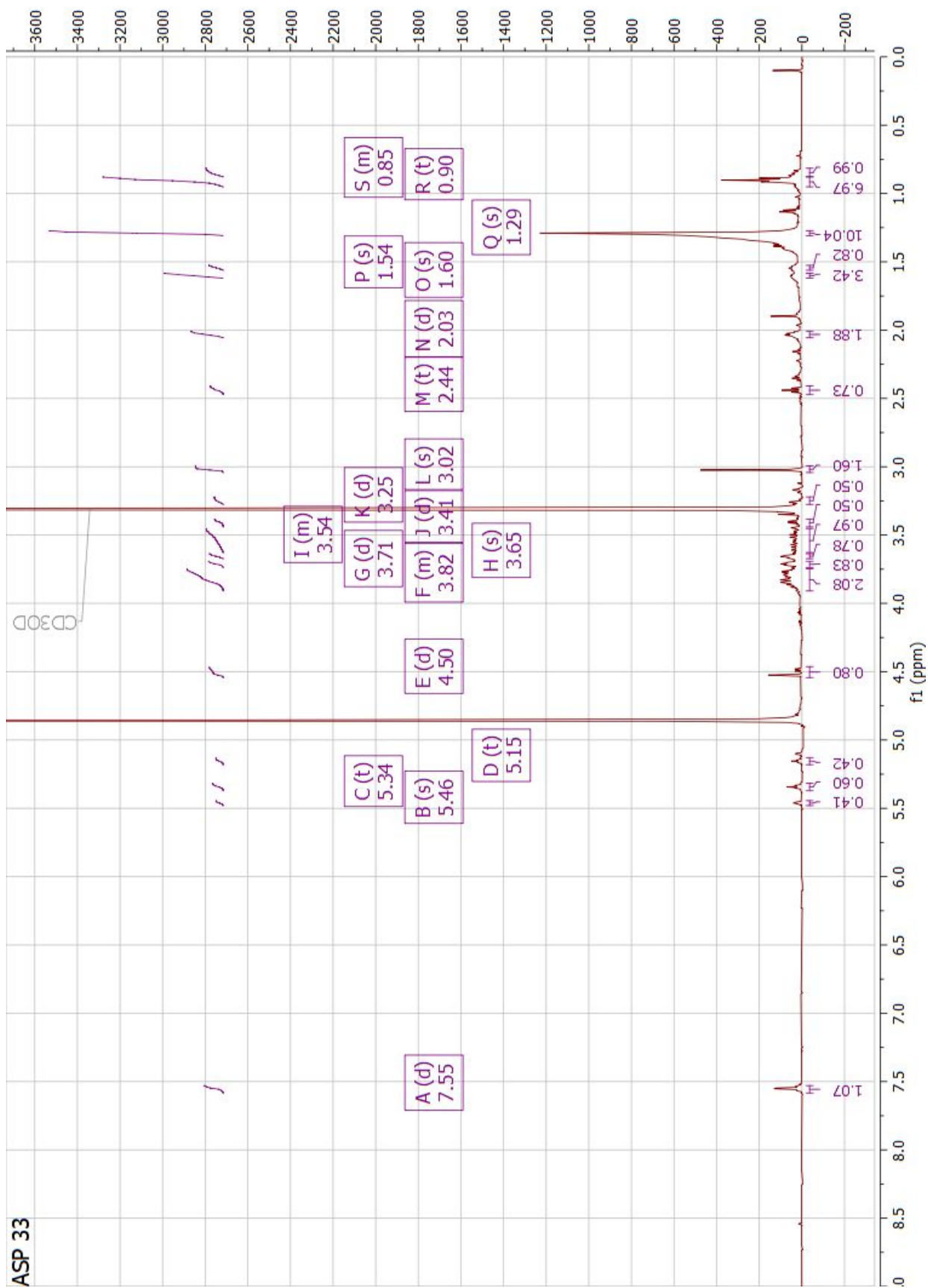


Figure S39. Labelled ¹H NMR of ASP33 in CD₃OD.

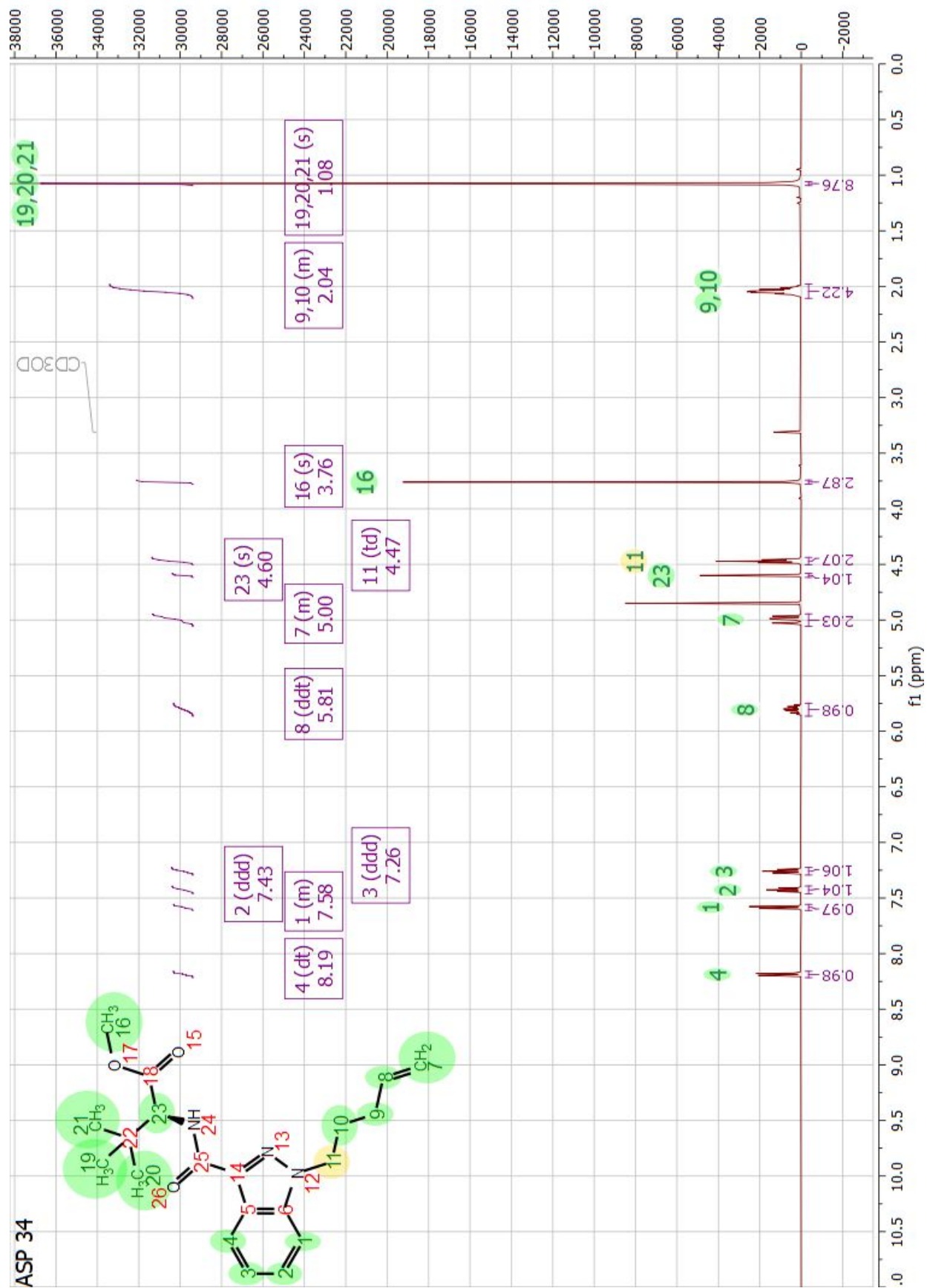


Figure S40. Labelled ¹H NMR of ASP34 in CD₃OD.

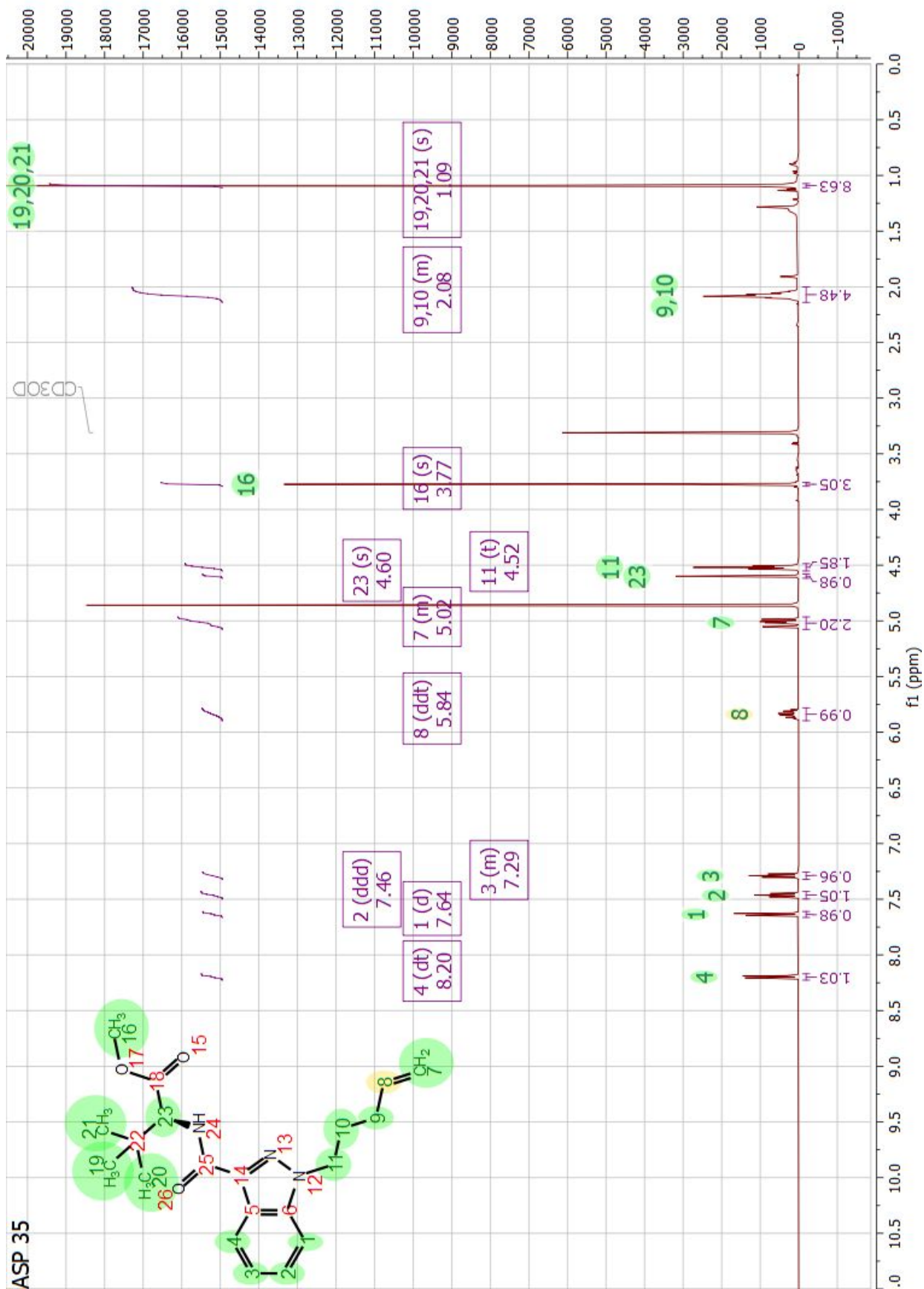


Figure S41. Labelled ^1H NMR of ASP35 in CD_3OD .

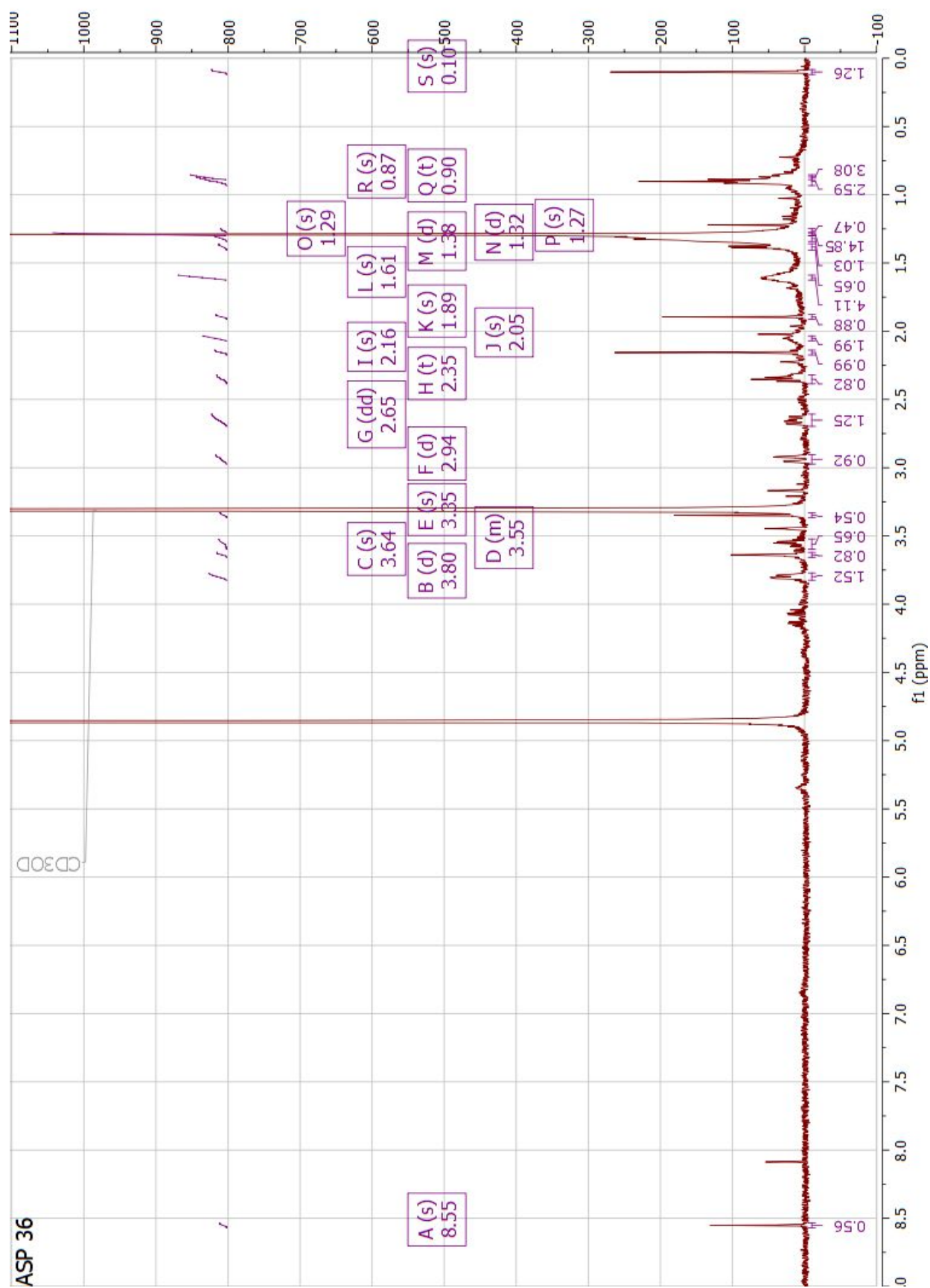


Figure S42. Labelled ^1H NMR of ASP36 in CD_3OD .

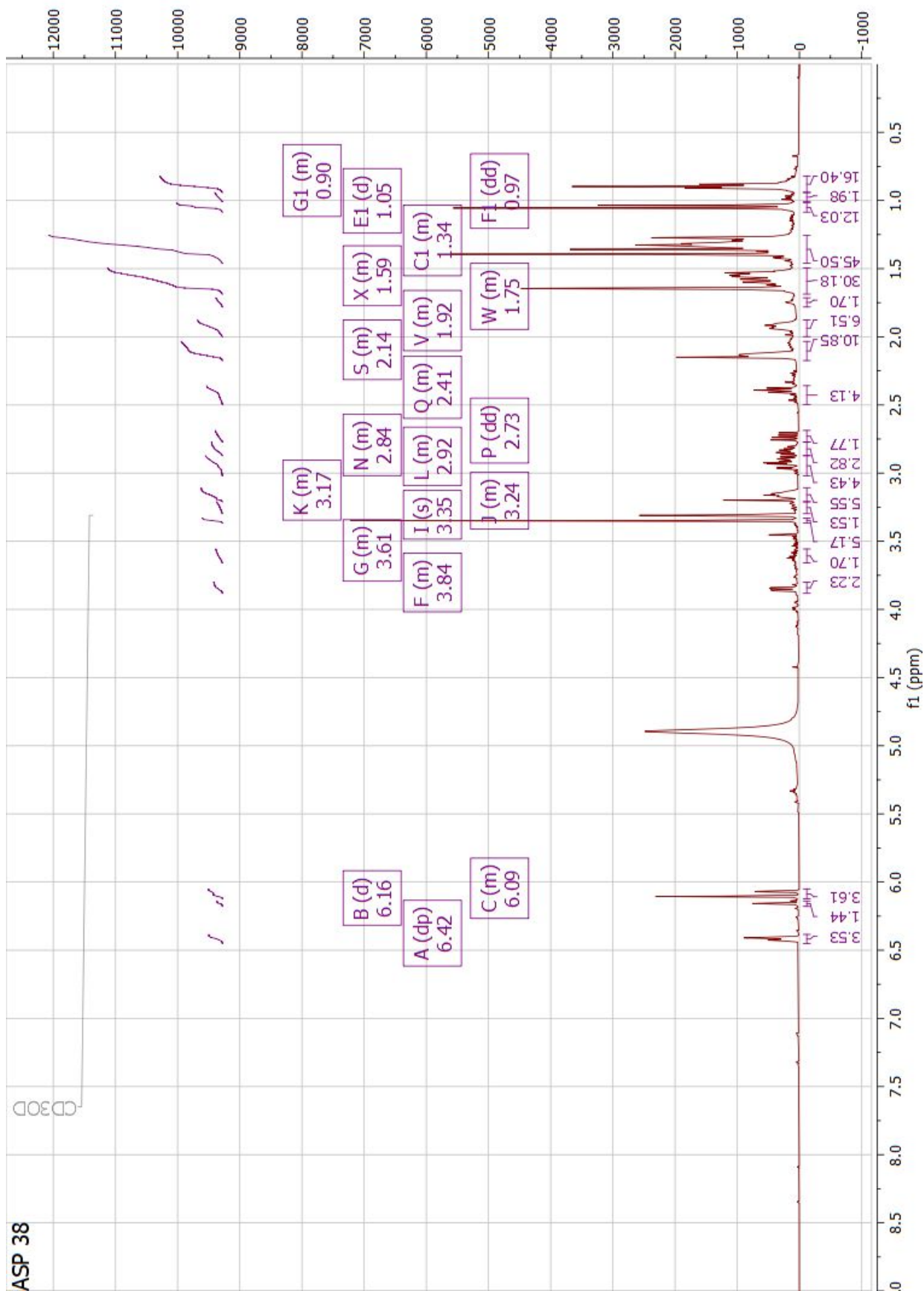


Figure S43. Labelled ^1H NMR of ASP38 in CD_3OD .

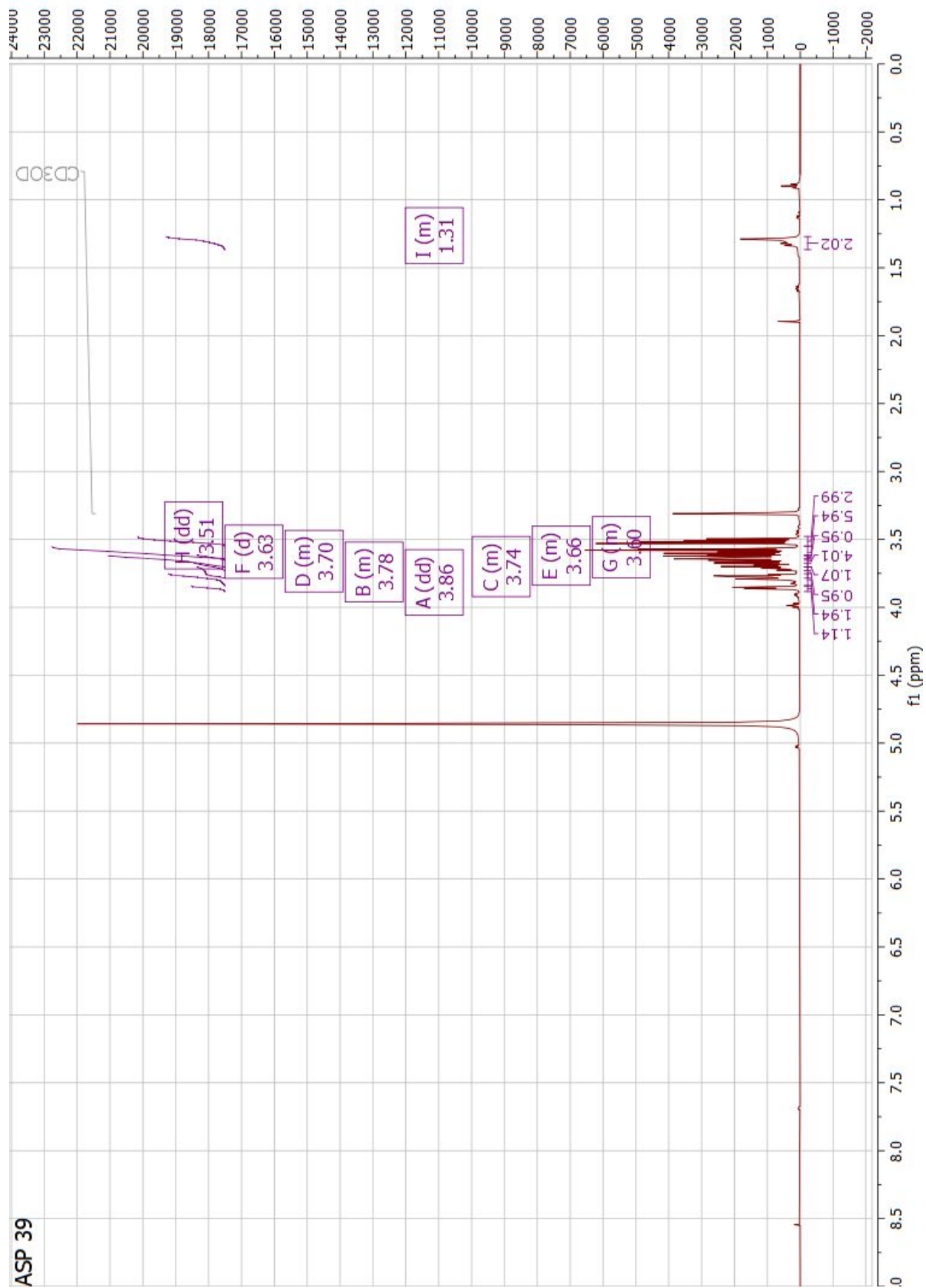


Figure S44. Labelled ^1H NMR of ASP39 in CD_3OD .

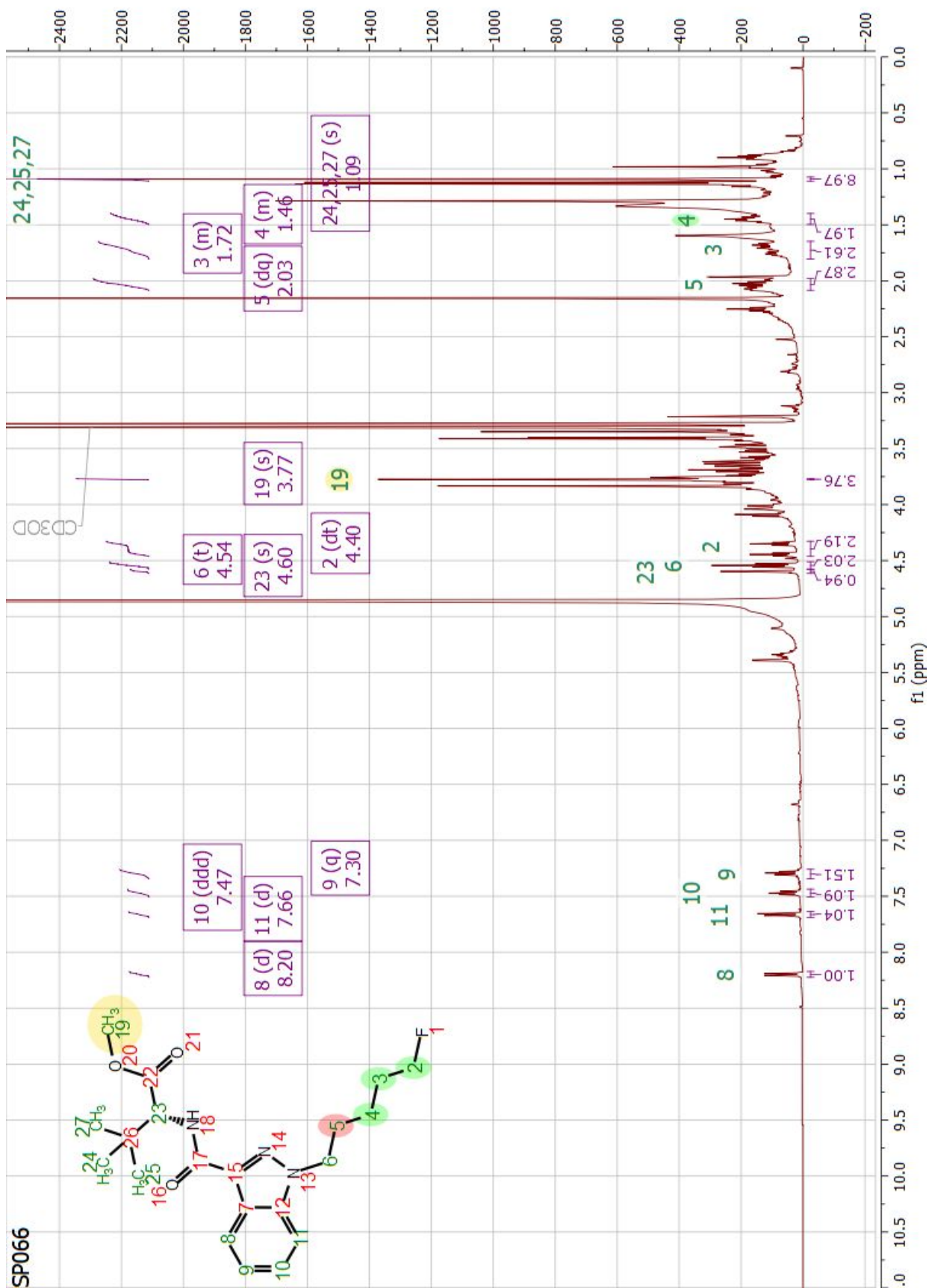


Figure S45. Labelled ¹H NMR of SP066 in CD₃OD.

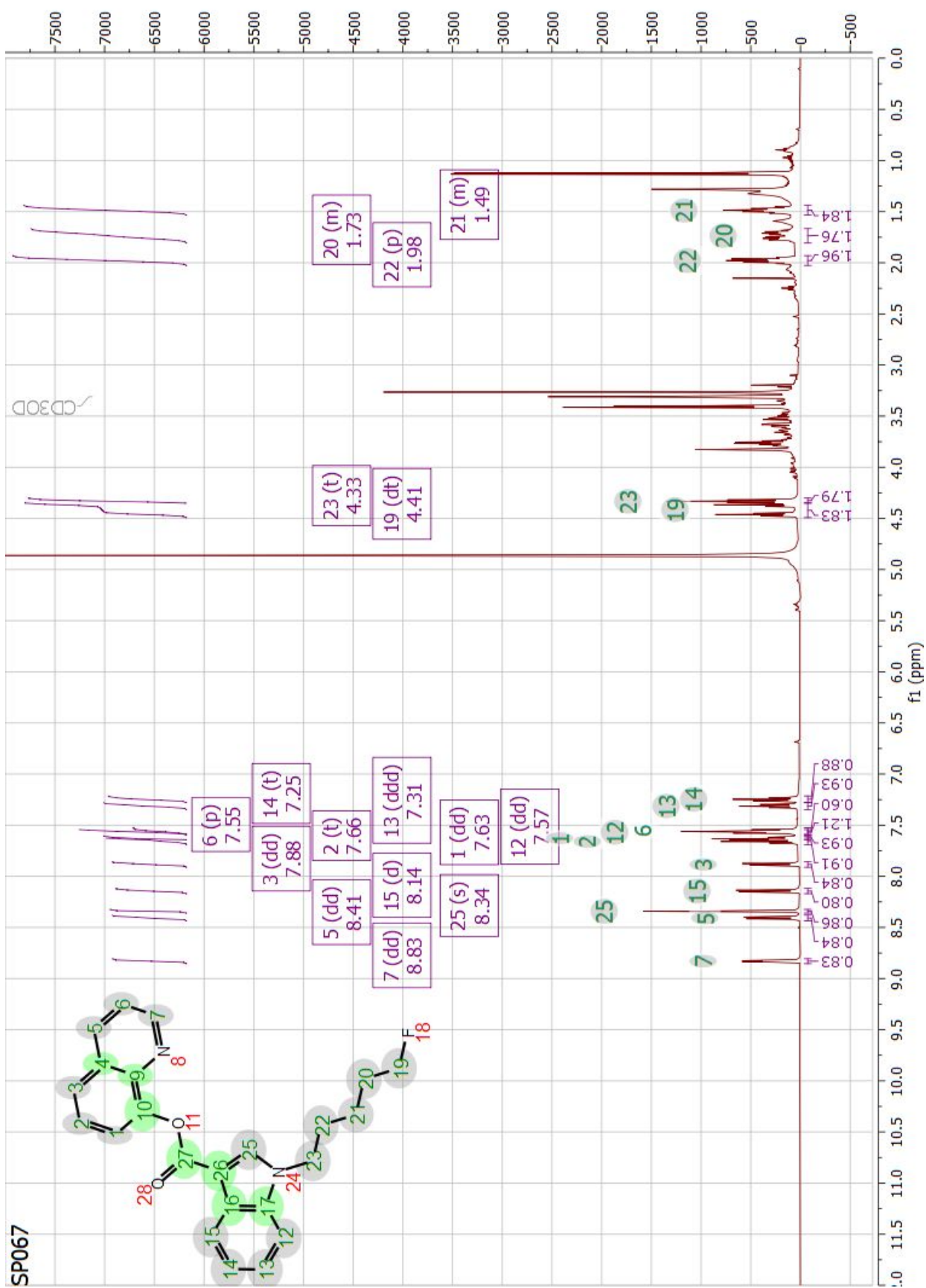


Figure S46. Labelled ¹H NMR of SP067 in CD₃OD.

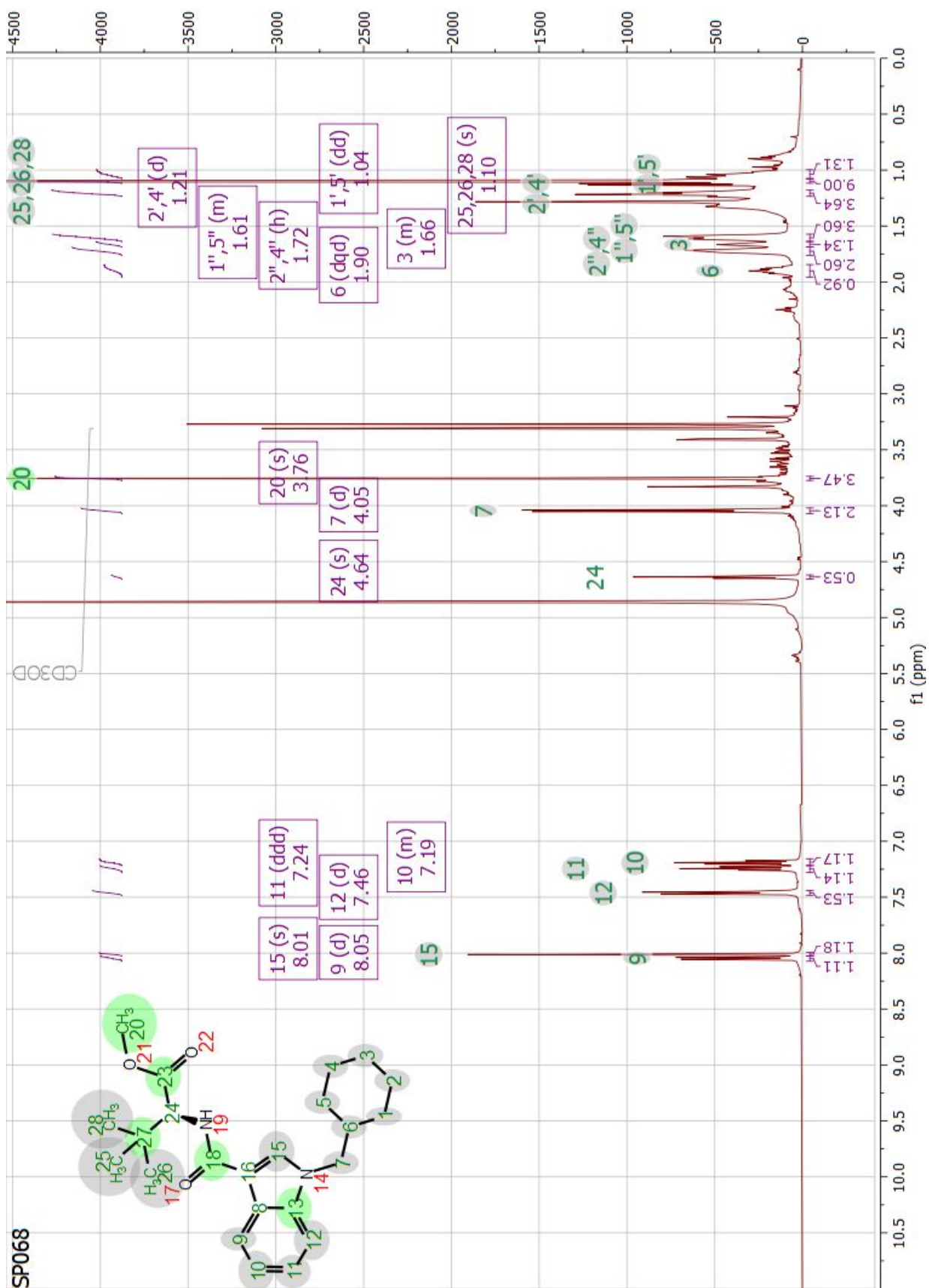


Figure S47. Labelled ¹H NMR of SP068 in CD₃OD.

ASP2: 5F-MDMB-PINACA

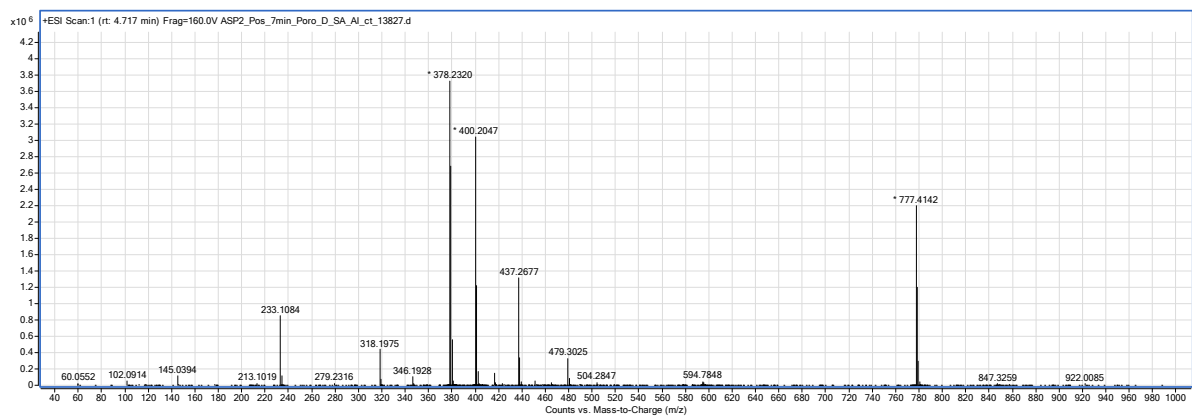
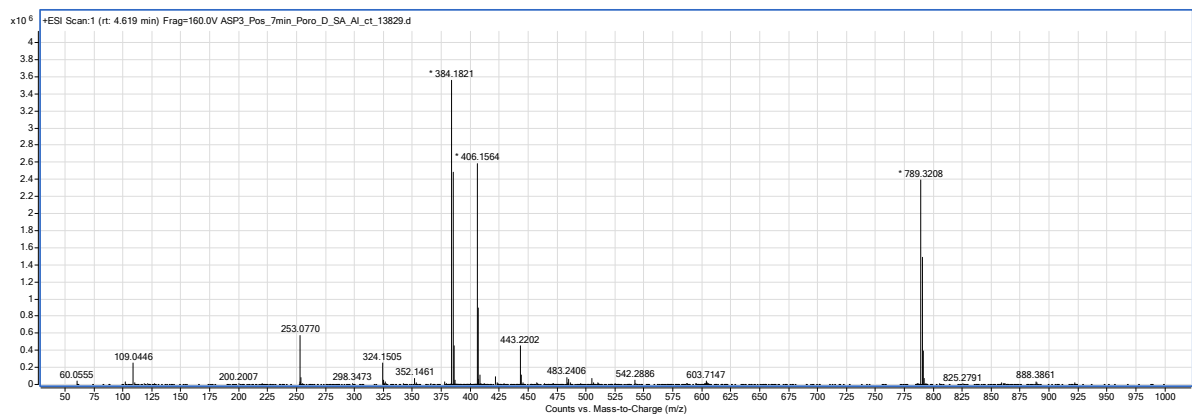


Figure S48. Extracted Mass Spectra from LC-MS Analysis for ASP2.

ASP3: AMB-FUBINACA



5F-MDMB-PINACA

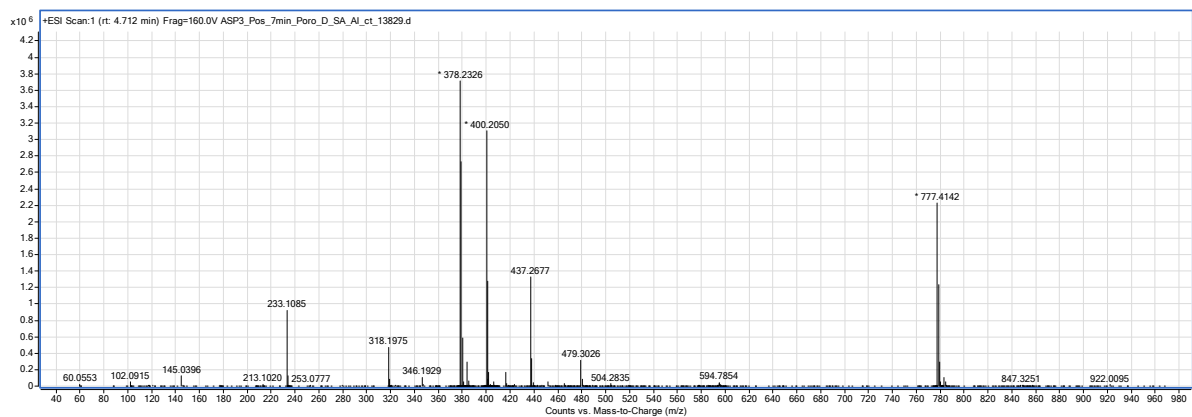


Figure S49. Extracted Mass Spectra from LC-MS Analysis for ASP3.

ASP4: MDMB-4en-PINACA

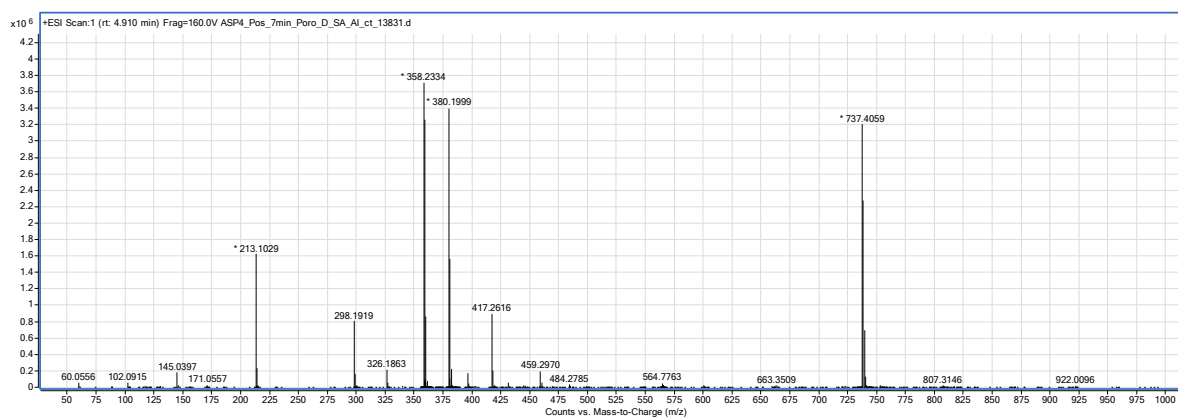


Figure S50. Extracted Mass Spectra from LC-MS Analysis for ASP4.

ASP5: 5F-MDMB-PICA

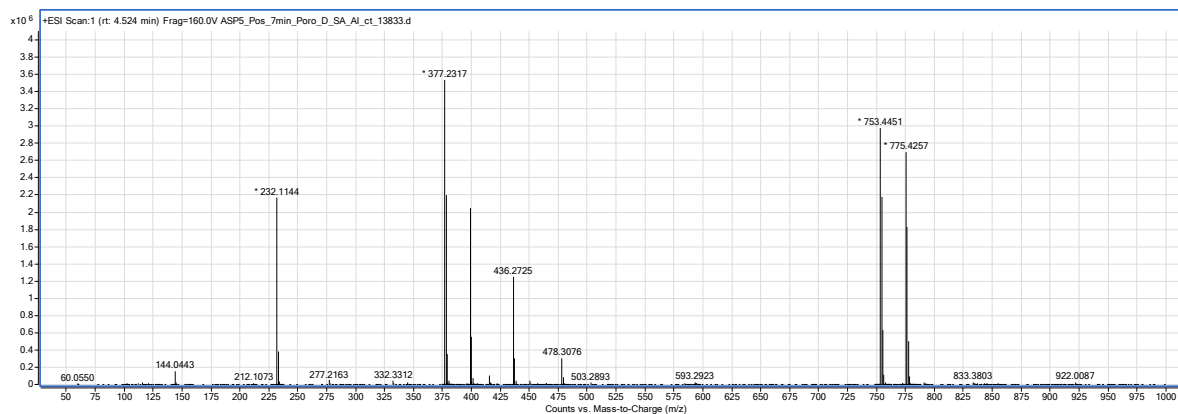


Figure S51. Extracted Mass Spectra from LC-MS Analysis for ASP5.

ASP6: MDMB-4en-PINACA

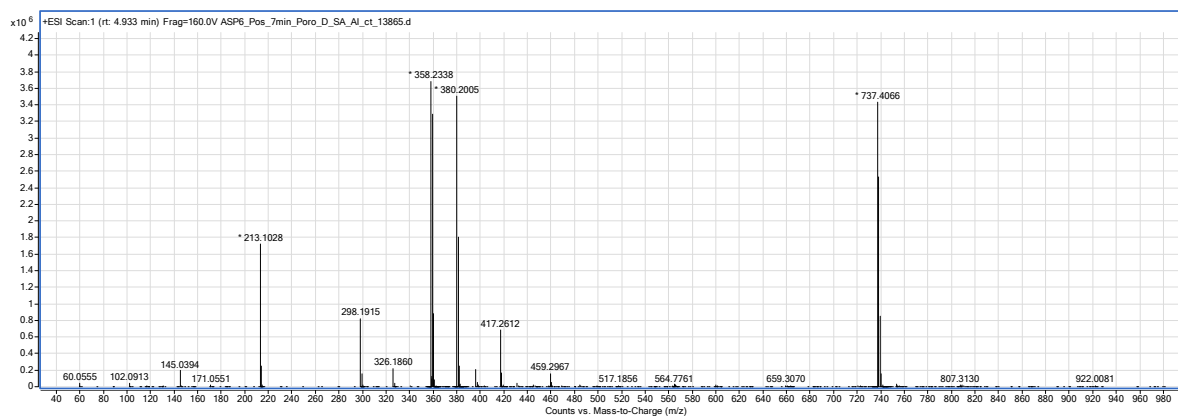


Figure S52. Extracted Mass Spectra from LC-MS Analysis for ASP6.

ASP8: 4F-MDMB-BINACA

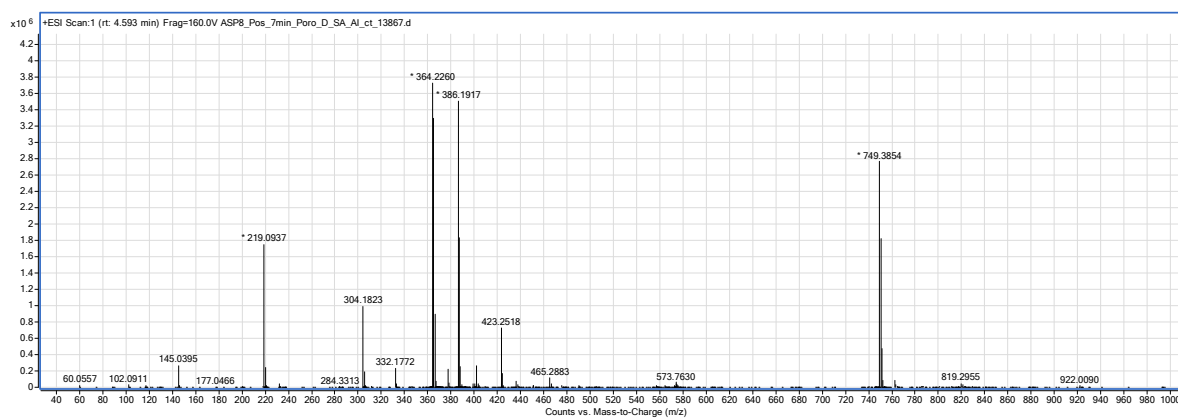


Figure S53. Extracted Mass Spectra from LC-MS Analysis for ASP8.

ASP11: MDMB-4en-PINACA

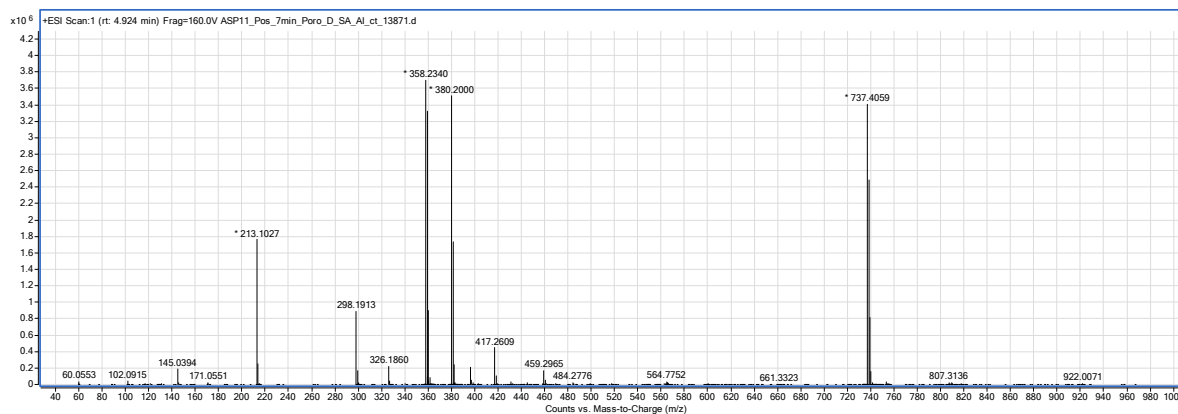


Figure S54. Extracted Mass Spectra from LC-MS Analysis for ASP11.

ASP12: MDMB-4en-PINACA

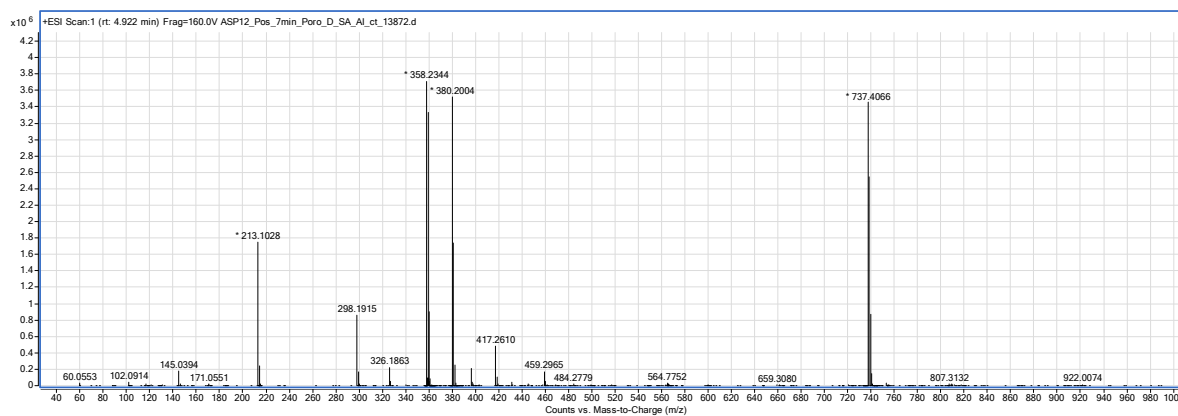


Figure S55. Extracted Mass Spectra from LC-MS Analysis for ASP12.

ASP13: MDMB-4en-PINACA

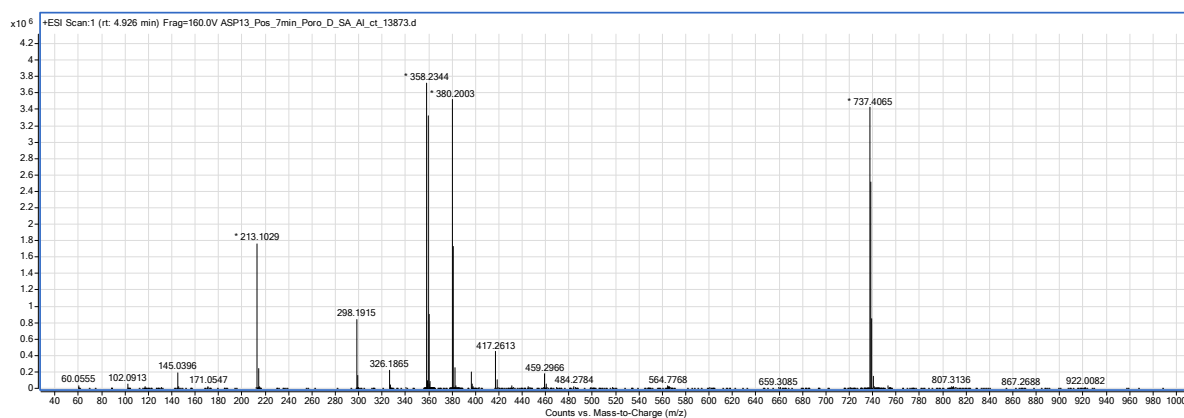


Figure S56. Extracted Mass Spectra from LC-MS Analysis for ASP13.

ASP14: 5F-MDMB-PINACA

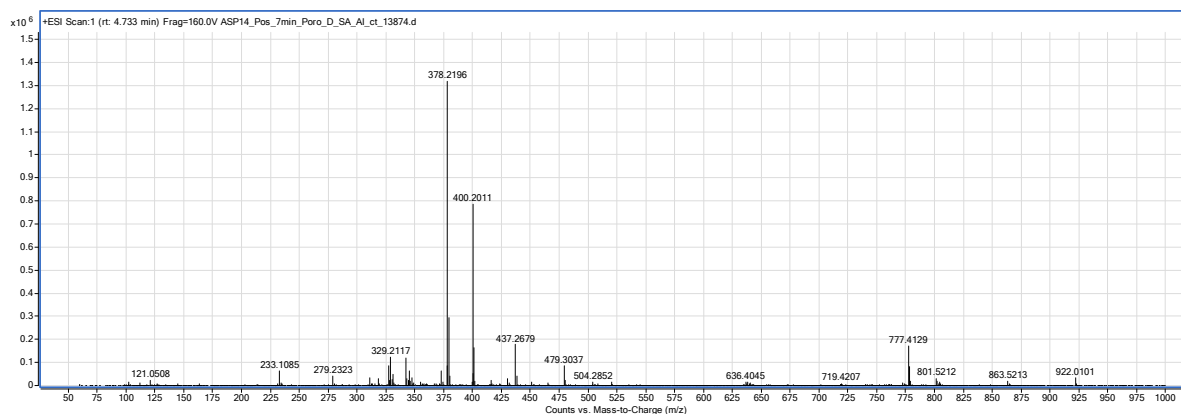


Figure S57. Extracted Mass Spectra from LC-MS Analysis for ASP14.

ASP15: 5F-MDMB-PINACA

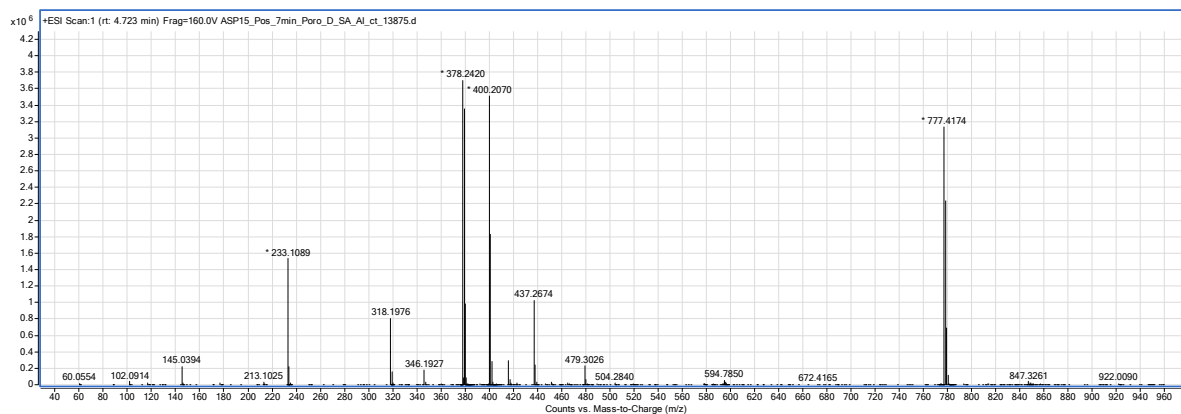


Figure S58. Extracted Mass Spectra from LC-MS Analysis for ASP15.

ASP16: 5F-MDMB-PINACA

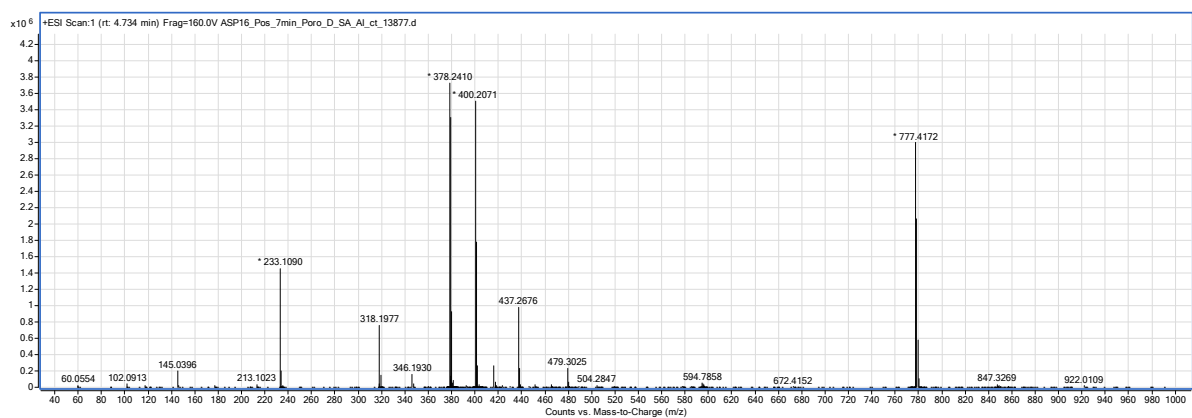


Figure S59. Extracted Mass Spectra from LC-MS Analysis for ASP16.

ASP17: 5F-MDMB-PINACA

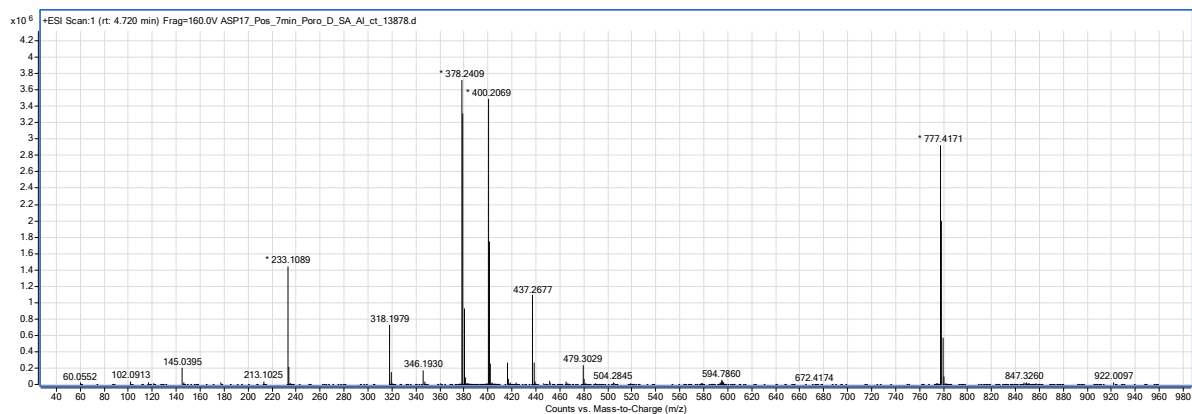
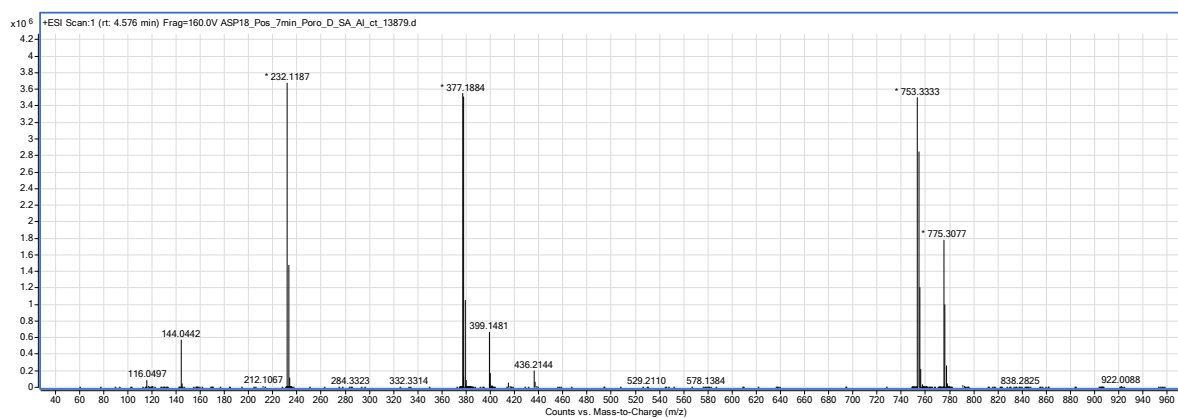


Figure S60. Extracted Mass Spectra from LC-MS Analysis for ASP17.

ASP18: 5F-PB-22



5F-AKB-48

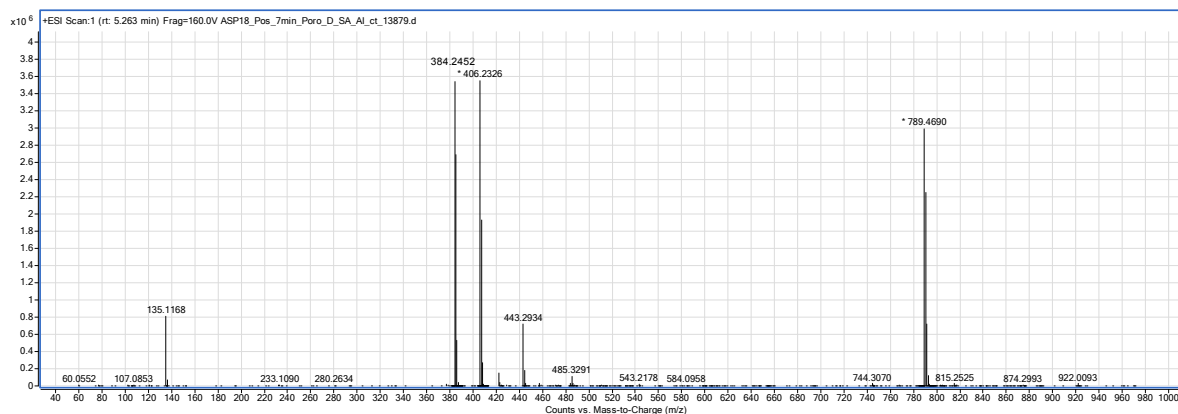
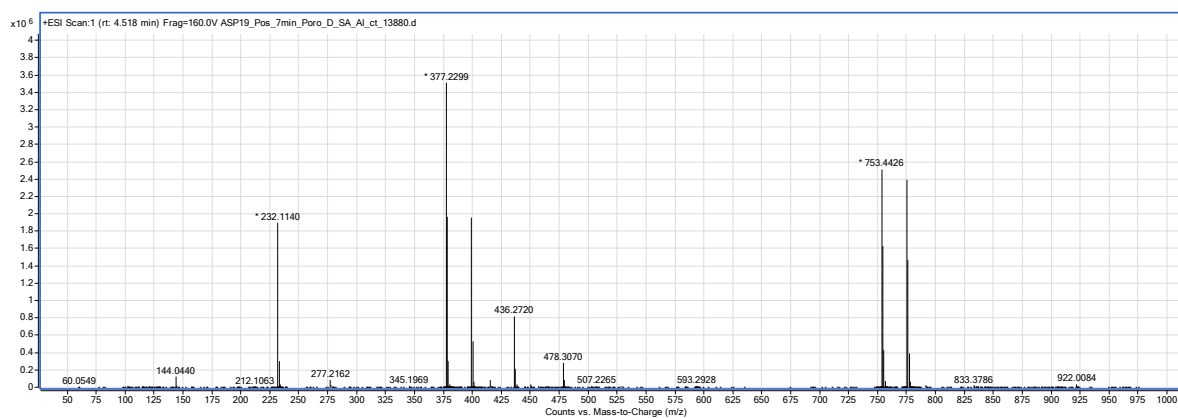
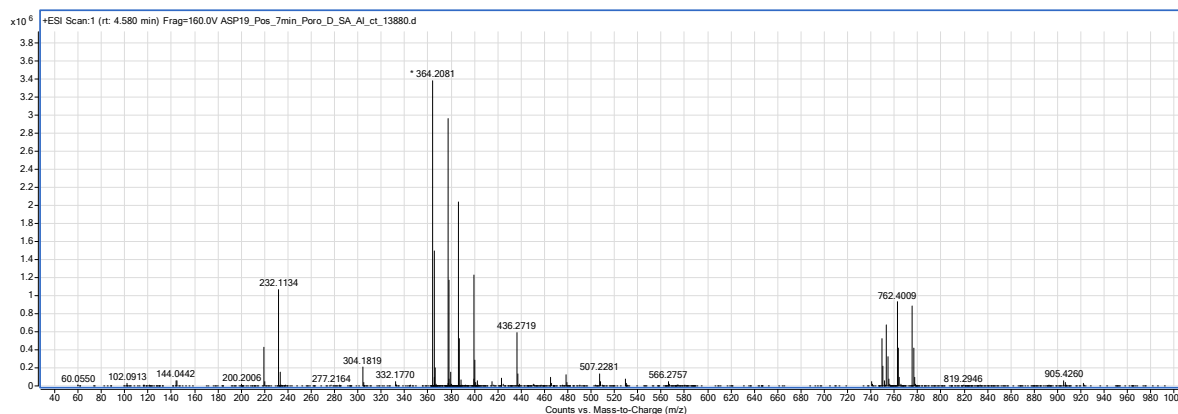


Figure S61. Extracted Mass Spectra from LC-MS Analysis for ASP18.

ASP19: 5F-MDMB-PICA



5F-AMB-PINACA



MDMB-4en-PINACA

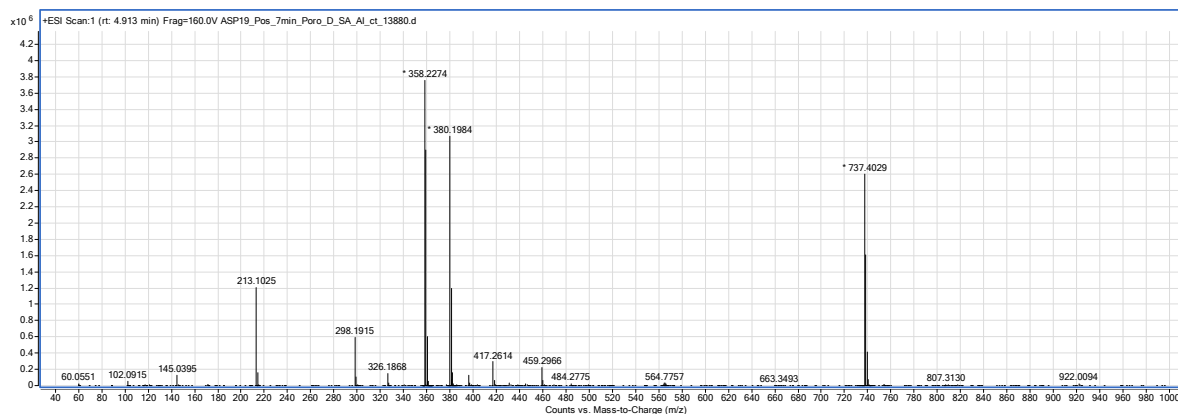


Figure S62. Extracted Mass Spectra from LC-MS Analysis for ASP19.

ASP22: MDMB-4en-PINACA

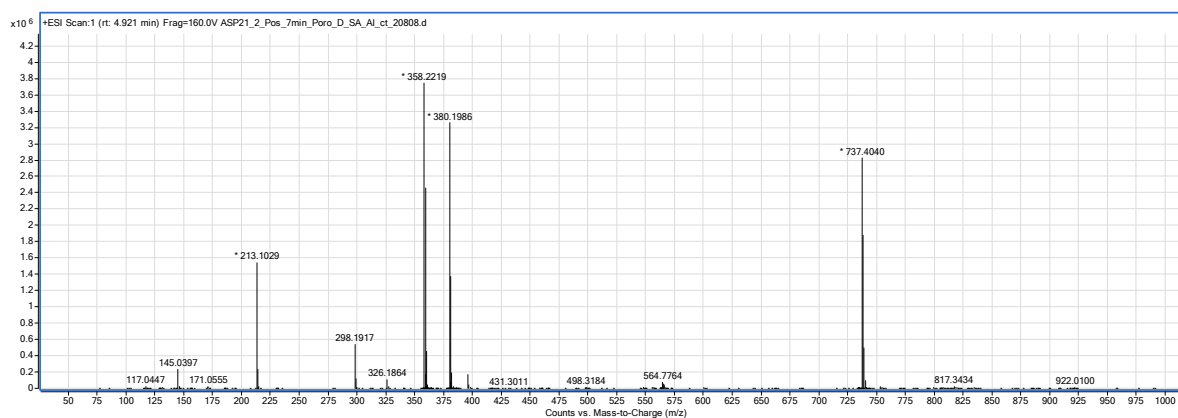


Figure S63. Extracted Mass Spectra from LC-MS Analysis for ASP22.

ASP23: MDMB-4en-PINACA

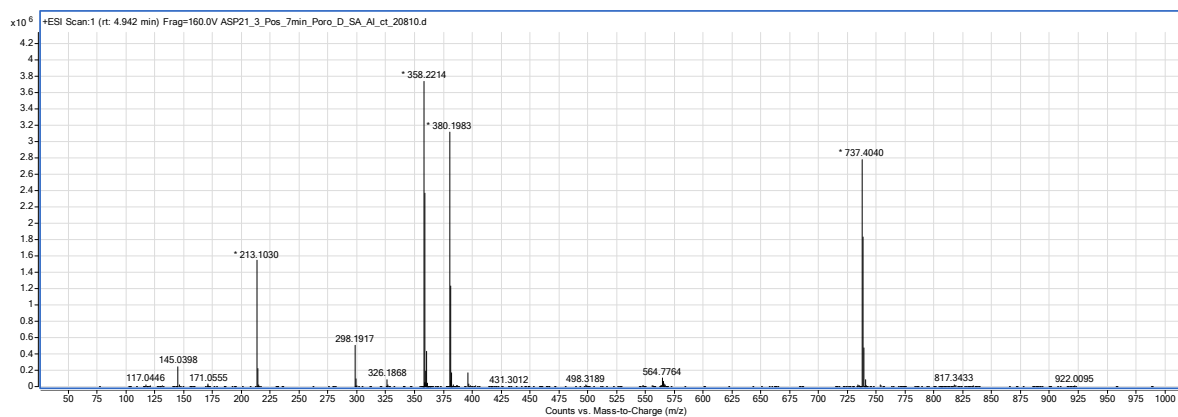


Figure S64. Extracted Mass Spectra from LC-MS Analysis for ASP23.

ASP24: MDMB-4en-PINACA

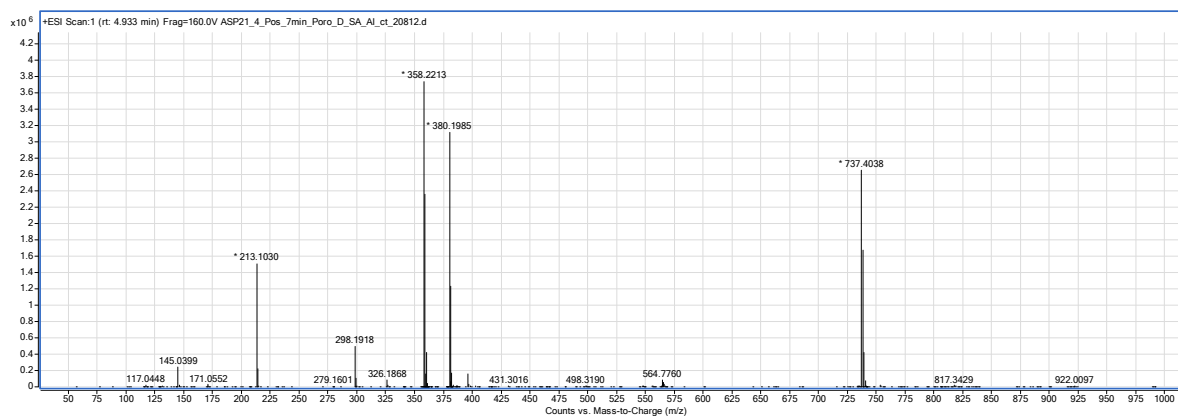
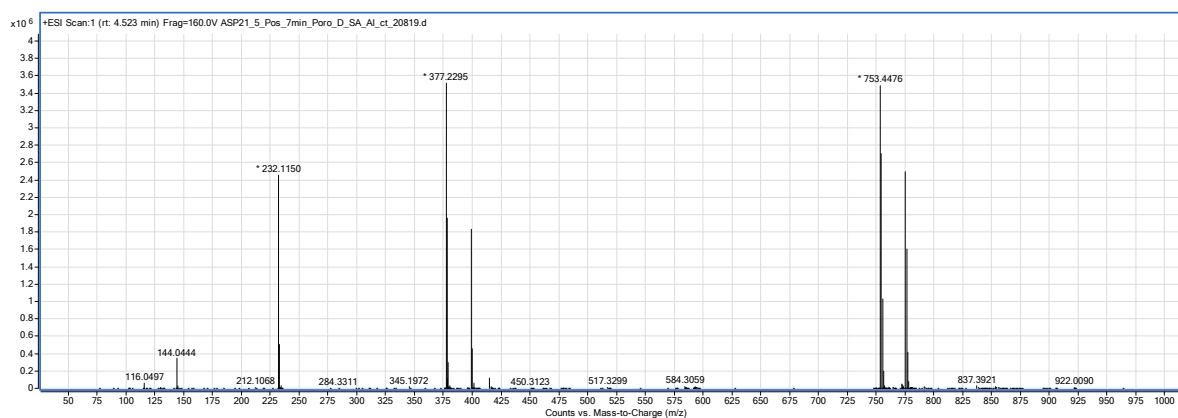


Figure S65. Extracted Mass Spectra from LC-MS Analysis for ASP24.

ASP25: 5F-MDMB-PICA



4F-MDMB-BINACA

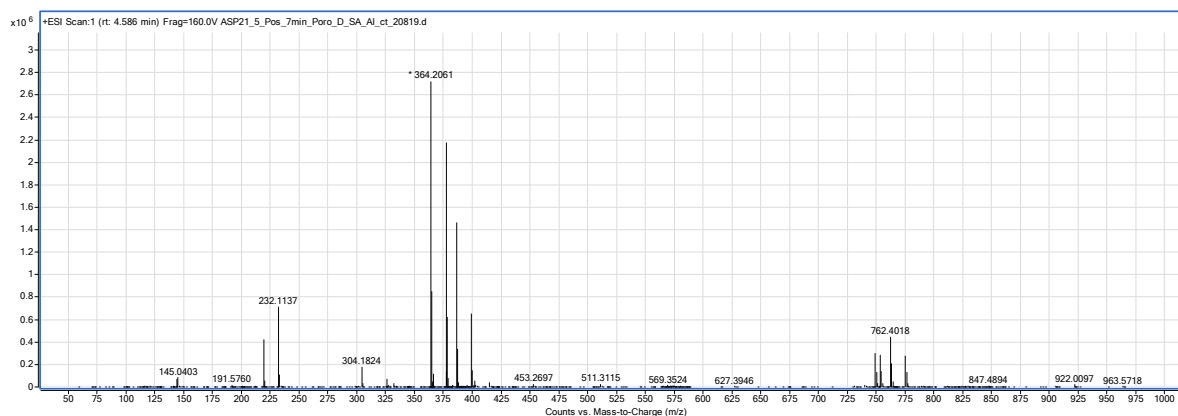


Figure S66. Extracted Mass Spectra from LC-MS Analysis for ASP25.

ASP26: MDMB-4en-PINACA

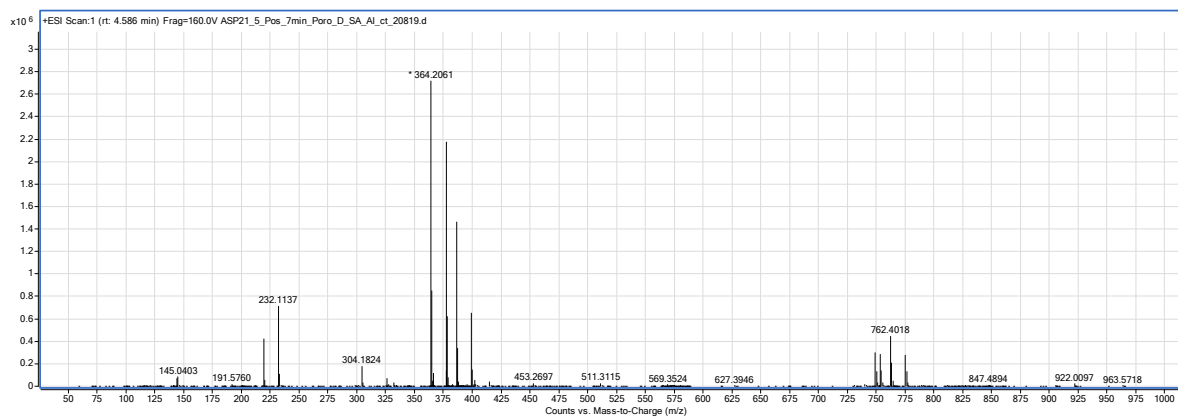
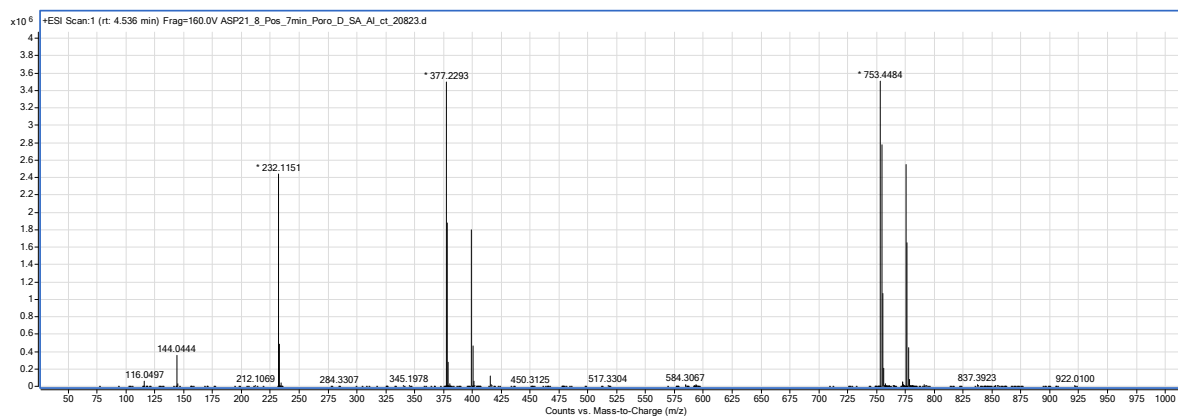
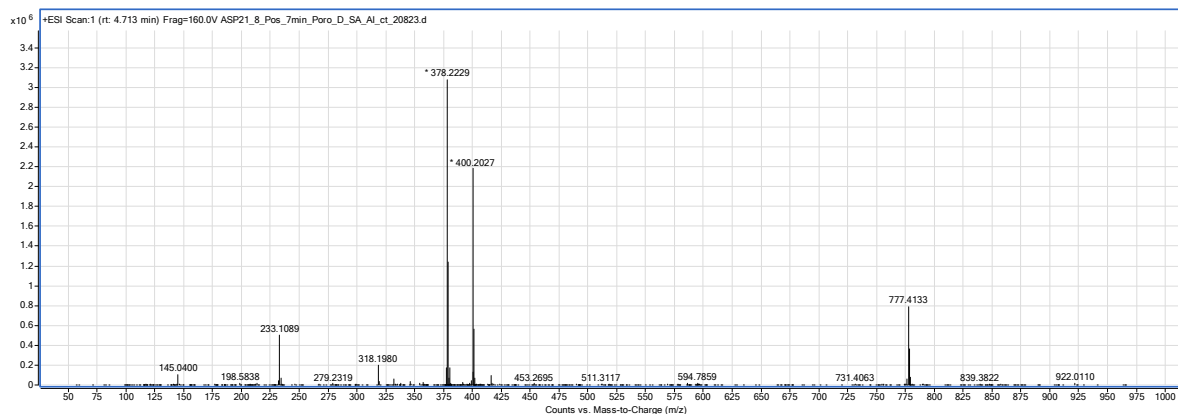


Figure S67. Extracted Mass Spectra from LC-MS Analysis for ASP26.

ASP28: 5F-MDMB-PICA



5F-MDMB-PINACA



FUB-144

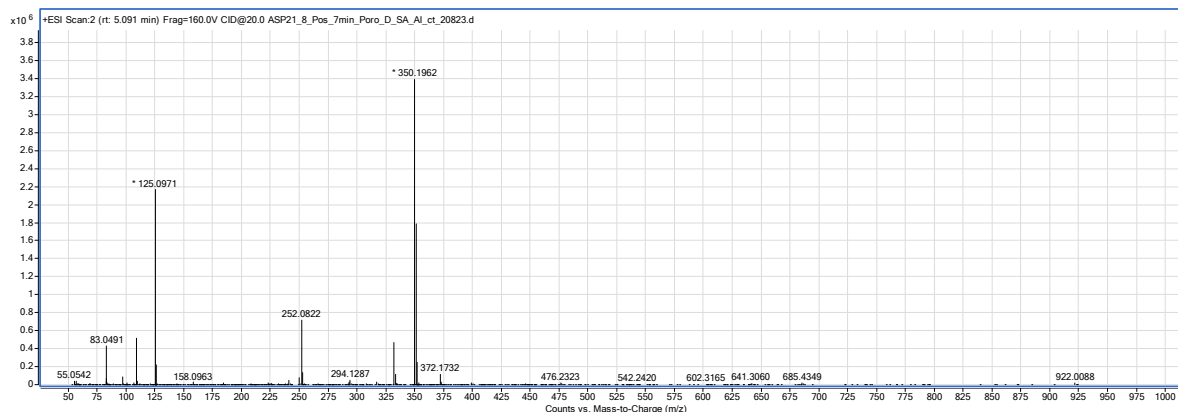


Figure S68. Extracted Mass Spectra from LC-MS Analysis for ASP28.

ASP29: MDMB-4en-PINACA

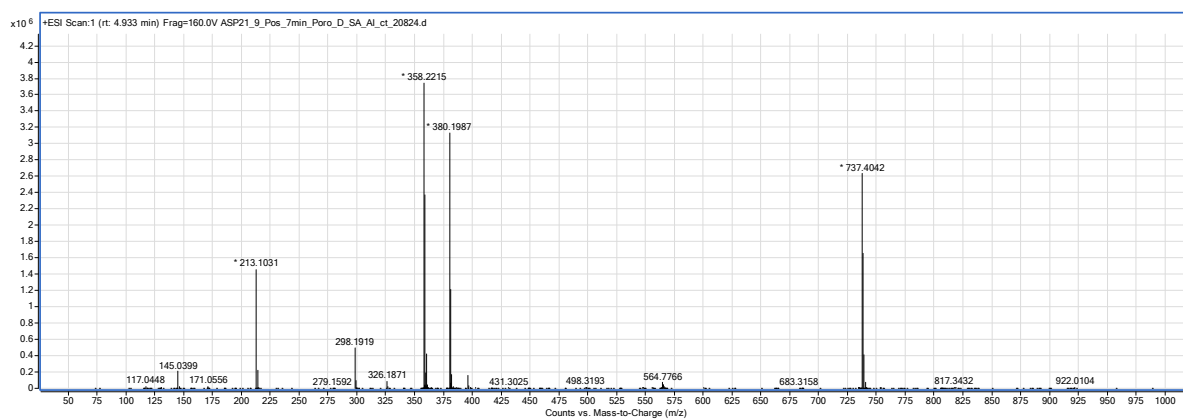
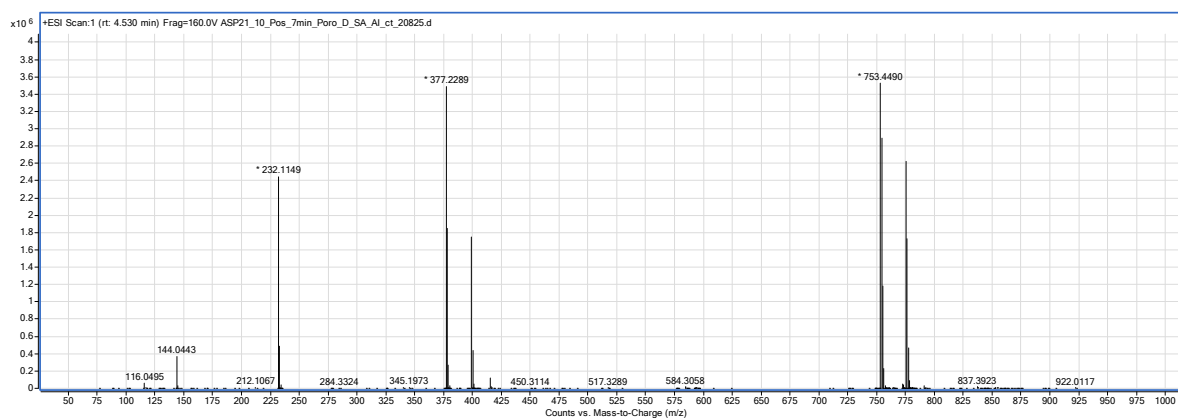
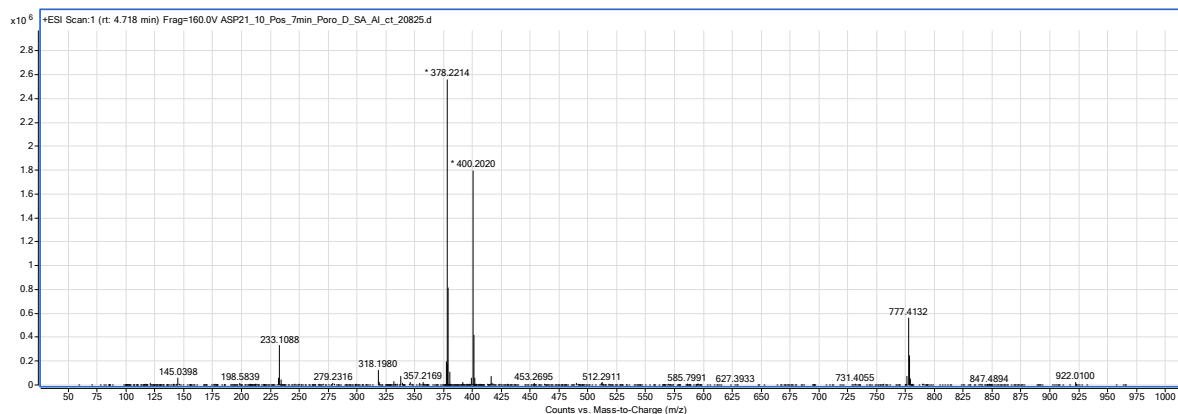


Figure S69. Extracted Mass Spectra from LC-MS Analysis for ASP29.

ASP30: 5F-MDMB-PICA



5F-MDMB-PINACA



FUB-144

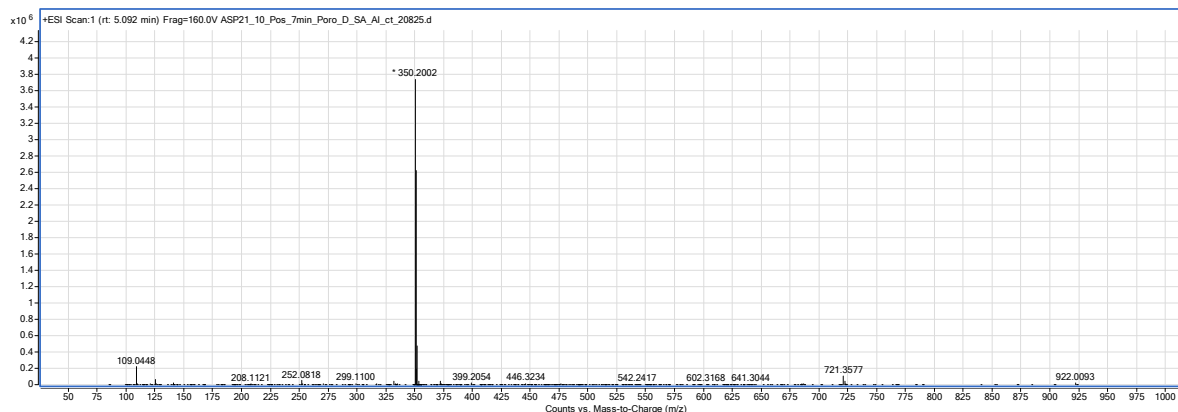


Figure S70. Extracted Mass Spectra from LC-MS Analysis for ASP30.

Tables

Table S1. Summary results for the confirmatory analysis using the combined TLC, NMR and LC-MS workflow. Only controlled substances are listed. Compounds that were detected in LC-MS but not identified in the NMR have been indicated with an Asterix (*).

Sample	Workflow Results
ASP 1	--
ASP 2	5F-MDMB-PINACA
ASP 3	5F-MDMB-PINACA, AMB-FUBINACA
ASP 4	MDMB-4en-PINACA
ASP 5	5F-MDMB-PICA
ASP 6	MDMB-4en-PINACA
ASP 7	--
ASP 8	4F-MDMB-BINACA
ASP 9	Cannabis*
ASP 10	--
ASP 11	MDMB-4en-PINACA
ASP 12	MDMB-4en-PINACA
ASP 13	MDMB-4en-PINACA
ASP 14	Cannabis*, 5F-MDMB-PINACA*
ASP 15	5F-MDMB-PINACA
ASP 16	5F-MDMB-PINACA
ASP 17	5F-MDMB-PINACA
ASP 18	5F-PB-22, 5F-AKB48
ASP 19	MDMB-4en-PINACA, 5F-MDMB-PICA, 5F-AMB-PINACA*
ASP 20	--
ASP 21	--
ASP 22	MDMB-4en-PINACA
ASP 23	MDMB-4en-PINACA
ASP 24	MDMB-4en-PINACA
ASP 25	5F-MDMB-PICA, 4F-MDMB-BINACA
ASP 26	MDMB-4en-PINACA

ASP 27	--
ASP 28	5F-MDMB-PICA, FUB-144, 5F-MDMB-PINACA*
ASP 29	MDMB-4en-PINACA
ASP 30	5F-MDMB-PICA, FUB-144, 5F-MDMB-PINACA*
SP066	5F-ADB
SP067	5F-PB-22
SP068	MDMB-CHMICA
ASP 31	--
ASP 32	--
ASP 33	--
ASP 34	MDMB-4en-PINACA
ASP 35	MDMB-4en-PINACA
ASP 36	--
ASP 38	--
ASP 39	--

Table S2. Results of trial of 181 paper (letters, cards etc.) samples seized from prisons highlighting the effect of changing detection threshold.

	High Sensitivity Threshold (~12% false positive threshold)	High Specificity Threshold (~6% false positive threshold)
Positive	50	47
False Negative	14	17
Negative	103	110
False Positive	14	7