

Supplementary Material

An efficient access to novel 2*H*-pyrazino[2,1-*b*]quinazoline-1,6-diones *via* intramolecular alkyne hydroamination

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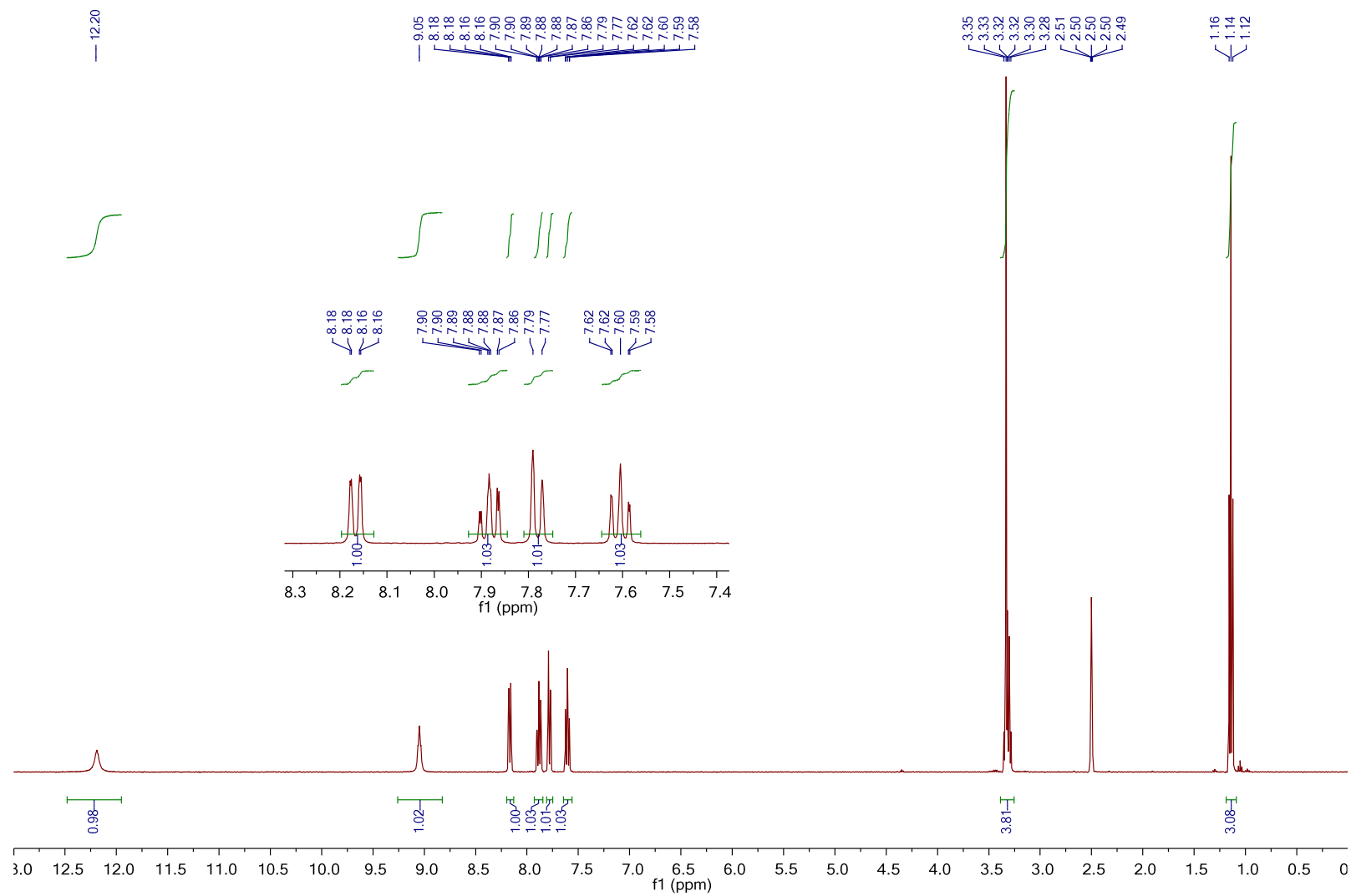
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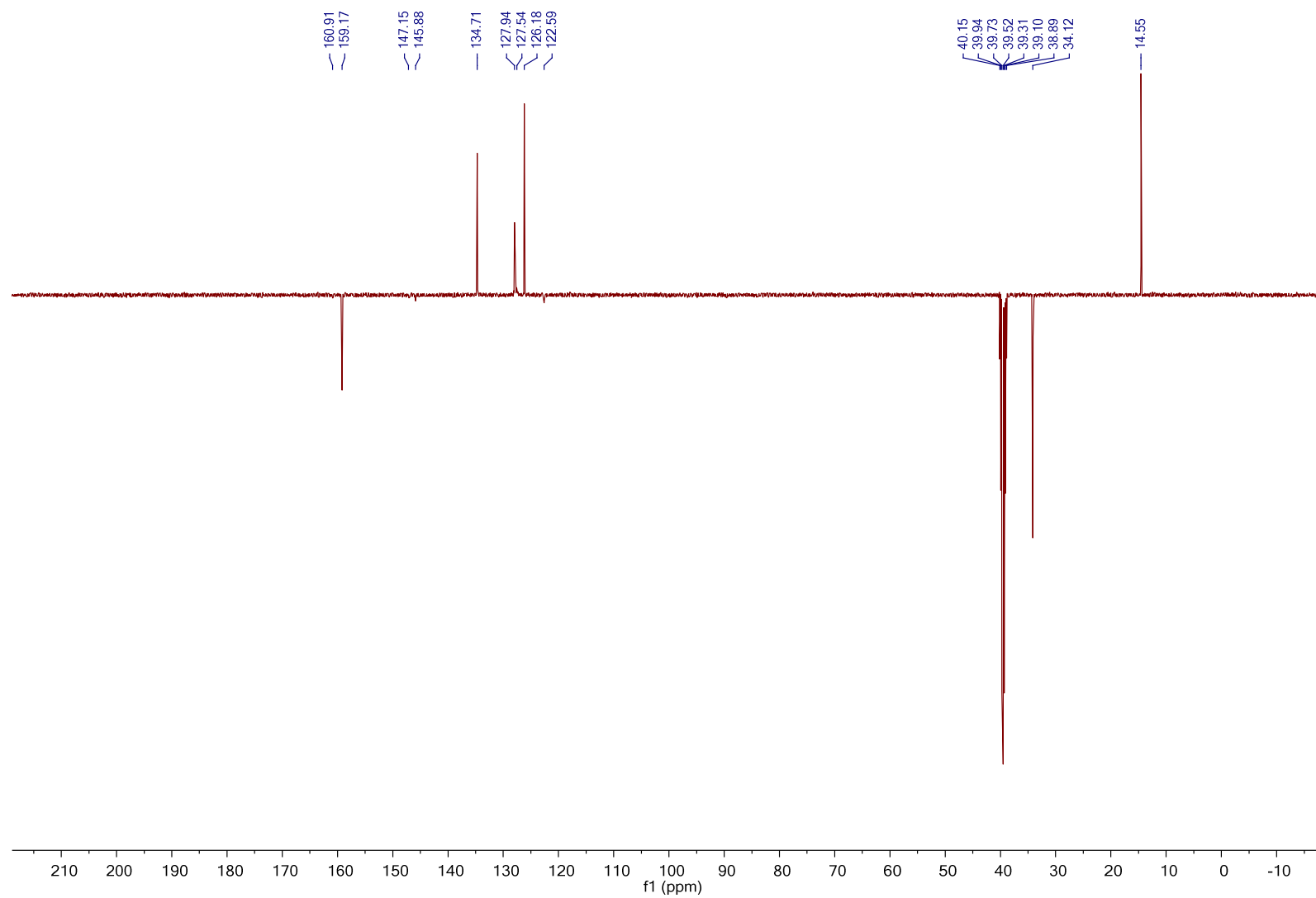
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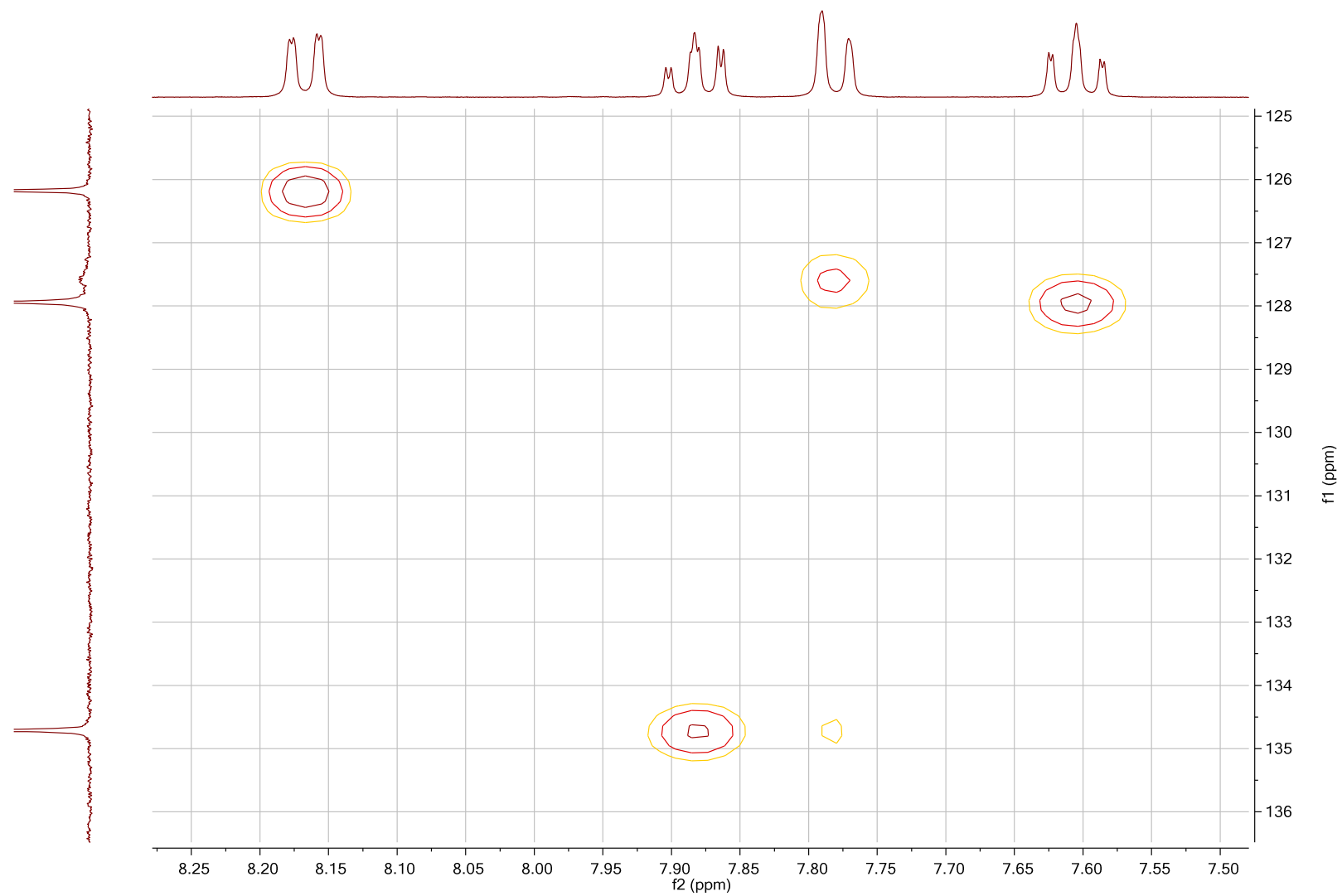
^1H NMR spectrum of *N*-ethyl-4-oxo-3,4-dihydroquinazoline-2-carboxamide (400 MHz, $\text{DMSO-}d_6$)



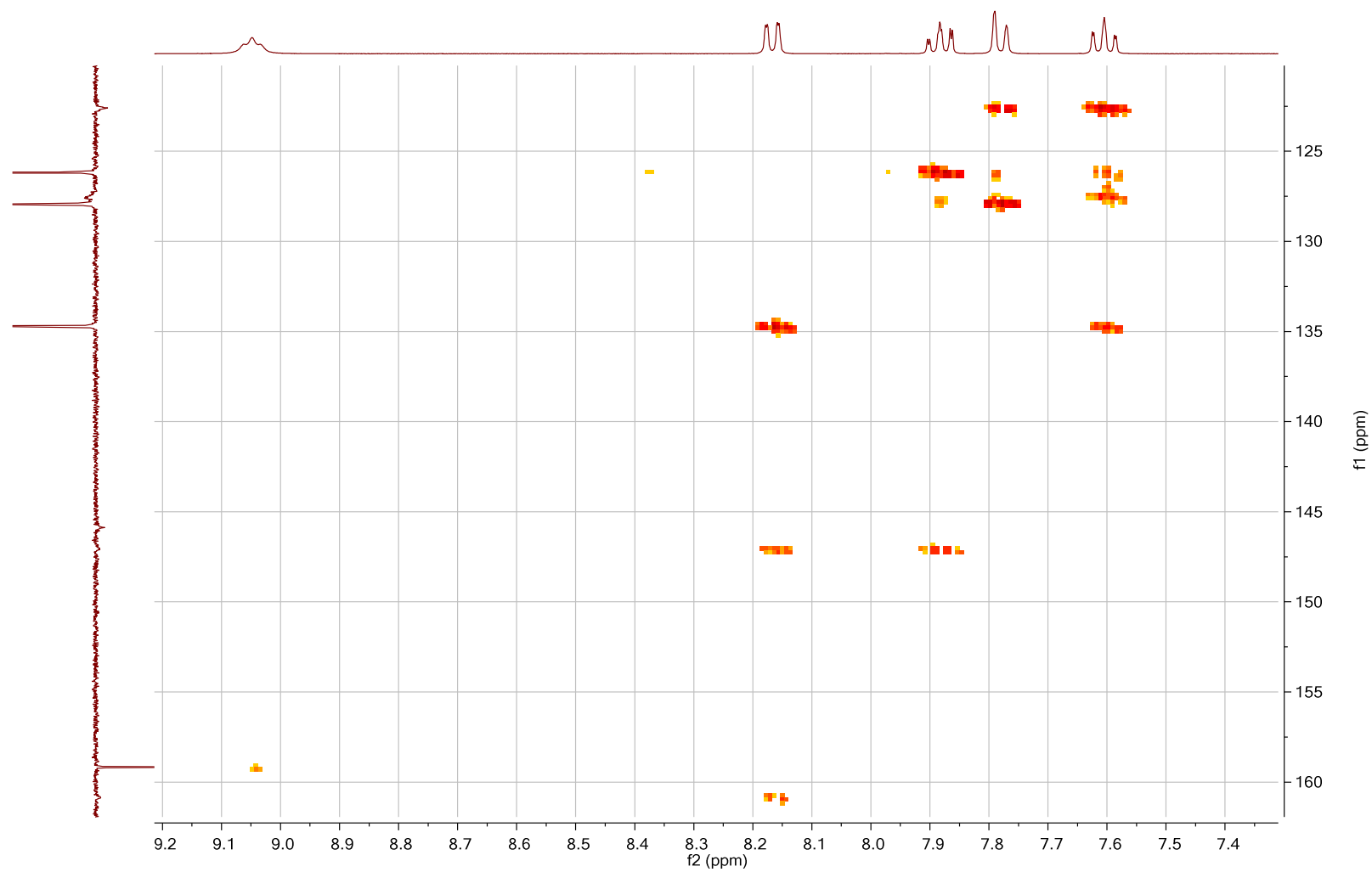
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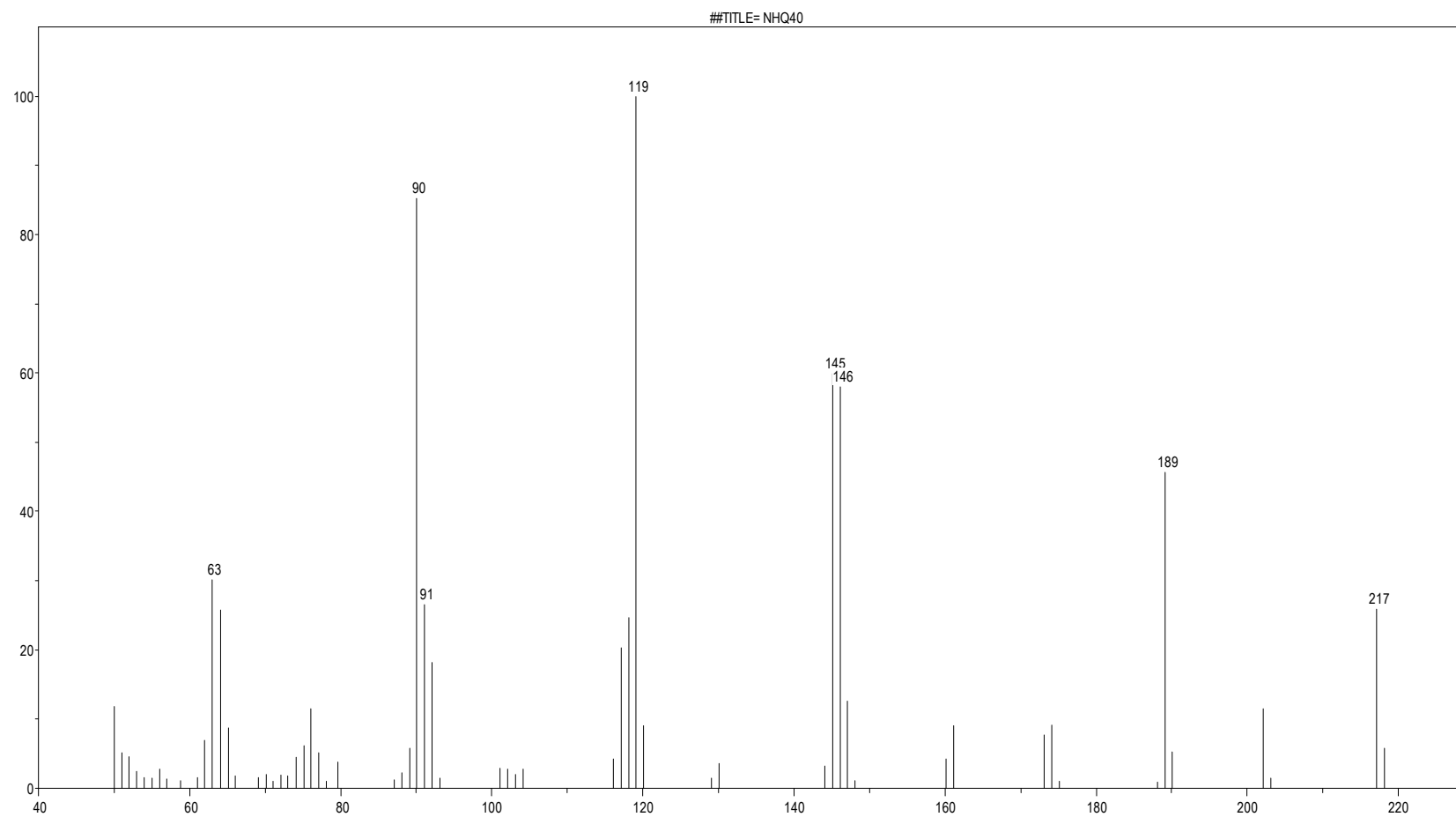


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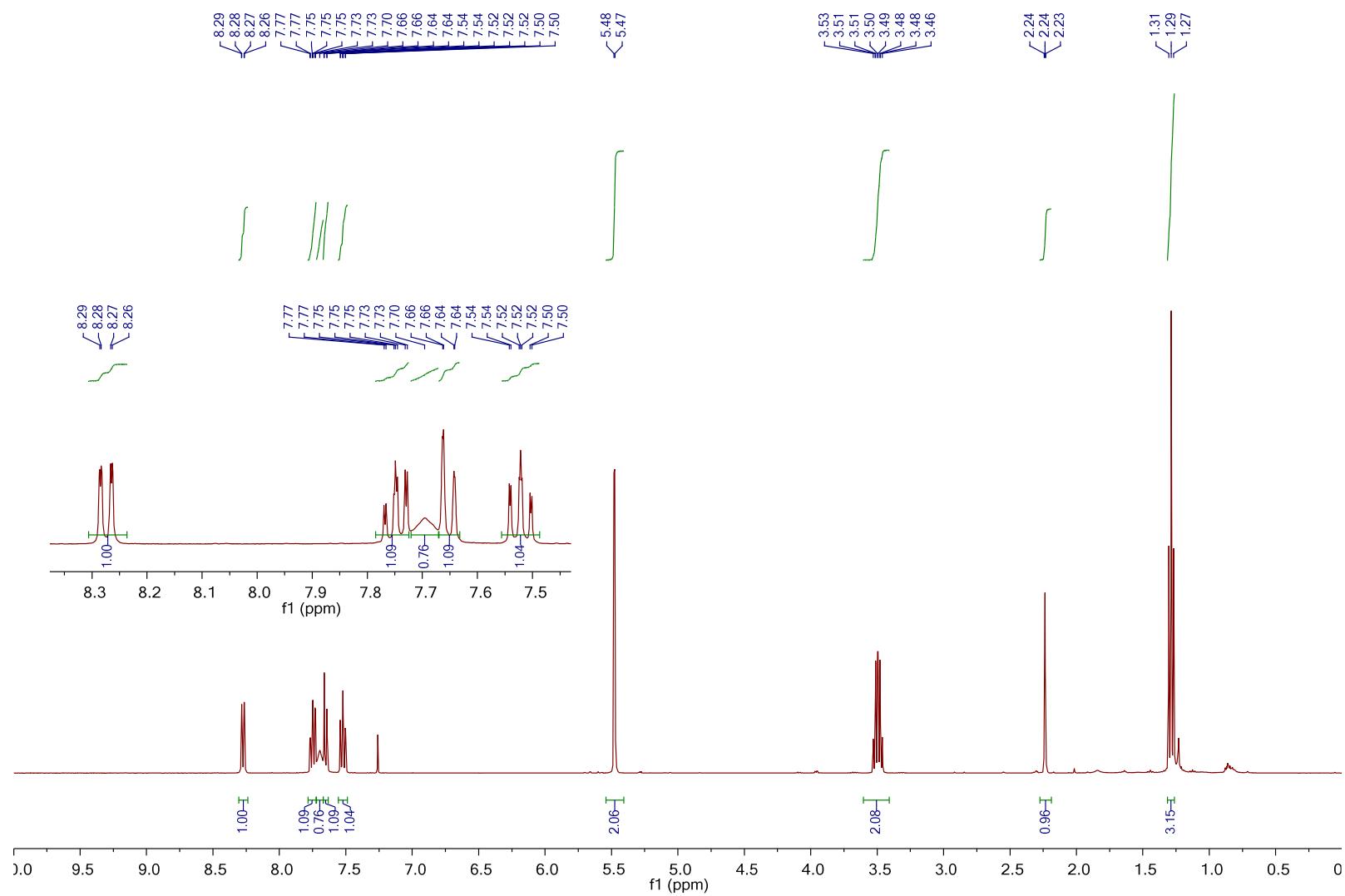


HMBC spectrum of *N*-ethyl-4-oxo-3,4-dihydroquinazoline-2-carboxamide (400 MHz, DMSO-*d*₆)

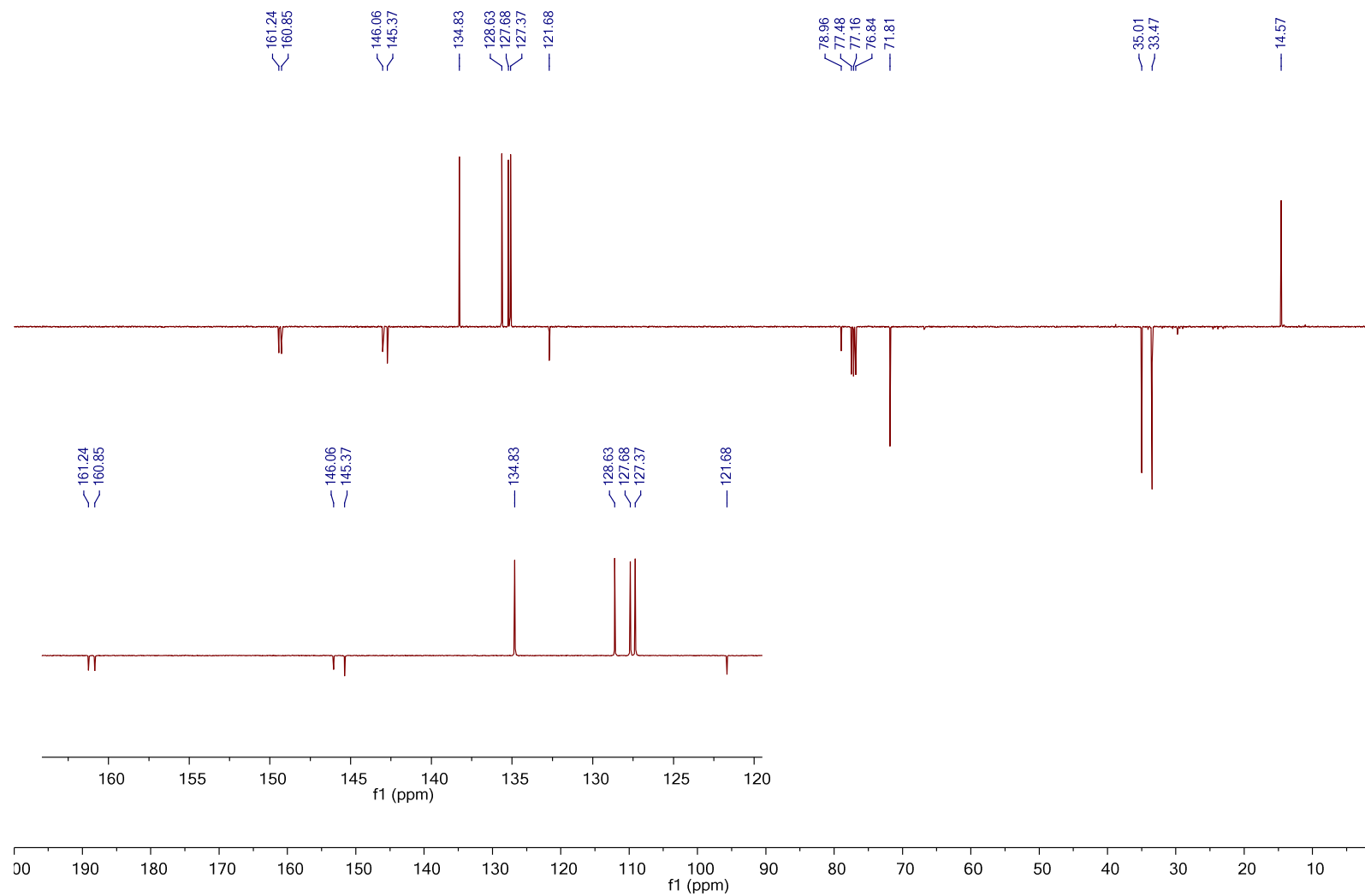


Mass spectrum of *N*-ethyl-4-oxo-3,4-dihydroquinazoline-2-carboxamide

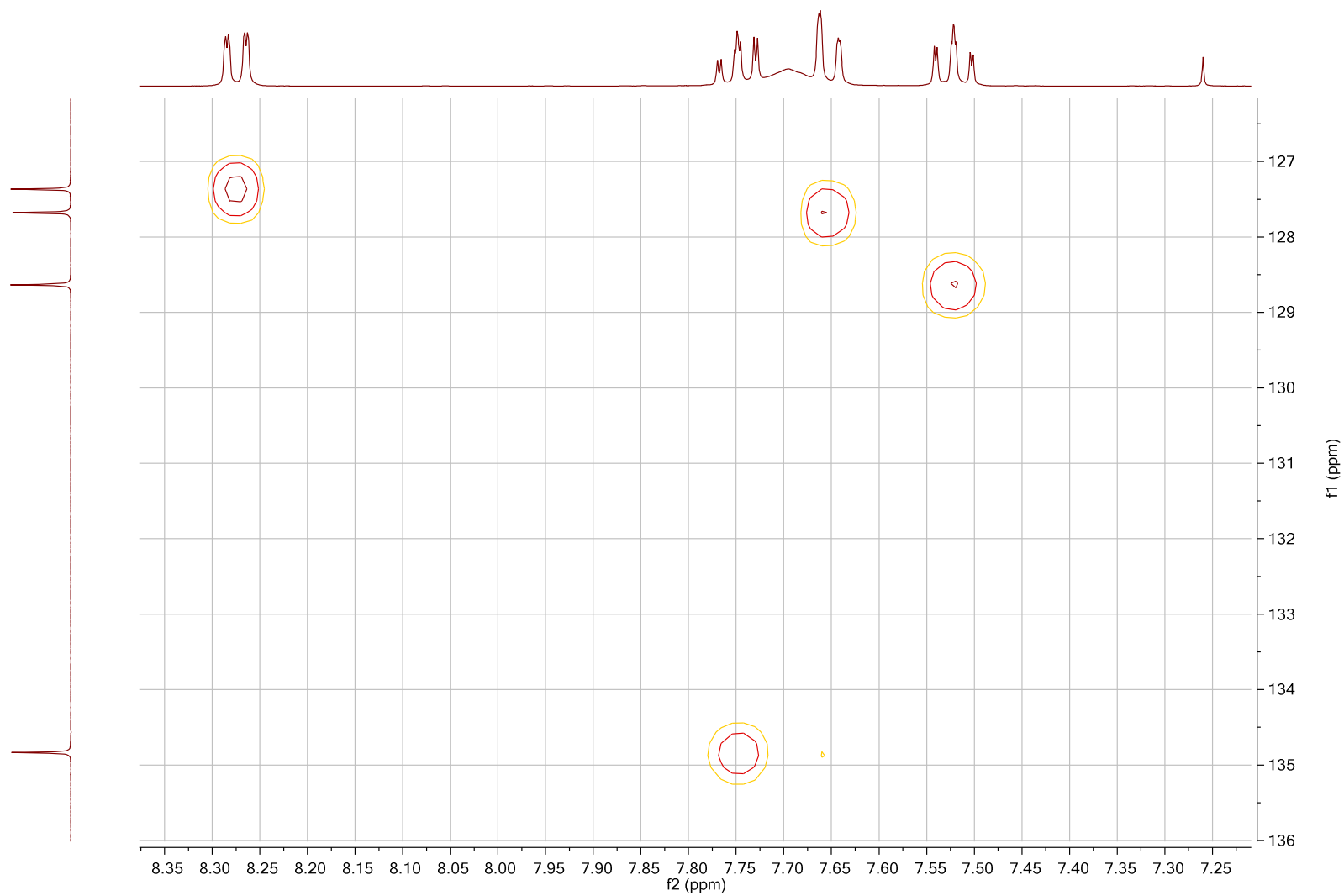
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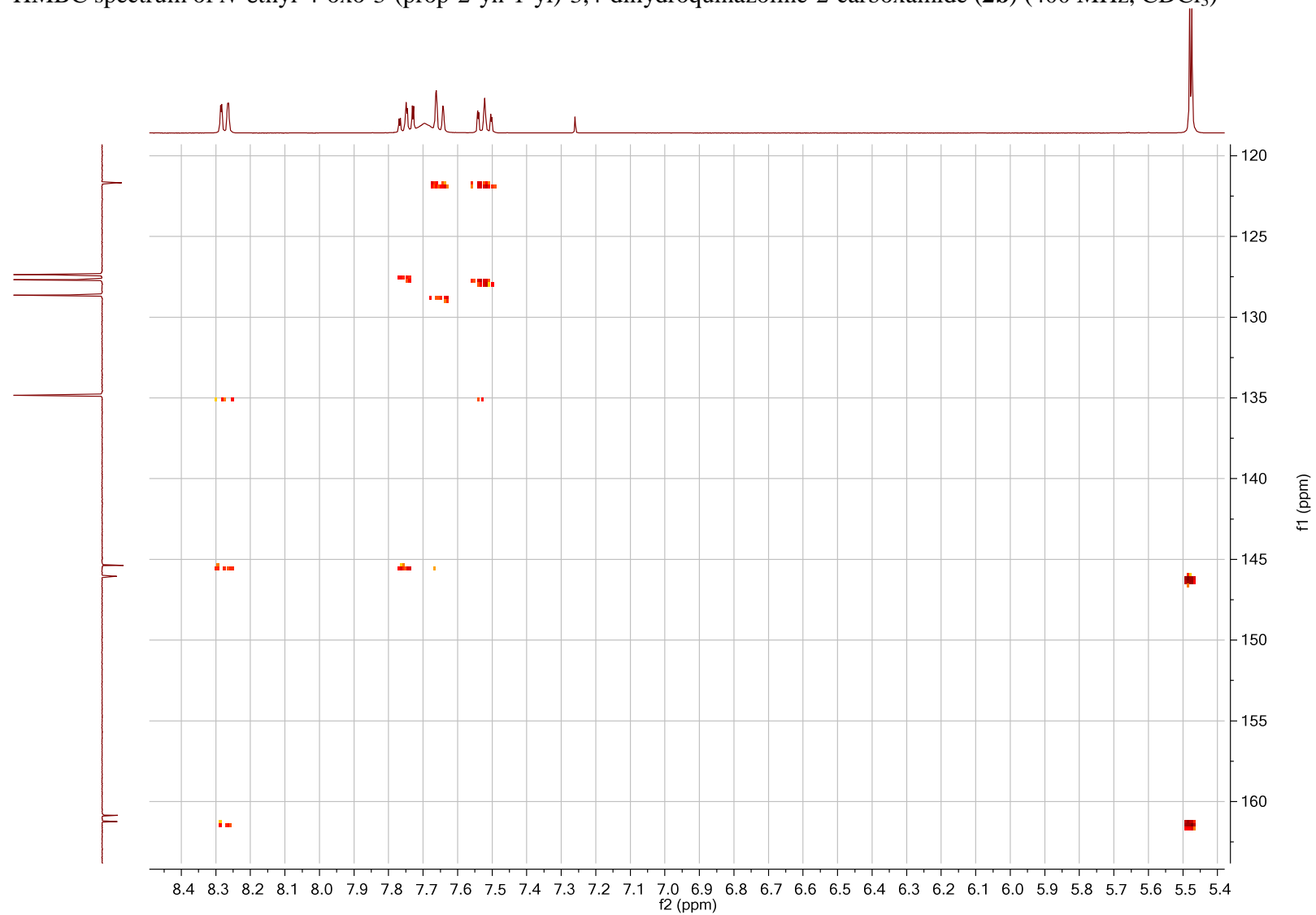
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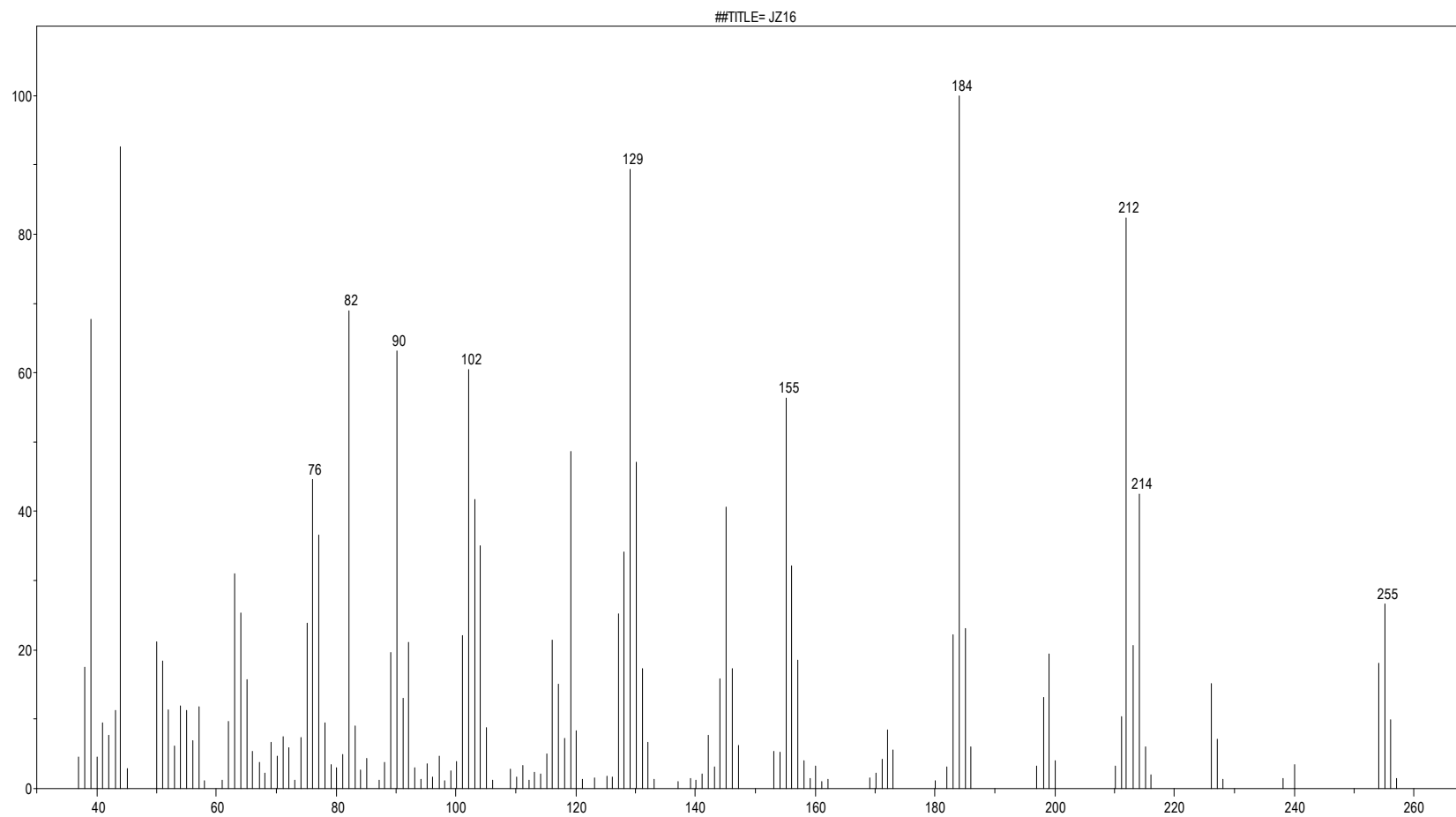


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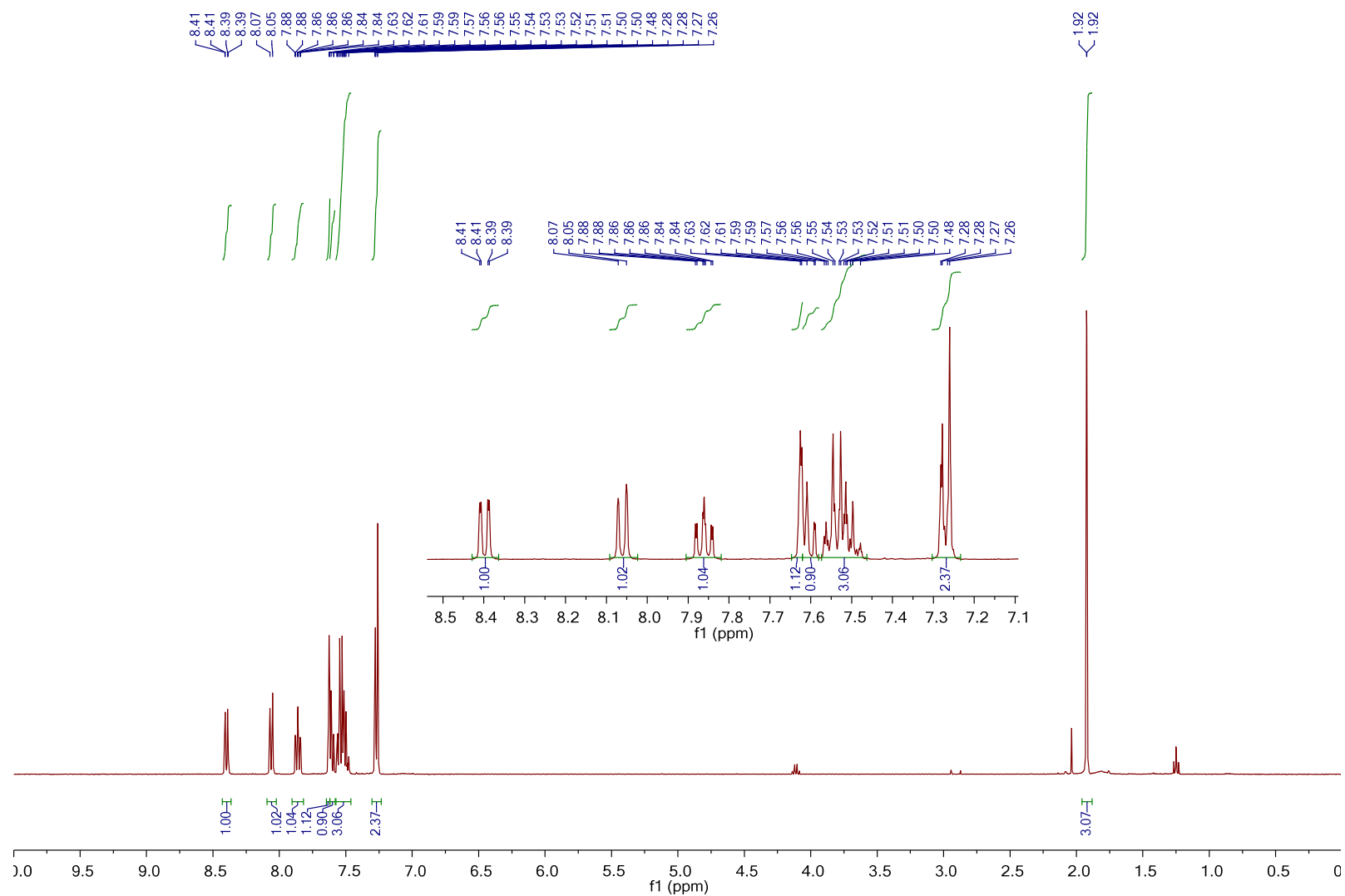


HMBC spectrum of *N*-ethyl-4-oxo-3-(prop-2-yn-1-yl)-3,4-dihydroquinazoline-2-carboxamide (**2b**) (400 MHz, CDCl₃)

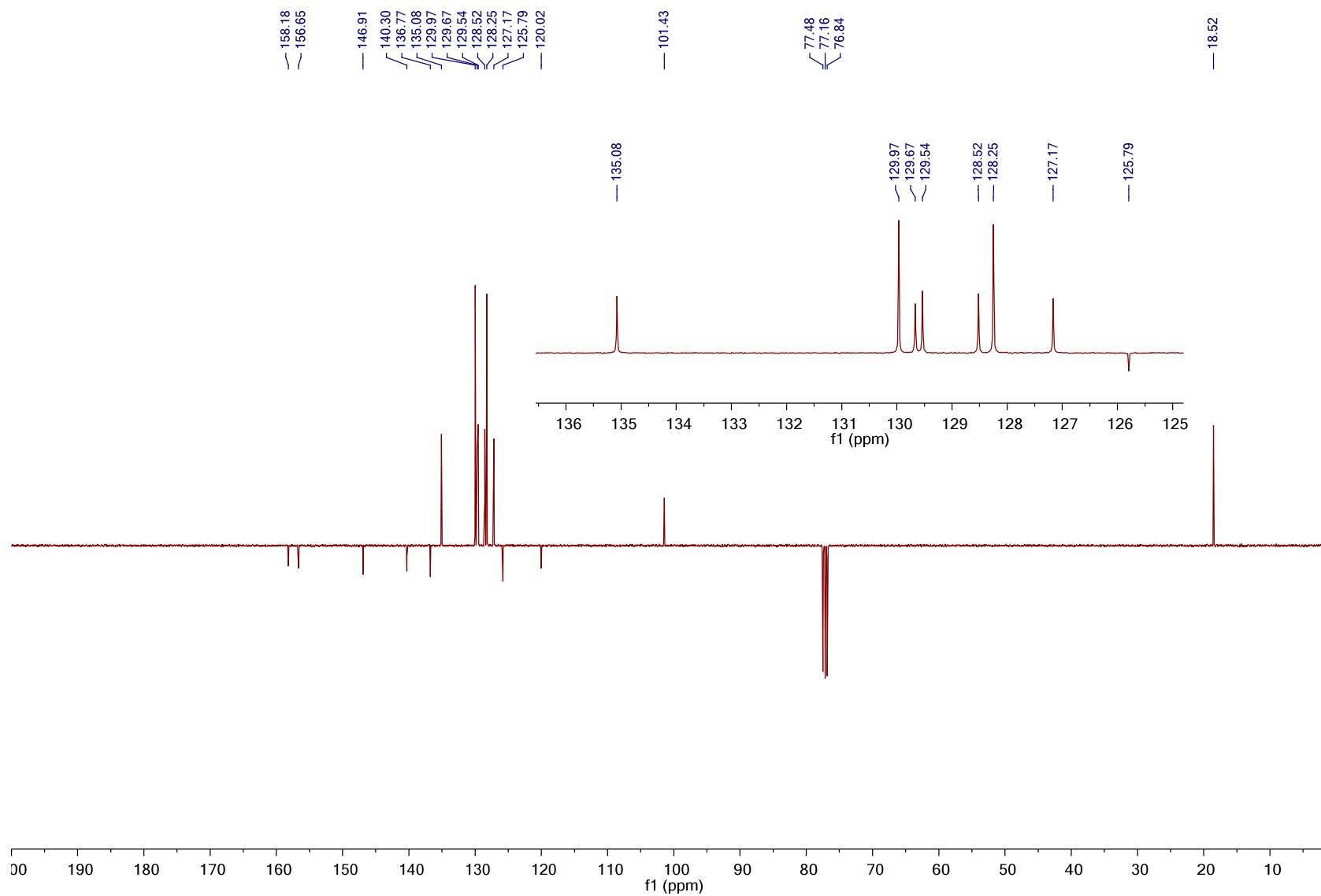


Mass spectrum of *N*-ethyl-4-oxo-3-(prop-2-yn-1-yl)-3,4-dihydroquinazoline-2-carboxamide (**2b**)

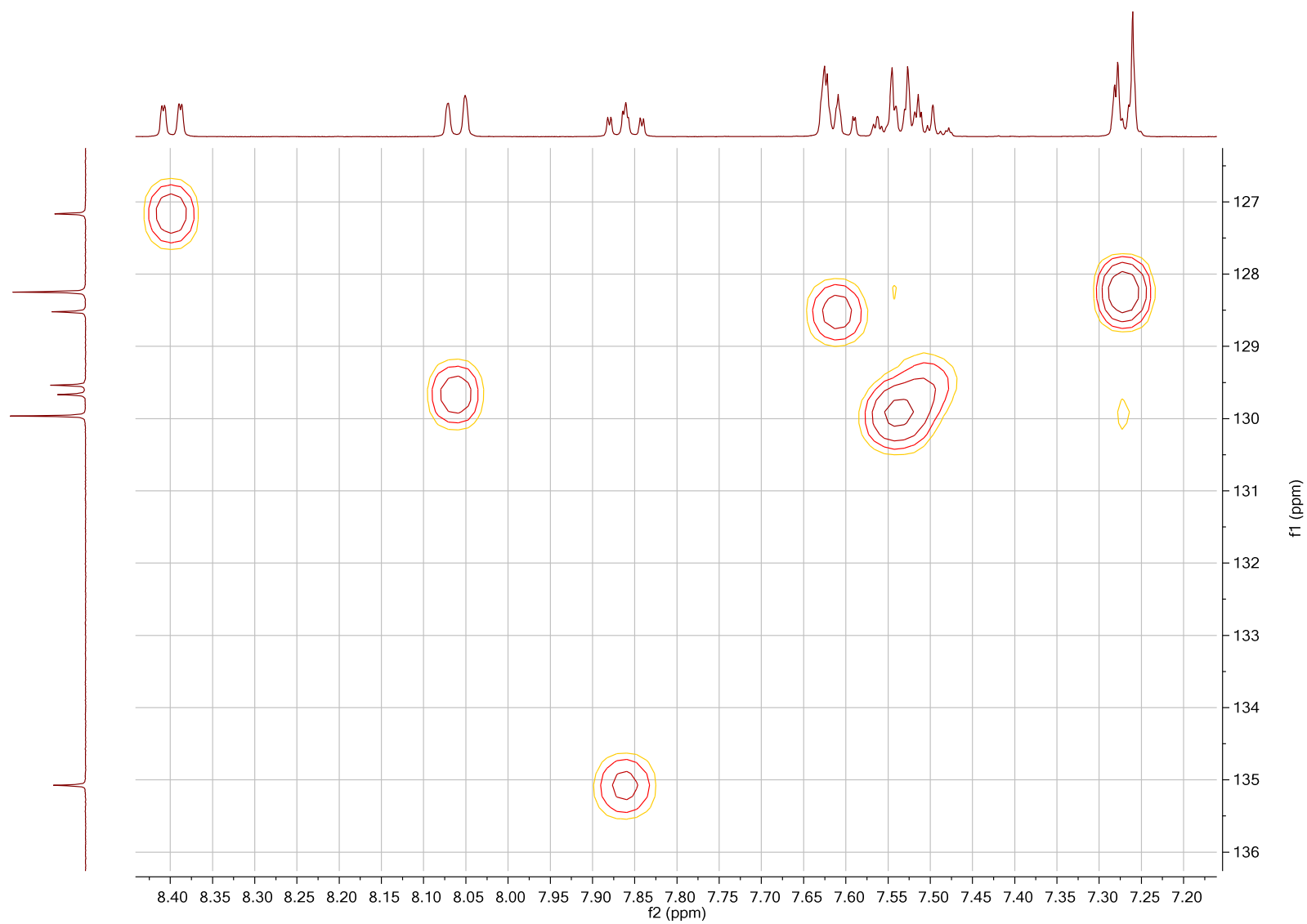
¹H NMR spectrum of 3-methyl-2-phenyl-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3a**) (400 MHz, CDCl₃)



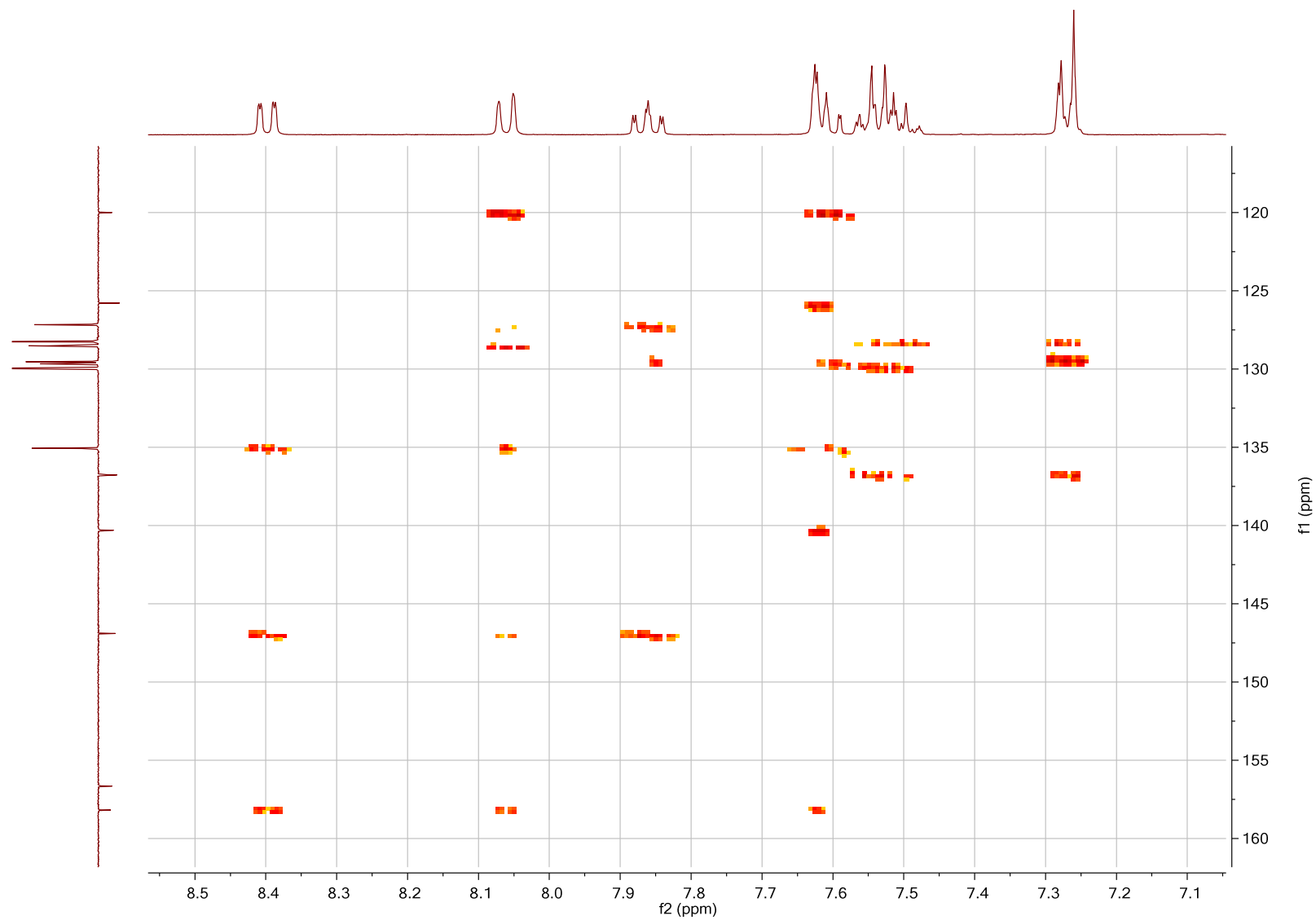
^{13}C NMR spectrum of 3-methyl-2-phenyl-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3a**) (100 MHz, CDCl_3)



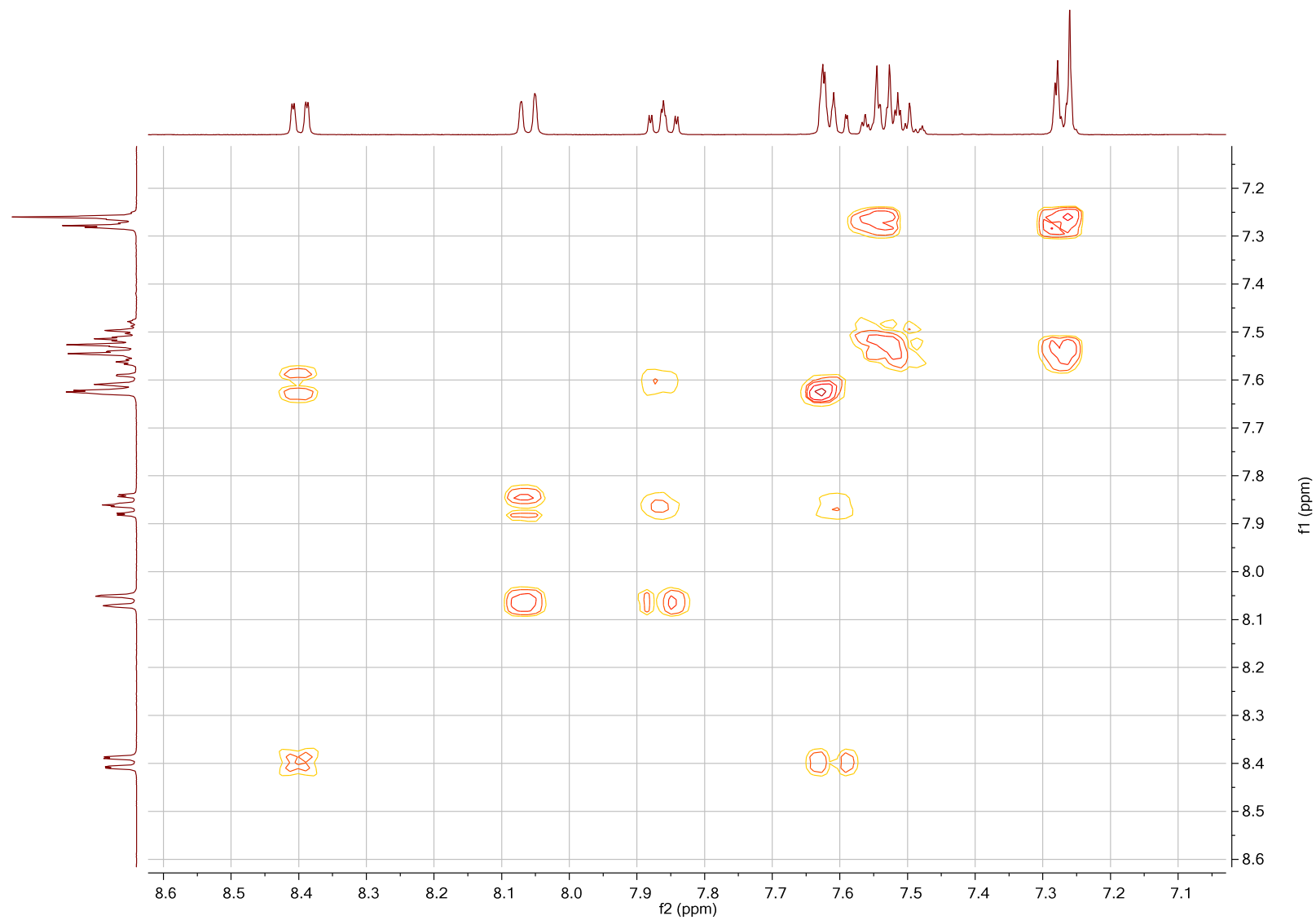
HSQC spectrum of 3-methyl-2-phenyl-2*H*-pyrazino[2,1-*b*]quanzoline-1,6-dione (**3a**) (400 MHz, CDCl₃)



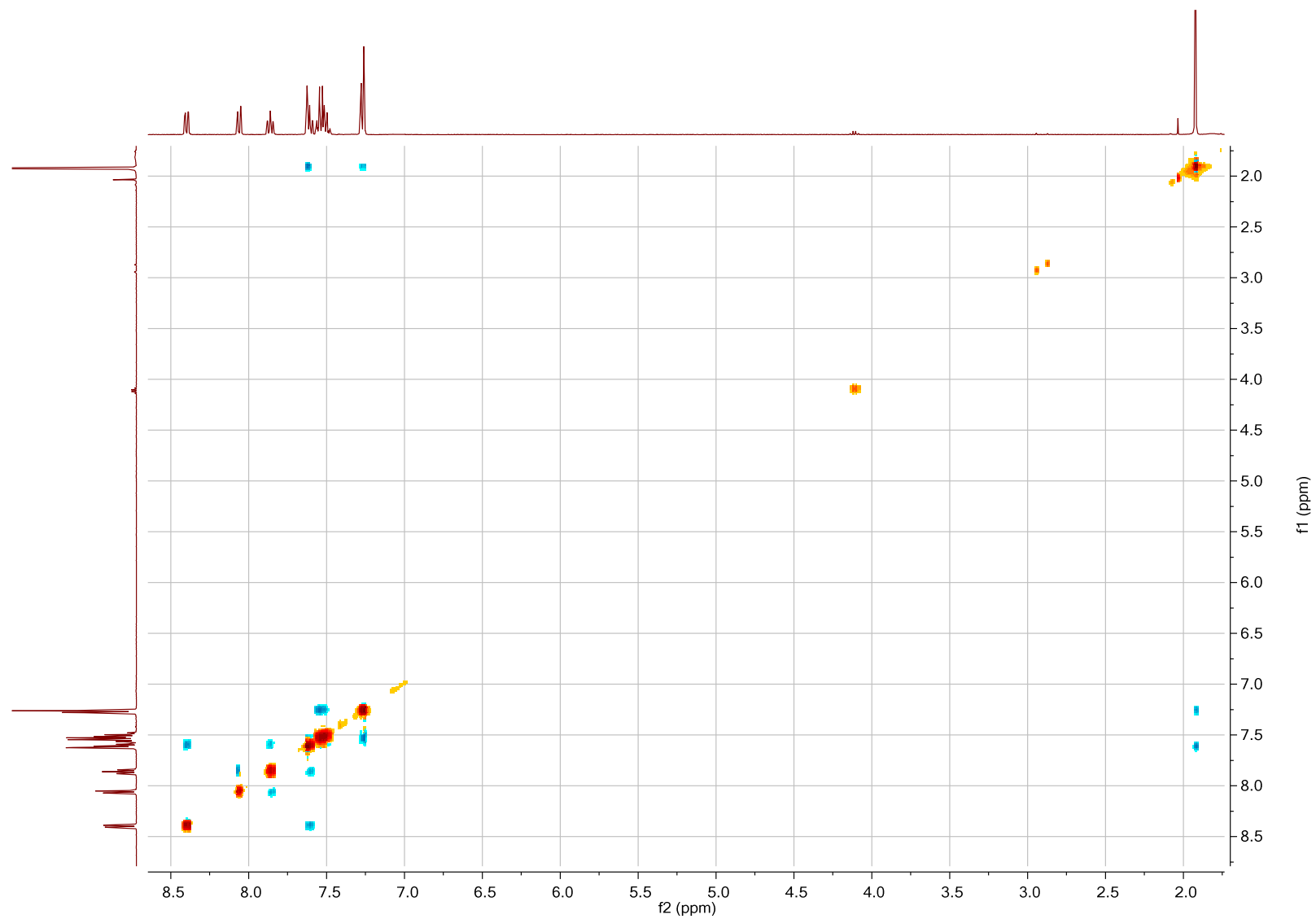
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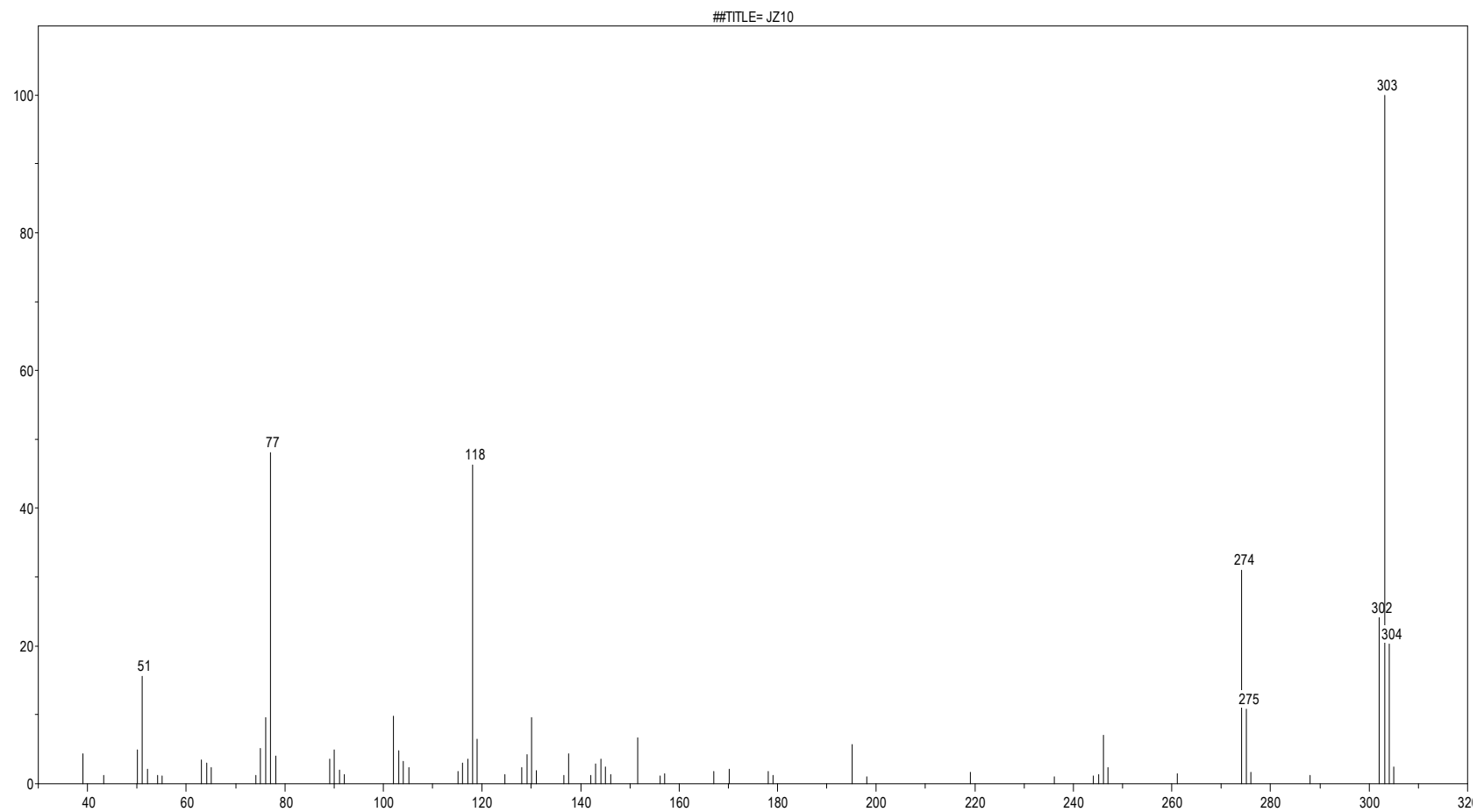


COSY spectrum of 3-methyl-2-phenyl-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3a**) (400 MHz, CDCl₃)

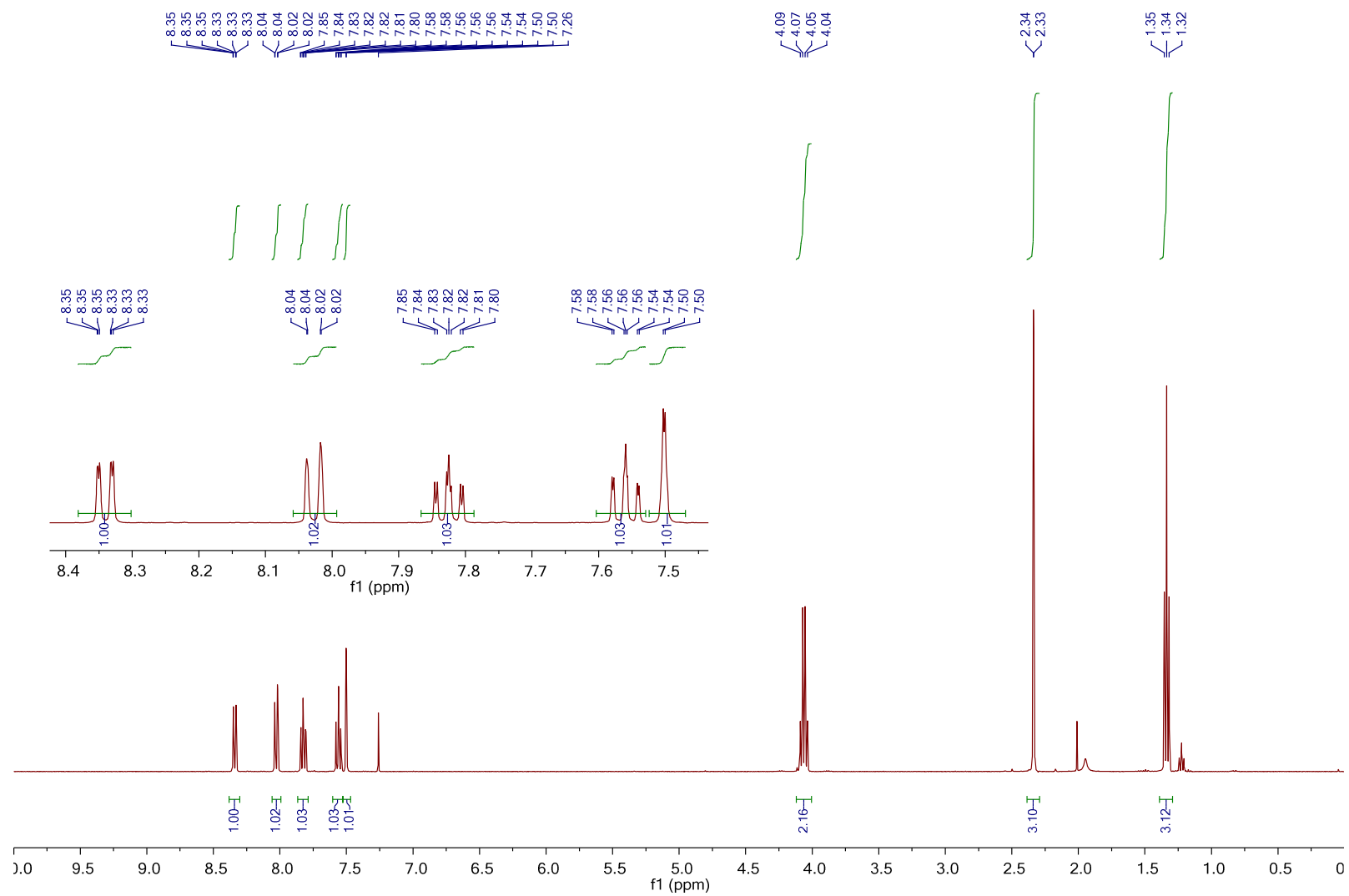


NOESY spectrum of 3-methyl-2-phenyl-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3a**) (400 MHz, CDCl₃)

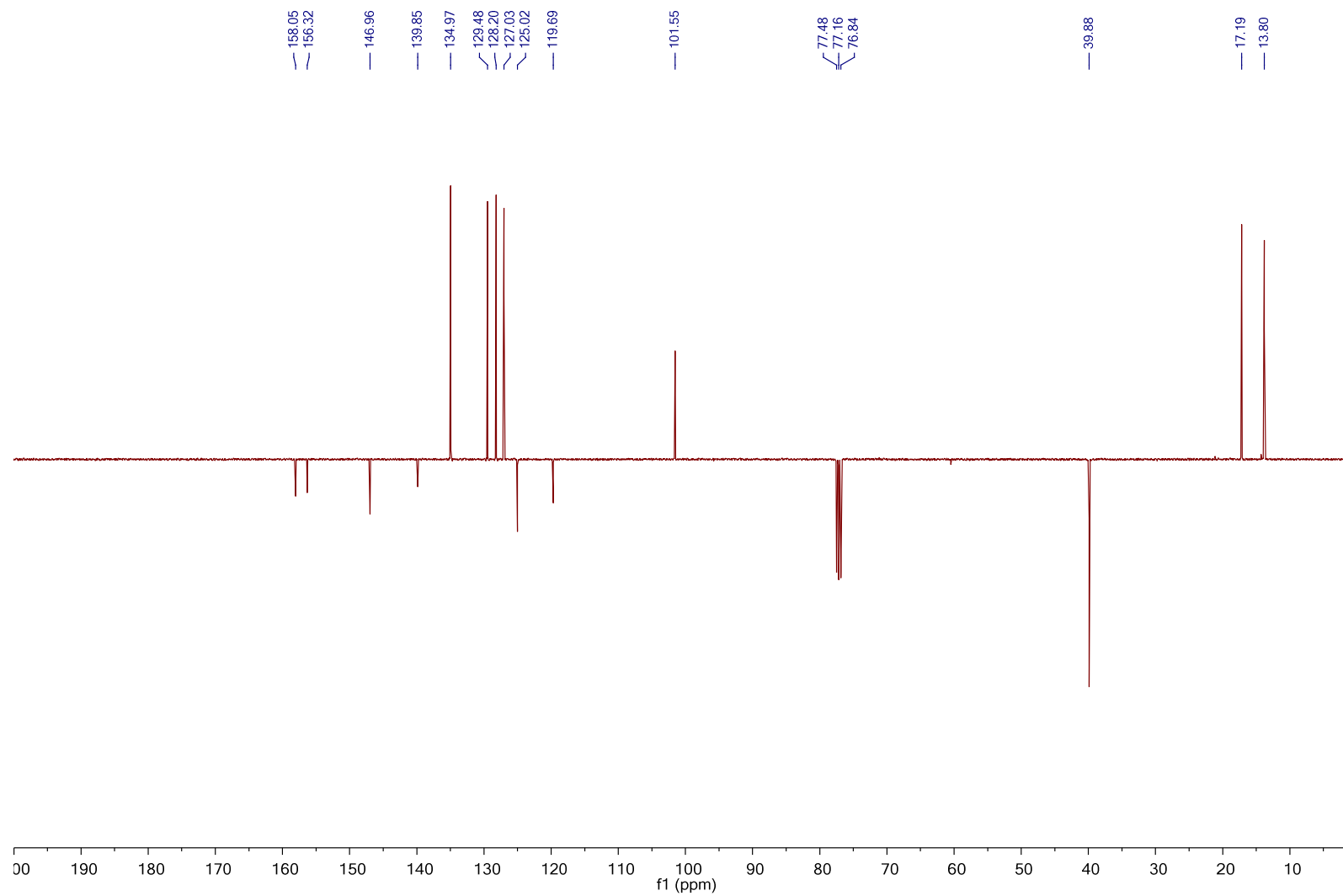


Mass spectrum of 3-methyl-2-phenyl-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3a**)

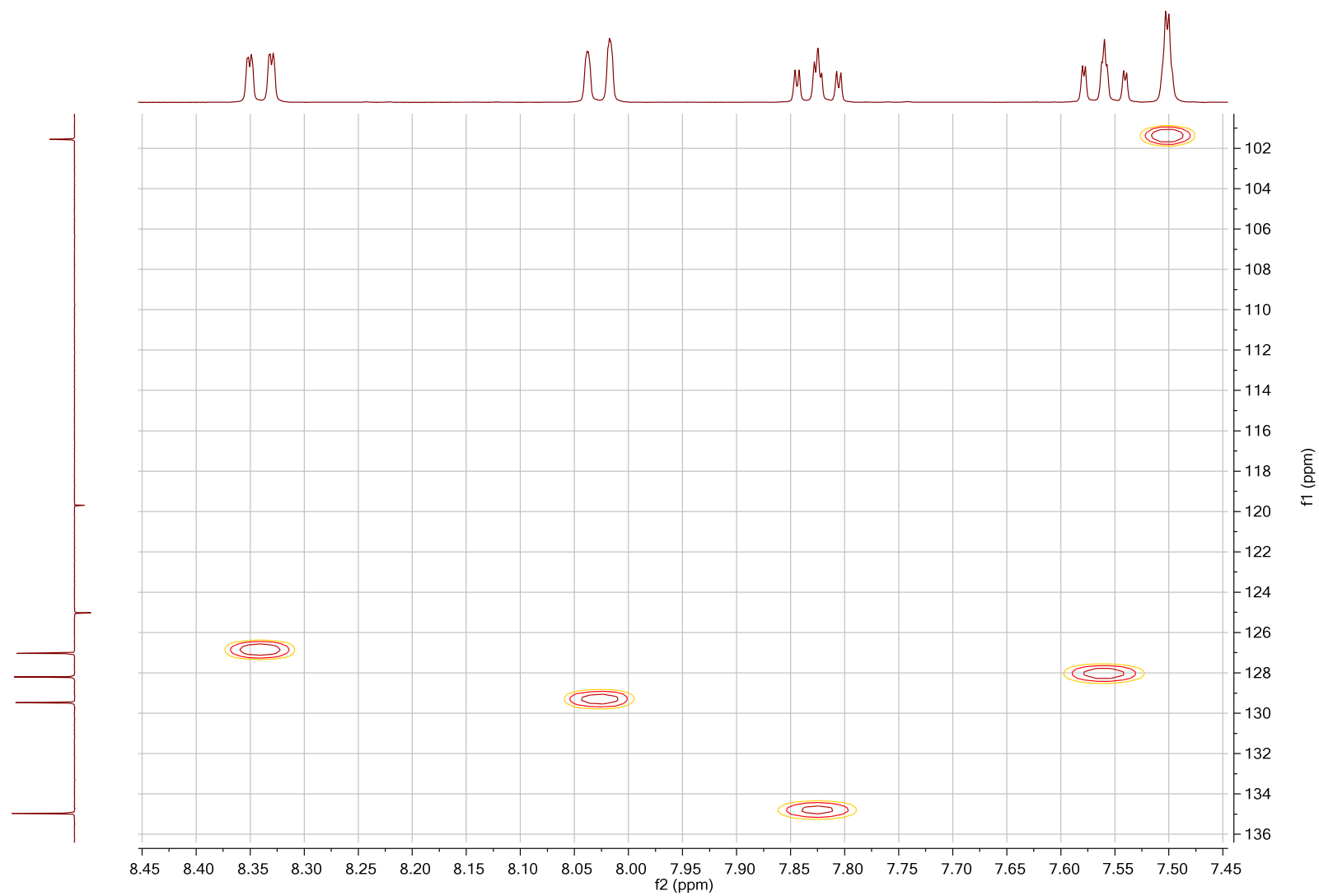
^1H NMR spectrum of 2-ethyl-3-methyl-2*H*-pyrazino[2,1-*b*]quinazoline-1,6-dione (**3b**) (400 MHz, CDCl_3)



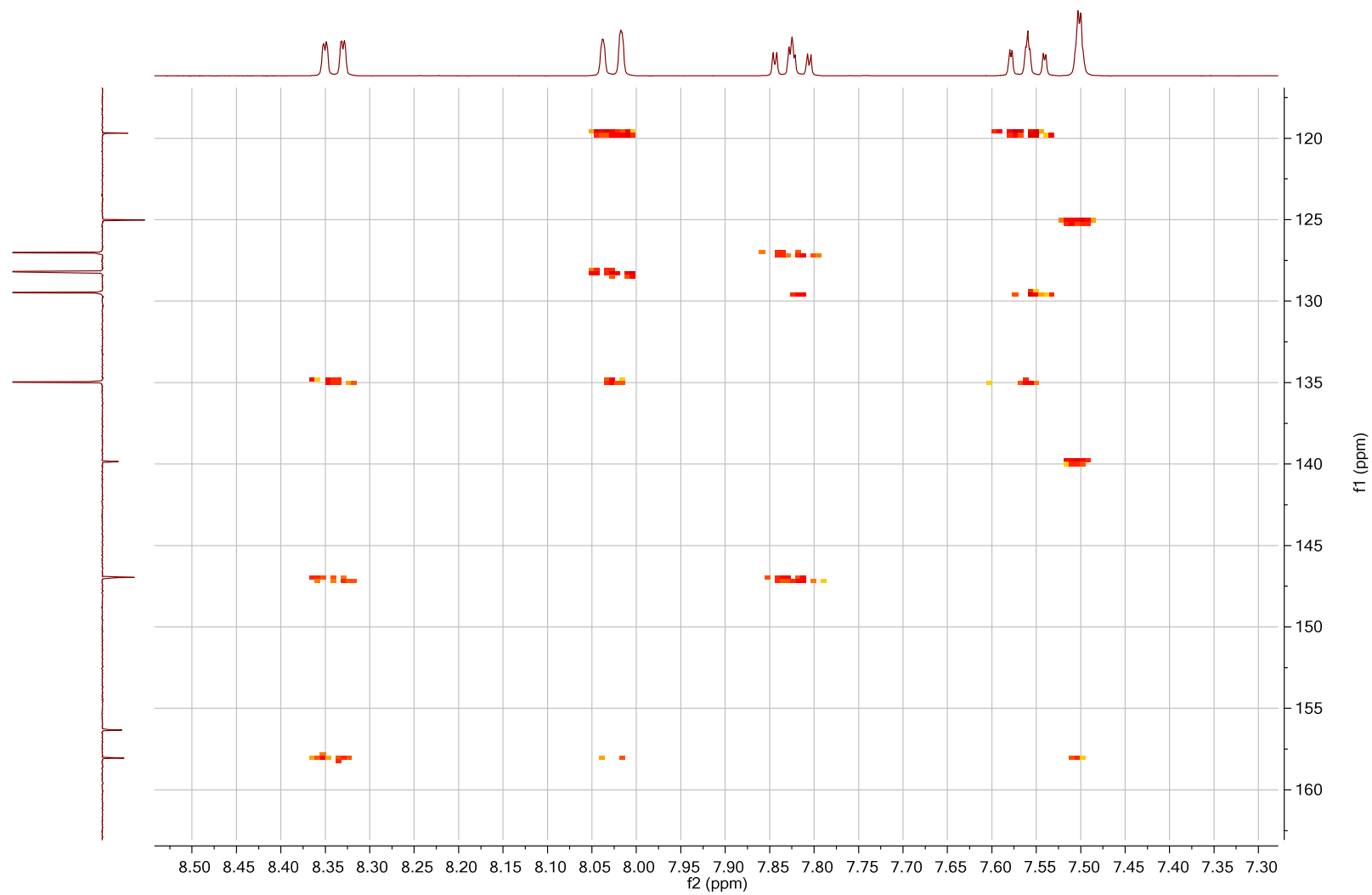
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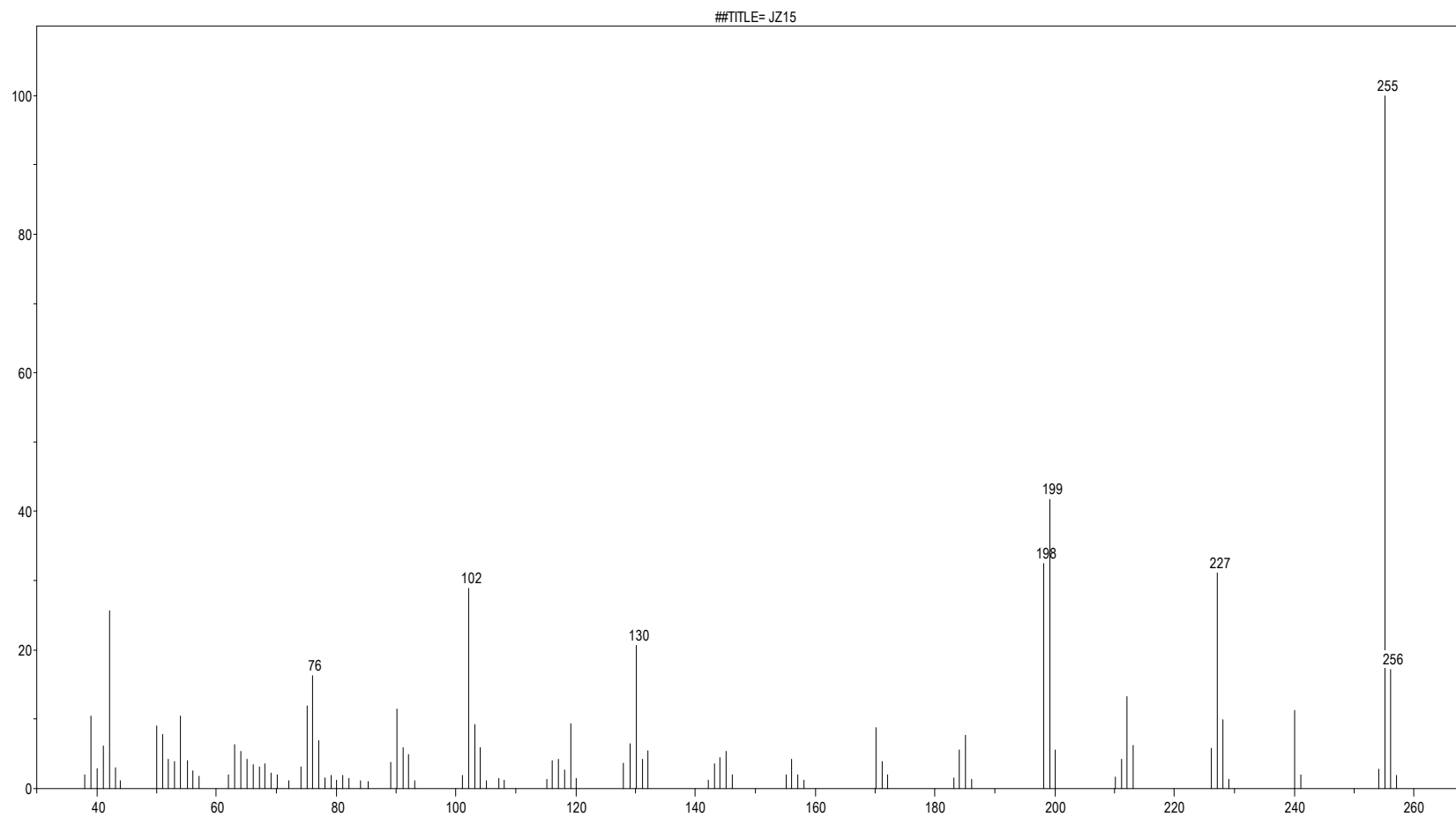


HSQC spectrum of 2-ethyl-3-methyl-2*H*-pyrazino[2,1-*b*]quinazoline-1,6-dione (**3b**) (400 MHz, CDCl₃)

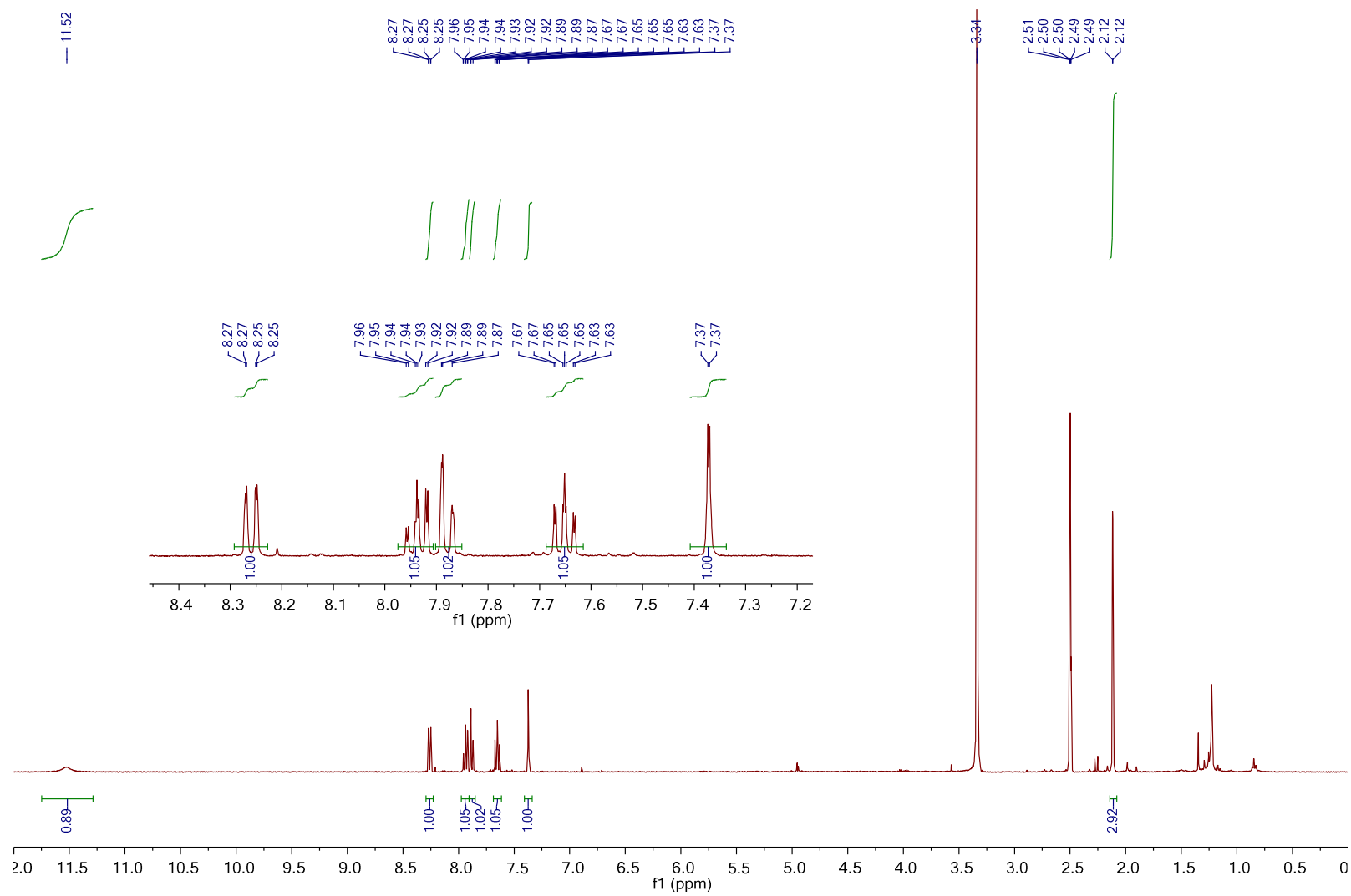


HMBC spectrum of 2-ethyl-3-methyl-2*H*-pyrazino[2,1-*b*]quinazoline-1,6-dione (**3b**) (400 MHz, CDCl₃)

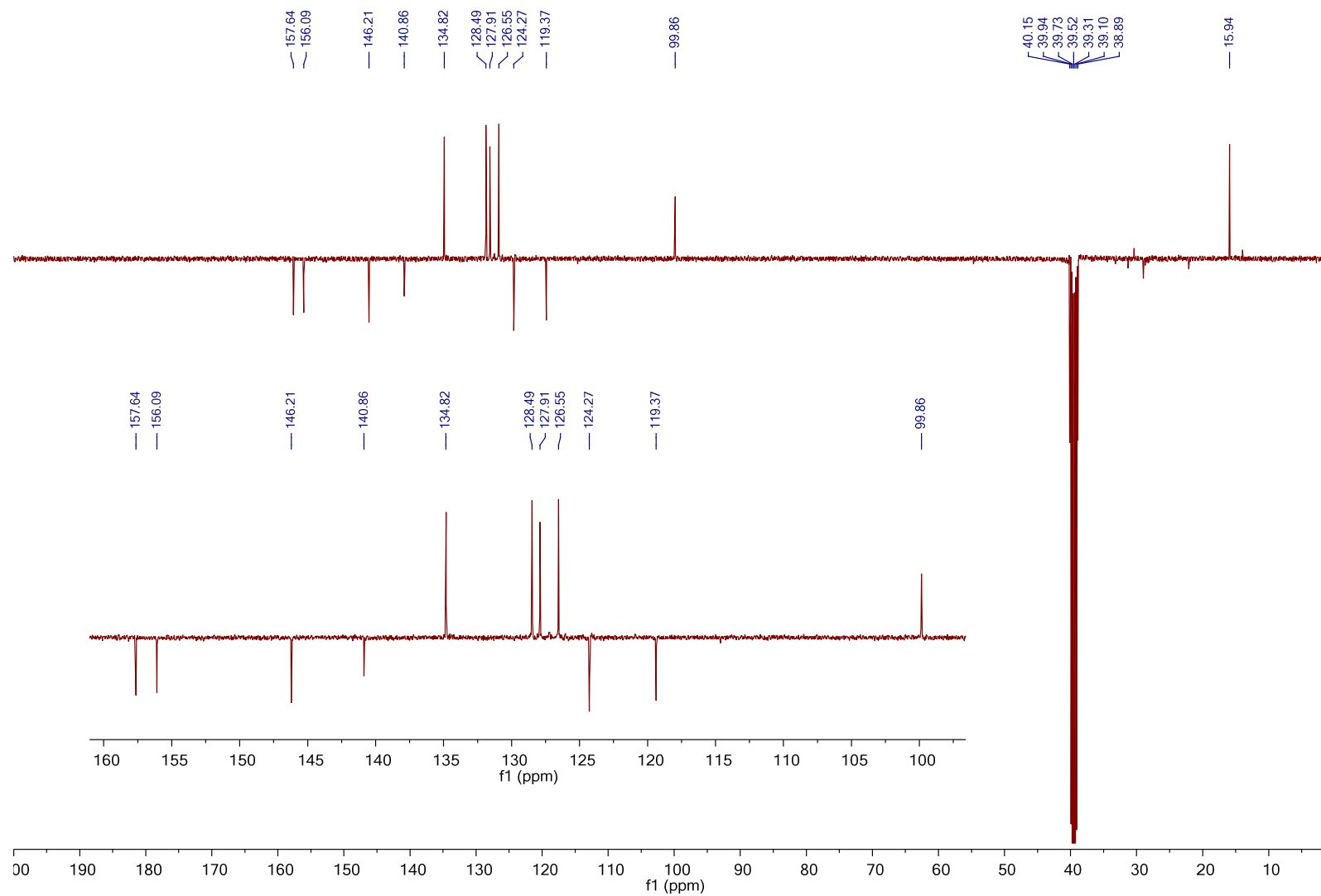


Mass spectrum of 2-ethyl-3-methyl-2*H*-pyrazino[2,1-*b*]quinazoline-1,6-dione (**3b**)

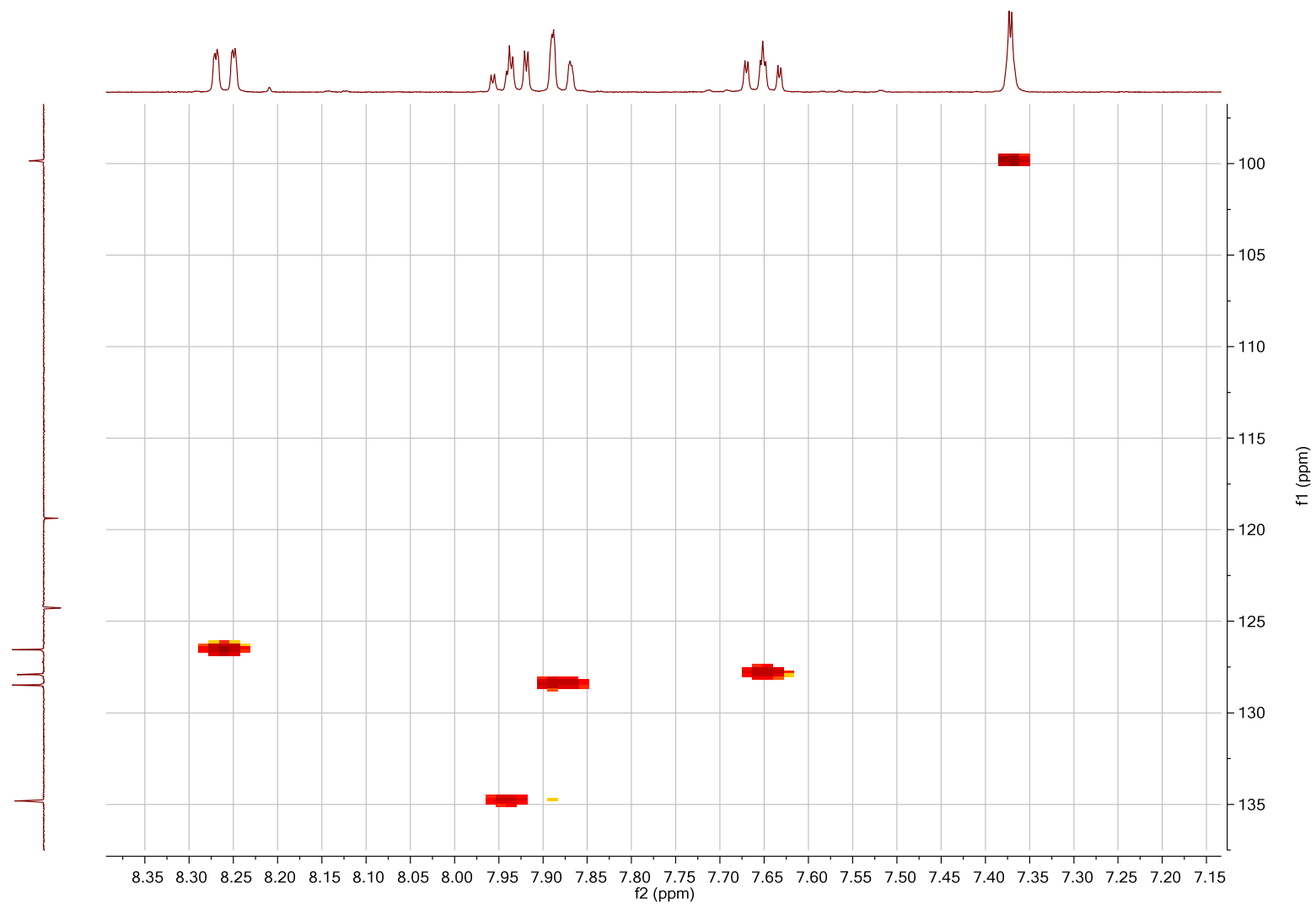
^1H NMR spectrum of 3-methyl-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3c**) (400 MHz, $\text{DMSO-}d_6$)



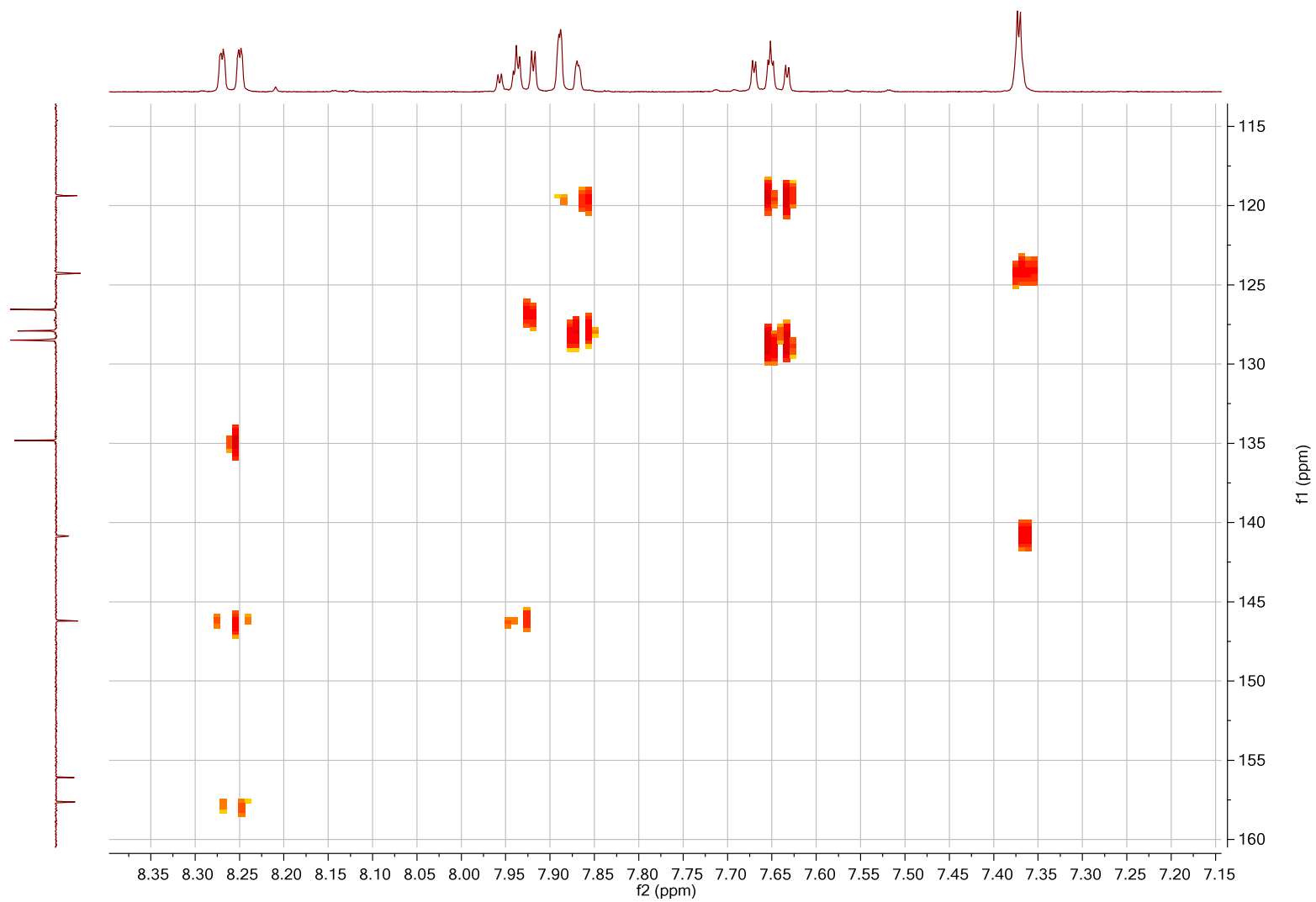
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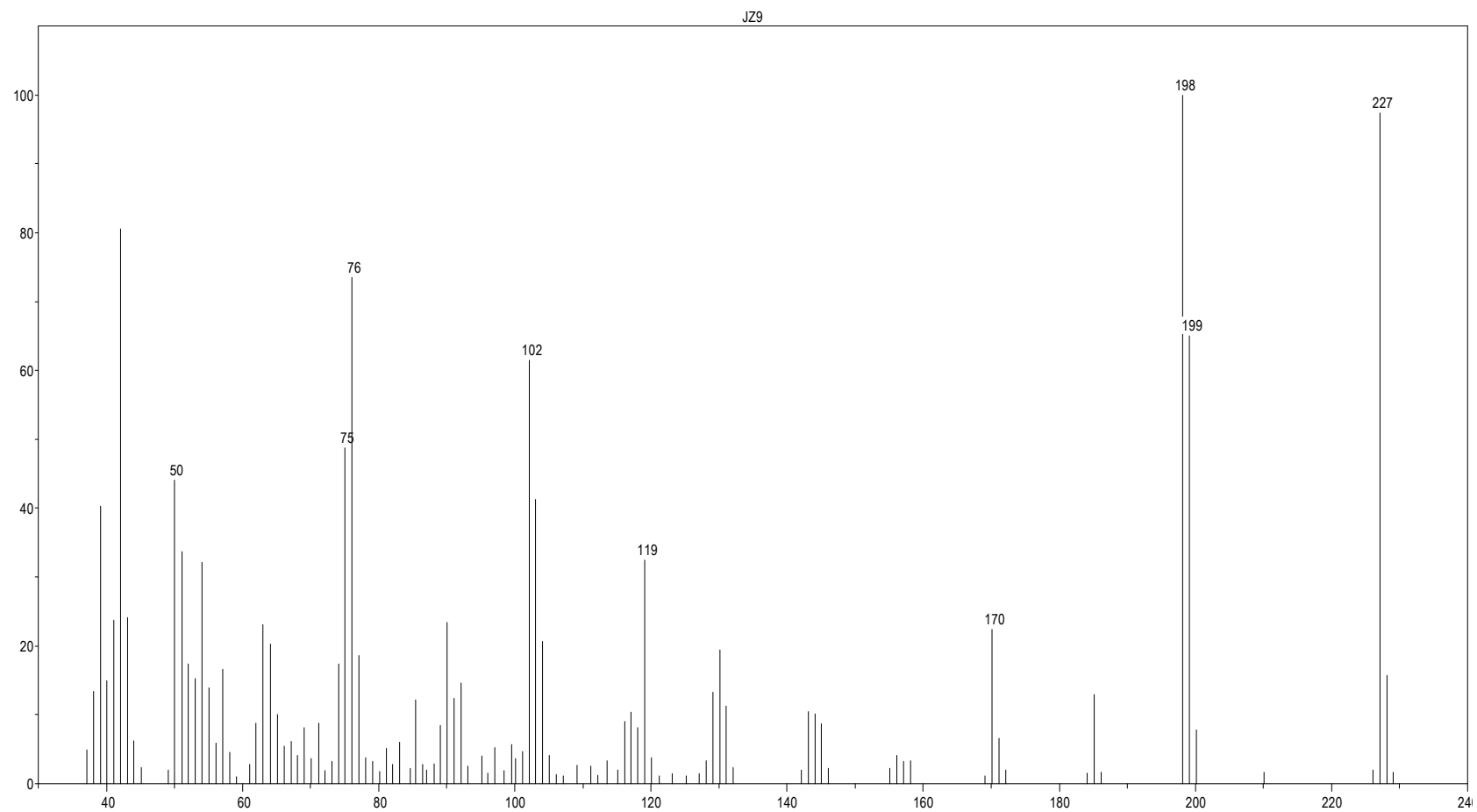


HSQC spectrum of 3-methyl-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3c**) (400 MHz, DMSO-*d*₆)

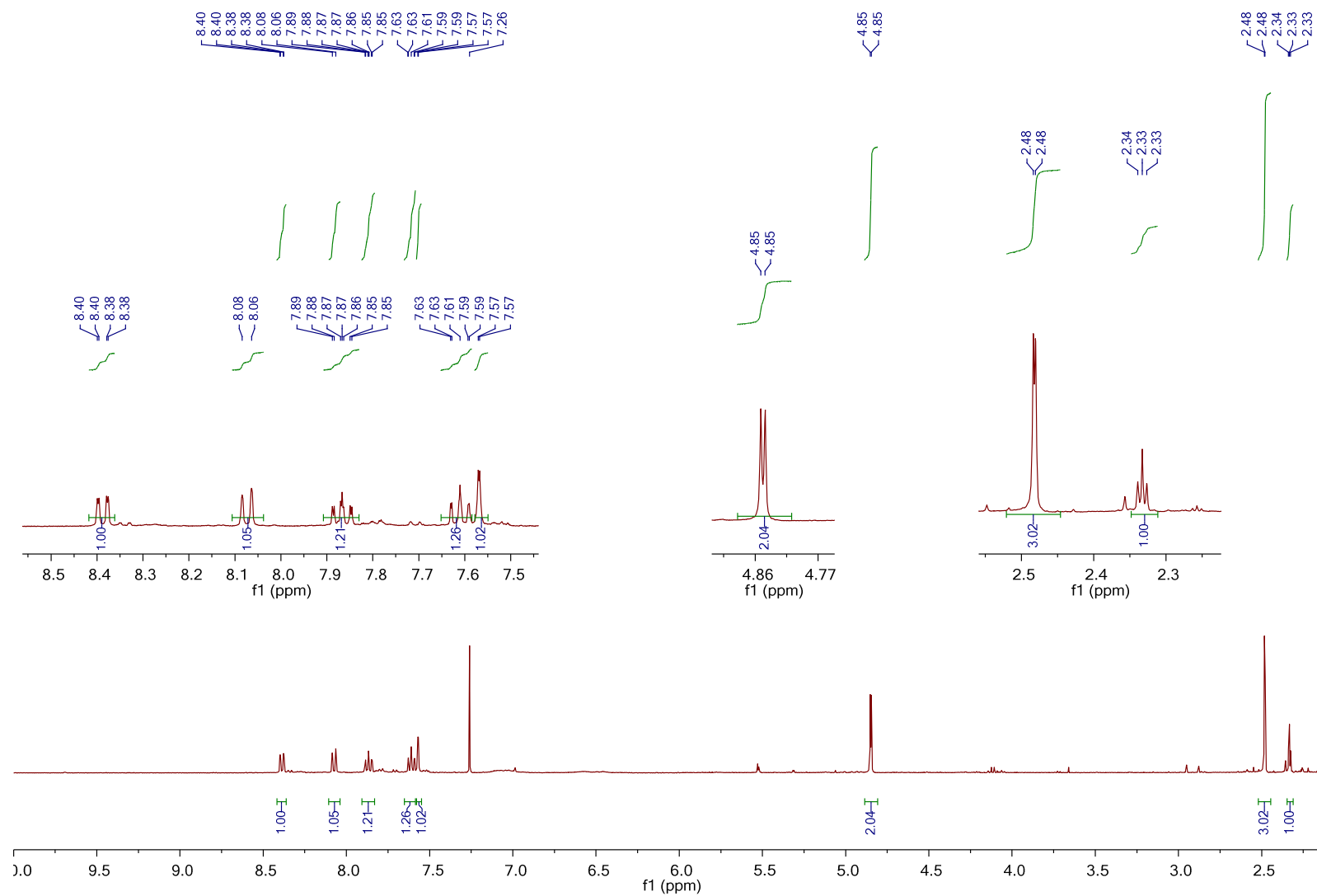


HMBC spectrum of 3-methyl-2*H*-pyrazino[2,1-*b*]quanzoline-1,6-dione (**3c**) (400 MHz, DMSO-*d*₆)

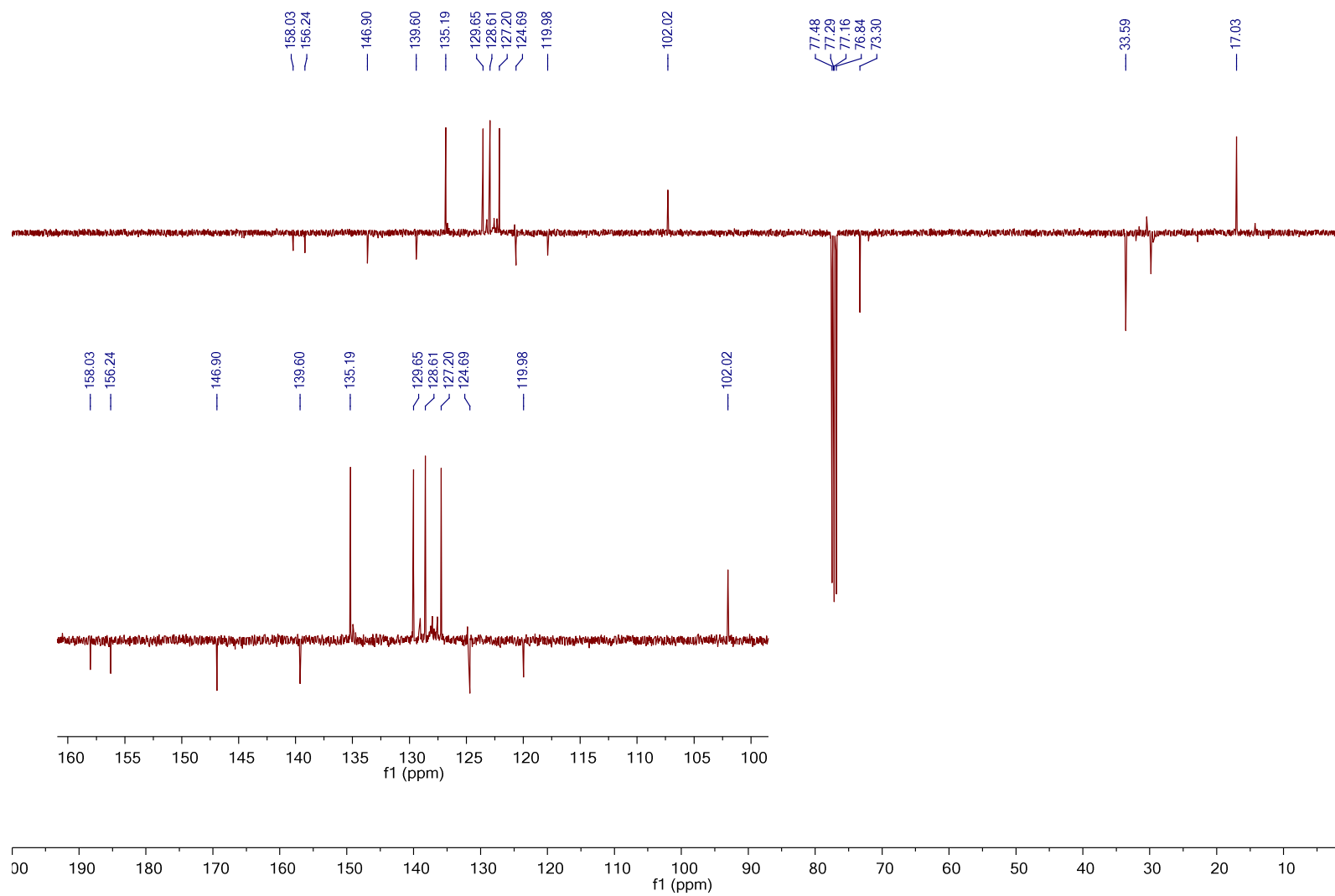


Mass spectrum of 3-methyl-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3c**)

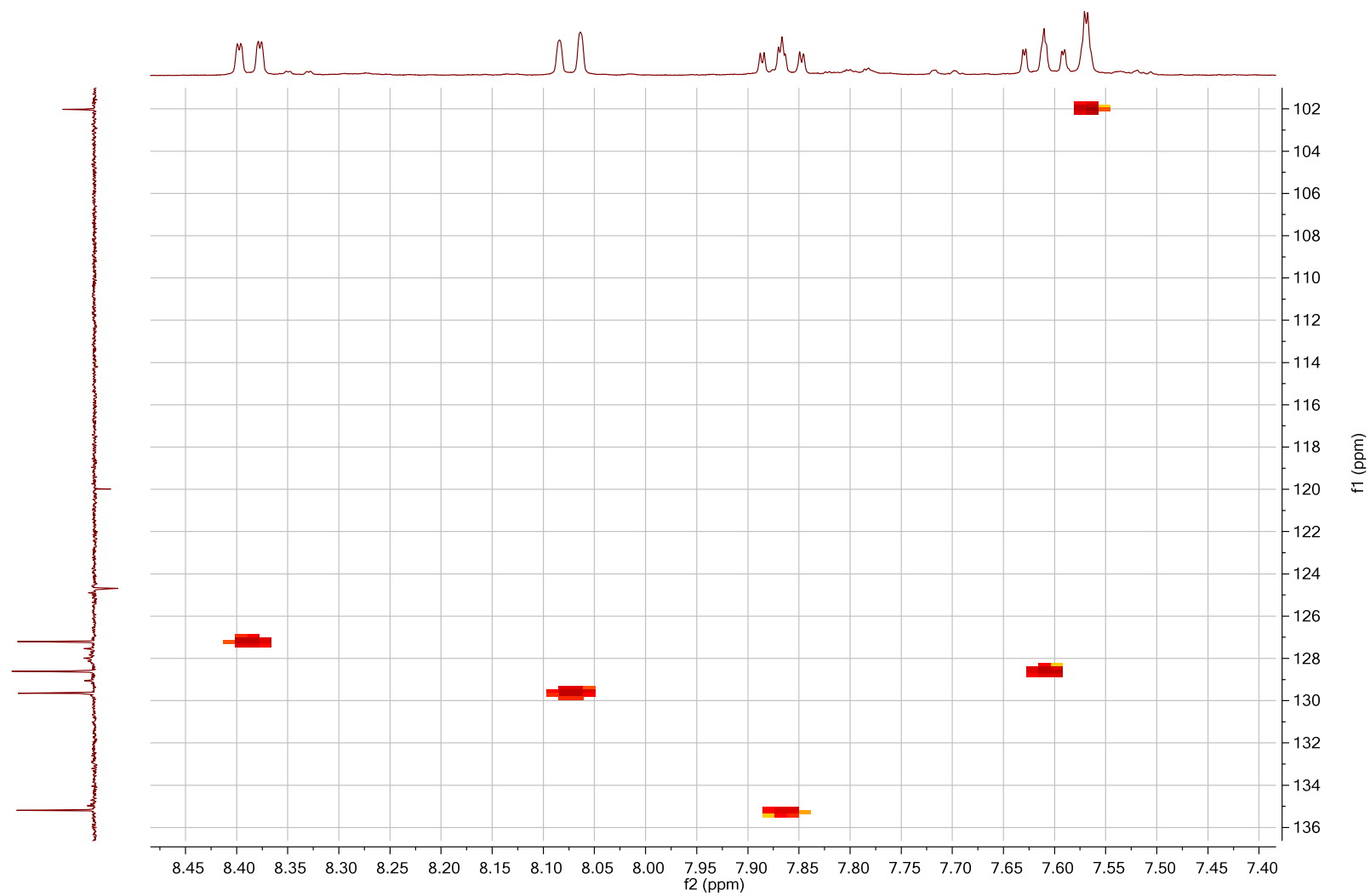
^1H NMR spectrum of 3-methyl-2-(prop-2-yn-1-yl)-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3d**) (400 MHz, CDCl_3)



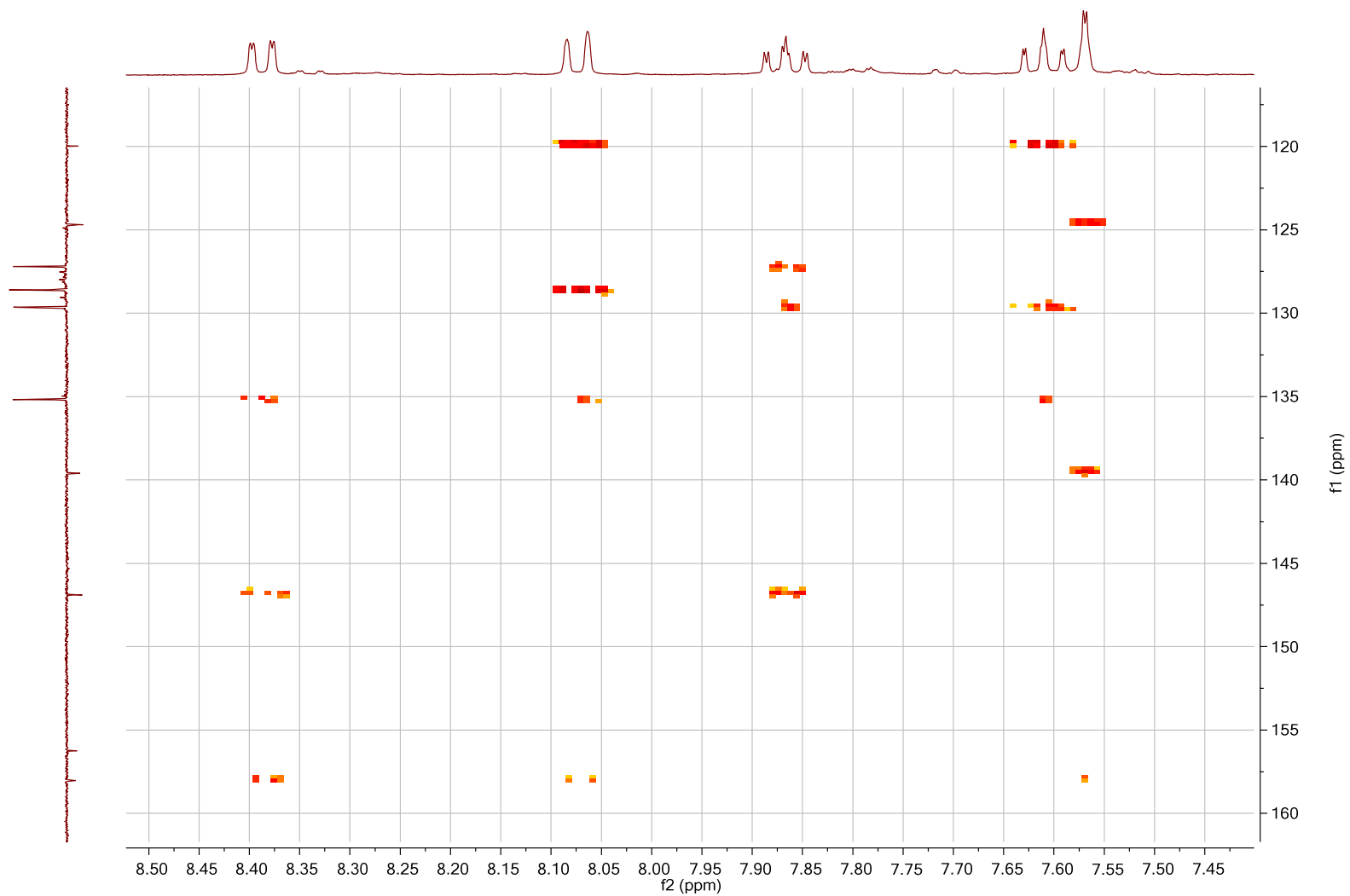
^{13}C NMR spectrum of 3-methyl-2-(prop-2-yn-1-yl)-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3d**) (100 MHz, CDCl_3)

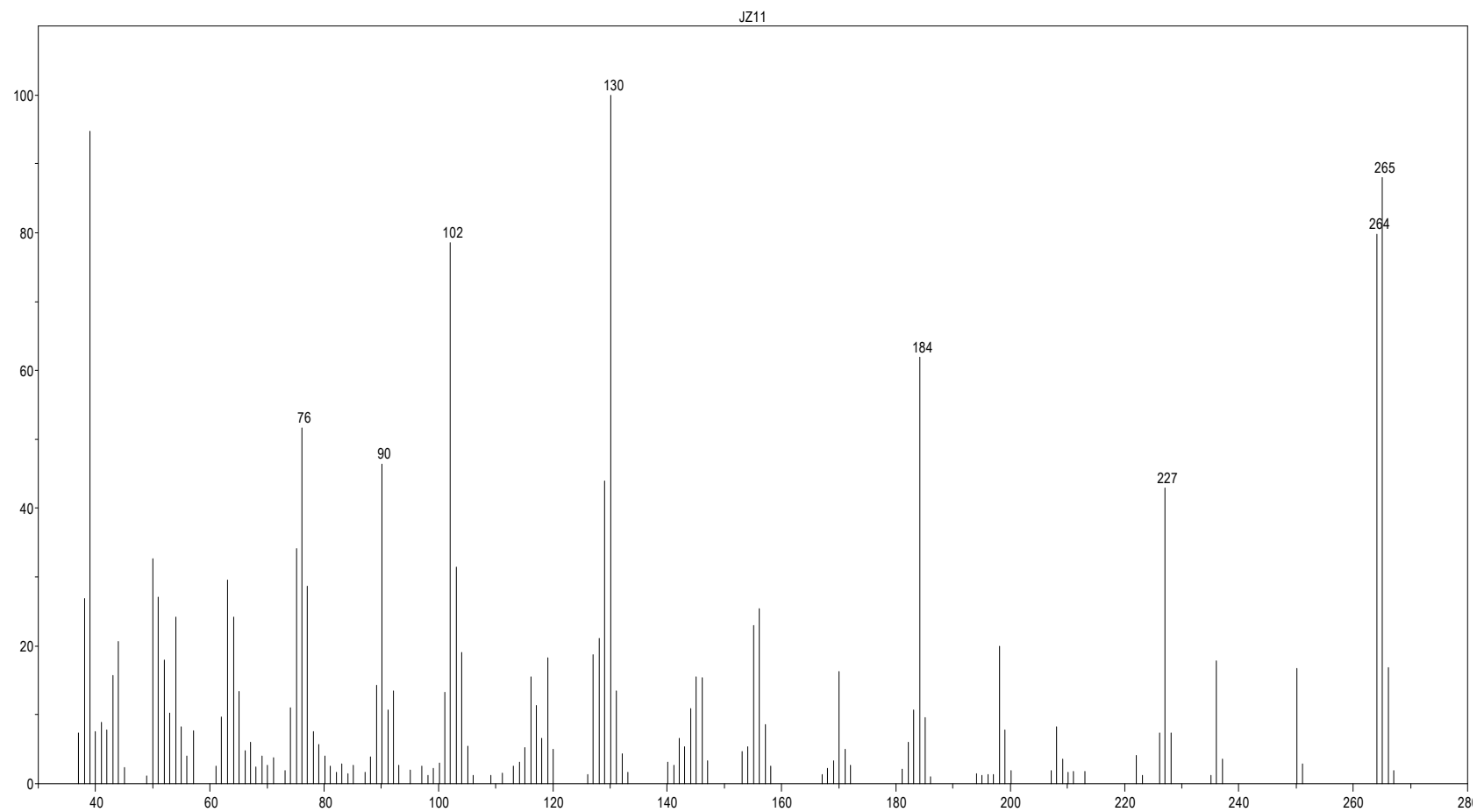


HSQC spectrum of 3-methyl-2-(prop-2-yn-1-yl)-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3d**) (400 MHz, CDCl₃)

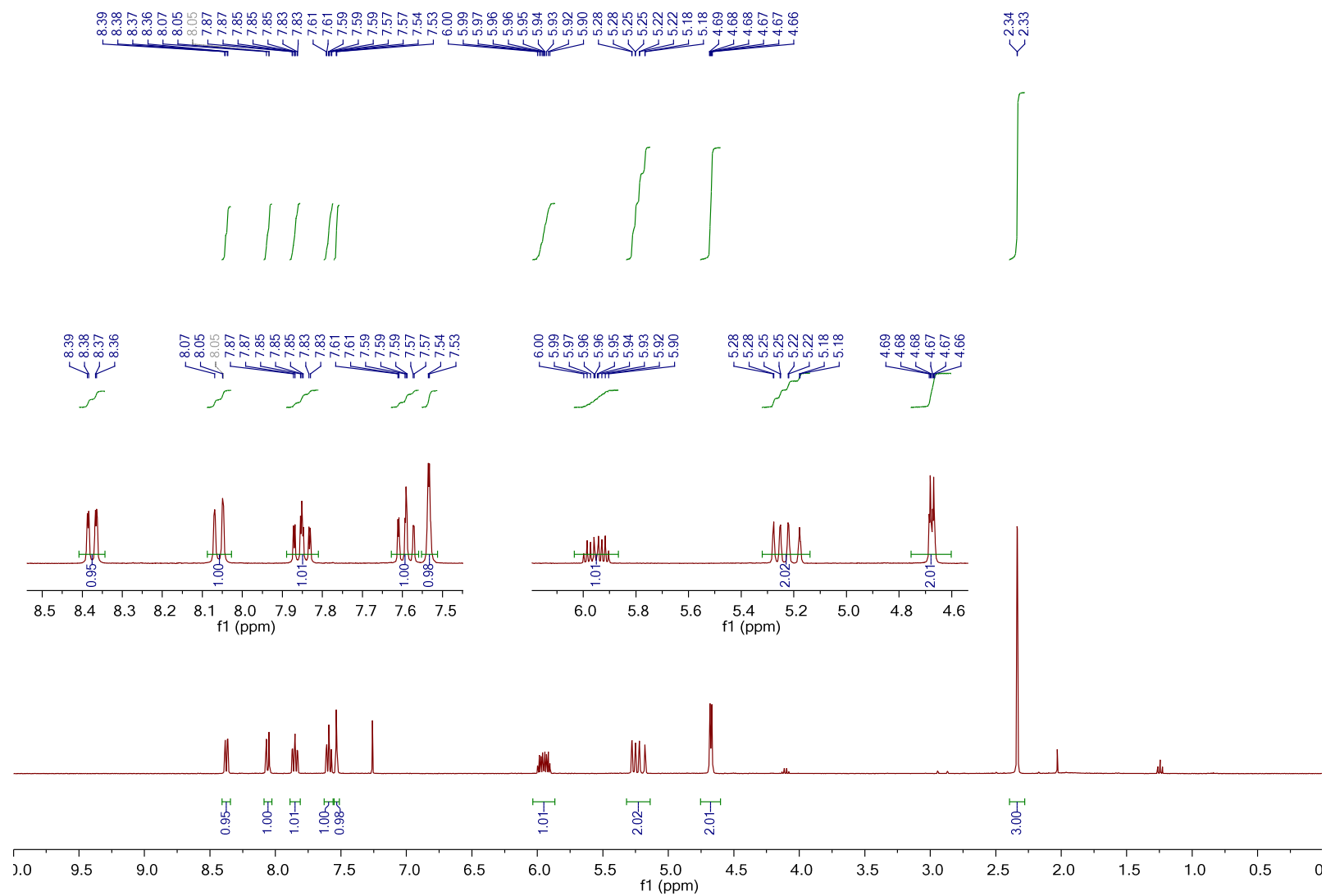


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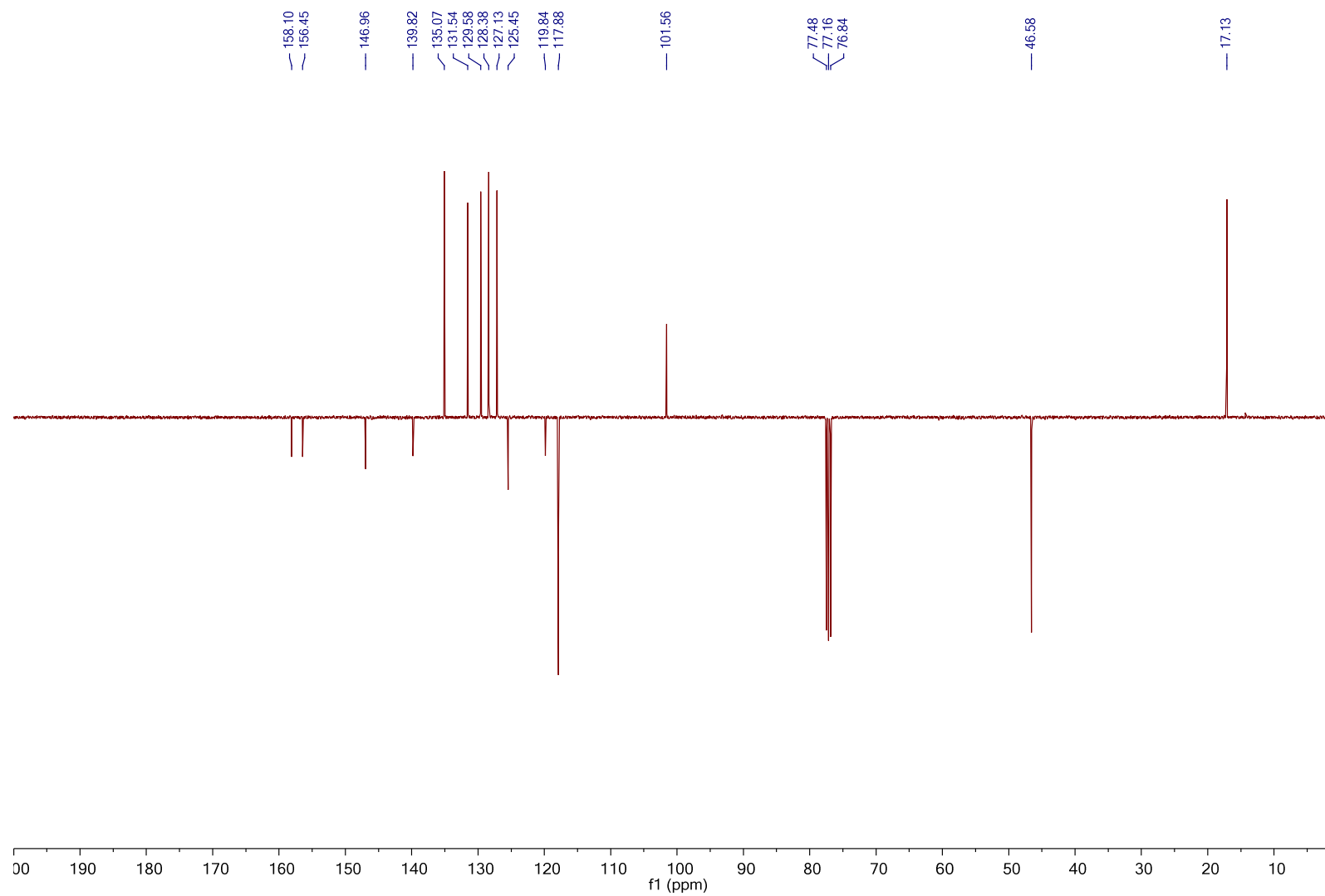


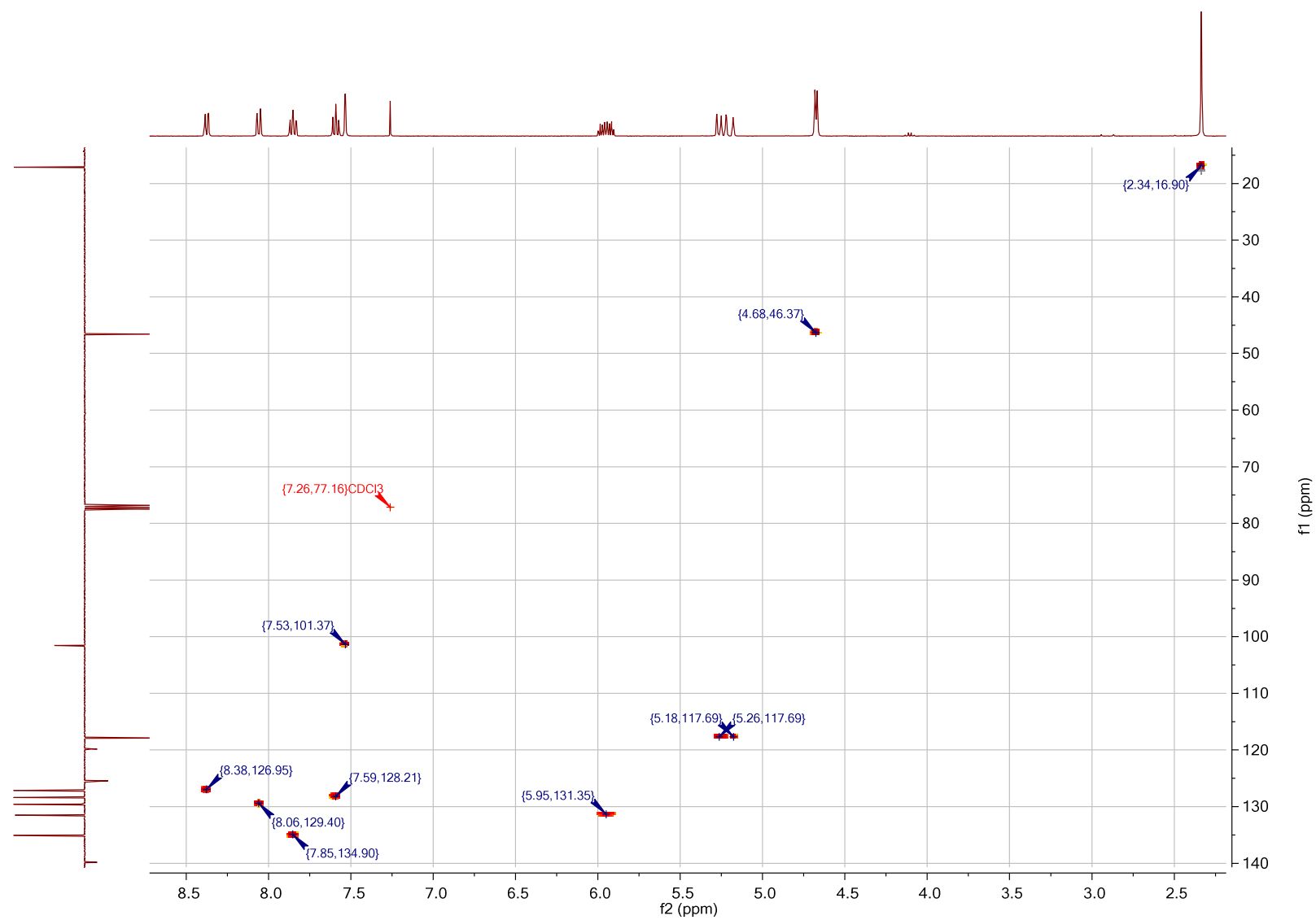
Mass spectrum of 3-methyl-2-(prop-2-yn-1-yl)-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3d**)

^1H NMR spectrum of 3-methyl-2-(prop-2-en-1-yl)-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3e**) (400 MHz, CDCl_3)

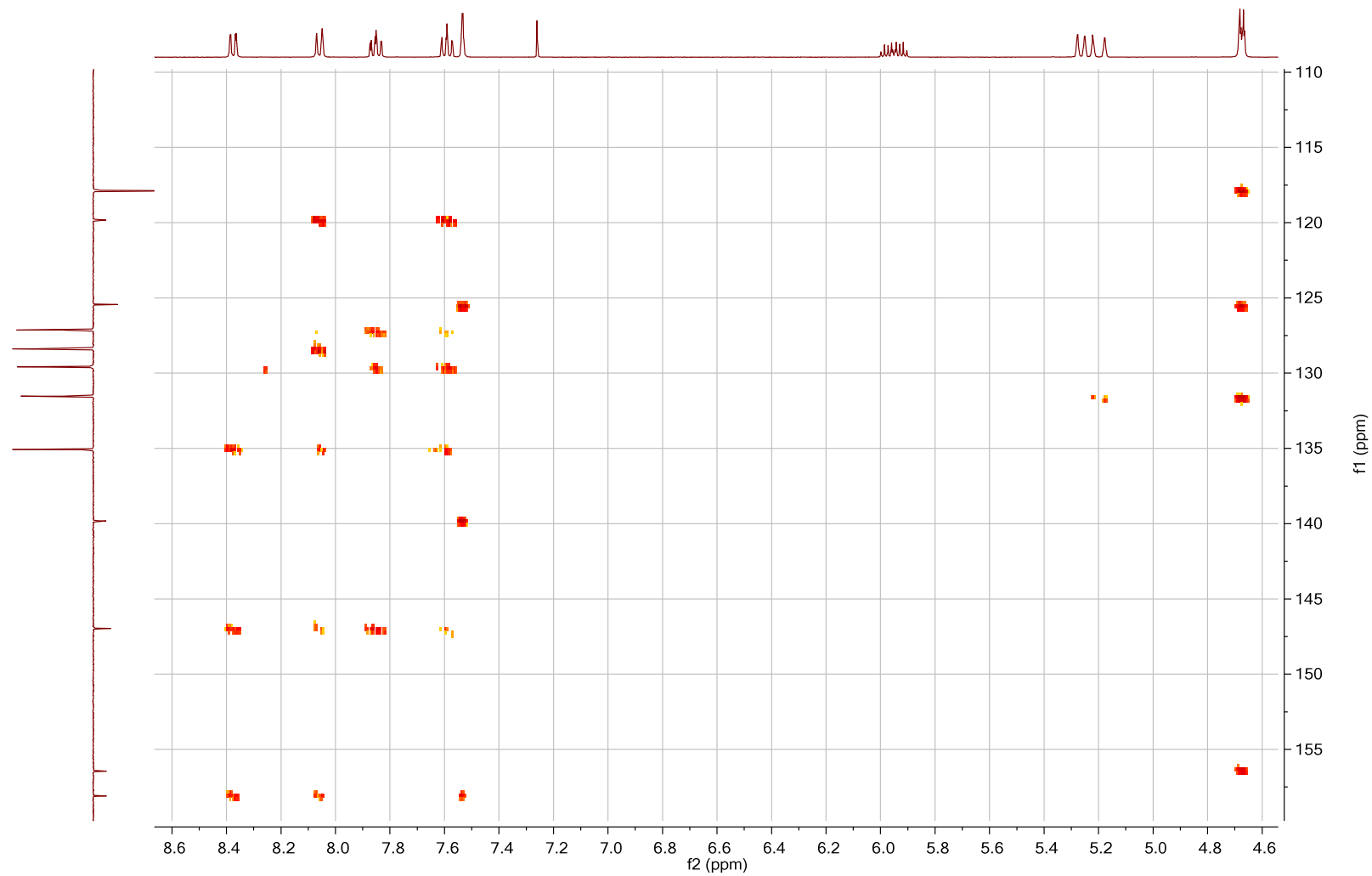


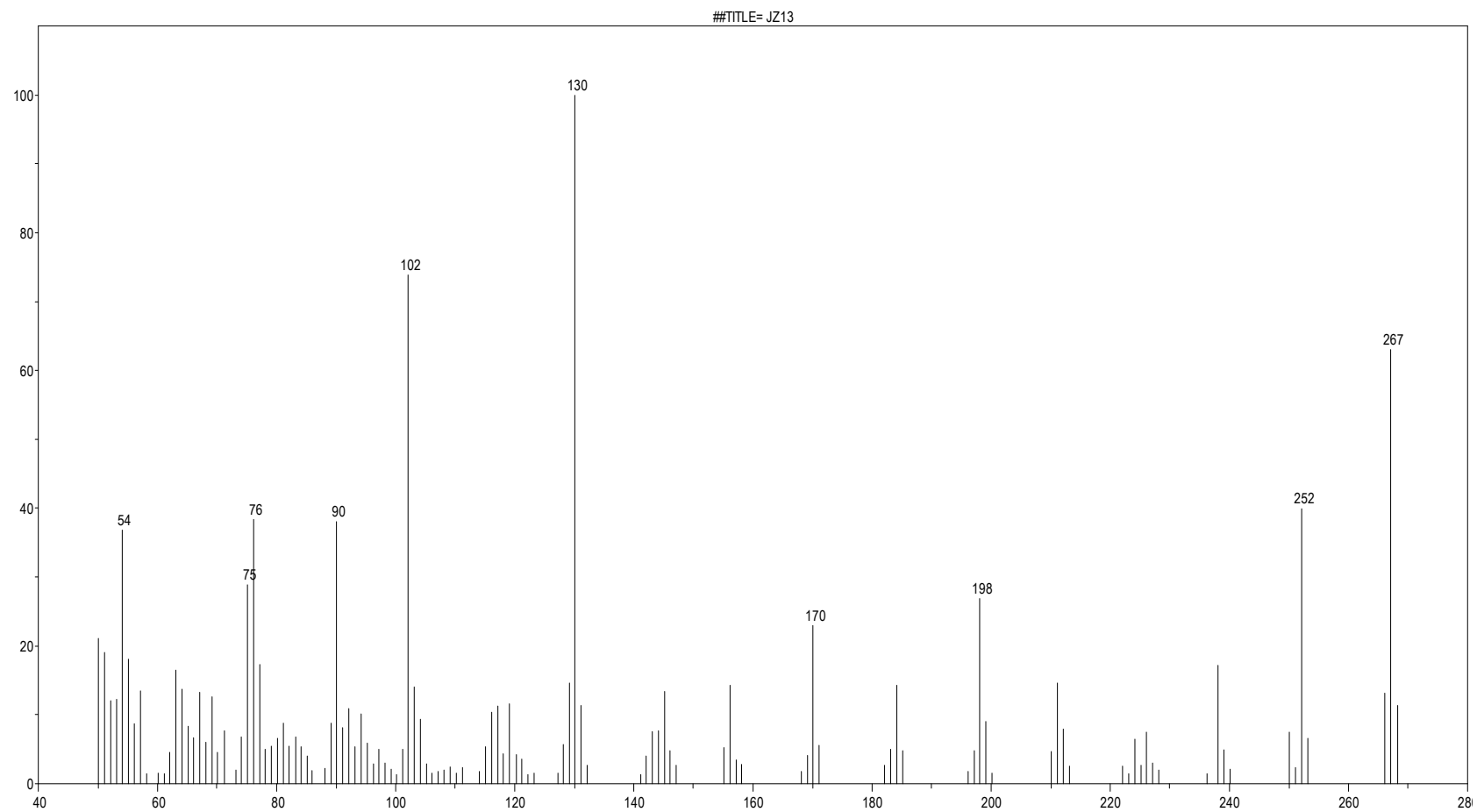
^{13}C NMR spectrum of 3-methyl-2-(prop-2-en-1-yl)-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3e**) (100 MHz, CDCl_3)



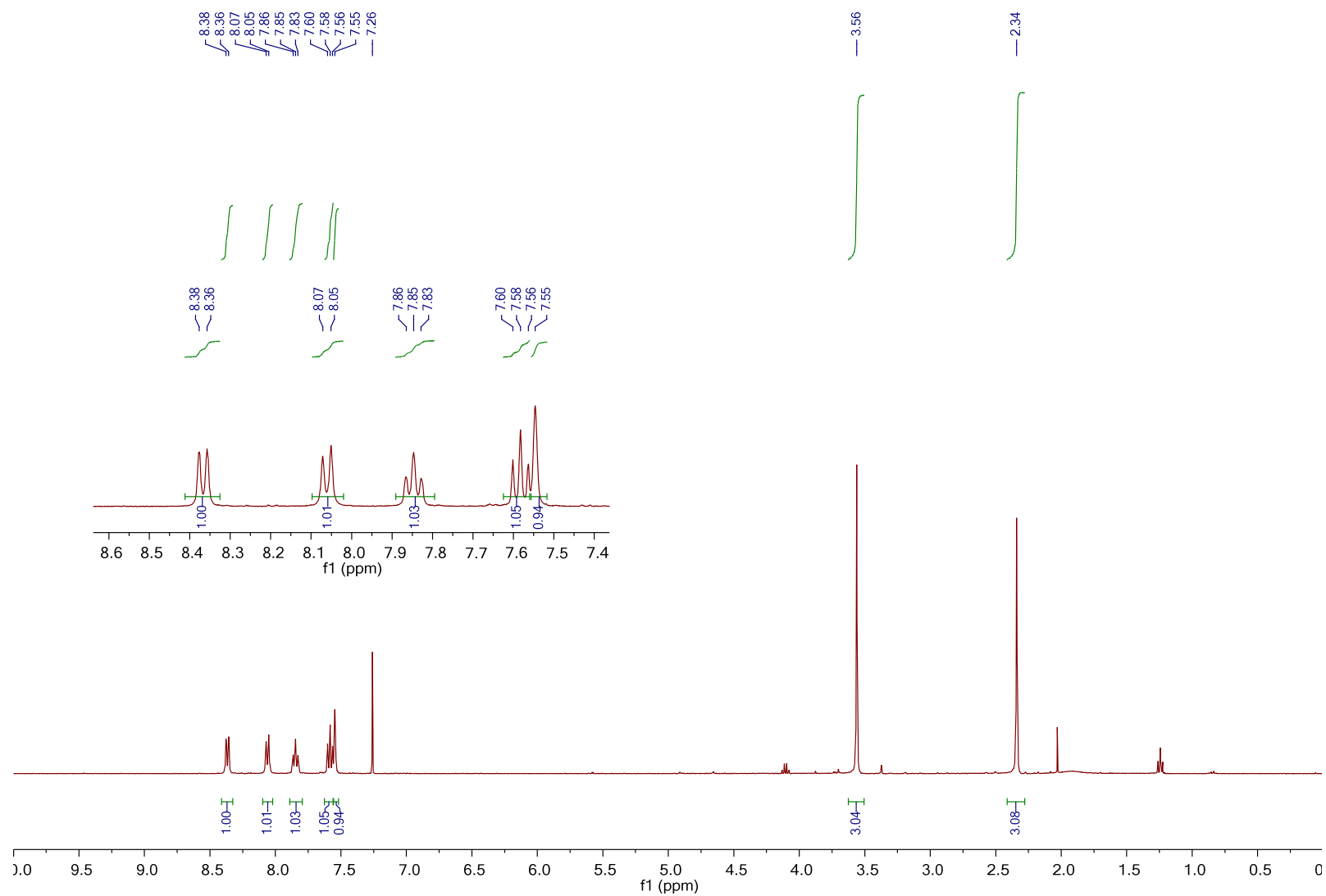
HSQC spectrum of 3-methyl-2-(prop-2-en-1-yl)-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3e**) (400 MHz, CDCl₃)

HMBC spectrum of 3-methyl-2-(prop-2-en-1-yl)-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3e**) (400 MHz, CDCl₃)

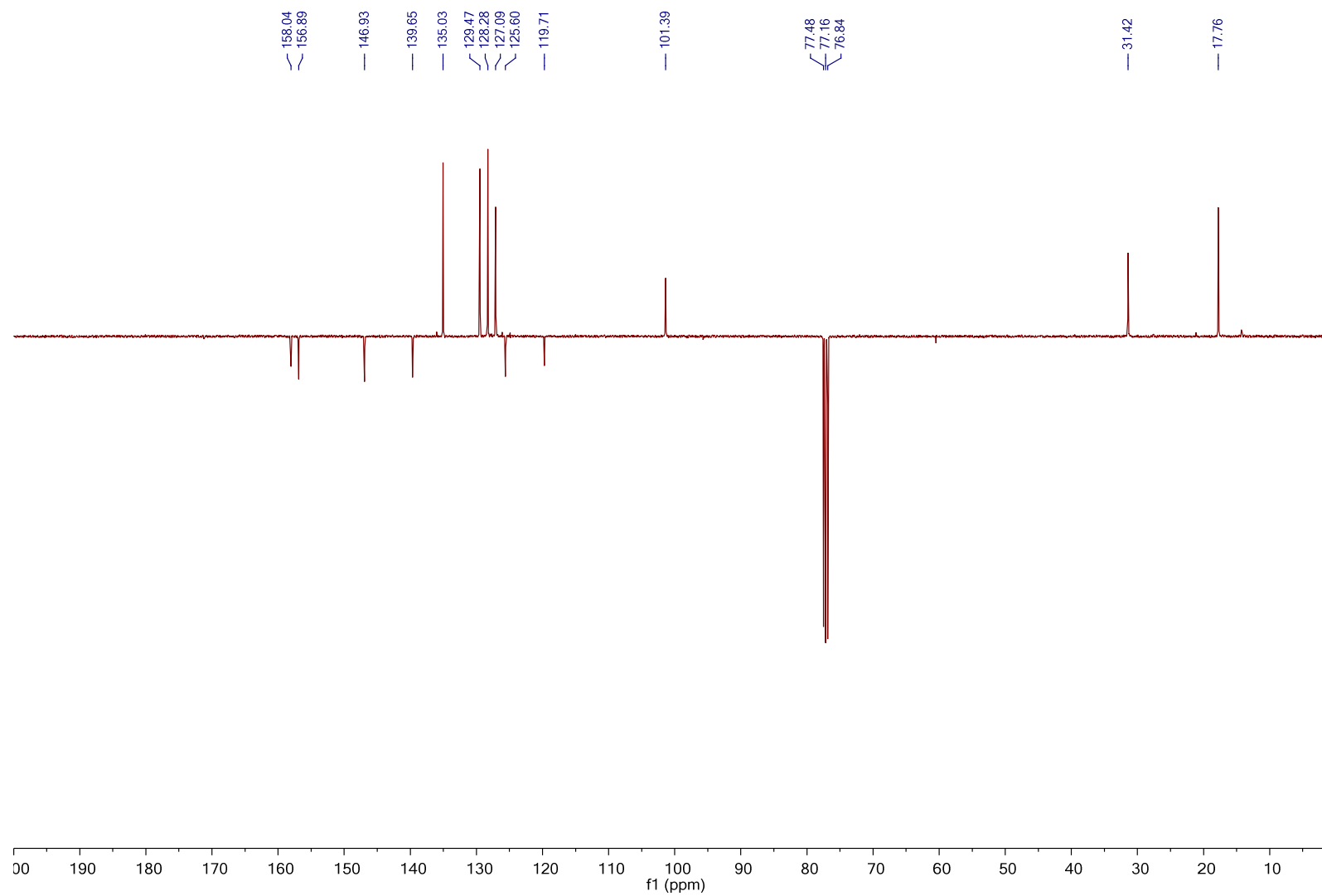


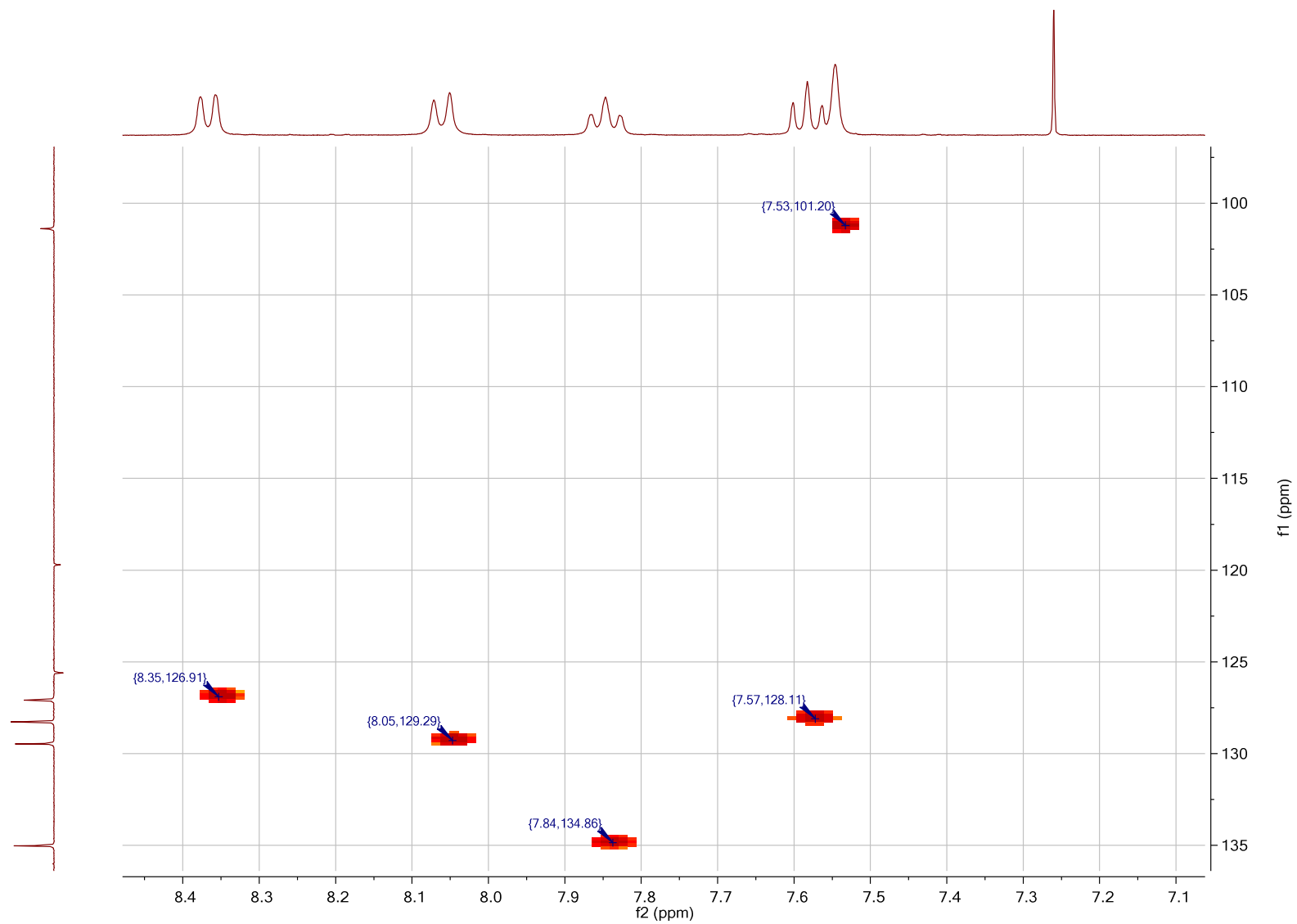
Mass spectrum of 3-methyl-2-(prop-2-en-1-yl)-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3e**)

^1H NMR spectrum of 2,3-dimethyl-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3f**) (400 MHz, CDCl_3)

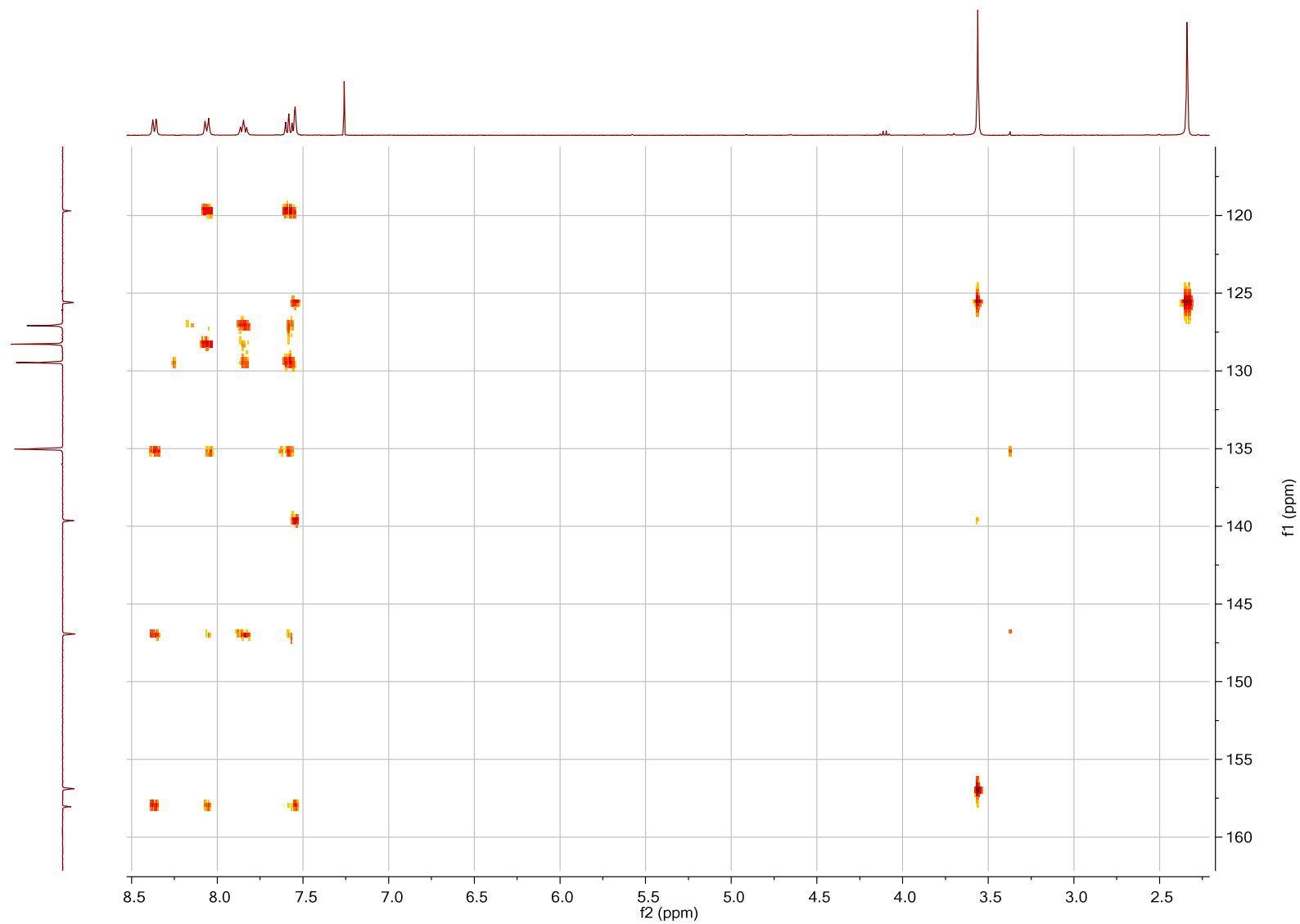


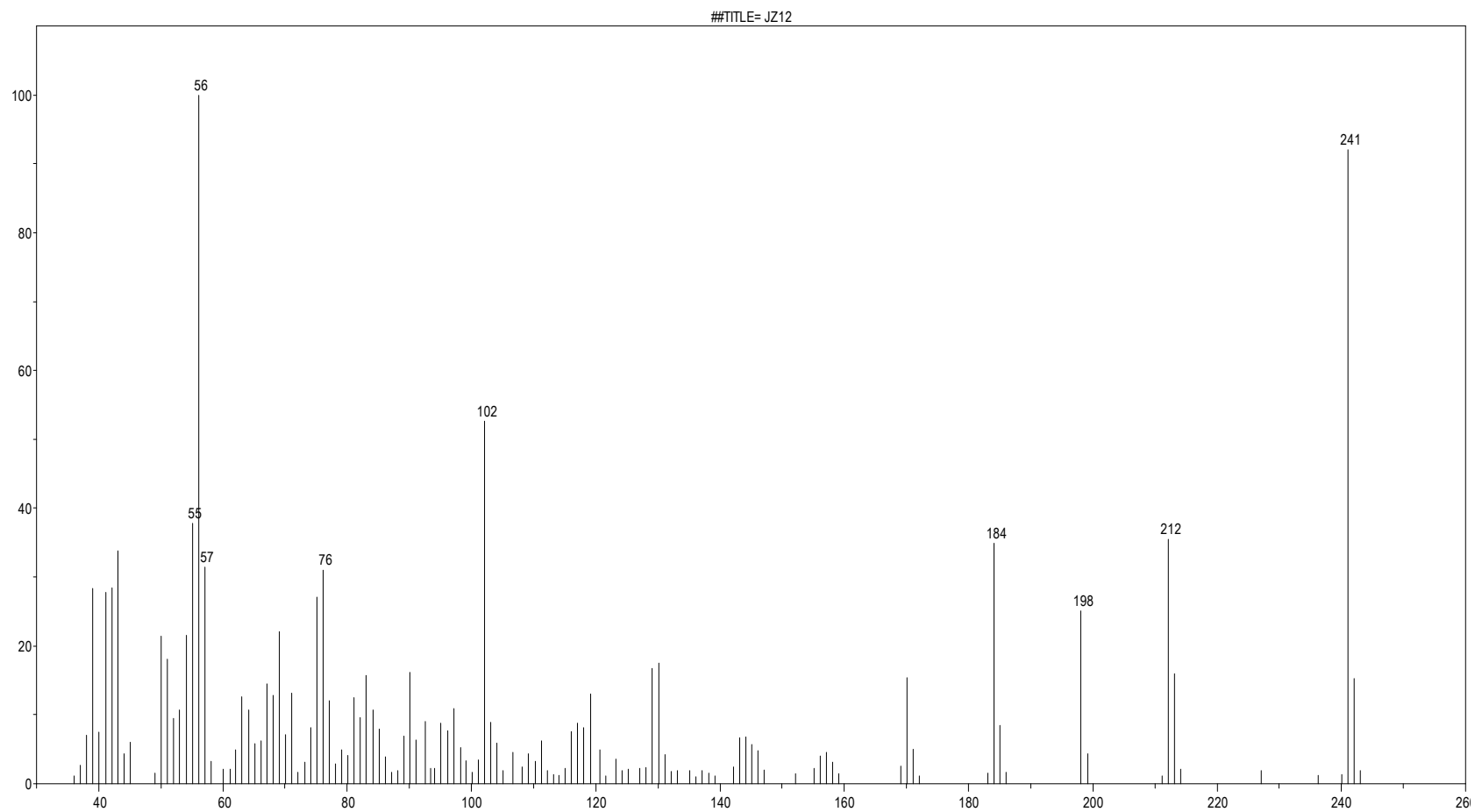
^{13}C NMR spectrum of 2,3-dimethyl-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3f**) (100 MHz, CDCl_3)



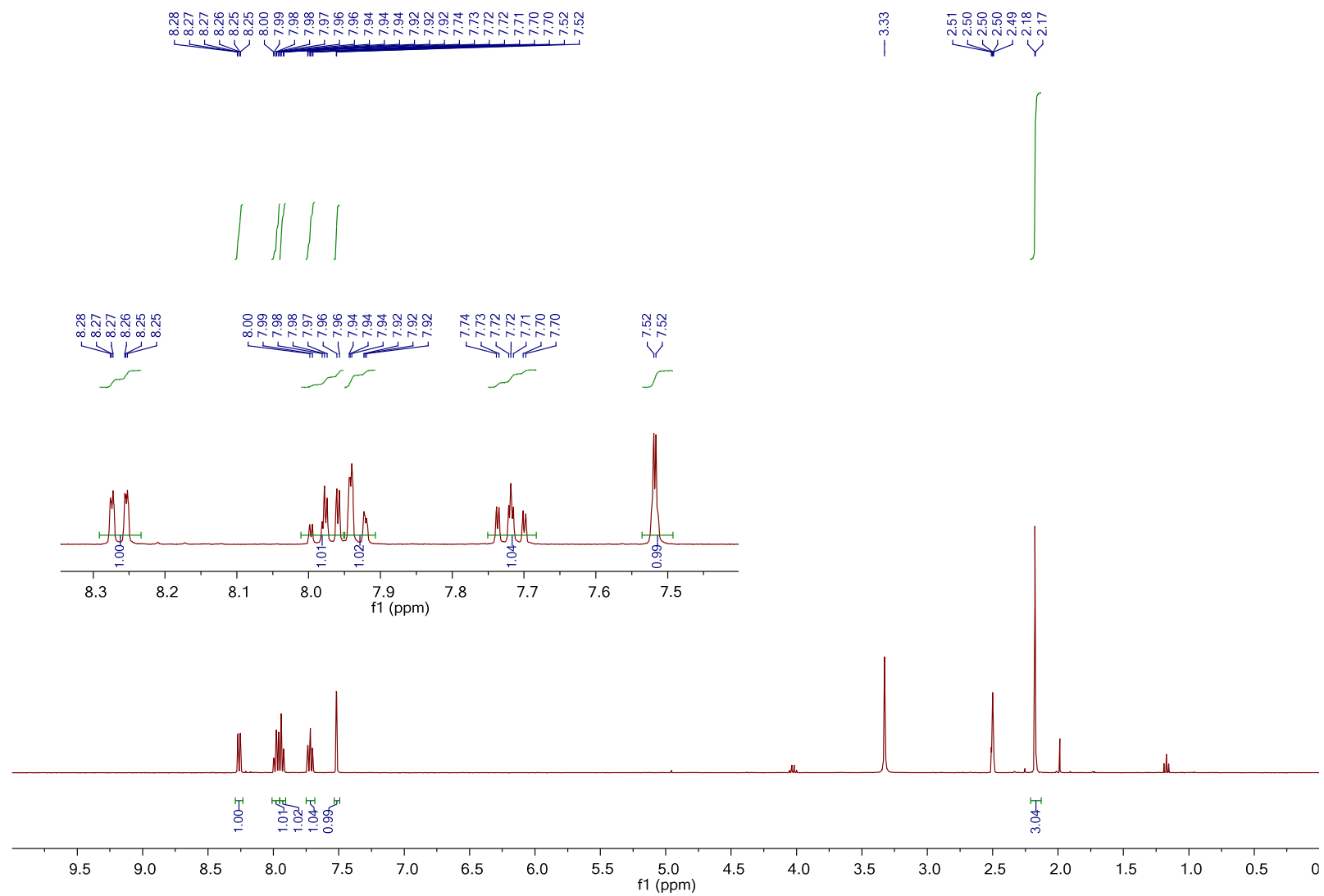
HSQC spectrum of 2,3-dimethyl-2*H*-pyrazino[2,1-*b*]quinoxaline-1,6-dione (**3f**) (400 MHz, CDCl₃)

HMBC spectrum of 2,3-dimethyl-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3f**) (400 MHz, CDCl₃)

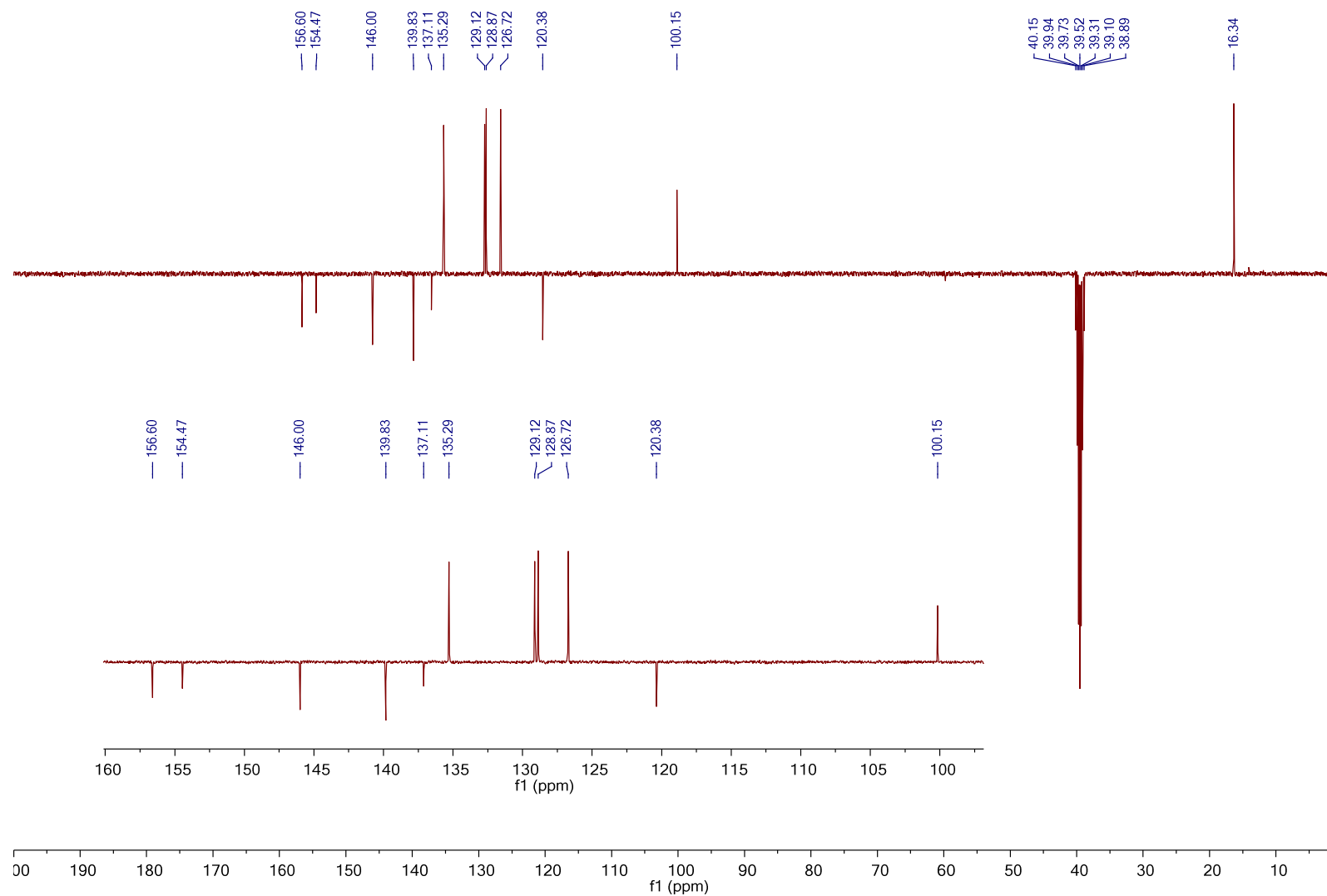


Mass spectrum of 2,3-dimethyl-2*H*-pyrazino[2,1-*b*]quiazoline-1,6-dione (**3f**)

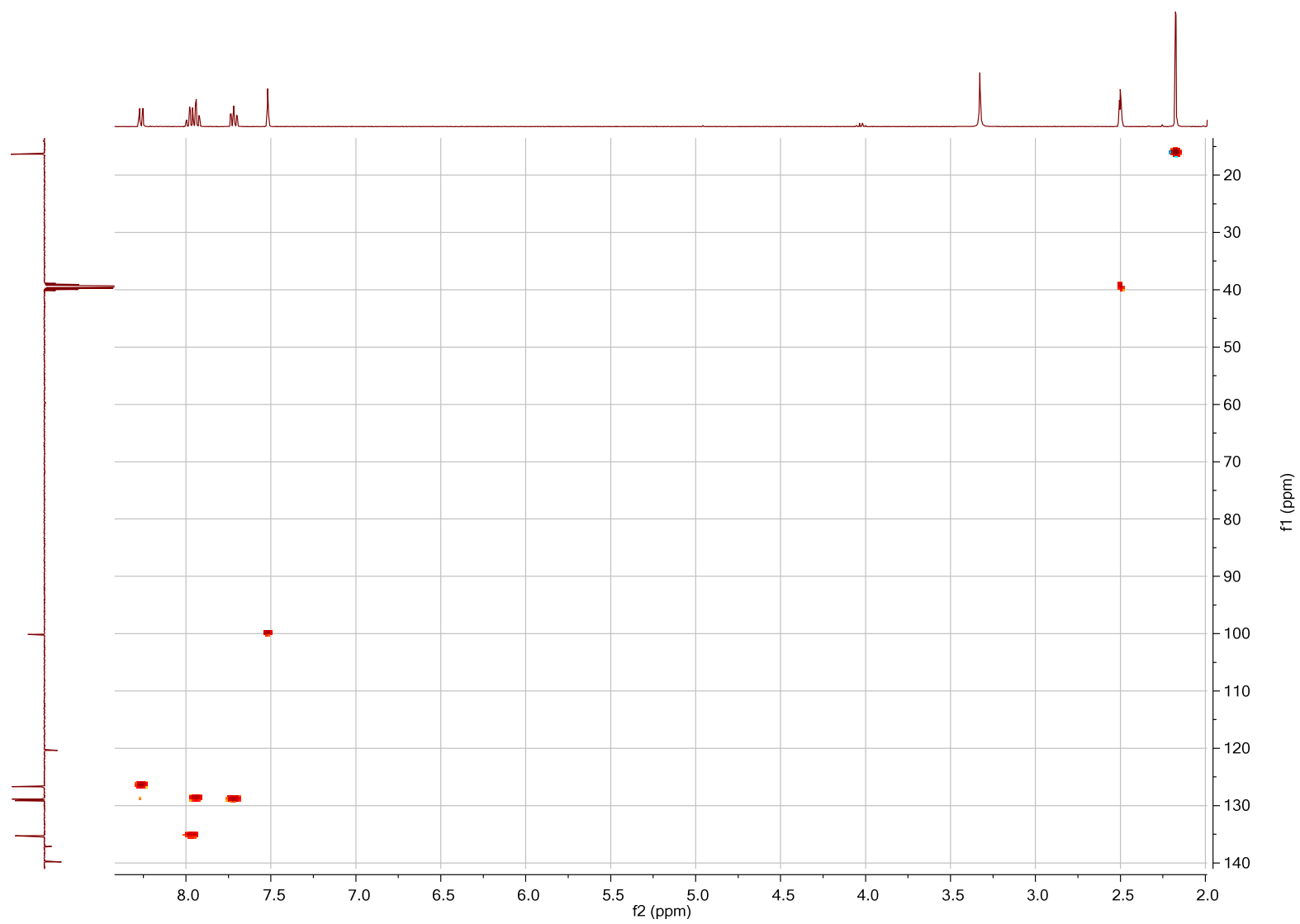
^1H NMR spectrum of 3-methyl[1,4]oxazino[3,4-*b*]quinazoline-1,6-dione (**5**) (400 MHz, $\text{DMSO-}d_6$)



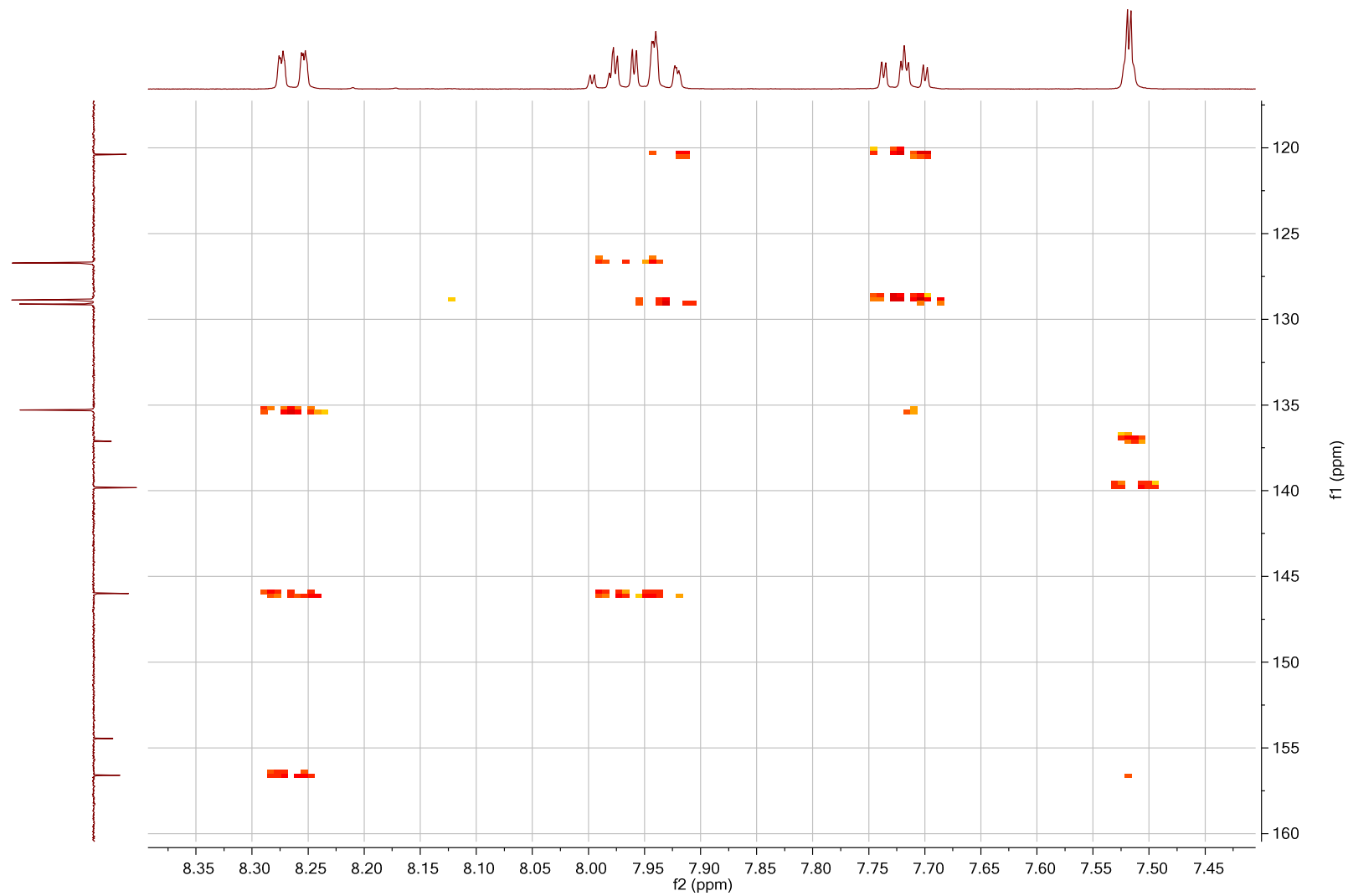
^{13}C NMR spectrum of 3-methyl[1,4]oxazino[3,4-*b*]quinazoline-1,6-dione (**5**) (100 MHz, $\text{DMSO-}d_6$)



HSQC spectrum of 3-methyl[1,4]oxazino[3,4-*b*]quinazoline-1,6-dione (**5**) (400 MHz, DMSO-*d*₆)



HMBC spectrum of 3-methyl[1,4]oxazino[3,4-*b*]quinazoline-1,6-dione (**5**) (400 MHz, DMSO-*d*₆)



Mass spectrum of 3-methyl[1,4]oxazino[3,4-*b*]quinazoline-1,6-dione (**5**)