



Supporting Information

for

Synthesis of new pyrazolo[1,2,3]triazines by cyclative cleavage of pyrazolyltriazenes

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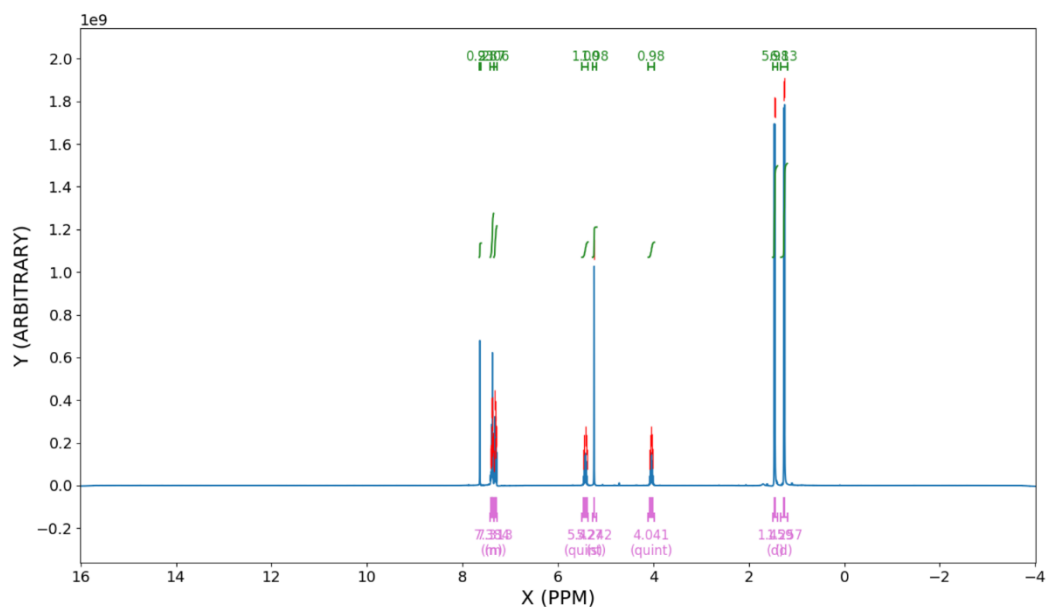
Copies of spectra

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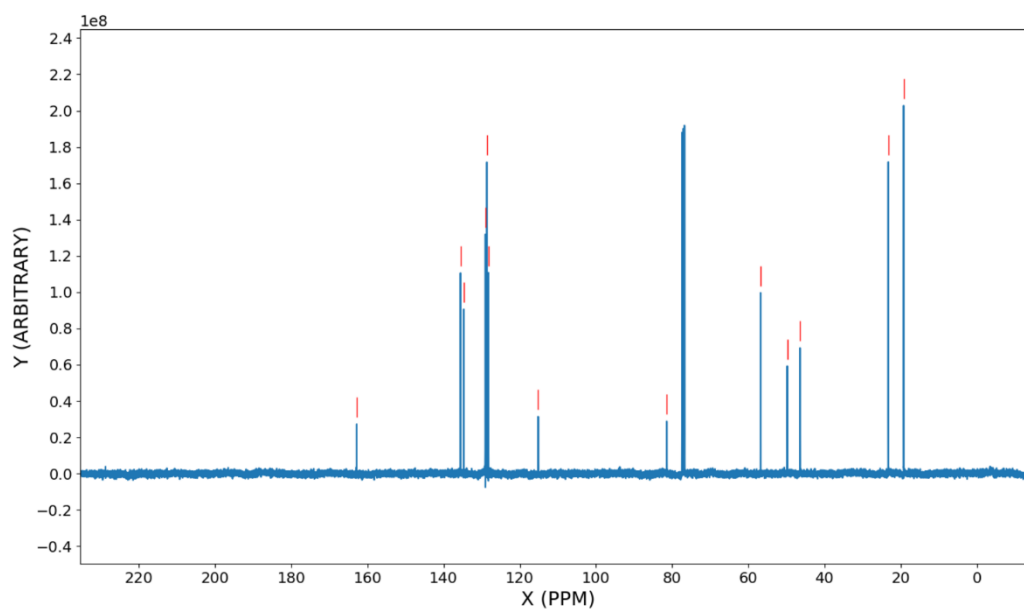
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(E)-1-Benzyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile (12a)

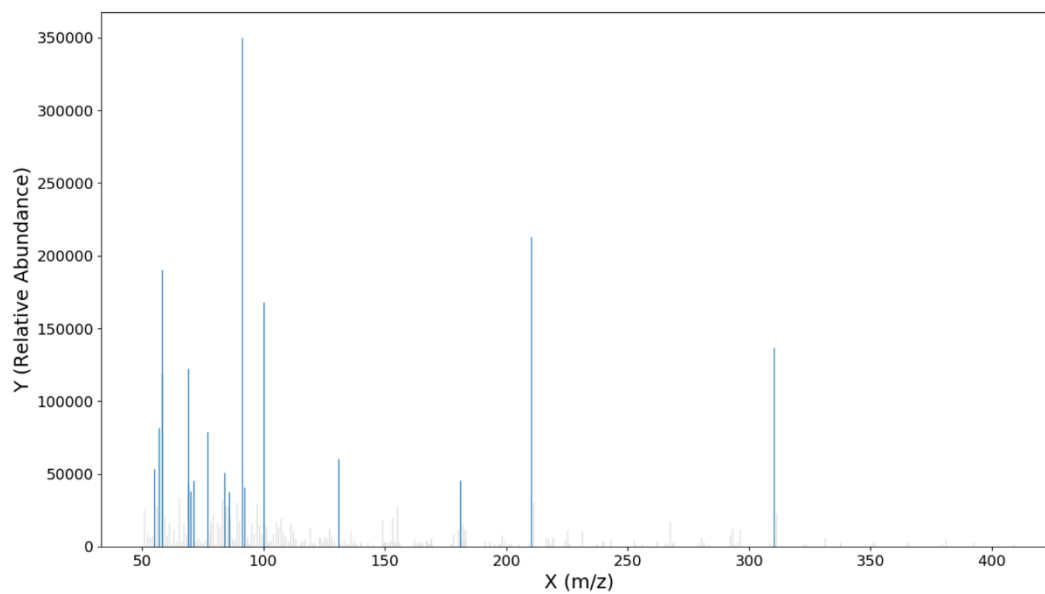
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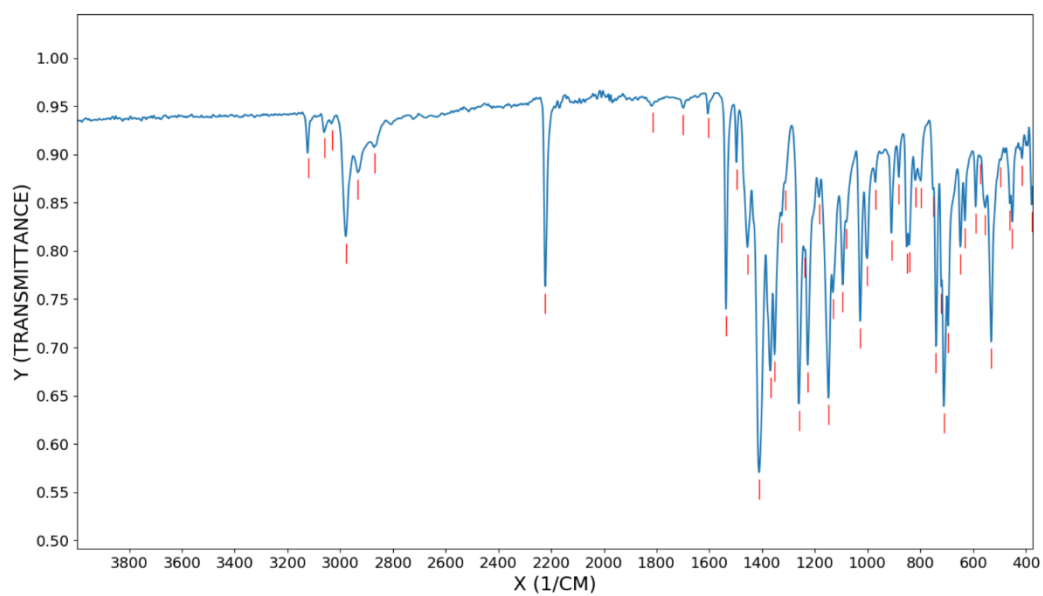
CHMO:0000593 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000470 | mass spectrometry (MS)

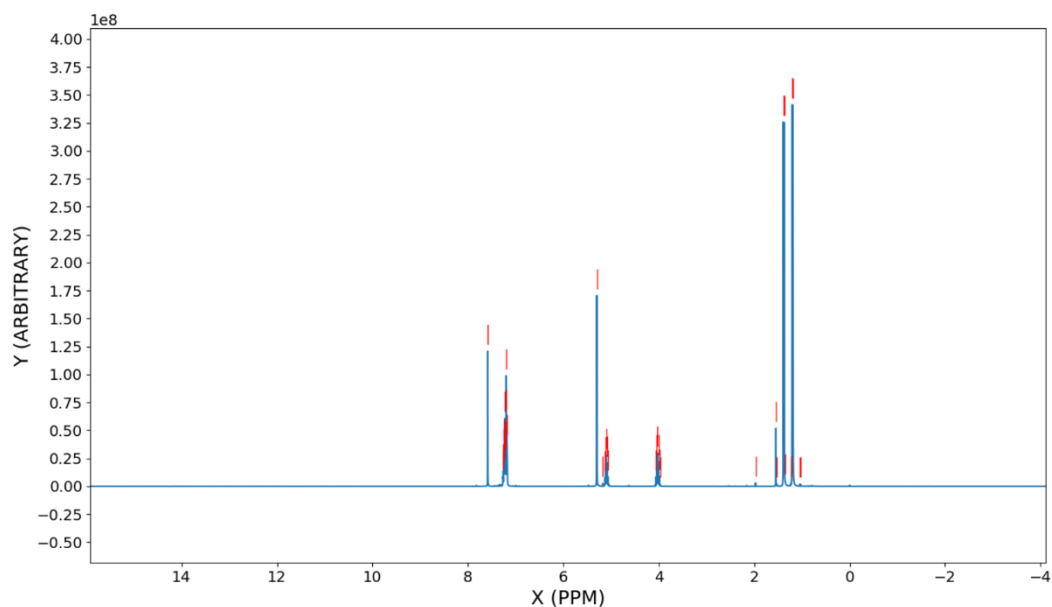


CHMO:0000630 | infrared absorption spectroscopy (IR)

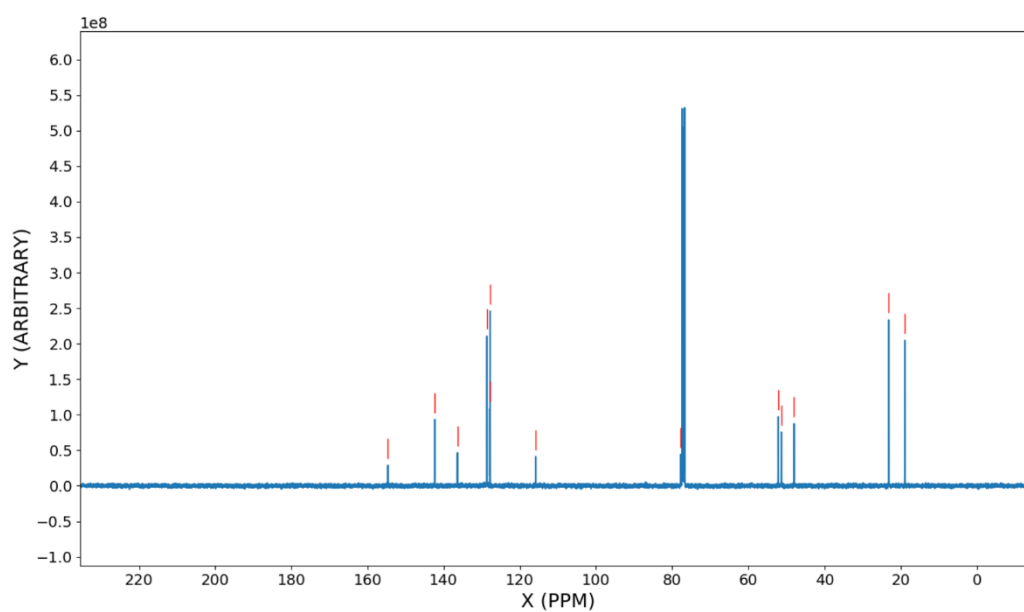


(*E*)-1-Benzyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazole-4-carbonitrile (13a)

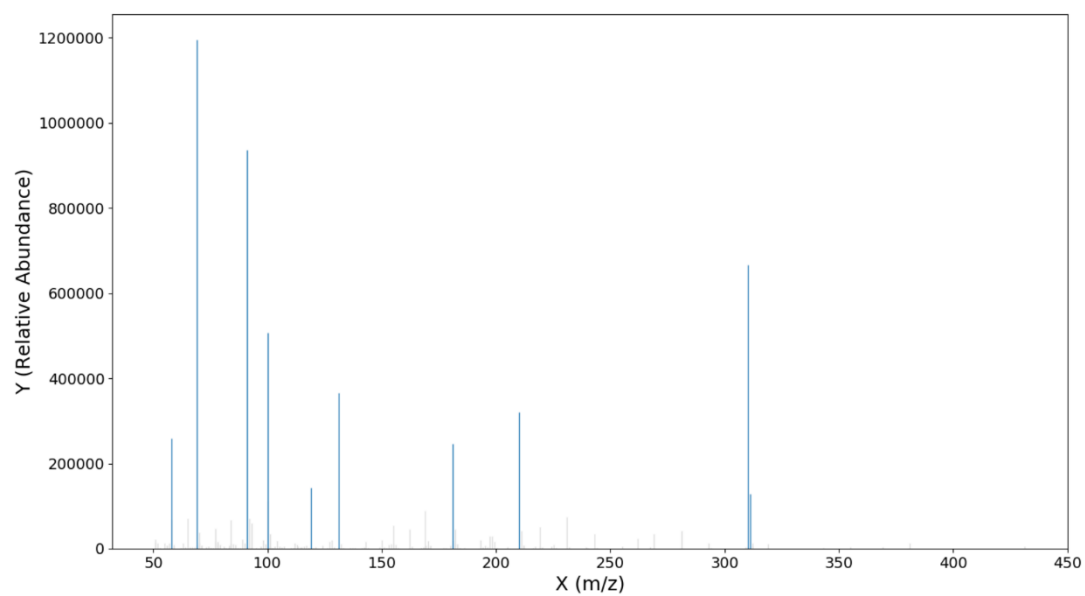
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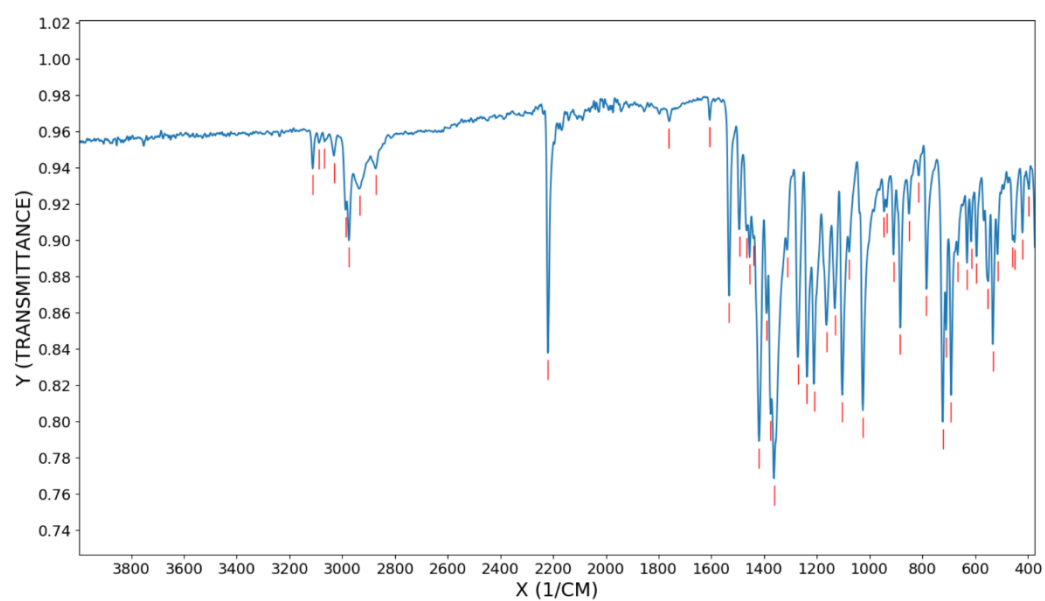
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000480 | electron ionisation mass spectrometry (EI-MS)

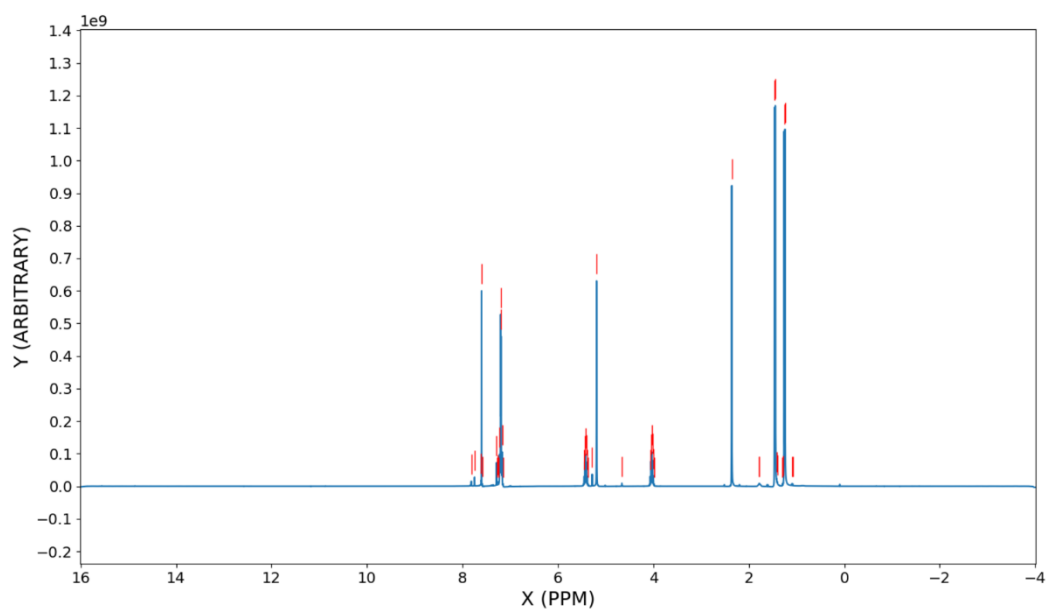


CHMO:0000630 | infrared absorption spectroscopy (IR)

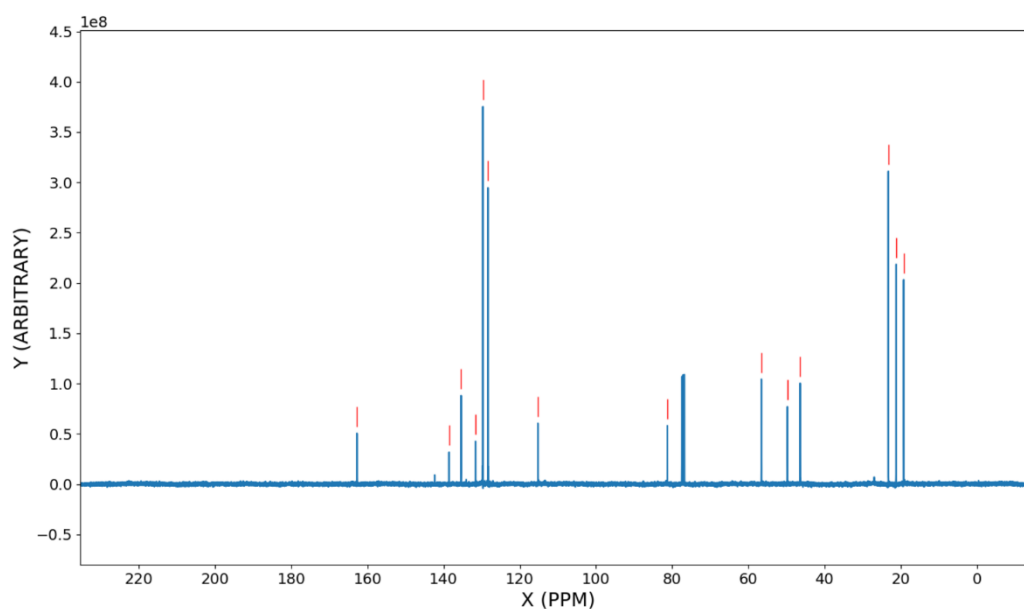


(*E*)-3-(3,3-Diisopropyltriaz-1-en-1-yl)-1-(4-methylbenzyl)-1*H*-pyrazole-4-carbonitrile (12b)

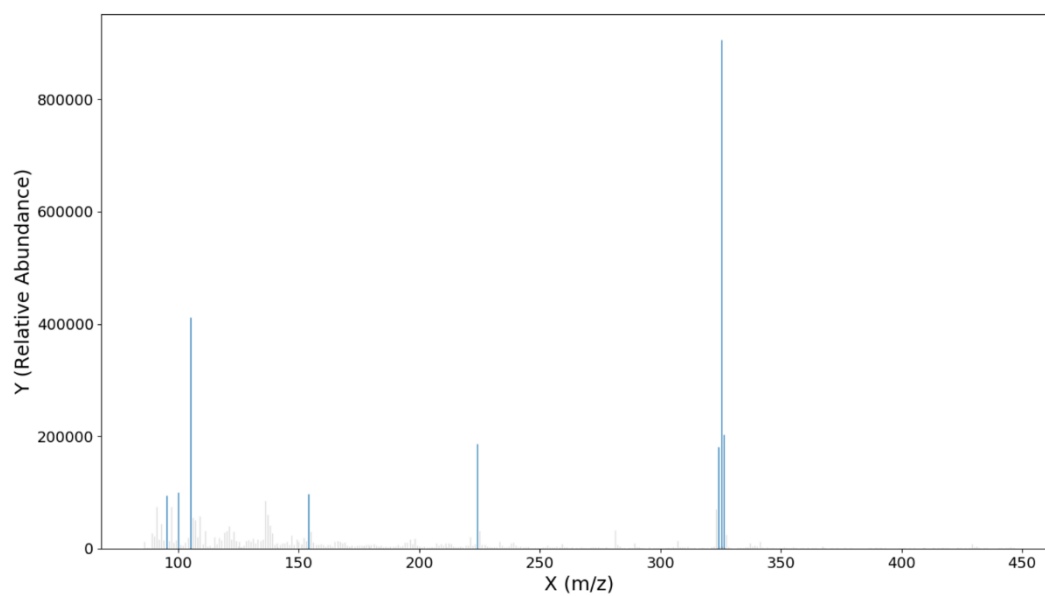
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



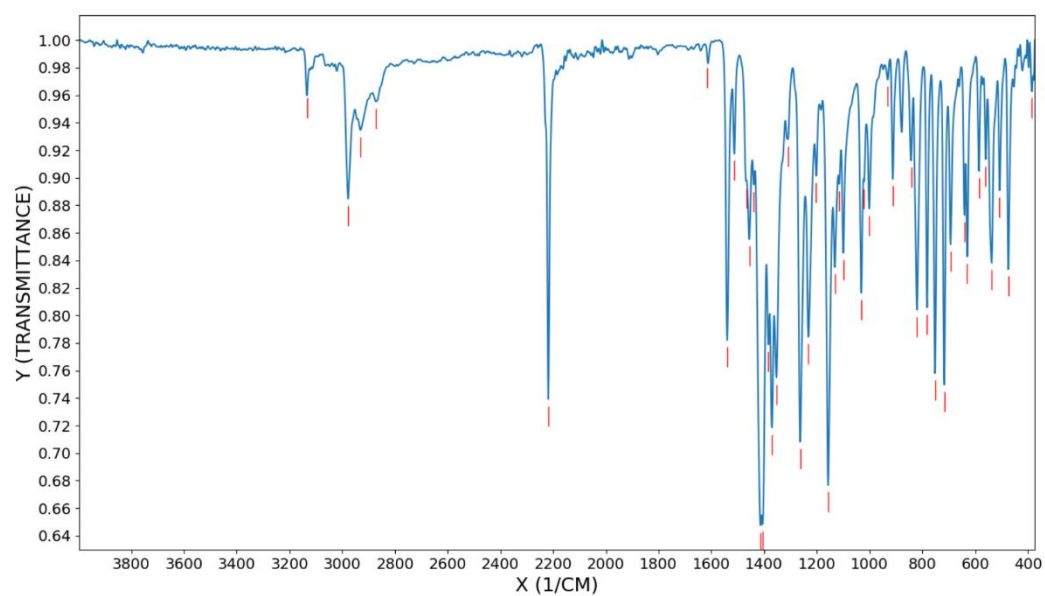
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

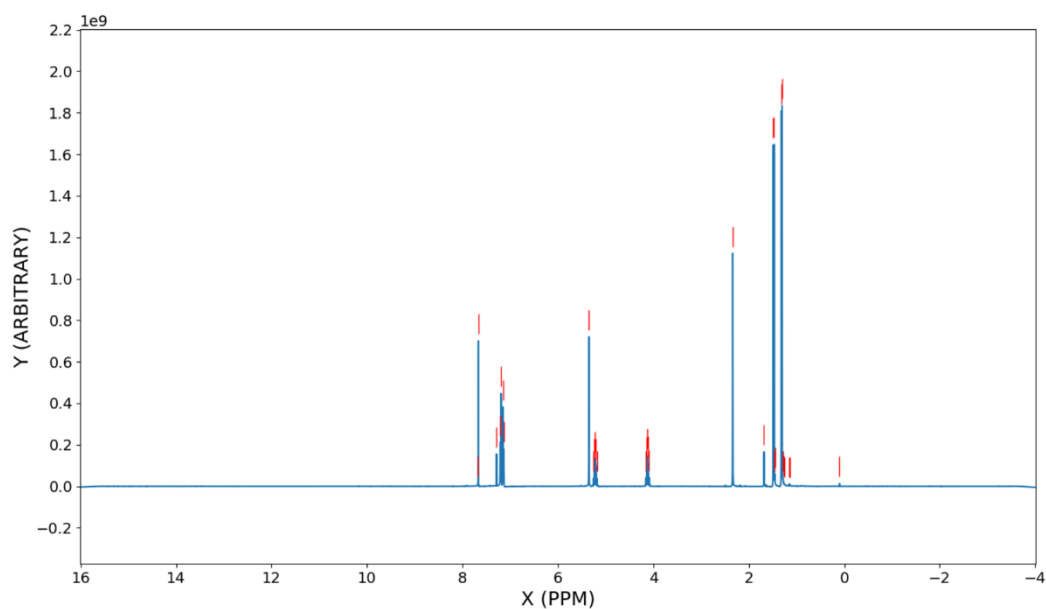


CHMO:0000630 | infrared absorption spectroscopy (IR)

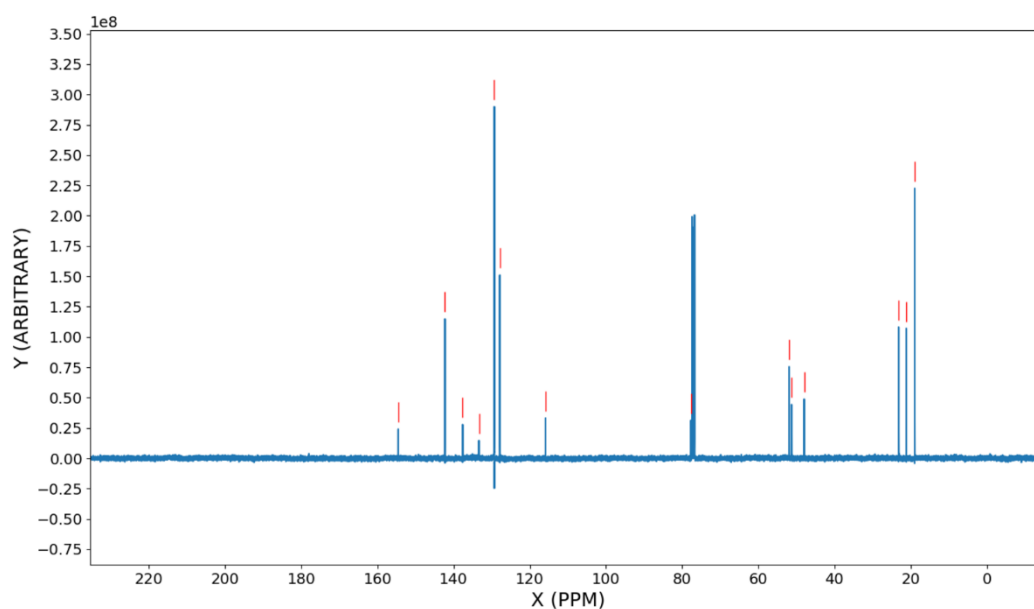


(*E*)-5-(3,3-Diisopropyltriaz-1-en-1-yl)-1-(4-methylbenzyl)-1*H*-pyrazole-4-carbonitrile (13b)

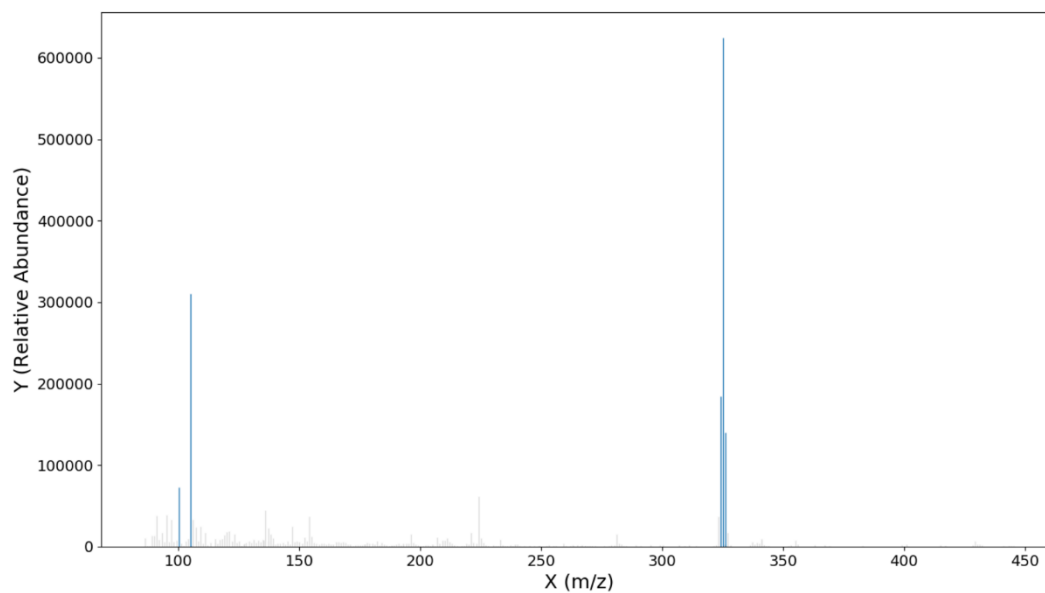
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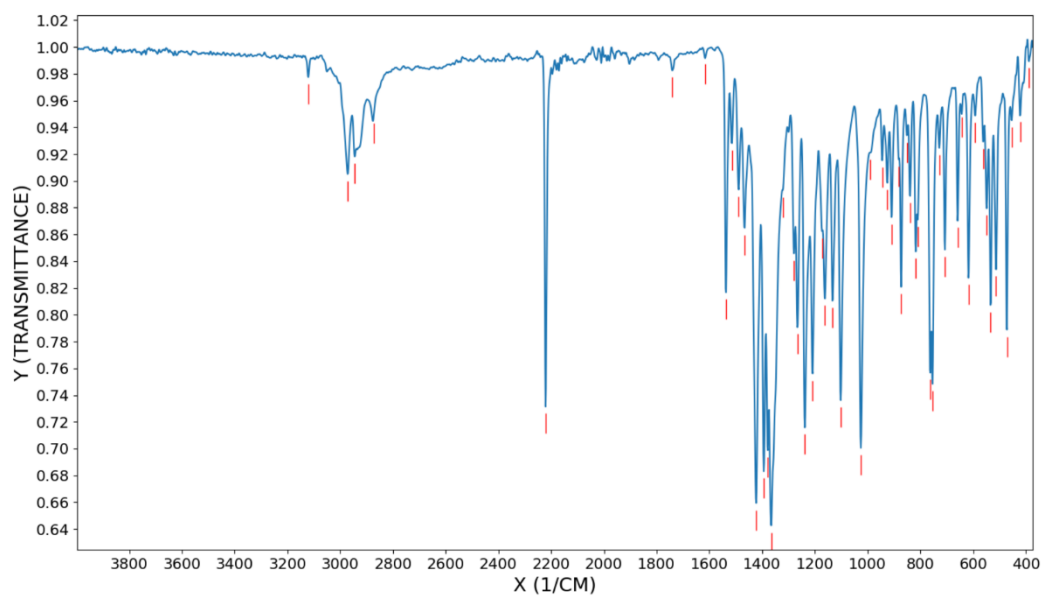
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CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

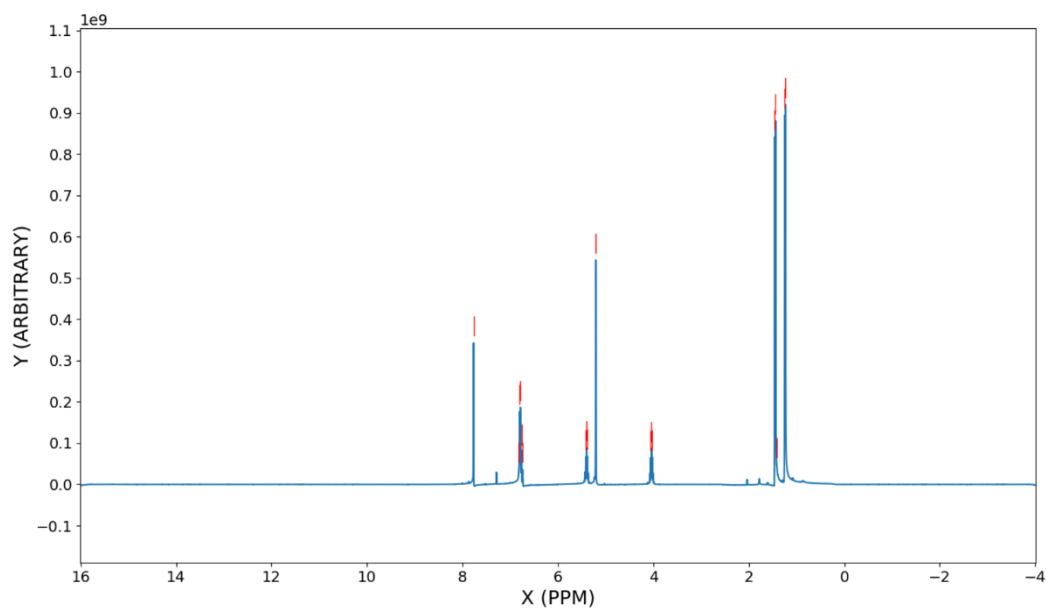


CHMO:0000630 | infrared absorption spectroscopy (IR)

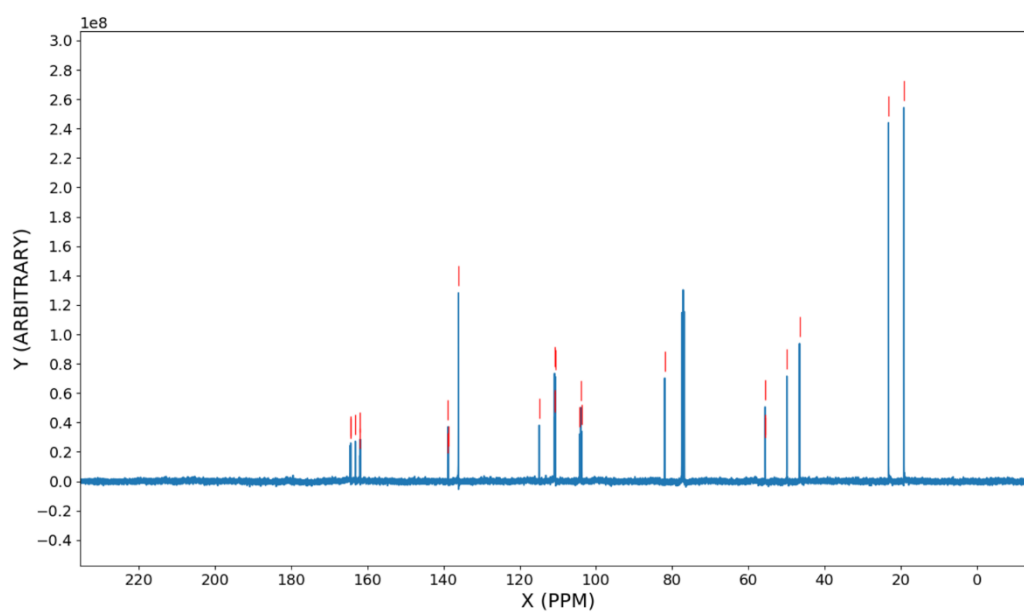


(*E*)-1-(3,5-Difluorobenzyl)-3-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazole-4-carbonitrile (12c)

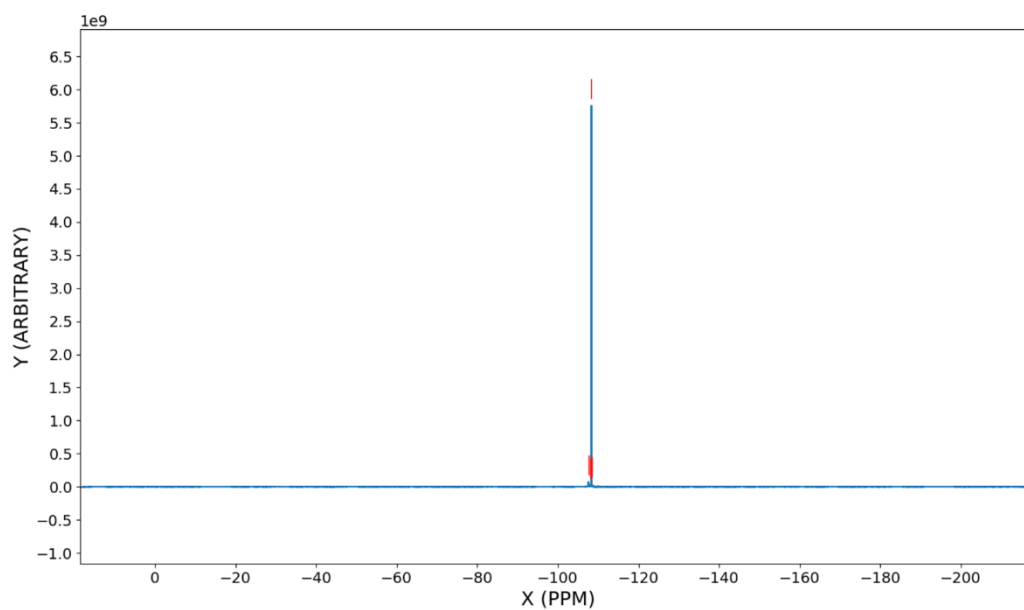
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)

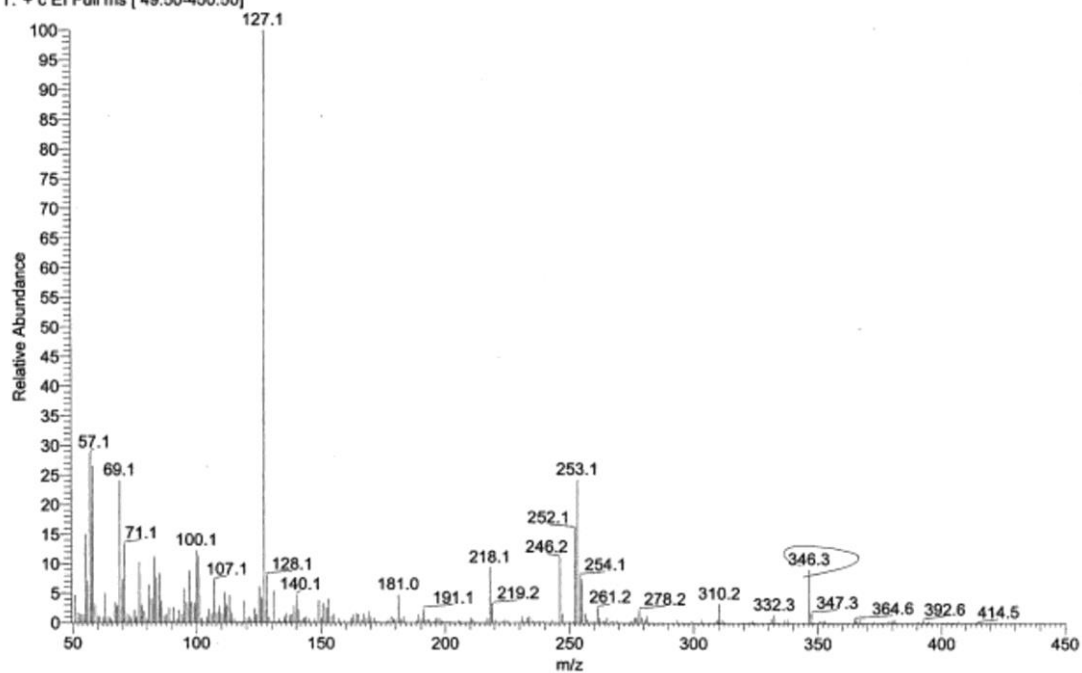


^{19}F nuclear magnetic resonance spectroscopy (^{19}F NMR)

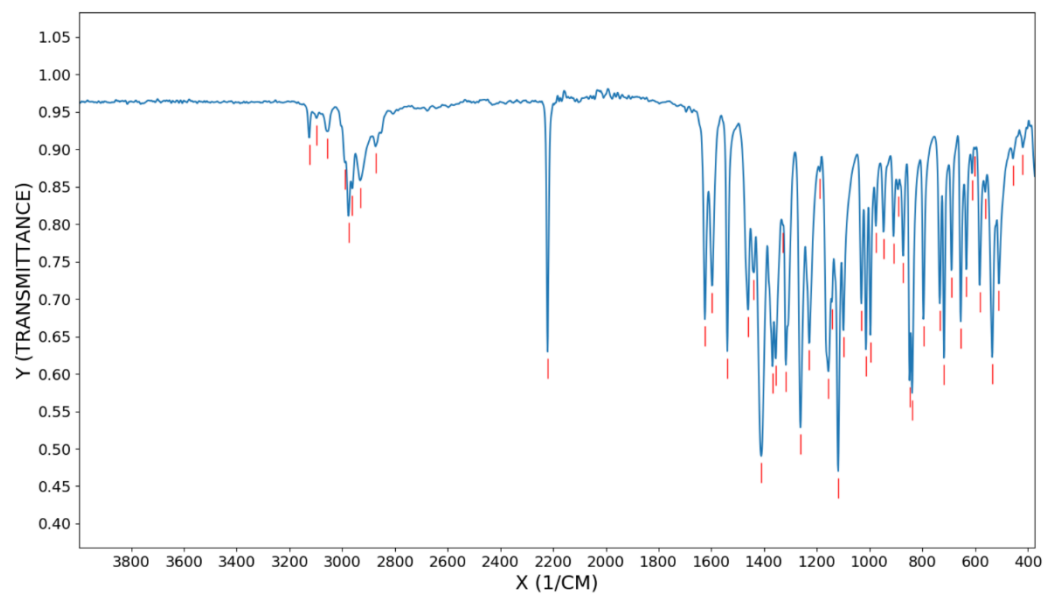


CHMO:0000480 | electron ionisation mass spectrometry (EI-MS)

T: + c EI Full ms [49.50-450.50]

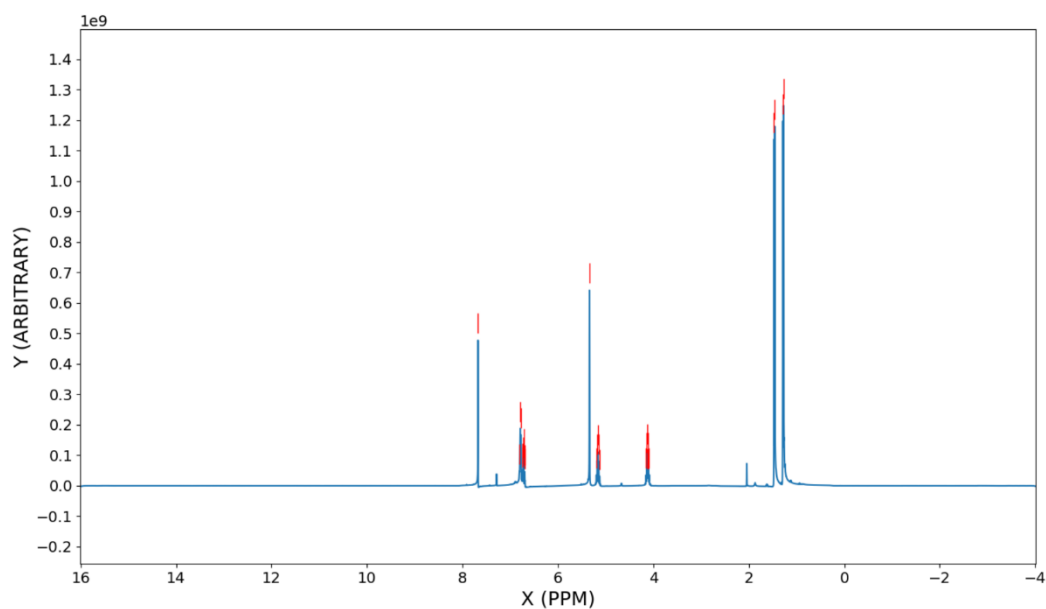


CHMO:0000630 | infrared absorption spectroscopy (IR)

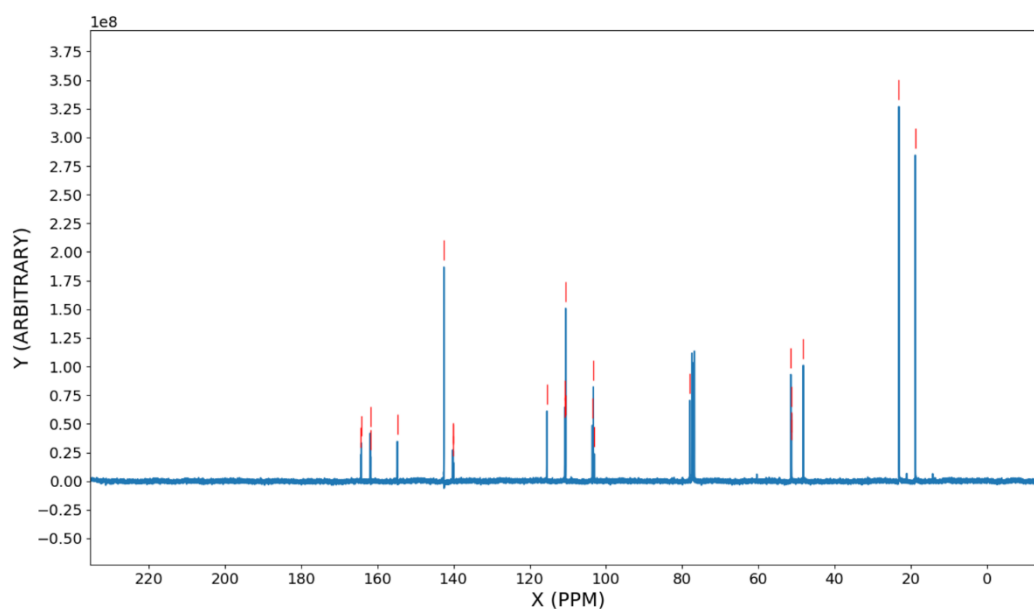


(*E*)-1-(3,5-Difluorobenzyl)-5-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazole-4-carbonitrile (13c)

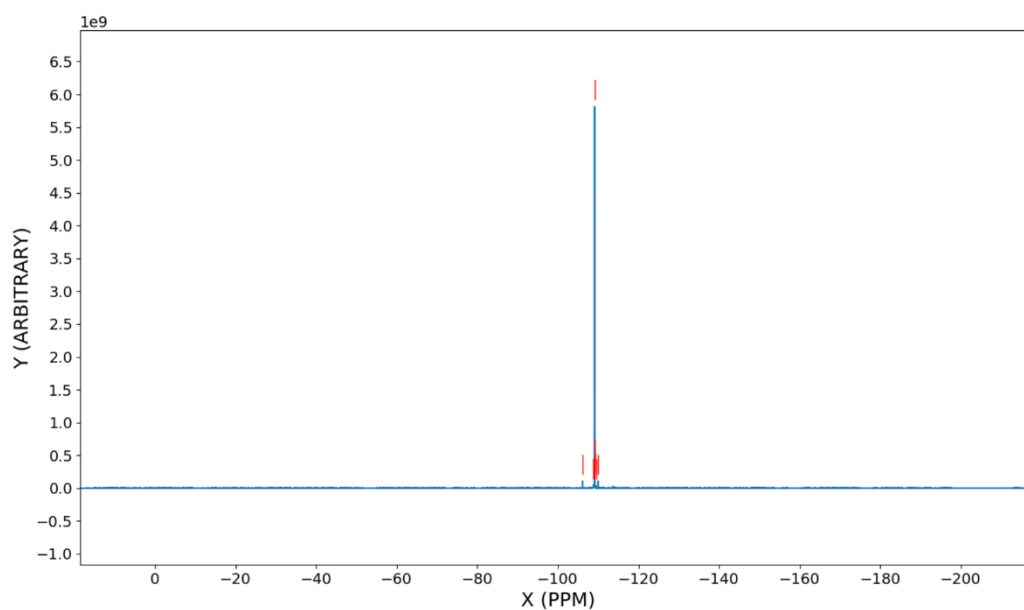
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



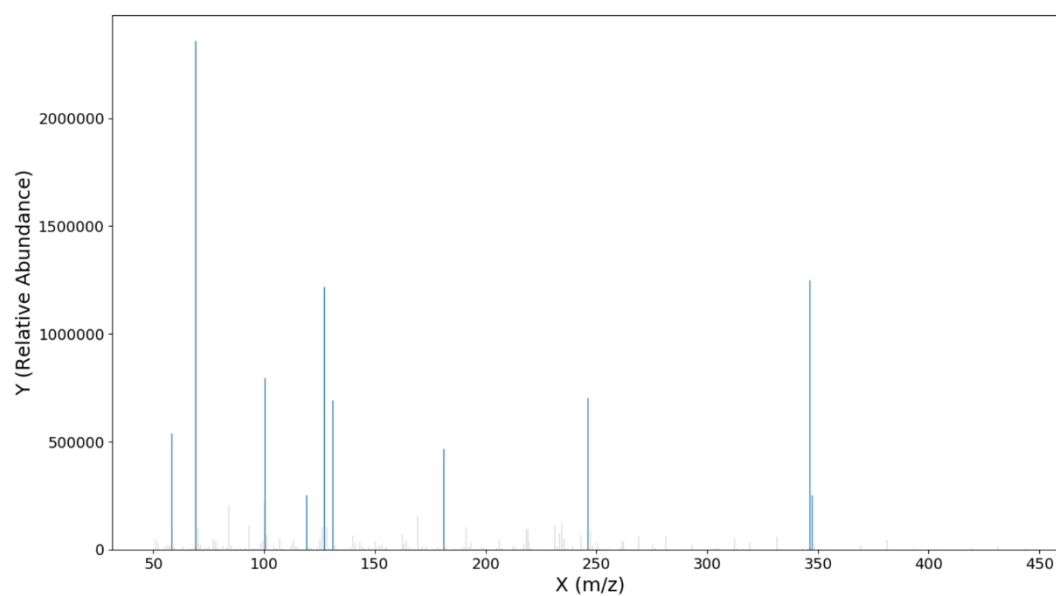
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



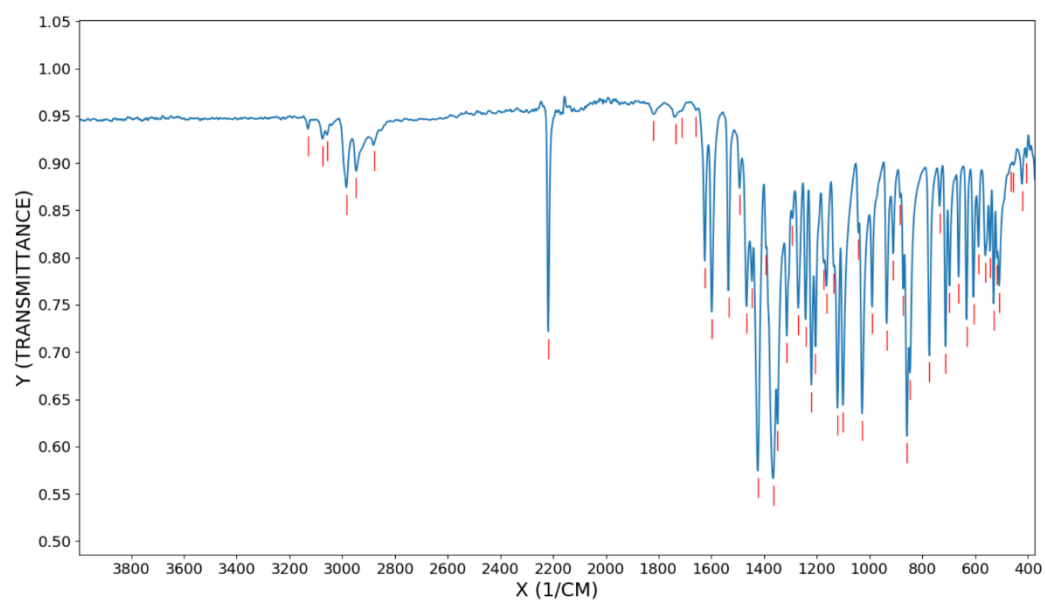
^{19}F nuclear magnetic resonance spectroscopy (^{19}F NMR)



CHMO:0000480 | electron ionisation mass spectrometry (EI-MS)

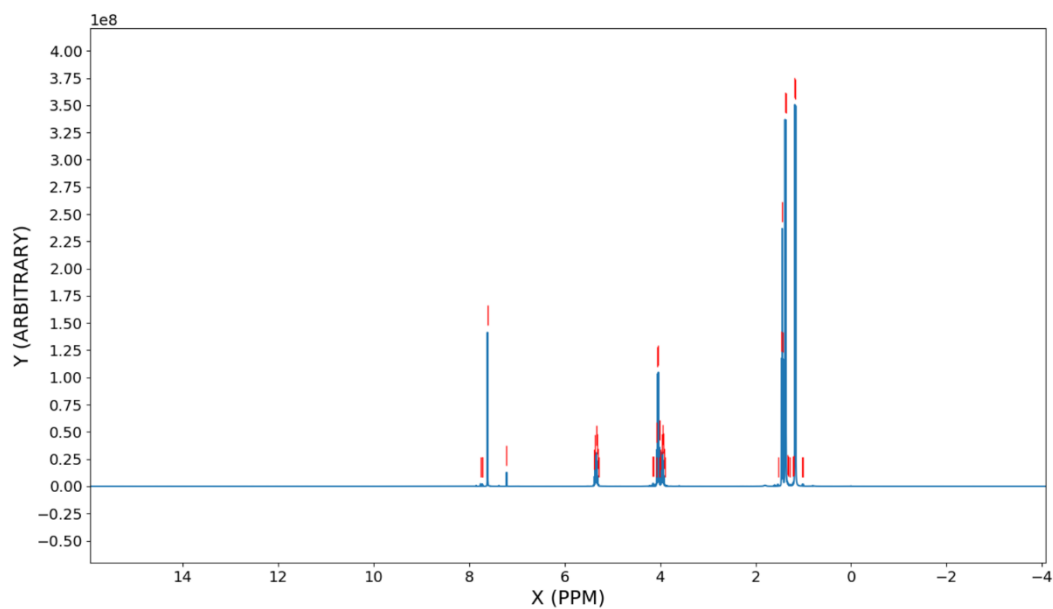


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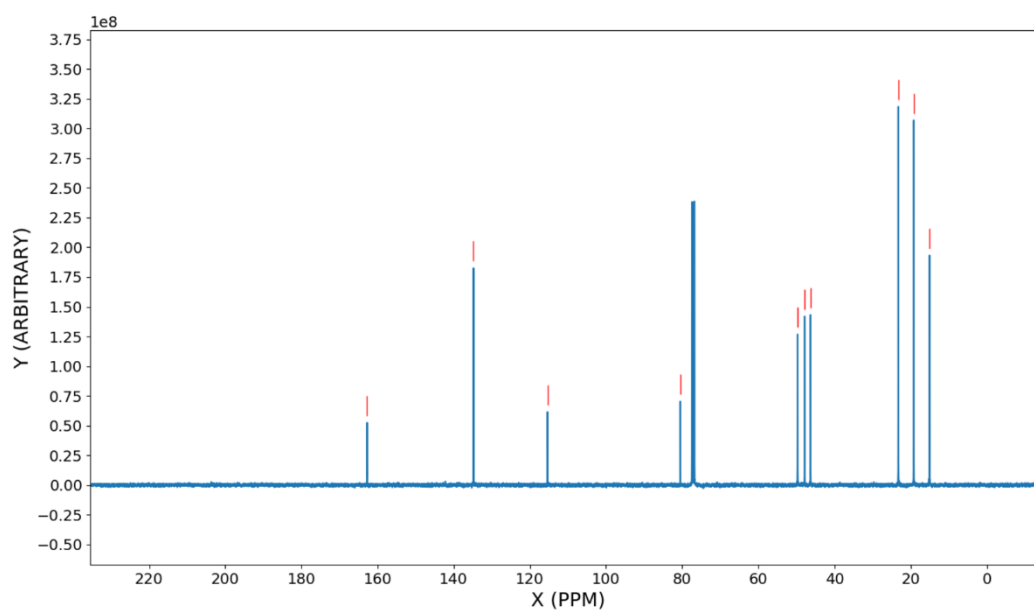


(*E*)-3-(3,3-Diisopropyltriaz-1-en-1-yl)-1-ethyl-1*H*-pyrazole-4-carbonitrile (12d)

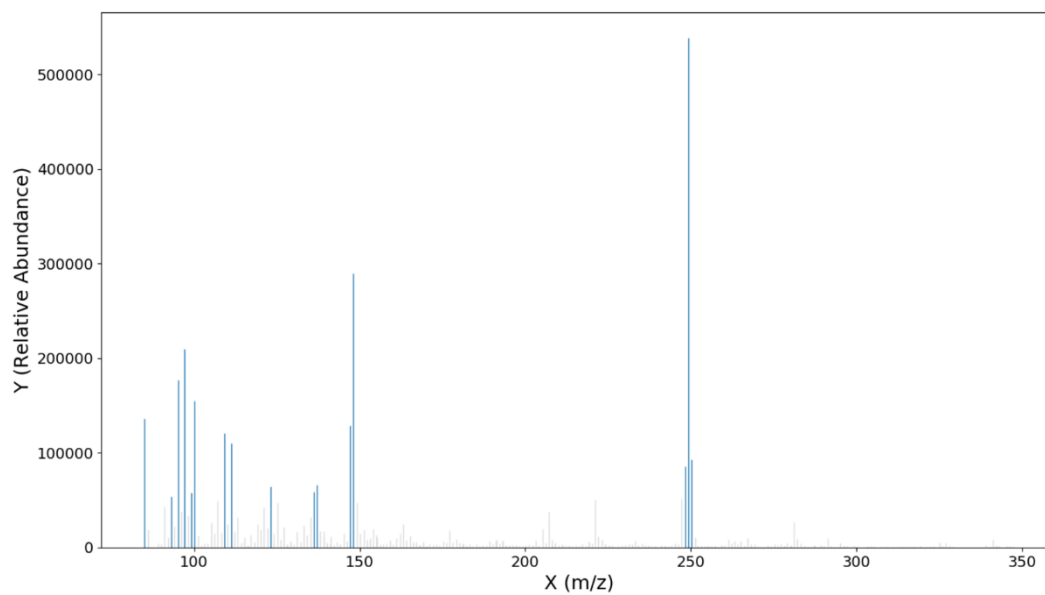
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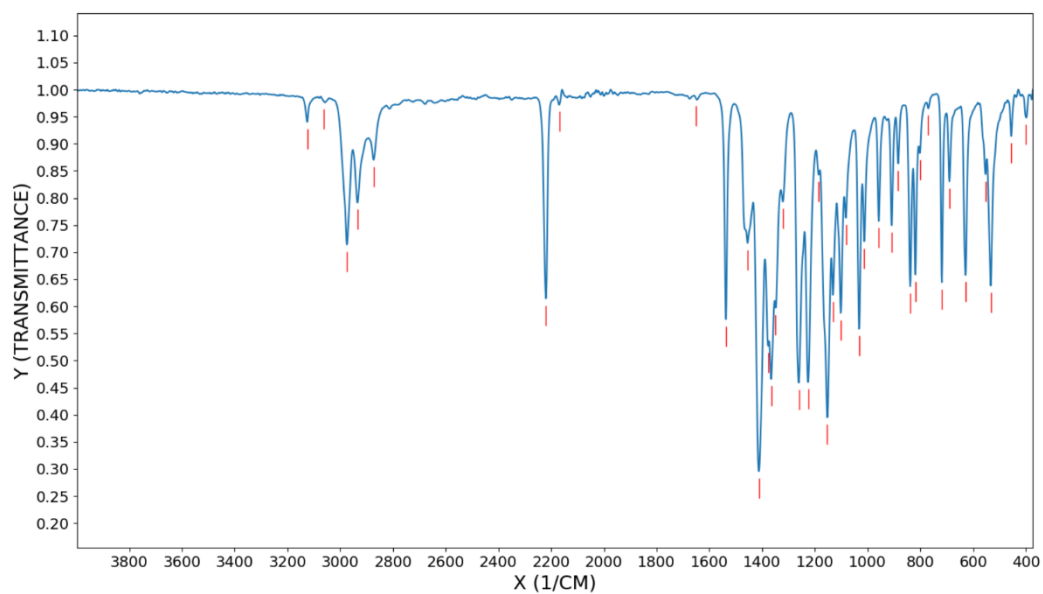
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

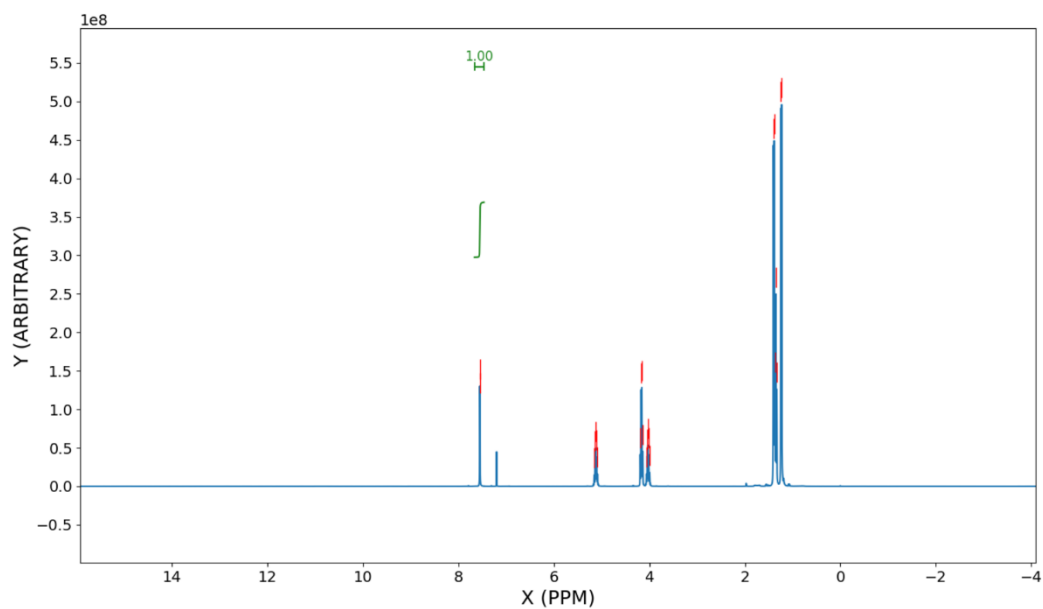


CHMO:0000630 | infrared absorption spectroscopy (IR)

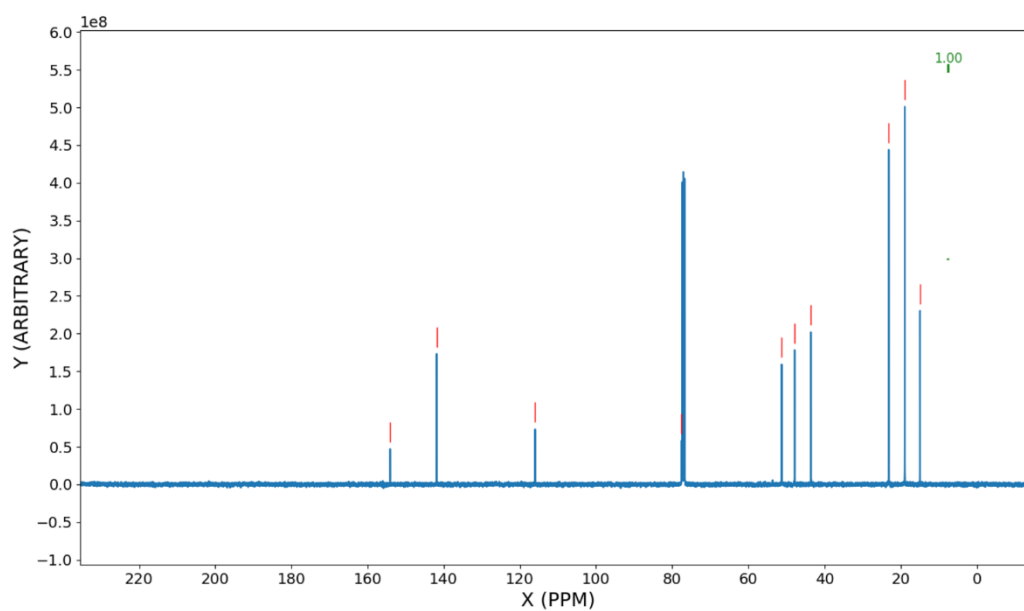


(*E*)-5-(3,3-Diisopropyltriaz-1-en-1-yl)-1-ethyl-1*H*-pyrazole-4-carbonitrile (13d)

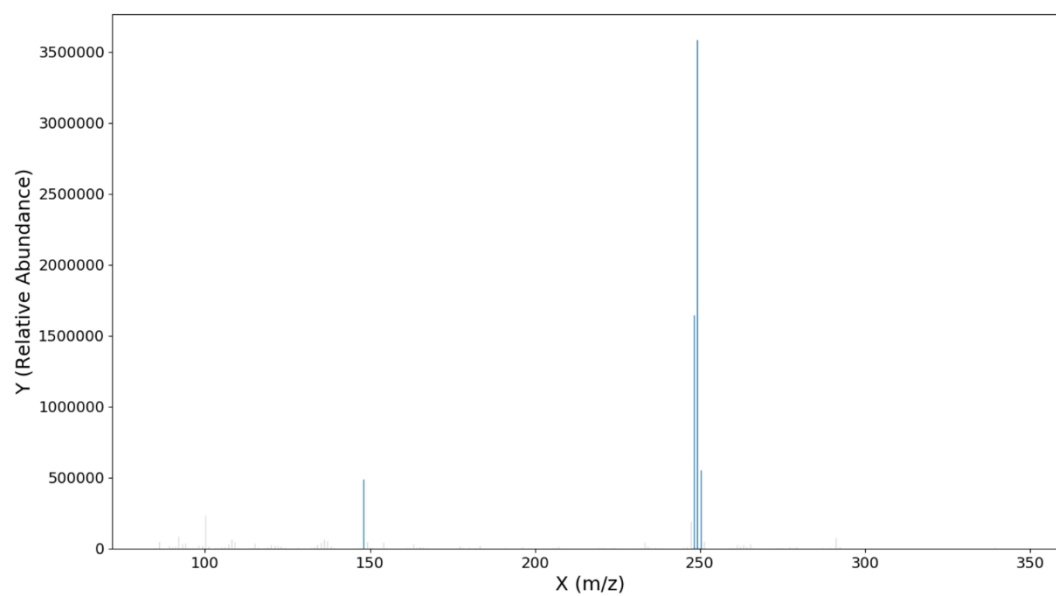
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



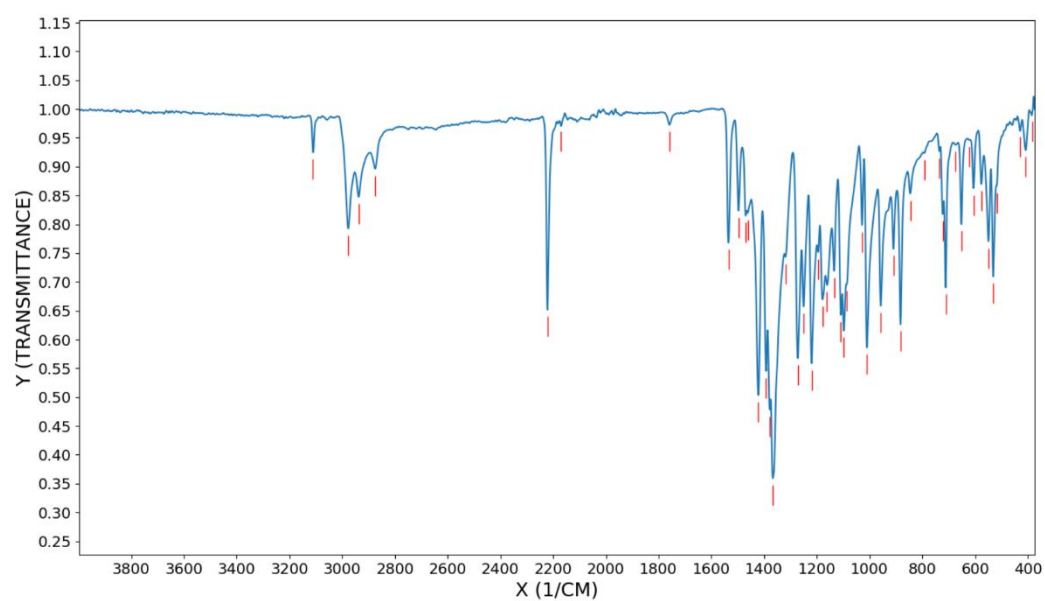
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

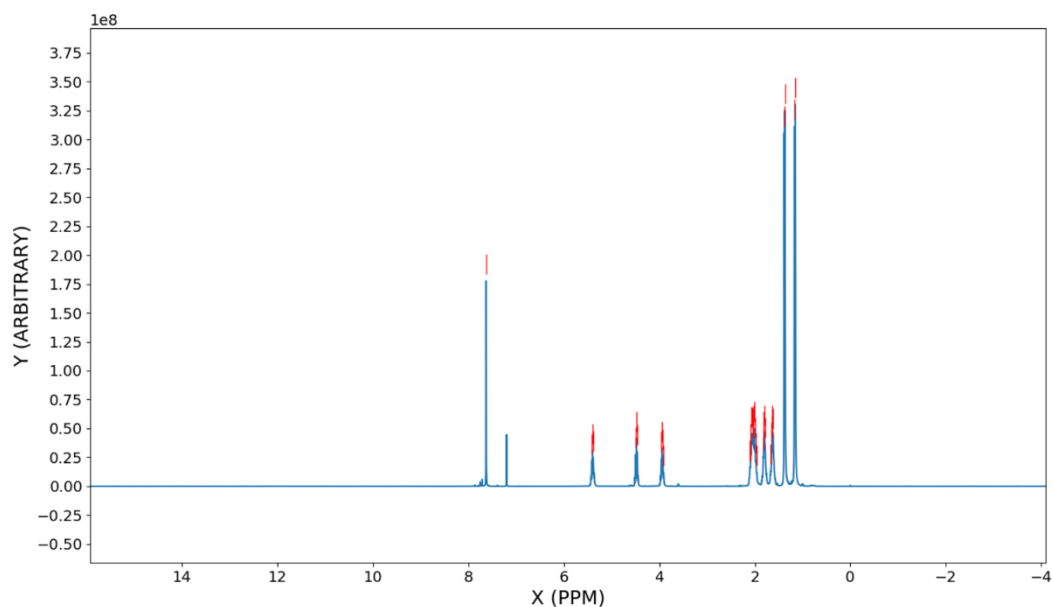


CHMO:0000630 | infrared absorption spectroscopy (IR)

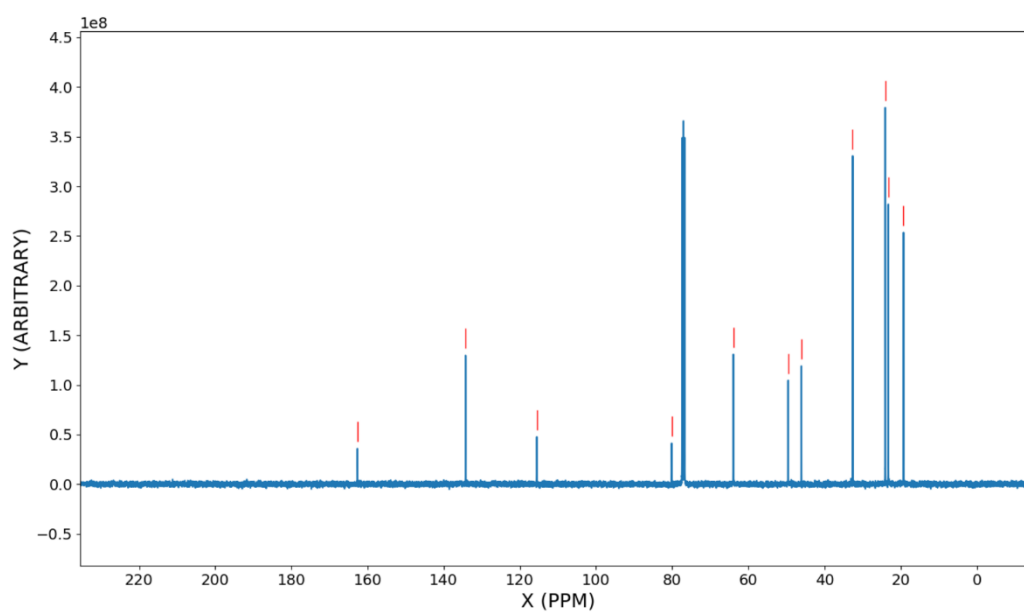


(*E*)-1-Cyclopentyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazole-4-carbonitrile (12e)

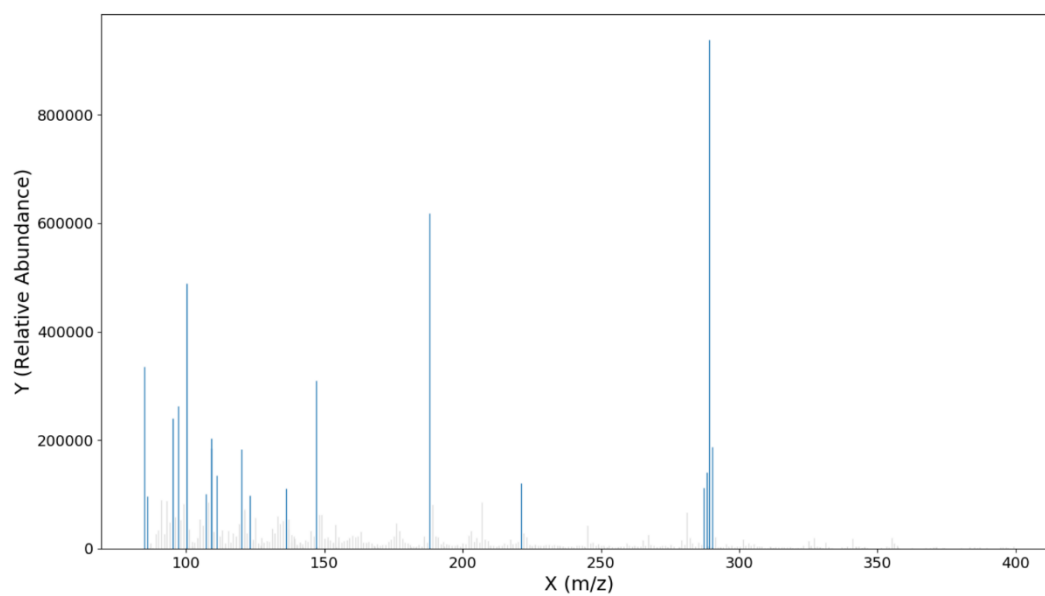
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



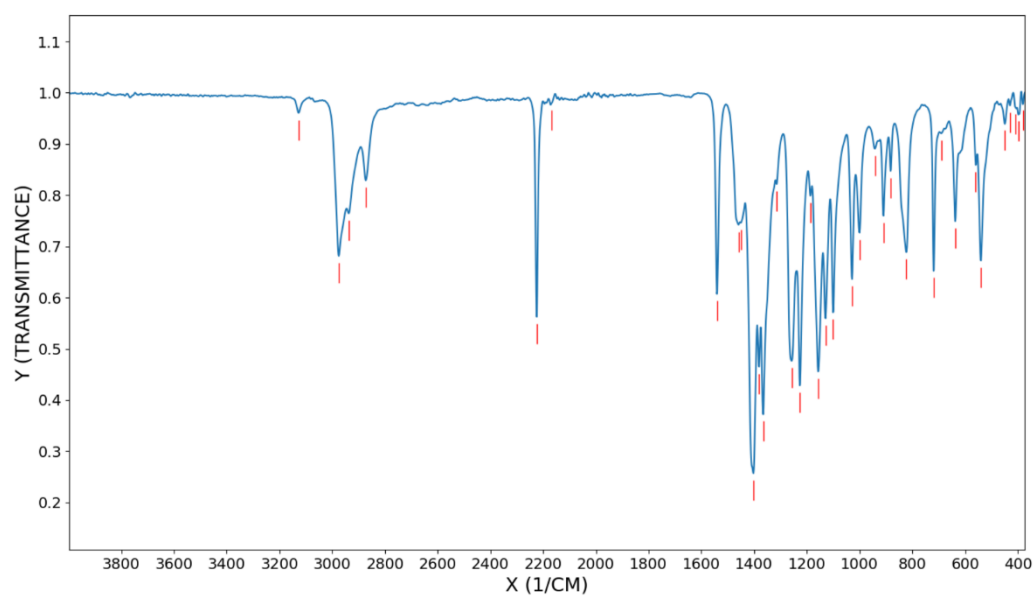
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

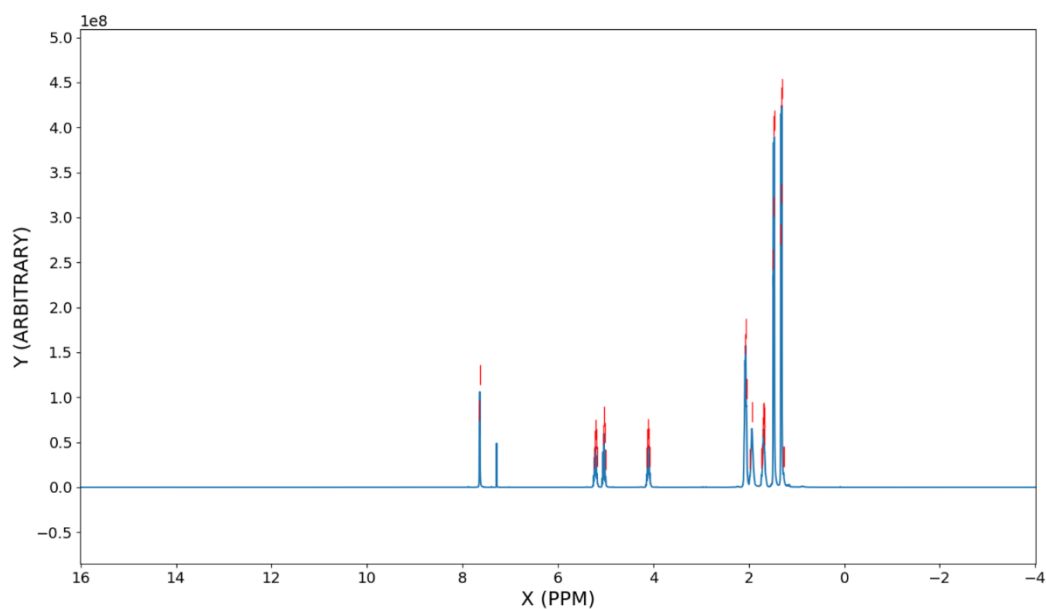


CHMO:0000630 | infrared absorption spectroscopy (IR)

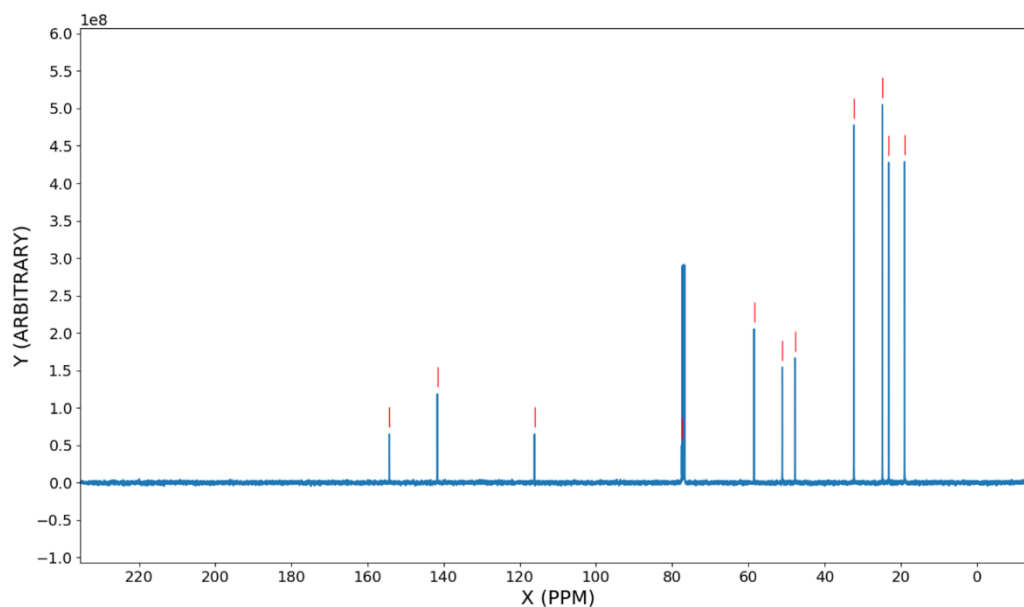


(*E*)-1-Cyclopentyl-5-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazole-4-carbonitrile (13e)

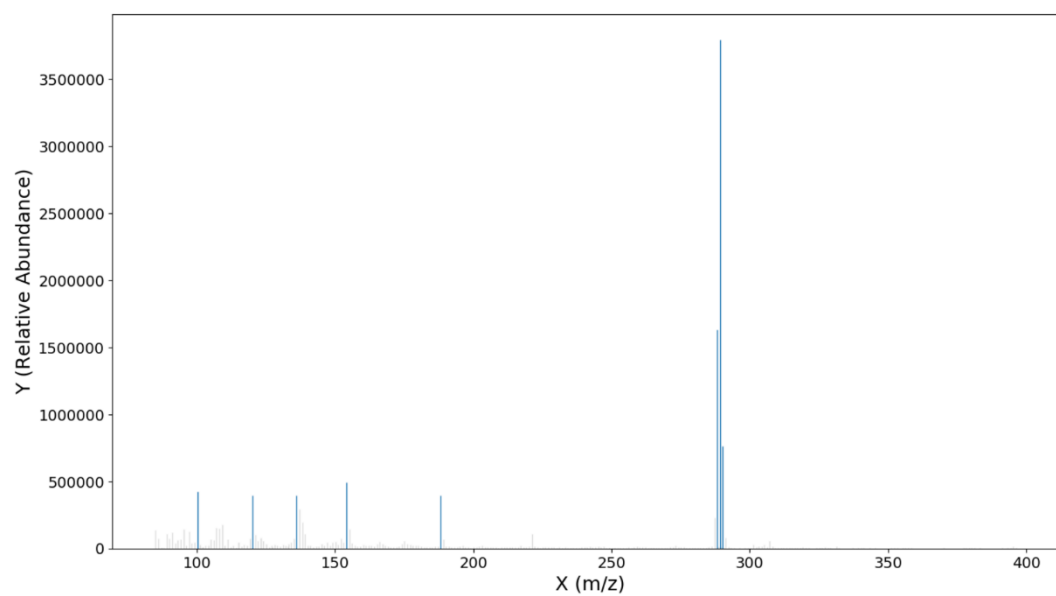
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



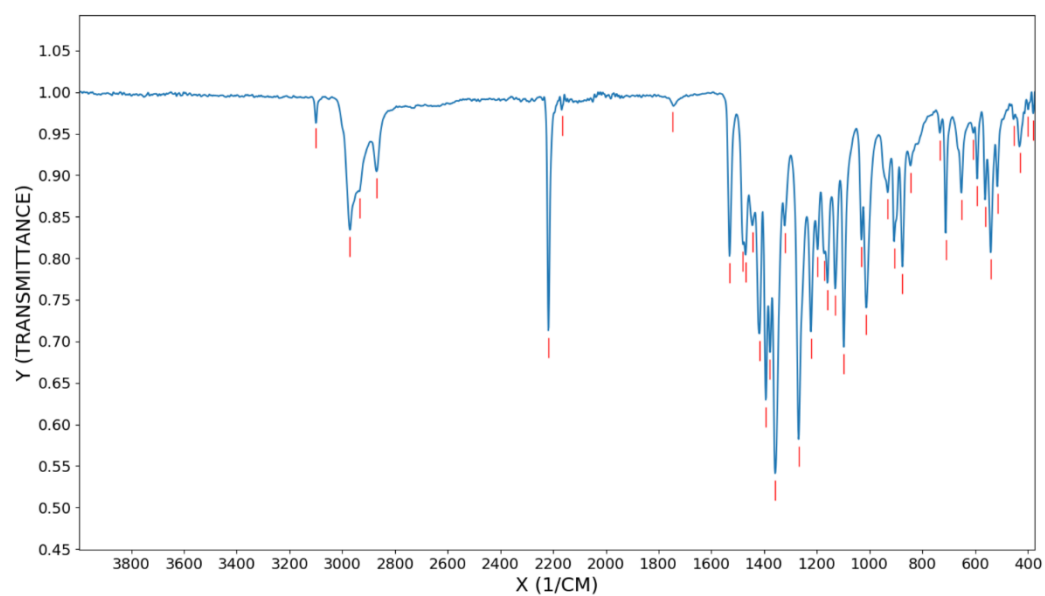
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

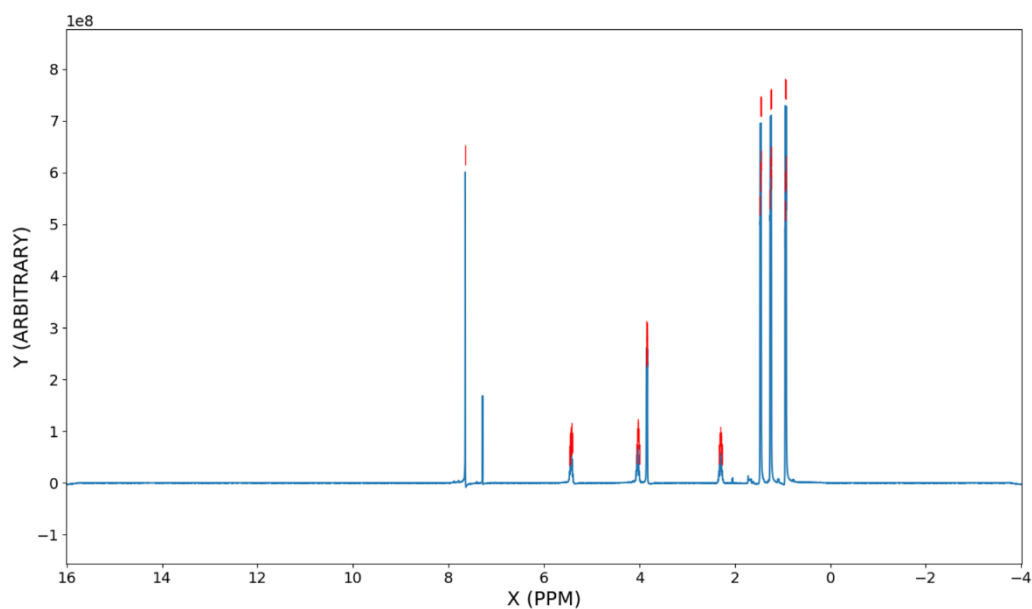


CHMO:0000630 | infrared absorption spectroscopy (IR)

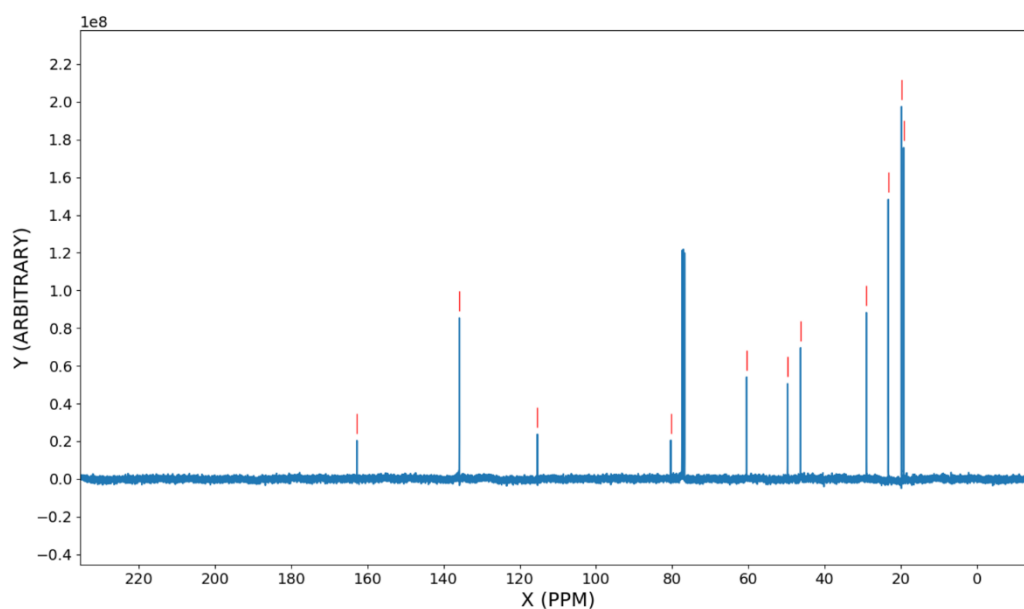


(*E*)-3-(3,3-Diisopropyltriaz-1-en-1-yl)-1-isobutyl-1*H*-pyrazole-4-carbonitrile (12f)

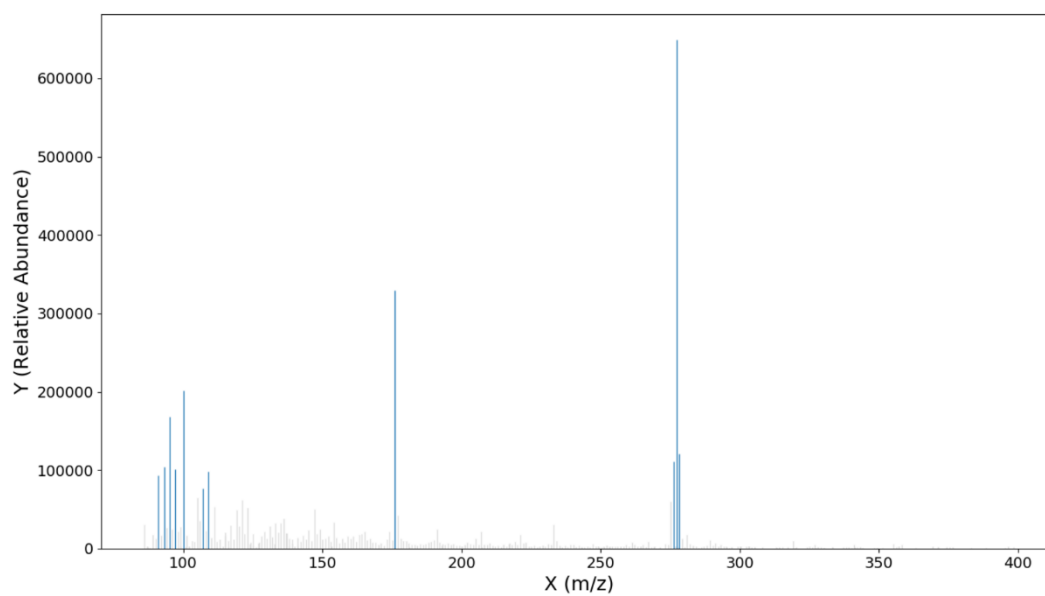
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



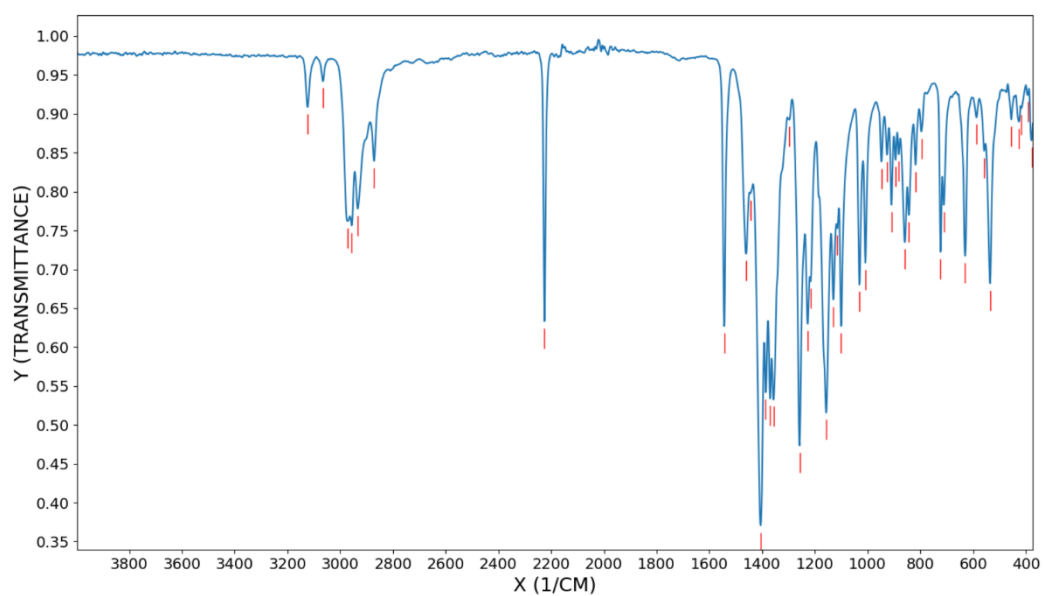
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

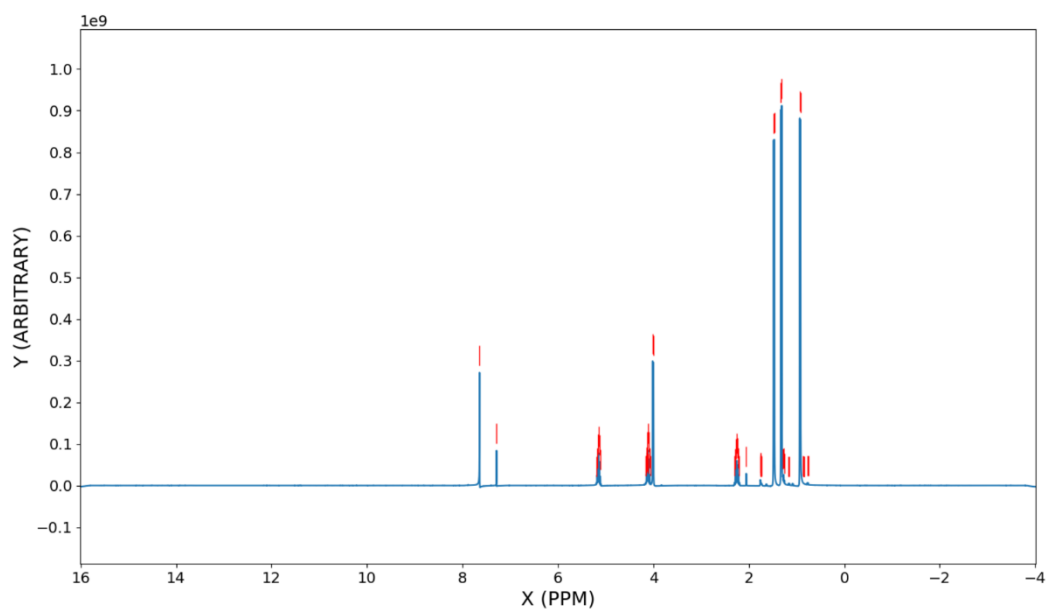


CHMO:0000630 | infrared absorption spectroscopy (IR)

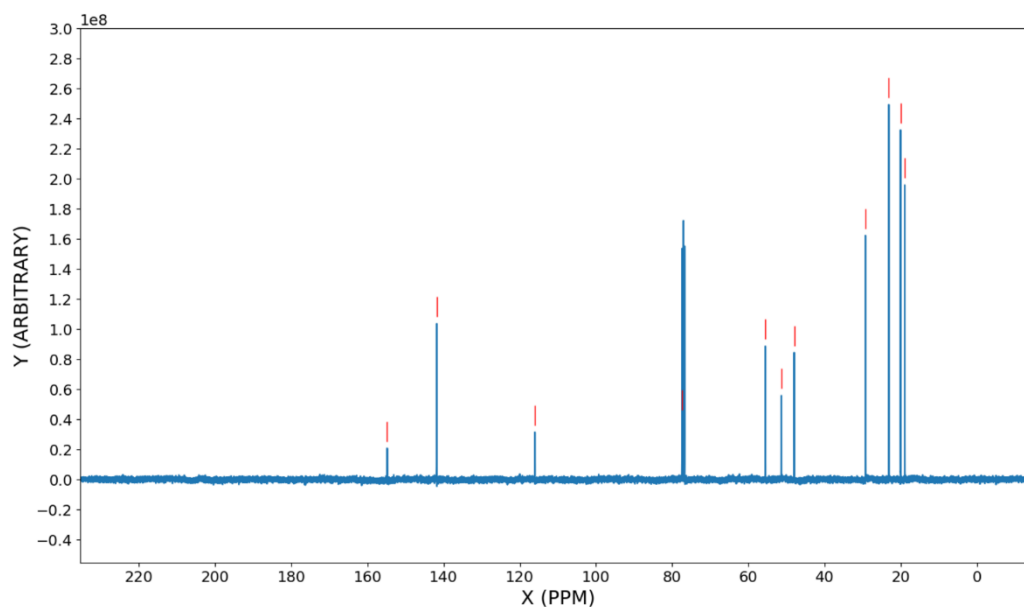


(*E*)-5-(3,3-Diisopropyltriaz-1-en-1-yl)-1-isobutyl-1*H*-pyrazole-4-carbonitrile (13f)

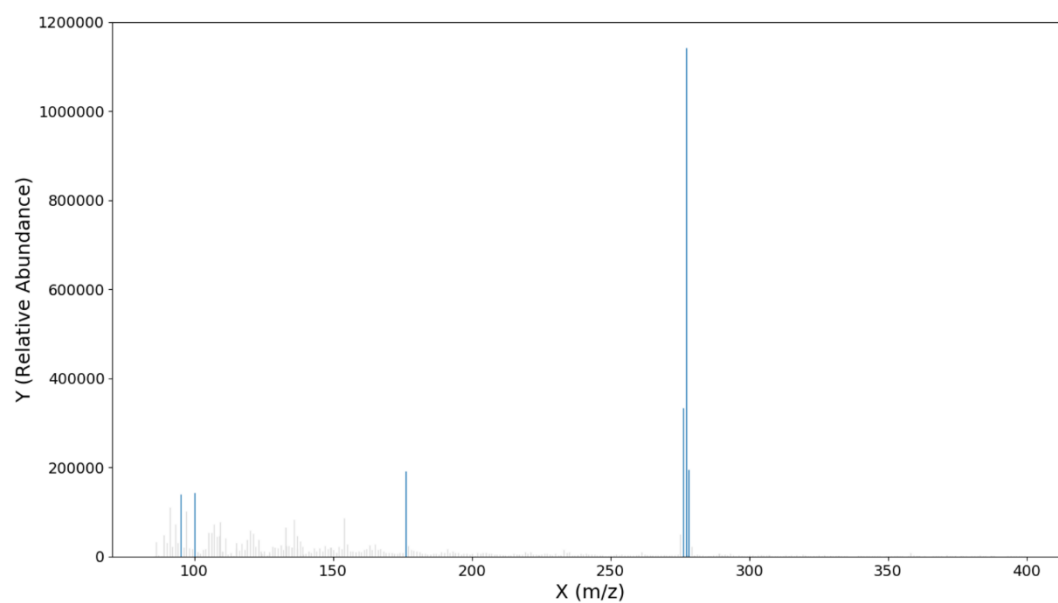
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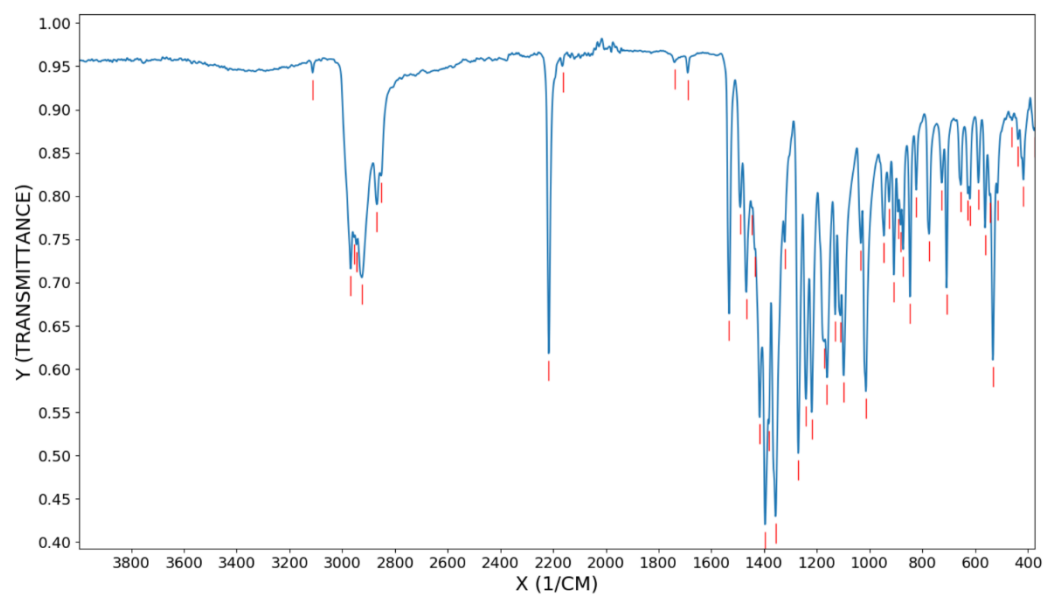
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CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

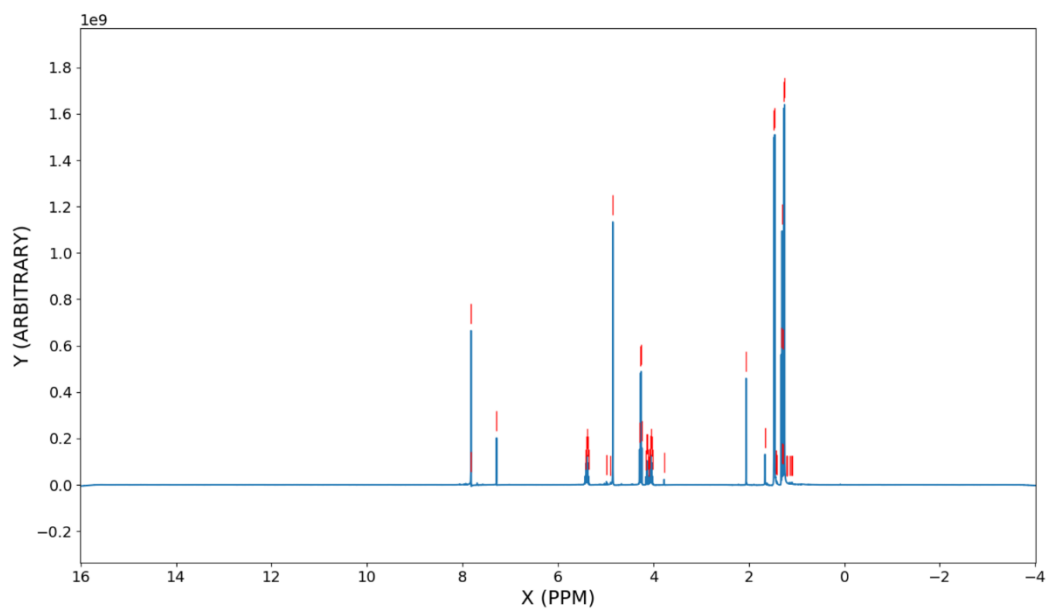


CHMO:0000630 | infrared absorption spectroscopy (IR)

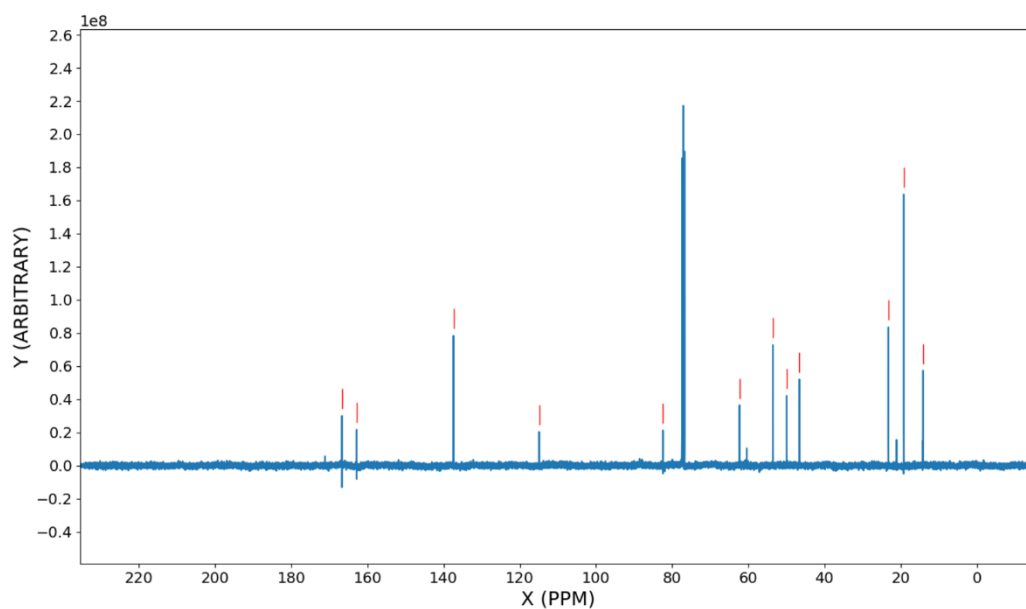


Ethyl (*E*)-2-(4-cyano-3-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazol-1-yl)acetate (12g)

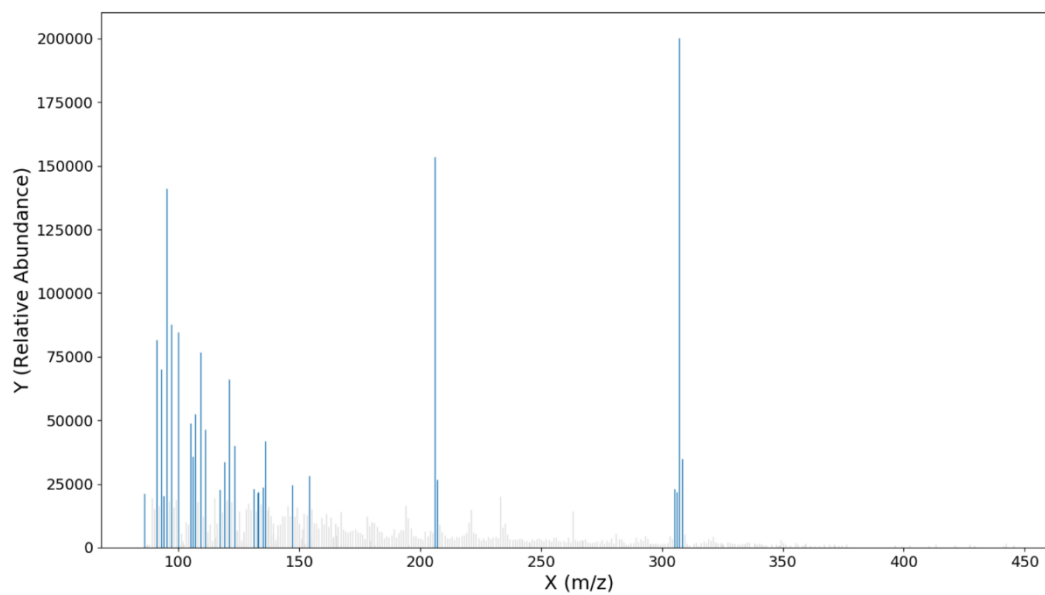
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



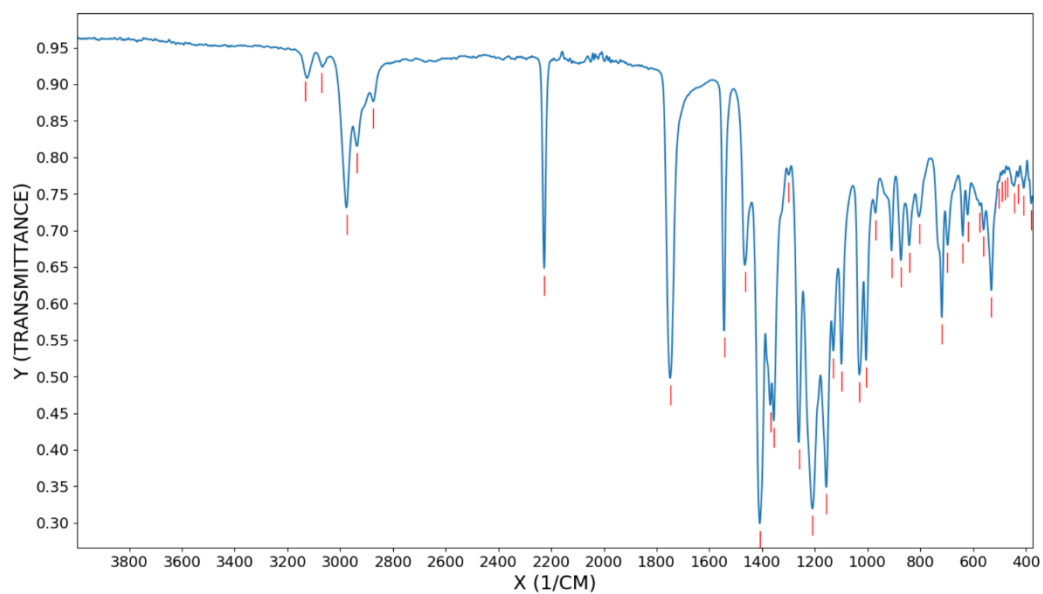
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

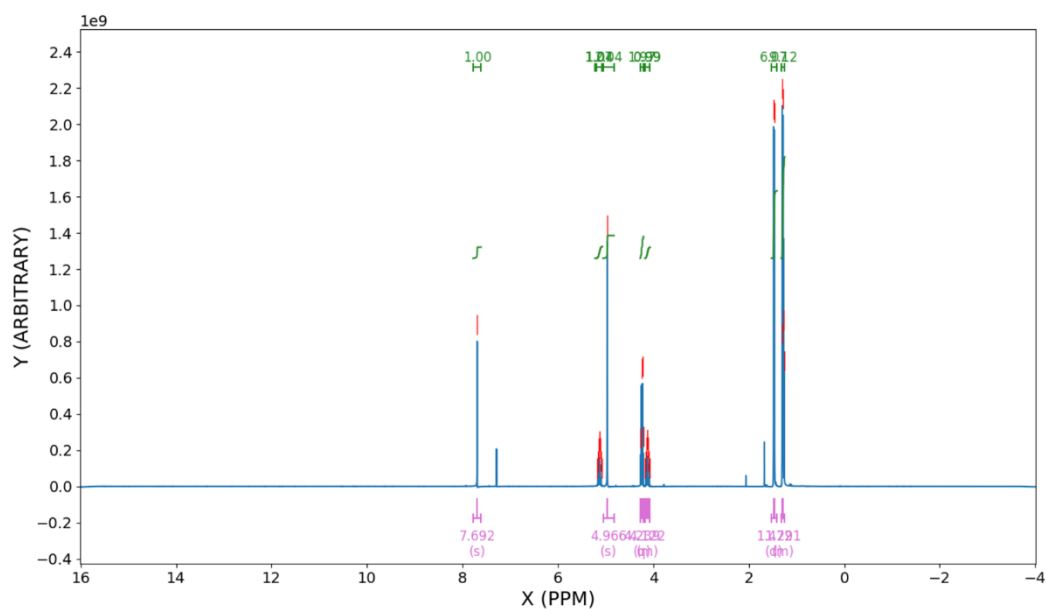


CHMO:0000630 | infrared absorption spectroscopy (IR)

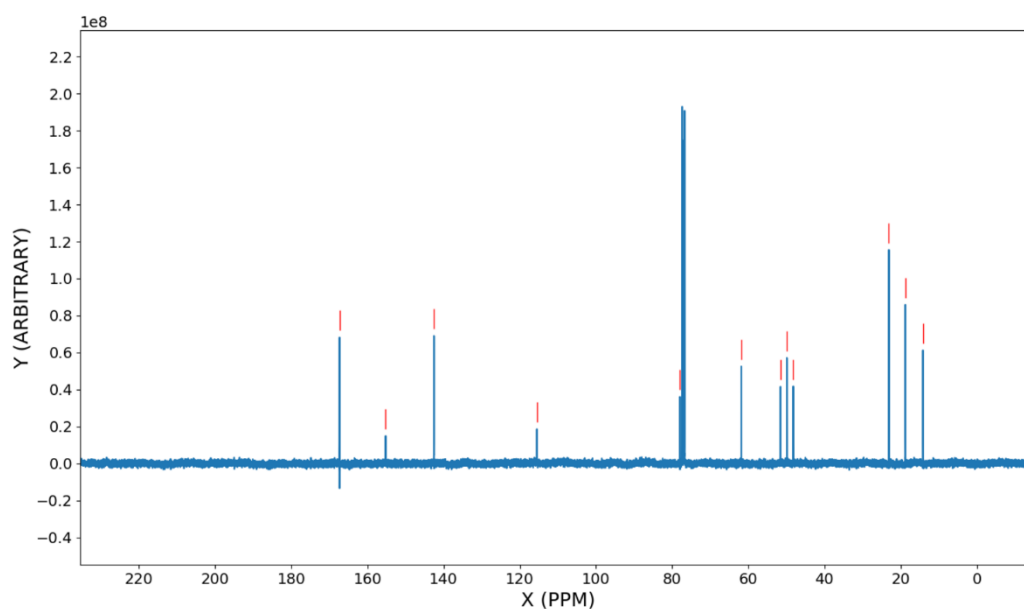


Ethyl (*E*)-2-(4-cyano-5-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazol-1-yl)acetate (13g)

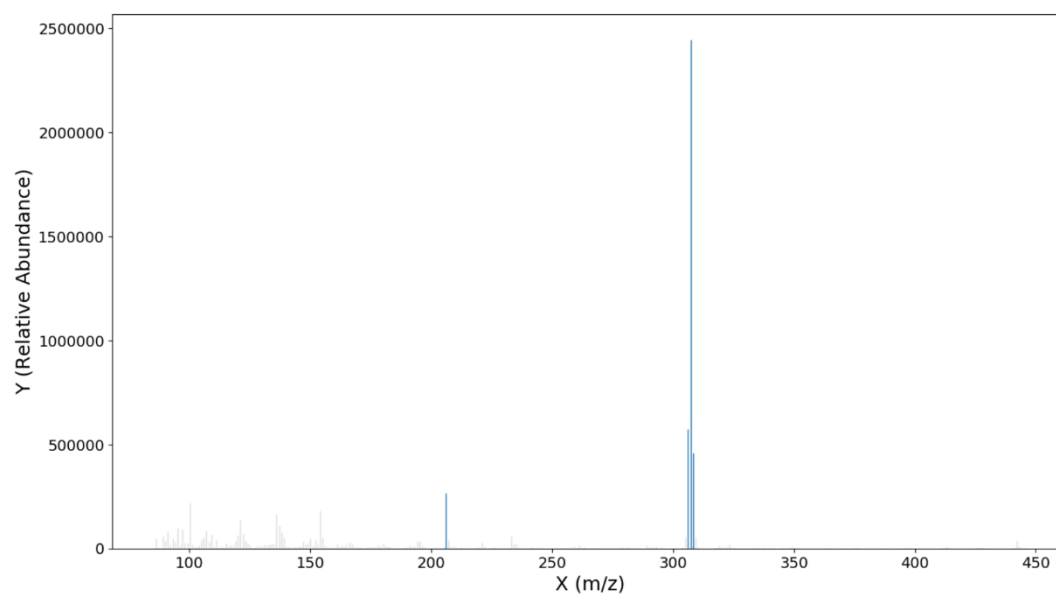
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



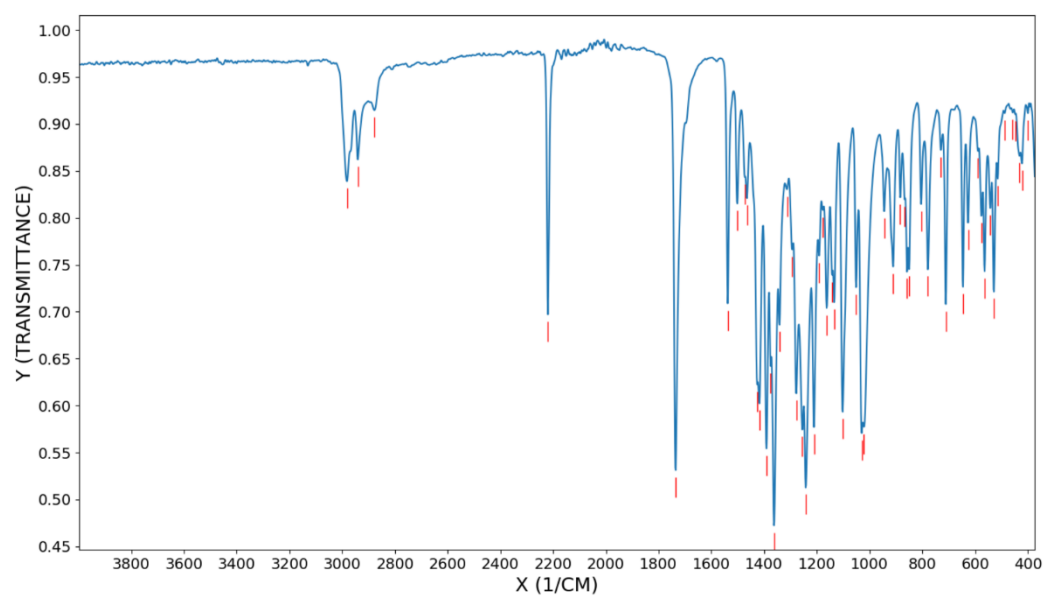
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

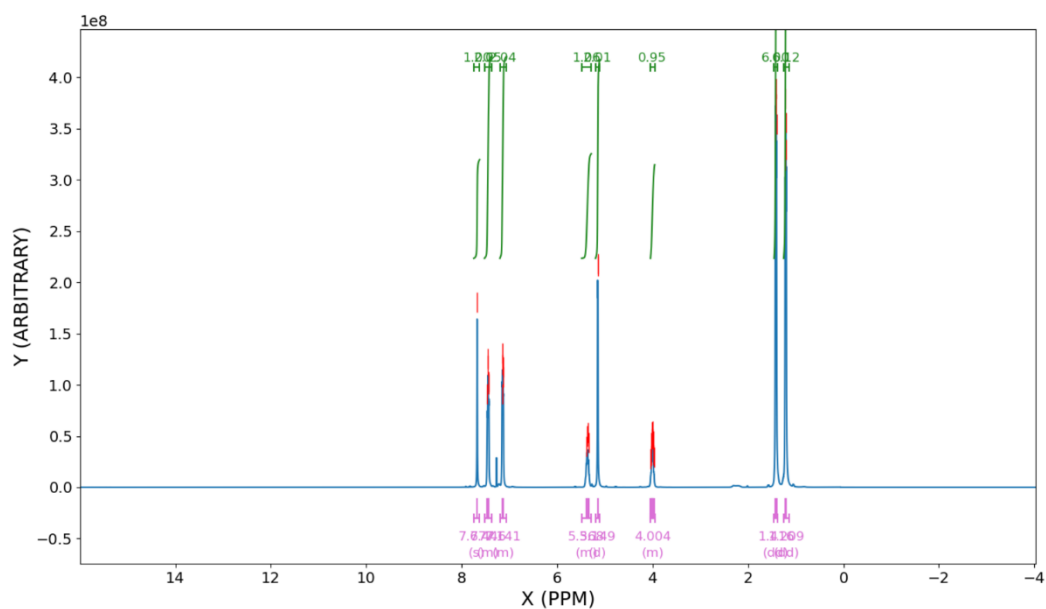


CHMO:0000630 | infrared absorption spectroscopy (IR)

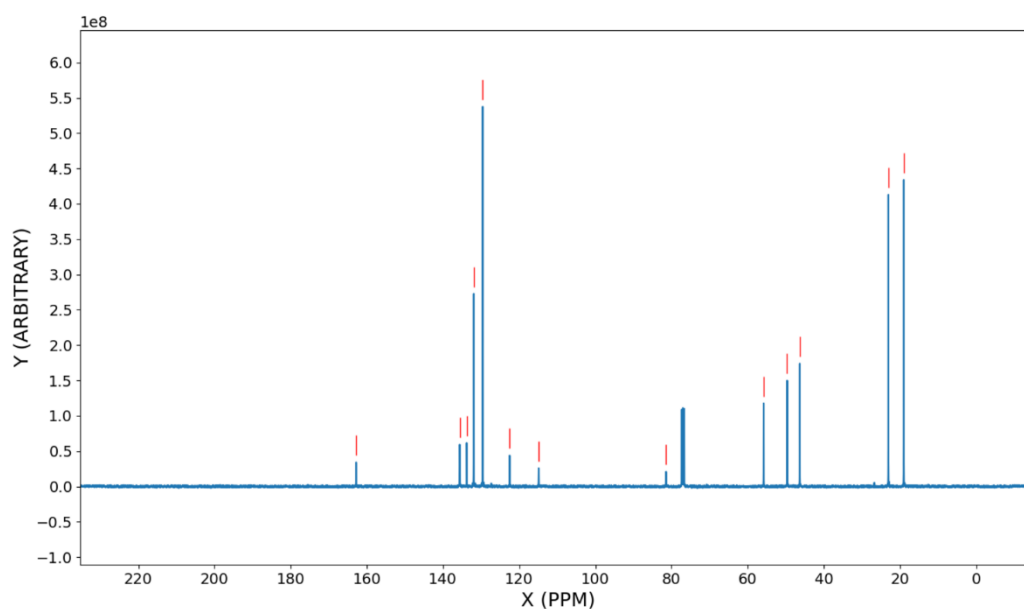


(*E*)-1-(4-Bromobenzyl)-3-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazole-4-carbonitrile (12h)

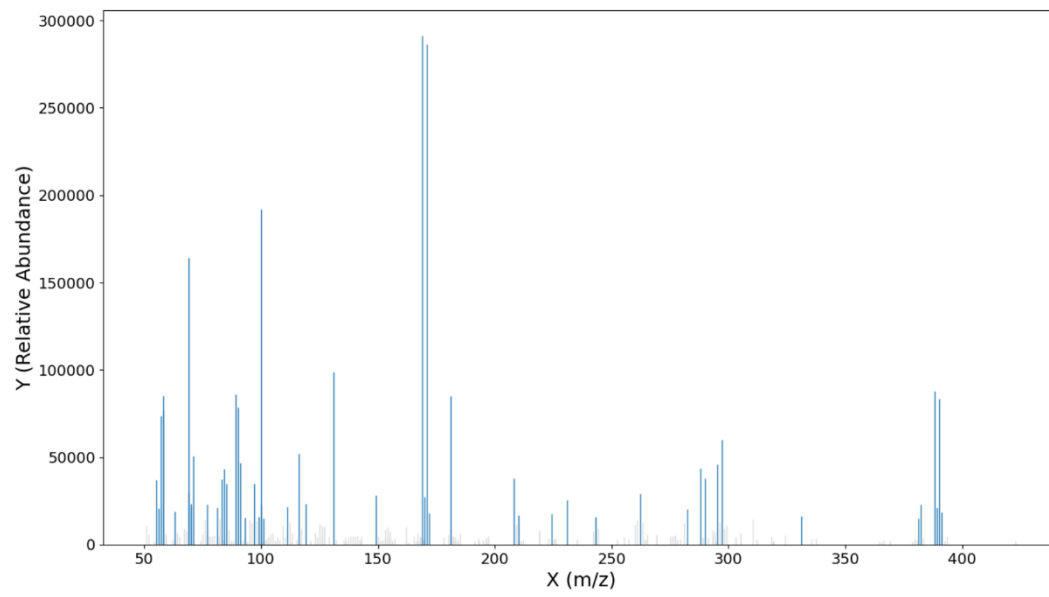
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)

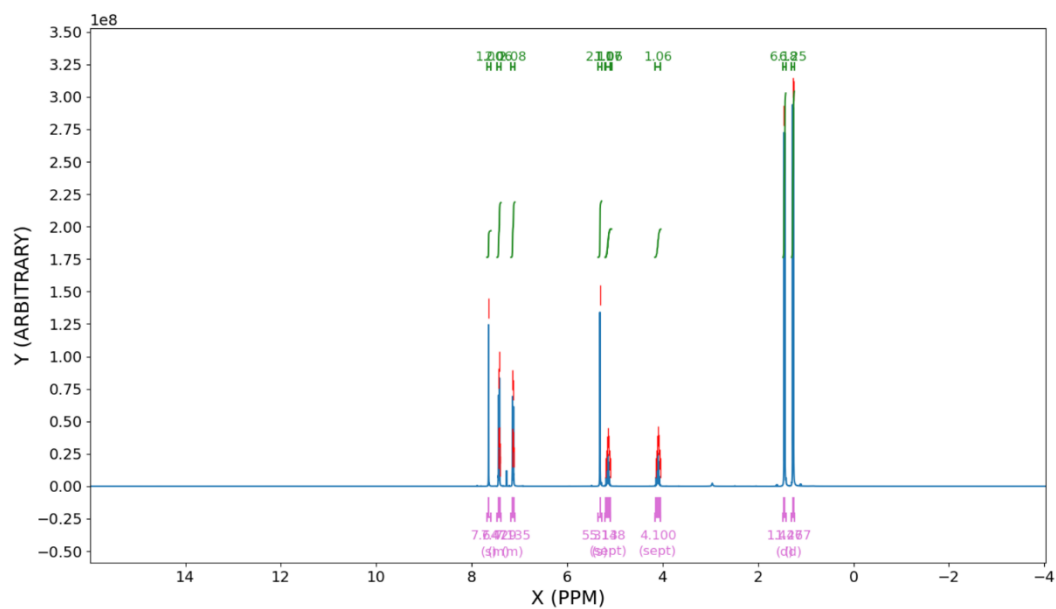


CHMO:0000470 | mass spectrometry (MS)

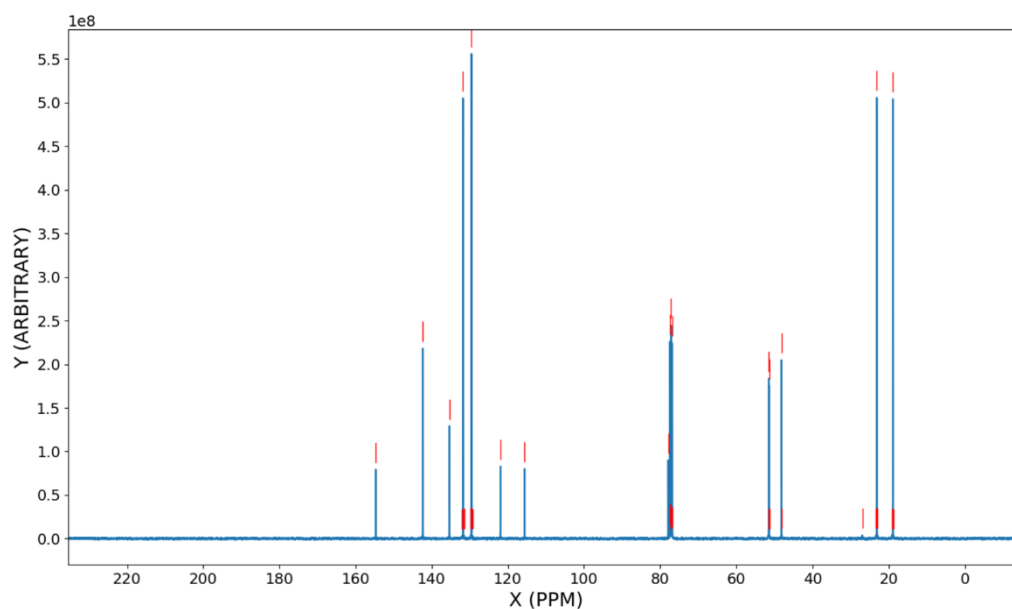


(E)-1-(4-Bromobenzyl)-5-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile (13h)

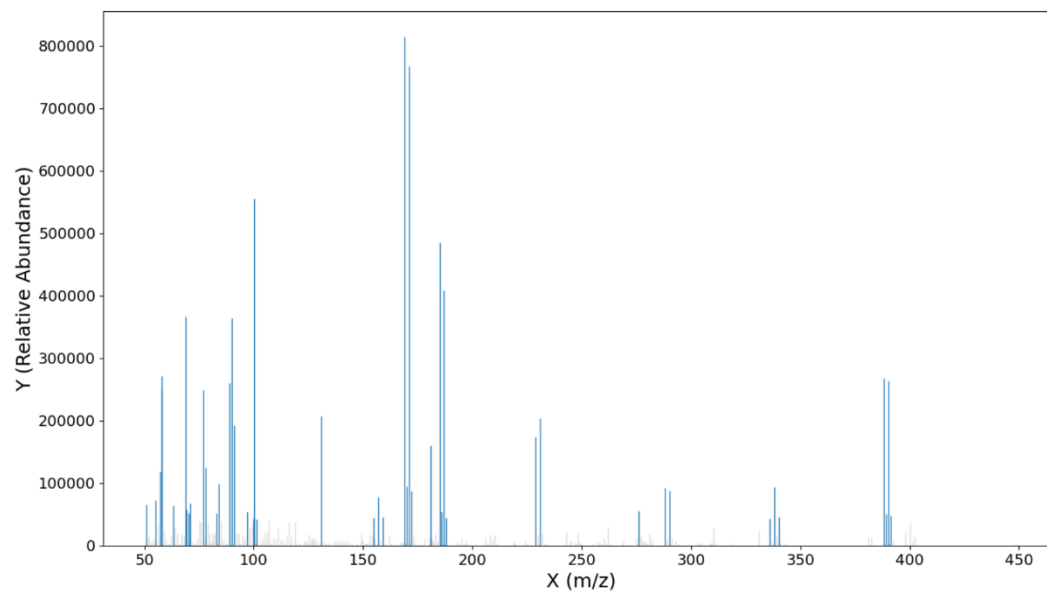
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)

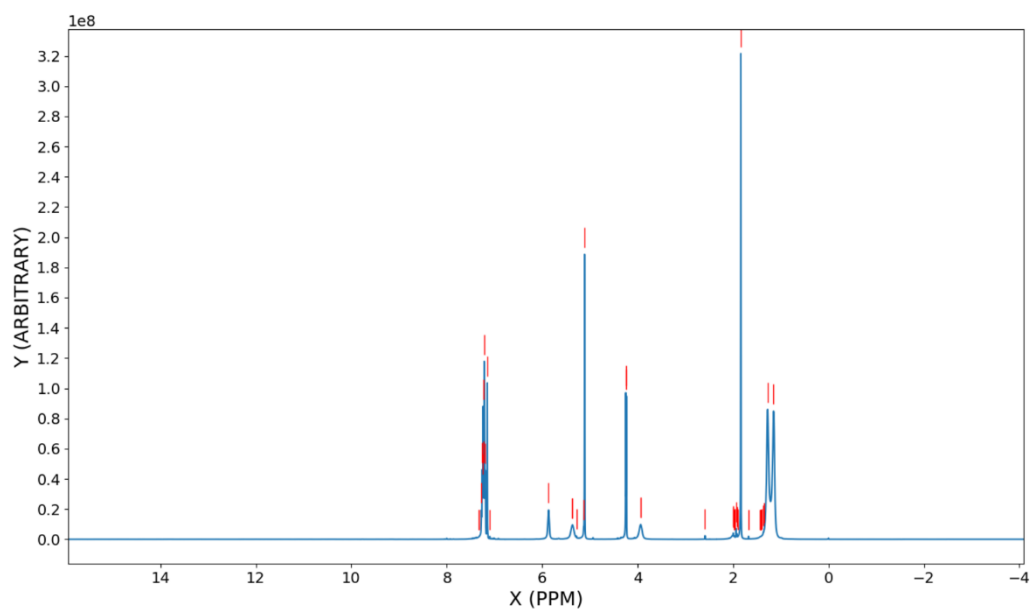


CHMO:0000470 | mass spectrometry (MS)

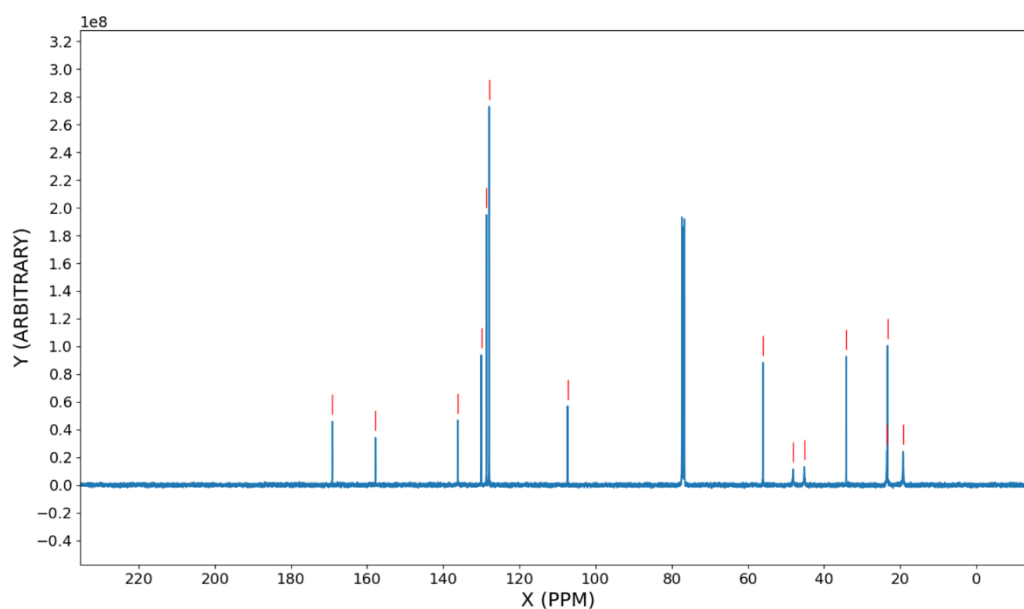


(*E*)-*N*-((1-Benzyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazol-4-yl)methyl)acetamido (9a)

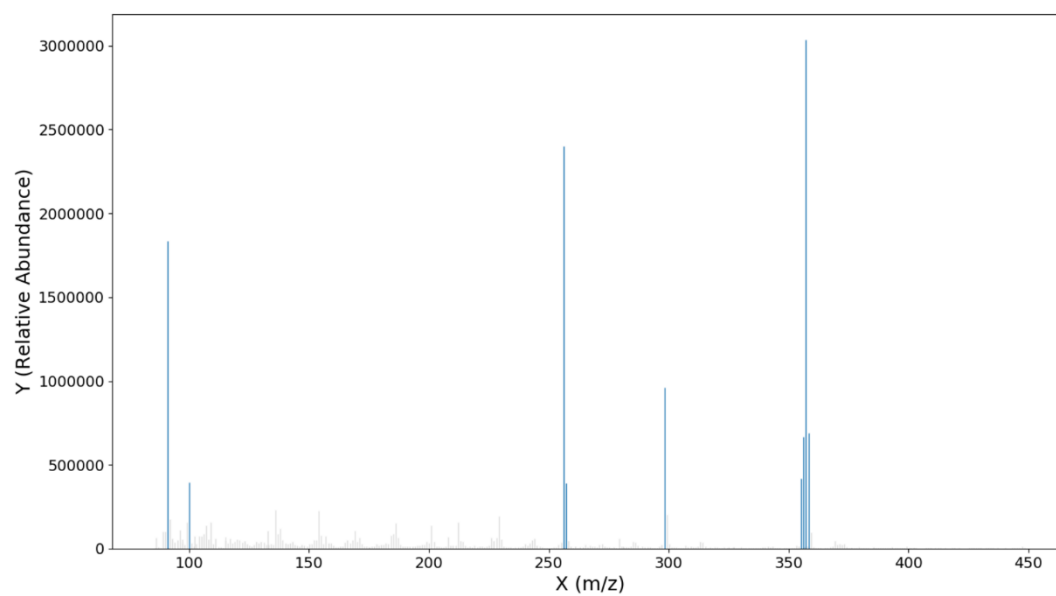
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



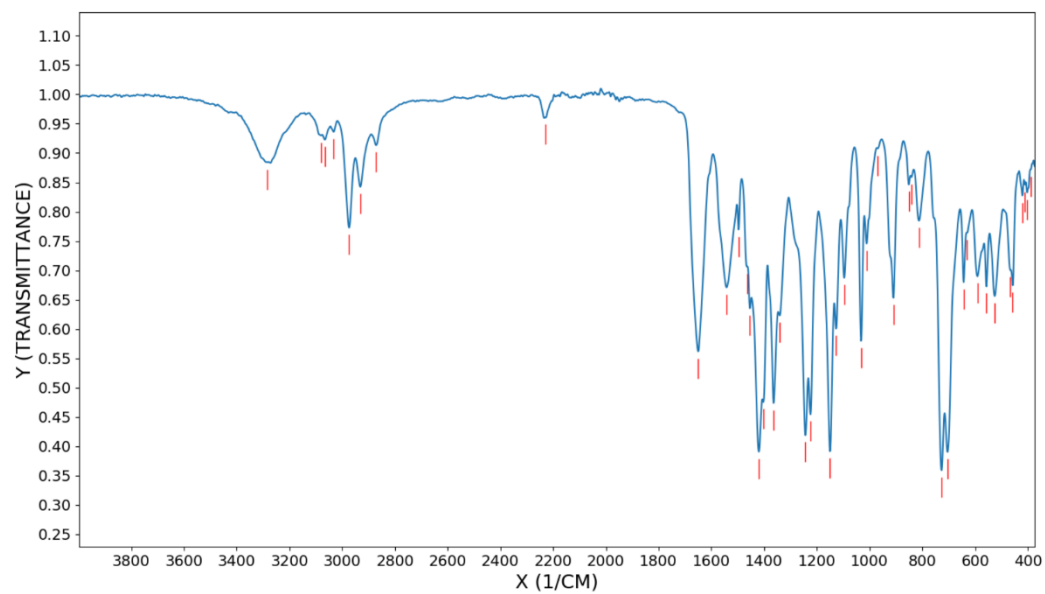
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

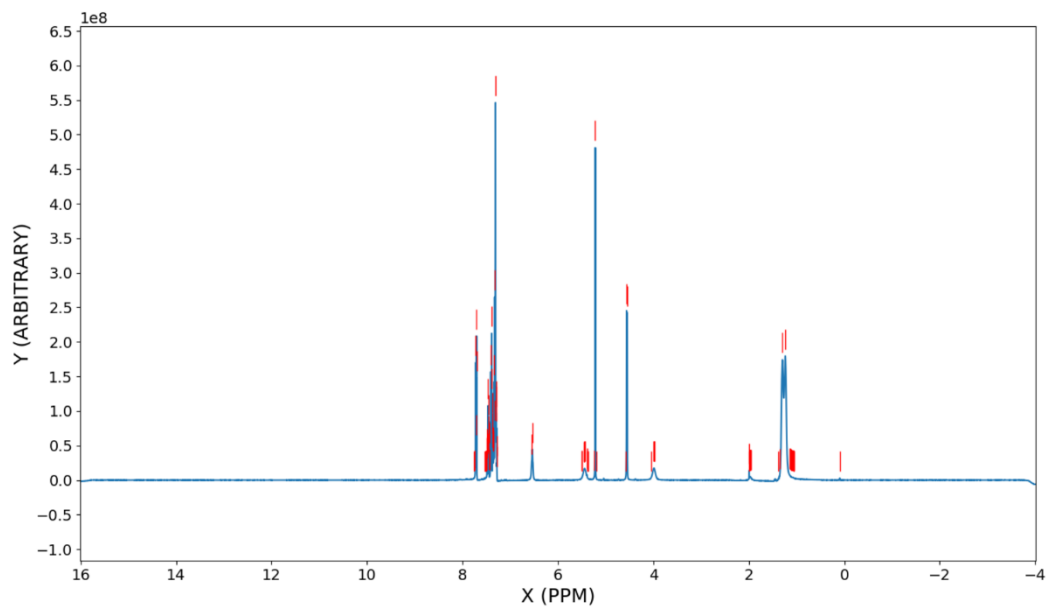


CHMO:0000630 | infrared absorption spectroscopy (IR)

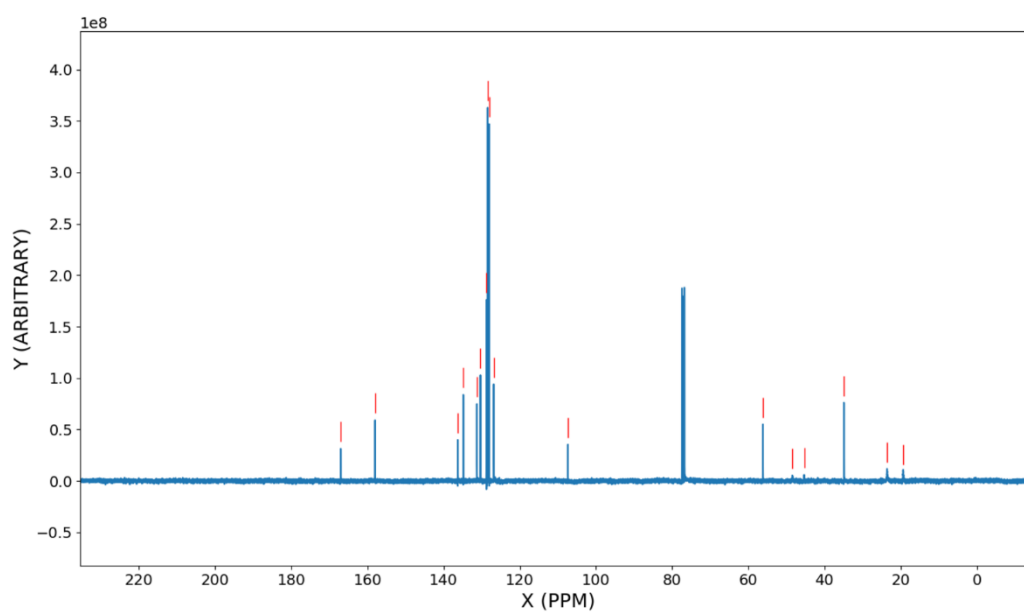


(*E*)-*N*-((1-Benzyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazol-4-yl)methyl)benzamide (9b)

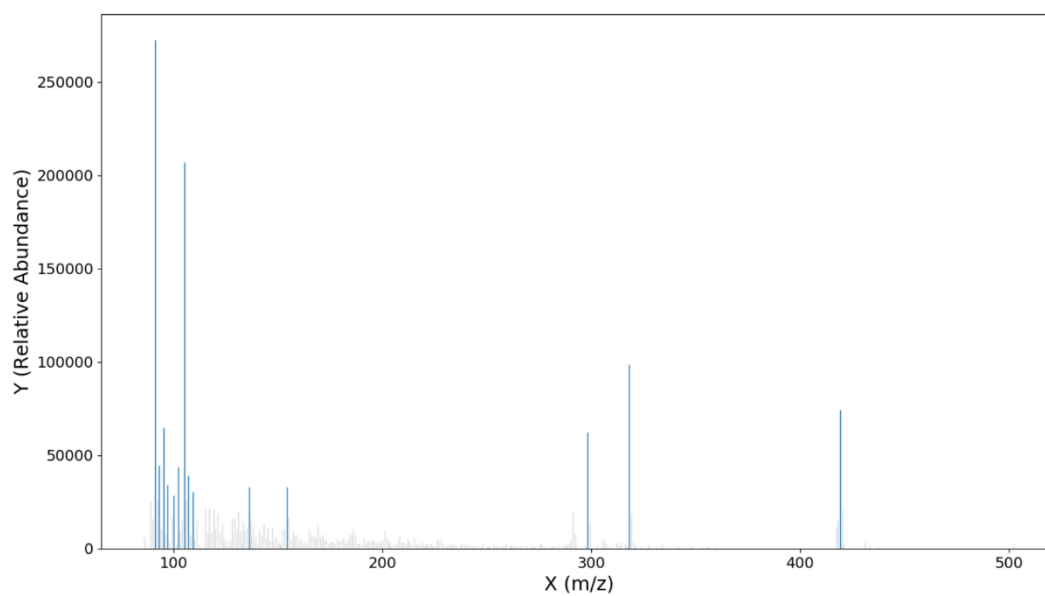
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



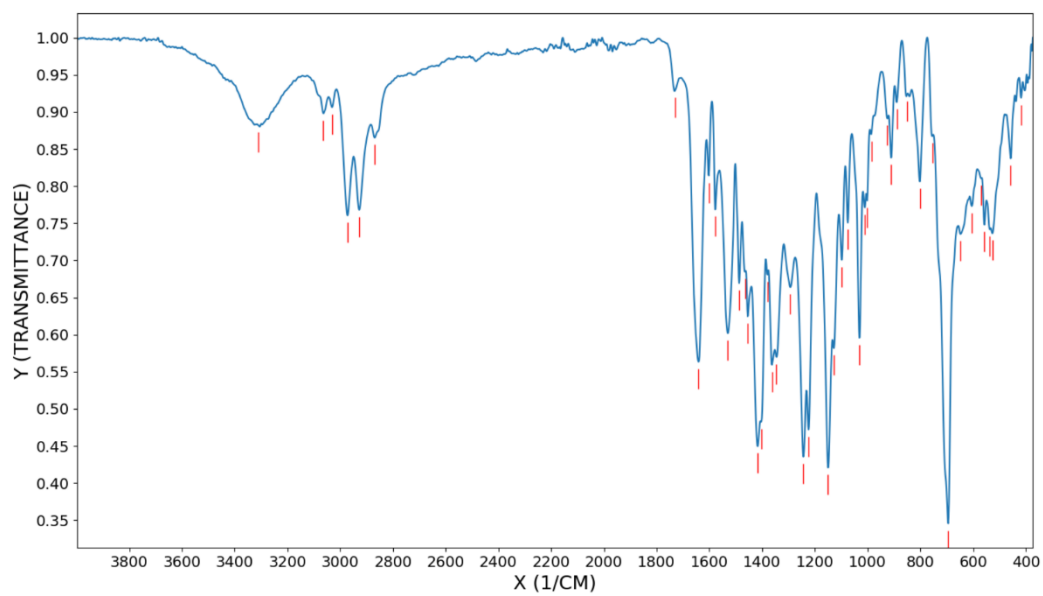
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

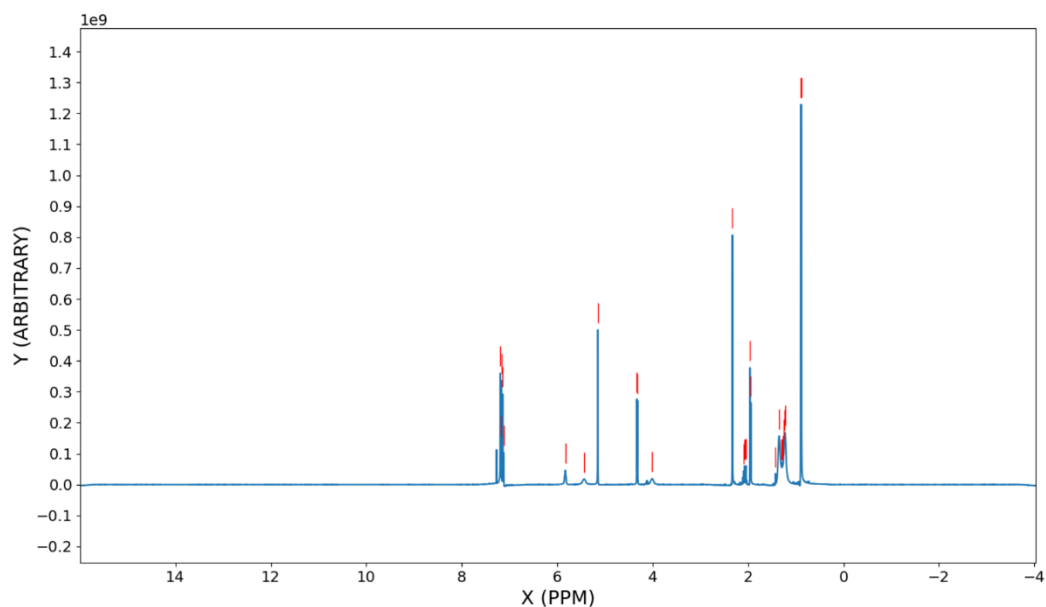


CHMO:0000630 | infrared absorption spectroscopy (IR)

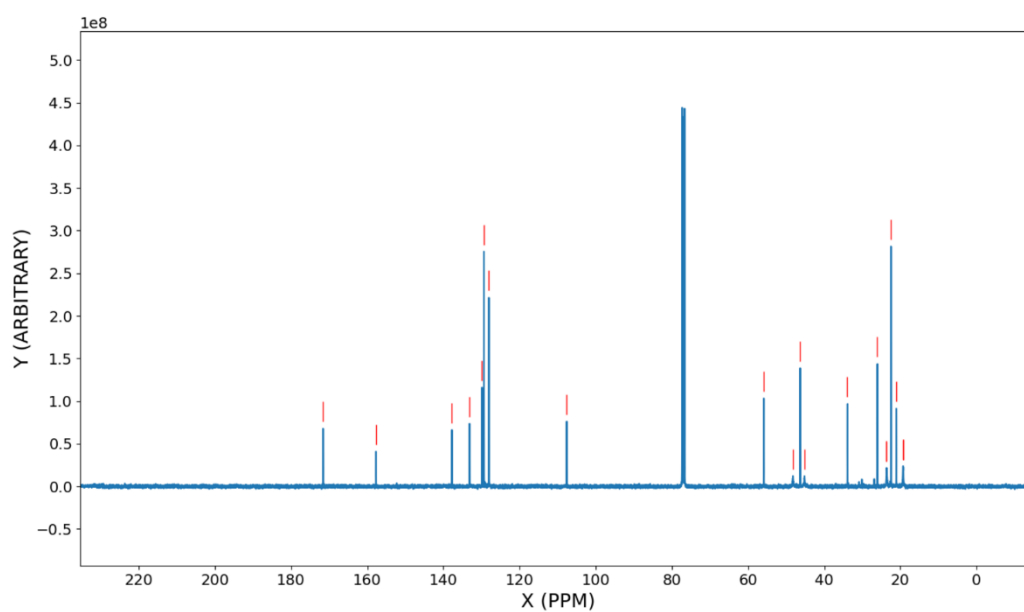


(*E*)-*N*-((3-(3,3-Diisopropyltriaz-1-en-1-yl)-1-(4-methylbenzyl)-1*H*-pyrazol-4-yl)methyl)-3-methylbutanamide (9c)

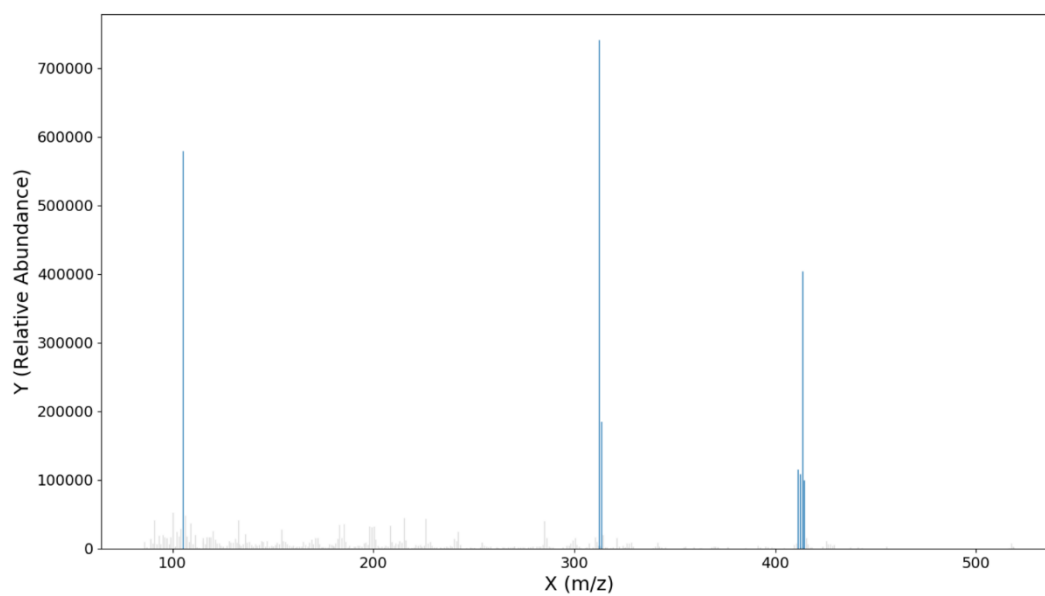
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



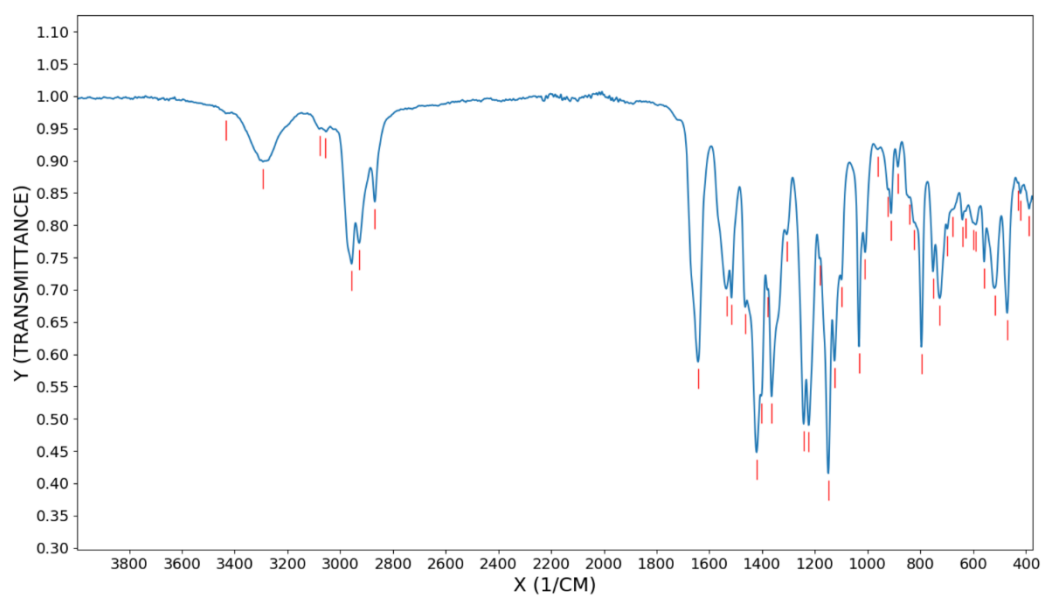
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

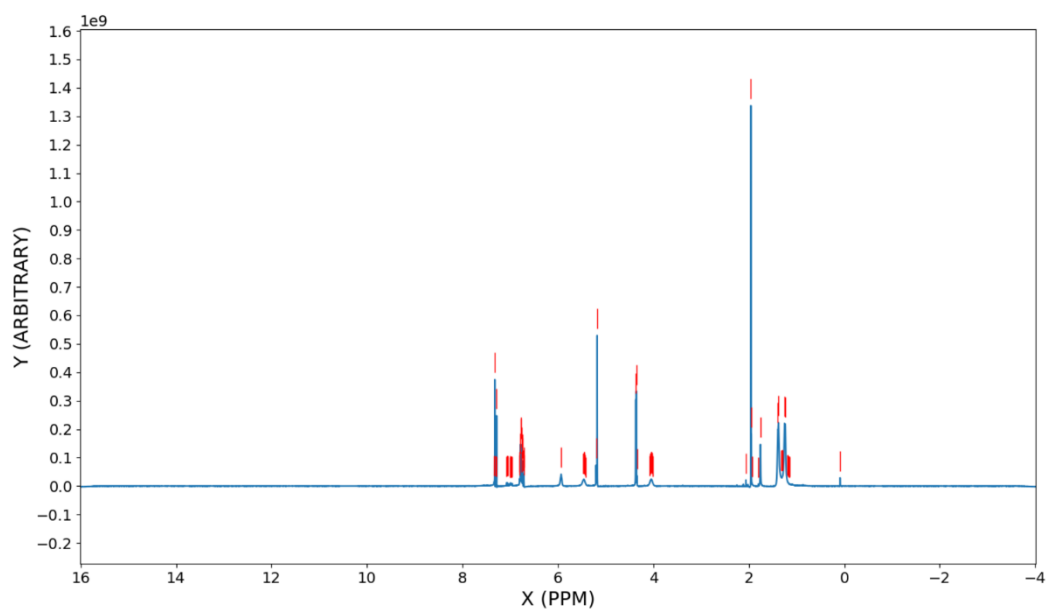


CHMO:0000630 | infrared absorption spectroscopy (IR)

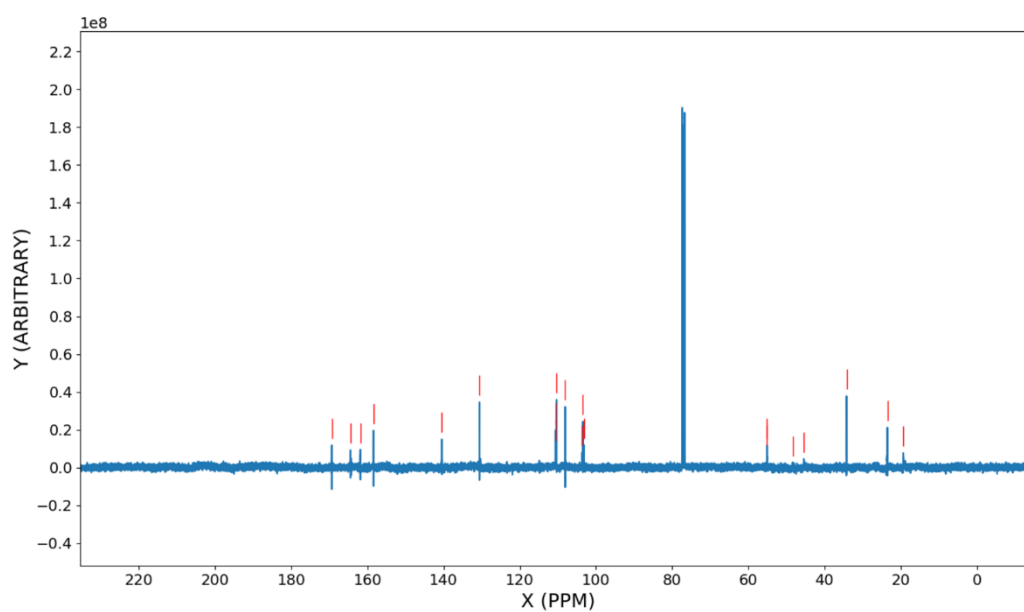


(*E*)-*N*-((1-(3,5-Difluorobenzyl)-3-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazol-4-yl)methyl)acetamido (9d)

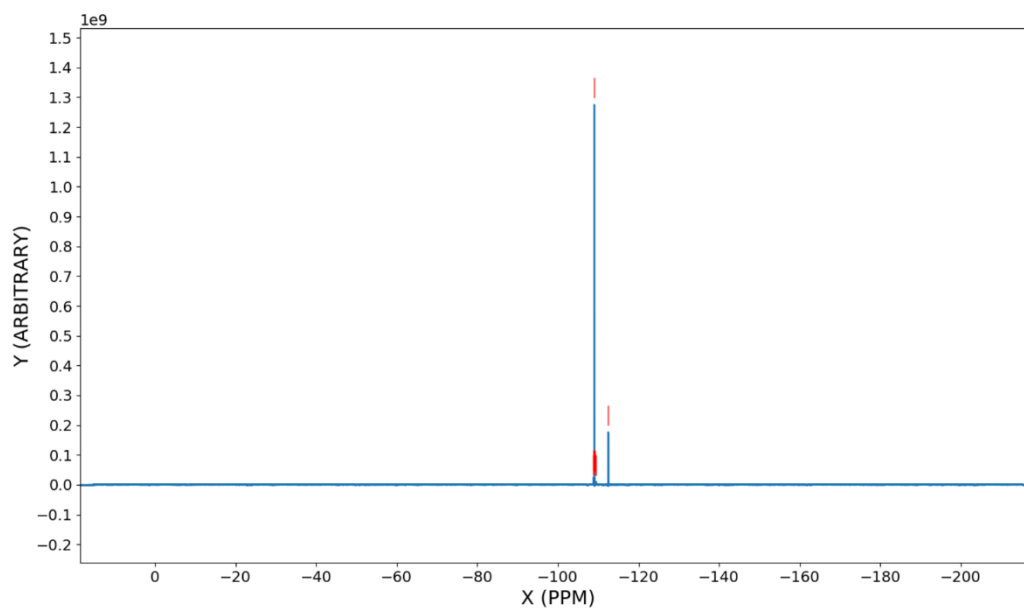
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



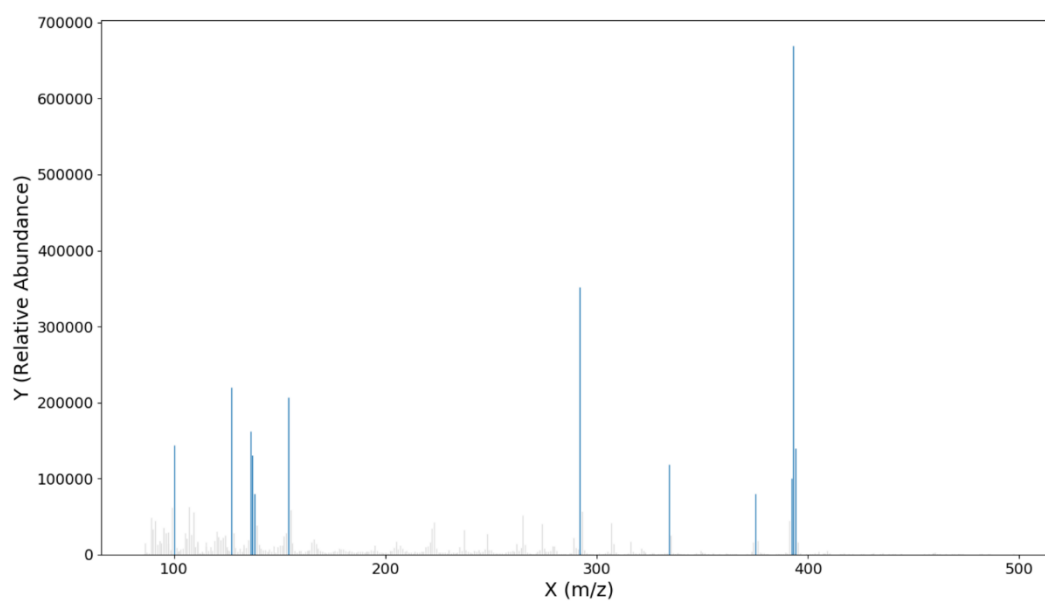
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



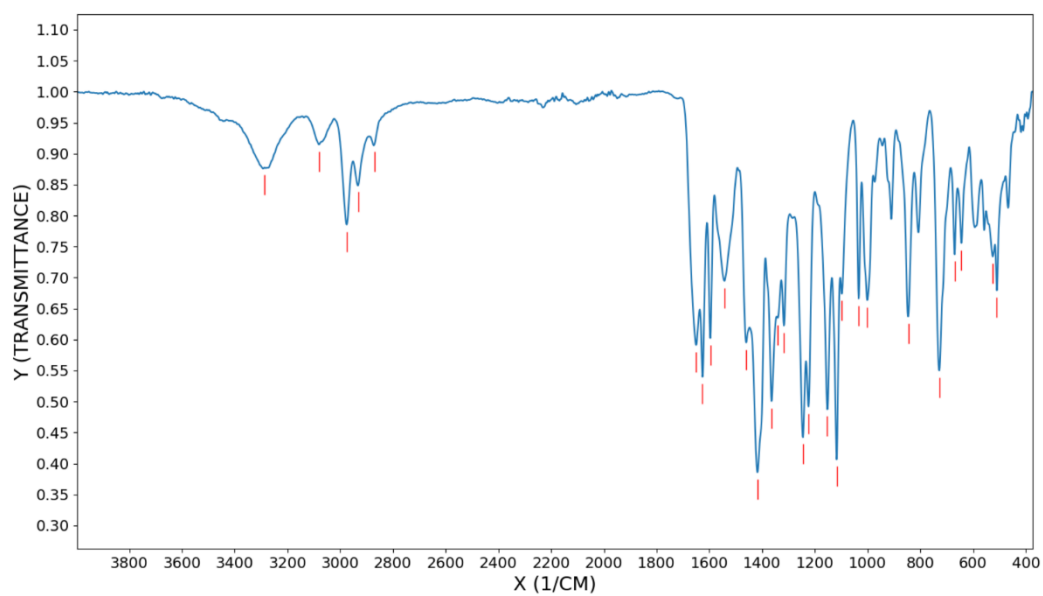
CHMO:0000597 | ^{19}F nuclear magnetic resonance spectroscopy (^{19}F NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

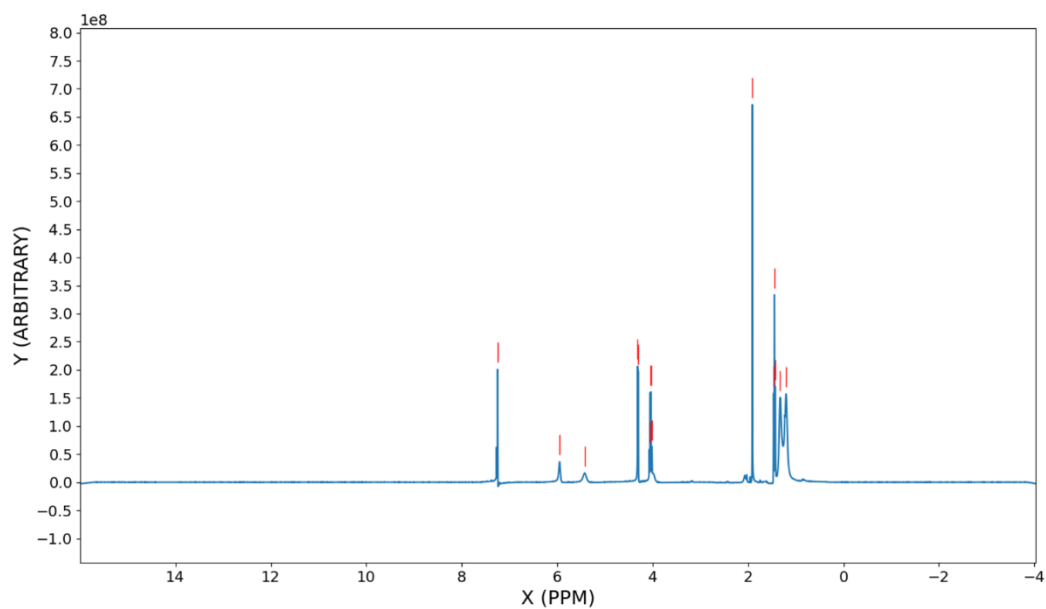


CHMO:0000630 | infrared absorption spectroscopy (IR)

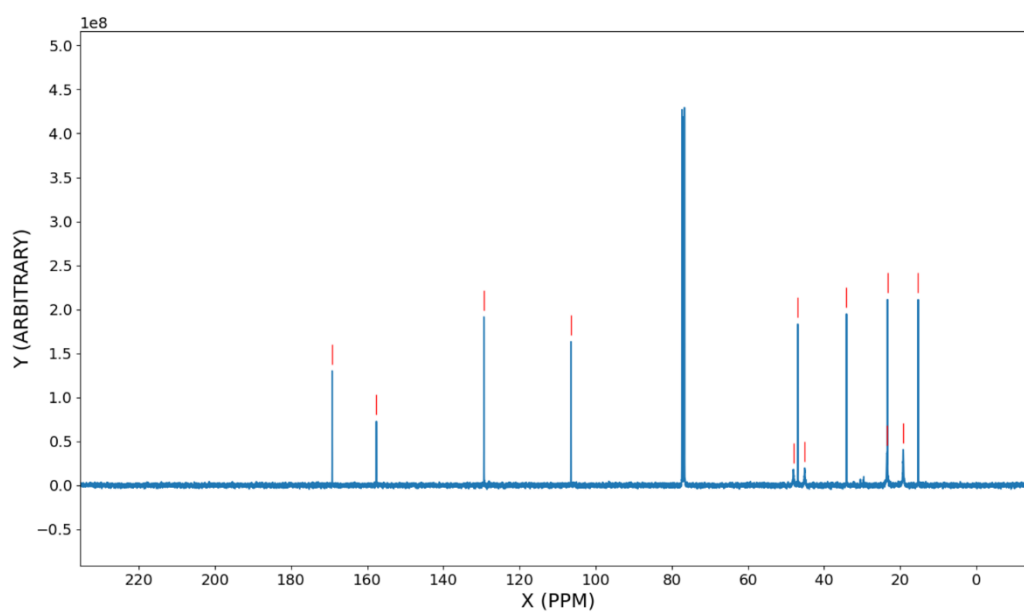


(*E*)-*N*-((3-(3,3-Diisopropyltriaz-1-en-1-yl)-1-ethyl-1*H*-pyrazol-4-yl)methyl)acetamido (9e)

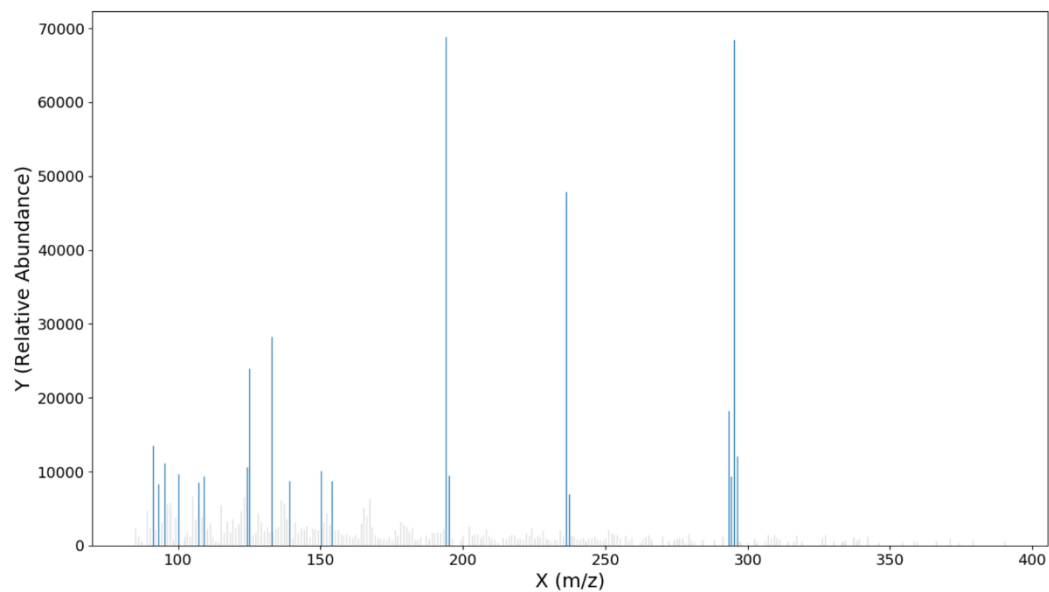
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



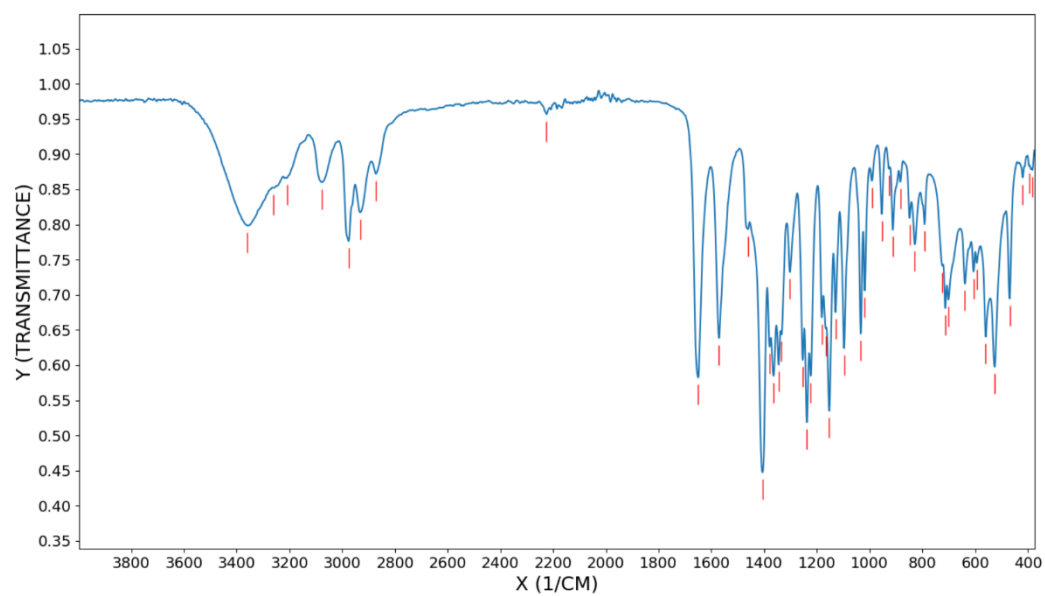
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

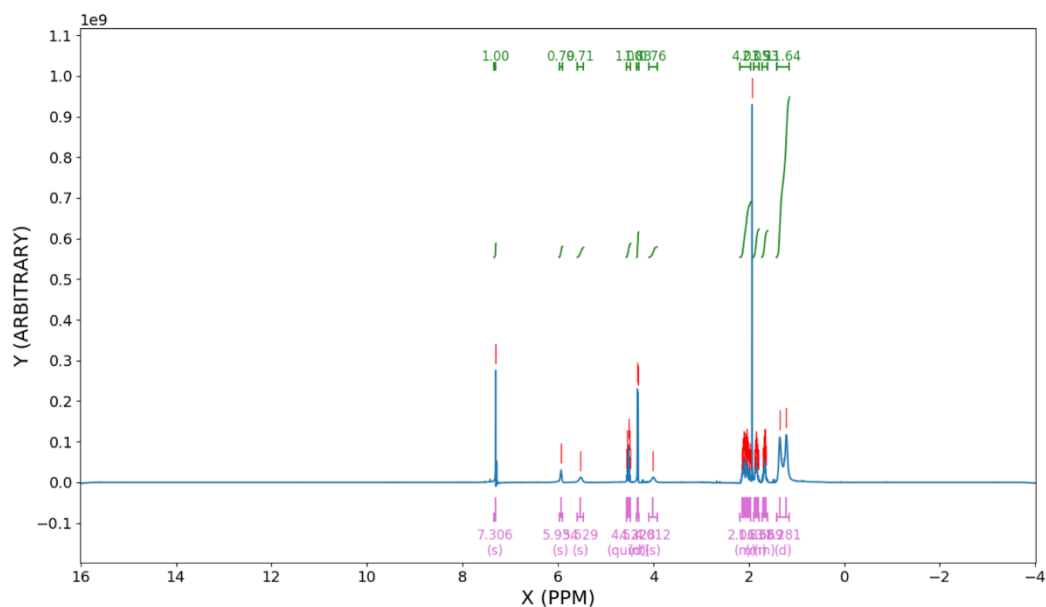


CHMO:0000630 | infrared absorption spectroscopy (IR)

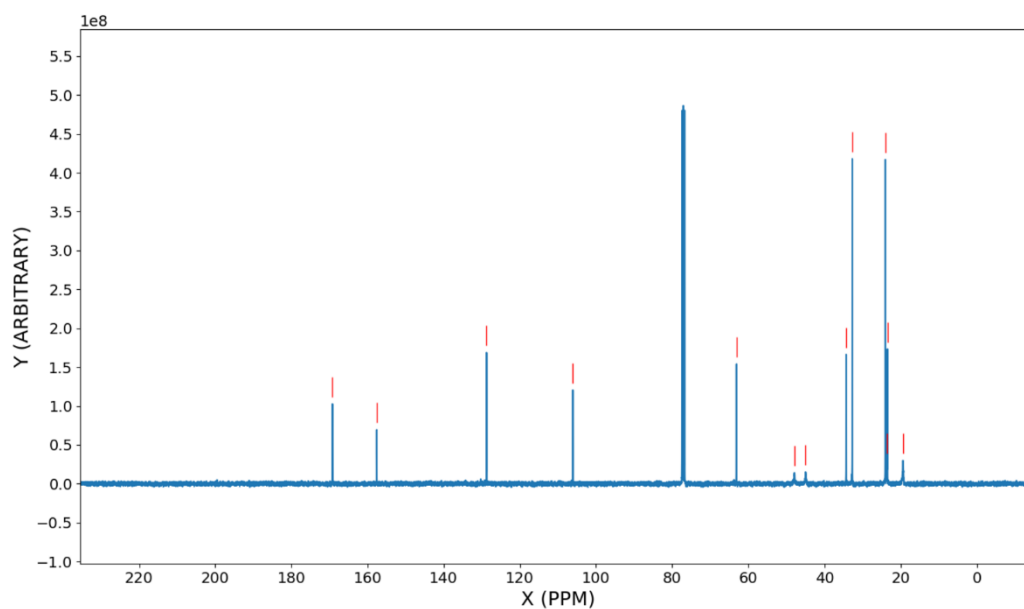


(E)-N-((1-Cyclopentyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1H-pyrazol-4-yl)methyl)acetamido (9f)

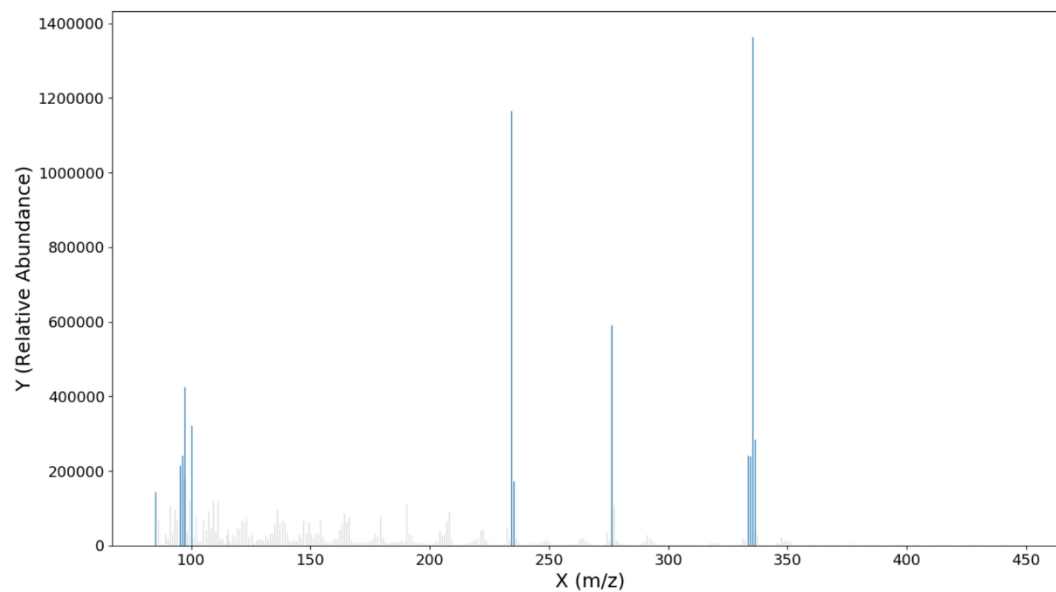
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



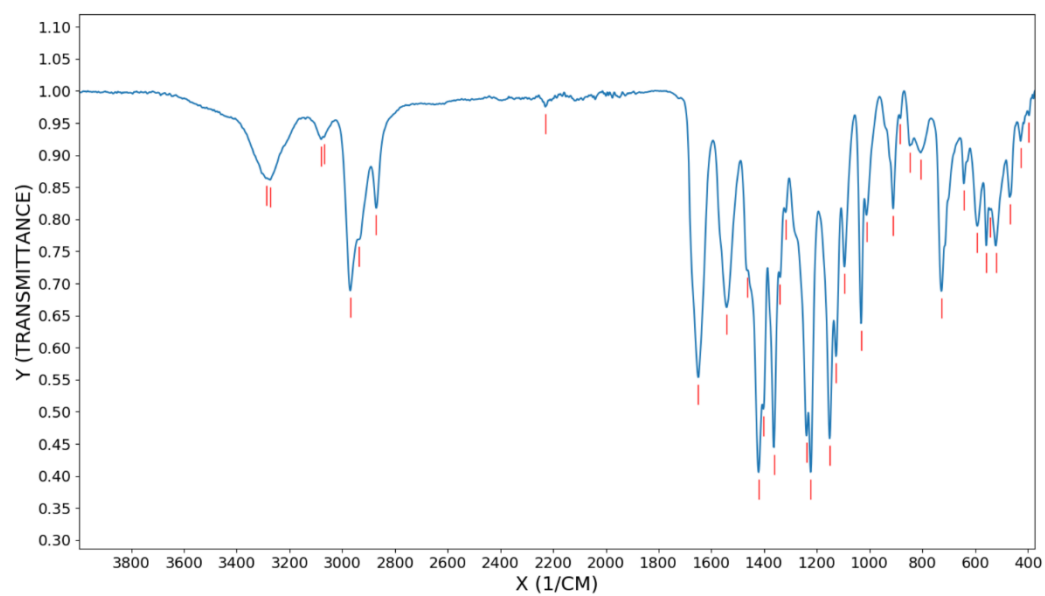
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

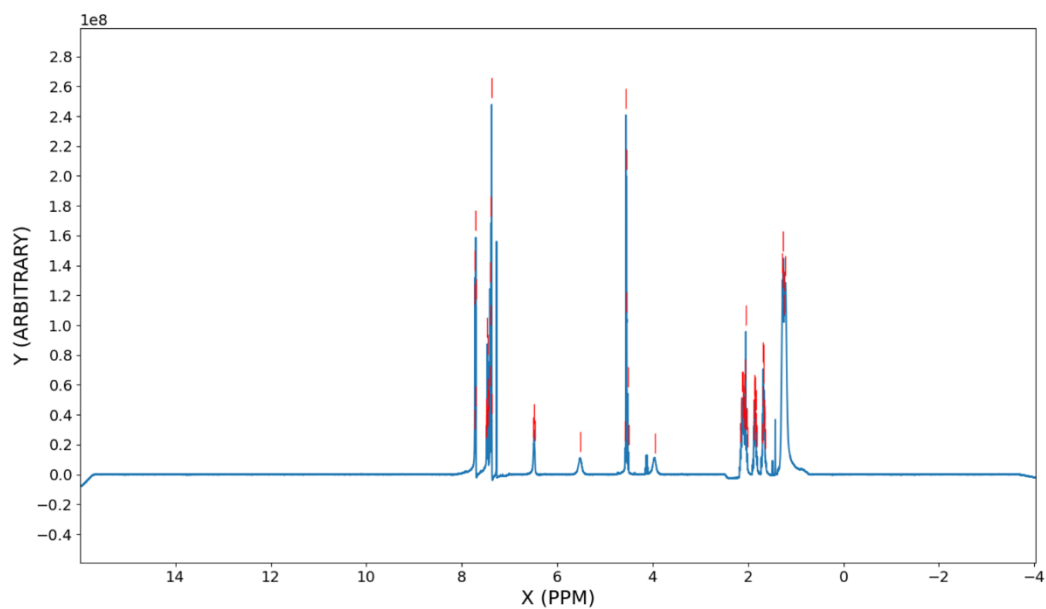


CHMO:0000630 | infrared absorption spectroscopy (IR)

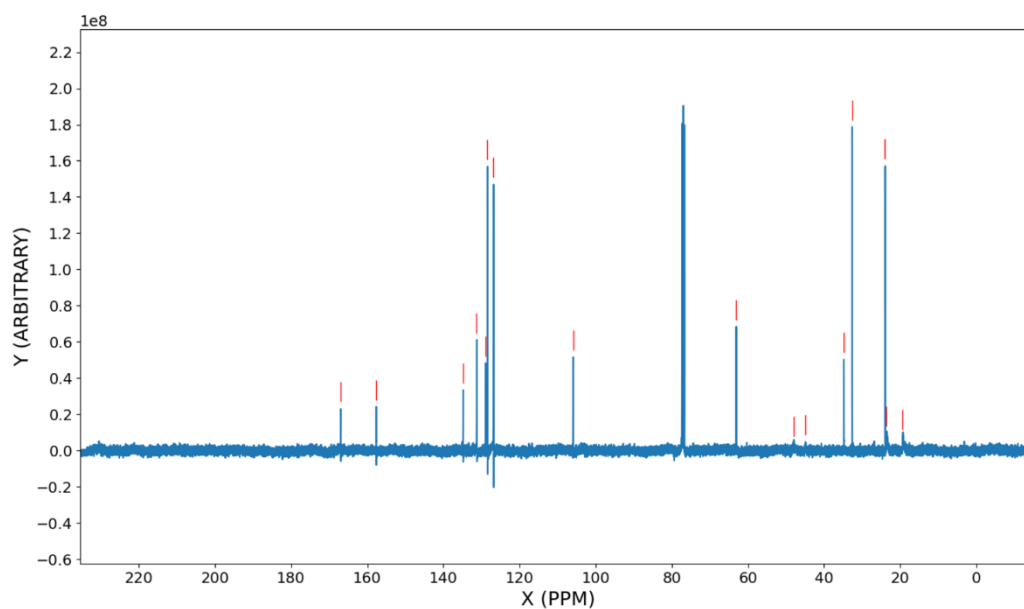


(*E*)-*N*-((1-Cyclopentyl-3-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazol-4-yl)methyl)benzamide (9g)

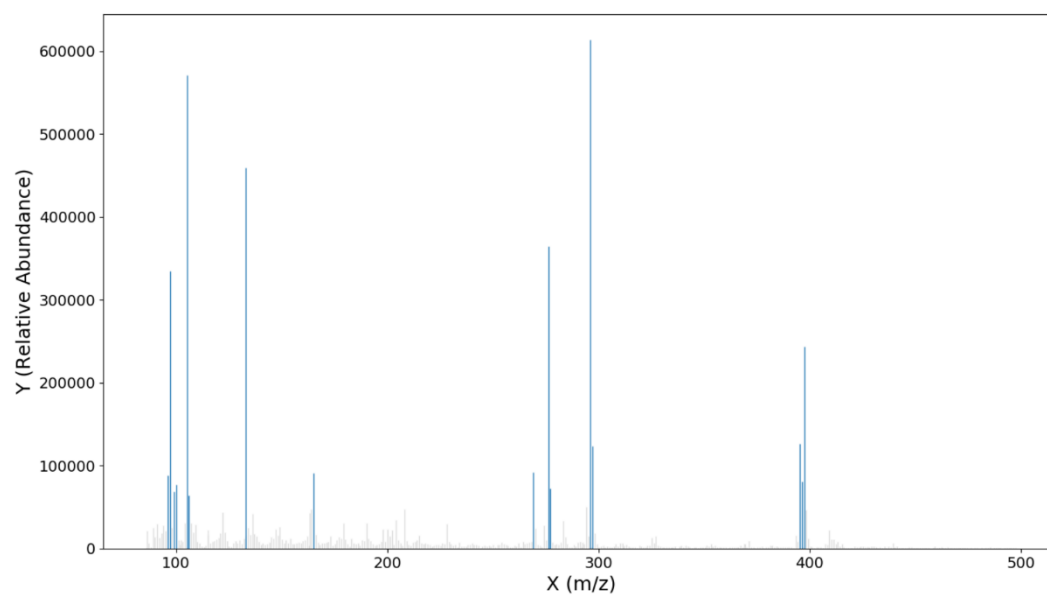
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



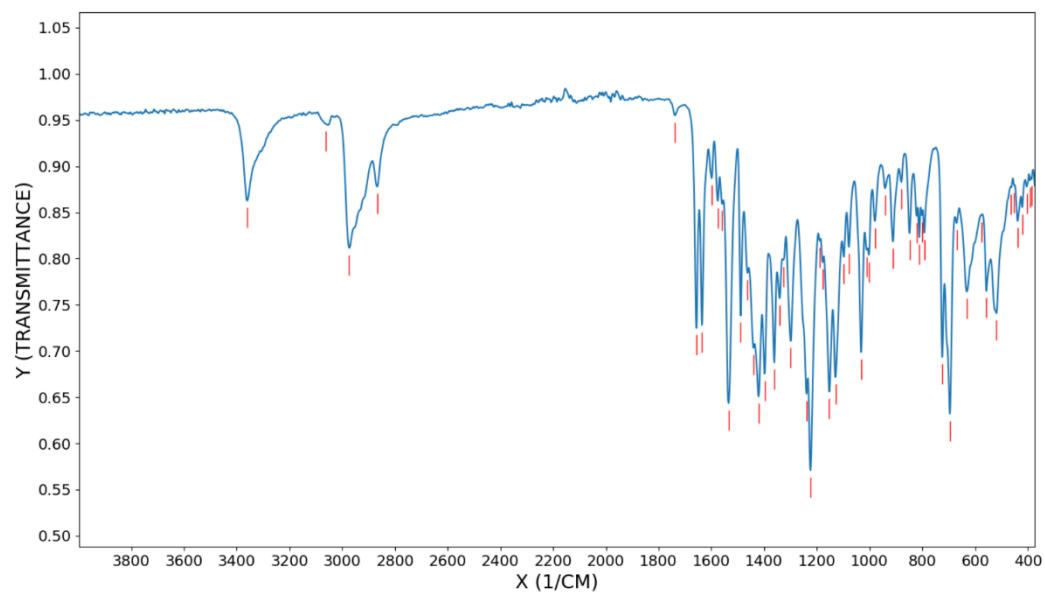
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

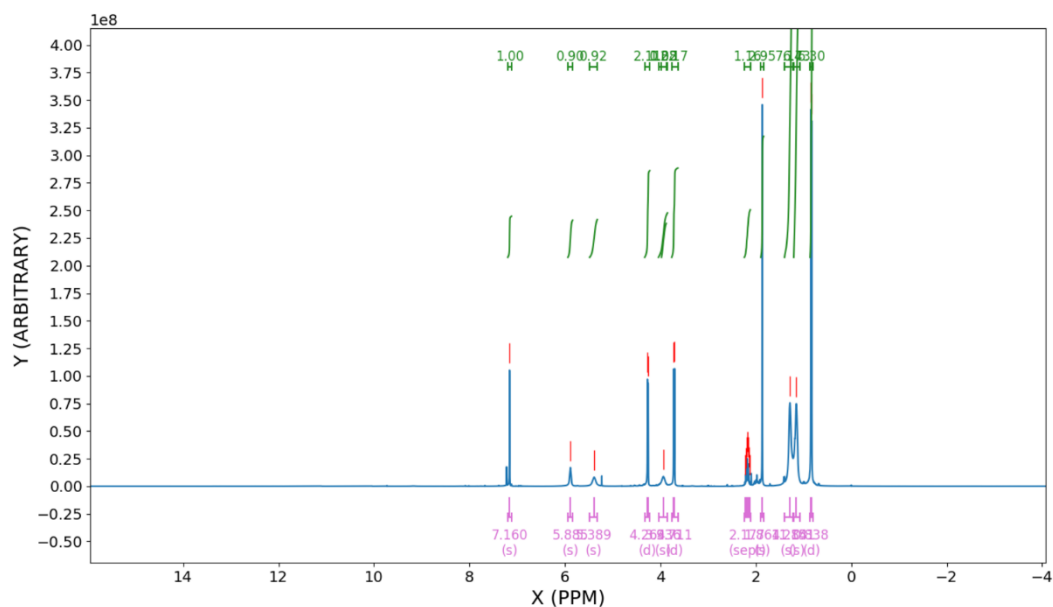


CHMO:0000630 | infrared absorption spectroscopy (IR)

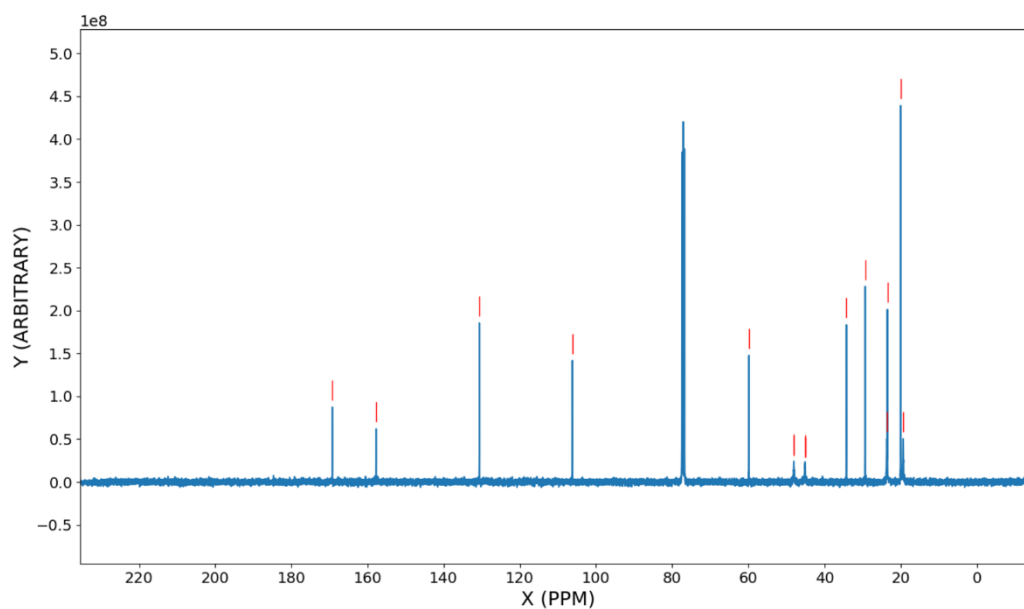


(E)-N-((3-(3,3-Diisopropyltriaz-1-en-1-yl)-1-isobutyl-1H-pyrazol-4-yl)methyl)acetamido (9h)

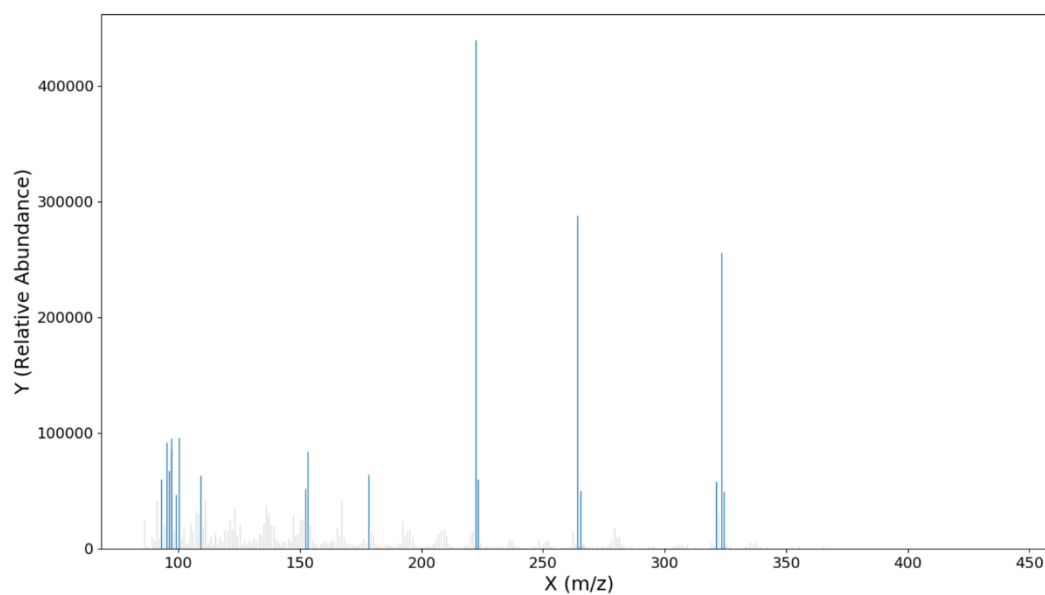
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



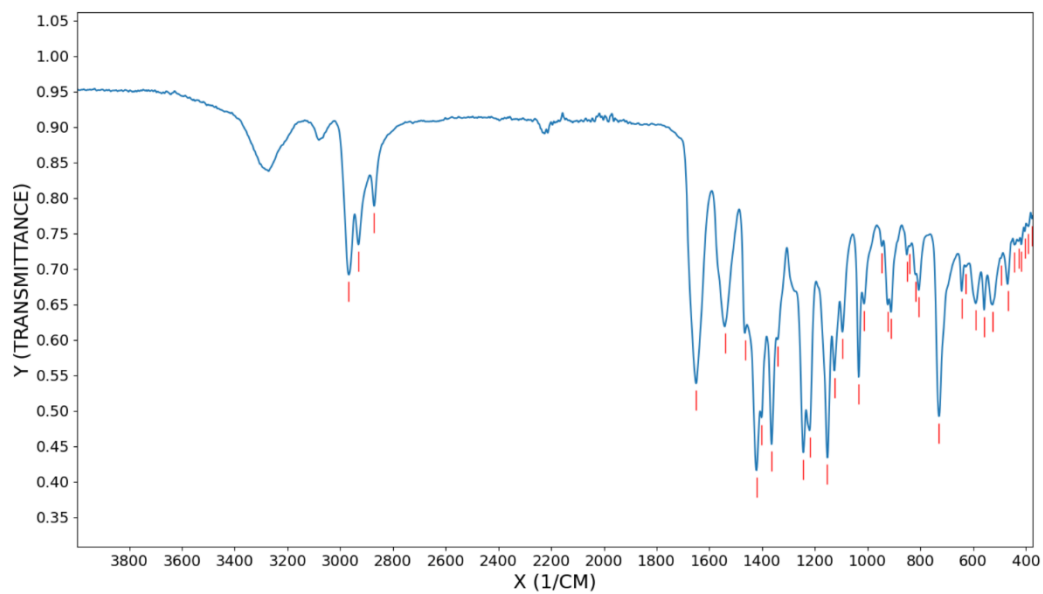
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

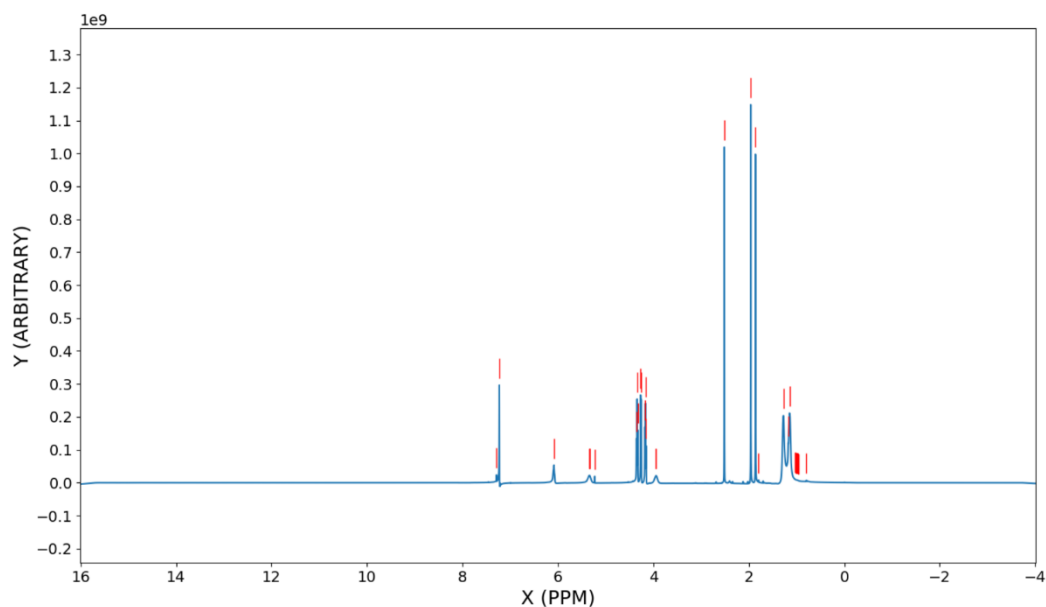


CHMO:0000630 | infrared absorption spectroscopy (IR)

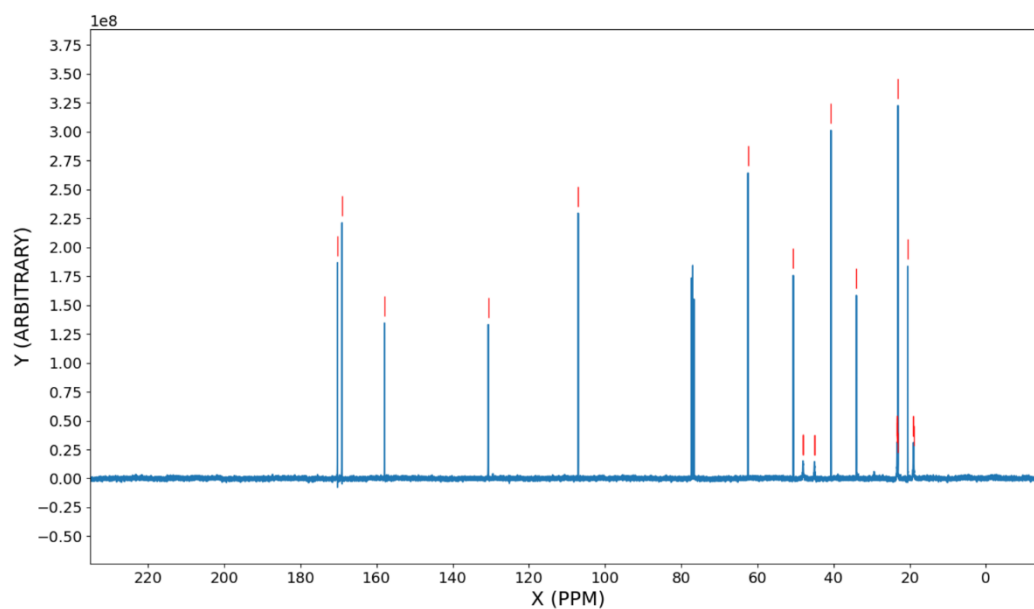


(*E*)-2-(4-(Acetamidomethyl)-3-(3,3-diisopropyltriaz-1-en-1-yl)-1*H*-pyrazol-1-yl)ethyl acetate (9i)

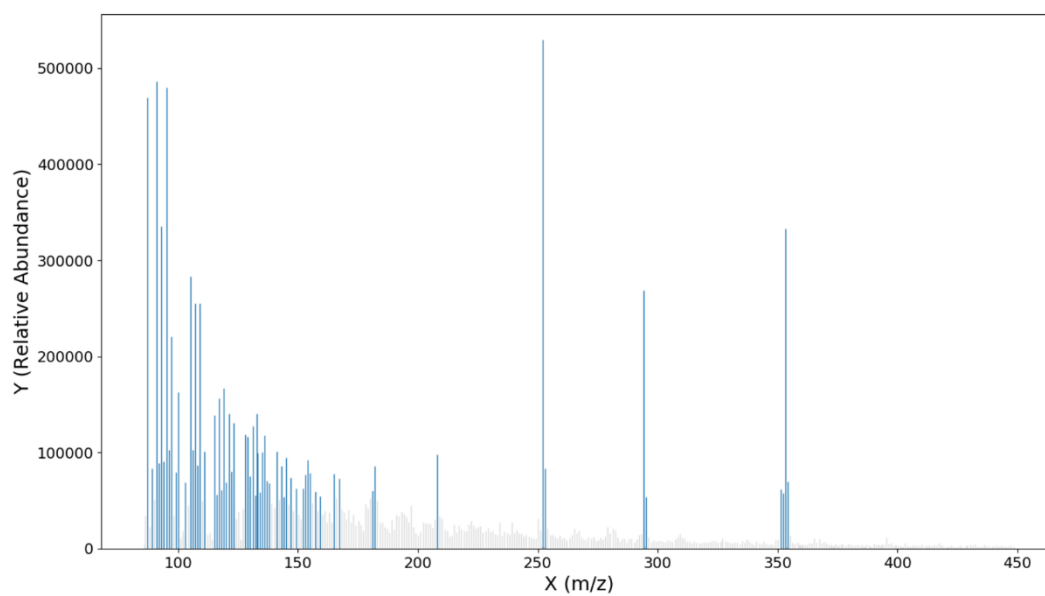
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



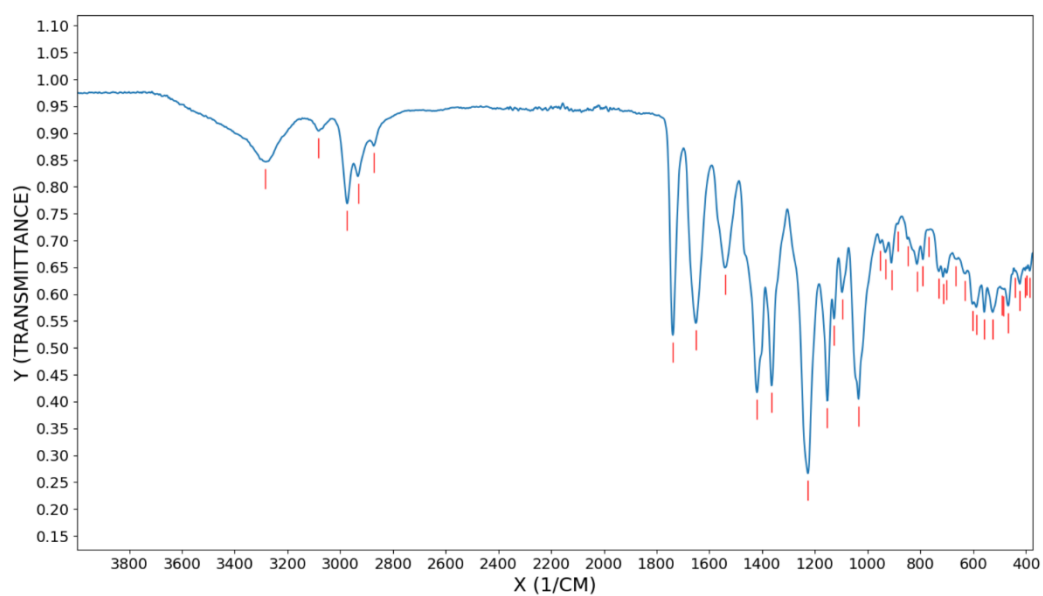
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

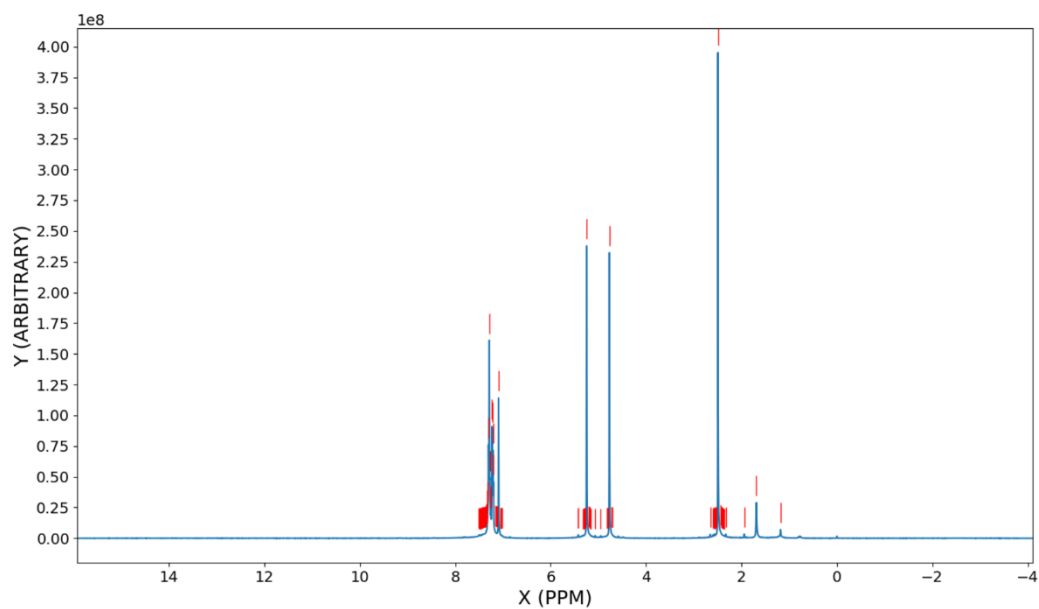


CHMO:0000630 | infrared absorption spectroscopy (IR)

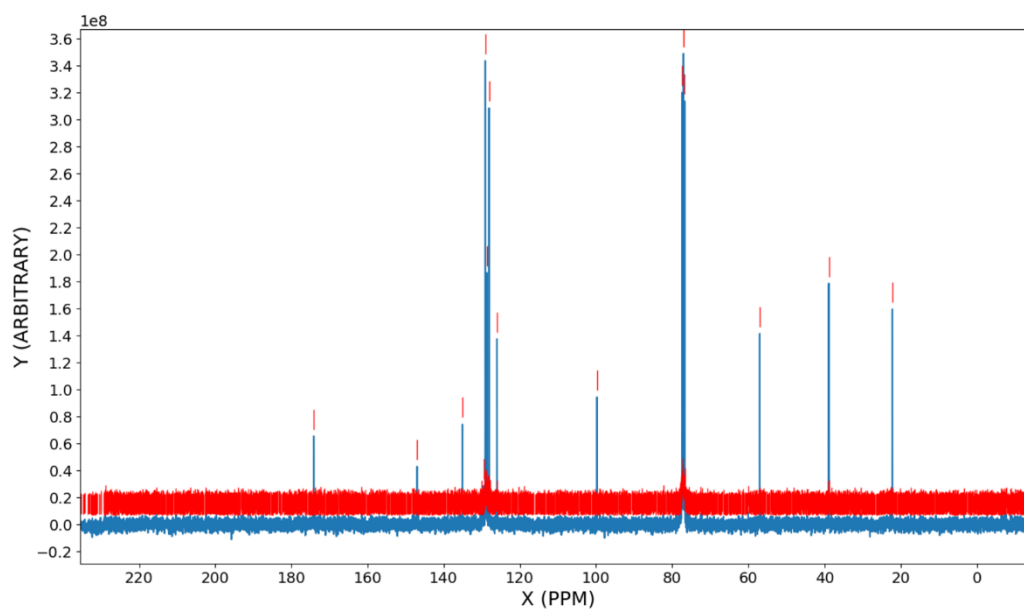


1-(6-Benzyl-4,6-dihydro-3H-pyrazolo[3,4-d][1,2,3]triazin-3-yl)ethan-1-one (5a)

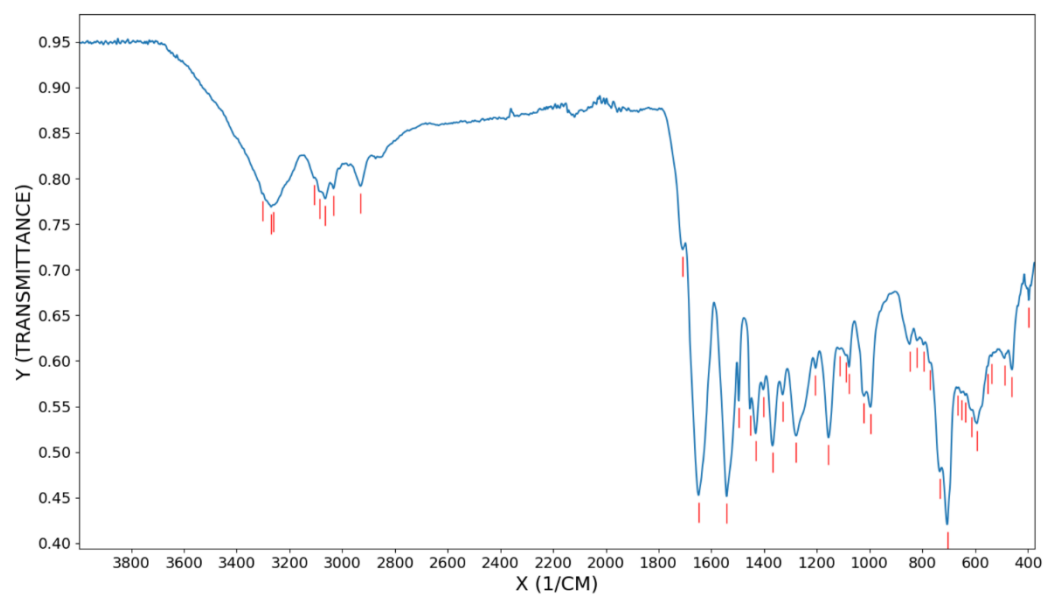
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



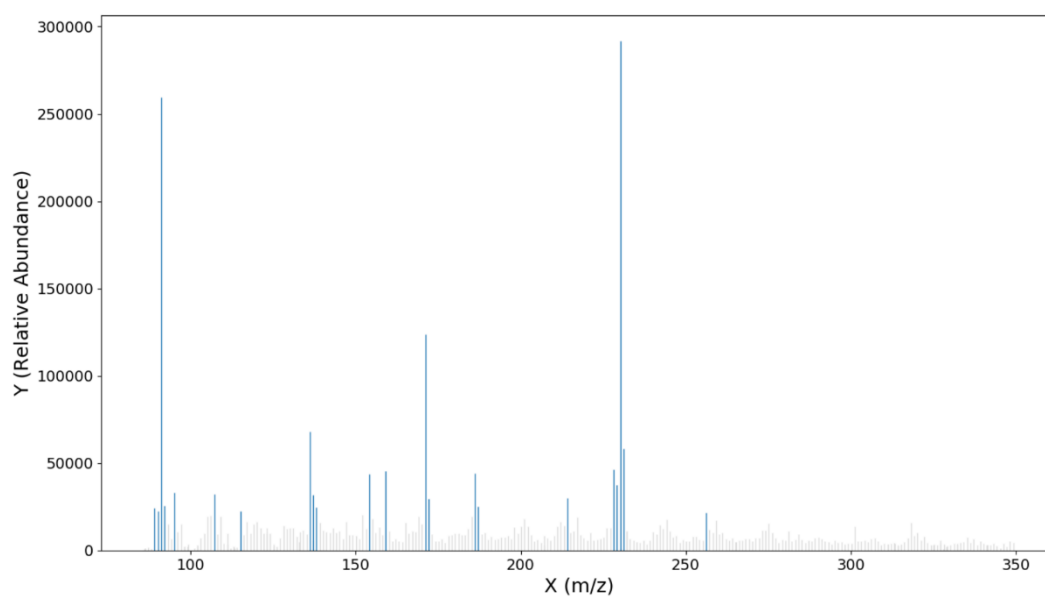
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000630 | infrared absorption spectroscopy (IR)

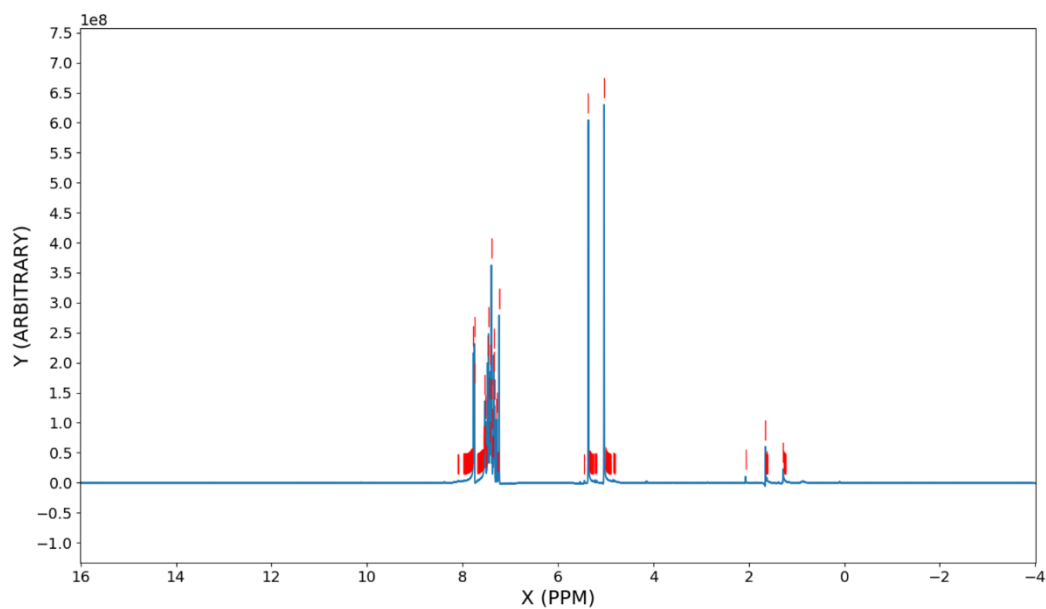


HMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

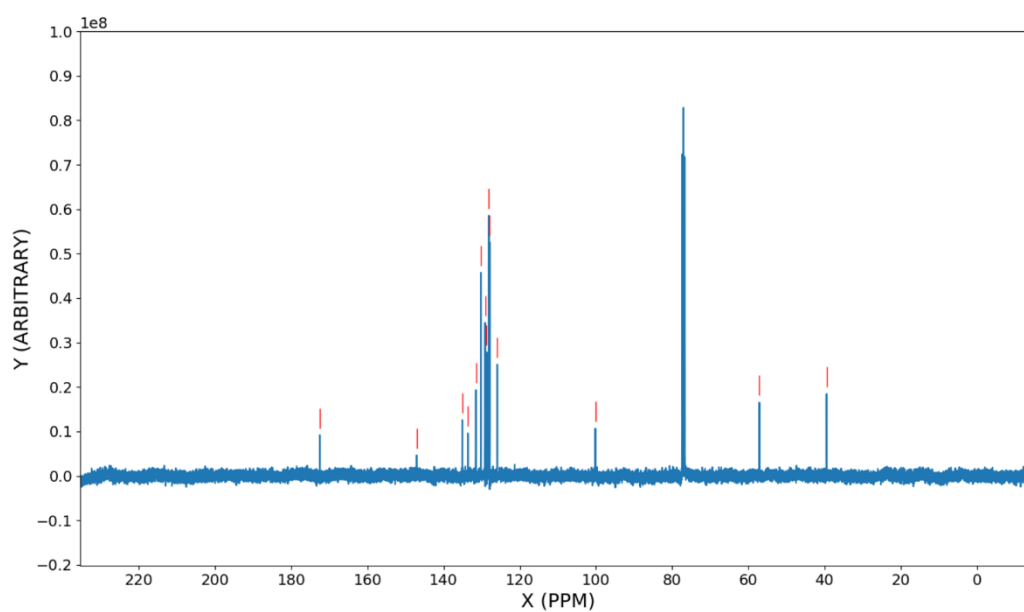


(6-Benzyl-4,6-dihydro-3H-pyrazolo[3,4-d][1,2,3]triazin-3-yl)(phenyl)methanone (5b)

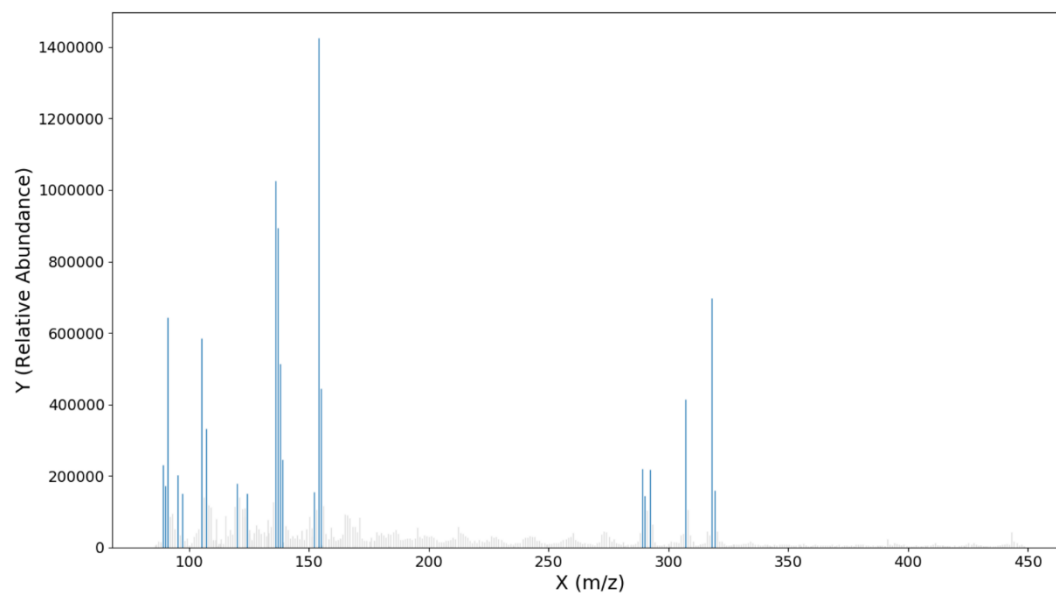
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



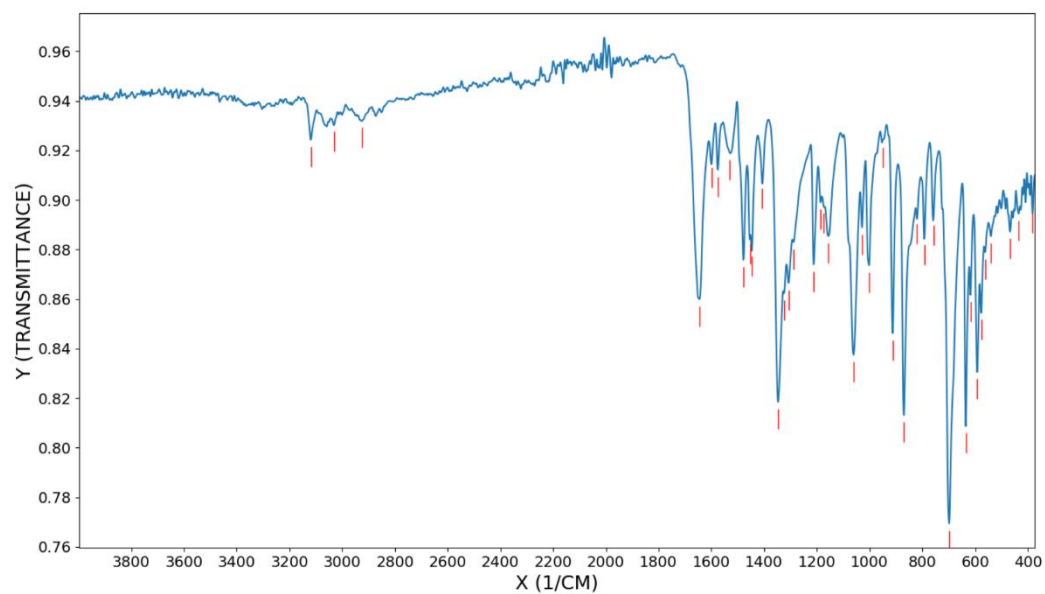
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

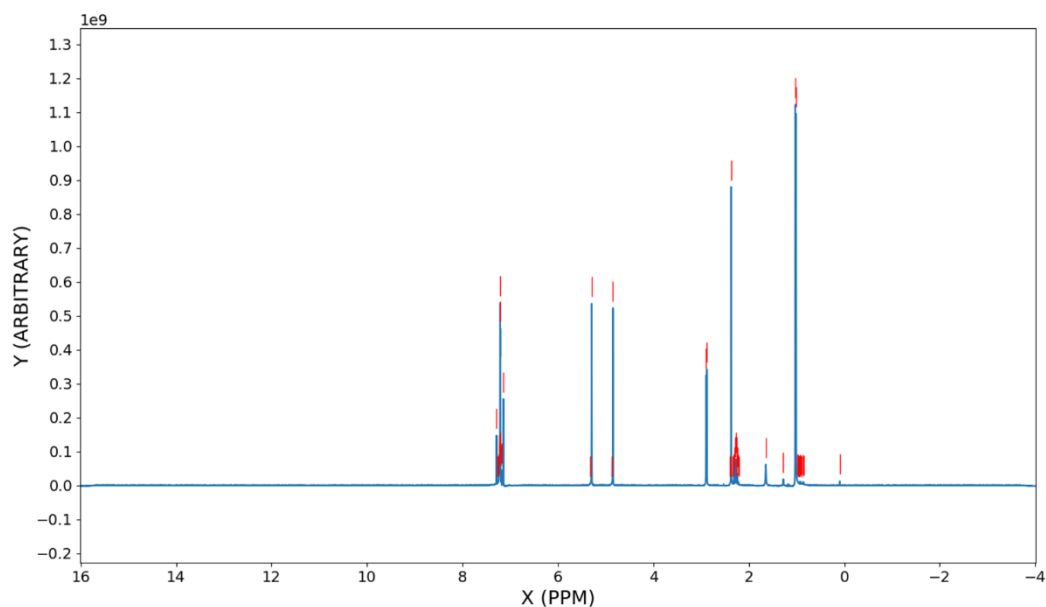


CHMO:0000630 | infrared absorption spectroscopy (IR)

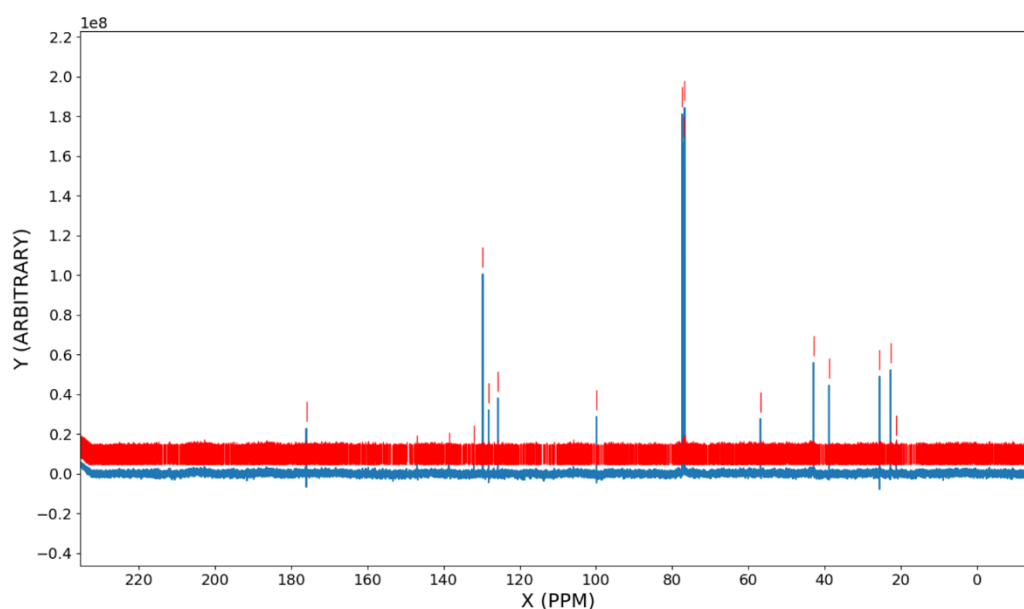


3-Methyl-1-(6-(4-methylbenzyl)-4,6-dihydro-3H-pyrazolo[3,4-d][1,2,3]triazin-3-yl)butan-1-one (5c)

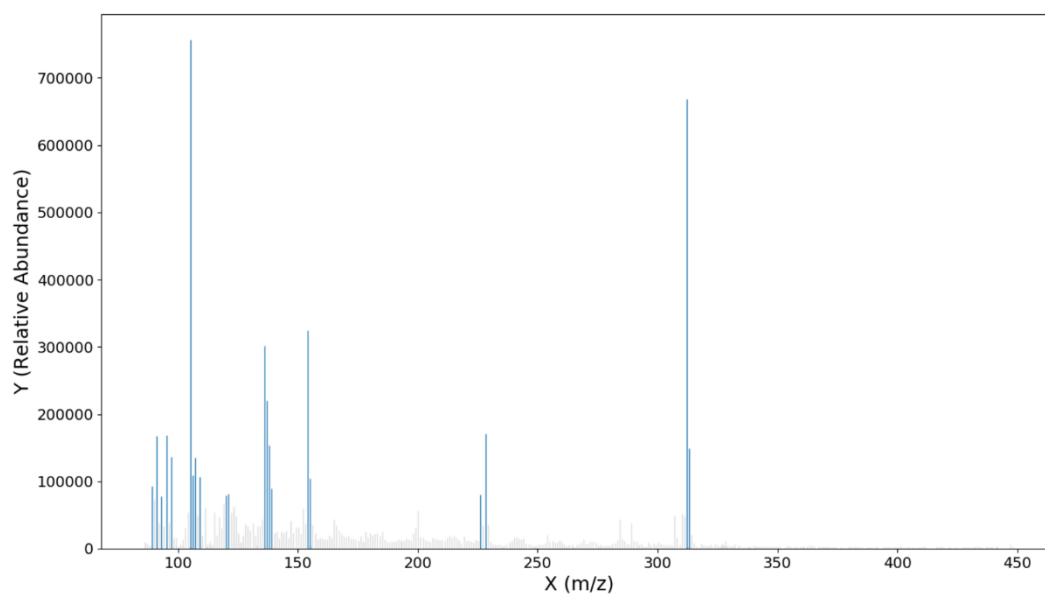
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



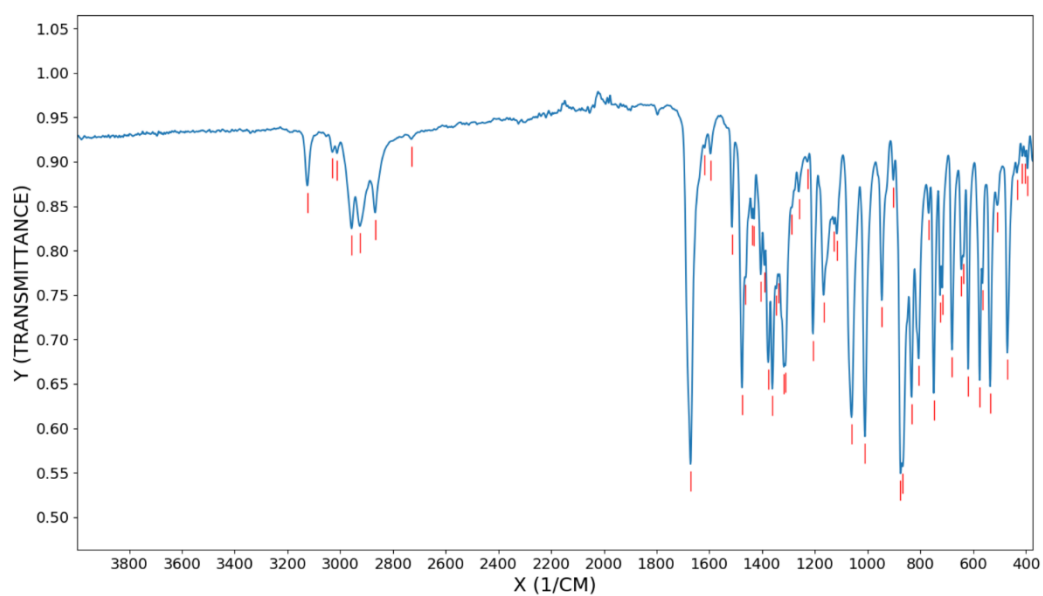
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

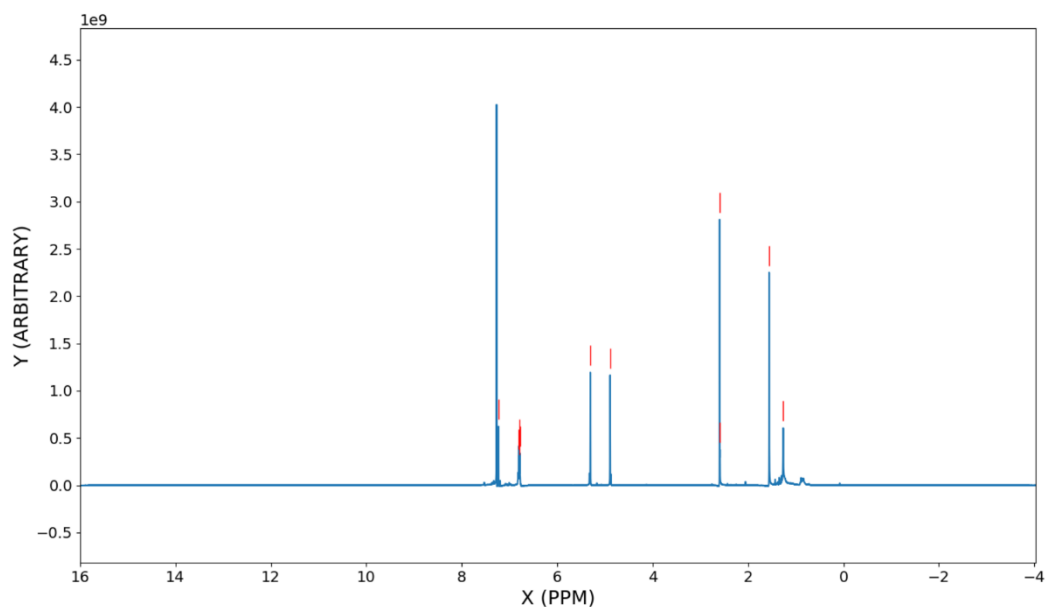


CHMO:0000630 | infrared absorption spectroscopy (IR)

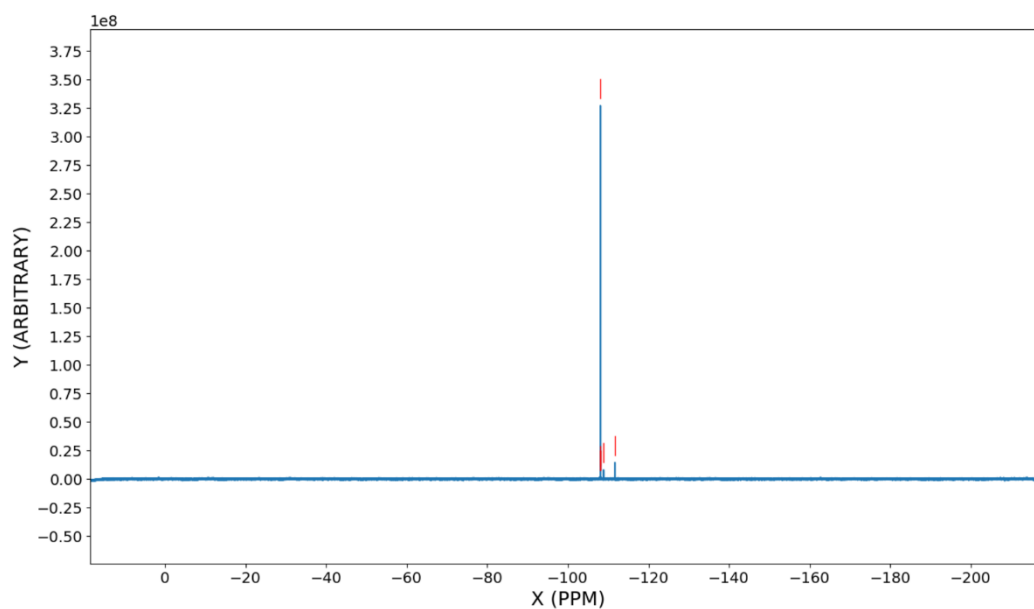


1-(6-(3,5-Difluorobenzyl)-4,6-dihydro-3H-pyrazolo[3,4-d][1,2,3]triazin-3-yl)ethan-1-one (5d)

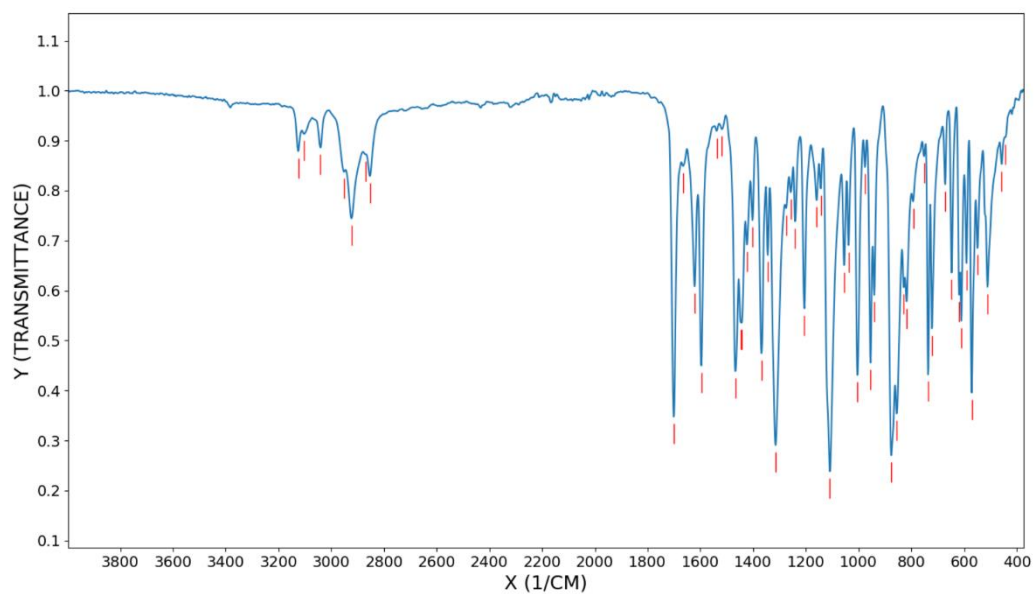
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



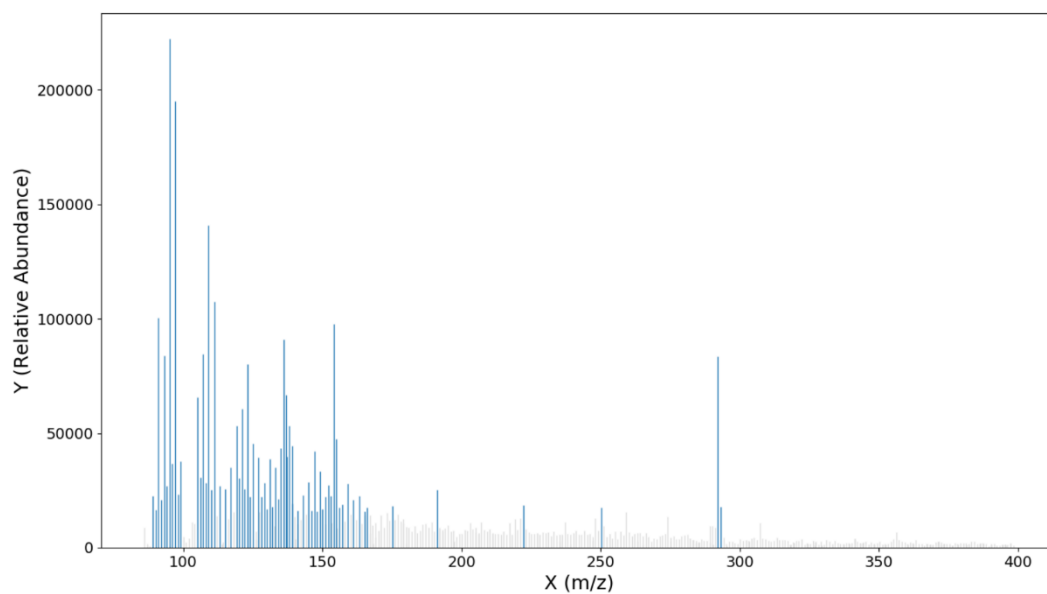
CHMO:0000597 | ¹⁹F nuclear magnetic resonance spectroscopy (¹⁹F NMR)



CHMO:0000630 | infrared absorption spectroscopy (IR)

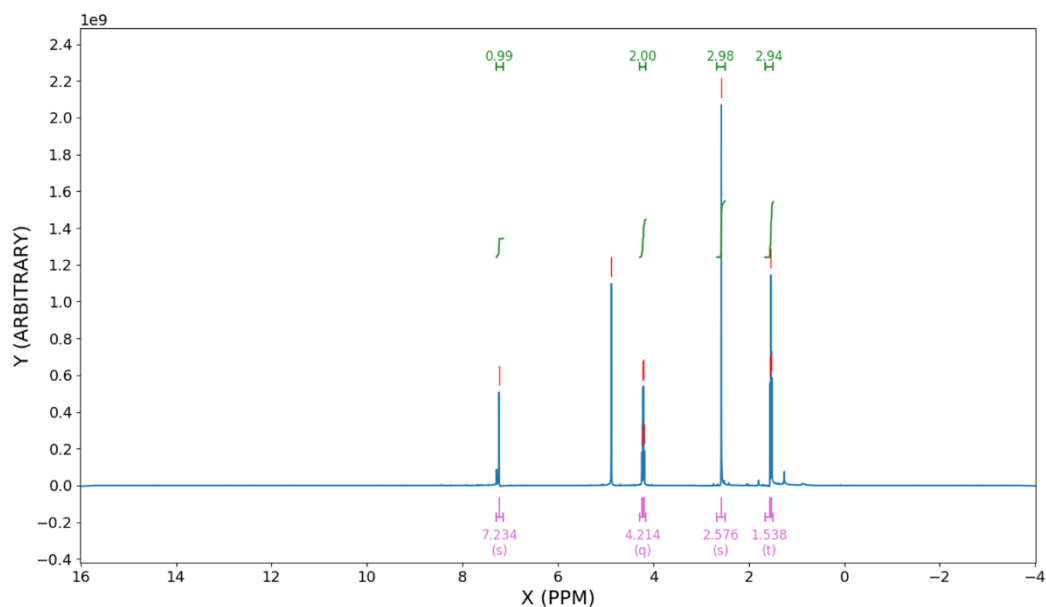


CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

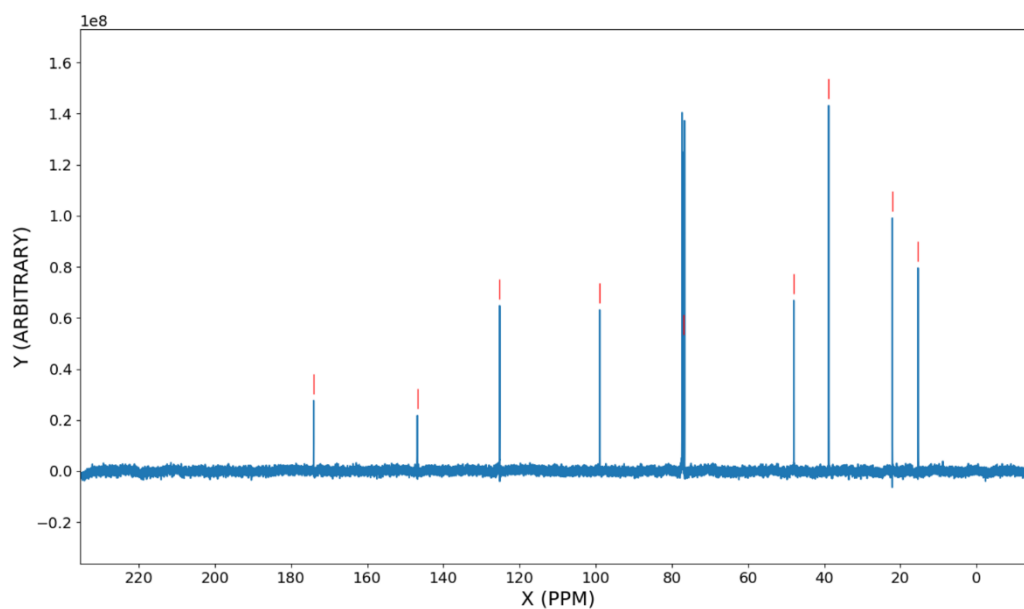


1-(6-Ethyl-4,6-dihydro-3H-pyrazolo[3,4-d][1,2,3]triazin-3-yl)ethan-1-one (5e)

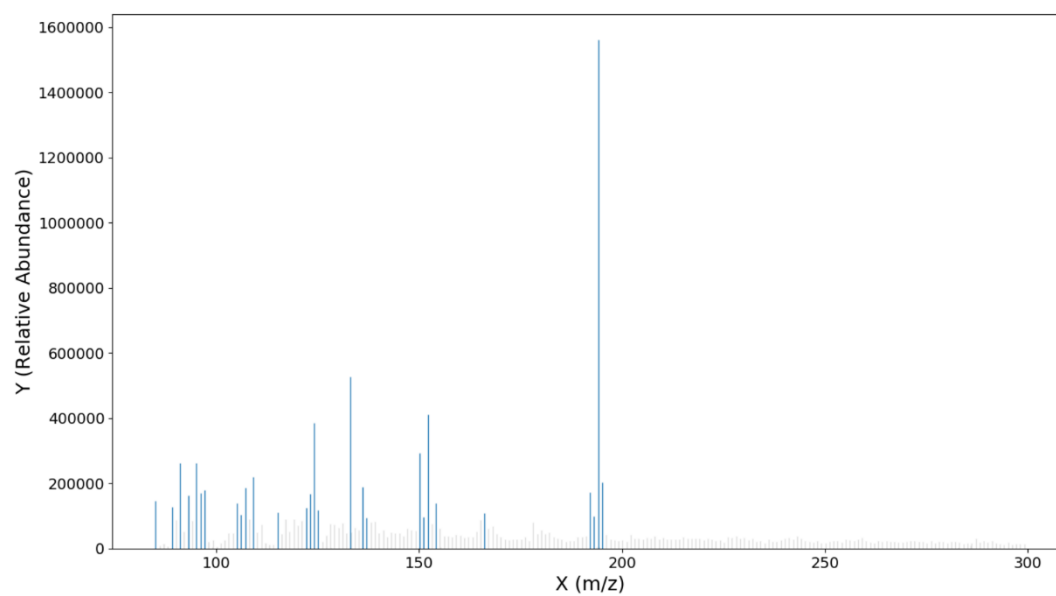
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



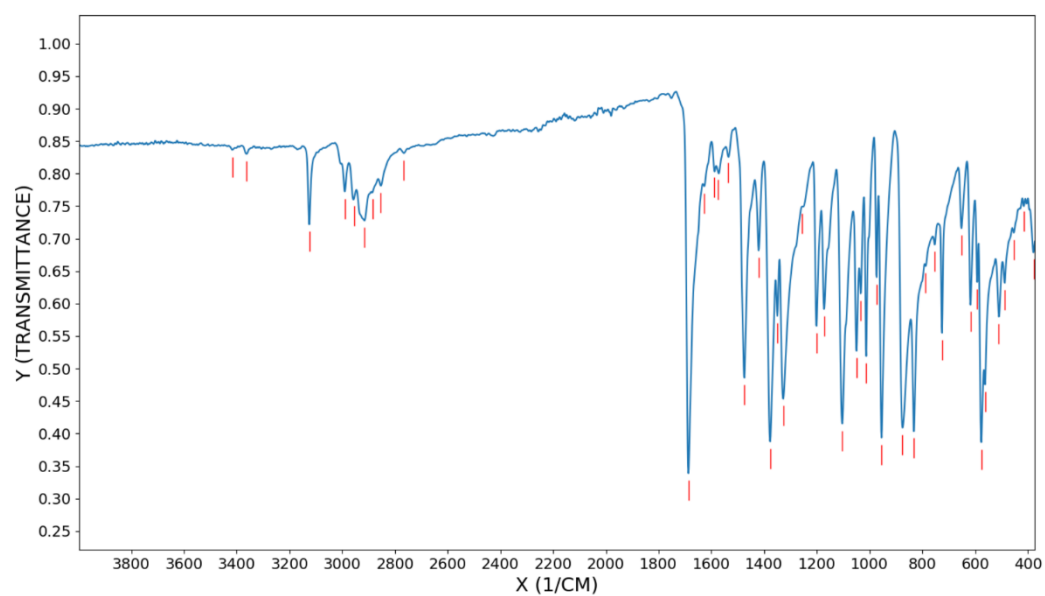
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

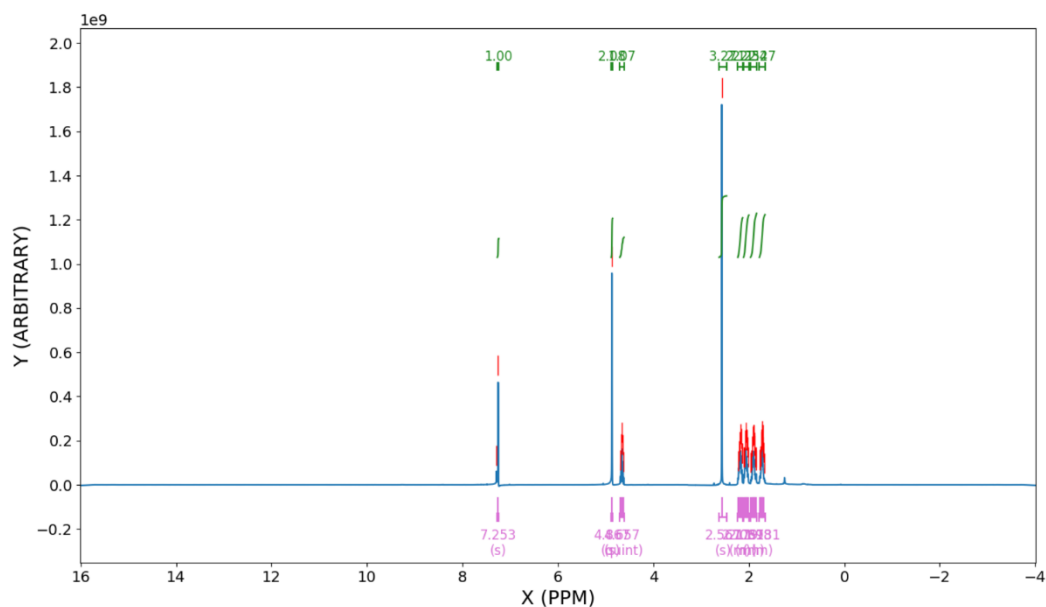


CHMO:0000630 | infrared absorption spectroscopy (IR)

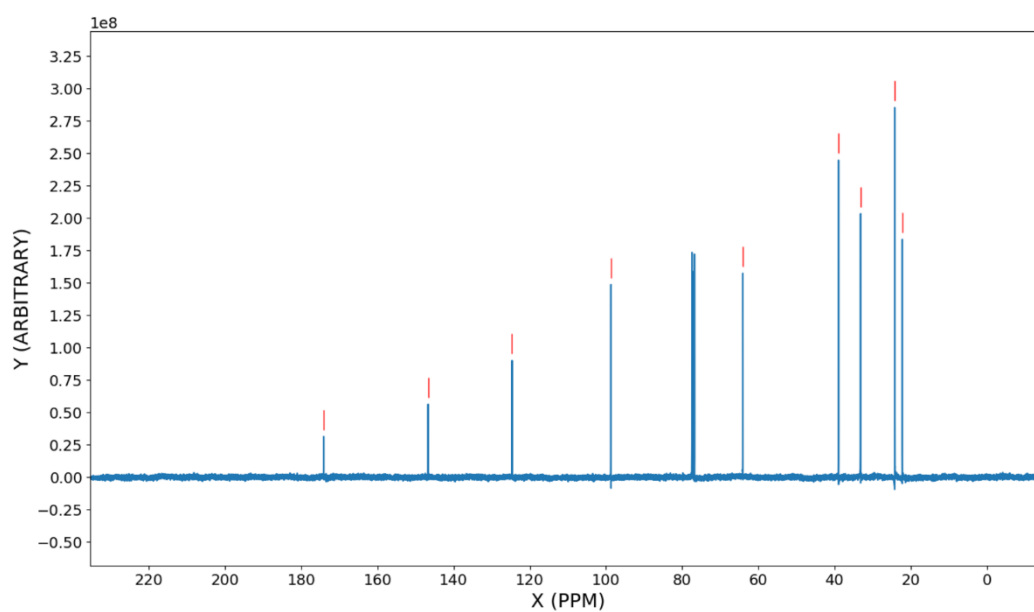


1-(6-Cyclopentyl-4,6-dihydro-3H-pyrazolo[3,4-d][1,2,3]triazin-3-yl)ethan-1-one (5f)

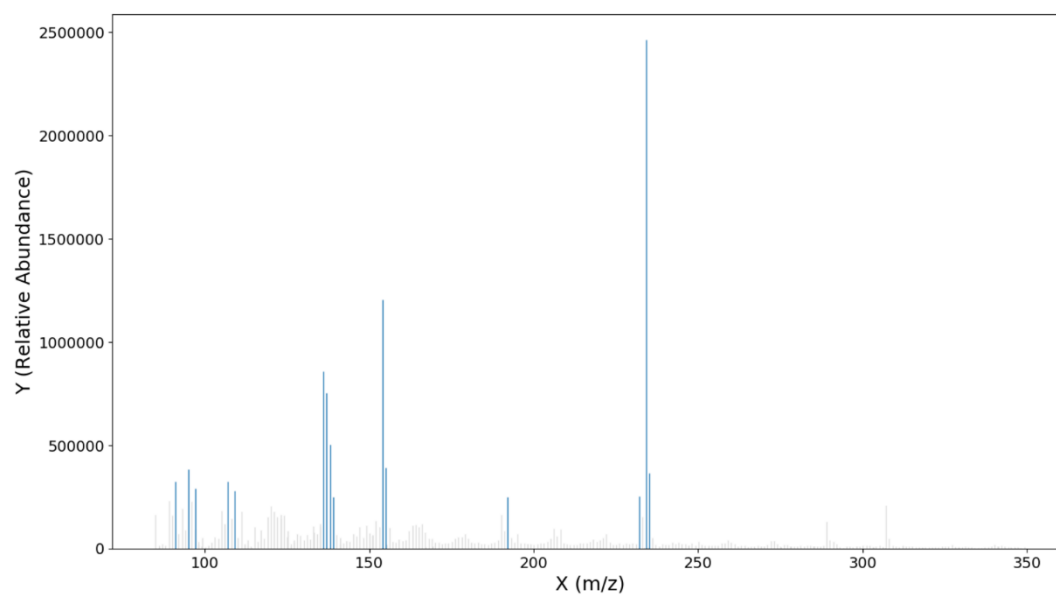
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



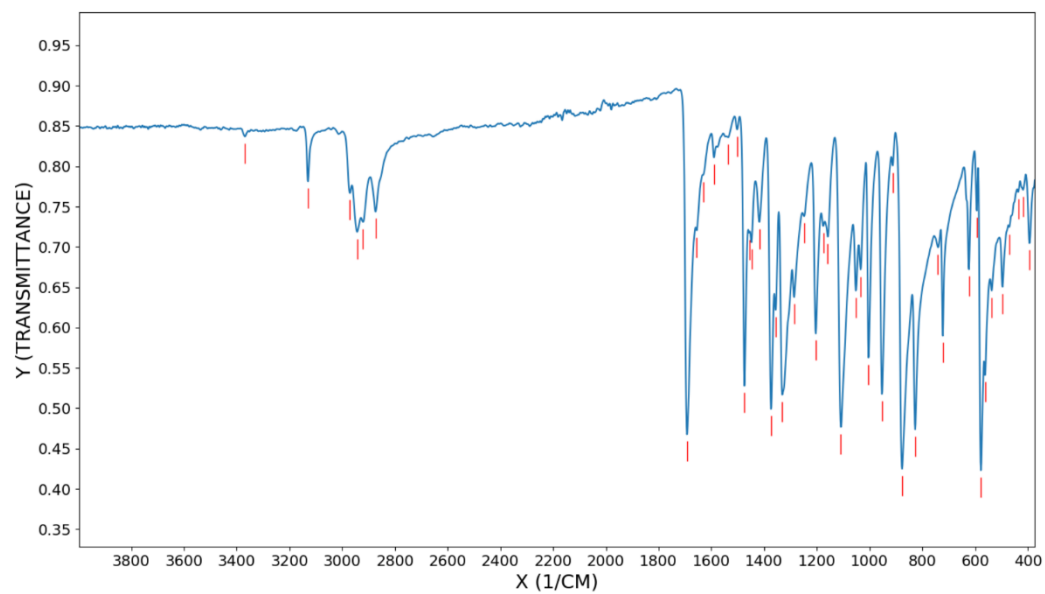
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

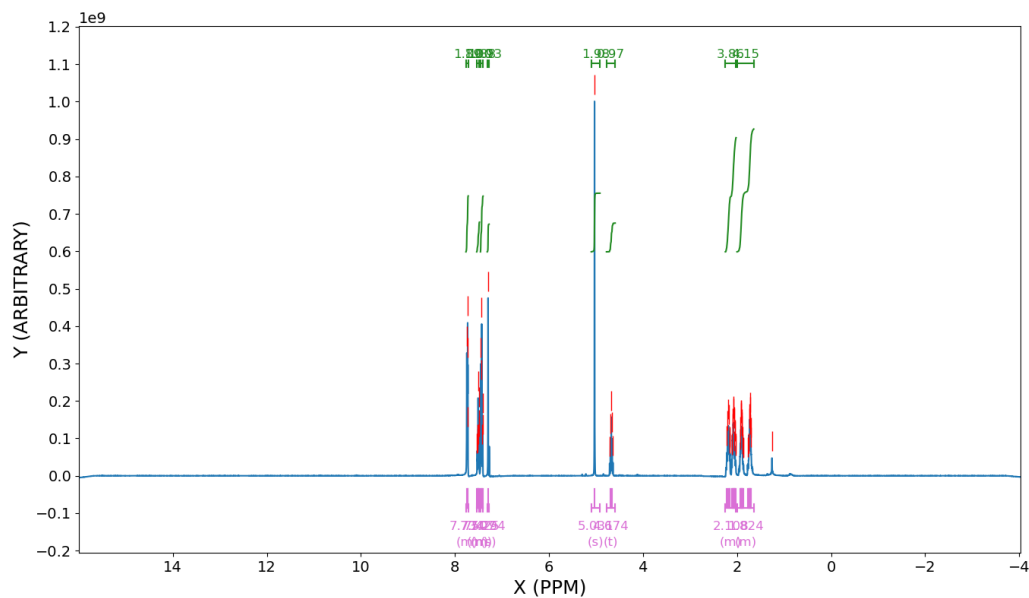


CHMO:0000630 | infrared absorption spectroscopy (IR)

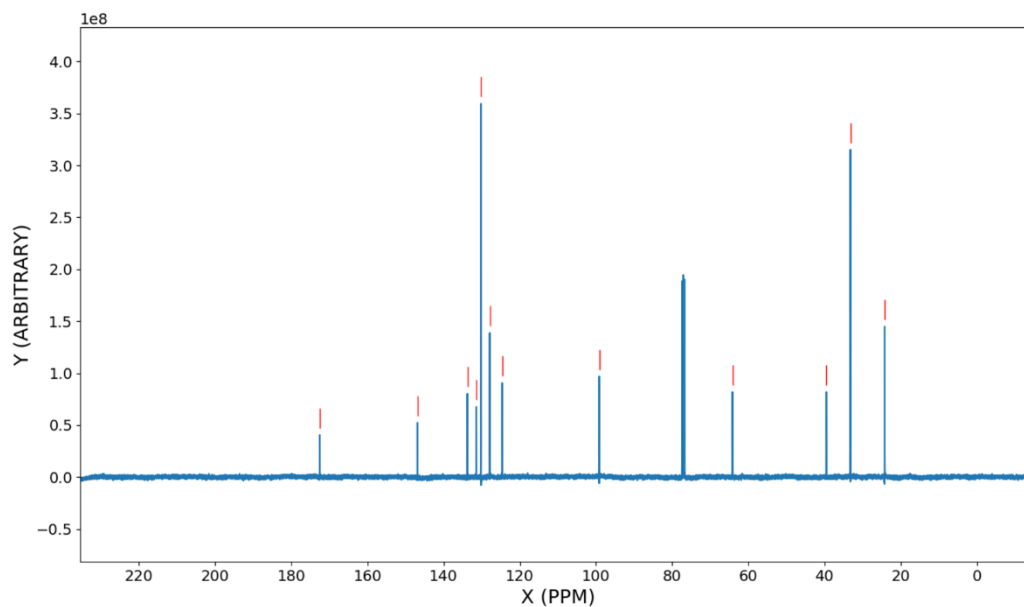


(6-Cyclopentyl-4,6-dihydro-3H-pyrazolo[3,4-*d*][1,2,3]triazin-3-yl)(phenyl)methanone (5g)

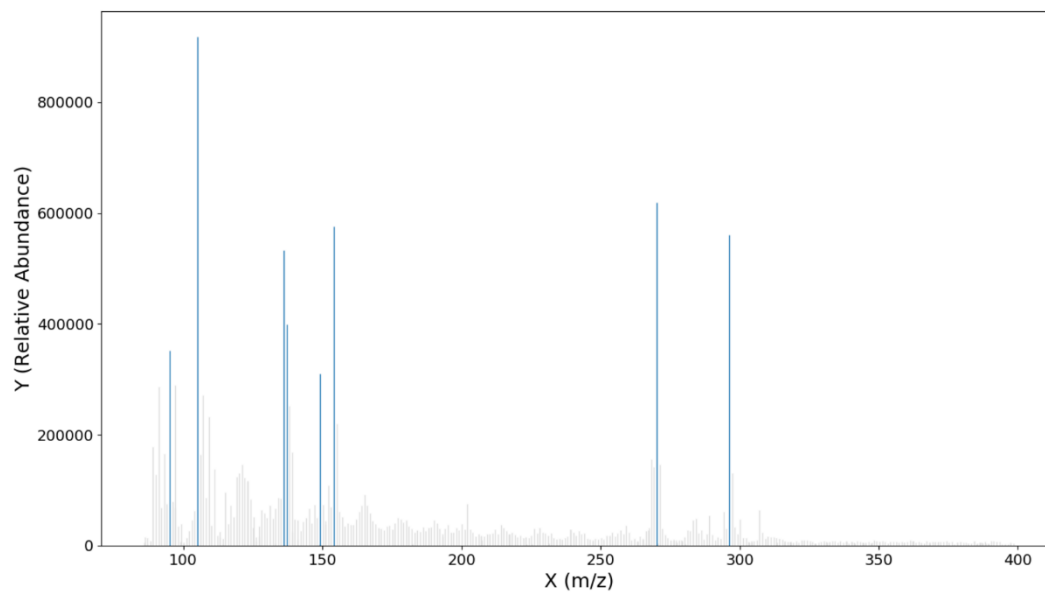
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



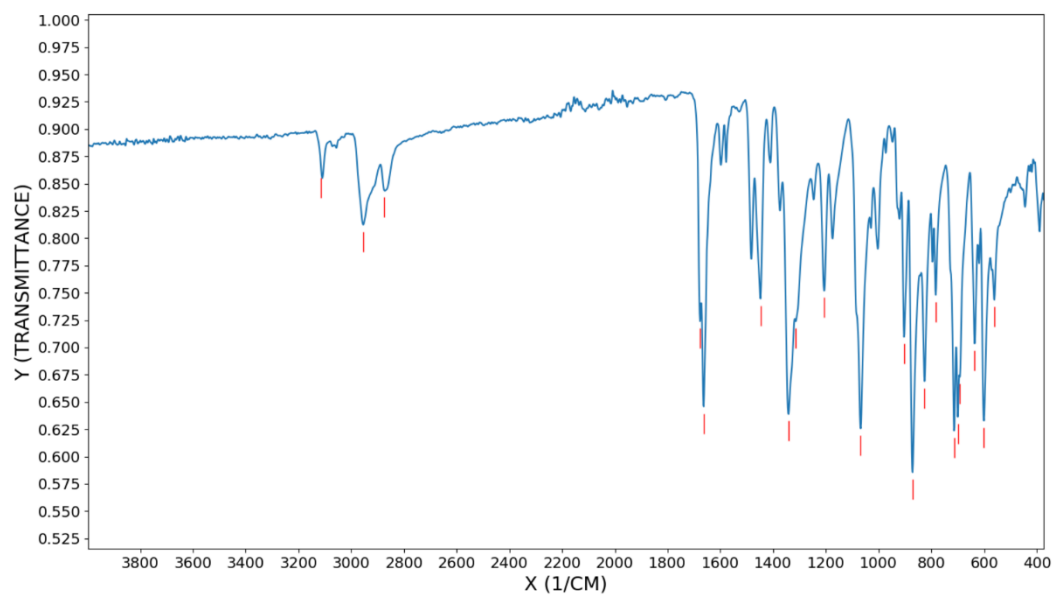
CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000470 | mass spectrometry (MS)

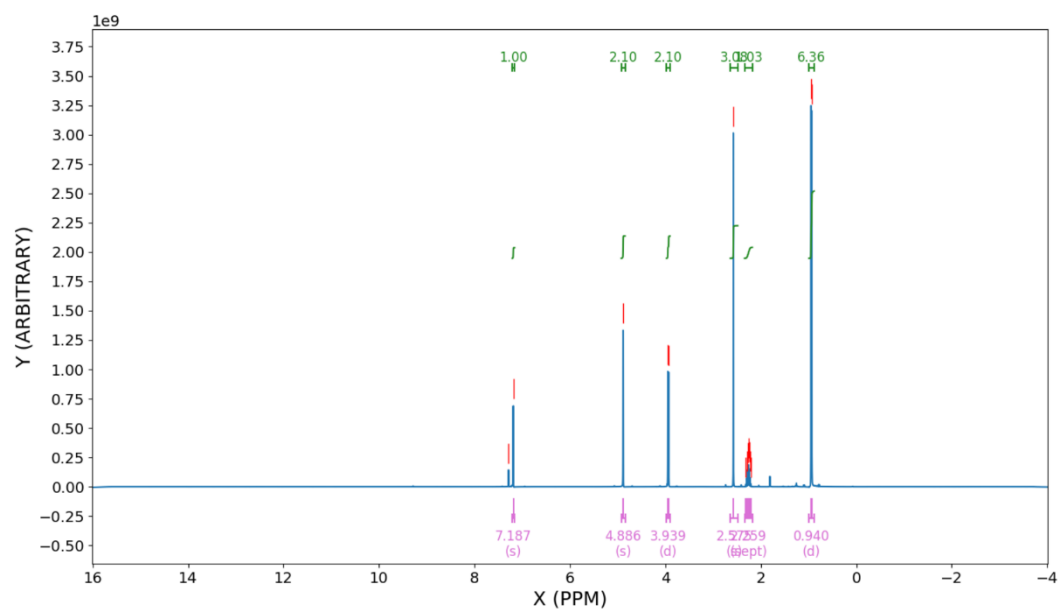


CHMO:0000630 | infrared absorption spectroscopy (IR)

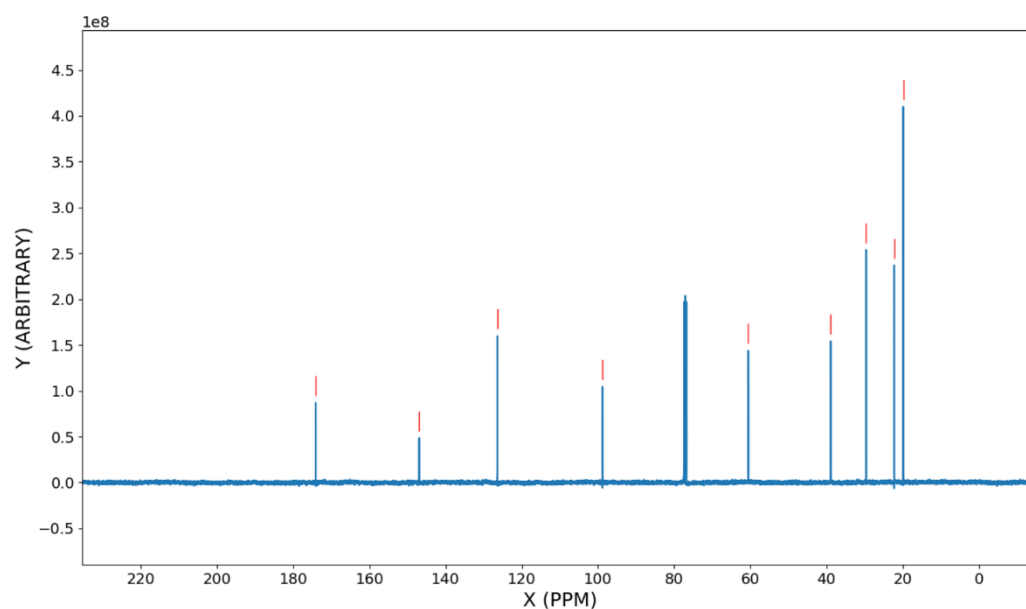


1-(6-Isobutyl-4,6-dihydro-3H-pyrazolo[3,4-d][1,2,3]triazin-3-yl)ethan-1-one (5h)

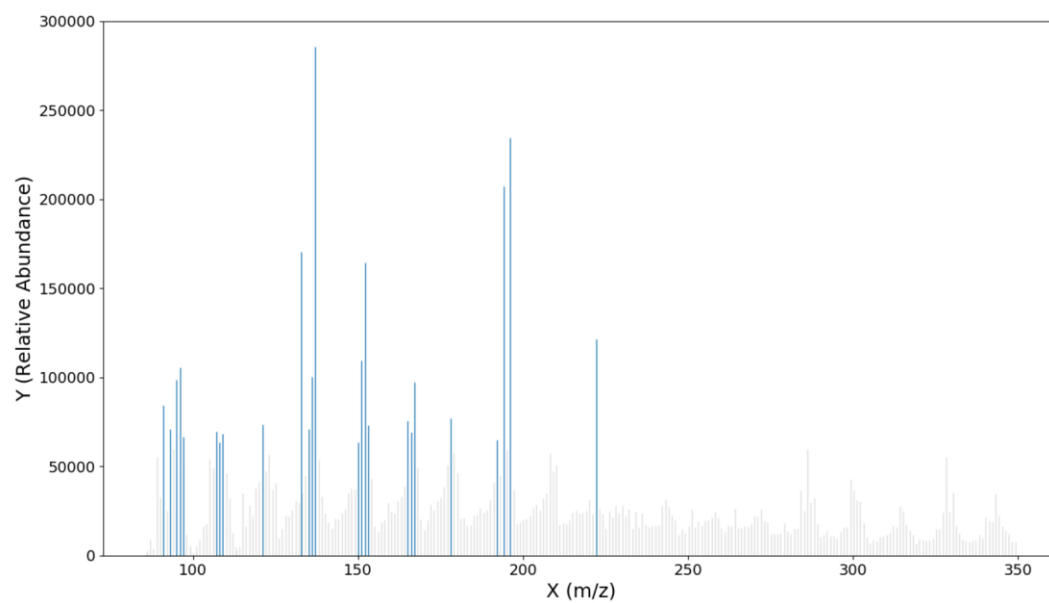
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)

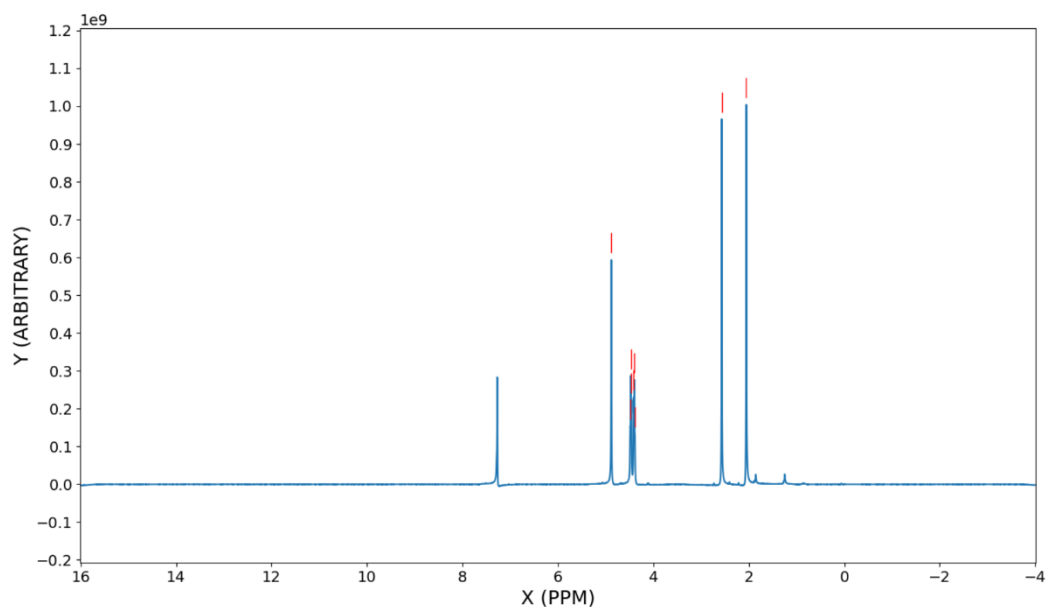


CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)

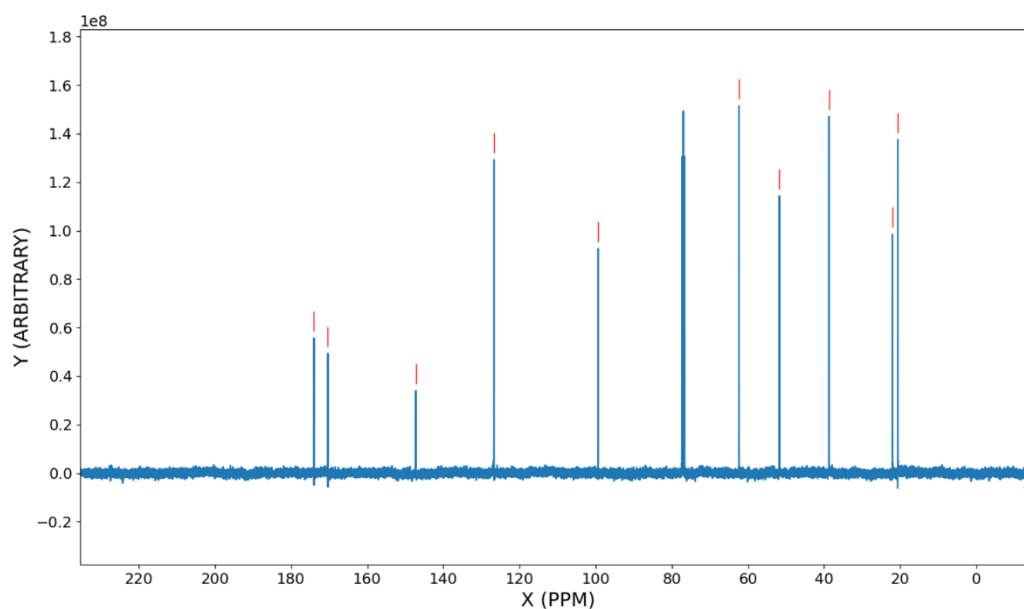


2-(3-Acetyl-3,4-dihydro-6*H*-pyrazolo[3,4-*d*][1,2,3]triazin-6-yl)ethyl acetate (5i)

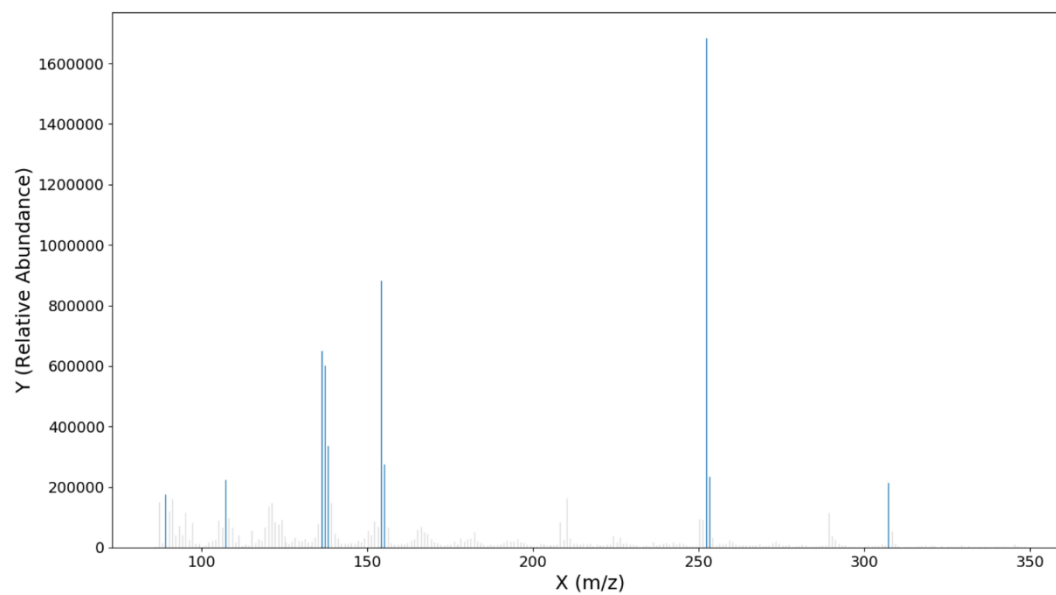
CHMO:0000593 | ¹H nuclear magnetic resonance spectroscopy (¹H NMR)



CHMO:0000595 | ¹³C nuclear magnetic resonance spectroscopy (¹³C NMR)



CHMO:0000563 | fast-atom bombardment mass spectrometry (FABMS)



CHMO:0000630 | infrared absorption spectroscopy (IR)

