

Regioselective Synthesis of 1,4-Disubstituted Imidazoles

*Chemical Development, Pharmaceutical Development, R&D, Bristol-Myers Squibb Company, 1 Squibb
Drive, New Brunswick, New Jersey 08903*

Michael.Schmidt@bms.com

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<u>Copy of Spectra:</u>	<u>S2</u>
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O=C1N(CCN1)C(=O)c2cnc(C3=CC=CC=C3Br)n2

VerticalScaleFactor = 1

CHLOROFORM-d

7.27

Normalized Intensity

1.00

0.75

0.50

0.25

0

0.88 0.99 2.00 2.02

2.02 6.09

Chemical Shift (ppm)

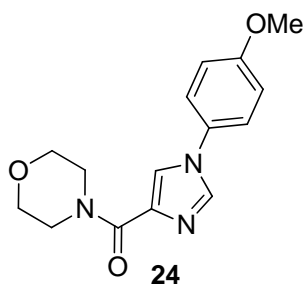
VerticalScaleFactor = 1

Normalized Intensity

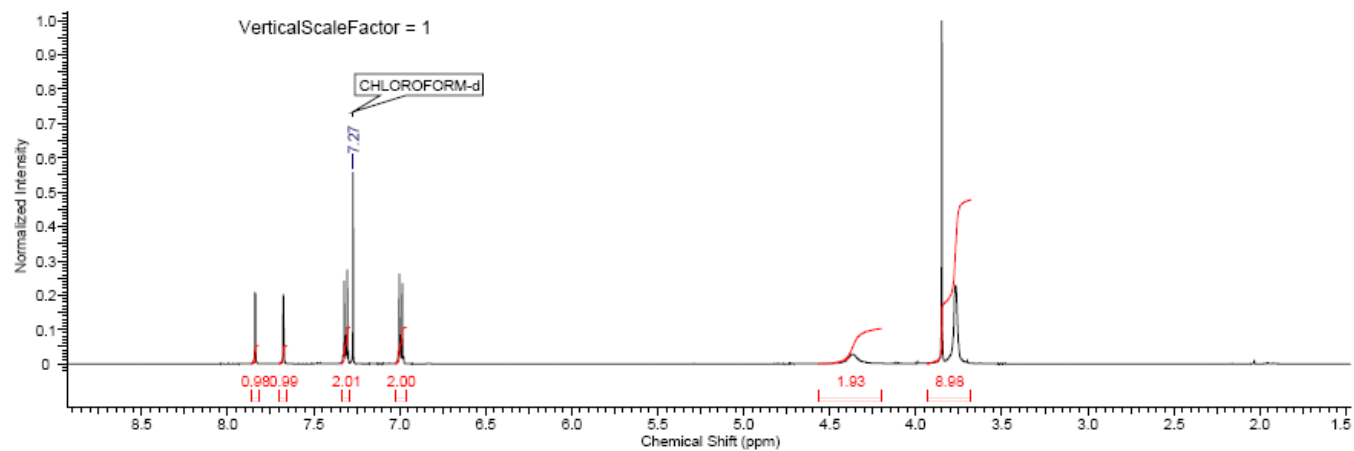
Chemical Shift (ppm)

CHLOROFORM-d

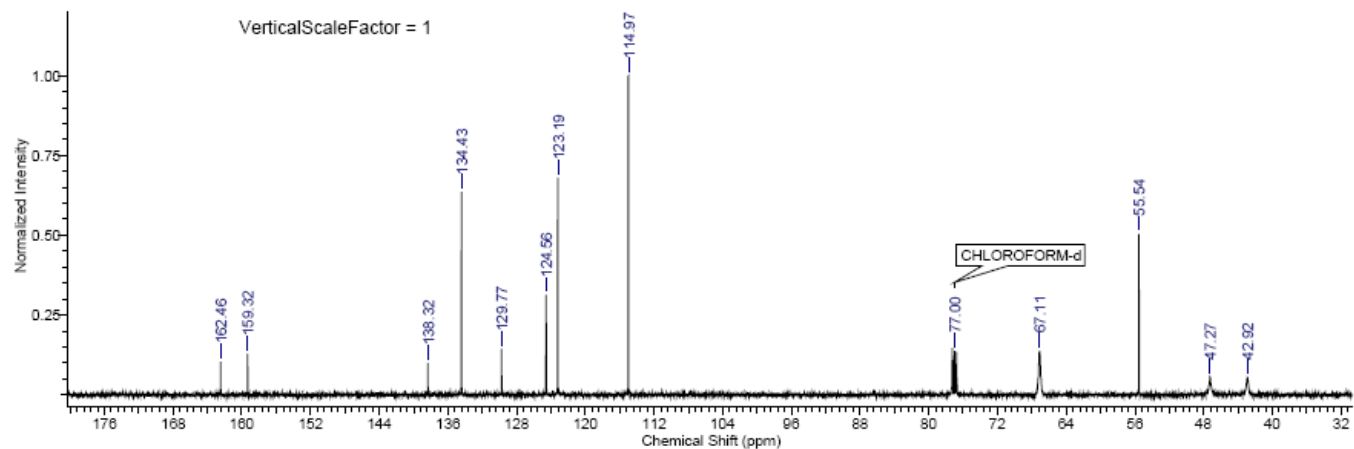
Chemical Shift (ppm)
162.20
139.06
135.58
134.03
133.21
123.95
123.08
121.83
77.00
67.12
47.27
42.98

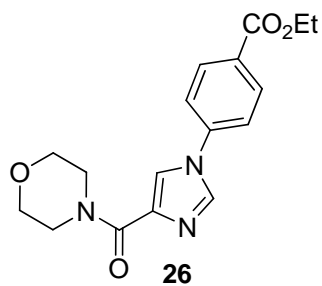


^1H NMR:

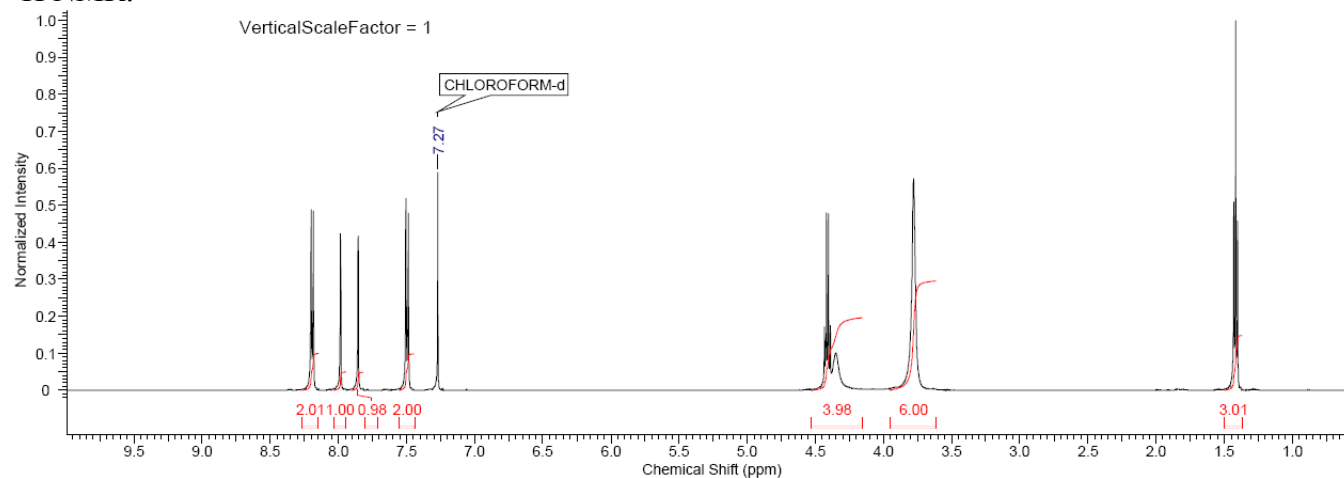


^{13}C NMR:

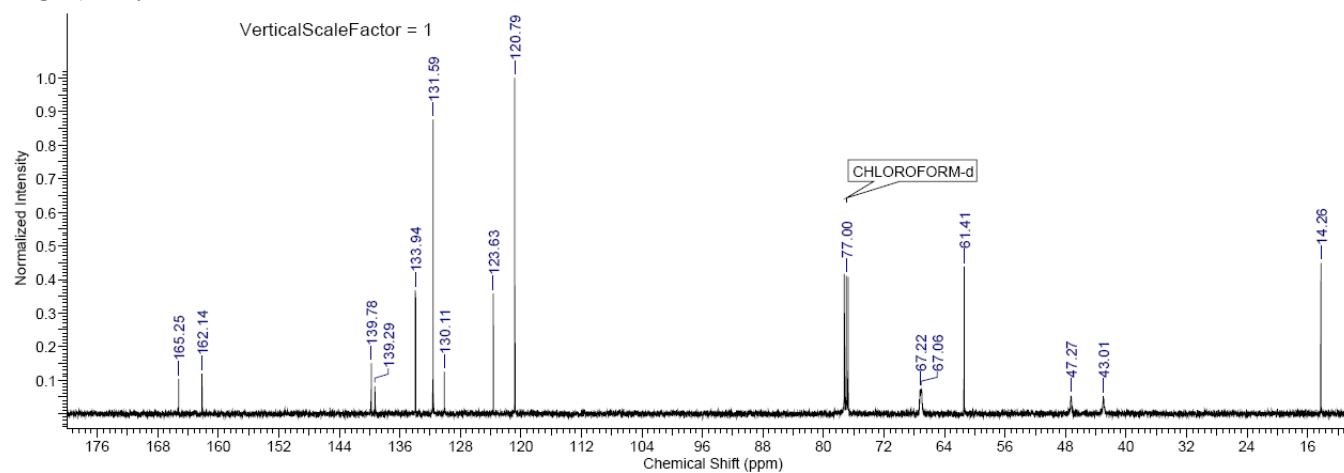




¹H NMR:

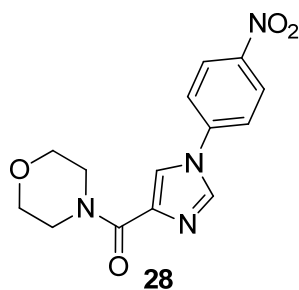


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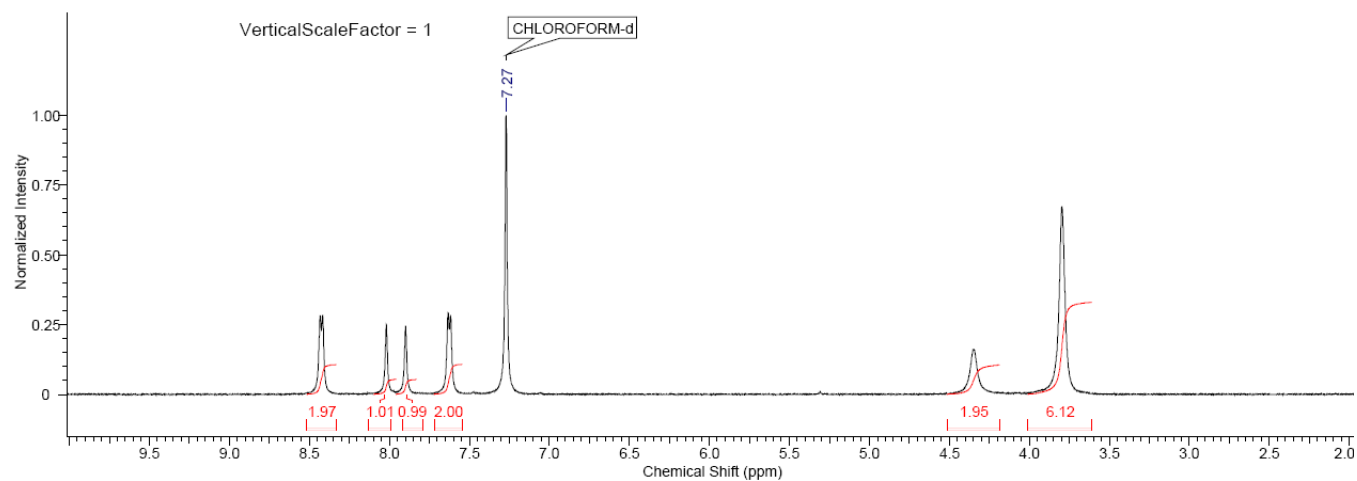


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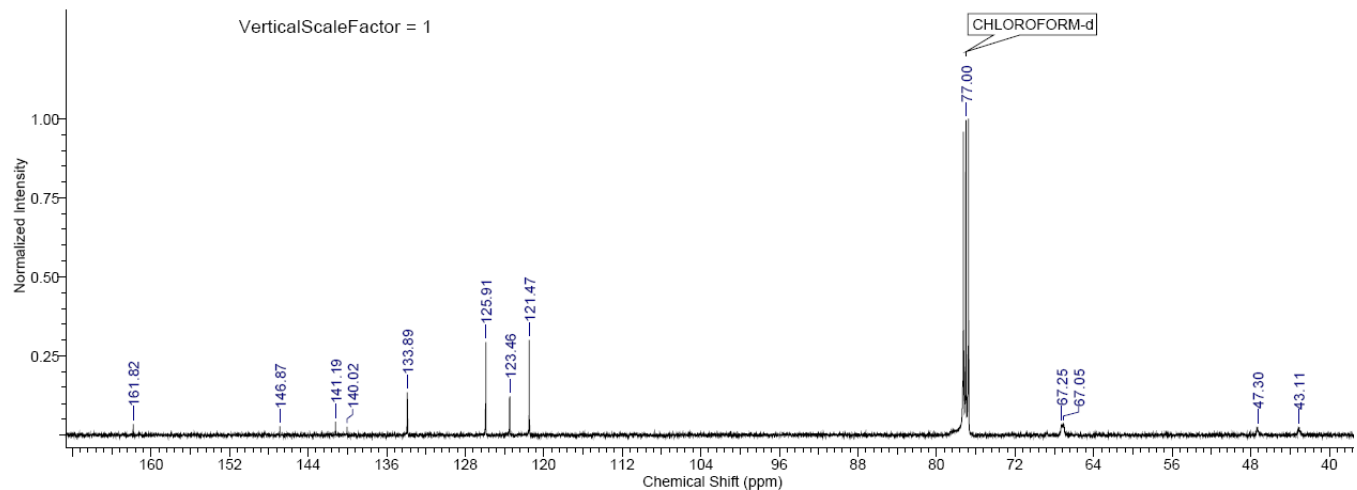
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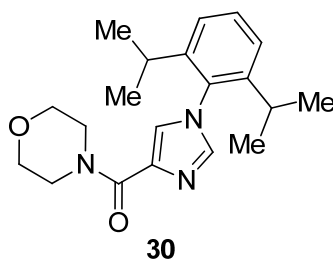


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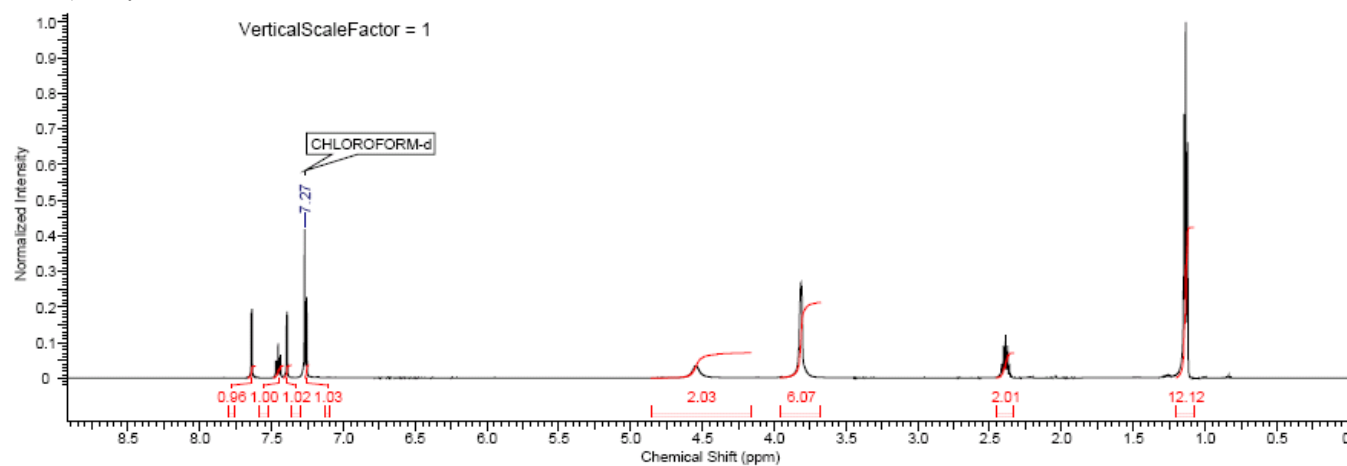


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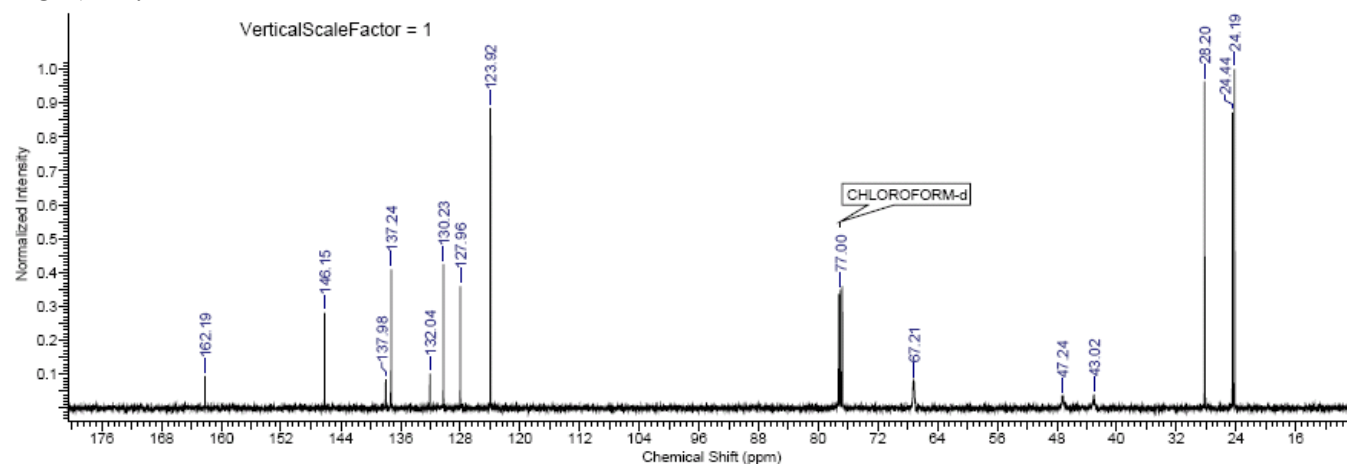


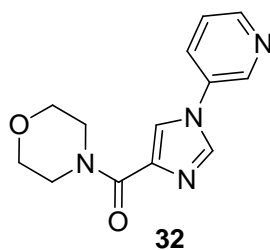


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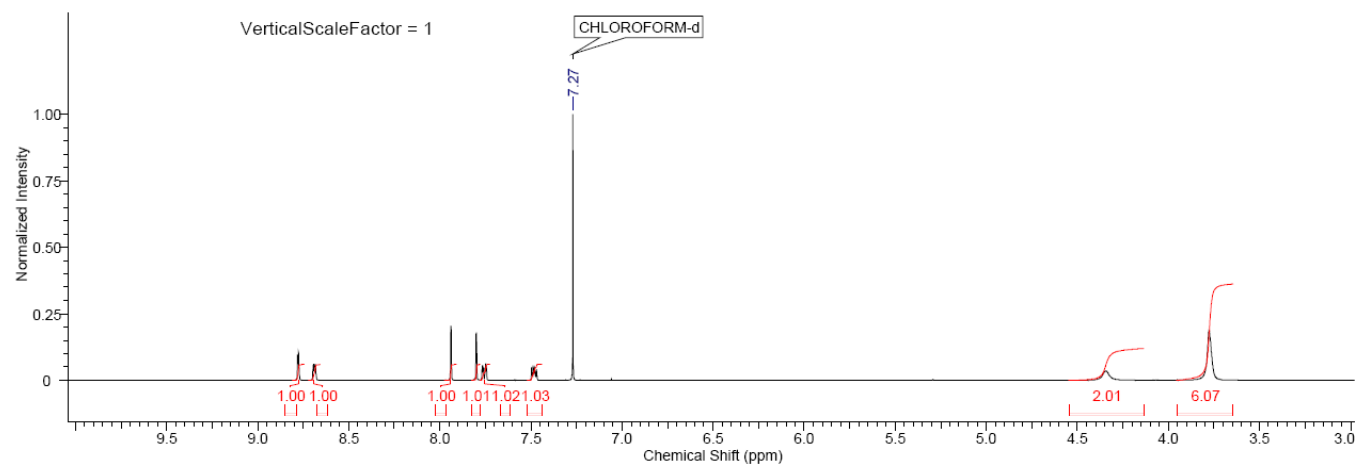


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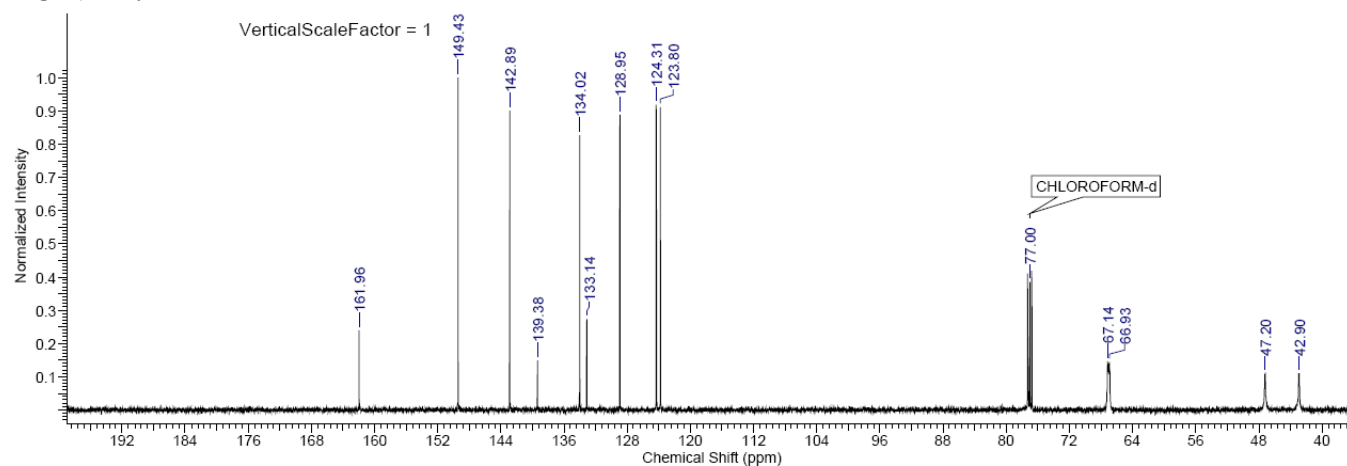




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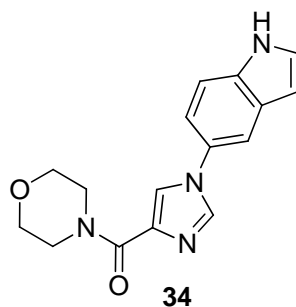


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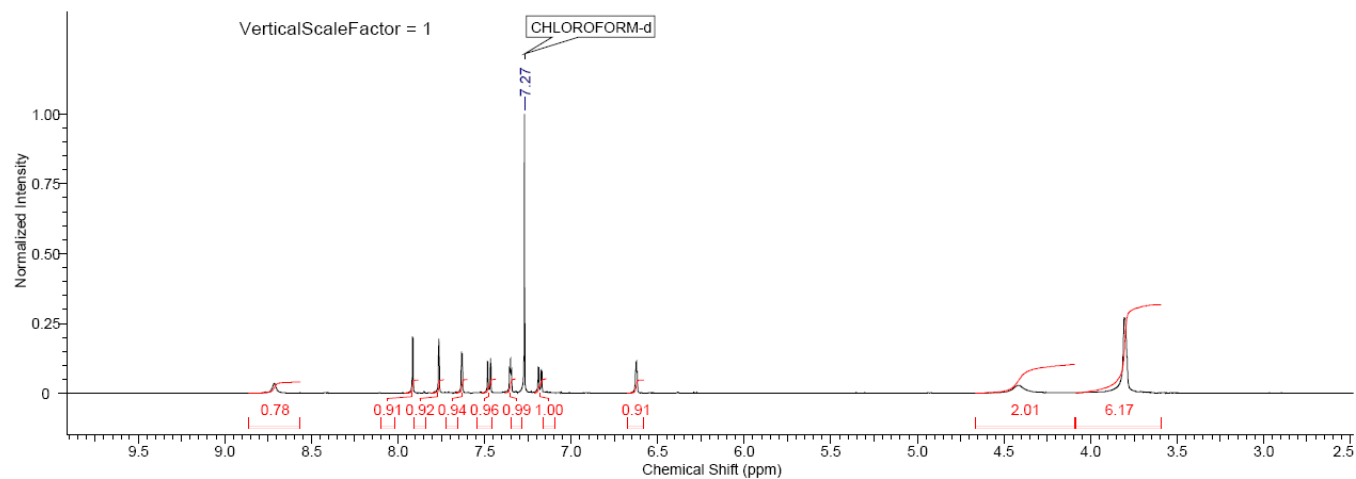


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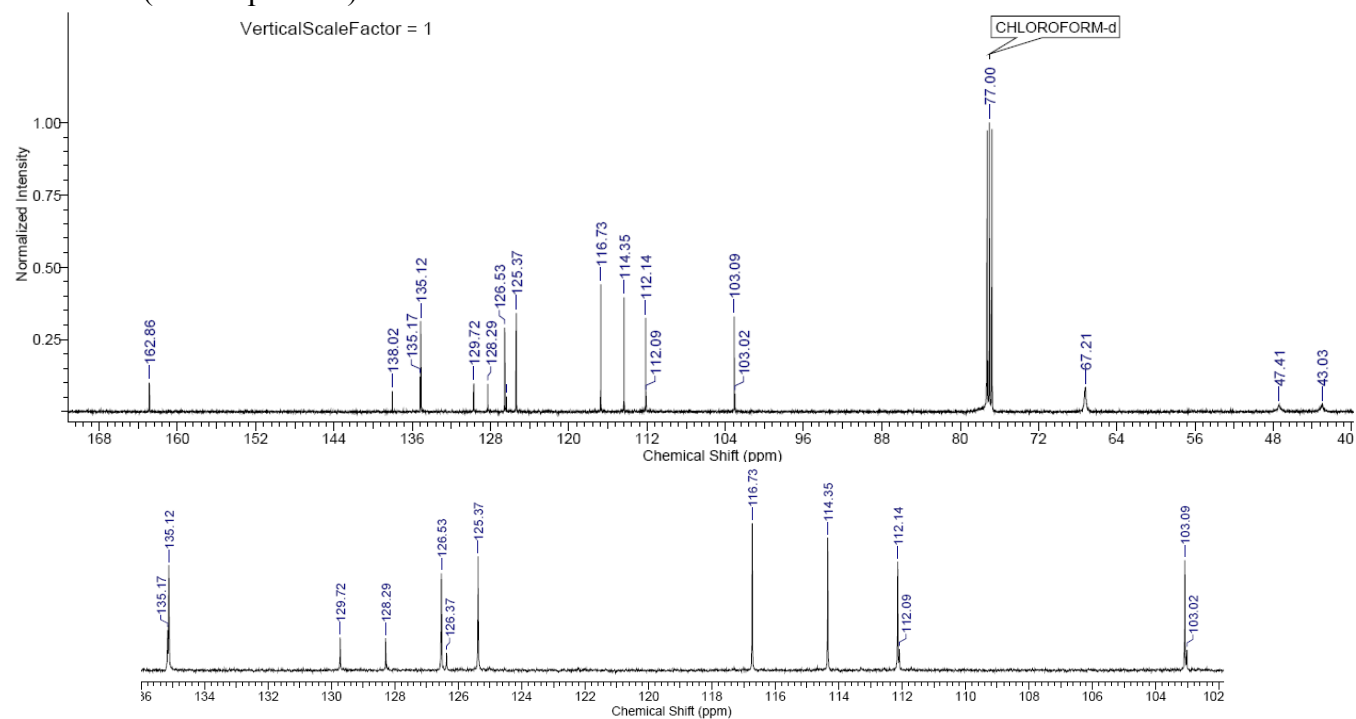
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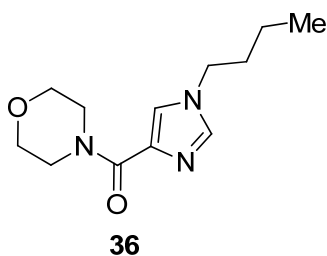


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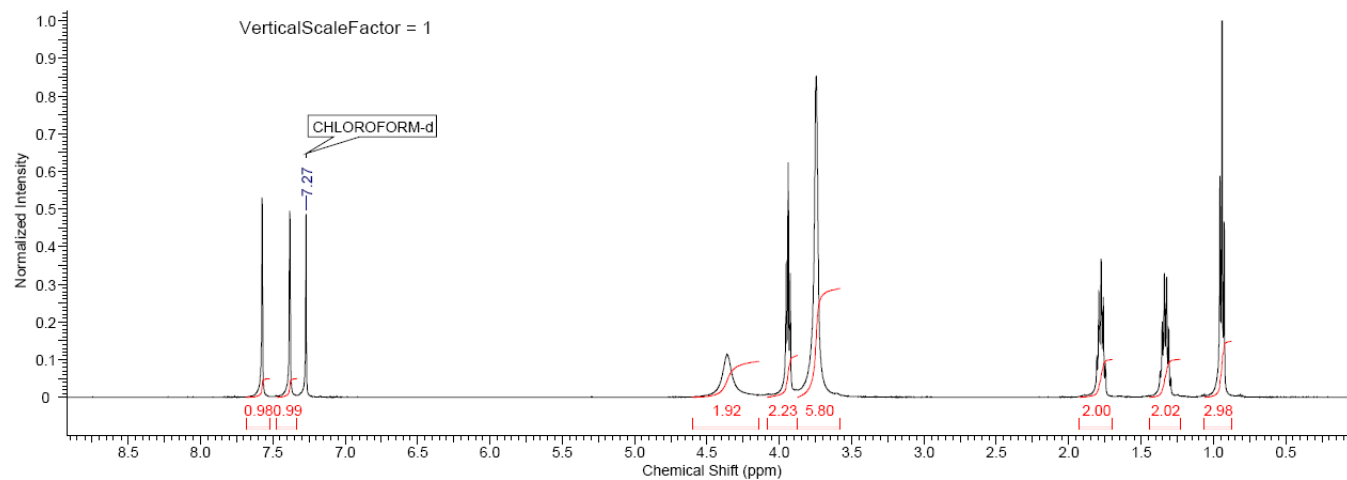


^{13}C NMR (with expansion):

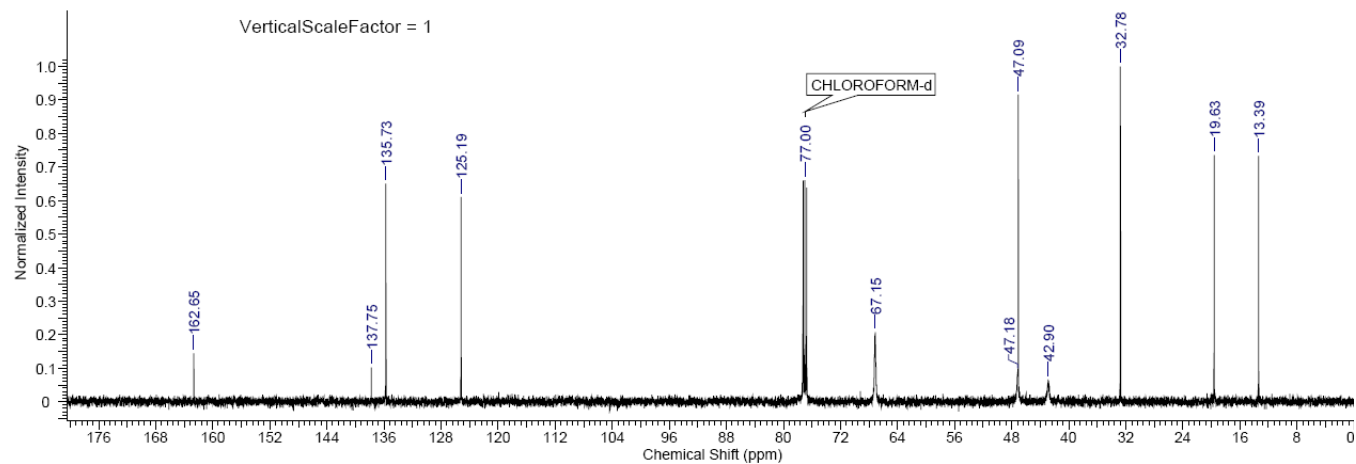




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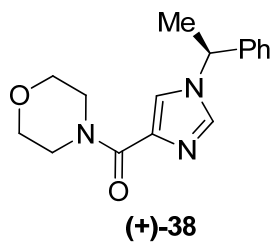


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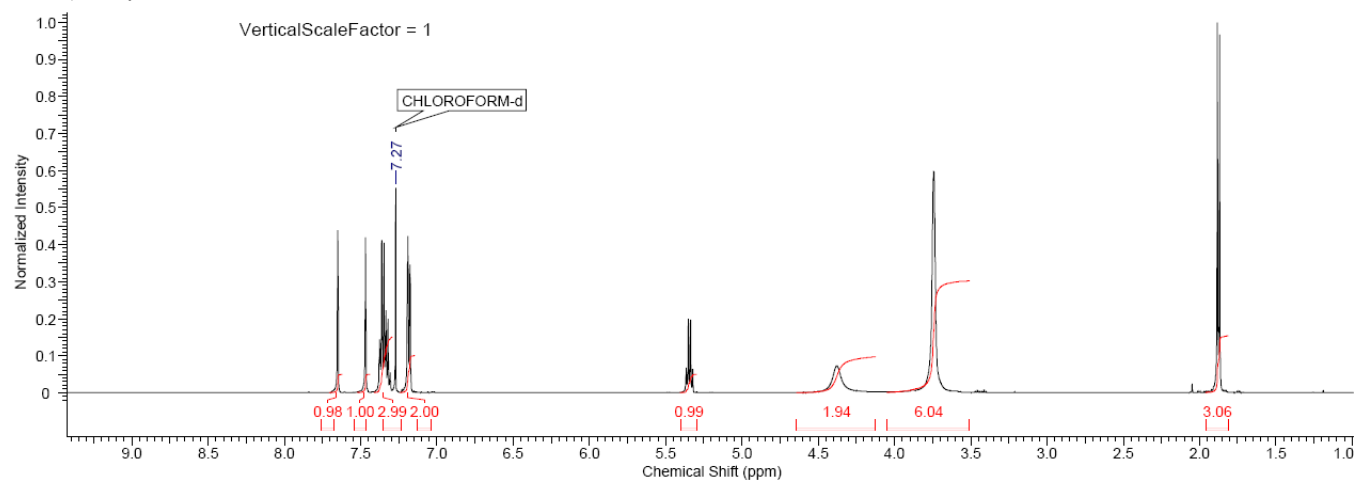


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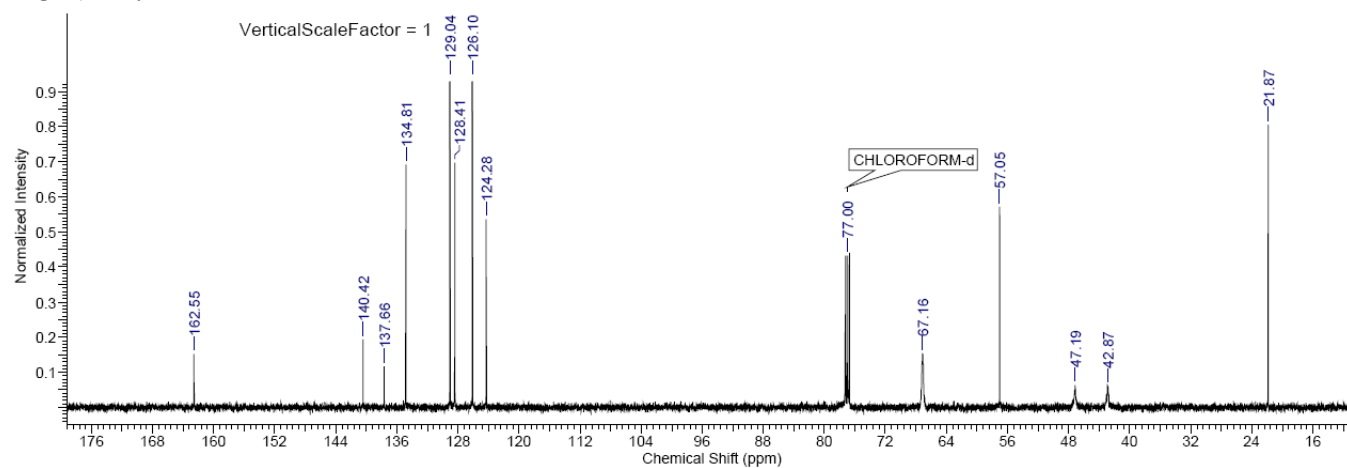
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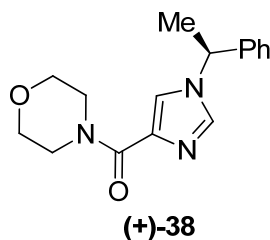


^1H NMR:

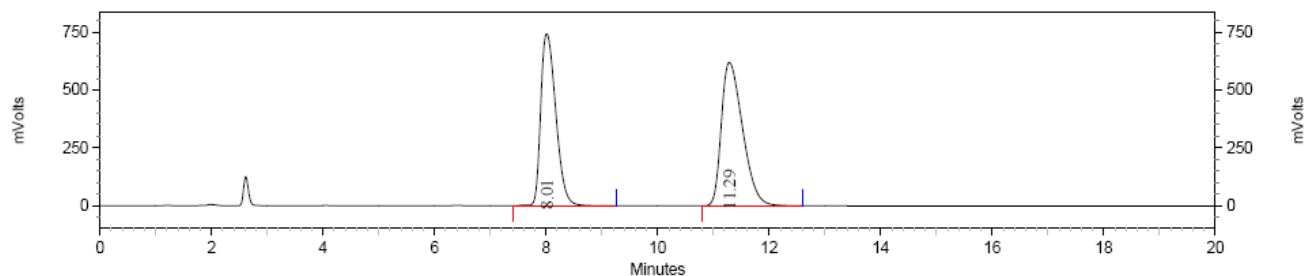


^{13}C NMR:



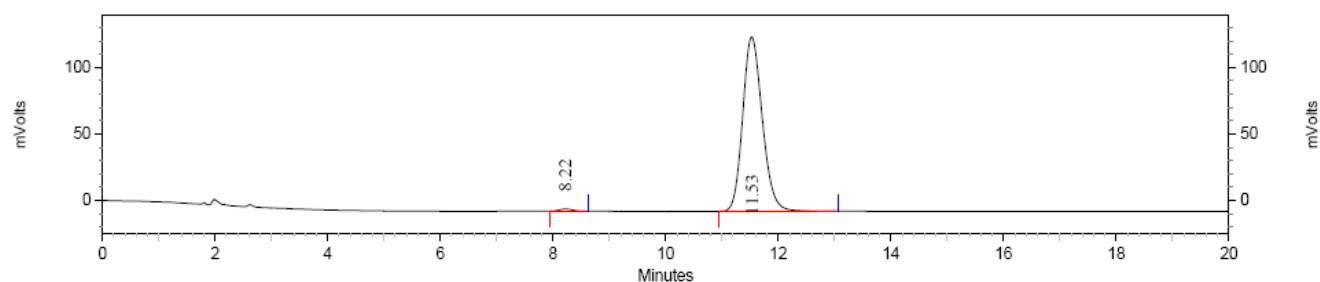


Mixture of Enantiomers:

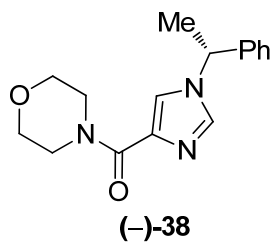


UV1 Results			
Pk #	Retention Time	Area	Area Percent
1	8.011	13949802	45.986
2	11.288	16385095	54.014
Totals		30334897	100.000

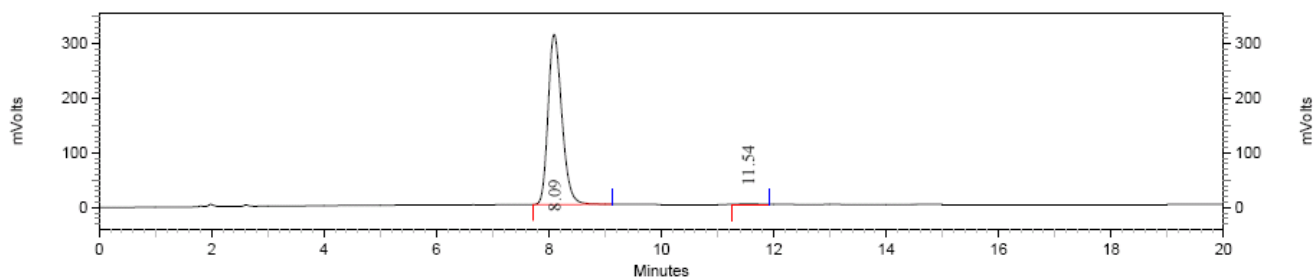
Compound (+)-38:



UV1 Results			
Pk #	Retention Time	Area	Area Percent
1	8.218	27658	0.863
2	11.528	3177223	99.137
Totals		3204881	100.000

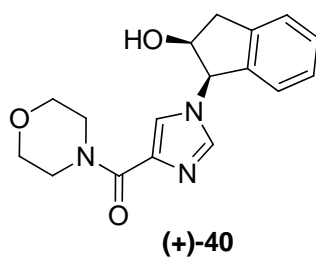


Compound (-)-38:

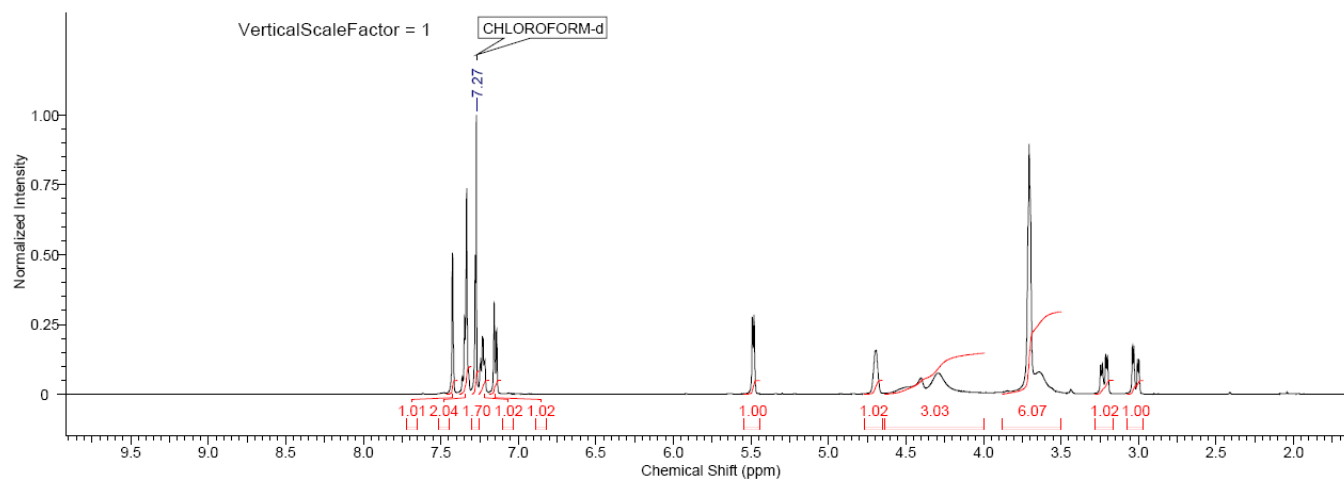


UV1 Results

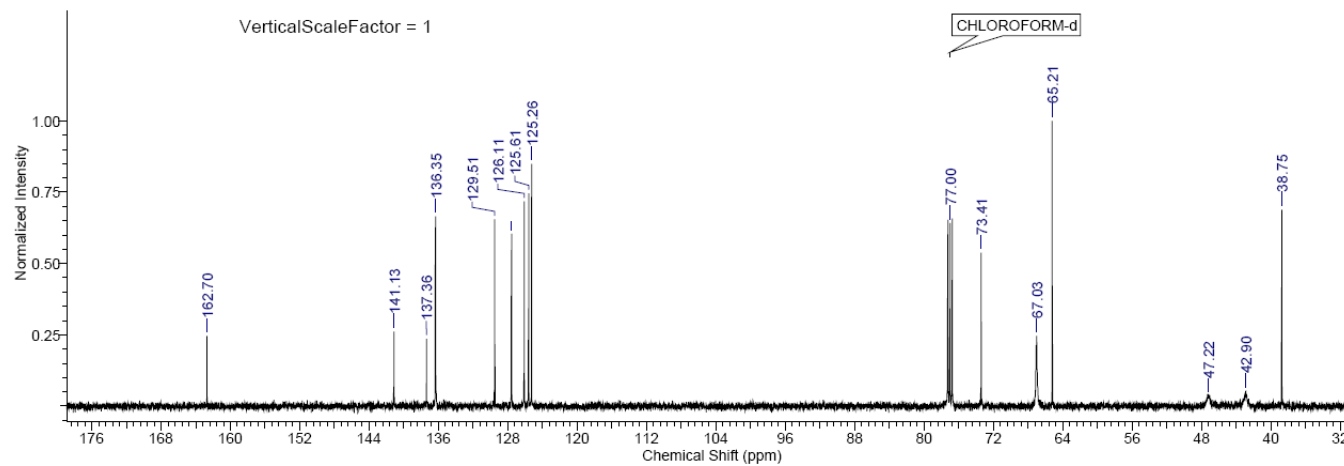
Pk #	Retention Time	Area	Area Percent
1	8.093	5311247	99.578
2	11.543	22489	0.422
Totals		5333736	100.000

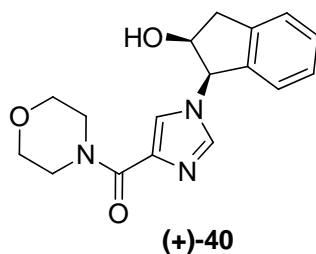


¹H NMR:

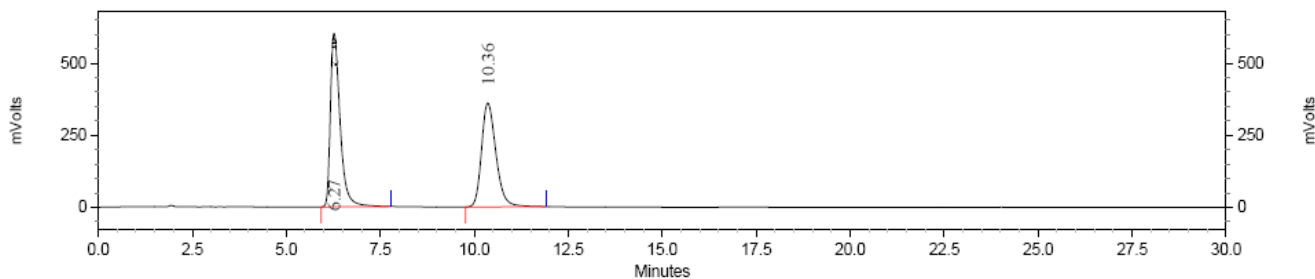


¹³C NMR:



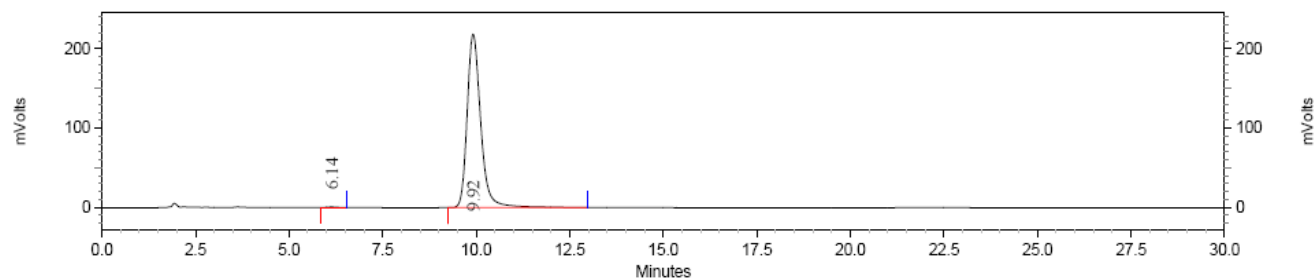


Mixture of Enantiomers:

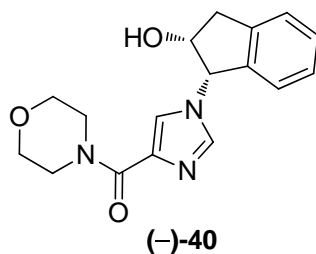


UV1 Results			
Pk #	Retention Time	Area	Area Percent
1	6.271	10792455	52.906
2	10.361	9606959	47.094
Totals		20399414	100.000

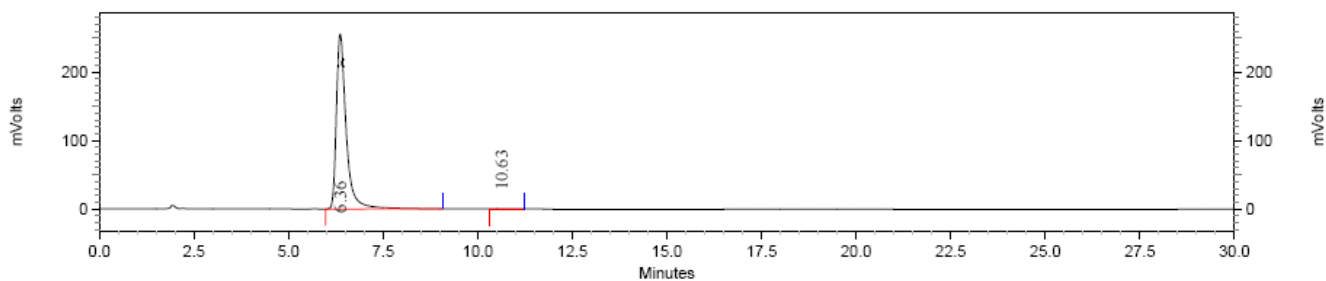
Compound (+)-40:



UV1 Results			
Pk #	Retention Time	Area	Area Percent
1	6.136	13438	0.242
2	9.919	5530116	99.758
Totals		5543554	100.000



Compound **(-)-40**:

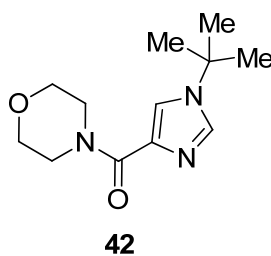


UVI Results

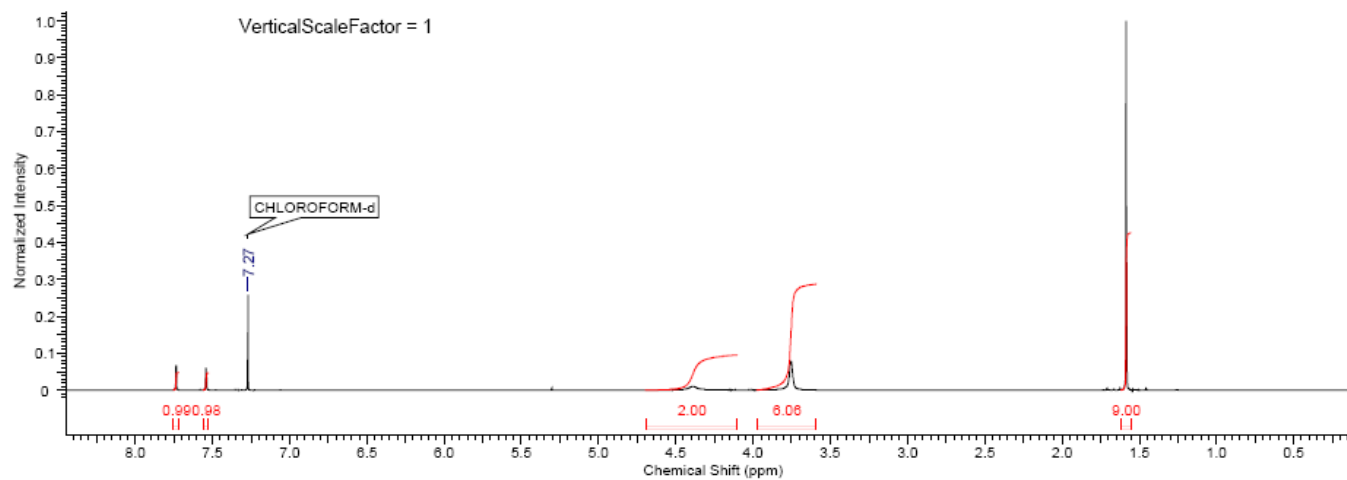
Pk #	Retention Time	Area	Area Percent
1	6.363	4636953	99.836
2	10.629	7637	0.164
Totals		4644590	100.000

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^1H NMR:



^{13}C NMR:

