Supporting Information

Synthesis of (Hetero)arylated Pyridazin-3(2*H*)-ones *via* Negishi reaction involving Zincated Pyridazin-3(2*H*)-ones.

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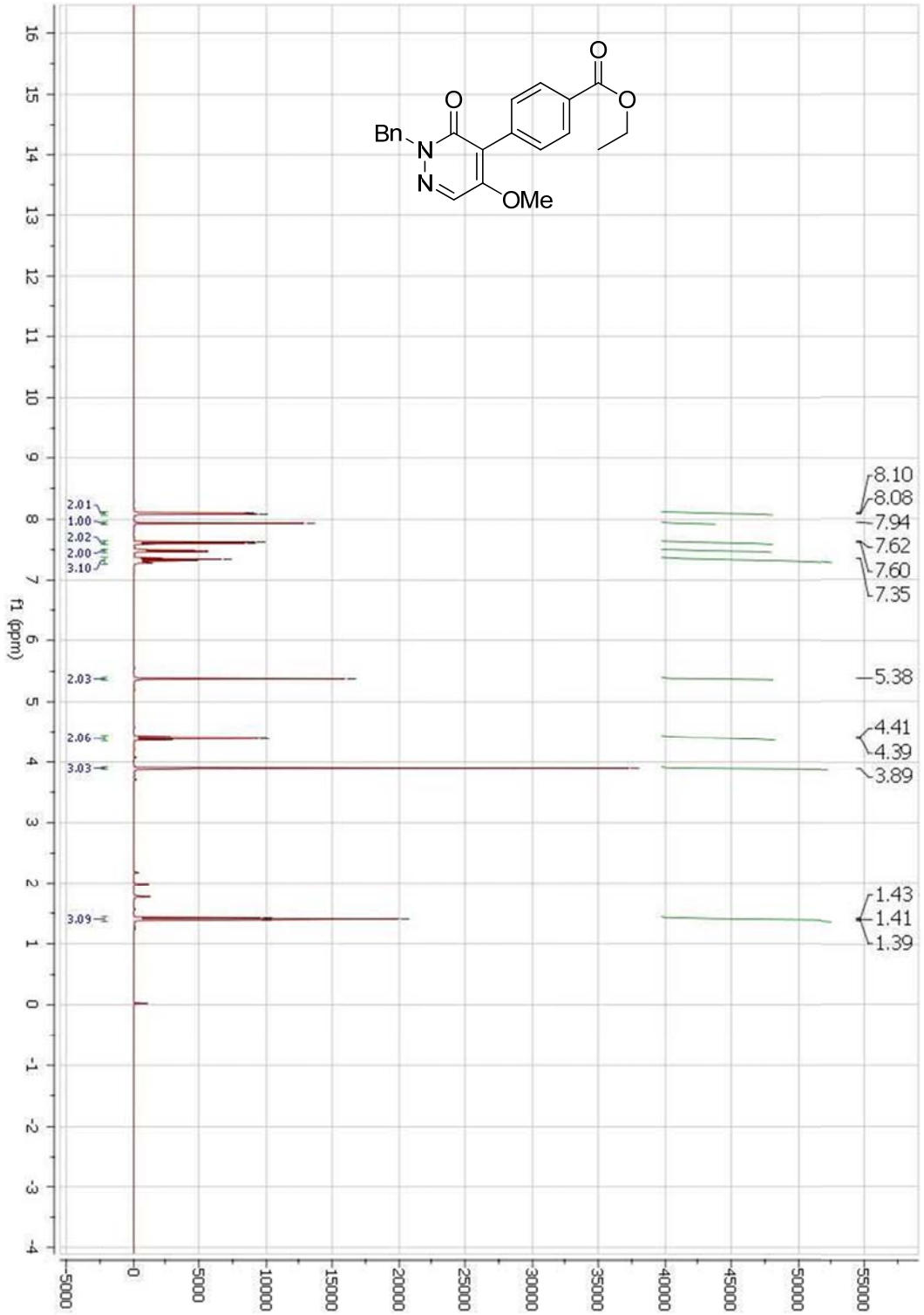
Contents

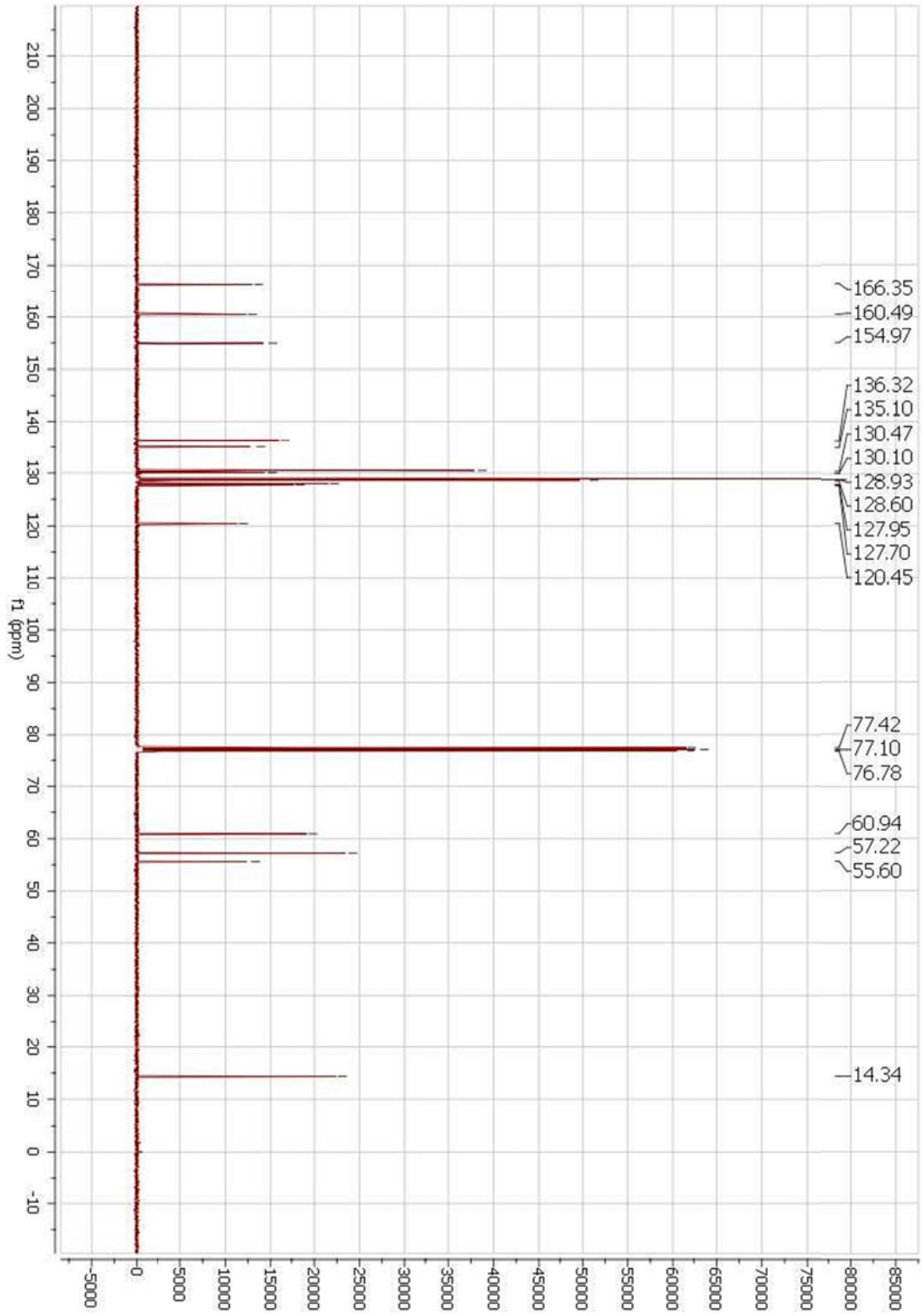
Spectra

Ethyl 4-(2-benzyl-5-methoxy-3-oxo-2,3-dihydropyridazin-4-yl)benzoate (**2a**)

^{1}H-NMR



^{13}C-NMR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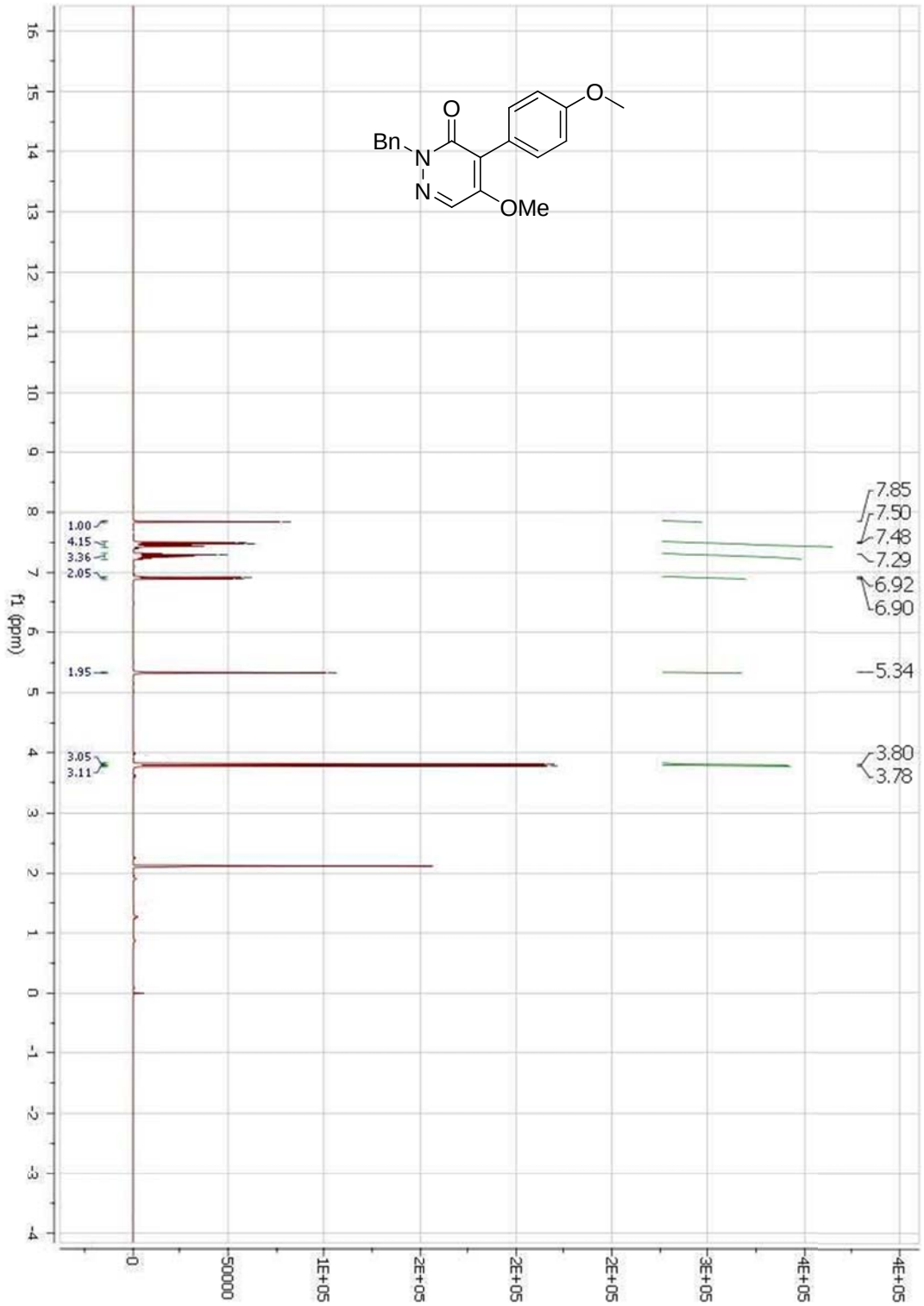
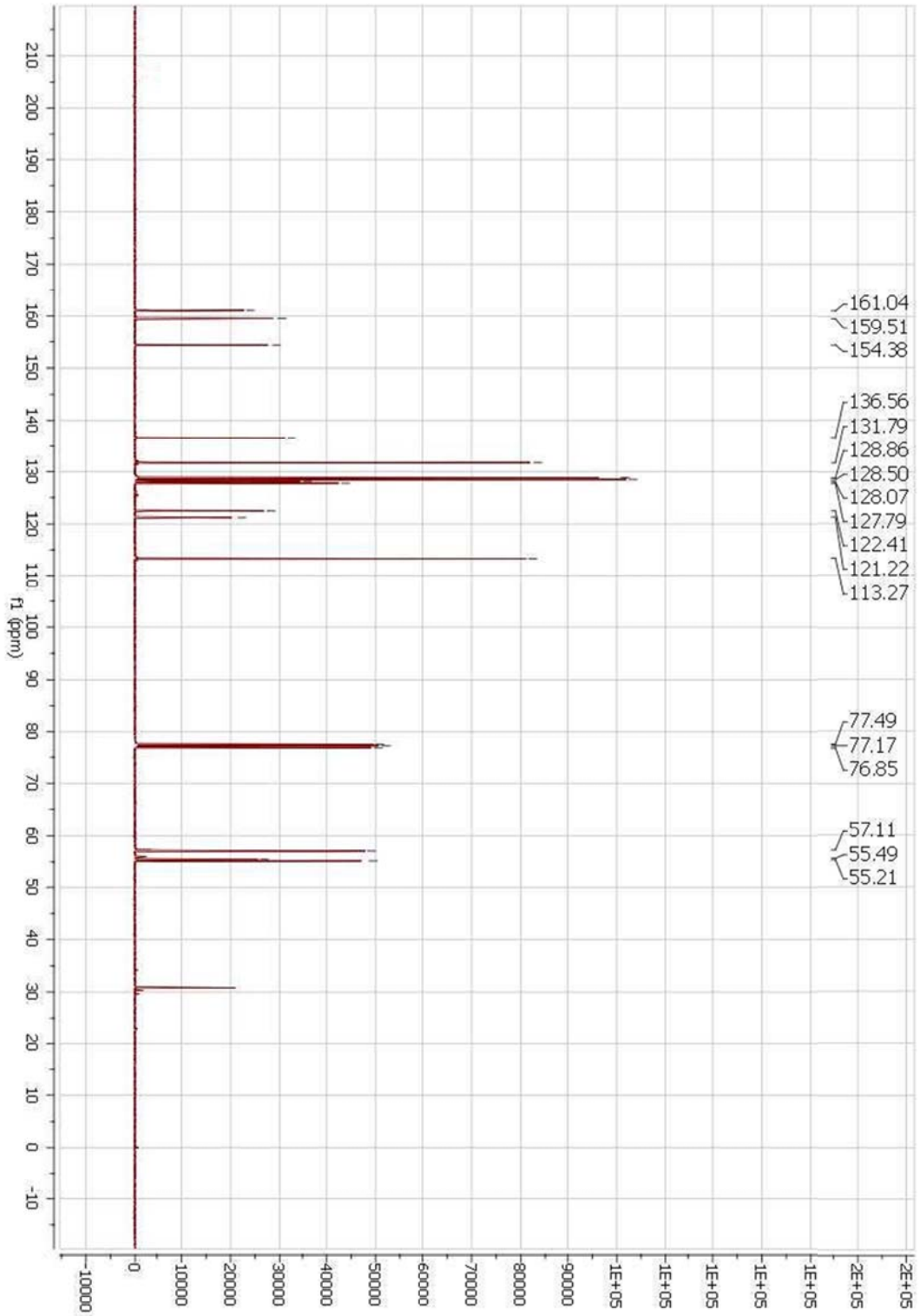
160.49
154.97
136.32
135.10
130.47
130.10
128.93
128.60
127.95
127.70
120.45
77.42
77.10
76.78
60.94
57.22
55.60
14.34
f1 (ppm)

2-Benzyl-5-methoxy-4-(4-methoxyphenyl)pyridazin-3(2*H*)-one (**2b**)

^{1}H-NMR



^{13}C-NMR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154.38
136.56
131.79
128.86
128.50
128.07
127.79
122.41
121.22
113.27
77.49
77.17
76.85
57.11
55.49
55.21
f1 (ppm)

2-Benzyl-4-(2-chlorophenyl)-5-methoxypyridazin-3(2*H*)-one (**2c**)

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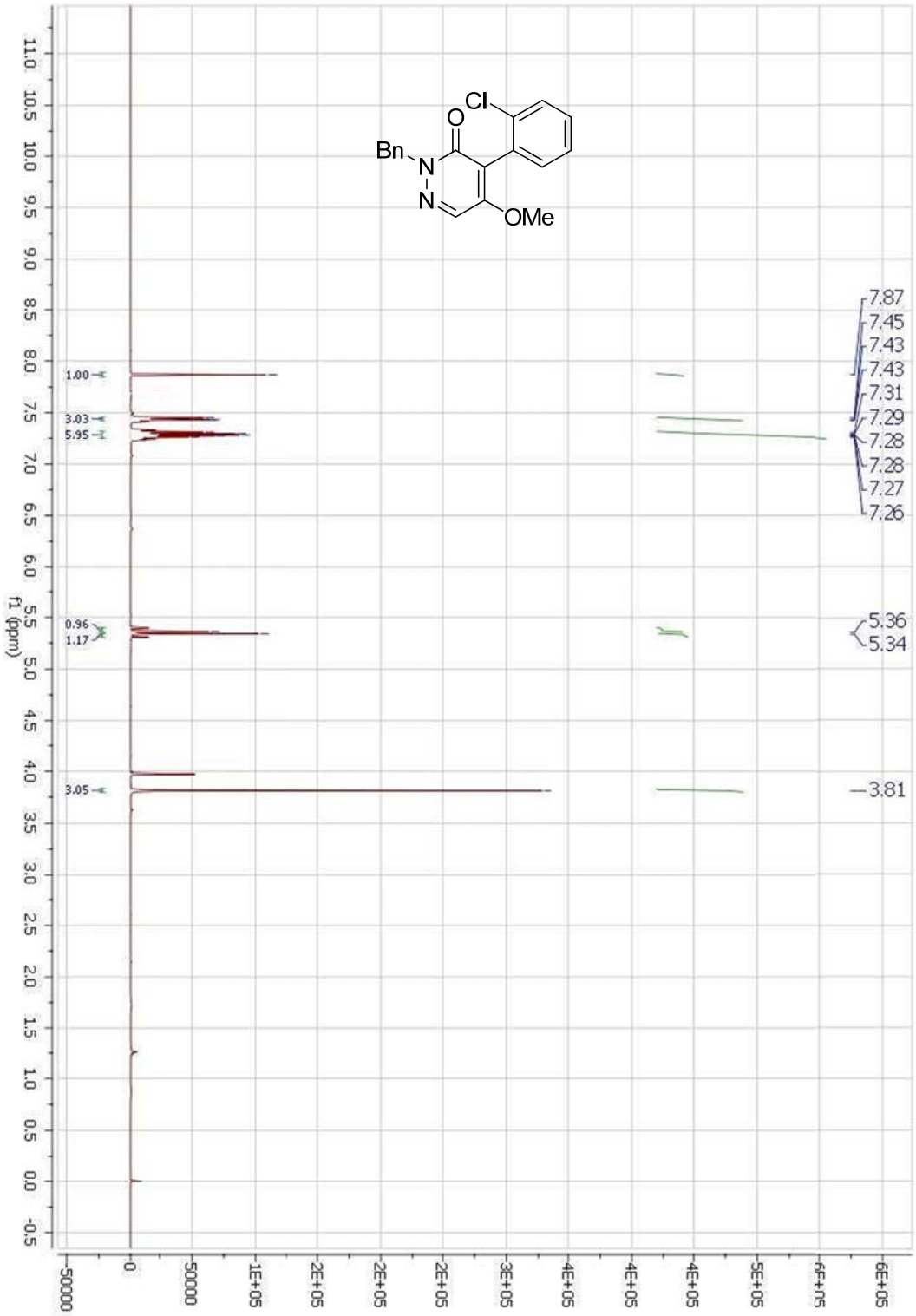

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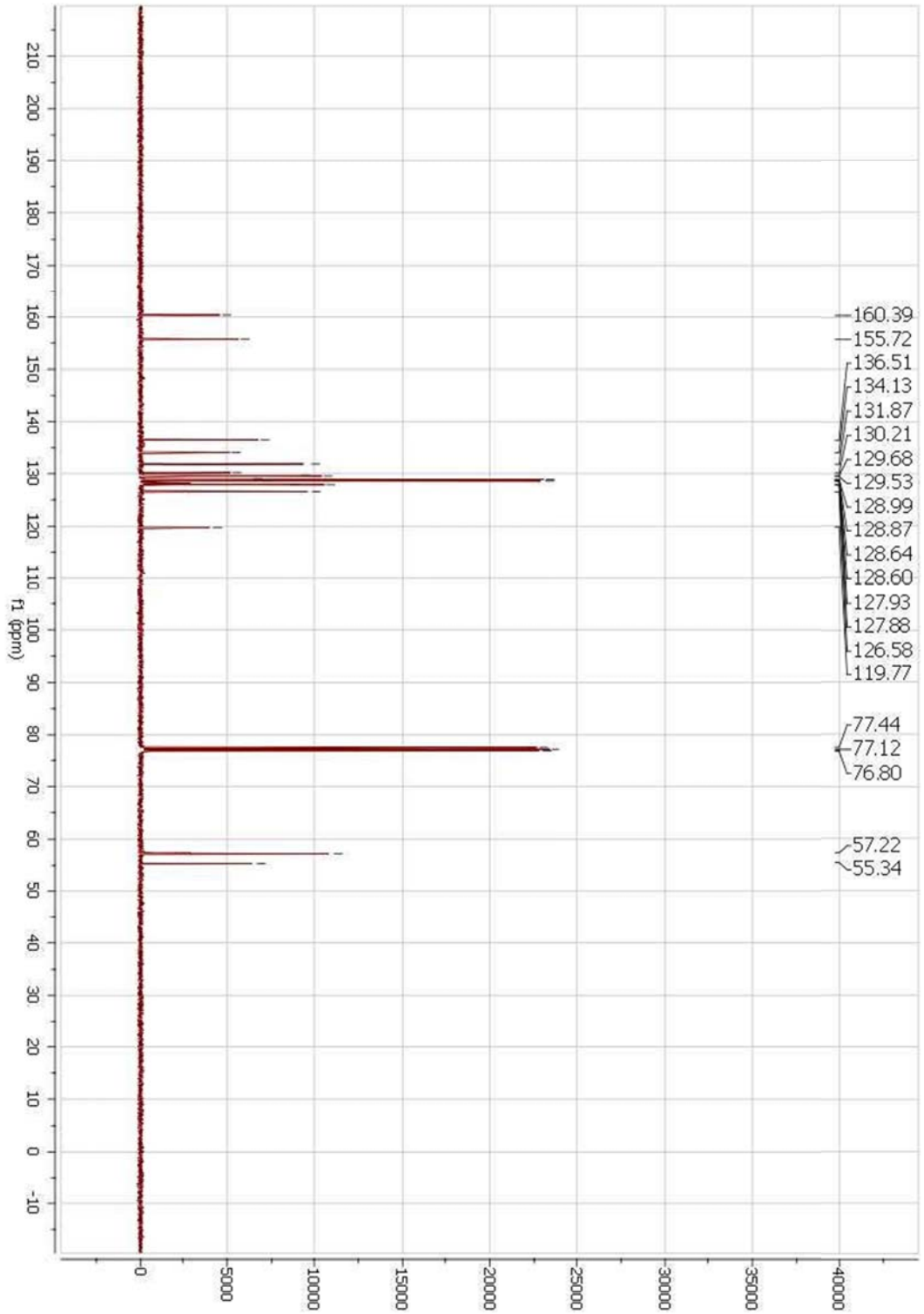
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127.93
127.88
126.58
119.77
77.44
77.12
76.80
57.22
55.34
f1 (ppm)

2-Benzyl-4-(3-chlorophenyl)-5-methoxypyridazin-3(2*H*)-one (**2d**)

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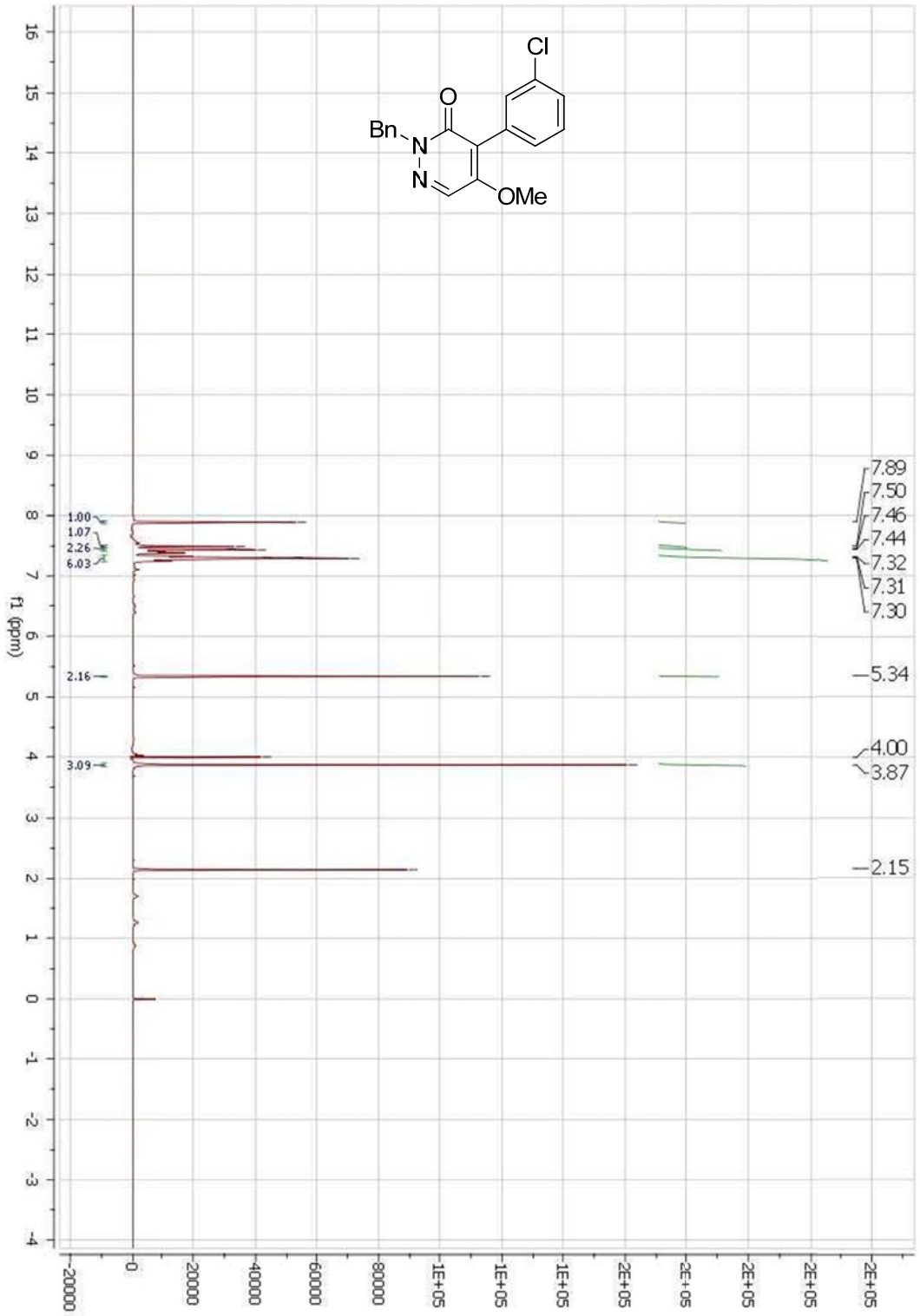

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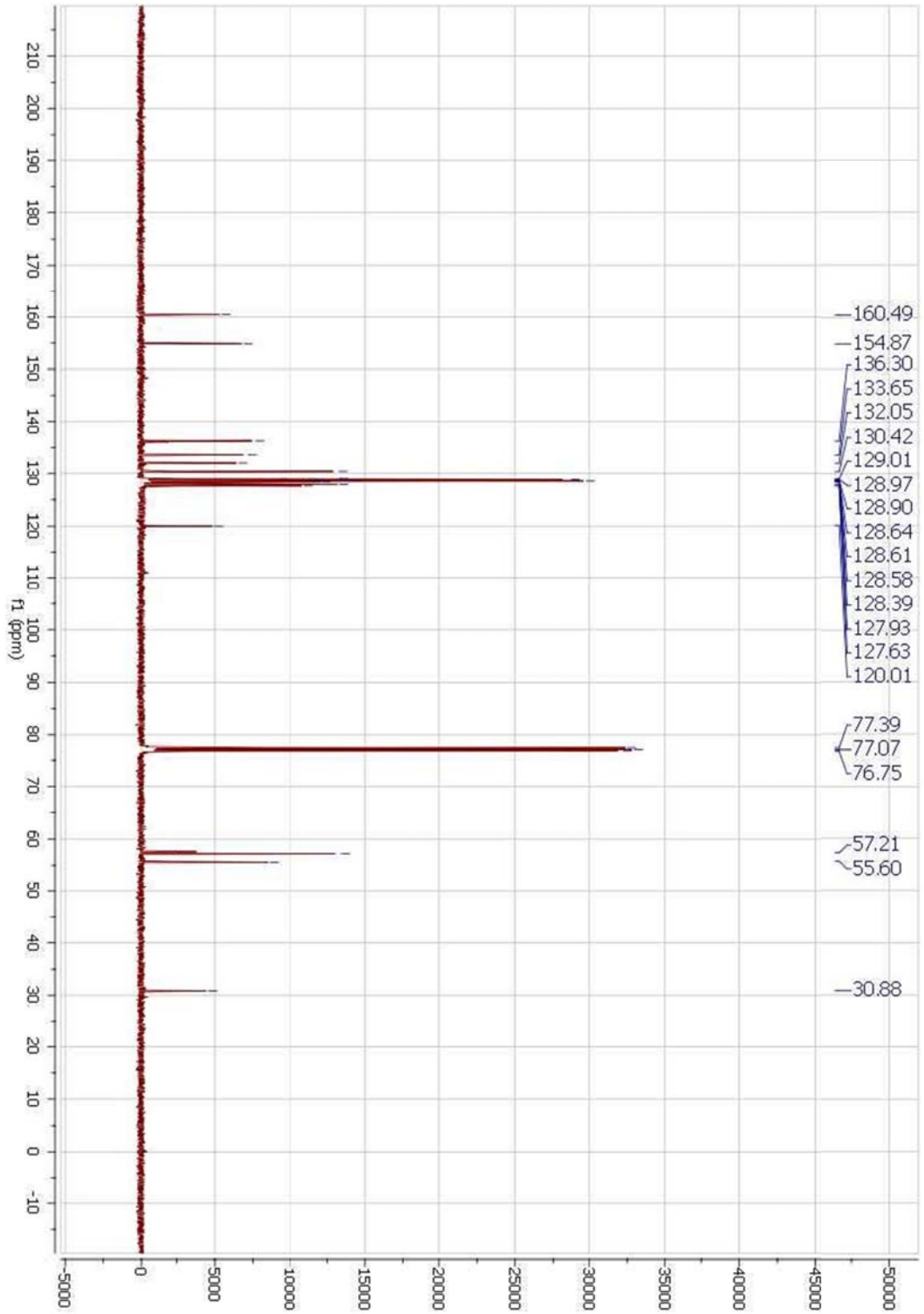
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128.58
128.39
127.93
127.63
120.01
77.39
77.07
76.75
57.21
55.60
30.88
f1 (ppm)

2-Benzyl-4-(4-chlorophenyl)-5-methoxypyridazin-3(2*H*)-one (**2e**)
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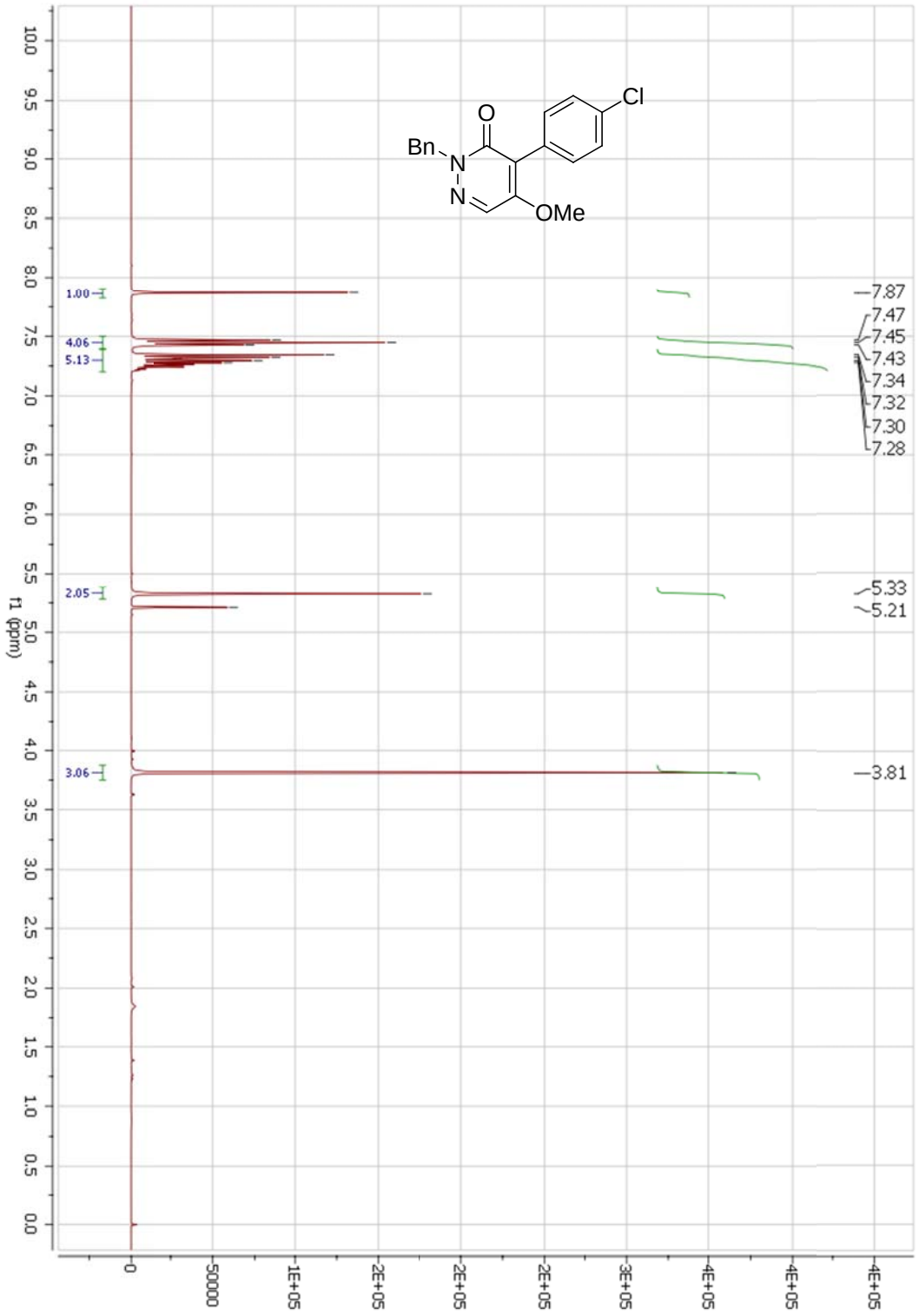

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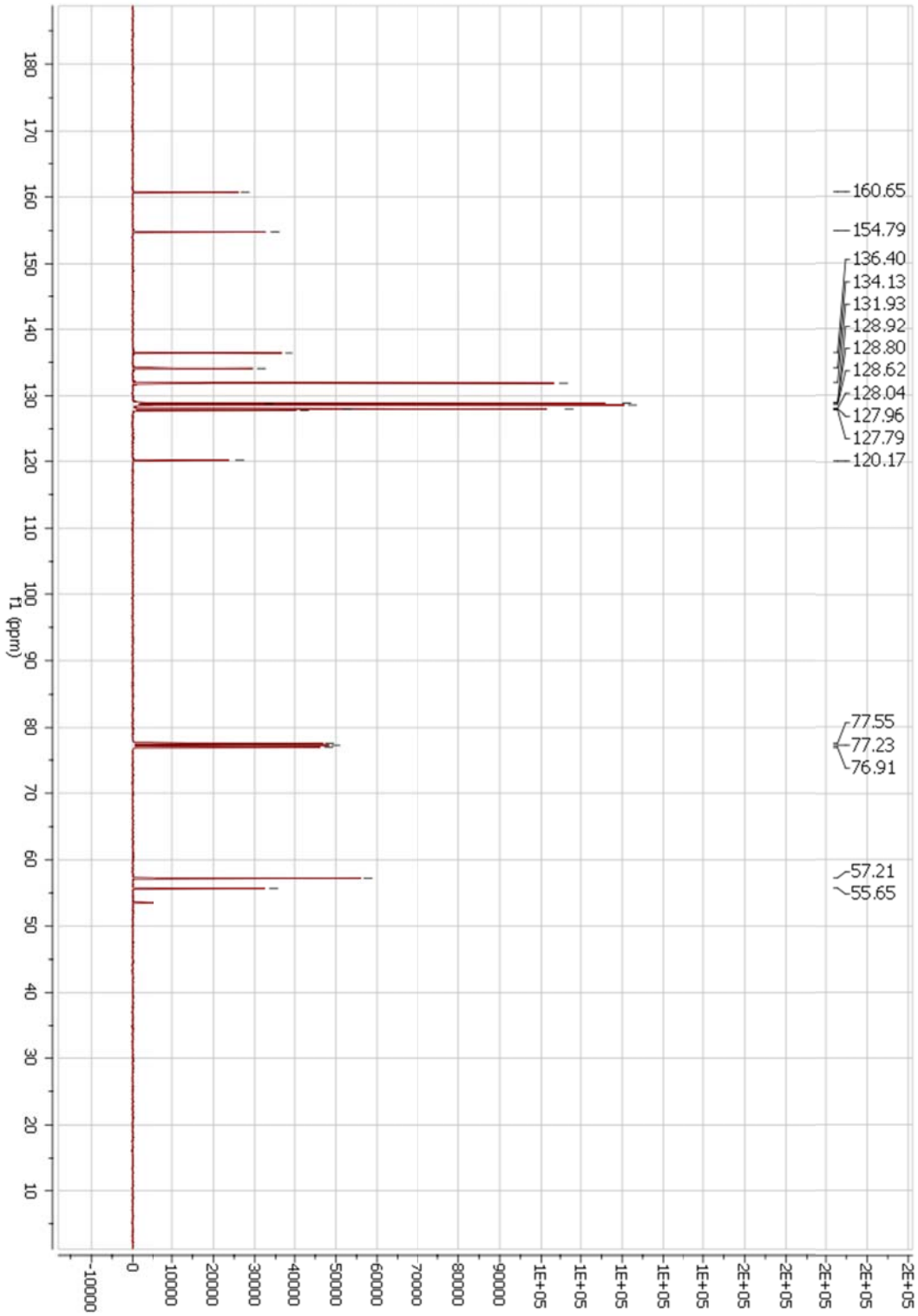
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128.04
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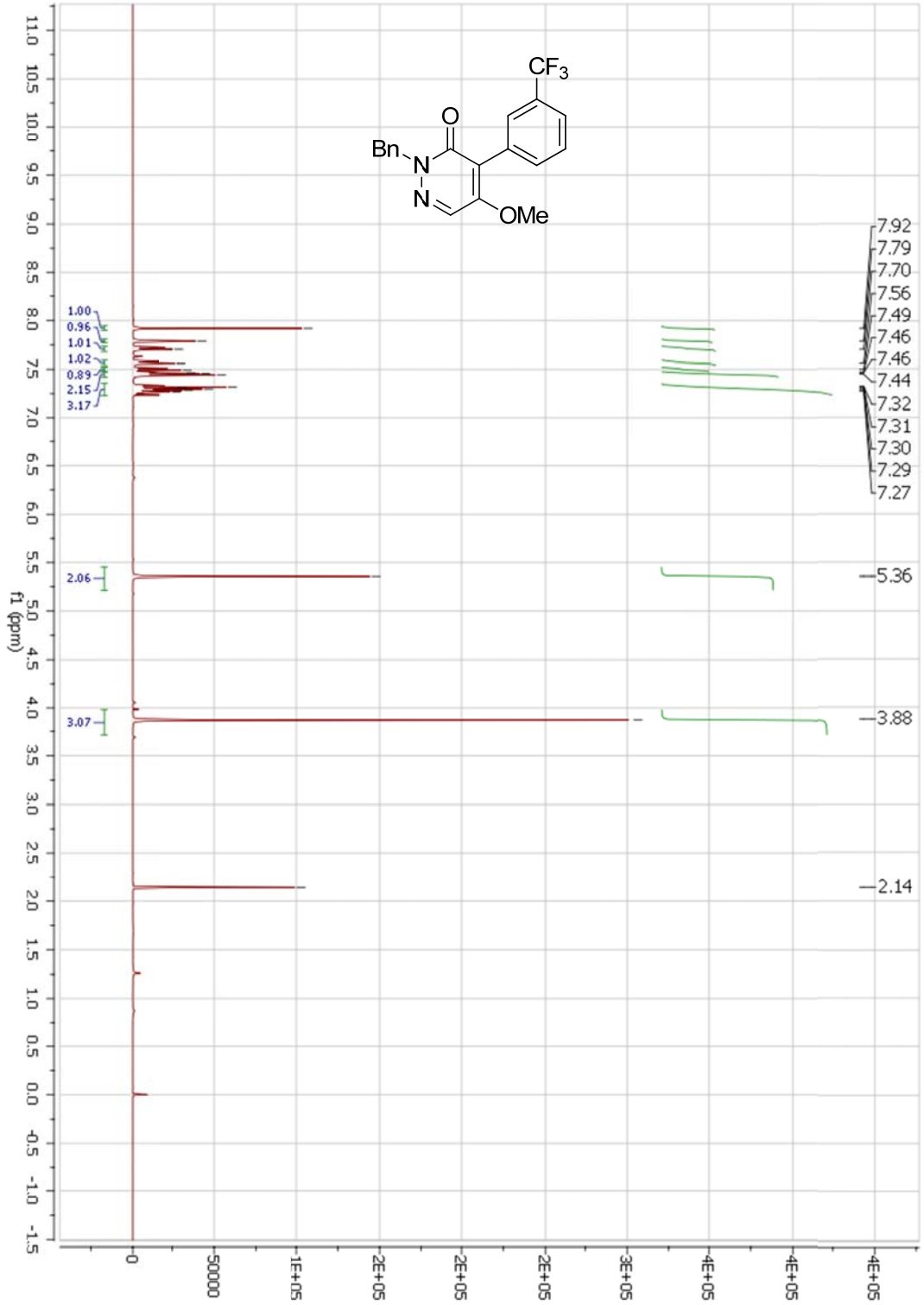
127.79
120.17
77.55
77.23
76.91
57.21
55.65
f1 (ppm)

2-Benzyl-5-methoxy-4-[3-(trifluoromethyl)phenyl]pyridazin-3(2*H*)-one (**2f**)

^{1}H-NMR



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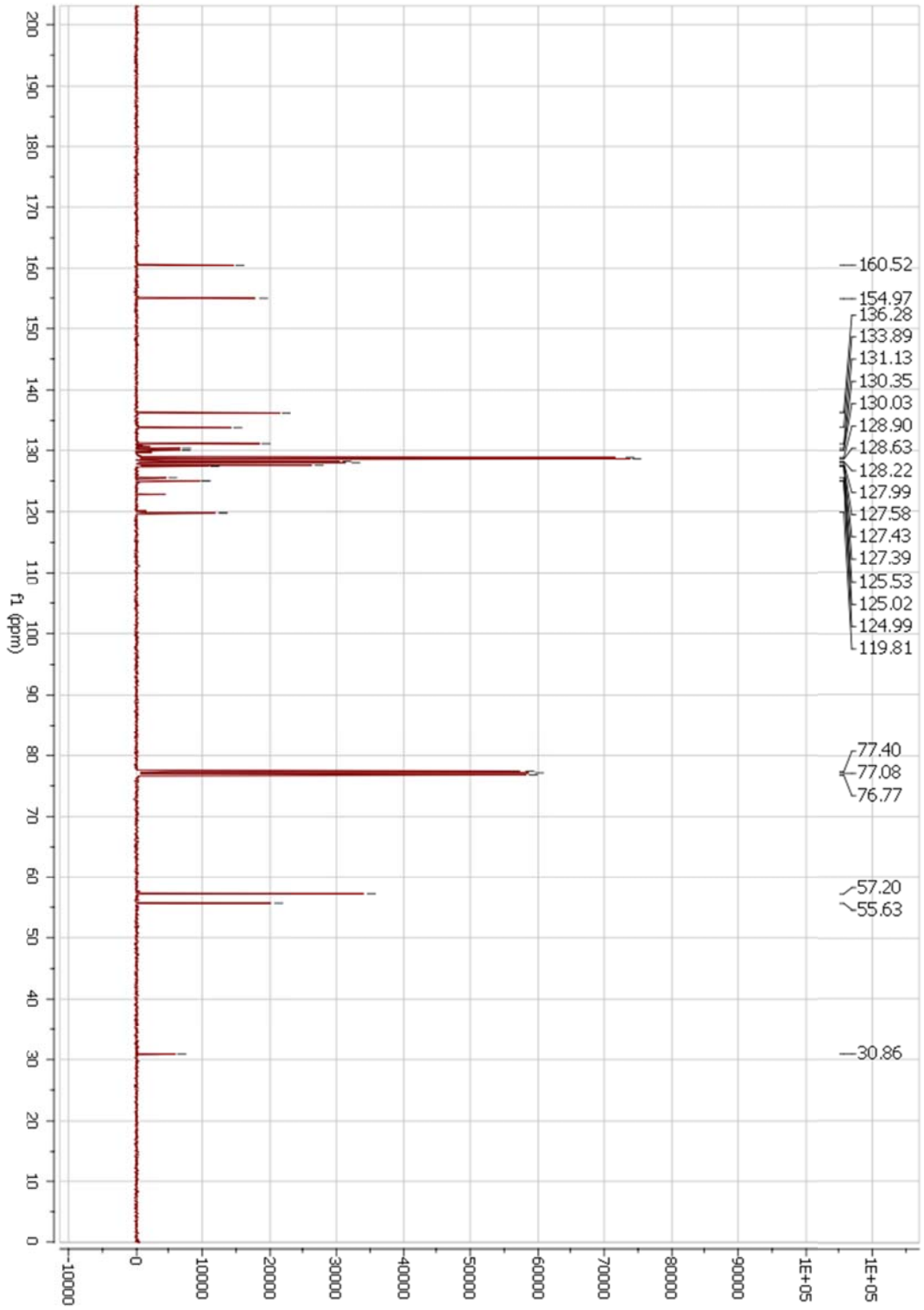
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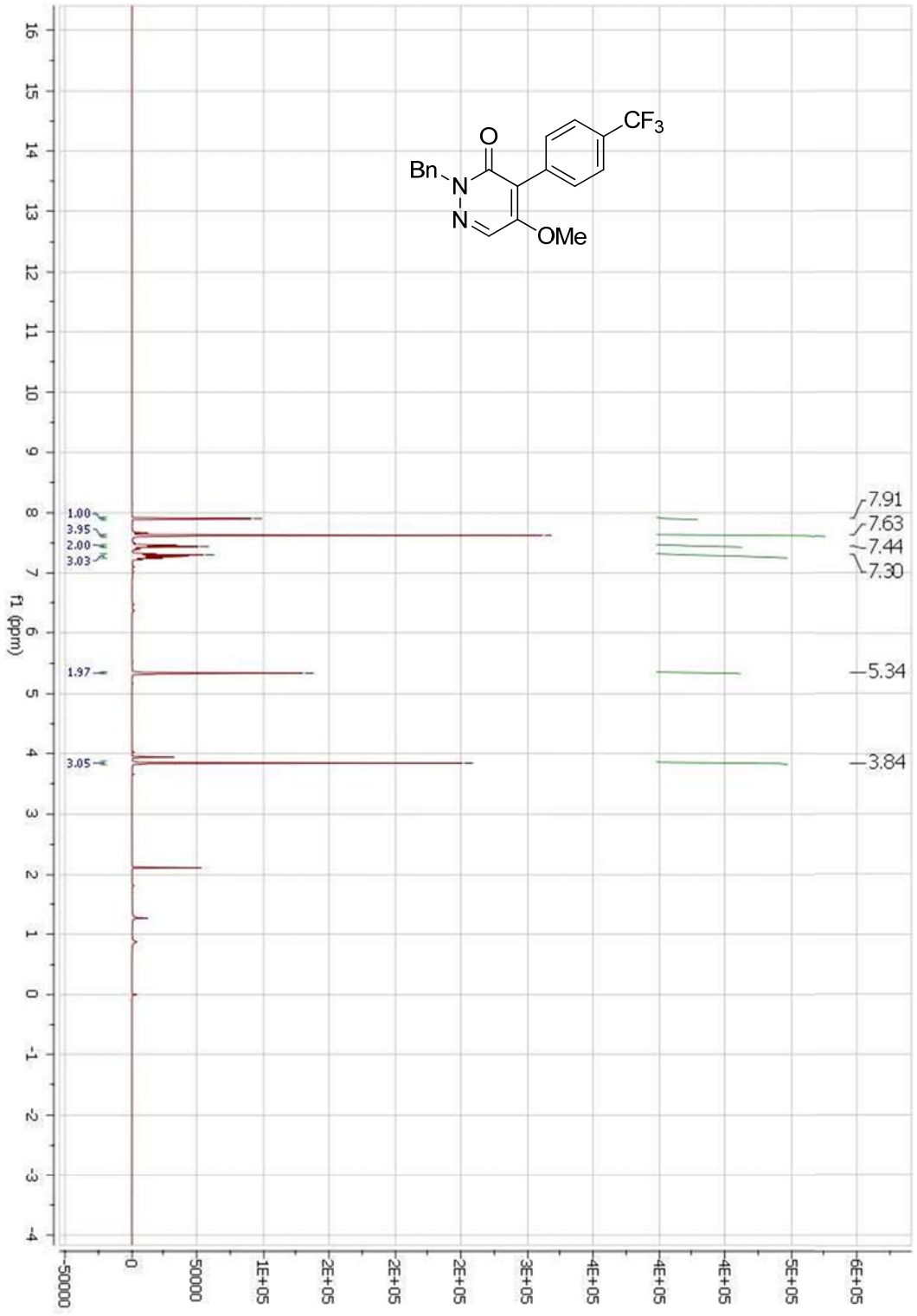
127.43
127.39
125.53
125.02
124.99
119.81
77.40
77.08
76.77
57.20
55.63
30.86
f1 (ppm)

2-Benzyl-5-methoxy-4-[4-(trifluoromethyl)phenyl]pyridazin-3(2*H*)-one (**2g**)

^{1}H-NMR



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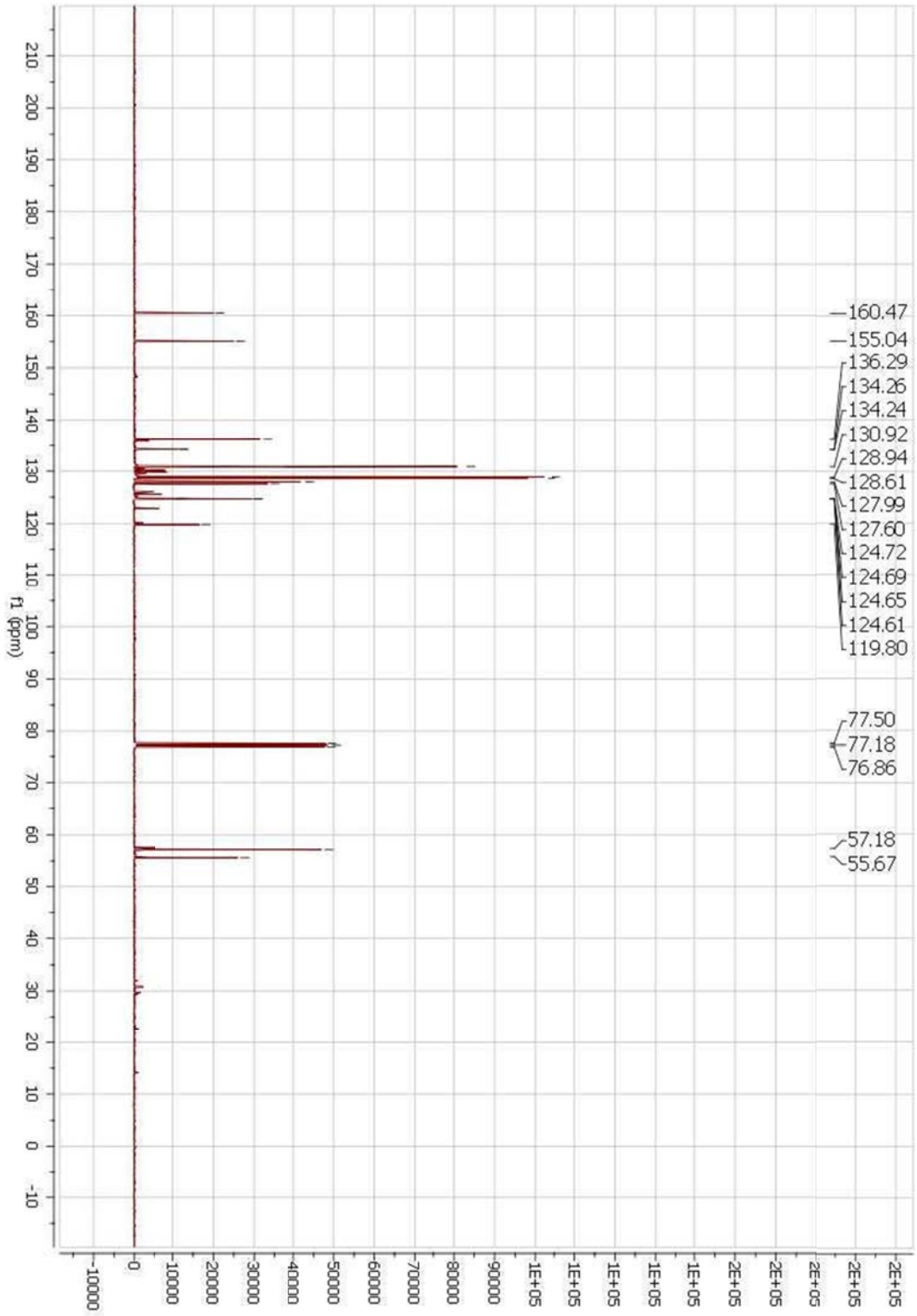
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127.99
127.60
124.72
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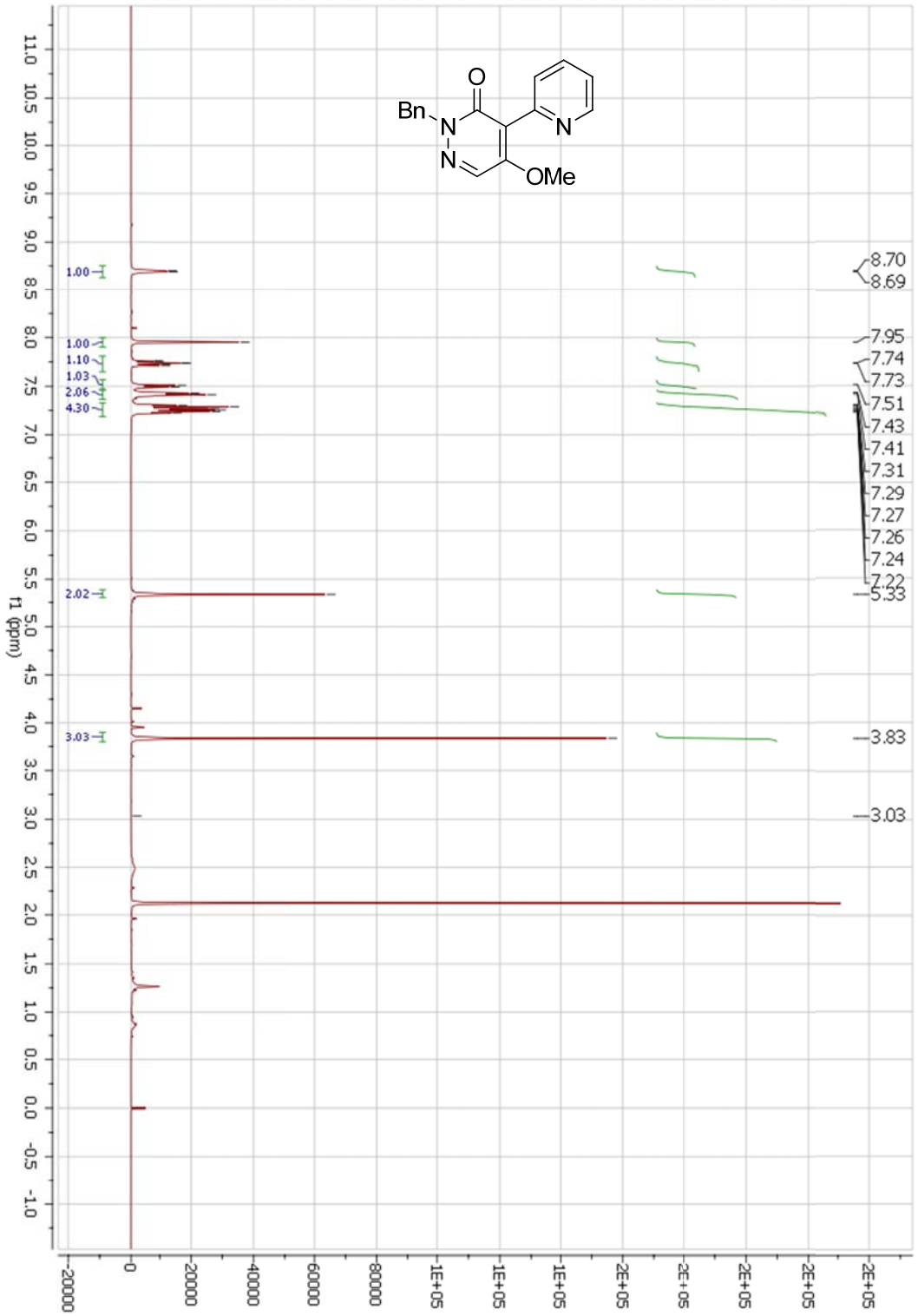
124.65
124.61
119.80
77.50
77.18
76.86
57.18
55.67
f1 (ppm)

2-Benzyl-5-methoxy-4-(pyridin-2-yl)pyridazin-3(2*H*)-one (**2h**)

^{1}H-NMR



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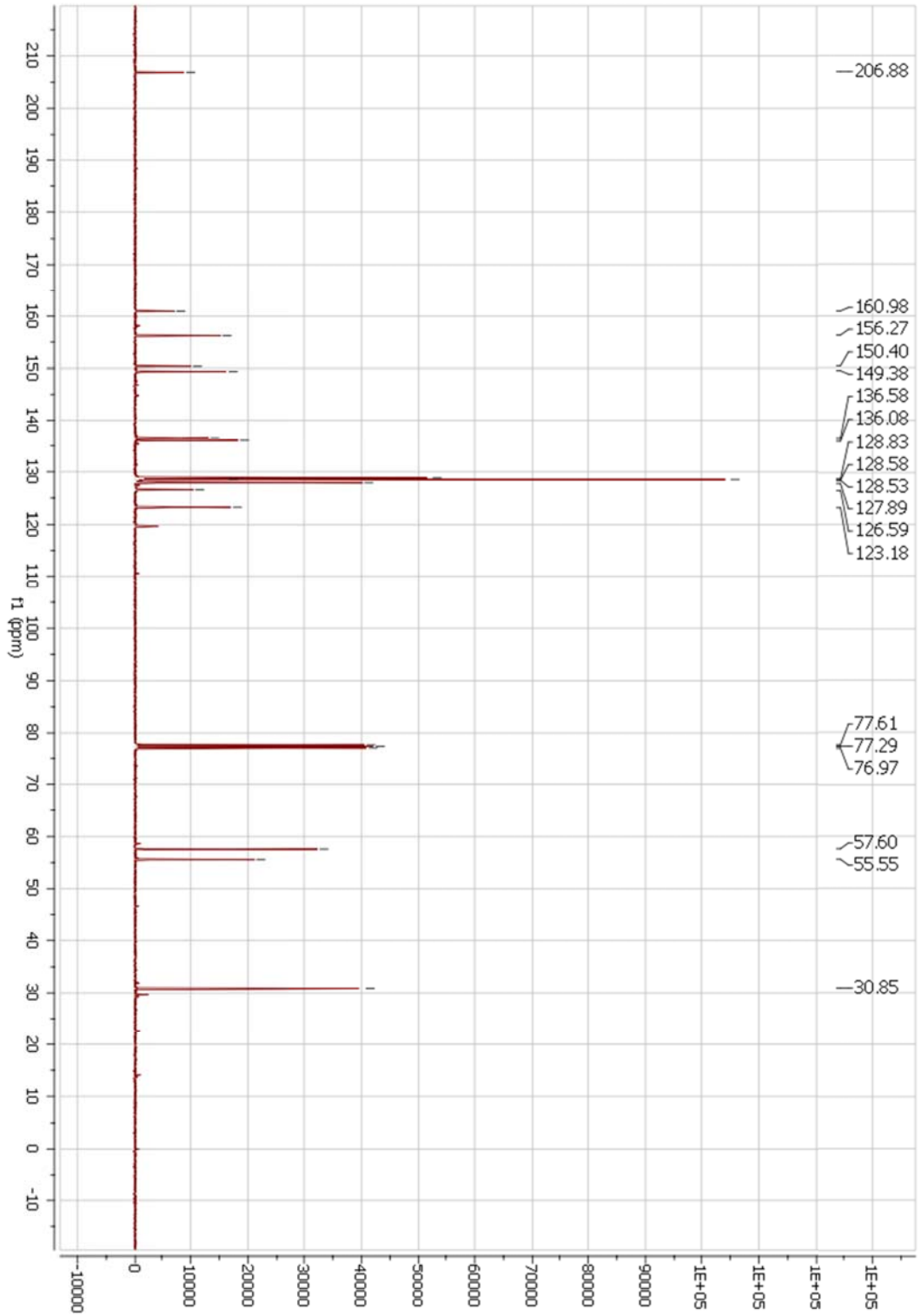
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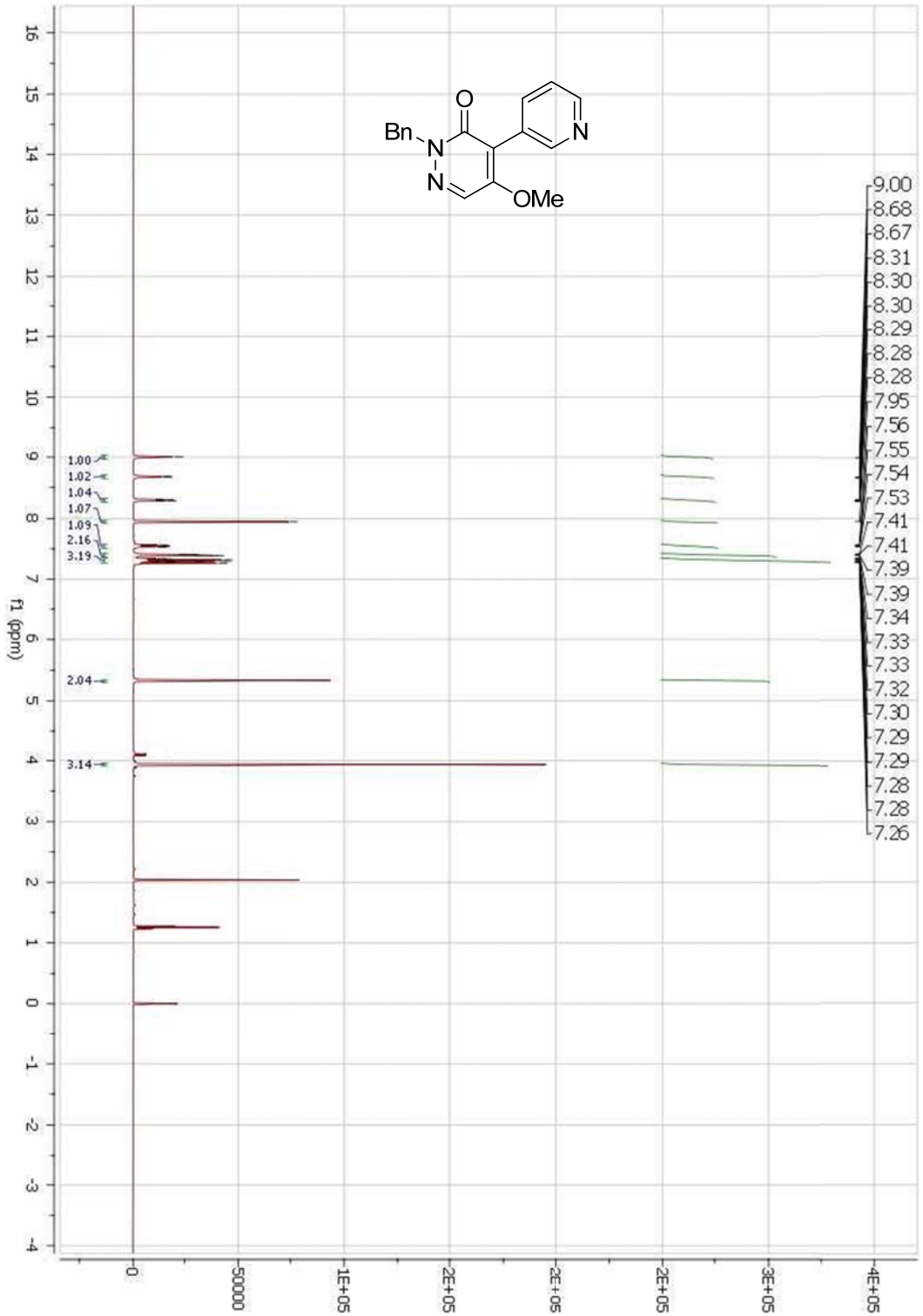
150.40
149.38
136.58
136.08
128.83
128.58
128.53
127.89
126.59
123.18
77.61
77.29
76.97
57.60
55.55
30.85
f1 (ppm)

2-Benzyl-5-methoxy-4-(pyridin-3-yl)pyridazin-3(2*H*)-one (**2i**)

^{1}H-NMR



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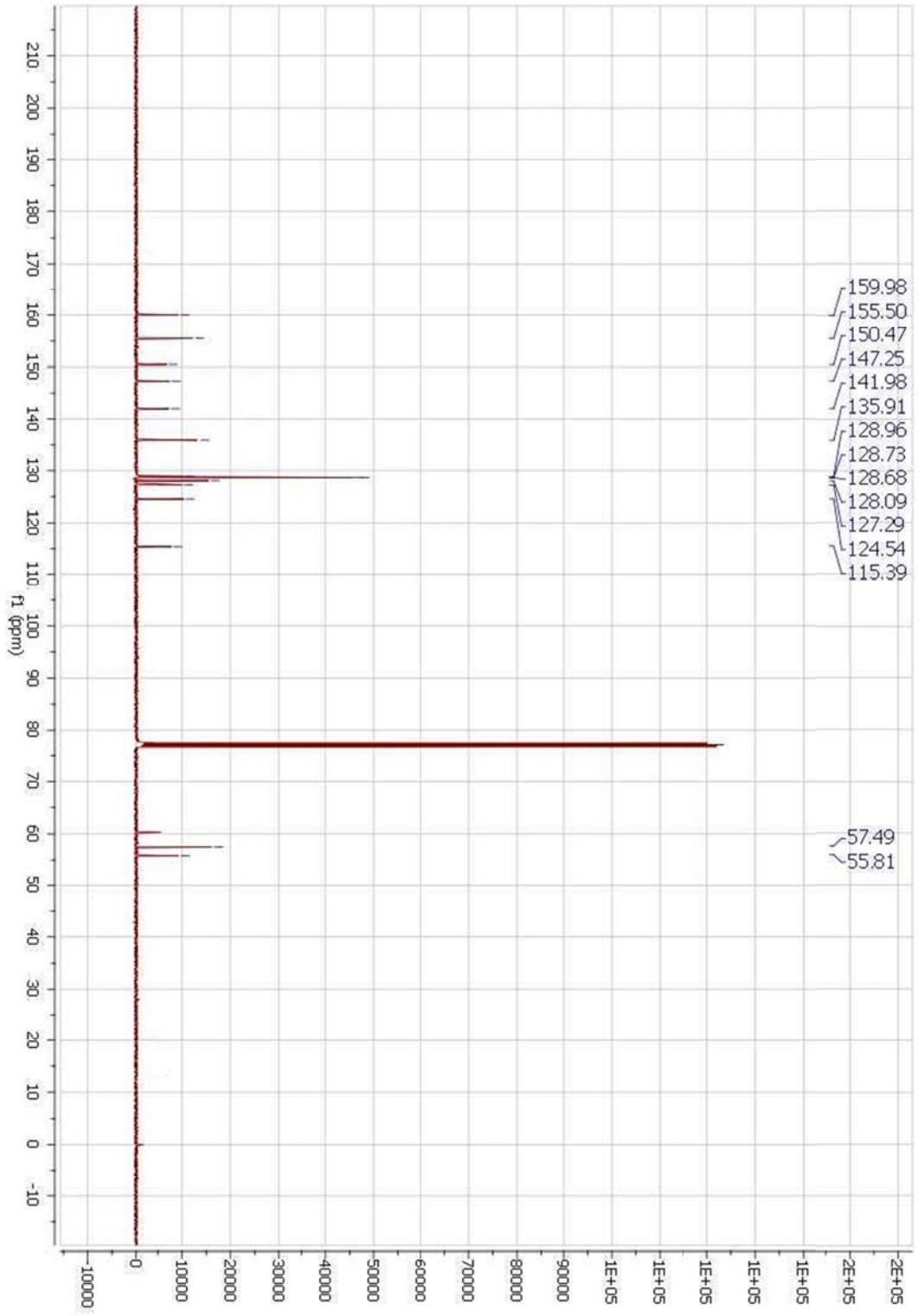
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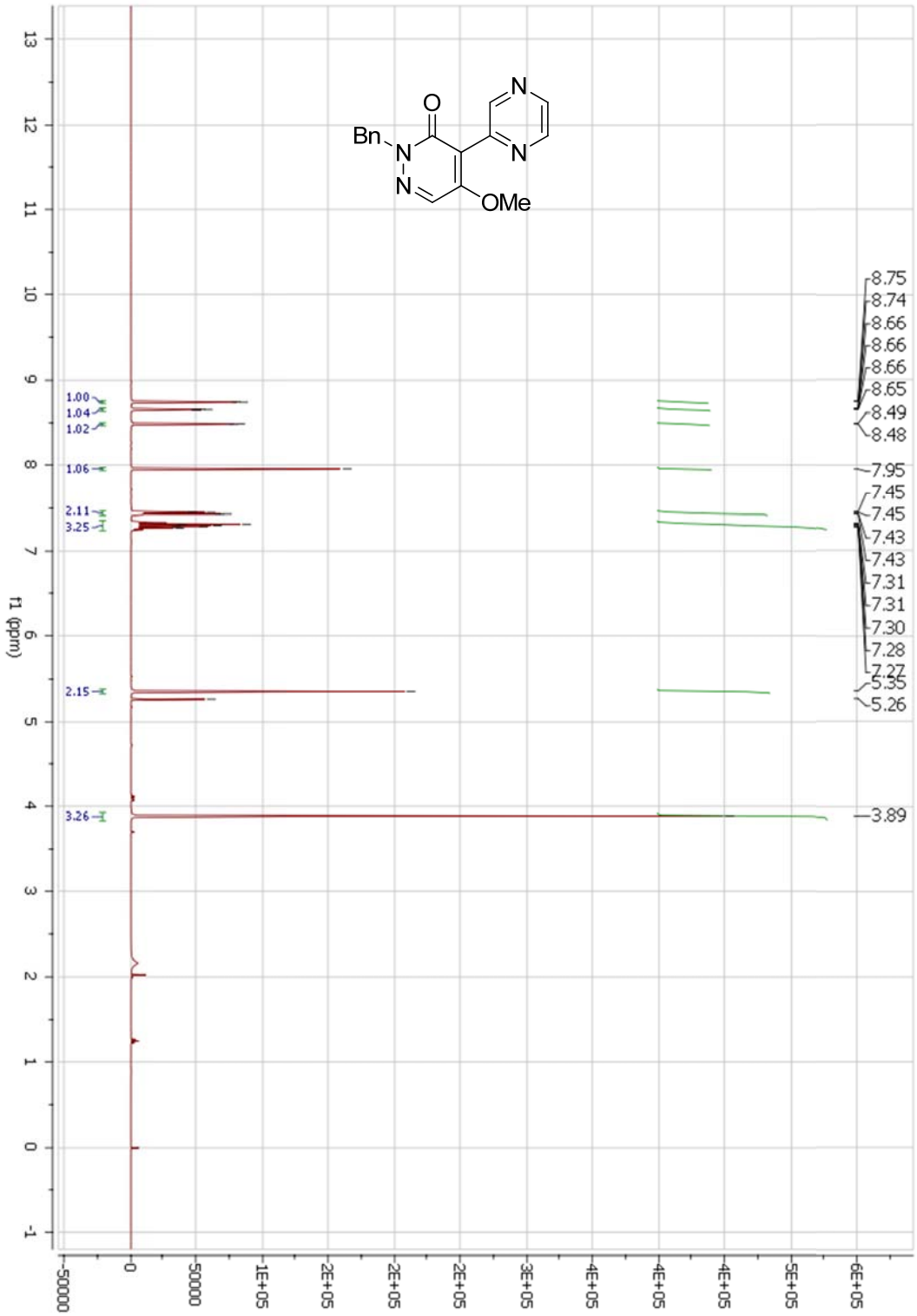
147.25
141.98
135.91
128.96
128.73
128.68
128.09
127.29
124.54
115.39
57.49
55.81
f1 (ppm)

2-Benzyl-5-methoxy-4-(pyrazin-2-yl)pyridazin-3(2*H*)-one (**2j**)

^{1}H-NMR



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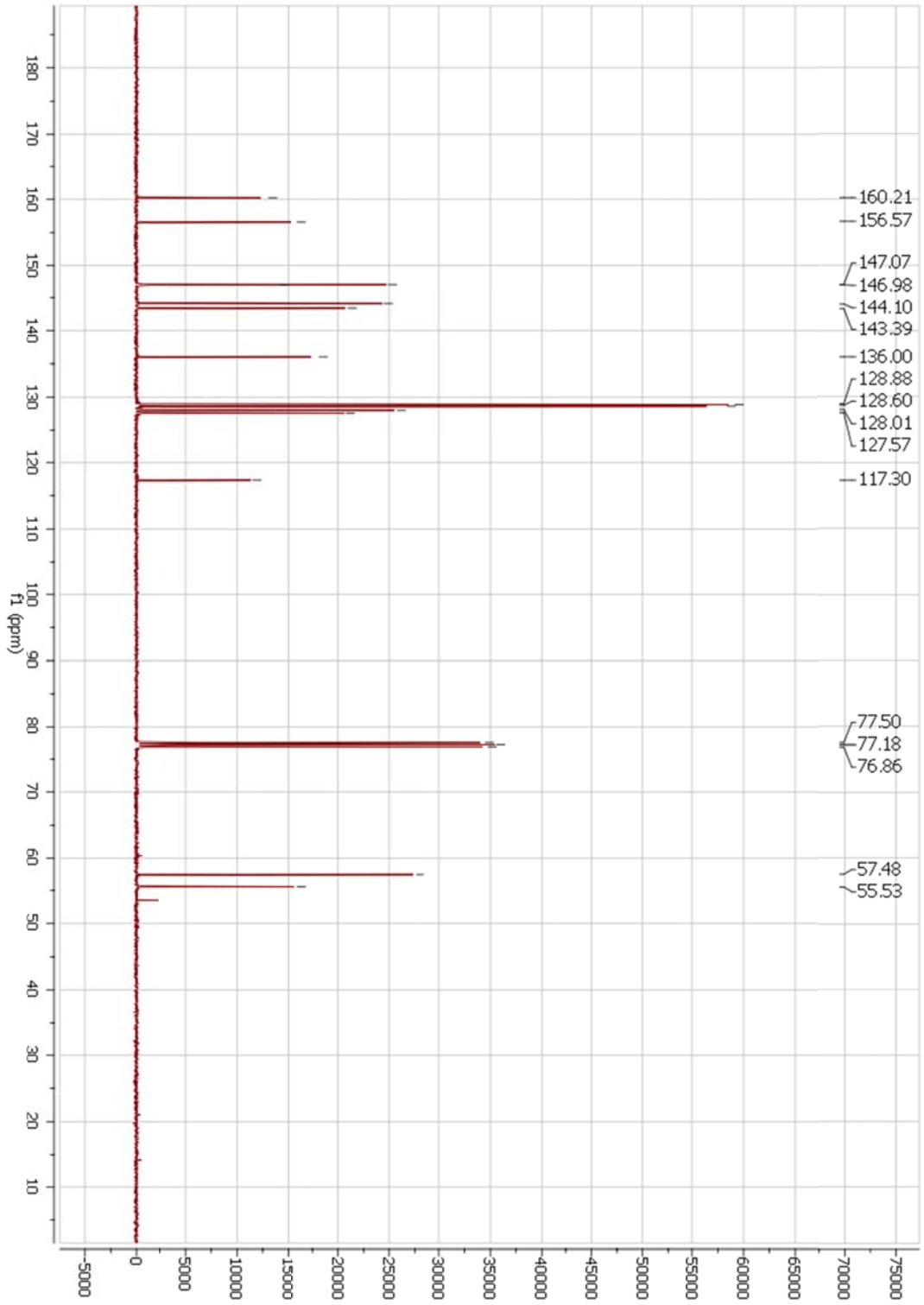
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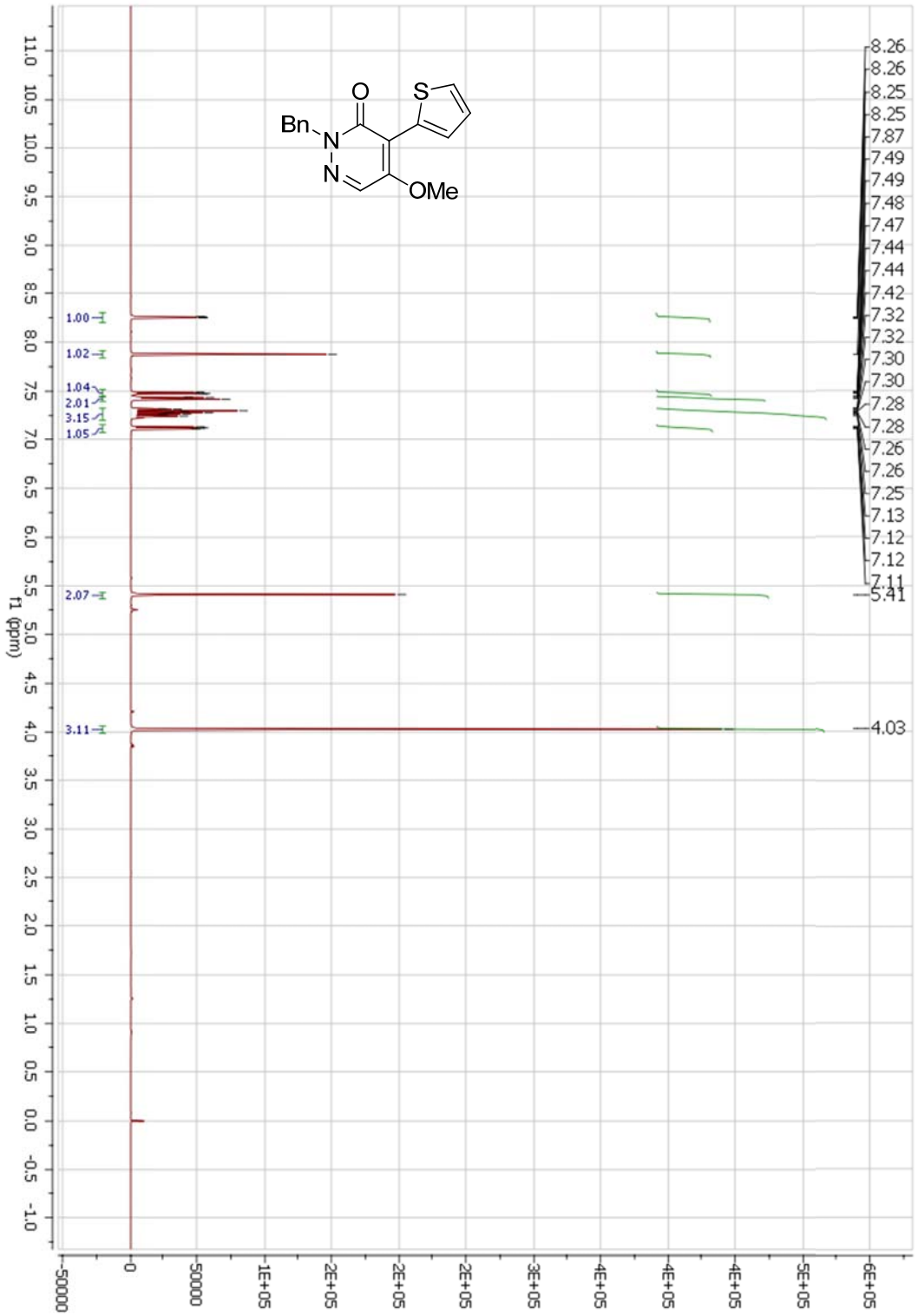
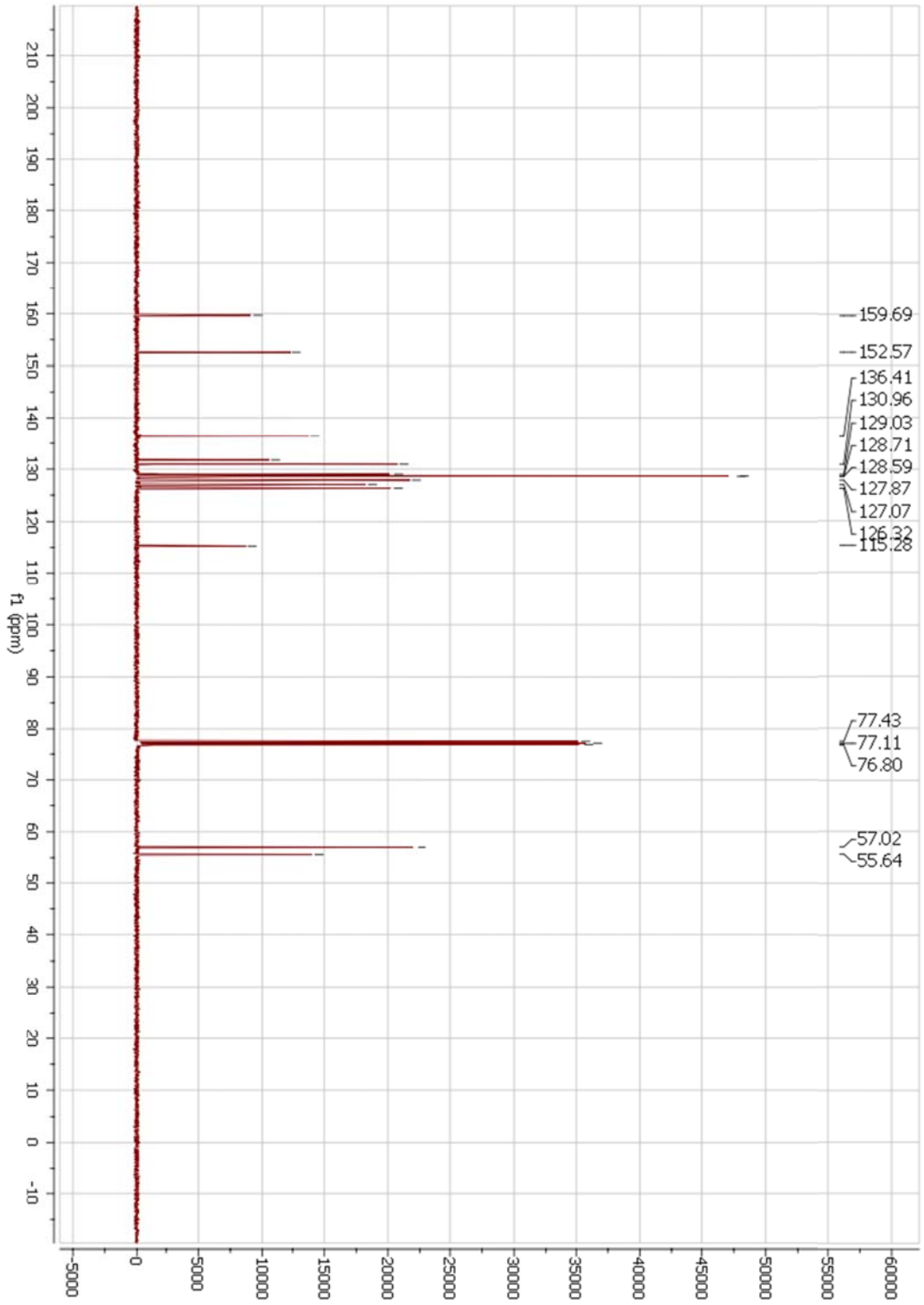
144.10
143.39
136.00
128.88
128.60
128.01
127.57
117.30
77.50
77.18
76.86
57.48
55.53
f1 (ppm)

2-Benzyl-5-methoxy-4-(thien-2-yl)pyridazin-3(2*H*)-one (**2k**)

^{1}H-NMR



^{13}C-NMR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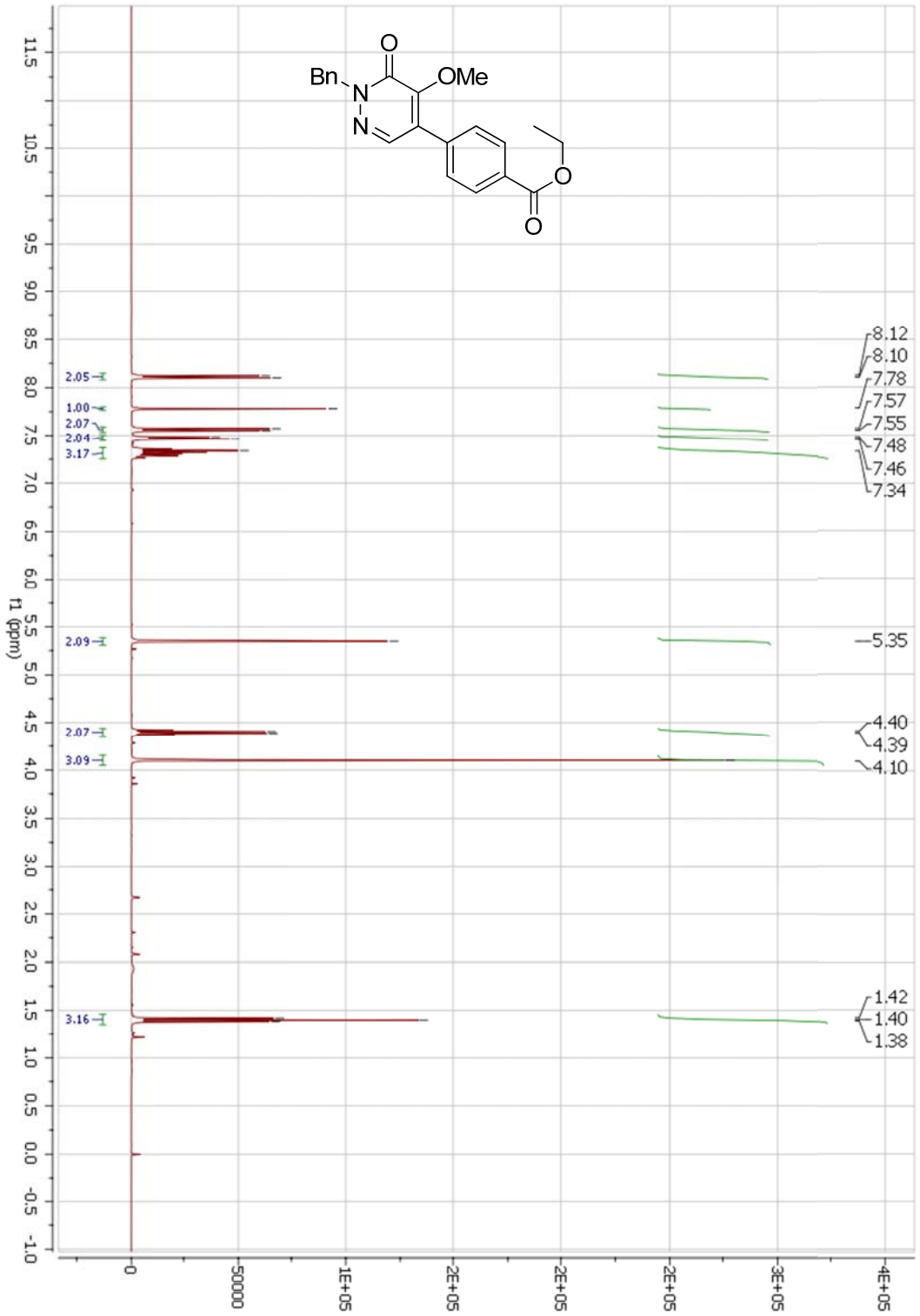
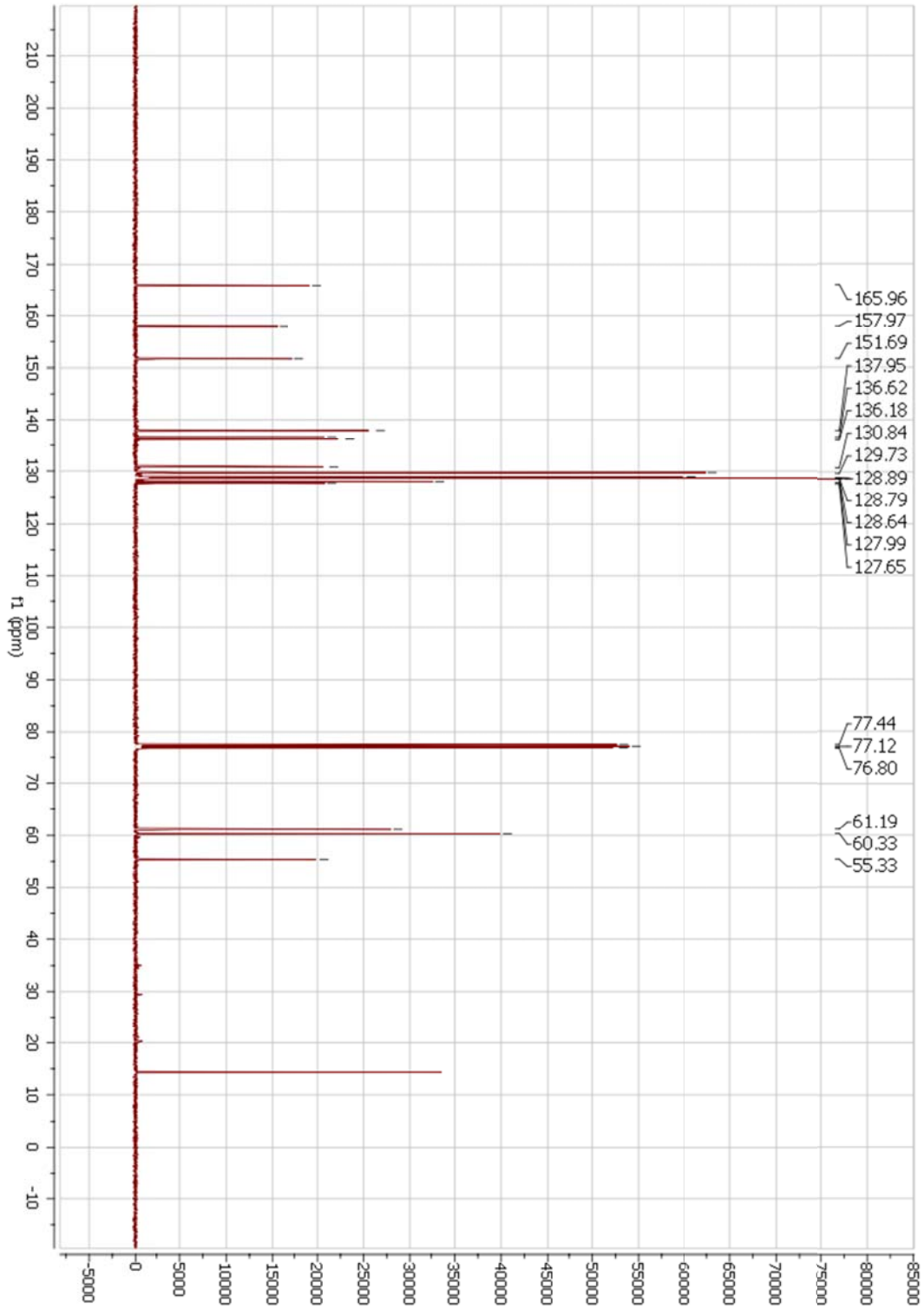
130.96
129.03
128.71
128.59
127.87
127.07
126.32
115.28
77.43
77.11
76.80
57.02
55.64
f1 (ppm)

Ethyl 4-(1-benzyl-5-methoxy-6-oxo-1,6-dihydropyridazin-4-yl)benzoate (**4a**)
^{1}H-NMR



^{13}C-NMR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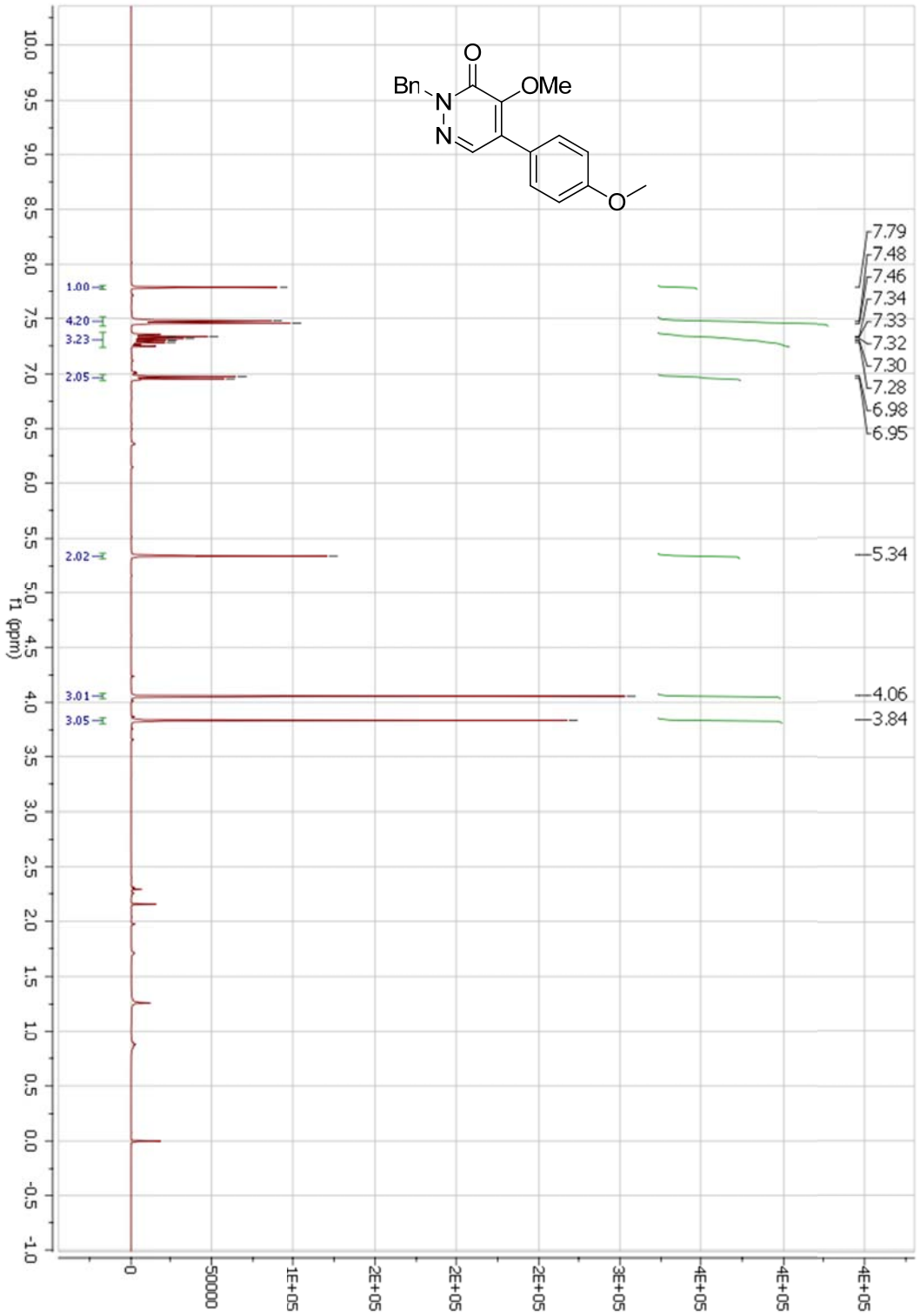
137.95
136.62
136.18
130.84
129.73
128.89
128.79
128.64
127.99
127.65
77.44
77.12
76.80
61.19
60.33
55.33
f1 (ppm)

2-Benzyl-4-methoxy-5-(4-methoxyphenyl)pyridazin-3(2*H*)-one (**4b**)

^{1}H-NMR



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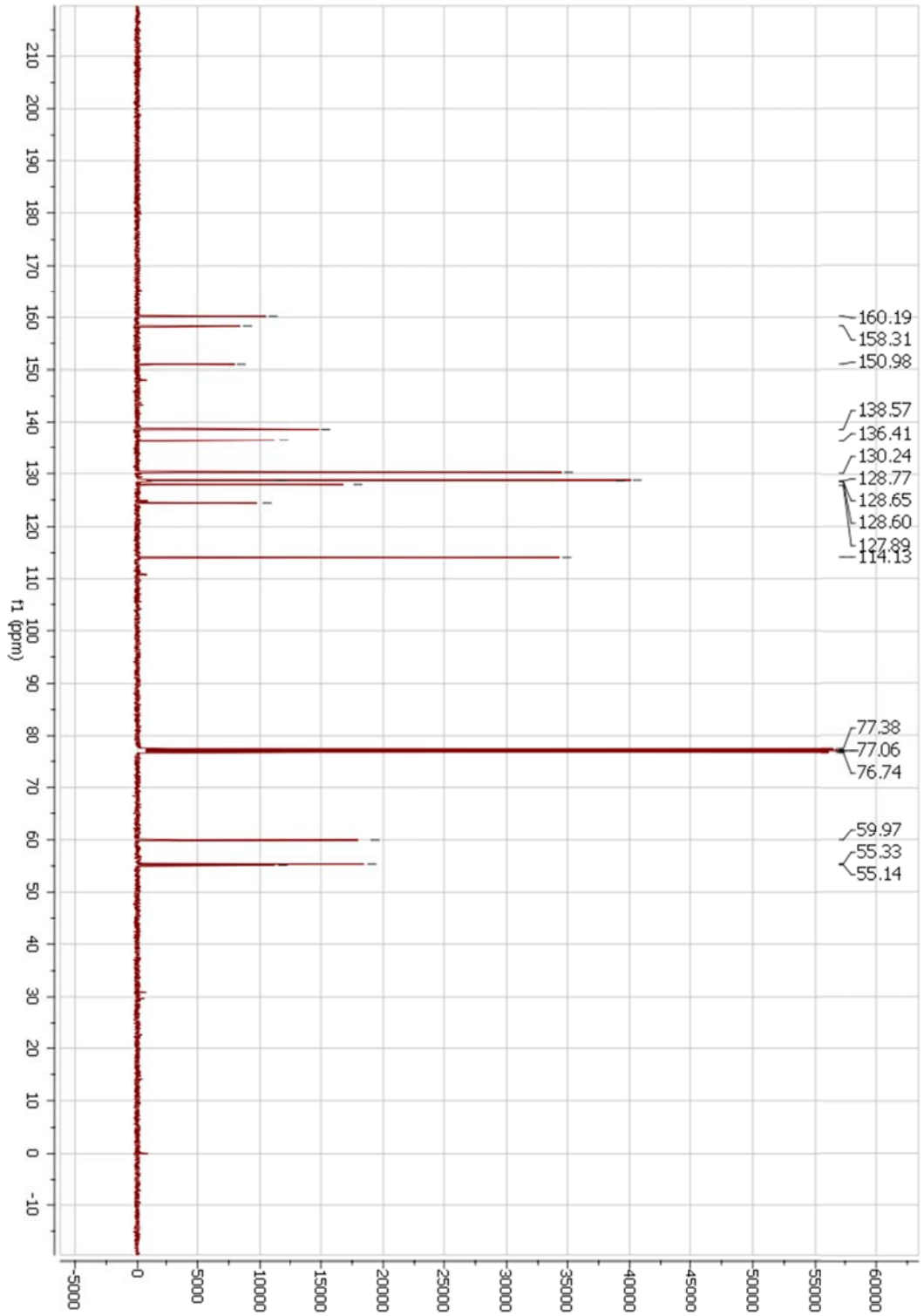
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136.41
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128.65
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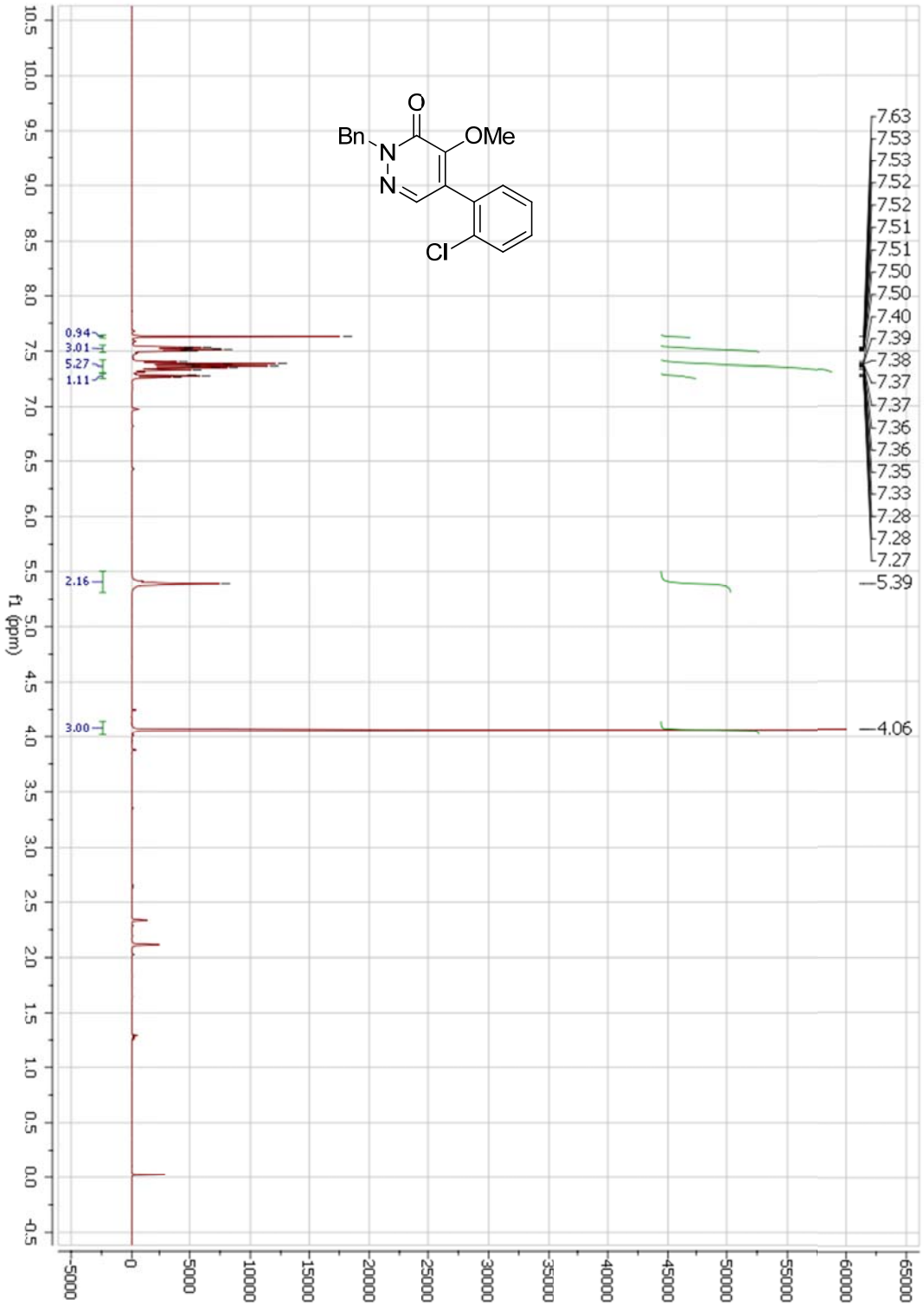
127.89
114.13
77.38
77.06
76.74
59.97
55.33
55.14
f1 (ppm)

2-Benzyl-5-(2-chlorophenyl)-4-methoxypyridazin-3(2*H*)-one (**4c**)

^{1}H-NMR



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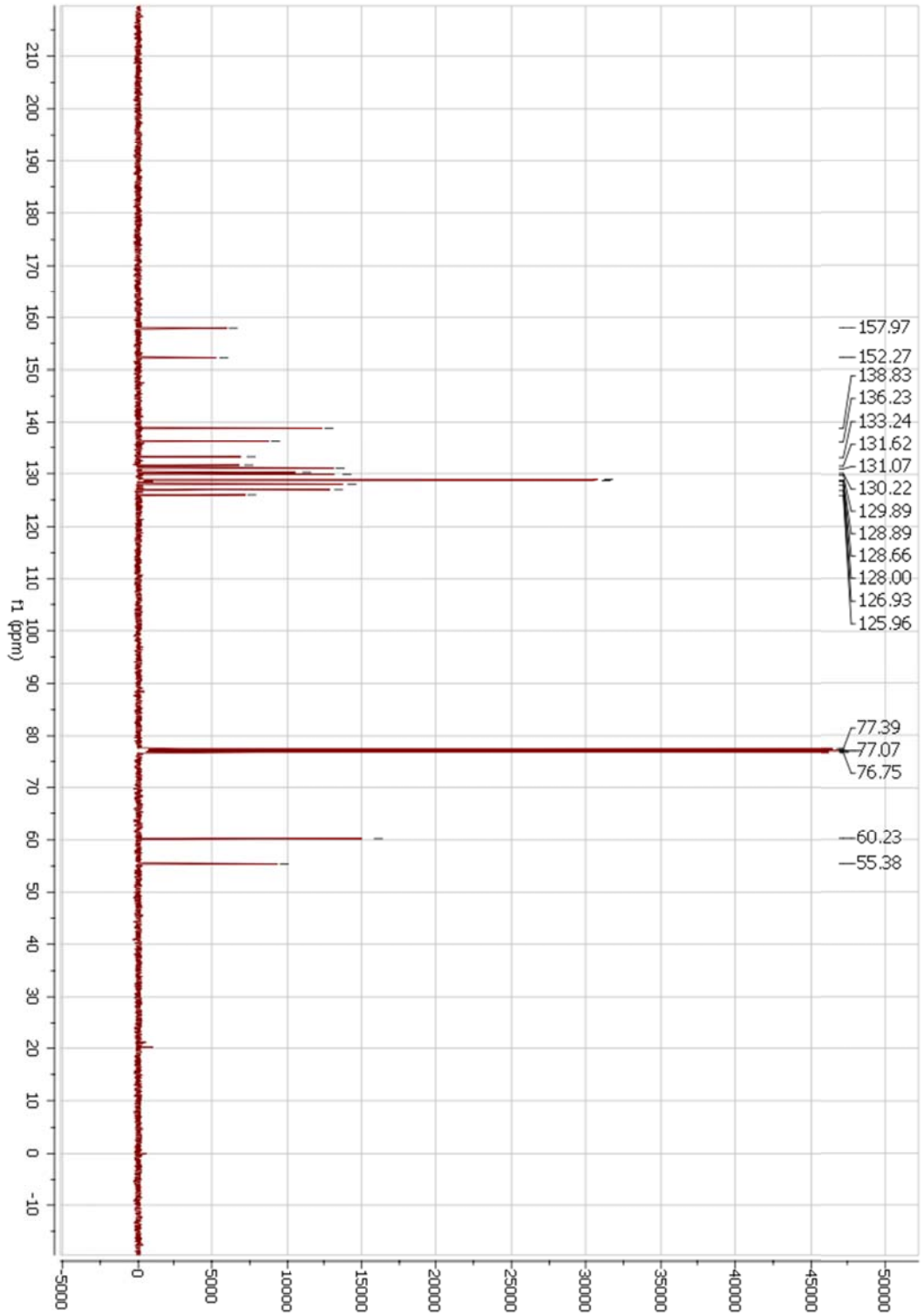
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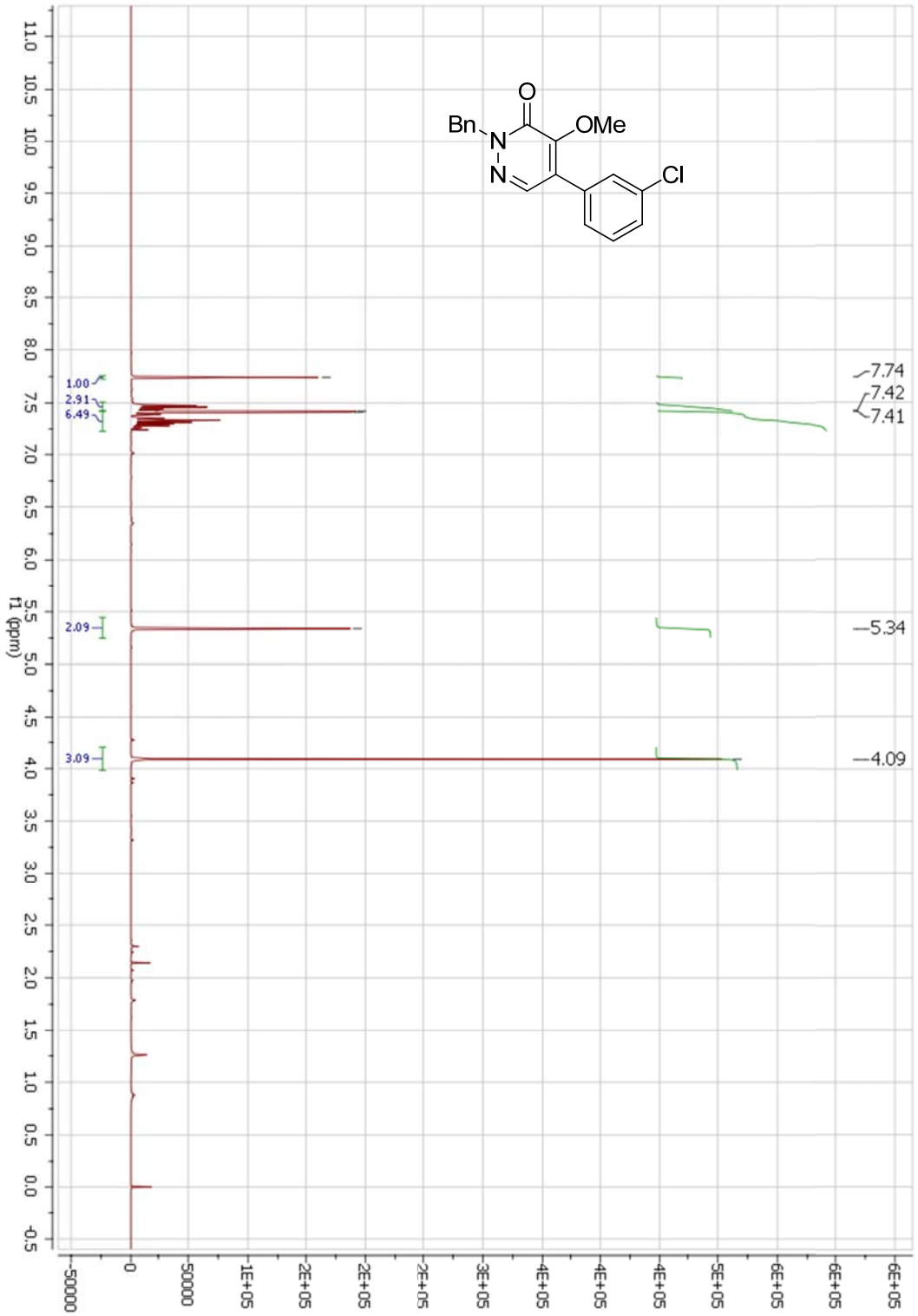
133.24
131.62
131.07
130.22
129.89
128.89
128.66
128.00
126.93
125.96
77.39
77.07
76.75
60.23
55.38
f1 (ppm)

2-Benzyl-5-(3-chlorophenyl)-4-methoxypyridazin-3(2*H*)-one (**4d**)

^{1}H-NMR



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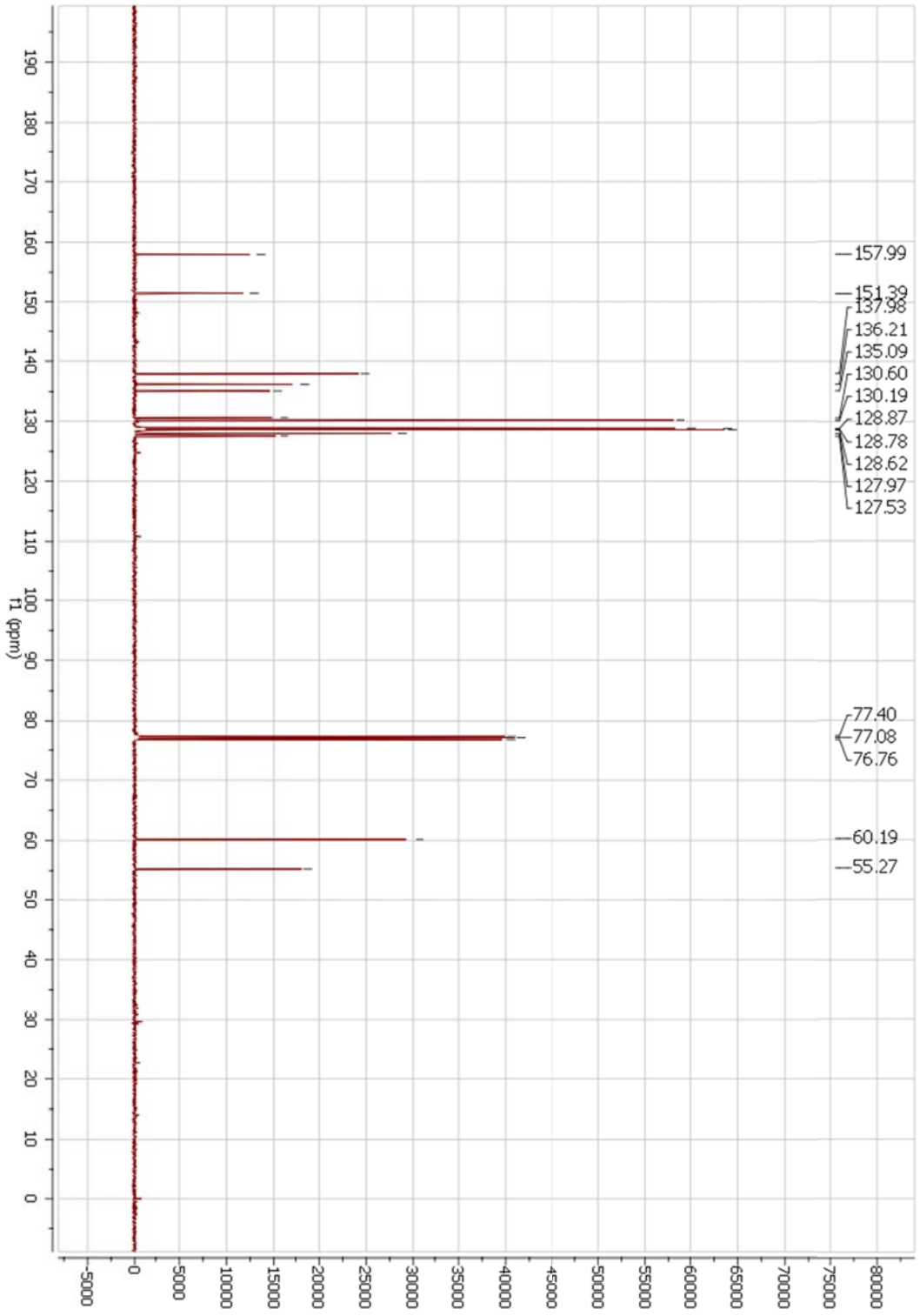
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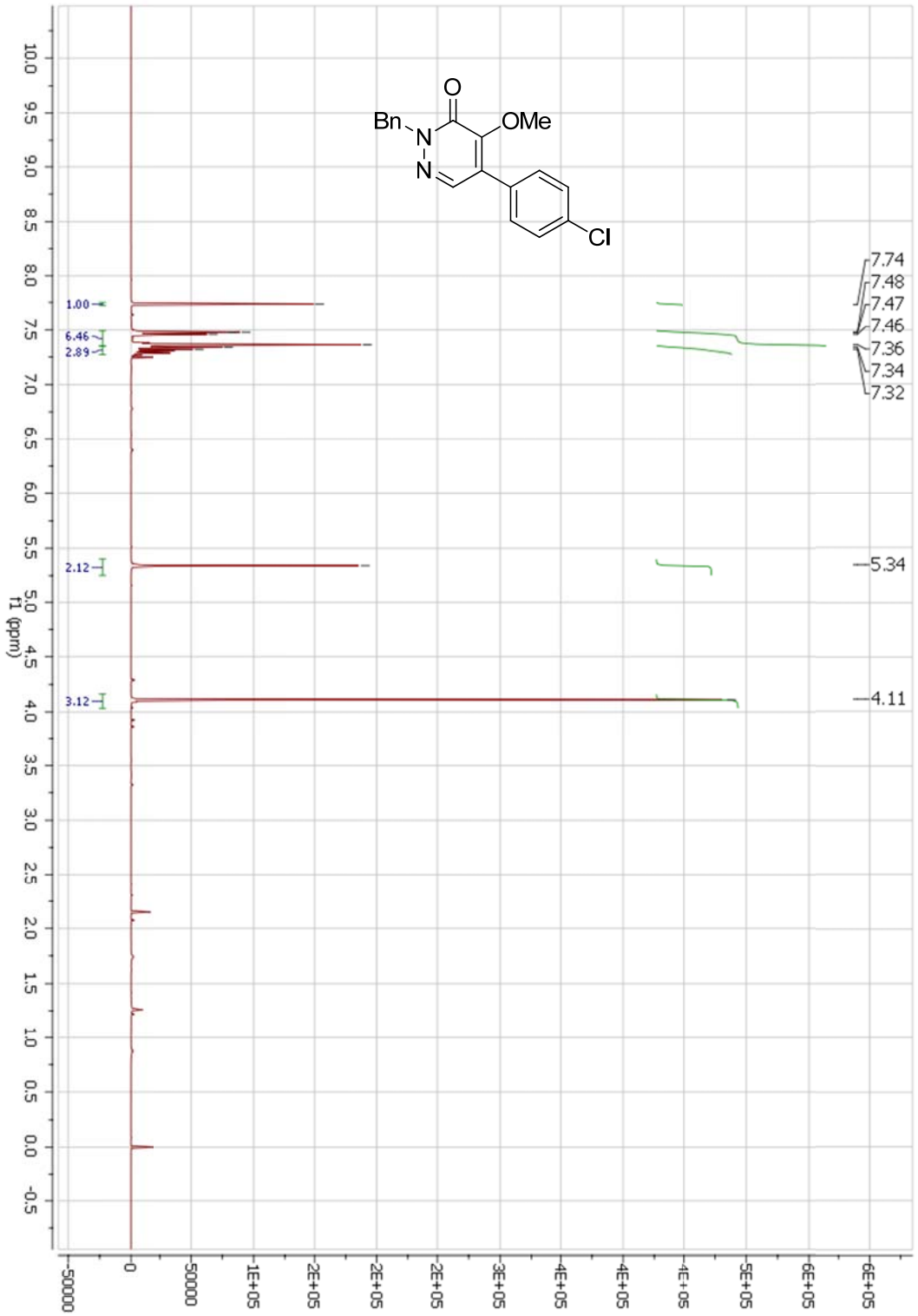
136.21
135.09
130.60
130.19
128.87
128.78
128.62
127.97
127.53
77.40
77.08
76.76
60.19
55.27
f1 (ppm)

2-Benzyl-5-(4-chlorophenyl)-4-methoxypyridazin-3(2*H*)-one (**4e**)

^{1}H-NMR



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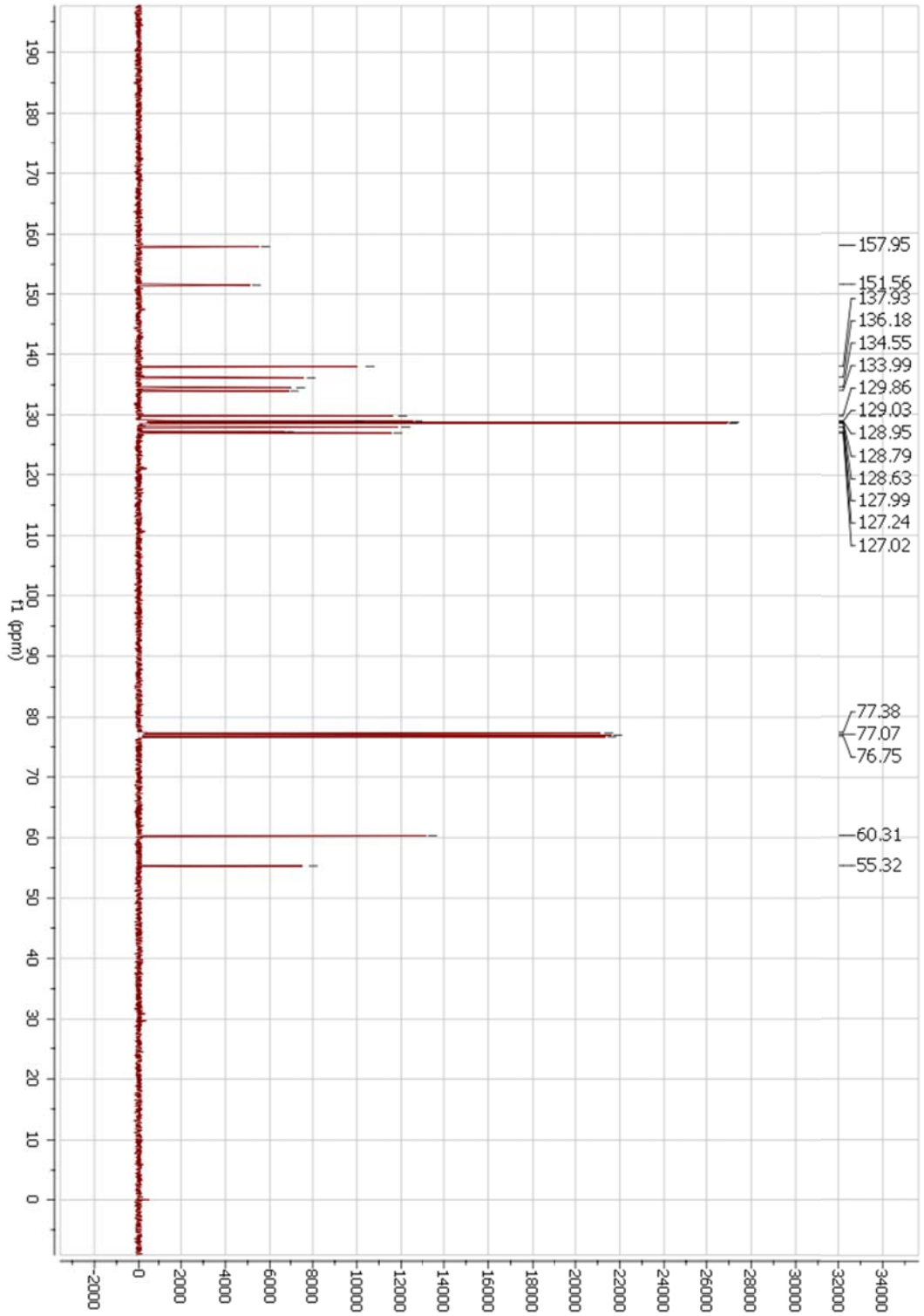
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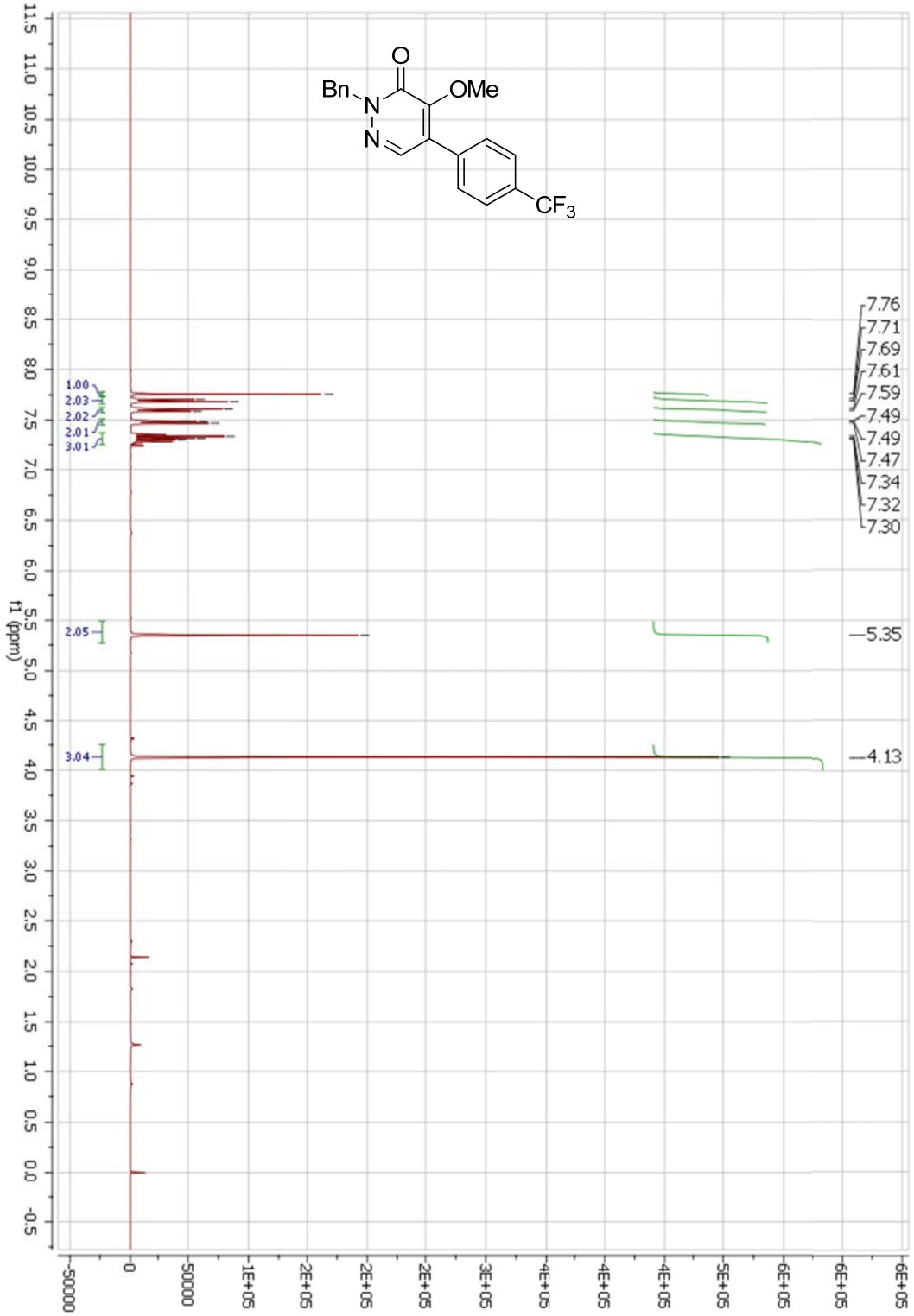
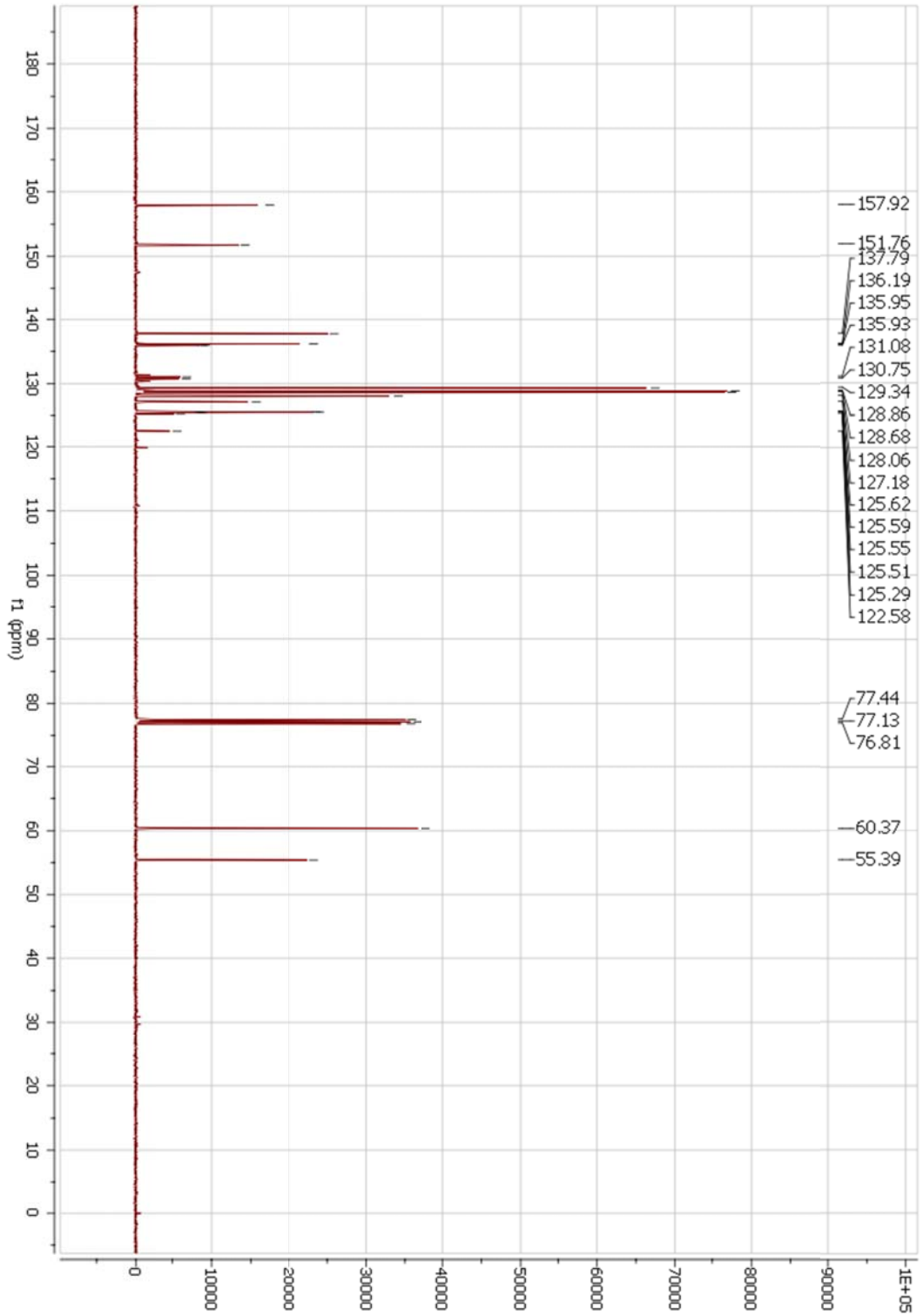
128.95
128.79
128.63
127.99
127.24
127.02
77.38
77.07
76.75
60.31
55.32
f1 (ppm)

2-Benzyl-4-methoxy-5-(4-(trifluoromethyl)phenyl)pyridazin-3(2*H*)-one (**4f**)

^{1}H-NMR



^{13}C-NMR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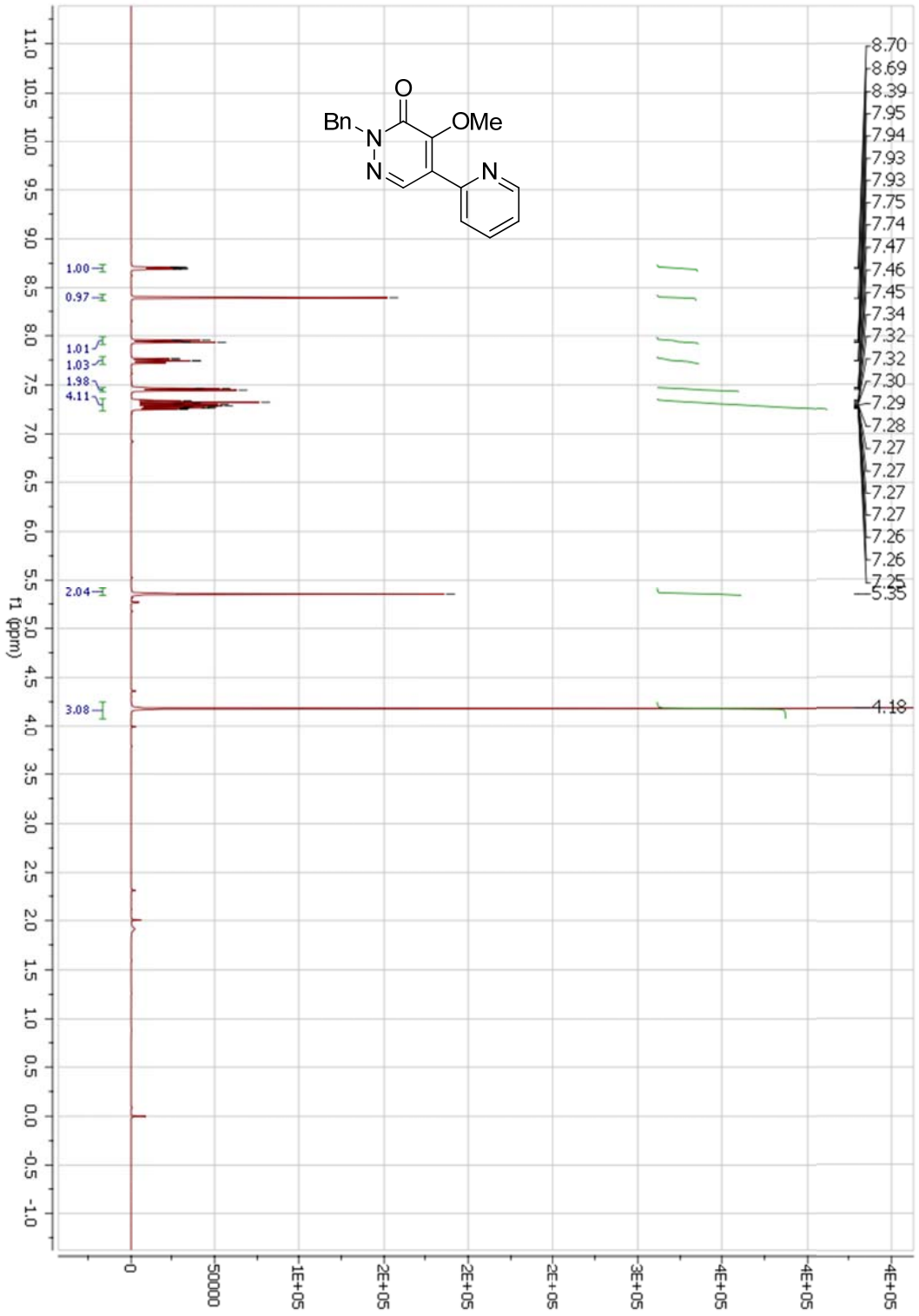
128.68
128.06
127.18
125.62
125.59
125.55
125.51
125.29
122.58
77.44
77.13
76.81
60.37
55.39
f1 (ppm)

2-Benzyl-4-methoxy-5-(pyridin-2-yl)pyridazin-3(2*H*)-one (**4g**)

^{1}H-NMR



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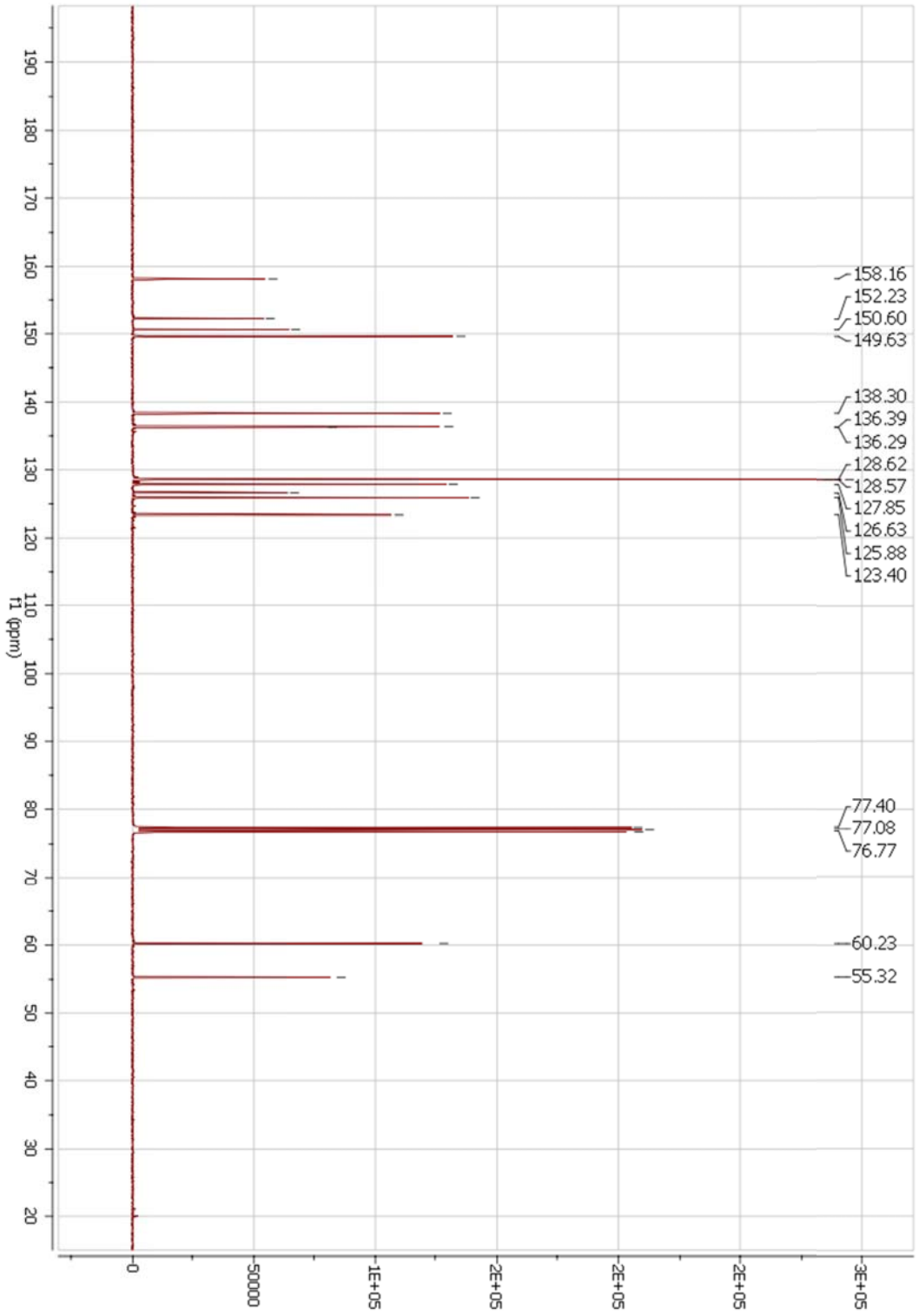
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152.23
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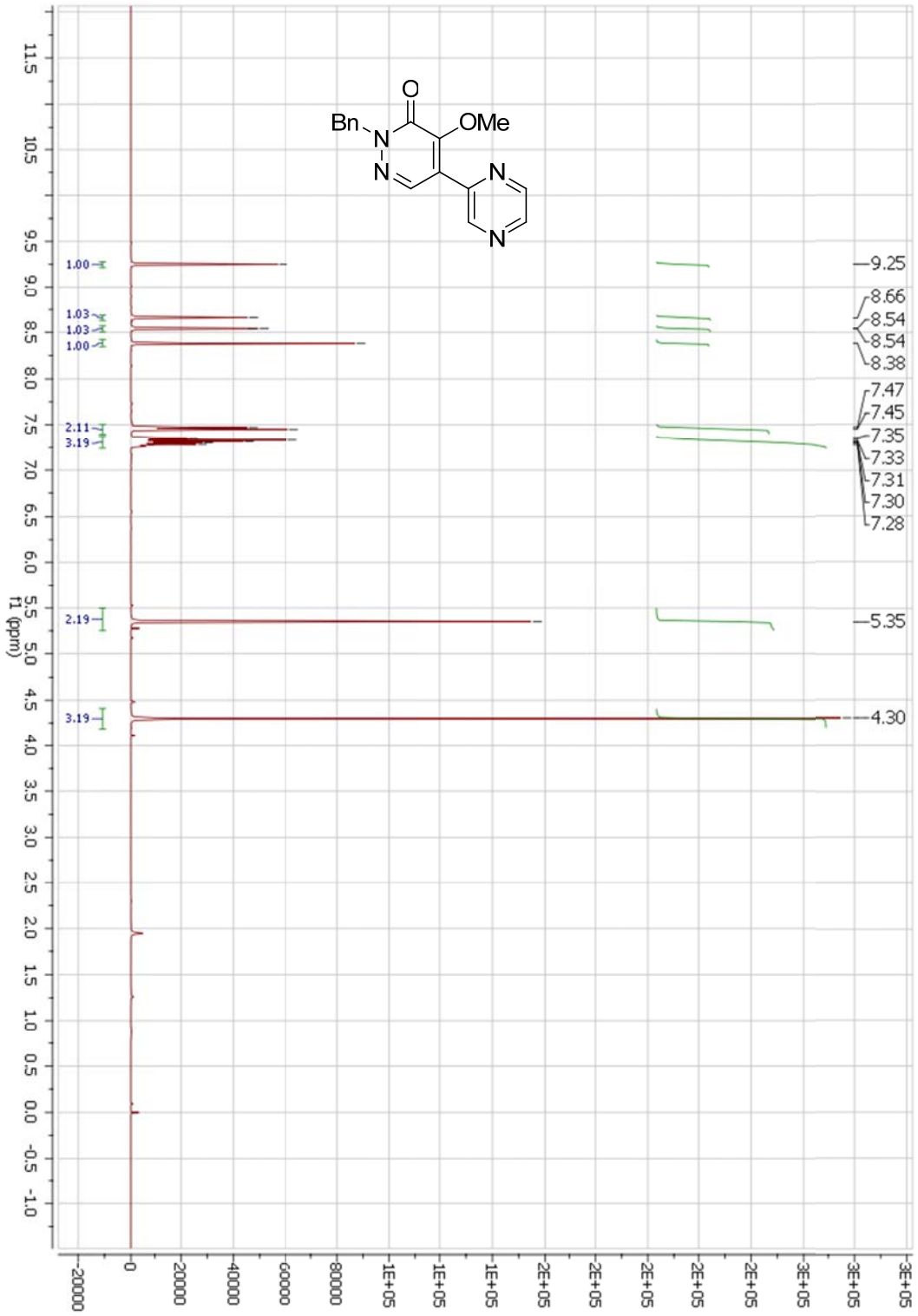
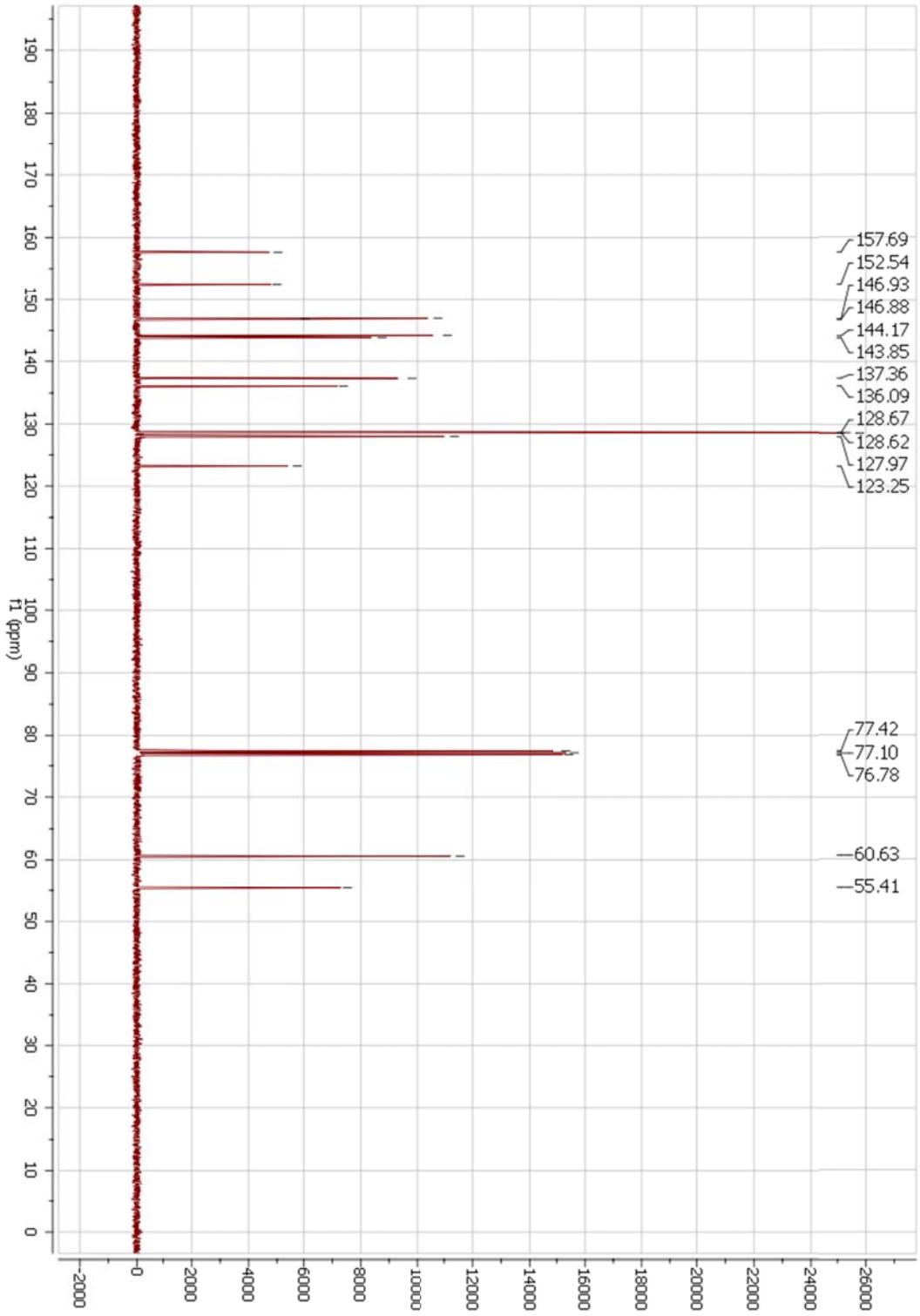
149.63
138.30
136.39
136.29
128.62
128.57
127.85
126.63
125.88
123.40
77.40
77.08
76.77
60.23
55.32
f1 (ppm)

2-Benzyl-4-methoxy-5-(pyrazin-2-yl)pyridazin-3(2*H*)-one (**4i**)

^{1}H-NMR

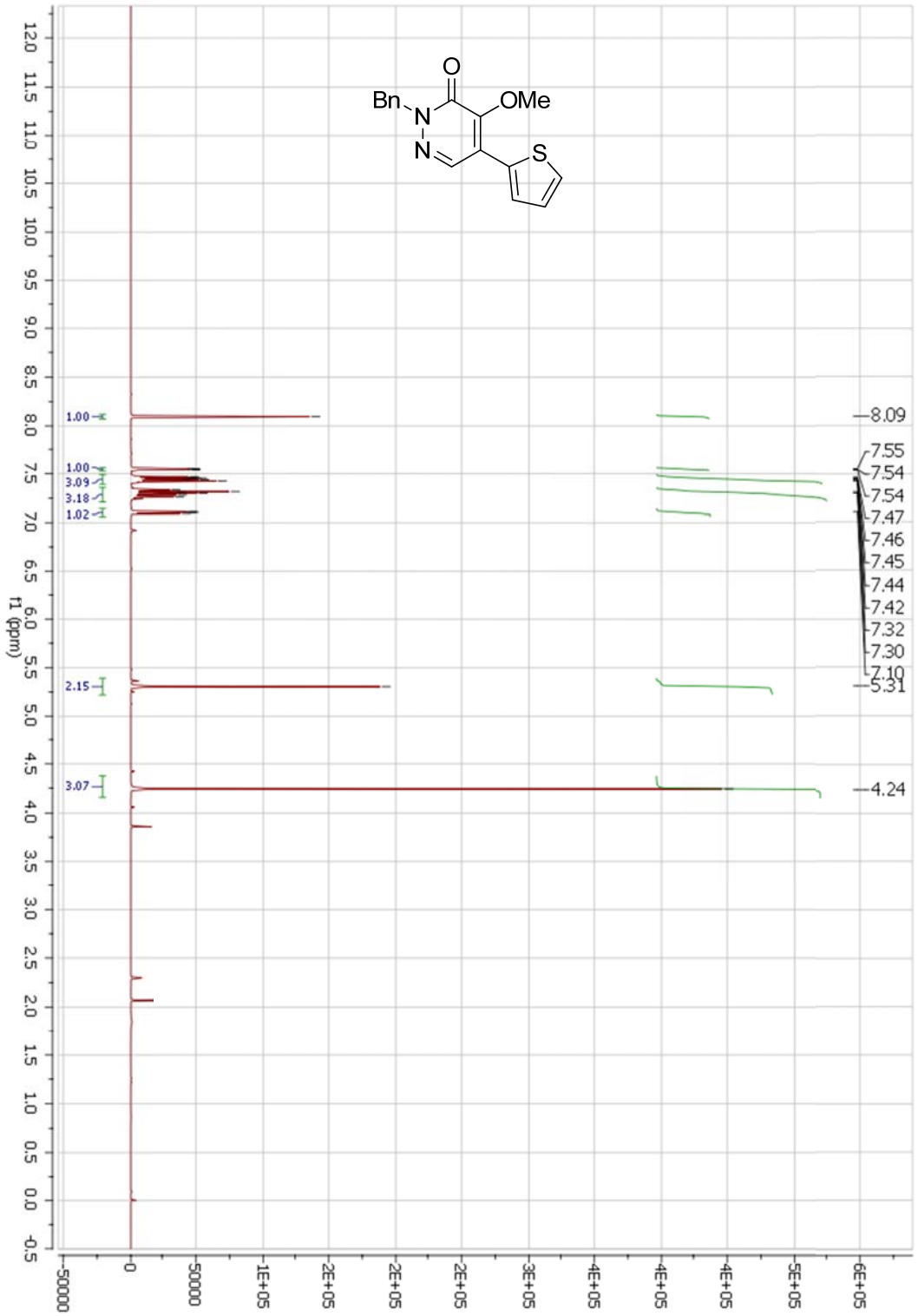


^{13}C-NMR

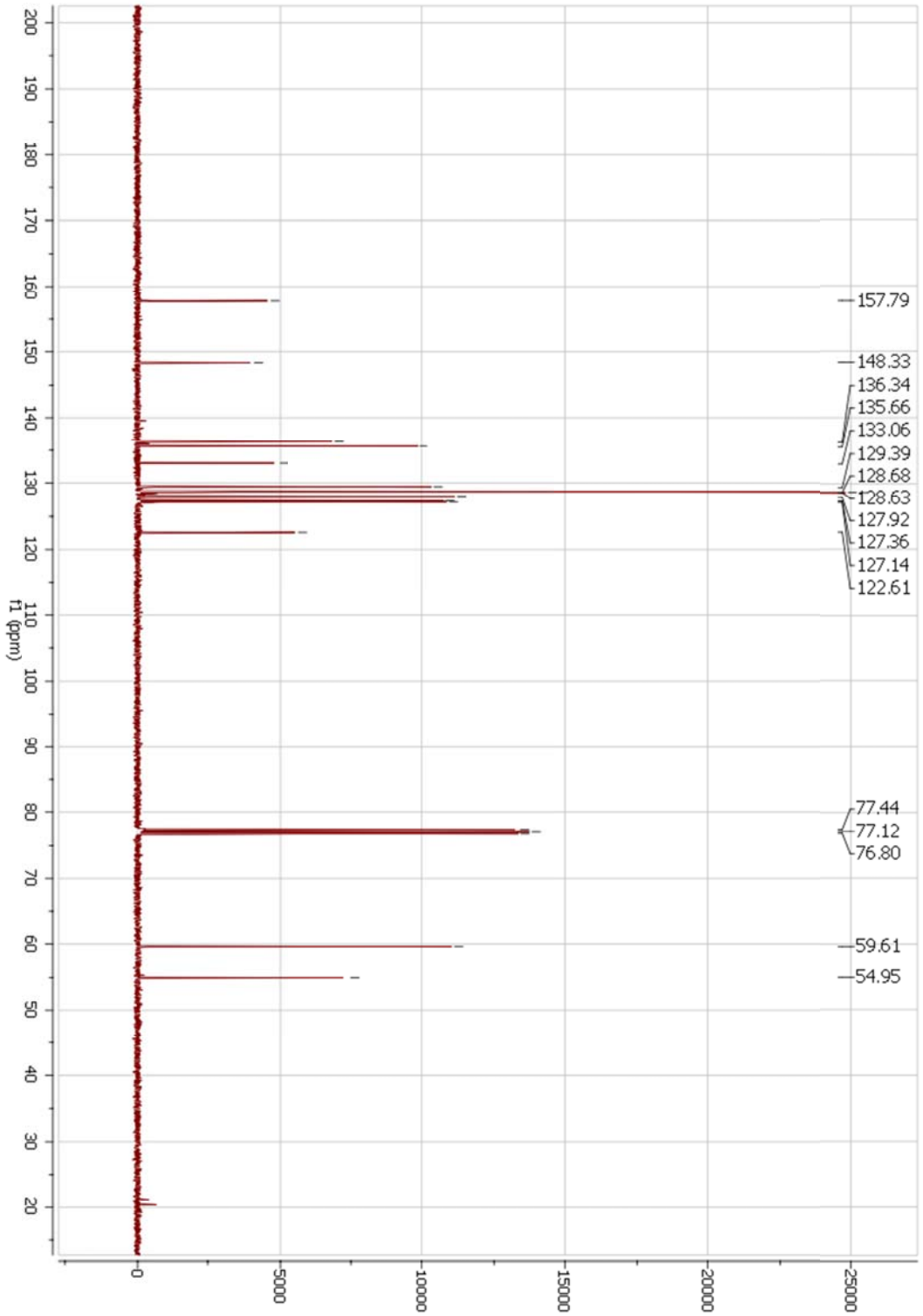

157.69
152.54
146.93
146.88
144.17
143.85
137.36
136.09
128.67
128.62
127.97
123.25
77.42
77.10
76.78
60.63
55.41
f1 (ppm)

2-Benzyl-4-methoxy-5-(thiophen-2-yl)pyridazin-3(2*H*)-one (**4j**)

^{1}H-NMR

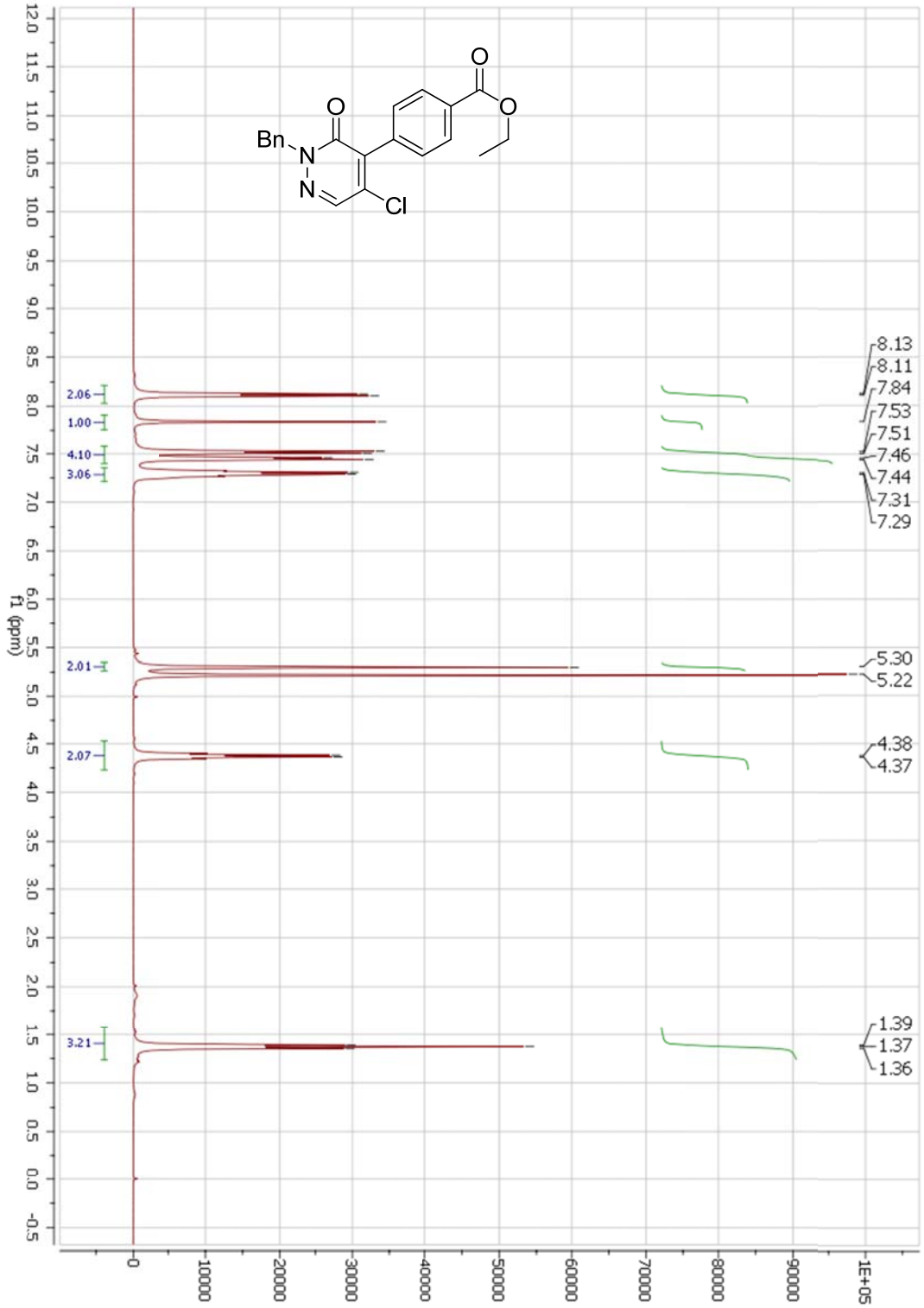


^{13}C-NMR

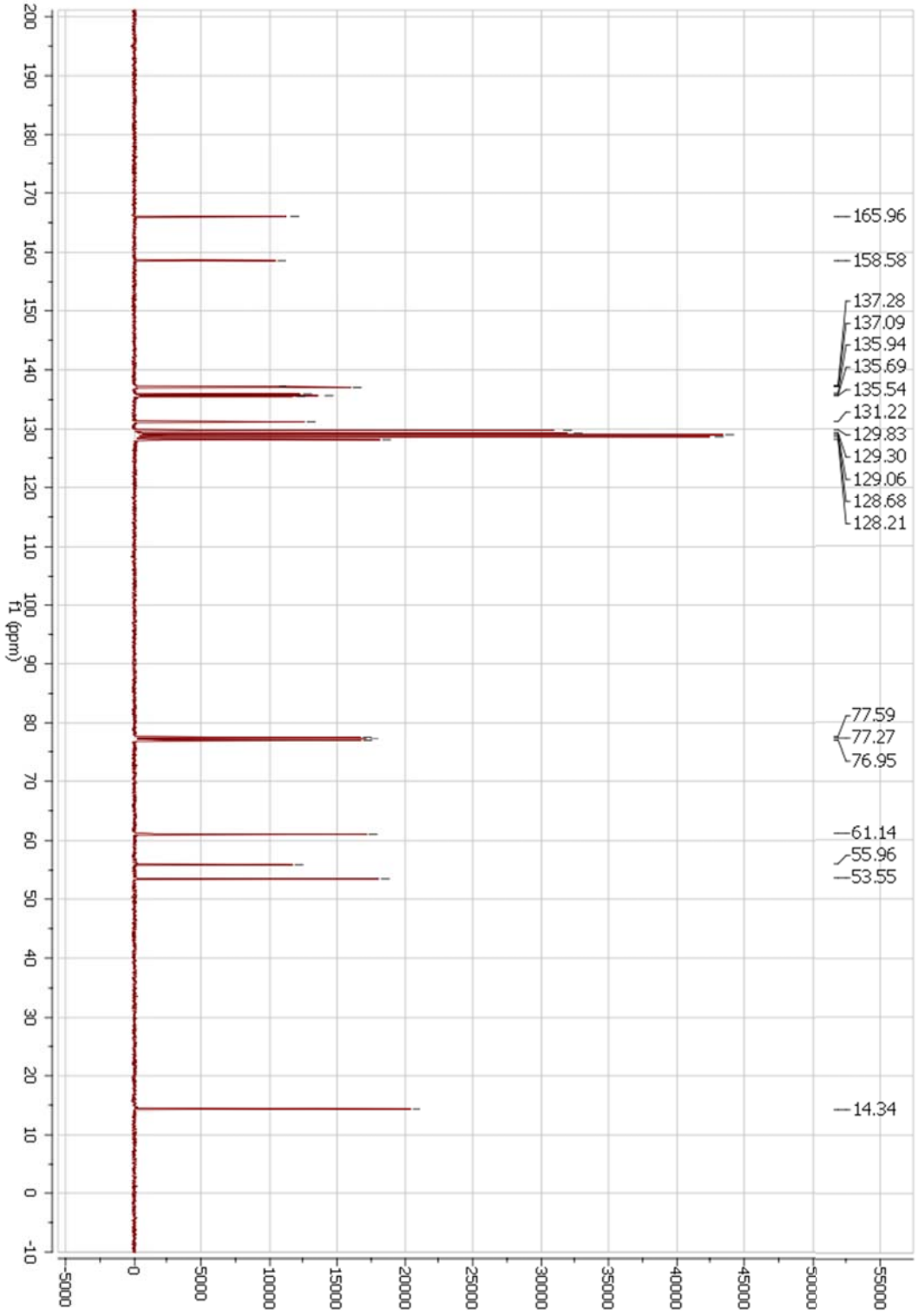

157.79
148.33
136.34
135.66
133.06
129.39
128.68
128.63
127.92
127.36
127.14
122.61
77.44
77.12
76.80
59.61
54.95
f1 (ppm)

Ethyl 4-(2-benzyl-5-chloro-3-oxo-2,3-dihydropyridazin-4-yl)benzoate (**7a**)

^{1}H-NMR

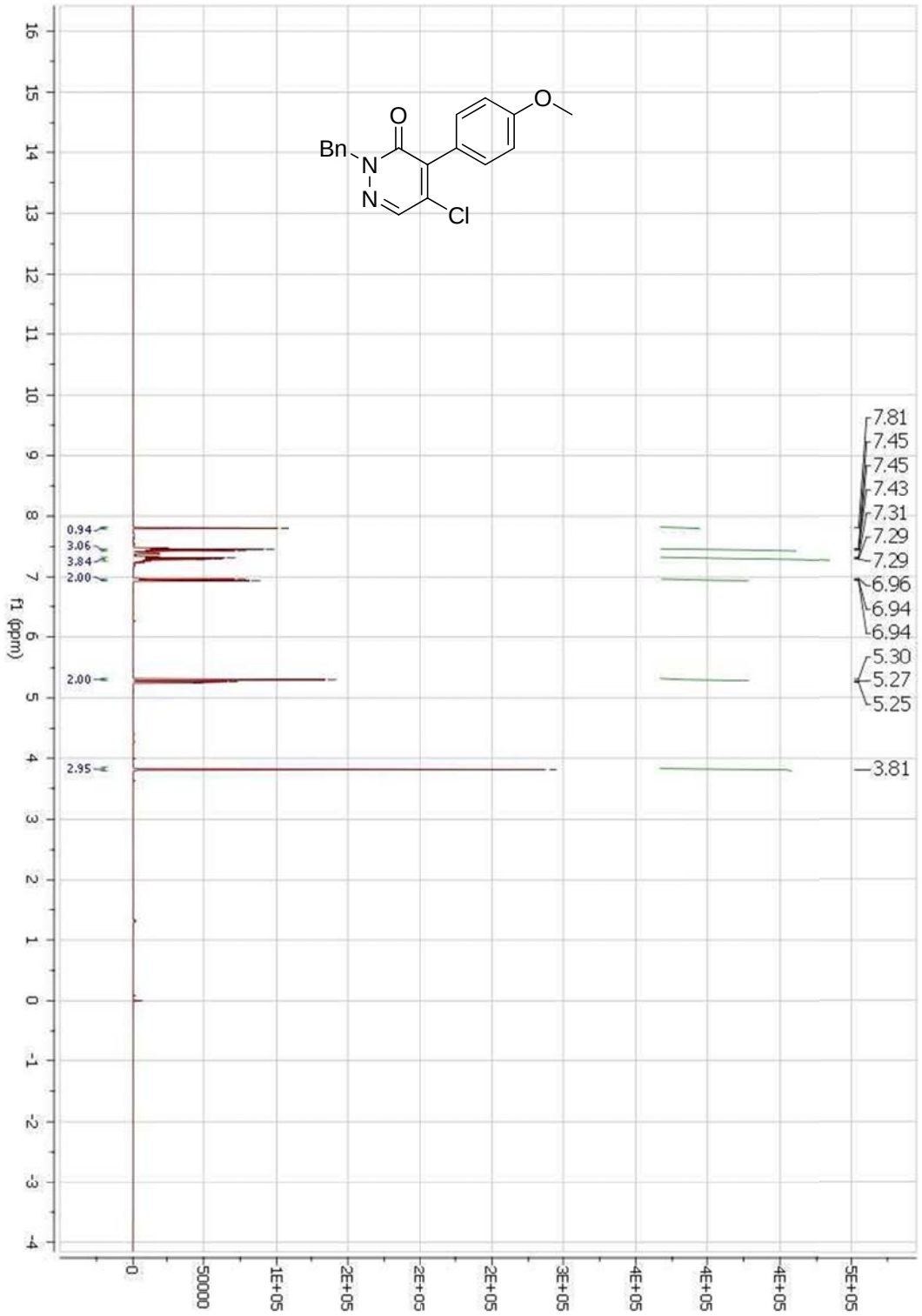


^{13}C-NMR

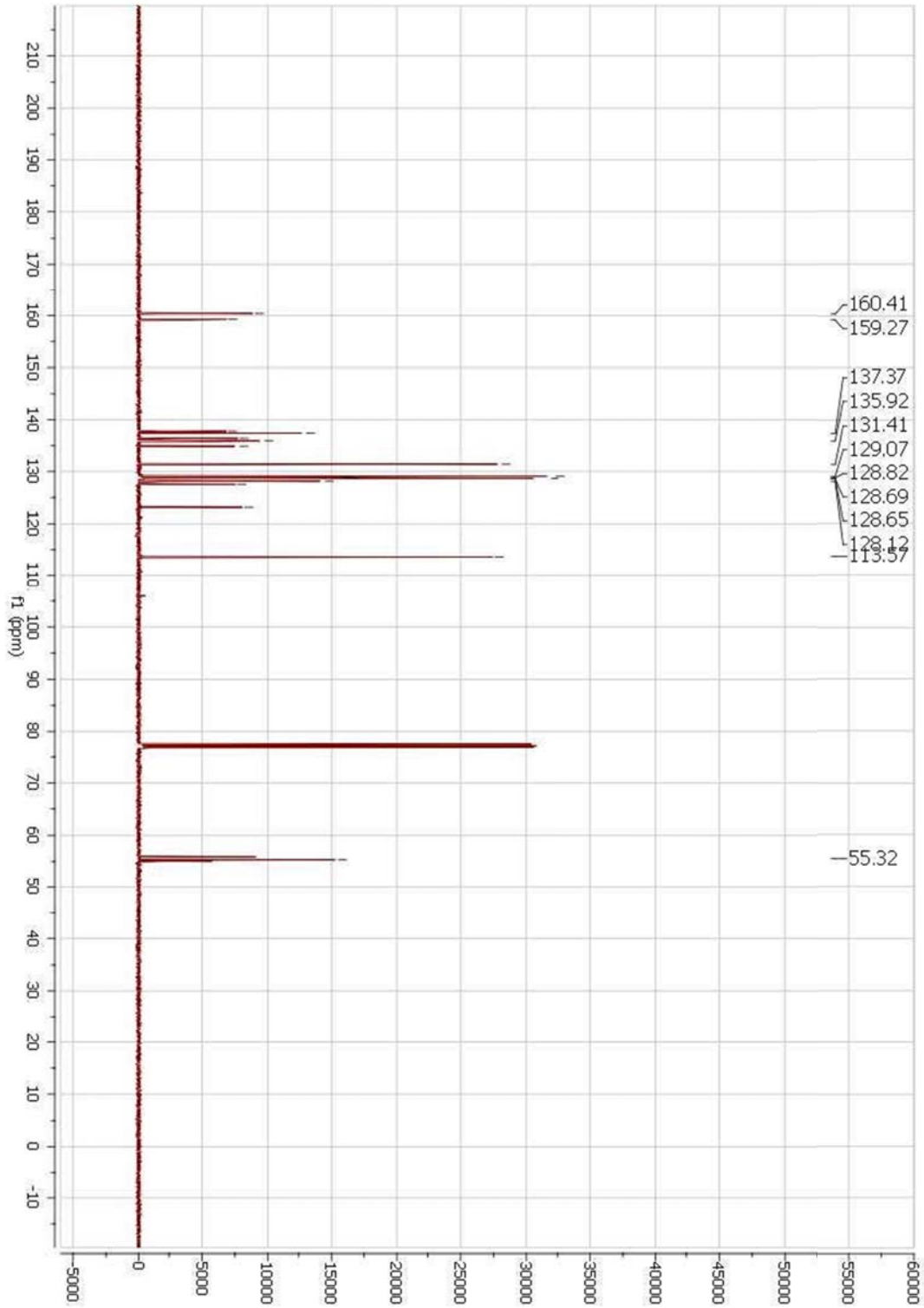

165.96
158.58
137.28
137.09
135.94
135.69
135.54
131.22
129.83
129.30
129.06
128.68
128.21
77.59
77.27
76.95
61.14
55.96
53.55
14.34
f1 (ppm)

2-Benzyl-5-chloro-4-(4-methoxyphenyl)pyridazin-3(2*H*)-one (**7b**)

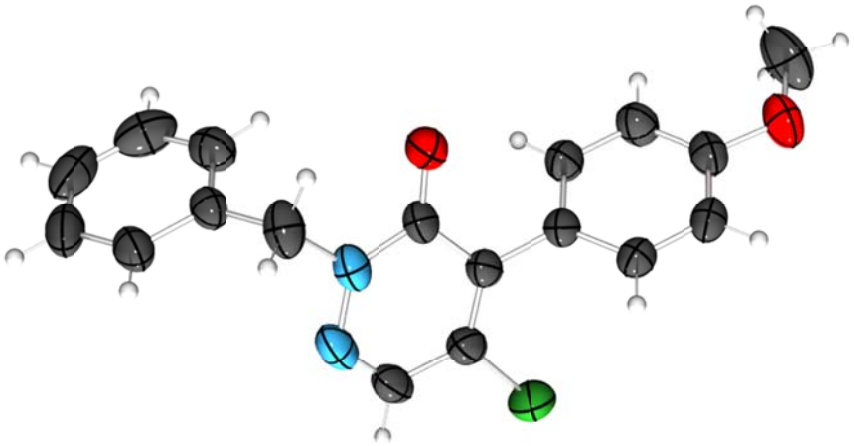
^{1}H-NMR



^{13}C-NMR


160.41
159.27
137.37
135.92
131.41
129.07
128.82
128.69
128.65
128.12
113.57
55.32
f1 (ppm)

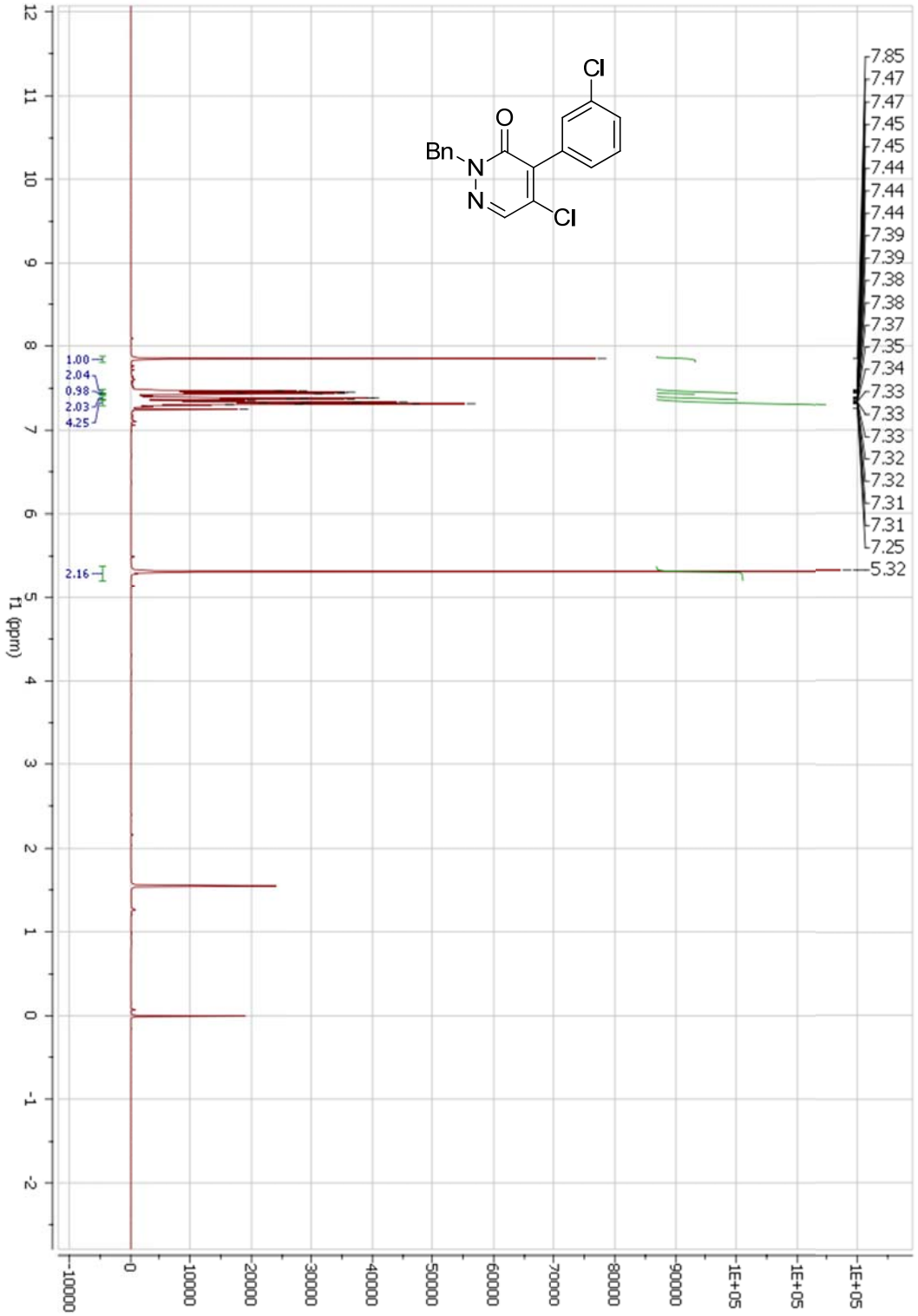
XRD structure



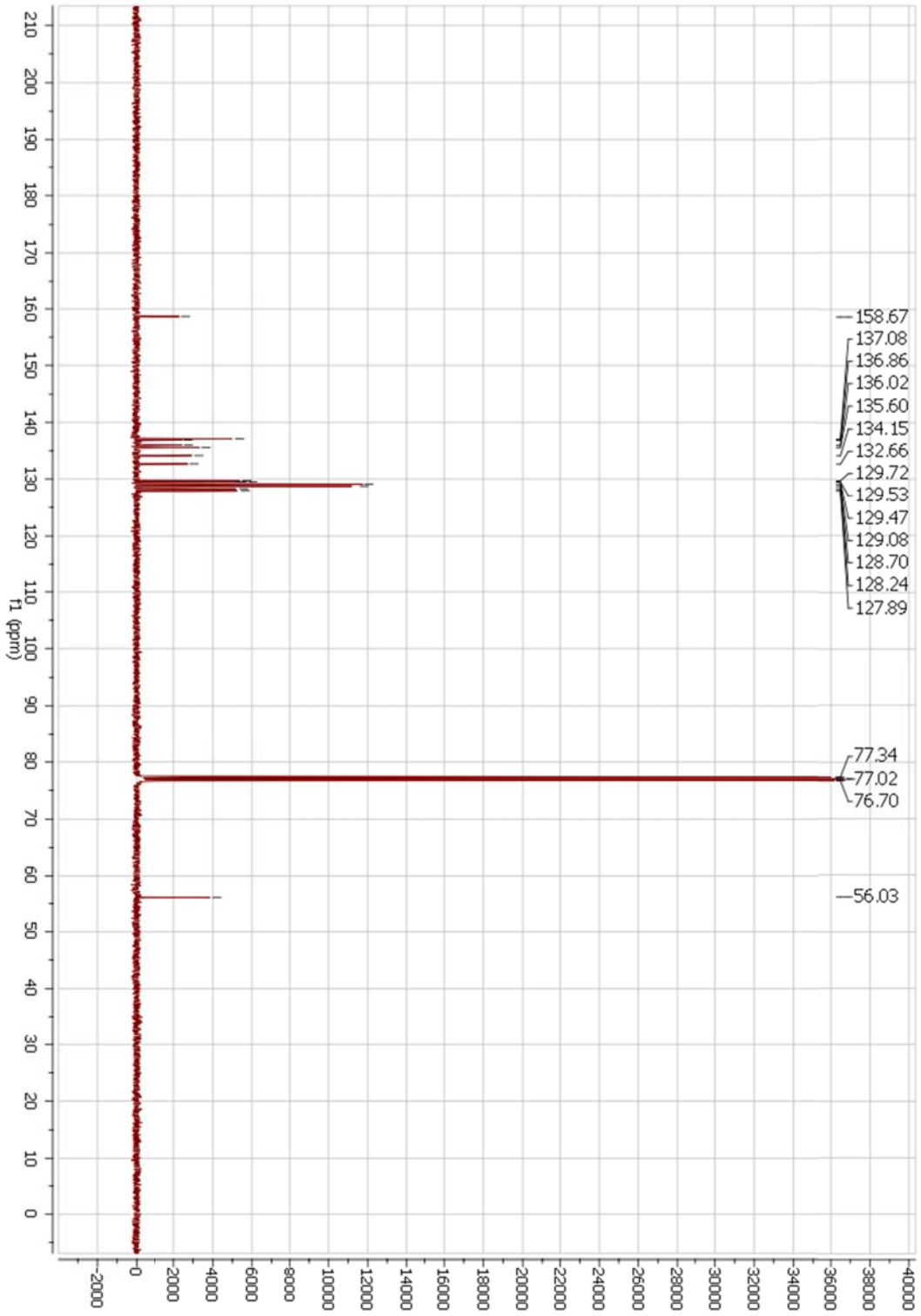
ORTEP-style plot of **7b** (C: grey, N: blue, O: red, F: light green, yellow, Cl: green, I: Purple). Thermal ellipsoids are drawn at 30% probability level, hydrogen atoms are drawn as spheres of 0.15 Å radius.

2-Benzyl-5-chloro-4-(3-chlorophenyl)pyridazin-3(2*H*)-one (**7d**)

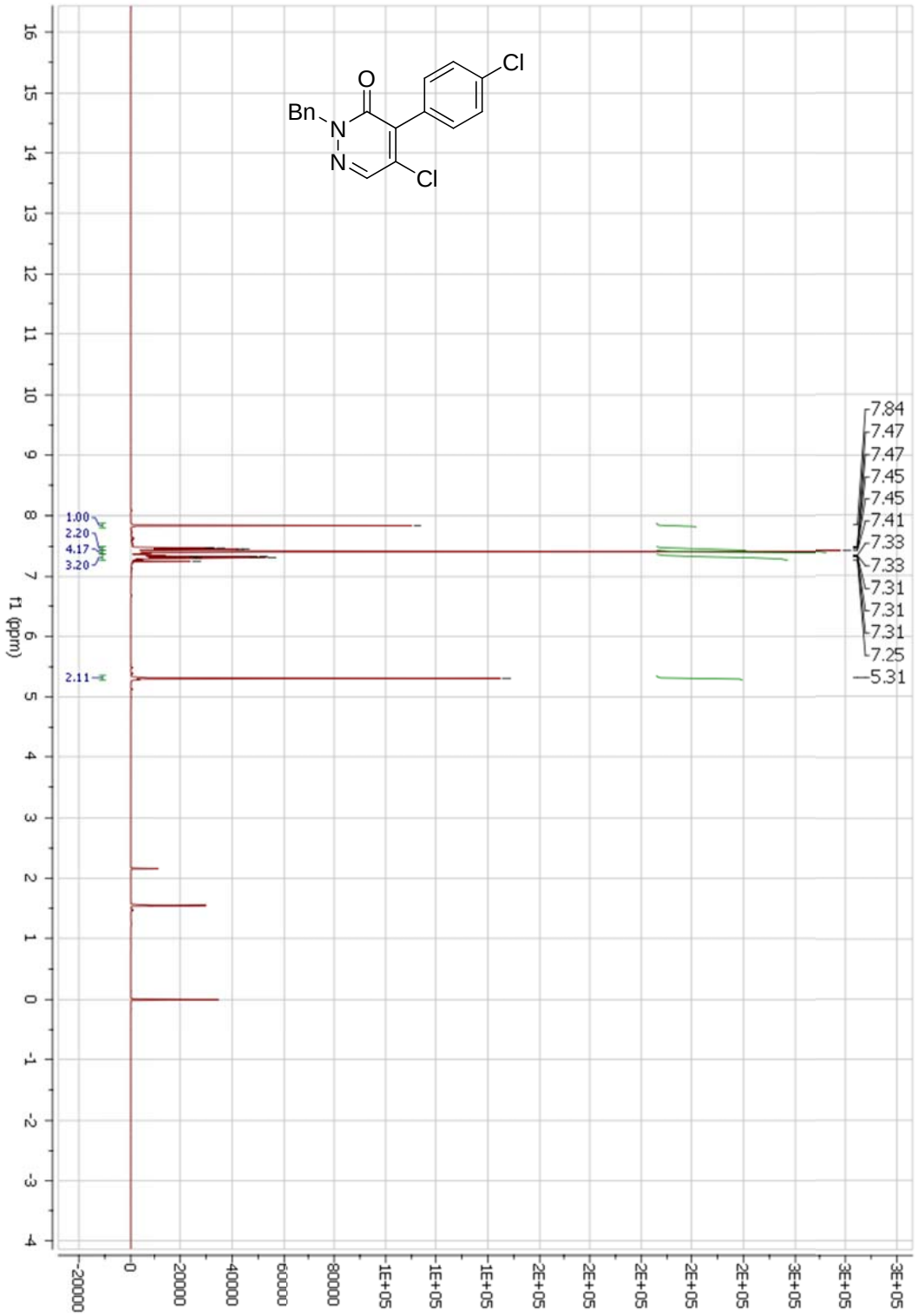
^{1}H-NMR



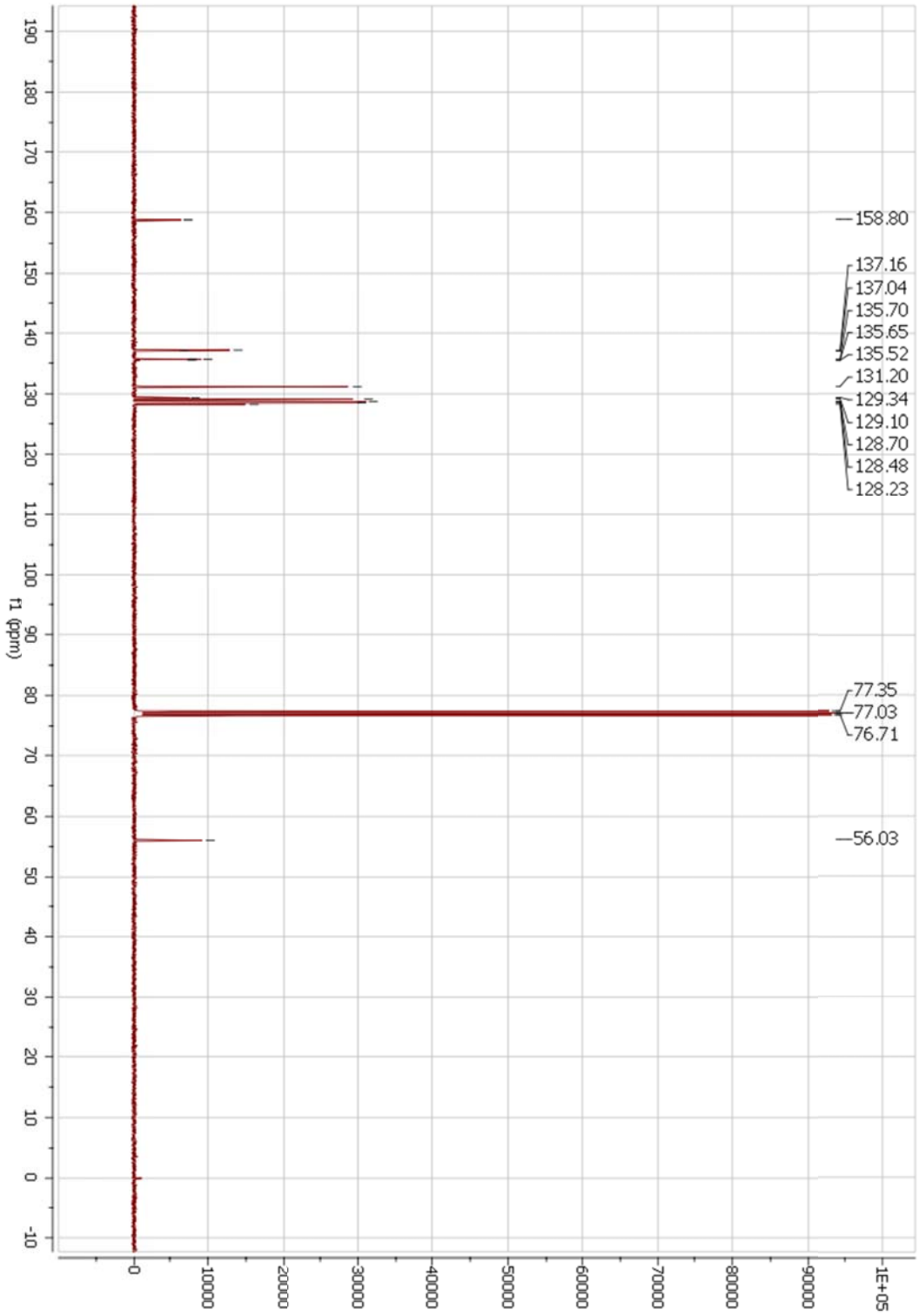
^{13}C-NMR


158.67
137.08
136.86
136.02
135.60
134.15
132.66
129.72
129.53
129.47
129.08
128.70
128.24
127.89
77.34
77.02
76.70
56.03
f1 (ppm)

2-Benzyl-5-chloro-4-(4-chlorophenyl)pyridazin-3(2*H*)-one (**7e**)
^{1}H-NMR

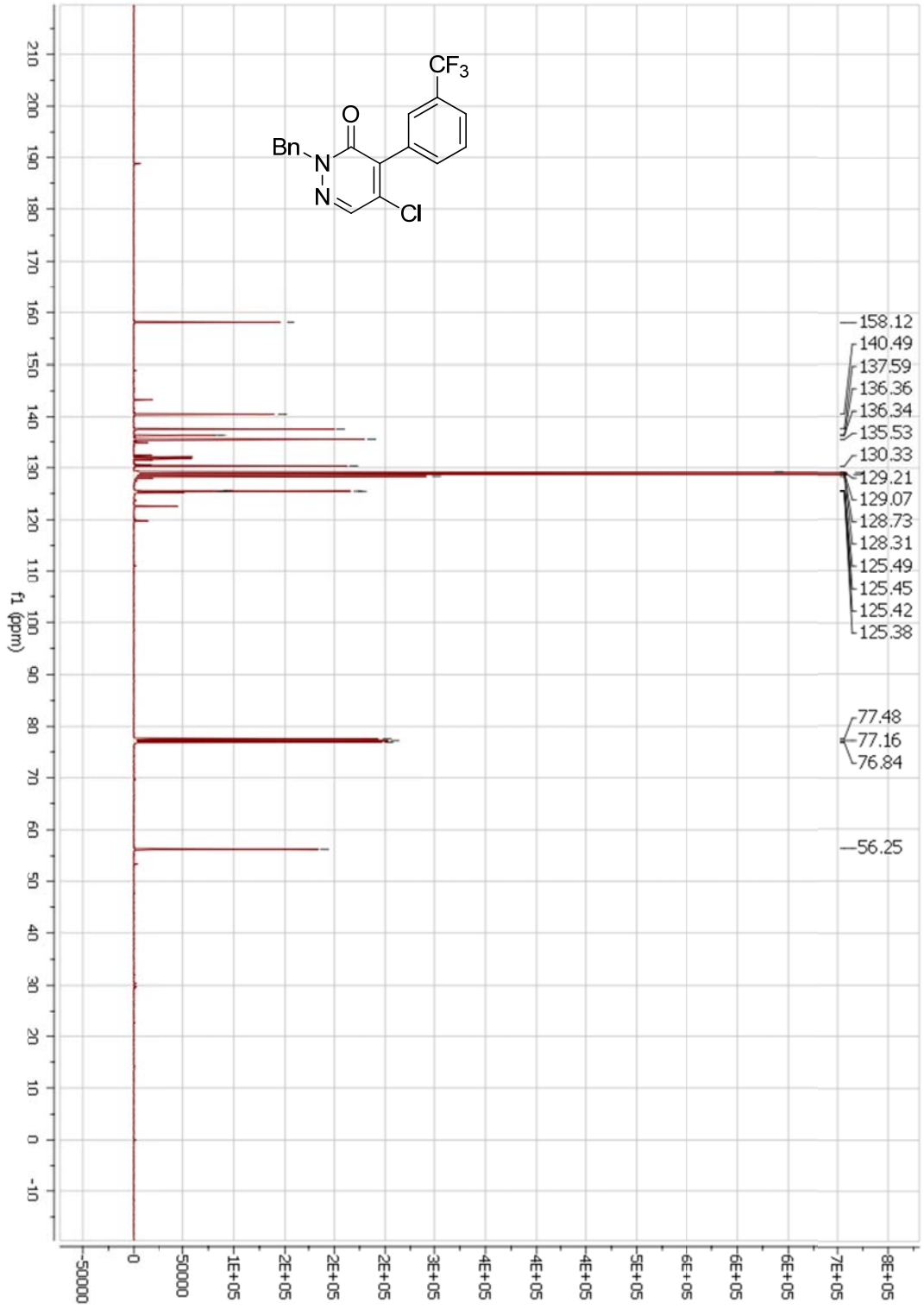


^{13}C-NMR

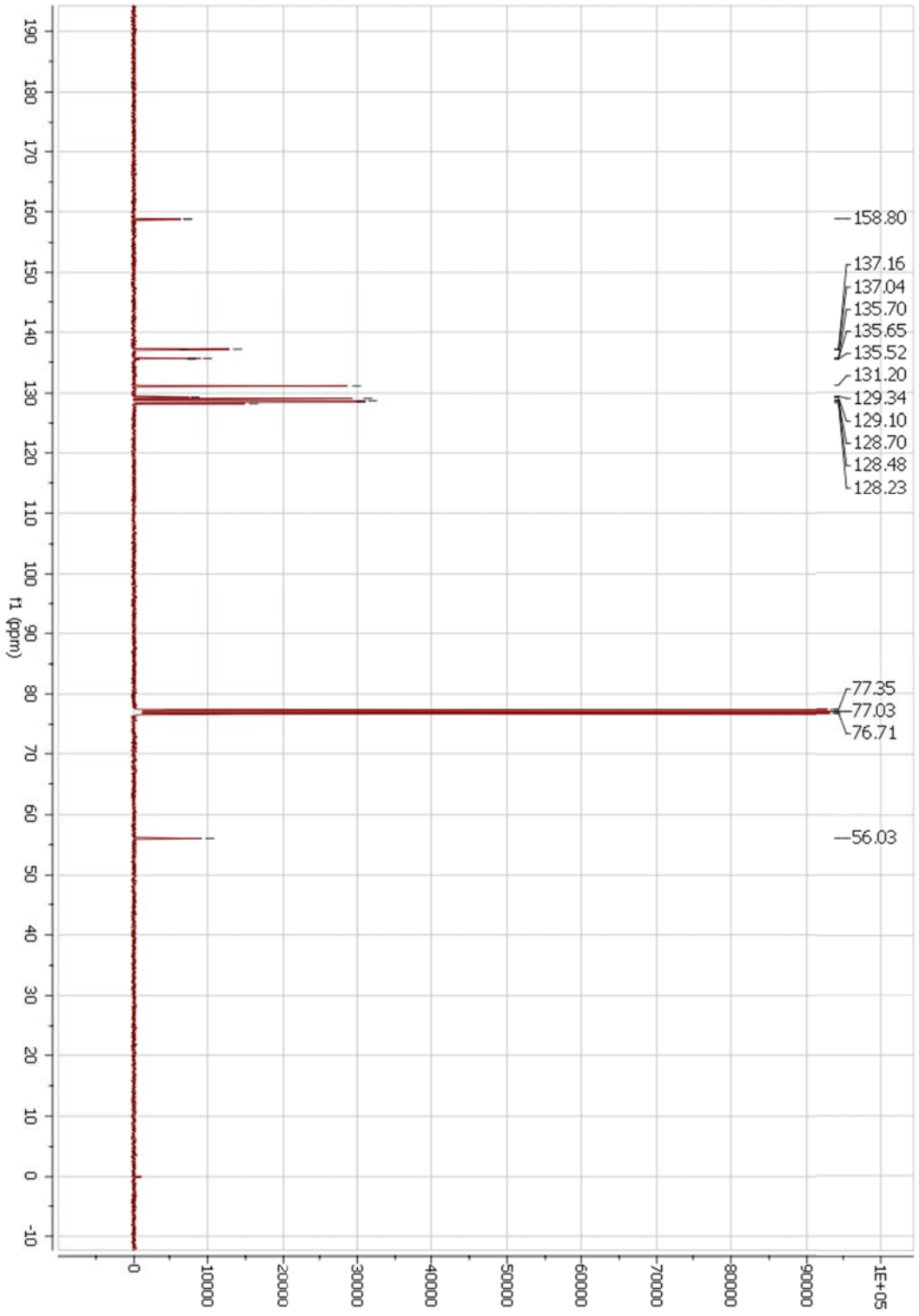

158.80
137.16
137.04
135.70
135.65
135.52
131.20
129.34
129.10
128.70
128.48
128.23
77.35
77.03
76.71
56.03
f1 (ppm)

2-Benzyl-5-chloro-4-(3-(trifluoromethyl)phenyl)pyridazin-3(2*H*)-one (**7f**)

^{1}H-NMR

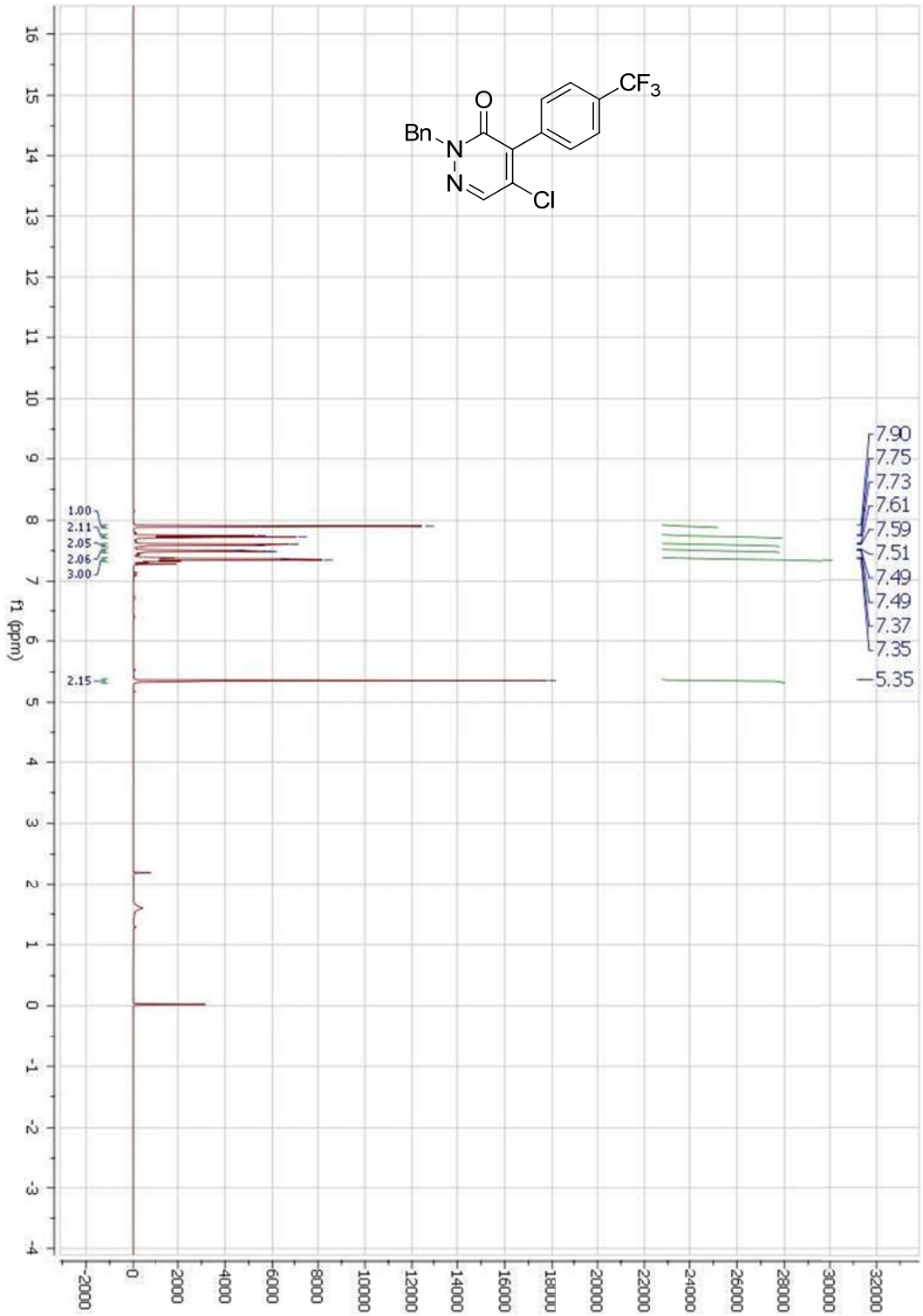


^{13}C-NMR


158.80
137.16
137.04
135.70
135.65
135.52
131.20
129.34
129.10
128.70
128.48
128.23
77.35
77.03
76.71
56.03
f1 (ppm)

2-Benzyl-5-chloro-4-(4-(trifluoromethyl)phenyl)pyridazin-3(2*H*)-one (**7g**)

^{1}H-NMR

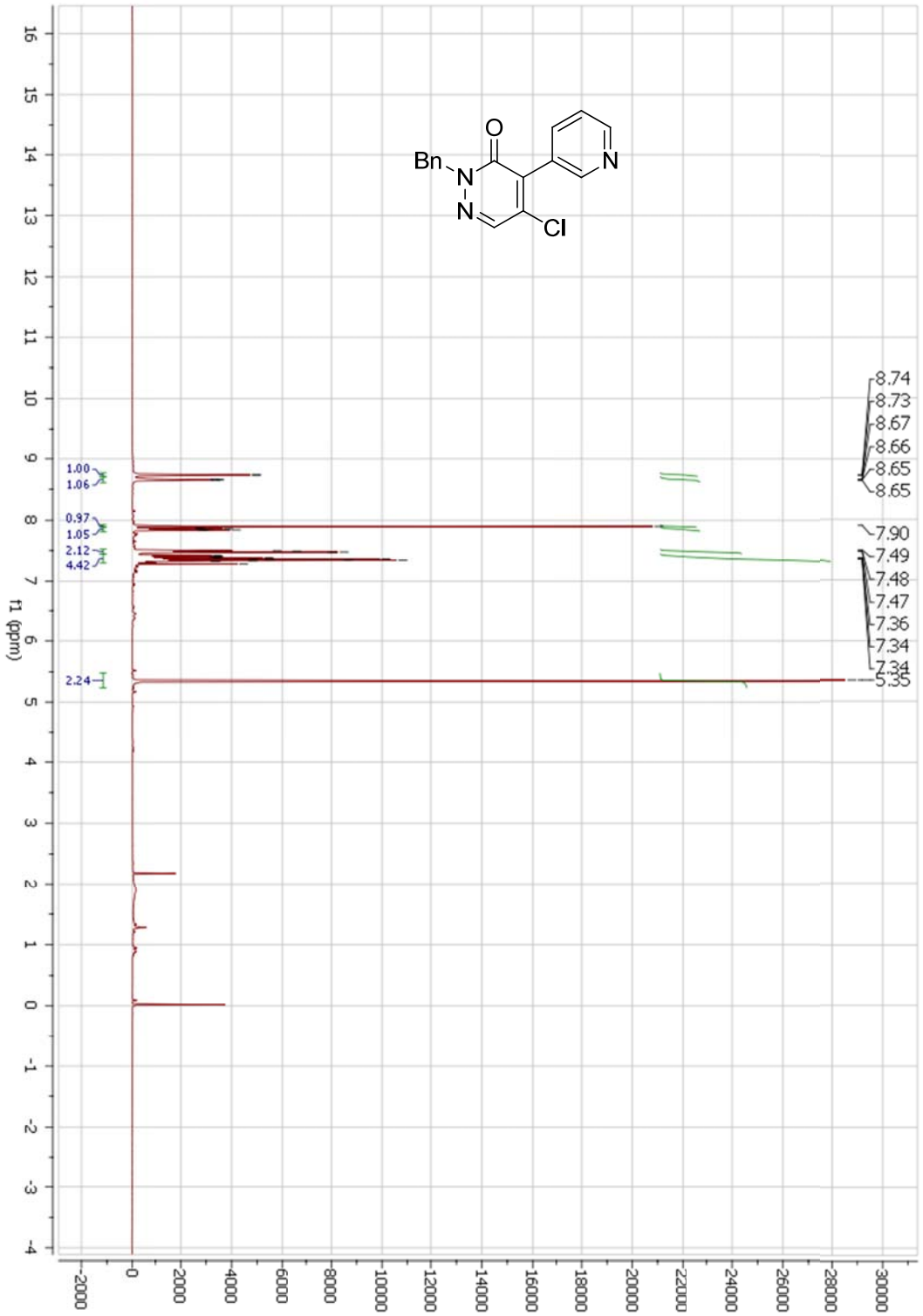


^{13}C-NMR

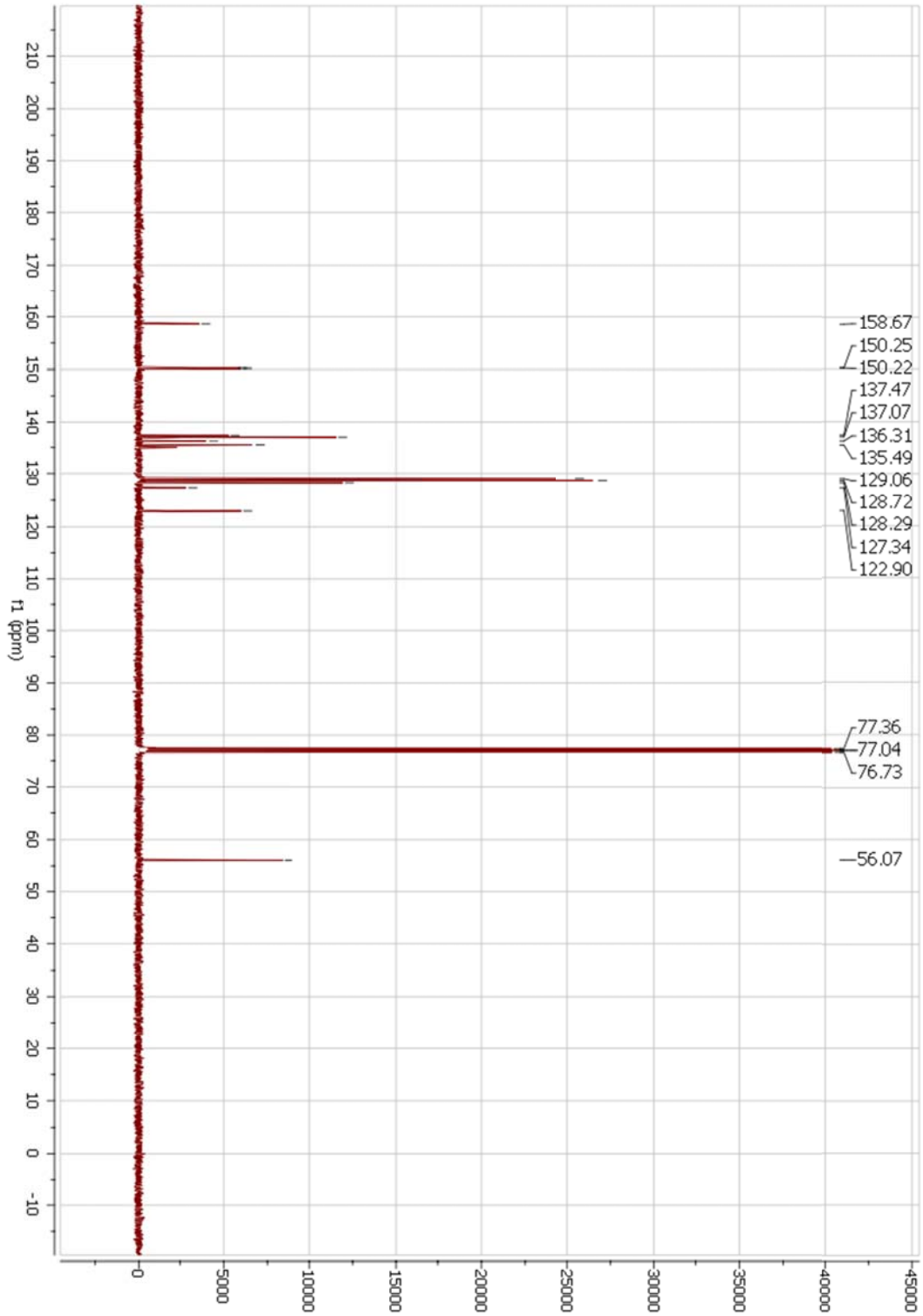

158.61
137.07
136.85
136.14
135.51
130.21
129.13
128.71
128.29
125.20
125.17
77.34
77.02
76.70
56.09
f1 (ppm)

2-Benzyl-5-chloro-4-(pyridin-3-yl)pyridazin-3(2*H*)-one (**7i**)

^{1}H-NMR

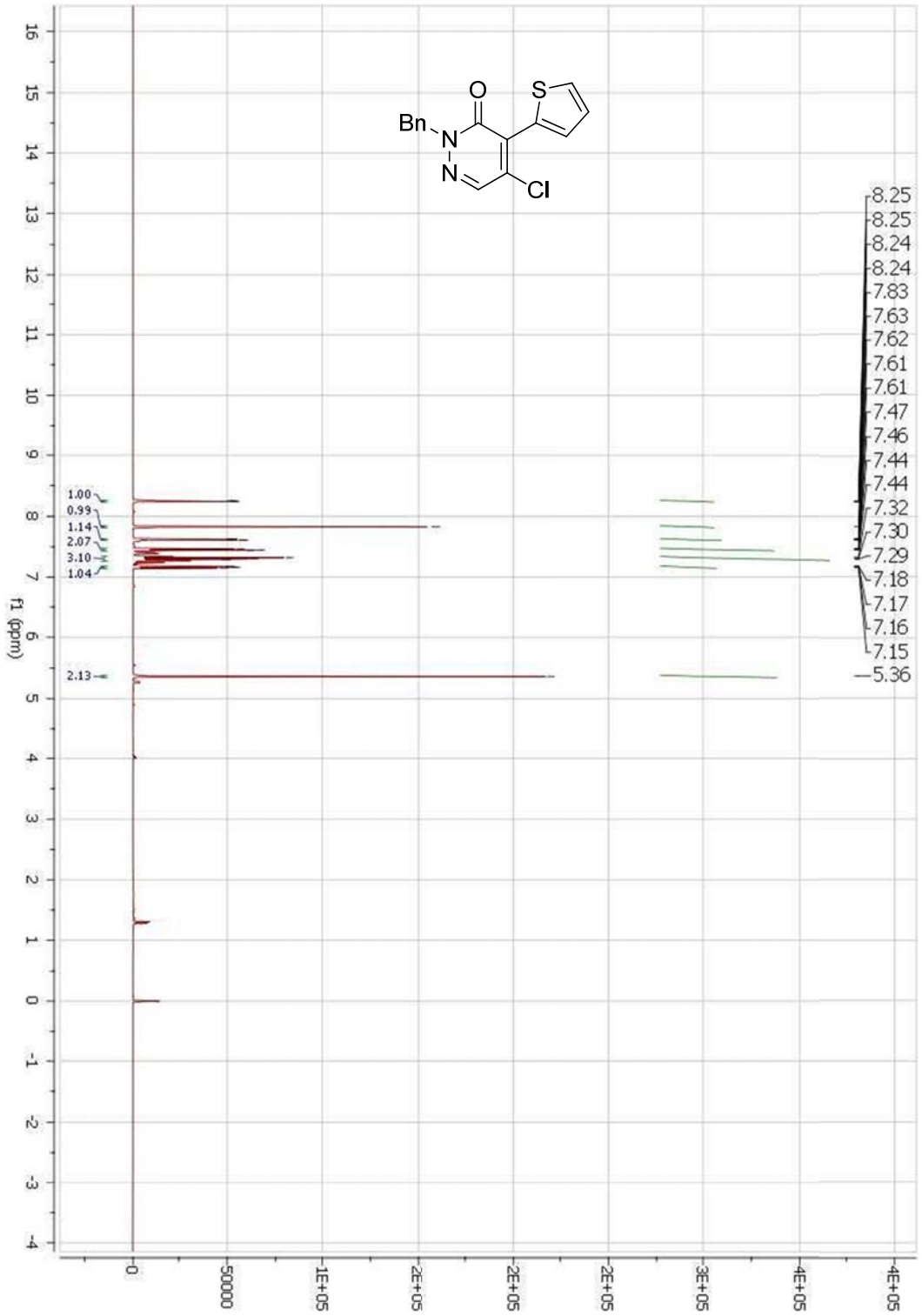


^{13}C-NMR

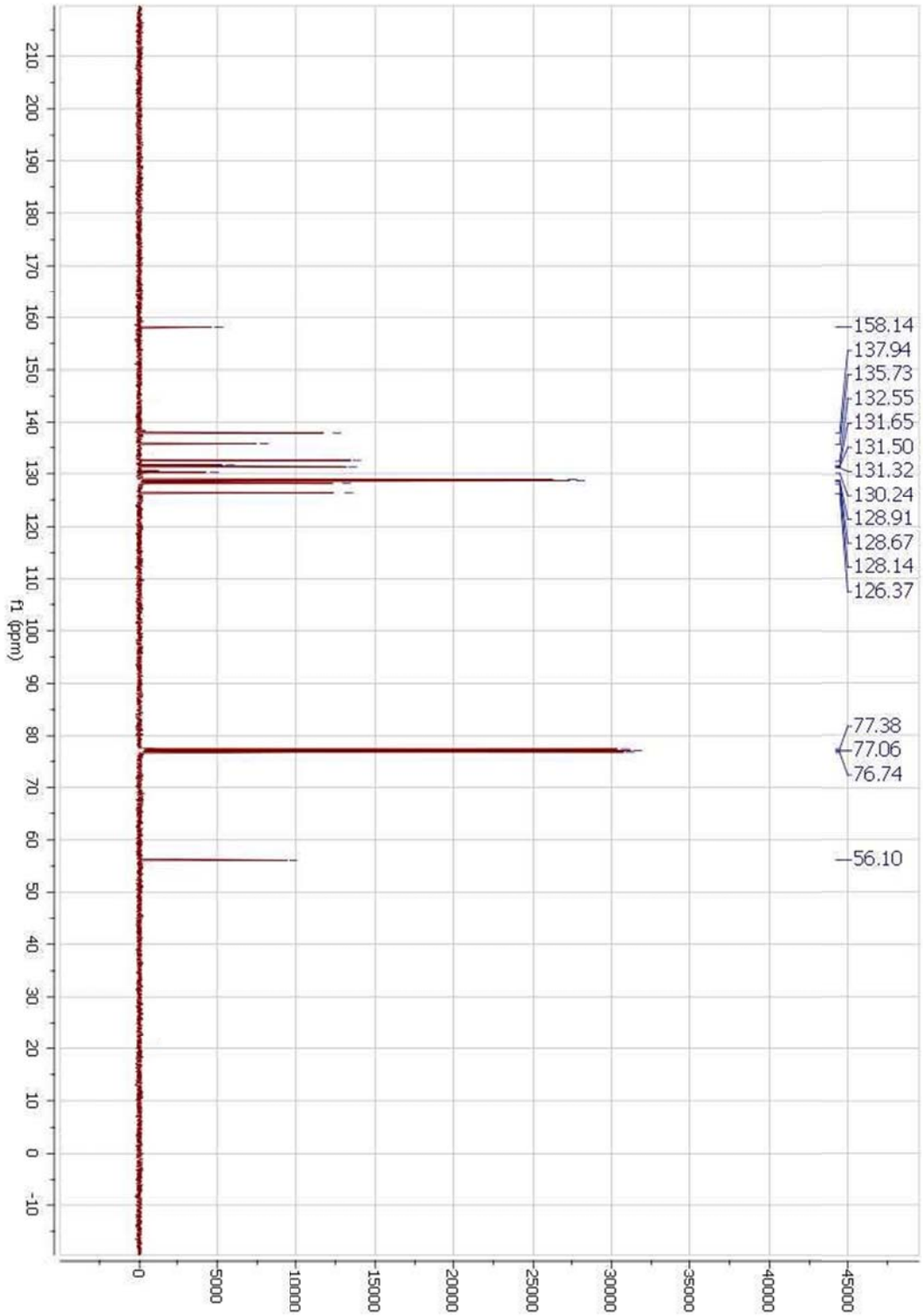

158.67
150.25
150.22
137.47
137.07
136.31
135.49
129.06
128.72
128.29
127.34
122.90
77.36
77.04
76.73
56.07
f1 (ppm)

2-Benzyl-5-chloro-4-(thien-2-yl)pyridazin-3(2*H*)-one (**7k**)

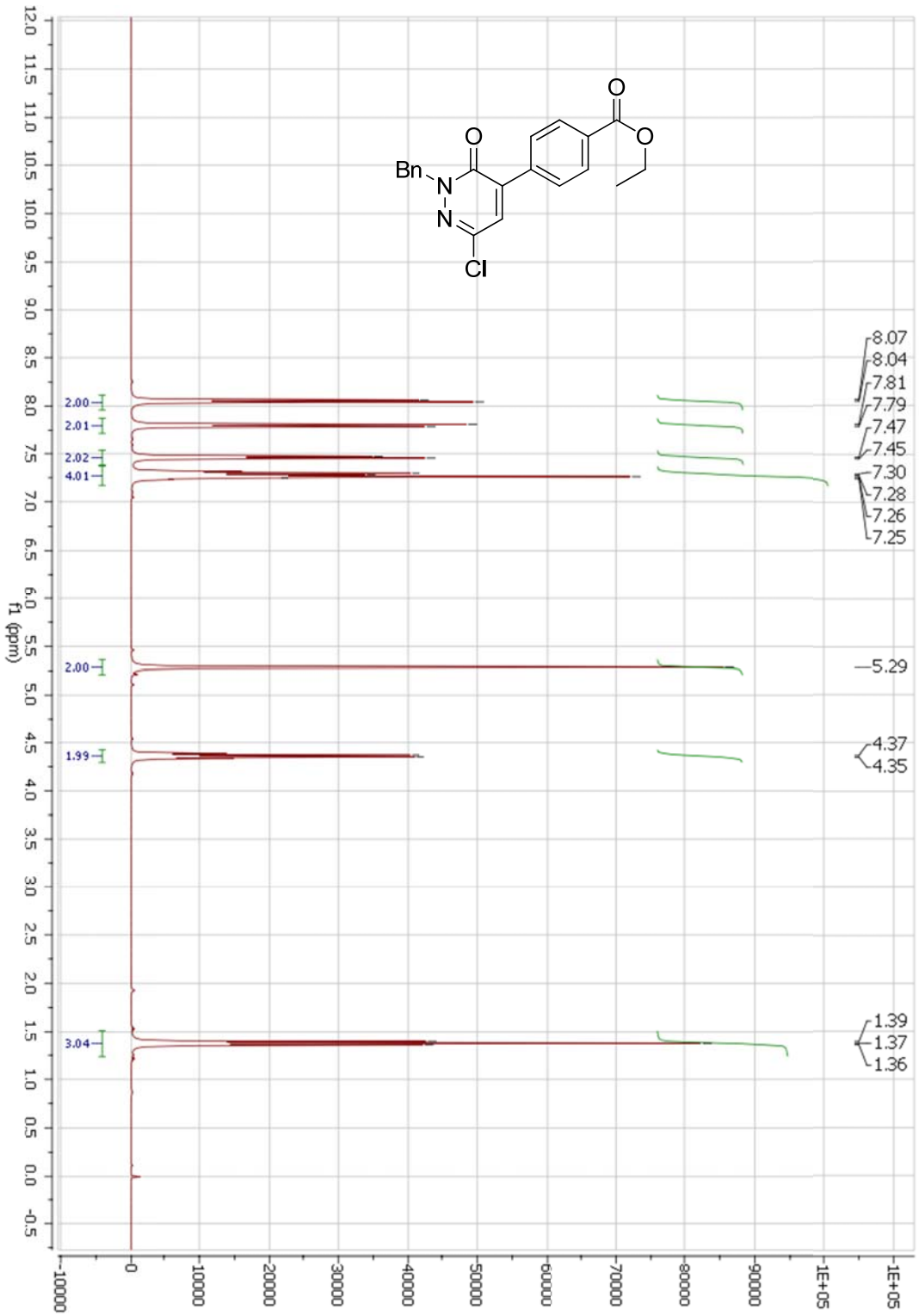
^{1}H-NMR



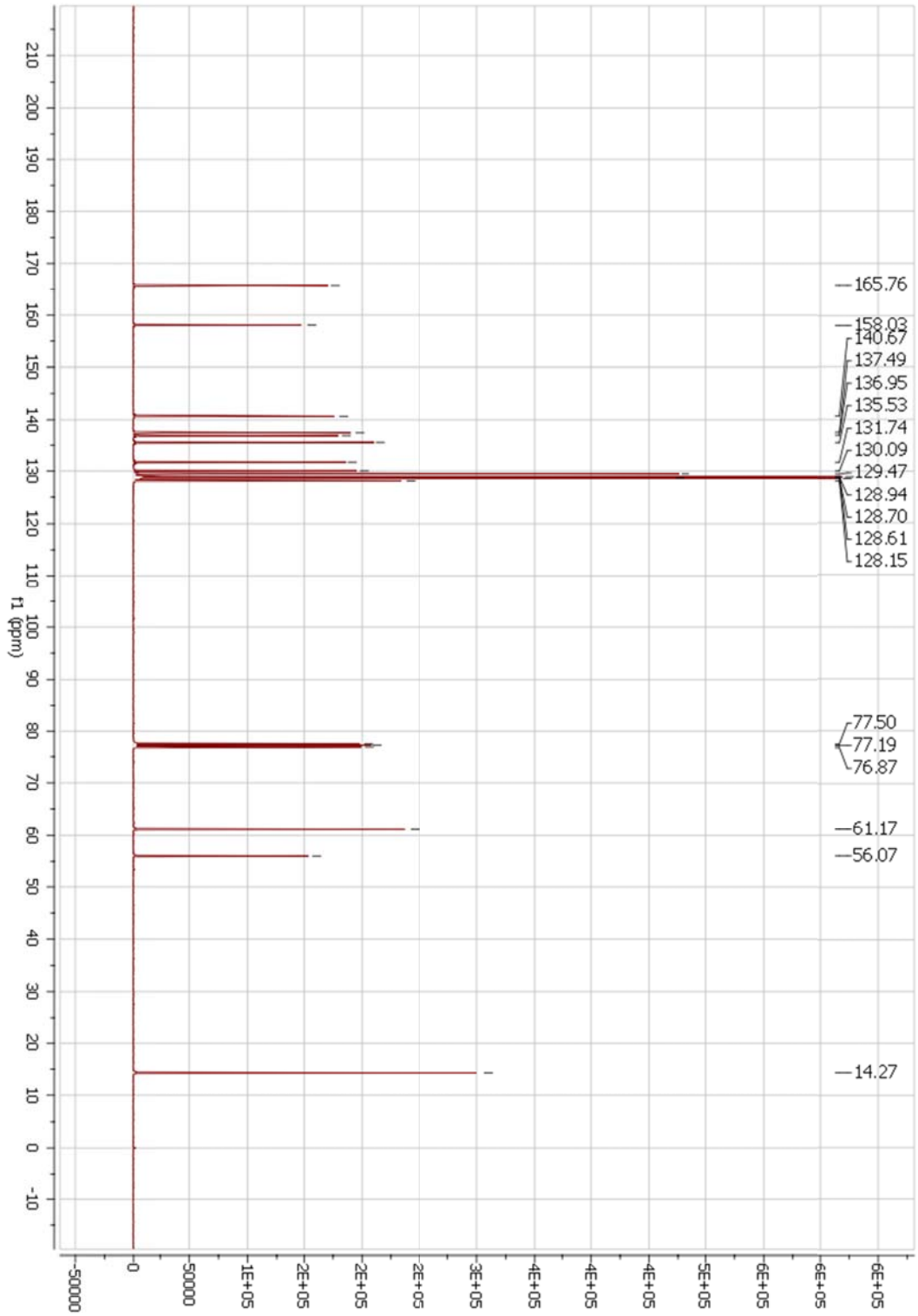
^{13}C-NMR


158.14
137.94
135.73
132.55
131.65
131.50
131.32
130.24
128.91
128.67
128.14
126.37
77.38
77.06
76.74
56.10
f1 (ppm)

Ethyl 4-(2-benzyl-6-chloro-3-oxo-2,3-dihydropyridazin-4-yl)benzoate (**9a**)
^{1}H-NMR

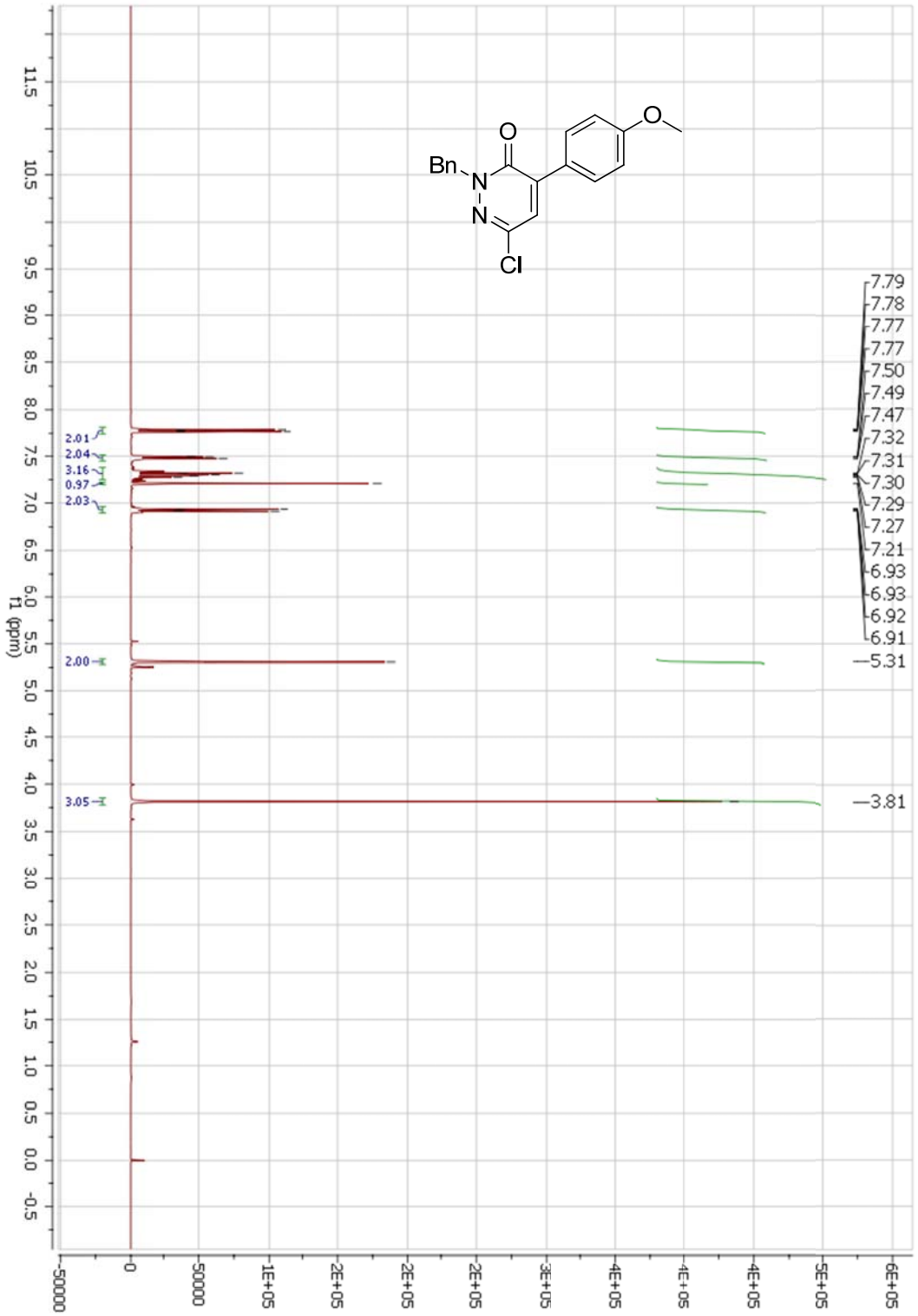


^{13}C-NMR

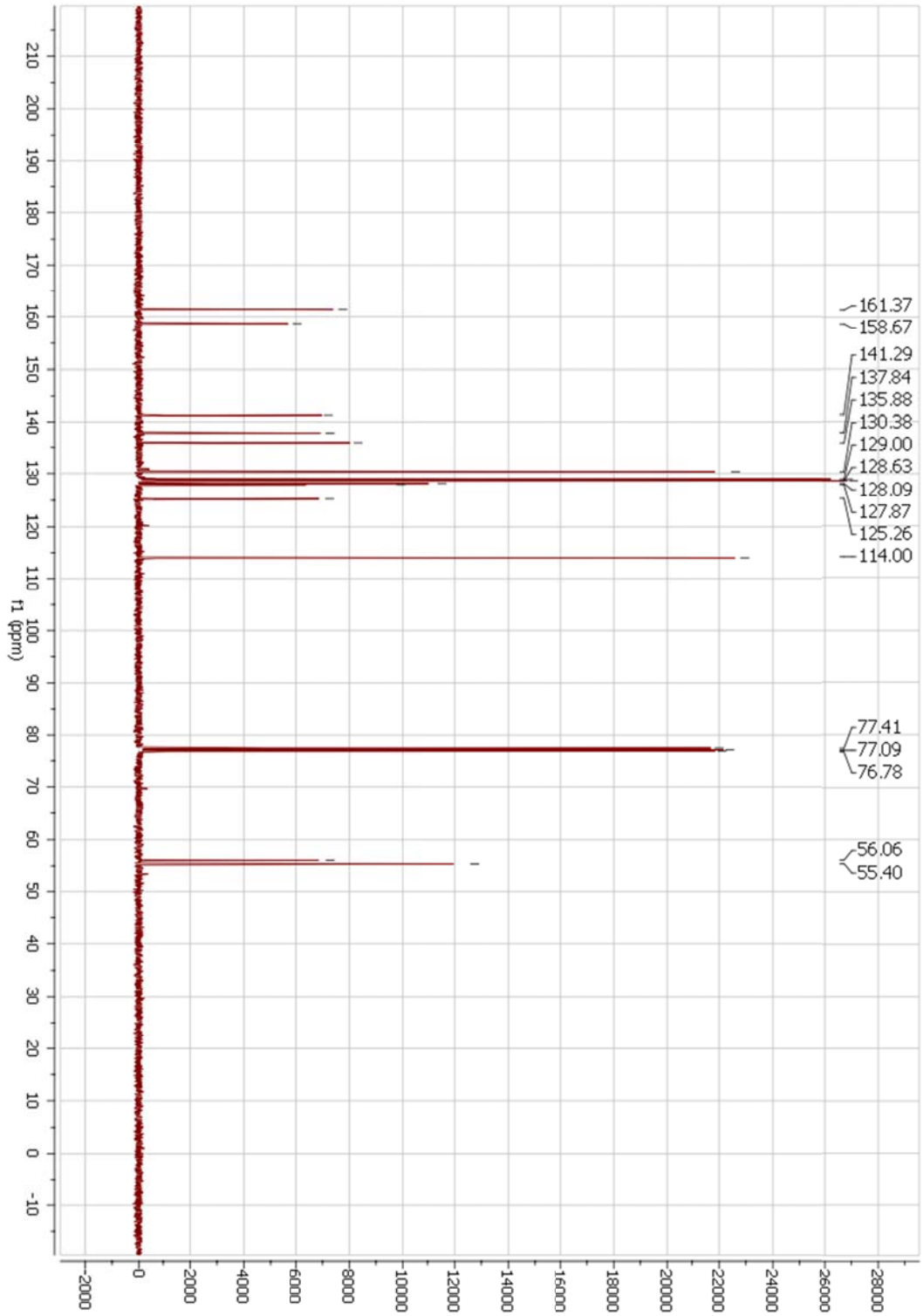

165.76
158.03
140.67
137.49
136.95
135.53
131.74
130.09
129.47
128.94
128.70
128.61
128.15
77.50
77.19
76.87
61.17
56.07
14.27
f1 (ppm)

2-Benzyl-6-chloro-4-(4-methoxyphenyl)pyridazin-3(2*H*)-one (**9b**)

^{1}H-NMR

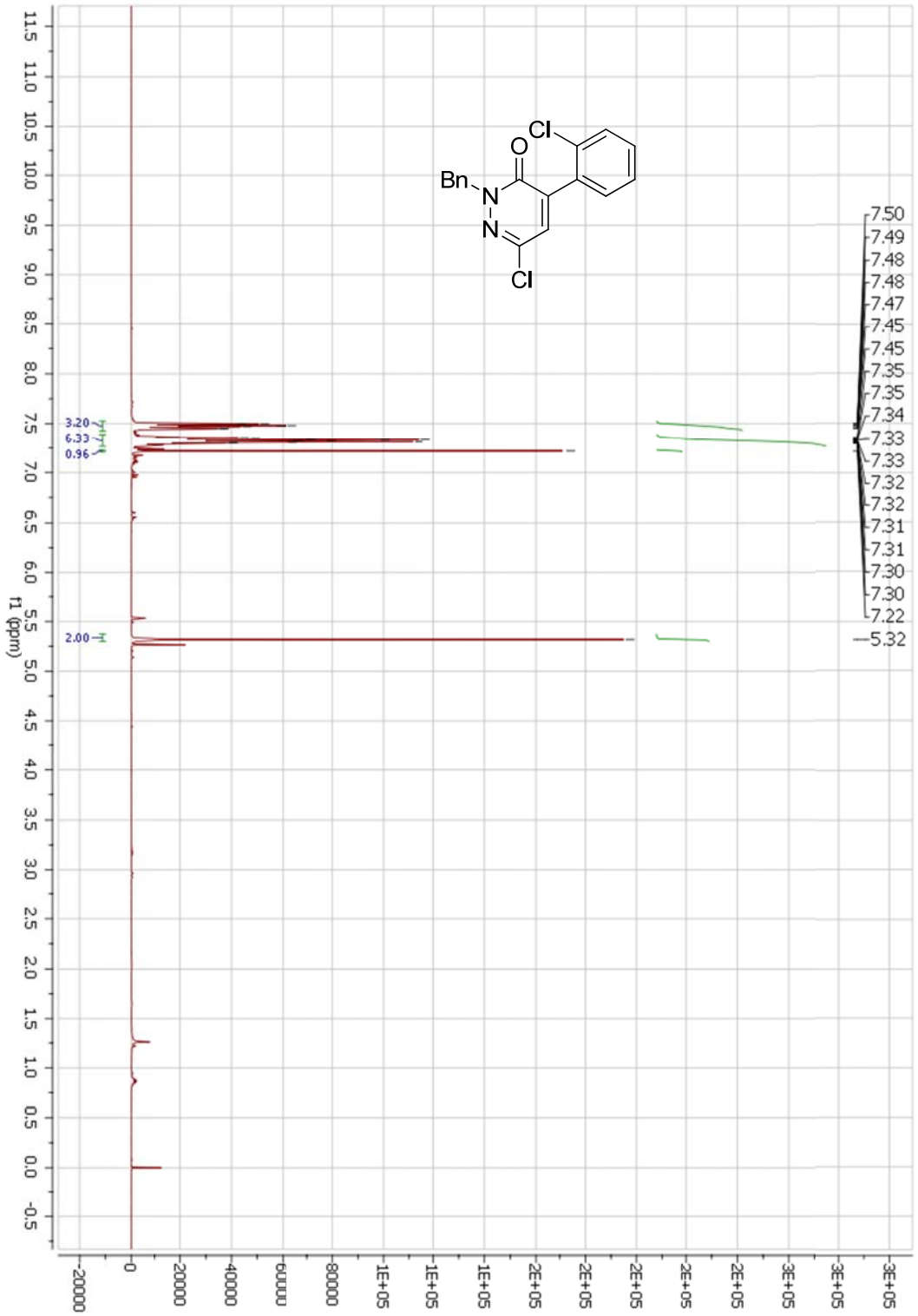


^{13}C-NMR

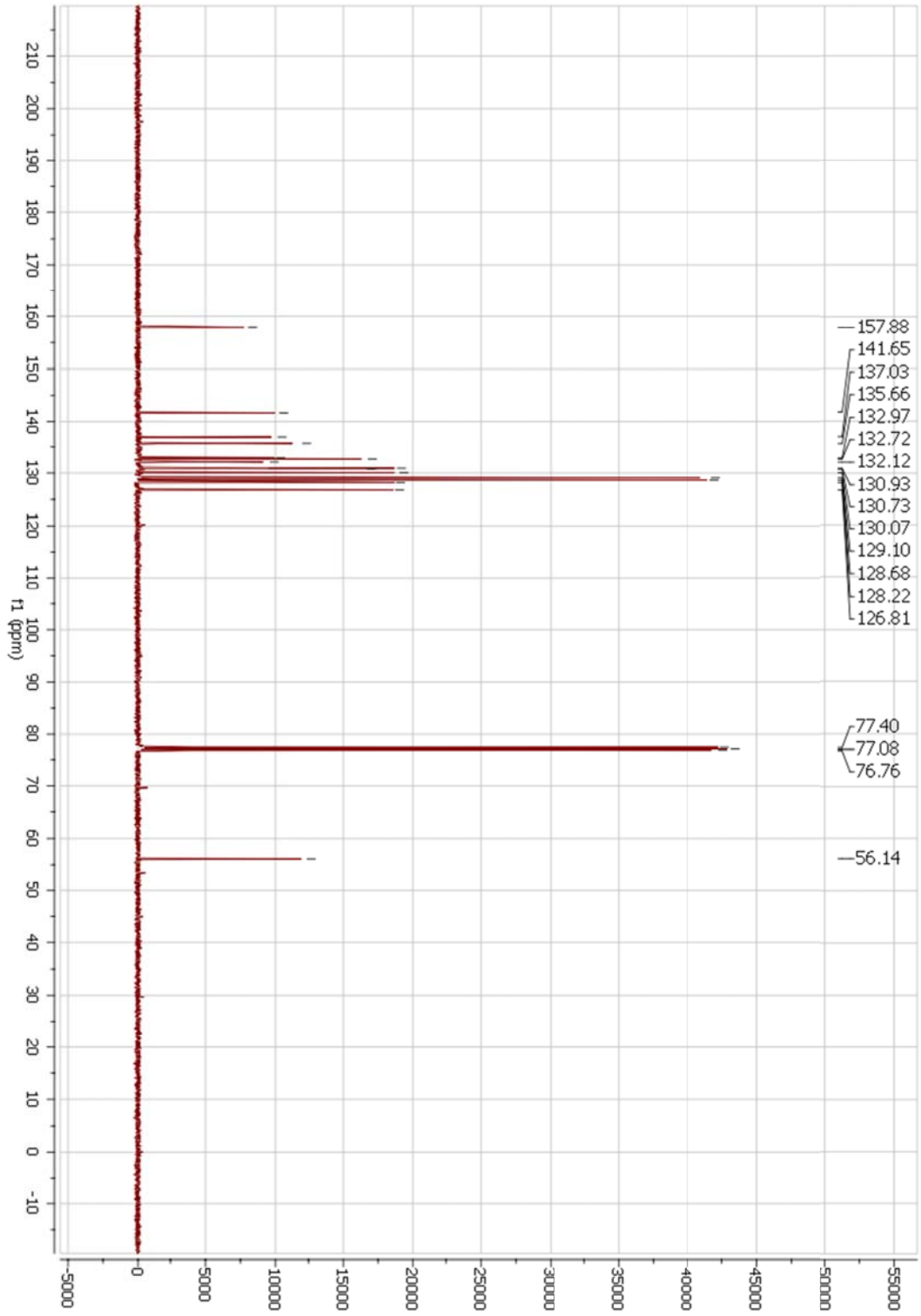

161.37
158.67
141.29
137.84
135.88
130.38
129.00
128.63
128.09
127.87
125.26
114.00
77.41
77.09
76.78
56.06
55.40
f1 (ppm)

2-Benzyl-6-chloro-4-(2-chlorophenyl)pyridazin-3(2*H*)-one (**9c**)

^{1}H-NMR

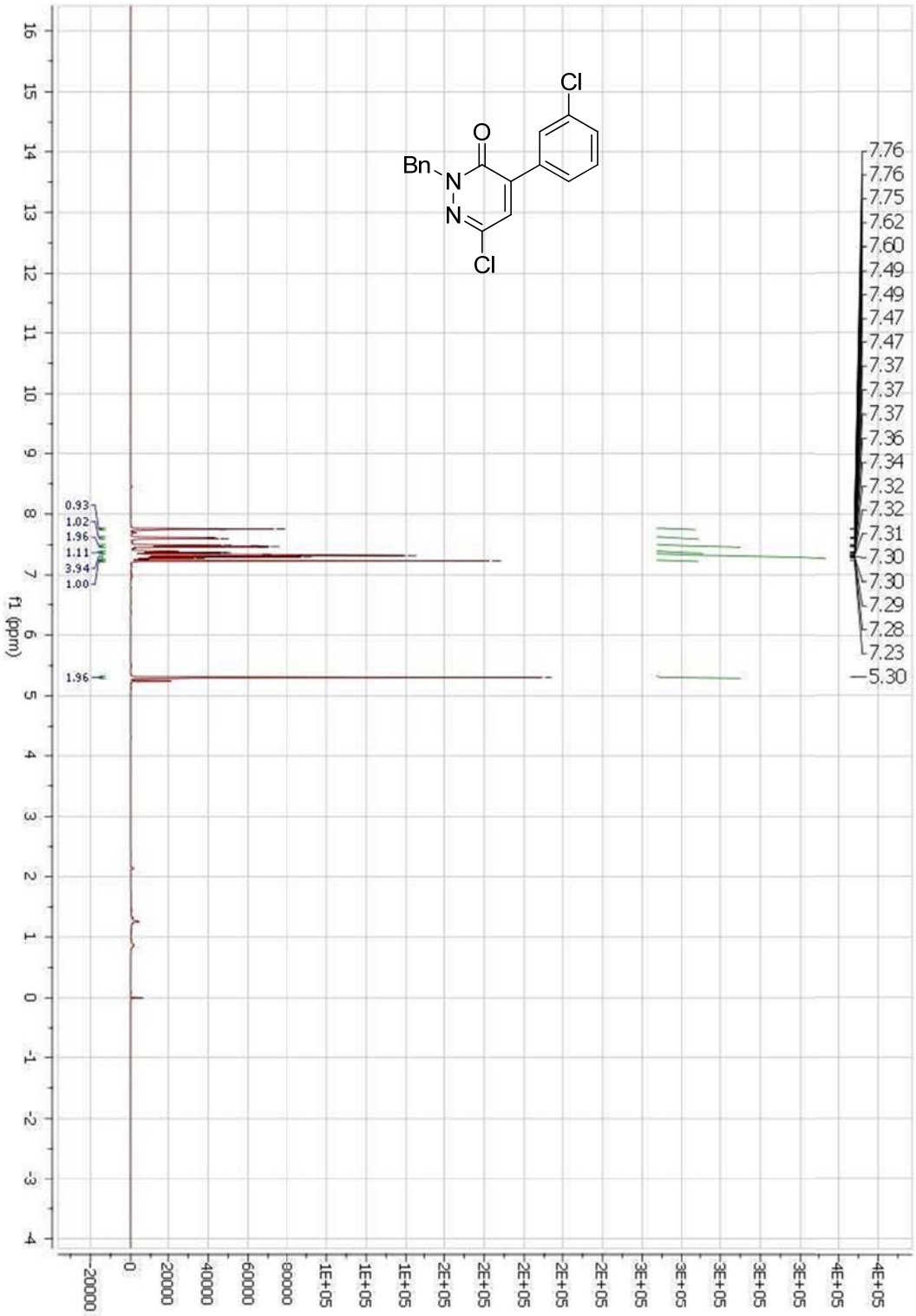


^{13}C-NMR

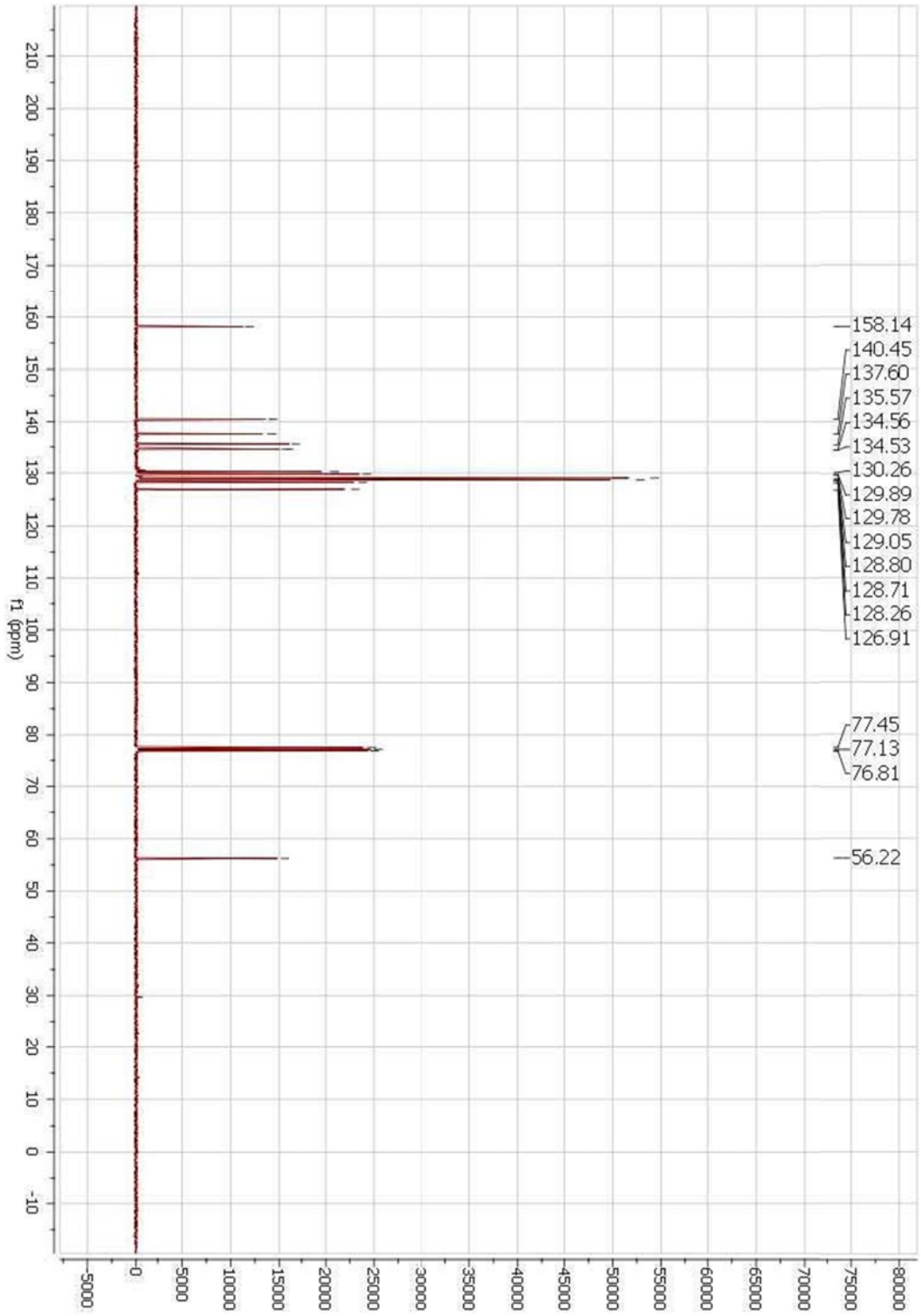

157.88
141.65
137.03
135.66
132.97
132.72
132.12
130.93
130.73
130.07
129.10
128.68
128.22
126.81
77.40
77.08
76.76
56.14
f1 (ppm)

2-Benzyl-6-chloro-4-(3-chlorophenyl)pyridazin-3(2*H*)-one (**9d**)

^{1}H-NMR

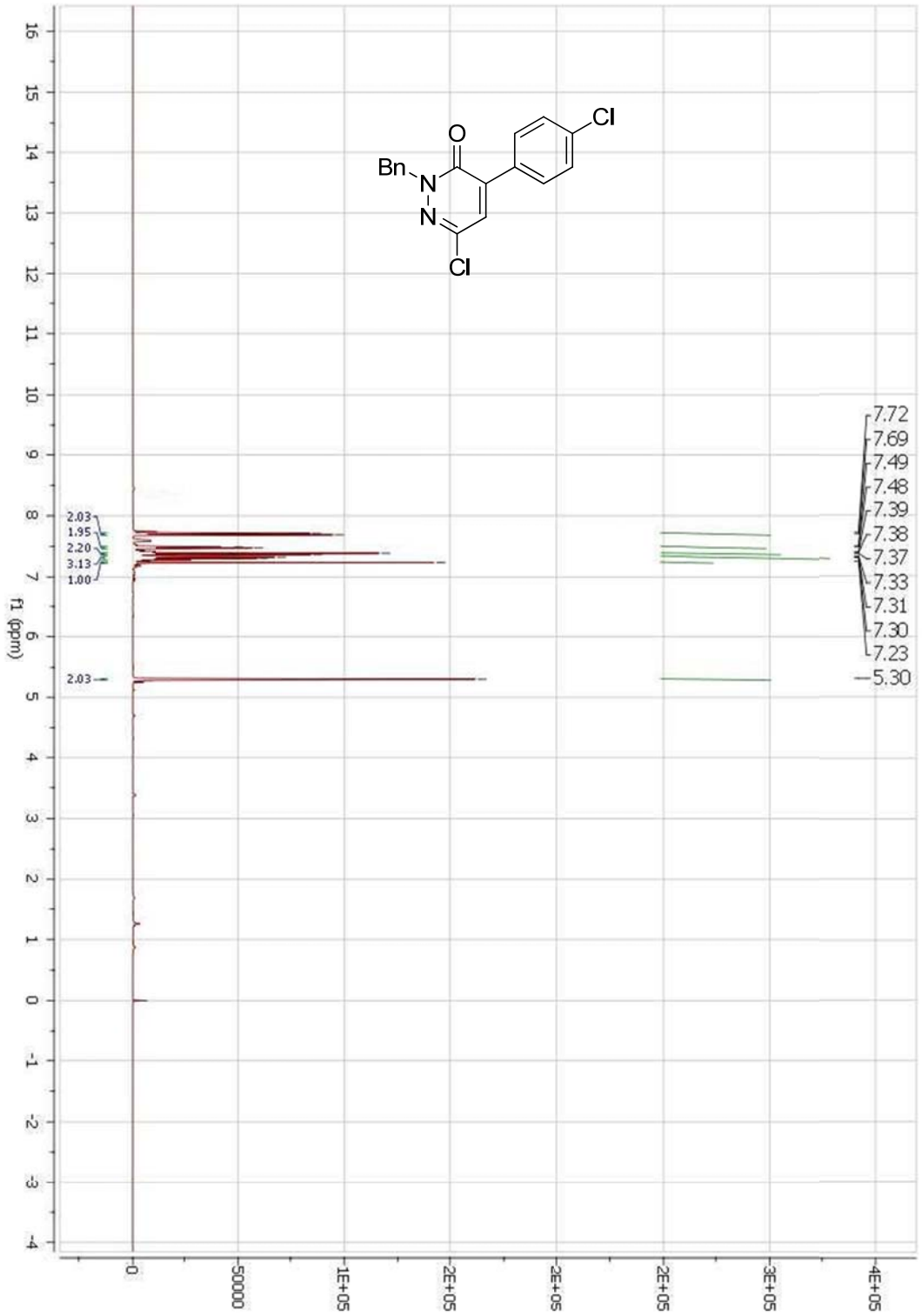


^{13}C-NMR

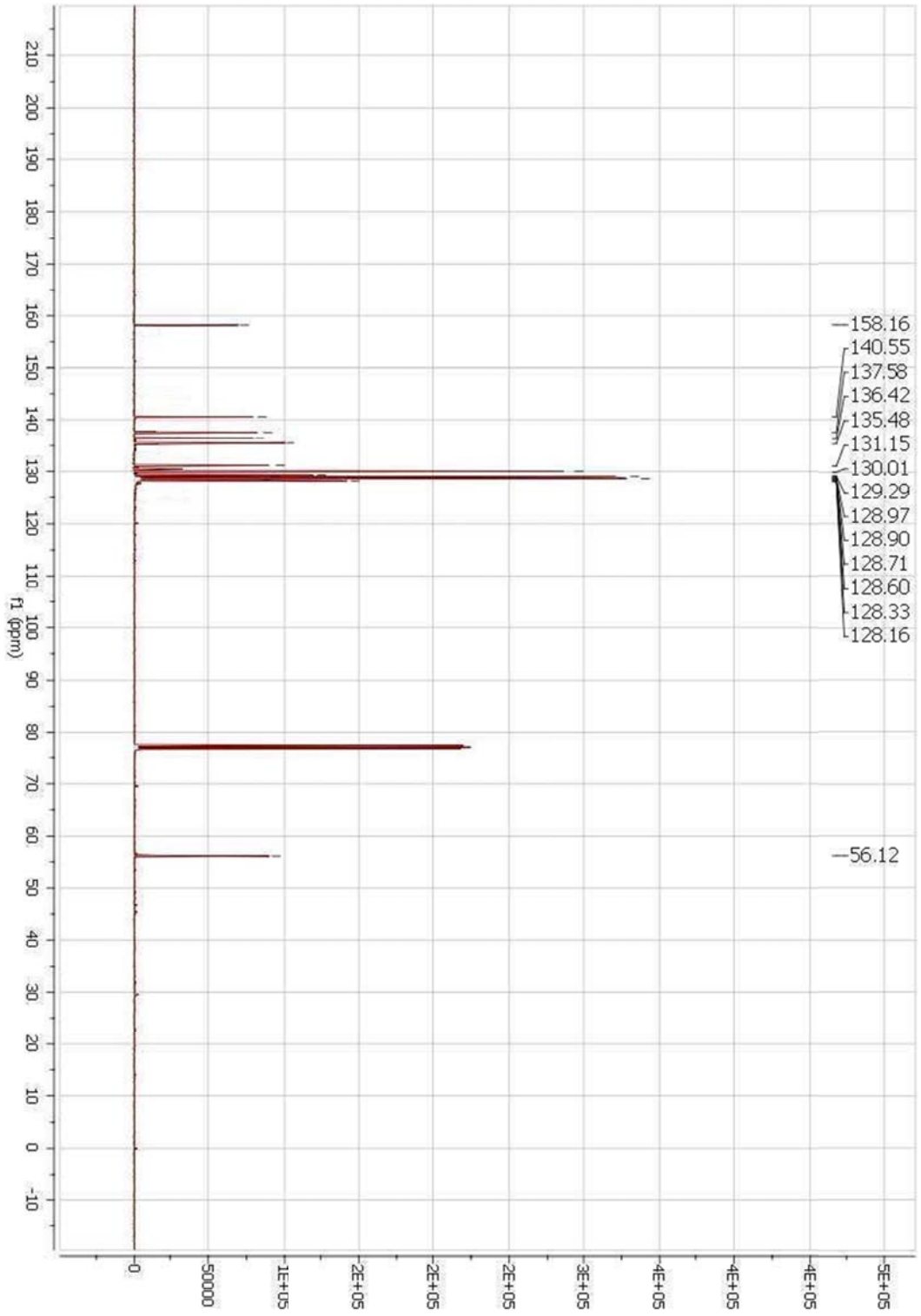

158.14
140.45
137.60
135.57
134.56
134.53
130.26
129.89
129.78
129.05
128.80
128.71
128.26
126.91
77.45
77.13
76.81
56.22
f1 (ppm)

2-Benzyl-6-chloro-4-(4-chlorophenyl)pyridazin-3(2*H*)-one (**9e**)

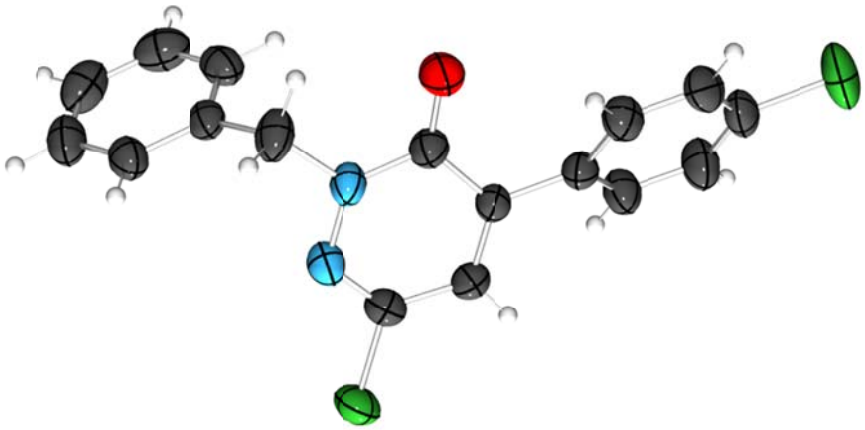
^{1}H-NMR



^{13}C-NMR

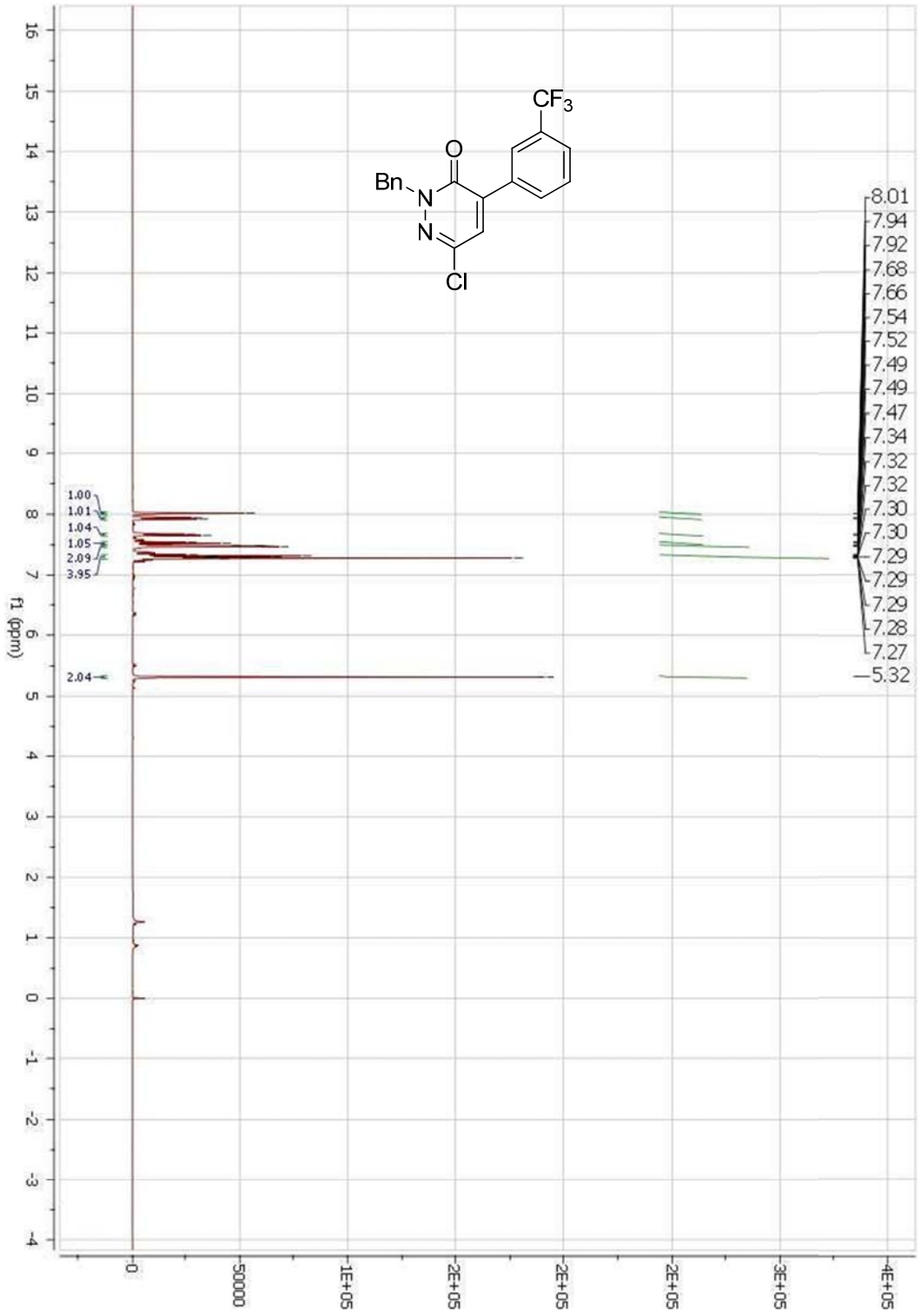

158.16
140.55
137.58
136.42
135.48
131.15
130.01
129.29
128.97
128.90
128.71
128.60
128.33
128.16
56.12
f1 (ppm)

XRD structure

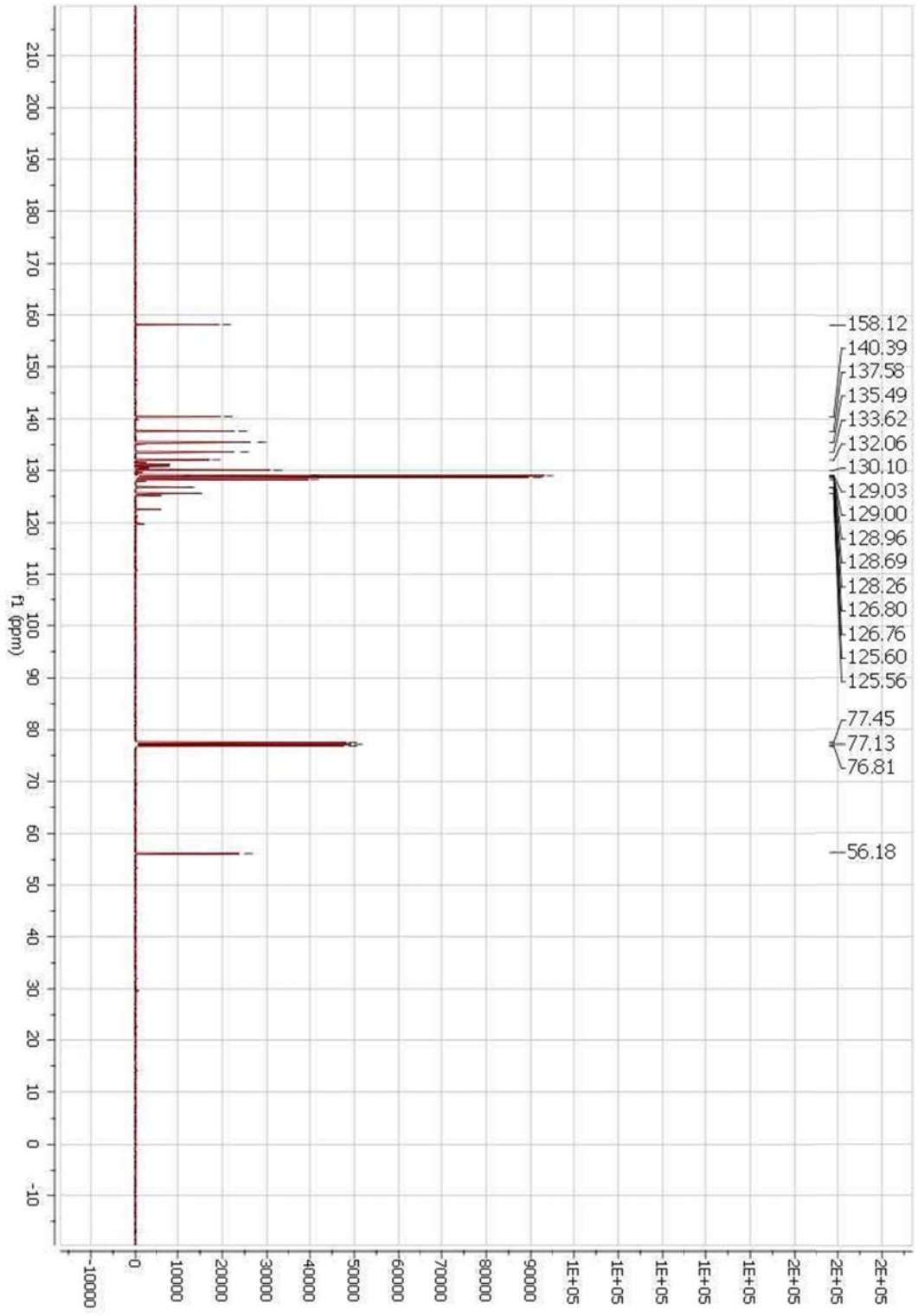


ORTEP-style plot of **9e** (C: grey, N: blue, O: red, F: light green, yellow, Cl: green, I: Purple). Thermal ellipsoids are drawn at 30% probability level, hydrogen atoms are drawn as spheres of 0.15 Å radius.

2-Benzyl-6-chloro-4-(3-(trifluoromethyl)phenyl)pyridazin-3(2*H*)-one (**9f**)
^{1}H-NMR

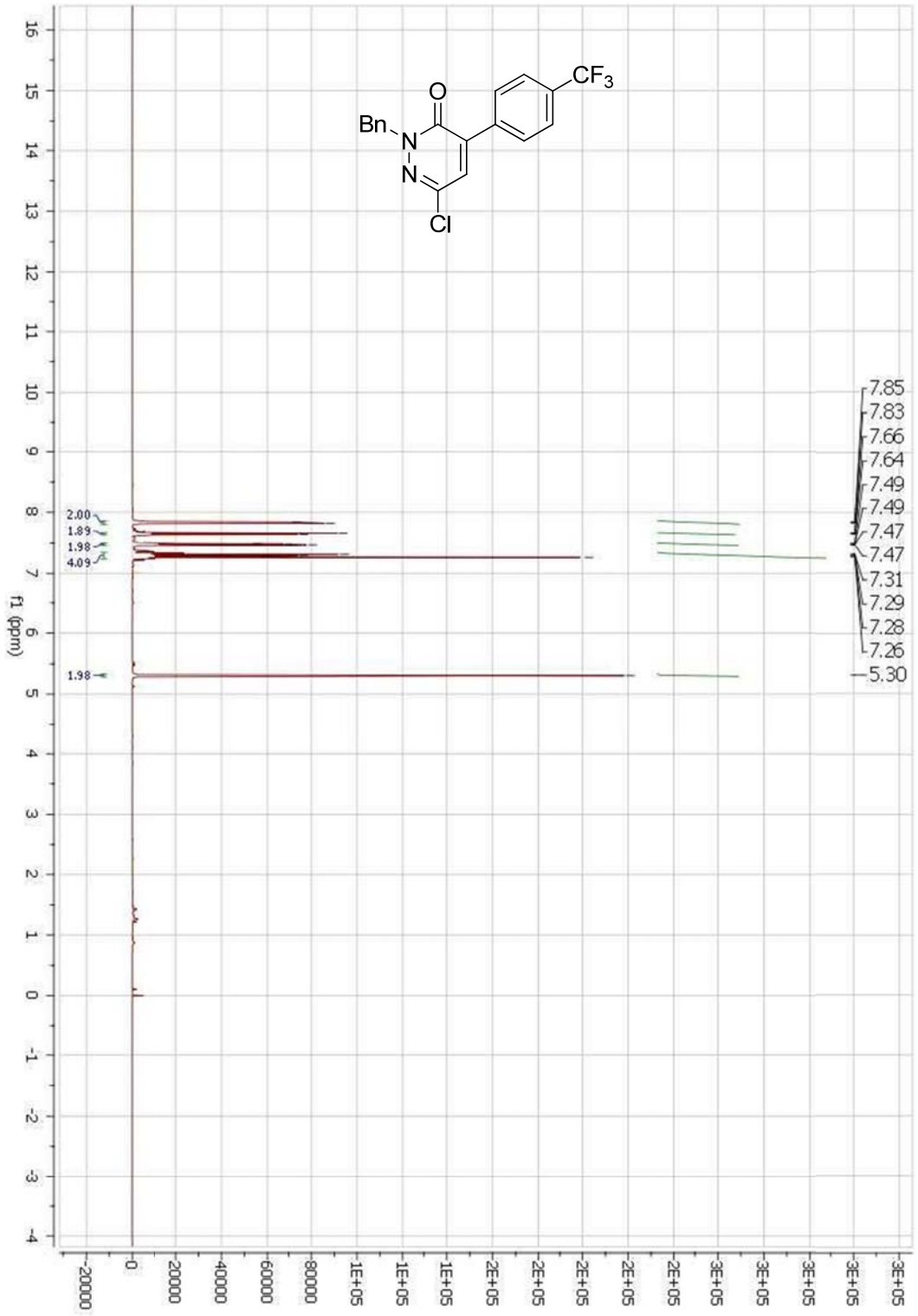


^{13}C-NMR

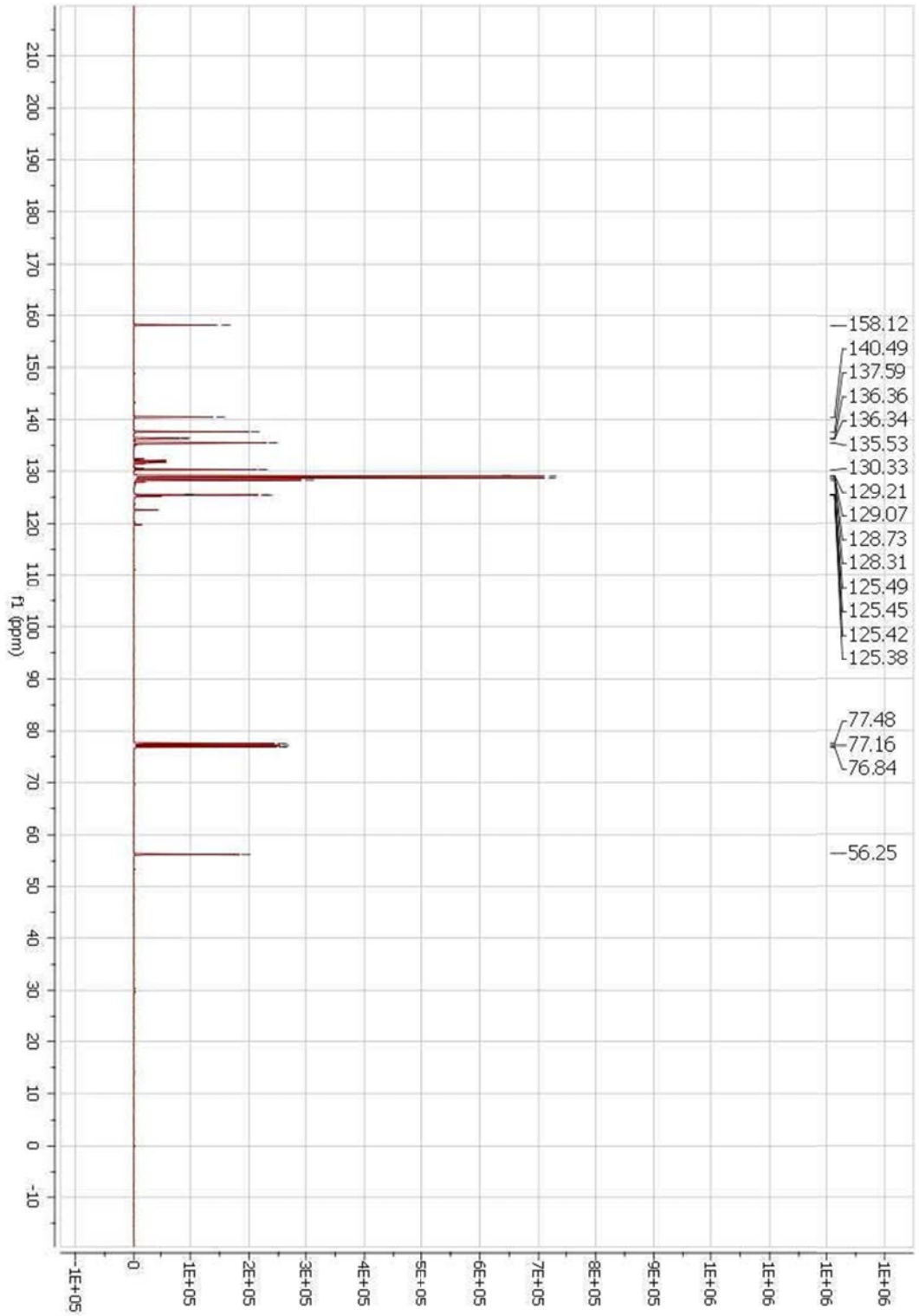

158.12
140.39
137.58
135.49
133.62
132.06
130.10
129.03
129.00
128.96
128.69
128.26
126.80
126.76
125.60
125.56
77.45
77.13
76.81
56.18
f1 (ppm)

2-Benzyl-6-chloro-4-(4-(trifluoromethyl)phenyl)pyridazin-3(2*H*)-one (**9g**)

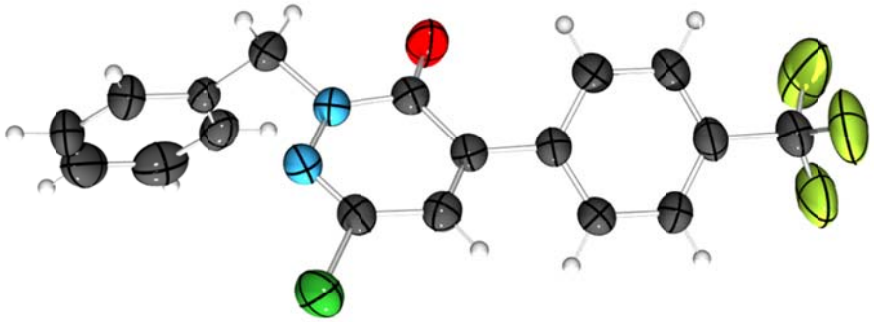
^{1}H-NMR



^{13}C-NMR


158.12
140.49
137.59
136.36
136.34
135.53
130.33
129.21
129.07
128.73
128.31
125.49
125.45
125.42
125.38
77.48
77.16
76.84
56.25
f1 (ppm)

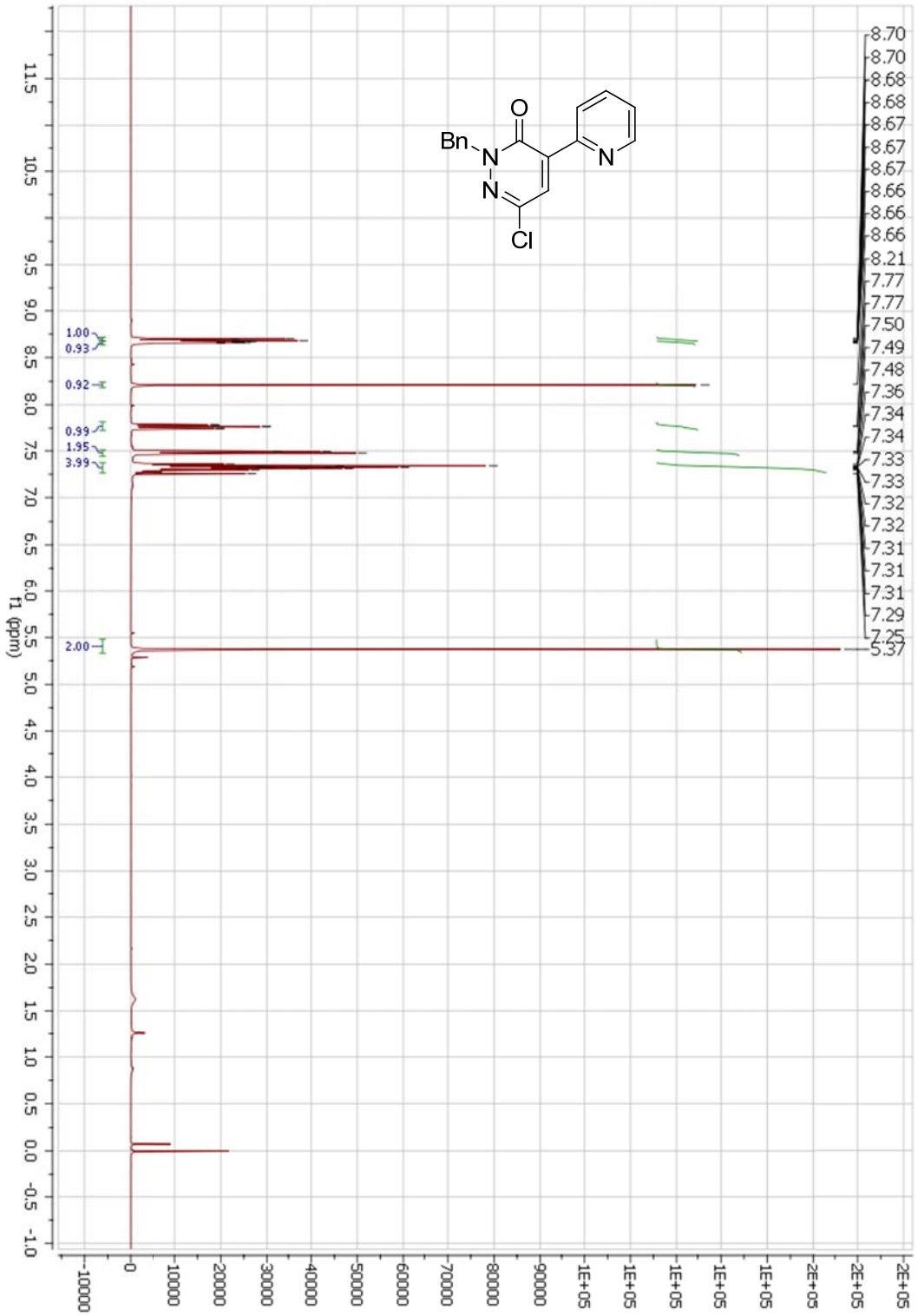
XRD structure



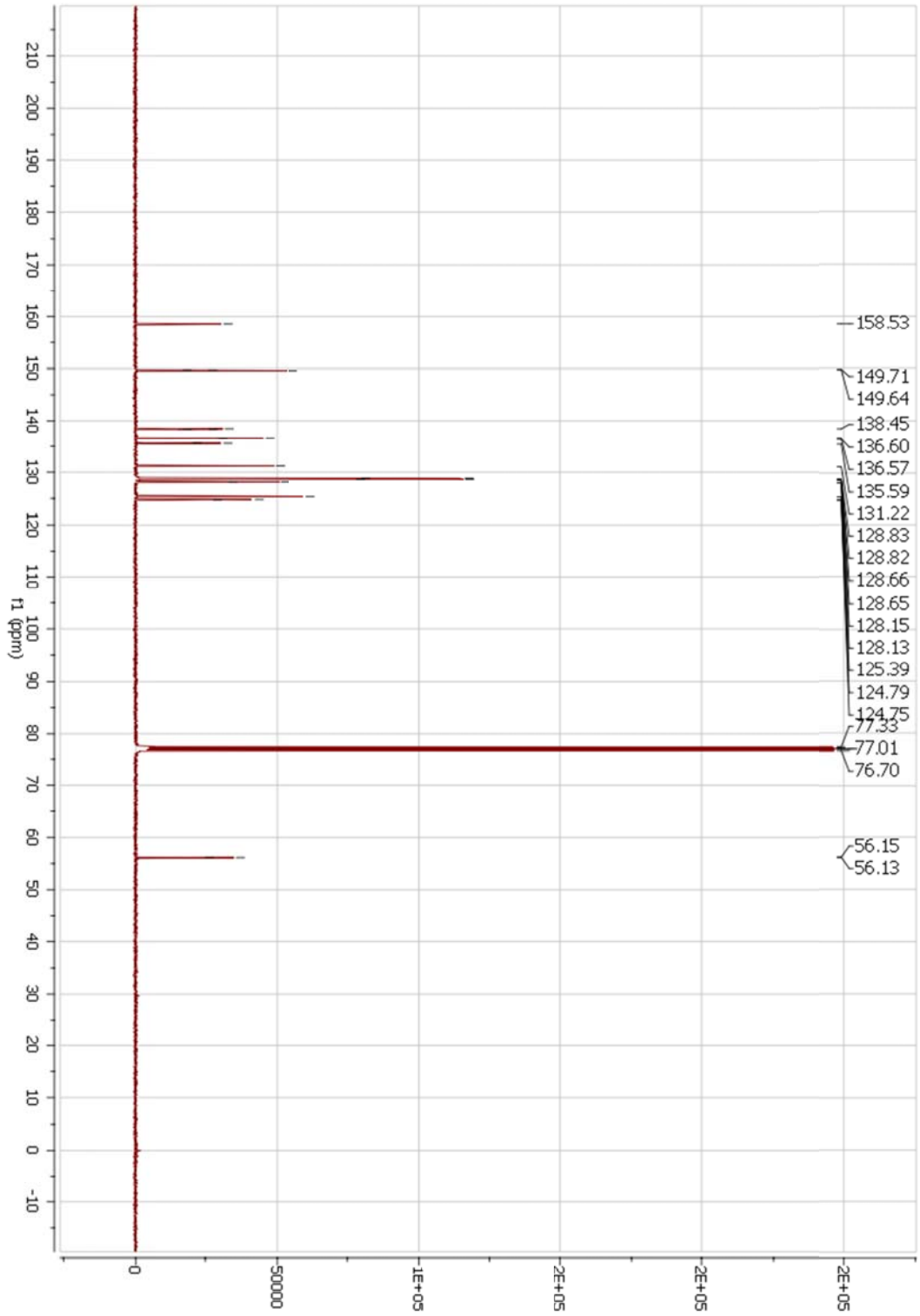
ORTEP-style plot of **9g** (C: grey, N: blue, O: red, F: light green, yellow, Cl: green, I: Purple). Thermal ellipsoids are drawn at 30% probability level, hydrogen atoms are drawn as spheres of 0.15 Å radius.

2-Benzyl-6-chloro-4-(pyridin-2-yl)pyridazin-3(2*H*)-one (**9h**)

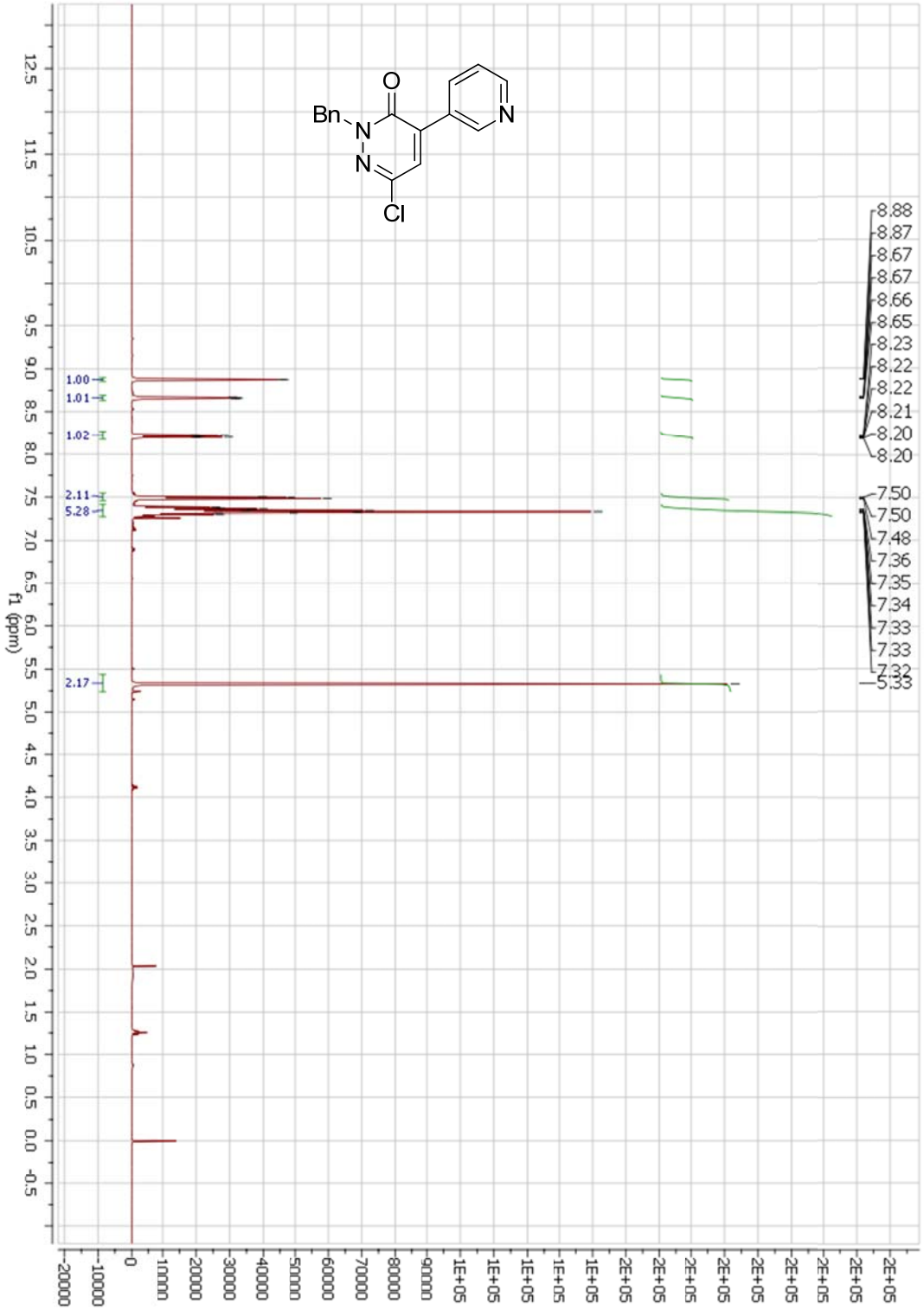
^{1}H-NMR



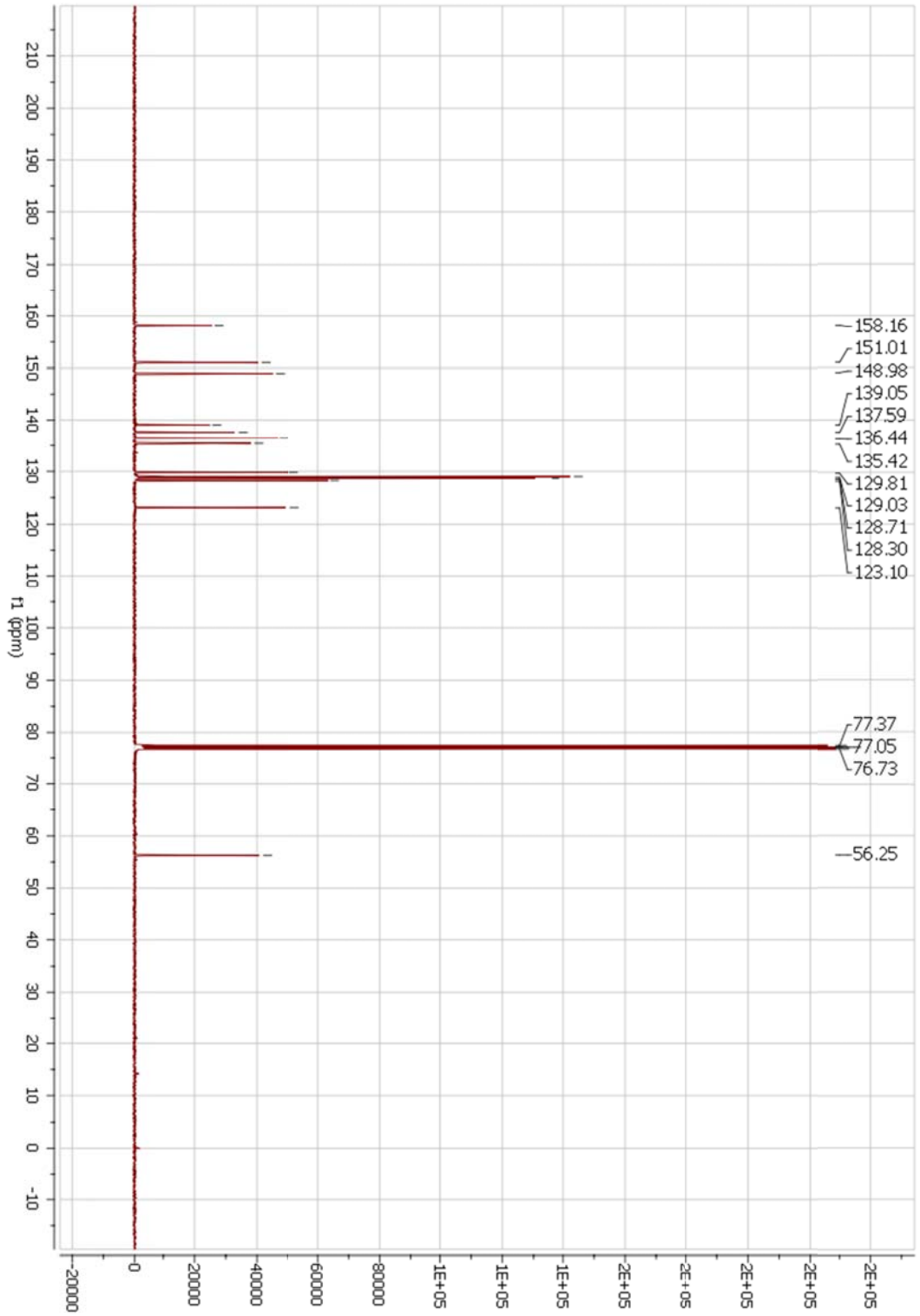
^{13}C-NMR


158.53
149.71
149.64
138.45
136.60
136.57
135.59
131.22
128.83
128.82
128.66
128.65
128.15
128.13
125.39
124.79
124.75
77.33
77.01
76.70
56.15
56.13
f1 (ppm)

2-Benzyl-6-chloro-4-(pyridin-3-yl)pyridazin-3(2H)-one (**9i**)
^{1}H-NMR

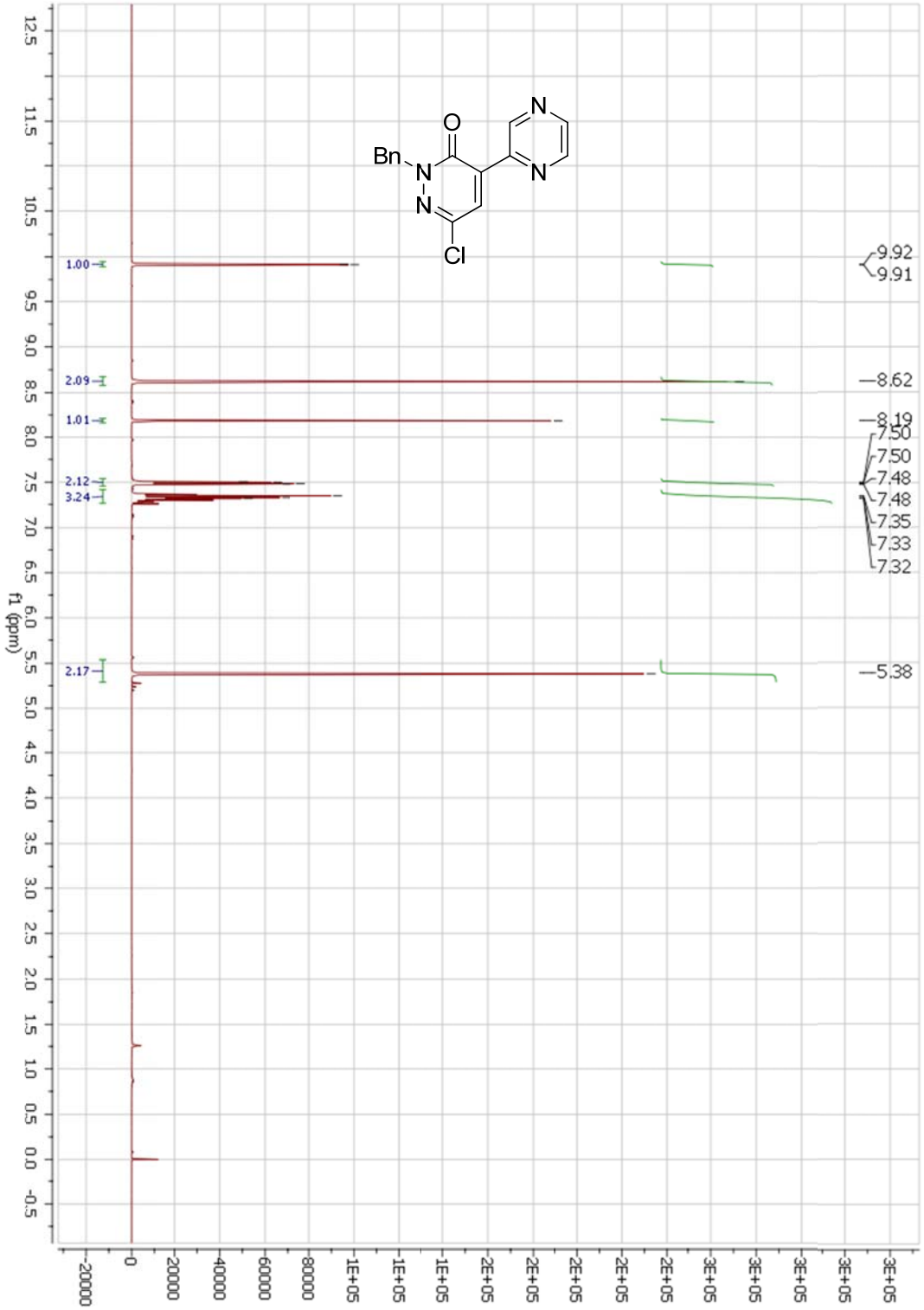


^{13}C-NMR

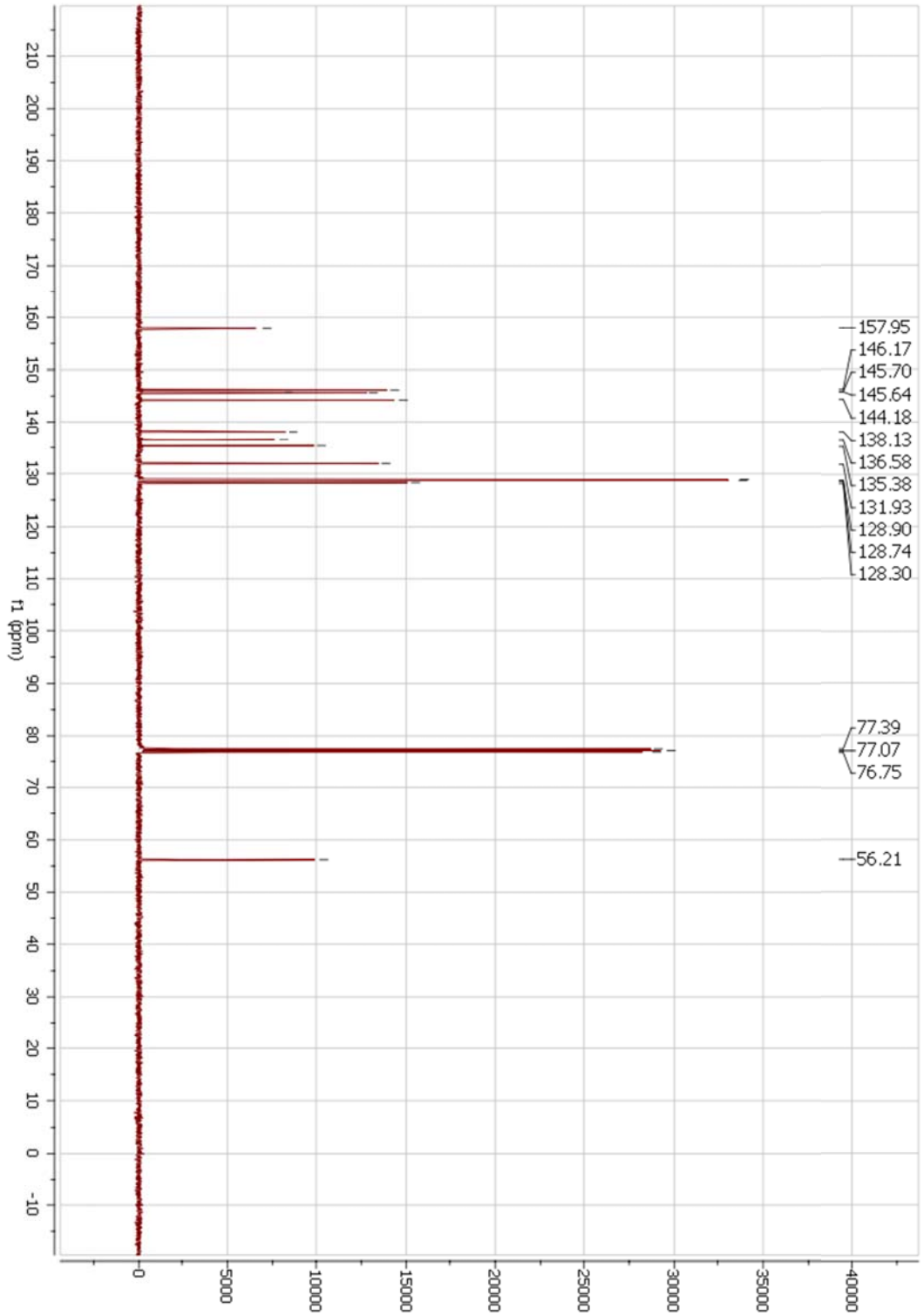

158.16
151.01
148.98
139.05
137.59
136.44
135.42
129.81
129.03
128.71
128.30
123.10
77.37
77.05
76.73
56.25
f1 (ppm)

2-Benzyl-6-chloro-4-(pyrazin-2-yl)pyridazin-3(2*H*)-one (**9j**)

^{1}H-NMR

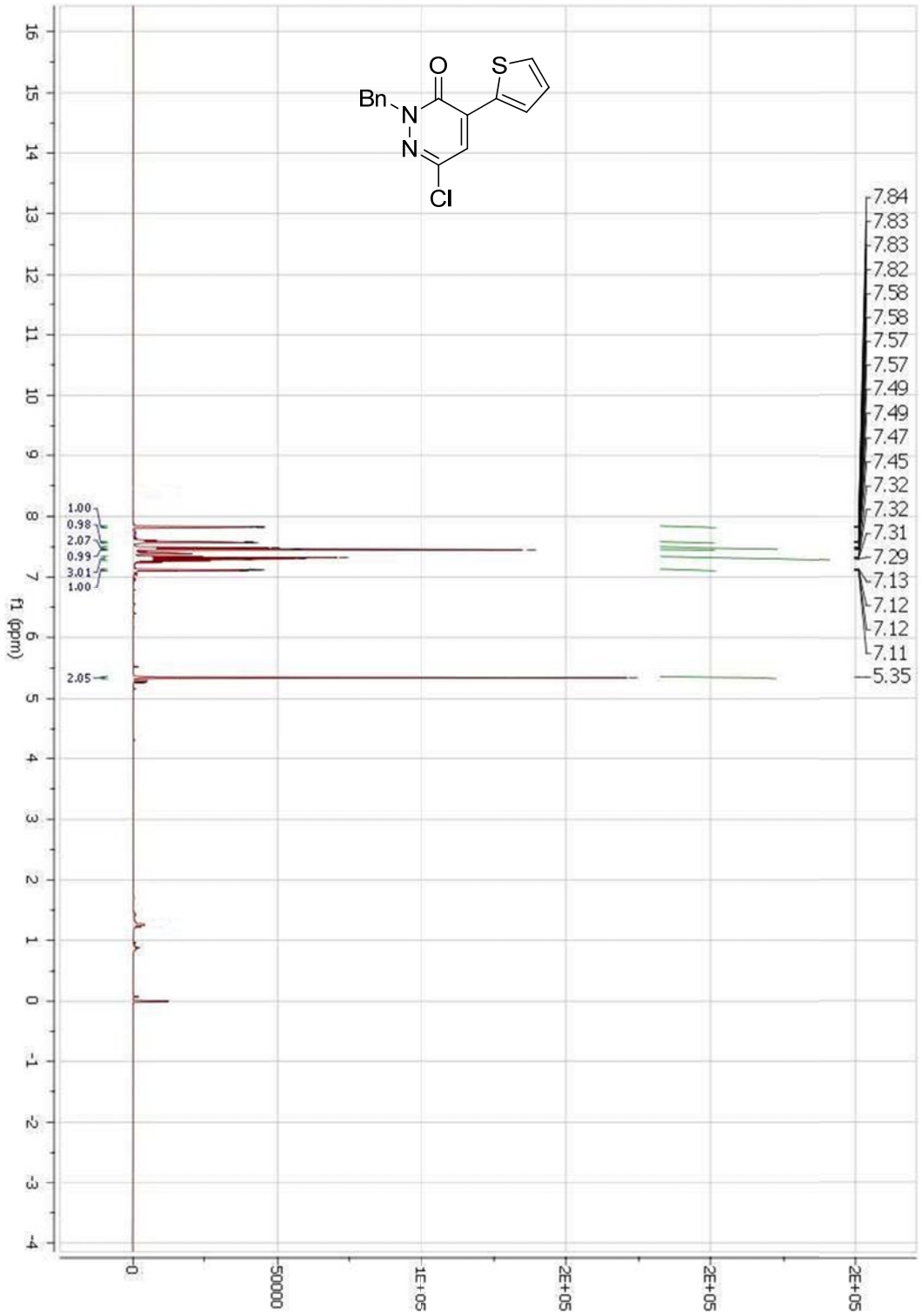


^{13}C-NMR

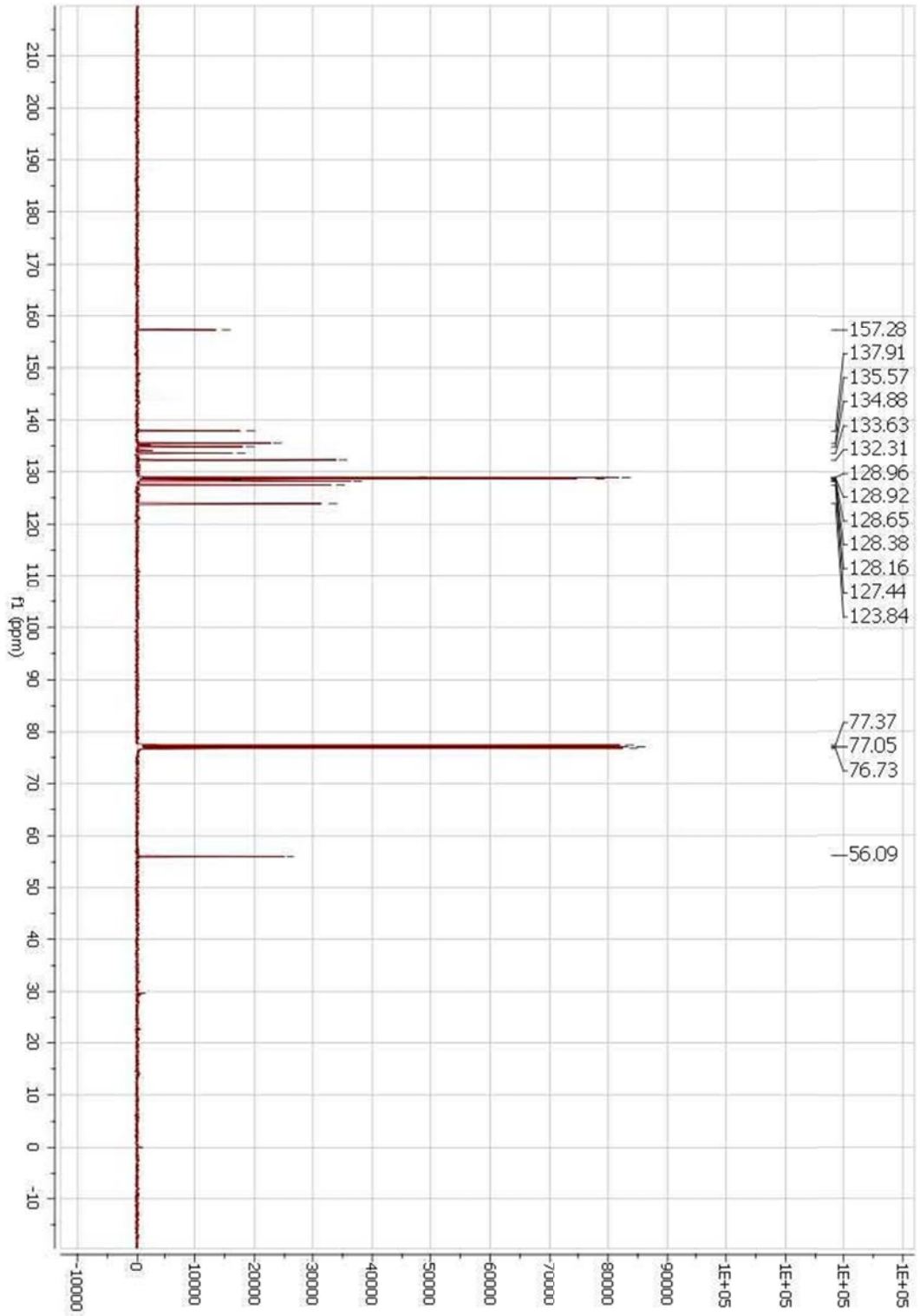

157.95
146.17
145.70
145.64
144.18
138.13
136.58
135.38
131.93
128.90
128.74
128.30
77.39
77.07
76.75
56.21
f1 (ppm)

2-Benzyl-6-chloro-4-(thien-2-yl)pyridazin-3(2*H*)-one (**9k**)

^{1}H-NMR

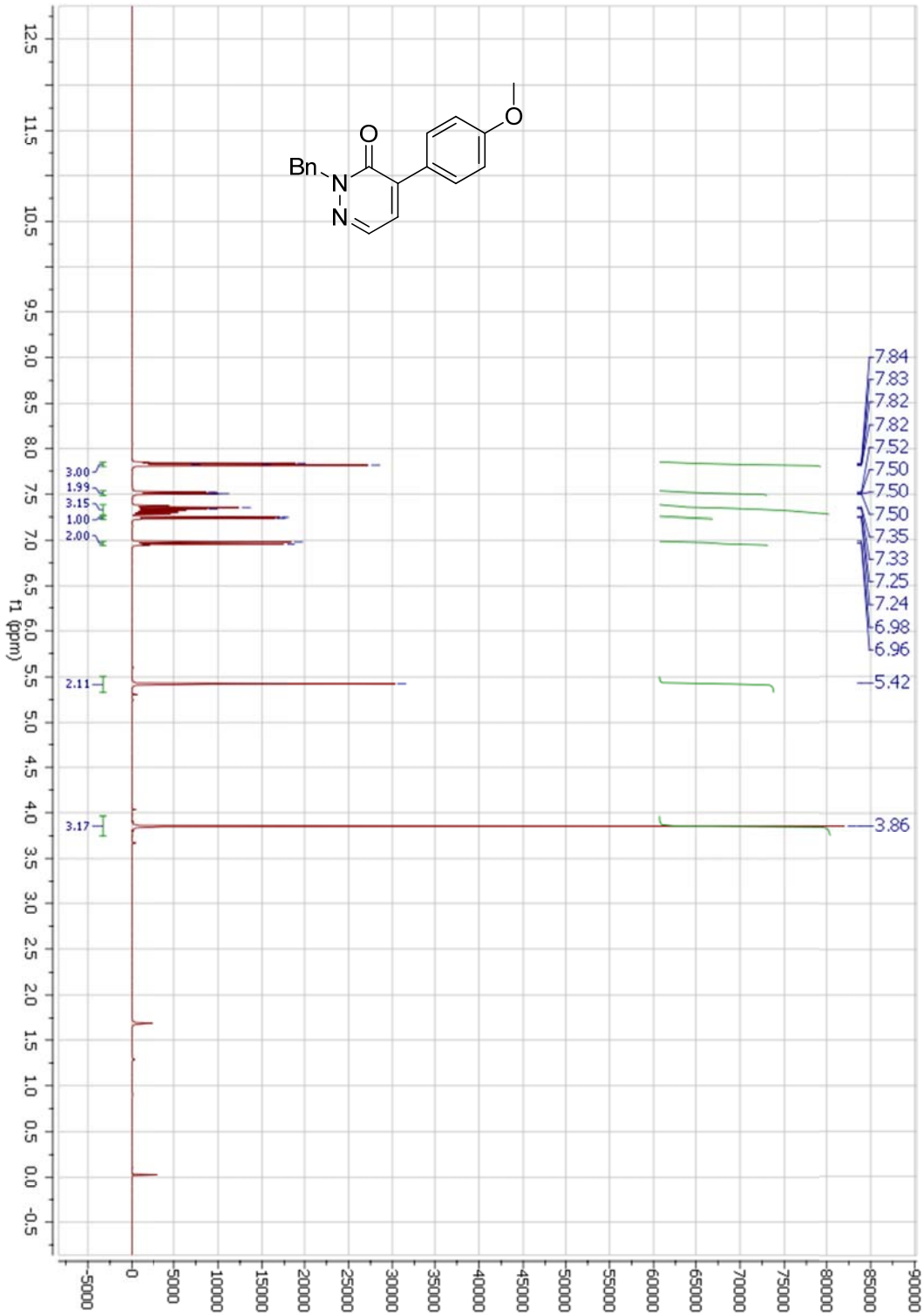


^{13}C-NMR

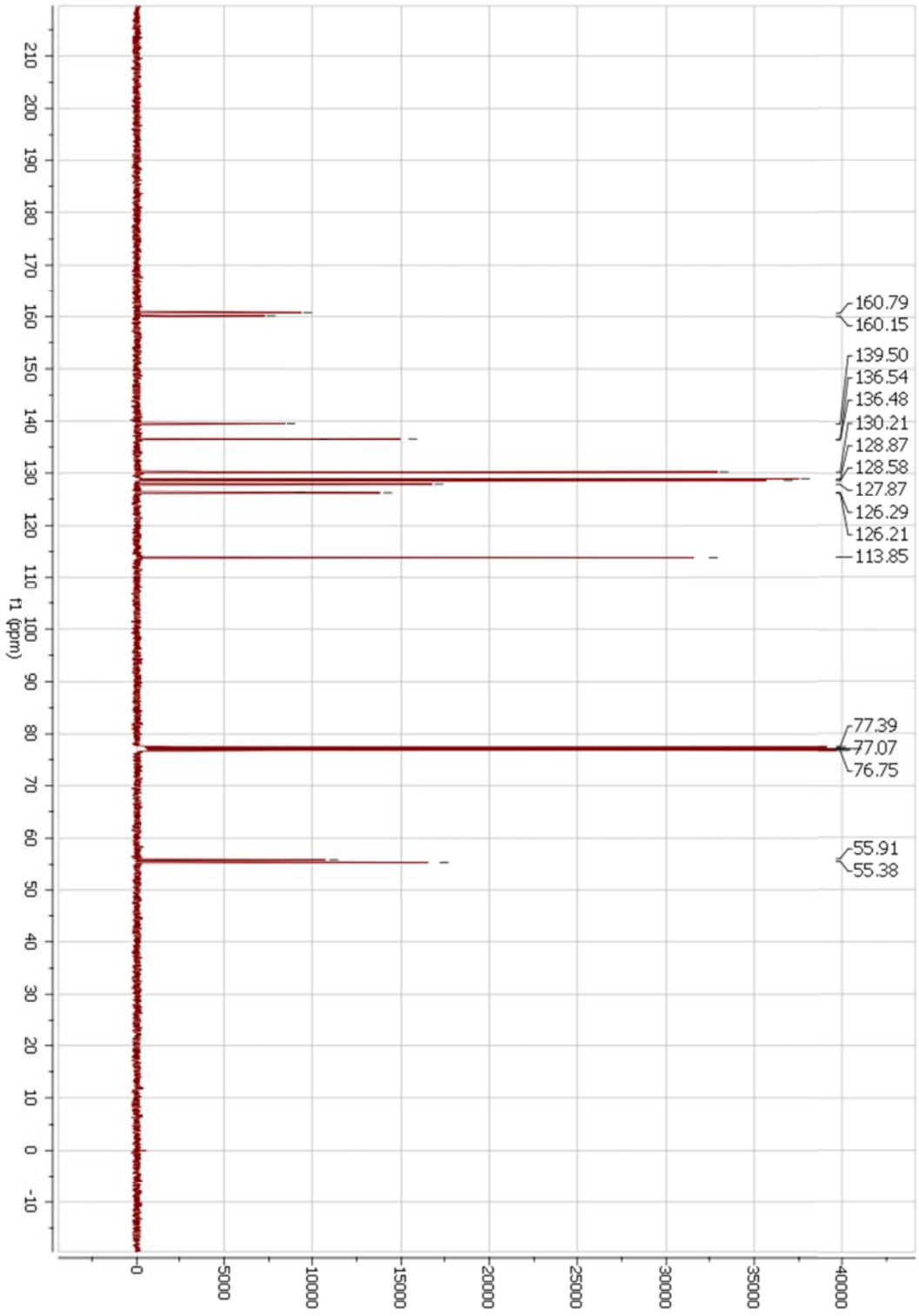

157.28
137.91
135.57
134.88
133.63
132.31
128.96
128.92
128.65
128.38
128.16
127.44
123.84
77.37
77.05
76.73
56.09
f1 (ppm)

2-Benzyl-4-(4-methoxyphenyl)pyridazin-3(2*H*)-one (**10**)

^{1}H-NMR

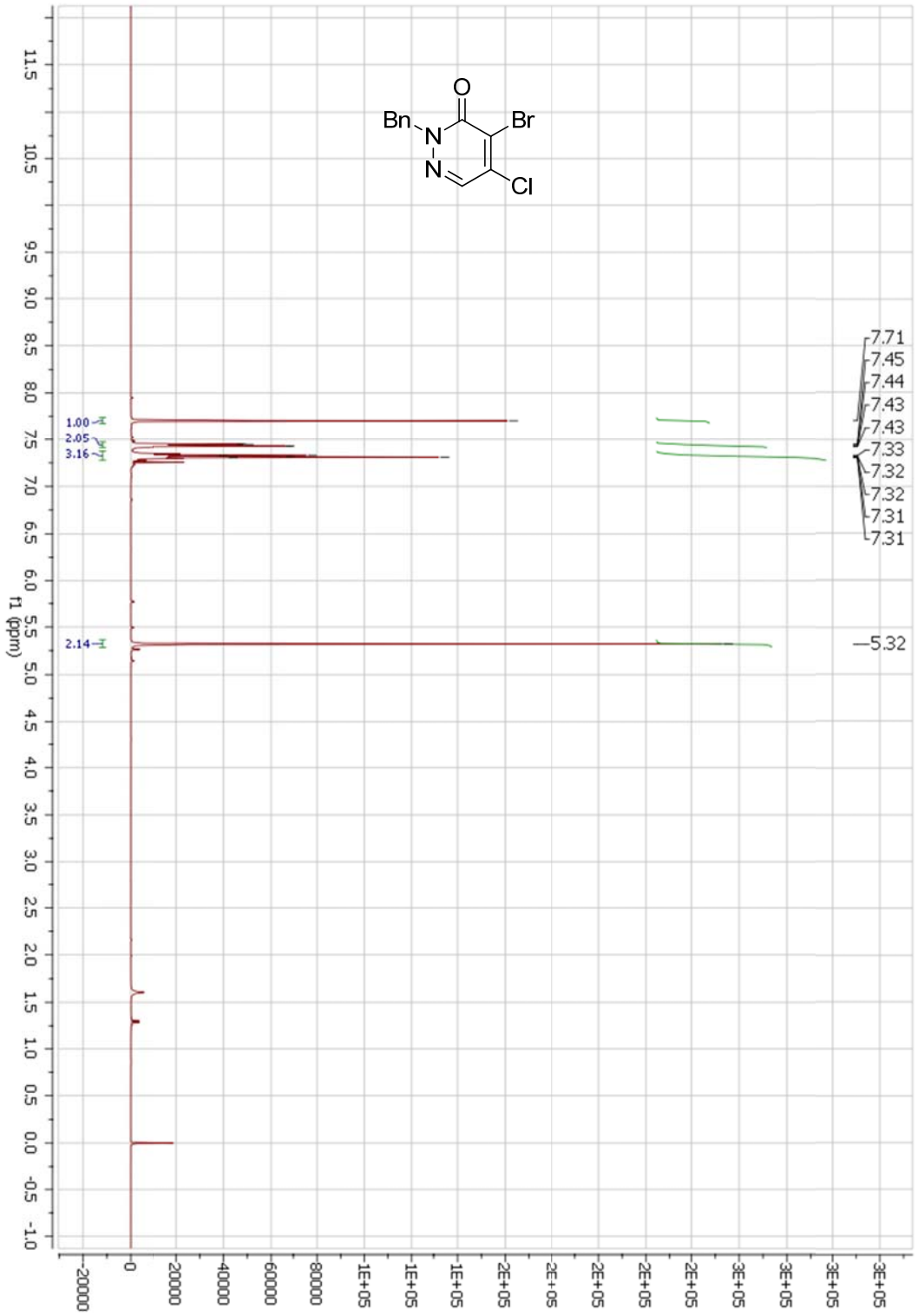


^{13}C-NMR

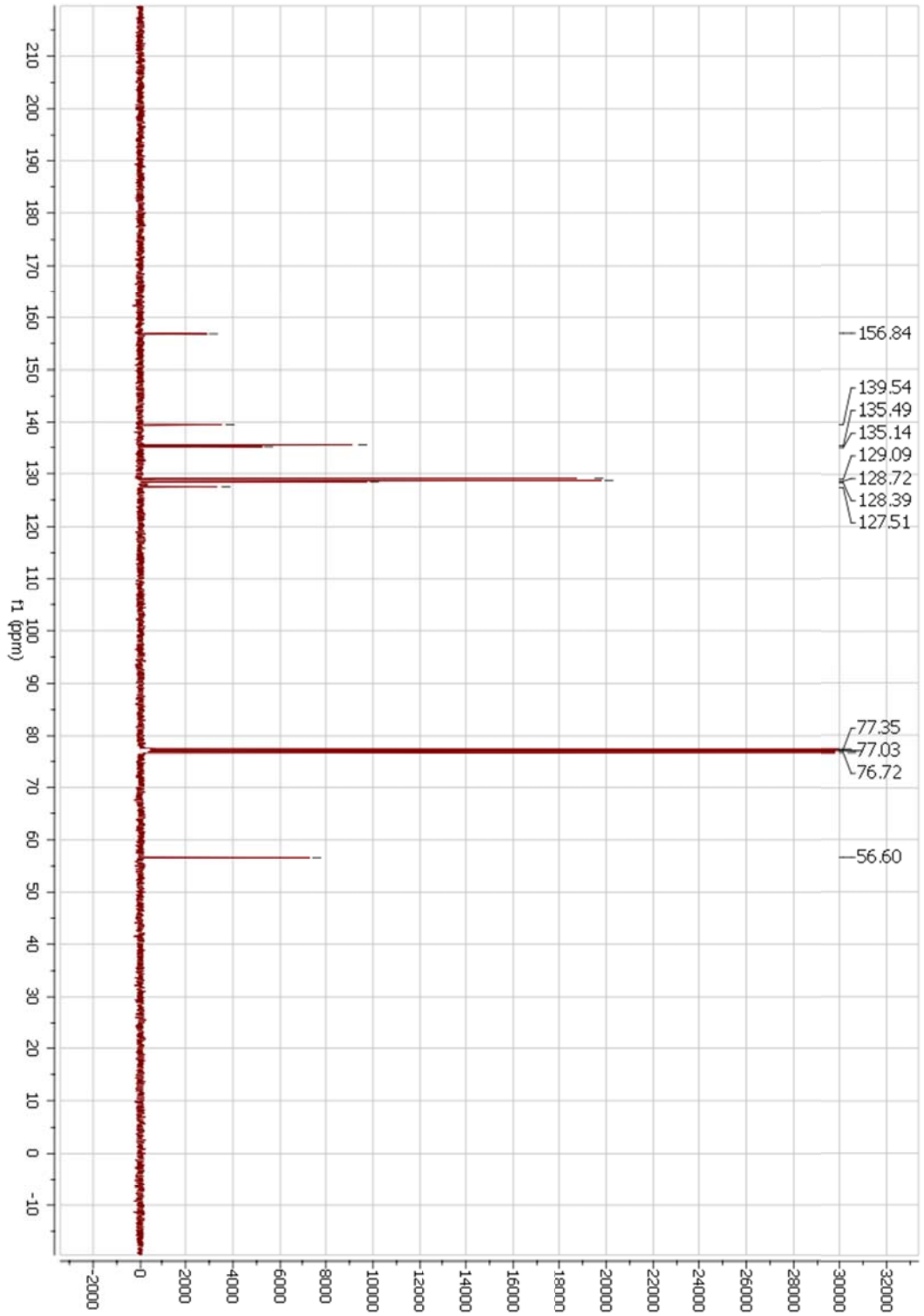

160.79
160.15
139.50
136.54
136.48
130.21
128.87
128.58
127.87
126.29
126.21
113.85
77.39
77.07
76.75
55.91
55.38
f1 (ppm)

2-Benzyl-4-bromo-5-chloropyridazin-3(2*H*)-one (**11a**)

^{1}H-NMR

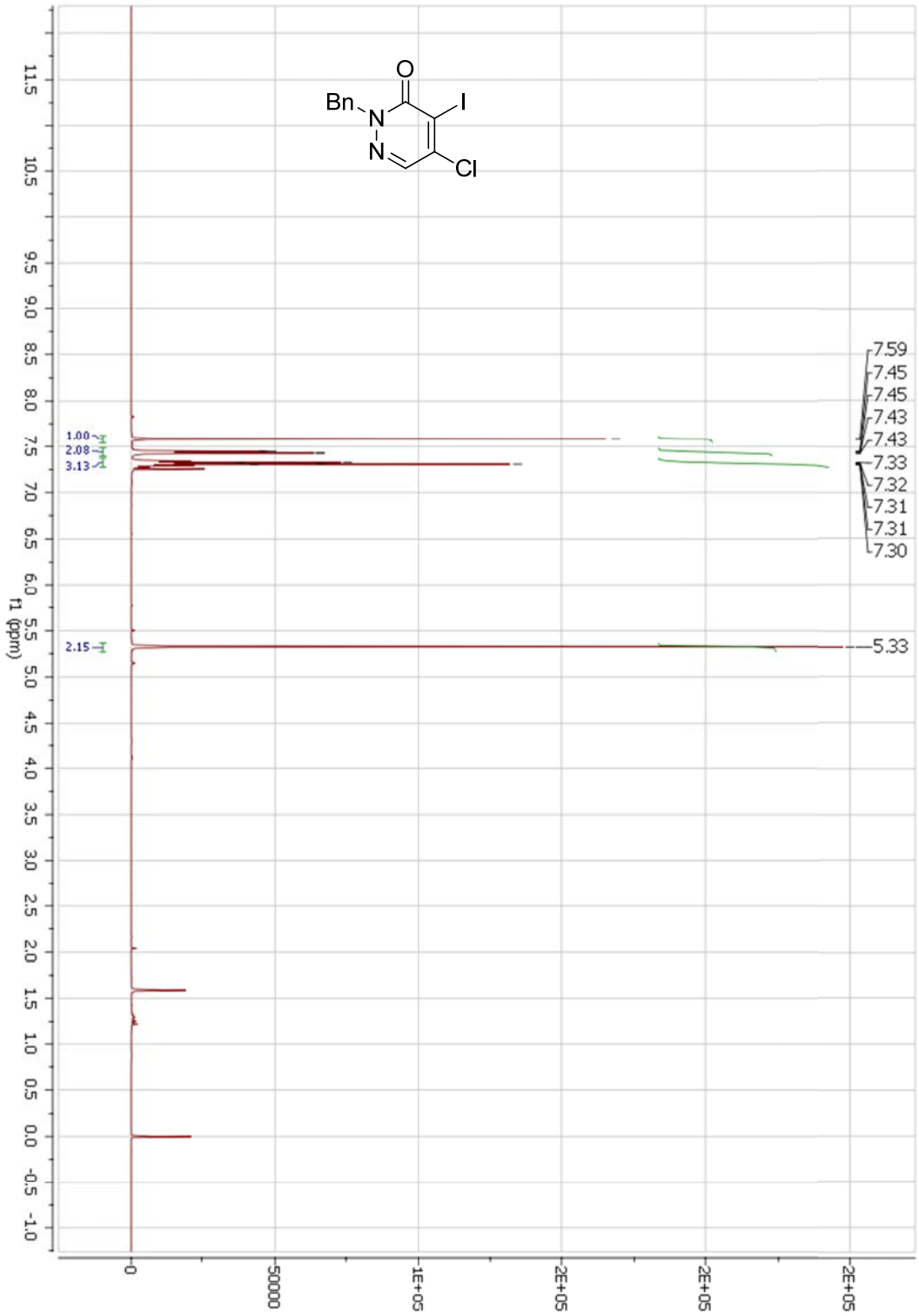


^{13}C-NMR

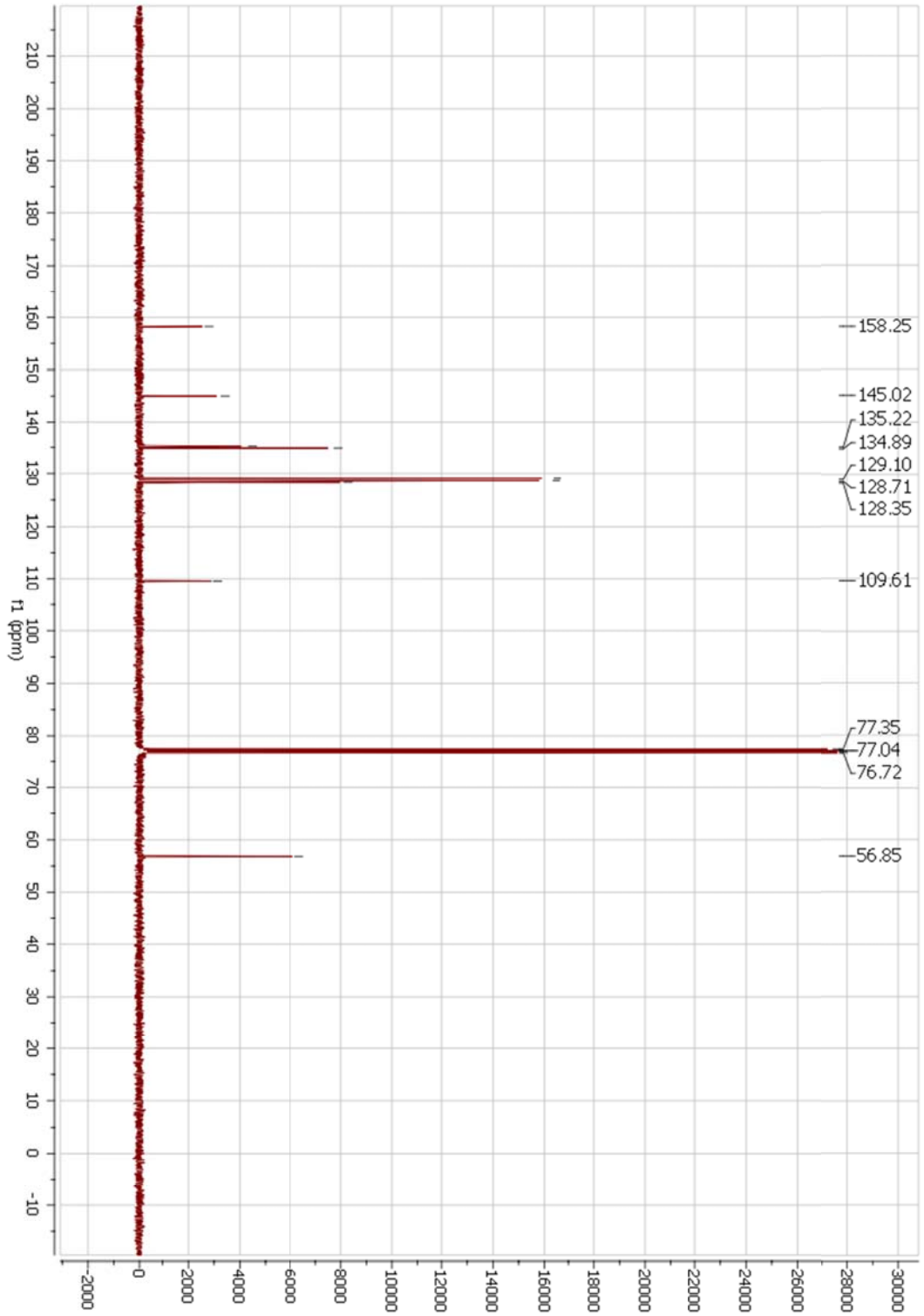

156.84
139.54
135.49
135.14
129.09
128.72
128.39
127.51
77.35
77.03
76.72
56.60
f1 (ppm)

2-Benzyl-5-chloro-4-iodopyridazin-3(2*H*)-one (**11b**)

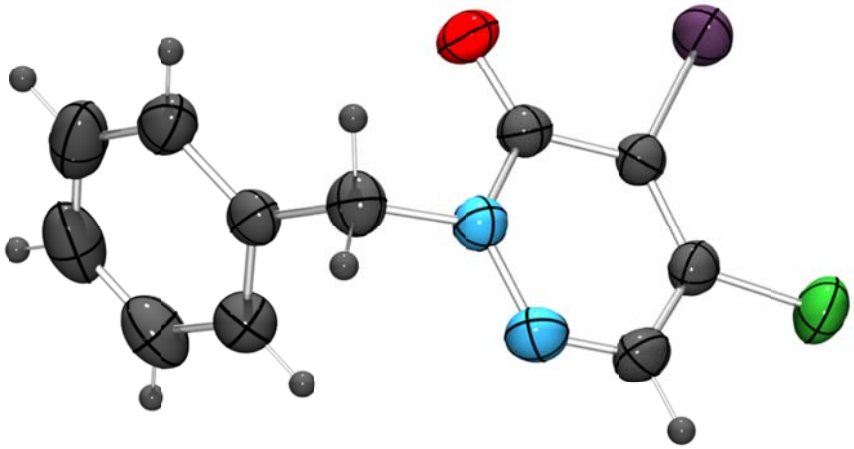
^{1}H-NMR



^{13}C-NMR


158.25
145.02
135.22
134.89
129.10
128.71
128.35
109.61
77.35
77.04
76.72
56.85
f1 (ppm)

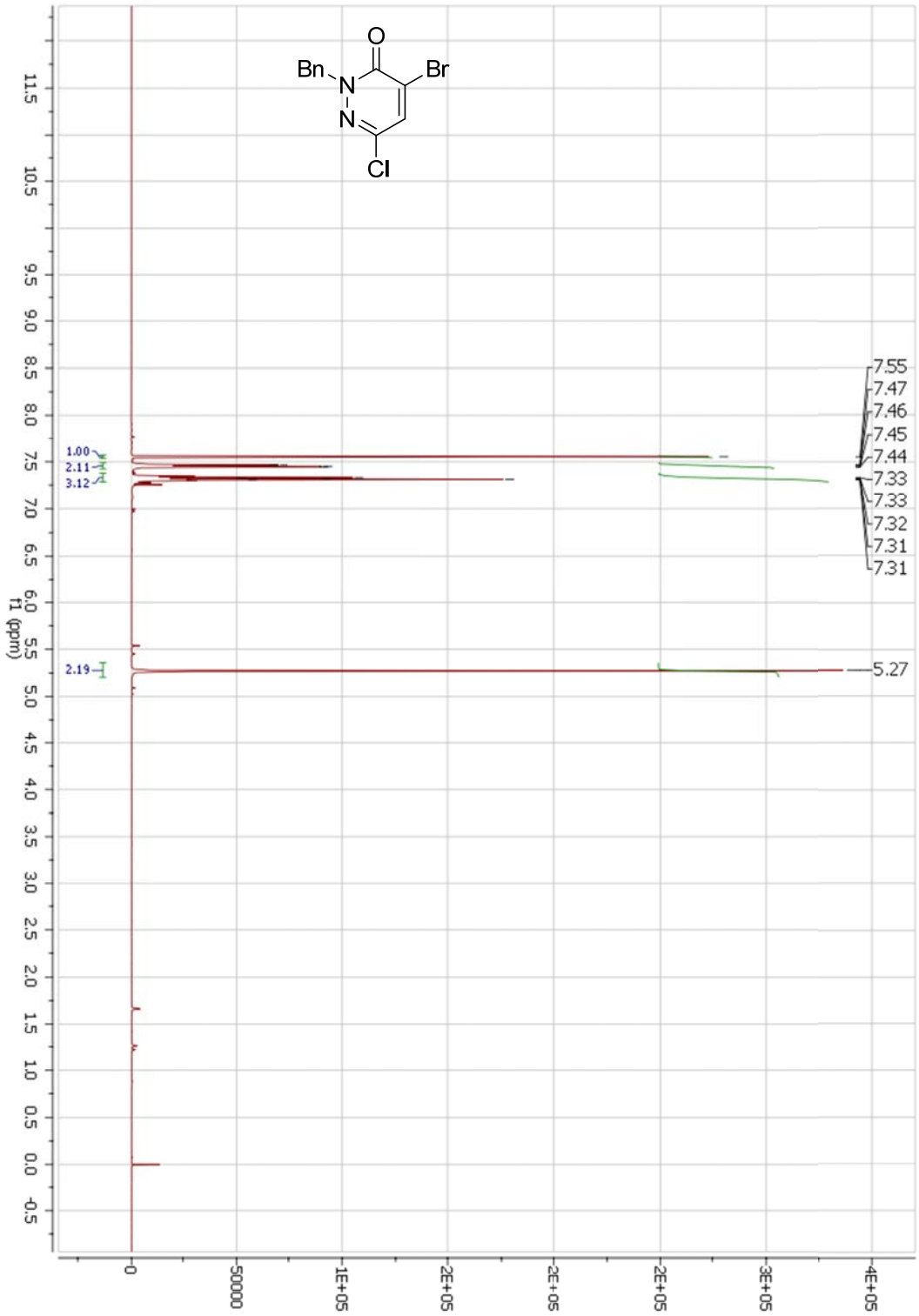
XRD structure



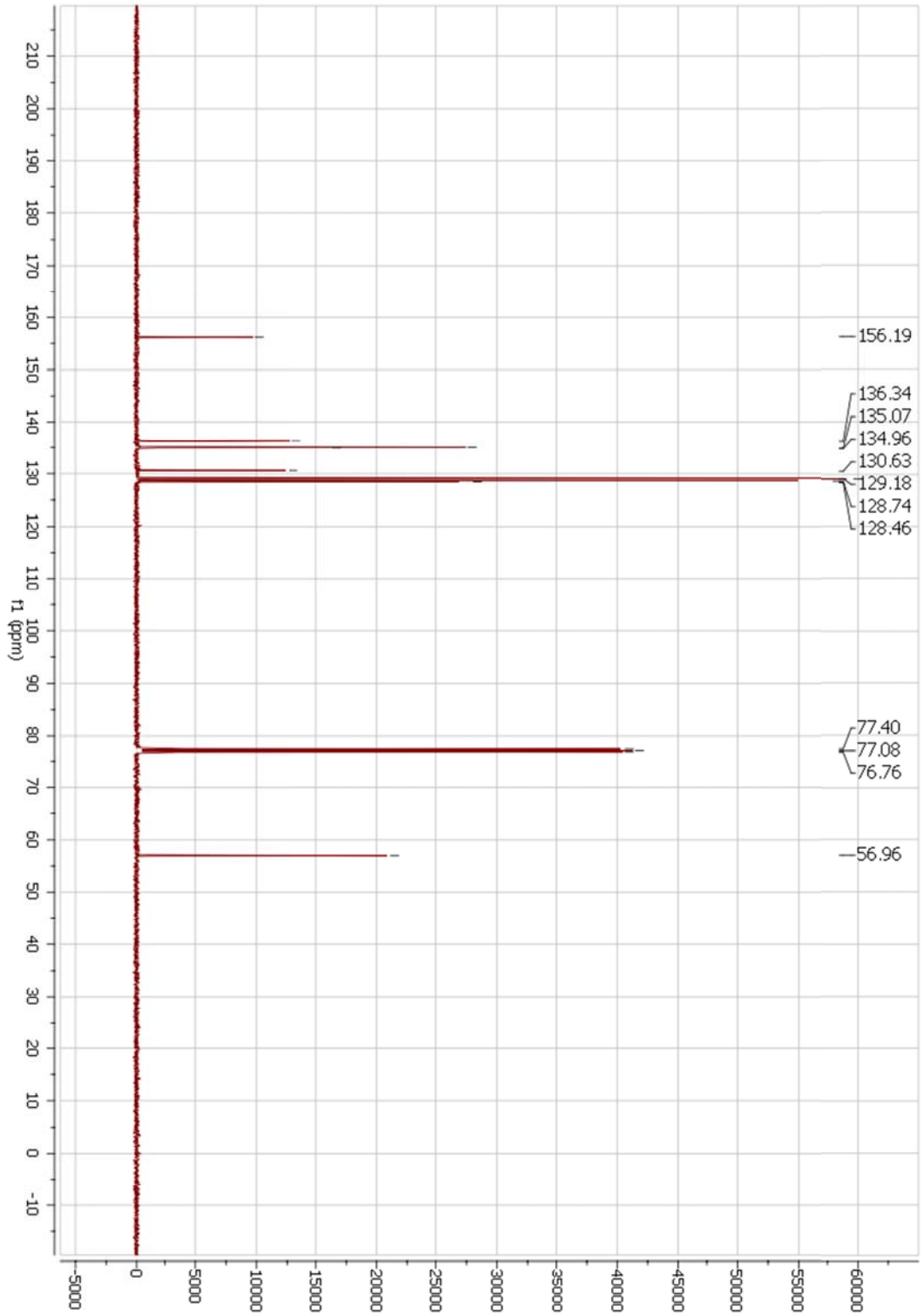
ORTEP-style plot of **11b** (C: grey, N: blue, O: red, F: light green, yellow, Cl: green, I: Purple). Thermal ellipsoids are drawn at 30% probability level, hydrogen atoms are drawn as spheres of 0.15 Å radius.

2-Benzyl-4-bromo-6-chloropyridazin-3(2*H*)-one (**12a**)

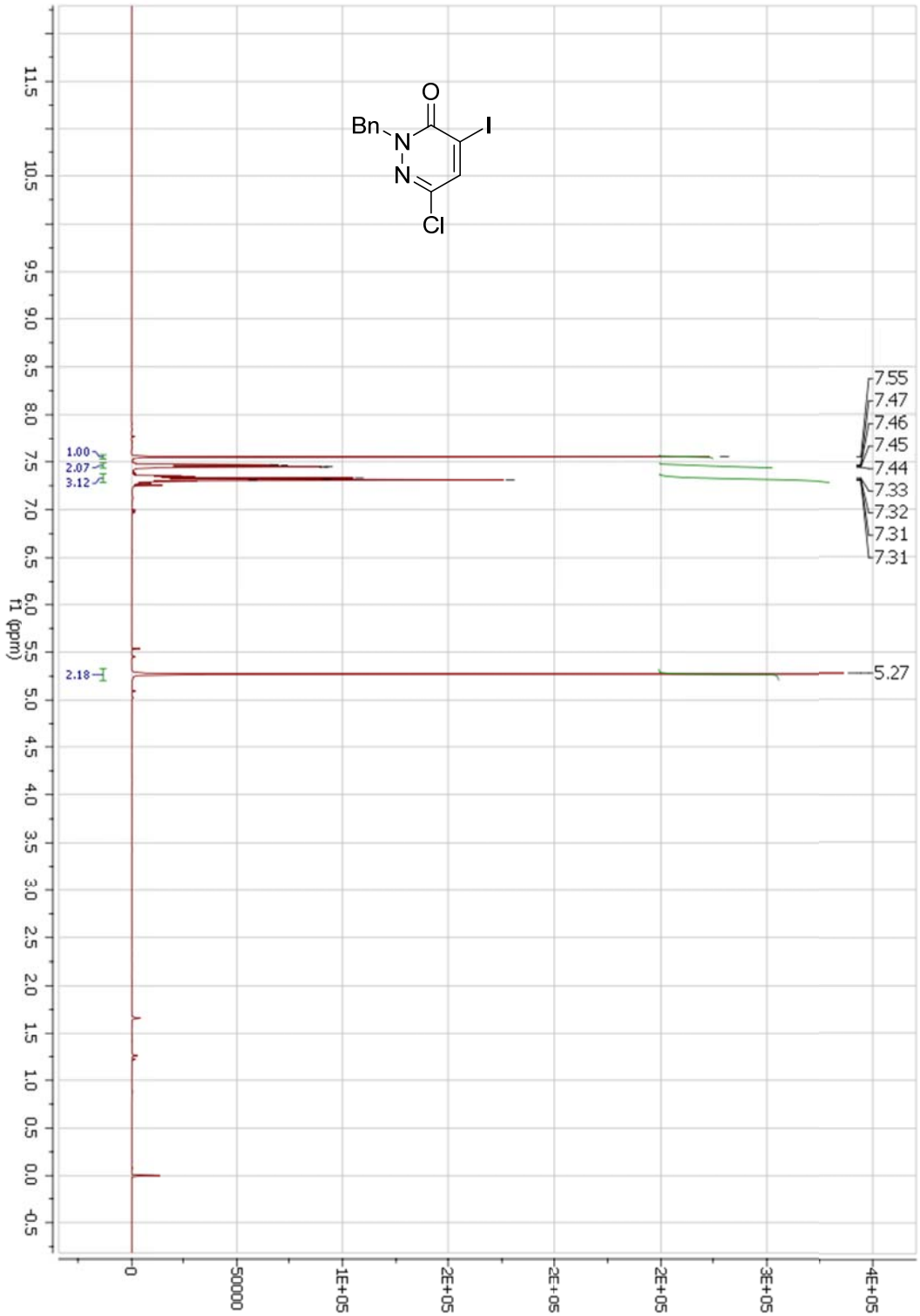
^{1}H-NMR



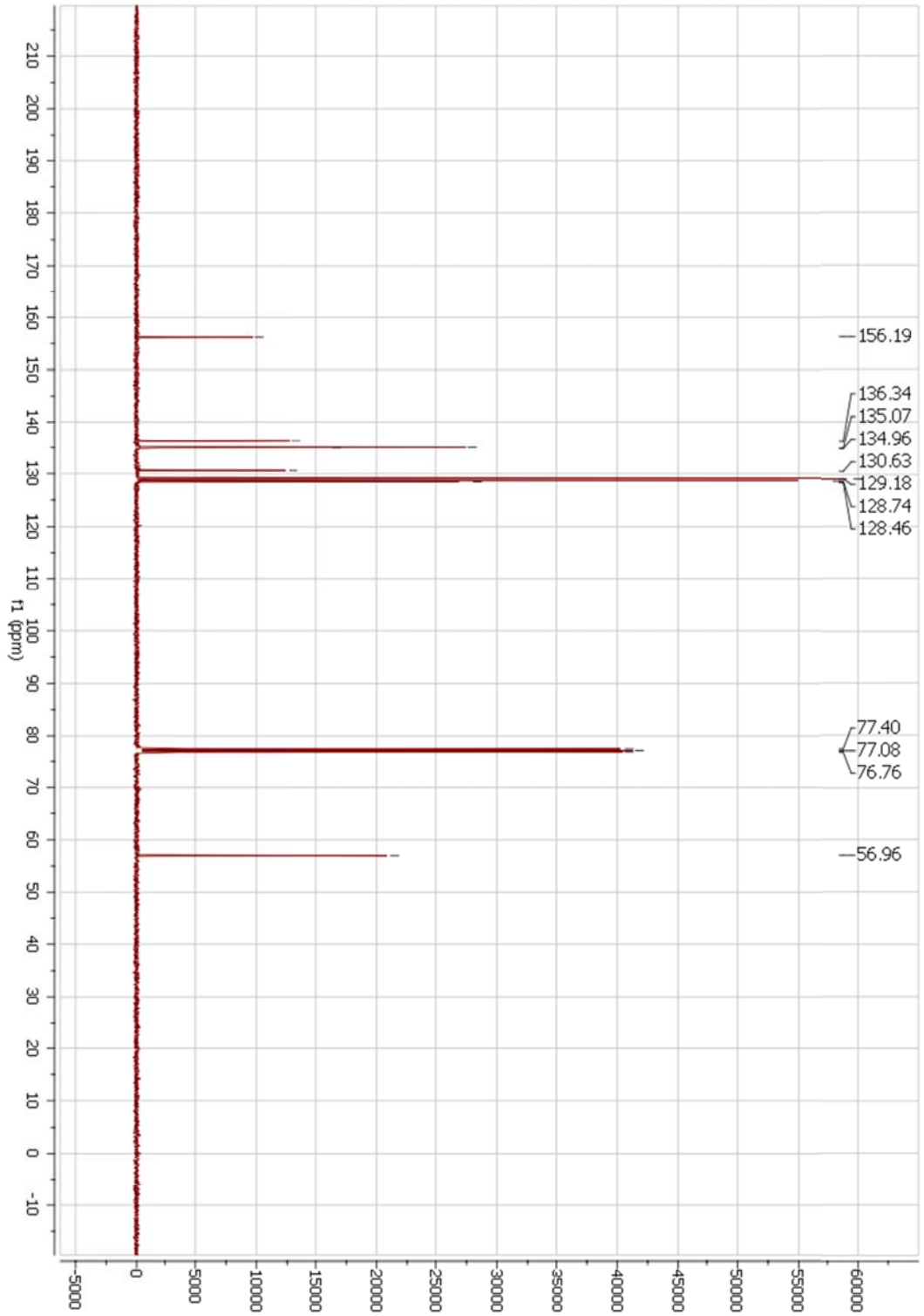
^{13}C-NMR


156.19
136.34
135.07
134.96
130.63
129.18
128.74
128.46
77.40
77.08
76.76
56.96
f1 (ppm)

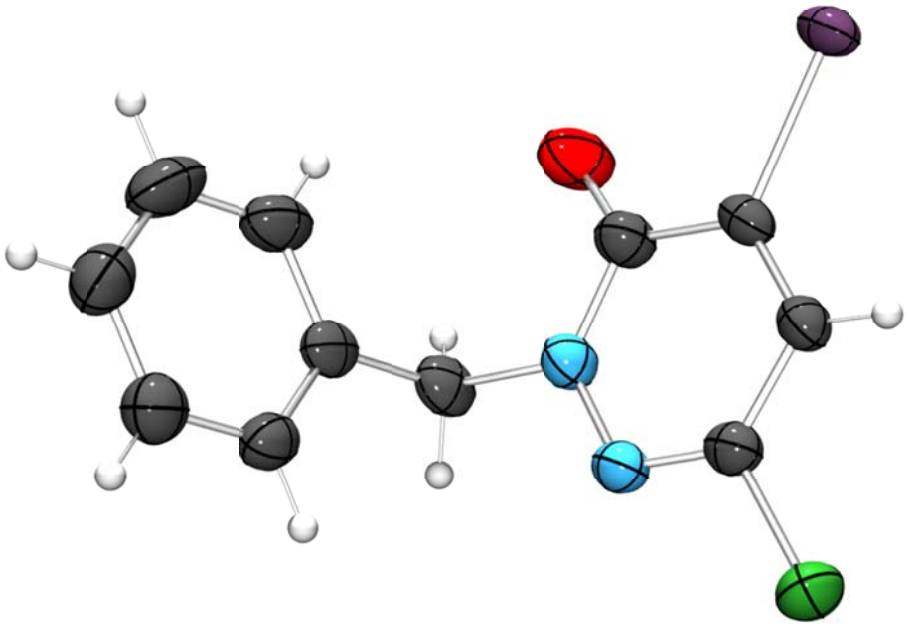
2-Benzyl-6-chloro-4-iodopyridazin-3(2*H*)-one (**12b**)
^{1}H-NMR



^{13}C-NMR


156.19
136.34
135.07
134.96
130.63
129.18
128.74
128.46
77.40
77.08
76.76
56.96
f1 (ppm)

XRD structure



ORTEP-style plot of **12b** (C: grey, N: blue, O: red, F: light green, yellow, Cl: green, I: Purple). Thermal ellipsoids are drawn at 30% probability level, hydrogen atoms are drawn as spheres of 0.15 Å radius.