

## Nickel-Catalyzed Reductive Conjugate Addition to Enones Via Allylnickel Intermediates

Ruja Shrestha,† Stephanie C. M. Dorn and Daniel J. Weix\*.

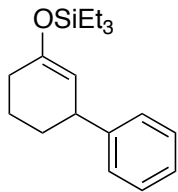
\*Department of Chemistry, University of Rochester, Rochester, NY 14627

†Present Address: Department of Chemistry, University of California, Berkeley, CA 94720

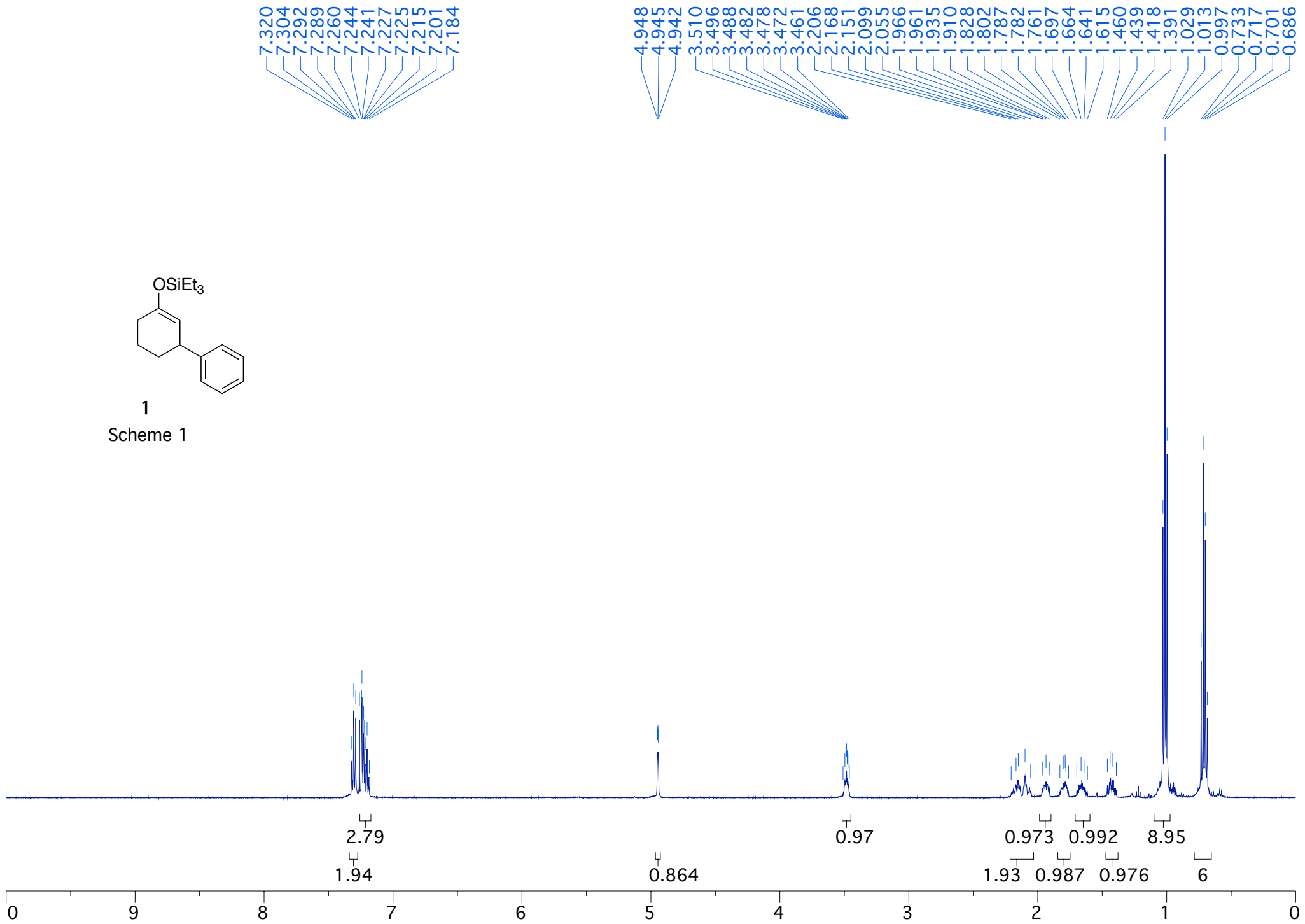
### Supporting Information – NMR Spectra

VIII.	NMR Spectra (separate pdf file)	
	Compound <b>1</b> <sup>1</sup> H NMR	S53
	Compound <b>1</b> <sup>13</sup> C NMR	S54
	Compound <b>1</b> IR spectrum	S55
	Compound <b>2</b> <sup>1</sup> H NMR	S56
	Compound <b>2</b> <sup>13</sup> C NMR	S57
	Compound <b>3</b> <sup>1</sup> H NMR	S58
	Compound <b>3</b> <sup>13</sup> C NMR	S59
	Compound <b>4</b> <sup>1</sup> H NMR	S60
	Compound <b>4</b> <sup>13</sup> C NMR	S61
	Compound <b>5</b> <sup>1</sup> H NMR	S62
	Compound <b>5</b> <sup>13</sup> C NMR	S63
	Compound <b>6</b> <sup>1</sup> H NMR	S64
	Compound <b>6</b> <sup>13</sup> C NMR	S65
	Compound <b>7</b> <sup>1</sup> H NMR	S66
	Compound <b>7</b> <sup>13</sup> C NMR	S67
	Compound <b>8</b> <sup>1</sup> H NMR	S68
	Compound <b>8</b> <sup>13</sup> C NMR	S69
	Compound <b>9</b> <sup>1</sup> H NMR	S70
	Compound <b>9</b> <sup>13</sup> C NMR	S71
	Compound <b>10</b> <sup>1</sup> H NMR	S72
	Compound <b>10</b> <sup>13</sup> C NMR	S73
	Compound <b>11</b> <sup>1</sup> H NMR	S74
	Compound <b>11</b> <sup>13</sup> C NMR	S75
	Compound <b>12</b> <sup>1</sup> H NMR	S76
	Compound <b>12</b> <sup>13</sup> C NMR	S77
	Compound <b>13</b> <sup>1</sup> H NMR	S78
	Compound <b>13</b> <sup>13</sup> C NMR	S79
	Compound <b>13</b> <sup>19</sup> F NMR	S80
	Compound <b>14</b> <sup>1</sup> H NMR	S81
	Compound <b>14</b> <sup>13</sup> C NMR	S82
	Compound <b>15</b> <sup>1</sup> H NMR	S83
	Compound <b>15</b> <sup>13</sup> C NMR	S84
	Compound <b>16</b> <sup>1</sup> H NMR	S85
	Compound <b>16</b> <sup>13</sup> C NMR	S86
	Compound <b>17</b> <sup>1</sup> H NMR	S87
	Compound <b>17</b> <sup>13</sup> C NMR	S88
	Compound <b>18</b> <sup>1</sup> H NMR	S89
	Compound <b>18</b> <sup>13</sup> C NMR	S90
	Compound <b>18</b> IR spectrum	S91
	Compound <b>19</b> <sup>1</sup> H NMR	S92
	Compound <b>19</b> <sup>13</sup> C NMR	S93
	Compound <b>20</b> <sup>1</sup> H NMR	S94
	Compound <b>20</b> <sup>13</sup> C NMR	S95
	Compound <b>21</b> <sup>1</sup> H NMR	S96

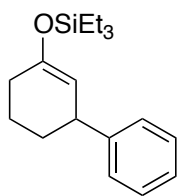
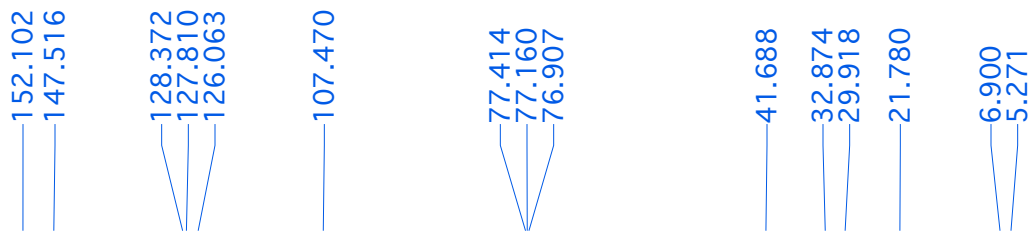
Compound <b>21</b>	<sup>13</sup> C NMR	S97
Compound <b>22</b>	<sup>1</sup> H NMR	S98
Compound <b>22</b>	<sup>13</sup> C NMR	S99
Compound <b>23</b>	<sup>1</sup> H NMR	S100
Compound <b>23</b>	<sup>13</sup> C NMR	S101
Compound <b>23</b>	<sup>19</sup> F NMR	S102
Compound <b>24</b>	<sup>1</sup> H NMR	S103
Compound <b>24</b>	<sup>13</sup> C NMR	S104
Compound <b>25</b>	<sup>1</sup> H NMR	S105
Compound <b>25</b>	<sup>13</sup> C NMR	S106
Compound <b>25</b>	<sup>19</sup> F NMR	S107
Compound <b>26</b>	<sup>1</sup> H NMR	S108
Compound <b>26</b>	<sup>13</sup> C NMR	S109
Compound <b>26</b>	<sup>19</sup> F NMR	S110
Compound <b>27</b>	<sup>1</sup> H NMR	S111
Compound <b>27</b>	<sup>13</sup> C NMR	S112
Compound <b>27</b>	<sup>19</sup> F NMR	S113
Compound <b>28</b>	<sup>1</sup> H NMR	S114
Compound <b>28</b>	<sup>13</sup> C NMR	S115
Compound <b>29</b>	<sup>1</sup> H NMR	S116
Compound <b>29</b>	<sup>13</sup> C NMR	S117
Compound <b>30</b>	<sup>1</sup> H NMR	S118
Compound <b>30</b>	<sup>13</sup> C NMR	S119
Compound <b>31</b>	<sup>1</sup> H NMR	S120
Compound <b>31</b>	<sup>13</sup> C NMR	S121
Compound <b>31</b>	<sup>19</sup> F NMR	S122
Compound <b>32</b>	<sup>1</sup> H NMR	S123
Compound <b>32</b>	<sup>13</sup> C NMR	S124
Compound <b>33</b>	<sup>1</sup> H NMR	S125
Compound <b>33</b>	<sup>13</sup> C NMR	S126
Compound <b>34</b>	<sup>1</sup> H NMR	S127
Compound <b>34</b>	<sup>13</sup> C NMR	S128

**1**

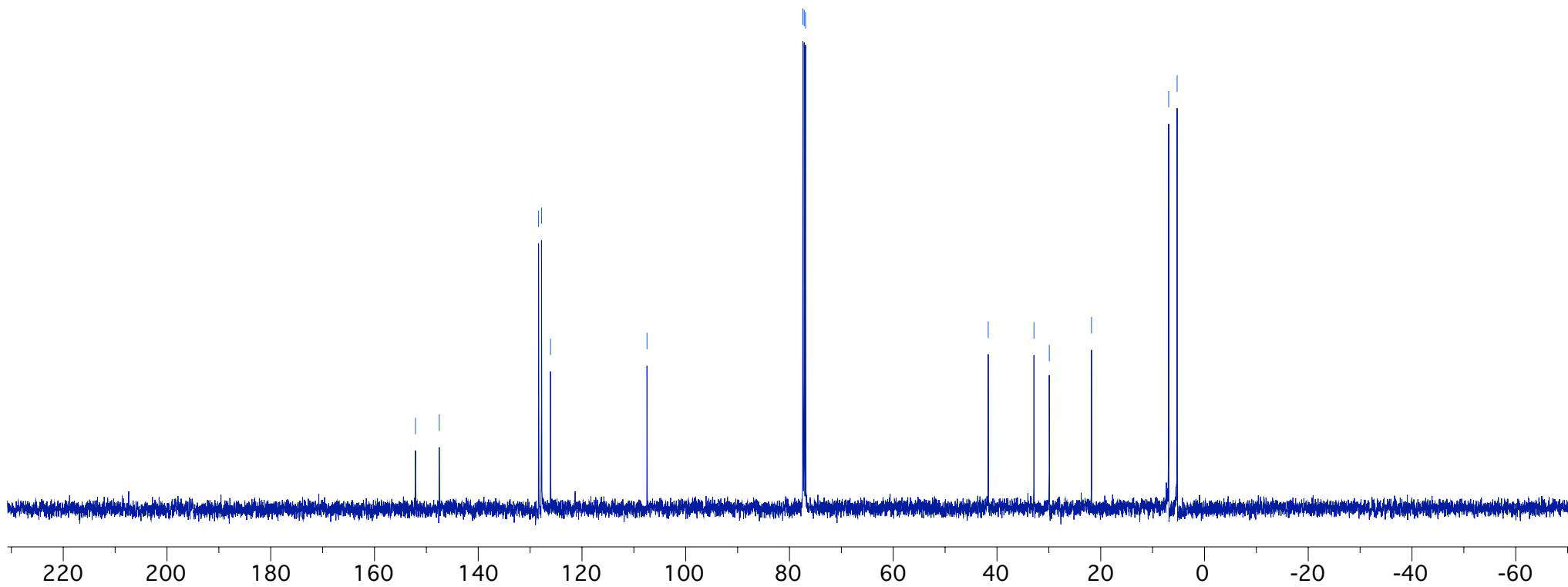
Scheme 1

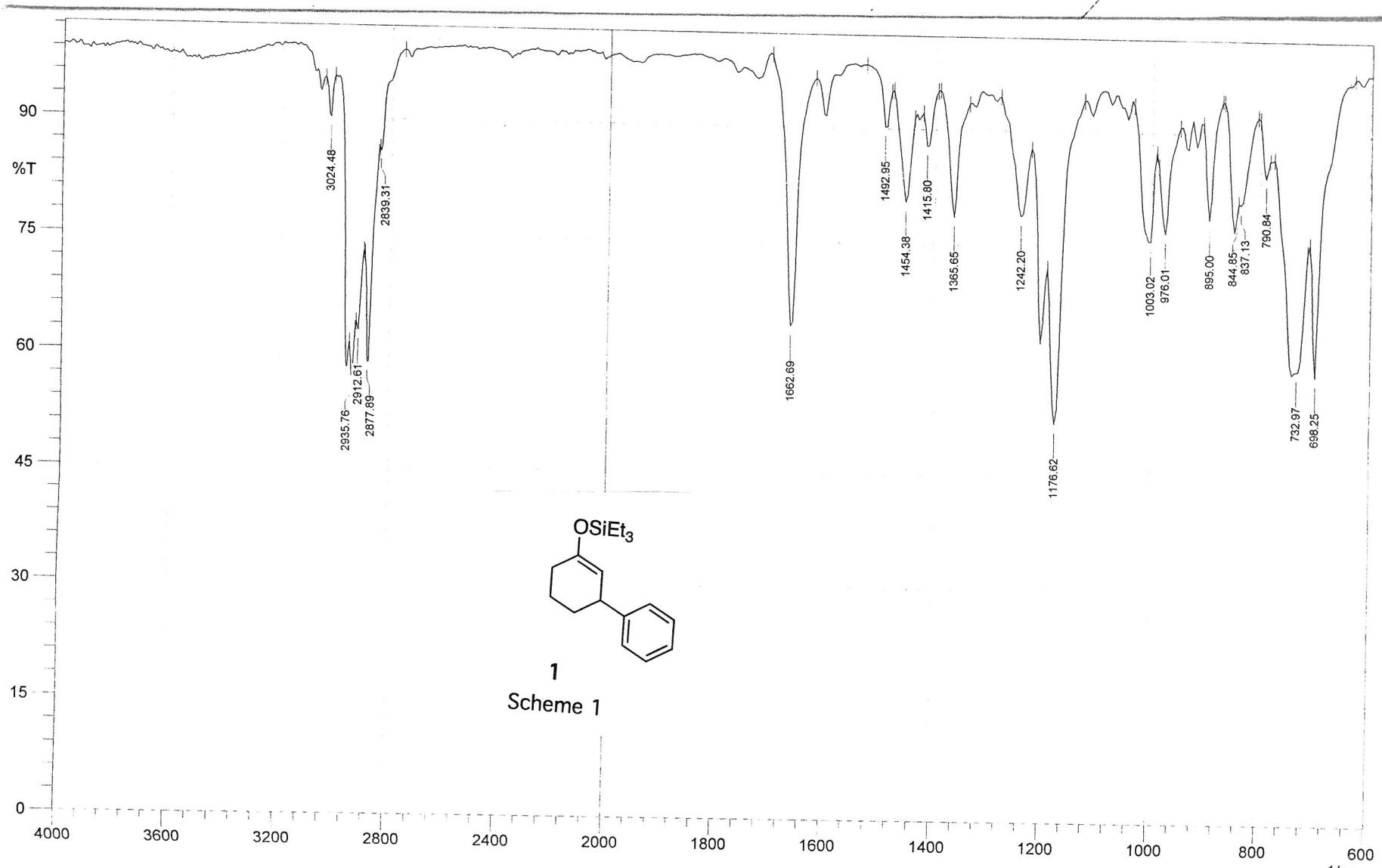


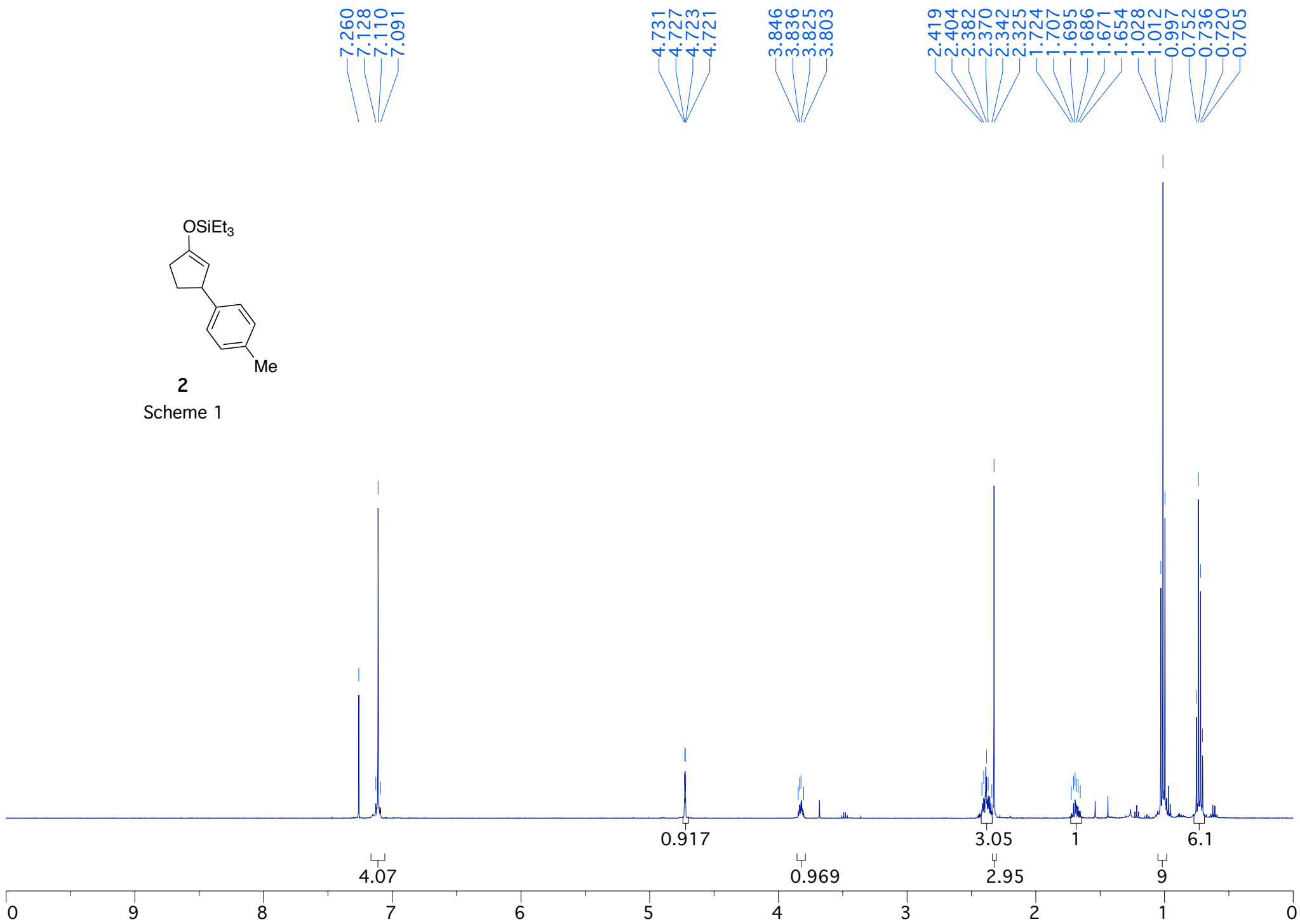
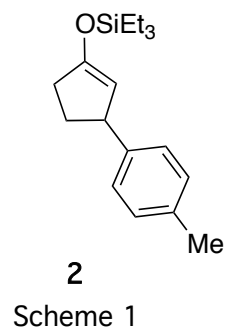
S54



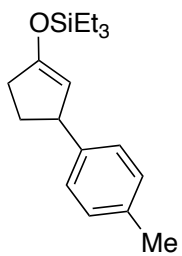
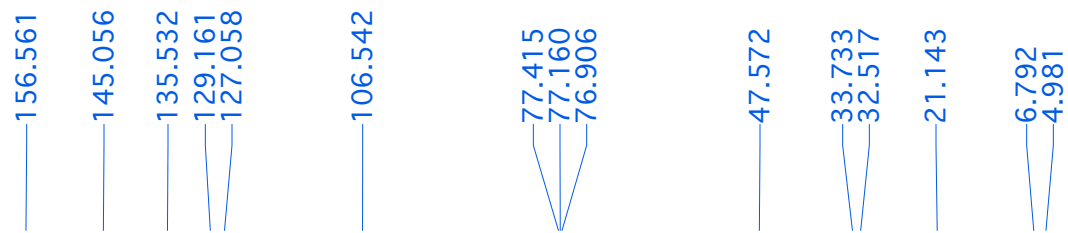
**1**  
Scheme 1



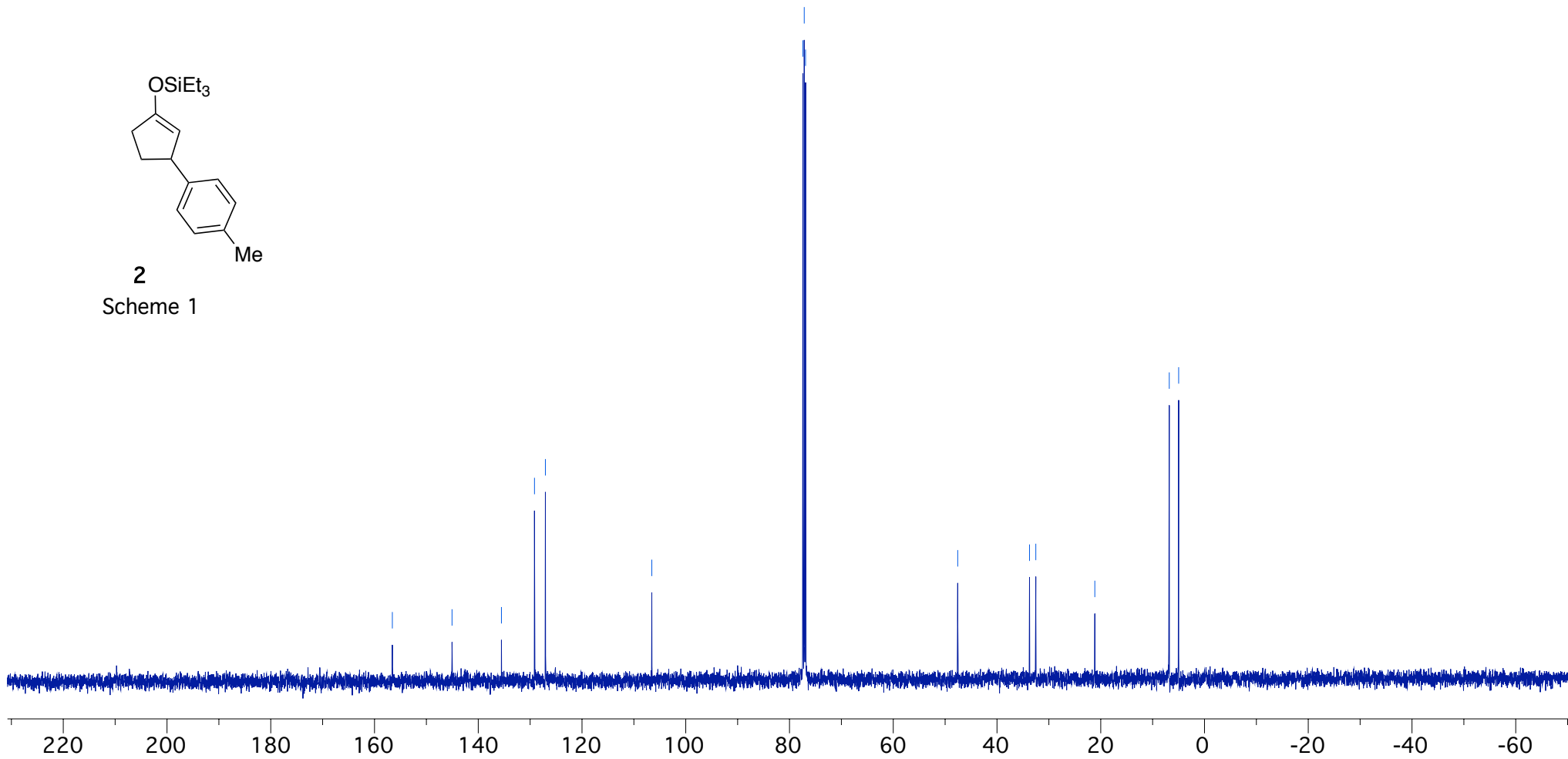


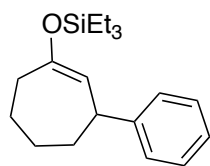


S57

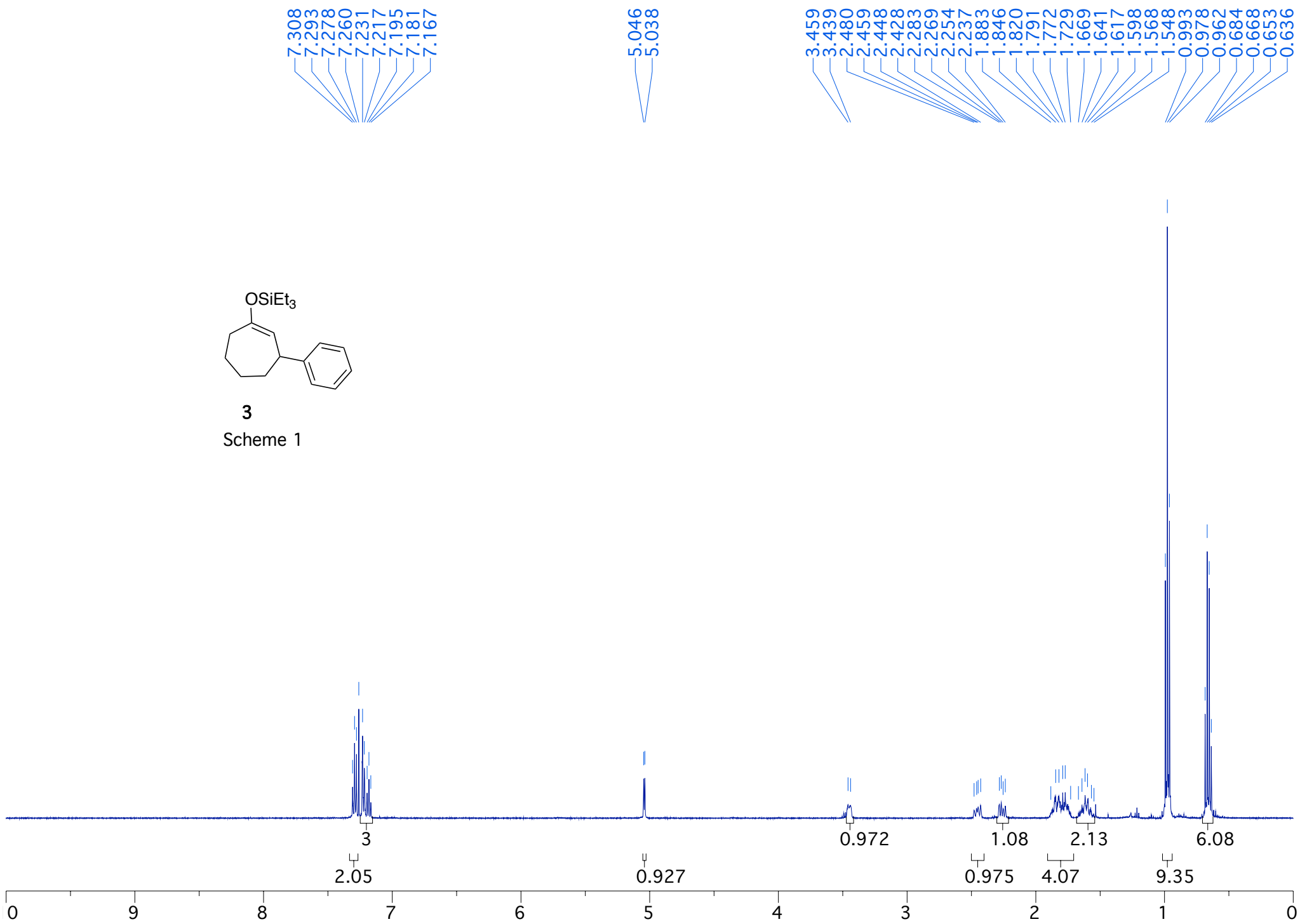


2  
Scheme 1



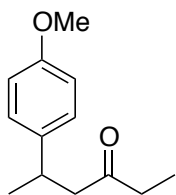
**3**

Scheme 1

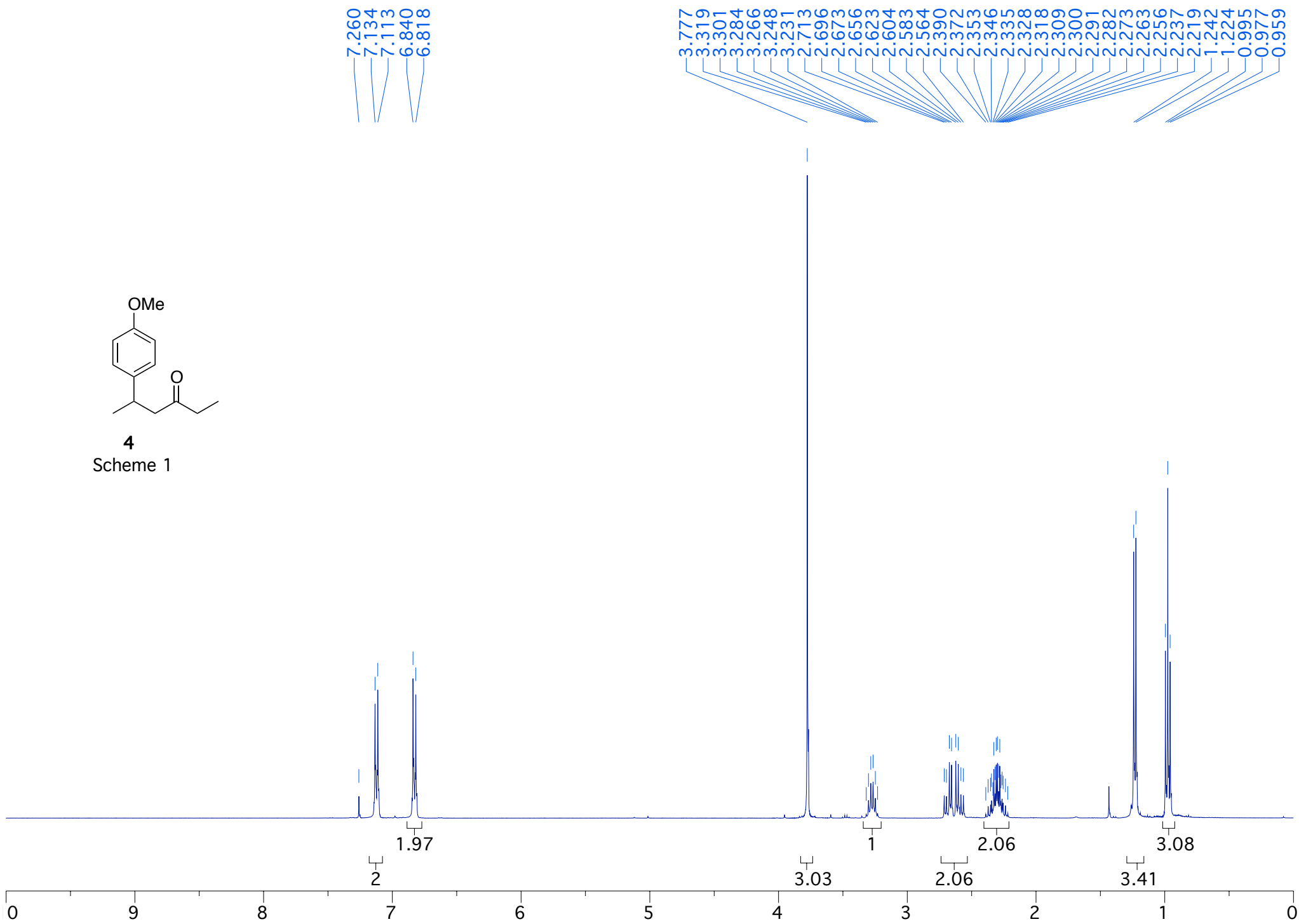


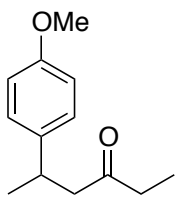




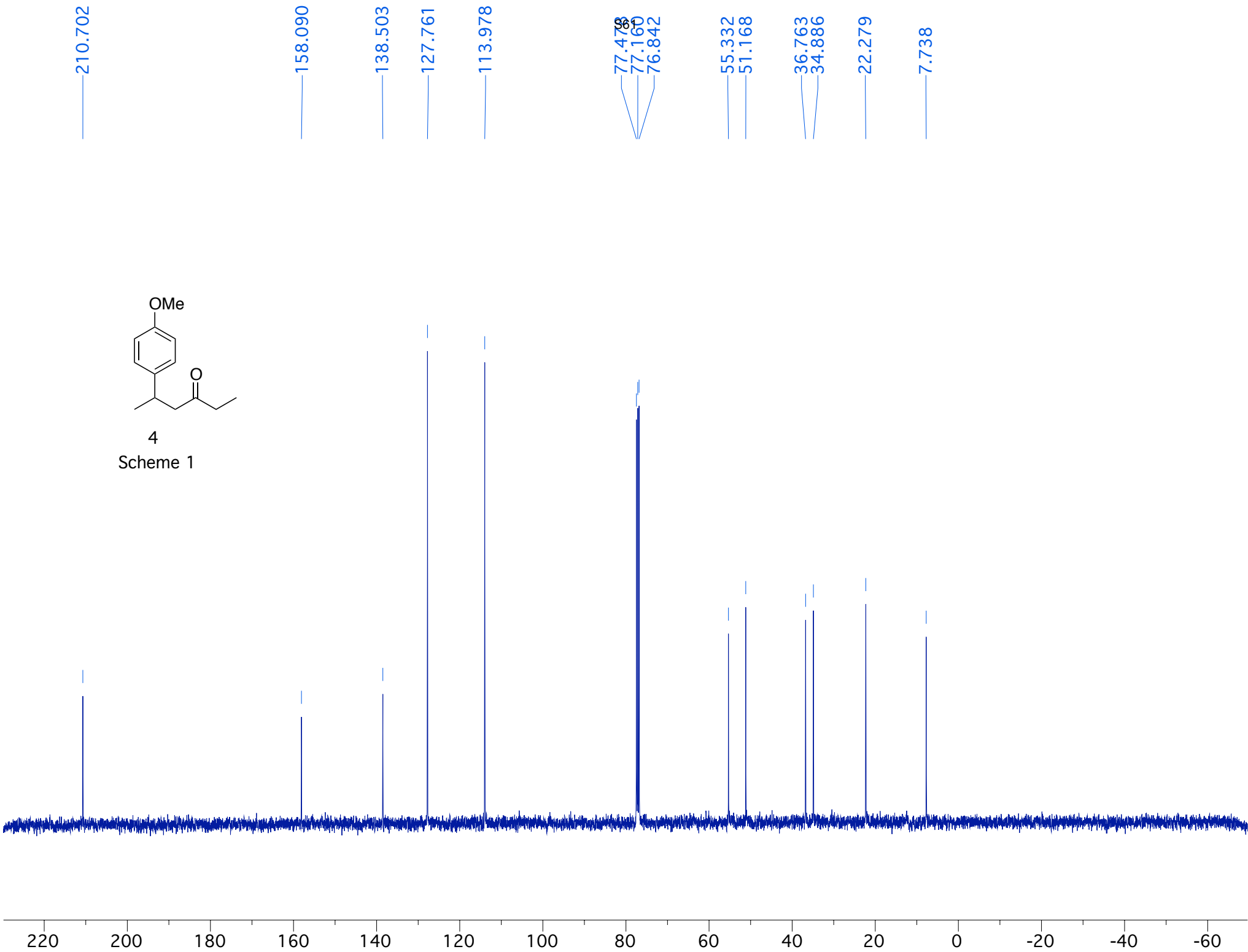
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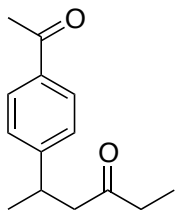
Scheme 1



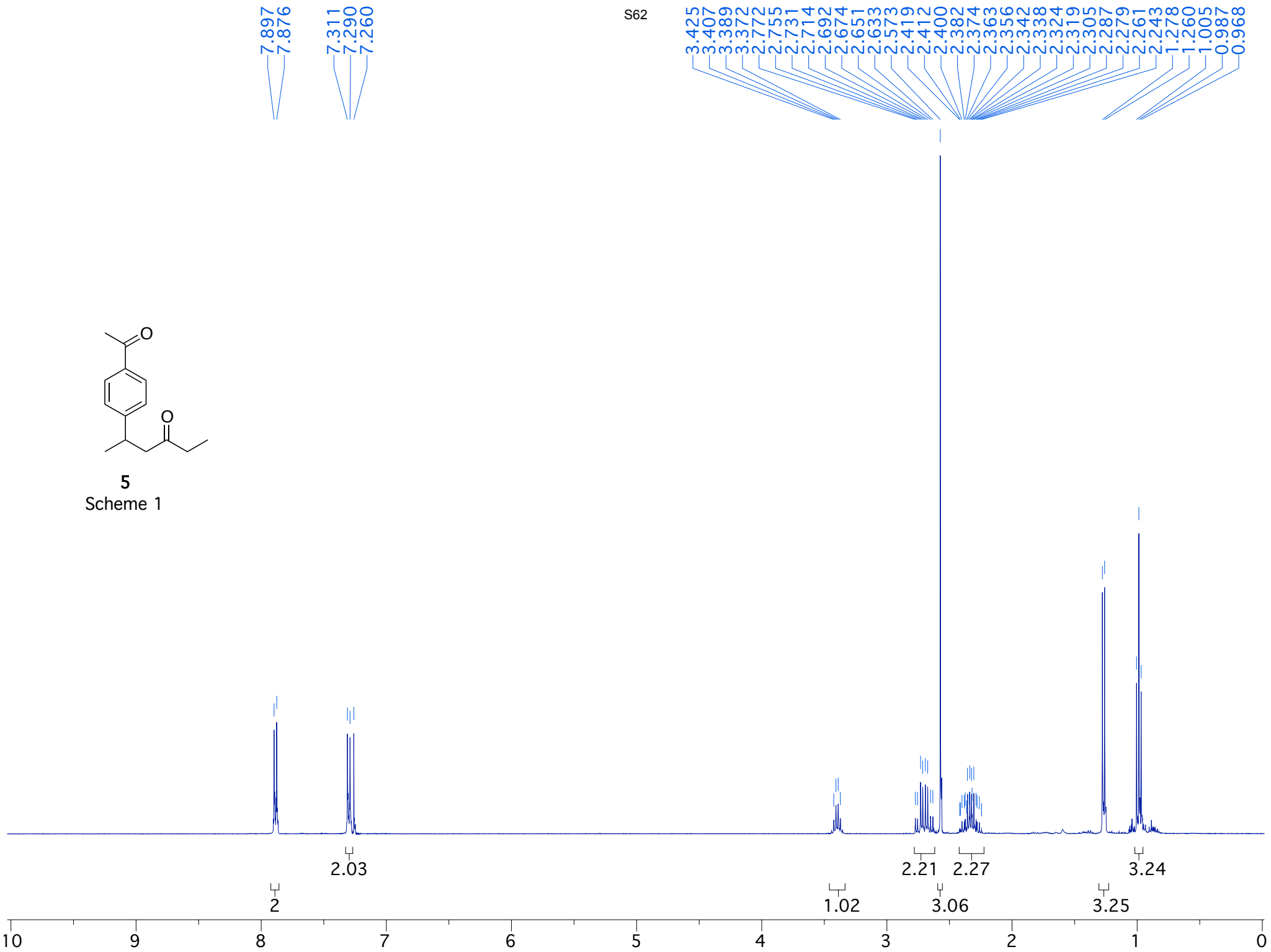


4  
Scheme 1





5  
Scheme 1



209.754

197.709

152.070

135.450

128.725

127.083

77.478

77.161

76.842

50.214

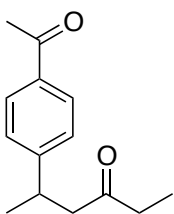
36.633

35.362

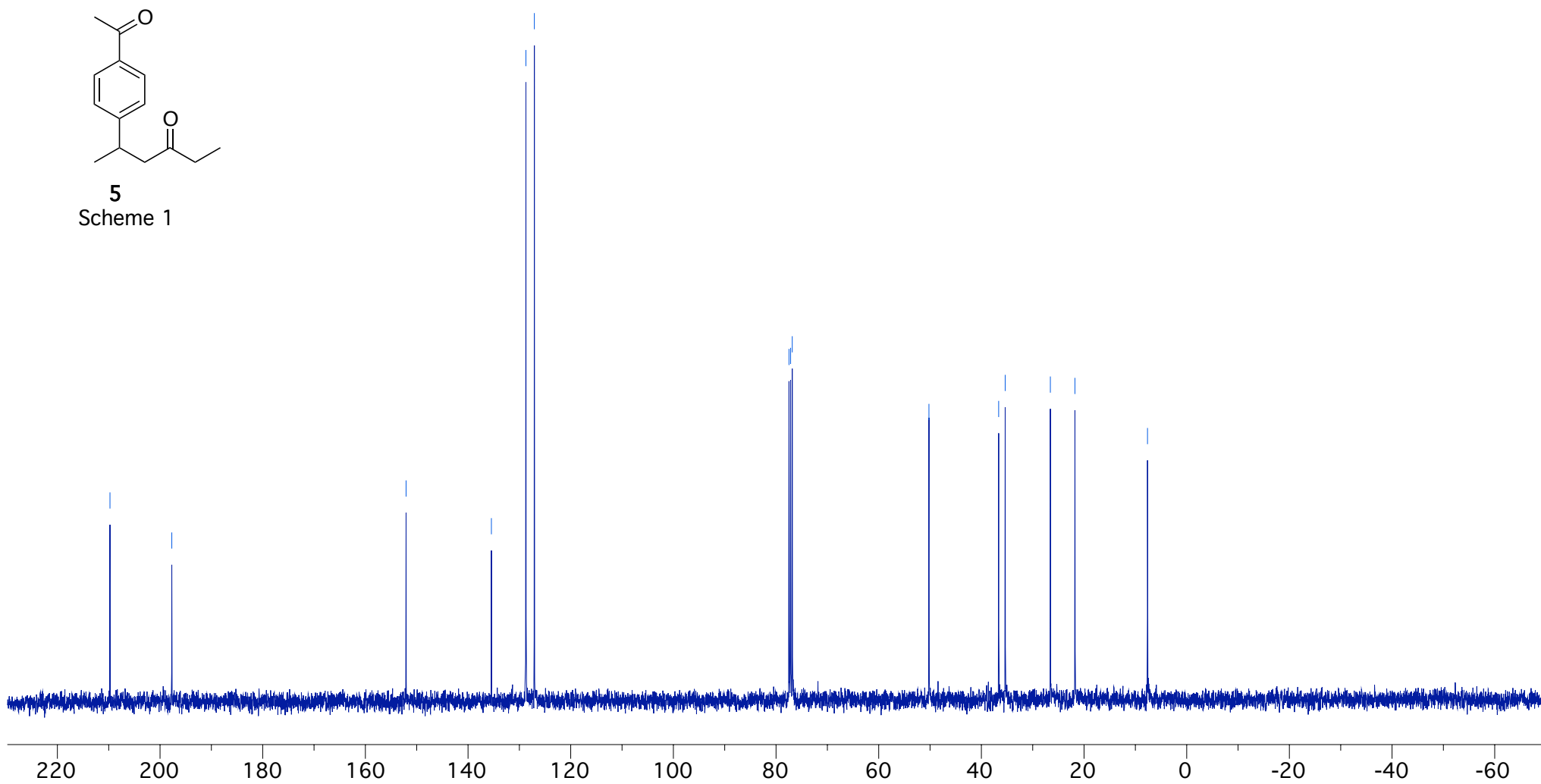
26.562

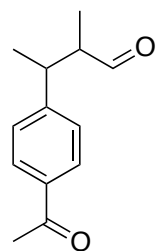
21.778

7.637



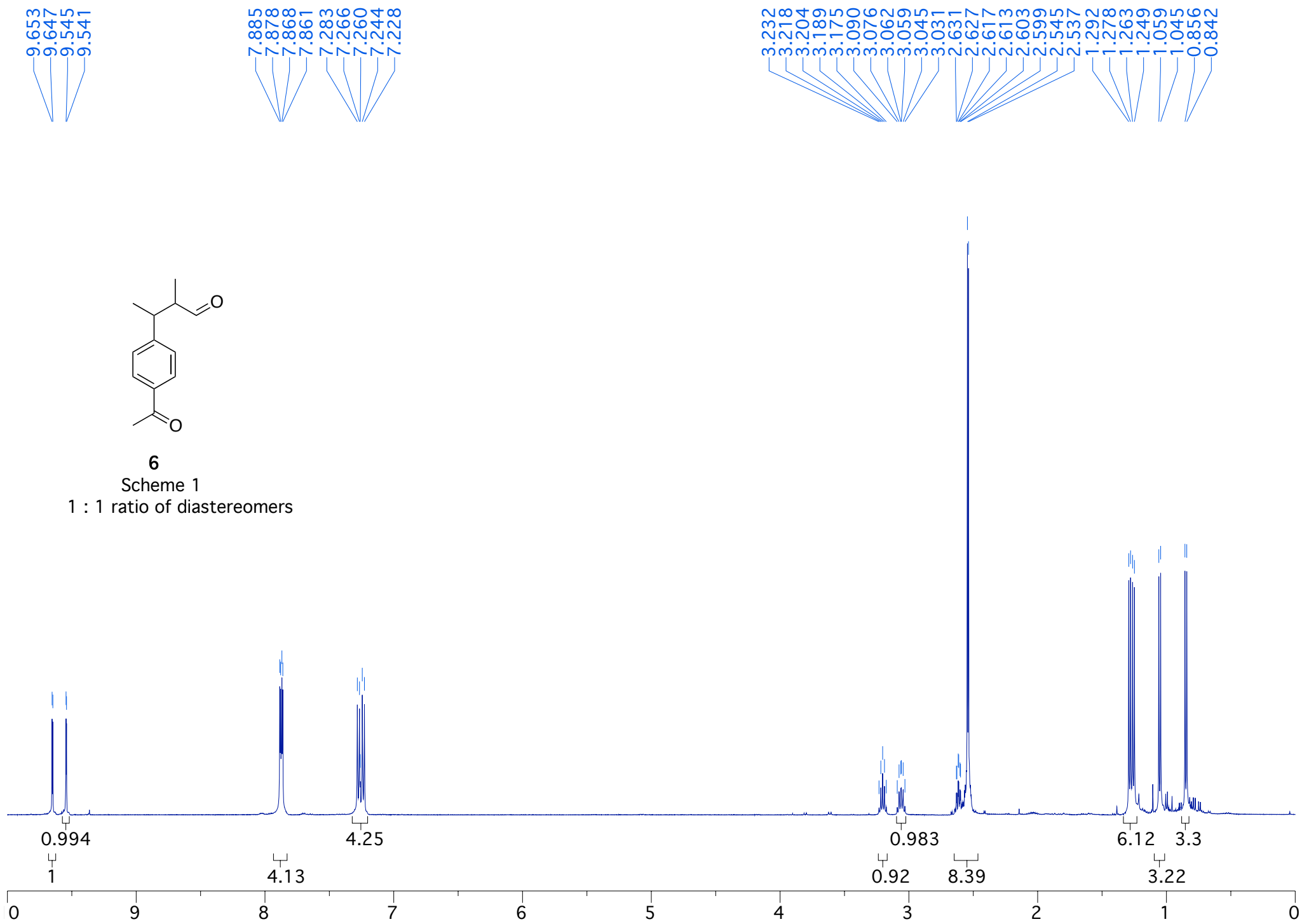
**5**  
Scheme 1



**6**

Scheme 1

1 : 1 ratio of diastereomers



204.116  
203.988  
197.676

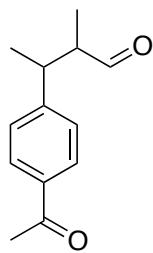
150.012  
149.405  
135.755  
135.650  
128.721  
127.893  
127.715

77.415  
77.160  
76.905

52.520  
52.263

40.779  
40.018

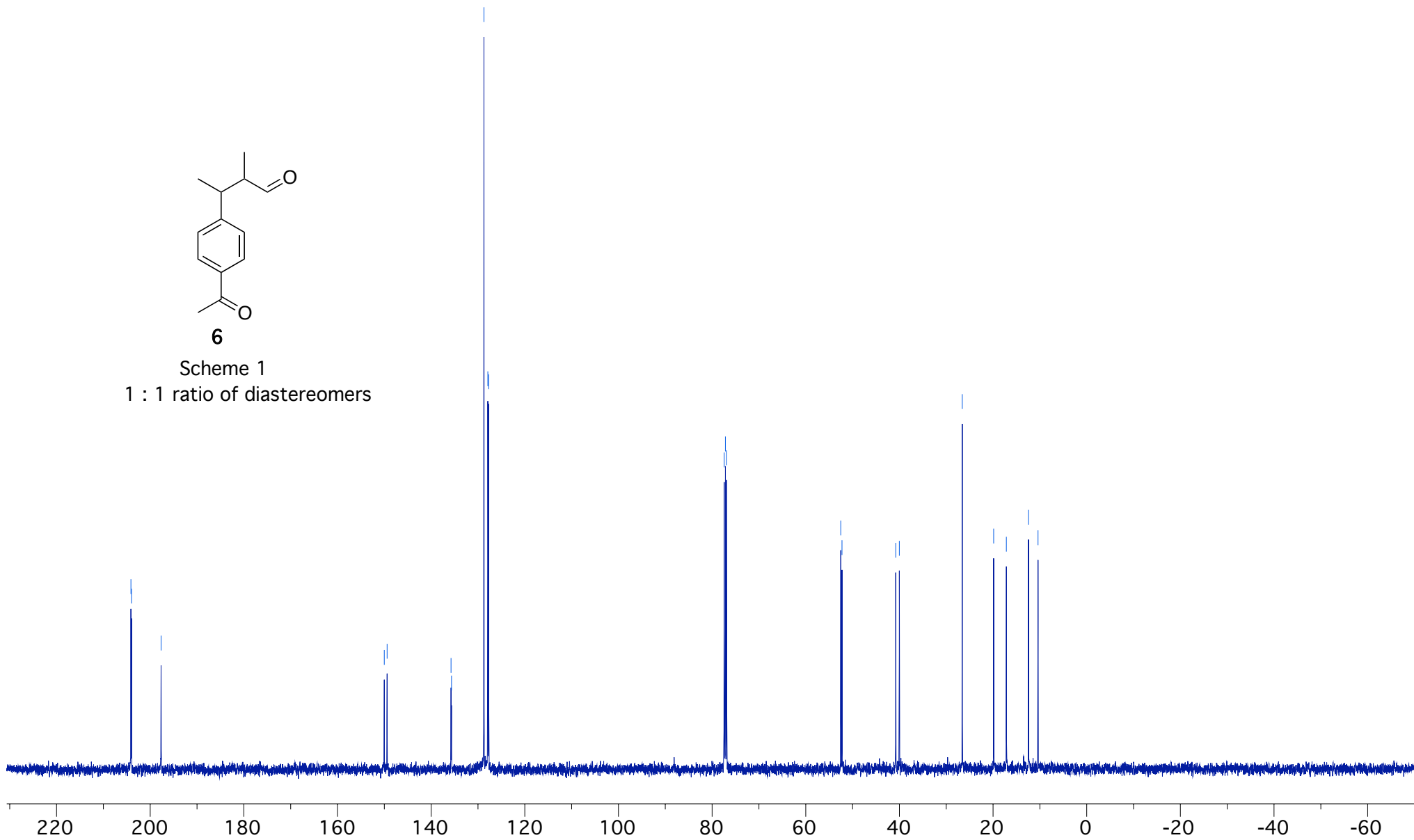
26.574  
19.869  
17.162  
12.435  
10.396

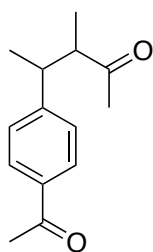


**6**

Scheme 1

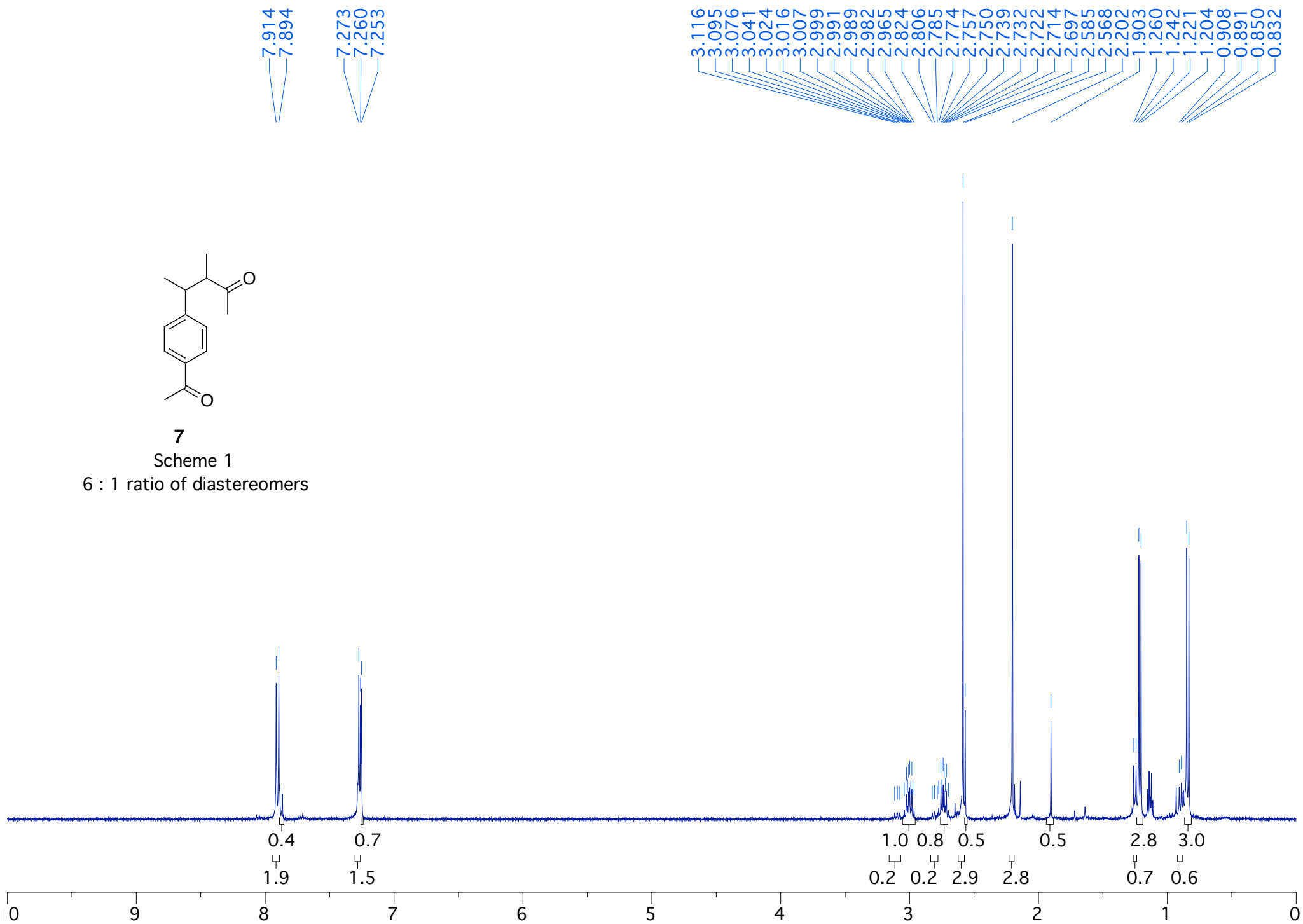
1 : 1 ratio of diastereomers



**7**

Scheme 1

6 : 1 ratio of diastereomers





212.301

197.823

150.466

135.804

128.825

127.937

77.413

77.160

76.906

53.636

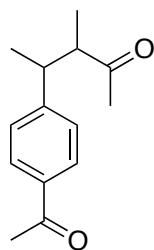
42.789

29.549

26.694

20.566

16.076

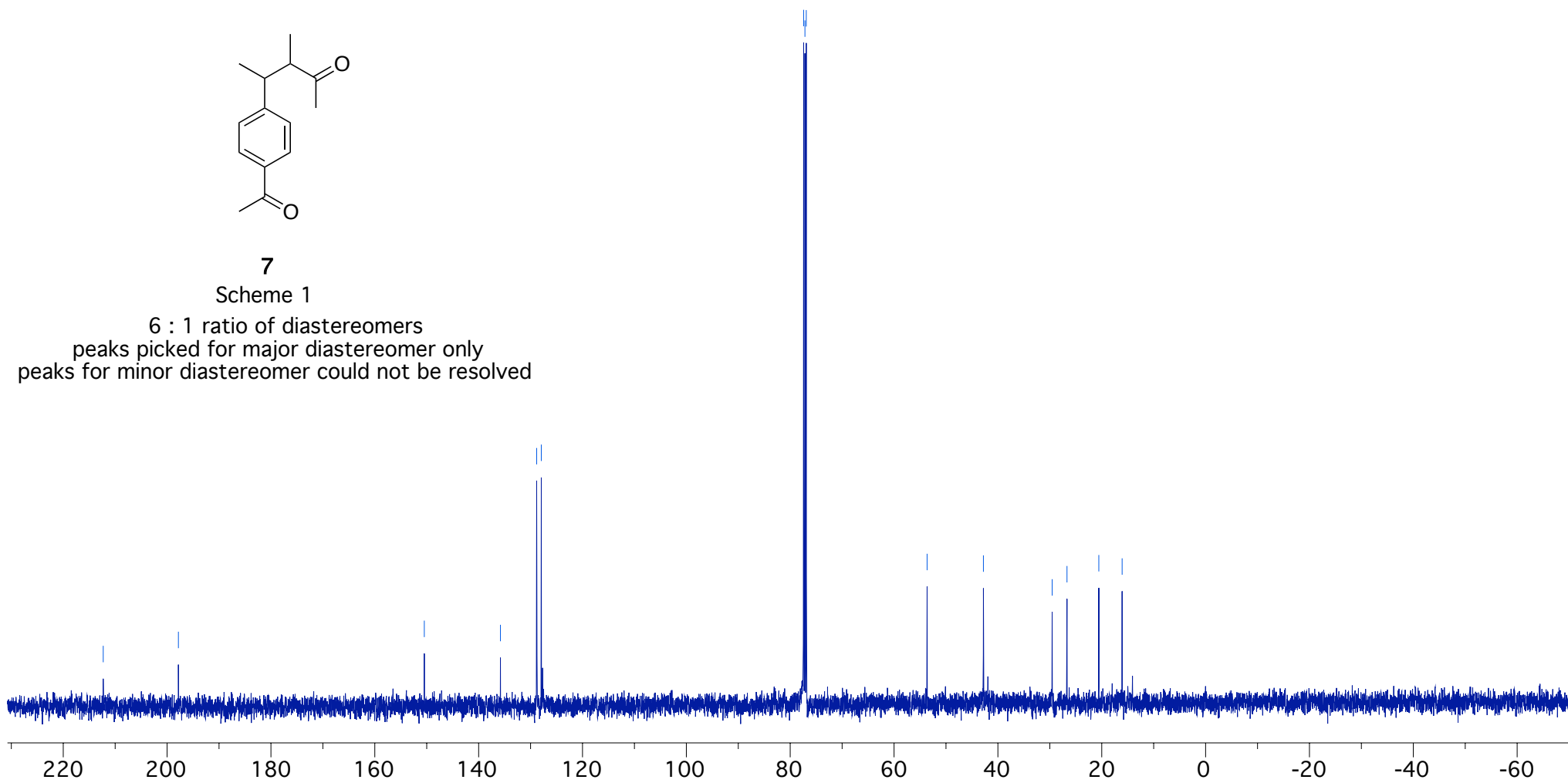
**7**

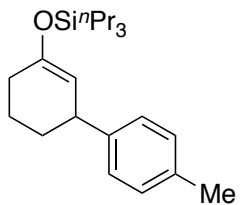
Scheme 1

6 : 1 ratio of diastereomers

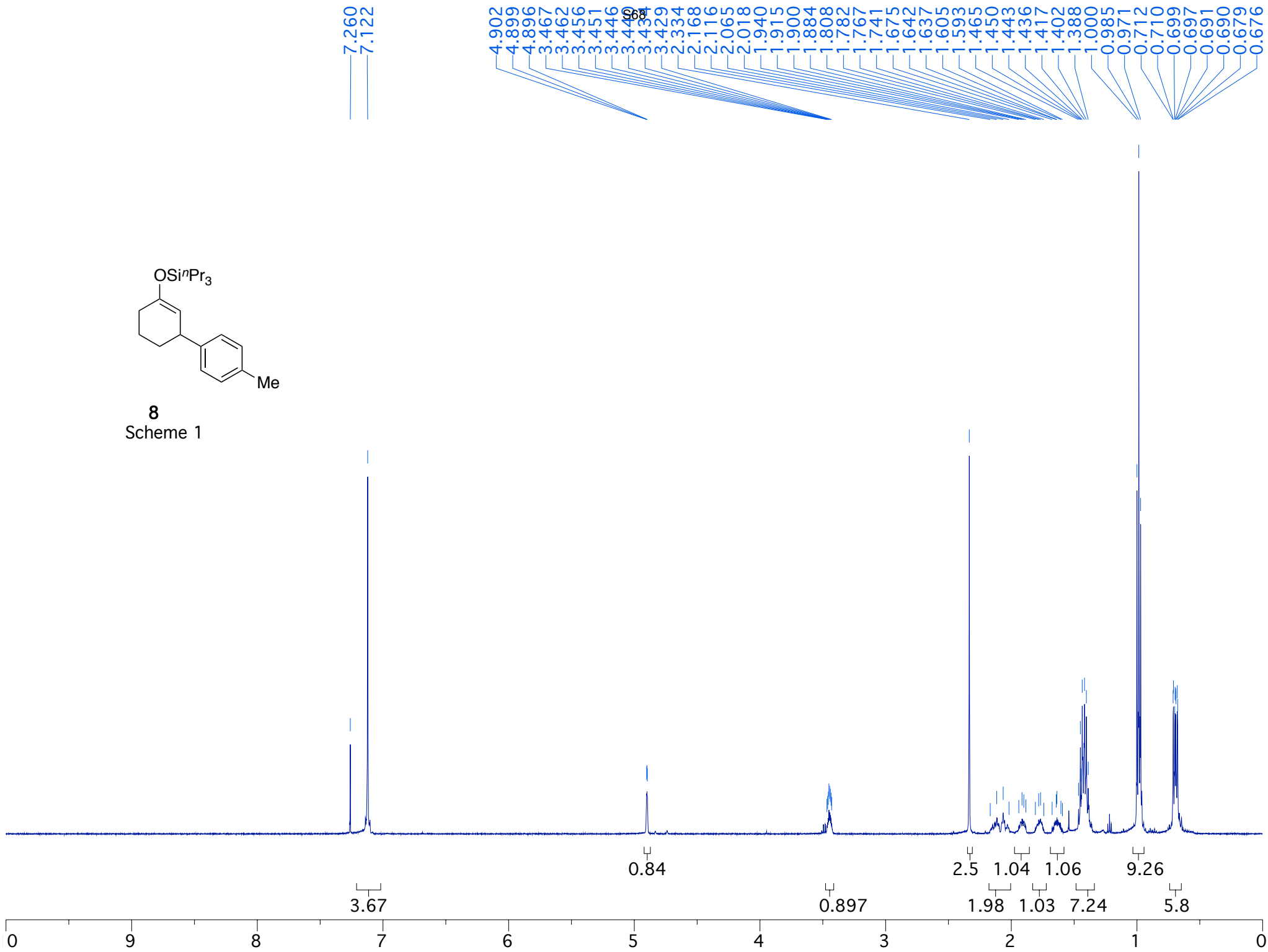
peaks picked for major diastereomer only

peaks for minor diastereomer could not be resolved

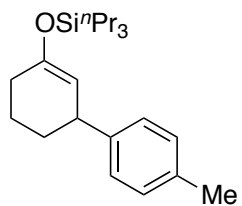
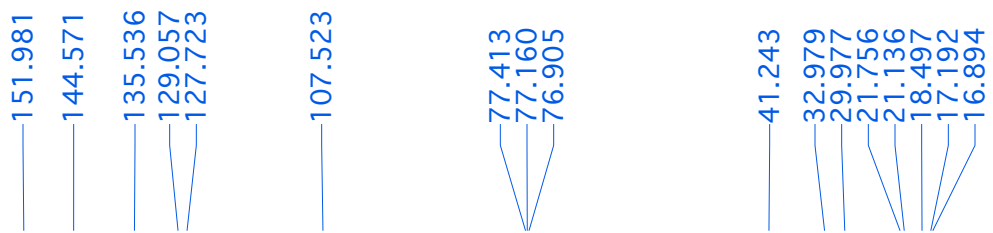




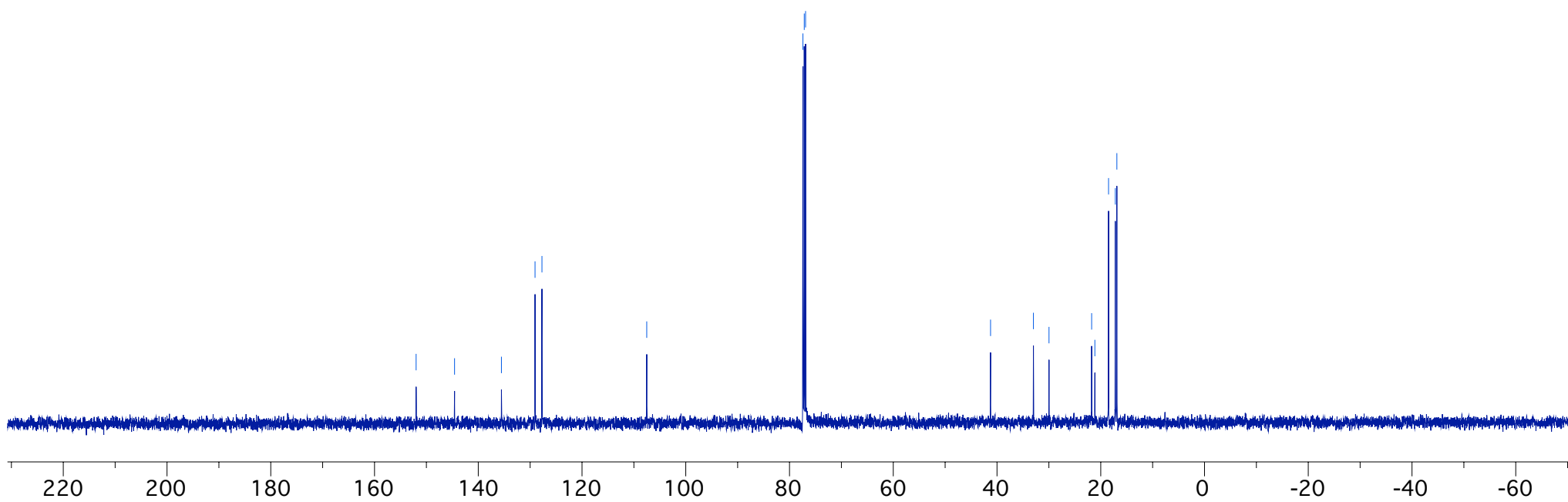
**8**  
Scheme 1

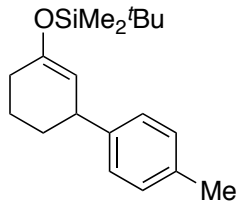


S69

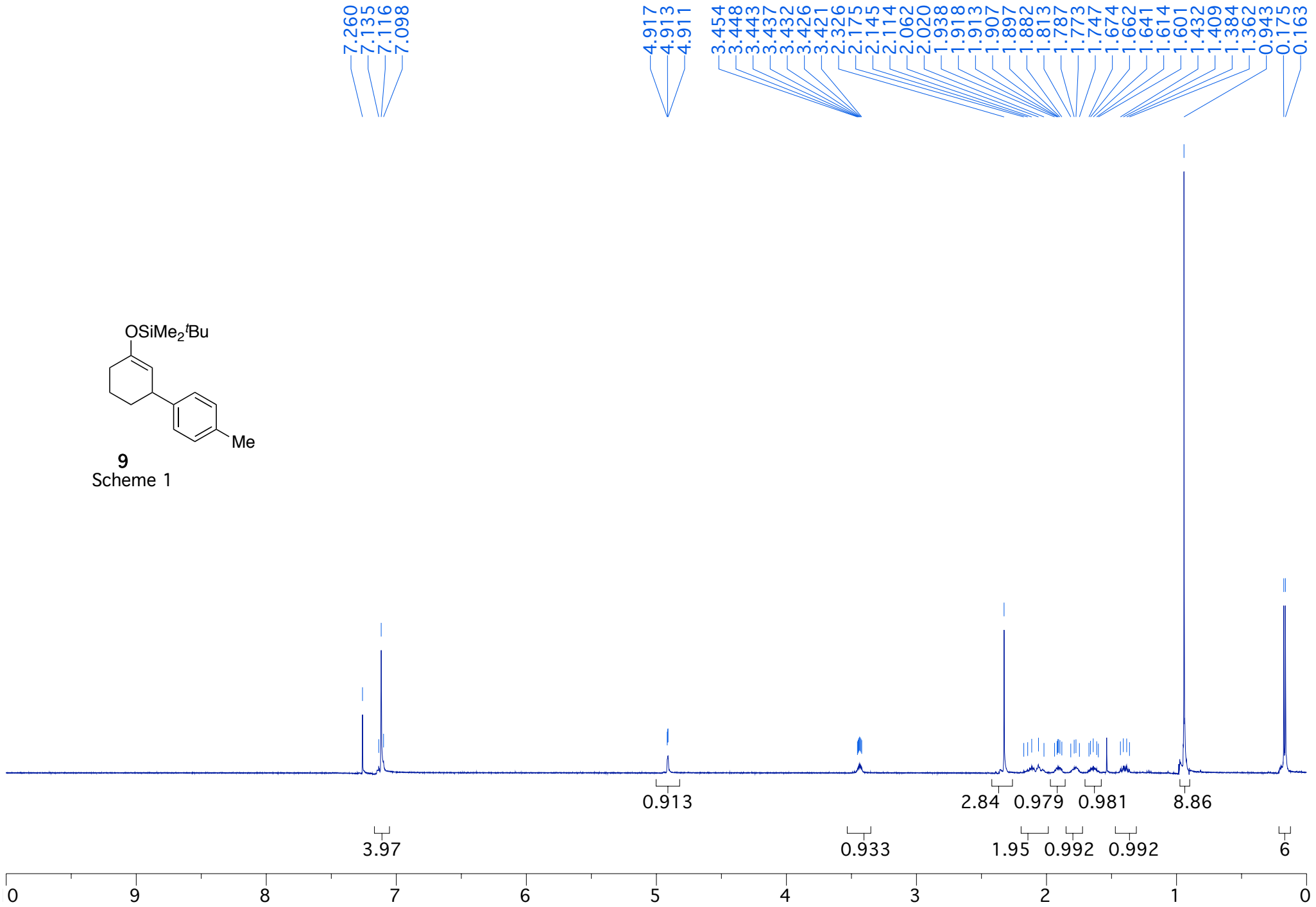


**8**  
Scheme 1

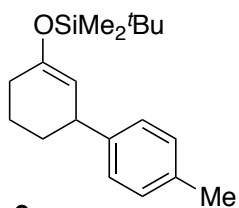
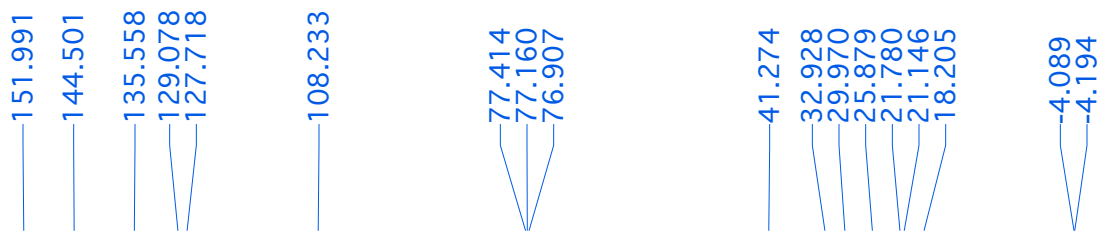




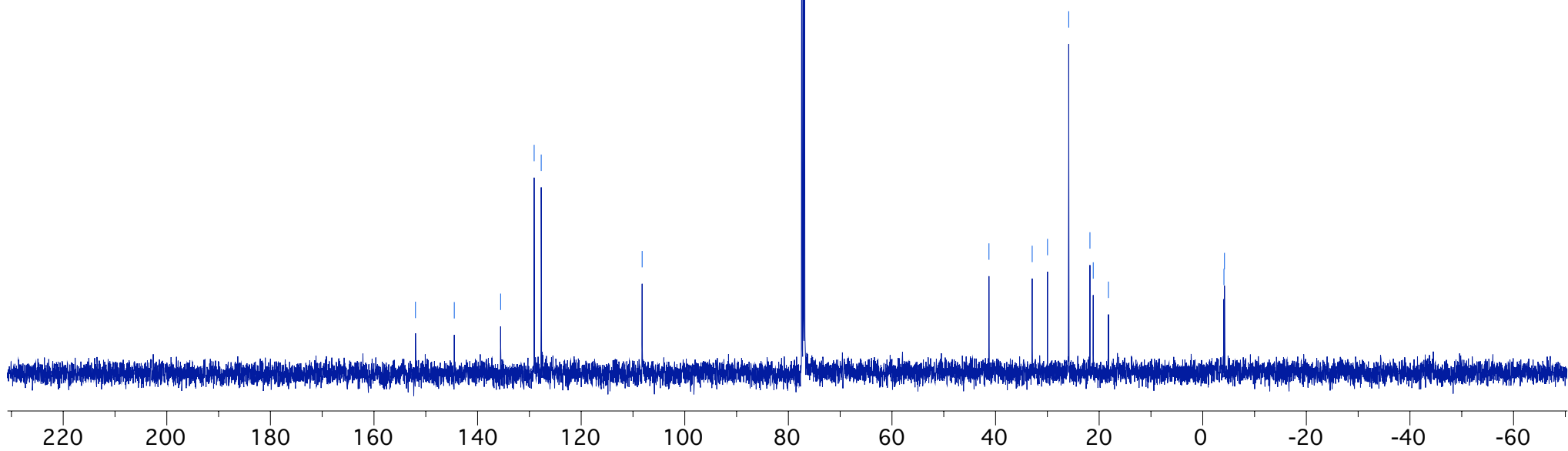
**9**  
Scheme 1

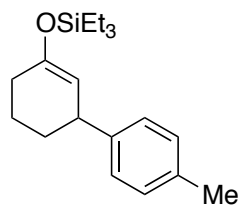


S71



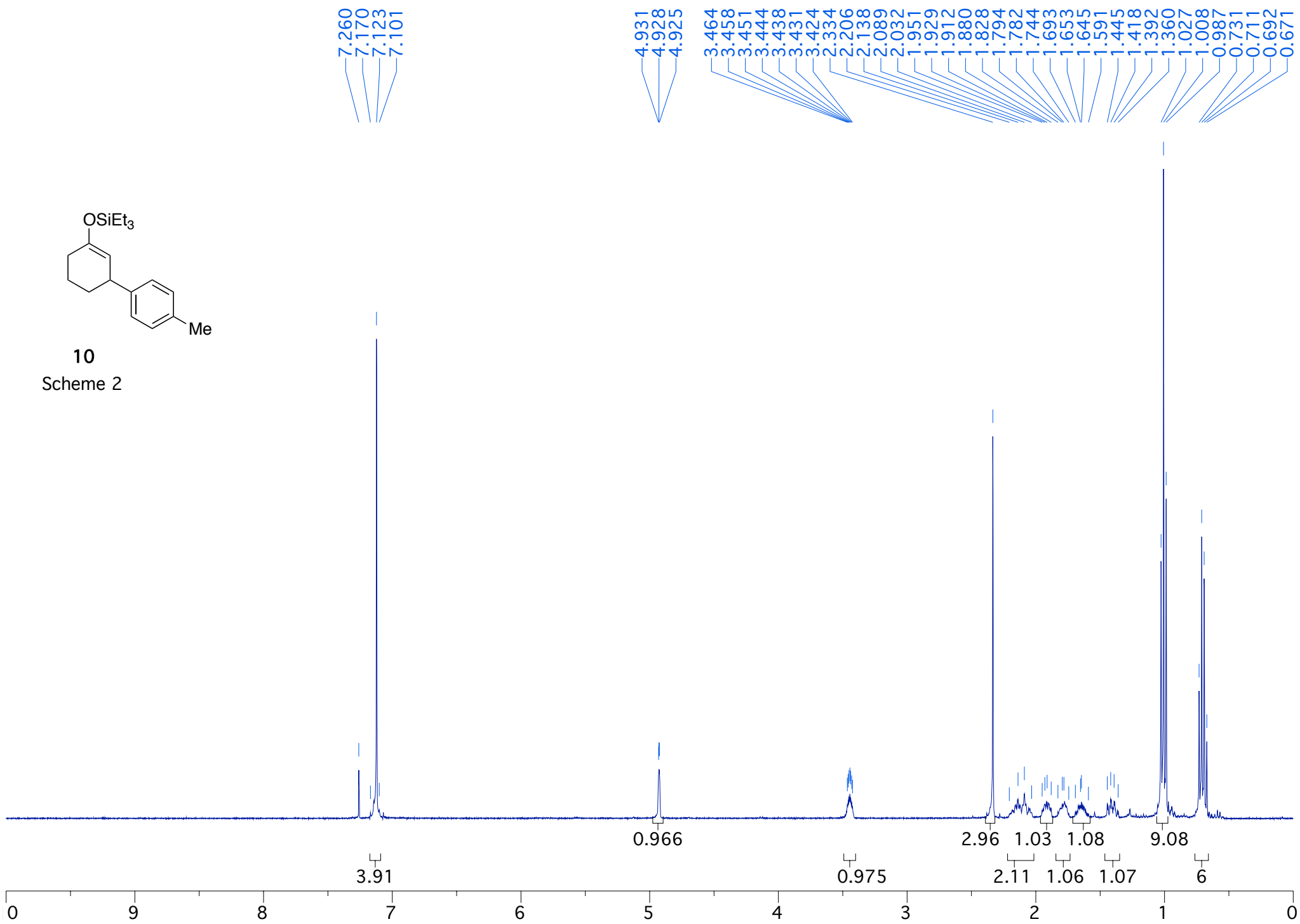
**9**  
Scheme 1



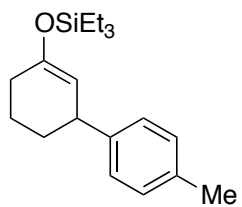
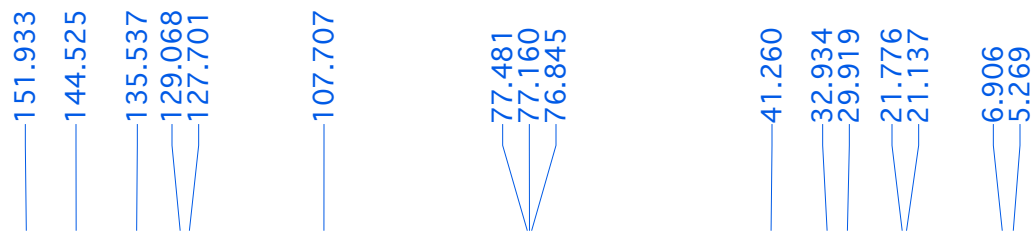


10

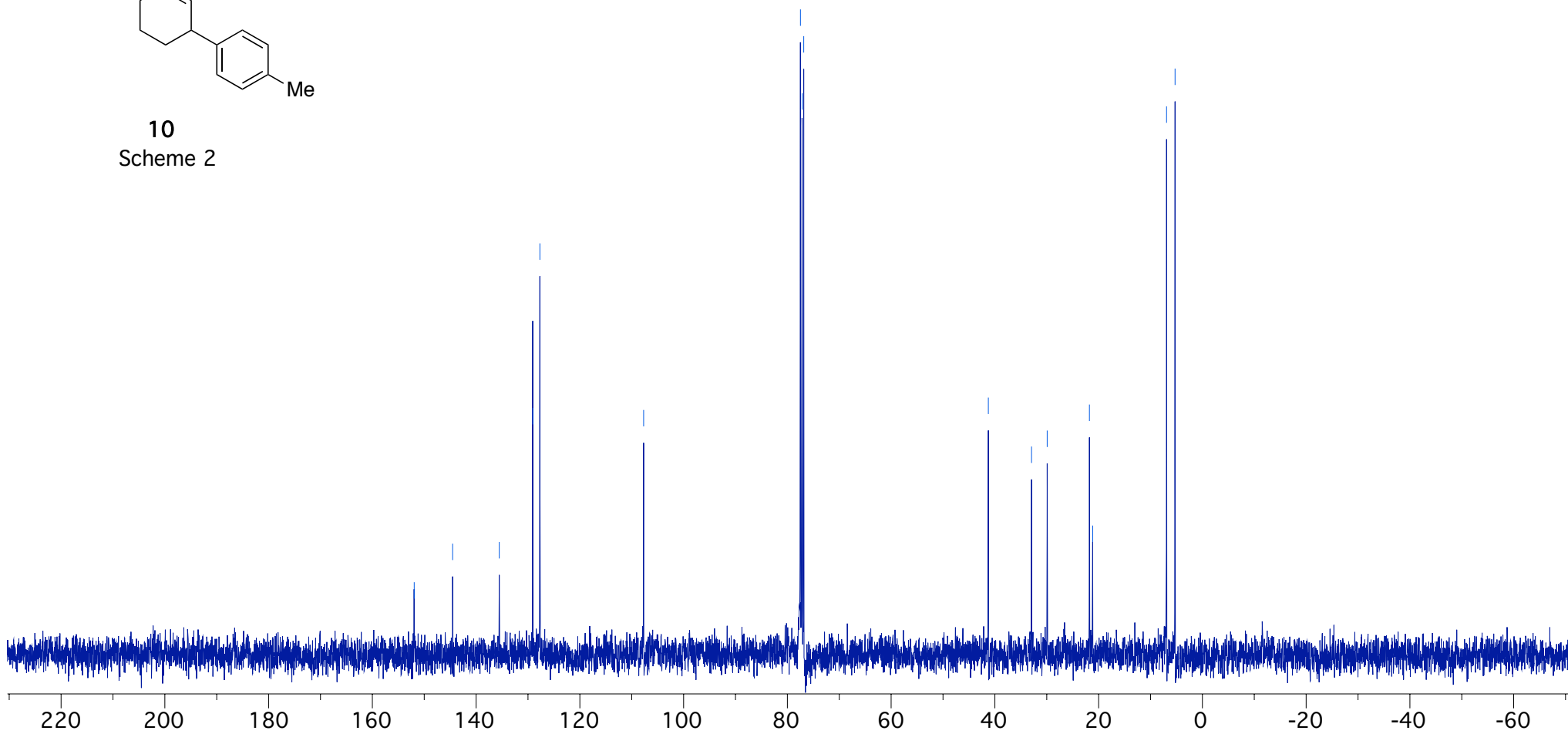
Scheme 2

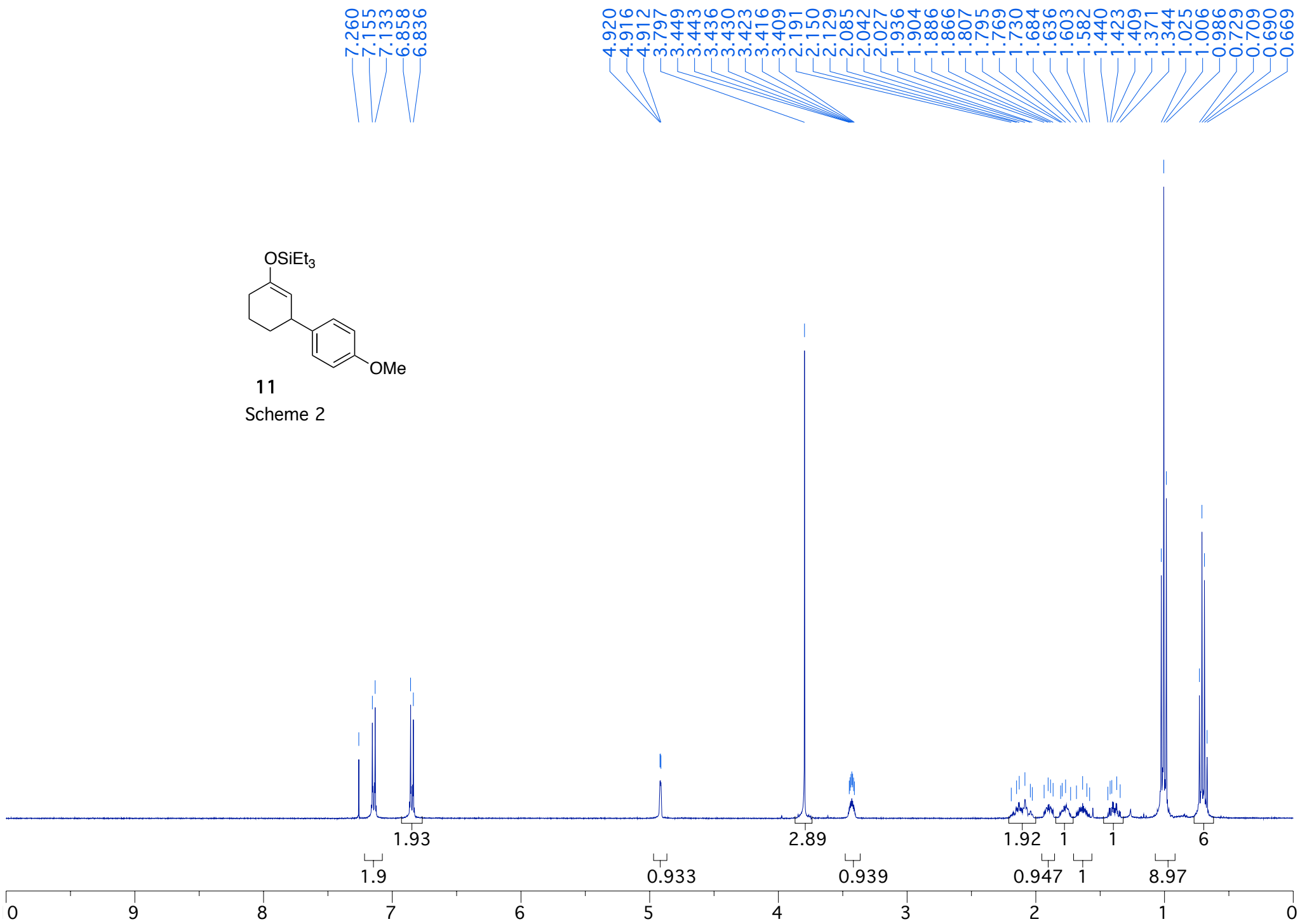
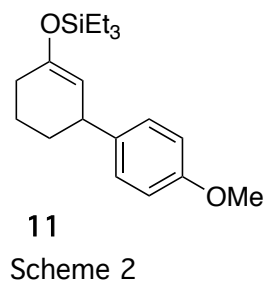


S73



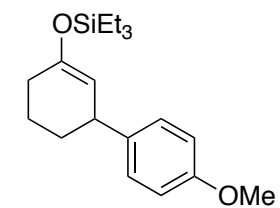
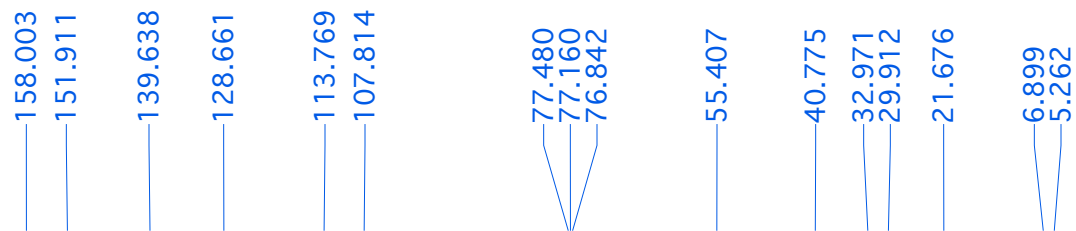
10  
Scheme 2



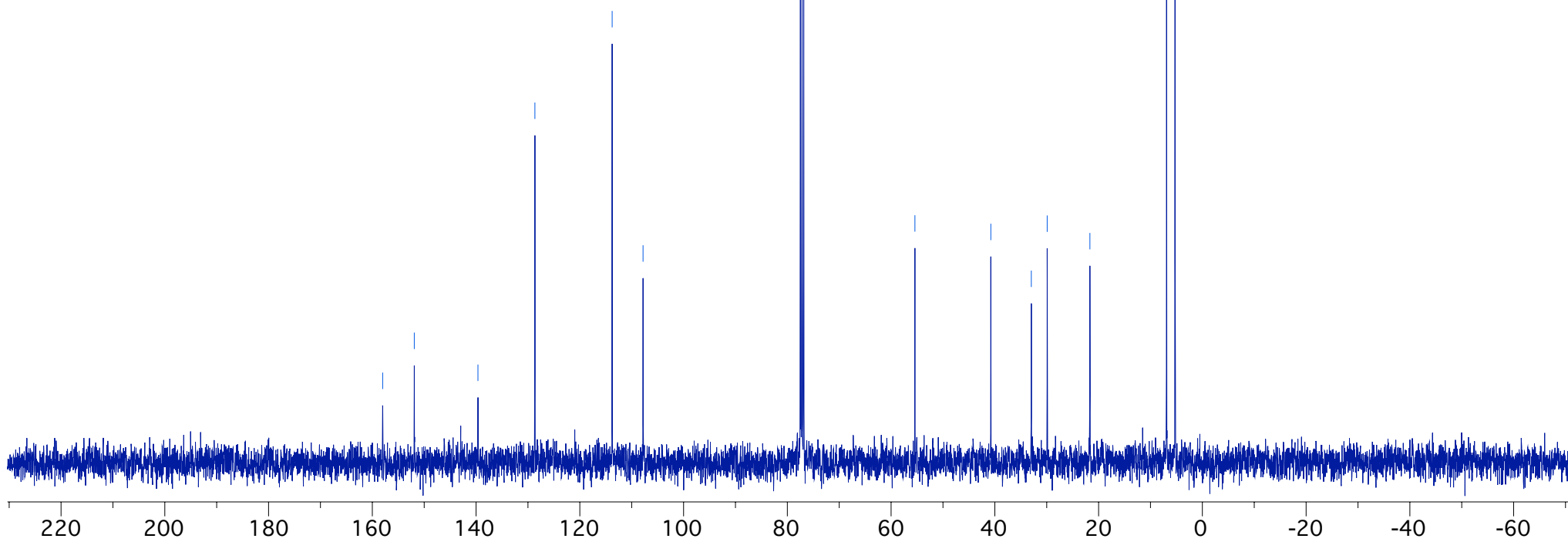


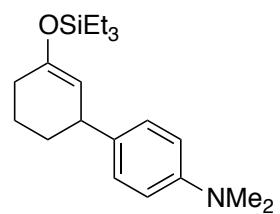


S75

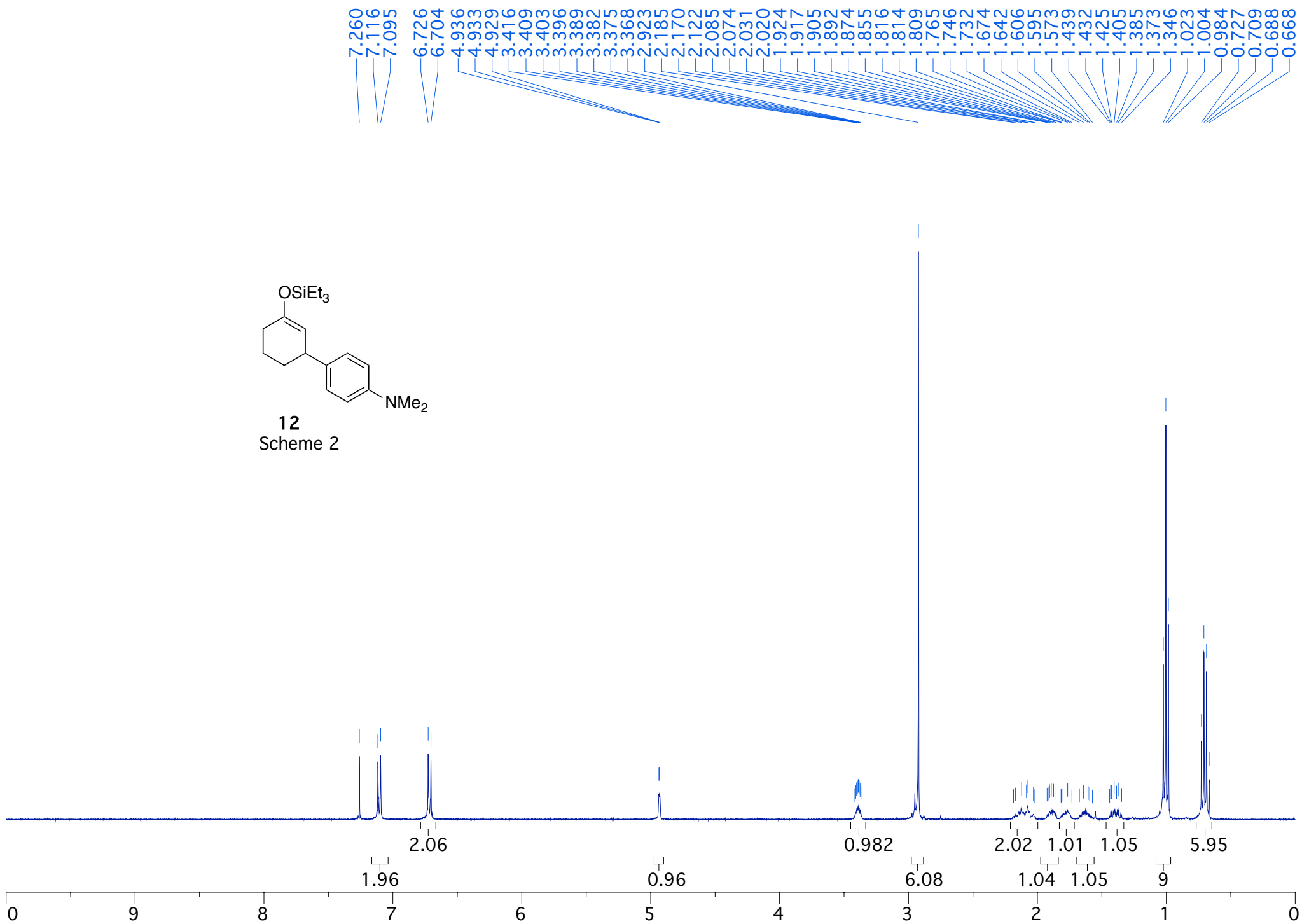


11  
Scheme 2

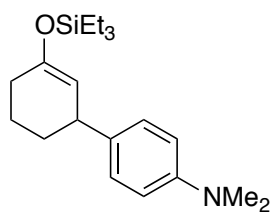




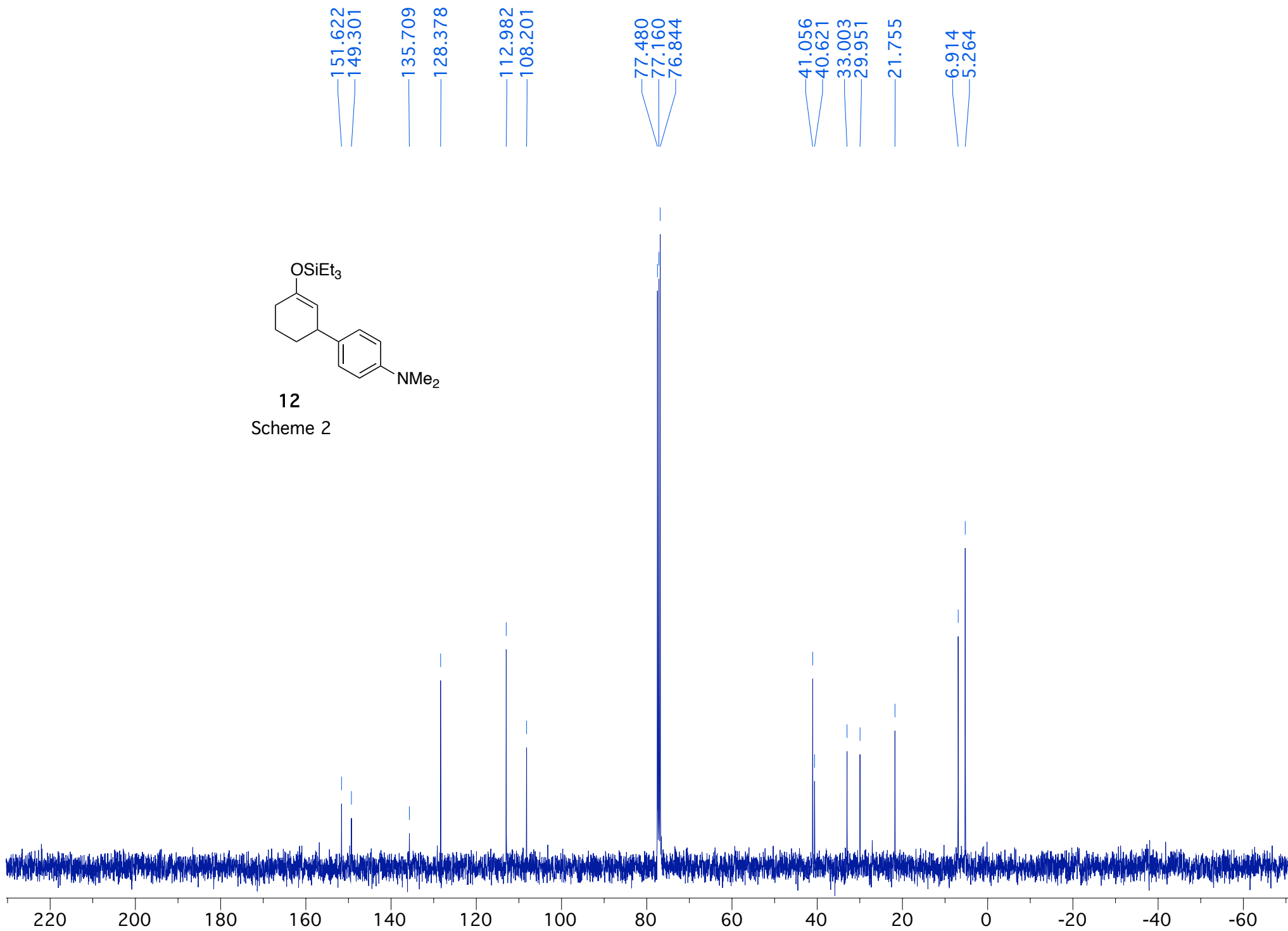
**12**  
Scheme 2

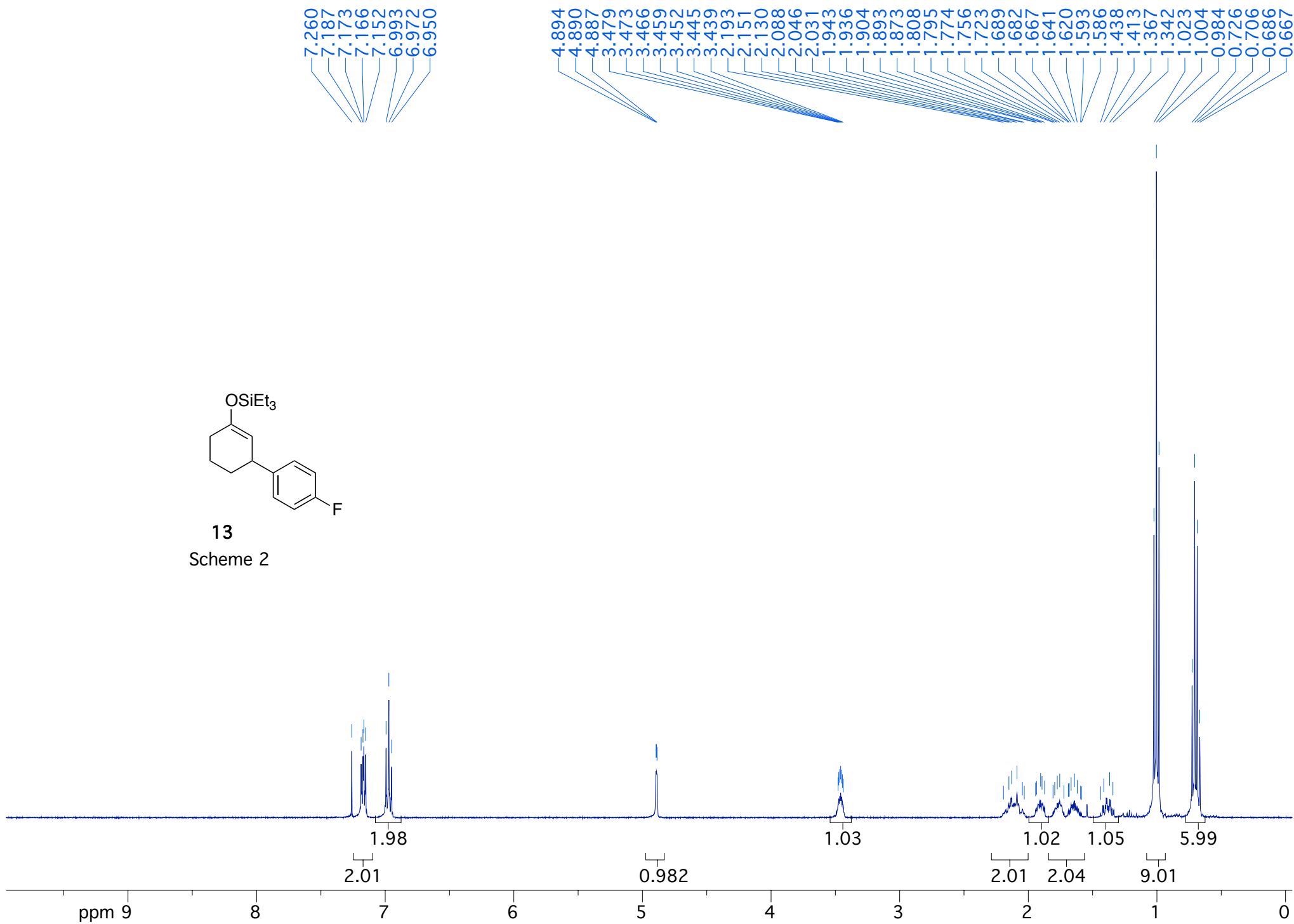
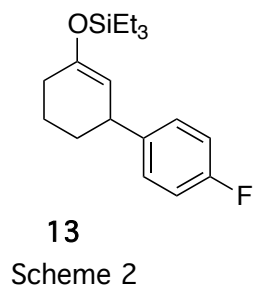


S77



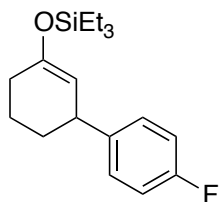
**12**  
Scheme 2



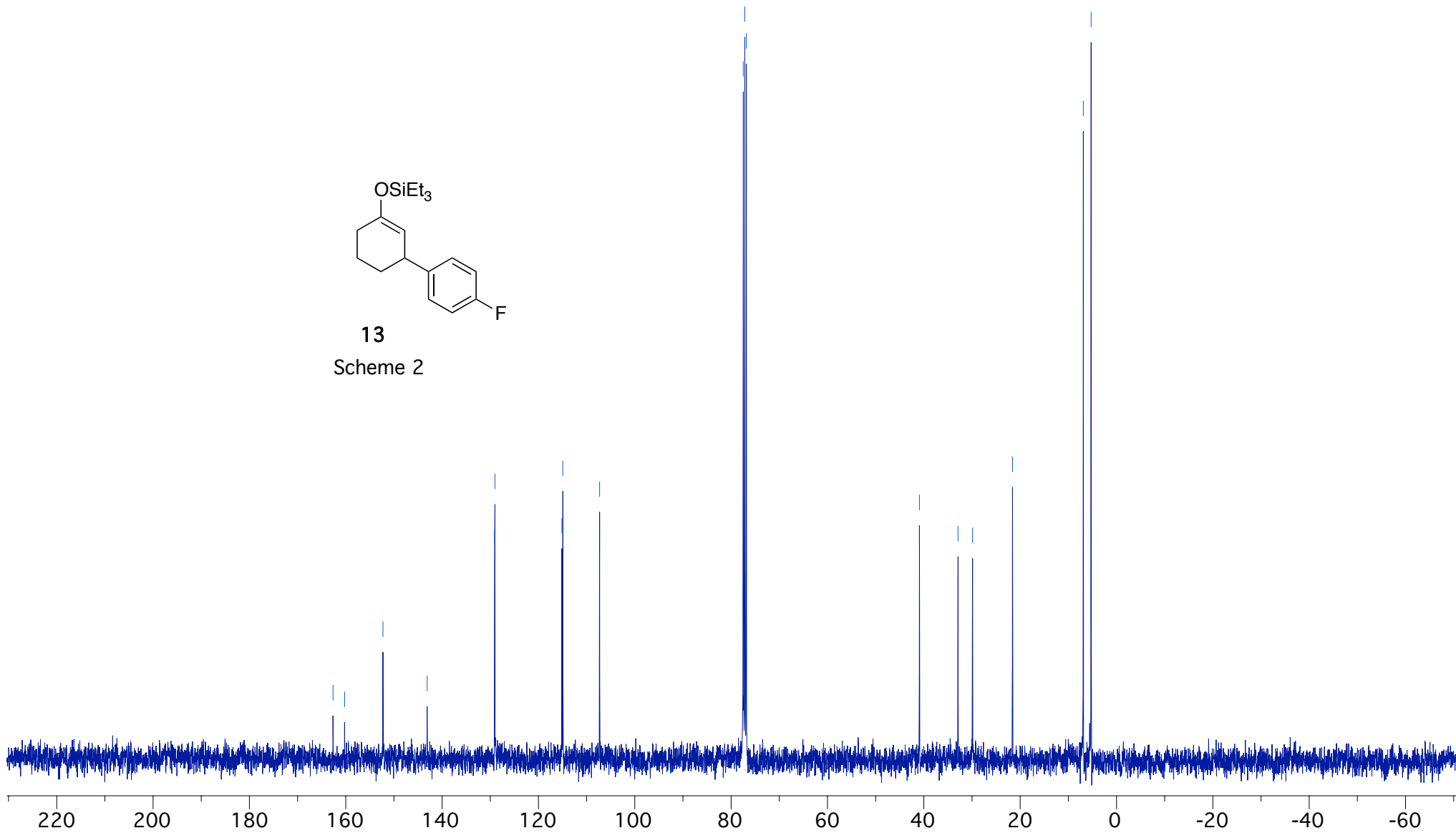


S79

162.648  
160.233  
152.279  
143.102  
129.110  
129.033  
115.140  
114.933  
107.305  
77.476  
77.160  
76.845  
40.910  
32.903  
29.875  
21.591  
6.885  
5.271

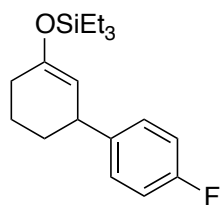


**13**  
Scheme 2



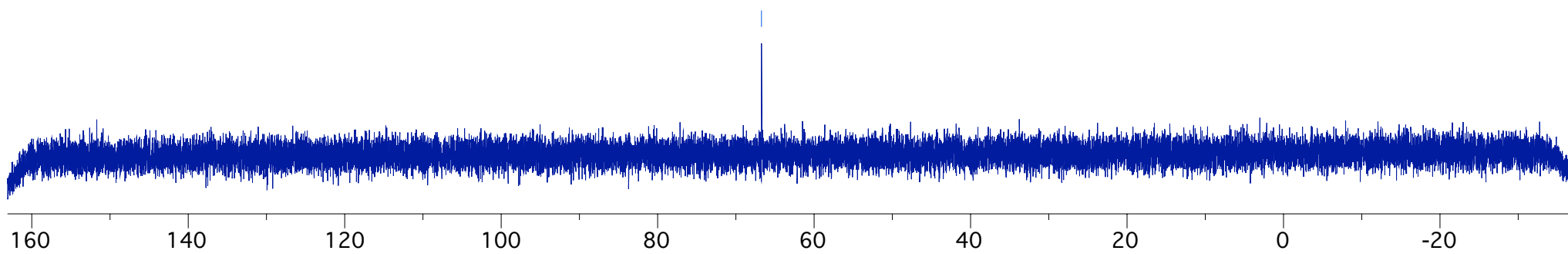
S80

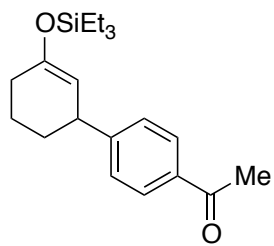
66.729



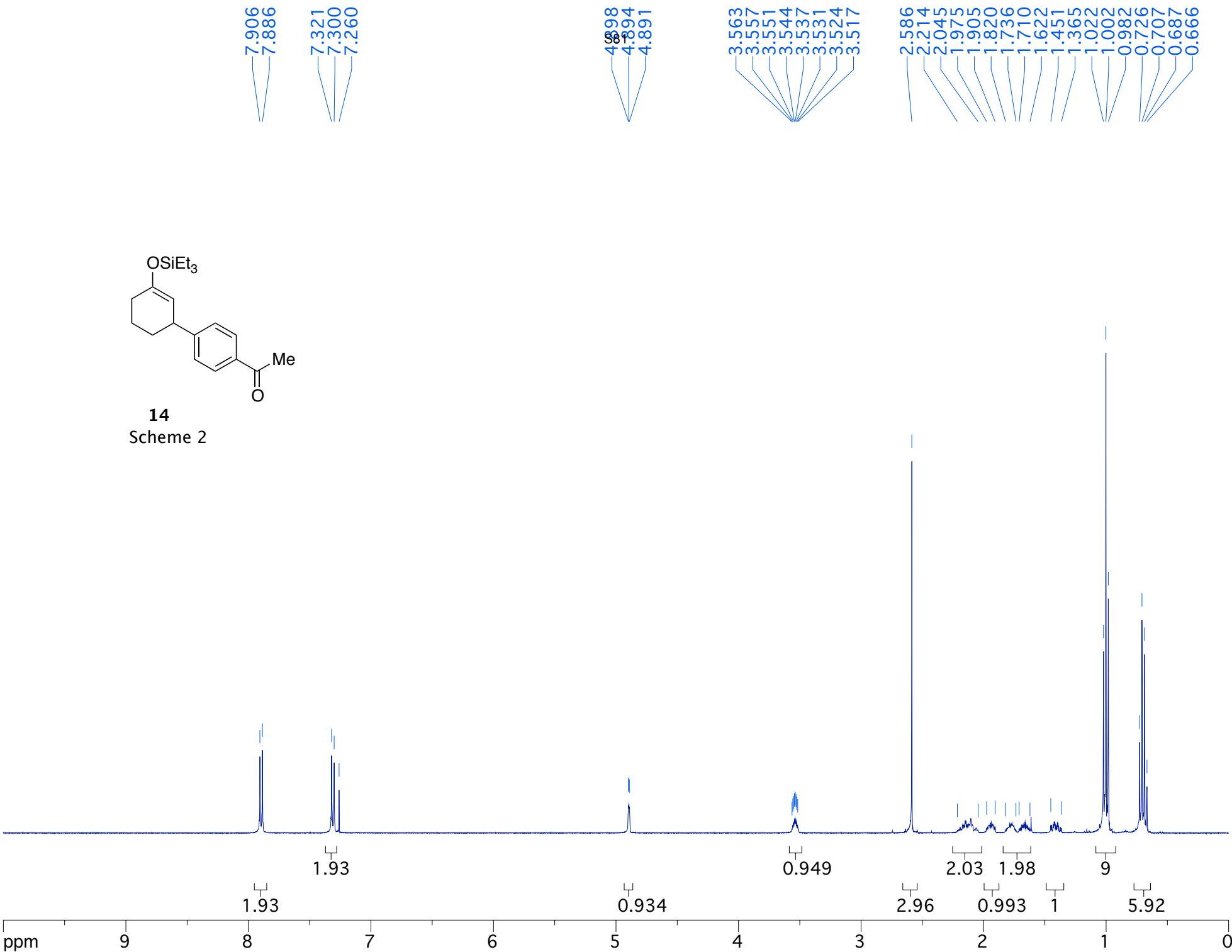
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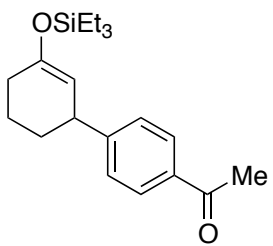
Scheme 2



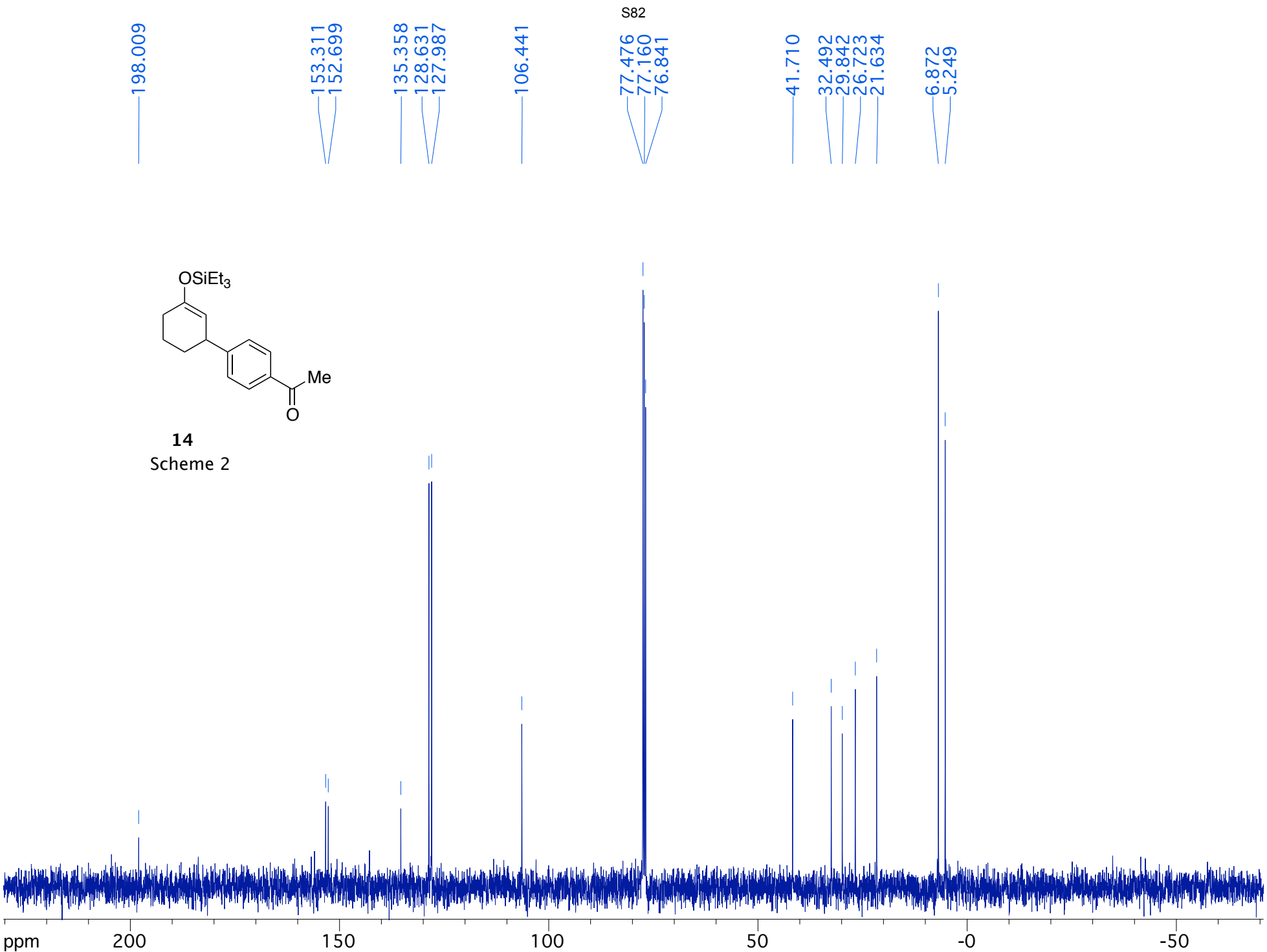


**14**  
Scheme 2

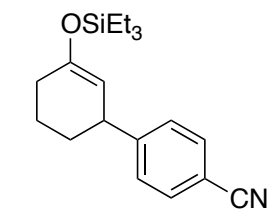




14  
Scheme 2

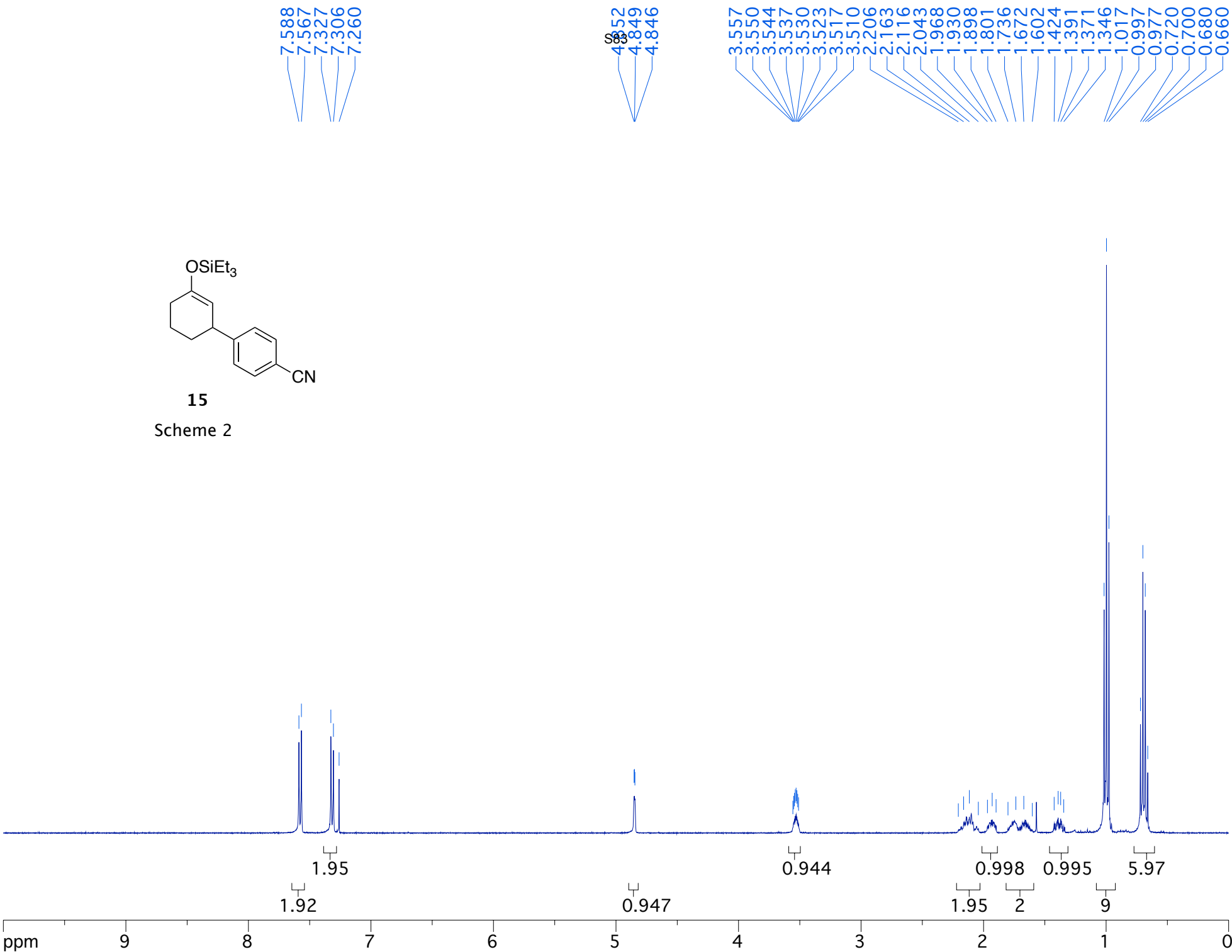


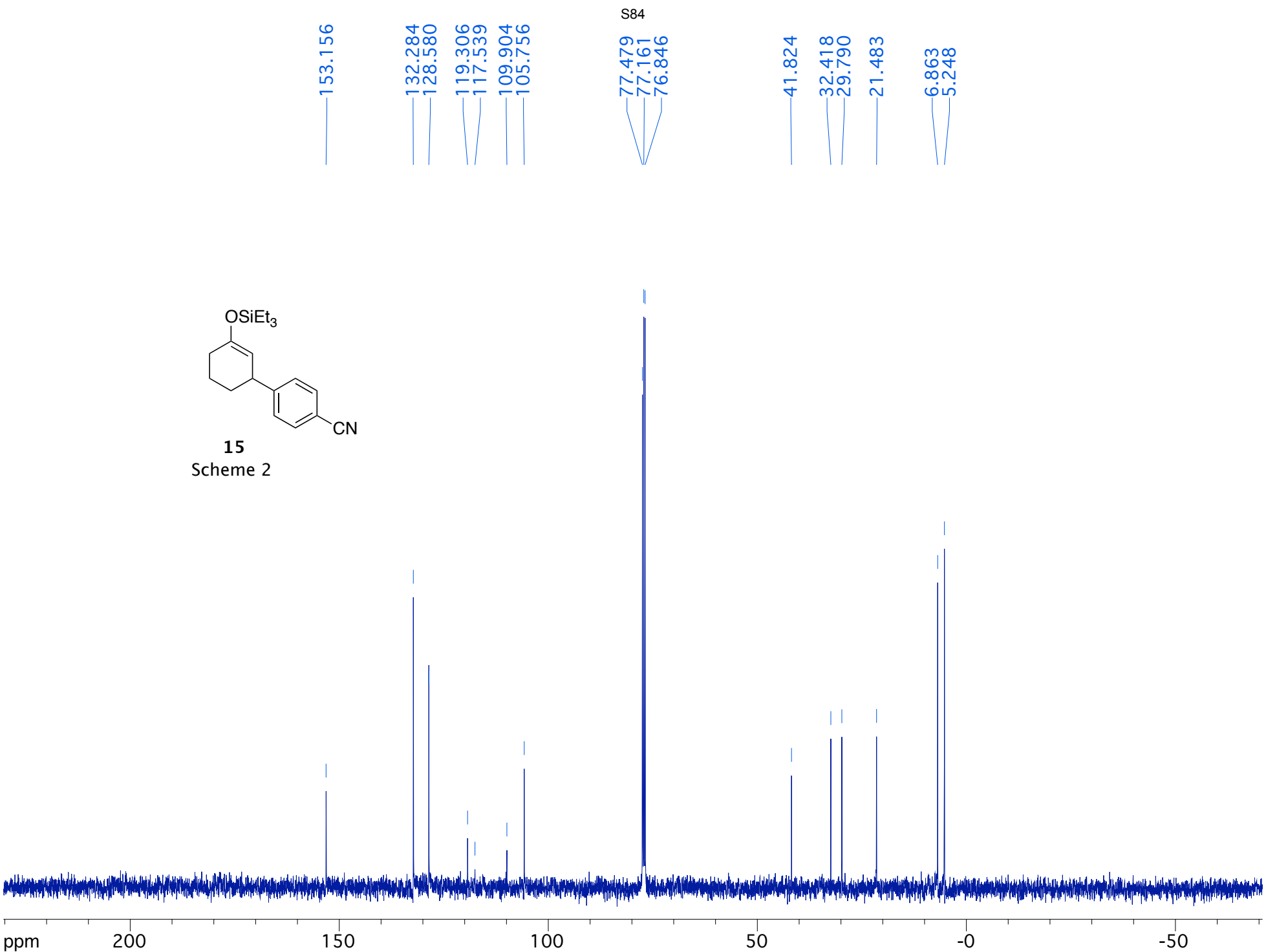
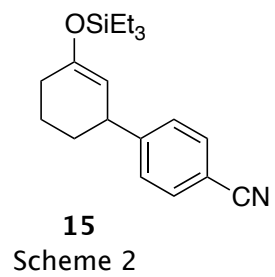


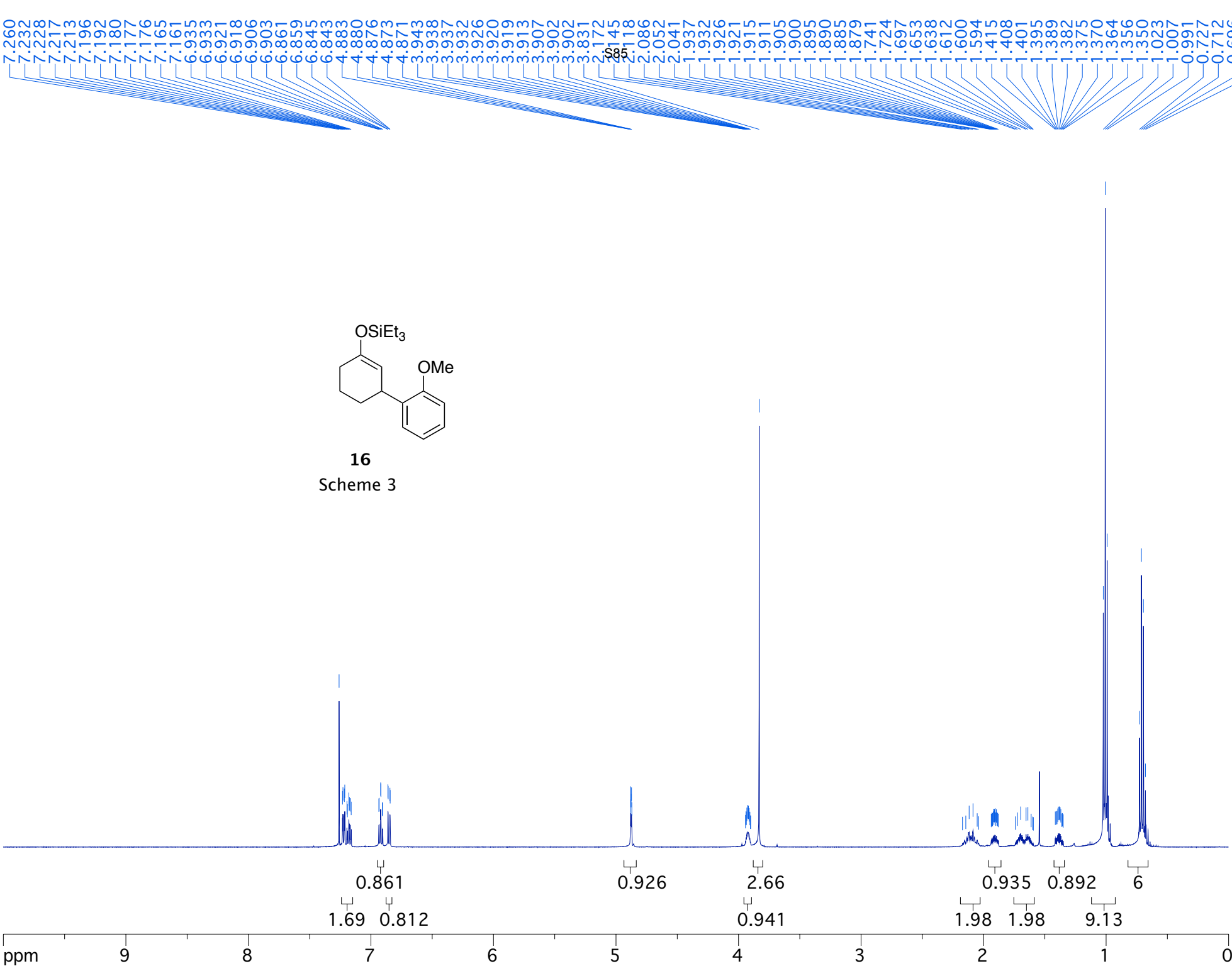


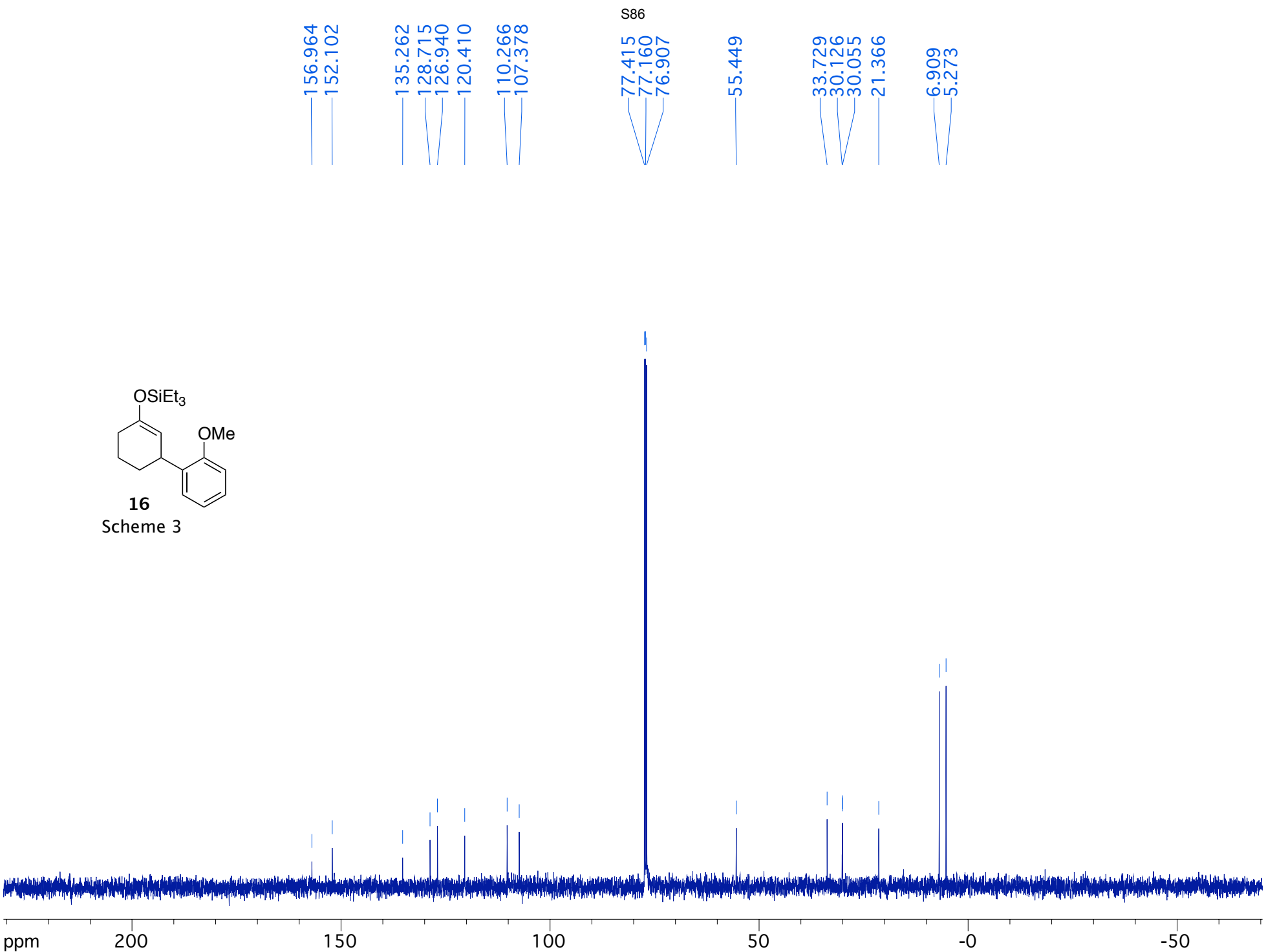
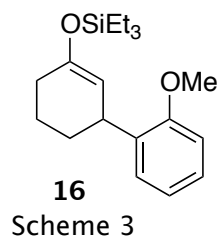
**15**

Scheme 2





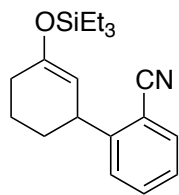




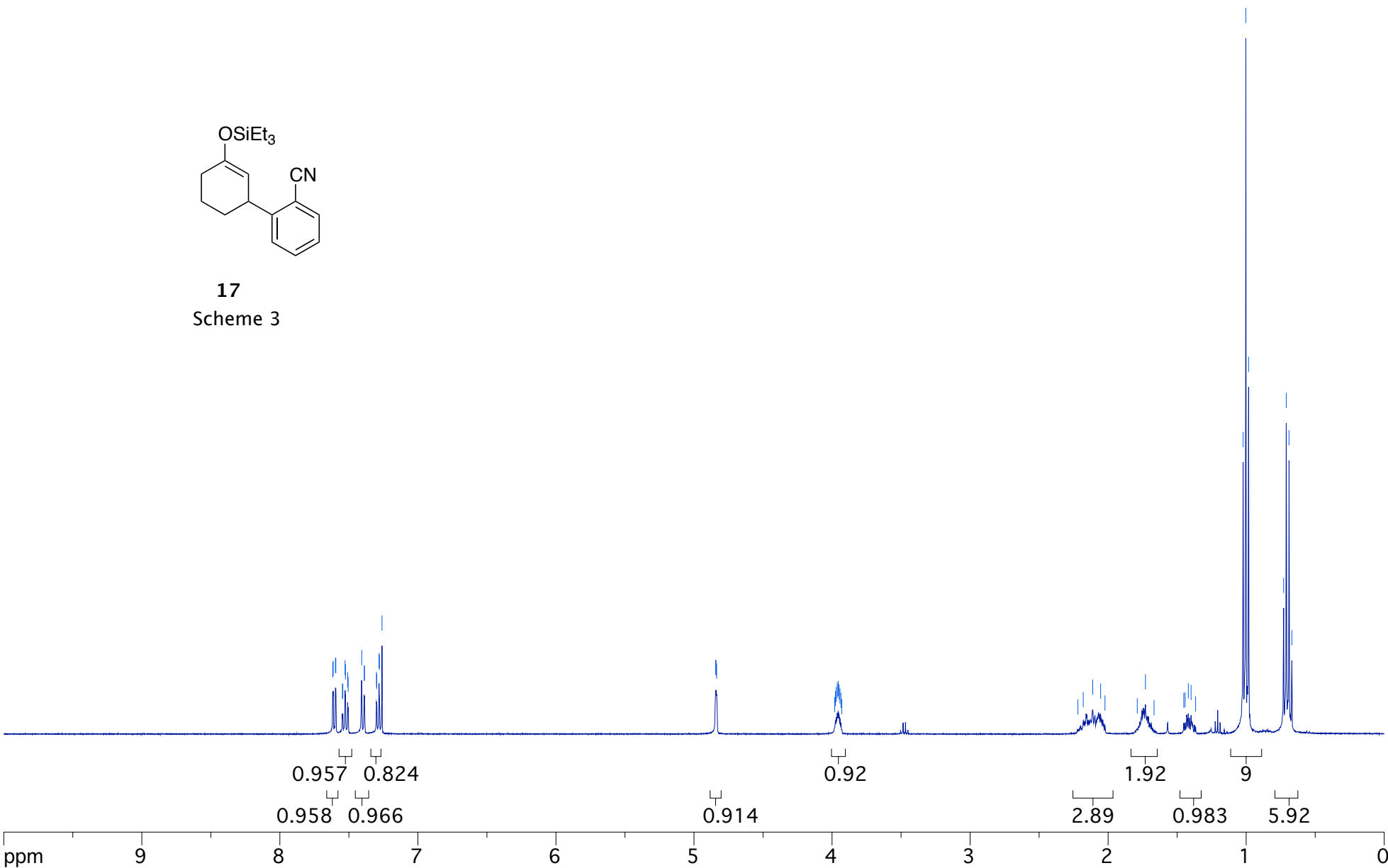
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7.614  
7.598  
7.595  
7.547  
7.544  
7.528  
7.525  
7.509  
7.505  
7.407  
7.389  
7.387  
7.301  
7.298  
7.282  
7.279  
7.260

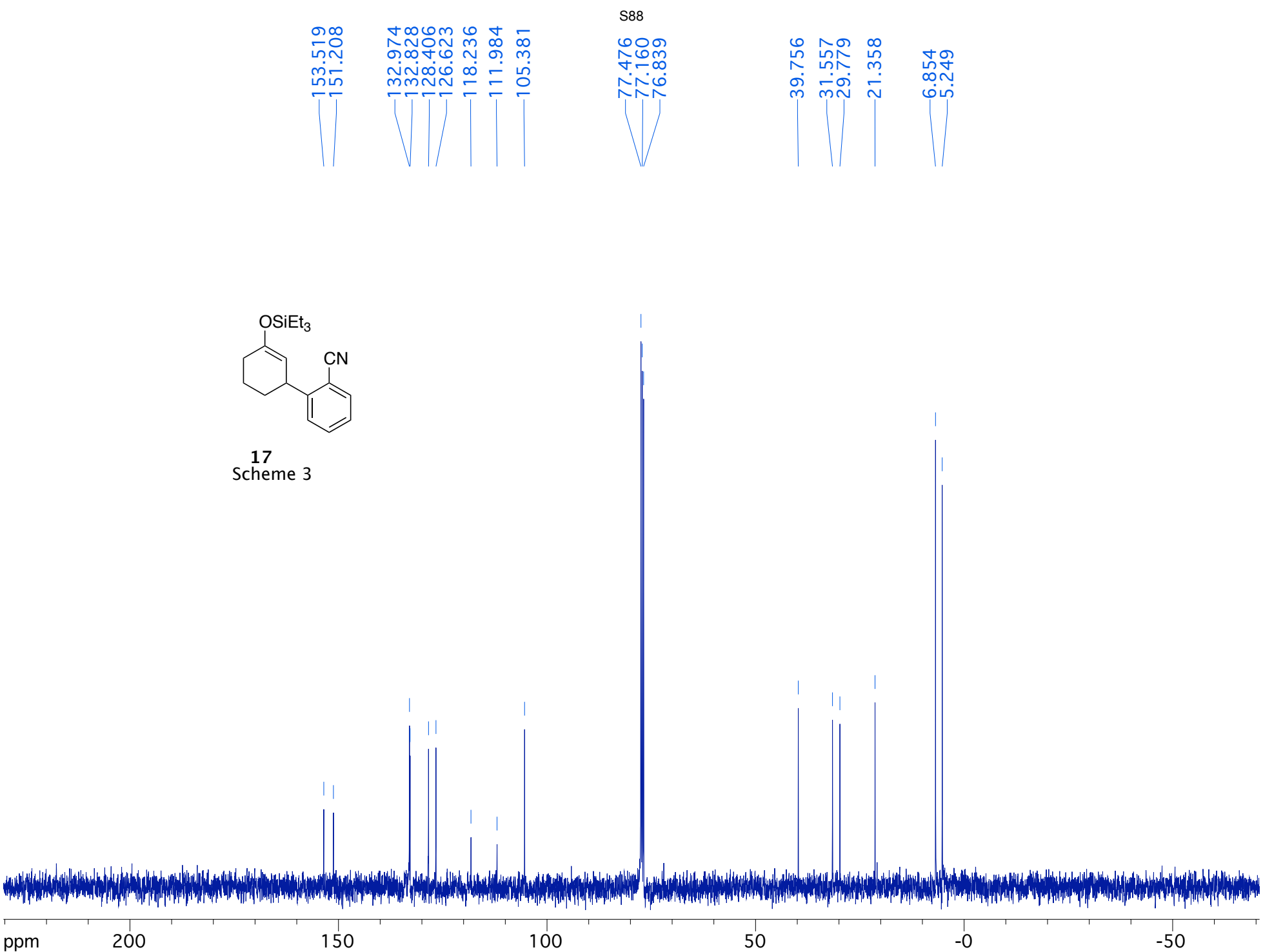
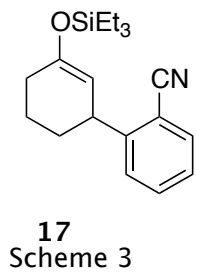
4.843  
4.840  
4.836  
3.981  
3.975  
3.969  
3.962  
3.956  
3.949  
3.943  
3.936  
3.929

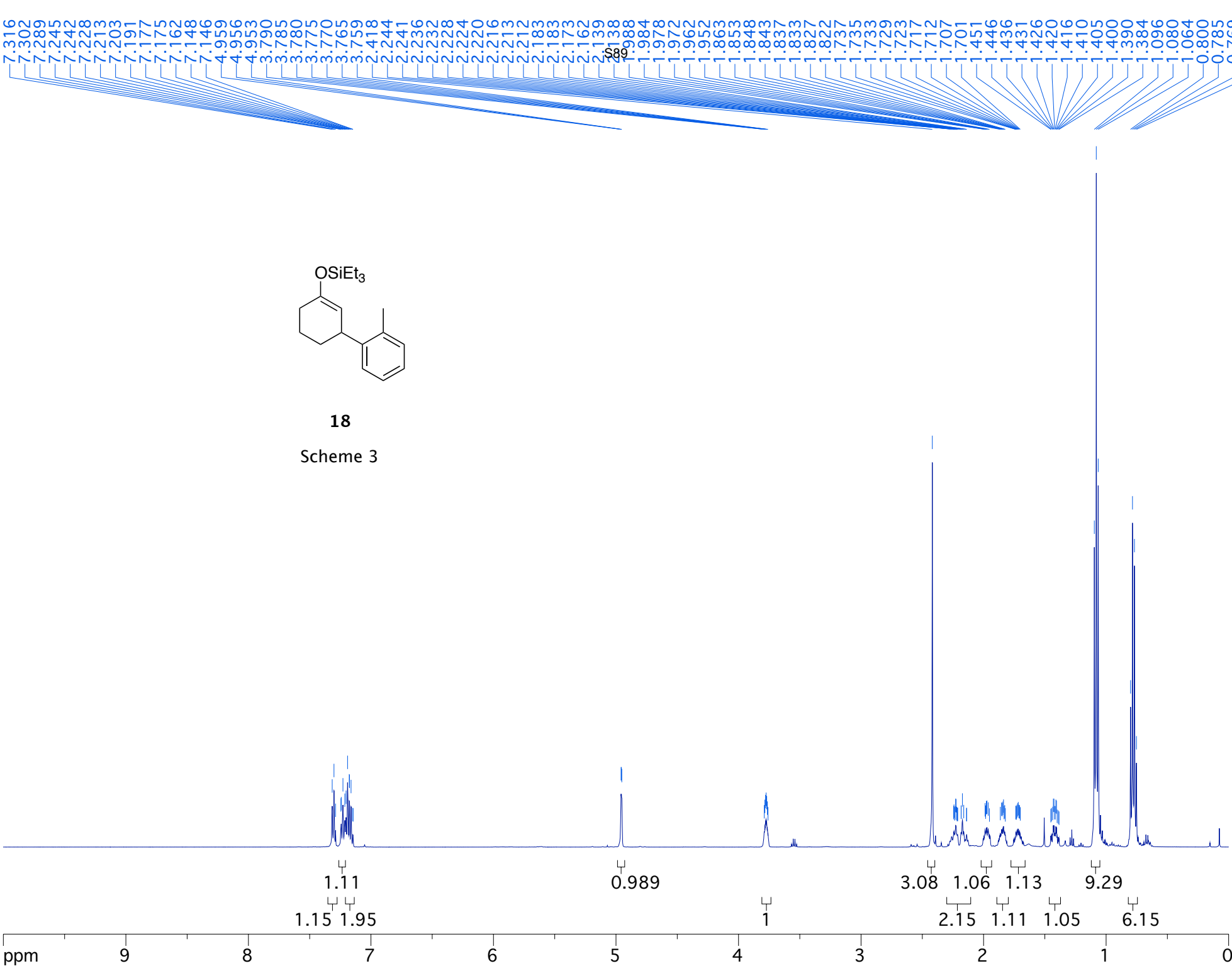
2.219  
2.180  
2.112  
2.054  
2.023  
1.789  
1.730  
1.667  
1.452  
1.442  
1.419  
1.399  
1.366  
1.022  
1.002  
0.983  
0.729  
0.710  
0.690  
0.669



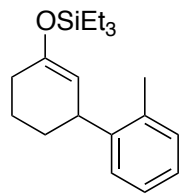
**17**  
Scheme 3





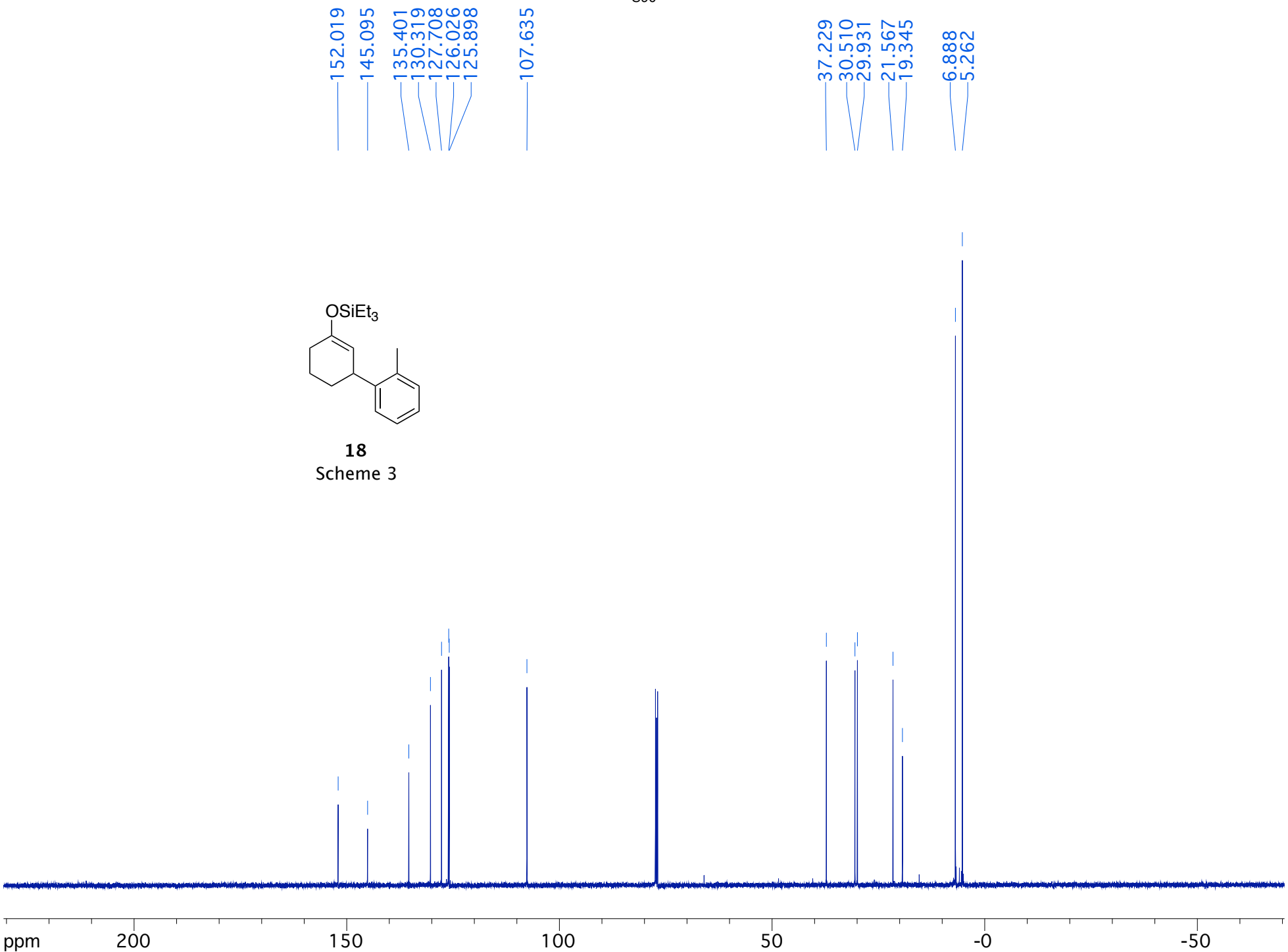


S90

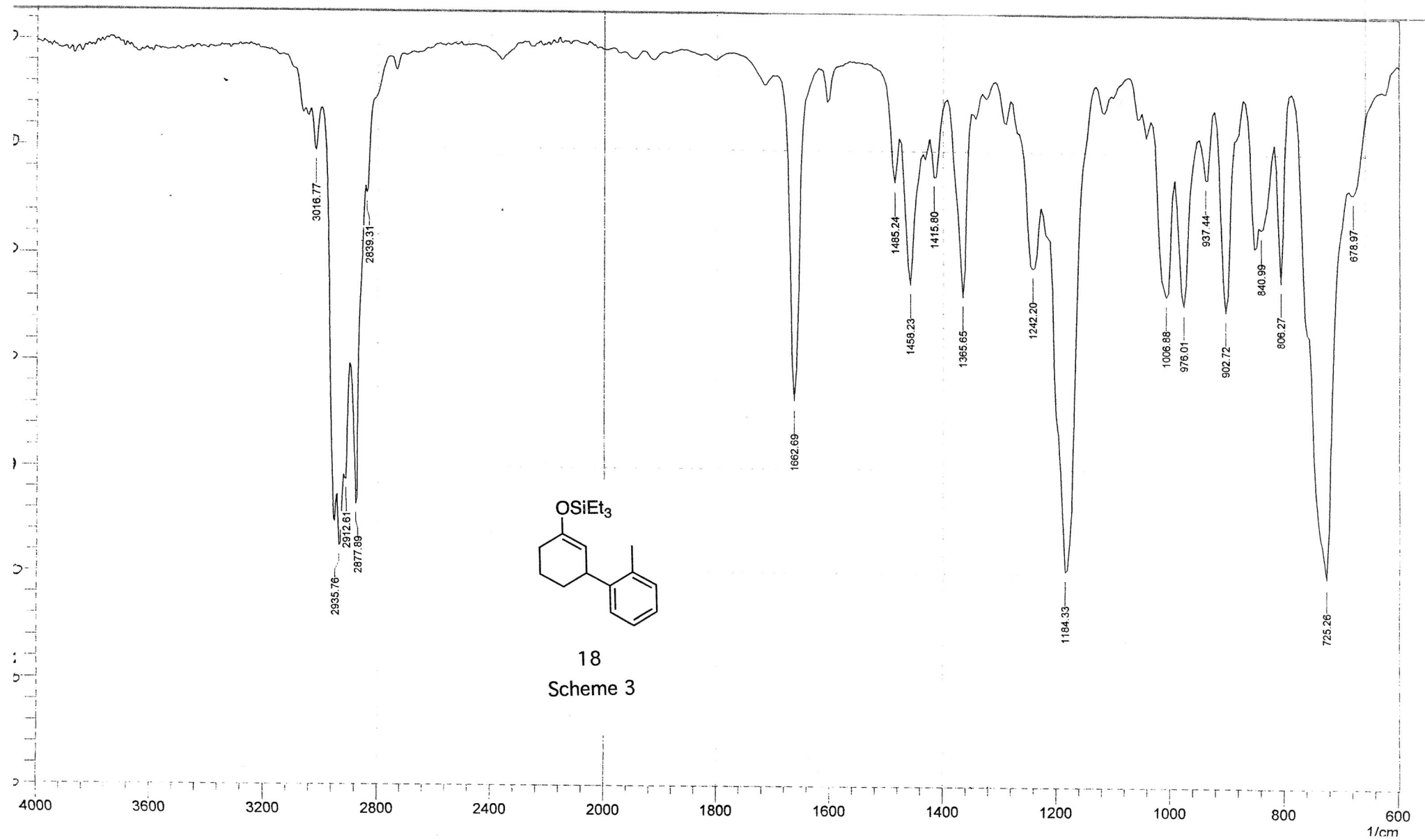


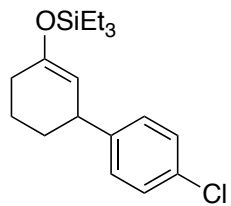
**18**

Scheme 3



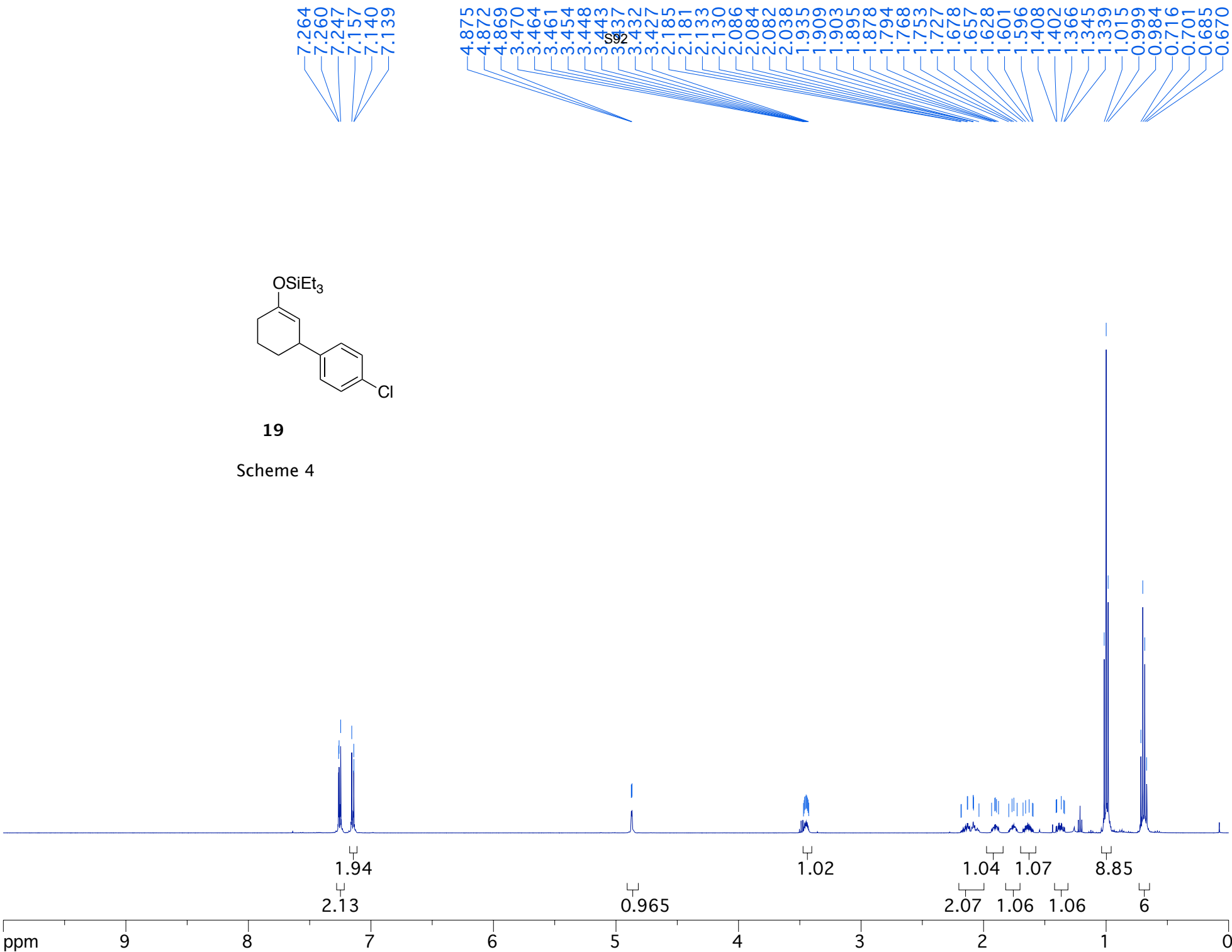


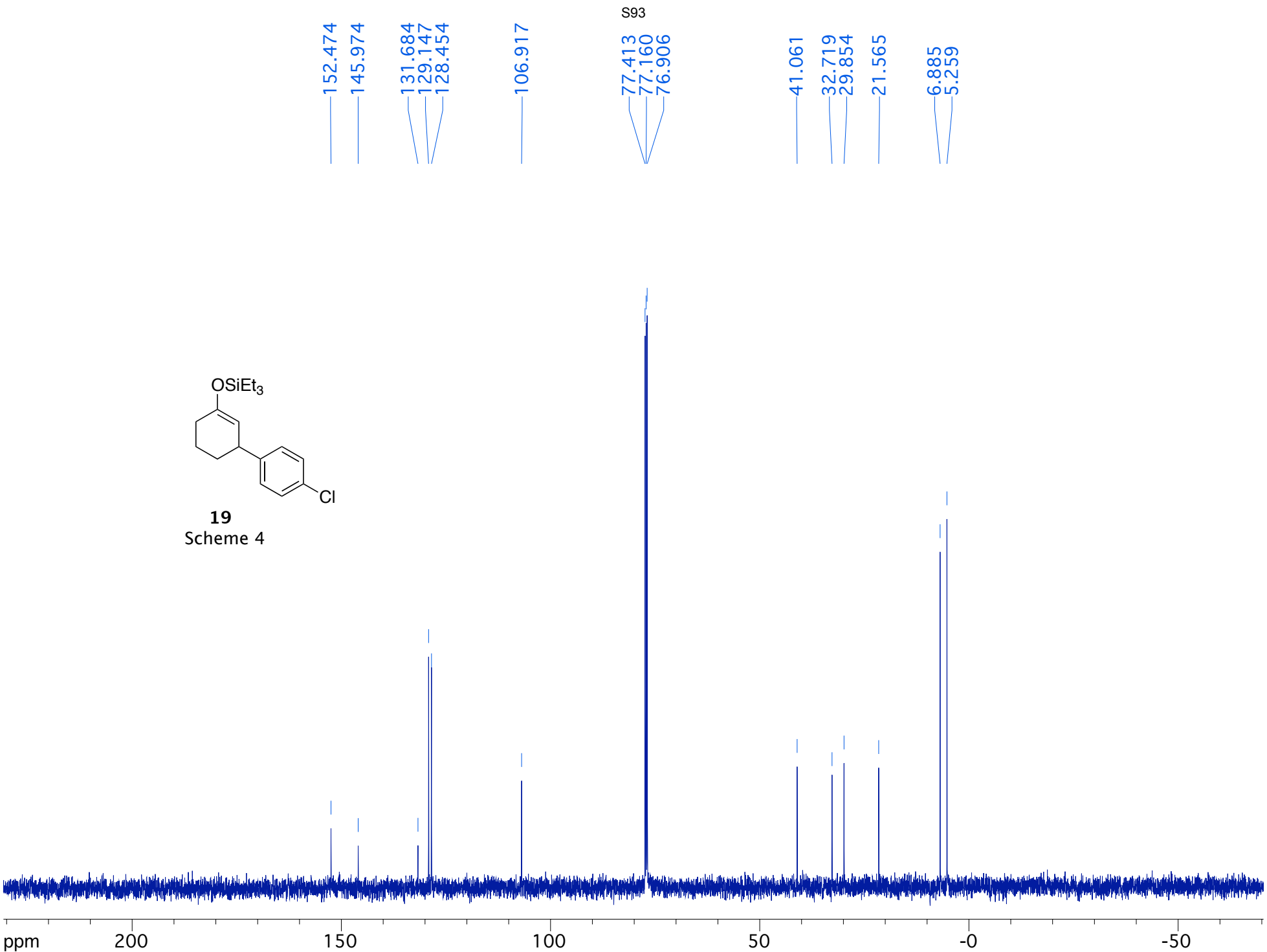
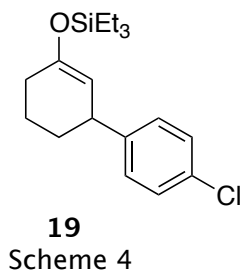


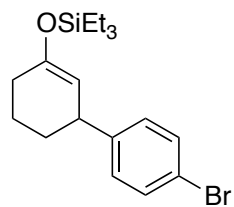


**19**

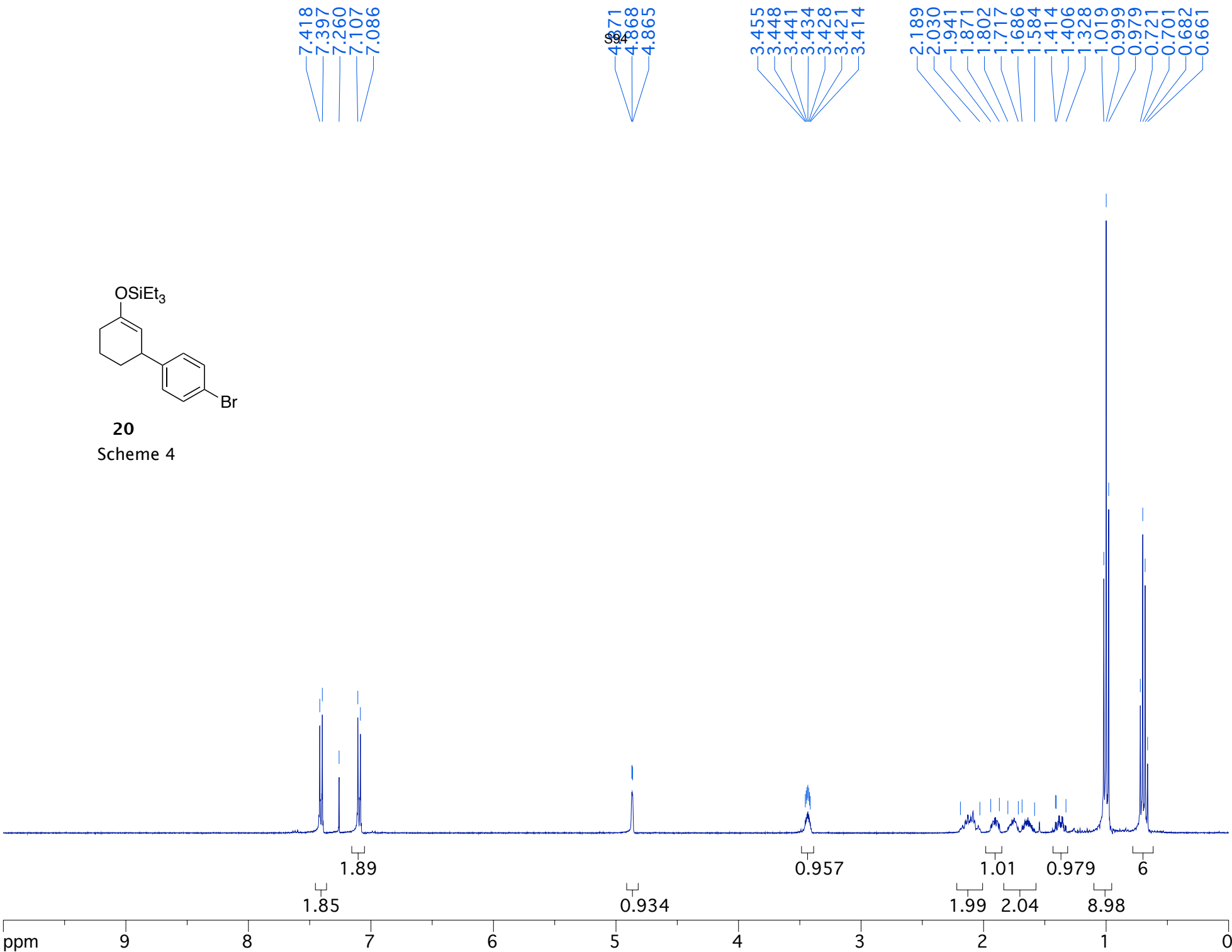
Scheme 4

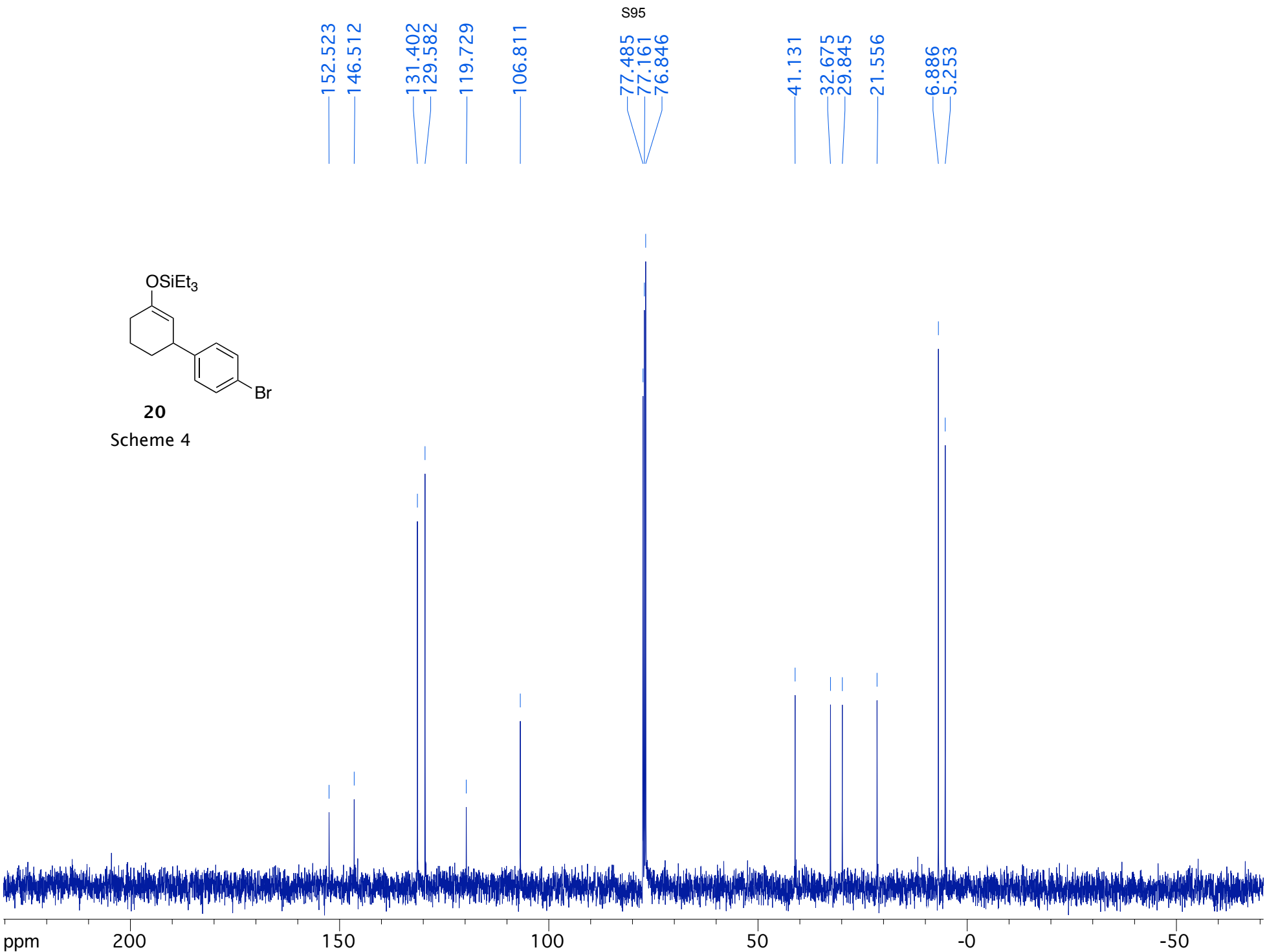
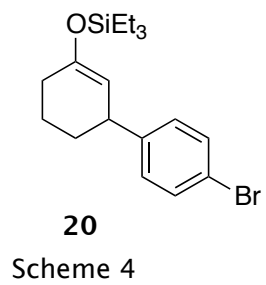


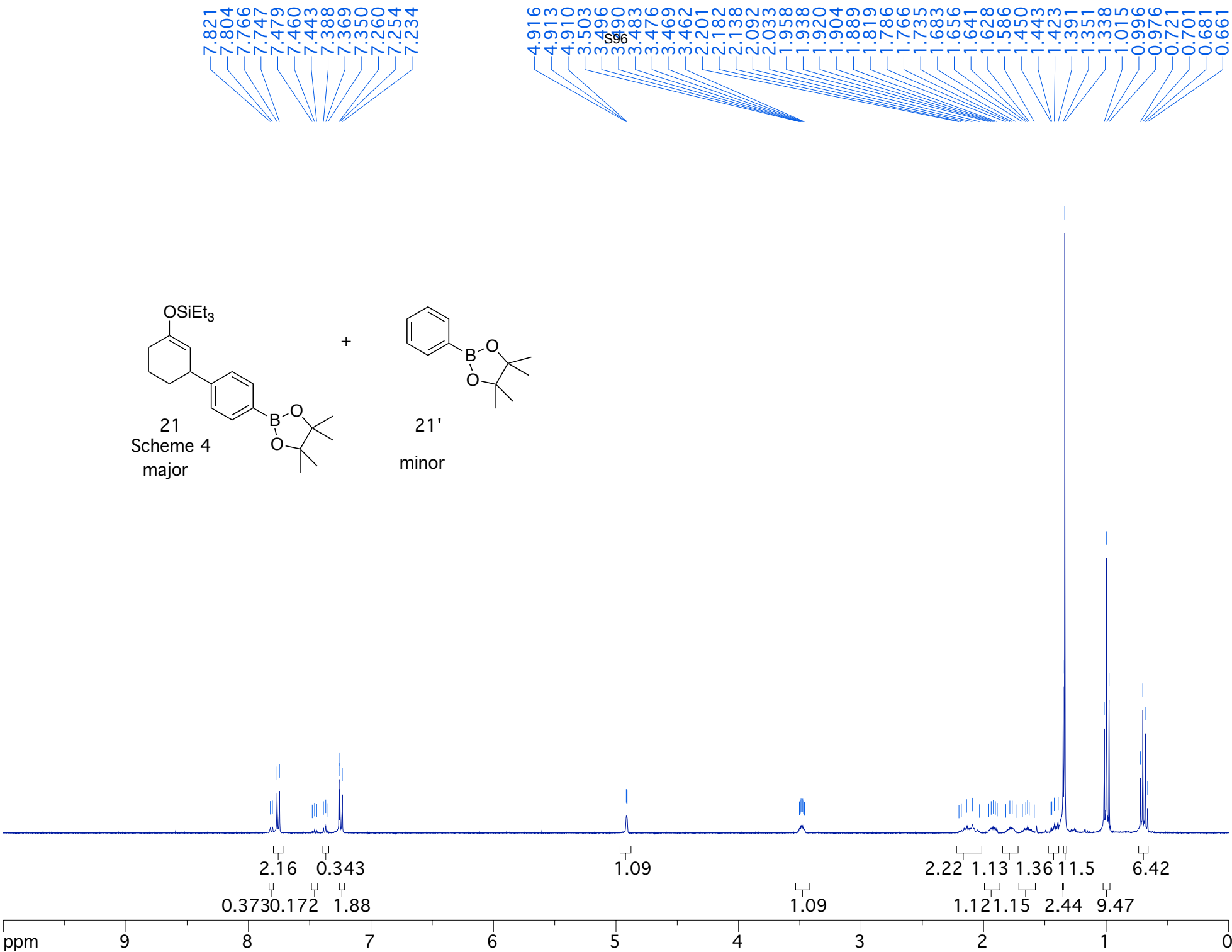
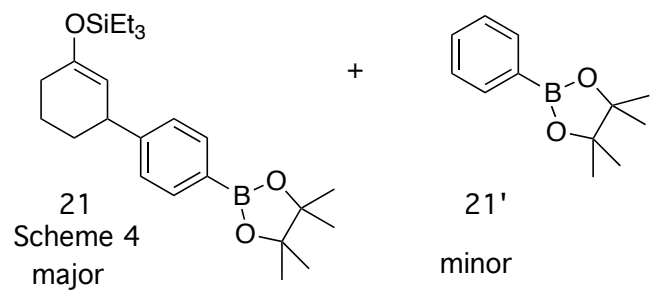


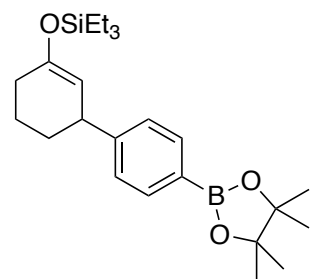


**20**  
Scheme 4

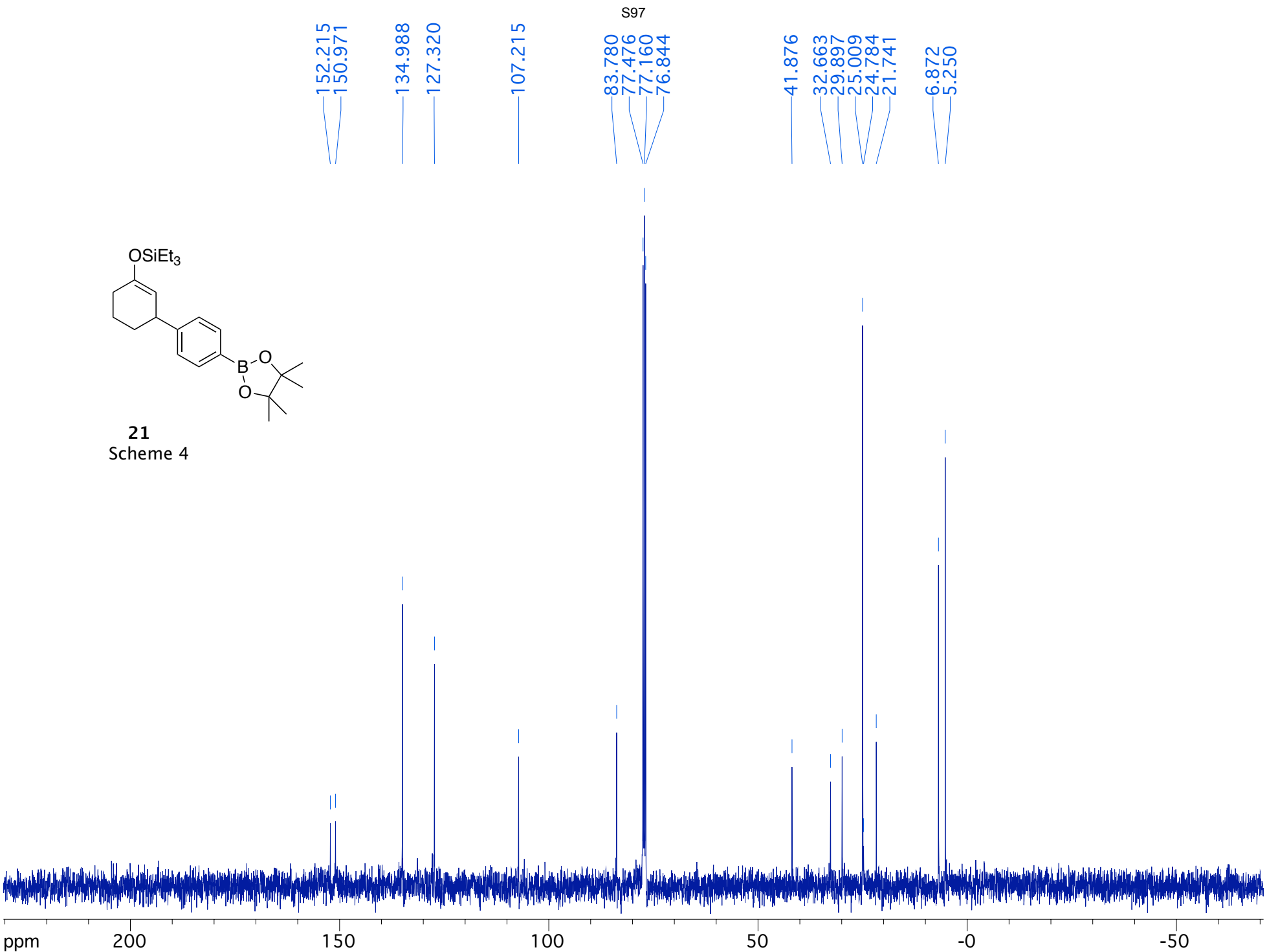


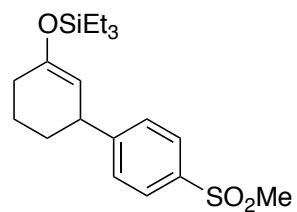






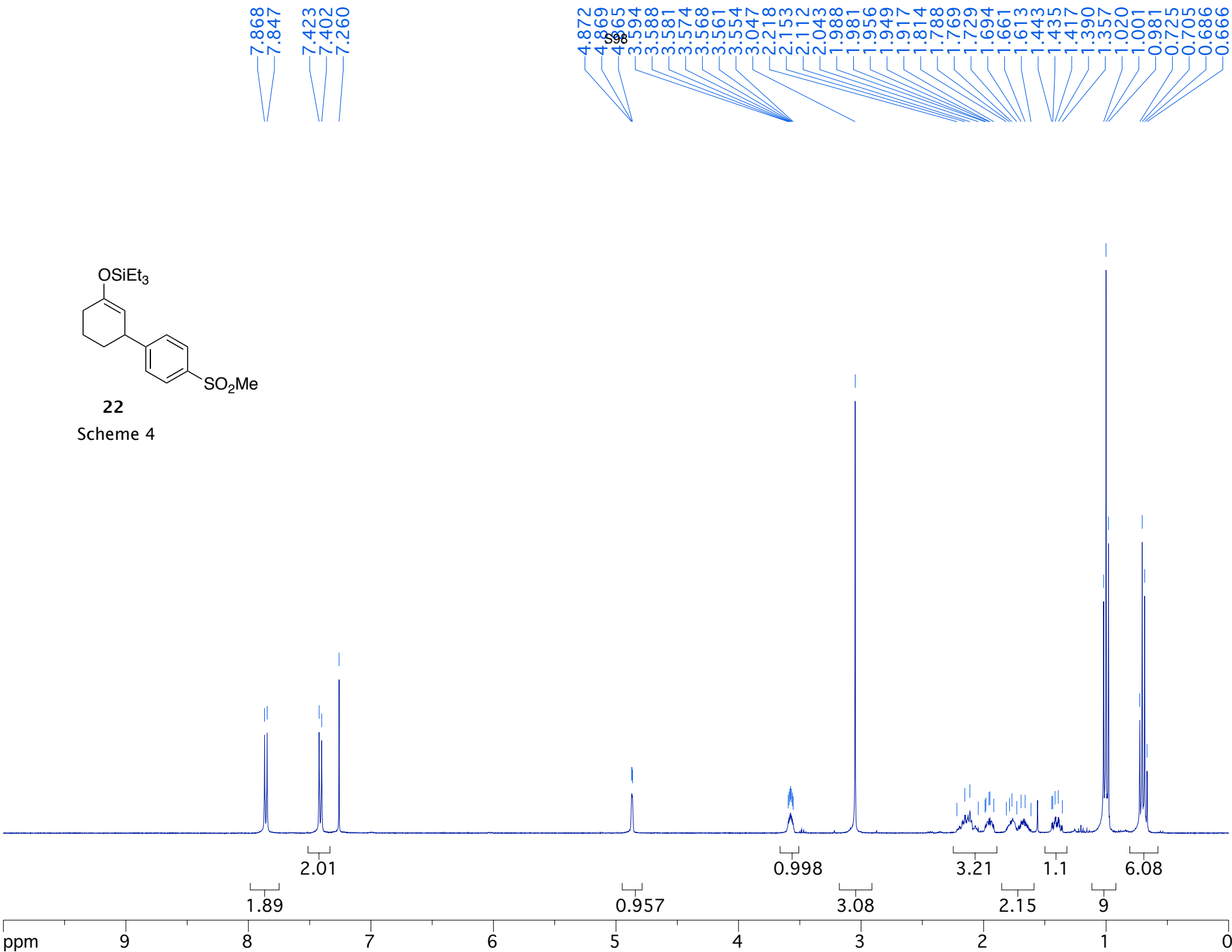
**21**  
Scheme 4



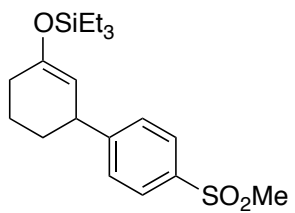


22

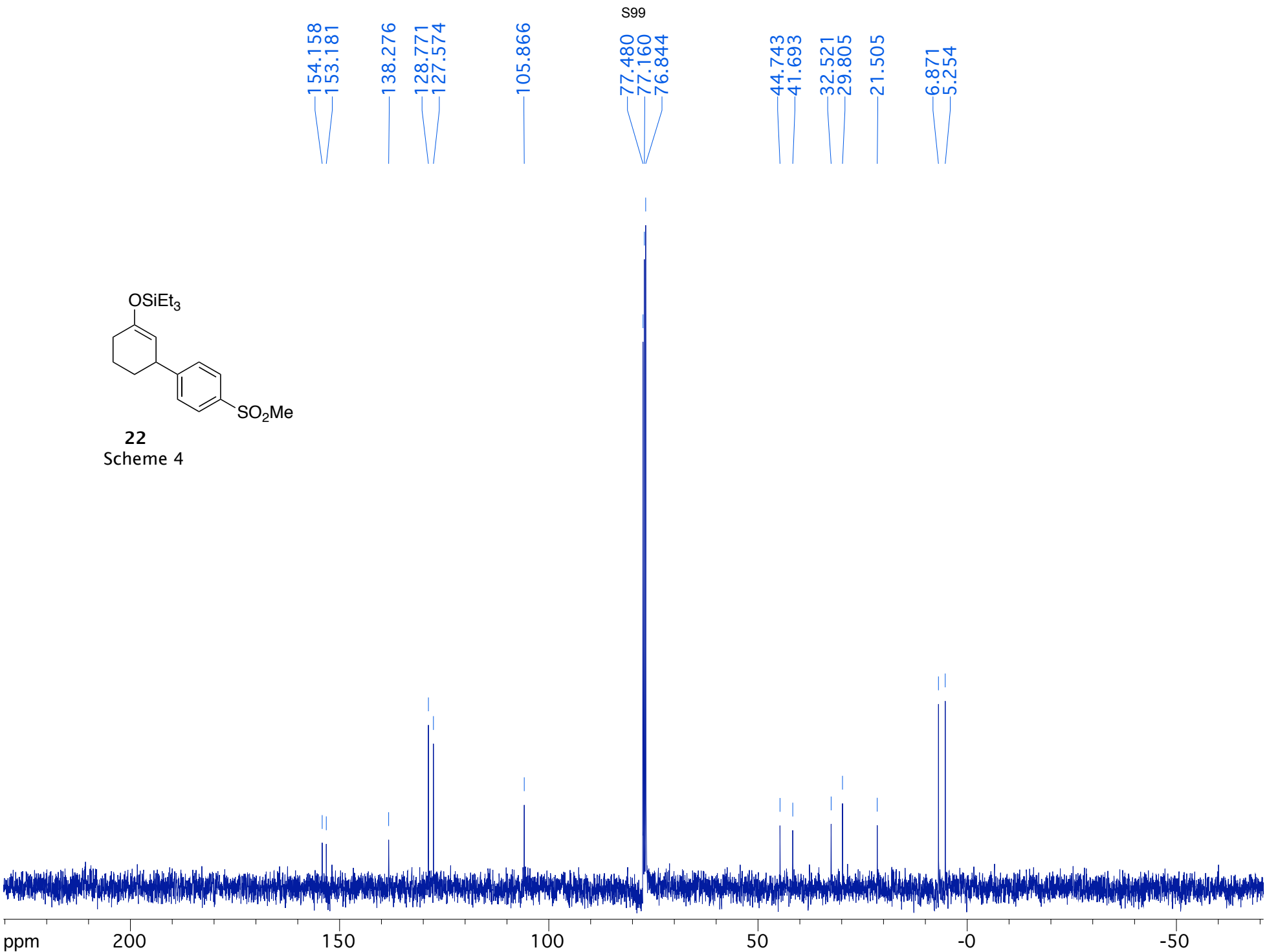
Scheme 4

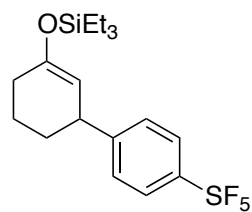
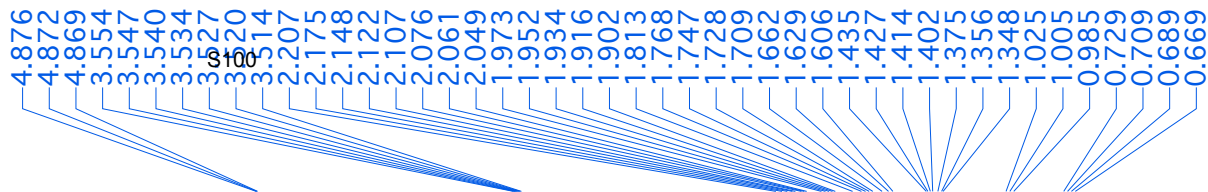
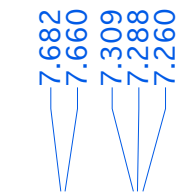




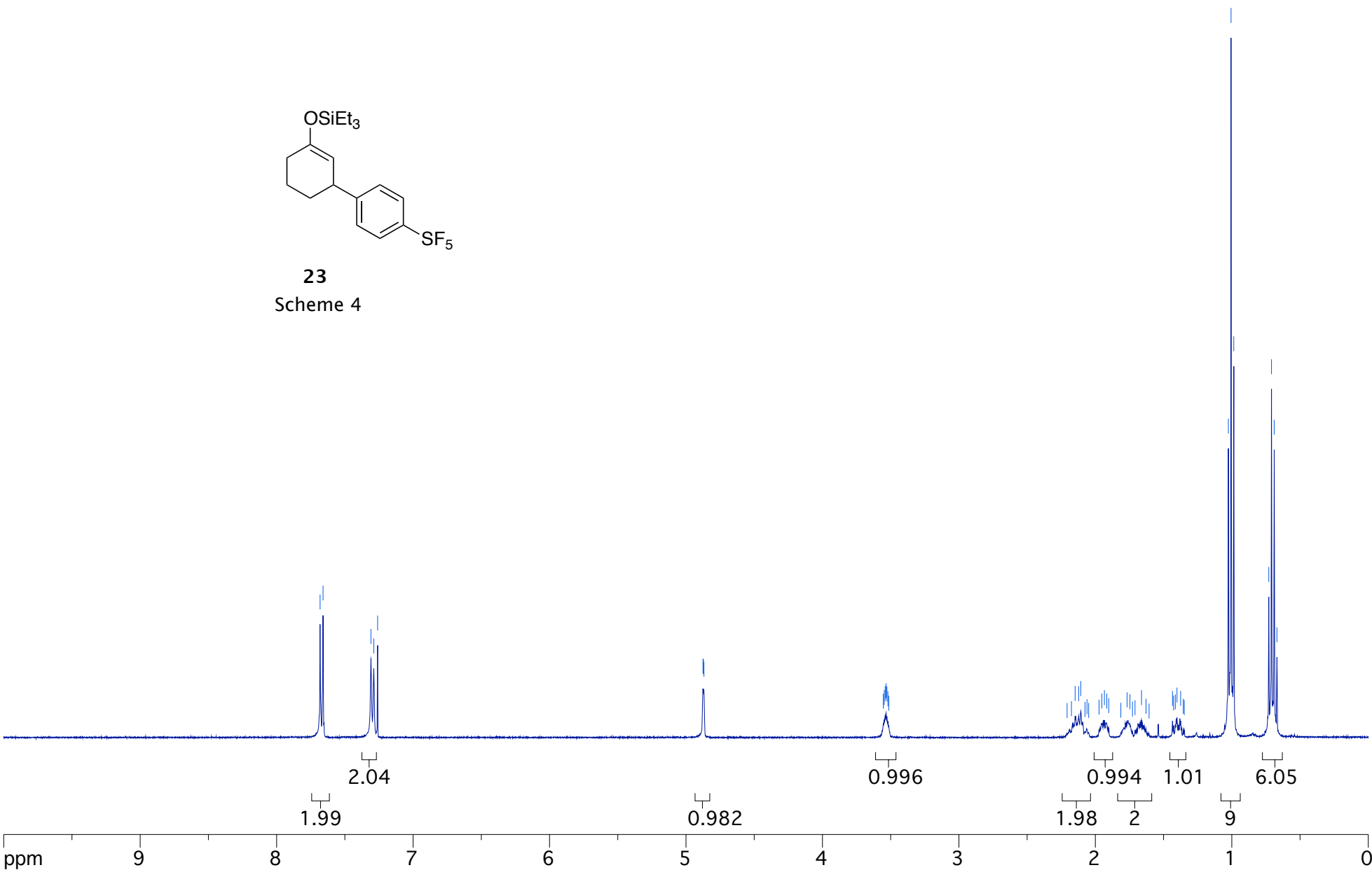


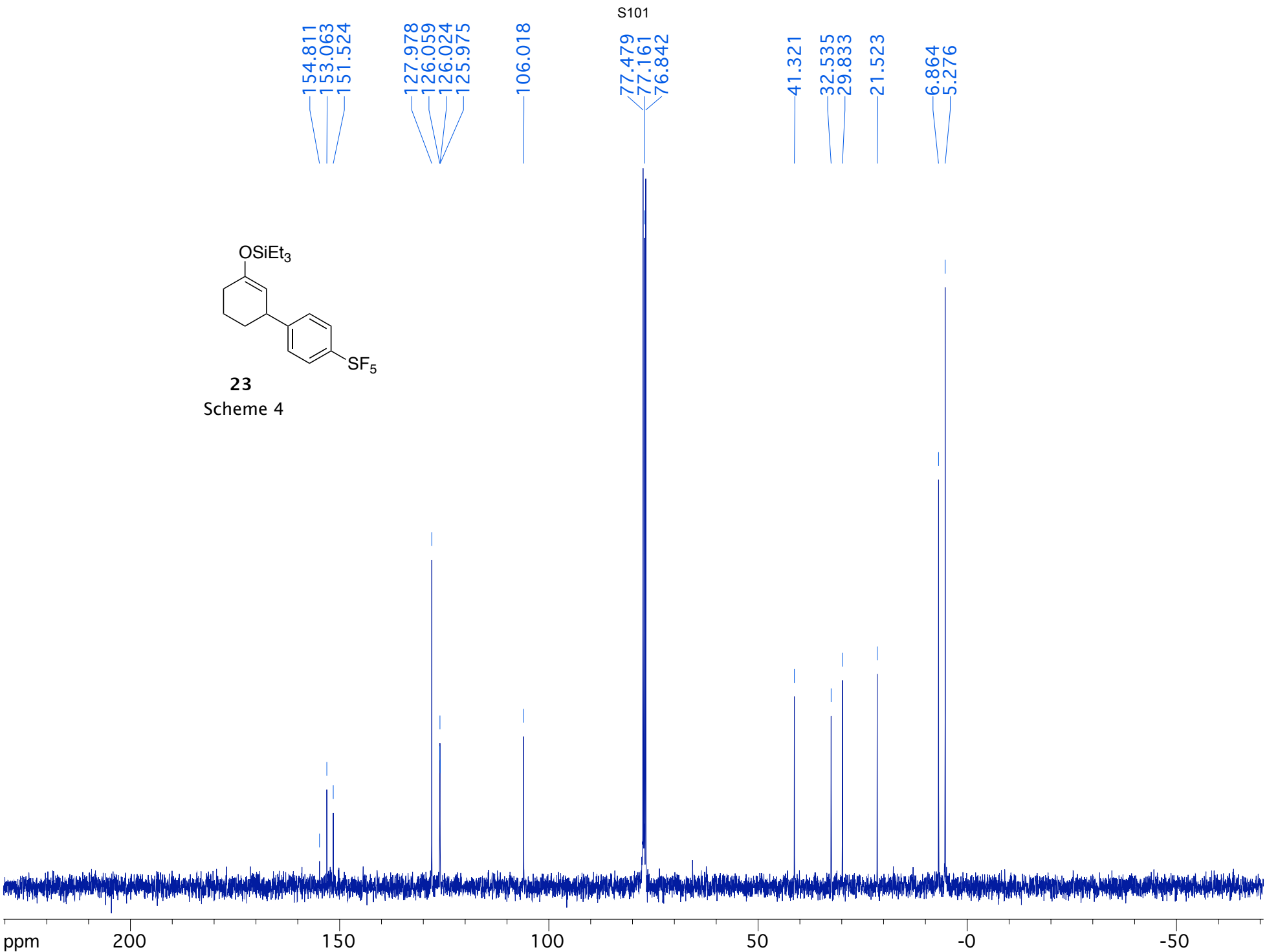
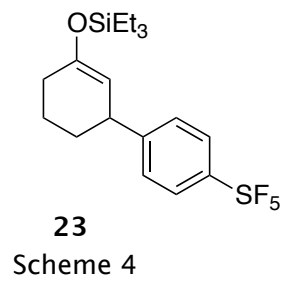
**22**  
Scheme 4



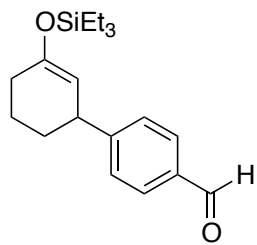


**23**  
Scheme 4

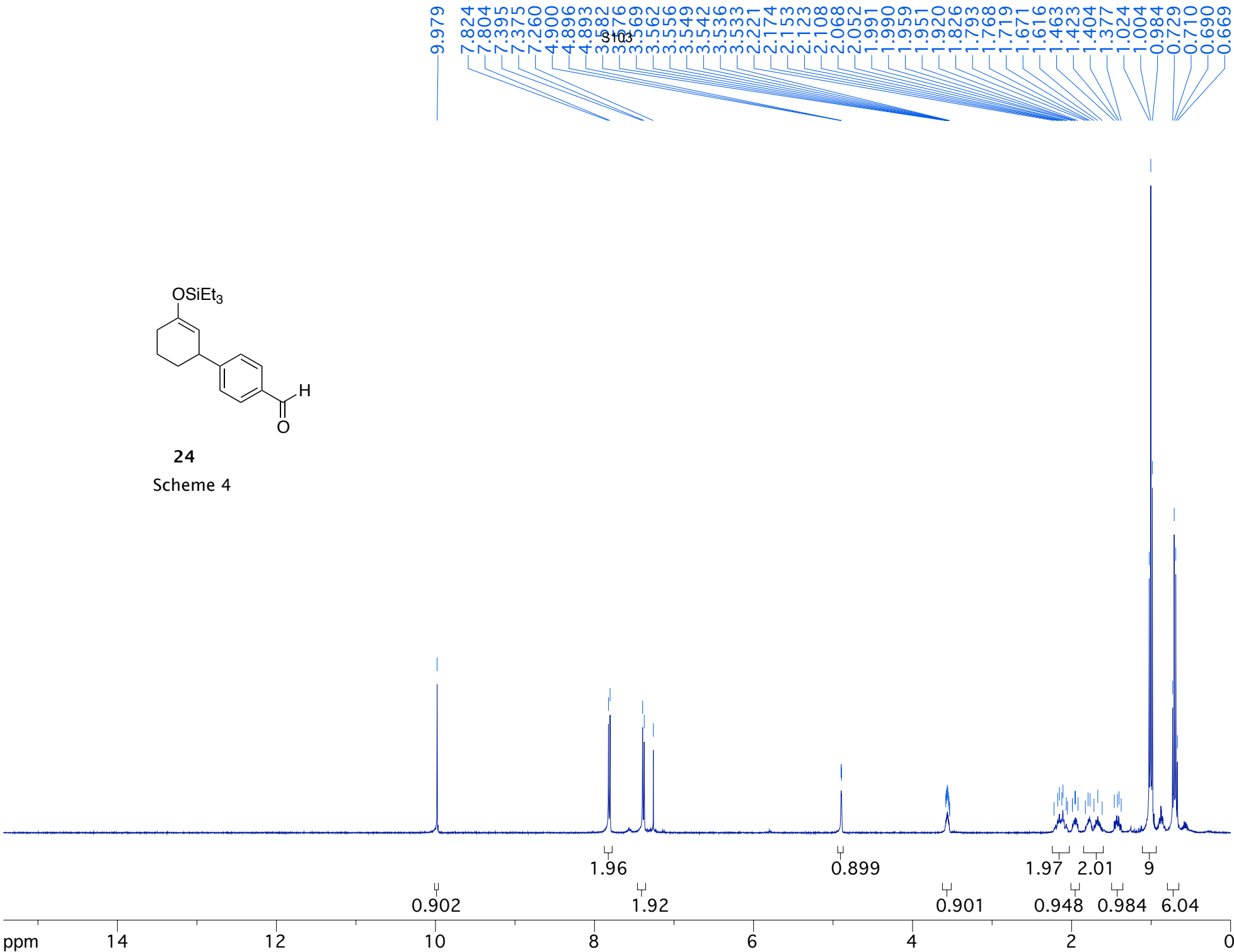


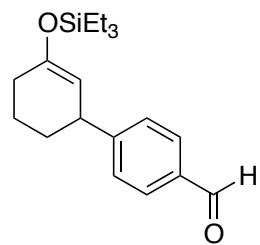




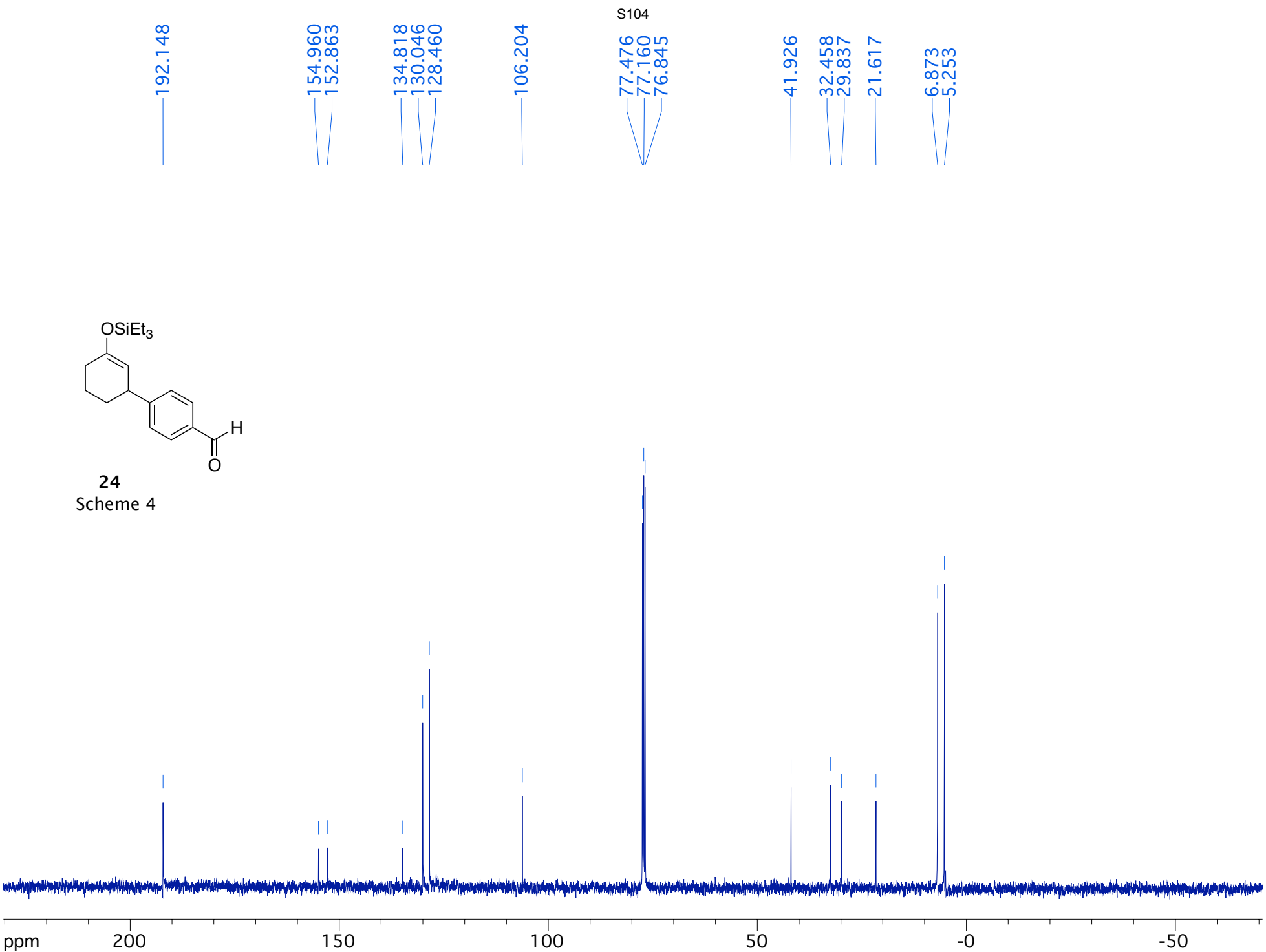


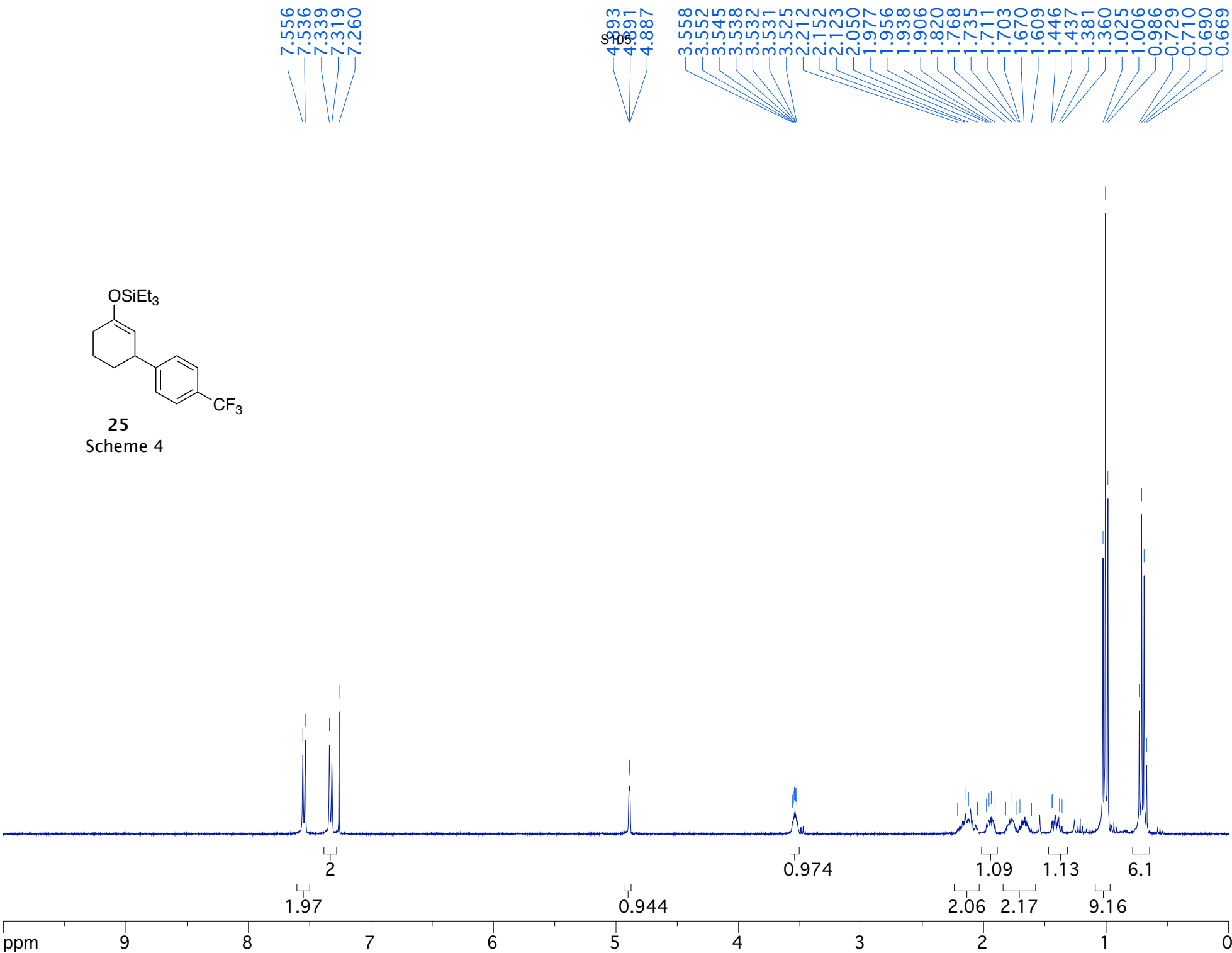
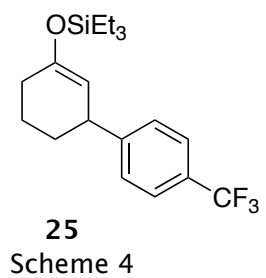
**24**  
Scheme 4

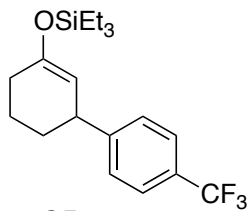




24  
Scheme 4

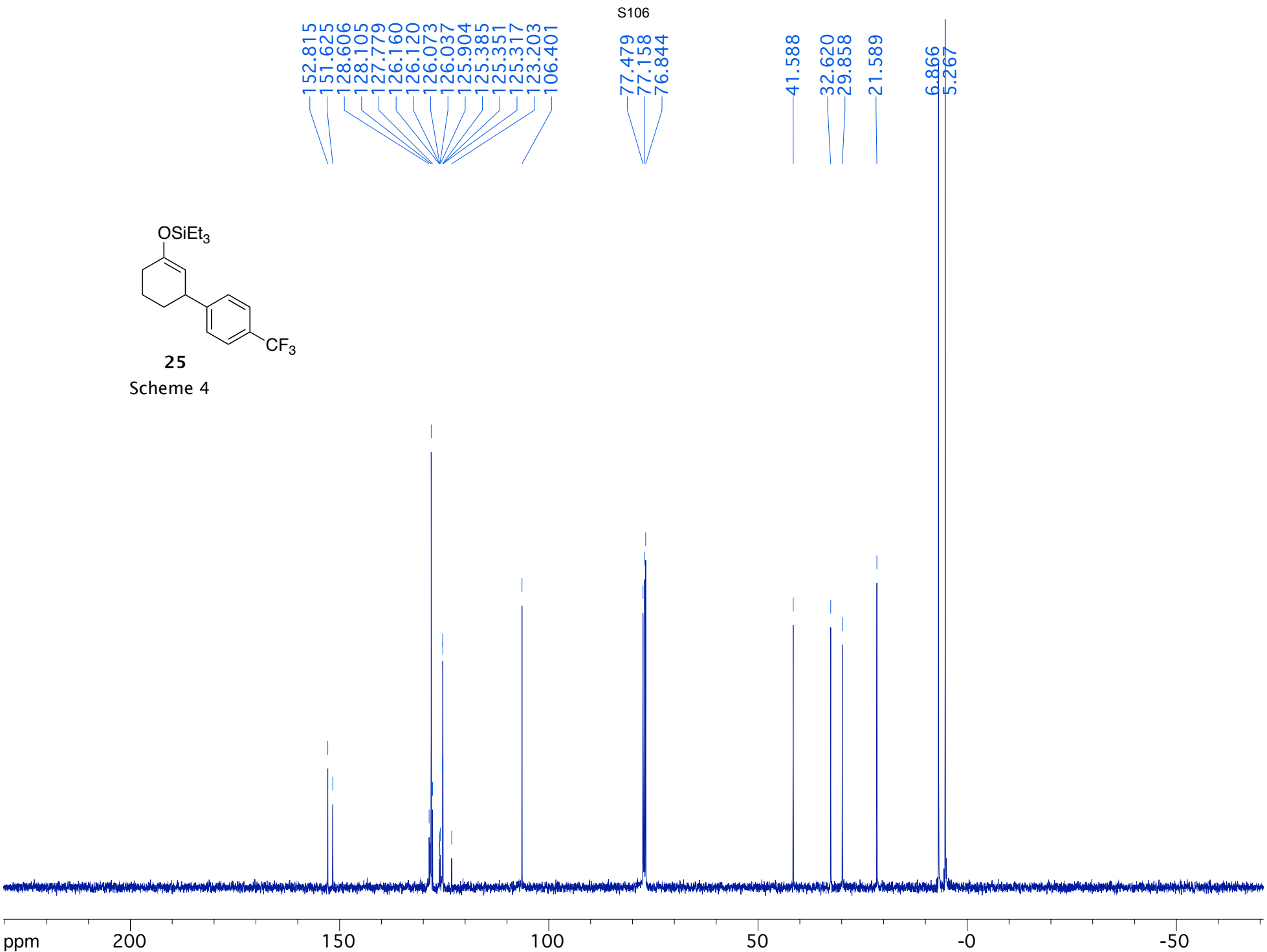




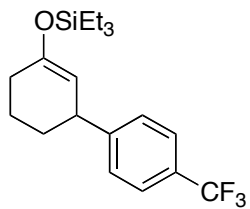


25

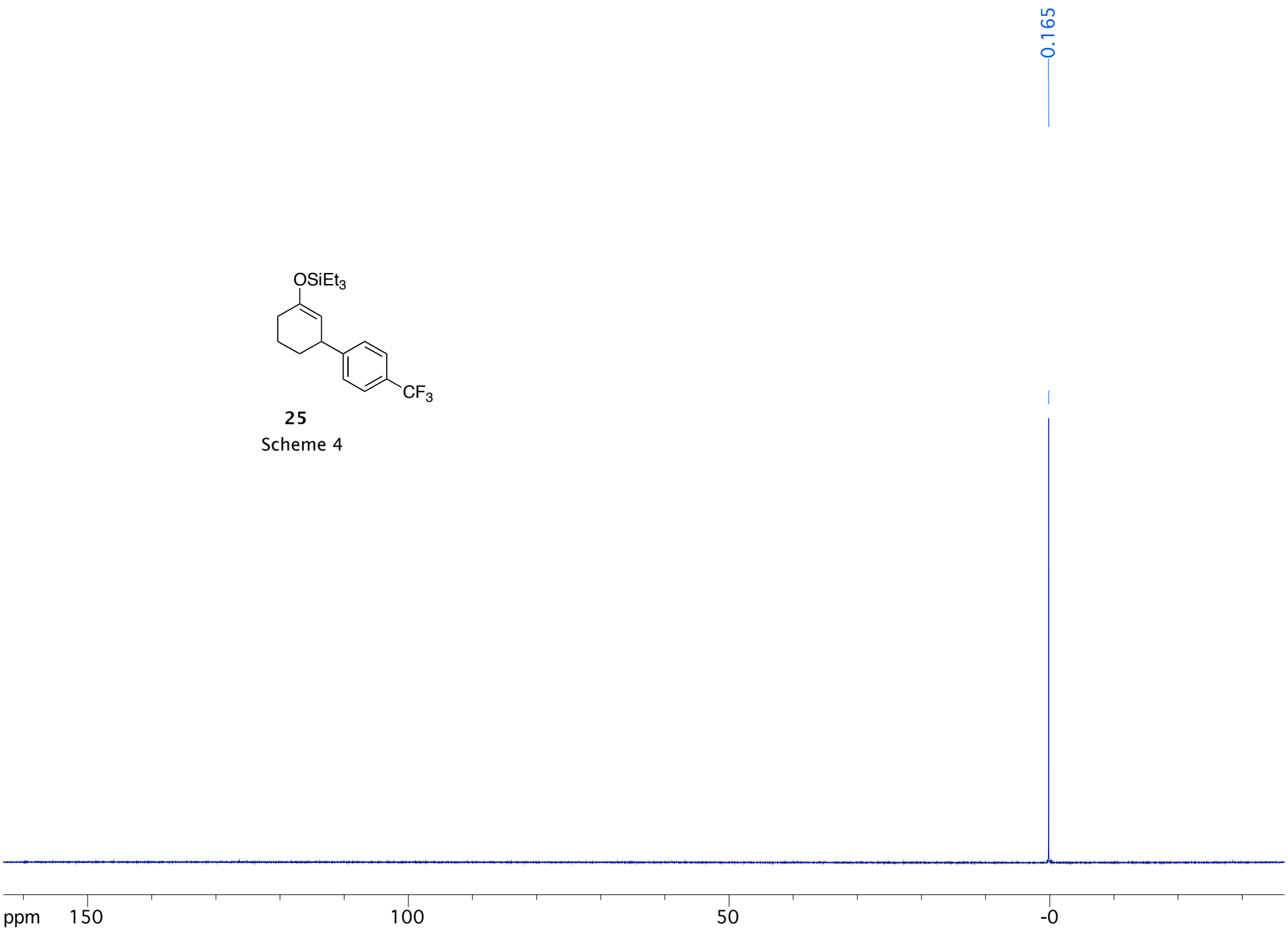
Scheme 4

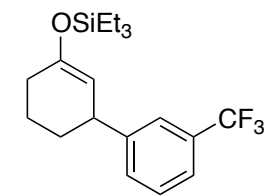




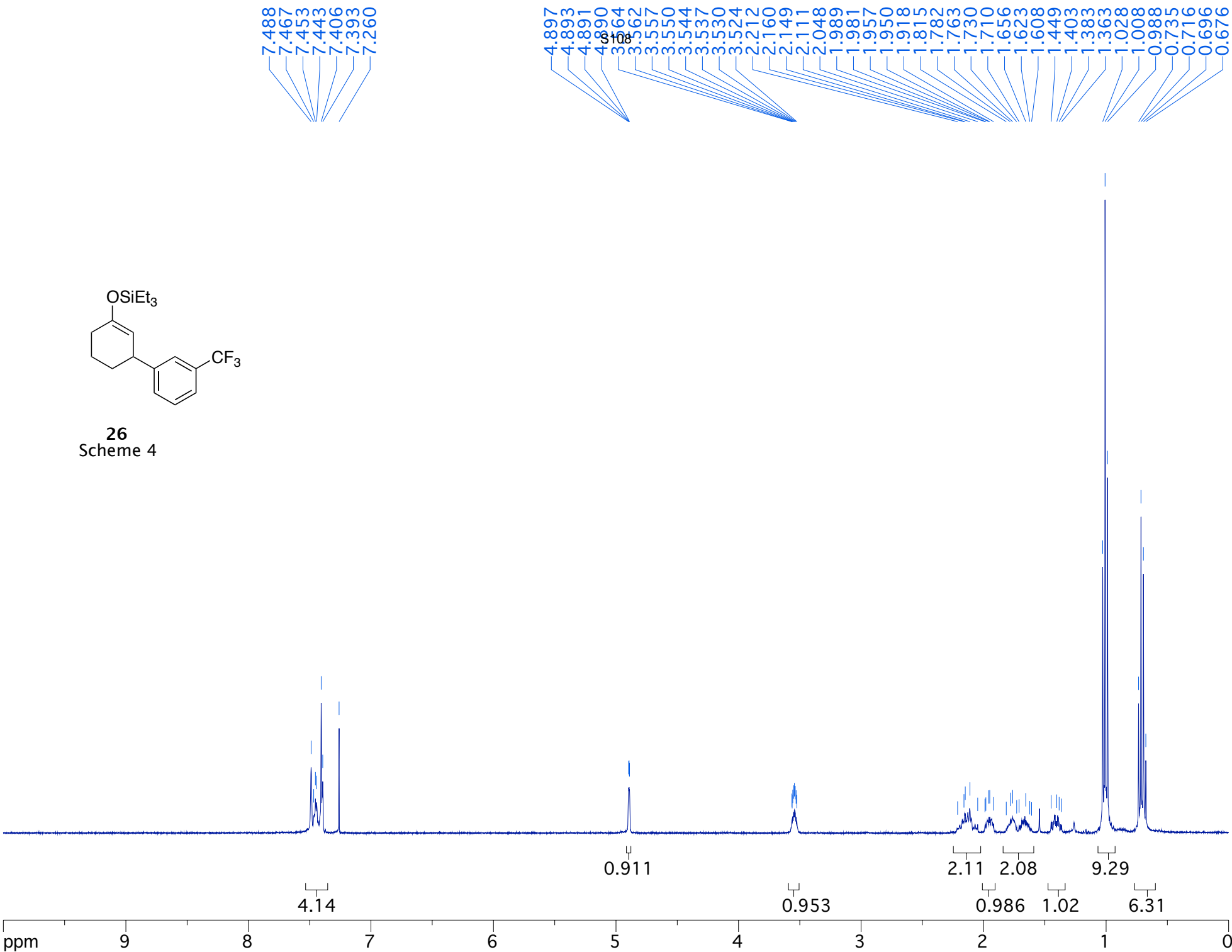


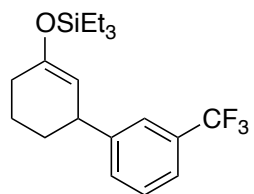
**25**  
Scheme 4





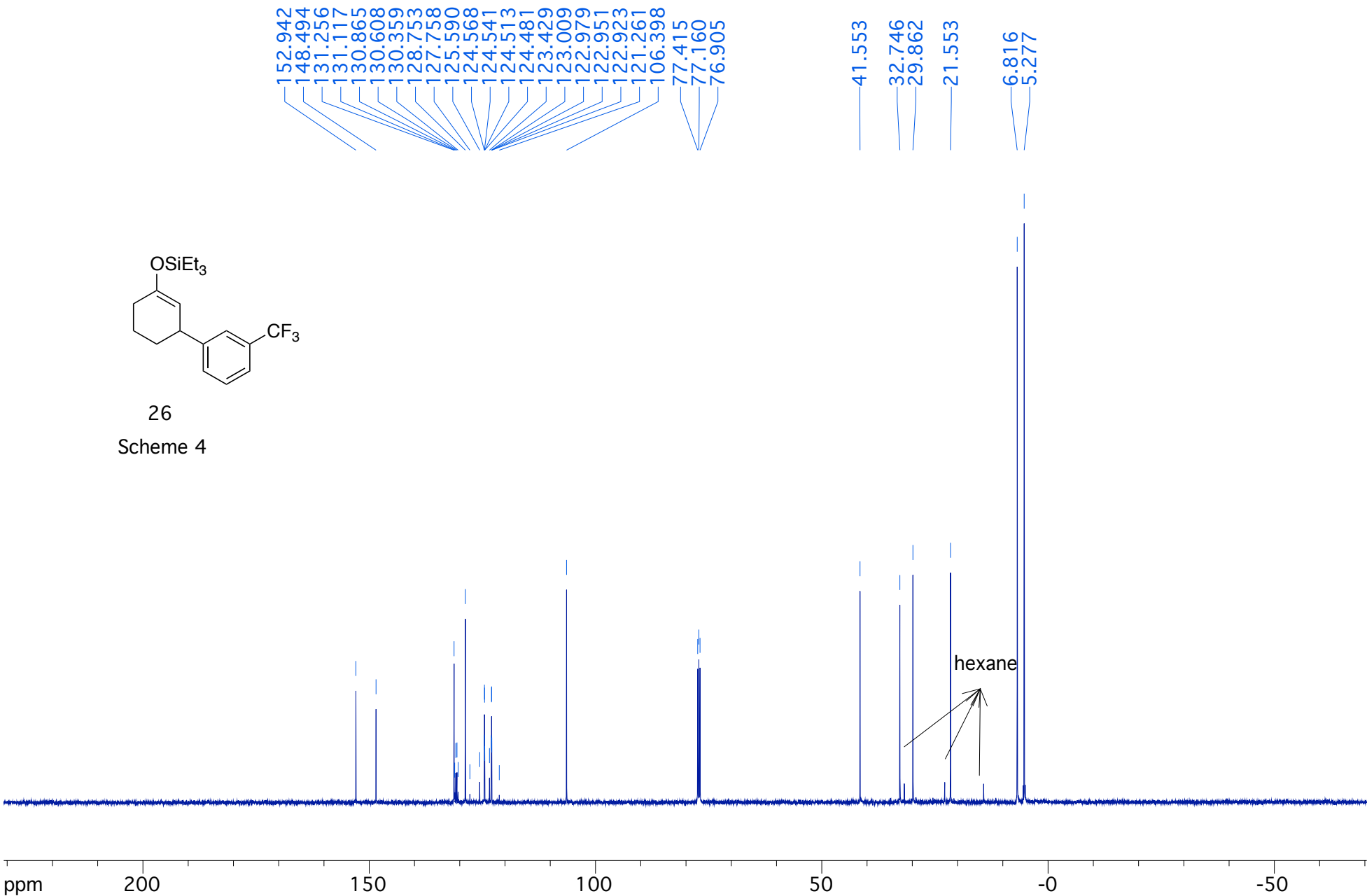
26  
Scheme 4

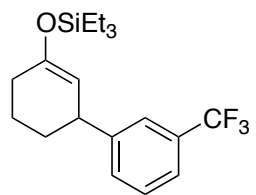




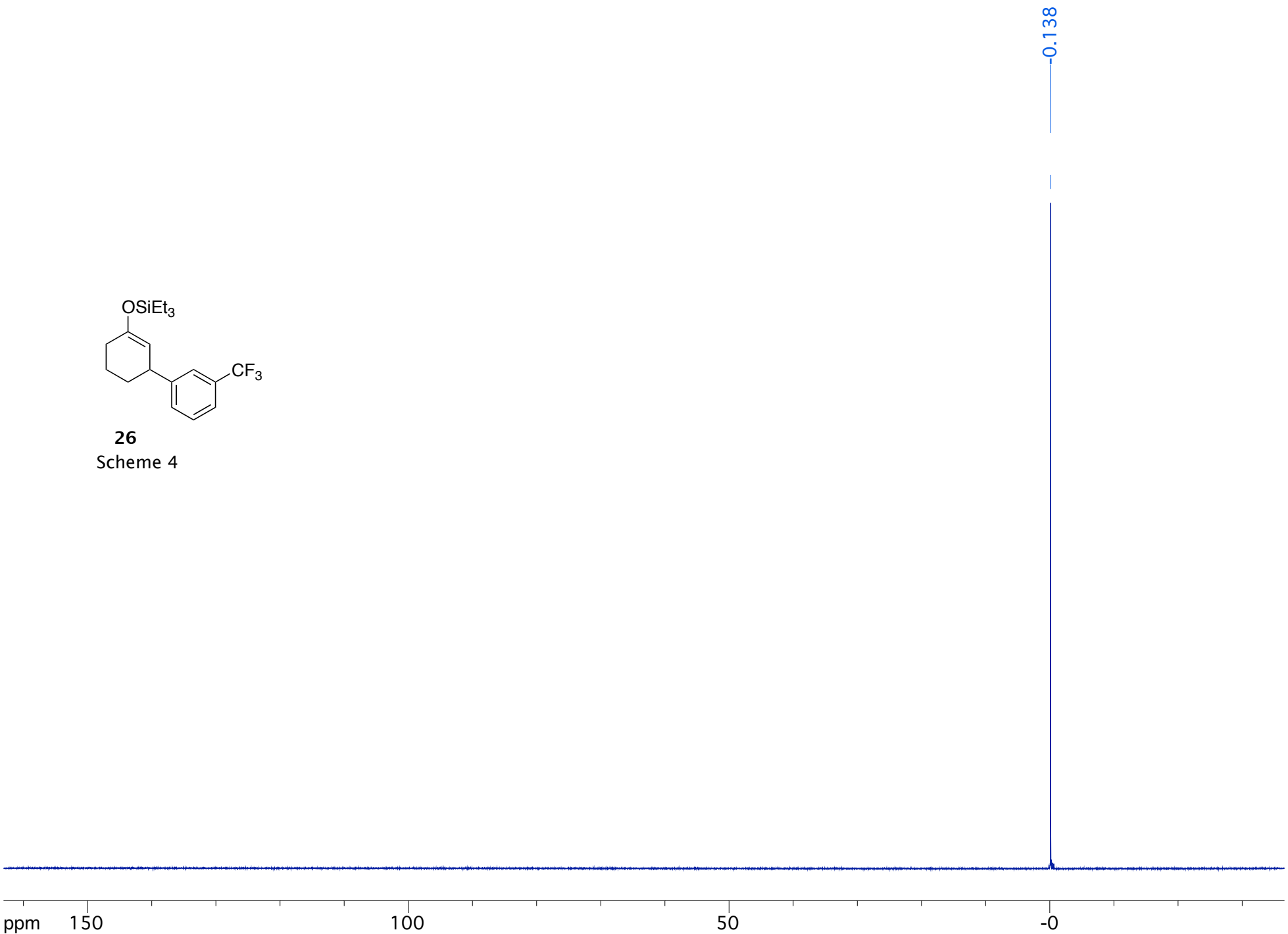
26

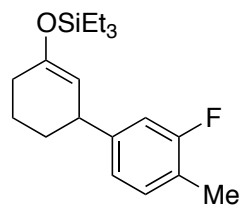
Scheme 4



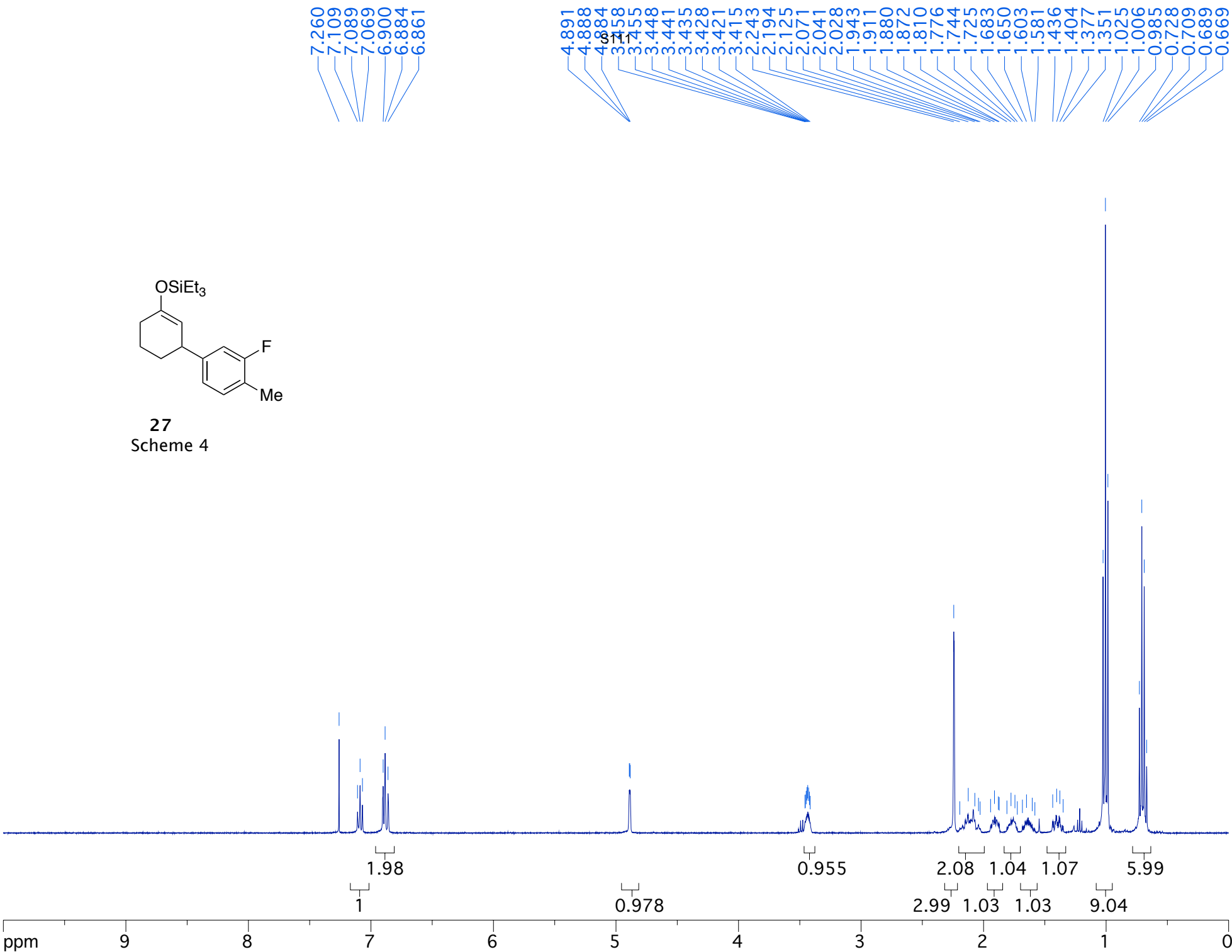


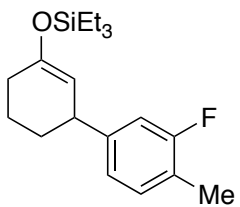
**26**  
Scheme 4



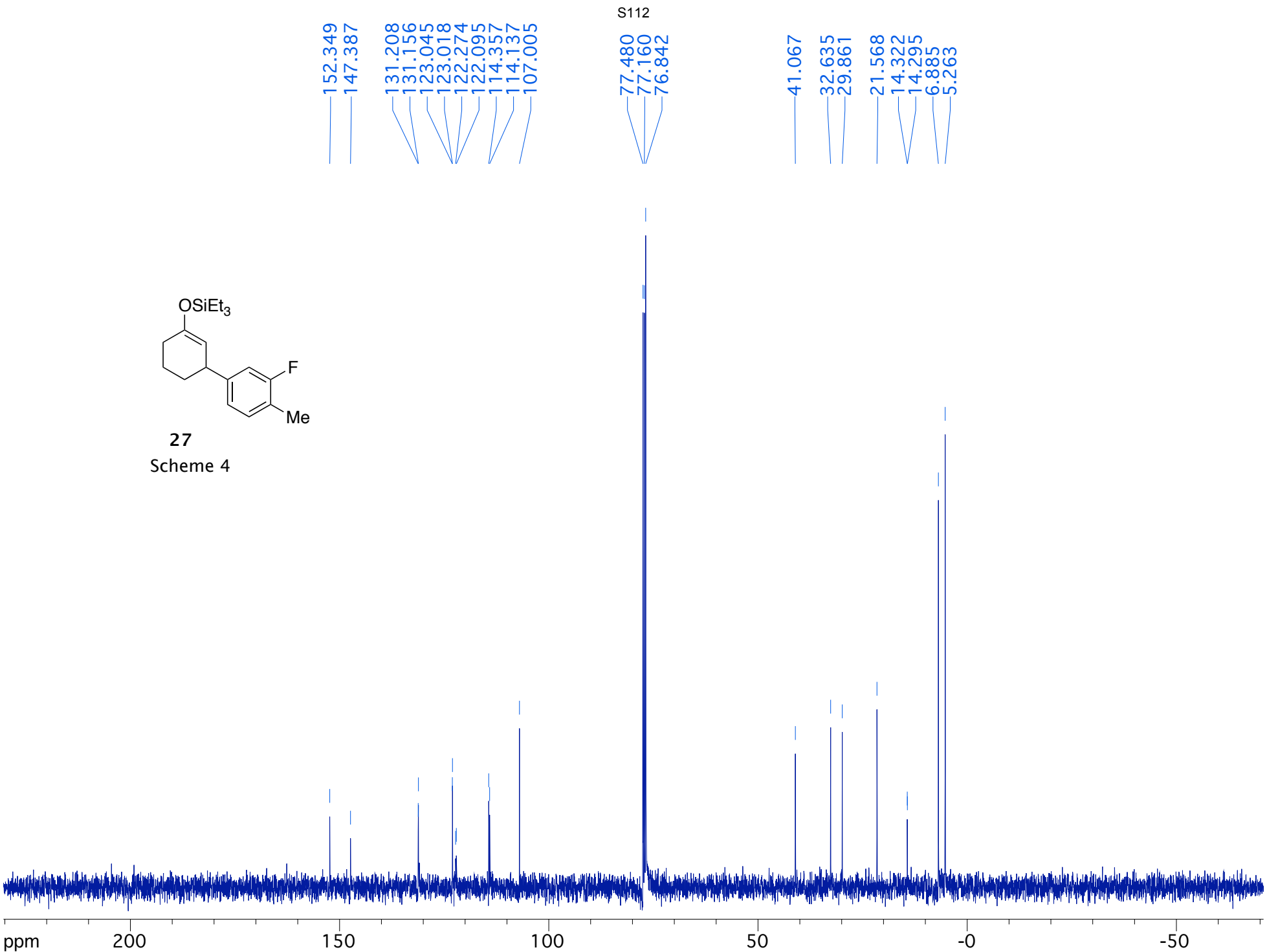


27  
Scheme 4

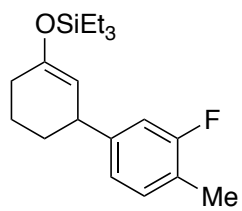




27  
Scheme 4



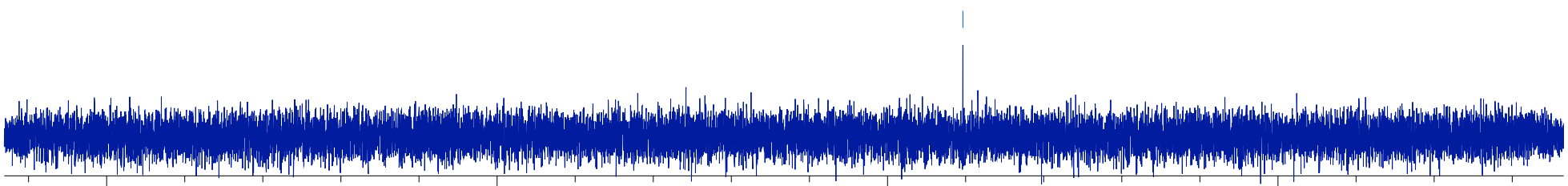
S113



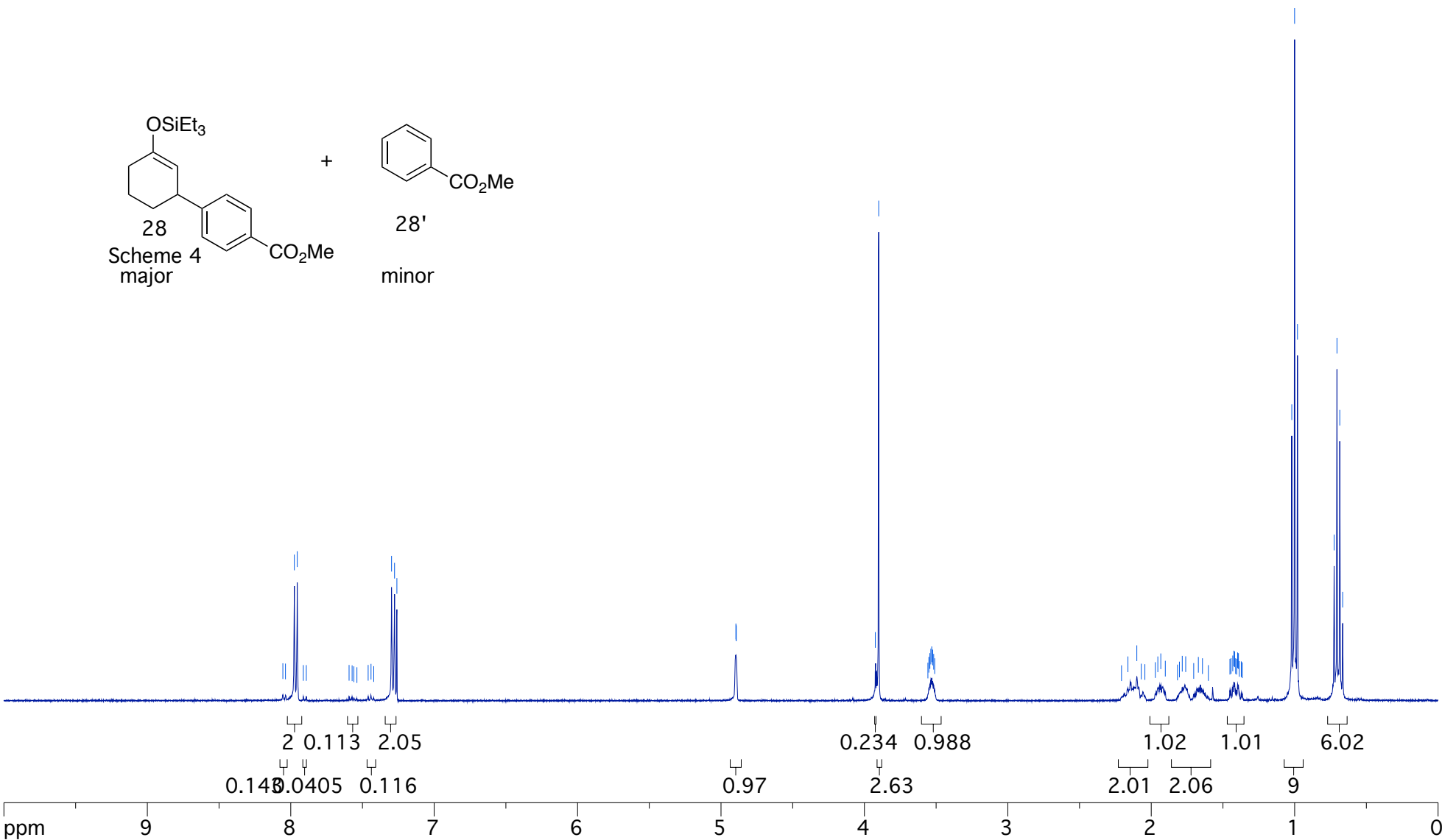
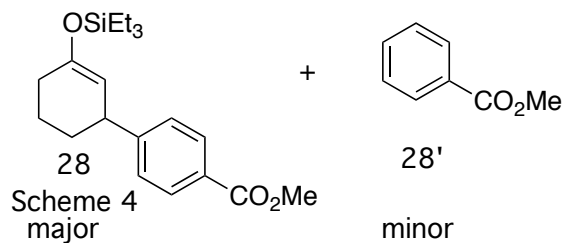
27  
Scheme 4

40.348

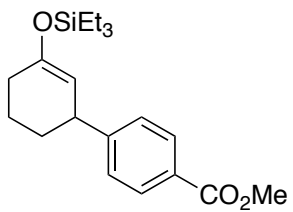
ppm 150 100 50 -0



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8.037  
7.975  
7.955  
7.912  
7.892  
7.593  
7.572  
7.560  
7.539  
7.460  
7.440  
7.421  
7.297  
7.276  
7.260  
4.896  
4.895  
4.893  
3.924  
3.900  
3.557  
3.551  
3.544  
3.537  
3.531  
3.524  
3.517  
3.510  
3.207  
2.207  
2.163  
2.101  
2.070  
2.044  
1.972  
1.954  
1.933  
1.902  
1.817  
1.803  
1.784  
1.760  
1.704  
1.671  
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1.602  
1.451  
1.444  
1.432  
1.424  
1.419  
1.412  
1.404  
1.398  
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0.685  
0.665

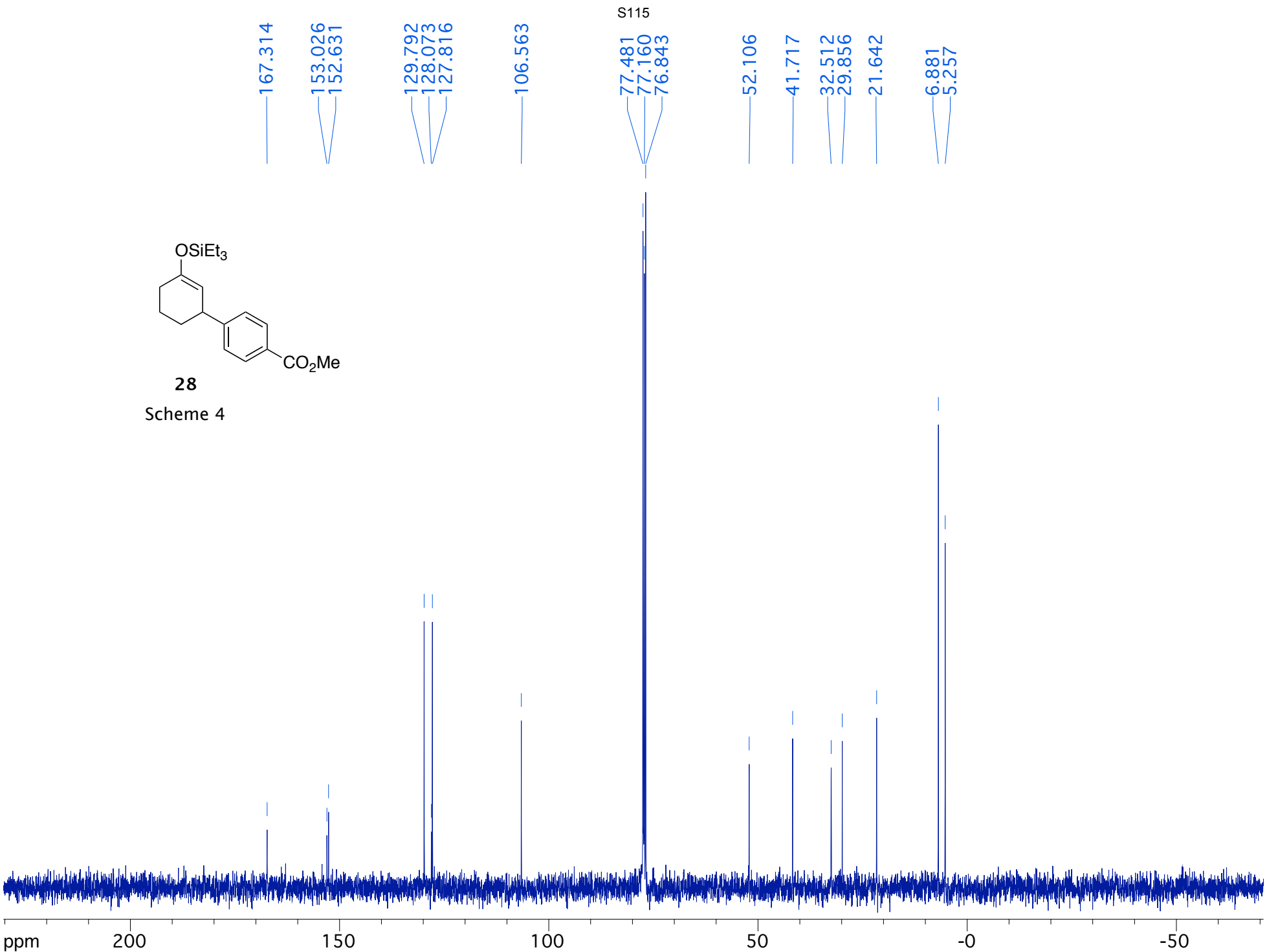






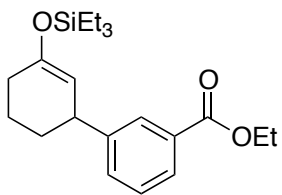
**28**

Scheme 4

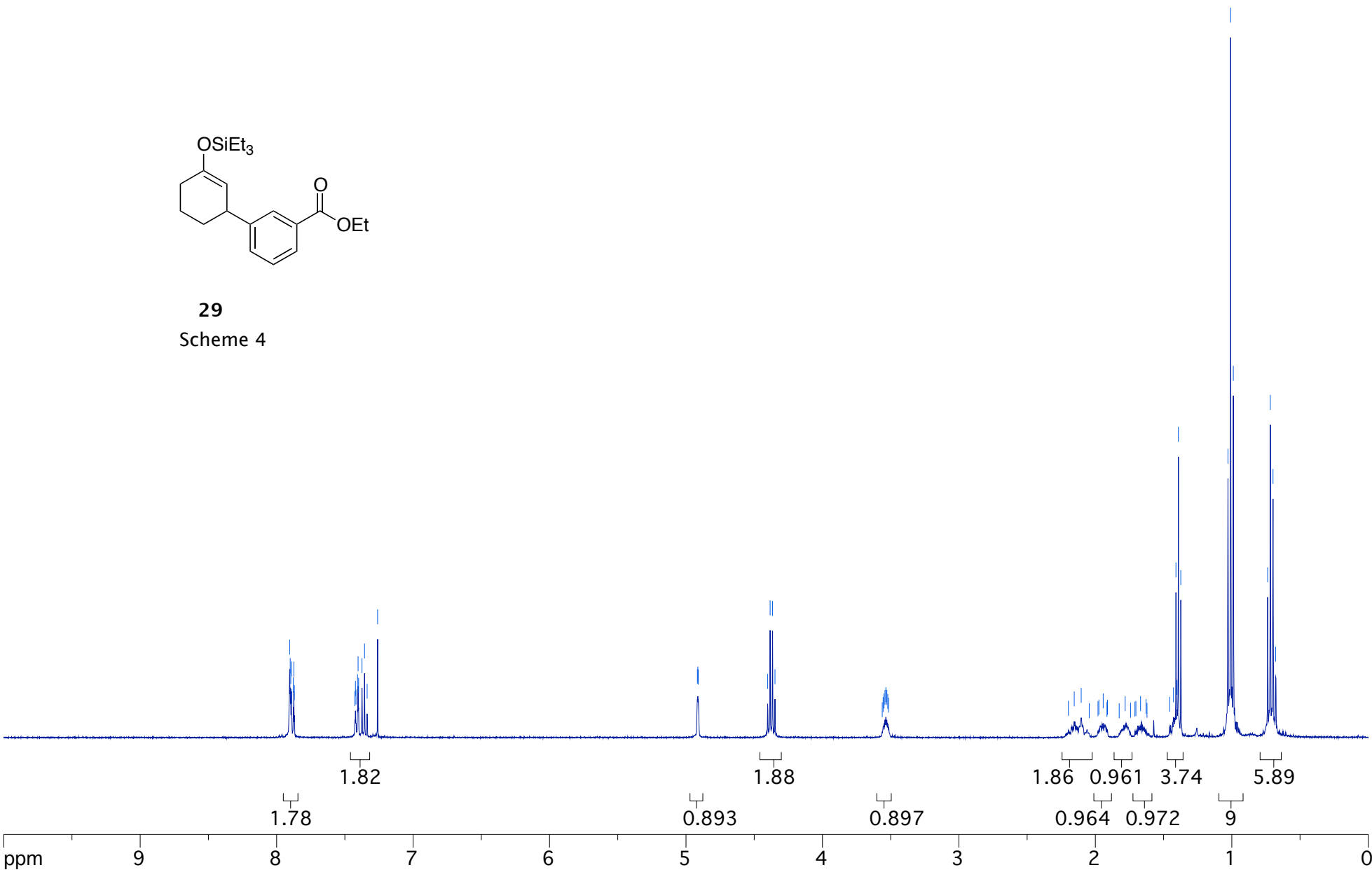


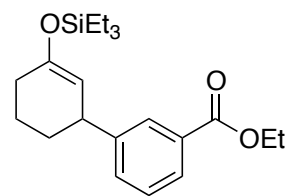
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7.900  
7.897  
7.893  
7.889  
7.878  
7.874  
7.870  
7.426  
7.422  
7.418  
7.407  
7.403  
7.399  
7.374  
7.356  
7.337  
7.260

4.916  
4.913  
4.910  
4.401  
4.383  
4.366  
4.348  
3.562  
3.555  
3.549  
3.542  
3.535  
3.528  
3.521  
3.515  
2.198  
2.155  
2.104  
2.045  
1.981  
1.974  
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1.915  
1.911  
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1.782  
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1.703  
1.669  
1.628  
1.622  
1.455  
1.427  
1.409  
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0.679

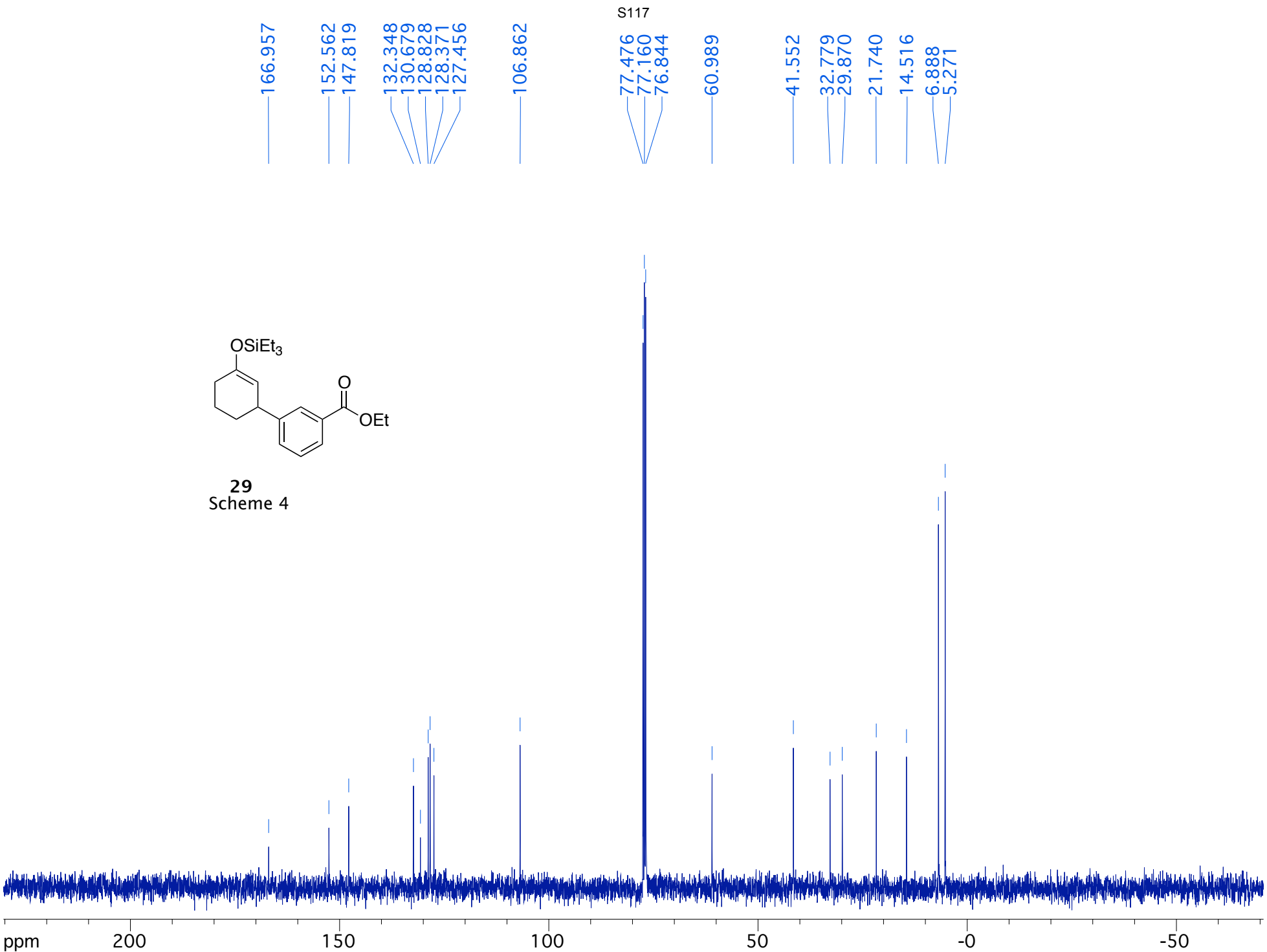


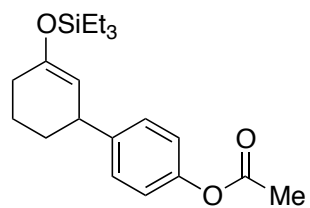
**29**  
Scheme 4



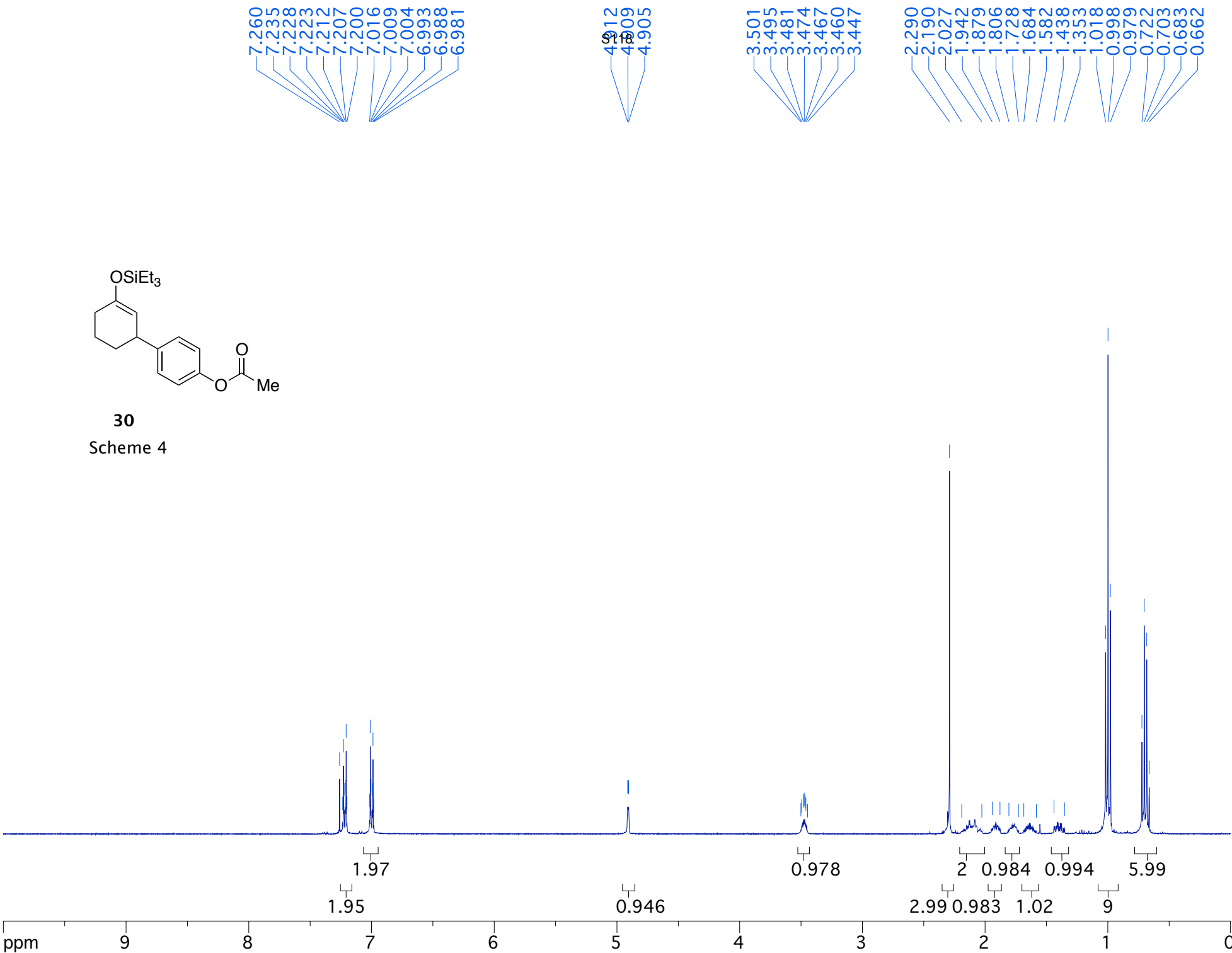


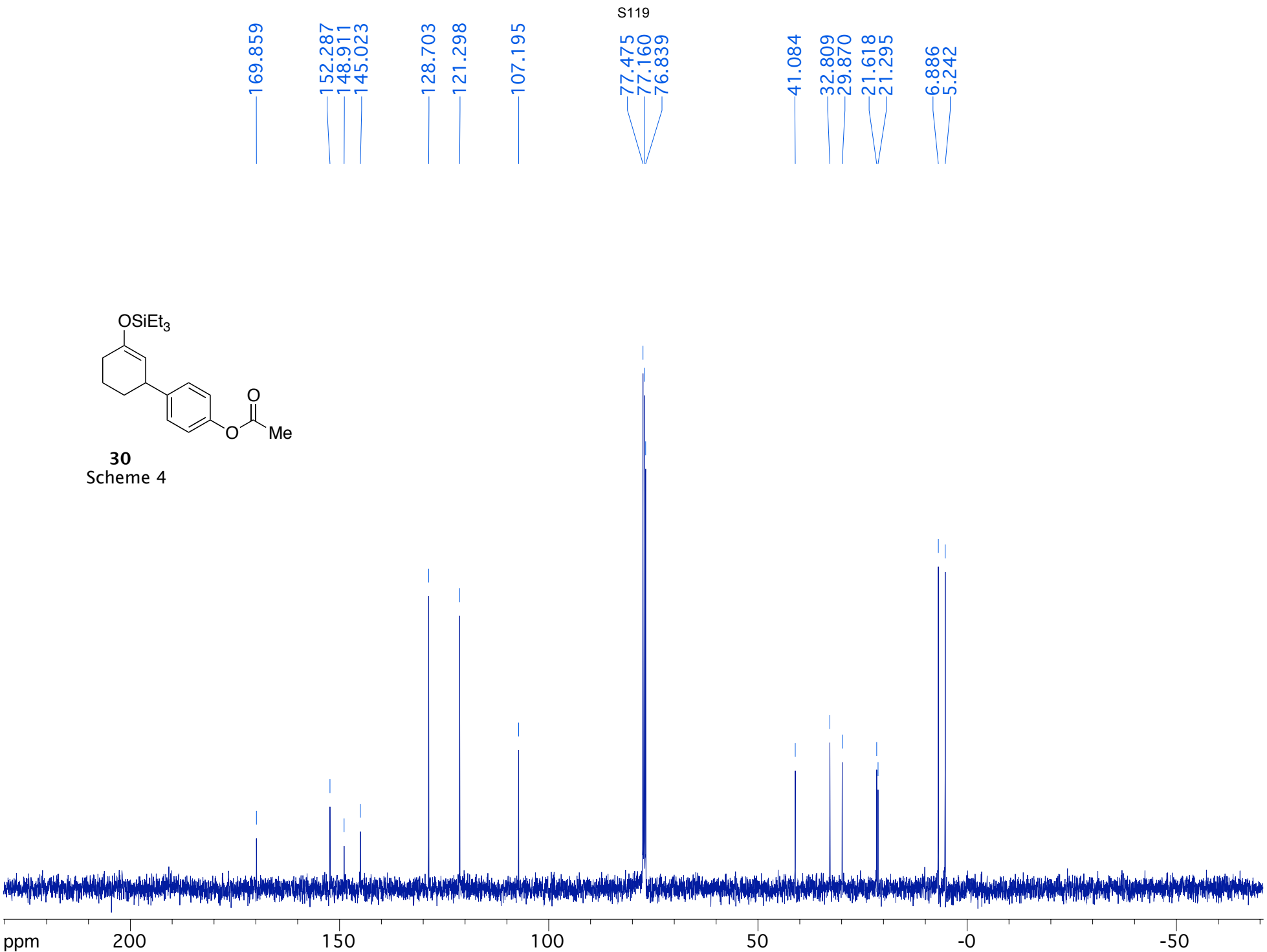
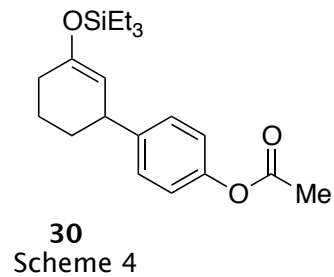
**29**  
Scheme 4

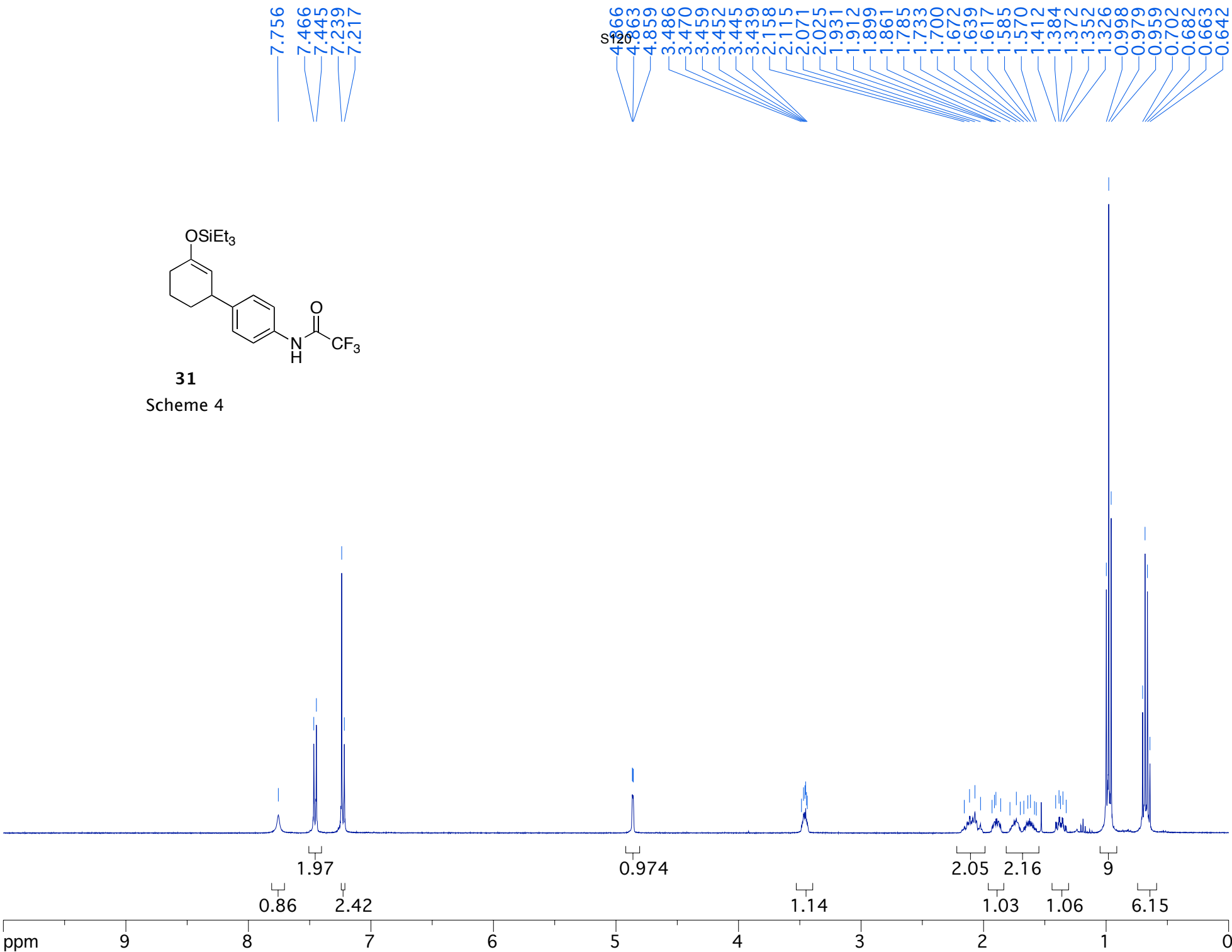
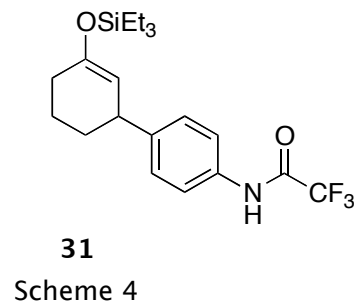


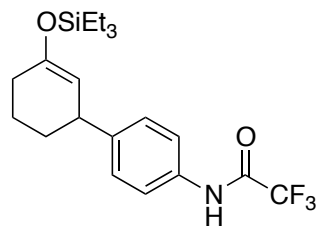


**30**  
Scheme 4



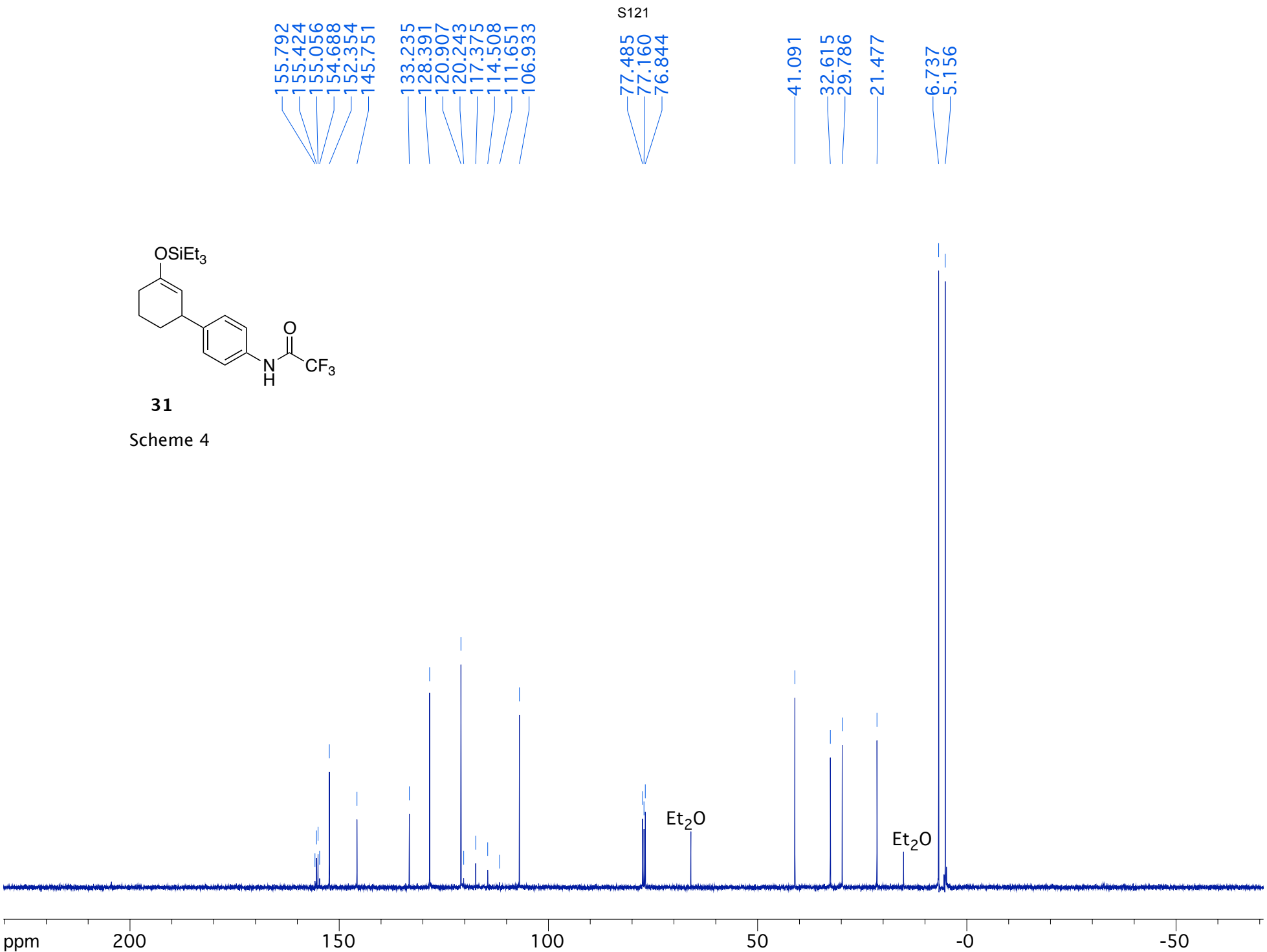


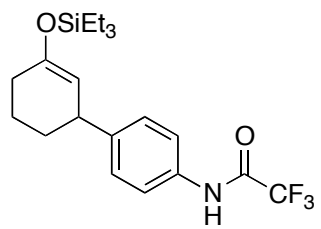




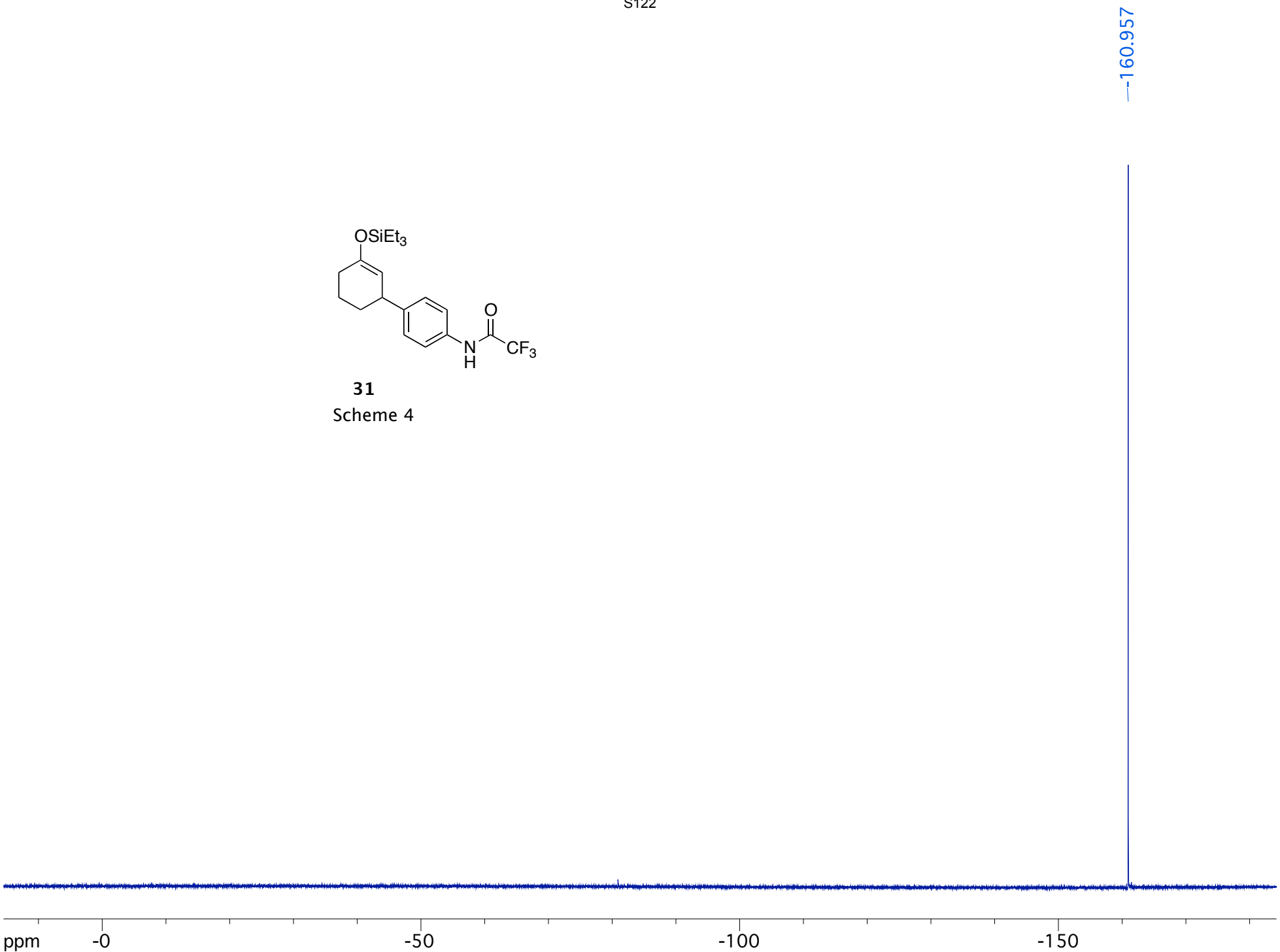
**31**

Scheme 4



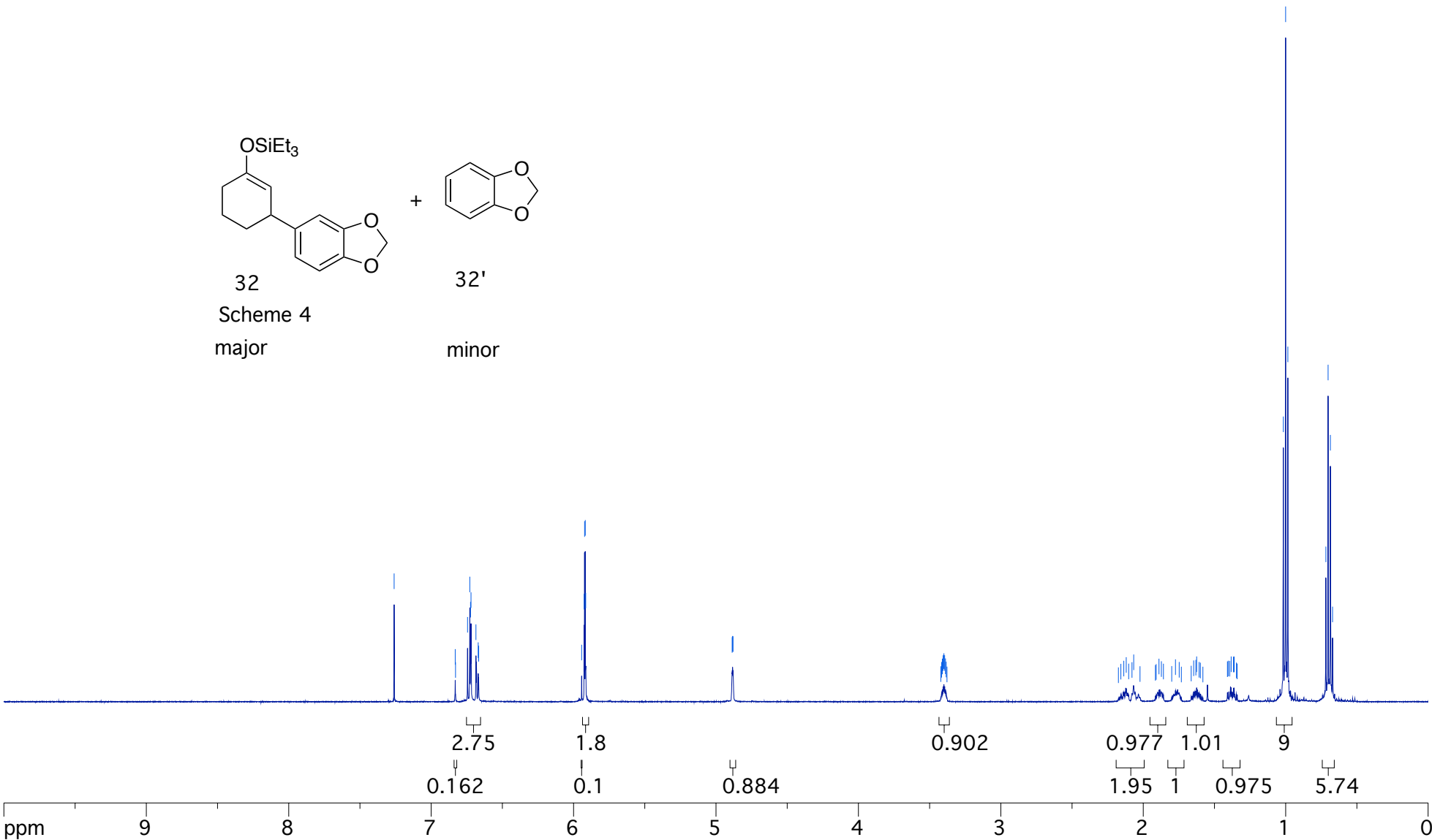
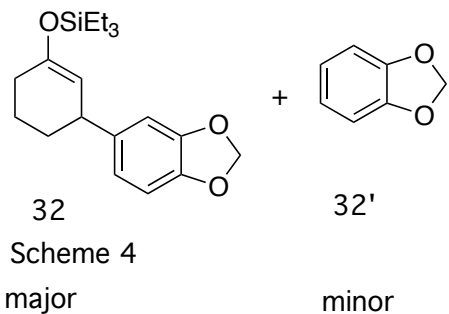


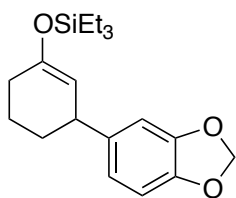
**31**  
Scheme 4



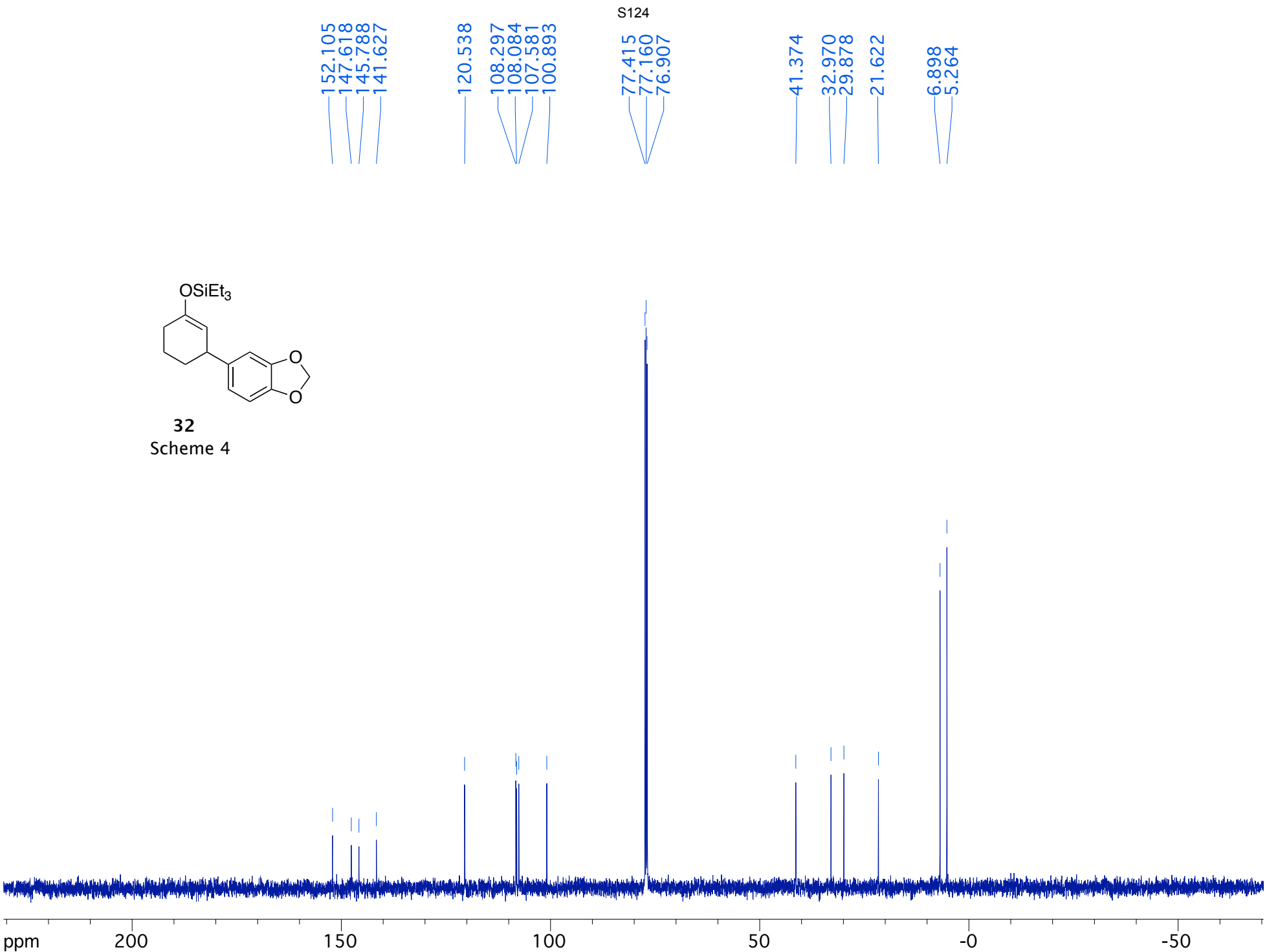


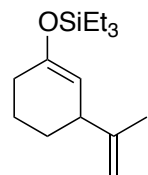
7.260  
6.831  
6.829  
6.744  
6.729  
6.724  
6.720  
6.686  
6.670  
6.667  
6.666  
5.943  
5.926  
5.923  
5.918  
5.915  
4.887  
4.883  
4.880  
4.422  
3.416  
3.411  
3.405  
3.400  
3.395  
3.389  
3.384  
3.378  
2.174  
2.157  
2.137  
2.120  
2.102  
2.079  
2.067  
2.023  
1.915  
1.909  
1.890  
1.873  
1.858  
1.800  
1.774  
1.748  
1.733  
1.663  
1.646  
1.631  
1.625  
1.608  
1.599  
1.581  
1.409  
1.403  
1.393  
1.383  
1.366  
1.362  
1.346  
1.340  
1.016  
1.000  
0.985  
0.718  
0.702  
0.686  
0.671



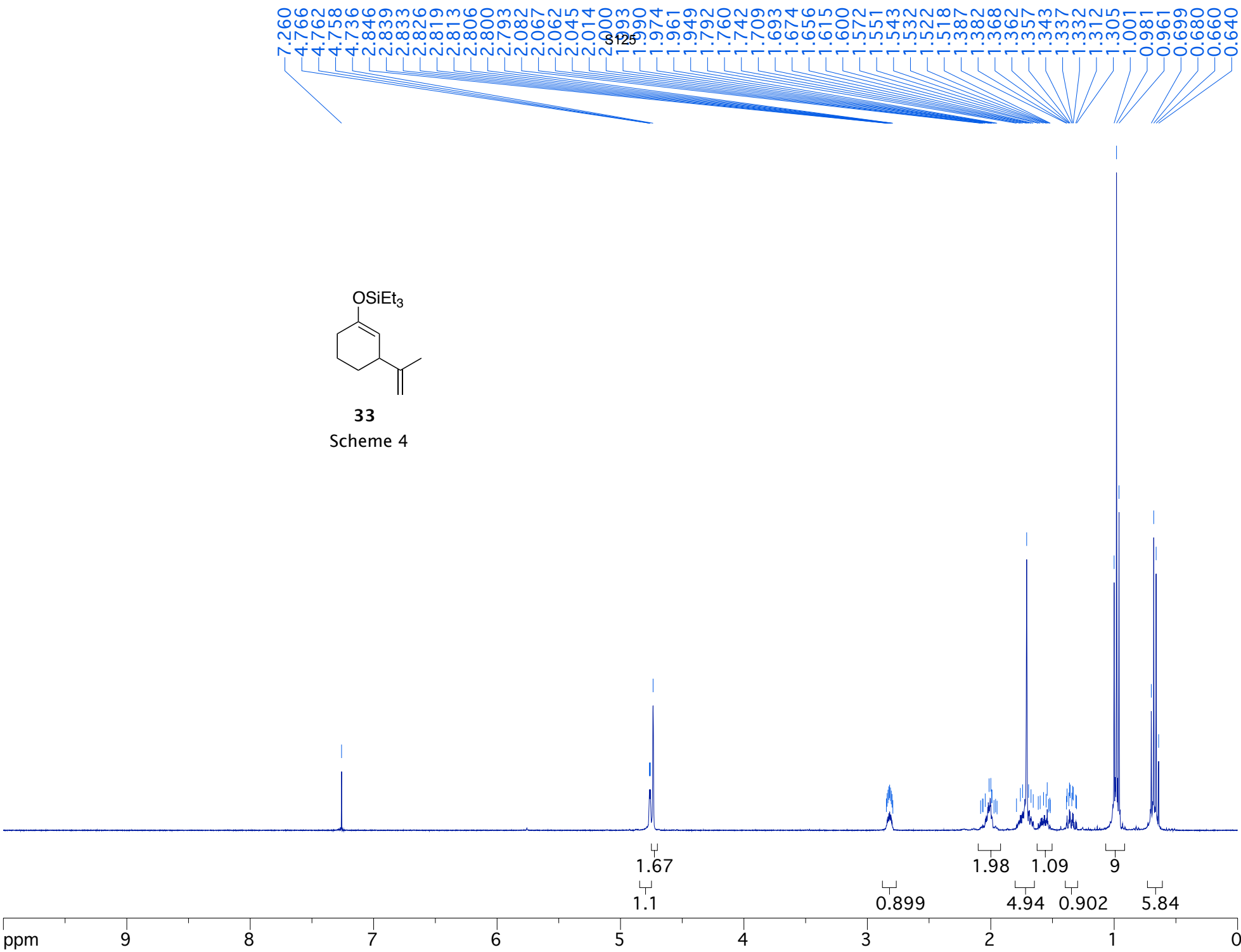


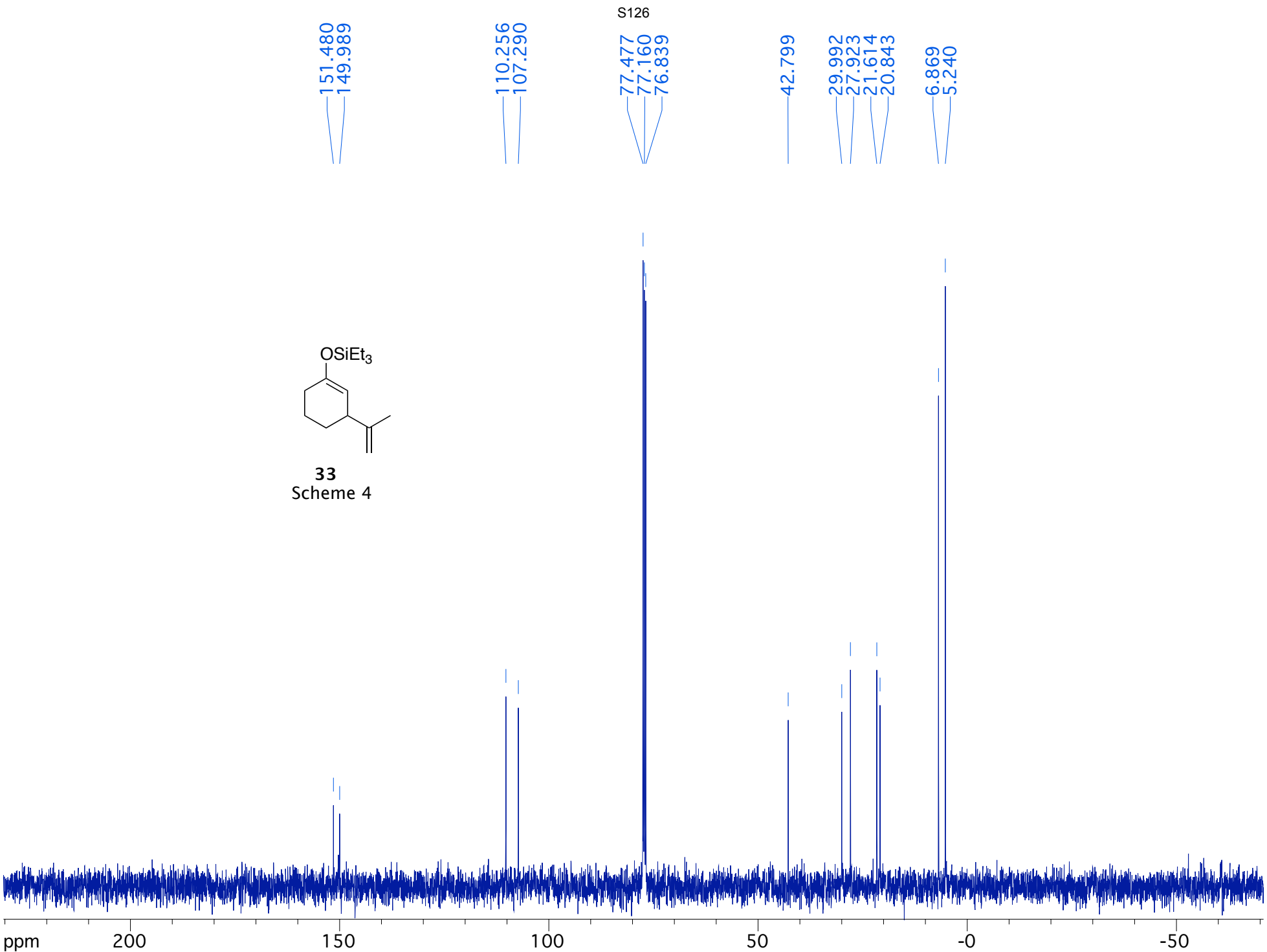
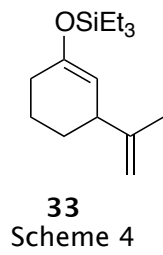
**32**  
Scheme 4

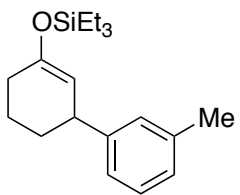




**33**  
Scheme 4







**34**  
Scheme 4

