Metal- and solvent-free approach to access 3-Se/S-chromones from the cyclization of enaminones in the presence of dichalcogenides catalyzed by KIO₃

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Table of Contents

I.   NMR Spectra
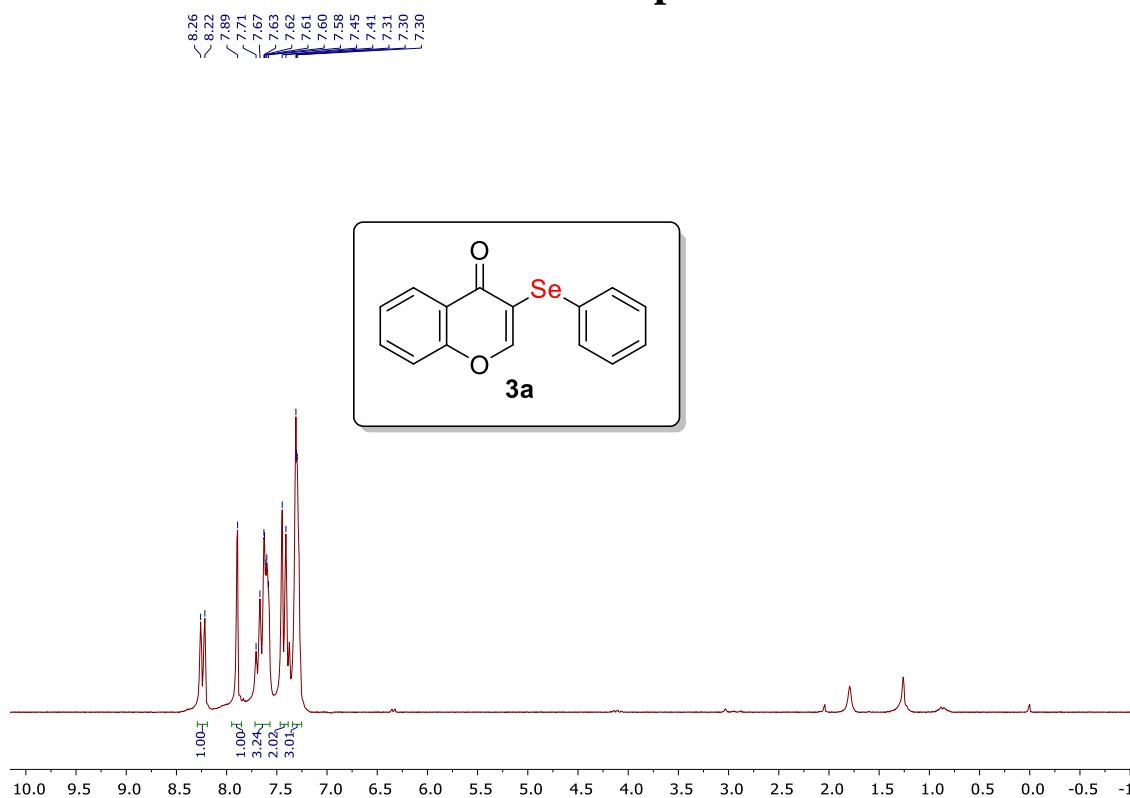
Figure S1. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3a**
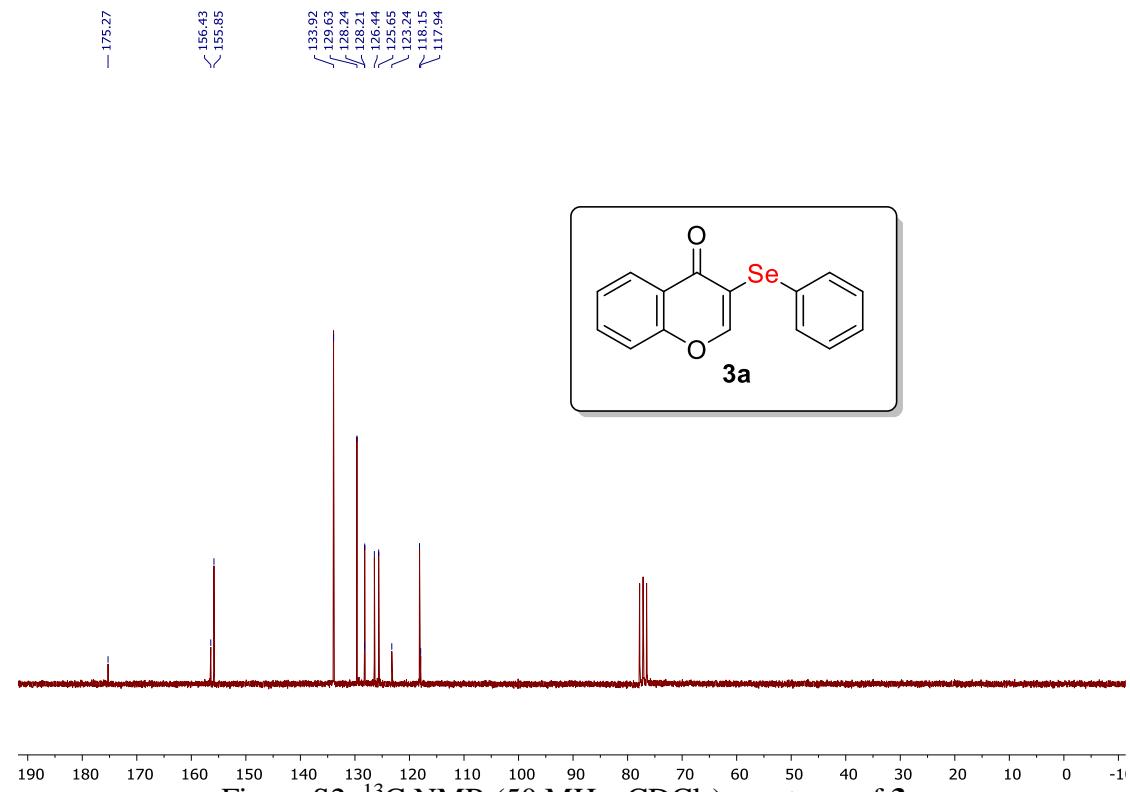
Figure S2. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3a**

303.06

463.15

3a
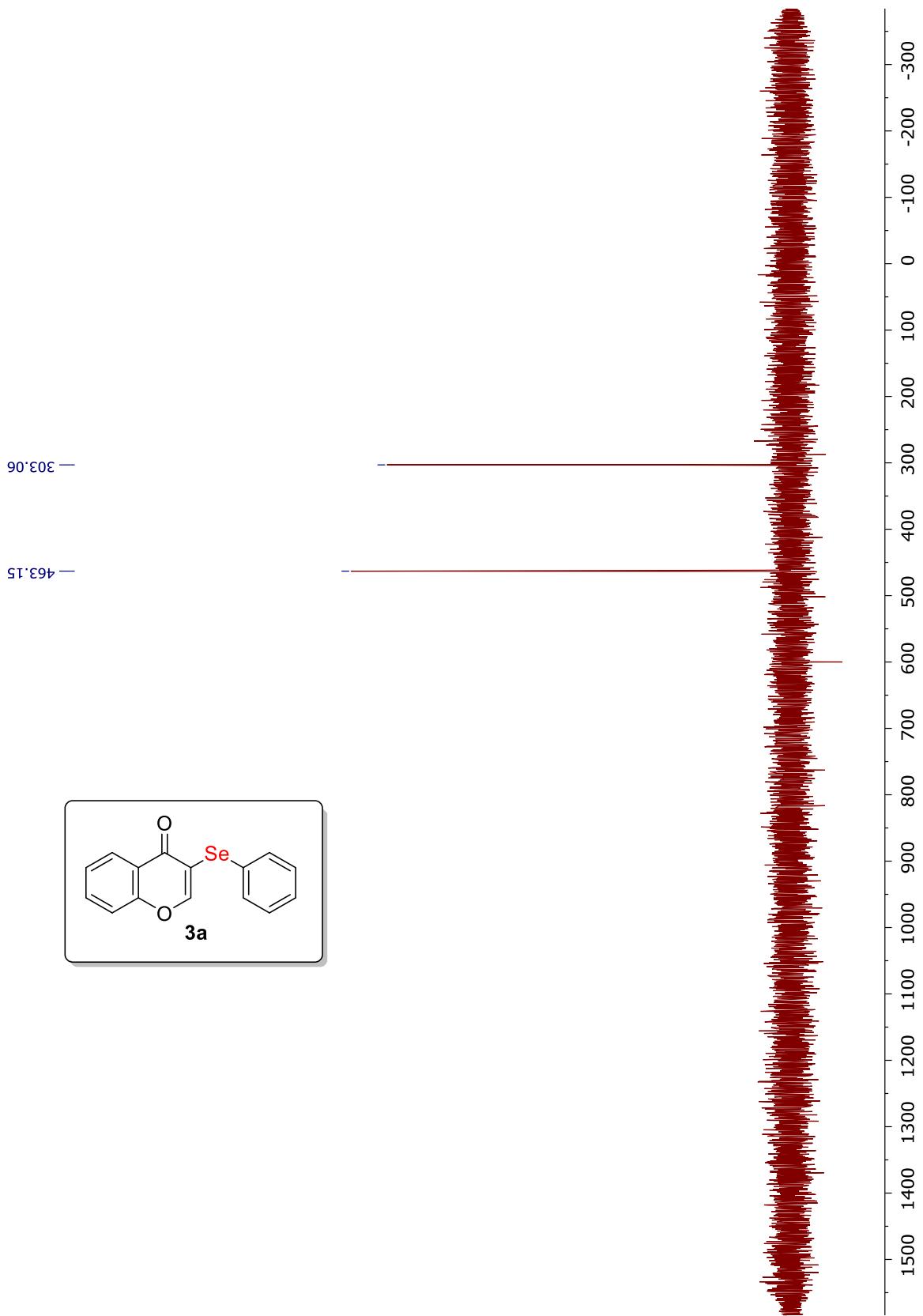
Figure S3. ^{77}Se NMR (38.14 MHz, CDCl$_3$) spectrum of **3a**
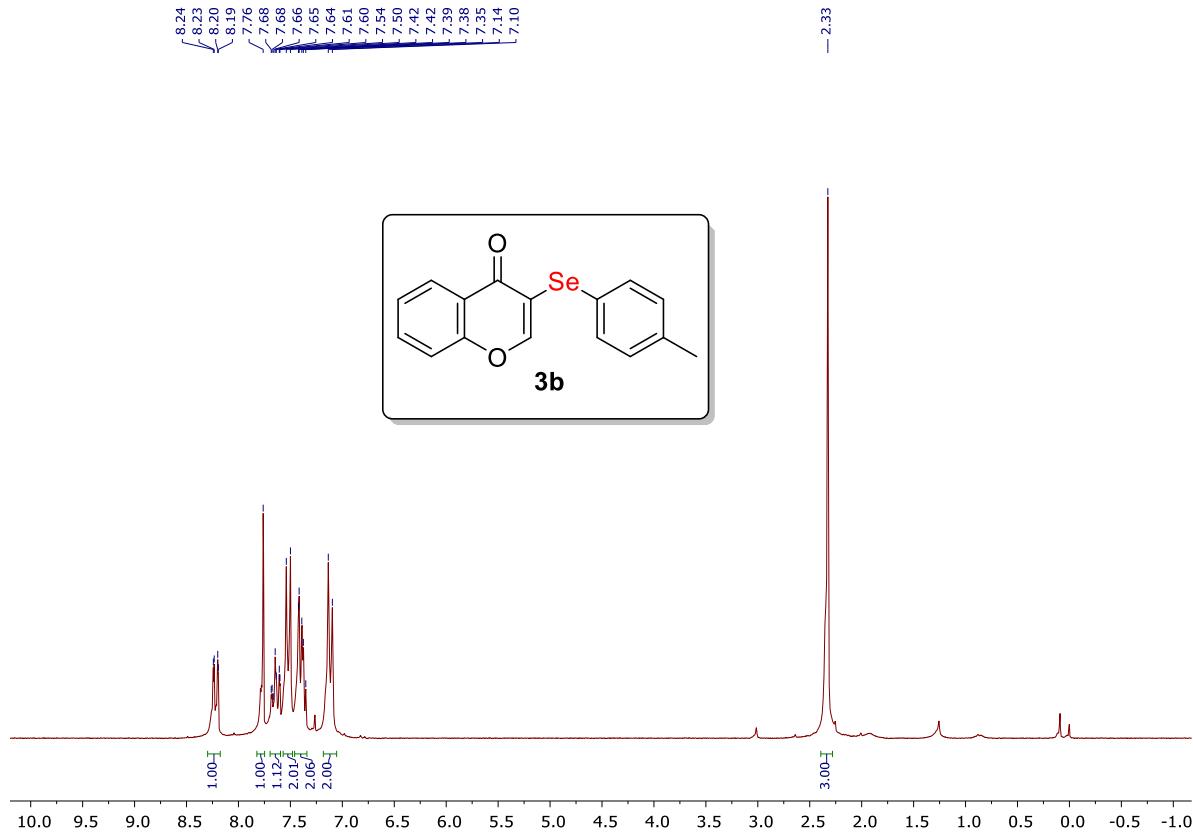
Figure S4. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3b**
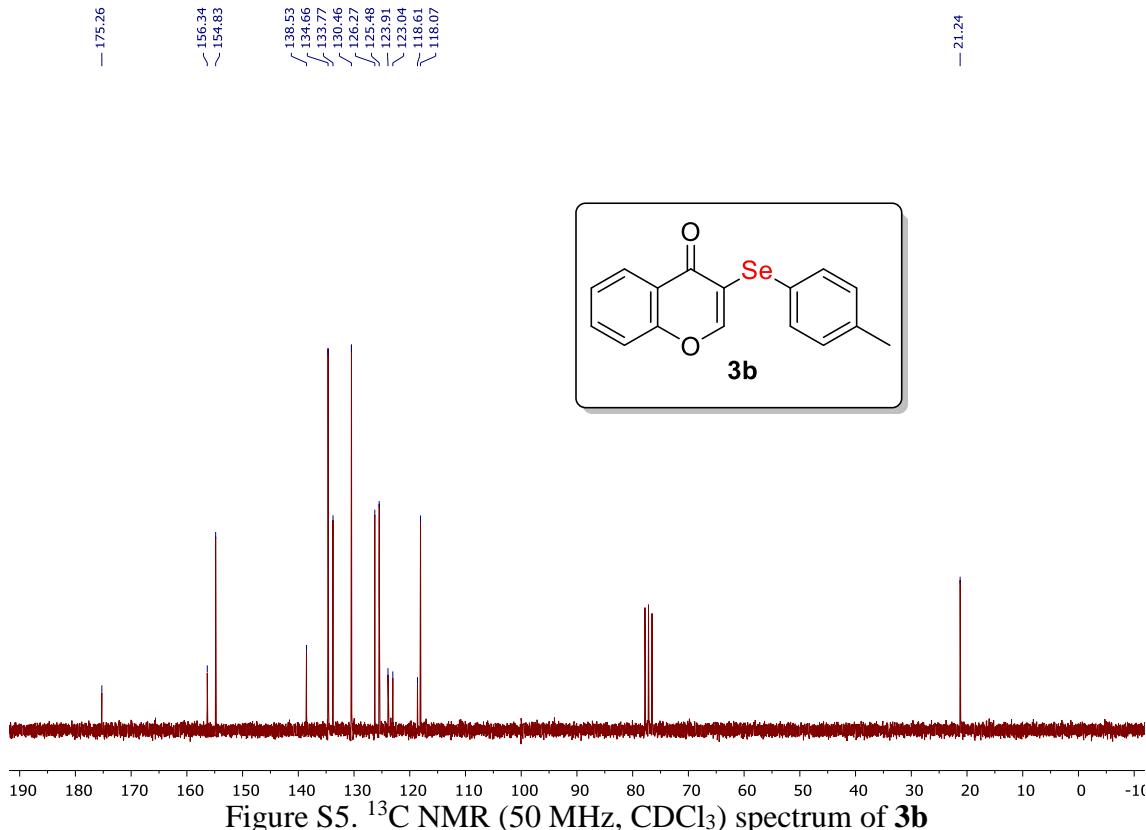
Figure S5. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3b**
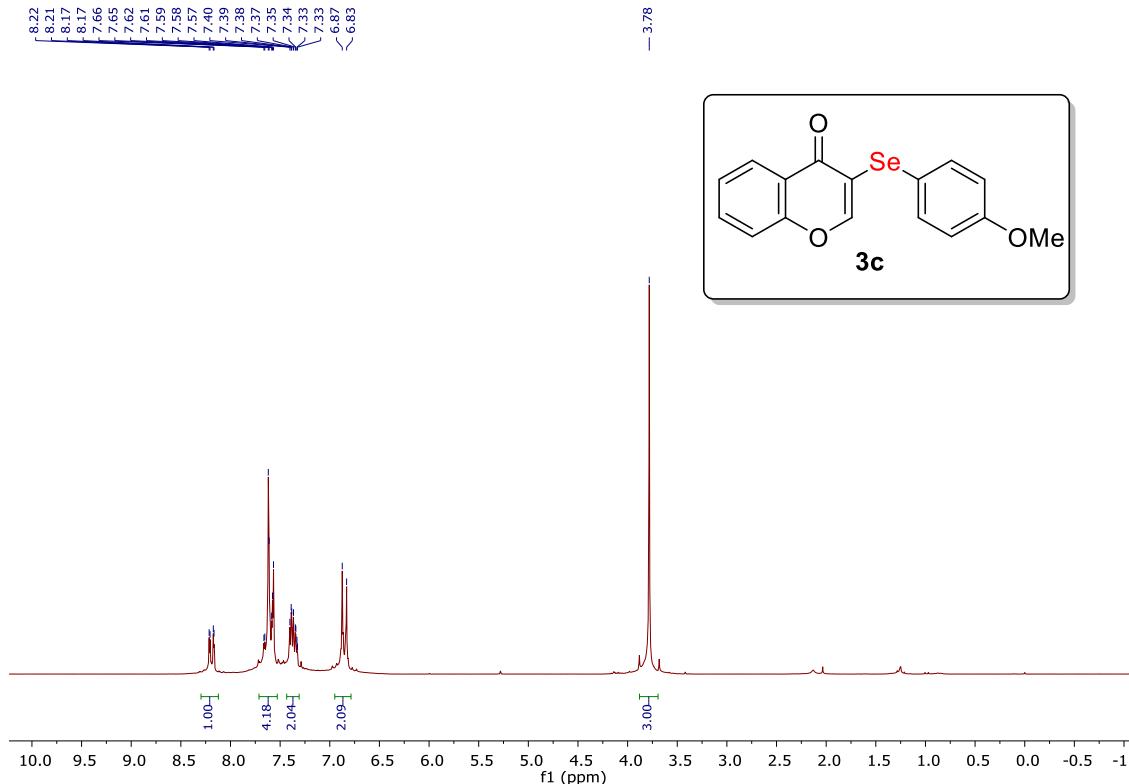
Figure S6. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3c**
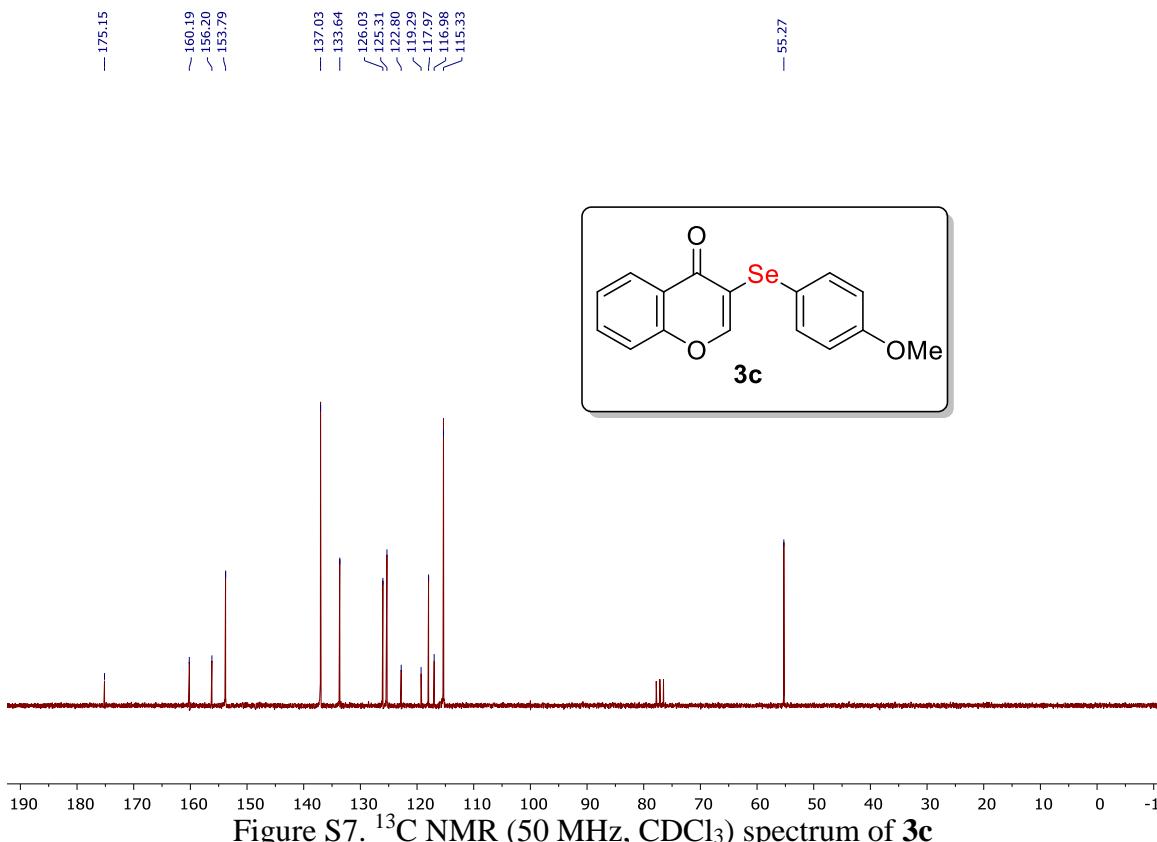
Figure S7. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3c**

8.24
8.23
8.20
8.19
7.89
7.71
7.67
7.65
7.64
7.63
7.62
7.61
7.59
7.58
7.44
7.41
7.40
7.04
7.03
7.00
6.99
6.96
6.95

1.00
1.00
3.21
2.12
2.17

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
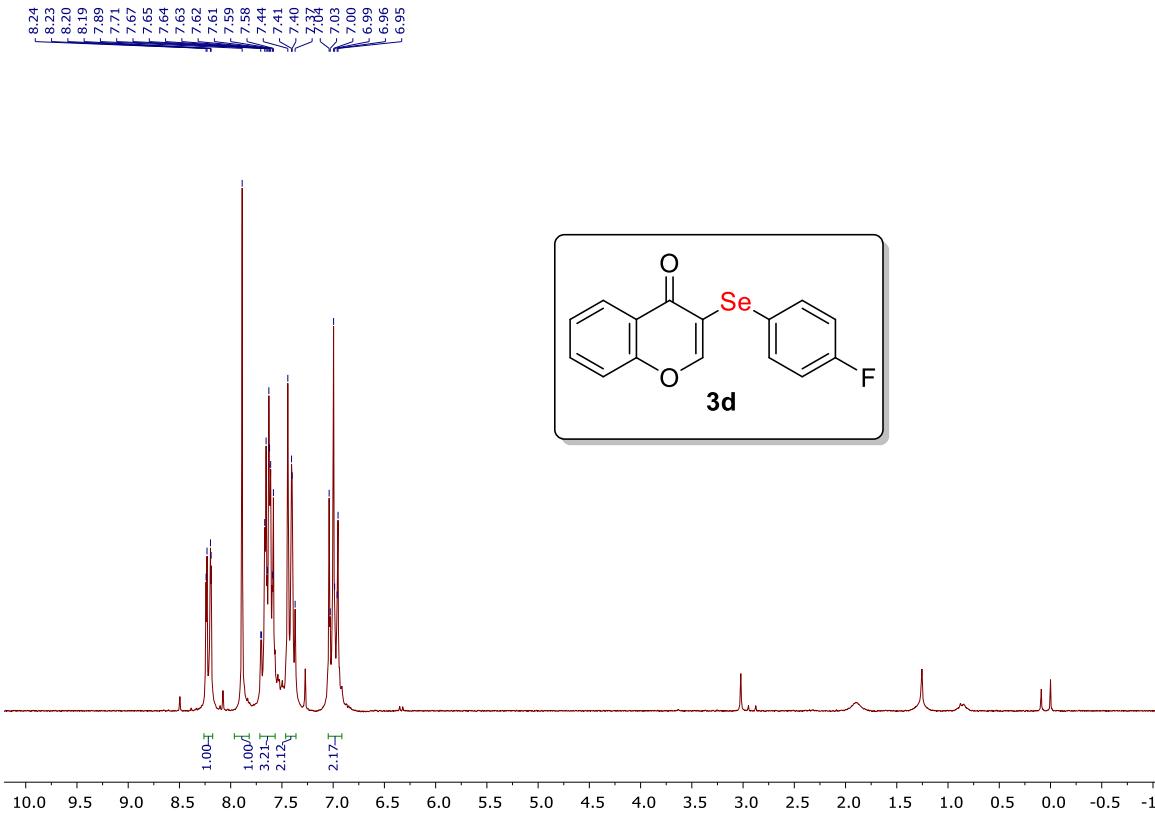
Figure S8. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3d**

175.19

165.48
160.54
156.38
155.62

136.55
136.39
133.97
126.35
125.68
123.18
122.65
122.58
118.14
118.09
117.02
116.60

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
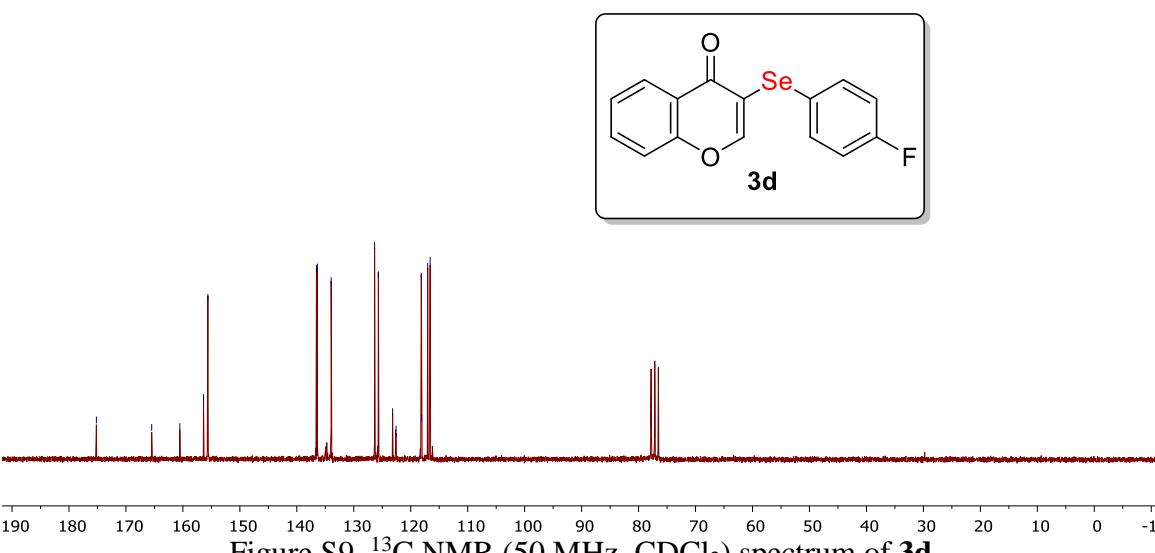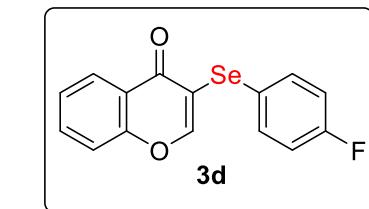
Figure S9. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3d**

8.24
8.23
8.19
8.19
8.00
7.71
7.71
7.67
7.63
7.63
7.53
7.49
7.48
7.45
7.41
7.37
7.26
7.21
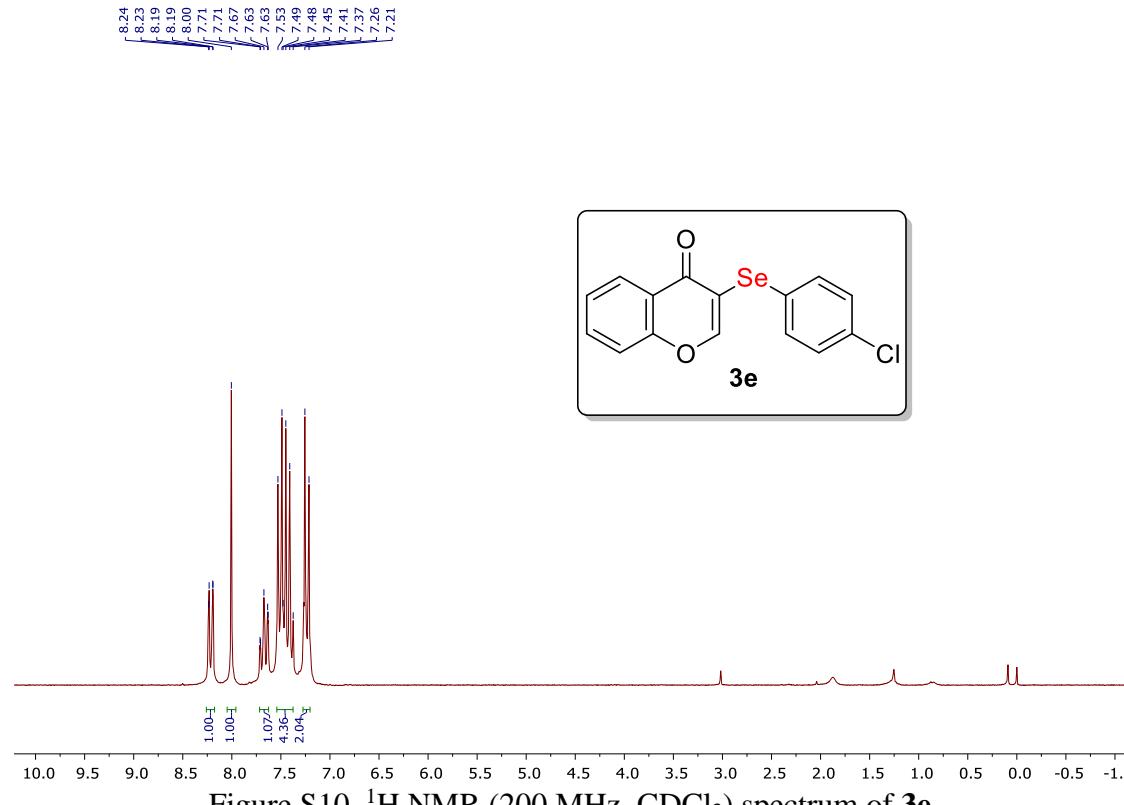
Figure S10. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3e**

175.07

156.55
156.38

134.86
134.37
134.04
129.68
126.76
126.41
125.77
123.29
118.17
117.23
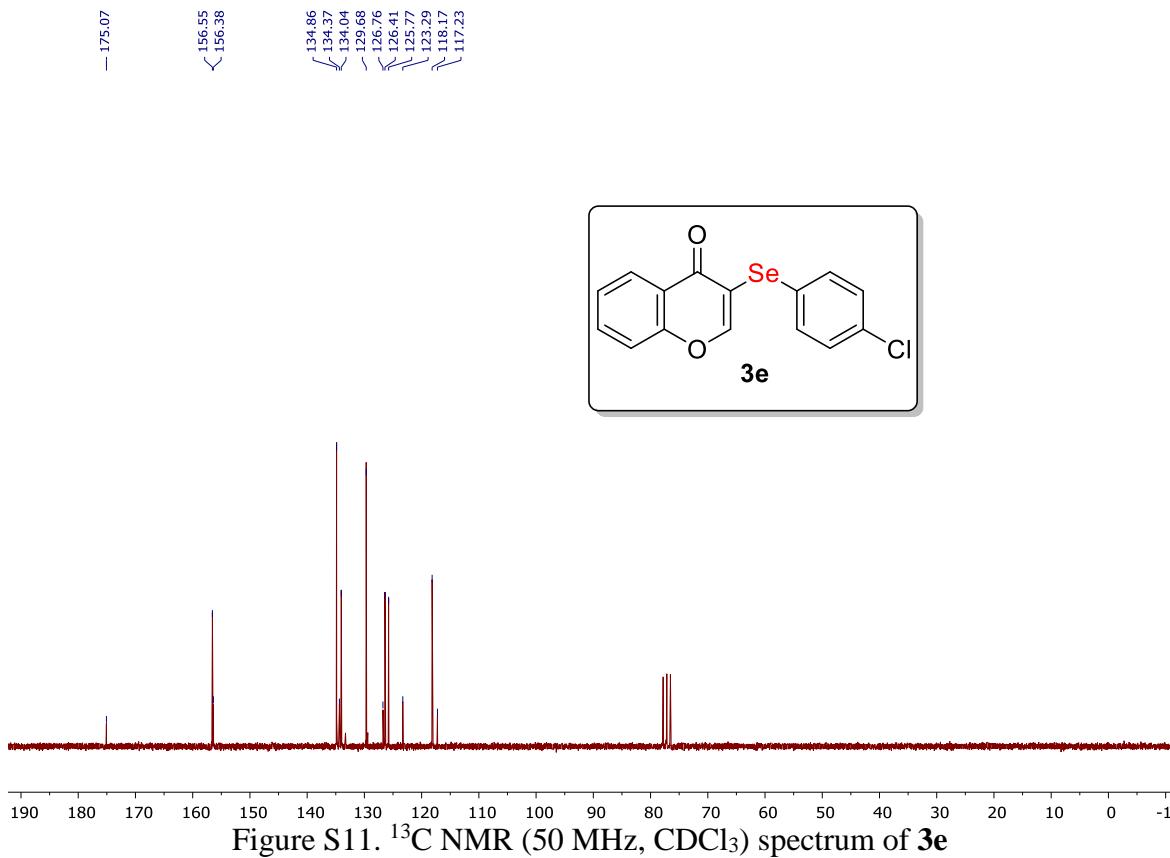
Figure S11. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3e**

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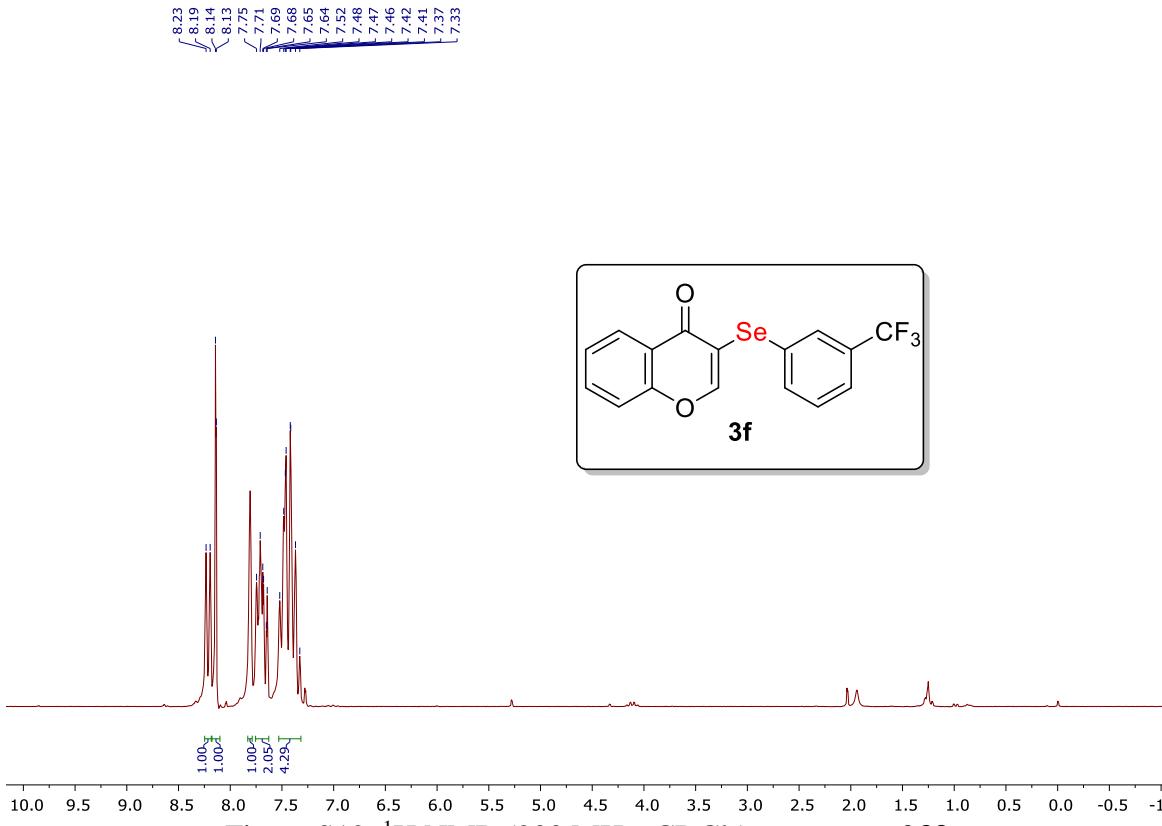
Figure S12. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3f**

174.93

157.55 156.42 136.10 134.14 132.60 131.96 131.78 131.31 130.67 130.25 129.76 129.34 129.27 126.44 125.88 124.61 124.55 123.40 120.94 118.20 116.33 115.52
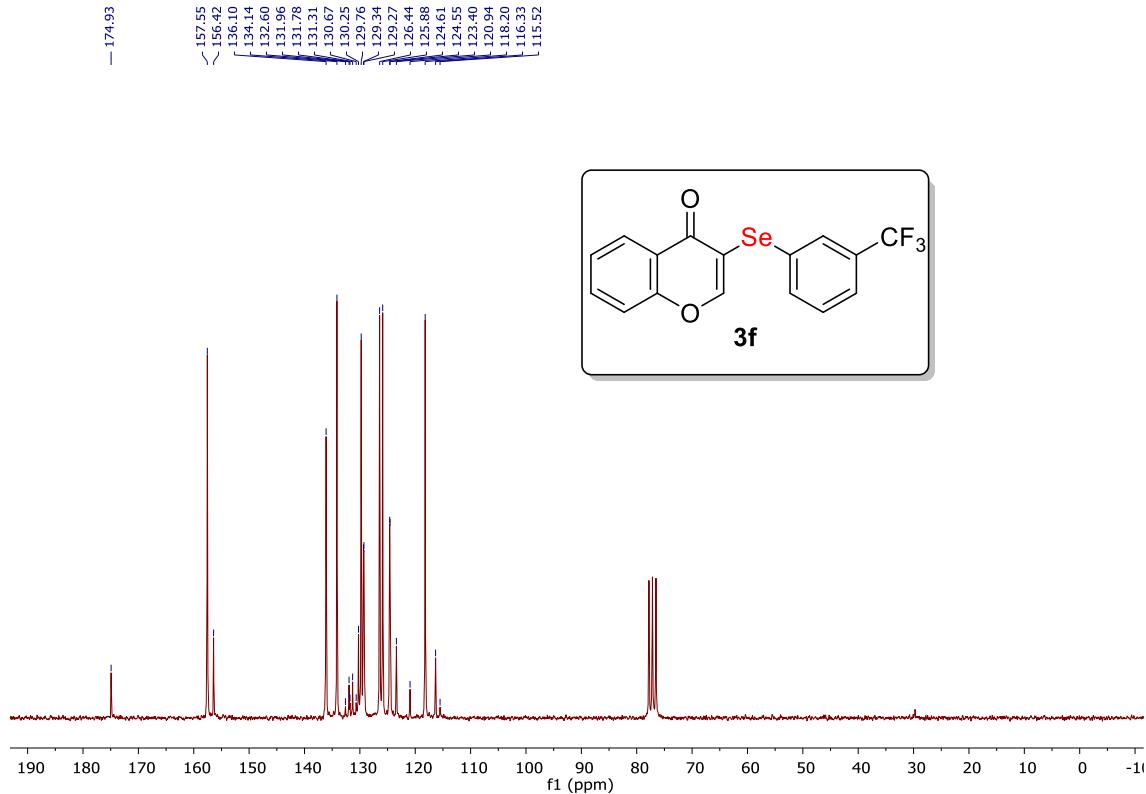
Figure S13. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3f**

8.25
8.24
8.20
8.20
7.68
7.65
7.64
7.61
7.61
7.49
7.45
7.43
7.39
7.38
7.36
7.26
7.24
7.23
7.21
7.21
7.17
7.17
7.12
7.11
7.09
7.08
7.05
2.48

1.00
2.00
3.01
3.15
3.00

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
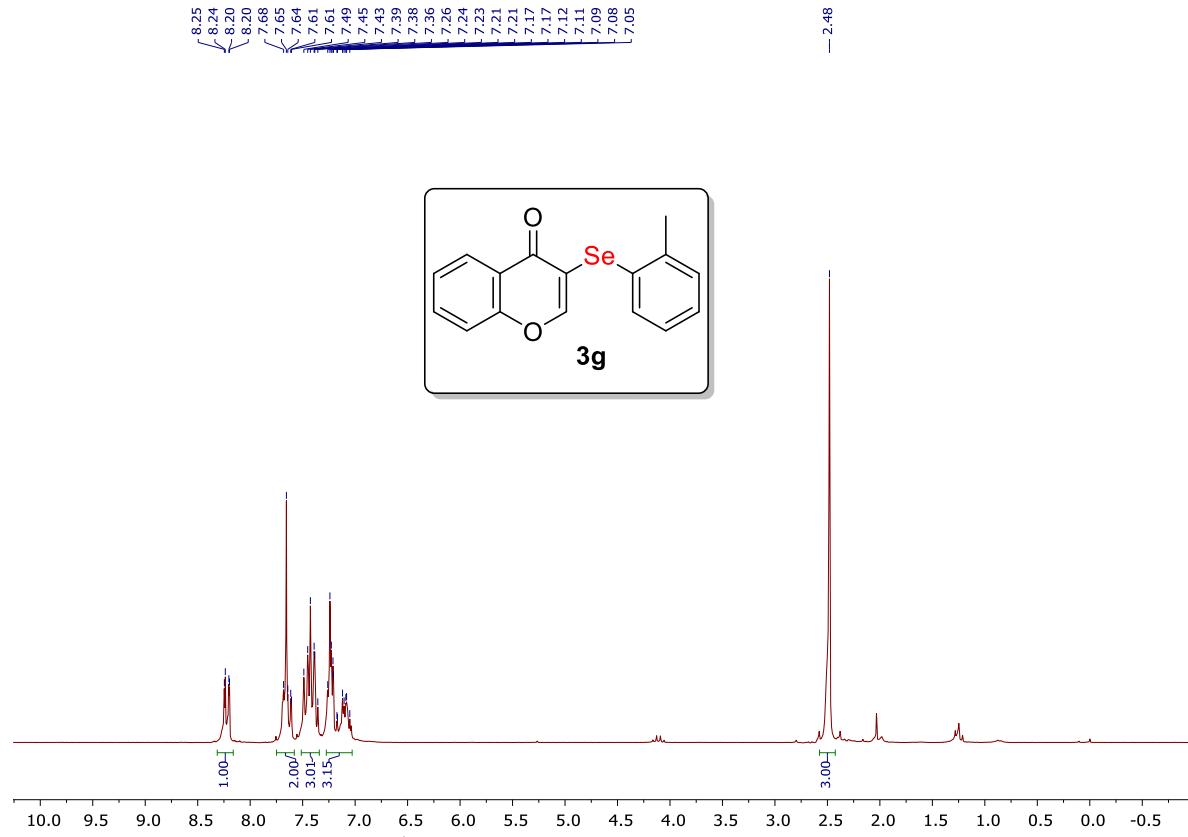
Figure S14. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3g**

175.22
156.34
154.69
140.57
134.50
133.78
130.48
128.56
128.48
127.03
126.21
125.49
122.95
118.05
117.30
22.35

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
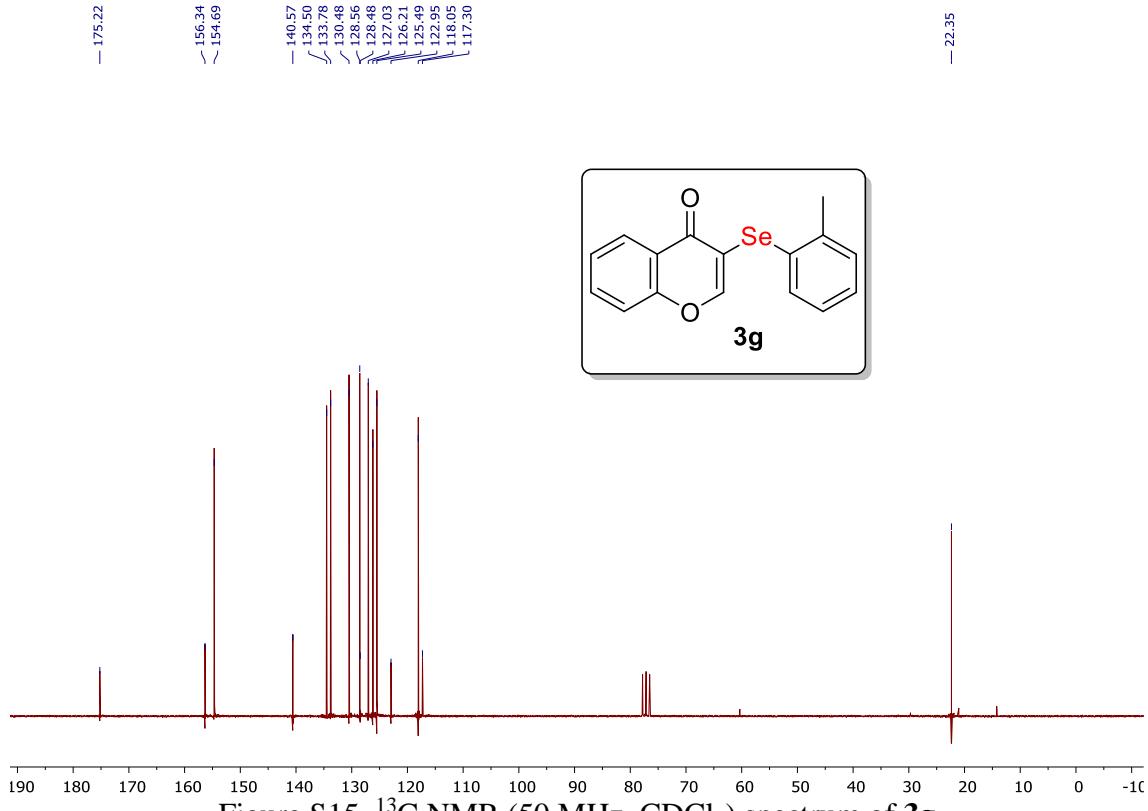
Figure S15. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3g**

8.29 8.29 8.26 8.25 8.08 7.74 7.73 7.70 7.69 7.66 7.65 7.48 7.48 7.44 7.43 7.40 7.40 7.28 7.26 7.24 7.23 7.22 7.21 7.20 7.19 7.18 7.17 6.89 6.87 6.85 6.83 6.80 6.79 3.89
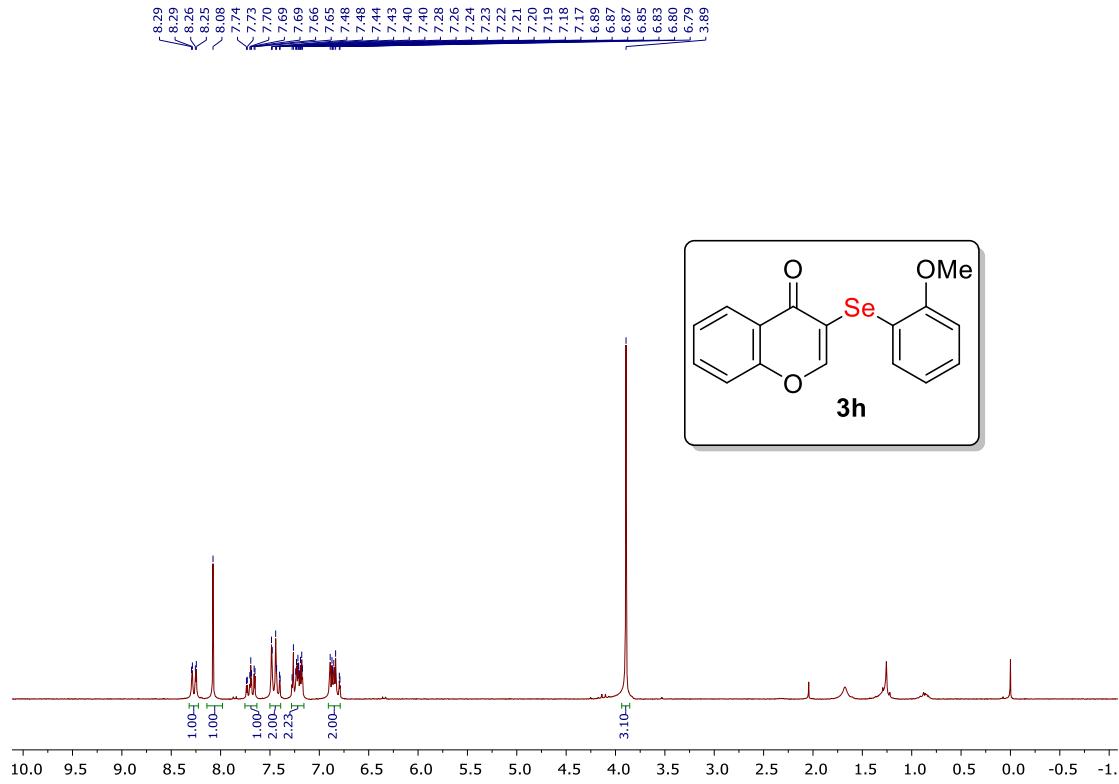
Figure S16. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3h**

175.51 157.80 157.57 156.57 133.94 131.89 128.73 126.61 125.74 123.47 121.87 118.55 118.21 114.98 110.88 56.06
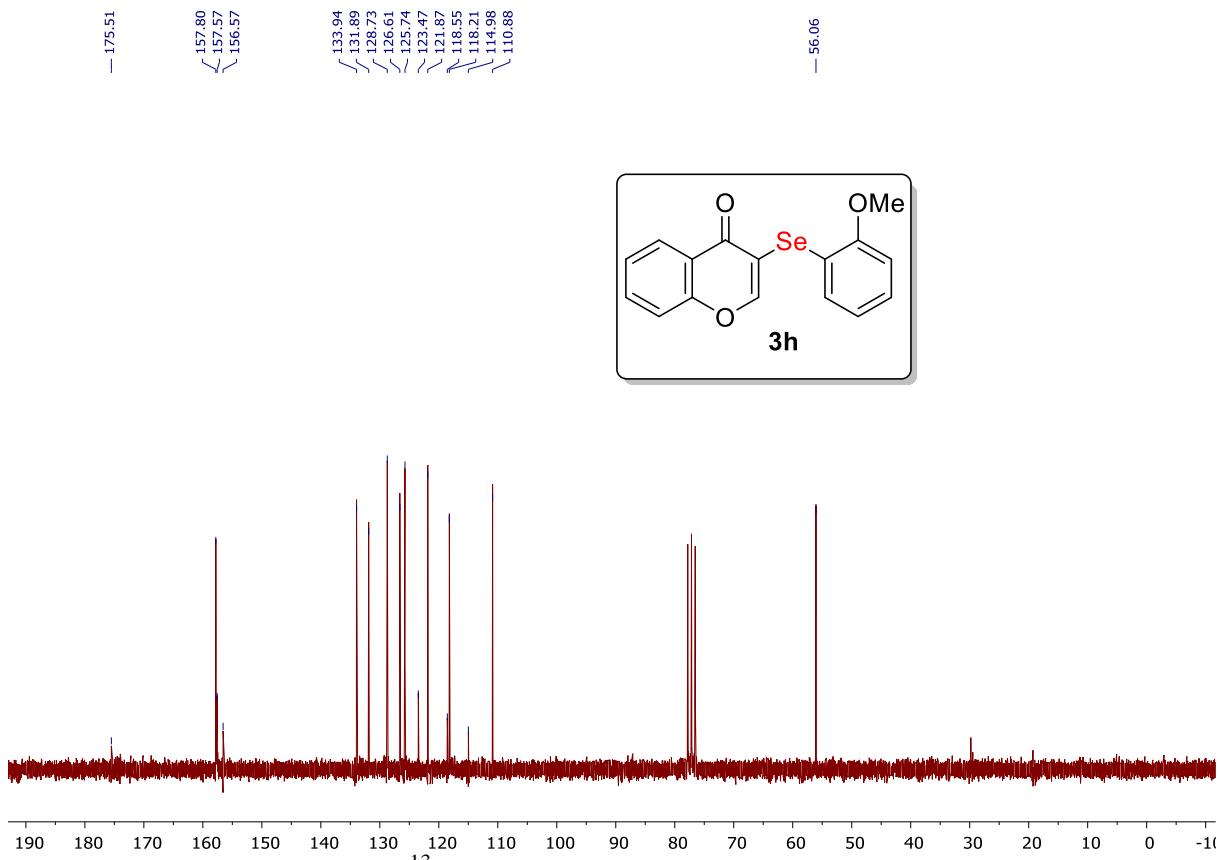
Figure S17. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3h**
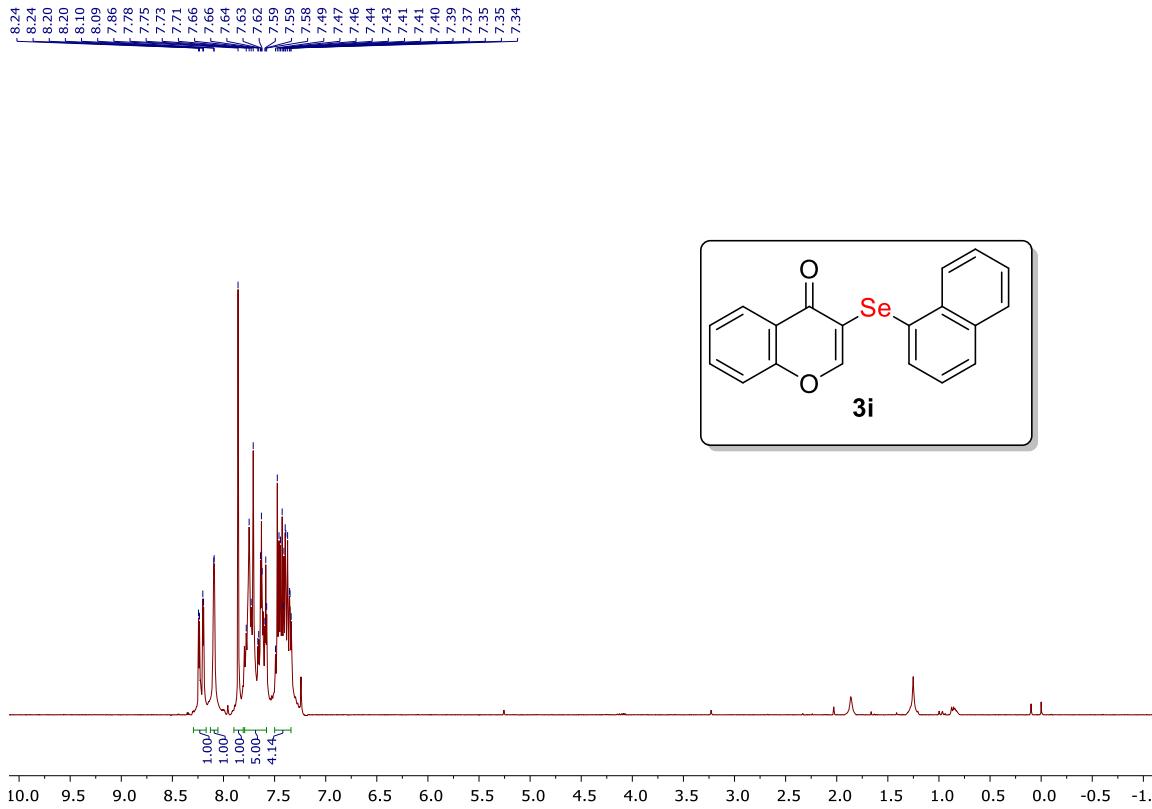
Figure S18. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3i**
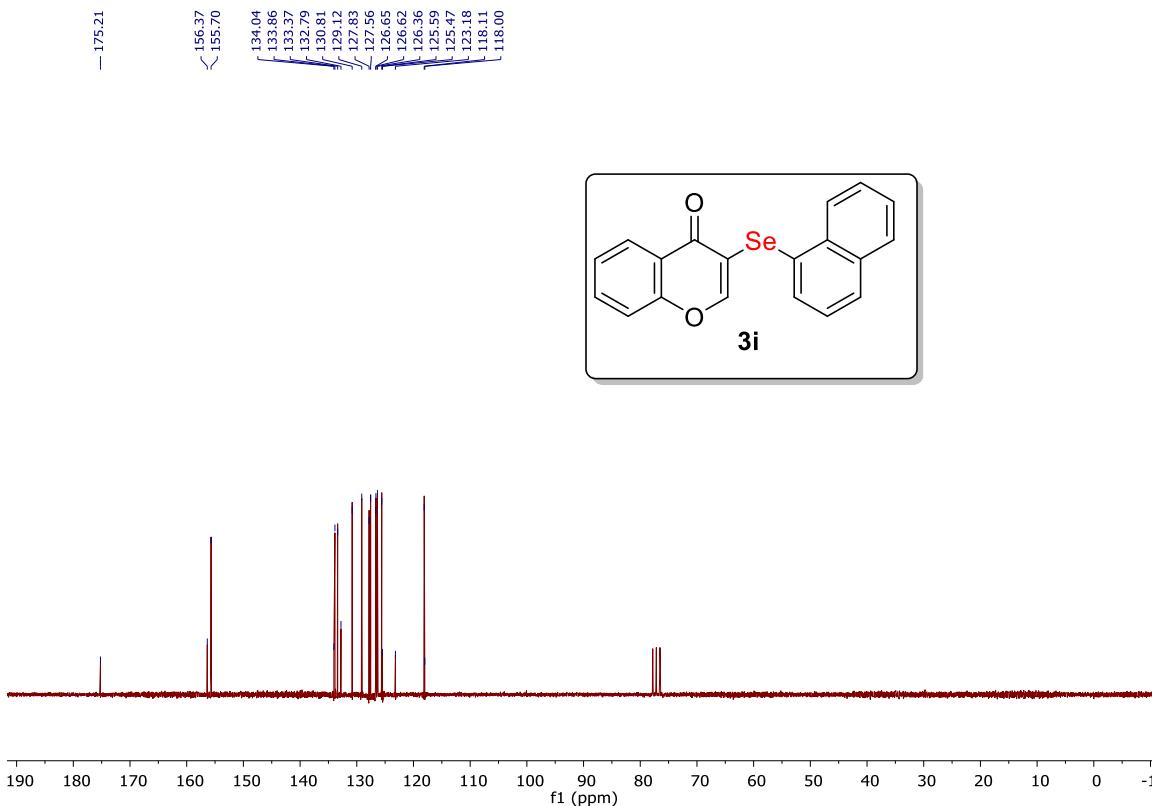
Figure S19. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3i**

8.22
8.22
8.18
8.18
7.68
7.68
7.65
7.64
7.63
7.61
7.60
7.56
7.50
7.50
7.48
7.47
7.43
7.42
7.41
7.40
7.39
7.38
7.37
7.36
7.35
7.08
7.06
7.05
7.03
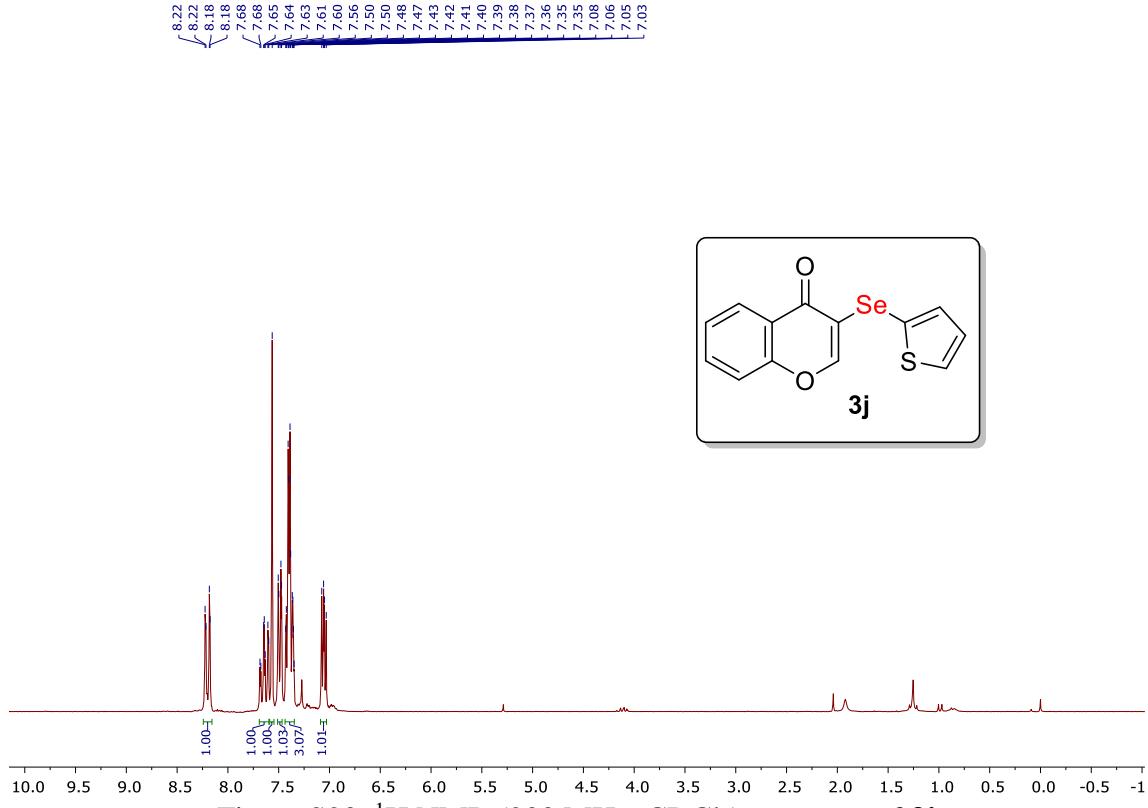
Figure S20. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3j**

175.03

156.33
153.33

137.99
133.86
132.82
128.66
126.07
125.52
122.77
120.05
119.92
118.10
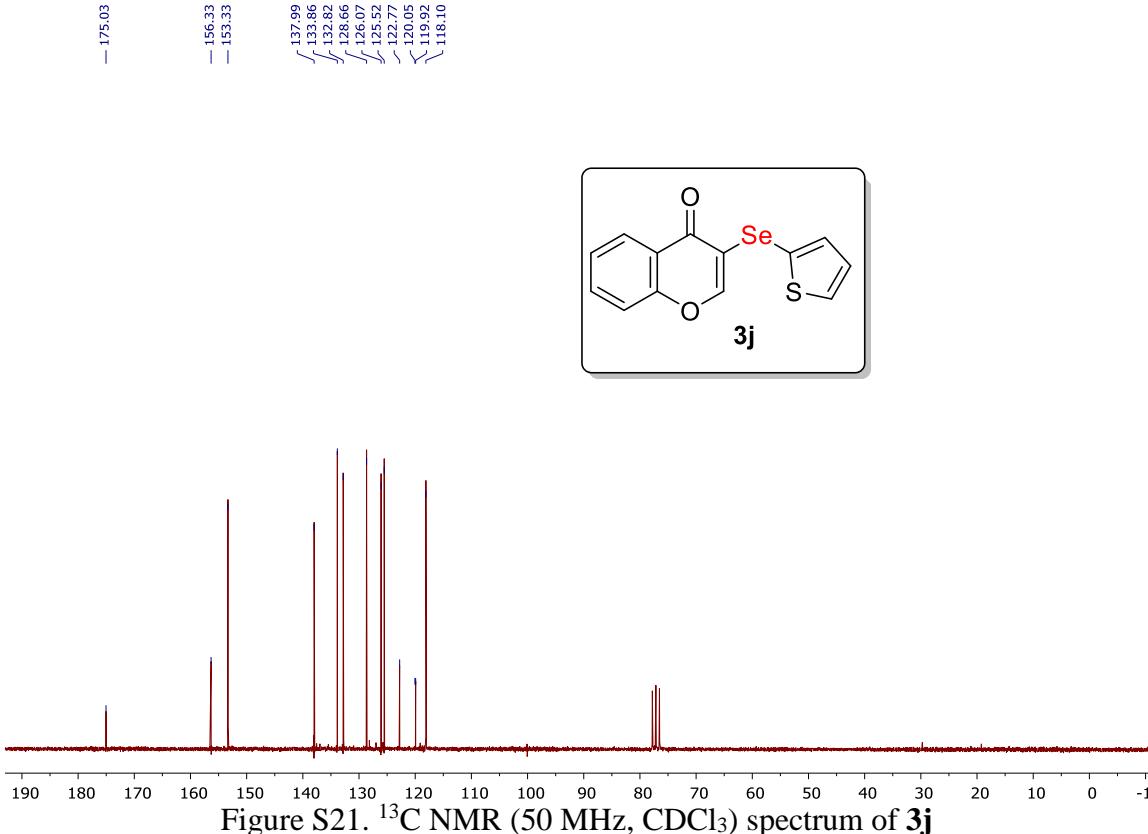
Figure S21. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3j**

8.27 8.26 8.26 8.24 8.23 8.22 8.22 8.18 7.72 7.71 7.69 7.68 7.67 7.64 7.63 7.47 7.43 7.39

2.93 2.89 2.85 1.73 1.70 1.66 1.62 1.58 1.51 1.47 1.44 1.40 1.36 1.33 0.94 0.90 0.87
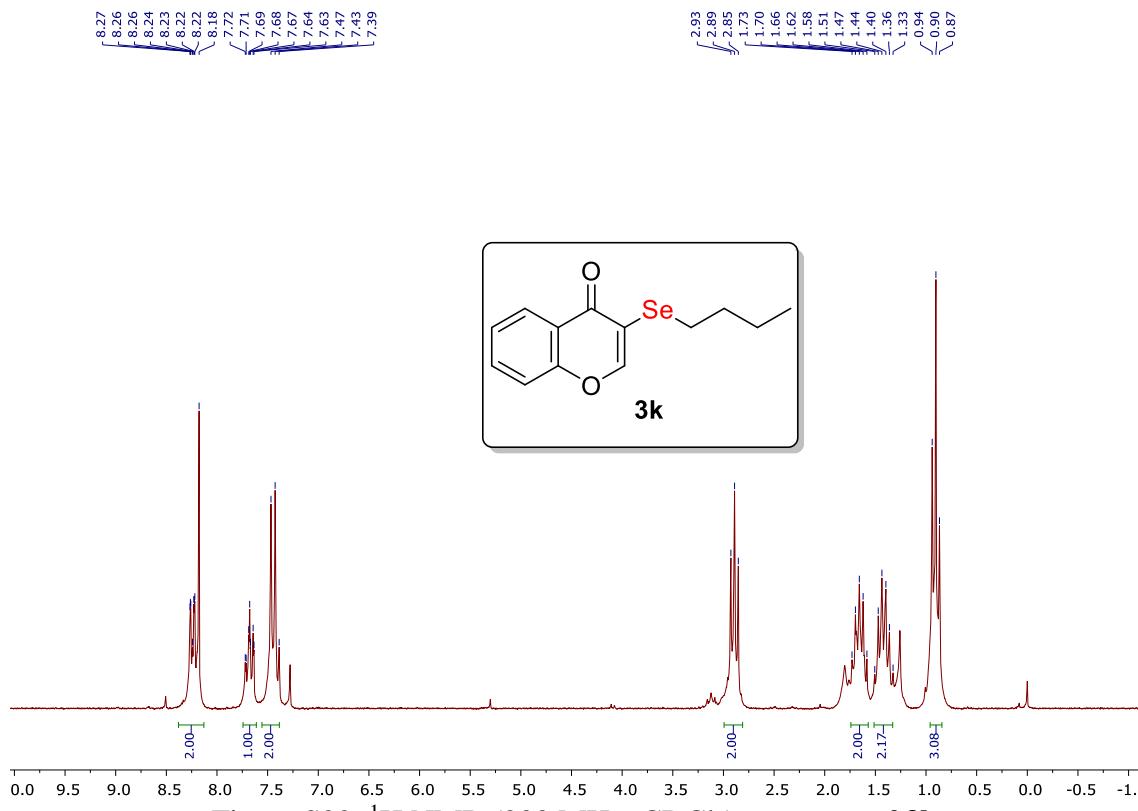
Figure S22. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3k**

175.99

156.46 156.35

133.80 126.41 125.58 123.31 118.14 114.87

32.26 26.11 22.90

13.66
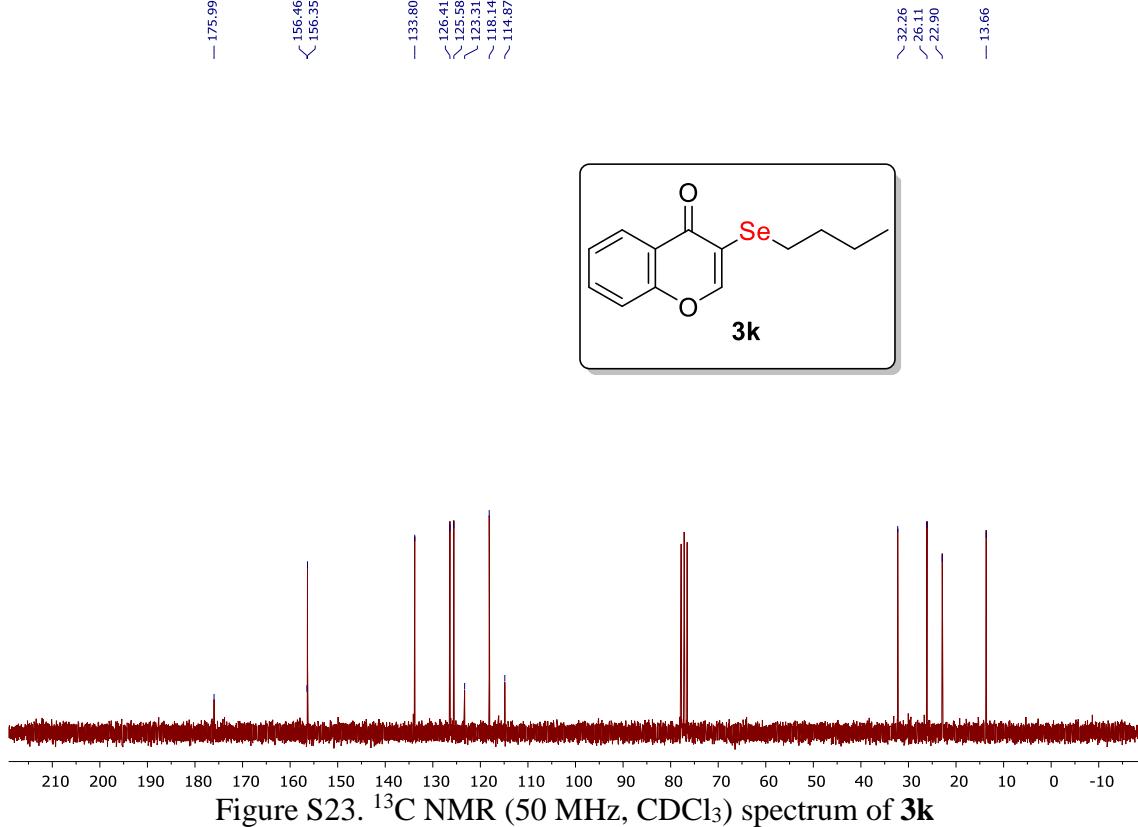
Figure S23. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3k**

8.28
8.25
8.24
7.87
7.71
7.70
7.67
7.66
7.63
7.62
7.47
7.46
7.42
7.39
7.38
7.27
7.26
7.22
7.21
7.19
7.16
7.14

4.10

3l

1.28
1.00
1.22
2.17
5.23
2.00

.0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
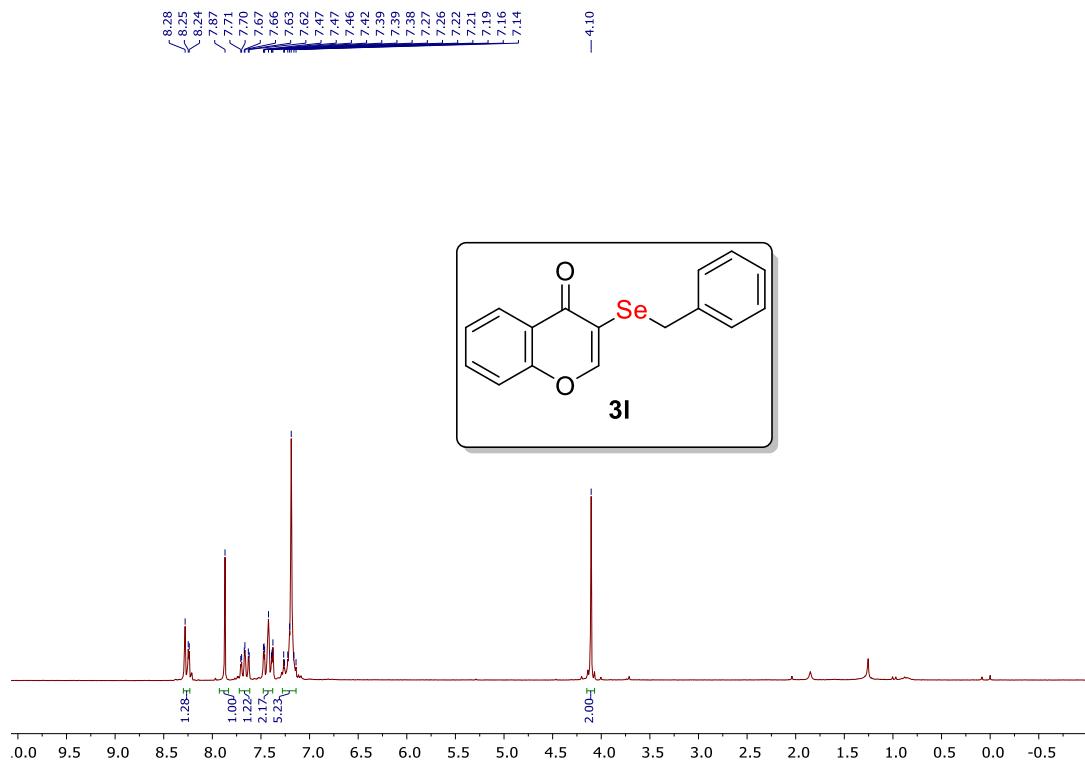
Figure S24. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **3l**

176.09

157.40
156.41

137.85
133.97
129.18
128.59
127.25
126.38
125.78
123.67
118.50
118.29

37.28

3l

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
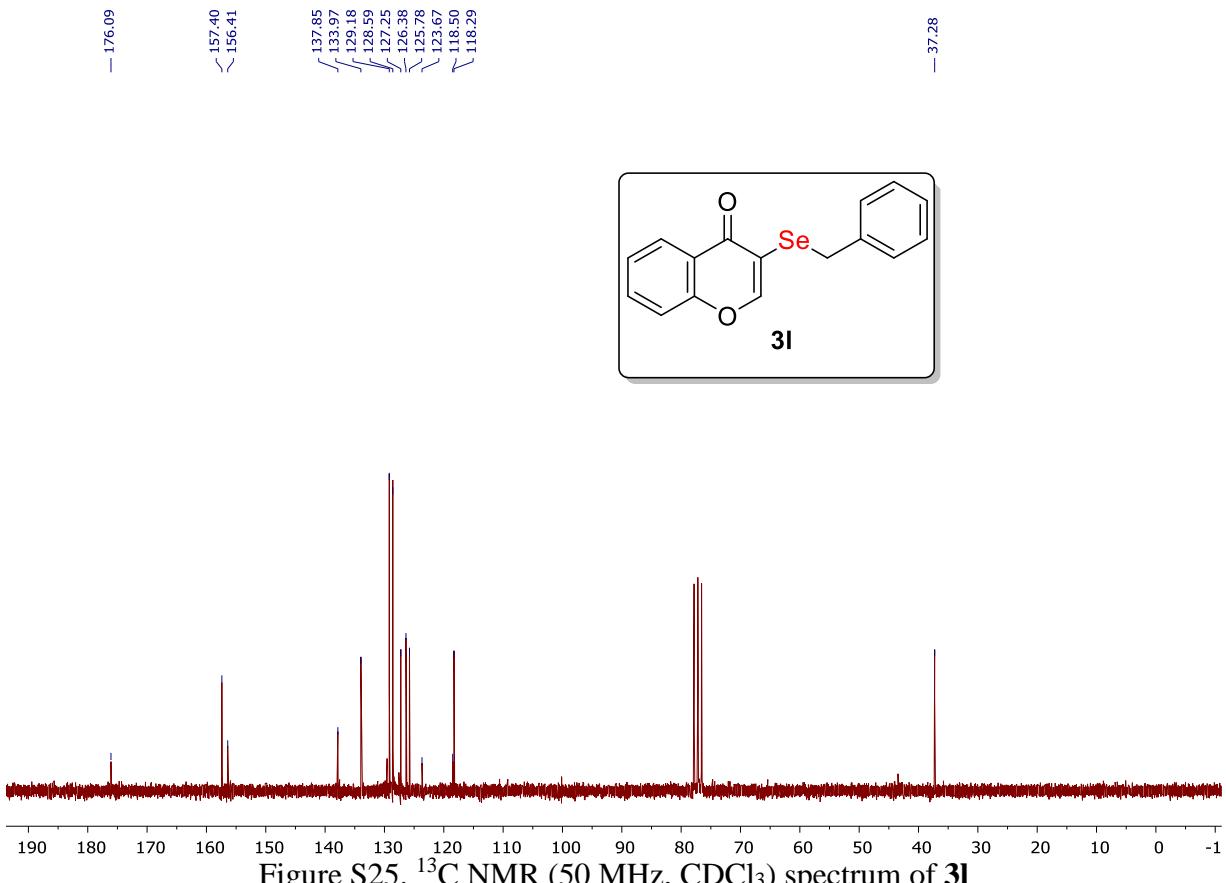
Figure S25. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **3l**

8.26
8.25
8.22
8.22
8.14
7.73
7.72
7.69
7.68
7.65
7.64
7.48
7.46
7.44
7.42
7.38
7.32
7.31
7.28
7.27
7.24
7.20
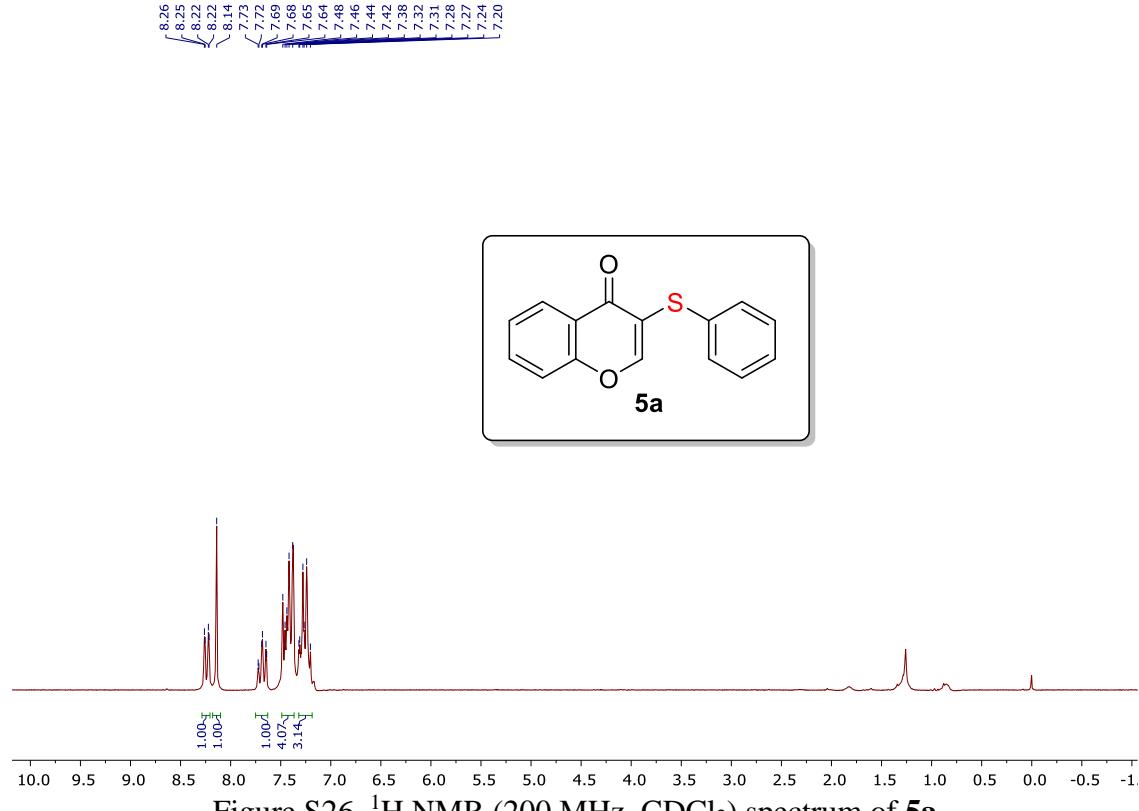
Figure S26. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **5a**

175.09

157.43
156.35

134.05
129.86
129.22
127.14
126.42
125.78
123.66
119.92
118.20
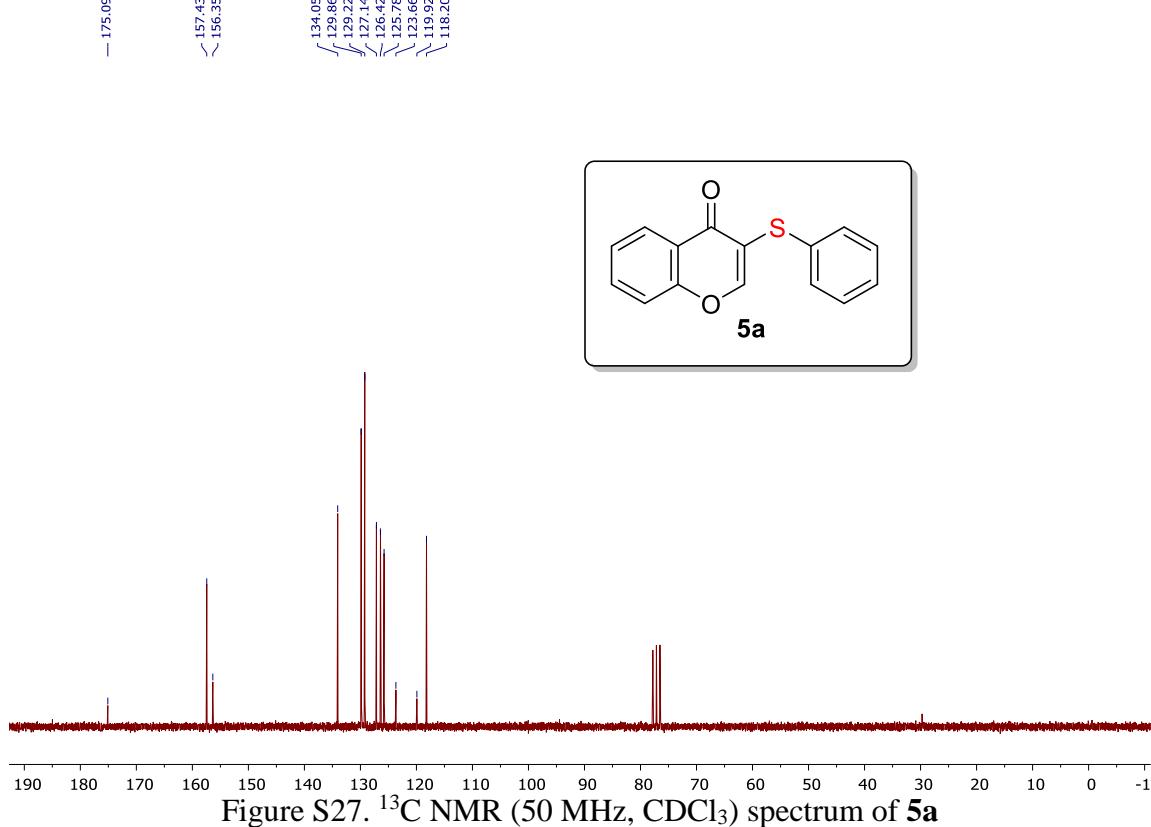
Figure S27. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **5a**
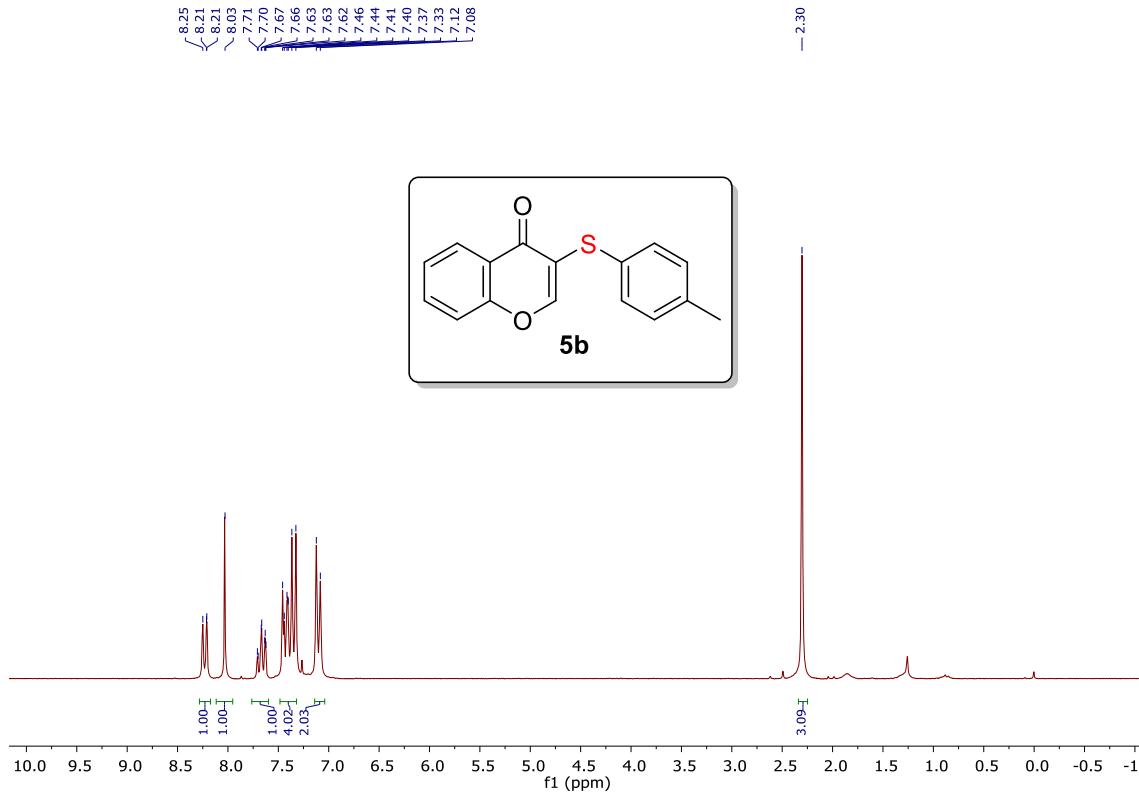
Figure S28. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **5b**
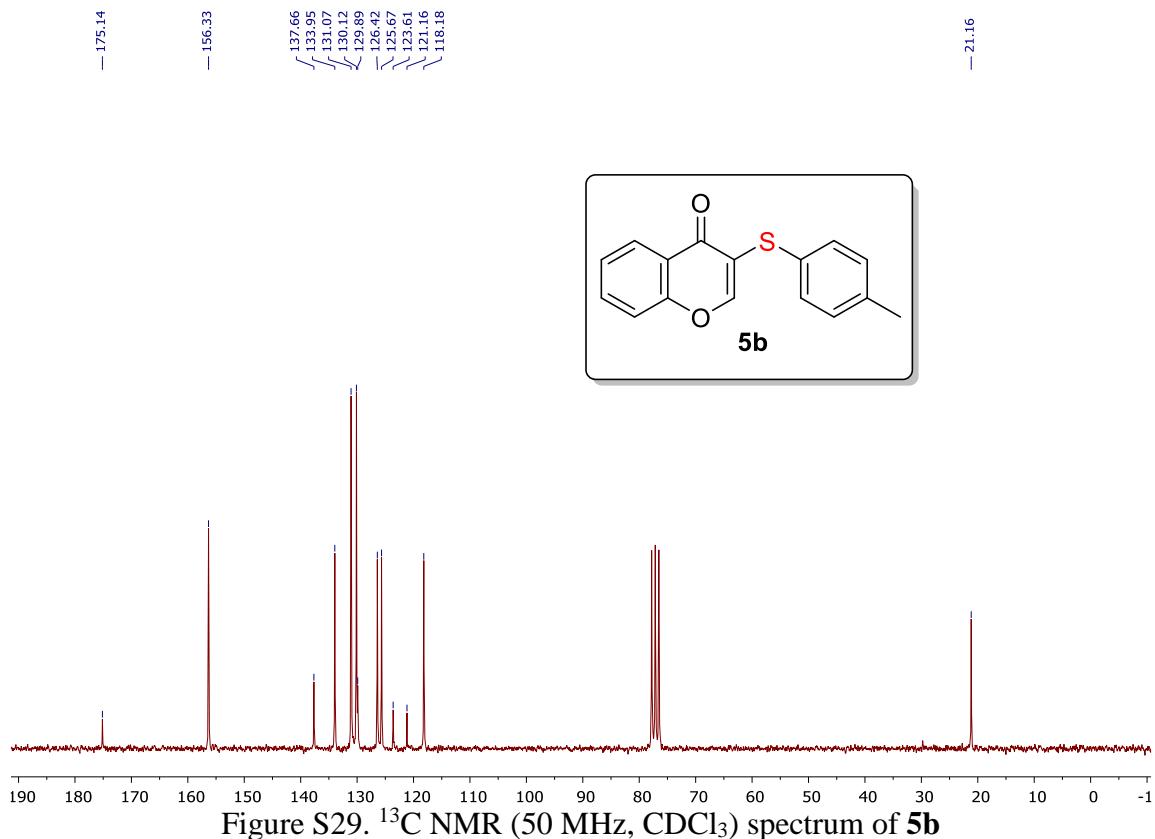
Figure S29. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **5b**
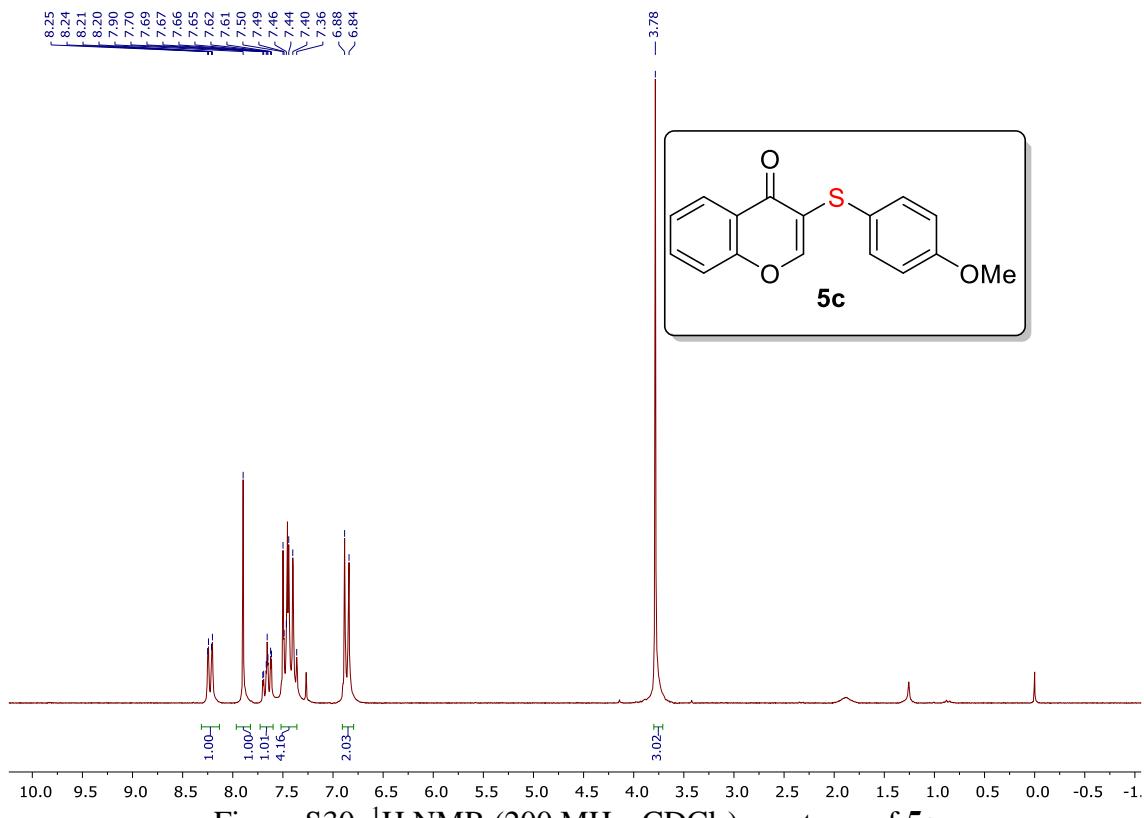
Figure S30. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **5c**
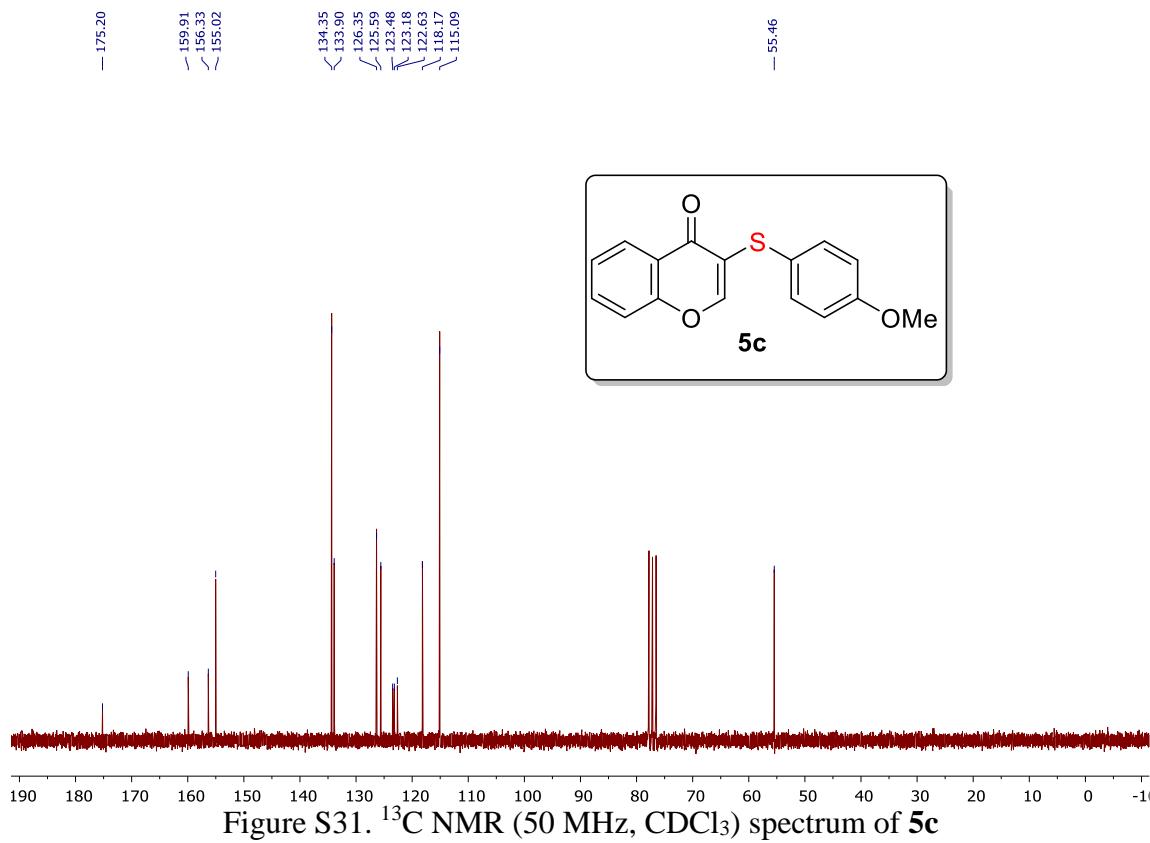
Figure S31. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **5c**

8.23
7.74
7.70
7.67
7.50
7.44
7.40
7.34
7.30
7.25

2.00
7.14
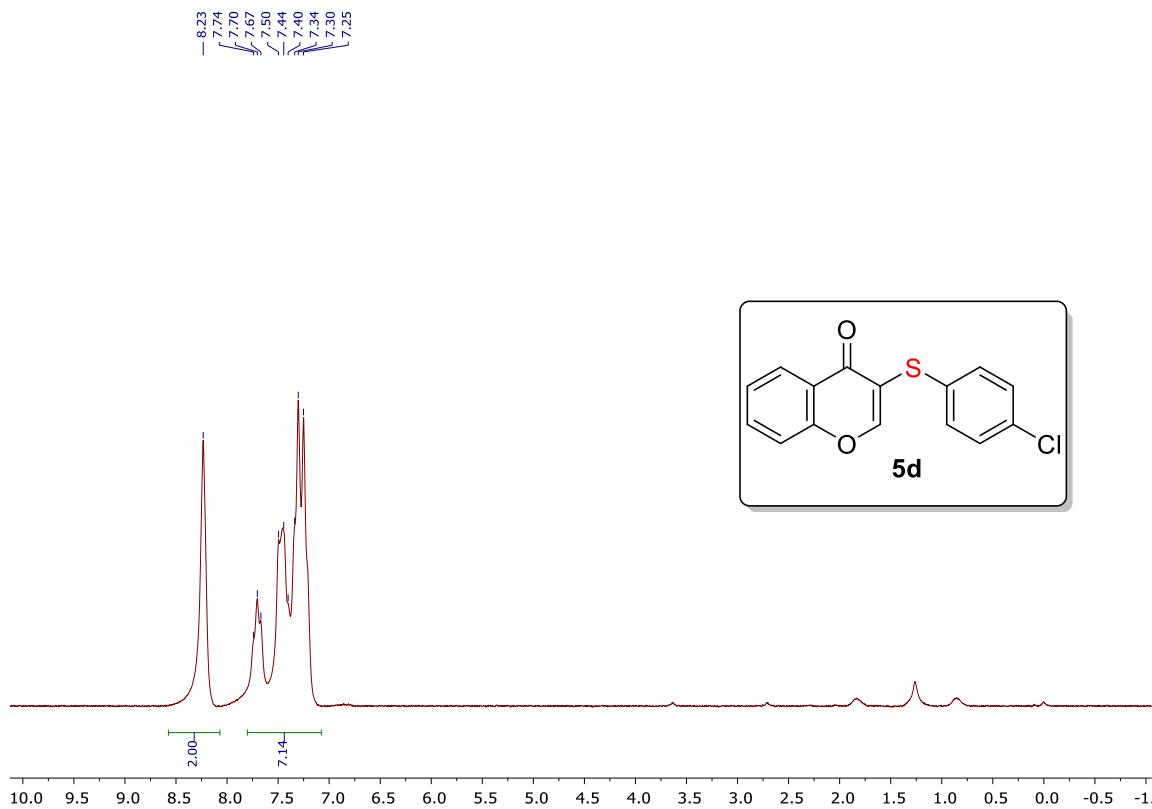
Figure S32. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **5d**

174.96
157.96
156.42
134.22
133.18
132.93
131.00
129.33
126.48
125.96
123.80
119.33
118.28
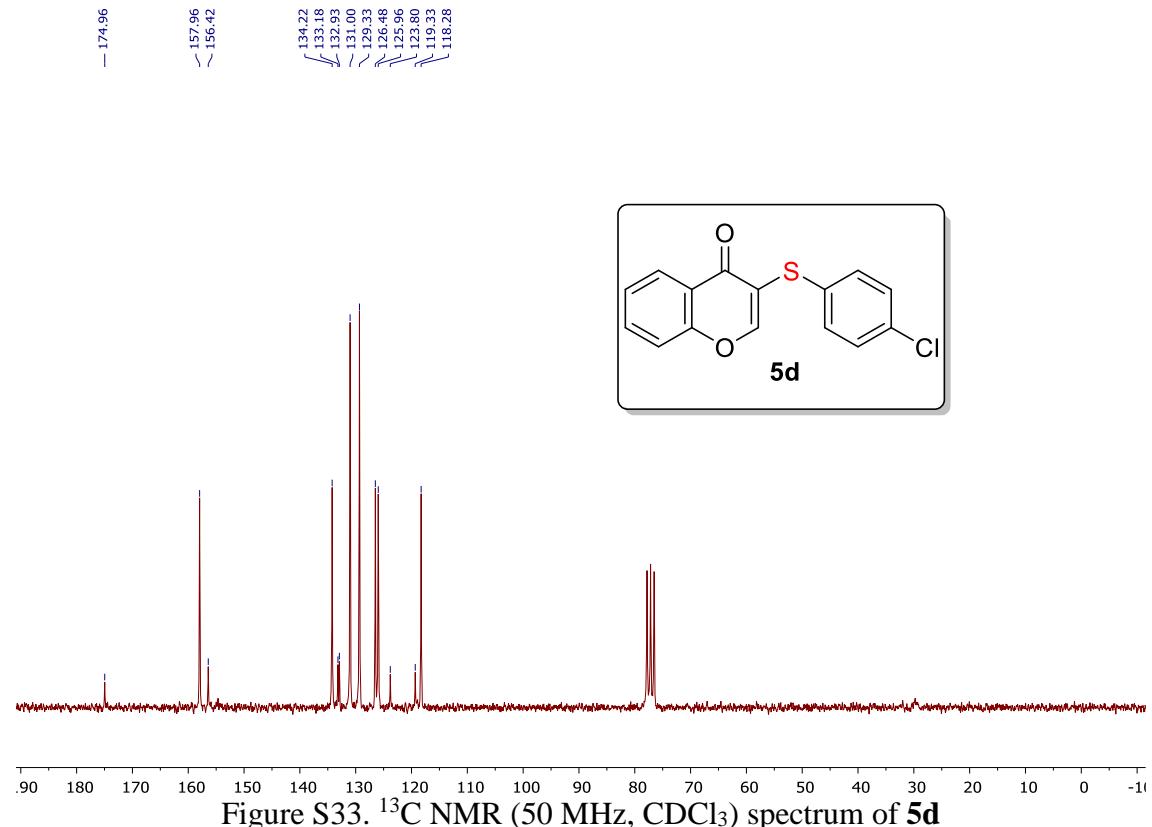
Figure S33. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **5d**
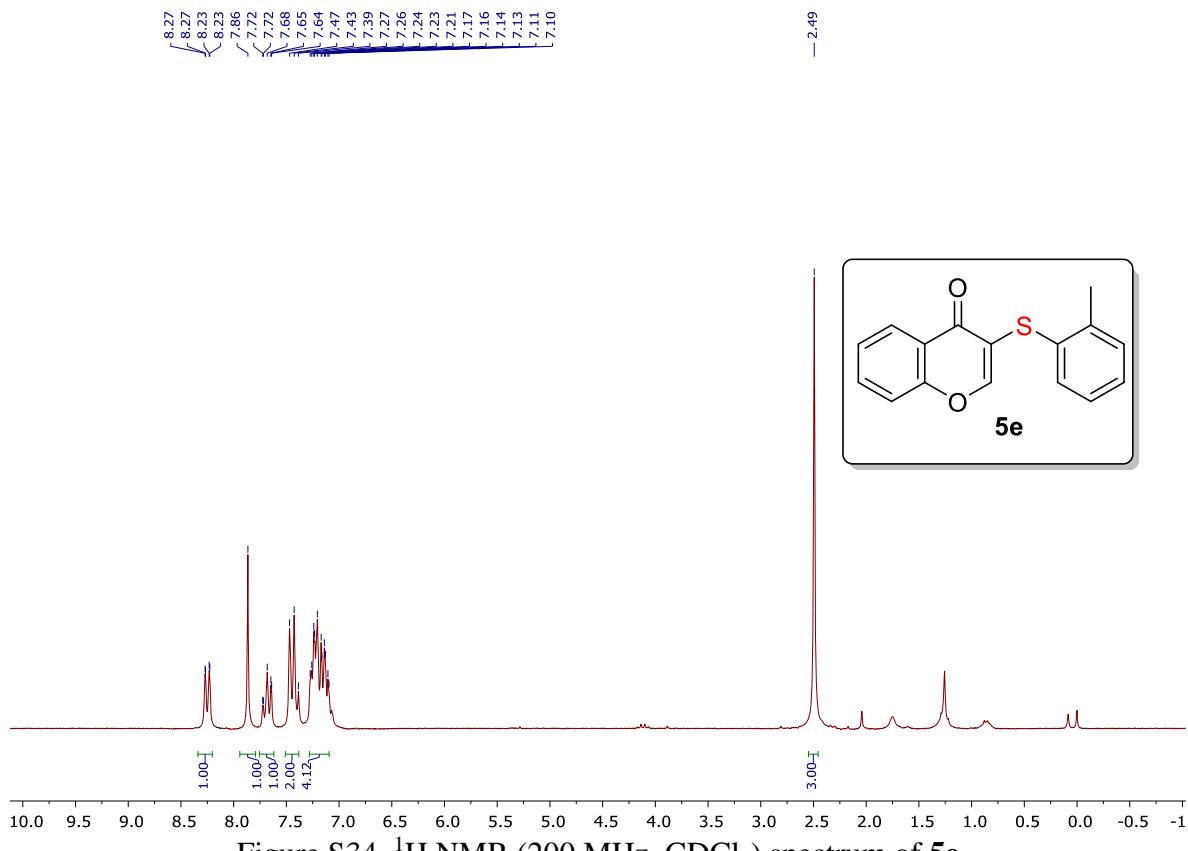
Figure S34. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **5e**
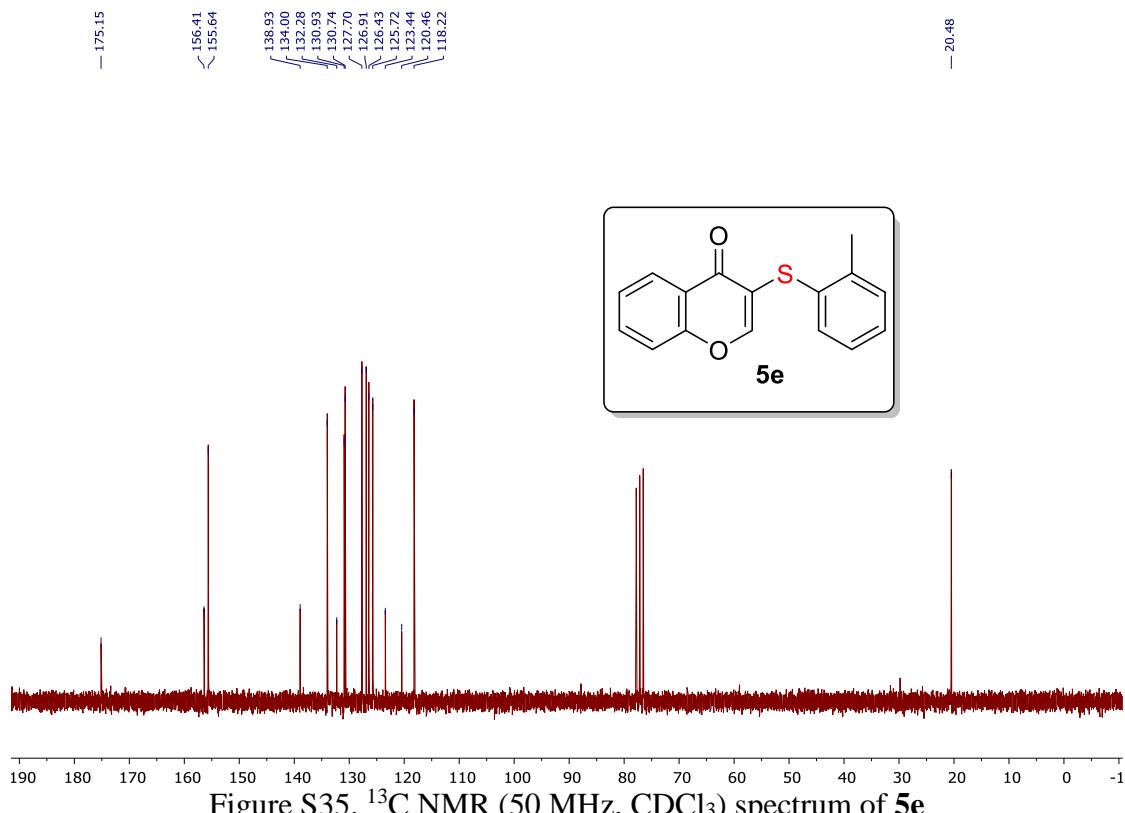
Figure S35. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **5e**
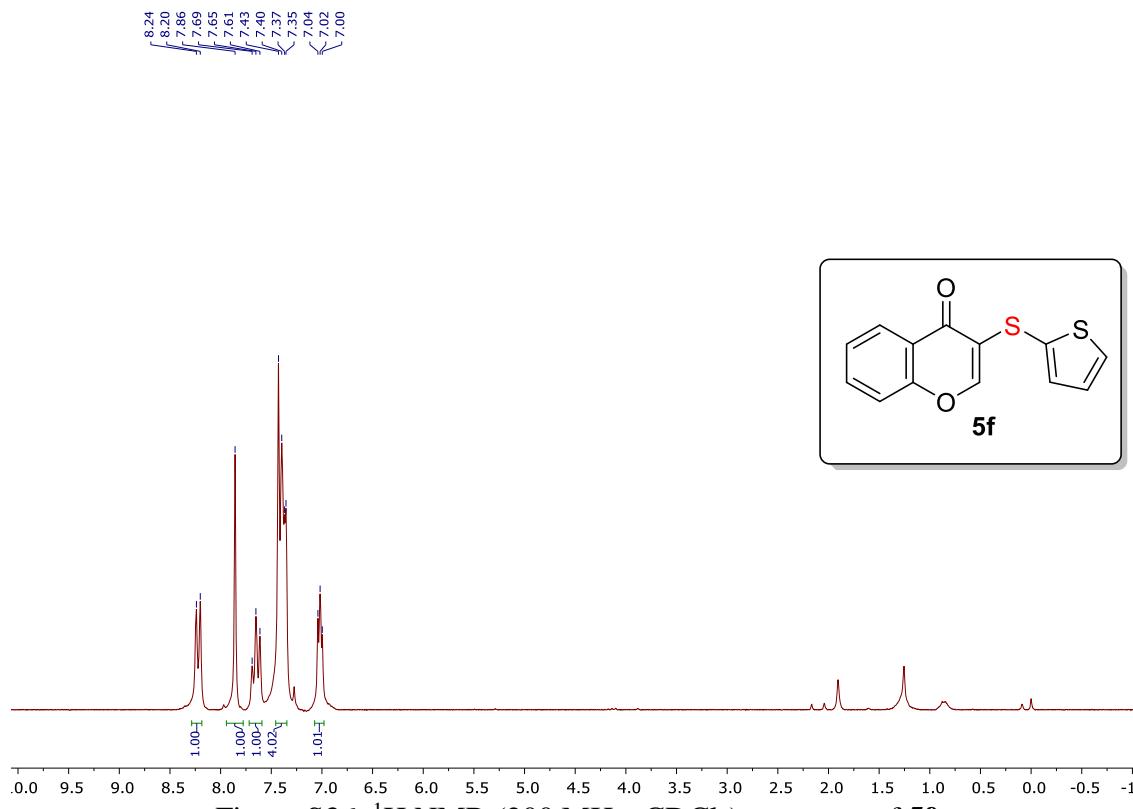
Figure S36. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **5f**
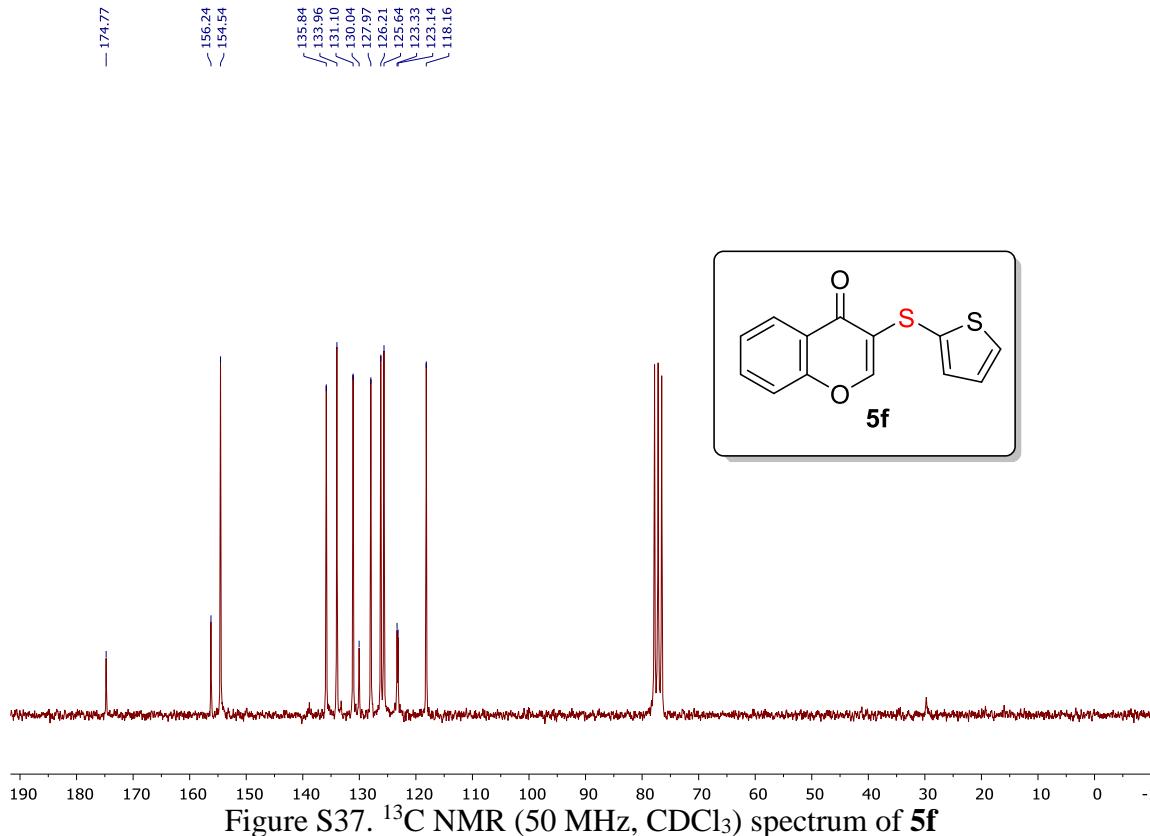
Figure S37. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **5f**
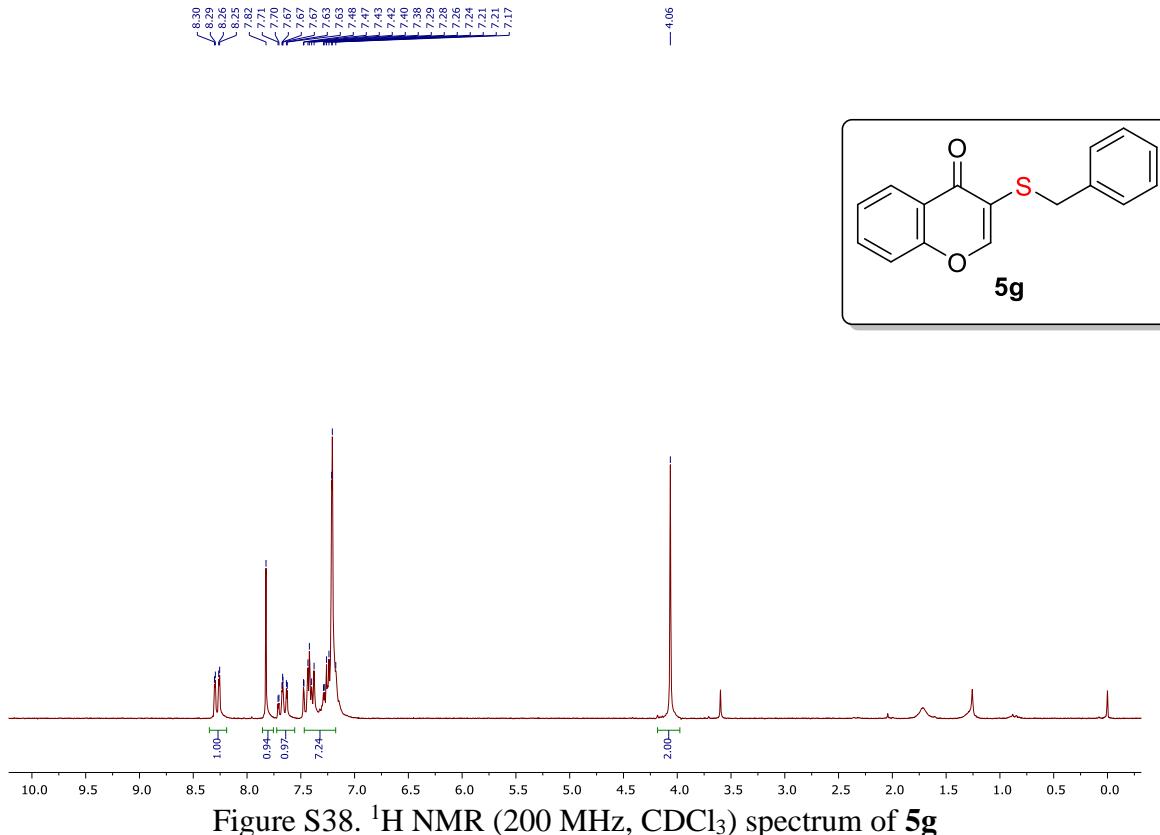
Figure S38. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **5g**
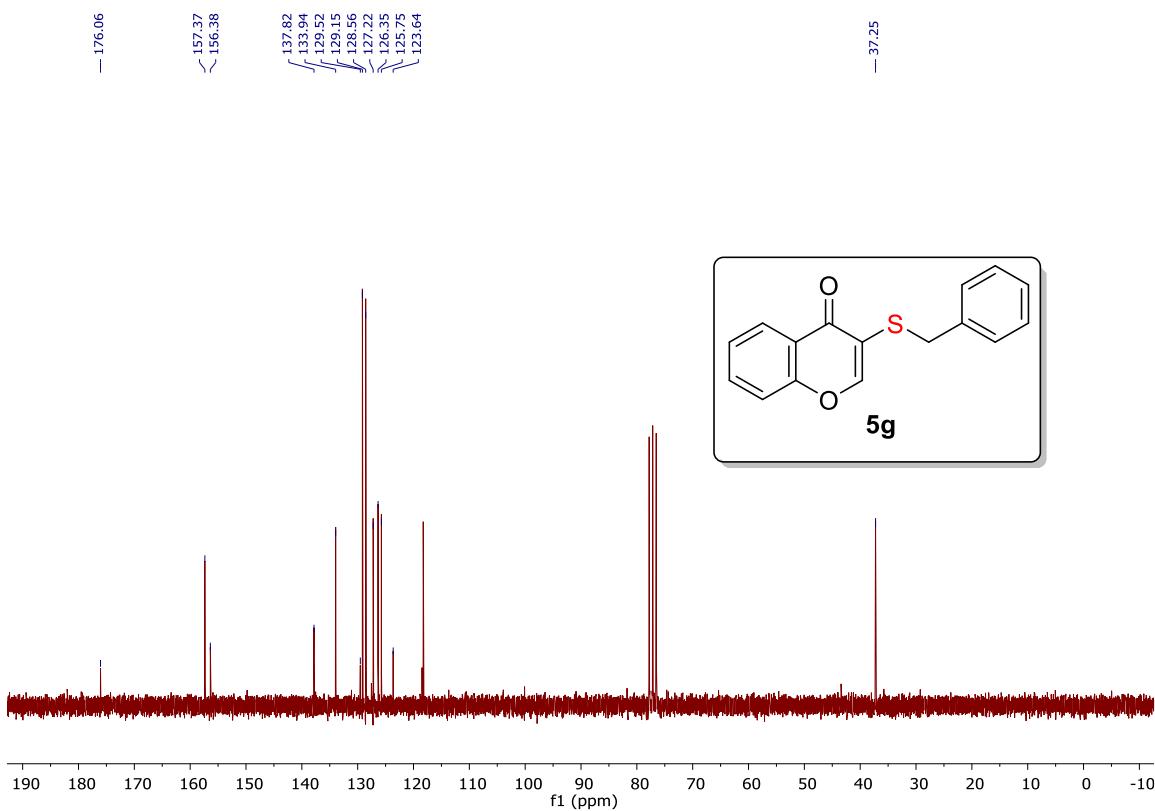
Figure S39. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **5g**
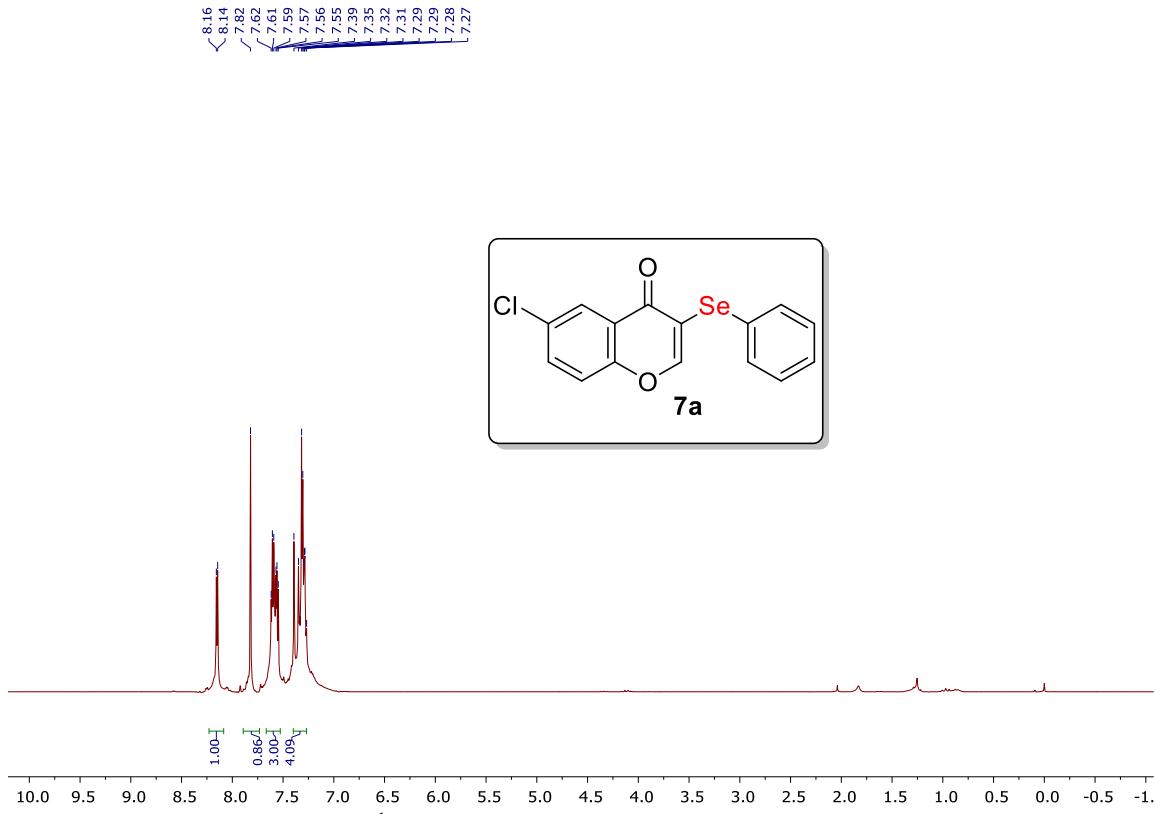
Figure S40. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7a**
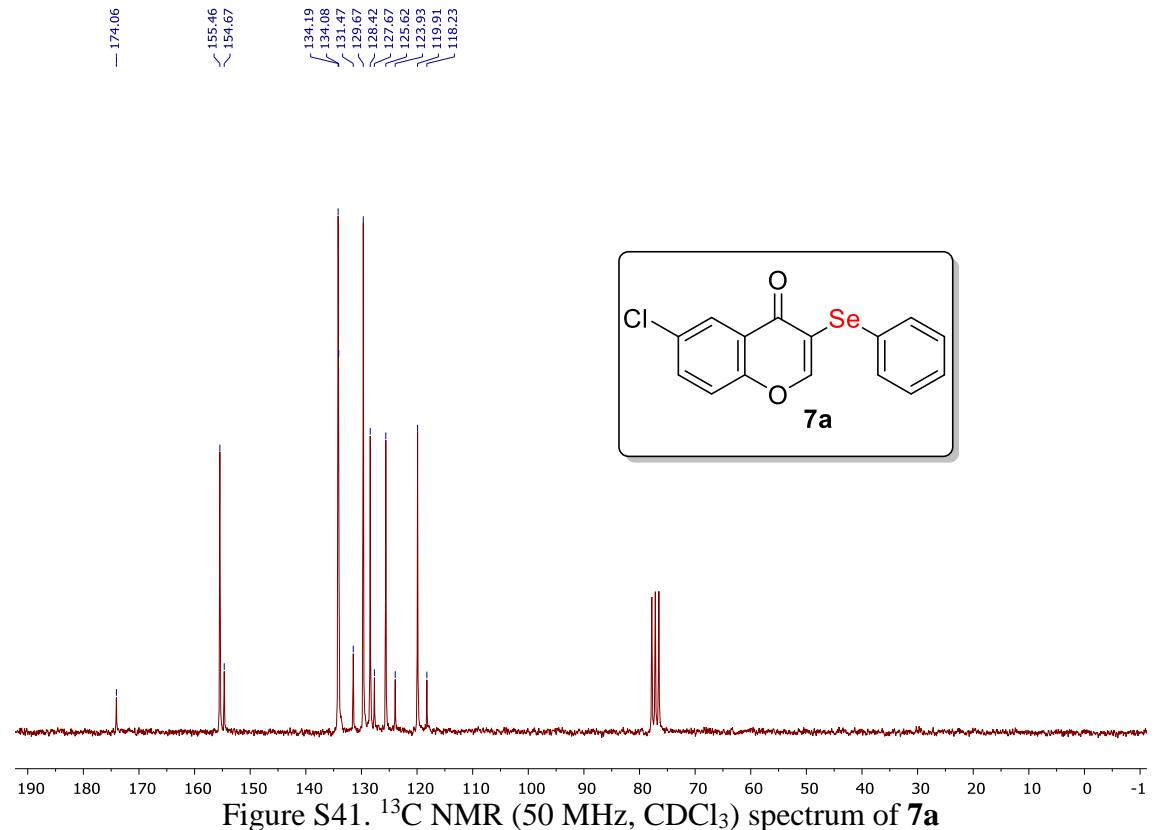
Figure S41. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7a**

8.16
8.15
8.08
7.62
7.61
7.58
7.57
7.43
7.41
7.40
7.38
7.37
7.36
7.32
7.31
7.28
7.27
7.25
7.24
7.23

1.00
1.00
1.00
6.12
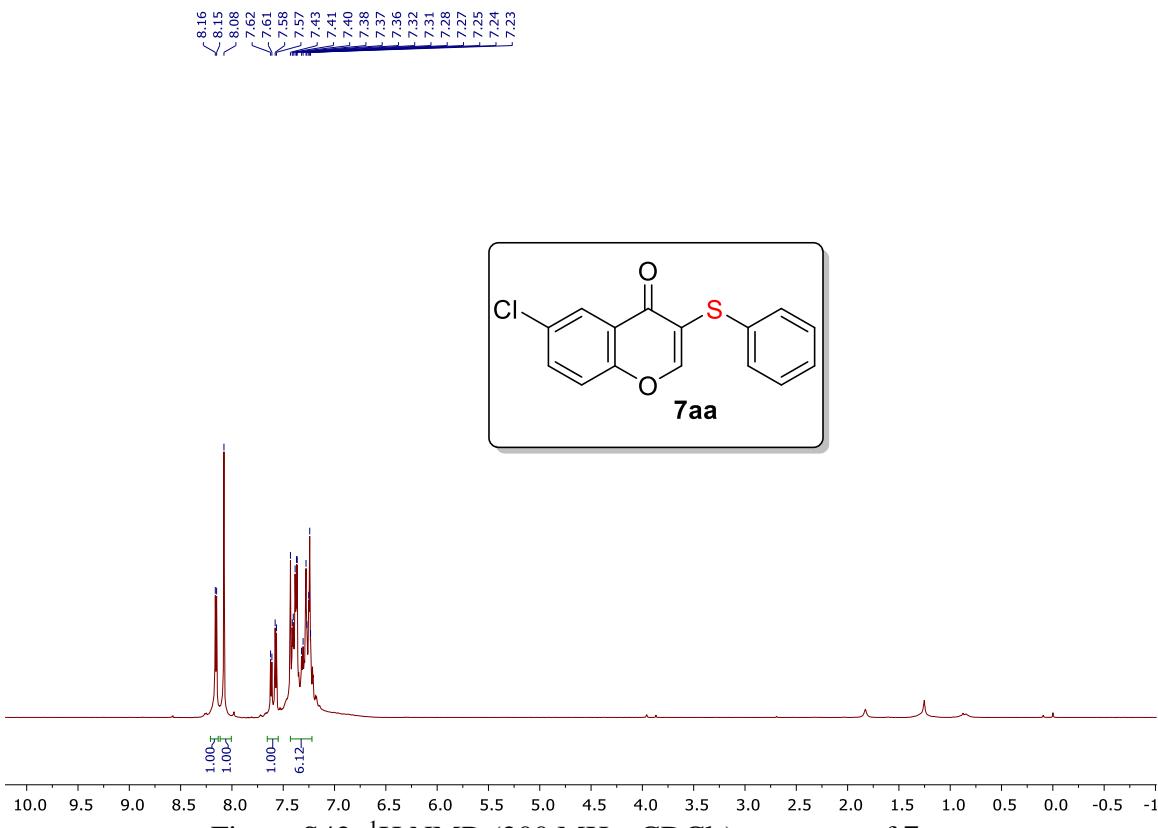
Figure S42. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7aa**

173.90
156.98
154.65
134.21
133.44
131.67
130.33
129.30
127.46
125.68
124.48
120.54
120.01
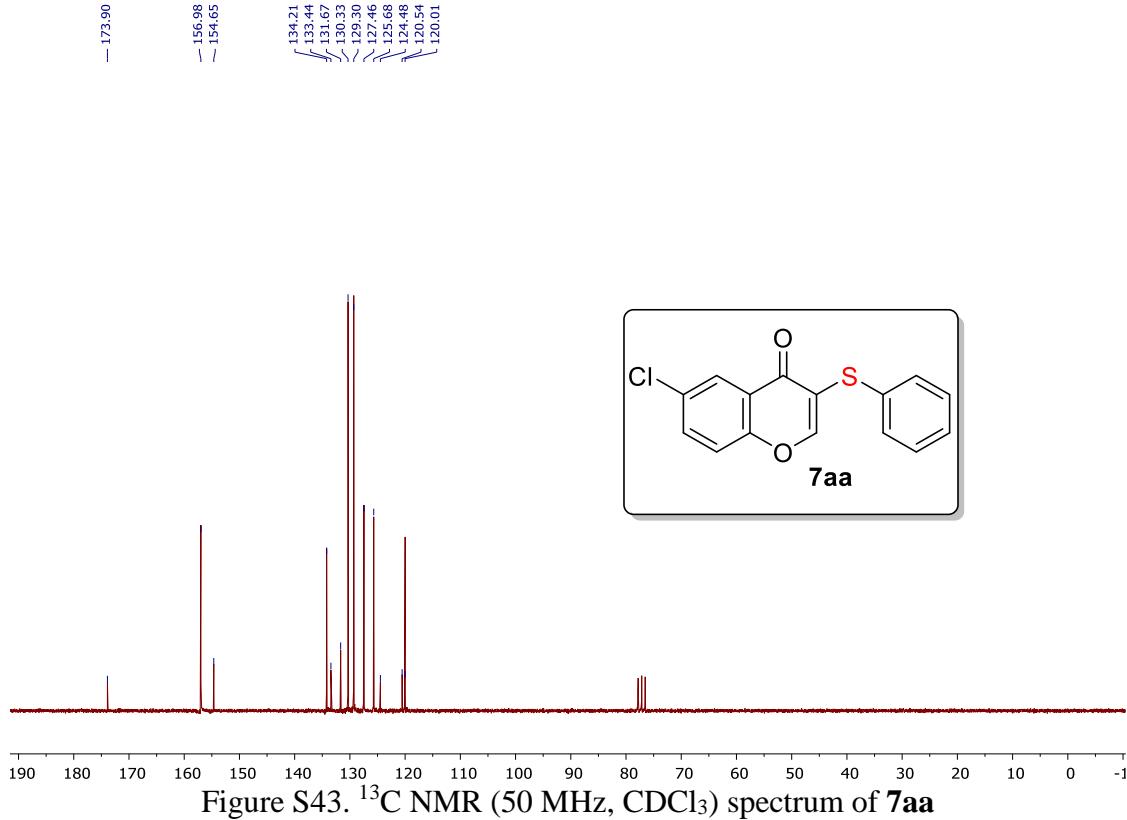
Figure S43. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7aa**

8.31
7.82
7.79
7.77
7.73
7.69
7.59
7.57
7.31
7.29

1.00
4.11
4.04

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
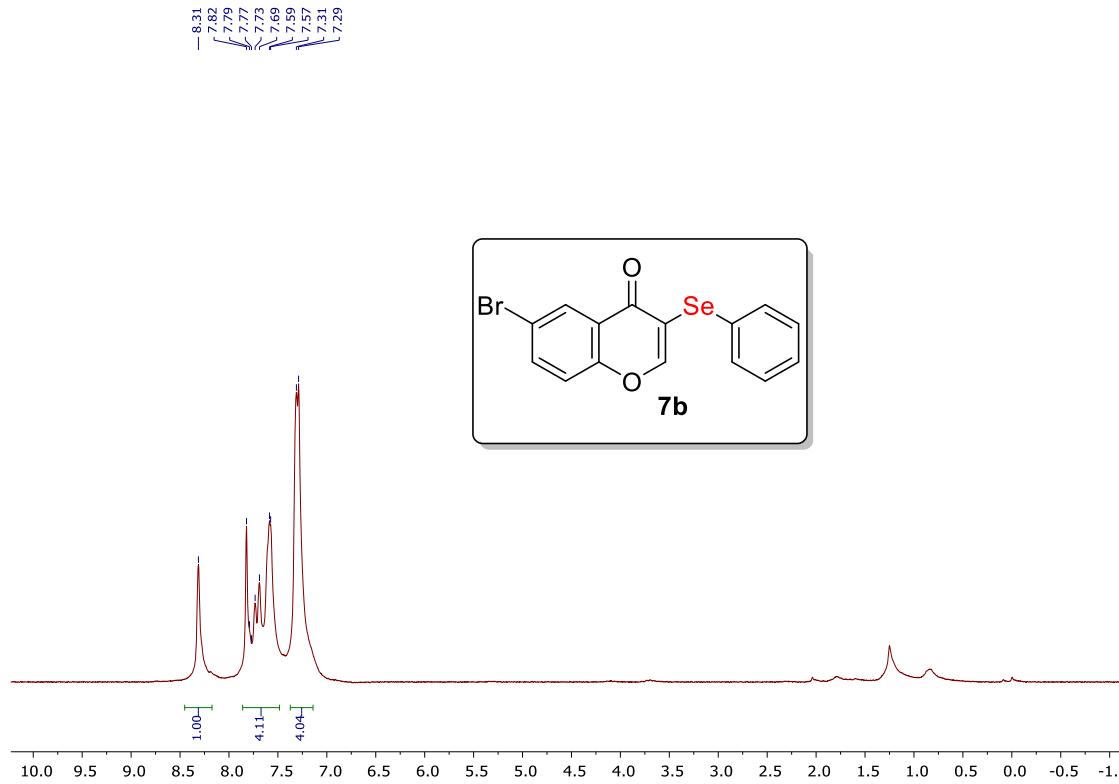
Figure S44. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7b**

173.92
155.45
155.11
136.84
134.21
129.69
128.85
128.44
127.67
124.30
120.13
118.95
118.34

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
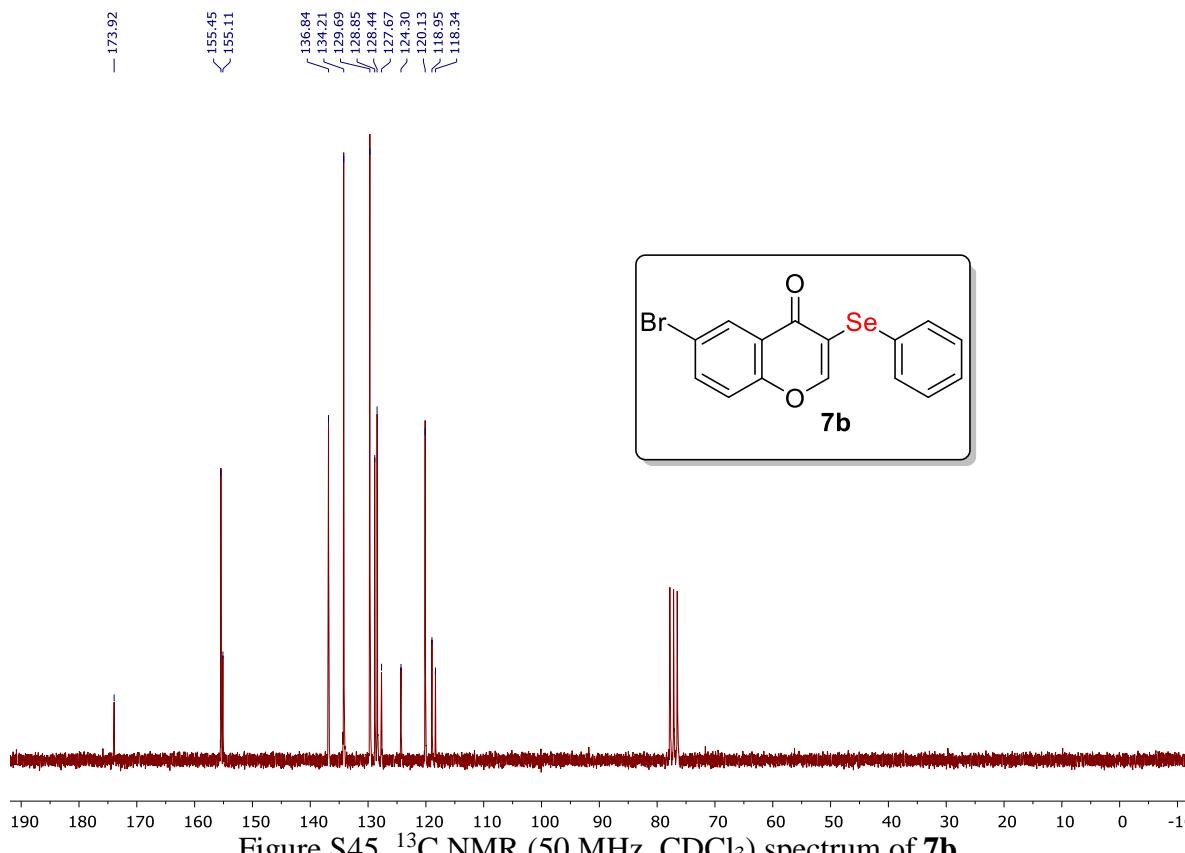
Figure S45. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7b**

8.34
8.33
8.08
7.77
7.76
7.73
7.72
7.41
7.38
7.33
7.29
7.25
7.23

1.00
1.00
1.00
6.08

0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
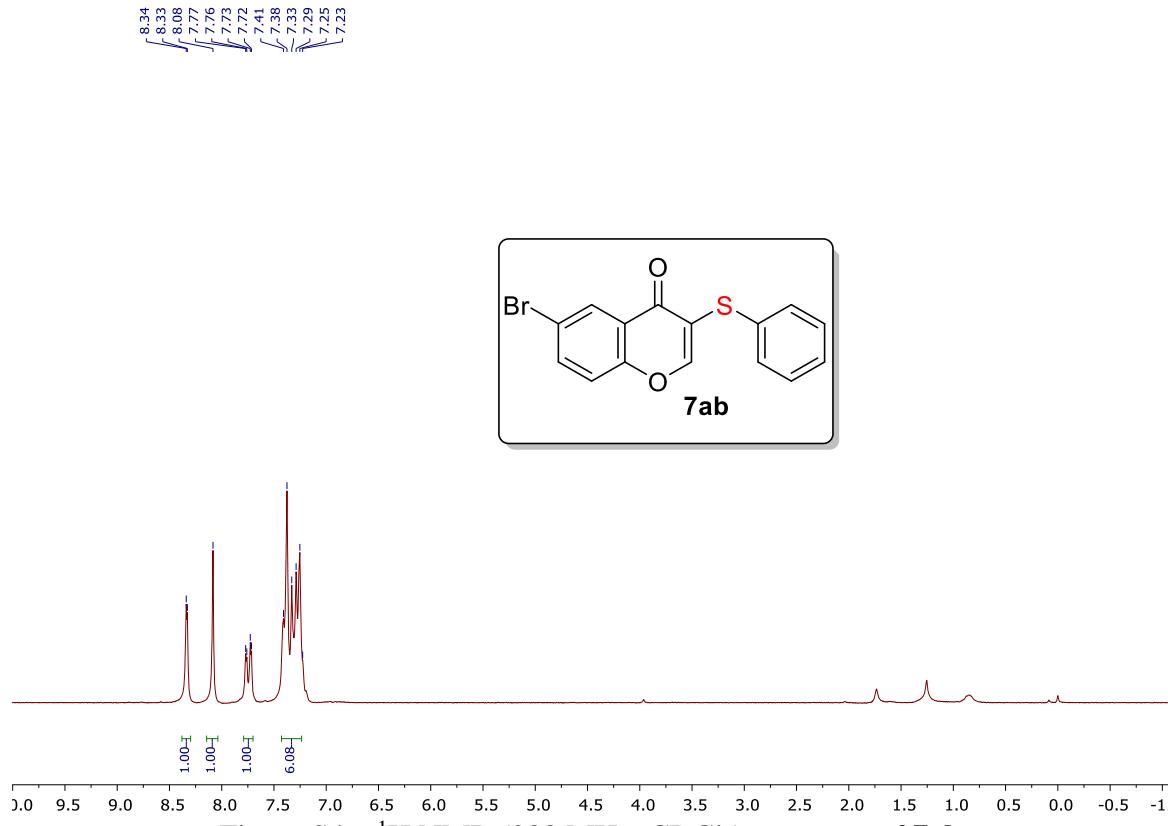
Figure S46. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7ab**

173.83

156.99
155.14

137.02
133.45
130.40
129.36
128.99
127.53
124.89
120.74
120.22
119.20

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
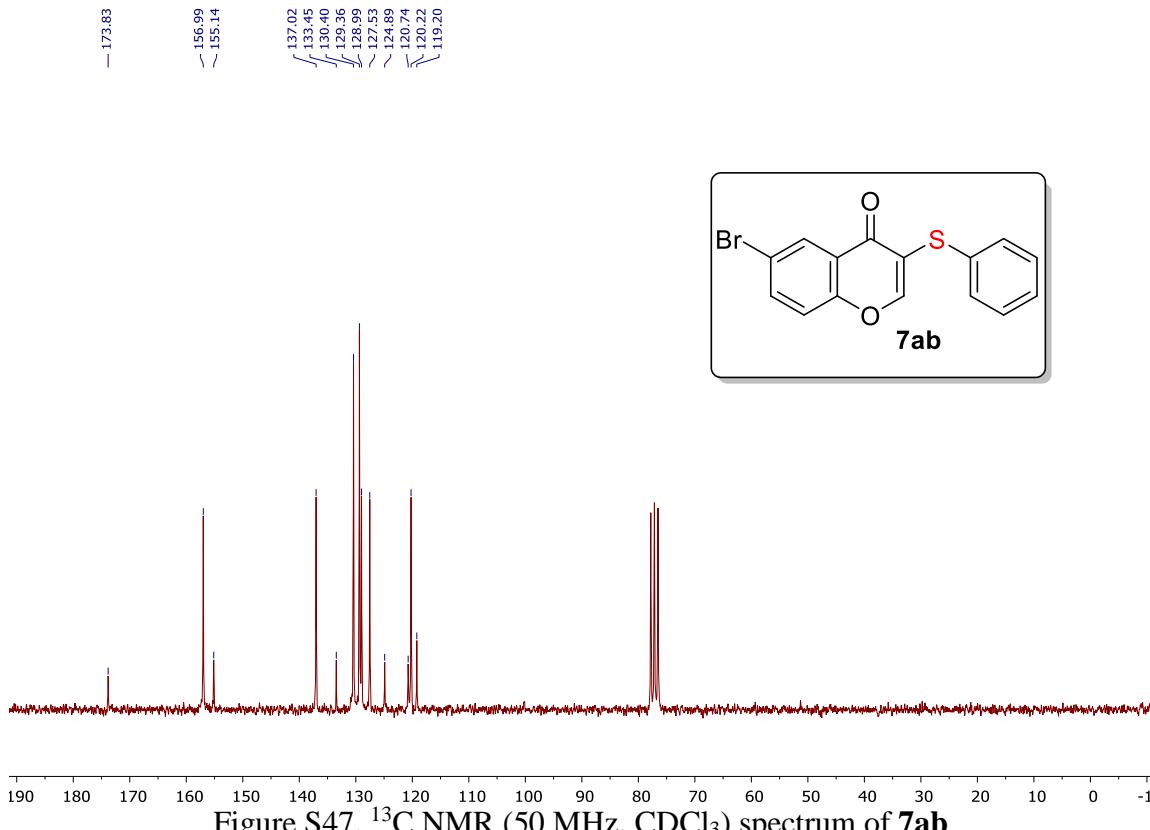
Figure S47. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7ab**
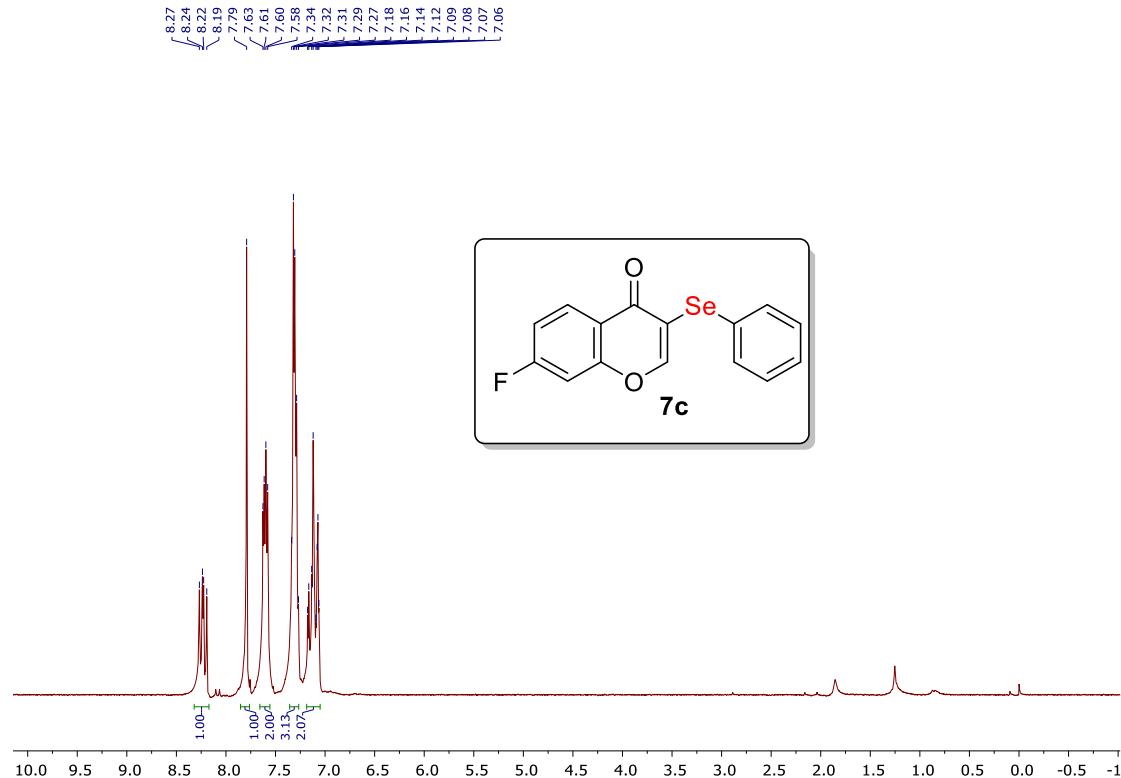
Figure S48. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7c**
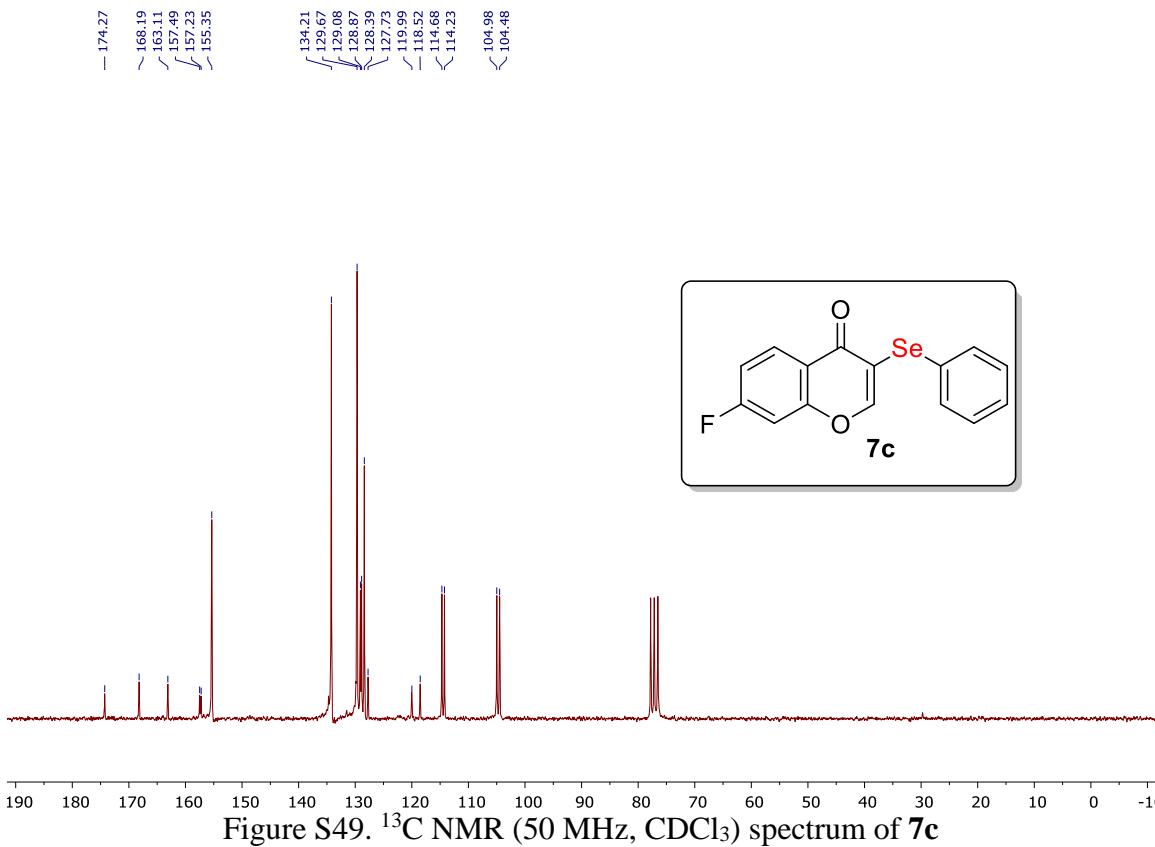
Figure S49. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7c**
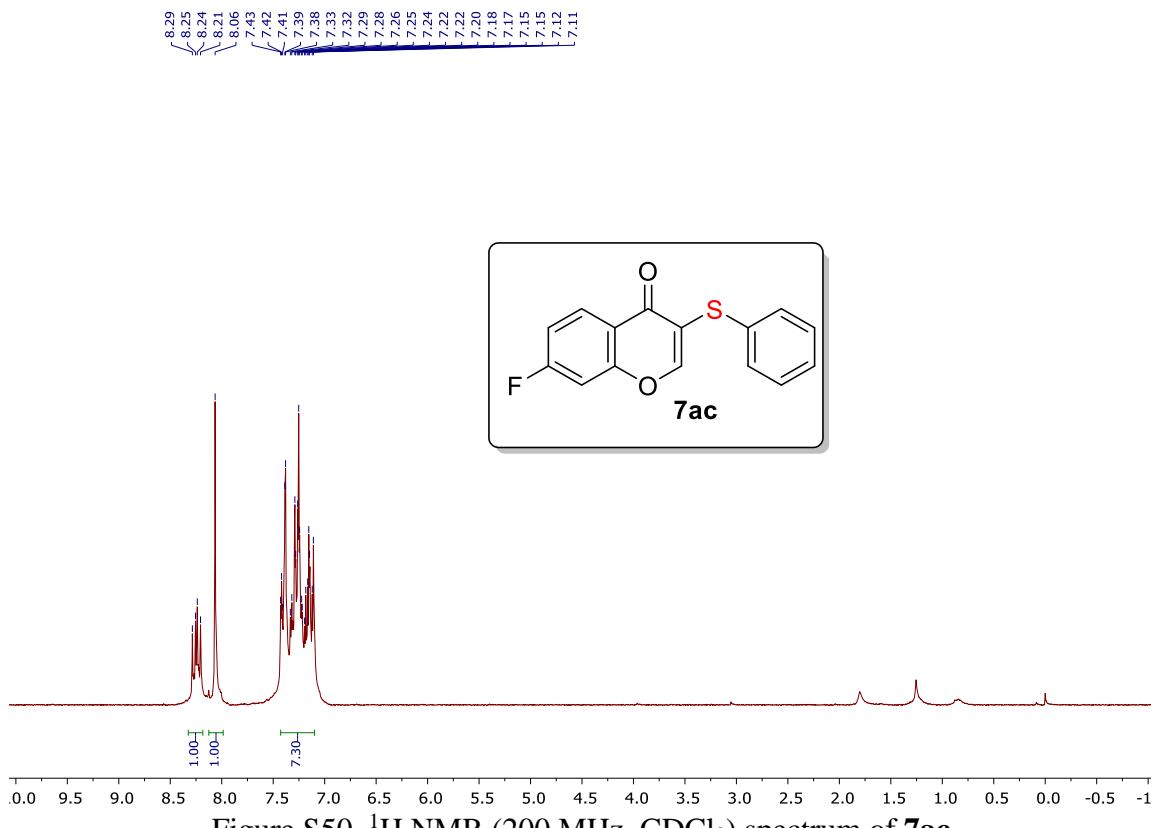
Figure S50. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7ac**
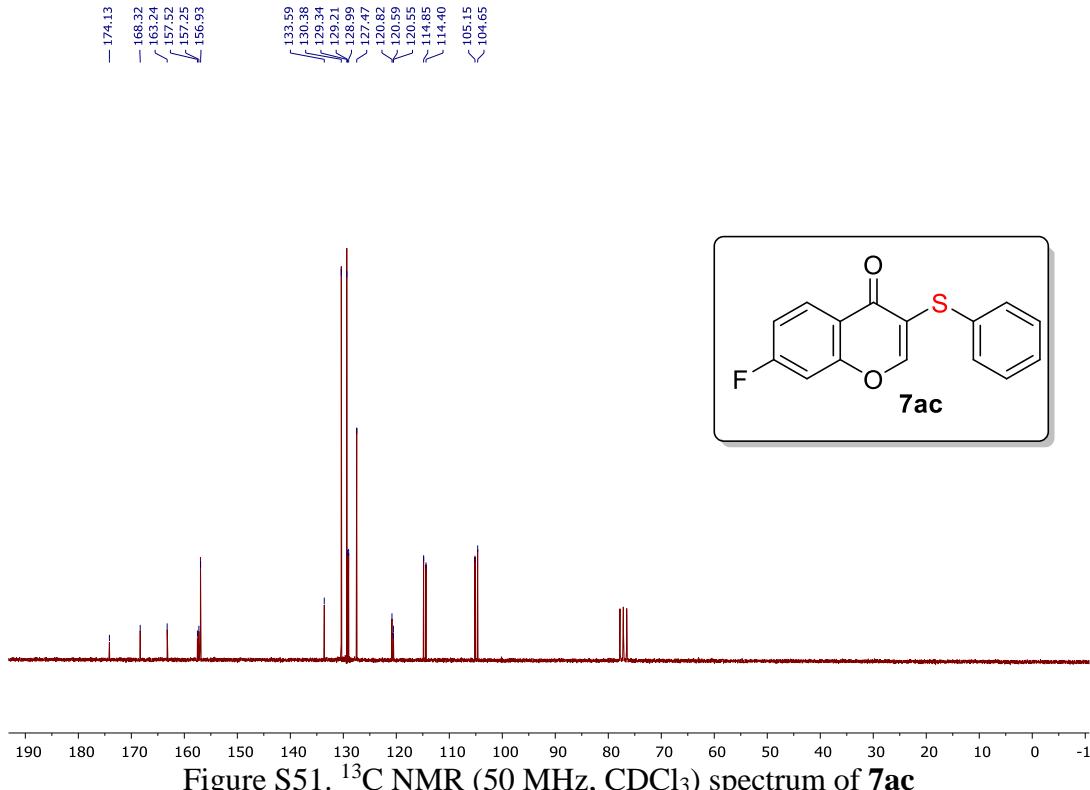
Figure S51. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7ac**
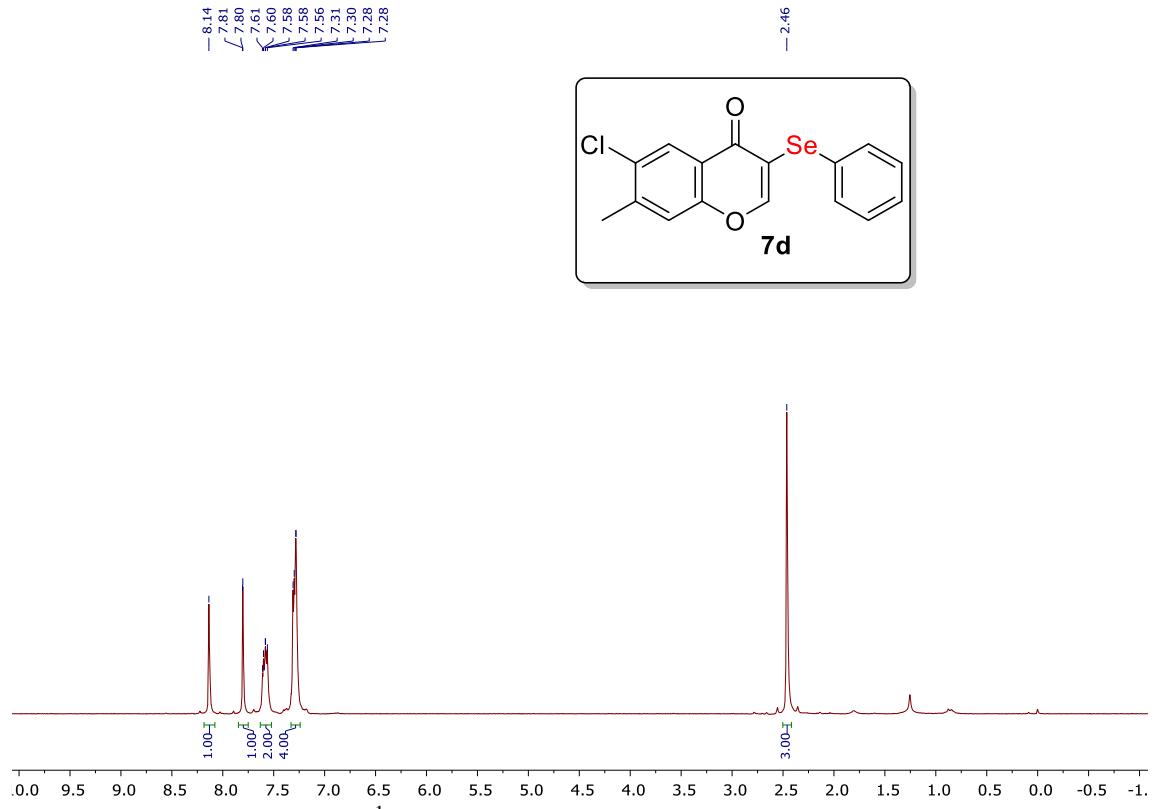
Figure S52. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7d**
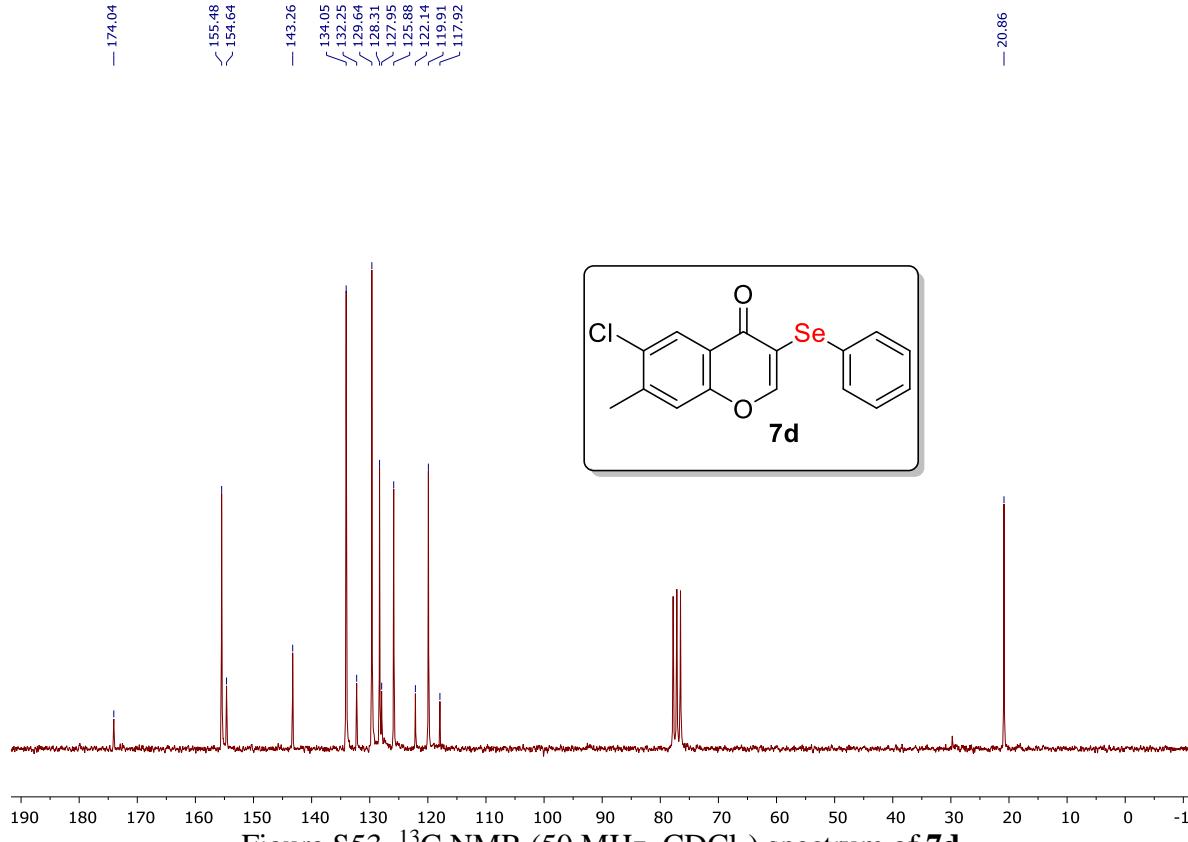
Figure S53. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7d**
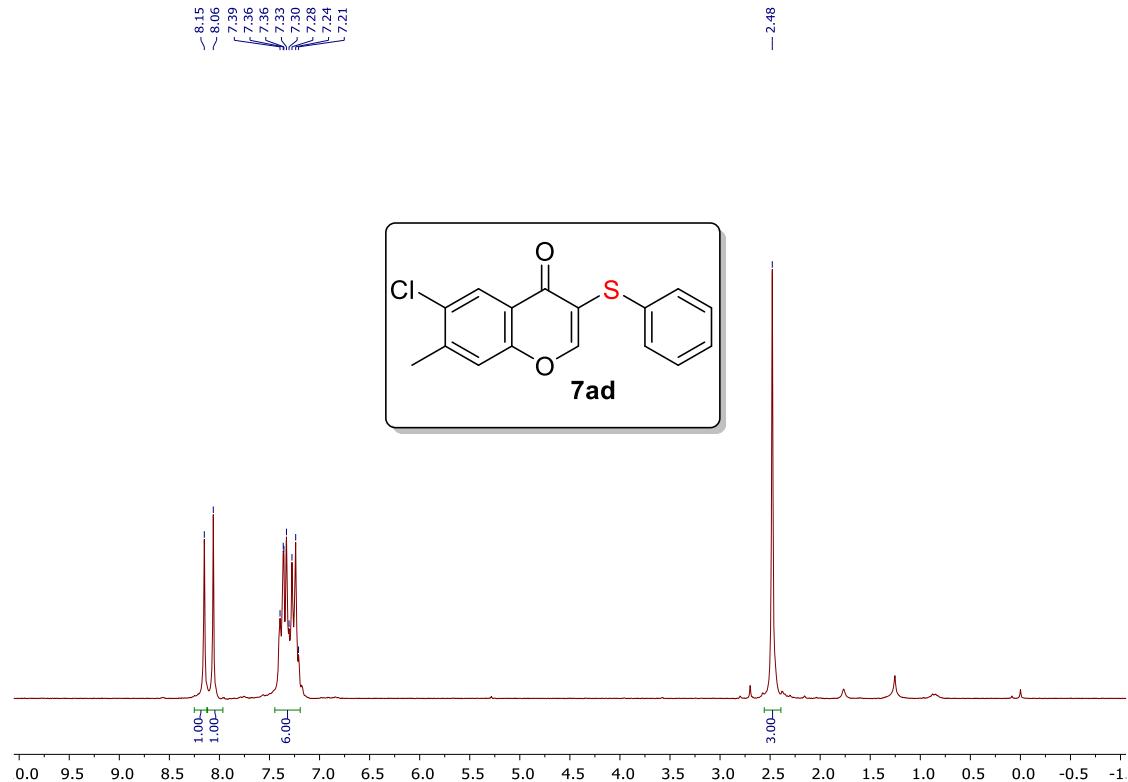
Figure S54. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7ad**
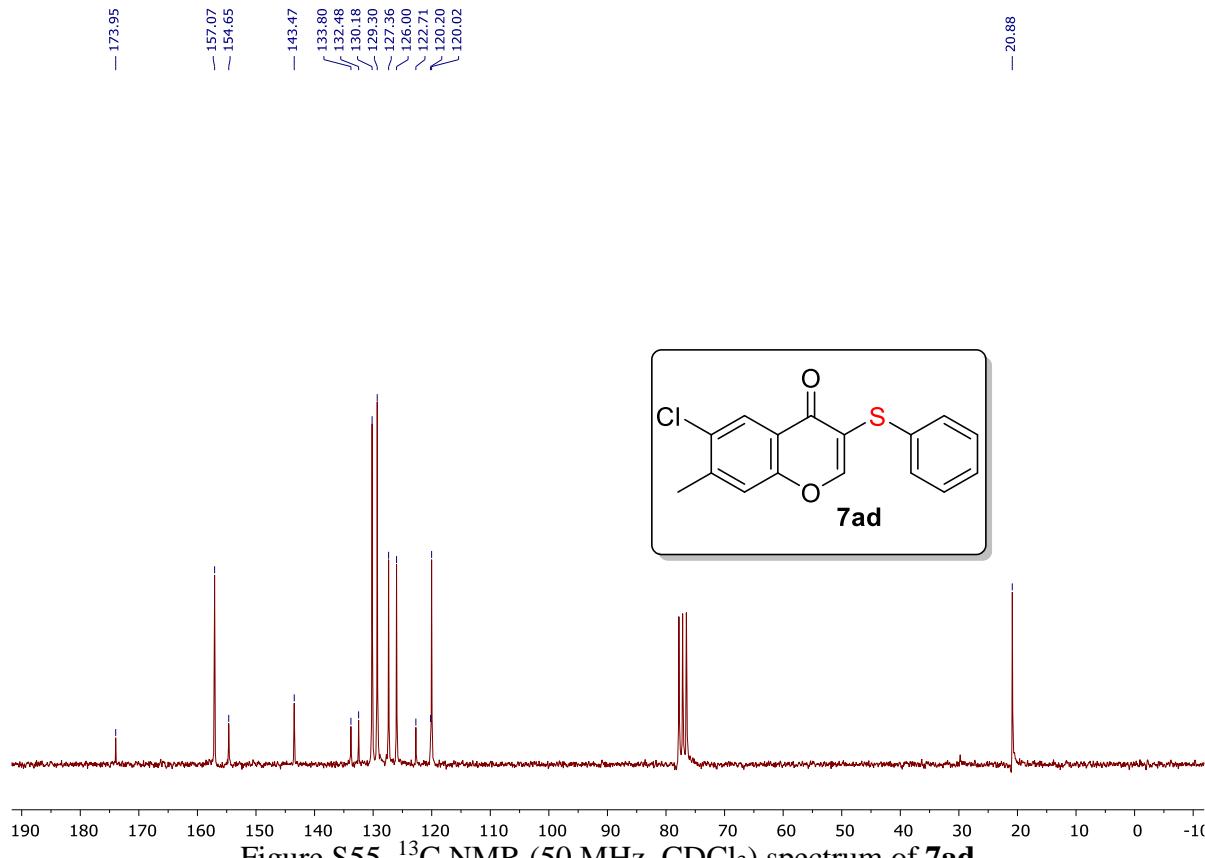
Figure S55. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7ad**
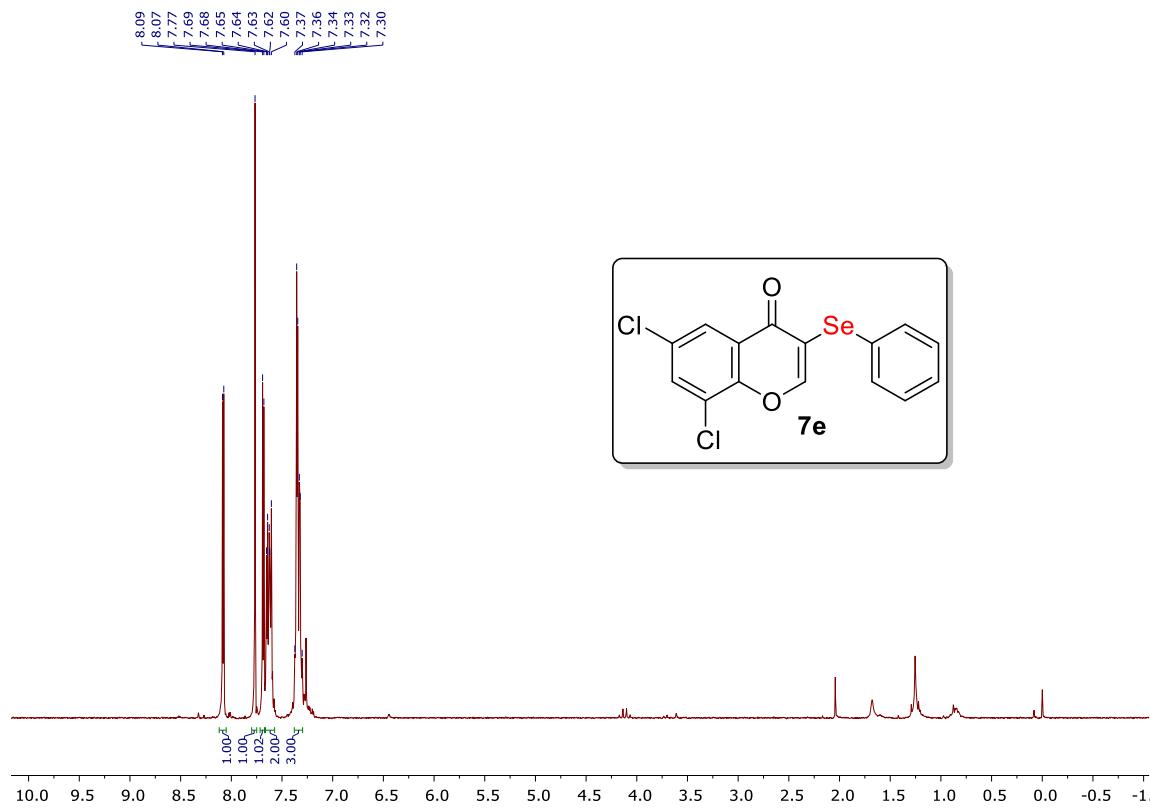
Figure S56. ¹H NMR (200 MHz, CDCl₃) spectrum of **7e**
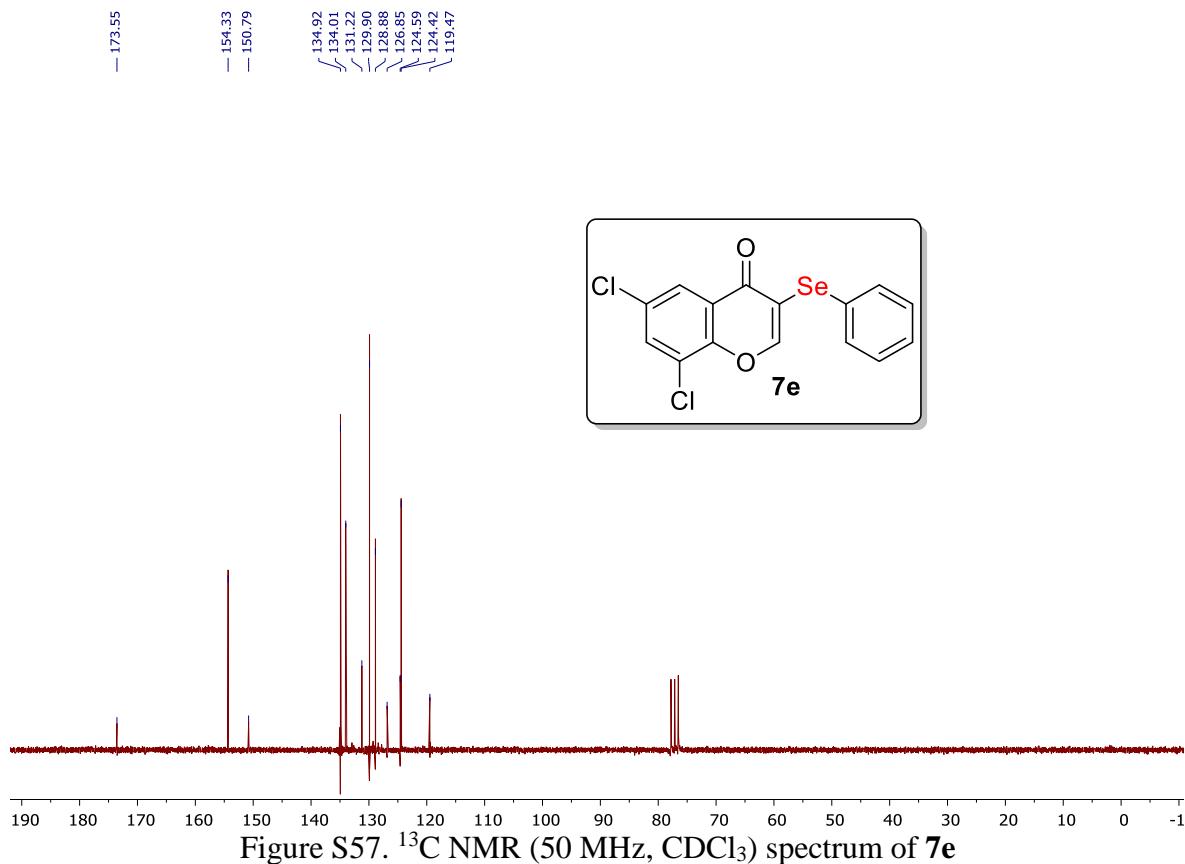
Figure S57. ¹³C NMR (50 MHz, CDCl₃) spectrum of **7e**
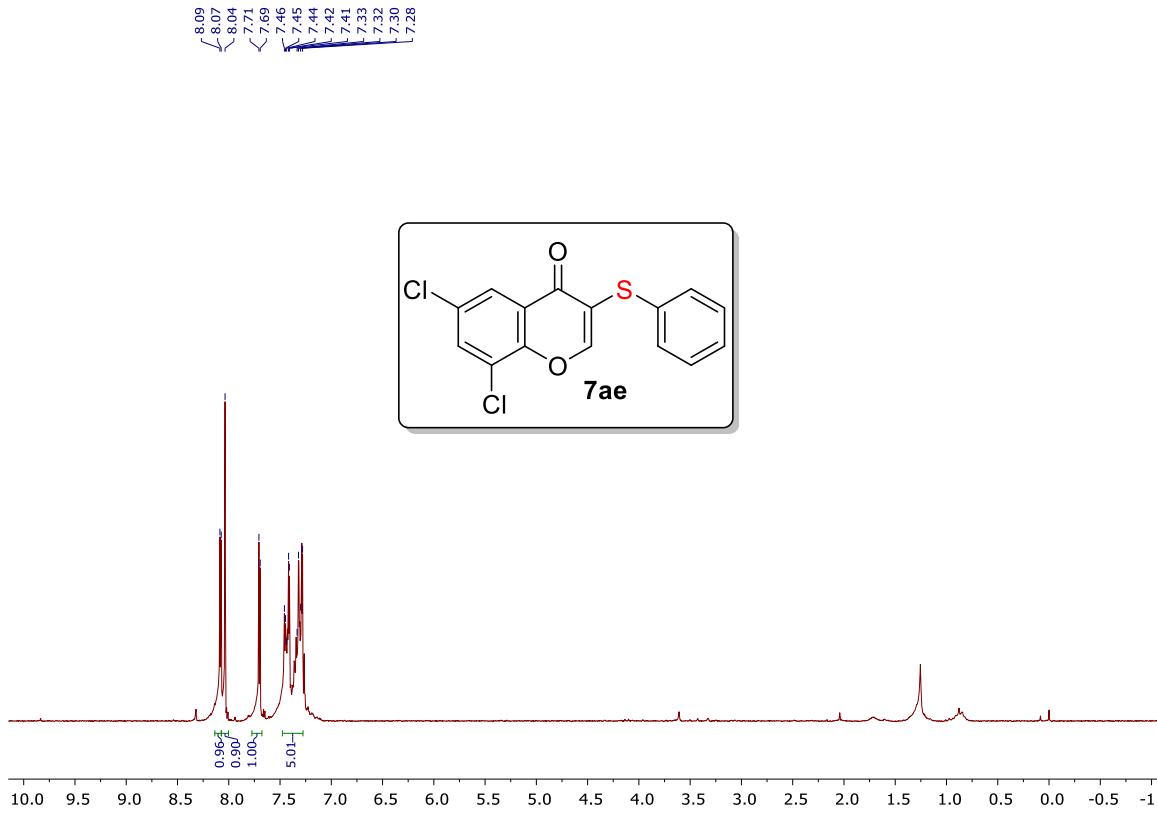
Figure S58. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7ae**
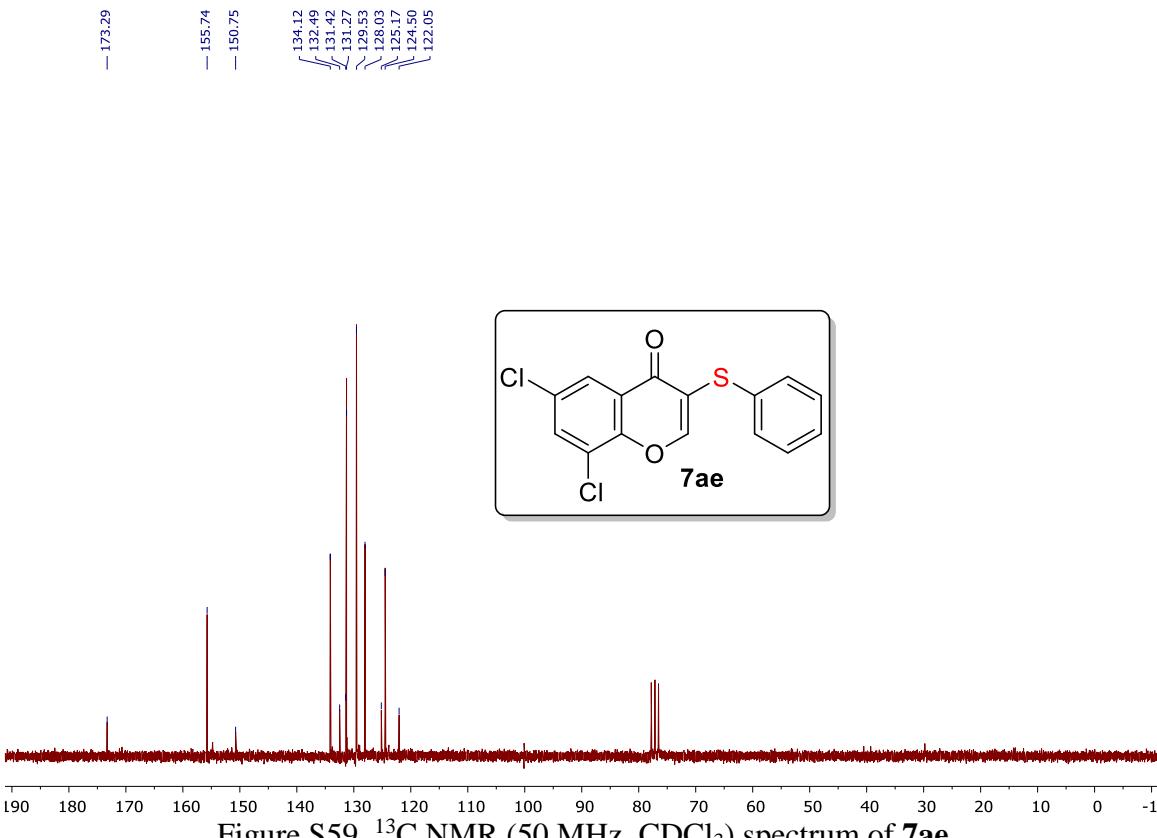

Figure S59. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7ae**

Figure S60. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7f**

Figure S61. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7f**

8.29
8.27
7.99
7.97
7.76
7.65
7.64
7.63
7.62
7.61
7.36
7.35
7.33
7.32
7.30
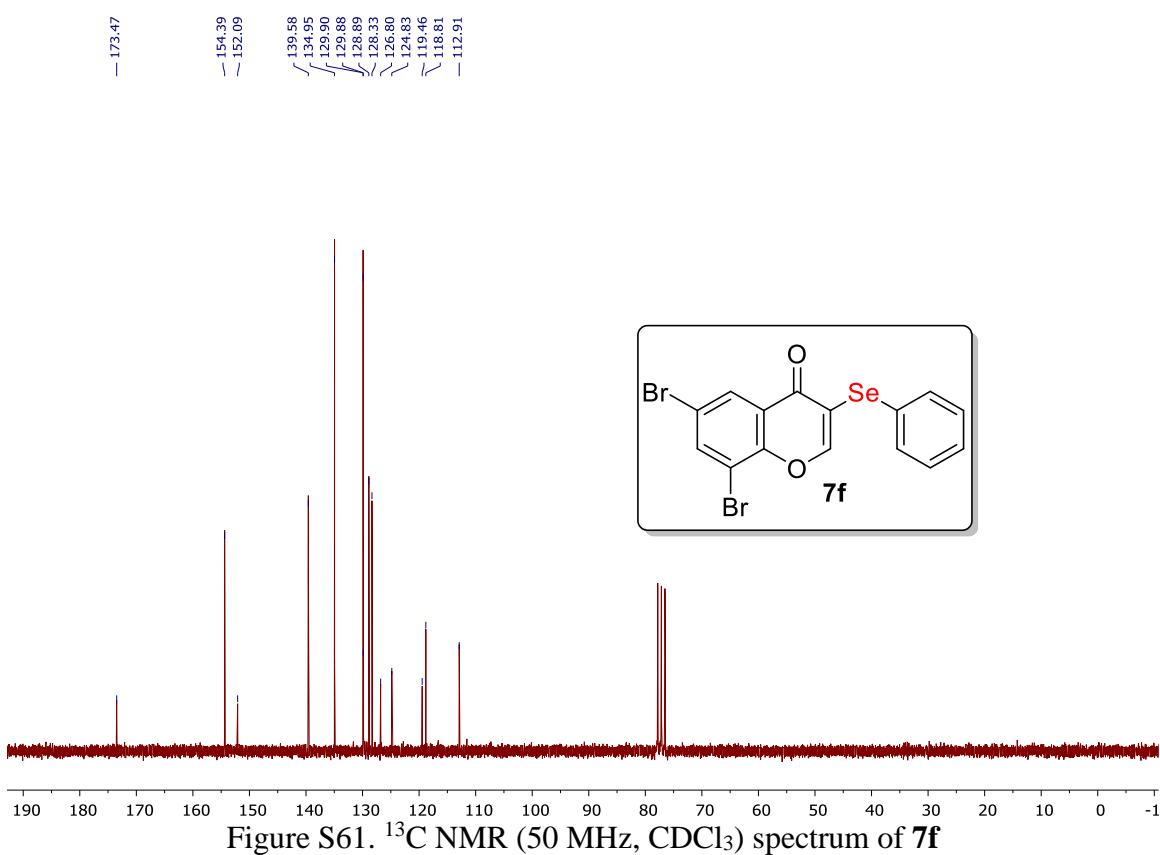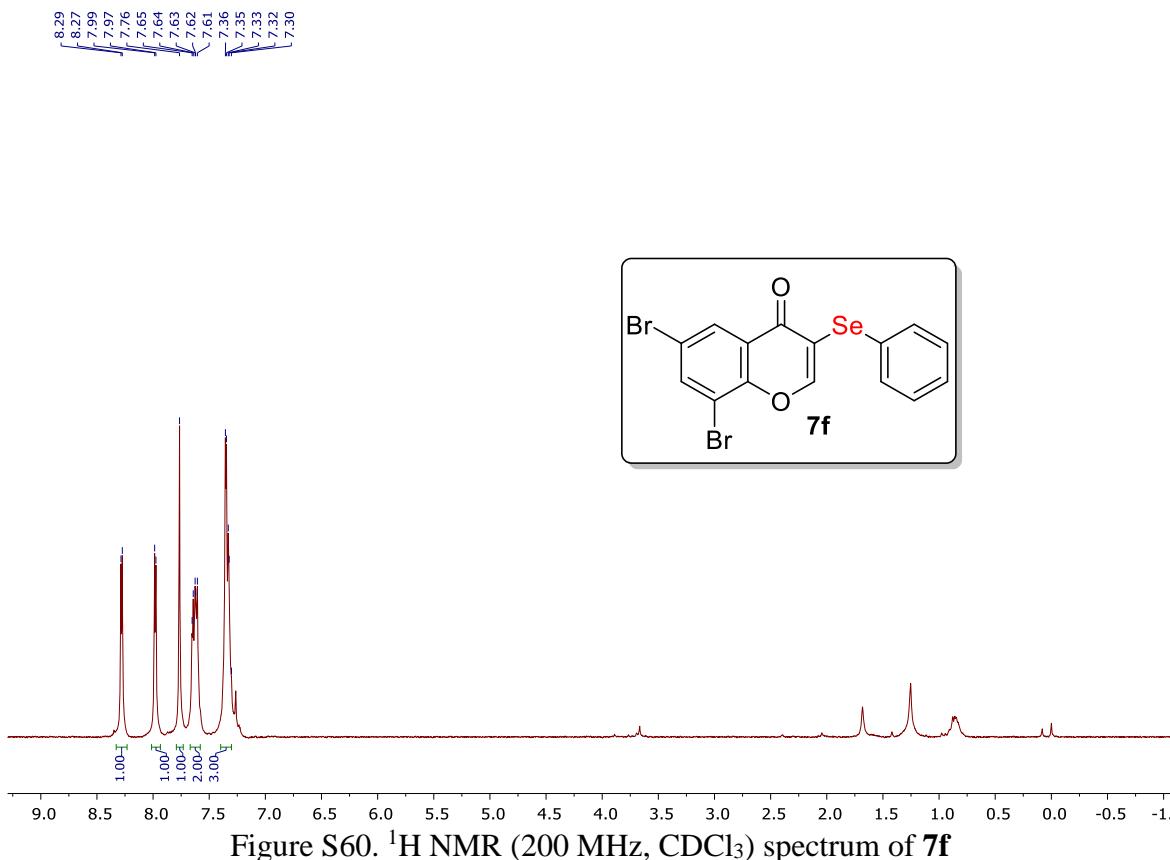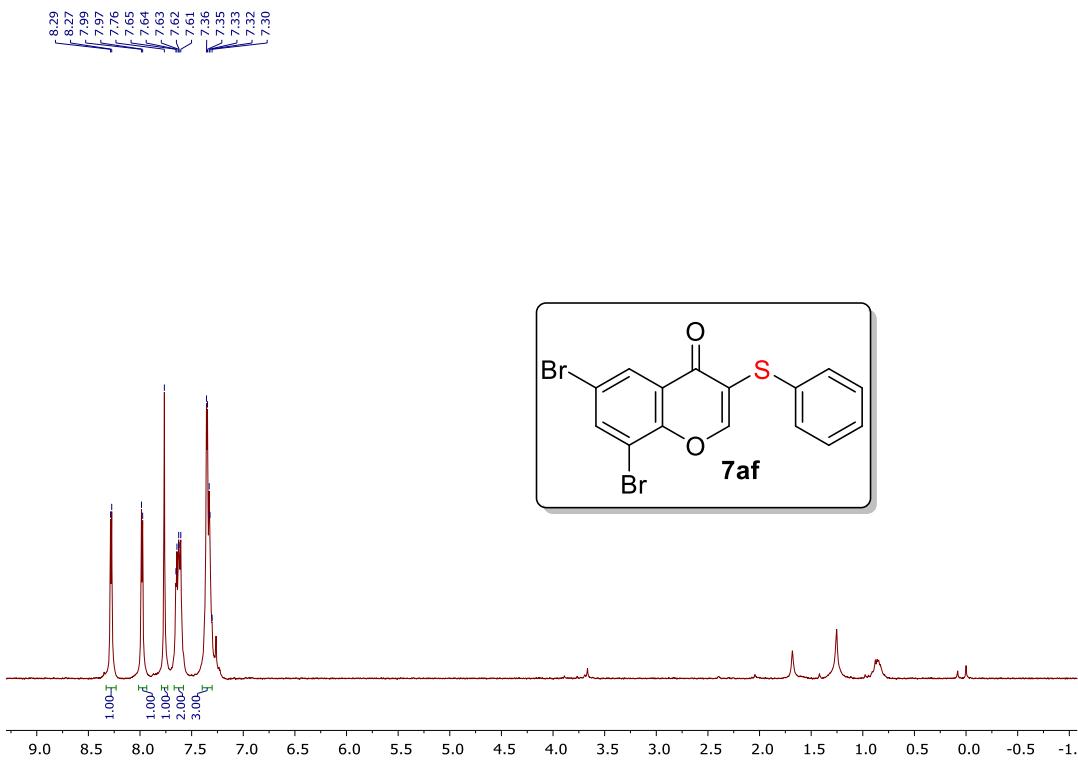
Figure S62. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7af**

173.28
155.82
152.11
139.78
132.47
131.36
129.59
128.48
128.10
125.46
122.13
119.07
113.02
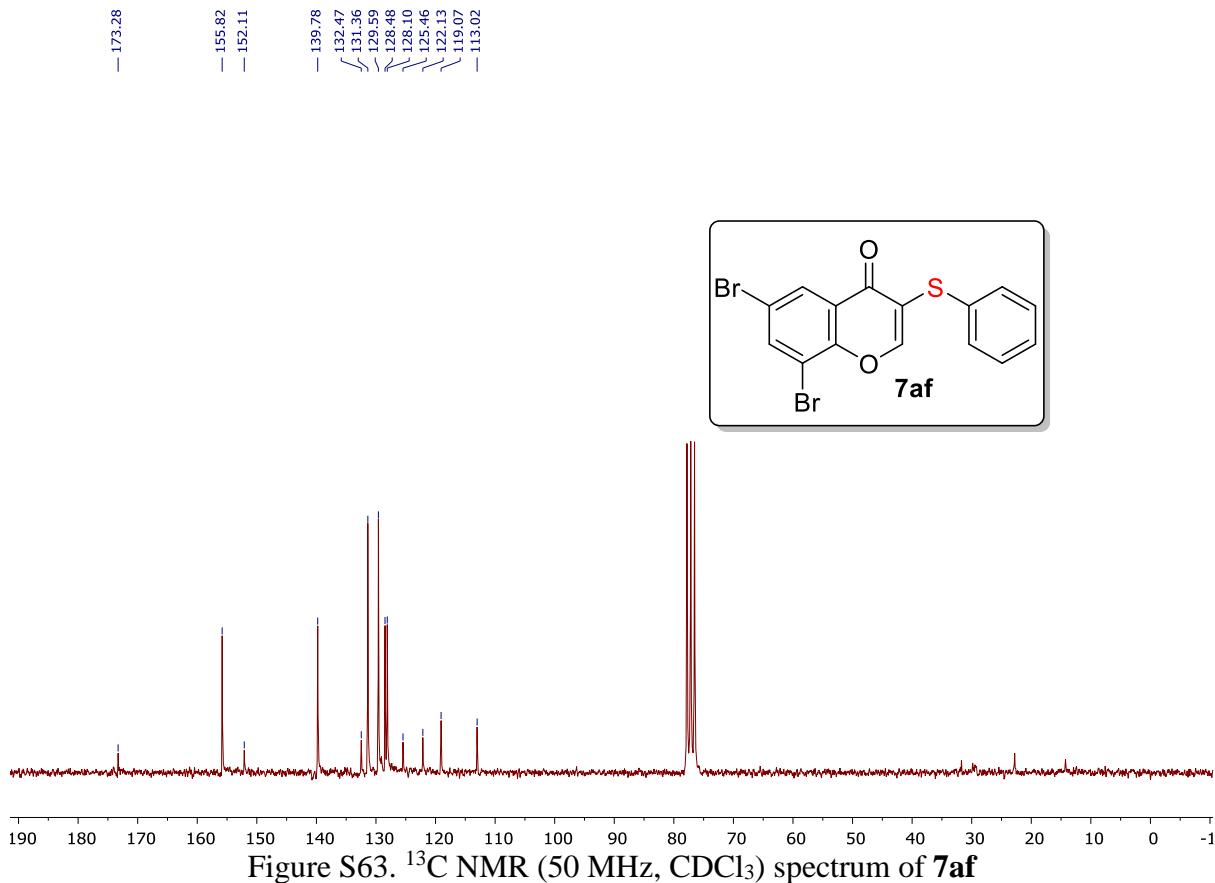
Figure S63. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7af**
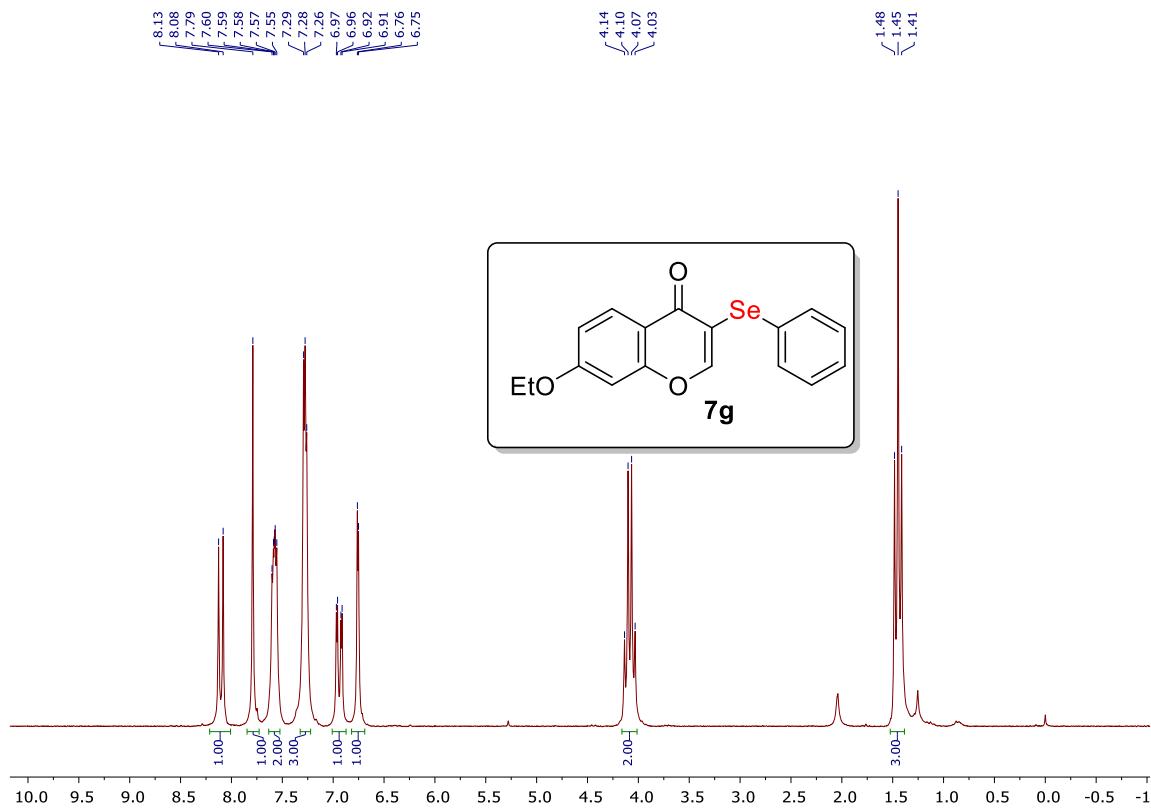
Figure S64. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7g**
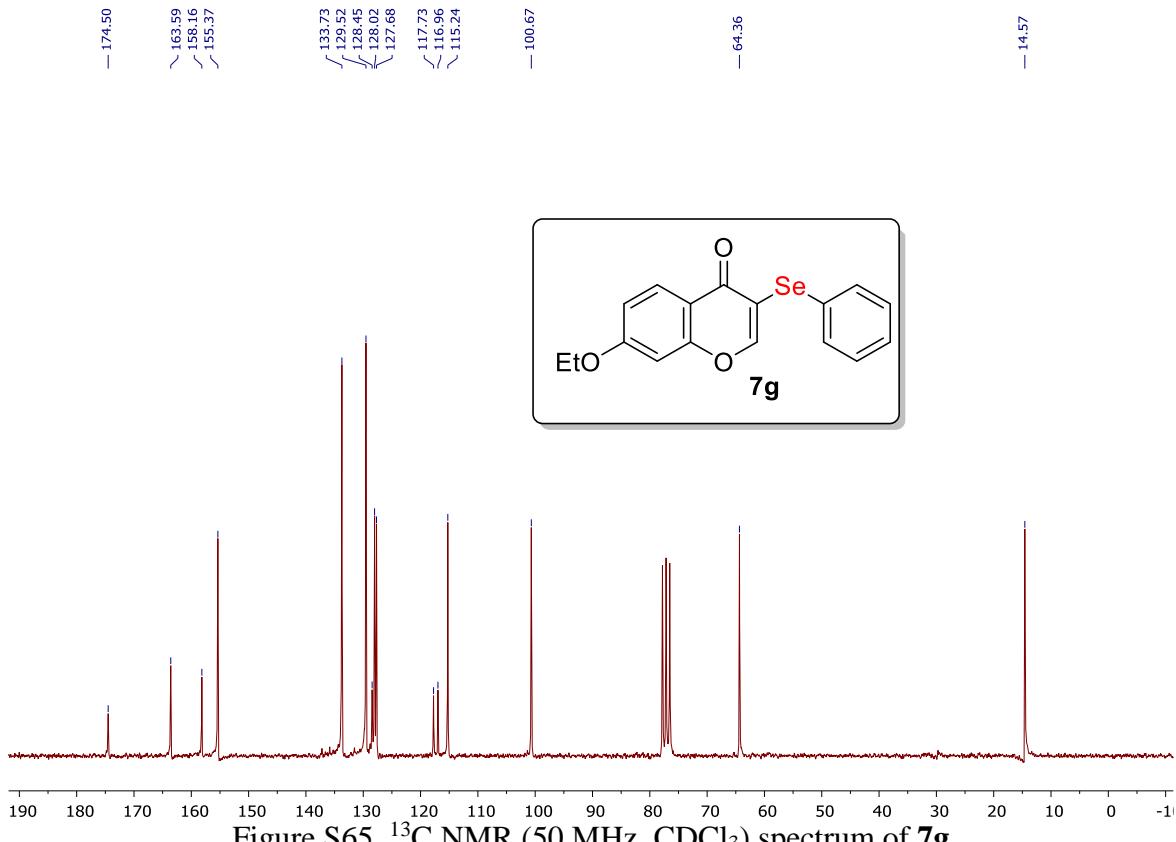
Figure S65. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7g**
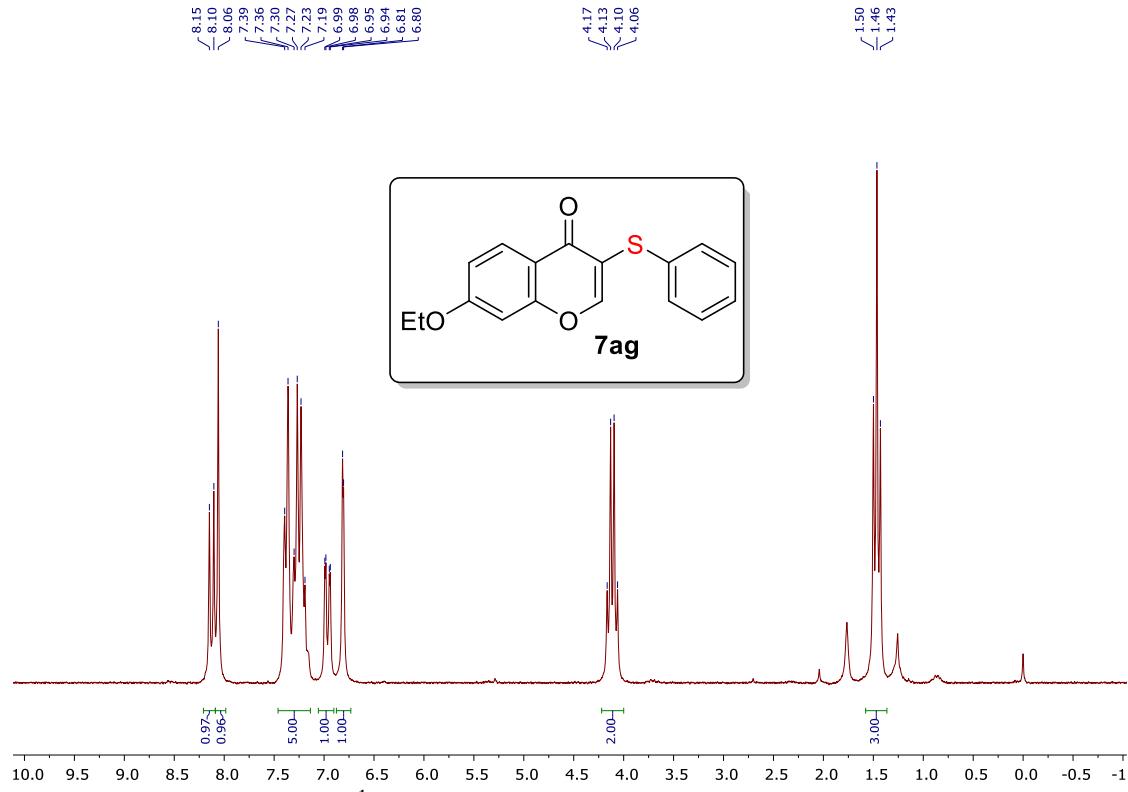
Figure S66. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7ag**
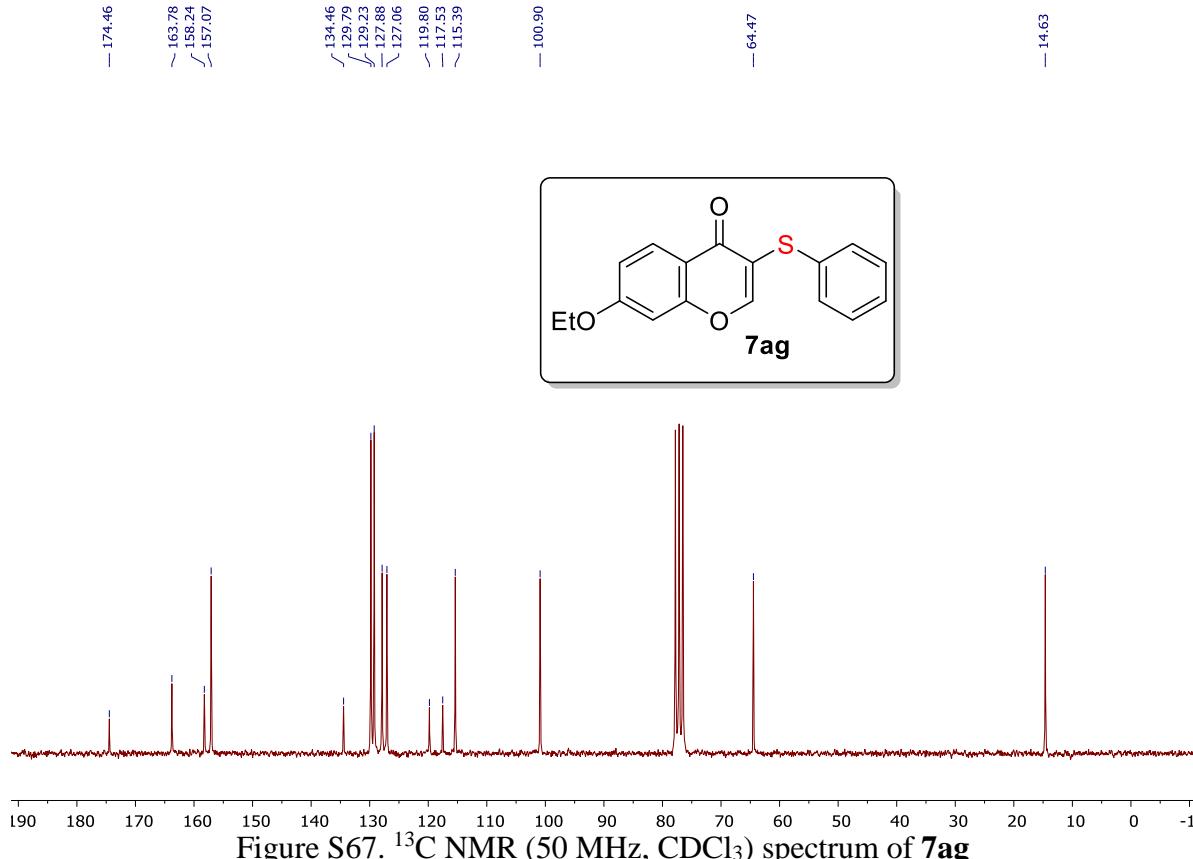
Figure S67. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7ag**
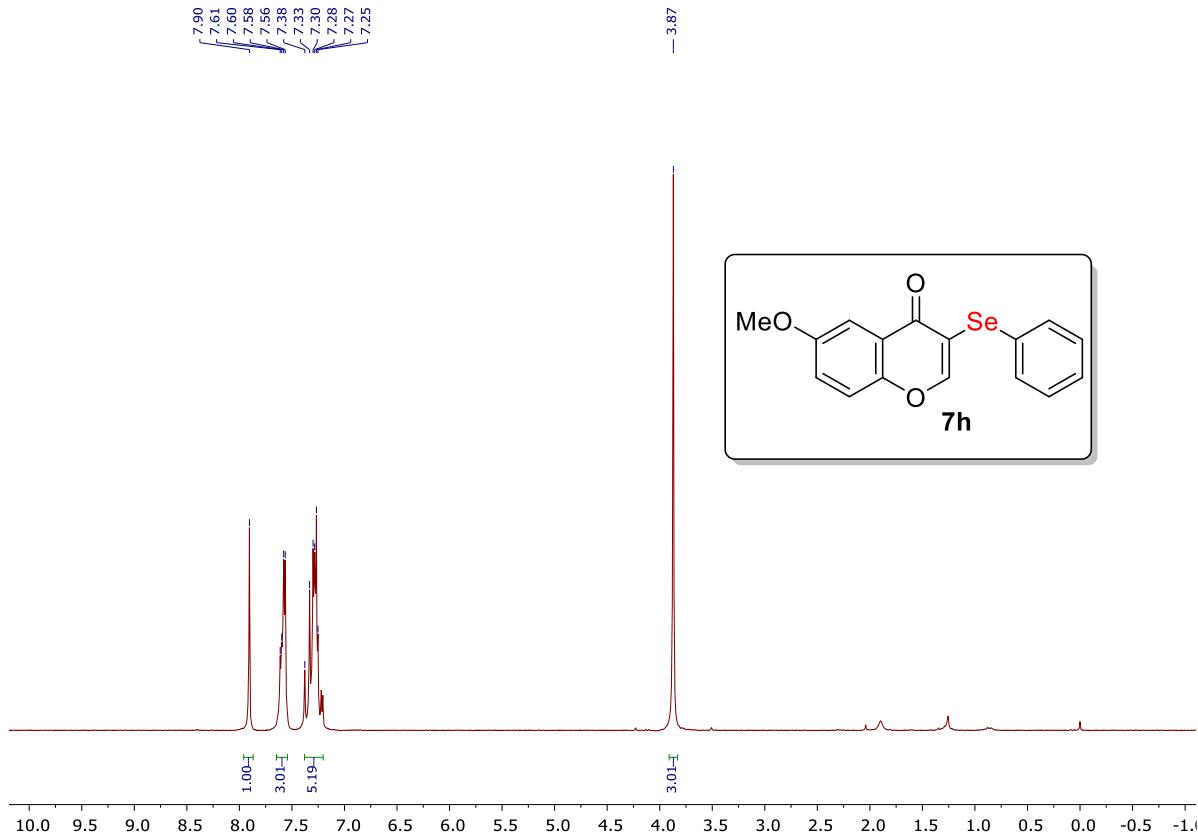
Figure S68. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7h**
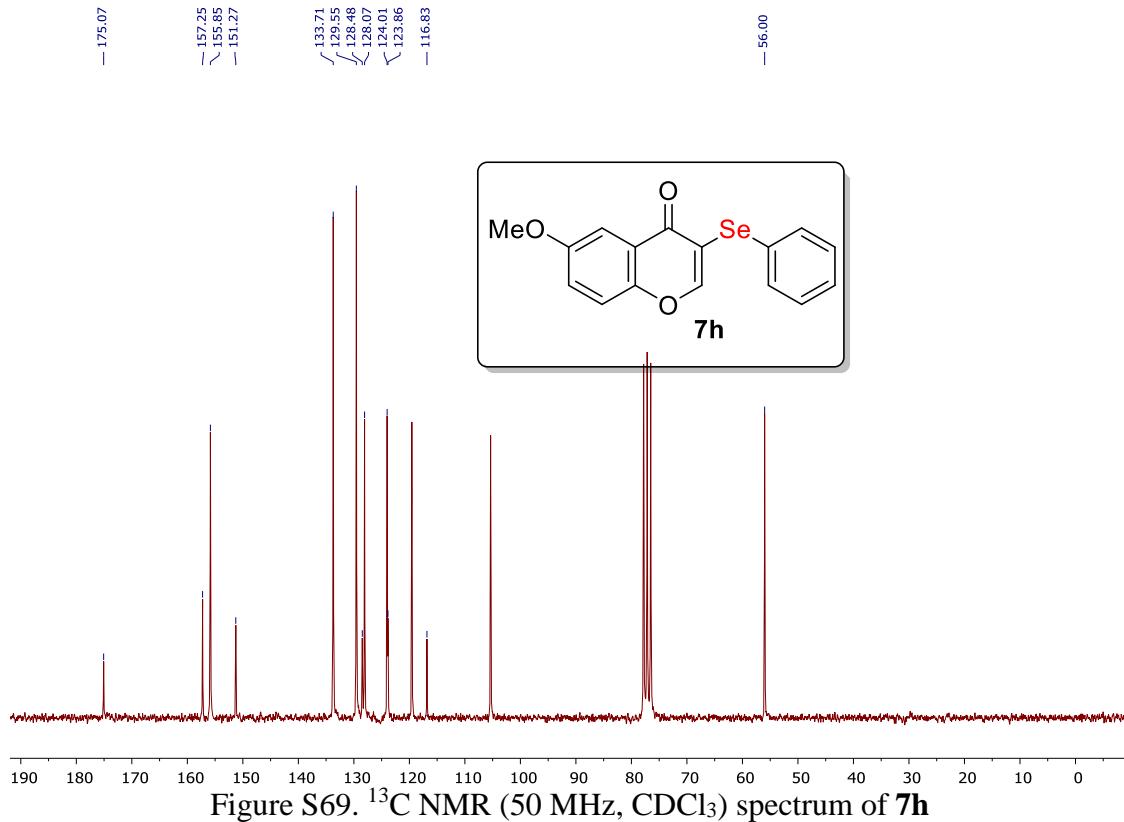
Figure S69. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7h**

7.87
7.31
7.29
7.14
7.11
7.09
7.08
7.01
6.99
6.98
6.95

3.59

MeO — 7ah

1.00
1.00
3.01
4.18
3.00

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
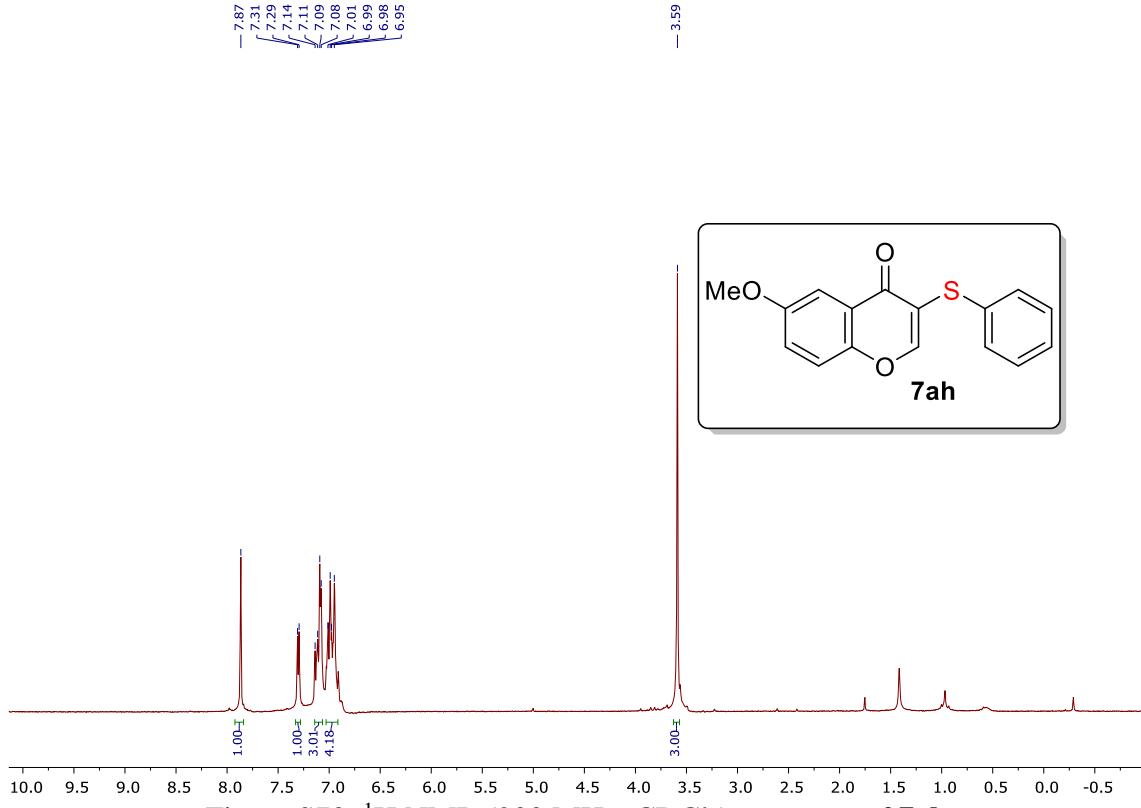
Figure S70. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7ah**

175.08
157.46
151.33
134.42
129.84
129.26
127.13
124.50
124.19
119.69
119.05
105.55
56.08

MeO — 7ah

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
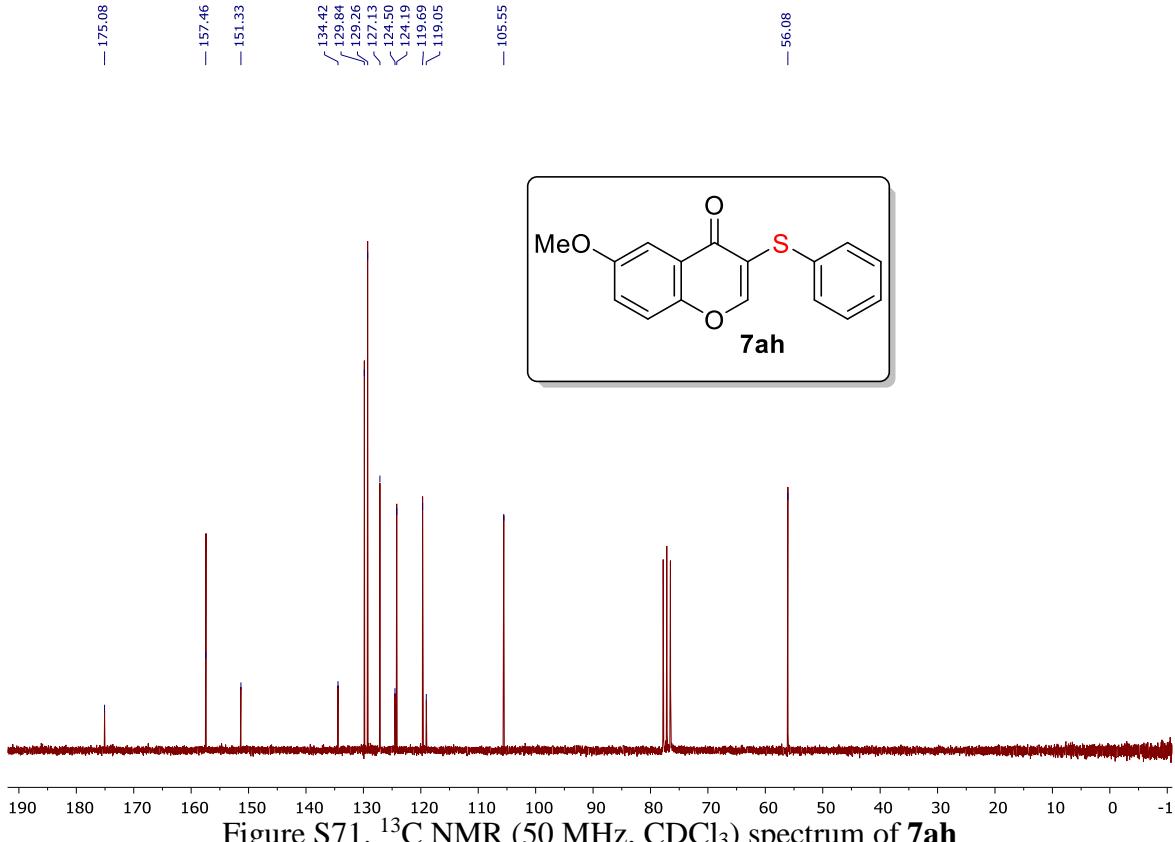
Figure S71. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7ah**

8.14
8.09
7.80
7.59
7.58
7.57
7.56
7.30
7.28
7.27
6.98
6.97
6.94
6.93
6.78
6.77

3.87

1.00
1.00
1.00
2.00
3.00
1.00
1.00

3.00

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
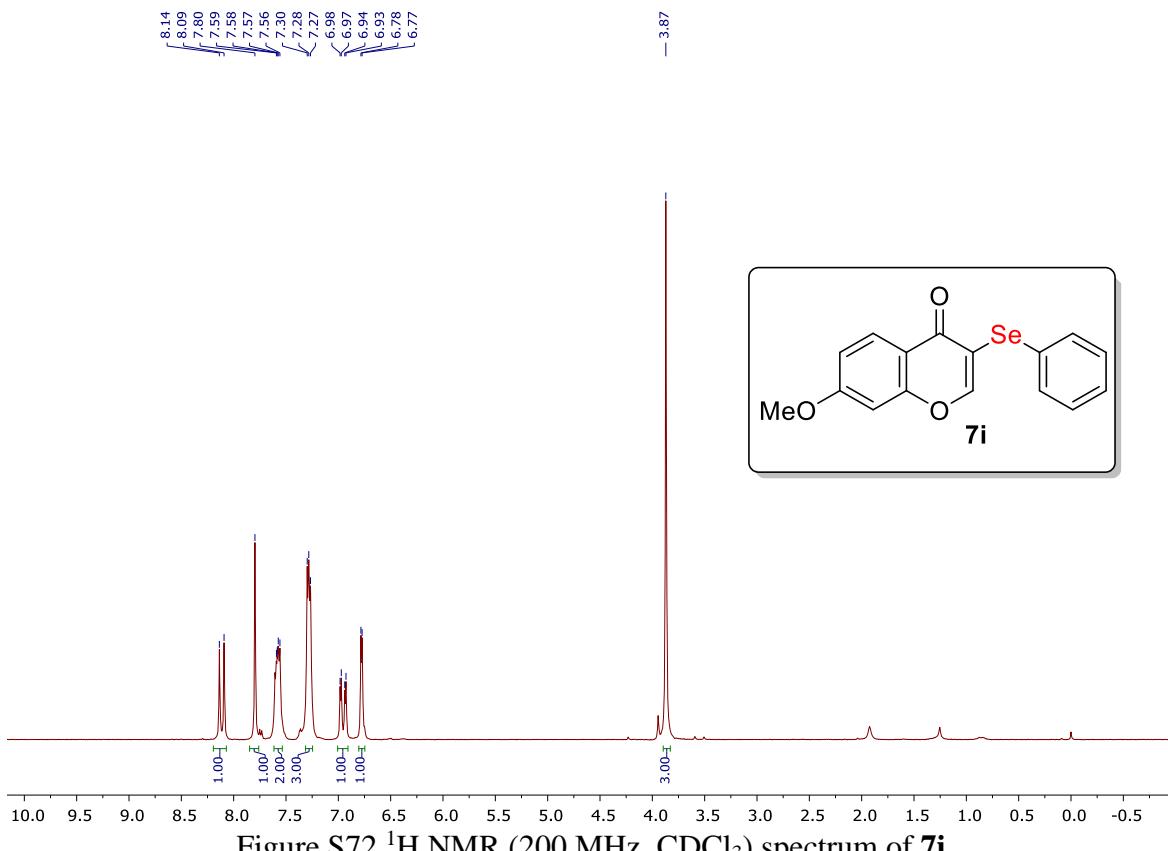
Figure S72. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7i**

174.51
164.21
158.16
155.35
133.76
129.54
128.40
128.06
127.75
117.81
117.11
114.95
100.23
55.93

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
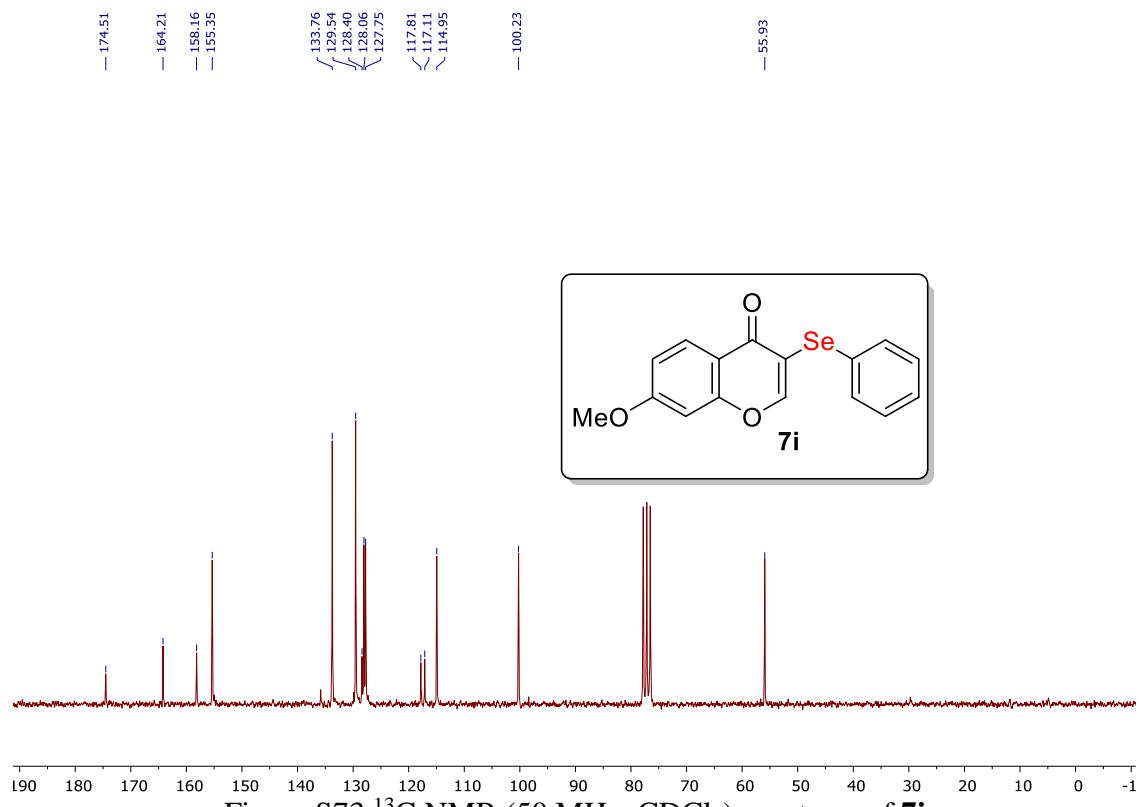
Figure S73. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7i**

8.15 8.10 8.05 7.40 7.39 7.36 7.35 7.31 7.30 7.26 7.23 7.19 6.99 6.98 6.95 6.94 6.83 6.81   3.88

0.97 0.97   5.00   1.00 1.00   3.01

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
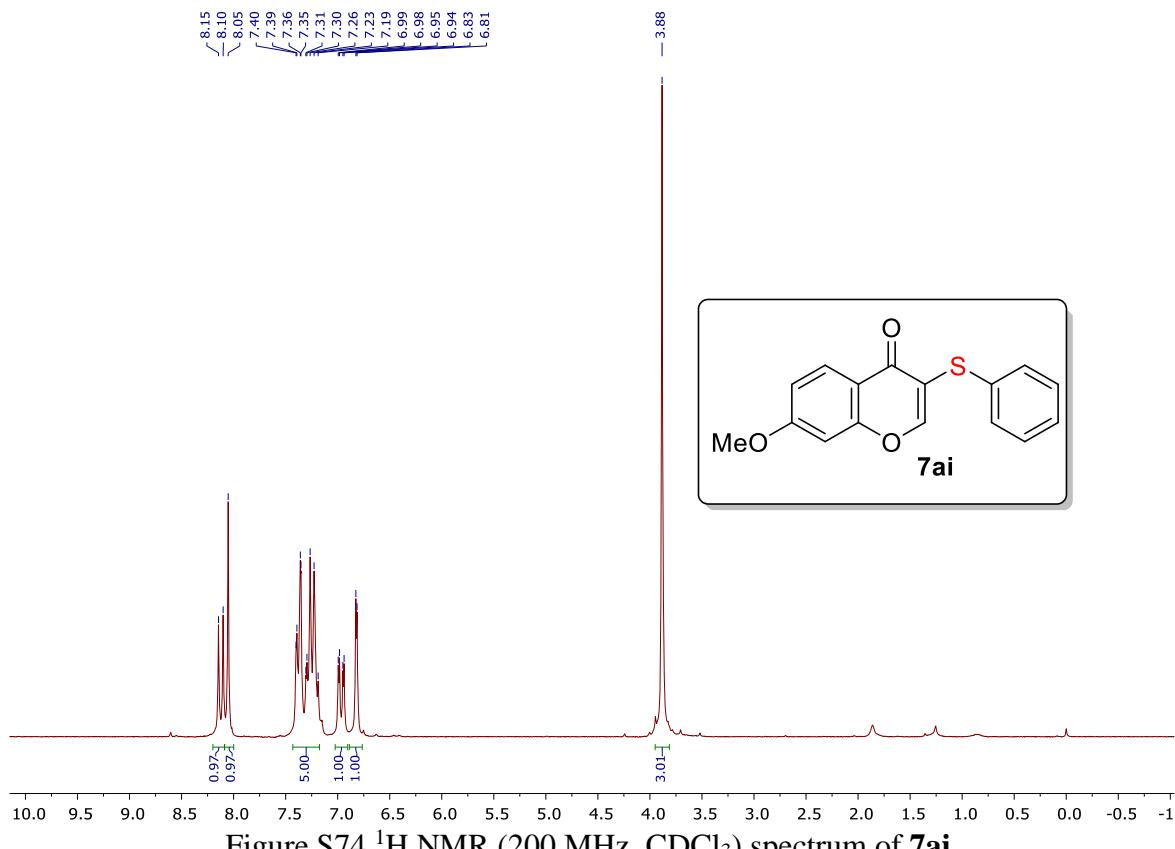
Figure S74. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7ai**

174.38   164.35   158.18 157.00   134.35 129.78 129.20 127.84 127.04   119.82 117.61 115.04   100.41   55.97

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
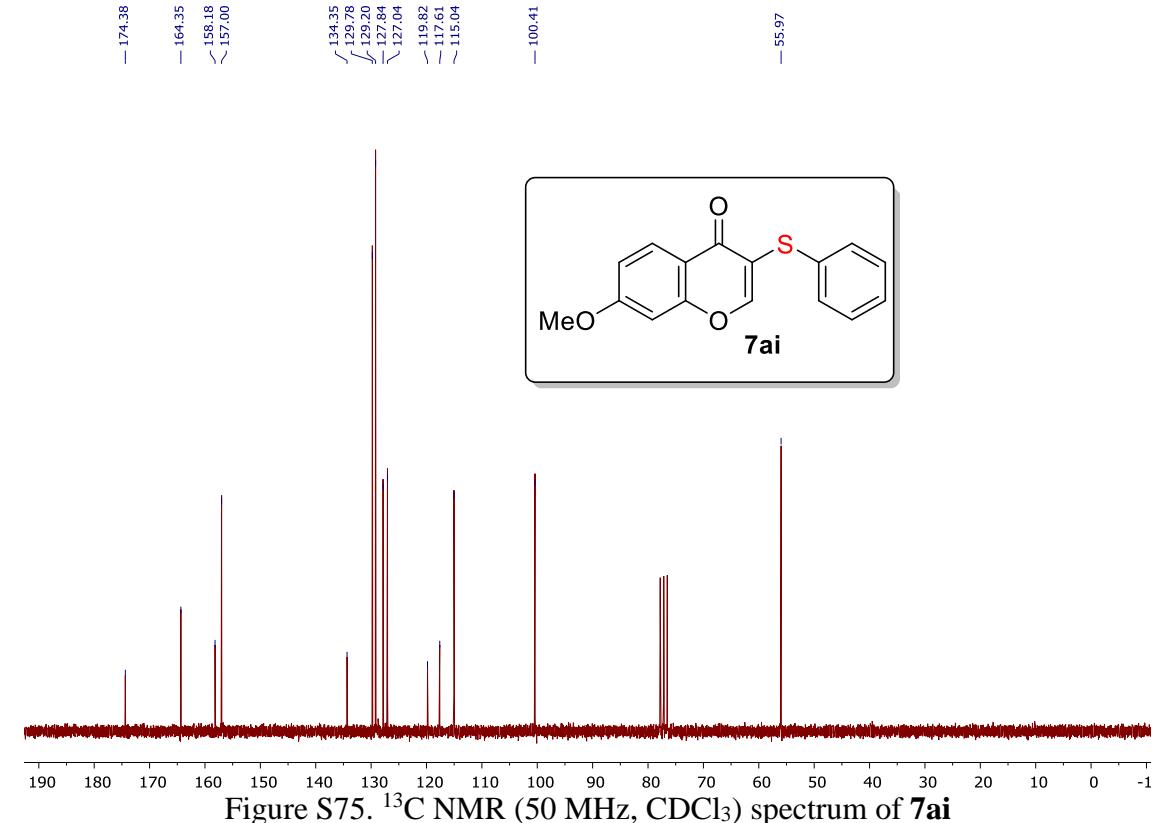
Figure S75. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7ai**
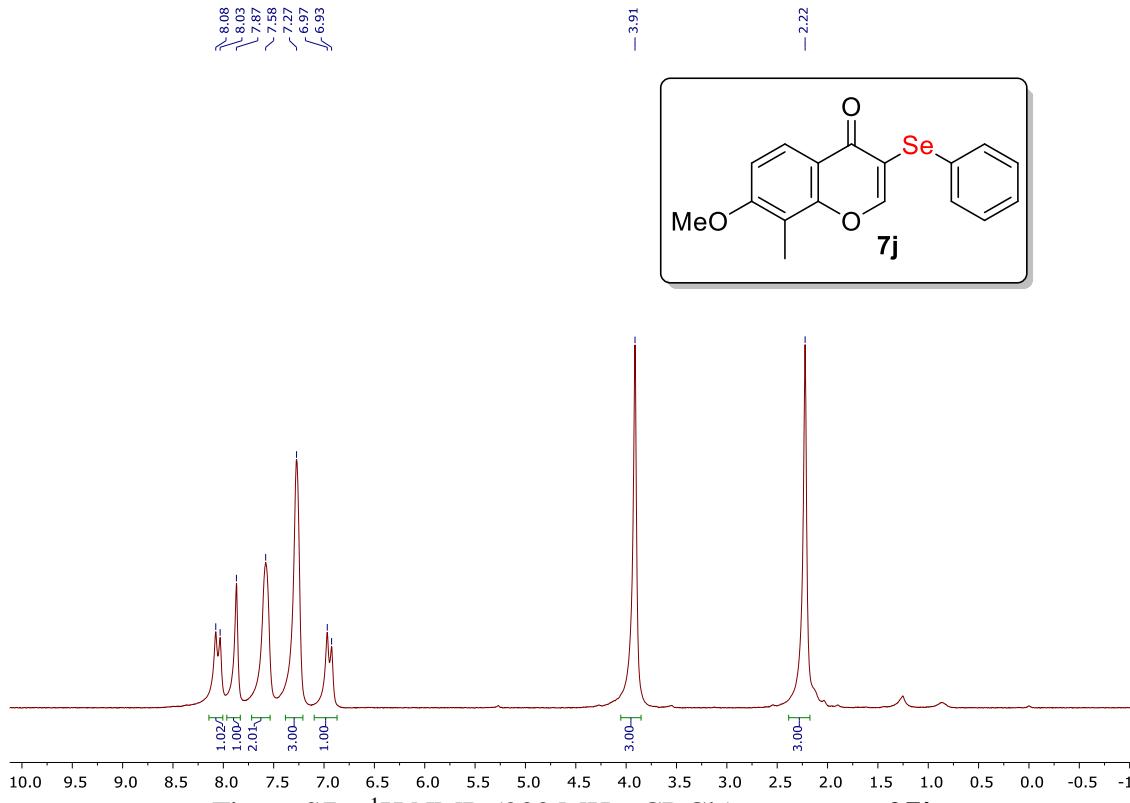
Figure S76. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7j**
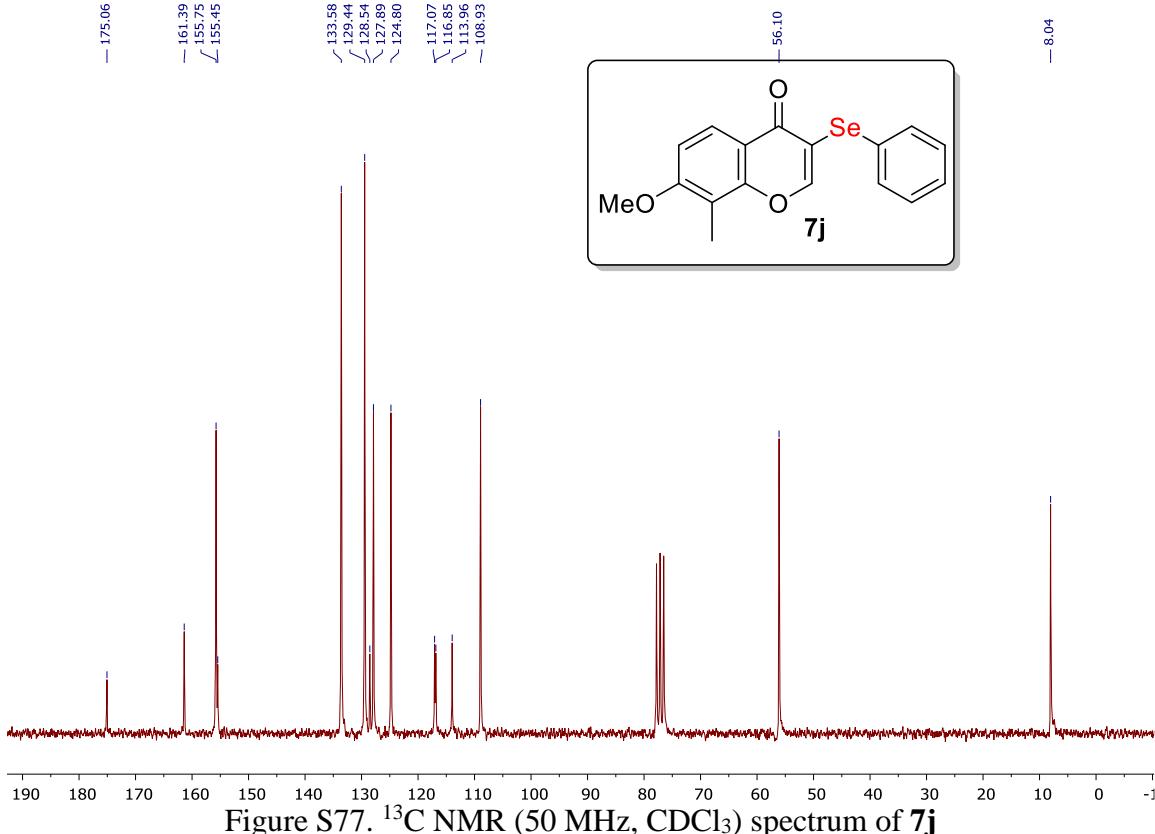
Figure S77. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7j**
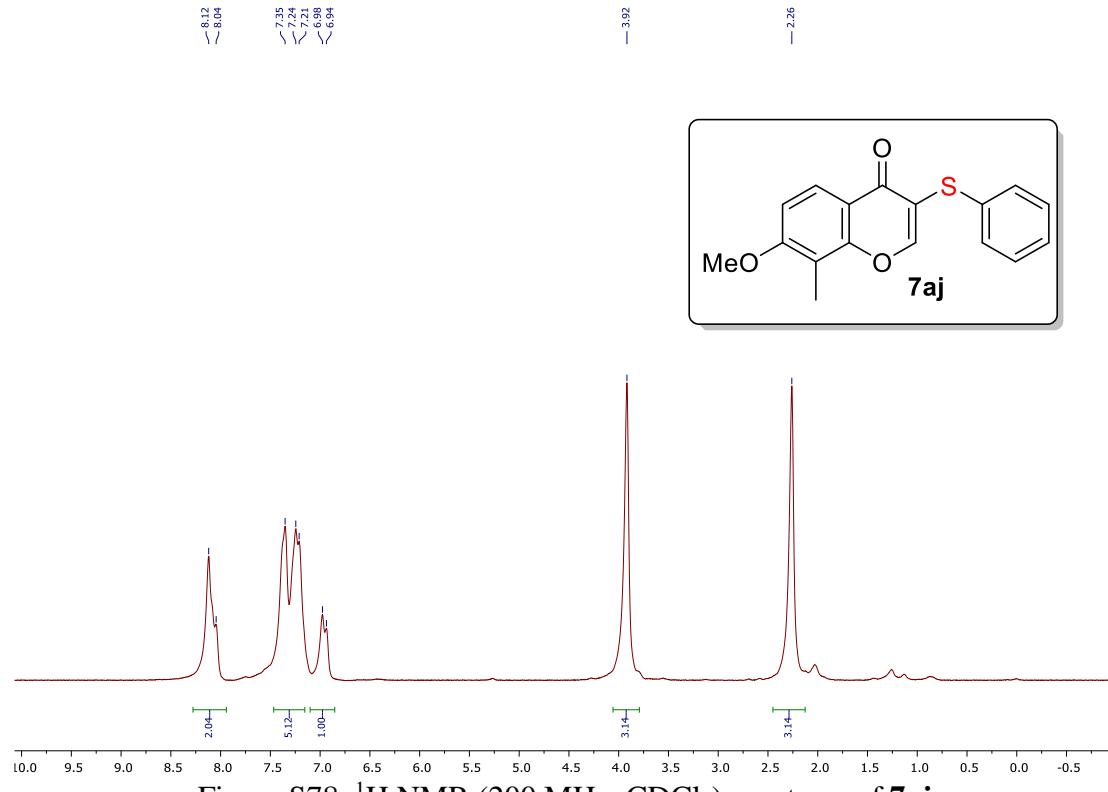
Figure S78. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7aj**
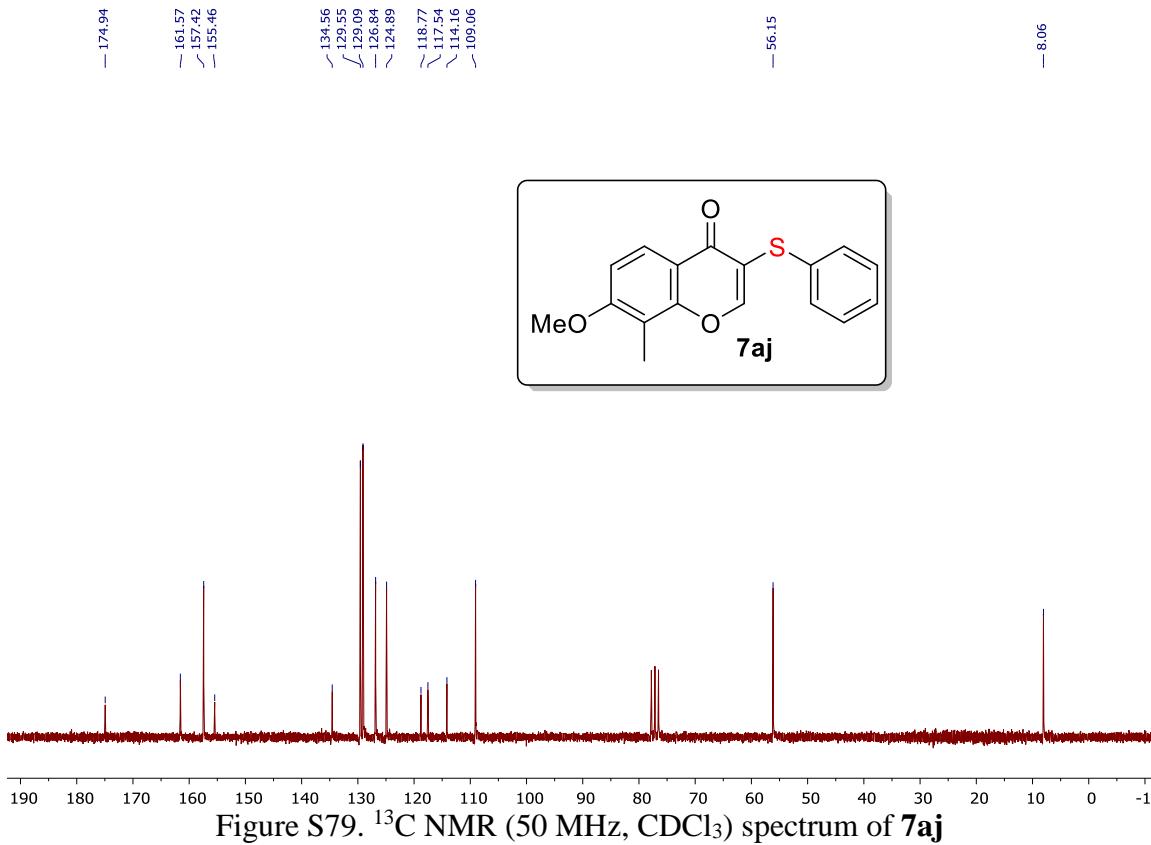
Figure S79. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7aj**
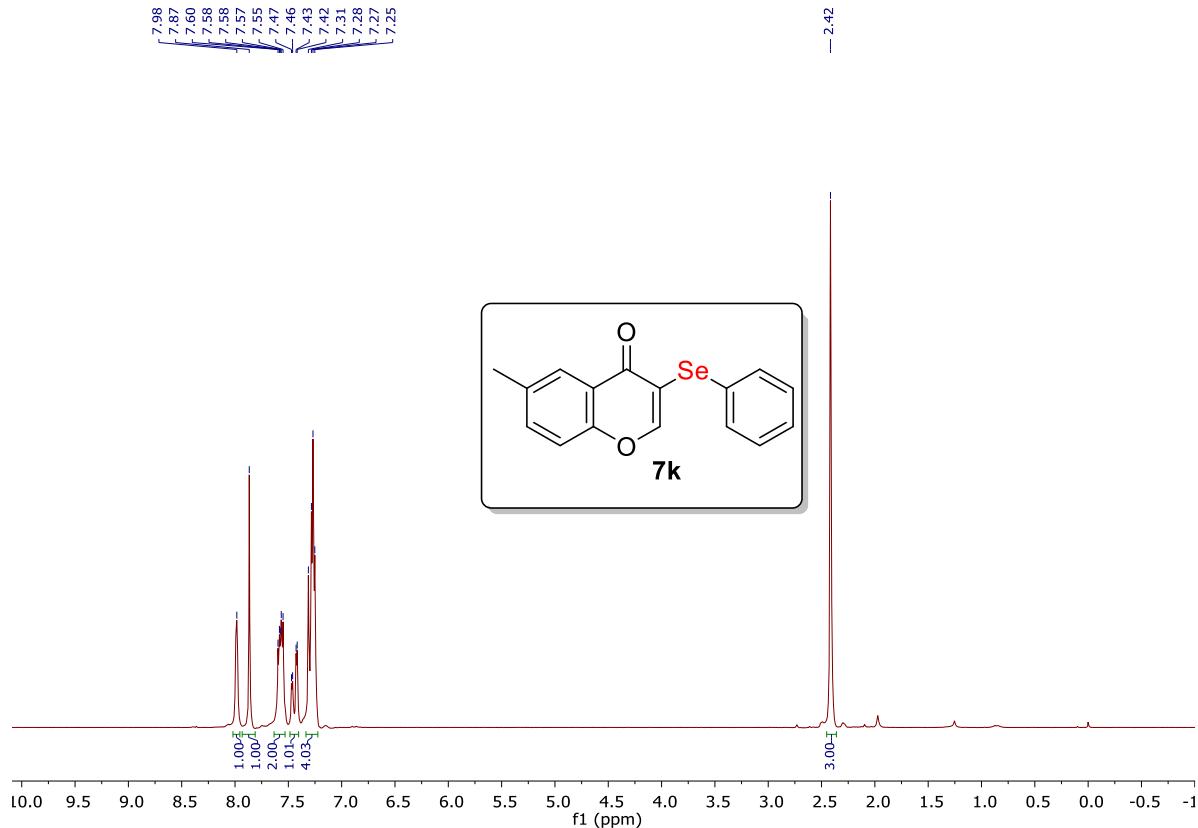
Figure S80. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7k**
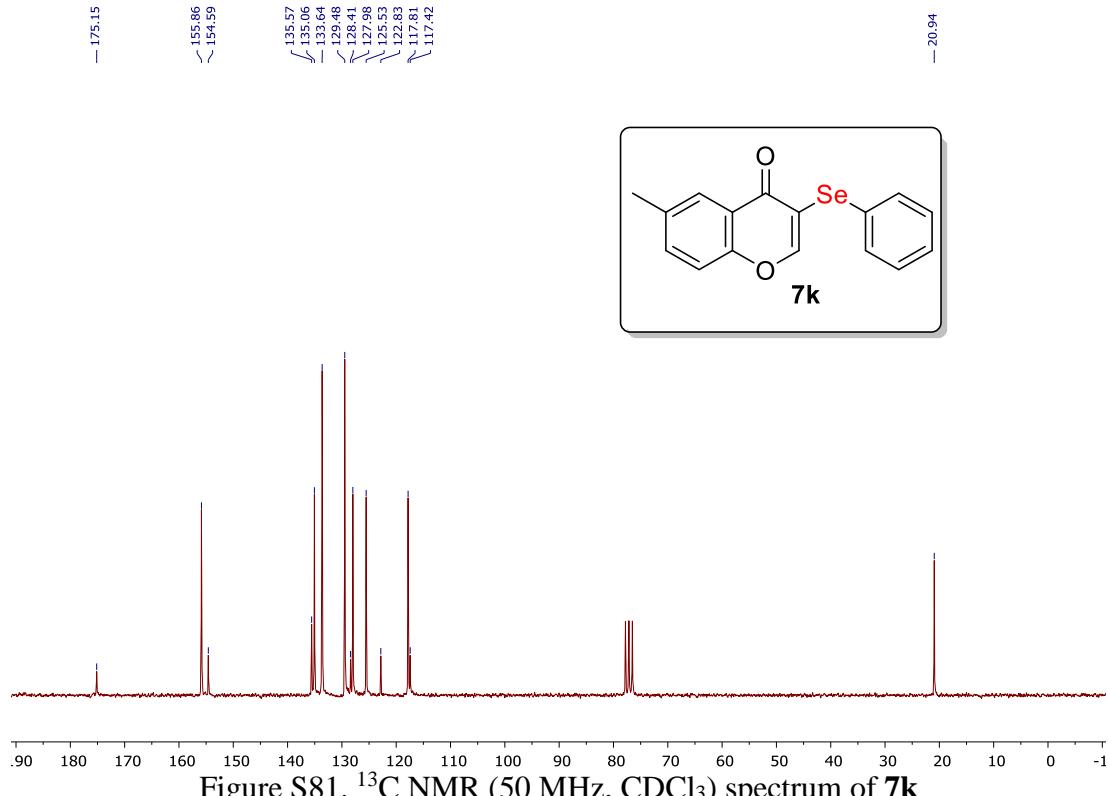
Figure S81. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7k**
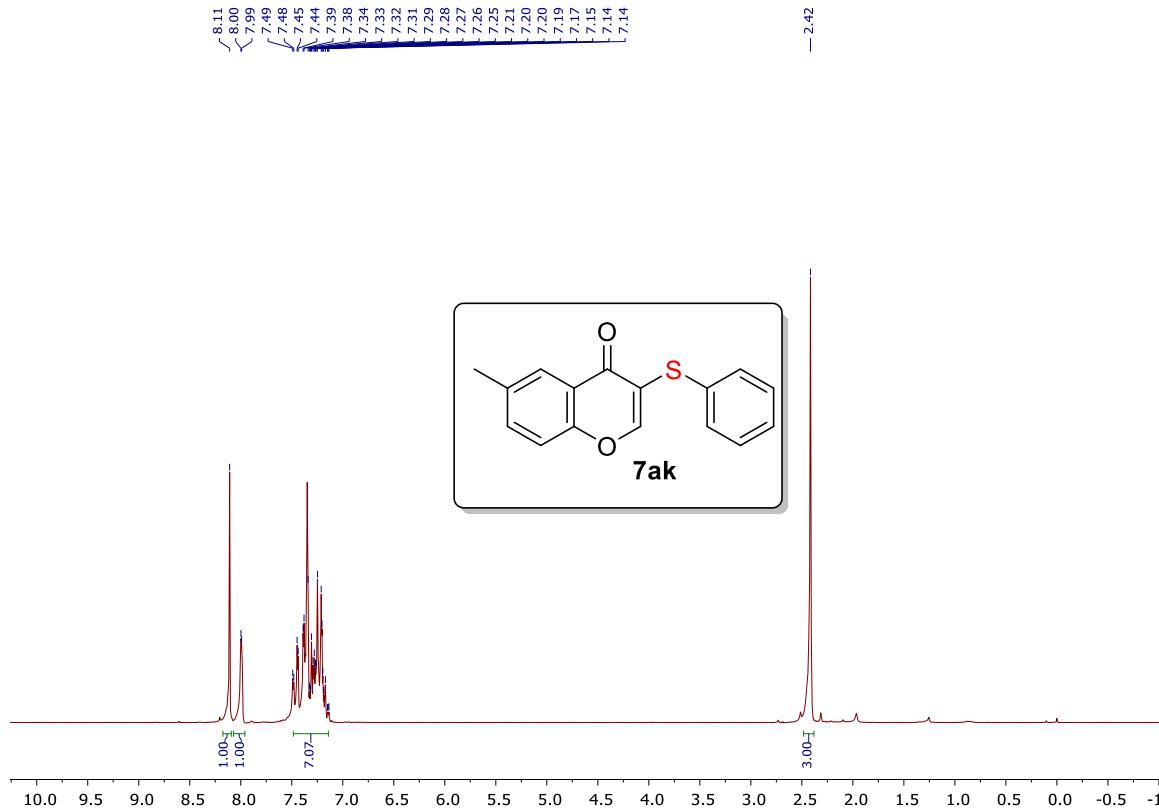
Figure S82. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7ak**
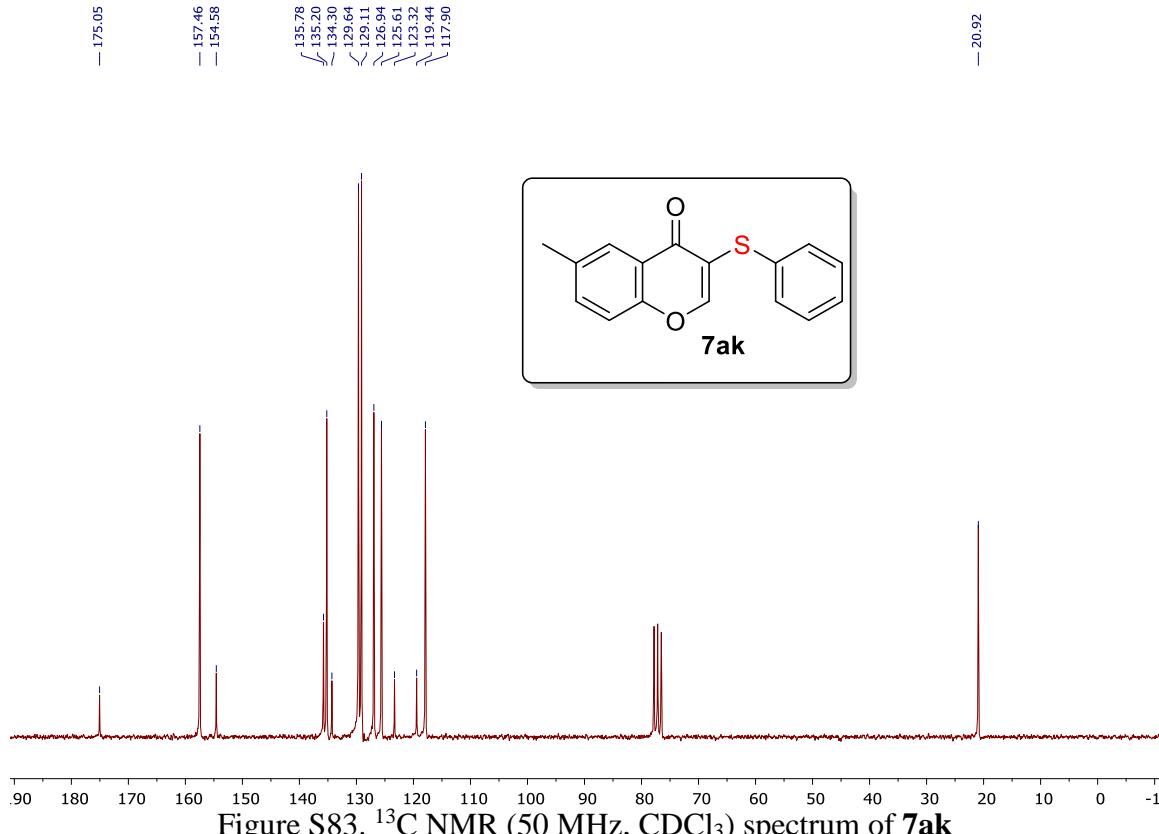
Figure S83. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7ak**
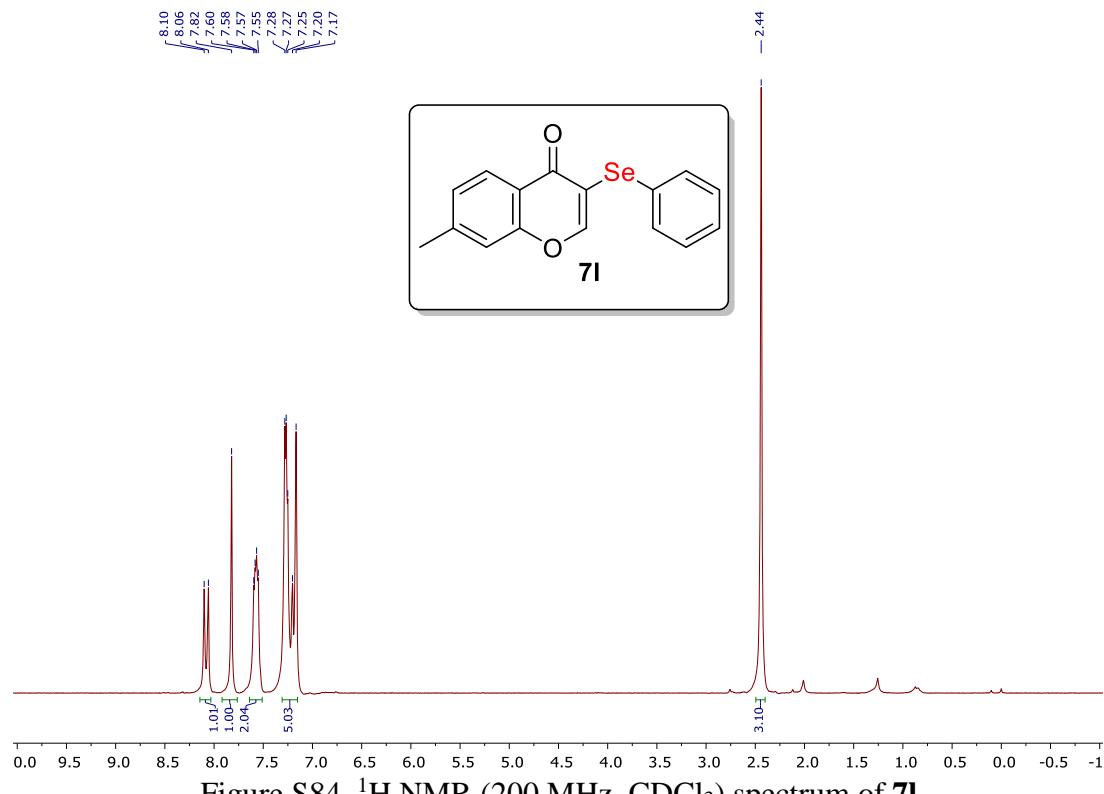
Figure S84. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7l**
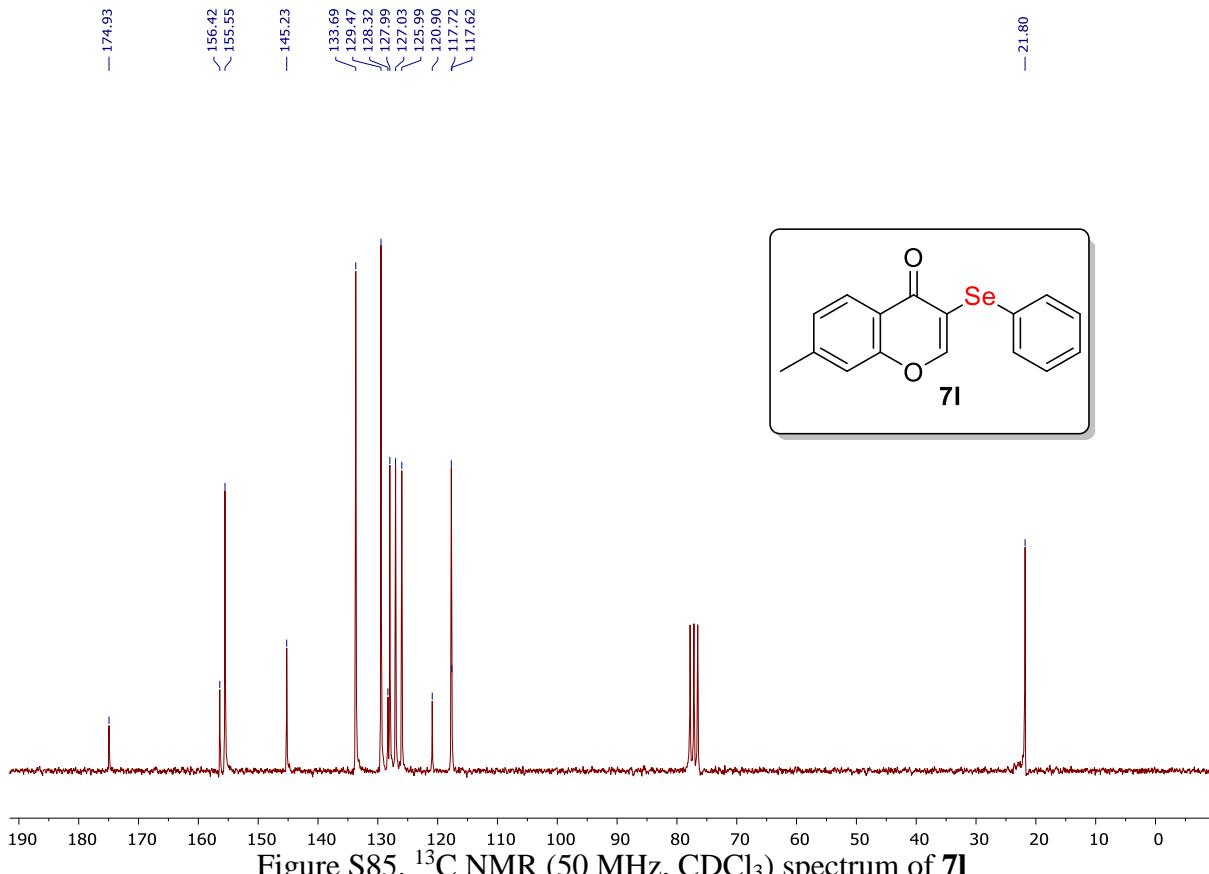
Figure S85. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7l**
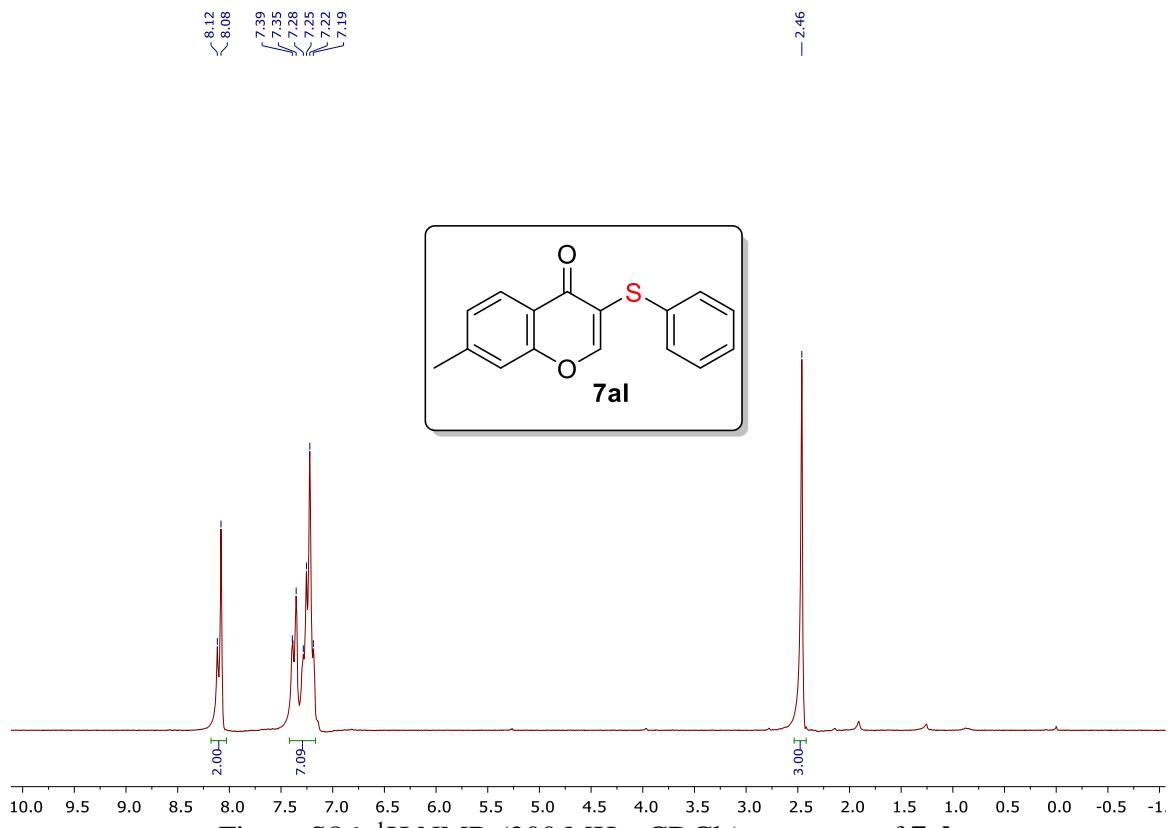
Figure S86. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7al**
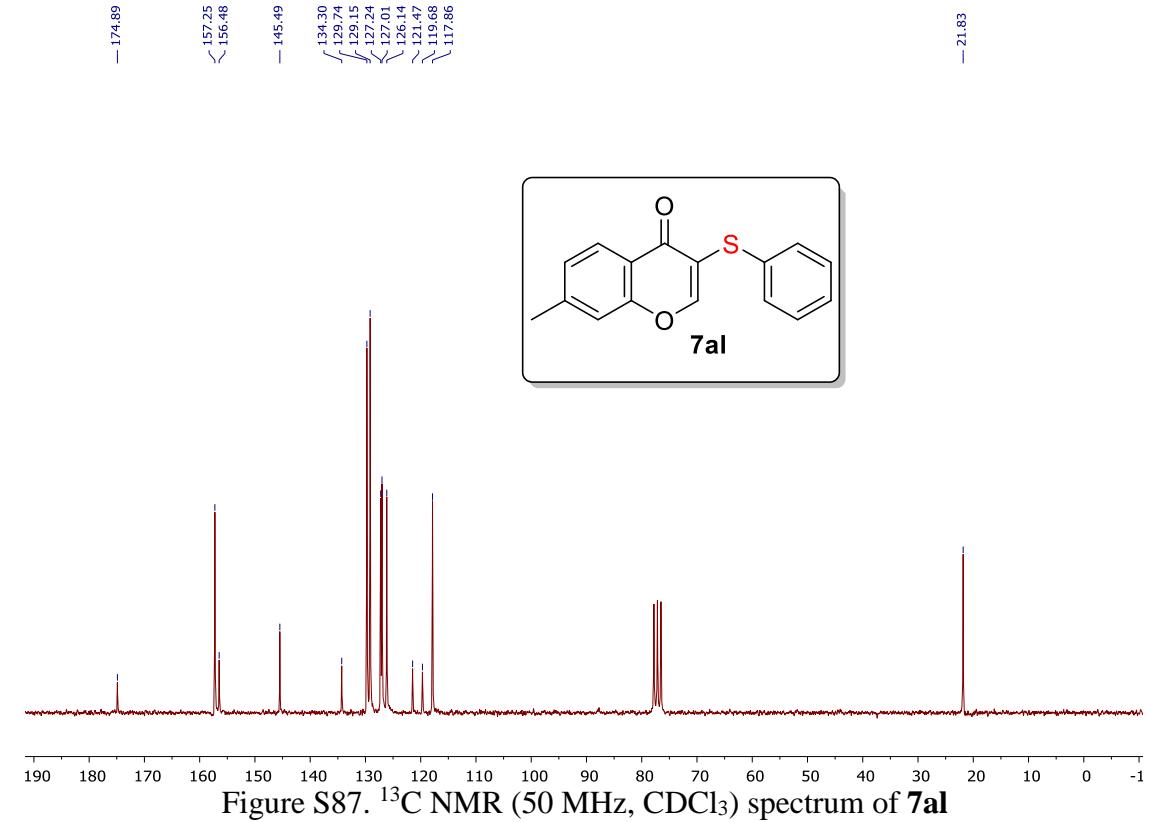
Figure S87. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7al**

8.47
8.43
8.23
8.20
8.16
7.96
7.95
7.92
7.81
7.77
7.73
7.72
7.72
7.70
7.68
7.67
7.48
7.45
7.35
7.32
7.28
7.26
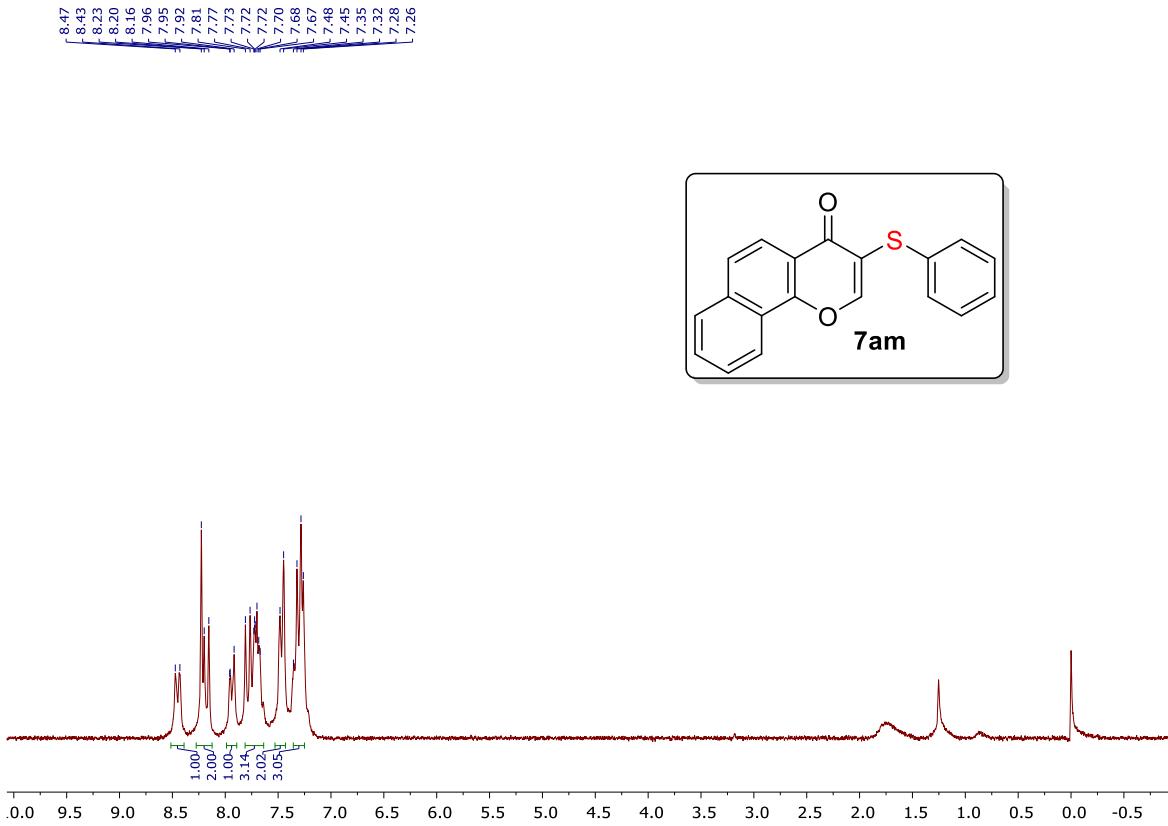
Figure S88. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7am**

174.98

153.86
135.80
132.20
129.50
128.46
128.17
127.67
127.30
125.71
123.87
122.22
121.12
120.26
119.23
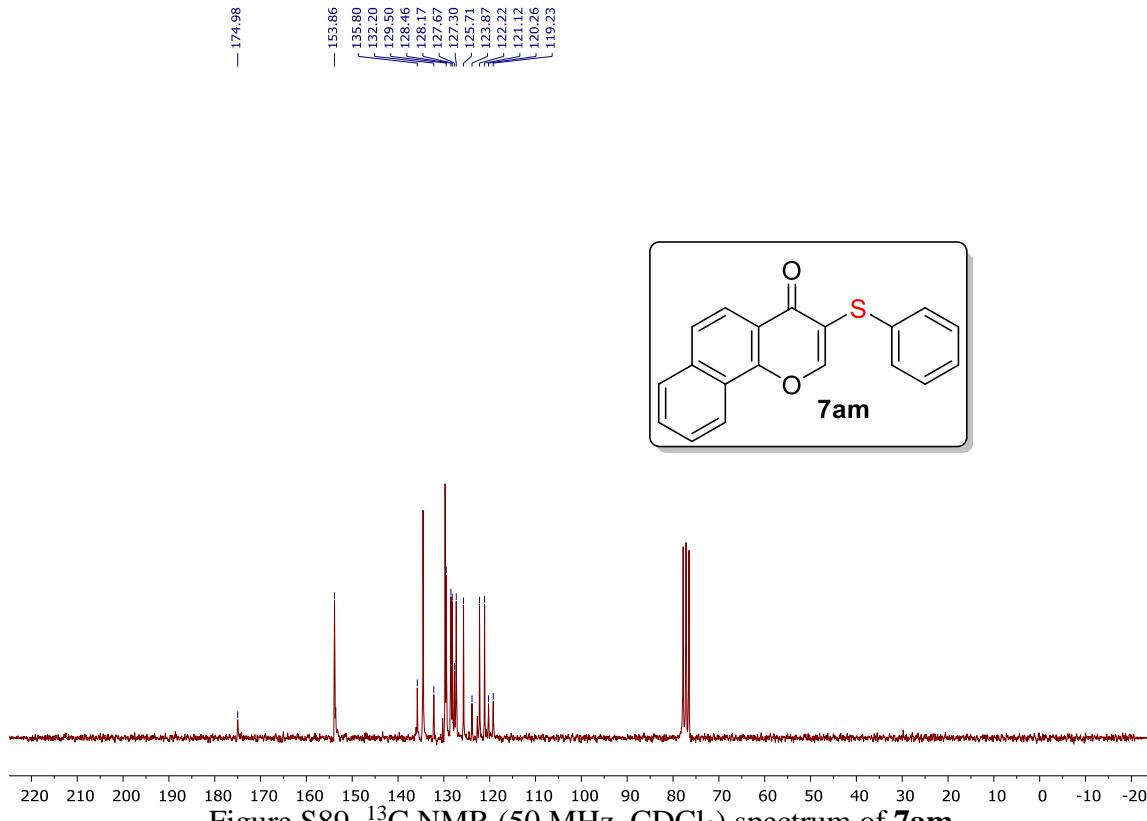
Figure S89. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7am**

8.43 8.39 8.19 8.16 8.12 7.92 7.91 7.88 7.77 7.72 7.70 7.67 7.66 7.47 7.44 7.31 7.27

1.00 2.00 1.00 3.00 5.02

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
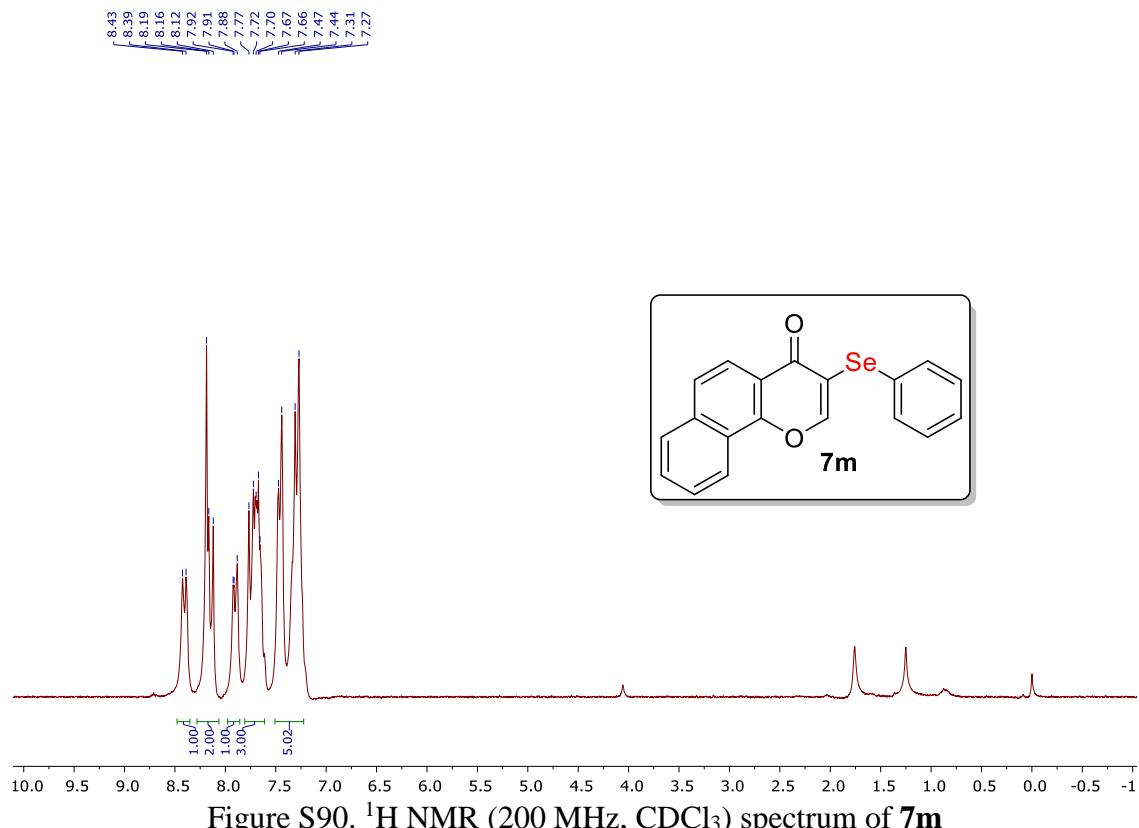
Figure S90. ^{1}H NMR (200 MHz, CDCl$_3$) spectrum of **7m**

174.82   155.54 153.85   135.90 133.55 130.67 129.61 129.38 128.19 127.51 127.41 125.88 123.86 122.31 122.23 121.11 119.87

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
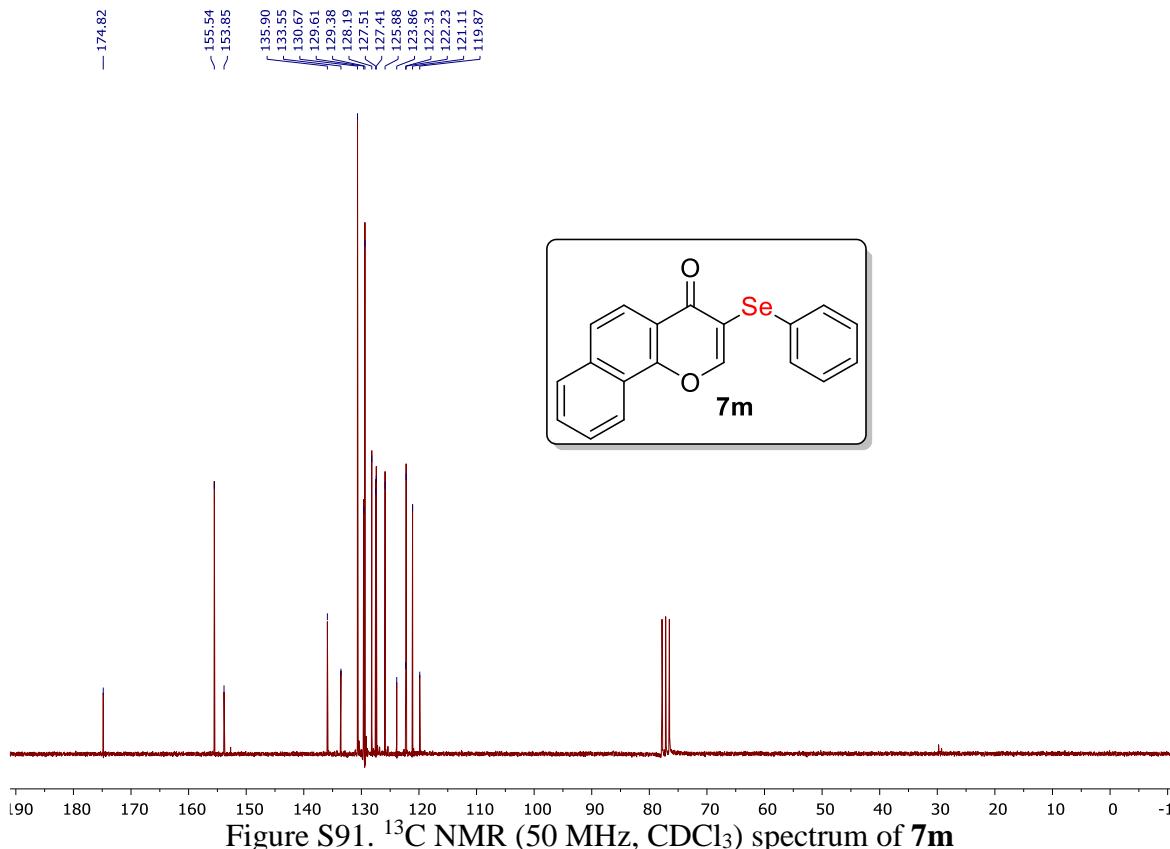
Figure S91. ^{13}C NMR (50 MHz, CDCl$_3$) spectrum of **7m**