Supporting information for the paper entitled:

Lewis Acids Promoted 3+2 Cycloaddition of Oxaziridines and Cyclic Allylic Alcohols through Carbonyl Imine Intermediates

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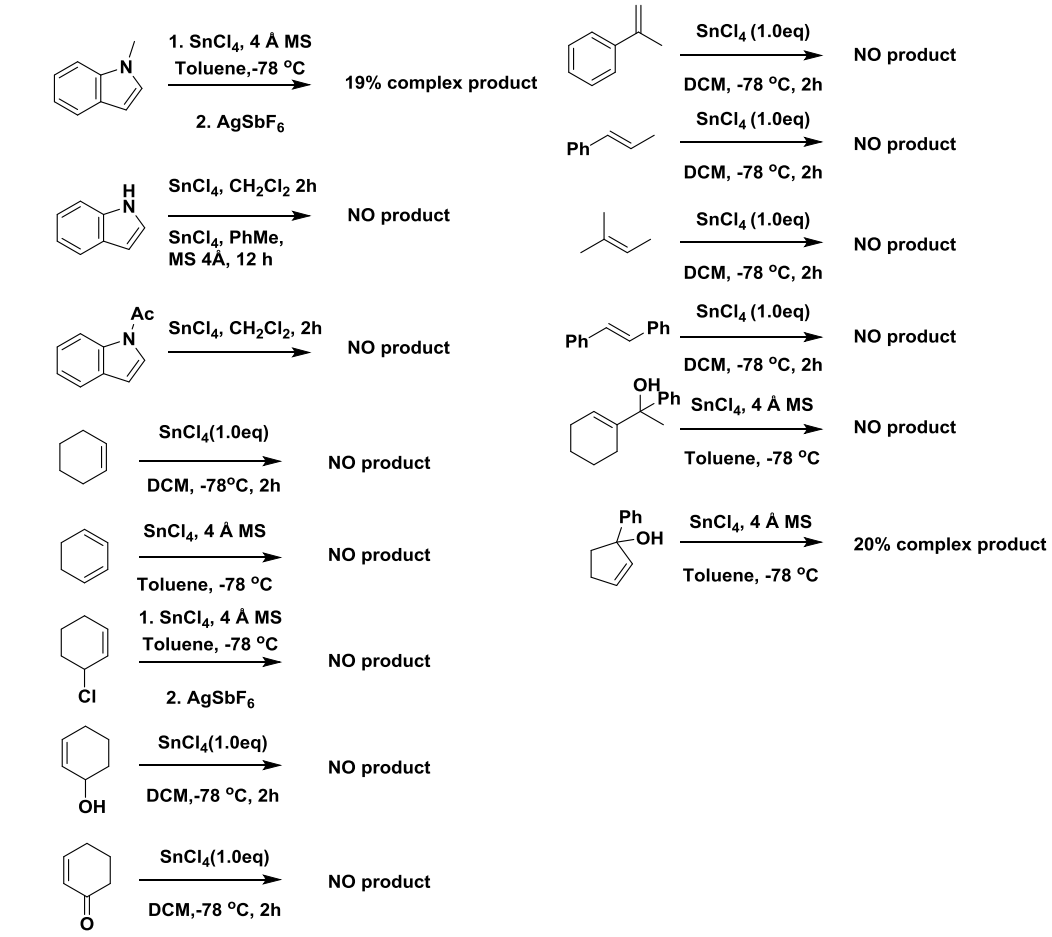
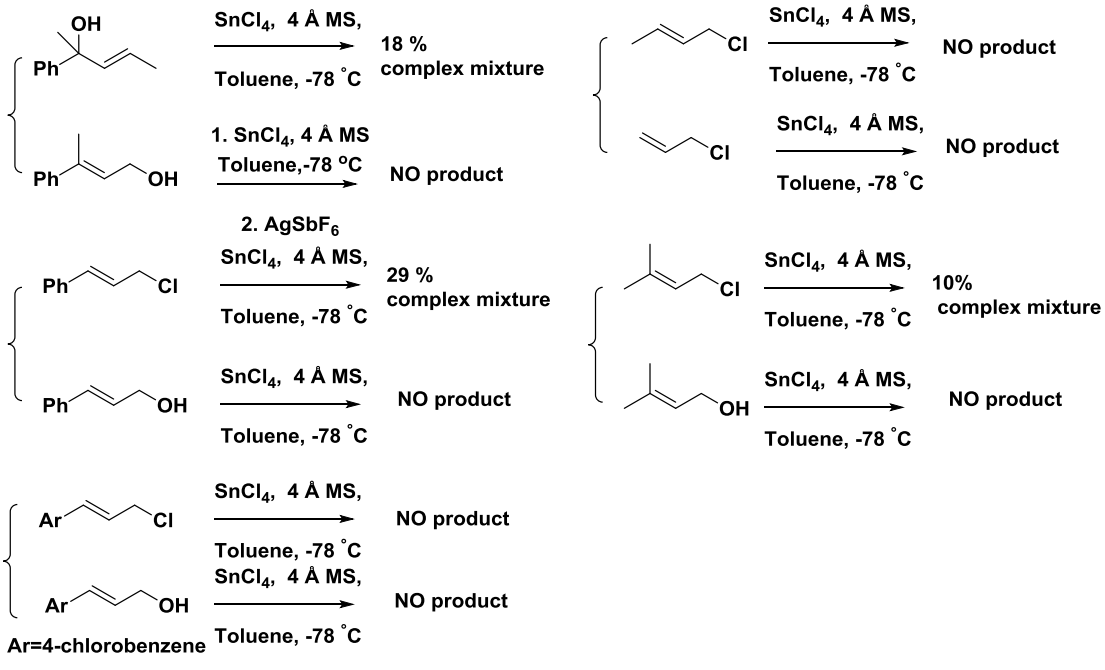
Scheme S1: Alkenes that are not suitable substrates for this reaction

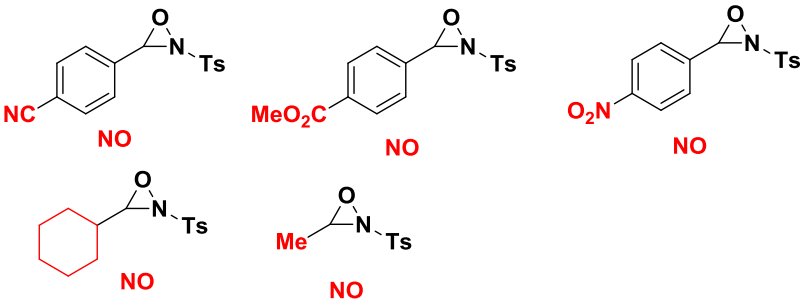
The following substrates have been tried but failed to yield desired products.



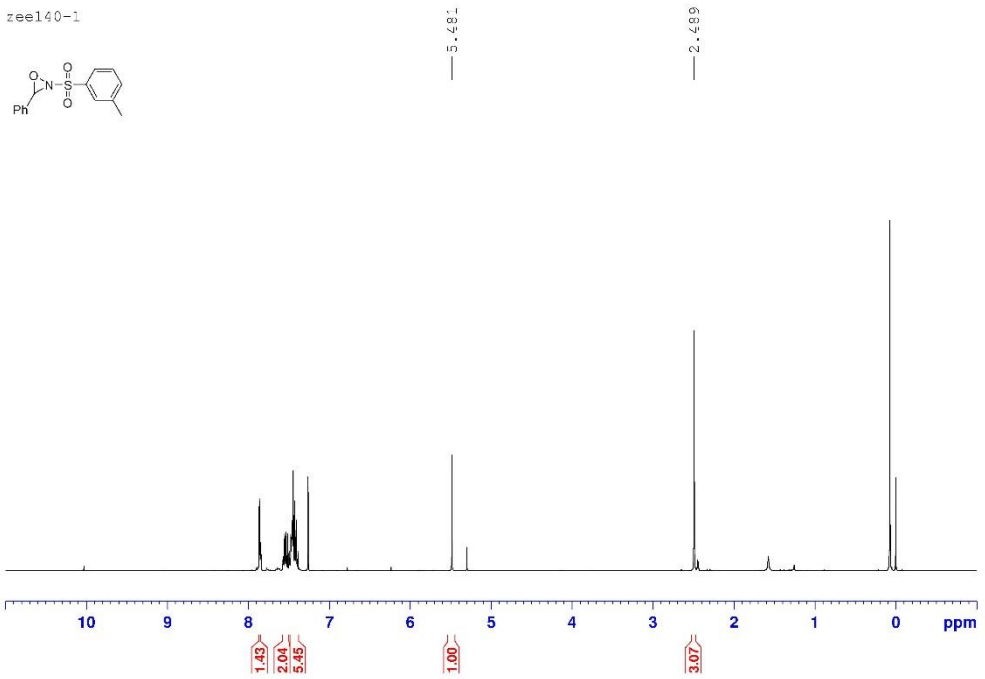


Scheme S2: Oxaziridines that are not suitable substrates for this reaction

The following substrates have been tried but failed to yield desired products.



I. Original spectra of ^{1}H and ^{13}C NMR



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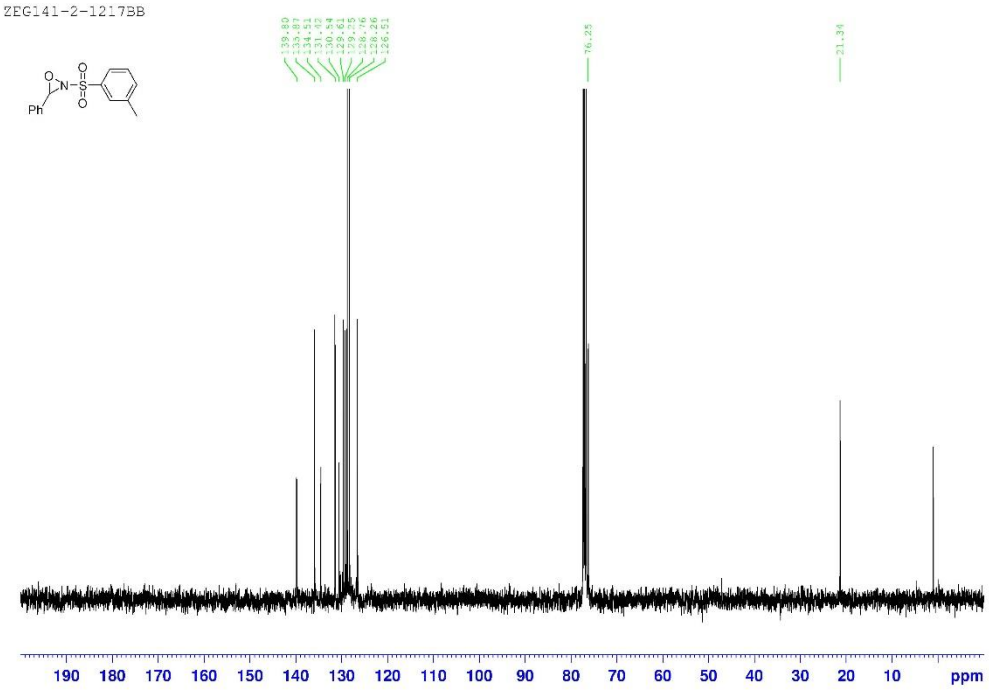
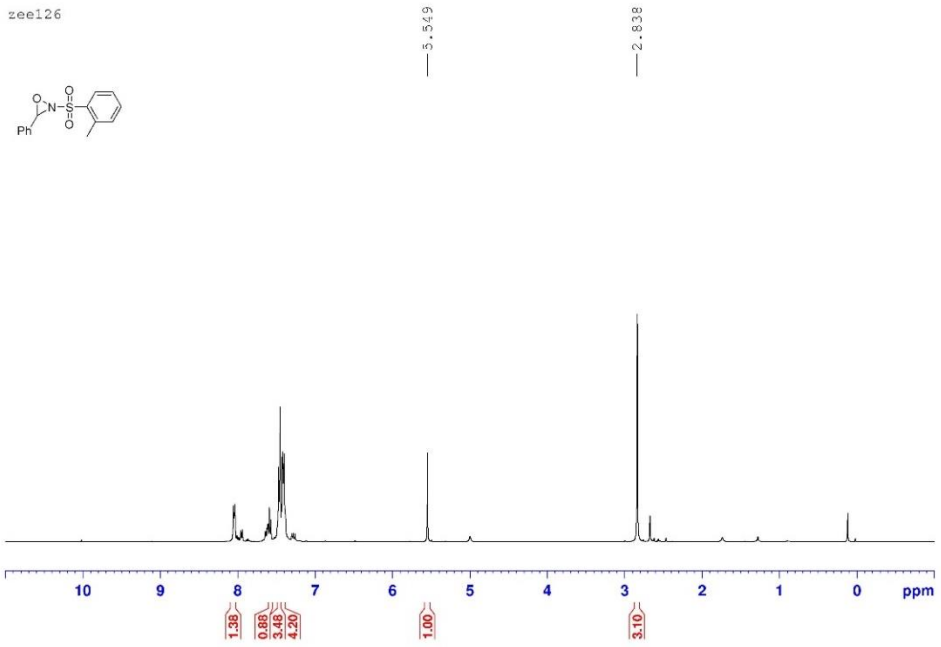
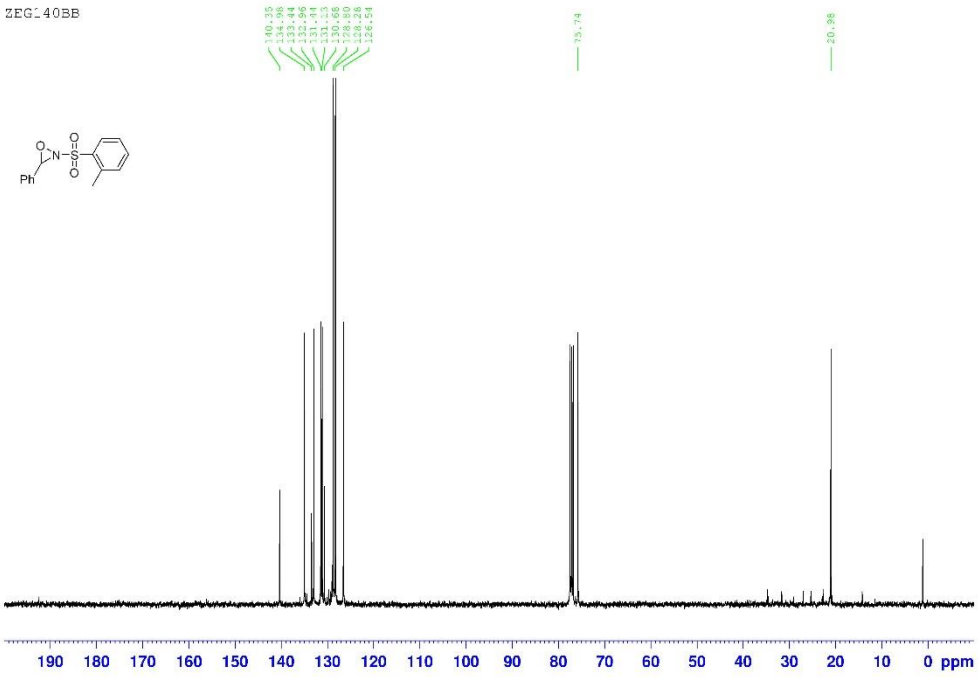


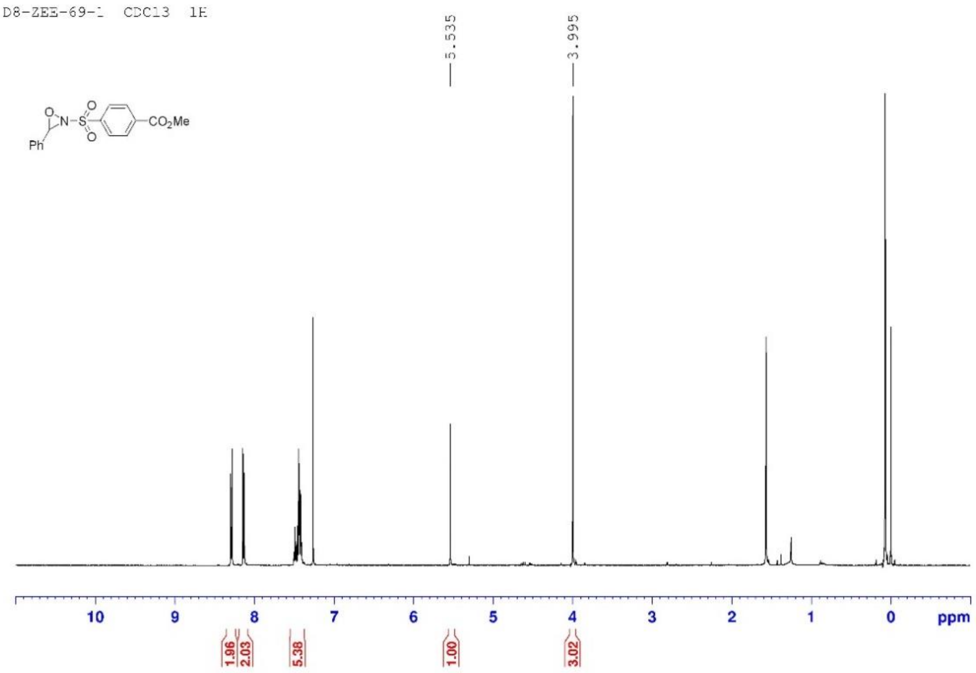
1b


zee126
5.549
2.838
Ph
10
9
8
7
6
5
4
3
2
1
0
ppm
1.38
0.88
3.48
4.20
1.00
3.10

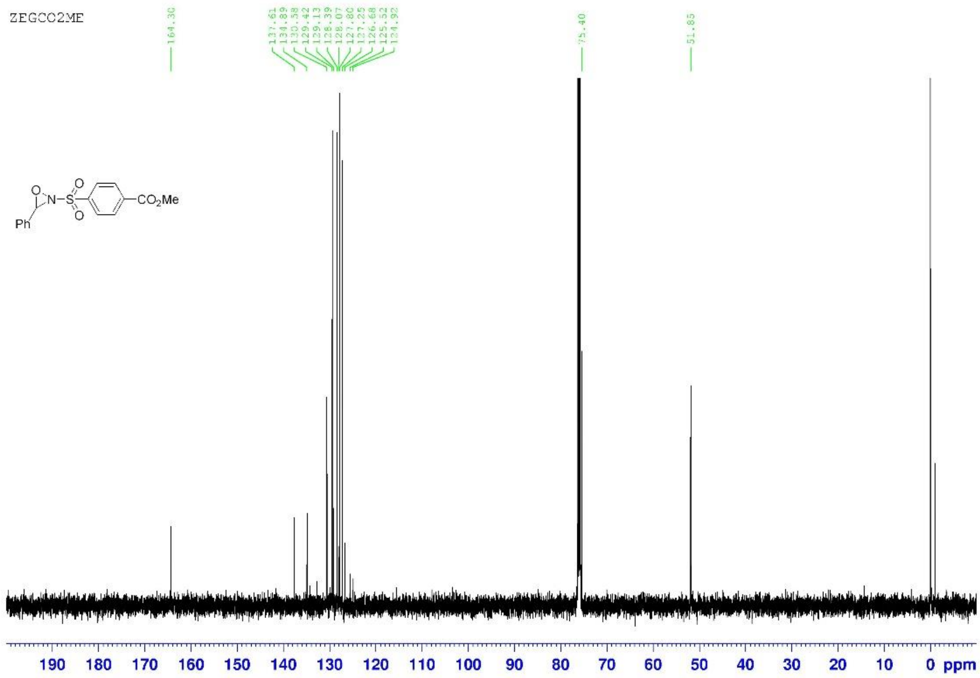
1c


ZEG140BB
140.35
134.96
133.44
132.96
131.74
131.15
130.68
128.80
128.28
126.54
75.74
20.98
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

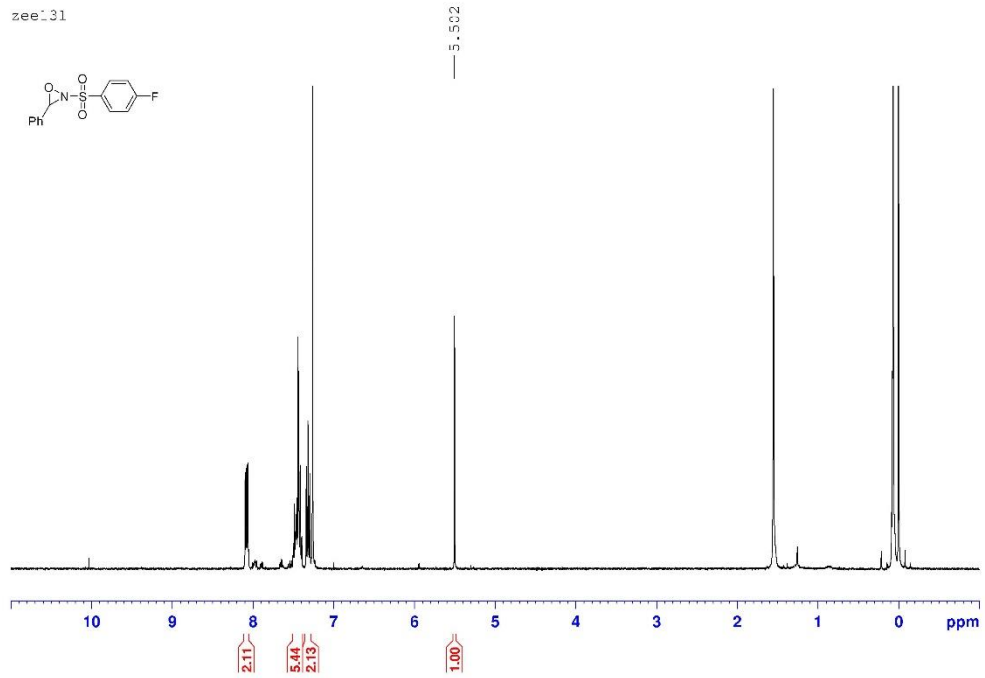
1c


D8-ZEE-69-1 CDCl3 1H
5.535
3.995
CO2Me
Ph
ppm
1.96
2.03
5.38
1.00
3.02

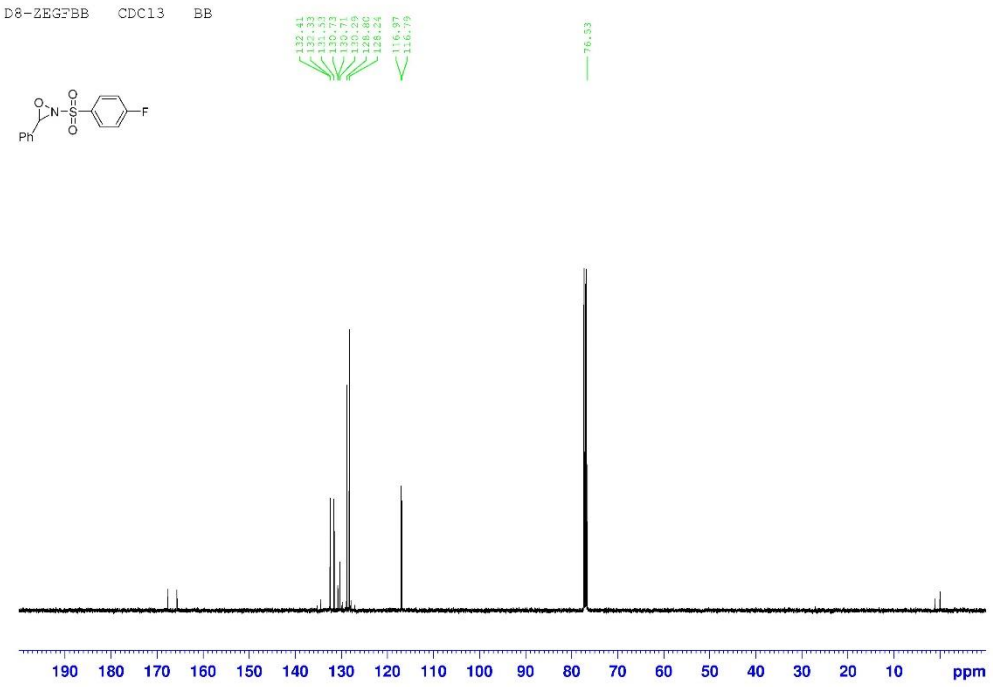
1f


ZEGCO2ME
164.30
75.40
51.85
CO2Me
Ph
ppm

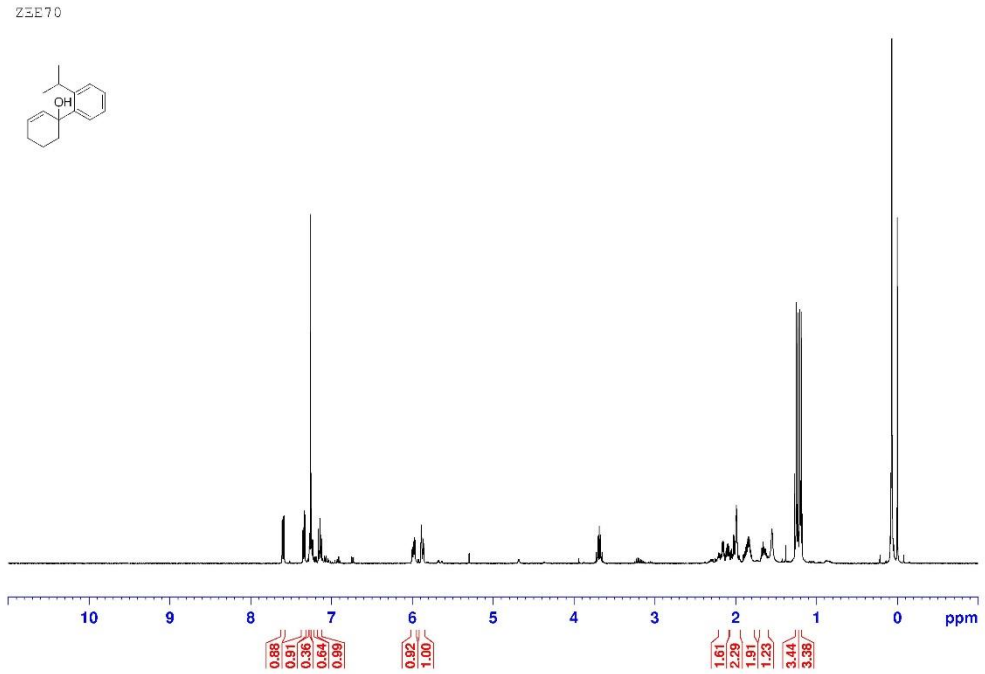
1f


zee_31
5.522
Ph
F
10
9
8
7
6
5
4
3
2
1
0
ppm
2.11
5.44
2.13
1.00

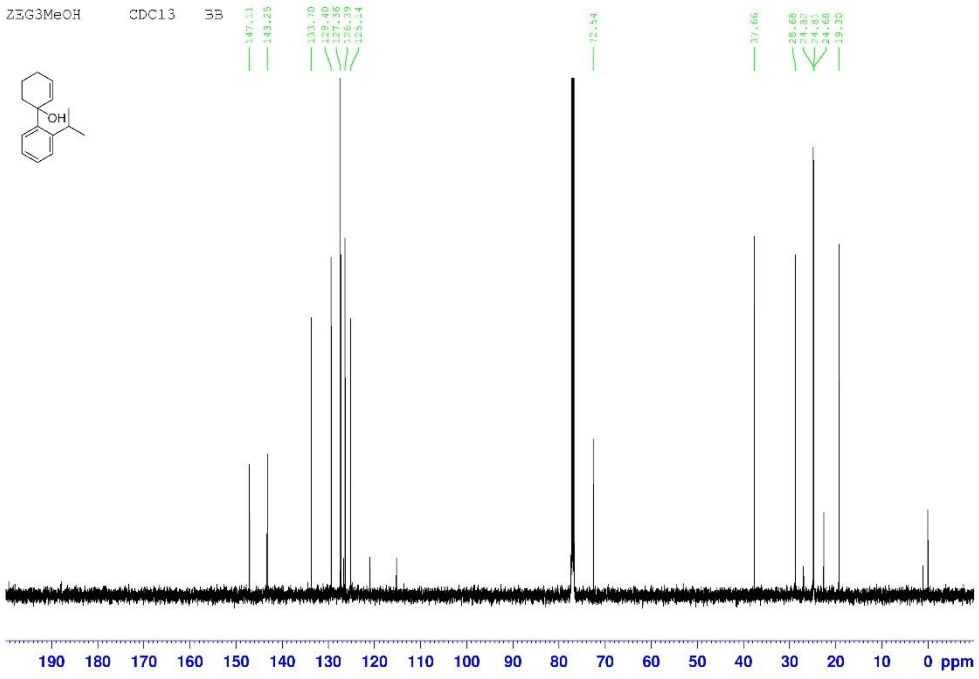
1g


D8-ZEGFBB CDC13 BB
132.41
132.33
131.33
130.73
130.71
130.29
129.60
128.24
116.97
116.79
76.53
Ph
F
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

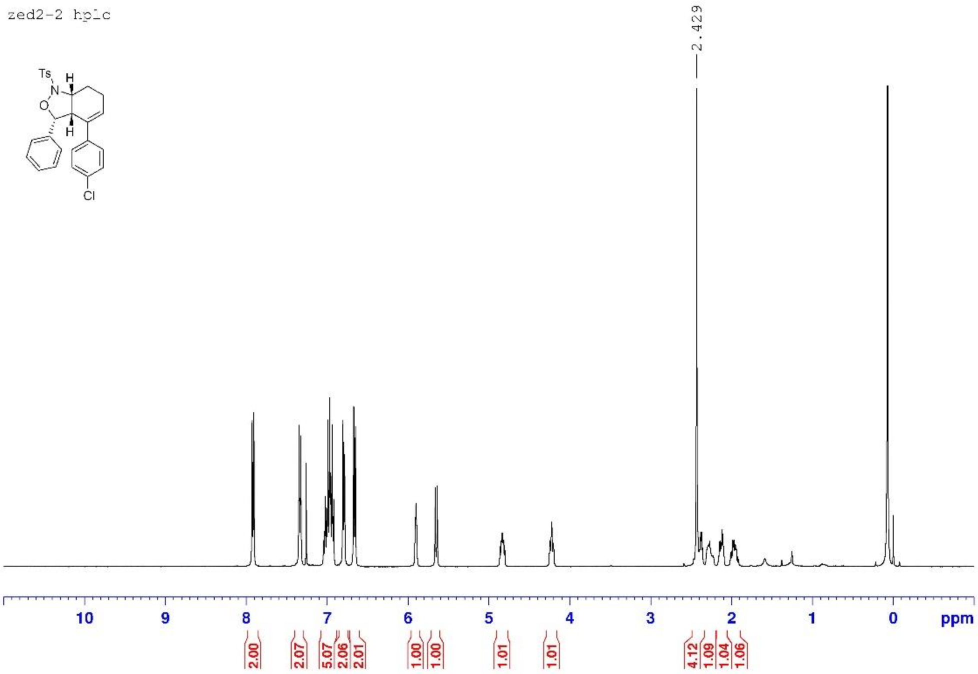
1g


ZEE70
OH
10
9
8
7
6
5
4
3
2
1
0
ppm
0.88
0.91
0.36
0.64
0.99
0.92
1.00
1.61
2.29
1.91
1.23
3.44
3.38

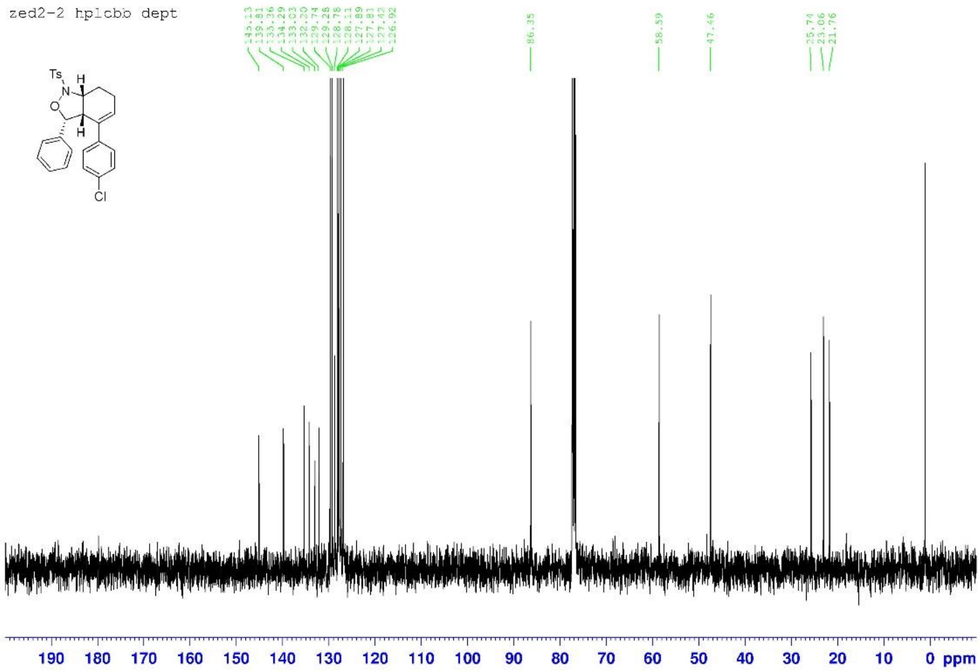
2j


ZEG3MeOH
CDCl3
BB
147.11
143.25
133.10
129.40
127.36
126.39
125.14
72.54
37.66
28.68
24.82
24.68
19.30
OH
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

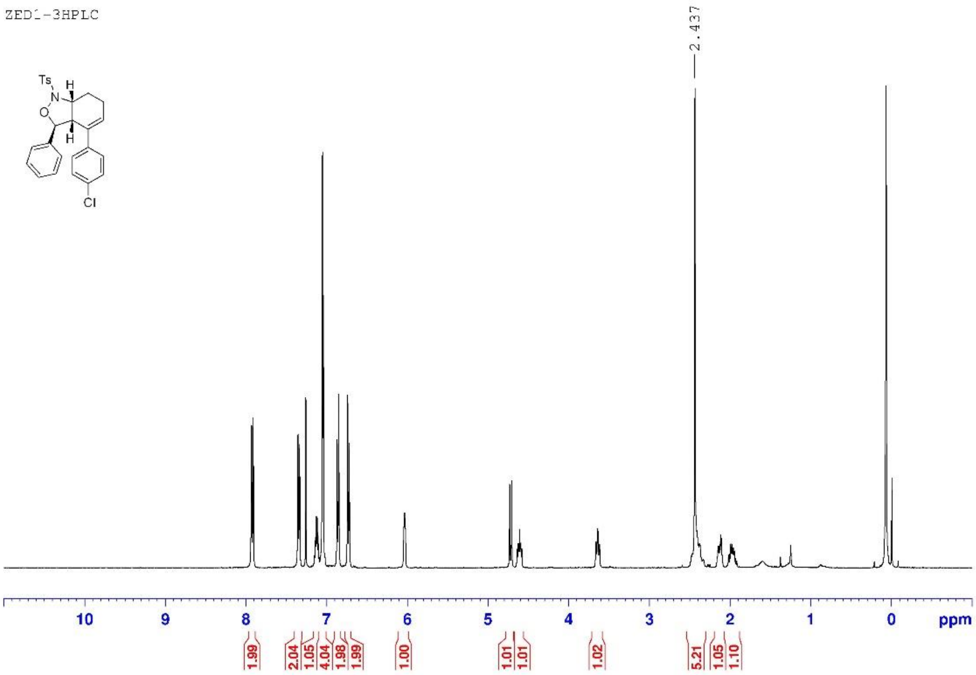
2j


zed2-2 hplc
2.429
ppm
2.00
2.07
5.07
2.06
2.01
1.00
1.00
1.01
1.01
4.12
1.09
1.04
1.06

3a

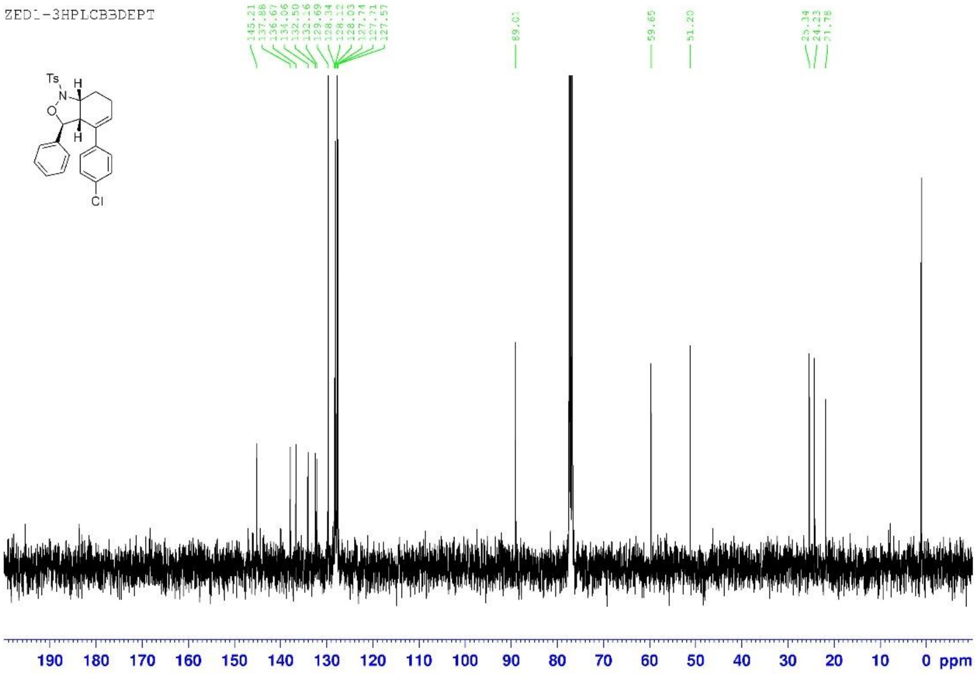

zed2-2 hplcbb dept
86.35
58.59
47.46
25.74
23.06
21.76
ppm

3a



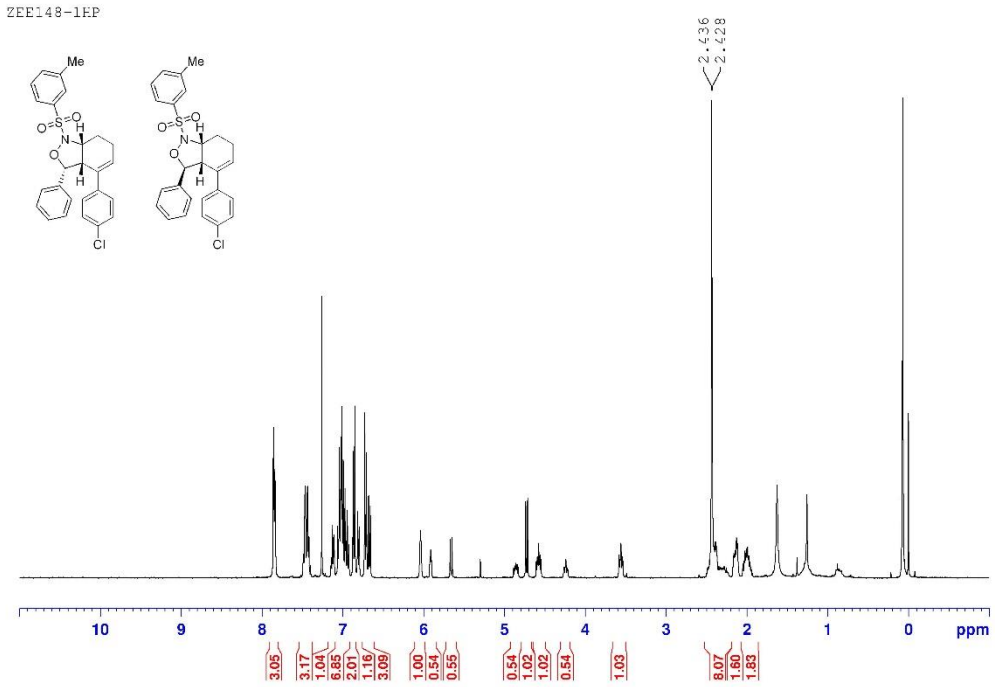
ZED1-3HPLC
2.437
Ts
N
H
O
H
Cl
10
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.04
1.05
4.04
1.98
1.99
1.00
1.01
1.01
1.02
5.21
1.05
1.10

4a

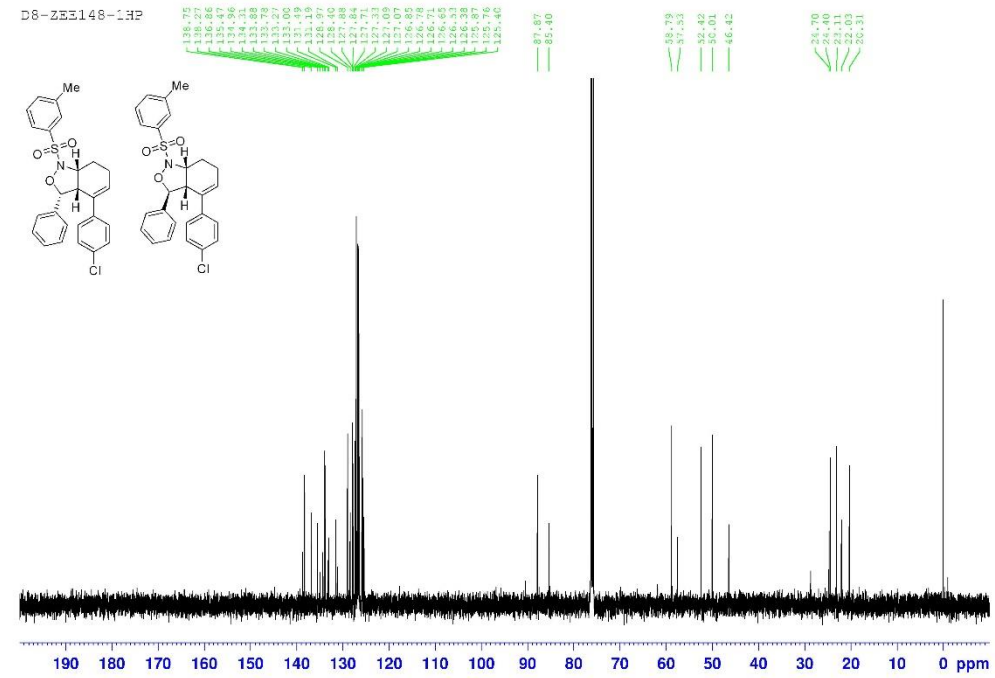


ZED1-3HPLCB3DEPT
145.21
137.86
136.67
134.06
132.50
132.16
129.69
128.34
128.12
128.03
127.74
127.71
127.57
89.01
59.65
51.20
25.34
24.23
21.78
Ts
N
H
O
H
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

4a



Left 3b, right 4b



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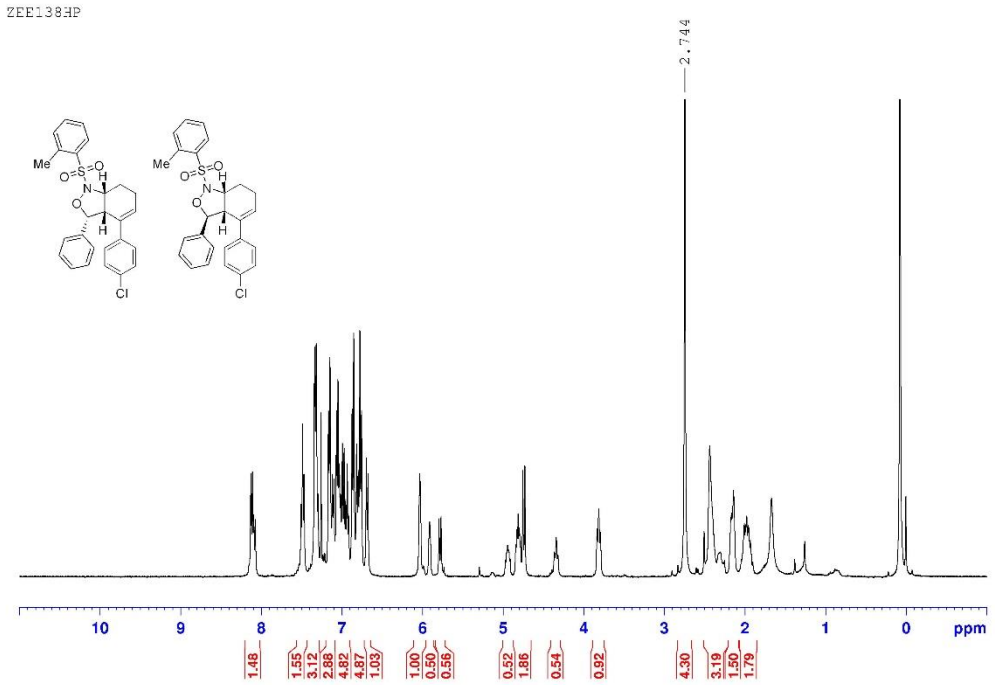

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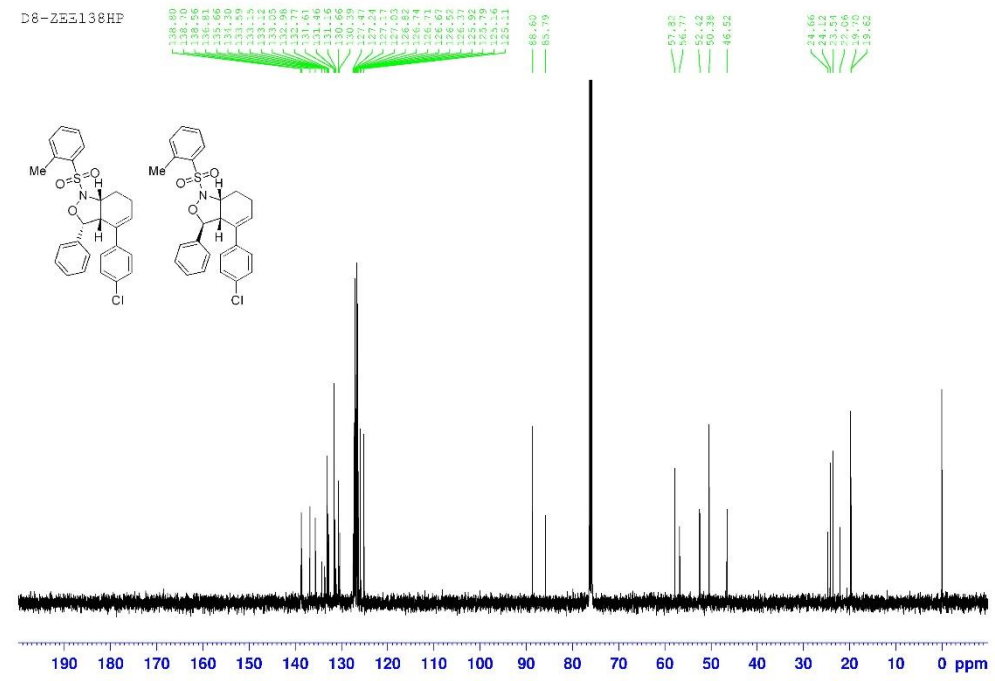

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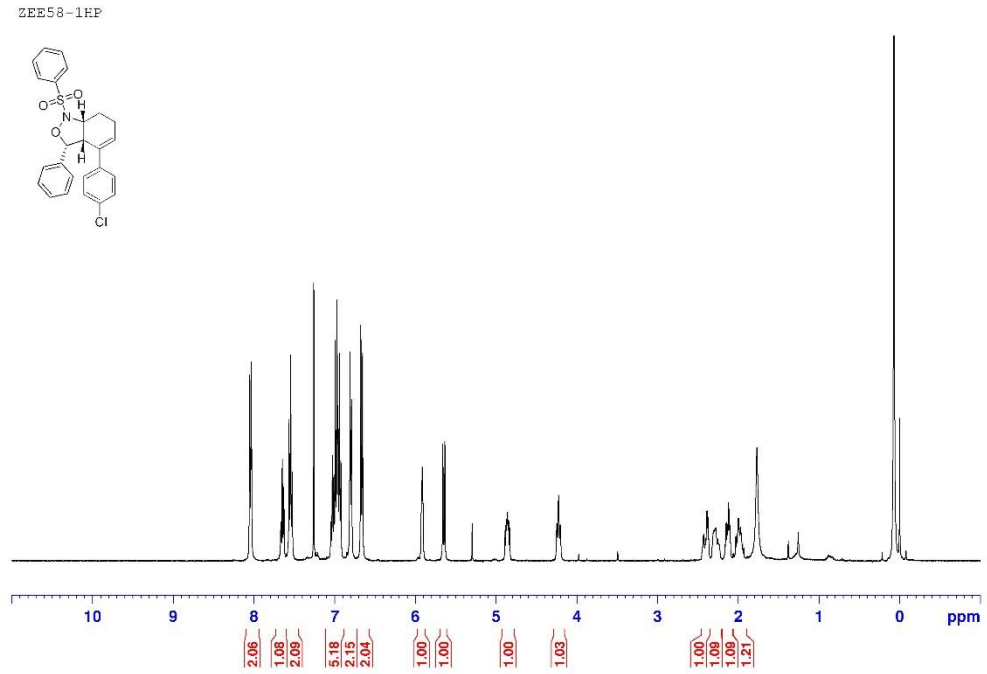
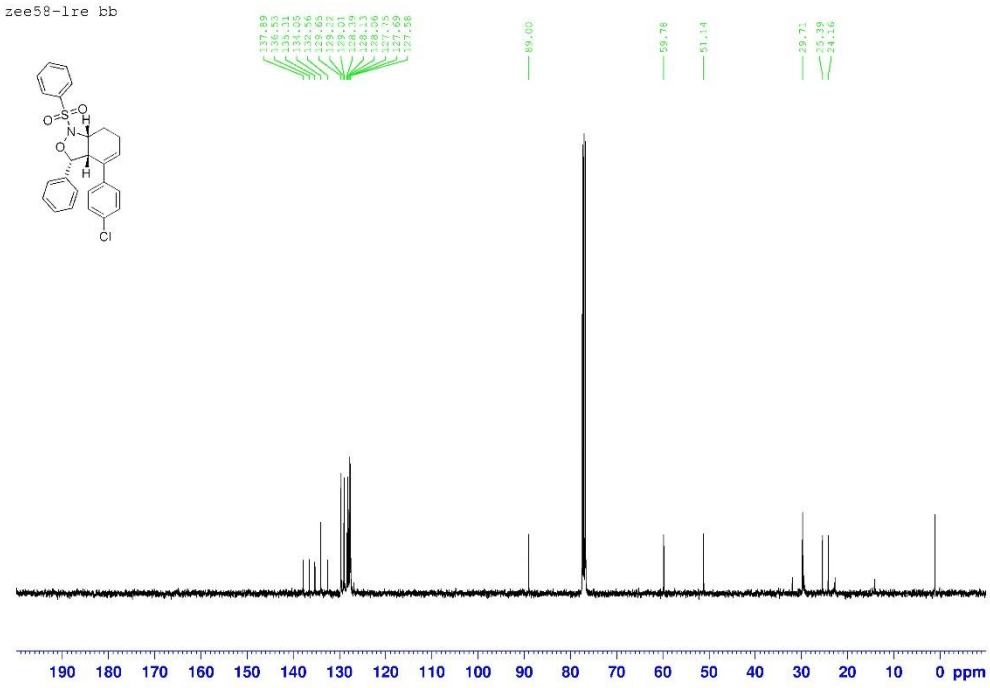
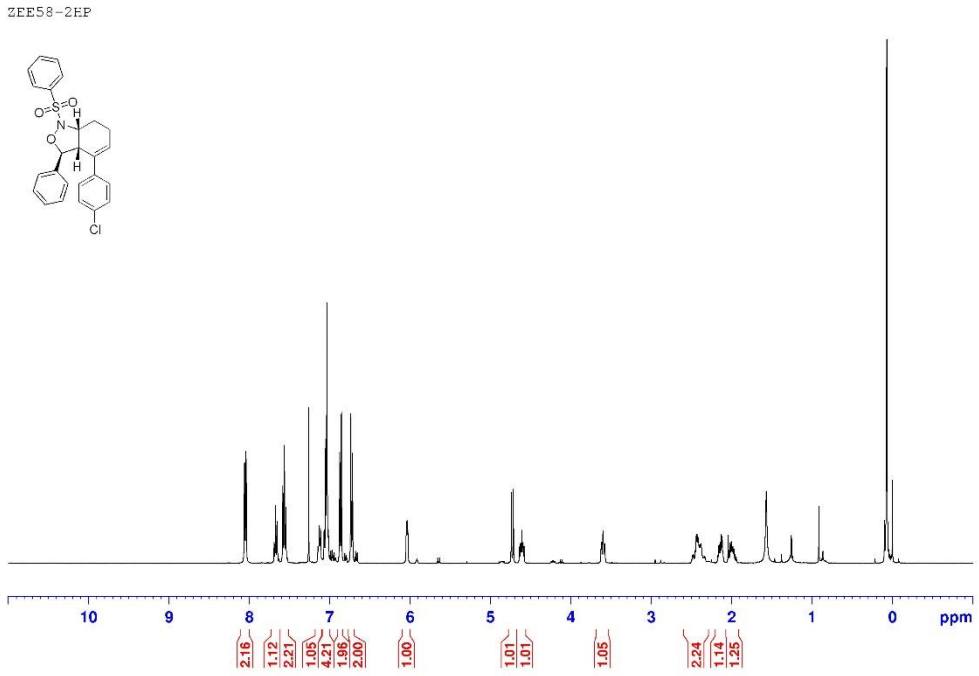

ZEE58-1HP
Cl
10
9
8
7
6
5
4
3
2
1
0
ppm
2.06
1.08
2.09
5.18
2.15
2.04
1.00
1.00
1.00
1.03
1.00
1.09
1.09
1.21

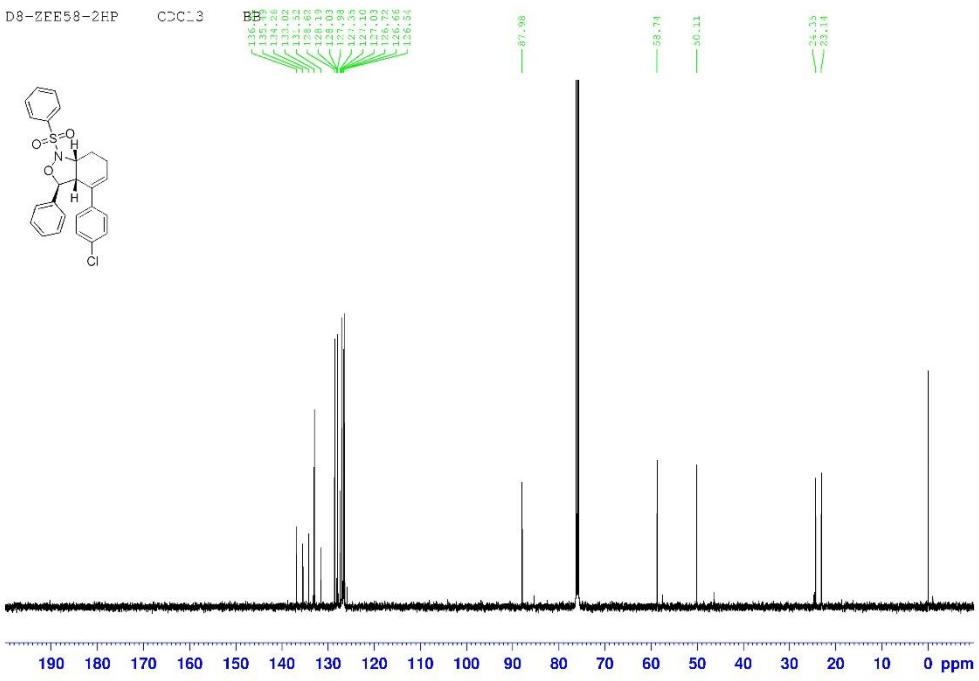
3d


zee58-1re bb
137.89
136.53
135.31
134.35
132.96
129.65
129.22
129.01
128.39
128.13
128.06
127.75
127.69
127.58
89.00
59.78
51.14
29.71
25.39
24.16
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

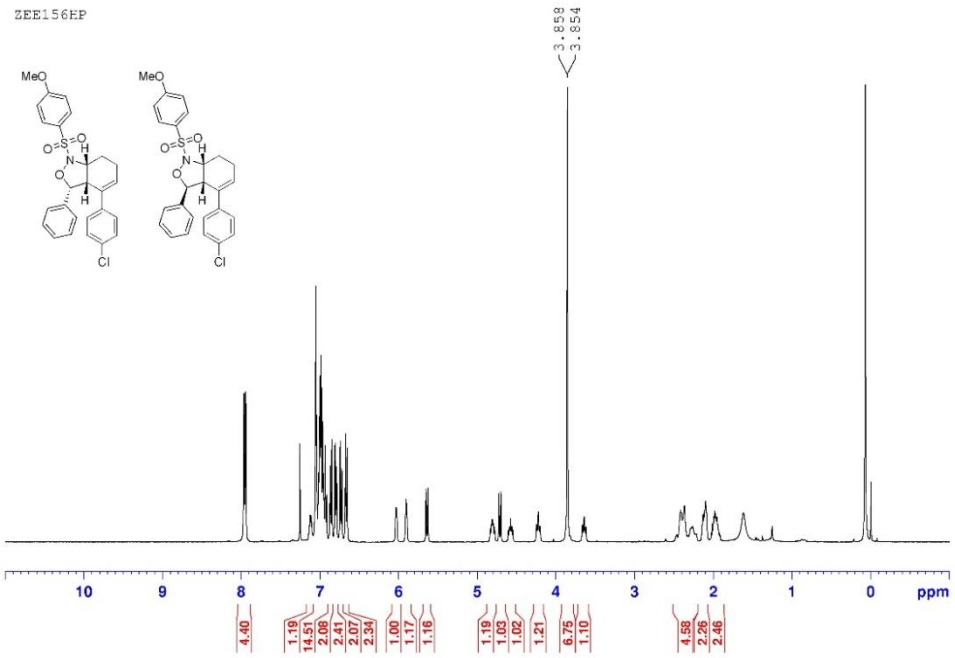
3d


ZEE58-2EP
10
9
8
7
6
5
4
3
2
1
0
ppm
2.16
1.12
2.21
1.05
4.21
1.96
2.00
1.00
1.01
1.01
1.05
2.24
1.14
1.25

4d


D8-ZEE58-2EP
CDCL3
87.98
58.74
50.11
24.33
23.14
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

4d



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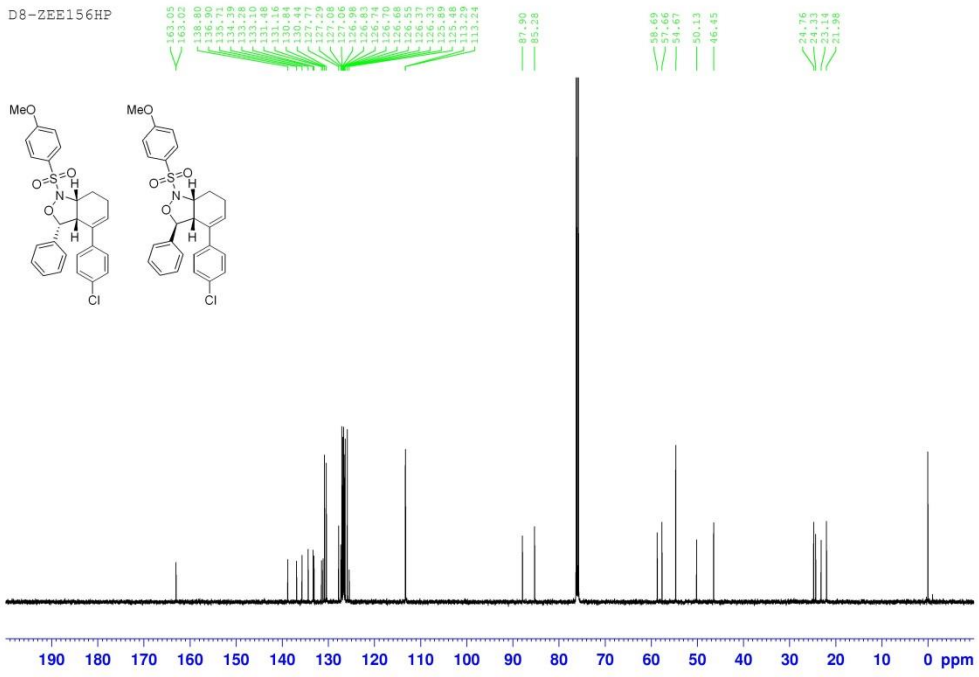

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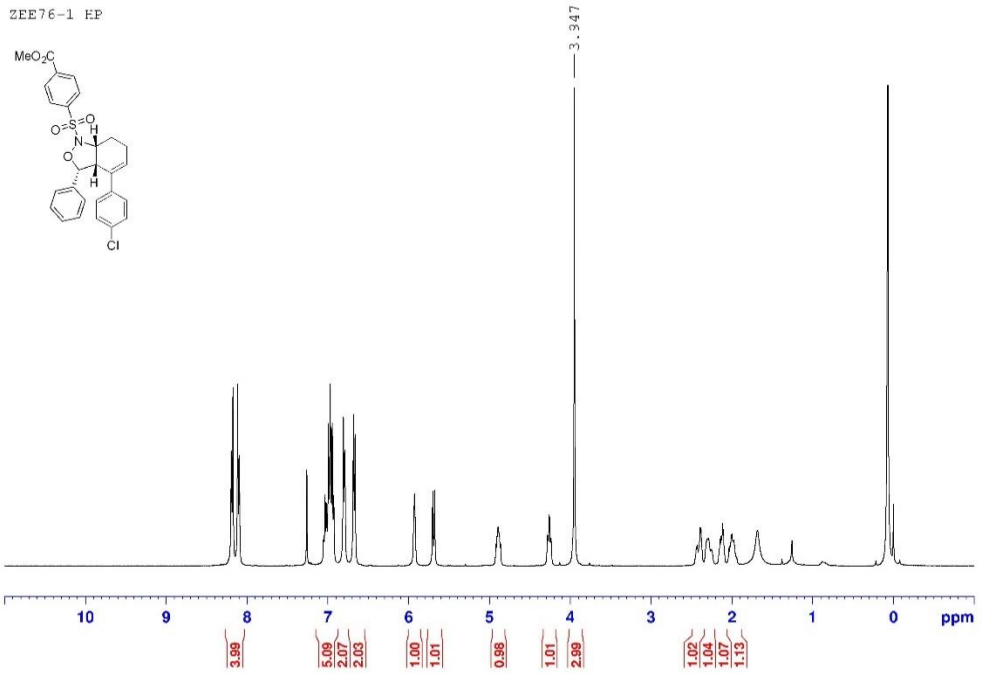
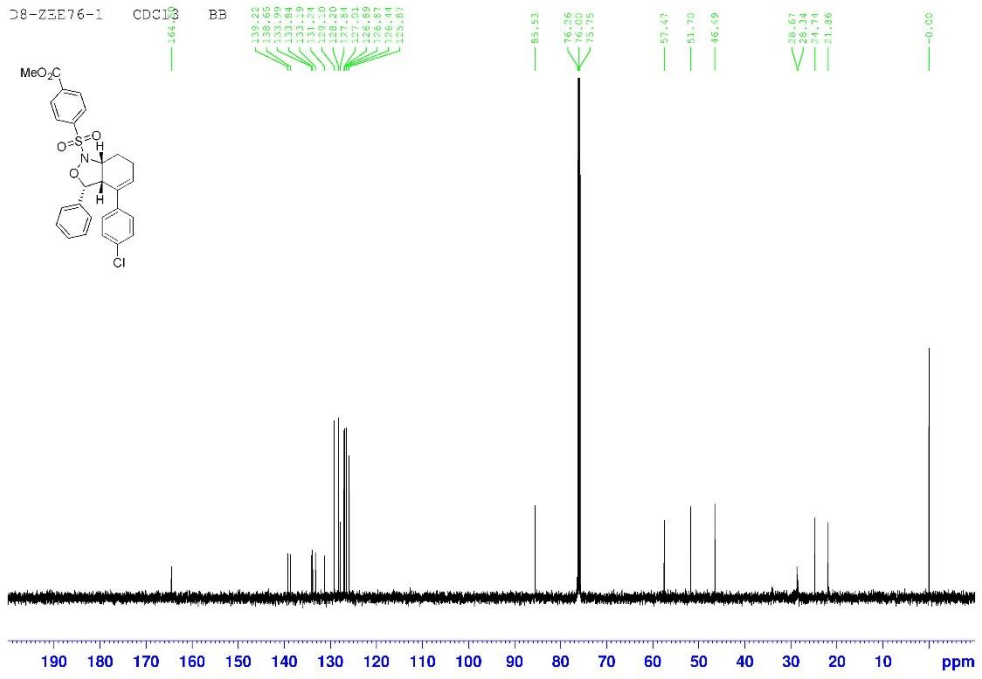
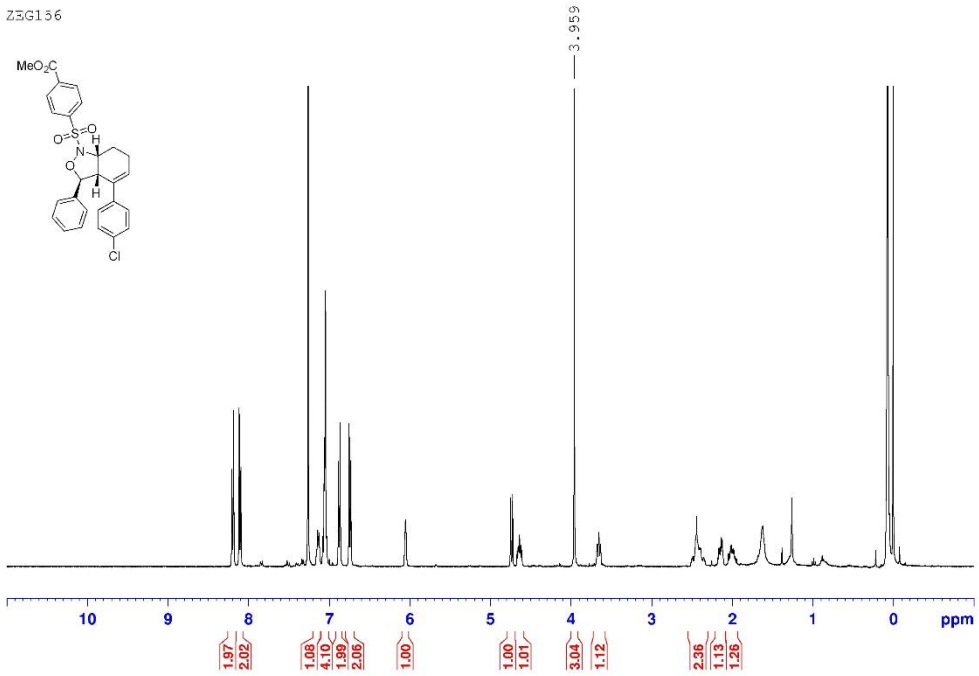

ZEE76-1 EP
MeO2C
3.347
10 9 8 7 6 5 4 3 2 1 0 ppm
3.99 5.09 2.07 2.03 1.00 1.01 0.98 1.01 2.99 1.02 1.04 1.07 1.13

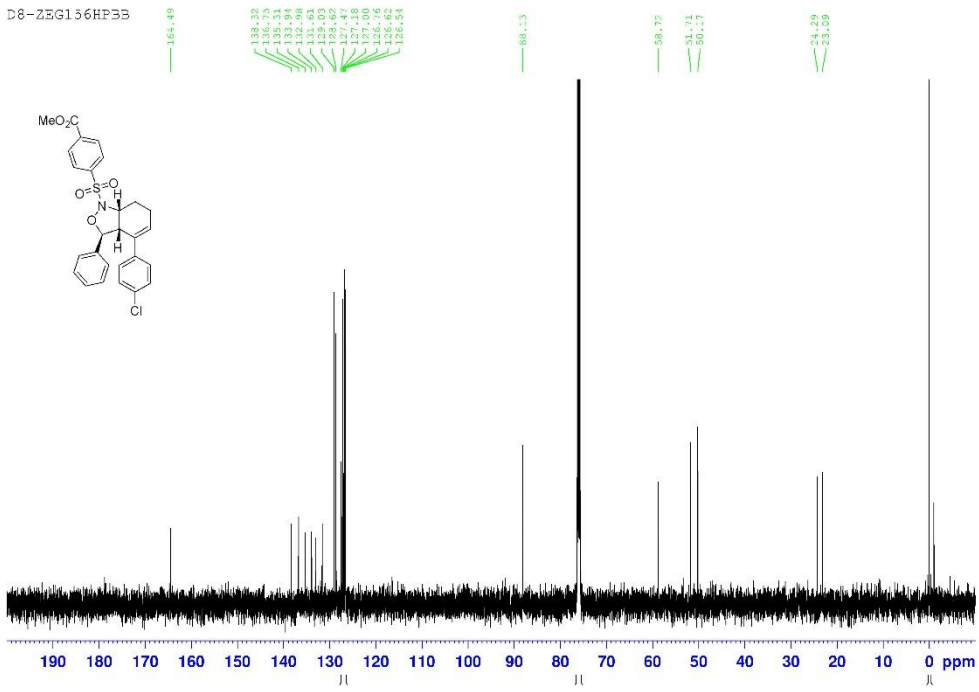
3f


D8-ZEE76-1 CDCl3 BB
MeO2C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

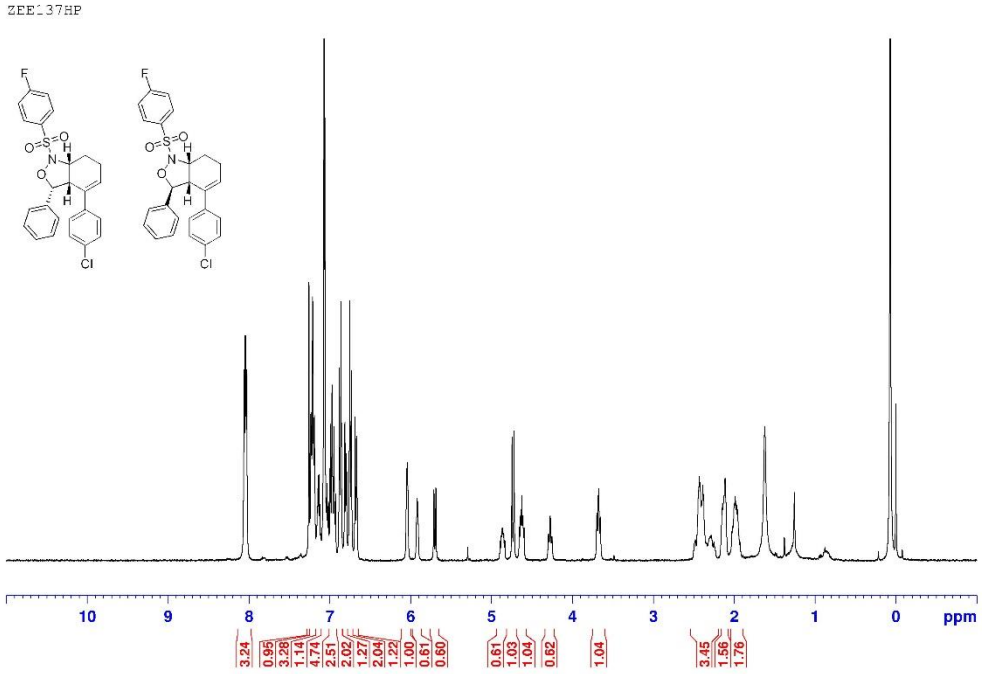
3f


ZEG136
3.959
10
9
8
7
6
5
4
3
2
1
0
ppm

4f


D8-ZEG156HP3B
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

4f



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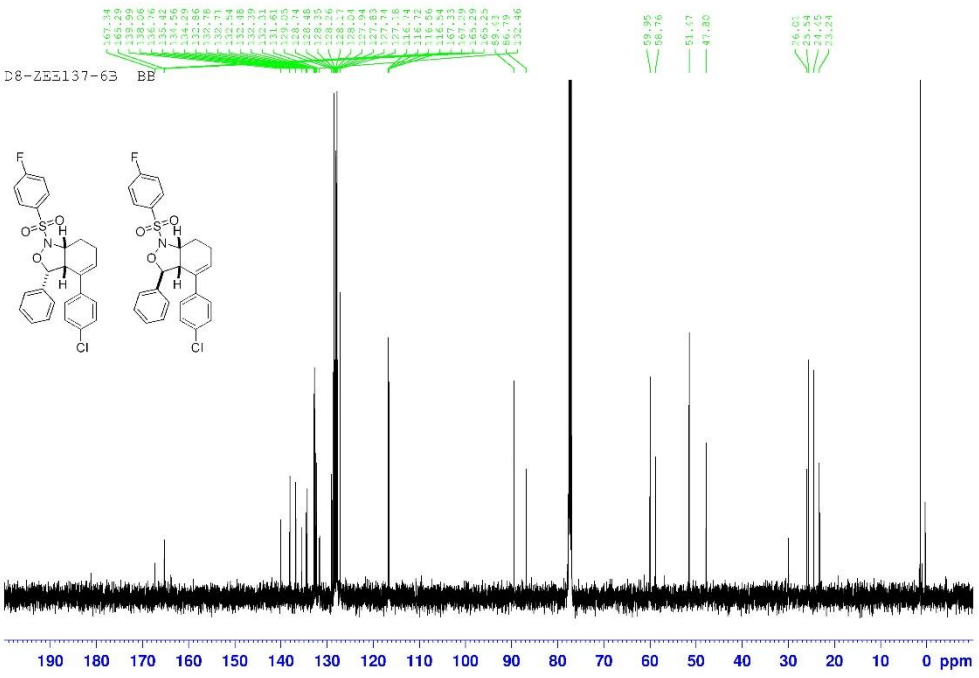

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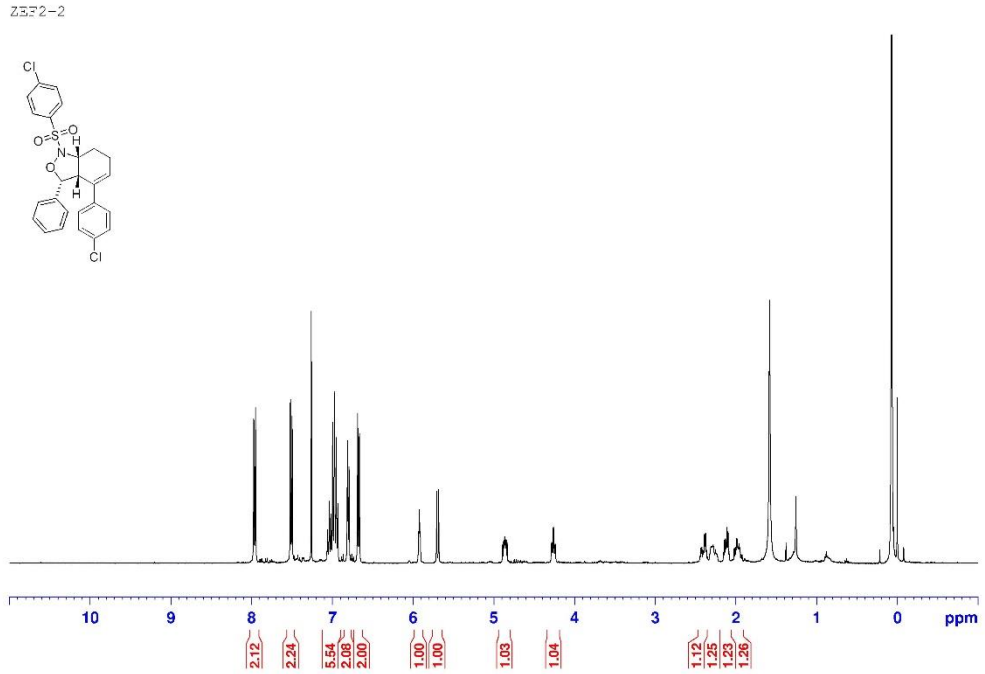
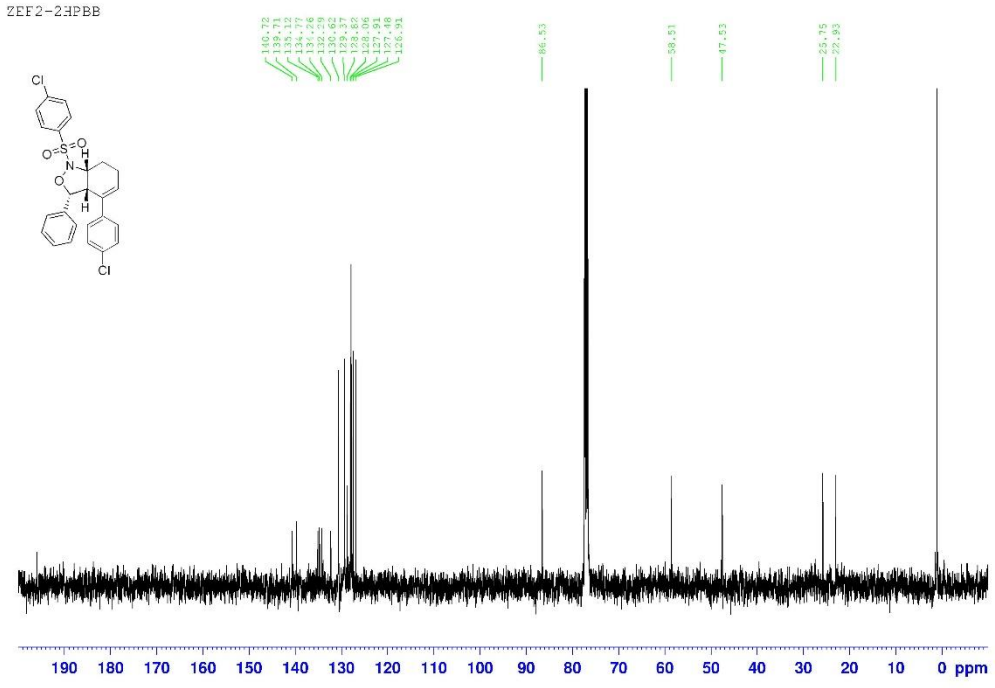
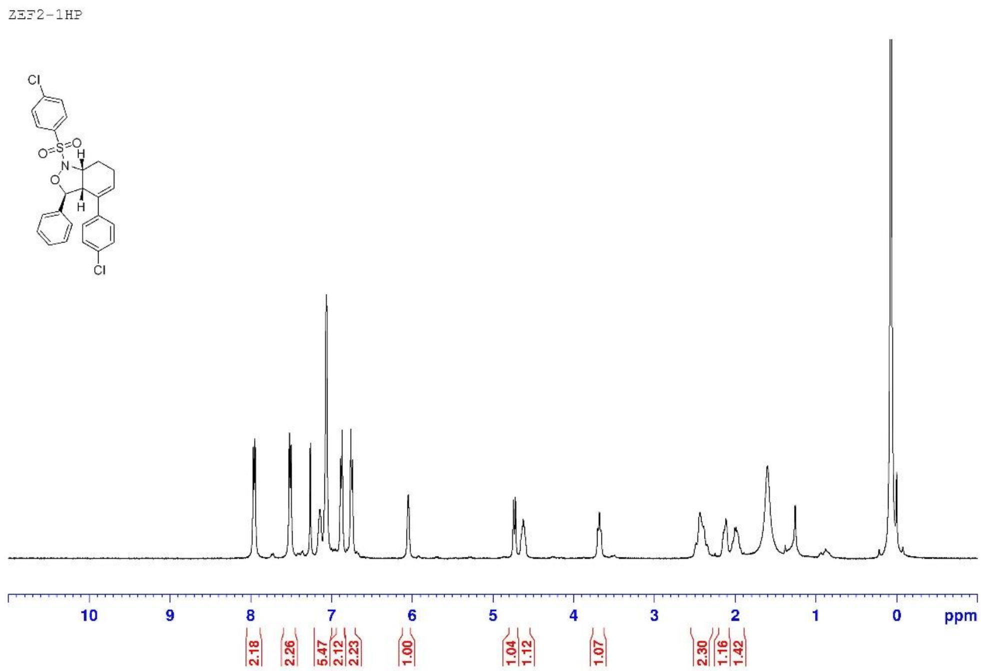

ZEF2-2
Cl
O
S
O
N
H
O
H
Cl
10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
2.24
5.54
2.08
2.00
1.00
1.00
1.03
1.04
1.12
1.25
1.23
1.26

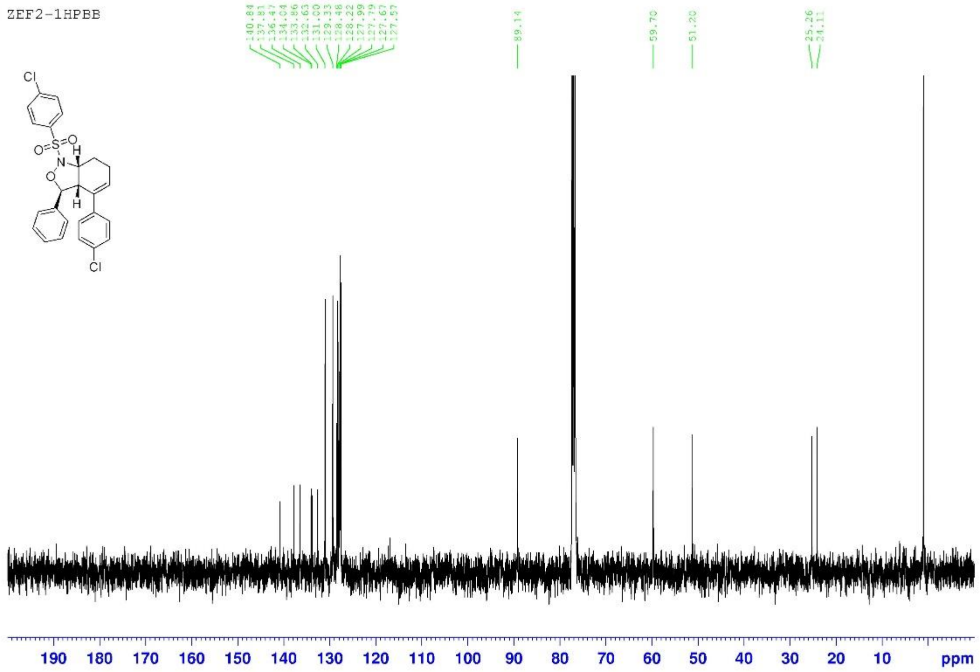
3h


ZEF2-2HPBB
140.72
139.71
135.12
134.77
134.26
132.29
130.62
129.37
128.96
128.06
127.91
127.48
126.91
86.53
58.51
47.53
25.75
22.93
Cl
O
S
O
N
H
O
H
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

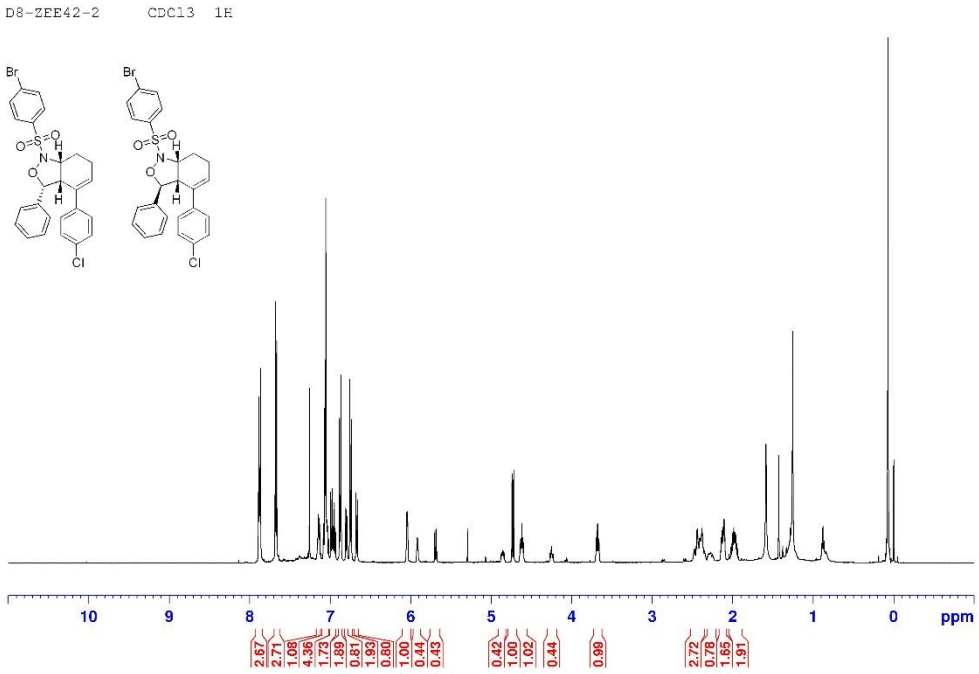
3h


ZEF2-1HP
Cl
N
O
H
Cl
10
9
8
7
6
5
4
3
2
1
0
ppm
2.18
2.26
5.47
2.12
2.23
1.00
1.04
1.12
1.07
2.30
1.16
1.42

4h


ZEF2-1HPBB
89.14
59.70
51.20
25.26
24.11
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

4h



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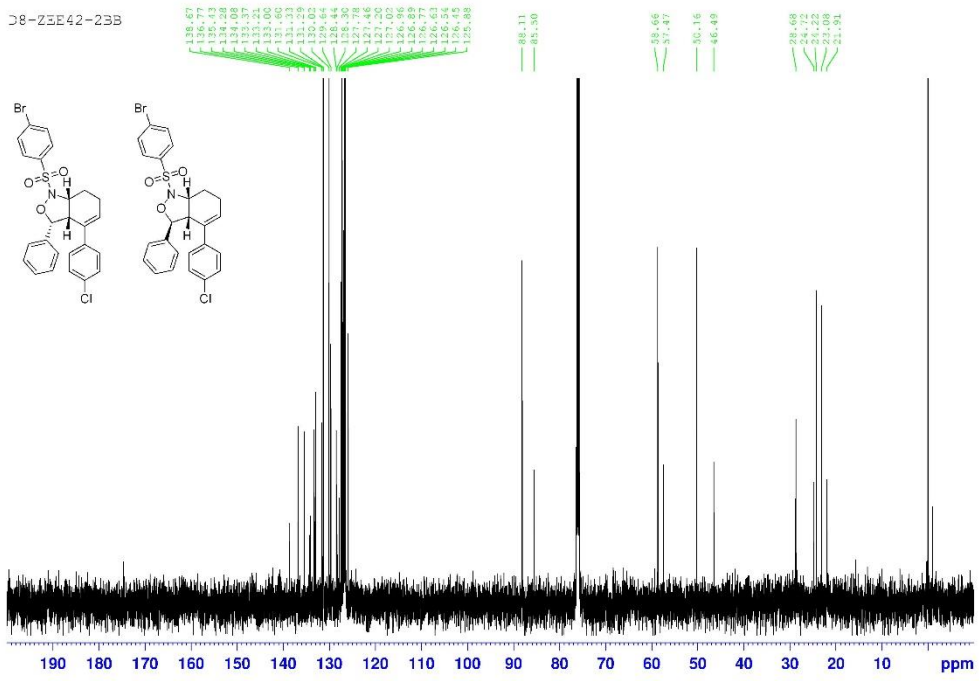
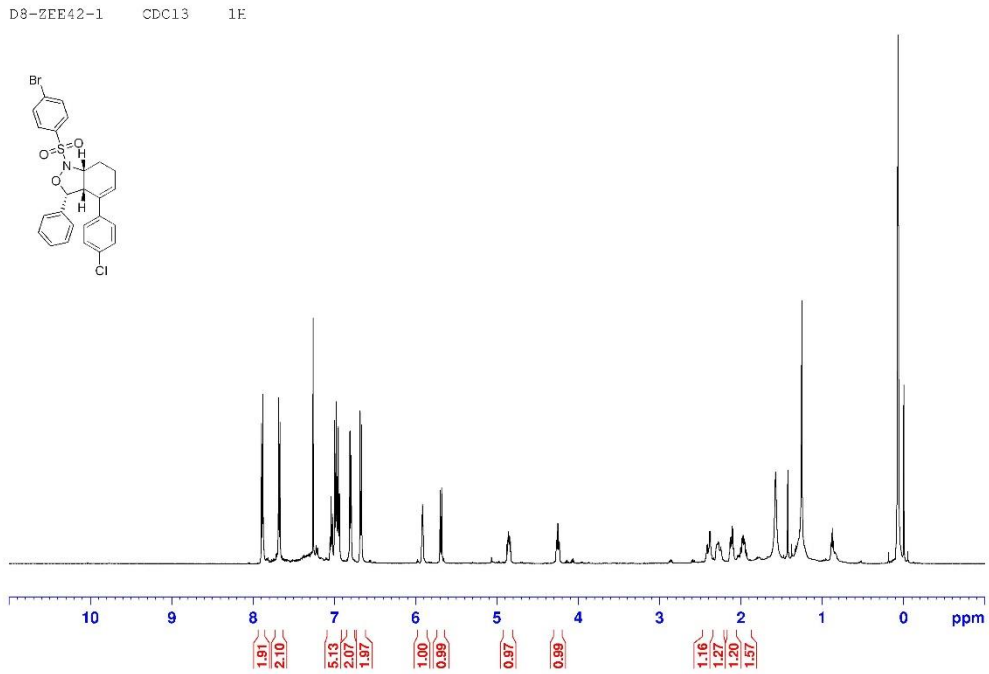
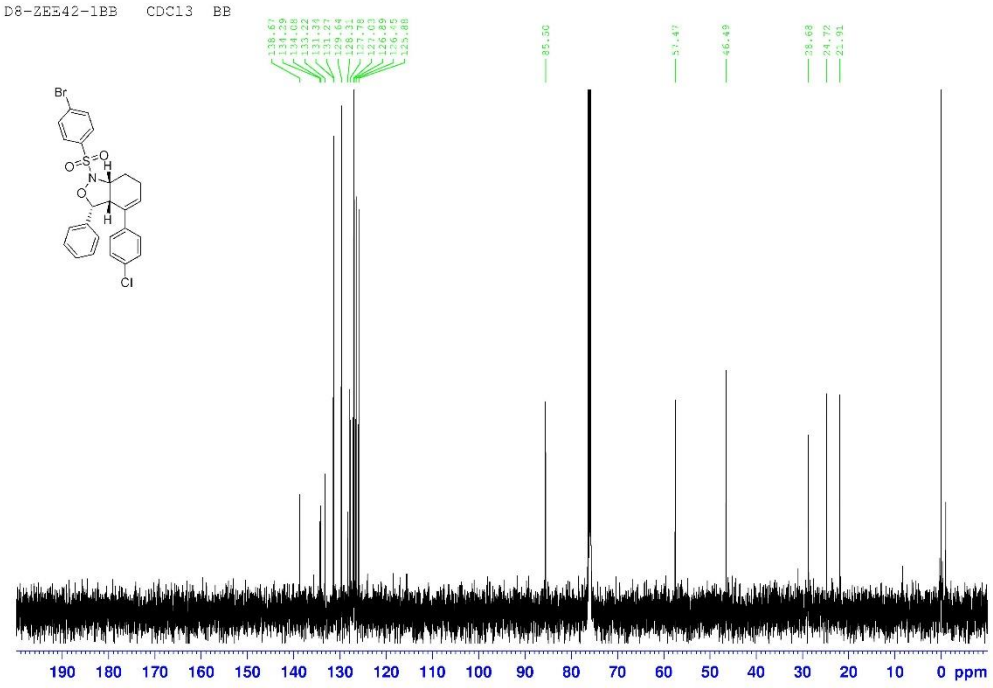


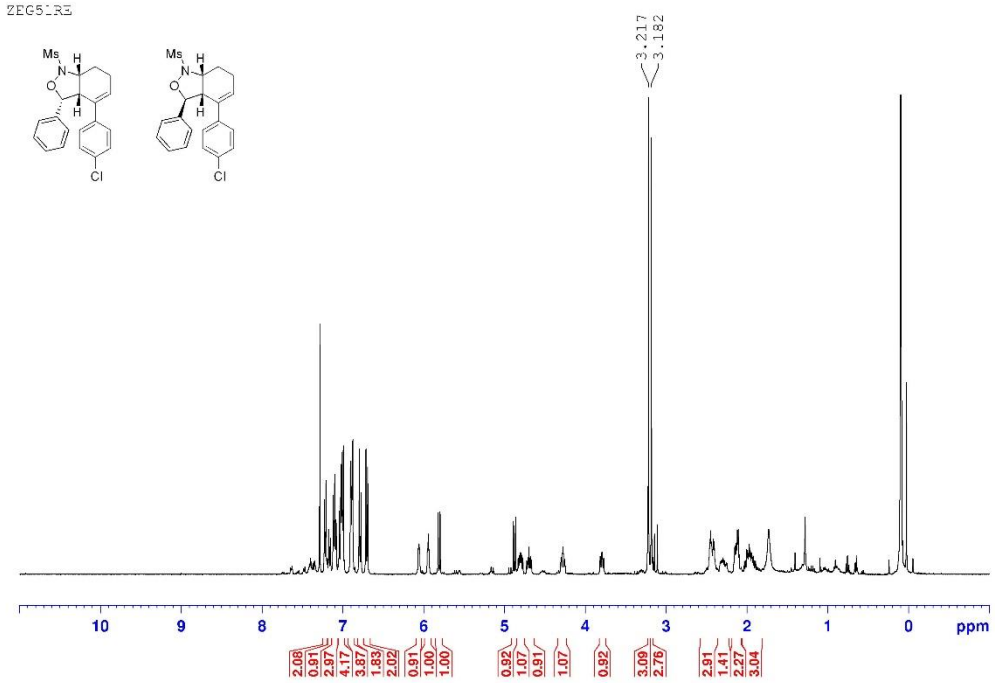
Left 3i, right 4i


D8-ZEE42-1 CDCl3 1E
Br
O
S
O
N
H
O
H
Cl
10 9 8 7 6 5 4 3 2 1 0 ppm
1.91 2.10 5.13 2.07 1.97 1.00 0.99 0.97 0.99 1.16 1.27 1.20 1.57

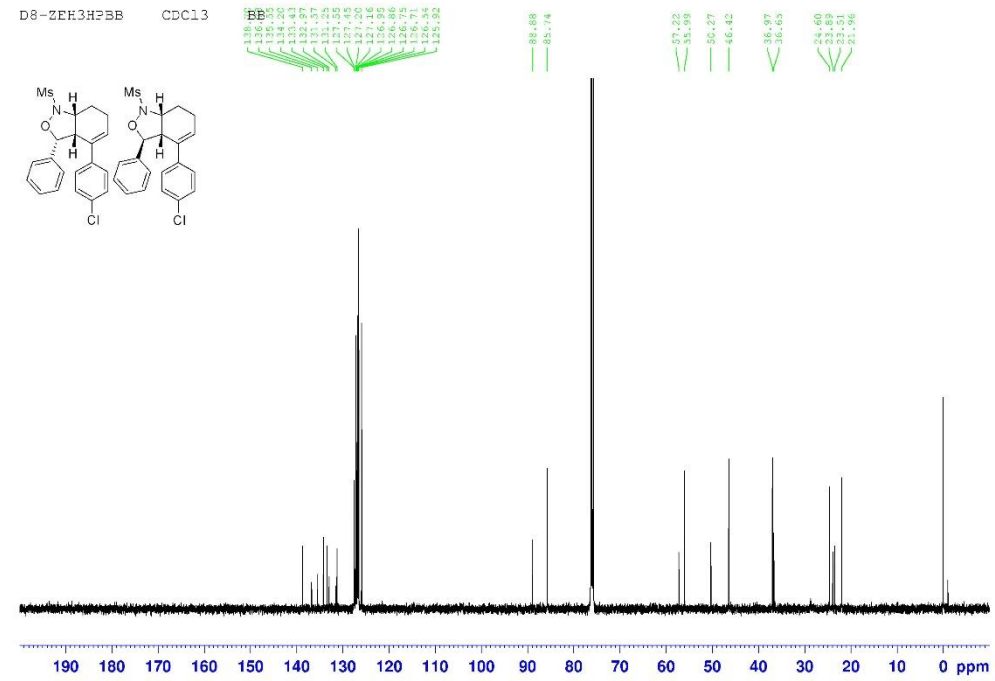
3i


D8-ZEE42-1BB CDCl3 BB
Br
O
S
O
N
H
O
H
Cl
95.50
51.47
46.49
28.68
24.72
21.91
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

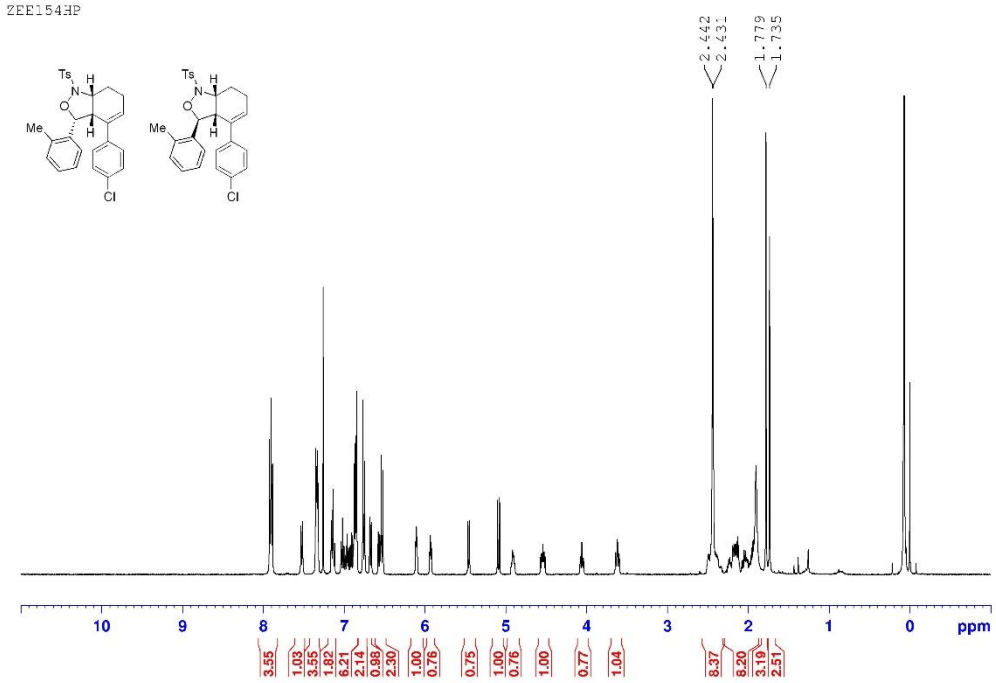
3i



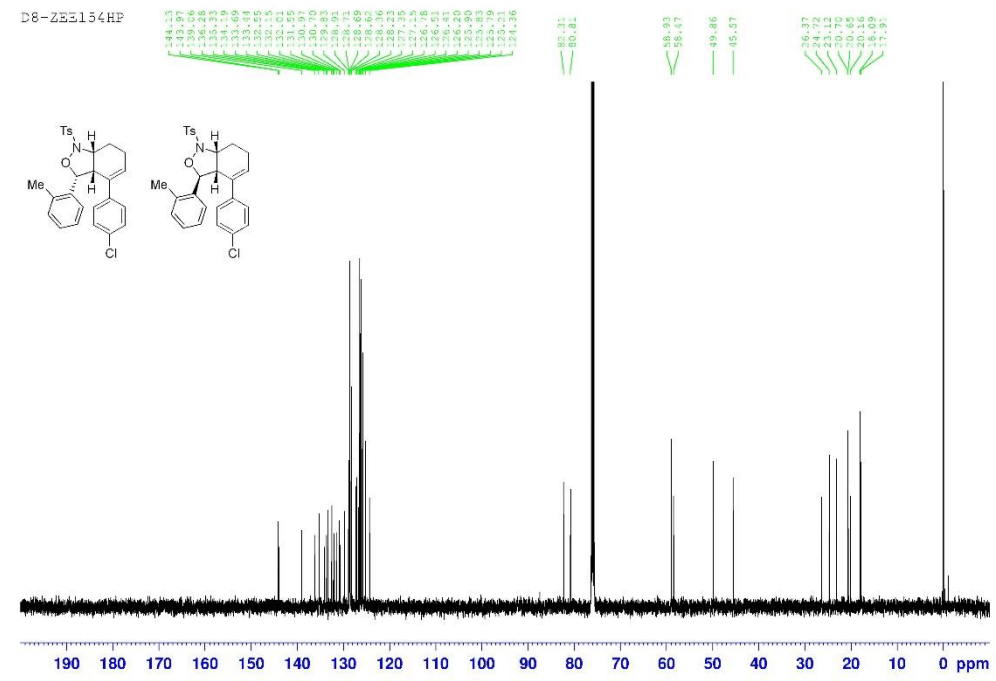
Left 3j, right 4j



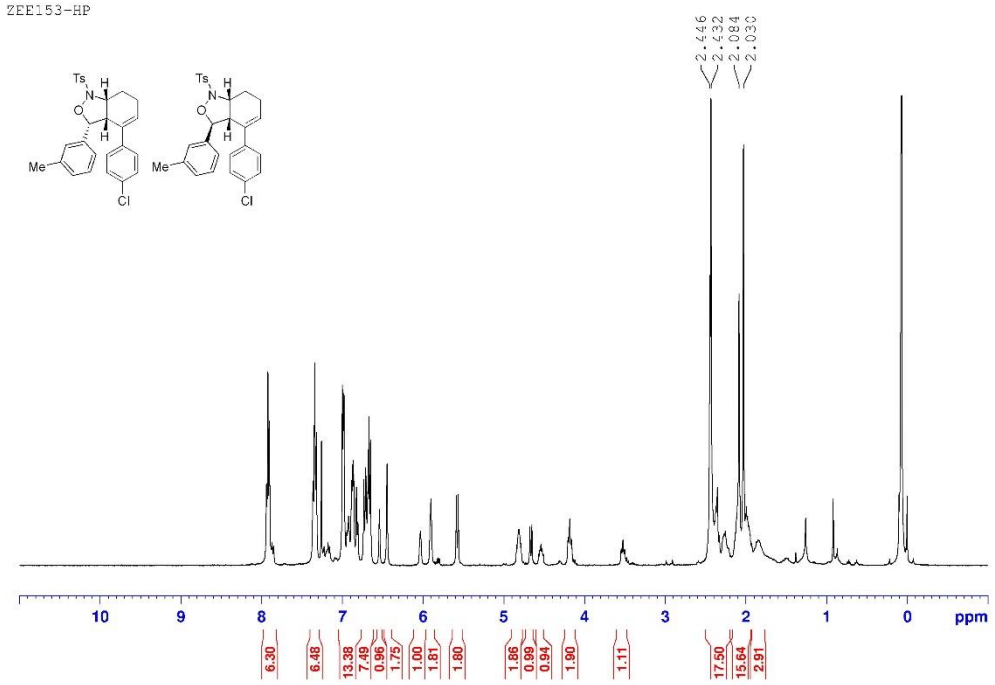
Left 3j, right 4j



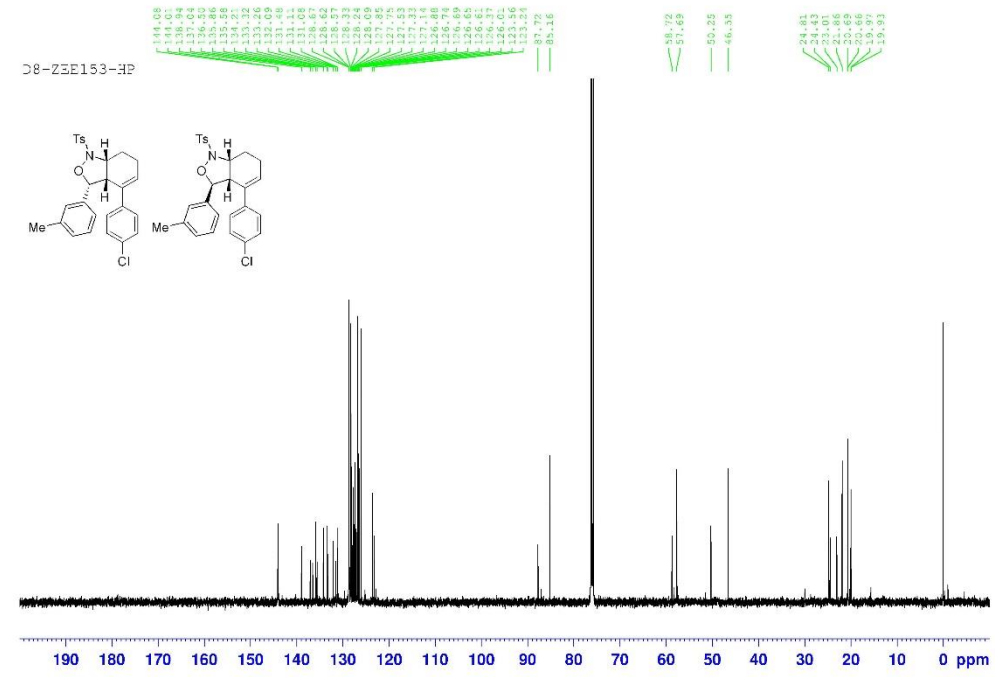
Left 3k, right 4k



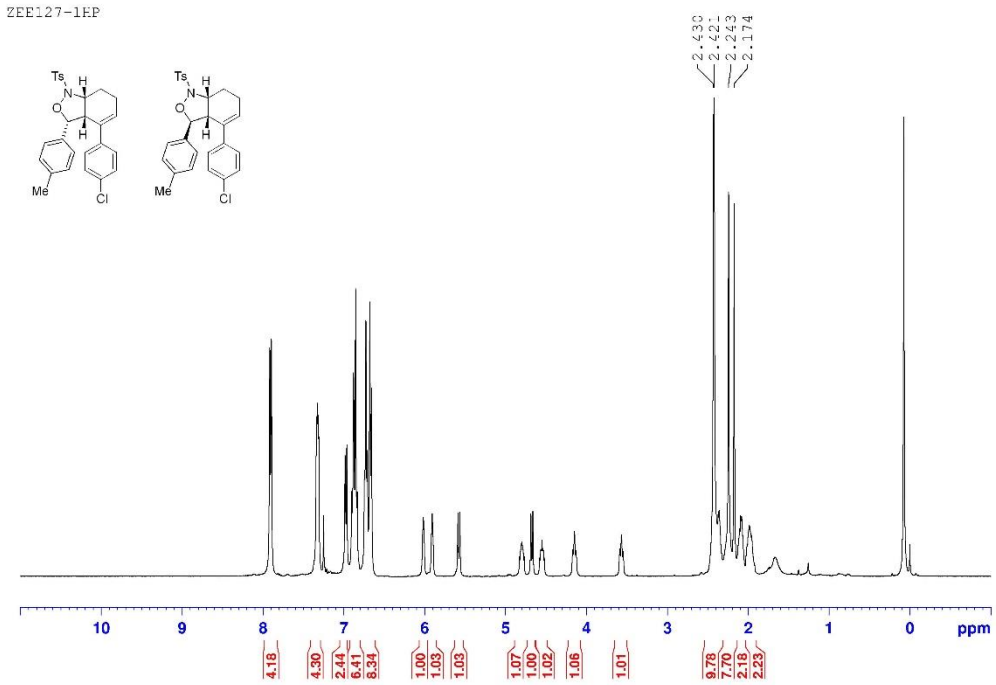
Left 3k, right 4k



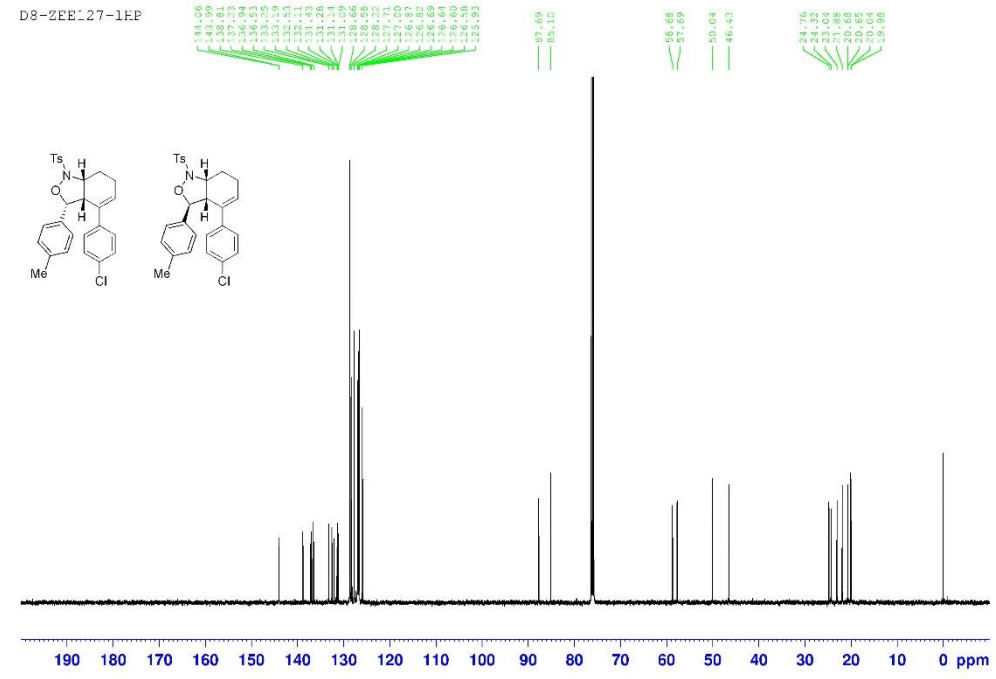
Left 3l, right 4l



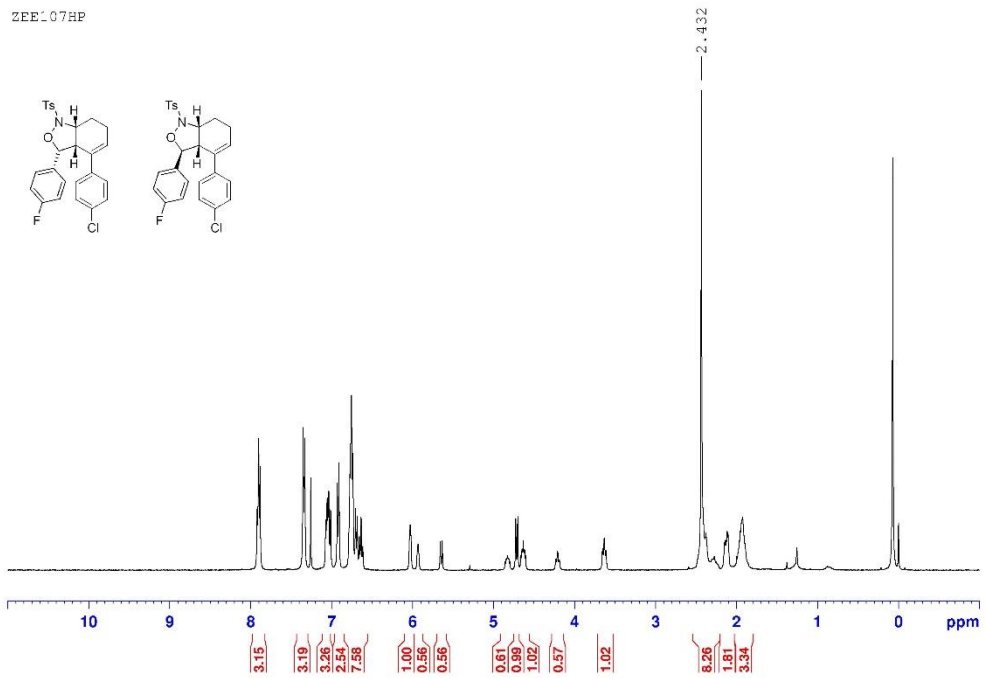
Left 3l, right 4l



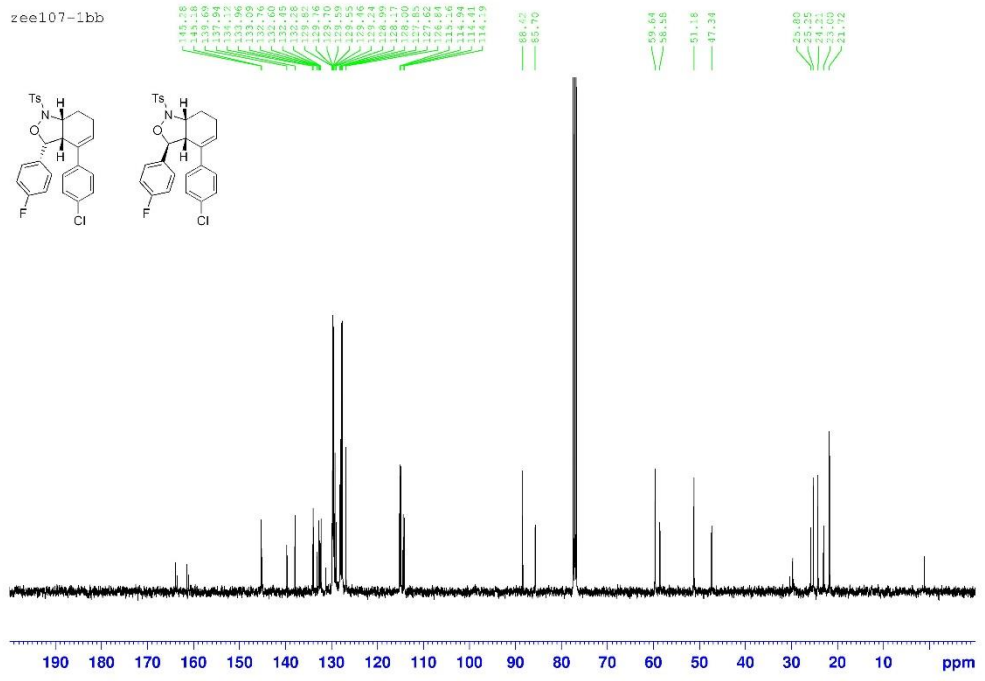
Left 3m, right 4m



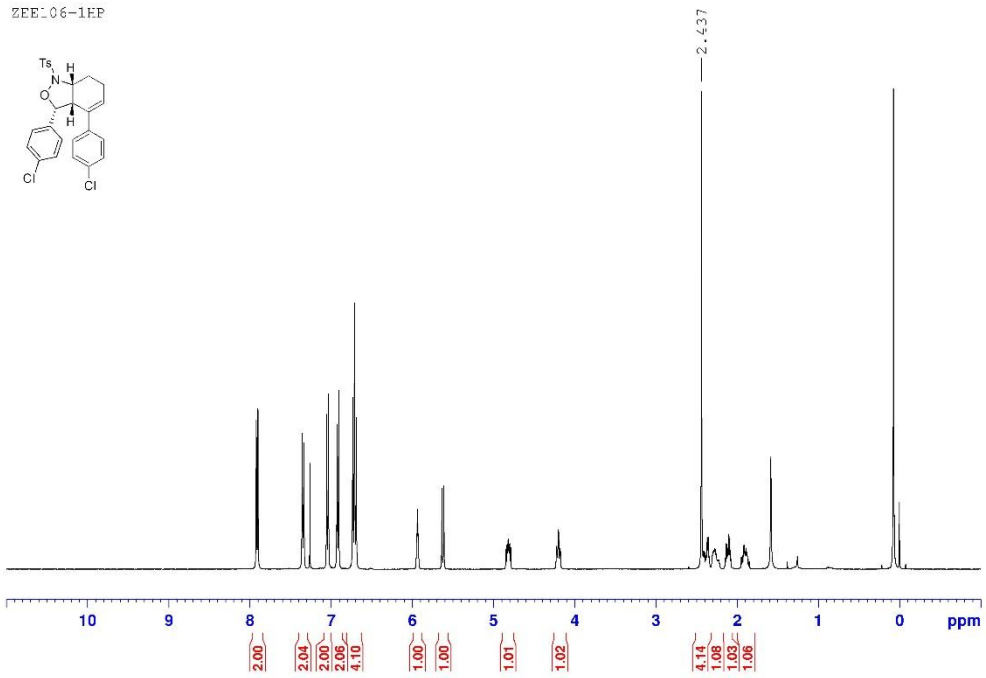
Left 3m, right 4m



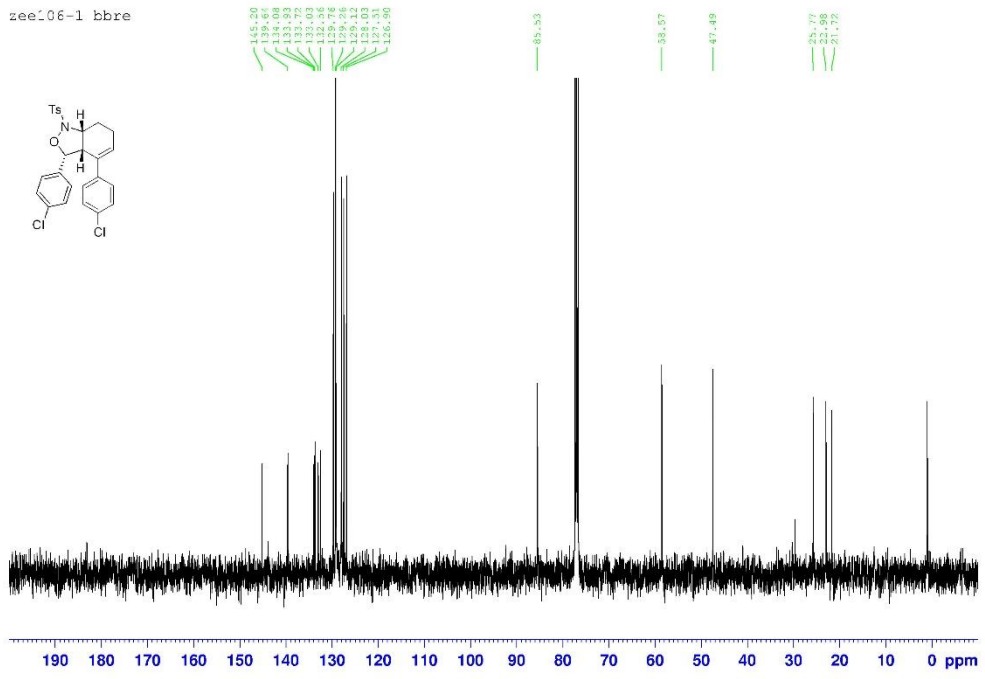
Left 3n, right 4n



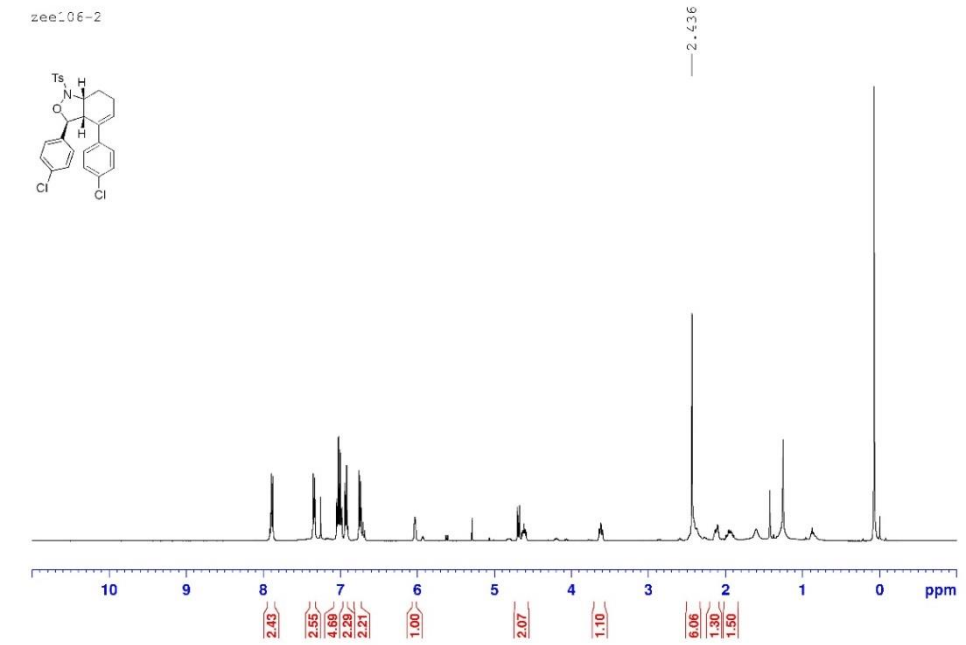
Left 3n, right 4n


ZEE_06-1EP
Ts
N
O
H
H
Cl
Cl
2.437
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.04
2.00
2.06
4.10
1.00
1.00
1.01
1.02
4.14
1.08
1.03
1.06

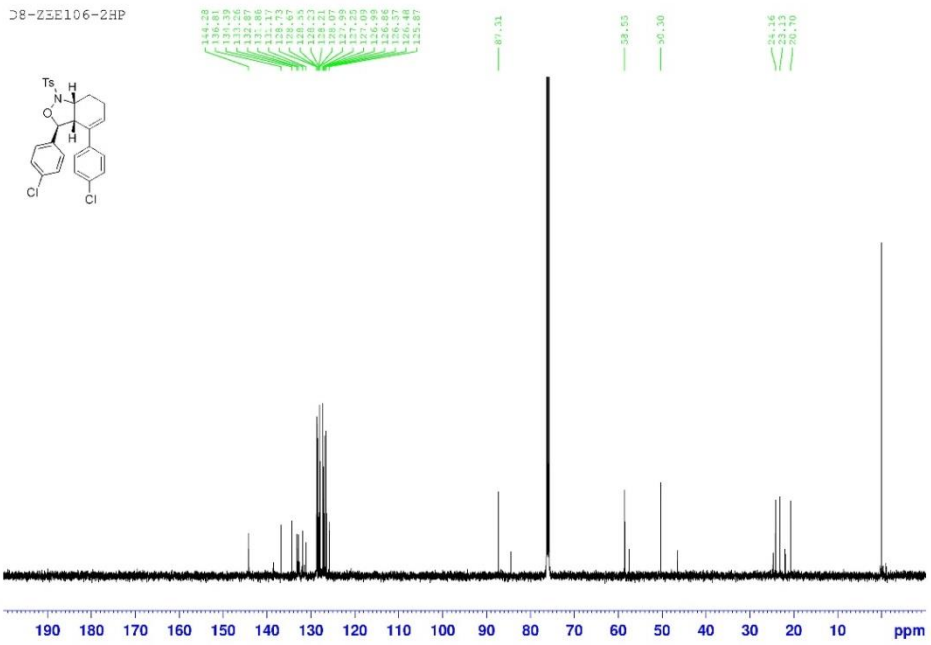
3p


zee_06-1 bbre
145.20
139.67
134.04
133.93
133.72
133.03
132.56
129.76
129.36
129.12
128.03
127.31
126.90
85.53
58.57
47.49
25.77
23.98
21.72
Ts
N
O
H
H
Cl
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

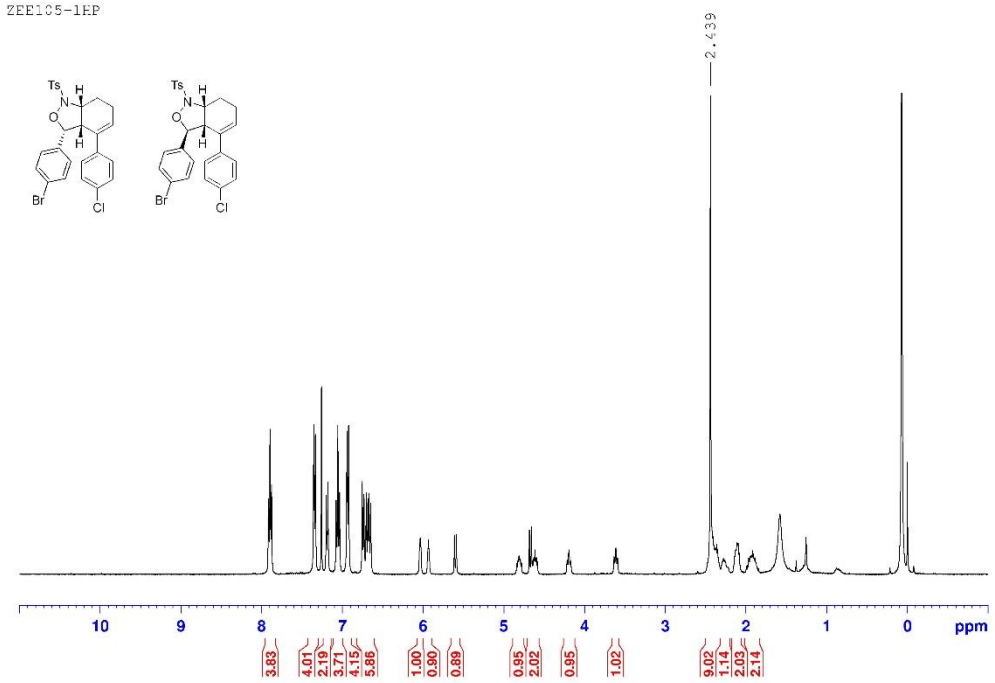
3p


zee106-2
2.436
10
9
8
7
6
5
4
3
2
1
0
ppm
2.43
2.55
4.69
2.29
2.21
1.00
2.07
1.10
6.06
1.30
1.50

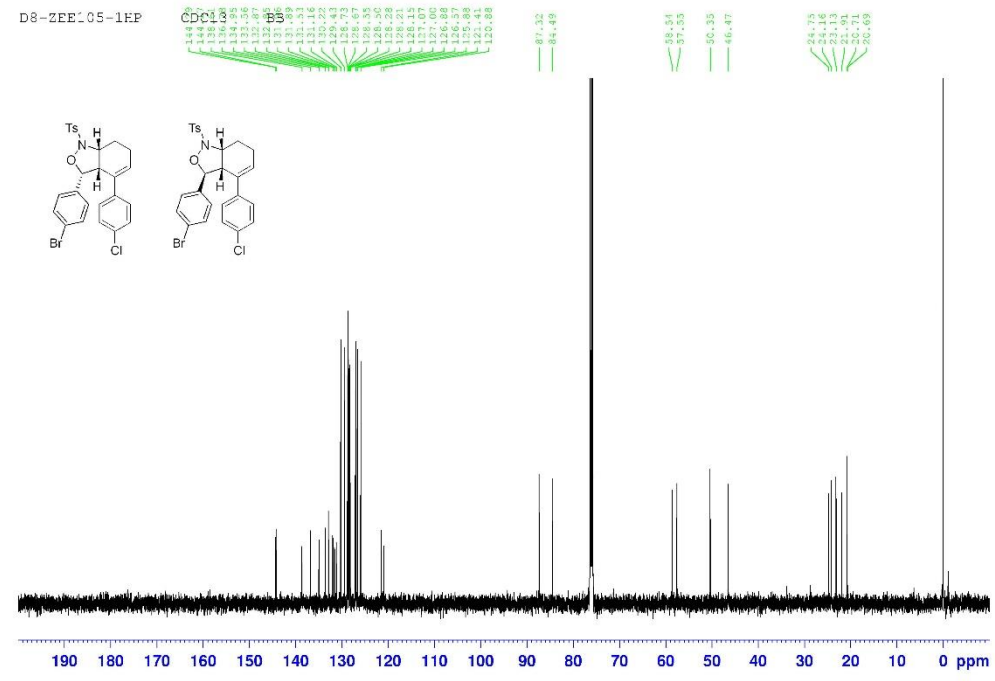
4p


D8-ZEE106-2HP
87.31
58.53
50.30
24.16
23.13
20.70
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

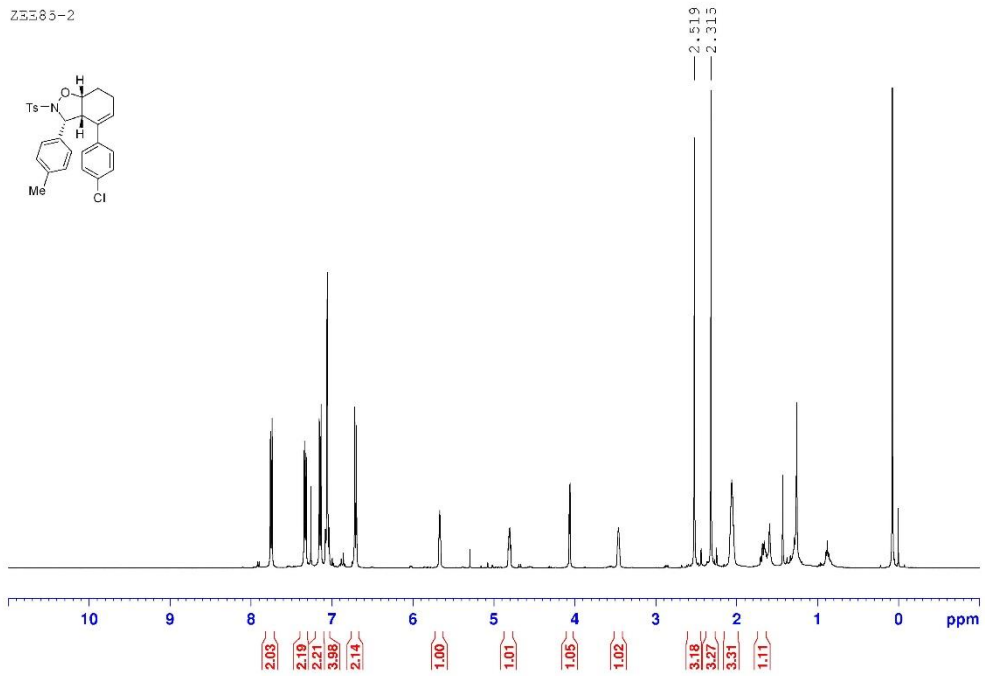
4p



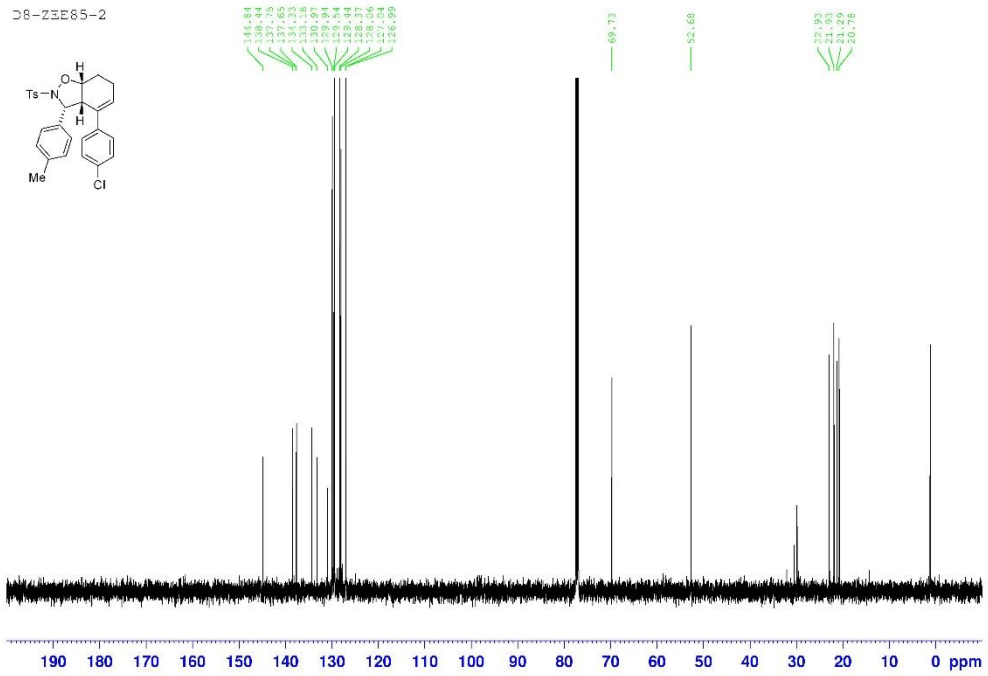
Left 3q, right 4q



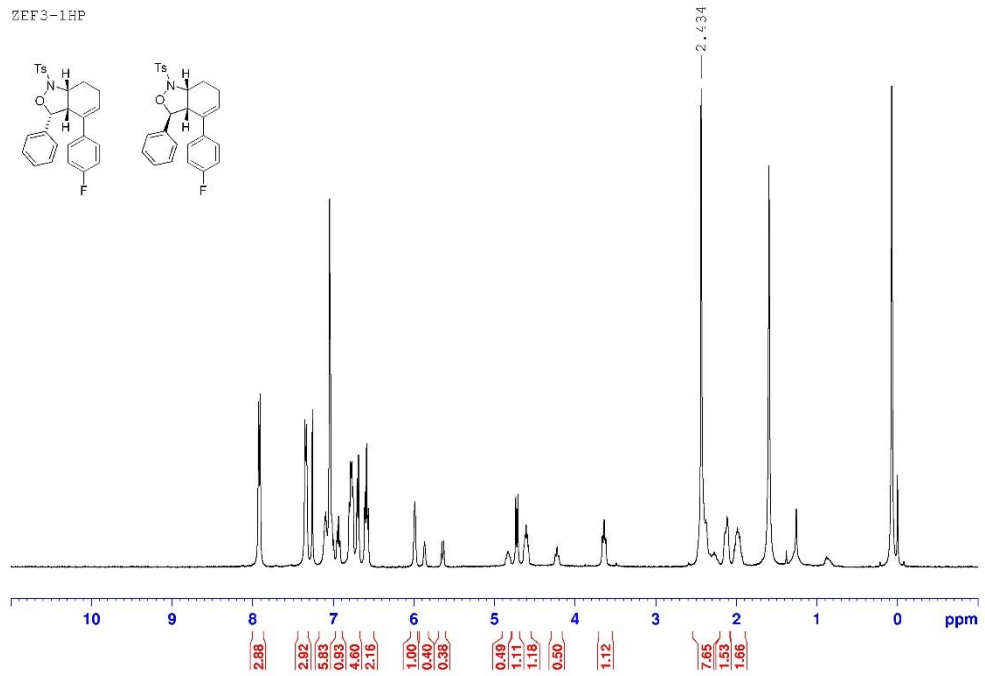
Left 3q, right 4q


Z3383-2
2.519
2.315
Ts
N
O
H
H
Me
Cl
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
2.19
2.21
3.98
2.14
1.00
1.01
1.05
1.02
3.18
3.27
3.31
1.11

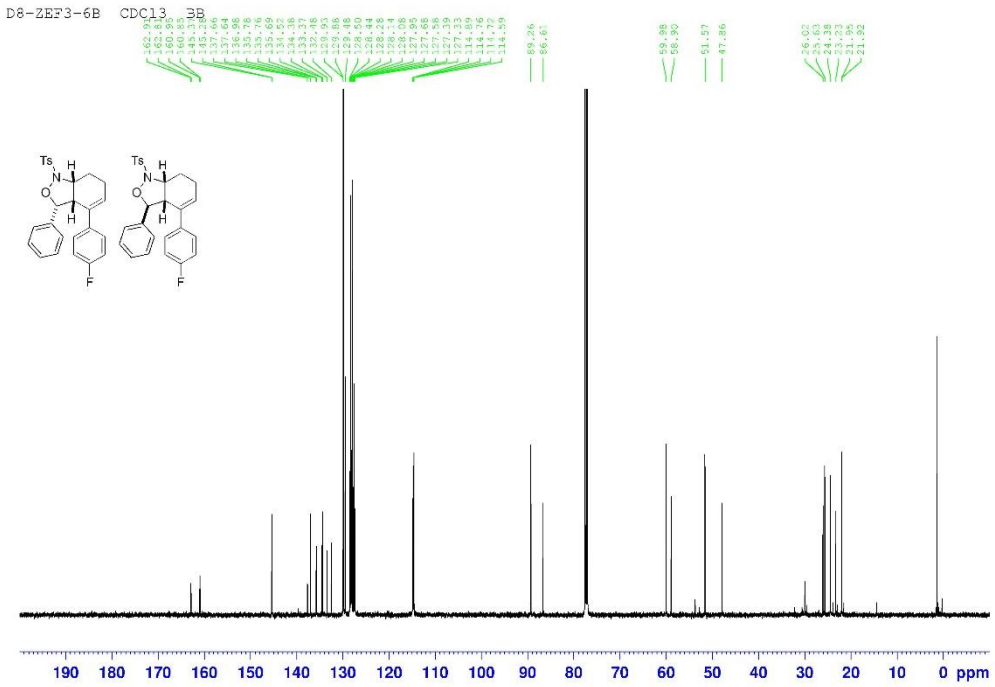
3x


D8-Z3E85-2
146.84
138.44
137.75
137.65
134.33
130.58
130.07
129.94
129.54
128.44
128.37
128.26
127.04
126.99
69.73
52.68
22.93
21.93
21.29
20.78
Ts
N
O
H
H
Me
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

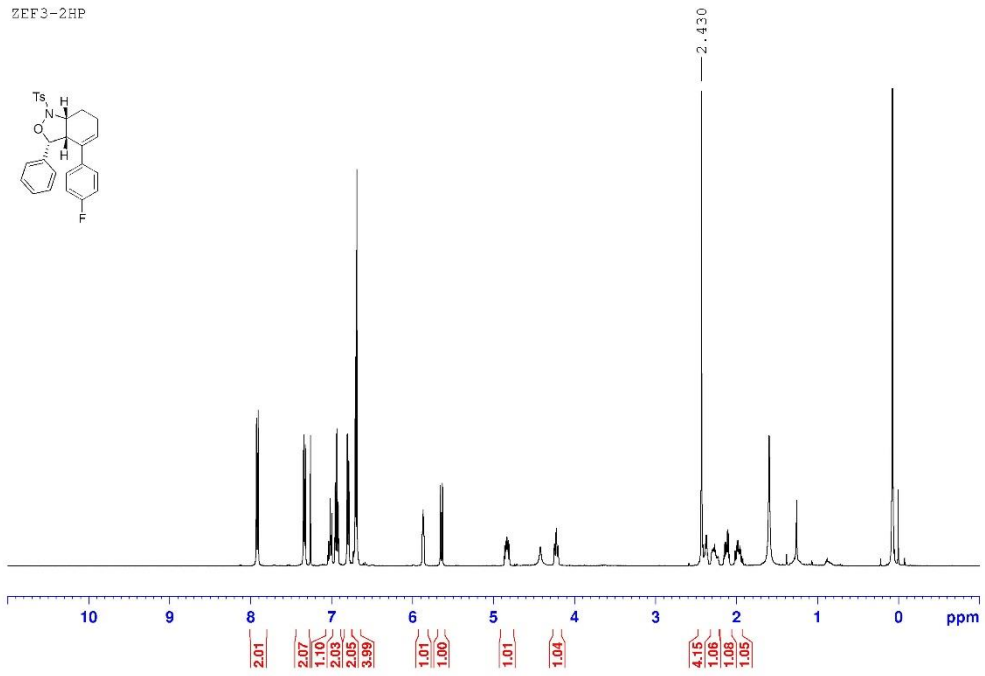
3x



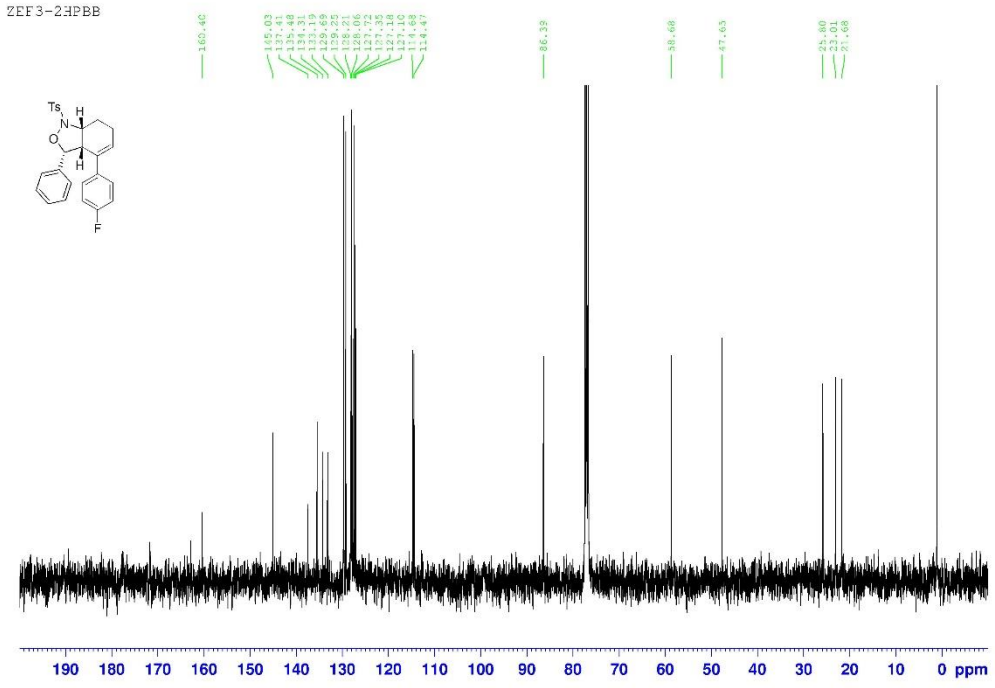
Left 5b, right 5b



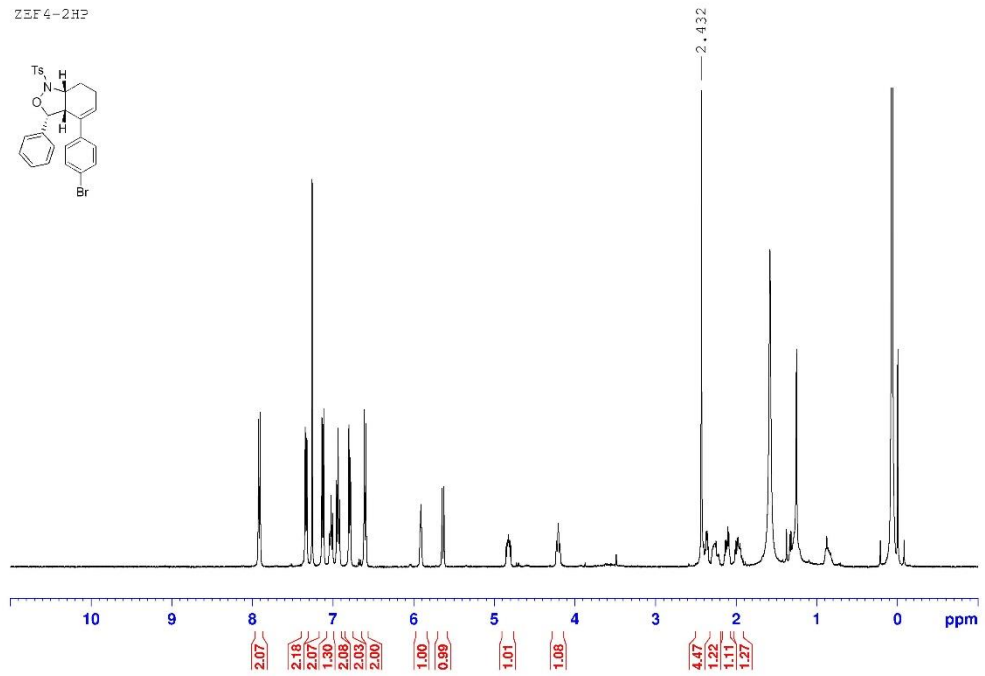
Left 5b, right 5b


ZEF3-2HP
2.430
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.07
1.10
2.03
2.05
3.99
1.01
1.00
1.01
1.04
4.15
1.06
1.08
1.05

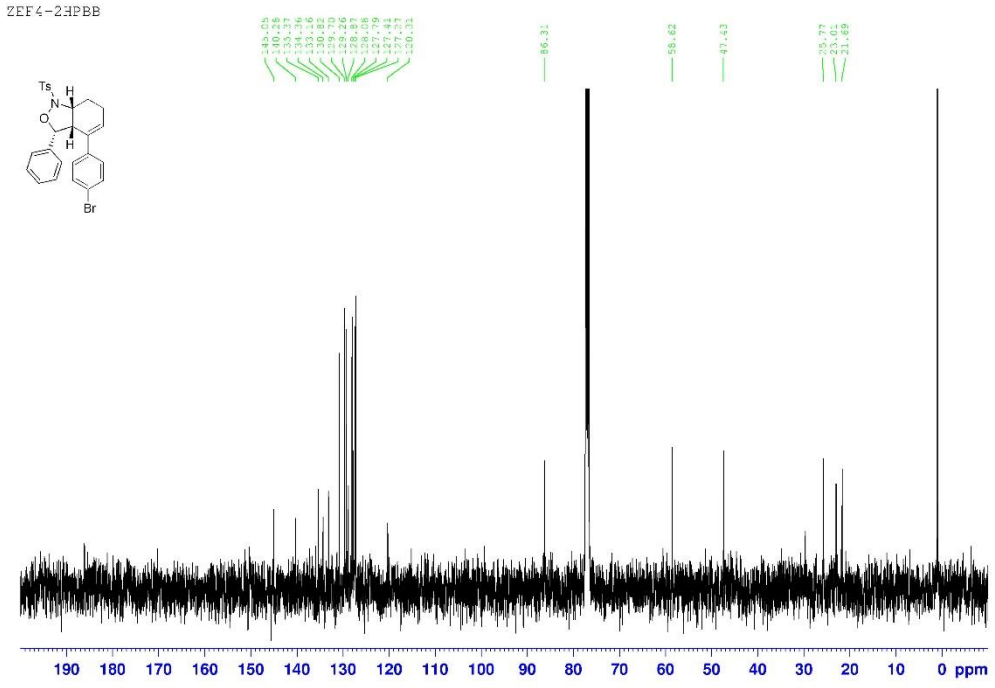
5b


ZEF3-2HPBB
160.46
145.03
137.41
135.48
134.31
133.69
129.49
129.25
128.21
128.06
127.72
127.35
127.18
127.10
114.68
114.47
86.39
58.68
47.63
25.80
23.01
21.68
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

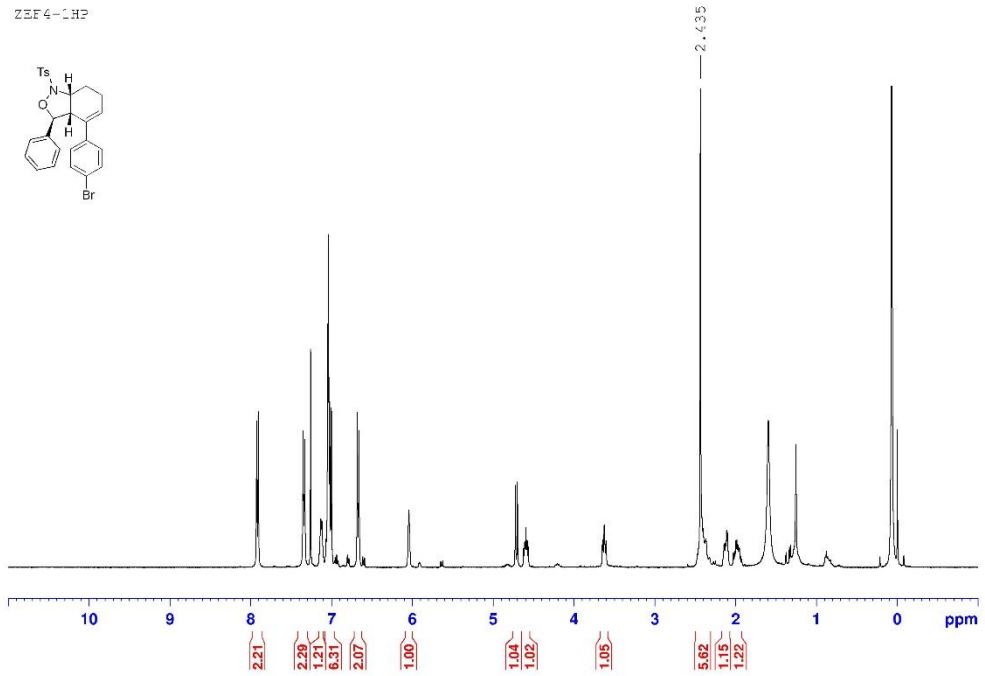
5b


ZEF4-2HP
Ts
N
O
H
H
Br
2.432
10
9
8
7
6
5
4
3
2
1
0
ppm
2.07
2.18
2.07
1.30
2.08
2.03
2.00
1.00
0.99
1.01
1.08
4.47
1.22
1.11
1.27

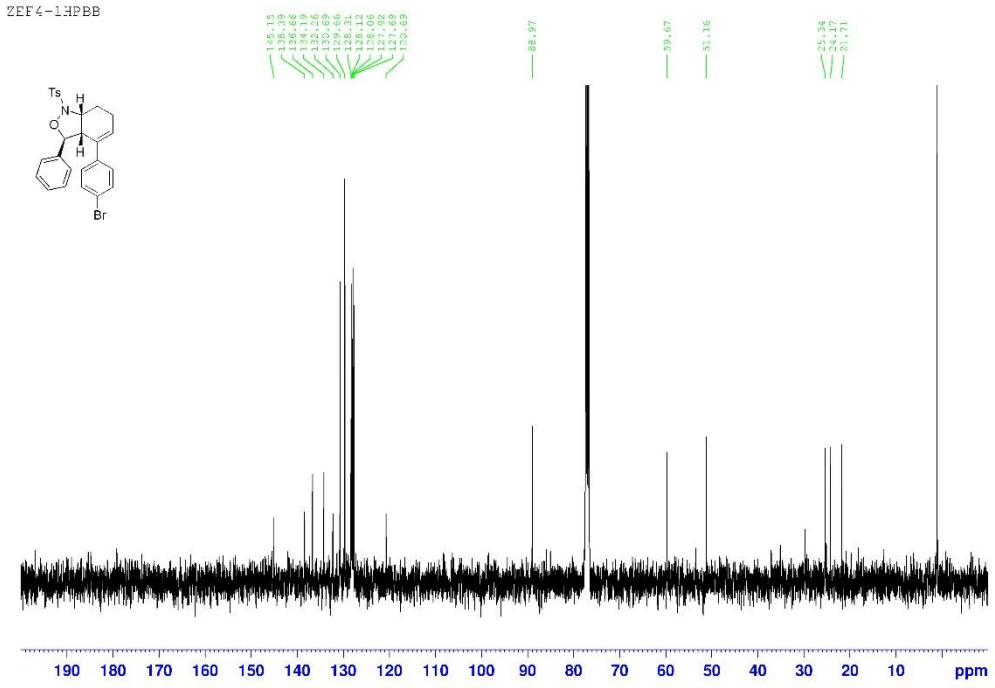
5c


ZEF4-2HPBB
Ts
N
O
H
H
Br
86.31
58.62
47.43
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

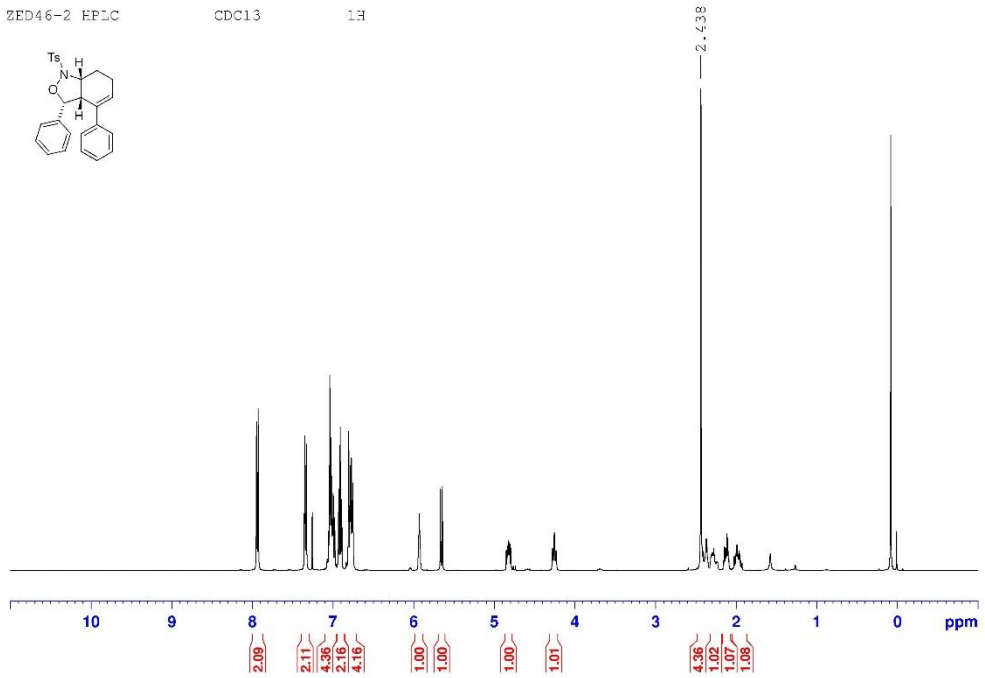
5c


ZEF4-1HP
Ts
N
H
O
H
Br
2.435
10
9
8
7
6
5
4
3
2
1
0
ppm
2.21
2.29
1.21
6.31
2.07
1.00
1.04
1.02
1.05
5.62
1.15
1.22

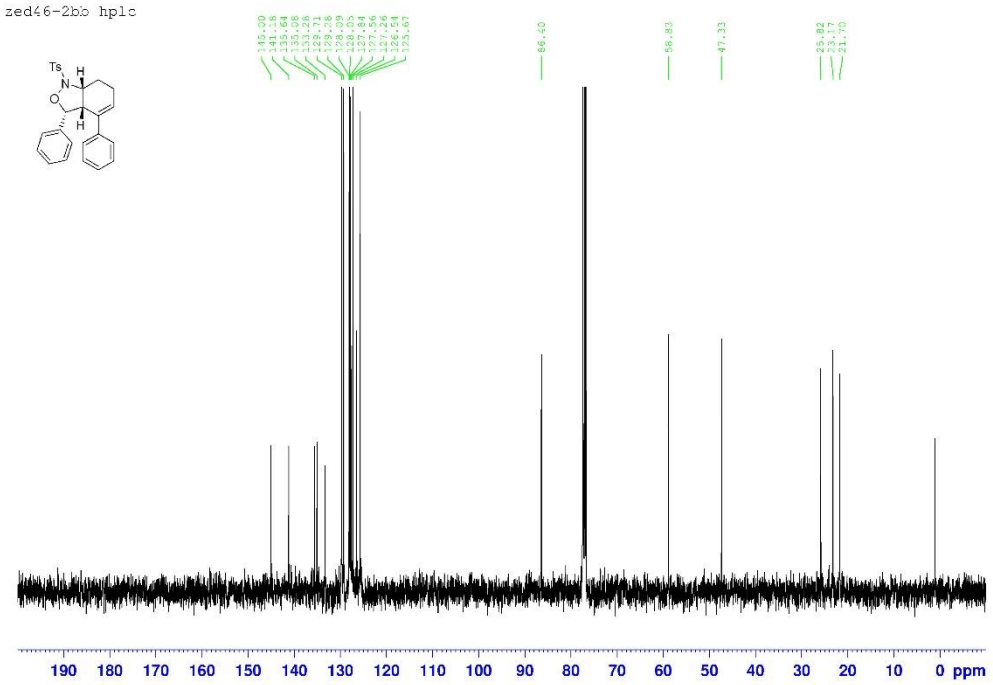
6c


ZEF4-1HPBB
Ts
N
H
O
H
Br
88.97
59.67
51.16
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

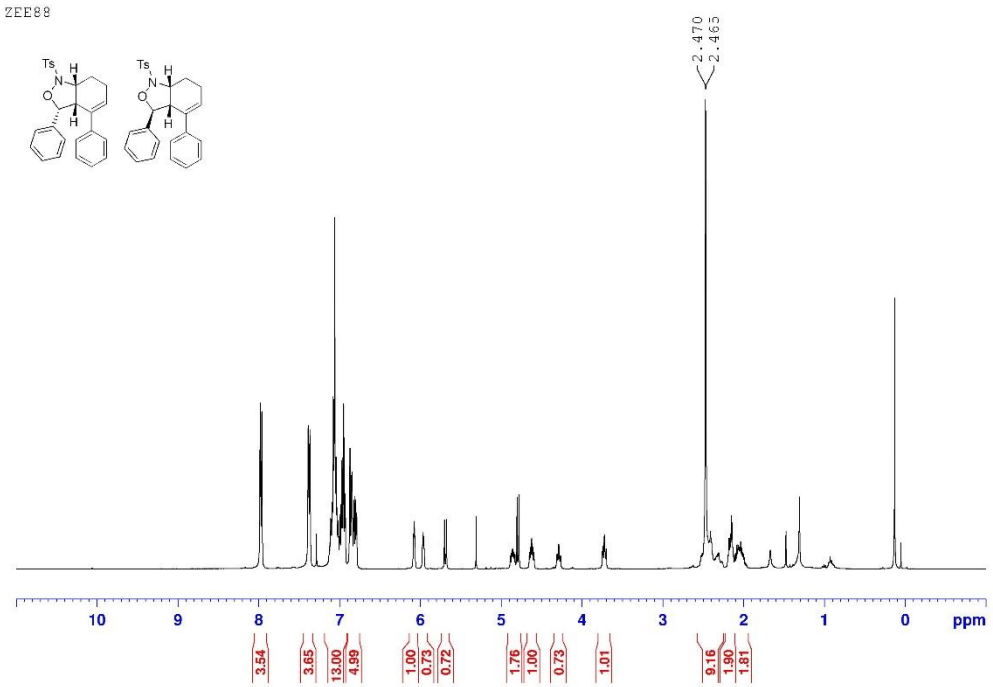
6c


ZED46-2 HPLC
CDC13
1H
Ts
N
H
O
H
2.4438
10
9
8
7
6
5
4
3
2
1
0
ppm
2.09
2.11
4.36
2.16
4.16
1.00
1.00
1.00
1.01
4.36
1.02
1.07
1.08

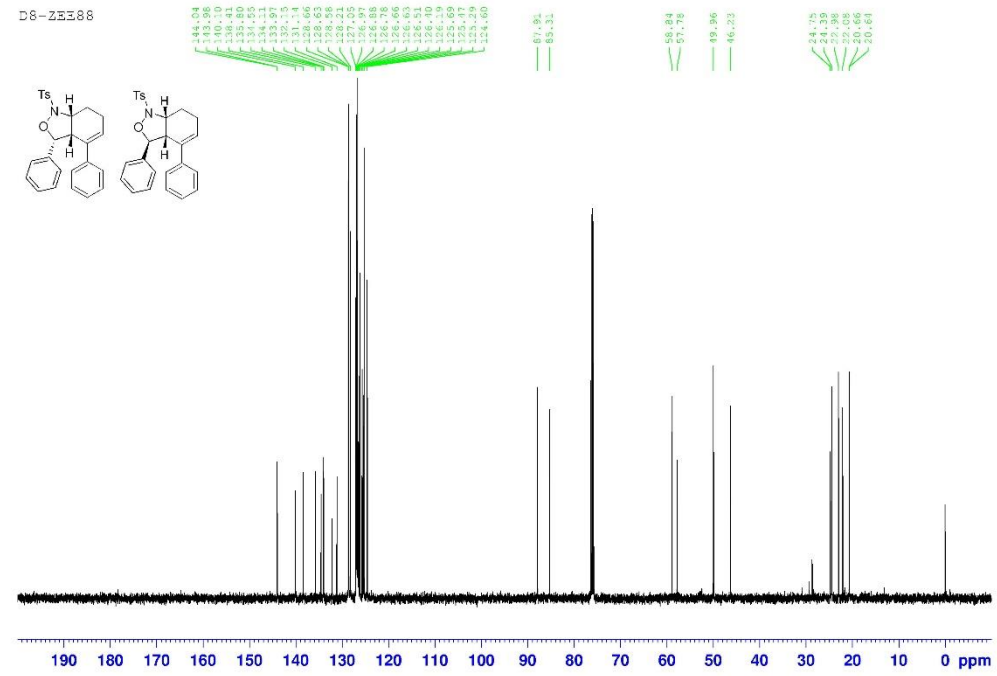
5d


zed46-2bb hplc
Ts
N
H
O
H
145.00
141.18
135.64
133.26
129.71
129.28
128.09
128.00
127.84
127.56
127.26
126.64
125.97
86.40
58.83
47.33
25.82
23.17
21.70
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

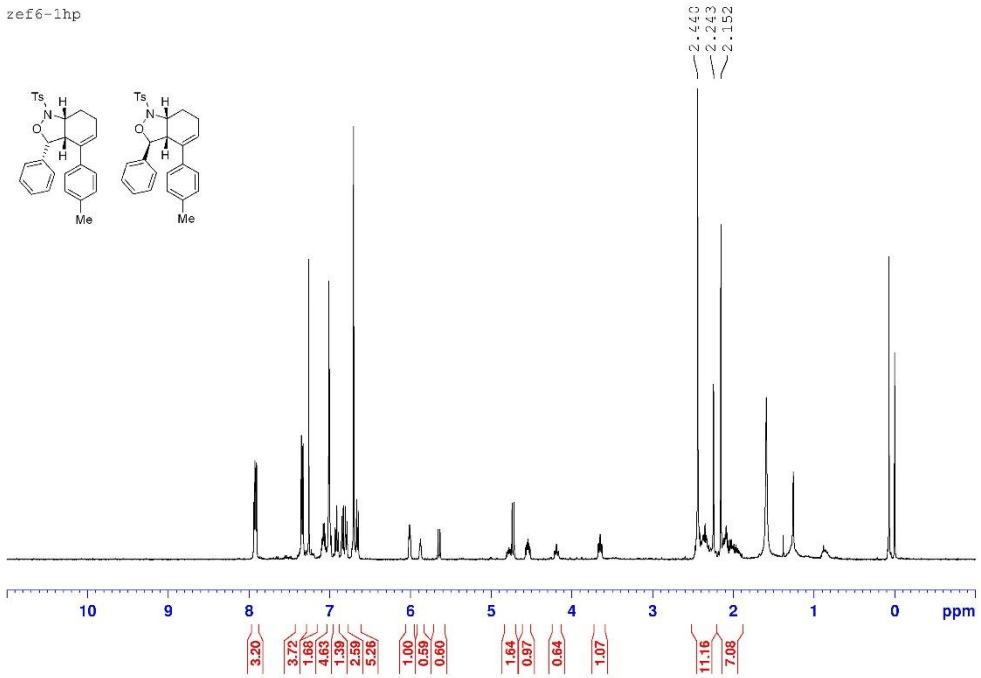
5d



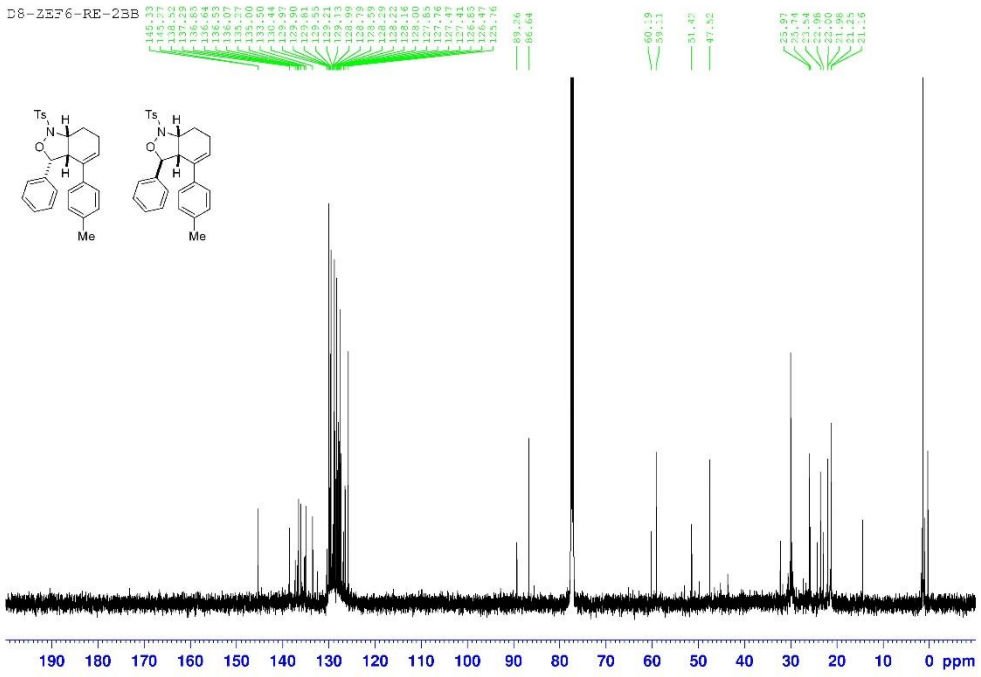
Left 5d, right 6d



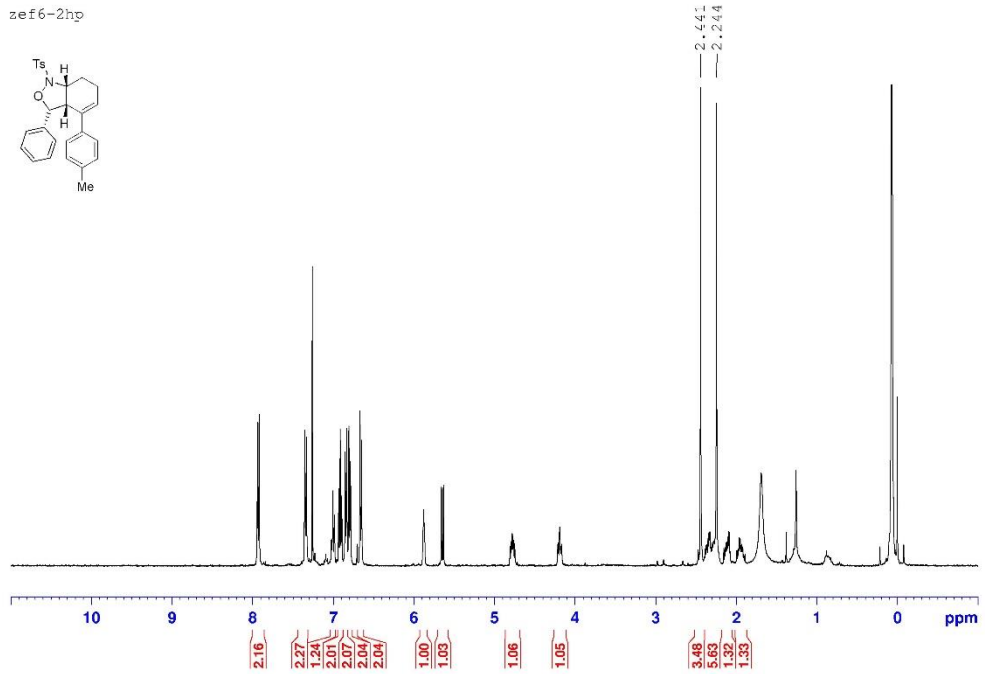
Left 5d, right 6d



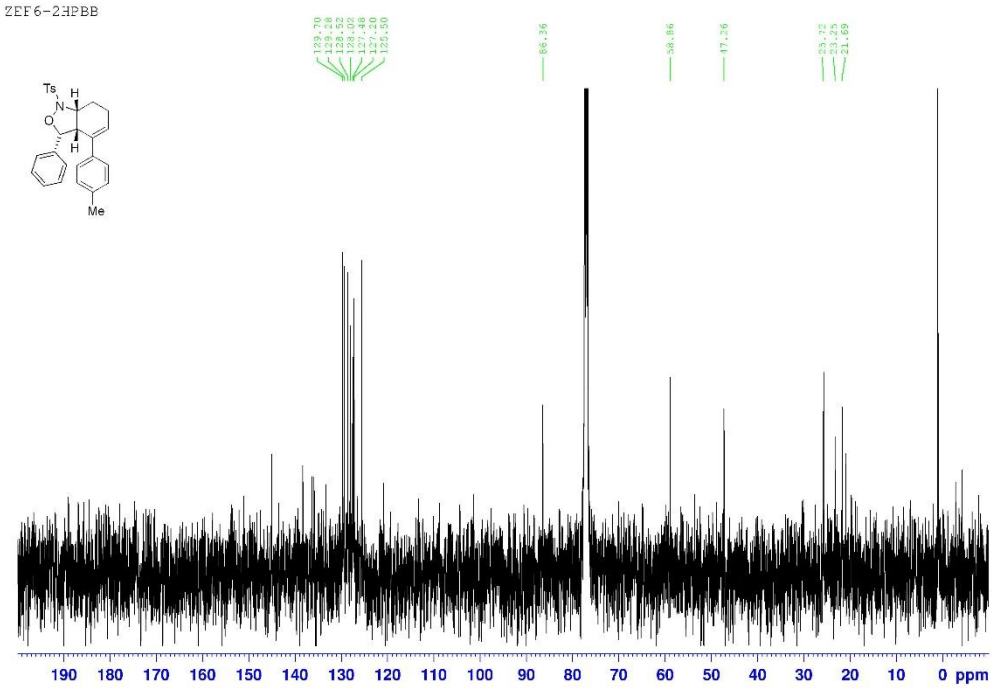
Left 5e, right 6e



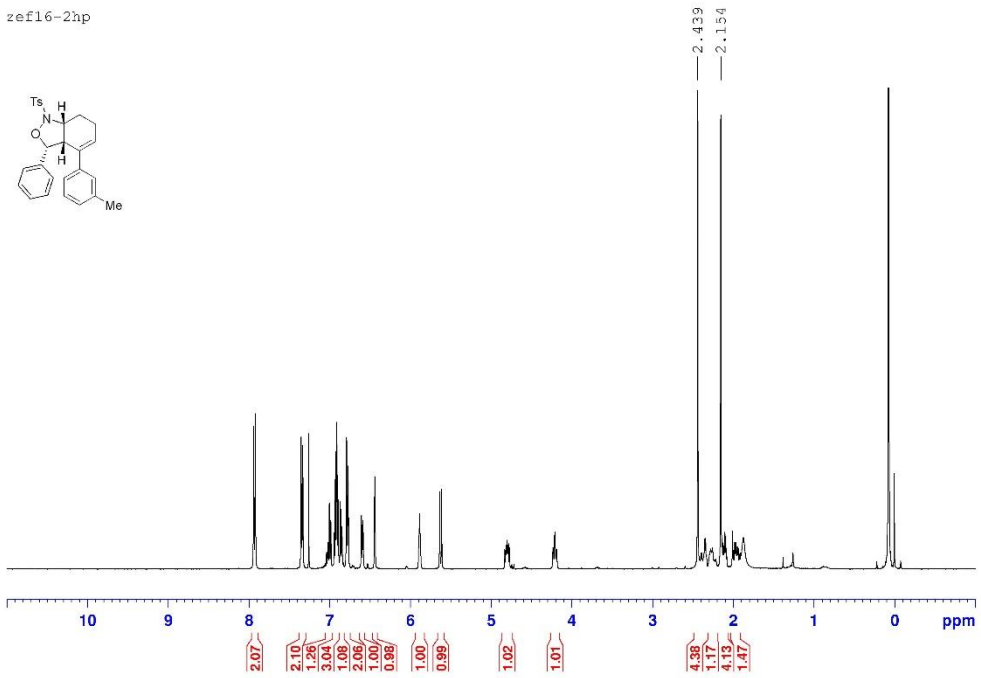
Left 5e, right 6e


zef6-2hp
Ts
H
N
O
H
Me
2.441
2.244
10
9
8
7
6
5
4
3
2
1
0
ppm
2.16
2.27
1.24
2.01
2.07
2.04
2.04
1.00
1.03
1.06
1.05
3.48
5.63
1.32
1.33

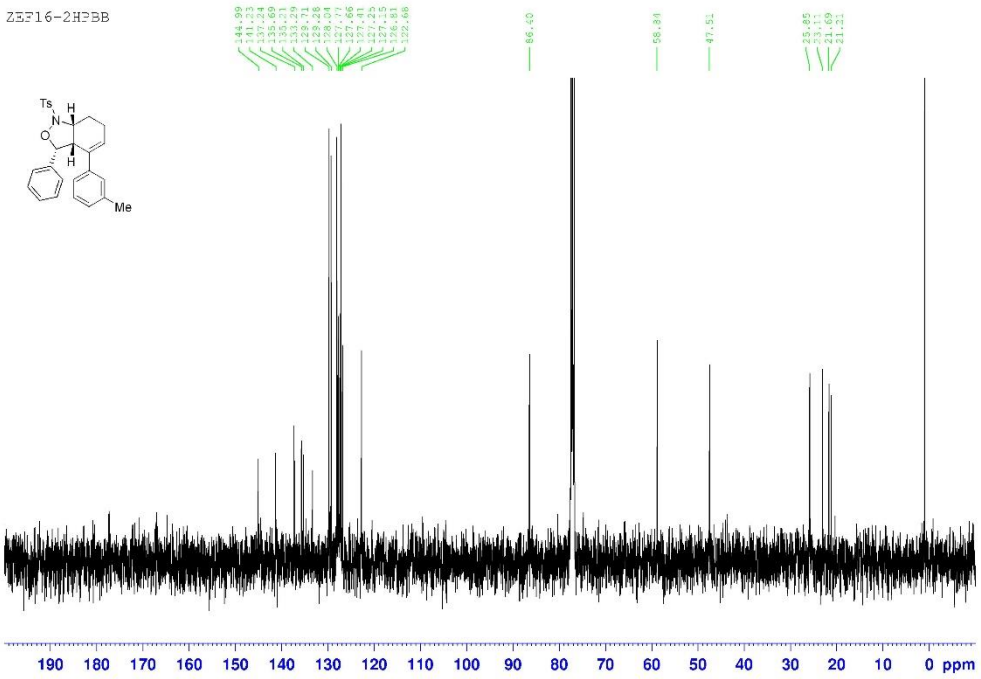
5e


ZEF6-2HPBB
Ts
H
N
O
H
Me
129.70
129.28
128.52
128.30
127.48
127.20
125.50
86.36
58.86
47.26
25.72
23.25
21.69
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

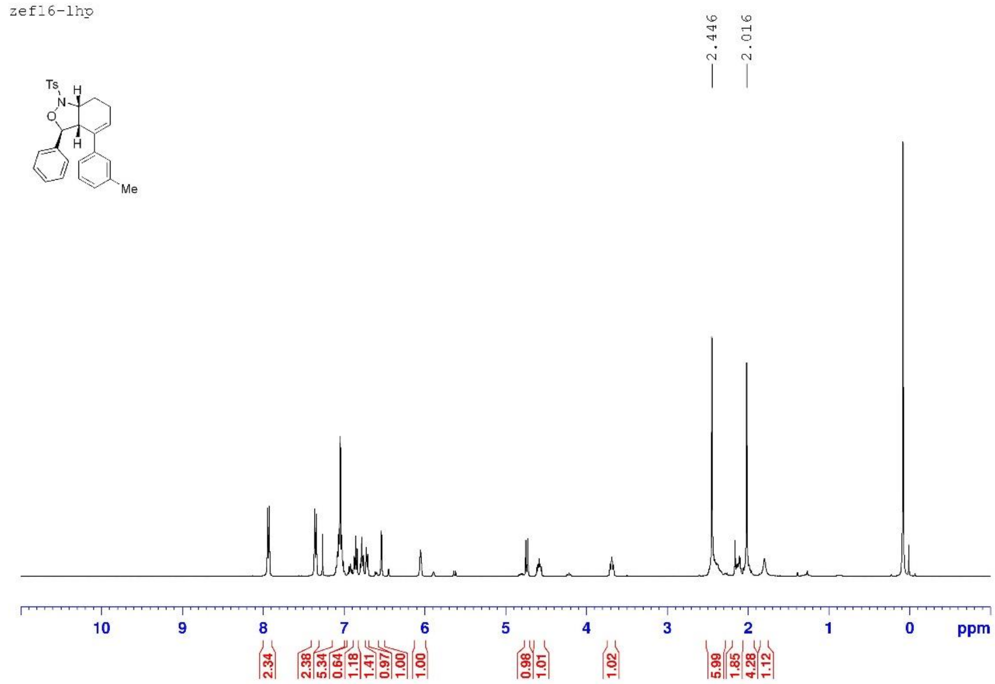
6e


zef16-2hp
Ts
N
O
H
H
Me
2.439
2.154
10
9
8
7
6
5
4
3
2
1
0
ppm
2.07
2.10
1.26
3.04
1.08
2.05
1.00
0.98
1.00
0.99
1.02
1.01
4.38
1.17
4.13
1.47

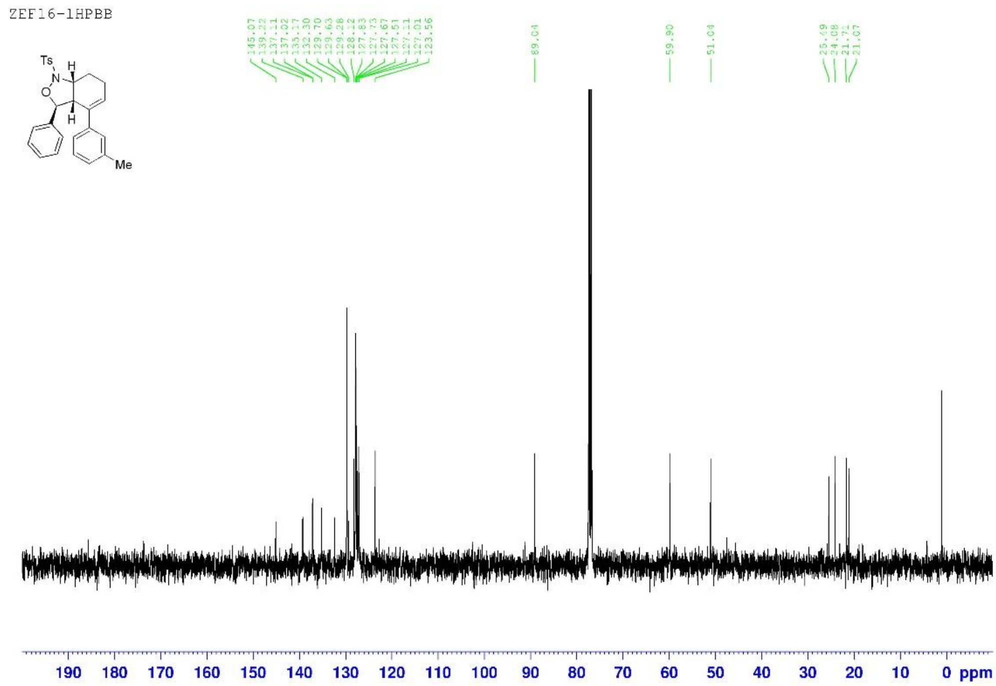
5f


ZEF16-2HPBB
144.99
141.23
137.24
135.69
135.11
133.29
129.71
129.28
128.04
127.77
127.66
127.41
127.25
126.53
126.31
122.66
86.40
58.34
47.51
25.85
23.15
21.69
21.32
Ts
N
O
H
H
Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

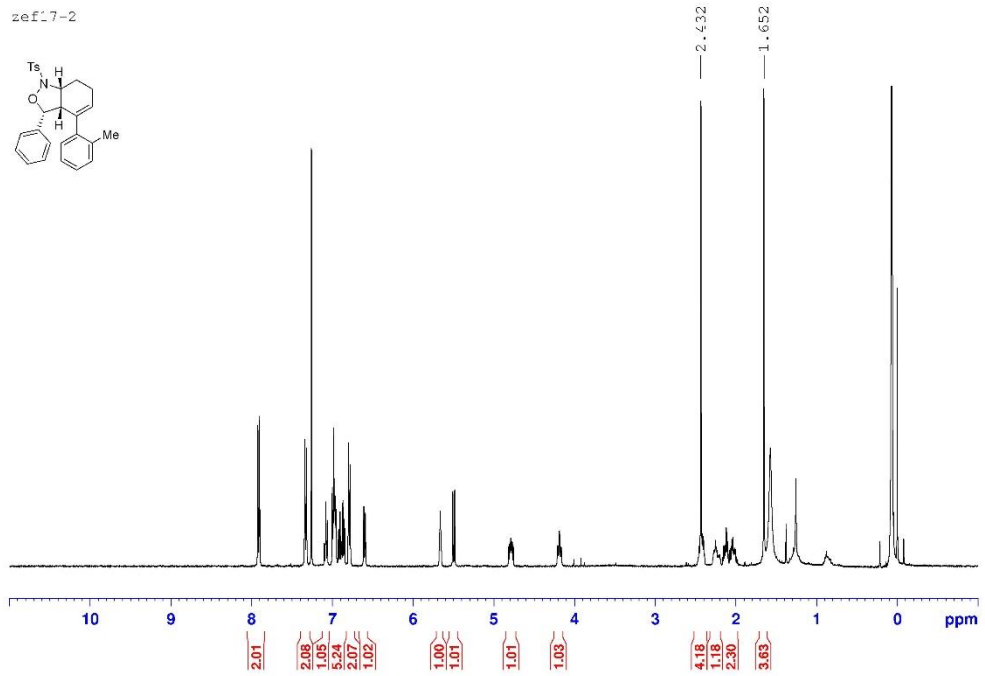
5f



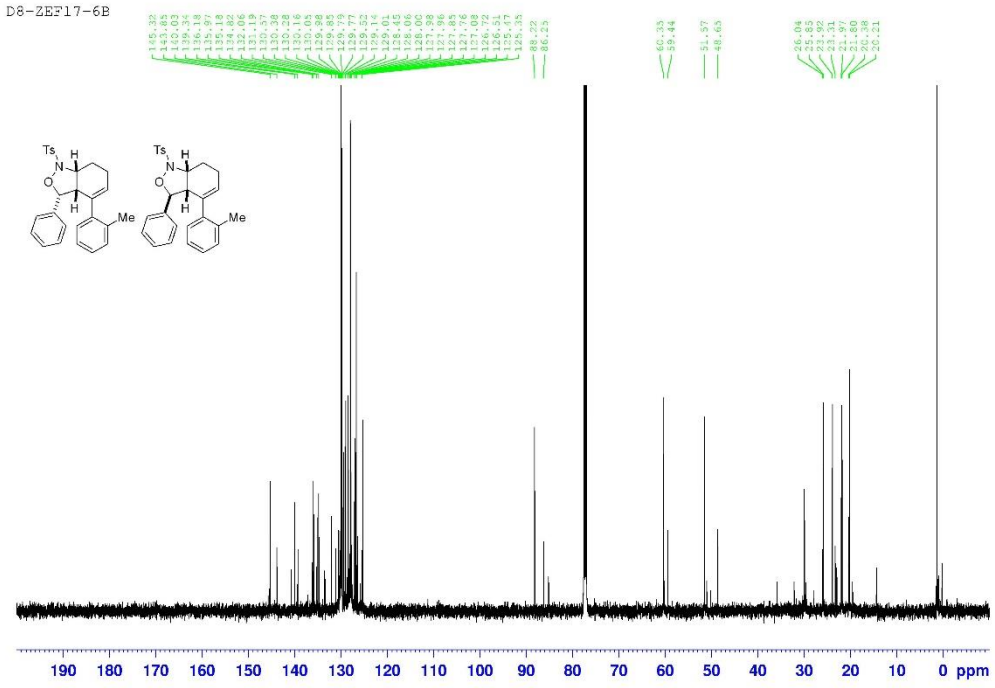
6f



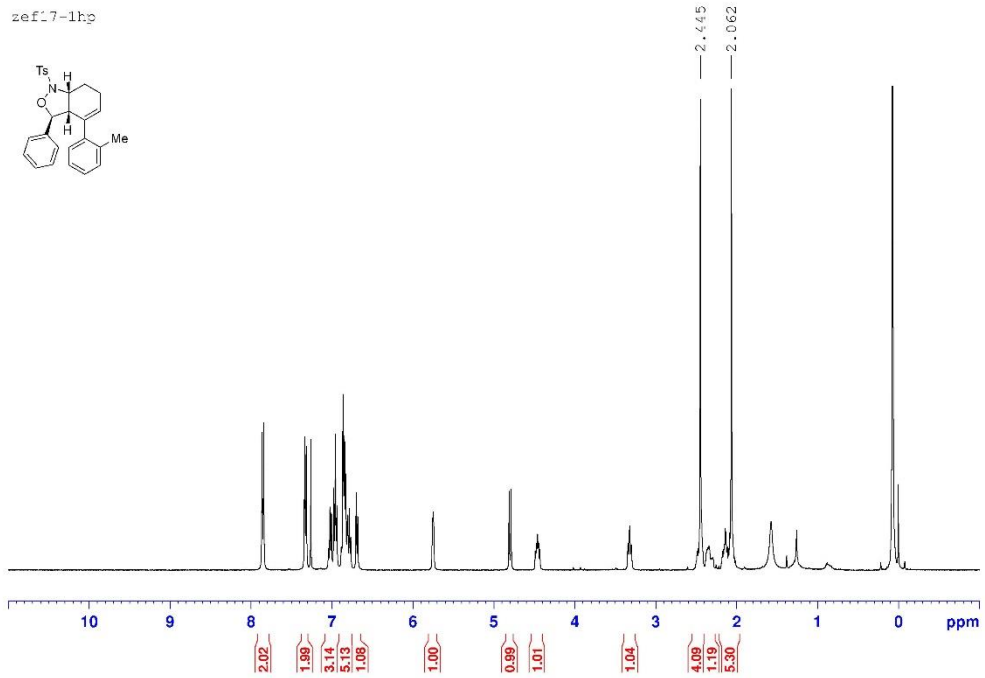
6f


zef17-2
Ts
H
N
O
H
Me
2.432
1.652
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.08
1.05
5.24
2.07
1.02
1.00
1.01
1.01
1.03
4.18
1.18
2.30
3.63

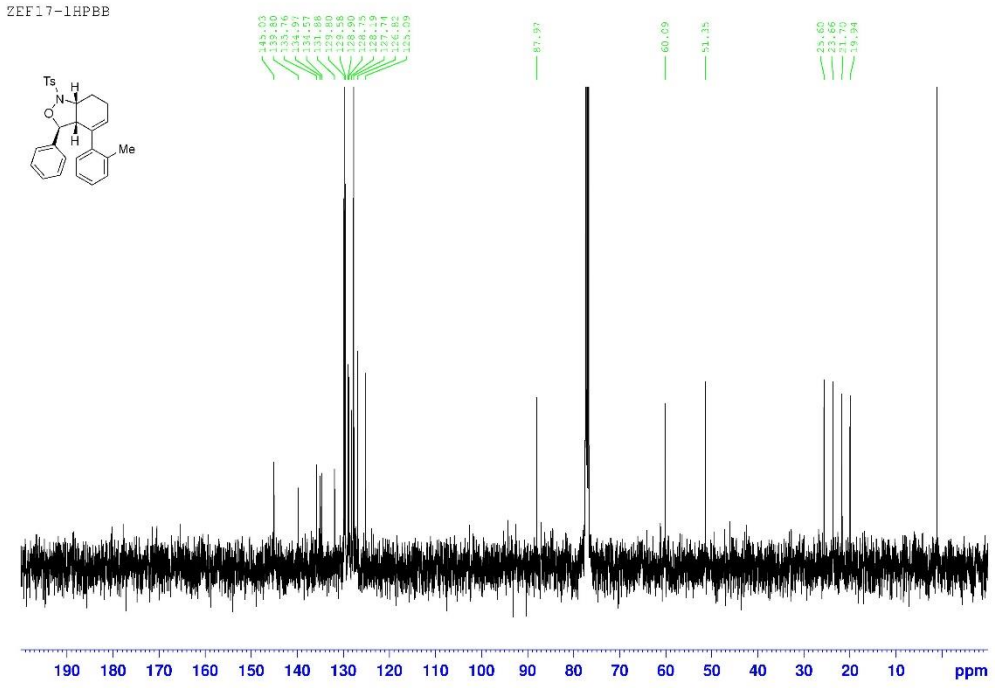
5g


D8-ZEF17-6B
Ts
H
N
O
H
Me
Ts
H
N
O
H
Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

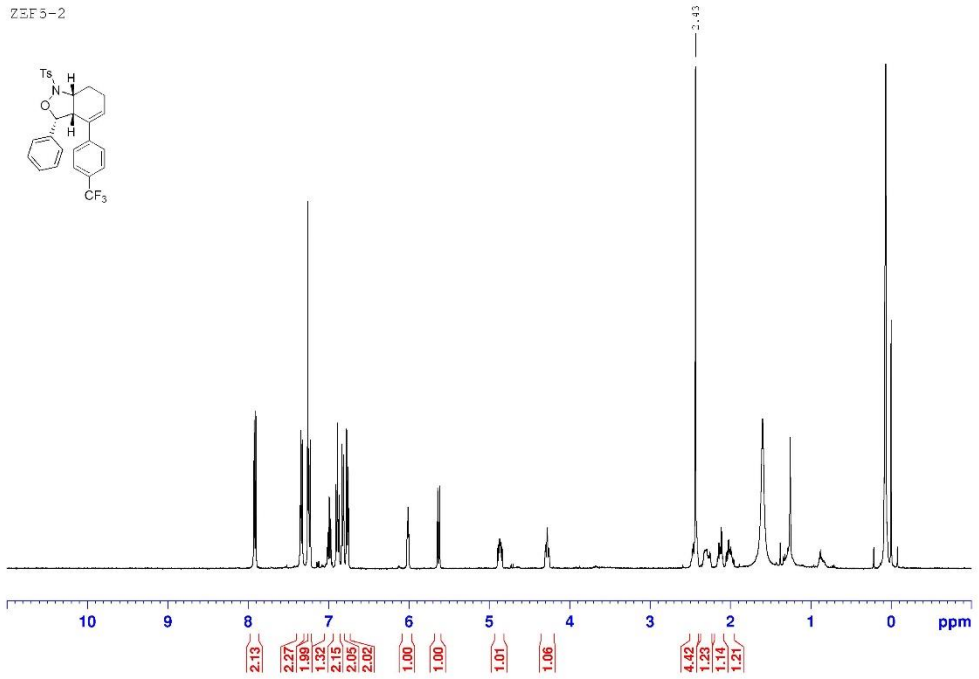
5g


zef17-1hp
Ts
N
O
H
H
Me
2.445
2.062
10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
1.99
3.14
5.13
1.08
1.00
0.99
1.01
1.04
4.09
1.19
5.30

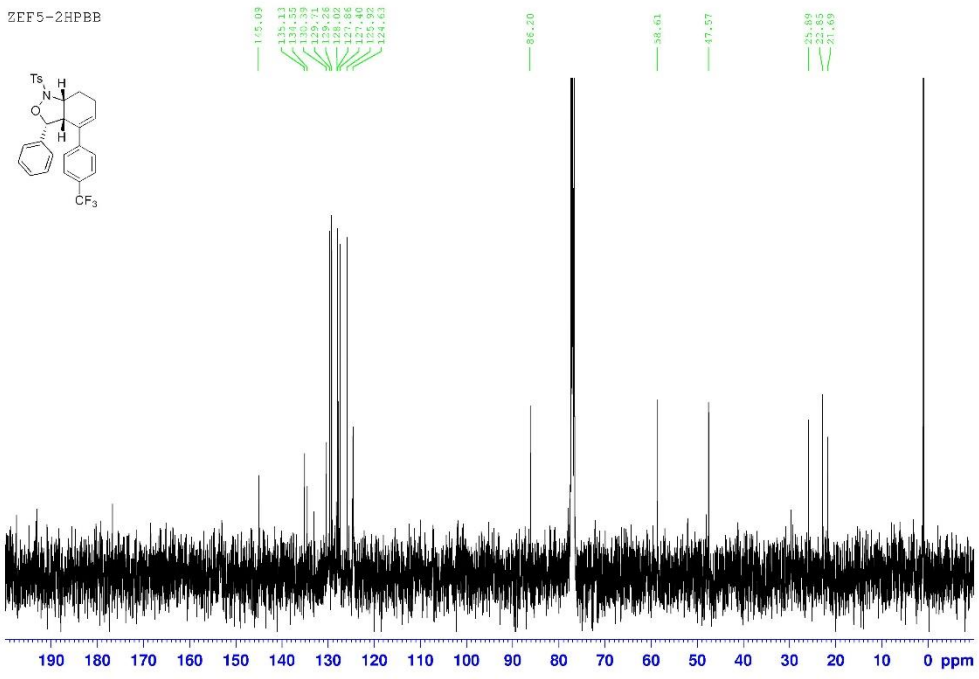
6g


ZEF17-1HPBB
Ts
N
O
H
H
Me
87.97
60.09
51.35
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

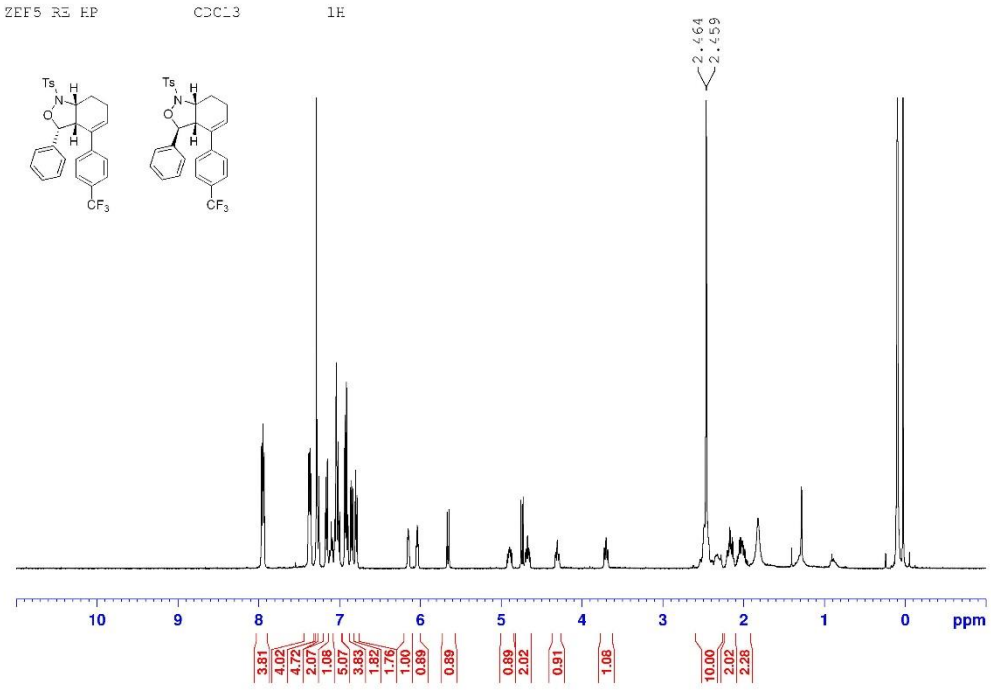
6g


ZEF5-2
Ts
N
O
H
H
CF3
2.43
10
9
8
7
6
5
4
3
2
1
0
ppm
2.13
2.27
1.99
1.32
2.15
2.05
2.02
1.00
1.00
1.01
1.06
4.42
1.23
1.14
1.21

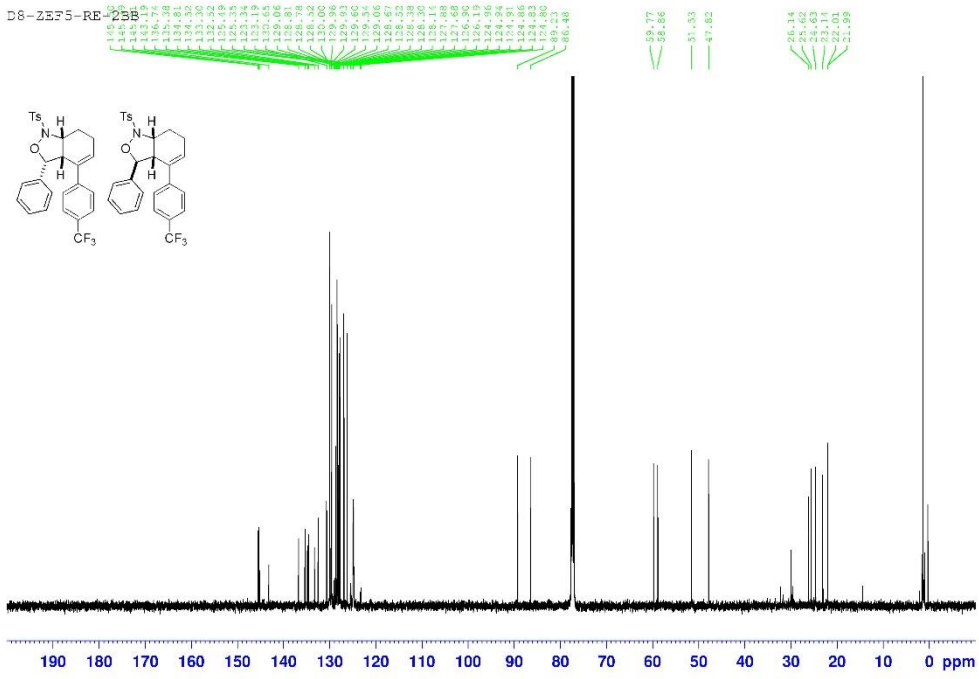
5h


ZEF5-2HPBB
Ts
N
O
H
H
CF3
148.09
135.13
134.55
130.39
129.71
128.58
128.02
127.86
127.40
125.92
124.63
86.20
58.61
47.57
25.89
22.85
21.69
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

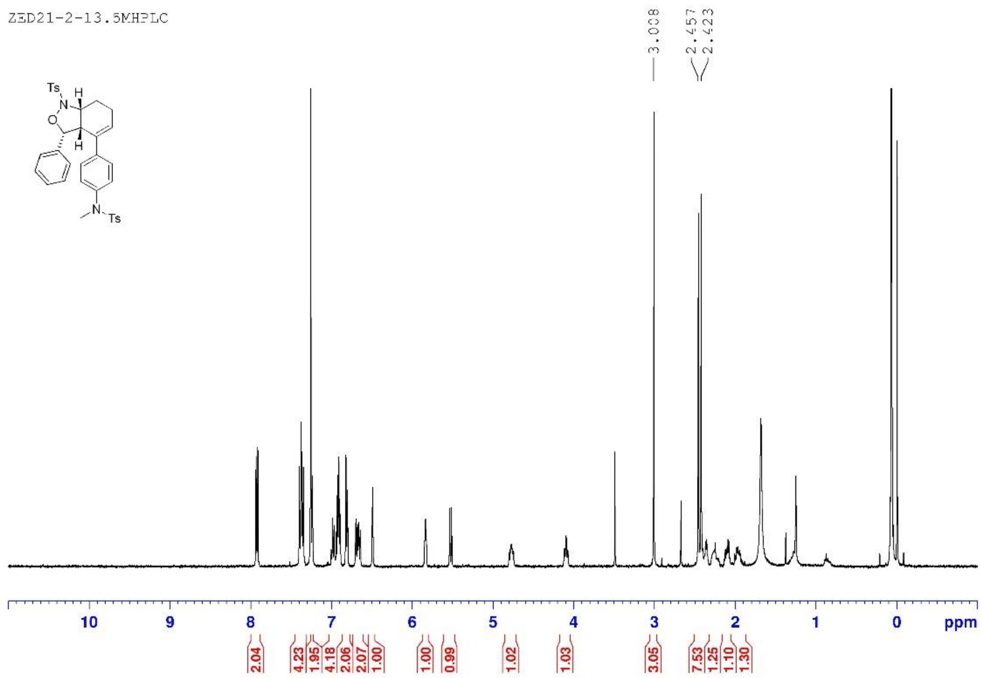
5h



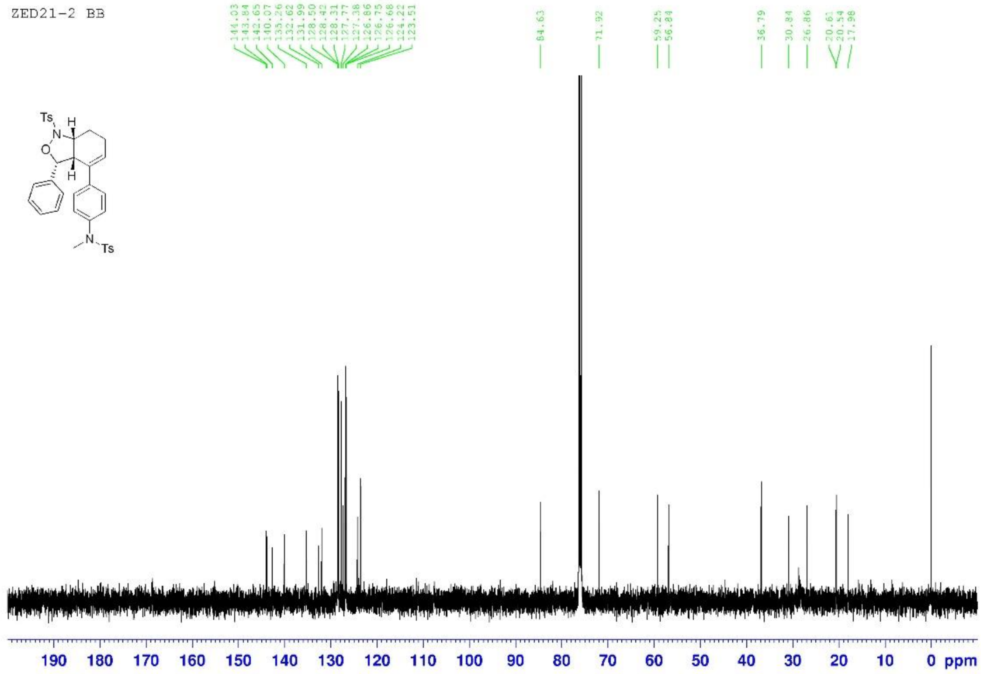
Left 5h, right 6h



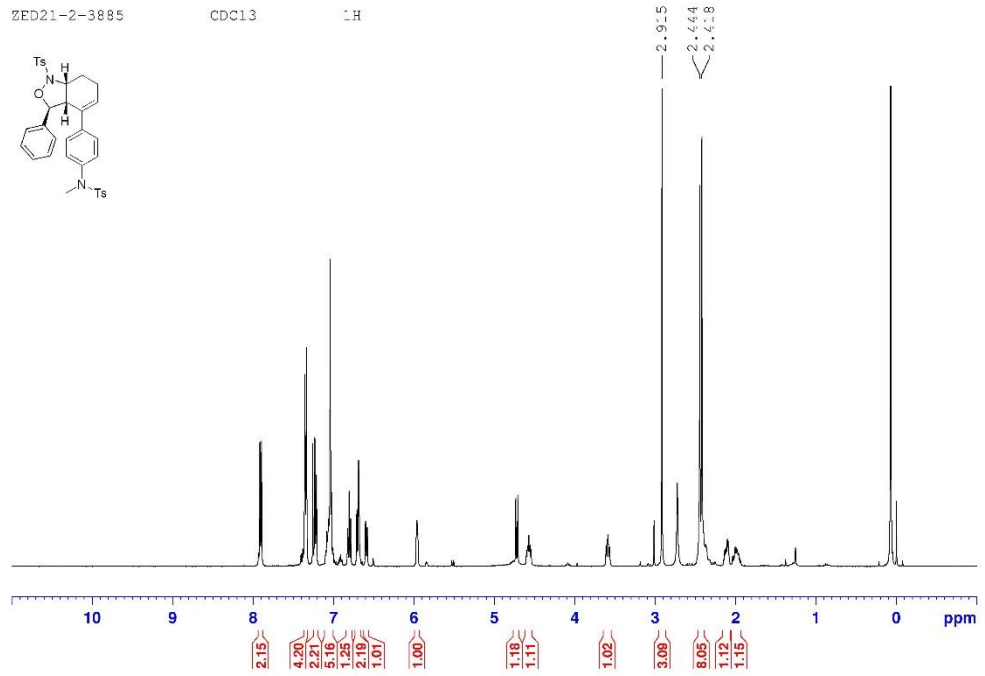
Left 5h, right 6h


ZED21-2-13.5MHPLC
Ts
N
H
O
H
N
Ts
3.008
2.457
2.423
10
9
8
7
6
5
4
3
2
1
0
ppm
2.04
4.23
1.95
4.18
2.06
2.07
1.00
1.00
0.99
1.02
1.03
3.05
7.53
1.25
1.10
1.30

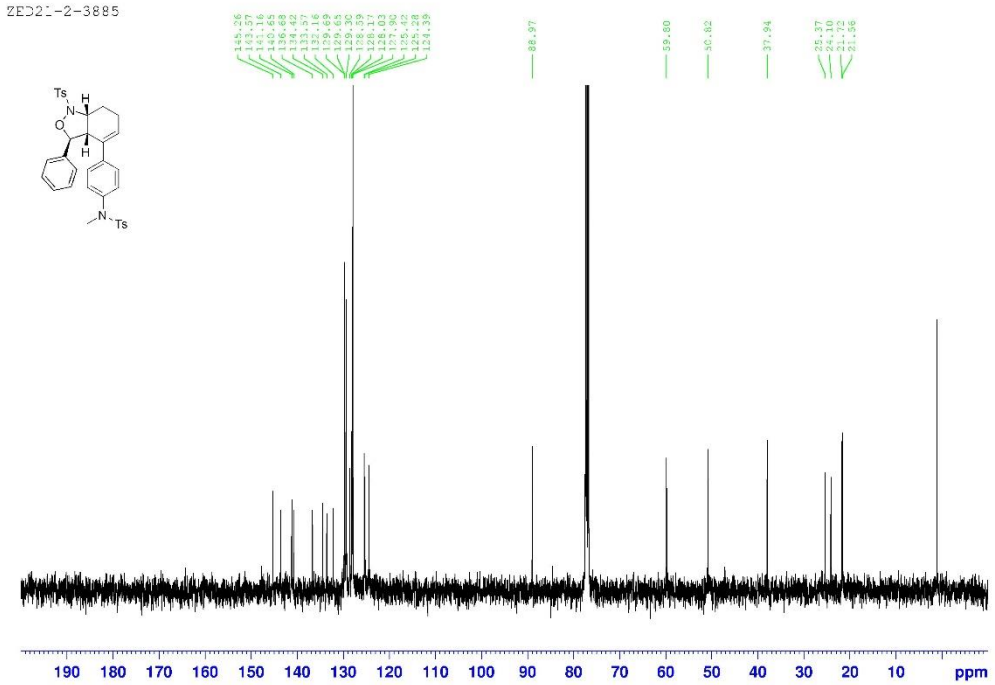
5i


ZED21-2 BB
Ts
N
H
O
H
N
Ts
84.63
71.92
36.79
30.84
26.86
20.54
17.98
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

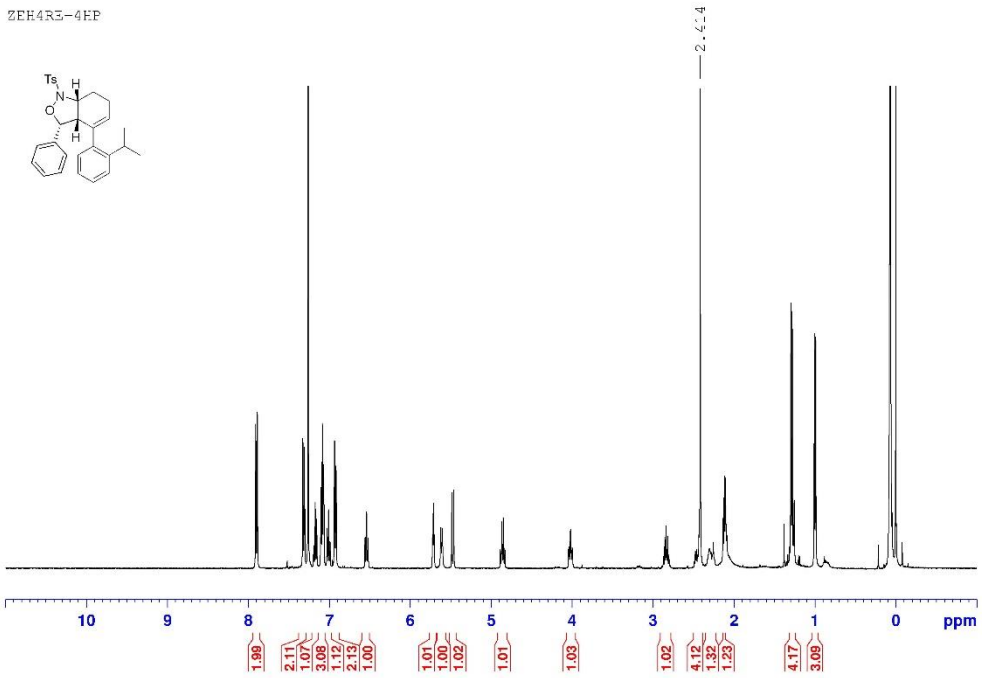
5i


ZED21-2-3885
CDCl3
1H
2.915
2.444
2.428
10
9
8
7
6
5
4
3
2
1
0
ppm
2.15
4.20
2.21
5.16
1.25
2.19
1.01
1.00
1.18
1.11
1.02
3.09
8.05
1.12
1.15

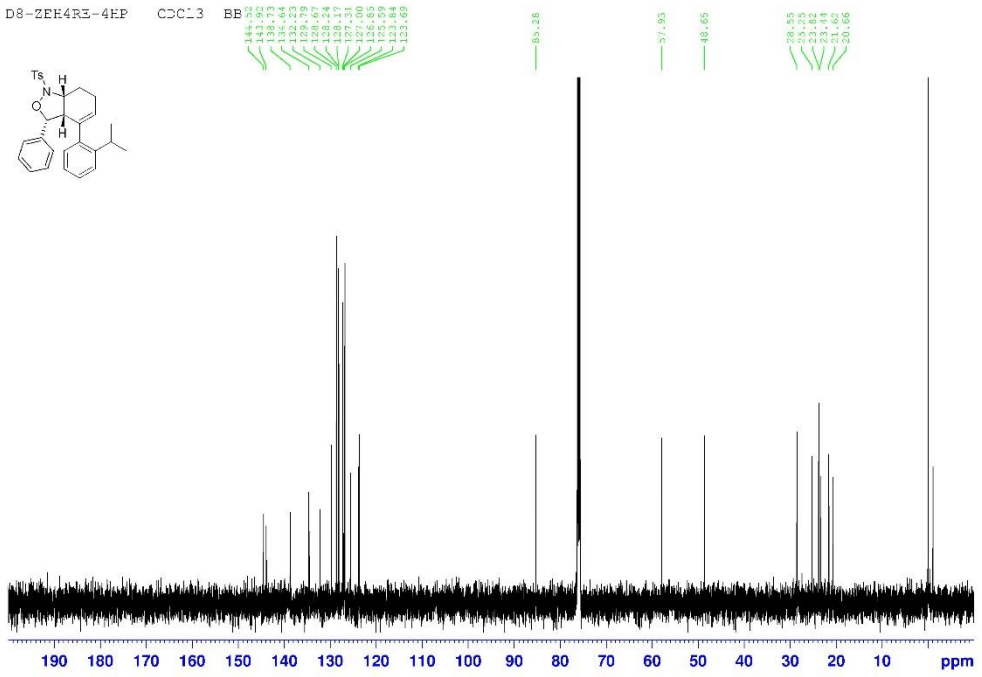
6i


ZED21-2-3885
88.97
59.80
50.82
37.94
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

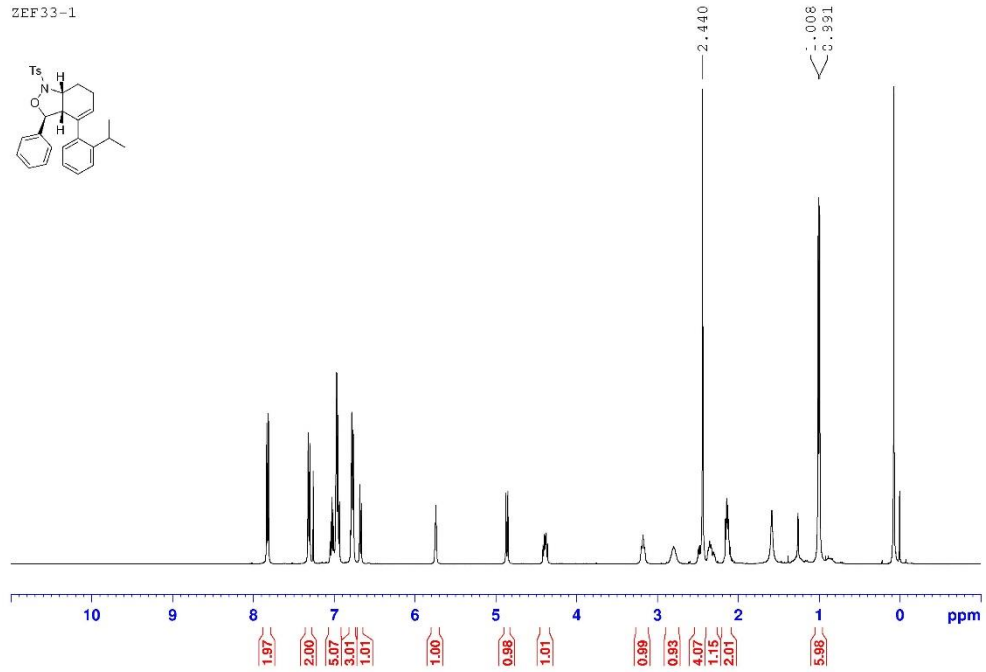
6i


ZEH4R3-4EP
Ts
N
O
H
H
2.414
10
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.11
1.07
3.08
1.12
2.13
1.00
1.01
1.00
1.02
1.01
1.03
1.02
4.12
1.32
1.23
4.17
3.09

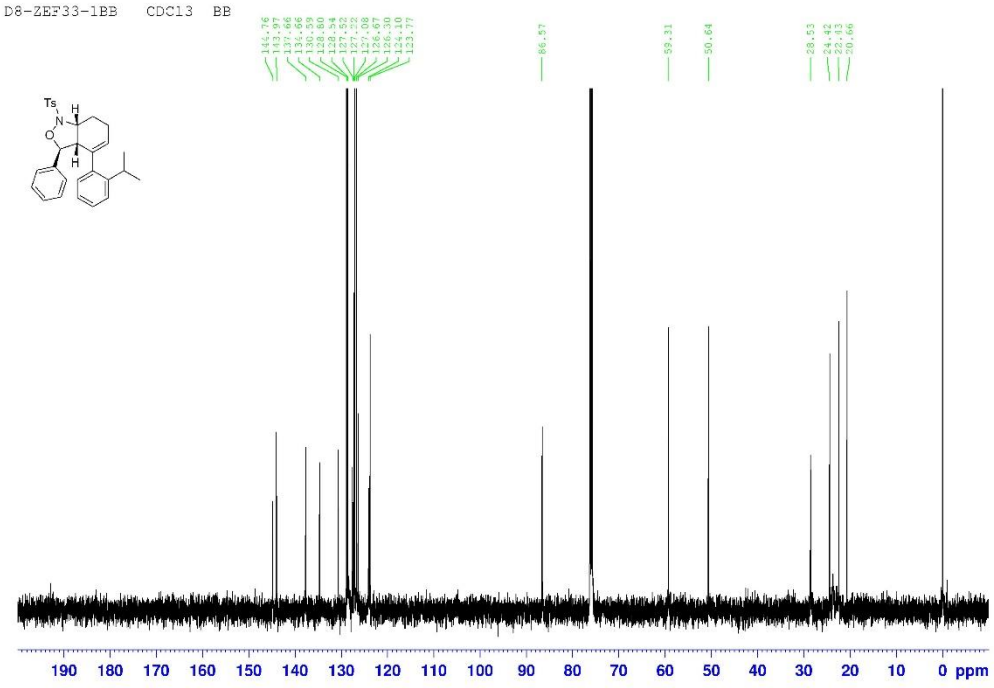
5j


D8-ZEH4R3-4EP CDCl3 BB
144.52
143.92
138.73
135.04
132.23
129.79
128.67
128.54
128.17
127.31
127.00
126.65
125.59
123.84
123.69
85.28
57.93
48.65
28.55
25.20
23.62
23.44
21.62
20.66
Ts
N
O
H
H
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

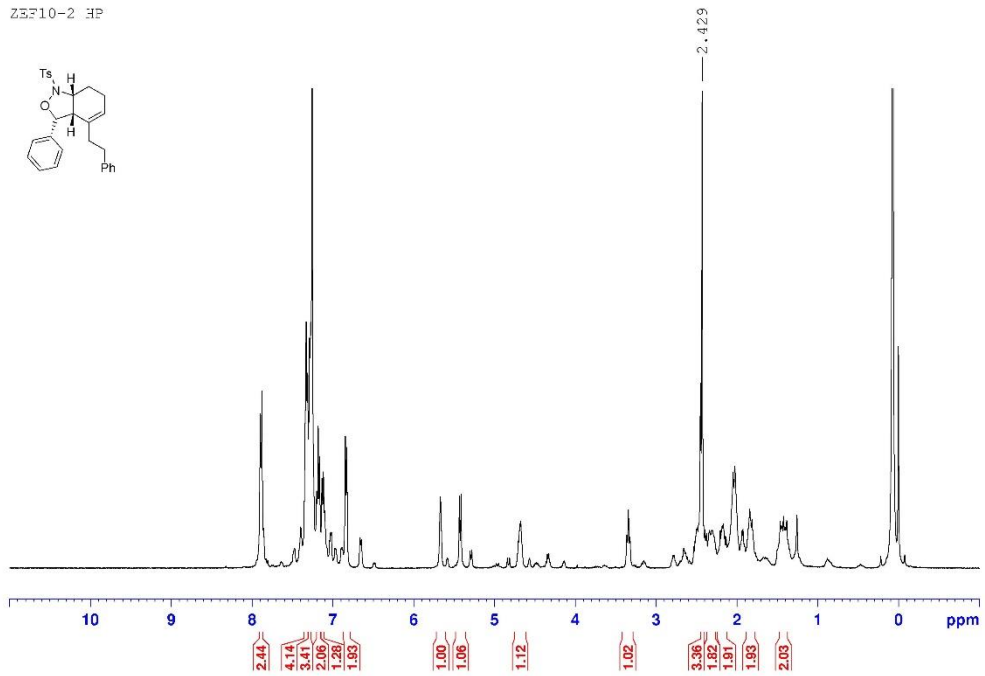
5j


ZEF33-1
Ts
H
N
O
H
2.440
1.008
3.931
10
9
8
7
6
5
4
3
2
1
0
ppm
1.97
2.00
5.07
3.01
1.01
1.00
0.98
1.01
0.99
0.93
4.07
1.15
2.01
5.98

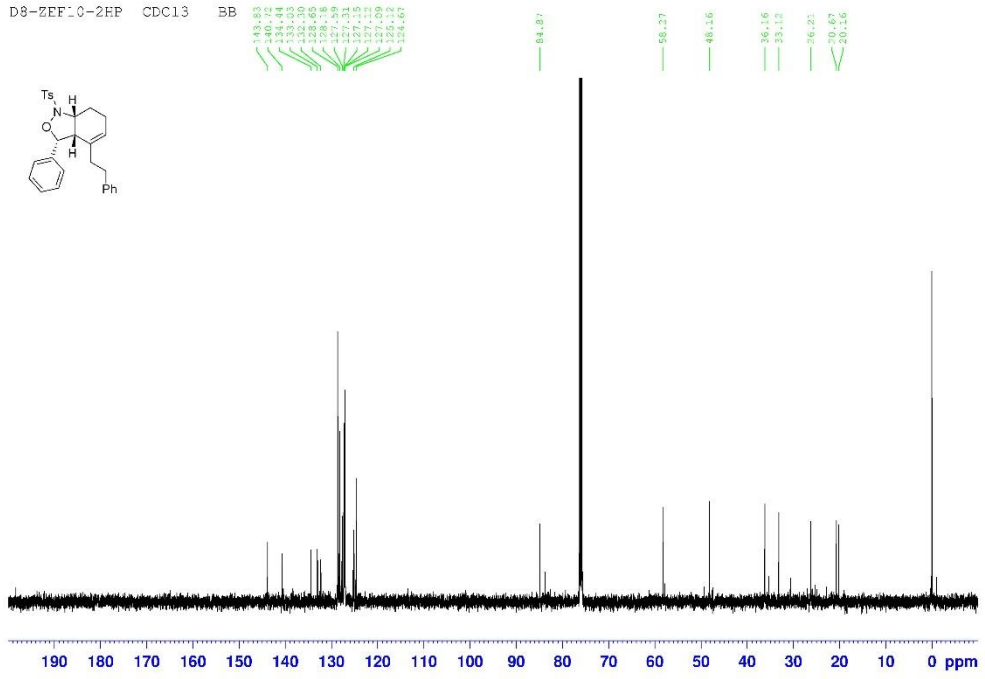
6j


D8-ZEF33-1BB CDCl3 BB
Ts
H
N
O
H
146.76
143.97
137.66
135.66
130.59
128.80
128.54
127.52
127.22
127.08
126.67
126.30
124.10
123.77
86.57
59.31
50.64
28.53
24.42
23.13
20.66
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

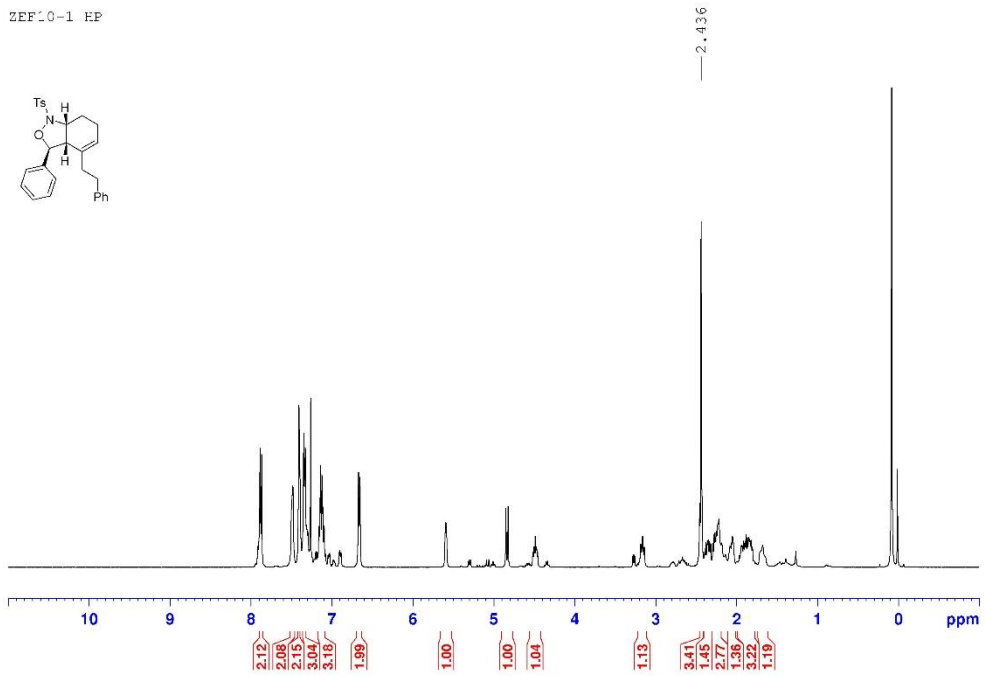
6j


ZEP10-2 HP
Ts
H
N
O
H
Ph
2.429
10
9
8
7
6
5
4
3
2
1
0
ppm
2.44
4.14
3.41
2.06
1.28
1.93
1.00
1.06
1.12
1.02
3.36
1.82
1.91
1.93
2.03

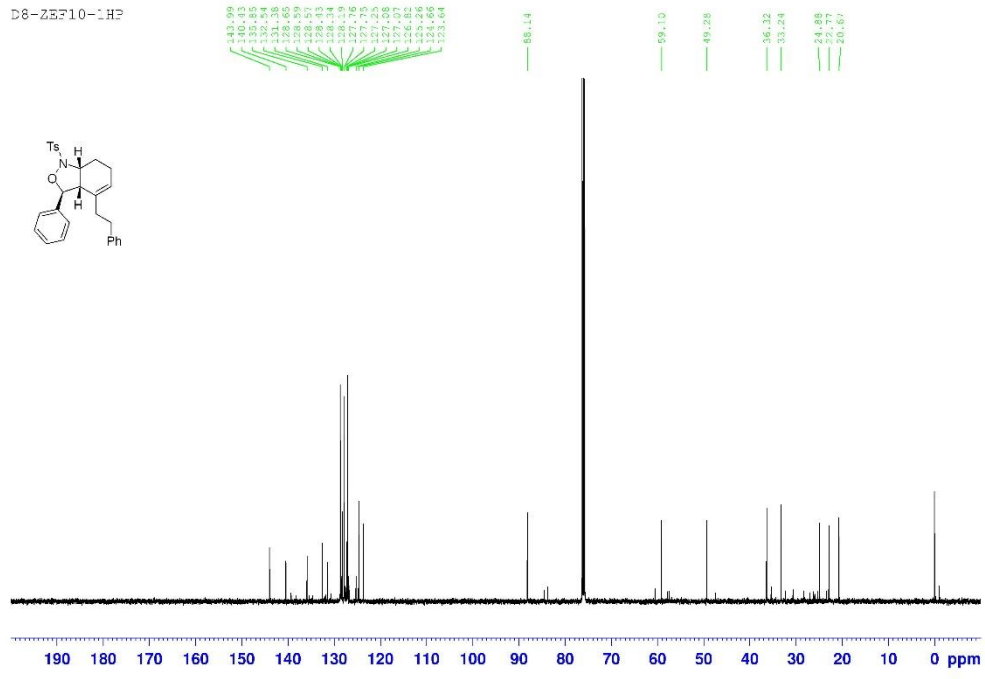
5l


D8-ZEP10-2HP CDCl3 BB
143.83
140.72
134.44
133.33
133.00
128.65
128.18
127.59
127.31
127.15
127.12
127.09
125.12
124.67
84.87
58.27
48.16
36.16
33.12
26.21
20.67
20.16
Ts
H
N
O
H
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

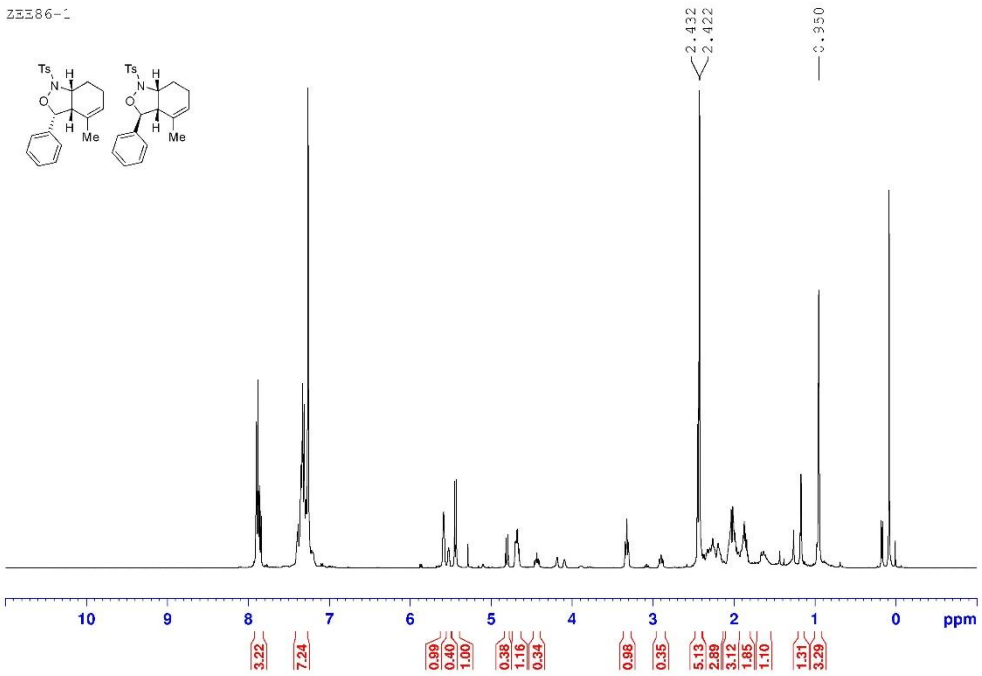
5l


ZEF10-1 HP
2.436
Ts
N
O
H
H
Ph
10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
2.08
2.15
3.04
3.18
1.99
1.00
1.00
1.04
1.13
3.41
1.45
2.77
1.36
3.22
1.19

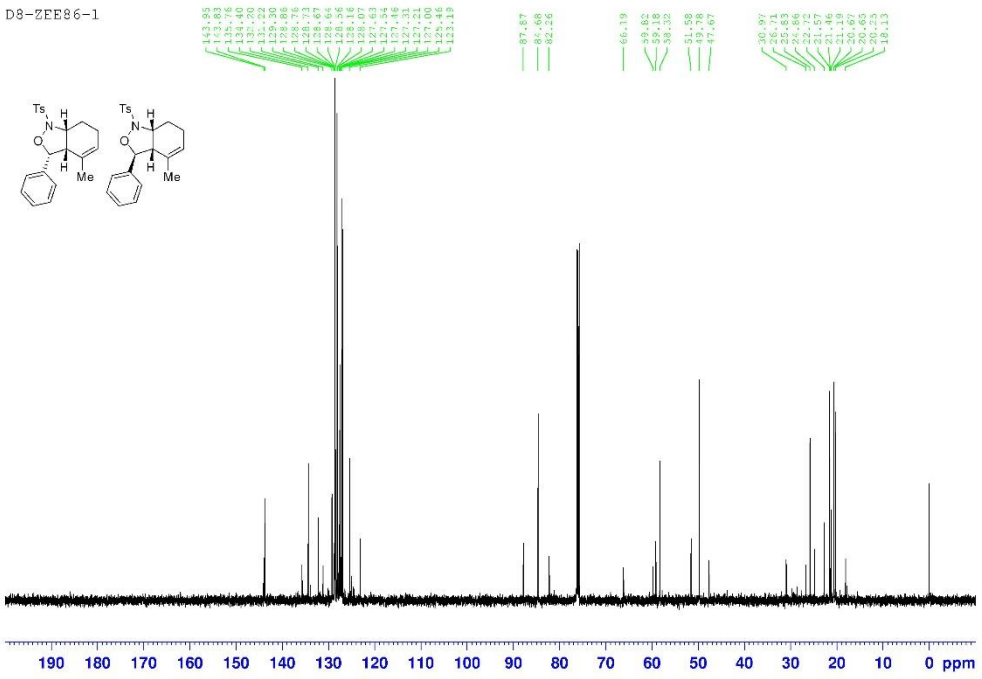
6l


D8-ZEF10-1HP
143.99
140.43
135.85
132.54
131.38
128.80
128.59
128.57
128.13
128.04
127.76
127.75
127.25
127.08
127.07
126.82
125.26
124.66
123.64
88.14
59.10
49.28
36.32
33.24
24.88
22.77
20.67
Ts
N
O
H
H
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

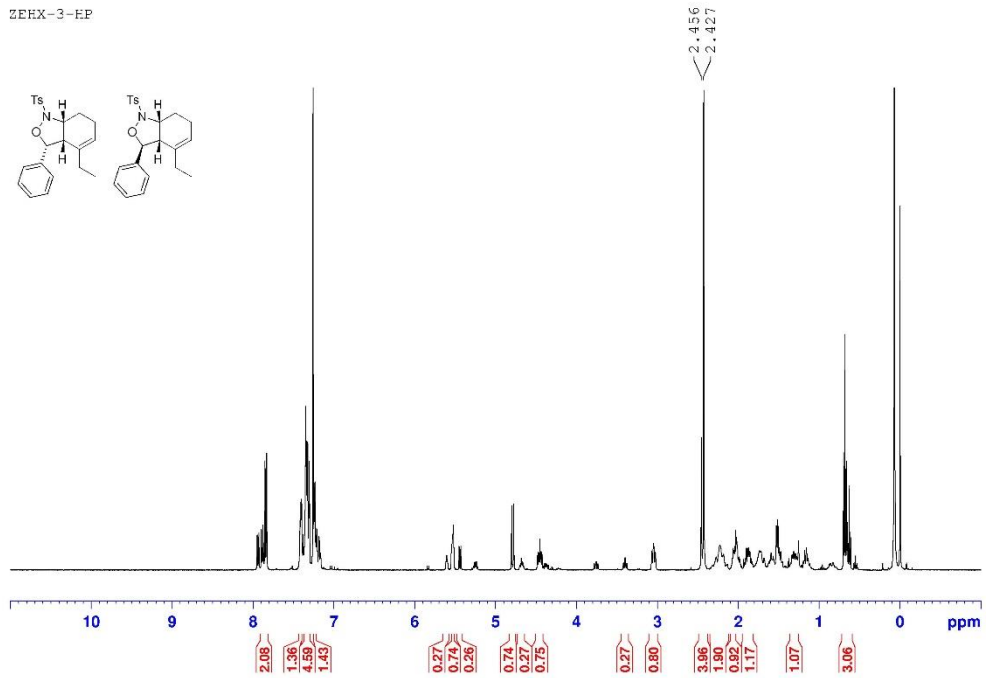
6l



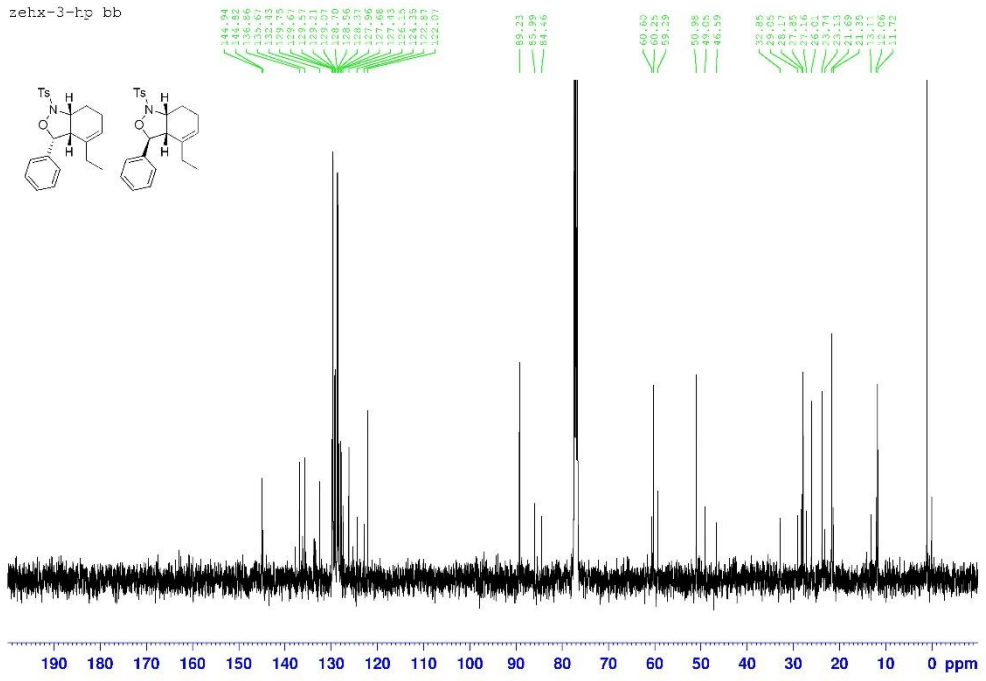
Left 5m, right 6m



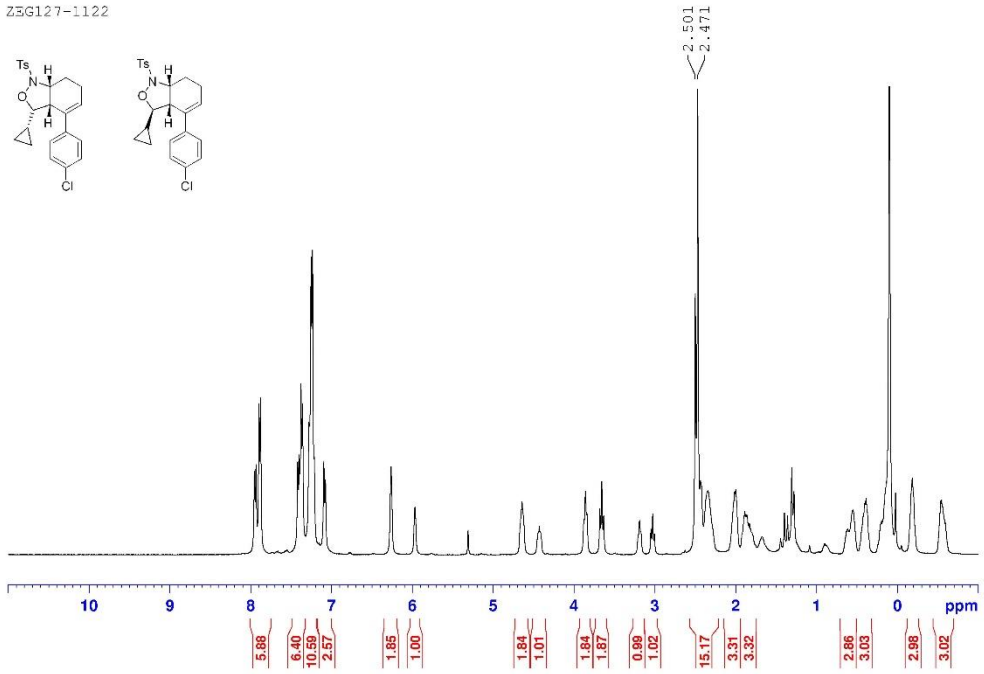
Left 5m, right 6m



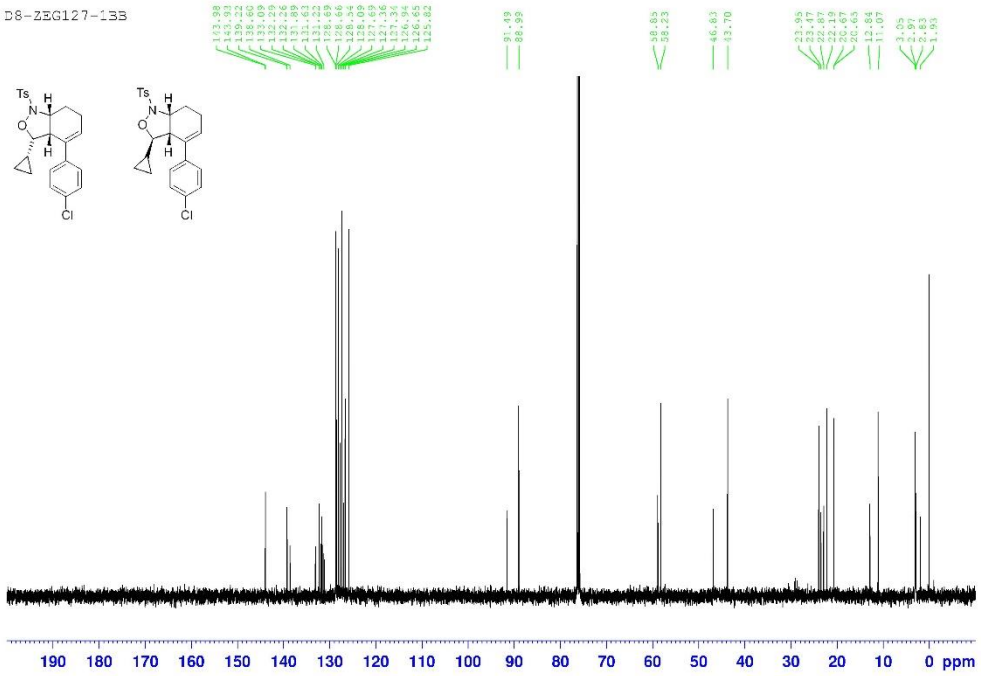
Left 5n, right 6n



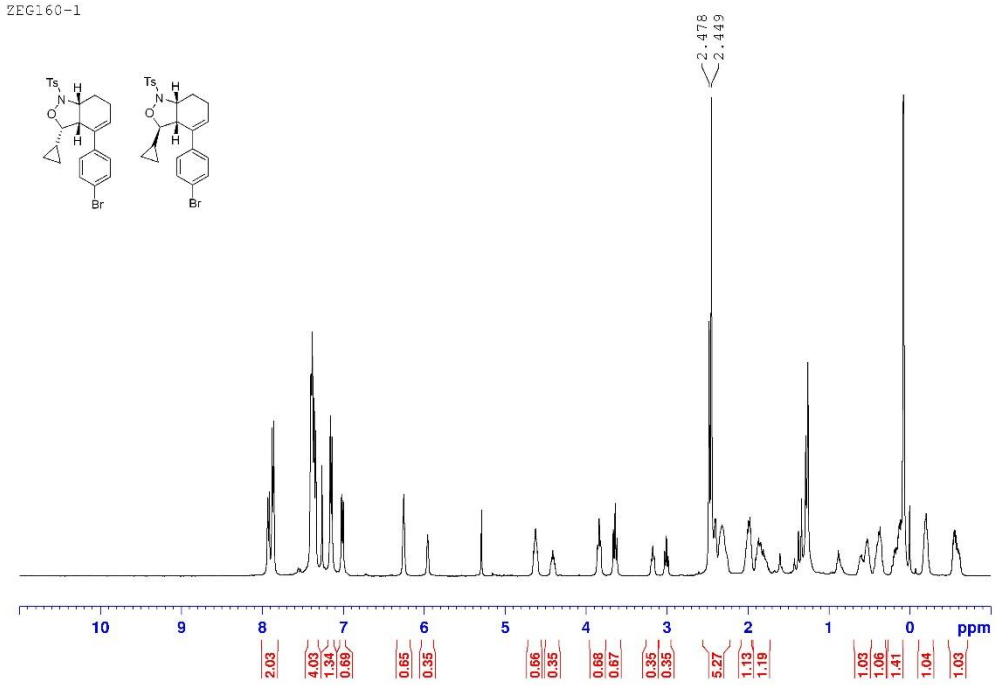
Left 5n, right 6n



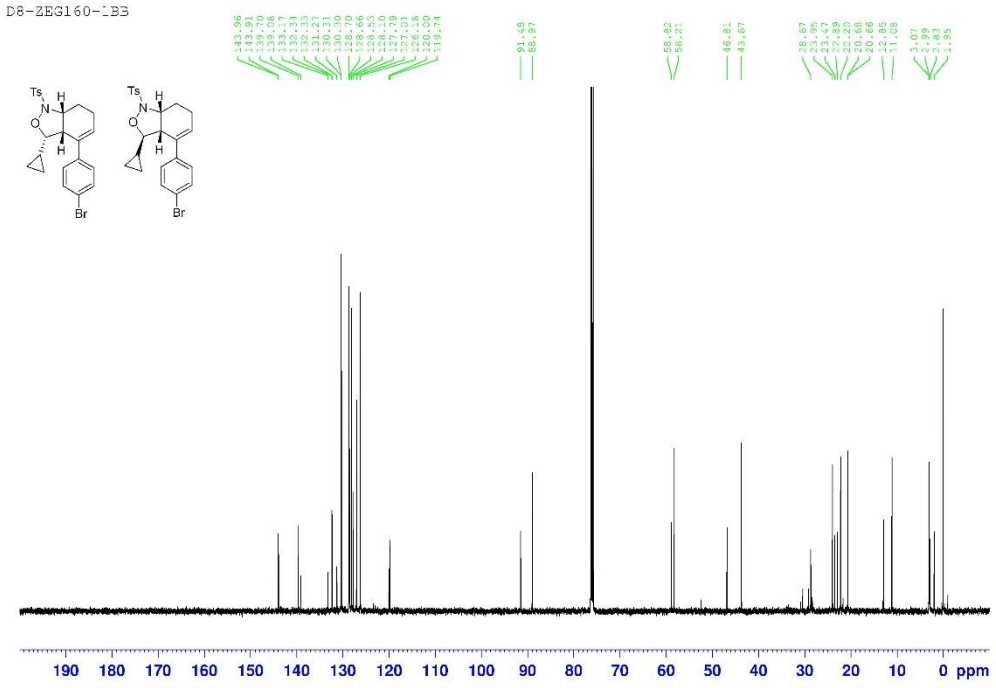
Left 10a, right 11a



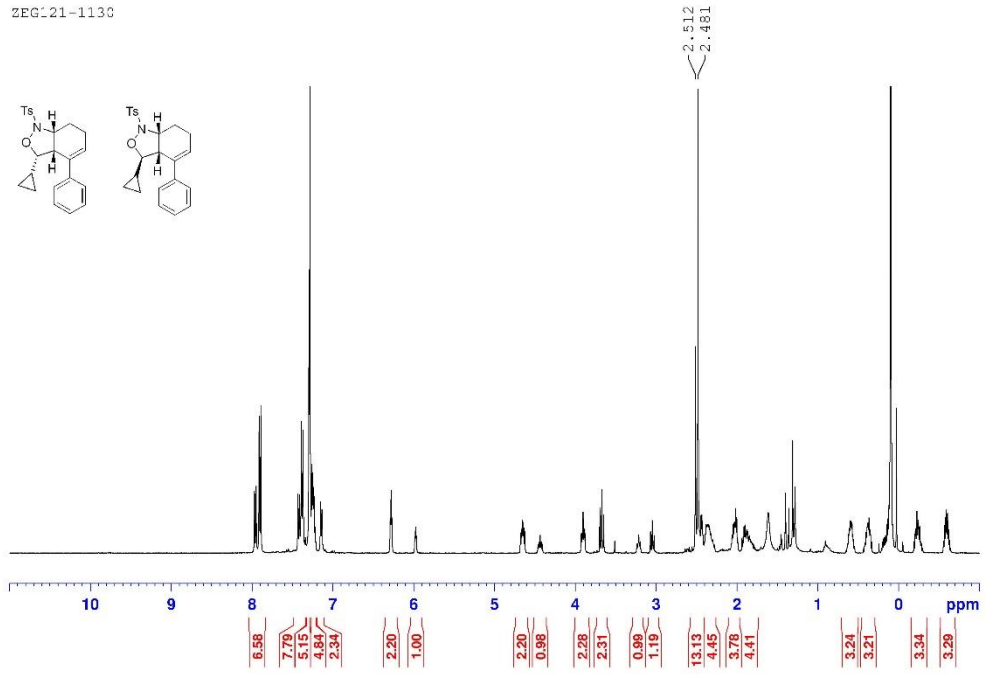
Left 10a, right 11a



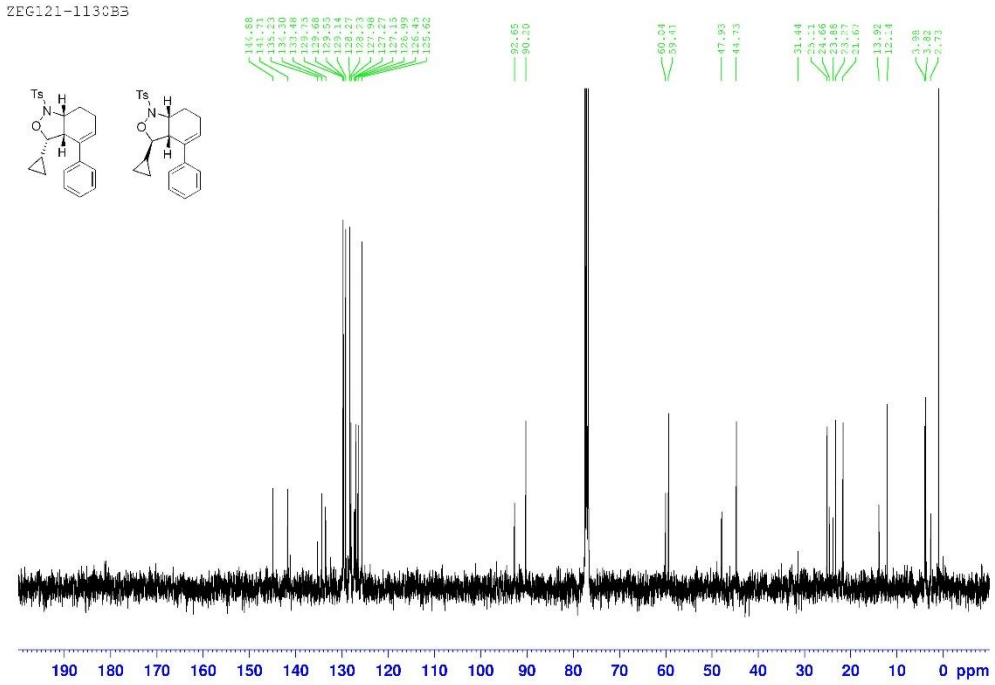
Left 10c, right 11c



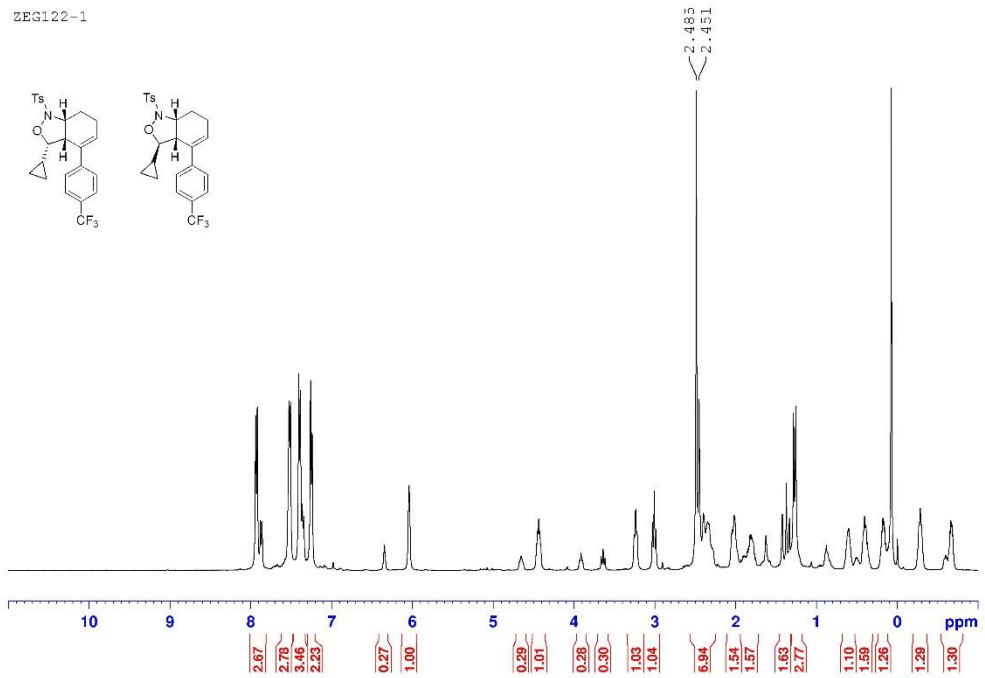
Left 10c, right 11c



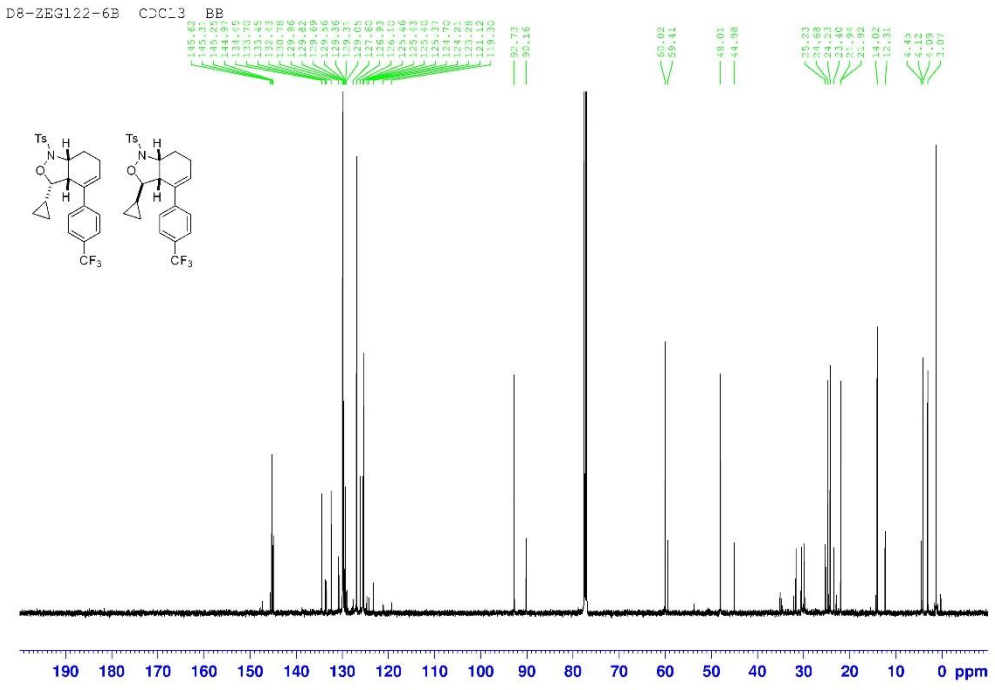
Left 10d, right 11d



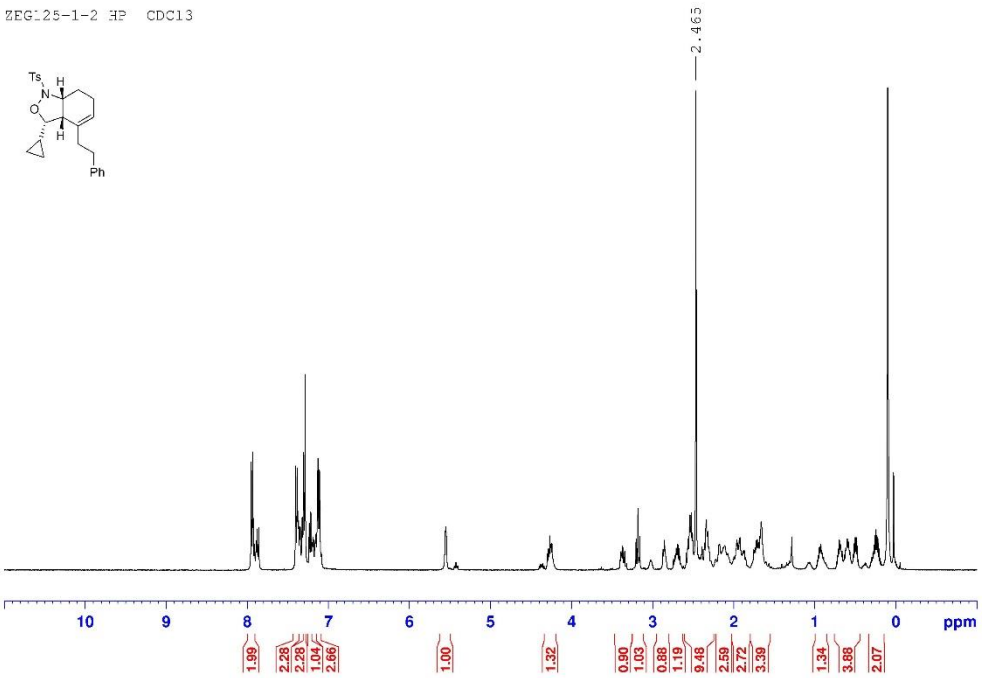
Left 10d, right 11d



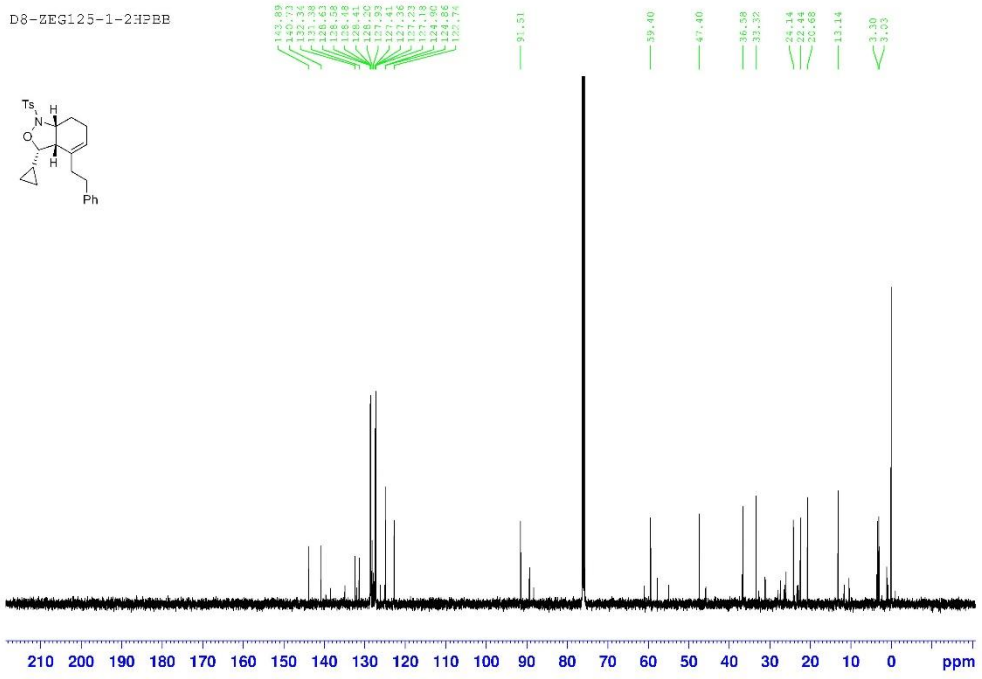
Left 10h, right 11h



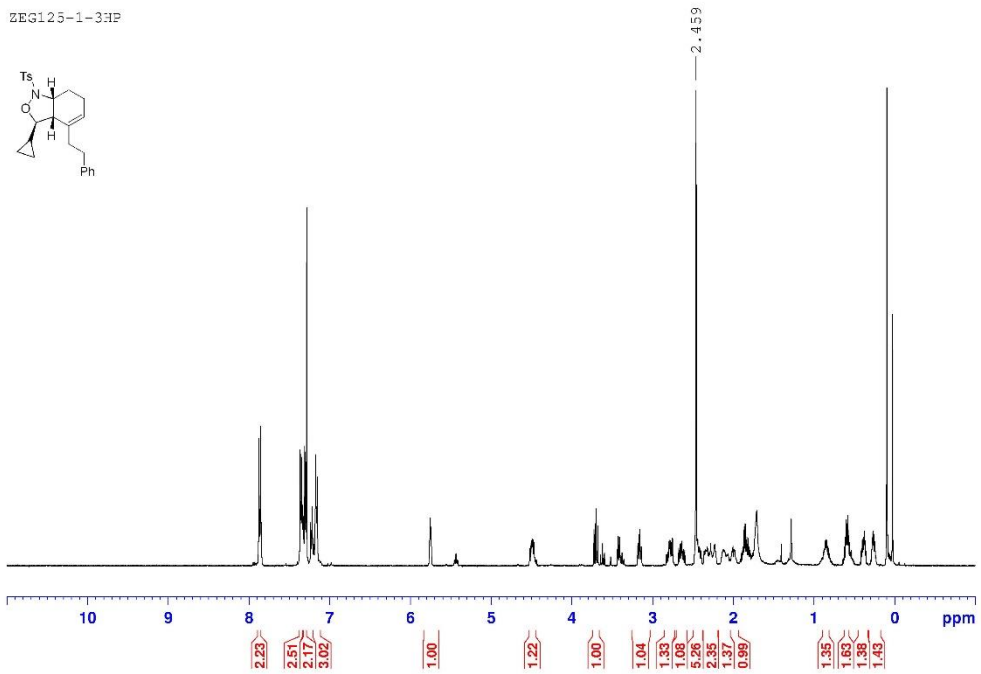
Left 10h, right 11h


ZEG125-1-2 HP CDCl3
Ts
N
H
O
H
Ph
2.465
10 9 8 7 6 5 4 3 2 1 0 ppm
1.99 2.28 2.28 1.04 2.66 1.00 1.32 0.90 1.03 0.88 1.19 9.48 2.59 2.72 3.39 1.34 3.88 2.07

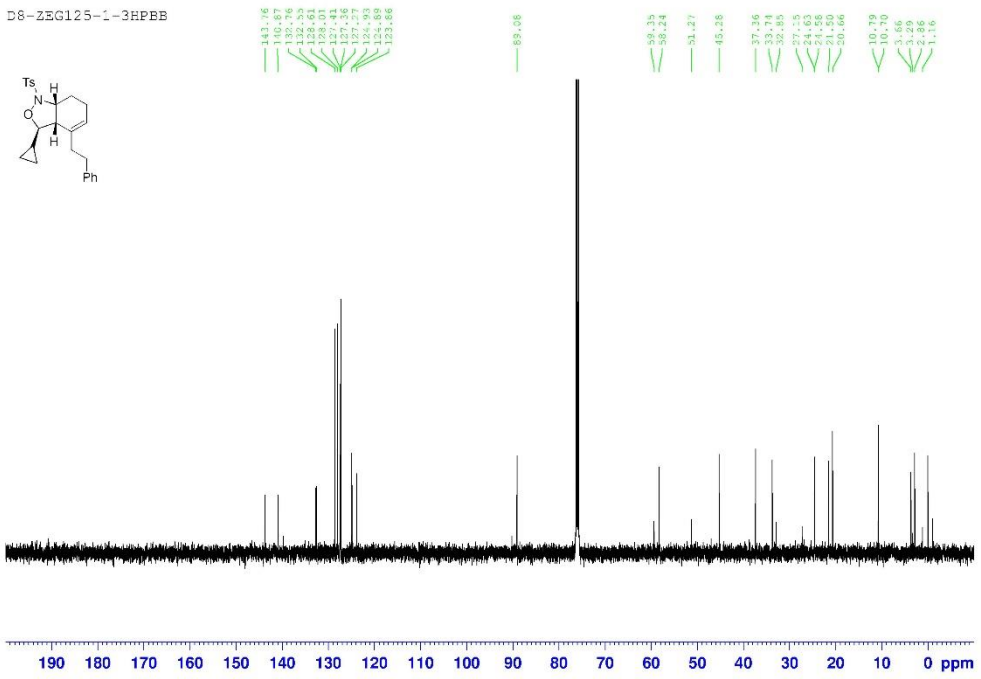
10l


D8-ZEG125-1-2HPBB
Ts
N
H
O
H
Ph
91.51
59.40
47.40
36.58
33.32
24.14
22.44
20.68
13.14
3.30
3.03
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

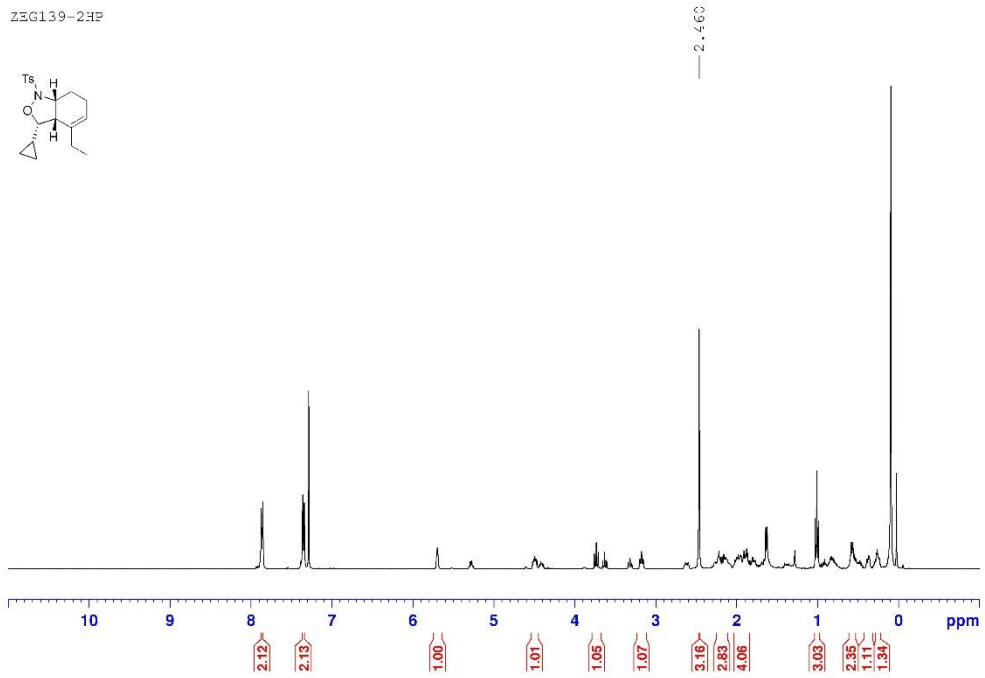
10l


ZEG125-1-3HP
Ts
N
O
H
H
Ph
2.459
10
9
8
7
6
5
4
3
2
1
0
ppm
2.23
2.51
2.17
3.02
1.00
1.22
1.00
1.04
1.33
1.08
5.26
2.35
1.37
0.99
1.35
1.63
1.38
1.43

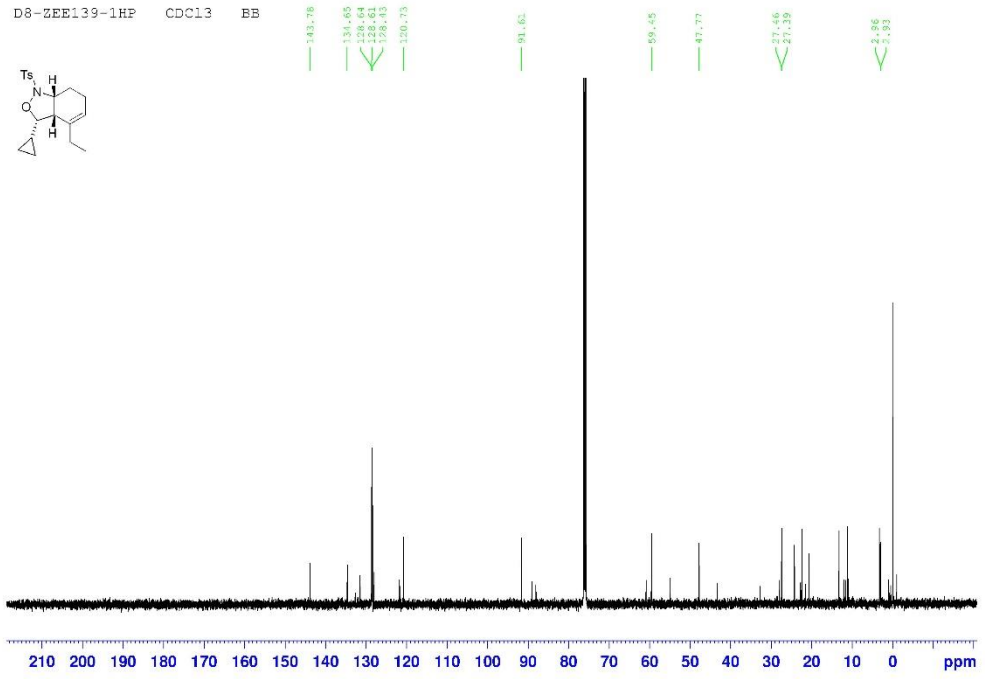
11l


D8-ZEG125-1-3HPBB
Ts
N
O
H
H
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

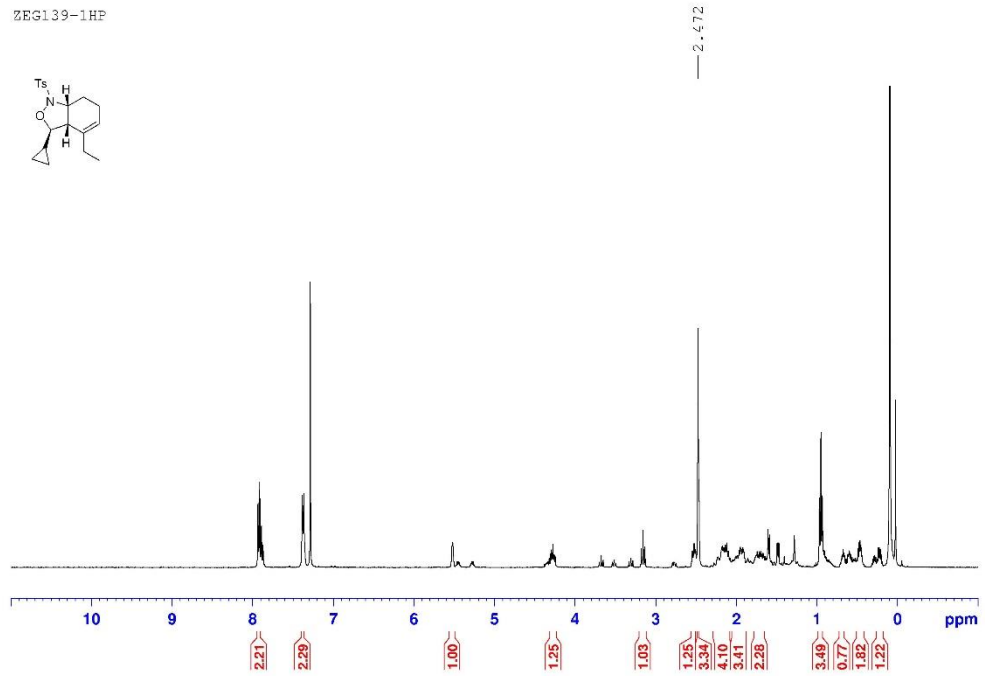
11l


ZEG139-2HP
2.463
10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
2.13
1.00
1.01
1.05
1.07
3.16
2.83
4.06
3.03
2.35
1.11
1.34

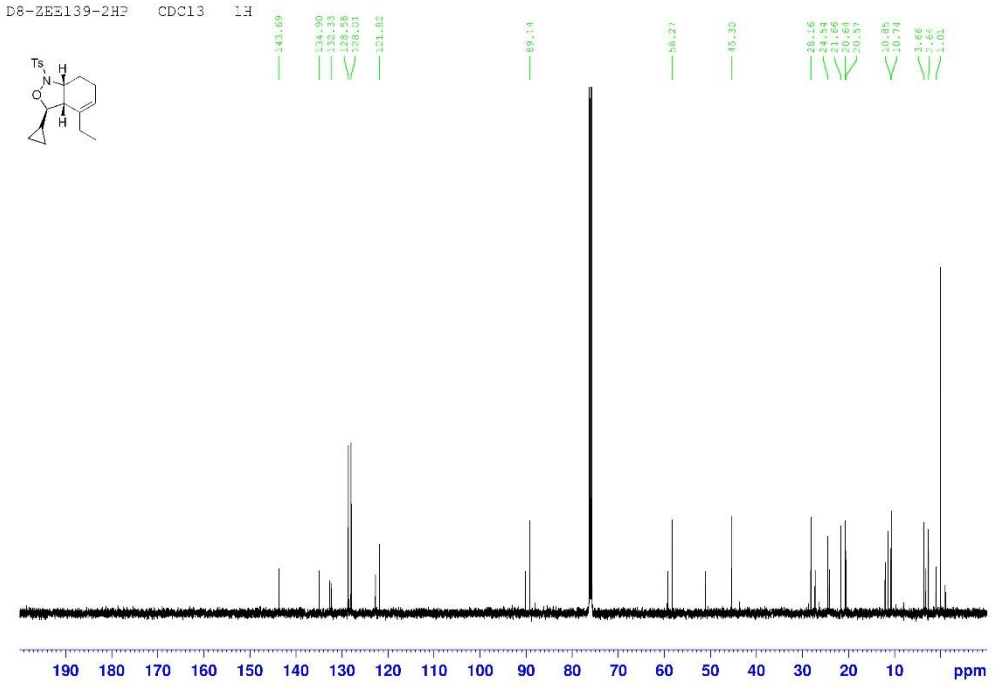
10m


D8-ZEE139-1HP CDCl3 BB
143.78
134.65
128.64
128.41
128.15
120.73
91.61
59.45
47.77
27.46
27.39
2.96
2.93
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

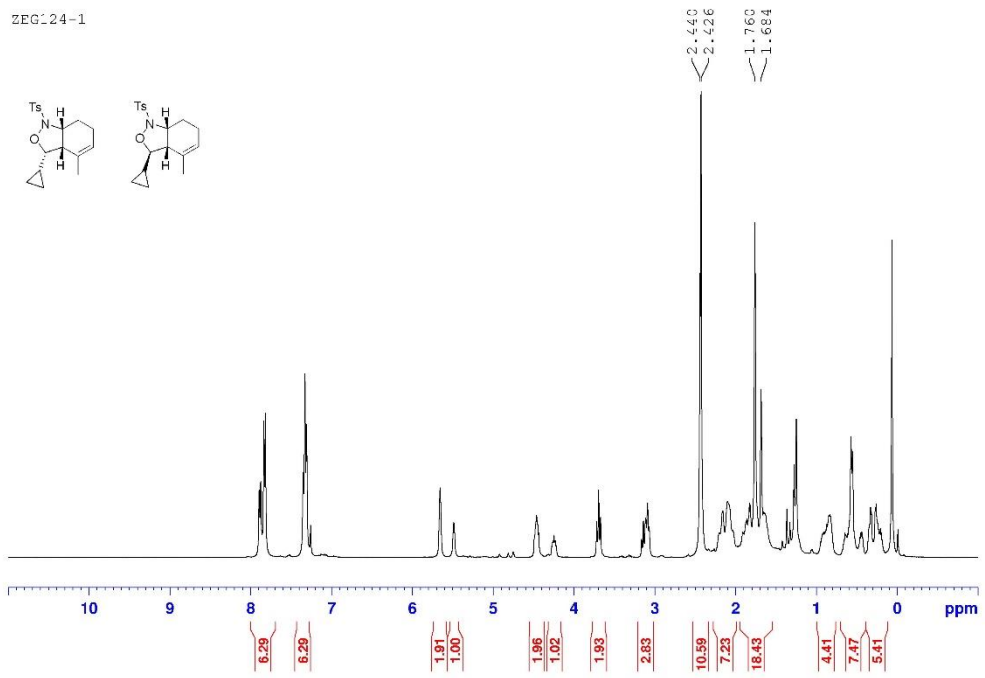
10m


ZEG139-1HP
2.472
10
9
8
7
6
5
4
3
2
1
0
ppm
2.21
2.29
1.00
1.25
1.03
1.25
3.34
4.10
3.41
2.28
3.49
0.77
1.82
1.22

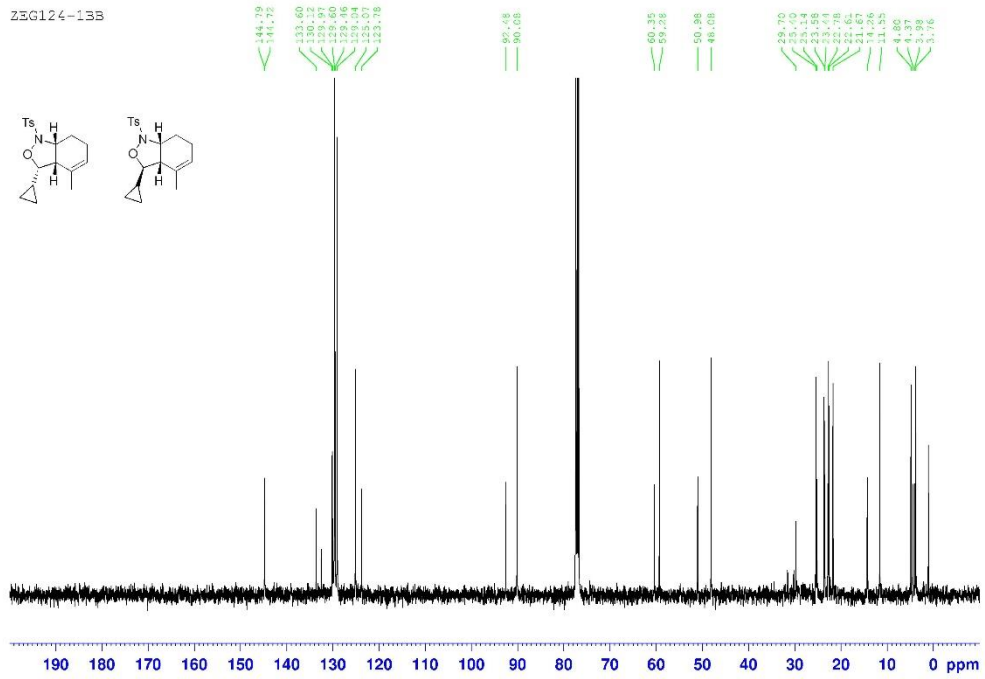
11m


D8-ZEE139-2HP CDCl3 1H
143.69
134.90
132.33
128.58
128.01
121.82
89.14
58.27
45.30
28.16
24.54
21.66
20.84
20.57
10.85
10.74
3.66
2.66
2.62
1.02
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

11m



Left 10n, right 11n



Left 10n, right 11n

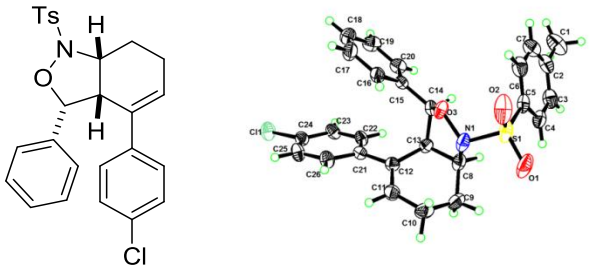
II. X-ray Crystal Structures of Selected Compounds:

X-ray crystallographic data (CIF files) of compounds **3a**, **3x**, **4a**, and **11a** have been deposited into CCDC with accessing codes as 1900624, 1900626, 1900625, and 1900627, respectively.

The ellipsoid contour % probability levels used were 50% for all crystal structures.

All crystals were prepared from the following procedures:

Firstly, each sample (ca. 20-30 mg) was dissolved in dichloromethane (5 mL, HPLC grade) in a glass sample vial (25 mL). Subsequently, hexane (10 mL, HPLC grade) was added carefully on top of the dichloromethane solution and two layers could be observed. The vial was kept in a fume hood to allow slow evaporation of solvents until crystals formed.



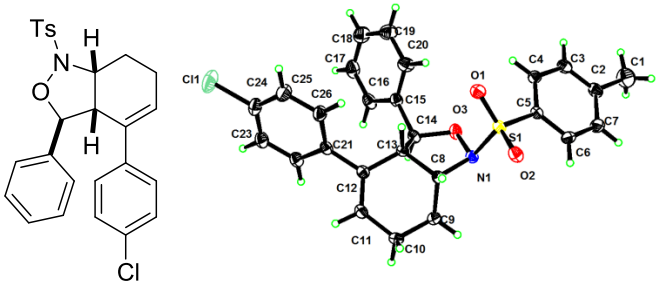
3a

Bond precision:	C-C = 0.0037 A Wavelength = 0.71073	
Cell:	a = 6.0404(10) b = 18.307(3) c = 20.483(3) alpha = 90 beta = 96.951(4) gamma = 90	
Temperature:	173 K	
	Calculated	Reported
Volume	2248.4(6)	2248.4(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C26 H24 Cl N O3 S	C26 H24 Cl N O3 S
Sum formula	C26 H24 Cl N O3 S	C26 H24 Cl N O3 S
Mr	465.97	465.97
Dx,g cm-3	1.377	1.377
Z	4	4
Mu (mm-1)	0.292	0.292
F000	976.0	976.0
F000’	977.47	
h,k,lmax	7,23,26	7,23,26
Nref	5188	5160
Tmin,Tmax	0.949,0.966	0.678,0.746
Tmin’	0.921	

Correction method= # Reported, T Limits: Tmin=0.678 Tmax=0.746
AbsCorr = MULTI-SCAN		

Data completeness = 0.995		

Theta(max) = 27.545
R(reflections) = 0.0523(3140)
wR2(reflections) = 0.1453(5160)
S = 0.994
Npar = 290

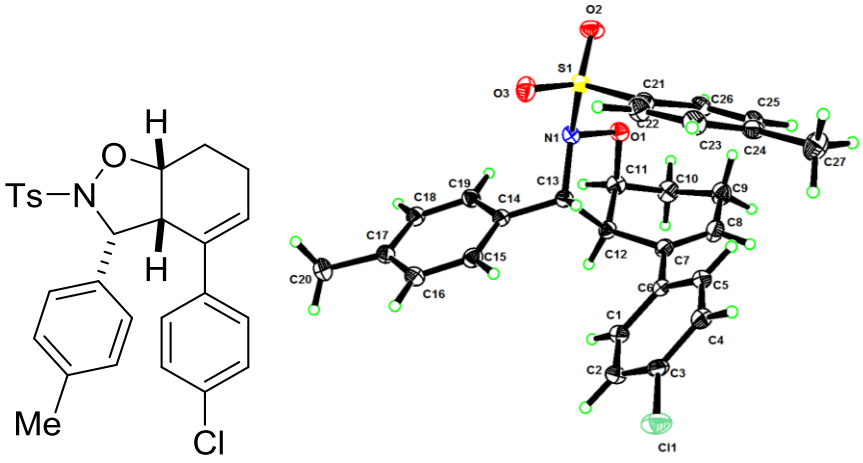


4a

Bond precision:	C-C = 0.0041 A Wavelength=0.71073	
Cell:	a = 8.2865(19) b = 10.144(3) c = 15.586(4) alpha = 77.546(6) beta = 84.113(6) gamma = 77.165(6)	
Temperature:	173 K	
	Calculated	Reported
Volume	1245.3(6)	1245.2(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26H24ClNO3S [+ solvent]	?
Sum formula	C26H24ClNO3S [+ solvent]	C26 H24 Cl N O3 S
Mr	465.97	465.97
Dx,g cm-3	1.243	1.243
Z	2	2
Mu (mm-1)	0.264	0.264
F000	488.0	488.0
F000’	488.74	
h,k,lmax	10,13,20	10,13,20
Nref	5663	5548
Tmin,Tmax	0.954,0.969	0.664,0.746
Tmin’	0.929	

Correction method = # Reported, T Limits: Tmin = 0.664 Tmax = 0.746,
AbsCorr = MULTI-SCAN		

Data completeness = 0.980		
Theta(max) = 27.399		
R(reflections) = 0.0556(3419)		
wR2(reflections) = 0.1567(5548)		
S = 0.982		
Npar = 290		

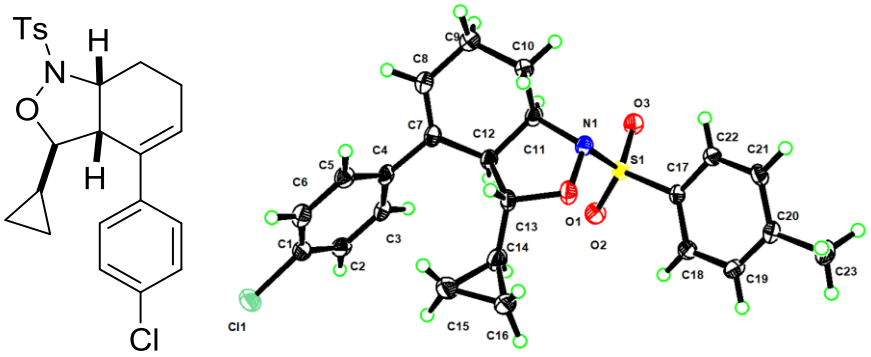


3x

Bond precision:	C-C = 0.0038 A Wavelength = 0.71073	
Cell:	a = 9.816(4) b = 17.033(7) c = 14.307(6) alpha = 90 beta = 98.619(9) gamma = 90	
Temperature:	173 K	
	Calculated	Reported
Volume	2365.1(17)	2364.9(18)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C27 H26 Cl N O3 S	C27 H26 Cl N O3 S
Sum formula	C27 H26 Cl N O3 S	C27 H26 Cl N O3 S
Mr	480.00	480.00
Dx,g cm-3	1.348	1.348
Z	4	4
Mu (mm-1)	0.280	0.280
F000	1008.0	1008.0
F000’	1009.48	
h,k,lmax	12,21,17	12,21,17
Nref	4867	4799
Tmin,Tmax	0.960,0.978	0.573,0.745
Tmin’	0.948	

Correction method = # Reported, T Limits: Tmin = 0.573 Tmax = 0.745
AbsCorr = MULTI-SCAN		

Data completeness = 0.986		
Theta(max) = 26.418		
R(reflections) = 0.0488(3447)		
wR2(reflections) = 0.1469(4799)		
S = 1.018		
Npar = 300		



11a

Bond precision:	C-C = 0.0044 A Wavelength = 0.71073	
Cell:	a = 8.2873(3) b = 11.2154(6) c = 13.2137(6) alpha = 104.220(2) beta = 107.154(2) gamma = 107.165(2)	
Temperature:	100 K	
	Calculated	Reported
Volume	1044.15(9)	1044.15(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C23 H24 Cl N O3 S	C23 H24 Cl N O3 S
Sum formula	C23 H24 Cl N O3 S	C23 H24 Cl N O3 S
Mr	429.94	429.94
Dx,g cm-3	1.367	1.367
Z	2	2
Mu (mm-1)	0.308	0.308
F000	452.0	452.0
F000’	452.72	
h,k,lmax	10,14,16	10,14,16
Nref	4270	4227
Tmin,Tmax	0.971,0.991	0.403,0.745
Tmin’	0.955	
Correction method= # Reported, T Limits: Tmin = 0.403 Tmax = 0.745,AbsCorr = MULTI-SCAN		
Data completeness = 0.990		
Theta(max) = 26.374		
R(reflections) = 0.0572(3022)		
wR2(reflections) = 0.1364(4227)		
S = 1.032		
Npar = 263		