Supplementary Materials: 1,3-Dipolar Cycloaddition in the Preparation of New Fused Heterocyclic Compounds via Thermal Initiation

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Table S1. Chemical shifts of hydrogen atoms at stereogenic centres in δ [ppm].

Compound	H10b	H3a	H2
9Aa	3.73	1.65	3.64
9Ab	3.86	1.96	3.81
9Ac	4.05	1.95	3.49
9Ad	4.24	2.03	3.74
9Ba	3.73	1.99	3.64
9Bc	4.58	2.84	3.61

Table S2. Reaction conditions and product yields in 1,3-DC.

Compound	R	X	T [°C]	Reaction Time [min]	Yield [%]
9Aa	Me	Ts	140	30	80
9Ab	Et	Ts	130	20	34
9Ac	Bn	Ts	140	35	57
9Ad	*i*-Pr	Ts	130	20	44
9Bc	Bn	Ms	130	25	29

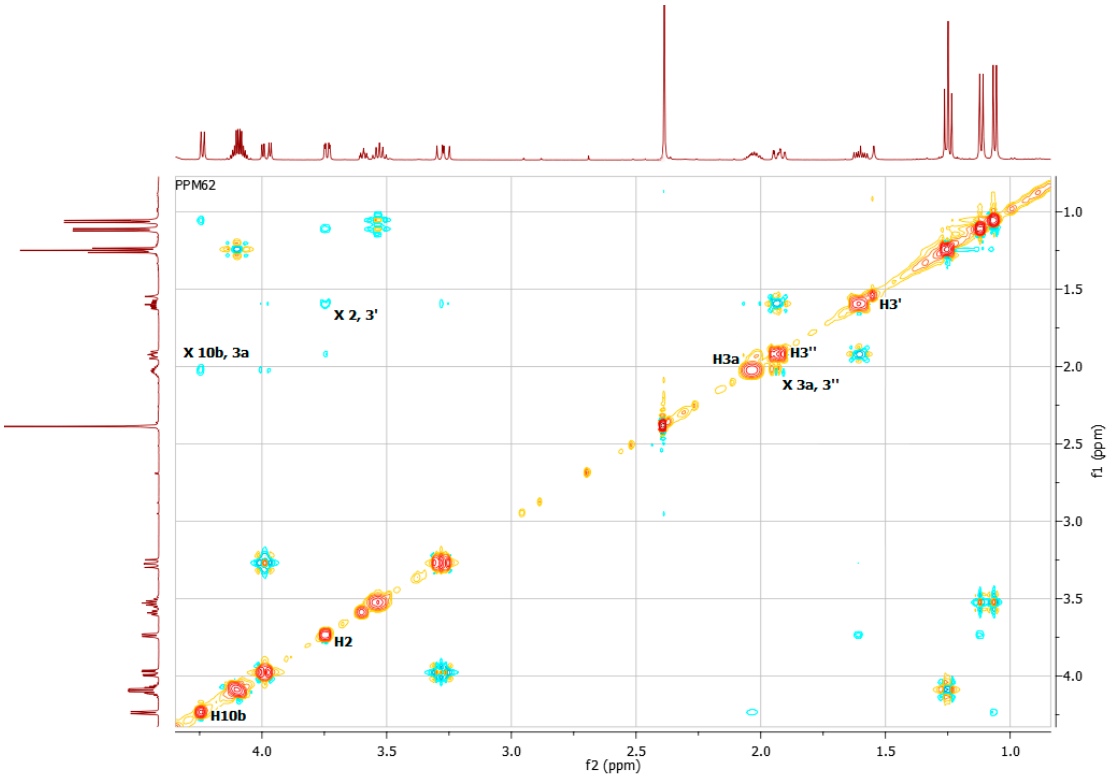
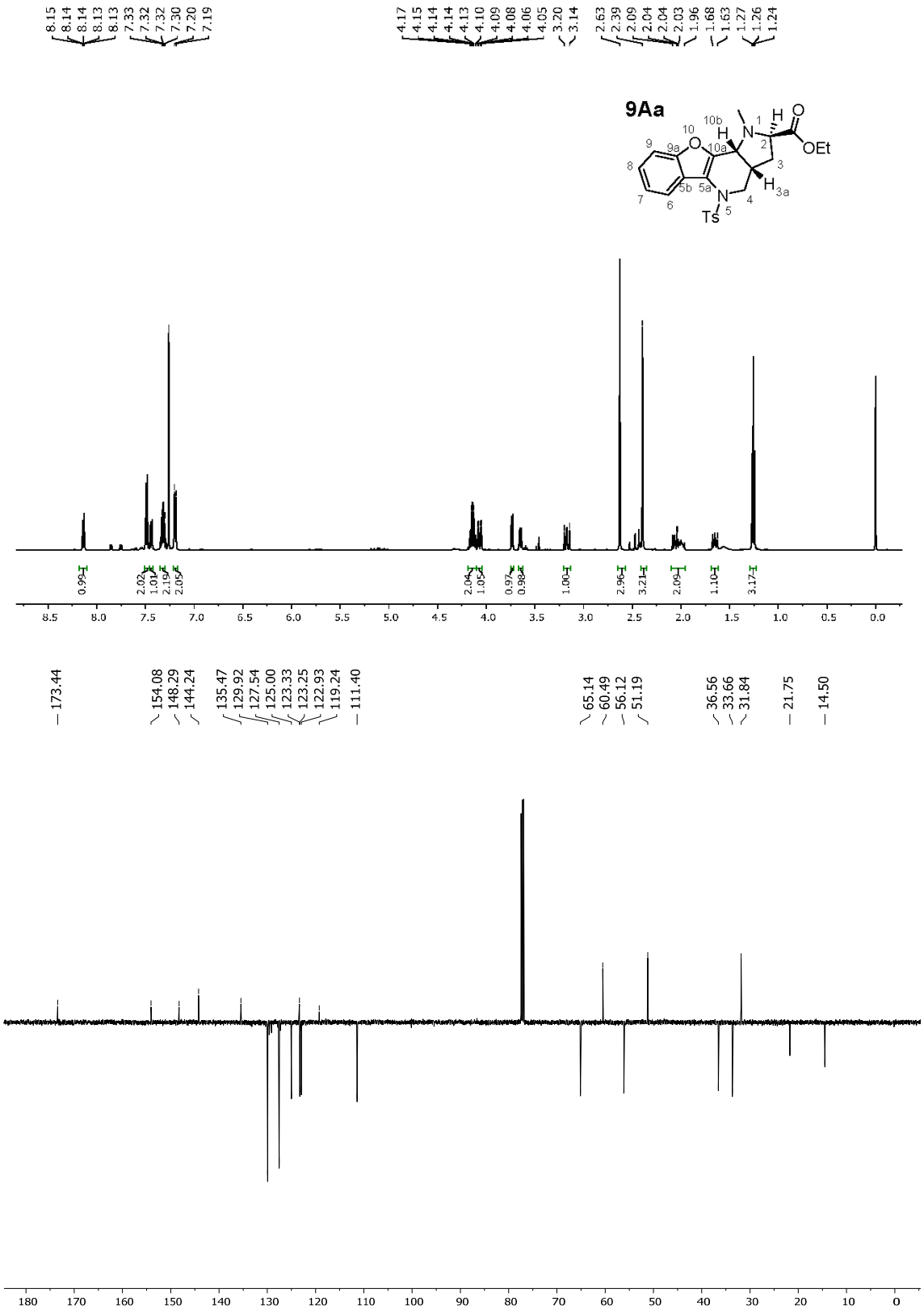
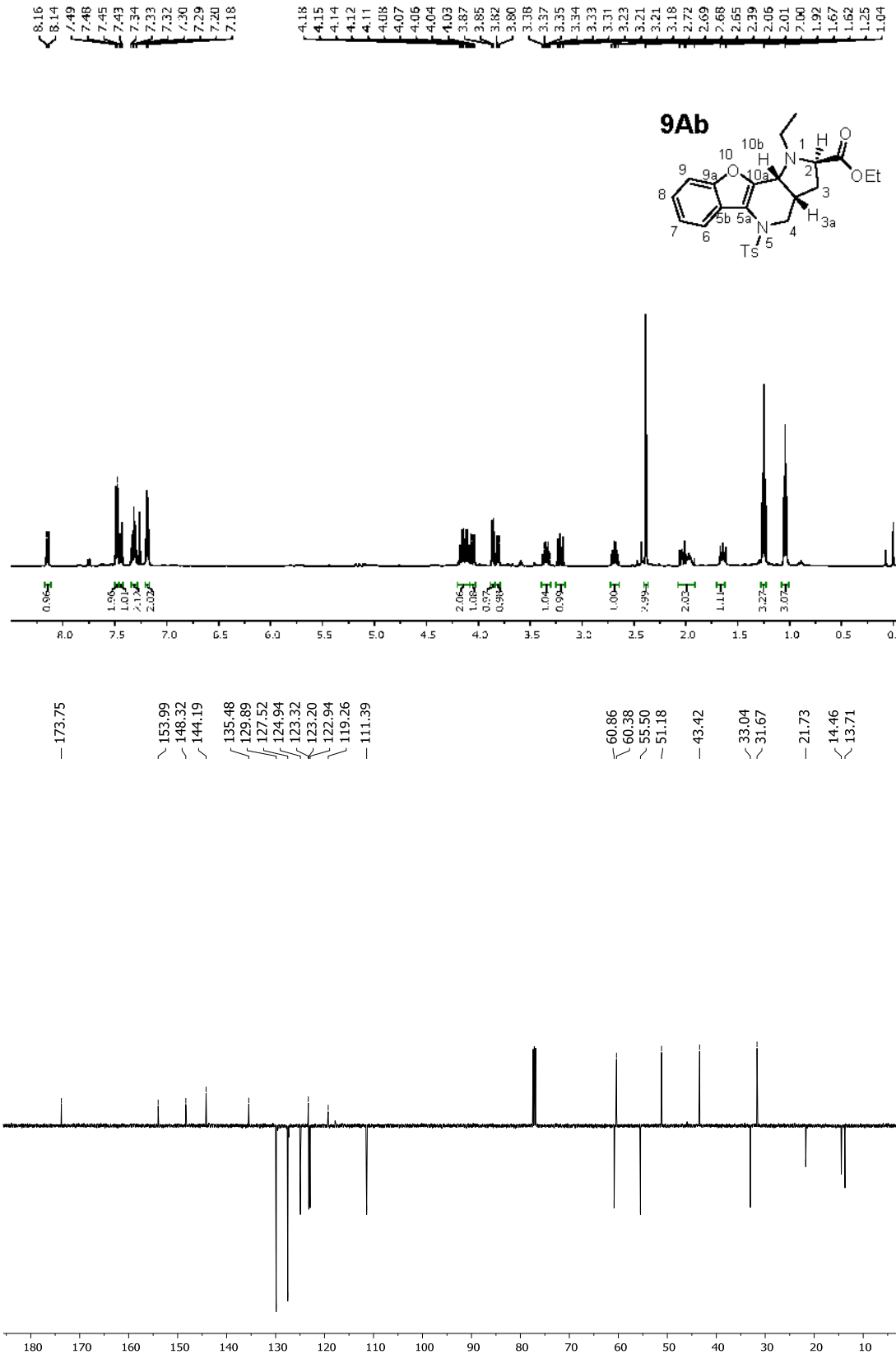
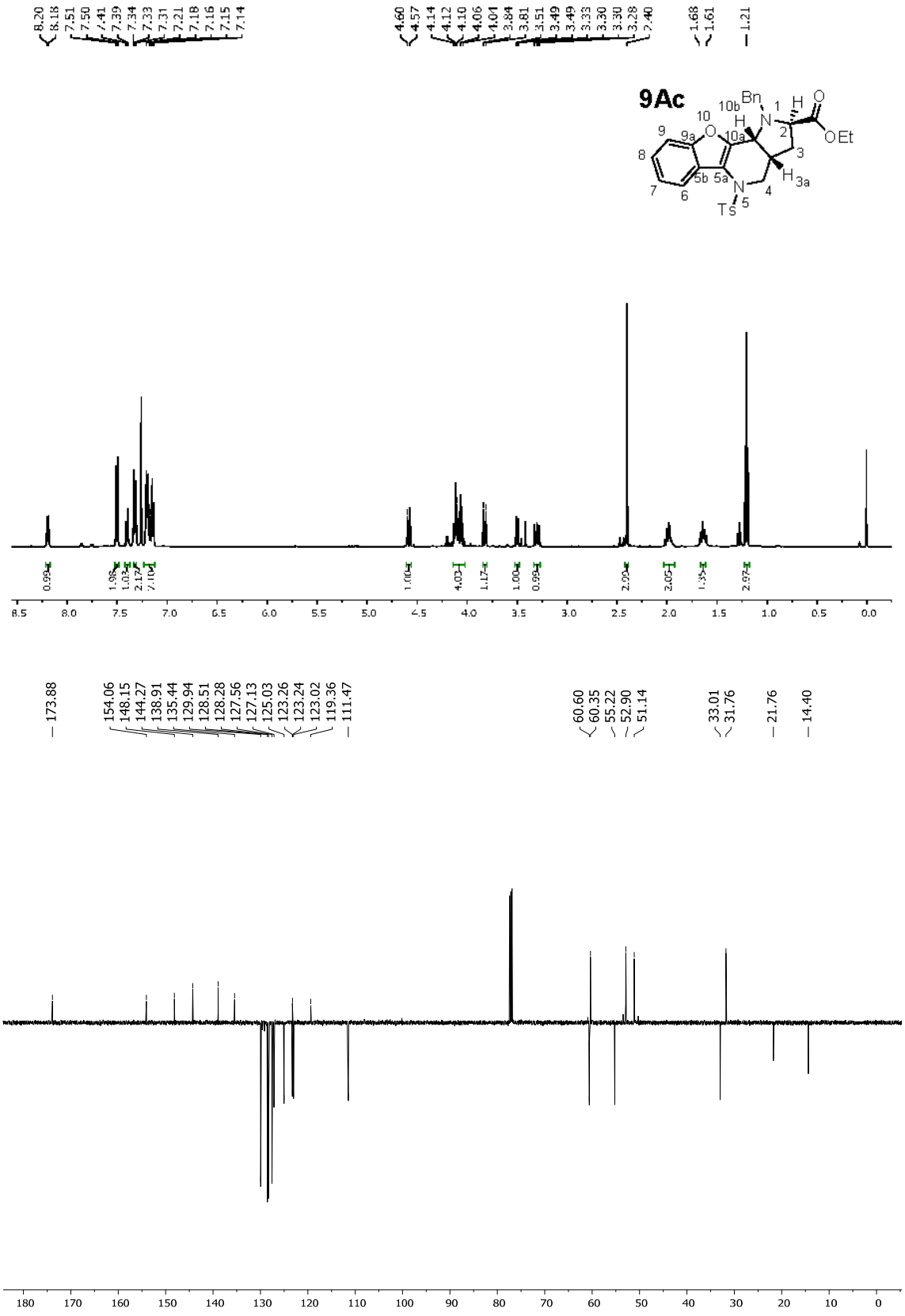


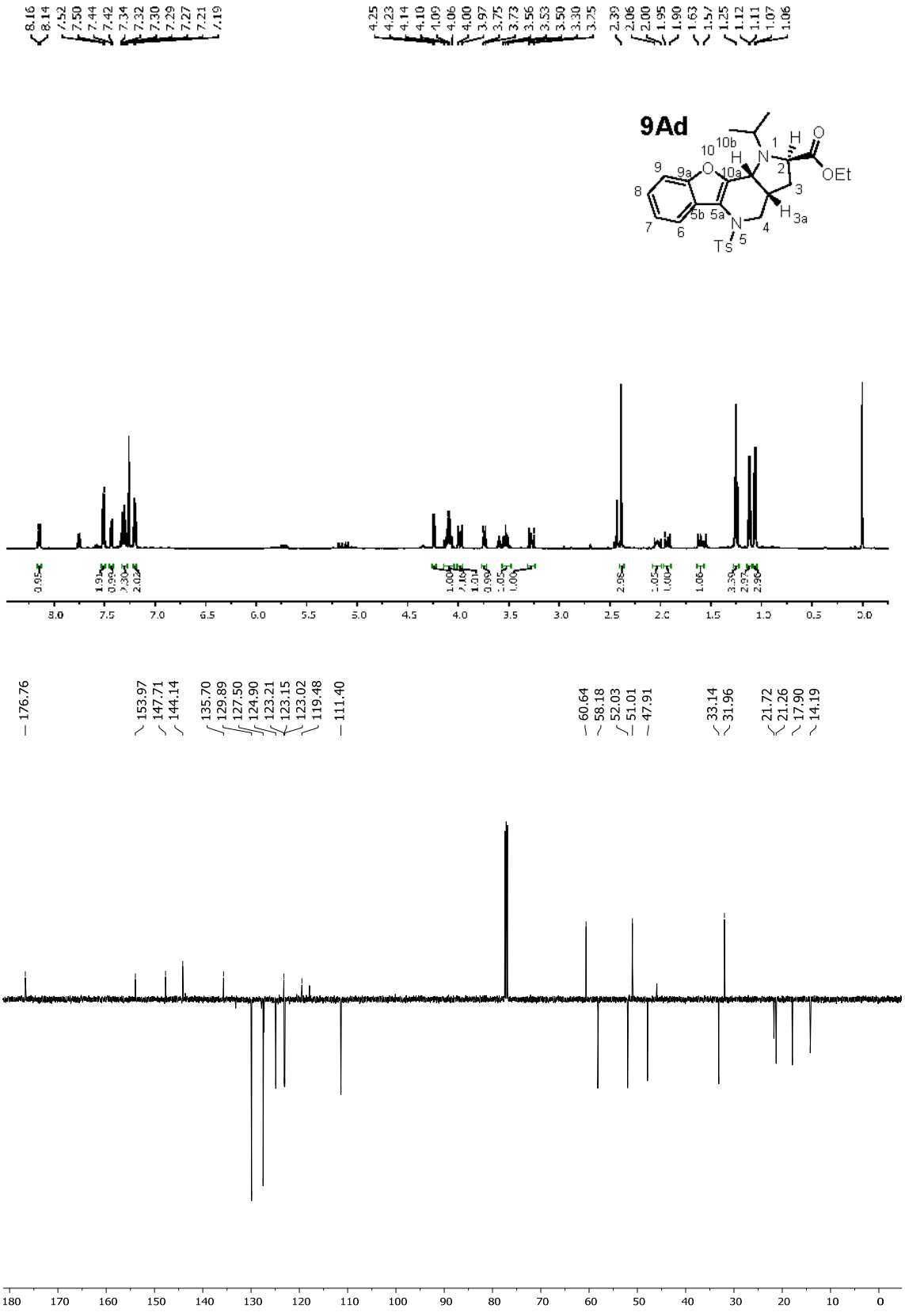
Figure S1. NOESY spectrum of compound **9Ad** (aliphatic fragment of the spectrum) picking up interactions between hydrogen atoms H10b, H3a and H2 at stereogenic centres.

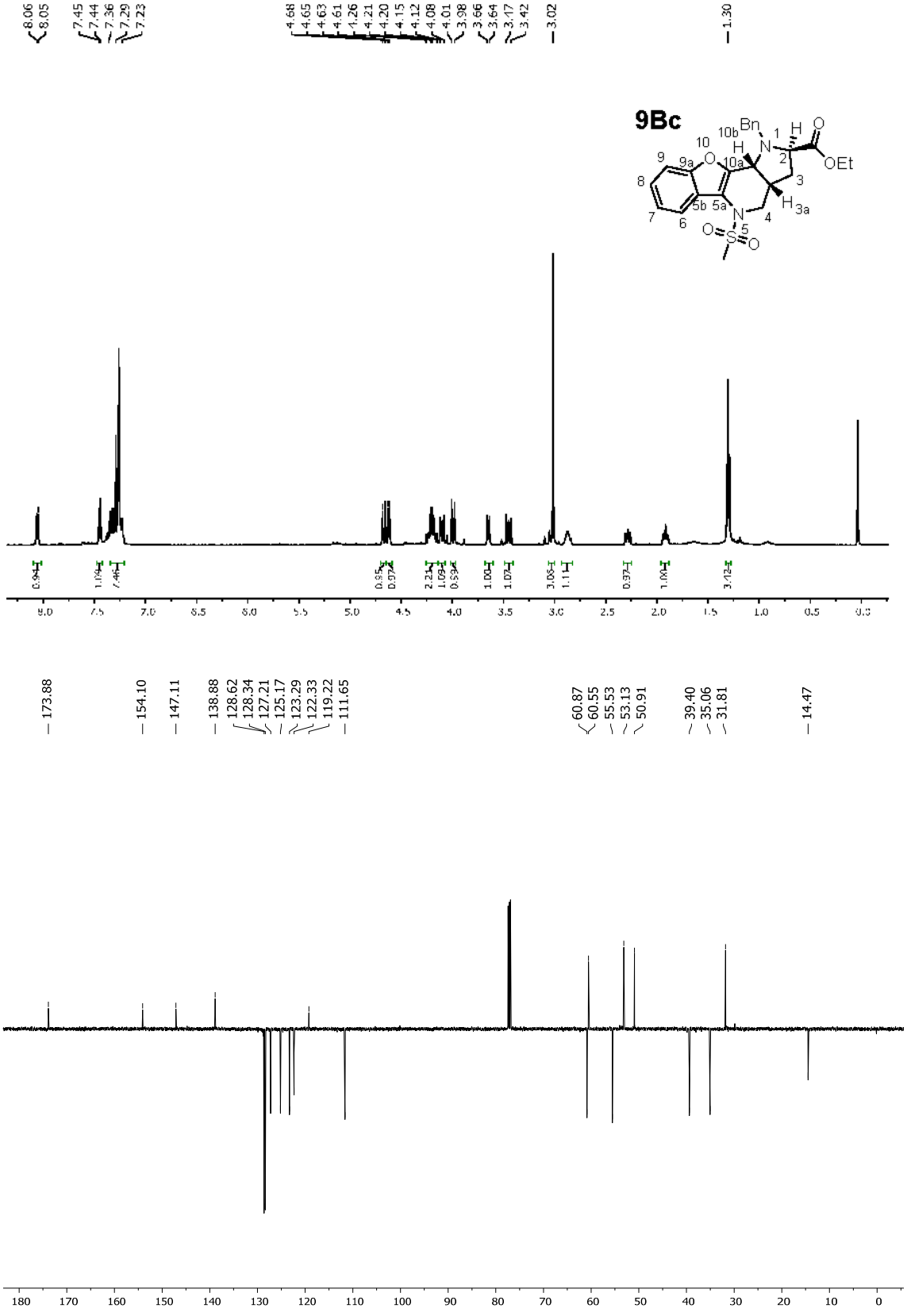
^{1}H-NMR and APT Spectra of Final Compounds 9Aa–d and 9Bc in $CDCl_3$




9Ab
OEt
Ts


9Ac
Bn
10b
H
N
1
H
O
10
9
9a
O
10a
2
OEt
8
3
5b
5a
H
3a
7
6
N
4
5
Ts


9Ad
OEt
Ts


8.06
8.05
7.45
7.44
7.36
7.29
7.23
4.68
4.65
4.63
4.61
4.26
4.21
4.20
4.15
4.12
4.08
4.01
3.98
3.66
3.64
3.47
3.42
3.02
1.30
9Bc
Bn
10b
H
N
1
H
O
10
9
9a
O
10a
2
OEt
8
3
5b
5a
H3a
7
6
4
N
O
S
5
O
0.94
1.09
2.46
0.95
0.97
2.25
1.09
0.93
1.00
1.07
3.05
1.11
0.97
1.00
3.12
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
173.88
154.10
147.11
138.88
128.62
128.34
127.21
125.17
123.29
122.33
119.22
111.65
60.87
60.55
55.53
53.13
50.91
39.40
35.06
31.81
14.47
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0