Supporting Information

Probing the Mechanism of Baylis-Hillman Reaction in Ionic Liquids

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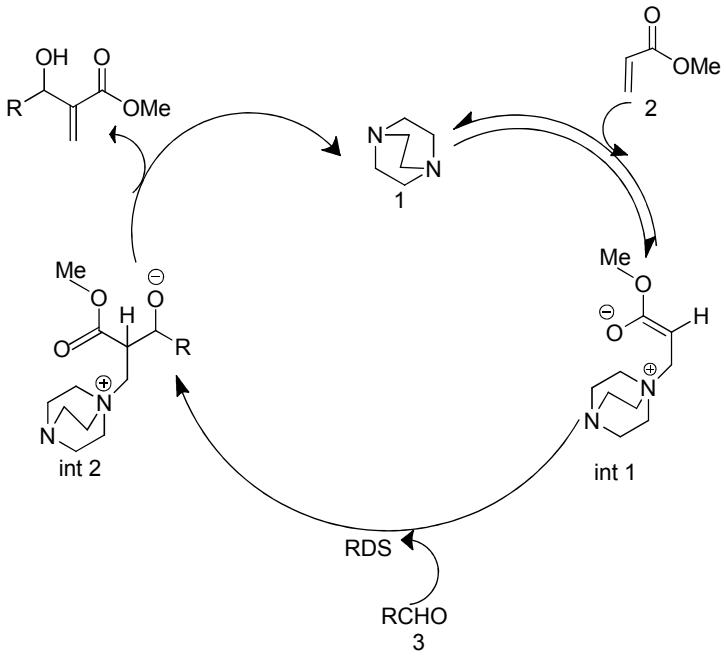
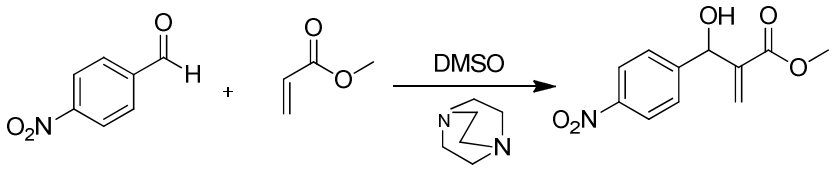
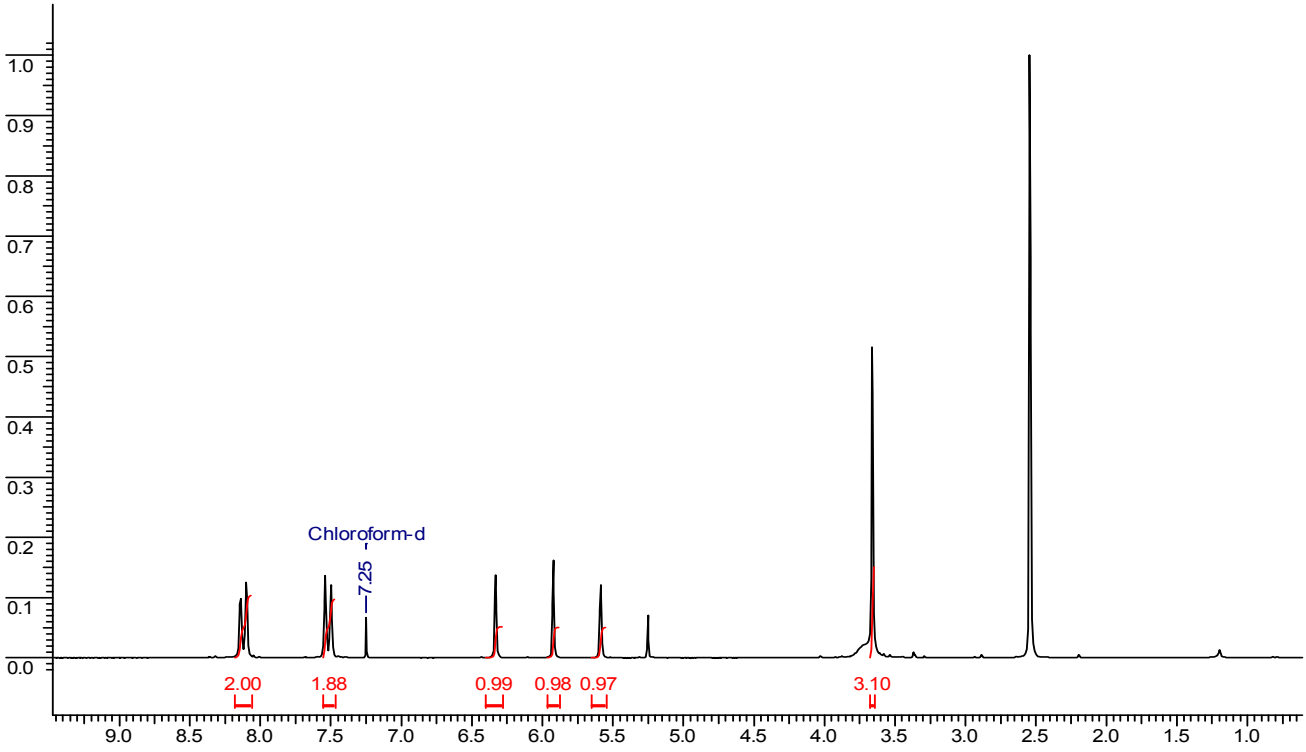
Contents:

Mechanism of B-H reaction (Hill and Isaacs)

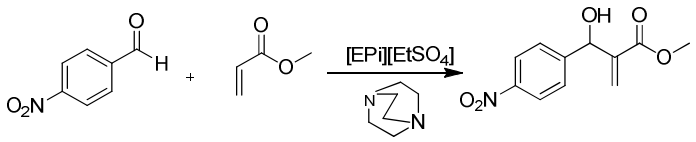


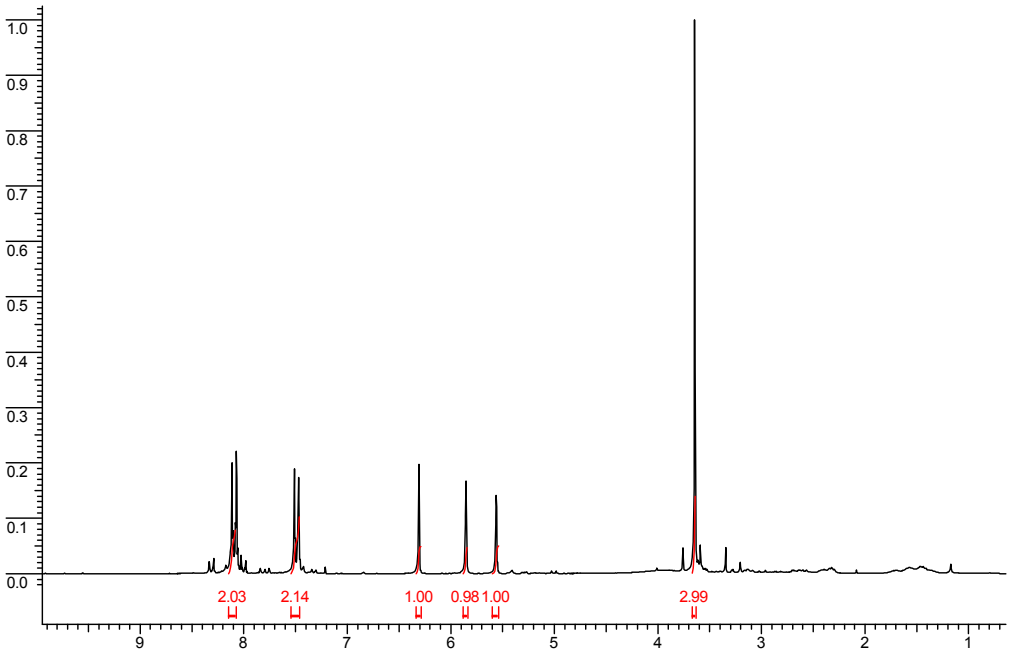
NMR of product

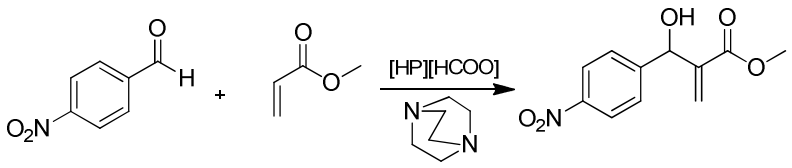


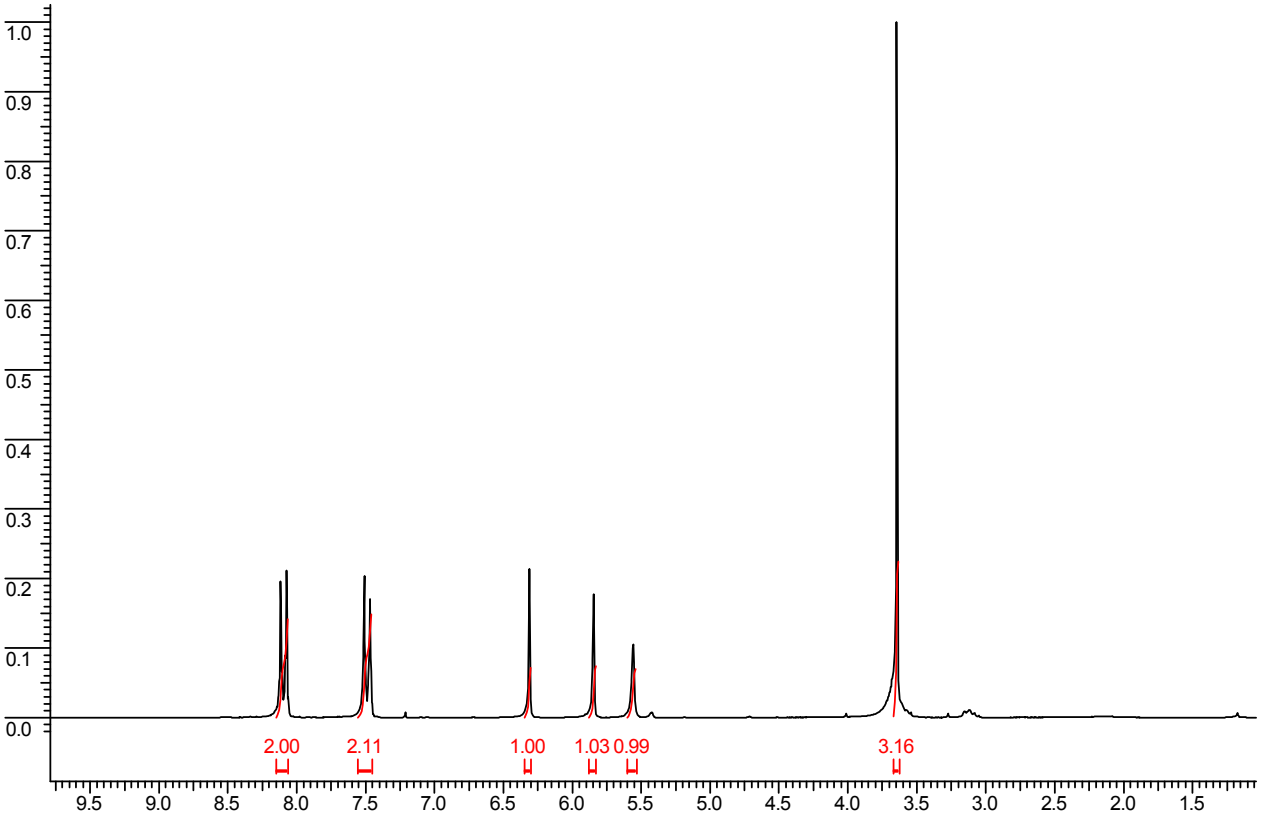


^{1}H NMR, 200 MHz, $CDCl_3$: 2-[Hydroxy(4-nitrophenyl)methyl]acrylic Acid Methyl Ester: δ 8.18 (d, 2H), δ 7.52 (d, 2H), δ 6.37 (s, 1H), δ 5.89 (s, 1H), δ 5.61 (s, 1H), δ 3.70 (s, 3H)

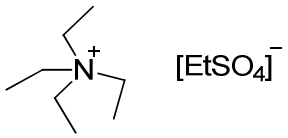

O
H
O_2N
+
O
O
[EPi][EtSO4]
N
N
OH
O
O
O_2N

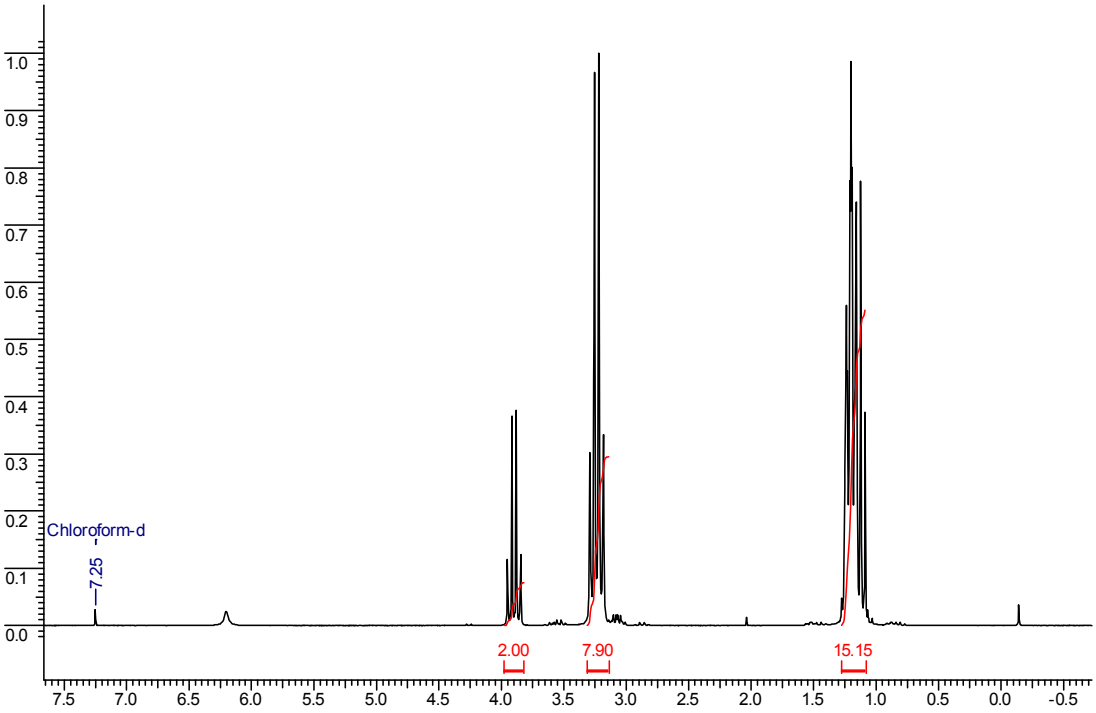

1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
2.03
2.14
1.00
0.98
1.00
2.99
9
8
7
6
5
4
3
2
1

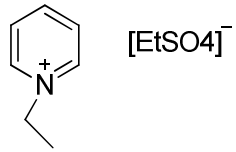

O
H
O2N
+
O
O
[HP][HCOO]
N
N
OH
O
O
O2N

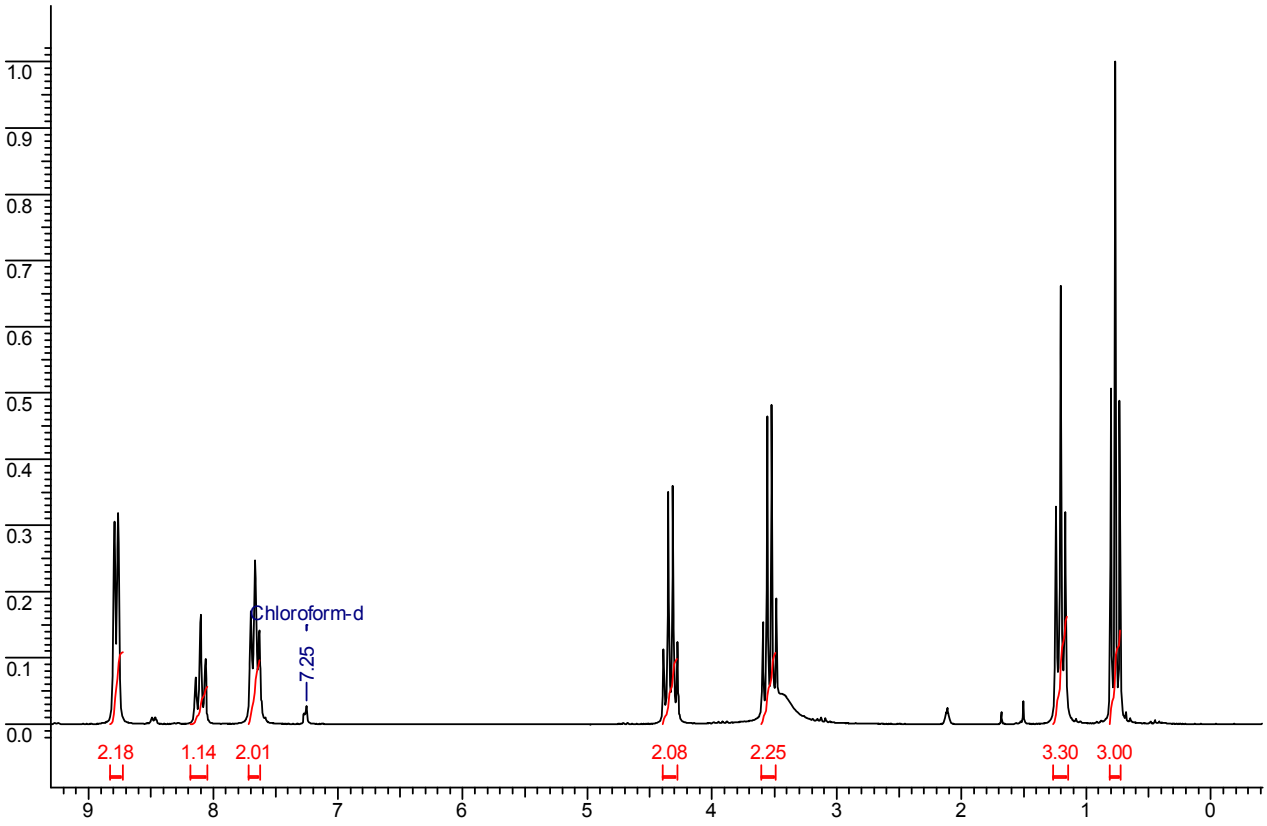

1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
2.00
2.11
1.00
1.03
0.99
3.16
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5

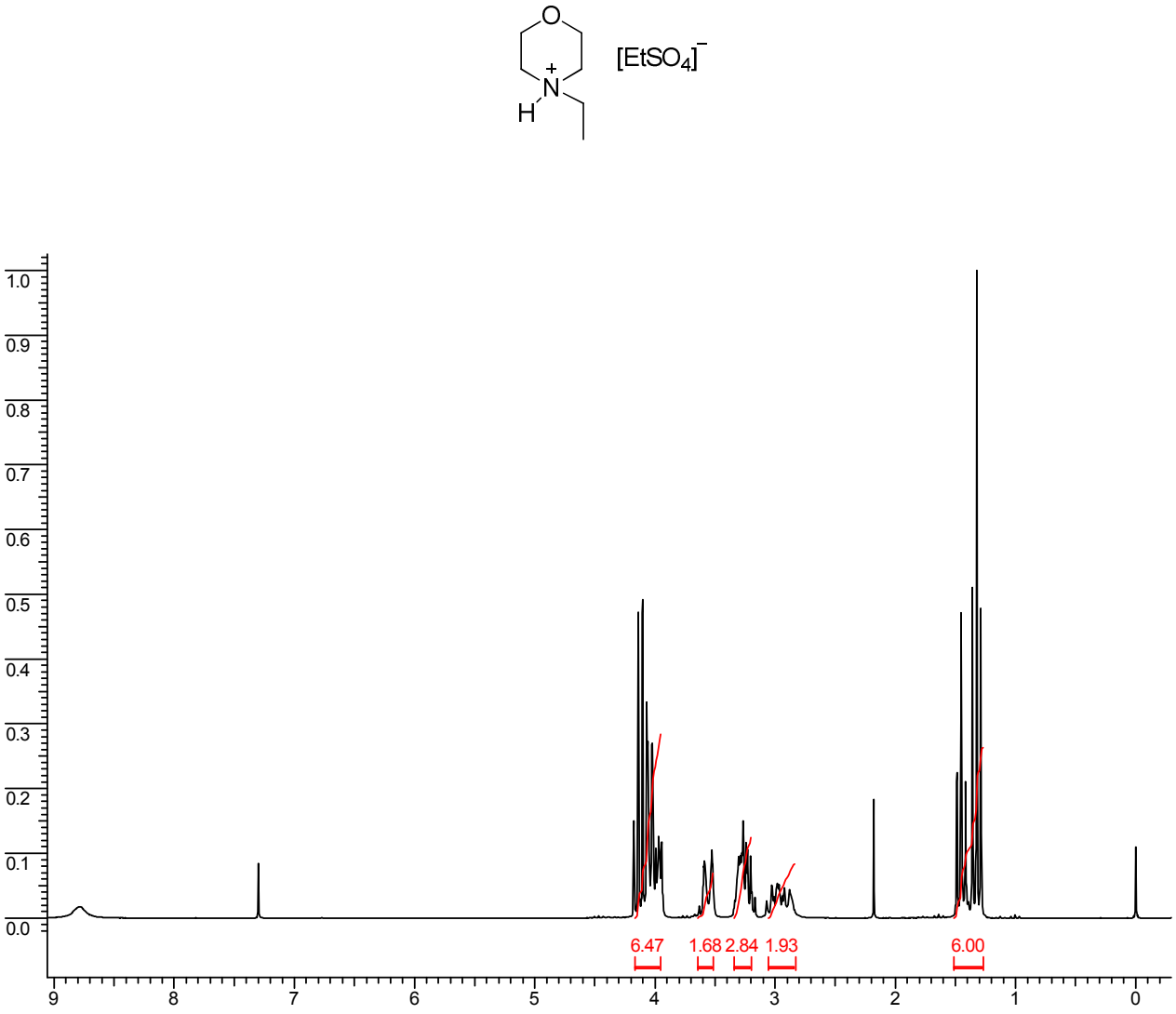
^{1}H NMR Of Ionic Liquids:

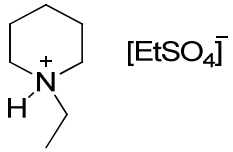




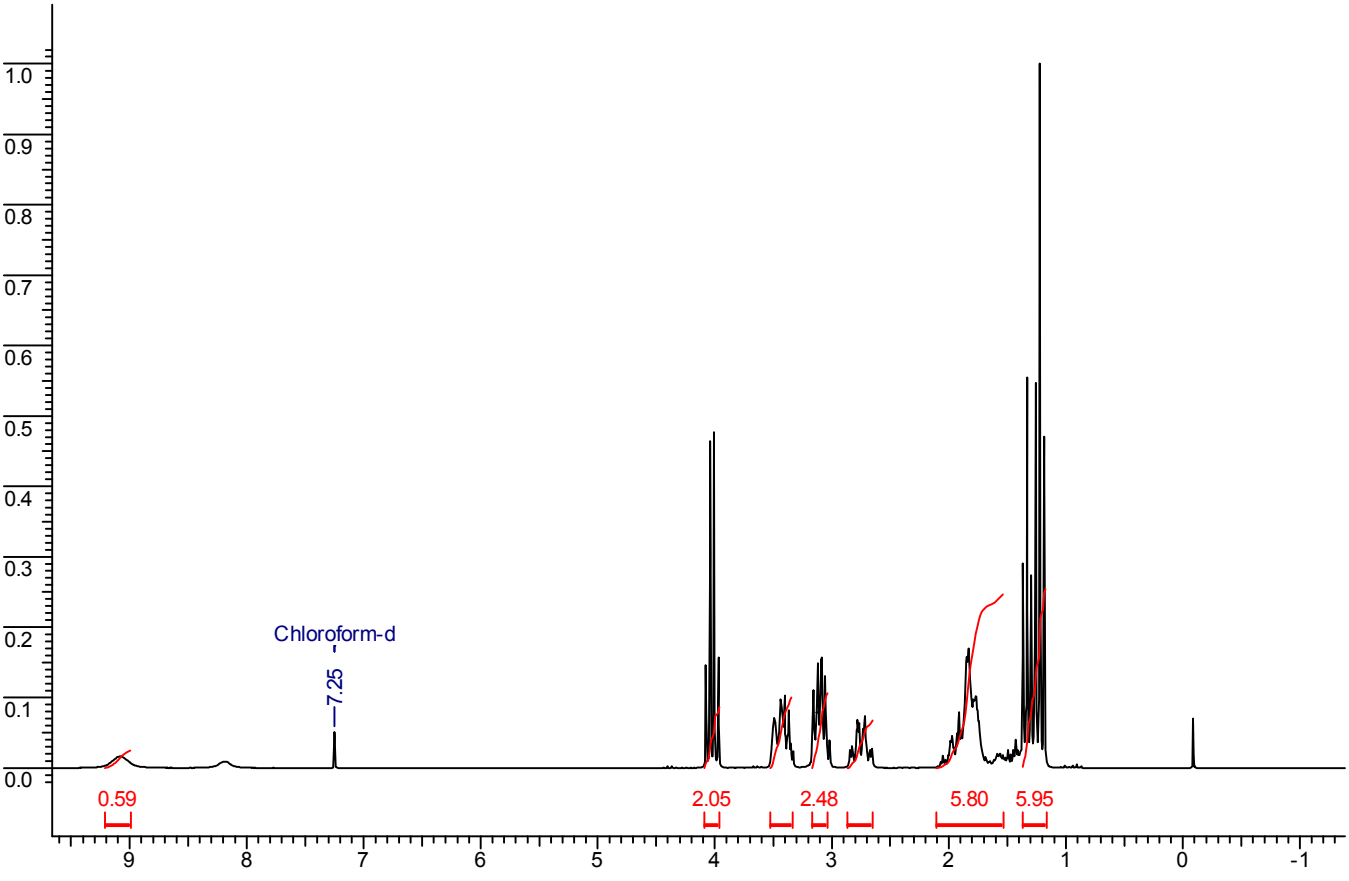

[EtSO4]⁻

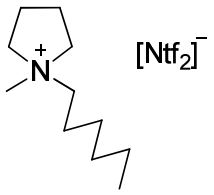

Chloroform-d
7.25
2.18
1.14
2.01
2.08
2.25
3.30
3.00

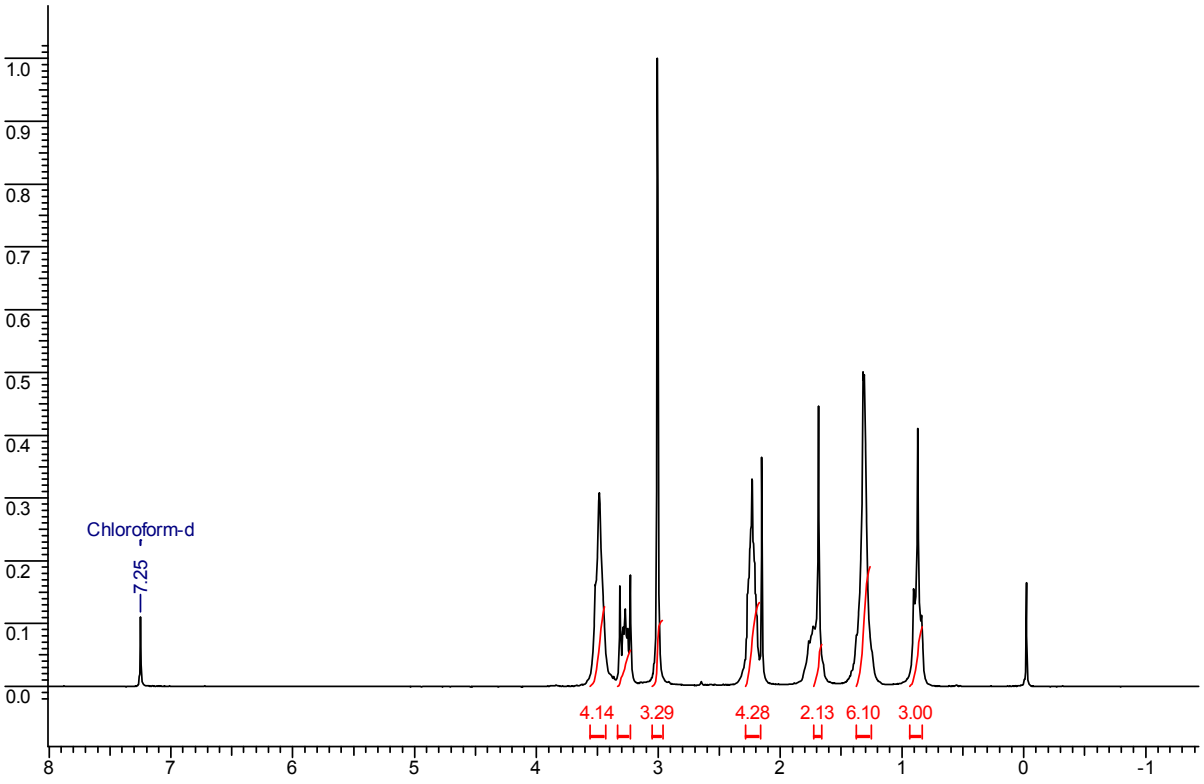

O
N
H
[EtSO4]−
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
6.47
1.68
2.84
1.93
6.00
9
8
7
6
5
4
3
2
1
0

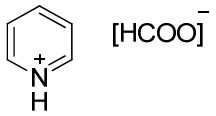

+
N
H

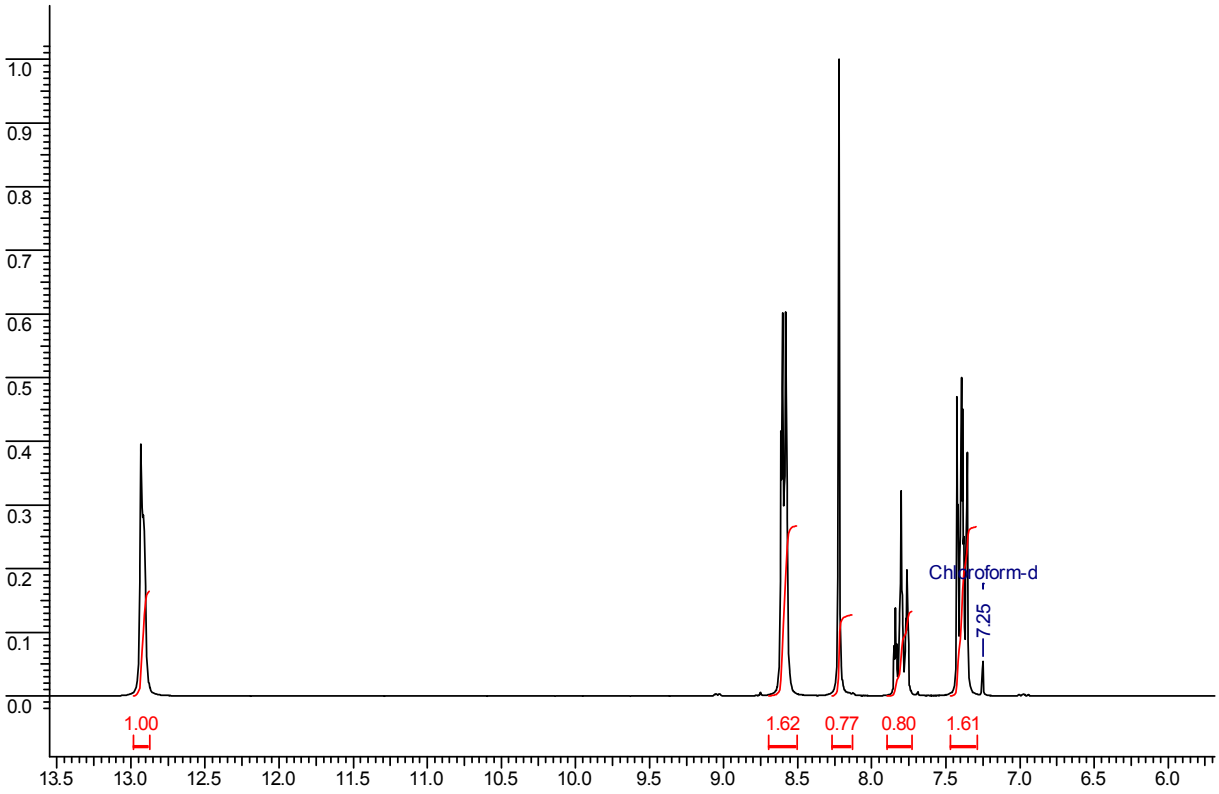
$[EtSO_4]^-$

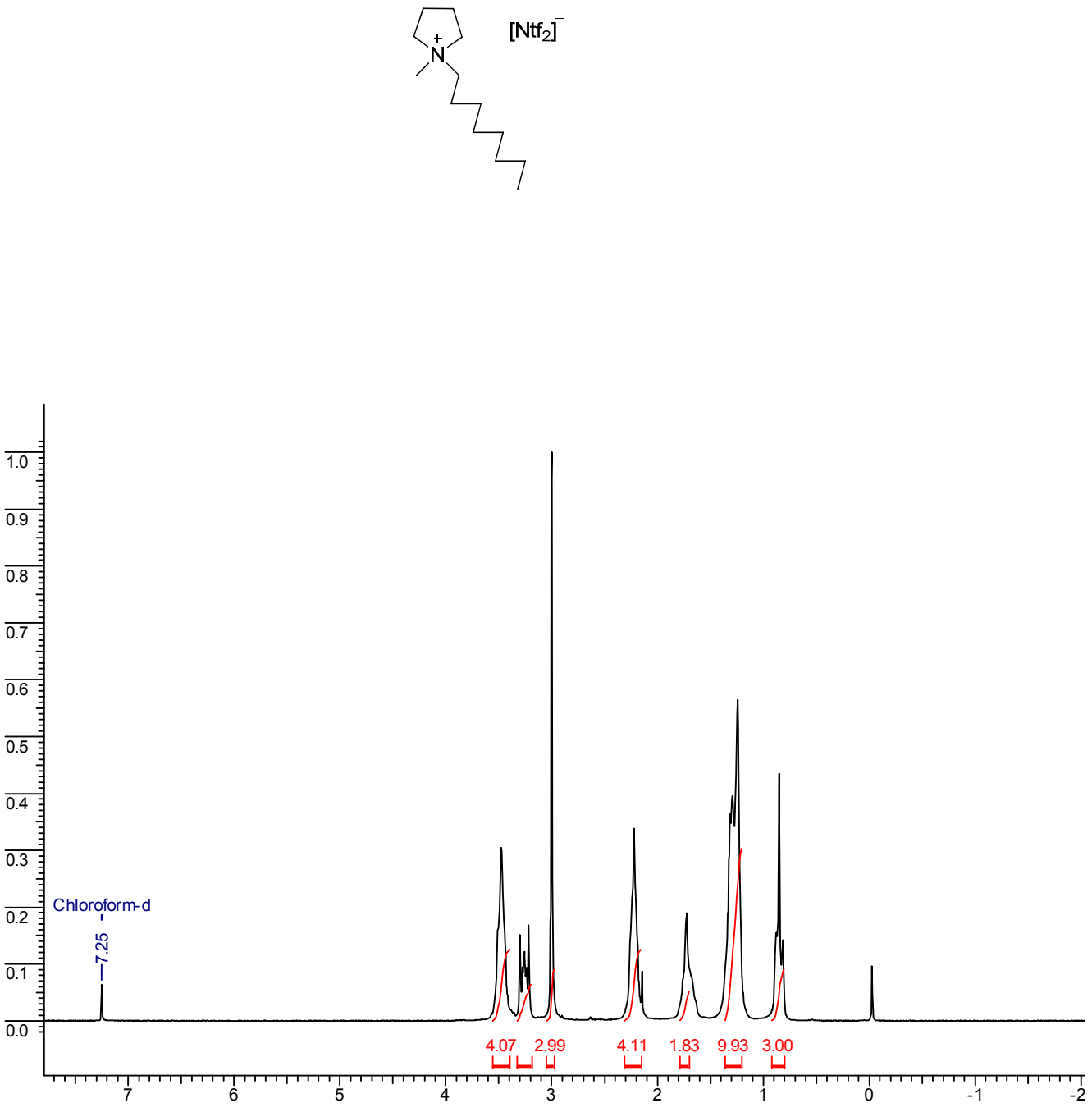

1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Chloroform-d
7.25
0.59
2.05
2.48
5.80
5.95
9
8
7
6
5
4
3
2
1
0
-1

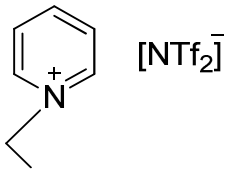

N
+
[Ntf2]-


Chloroform-d
7.25
4.14
3.29
4.28
2.13
6.10
3.00

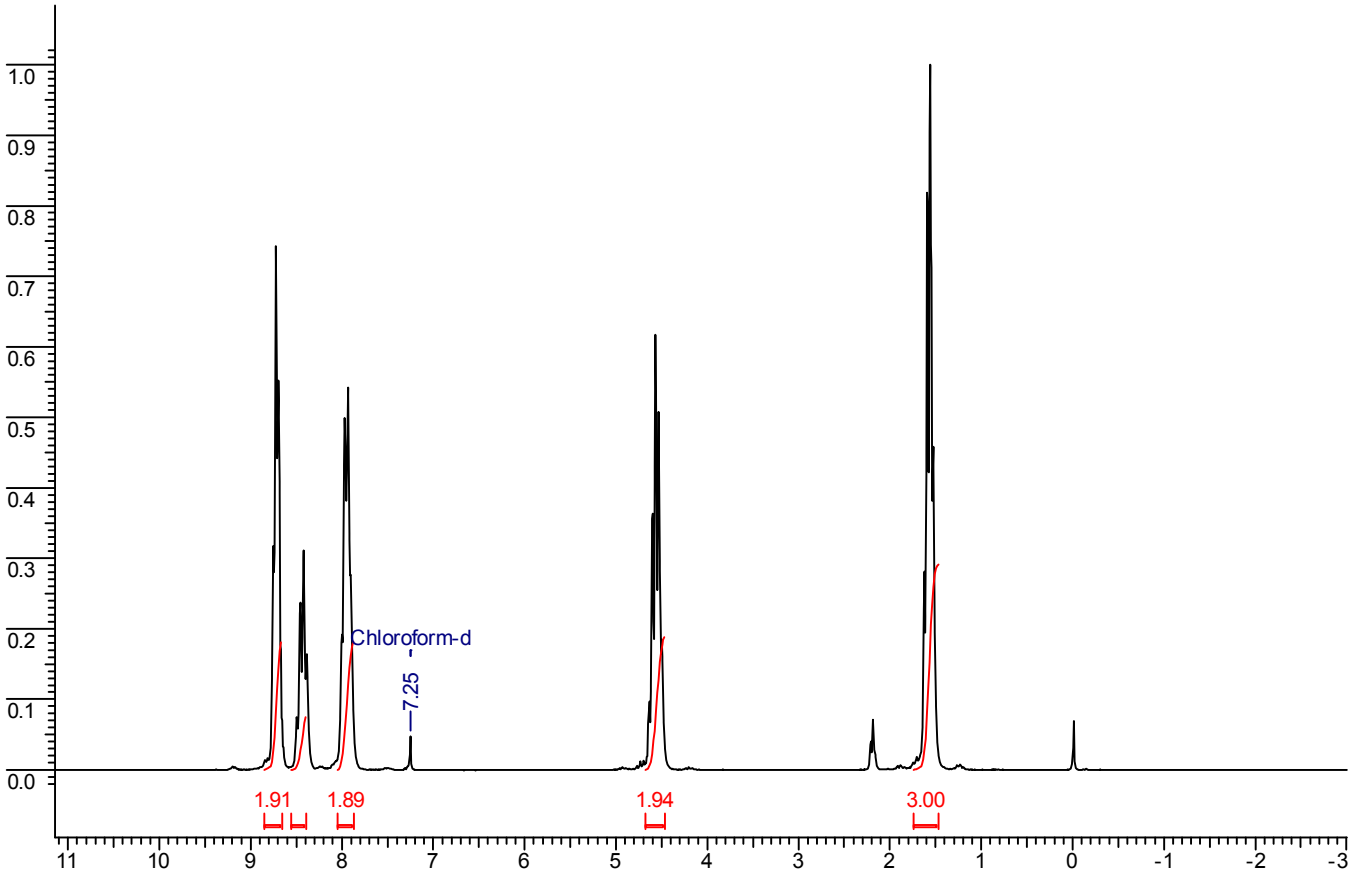

[HCOO]⁻
N
H


1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Chloroform-d
7.25
1.00
1.62
0.77
0.80
1.61
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0


[Ntf2]−
N
+
Chloroform-d
7.25
4.07
2.99
4.11
1.83
9.93
3.00
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
7
6
5
4
3
2
1
0
-1
-2


+
N

$[NTf_2^-]$


1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Chloroform-d
7.25
1.91
1.89
1.94
3.00
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3