Electronic supplementary information

RSC Advances

# Renewable sources from the plants as the starting material for designing new terpene chiral ionic liquids used for the chromatographic separation of acidic enantiomers

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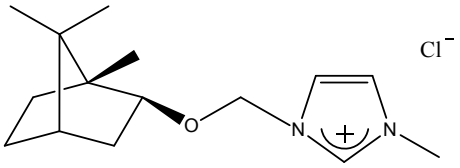
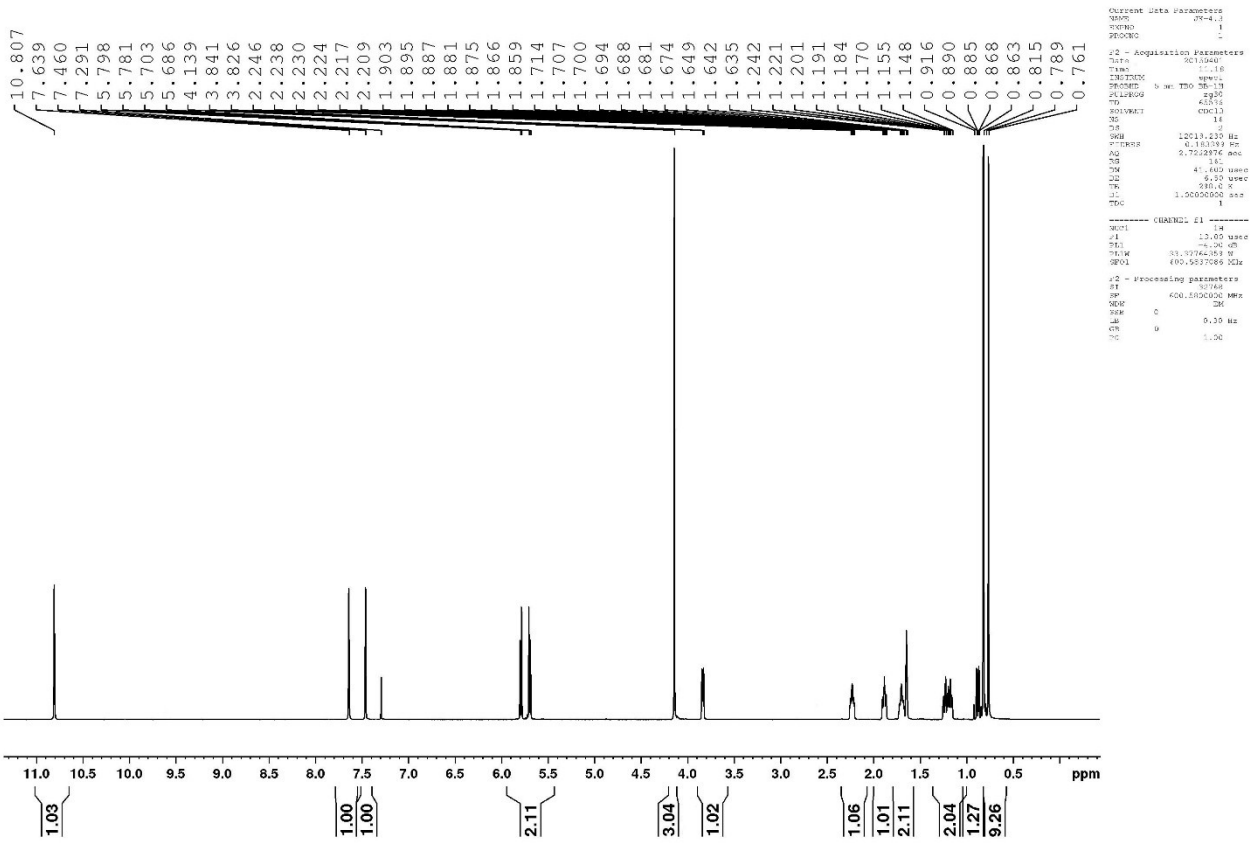
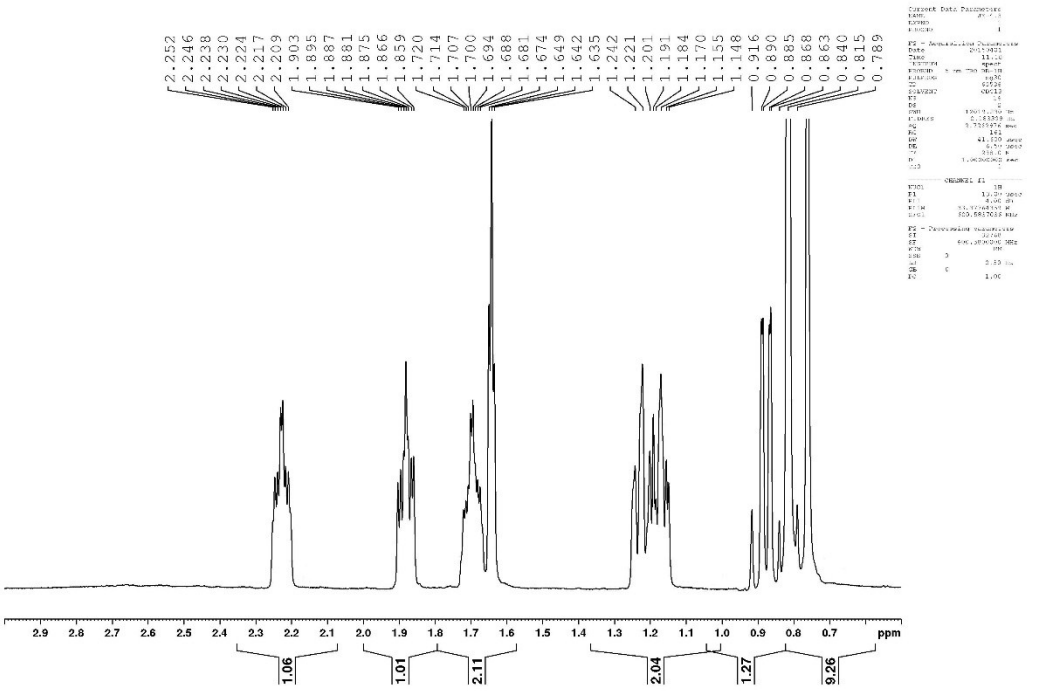
NMR spectra of the discussed CILs in $CDCl_3$

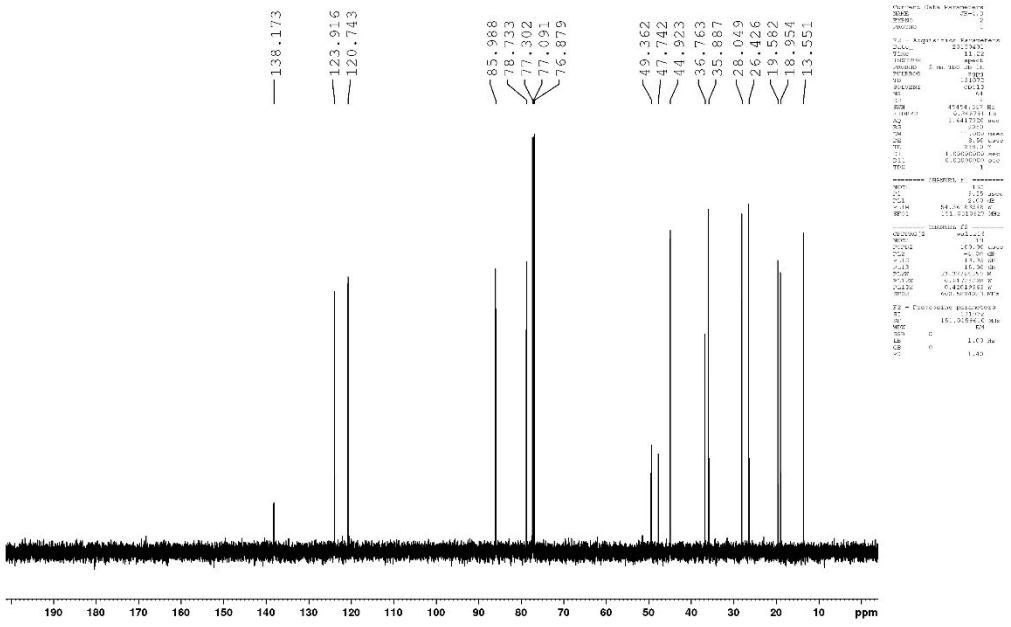
A)

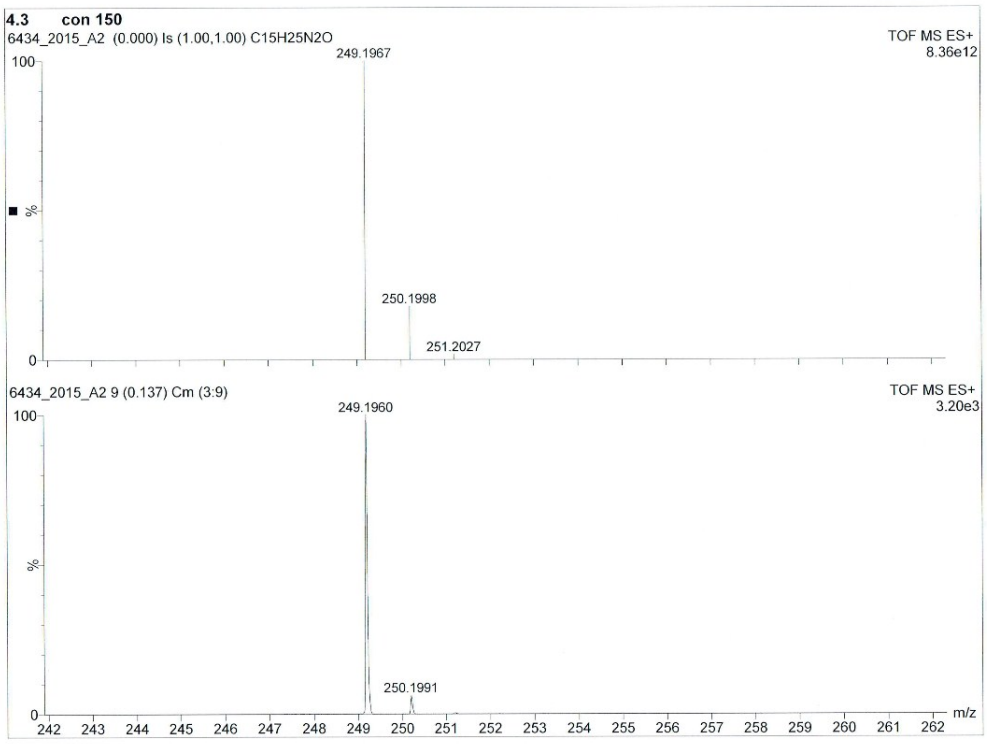
1-[(1*S*)-*endo*-(–)-Borneoxymethyl]-3-methylimidazolium chloride [$C_1$-Im-$CH_2$O-Bor][Cl] (**1b**)

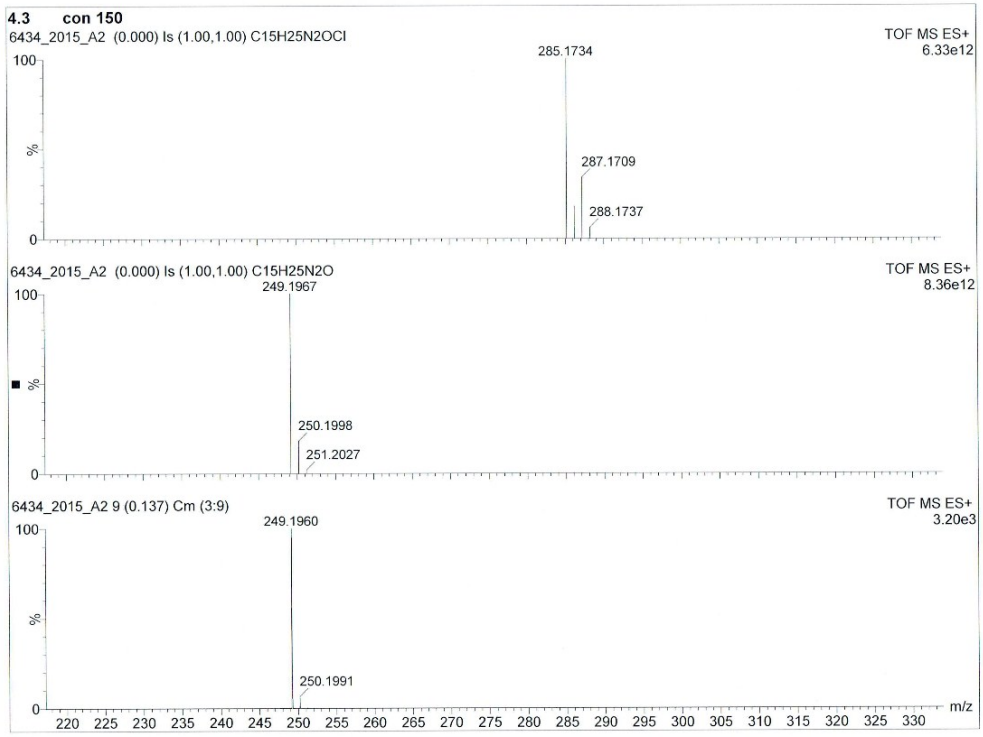



2.252
2.246
2.238
2.230
2.224
2.217
2.209
1.903
1.895
1.887
1.881
1.875
1.866
1.859
1.720
1.714
1.707
1.700
1.694
1.688
1.681
1.674
1.649
1.642
1.635
1.242
1.221
1.201
1.191
1.184
1.170
1.155
1.148
0.916
0.890
0.885
0.868
0.863
0.840
0.815
0.789
2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 ppm
1.06
1.01
2.11
2.04
1.27
9.26

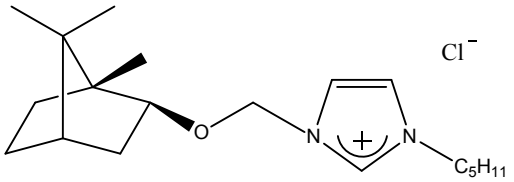

138.173
123.916
120.743
85.988
78.733
77.302
77.091
76.879
49.362
47.742
44.923
36.763
35.887
28.049
26.426
19.562
18.954
13.551
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

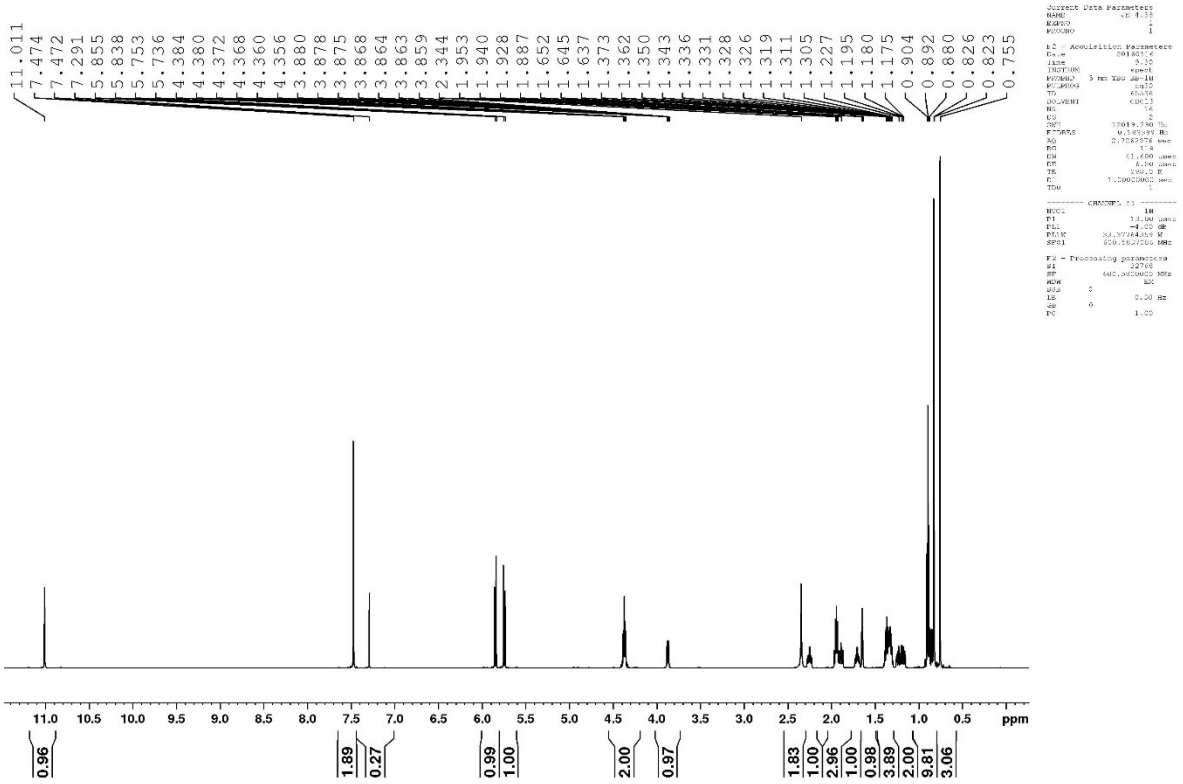

4.3 con 150
6434_2015_A2 (0.000) Is (1.00,1.00) C15H25N2O
TOF MS ES+
8.36e12
249.1967
250.1998
251.2027
6434_2015_A2 9 (0.137) Cm (3:9)
TOF MS ES+
3.20e3
249.1960
250.1991
m/z

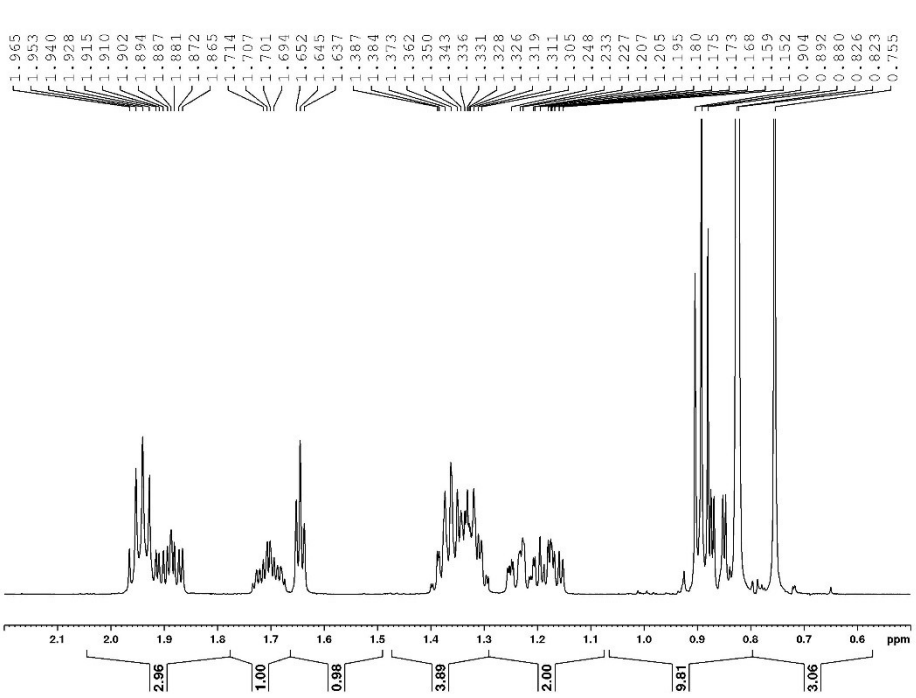

4.3 con 150
6434_2015_A2 (0.000) Is (1.00,1.00) C15H25N2OCl
TOF MS ES+
6.33e12
285.1734
287.1709
288.1737
6434_2015_A2 (0.000) Is (1.00,1.00) C15H25N2O
TOF MS ES+
8.36e12
249.1967
250.1998
251.2027
6434_2015_A2 9 (0.137) Cm (3:9)
TOF MS ES+
3.20e3
249.1960
250.1991
m/z

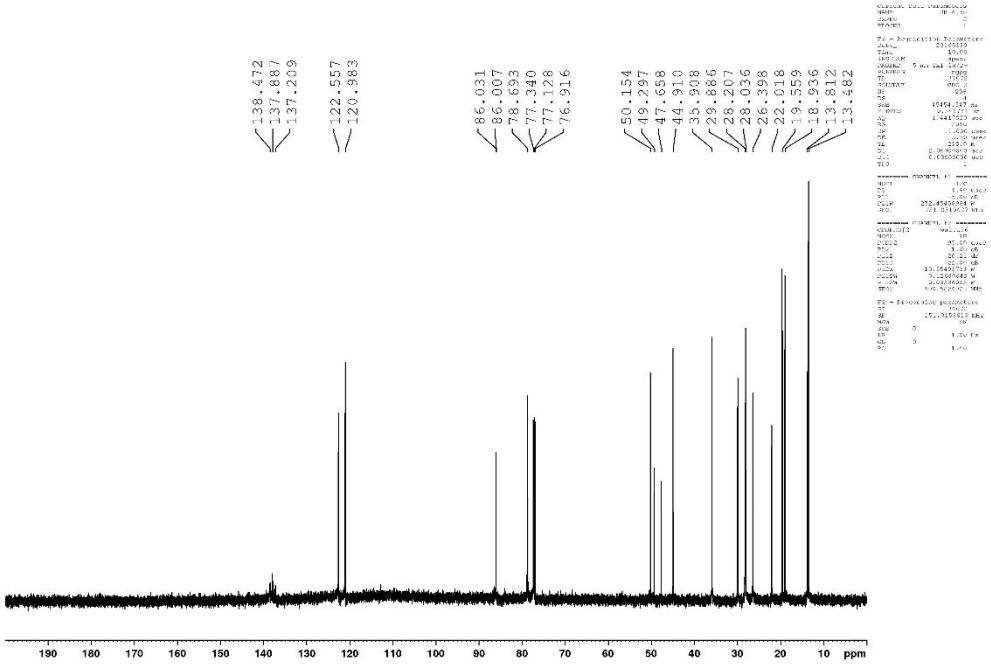
B)

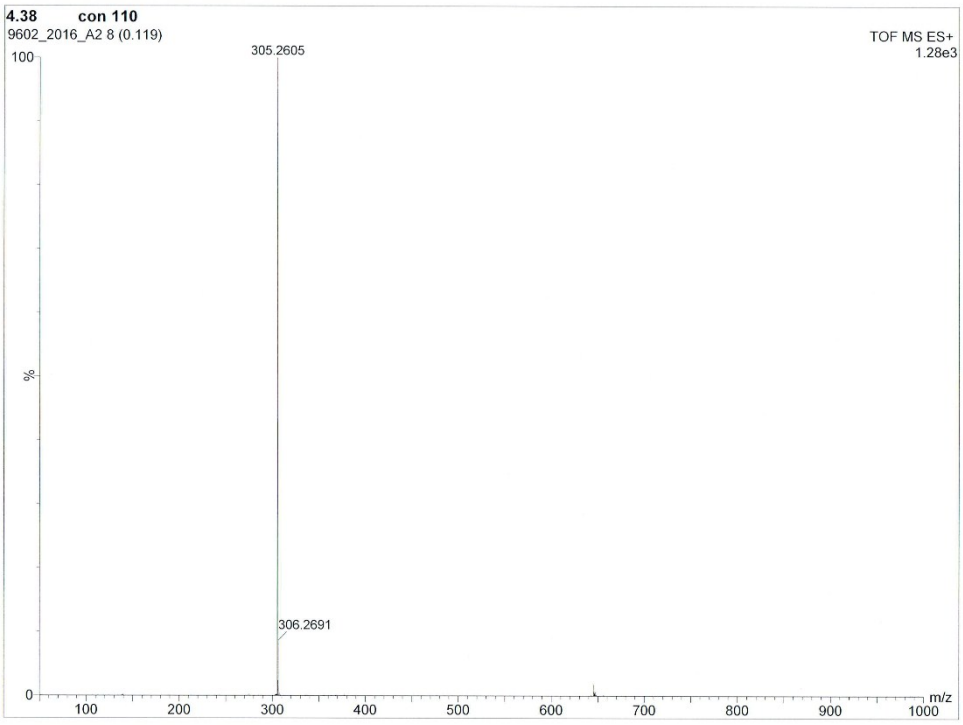
1-[(1*S*)-*endo*-(–)-Borneoxymethyl]-3-pentylimidazolium chloride [$C_5$-Im-$CH_2O$-Bor][Cl] (**1c**)

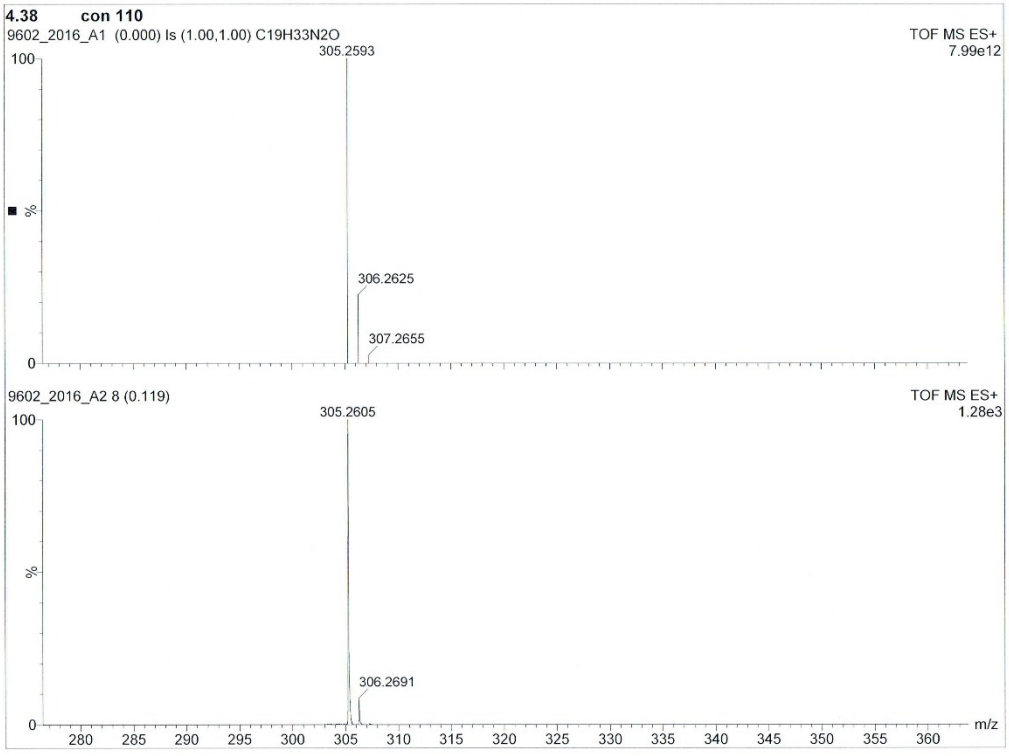



1.965
1.953
1.940
1.928
1.915
1.910
1.902
1.894
1.887
1.881
1.872
1.865
1.714
1.707
1.701
1.694
1.652
1.645
1.637
1.387
1.384
1.373
1.362
1.350
1.343
1.336
1.331
1.328
1.326
1.319
1.311
1.305
1.248
1.233
1.227
1.207
1.205
1.195
1.180
1.175
1.173
1.168
1.159
1.152
0.904
0.892
0.880
0.826
0.823
0.755
2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 0.6 ppm
2.96
1.00
0.98
3.89
2.00
9.81
3.06

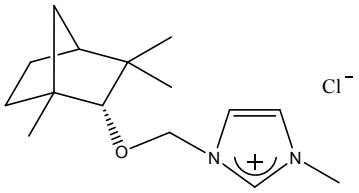

138.472
137.887
137.209
122.557
120.983
86.031
86.007
78.693
77.340
77.128
76.916
50.154
49.297
47.658
44.910
35.908
29.886
28.207
28.036
26.398
22.018
19.559
18.536
13.812
13.482
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

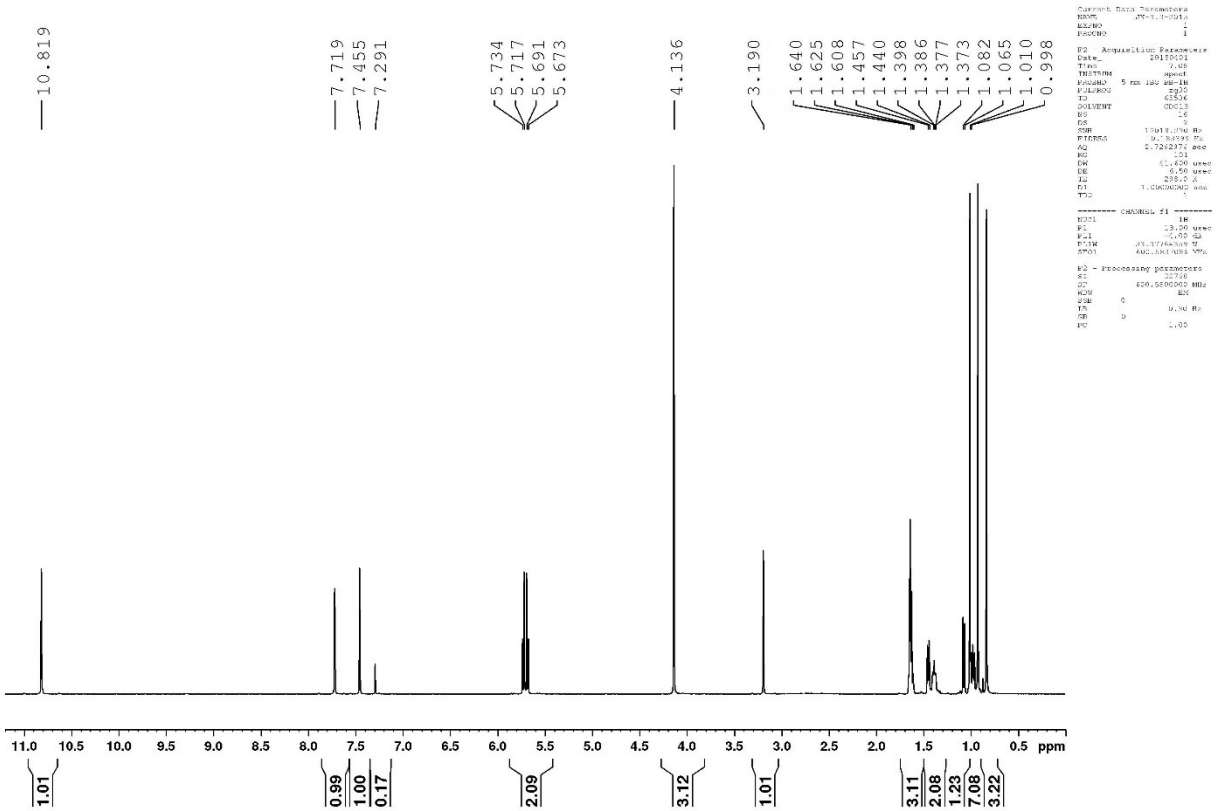

4.38 con 110
9602_2016_A2 8 (0.119)
TOF MS ES+
1.28e3
305.2605
306.2691
100
%
0
100 200 300 400 500 600 700 800 900 1000
m/z

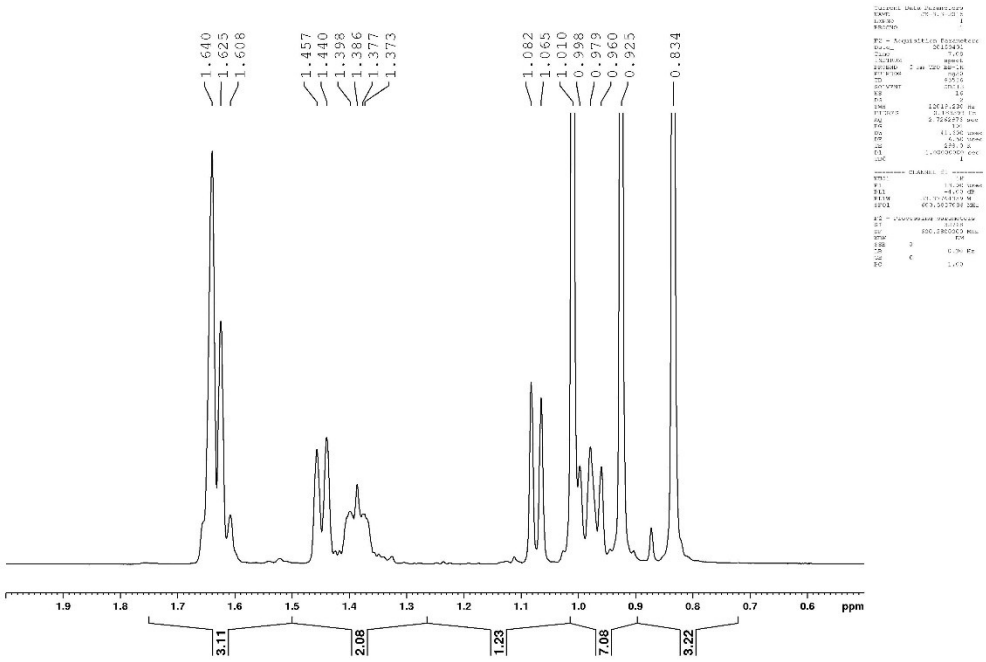

4.38 con 110
9602_2016_A1 (0.000) Is (1.00,1.00) C19H33N2O
TOF MS ES+
7.99e12
305.2593
306.2625
307.2655
100
%
0
9602_2016_A2 8 (0.119)
TOF MS ES+
1.28e3
305.2605
306.2691
100
%
0
280 285 290 295 300 305 310 315 320 325 330 335 340 345 350 355 360
m/z

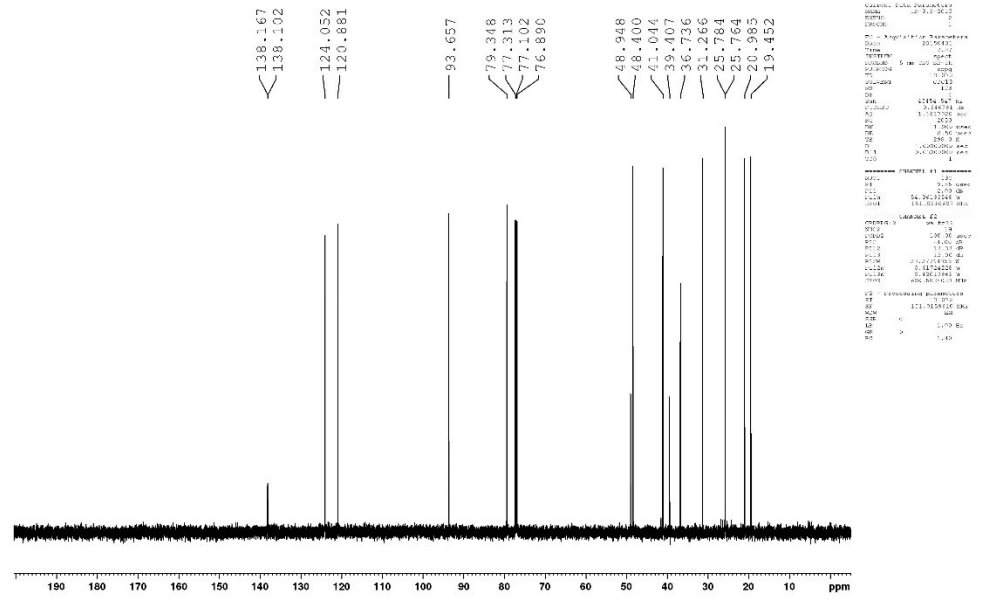
C)

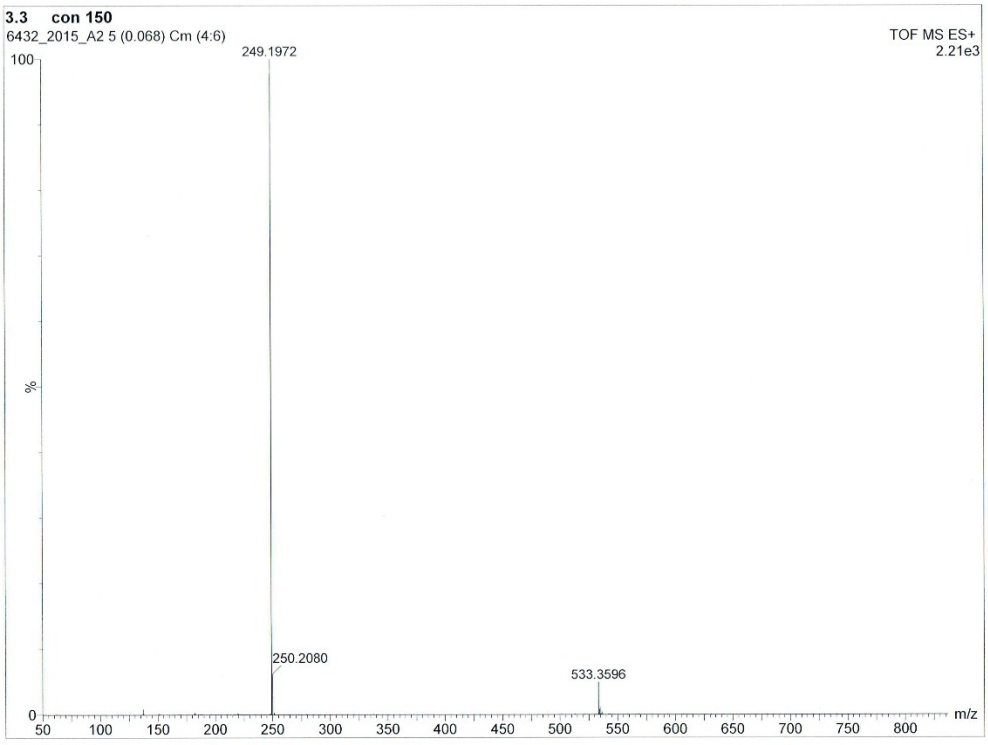
1-[(1*R*)-*endo*-(+)-Fenchoxymethyl]-3-methylimidazolium chloride [$C_1$-Im-$CH_2$O-Fen][Cl] (**2b**)

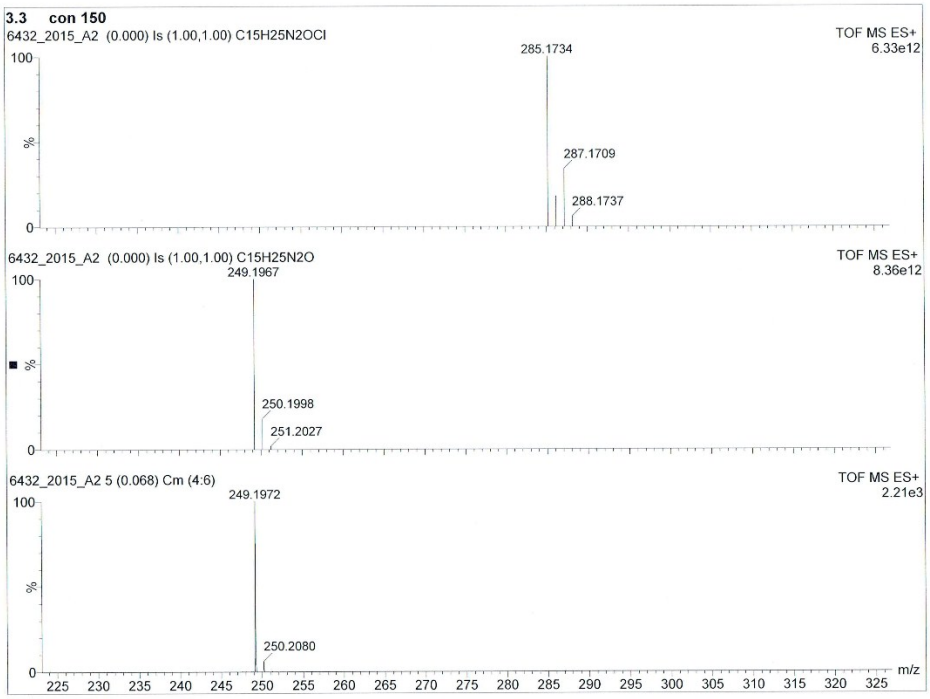



1.640
1.625
1.608
1.457
1.440
1.398
1.386
1.377
1.373
1.082
1.065
1.010
0.998
0.979
0.960
0.925
0.834
1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 0.6 ppm
3.11
2.08
1.23
7.08
3.22

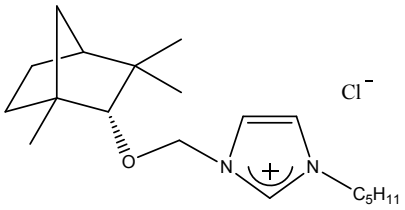

138.167
138.102
124.052
120.881
93.657
79.348
77.313
77.102
76.890
68.948
68.400
41.044
39.407
36.736
31.266
25.784
25.764
20.985
19.452
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

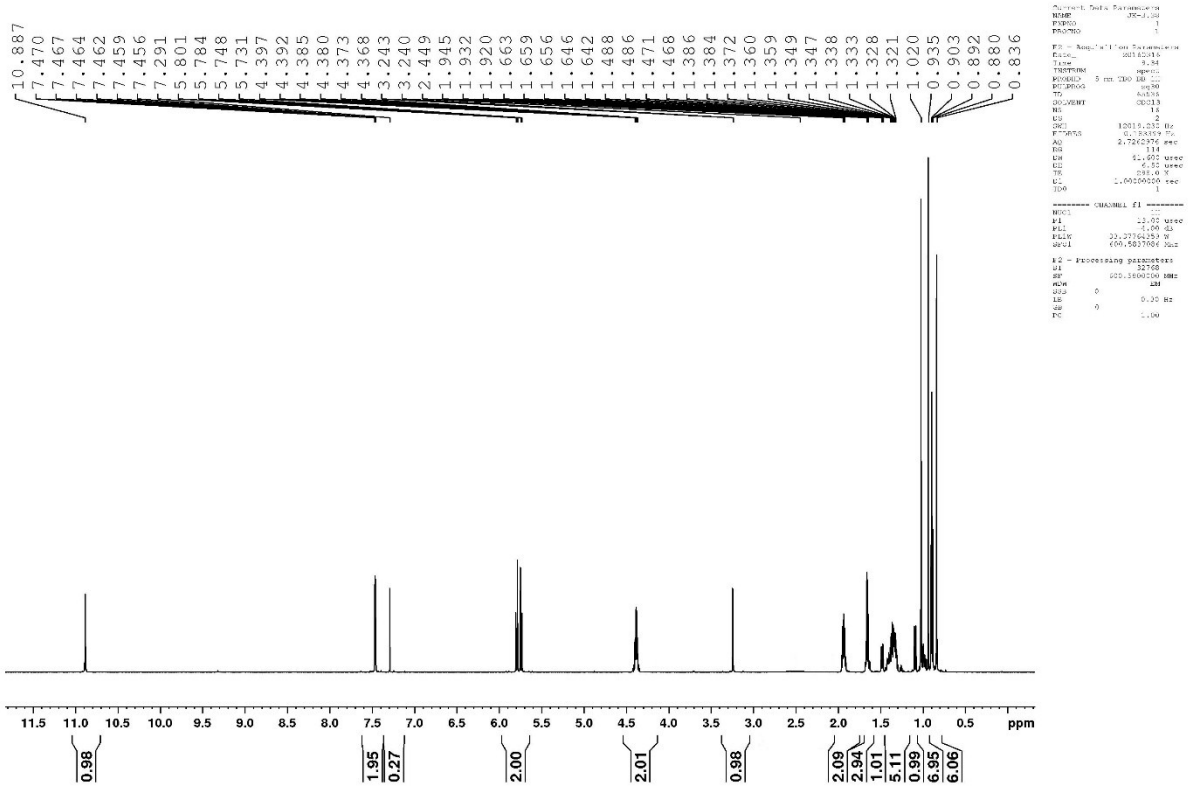

3.3 con 150
6432_2015_A2 5 (0.068) Cm (4:6)
TOF MS ES+
2.21e3
249.1972
250.2080
533.3596
100
%
0
m/z
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800

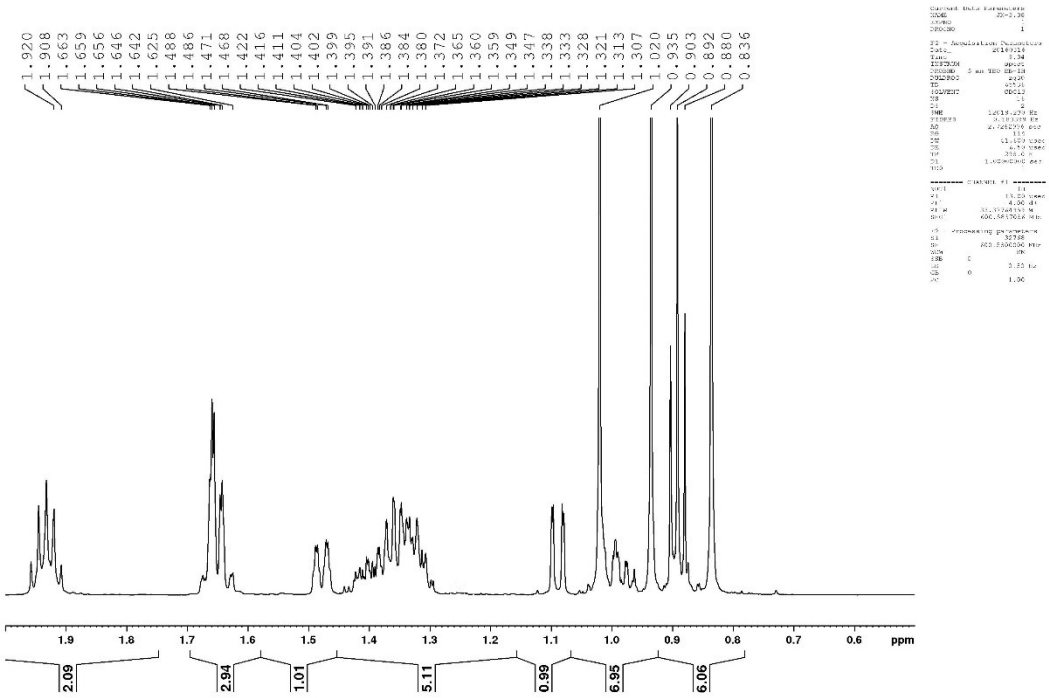

3.3 con 150
6432_2015_A2 (0.000) Is (1.00,1.00) C15H25N2OCl
TOF MS ES+
6.33e12
285.1734
287.1709
288.1737
6432_2015_A2 (0.000) Is (1.00,1.00) C15H25N2O
TOF MS ES+
8.36e12
249.1967
250.1998
251.2027
6432_2015_A2 5 (0.068) Cm (4:6)
TOF MS ES+
2.21e3
249.1972
250.2080
100
%
0
m/z
225 230 235 240 245 250 255 260 265 270 275 280 285 290 295 300 305 310 315 320 325

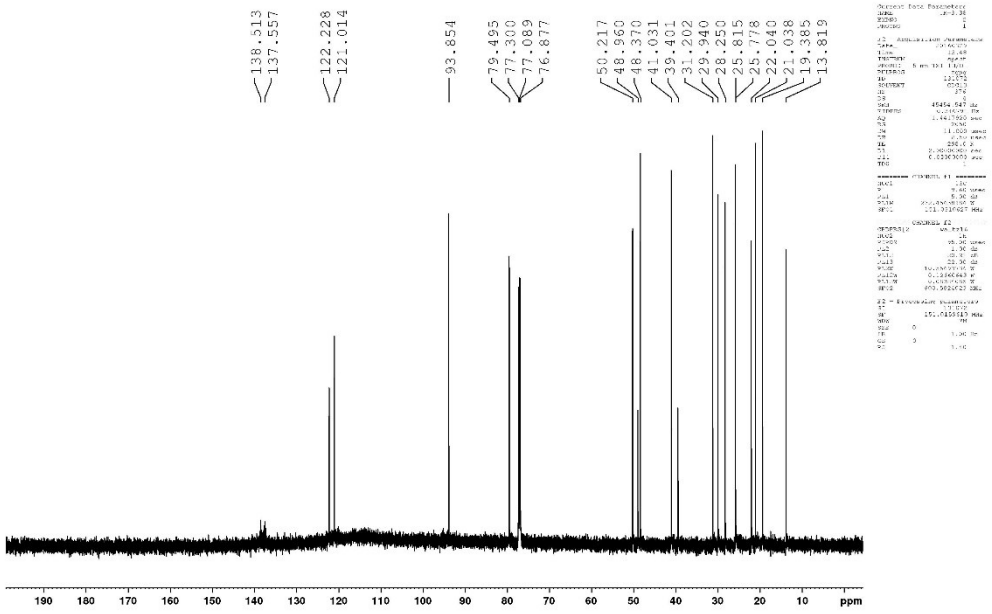
D)

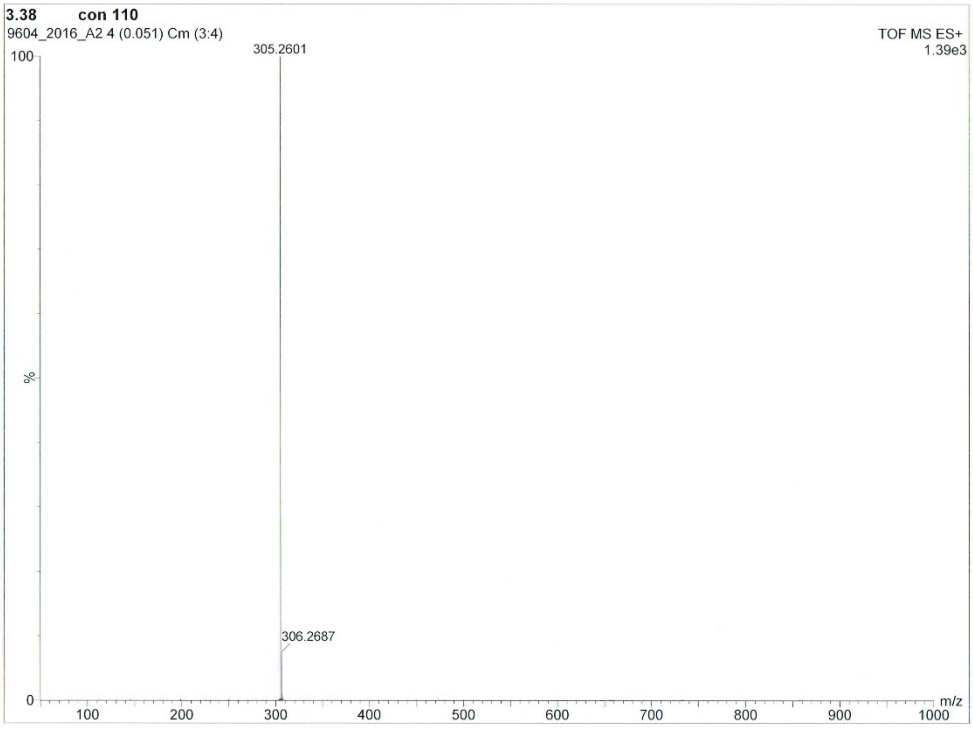
1-[(1*R*)-*endo*-(+)-Fenchoxymethyl]-3-pentylimidazolium chloride [$C_5$-Im-$CH_2$O-Fen][Cl] (**2c**)

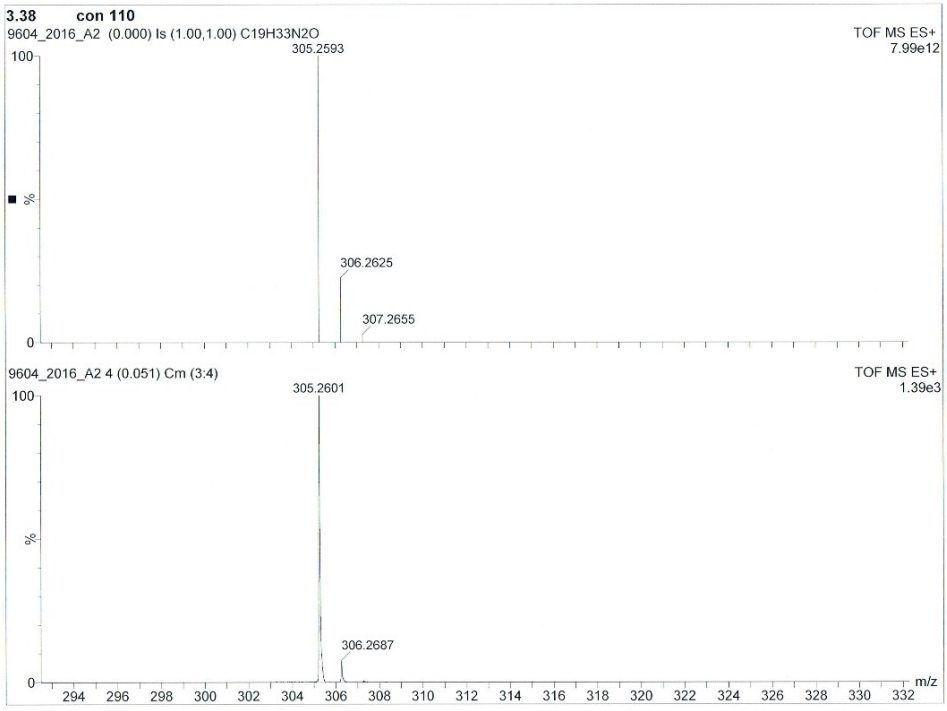



1.920
1.908
1.663
1.659
1.656
1.646
1.642
1.625
1.488
1.486
1.471
1.468
1.422
1.416
1.411
1.404
1.402
1.399
1.395
1.391
1.386
1.384
1.380
1.372
1.365
1.360
1.359
1.349
1.347
1.338
1.333
1.328
1.321
1.313
1.307
1.020
0.935
0.903
0.892
0.880
0.836
1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 0.6 ppm
2.09
2.94
1.01
5.11
0.99
6.95
6.06


138.513
137.557
122.228
121.014
93.854
79.495
77.300
77.089
76.877
50.217
48.960
46.370
41.031
39.401
31.202
29.940
28.250
25.815
25.778
22.040
21.038
19.385
13.819
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


3.38 con 110
9604_2016_A2 4 (0.051) Cm (3:4)
TOF MS ES+
1.39e3
305.2601
306.2687
100
%
0
m/z
100 200 300 400 500 600 700 800 900 1000


3.38 con 110
9604_2016_A2 (0.000) Is (1.00,1.00) C19H33N2O
TOF MS ES+
7.99e12
305.2593
306.2625
307.2655
9604_2016_A2 4 (0.051) Cm (3:4)
TOF MS ES+
1.39e3
305.2601
306.2687
100
%
0
m/z
294 296 298 300 302 304 306 308 310 312 314 316 318 320 322 324 326 328 330 332

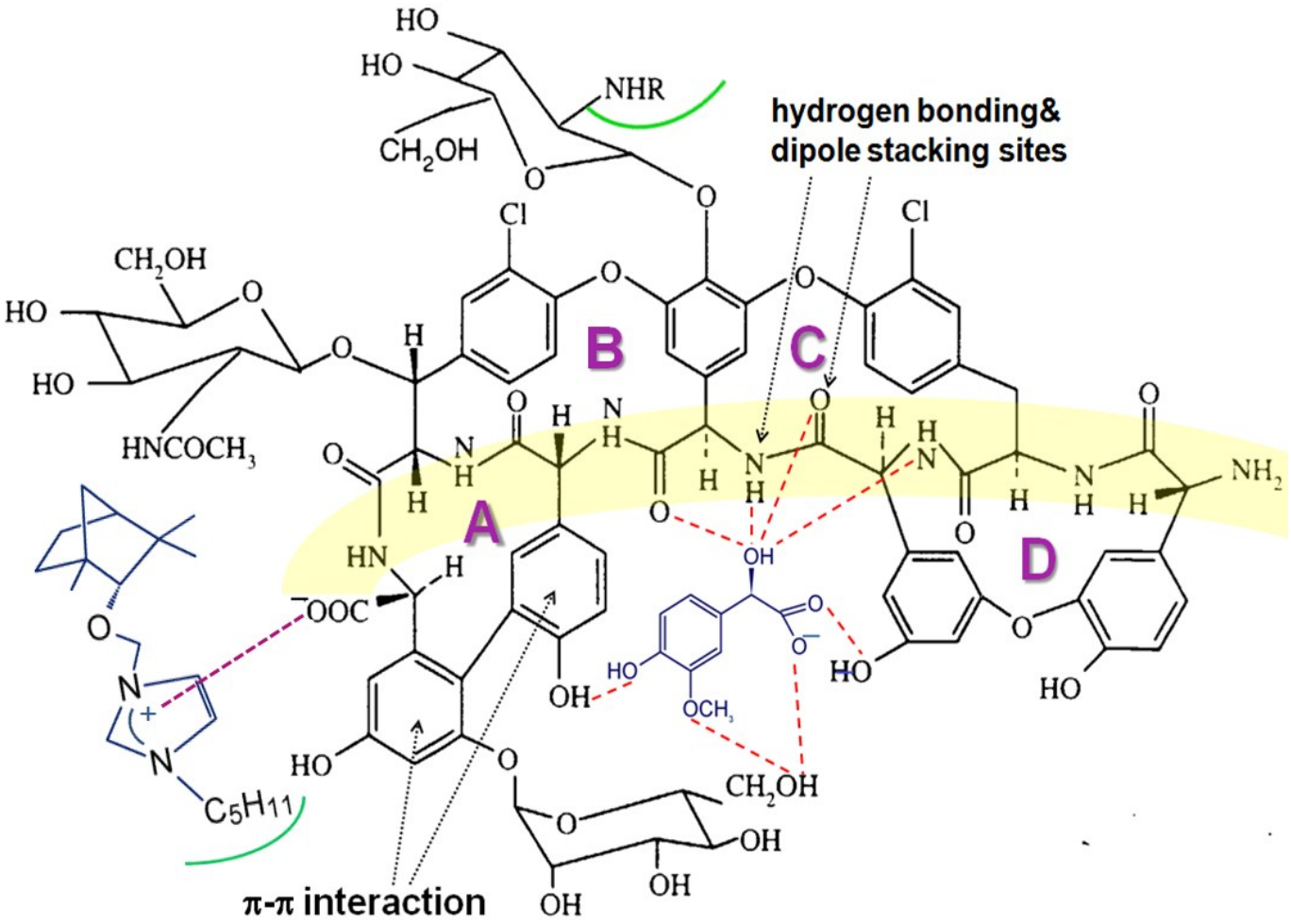



Fig. S1 The scheme of the interactions between *R*-4-hydroxy-3-methoxy mandelic acid and teicoplanin. The *R*-enantiomer binds simultaneously to cavities A, C and D. Red dashed lines indicate the possibility of creating hydrogen bonds. Purple dashed line indicates the ionic bridge created between carboxyl group of teicoplanin and the imidazolium moiety of terpen**e** CIL. Green solid line shows hydrophobic interactions between the alkyl group (pentyl) of **1b** CIL and the aliphatic decanoic chain of teicoplanin (R).

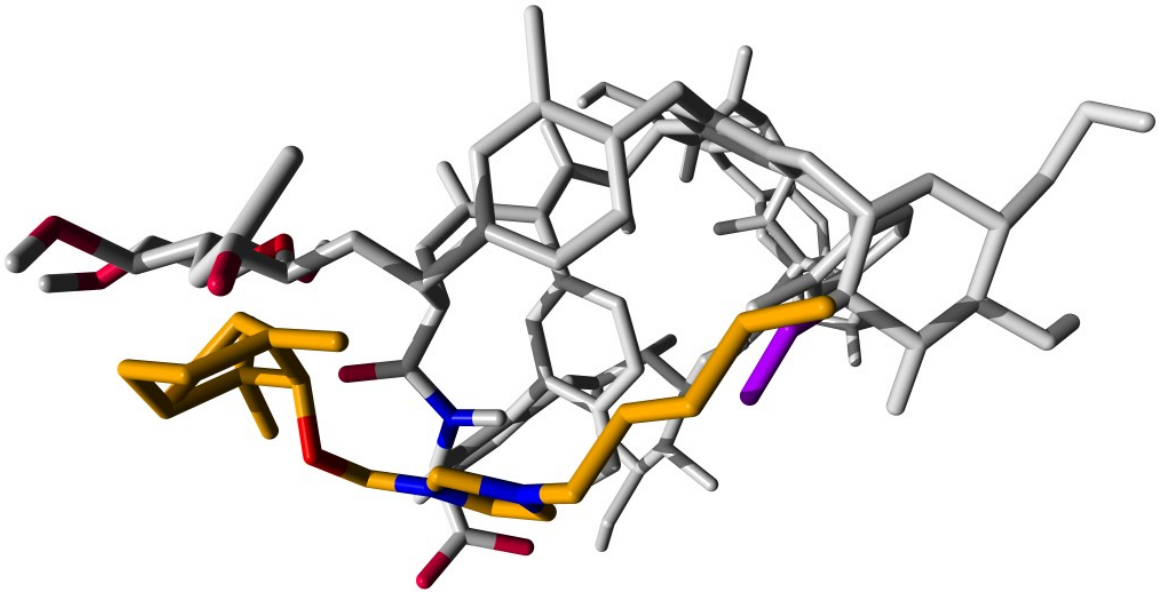


Fig. S2 The teicoplanin – **2c** CIL complex. The decanoic chain (purple) was shorten for clarity. The **2c** CIL was colored in orange.