Supporting Information

For

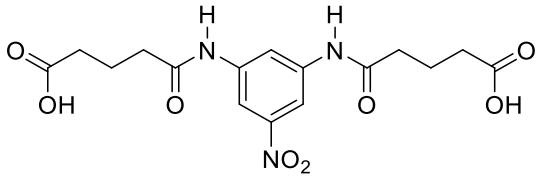
The Colorimetric Detection of the Hydroxyl Radical

Yandong Ran, Mohammed Moursy, Robert Hider and Agostino Cilibrizzi*

Institute of Pharmaceutical Sciences, King's College London, SE1 9NH, United Kingdom

*agostino.cilibrizzi@kcl.ac.uk

Content: spectral data for NPBG.

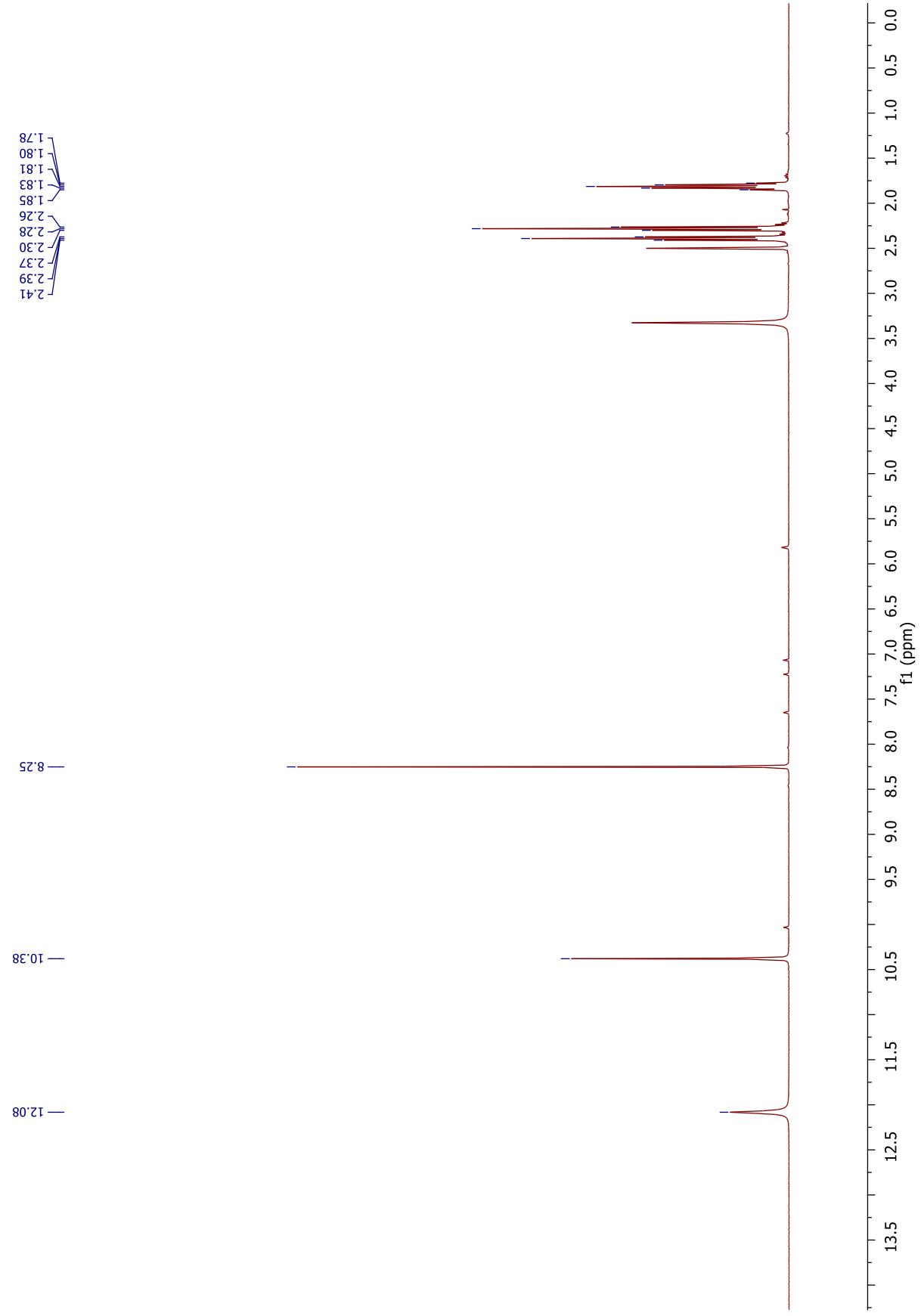


N,N'-(5-nitro-1,3-phenylene)bisglutoramide (**NPBG**)

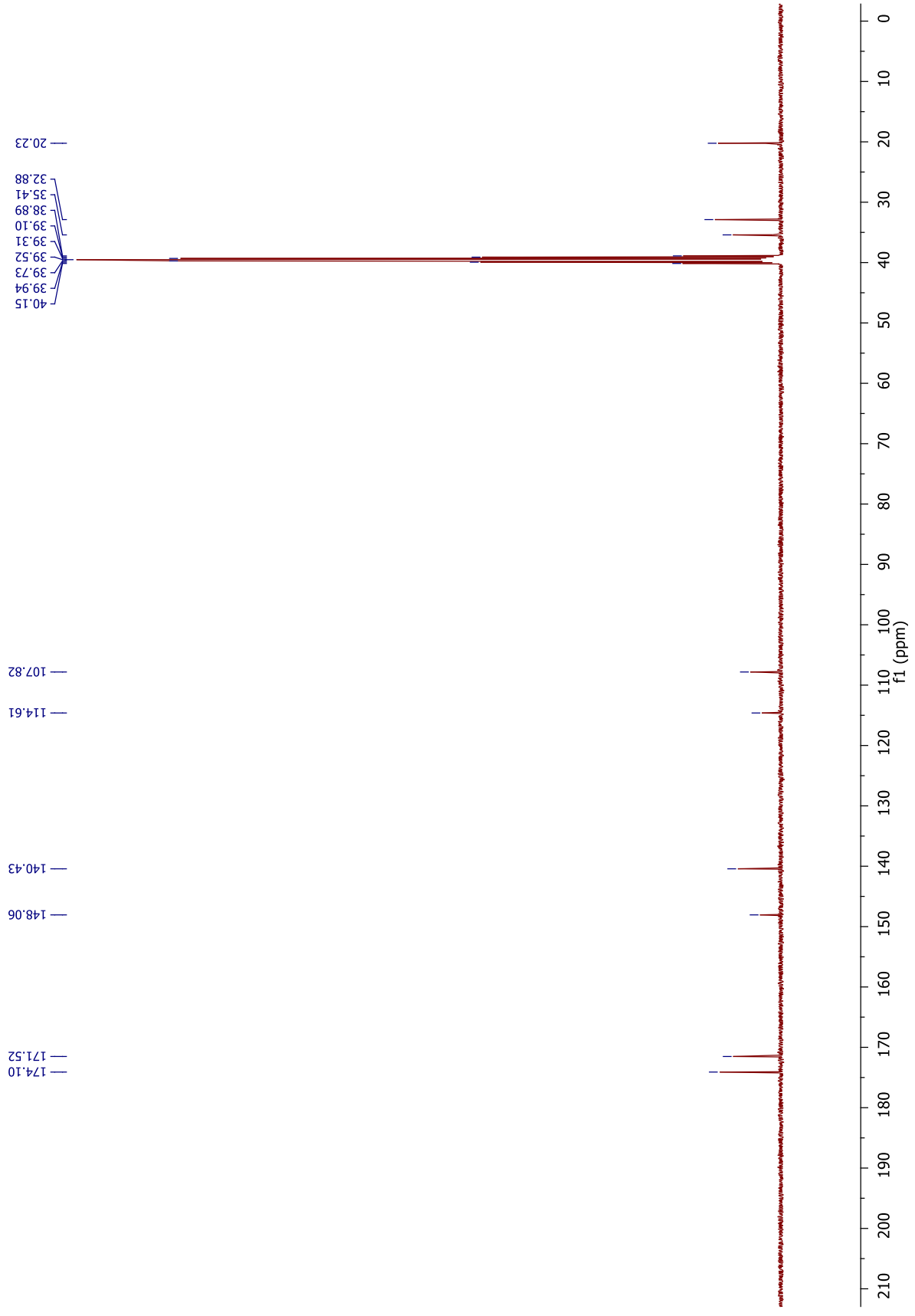
$C_{16}H_{19}N_3O_8$
MW: 381.34

1. ^{1}H NMR – NPBG
2. ^{13}C NMR – NPBG
3. DEPT ^{13}C NMR – NPBG
4. MS (ESI^-) – NPBG
5. FT-IR – NPBG
6. UV spectra of the *ortho*- (a) and *para*- (b) hydroxy and phenolate NPBG species
7. HPLC chromatograms of *ortho*- and *para*-hydroxy-NPBG isomers monitored at 430 nm (a) and 232 nm (b)

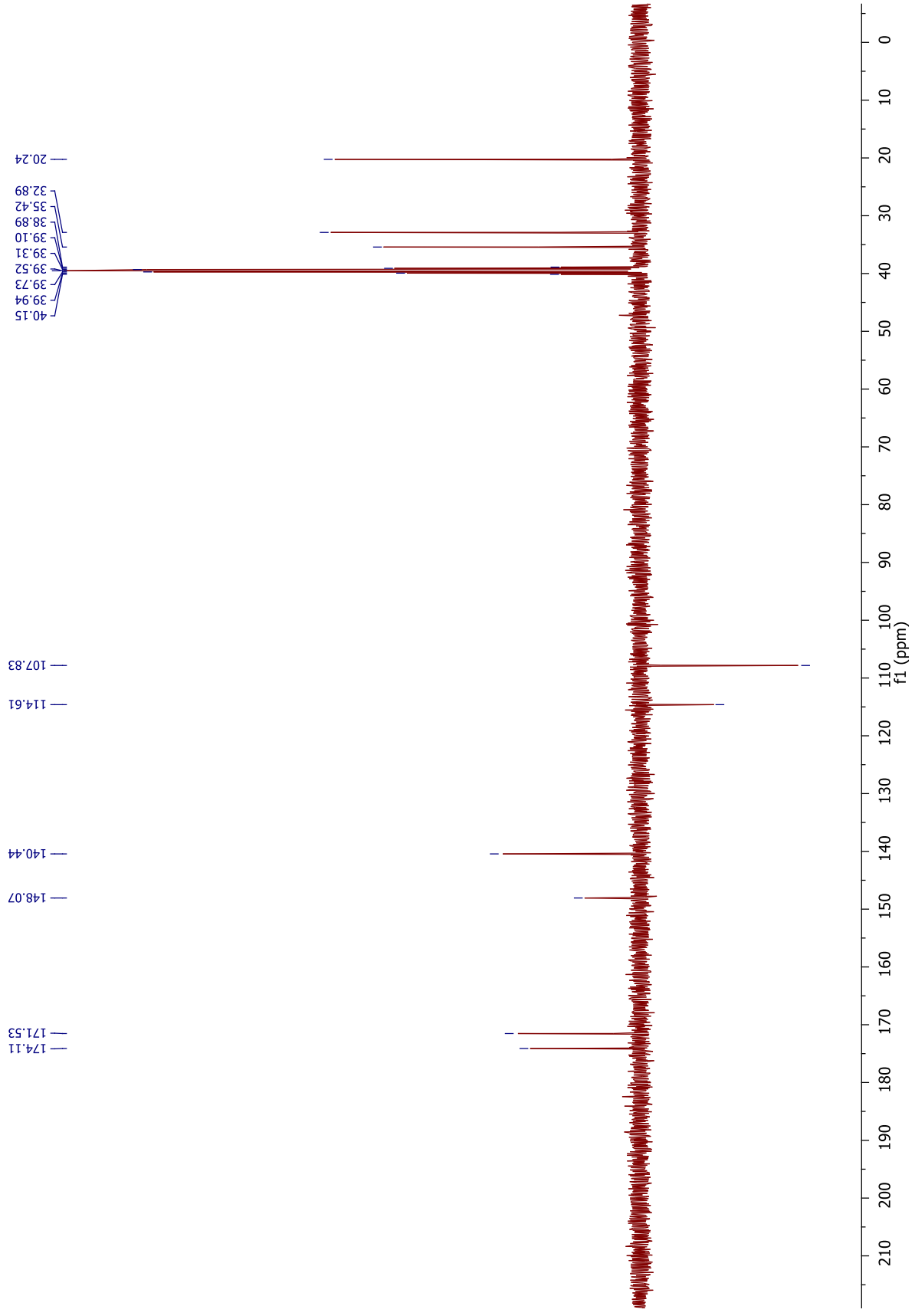
1. ^{1}H NMR - NPBG


1.78
1.80
1.81
1.83
1.85
2.26
2.28
2.30
2.37
2.39
2.41
8.25
10.38
12.08
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
8.5
9.0
9.5
10.5
11.5
12.5
13.5
f1 (ppm)

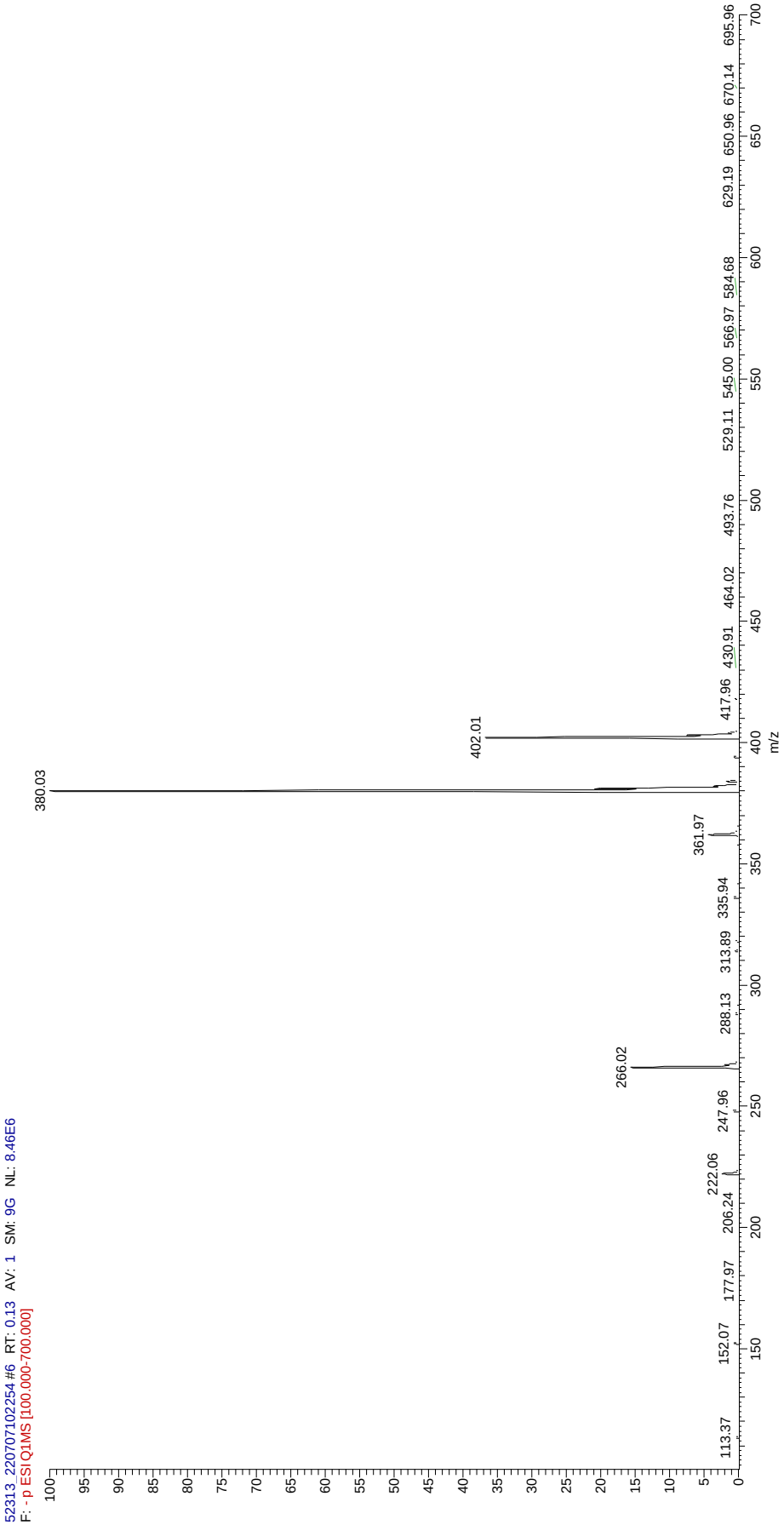
2. ^{13}C NMR – NPBG



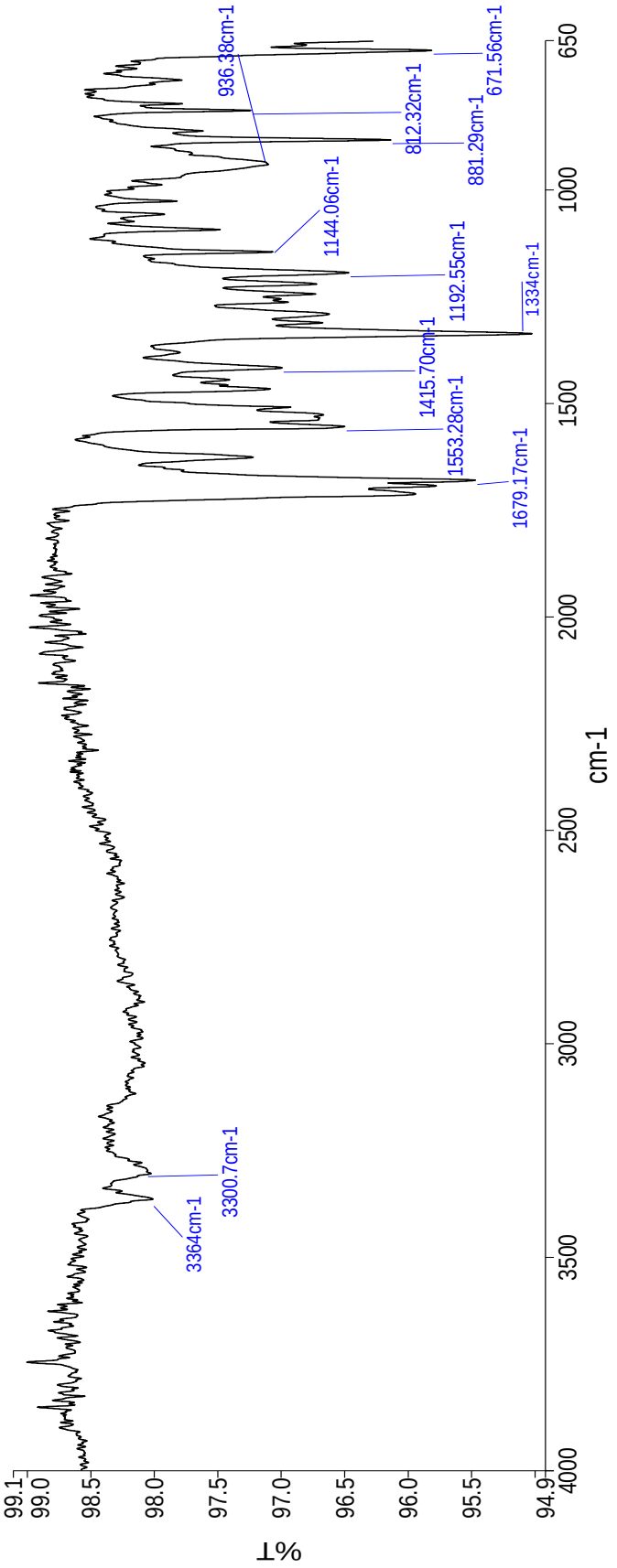
3. DEPT ^{13}C NMR - NPBG



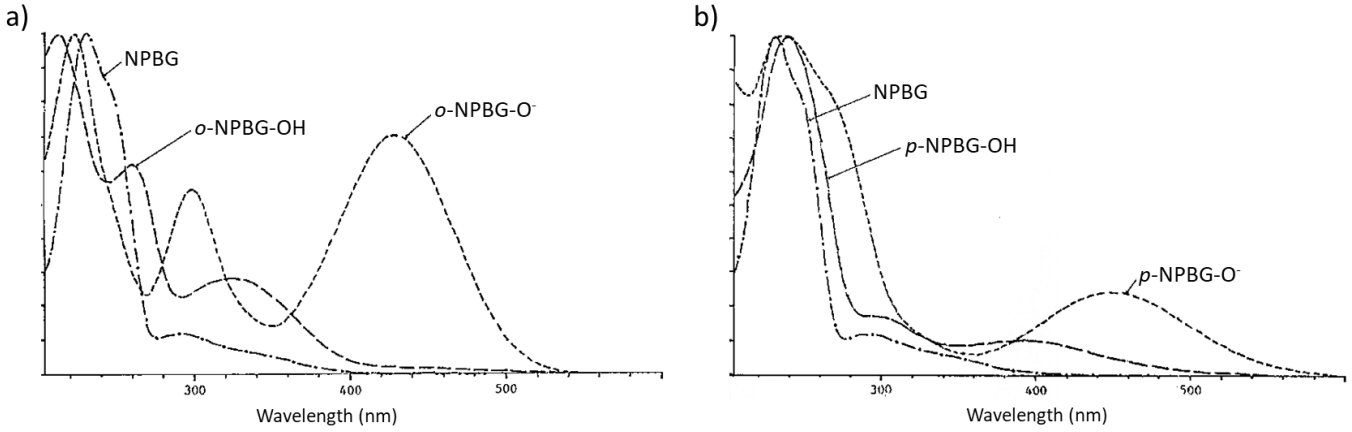
4. MS (ESI$^-$) - NPBG


52313_220707102254 #6 RT: 0.13 AV: 1 SM: 9G NL: 8.46E6
F: - p ESI Q1MS [100.000-700.000]
380.03
402.01
361.97
266.02
m/z

5. FT-IR - NPBG


936.38cm-1
812.32cm-1
671.56cm-1
881.29cm-1
1144.06cm-1
1192.55cm-1
1334cm-1
1415.70cm-1
1553.28cm-1
1679.17cm-1
3364cm-1
3300.7cm-1
%T
cm-1
99.1
99.0
98.5
98.0
97.5
97.0
96.5
96.0
95.5
94.9
4000
3500
3000
2500
2000
1500
1000
650

6. **UV spectra** of the *ortho*- (a) and *para*- (b) hydroxy and phenolate NPBG species



7. **HPLC chromatograms** of *ortho*- and *para*-hydroxy-NPBG isomers monitored at 430 nm (a) and 232 nm (b)

