Supplementary Materials

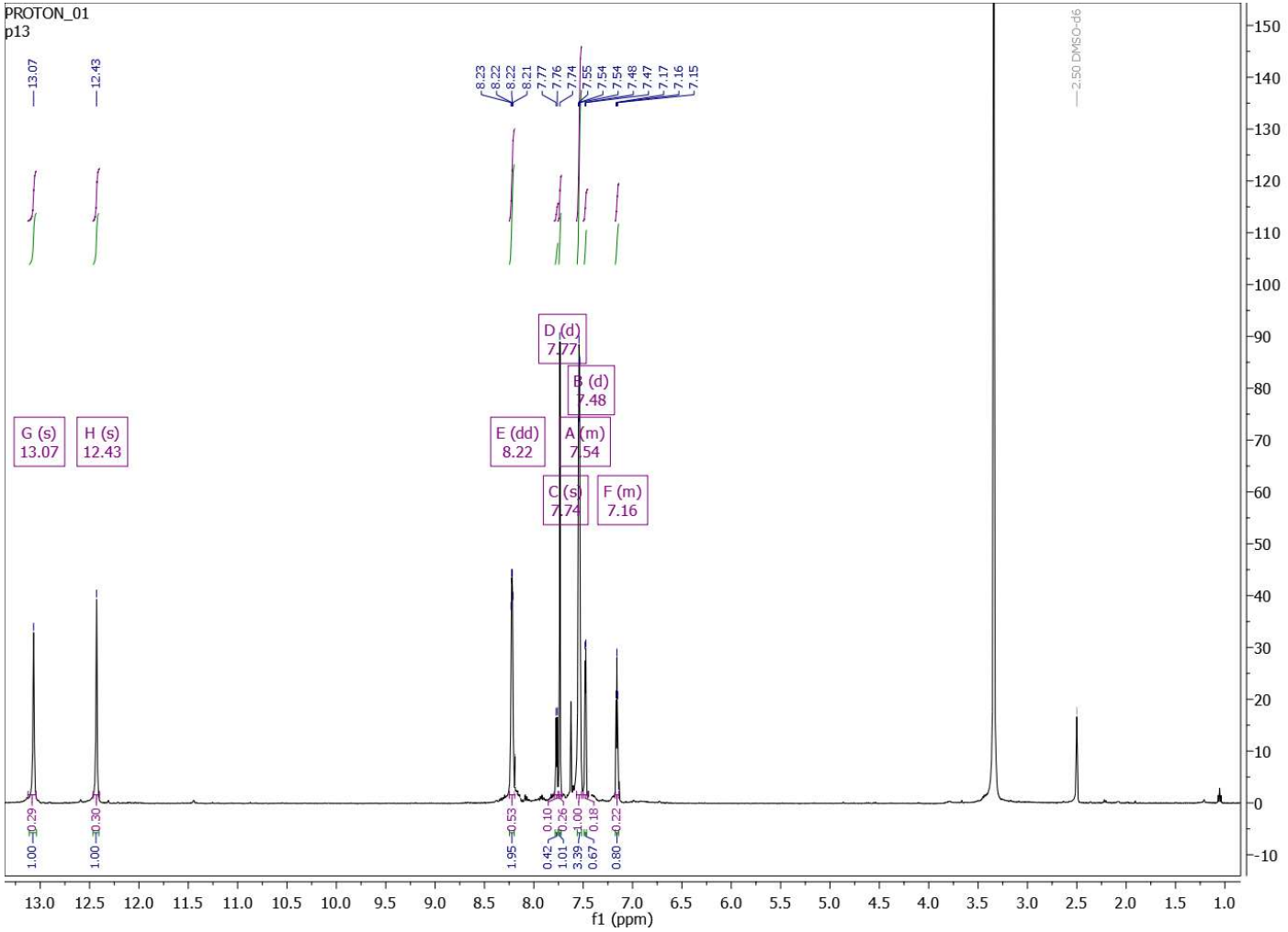
Novel Pyrimidine Derivatives as Antioxidant and Anticancer Agents: Design, Synthesis and Molecular Modeling Studies

Malama Myriagkou [1], Evangelia Papakonstantinou [2], Georgia-Eirini Deligiannidou [2], Alexandros Patsilinakos [3,†], Christos Kontogiorgis [2] and Eleni Pontiki [1,*]

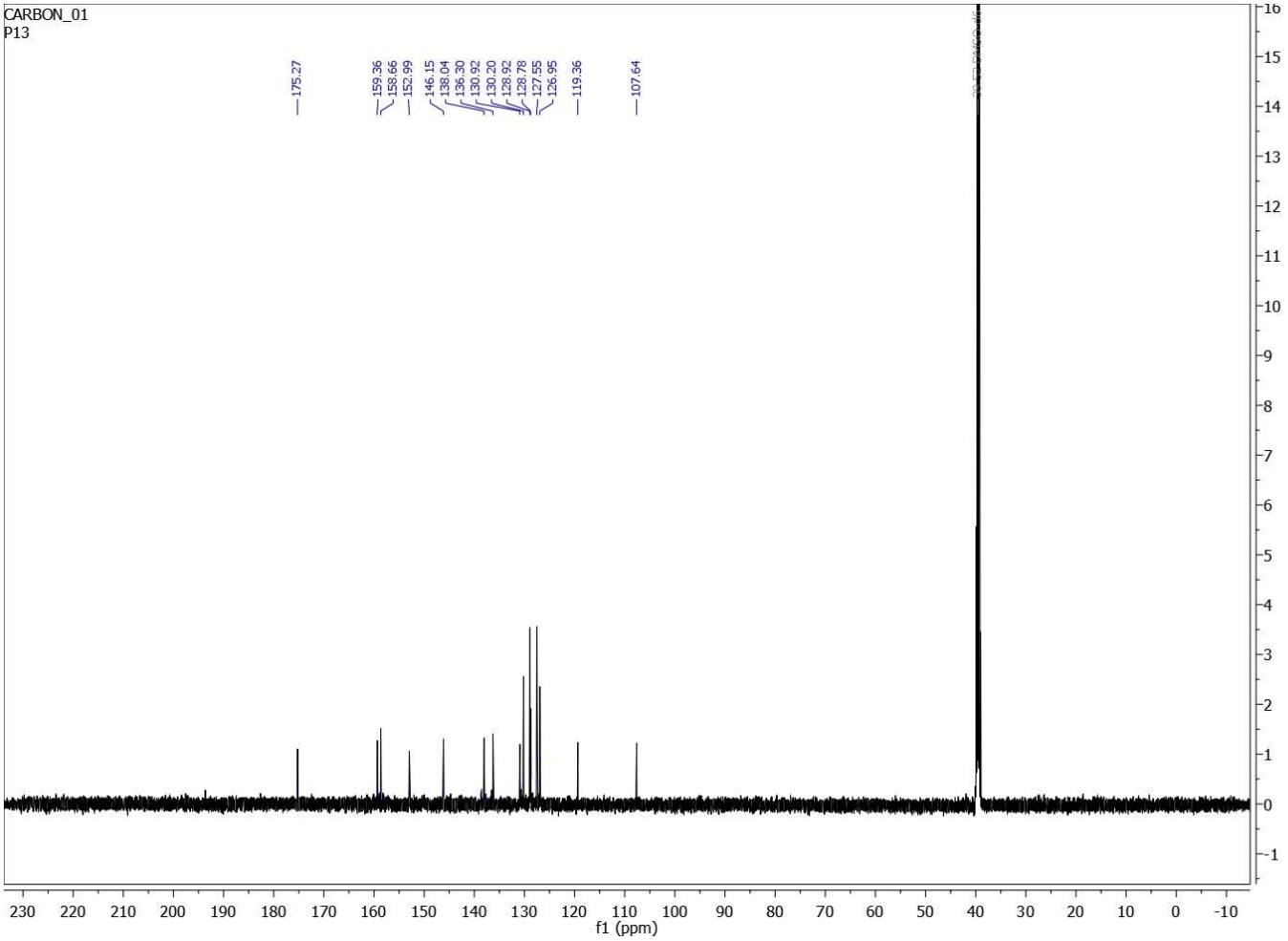
[1] Department of Pharmaceutical Chemistry, School of Pharmacy, Faculty of Health Sciences, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece; myriagkou@pharm.auth.gr
[2] Laboratory of Hygiene and Environmental Protection, School of Medicine, Democritus University of Thrace, 25510 Alexandroupoli, Greece; evangeliapapakonstantinou7@gmail.com (E.P.); edeligia@med.duth.gr (G.-E.D.); ckontogi@med.duth.gr (C.K.)
[3] Department of Drug Chemistry and Technology, Sapienza University, 00185 Rome, Italy; alexandros.patsilinakos@gmail.com
* Correspondence: epontiki@pharm.auth.gr
† Current address: Sibylla Biotech S.p.A., 37121 Verona, Italy

Figure S1: ^{1}H-NMR and ^{13}C-NMR data for the novel synthesized derivatives

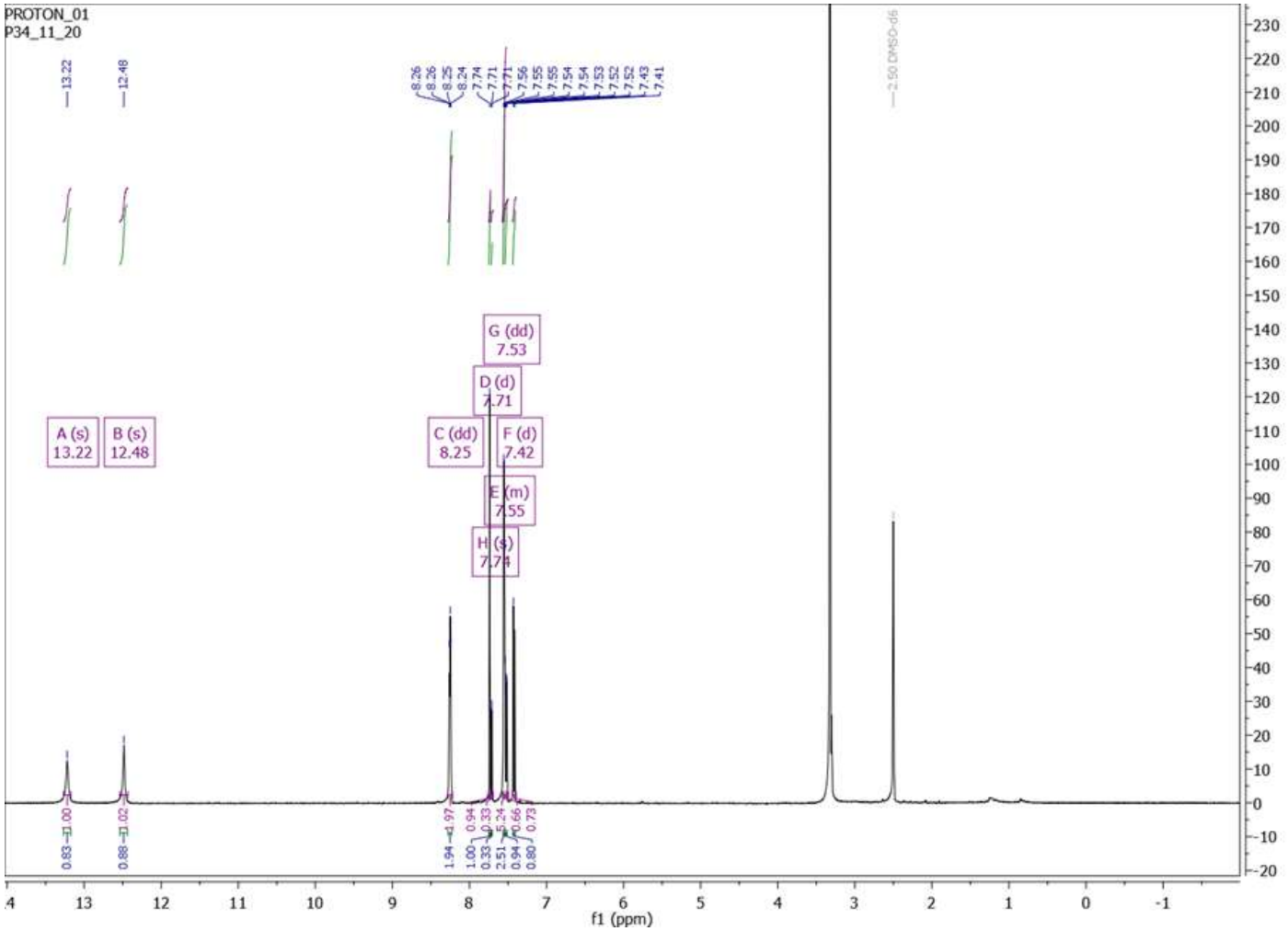
2c – ^{1}H-NMR



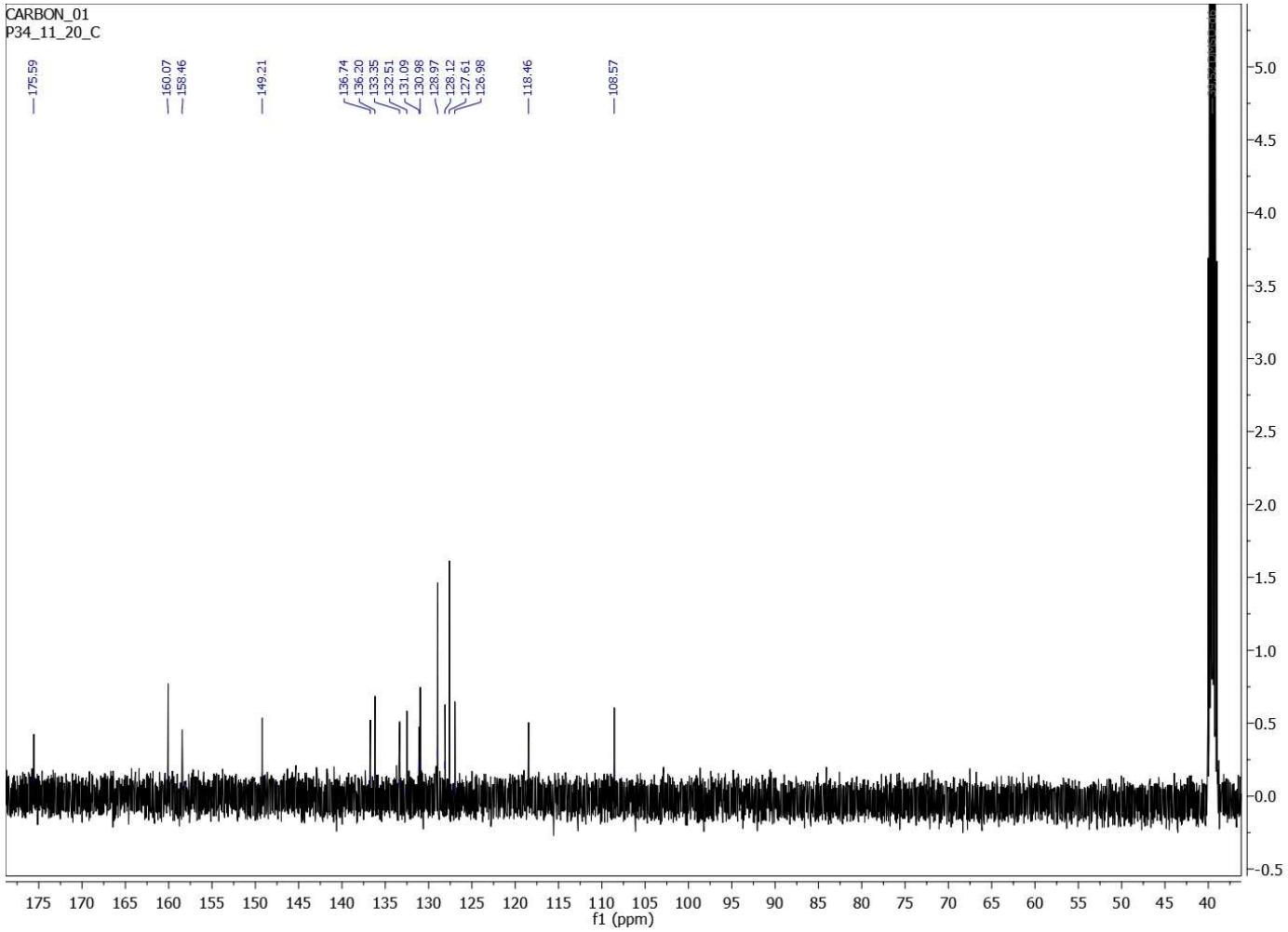
2c – ^{13}C-NMR


CARBON_01
P13
175.27
159.36
158.66
152.99
146.15
138.04
136.30
130.92
130.20
128.92
128.78
127.55
126.95
119.36
107.64
f1 (ppm)

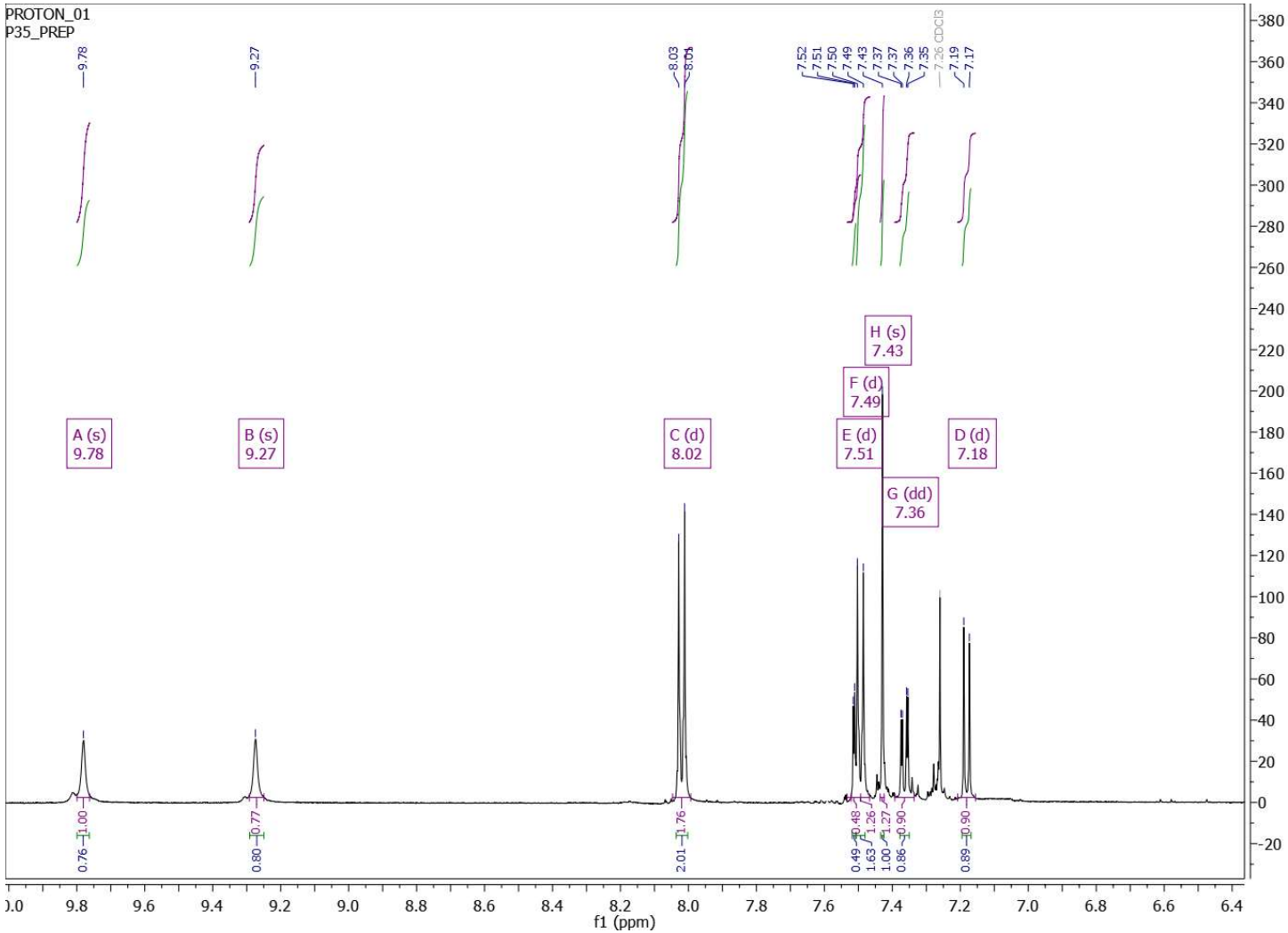
2g - ^{1}H-NMR


PROTON_01
P34_11_20
13.22
12.48
8.26
8.26
8.25
8.24
7.74
7.71
7.71
7.56
7.55
7.55
7.54
7.54
7.53
7.52
7.52
7.43
7.41
2.50 DMSO-d6
G (dd)
7.53
D (d)
7.71
A (s)
13.22
B (s)
12.48
C (dd)
8.25
F (d)
7.42
E (m)
7.55
H (s)
7.74
0.83
1.00
0.88
1.02
1.94
4.97
1.00
0.94
0.33
0.33
2.51
5.24
0.94
0.66
0.80
0.73
f1 (ppm)

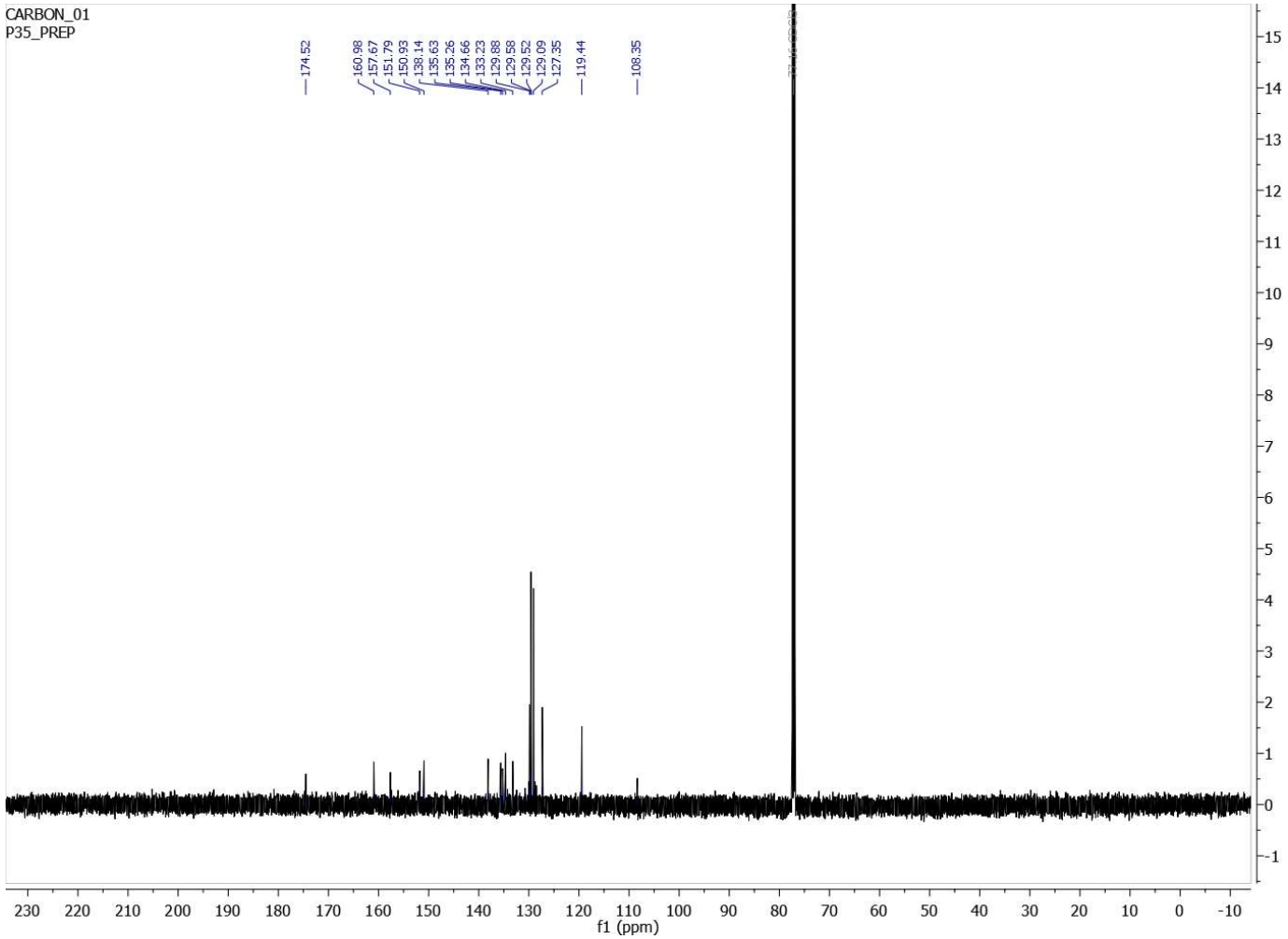
2g – ^{13}C-NMR


CARBON_01
P34_11_20_C
175.59
160.07
158.46
149.21
136.74
136.20
133.35
132.51
131.09
130.98
128.97
128.12
127.61
126.98
118.46
108.57
f1 (ppm)

2h – ^{1}H-NMR


PROTON_01
P35_PREP
9.78
9.27
8.03
8.01
7.52
7.51
7.50
7.49
7.43
7.37
7.37
7.36
7.35
7.26 CDCl3
7.19
7.17
A (s)
9.78
B (s)
9.27
C (d)
8.02
H (s)
7.43
F (d)
7.49
E (d)
7.51
G (dd)
7.36
D (d)
7.18
1.00
0.77
1.76
0.48
1.26
1.27
0.90
0.90
f1 (ppm)

2h – ^{13}C-NMR


CARBON_01
P35_PREP
174.52
160.98
157.67
151.79
150.93
138.14
135.63
135.26
134.66
133.23
129.88
129.58
129.52
129.09
127.35
119.44
108.35
f1 (ppm)