

Supporting Information

Chlorotrimethylsilane Catalyzed Synthesis of 1,3-Diphenyl-2-Propenones and their Antimicrobial Activities

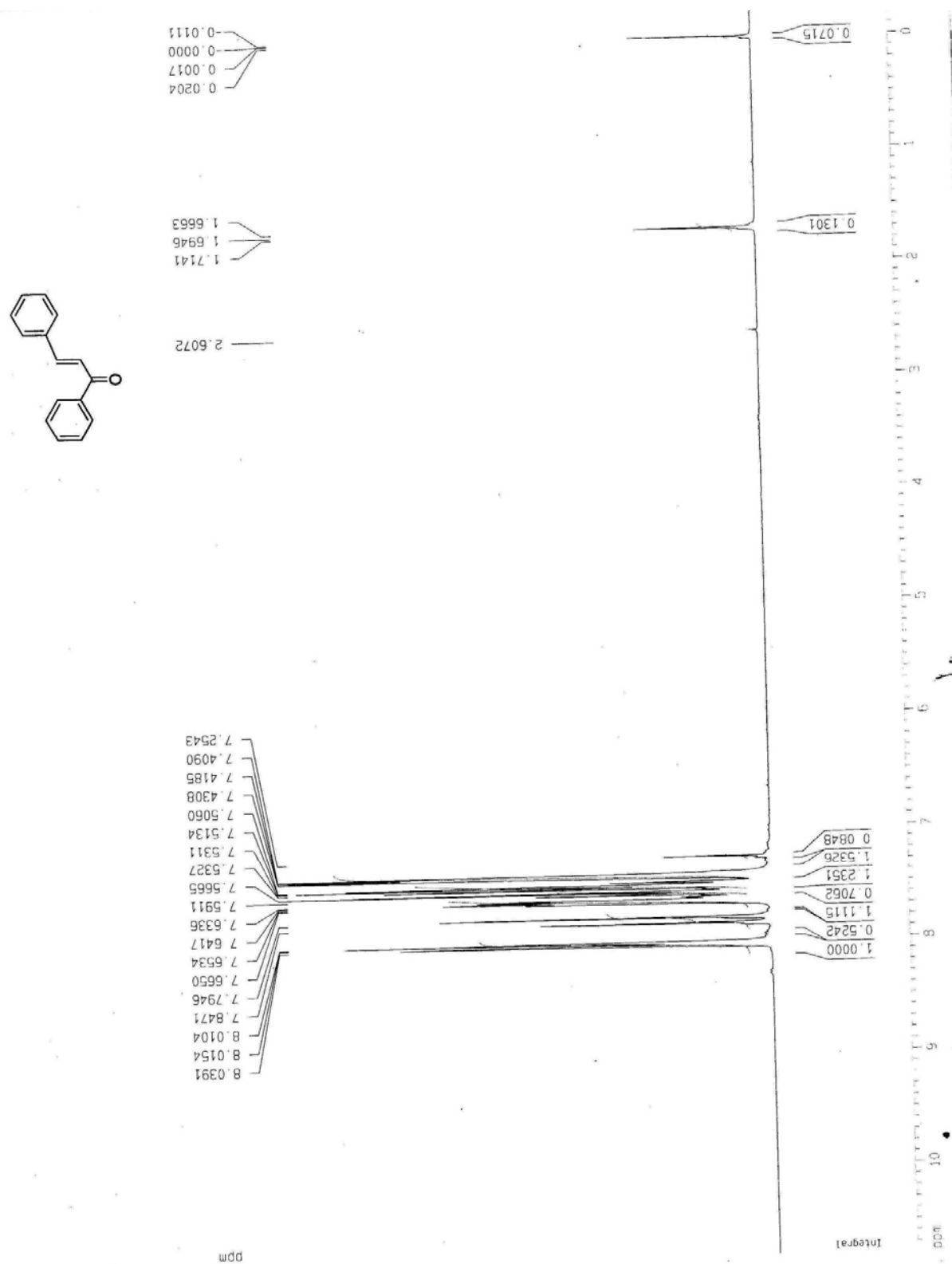
Progyashree Goswami^{a,b}, Madhumita Talukdar^b, Tarun C. Bora^b, Prodeep Phukan^{a*} and Jadab C. Sarma^{b*}

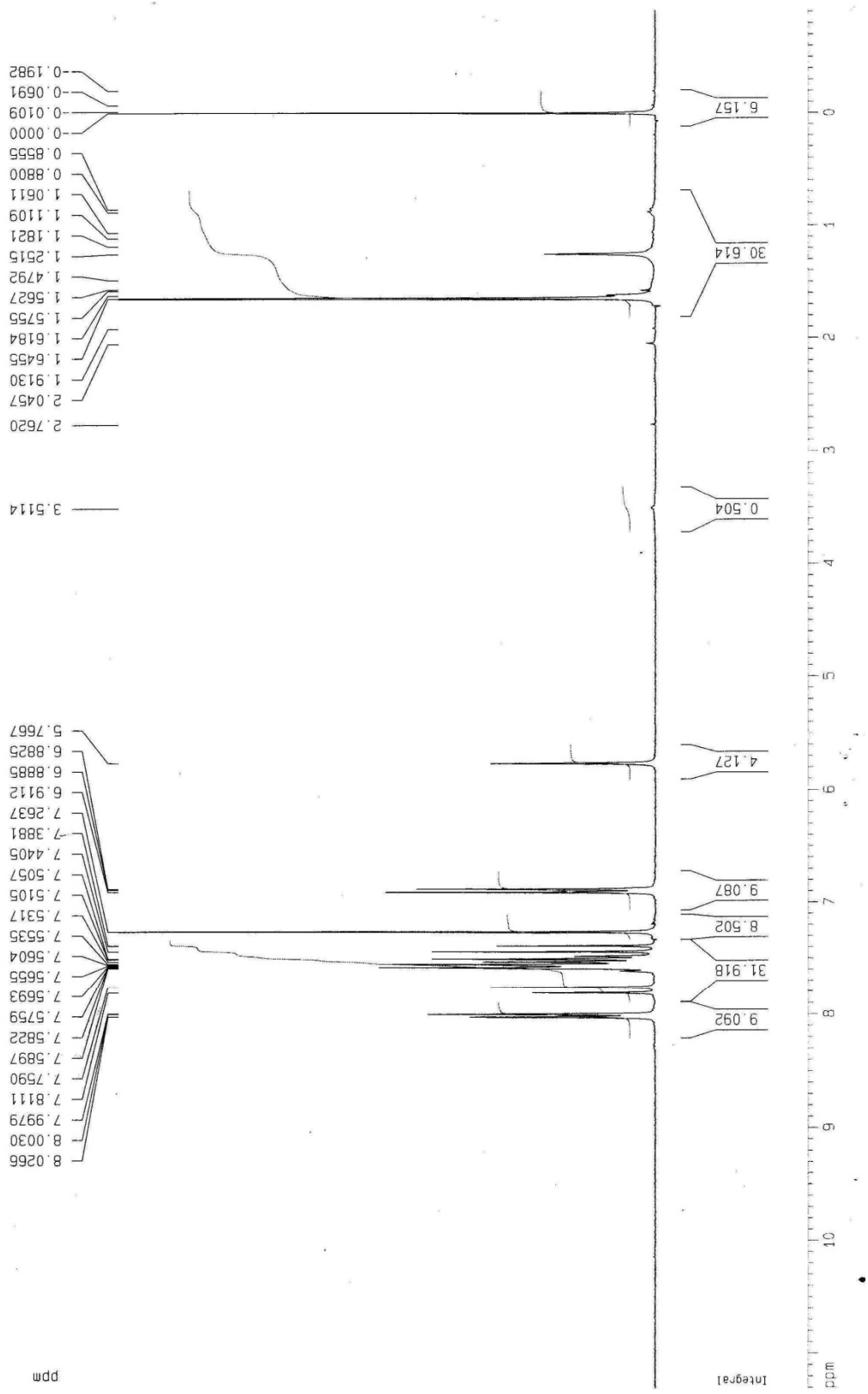
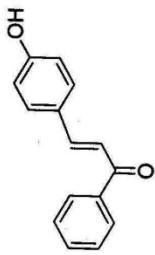
(^aDepartment of Chemistry, Gauhati University, Guwahati 781014, Assam, India)

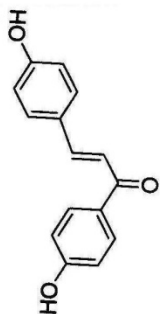
(^bCSIR- North-East Institute of Science and Technology, Jorhat 785006, Assam, India)

*E-Mail: pphukan@yahoo.com

Figure S1: ^1H -NMR spectra of synthesized chalcones. ^{13}C -NMR spectra are provided only for new entries such as **6**, **7**, **8**, and **9**.







1.28799
1.27304
1.24927

2.02453

3.14762
3.31627
3.32110
3.32624
3.33159
3.33662
3.55889

4.65258
4.92062

5.18464

6.84373
6.87245
6.88231
6.89471
6.90069
6.91767
6.92382
7.04533
7.56577
7.60615
7.61722
7.63480
7.70219
7.75389
7.82627
7.85648
7.86351
7.88726
7.99459
8.00322
8.00920
8.03235

ppm

0.456

9.288

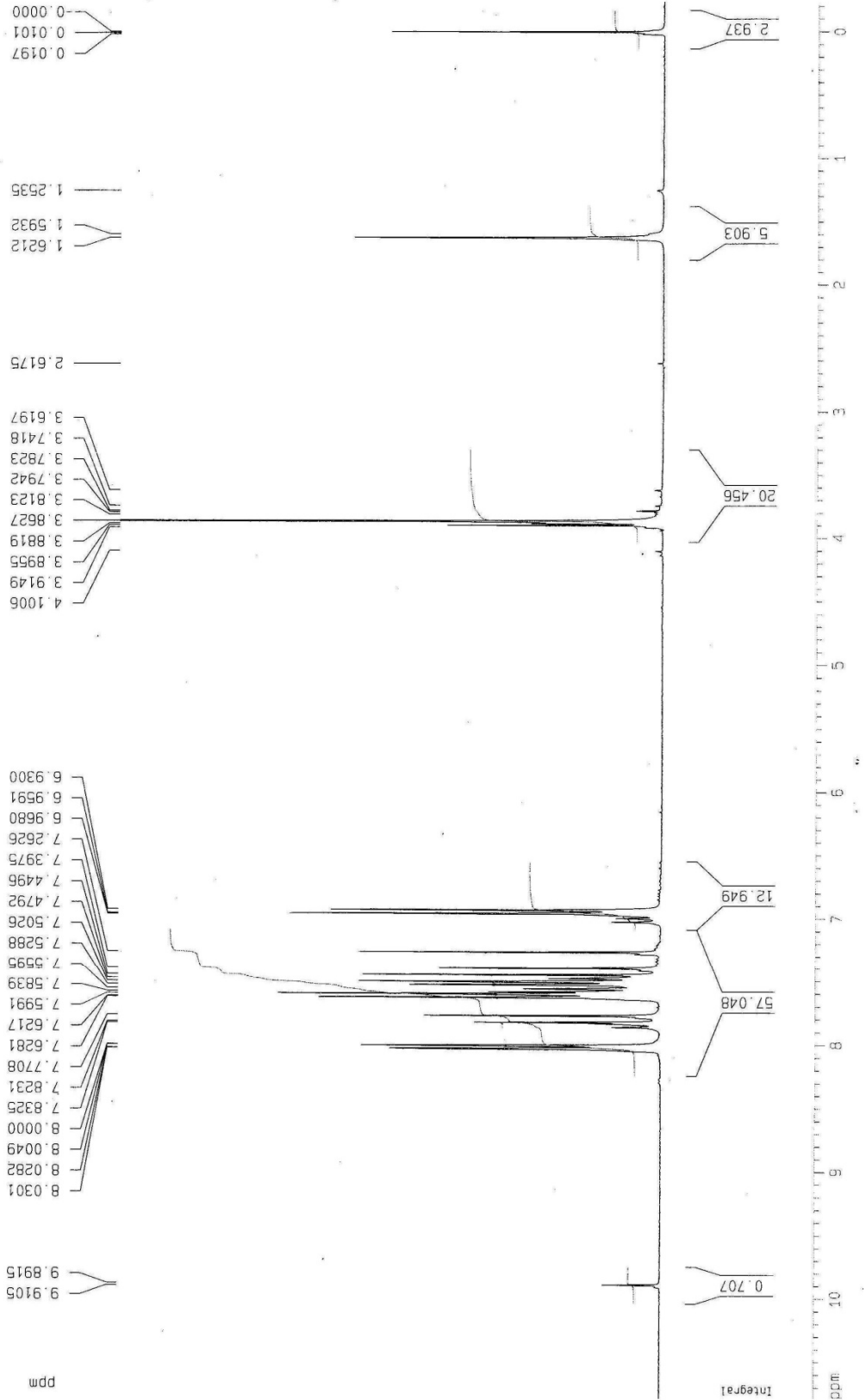
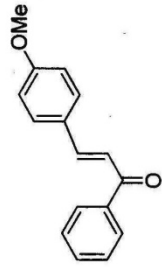
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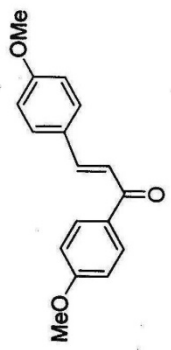
18.453

27.516

Integral

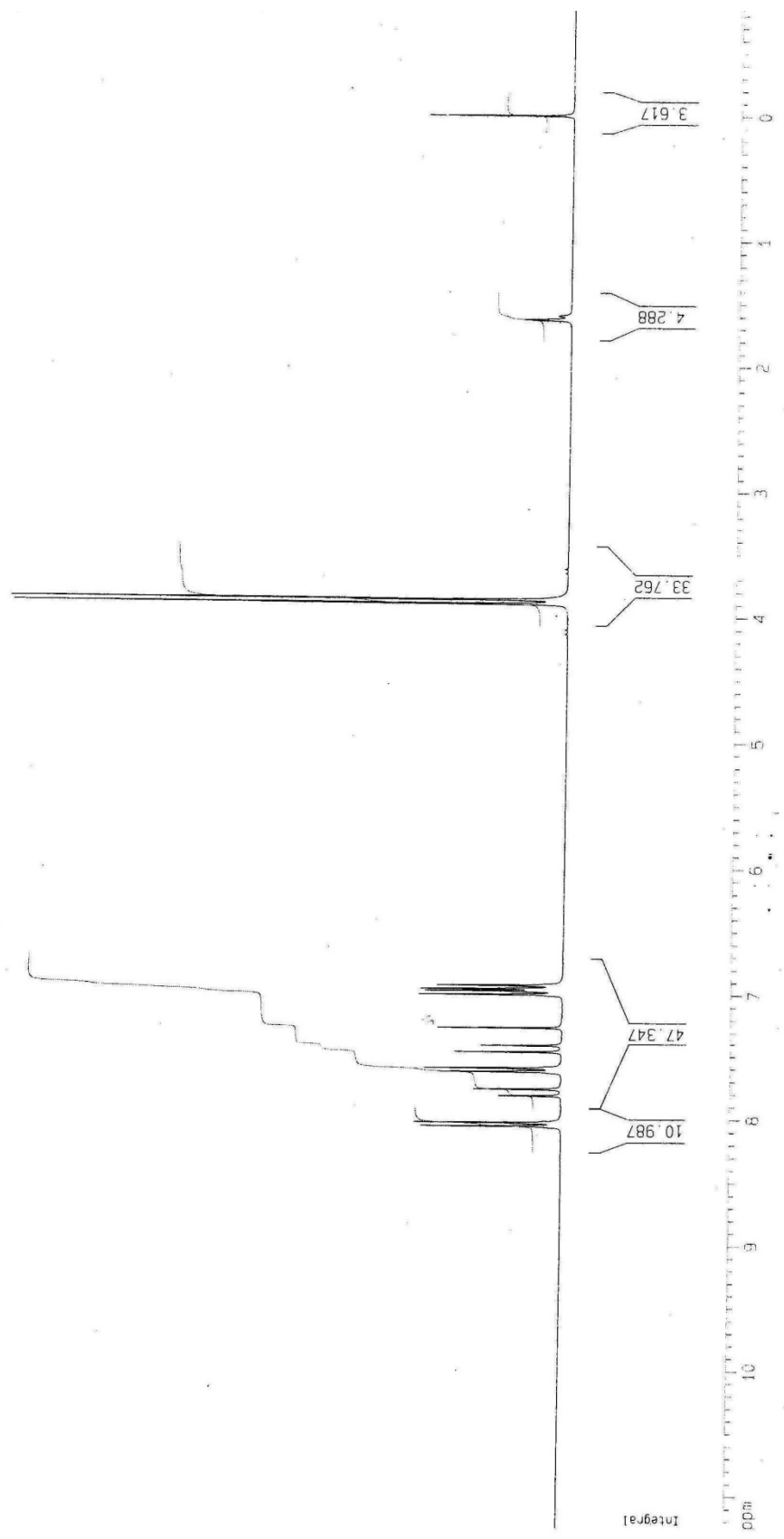


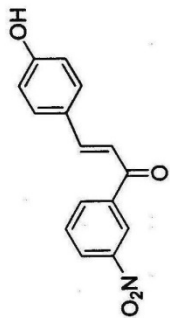




Chemical shift (ppm) values for the structure above:

- 3.89512, 3.86184
- 1.62505, 1.59605
- 0.01066, 0.00001
- 8.06681, 8.05770, 8.02836, 8.01958, 7.81577, 7.76383, 7.62604, 7.59691, 7.46815, 7.41631, 7.26470, 7.00908, 7.00030, 6.97083, 6.95597, 6.92682





ppm

10.2440

8.8102

8.8044

8.7982

8.5952

8.5691

8.5014

8.4991

8.4942

8.4745

8.4717

8.4669

7.8952

7.8587

7.8603

7.8421

7.8217

7.8082

7.7972

7.7460

6.8714

6.8427

3.6726

3.5455

3.4962

3.4067

3.2745

3.1763

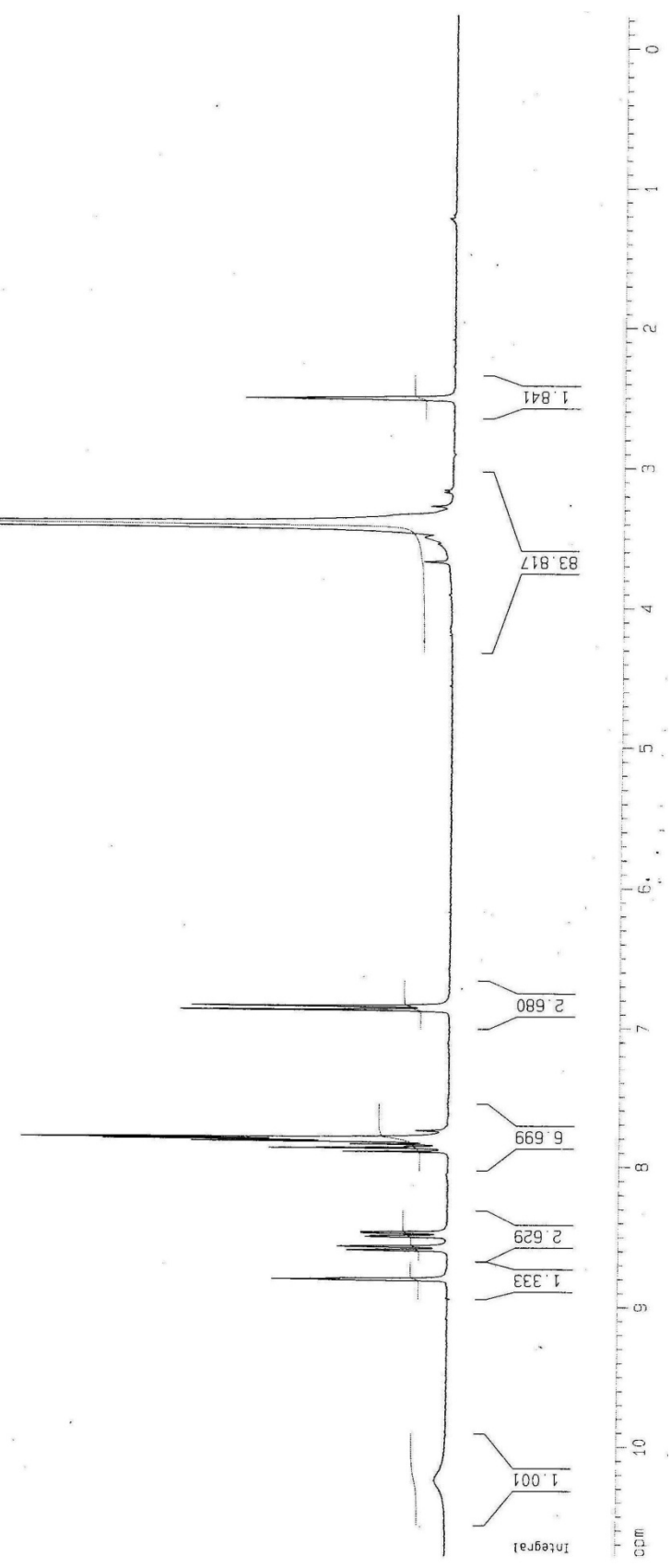
3.1599

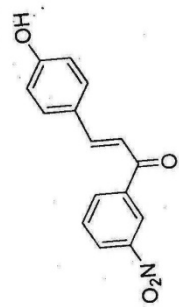
2.8119

2.5061

2.5002

1.2193





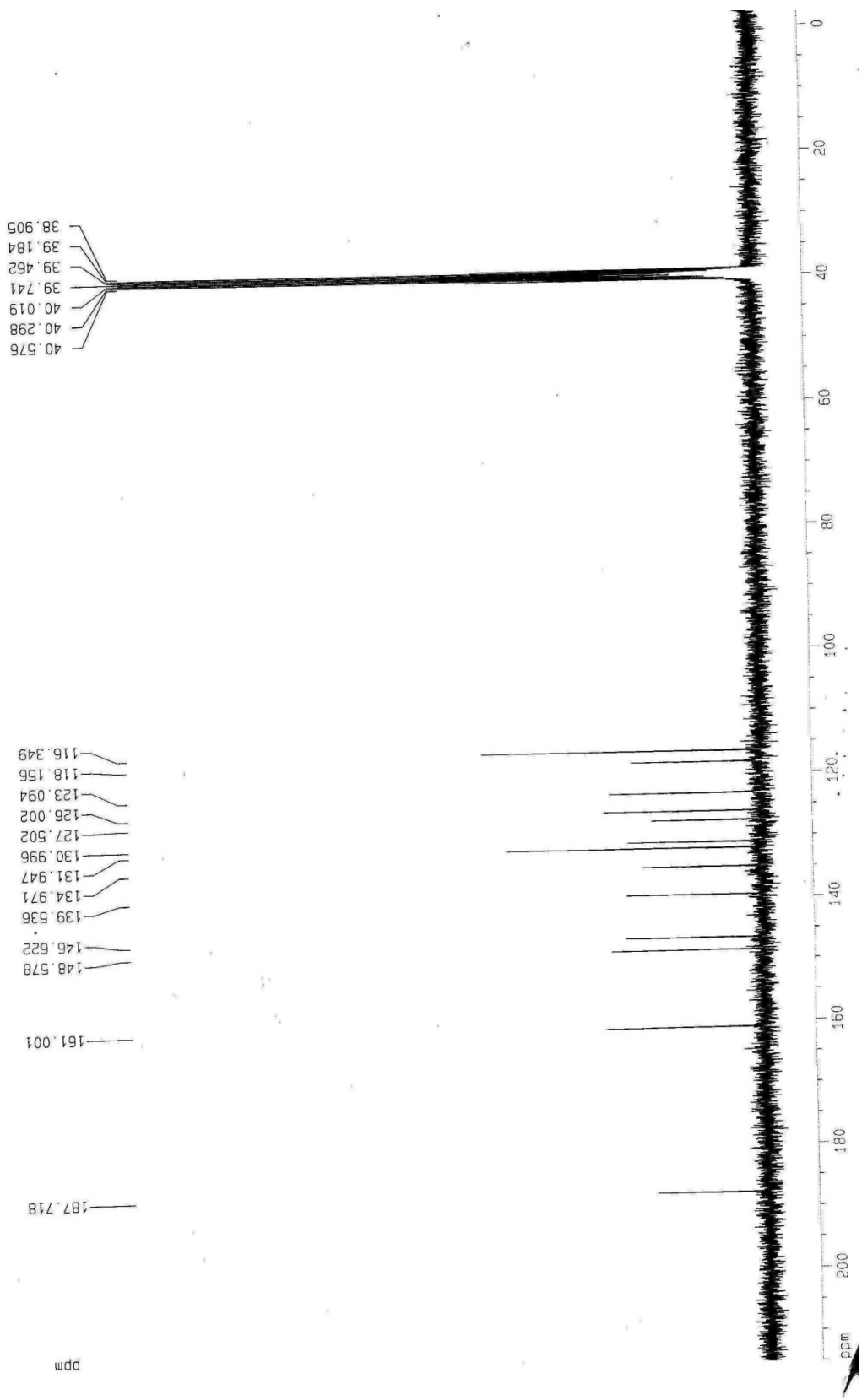
- 40.576
- 40.298
- 40.019
- 39.741
- 39.462
- 39.184
- 38.905

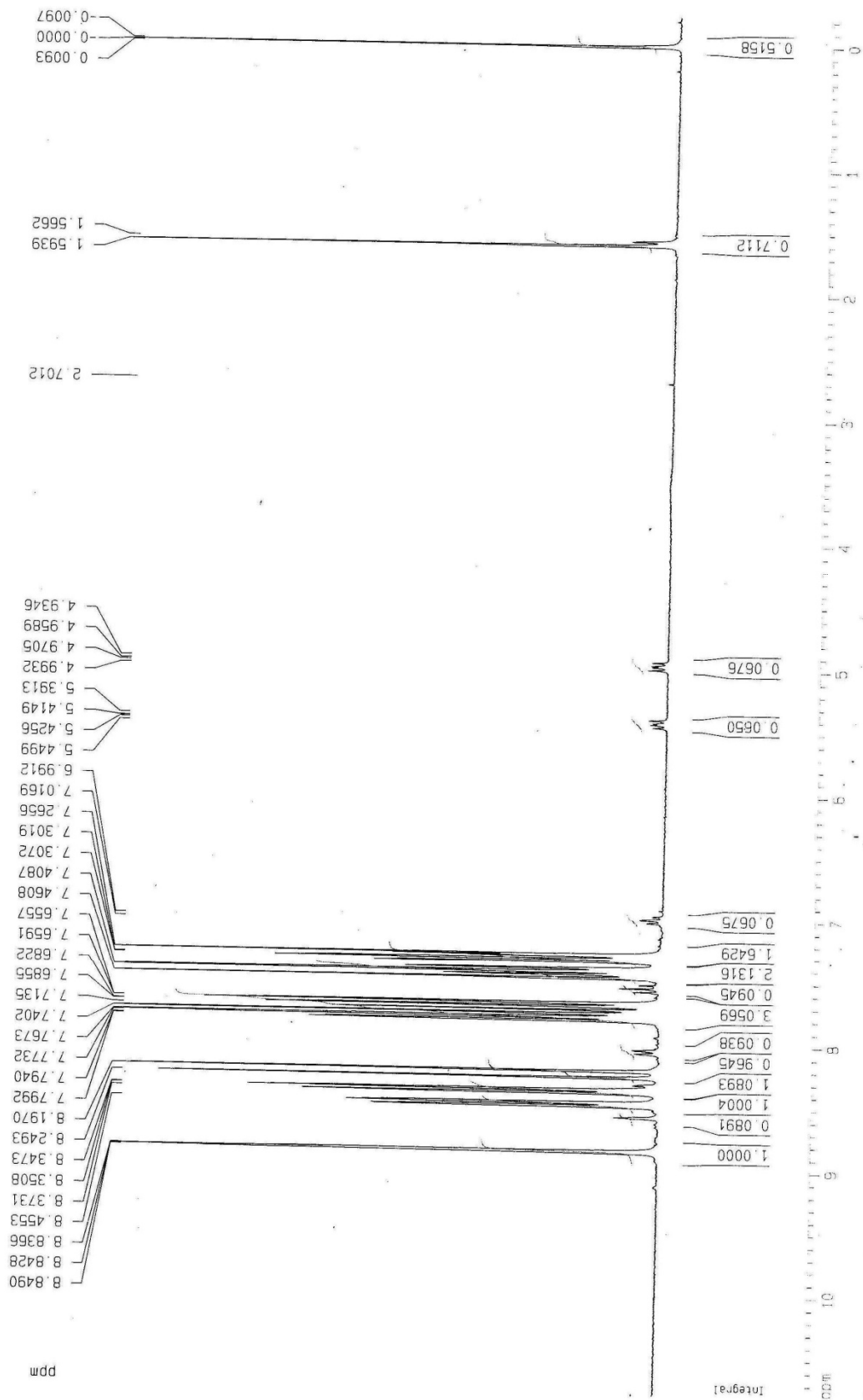
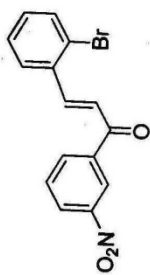
- 148.578
- 146.622
- 139.536
- 134.971
- 131.947
- 130.996
- 127.502
- 126.002
- 123.094
- 118.156
- 116.349

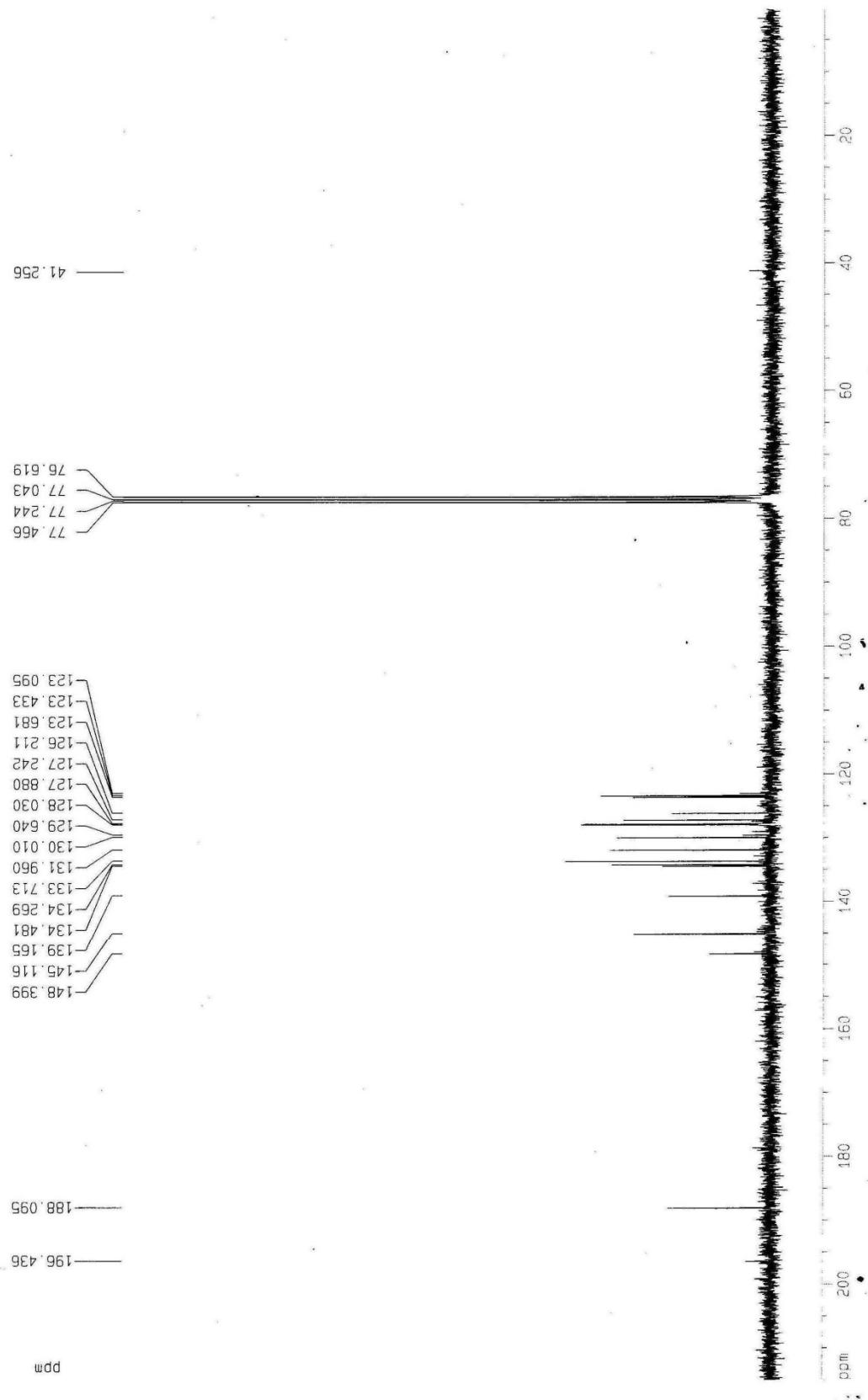
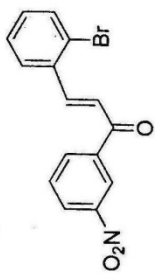
161.001

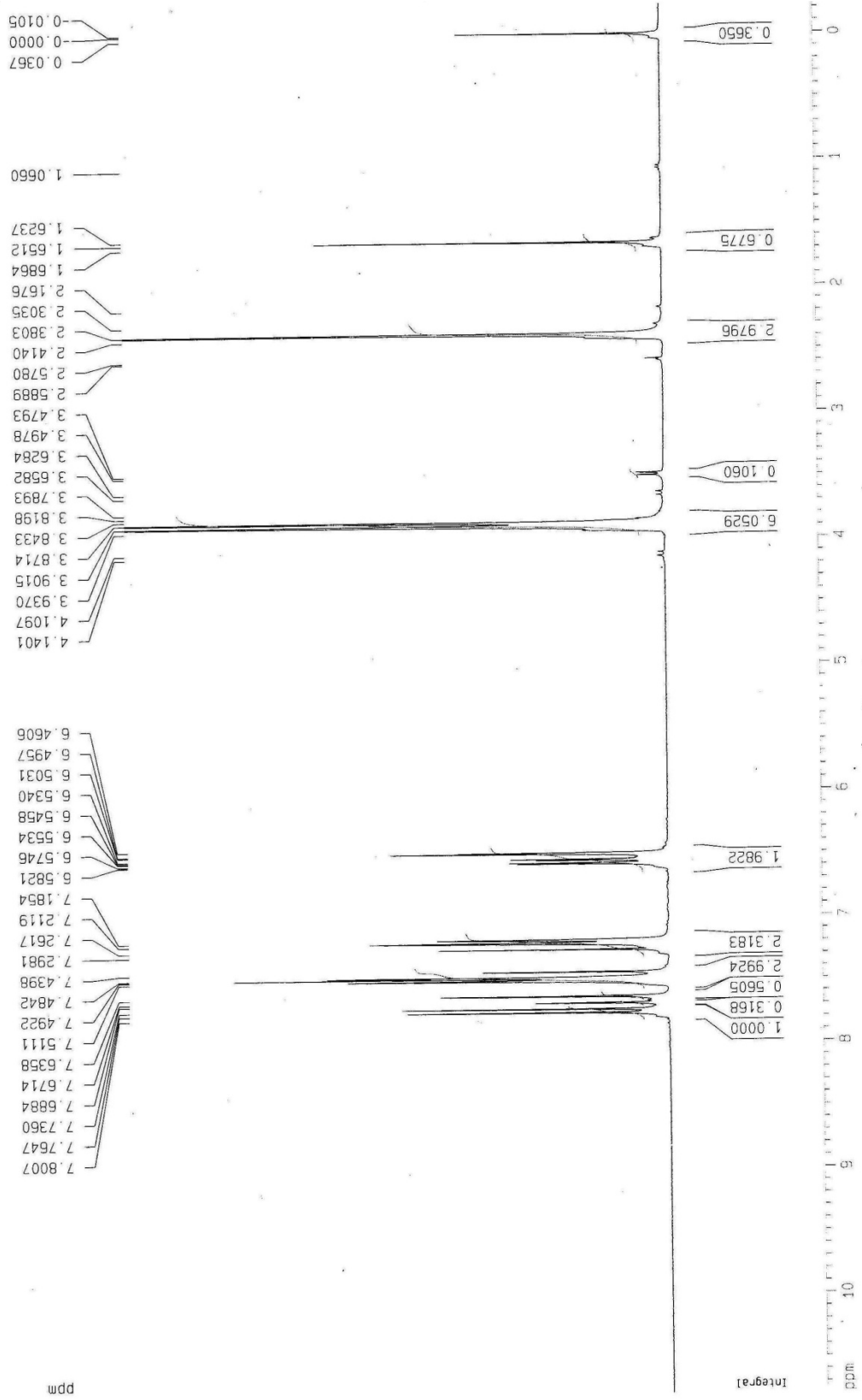
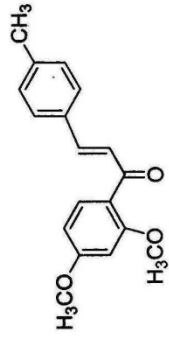
187.718

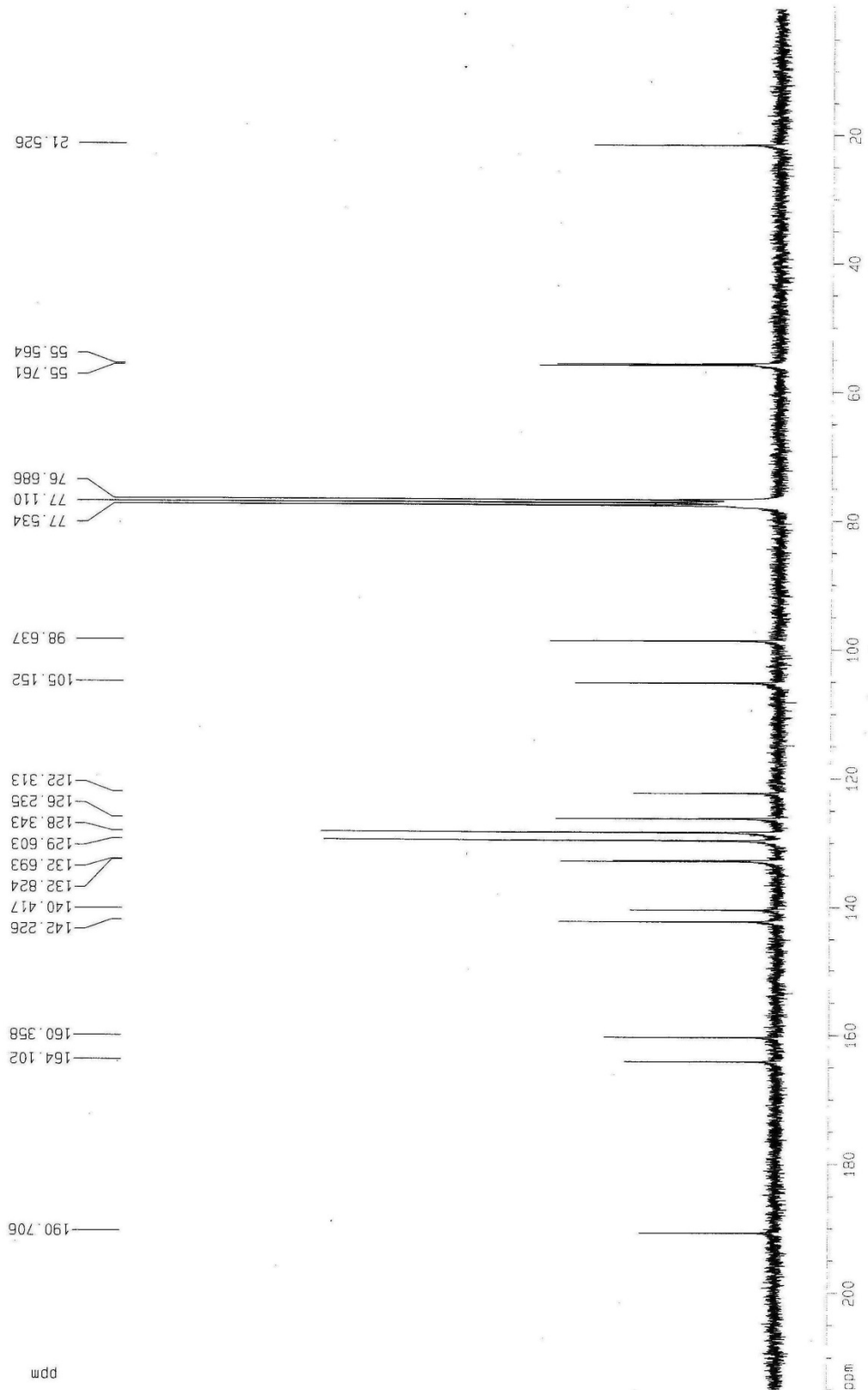
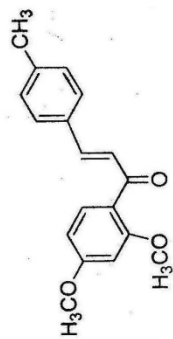
ppm

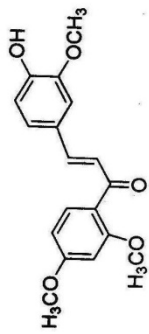








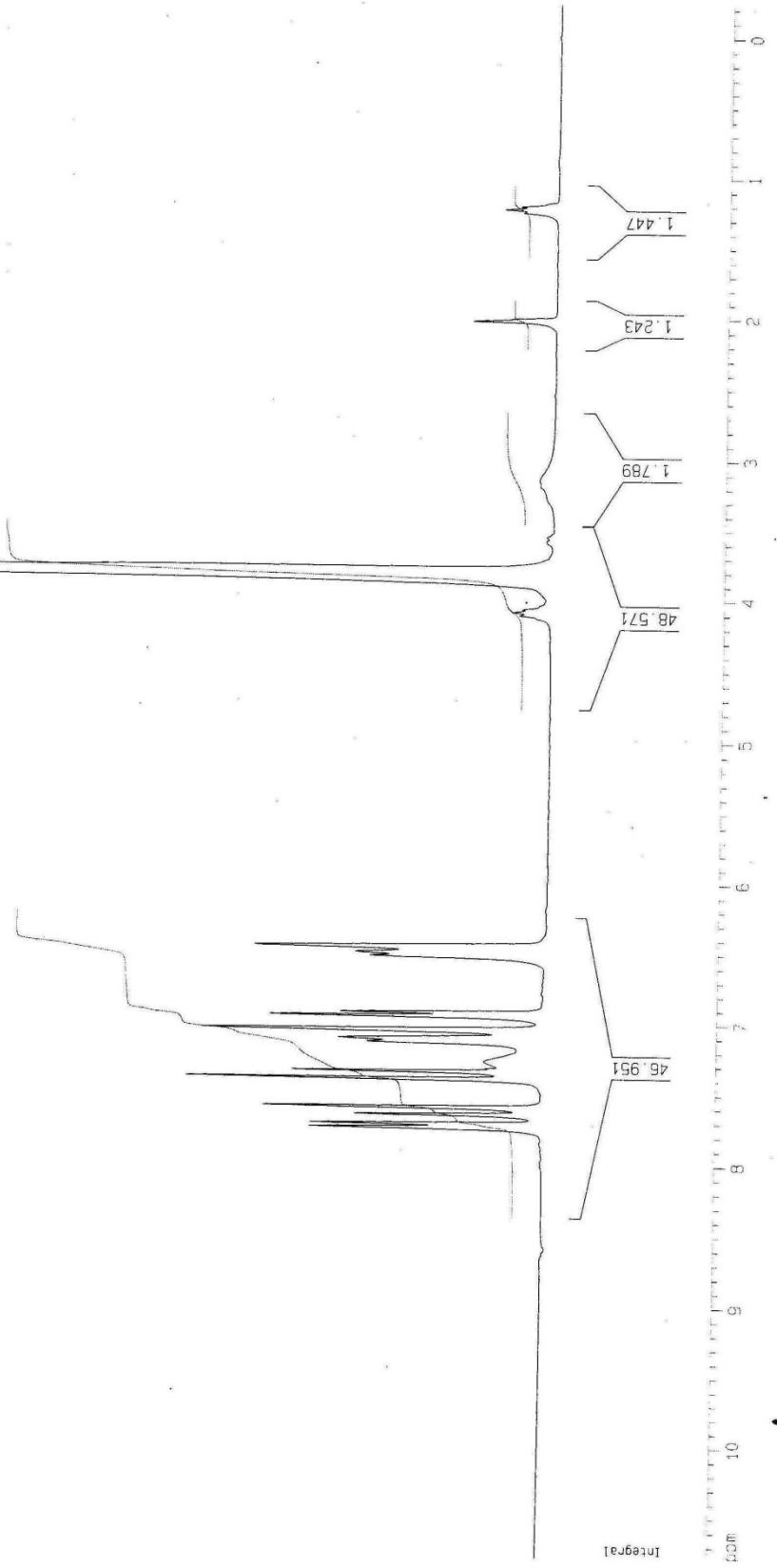


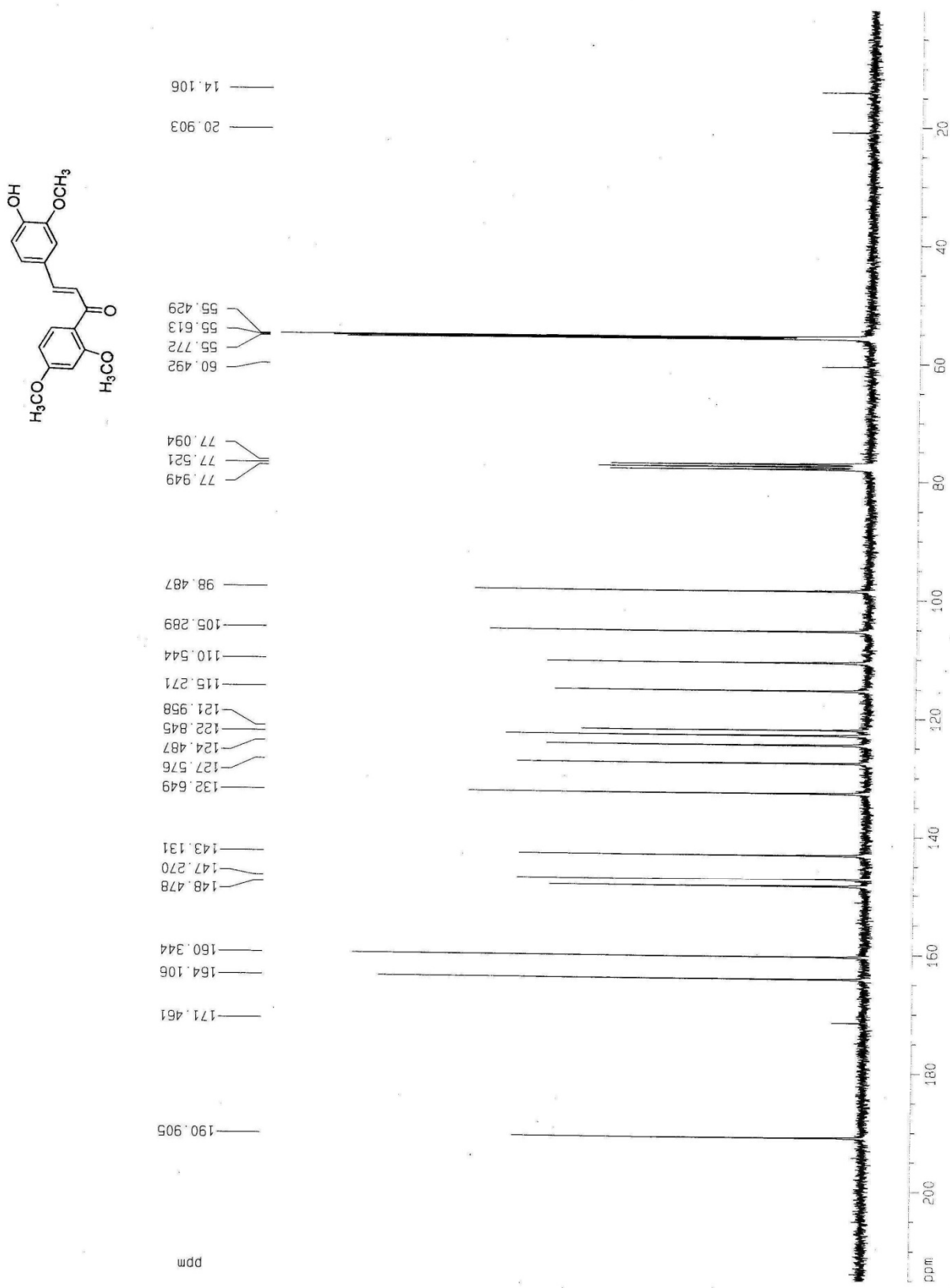


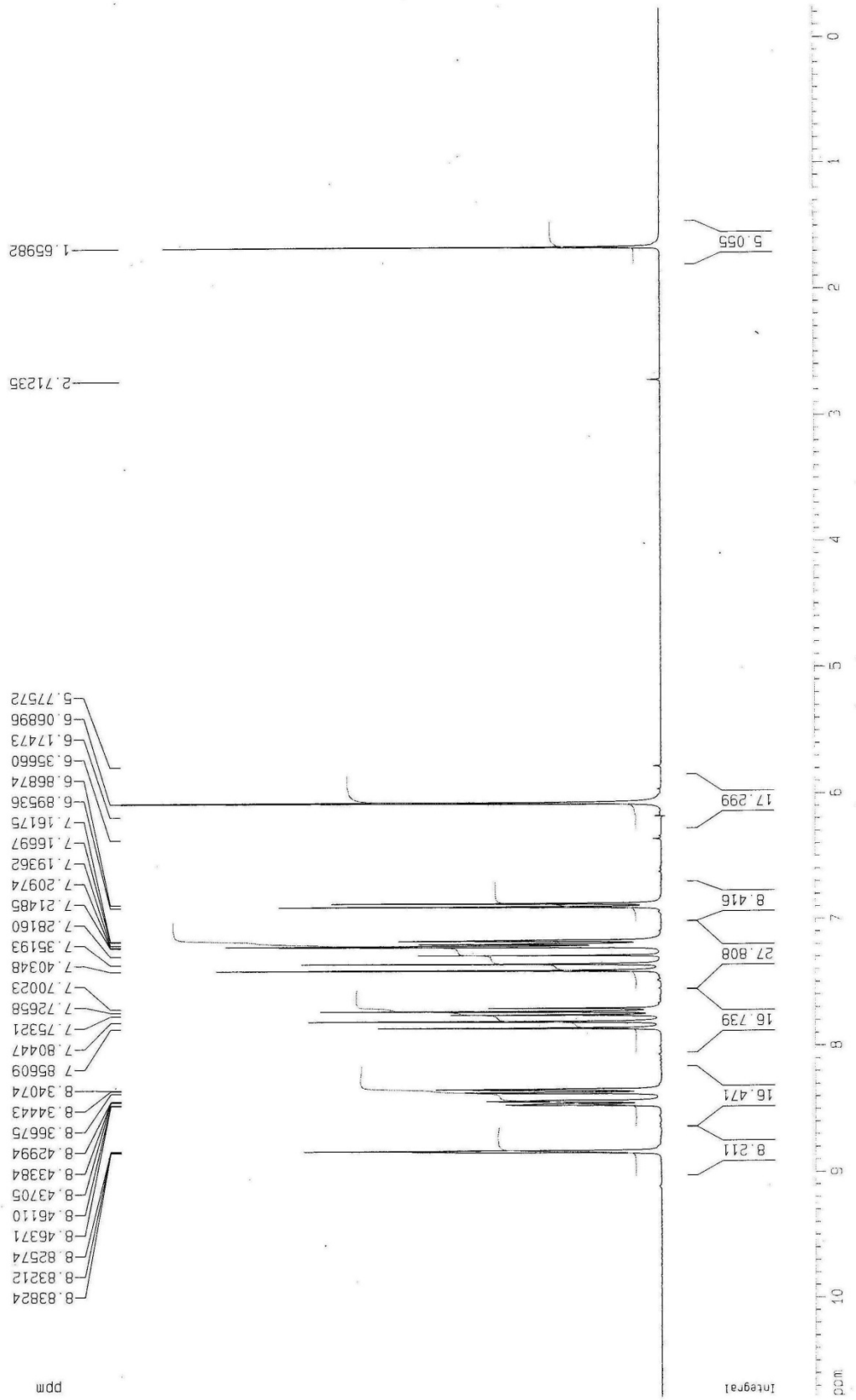
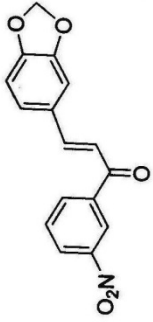
- 1.20703
- 1.22644
- 1.24764
- 2.00373
- 2.02013
- 3.14048
- 3.55137
- 3.57986
- 3.77199
- 3.79679
- 3.82347
- 3.83572
- 4.06305
- 4.08234
- 4.10547

- 6.45528
- 6.49443
- 6.51998
- 6.91907
- 6.94583
- 7.04349
- 7.10382
- 7.12958
- 7.18946
- 7.26913
- 7.32047
- 7.34123
- 7.39347
- 7.59438
- 7.64553
- 7.71212
- 7.74032

ppm







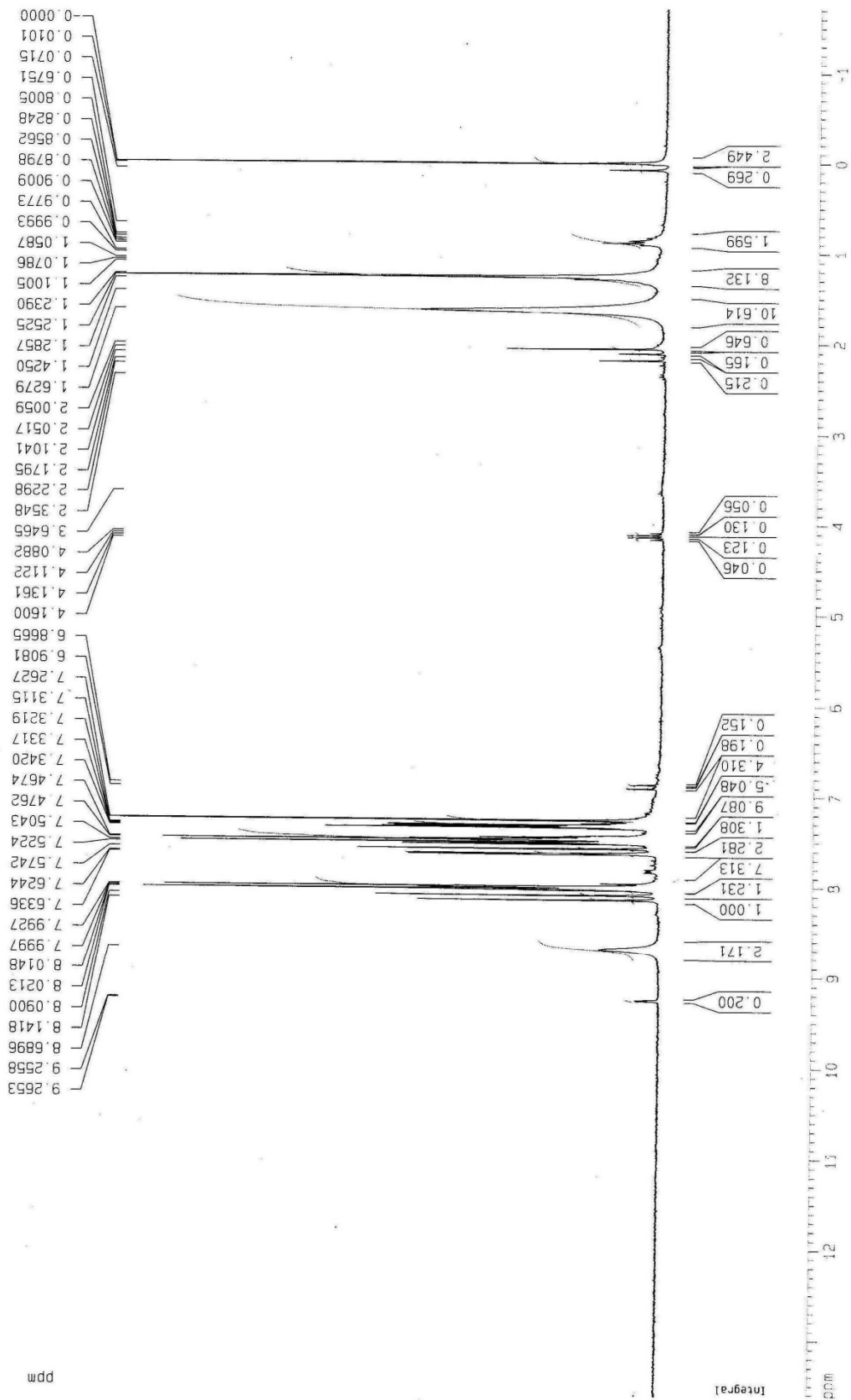
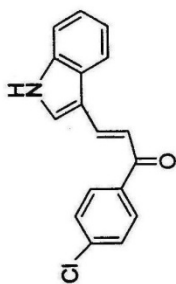
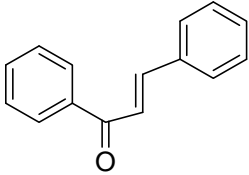
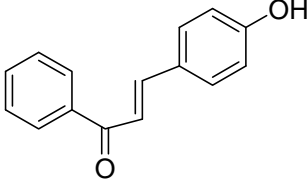
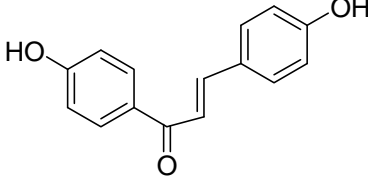
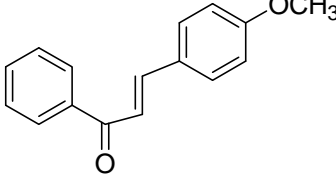
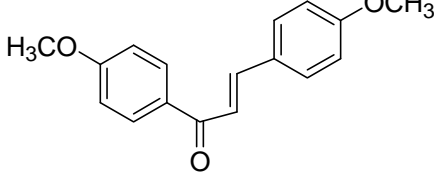
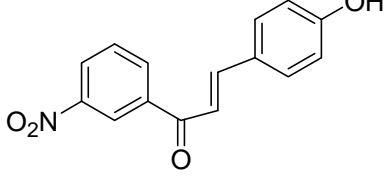
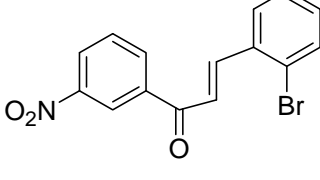


Table S1: Effects of substituent on 309.3 band of chalcone in methanol. The absorption wavelength of C=O, N=O and C=C groups in UV-vis spectroscopy show a bathochromic or red shift due to extended conjugation.

No	Chalcone	λ (nm)	Absorption
1		309.3	2.2540
		227.3	1.0048
		206.7	1.3688
2		344.3	2.3606
		247.3	1.2585
		206.7	1.4253
3		348.2	1.0429
		235.3	0.4436
		204.3	0.4999
4		341.5	0.8120
		245.5	0.4160
		203.0	0.7440
5		343.5	0.7546
		233.7	0.3324
		204.3	0.3391
6		357.5	0.9440
		245.5	0.9520
		203.0	0.7400
7		304.5	0.1370
		232.0	0.4300
		204.5	0.5340

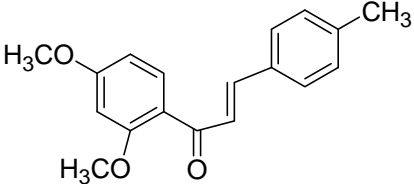
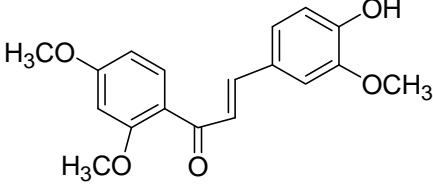
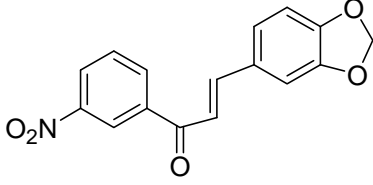
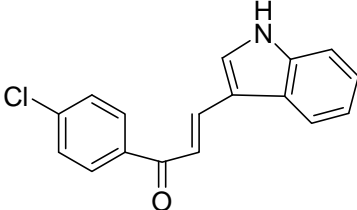
8		328.3	0.5384
		230.5	0.2893
		205.9	0.6124
9		362.5	1.6712
		246.5	0.8063
		209.1	1.9045
10		368.1	0.1253
		244.8	0.1439
		211.5	0.1551
		197.9	0.1346
11		392.0	0.097
		267.5	0.072
		219.0	0.114

Figure S2: (a) Molecular packing diagram of **6** via O–H···O hydrogen bonds along *b*-axis.

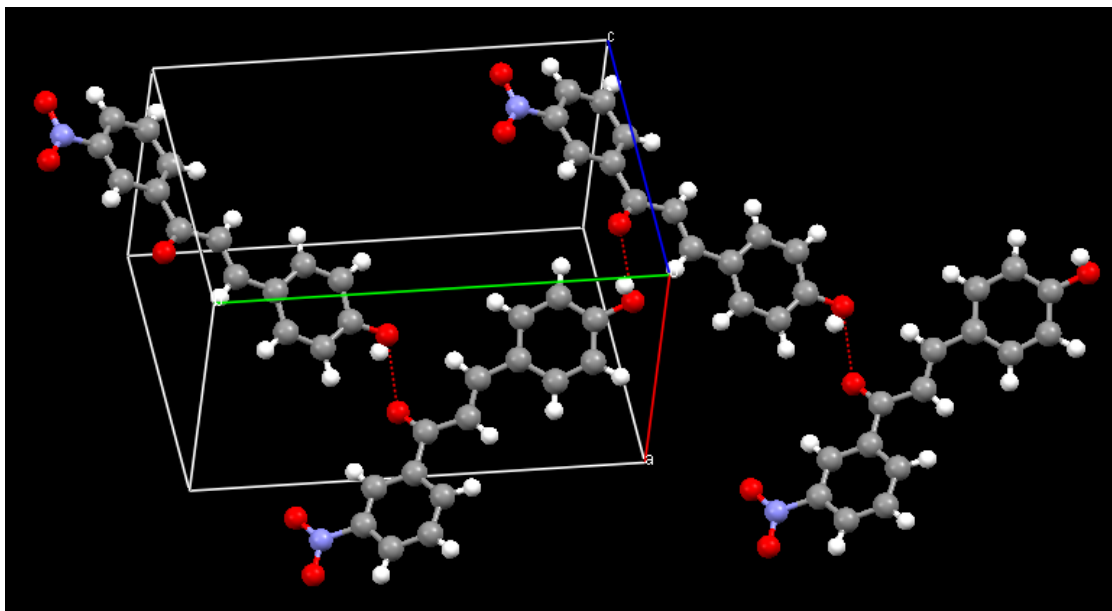


Figure S2: (b) Molecular packing diagram of **7**. The C–H···O hydrogen bond between NO₂ and C–H of phenyl ring held molecules together in the crystal.

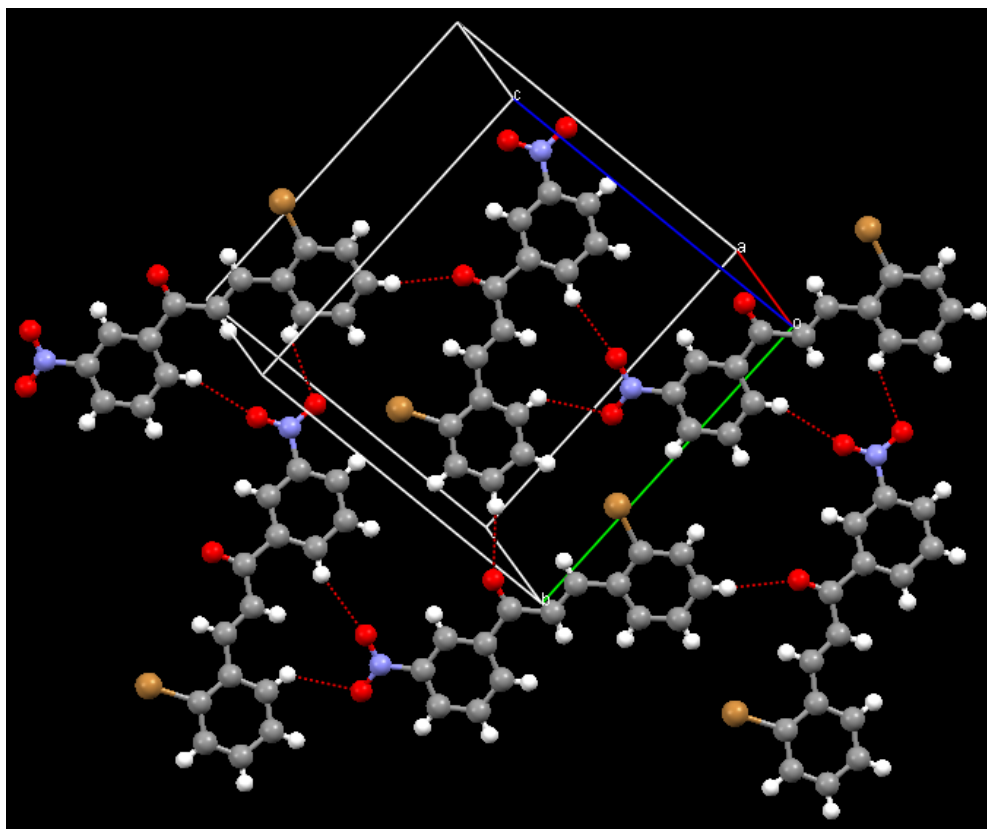


Figure S2: (c) Molecules are arranged in **8** via C–H···O hydrogen bonds. Ketone and ether group oxygen acts as hydrogen bond acceptor.

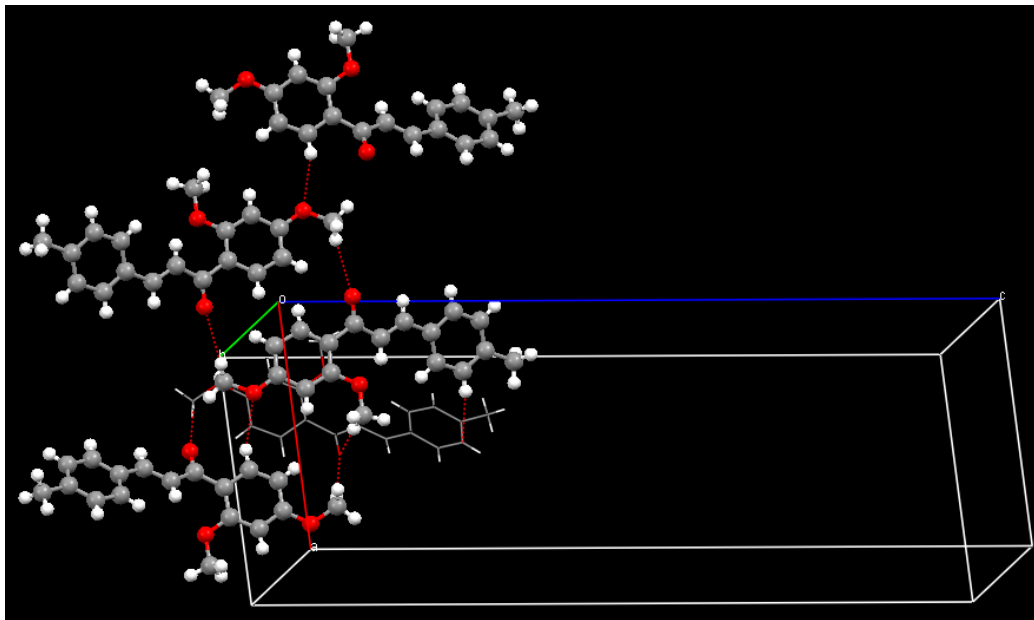


Figure S2: (d) In **10** molecules are arranged via C–H···O hydrogen bonds. Oxygen from piperinol ring, NO₂ and C=O groups are involved in hydrogen bonding.

