Supplementary Material

Microwave-Assisted synthesis of 2,8-di(alkyl/ aryl)-4,6-dichloro-2,8-dihydropyrano[3,2-g] chromene-3,7-dicarbaldehydes and their antimicrobial activity

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e-mail: ***vrr9@yahoo.com***

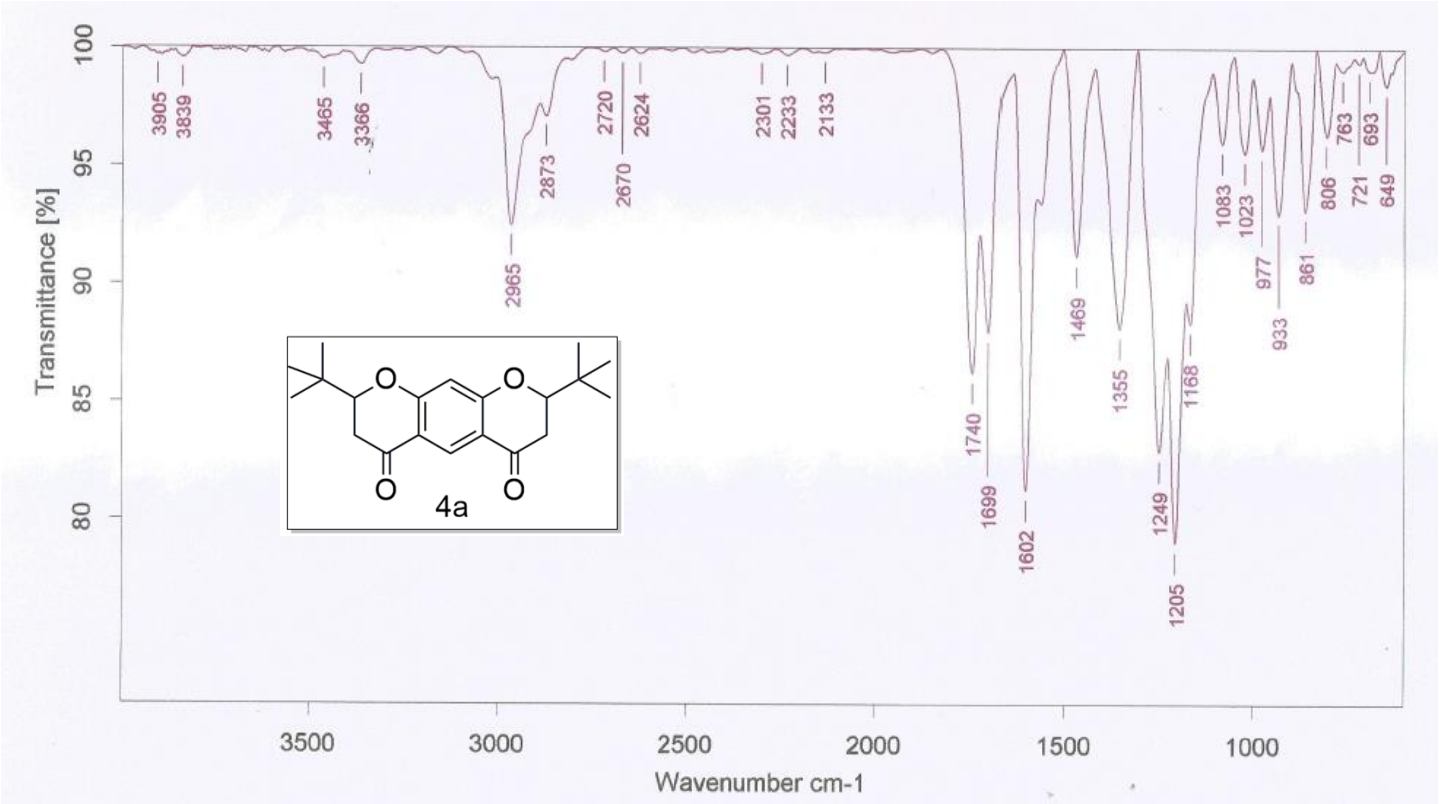


Figure 1: IR data of 2,8-di-tert-butyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4a)

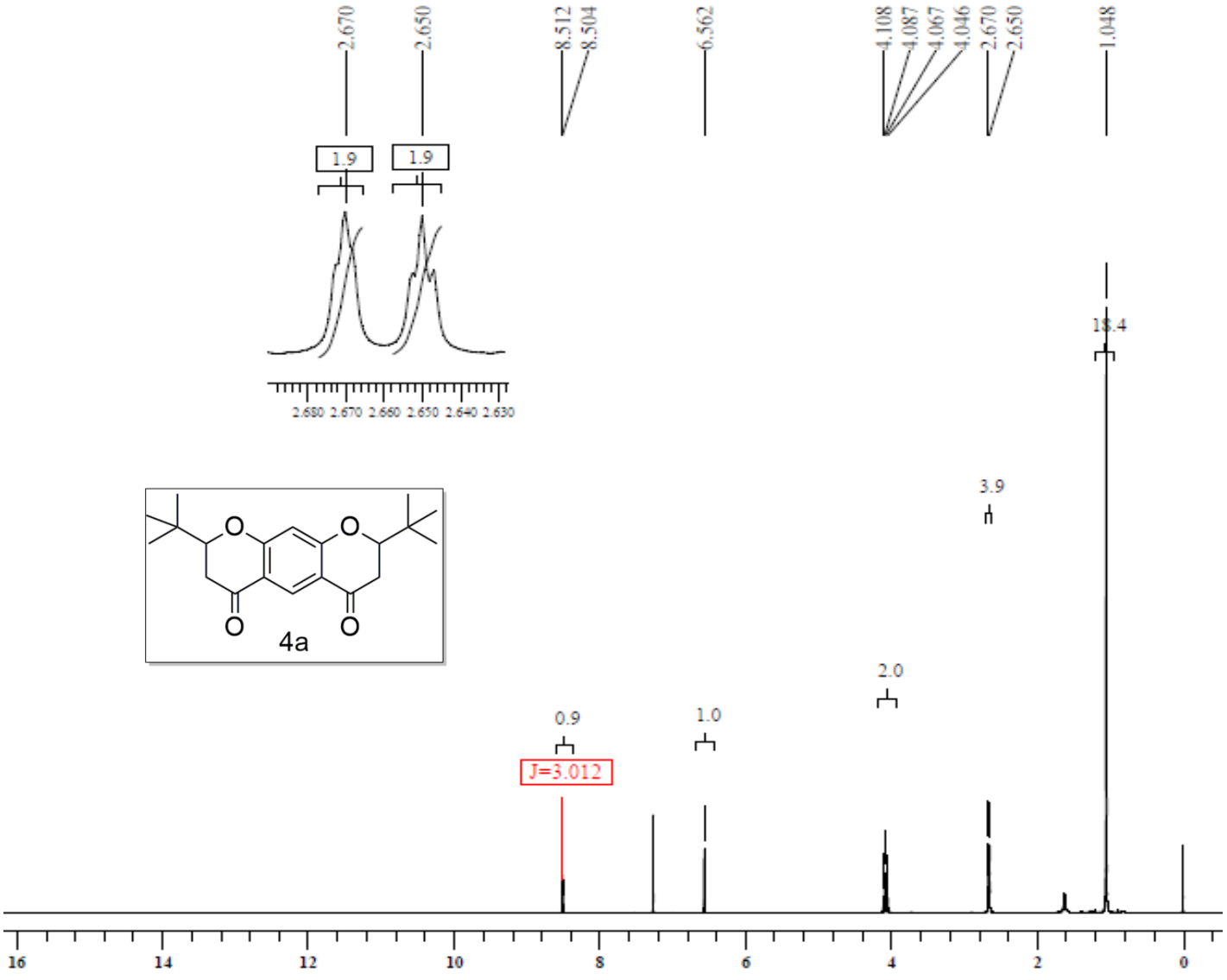


Figure -2: ^{1}H NMR of 2,8-di-tert-butyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4a).

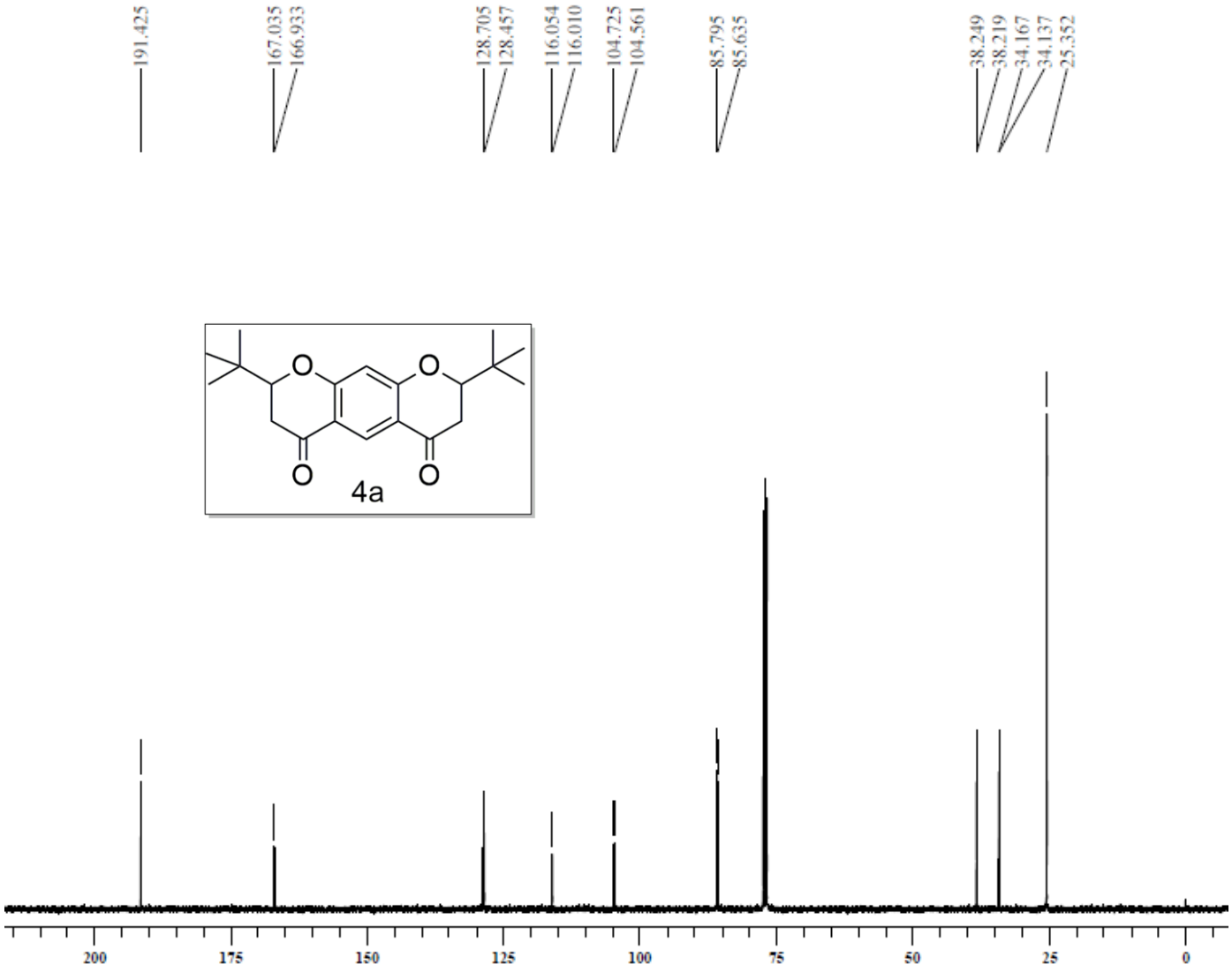
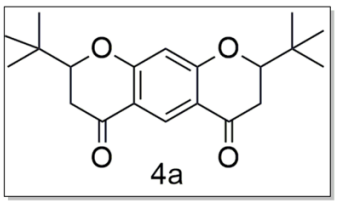
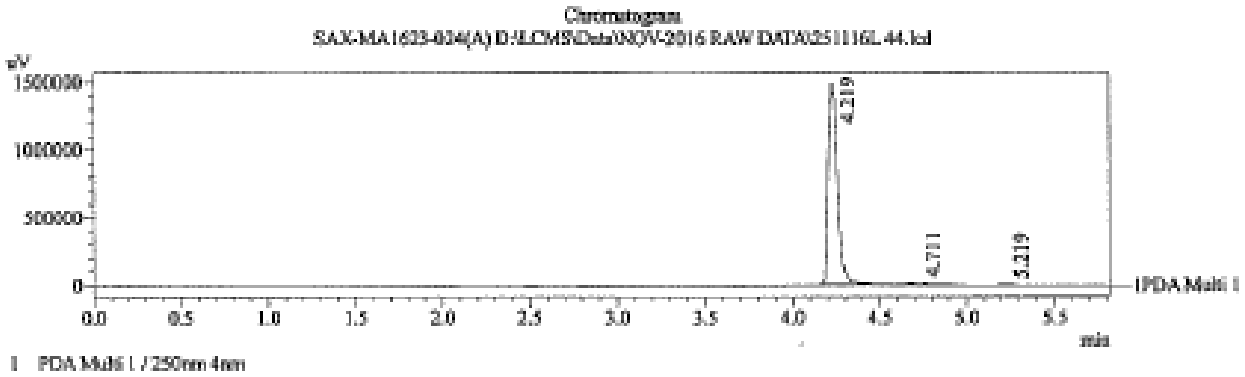
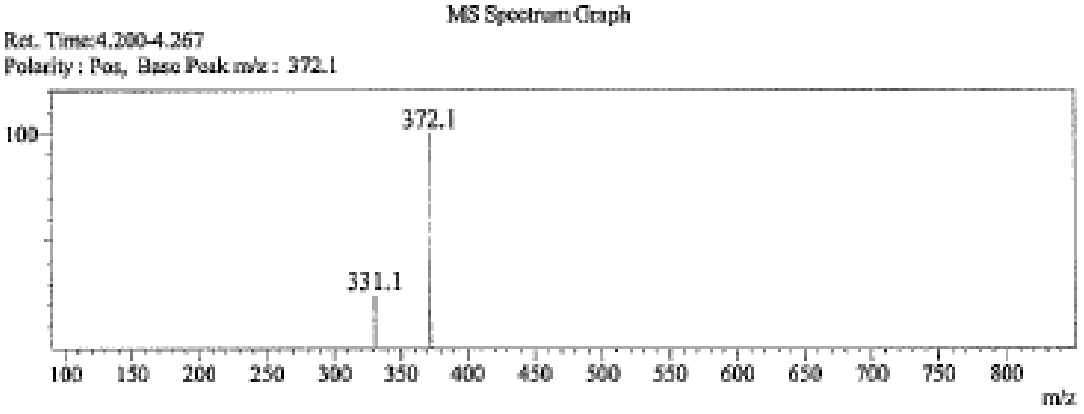


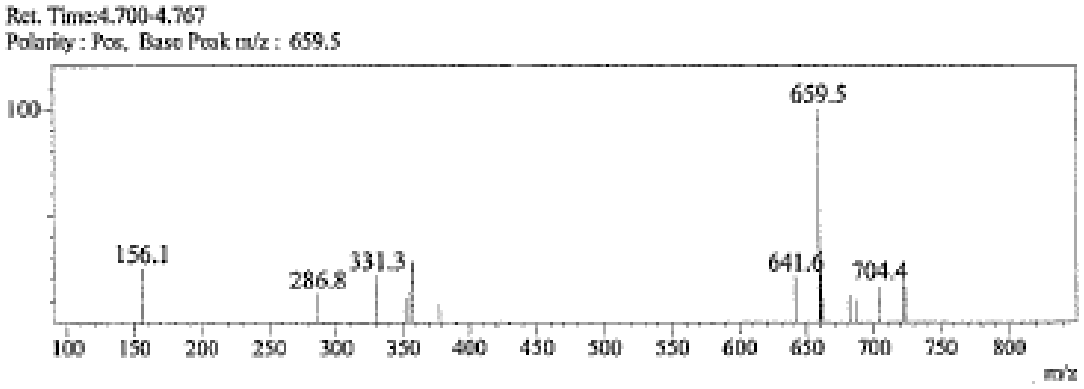
Figure 3: ^{13}C NMR of 2,8-di-tert-butyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4a).

Tuning File :D:\LCMS\Tuning Files\Tuning-ESI-15092014.lct
Vial No :25
Description :Kinetex EVO C-18 (50 X3.0mm,2.6um)
Mobile Phase : A :2.5mM NH4OOCH in water+5%ACN,
B:ACN+ 5% 2.5mM NH4OOCH in Water
T/B% :0.01/5,4/95,5.5/95
Flow : 0.8ml / min(Gradient).









Peak Table

PDA Ch1 250nm 4nm

Peak#	Ret. Time	Area	Area %
1	4.219	5312277	97.294
2	4.711	125241	2.294
3	5.219	22483	0.412
Total		5460000	100.000

Figure 4: LCMS of 2,8-di-tert-butyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4a)

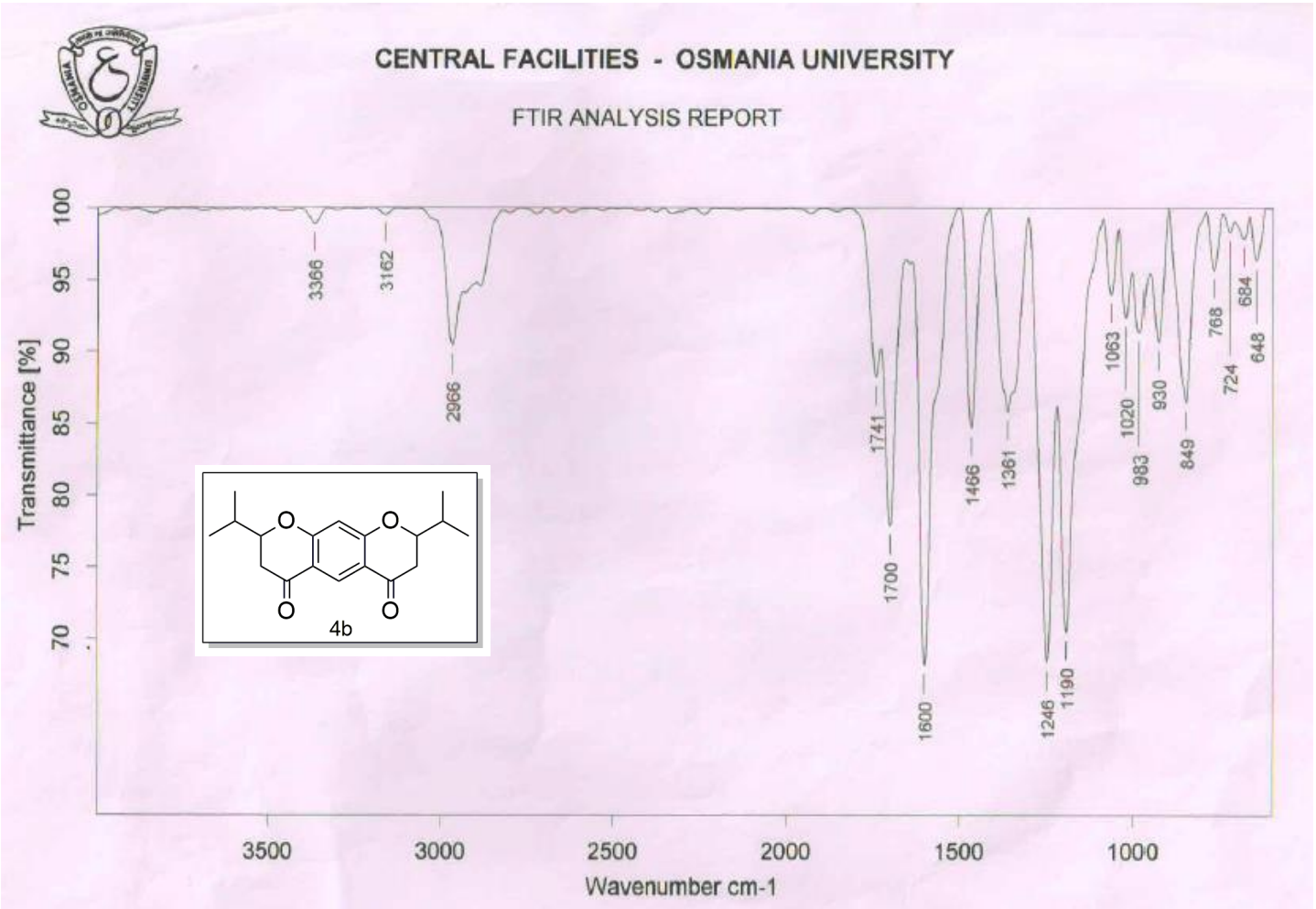


Figure 5: IR data of 2,8-diisopropyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione(4b)

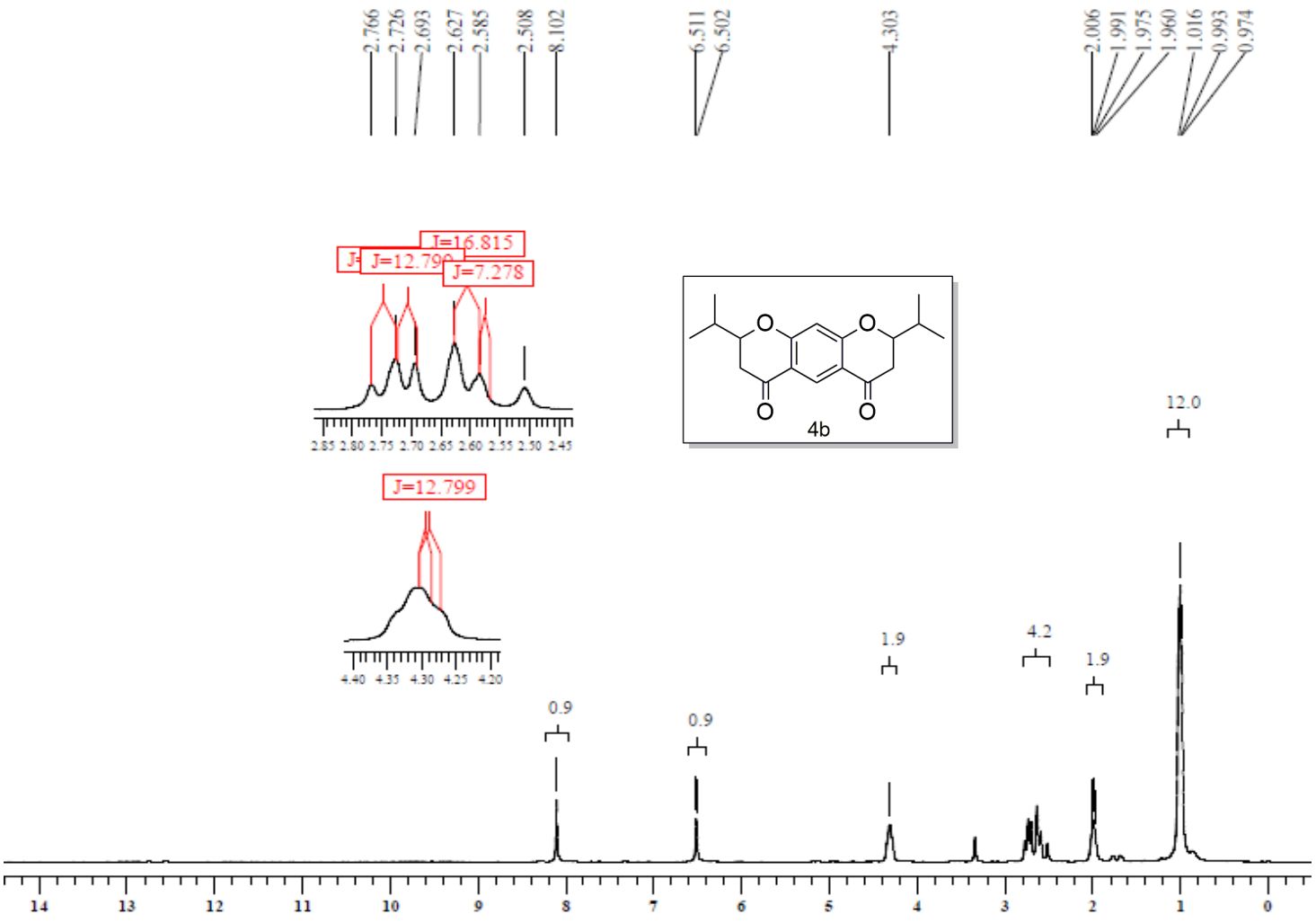


Figure 6: ^{1}H NMR of 2,8-diisopropyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione(4b)

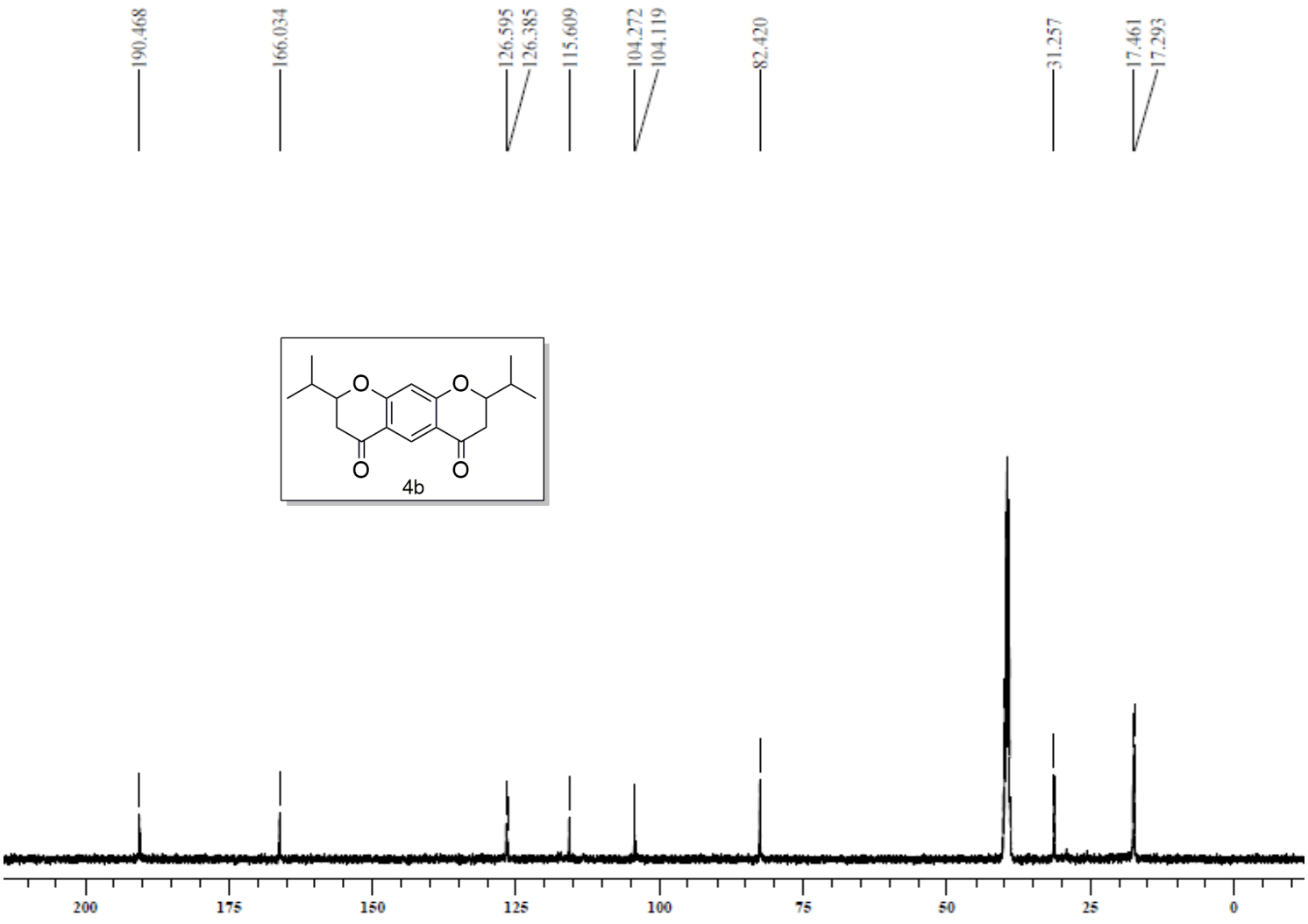
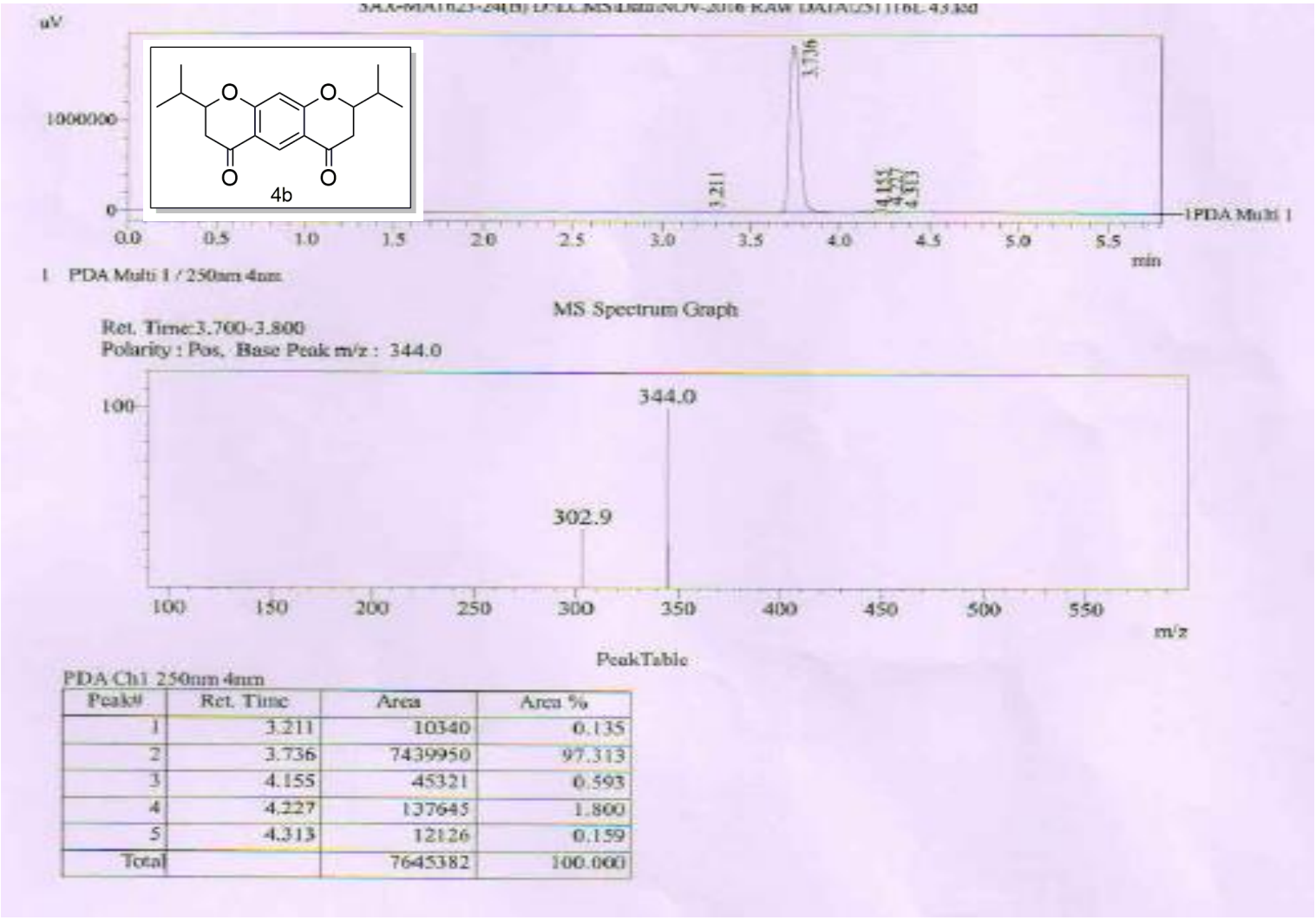


Figure 7: ^{13}C NMR of 2,8-diisopropyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione(4b)



PeakTable

PDA Ch1 250nm 4nm

Peak#	Ret. Time	Area	Area %
1	3.211	10340	0.135
2	3.736	7439950	97.313
3	4.155	45321	0.593
4	4.227	137645	1.800
5	4.313	12126	0.159
Total		7645382	100.000

Figure 8: LCMS of 2,8-diisopropyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4b)

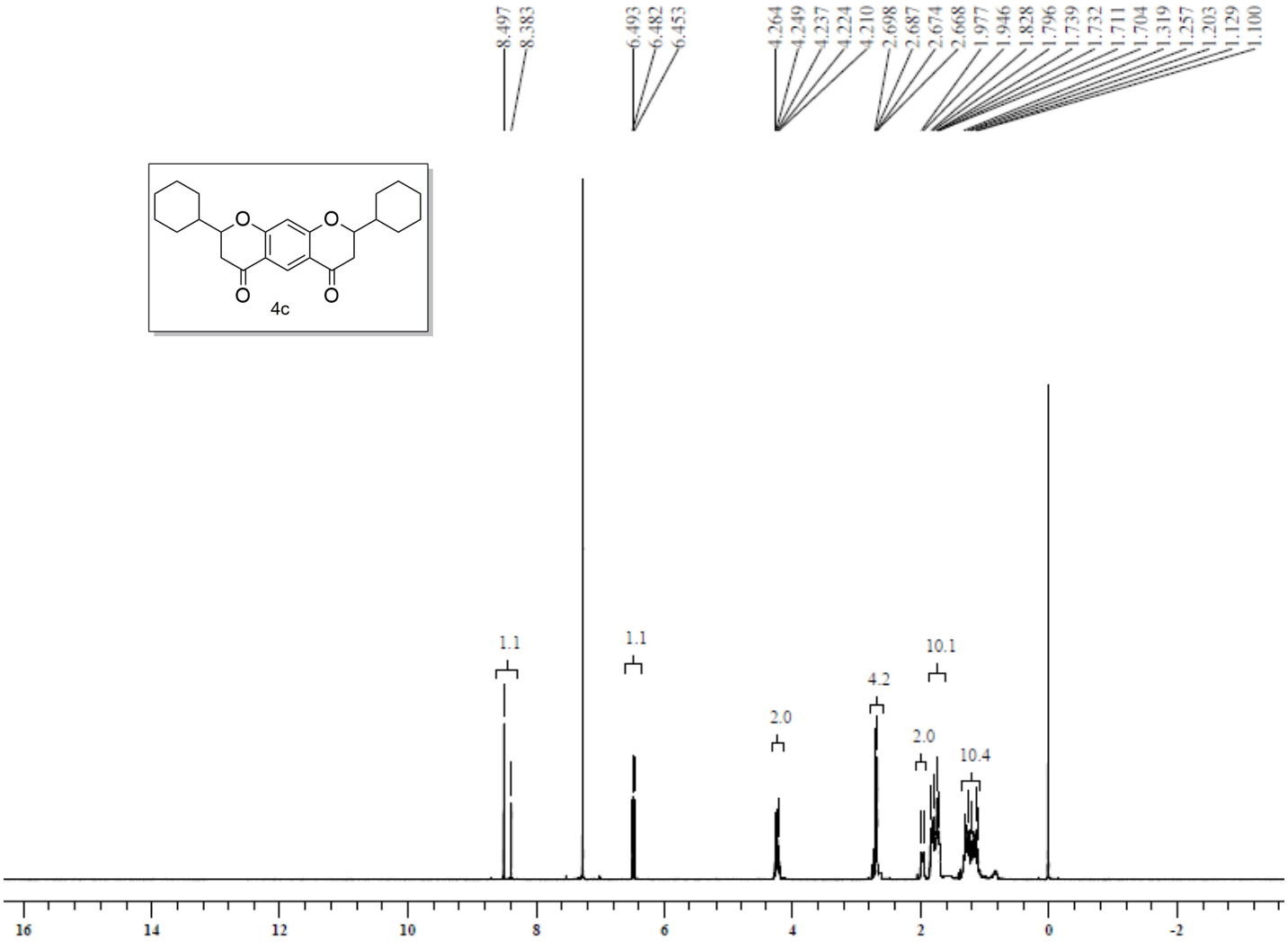


Figure 9: ^{1}H NMR of 2,8-dicyclohexyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione(4c)

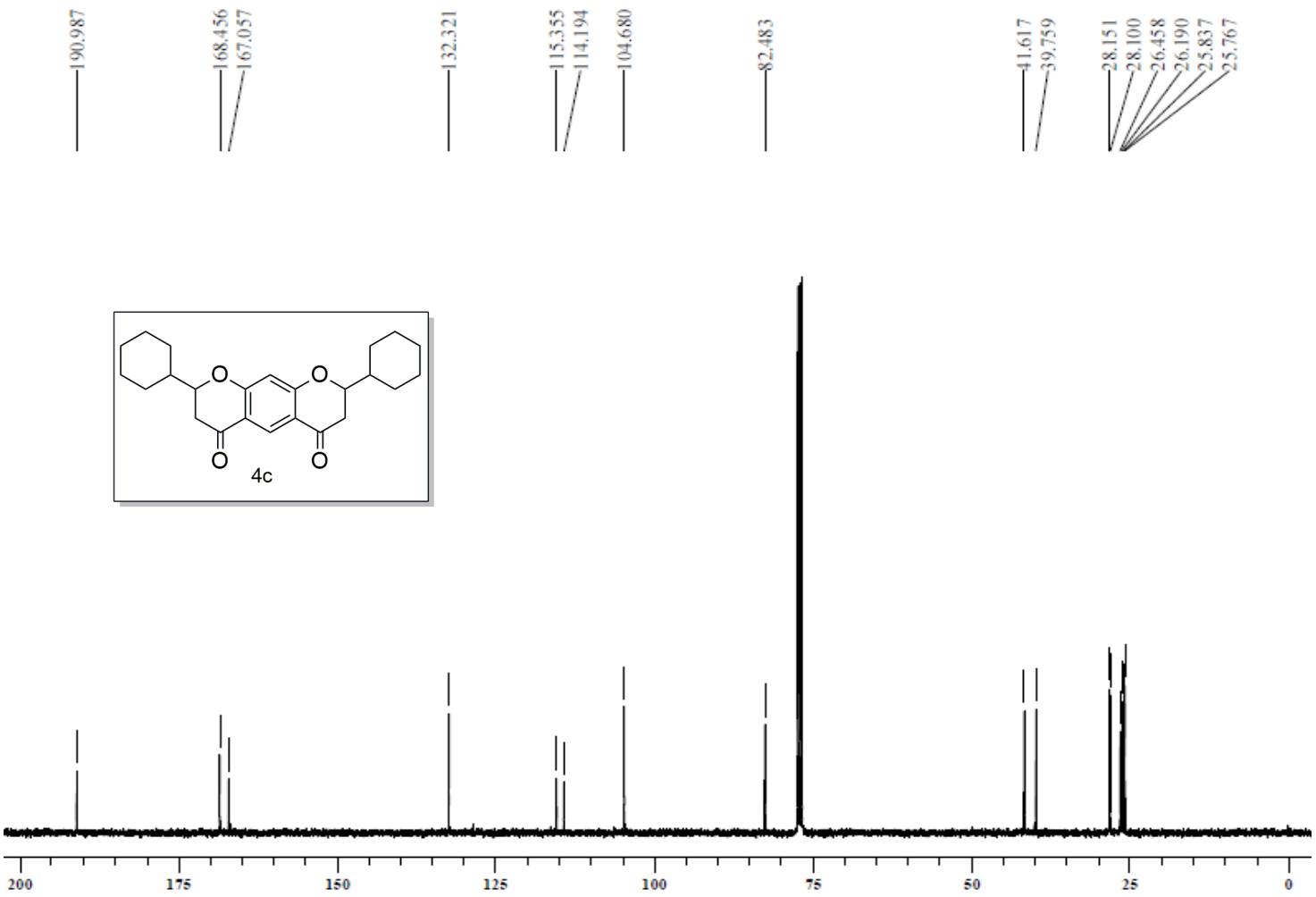


Figure 10: ^{13}C NMR of 2,8-dicyclohexyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione(4c)

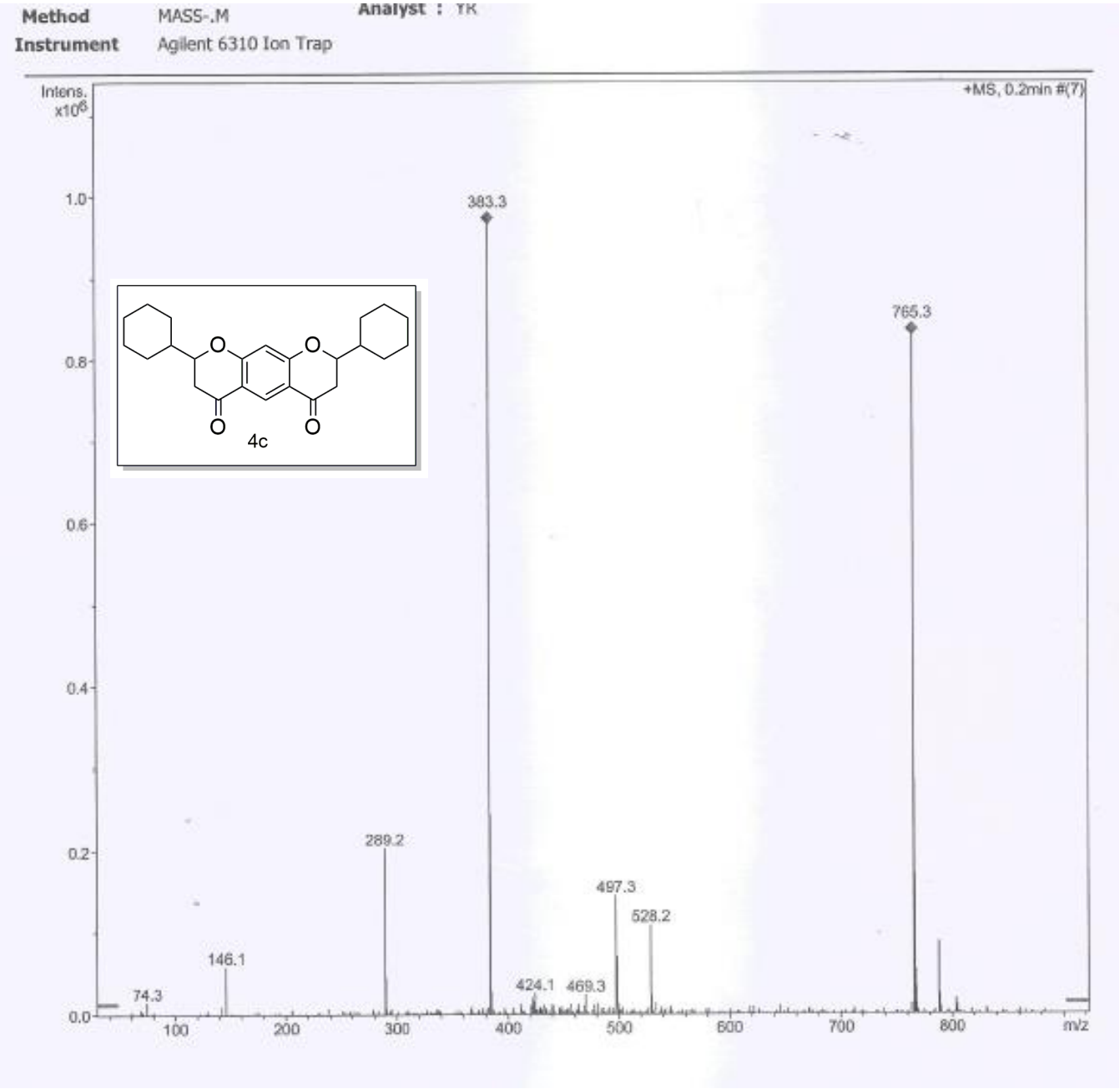


Figure 11: Mass data of 2,8-dicyclohexyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione(4c)

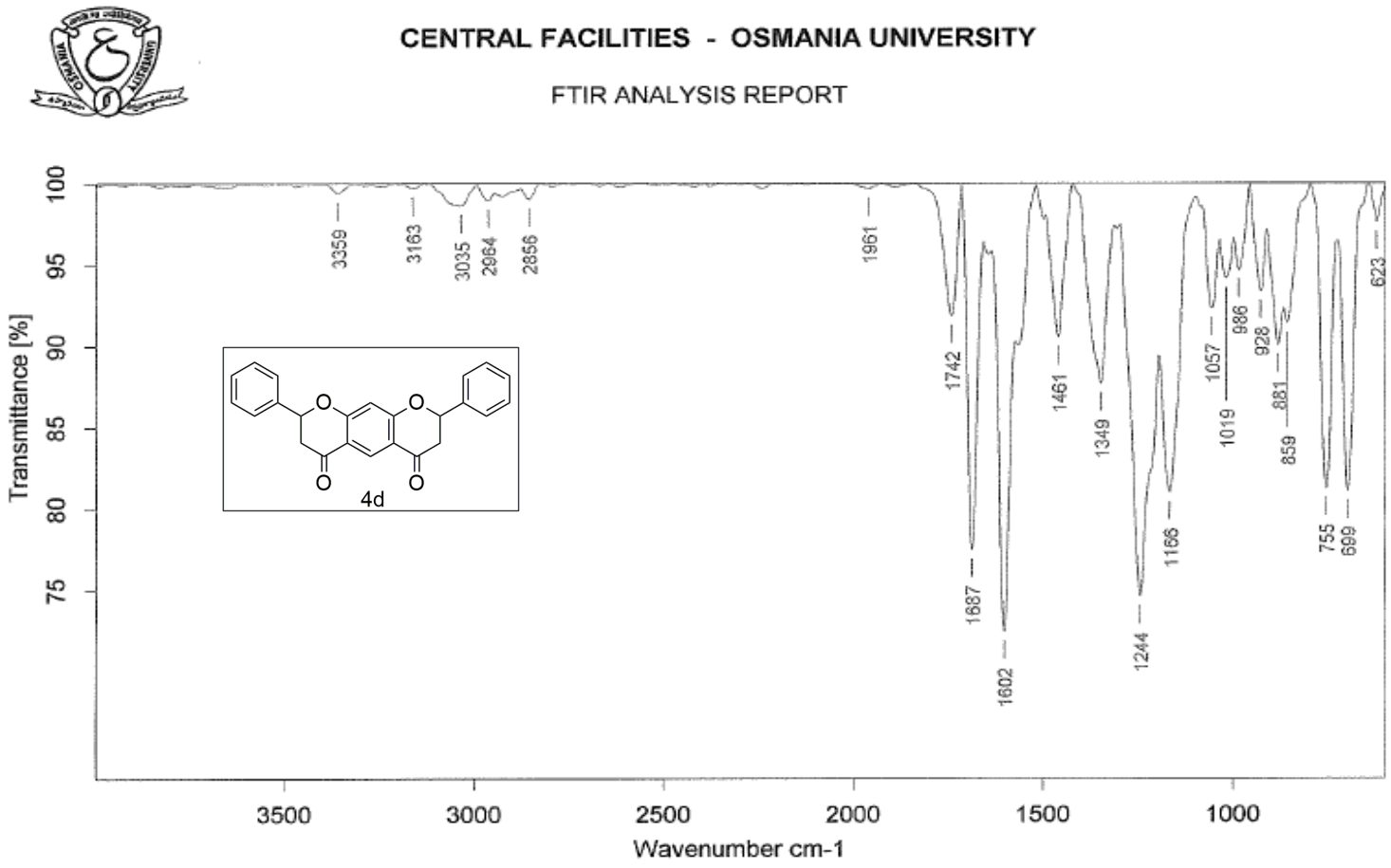


Figure 12: IR data of 2,8-diphenyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4d)

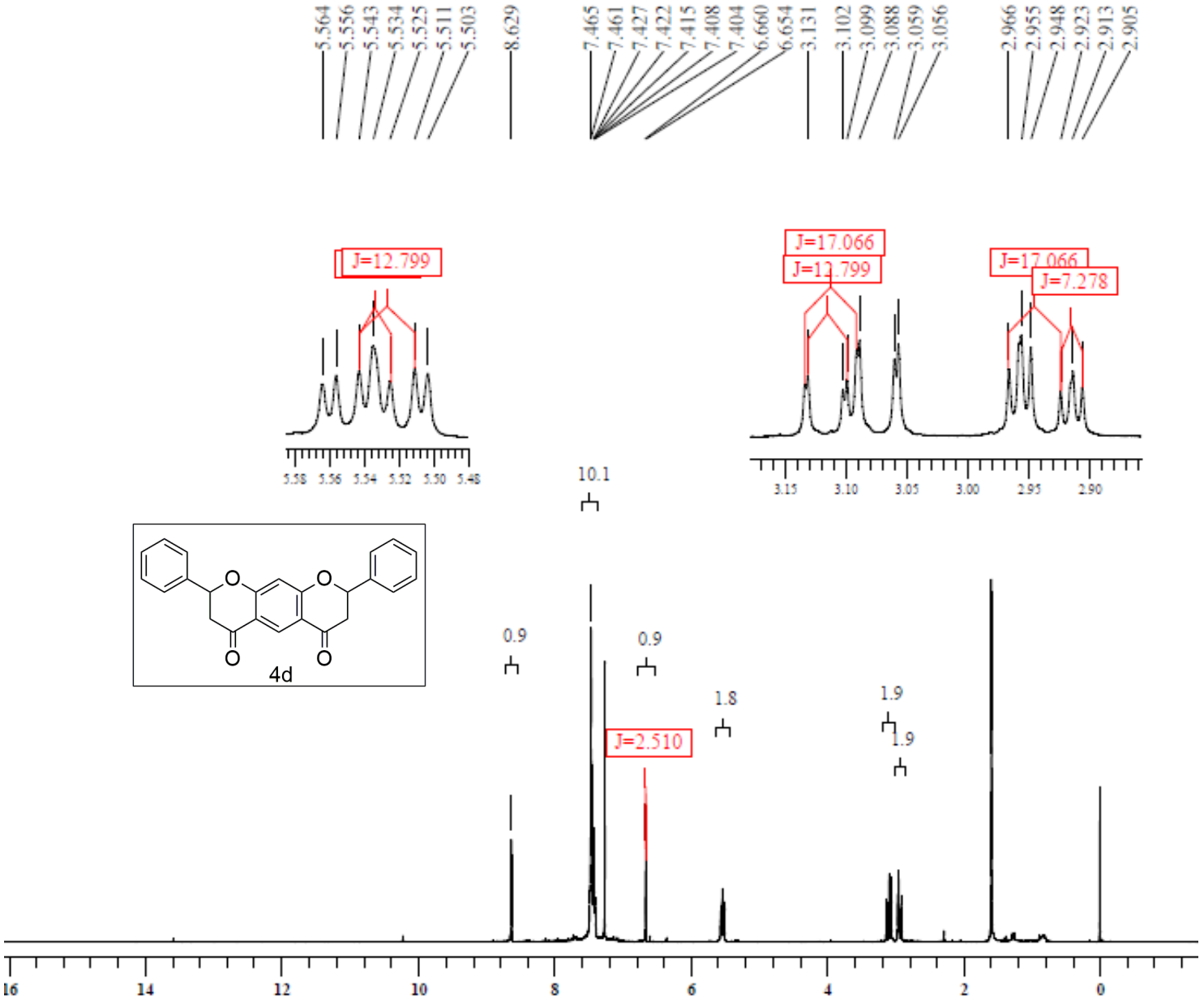


Figure 13: [1]HNMR of 2,8-diphenyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4d)

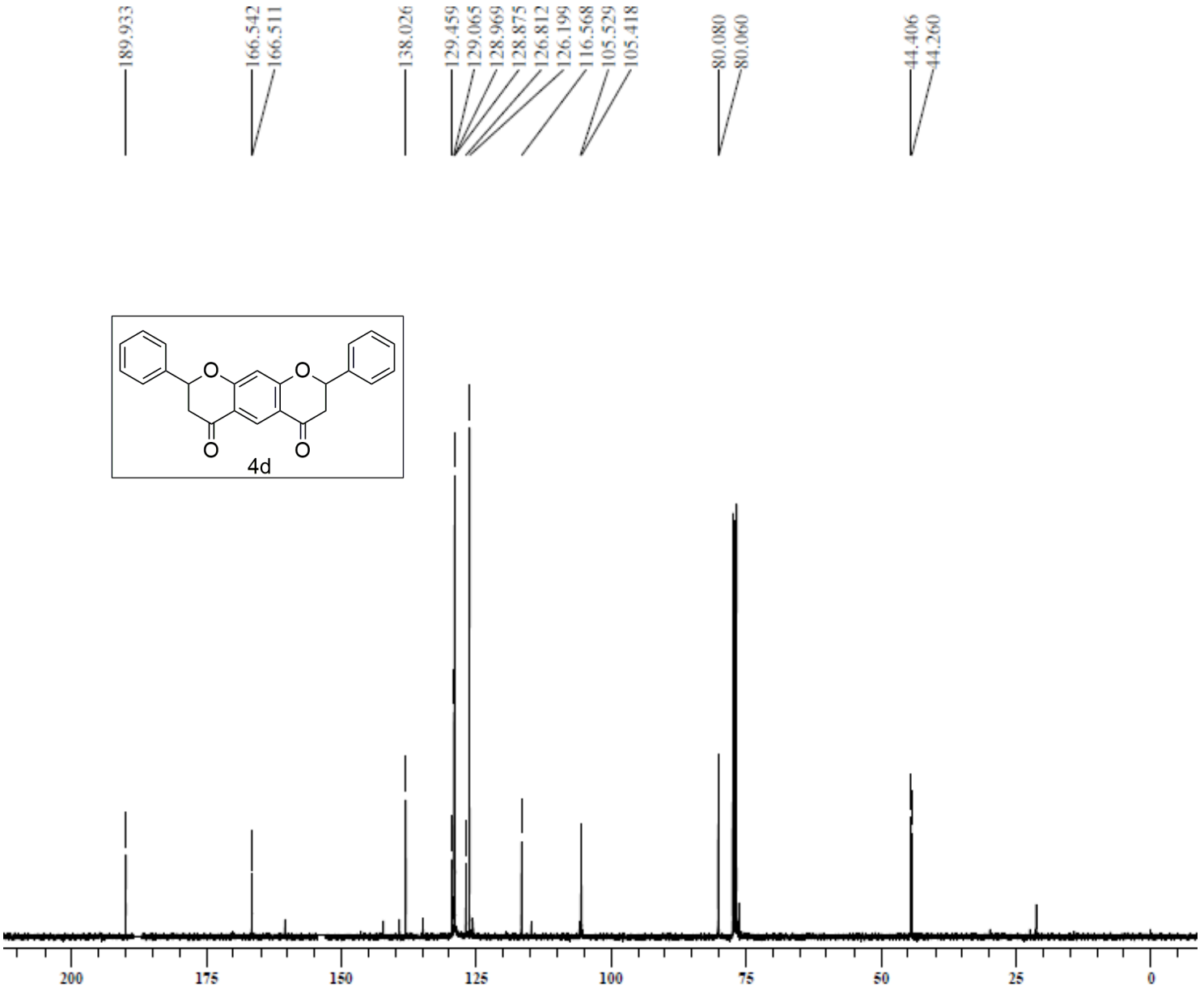
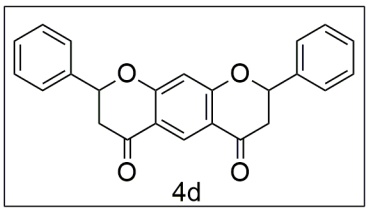
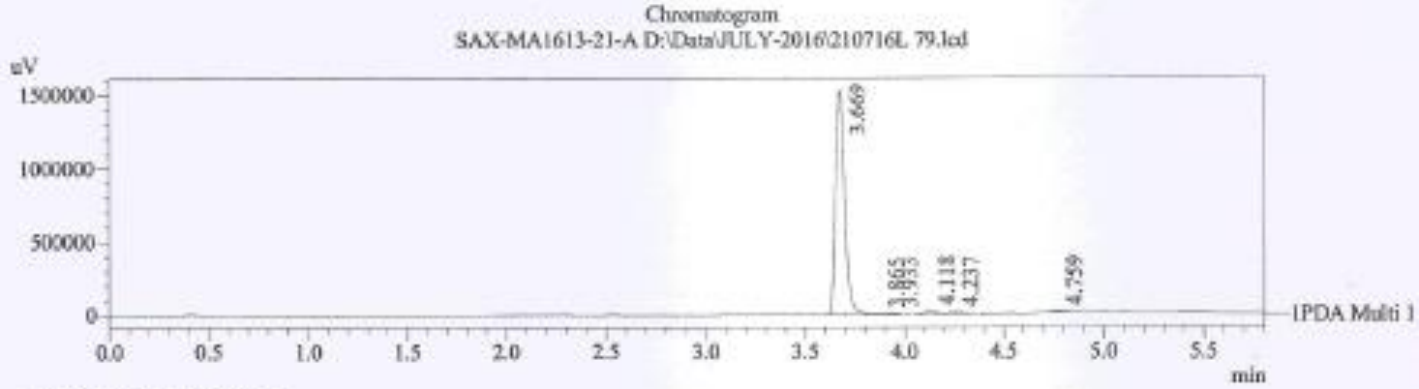


Figure 14: ^{13}CNMR of 2,8-diphenyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4d)

Method File : AF- KE-5.5.lcm
Tuning File :D:\Data\Tuning Files\Tuning-ESI-15092014.lct
Vial No :41
Description :Kinetex EVO C-18 (50 X3.0mm,2.6um)
Mobile Phase : A :2.5mM NH4OOCH in water+5%ACN,
B:ACN+ 5% 2.5mM NH4OOCH in Water
T/B% :0.01/5,4/95,5.5/95
Flow : 0.8ml / min(Gradient).

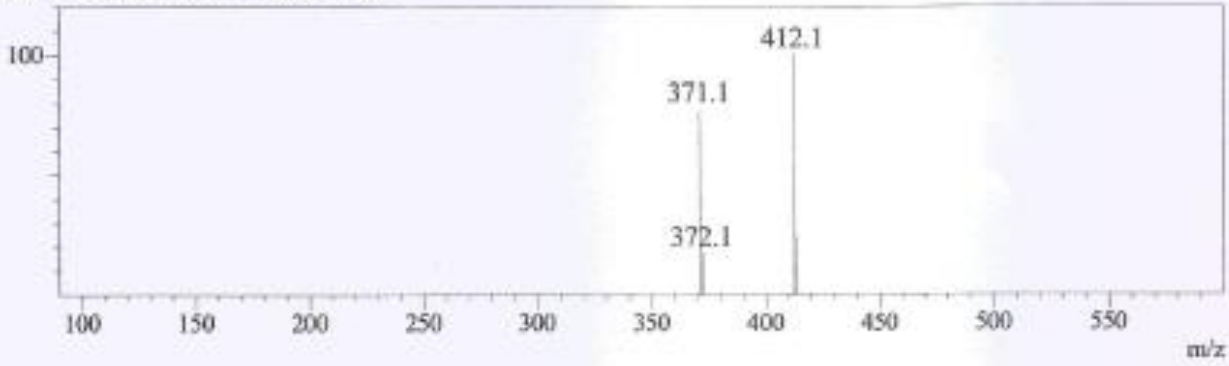




1 PDA Multi 1 / 252nm 4nm

MS Spectrum Graph

Ret. Time:3.667-3.733
Polarity : Pos. Base Peak m/z : 412.1



PeakTable

PDA Ch1 252nm 4nm

Peak#	Ret. Time	Area	Area %
1	3.669	4736931	97.208
* 2	3.865	5104	0.105
3	3.933	16191	0.332
4	4.118	56566	1.161
5	4.237	26692	0.548
* 6	4.759	31476	0.646
Total		4872961	100.000

Figure 15: LCMS of 2,8-diphenyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4d)

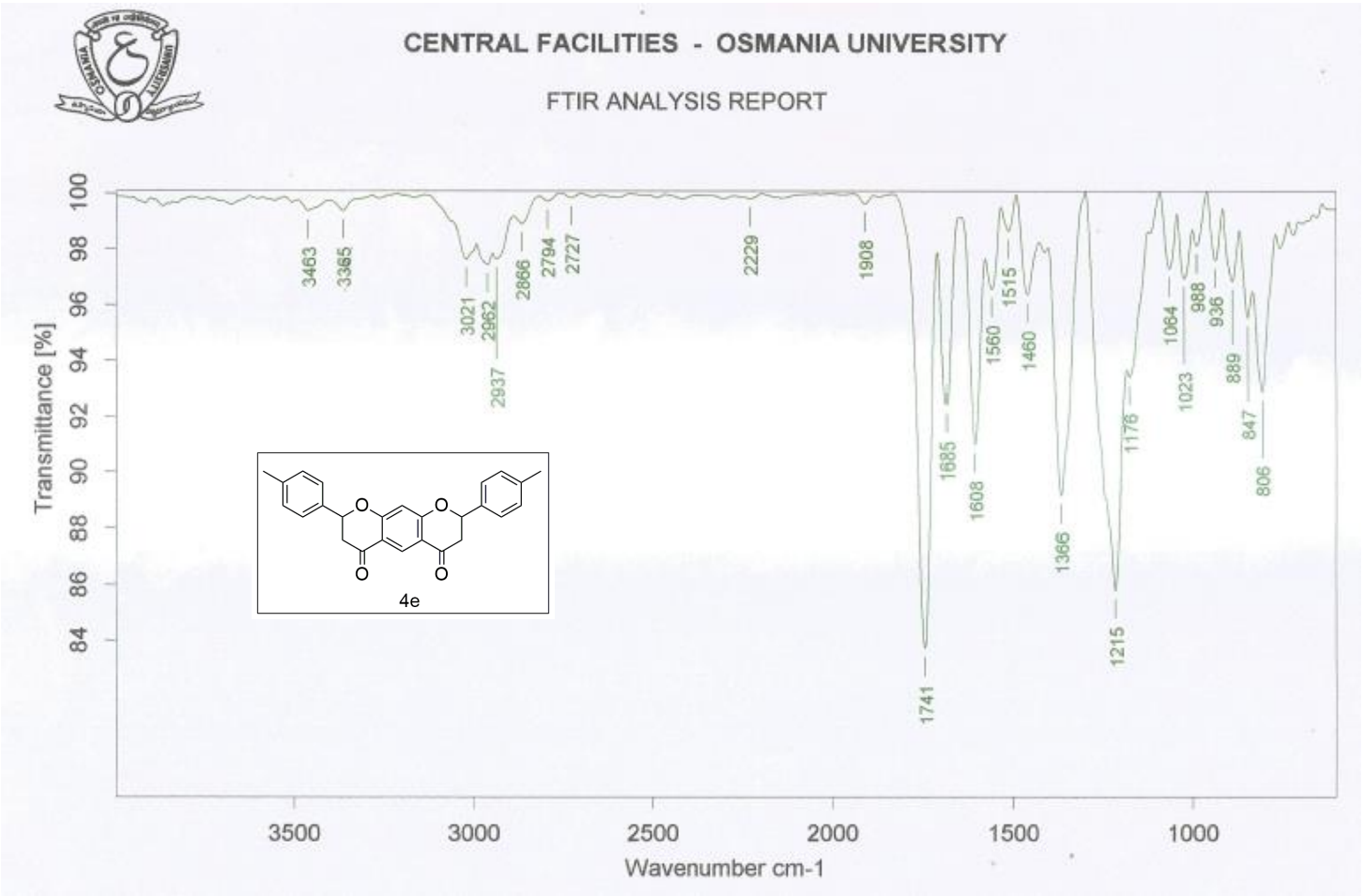


Figure 16: IR data of 2,8-di-p-tolyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione(4e)

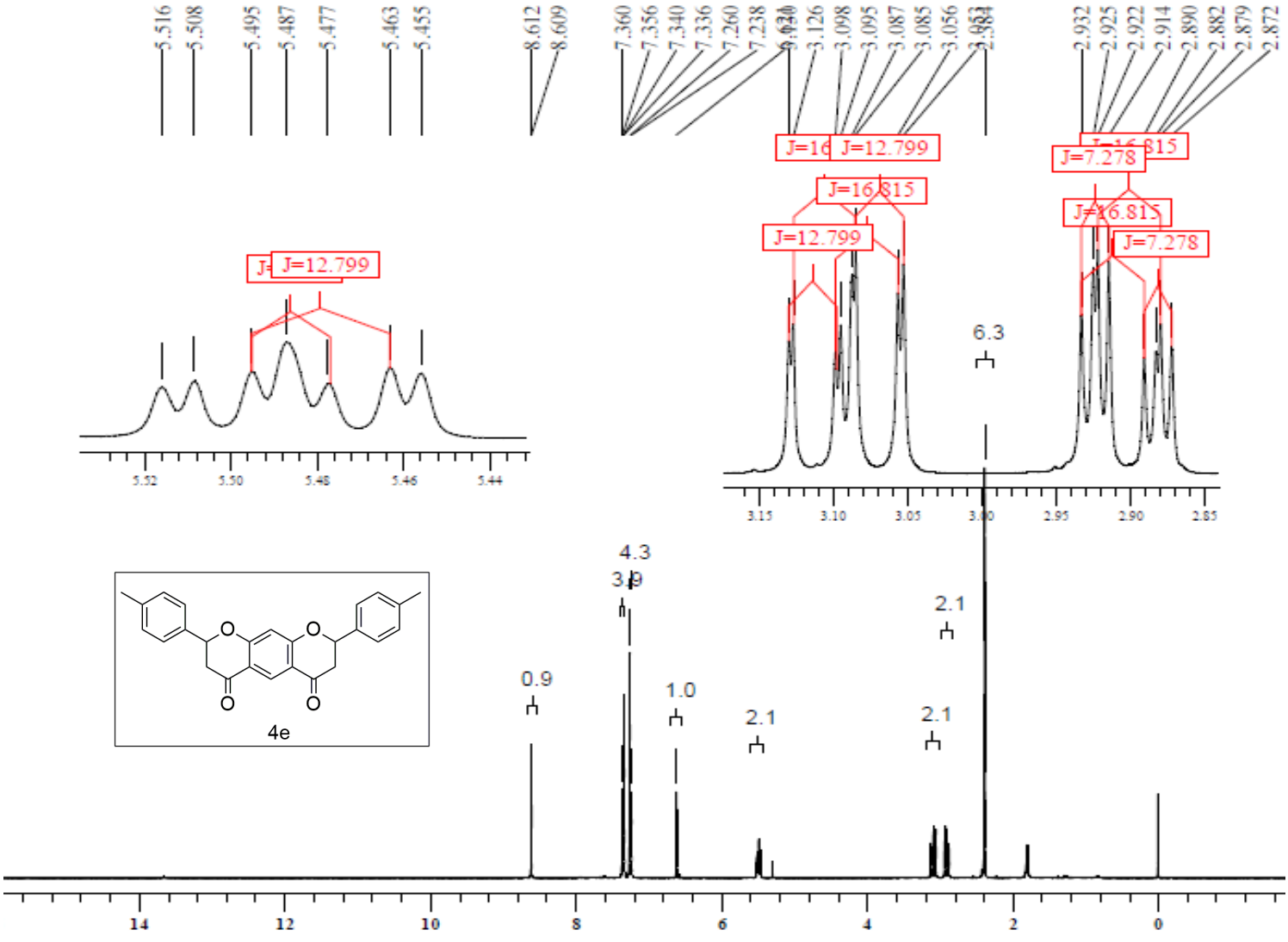


Figure 17: ^{1}H NMR of 2,8-di-p-tolyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione(4e)

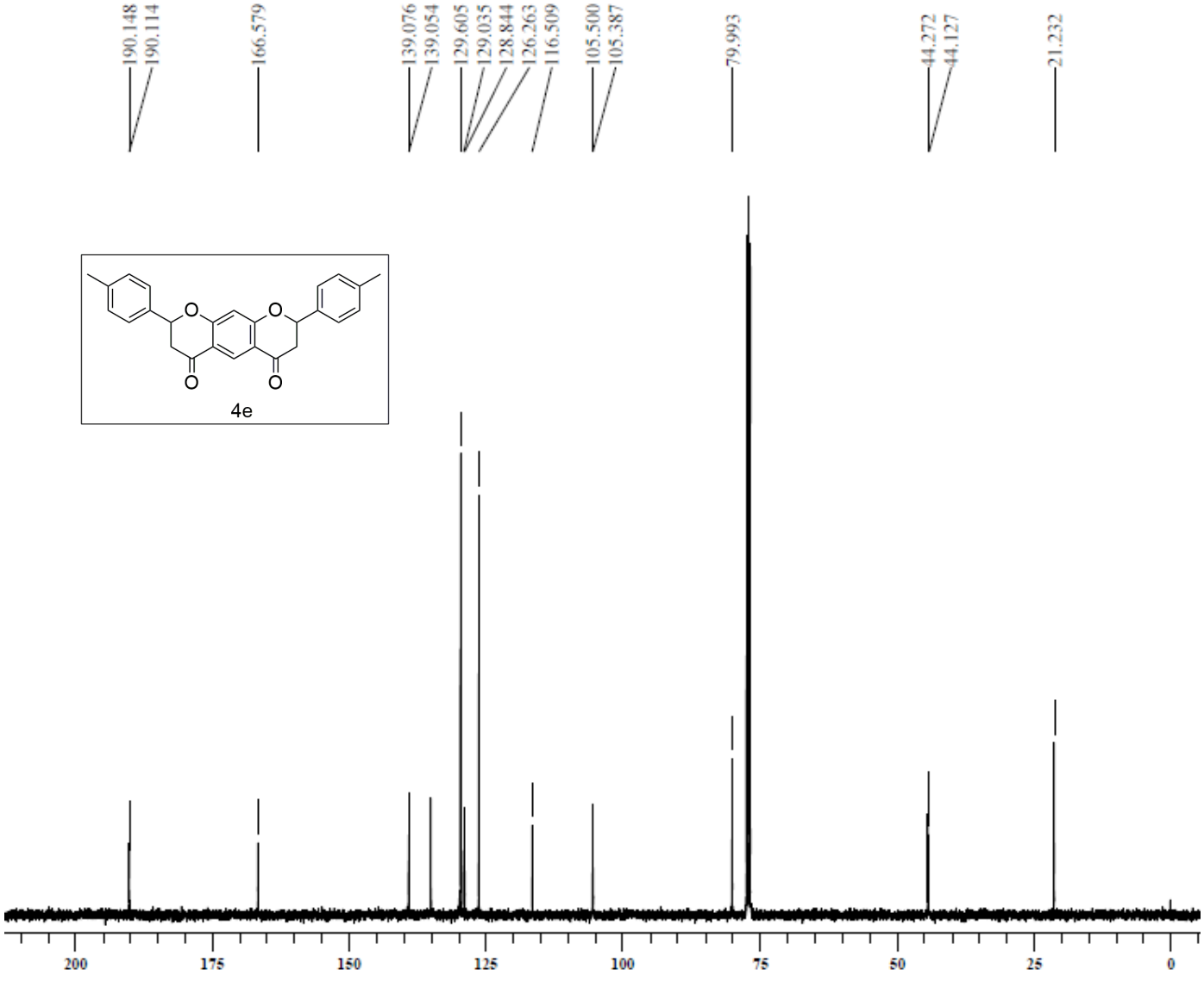


Figure 18: ^{13}C NMR of 2,8-di-p-tolyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione (4e)

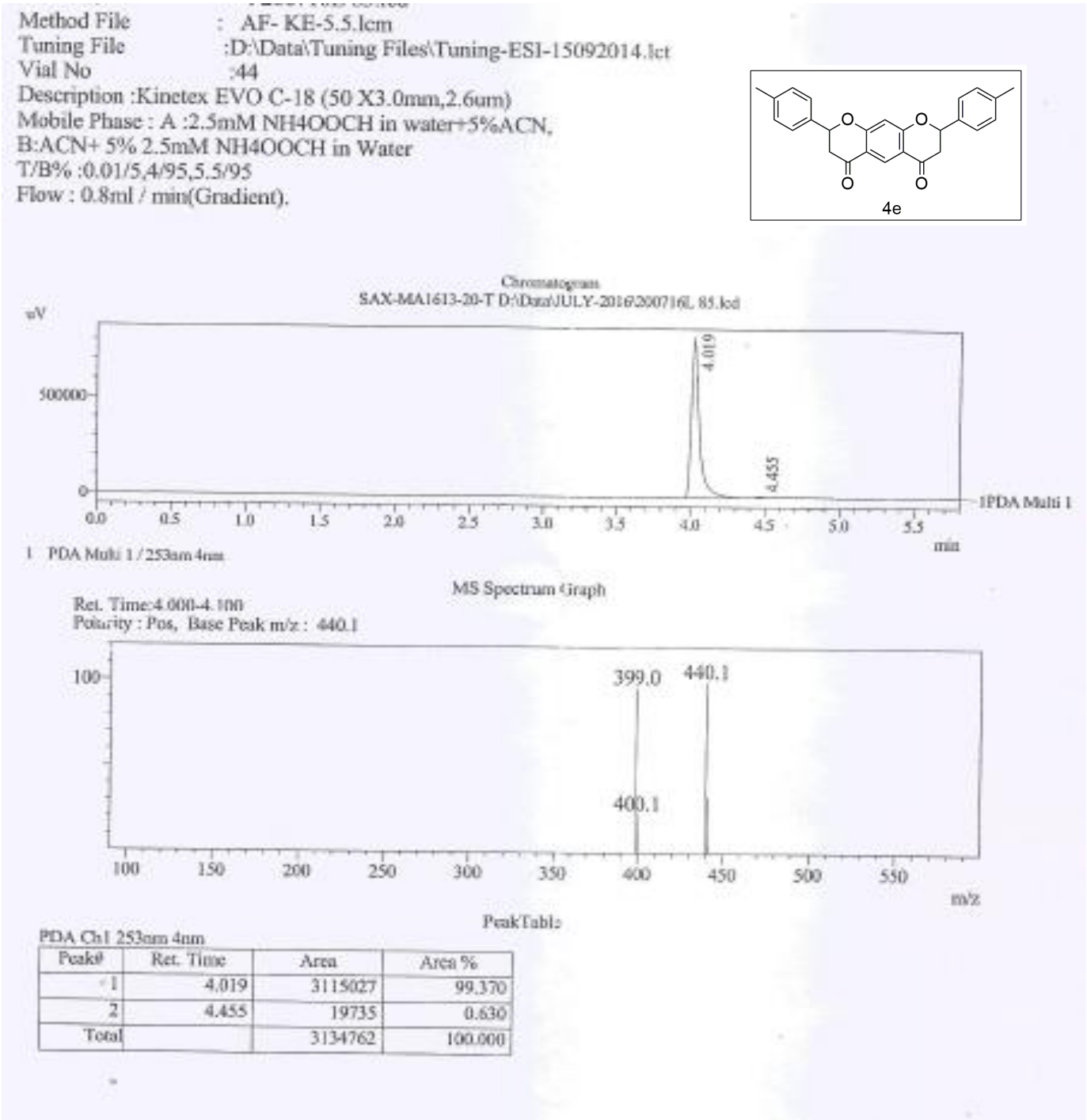


Figure 19: LCMS data of 2,8-di-p-tolyl-2,3,7,8-tetrahydropyrano[3,2-g]chromene-4,6-dione(4e)

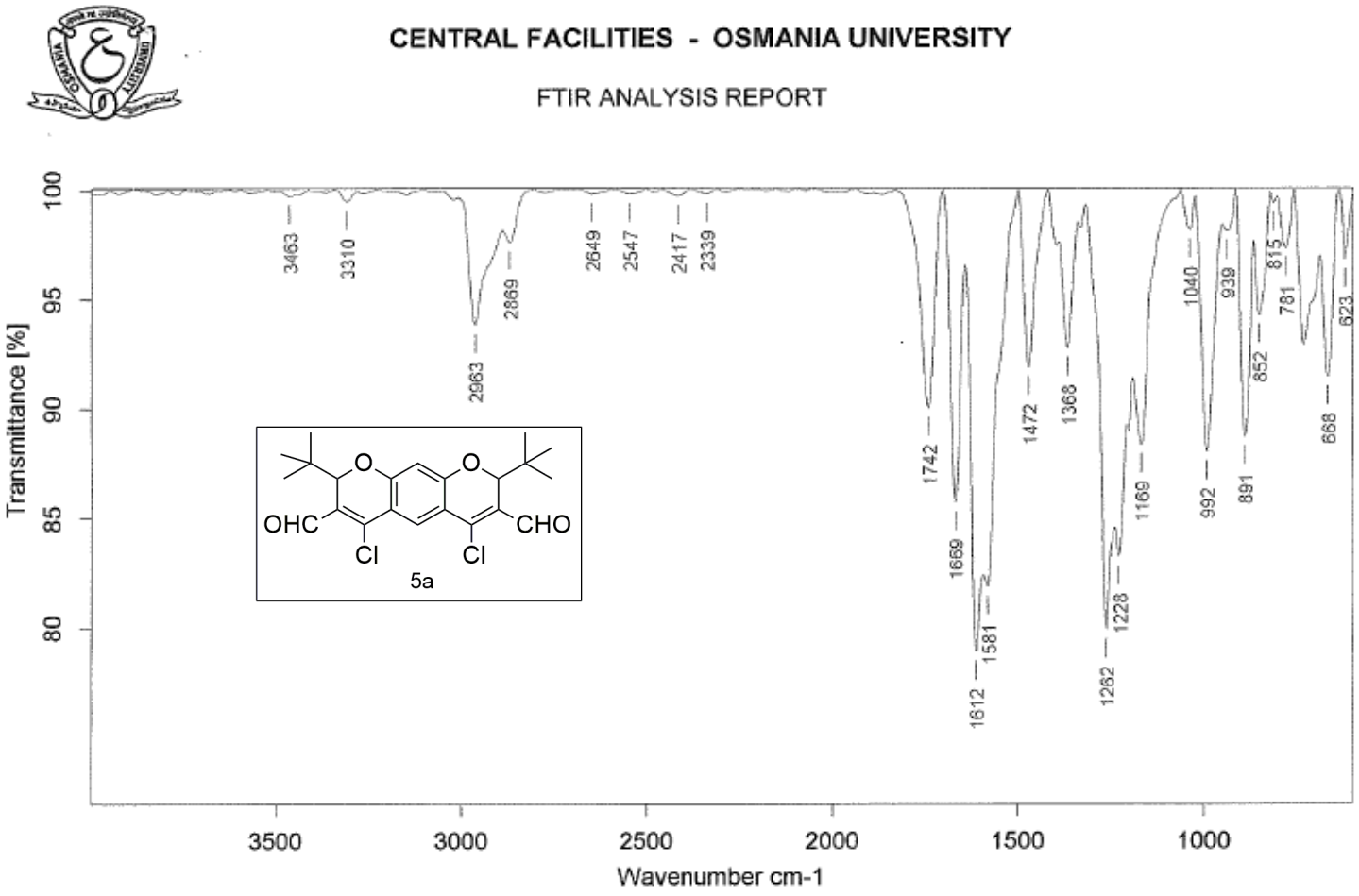


Figure 20: IR data of 2,8-di-tert-butyl-4,6-dichloro-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5a)

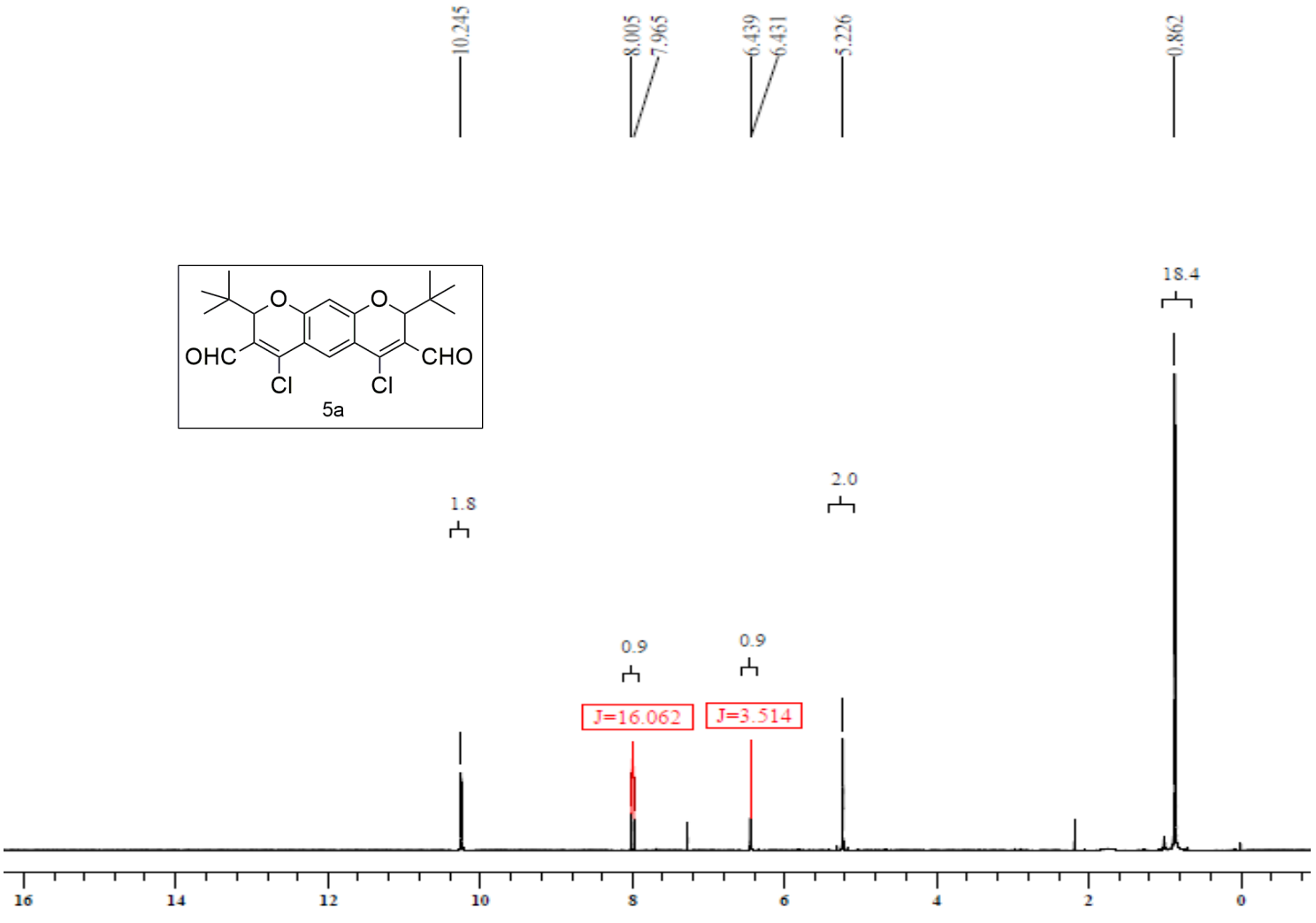


Figure 21: ^{1}H NMR of 2,8-di-tert-butyl-4,6-dichloro-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5a)

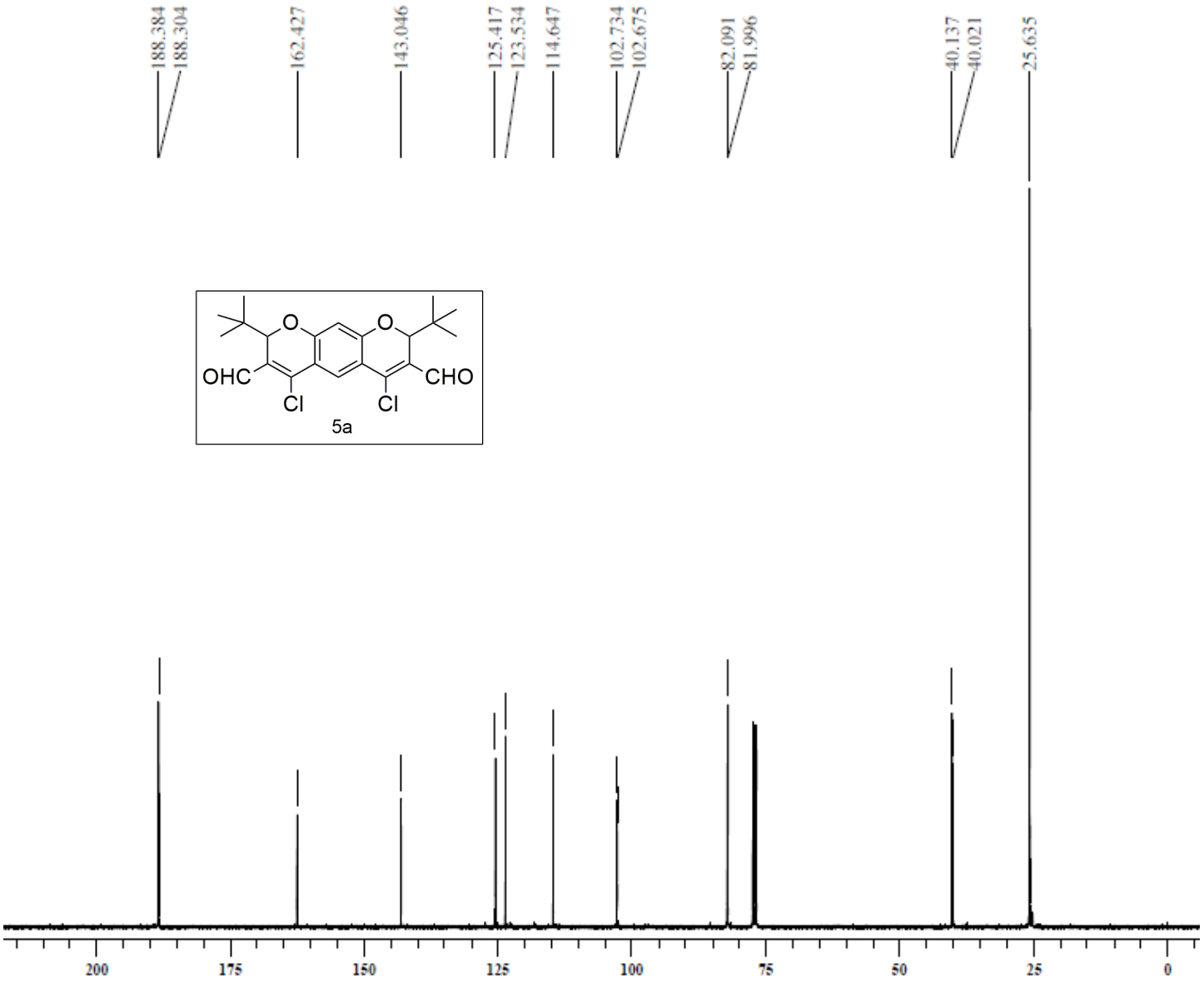
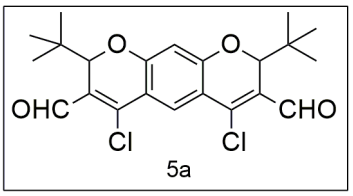
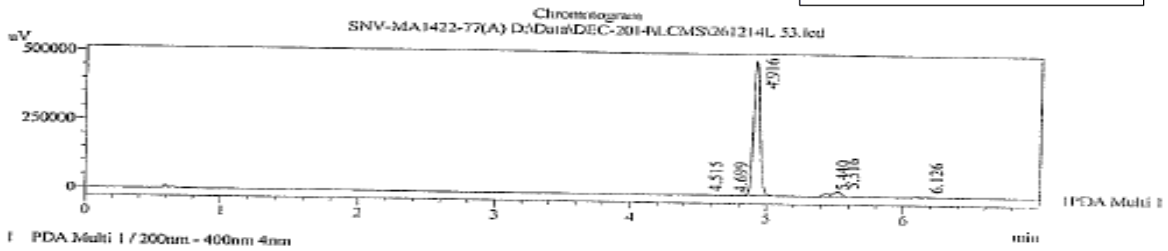


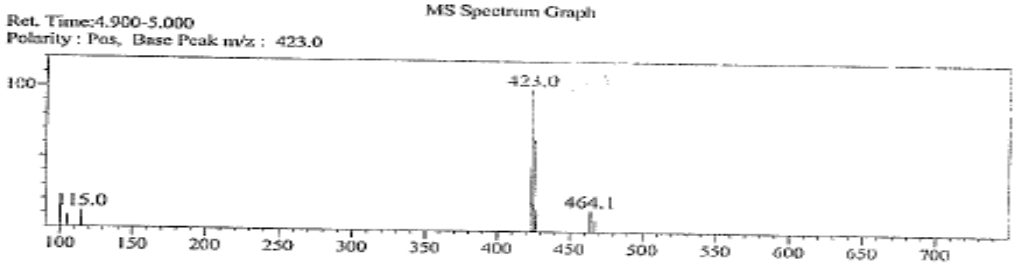
Figure 22: ^{13}C NMR of 2,8-di-tert-butyl-4,6-dichloro-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde(5a)

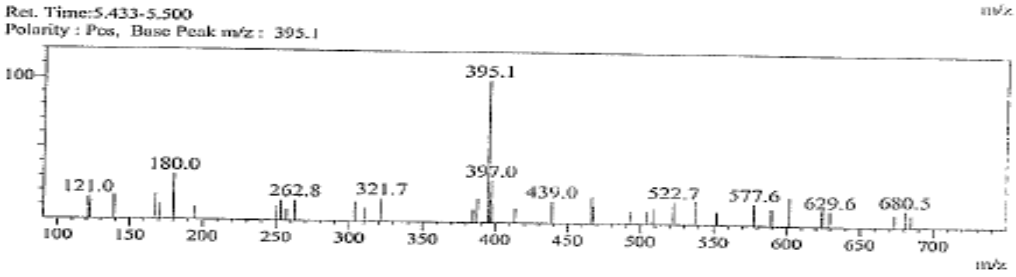
Method File : lcms.lcm
Tuning File :D:\Data\Tuning Files\Tuning-ESI-15092014.lct
Vial No :26
[Description] : Description :Gemini NX C-18 (50 X4.6mm,3.0um)
Mobile Phase : A :2.5mM NH4OOCH in water+5%ACN,
B:ACN+ 5% 2.5mM NH4OOCH in Water
T/B% :0.01/5,0.5/5,3.5/100,7/100
Flow : 1.2ml / min(Gradient).

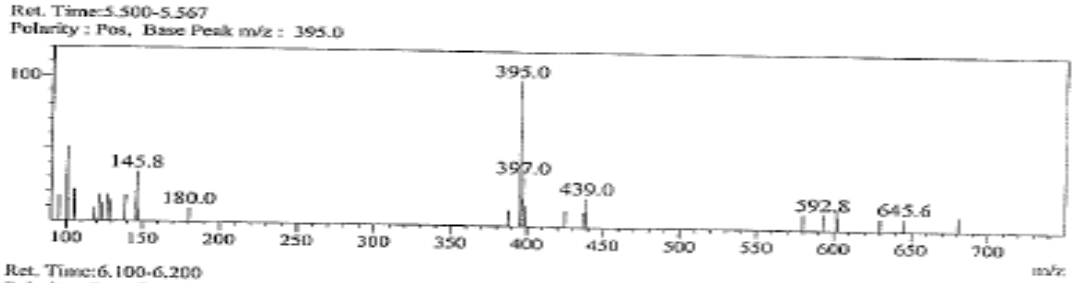


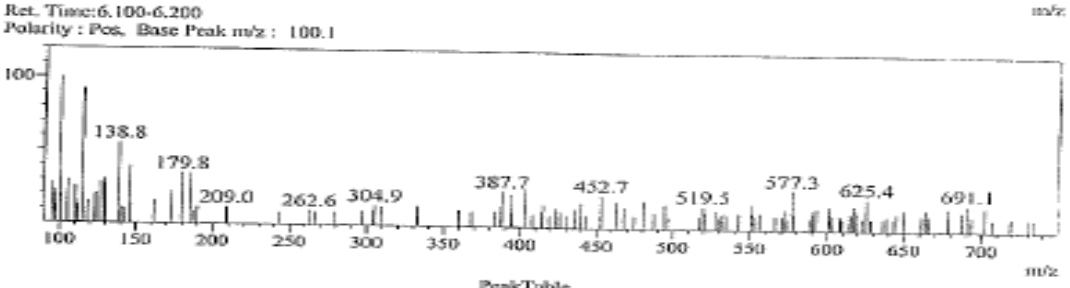
5a











PDA Ch1 200nm - 400nm 4nm

PeakTable

Peak#	Ret. Time	Area	Area %
1	4.515	6354	0.362
2	4.699	545	0.031
3	4.916	1592568	90.703
4	5.440	43341	2.468
5	5.516	77170	4.395
6	6.126	35828	2.041
Total		1755806	100.000

Figure 23: LCMS of 2,8-di-tert-butyl-4,6-dichloro-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde(5a)

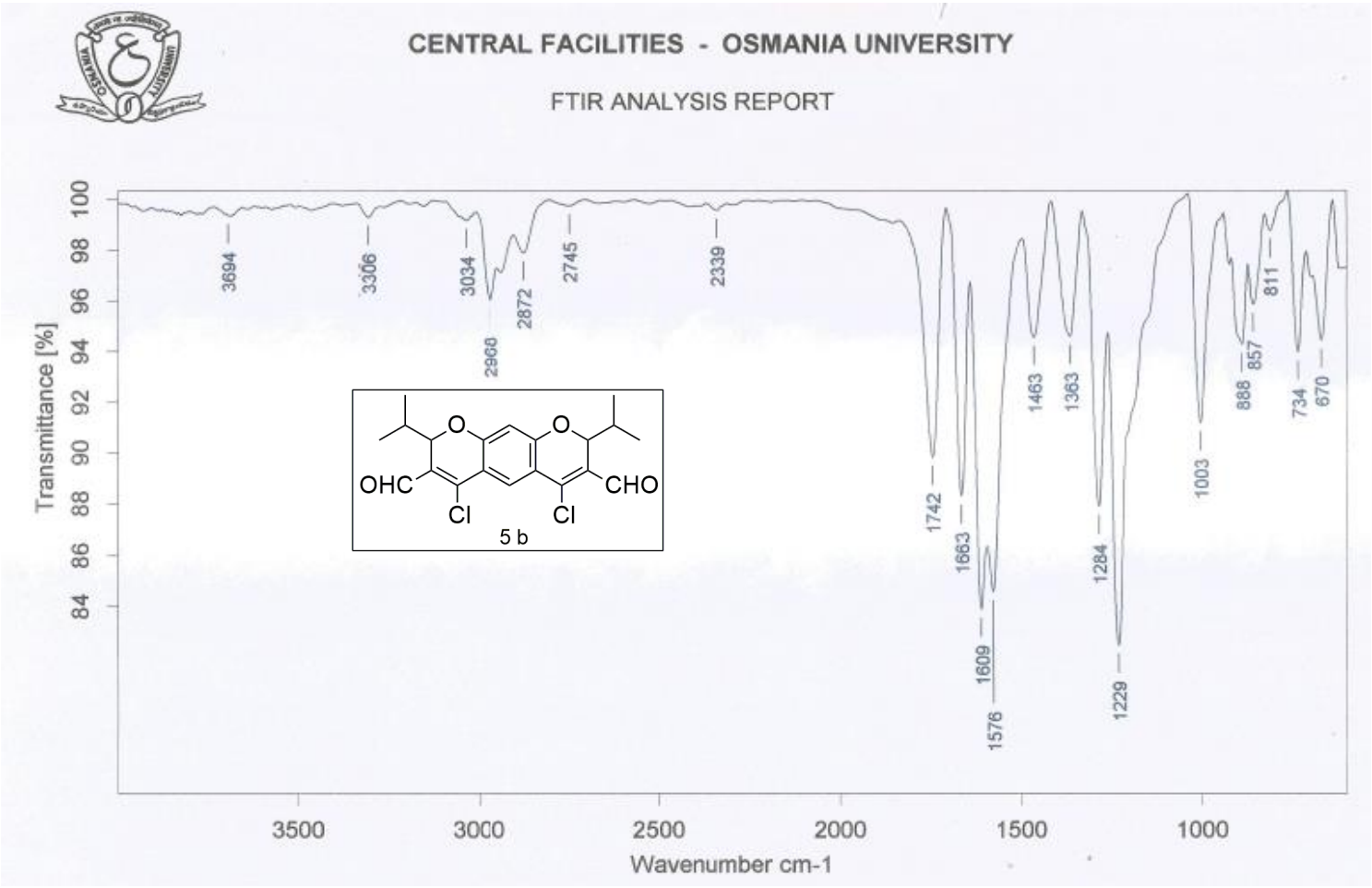


Figure 24: IR data of 4,6-dichloro-2,8-diisopropyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5b)

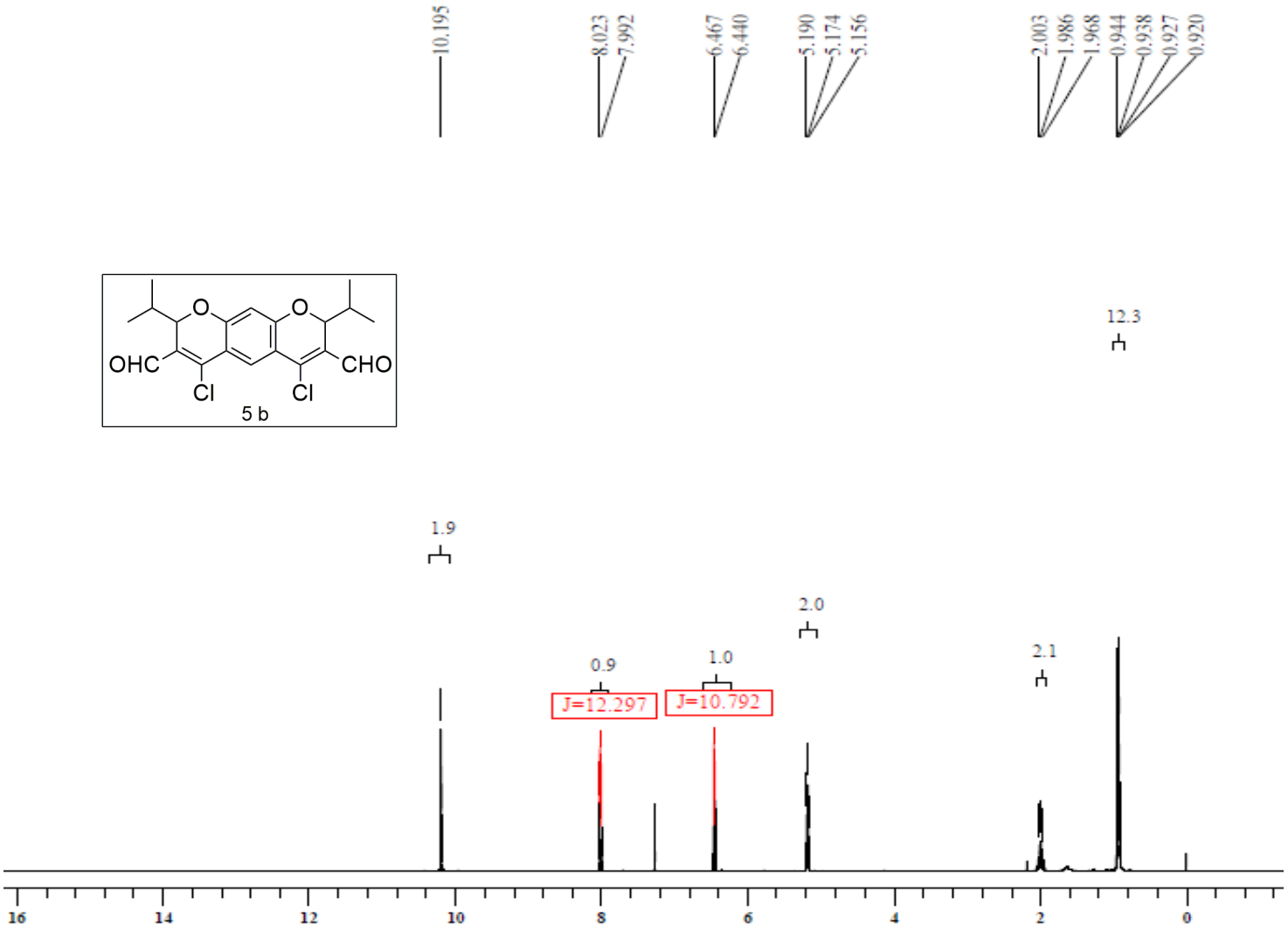


Figure 25: ^{1}H NMR of 4,6-dichloro-2,8-diisopropyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5b)

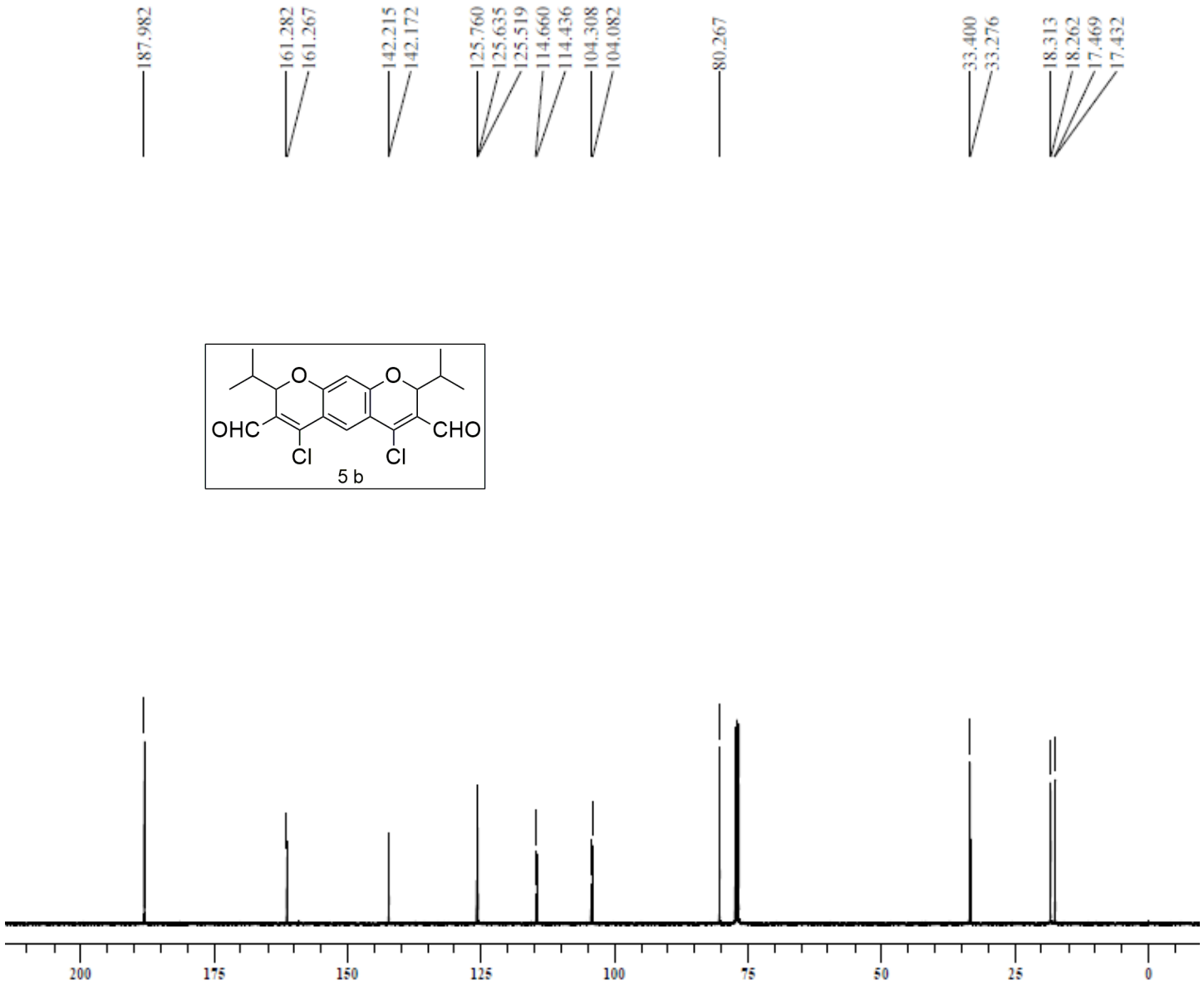
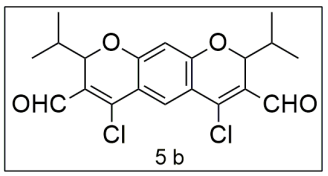
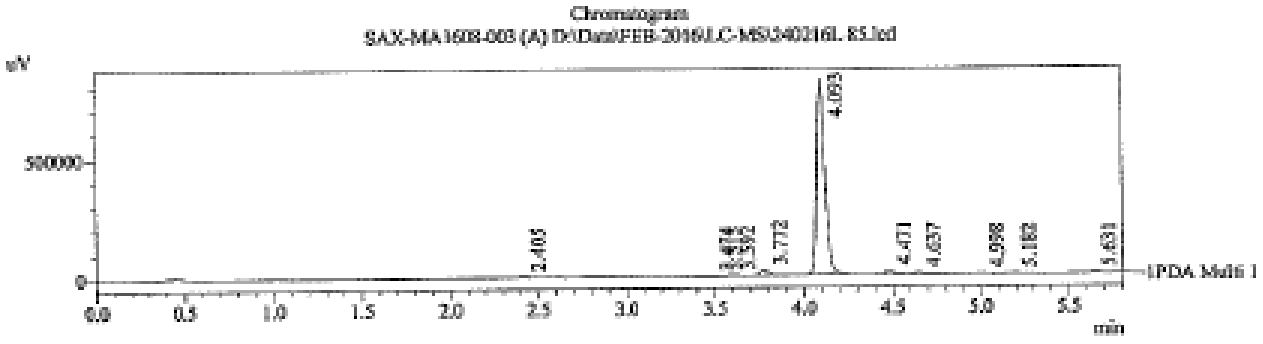


Figure 26: ^{13}C NMR data of 4,6-dichloro-2,8-diisopropyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5b)

Tuning File :D:\Data\Tuning Files\Tuning-ESI-15092014.lct
Vial No :27
Description :Kinetex EVO C-18 (50 X3.0mm,2.6um)
Mobile Phase : A :2.5mM NH4OOCH in water+5%ACN,
B:ACN+ 5% 2.5mM NH4OOCH in Water
T/B% :0.01/5,4/95,5.5/95
Flow : 0.8ml / min(Gradient).



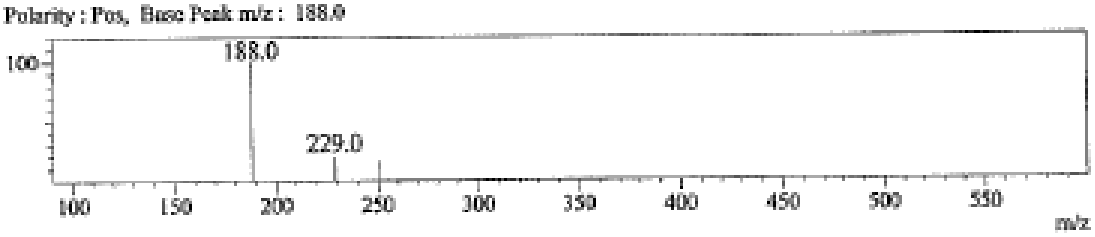
5 b



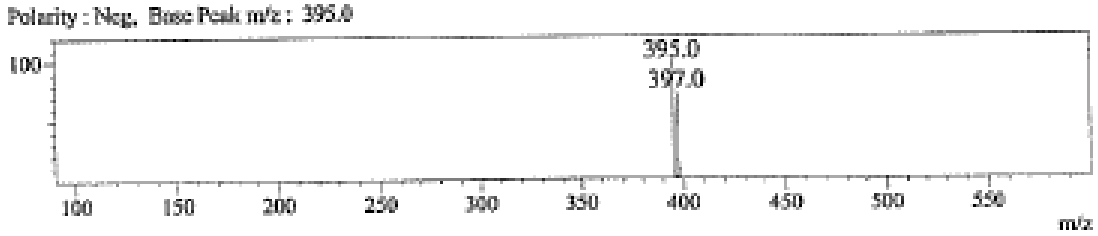
1 PDA Multi 1 / 246nm 4nm

MS Spectrum Graph

Ret. Time:3.767-3.833
Polarity : Pos, Base Peak m/z : 188.0



Ret. Time:4.083-4.150
Polarity : Neg, Base Peak m/z : 395.0



PeakTable

PDA Ch1 246nm 4nm

Peak#	Ret. Time	Area	Area %
1	2.405	14214	0.521
2	3.474	5378	0.197
3	3.515	4192	0.154
4	3.592	11212	0.411
5	3.772	70021	2.568
6	4.093	2528277	92.718
7	4.471	46638	1.710
8	4.637	16009	0.587
9	4.998	3736	0.137
10	5.182	8149	0.299
11	5.631	19014	0.697
Total		2726839	100.000

Figure 27: LCMS of 4,6-dichloro-2,8-diisopropyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5b)

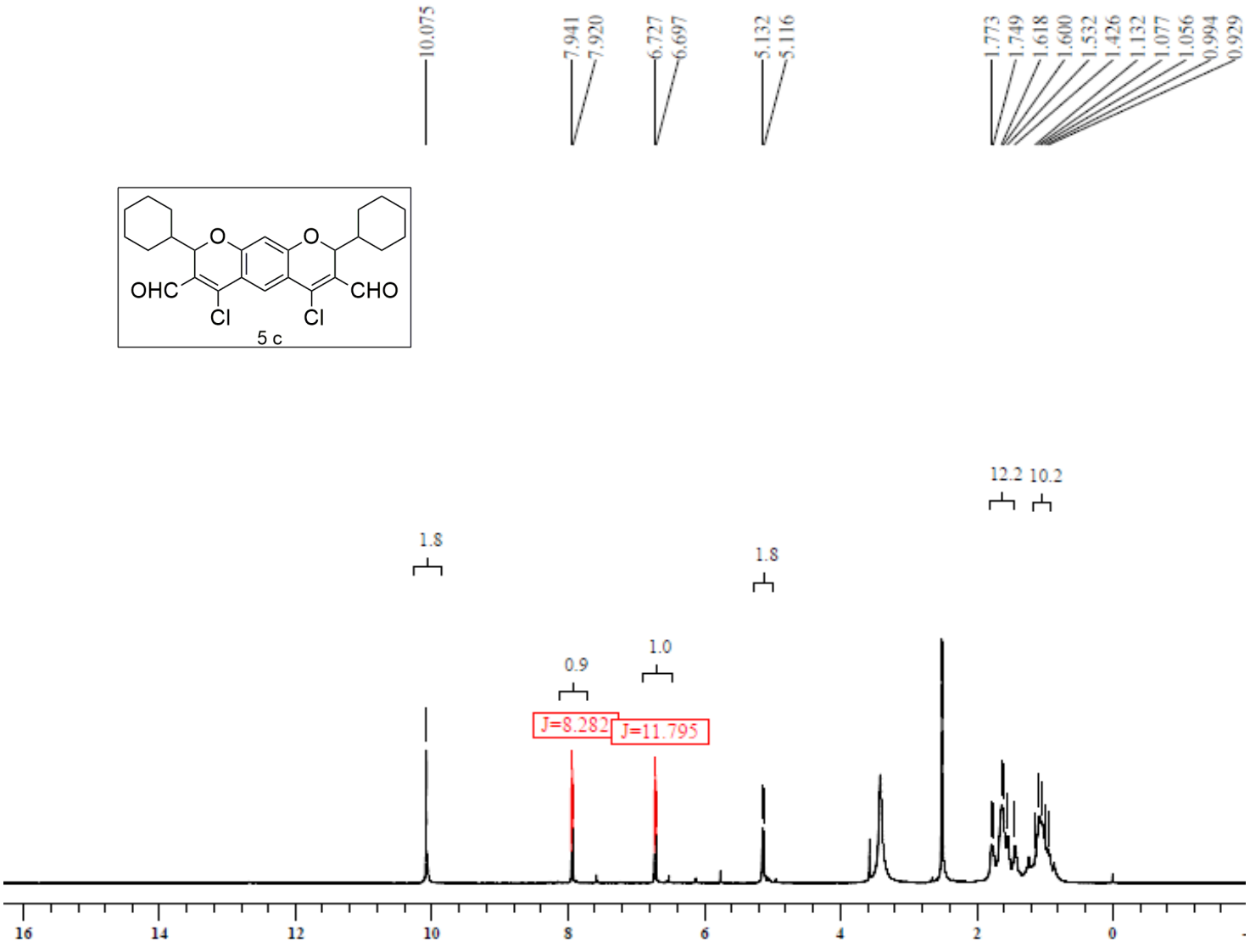


Figure 28: ^{1}H NMR of 4,6-dichloro-2,8-dicyclohexyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5c)

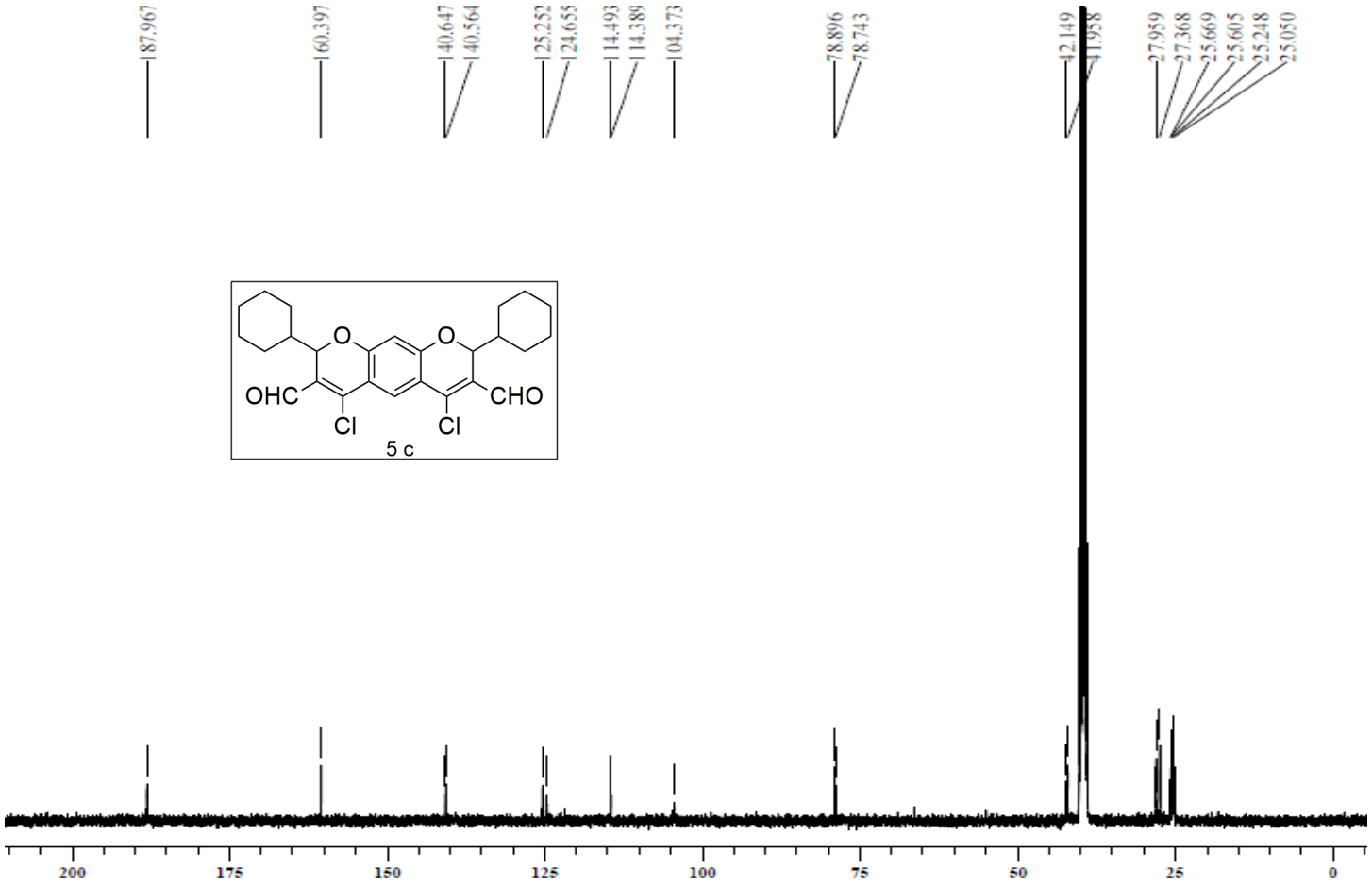


Figure 29: ^{13}CNMR of 4,6-dichloro-2,8-dicyclohexyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5c)

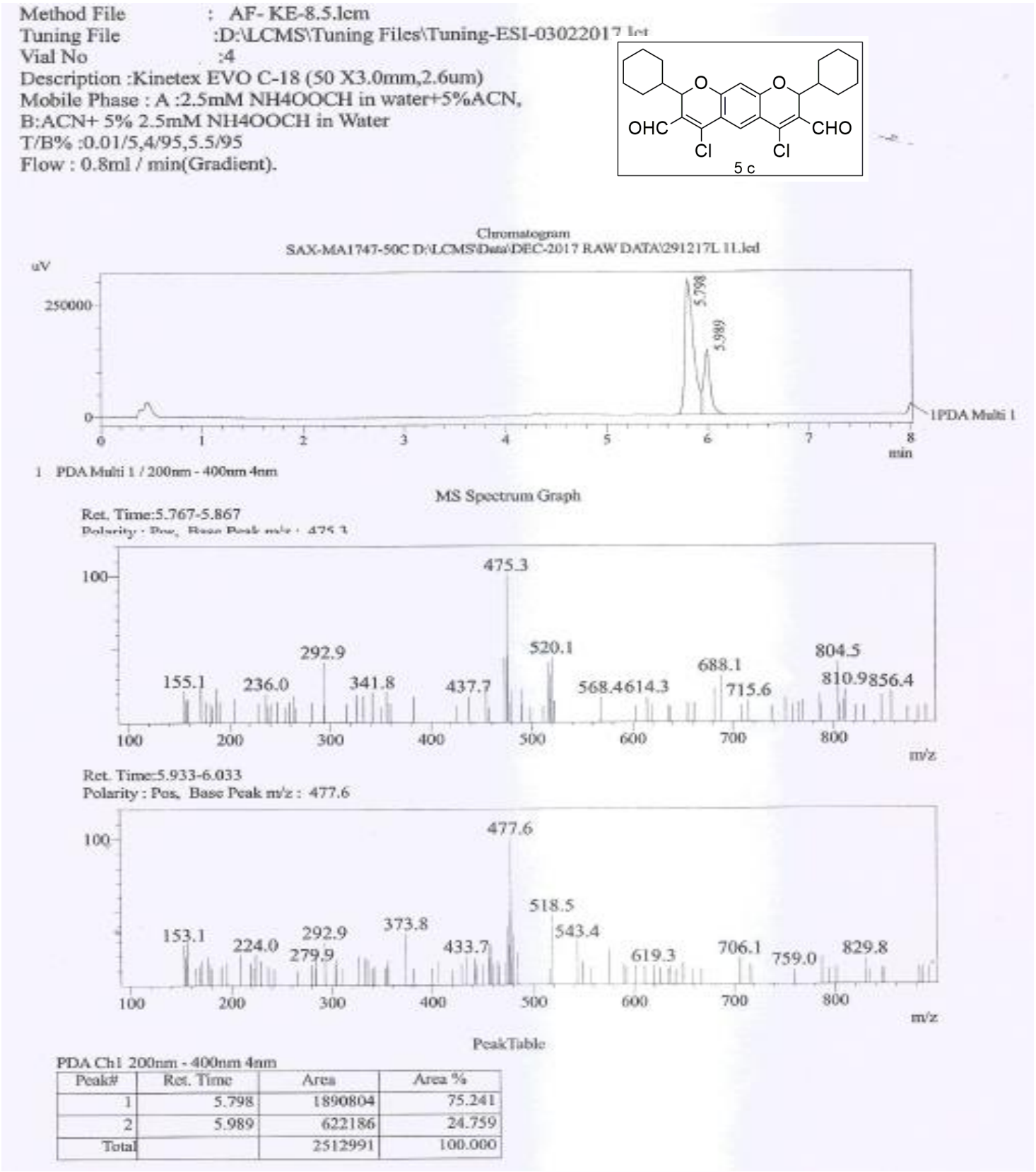


Figure 30: LCMS of 4,6-dichloro-2,8-dicyclohexyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5c)

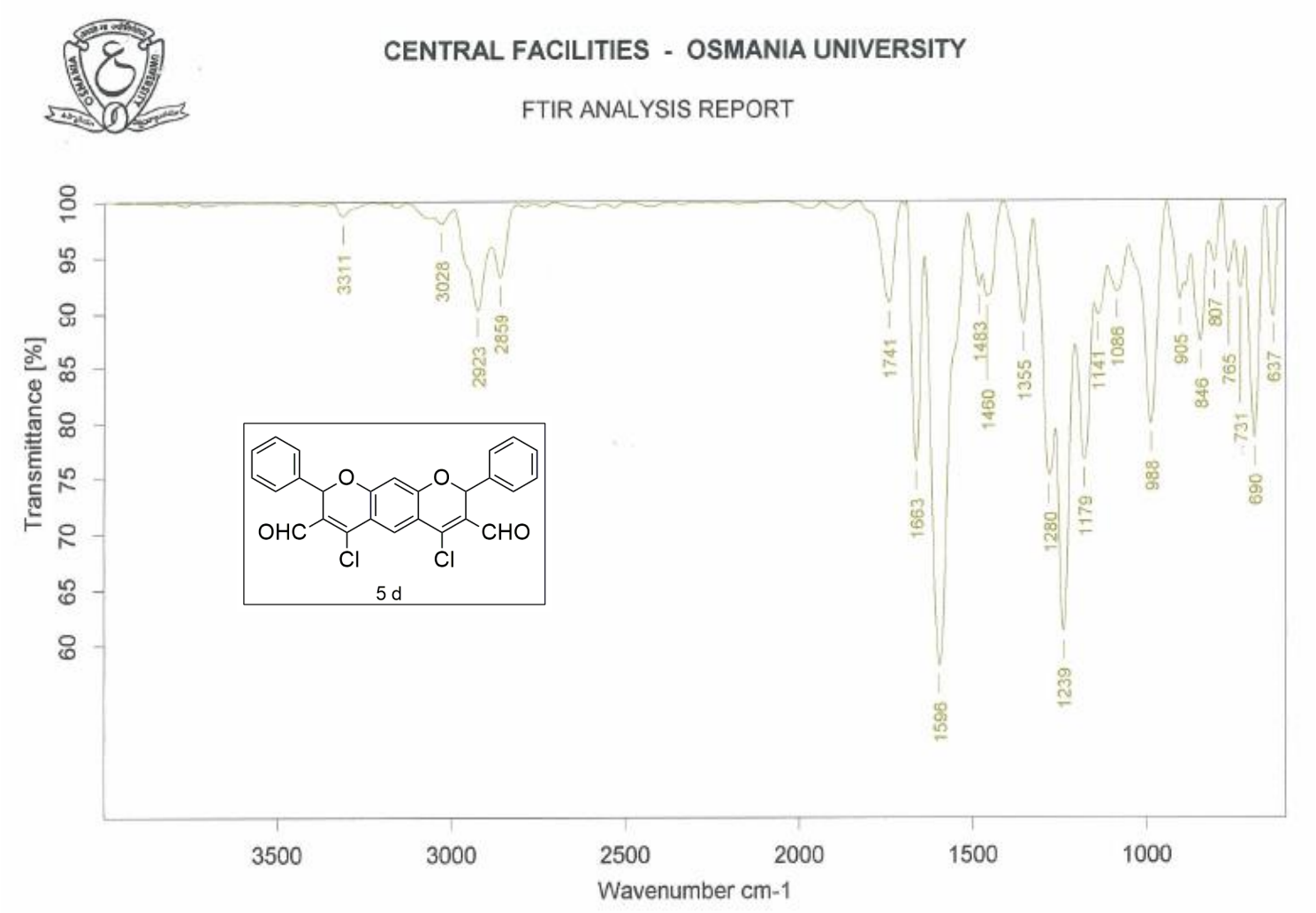


Figure 31: IR data of 4,6-dichloro-2,8-diphenyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5d)

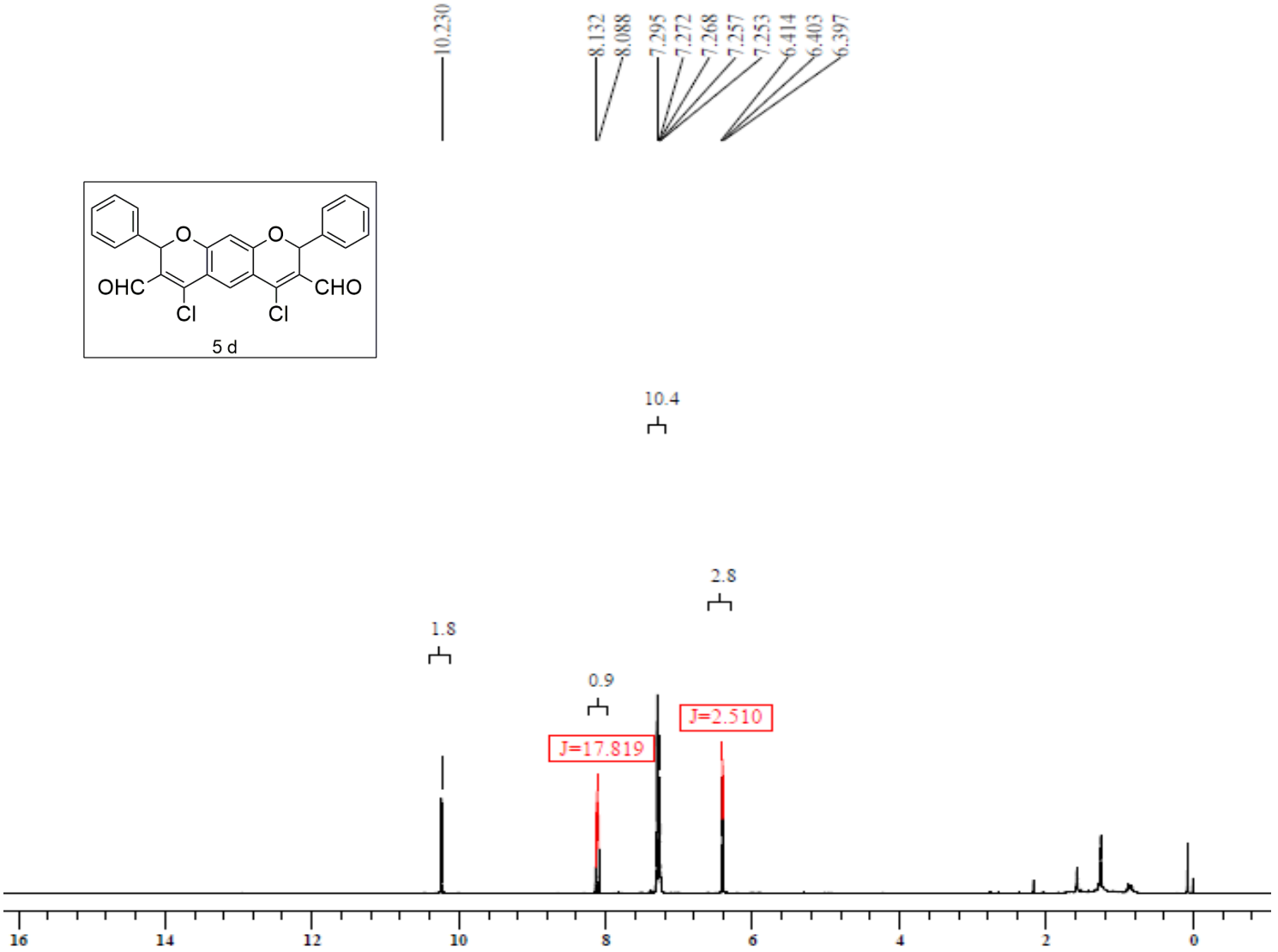


Figure 32: ^{1}H NMR of 4,6-dichloro-2,8-diphenyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde(5d)

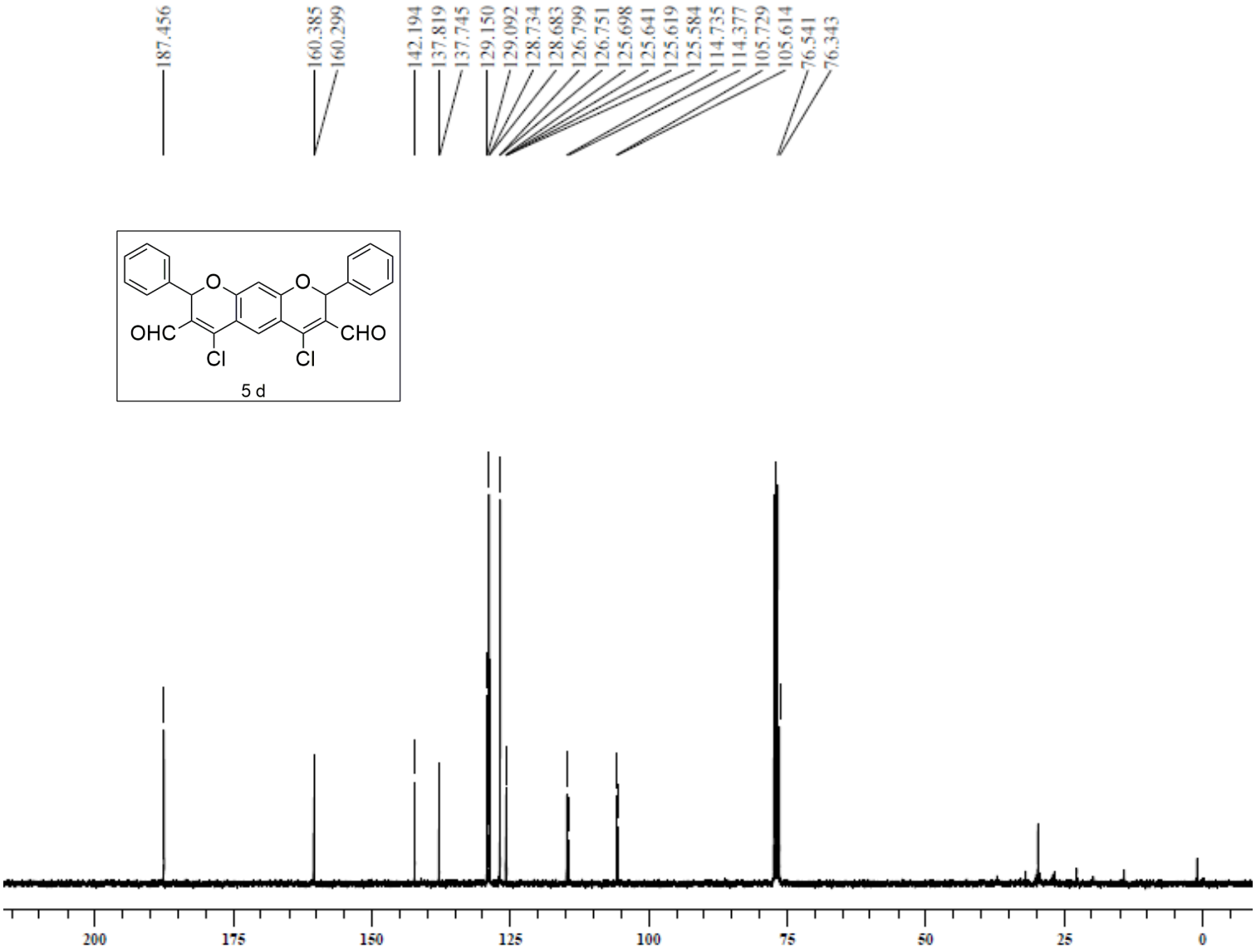


Figure 33: ^{13}C NMR of 4, 6-dichloro-2, 8-diphenyl-2, 8-dihydropyrano [3, 2-g] chromene-3,7-dicarbaldehyde (5d)

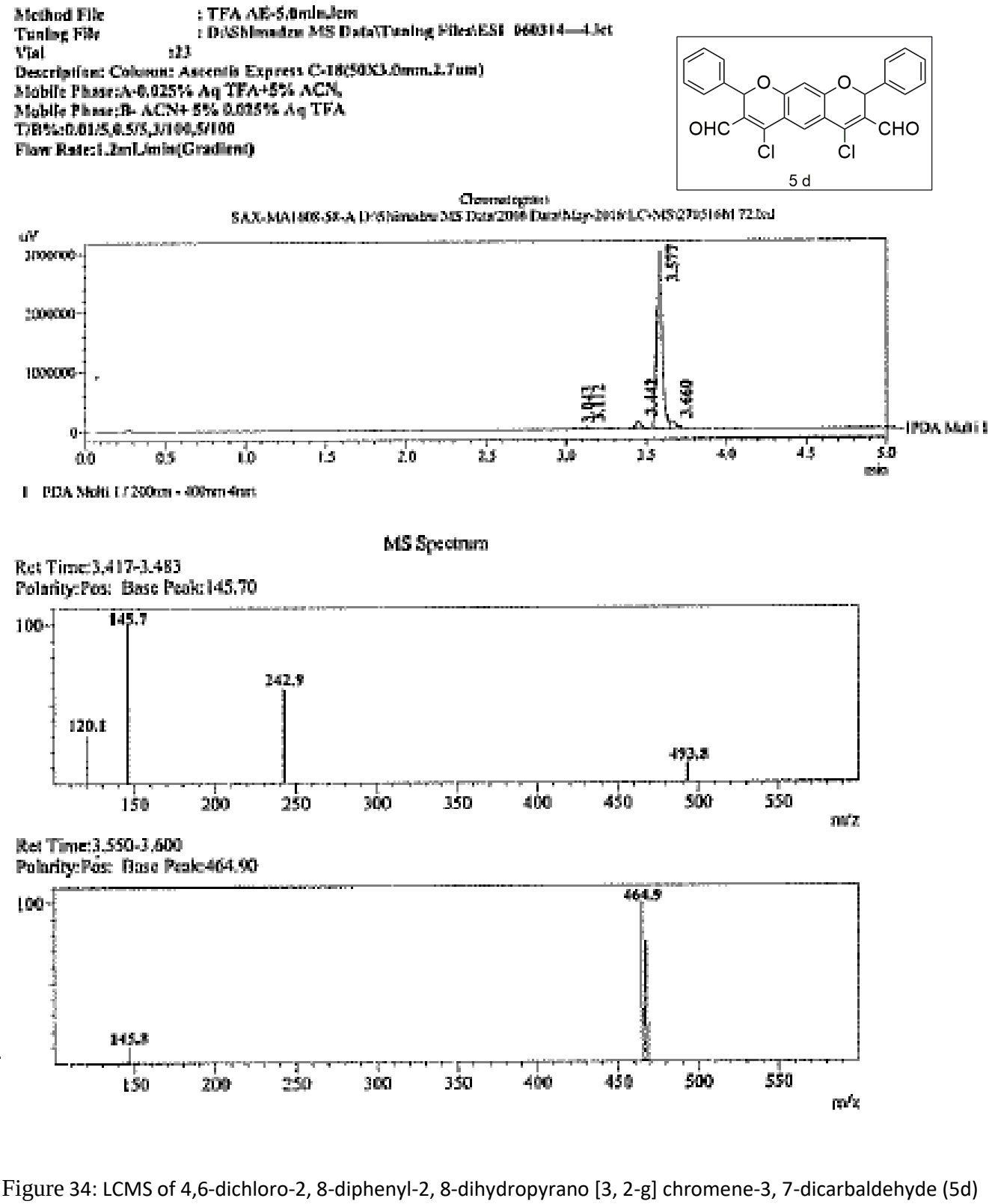


Figure 34: LCMS of 4,6-dichloro-2, 8-diphenyl-2, 8-dihydropyrano [3, 2-g] chromene-3, 7-dicarbaldehyde (5d)

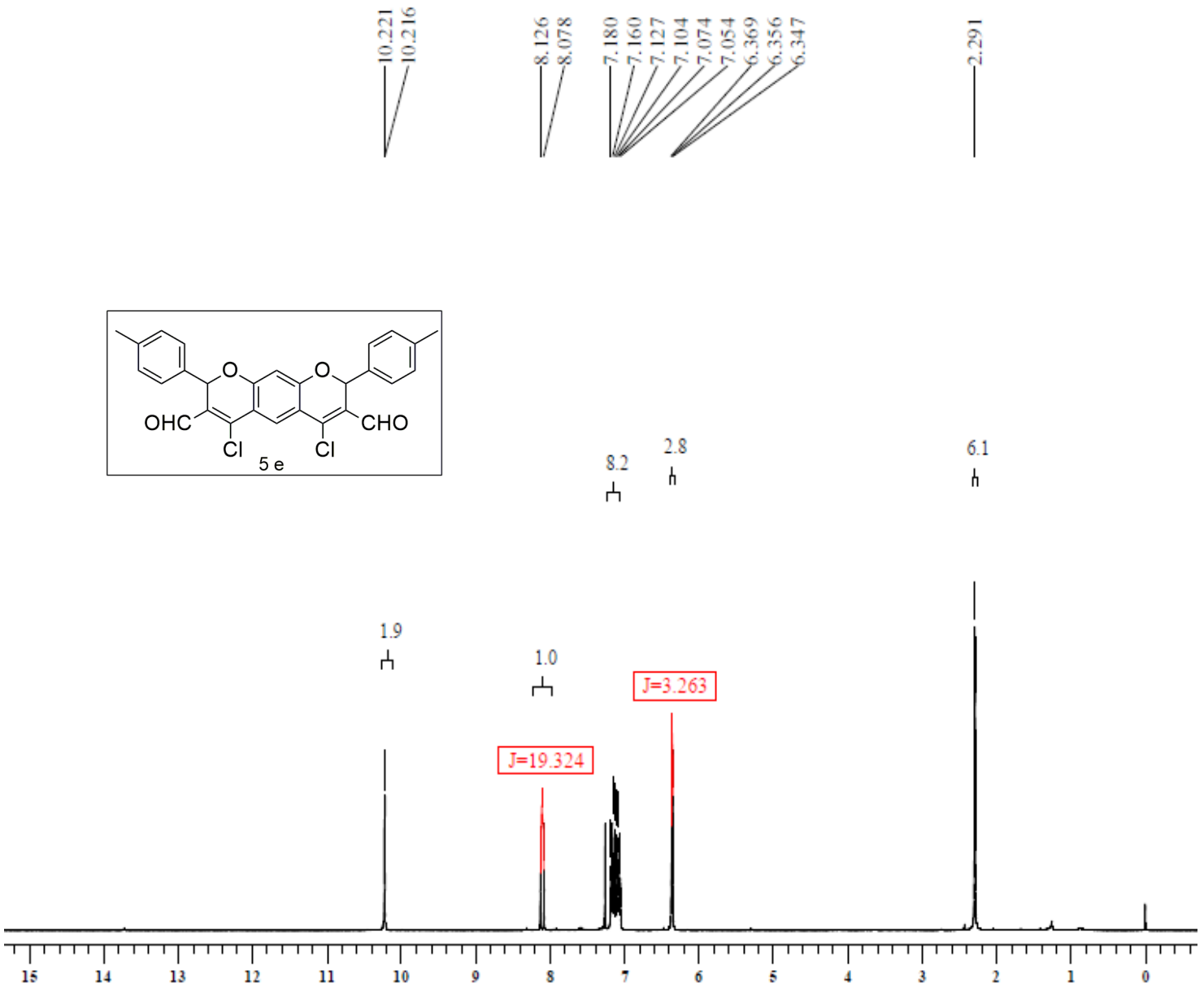


Figure 35: ^{1}H NMR of 4,6-dichloro-2,8-di-p-tolyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde (5e)

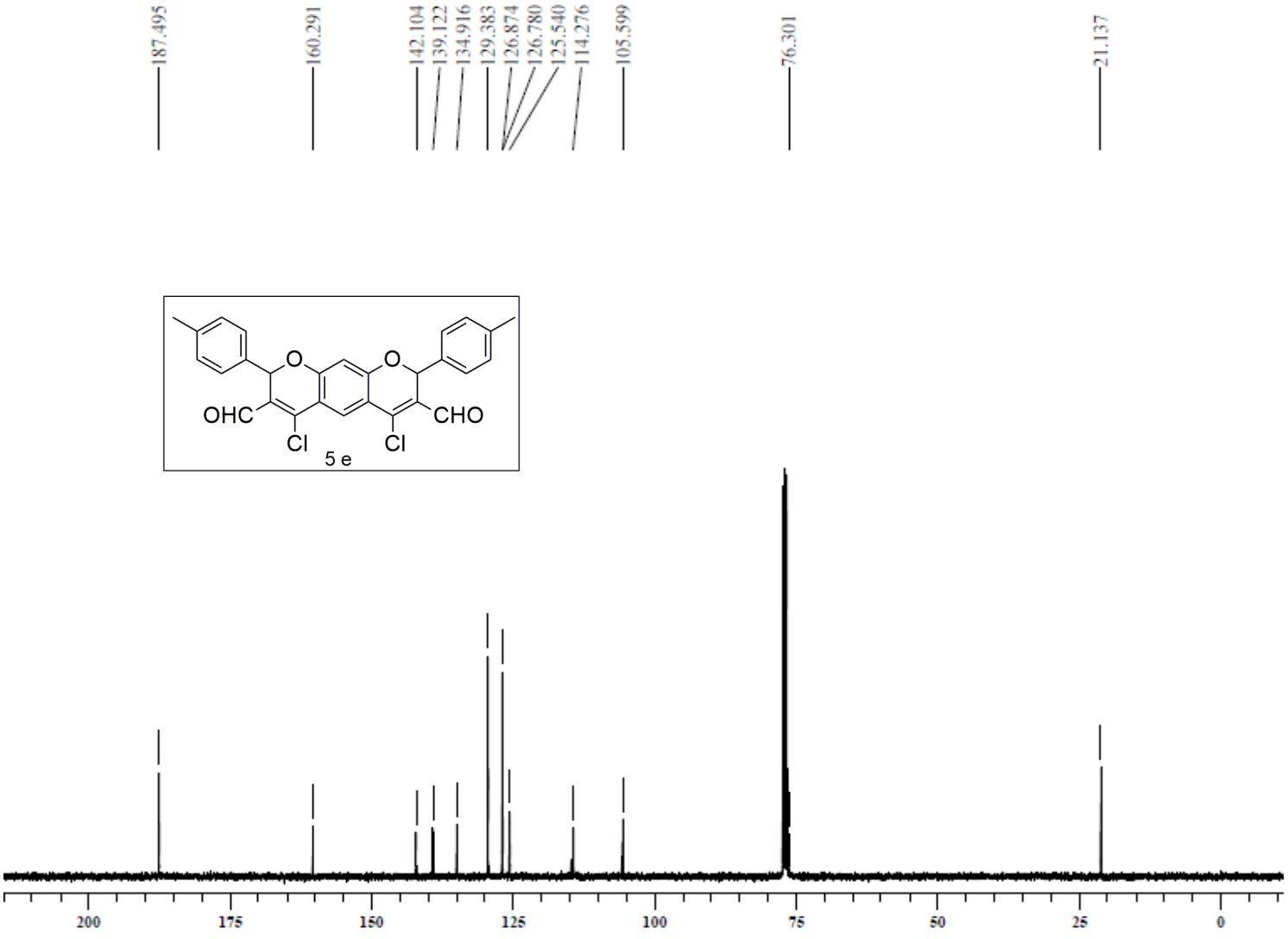
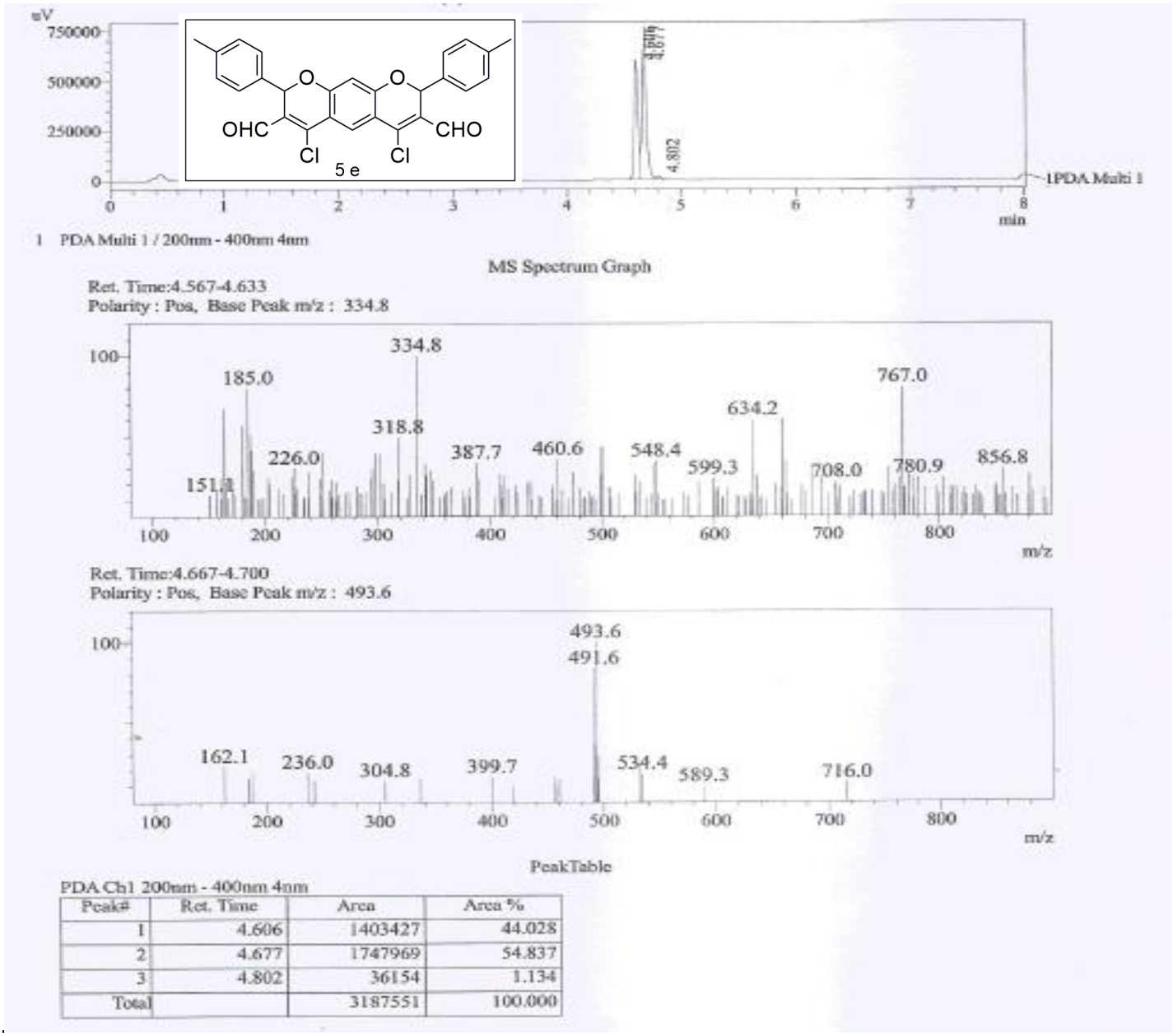


Figure 36: ^{13}C NMR of 4,6-dichloro-2,8-di-p-tolyl-2,8-dihydropyrano[3,2-g]chromene-3,7-dicarbaldehyde(5e)



Peak#	Ret. Time	Area	Area %
1	4.606	1403427	44.028
2	4.677	1747969	54.837
3	4.802	36154	1.134
Total		3187551	100.000

Figure 37: LCMS of 4,6-dichloro-2,8-di-p-tolyl-2,8-dihydropyrano[3,2-g]chromene-3,7dicarbaldehyde (5e)