The synthesis of highly functionalized *bis*(4H-chromene-) and 4H-benzo[*g*]chromenes derivatives *via* an isocyanide based pseudo-five-component reaction

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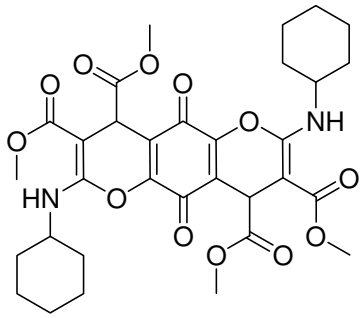
SUPPORTING INFORMATION

Experimental Section

General

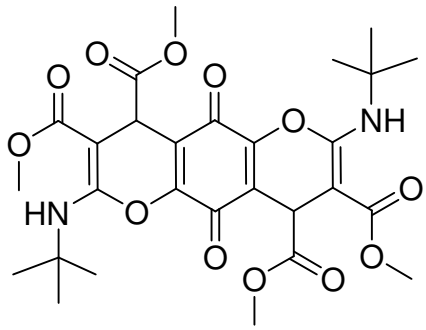
Melting points are uncorrected. Mass spectra were recorded at an ionization potential of 70 eV. ^{1}H and ^{13}C NMR spectra were recorded at 500.13, 300.13 and 125.77, 75.47 MHz. NMR spectra were obtained on solution in $CDCl_3$ using TMS as internal standard. The chemicals used in this work were in synthesis grade and were used without purification.

Tetramethyl 2,7-bis(cyclohexylamino)-5,10-dioxo-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4a):



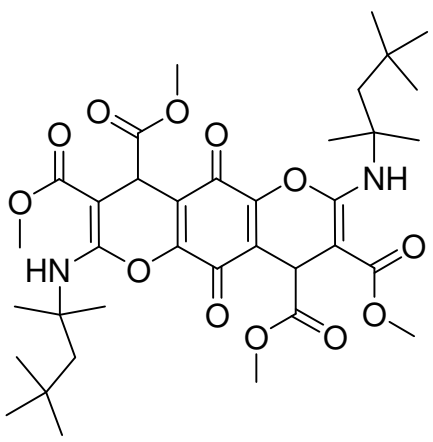
Brownish red powder (0.55 g, yield 86%). mp 257-258 ºC.IR (KBr) (ν_{max}/cm^{-1}): 2933, 2859, 1751, 1673, 1602, 1446. MS, m/z (%): 643 (M^{+}+1, 2), 611 (3), 585 (5), 553 (3), 525 (4), 486 (5), 402 (5), 327 (5), 297 (5), 269 (5), 170 (5), 96 (20), 83 (30), 55 (80), 41 (80), 31 (100). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 1.35-1.96 (20H, m, $10CH_2$ of 2cyclohexyl), 3.66 (6H, s, $2O\text{-}CH_3$), 3.71 (6H, s, $2O\text{-}CH_3$), 3.79 (2H, bs, C*H*-NH), 4.64 (2H, s, 2C*H*-CO_2Me), 8.57 (2H, bs, 2CH-N*H*). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 24.3, 25.4, 33.5, (C-cyclohexyl), 35.2 (*C*H-CO_2Me), 50.3 (CH-NH), 51.2, 52.8 ($2O\text{-}CH_3$), 70.7, 117.7, 147.8, 158.3 (C-alkene), 169.1, 172.2, 176.9 (3C=O). Anal. Calcd for $C_{32}H_{38}N_2O_{12}$: C, 59.81; H, 5.96; N, 4.36; Found: C, 59.76; H, 5.84; N, 4.28.

Tetramethyl 2,7-bis(tert-butylamino)-5,10-dioxo-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4b):



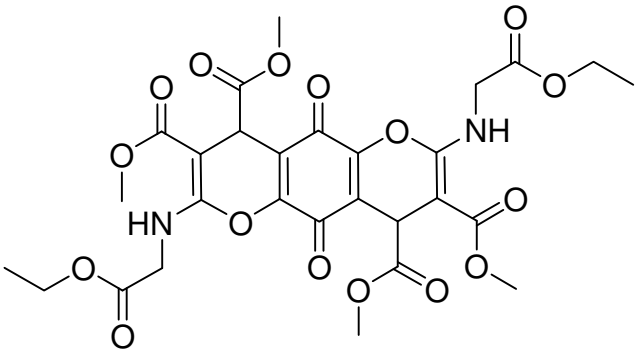
Dark red powder (0.41 g, yield 70%). mp 238-240 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2947, 2839, 1757, 1679, 1604, 1441. MS, m/z (%): 531 (M^+-59, 20), 419 (50), 359(15), 327 (13), 295 (15), 57 (75), 41 (100). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 1.45 (18H, s, 2C$(CH_3)_3$), 3.67 (6H, s, 2O-CH_3), 3.72 (6H, s, 2O-CH_3), 4.68 (2H, s, 2C*H*-CO_2Me), 8.73 (2H, bs, 2N*H*). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 30.2 (C(*C*$H_3)_3$) 35.0 (*C*H-CO_2Me), 51.3 (C-NH), 52.8, 53.5 (2O-CH_3), 71.4, 117.5, 147.8, 159.6 (C-alkene), 169.1, 172.1, 177.0 (3C=O). Anal. Calcd for $C_{28}H_{34}N_2O_{12}$: C, 56.94; H, 5.80; N, 4.74; Found: C, 56.86; H, 5.74; N, 4.82.

Tetramethyl 5,10-dioxo-2,7-bis(2,4,4-trimethylpentan-2-ylamino)-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4c):



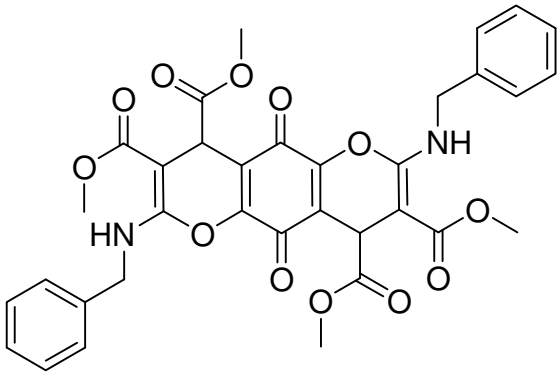
Brownish red powder (0.51 g, yield 73%). mp 211-213 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2952, 2843, 1750, 1672, 1591, 1437. MS, m/z (%): 704 (M^++2, 3), 645 (50), 533 (30), 419 (80), 389 (23), 361 (25), 327 (15), 297 (13), 250 (73), 218 (30), 142 (25), 57 (75), 31 (100) . ^{1}H NMR (500 MHz, $CDCl_3$): δ_H (ppm) 0.96 (18H, s, 2C$(CH_3)_3$), 1.49 (12H, s, 4CH_3), 1.82 (4H, s, 2CH_2), 3.64 (6H, s, 2O-CH_3), 3.71 (6H, s, 2O-CH_3), 4.69 (2H, s, 2C*H*-CO_2Me), 8.75 (2H, bs, 2NH). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C (ppm) 31.3, 31.7 (2CH_3), 31. 8 (C(*C*$H_3)_3$), 32.0 (CH_2), 35.4 (*C*H-CO_2Me), 51.6 (*C*$(CH_3)_3$), 53.1, 53.3 (2O-CH_3), 57.5 (C-NH), 71. 8, 118.2, 148.3, 160.1 (C-alkene), 169.6, 172.4, 177.4 (3C=O). Anal. Calcd for $C_{36}H_{50}N_2O_{12}$: C, 61.52; H, 7.17; N, 3.99; Found: C, 61.46; H, 7.23; N, 3.84.

Tetramethyl 2,7-bis(2-ethoxy-2-oxoethylamino)-5,10-dioxo-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4d):



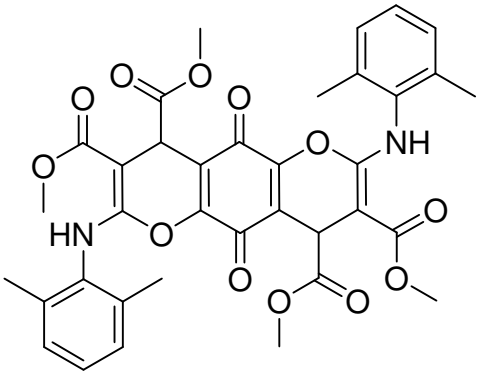
Brownish red powder (0.40 g, yield 62%). mp 240-241 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2952, 1750, 1678, 1605, 1452. MS, m/z (%): 619 (M^+-31, 15), 593 (100), 561 (80), 532 (30), 490 (20), 415 (21), 387 (25), 341 (25), 267 (45), 193 (70), 142 (100), 59 (15), 31 (75). ^{1}H NMR (500 MHz, $CDCl_3$): δ_H (ppm) 1.29 (6H, t, $^3J_{HH}$=6.9 Hz, 2OCH$_2$C*H$_3$*), 3.66 (6H, s, 2O-CH$_3$), 3.76 (6H, s, 2O-CH$_3$), 4.13-4.27 (8H, m, 2NH-C*H$_2$*, 2OC*H$_2$*CH$_3$), 4.68 (2H, s, 2C*H*-CO$_2$Me), 8.78 (2H, bs, 2NH). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C (ppm) 14.6 (OCH$_2$*C*H$_3$), 35.7 (*C*H-CO$_2$Me), 43.4 (NH-CH$_2$), 51.9, 53.2 (2O-CH$_3$), 62.2 (O*C*H$_2$CH$_3$), 73.9, 118.3, 148.0, 158.8 (C-alkene), 169.0, 169.6, 171.9, 176.9 (4C=O). Anal. Calcd for $C_{36}H_{50}N_2O_{12}$: C, 61.52; H, 7.17; N, 3.99; Found: C, 61.48; H, 7.20; N, 3.86.

Tetramethyl 2,7-bis(benzylamino)-5,10-dioxo-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4e):



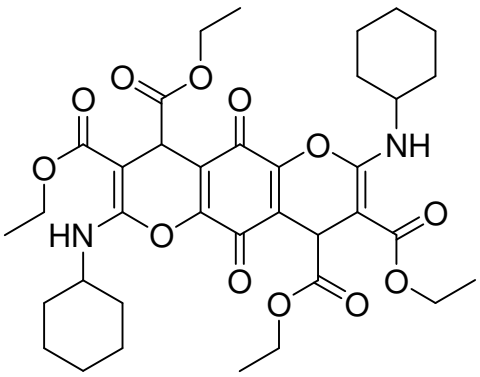
Dark red powder (0.55 g, yield 83%). mp 215-217 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2952, 2921, 1746, 1683, 1600. MS, m/z (%): 627 (M^+-31, 3), 601 (5), 569 (5), 511 (2), 494 (5), 451 (5), 197 (20), 165 (3), 133 (5), 91 (100), 65 (5), 31 (30). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 3.72 (6H, s, 2O-CH$_3$), 3.74 (6H, s, 2O-CH$_3$), 4.52-4.67 (4H, m, 2C*H$_2$*NH), 4.70 (2H, s, 2C*H*-CO$_2$Me), 7.28-7.35 (10H, m, arom), 8.92 (2H, bs, 2CH$_2$-N*H*). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 35.2 (*C*H-CO$_2$Me), 45.2 (CH$_2$NH), 51.4, 53.0 (2O-CH$_3$), 72.1, 117.4, 127.7, 127.8, 128.8, 137.7, 147.6, 158.6 (C-alkene, arom), 168.9, 171.7, 176.6 (3C=O). Anal. Calcd for $C_{34}H_{30}N_2O_{12}$: C, 62.00; H, 4.59; N, 4.25; Found: C, 62.09; H, 4.62; N, 4.19.

Tetramethyl 2,7-bis(2,6-dimethylphenylamino)-5,10-dioxo-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4f):



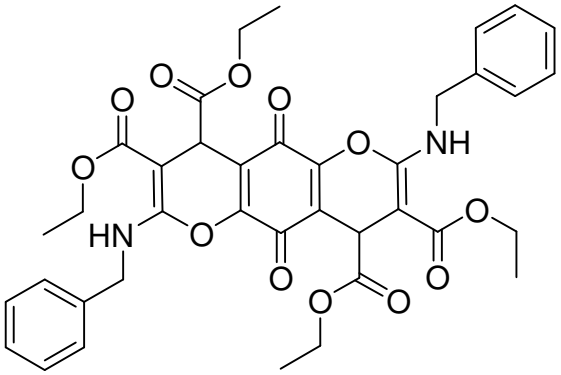
Brownish red powder (0.48 g, yield 70%). mp 264-266 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2931, 2855, 1697, 1643, 1530, 1451. MS, m/z (%): 627 (M$^+$-59, 50), 597 (20), 568 (10), 427 (40), 284 (20), 274 (10), 168 (20), 144 (20), 105 (90), 79 (100), 59 (50). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 2.19 (12H, s, 4CH_3), 3.67 (6H, s, 2O-CH_3), 3.78 (6H, s, 2O-CH_3), 4.66 (2H, s, 2C*H*-CO_2Me), 7.13 (6H, m, arom), 9.91 (2H, bs, NH). Anal. Calcd for $C_{36}H_{34}N_2O_{12}$: C, 62.97; H, 4.99; N, 4.08; Found: C, 62.88; H, 4.94; N, 4.12.

Tetraethyl 2,7-bis(cyclohexylamino)-5,10-dioxo-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4g):



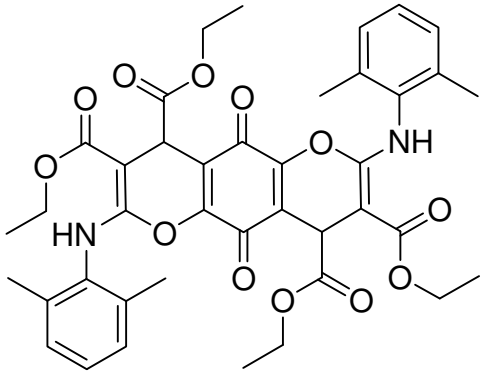
Brownish red powder (0.57 g, 82%). mp 236-238 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2931, 2854, 1726, 1676, 1602, 1435. MS, m/z (%): 653 (M$^+$-45, 3), 627 (5), 552 (5), 471 (5), 430 (3), 341 (5), 297 (5), 269 (5), 120 (5), 83 (30), 55 (100), 41 (80). ^{1}H NMR (500 MHz, $CDCl_3$): δ_H (ppm) 1.23-1.99 (32H, m, 10CH_2 of 2cyclohexyl, 4OCH_2C*H*$_3$), 3.81 (2H, bs, 2C*H*-NH), 4.12-4.18 (8H, m, 4OC*H*$_2$CH$_3$), 4.65 (2H, s, 2C*H*-CO_2Me), 8.55 (2H, bs, 2CH-N*H*). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C (ppm) 14.5, 14.8, (2CH_3), 24.8, 25.8, 34.0 (C-cyclohexyl), 35.9 (*C*H-CO_2Et), 50.8 (CH-NH), 60.2, 61.9 (2O*C*H$_2$CH$_3$), 71.5, 118.2, 148.3, 158.8 (C-alkene), 169.2, 171.4, 177.6 (3C=O). Anal. Calcd for $C_{36}H_{46}N_2O_{12}$: C, 61.88; H, 6.64; N, 4.01; Found: C, 61.93; H, 6.70; N, 4.10.

Tetraethyl 2,7-bis(benzylamino)-5,10-dioxo-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4h):



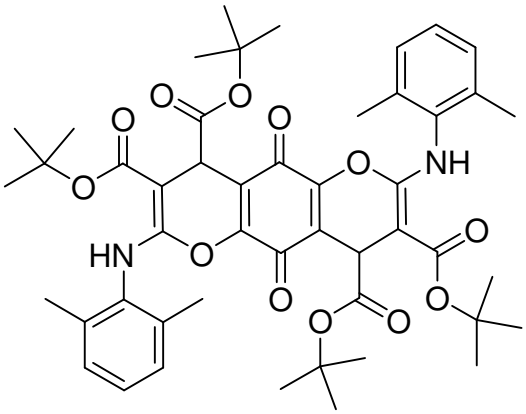
Dark red powder (0.54 g, 75%). mp 211-212 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2964, 1742, 1701, 1645, 1602. MS, m/z (%): 669 (M^+-45, 3), 643 (5), 536 (5), 505 (5), 479 (5), 194 (5), 152 (5), 133 (6), 91 (100), 58 (5), 45 (20), 31 (5). ^{1}H NMR (500 MHz, $CDCl_3$): δ_H (ppm) 1.25-1.27 (12H, m, 4OCH$_2$C*H$_3$*), 4.14 (8H, m, 4OC*H$_2$*CH$_3$), 4.60 (4H, bs, 2C*H$_2$*NH), 4.66 (2H, s, 2C*H*-CO$_2$Et), 7.35 (10H, m, arom), 8.95 (2H, bs, 2NH).. ^{13}C NMR (125 MHz, $CDCl_3$): δ_C (ppm) 14.1, 14.4 (2CH$_3$), 35.6 (*C*H-CO$_2$Et), 45.2 (CH$_2$NH), 60.0, 61.6 (2O*C*H$_2$CH$_3$), 72.2, 117.8, 127.6, 127.7, 128.7, 137.8, 147.6, 158.5 (C-alkene, arom), 168.6, 171.8, 175.7 (3C=O). Anal. Calcd for $C_{38}H_{38}N_2O_{12}$: C, 63.86; H, 5.36; N, 3.92; Found: C, 63.91; H, 5.42; N, 3.86.

Tetraethyl 2,7-bis(2,6-dimethylphenylamino)-5,10-dioxo-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4i)

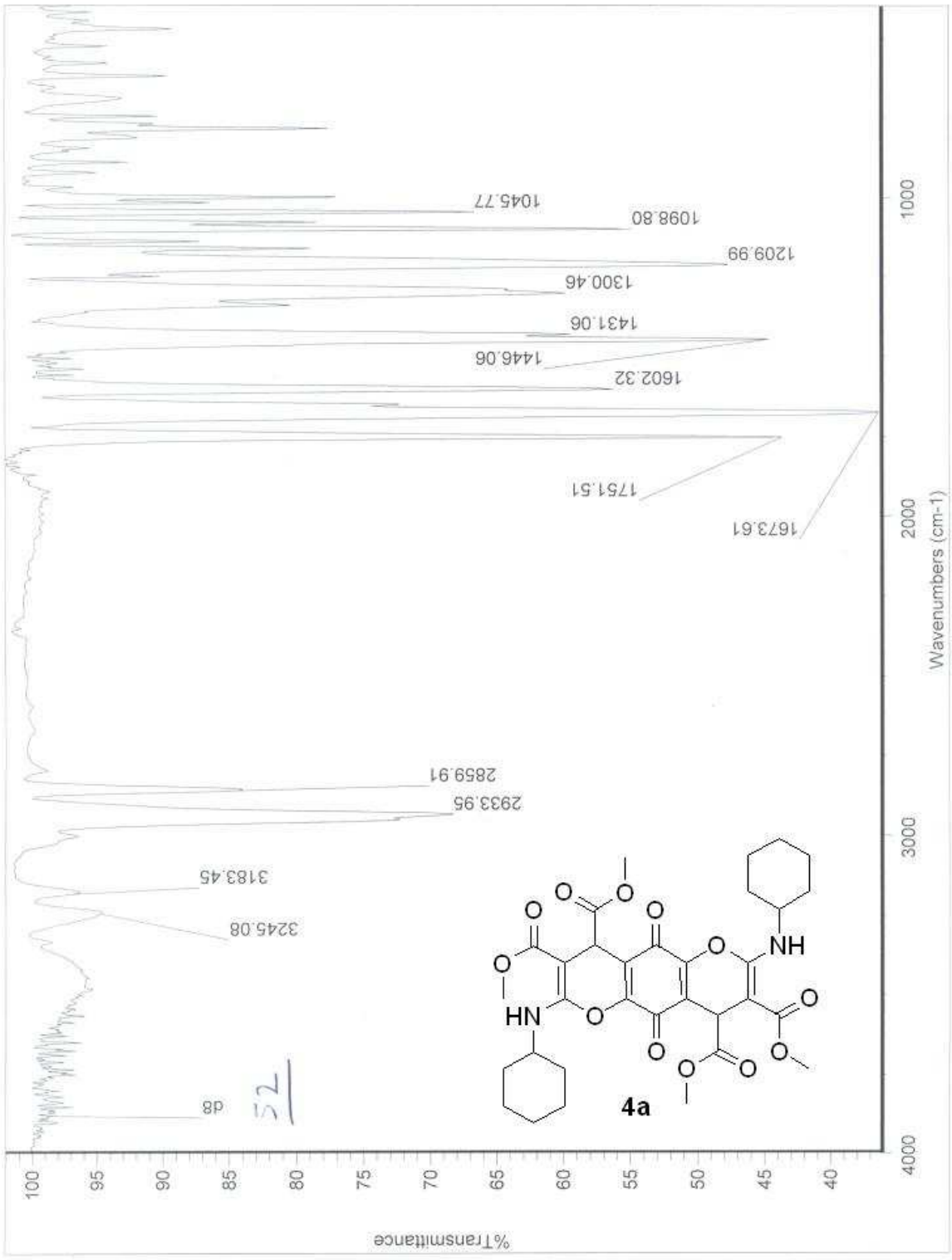


Dark red powder (0.48 g, 65%). mp 245-248 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2972, 1731, 1678, 1642, 1584. MS, m/z (%): 697 (M^+-45, 5), 669 (10), 625 (11), 597 (8), 452 (10), 299 (5), 196 (4), 156 (28), 105 (50), 79 (50), 31 (100). ^{1}H NMR (500 MHz, $CDCl_3$): δ_H (ppm) 1.20 (6H, t, $^3J_{HH}$=6.9 Hz, 2OCH$_2$C*H$_3$*), 1.30 (6H, t, $^3J_{HH}$=6.9 Hz, 2OCH$_2$C*H$_3$*), 2.22 (12H, s, 4CH$_3$), 4.10 (4H, m, 2OC*H$_2$*CH$_3$), 4.21 (4H, m, 2OC*H$_2$*CH$_3$), 4.65 (2H, s, 2C*H*-CO$_2$Et), 7.09 (6H, m, arom), 9.81 (2H, bs, 2NH).. ^{13}C NMR (125 MHz, $CDCl_3$): δ_C (ppm) 14.4, 14.7, 18.8 (3CH$_3$), 35.9 (*C*H-CO$_2$Et), 60.7, 62.0 (2O*C*H$_2$CH$_3$), 73.5, 118.2, 127.7, 128.6, 128.7, 133.9, 149.1, 158.2 (C-alkene, arom), 169.8, 171.9, 176.8 (3C=O). Anal. Calcd for $C_{40}H_{42}N_2O_{12}$: C, 64.68; H, 5.70; N, 3.77; Found: C, 64.72; H, 5.80; N, 3.73.

Tetra-tert-butyl 2,7-bis(2,6-dimethylphenylamino)-5,10-dioxo-4,5,9,10-tetrahydropyrano[2,3-g]chromene-3,4,8,9-tetracarboxylate (4j):



Dark red powder (0.60 g, 70%). mp 225-227 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2978, 2926, 1740, 1668, 1614. MS, m/z (%):709 (M^+-146, 3), 653 (5), 496 (10), 455 (3), 372 (5), 287 (5), 271 (5), 213 (10), 57 (60), 41 (100). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 1.20 (6H, t, $^3J_{HH}$=6.9 Hz, 2OCH$_2$C*H$_3$*), 1.39 (18H, s, 2OC(C*H$_3$*)$_3$), 1.53 (18H, s, 2OC(C*H$_3$*)$_3$), 2.19 (12H, s, 4CH$_3$), 4.70 (2H, s, 2C*H*-CO$_2$^{t}Bu), 7.10 (6H, m, arom), 9.85 (2H, bs, 2NH).. ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 18.4 (CH$_3$), 27.7, 28.5 (2OC(*C*H$_3$)$_3$), 36.6 (*C*H-CO$_2$Et), 73.0(C-alkene), 80.6, 81.6 (2O*C*(CH$_3$)$_3$), 109.2, 118.0, 127.1, 128.1, 134.4, 135.2, 147.7, 158.9 (C-alkene, arom), 168.5, 169.8, 173.3 (3C=O). Anal. Calcd for $C_{48}H_{58}N_2O_{12}$: C, 67.43; H, 6.84; N, 3.28; Found: C, 67.49; H, 6.79; N, 3.31.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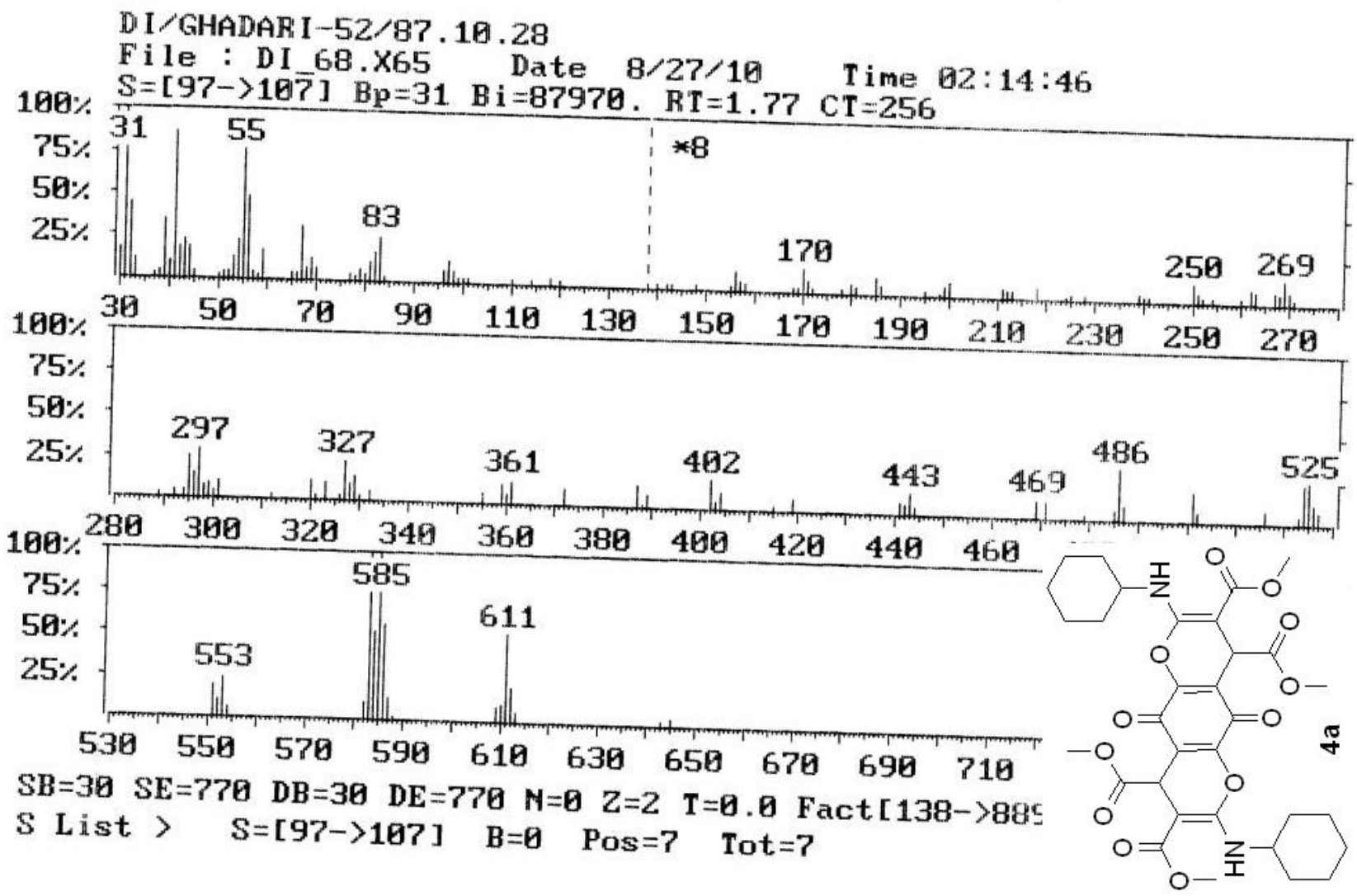
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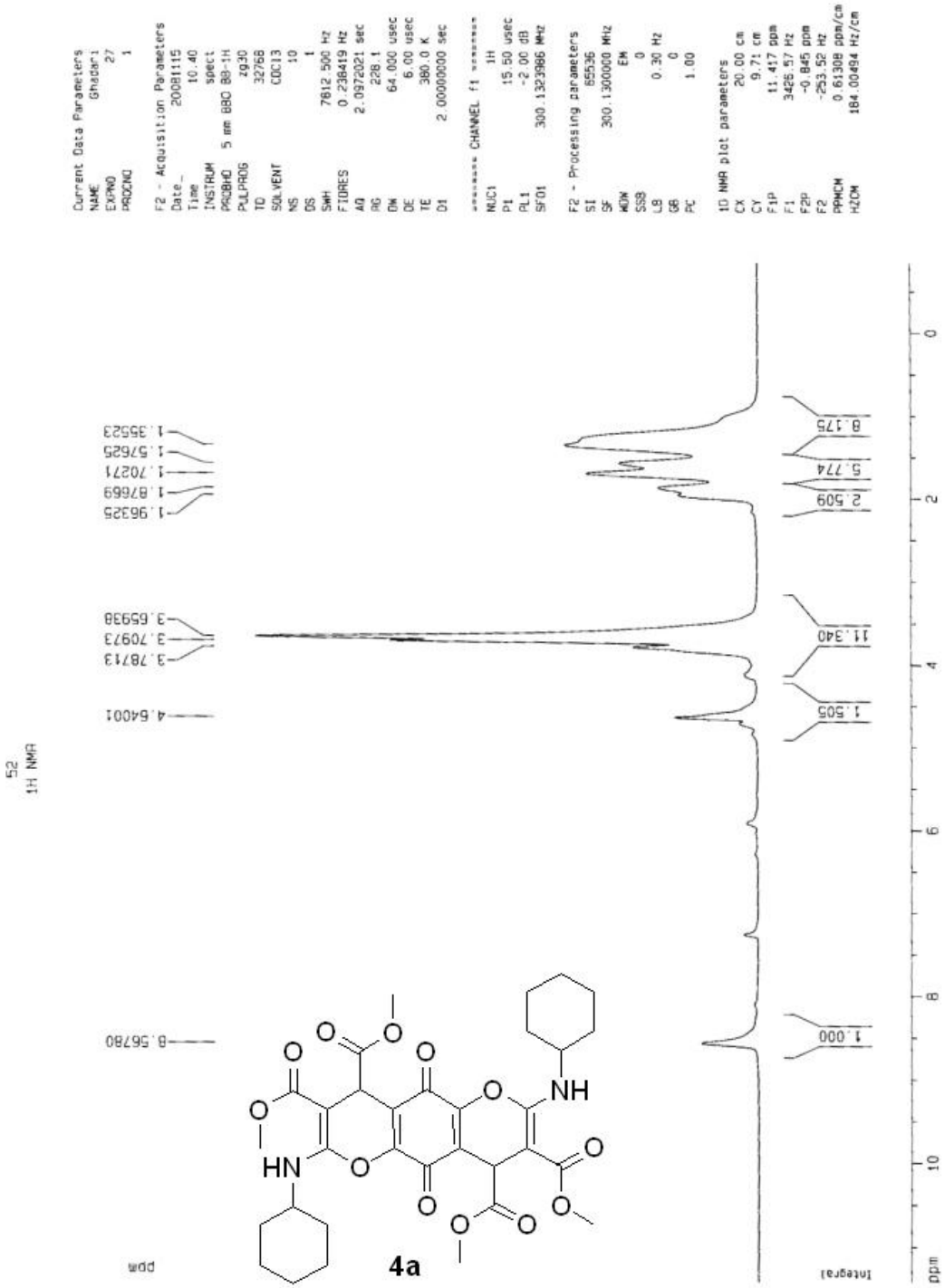
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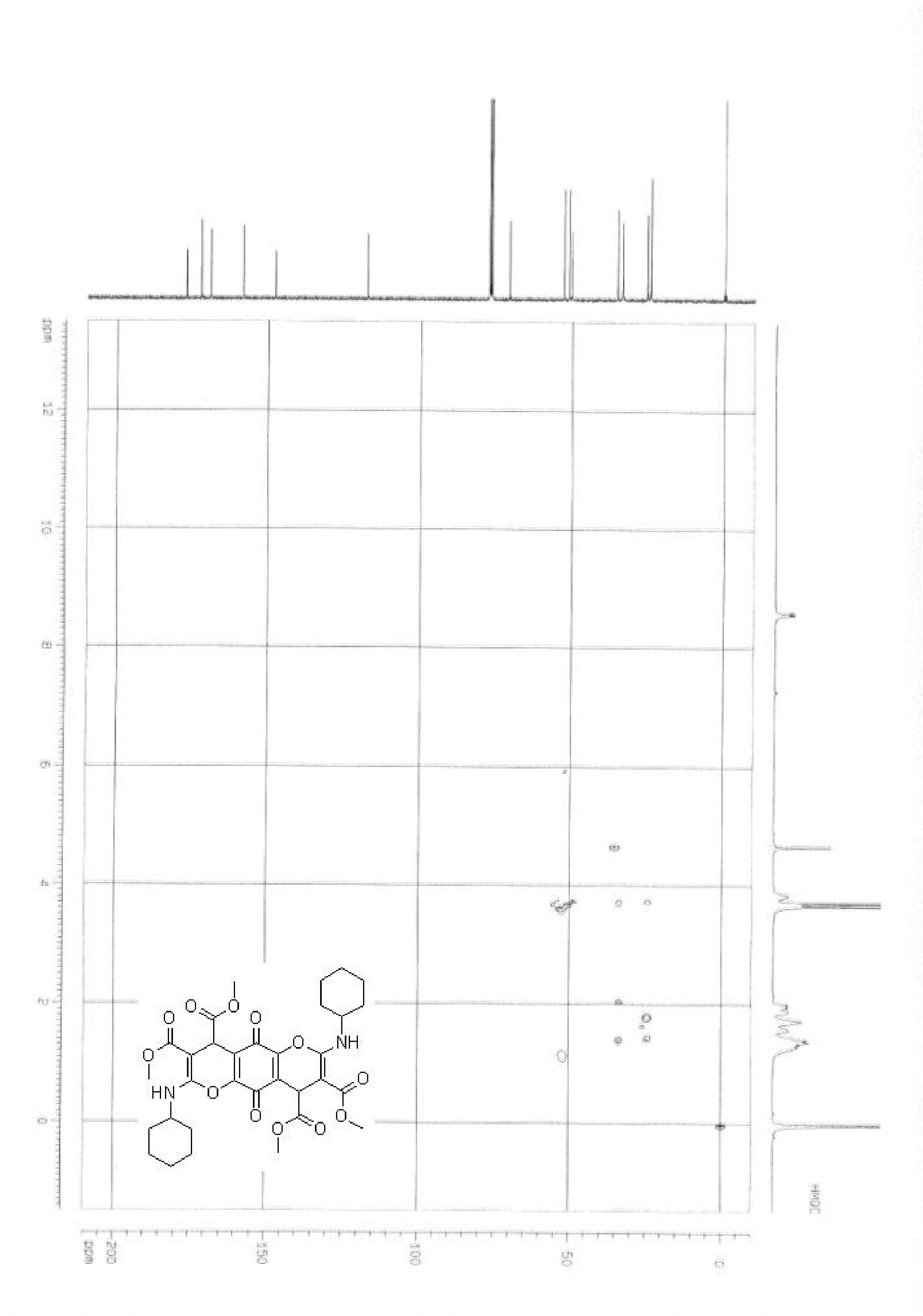
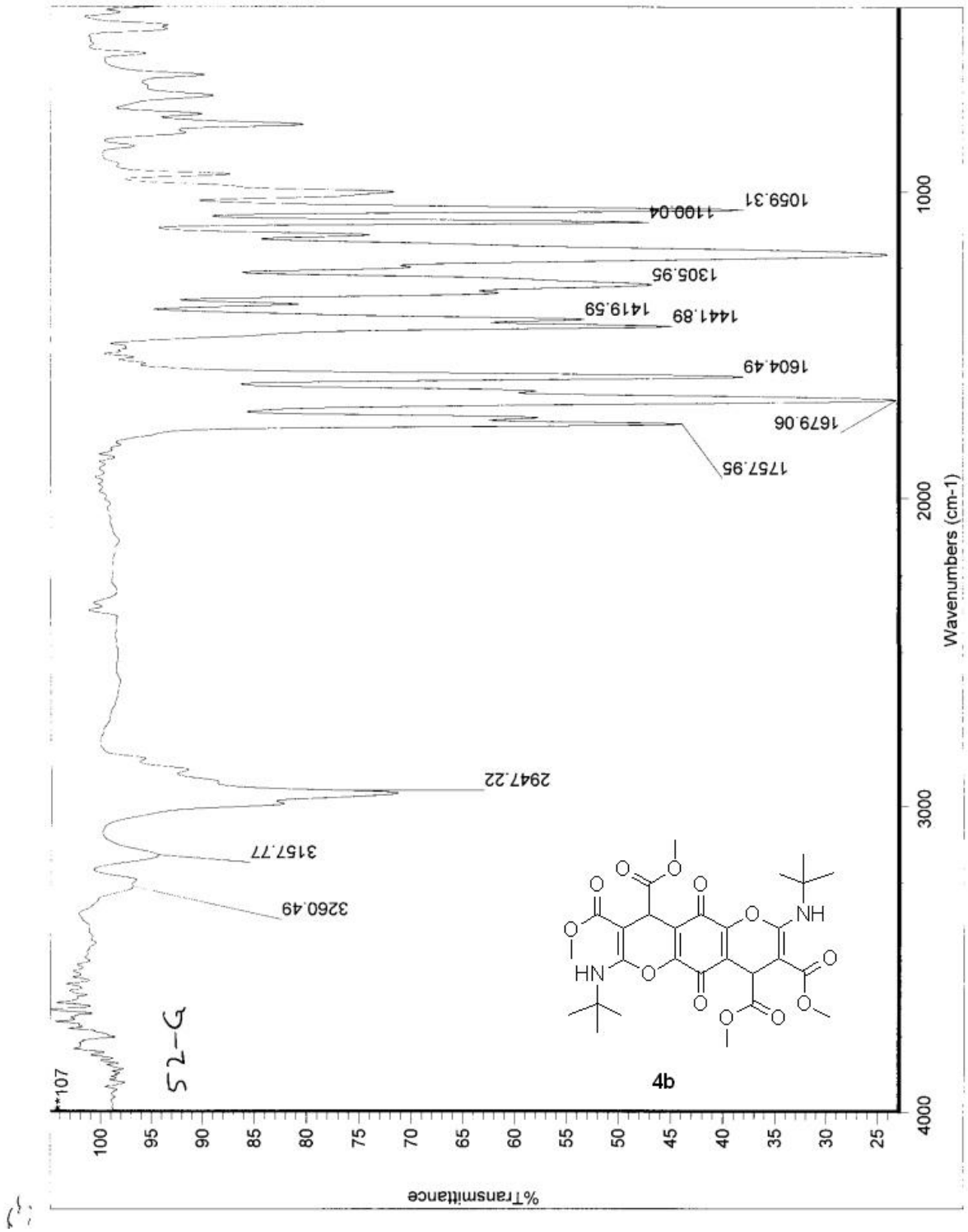
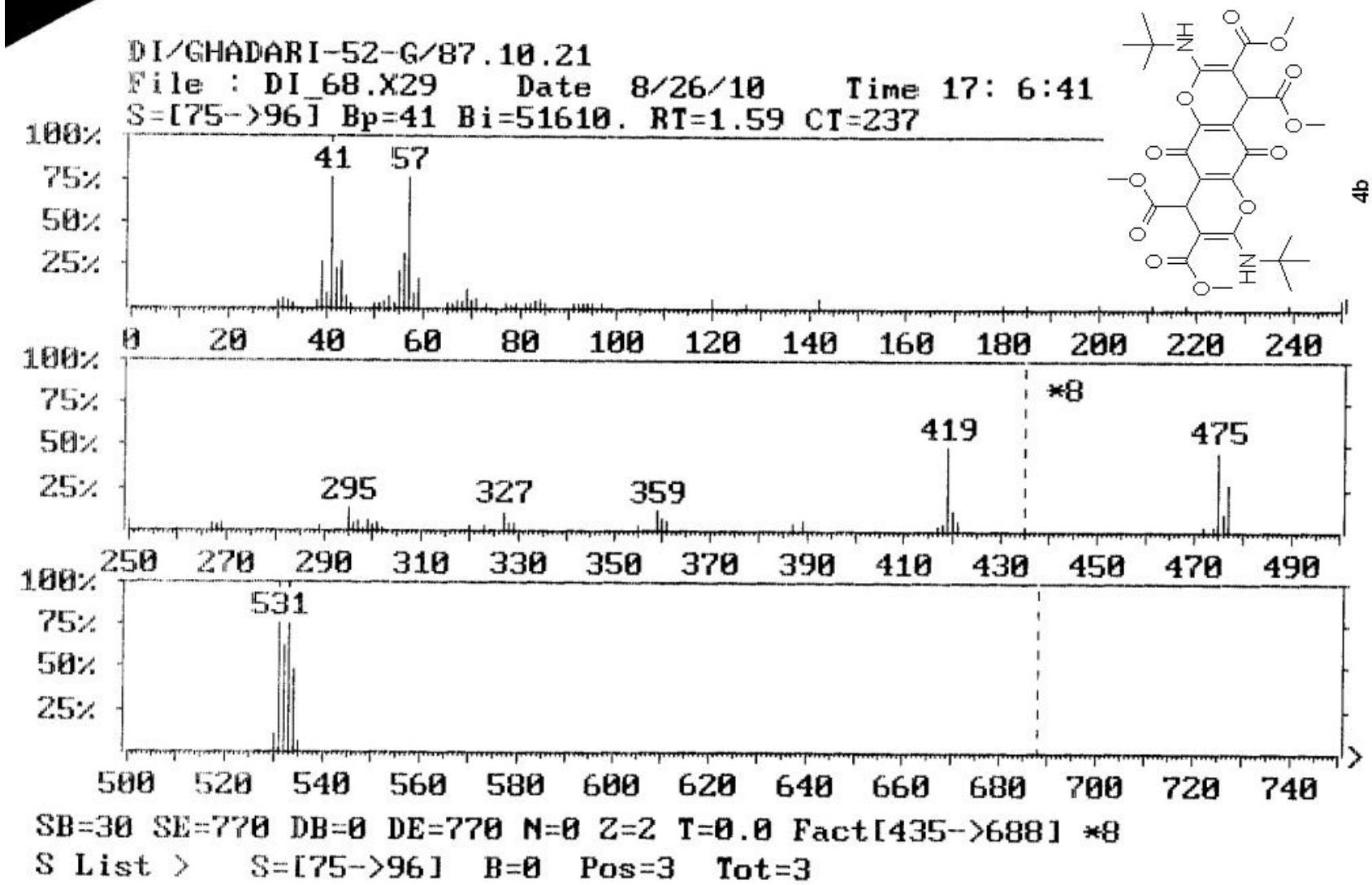
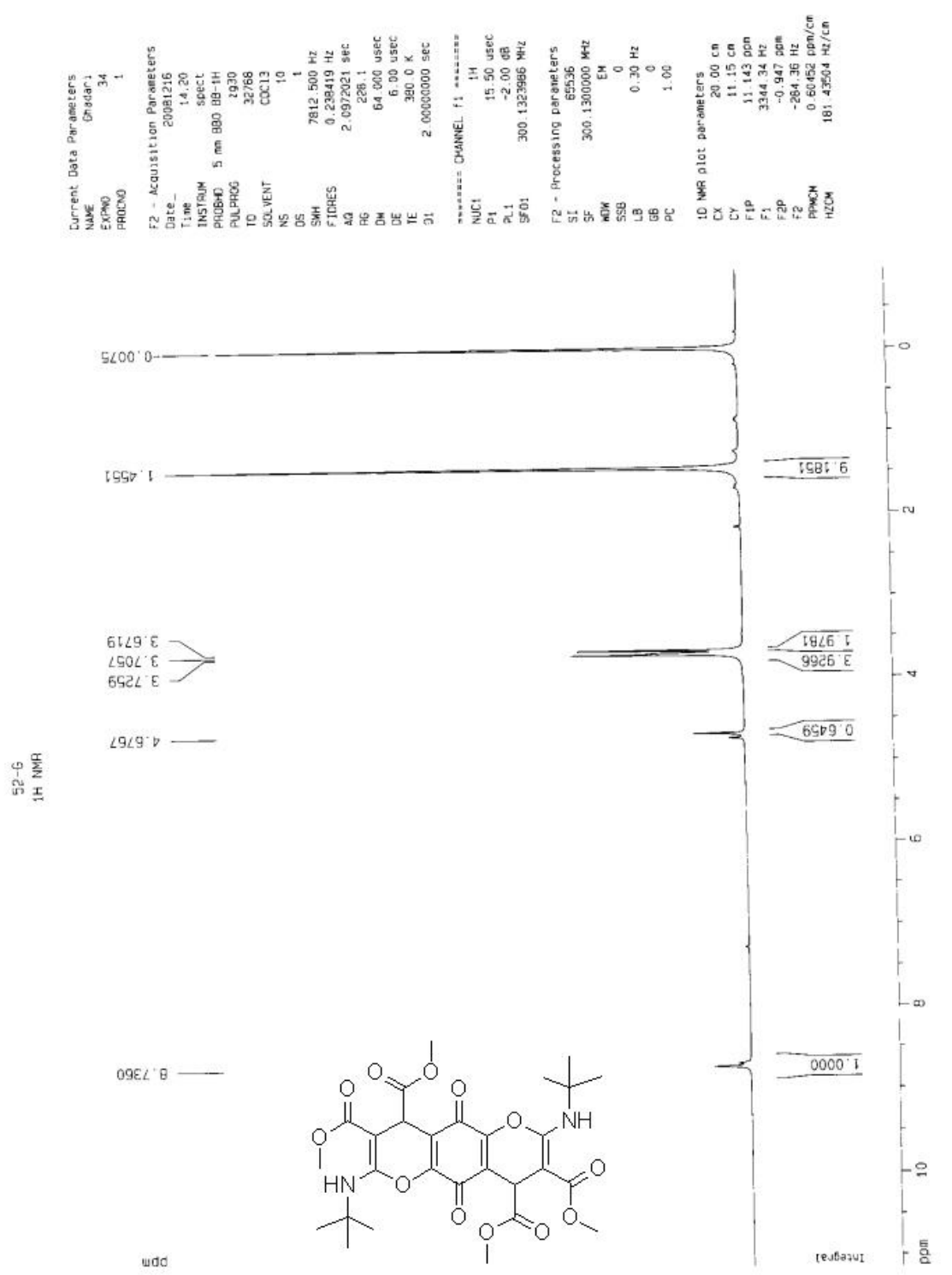
117.687
147.796
158.348
169.073
172.167
176.968
4a
ppm


HMQC


%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
3260.49
3157.77
2947.22
1757.95
1679.06
1604.49
1441.89
1419.59
1305.95
1100.04
1059.31
S2-G
4b

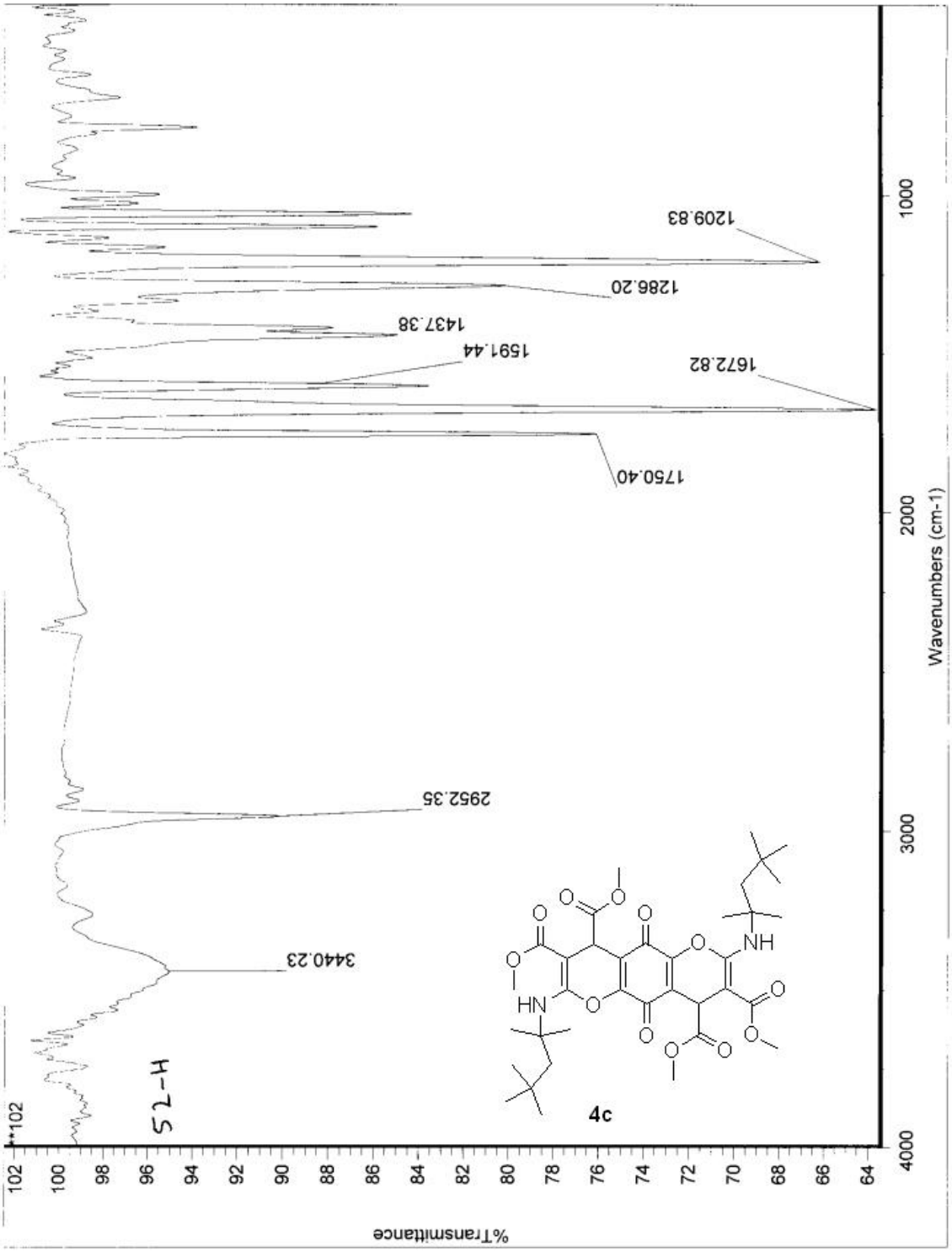

DI/GHADARI-52-G/87.10.21
File : DI_68.X29 Date 8/26/10 Time 17: 6:41
S=[75->96] Bp=41 Bi=51610. RT=1.59 CT=237
100%
75%
50%
25%
41
57
0 20 40 60 80 100 120 140 160 180 200 220 240
*8
419
475
295
327
359
250 270 290 310 330 350 370 390 410 430 450 470 490
531
500 520 540 560 580 600 620 640 660 680 700 720 740
SB=30 SE=770 DB=0 DE=770 N=0 Z=2 T=0.0 Fact[435->688] *8
S List > S=[75->96] B=0 Pos=3 Tot=3

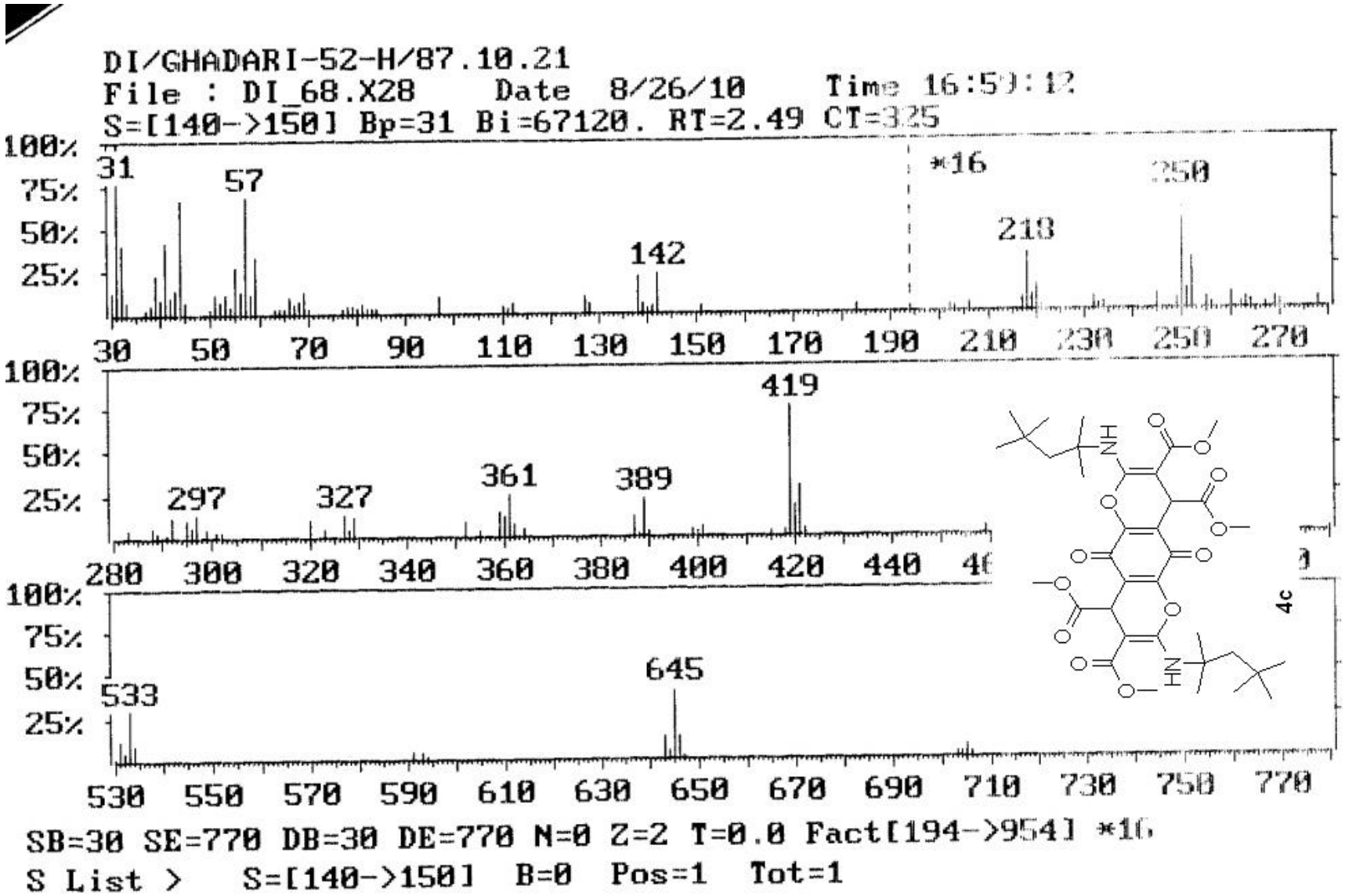
4b


52-G
1H NMR
Current Data Parameters
NAME Ghadari
EXPNO 34
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081216
Time 14.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG 1930
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.09720021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 390.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 11.15 cm
F1P 11.143 ppm
F1 3344.34 Hz
F2P -0.947 ppm
F2 -284.36 Hz
PPMCM 0.66452 ppm/cm
HZCM 181.43504 Hz/cm
0.0075
1.4551
3.6719
3.7057
3.7259
4.6767
8.7360
9.1851
1.9781
3.9266
0.6459
1.0000
Integral
ppm

4b

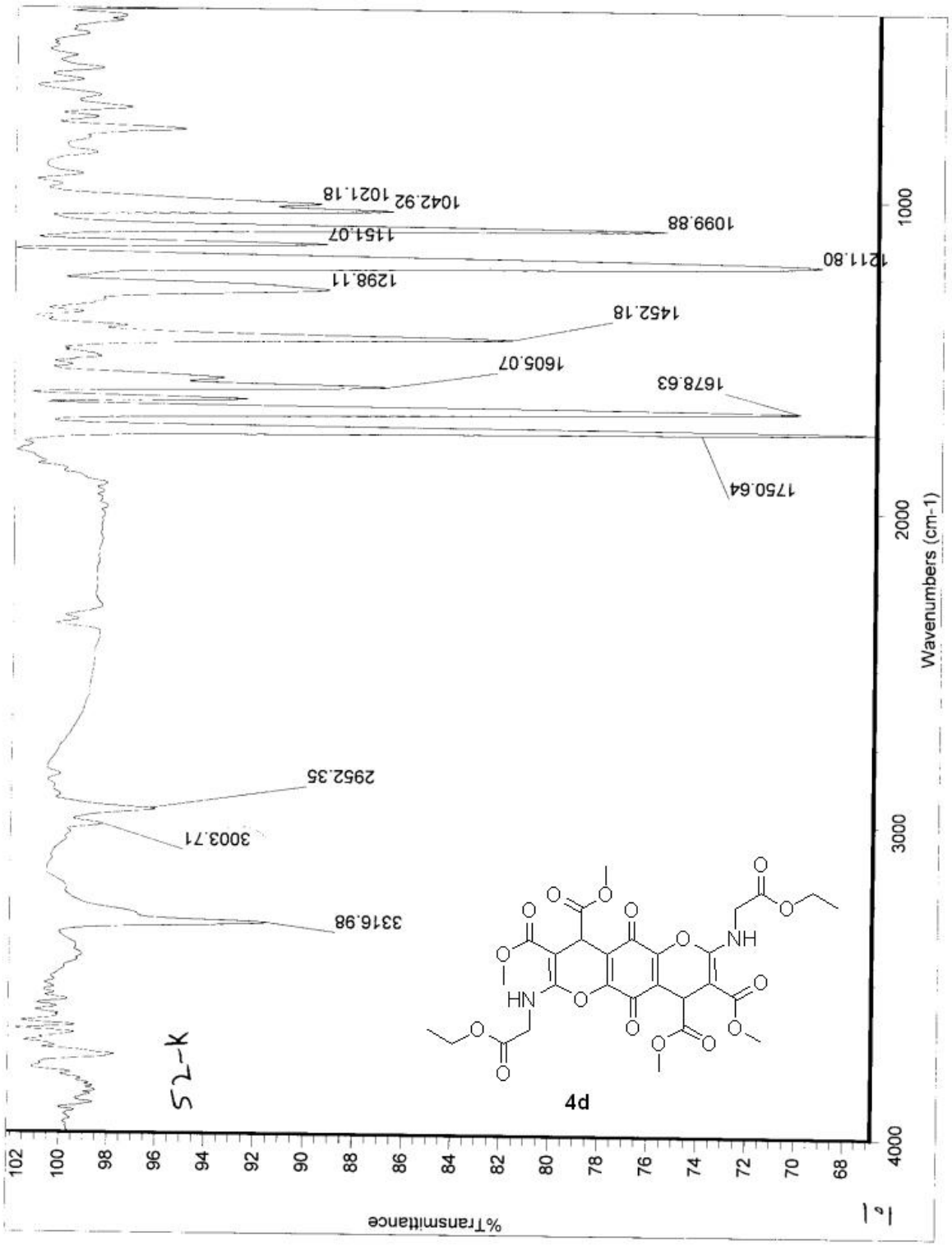
52-G
13C{1H} NMR
Current Data Parameters
NAME Ghagari
EXPNO 35
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081220
Time 10.52
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 172
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
AQ 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.50 cm
F1P 219.155 ppm
F1 16539.11 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28052 Hz/cm
-0.032
30.212
30.254
34.845
35.000
51.259
52.798
52.913
53.482
71.443
71.669
76.640
77.064
77.488
117.420
117.557
147.836
147.892
159.641
159.775
169.073
169.127
171.825
172.128
176.918
177.016
ppm
0
25
50
75
100
125
150
175
200
4b

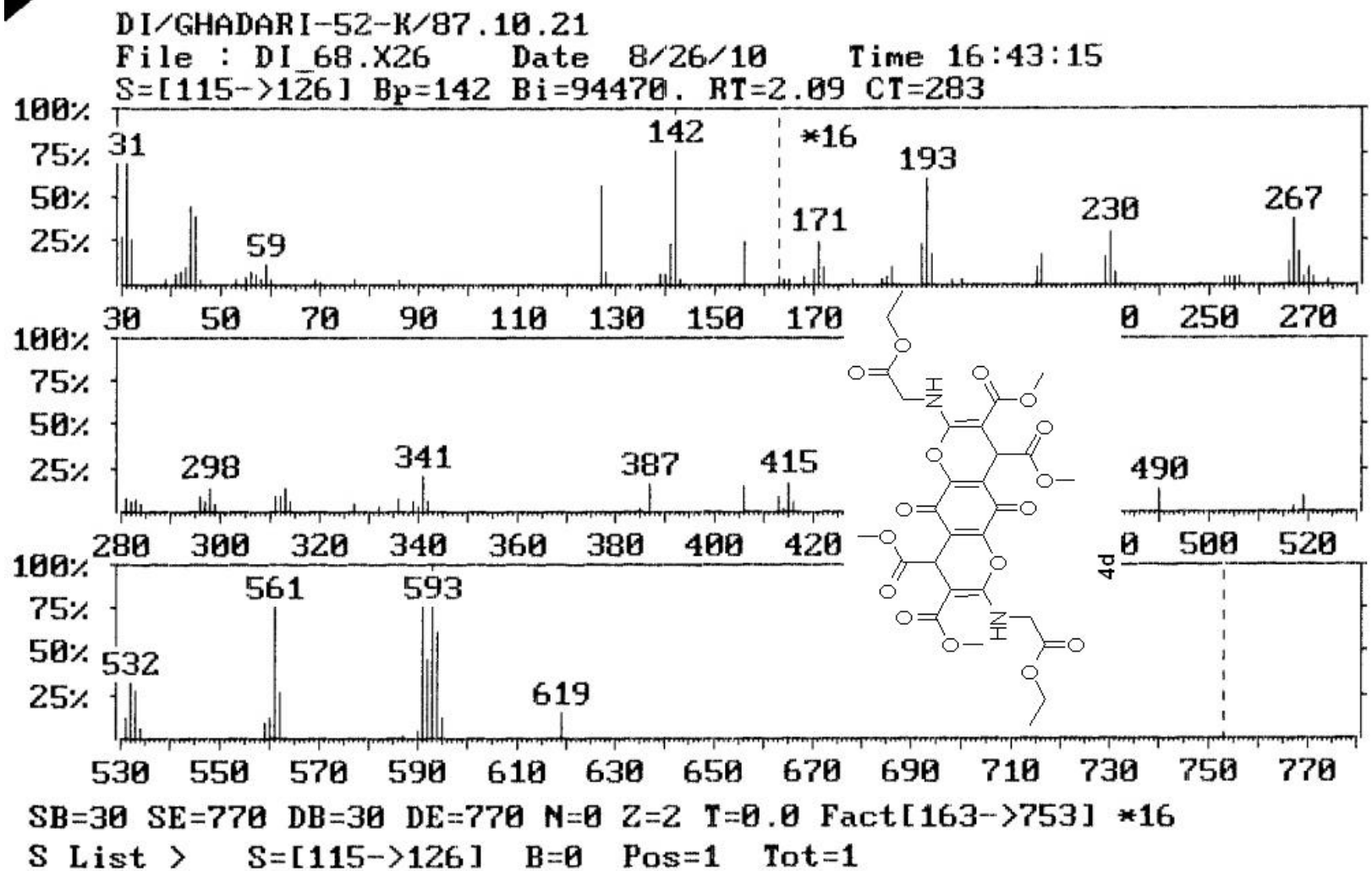

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
102
100
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
3440.23
2952.35
1750.40
1672.82
1591.44
1437.38
1286.20
1209.83
4c


DI/GHADARI-52-H/87.10.21
File : DI_68.X28 Date 8/26/10 Time 16:50:12
S=[140->150] Bp=31 Bi=67120. RT=2.49 CT=325
100%
75%
50%
25%
31
57
142
*16
218
250
30 50 70 90 110 130 150 170 190 210 230 250 270
419
361
389
297
327
280 300 320 340 360 380 400 420 440
533
645
530 550 570 590 610 630 650 670 690 710 730 750 770
4c
SB=30 SE=770 DB=30 DE=770 N=0 Z=2 T=0.0 Fact[194->954] *16
S List > S=[140->150] B=0 Pos=1 Tot=1

52H 1HNMR in CDCl3 at 298 K 87/9/17
Current Data Parameters
NAME Shaban
EXPNO 28
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081207
Time 14.21
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 203.2
DW 48.400 usec
DE 6.50 usec
TE 298.1 K
D1 5.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300231 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.28 cm
F1P 11.898 ppm
F1 5950.48 Hz
F2P 0.267 ppm
F2 133.71 Hz
PPMCM 0.59153 ppm/cm
HZCM 290.83835 Hz/cm
0.95822
1.49106
1.49852
1.82004
3.64187
3.71391
4.69274
7.25794
8.75599
9.0294
6.1867
2.1163
3.2360
3.2391
1.0705
1.0000
Integral
ppm
4c

52H 13CNMR in CDCl3 at 298 K 87/9/17
Current Data Parameters
NAME Shabani
EXPNO 27
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061207
Time 14.12
INSTRUM spect
PROBHD 5 mm BNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 311
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5456039 sec
RG 4096
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SF01 125.7703643 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SF02 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 4.99 cm
F1P 212.261 ppm
F1 26693.42 Hz
F2P 8.695 ppm
F2 1093.50 Hz
PPMCM 10.17827 ppm/cm
HZCM 1279.99622 Hz/cm
31.328
31.690
31.778
32.017
35.434
51.629
53.109
53.273
57.460
71.781
77.182
77.435
77.690
118.250
148.322
160.121
169.573
172.402
177.405
ppm
25
50
75
100
125
150
175
200
ppm
NH
HN
4c

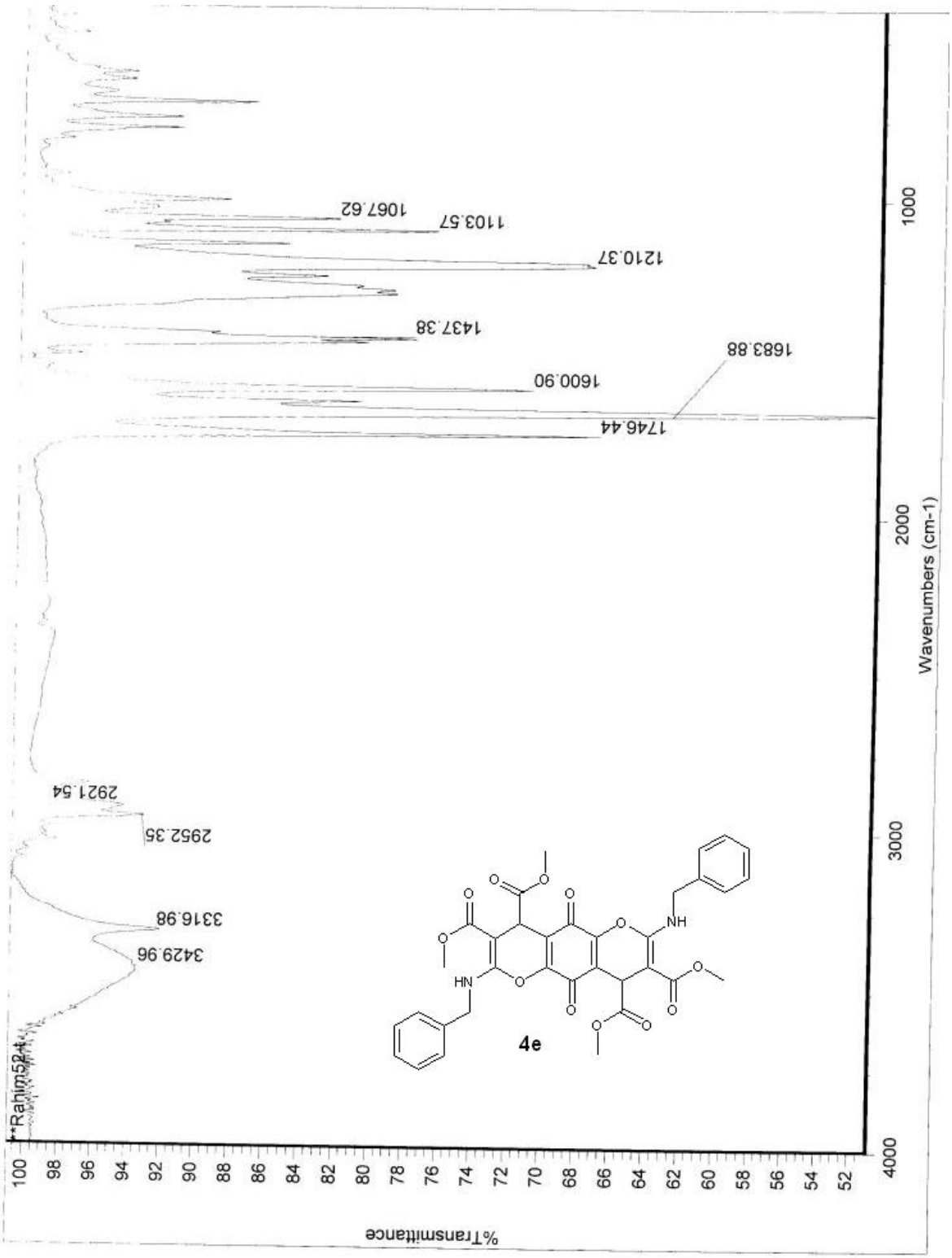

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3316.98
3003.71
2952.35
1750.64
1678.63
1605.07
1452.18
1298.11
1211.80
1151.07
1099.88
1042.92
1021.18
4d

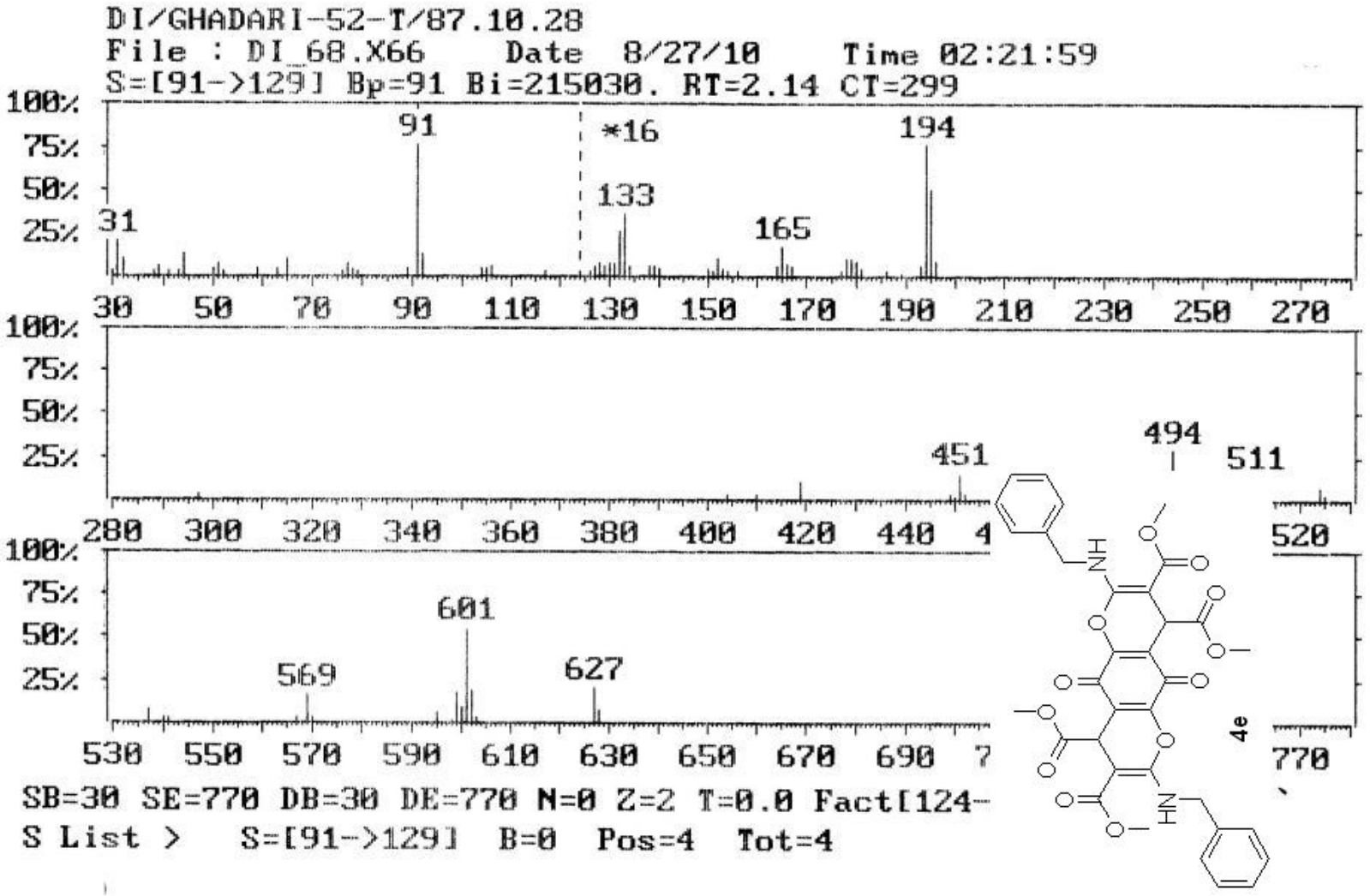

DI/GHADARI-52-K/87.10.21
File : DI_68.X26 Date 8/26/10 Time 16:43:15
S=[115->126] Bp=142 Bi=94470. RT=2.09 CT=283
100%
75%
50%
25%
31
59
142
*16
171
193
230
267
30 50 70 90 110 130 150 170 0 250 270
298
341
387
415
490
280 300 320 340 360 380 400 420 0 500 520
4d
561
593
532
619
530 550 570 590 610 630 650 670 690 710 730 750 770
SB=30 SE=770 DB=30 DE=770 N=0 Z=2 T=0.0 Fact[163->753] *16
S List > S=[115->126] B=0 Pos=1 Tot=1

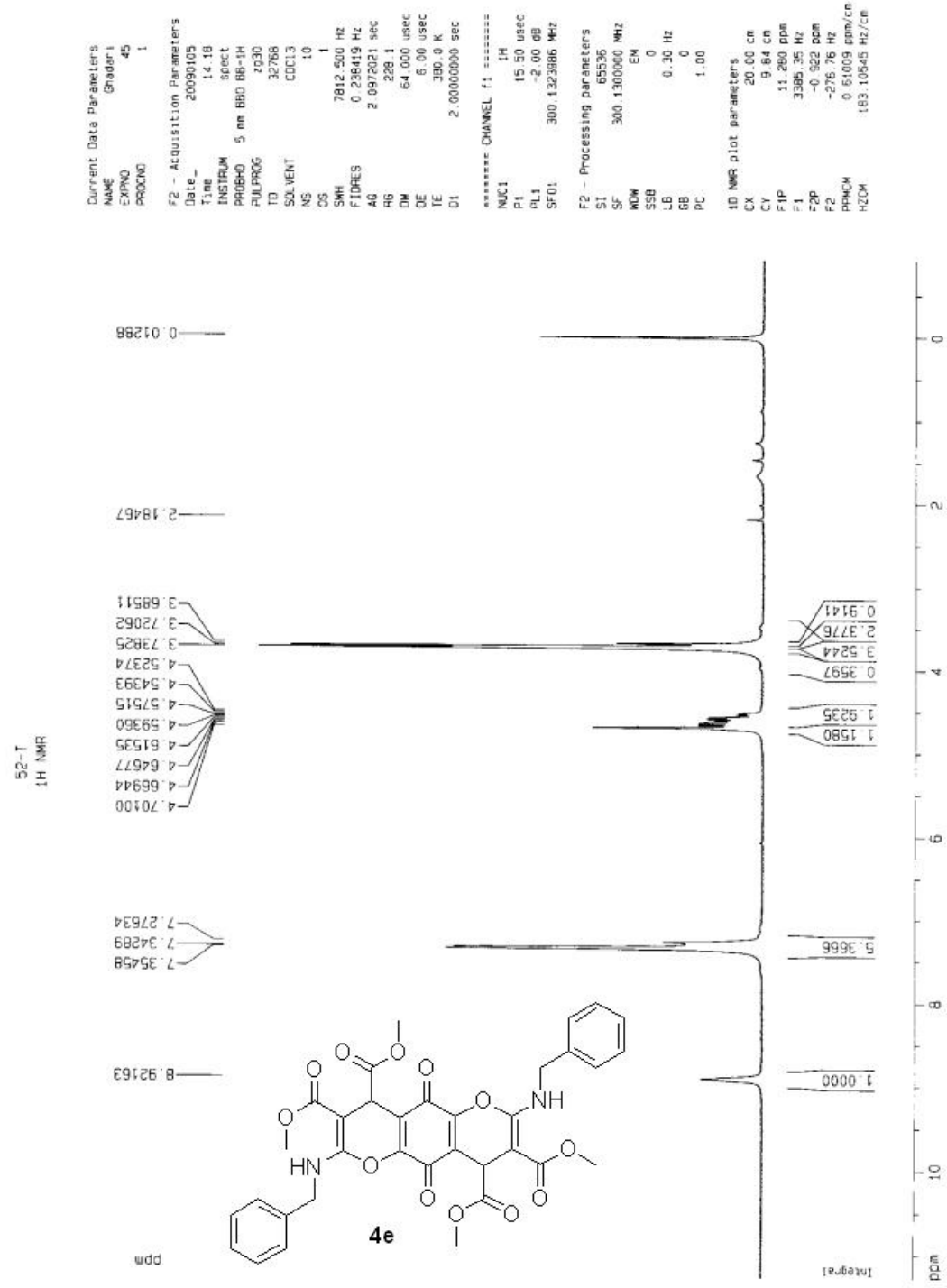
52-K 1HNMR in CDCl3 at 298 K 87/9/17
Current Data Parameters
NAME Shabani
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081207
Time 13.20
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 1
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 456.1
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 6.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300231 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.25 cm
F1P 11.526 ppm
F1 5764.34 Hz
F2P 0.477 ppm
F2 238.41 Hz
PPMCM 0.55245 ppm/cm
HZCM 276.29642 Hz/cm
1.27552
1.28941
1.30303
3.65587
3.76005
4.13265
4.14209
4.21028
4.21996
4.23427
4.24620
4.27319
4.67710
7.25957
8.77866
3.3287
3.2384
3.3391
1.2576
3.6451
1.1294
1.0000
ppm
Integral
ppm

4d

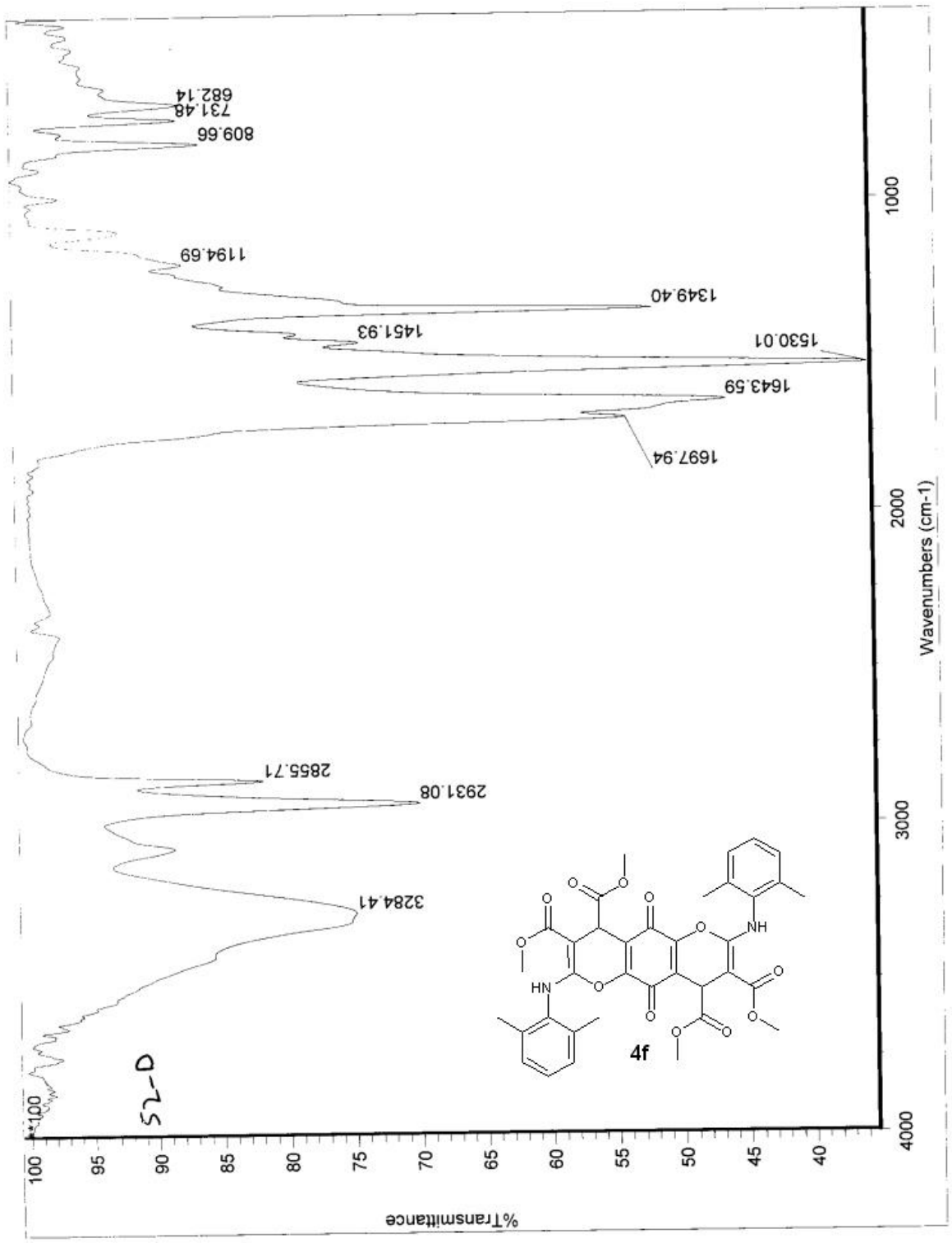
52k 13CNMR in CDCl3 at 298 K 07/9/17
Current Data Parameters
NAME Shabani
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061207
Time 13.26
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 330
DS 4
SWH 30030.029 Hz
FIDRES 0.916444 Hz
AQ 0.5456539 sec
RG 6502
DW 16.650 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.10 usec
PL1 3.00 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.50 dB
PL13 15.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 5.17 cm
F1P 213.336 ppm
F1 26828.70 Hz
F2P 4.124 ppm
F2 518.60 Hz
PPMCM 10.46063 ppm/cm
HZCM 1315.50464 Hz/cm
14.561
35.684
43.402
51.933
53.248
62.146
73.882
77.184
77.438
77.692
118.319
148.012
158.785
169.021
169.581
171.894
176.942
ppm
25
50
75
100
125
150
175
200
ppm
HN
NH
4d

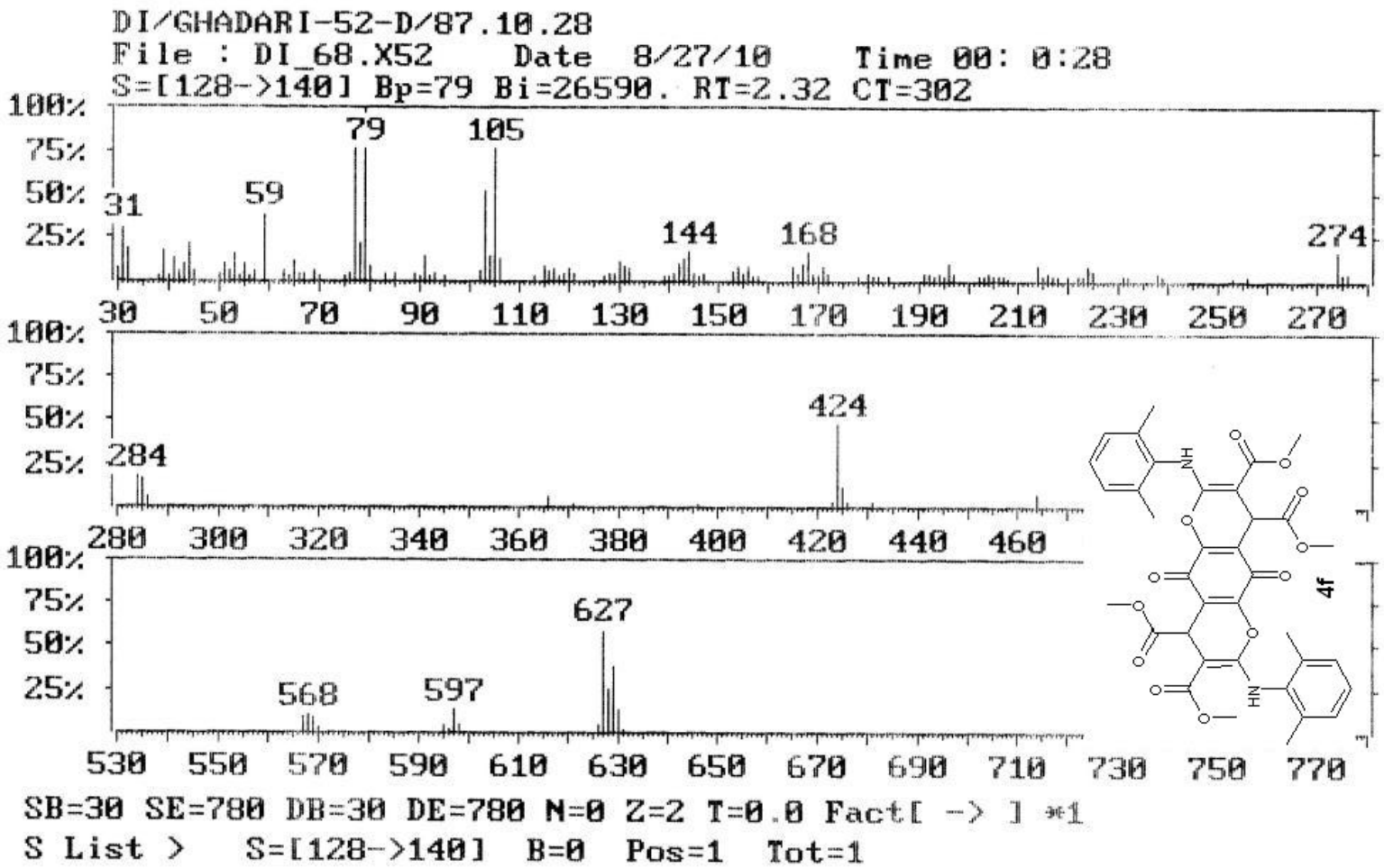

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3429.96
3316.98
2952.35
2921.54
1746.44
1600.90
1683.88
1437.38
1210.37
1103.57
1067.62
4e

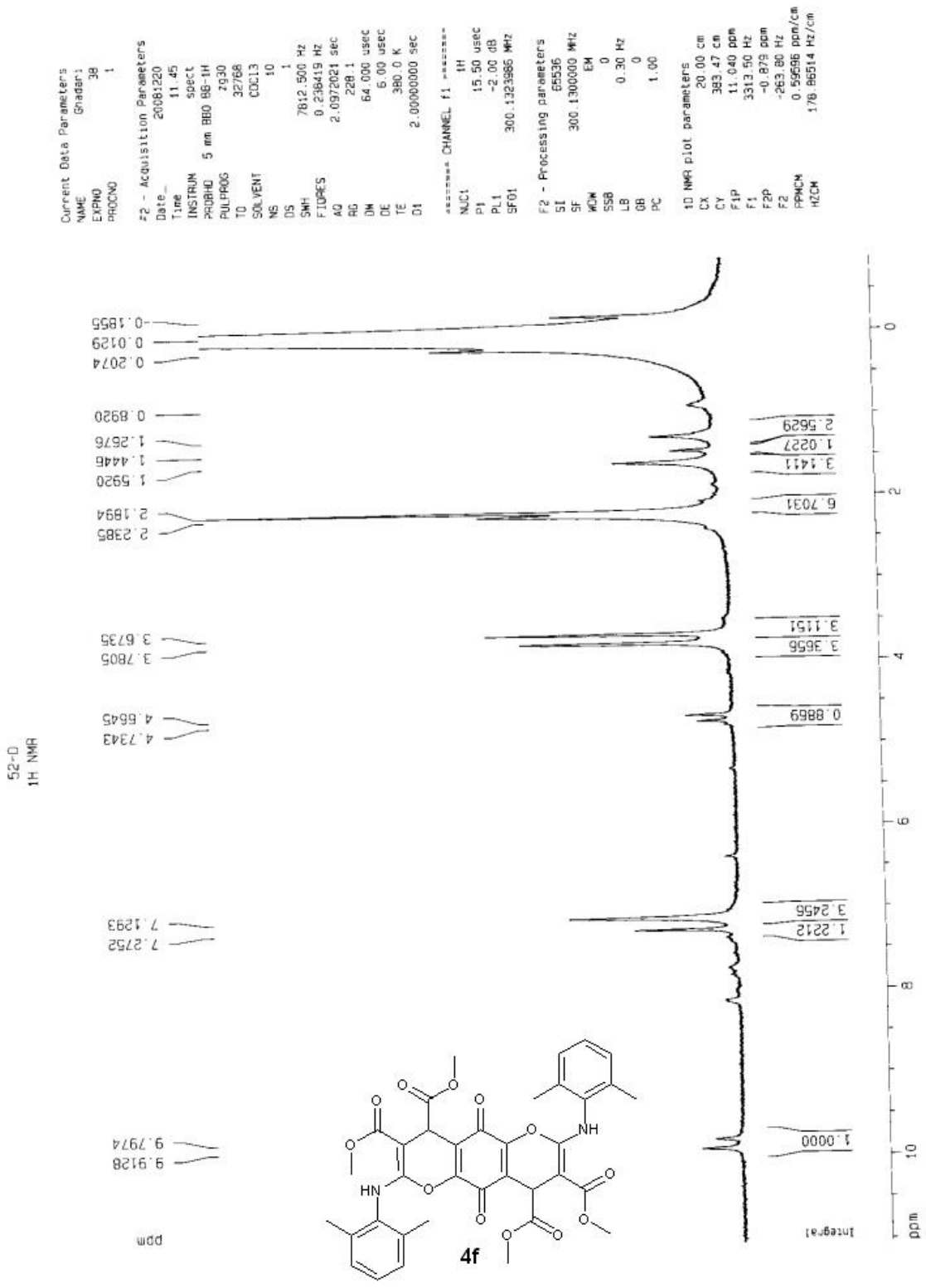

DI/GHADARI-52-T/87.10.28
File : DI_68.X66 Date 8/27/10 Time 02:21:59
S=[91->129] Bp=91 Bi=215030. RT=2.14 CT=299
100%
75%
50%
25%
91
*16
194
133
31
165
30 50 70 90 110 130 150 170 190 210 230 250 270
451
494
511
280 300 320 340 360 380 400 420 440 4
520
601
569
627
530 550 570 590 610 630 650 670 690 7
770
4e
SB=30 SE=770 DB=30 DE=770 N=0 Z=2 T=0.0 Fact[124-
S List > S=[91->129] B=0 Pos=4 Tot=4

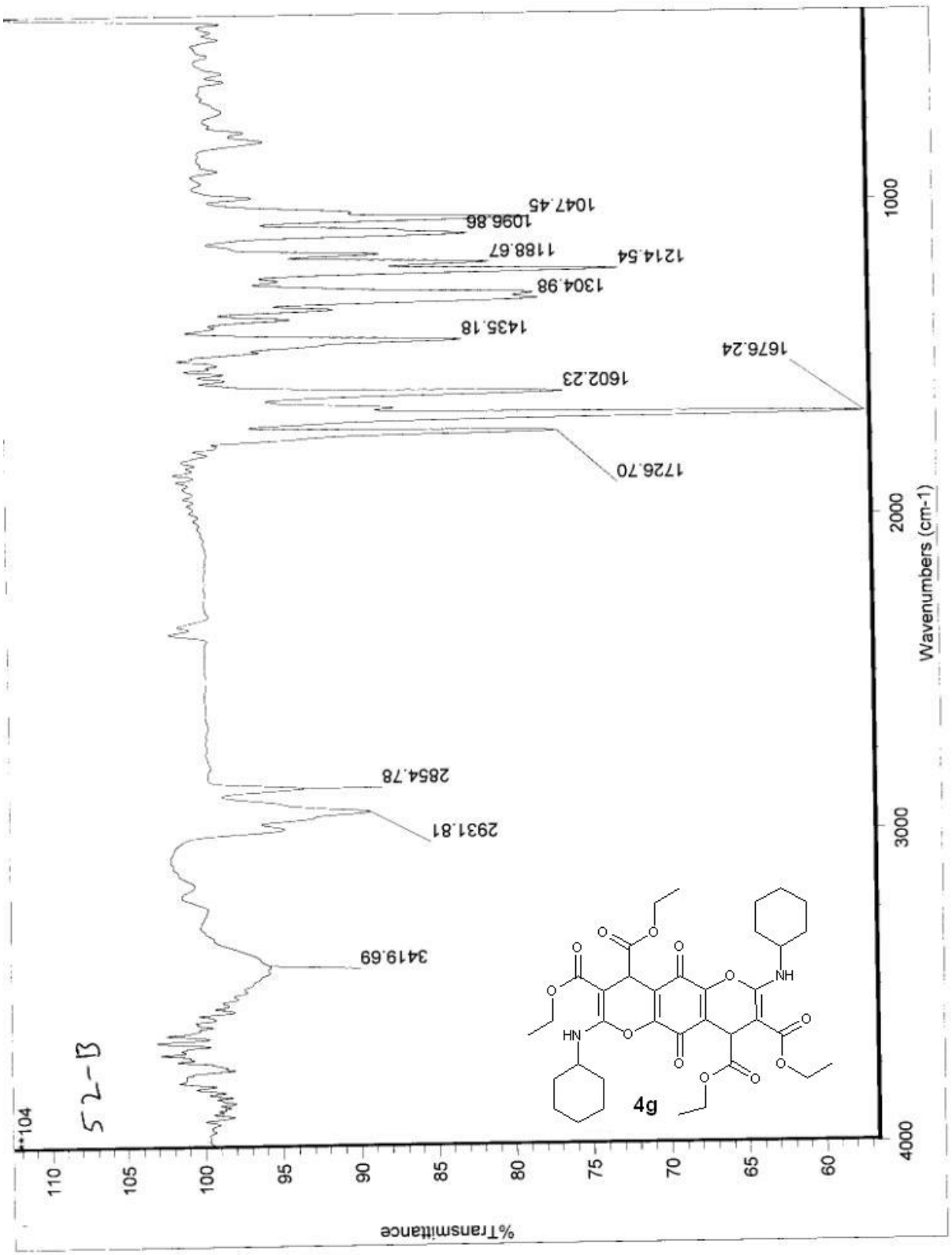

Current Data Parameters
NAME Ghaderi
EXPNO 45
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090105
Time 14.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 330.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 9.84 cm
F1P 11.280 ppm
F1 3385.35 Hz
F2P -0.922 ppm
F2 -276.76 Hz
PPMCM 0.61009 ppm/cm
HZCM 183.10545 Hz/cm
0.01288
2.18467
3.68511
3.72062
3.73825
4.52374
4.54393
4.57515
4.59360
4.61535
4.64677
4.66944
4.70100
7.27634
7.32289
7.35458
8.92163
0.9141
2.3776
3.5244
0.3597
1.9235
1.1580
5.3666
1.0000
52-T
1H NMR
4e
ppm
Integral

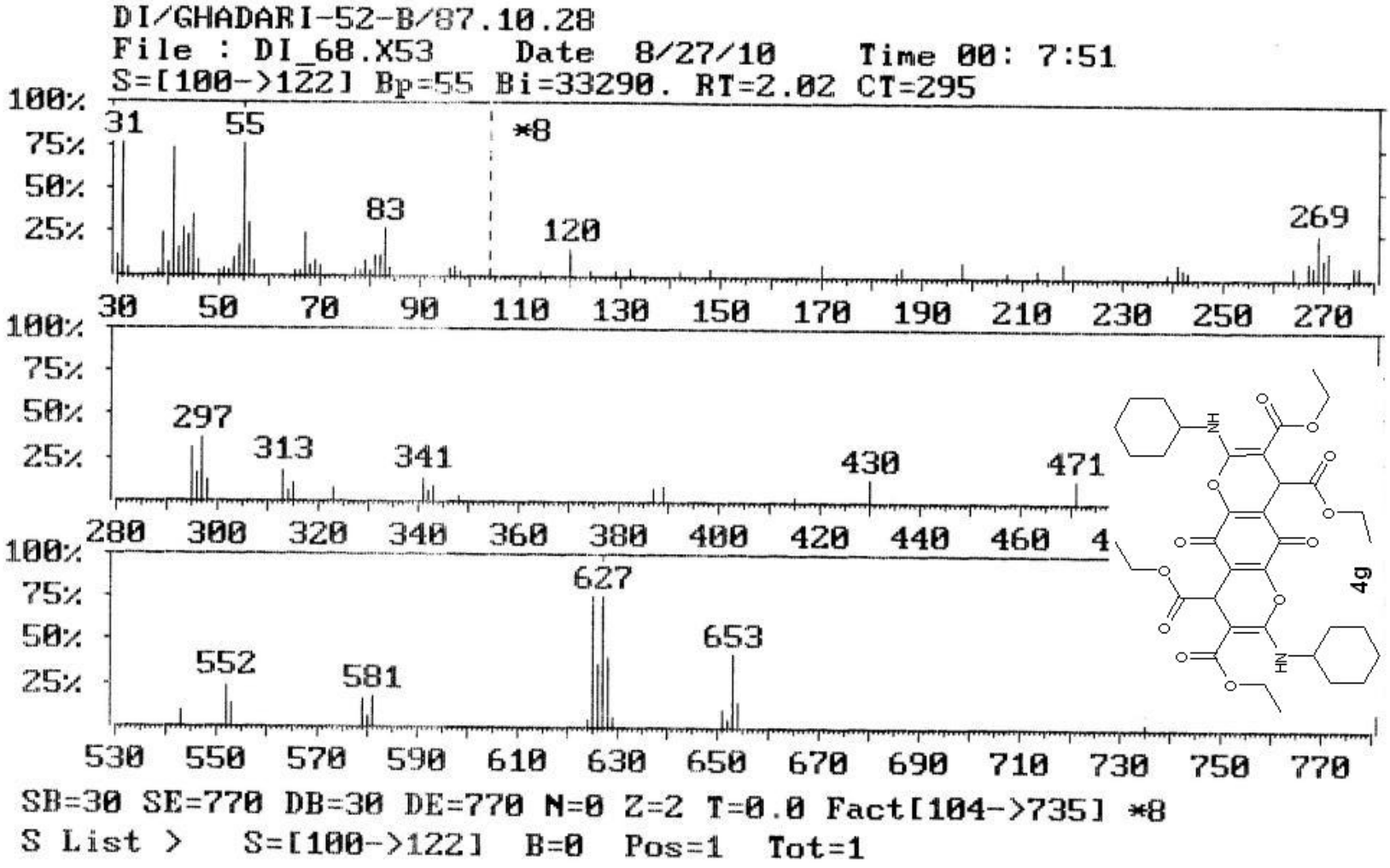
52-T
13C{1H} NMR
Current Data Parameters
NAME Ghadari
EXPNO 46
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090105
Time 14.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 123
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 14.05 cm
F1P 219.155 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm
0.013
35.217
45.186
51.387
52.999
72.145
76.625
77.049
77.472
117.434
127.573
127.769
128.796
137.677
147.621
158.633
168.910
171.760
176.636
4e
ppm
0
50
100
150
200

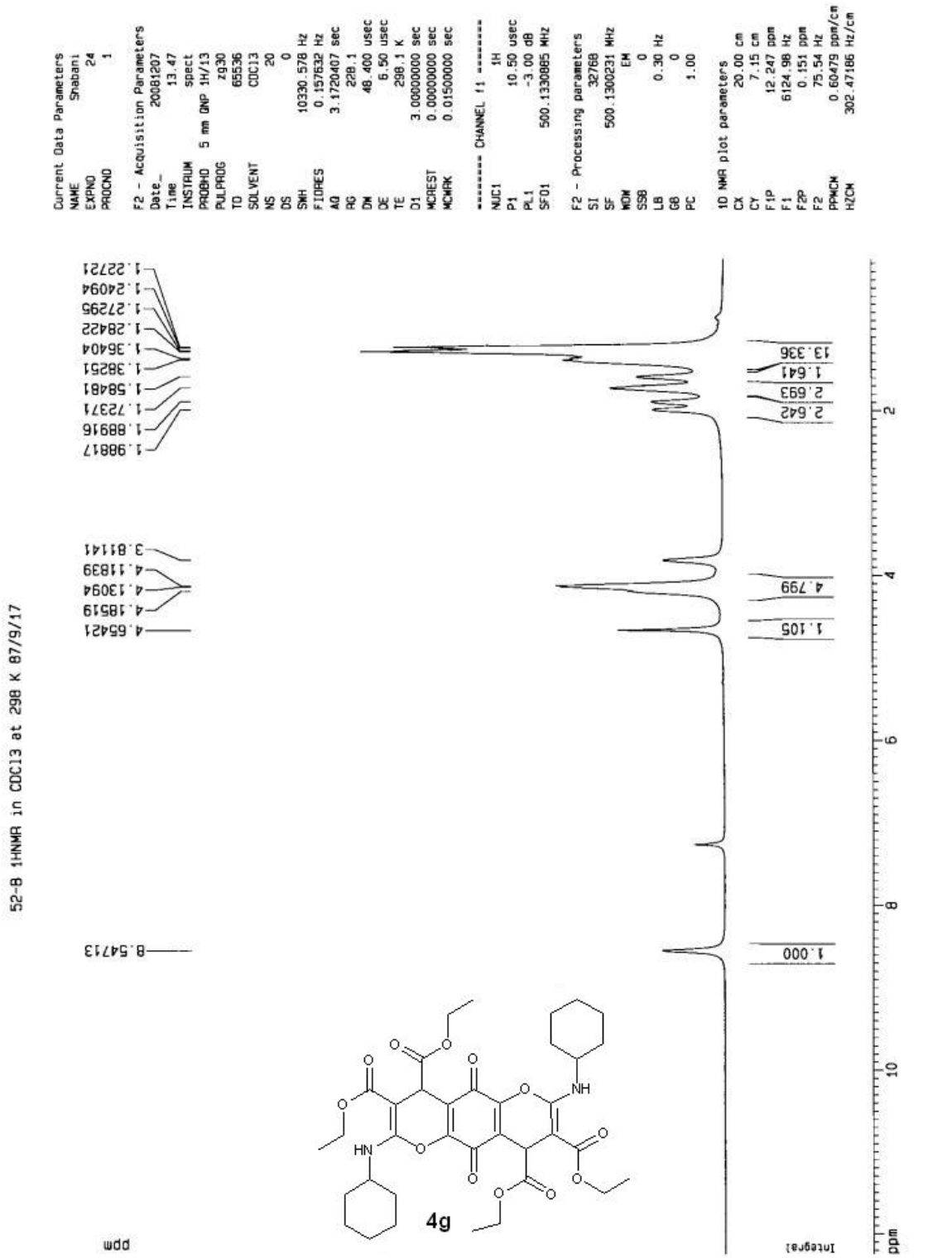

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
100
95
90
85
80
75
70
65
60
55
50
45
40
3284.41
2931.08
2855.71
1697.94
1643.59
1530.01
1451.93
1349.40
1194.69
809.66
731.48
682.14
4f
57-D

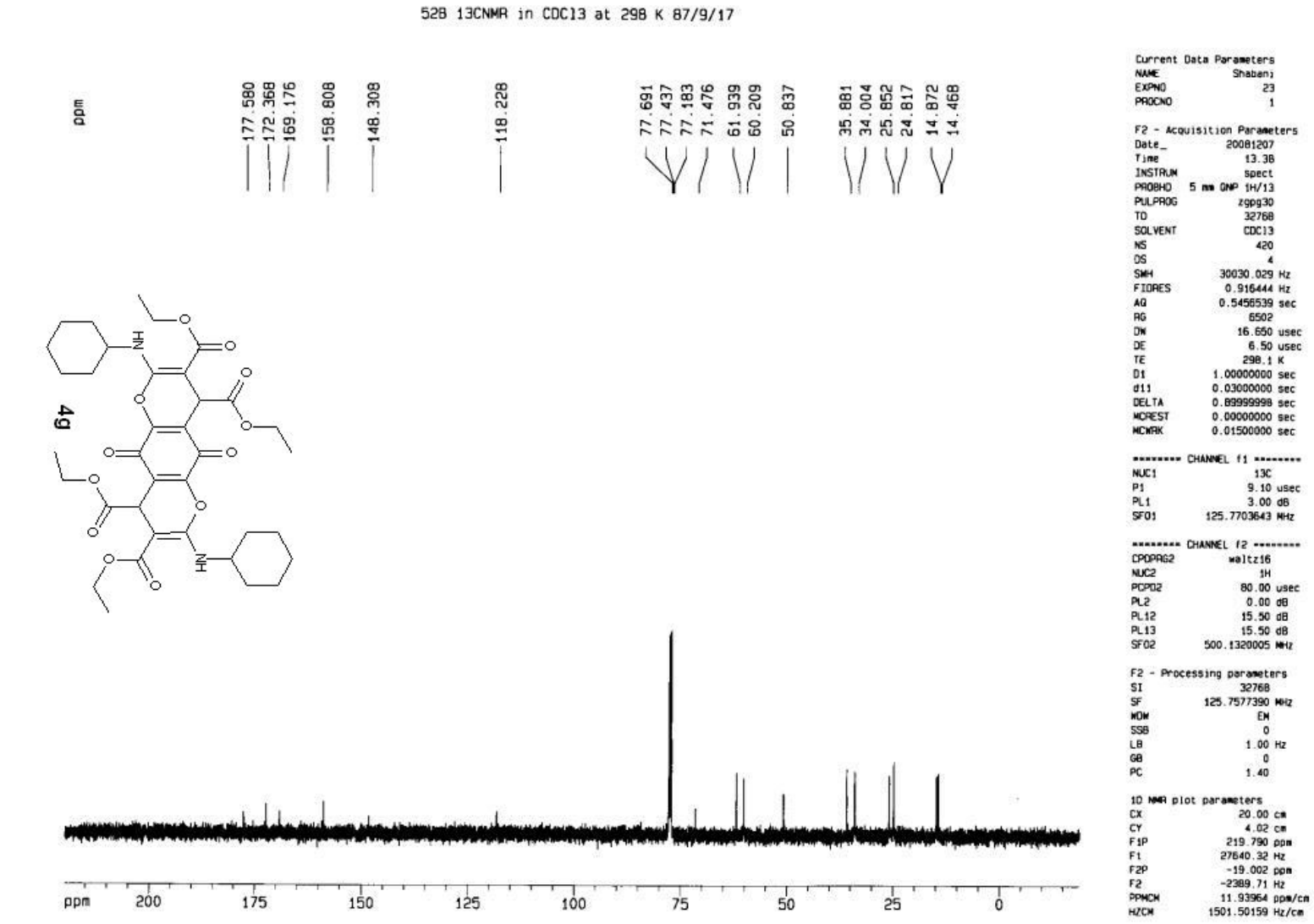

DI/GHADARI-52-D/87.10.28
File : DI_68.X52 Date 8/27/10 Time 00: 0:28
S=[128->140] Bp=79 Bi=26590. RT=2.32 CT=302
100%
75%
50%
25%
31
59
79
105
144
168
274
30 50 70 90 110 130 150 170 190 210 230 250 270
284
424
280 300 320 340 360 380 400 420 440 460
627
568
597
530 550 570 590 610 630 650 670 690 710 730 750 770
4f
SB=30 SE=780 DB=30 DE=780 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[128->140] B=0 Pos=1 Tot=1


52-D
1H NMR
4f
ppm
integral


%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
110
105
100
95
90
85
80
75
70
65
60
3419.69
2931.81
2854.78
1726.70
1676.24
1602.23
1435.18
1304.98
1214.54
1188.67
1096.86
1047.45
S2-B
4g


DI/GHADARI-52-B/87.10.28
File : DI_68.X53 Date 8/27/10 Time 00: 7:51
S=[100->122] Bp=55 Bi=33290. RT=2.02 CT=295
100%
75%
50%
25%
31
55
*8
83
120
269
30 50 70 90 110 130 150 170 190 210 230 250 270
297
313
341
430
471
280 300 320 340 360 380 400 420 440 460 4
627
653
552
581
530 550 570 590 610 630 650 670 690 710 730 750 770
4g
SB=30 SE=770 DB=30 DE=770 N=0 Z=2 T=0.0 Fact[104->735] *8
S List > S=[100->122] B=0 Pos=1 Tot=1


52-B 1HNMR in CDCl3 at 298 K 87/9/17
Current Data Parameters
NAME Shabani
EXPNO 24
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081207
Time 13.47
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 20
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 228.1
DW 48.400 usec
DE 6.50 usec
TE 298.1 K
D1 3.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300231 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 7.15 cm
F1P 12.247 ppm
F1 6124.98 Hz
F2P 0.151 ppm
F2 75.54 Hz
PPMCM 0.60479 ppm/cm
HZCM 302.47186 Hz/cm
1.22721
1.24094
1.27295
1.28422
1.36404
1.38251
1.58481
1.72371
1.88916
1.98817
3.81141
4.11839
4.13094
4.18519
4.65421
8.54713
13.336
1.641
2.693
2.642
4.799
1.105
1.000
4g
ppm
Integral



Current Data Parameters

NAME	Shaban;
EXPNO	23
PROCNO	1

F2 - Acquisition Parameters

Date_	20081207
Time	13.38
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	420
DS	4
SWH	30030.029 Hz
FIDRES	0.916444 Hz
AQ	0.5456539 sec
RG	8502
DW	16.650 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	9.10 usec
PL1	3.00 dB
SF01	125.7703643 MHz

======== CHANNEL f2 ========

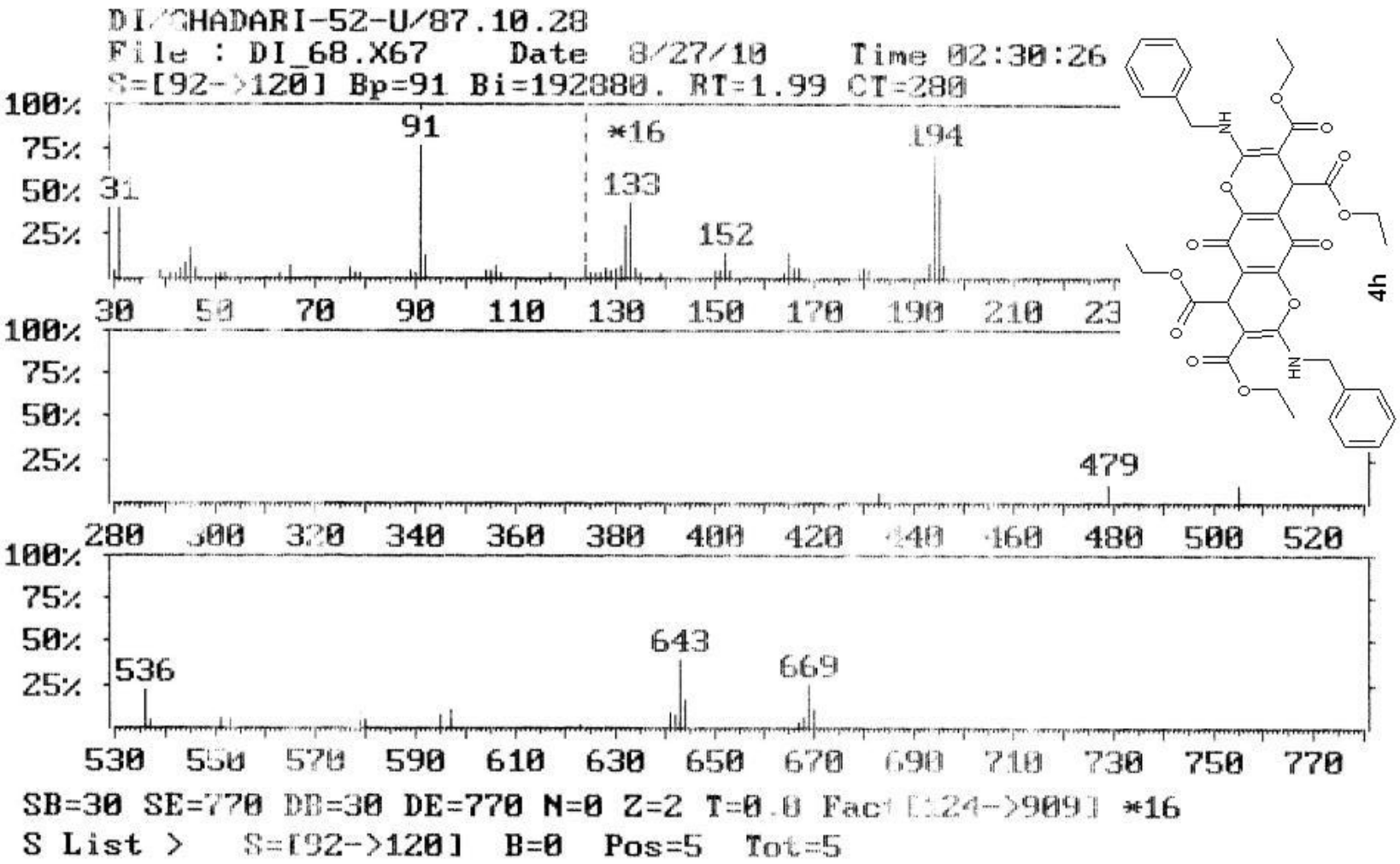
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.50 dB
PL13	15.50 dB
SF02	500.1320005 MHz

F2 - Processing parameters

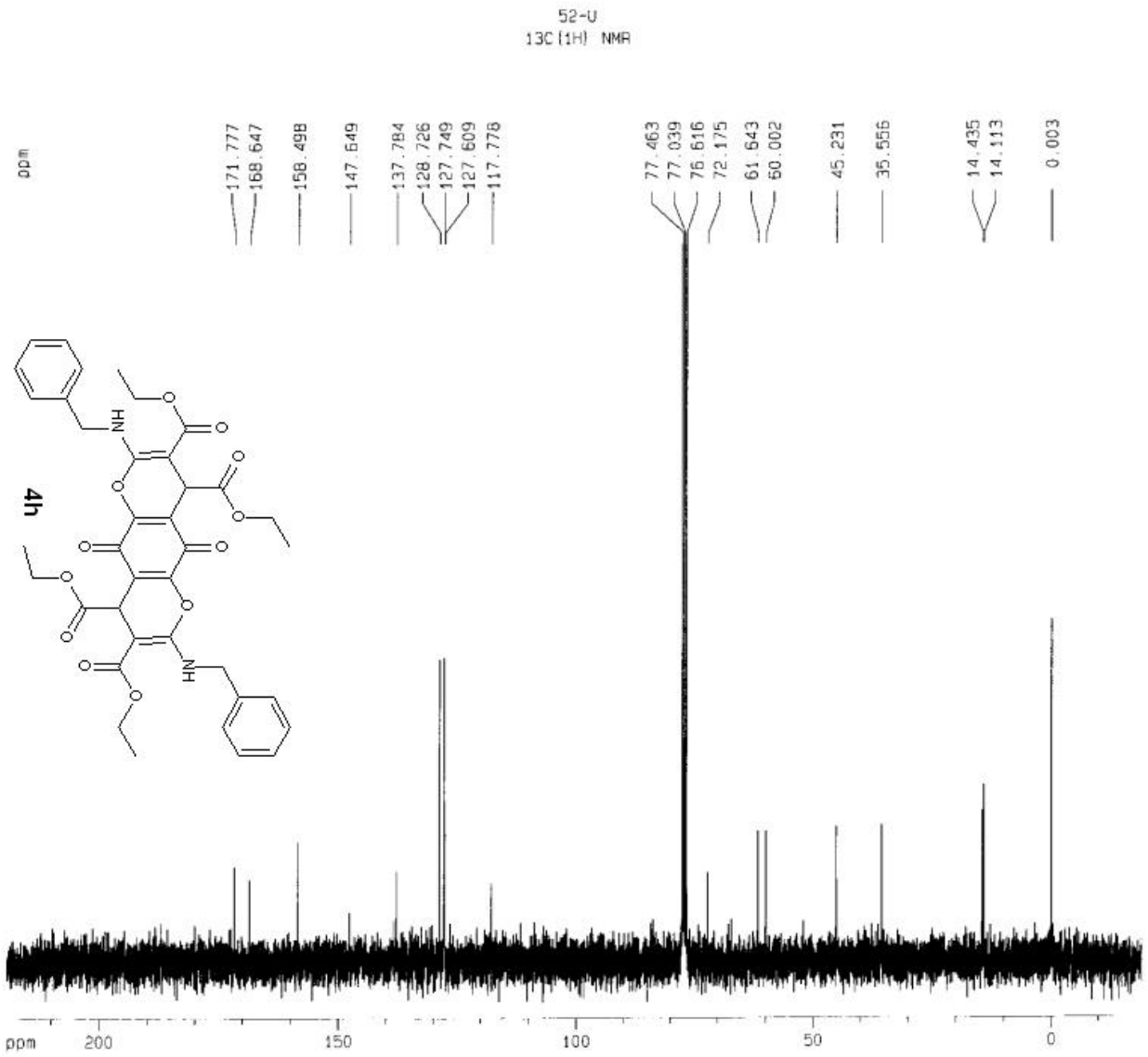
SI	32768
SF	125.7577390 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

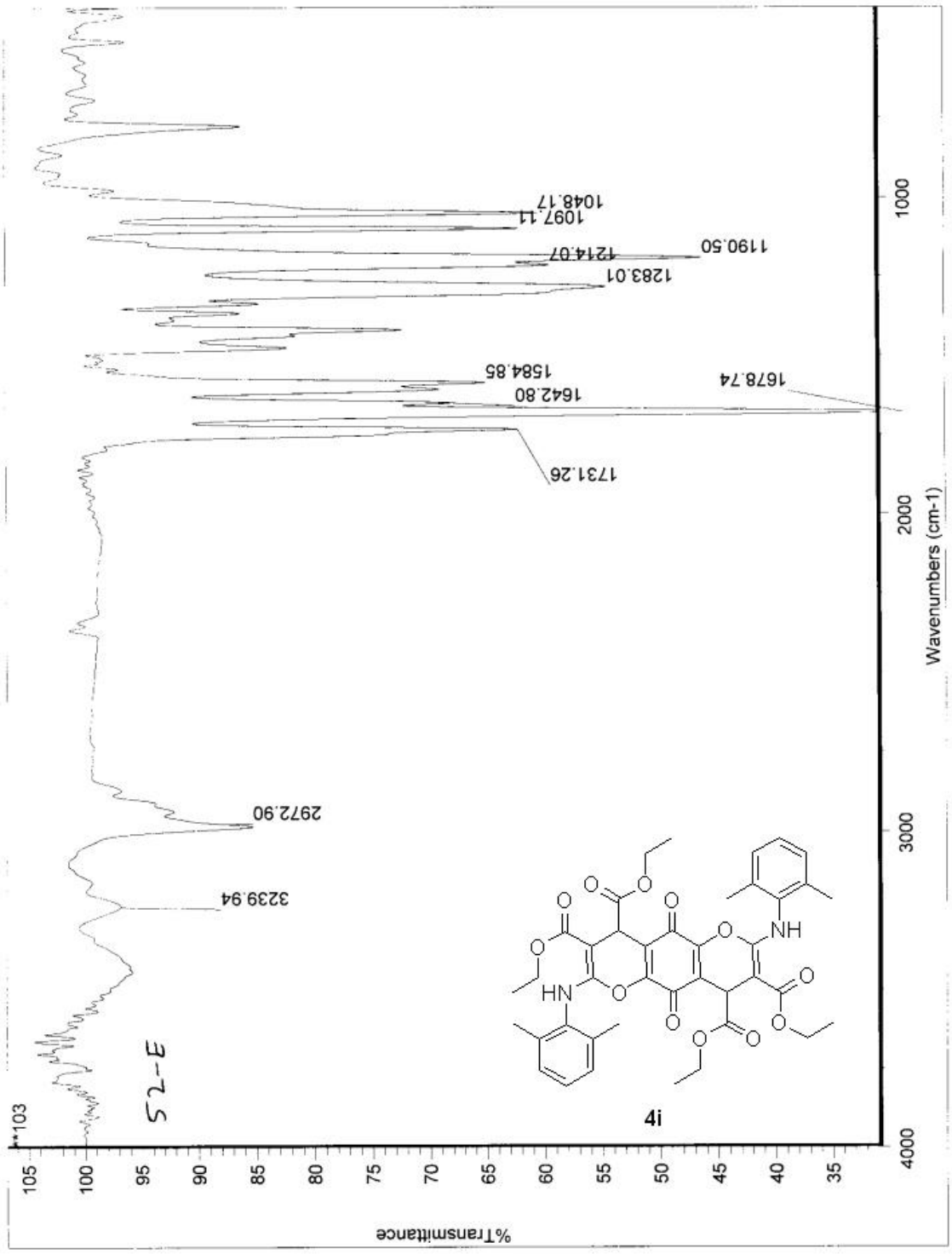
CX	20.00 cm
CY	4.02 cm
F1P	219.790 ppm
F1	27640.32 Hz
F2P	-19.002 ppm
F2	-2389.71 Hz
PPMCM	11.93964 ppm/cm
HZCM	1501.50159 Hz/cm

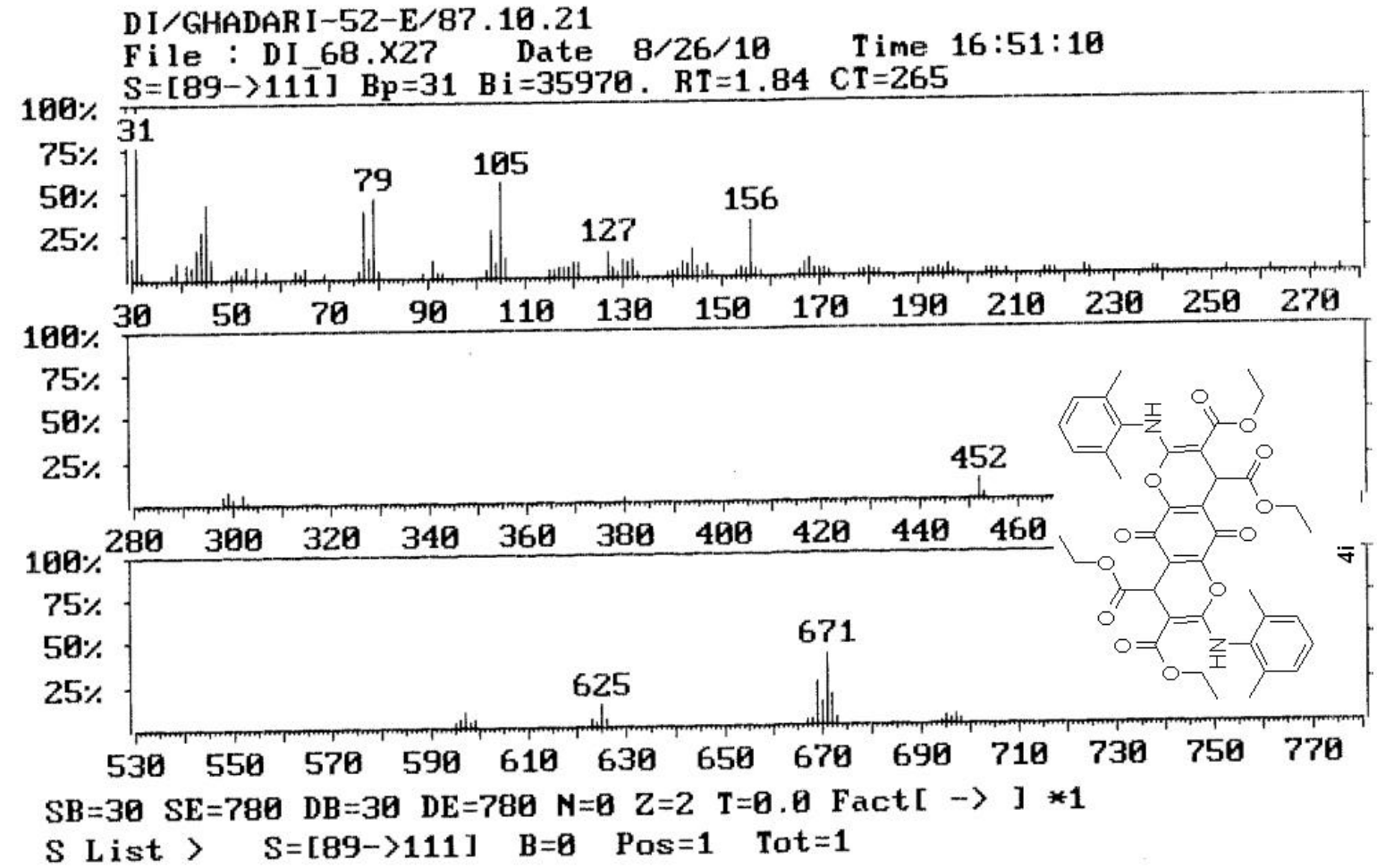

DI/GHADARI-52-U/87.10.28
File : DI_68.X67 Date 8/27/10 Time 02:30:26
S=[92->120] Bp=91 Bi=192880. RT=1.99 CT=280
100%
75%
50%
25%
91
*16
194
31
133
152
30 50 70 90 110 130 150 170 190 210 23
479
280 300 320 340 360 380 400 420 440 460 480 500 520
536
643
669
530 550 570 590 610 630 650 670 690 710 730 750 770
SB=30 SE=770 DB=30 DE=770 N=0 Z=2 T=0.0 Fact [124->909] *16
S List > S=[92->120] B=0 Pos=5 Tot=5
4h

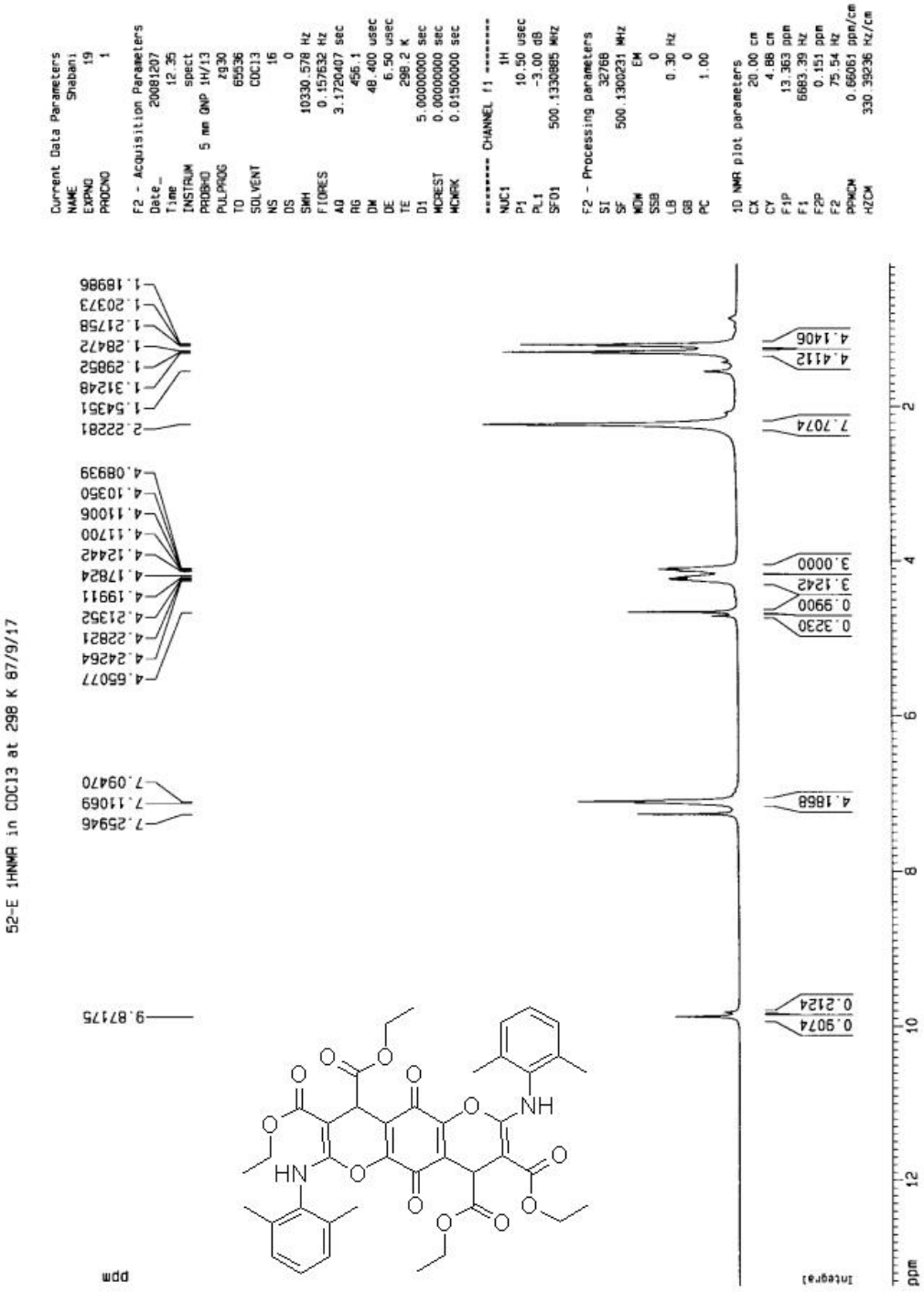
52-U
1H NMR
Current Data Parameters
NAME Ghadar1
EXPNO 47
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090105
Time 14.31
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323985 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 9.84 cm
F1P 11.314 ppm
F1 3395.52 Hz
F2P -0.990 ppm
F2 -297.10 Hz
PPMCM 0.61517 ppm/cm
HZCM 184.63135 Hz/cm
0.00991
1.24875
1.27239
4.13936
4.60392
4.65561
7.35117
5.4511
4.1990
3.0429
1.0000
5.1961
Integral
ppm
4h



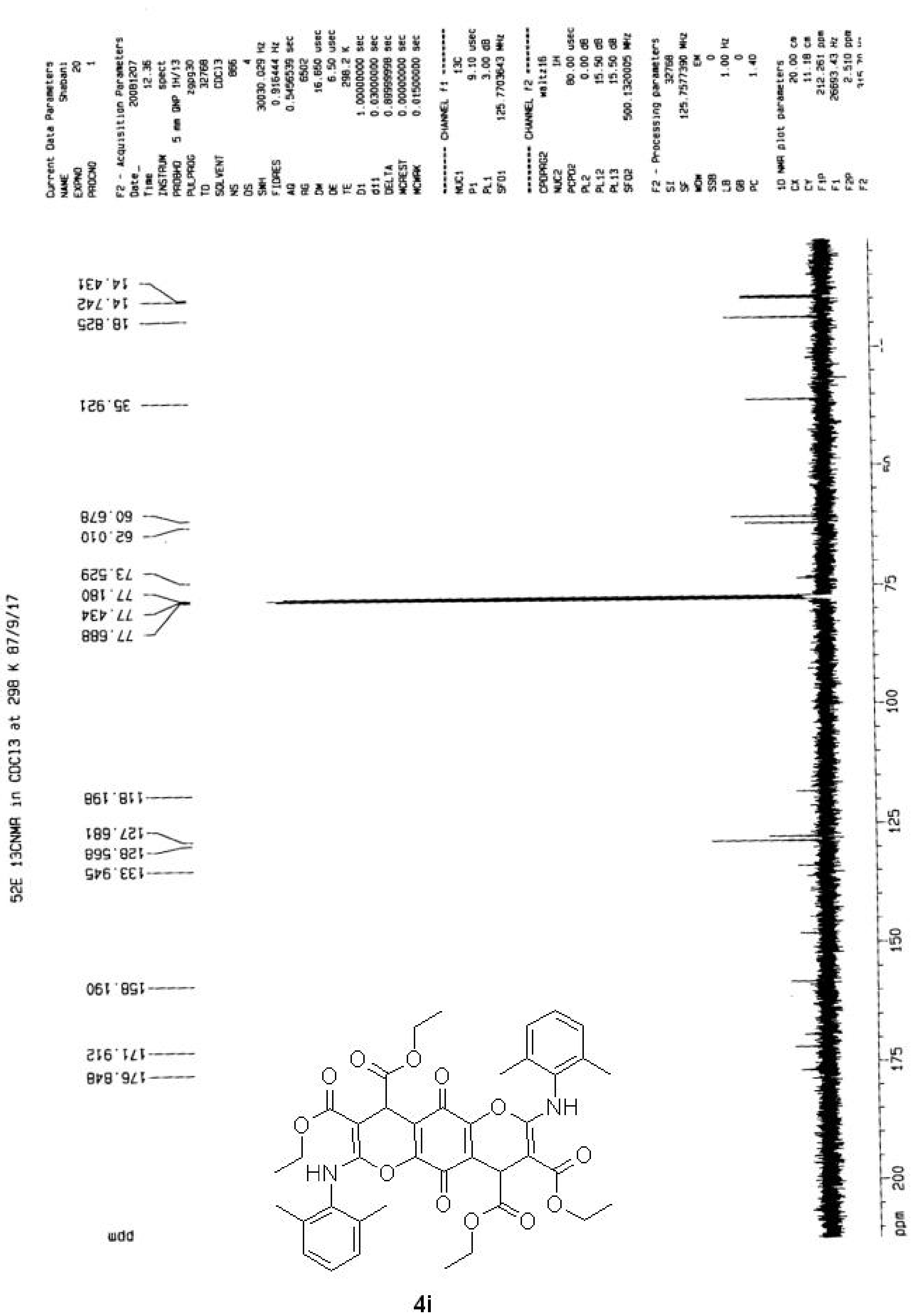

```
Current Data Parameters
NAME                  Ghadari
EXPNO                      48
PROCNO                      1

F2 - Acquisition Parameters
Date_               20090105
Time                   14.39
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                CDCl3
NS                        127
DS                          2
SWH                17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                       2048
DW                   27.800 usec
DE                    6.00 usec
TE                   300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
d12                0.00002000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                       8.75 usec
PL1                     -2.00 dB
SFO1               75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   87.00 usec
PL2                     -2.00 dB
PL12                    12.00 dB
PL13                    18.00 dB
SFO2              300.1312005 MHz

F2 - Processing parameters
SI                        65536
SF                 75.4677490 MHz
WDW                          EM
SSB                           0
LB                       1.00 Hz
GB                            0
PC                         1.00

1D NMR plot parameters
CX                       20.00 cm
CY                       14.05 cm
F1P                    219.155 ppm
F1                   16539.10 Hz
F2P                    -19.167 ppm
F2                   -1446.51 Hz
PPMCM                 11.91609 ppm/cm
HZCM                899.28058 Hz/cm
```


%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3239.94
2972.90
1731.26
1678.74
1642.80
1584.85
1283.01
1214.07
1190.50
1097.11
1048.17
S2-E
4i

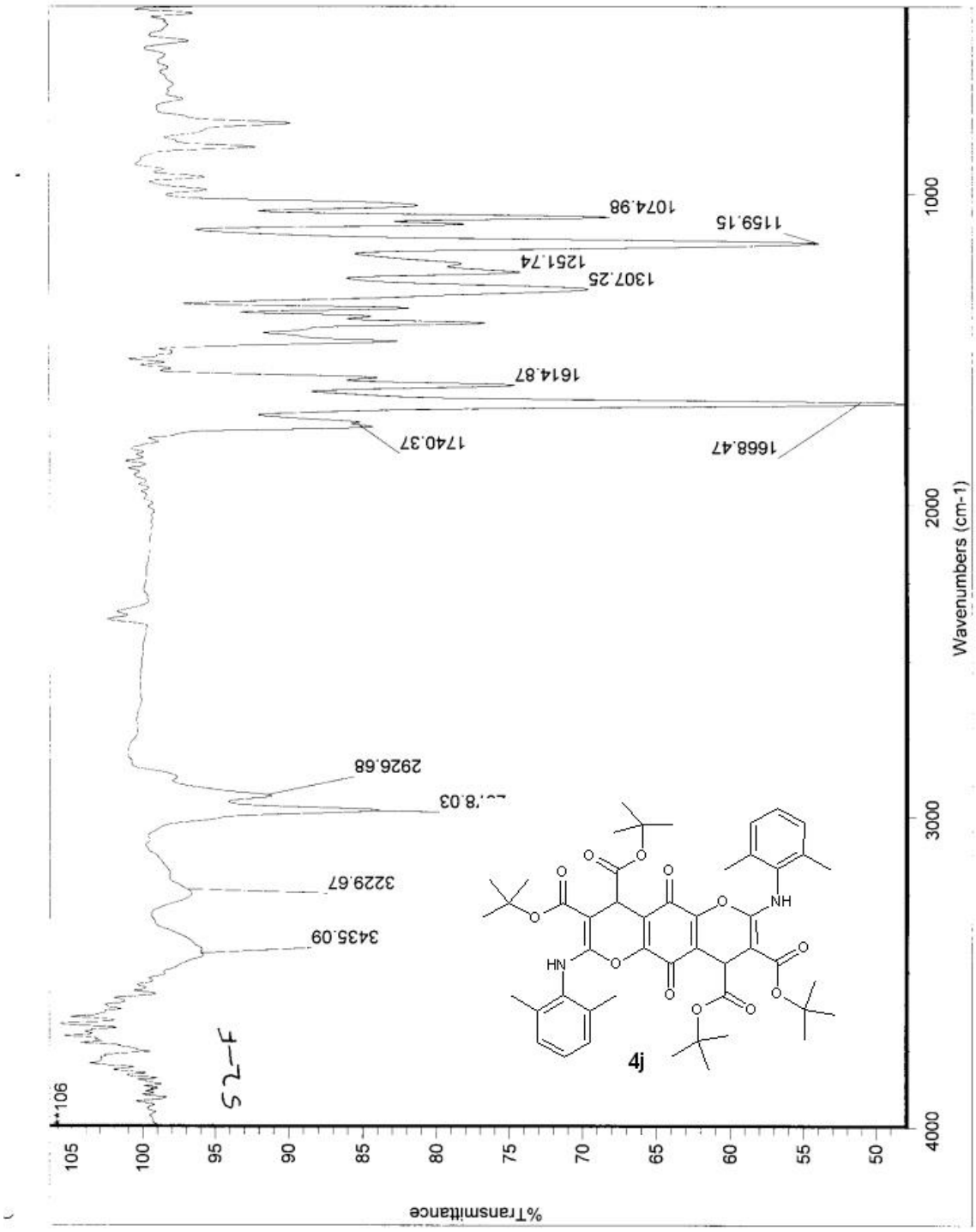

DI/GHADARI-52-E/87.10.21
File : DI_68.X27 Date 8/26/10 Time 16:51:10
S=[89->111] Bp=31 Bi=35970. RT=1.84 CT=265
100%
75%
50%
25%
31
79
105
127
156
30 50 70 90 110 130 150 170 190 210 230 250 270
452
280 300 320 340 360 380 400 420 440 460
671
625
530 550 570 590 610 630 650 670 690 710 730 750 770
4i
SB=30 SE=780 DB=30 DE=780 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[89->111] B=0 Pos=1 Tot=1

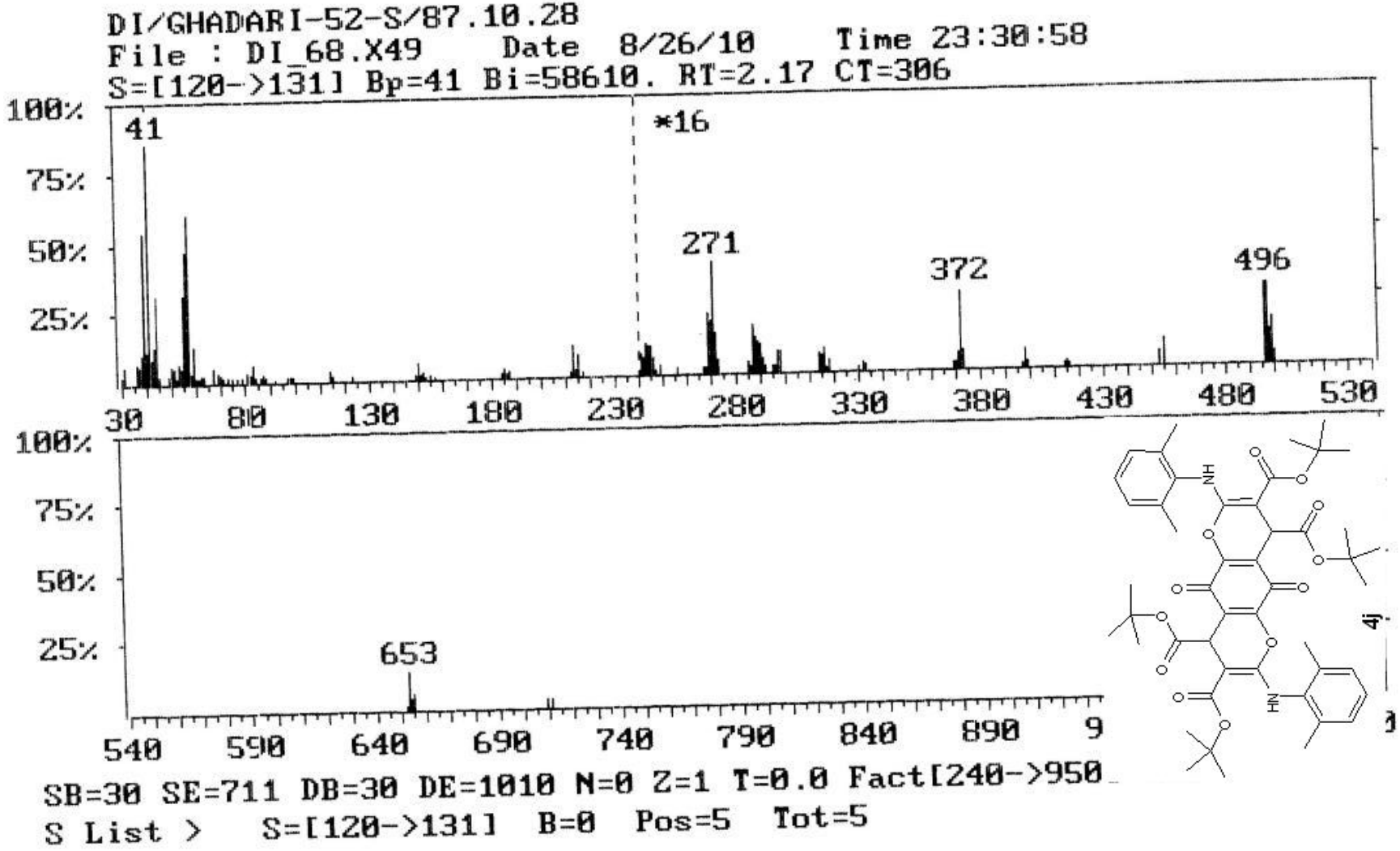

52-E 1HNMR in CDCl3 at 298 K 07/9/17
Current Data Parameters
NAME Shabani
EXPNO 19
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081207
Time 12.25
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 456.1
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 5.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300231 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.88 cm
F1P 13.363 ppm
F1 6683.39 Hz
F2P 0.151 ppm
F2 75.54 Hz
PPMCM 0.66061 ppm/cm
HZCM 330.39236 Hz/cm
9.87175
7.25946
7.11069
7.09470
4.65077
4.24264
4.22821
4.21352
4.19911
4.17824
4.12442
4.11700
4.11006
4.10350
4.08939
2.22281
1.54351
1.31248
1.29852
1.28472
1.21758
1.20373
1.18986
0.2124
0.9074
4.1868
7.7074
4.4112
4.1406
0.3230
0.9900
3.1242
3.0000
ppm
Integral

4i

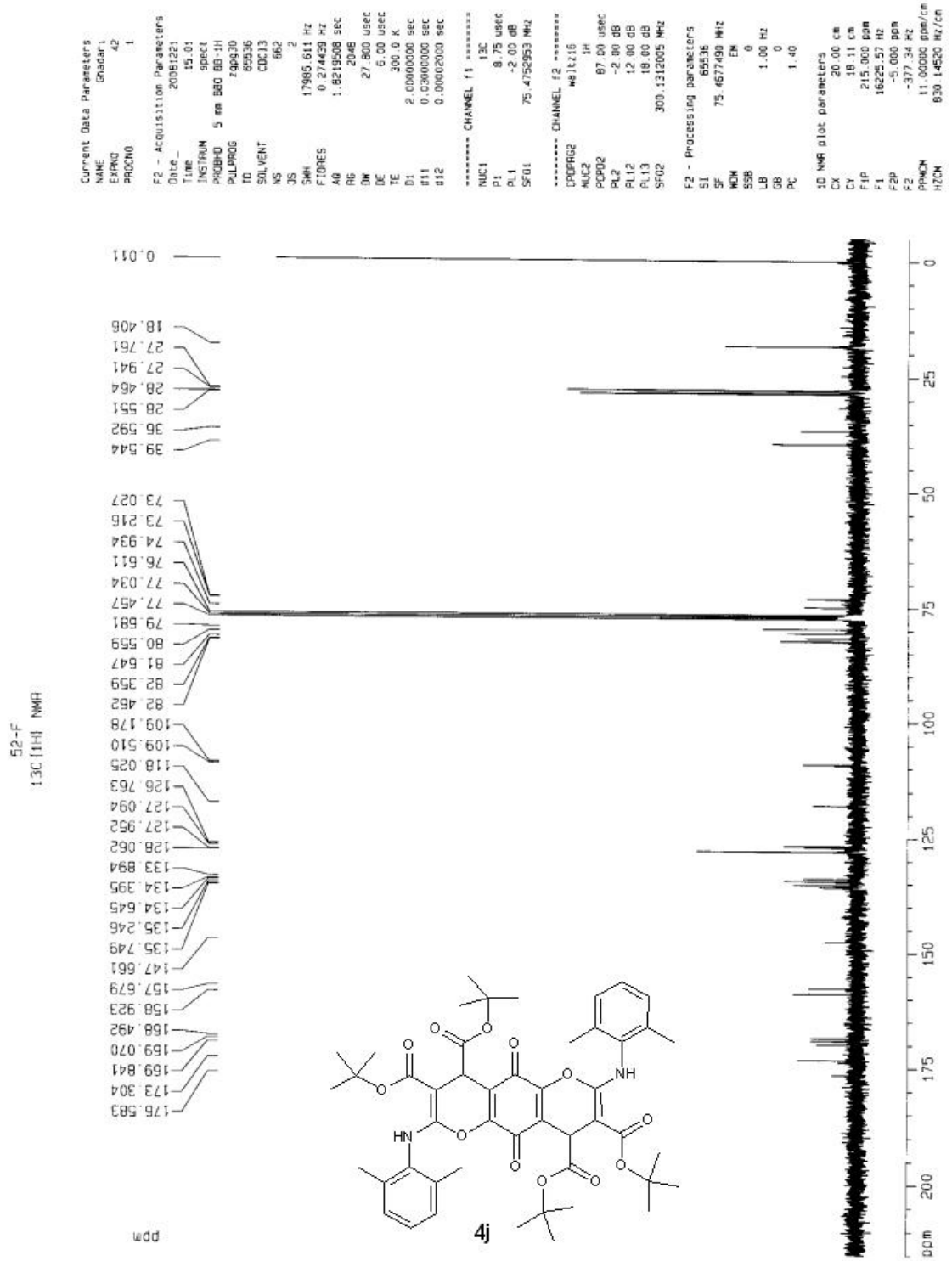

52E 13CNMR in CDCl3 at 298 K 87/9/17
14.431
14.742
18.825
35.921
60.678
62.010
73.529
77.180
77.434
77.688
118.198
127.681
128.568
133.945
158.190
171.912
176.848
ppm
HN
NH
O

4i

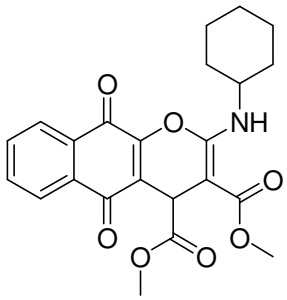

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
3435.09
3229.67
2926.68
1740.37
1668.47
1614.87
1307.25
1251.74
1159.15
1074.98
4j


DI/GHADARI-52-S/87.10.28
File : DI_68.X49 Date 8/26/10 Time 23:30:58
S=[120->131] Bp=41 Bi=58610. RT=2.17 CT=306
100%
75%
50%
25%
41
*16
271
372
496
30 80 130 180 230 280 330 380 430 480 530
100%
75%
50%
25%
653
540 590 640 690 740 790 840 890 9
SB=30 SE=711 DB=30 DE=1010 N=0 Z=1 T=0.0 Fact[240->950
S List > S=[120->131] B=0 Pos=5 Tot=5

52-F
1H NMR
Current Data Parameters
NAME Ghadari
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081216
Time 13.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 226.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323985 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 35.09 cm
F1P 11.040 ppm
F1 3313.50 Hz
F2P -1.119 ppm
F2 -335.76 Hz
PPMCM 0.60795 ppm/cm
HZCM 182.46300 Hz/cm
9.8531
7.1043
6.6538
4.5961
4.5568
2.2771
2.1898
2.1321
1.5263
1.4181
1.3989
1.3930
1.2785
0.9021
0.2140
0.0195
0.0133
-0.1792
1.000
3.462
0.404
0.461
6.618
1.901
11.642
11.520
1.378
ppm
Integral
4j

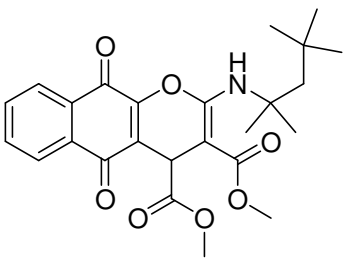

52-F
13C{1H} NMR
Current Data Parameters
NAME Ghadari
EXPNO 42
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061221
Time 15.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 662
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
CHANNEL f1
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 18.11 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 11.00000 ppm/cm
HZCM 830.14520 Hz/cm
0.011
18.406
27.761
27.941
28.464
28.551
36.592
39.544
73.027
73.216
74.934
76.611
77.034
77.457
79.681
80.559
81.647
82.359
82.462
109.178
109.510
118.025
126.763
127.094
127.952
128.062
133.894
134.395
134.645
135.246
135.749
147.661
157.679
158.923
168.492
169.070
169.841
173.304
176.583
ppm
4j

Dimethyl 2-(cyclohexylamino)-5,10-dihydro-5,10-dioxo-4H-benzo[g]chromene-3,4-dicarboxylate (10a):



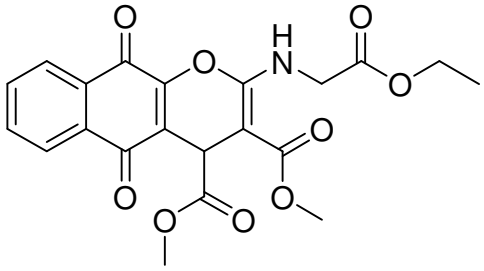
Brownish red powder (0.38 g, yield 89%). mp 177-178 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2936, 2859, 1732, 1680, 1637, 1598. MS, m/z (%): 425 (M^++1, 3), 366 (100), 284 (75), 252 (73), 196 (20), 140(25), 10 (76), 59 (50), 41 (85). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 1.42-2.08 (10H, m, 5CH_2 of cyclohexyl), 3.67 (3H, s, O-CH_3), 3.74 (3H, s, O-CH_3), 3.86 (1H, bs, C*H*-NH), 4.74 (1H, s, C*H*-CO_2Me), 7.27-8.15 (4H, m, arom), 8.64 (1H, bs, CH-N*H*). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 24.4, 24.5, 25.4, 33.4, 33.7, (C-cyclohexyl), 35.0 (*C*H-CO_2Me), 50.7 (CH-NH), 51.3, 52.7 (2O-CH_3), 72.3, 114.2, 123.8, 129.8, 130.0, 131.8, 135.1, 135.4, 156.9, 158.2 (C-alkene, C-arom), 169.3, 172.9, 177.7, 177.9 (4C=O). Anal. Calcd for $C_{23}H_{23}NO_7$: C, 64.93; H, 5.45; N, 3.29; Found: C, 64.88; H, 5.49; N, 3.32.

dimethyl 2-(2,4,4-trimethylpentan-2-ylamino)-5,10-dihydro-5,10-dioxo-4H-benzo[g]chromene-3,4-dicarboxylate (10b):



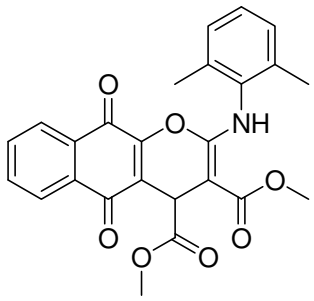
Dark orange powder (0.34 g, yield 75%). mp 183-185 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2957, 2865, 1724, 1673, 1607. MS, m/z (%): 455 (M^+-59, 50), 324 (45), 284 (100), 252 (25), 57 (24), 41 (25). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 0.99 (9H, s, $C(CH_3)_3$), 1.54 (6H, s, 2CH_3), 1.89 (2H, s, CH_2), 3.66 (3H, s, O-CH_3), 3.74 (3H, s, O-CH_3), 4.87 (1H, s, C*H*-CO_2Me), 7.57-7.77 (2H, m, arom), 8.11-8.14 (2H, m, arom), 8.80 (1H, bs, NH). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 30.9, 31.2 (2CH_3), 31.4 (C(*C*H_3)$_3$), 31.6 (CH_2), 35.5 (*C*H-CO_2Me), 51.2, 52.7 (2O-CH_3), 52.9 (C-NH), 56.9 (*C*$(CH_3)_3$), 71.4, 122.1, 126.5, 126.7, 130.6, 131.5, 133.9, 134.5, 149.7, 159.9 (C-alkene, C-arom), 169.3, 171.2, 177.2, 182.7 (4C=O). Anal. Calcd for $C_{25}H_{29}NO_7$: C, 65.92; H, 6.42; N, 3.08; Found: C, 65.87; H, 6.49; N, 3.11.

dimethyl 2-((ethoxycarbonyl)methylamino)-5,10-dihydro-5,10-dioxo-4H-benzo[g]chromene-3,4-dicarboxylate (10c):



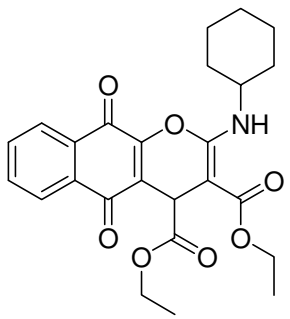
Yellow powder (0.26 g, yield 60%). mp 167-169 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2988, 2952, 1739, 1691, 1613, 1455. MS, m/z (%): 370 (M^+-59, 100), 296 (27), 253 (40), 45 (75). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 1.23 (3H, bs,CH_3), 3.63 (3H, s, O-CH_3), 3.70 (3H, s, O-CH_3), 4.16 (4H, bs, OC*H*$_2$CH$_3$, CO-C*H*$_2$-NH), 4.81 (1H, s, C*H*-CO_2Me), 7.70 (2H, bs, arom), 8.05 (2H, bs, arom), 8.74 (1H, bs, NH). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm)14.1 (OCH$_2$*C*H$_3$) 35.6 (*C*H-CO_2Me), 42.9(CO-*C*H$_2$-NH), 51.5, 52.8 (2O-CH_3), 61.7 (O*C*H$_2$CH$_3$), 73.5, 122.0, 126.5, 126.7, 130.5, 131.4, 133.9, 134.6, 134.9, 149.4, 158.6 (C-alkene, C-arom), 168.8, 169.7, 171.9, 176.8, 182.6 (5C=O). Anal. Calcd for $C_{21}H_{19}NO_9$: C, 58.74; H, 4.46; N, 3.26; Found: C, 58.79; H, 4.43; N, 3.32.

dimethyl 2-(2,6-dimethylphenylamino)-5,10-dihydro-5,10-dioxo-4H-benzo[g]chromene-3,4-dicarboxylate (10d):



Dark yellow powder (0.34 g, 77%). mp 215-217 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2957, 2844, 1734, 1681, 1617, 1586. MS, m/z (%): 447 (M^+, 2), 388 (100), 105 (25), 77 (35), 59 (20). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 2.28 (6H, s, 2CH_3), 3.71 (3H, s, O-CH_3), 3.83 (3H, s, O-CH_3), 4.95 (1H, s, C*H*-CO_2Me), 7.15 (3H, bs, arom) 7.72 (2H, m, arom), 8.04 (1H, d, $^3J_{HH}$=6.5 Hz, arom), 8.10 (1H, d, $^3J_{HH}$=6.5 Hz, arom), 9.90 (1H, bs, NH). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 18.4 (CH_3), 35.8 (*C*H-CO_2Me), 51.5, 52.8 (2O-CH_3), 73.1, 121.8, 126.5, 126.7, 127.4, 128.2, 128.3, 128.9, 132.9, 133.9, 134.5, 135.1, 148.3, 158.2 (C-alkene, C-arom), 168.5, 171.2, 175.9, 182.8 (4C=O). Anal. Calcd for $C_{25}H_{21}NO_7$: C, 67.11; H, 4.73; N, 3.13; Found: C, 67.19; H, 4.76; N, 3.17.

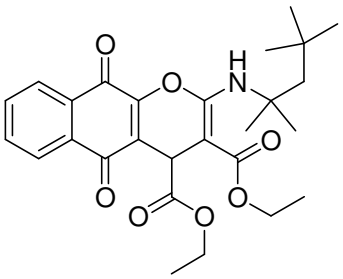
diethyl 2-(cyclohexylamino)-5,10-dihydro-5,10-dioxo-4H-benzo[g]chromene-3,4-dicarboxylate(10e):



Orange powder (0.38 g, 84%). mp: 164-166 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2926, 2854, 1740, 1683, 1632, 1586. MS, m/z (%): 380 (M^+-73, 50), 298 (25), 252 (25), 105 (20), 82 (18), 55 (73), 31 (100). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 1.10-2.17

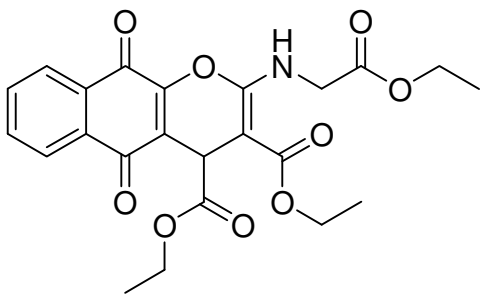
(16H, m, $5CH_2$ of cyclohexyl, $2OCH_2C\mathit{H_3}$), 3.54 (1H, bs, C*H*-NH), 3.88-4.4.24 (4H, m, $2OC\mathit{H_2}CH_3$), 4.72 (1H, s, C*H*-CO_2Me), 7.27-8.17 (4H, m, arom), 8.69 (1H, d, ^{3}J= 6.3 Hz, CH-N*H*). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 14.2, 14.5, ($2CH_3$), 24.4, 24.6, 25.41, 33.5, 33.8 (C-cyclohexyl), 35.40 (*C*H-CO_2Et), 50.7 (CH-NH), 59.9, 61.5 ($2OC\mathit{H_2}CH_3$), 72.5, 114.3, 123.9, 129.6, 129.9, 131.8, 135.2, 135.4, 156.9, 158.0 (C-alkene, C-arom), 168.9, 173.2, 177.8, 177.9, (4C=O). Anal. Calcd for $C_{25}H_{27}NO_7$: C, 66.21; H, 6.00; N, 3.09; Found: C, 66.27; H, 6.04; N, 3.15.

diethyl 2-(2,4,4-trimethylpentan-2-ylamino)-5,10-dihydro-5,10-dioxo-4H-benzo[g]chromene-3,4-dicarboxylate (10f):



Brownish red powder (0.36 g, 74%). mp 164-166 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2993, 2957, 1720, 1673, 1606. MS, m/z (%): 484 (M^++1, 4), 410 (60), 372 (15), 338 (45), 298 (100), 252 (30), 57 (27), 41 (30). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 0.97 (9H, s, $C(CH_3)_3$), 1.21 (3H, t, $^3J_{HH}$=7.0 Hz, $OCH_2C\mathit{H_3}$), 1.29 (3H, t, $^3J_{HH}$=7.0 Hz, $OCH_2C\mathit{H_3}$), 1.53 (6H, s, $2CH_3$), 1.88 (2H, bs, CH_2), 4.08-4.22 (4H, m, $2OC\mathit{H_2}CH_3$), 4.84 (1H, S, C*H*-CO_2Et), 7.73-7.76 (2H, m, arom), 8.09-8.12 (2H, m, arom), 8.81 (1H, bs, NH). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 14.1, 14.5 (2 $OCH_2\mathit{C}H_3$), 30.9, 31.3 ($2CH_3$), 31.4($C(\mathit{C}H_3)_3$), 31.6 (CH_2), 35.8 (*C*H-CO_2Et), 52.8 ($\mathit{C}(CH_3)_3$), 56.8 (C-NH), 59.7, 61.4 ($2OC\mathit{H_2}CH_3$), 71.6, 122.1, 126.5, 126.7, 130.6, 131.5, 133.9, 134.5, 149.6, 159.7 (C-alkene, C-arom), 169.0, 172.0, 177.2, 182.8 (4C=O). Anal. Calcd for $C_{27}H_{33}NO_7$: C, 67.06; H, 6.88; N, 2.90; Found: C, 67.11; H, 6.91; N, 2.93.

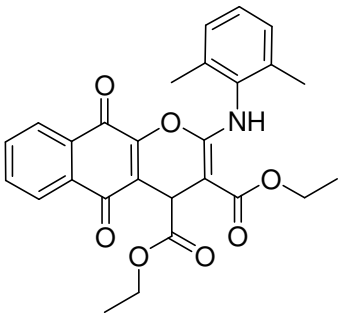
diethyl 2-((ethoxycarbonyl)methylamino)-5,10-dihydro-5,10-dioxo-4H-benzo[g]chromene-3,4-dicarboxylate (10g):



Dark yellow powder (0.28 g, yield 62%). mp 156-158 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2988, 2967, 1740, 1719, 1689, 1609. MS, m/z (%): 457 (M^++1, 5), 456 (M^+, 3), 384 (100), 310 (15), 282 (20), 253 (35), 59 (15), 31 (25). ^{1}H NMR (300 MHz, $CDCl_3$): δ_H (ppm) 1.12-1.30 (9H, m, $3OCH_2C\mathit{H_3}$),

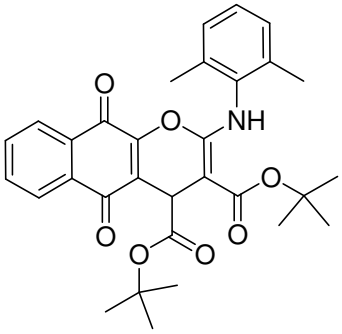
4.21-4.34 (8H, m, 3OC*H*$_2$CH$_3$, CO-C*H*$_2$-NH), 4.93 (1H, s, C*H*-CO$_2$Me), 7.74 (2H, bs, arom), 8.10 (2H, bs, arom), 8.83 (1H, bs, NH). ^{13}C NMR (75 MHz, CDCl$_3$): δ_C (ppm)13.9, 14.1, 14.1 (3OCH$_2$*C*H$_3$), 35.9 (*C*H-CO$_2$Me), 42.9(CO-*C*H$_2$-NH), 60.1, 61.3, 61.6 (3O*C*H$_2$CH$_3$), 73.7, 122.2, 126.2, 126.5, 130.6, 131.4, 133.0, 134.5, 134.9, 154.6, 158.5 (C-alkene, C-arom), 168.5, 169.0, 171.8, 176.9, 182.7 (5C=O). Anal. Calcd for $C_{23}H_{23}NO_9$: C, 60.39; H, 5.07; N, 3.06; Found: C, 60.42; H, 5.10; N, 3.11.

diethyl 2-(2,6-dimethylphenylamino)-5,10-dihydro-5,10-dioxo-4H-benzo[g]chromene-3,4-dicarboxylate (10h):



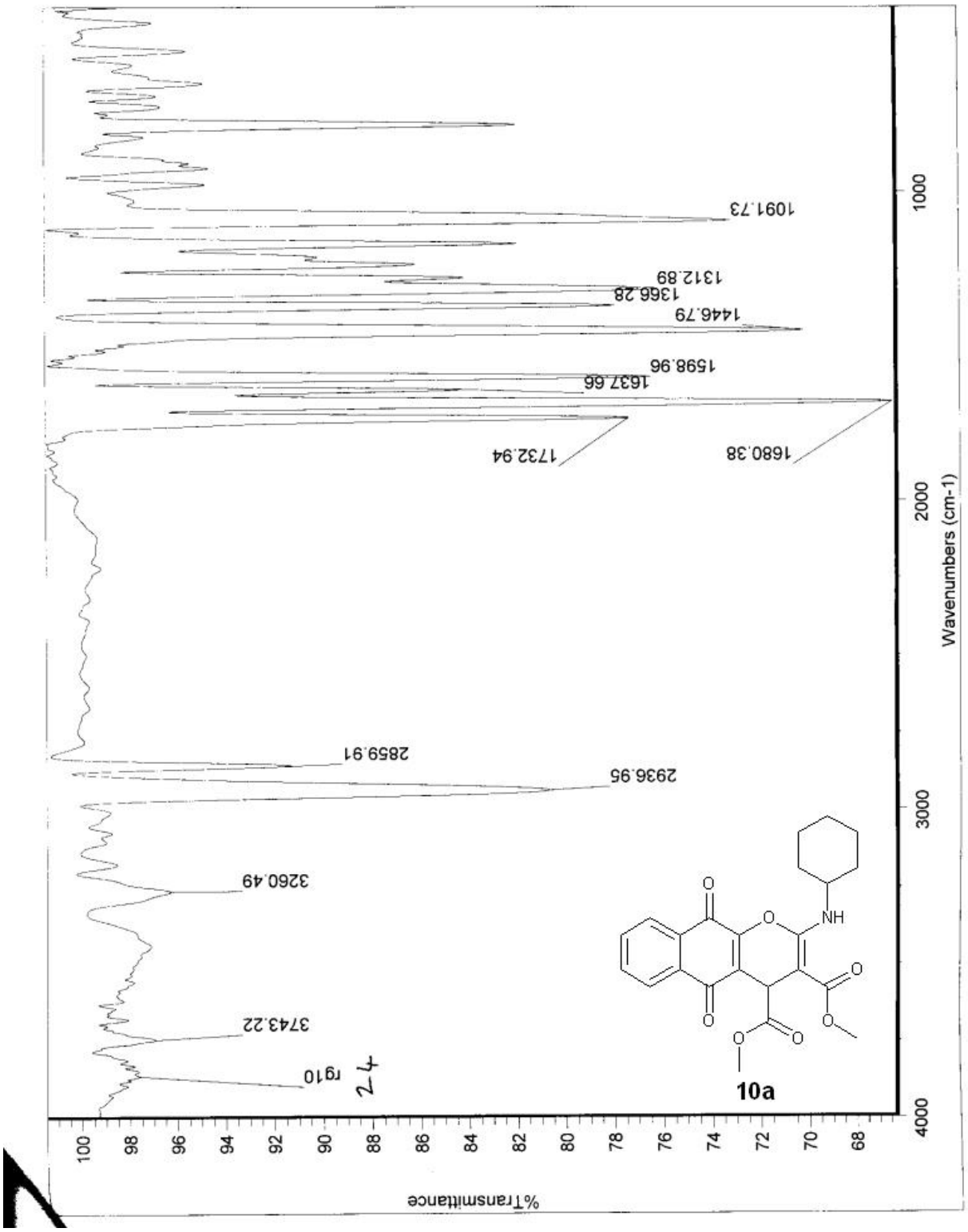
Brownish red powder (0.35 g, 74%). mp 172-174 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2978, 2895, 1723, 1672, 1597. MS, m/z (%): 475 (M$^+$, 30), 402 (100), 105 (20), 77 (28). ^{1}H NMR (300 MHz, CDCl$_3$): δ_H (ppm), 1.25-1.39 (6H, m, 2OCH$_2$C*H$_3$*), 2.28 (6H, s, 2CH$_3$), 4.16-4.34 (4H, m, 2OC*H*$_2$CH$_3$), 4.93 (1H, s, C*H*-CO$_2$Et), 7.14 (3H, bs, arom) 7.70-7.74 (2H, m, arom), 7.99 (1H, d, $^3J_{HH}$=6.6 Hz, arom), 8.10 (1H, d, $^3J_{HH}$=6.6 Hz, arom), 9.94 (1H, bs, NH). ^{13}C NMR (75 MHz, CDCl$_3$): δ_C (ppm) 14.1, 14.5 (2OCH$_2$*C*H$_3$), 18.4 (CH$_3$), 36.1 (*C*H-CO$_2$Me), 60.2, 61.5 (2O*C*H$_2$CH$_3$), 73.2, 121.9, 126.4, 126.6, 127.3, 128.1, 130.5, 131.4, 133.7, 133.9, 134.4, 135.8, 149.6, 158.0 (C-alkene, C-arom), 169.0, 171.8, 176.6, 182.7 (4C=O). Anal. Calcd for $C_{27}H_{25}NO_7$: C, 68.20; H, 5.30; N, 2.95; Found: C, 68.31; H, 5.27; N, 2.87.

di-tert-butyl 2-(2,6-dimethylphenylamino)-5,10-dihydro-5,10-dioxo-4H-benzo[g]chromene-3,4-dicarboxylate (10i):



Dark yellow powder (0.34 g, 64%). mp 171-173 ºC. IR (KBr) (ν_{max}/cm^{-1}): 2972, 2957, 1722, 1681, 1578. MS, m/z (%): 430 (M$^+$-101, 8), 374 (100), 105 (20), 77 (20), 57 (30), 41 (25). ^{1}H NMR (300 MHz, CDCl$_3$): δ_H (ppm) 1.44 (9H, s, C(CH$_3$)$_3$), 1.74 (9H, s, C(CH$_3$)$_3$) 2.17 (6H, s, 2CH$_3$), 4.76

(1H, s, C*H*-CO_2t-Bu), 7.13 (3H, bs, arom) 7.72-7.76 (2H, m, arom), 8.02-8.12 (2H, m, arom), 9.92 (1H, bs, NH). ^{13}C NMR (75 MHz, $CDCl_3$): δ_C (ppm) 18.4 (CH_3), 27.8, 28.5 (2OC(*C*H_3)$_3$), 37.5 (*C*H- CO_2t-Bu), 74.0 (C-alkene), 80.5, 81.5 (2O*C*(CH_3)$_3$), 121.4, 122.5, 127.5, 128.0, 130.6, 131.5, 133.7, 133.9, 134.0, 134.3, 135.6, 149.5, 157.7 (C-alkene, C-arom), 168.6, 170.7, 176.8, 182.7 (4C=O). Anal. Calcd for $C_{31}H_{33}NO_7$: C, 70.04; H, 6.26; N, 2.63; Found: C, 70.11; H, 6.28; N, 2.71.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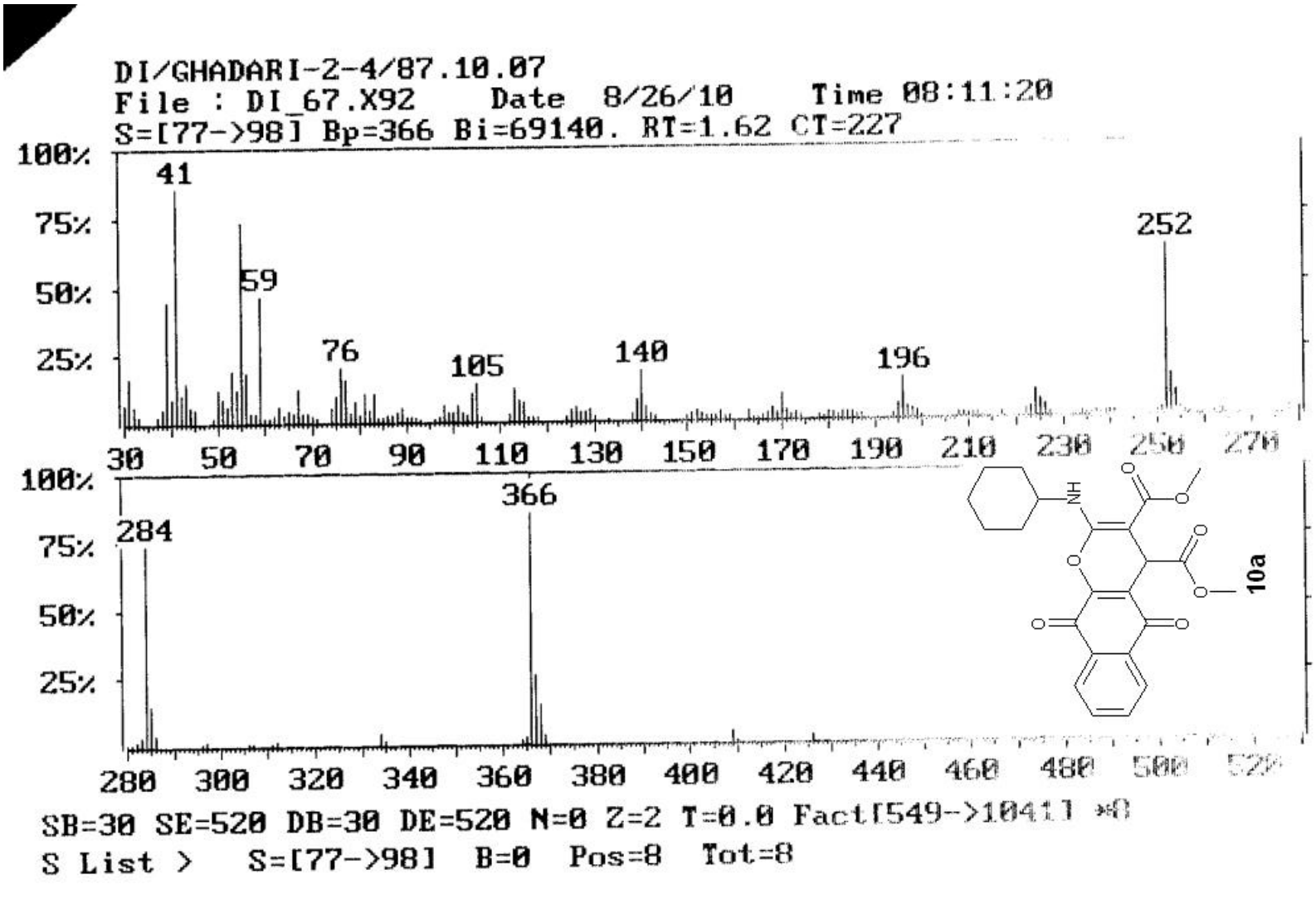
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24
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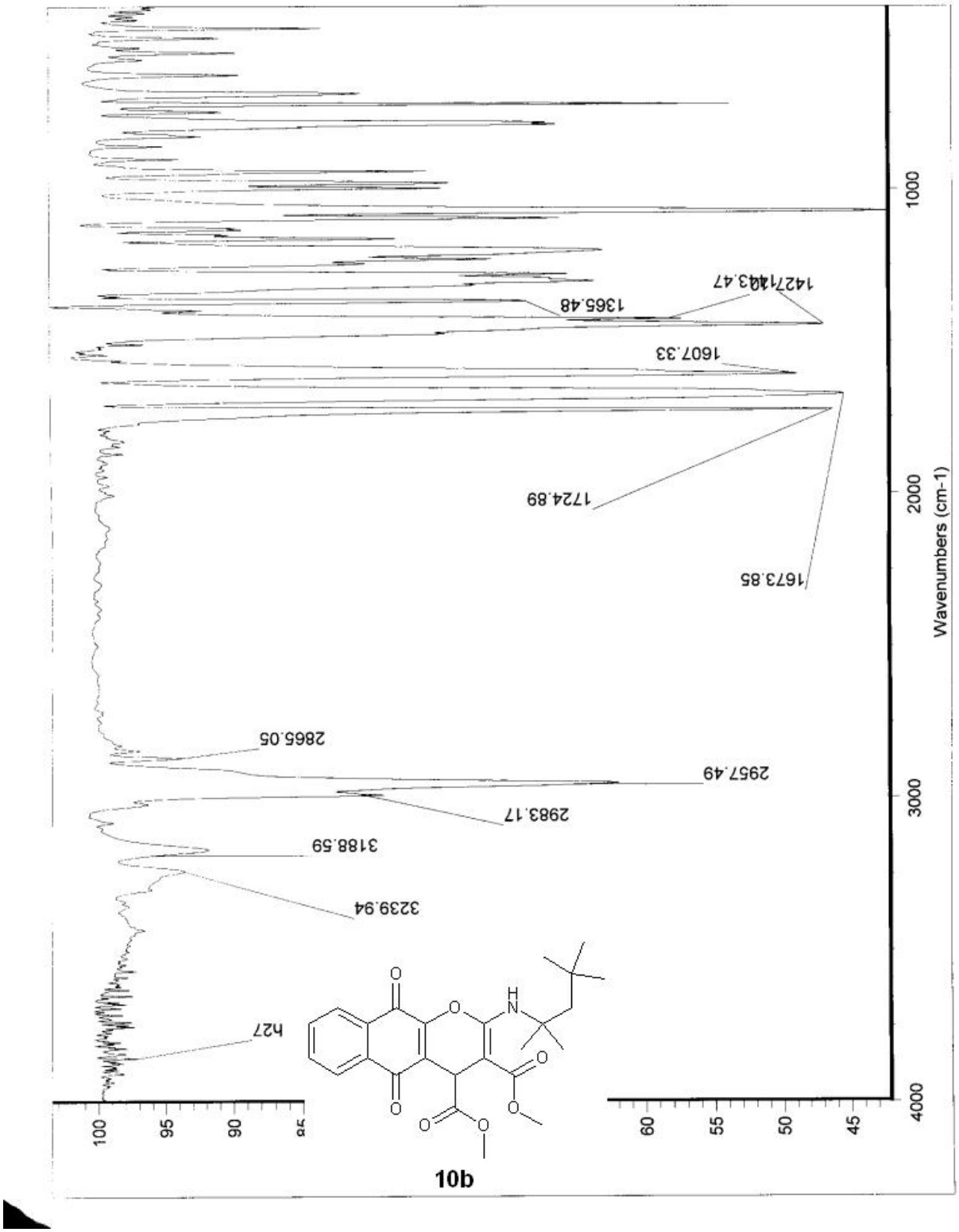
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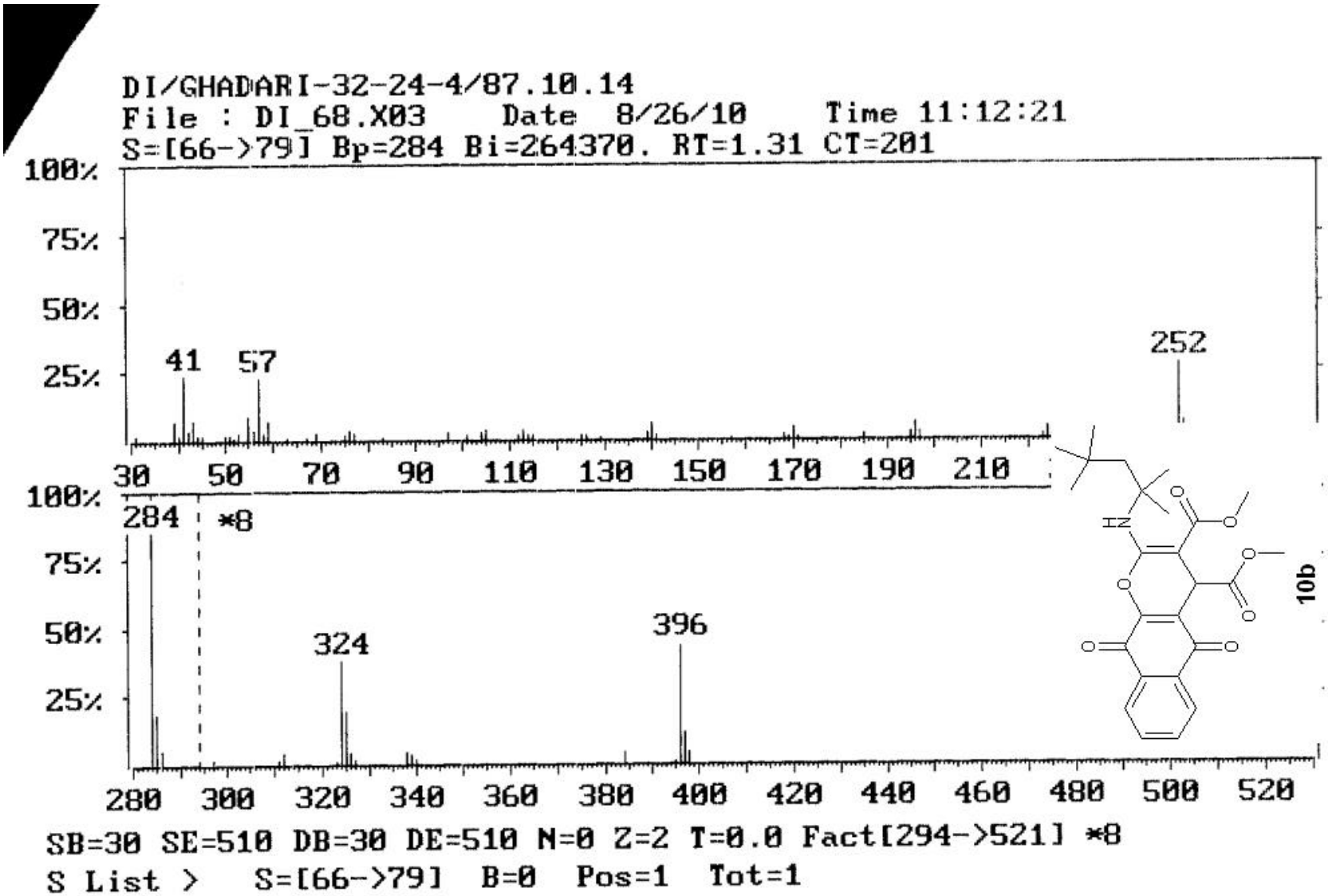
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24-4
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24-4
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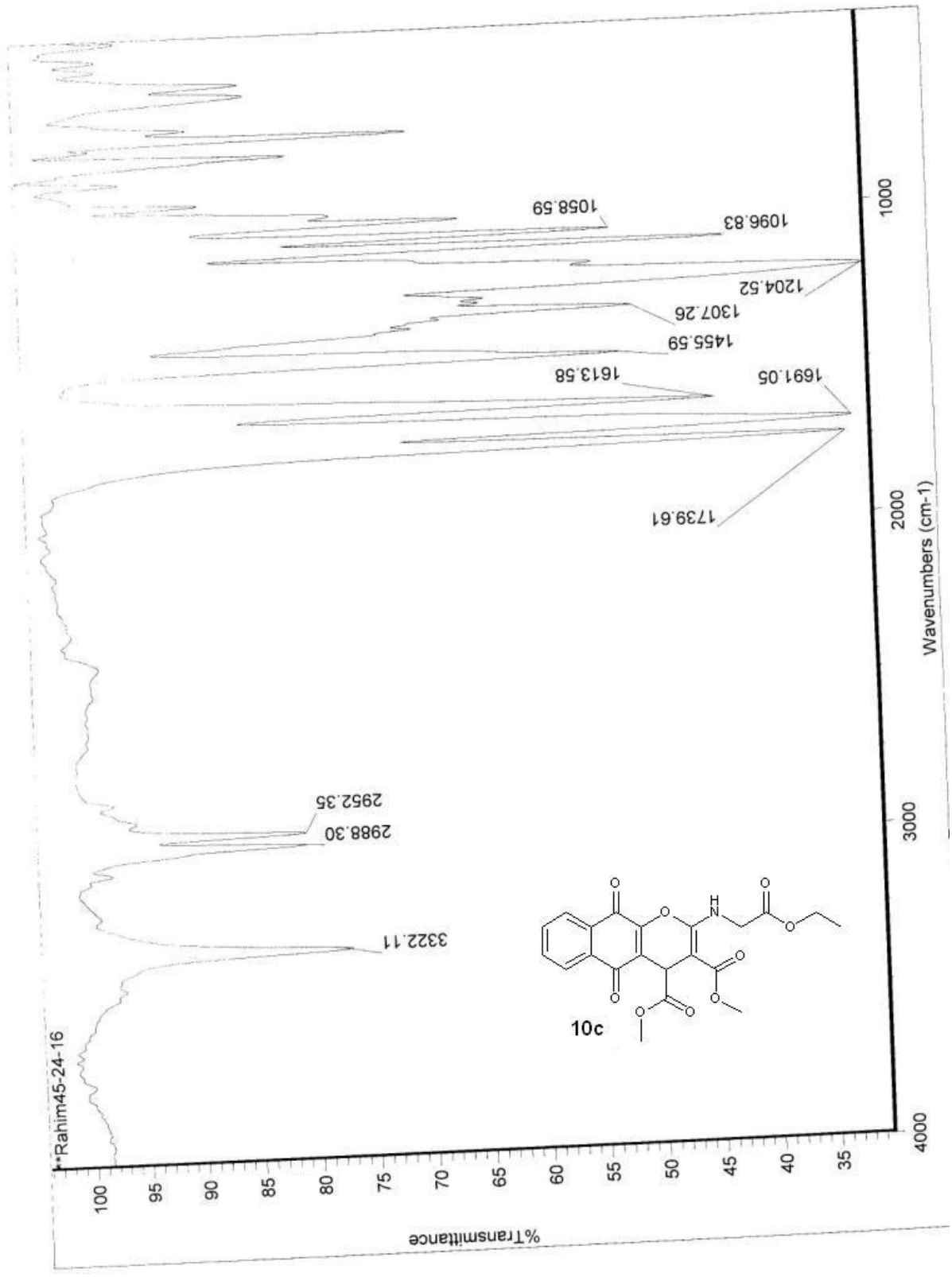
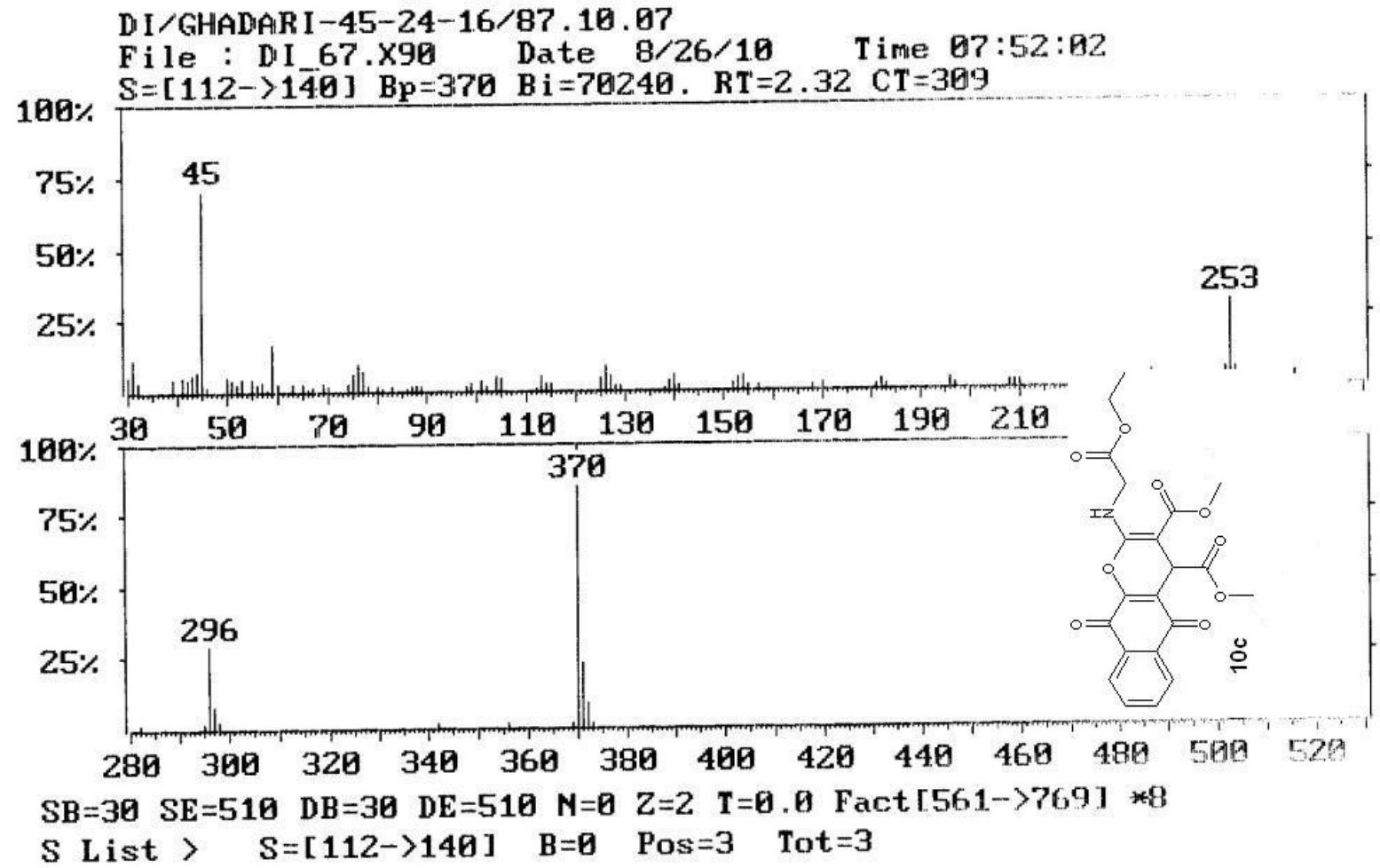
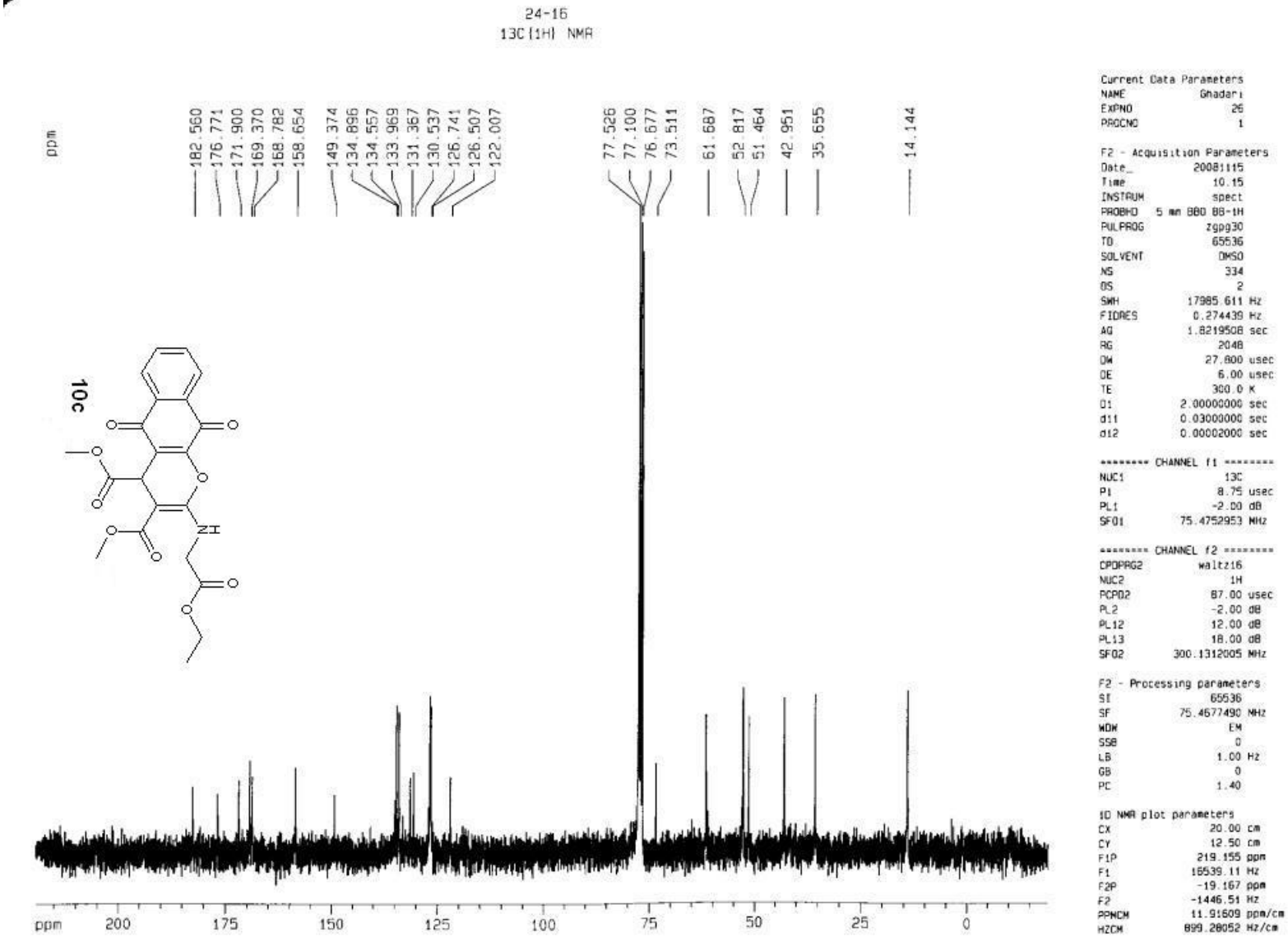
133.921
131.513
130.603
126.750
126.535
126.457
122.076
77.496
77.272
77.072
76.648
71.429
56.884
52.888
52.704
51.176
35.526
31.539
31.537
31.405
31.266
31.164
30.883
10b
ppm
0
50
100
150
200


Rahim45-24-16
%Transmittance
Wavenumbers (cm-1)
3322.11
2988.30
2952.35
1739.61
1691.05
1613.58
1455.59
1307.26
1204.52
1096.83
1058.59
10c


DI/GHADARI-45-24-16/87.10.07
File : DI_67.X90 Date 8/26/10 Time 07:52:02
S=[112->140] Bp=370 Bi=70240. RT=2.32 CT=309
100%
75%
50%
25%
45
253
30 50 70 90 110 130 150 170 190 210
100%
75%
50%
25%
370
296
280 300 320 340 360 380 400 420 440 460 480 500 520
10c
SB=30 SE=510 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[561->769] *8
S List > S=[112->140] B=0 Pos=3 Tot=3

Current Data Parameters
NAME Ghadari
EXPNO 25
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081115
Time 9.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.97 cm
F1P 11.485 ppm
F1 3447.13 Hz
F2P -0.913 ppm
F2 -274.08 Hz
PPMCM 0.61993 ppm/cm
HZCM 186.06088 Hz/cm
24-16
1H NMR
1.23559
3.53369
3.69732
3.72455
4.16121
4.81094
4.84052
7.70238
8.04900
8.74302
3.5370
8.0465
4.3368
1.3296
2.2418
2.7302
1.0000
10c
integral
ppm



Current Data Parameters
NAME Ghadari
EXPNO 26
PROCNO 1

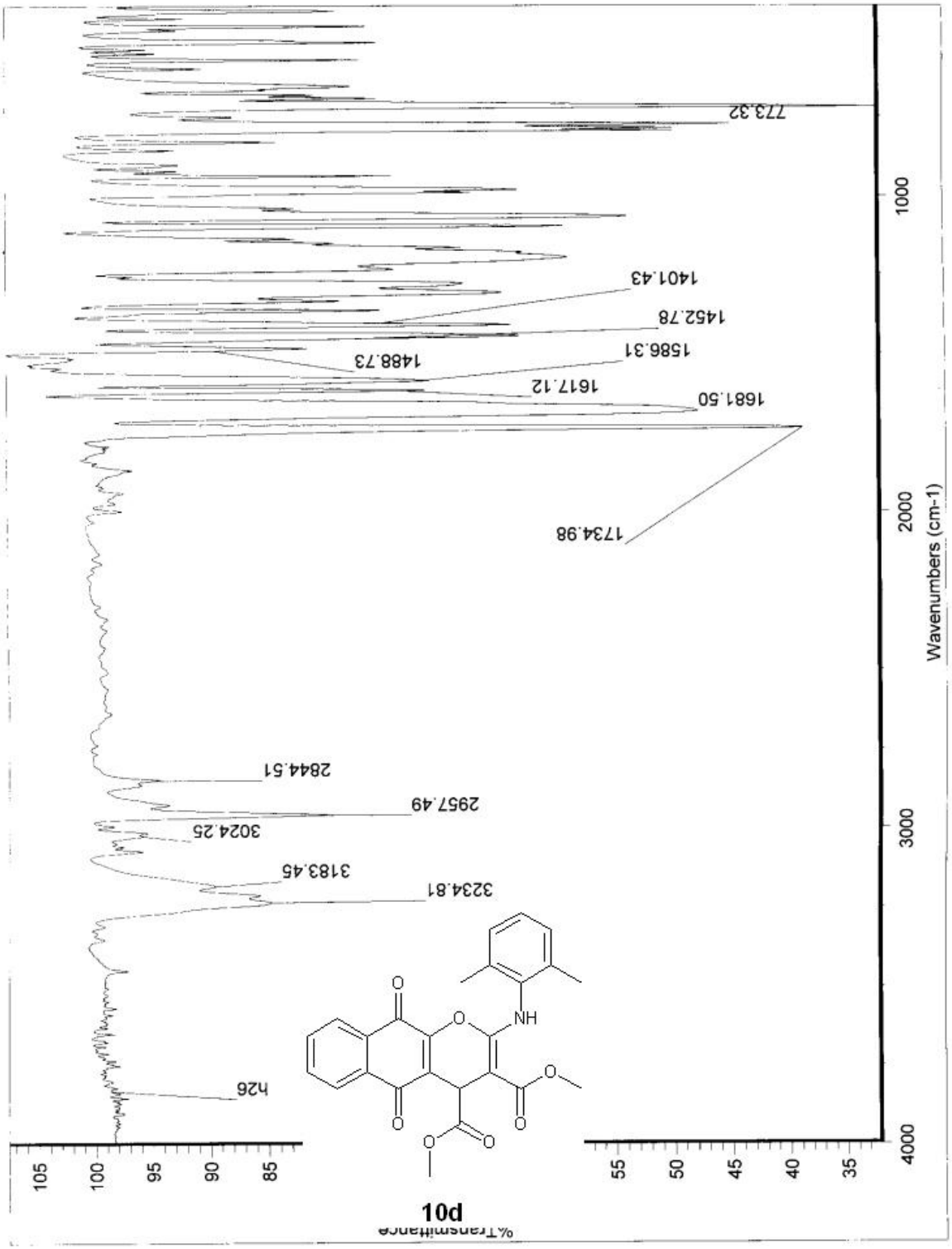
F2 - Acquisition Parameters
Date_ 20081115
Time 10.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 334
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

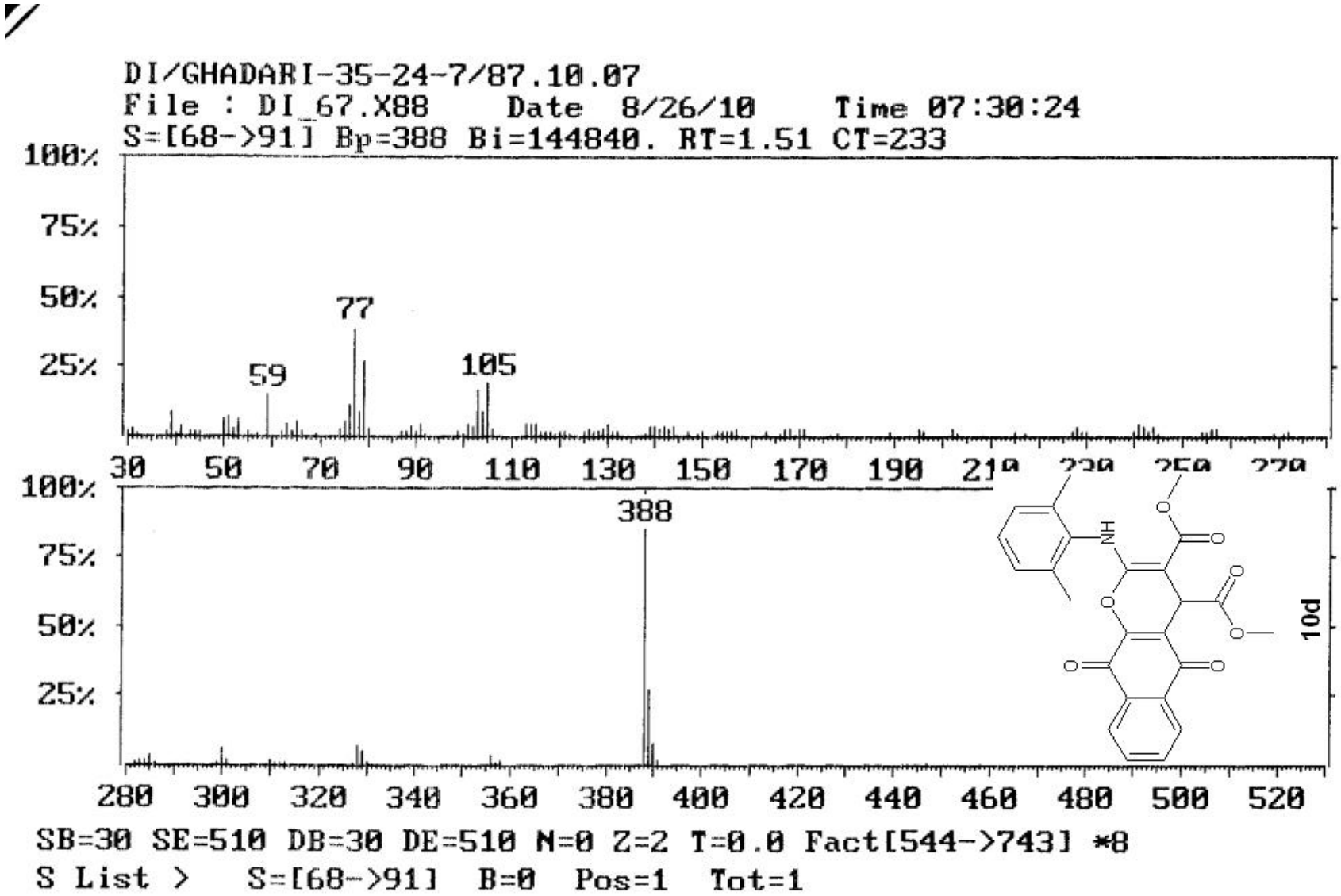
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

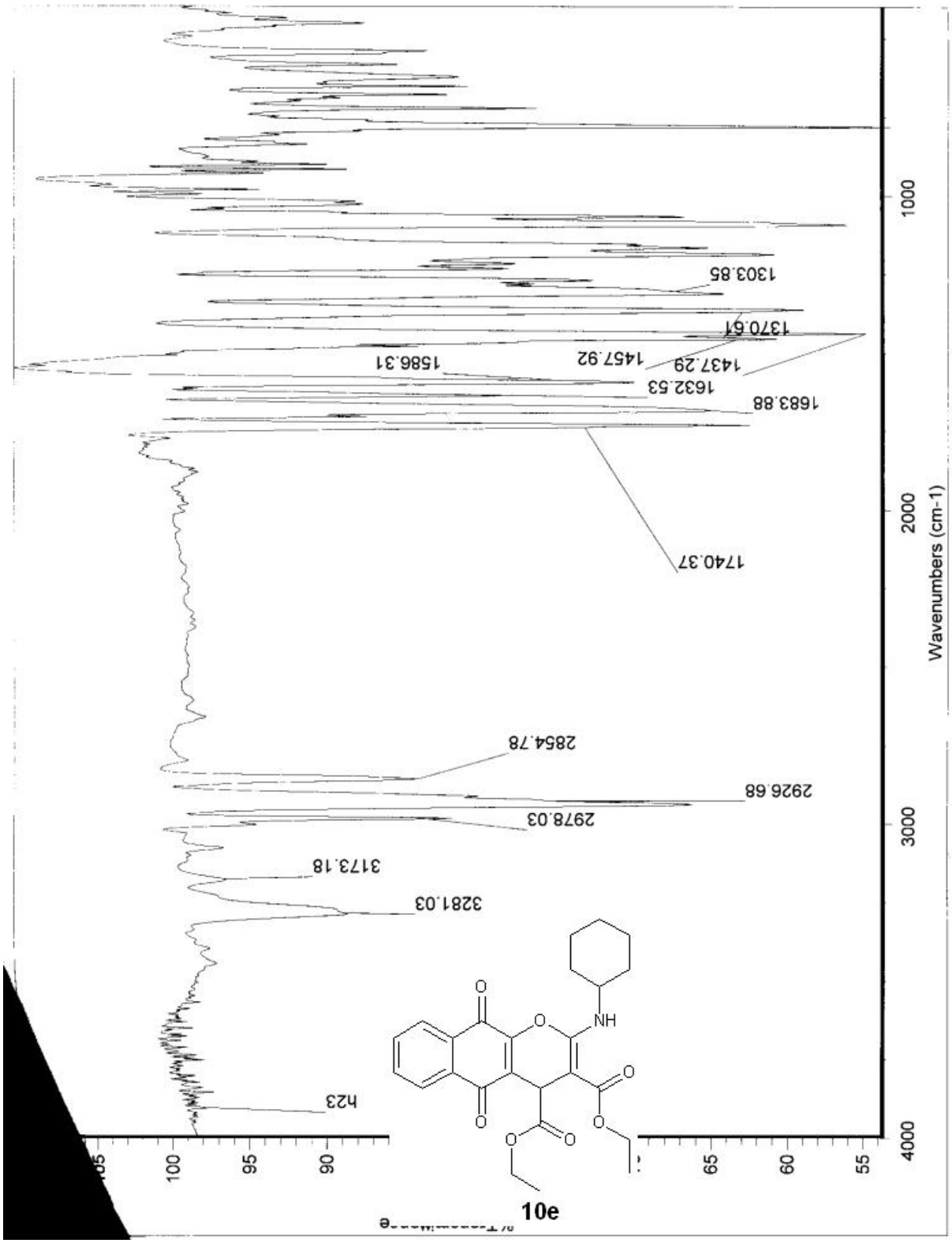
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 219.155 ppm
F1 16539.11 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28052 Hz/cm

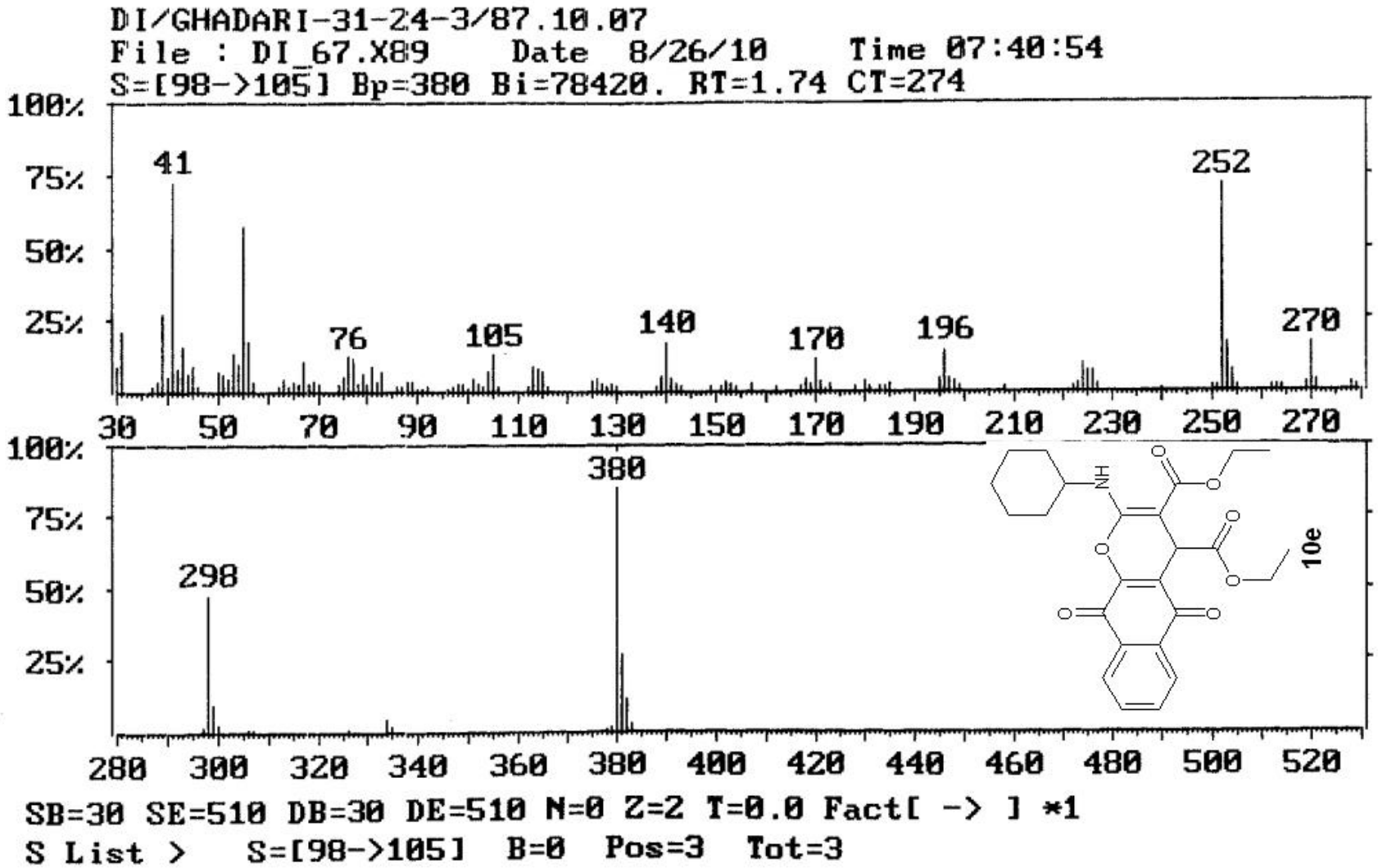

10d
%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
105
100
95
90
85
55
50
45
40
35
h26
3234.81
3183.45
3024.25
2957.49
2844.51
1734.98
1681.50
1617.12
1586.31
1488.73
1452.78
1401.43
773.32
O
NH
O
O
O
O
O
O

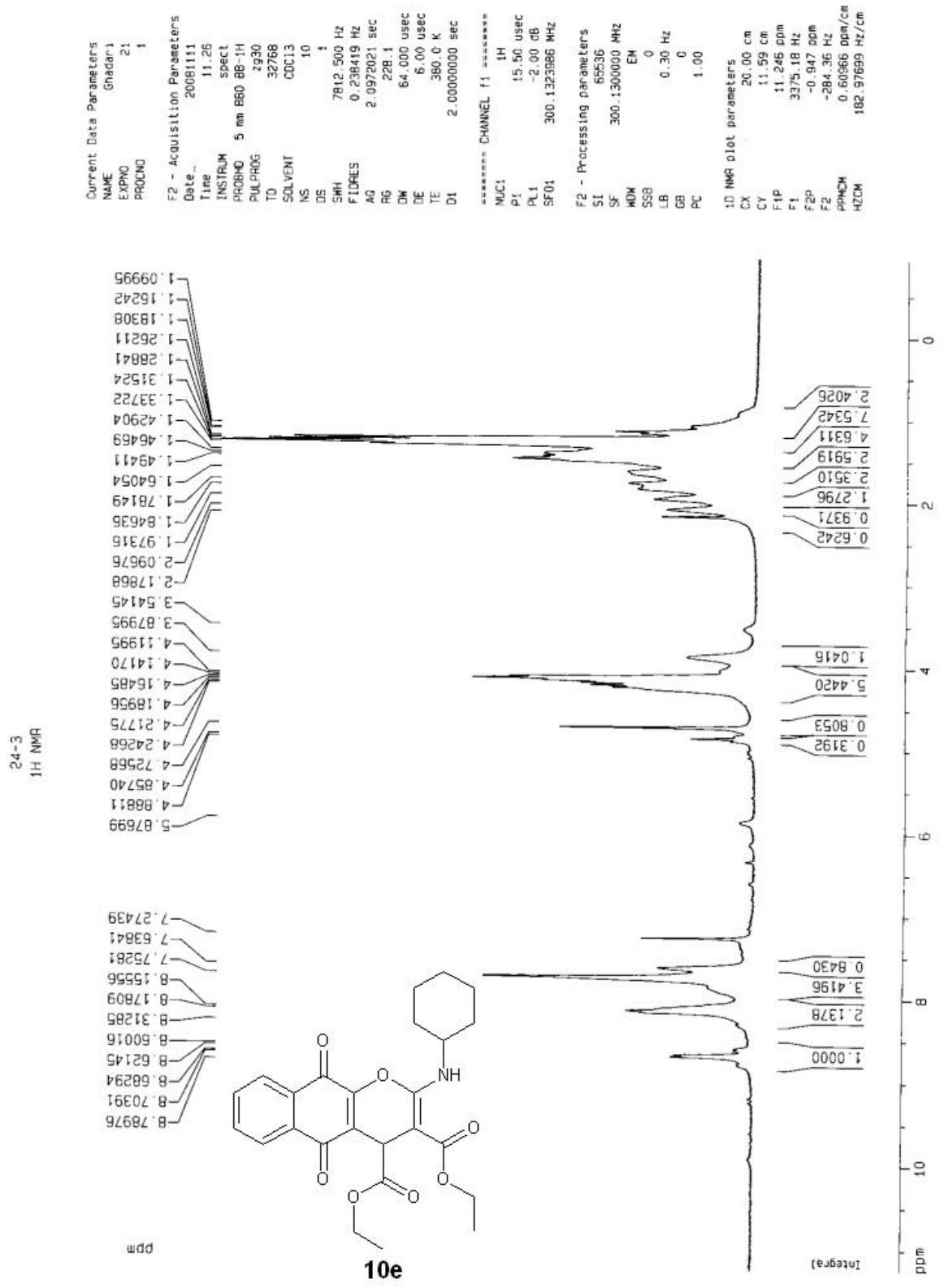

DI/GHADARI-35-24-7/87.10.07
File : DI_67.X88 Date 8/26/10 Time 07:30:24
S=[68->91] Bp=388 Bi=144840. RT=1.51 CT=233
100%
75%
50%
25%
77
59
105
30 50 70 90 110 130 150 170 190
100%
75%
50%
25%
388
280 300 320 340 360 380 400 420 440 460 480 500 520
10d
SB=30 SE=510 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[544->743] *8
S List > S=[68->91] B=0 Pos=1 Tot=1

24-7
1H NMR
Current Data Parameters
NAME Ghadari
EXPNO 16
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081103
Time 10.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.41 cm
F1P 11.380 ppm
F1 3415.45 Hz
F2P -0.864 ppm
F2 -259.25 Hz
PPMCM 0.61218 ppm/cm
HZCM 183.73471 Hz/cm
2.27737
3.71835
3.83501
4.95818
7.15445
7.72447
7.99637
8.01782
8.09853
8.12084
9.89837
6.1941
3.1413
3.3205
1.0000
3.1823
2.2330
1.0733
1.1389
0.9812
NH
O
O
O
O
O
O
O
O
10d
ppm
Integral

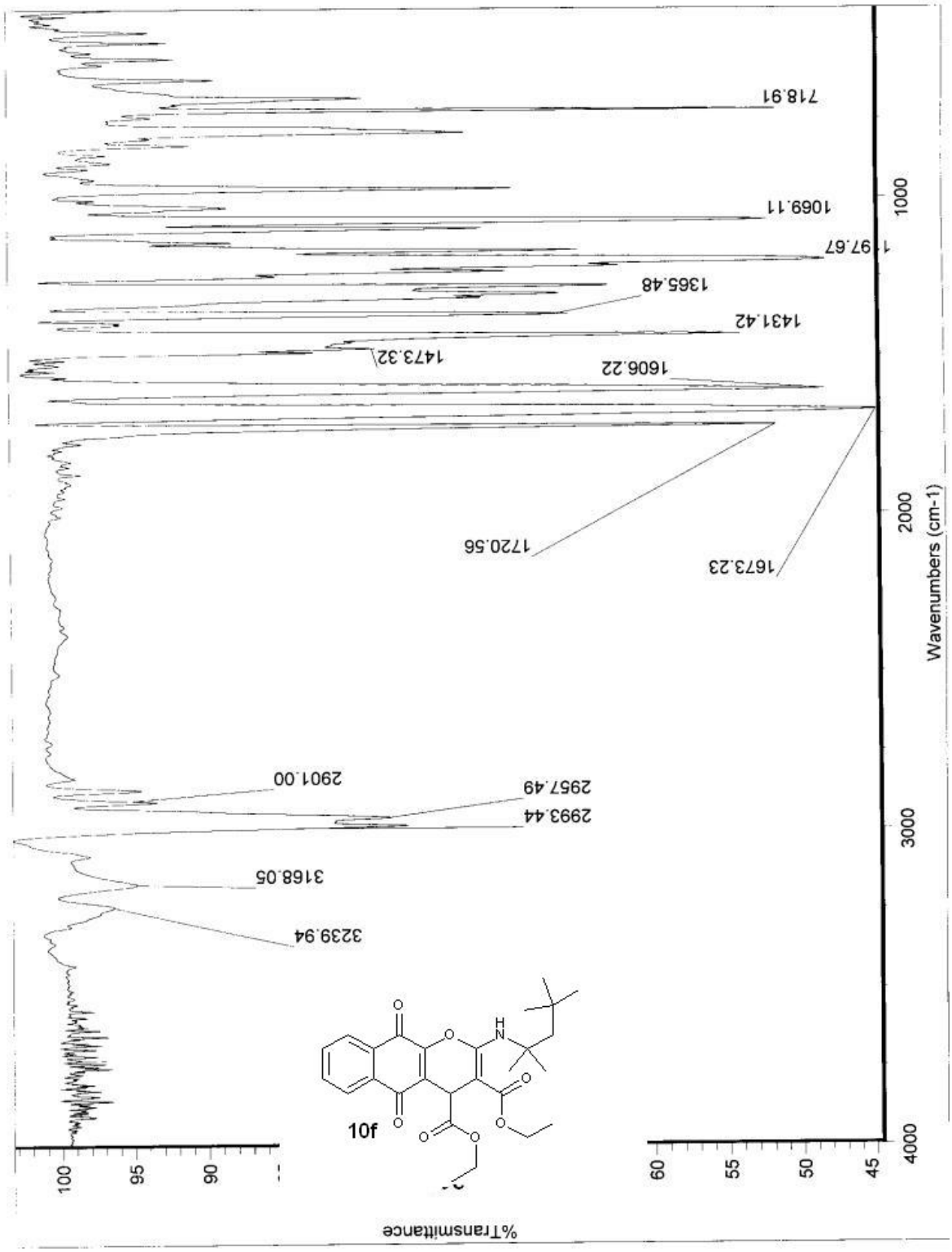
24-7
13C{1H} NMR
Current Data Parameters
NAME Chaderi
EXPNO 17
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081103
Time 10.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 658
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 10.80 cm
F1P 219.155 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm
18.465
35.833
51.539
52.875
73.073
76.690
77.114
77.538
126.510
126.681
127.428
128.174
133.983
134.478
158.231
NH
10d
ppm
0
50
100
150
200

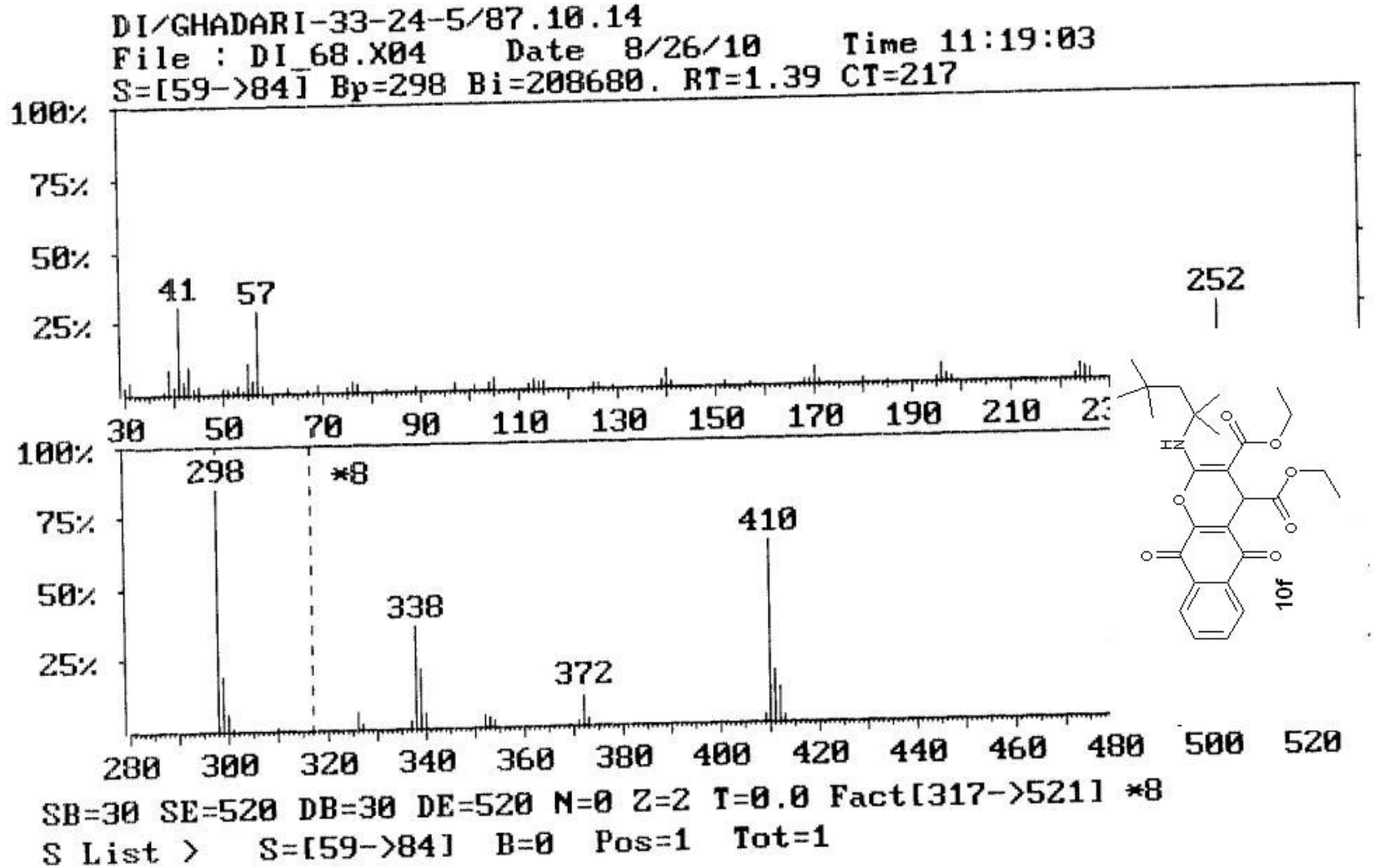

3281.03
3173.18
2978.03
2926.68
2854.78
1740.37
1683.88
1632.53
1586.31
1457.92
1437.29
1370.61
1303.85
Wavenumbers (cm-1)
4000
3000
2000
1000
NH
O
10e


DI/GHADARI-31-24-3/87.10.07
File : DI_67.X89 Date 8/26/10 Time 07:40:54
S=[98->105] Bp=380 Bi=78420. RT=1.74 CT=274
100%
75%
50%
25%
41
252
76
105
140
170
196
270
30 50 70 90 110 130 150 170 190 210 230 250 270
380
298
280 300 320 340 360 380 400 420 440 460 480 500 520
NH
O
10e
SB=30 SE=510 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[98->105] B=0 Pos=3 Tot=3


24-3
1H NMR
Current Data Parameters
NAME Ghadari
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081111
Time 11.26
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323886 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 11.59 cm
F1P 11.246 ppm
F1 3375.18 Hz
F2P -0.947 ppm
F2 -284.36 Hz
PPMCM 0.60966 ppm/cm
HZCM 182.97699 Hz/cm
1.0999
1.1524
1.1830
1.2621
1.2884
1.3152
1.3372
1.4290
1.4646
1.4941
1.6405
1.7814
1.8463
1.9731
2.0967
2.1786
3.5414
3.8799
4.1199
4.1417
4.1648
4.1895
4.2177
4.2426
4.7556
4.8574
4.8881
5.8769
7.2743
7.5384
7.7528
8.1555
8.1780
8.3128
8.5001
8.6214
8.6829
8.7039
8.7897
0.6242
0.9371
1.2796
2.3510
2.5919
4.6311
7.5342
2.4026
1.0000
2.1378
3.4196
0.8430
5.4420
1.0416
0.8053
0.3192
Integral
ppm
10e

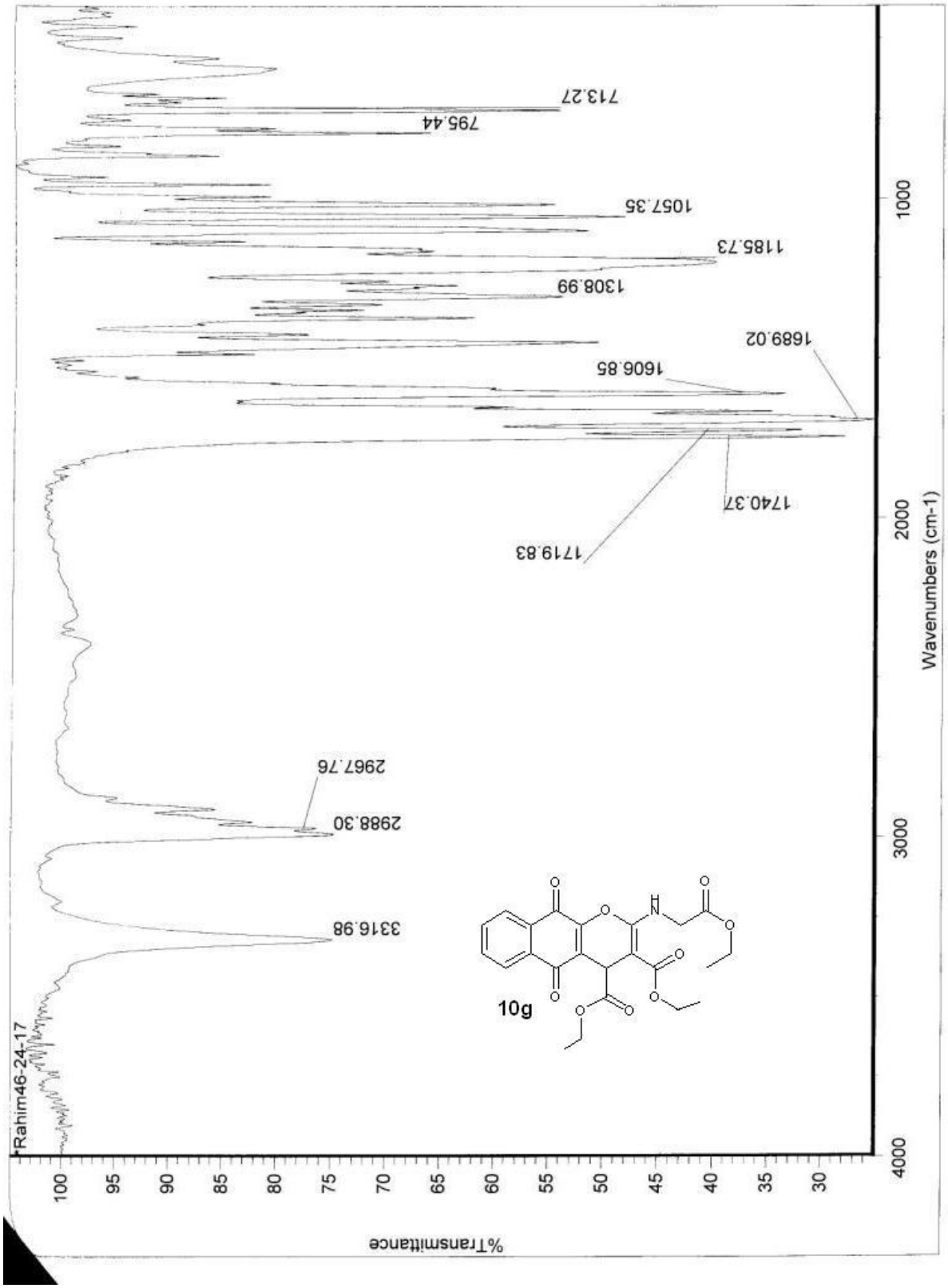
24-3
13C(1H) NMR
Current Data Parameters
NAME Ghadari
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081111
Time 11.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 282
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 40.77 cm
F1P 219.155 ppm
F1 16539.11 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28052 Hz/cm
14.160
14.525
24.422
24.459
24.601
25.409
33.462
33.805
35.400
50.701
59.903
61.458
72.510
76.669
77.092
77.299
77.388
77.515
77.808
114.341
123.878
129.988
131.775
135.250
135.449
156.932
158.014
168.998
177.804
177.863
NH
10e
ppm
0
50
100
150
200

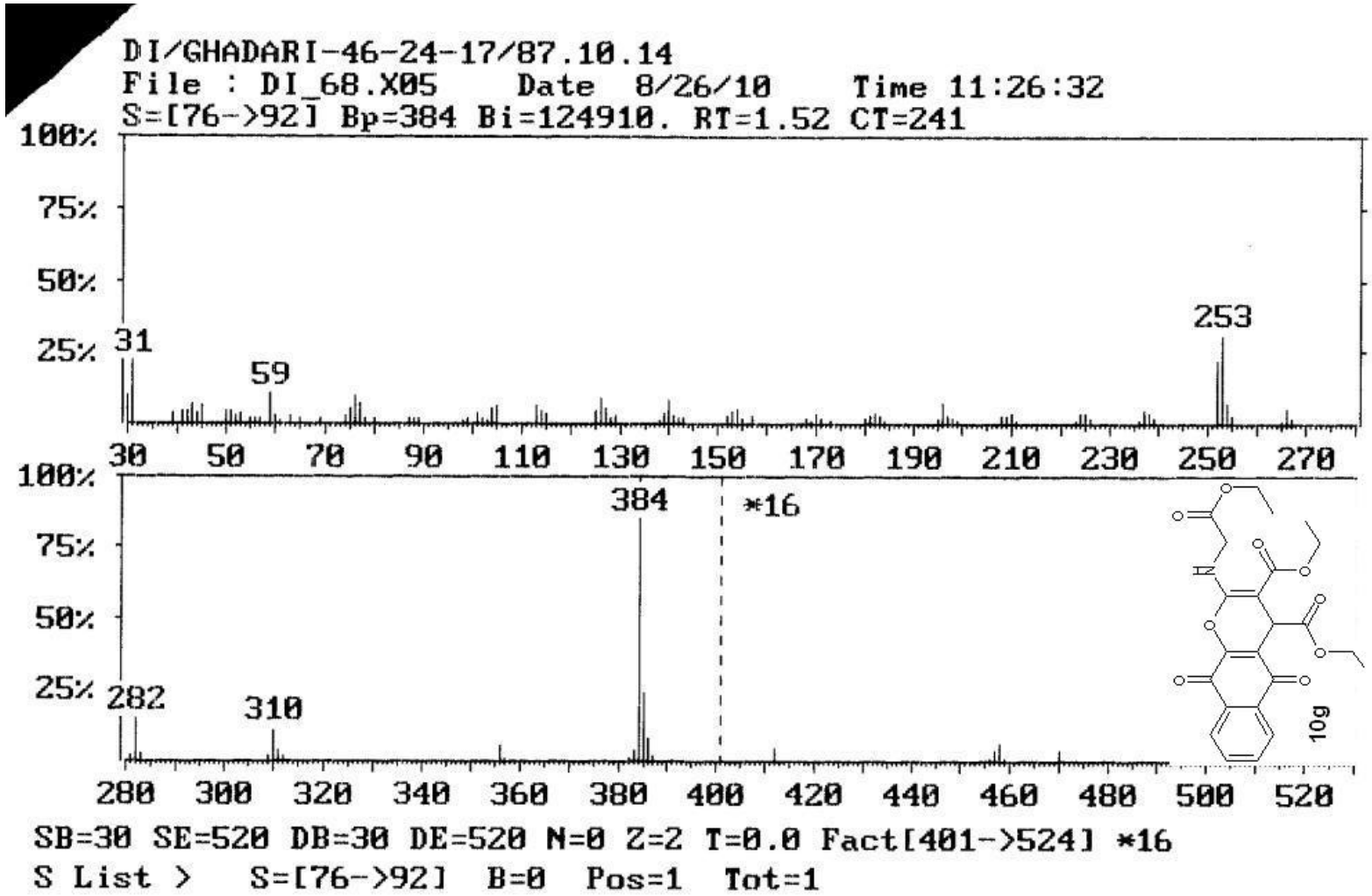

718.91
1069.11
1197.67
1365.48
1431.42
1473.32
1606.22
1673.23
1720.56
2901.00
2957.49
2993.44
3168.05
3239.94
10f
%Transmittance
Wavenumbers (cm-1)

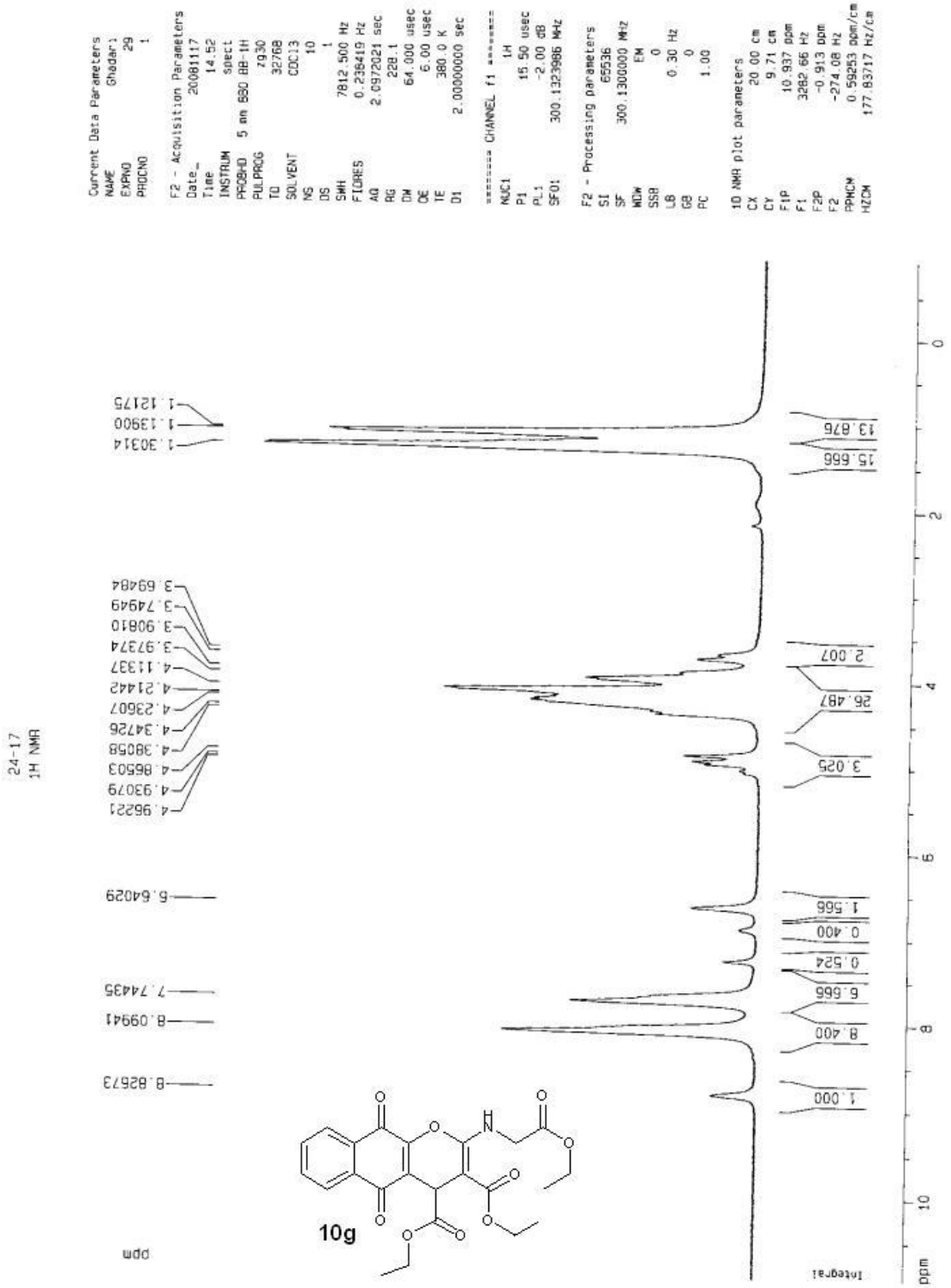

DI/GHADARI-33-24-5/87.10.14
File : DI_68.X04 Date 8/26/10 Time 11:19:03
S=[59->84] Bp=298 Bi=208680. RT=1.39 CT=217
100%
75%
50%
25%
41
57
252
30 50 70 90 110 130 150 170 190 210
100%
298
*8
410
338
372
280 300 320 340 360 380 400 420 440 460 480 500 520
10f
SB=30 SE=520 DB=30 DE=520 N=0 Z=2 T=0.0 Fact[317->521] *8
S List > S=[59->84] B=0 Pos=1 Tot=1

24-5
1H NMR
Current Data Parameters
NAME Gnadari
EXPNO 14
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081103
Time 10.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323985 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 11.91 cm
F1P 11.380 ppm
F1 3415.45 Hz
F2P -0.864 ppm
F2 -259.25 Hz
PPMCM 0.61218 ppm/cm
HZCM 183.73471 Hz/cm
0.83699
0.97601
1.18361
1.20690
1.23024
1.27004
1.29328
1.31663
1.53181
1.87694
4.08571
4.10815
4.13063
4.15570
4.19116
4.21524
4.84285
7.73225
7.74439
8.09444
8.10686
8.81360
10.224
3.809
3.869
7.203
2.574
4.546
0.995
2.176
2.245
1.000
10f
ppm
Integral

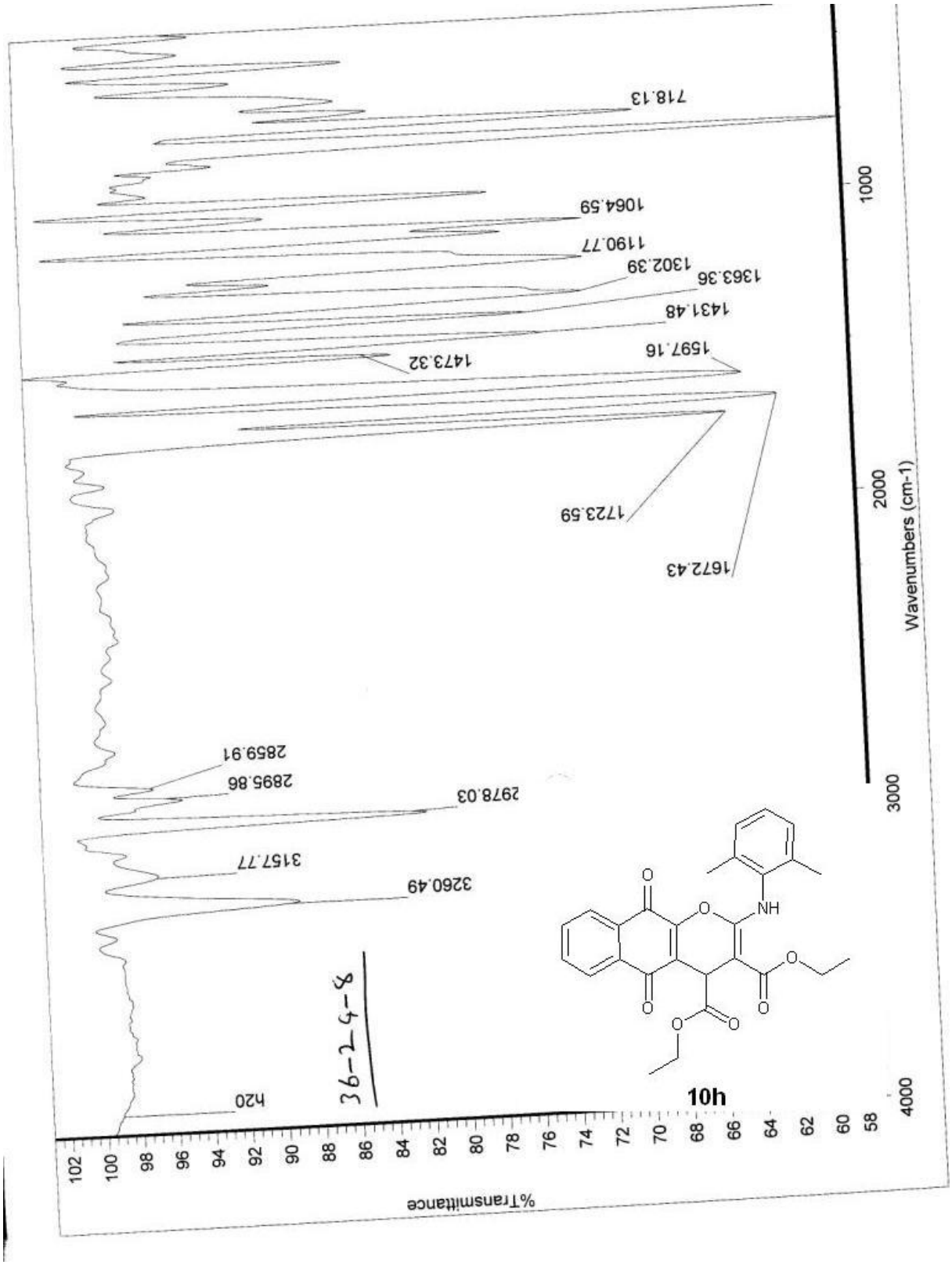
24-5
13C{1H} NMR
Current Data Parameters
NAME Ghadari
EXPNO 15
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081103
Time 10.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 159
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 9.59 cm
F1P 219.155 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm
182.767
177.220
172.011
169.003
159.743
149.648
134.496
133.862
131.535
130.589
126.677
126.485
122.145
77.522
77.098
76.675
71.577
61.390
59.721
56.768
52.843
35.809
31.625
31.410
31.261
30.931
14.520
14.097
10f
ppm
ppm

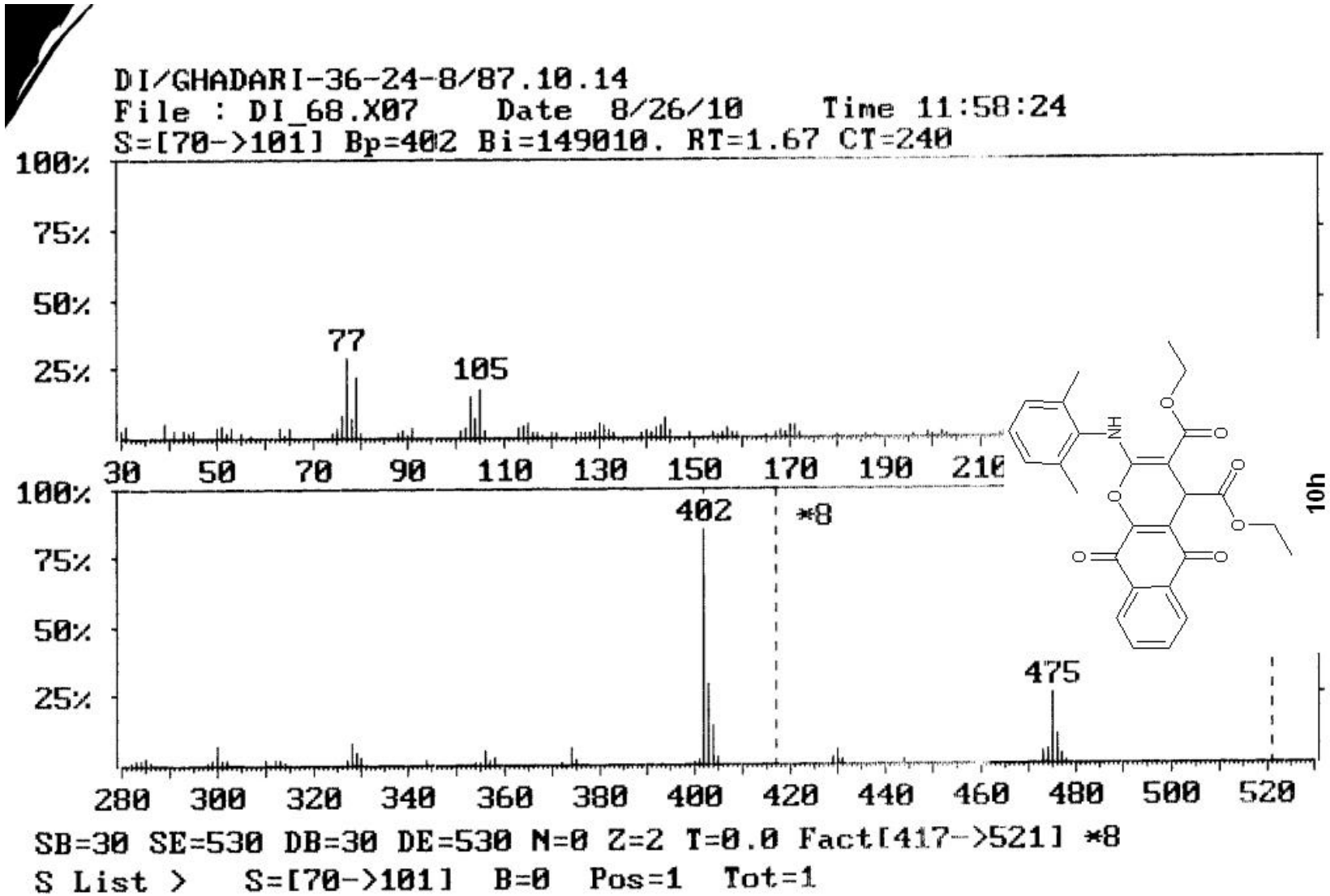

Rahim46-24-17
%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
3316.98
2988.30
2967.76
1719.83
1740.37
1689.02
1606.85
1308.99
1185.73
1057.35
795.44
713.27
10g

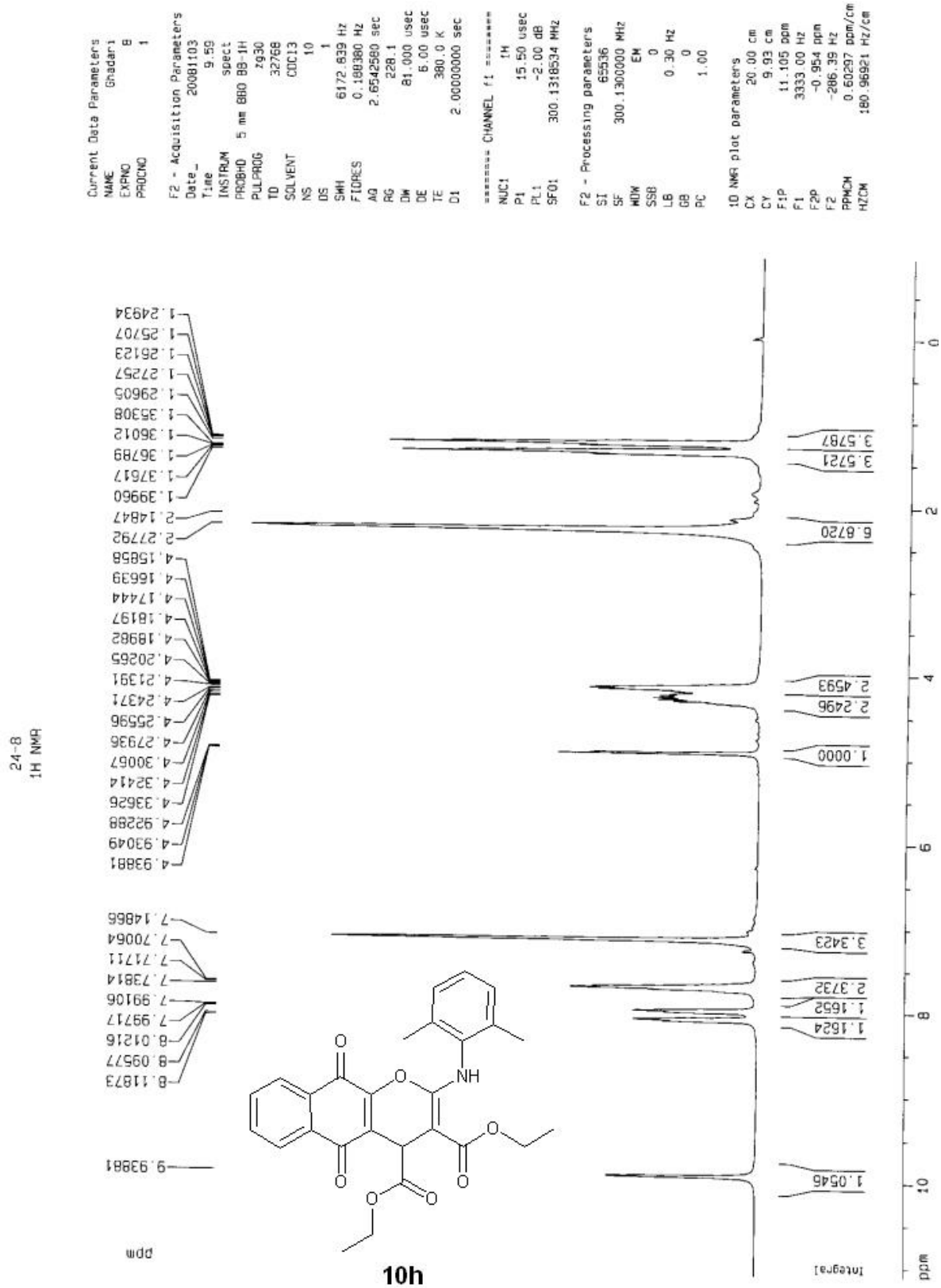

DI/GHADARI-46-24-17/87.10.14
File : DI_68.X05 Date 8/26/10 Time 11:26:32
S=[76->92] Bp=384 Bi=124910. RT=1.52 CT=241
100%
75%
50%
25%
31
59
253
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
282
310
384
*16
10g
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=520 DB=30 DE=520 N=0 Z=2 T=0.0 Fact[401->524] *16
S List > S=[76->92] B=0 Pos=1 Tot=1


24-17
1H NMR
10g
ppm
integral

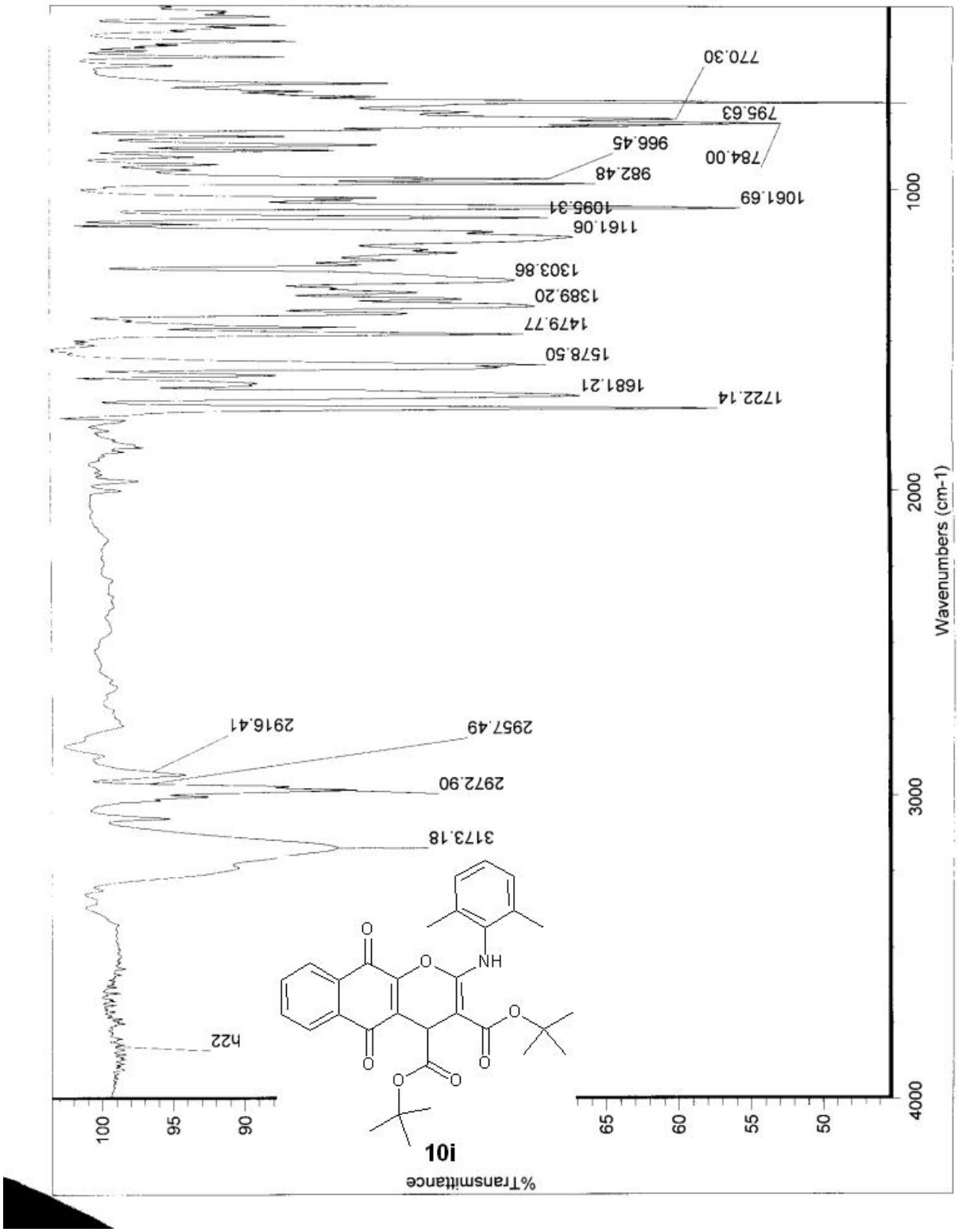
24-17
13C{1H} NMR
Current Data Parameters
NAME Ghaderi
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081117
Time 15.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 444
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752963 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 23.10 cm
F1P 219.155 ppm
F1 16539.11 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28052 Hz/cm
10g
ppm

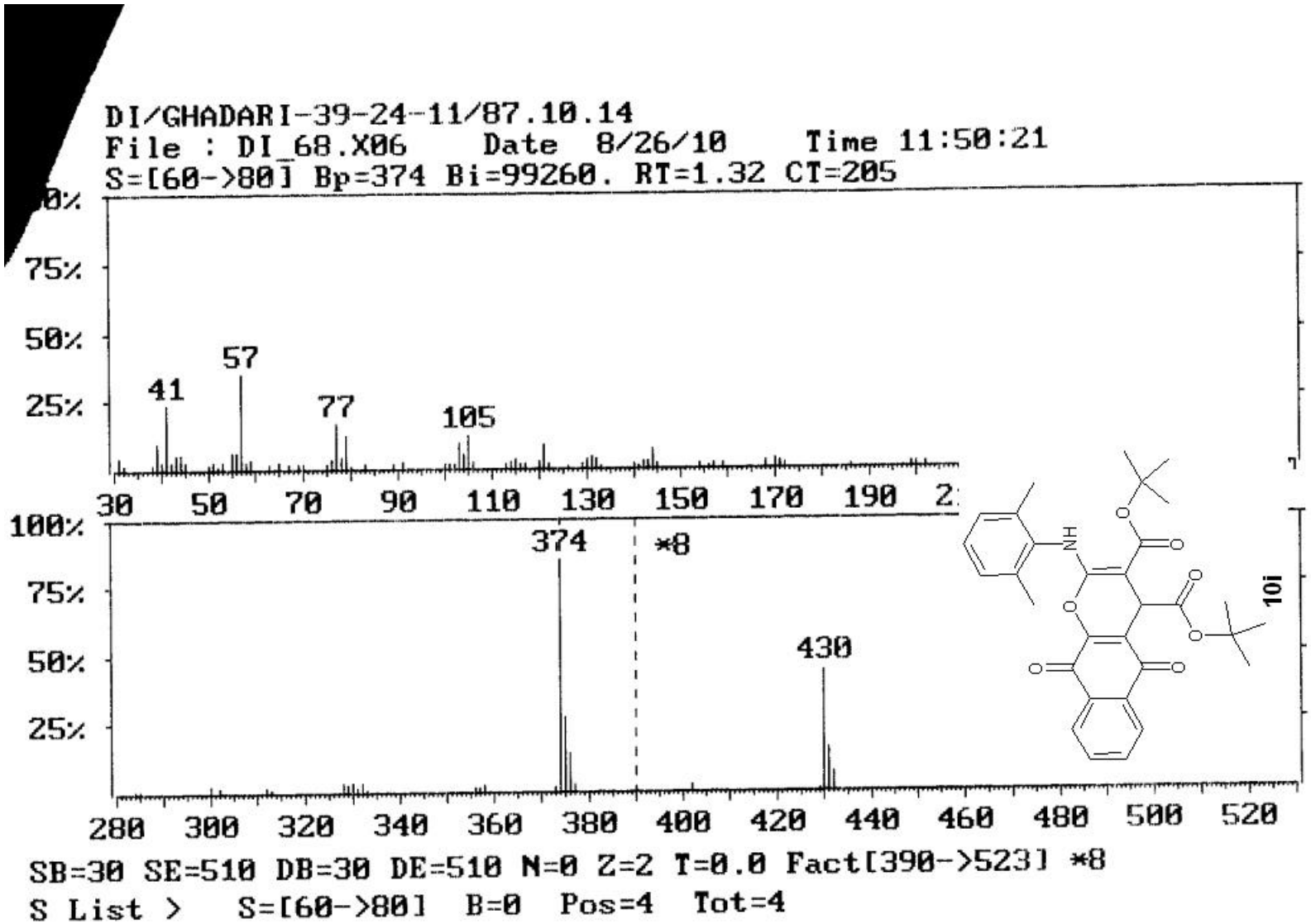

%Transmittance
Wavenumbers (cm-1)
4000
3000
2000
1000
102
100
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
62
60
58
h20
3260.49
3157.77
2978.03
2895.86
2859.91
1672.43
1723.59
1597.16
1473.32
1431.48
1363.36
1302.39
1190.77
1064.59
718.13
36-2-4-8
NH
O
10h


DI/GHADARI-36-24-8/87.10.14
File : DI_68.X07 Date 8/26/10 Time 11:58:24
S=[70->101] Bp=402 Bi=149010. RT=1.67 CT=240
100%
75%
50%
25%
77
105
30 50 70 90 110 130 150 170 190 210
100%
75%
50%
25%
402
*8
475
280 300 320 340 360 380 400 420 440 460 480 500 520
NH
O
O
O
O
O
O
10h
SB=30 SE=530 DB=30 DE=530 N=0 Z=2 T=0.0 Fact[417->521] *8
S List > S=[70->101] B=0 Pos=1 Tot=1


24-8
1H NMR
Current Data Parameters
NAME Ghadari
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081103
Time 9.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 228.1
DW 81.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1318534 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 9.93 cm
F1P 11.105 ppm
F1 3333.00 Hz
F2P -0.954 ppm
F2 -286.39 Hz
PPMCM 0.60297 ppm/cm
HZCM 180.96921 Hz/cm
1.24934
1.25707
1.26123
1.27257
1.29605
1.35308
1.36012
1.36789
1.37617
1.39960
2.14847
2.27792
4.15858
4.16639
4.17444
4.18197
4.18982
4.20265
4.21391
4.24371
4.25596
4.27936
4.30067
4.32414
4.33626
4.92288
4.93049
4.93881
7.14866
7.70064
7.71711
7.73814
7.99106
7.99717
8.01216
8.09577
8.11873
9.93881
3.57871
3.57221
6.87201
2.45931
2.24961
1.00000
3.34231
2.37321
1.16521
1.16241
1.05461
integral
ppm
10h

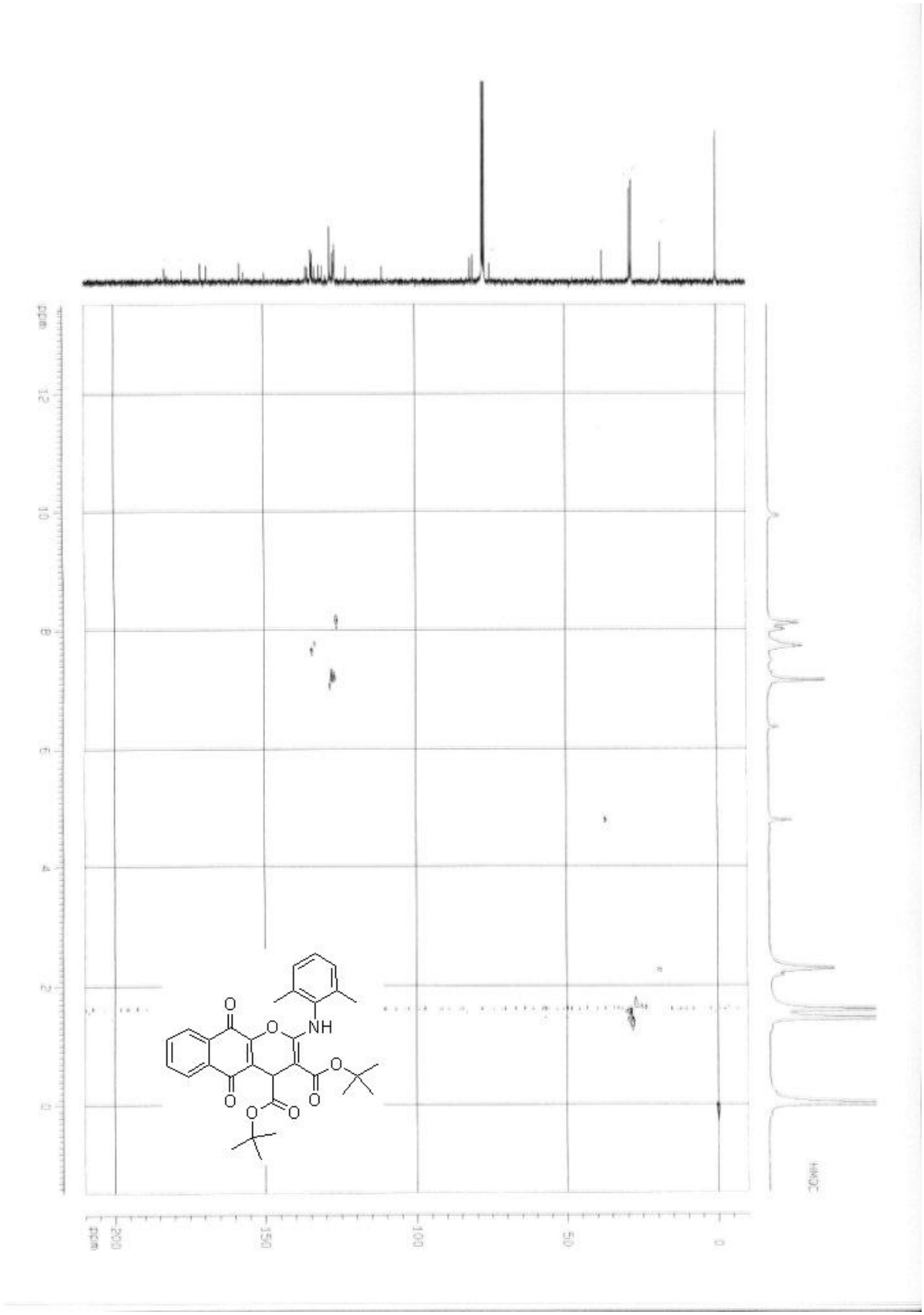
24-B
13C{1H} NMR
Current Data Parameters
NAME Chaddari
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081103
Time 10.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 78
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
CHANNEL f1
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.50
1D NMR plot parameters
CX 20.00 cm
CY 6.17 cm
F1P 219.155 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm
14.157
14.512
18.468
36.182
60.212
61.571
73.229
76.720
77.144
77.569
121.912
126.462
126.621
127.336
128.145
130.557
131.415
133.728
133.931
134.437
135.809
149.637
158.046
169.004
171.841
176.602
182.720
ppm
0
50
100
150
200
10h


10i
%Transmittance
Wavenumbers (cm-1)
h22
3173.18
2972.90
2957.49
2916.41
1722.14
1681.21
1578.50
1479.77
1389.20
1303.86
1161.06
1095.31
1061.69
982.48
966.45
784.00
795.63
770.30


DI/GHADARI-39-24-11/87.10.14
File : DI_68.X06 Date 8/26/10 Time 11:50:21
S=[60->80] Bp=374 Bi=99260. RT=1.32 CT=205
75%
50%
25%
41
57
77
105
30 50 70 90 110 130 150 170 190
100%
75%
50%
25%
374
*8
430
280 300 320 340 360 380 400 420 440 460 480 500 520
10i
SB=30 SE=510 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[390->523] *8
S List > S=[60->80] B=0 Pos=4 Tot=4

24-11
1H NMR
Current Data Parameters
NAME Keshipoor
EXPNO 51
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081111
Time 13.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.10
1D NMR plot parameters
CX 20.00 cm
CY 9.90 cm
F1P 11.931 ppm
F1 3580.77 Hz
F2P -0.947 ppm
F2 -284.36 Hz
PPMCM 0.64391 ppm/cm
HZCM 193.25661 Hz/cm
9.92412
8.12560
8.10483
8.02012
7.99729
7.90333
7.76364
7.73816
7.71979
7.71527
7.70296
7.69715
7.13979
7.04135
6.94470
4.77738
4.76076
2.81656
2.17862
2.17412
1.76699
1.74647
1.73051
1.59404
1.57775
1.44484
1.42851
1.000
2.093
1.180
3.247
3.679
1.008
11.286
11.941
integral
ppm
10i

24-11
13C{1H} NMR
182.762
176.824
170.756
170.603
168.693
157.700
149.589
135.652
134.312
134.057
133.956
133.750
131.549
130.612
128.054
127.590
127.089
126.541
126.400
122.581
119.565
110.043
81.495
80.505
77.478
77.054
76.631
75.778
74.801
74.082
37.555
28.532
27.971
27.878
18.476
18.393
Current Data Parameters
NAME Keshipoor
EXPNO 52
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081112
Time 13.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 9.90 cm
F1P 219.195 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm
NH
10i
ppm
0
50
100
150
200


ppm
12
10
8
6
4
2
0
ppm
200
150
100
50
0
HMQC
O
NH
O
O
O
O
O
O