Supporting Information

Synthesis and Properties of Imidazolo Fused Benzotriazinyl Radicals

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Supporting Information

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Cyclic Voltammetry Spectra of Radicals 4a-i and 5

Figure S1. Cyclic voltammogram of radical **4a**

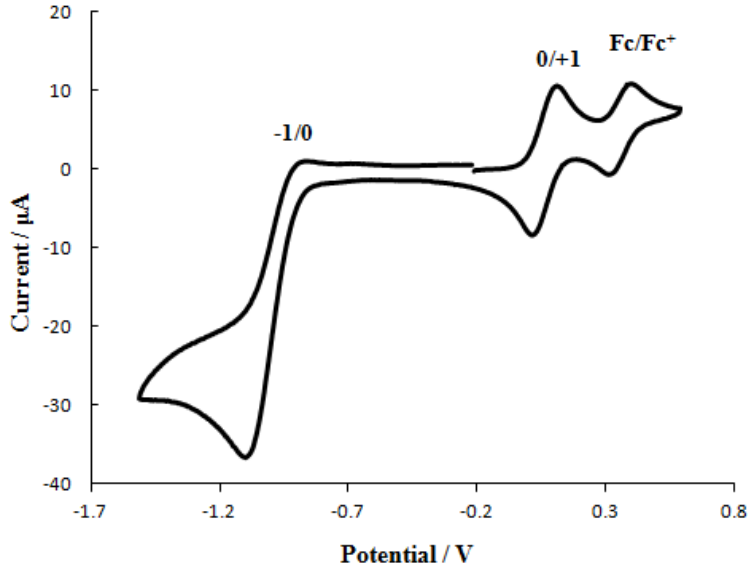


Figure S2. Cyclic voltammogram of radical **4b**

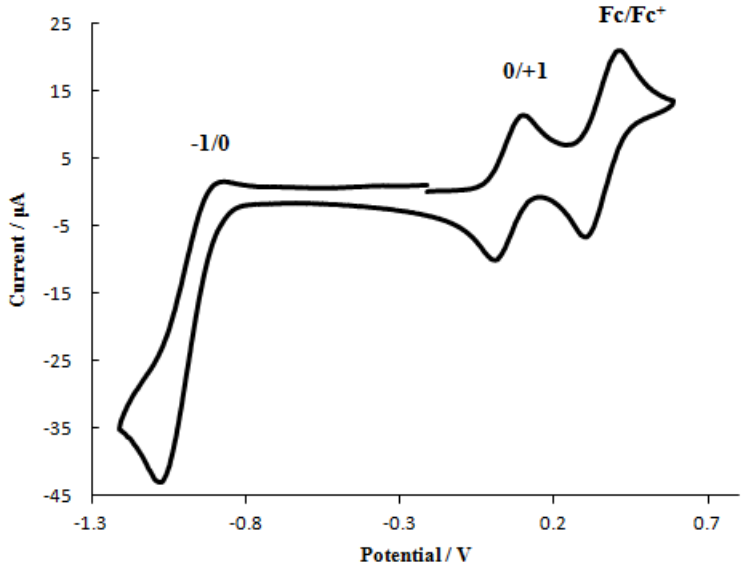


Figure S3. Cyclic voltammogram of radical **4c**

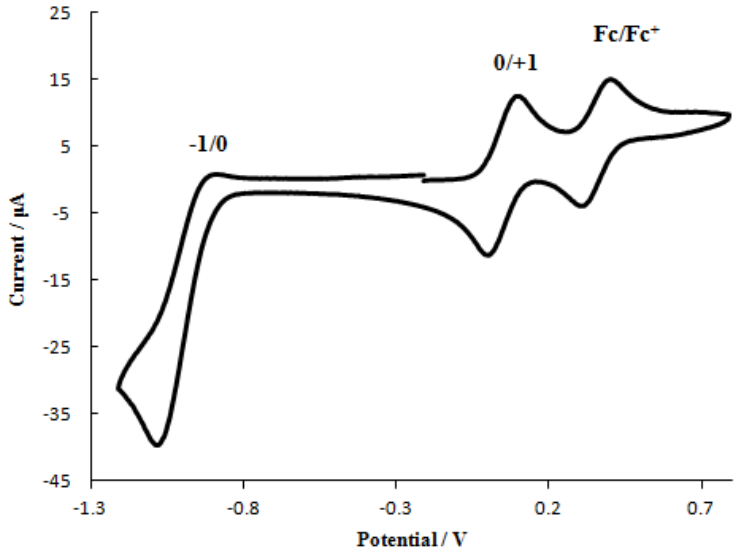


Figure S4. Cyclic voltammogram of radical **4d**

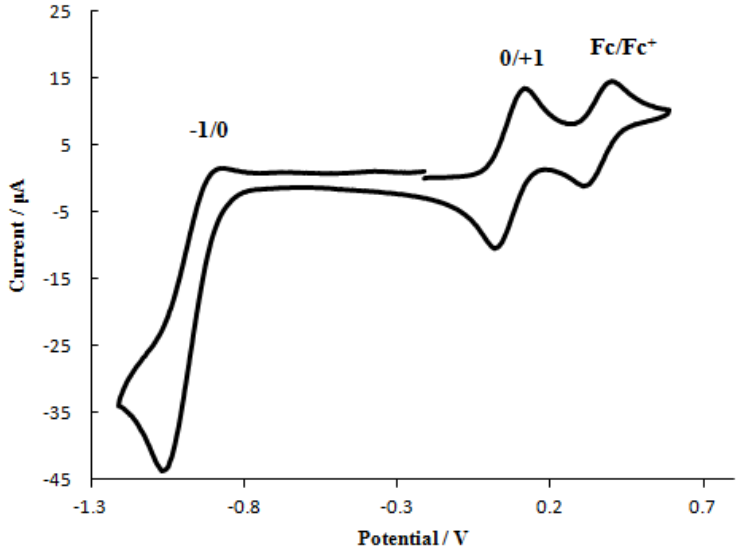


Figure S5. Cyclic voltammogram of radical **4e**

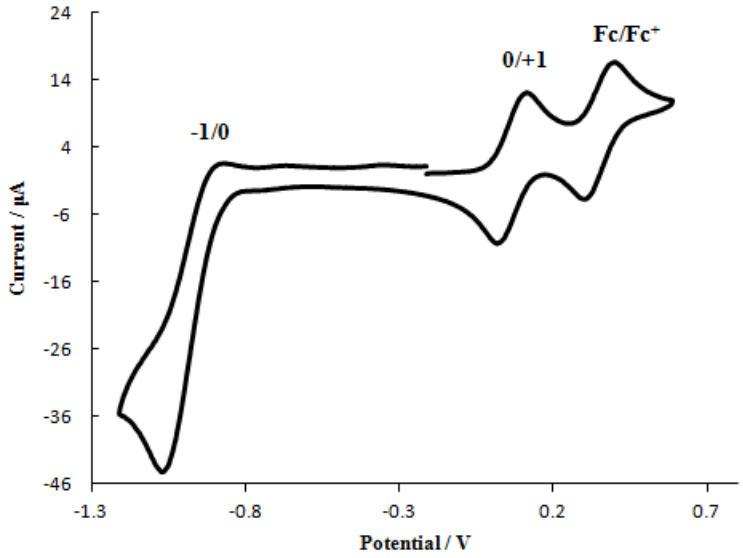


Figure S6. Cyclic voltammogram of radical **4f**

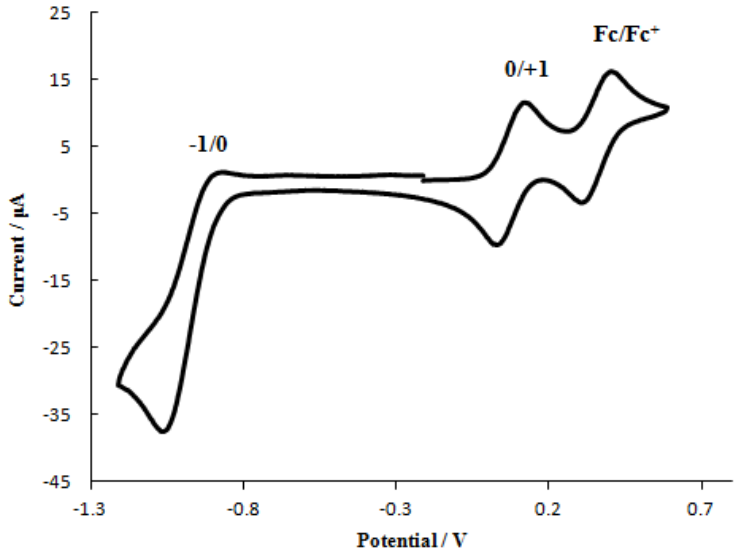


Figure S7. Cyclic voltammogram of radical **4g**

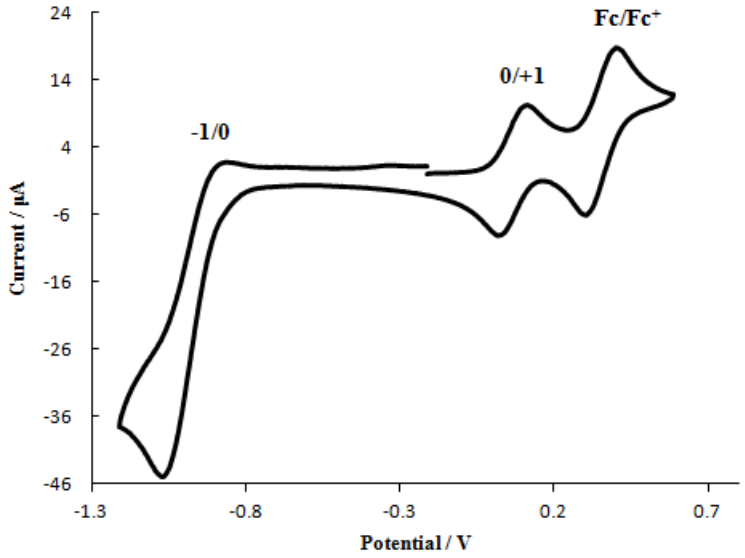


Figure S8. Cyclic voltammogram of radical **4h**

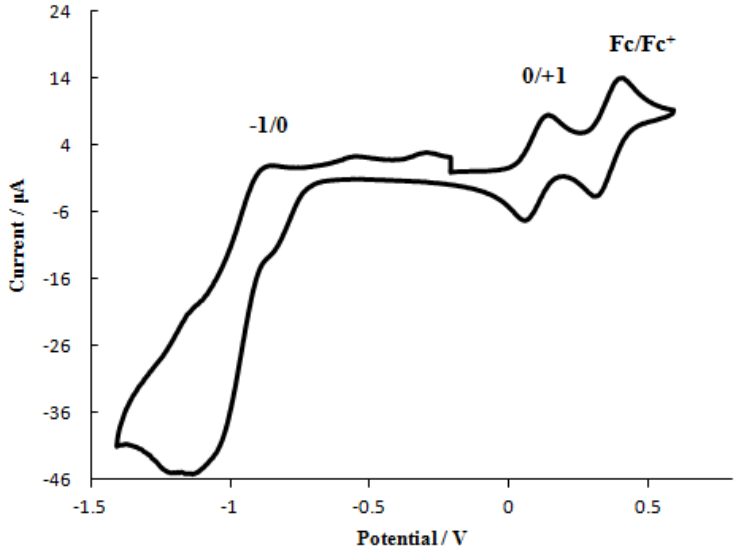


Figure S9. Cyclic voltammogram of radical **4i**

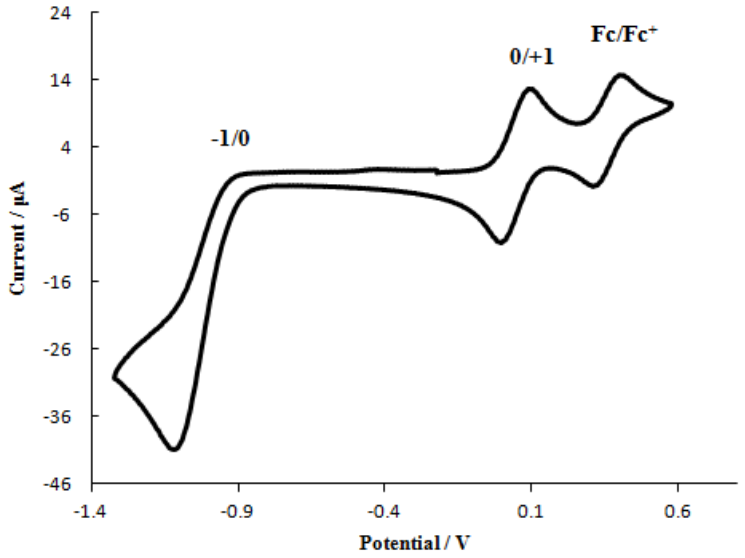
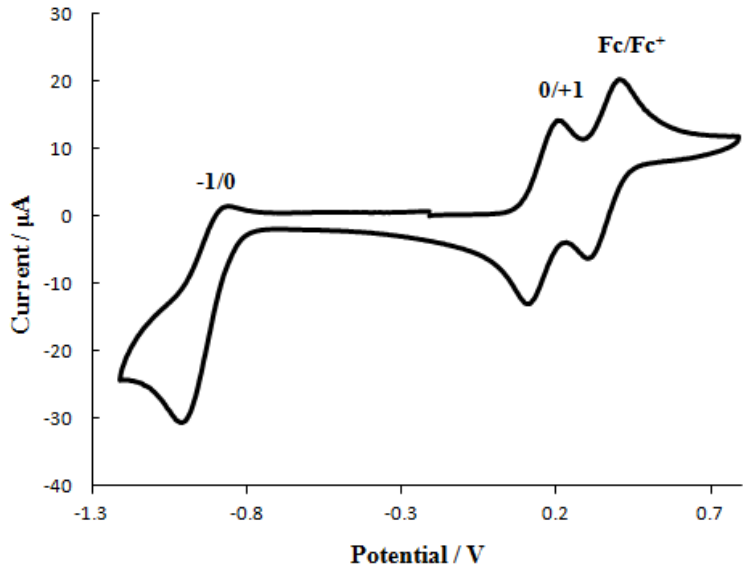


Figure S10. Cyclic voltammogram of radical **5**



Solid-State EPR Spectra of Radicals 4a-i and 5

Figure S11. Solid-state EPR spectrum of radical **4a**

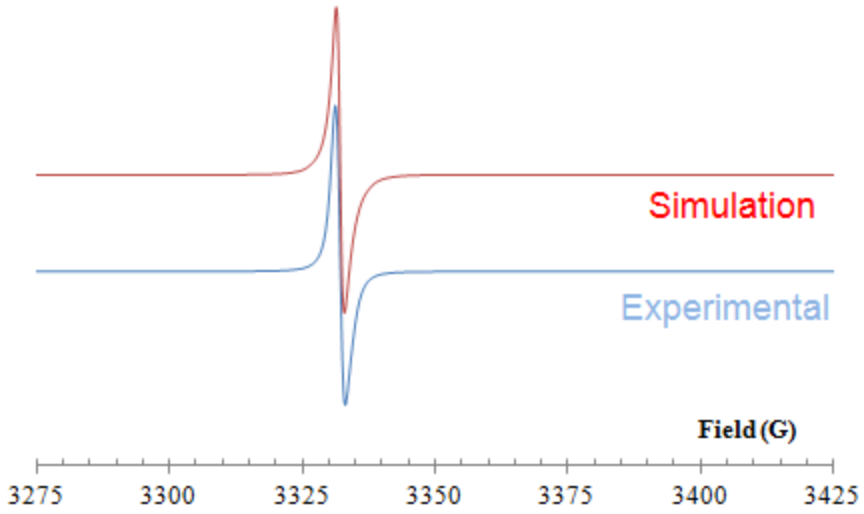


Figure S12. Solid-state EPR spectrum of radical **4b**

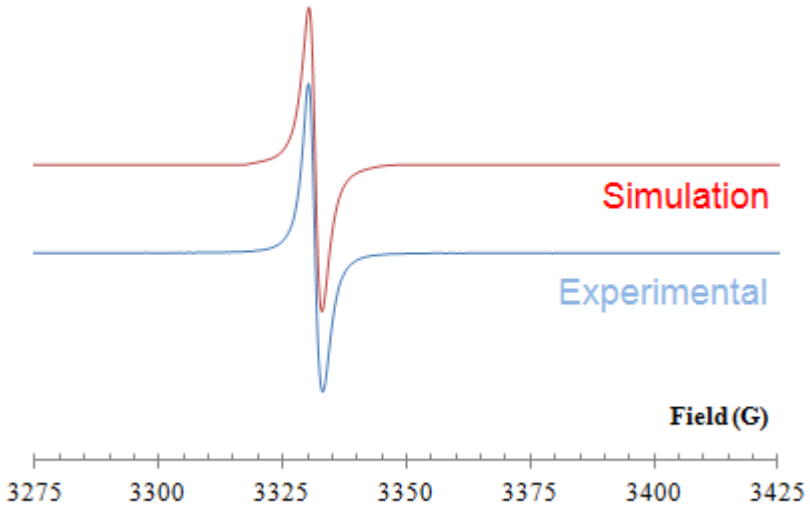


Figure S13. Solid-state EPR spectrum of radical **4c**

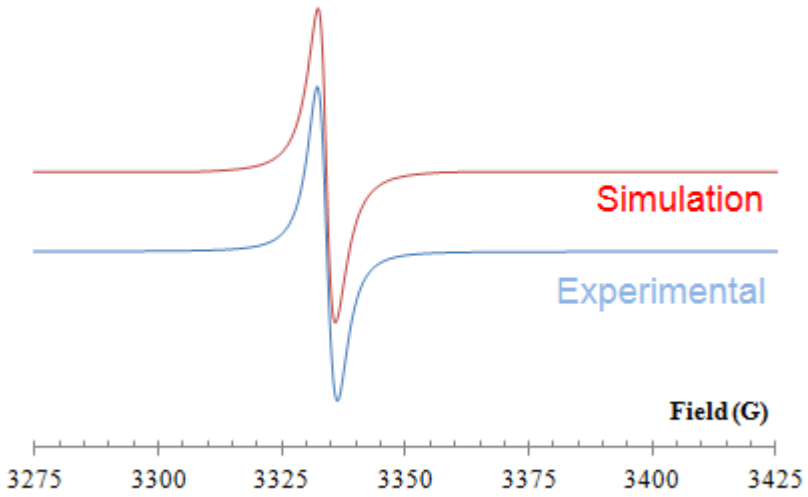


Figure S14. Solid-state EPR spectrum of radical **4d**

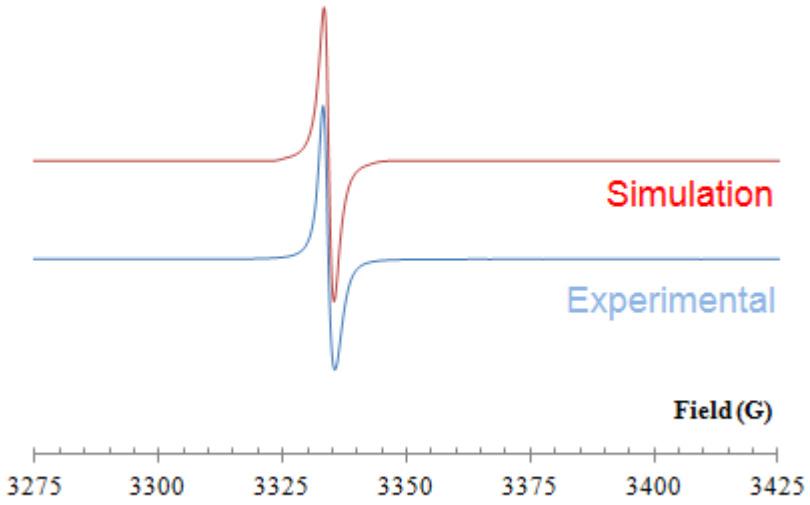


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Figure S15. Solid-state EPR spectrum of radical **4e**

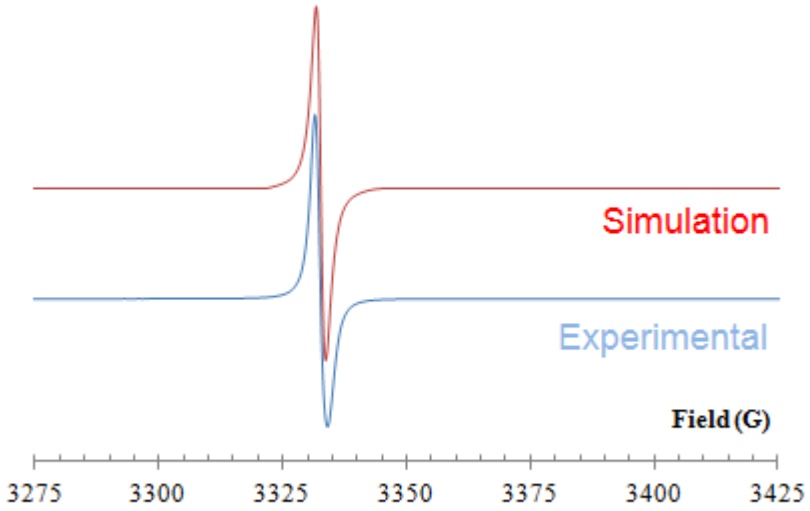


Figure S16. Solid-state EPR spectrum of radical **4f**

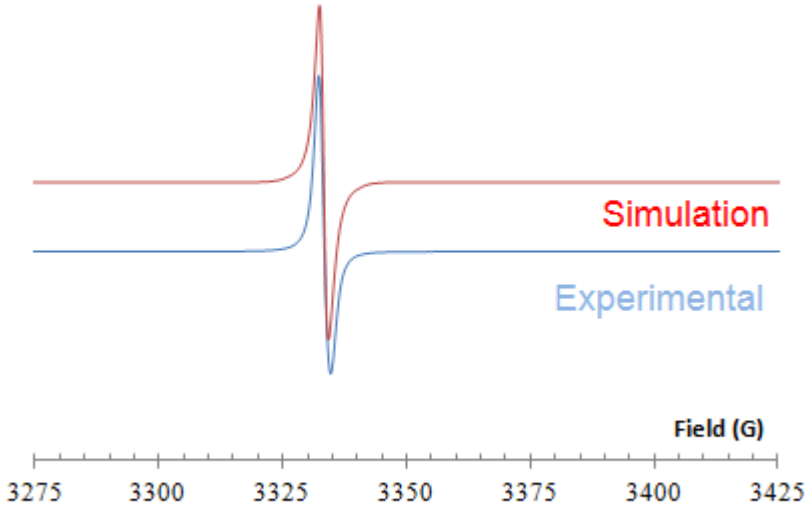
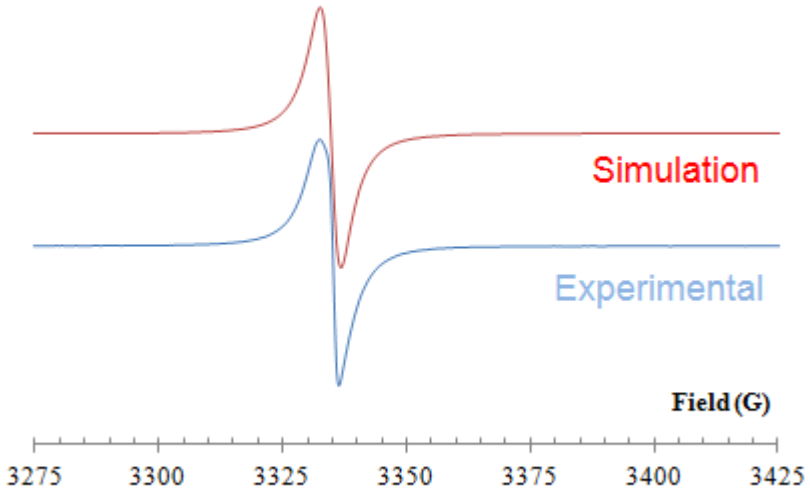


Figure S17. Solid-state EPR spectrum of radical **4g**



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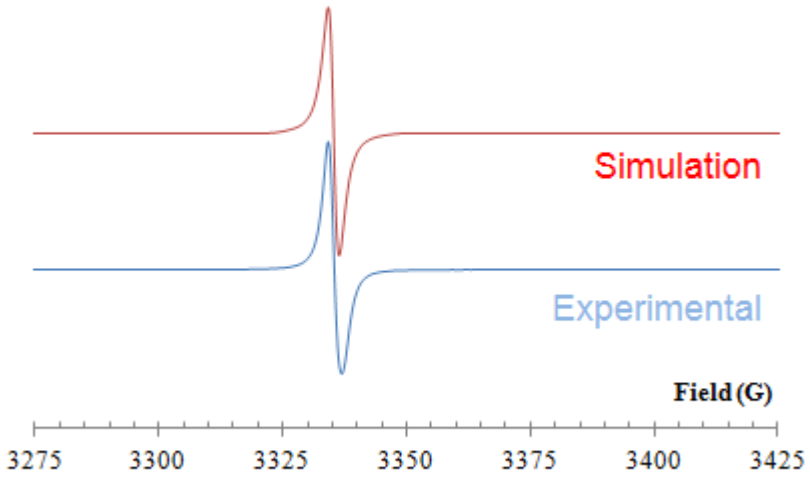


Figure S19. Solid-state EPR spectrum of radical **4i**

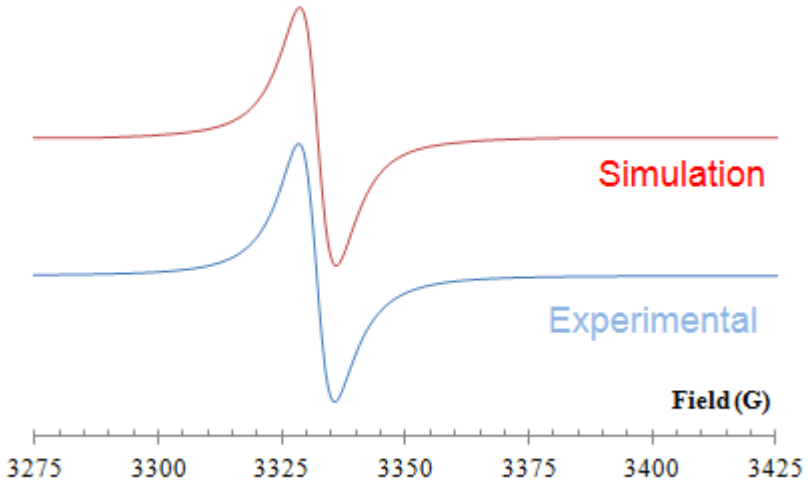
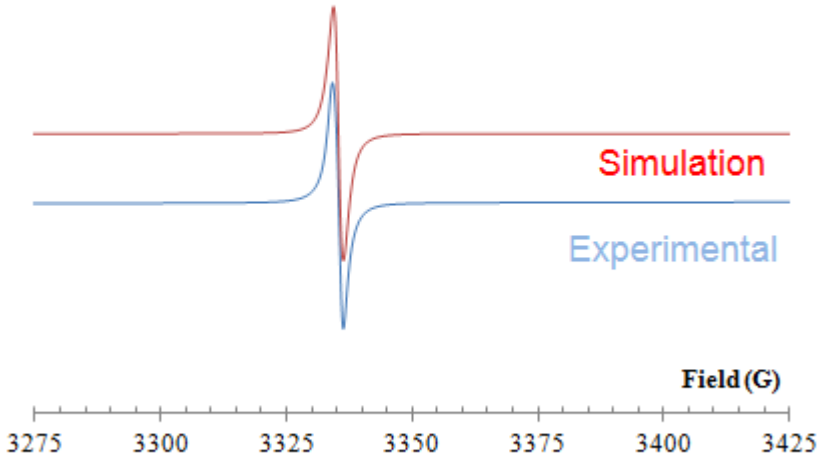


Figure S20. Solid-state EPR spectrum of radical **5**



Solution EPR Spectra of Radicals 5 and 4a-i

Figure S21. Solution EPR spectrum of radical **4a**

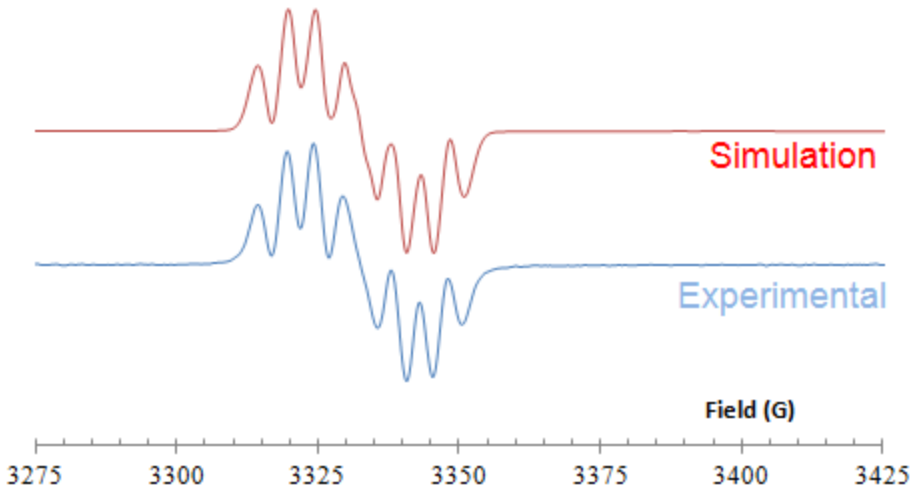


Figure S22. Solution EPR spectrum of radical **4b**

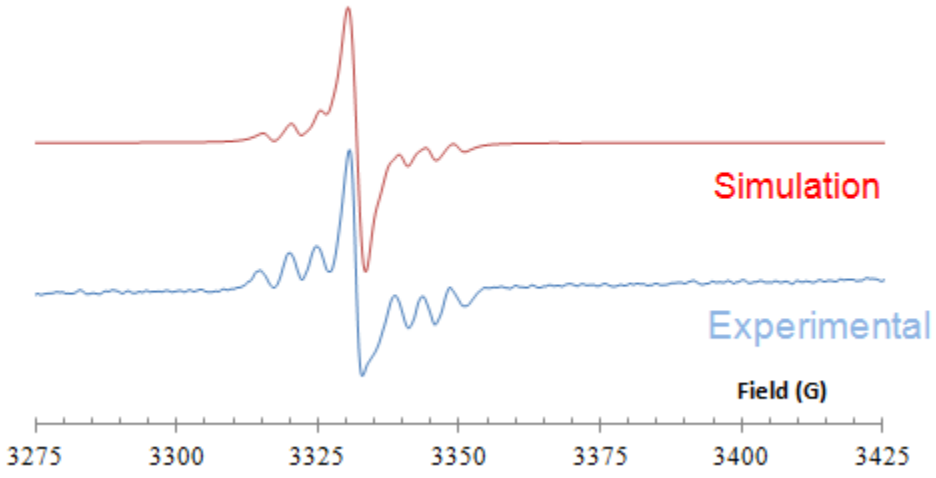


Figure S23. Solution EPR spectrum of radical **4c**

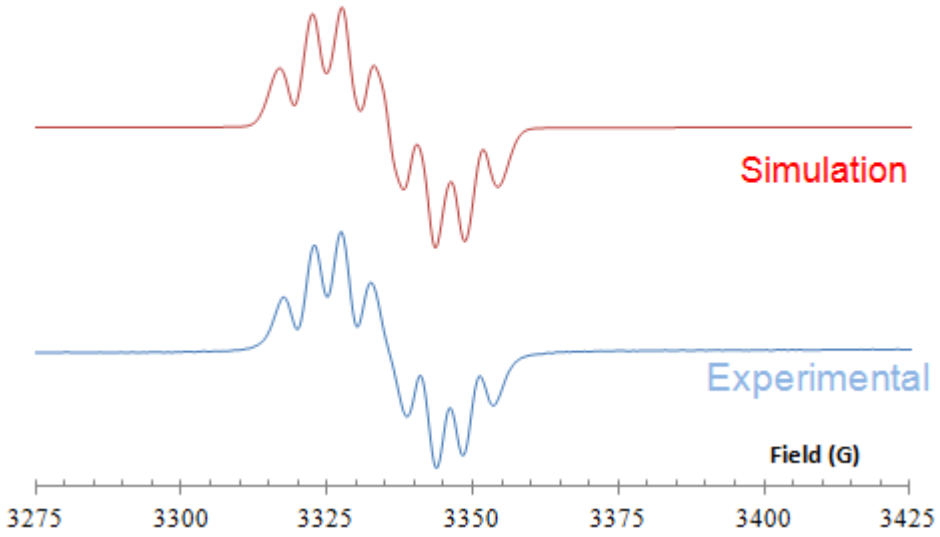


Figure S24. Solution EPR spectrum of radical **4d**

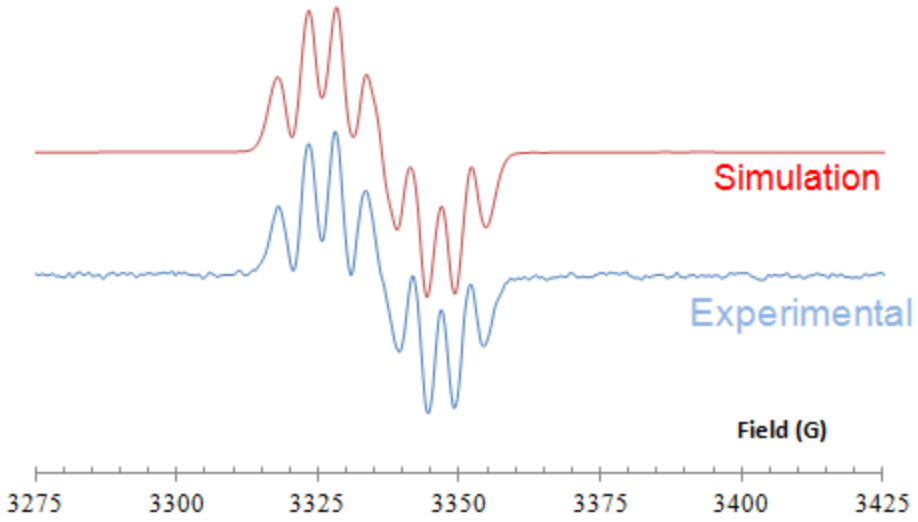


Figure S25. Solution EPR spectrum of radical **4e**

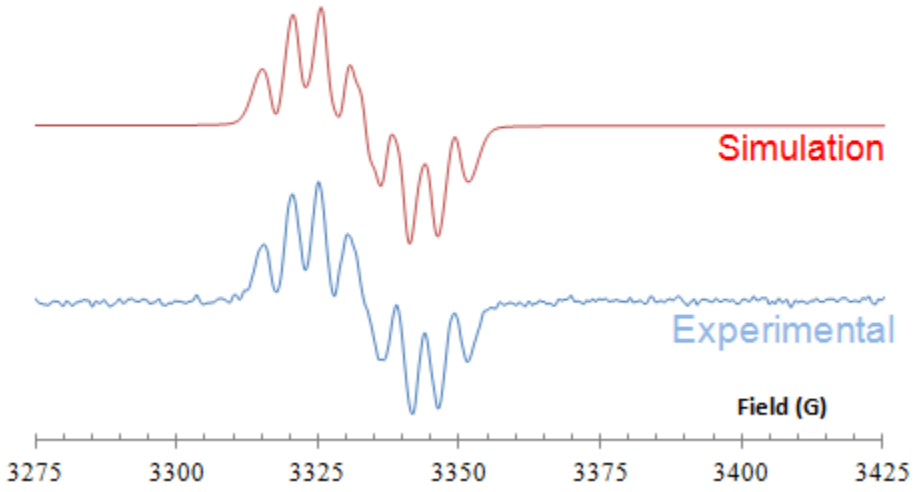


Figure S26. Solution EPR spectrum of radical **4f**

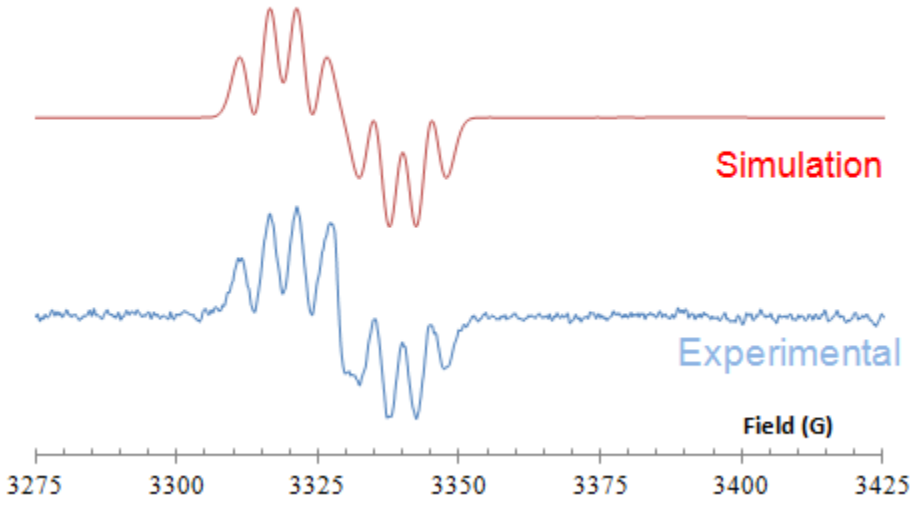


Figure S27. Solution EPR spectrum of radical **4g**

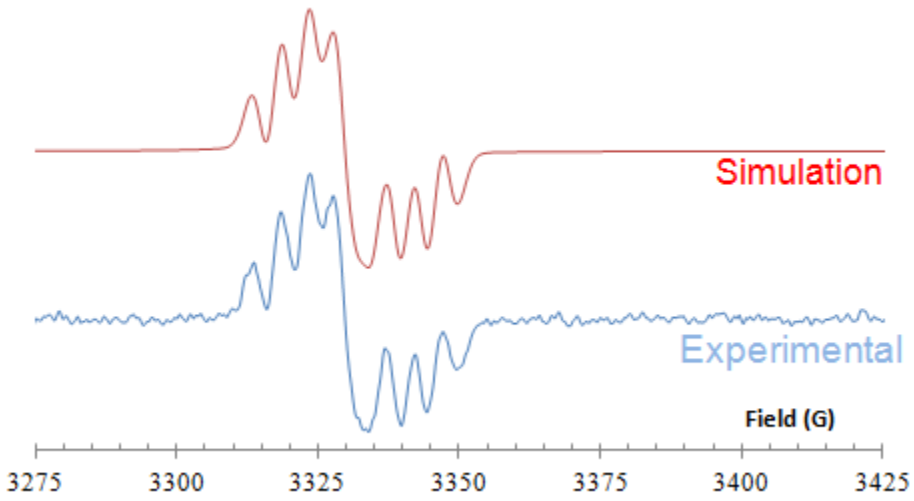


Figure S28. Solution EPR spectrum of radical **4h**

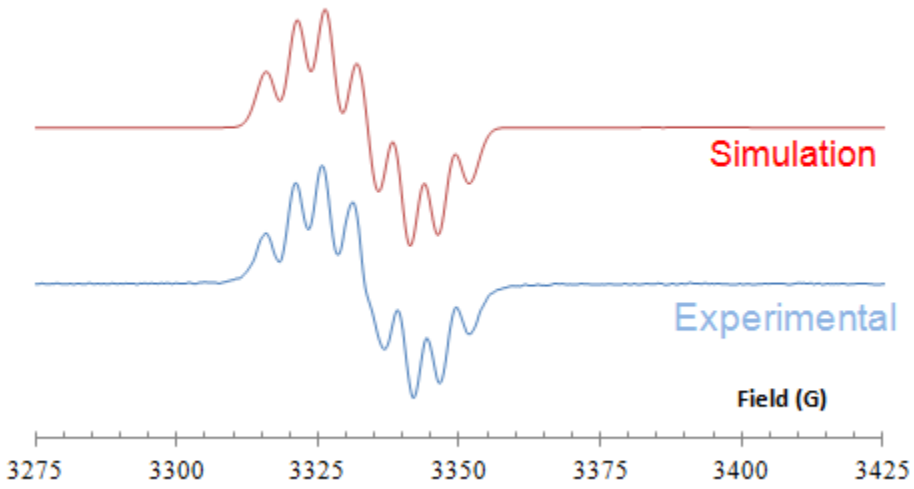
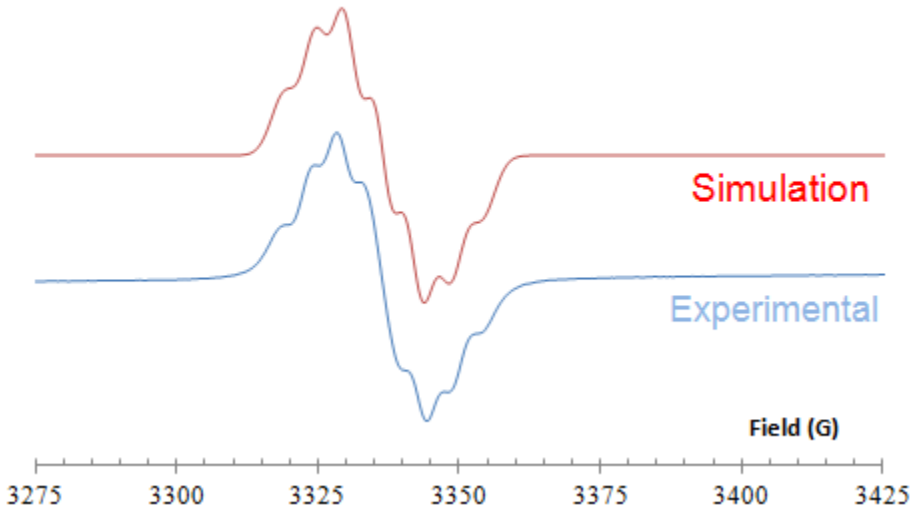


Figure S29. Solution EPR spectrum of radical **4i**

Figure S30. Solution EPR spectrum of radical **5**



X-Ray Crystallography. Radical 4a (CCDC 940089)

Data were collected on an Oxford-Diffraction Supernova diffractometer, equipped with a CCD area detector utilizing Cu-Kα radiation (λ = 1.5418 Å). A suitable crystal was attached to glass fibers using paratone-N oil and transferred to a goniostat where they were cooled for data collection. Unit cell dimensions were determined and refined by using 3520 ($3.34 \leq \theta \leq 72.47$) reflections. Empirical absorption corrections (multi-scan based on symmetry-related measurements) were applied using CrysAlis RED software.[1] The structures were solved by direct method and refined on F^2 using full-matrix least squares using SHELXL97.[2] Software packages used: CrysAlis CCD[1] for data collection, CrysAlis RED[1] for cell refinement and data reduction, WINGX for geometric calculations,[3] and DIAMOND[4] for molecular graphics. The non-H atoms were treated anisotropically. The hydrogen atoms were placed in calculated, ideal positions and refined as riding on their respective carbon atoms.

Crystal refinement data (**4a**): $C_{32}H_{22}N_5$, M = 476.55, Triclinic, space group *P -1*, a = 7.8924(8) Å, b = 11.3721(9) Å, c = 13.2802(12) Å, α = 96.019(7)°, β = 90.262(8)°, γ = 96.237(8)°, V = 1178.20(19) Å^3, Z = 2, T = 100(2) K, ρ_{calcd} = 1.343 g cm^{-3}, $2\theta_{max}$ = 67. Refinement of 334 parameters on 4186 independent reflections out of 7408 measured reflections (R_{int} = 0.0284) led to R_1 = 0.0452 [I>2s(I)], wR_2 = 0.1356 (all data), and S = 1.044 with the largest difference peak and hole of 0.220 and -0.315 e^{-3}, respectively.

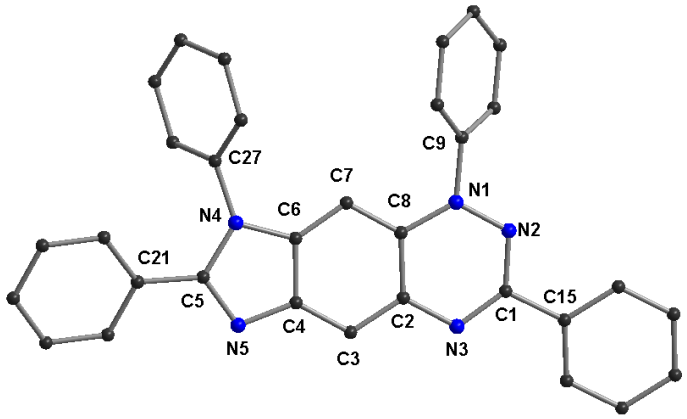


Figure S31. A partially labelled plot of 1,3,7,8-tetraphenyl-4,8-dihydro-1*H*-imidazo[4,5-*g*][1,2,4]benzotriazin-4-yl (**4a**). The hydrogen atoms were omitted for clarity.

X-Ray Crystallography. Radical 5 (CCDC 940088)

Data were collected on an Oxford-Diffraction Supernova diffractometer, equipped with a CCD area detector utilizing Cu-Kα radiation (λ = 1.5418 Å). A suitable crystal was attached to glass fibers using paratone-N oil and transferred to a goniostat where they were cooled for data collection. Unit cell dimensions were determined and refined by using 2999 ($4.99 \leq \theta \leq 66.99^{o}$) reflections. Empirical absorption corrections (multi-scan based on symmetry-related measurements) were applied using CrysAlis RED software.[1] The structures were solved by direct method and refined on F^2 using full-matrix least squares using SHELXL97.[2] Software packages used: CrysAlis CCD[1] for data collection, CrysAlis RED[1] for cell refinement and data reduction, WINGX for geometric calculations,[3] and DIAMOND[4] for molecular graphics. The non-H atoms were treated anisotropically. The hydrogen atoms were placed in calculated, ideal positions and refined as riding on their respective carbon atoms.

Crystal refinement data (**5**): $C_{29}H_{20}N_4O$, M = 440.49, Triclinic, space group P -1, a = 7.8405(13) Å, b = 9.2163(12) Å, c = 15.484(2) Å, α = 96.813(11)^{o}, β = 90.713(13)^{o}, γ = 104.161(13)^{o}, V = 1076.2(3) Å^3, Z = 2, T = 100(2) K, ρ_{calcd} = 1.359 g cm^{-3}, $2\theta_{max}$ = 67. Refinement of 307 parameters on 3820 independent reflections out of 6475 measured reflections (R_{int} = 0.0260) led to R_1 = 0.0471 [I>2s(I)], wR_2= 0.1323 (all data), and S = 1.028 with the largest difference peak and hole of 0.217and -0.257 e^{-3}, respectively.

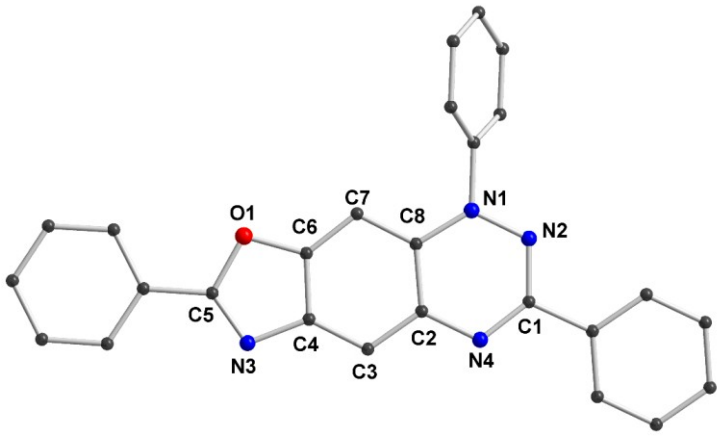


Figure S32. A partially labelled plot of 1,3,7-triphenyl-1,4-dihydro[1,3]oxazolo[4,5-*g*][1,2,4]benzotriazin-4-yl (**5**). The hydrogen atoms were omitted for clarity.

References

[1] Oxford Diffraction (2008). CrysAlis CCD and CrysAlis RED, version 1.171.32.15, Oxford Diffraction Ltd, Abingdon, Oxford, England.

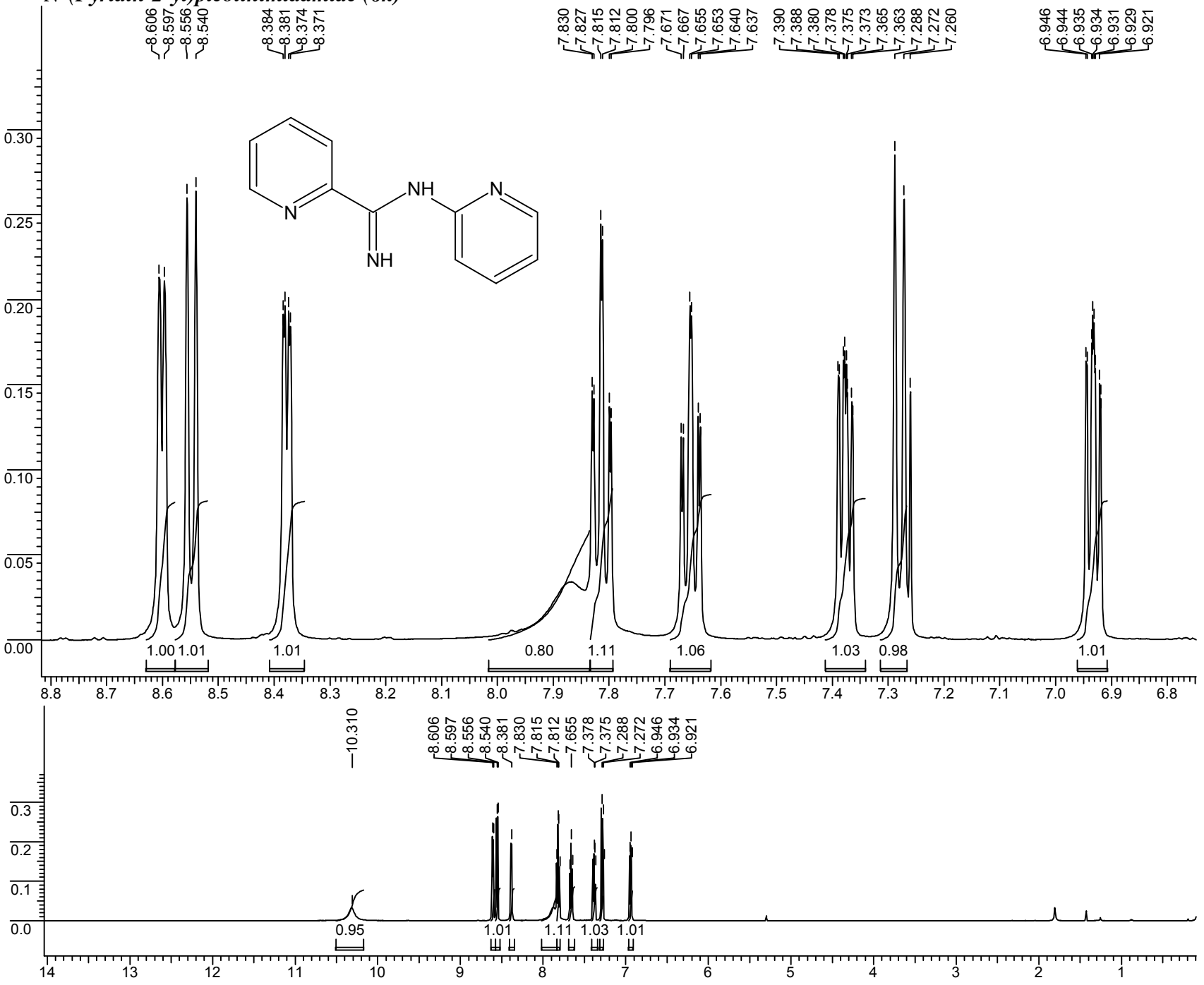
[2] Sheldrick, G. M. "SHELXL97-A program for the refinement of crystal structure", University of Göttingen, Germany.

[3] Farrugia, L. J. "WinGX suite for single crystal small molecule crystallography", *J. Appl. Crystallogr.*, 1999, **32**, 837.

[4] Brandenburg, K. 2006, DIAMOND. Version 3.1d. Crystal Impact GbR, Bonn, Germany.

^{1}H and ^{13}C NMR Spectra for All New Compounds and ^{1}H NMR Spectra of Known Compounds 13a, 13b, 14 and *N*-(4-nitrophenyl)acetamide Prepared *via* New Routes

N-(Pyridin-2-yl)picolinimidamide (6k)



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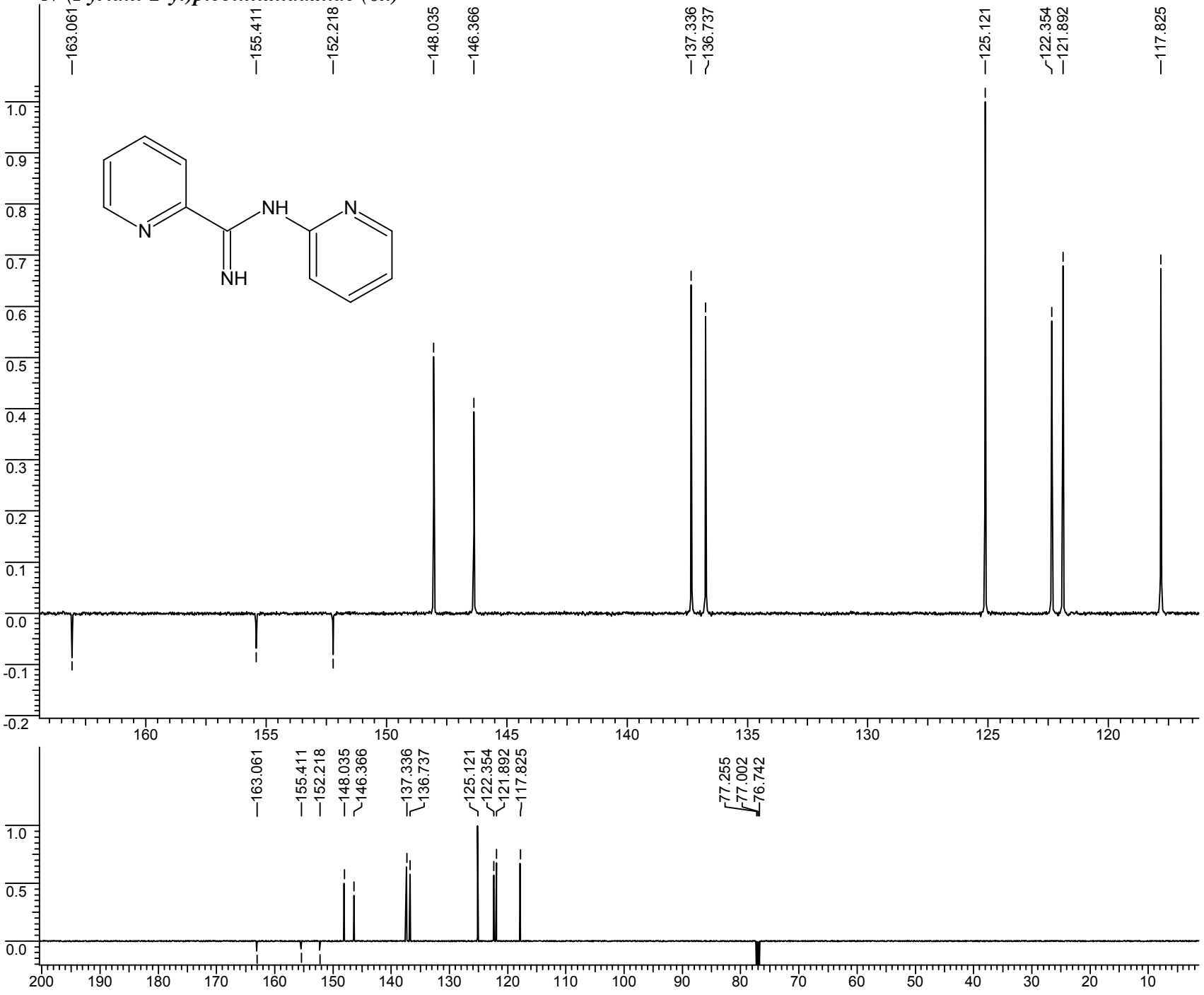
N-(Pyridin-2-yl)picolinimidamide (6k)



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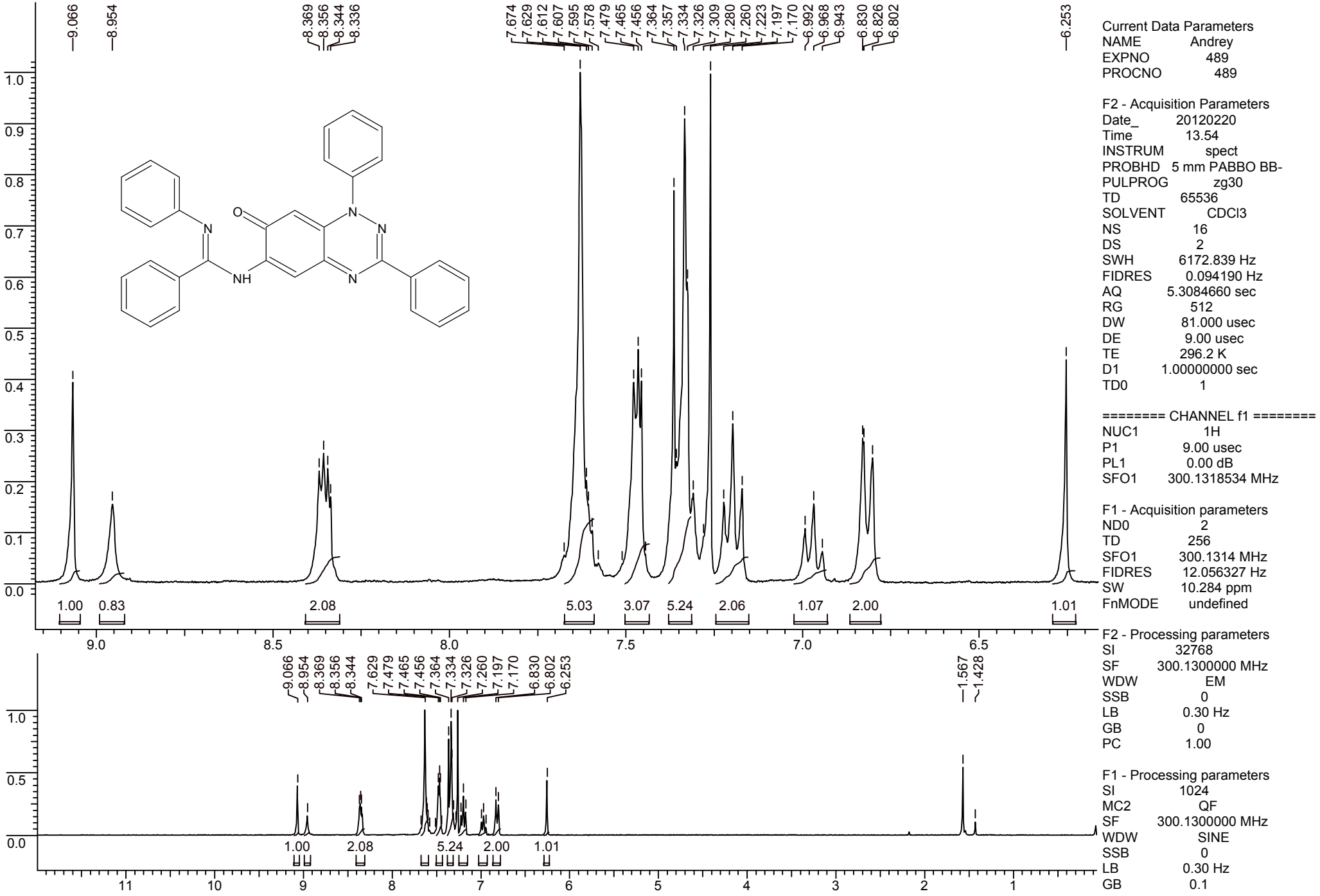

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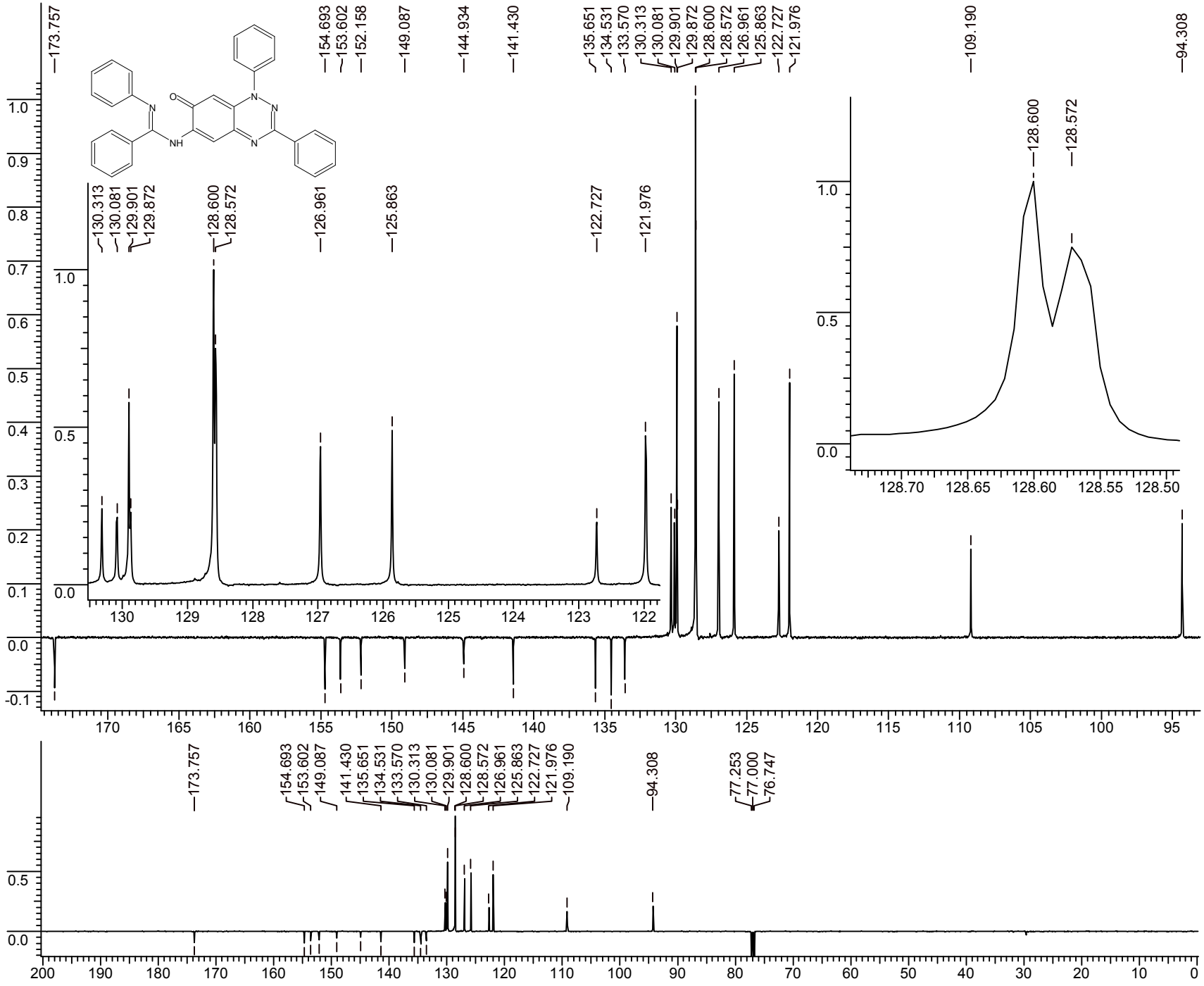
GB 0.1

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)-N'-phenylbenzimidamide (7a)



Current Data Parameters
NAME Andrey
EXPNO 50
PROCNO 1

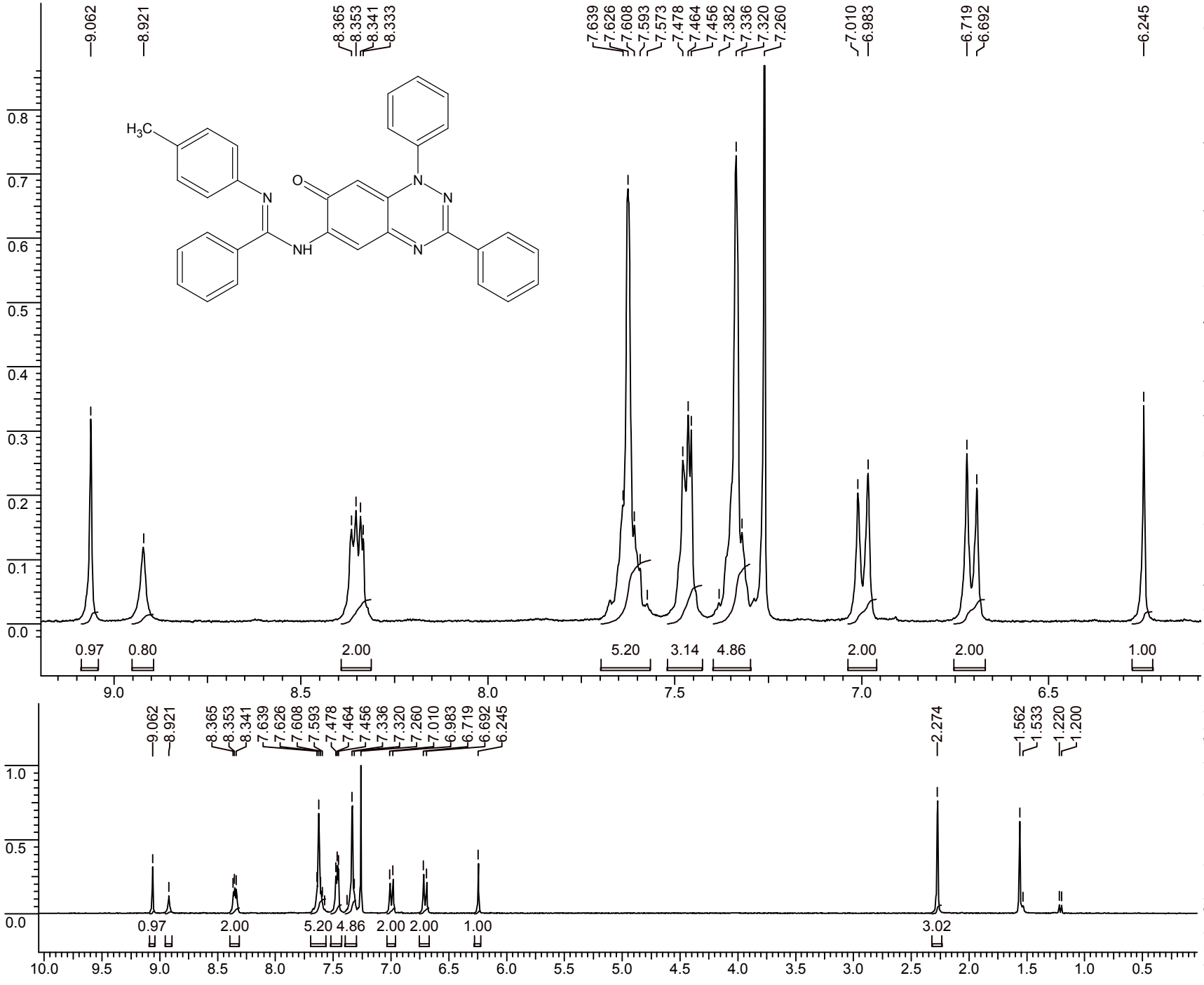
F2 - Acquisition Parameters
Date_ 20120221
Time 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.38 usec
P2 16.76 usec
PLW1 138.00000000 W
SFO1 125.7459782 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 15.41699982 W
PLW12 0.33258000 W
SFO2 500.0350280 MHz

F2 - Processing parameters
SI 32768
SF 125.7334160 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)-N'-p-tolylbenzimidamide (7b)



Current Data Parameters
NAME Andrey
EXPNO 571
PROCNO 571

F2 - Acquisition Parameters
Date_ 20121017
Time 21.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 usec
DE 9.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

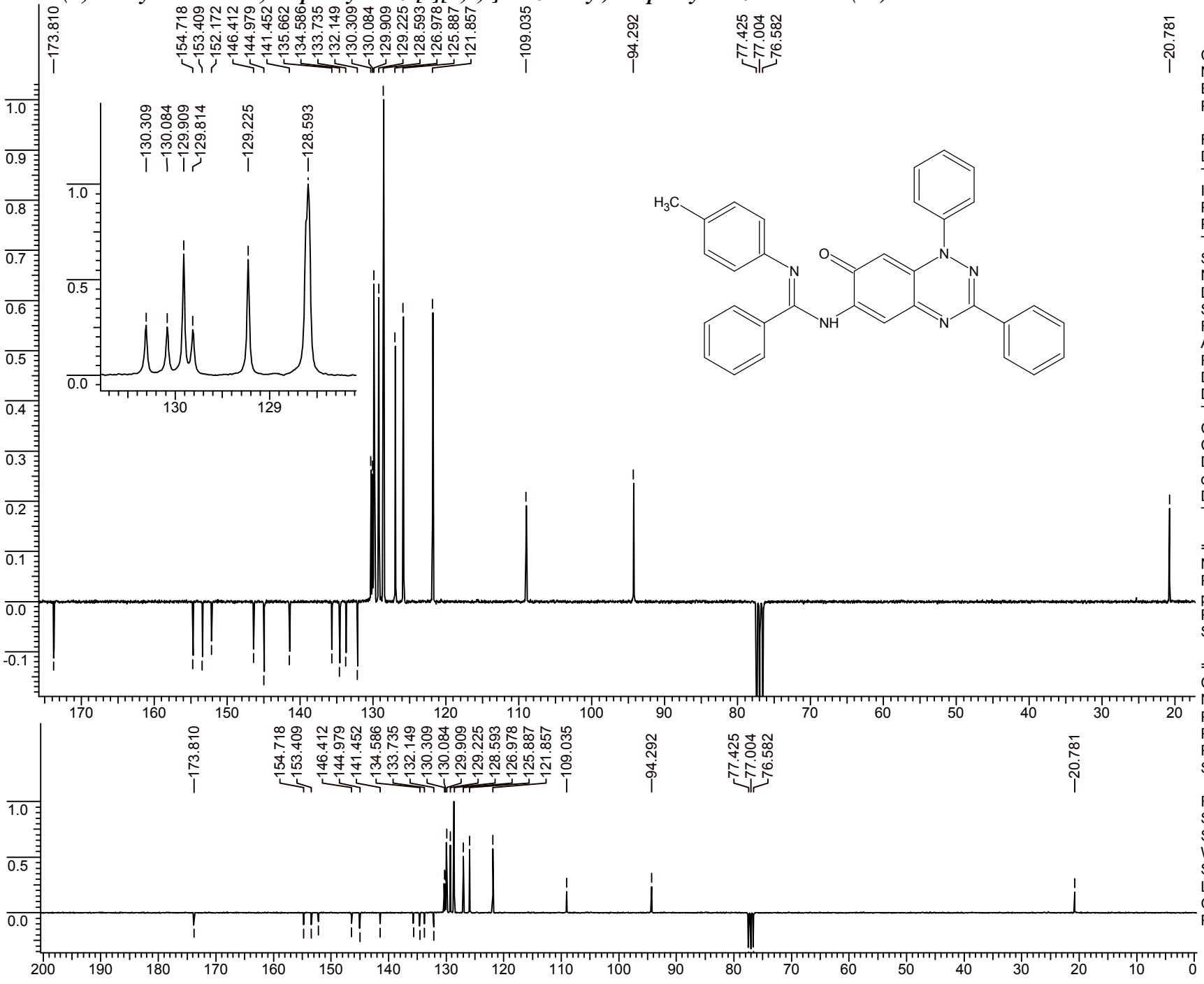
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)-N'-p-tolylbenzimidamide (7b)



Current Data Parameters
NAME Andrey
EXPNO 572
PROCNO 572

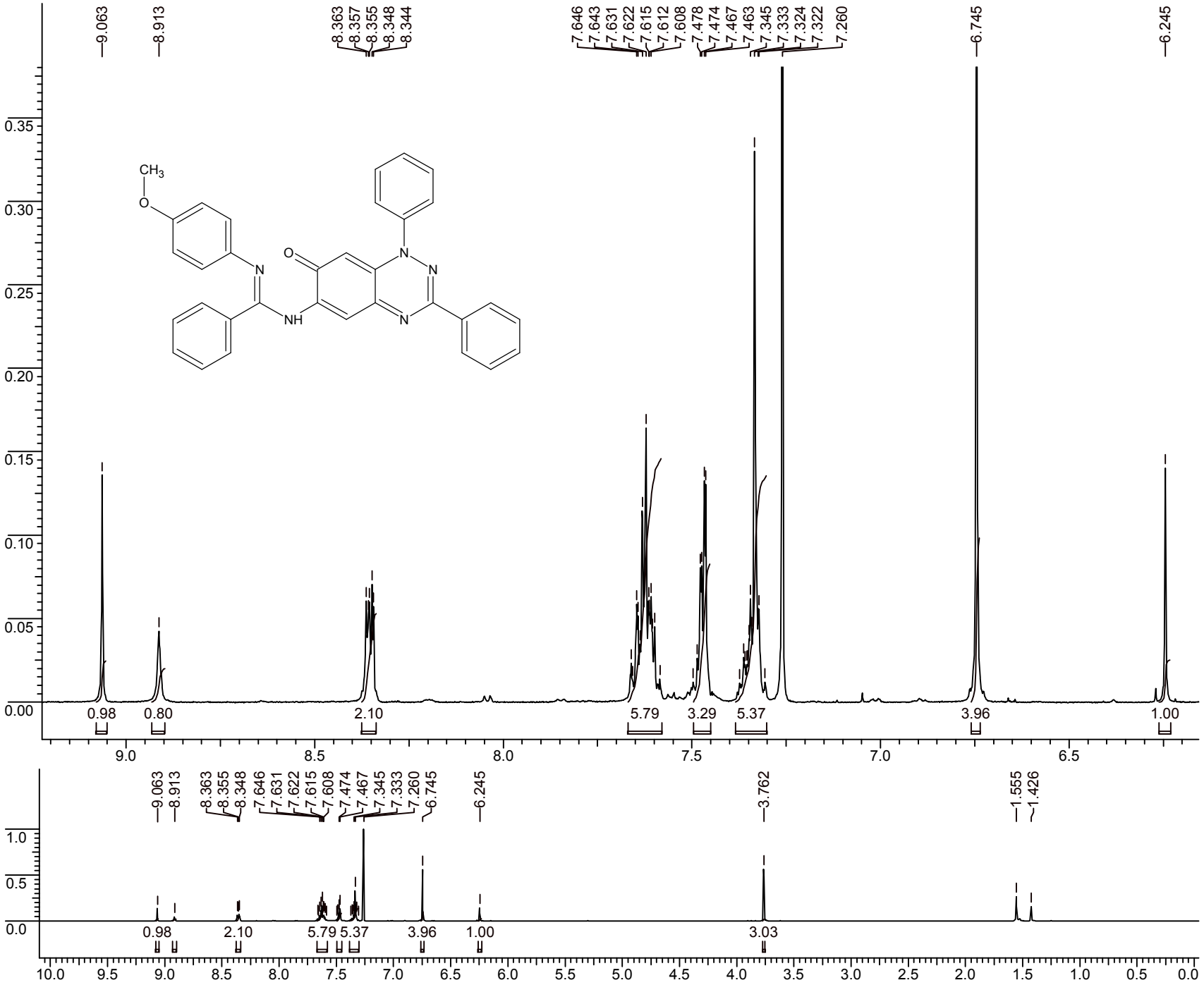
F2 - Acquisition Parameters
Date_ 20121017
Time 21.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 6000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 297.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)-N'-(4-methoxyphenyl)benzimidamide (7c)



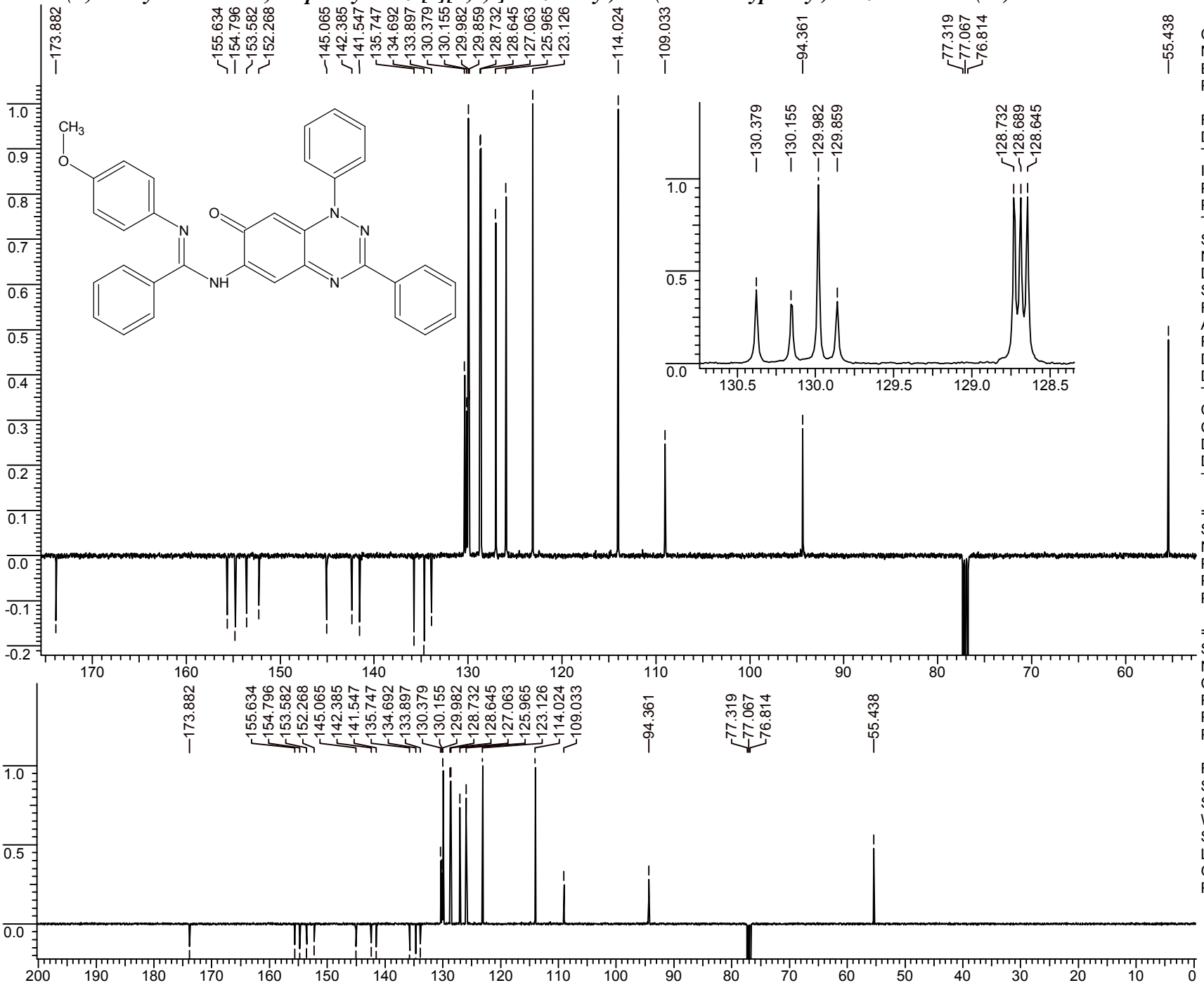
Current Data Parameters
NAME Andrey
EXPNO 142
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121016
Time 15.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.0361158 MHz
NUC1 1H
P1 11.75 usec
PLW1 15.41699982 W

F2 - Processing parameters
SI 65536
SF 500.0330400 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)-N'-(4-methoxyphenyl)benzimidamide (7c)



Current Data Parameters
NAME Andrey
EXPNO 144
PROCNO 1

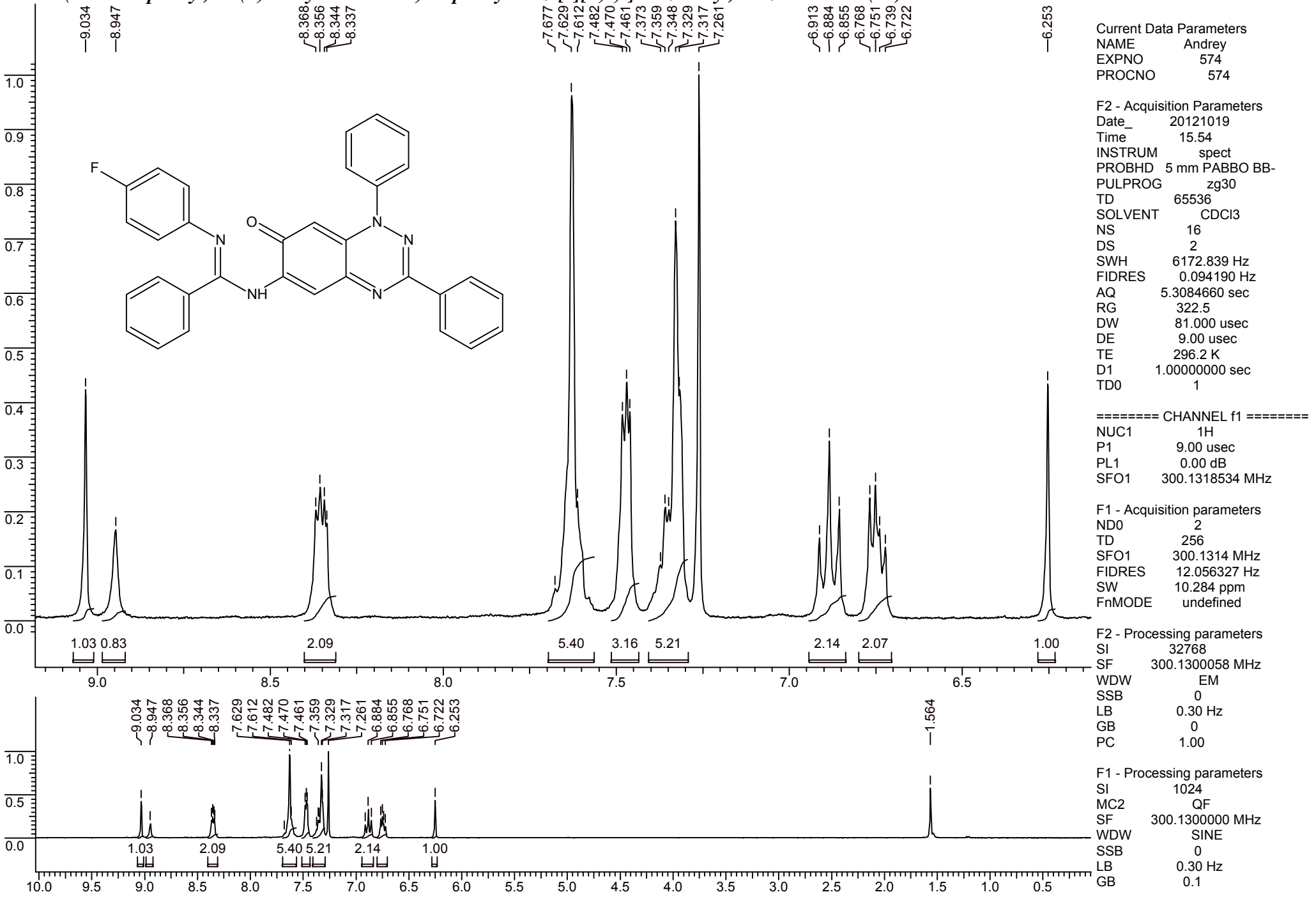
F2 - Acquisition Parameters
Date_ 20121016
Time 16.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1256
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 297.1 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7459782 MHz
NUC1 13C
P1 8.70 usec
P2 17.40 usec
PLW1 138.00000000 W

======== CHANNEL f2 ========
SFO2 500.0350280 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.41699982 W
PLW12 0.33258000 W

F2 - Processing parameters
SI 32768
SF 125.7334050 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N'-(4-Fluorophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7d)



Current Data Parameters
NAME Andrey
EXPNO 574
PROCNO 574

F2 - Acquisition Parameters
Date_ 20121019
Time 15.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 usec
DE 9.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

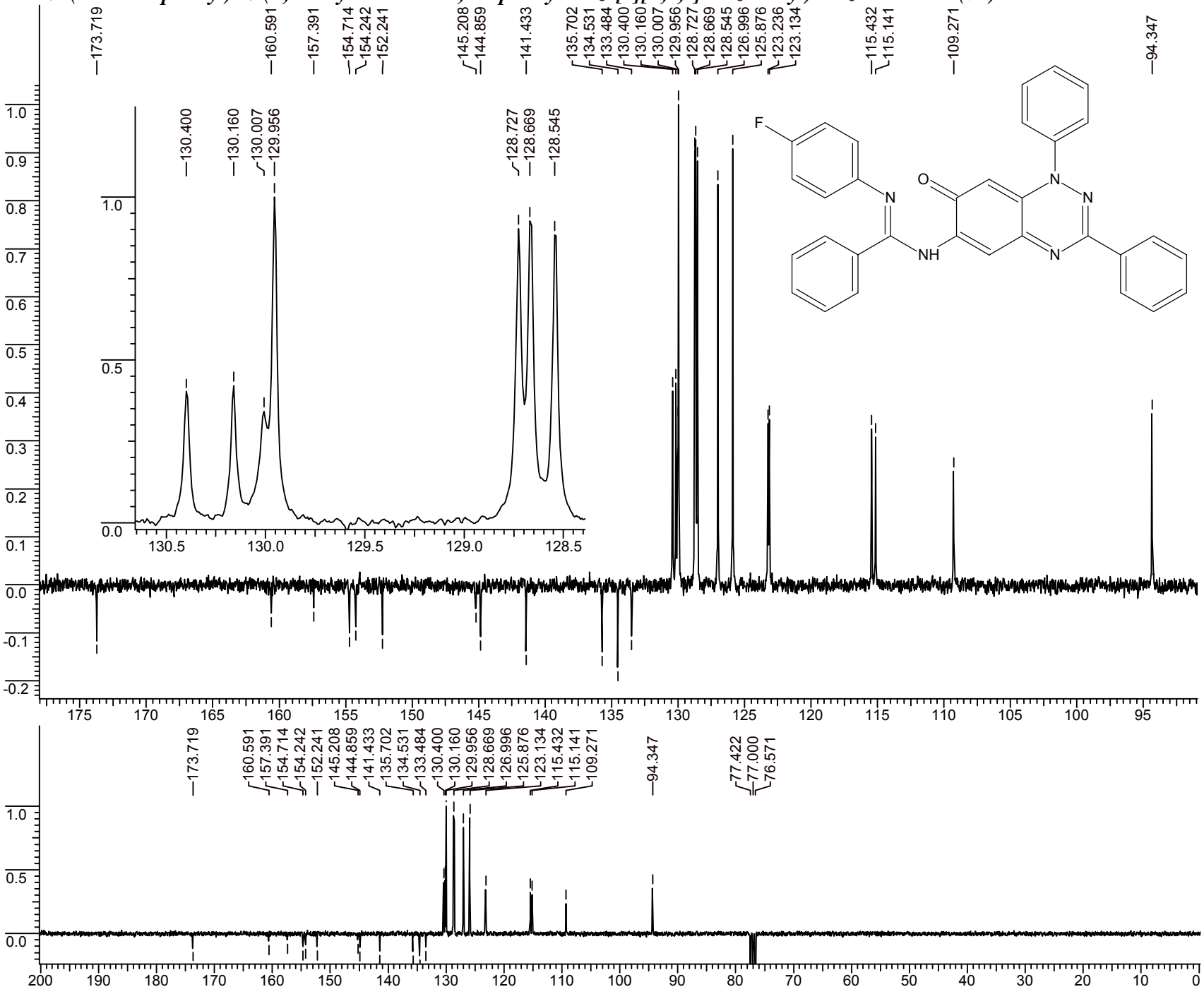
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300058 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

N'-(4-Fluorophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7d)



Current Data Parameters
NAME Andrey
EXPNO 575
PROCNO 575

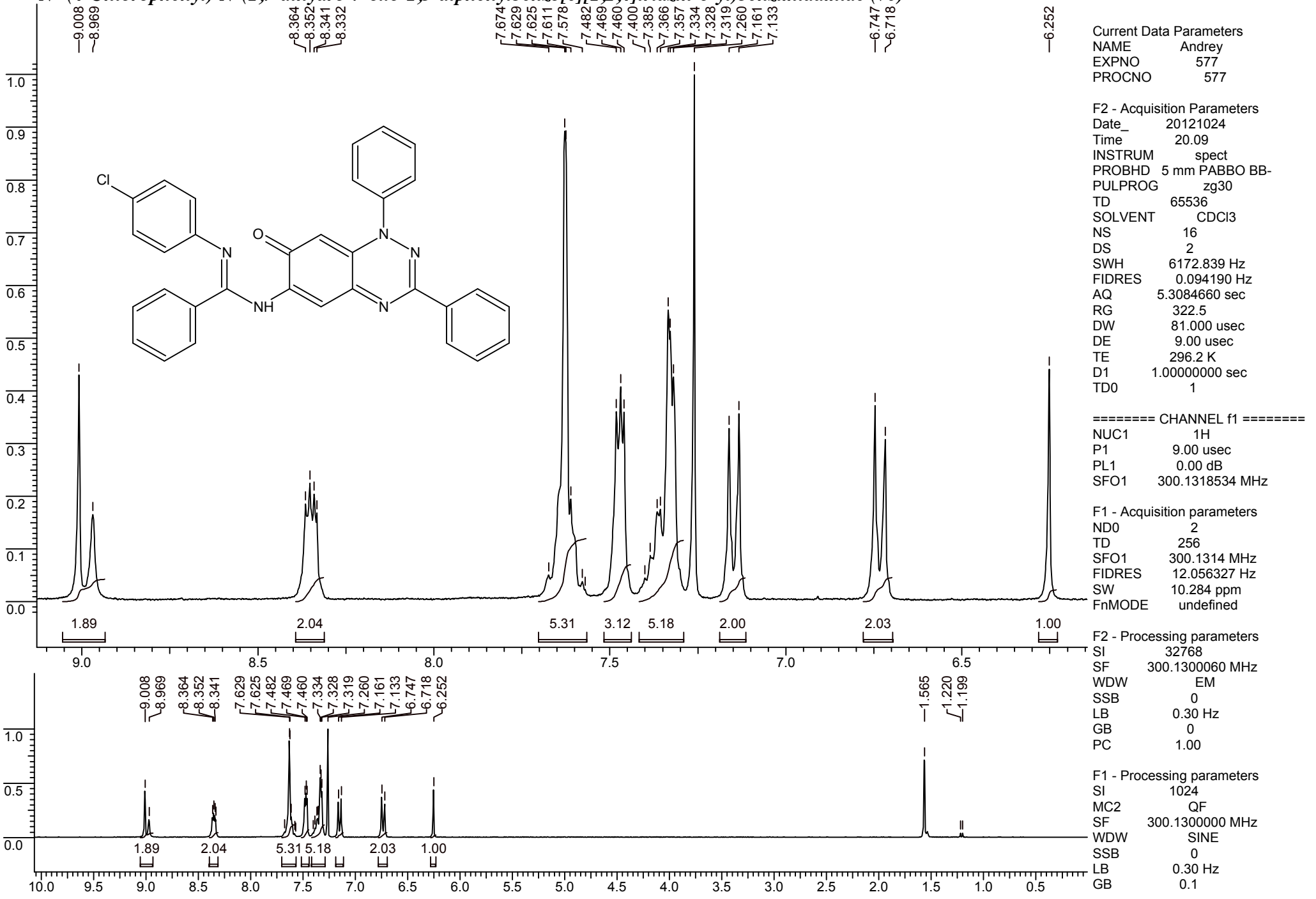
F2 - Acquisition Parameters
Date_ 20121019
Time 16.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1200
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DW 27.800 usec
DE 6.00 usec
TE 296.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N'-(4-Chlorophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7e)



Current Data Parameters
NAME Andrey
EXPNO 577
PROCNO 577

F2 - Acquisition Parameters
Date_ 20121024
Time 20.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 usec
DE 9.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

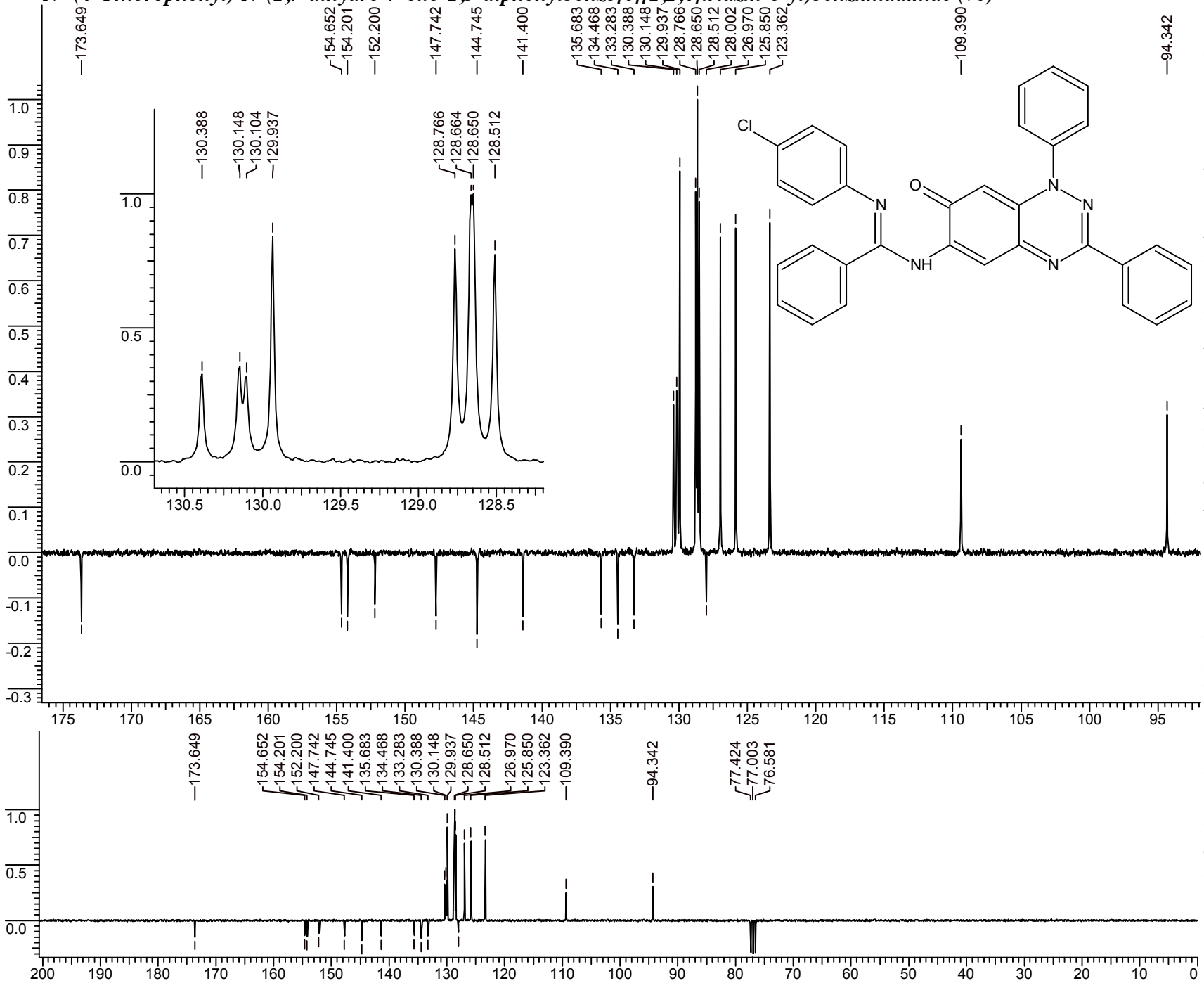
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

N'-(4-Chlorophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7e)



Current Data Parameters
NAME Andrey
EXPNO 578
PROCNO 578

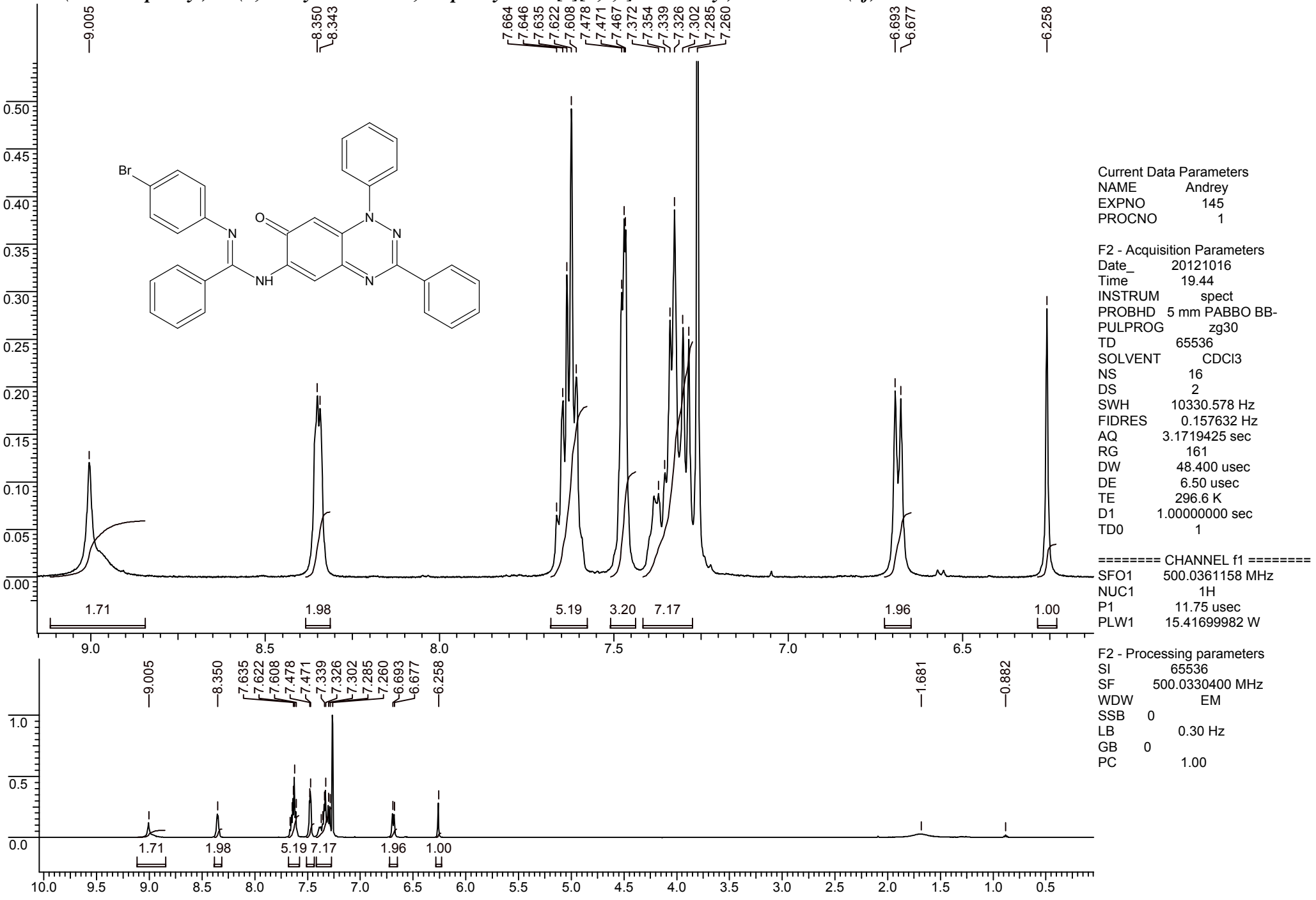
F2 - Acquisition Parameters
Date_ 20121024
Time 20.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1200
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 296.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677532 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N'-(4-Bromophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzamidine (7f)



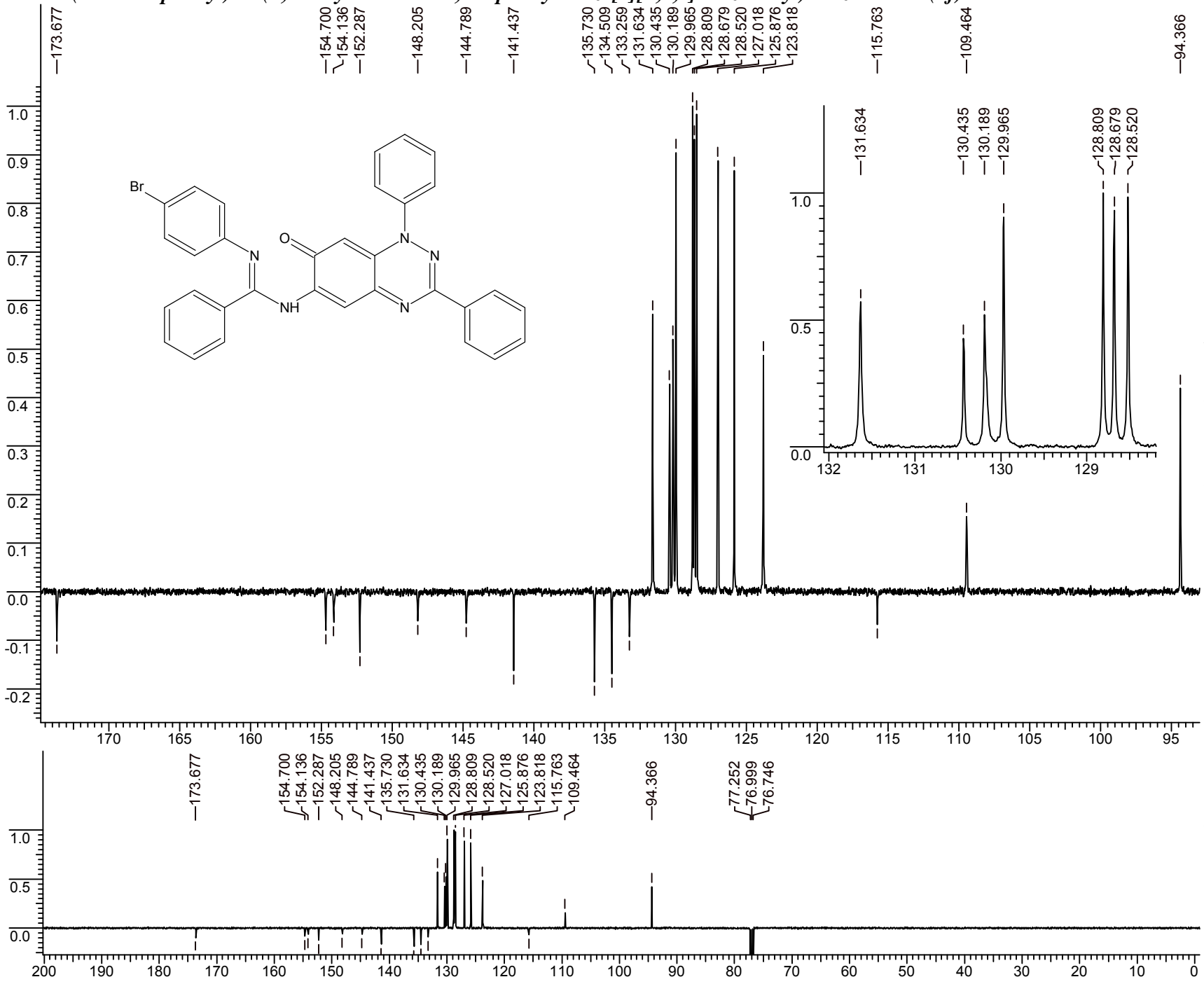
Current Data Parameters
NAME Andrey
EXPNO 145
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121016
Time 19.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.0361158 MHz
NUC1 1H
P1 11.75 usec
PLW1 15.41699982 W

F2 - Processing parameters
SI 65536
SF 500.0330400 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N'-(4-Bromophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzamidine (7f)



Current Data Parameters
NAME Andrey
EXPNO 147
PROCNO 1

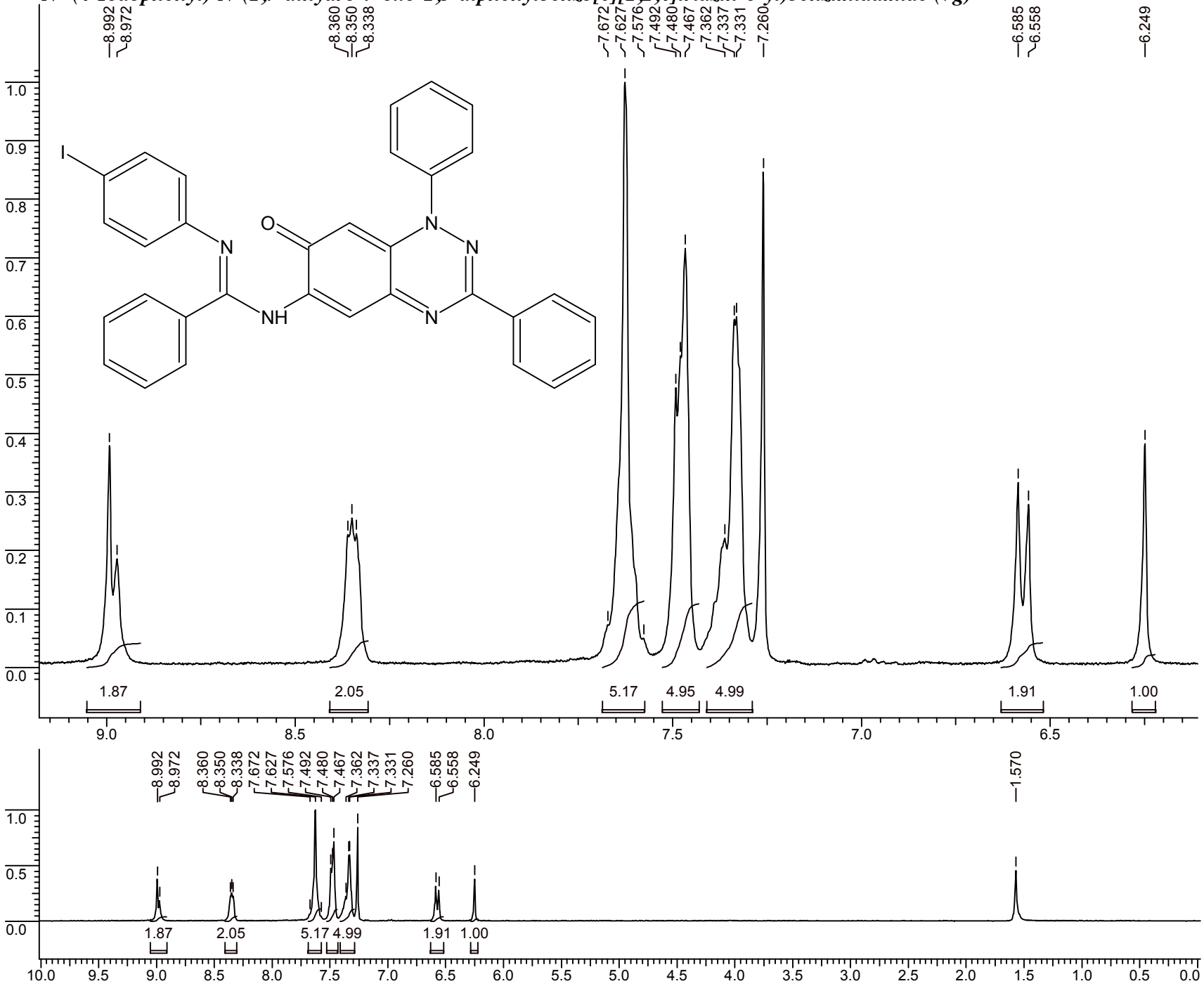
F2 - Acquisition Parameters
Date_ 20121016
Time 21.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 2400
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7459782 MHz
NUC1 13C
P1 8.70 usec
P2 17.40 usec
PLW1 138.00000000 W

======== CHANNEL f2 ========
SFO2 500.0350280 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.41699982 W
PLW12 0.33258000 W

F2 - Processing parameters
SI 32768
SF 125.7334098 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N'-(4-Iodophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7g)



Current Data Parameters
NAME Andrey
EXPNO 579
PROCNO 579

F2 - Acquisition Parameters
Date_ 20121027
Time 22.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 usec
DE 9.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

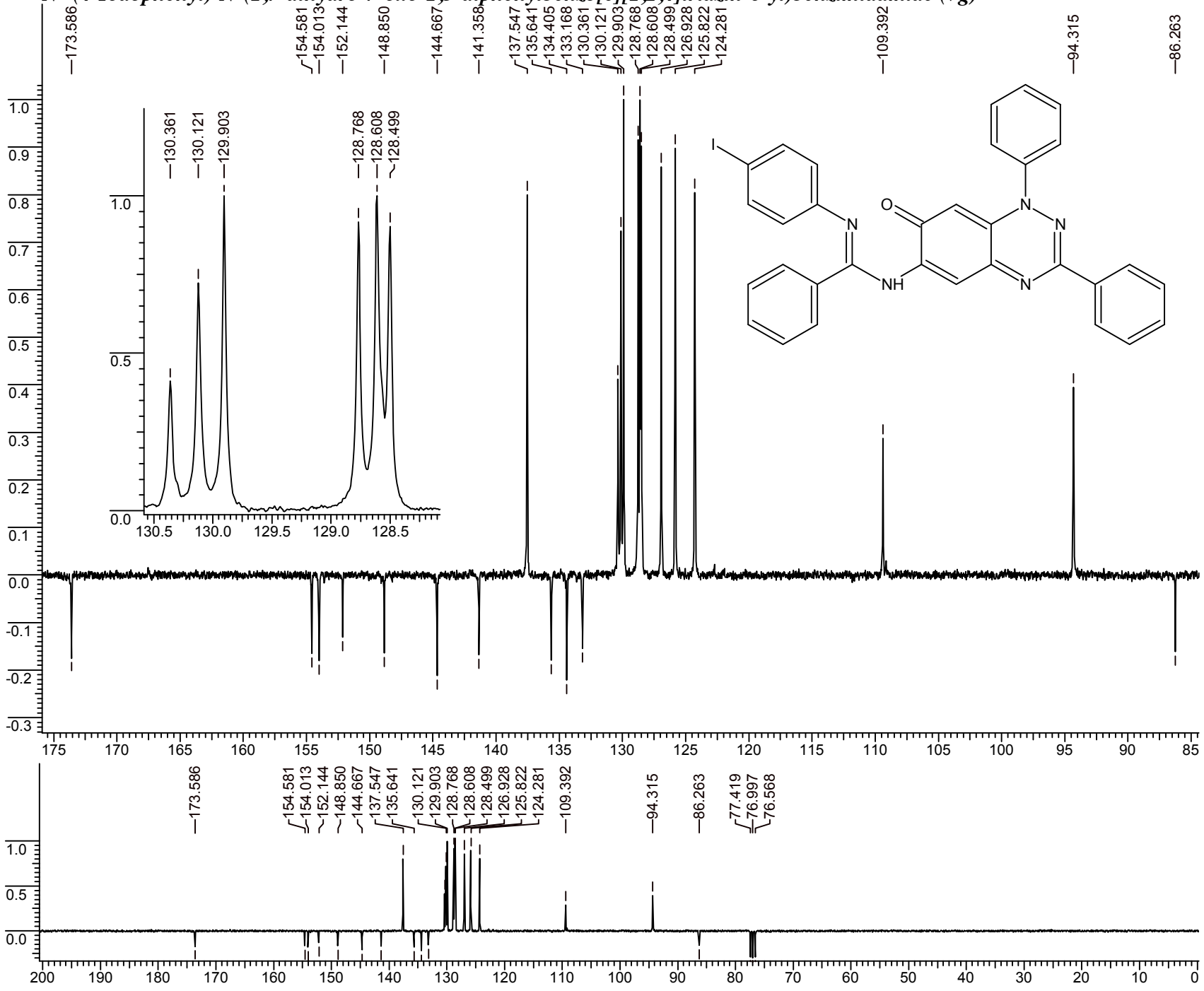
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300057 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

N'-(4-Iodophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7g)



Current Data Parameters
NAME Andrey
EXPNO 580
PROCNO 580

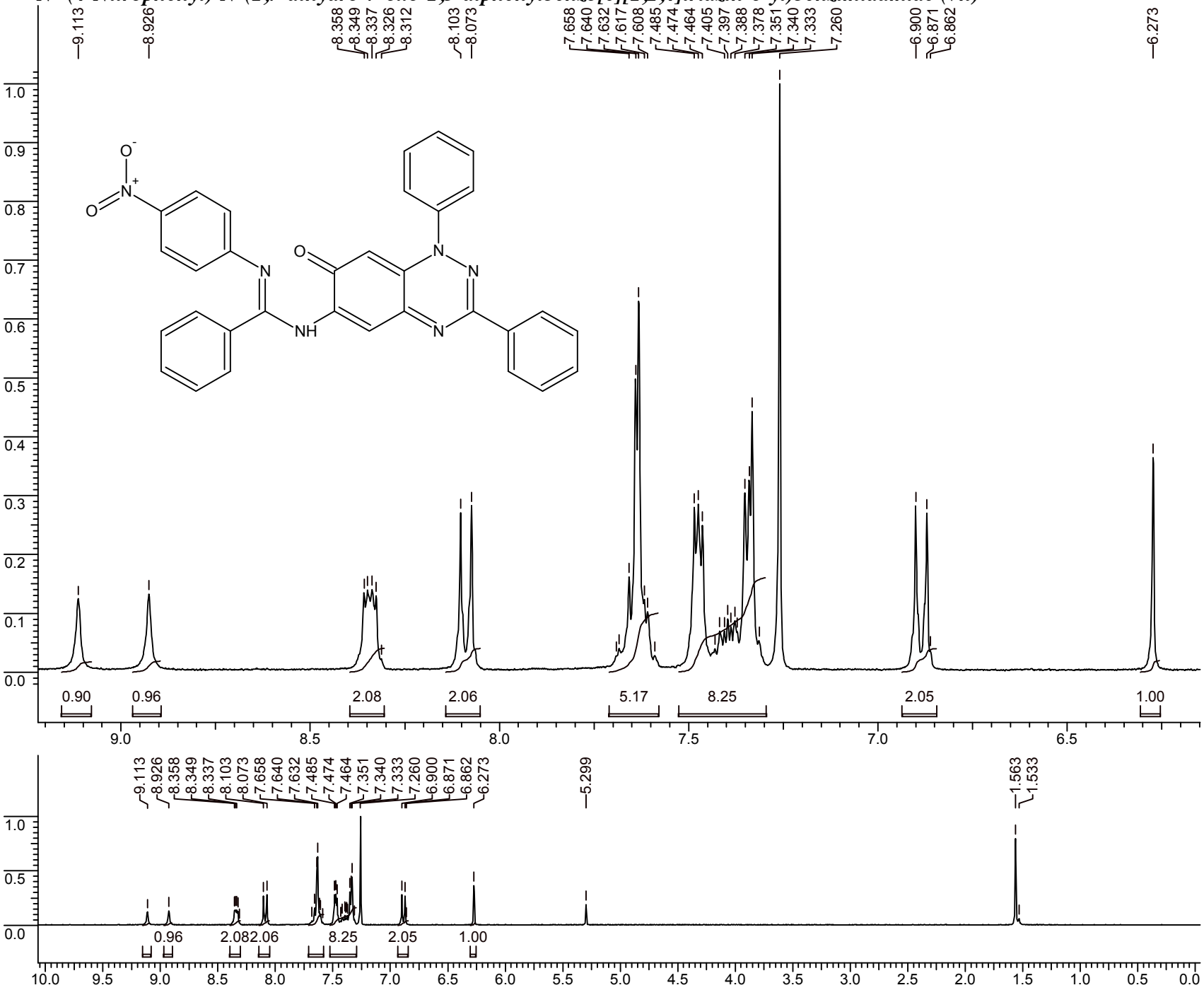
F2 - Acquisition Parameters
Date_ 20121027
Time 22.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1200
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 296.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677552 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N'-(4-Nitrophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7h)



Current Data Parameters
NAME Andrey
EXPNO 581
PROCNO 581

F2 - Acquisition Parameters
Date_ 20121029
Time 22.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 usec
DE 9.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

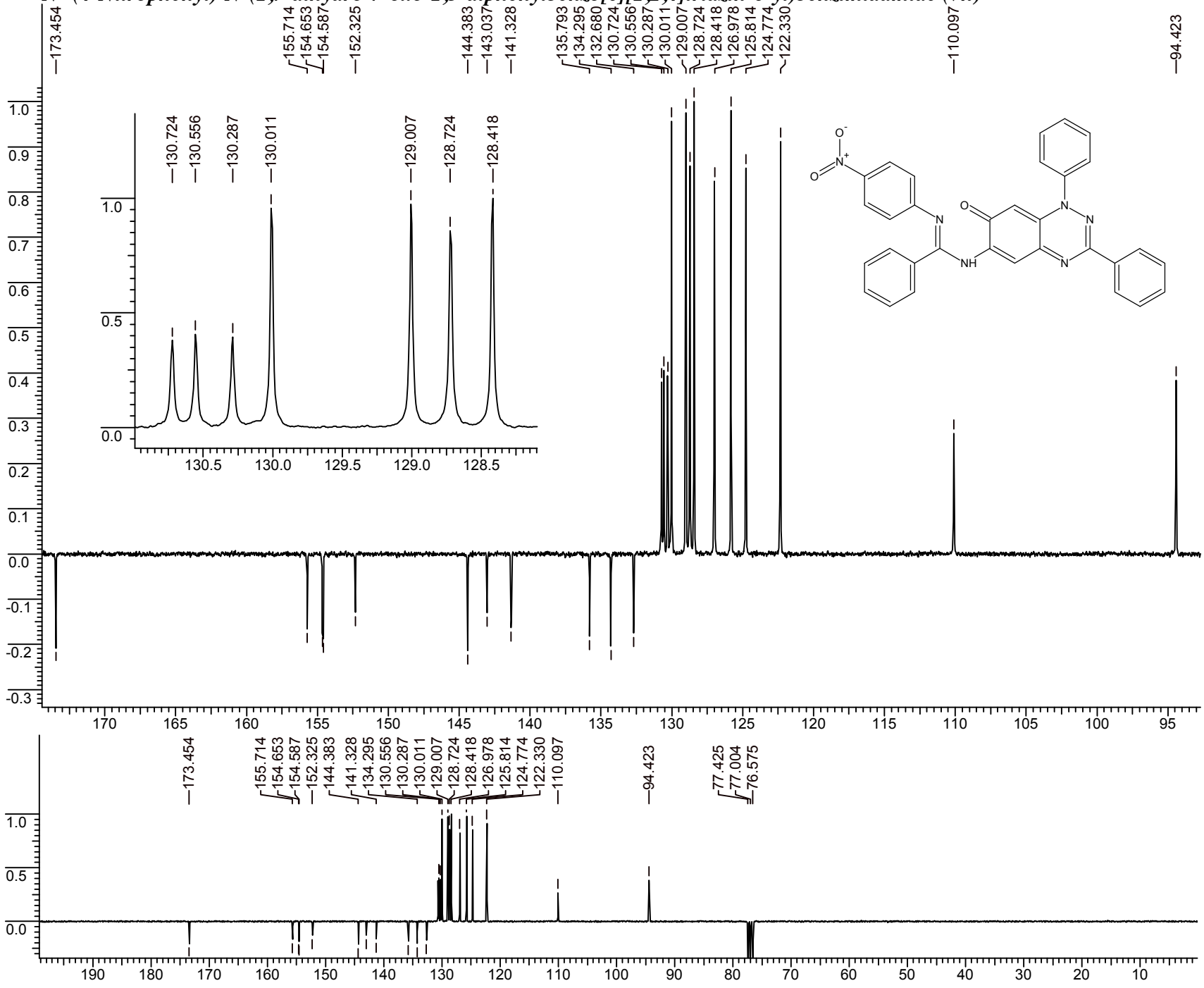
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

N'-(4-Nitrophenyl)-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7h)



Current Data Parameters
NAME Andrey
EXPNO 582
PROCNO 582

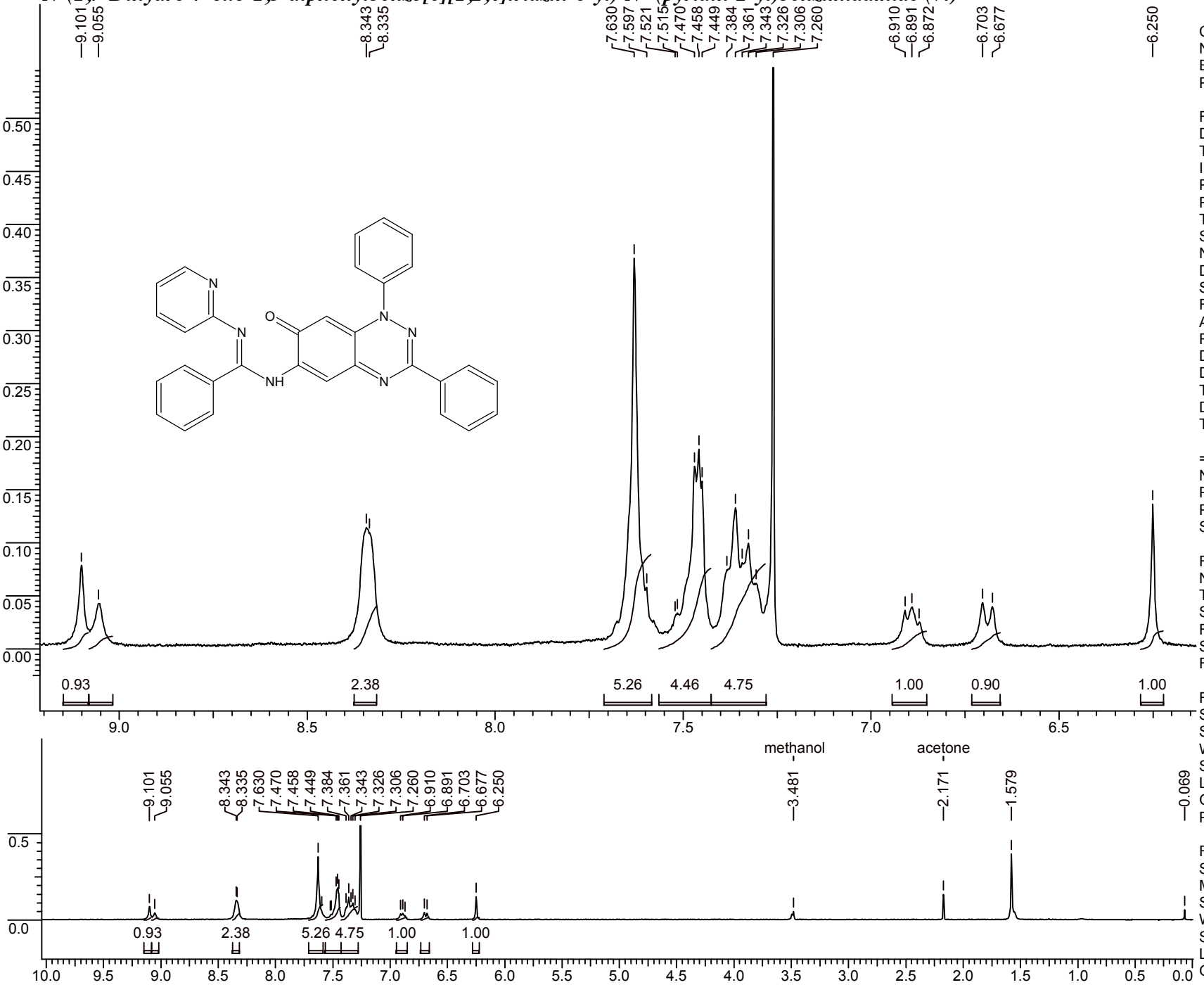
F2 - Acquisition Parameters
Date_ 20121029
Time 22.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 8611
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 296.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677520 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)-N'-(pyridin-2-yl)benzimidamide (7i)



Current Data Parameters
NAME Andrey
EXPNO 619
PROCNO 619

F2 - Acquisition Parameters
Date_ 20121226
Time 12.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 574.7
DW 81.000 usec
DE 9.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

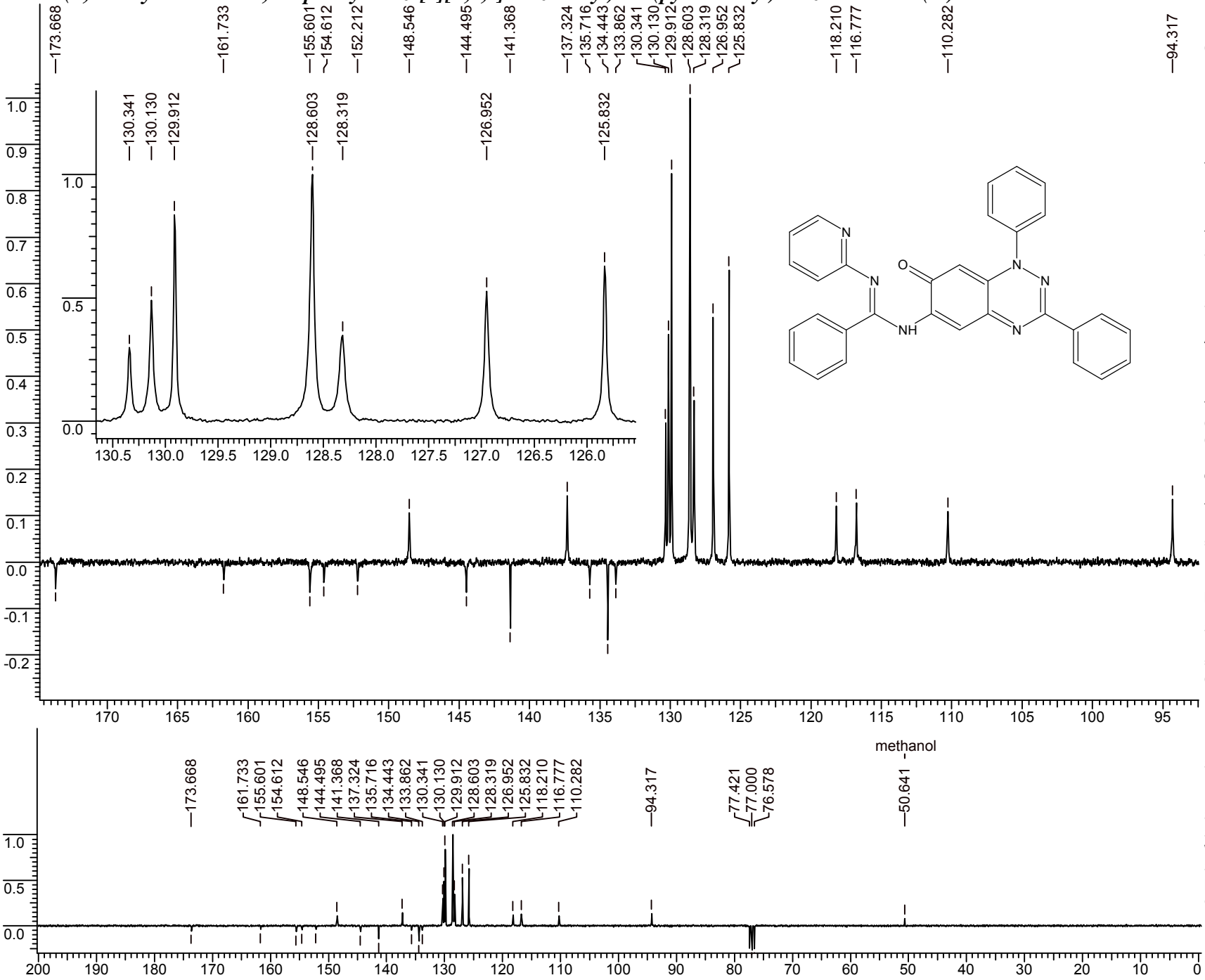
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)-N'-(pyridin-2-yl)benzimidamide (7i)



Current Data Parameters
NAME Andrey
EXPNO 594
PROCNO 594

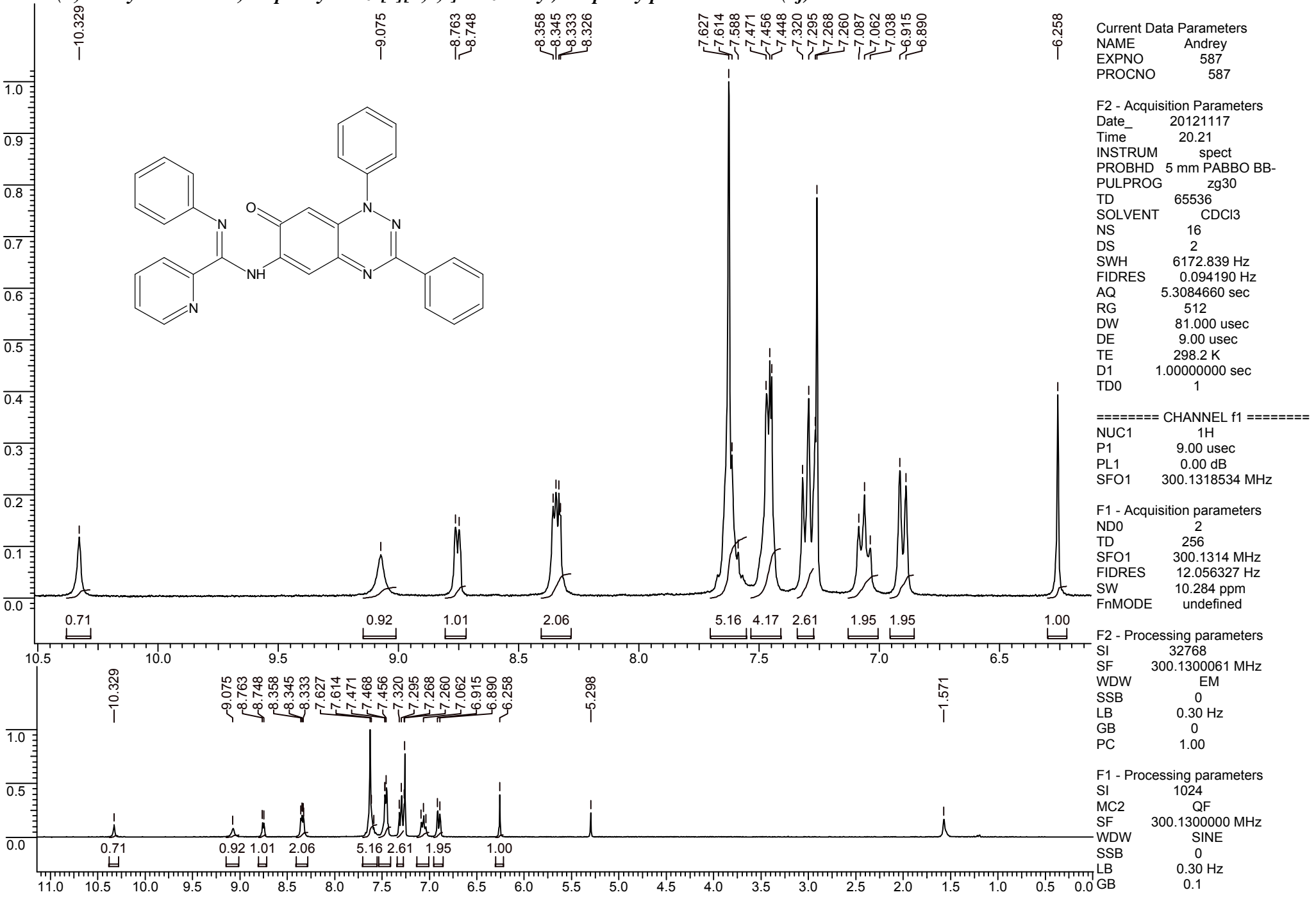
F2 - Acquisition Parameters
Date_ 20121127
Time 16.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 921
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 297.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677546 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)-N'-phenylpicolinidamide (7j)



Current Data Parameters
NAME Andrey
EXPNO 587
PROCNO 587

F2 - Acquisition Parameters
Date_ 20121117
Time 20.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DW 81.000 usec
DE 9.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

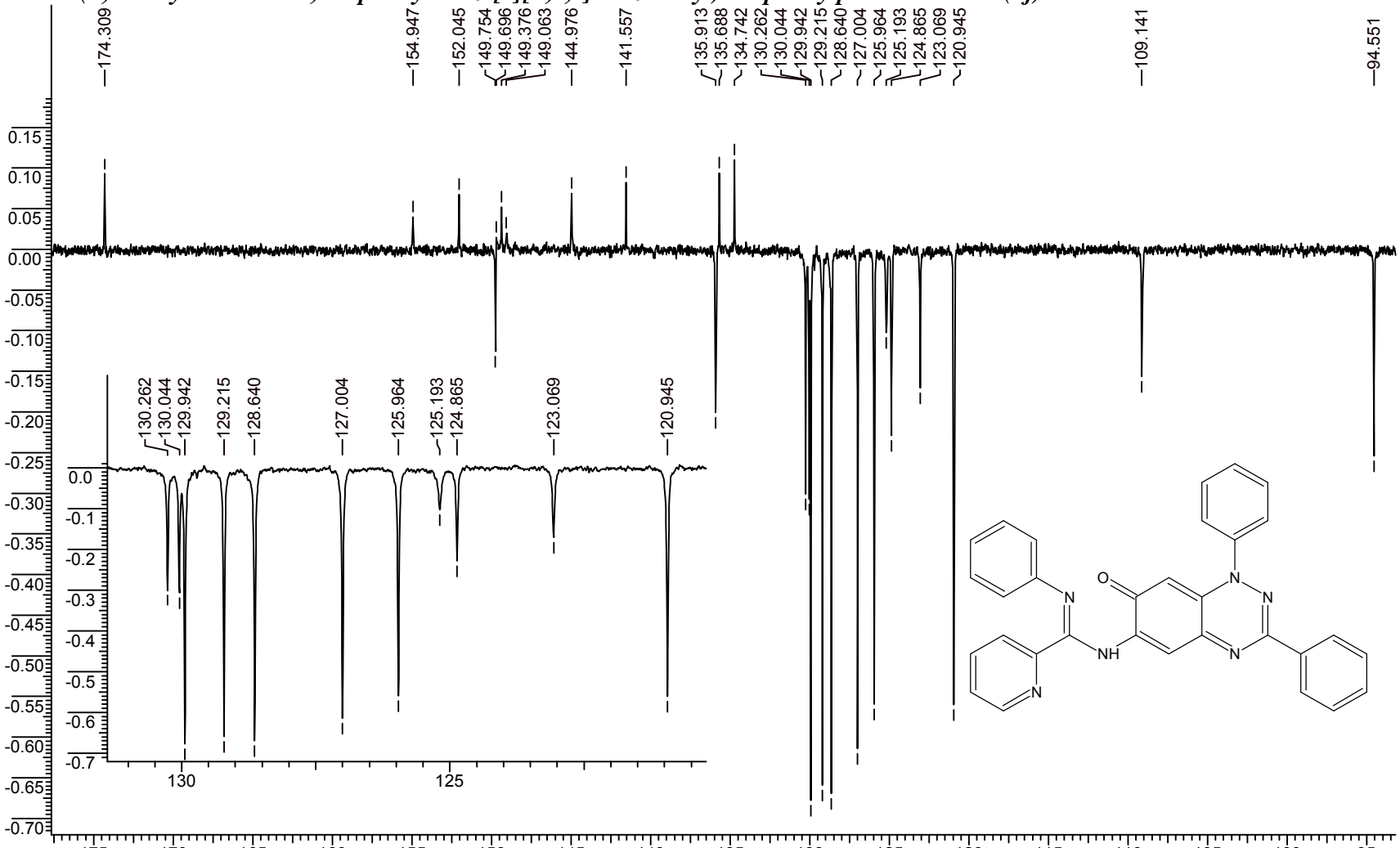
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

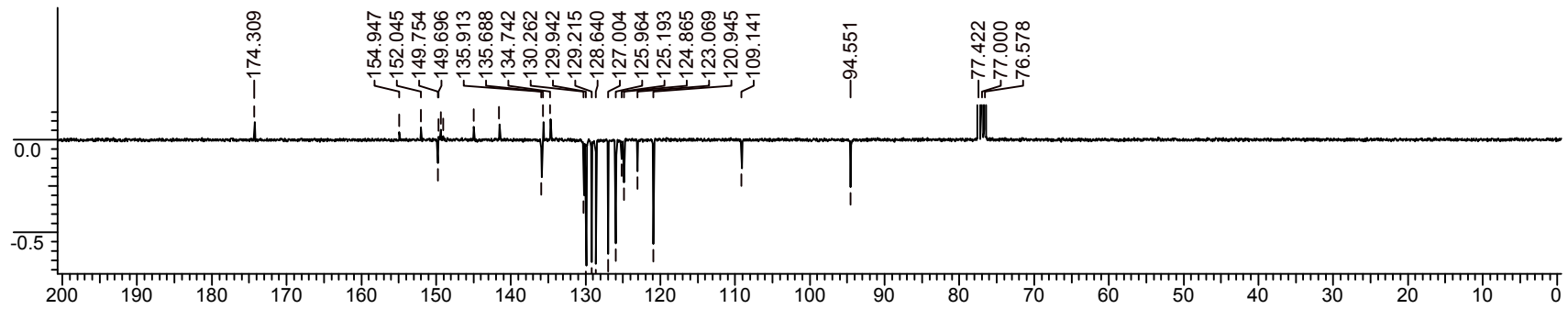
F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)-N'-phenylpicolinidamide (7j)





Current Data Parameters
NAME Andrey
EXPNO 588
PROCNO 588

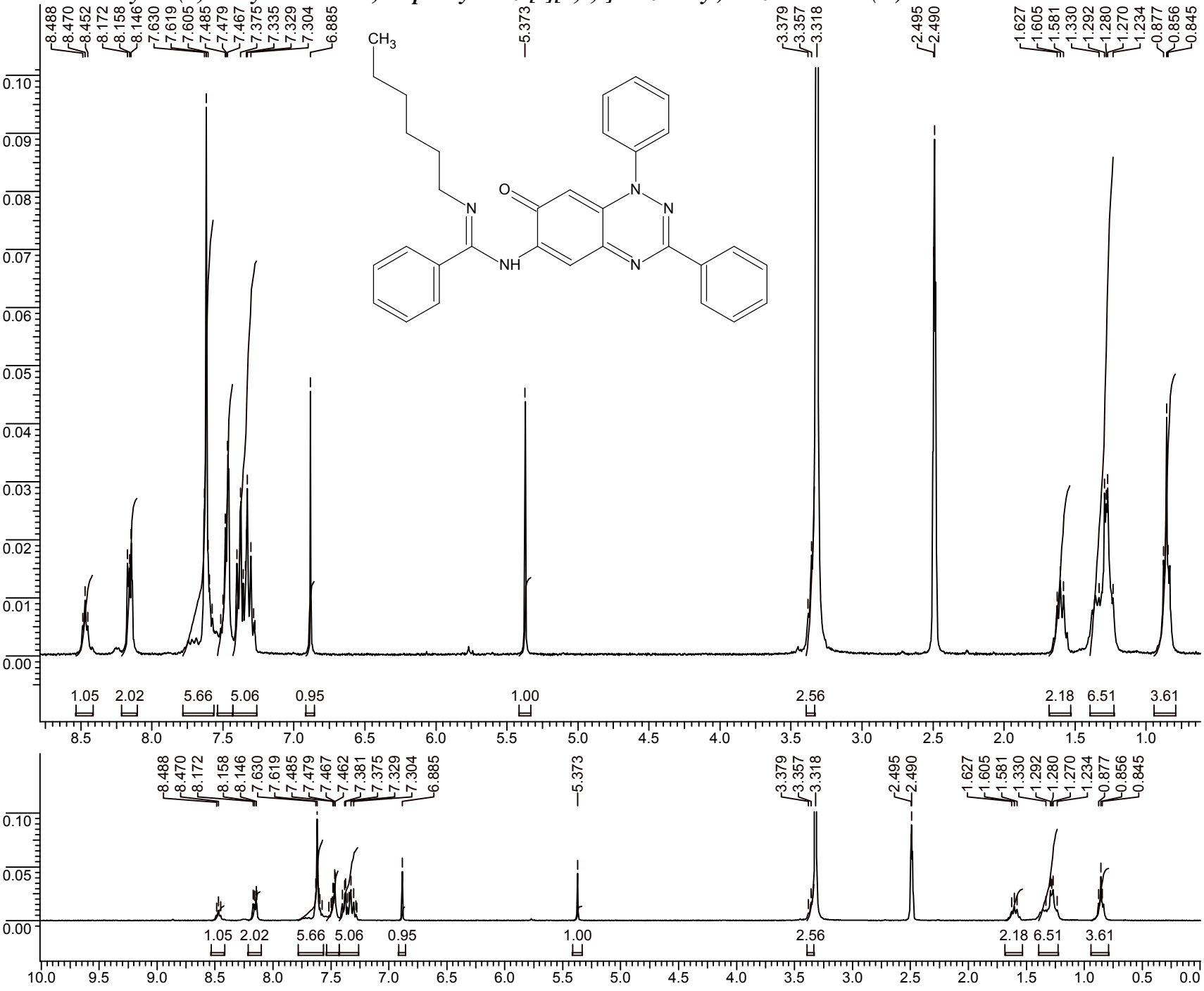
F2 - Acquisition Parameters
Date_ 20121117
Time 21.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 15000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 6502
DW 27.800 usec
DE 6.00 usec
TE 299.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677501 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N'-n-Hexyl-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7l)



Current Data Parameters
NAME Andrey
EXPNO 610
PROCNO 610

F2 - Acquisition Parameters
Date_ 20121208
Time 16.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 9.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

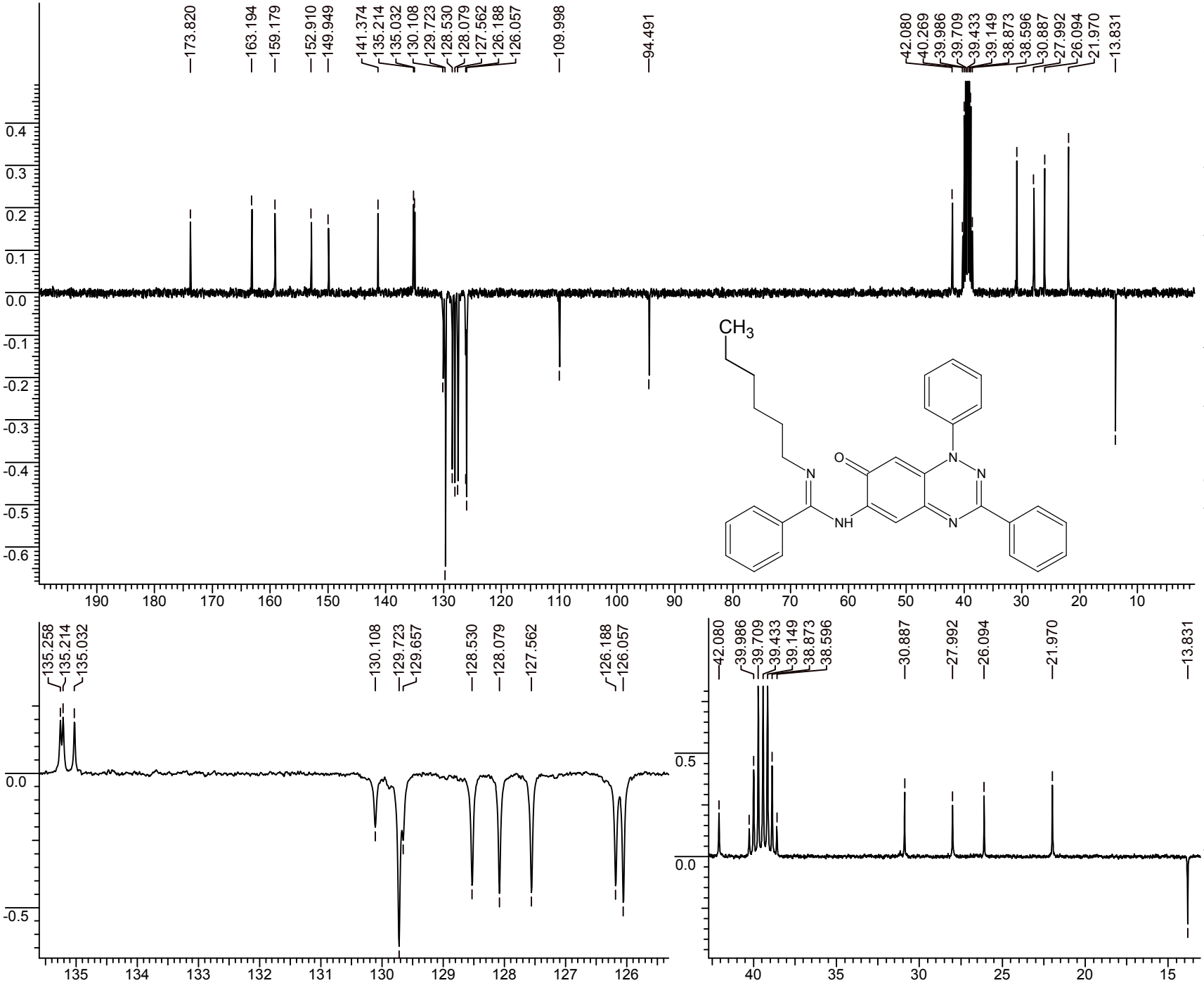
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300012 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

N'-n-Hexyl-N-(1,7-dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzimidamide (7l)



Current Data Parameters
NAME Andrey
EXPNO 612
PROCNO 612

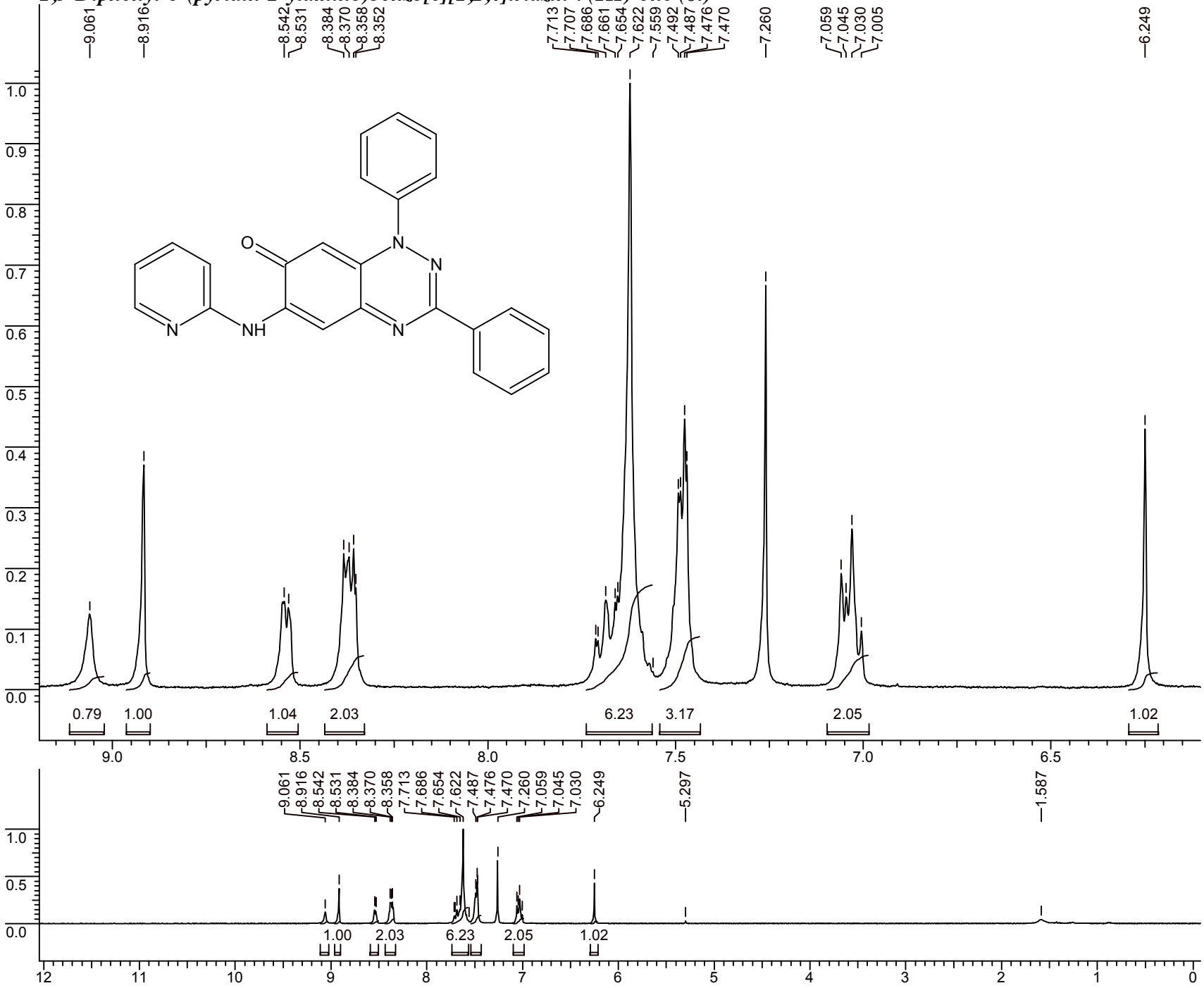
F2 - Acquisition Parameters
Date_ 20121208
Time 17.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 7298.2
DW 27.800 usec
DE 6.00 usec
TE 298.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677913 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1,3-Diphenyl-6-(pyridin-2-ylamino)benzo[e][1,2,4]triazin-7(1H)-one (8i)



Current Data Parameters
NAME Andrey
EXPNO 498
PROCNO 498

F2 - Acquisition Parameters
Date_ 20120308
Time 20.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 574.7
DW 81.000 usec
DE 9.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

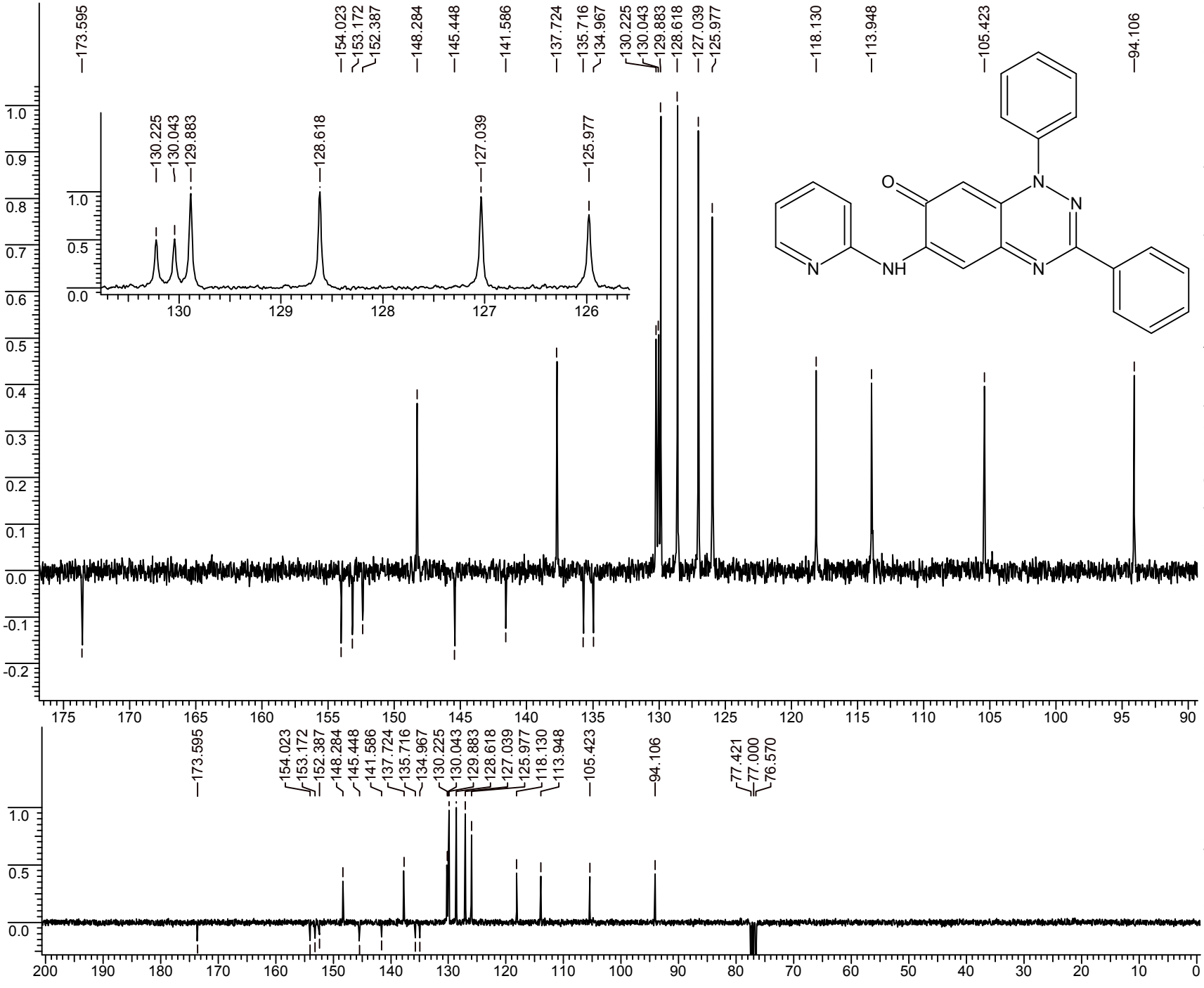
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

1,3-Diphenyl-6-(pyridin-2-ylamino)benzo[e][1,2,4]triazin-7(1H)-one (8i)



Current Data Parameters
NAME Andrey
EXPNO 499
PROCNO 499

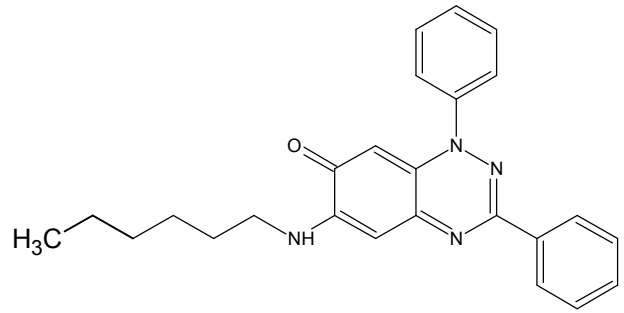
F2 - Acquisition Parameters
Date_ 20120308
Time 20.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1200
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 297.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677515 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

6-(n-Hexylamino)-1,3-diphenylbenzo[e][1,2,4]triazin-7(1H)-one (8l)



8.319 8.308 8.295 7.607 7.588 7.580 7.465 7.453 7.260 6.888 6.629 6.116 3.436 3.415 3.394 3.372 2.170 1.788 1.764 1.740 1.715 1.565 1.473 1.452 1.401 1.361 1.352 1.340 0.934 0.913

2.00 4.96 0.87 1.03 1.00 2.01 2.04 6.19 3.04

Current Data Parameters
NAME Andrey
EXPNO 600
PROCNO 600

F2 - Acquisition Parameters
Date_ 20121201
Time 16.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 usec
DE 9.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

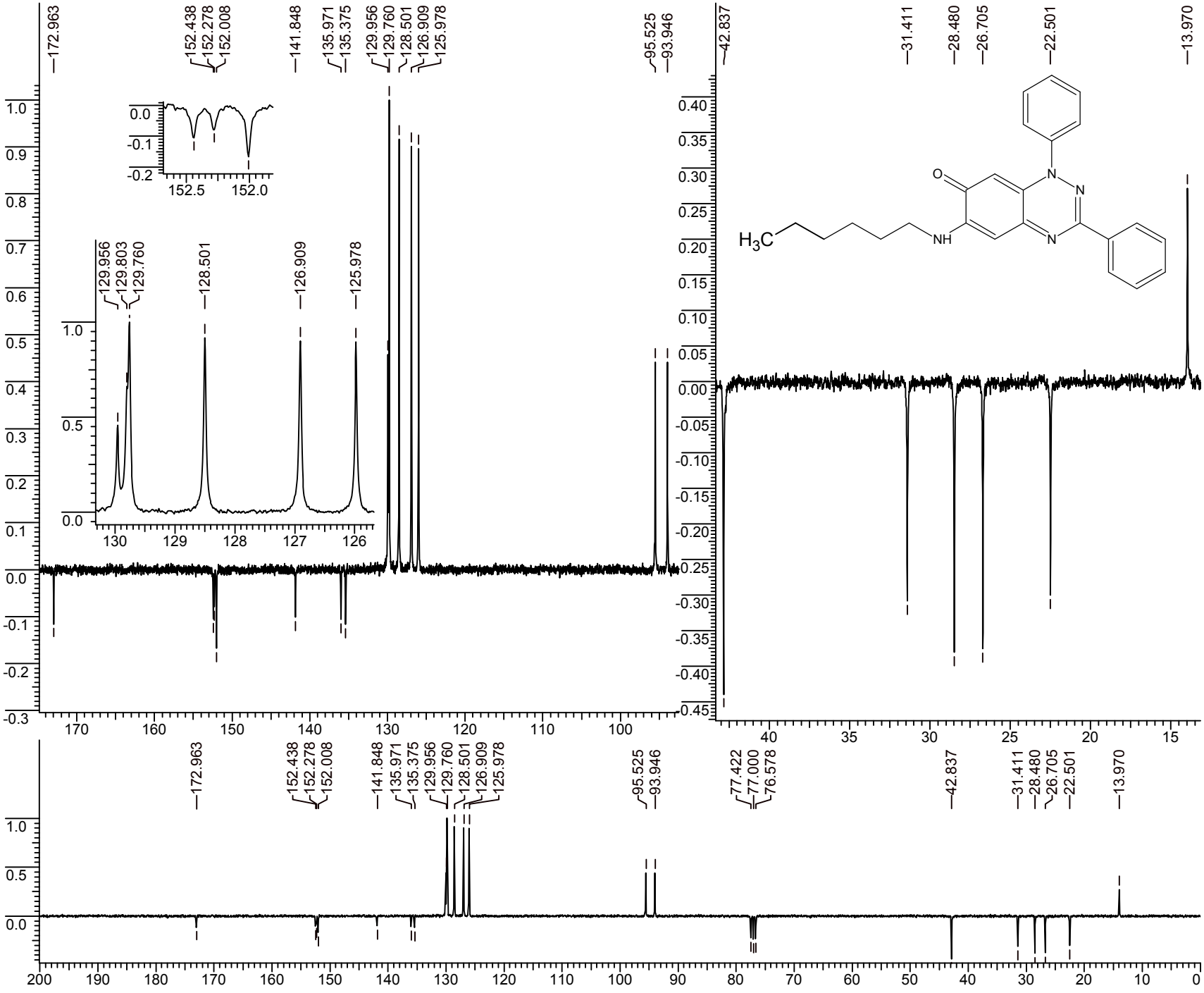
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

6-(n-Hexylamino)-1,3-diphenylbenzo[e][1,2,4]triazin-7(1H)-one (8l)



Current Data Parameters
NAME Andrey
EXPNO 601
PROCNO 601

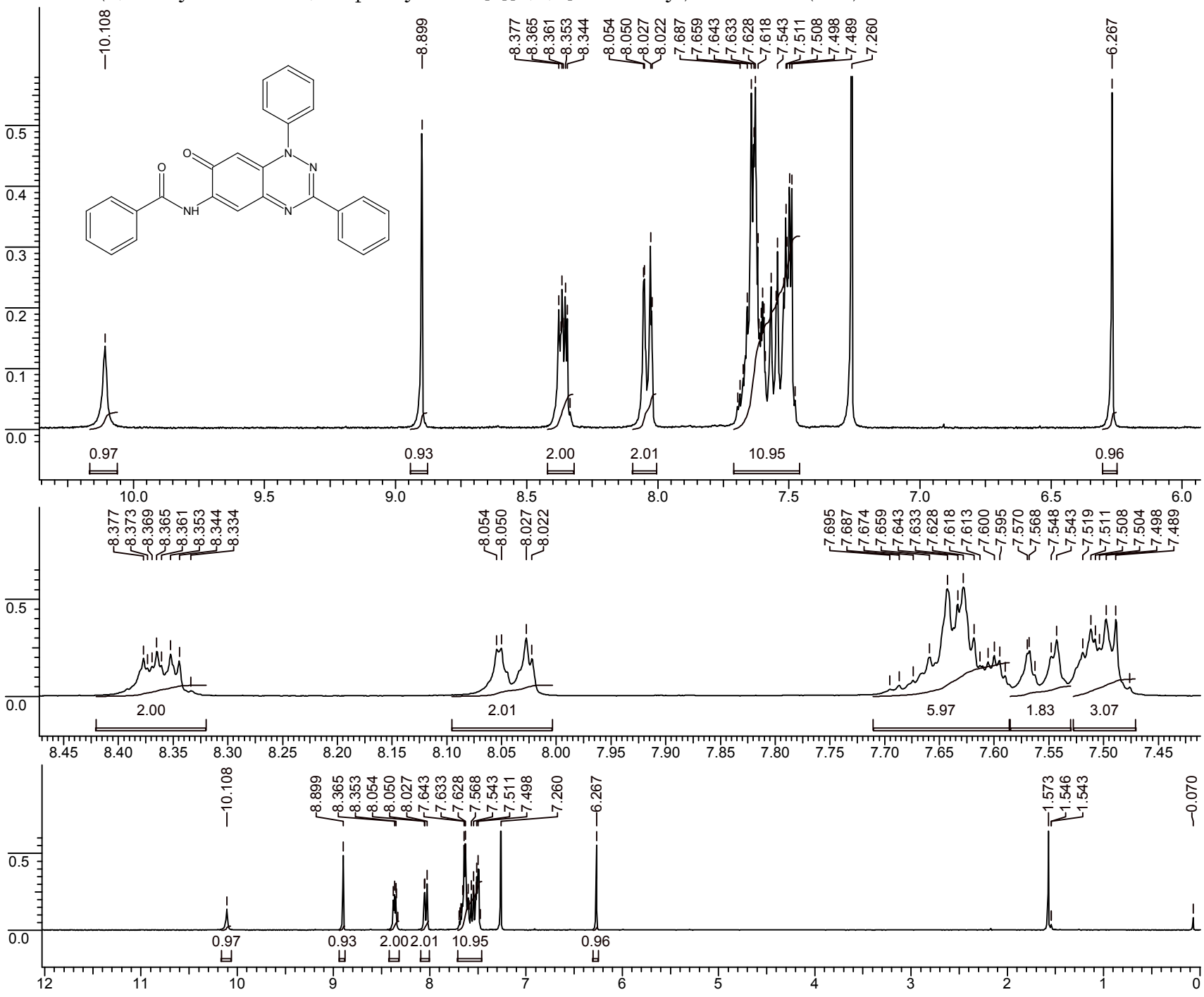
F2 - Acquisition Parameters
Date_ 20121201
Time 17.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1129
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 298.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00000908 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.13 usec
p2 14.26 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)benzamide (13a)



Current Data Parameters
NAME Andrey
EXPNO 494
PROCNO 494

F2 - Acquisition Parameters
Date_ 20120302
Time 18.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 574.7
DW 81.000 usec
DE 9.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

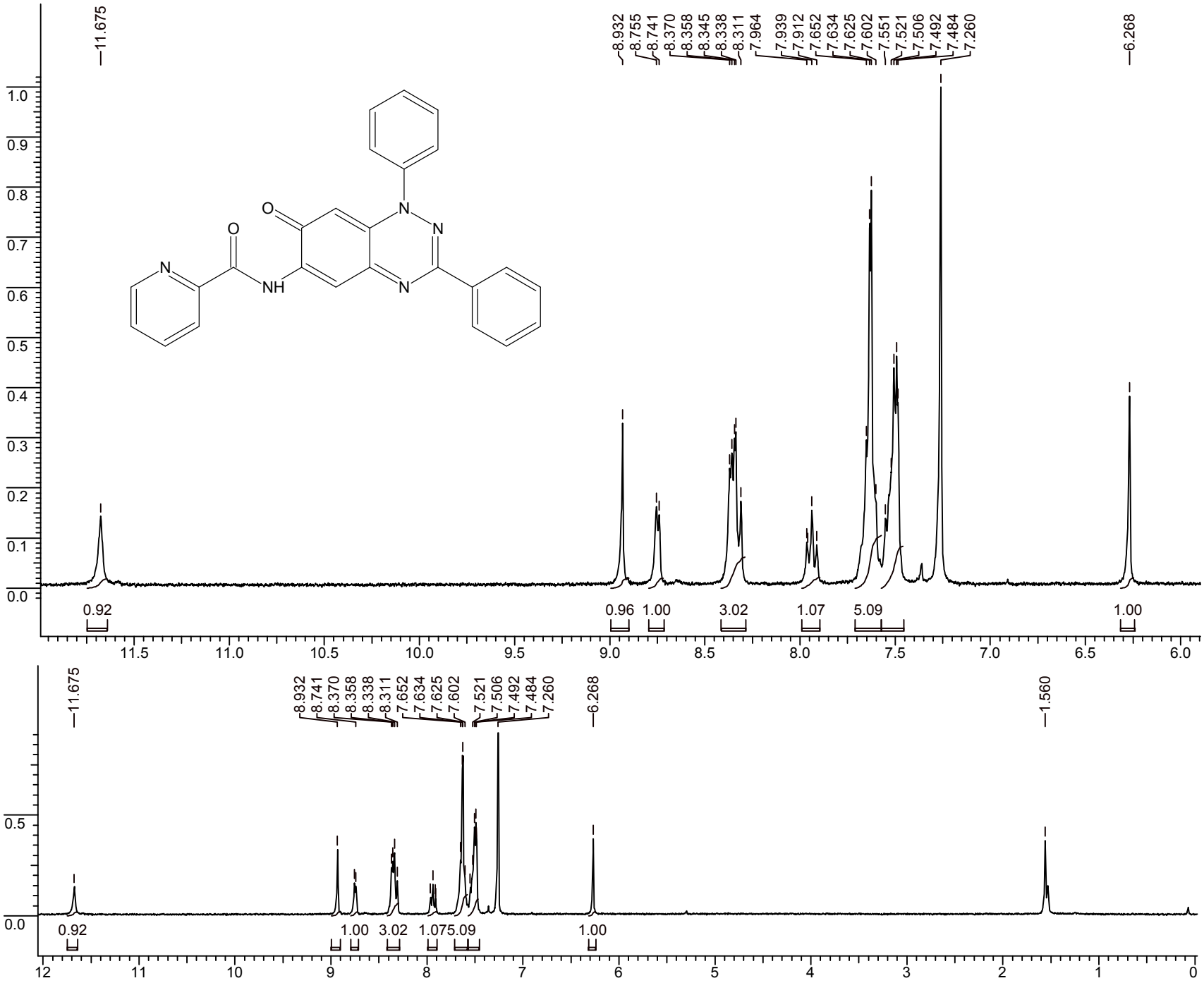
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

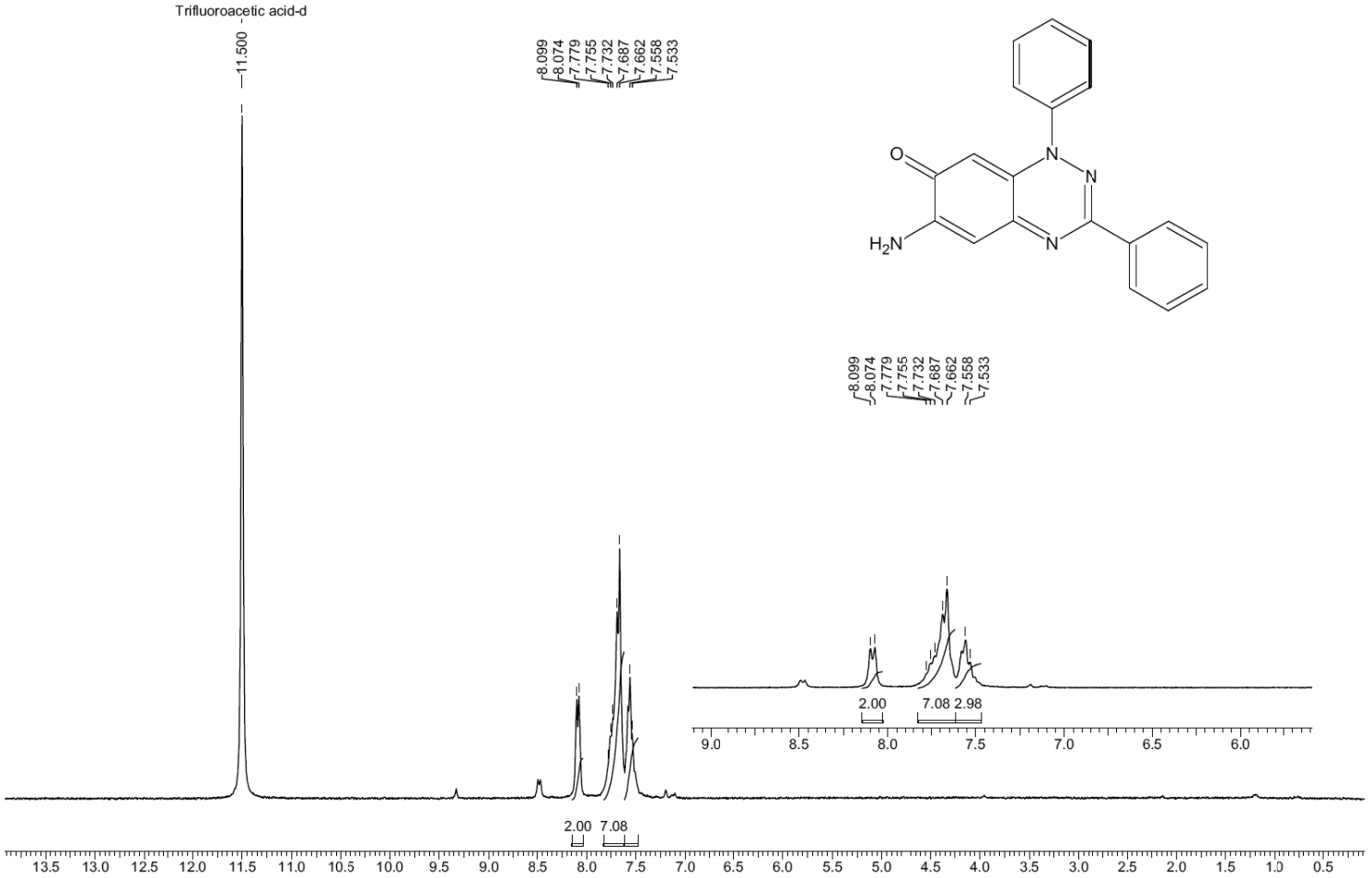
F2 - Processing parameters
SI 32768
SF 300.1300058 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

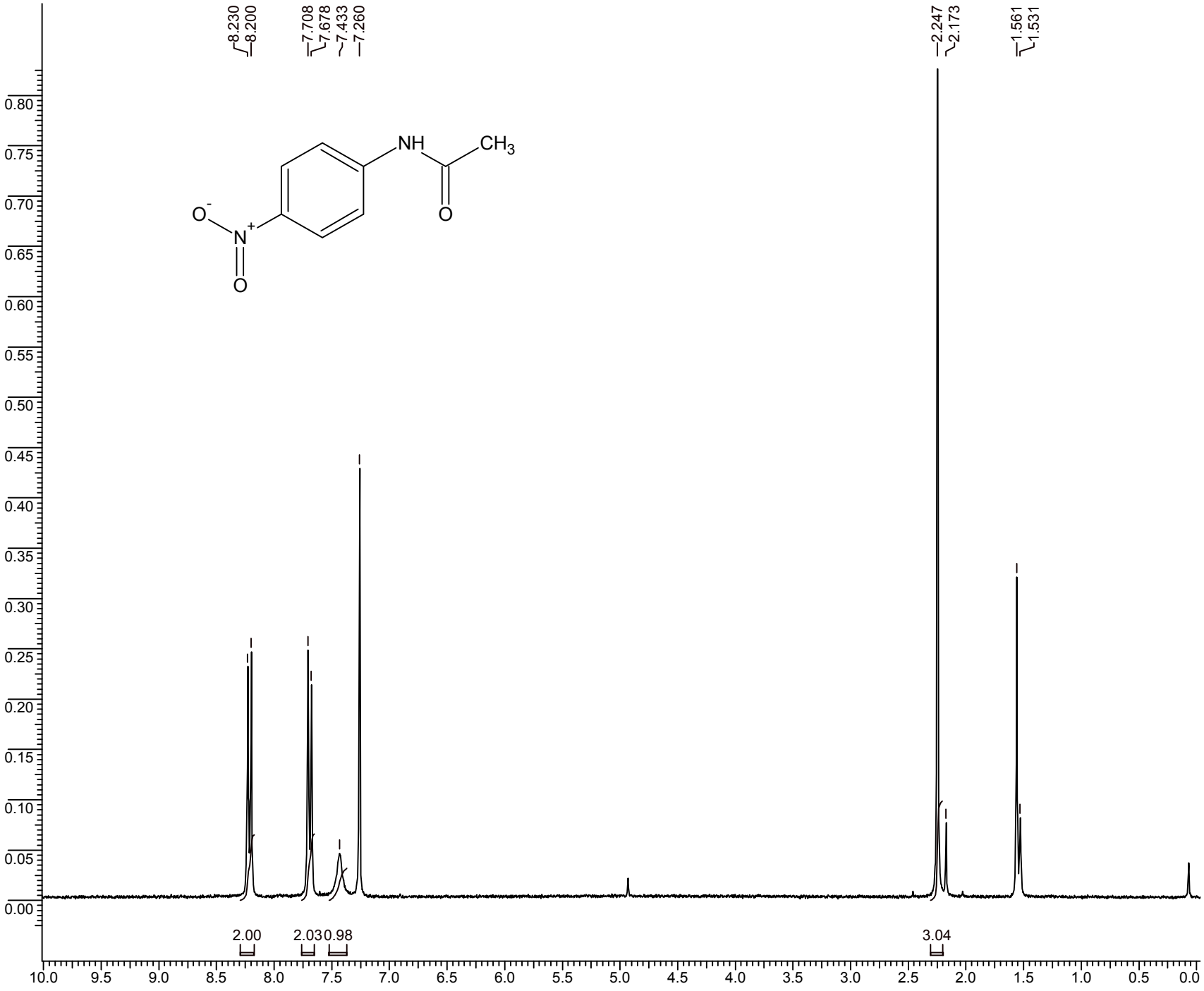
N-(1,7-Dihydro-7-oxo-1,3-diphenylbenzo[e][1,2,4]triazin-6-yl)picolinamide (13b)



1H NMR of 6-Amino-1,3-diphenylbenzo[e][1,2,4]triazin-7(1H)-one（1 4）



N-(4-nitrophenyl)acetamide



Current Data Parameters
NAME Andrey
EXPNO 613
PROCNO 613

F2 - Acquisition Parameters
Date_ 20121213
Time 13.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 574.7
DW 81.000 usec
DE 9.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined

F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1