Electronic Supplementary Information

Studies on the Interactions of 5-*R*-3-(2-Pyridyl)-1,2,4-triazines with Arynes: Inverse Demand *Aza*-Diels-Alder Reaction Versus Aryne-Mediated Domino Process

Dmitry S. Kopchuk,[a,b] Igor L. Nikonov,[a] Albert F. Khasanov,[a] Kousik Giri,[c] Sougata Santra,*[a] Igor S. Kovalev,[a] Emiliya V. Nosova,[a,b] Sravya Gundala,[a] Padmavathi Venkatapuram,[d] Grigory V. Zyryanov,[a,b] Adinath Majee,[e] Oleg N. Chupakhin[a,b]

[a]*Department of Organic and Biomolecular Chemistry, Chemical Engineering Institute, Ural Federal University, 19 Mira Str., Yekaterinburg, K-2, 620002, Russian Federation.*

[b]*I. Ya. Postovskiy Institute of Organic Synthesis, Ural Division of the Russian Academy of Sciences, 22 S. Kovalevskoy Str., Yekaterinburg, 620219, Russian Federation*

[c]*Centre for Computational Sciences, School of Basic and Applied Sciences, Central University of Punjab, City Campus, Mansa Road, Bathinda-151001, India*

[d]*Department of Chemistry, Sri Venkateswara University, Tirupati-517502, Andhra Pradesh, India*

[e]*Department of Chemistry, Visva-Bharati (A Central University), Santiniketan-731235, India*

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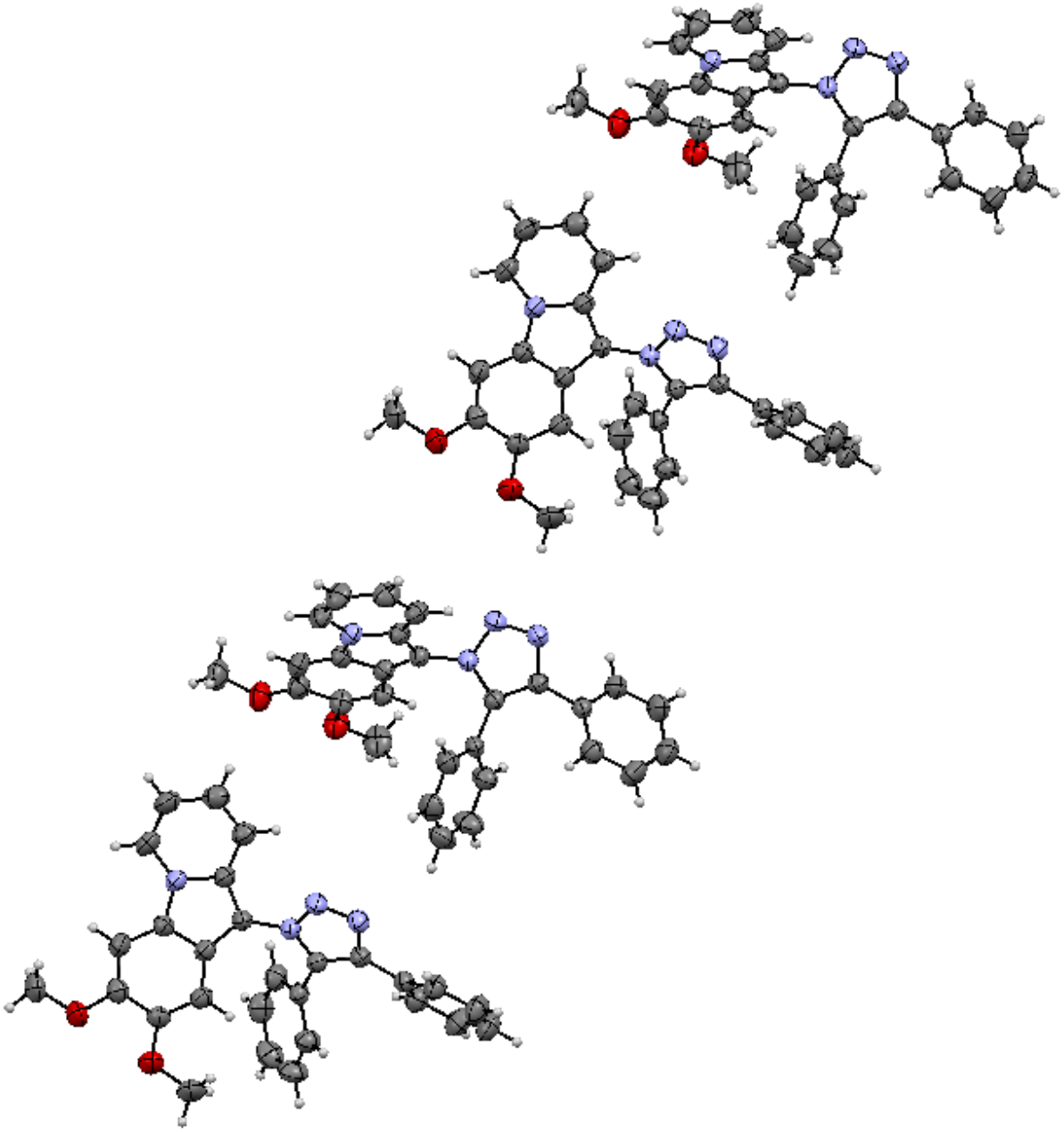


Figure S1 The crystal packing for the pyrido[1,2-*a*]indole **2j**

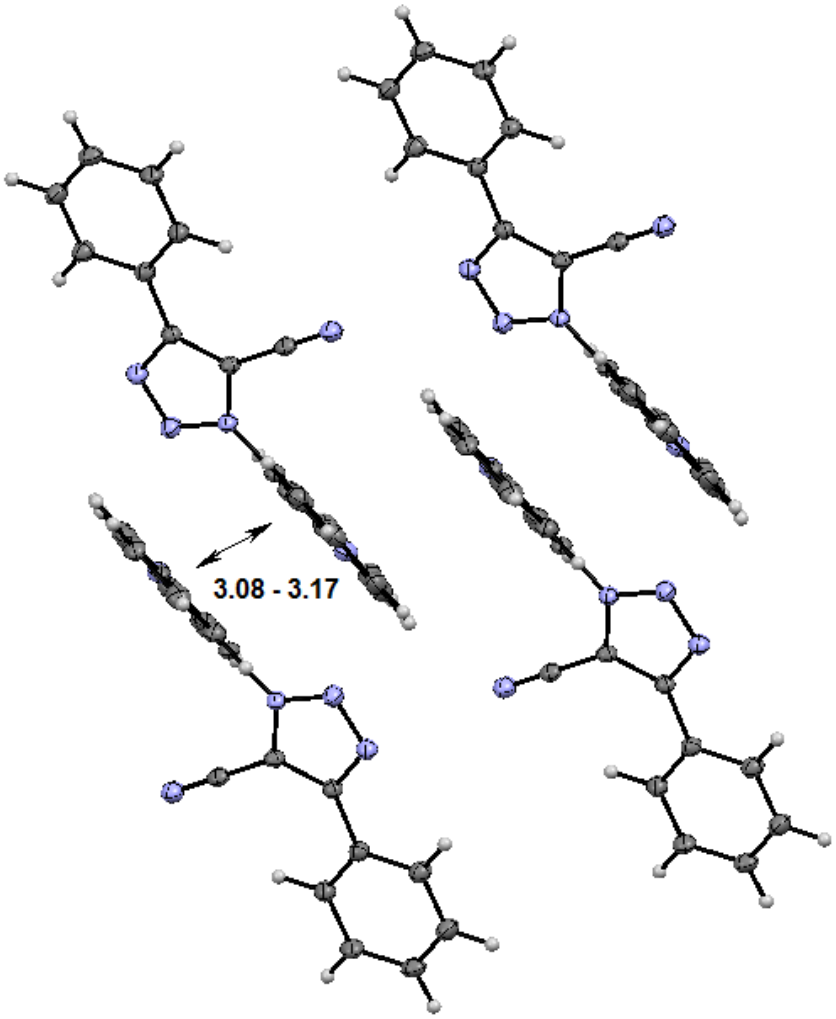


Figure S2 The crystal packing for the pyrido[1,2-*a*]indole **2d**

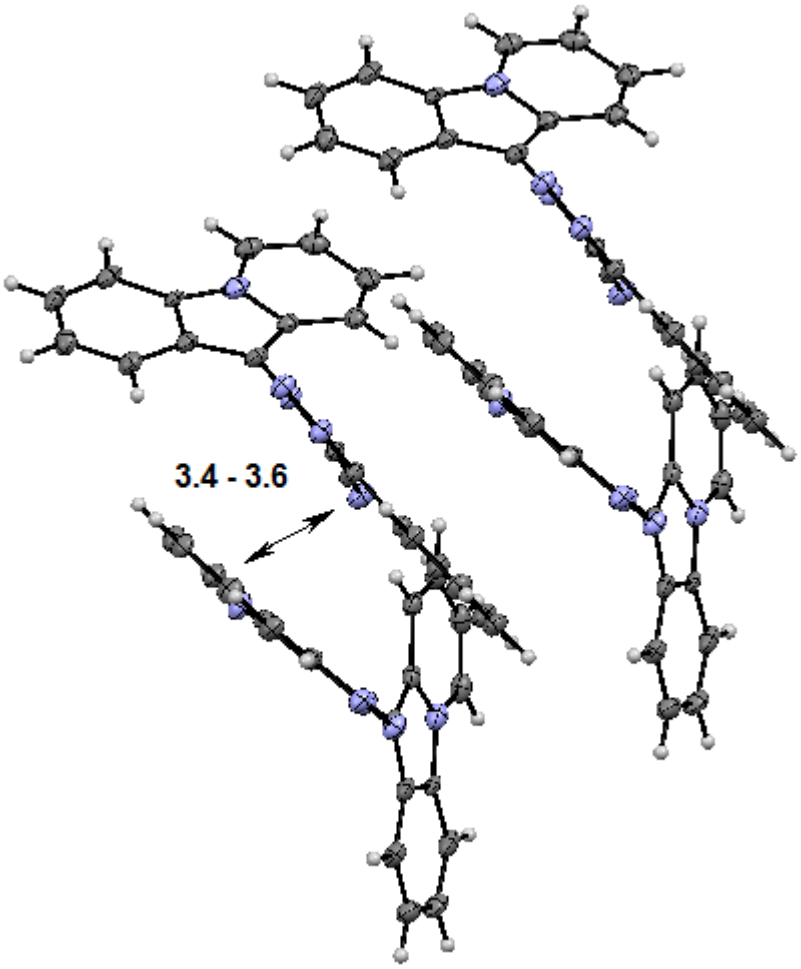


Figure S3 The crystal packing for the pyrido[1,2-*a*]indole **2d**

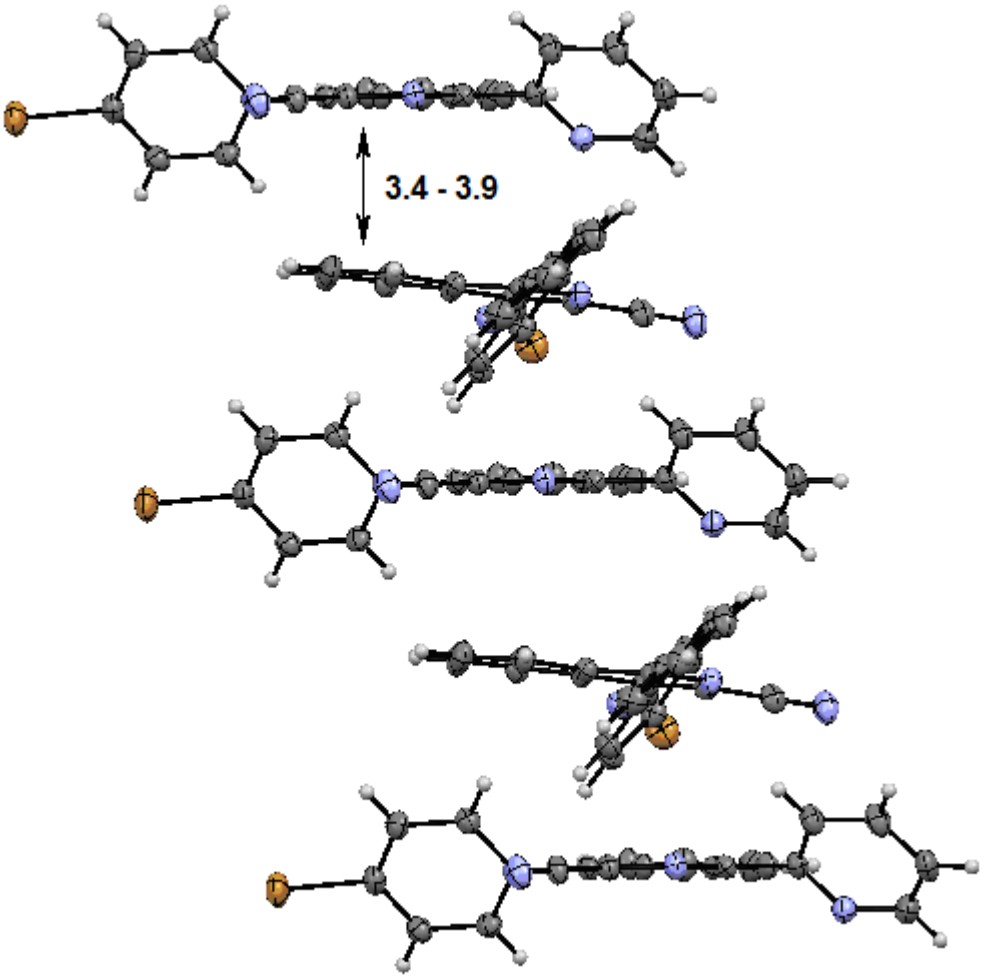


Figure S4 The crystal packing for the isoquinoline **3c**

Table S1. Crystallographic data for compounds **2d,2j,3c**

Crystal data	**Compound 2d**	**Compound 2j**	**Compound 3c**
CCDC-No.			
Temperature, K	150.00(10)	294(2)	120.01(10)
Empirical formula	$C_{21}H_{12}BrN_3$	$C_{28}H_{22}N_4O_2$	$C_{21}H_{13}N_5$
Formula weight	386.25	446.50	335.36
Crystal size, mm	0.19 × 0.13 × 0.07	0.25 × 0.2 × 0.15	0.24 × 0.19 × 0.14
Crystal system, space group	Monoclinic, $P2_1/c$	Orthorhombic, Pbca	Monoclinic, $P2_1/c$
Unit cell dimensions:			
a, Å	18.8659(10)	9.2421(5)	13.2575(7)
b, Å	10.1158(4)	17.3468(11)	15.3061(7)
c, Å	8.8637(5)	28.1793(14)	7.8541(3)
α, °	90.00	90.00	90.00
β, °	99.138(6)	90.00	98.654(5)
γ, °	90.00	90.00	90.00
Volume, $Å^3$	1670.12(15)	4517.7(4)	1575.61(13)
Z	4	8	4
Calculated density, mg/mm^3	1.536	1.313	1.414
Linear absorbtion coefficient μ, mm^{-1}	2.469	0.085	0.088
F(000)	776.0	1872.0	696.0
2Θ range for data collection	4.38 to 61.66°	4.7 to 61.9°	5.32 to 61.54°
Index ranges	$-27 \leq h \leq 24$, $-14 \leq k \leq 13$, $-12 \leq l \leq 11$	$-12 \leq h \leq 9$, $-23 \leq k \leq 7$, $-35 \leq l \leq 39$	$-9 \leq h \leq 19$, $-20 \leq k \leq 19$, $-10 \leq l \leq 11$

	14628	16469	8647
Reflections collected	4697	6245	4303
Independent reflections	0.0428	0.0798	0.0373
R (int)	4697/0/226	6245/0/317	4303/0/287
Data/restraints/parameters	1.001	0.932	1.002
Goodness-of-fit on F^2	R_1 = 0.0473,	R_1 = 0.0624,	R_1 = 0.0524,
Final R indexes [I>=2σ (I)]	wR_2 = 0.1155	wR_2 = 0.1014	wR_2 = 0.1202
	R_1 = 0.0792,	R_1 = 0.2187,	R_1 = 0.0909,
Final R indexes [all data]	wR_2 = 0.1341	wR_2 = 0.1520	wR_2 = 0.1391
	1.18/-0.83	0.20/-0.21	0.43/-0.35
Largest diff. peak/hole / $\bar{e}Å^{-3}$			

Possible reaction pathways (for DFT calculations) for the interactions of 1,2,4-triazine 1d with benzyne and 4,5-difluoro-1,2-dehydro-benzene

Benzyne:

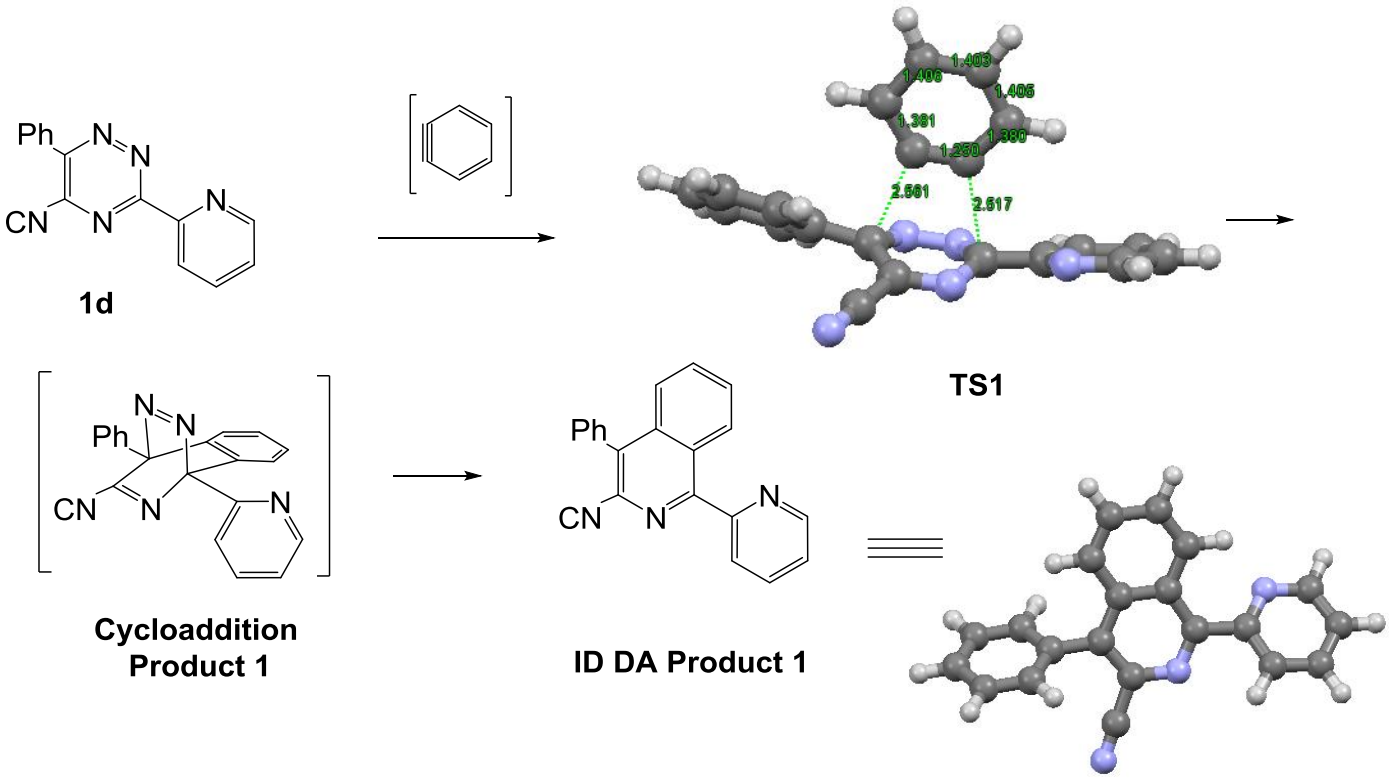


Figure S5. Inverse Demand Diels-Alder reaction through TS1

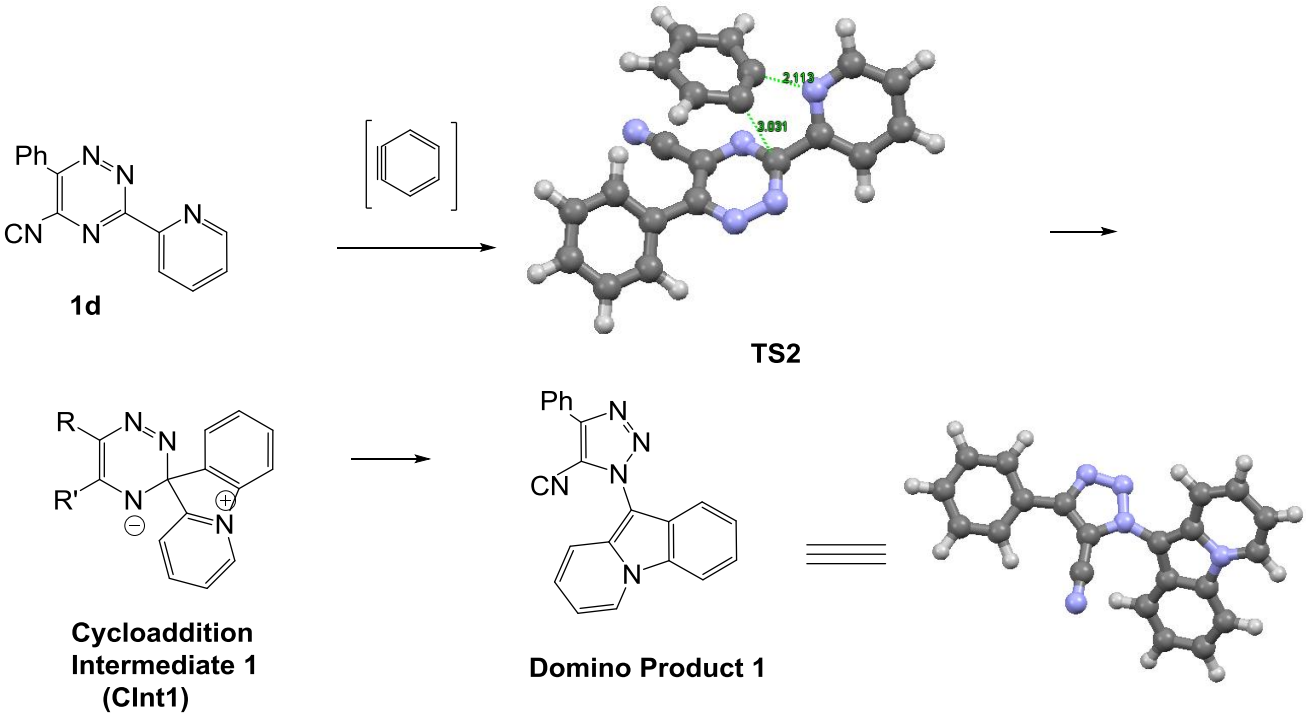


Figure S6. Aryne-mediated domino process through TS2

4,5-Difluoro-1,2-Dehydro-benzene:

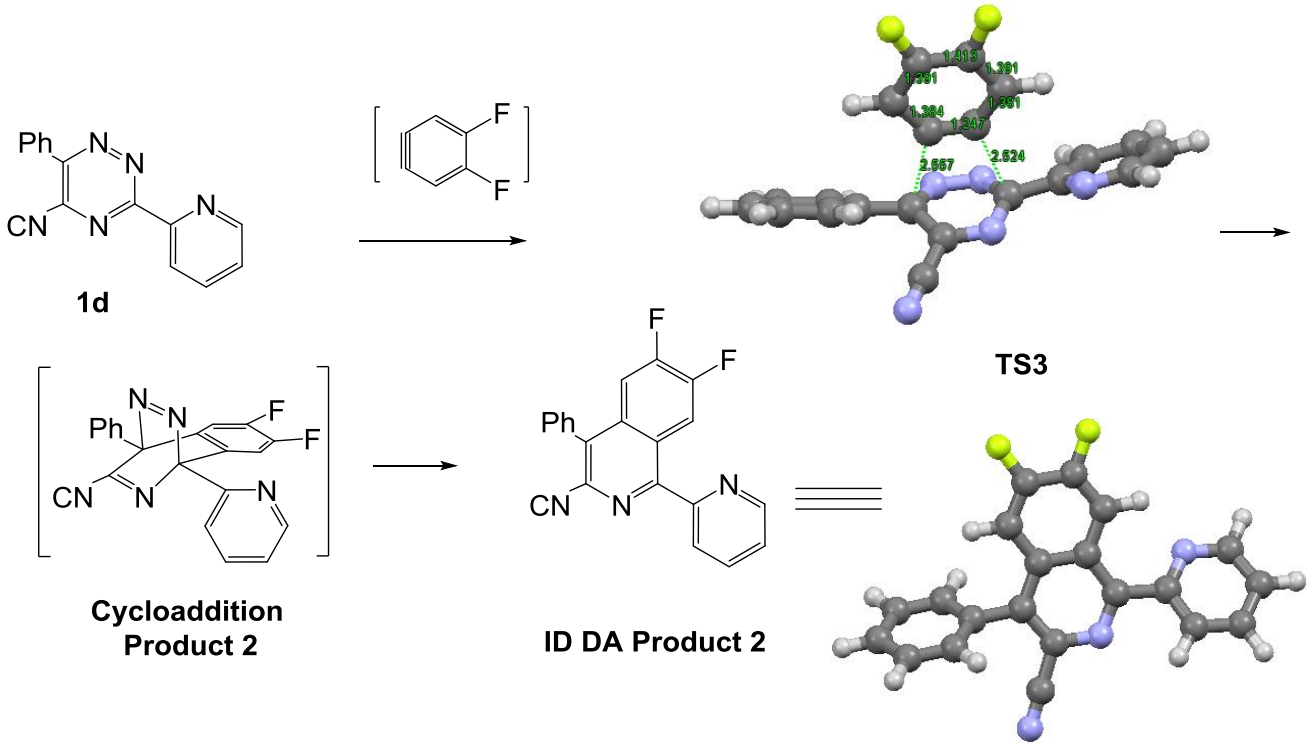


Figure S7. Inverse Demand Diels-Alder reaction through TS3

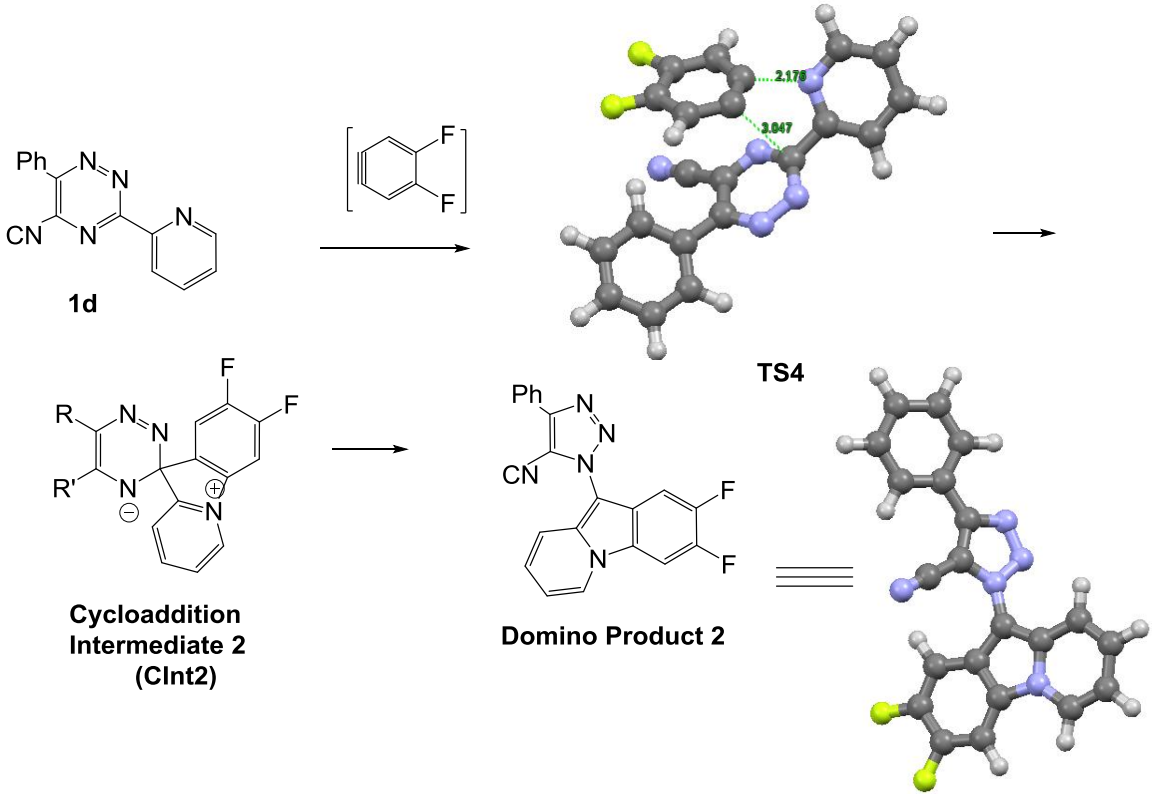
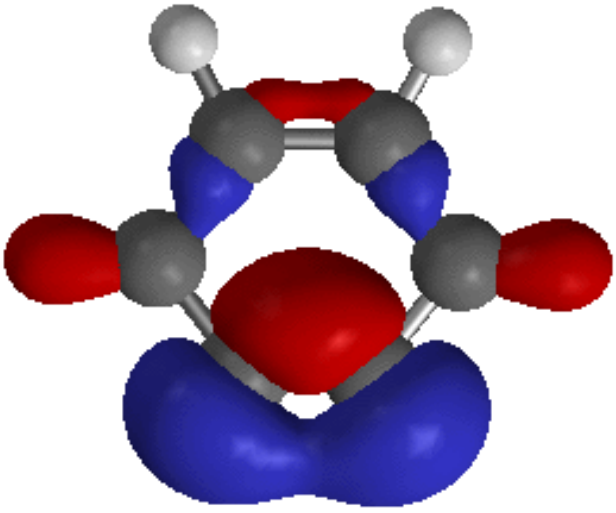
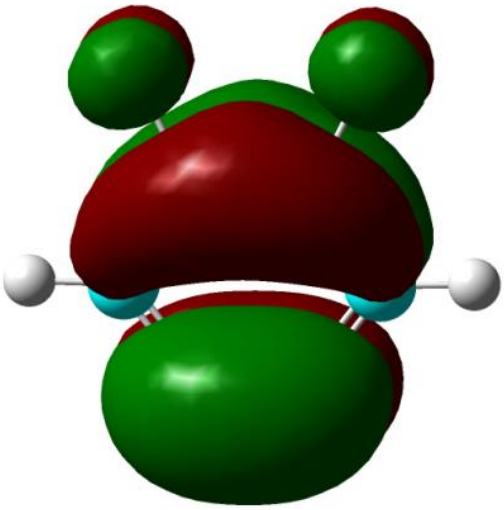


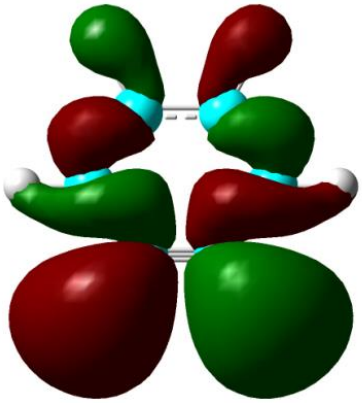
Figure S8. Aryne-mediated domino process through TS4

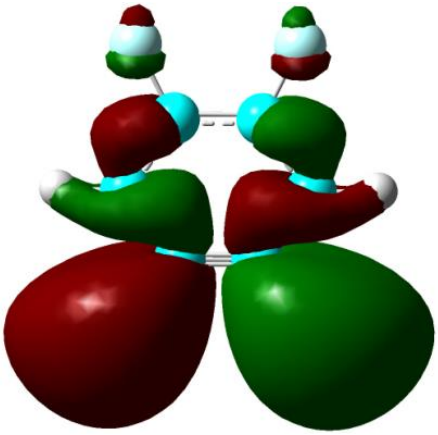




HOMO Benzyne[1] HOMO 4,5-difluoro-1,2-Dehydro-benzene

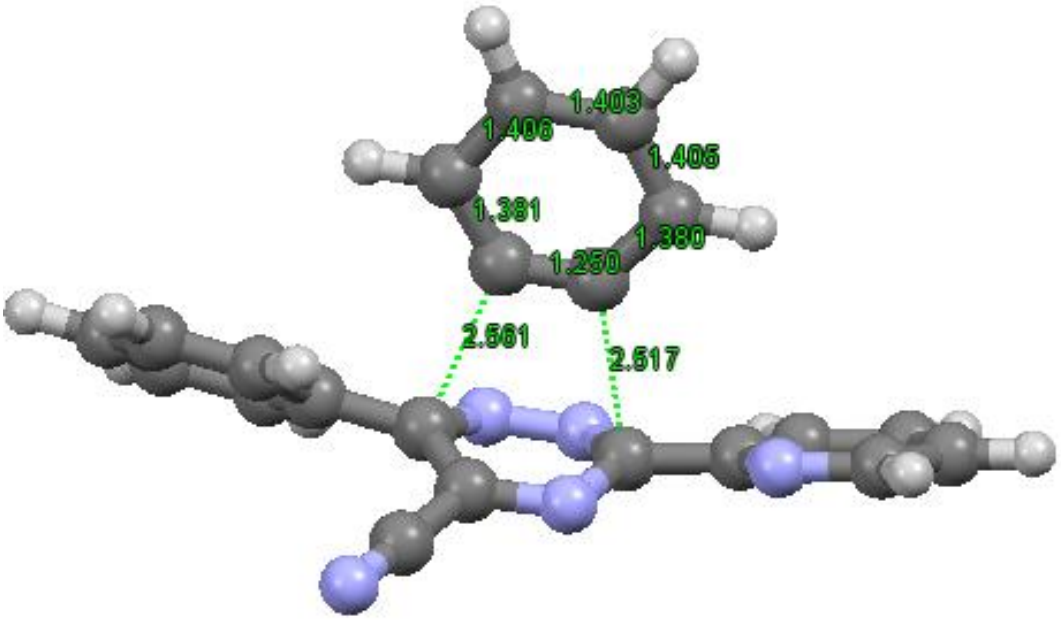
Figure S9 HOMO lobes distirbutions in benzyne vs 4,5-difluoro-1,2-dehydro-benzene



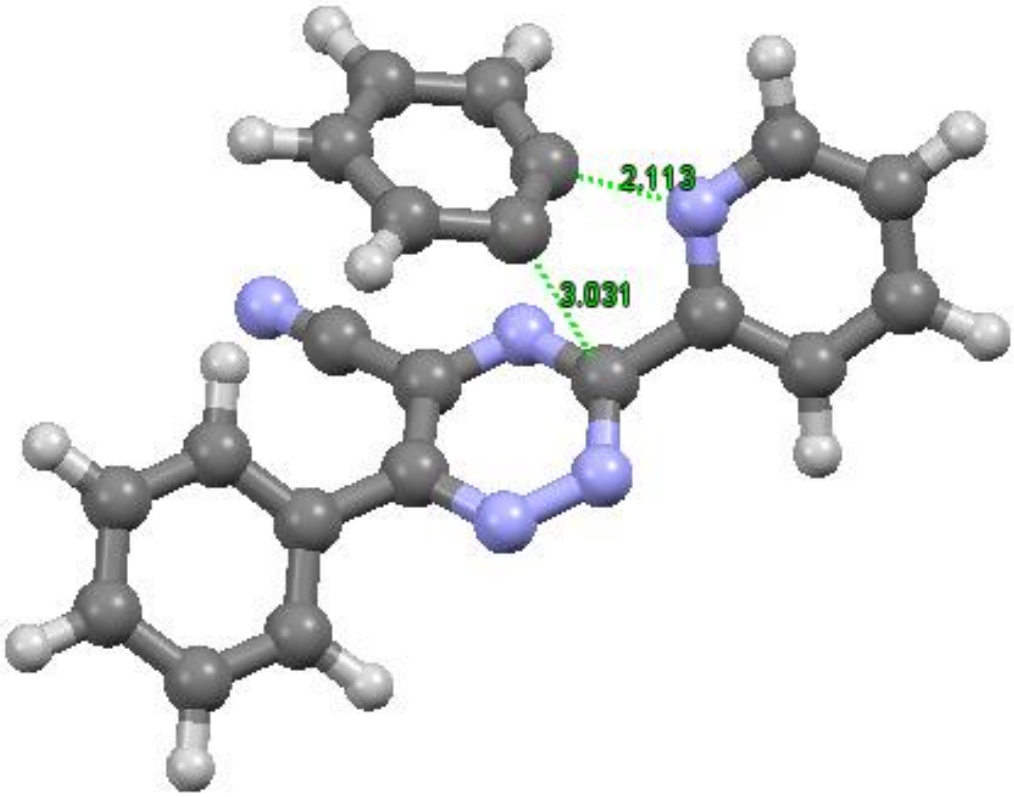


LUMO Benzyne LUMO 4,5-difluoro-1,2-Dehydro-benzene

Figure S10 LUMO distributions

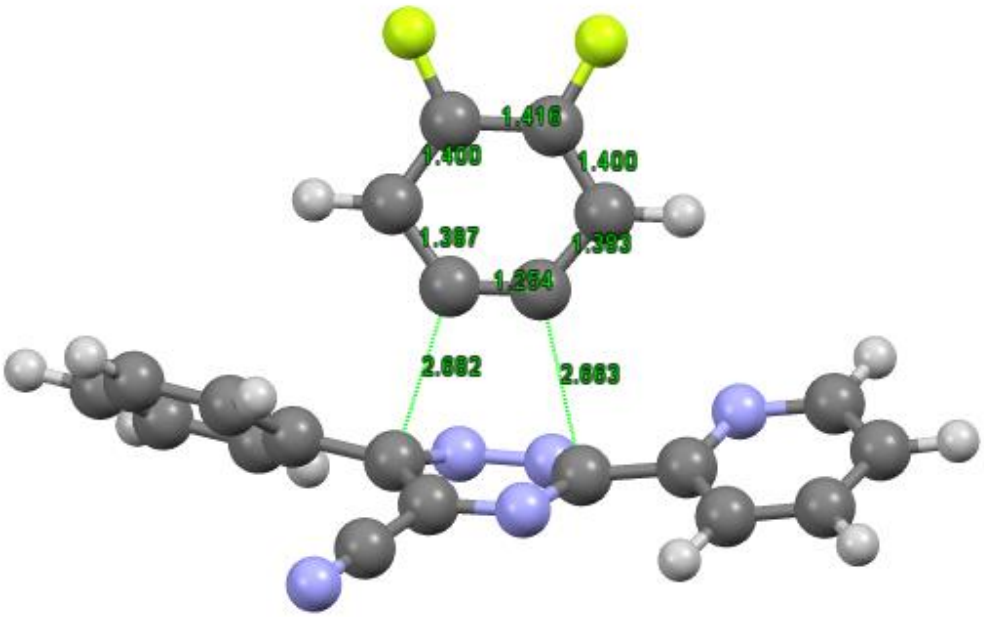


TS1

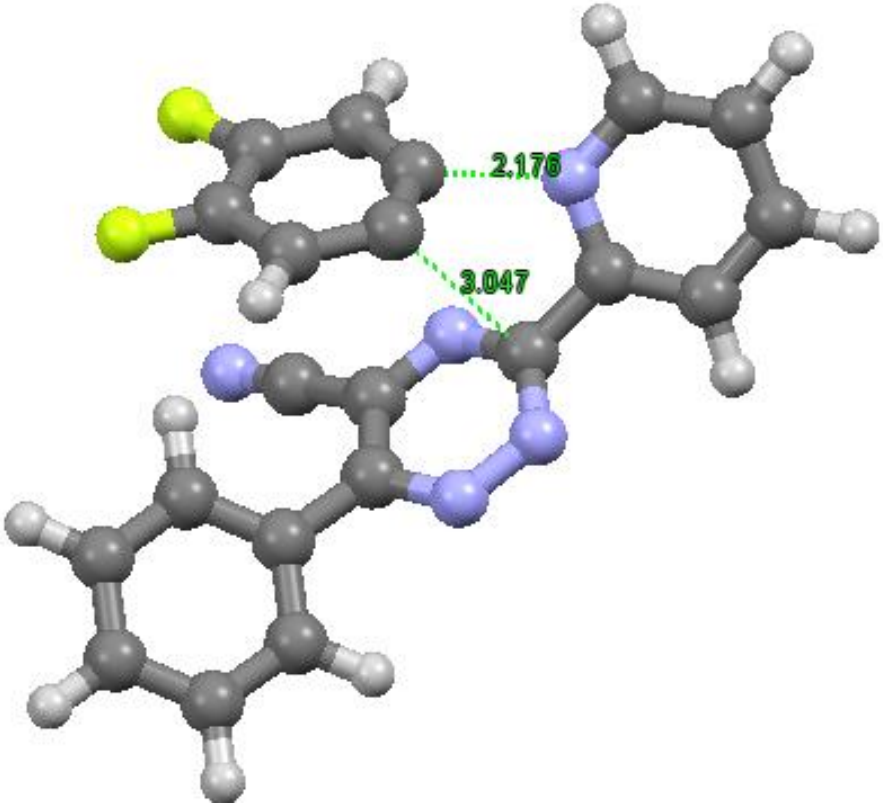


TS2

Figure S11 Two possible types of transition states in the reaction of **1d** and benzyne



TS3



TS4

Figure S12 Two possible types of transition states in the reaction of **1d** and 4,5-difluoro-1,2-dehydro-benzene

Table S2. The activation enthalpy (ΔH‡), activation free energy (ΔG‡) and reaction free energy (ΔGrxn) for the interaction of **1d** and arynes

Transition state	**$\Delta H^{\neq}$**	**$\Delta G^{\neq}$**	**ΔG_{rxn}**	**k_2 ($M^{-1}s^{-1}$)**
1,2-Dehydro-Benzene				
TS1	-3.887	**8.826**	-141.039	**$2.10x10^6$**
TS2	-2.040	11.594	-81.913	$1.97x10^4$
4,5-Difluoro-1,2-Dehydro-benzene				
TS3	-4.300	8.550	-144.821	$3.36x10^6$
TS4	-4.715	9.004	-83.901	$1.56x10^6$

Table S3. DFT calculations (M062X, 6-311+G(d,p)) for ΔH# (Activation Enthalpy), ΔG# (Activation Free Energy), ΔGrxn (Reaction Free Energy) for TS1-TS4 for interaction between 1,2,4-triazine **1d** and arynes

Product	Prd1 (E_0 + H_{corr})	Prod2 (E_0 + H_{corr})	$\Delta_r H^0$ (298.15 K) (kcal/mol)	Prd1 (E_0 + G_{corr})	Prod2 (E_0 + G_{corr})	$\Delta_r G^0$ (298.15 K) (kcal/mol)	TS (E_0 + H_{corr})	$\Delta H^{\#}$ (298.15 K) (kcal/mol)	TS (E_0 + G_{corr})	$\Delta G^{\#}$ (298.15 K) (kcal/mol)
ID DA Product 1	-971,8685970	-109,5132190	**-144,5637561**	-971,9356770	-109,5349470	**-141,0390352**	-1081,1576340	**-3,887**	-1081,2317990	**8,826**
ID DA Product 2	-1170,359337	-109,5132190	**-148,2754748**	-1170,4307480	-109,5349470	**-144,8216625**	-1279,6431160	**-4,300**	-1279,7212830	**8,549**
Domino Product 1	-1081,305845	0,0000000	**-96,8912319**	-1081,3764020	0,0000000	**-81,9138351**	-1081,1546900	**-2,040**	-1081,2273880	**11,594**
Domino Product 2	-1279,7932510	0,0000000	**-98,5108339**	-1279,8681340	0,0000000	**-83,6012082**	-1279,6437780	**-4,715**	-1279,7205590	**9,004**

Table S4. DFT calculations (M062X, 6-311+G(d,p)) for ΔH# (Activation Enthalpy), ΔG# (Activation Free Energy), ΔGrxn (Reaction Free Energy) for TS1-TS4 for interaction between 1,2,4-triazine **1d** and arynes

Product	TS (E)	dist_phpy ($E^{\#}$)	dist_bnzy(/F) ($E^{\#}$)	$\Delta E^{\#}$ (dist_phpy)	$\Delta E^{\#}$ (dist_bnzy (F))	$\Delta E^{\#}$(total_distor)	$\Delta E^{\#}$(activation E)	$\Delta E^{\#}$(interaction E)	
ID DA Product 1	-1081,4611043	-850,5815147	-230,8665170	3,734	0,1514808	**3,885**	**-4,318**	**-8,203**	**1d + Benzyne**
ID DA Product 2	-1279,9327849	-850,5820011	-429,3375560	3,428	0,1696158	**3,598**	**-4,702**	**-8,301**	**1d + F2-Benzyne**
Domino Product 1	-1081,4584468	-850,5837682	-230,8613277	2,320	3,4078158	**5,727**	**-2,650**	**-8,378**	**1d + Benzyne**
Domino Product 2	-1279,9337068	-850,5838668	-429,3337741	2,258	2,5427940	**4,801**	**-5,281**	**-10,082**	**1d + F2-Benzyne**

Cartesian coordinates (Angstroms) and total energies (hartree) of the geometry-optimized structures of all computed compounds:

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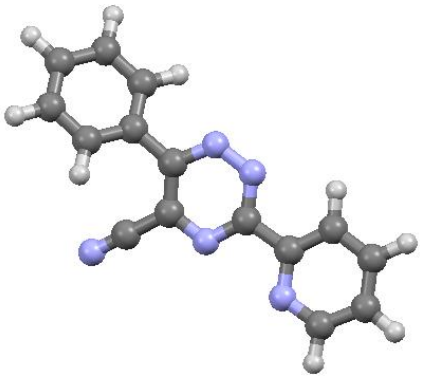
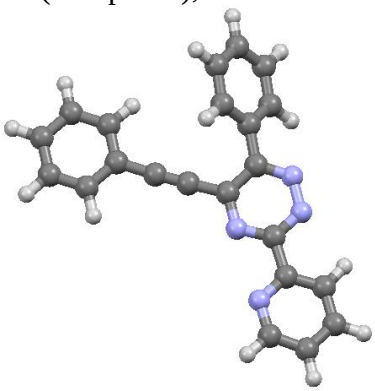


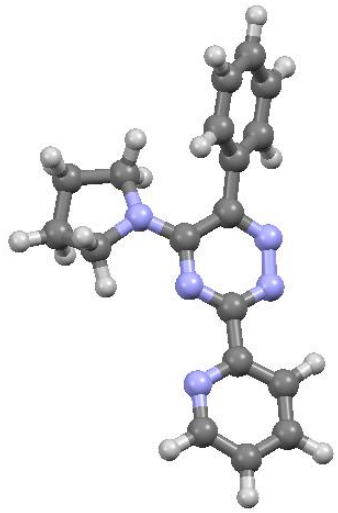
C	-1.46380700	-0.14429200	0.00452600
N	-0.83235300	-1.31684000	0.12844600
N	0.47559200	-1.34563700	0.14410700
C	1.17679700	-0.21437500	0.01874100
C	0.46698500	0.98269900	-0.20469300
N	-0.85139000	1.02309400	-0.19582100
C	-2.95337300	-0.17633900	0.06882300
N	-3.57557800	1.00161800	0.04379000
C	-4.90251000	1.00059800	0.10134100
C	-5.66794000	-0.16025900	0.18406800
C	-5.00971800	-1.38211300	0.21130100
C	-3.62321600	-1.39809000	0.15454100
C	2.64722600	-0.33150700	0.08341400
C	3.25816700	-1.46623500	-0.45875600
C	4.63722400	-1.60656100	-0.40353900
C	5.41556300	-0.62486000	0.20389200
C	4.81028900	0.49683100	0.75967700
C	3.43039800	0.64714500	0.69934800
C	1.14104700	2.22721400	-0.51049200
N	1.67106100	3.21476200	-0.76081100
H	-3.06047900	-2.32094500	0.17557600
H	-5.56516500	-2.31003700	0.27630700
H	-5.38022100	1.97506300	0.08111900
H	-6.74798300	-0.09935500	0.22687800
H	2.64166100	-2.22791400	-0.91947600
H	2.96971700	1.51711300	1.15116700
H	5.10597300	-2.48283800	-0.83441200
H	5.41060400	1.25667300	1.24446500
H	6.49232500	-0.73661100	0.24745200

4a (Gas phase), -1065.5176721 hartree, n_{imag} = 0:



C	-1.49600000	-0.11100000	0.06100000
N	-0.85600000	-1.28200000	0.06100000
N	0.45600000	-1.28900000	-0.02000000
C	1.12600000	-0.14400000	-0.11700000
C	0.40300000	1.07400000	-0.21100000
N	-0.91700000	1.07900000	-0.09900000
C	-2.98000000	-0.17000000	0.22900000
N	-3.61600000	0.99300000	0.36900000
C	-4.93500000	0.96200000	0.52100000
C	-5.68200000	-0.21300000	0.53900000
C	-5.01000000	-1.41900000	0.39400000
C	-3.63200000	-1.40500000	0.23800000
C	2.60200000	-0.24600000	-0.16700000
C	3.18600000	-1.29100000	-0.88700000
C	4.56800000	-1.41700000	-0.93800000
C	5.37800000	-0.51300000	-0.25800000
C	4.80000000	0.51700000	0.47800000
C	3.41800000	0.65400000	0.52100000
C	1.05900000	2.31400000	-0.48100000
H	-3.05800000	-2.31400000	0.12600000
H	-5.55000000	-2.35900000	0.40200000
H	-5.42300000	1.92500000	0.63500000
H	-6.75700000	-0.17500000	0.66400000
H	2.54600000	-1.99700000	-1.40100000
H	2.97500000	1.45100000	1.10700000
H	5.01300000	-2.22500000	-1.50700000
H	5.42600000	1.21100000	1.02600000
H	6.45600000	-0.61600000	-0.29500000
C	1.64700000	3.33700000	-0.72600000
C	2.38900000	4.52500000	-1.00200000
C	3.76400000	4.43600000	-1.25300000
C	1.75600000	5.77400000	-1.02000000
C	4.49500000	5.58700000	-1.51700000
H	4.24100000	3.46300000	-1.24100000
C	2.49500000	6.91800000	-1.28500000
H	0.69200000	5.83100000	-0.82700000
C	3.86300000	6.82700000	-1.53300000
H	5.55800000	5.51600000	-1.71200000
H	2.00400000	7.88400000	-1.29800000
H	4.43500000	7.72300000	-1.74000000

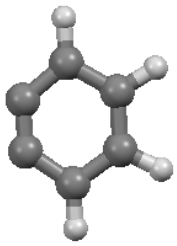
4b (Gas phase), -969.7286212 hartree, n_{imag} = 0:



C	-1.64460300	-0.16899300	0.04339900
N	-1.01107800	-1.25973600	-0.38151100
N	0.30166800	-1.17706400	-0.52338500
C	0.93697800	-0.03082500	-0.36730400
C	0.17333000	1.16950300	-0.16074900
N	-1.10848000	1.04013500	0.16335400
C	-3.09180100	-0.33565500	0.38243300
N	-3.78271300	0.77081700	0.66017500
C	-5.06985300	0.63687500	0.96492000
C	-5.73021400	-0.58743100	1.00720100
C	-5.00326500	-1.73443900	0.71524900
C	-3.65890500	-1.61238800	0.39718300
C	2.41641300	-0.12083900	-0.32819300
C	3.09896300	-0.90956900	-1.25485300
C	4.47978200	-1.04371200	-1.17583300
C	5.18891900	-0.40648000	-0.16155700
C	4.51032000	0.36474800	0.77738100
C	3.13066200	0.50939300	0.69299700
H	-3.04251900	-2.46908000	0.16262200
H	-5.47460400	-2.70998800	0.73699100
H	-5.60444100	1.55594700	1.18572500
H	-6.78154100	-0.63273800	1.26209200
H	2.53461400	-1.41871000	-2.02682600
H	2.59822800	1.10890000	1.42480300
H	5.00337900	-1.65146800	-1.90421000
H	5.05472500	0.85003900	1.57877600
H	6.26499400	-0.51608600	-0.09879800
C	1.84907700	2.73556800	-1.13640900
C	-0.20007500	3.59737100	-0.15510900
C	1.67604700	4.22093000	-1.47992200
H	1.82905100	2.10437000	-2.03108700
H	2.78999400	2.55012000	-0.62063800
C	0.16947100	4.45251300	-1.36261500
H	0.03078000	4.11614500	0.78118700
H	-1.23944700	3.28074300	-0.12787900

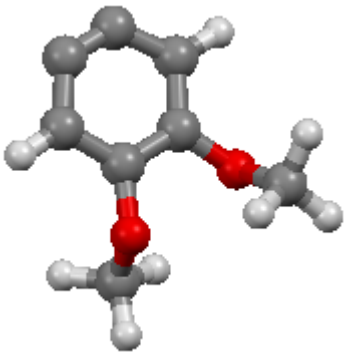
H	2.20247200	4.83293300	-0.74299700
H	2.08142000	4.45620800	-2.46379600
H	-0.09617400	5.50145800	-1.23107900
H	-0.34459500	4.07354700	-2.25014400
N	0.68072400	2.42178200	-0.29040100

Benzyne (Gas phase), -230.8667584 hartree, n_{imag} = 0:



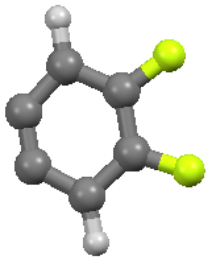
C	0.51800000	0.21500000	-0.00300000
C	1.92200000	0.21500000	0.00000000
C	2.68000000	1.39900000	0.00500000
C	1.84100000	2.49700000	0.00400000
C	0.60200000	2.49800000	0.00100000
C	-0.23800000	1.40000000	-0.00300000
H	-0.00500000	-0.73500000	-0.00600000
H	2.44500000	-0.73600000	0.00000000
H	3.76100000	1.40000000	0.00700000
H	-1.32000000	1.40300000	-0.00600000

4,5-Dimethoxy-1,2-dehydro-benzene (Gas phase), -459.8815837 hartree, n_{imag} = 0:



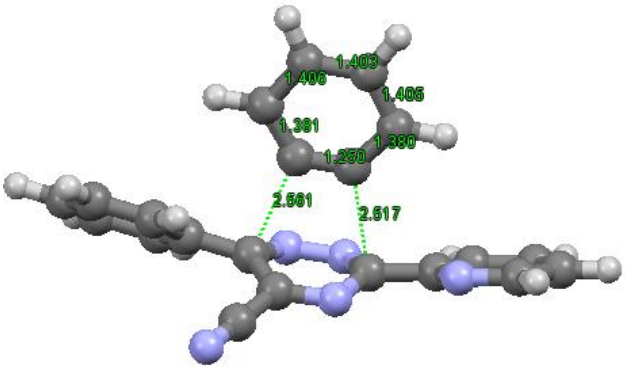
C	-1.31986300	1.37798900	-0.49257500
C	-2.41637600	0.58390100	-0.20331500
C	-2.41636600	-0.58391200	0.20331400
C	-1.31985100	-1.37799400	0.49258100
C	-0.13936300	-0.67321700	0.23622000
C	-0.13936800	0.67322100	-0.23621700
H	-1.30049900	-2.39714100	0.85464700
H	-1.30050300	2.39713500	-0.85464500
O	1.06252900	-1.28514300	0.46556300
O	1.06251600	1.28515700	-0.46556500
C	1.72522000	-1.70896500	-0.72543400
H	2.66716800	-2.15476200	-0.41165200
H	1.11959500	-2.45650700	-1.24593100
H	1.91578300	-0.85875500	-1.38372900
C	1.72522300	1.70896200	0.72543000
H	2.66715500	2.15478200	0.41163700
H	1.11959400	2.45648100	1.24595600
H	1.91581300	0.85873800	1.38370000

4,5-Difluoro-1,2-dehydro-benzene (Gas phase), -429.3378263 hartree, n_{imag} = 0:



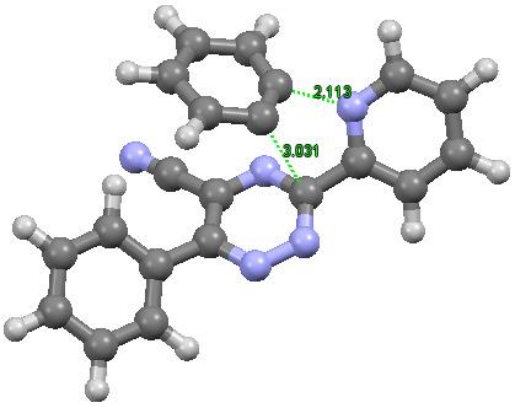
C	-0.38958100	-0.70732200	0.00000000
C	-0.38958200	0.70732200	0.00000000
C	0.77297000	1.47058400	0.00000000
C	1.86314700	0.61774100	0.00000000
C	1.86314800	-0.61774000	0.00000000
C	0.77297000	-1.47058300	0.00000000
H	0.75113100	2.55143500	0.00000000
H	0.75113200	-2.55143500	0.00000000
F	-1.58115000	1.30886600	0.00000000
F	-1.58115000	-1.30886700	0.00000000

TS1 (Gas phase), -1081.4611043 hartree, n_{imag} = 1:



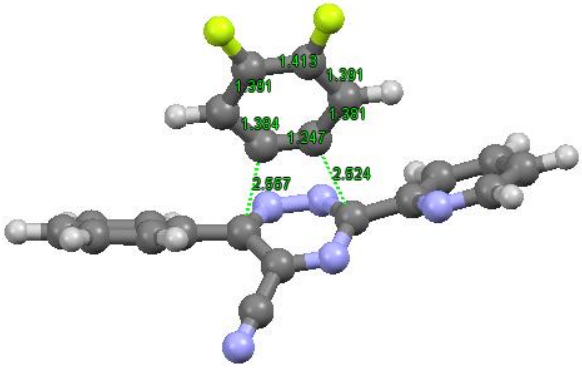
C	-1.24331500	2.17928900	0.45908600
C	-0.47722000	1.06563900	0.17454000
C	0.77092900	0.99145900	0.19187200
C	1.66436300	1.99174400	0.51459300
C	0.97830800	3.17875400	0.82348800
C	-0.42248200	3.26924300	0.79575500
C	1.30245000	-1.39040000	-0.42588200
N	0.68232800	-1.26270200	-1.62479000
N	-0.60530600	-1.19524900	-1.64616900
C	-1.30079300	-1.26627600	-0.48790000
C	-0.62372400	-1.85293700	0.61175300
N	0.68693000	-1.89255600	0.65211700
C	2.78340000	-1.22494400	-0.41074900
C	4.66994100	-0.97315900	0.83920700
C	5.47658400	-0.89112300	-0.29333500
C	4.87130500	-0.97680900	-1.54009100
C	3.49498300	-1.14403300	-1.60805700
H	2.97099200	-1.21286200	-2.55139500
H	5.46031300	-0.91572200	-2.44743300
H	5.10460400	-0.90284700	1.83148100
H	6.54659000	-0.76080500	-0.19253200
H	2.74305400	1.90682900	0.54006300
H	-2.32419800	2.23905800	0.43578700
N	3.35150100	-1.13346900	0.79113100
C	-1.34086900	-2.46410900	1.70804500
N	-1.91726200	-2.95137400	2.57402900
H	1.55355500	4.05709400	1.09495600
H	-0.89047000	4.21504800	1.04573700
C	-2.75286000	-1.00674800	-0.54550200
C	-3.43577900	-0.54379000	0.58237900
C	-3.44623000	-1.20113100	-1.74299300
C	-4.80026400	-0.29362400	0.51648700
H	-2.89918400	-0.36166400	1.50692900
C	-4.81061600	-0.95138400	-1.80197900
H	-2.90649100	-1.54848900	-2.61459900
C	-5.49012600	-0.50017400	-0.67414400
H	-5.32322400	0.06395100	1.39502600
H	-5.34557200	-1.11145800	-2.73021600
H	-6.55515100	-0.30740600	-0.72350100

TS2 (Gas phase), -1081.4584468 hartree, n_{imag} = 1:



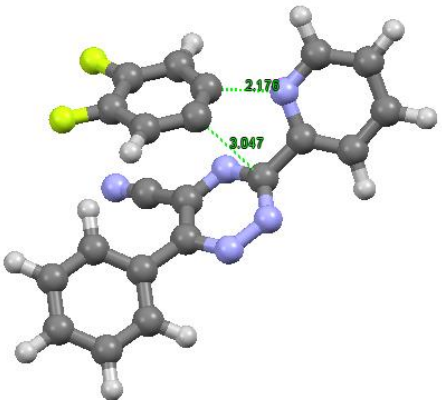
C	-1.22254100	-1.12655300	0.37443300
N	-0.56794600	-2.07035300	-0.29772600
N	0.73956600	-1.98575400	-0.37087200
C	1.38098700	-0.98051500	0.22896600
C	0.65417600	-0.17693500	1.13446600
N	-0.65924400	-0.24700300	1.20153800
C	-2.69284200	-1.04720600	0.17217100
N	-3.18840200	0.18733100	0.04500600
C	-4.48920600	0.34544500	-0.17567000
C	-5.36301800	-0.73201000	-0.27119700
C	-4.84762100	-2.01600300	-0.15138800
C	-3.48540600	-2.18246500	0.06754000
C	2.82034800	-0.82808200	-0.04840600
C	3.60591700	-1.96195000	-0.27244000
C	4.95855400	-1.82257500	-0.54763400
C	5.53092600	-0.55474700	-0.61561100
C	4.74691800	0.57581100	-0.41210700
C	3.39350200	0.44311500	-0.12775700
C	1.30435800	0.71752600	2.06668900
N	1.81393300	1.42164400	2.81764900
H	-3.03059800	-3.16040400	0.15517800
H	-5.49682100	-2.87923000	-0.23333500
H	-4.83243900	1.36778100	-0.29533300
H	-6.41629000	-0.56091200	-0.45092200
H	3.14505800	-2.94077400	-0.22663100
H	2.77914800	1.32665200	0.00563900
H	5.56802900	-2.70307100	-0.71061800
H	5.18696800	1.56318000	-0.47848000
H	6.58723200	-0.44874600	-0.83227100
C	-0.55209000	3.38412200	0.08043500
C	0.34204000	3.06066400	-0.95283300
C	0.11292300	1.97588400	-1.80639000
C	-1.03096200	1.18708500	-1.57429800
C	-1.76161300	1.59889800	-0.61540800
C	-1.70043100	2.61513500	0.30258100
H	0.82624400	1.75092900	-2.59439900
H	-2.39835500	2.80164500	1.10748700
H	1.23374900	3.66624400	-1.08154700
H	-0.34678600	4.22778700	0.72921800

TS3 (Gas phase), -1279.9327849 hartree, n_{imag} = 1:



C	-1.26788300	2.16865700	0.46051400
C	-0.47976900	1.06675500	0.17988000
C	0.76498700	0.99877400	0.21062800
C	1.66078400	1.99408200	0.55128200
C	0.95805600	3.15572800	0.85333600
C	-0.45201000	3.24001800	0.80856400
C	1.30851800	-1.37765100	-0.44090700
N	0.68410700	-1.23386900	-1.63516800
N	-0.60402000	-1.16758900	-1.65139100
C	-1.29779900	-1.25996900	-0.49343000
C	-0.61467800	-1.84903900	0.60140400
N	0.69665100	-1.88236500	0.63793200
C	2.78938400	-1.21434900	-0.42935900
C	4.66857900	-0.89407500	0.81570600
C	5.48279400	-0.89338300	-0.31475300
C	4.88552500	-1.05513700	-1.55750400
C	3.50796100	-1.21556300	-1.62439800
H	2.98962900	-1.34045900	-2.56518700
H	5.48126900	-1.05774600	-2.46240500
H	5.09726500	-0.76036000	1.80395200
H	6.55306500	-0.76477300	-0.21518000
H	2.74024000	1.93676100	0.59838300
H	-2.34737800	2.24596600	0.43234700
N	3.34922700	-1.04805300	0.76876000
C	-1.32487300	-2.46777200	1.69768200
N	-1.89548700	-2.96171800	2.56359200
C	-2.75020800	-1.00213200	-0.54521300
C	-3.43232300	-0.55407900	0.58952700
C	-3.44394000	-1.17963100	-1.74529400
C	-4.79634800	-0.30066800	0.52715500
H	-2.89691200	-0.38668300	1.51760200
C	-4.80798500	-0.92762300	-1.80021100
H	-2.90522500	-1.51556100	-2.62198200
C	-5.48638000	-0.49031000	-0.66622500
H	-5.31863300	0.04601600	1.41037000
H	-5.34347400	-1.07447000	-2.73024800
H	-6.55099100	-0.29491600	-0.71285300
F	1.61692900	4.26124800	1.20832800
F	-0.99617400	4.41732600	1.12539900

TS4 (Gas phase), -1279.9337068 hartree, n_{imag} = 1:



C	-1.26731400	-1.09057200	0.35340100
N	-0.60961300	-2.02800300	-0.32481700
N	0.69823100	-1.94067700	-0.39642600
C	1.33951400	-0.94039900	0.21258700
C	0.60933300	-0.14277000	1.12119700
N	-0.70498400	-0.21250500	1.18285900
C	-2.73718000	-1.00956900	0.14555200
N	-3.23355500	0.22561100	0.02332400
C	-4.53432300	0.37905800	-0.20393300
C	-5.40506700	-0.69998100	-0.30988900
C	-4.88725600	-1.98341900	-0.19484900
C	-3.52582000	-2.14697800	0.02937500
C	2.77710400	-0.78012200	-0.06836600
C	3.56123500	-1.90930300	-0.32197800
C	4.91104800	-1.76385600	-0.60662000
C	5.48233700	-0.49445400	-0.65611000
C	4.70046100	0.63166400	-0.42293600
C	3.35008600	0.49283400	-0.12718200
C	1.25270000	0.75194700	2.05725000
N	1.75227700	1.45932500	2.81201100
H	-3.06851200	-3.12412500	0.11291400
H	-5.53377600	-2.84789400	-0.28439100
H	-4.88345600	1.39996200	-0.31819700
H	-6.45802600	-0.53023800	-0.49275800
H	3.10155700	-2.88922900	-0.29118000
H	2.74545500	1.37833700	0.03229800
H	5.51928400	-2.64079600	-0.79182100
H	5.13692300	1.62136300	-0.47449300
H	6.53639400	-0.38389500	-0.88124600
C	-0.40610300	3.27793600	0.09504100
C	0.48657800	2.90608200	-0.92995400
C	0.21112000	1.88531400	-1.82800000
C	-1.00615700	1.22130100	-1.61489600
C	-1.73454100	1.64234400	-0.67211500
C	-1.61396800	2.62143500	0.28522200
H	0.93955900	1.63630000	-2.59289400
H	-2.29134100	2.86470800	1.09216700
F	-0.04910900	4.28126200	0.90007000
F	1.65002700	3.57220500	-0.99302700

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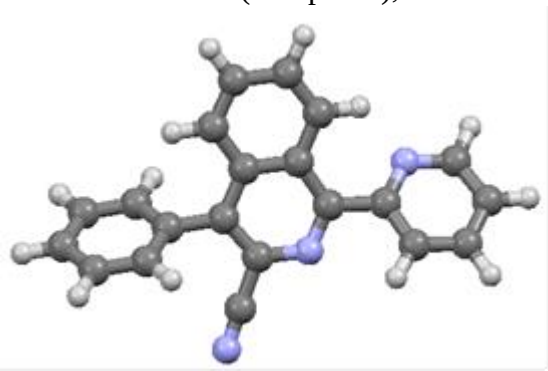

C	1.22859700	2.32696300	-0.27016100
C	0.55545900	1.08601000	-0.12470900
C	-0.86661000	1.06175200	-0.12669800
C	-1.57201800	2.28244800	-0.28056200
C	-0.89299100	3.46539200	-0.41572900
C	0.51744700	3.48892100	-0.40896200
C	-1.50964700	-0.22041100	-0.03073900
C	1.27001900	-0.14746300	-0.02726900
C	0.51893100	-1.30189900	-0.00259300
N	-0.83501100	-1.34212100	-0.00585600
C	-2.99437200	-0.39935200	0.03185000
N	-3.71226100	0.50390100	0.70282100
C	-5.02584000	0.30749800	0.80589900
C	-5.68656400	-0.77764700	0.24318800
C	-4.93462400	-1.71167400	-0.45989700
C	-3.56535000	-1.52708300	-0.56461000
C	2.75282300	-0.18848800	0.04054200
C	3.41962300	0.40630500	1.11489000
C	4.80561300	0.35653500	1.19388000
C	5.53823800	-0.28295600	0.19799300
C	4.88009000	-0.87634500	-0.87340800
C	3.49269900	-0.83215800	-0.95161800
C	1.16085300	-2.59650700	0.06360800
N	1.66430200	-3.62907500	0.10689700
H	-2.93117500	-2.23475800	-1.08077900
H	-5.40763100	-2.57349400	-0.91560200
H	-5.57487100	1.05574800	1.36896800
H	-6.75780400	-0.88378900	0.35722300
H	2.84464400	0.89778000	1.89235000
H	2.97886900	-1.30017900	-1.78367500
H	5.31323800	0.81188700	2.03572400
H	5.44525500	-1.37948900	-1.64848900
H	6.61910000	-0.32241900	0.26032100
H	-2.65075600	2.27041300	-0.28208300
H	2.31047600	2.34045500	-0.29264000
H	-1.44404400	4.39016200	-0.53702200
H	1.04013400	4.43046000	-0.52886200

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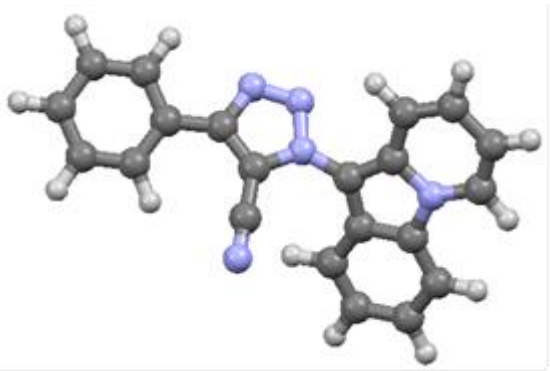

C	-2.42481100	0.17695000	-0.31815600
C	-3.56452900	-0.43070900	0.18543500
C	-0.01010400	-0.17668400	0.20931600
C	0.93424700	-1.16701600	0.01281900
C	0.65312000	1.08226300	0.27261000
C	2.02922500	0.82136300	0.09296100
C	0.87098100	-2.58259200	-0.11272900
C	2.01770300	-3.28495500	-0.31187700
H	-0.09502400	-3.06257500	-0.03058900
C	3.28120200	-2.61614200	-0.38565600
H	1.98241800	-4.36252900	-0.40923100
C	3.33763200	-1.26983600	-0.25613800
H	4.19477200	-3.17253000	-0.53864500
H	4.25388500	-0.69782100	-0.29685200
C	0.23180500	2.40828800	0.47587700
C	1.18109100	3.40776400	0.48357300
H	-0.81651300	2.63967800	0.62052500
C	2.54917100	3.12667000	0.29172600
H	0.87142500	4.43417700	0.63671500
C	2.99063700	1.83273500	0.09646800
H	3.26513500	3.93873600	0.29886600
H	4.04300300	1.62004500	-0.04612400
N	2.18596300	-0.55100900	-0.05907400
C	-2.22272000	1.13887400	-1.33771600
N	-2.07371800	1.92389900	-2.16594300
N	-3.15137400	-1.35108600	1.09517600
N	-1.86271000	-1.33042100	1.19466500
N	-1.39059900	-0.41547400	0.34940800
C	-4.98371100	-0.22987100	-0.12696000
C	-5.91762700	-1.16174900	0.33668100
C	-5.42151400	0.86886000	-0.87093000
C	-7.26628300	-0.99672100	0.05423100
H	-5.57122900	-2.00780500	0.91690900
C	-6.77303100	1.02690200	-1.15243300
H	-4.71498800	1.60807200	-1.22867200
C	-7.69832300	0.09613400	-0.69227200
H	-7.98283600	-1.72405100	0.41658400
H	-7.10219600	1.88222700	-1.72993300
H	-8.75154000	0.22233100	-0.91271000

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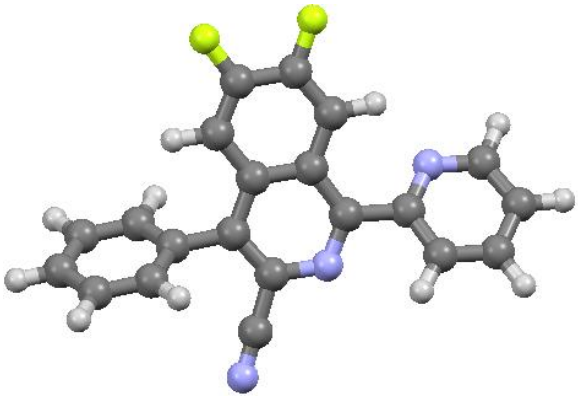
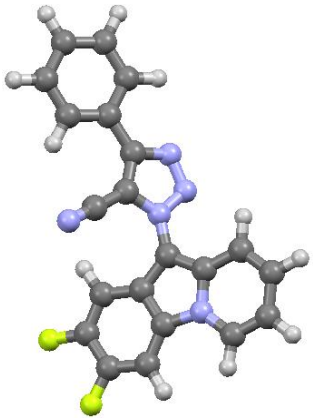
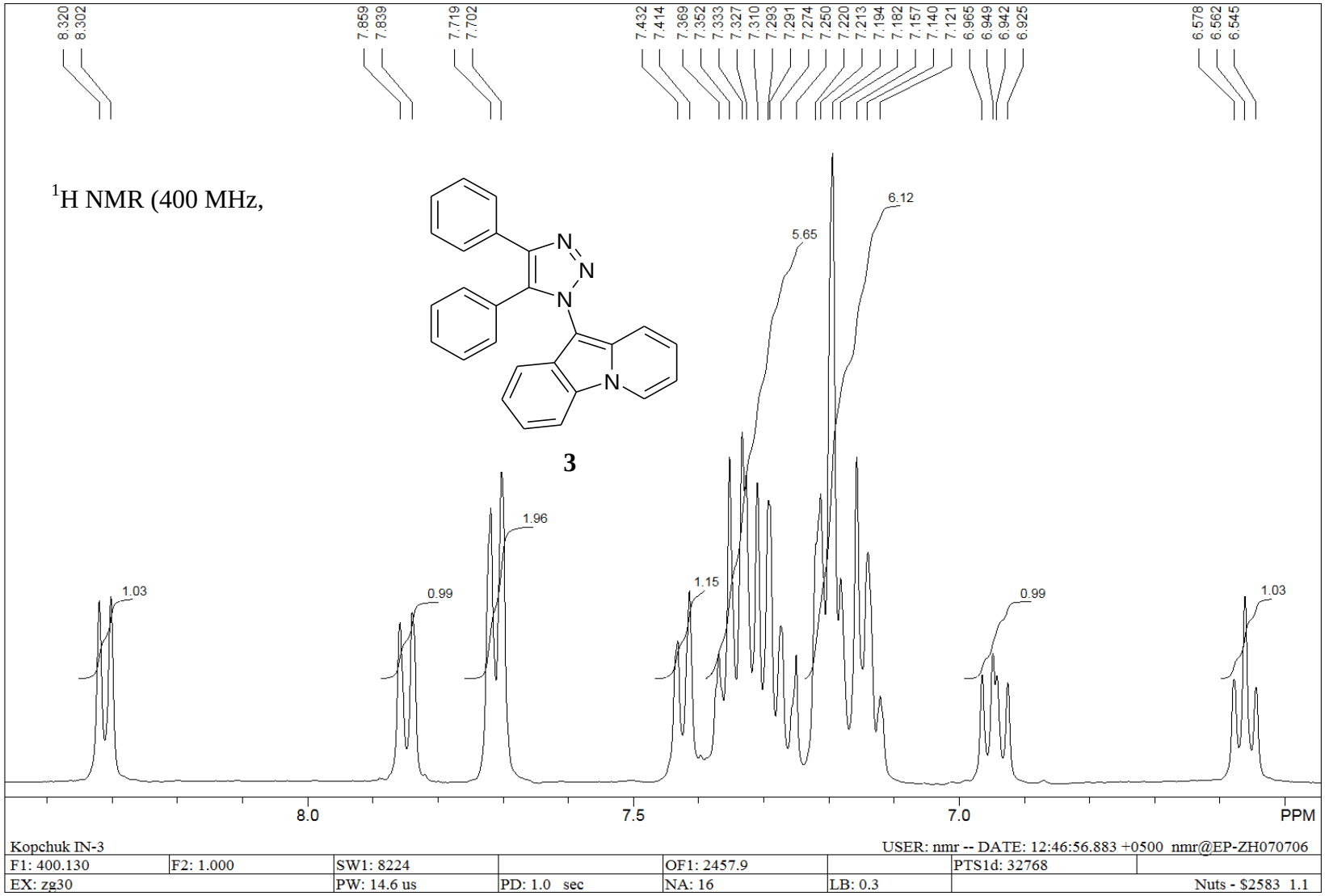


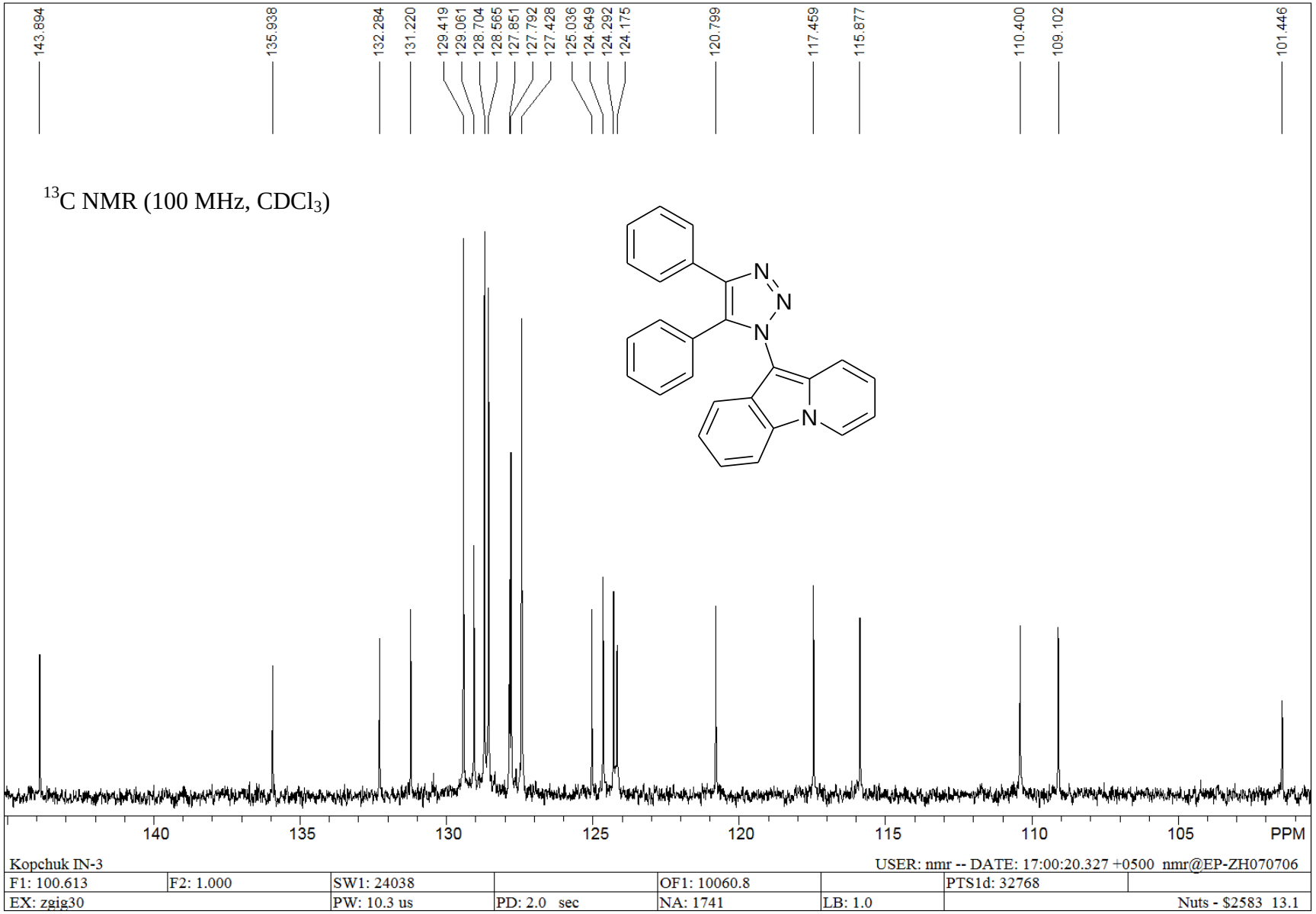
C	1.23942200	2.31887800	-0.25048400
C	0.55545600	1.08296400	-0.11345900
C	-0.86726400	1.06219700	-0.11192700
C	-1.57464400	2.28415200	-0.24757300
C	-0.88484000	3.44979100	-0.37226500
C	0.52440700	3.46888700	-0.37384600
C	-1.51359700	-0.21825800	-0.02636500
C	1.27025700	-0.14856700	-0.02278300
C	0.51622000	-1.30178500	0.00403300
N	-0.83551900	-1.33869000	-0.00052300
C	-2.99876400	-0.39949600	0.02274200
N	-3.73258200	0.54007900	0.62278900
C	-5.04758700	0.34731100	0.71293400
C	-5.69421300	-0.77294100	0.20578100
C	-4.92659300	-1.74464800	-0.42534000
C	-3.55593900	-1.56257400	-0.51614200
C	2.75301100	-0.18825000	0.03574000
C	3.42646100	0.40674900	1.10591900
C	4.81320200	0.36009700	1.17347200
C	5.53869700	-0.27676800	0.17086500
C	4.87353600	-0.87104900	-0.89577800
C	3.48563900	-0.82997700	-0.96318300
C	1.15732800	-2.59674700	0.07007000
N	1.66041700	-3.62928600	0.11397900
H	-2.91171600	-2.29733700	-0.97880500
H	-5.38883000	-2.63366600	-0.83764500
H	-5.60852500	1.12774300	1.21719000
H	-6.76712800	-0.87581900	0.30547500
H	2.85737600	0.89438700	1.89024100
H	2.96624600	-1.29819000	-1.79167200
H	5.32660500	0.81583800	2.01146700
H	5.43377700	-1.37186900	-1.67583100
H	6.62008800	-0.31326400	0.22404900
H	-2.65327800	2.30700500	-0.23708100
H	2.32010500	2.36072200	-0.28038300
F	-1.52057300	4.61288200	-0.50676500
F	1.13215600	4.64433600	-0.51454100

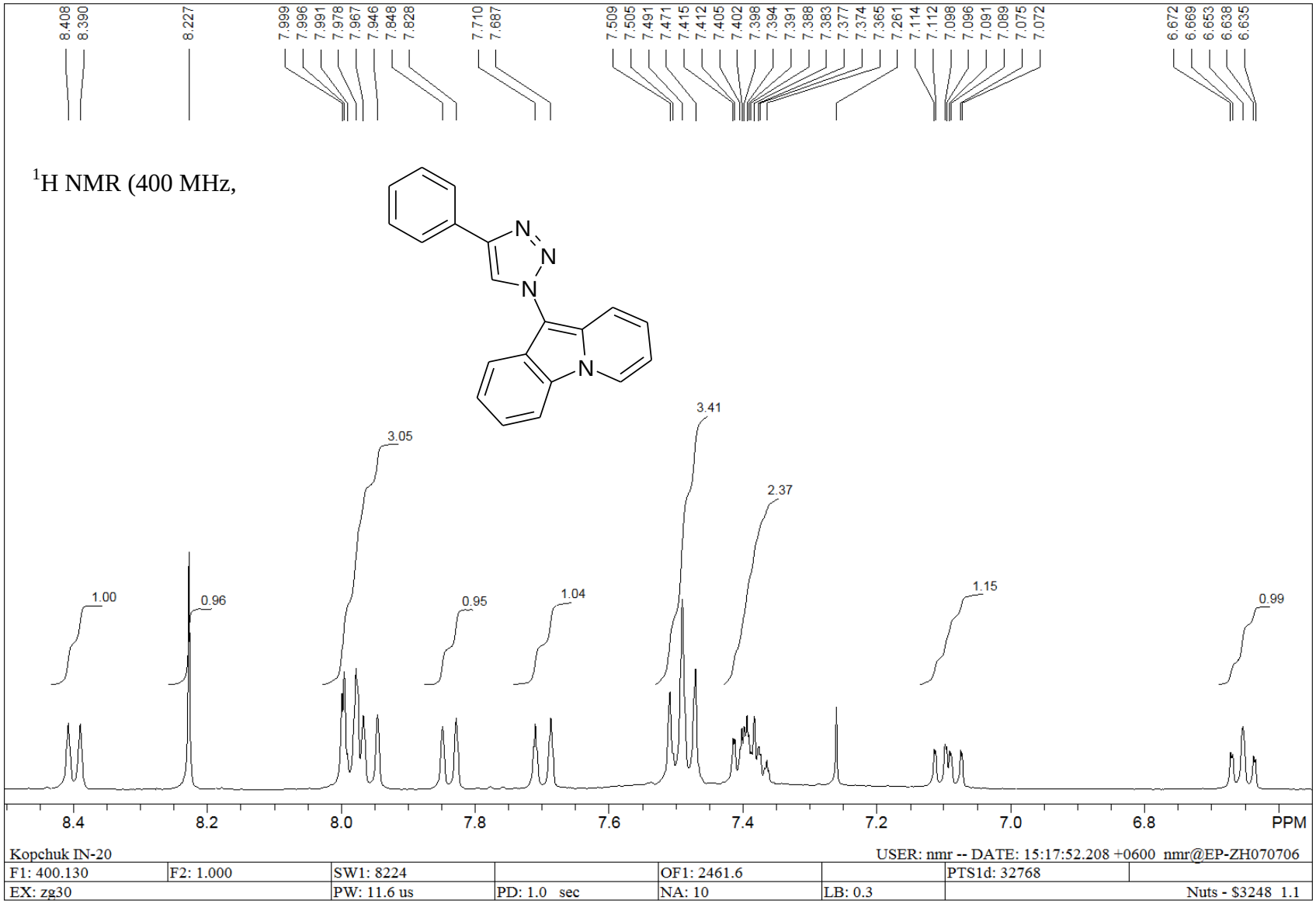
Domino Product 2 (Gas phase), -1280.0881859 hartree, n_{imag} = 0:

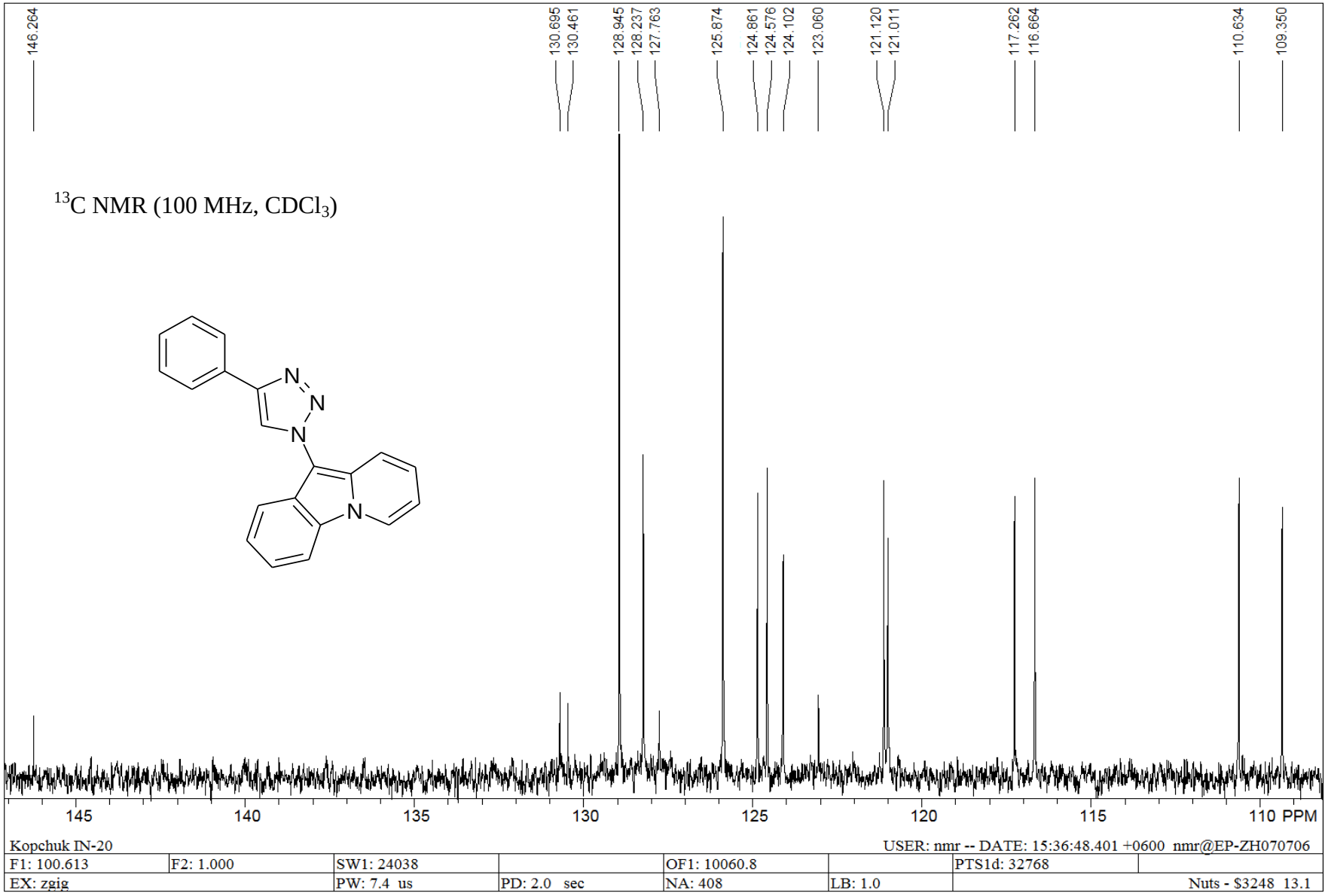


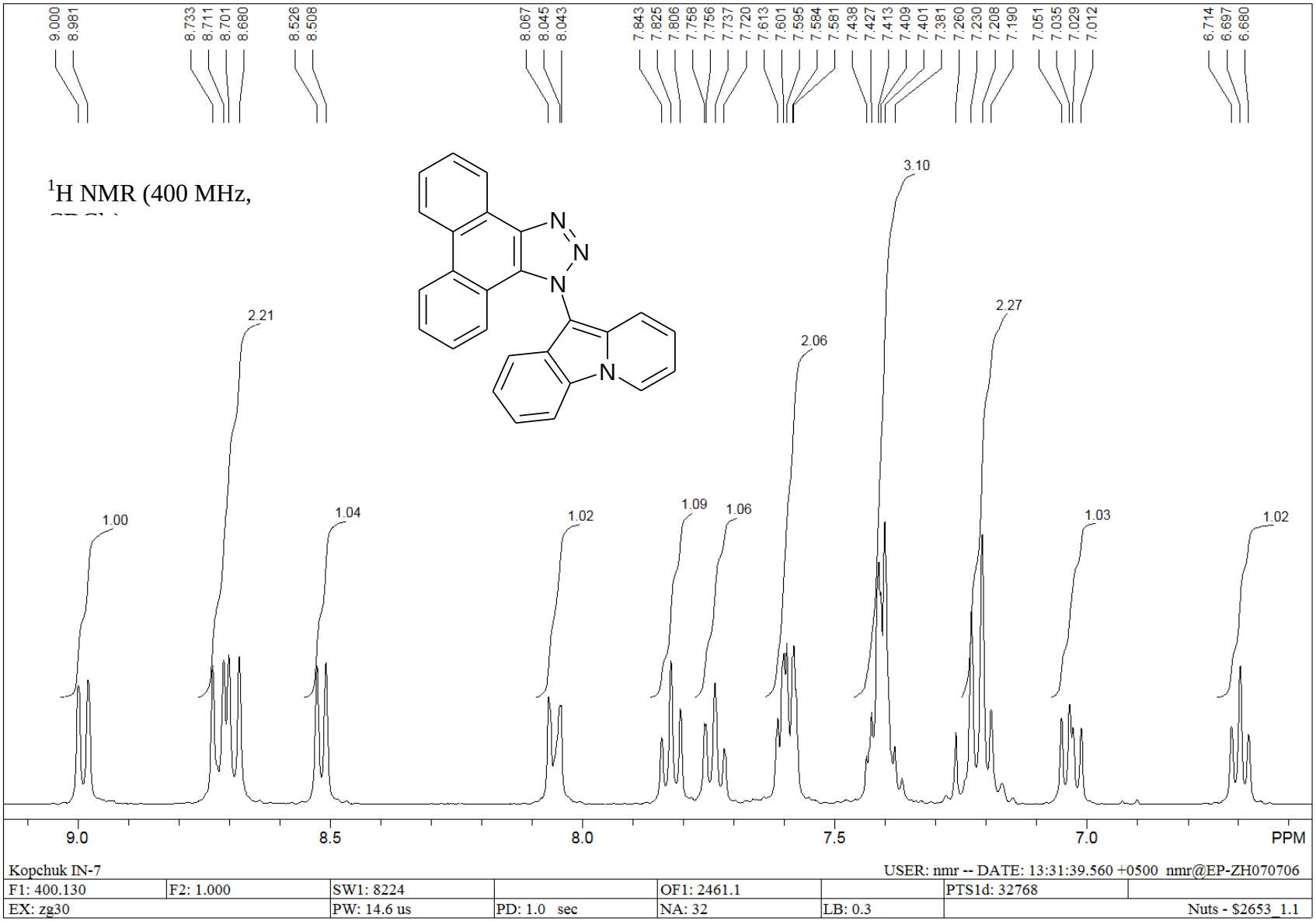
C	-2.42578900	0.17555200	-0.31607200
C	-3.56538700	-0.42906600	0.19008200
C	-0.01186500	-0.17547800	0.21473700
C	0.93295600	-1.16490200	0.01338100
C	0.65240000	1.08161700	0.27680100
C	2.02700100	0.81979100	0.09223800
C	0.86902500	-2.57983100	-0.11364500
C	2.01507600	-3.28212300	-0.31644900
H	-0.09711300	-3.05925800	-0.02970700
C	3.27855600	-2.61346100	-0.39258800
H	1.97959300	-4.35948000	-0.41498400
C	3.33731600	-1.26791700	-0.26202100
H	4.19142600	-3.17022800	-0.54836900
H	4.25412000	-0.69678000	-0.30441800
C	0.22393400	2.40549700	0.48297100
C	1.17604000	3.38934900	0.48722900
H	-0.81520000	2.66891500	0.63320000
C	2.54151400	3.10811200	0.29118500
C	2.99322300	1.82864700	0.09295300
H	4.05115600	1.65180600	-0.04975200
N	2.18465100	-0.54896400	-0.06131900
C	-2.21692300	1.13304700	-1.33823400
N	-2.05169700	1.91555100	-2.16580000
N	-3.15212500	-1.34390500	1.10655200
N	-1.86439100	-1.32246000	1.20779600
N	-1.39174300	-0.41212900	0.35713600
C	-4.98384900	-0.23010500	-0.12542900
C	-5.91824500	-1.16072400	0.33944200
C	-5.41953900	0.86644800	-0.87380400
C	-7.26623200	-0.99655300	0.05333400
H	-5.57336000	-2.00488600	0.92332400
C	-6.77030500	1.02362500	-1.15874900
H	-4.71238800	1.60514200	-1.23163900
C	-7.69632300	0.09399800	-0.69758200
H	-7.98370700	-1.72253300	0.41643900
H	-7.09841100	1.87732600	-1.73915100
H	-8.74905500	0.21961400	-0.92053000
F	3.40097800	4.13047900	0.30562800
F	0.83202300	4.66416200	0.68128600

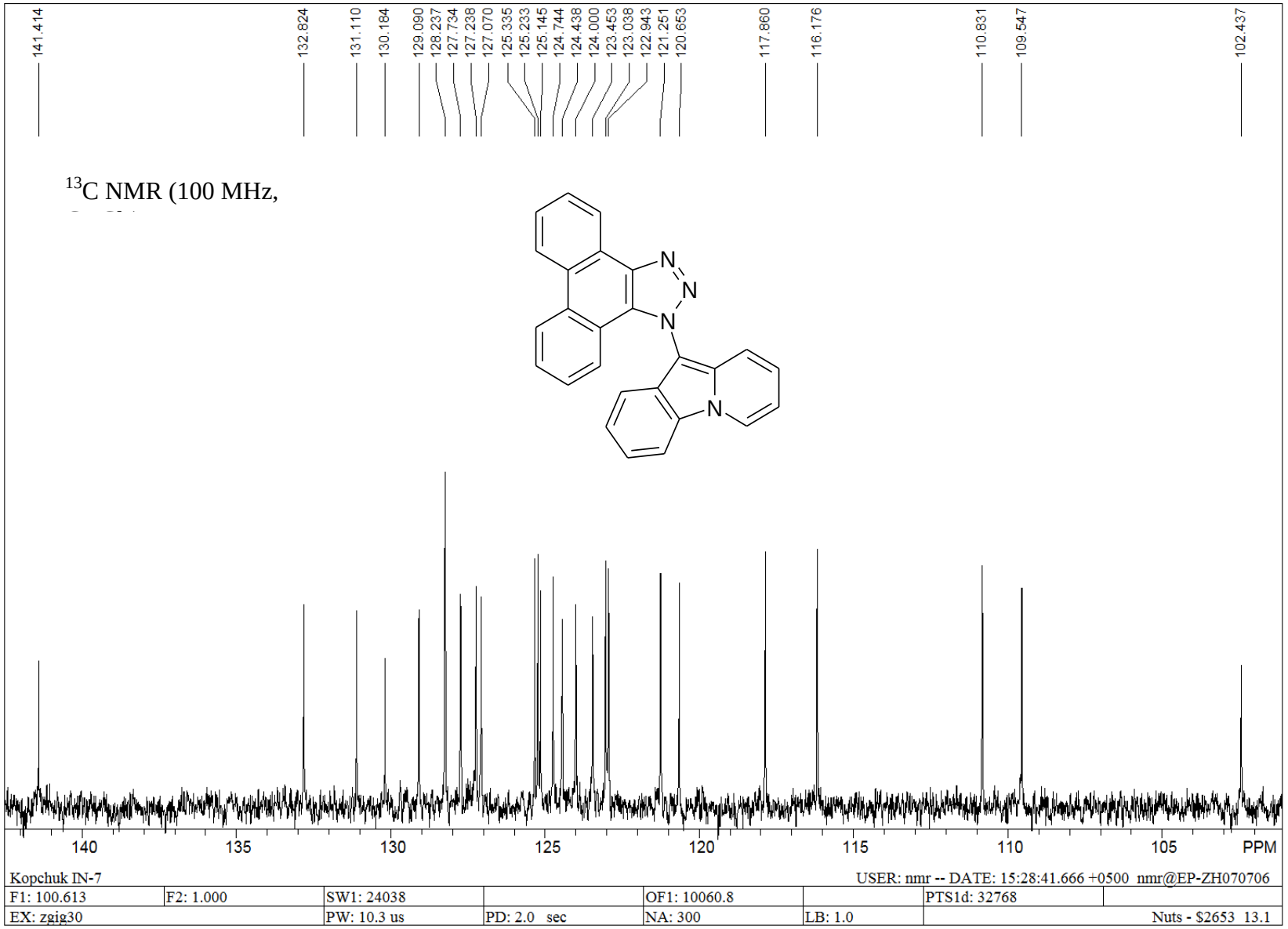

8.320
8.302
7.859
7.839
7.719
7.702
7.432
7.414
7.369
7.352
7.333
7.327
7.310
7.293
7.291
7.274
7.250
7.220
7.213
7.194
7.182
7.157
7.140
7.121
6.965
6.949
6.942
6.925
6.578
6.562
6.545
1H NMR (400 MHz,
N
N
N
N
3
6.12
5.65
1.96
1.03
0.99
1.15
0.99
1.03
8.0
7.5
7.0
PPM
Kopchuk IN-3
USER: nmr -- DATE: 12:46:56.883 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2457.9
PTS1d: 32768
EX: zg30
PW: 14.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $2583 1.1

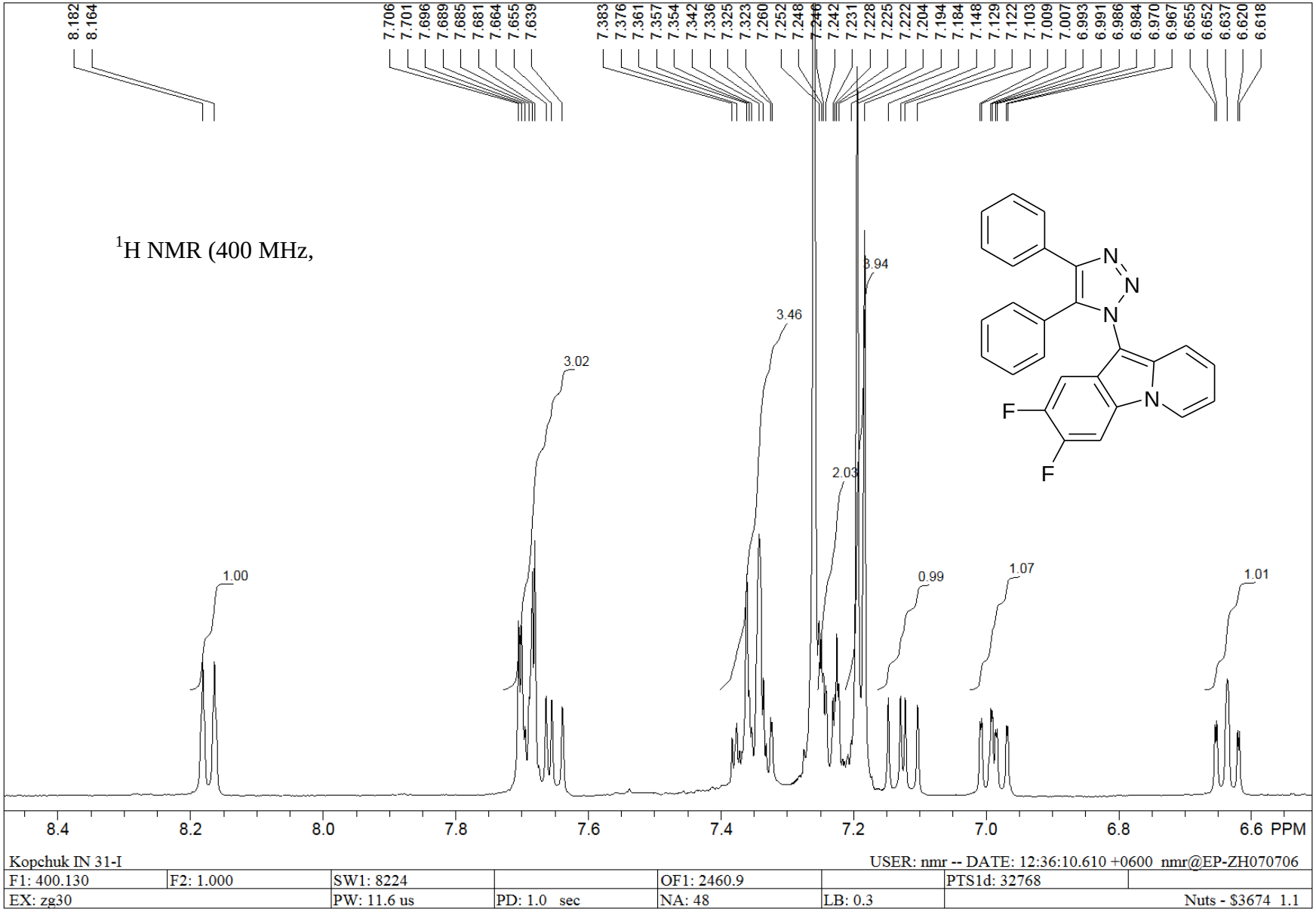

143.894
135.938
132.284
131.220
129.419
129.061
128.704
128.565
127.851
127.792
127.428
125.036
124.649
124.292
124.175
120.799
117.459
115.877
110.400
109.102
101.446
13C NMR (100 MHz, CDCl3)
N
N
N
N
140
135
130
125
120
115
110
105
PPM
Kopchuk IN-3
USER: nmr -- DATE: 17:00:20.327 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 10.3 us
PD: 2.0 sec
NA: 1741
LB: 1.0
Nuts - $2583 13.1

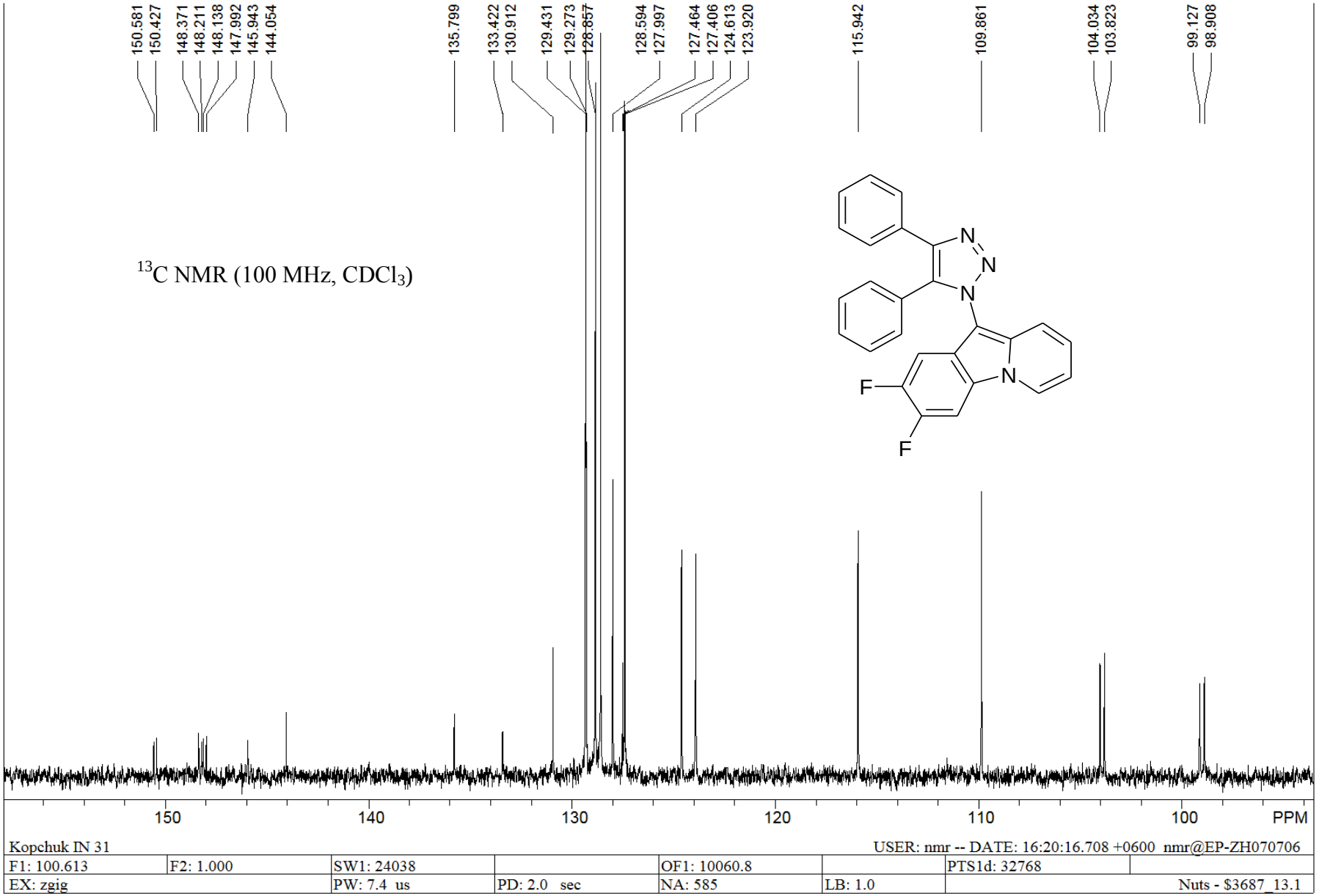

8.408
8.390
8.227
7.999
7.996
7.991
7.978
7.967
7.946
7.848
7.828
7.710
7.687
7.509
7.505
7.491
7.471
7.415
7.412
7.405
7.402
7.398
7.394
7.391
7.388
7.383
7.377
7.374
7.365
7.261
7.114
7.112
7.098
7.096
7.091
7.089
7.075
7.072
6.672
6.669
6.653
6.638
6.635
1H NMR (400 MHz,
N
N
N
N
3.41
3.05
2.37
1.15
1.00
0.96
0.95
1.04
0.99
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
PPM
Kopchuk IN-20
USER: nmr -- DATE: 15:17:52.208 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.6
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 10
LB: 0.3
Nuts - $3248 1.1


146.264
130.695
130.461
128.945
128.237
127.763
125.874
124.861
124.576
124.102
123.060
121.120
121.011
117.262
116.664
110.634
109.350
^{13}C NMR (100 MHz, CDCl$_3$)
N
N
N
N
145
140
135
130
125
120
115
110 PPM
Kopchuk IN-20
USER: nmr -- DATE: 15:36:48.401 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig
PW: 7.4 us
PD: 2.0 sec
NA: 408
LB: 1.0
Nuts - $3248 13.1

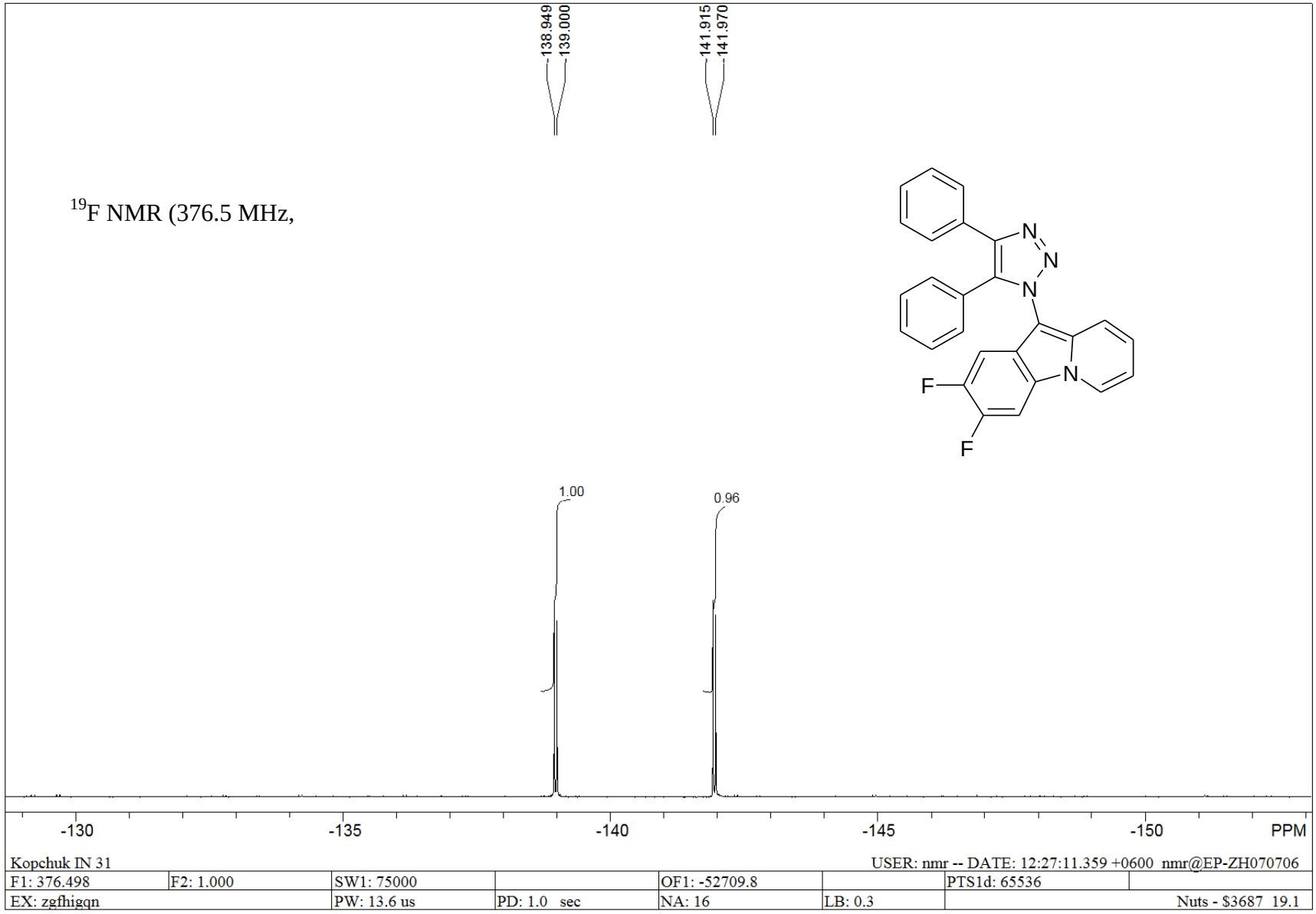

9.000
8.981
8.733
8.711
8.701
8.680
8.526
8.508
8.067
8.045
8.043
7.843
7.825
7.806
7.758
7.756
7.737
7.720
7.613
7.601
7.595
7.584
7.581
7.438
7.427
7.413
7.409
7.401
7.381
7.260
7.230
7.208
7.190
7.051
7.035
7.029
7.012
6.714
6.697
6.680
1H NMR (400 MHz,
N
N
N
N
1.00
2.21
1.04
1.02
1.09
1.06
2.06
3.10
2.27
1.03
1.02
9.0
8.5
8.0
7.5
7.0
PPM
Kopchuk IN-7
USER: nmr -- DATE: 13:31:39.560 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.1
PTS1d: 32768
EX: zg30
PW: 14.6 us
PD: 1.0 sec
NA: 32
LB: 0.3
Nuts - $2653_1.1

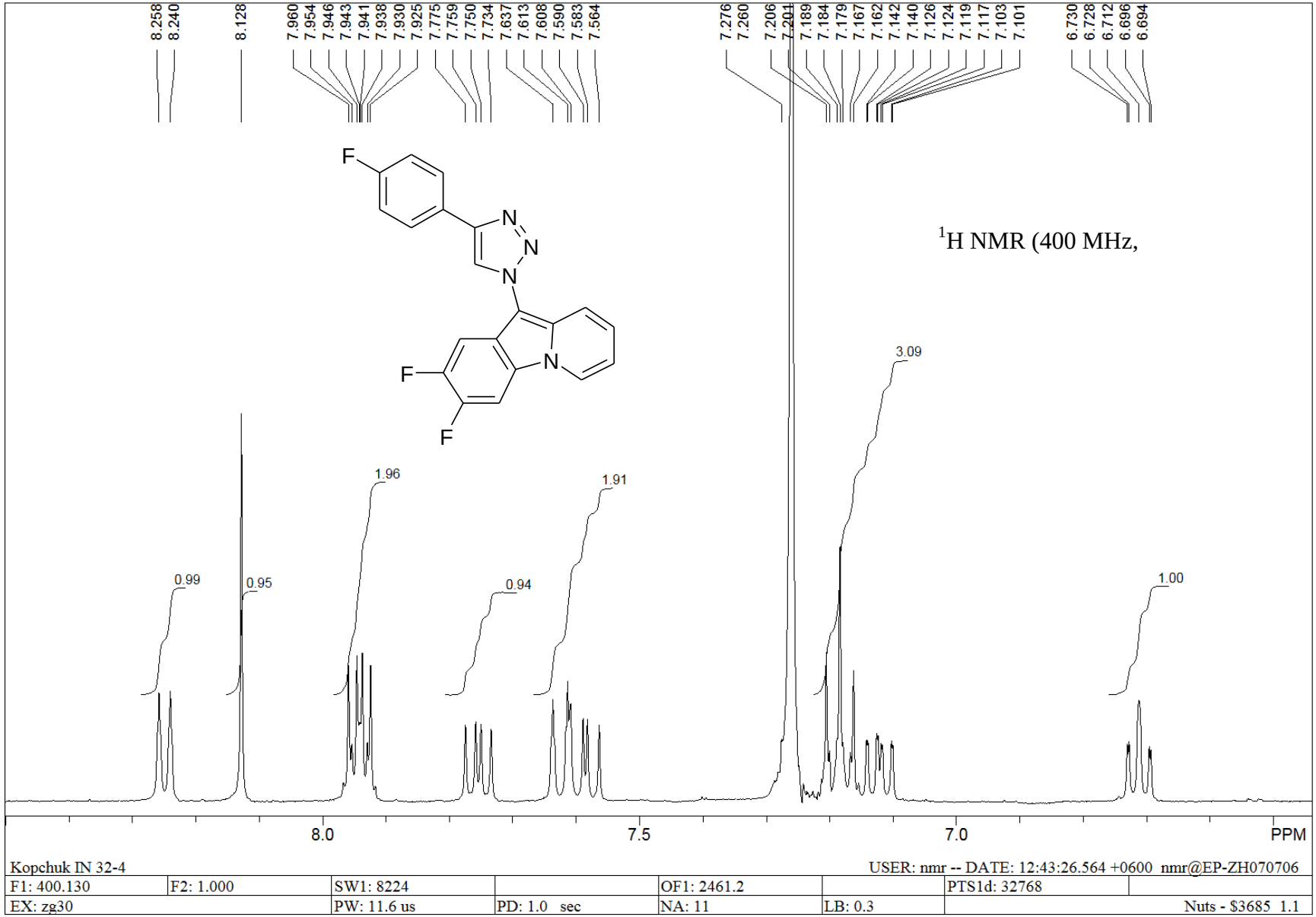

141.414
132.824
131.110
130.184
129.090
128.237
127.734
127.238
127.070
125.335
125.233
125.145
124.744
124.438
124.000
123.453
123.038
122.943
121.251
120.653
117.860
116.176
110.831
109.547
102.437
13C NMR (100 MHz,
N
N
N
N
140
135
130
125
120
115
110
105
PPM
Kopchuk IN-7
USER: nmr -- DATE: 15:28:41.666 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 10.3 us
PD: 2.0 sec
NA: 300
LB: 1.0
Nuts - $2653 13.1

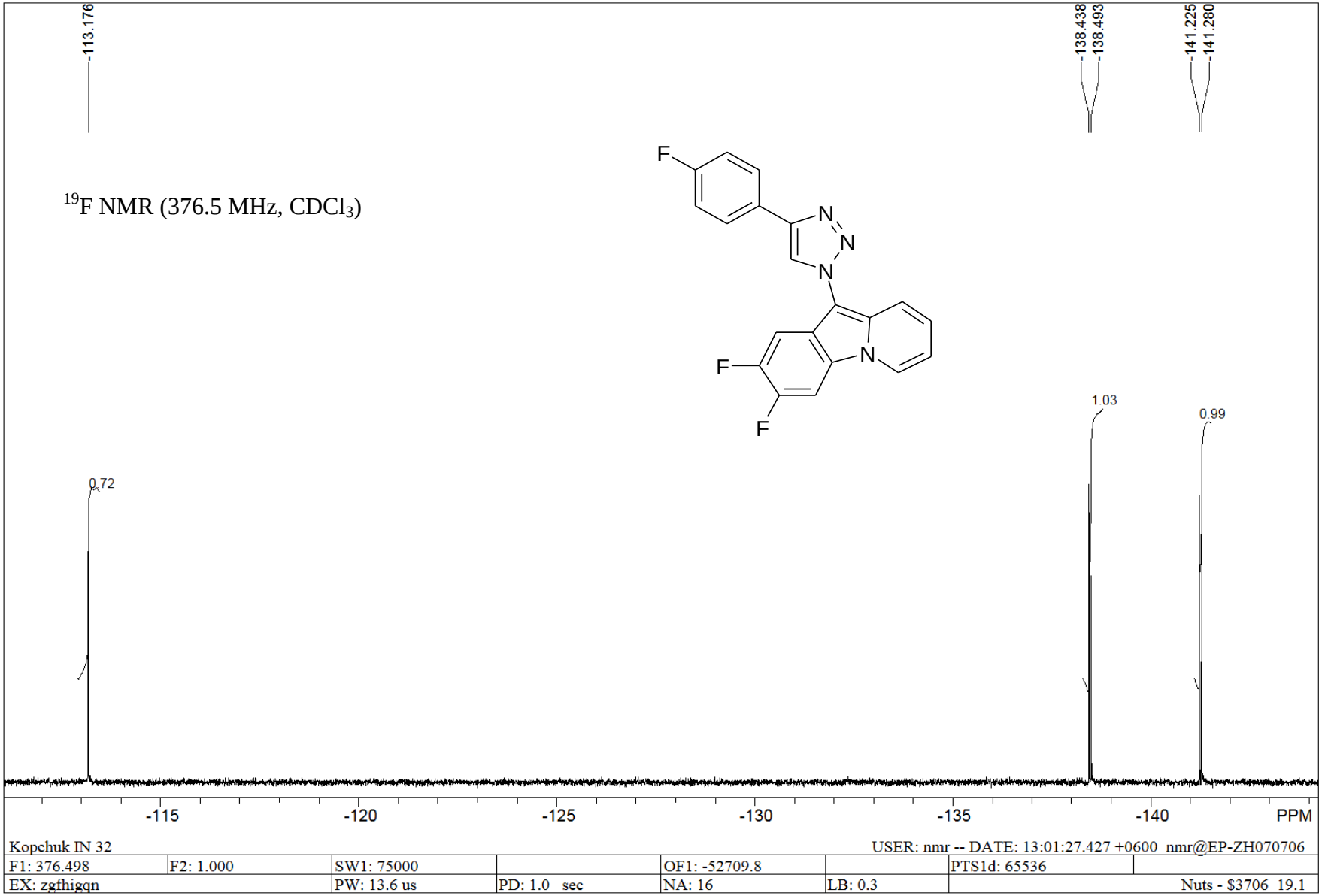

8.182
8.164
7.706
7.701
7.696
7.689
7.685
7.681
7.664
7.655
7.639
7.383
7.376
7.361
7.357
7.354
7.342
7.336
7.325
7.323
7.260
7.252
7.248
7.246
7.242
7.231
7.228
7.225
7.222
7.204
7.194
7.184
7.148
7.129
7.122
7.103
7.009
7.007
6.993
6.991
6.986
6.984
6.970
6.967
6.655
6.652
6.637
6.620
6.618
1H NMR (400 MHz,
3.94
3.46
3.02
2.03
1.00
0.99
1.07
1.01
N
N
N
N
F
F
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6 PPM
Kopchuk IN 31-I
USER: nmr -- DATE: 12:36:10.610 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 48
LB: 0.3
Nuts - $3674 1.1

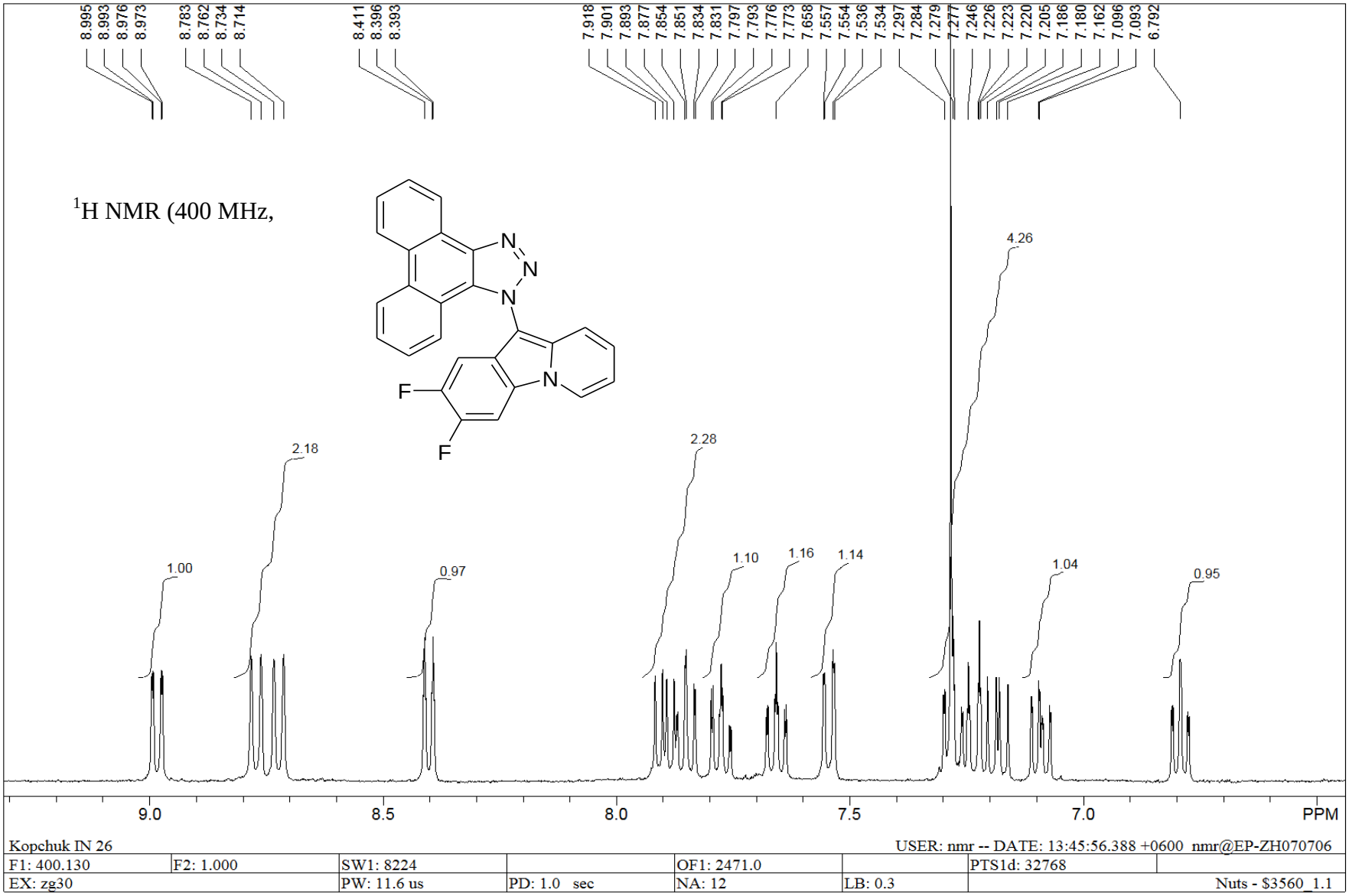

150.581
150.427
148.371
148.211
148.138
147.992
145.943
144.054
135.799
133.422
130.912
129.431
129.273
128.857
128.594
127.997
127.464
127.406
124.613
123.920
115.942
109.861
104.034
103.823
99.127
98.908
^{13}C NMR (100 MHz, $CDCl_3$)
N
N
N
N
F
F
150
140
130
120
110
100
PPM
Kopchuk IN 31
USER: nmr -- DATE: 16:20:16.708 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig
PW: 7.4 us
PD: 2.0 sec
NA: 585
LB: 1.0
Nuts - $3687_13.1

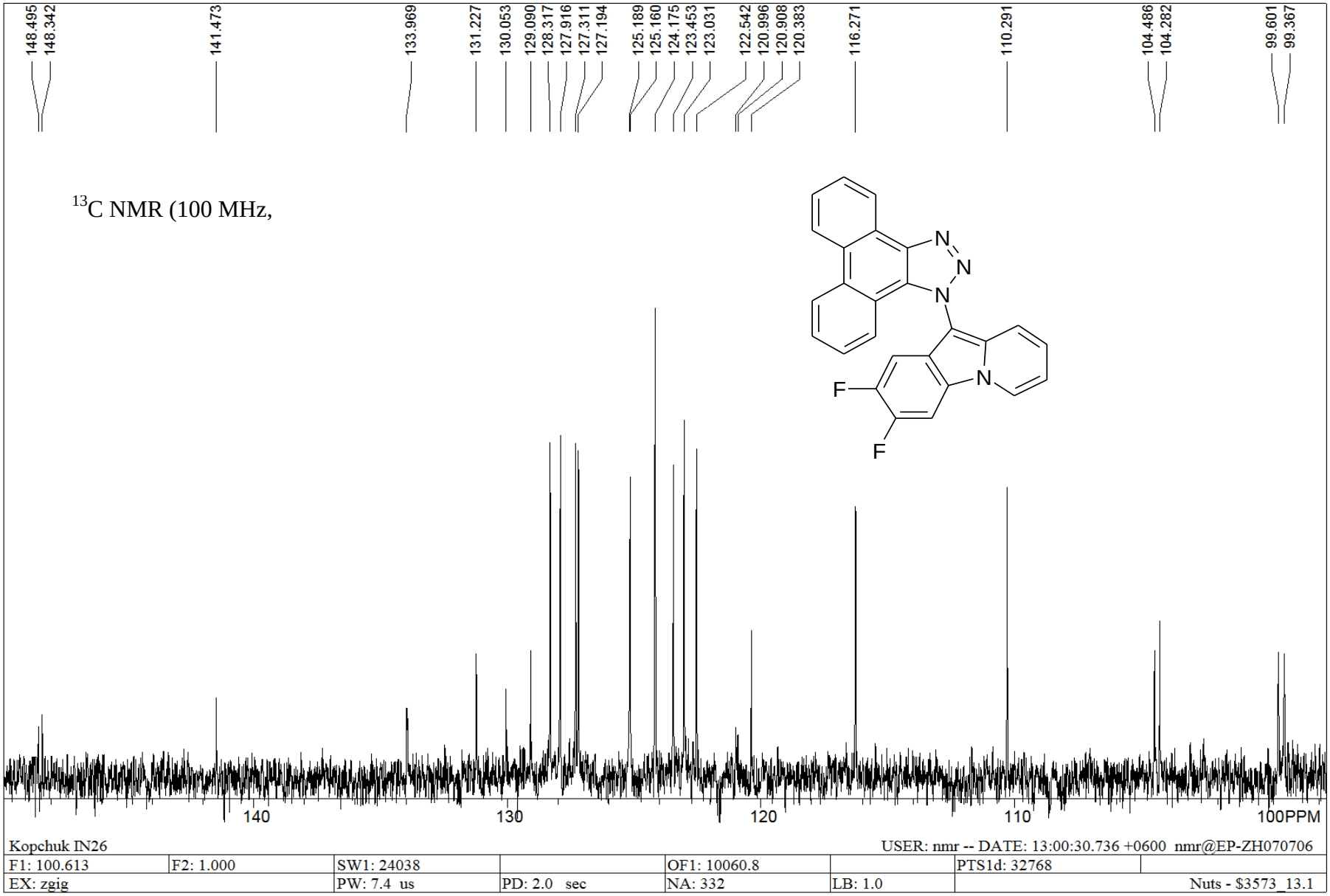
^{19}F NMR (376.5 MHz,



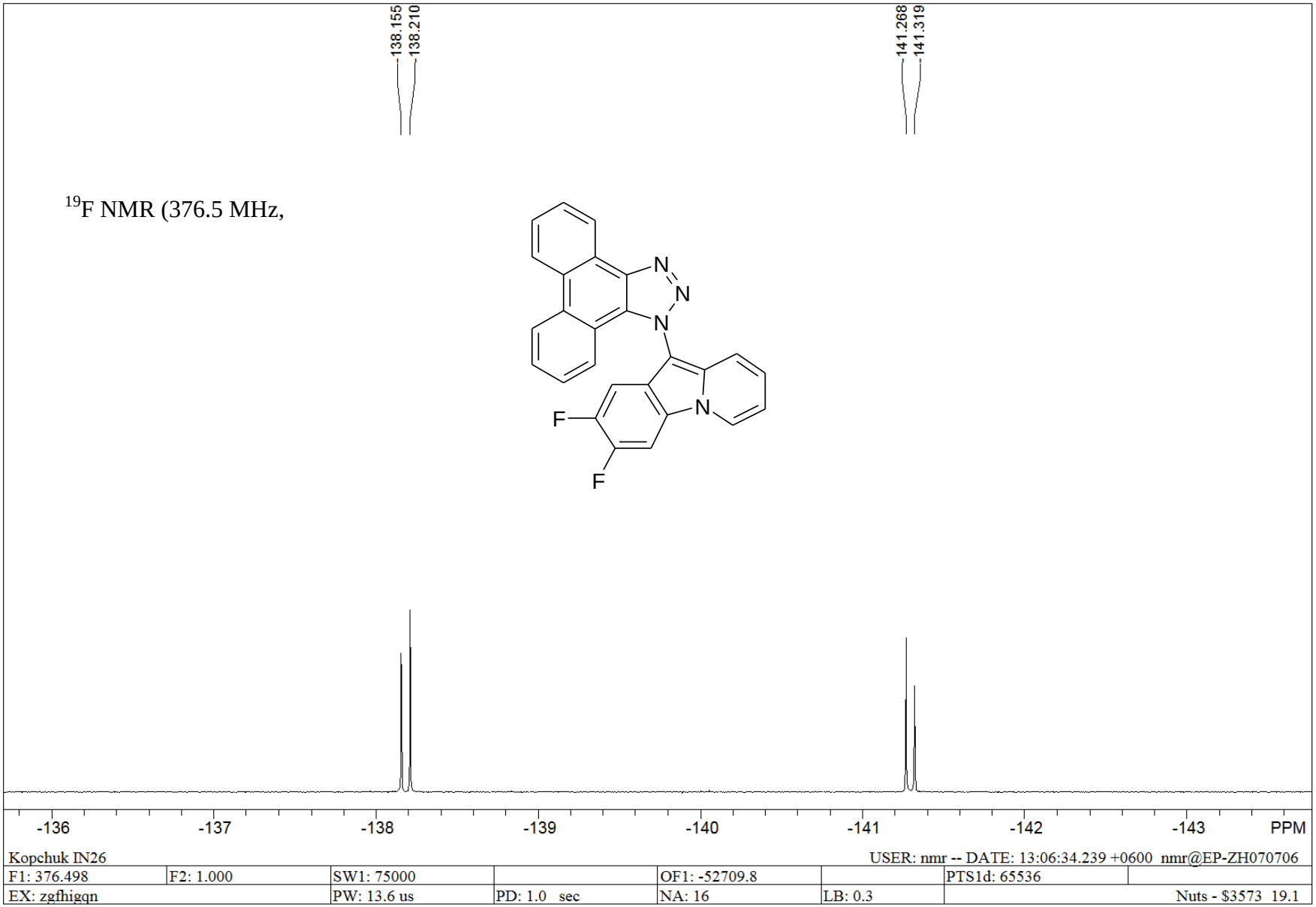

8.258
8.240
8.128
7.960
7.954
7.946
7.943
7.941
7.938
7.930
7.925
7.775
7.759
7.750
7.734
7.637
7.613
7.608
7.590
7.583
7.564
7.276
7.260
7.206
7.201
7.189
7.184
7.179
7.167
7.162
7.142
7.140
7.126
7.124
7.119
7.117
7.103
7.101
6.730
6.728
6.712
6.696
6.694
F
N
N
N
F
F
N
1H NMR (400 MHz,
3.09
1.96
1.91
0.99
0.95
0.94
1.00
8.0
7.5
7.0
PPM
Kopchuk IN 32-4
USER: nmr -- DATE: 12:43:26.564 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.2
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 11
LB: 0.3
Nuts - $3685 1.1

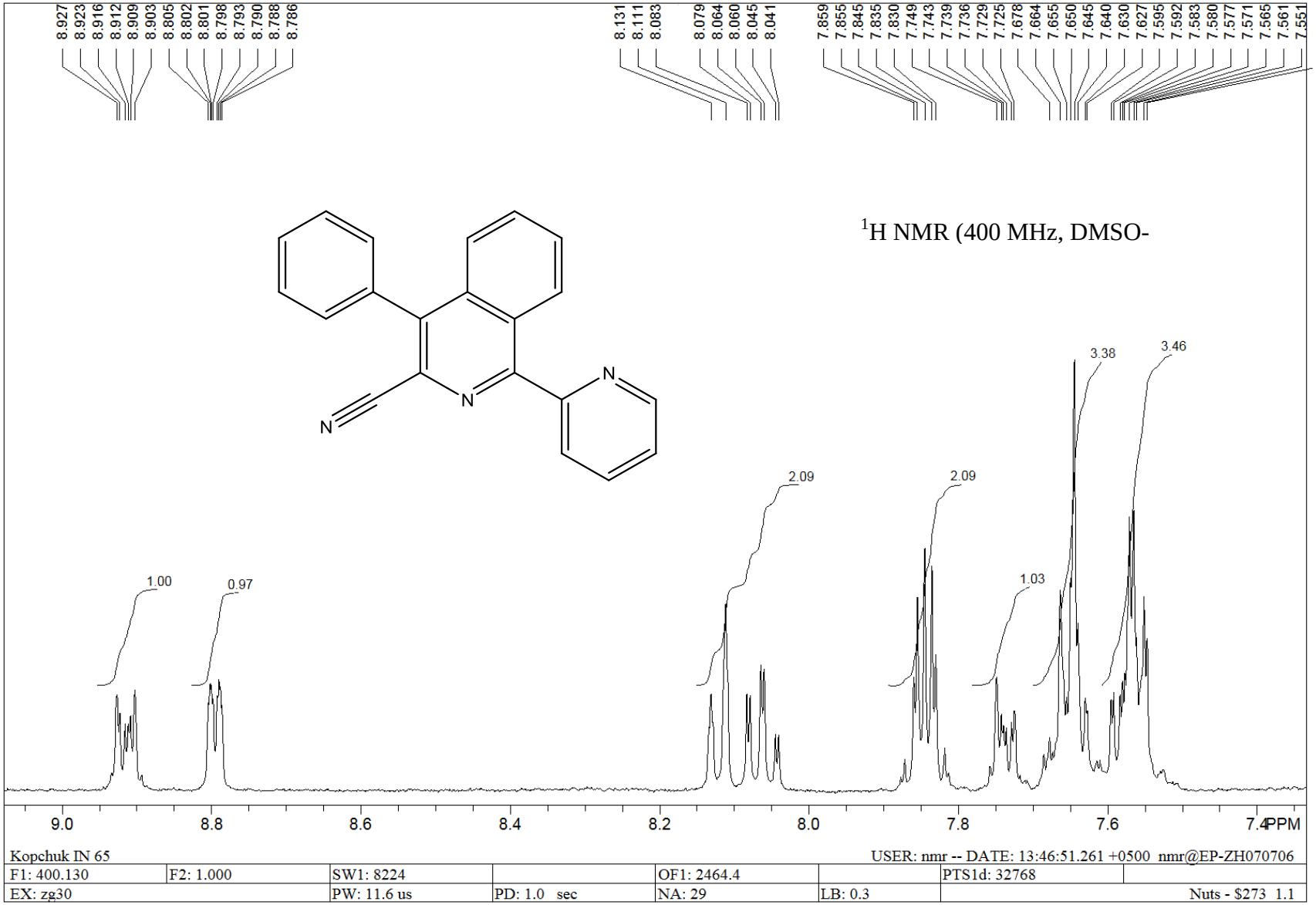

113.176
138.438
138.493
141.225
141.280
^{19}F NMR (376.5 MHz, CDCl$_3$)
F
N
N
N
F
F
N
1.03
0.99
0.72
-115
-120
-125
-130
-135
-140
PPM
Kopchuk IN 32
USER: nmr -- DATE: 13:01:27.427 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 13.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3706 19.1

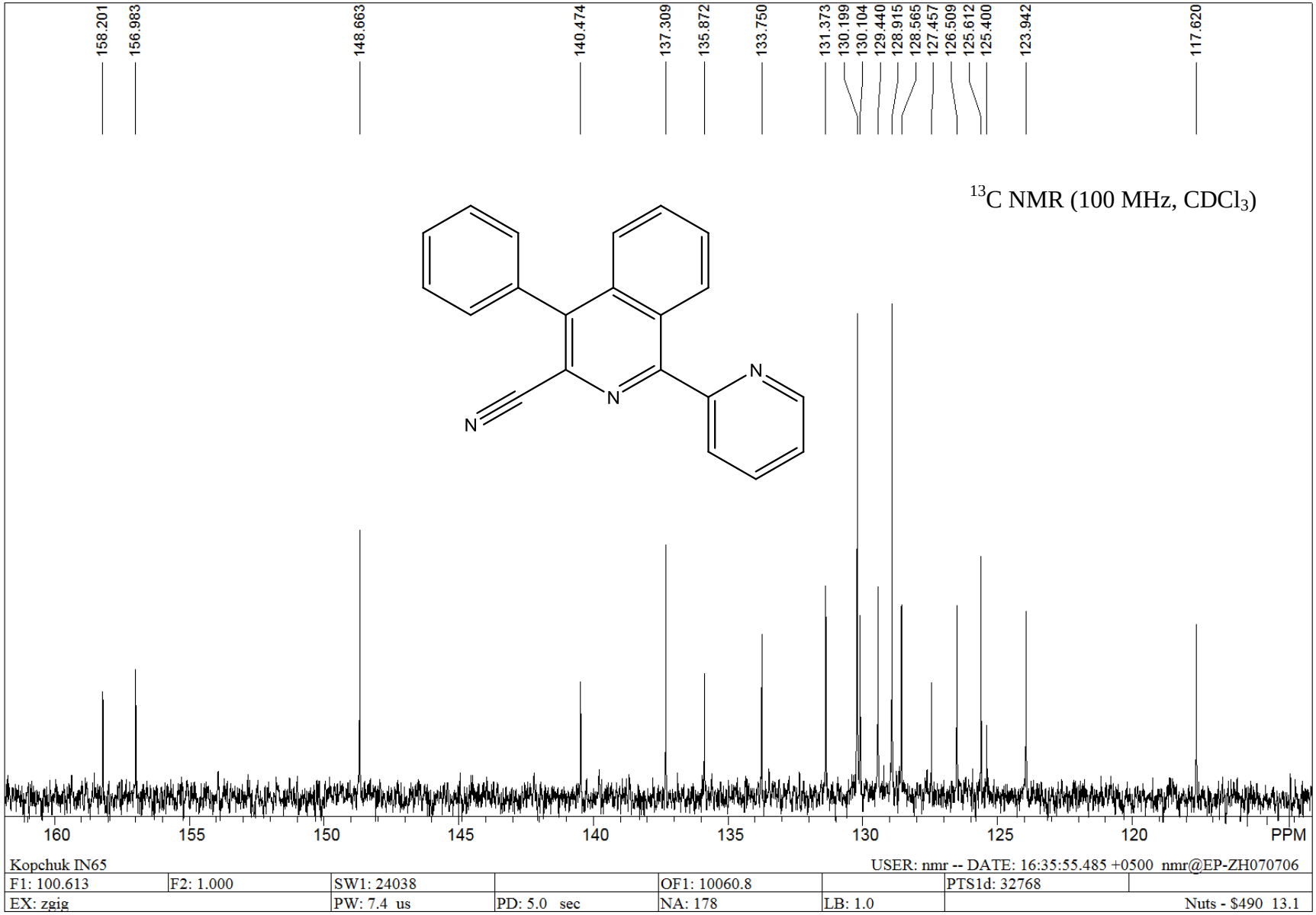

8.995
8.993
8.976
8.973
8.783
8.762
8.734
8.714
8.411
8.396
8.393
7.918
7.901
7.893
7.877
7.854
7.851
7.834
7.831
7.797
7.793
7.776
7.773
7.658
7.557
7.554
7.536
7.534
7.297
7.284
7.279
7.277
7.246
7.226
7.223
7.220
7.205
7.186
7.180
7.162
7.096
7.093
6.792
1H NMR (400 MHz,
N
N
N
F
F
N
4.26
2.18
2.28
1.00
0.97
1.10
1.16
1.14
1.04
0.95
9.0
8.5
8.0
7.5
7.0
PPM
Kopchuk IN 26
USER: nmr -- DATE: 13:45:56.388 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 12
LB: 0.3
Nuts - $3560_1.1

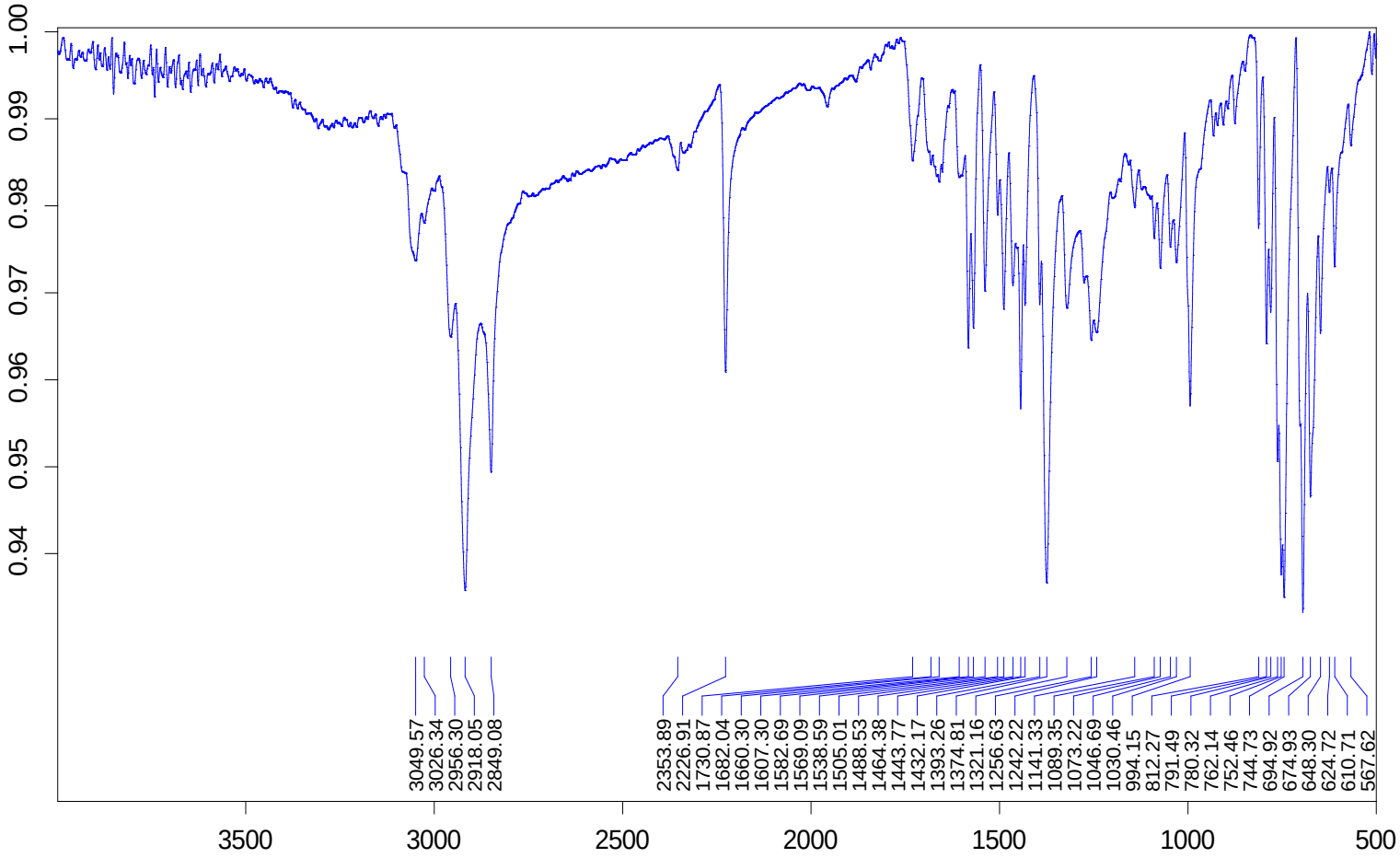

148.495
148.342
141.473
133.969
131.227
130.053
129.090
128.317
127.916
127.311
127.194
125.189
125.160
124.175
123.453
123.031
122.542
120.996
120.908
120.383
116.271
110.291
104.486
104.282
99.601
99.367
^{13}C NMR (100 MHz,
N
N
N
N
F
F
140
130
120
110
100PPM
Kopchuk IN26
USER: nmr -- DATE: 13:00:30.736 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig
PW: 7.4 us
PD: 2.0 sec
NA: 332
LB: 1.0
Nuts - $3573_13.1

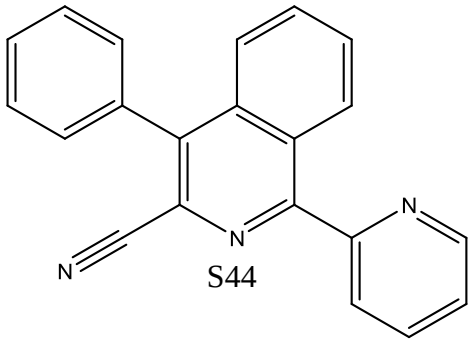
^{19}F NMR (376.5 MHz,

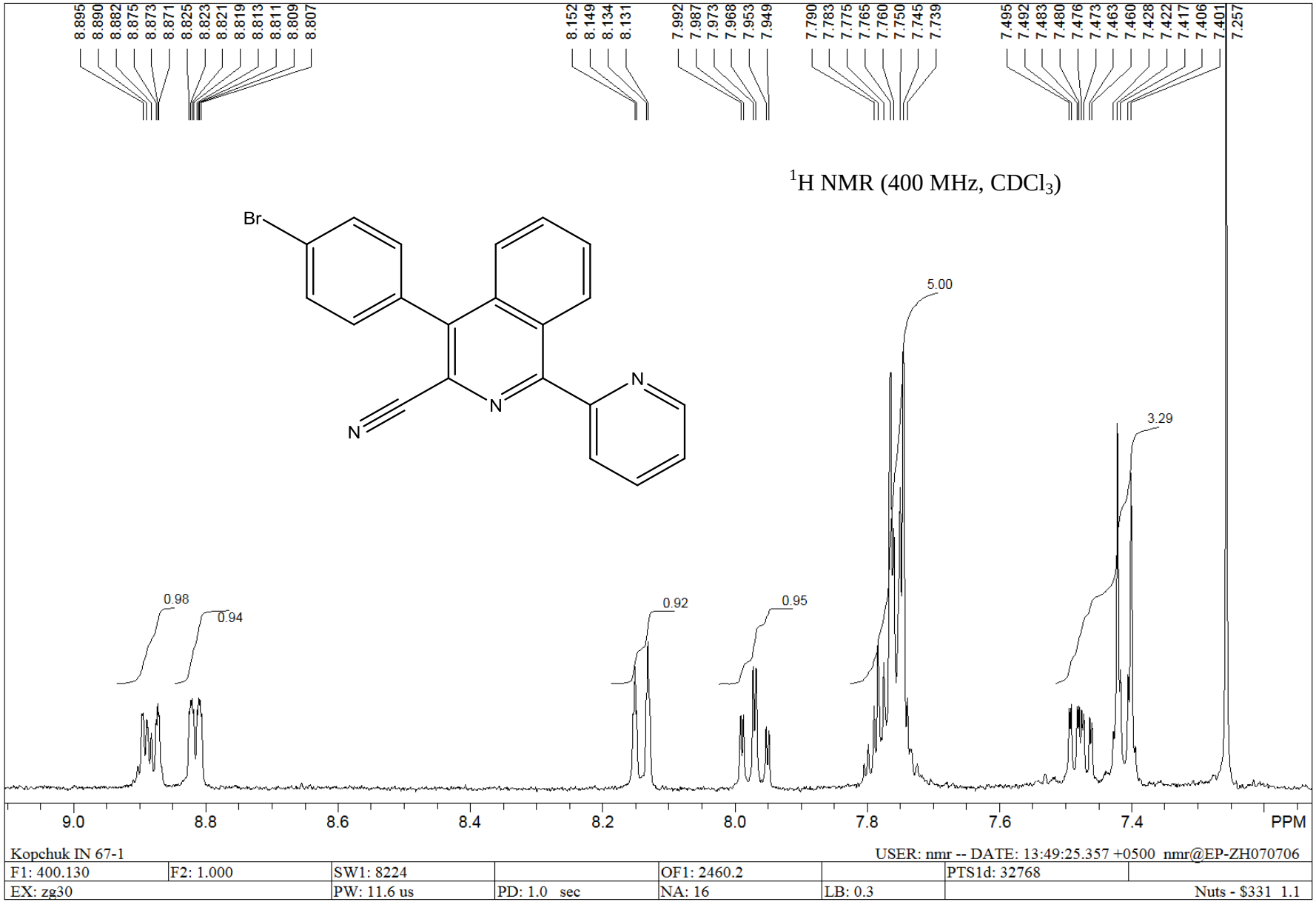


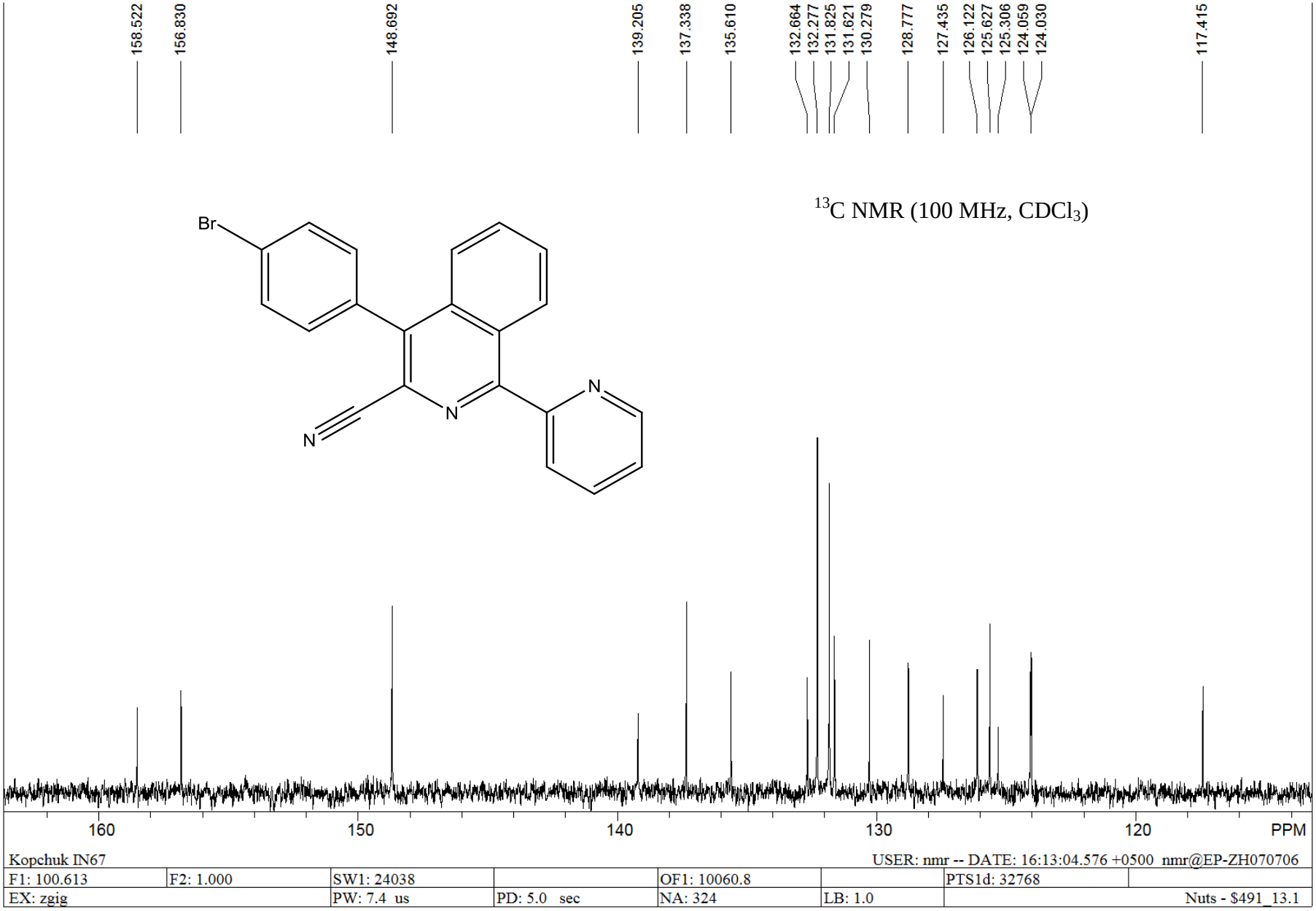

8.927
8.923
8.916
8.912
8.909
8.903
8.805
8.802
8.801
8.798
8.793
8.790
8.788
8.786
8.131
8.111
8.083
8.079
8.064
8.060
8.045
8.041
7.859
7.855
7.845
7.835
7.830
7.749
7.743
7.739
7.736
7.729
7.725
7.678
7.664
7.655
7.650
7.645
7.640
7.630
7.627
7.595
7.592
7.583
7.580
7.577
7.571
7.565
7.561
7.551
N
N
N
1H NMR (400 MHz, DMSO-
1.00
0.97
2.09
2.09
1.03
3.38
3.46
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
PPM
Kopchuk IN 65
USER: nmr -- DATE: 13:46:51.261 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2464.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 29
LB: 0.3
Nuts - $273 1.1

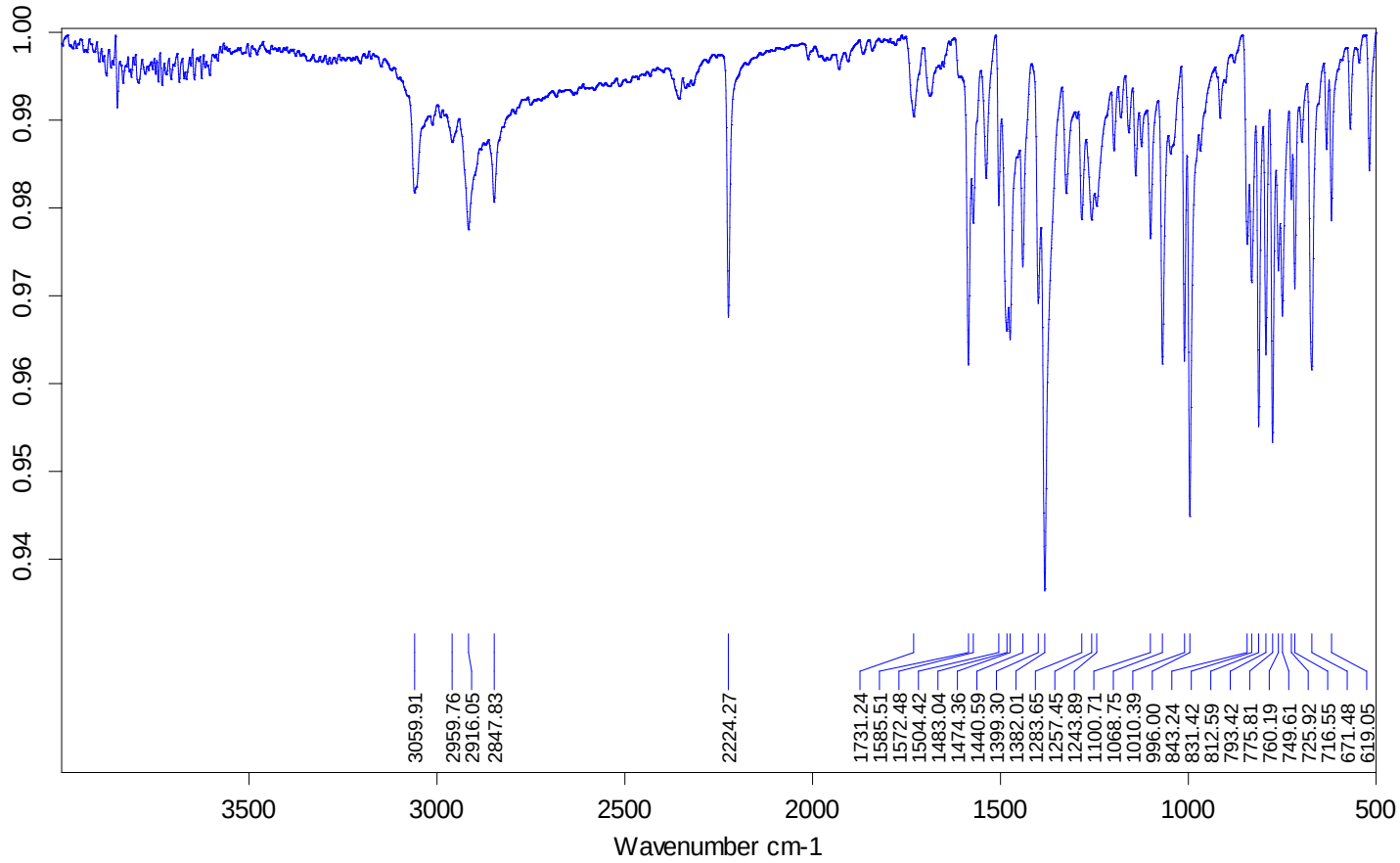

158.201
156.983
148.663
140.474
137.309
135.872
133.750
131.373
130.199
130.104
129.440
128.915
128.565
127.457
126.509
125.612
125.400
123.942
117.620
^{13}C NMR (100 MHz, CDCl$_3$)
N
N
N
160
155
150
145
140
135
130
125
120
PPM
Kopchuk IN65
USER: nmr -- DATE: 16:35:55.485 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig
PW: 7.4 us
PD: 5.0 sec
NA: 178
LB: 1.0
Nuts - $490 13.1

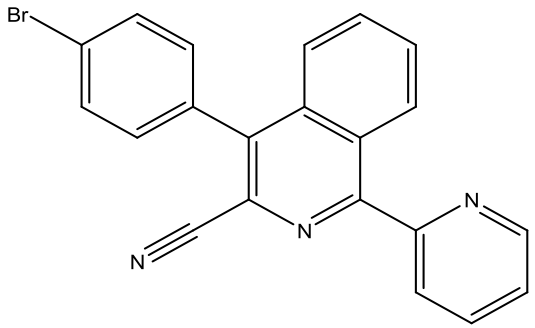

1.00
0.99
0.98
0.97
0.96
0.95
0.94
3049.57
3026.34
2956.30
2918.05
2849.08
2353.89
2226.91
1730.87
1682.04
1660.30
1607.30
1582.69
1569.09
1538.59
1505.01
1488.53
1464.38
1443.77
1432.17
1393.26
1374.81
1321.16
1256.63
1242.22
1141.33
1089.35
1073.22
1046.69
1030.46
994.15
812.27
791.49
780.32
762.14
752.46
744.73
694.92
674.93
648.30
624.72
610.71
567.62
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

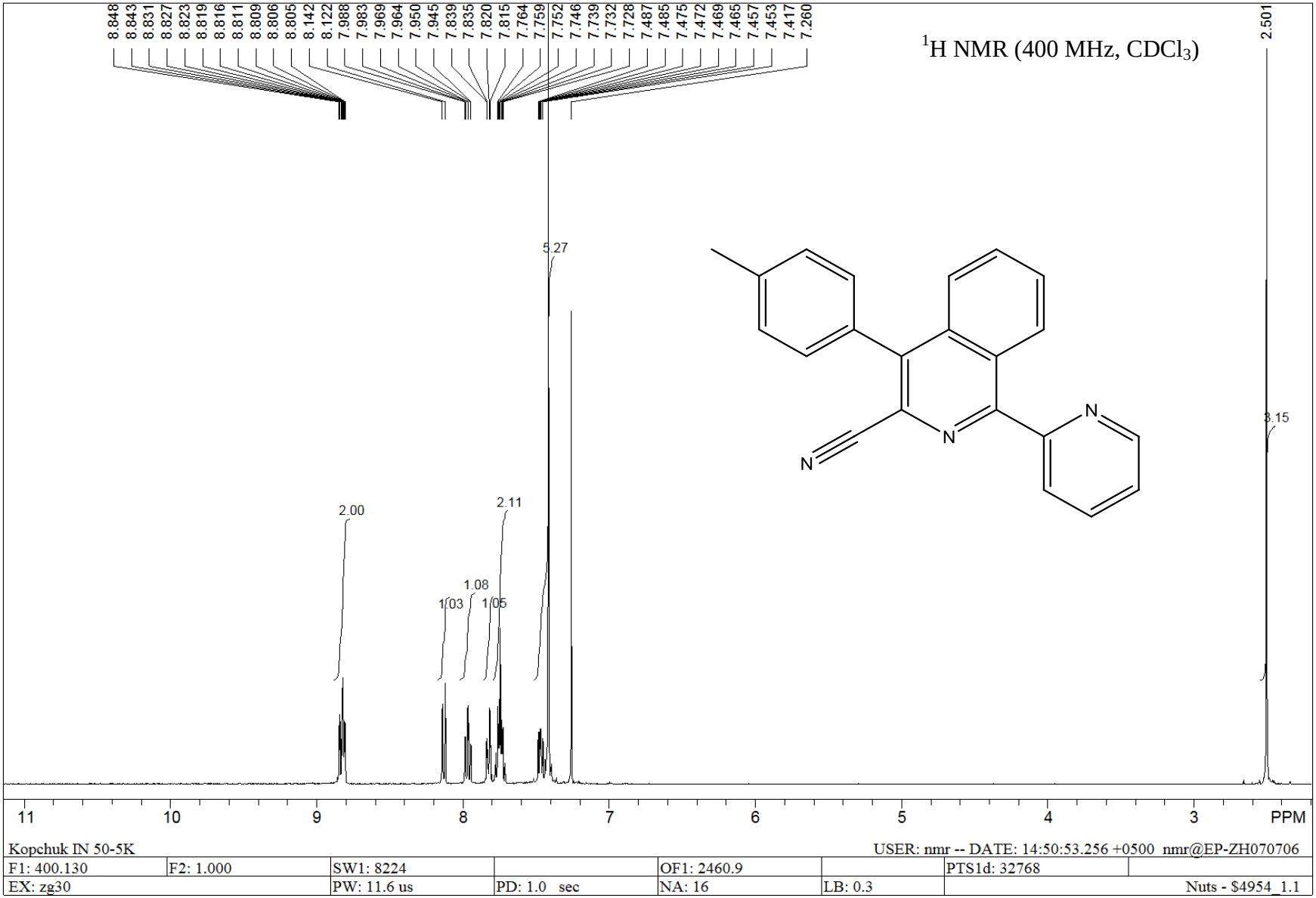

N
N
N

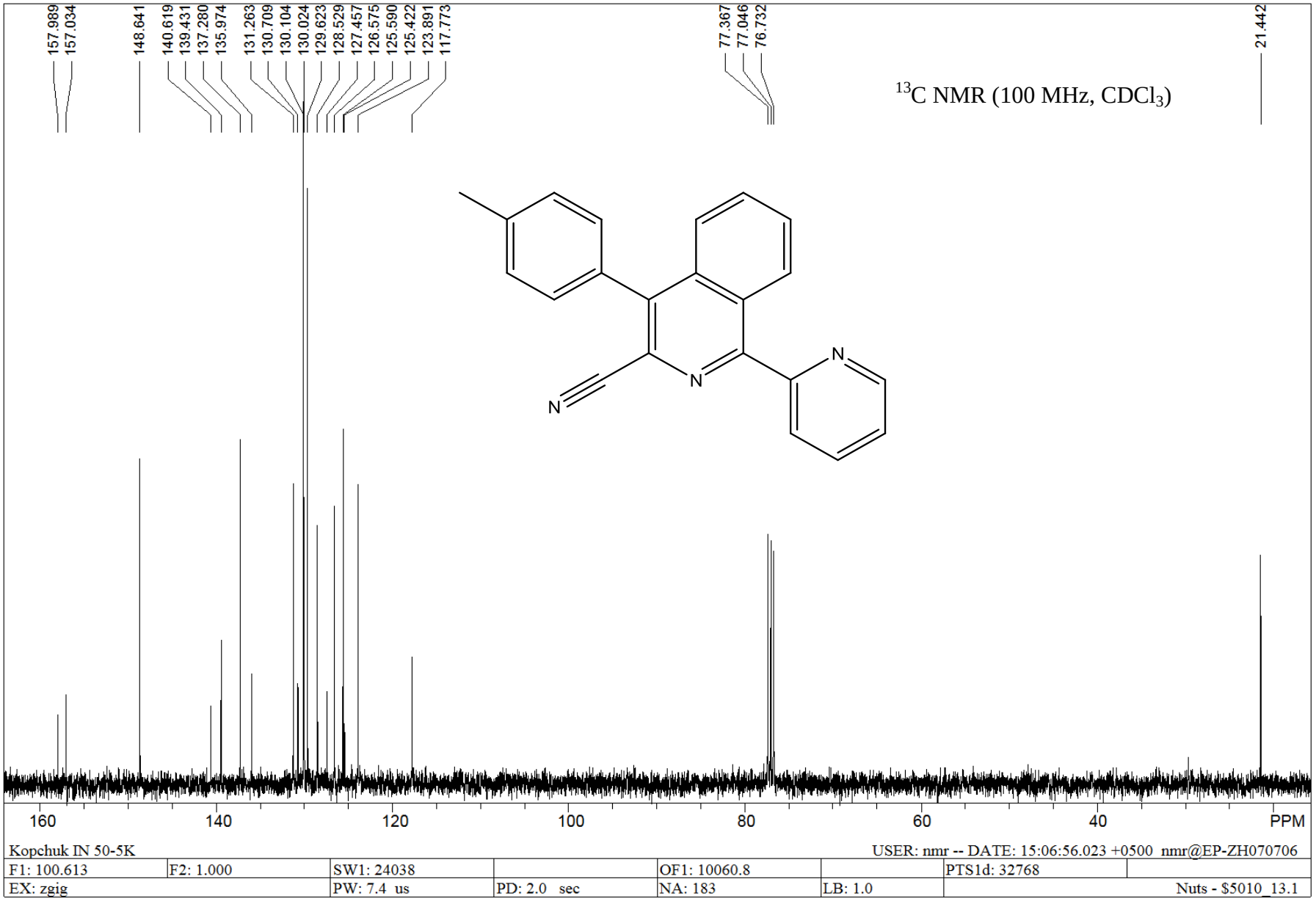

8.895
8.890
8.882
8.875
8.873
8.871
8.825
8.823
8.821
8.819
8.813
8.811
8.809
8.807
8.152
8.149
8.134
8.131
7.992
7.987
7.973
7.968
7.953
7.949
7.790
7.783
7.775
7.765
7.760
7.750
7.745
7.739
7.495
7.492
7.483
7.480
7.476
7.473
7.463
7.460
7.428
7.422
7.417
7.406
7.401
7.257
^{1}H NMR (400 MHz, $CDCl_3$)
Br
N
N
N
5.00
3.29
0.98
0.94
0.92
0.95
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
PPM
Kopchuk IN 67-1
USER: nmr -- DATE: 13:49:25.357 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.2
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $331 1.1

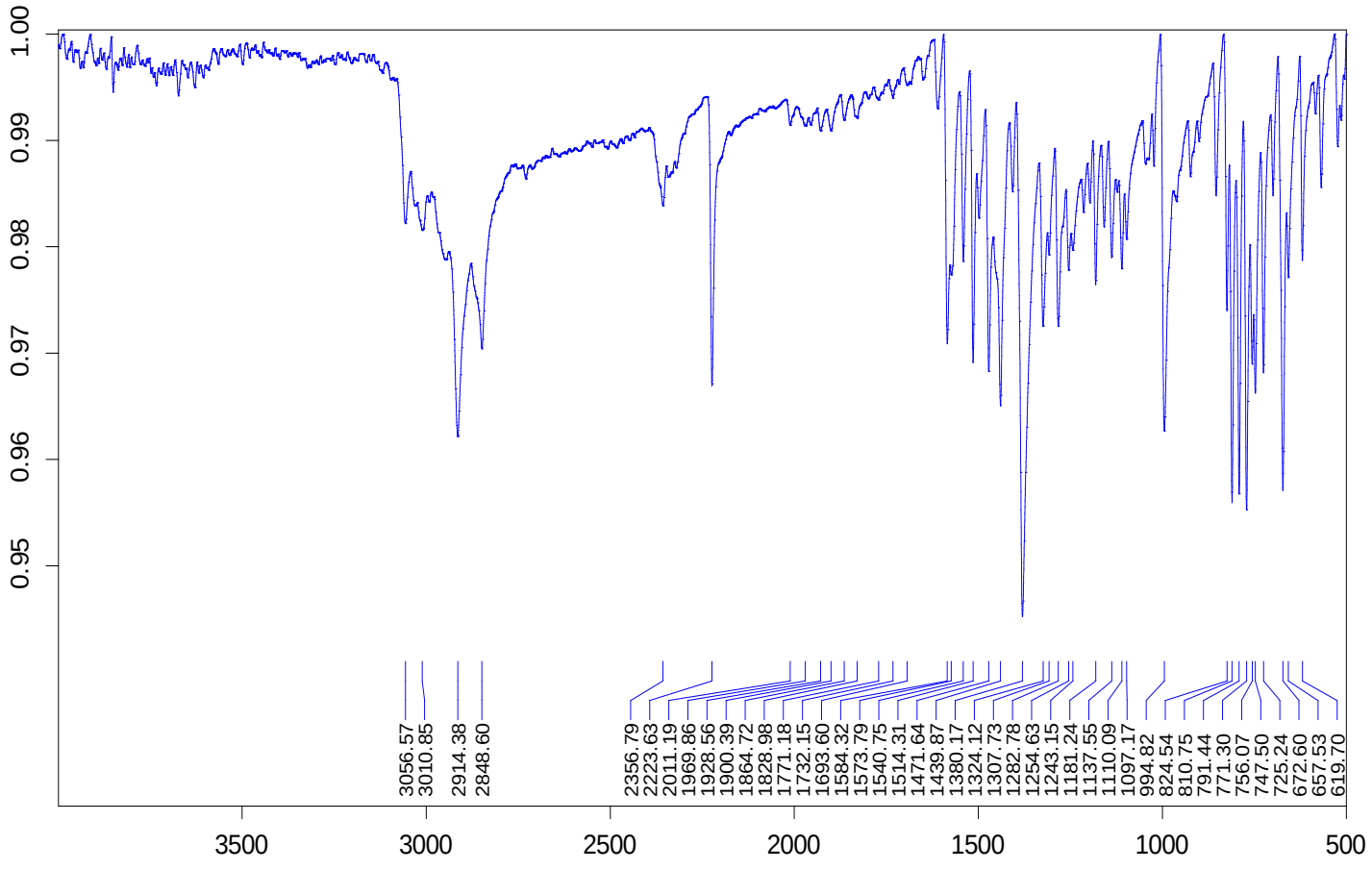

158.522
156.830
148.692
139.205
137.338
135.610
132.664
132.277
131.825
131.621
130.279
128.777
127.435
126.122
125.627
125.306
124.059
124.030
117.415
Br
N
N
N
^{13}C NMR (100 MHz, CDCl$_3$)
160
150
140
130
120
PPM
Kopchuk IN67
USER: nmr -- DATE: 16:13:04.576 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig
PW: 7.4 us
PD: 5.0 sec
NA: 324
LB: 1.0
Nuts - $491_13.1

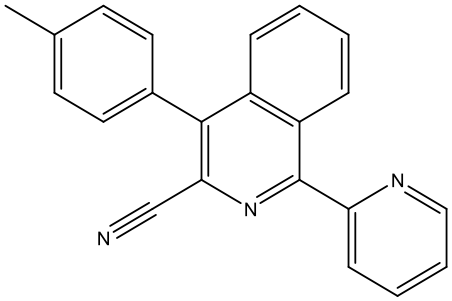

1.00
0.99
0.98
0.97
0.96
0.95
0.94
3059.91
2959.76
2916.05
2847.83
2224.27
1731.24
1585.51
1572.48
1504.42
1483.04
1474.36
1440.59
1399.30
1382.01
1283.65
1257.45
1243.89
1100.71
1068.75
1010.39
996.00
843.24
831.42
812.59
793.42
775.81
760.19
749.61
725.92
716.55
671.48
619.05
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

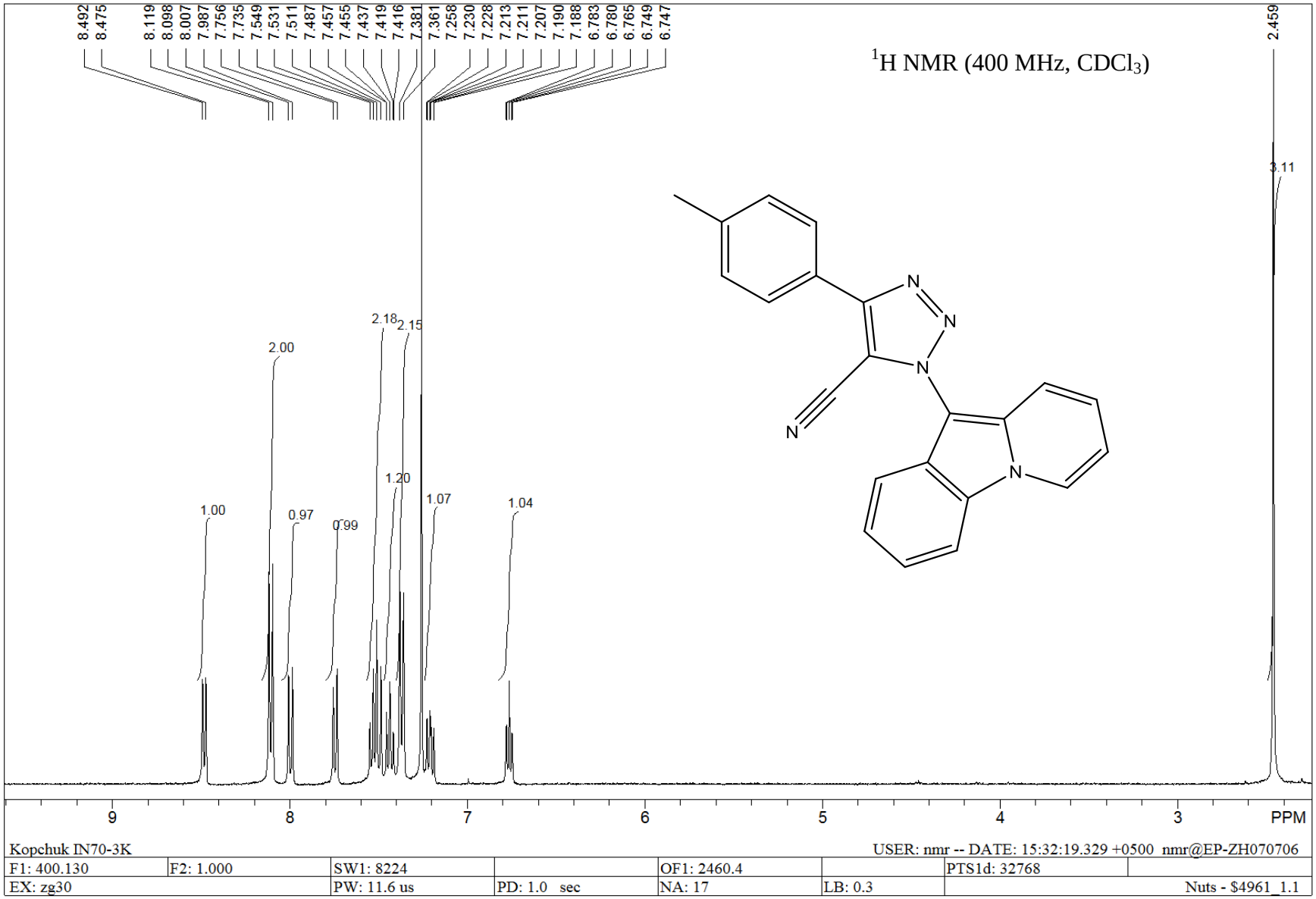

Br
N
N
N

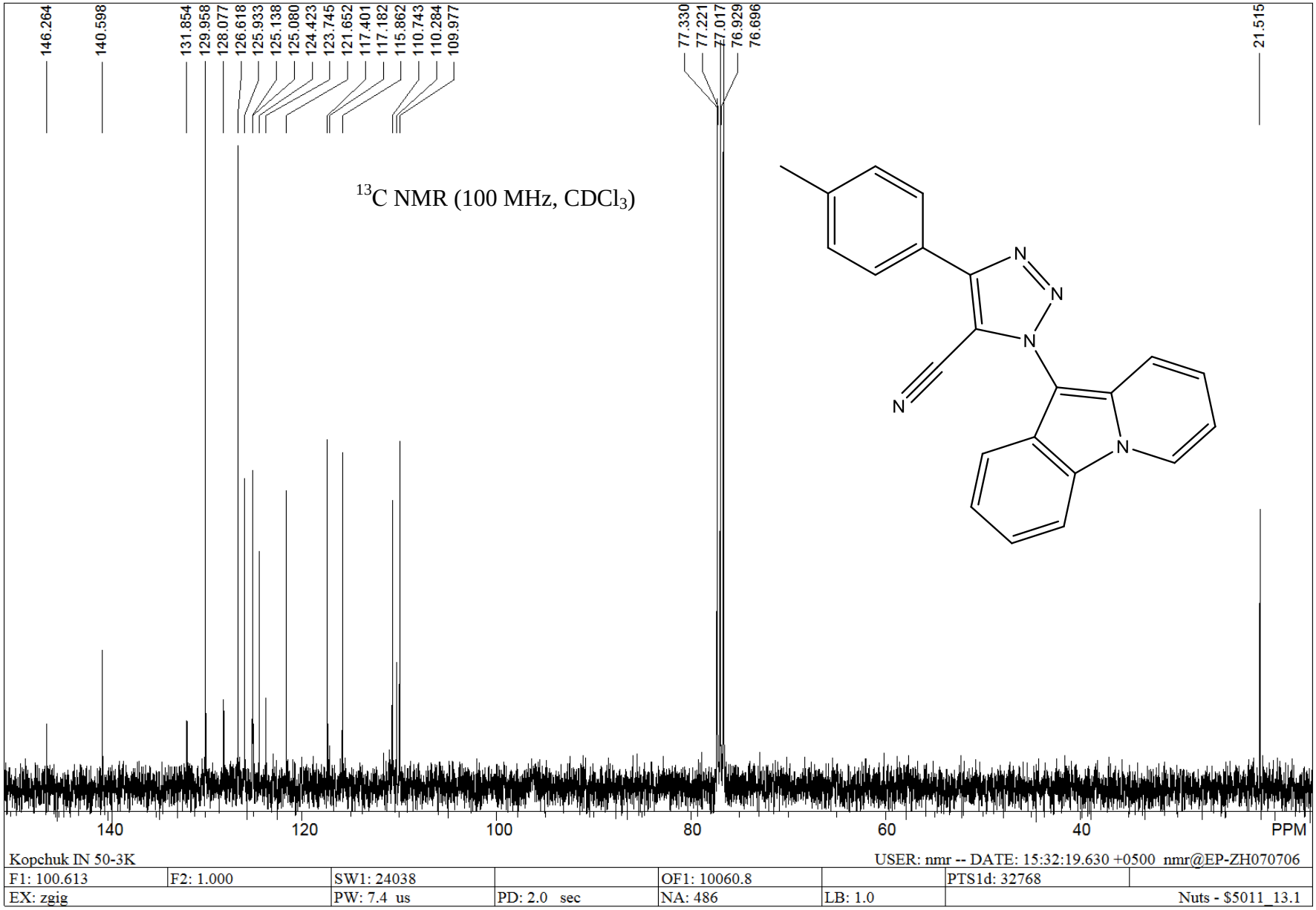

^{1}H NMR (400 MHz, $CDCl_3$)
8.848
8.843
8.831
8.827
8.823
8.819
8.816
8.811
8.809
8.806
8.805
8.142
8.122
7.988
7.983
7.969
7.964
7.950
7.945
7.839
7.835
7.820
7.815
7.764
7.759
7.752
7.746
7.739
7.732
7.728
7.487
7.485
7.475
7.472
7.469
7.465
7.457
7.453
7.417
7.260
2.501
5.27
3.15
2.00
2.11
1.08
1.03
1.05
N
N
N
11
10
9
8
7
6
5
4
3
PPM
Kopchuk IN 50-5K
USER: nmr -- DATE: 14:50:53.256 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $4954_1.1

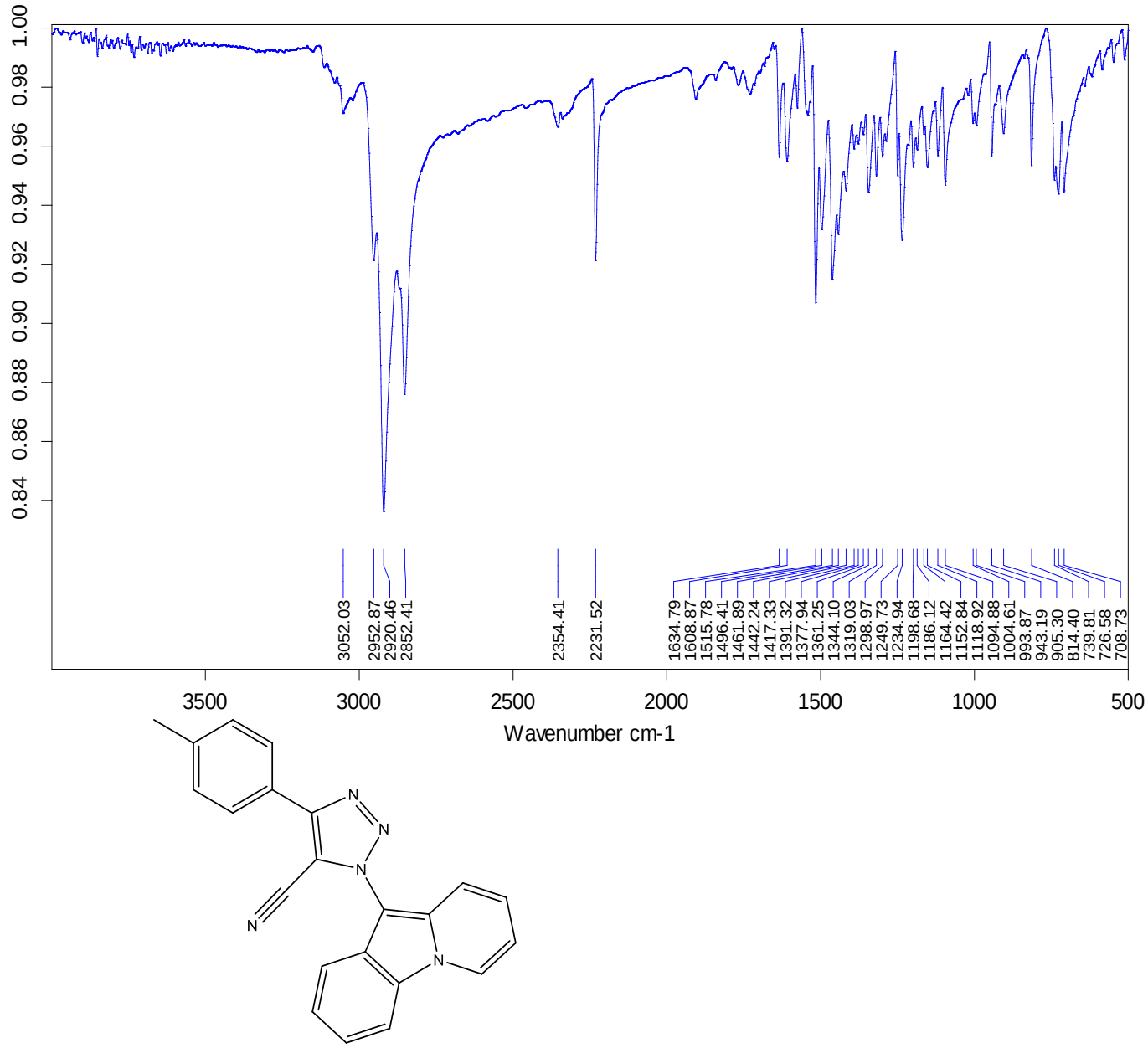

157.989
157.034
148.641
140.619
139.431
137.280
135.974
131.263
130.709
130.104
130.024
129.623
128.529
127.457
126.575
125.590
125.422
123.891
117.773
77.367
77.046
76.732
21.442
^{13}C NMR (100 MHz, $CDCl_3$)
N
N
N
160
140
120
100
80
60
40
PPM
Kopchuk IN 50-5K
USER: nmr -- DATE: 15:06:56.023 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig
PW: 7.4 us
PD: 2.0 sec
NA: 183
LB: 1.0
Nuts - $5010_13.1

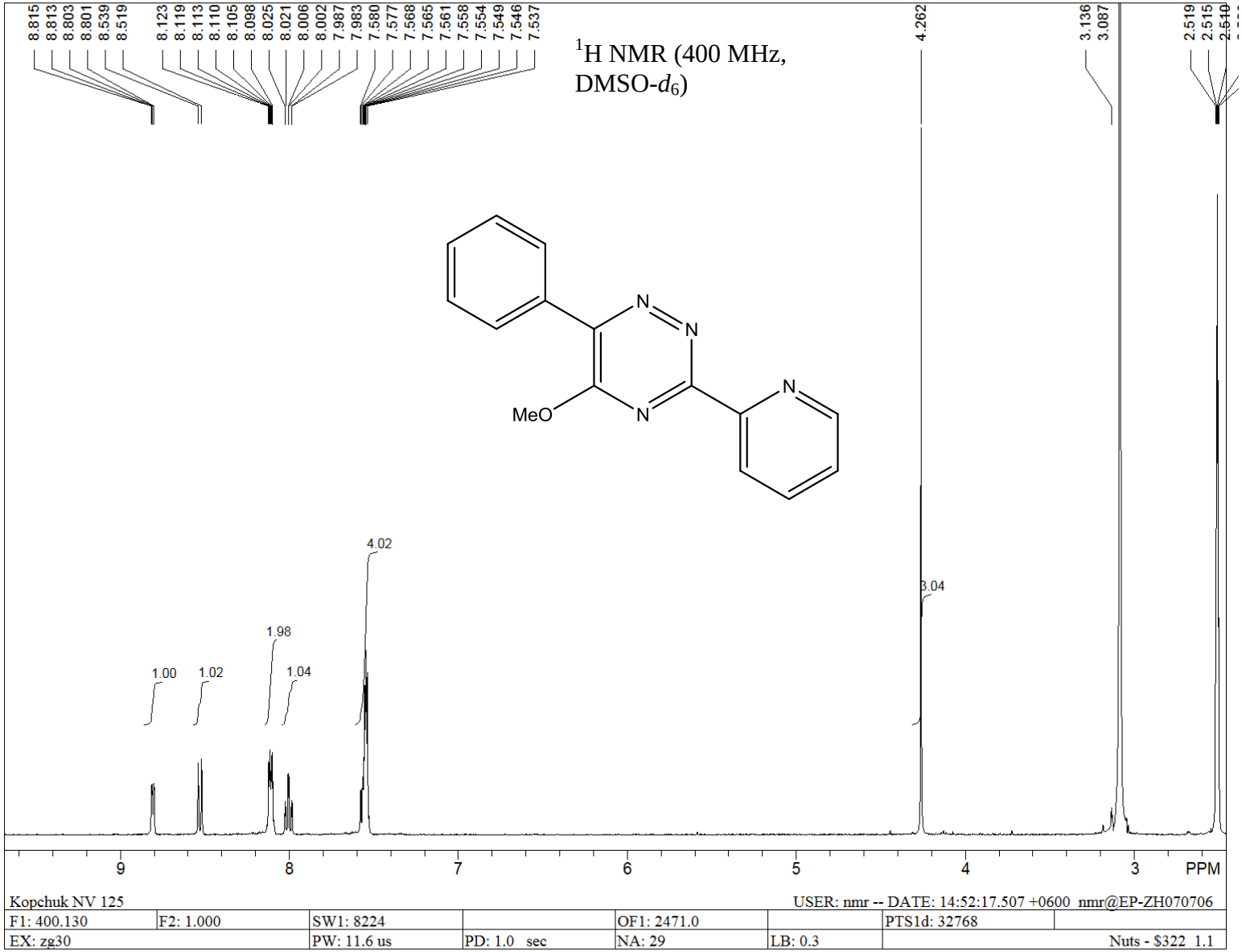

1.00
0.99
0.98
0.97
0.96
0.95
3056.57
3010.85
2914.38
2848.60
2356.79
2223.63
2011.19
1969.86
1928.56
1900.39
1864.72
1828.98
1771.18
1732.15
1693.60
1584.32
1573.79
1540.75
1514.31
1471.64
1439.87
1380.17
1324.12
1307.73
1282.78
1254.63
1243.15
1181.24
1137.55
1110.09
1097.17
994.82
824.54
810.75
791.44
771.30
756.07
747.50
725.24
672.60
657.53
619.70
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

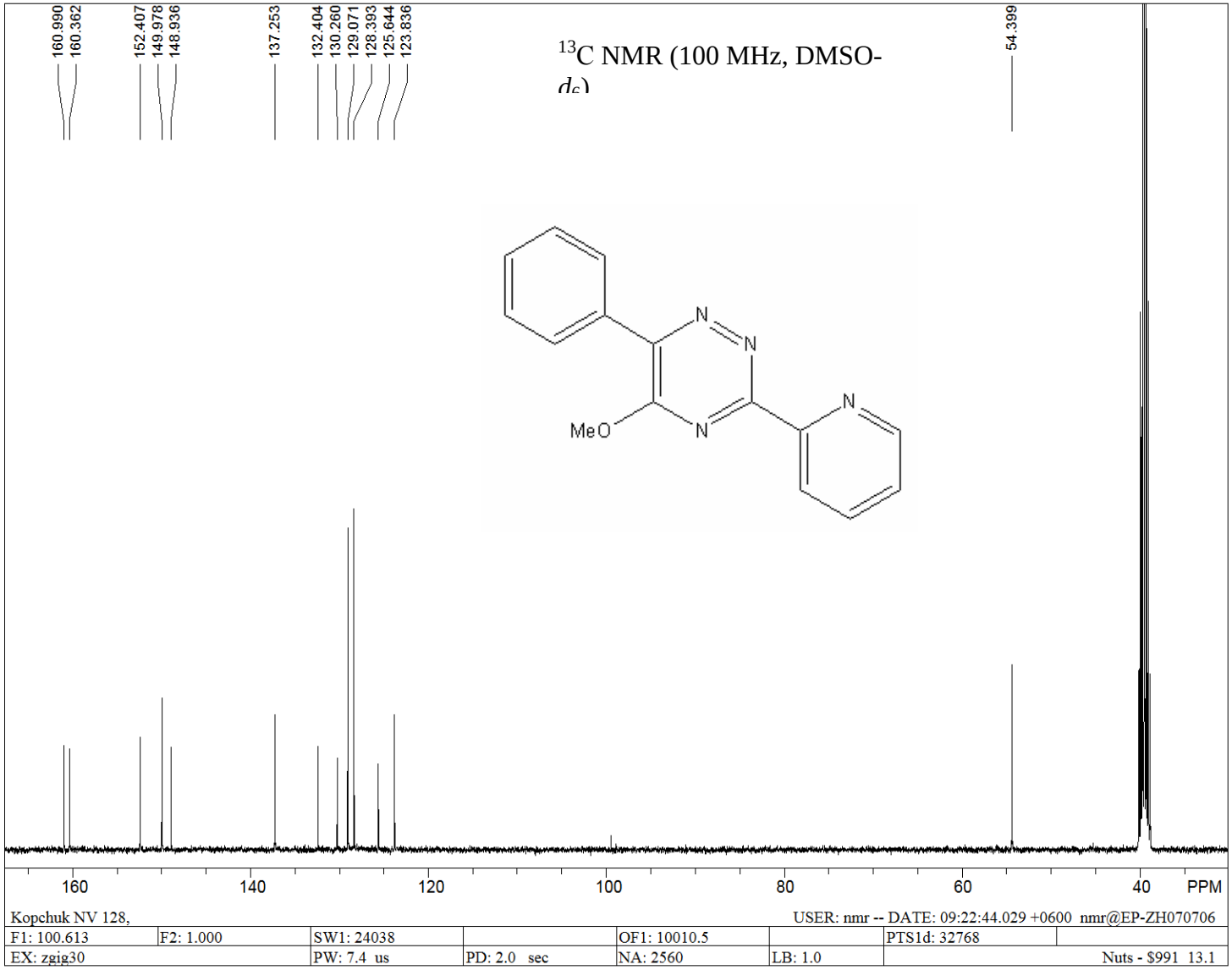

N
N
N

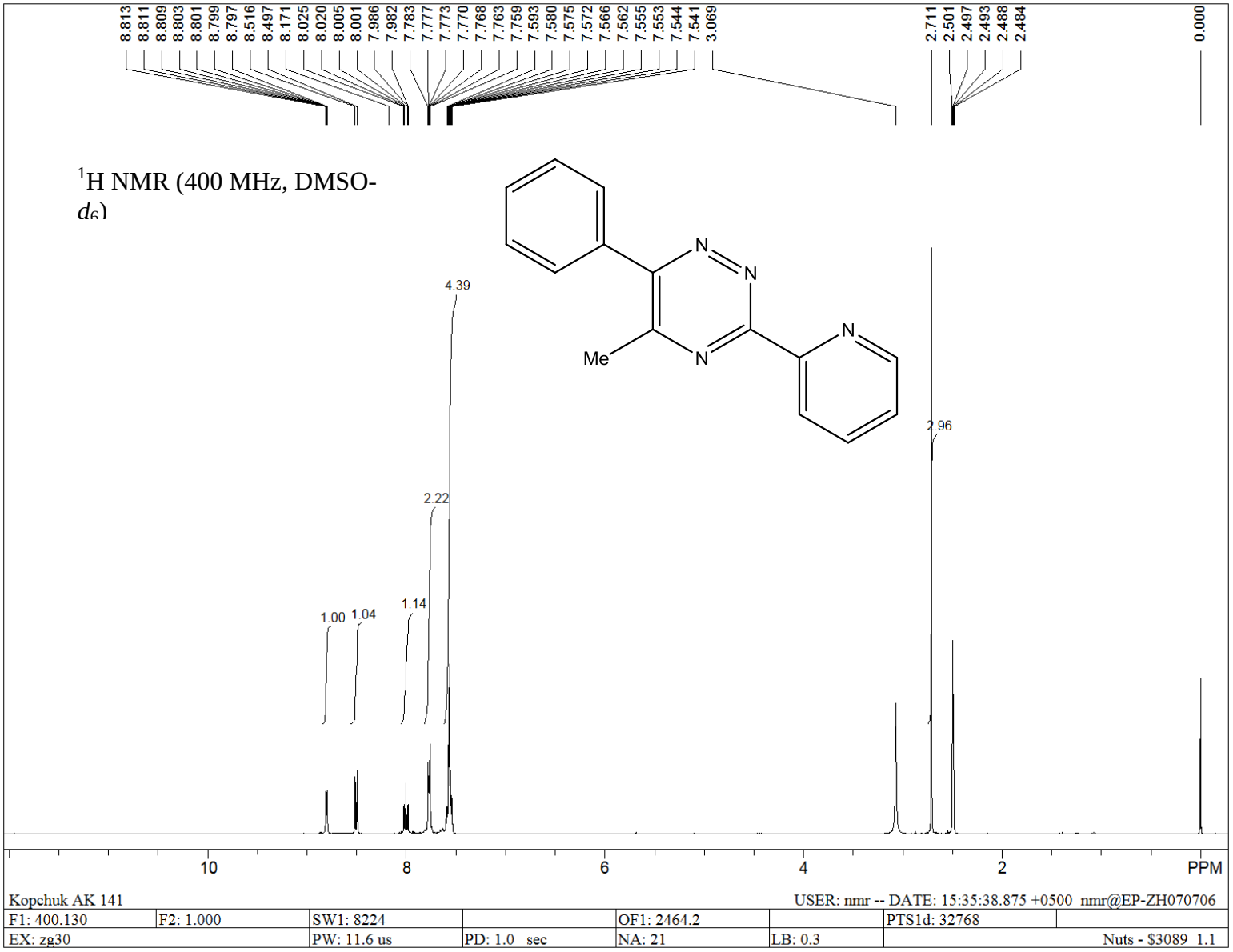

8.492
8.475
8.119
8.098
8.007
7.987
7.756
7.735
7.549
7.531
7.511
7.487
7.457
7.455
7.437
7.419
7.416
7.381
7.361
7.258
7.230
7.228
7.213
7.211
7.207
7.190
7.188
6.783
6.780
6.765
6.749
6.747
2.459
^{1}H NMR (400 MHz, $CDCl_3$)
3.11
2.18
2.15
2.00
1.20
1.07
1.04
1.00
0.97
0.99
N
N
N
N
9
8
7
6
5
4
3
PPM
Kopchuk IN70-3K
USER: nmr -- DATE: 15:32:19.329 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 17
LB: 0.3
Nuts - $4961_1.1

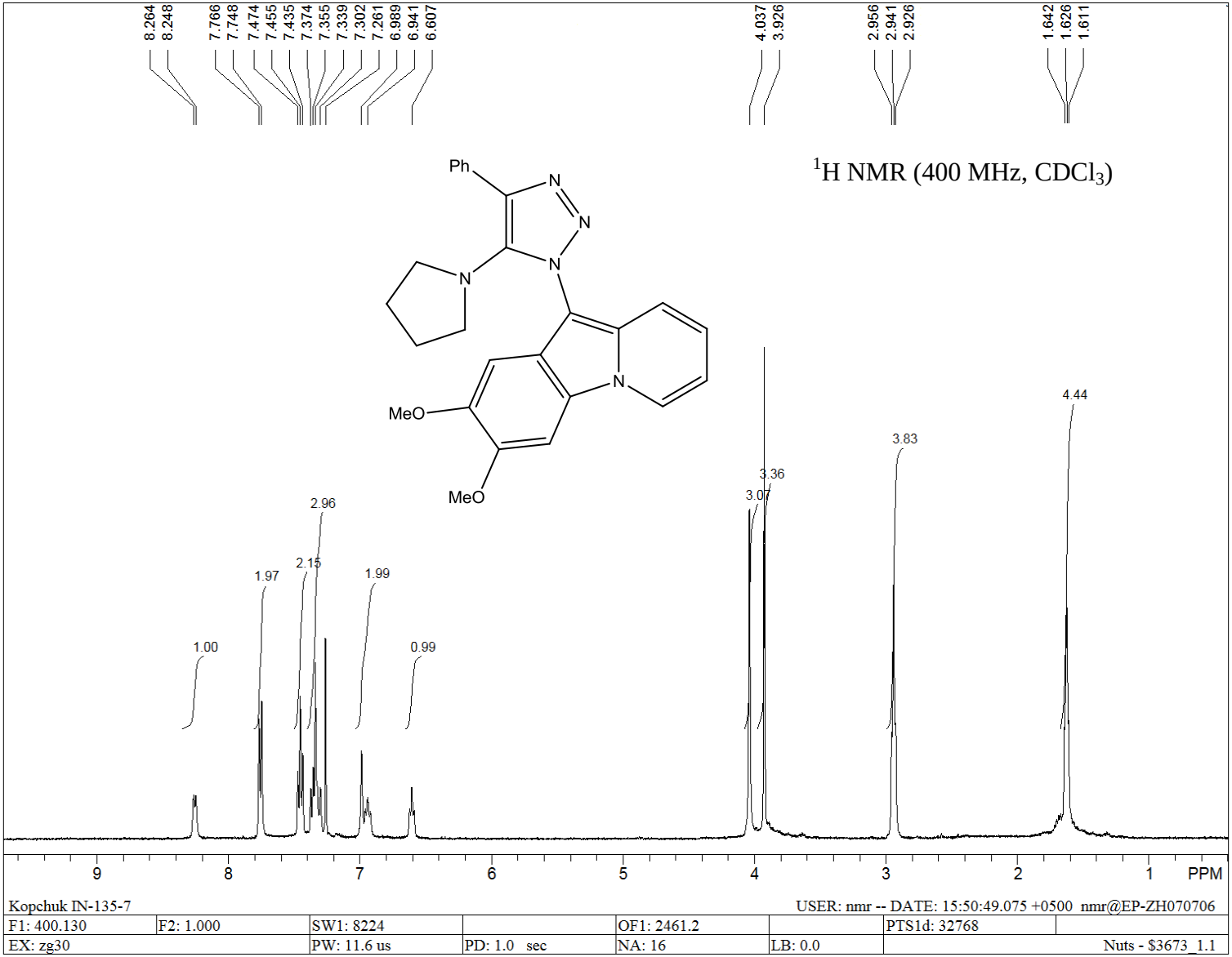

146.264
140.598
131.854
129.958
128.077
126.618
125.933
125.138
125.080
124.423
123.745
121.652
117.401
117.182
115.862
110.743
110.284
109.977
77.330
77.221
77.017
76.929
76.696
21.515
^{13}C NMR (100 MHz, $CDCl_3$)
N
N
N
N
N
140
120
100
80
60
40
PPM
Kopchuk IN 50-3K
USER: nmr -- DATE: 15:32:19.630 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig
PW: 7.4 us
PD: 2.0 sec
NA: 486
LB: 1.0
Nuts - $5011_13.1

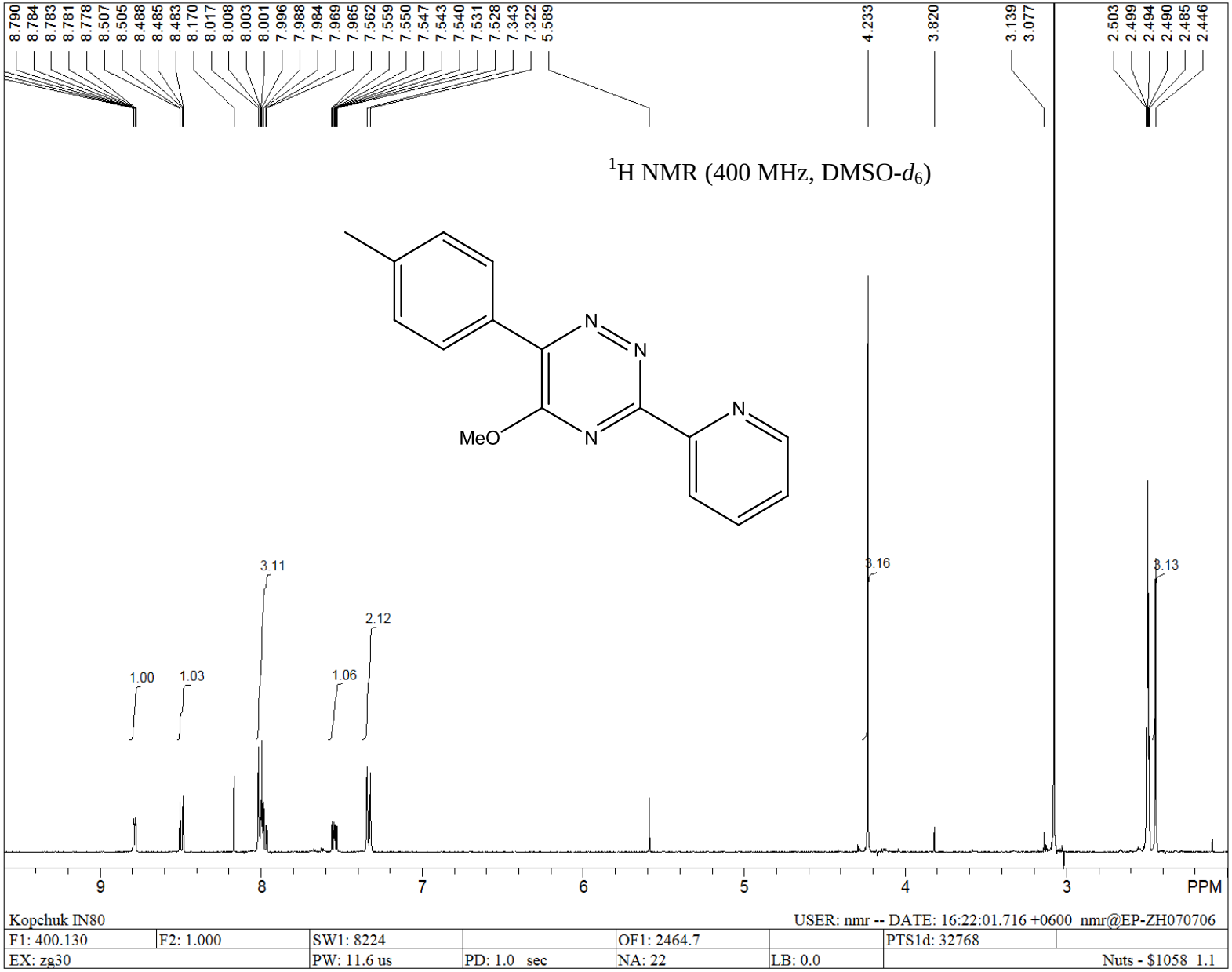

1.00
0.98
0.96
0.94
0.92
0.90
0.88
0.86
0.84
3052.03
2952.87
2920.46
2852.41
2354.41
2231.52
1634.79
1608.87
1515.78
1496.41
1461.89
1442.24
1417.33
1391.32
1377.94
1361.25
1344.10
1319.03
1298.97
1249.73
1234.94
1198.68
1186.12
1164.42
1152.84
1118.92
1094.88
1004.61
993.87
943.19
905.30
814.40
739.81
726.58
708.73
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
N
N
N
N
N

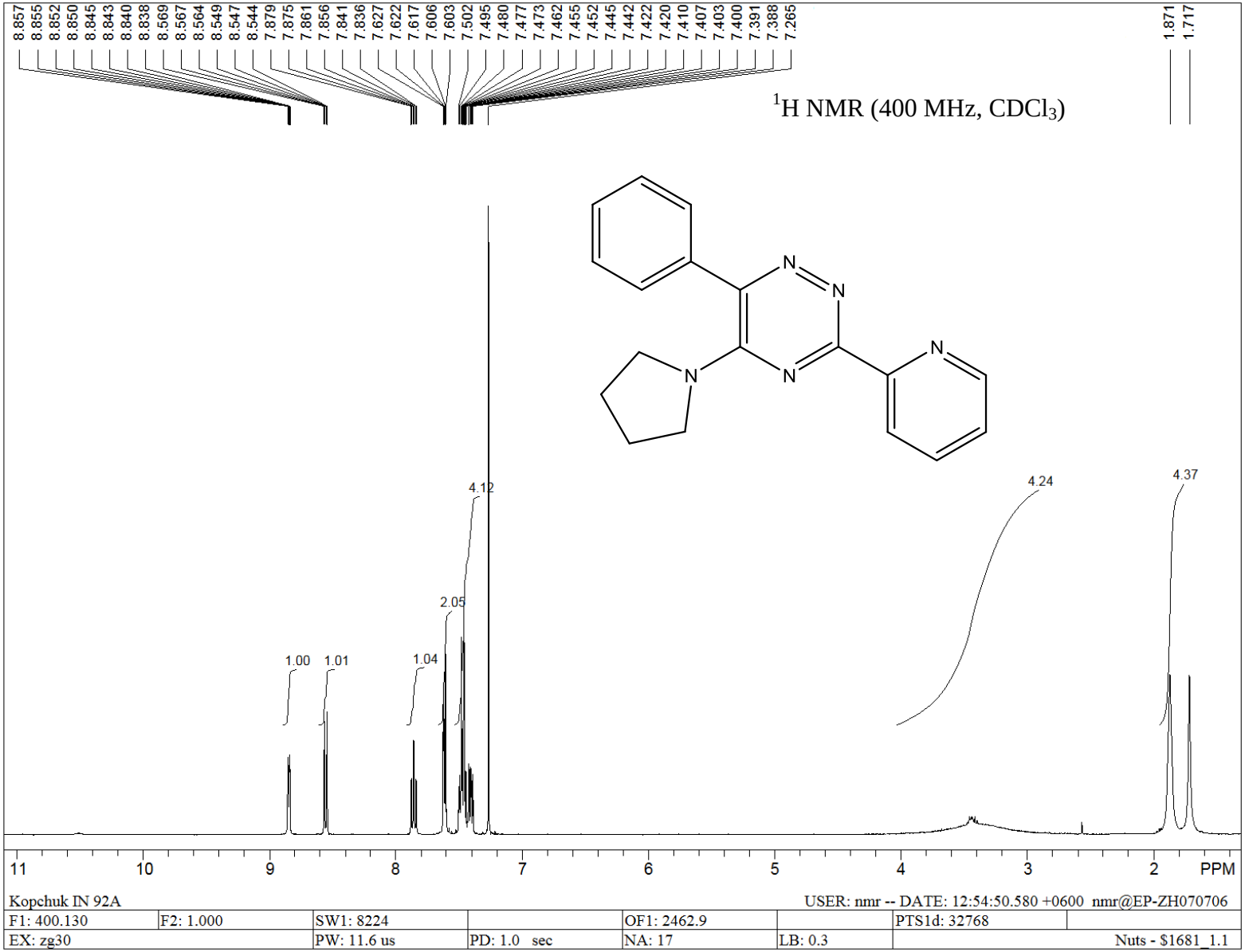

8.815
8.813
8.803
8.801
8.539
8.519
8.123
8.119
8.113
8.110
8.105
8.098
8.025
8.021
8.006
8.002
7.987
7.983
7.580
7.577
7.568
7.565
7.561
7.558
7.554
7.549
7.546
7.537
4.262
3.136
3.087
2.519
2.515
2.510
^{1}H NMR (400 MHz, DMSO-d_6)
N
N
N
N
MeO
1.00
1.02
1.98
1.04
4.02
3.04
9
8
7
6
5
4
3
PPM
Kopchuk NV 125
USER: nmr -- DATE: 14:52:17.507 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 29
LB: 0.3
Nuts - $322 1.1

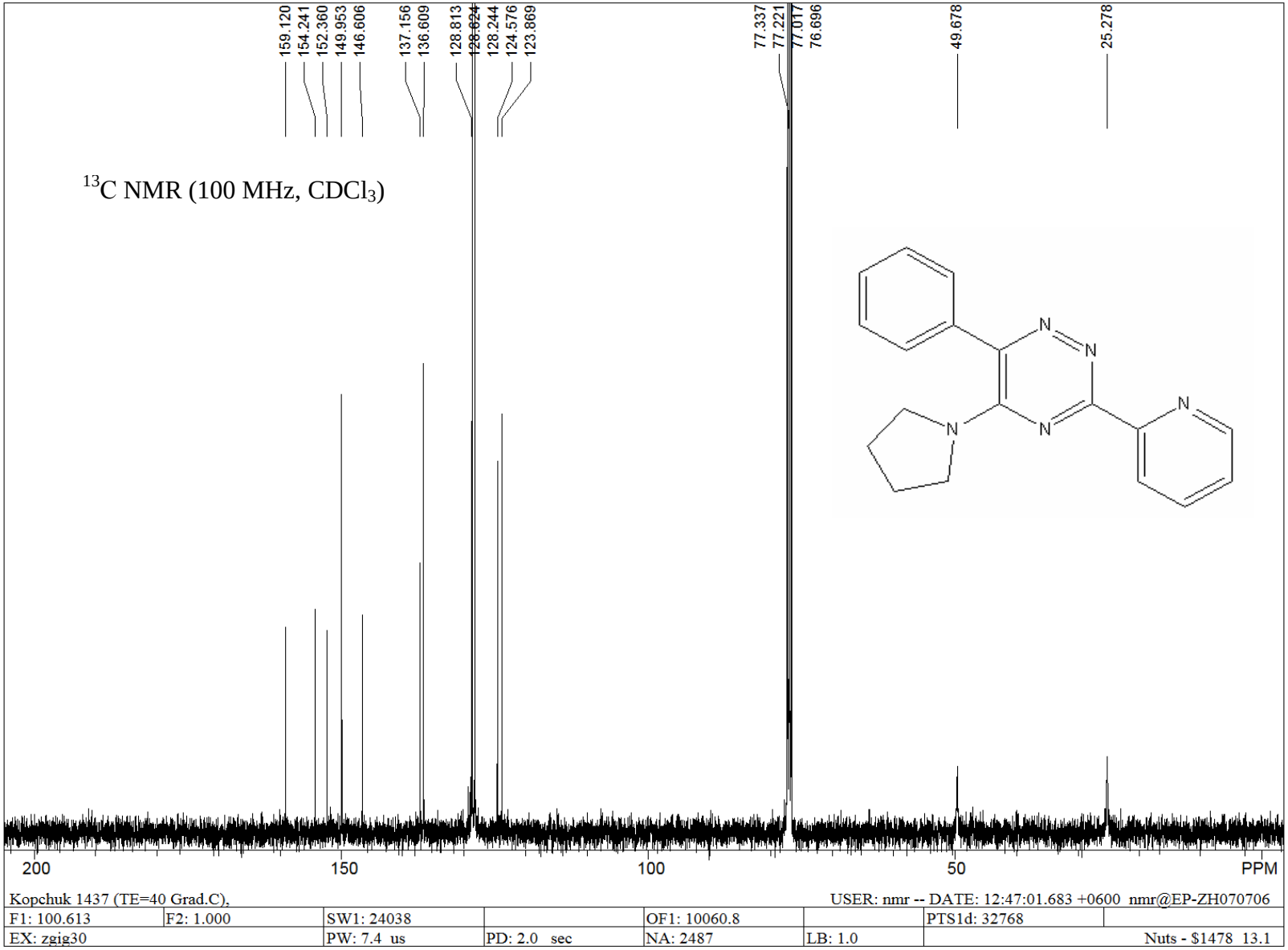

160.990
160.362
152.407
149.978
148.936
137.253
132.404
130.260
129.071
128.393
125.644
123.836
54.399
^{13}C NMR (100 MHz, DMSO-d_6)
N
N
N
MeO
N
160
140
120
100
80
60
40
PPM
Kopchuk NV 128,
USER: nmr -- DATE: 09:22:44.029 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10010.5
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 2560
LB: 1.0
Nuts - $991 13.1

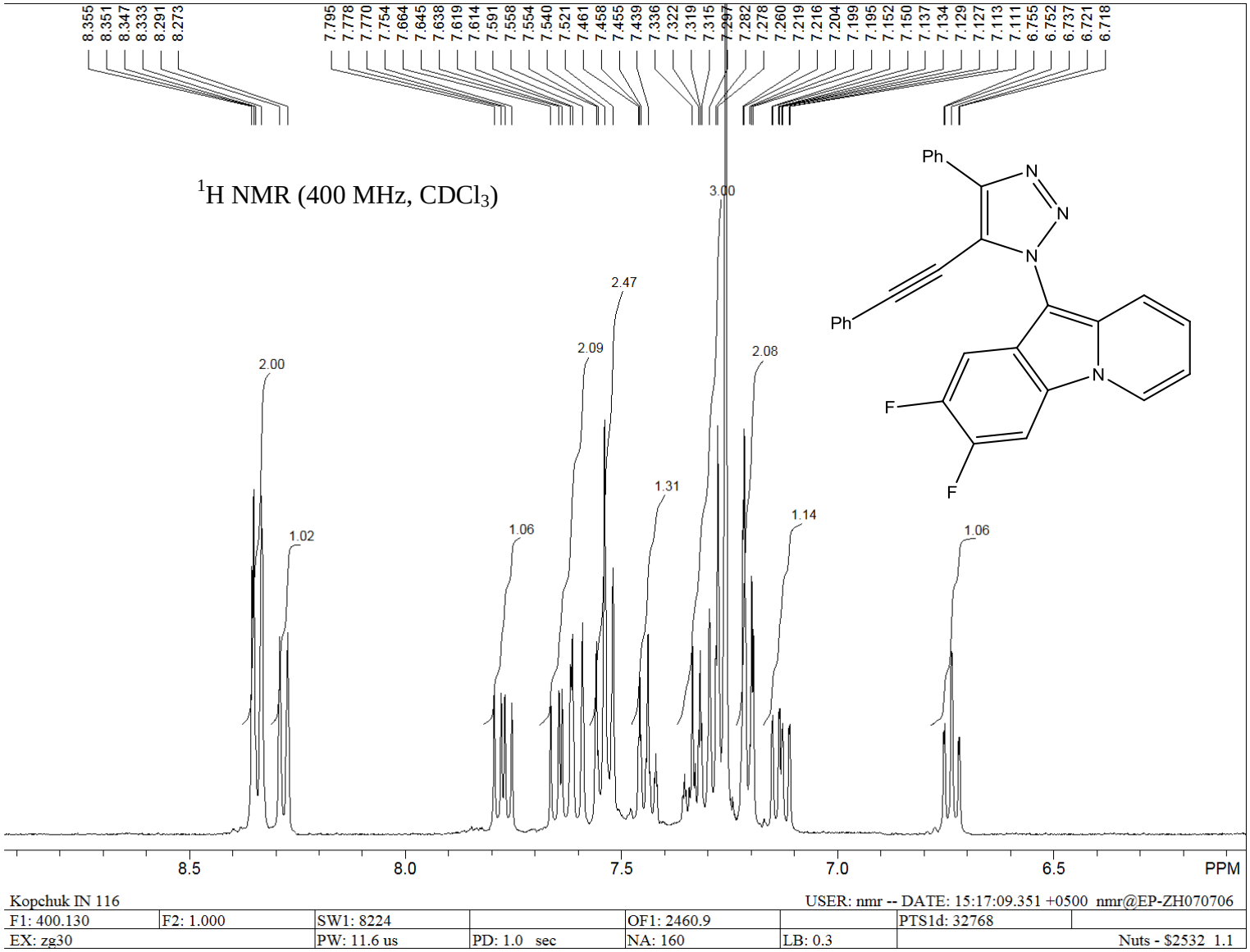

8.813
8.811
8.809
8.803
8.801
8.799
8.797
8.516
8.497
8.171
8.025
8.020
8.005
8.001
7.986
7.982
7.783
7.777
7.773
7.770
7.768
7.763
7.759
7.593
7.580
7.575
7.572
7.566
7.562
7.555
7.553
7.544
7.541
3.069
2.711
2.501
2.497
2.493
2.488
2.484
0.000
1H NMR (400 MHz, DMSO-d6)
N
N
N
Me
4.39
2.96
2.22
1.14
1.00
1.04
10
8
6
4
2
PPM
Kopchuk AK 141
USER: nmr -- DATE: 15:35:38.875 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2464.2
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 21
LB: 0.3
Nuts - $3089 1.1

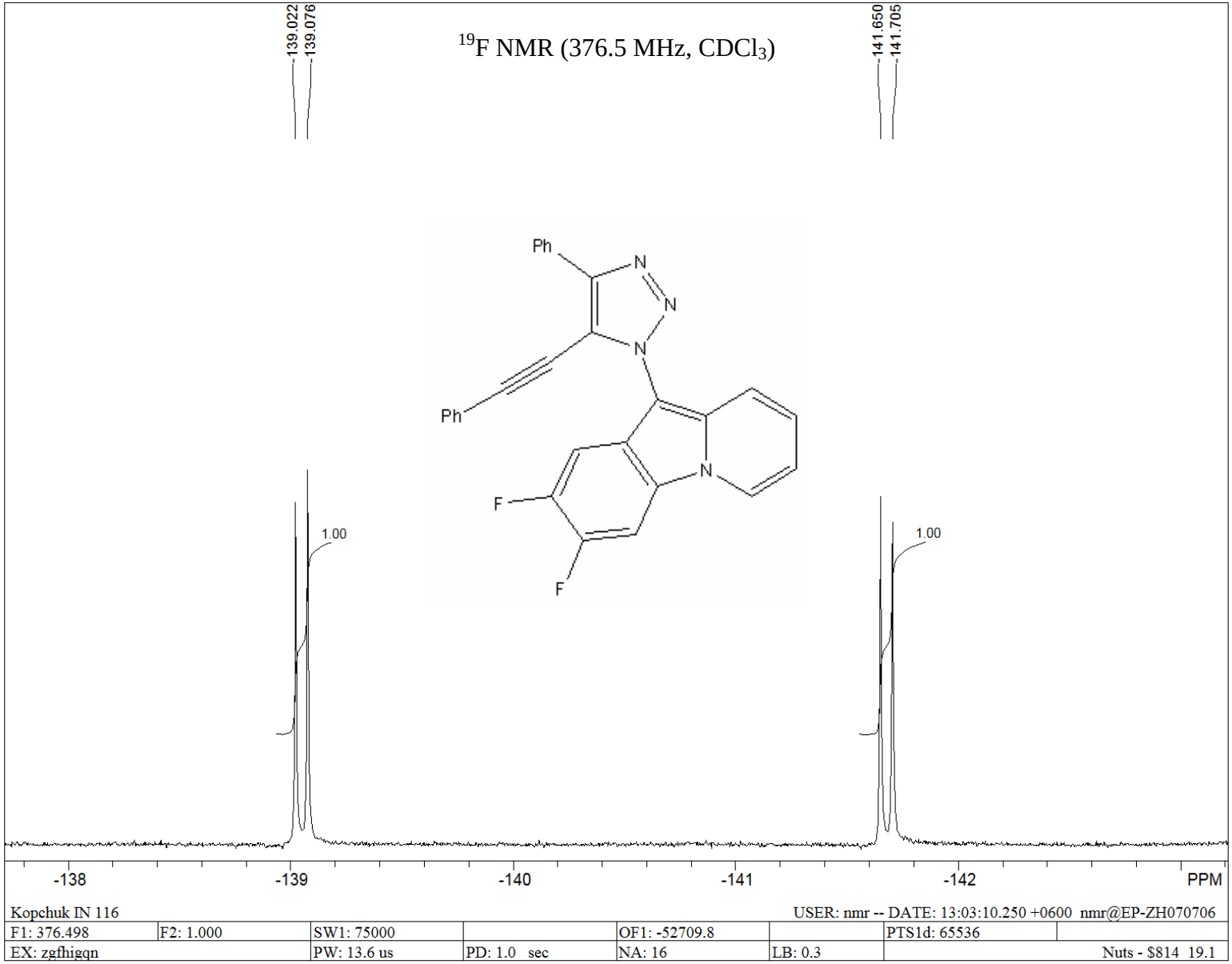

8.264
8.248
7.766
7.748
7.474
7.455
7.435
7.374
7.355
7.339
7.302
7.261
6.989
6.941
6.607
4.037
3.926
2.956
2.941
2.926
1.642
1.626
1.611
^{1}H NMR (400 MHz, $CDCl_3$)
Ph
N
N
N
N
MeO
MeO
4.44
3.83
3.36
3.07
2.96
2.15
1.99
1.97
1.00
0.99
9
8
7
6
5
4
3
2
1
PPM
Kopchuk IN-135-7
USER: nmr -- DATE: 15:50:49.075 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.2
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $3673_1.1

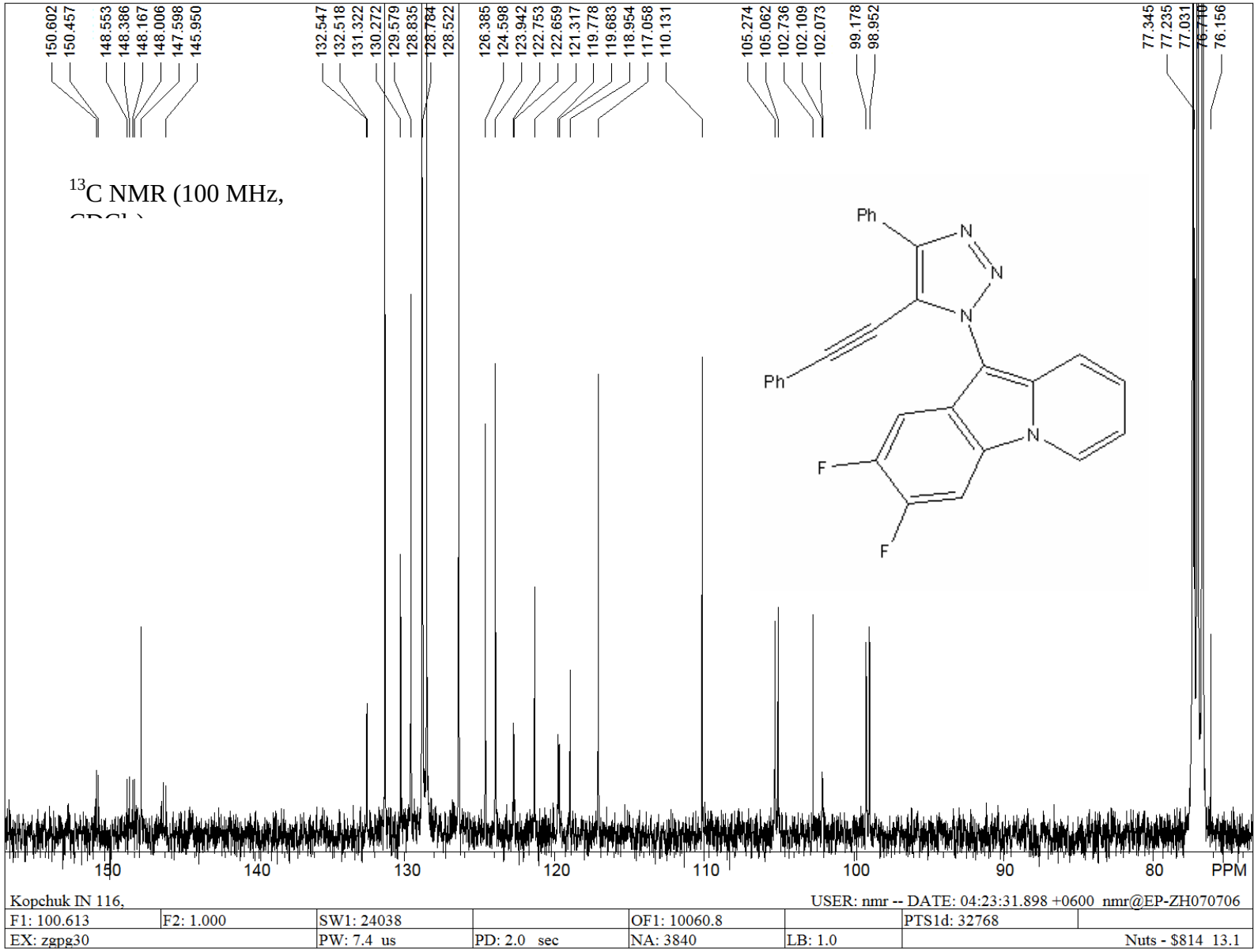

8.790
8.784
8.783
8.781
8.778
8.507
8.505
8.488
8.485
8.483
8.170
8.017
8.008
8.003
8.001
7.996
7.988
7.984
7.969
7.965
7.562
7.559
7.550
7.547
7.543
7.540
7.531
7.528
7.343
7.322
5.589
4.233
3.820
3.139
3.077
2.503
2.499
2.494
2.490
2.485
2.446
1H NMR (400 MHz, DMSO-d6)
MeO
N
N
N
N
3.11
3.16
3.13
2.12
1.00
1.03
1.06
9
8
7
6
5
4
3
PPM
Kopchuk IN80
USER: nmr -- DATE: 16:22:01.716 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2464.7
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 22
LB: 0.0
Nuts - $1058 1.1

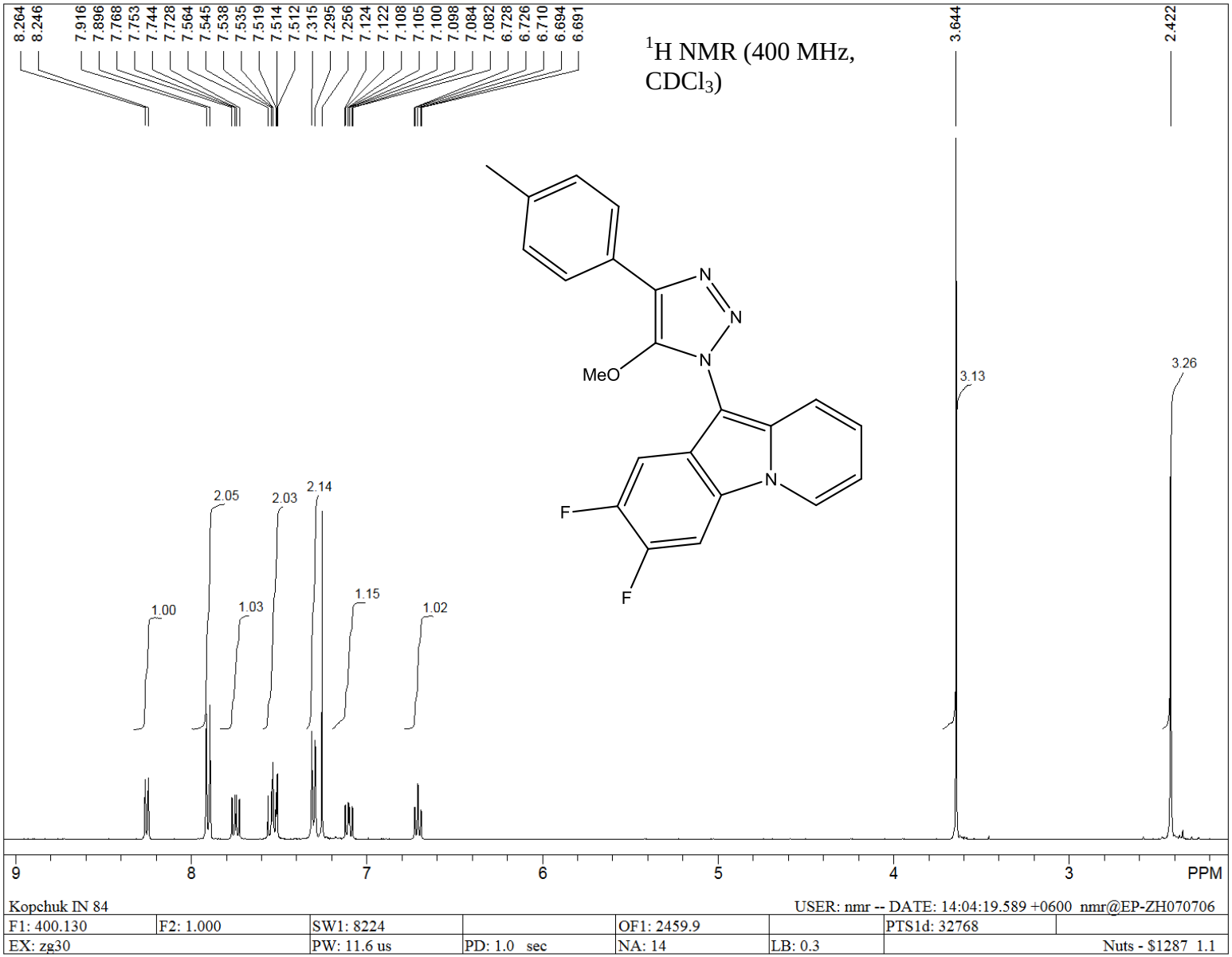

8.857 8.855 8.852 8.850 8.845 8.843 8.840 8.838 8.569 8.567 8.564 8.549 8.547 8.544 8.879 7.875 7.861 7.856 7.841 7.836 7.627 7.622 7.617 7.606 7.603 7.502 7.495 7.480 7.477 7.473 7.462 7.455 7.452 7.445 7.442 7.422 7.420 7.410 7.407 7.403 7.400 7.391 7.388 7.265
1.871 1.717
^{1}H NMR (400 MHz, $CDCl_3$)
N N N N N
4.12
4.24
4.37
2.05
1.00 1.01 1.04
11 10 9 8 7 6 5 4 3 2 PPM
Kopchuk IN 92A
USER: nmr -- DATE: 12:54:50.580 +0600 nmr@EP-ZH070706
F1: 400.130 F2: 1.000 SW1: 8224 OF1: 2462.9 PTS1d: 32768
EX: zg30 PW: 11.6 us PD: 1.0 sec NA: 17 LB: 0.3 Nuts - $1681_1.1

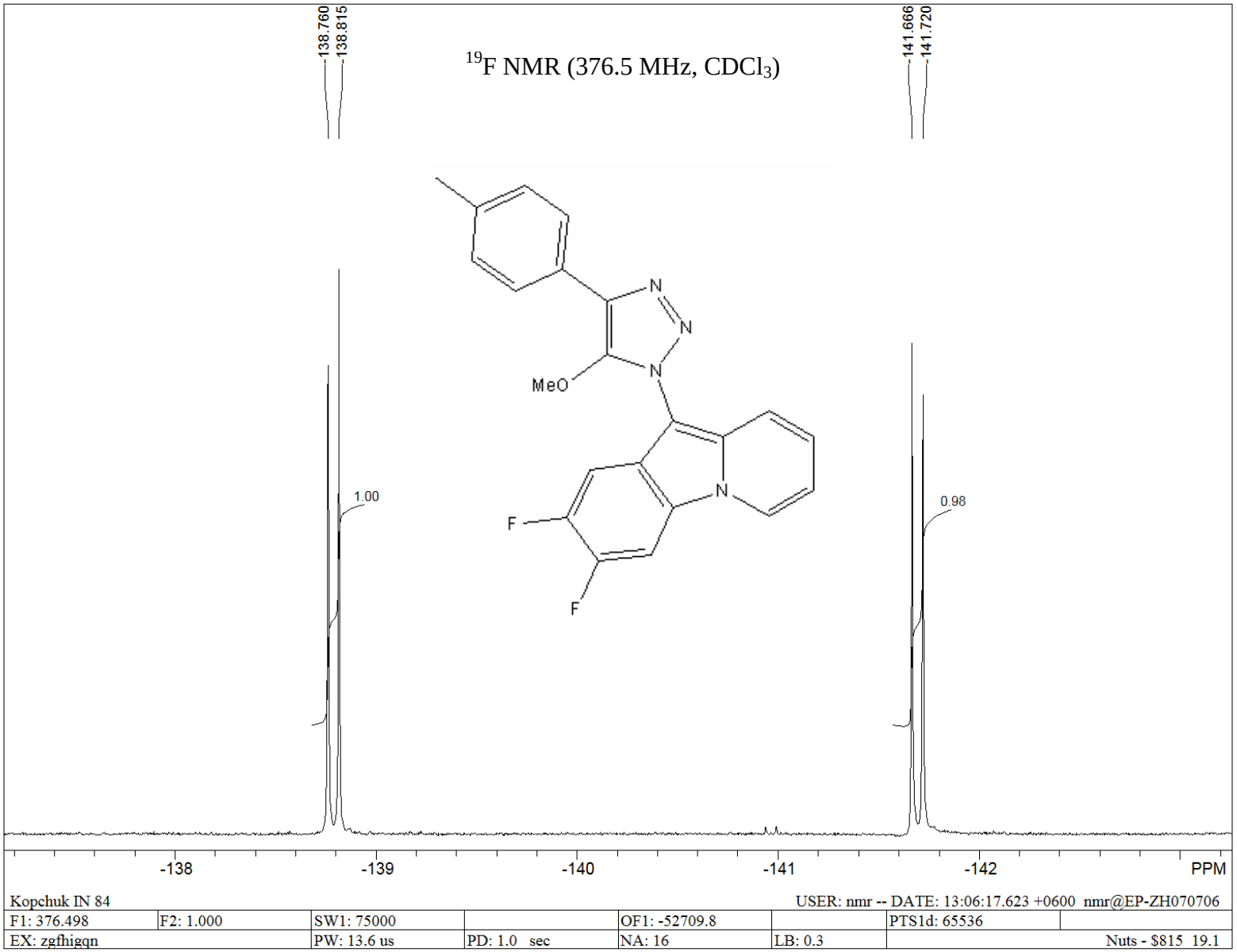

159.120
154.241
152.360
149.953
146.606
137.156
136.609
128.813
128.624
128.244
124.576
123.869
77.337
77.221
77.017
76.696
49.678
25.278
^{13}C NMR (100 MHz, $CDCl_3$)
N
N
N
N
200
150
100
50
PPM
Kopchuk 1437 (TE=40 Grad.C),
USER: nmr -- DATE: 12:47:01.683 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 2487
LB: 1.0
Nuts - $1478 13.1

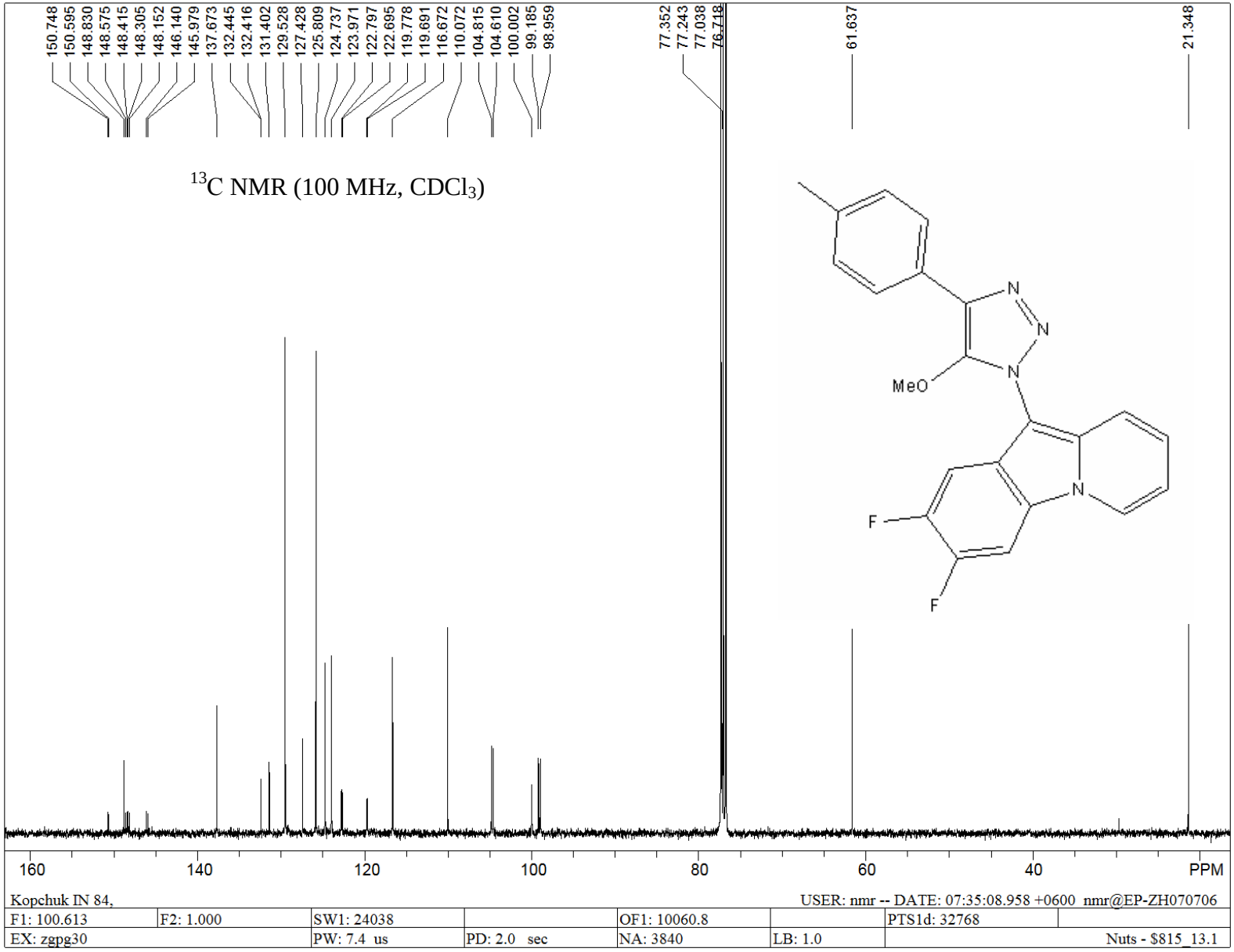

8.355
8.351
8.347
8.333
8.291
8.273
7.795
7.778
7.770
7.754
7.664
7.645
7.638
7.619
7.614
7.591
7.558
7.554
7.540
7.521
7.461
7.458
7.455
7.439
7.336
7.322
7.319
7.315
7.297
7.282
7.278
7.260
7.219
7.216
7.204
7.199
7.195
7.152
7.150
7.137
7.134
7.129
7.127
7.113
7.111
6.755
6.752
6.737
6.721
6.718
^{1}H NMR (400 MHz, $CDCl_3$)
3.00
2.47
2.09
2.08
2.00
1.31
1.14
1.06
1.06
1.02
Ph
N
N
N
Ph
N
F
F
8.5
8.0
7.5
7.0
6.5
PPM
Kopchuk IN 116
USER: nmr -- DATE: 15:17:09.351 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 160
LB: 0.3
Nuts - $2532 1.1

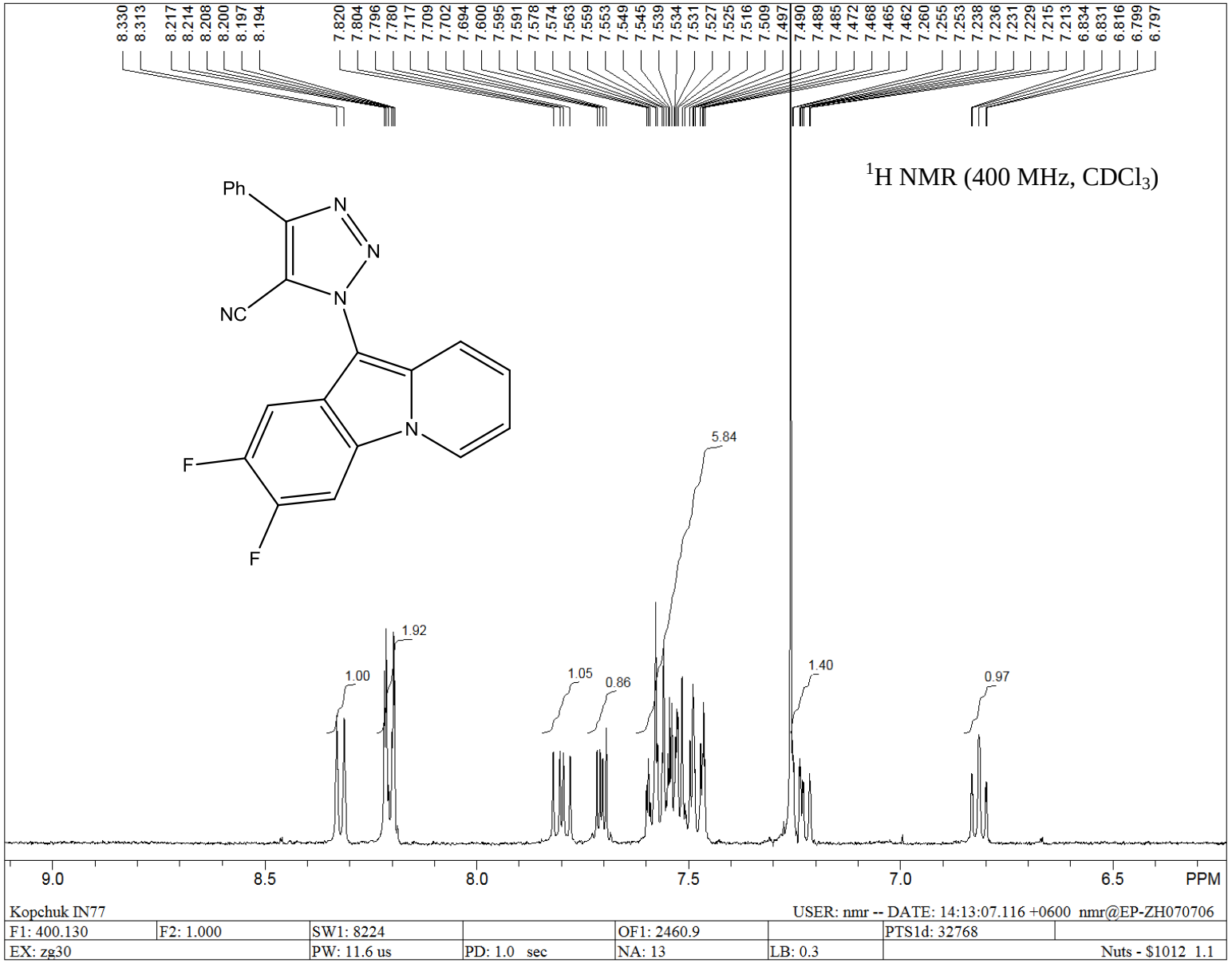

^{19}F NMR (376.5 MHz, $CDCl_3$)
139.022
139.076
141.650
141.705
Ph
N
N
N
Ph
N
F
F
1.00
1.00
-138
-139
-140
-141
-142
PPM
Kopchuk IN 116
USER: nmr -- DATE: 13:03:10.250 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 13.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $814 19.1


150.602
150.457
148.553
148.386
148.167
148.006
147.598
145.950
132.547
132.518
131.322
130.272
129.579
128.835
128.784
128.522
126.385
124.598
123.942
122.753
122.659
121.317
119.778
119.683
118.954
117.058
110.131
105.274
105.062
102.736
102.109
102.073
99.178
98.952
77.345
77.235
77.031
76.710
76.156
^{13}C NMR (100 MHz,
Ph
N
N
N
Ph
N
F
F
150
140
130
120
110
100
90
80
PPM
Kopchuk IN 116,
USER: nmr -- DATE: 04:23:31.898 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgpg30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $814 13.1

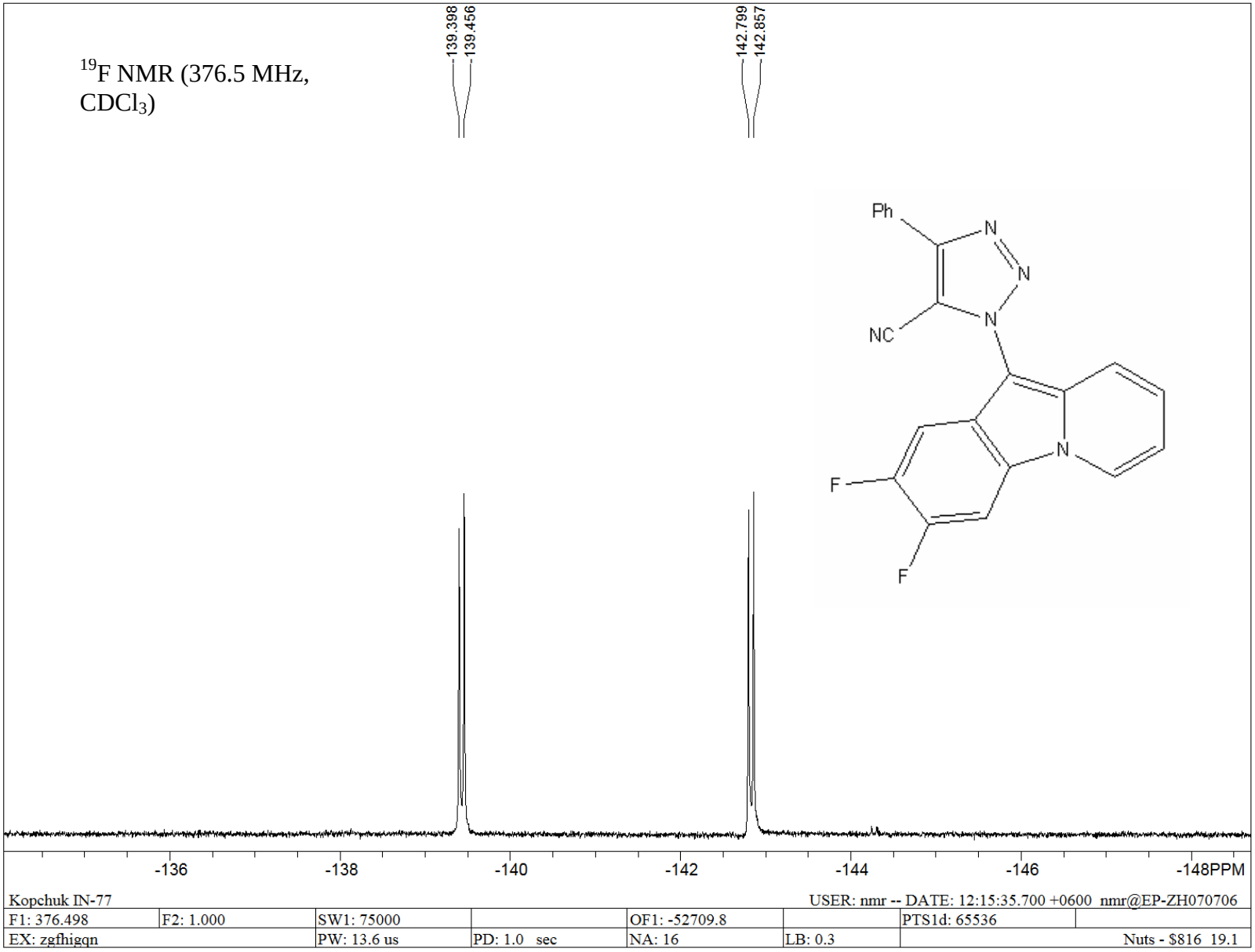

8.264
8.246
7.916
7.896
7.768
7.753
7.744
7.728
7.564
7.545
7.538
7.535
7.519
7.514
7.512
7.315
7.295
7.256
7.124
7.122
7.108
7.105
7.100
7.098
7.084
7.082
6.728
6.726
6.710
6.694
6.691
3.644
2.422
^{1}H NMR (400 MHz, $CDCl_3$)
MeO
N
N
N
N
F
F
3.13
3.26
1.00
2.05
1.03
2.03
2.14
1.15
1.02
9
8
7
6
5
4
3
PPM
Kopchuk IN 84
USER: nmr -- DATE: 14:04:19.589 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2459.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 14
LB: 0.3
Nuts - $1287 1.1

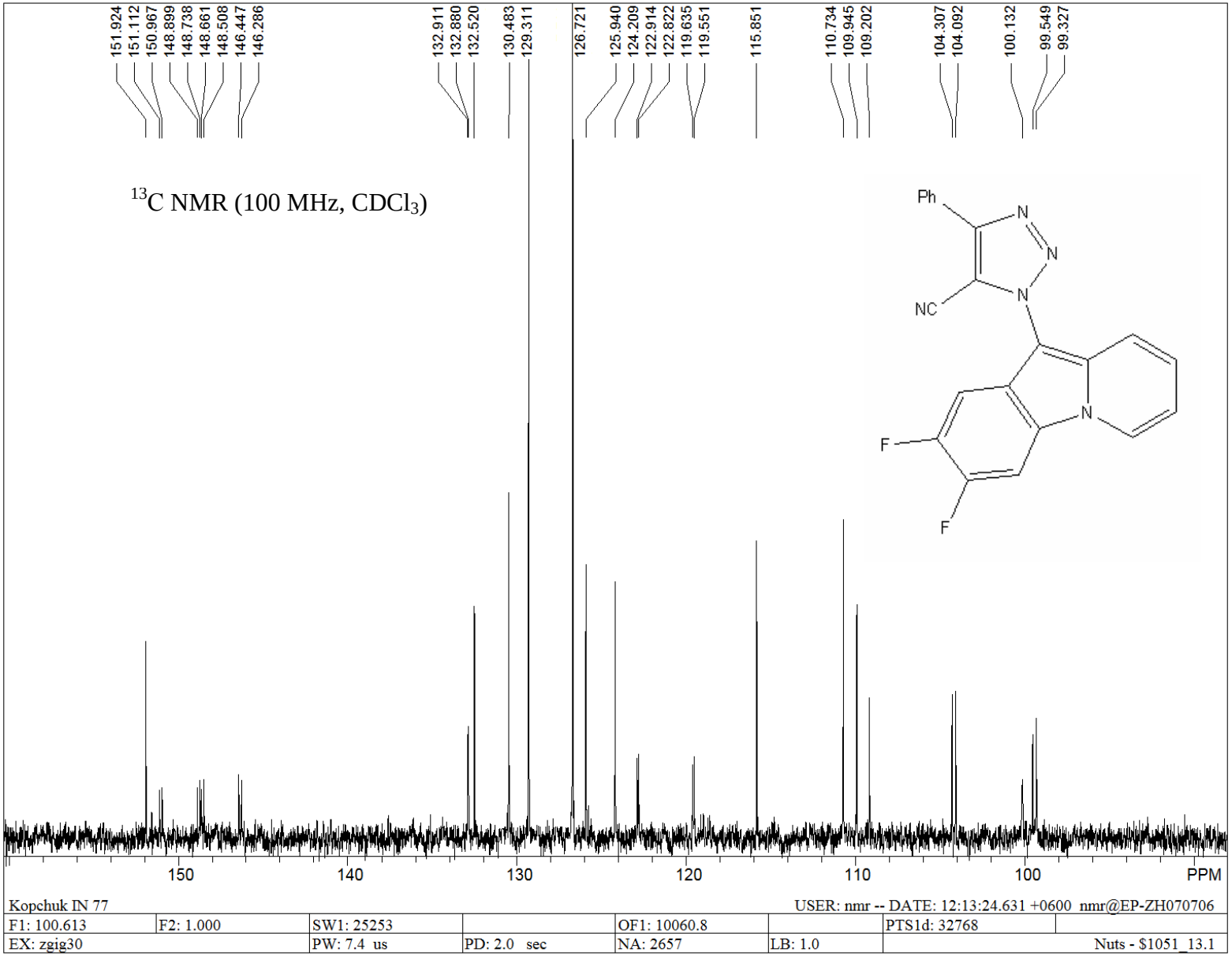

^{19}F NMR (376.5 MHz, $CDCl_3$)
138.760
138.815
141.666
141.720
1.00
0.98
MeO
N
N
N
N
F
F
-138
-139
-140
-141
-142
PPM
Kopchuk IN 84
USER: nmr -- DATE: 13:06:17.623 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 13.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $815 19.1

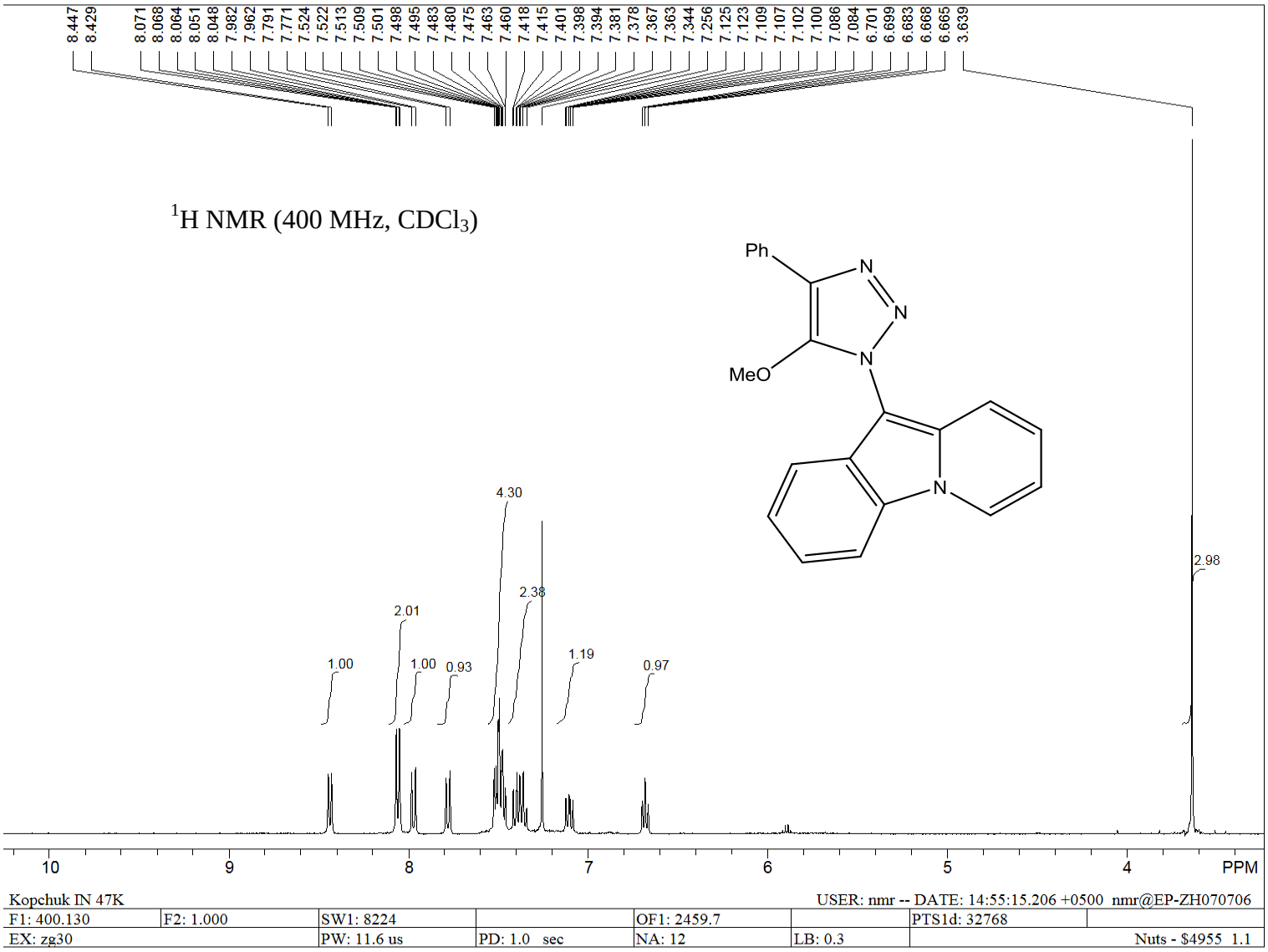

150.748
150.595
148.830
148.575
148.415
148.305
148.152
146.140
145.979
137.673
132.445
132.416
131.402
129.528
127.428
125.809
124.737
123.971
122.797
122.695
119.778
119.691
116.672
110.072
104.815
104.610
100.002
99.185
98.959
77.352
77.243
77.038
76.718
61.637
21.348
^{13}C NMR (100 MHz, $CDCl_3$)
MeO
N
N
N
N
F
F
160
140
120
100
80
60
40
PPM
Kopchuk IN 84,
USER: nmr -- DATE: 07:35:08.958 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgpg30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $815_13.1

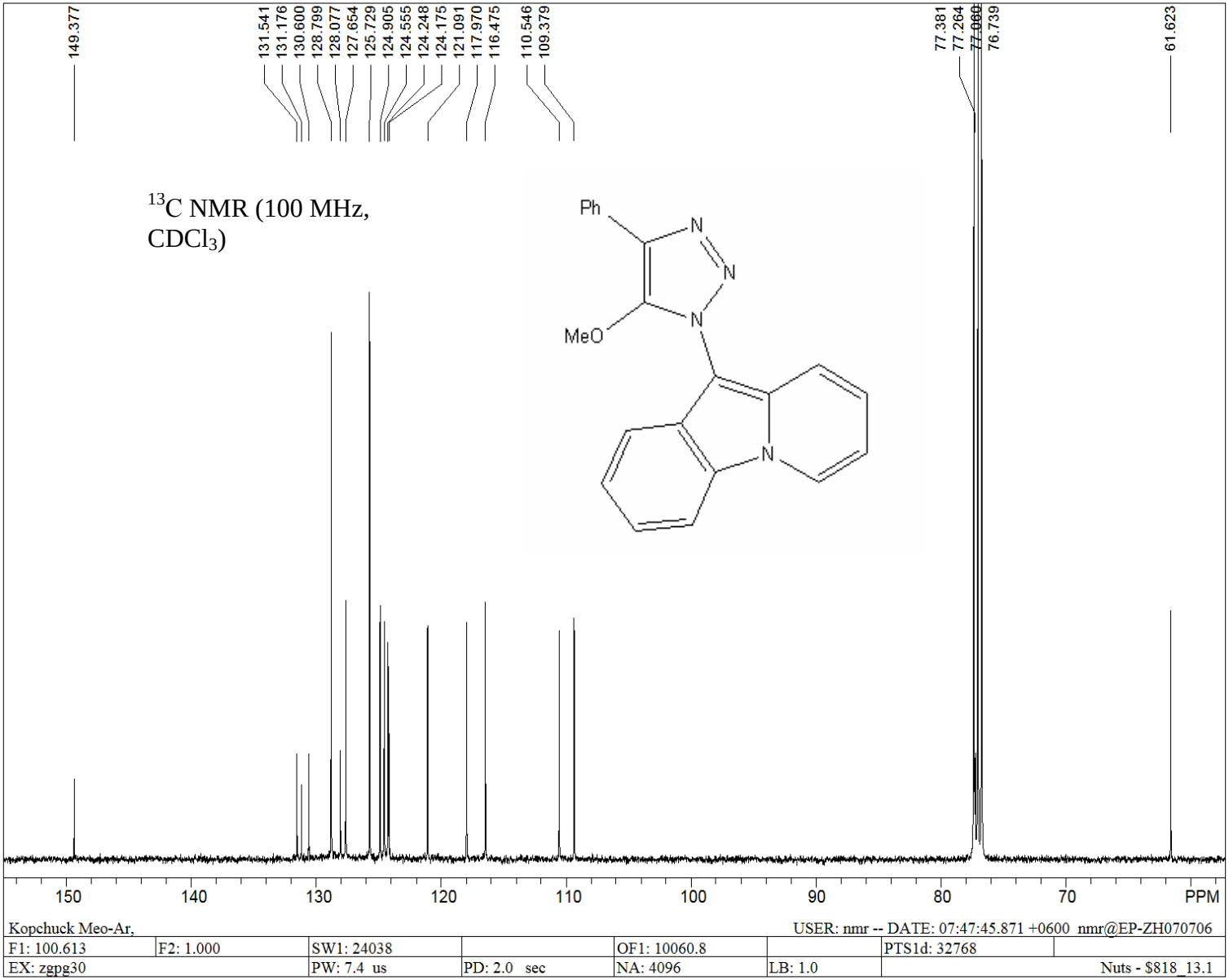

8.330
8.313
8.217
8.214
8.208
8.200
8.197
8.194
7.820
7.804
7.796
7.780
7.717
7.709
7.702
7.694
7.600
7.595
7.591
7.578
7.574
7.563
7.559
7.553
7.549
7.545
7.539
7.534
7.531
7.527
7.525
7.516
7.509
7.497
7.490
7.489
7.485
7.472
7.468
7.465
7.462
7.260
7.255
7.253
7.238
7.236
7.231
7.229
7.215
7.213
6.834
6.831
6.816
6.799
6.797
^{1}H NMR (400 MHz, $CDCl_3$)
Ph
N
N
N
NC
N
F
F
5.84
1.92
1.00
1.05
0.86
1.40
0.97
9.0
8.5
8.0
7.5
7.0
6.5
PPM
Kopchuk IN77
USER: nmr -- DATE: 14:13:07.116 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 13
LB: 0.3
Nuts - $1012 1.1

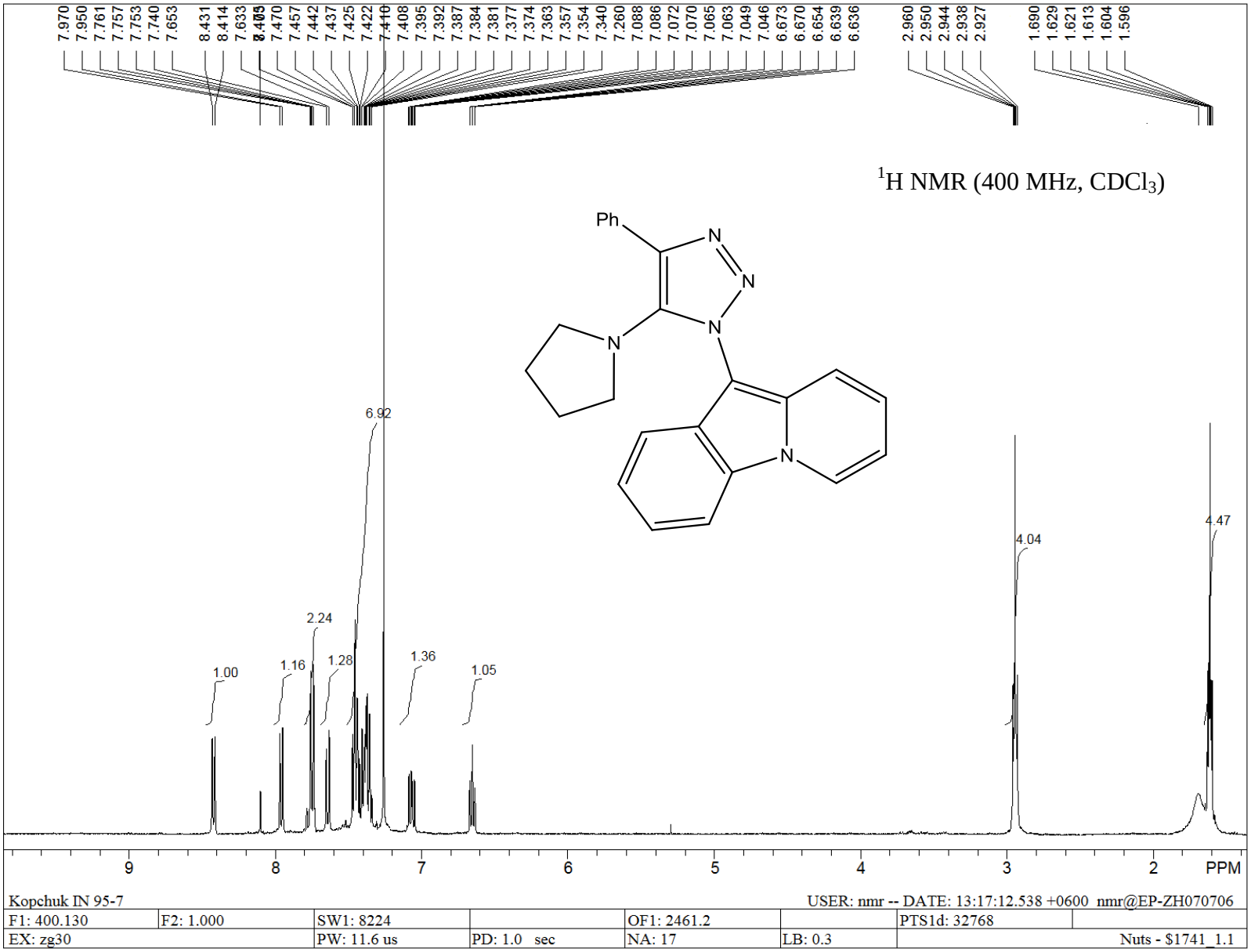
^{19}F NMR (376.5 MHz, $CDCl_3$)

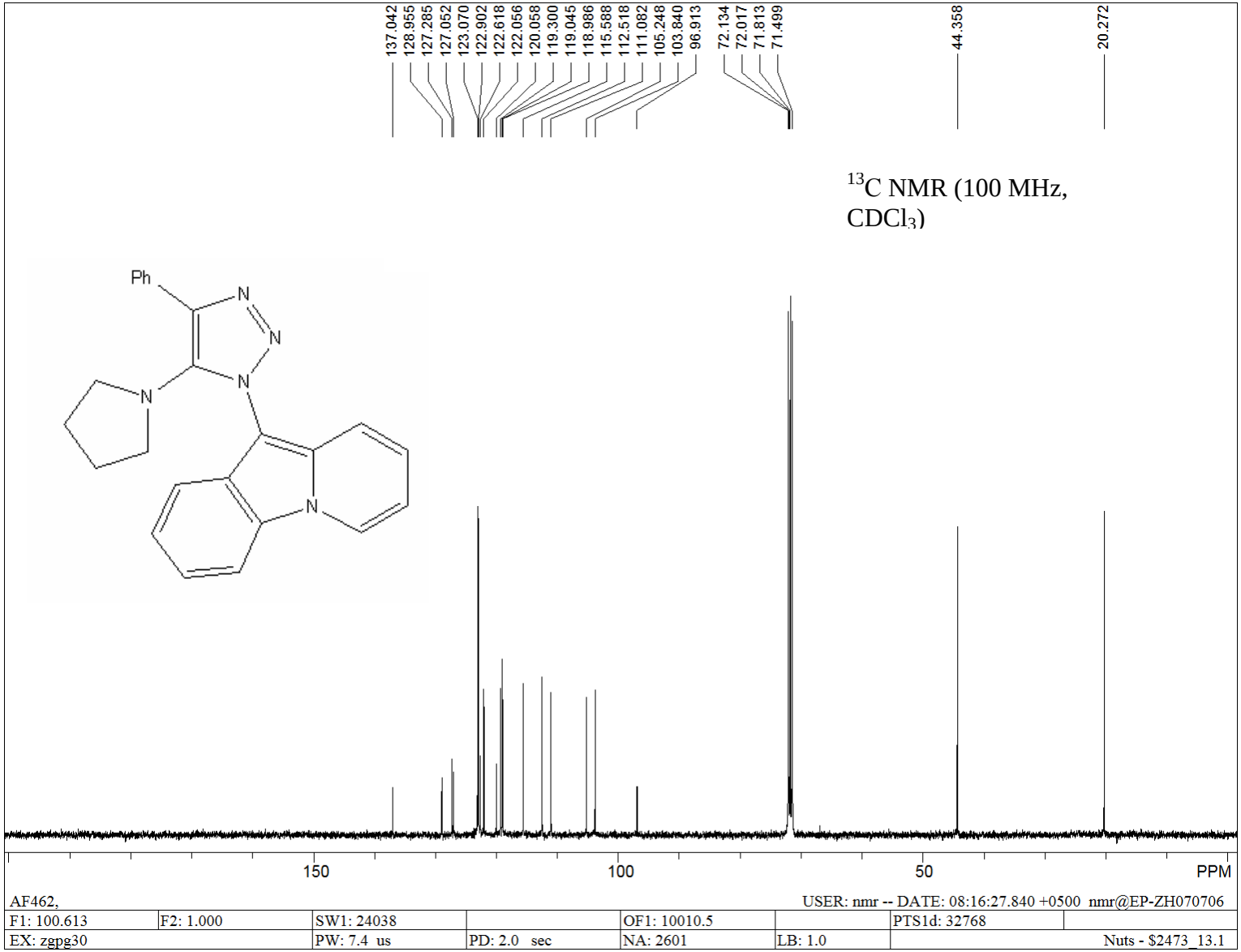



151.924
151.112
150.967
148.899
148.738
148.661
148.508
146.447
146.286
132.911
132.880
132.520
130.483
129.311
126.721
125.940
124.209
122.914
122.822
119.635
119.551
115.851
110.734
109.945
109.202
104.307
104.092
100.132
99.549
99.327
13C NMR (100 MHz, CDCl3)
Ph
N
N
N
NC
N
F
F
150
140
130
120
110
100
PPM
Kopchuk IN 77
USER: nmr -- DATE: 12:13:24.631 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 25253
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 2657
LB: 1.0
Nuts - $1051_13.1

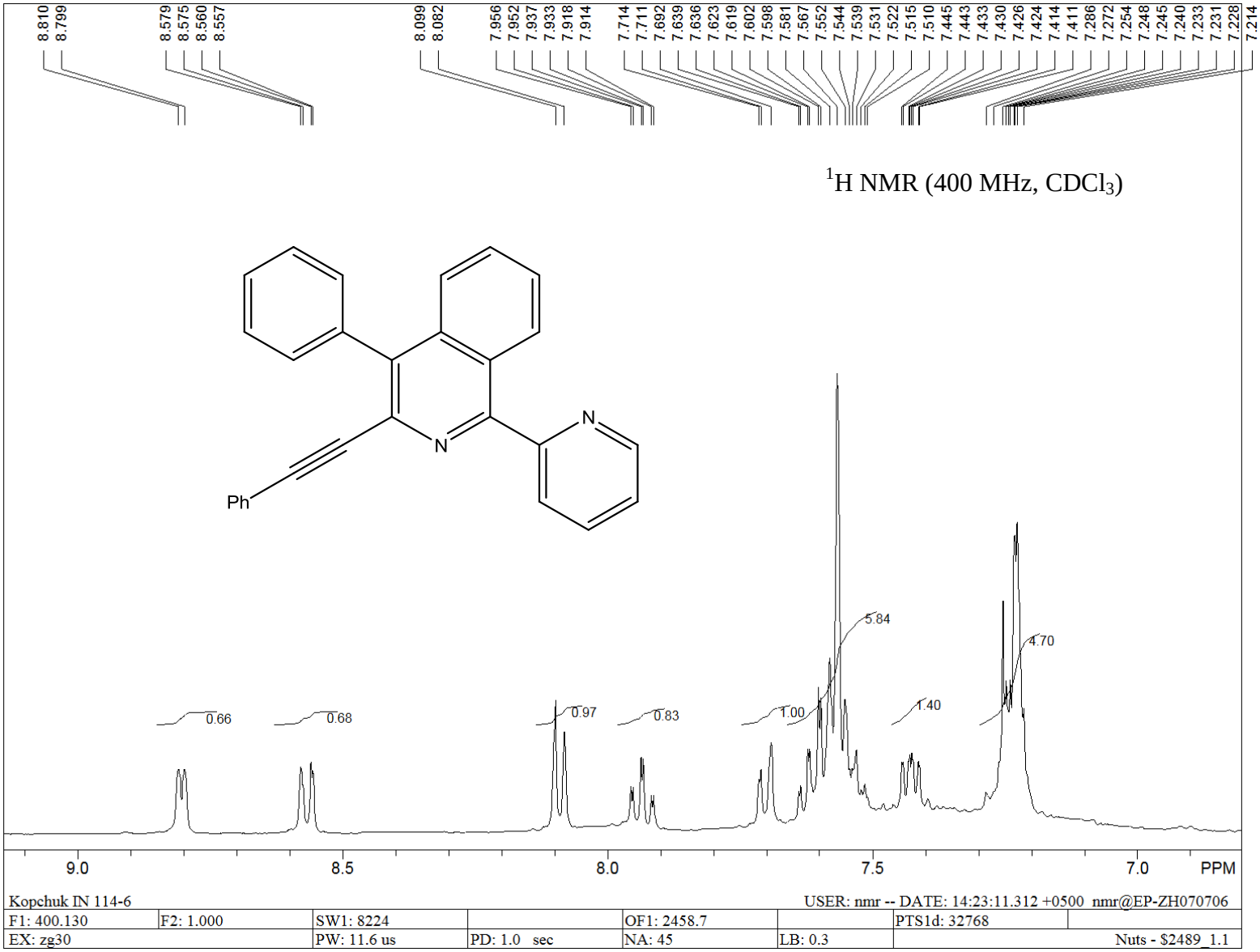

8.447
8.429
8.071
8.068
8.064
8.051
8.048
7.982
7.962
7.791
7.771
7.524
7.522
7.513
7.509
7.501
7.498
7.495
7.483
7.480
7.475
7.463
7.460
7.418
7.415
7.401
7.398
7.394
7.381
7.378
7.367
7.363
7.344
7.256
7.125
7.123
7.109
7.107
7.102
7.100
7.086
7.084
6.701
6.699
6.683
6.668
6.665
3.639
1H NMR (400 MHz, CDCl3)
Ph
N
N
N
MeO
N
4.30
2.38
2.01
1.00
1.00
0.93
1.19
0.97
2.98
10
9
8
7
6
5
4
PPM
Kopchuk IN 47K
USER: nmr -- DATE: 14:55:15.206 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2459.7
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 12
LB: 0.3
Nuts - $4955 1.1

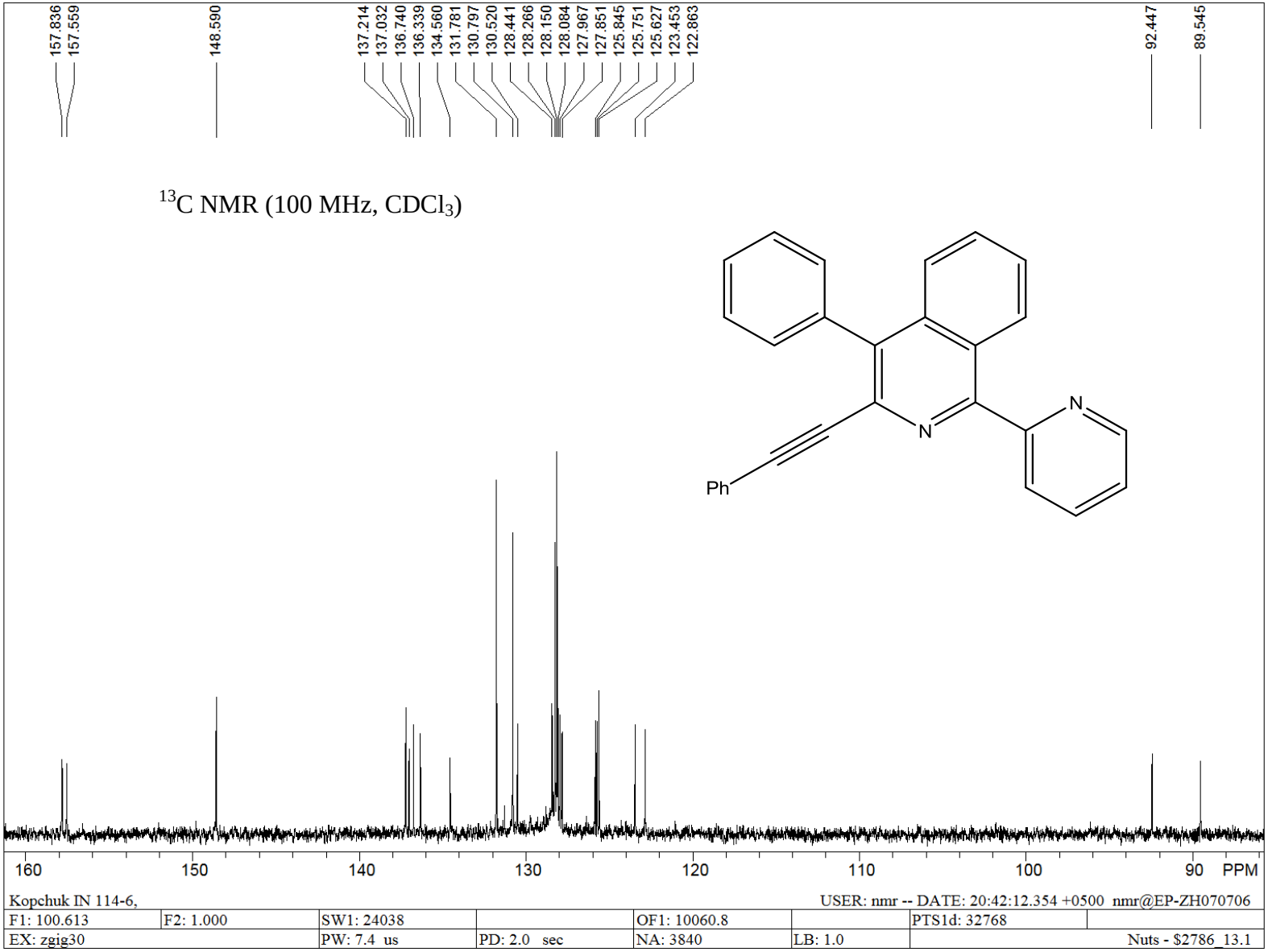

149.377
131.541
131.176
130.600
128.799
128.077
127.654
125.729
124.905
124.555
124.248
124.175
121.091
117.970
116.475
110.546
109.379
77.381
77.264
77.060
76.739
61.623
^{13}C NMR (100 MHz, $CDCl_3$)
Ph
N
N
N
MeO
N
150
140
130
120
110
100
90
80
70
PPM
Kopchuck Meo-Ar,
USER: nmr -- DATE: 07:47:45.871 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgpg30
PW: 7.4 us
PD: 2.0 sec
NA: 4096
LB: 1.0
Nuts - $818_13.1

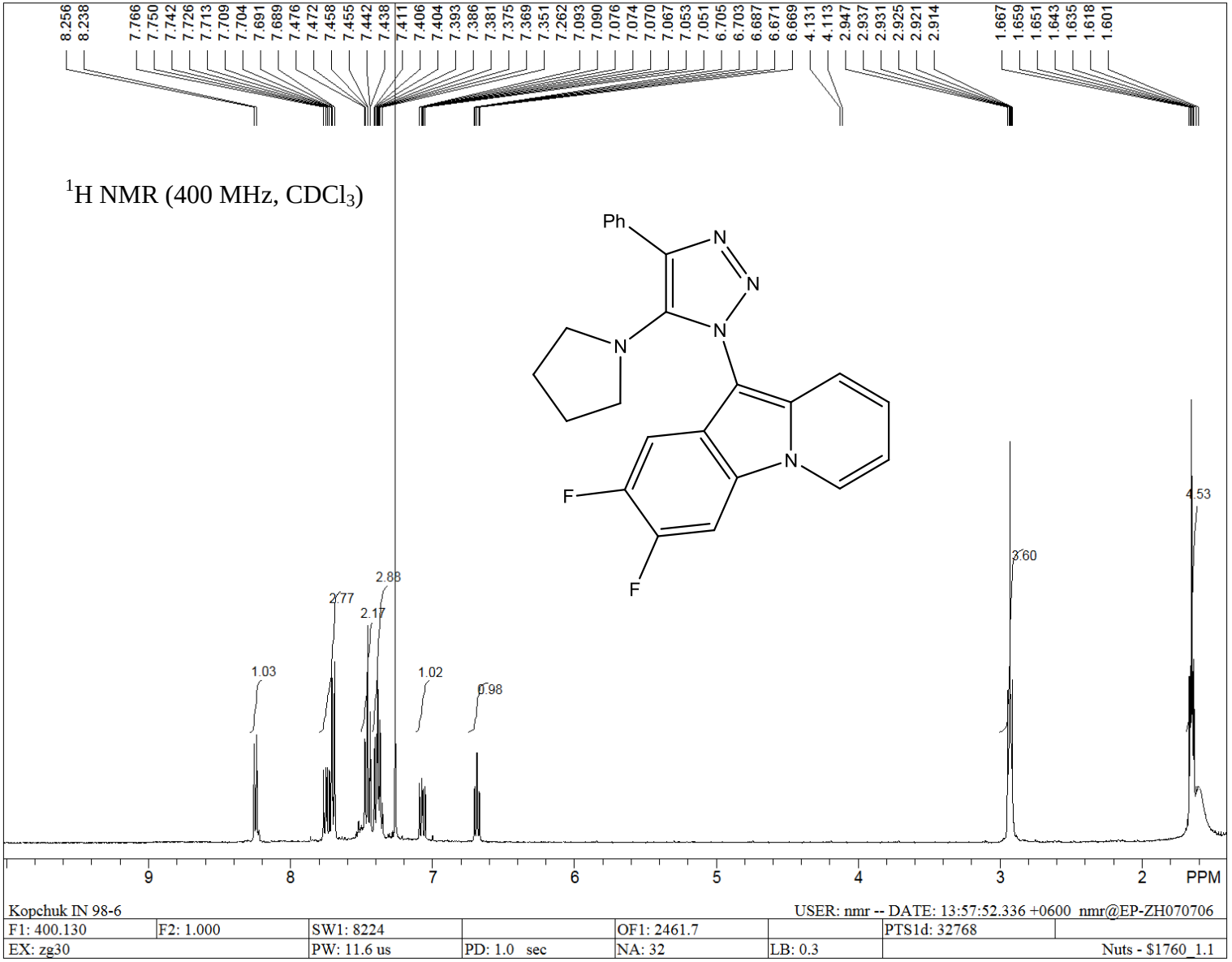

7.970
7.950
7.761
7.757
7.753
7.740
7.653
8.431
8.414
7.633
7.470
7.457
7.442
7.437
7.425
7.422
7.408
7.395
7.392
7.387
7.384
7.381
7.377
7.374
7.363
7.357
7.354
7.340
7.260
7.088
7.086
7.072
7.070
7.065
7.063
7.049
7.046
6.673
6.670
6.654
6.639
6.636
2.960
2.950
2.944
2.938
2.927
1.690
1.629
1.621
1.613
1.604
1.596
^{1}H NMR (400 MHz, $CDCl_3$)
Ph
N
N
N
N
N
6.92
2.24
1.00
1.16
1.28
1.36
1.05
4.04
4.47
9
8
7
6
5
4
3
2
PPM
Kopchuk IN 95-7
USER: nmr -- DATE: 13:17:12.538 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.2
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 17
LB: 0.3
Nuts - $1741_1.1

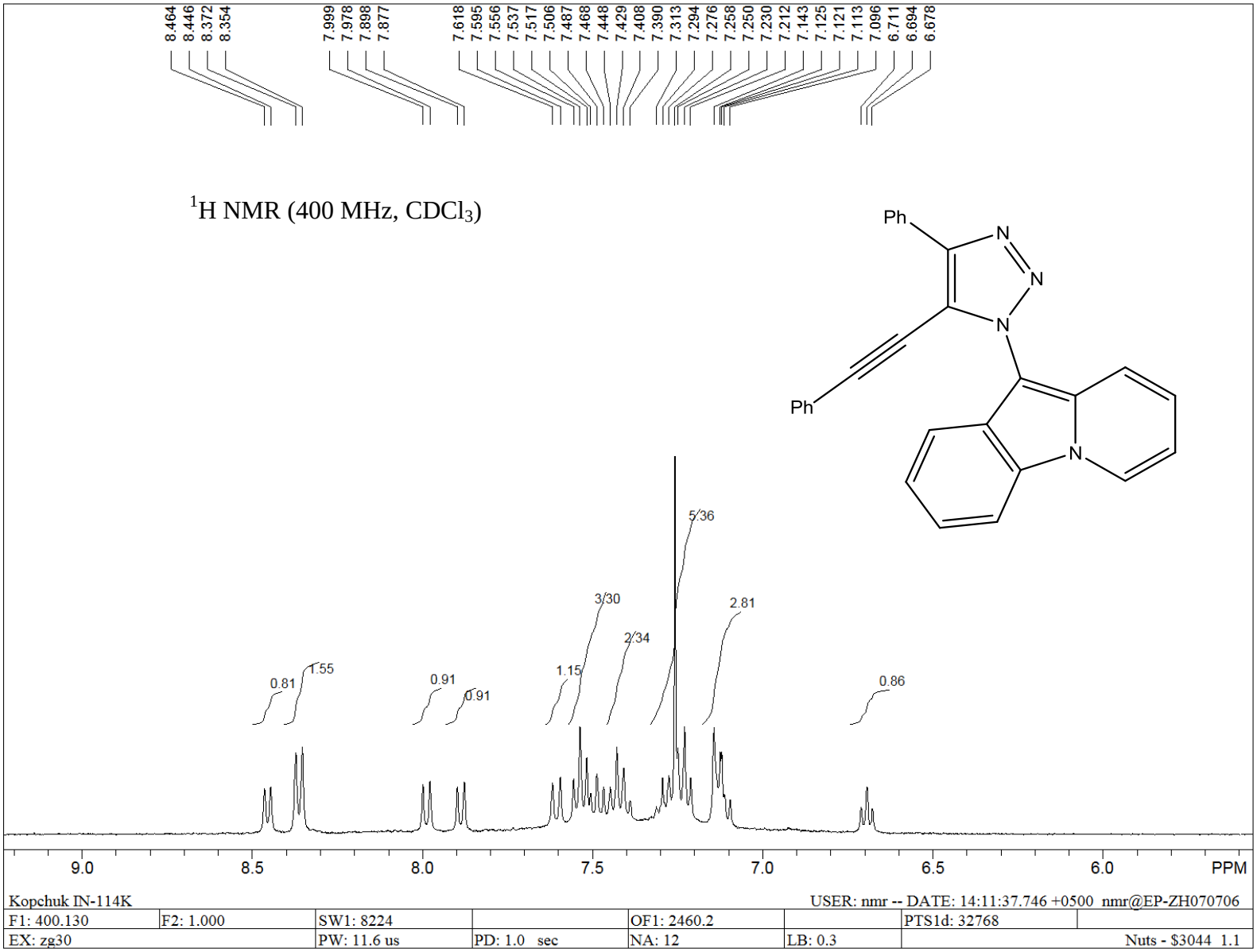


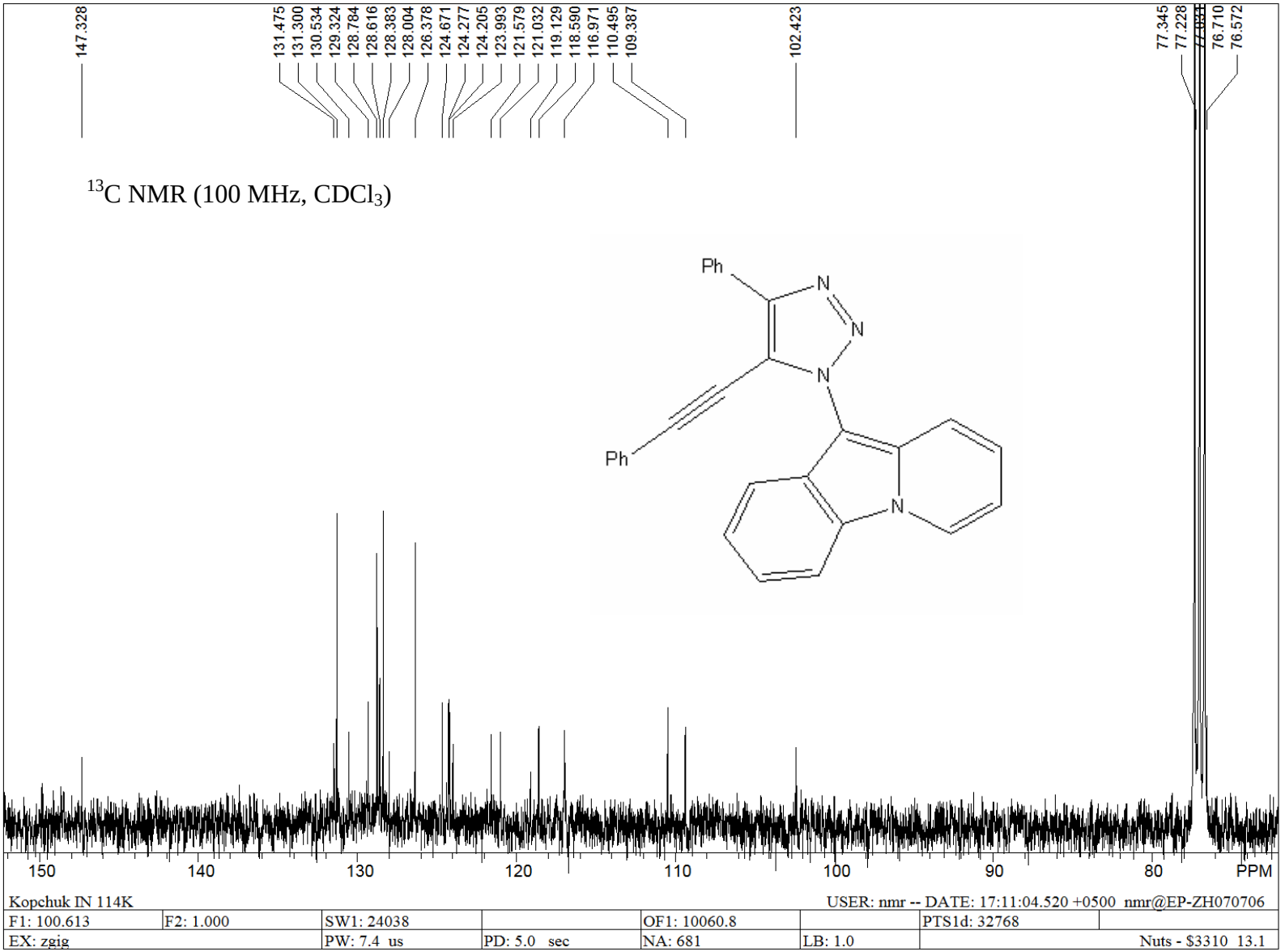
^{13}C NMR (100 MHz, $CDCl_3$)


8.810
8.799
8.579
8.575
8.560
8.557
8.099
8.082
7.956
7.952
7.937
7.933
7.918
7.914
7.714
7.711
7.692
7.639
7.636
7.623
7.619
7.602
7.598
7.581
7.567
7.552
7.544
7.539
7.531
7.522
7.515
7.510
7.445
7.443
7.433
7.430
7.426
7.424
7.414
7.411
7.286
7.272
7.254
7.248
7.245
7.240
7.233
7.231
7.228
7.214
^{1}H NMR (400 MHz, $CDCl_3$)
N
N
Ph
0.66
0.68
0.97
0.83
1.00
5.84
1.40
4.70
9.0
8.5
8.0
7.5
7.0
PPM
Kopchuk IN 114-6
USER: nmr -- DATE: 14:23:11.312 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2458.7
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 45
LB: 0.3
Nuts - $2489_1.1

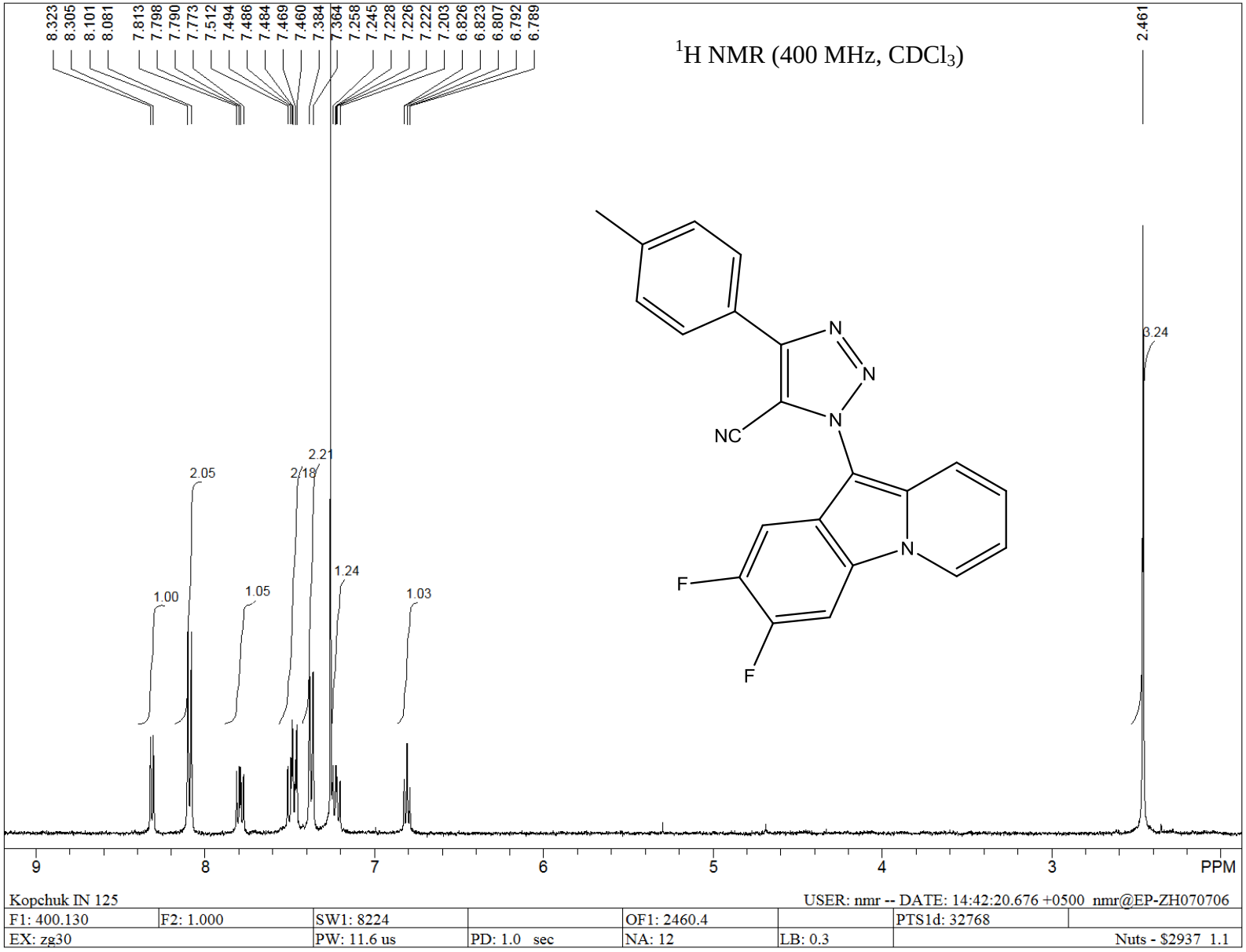

157.836
157.559
148.590
137.214
137.032
136.740
136.339
134.560
131.781
130.797
130.520
128.441
128.266
128.150
128.084
127.967
127.851
125.845
125.751
125.627
123.453
122.863
92.447
89.545
^{13}C NMR (100 MHz, CDCl$_3$)
N
N
Ph
160
150
140
130
120
110
100
90
PPM
Kopchuk IN 114-6,
USER: nmr -- DATE: 20:42:12.354 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $2786_13.1

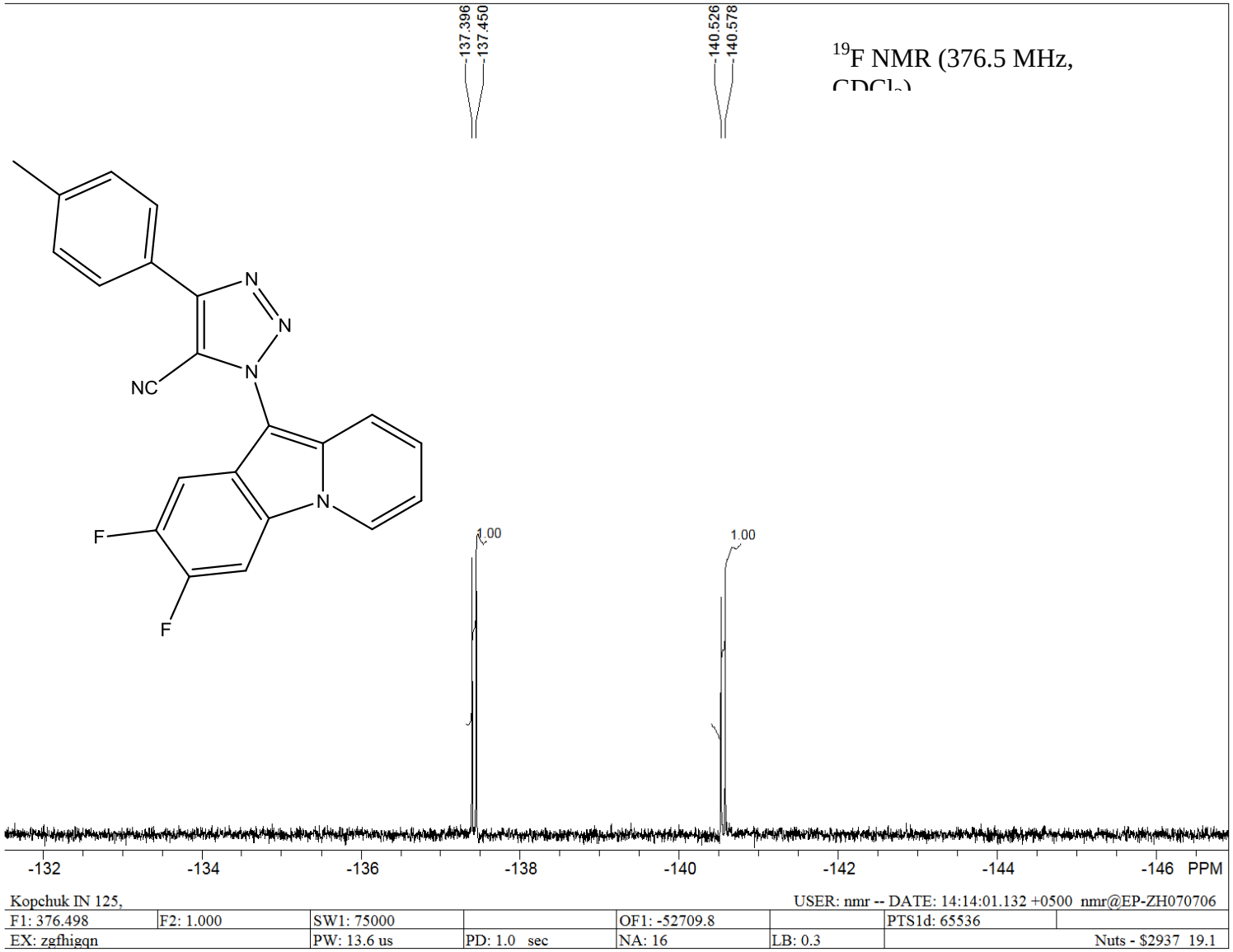

8.256
8.238
7.766
7.750
7.742
7.726
7.713
7.709
7.704
7.691
7.689
7.476
7.472
7.458
7.455
7.442
7.438
7.411
7.406
7.404
7.393
7.386
7.381
7.375
7.369
7.351
7.262
7.093
7.090
7.076
7.074
7.070
7.067
7.053
7.051
6.705
6.703
6.687
6.671
6.669
4.131
4.113
2.947
2.937
2.931
2.925
2.921
2.914
1.667
1.659
1.651
1.643
1.635
1.618
1.601
1H NMR (400 MHz, CDCl3)
Ph
N
N
N
N
F
F
N
1.03
2.77
2.17
2.88
1.02
0.98
3.60
4.53
9
8
7
6
5
4
3
2
PPM
Kopchuk IN 98-6
USER: nmr -- DATE: 13:57:52.336 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.7
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 32
LB: 0.3
Nuts - $1760_1.1

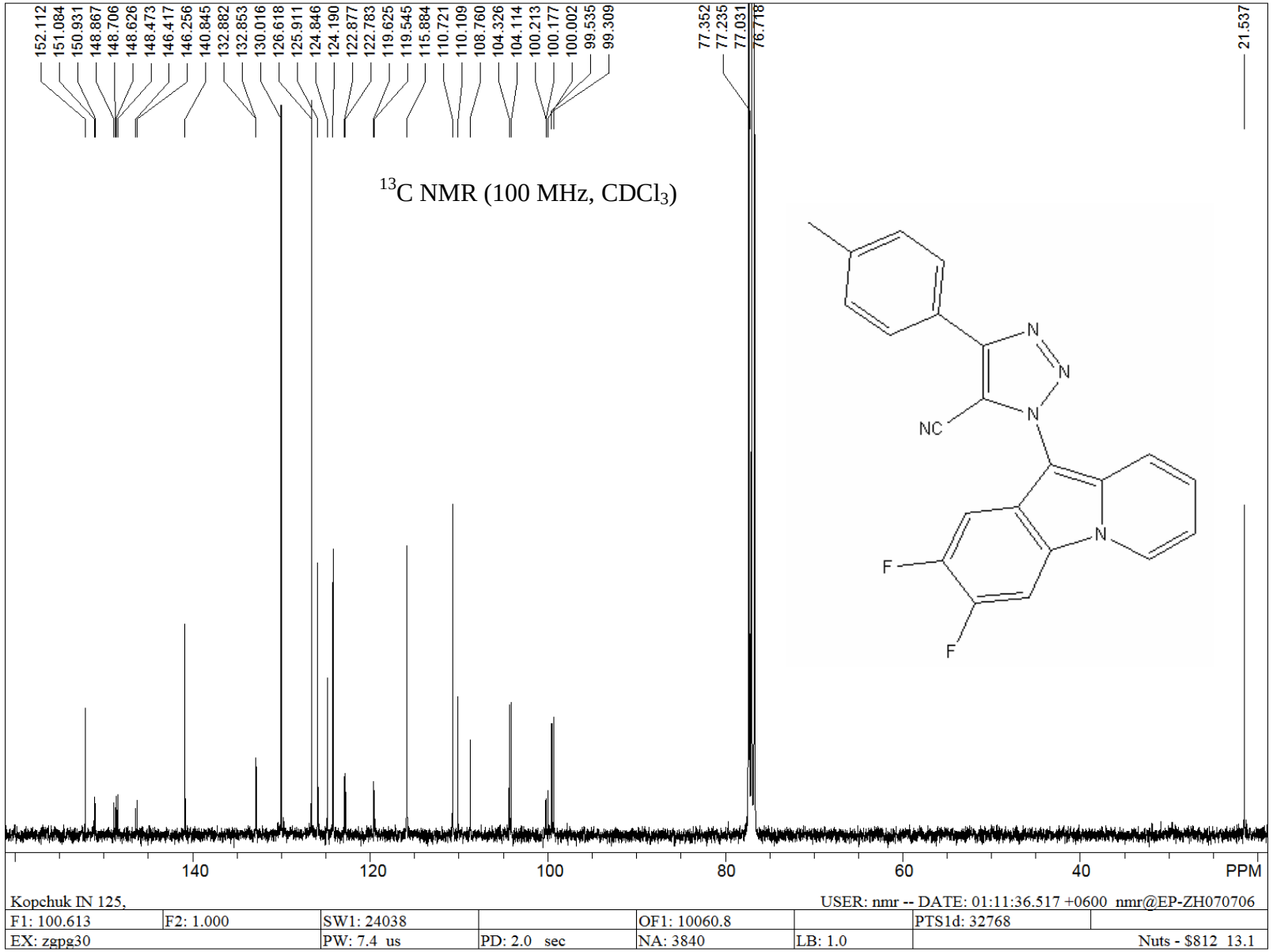

8.464
8.446
8.372
8.354
7.999
7.978
7.898
7.877
7.618
7.595
7.556
7.537
7.517
7.506
7.487
7.468
7.448
7.429
7.408
7.390
7.313
7.294
7.276
7.258
7.250
7.230
7.212
7.143
7.125
7.121
7.113
7.096
6.711
6.694
6.678
^{1}H NMR (400 MHz, $CDCl_3$)
Ph
N
N
N
Ph
N
0.81
1.55
0.91
0.91
1.15
3.30
2.34
5.36
2.81
0.86
9.0
8.5
8.0
7.5
7.0
6.5
6.0
PPM
Kopchuk IN-114K
USER: nmr -- DATE: 14:11:37.746 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.2
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 12
LB: 0.3
Nuts - $3044 1.1

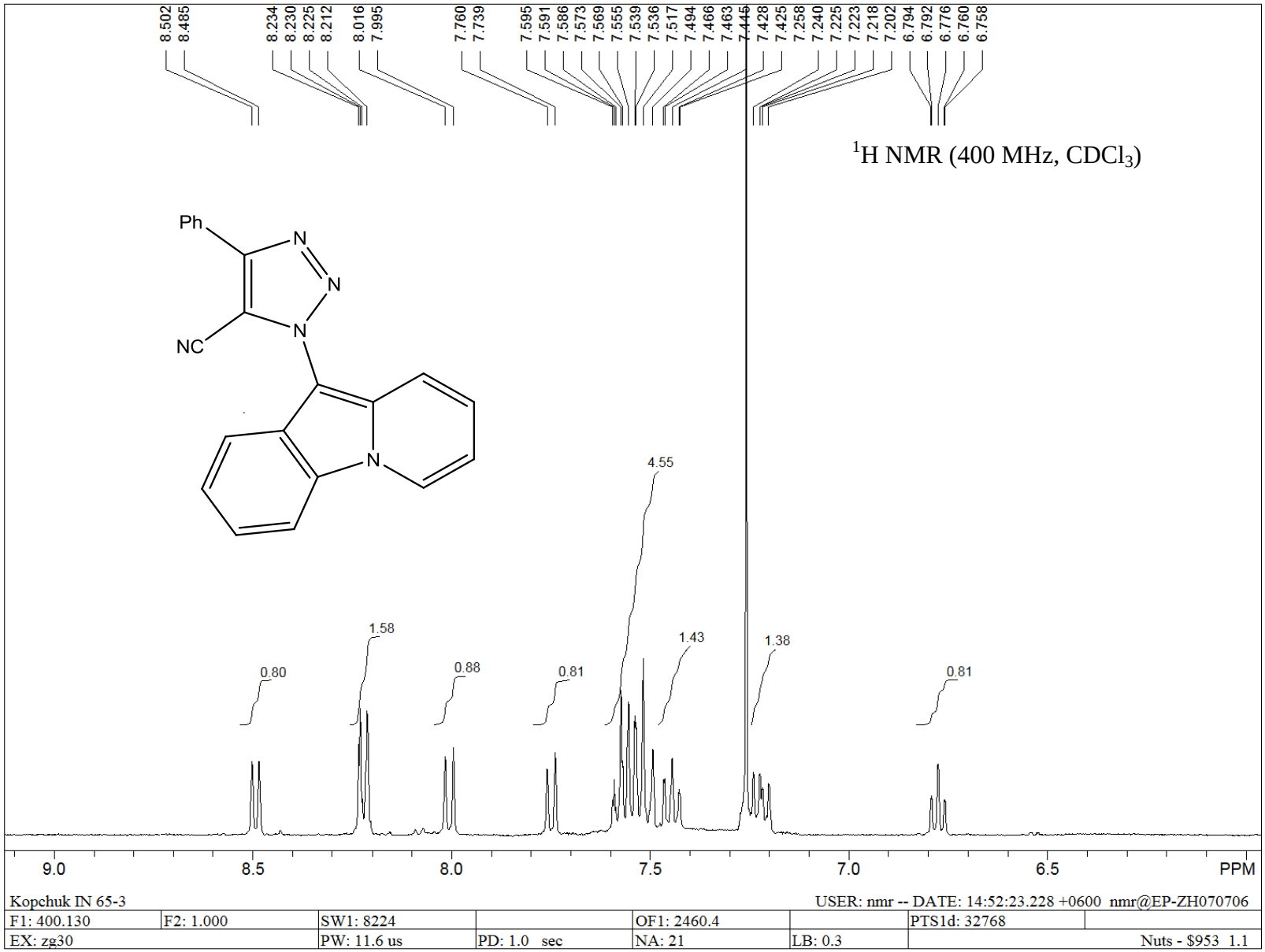


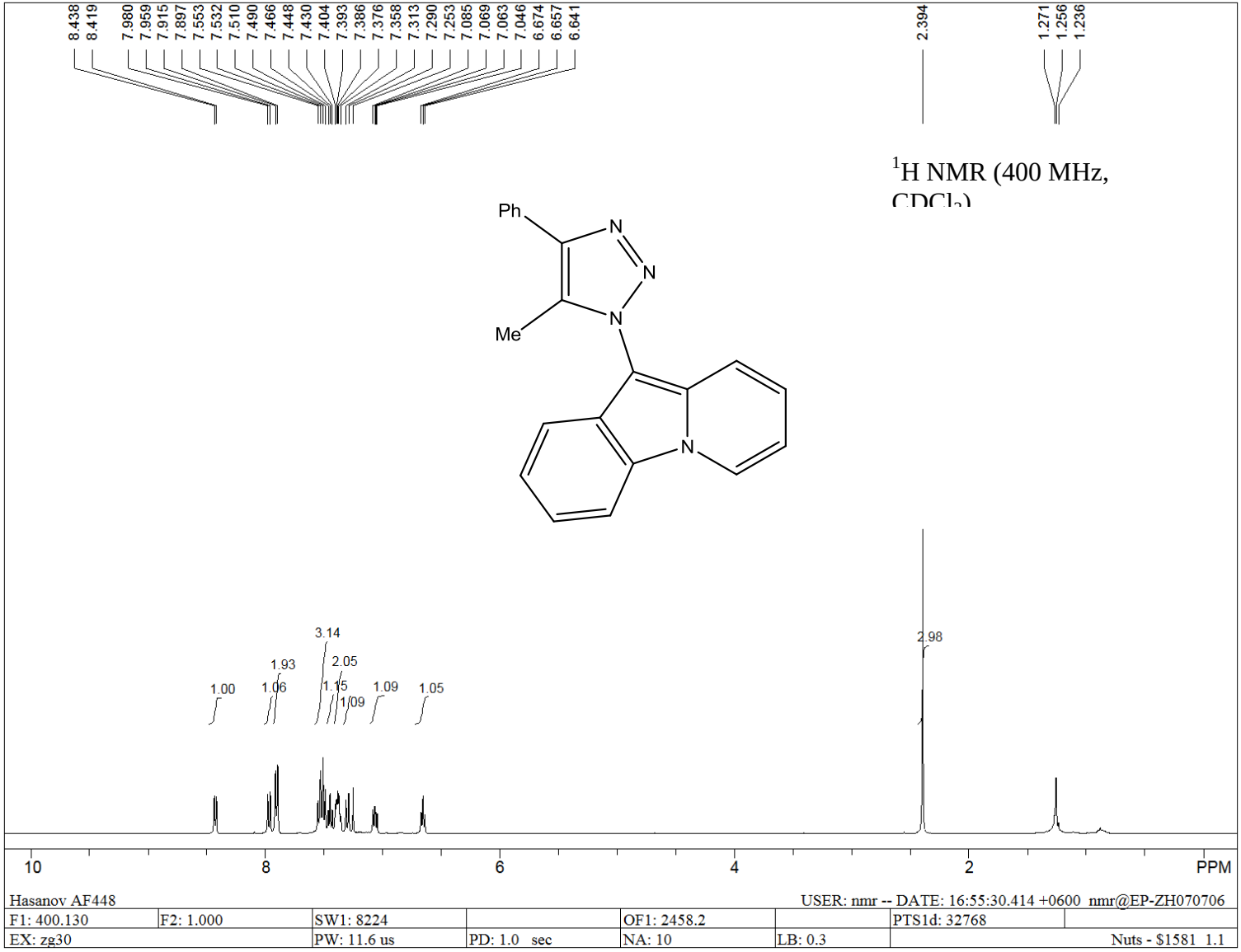
^{13}C NMR (100 MHz, $CDCl_3$)


8.323
8.305
8.101
8.081
7.813
7.798
7.790
7.773
7.512
7.494
7.486
7.484
7.469
7.460
7.384
7.364
7.258
7.245
7.228
7.226
7.222
7.203
6.826
6.823
6.807
6.792
6.789
2.461
^{1}H NMR (400 MHz, $CDCl_3$)
3.24
2.21
2.18
2.05
1.24
1.03
1.00
1.05
N
N
N
NC
N
F
F
9
8
7
6
5
4
3
PPM
Kopchuk IN 125
USER: nmr -- DATE: 14:42:20.676 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 12
LB: 0.3
Nuts - $2937 1.1

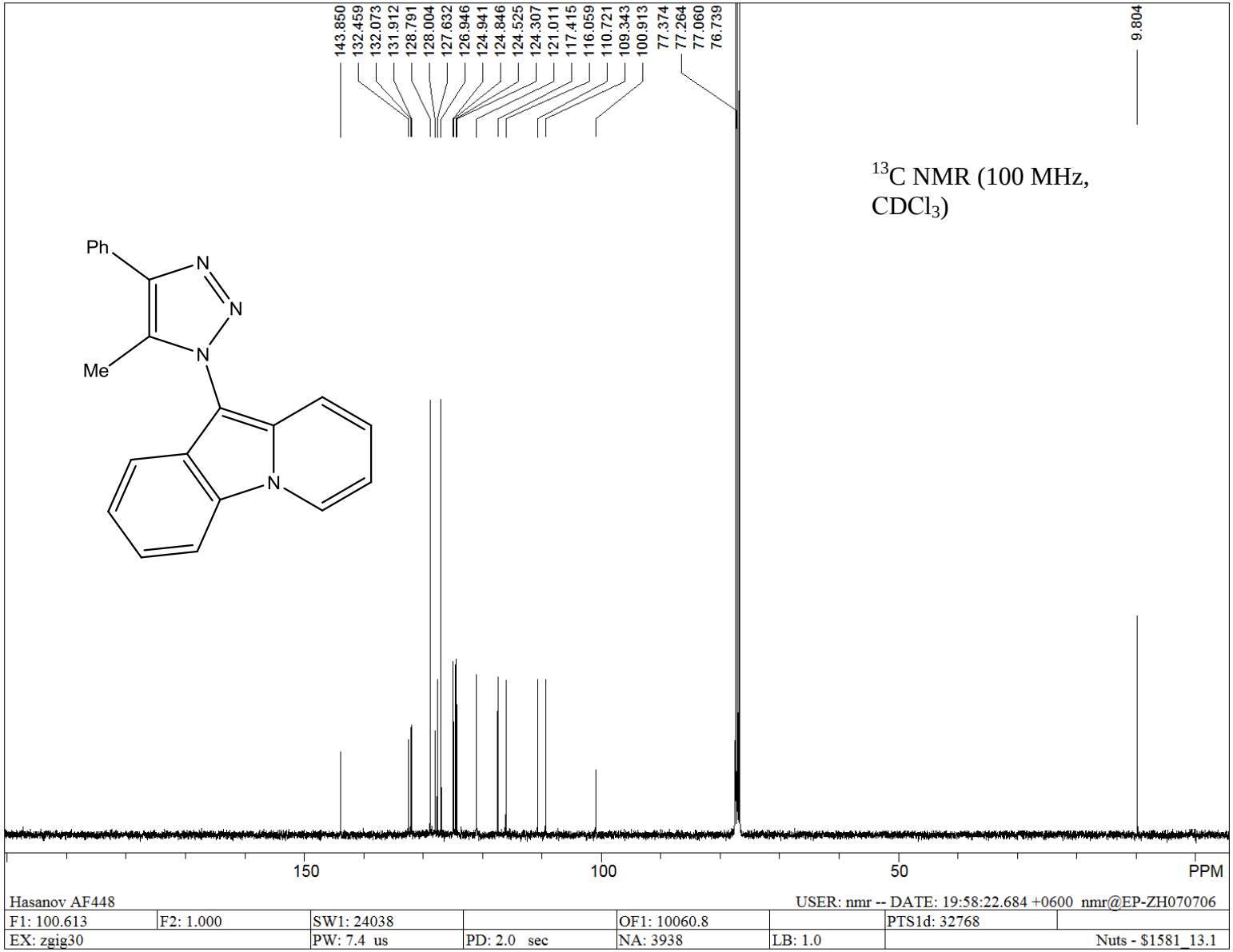

137.396
137.450
140.526
140.578
^{19}F NMR (376.5 MHz,
CDCl$_3$)
N
N
N
NC
F
F
N
1.00
1.00
-132
-134
-136
-138
-140
-142
-144
-146 PPM
Kopchuk IN 125,
USER: nmr -- DATE: 14:14:01.132 +0500 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 13.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $2937 19.1

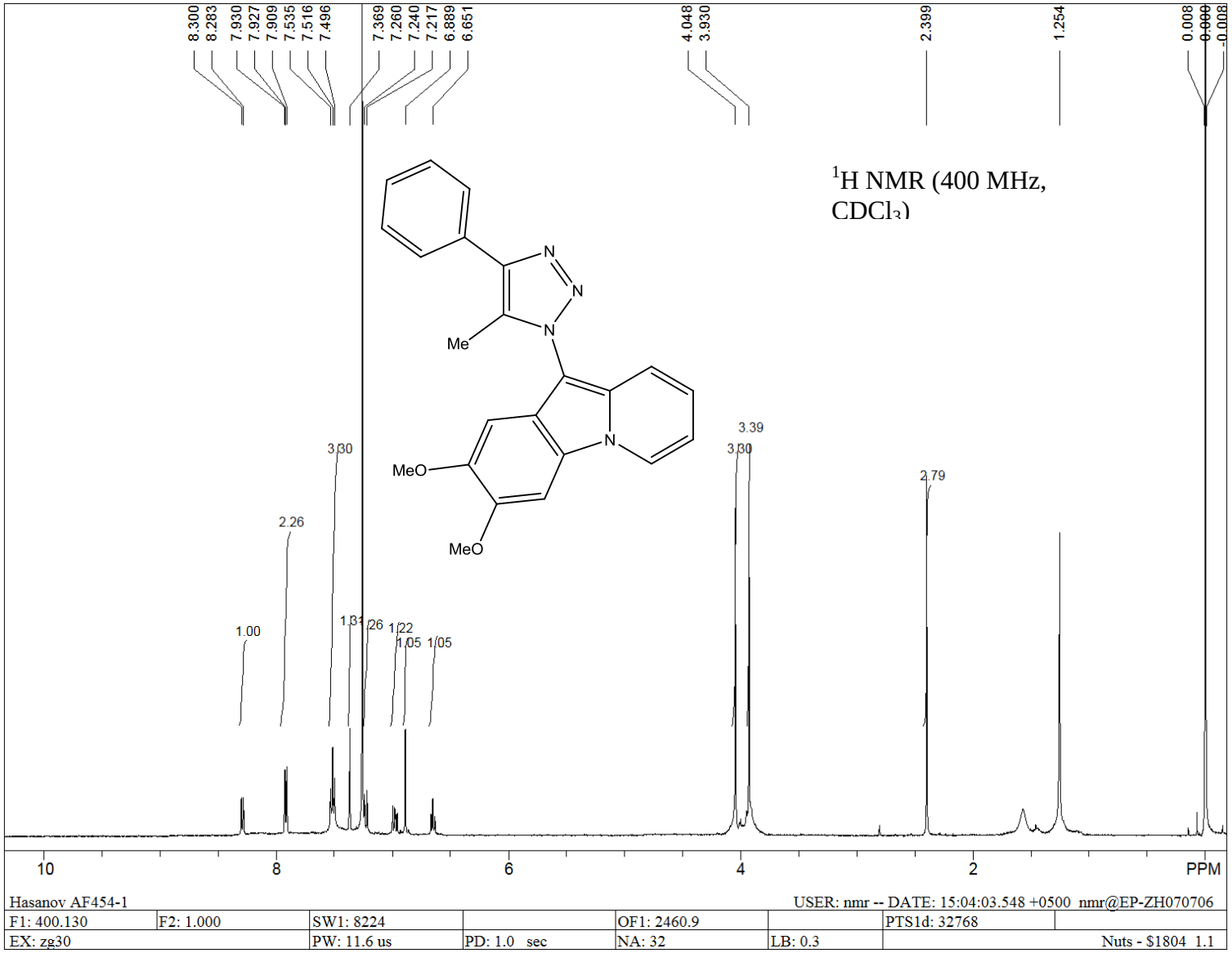

152.112
151.084
150.931
148.867
148.706
148.626
148.473
146.417
146.256
140.845
132.882
132.853
130.016
126.618
125.911
124.846
124.190
122.877
122.783
119.625
119.545
115.884
110.721
110.109
108.760
104.326
104.114
100.213
100.177
100.002
99.535
99.309
77.352
77.235
77.031
76.718
21.537
^{13}C NMR (100 MHz, $CDCl_3$)
N
N
N
NC
N
F
F
140
120
100
80
60
40
PPM
Kopchuk IN 125,
USER: nmr -- DATE: 01:11:36.517 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgpg30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $812 13.1

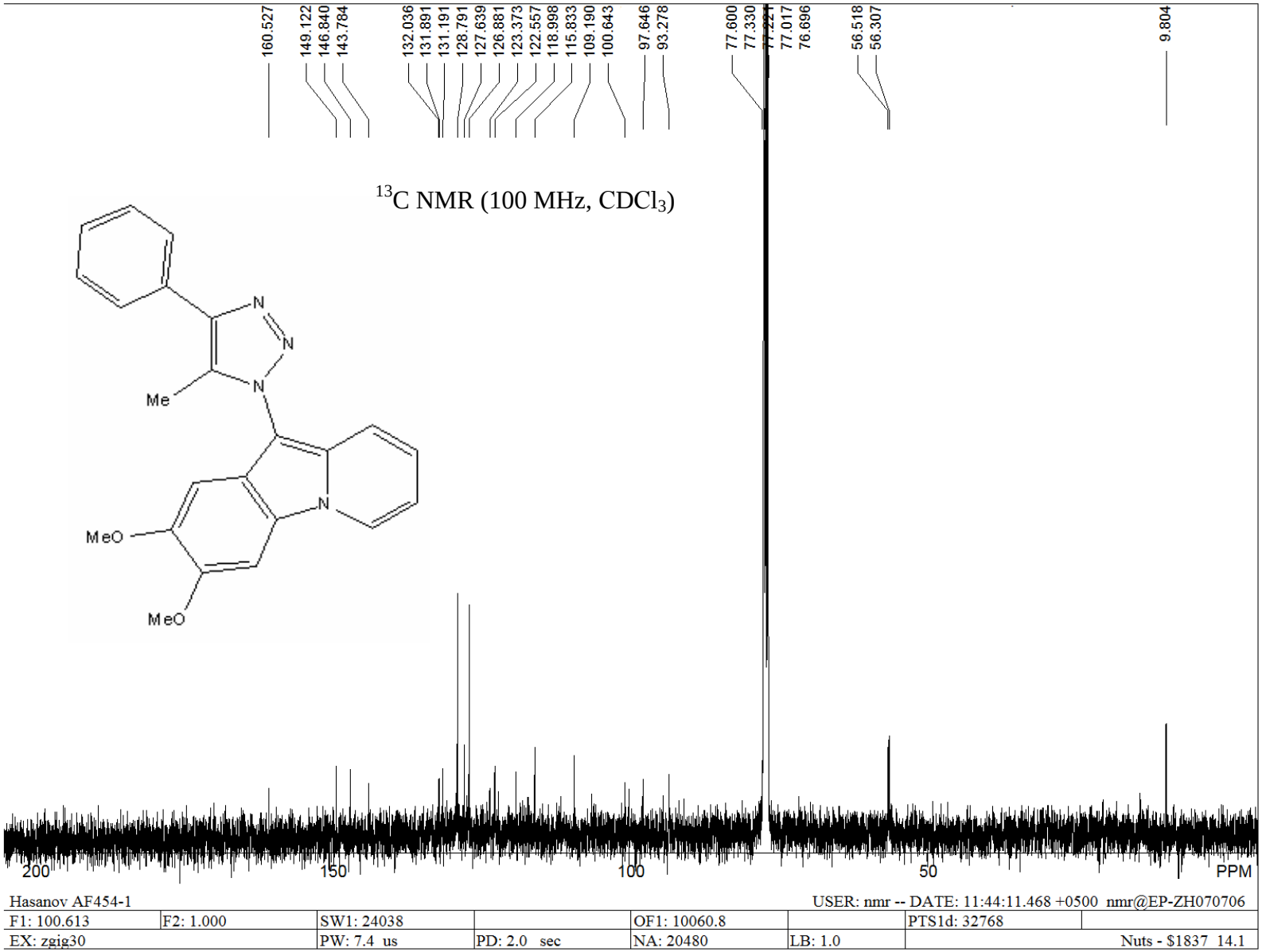

8.502
8.485
8.234
8.230
8.225
8.212
8.016
7.995
7.760
7.739
7.595
7.591
7.586
7.573
7.569
7.555
7.539
7.536
7.517
7.494
7.466
7.463
7.445
7.428
7.425
7.258
7.240
7.225
7.223
7.218
7.202
6.794
6.792
6.776
6.760
6.758
^{1}H NMR (400 MHz, $CDCl_3$)
Ph
N
N
N
NC
N
4.55
1.58
1.43
1.38
0.80
0.88
0.81
0.81
9.0
8.5
8.0
7.5
7.0
6.5
PPM
Kopchuk IN 65-3
USER: nmr -- DATE: 14:52:23.228 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 21
LB: 0.3
Nuts - $953 1.1



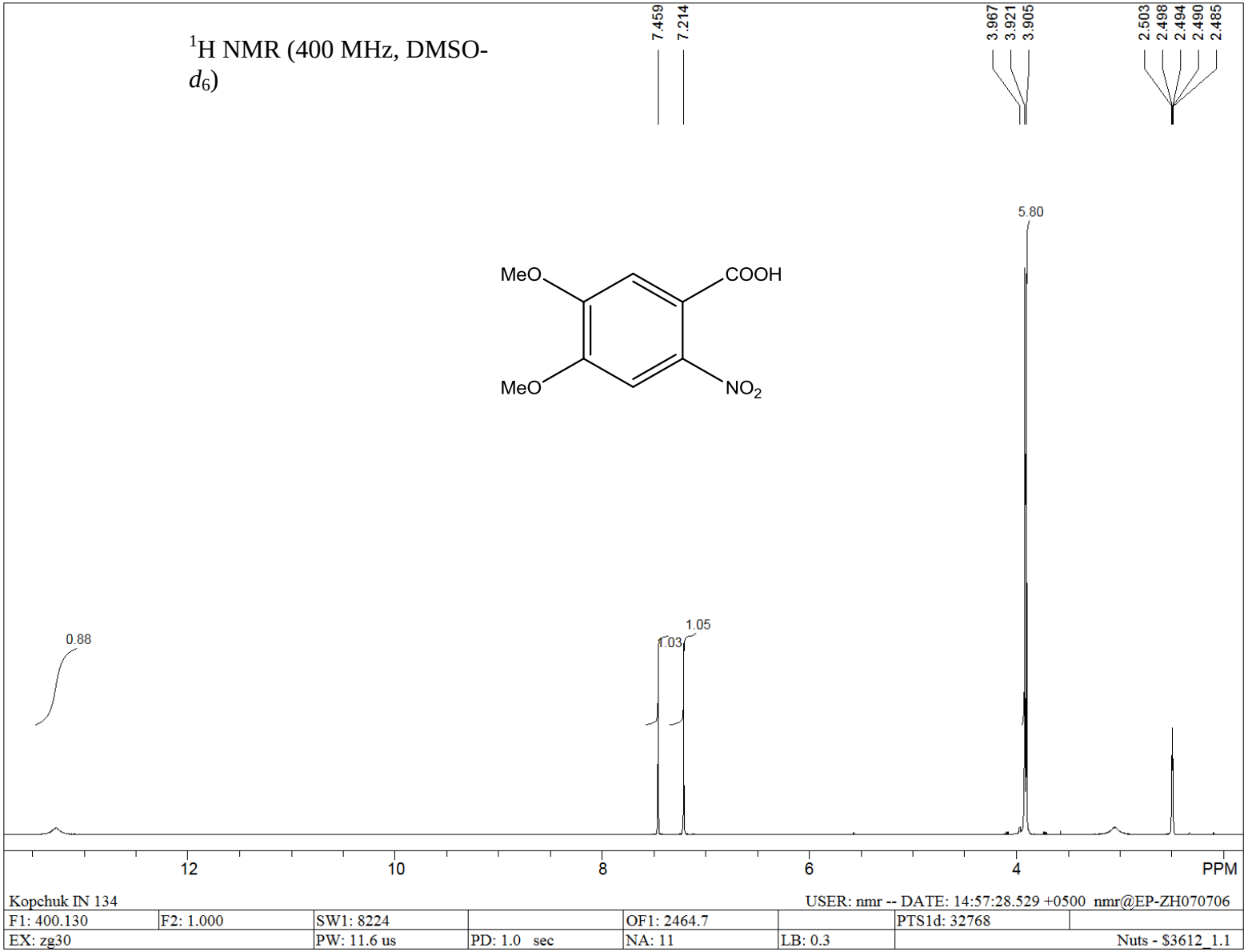
^{1}H NMR (400 MHz, $CDCl_3$)

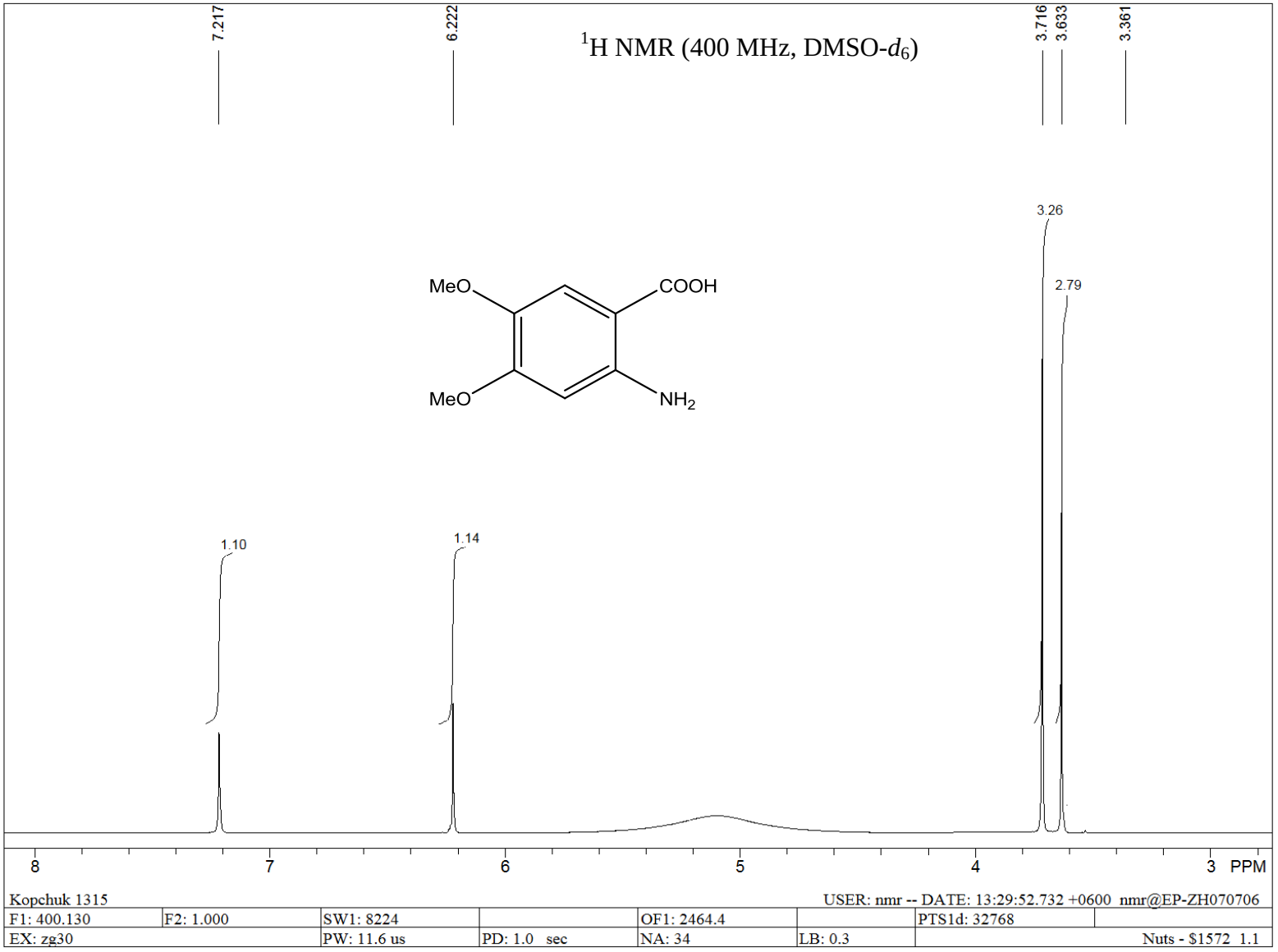

143.850
132.459
132.073
131.912
128.791
128.004
127.632
126.946
124.941
124.846
124.525
124.307
121.011
117.415
116.059
110.721
109.343
100.913
77.374
77.264
77.060
76.739
9.804
^{13}C NMR (100 MHz, $CDCl_3$)
Ph
N
N
N
Me
N
150
100
50
PPM
Hasanov AF448
USER: nmr -- DATE: 19:58:22.684 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3938
LB: 1.0
Nuts - $1581_13.1

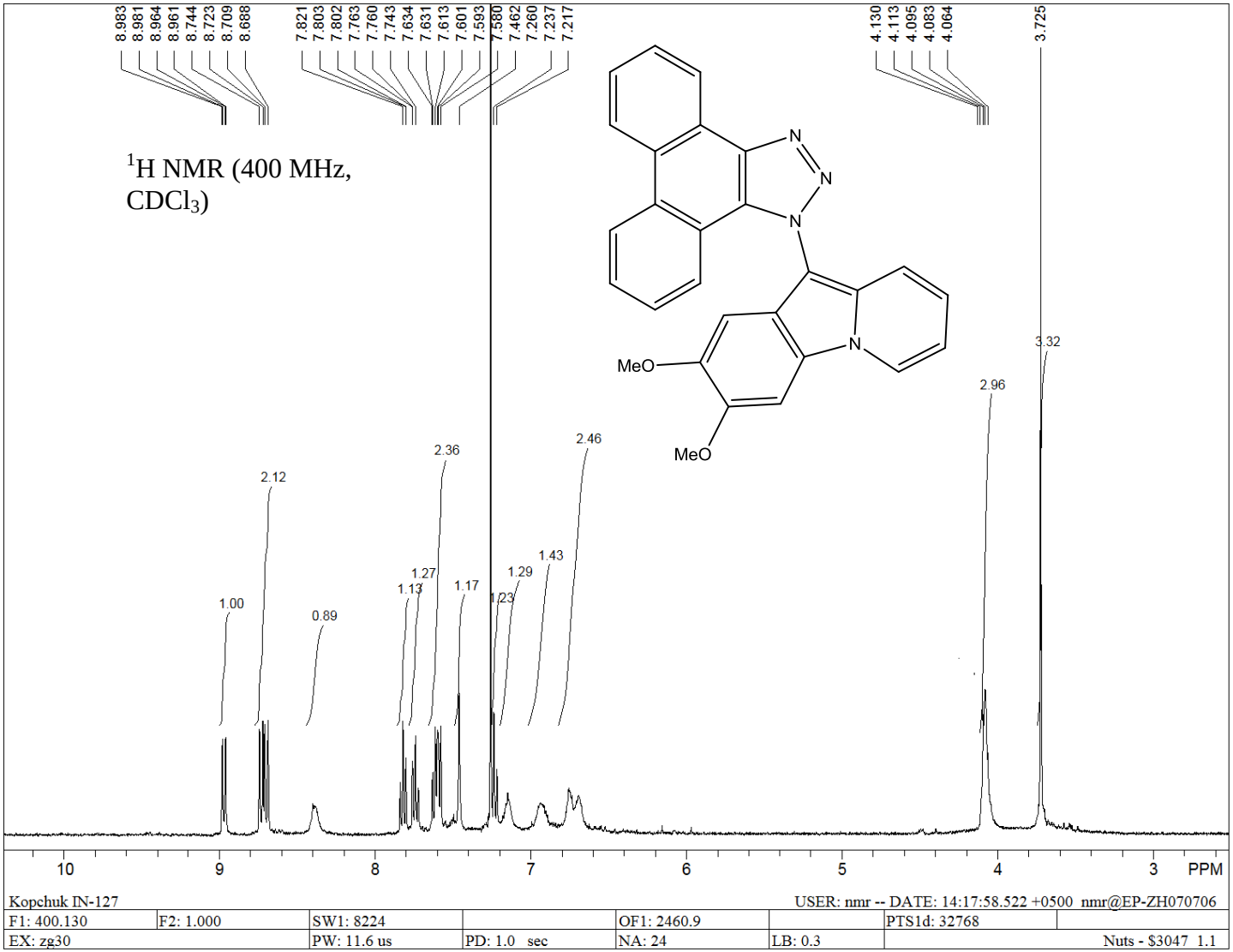

8.300
8.283
7.930
7.927
7.909
7.535
7.516
7.496
7.369
7.260
7.240
7.217
6.889
6.651
4.048
3.930
2.399
1.254
0.008
0.000
-0.008
1H NMR (400 MHz, CDCl3)
Me
N
N
N
MeO
MeO
N
3.30
2.26
1.00
1.31
1.26
1.22
1.05
1.05
3.39
3.30
2.79
10
8
6
4
2
PPM
Hasanov AF454-1
USER: nmr -- DATE: 15:04:03.548 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 32
LB: 0.3
Nuts - $1804 1.1

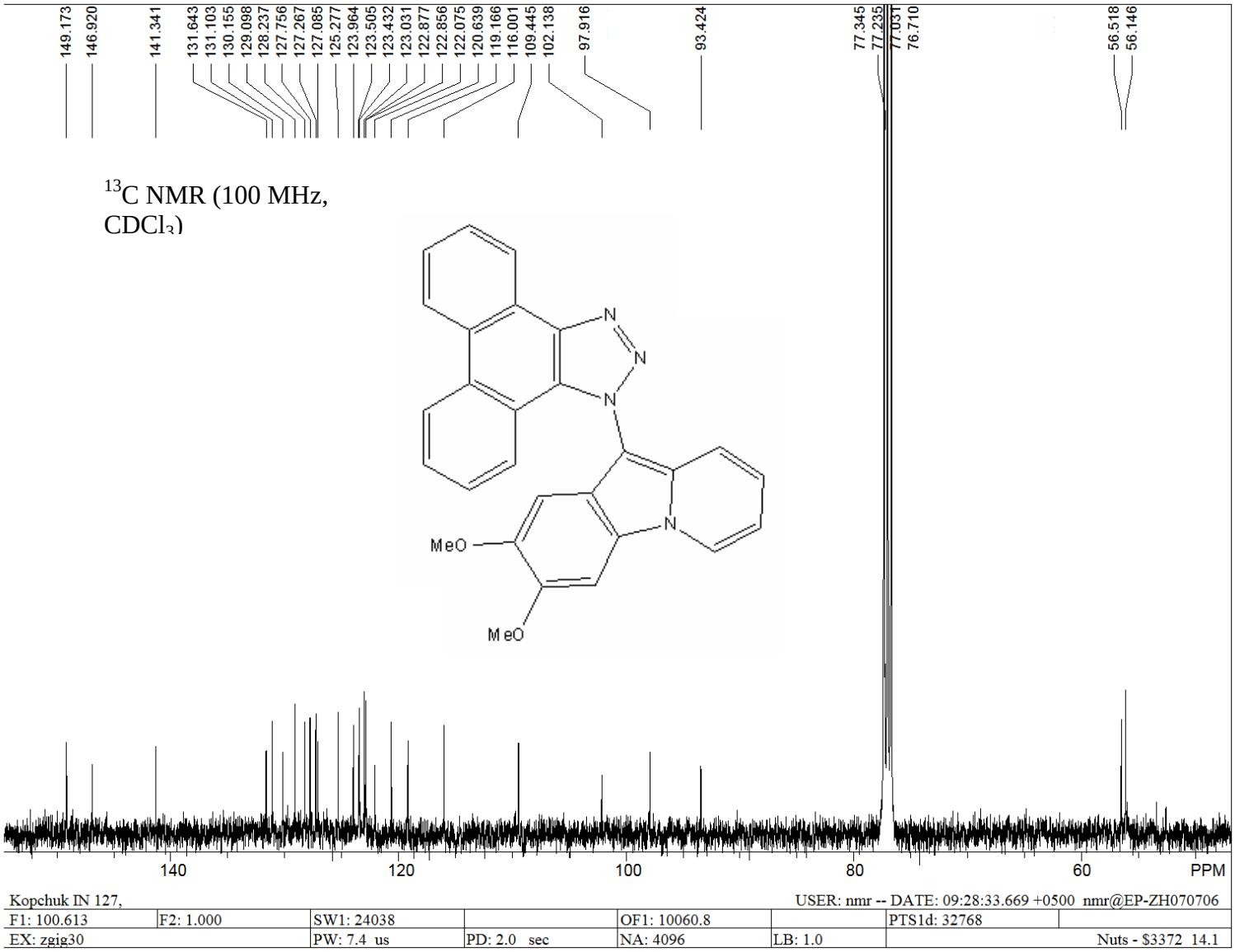

160.527
149.122
146.840
143.784
132.036
131.891
131.191
128.791
127.639
126.881
123.373
122.557
118.998
115.833
109.190
100.643
97.646
93.278
77.600
77.330
77.017
76.696
56.518
56.307
9.804
^{13}C NMR (100 MHz, $CDCl_3$)
N
N
N
Me
N
MeO
MeO
200
150
100
50
PPM
Hasanov AF454-1
USER: nmr -- DATE: 11:44:11.468 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 20480
LB: 1.0
Nuts - $1837 14.1

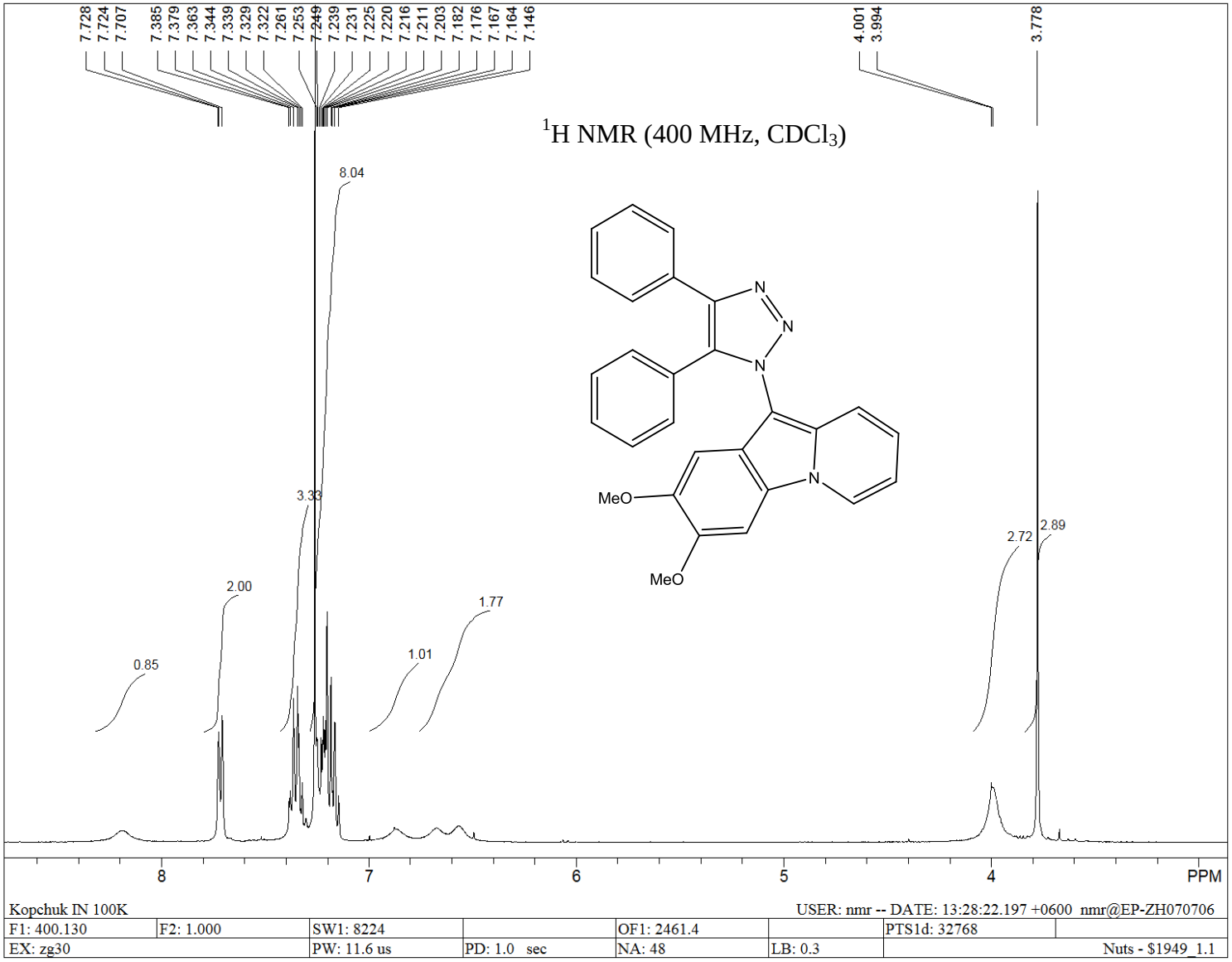
^{1}H NMR (400 MHz, DMSO-d_6)

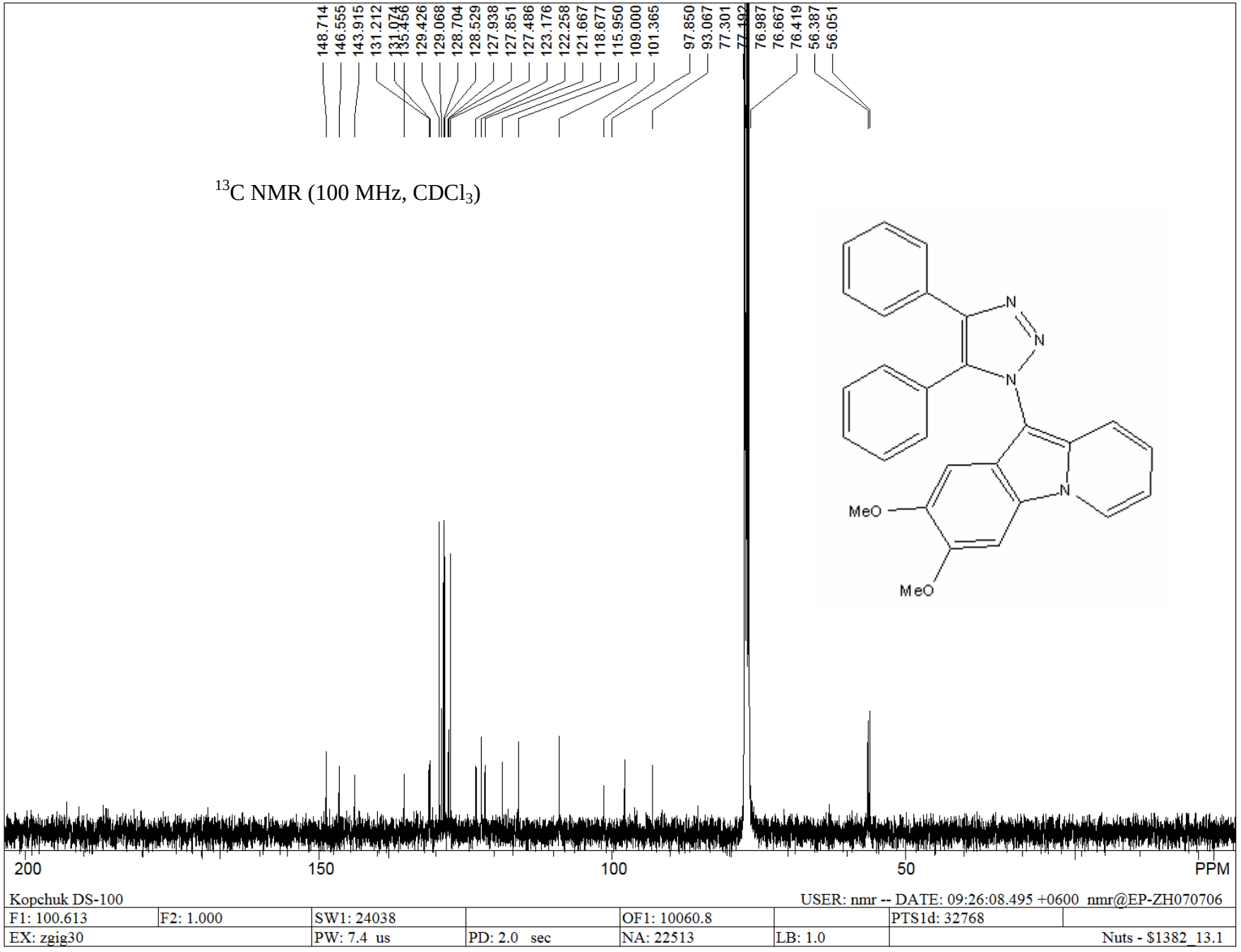


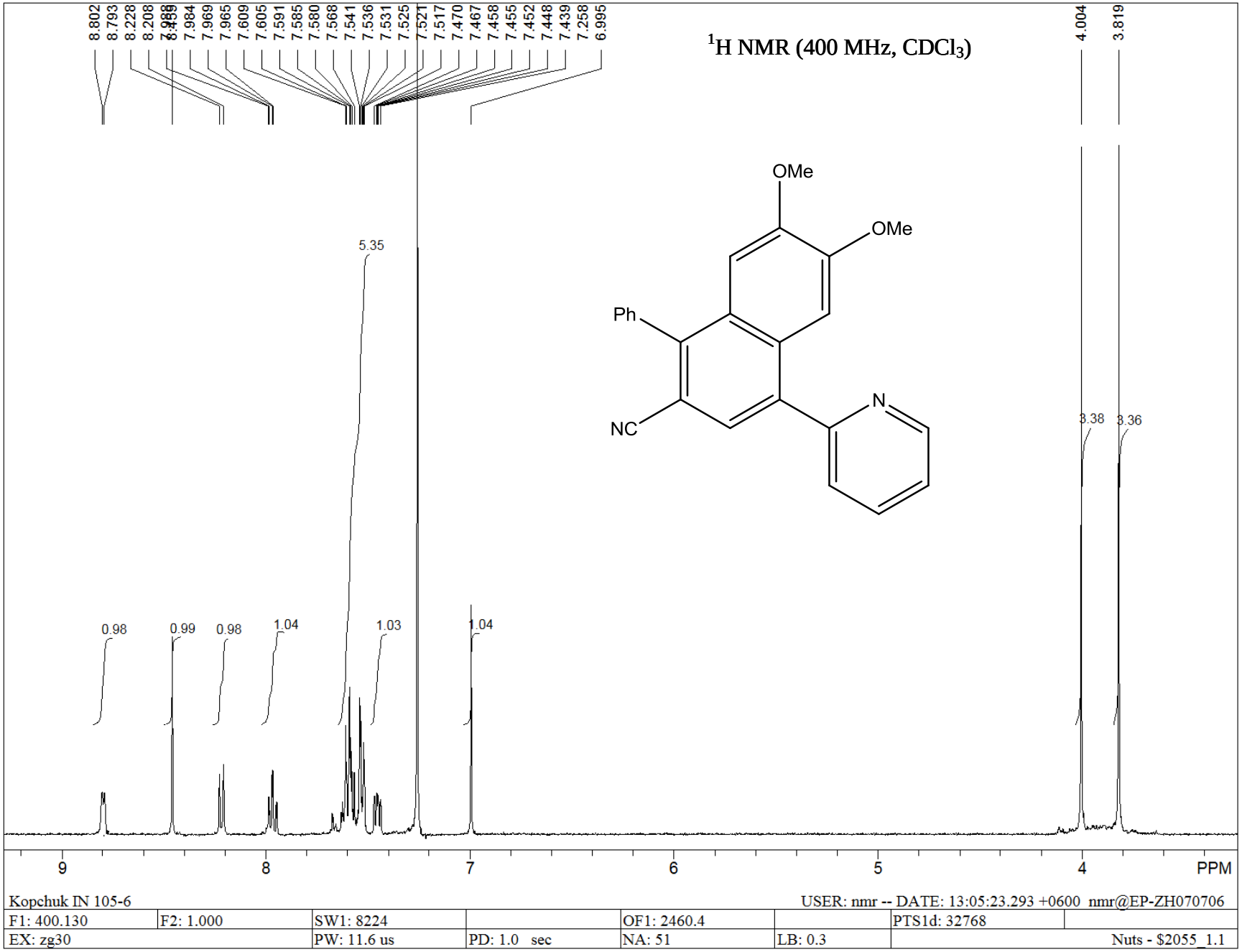

^{1}H NMR (400 MHz, DMSO-d_6)
7.217
6.222
3.716
3.633
3.361
3.26
2.79
1.10
1.14
MeO
COOH
MeO
NH2
8
7
6
5
4
3 PPM
Kopchuk 1315
USER: nmr -- DATE: 13:29:52.732 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2464.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 34
LB: 0.3
Nuts - $1572 1.1

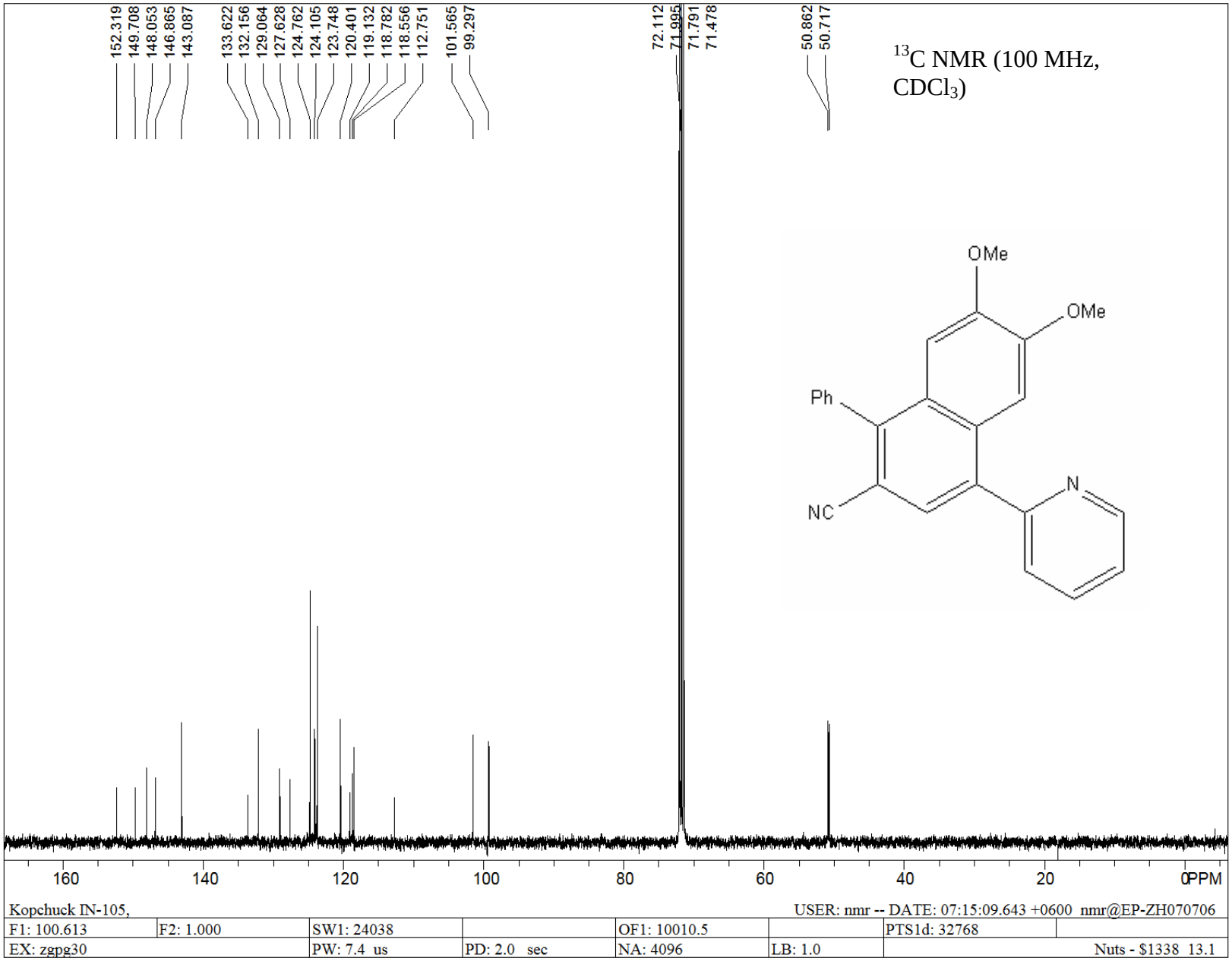

8.983
8.981
8.964
8.961
8.744
8.723
8.709
8.688
7.821
7.803
7.802
7.763
7.760
7.743
7.634
7.631
7.613
7.601
7.593
7.580
7.462
7.260
7.237
7.217
4.130
4.113
4.095
4.083
4.064
3.725
1H NMR (400 MHz, CDCl3)
N
N
N
N
MeO
MeO
3.32
2.96
2.46
2.36
2.12
1.43
1.29
1.27
1.17
1.13
1.23
1.00
0.89
10
9
8
7
6
5
4
3
PPM
Kopchuk IN-127
USER: nmr -- DATE: 14:17:58.522 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 24
LB: 0.3
Nuts - $3047 1.1

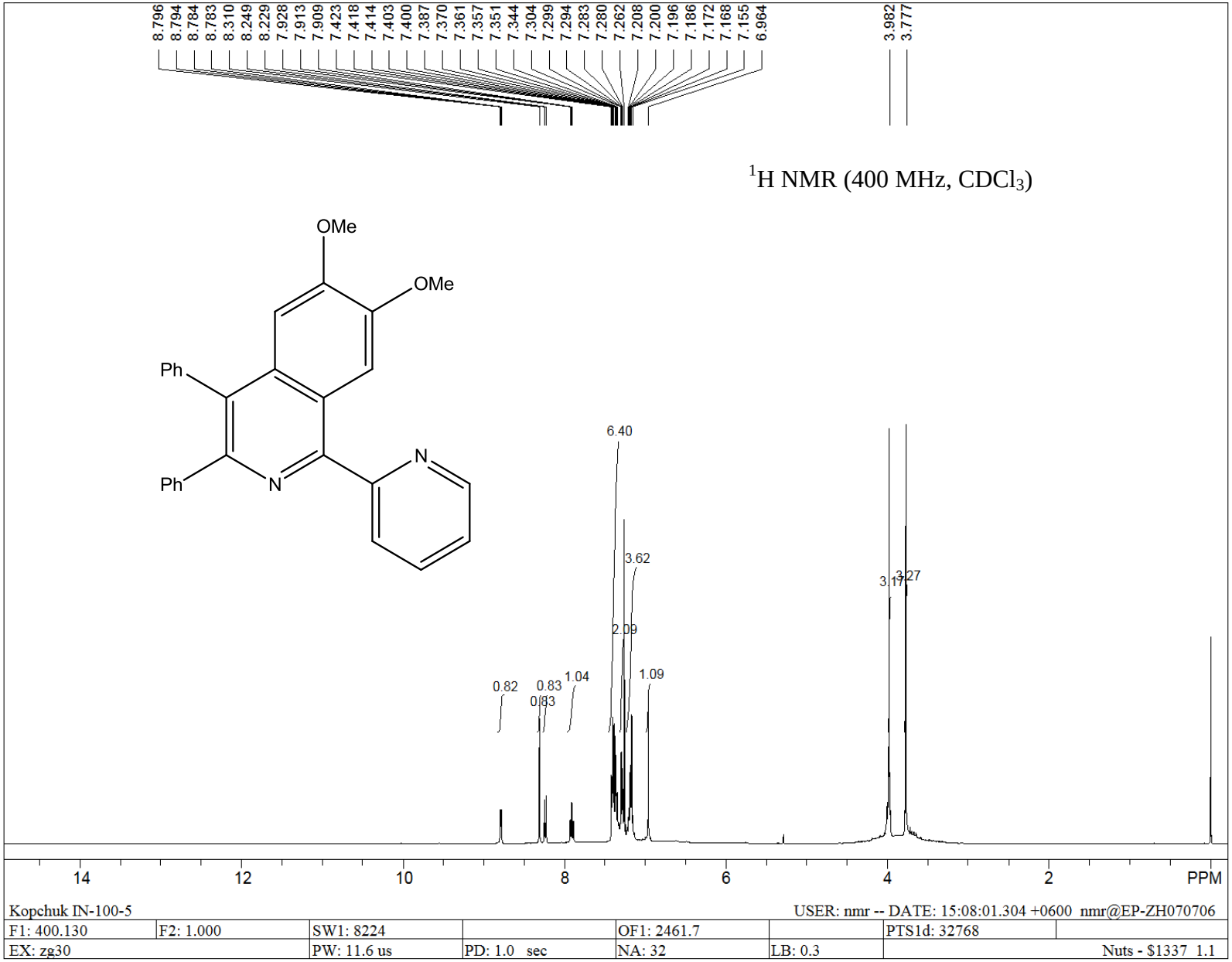

149.173
146.920
141.341
131.643
131.103
130.155
129.098
128.237
127.756
127.267
127.085
125.277
123.964
123.505
123.432
123.031
122.877
122.856
122.075
120.639
119.166
116.001
109.445
102.138
97.916
93.424
77.345
77.235
77.031
76.710
56.518
56.146
13C NMR (100 MHz, CDCl3)
N
N
N
N
MeO
MeO
140
120
100
80
60
PPM
Kopchuk IN 127,
USER: nmr -- DATE: 09:28:33.669 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 4096
LB: 1.0
Nuts - $3372 14.1

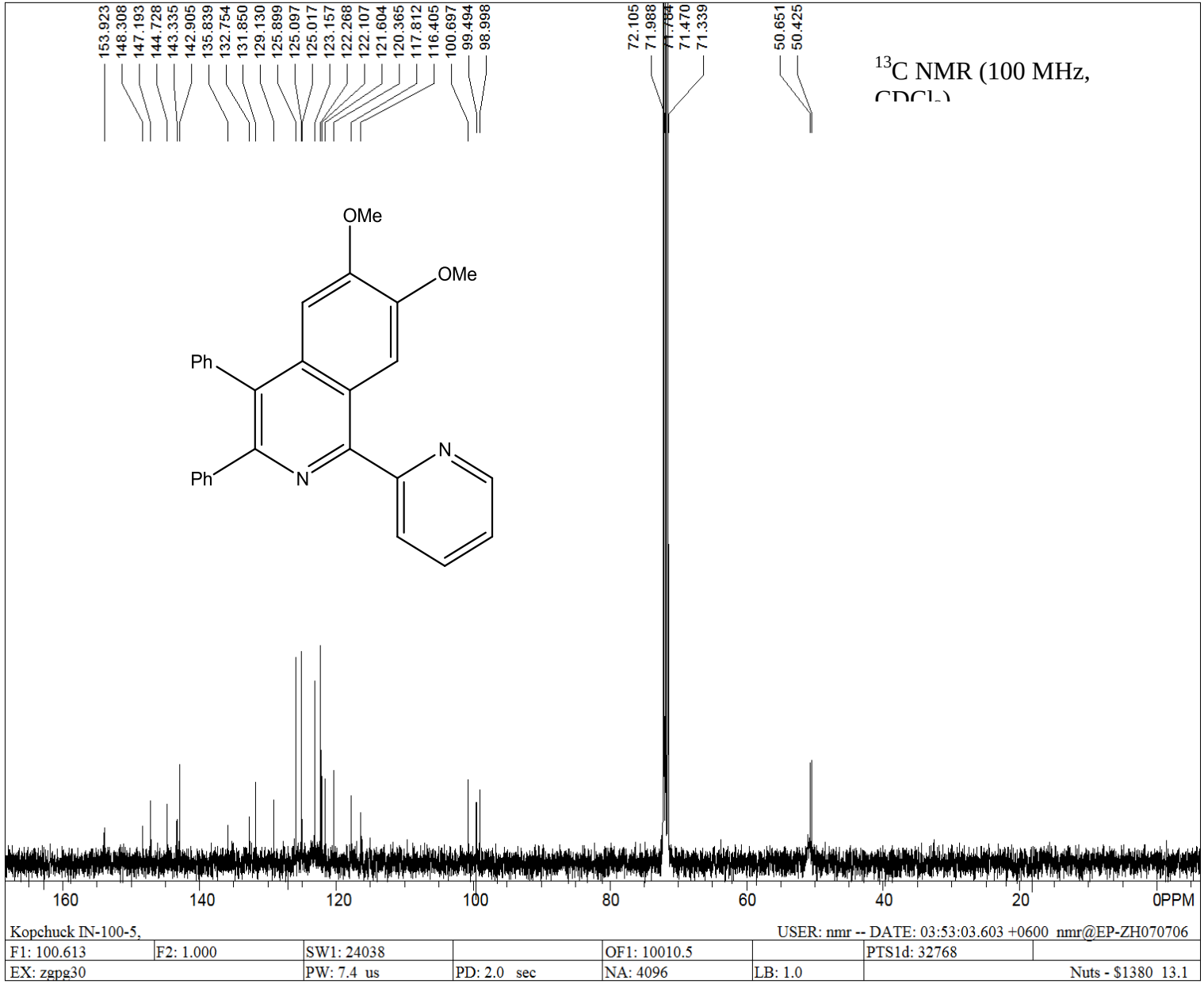

7.728
7.724
7.707
7.385
7.379
7.363
7.344
7.339
7.329
7.322
7.261
7.253
7.249
7.239
7.231
7.225
7.220
7.216
7.211
7.203
7.182
7.176
7.167
7.164
7.146
4.001
3.994
3.778
^{1}H NMR (400 MHz, $CDCl_3$)
8.04
3.33
2.00
0.85
1.01
1.77
2.72
2.89
N
N
N
N
MeO
MeO
8
7
6
5
4
PPM
Kopchuk IN 100K
USER: nmr -- DATE: 13:28:22.197 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 48
LB: 0.3
Nuts - $1949_1.1

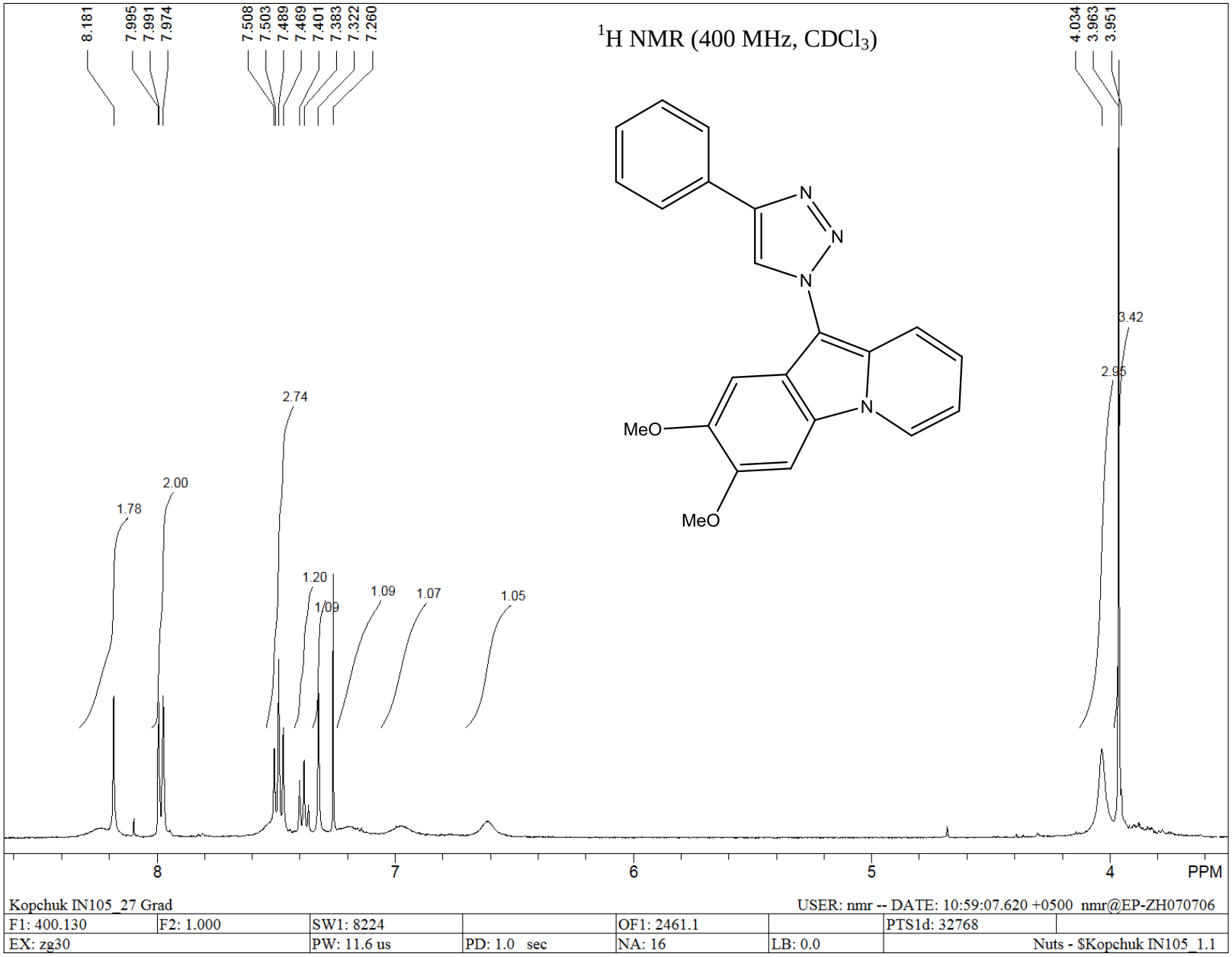

148.714
146.555
143.915
131.212
131.074
135.456
129.426
129.068
128.704
128.529
127.938
127.851
127.486
123.176
122.258
121.667
118.677
115.950
109.000
101.365
97.850
93.067
77.301
77.192
76.987
76.667
76.419
56.387
56.051
^{13}C NMR (100 MHz, $CDCl_3$)
N
N
N
N
MeO
MeO
200
150
100
50
PPM
Kopchuk DS-100
USER: nmr -- DATE: 09:26:08.495 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 22513
LB: 1.0
Nuts - $1382_13.1

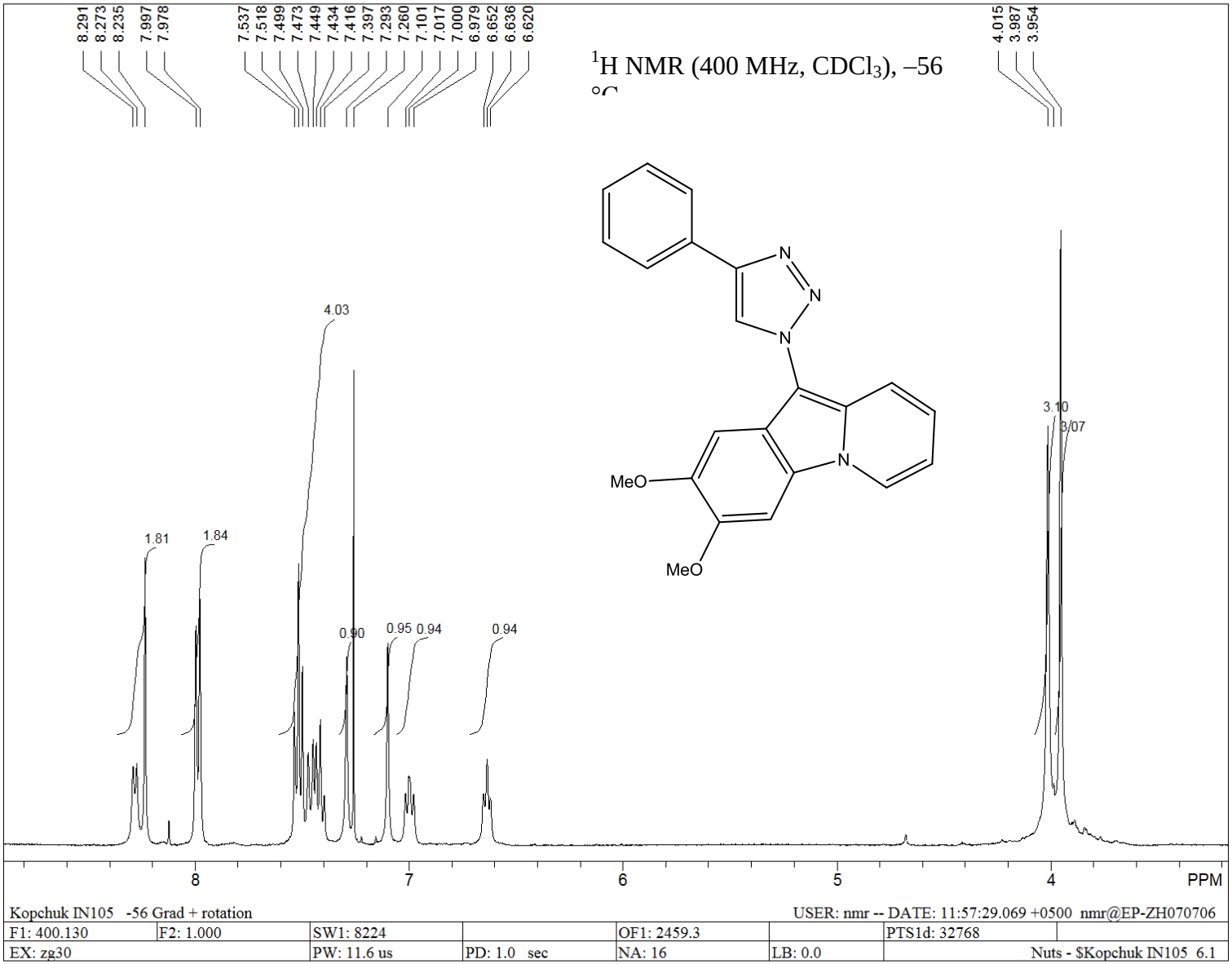

^{1}H NMR (400 MHz, $CDCl_3$)
8.802
8.793
8.228
8.208
7.984
7.969
7.965
7.609
7.605
7.591
7.585
7.580
7.568
7.541
7.536
7.531
7.525
7.521
7.517
7.470
7.467
7.458
7.455
7.452
7.448
7.439
7.258
6.995
4.004
3.819
OMe
OMe
Ph
NC
N
5.35
0.98
0.99
0.98
1.04
1.03
1.04
3.38
3.36
9
8
7
6
5
4
PPM
Kopchuk IN 105-6
USER: nmr -- DATE: 13:05:23.293 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 51
LB: 0.3
Nuts - $2055_1.1

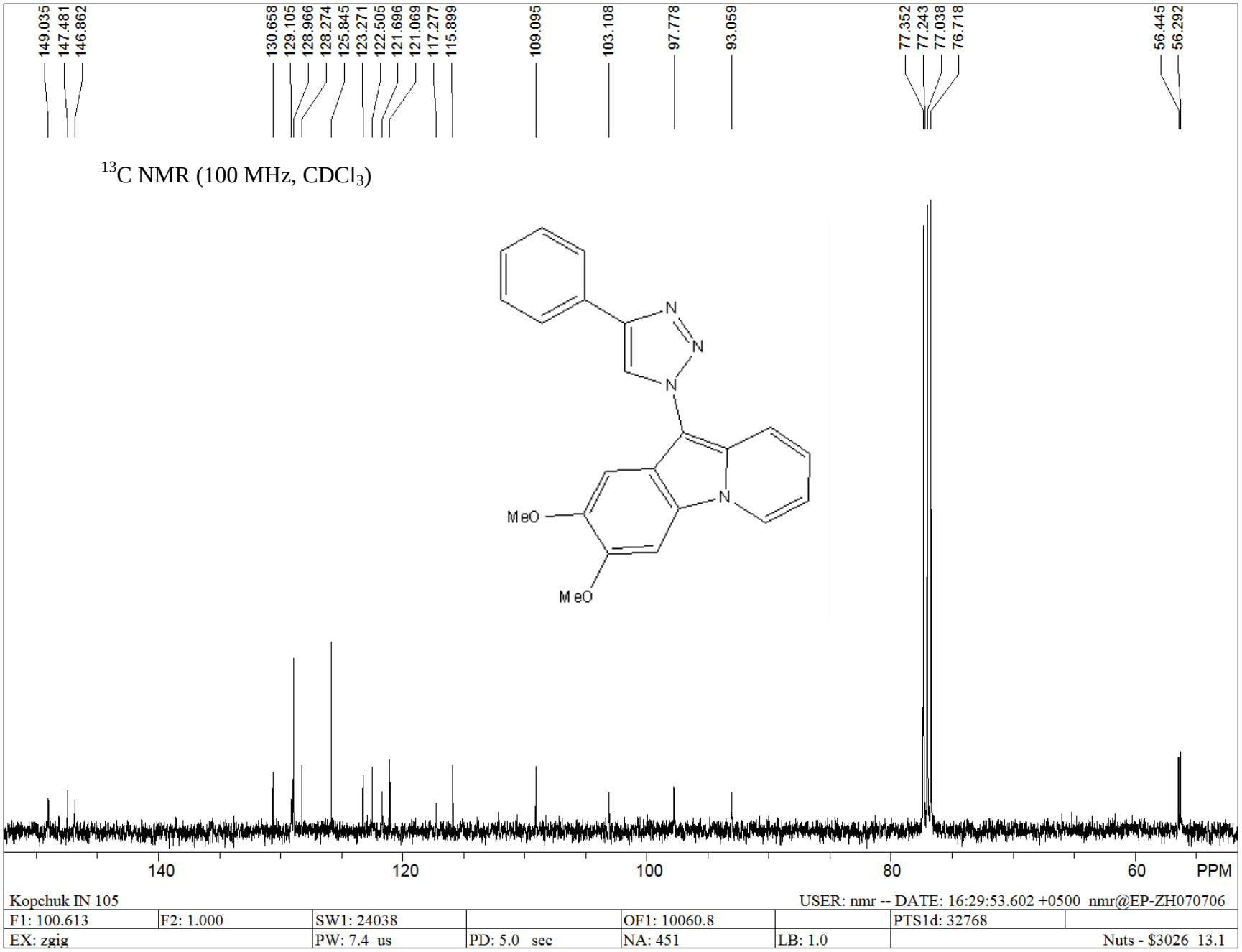

152.319
149.708
148.053
146.865
143.087
133.622
132.156
129.064
127.628
124.762
124.105
123.748
120.401
119.132
118.782
118.556
112.751
101.565
99.297
72.112
71.995
71.791
71.478
50.862
50.717
^{13}C NMR (100 MHz, $CDCl_3$)
OMe
OMe
Ph
NC
N
160
140
120
100
80
60
40
20
0PPM
Kopchuck IN-105,
USER: nmr -- DATE: 07:15:09.643 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10010.5
PTS1d: 32768
EX: zgpg30
PW: 7.4 us
PD: 2.0 sec
NA: 4096
LB: 1.0
Nuts - $1338 13.1

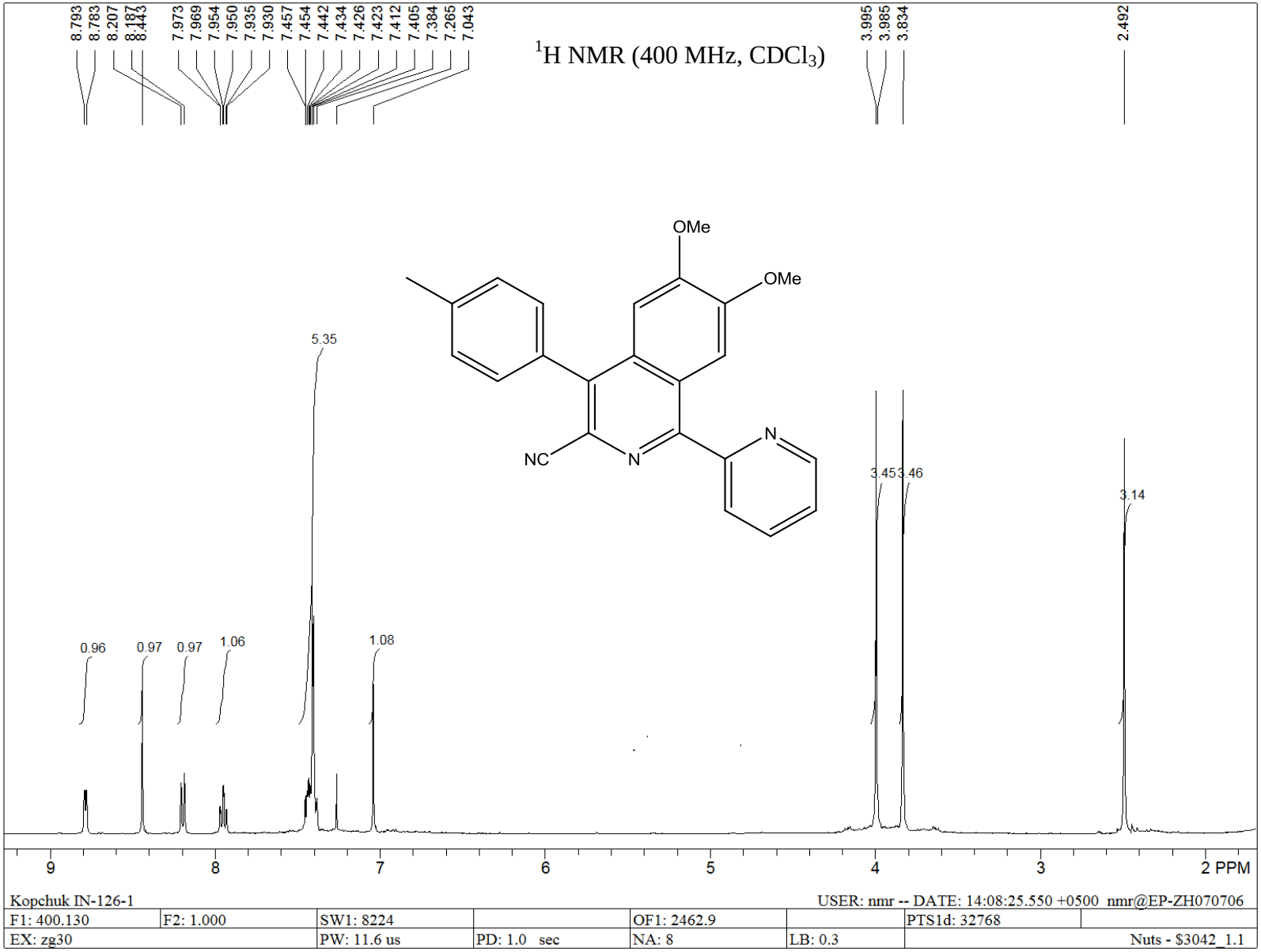

8.796
8.794
8.784
8.783
8.310
8.249
8.229
7.928
7.913
7.909
7.423
7.418
7.414
7.403
7.400
7.387
7.370
7.361
7.357
7.351
7.344
7.304
7.299
7.294
7.283
7.280
7.262
7.208
7.200
7.196
7.186
7.172
7.168
7.155
6.964
3.982
3.777
^{1}H NMR (400 MHz, $CDCl_3$)
OMe
OMe
Ph
Ph
N
N
6.40
3.62
3.17
3.27
2.09
1.09
1.04
0.83
0.83
0.82
14
12
10
8
6
4
2
PPM
Kopchuk IN-100-5
USER: nmr -- DATE: 15:08:01.304 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.7
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 32
LB: 0.3
Nuts - $1337 1.1

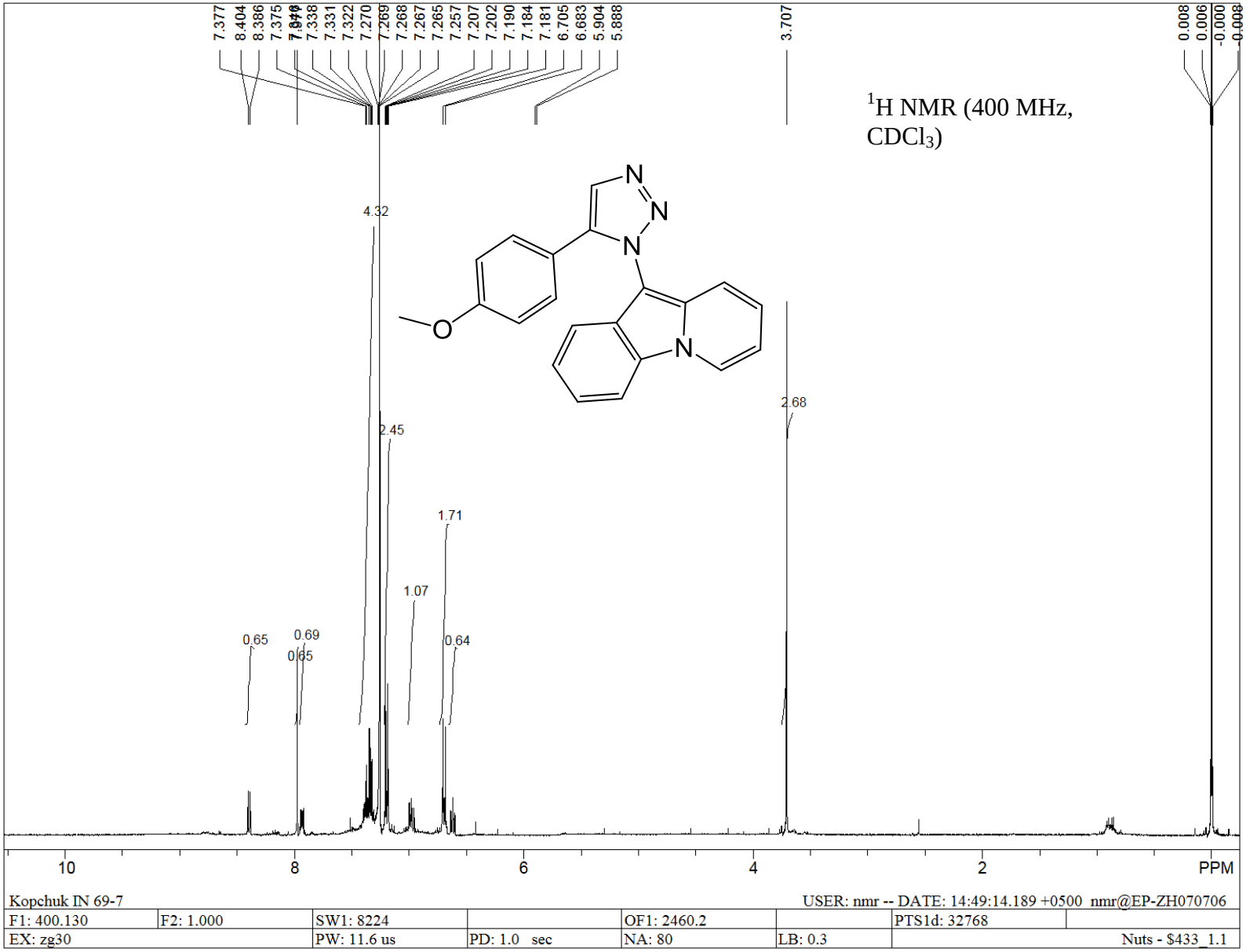

153.923
148.308
147.193
144.728
143.335
142.905
135.839
132.754
131.850
129.130
125.899
125.097
125.017
123.157
122.268
122.107
121.604
120.365
117.812
116.405
100.697
99.494
98.998
72.105
71.988
71.784
71.470
71.339
50.651
50.425
13C NMR (100 MHz,
OMe
OMe
Ph
Ph
N
N
160
140
120
100
80
60
40
20
0PPM
Kopchuck IN-100-5,
USER: nmr -- DATE: 03:53:03.603 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10010.5
PTS1d: 32768
EX: zgpg30
PW: 7.4 us
PD: 2.0 sec
NA: 4096
LB: 1.0
Nuts - $1380 13.1

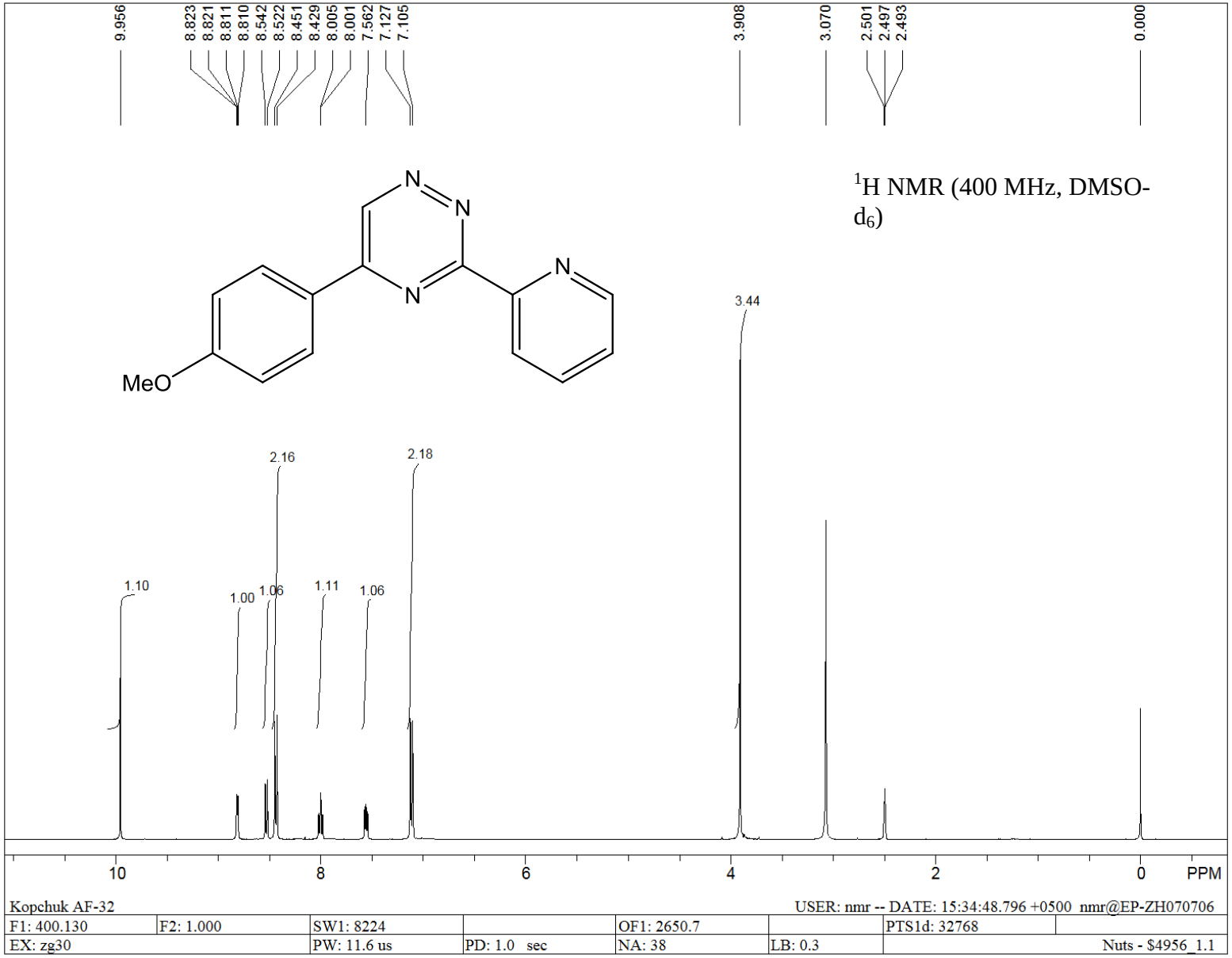

^{1}H NMR (400 MHz, $CDCl_3$)
8.181
7.995
7.991
7.974
7.508
7.503
7.489
7.469
7.401
7.383
7.322
7.260
4.034
3.963
3.951
3.42
2.95
2.74
2.00
1.78
1.20
1.09
1.09
1.07
1.05
MeO
MeO
N
N
N
N
8
7
6
5
4
PPM
Kopchuk IN105_27 Grad
USER: nmr -- DATE: 10:59:07.620 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.1
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $Kopchuk IN105_1.1

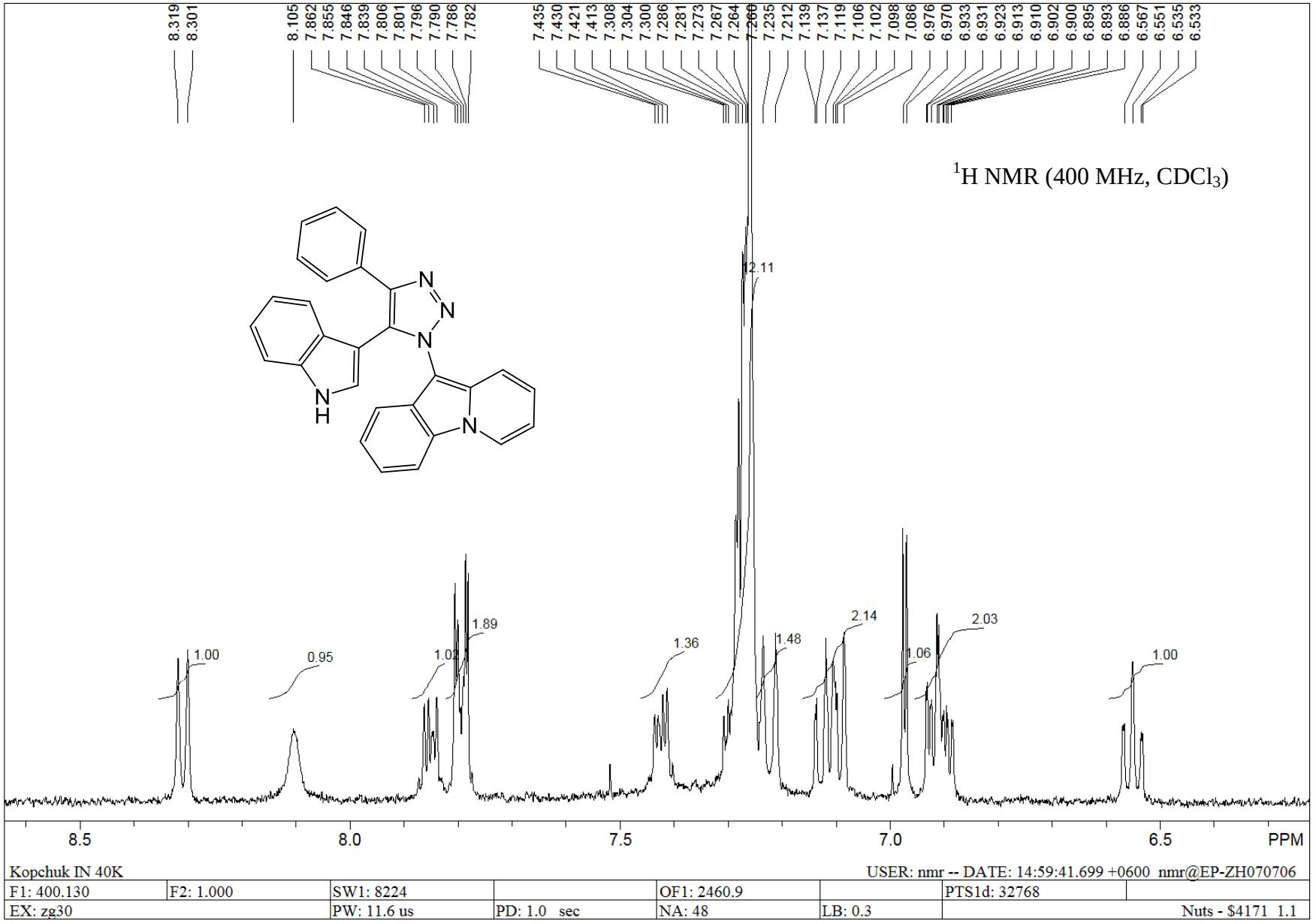

8.291
8.273
8.235
7.997
7.978
7.537
7.518
7.499
7.473
7.449
7.434
7.416
7.397
7.293
7.260
7.101
7.017
7.000
6.979
6.652
6.636
6.620
4.015
3.987
3.954
^{1}H NMR (400 MHz, CDCl$_3$), –56 °C
4.03
1.81
1.84
0.90
0.95
0.94
0.94
3.10
3.07
MeO
MeO
N
N
N
N
8
7
6
5
4
PPM
Kopchuk IN105 -56 Grad + rotation
USER: nmr -- DATE: 11:57:29.069 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2459.3
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $Kopchuk IN105 6.1

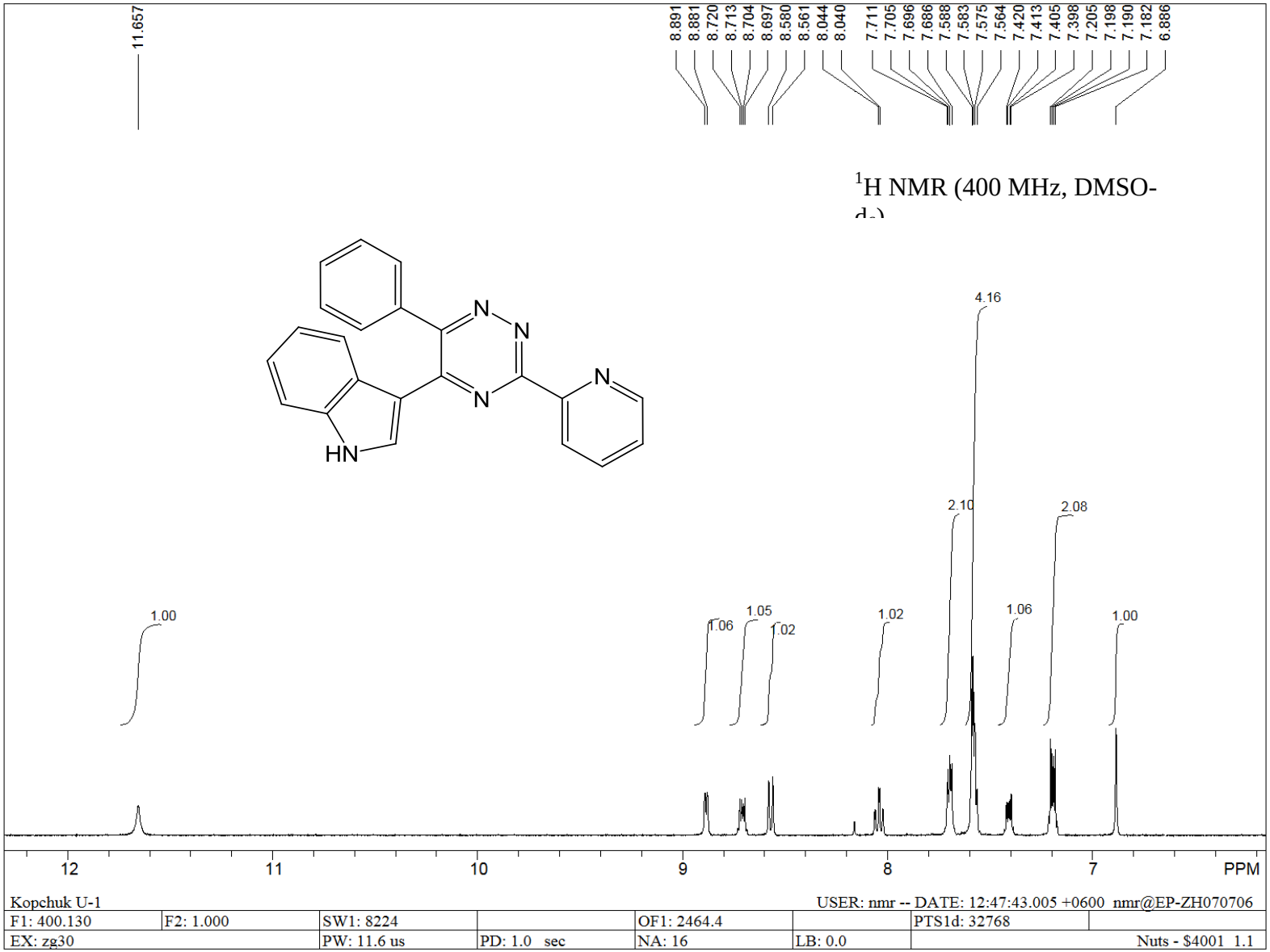

149.035
147.481
146.862
130.658
129.105
128.966
128.274
125.845
123.271
122.505
121.696
121.069
117.277
115.899
109.095
103.108
97.778
93.059
77.352
77.243
77.038
76.718
56.445
56.292
13C NMR (100 MHz, CDCl3)
N
N
N
N
MeO
MeO
140
120
100
80
60
PPM
Kopchuk IN 105
USER: nmr -- DATE: 16:29:53.602 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig
PW: 7.4 us
PD: 5.0 sec
NA: 451
LB: 1.0
Nuts - $3026 13.1

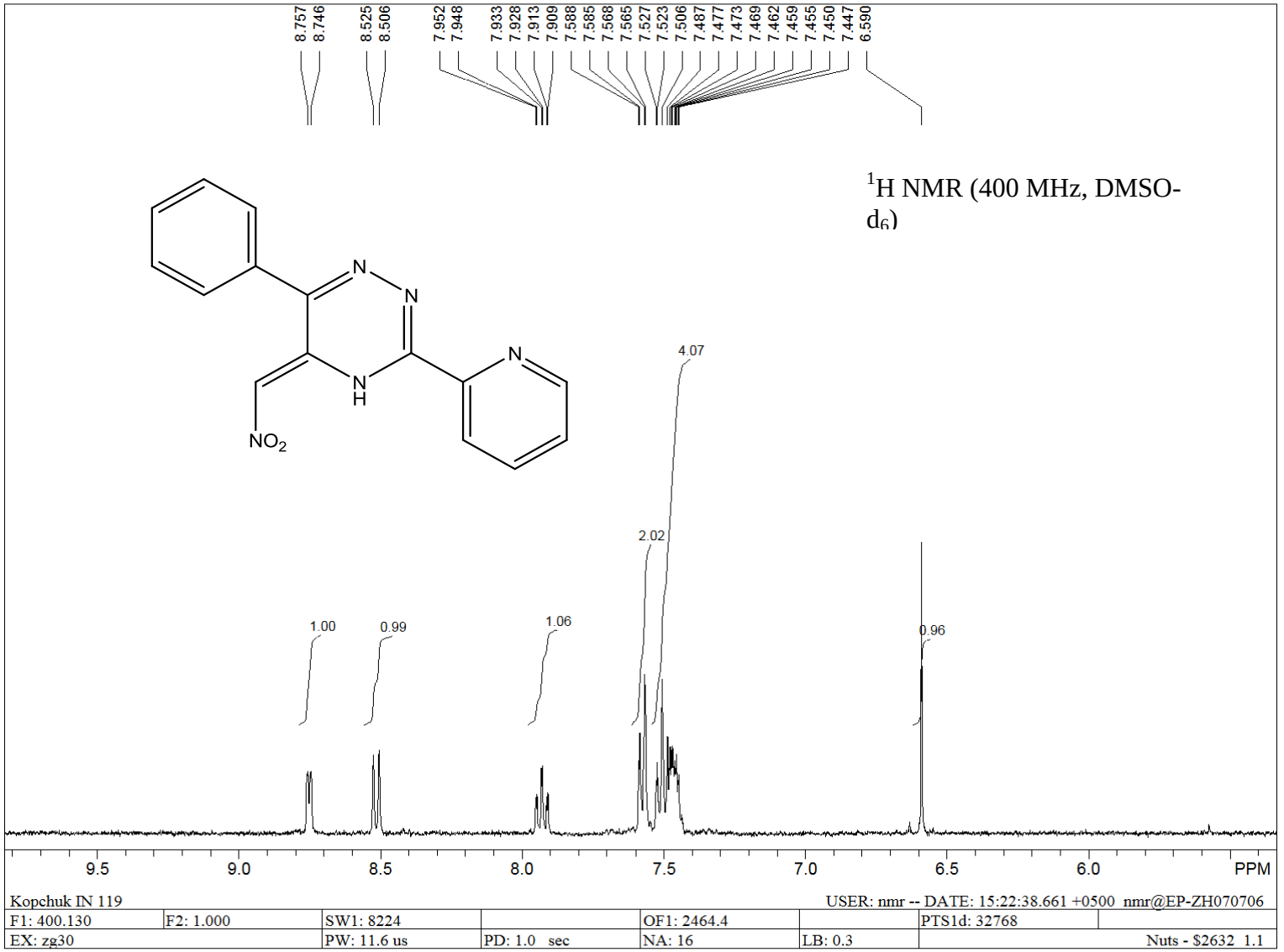

8.793
8.783
8.207
8.187
8.443
7.973
7.969
7.954
7.950
7.935
7.930
7.457
7.454
7.442
7.434
7.426
7.423
7.412
7.405
7.384
7.265
7.043
3.995
3.985
3.834
2.492
^{1}H NMR (400 MHz, $CDCl_3$)
OMe
OMe
N
NC
N
5.35
3.45
3.46
3.14
0.96
0.97
0.97
1.06
1.08
9
8
7
6
5
4
3
2 PPM
Kopchuk IN-126-1
USER: nmr -- DATE: 14:08:25.550 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2462.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 8
LB: 0.3
Nuts - $3042_1.1

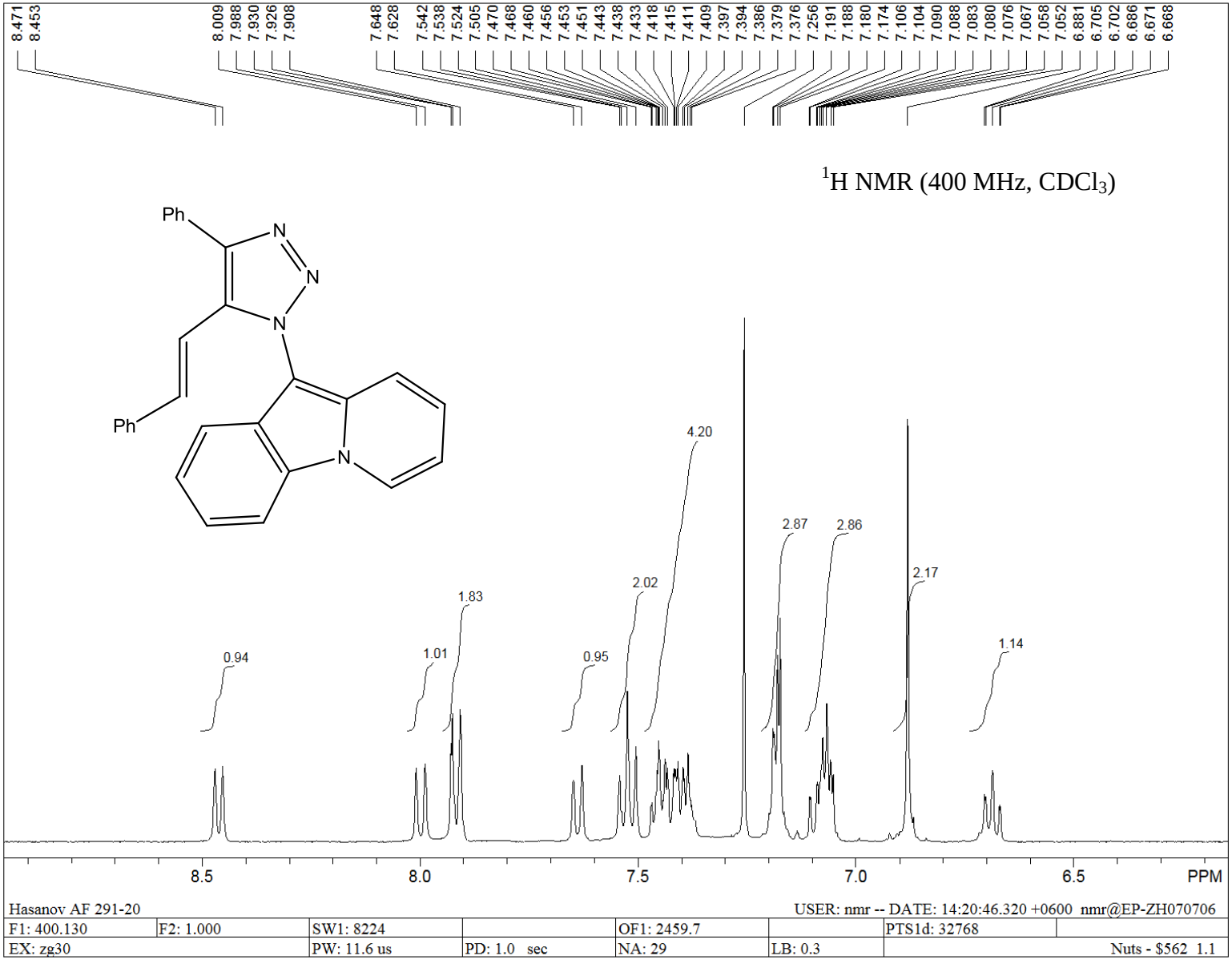

7.377
8.404
8.386
7.375
7.338
7.331
7.322
7.270
7.269
7.268
7.267
7.265
7.257
7.207
7.202
7.190
7.184
7.181
6.705
6.683
5.904
5.888
3.707
0.008
0.006
-0.000
-0.008
^{1}H NMR (400 MHz, $CDCl_3$)
4.32
2.45
2.68
1.71
1.07
0.65
0.69
0.65
0.64
10
8
6
4
2
PPM
Kopchuk IN 69-7
USER: nmr -- DATE: 14:49:14.189 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.2
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 80
LB: 0.3
Nuts - $433_1.1

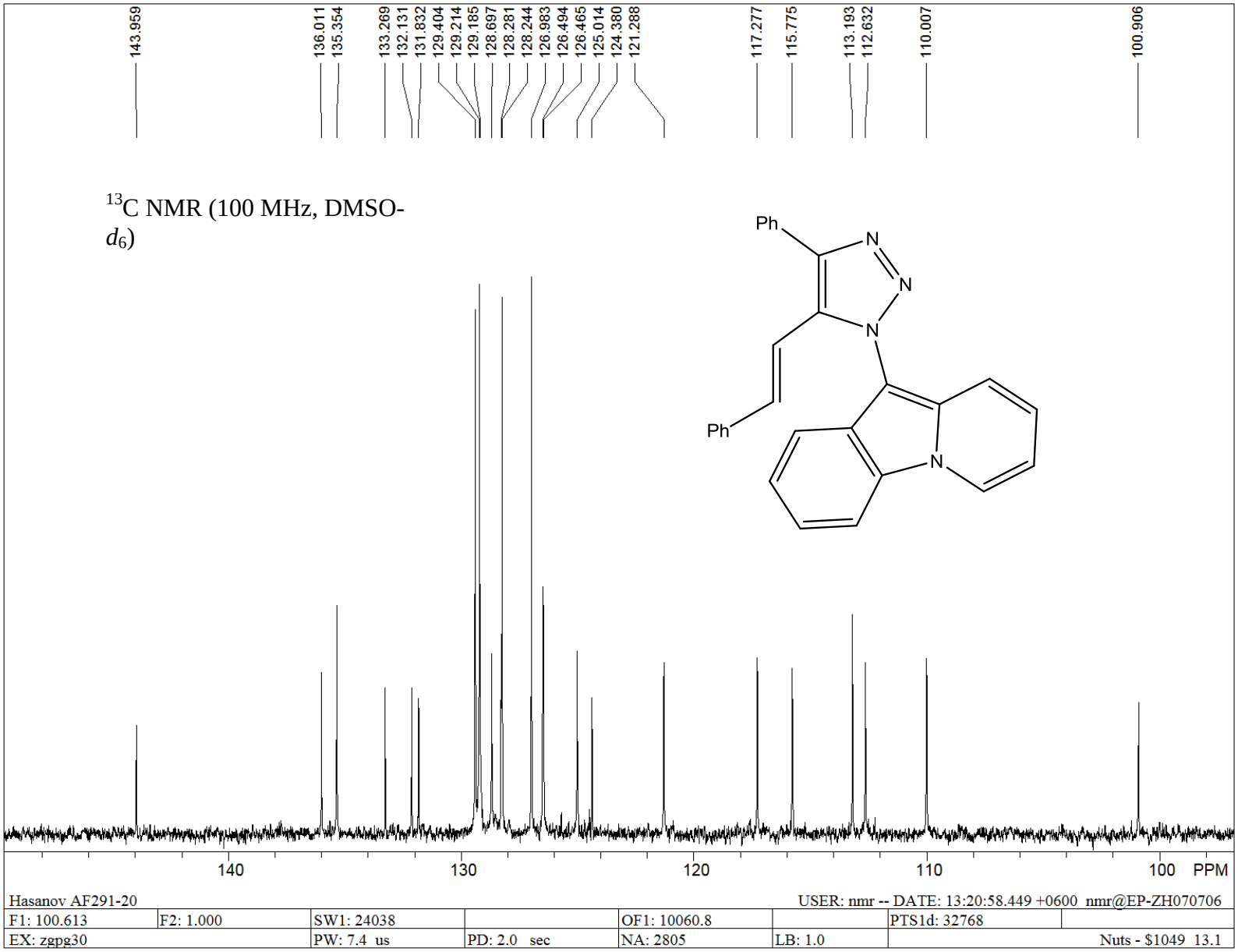

9.956
8.823
8.821
8.811
8.810
8.542
8.522
8.451
8.429
8.005
8.001
7.562
7.127
7.105
3.908
3.070
2.501
2.497
2.493
0.000
N
N
N
N
MeO
^{1}H NMR (400 MHz, DMSO-d_6)
3.44
2.16
2.18
1.10
1.00
1.06
1.11
1.06
10
8
6
4
2
0
PPM
Kopchuk AF-32
USER: nmr -- DATE: 15:34:48.796 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2650.7
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 38
LB: 0.3
Nuts - $4956_1.1

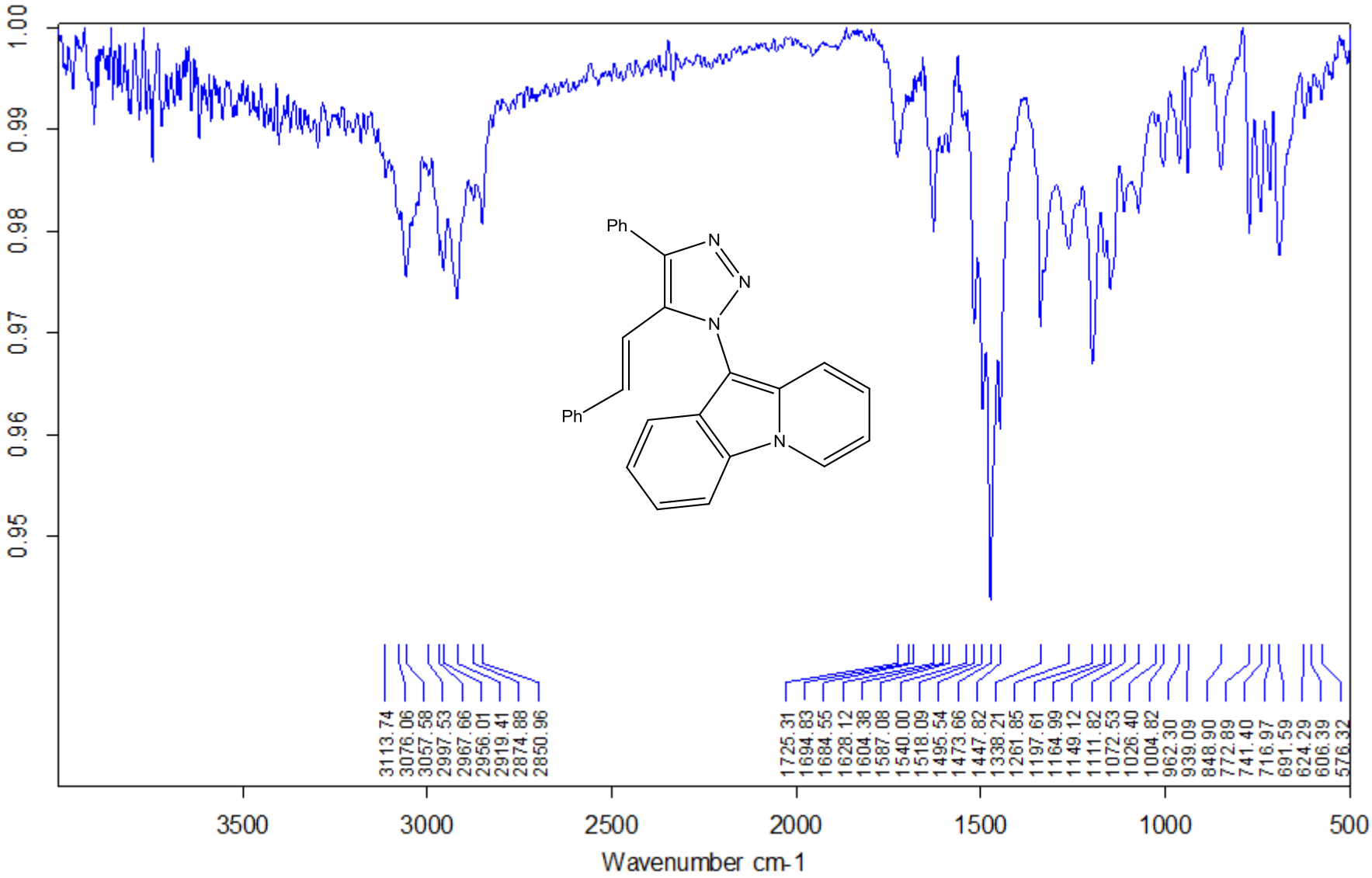

8.319
8.301
8.105
7.862
7.855
7.846
7.839
7.806
7.801
7.796
7.790
7.786
7.782
7.435
7.430
7.421
7.413
7.308
7.304
7.300
7.286
7.281
7.273
7.267
7.264
7.260
7.235
7.212
7.139
7.137
7.119
7.106
7.102
7.098
7.086
6.976
6.970
6.933
6.931
6.923
6.913
6.910
6.902
6.900
6.895
6.893
6.886
6.567
6.551
6.535
6.533
^{1}H NMR (400 MHz, $CDCl_3$)
N
N
N
N
H
12.11
1.00
0.95
1.02
1.89
1.36
1.48
2.14
1.06
2.03
1.00
8.5
8.0
7.5
7.0
6.5
PPM
Kopchuk IN 40K
USER: nmr -- DATE: 14:59:41.699 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 48
LB: 0.3
Nuts - $4171 1.1

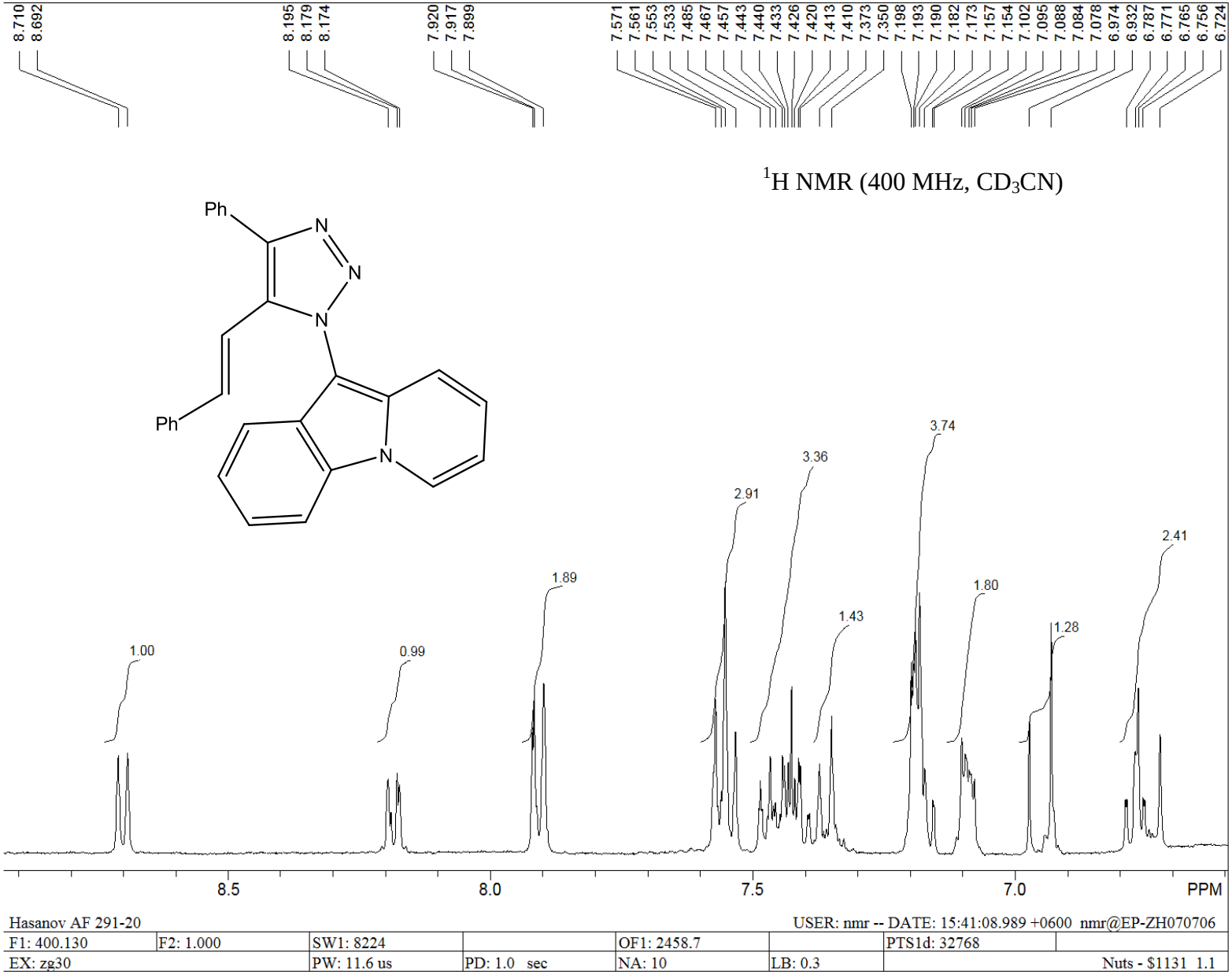

11.657
8.891
8.881
8.720
8.713
8.704
8.697
8.580
8.561
8.044
8.040
7.711
7.705
7.696
7.686
7.588
7.583
7.575
7.564
7.420
7.413
7.405
7.398
7.205
7.198
7.190
7.182
6.886
1H NMR (400 MHz, DMSO-
N
N
N
HN
4.16
2.10
2.08
1.00
1.06
1.05
1.02
1.02
1.06
1.00
12
11
10
9
8
7
PPM
Kopchuk U-1
USER: nmr -- DATE: 12:47:43.005 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2464.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $4001 1.1

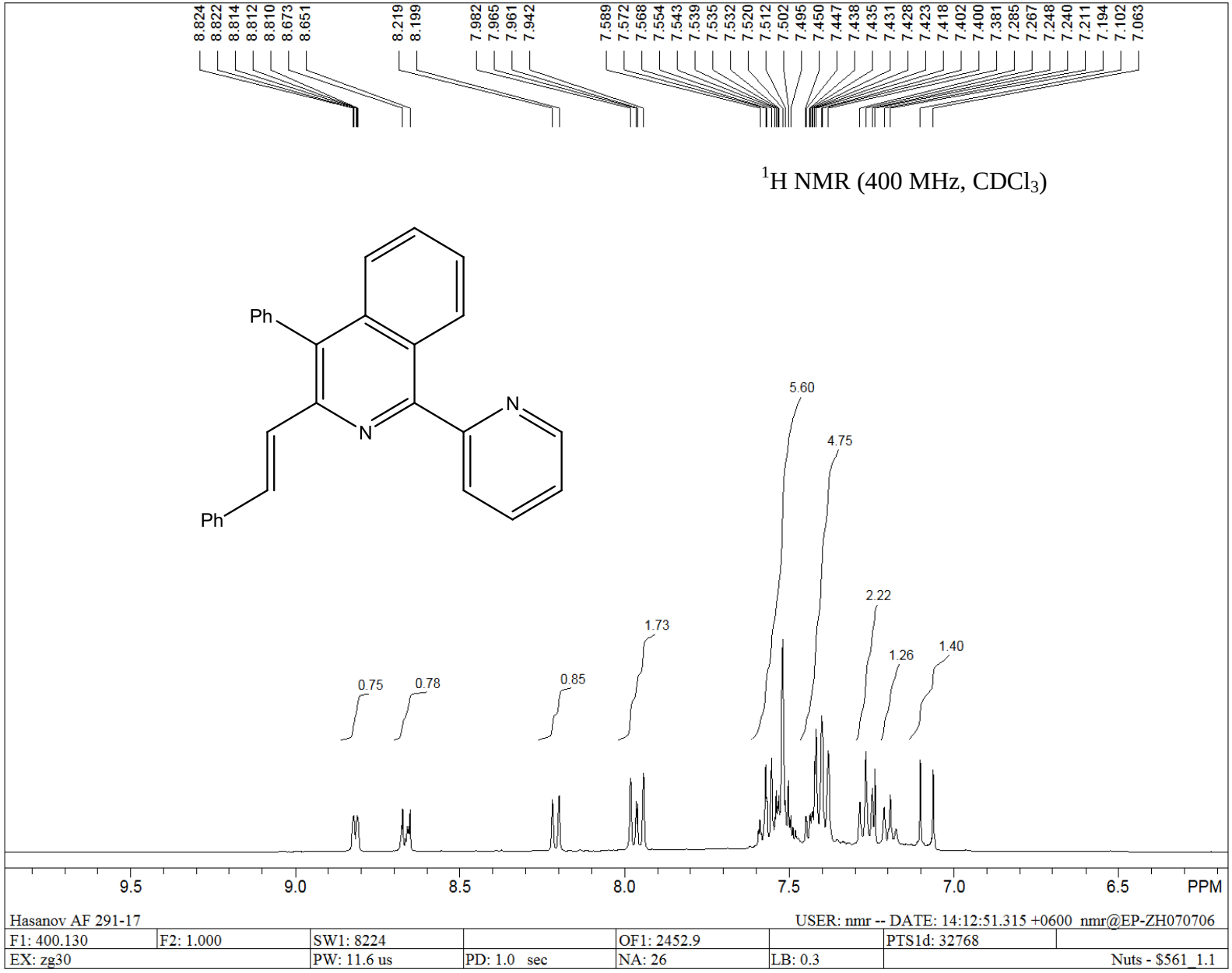

8.757
8.746
8.525
8.506
7.952
7.948
7.933
7.928
7.913
7.909
7.588
7.585
7.568
7.565
7.527
7.523
7.506
7.487
7.477
7.473
7.469
7.462
7.459
7.455
7.450
7.447
6.590
^{1}H NMR (400 MHz, DMSO-d_6)
N
N
N
H
NO_2
4.07
2.02
1.00
0.99
1.06
0.96
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
PPM
Kopchuk IN 119
USER: nmr -- DATE: 15:22:38.661 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2464.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $2632 1.1

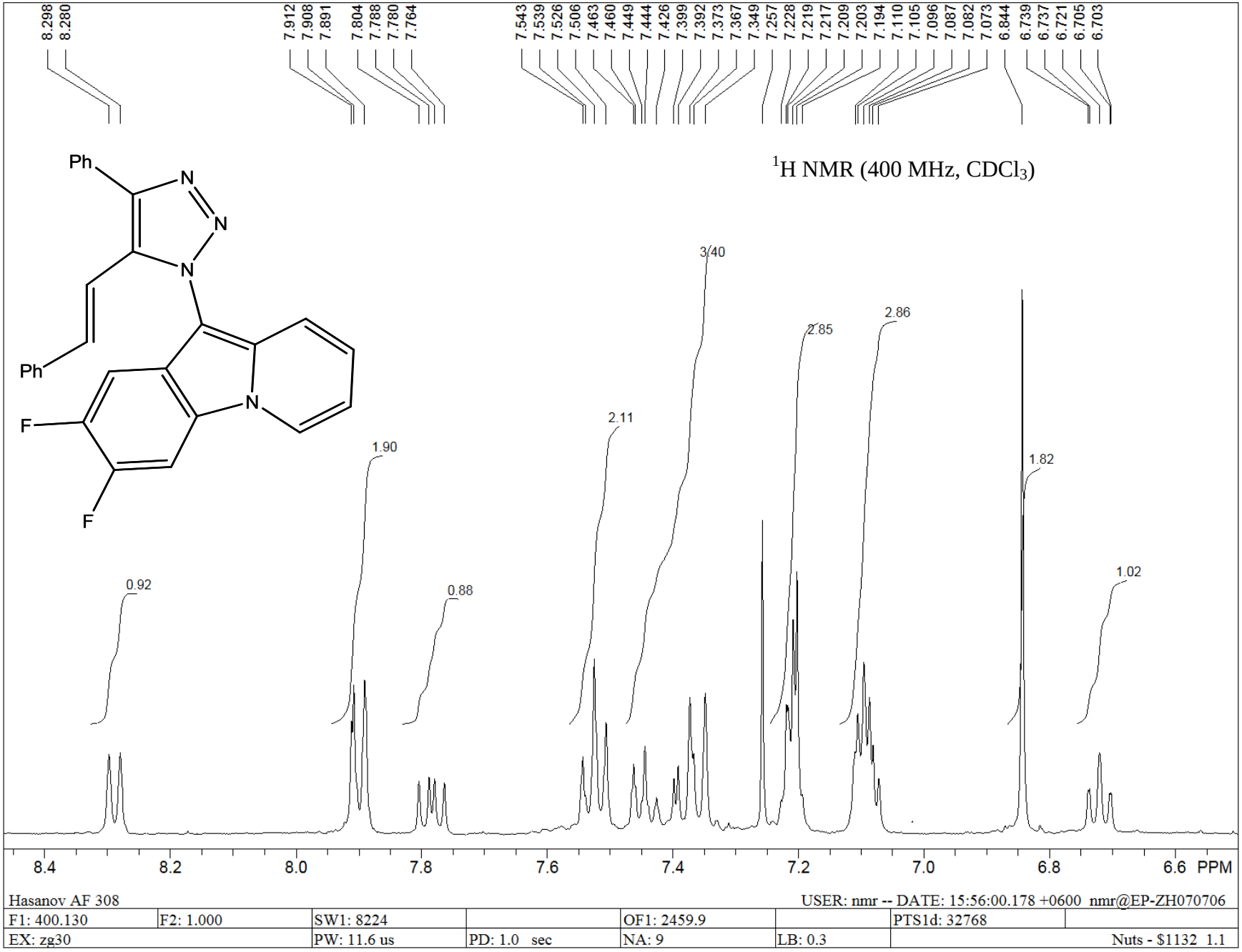

8.471
8.453
8.009
7.988
7.930
7.926
7.908
7.648
7.628
7.542
7.538
7.524
7.505
7.470
7.468
7.460
7.456
7.453
7.451
7.443
7.438
7.433
7.418
7.415
7.411
7.409
7.397
7.394
7.386
7.379
7.376
7.256
7.191
7.188
7.180
7.174
7.106
7.104
7.090
7.088
7.083
7.080
7.076
7.067
7.058
7.052
6.881
6.705
6.702
6.686
6.671
6.668
1H NMR (400 MHz, CDCl3)
Ph
N
N
N
Ph
N
0.94
1.01
1.83
0.95
2.02
4.20
2.87
2.86
2.17
1.14
8.5
8.0
7.5
7.0
6.5
PPM
Hasanov AF 291-20
USER: nmr -- DATE: 14:20:46.320 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2459.7
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 29
LB: 0.3
Nuts - $562 1.1


143.959
136.011
135.354
133.269
132.131
131.832
129.404
129.214
129.185
128.697
128.281
128.244
126.983
126.494
126.465
125.014
124.380
121.288
117.277
115.775
113.193
112.632
110.007
100.906
^{13}C NMR (100 MHz, DMSO-d_6)
Ph
N
N
N
Ph
N
140
130
120
110
100
PPM
Hasanov AF291-20
USER: nmr -- DATE: 13:20:58.449 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgpg30
PW: 7.4 us
PD: 2.0 sec
NA: 2805
LB: 1.0
Nuts - $1049 13.1

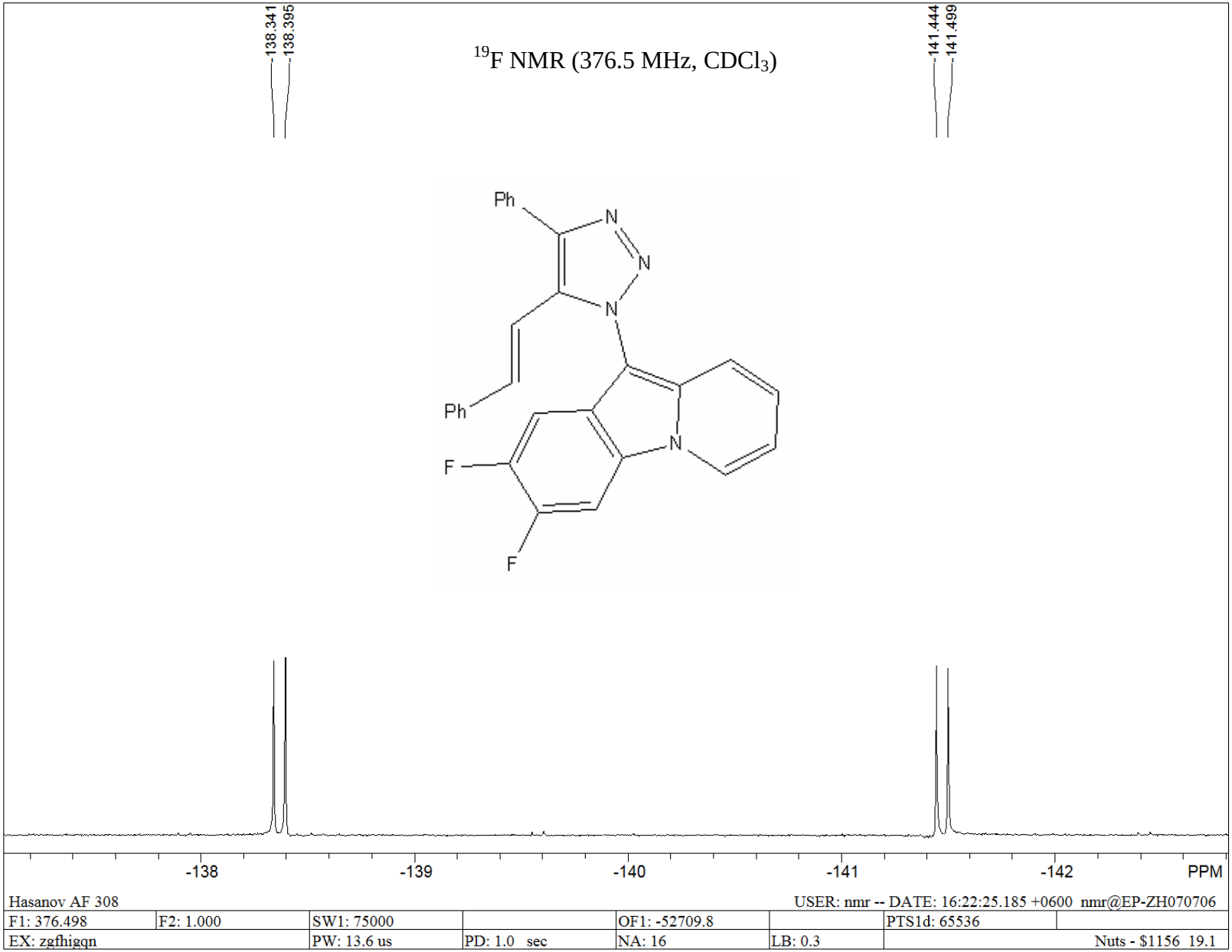

1.00
0.99
0.98
0.97
0.96
0.95
Ph
N
N
N
Ph
3113.74
3076.06
3057.58
2997.53
2967.66
2956.01
2919.41
2874.88
2850.96
1725.31
1694.83
1684.55
1628.12
1604.38
1587.08
1540.00
1518.09
1495.54
1473.66
1447.82
1338.21
1261.85
1197.61
1164.99
1149.12
1111.82
1072.53
1026.40
1004.82
962.30
939.09
848.90
772.89
741.40
716.97
691.59
624.29
606.39
576.32
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

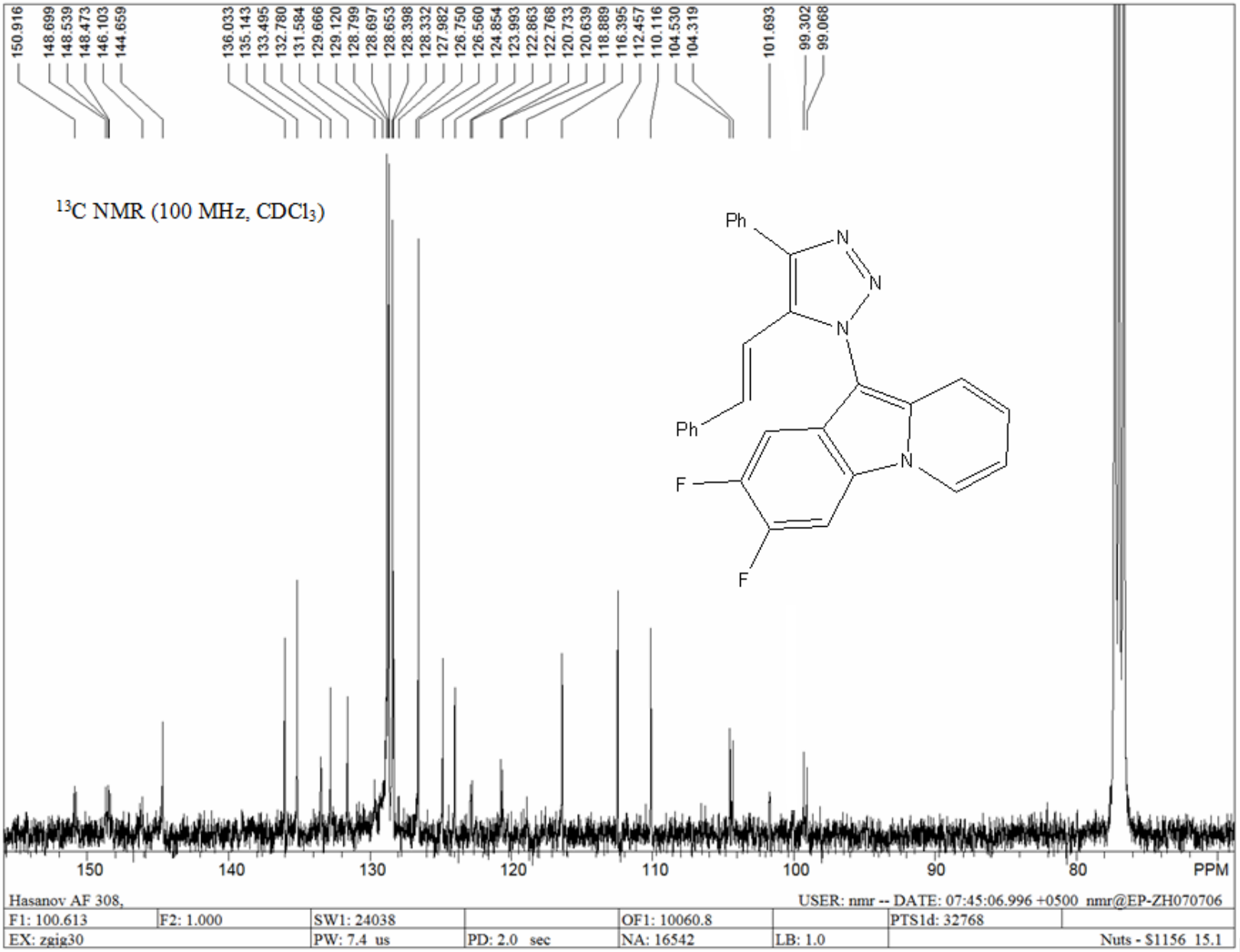

8.710
8.692
8.195
8.179
8.174
7.920
7.917
7.899
7.571
7.561
7.553
7.533
7.485
7.467
7.457
7.443
7.440
7.433
7.426
7.420
7.413
7.410
7.373
7.350
7.198
7.193
7.190
7.182
7.173
7.157
7.154
7.102
7.095
7.088
7.084
7.078
6.974
6.932
6.787
6.771
6.765
6.756
6.724
1H NMR (400 MHz, CD3CN)
Ph
N
N
N
Ph
N
1.00
0.99
1.89
2.91
3.36
1.43
3.74
1.80
1.28
2.41
8.5
8.0
7.5
7.0
PPM
Hasanov AF 291-20
USER: nmr -- DATE: 15:41:08.989 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2458.7
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 10
LB: 0.3
Nuts - $1131 1.1

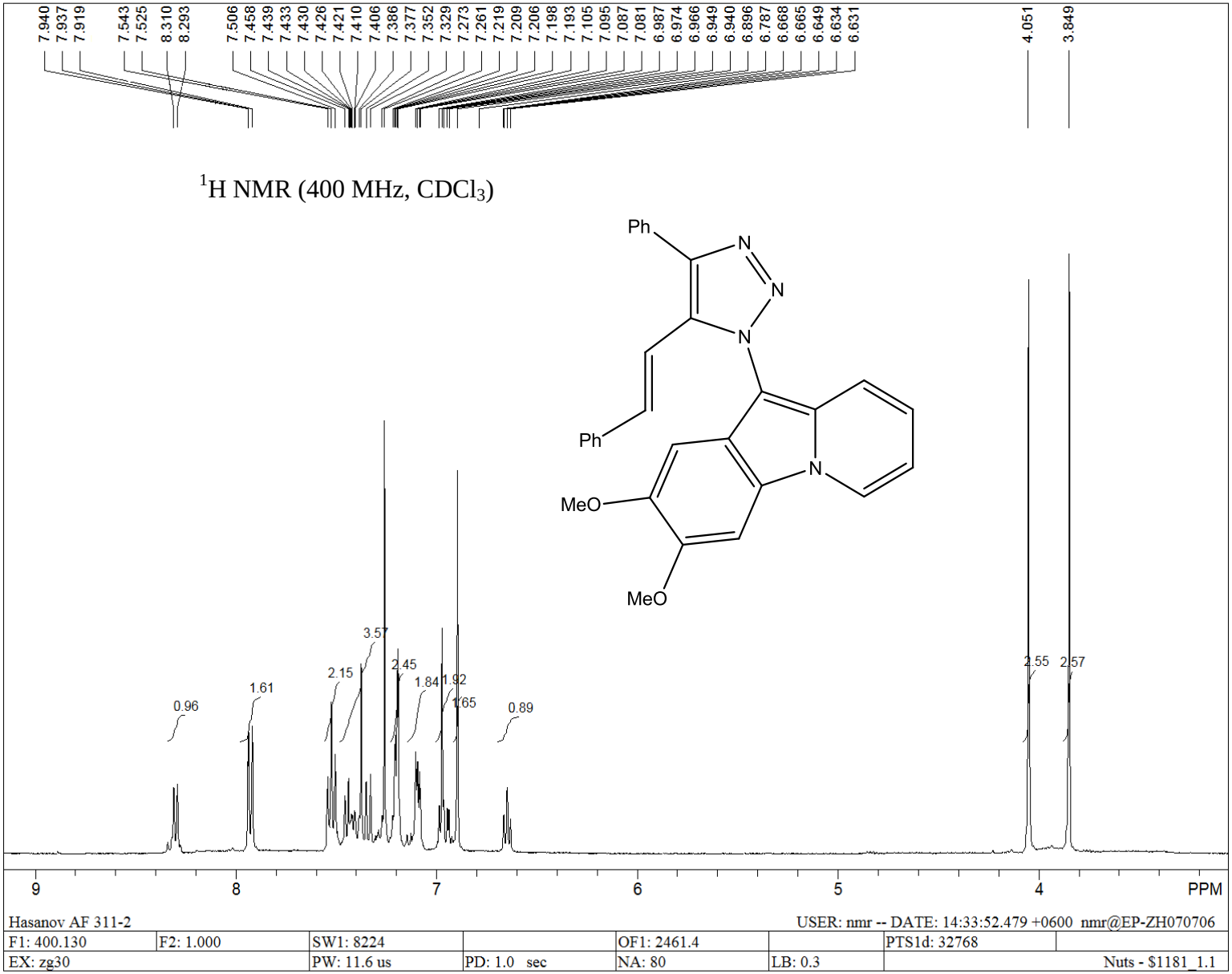

8.824
8.822
8.814
8.812
8.810
8.673
8.651
8.219
8.199
7.982
7.965
7.961
7.942
7.589
7.572
7.568
7.554
7.543
7.539
7.535
7.532
7.520
7.512
7.502
7.495
7.450
7.447
7.438
7.435
7.431
7.428
7.423
7.418
7.402
7.400
7.381
7.285
7.267
7.248
7.240
7.211
7.194
7.102
7.063
^{1}H NMR (400 MHz, $CDCl_3$)
Ph
N
N
Ph
5.60
4.75
2.22
1.73
1.26
1.40
0.75
0.78
0.85
9.5
9.0
8.5
8.0
7.5
7.0
6.5
PPM
Hasanov AF 291-17
USER: nmr -- DATE: 14:12:51.315 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2452.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 26
LB: 0.3
Nuts - $561_1.1

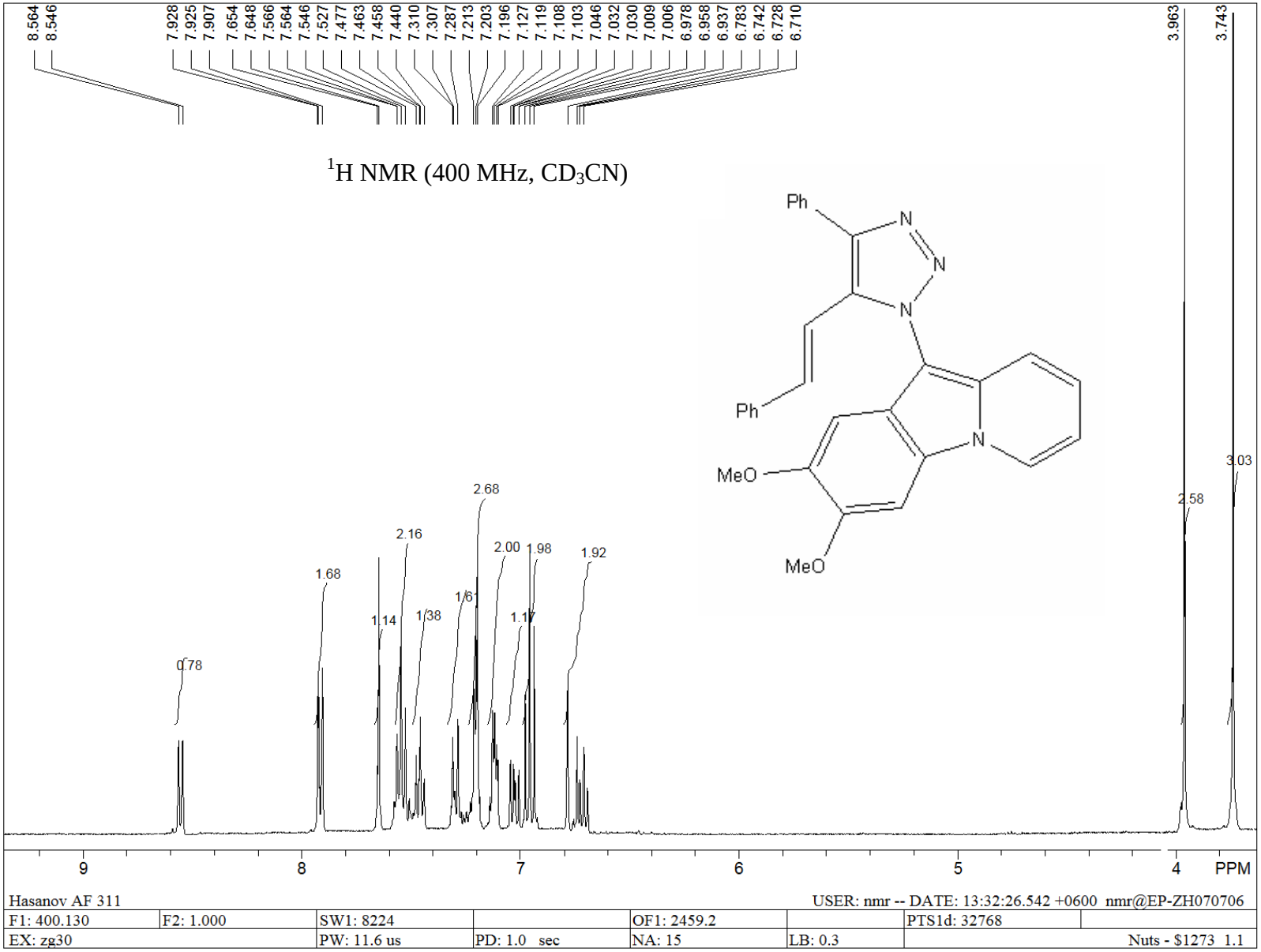

8.298
8.280
7.912
7.908
7.891
7.804
7.788
7.780
7.764
7.543
7.539
7.526
7.506
7.463
7.460
7.449
7.444
7.426
7.399
7.392
7.373
7.367
7.349
7.257
7.228
7.219
7.217
7.209
7.203
7.194
7.110
7.105
7.096
7.087
7.082
7.073
6.844
6.739
6.737
6.721
6.705
6.703
Ph
N
N
N
Ph
F
F
N
^{1}H NMR (400 MHz, $CDCl_3$)
3.40
2.86
2.85
2.11
1.90
1.82
1.02
0.92
0.88
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6 PPM
Hasanov AF 308
USER: nmr -- DATE: 15:56:00.178 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2459.9
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 9
LB: 0.3
Nuts - $1132 1.1

^{19}F NMR (376.5 MHz, $CDCl_3$)

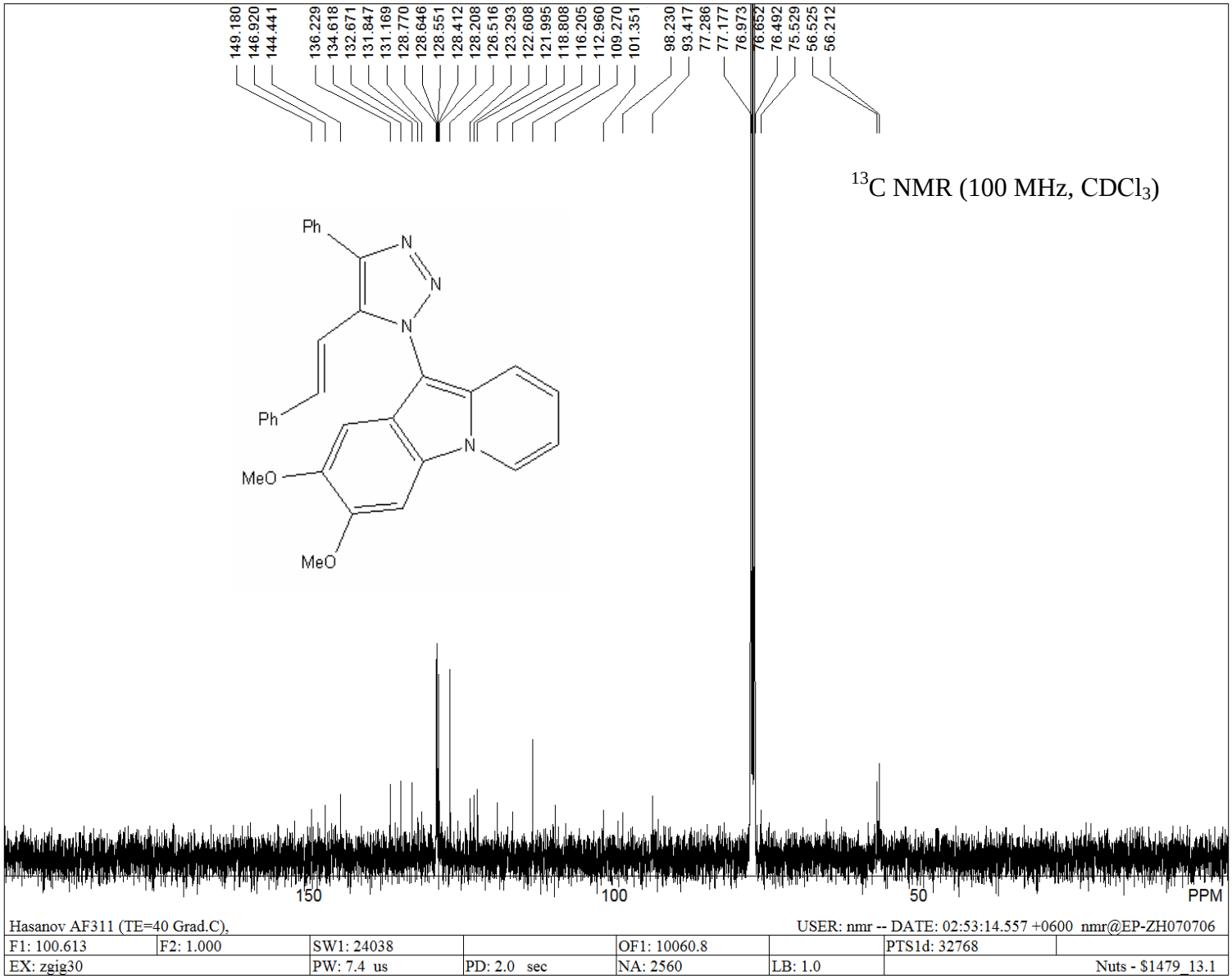



150.916
148.699
148.539
148.473
146.103
144.659
136.033
135.143
133.495
132.780
131.584
129.666
129.120
128.799
128.697
128.653
128.398
128.332
127.982
126.750
126.560
124.854
123.993
122.863
122.768
120.733
120.639
118.889
116.395
112.457
110.116
104.530
104.319
101.693
99.302
99.068
^{13}C NMR (100 MHz, CDCl$_3$)
Ph
N
N
N
Ph
F
F
N
150
140
130
120
110
100
90
80
PPM
Hasanov AF 308,
USER: nmr -- DATE: 07:45:06.996 +0500 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 16542
LB: 1.0
Nuts - $1156 15.1


7.940
7.937
7.919
7.543
7.525
8.310
8.293
7.506
7.458
7.439
7.433
7.430
7.426
7.421
7.410
7.406
7.386
7.377
7.352
7.329
7.273
7.261
7.219
7.209
7.206
7.198
7.193
7.105
7.095
7.087
7.081
6.987
6.974
6.966
6.949
6.940
6.896
6.787
6.668
6.665
6.649
6.634
6.631
4.051
3.849
1H NMR (400 MHz, CDCl3)
Ph
N
N
N
Ph
N
MeO
MeO
0.96
1.61
2.15
3.57
2.45
1.84
1.92
1.65
0.89
2.55
2.57
9
8
7
6
5
4
PPM
Hasanov AF 311-2
USER: nmr -- DATE: 14:33:52.479 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2461.4
PTS1d: 32768
EX: zg30
PW: 11.6 us
PD: 1.0 sec
NA: 80
LB: 0.3
Nuts - $1181_1.1



^{1}H NMR (400 MHz, CD_3CN)


149.180
146.920
144.441
136.229
134.618
132.671
131.847
131.169
128.770
128.646
128.551
128.412
128.208
126.516
123.293
122.608
121.995
118.808
116.205
112.960
109.270
101.351
98.230
93.417
77.286
77.177
76.973
76.852
76.492
75.529
56.525
56.212
^{13}C NMR (100 MHz, CDCl$_3$)
Ph
N
N
N
Ph
N
MeO
MeO
150
100
50
PPM
Hasanov AF311 (TE=40 Grad.C),
USER: nmr -- DATE: 02:53:14.557 +0600 nmr@EP-ZH070706
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 2560
LB: 1.0
Nuts - $1479_13.1

References:

1. http://www.chemgapedia.de/vsengine/vlu/vsc/en/ch/12/oc/vlu_organik/aromaten/reaktionen/reaktionen_aromaten.vlu/Page/vsc/en/ch/12/oc/aromaten/reaktionen/ar_sn/arine/arine.vscml.html