Chemistry of Heterocyclic Compounds **2024**, *60*(5/6), 289–298

2,5-Di(het)arylpyridines: synthesis by "1,2,4-triazine" methodology and photophysical properties

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Supplementary Information

Table S1 The selected bond distances and angles for compound **3b**.

Molecule 1		Molecule 2	
Bond/angle	Å/°	Bond/angle	Å/°
Cl1 C16	1.731(2)	Cl1A C16A	1.725(2)
N2 N1	1.339(2)	N2A N1A	1.337(2)
N2 C3	1.315(2)	N2A C3A	1.327(2)
N4 C3	1.349(2)	N4A C3A	1.348(2)
C6 C7	1.470(3)	C6A C7A	1.465(3)
N2 C3 N4	124.32(18)	N2A C3A N4A	123.74(18)
C3 N2 N1	119.57(17)	C3A N2A N1A	119.65(17)
N1 C6 C7 C12	-1.9(3)	N1A C6A C7A C12A	28.0(3)

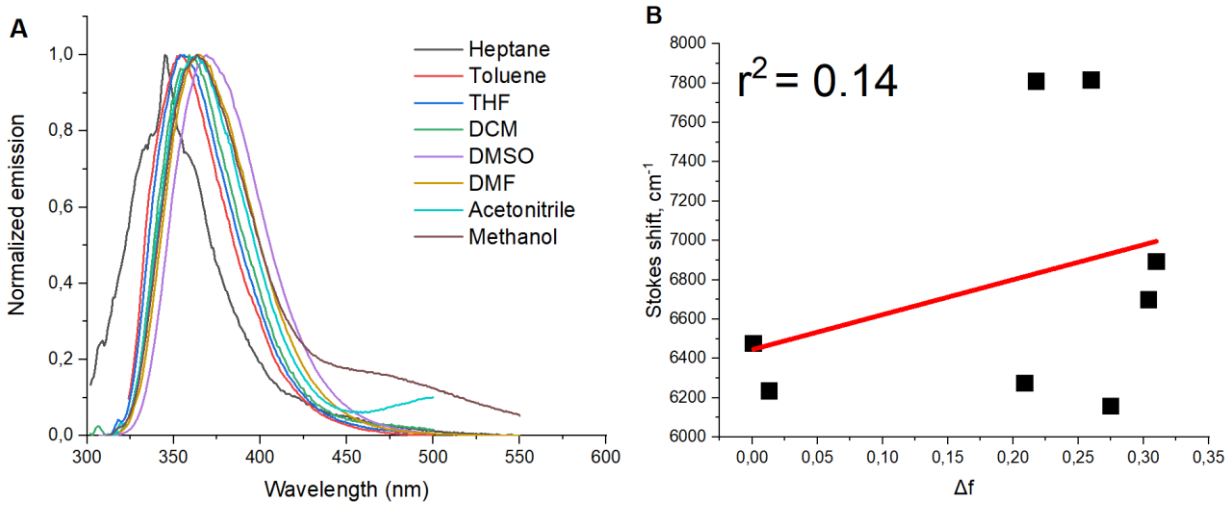


Figure S1 Solvatochromic behavior of **6c** in solvents with different polarity (A) and the Lippert-Mataga plot for **6c** (B), where Δf – orientation polarizability of the solvents.

Table S2 Photophysical properties of **6c** in solvents with different polarity

Solvent	Δf	λ_{abs}, nm	λ_{em}, nm	Stokes shift, nm (cm^{-1})
n-Heptane	0.0001	282	335sh, 345, 359sh	63 (6475)
Toluene	0.013	290	354	64 (6234)
THF	0.209	291	356	65 (6274)
DCM	0.218	281	360	79 (7809)
DMSO	0.26	287	370	83 (7816)
DMF	0.275	292	356	73 (6849)
MeCN	0.304	292	364	72 (6774)
MeOH	0.310	291	364	73 (6892)

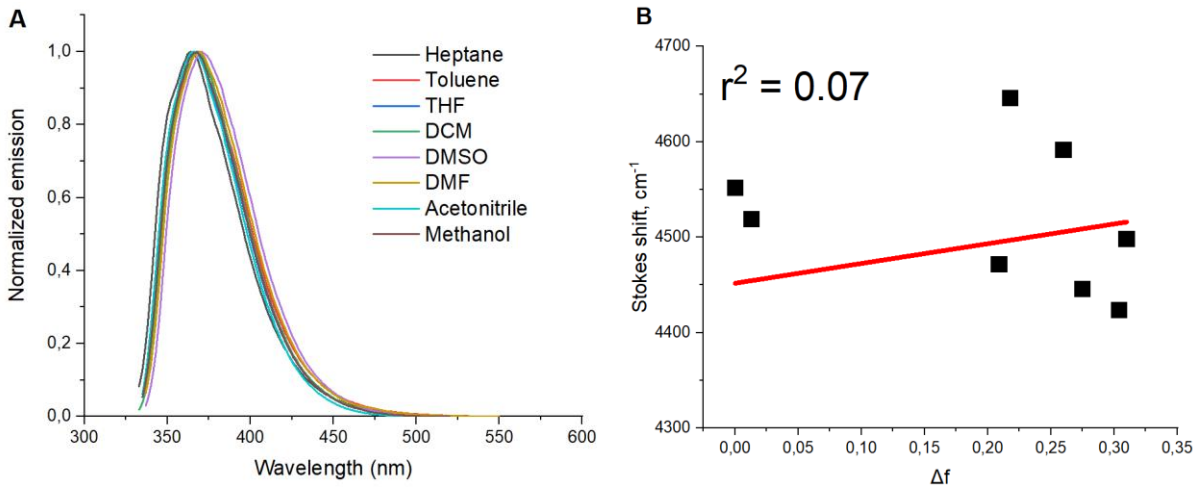
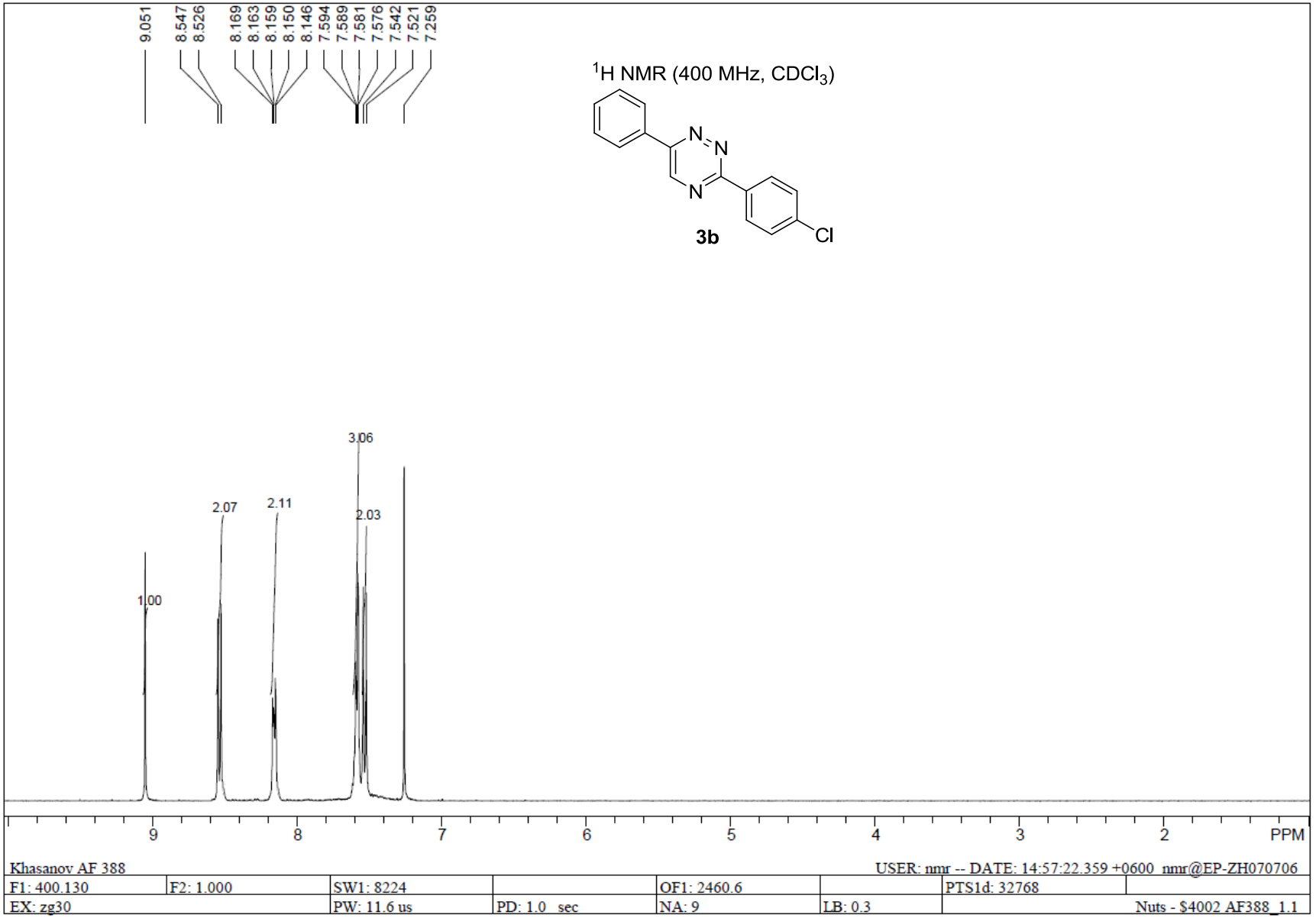


Figure S2 Solvatochromic behavior of **6f** in solvents with different polarity (A) and the Lippert-Mataga plot for **6f** (B), where Δf – orientation polarizability of the solvents

Table S3 Photophysical properties of **6f** in solvents with different polarity

Solvent	**Δf**	**λ_{abs}, nm**	**λ_{em}, nm**	**Stokes shift, nm (cm^{-1})**
n-Heptane	0.0001	313	365	52 (4552)
Toluene	0.013	317	370	53 (4519)
THF	0.209	316	368	52 (4472)
DCM	0.218	315	369	54 (4646)
DMSO	0.26	317	371	54 (4592)
DMF	0.275	317	369	52 (4445)
MeCN	0.304	315	366	51 (4423)
MeOH	0.310	315	367	52 (4498)


9.051
8.547
8.526
8.169
8.163
8.159
8.150
8.146
7.594
7.589
7.581
7.576
7.542
7.521
7.259
^{1}H NMR (400 MHz, $CDCl_3$)
N
N
N
Cl
3b
3.06
2.07
2.11
2.03
1.00
9
8
7
6
5
4
3
2
PPM
Khasanov AF 388
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F2: 1.000
SW1: 8224
OF1: 2460.6
PTS1d: 32768
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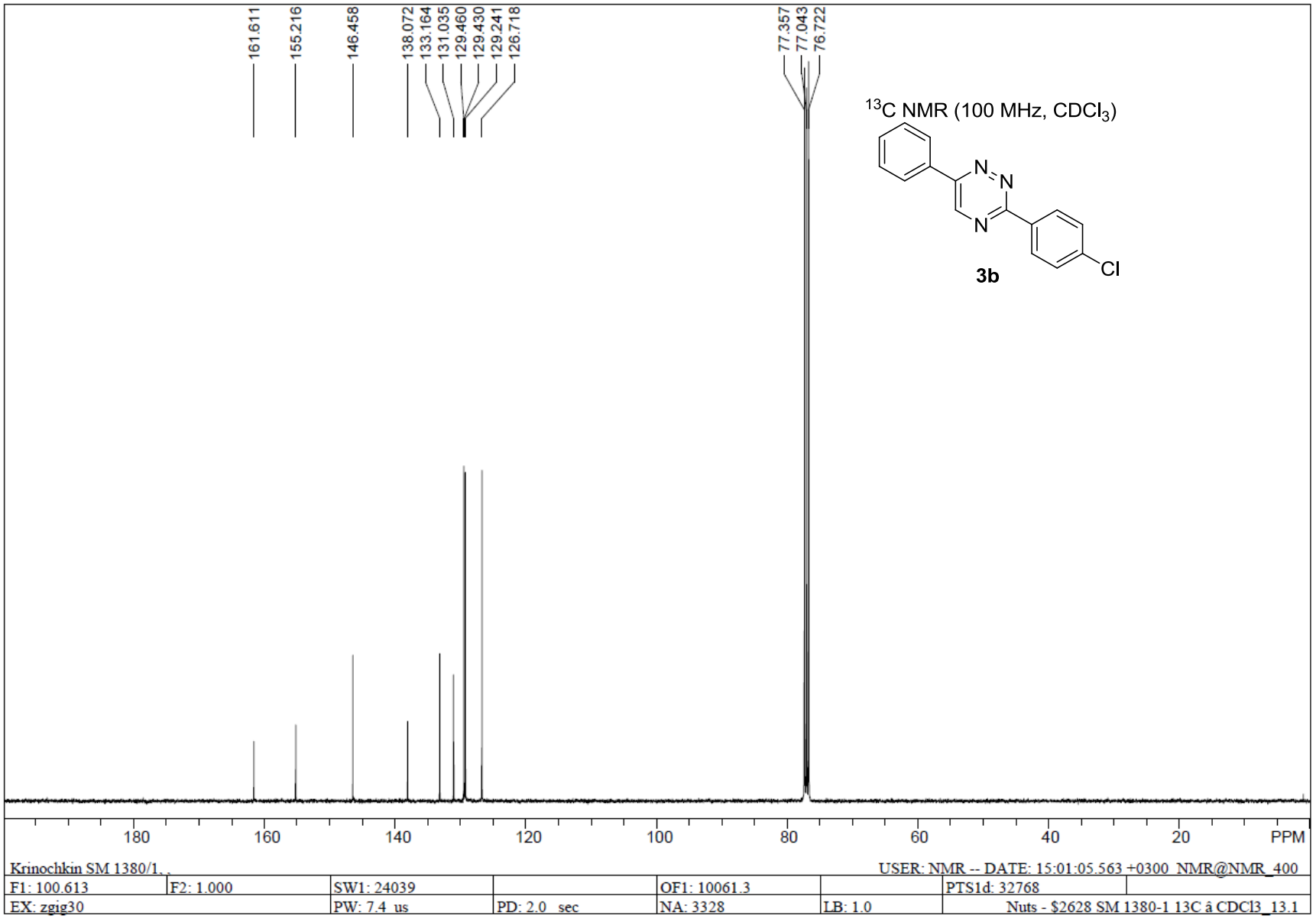
PW: 11.6 us
PD: 1.0 sec
NA: 9
LB: 0.3
Nuts - $4002 AF388_1.1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155.216
146.458
138.072
133.164
131.035
129.460
129.430
129.241
126.718
77.357
77.043
76.722
^{13}C NMR (100 MHz, $CDCl_3$)
N
N
N
Cl
3b
180
160
140
120
100
80
60
40
20
PPM
Krinochkin SM 1380/1, ,
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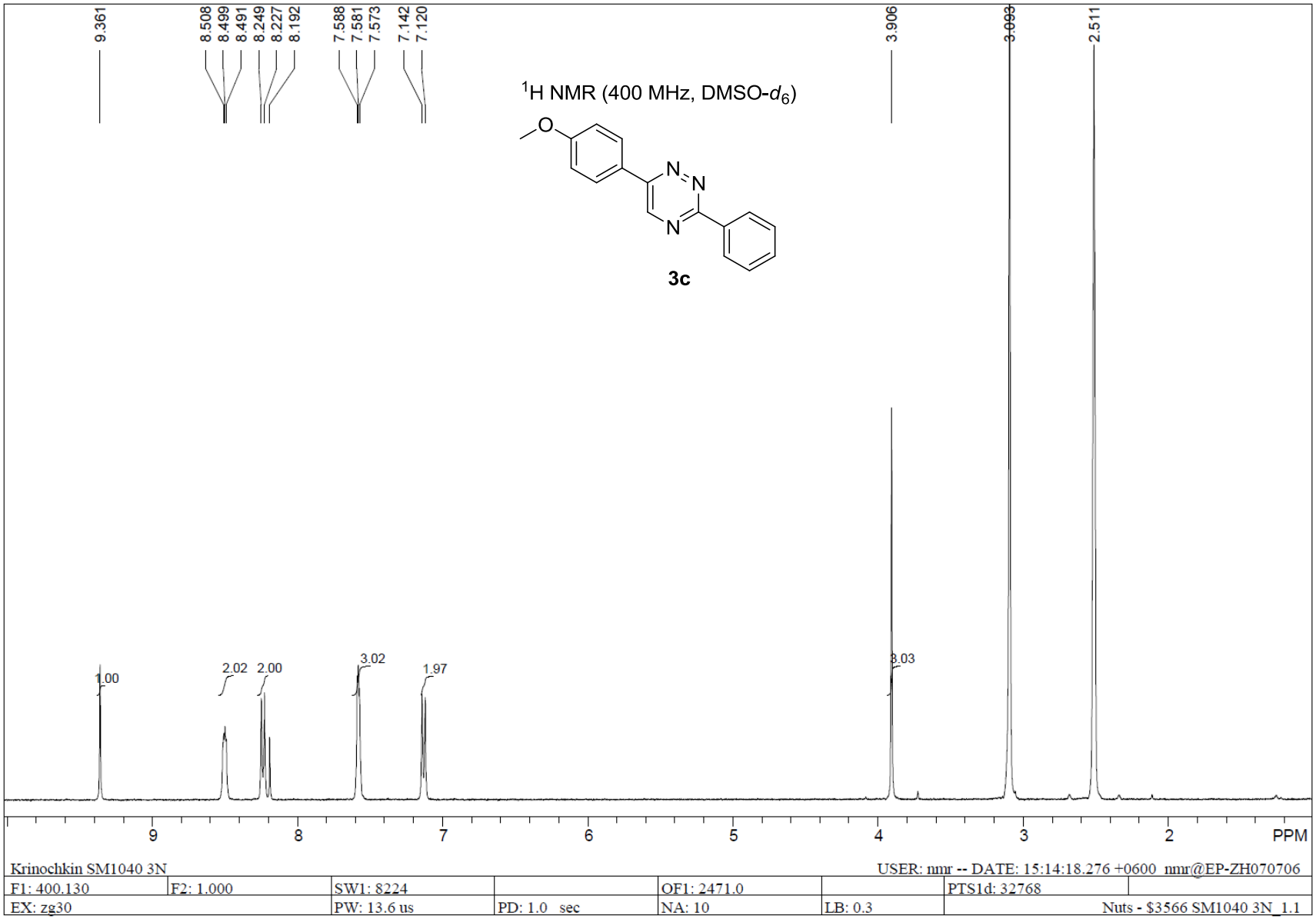
F2: 1.000
SW1: 24039
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3328
LB: 1.0
Nuts - $2628 SM 1380-1 13C â CDCl3 13.1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8.508
8.499
8.491
8.249
8.227
8.192
7.588
7.581
7.573
7.142
7.120
3.906
3.093
2.511
^{1}H NMR (400 MHz, DMSO-d_6)
O
N
N
N
3c
1.00
2.02
2.00
3.02
1.97
3.03
9
8
7
6
5
4
3
2
PPM
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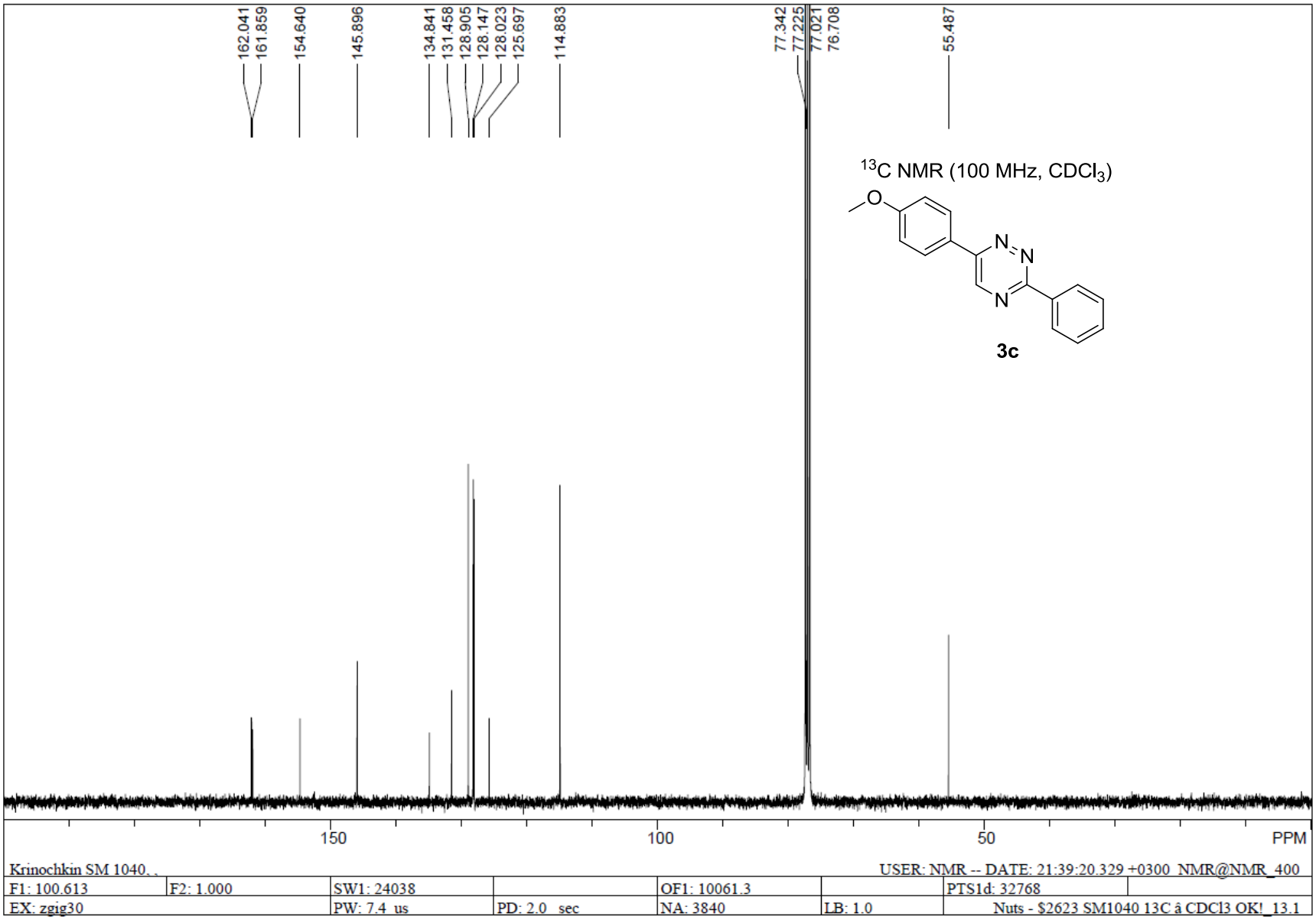
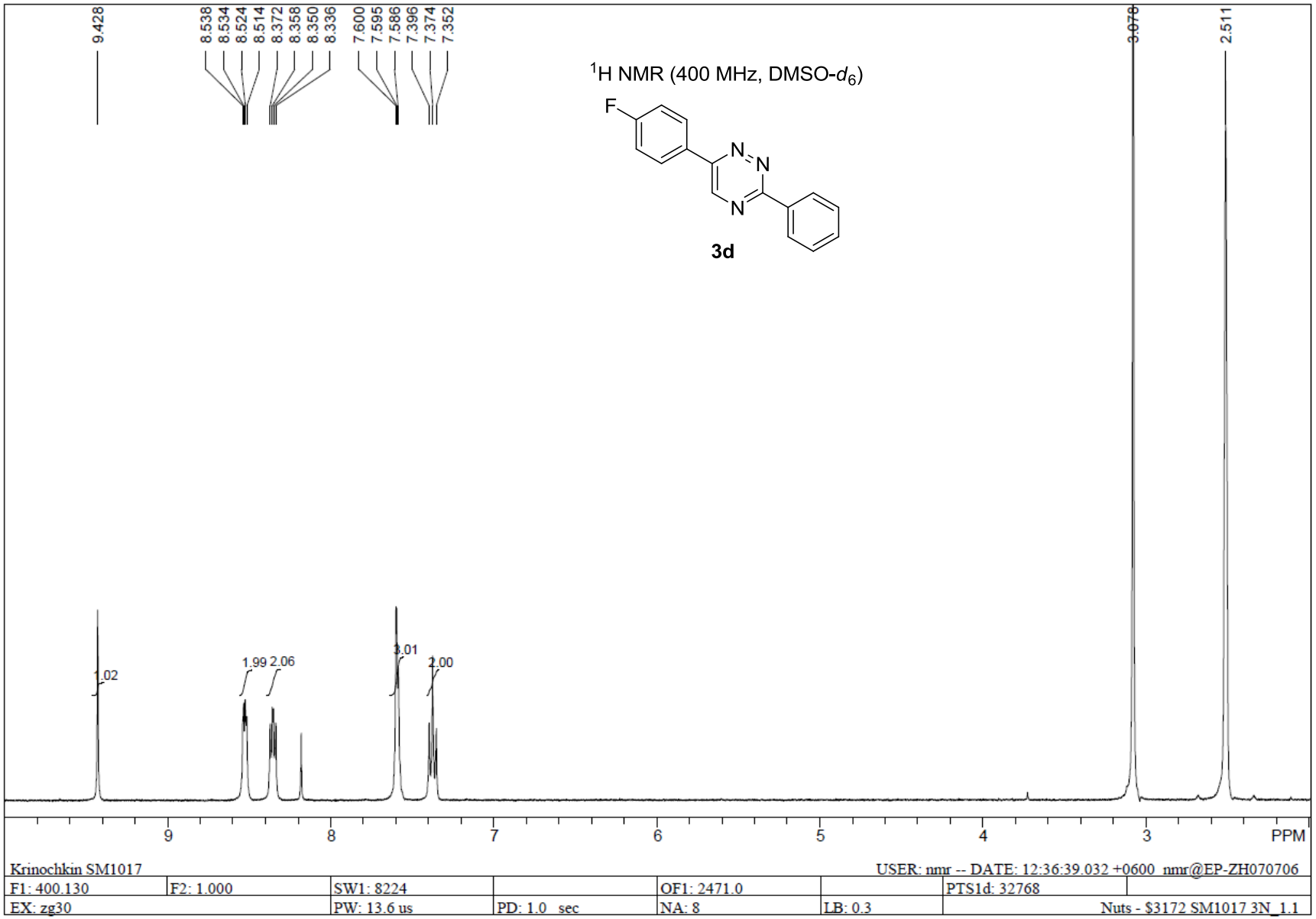
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 10
LB: 0.3
Nuts - $3566 SM1040 3N_1.1


162.041
161.859
154.640
145.896
134.841
131.458
128.905
128.147
128.023
125.697
114.883
77.342
77.225
77.021
76.708
55.487
^{13}C NMR (100 MHz, CDCl$_3$)
O
N
N
N
3c
150
100
50
PPM
Krinochkin SM 1040, ,
USER: NMR -- DATE: 21:39:20.329 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $2623 SM1040 13C â CDCl3 OK!_13.1


9.428
8.538
8.534
8.524
8.514
8.372
8.358
8.350
8.336
7.600
7.595
7.586
7.396
7.374
7.352
3.078
2.511
^{1}H NMR (400 MHz, DMSO-d_6)
F
N
N
N
3d
1.02
1.99
2.06
3.01
2.00
9
8
7
6
5
4
3
PPM
Krinochkin SM1017
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F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
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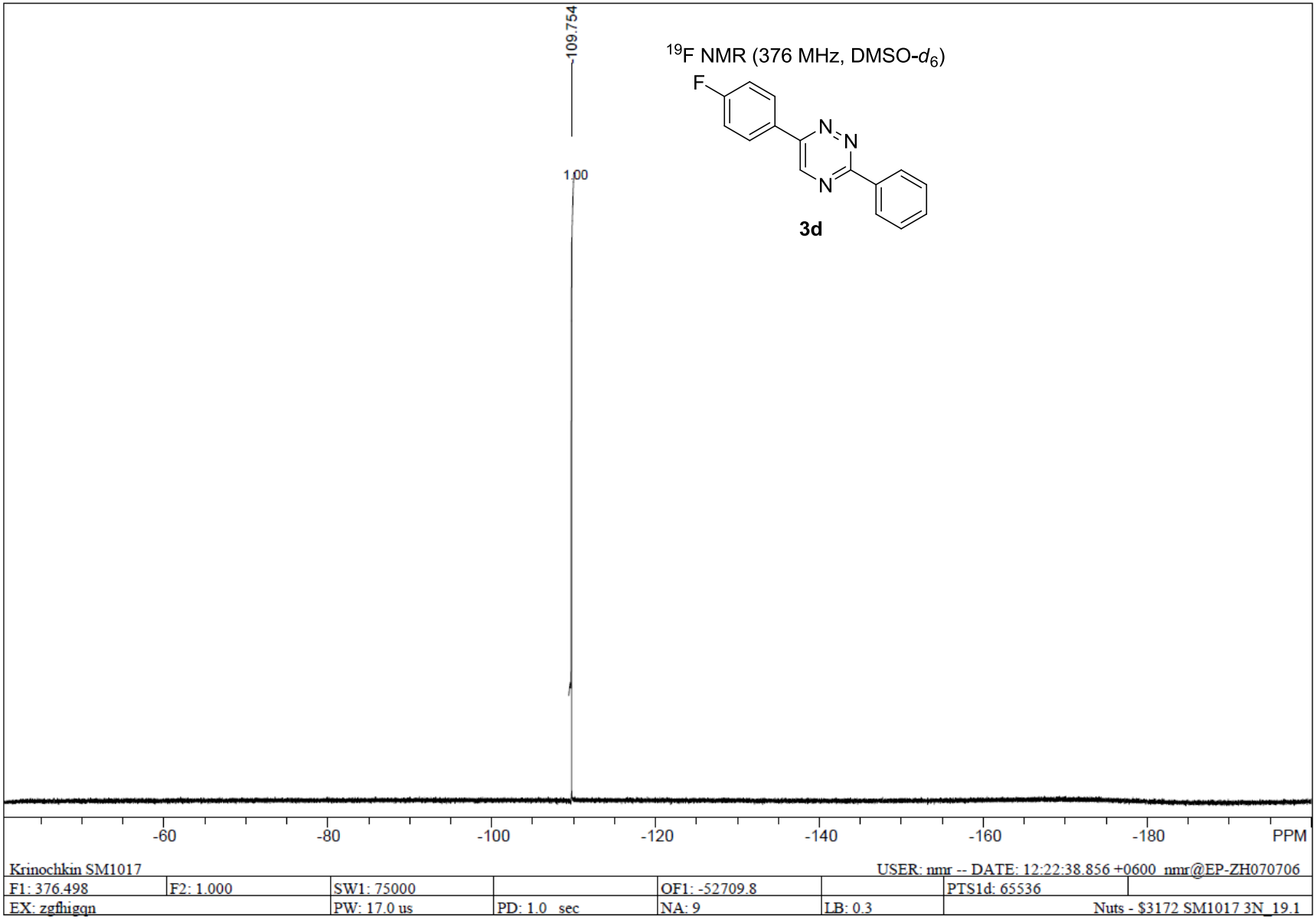
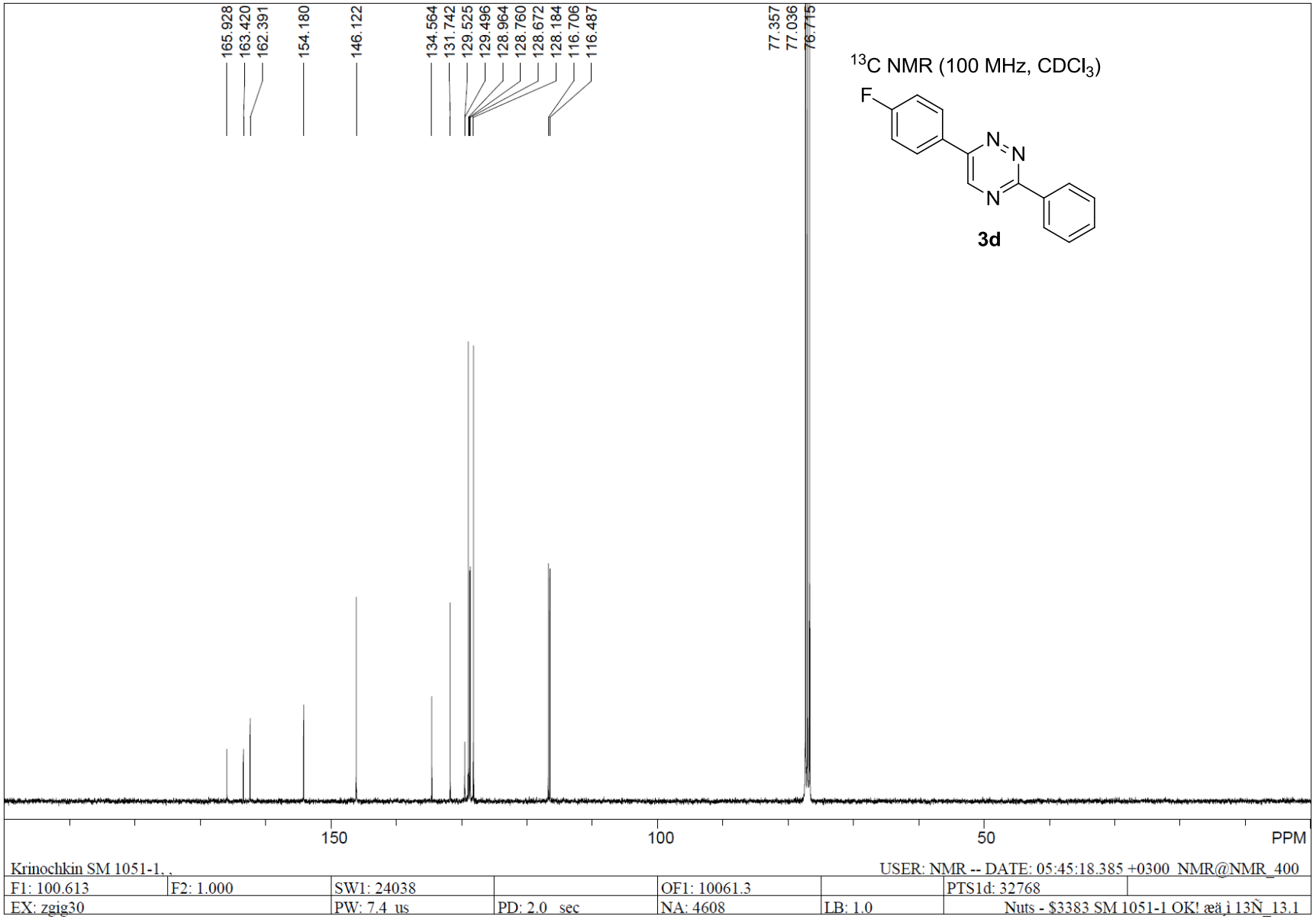
PW: 13.6 us
PD: 1.0 sec
NA: 8
LB: 0.3
Nuts - $3172 SM1017 3N_1.1


109.754
1.00
^{19}F NMR (376 MHz, DMSO-d_6)
F
N
N
N
3d
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1017
USER: nmr -- DATE: 12:22:38.856 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 9
LB: 0.3
Nuts - $3172 SM1017 3N_19.1



Krinochkin SM 1051-1, ,

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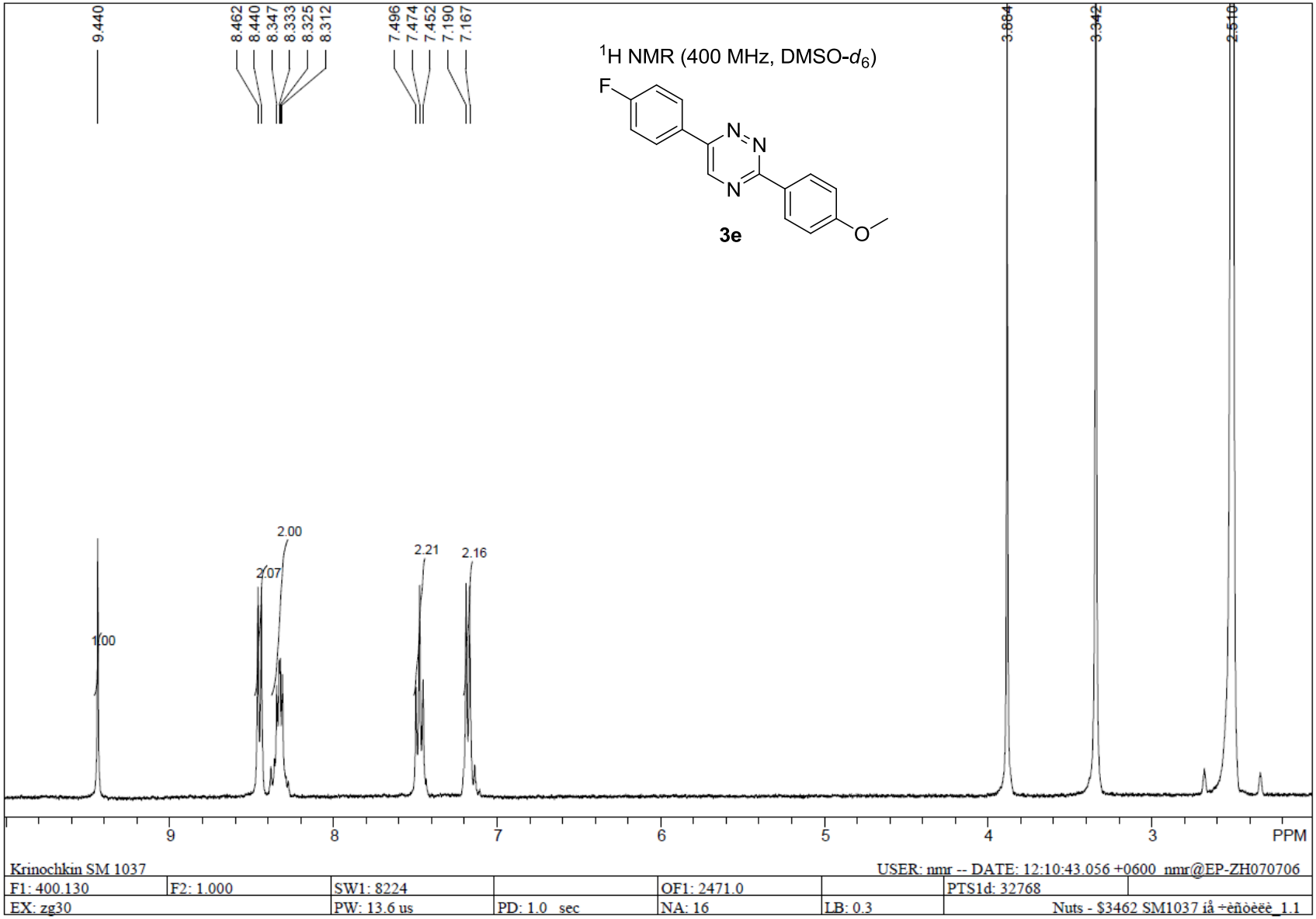
EX: zgig30		PW: 7.4 us	PD: 2.0 sec	NA: 4608	LB: 1.0	Nuts - $3383 SM 1051-1 OK! æä¡ì 13Ñ_13.1	


9.440
8.462
8.440
8.347
8.333
8.325
8.312
7.496
7.474
7.452
7.190
7.167
3.884
3.342
2.510
^{1}H NMR (400 MHz, DMSO-d_6)
F
N
N
N
O
3e
2.00
2.07
2.21
2.16
1.00
9
8
7
6
5
4
3
PPM
Krinochkin SM 1037
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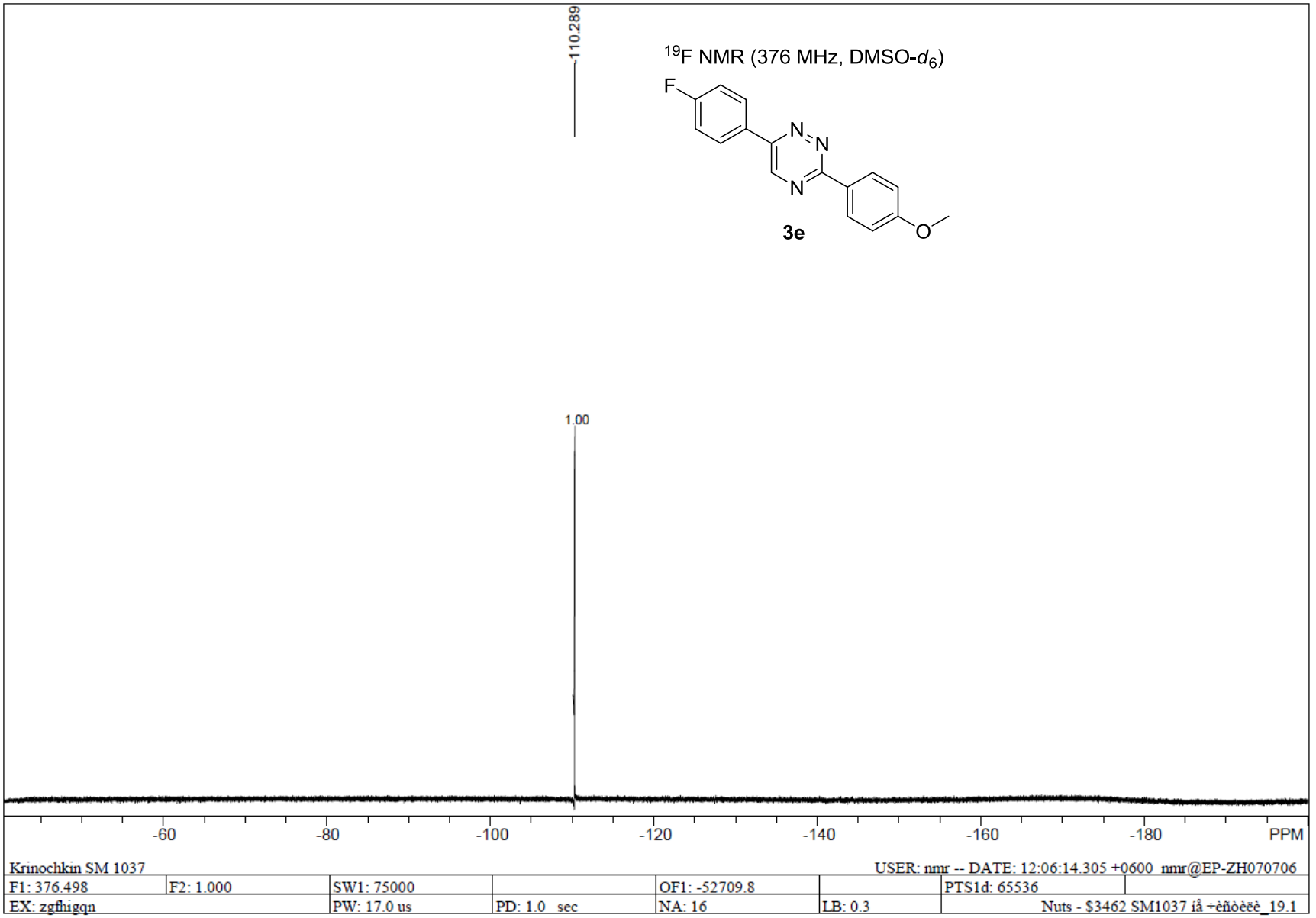
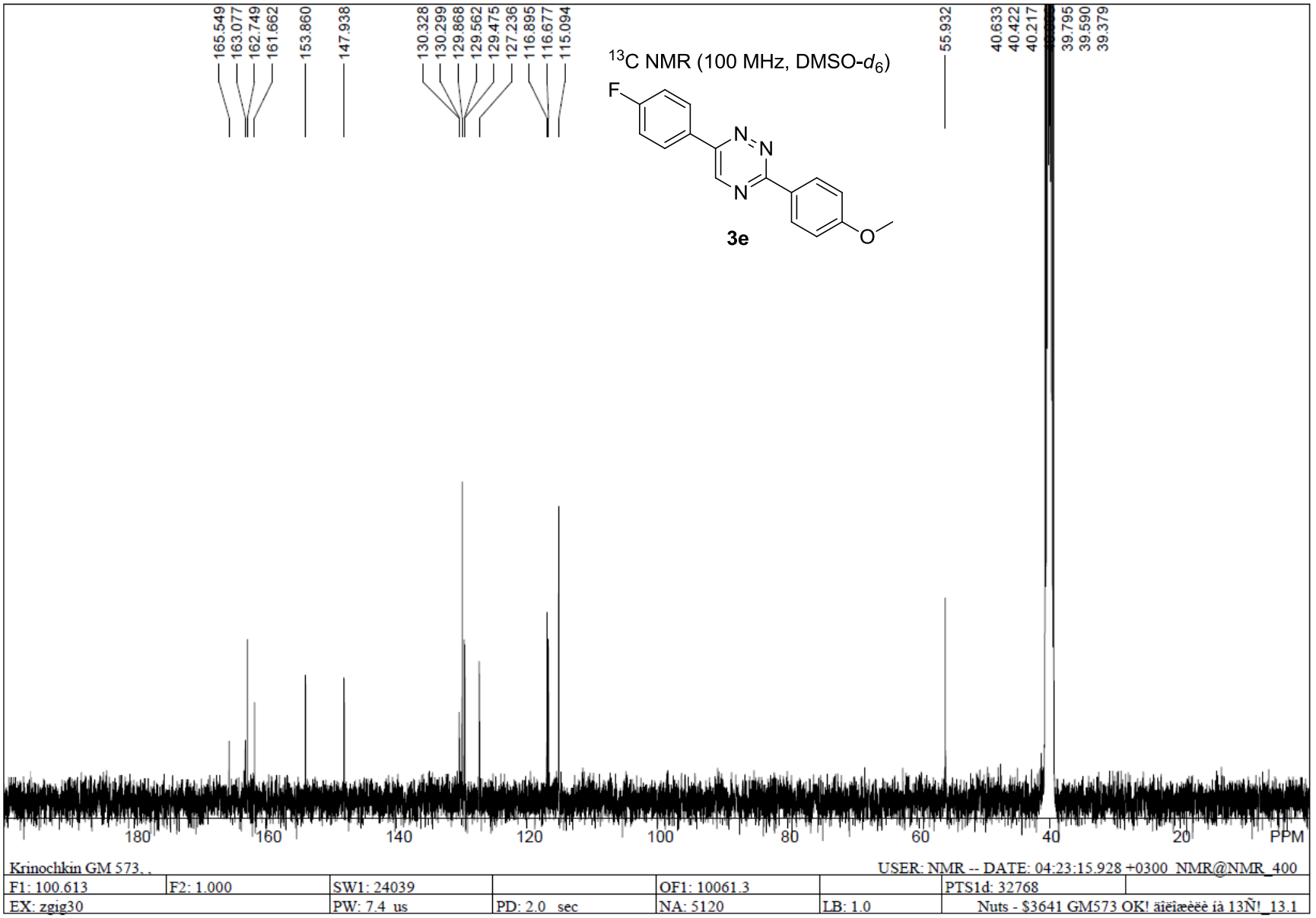
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3462 SM1037 iå ÷èñòèëü_1.1


110.289
^{19}F NMR (376 MHz, DMSO-d_6)
F
N
N
N
O
3e
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM 1037
USER: nmr -- DATE: 12:06:14.305 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3462 SM1037 íå ÷èñòèëè_19.1


165.549
163.077
162.749
161.662
153.860
147.938
130.328
130.299
129.868
129.562
129.475
127.236
116.895
116.677
115.094
55.932
40.633
40.422
40.217
39.795
39.590
39.379
^{13}C NMR (100 MHz, DMSO-d_6)
F
N
N
N
O
3e
180
160
140
120
100
80
60
40
20
PPM
Krinochkin GM 573. .
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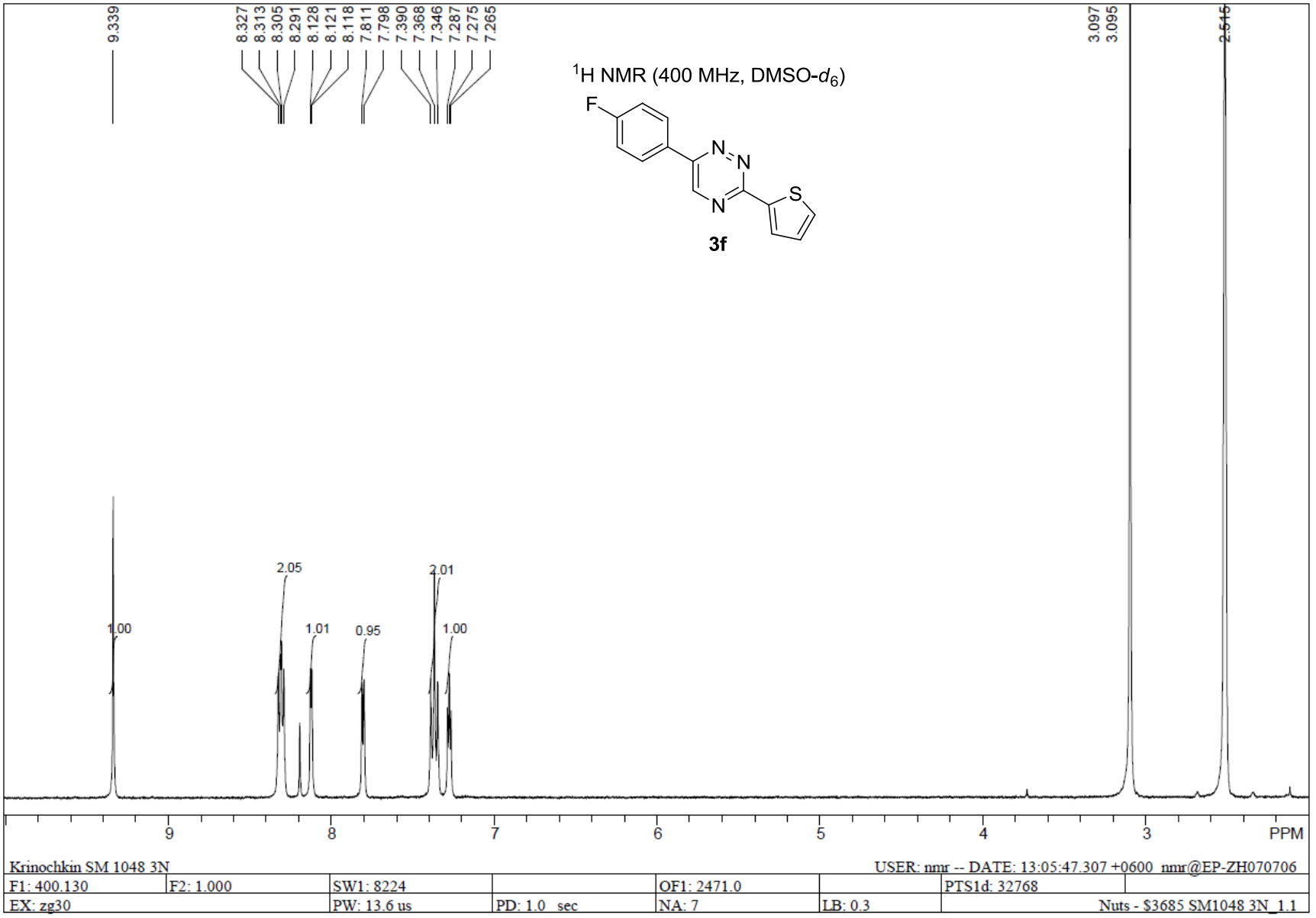
F1: 100.613
F2: 1.000
SW1: 24039
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 5120
LB: 1.0
Nuts - $3641 GM573 OK! äîëîæèëè íà 13Ñ!_13.1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8.327
8.313
8.305
8.291
8.128
8.121
8.118
7.811
7.798
7.390
7.368
7.346
7.287
7.275
7.265
3.097
3.095
2.515
^{1}H NMR (400 MHz, DMSO-d_6)
F
N
N
N
S
3f
1.00
2.05
1.01
0.95
2.01
1.00
9
8
7
6
5
4
3
PPM
Krinochkin SM 1048 3N
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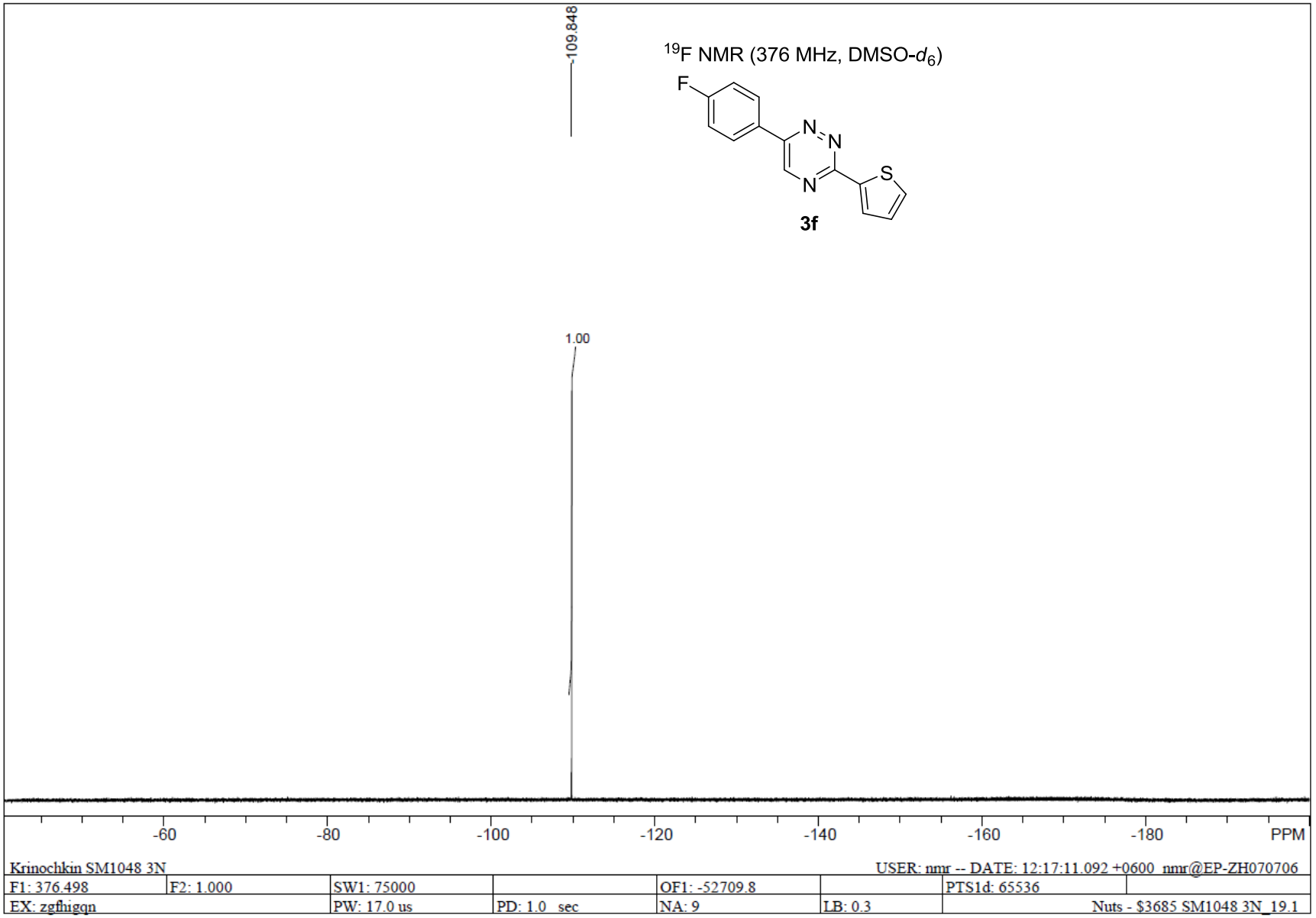
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 7
LB: 0.3
Nuts - $3685 SM1048 3N_1.1


-109.848
^{19}F NMR (376 MHz, DMSO-d_6)
F
N
N
N
S
3f
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1048 3N
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F1: 376.498
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SW1: 75000
OF1: -52709.8
PTS1d: 65536
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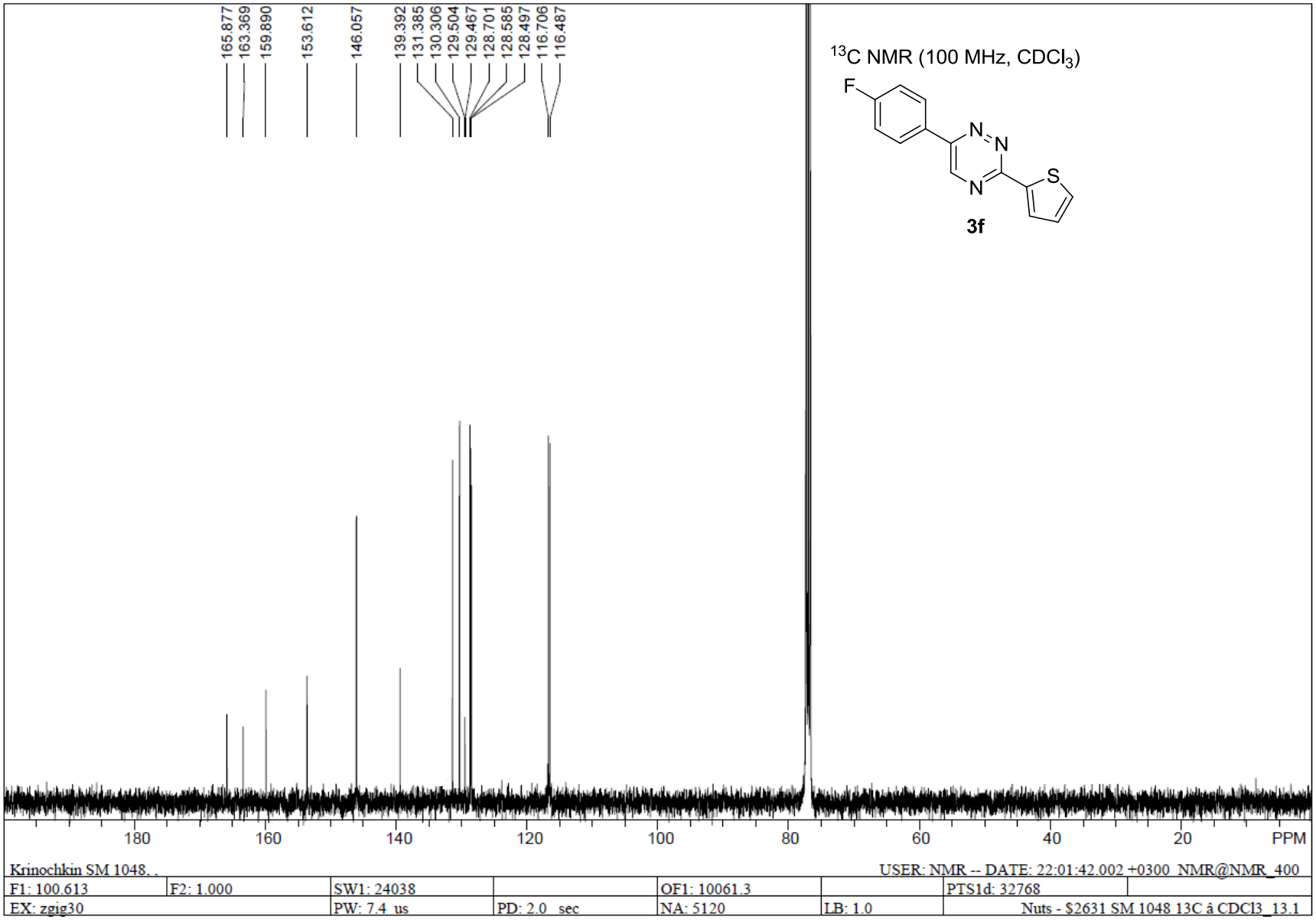
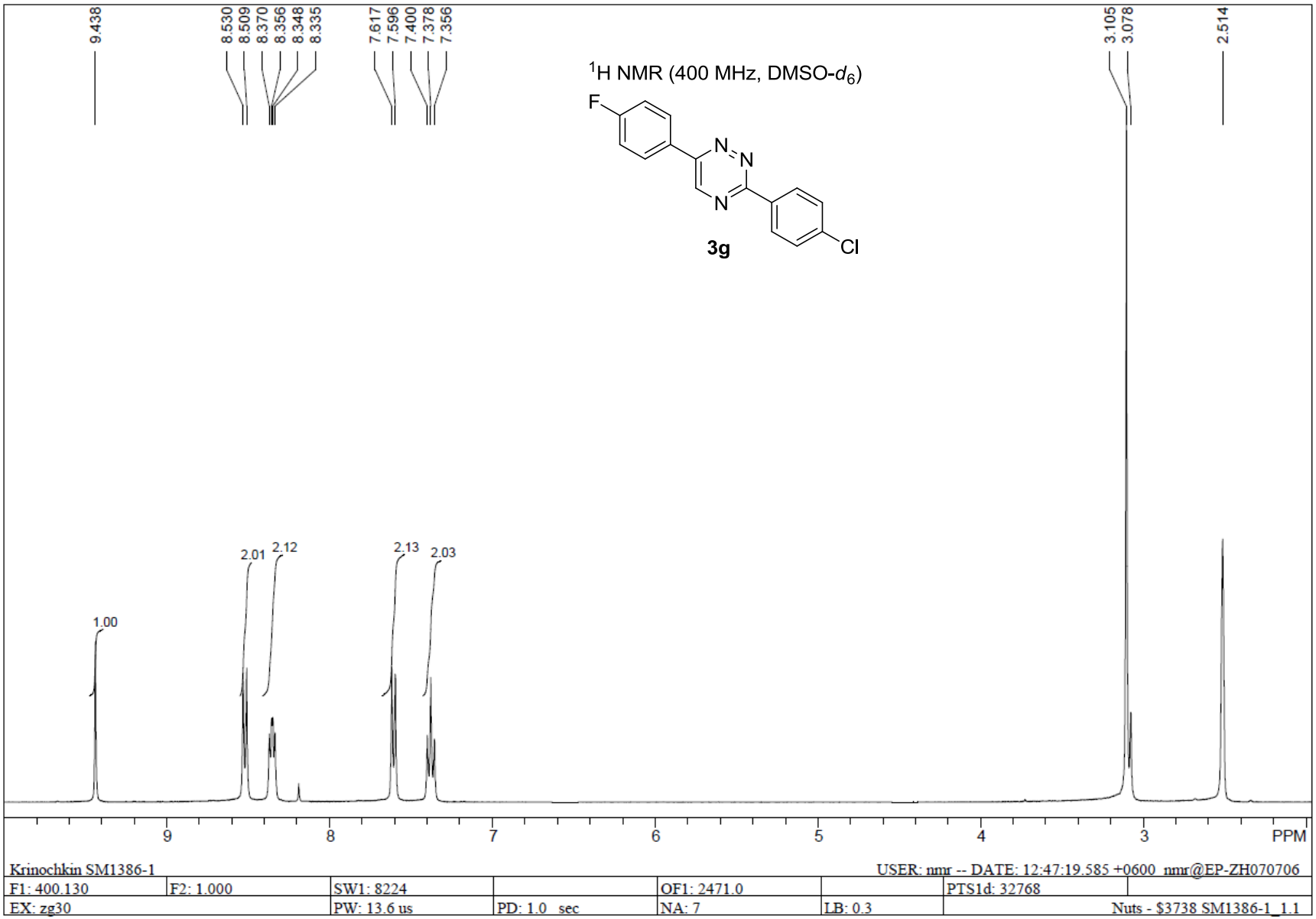
PW: 17.0 us
PD: 1.0 sec
NA: 9
LB: 0.3
Nuts - $3685 SM1048 3N_19.1


165.877
163.369
159.890
153.612
146.057
139.392
131.385
130.306
129.504
129.467
128.701
128.585
128.497
116.706
116.487
^{13}C NMR (100 MHz, CDCl$_3$)
F
N
N
N
S
3f
180
160
140
120
100
80
60
40
20
PPM
Krinochkin SM 1048. .
USER: NMR -- DATE: 22:01:42.002 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 5120
LB: 1.0
Nuts - $2631 SM 1048 13C â CDCl3 13.1


9.438
8.530
8.509
8.370
8.356
8.348
8.335
7.617
7.596
7.400
7.378
7.356
3.105
3.078
2.514
^{1}H NMR (400 MHz, DMSO-d_6)
F
N
N
N
Cl
3g
1.00
2.01
2.12
2.13
2.03
9
8
7
6
5
4
3
PPM
Krinochkin SM1386-1
USER: nmr -- DATE: 12:47:19.585 +0600 nmr@EP-ZH070706
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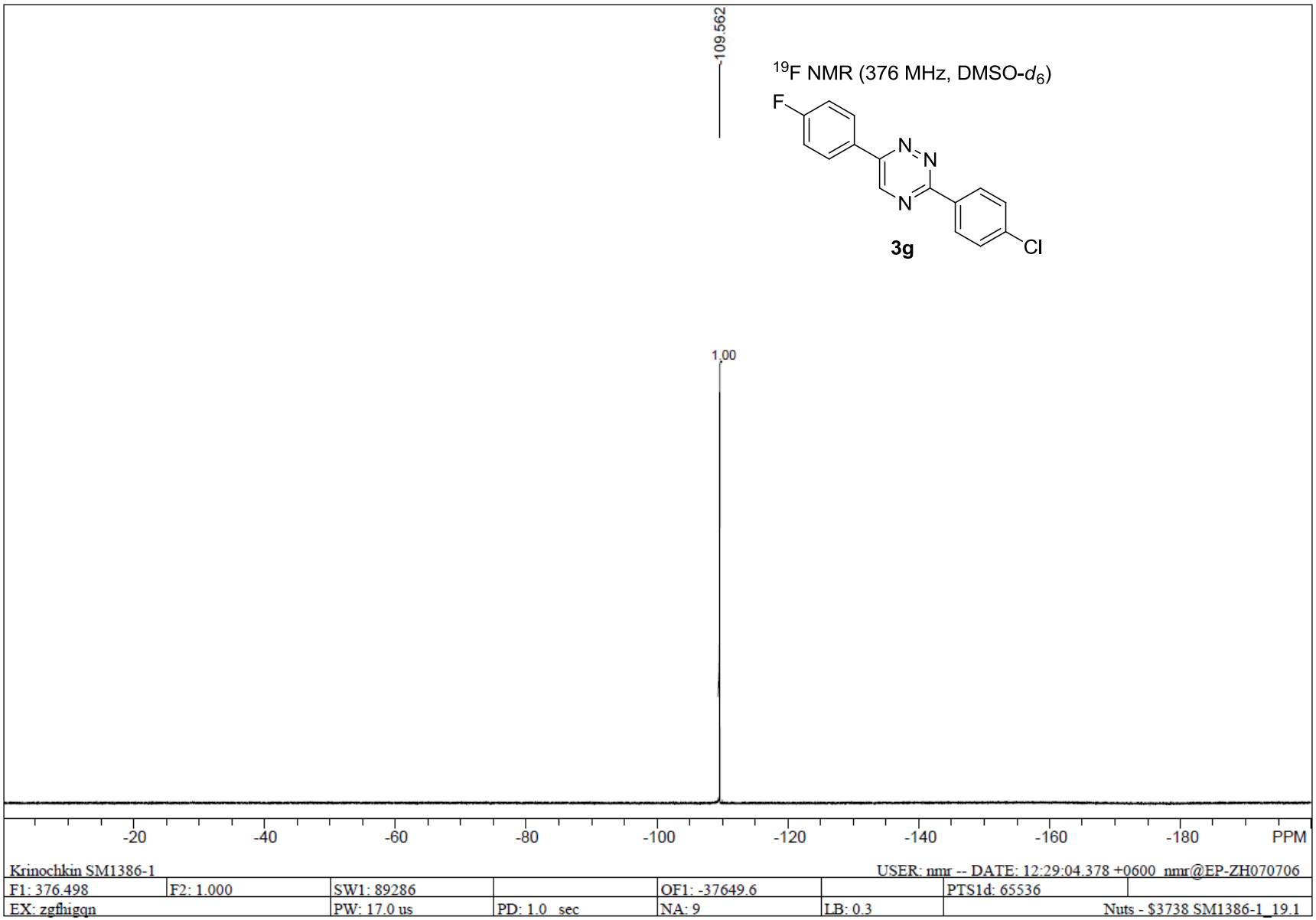
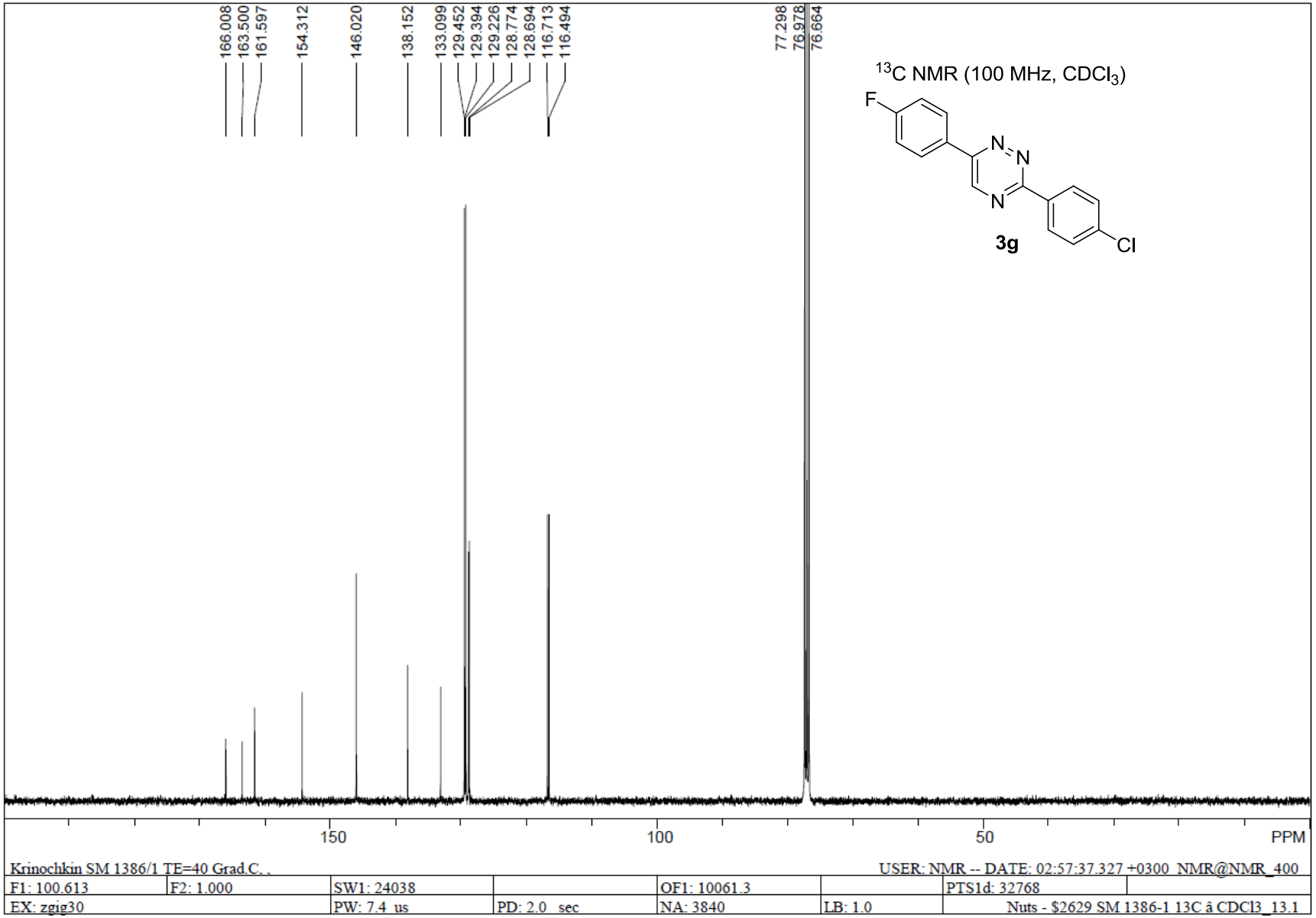
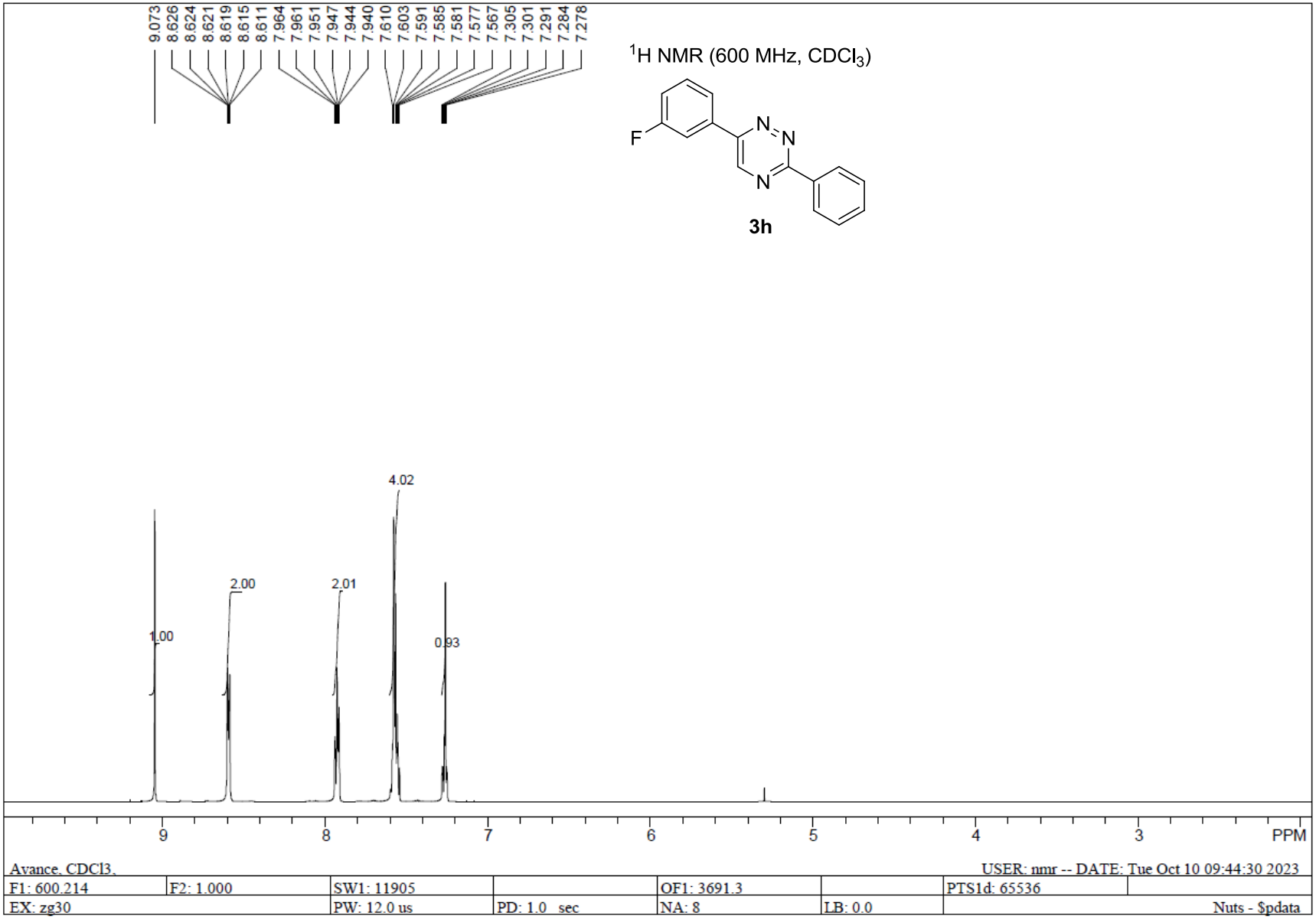
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 7
LB: 0.3
Nuts - $3738 SM1386-1_1.1


109.562
^{19}F NMR (376 MHz, DMSO-d_6)
F
N
N
N
Cl
3g
1.00
-20
-40
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1386-1
USER: nmr -- DATE: 12:29:04.378 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 89286
OF1: -37649.6
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 9
LB: 0.3
Nuts - $3738 SM1386-1_19.1


166.008
163.500
161.597
154.312
146.020
138.152
133.099
129.452
129.394
129.226
128.774
128.694
116.713
116.494
77.298
76.978
76.664
^{13}C NMR (100 MHz, $CDCl_3$)
F
N
N
N
Cl
3g
150
100
50
PPM
Krinochkin SM 1386/1 TE=40 Grad.C. .
USER: NMR -- DATE: 02:57:37.327 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $2629 SM 1386-1 13C â CDCl3 13.1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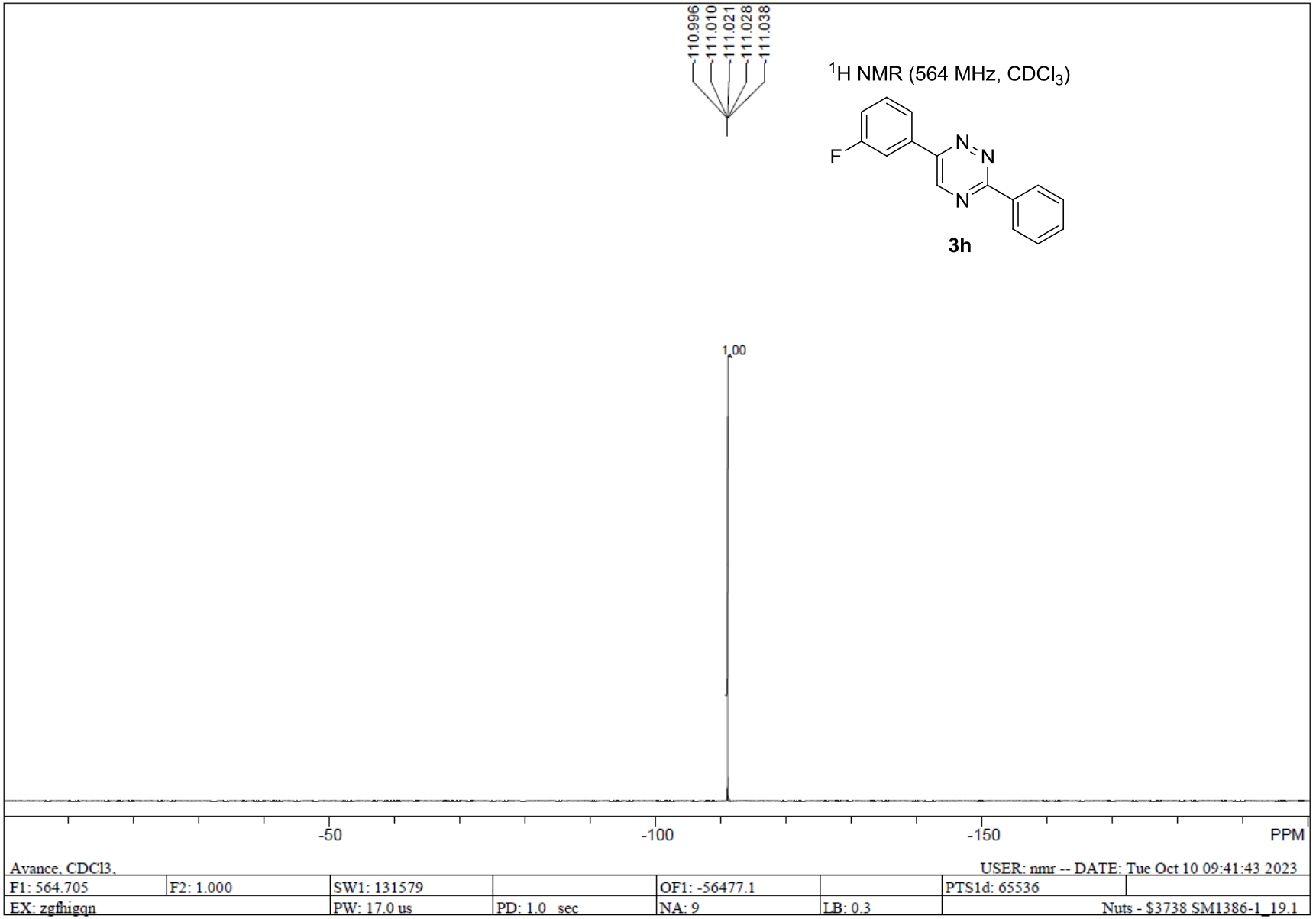
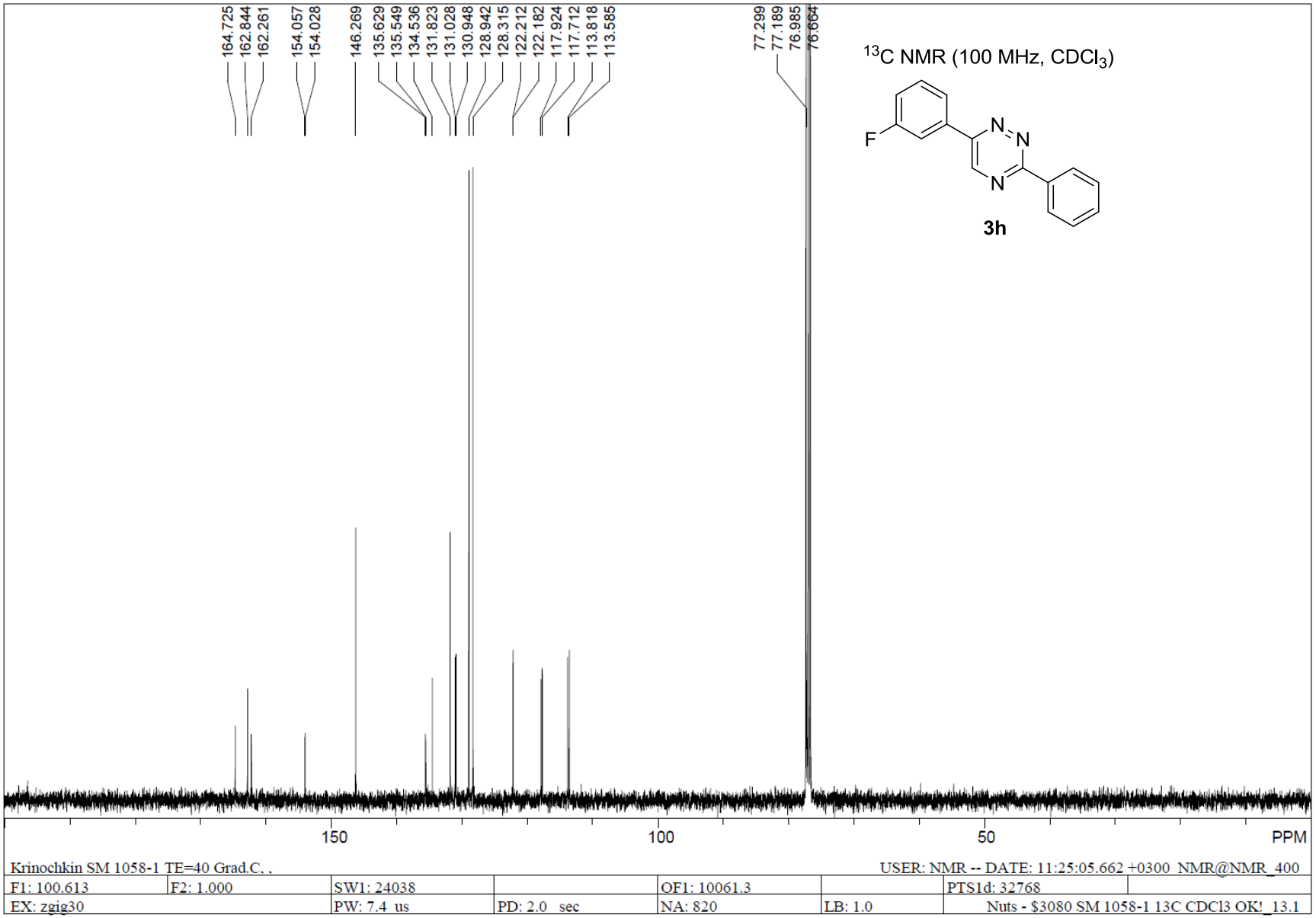
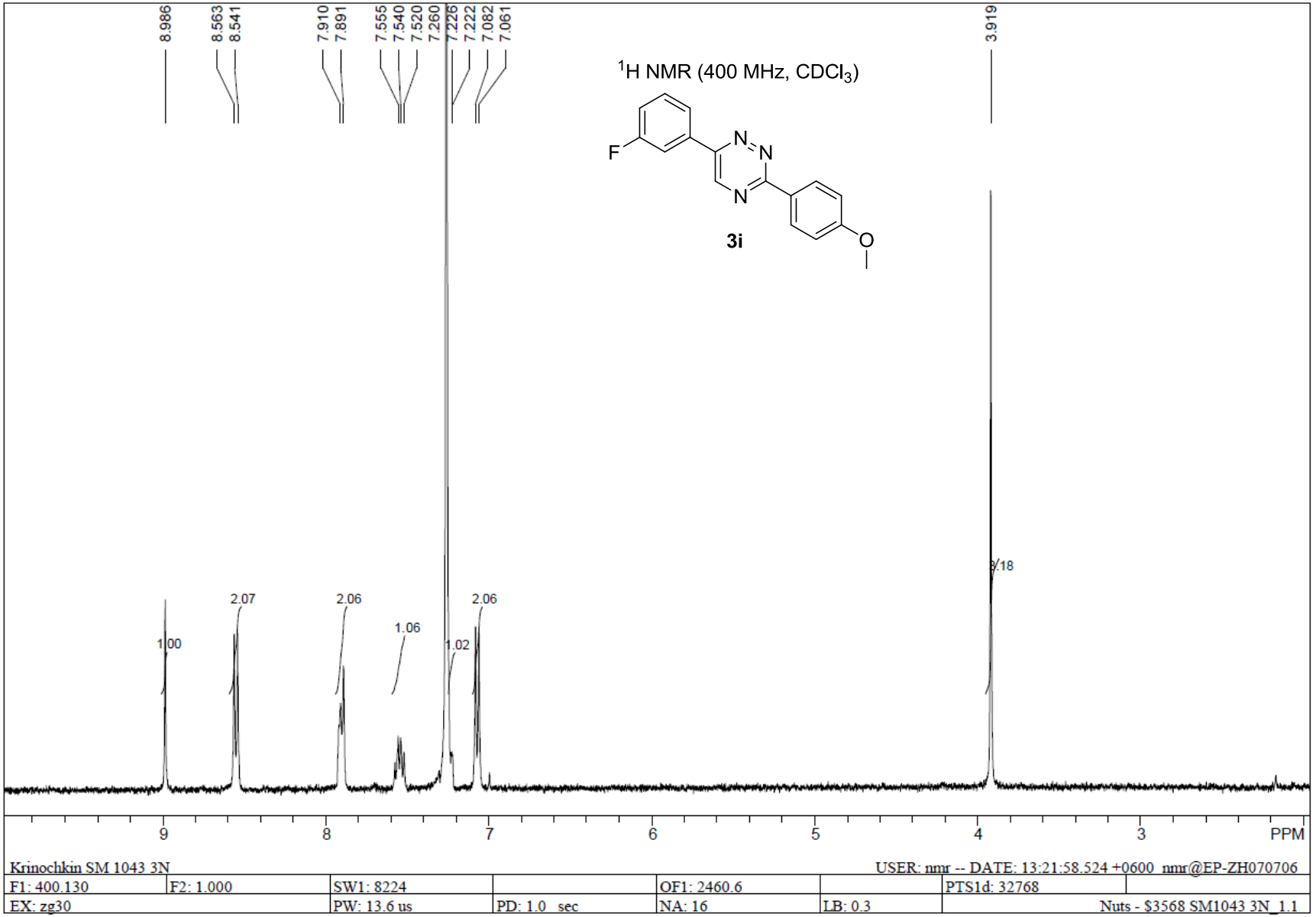
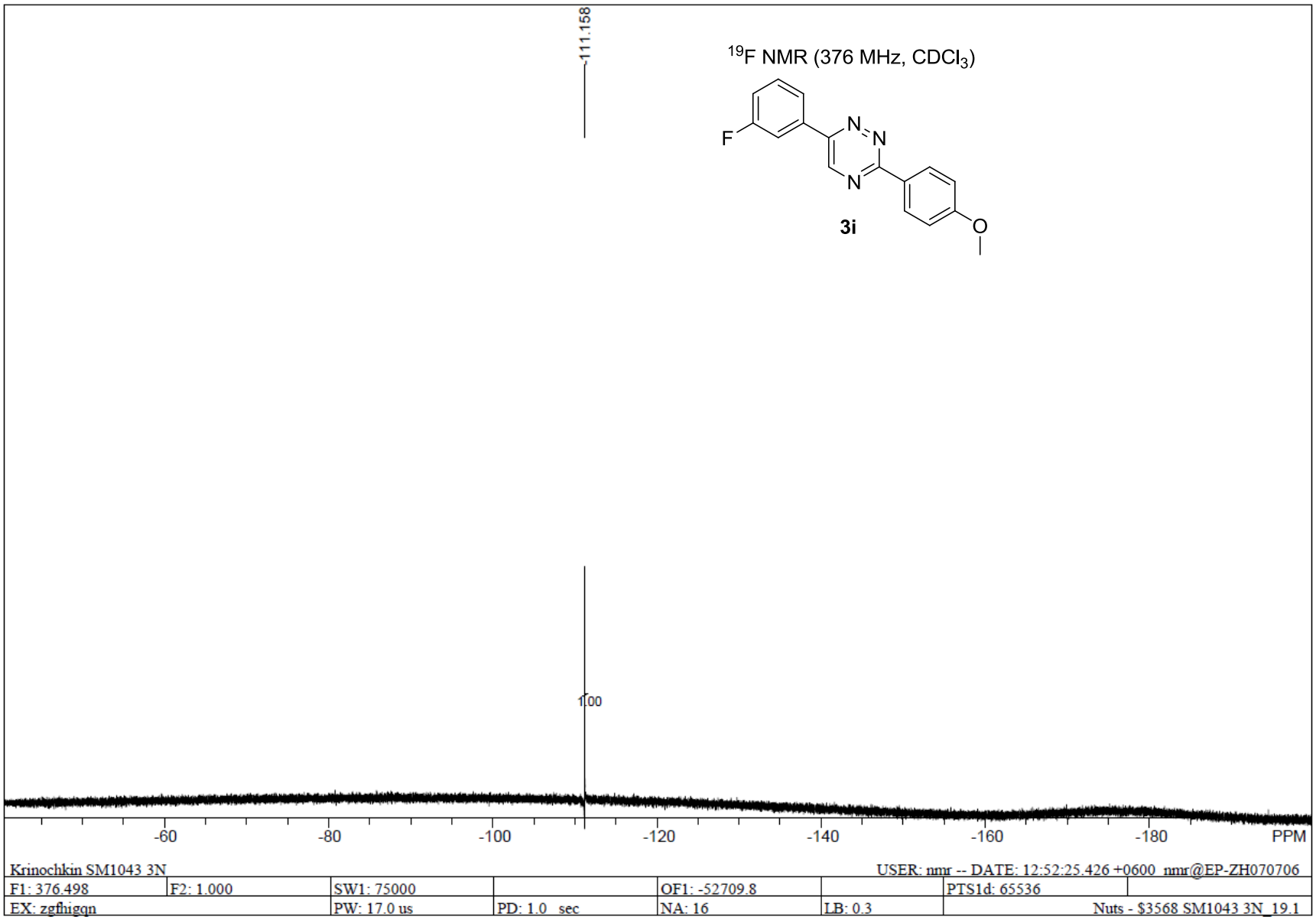
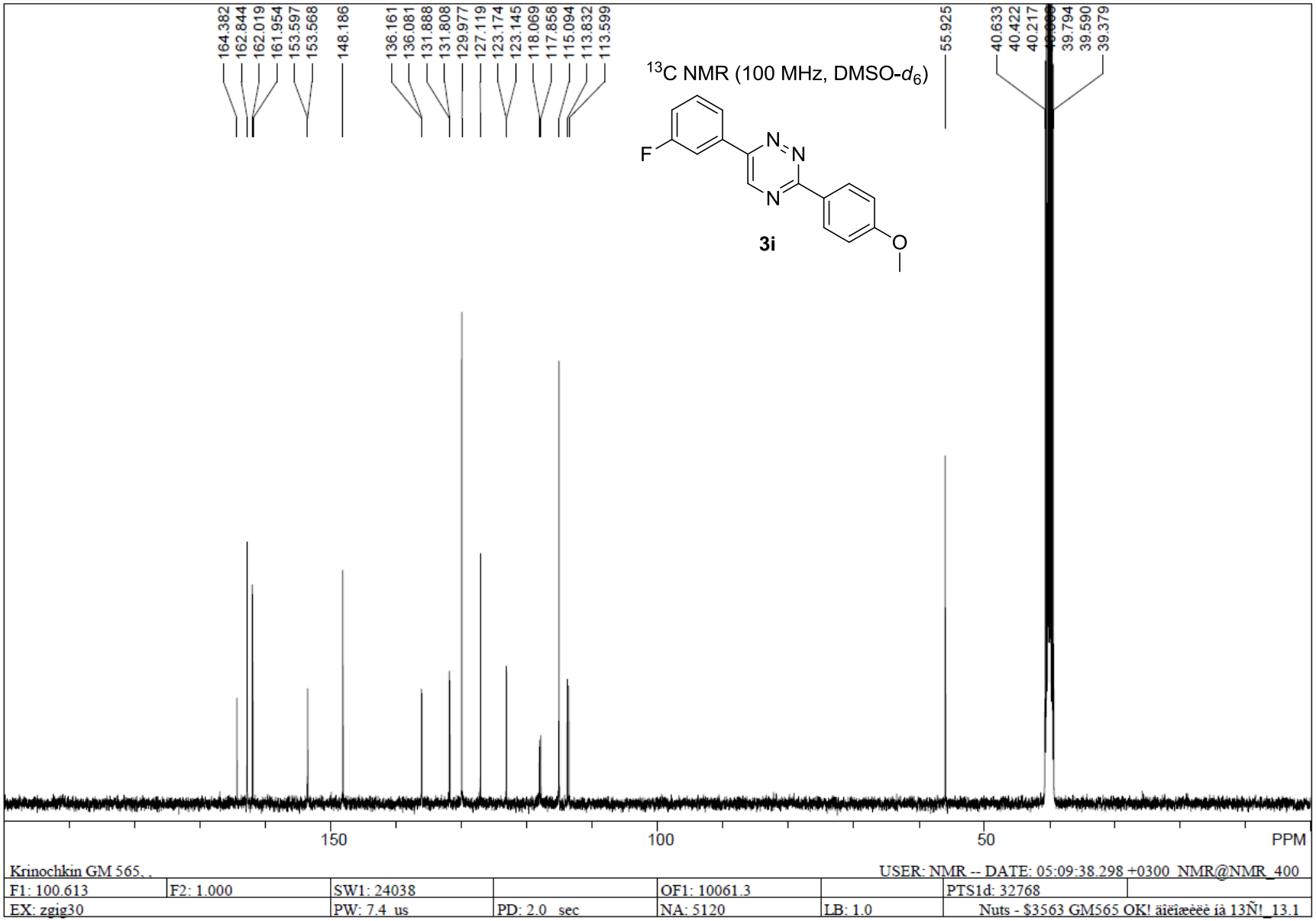
8.626
8.624
8.621
8.619
8.615
8.611
7.964
7.961
7.951
7.947
7.944
7.940
7.610
7.603
7.591
7.585
7.581
7.577
7.567
7.305
7.301
7.291
7.284
7.278
1H NMR (600 MHz, CDCl3)
F
N
N
N
3h
4.02
2.00
2.01
1.00
0.93
9
8
7
6
5
4
3
PPM
Avance, CDCl3,
USER: nmr -- DATE: Tue Oct 10 09:44:30 2023
F1: 600.214
F2: 1.000
SW1: 11905
OF1: 3691.3
PTS1d: 65536
EX: zg30
PW: 12.0 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $pdata

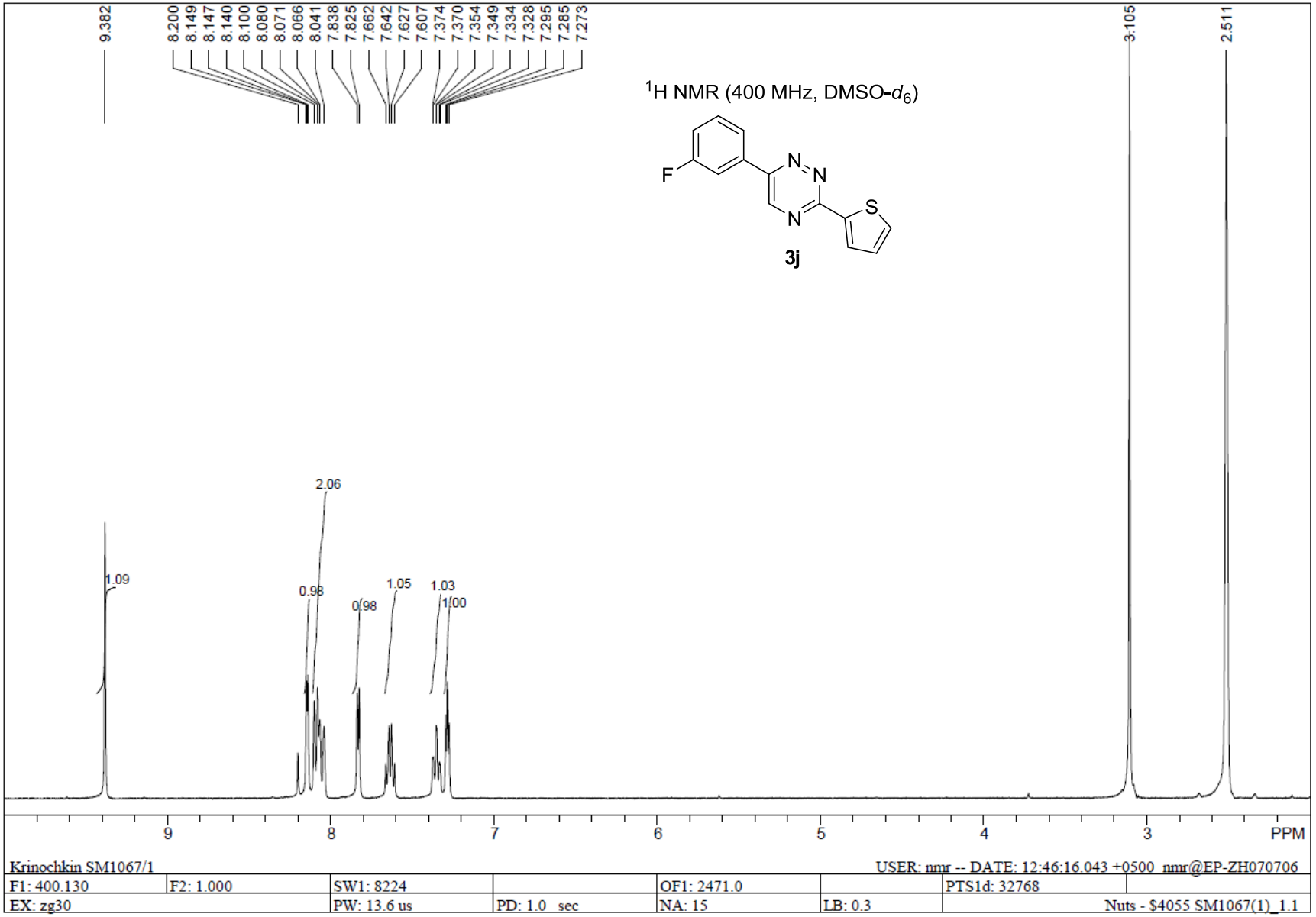

110.996
111.010
111.021
111.028
111.038
^{1}H NMR (564 MHz, $CDCl_3$)
F
N
N
N
3h
1.00
-50
-100
-150
PPM
Avance, CDCl3,
USER: nmr -- DATE: Tue Oct 10 09:41:43 2023
F1: 564.705
F2: 1.000
SW1: 131579
OF1: -56477.1
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 9
LB: 0.3
Nuts - $3738 SM1386-1_19.1


164.725
162.844
162.261
154.057
154.028
146.269
135.629
135.549
134.536
131.823
131.028
130.948
128.942
128.315
122.212
122.182
117.924
117.712
113.818
113.585
77.299
77.189
76.985
76.664
13C NMR (100 MHz, CDCl3)
F
N
N
N
3h
150
100
50
PPM
Krinochkin SM 1058-1 TE=40 Grad.C, ,
USER: NMR -- DATE: 11:25:05.662 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 820
LB: 1.0
Nuts - $3080 SM 1058-1 13C CDCl3 OK!_13.1

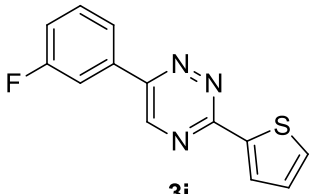

8.986
8.563
8.541
7.910
7.891
7.555
7.540
7.520
7.260
7.226
7.222
7.082
7.061
3.919
^{1}H NMR (400 MHz, $CDCl_3$)
F
N
N
N
O
3i
1.00
2.07
2.06
1.06
1.02
2.06
3.18
9
8
7
6
5
4
3
PPM
Krinochkin SM 1043 3N
USER: nmr -- DATE: 13:21:58.524 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.6
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3568 SM1043 3N_1.1


-111.158
^{19}F NMR (376 MHz, $CDCl_3$)
F
N
N
N
O
3i
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1043 3N
USER: nmr -- DATE: 12:52:25.426 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3568 SM1043 3N_19.1


164.382
162.844
162.019
161.954
153.597
153.568
148.186
136.161
136.081
131.888
131.808
129.977
127.119
123.174
123.145
118.069
117.858
115.094
113.832
113.599
55.925
40.633
40.422
40.217
39.794
39.590
39.379
13C NMR (100 MHz, DMSO-d6)
F
N
N
N
O
3i
150
100
50
PPM
Krinochkin GM 565, .
USER: NMR -- DATE: 05:09:38.298 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 5120
LB: 1.0
Nuts - $3563 GM565 OK! äïëíæèëè íà 13Ñ!_13.1


9.382
8.200
8.149
8.147
8.140
8.100
8.080
8.071
8.066
8.041
7.838
7.825
7.662
7.642
7.627
7.607
7.374
7.370
7.354
7.349
7.334
7.328
7.295
7.285
7.273
3.105
2.511
1H NMR (400 MHz, DMSO-d6)
F
N
N
N
S
3j
2.06
1.09
0.98
0.98
1.05
1.03
1.00
9
8
7
6
5
4
3
PPM
Krinochkin SM1067/1
USER: nmr -- DATE: 12:46:16.043 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 15
LB: 0.3
Nuts - $4055 SM1067(1)_1.1

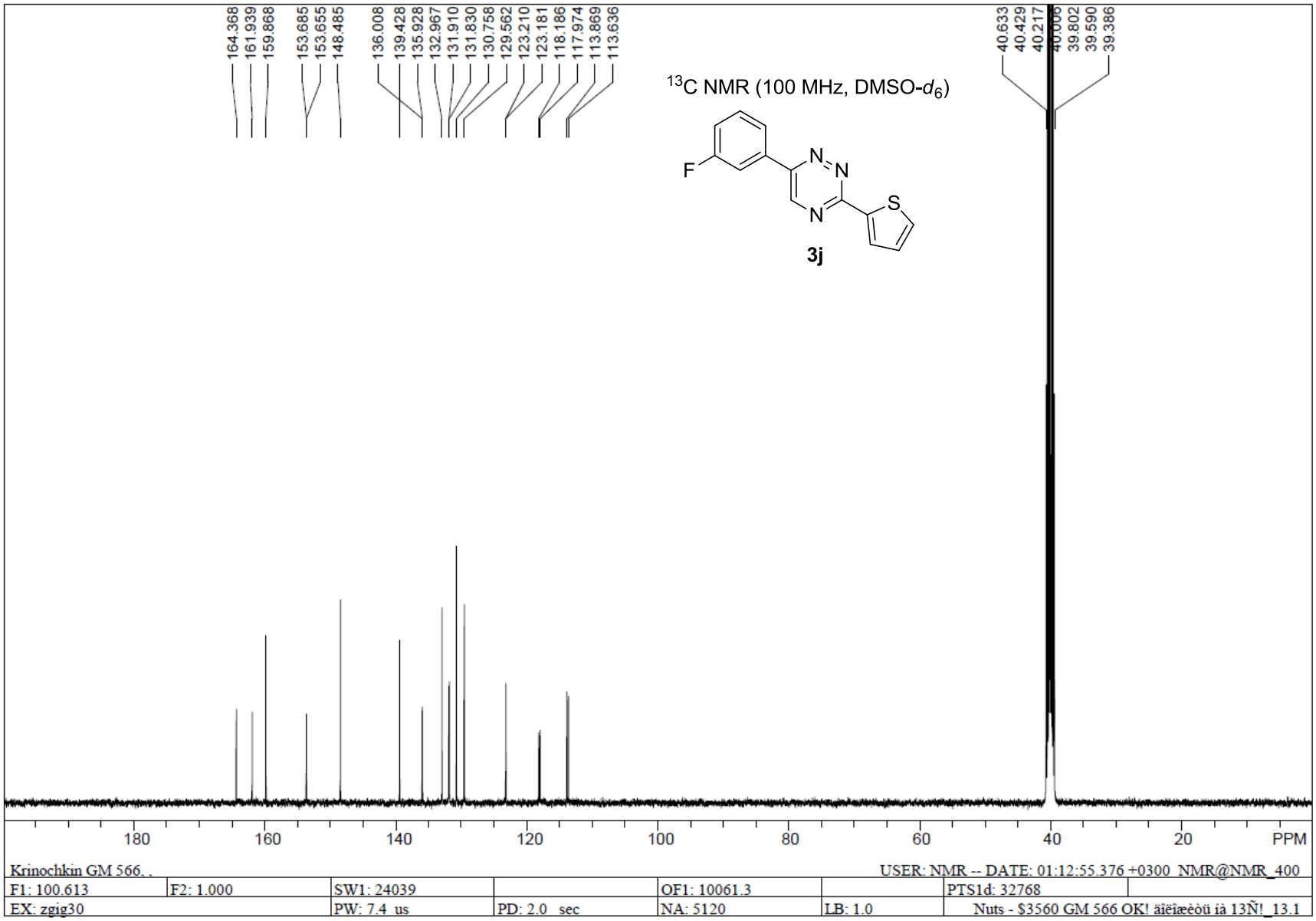
^{19}F NMR (376 MHz, DMSO-d_6)

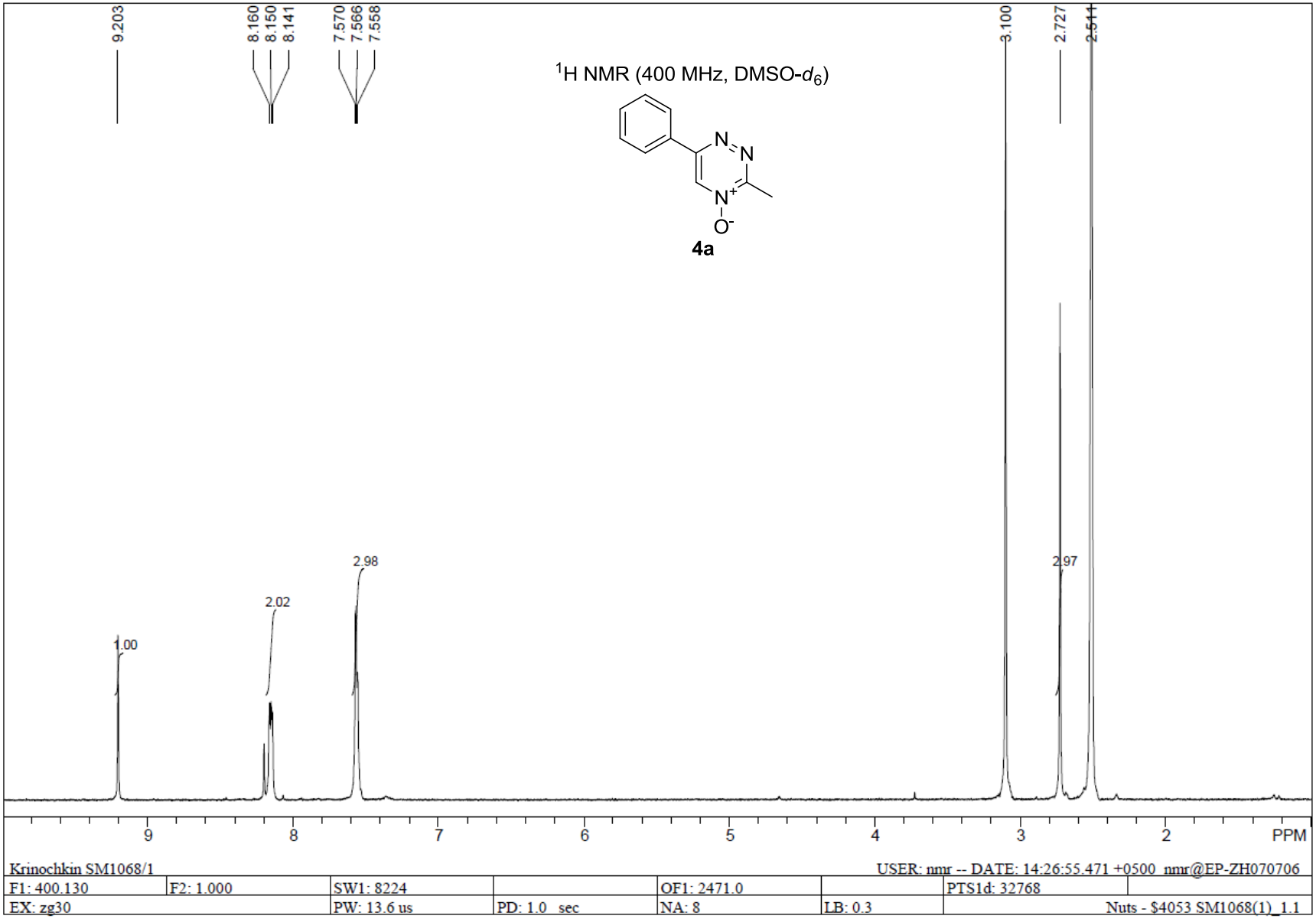


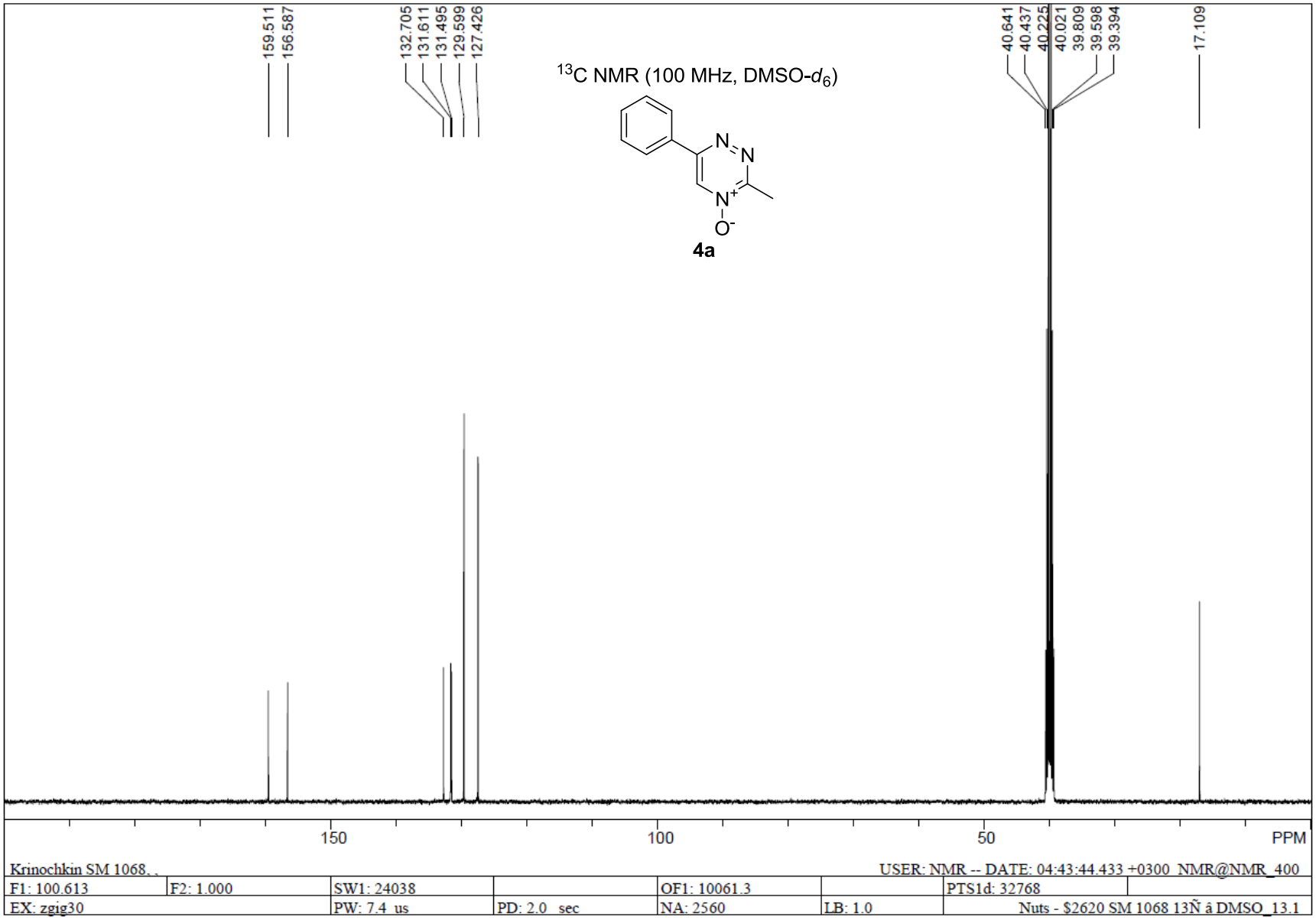
3j

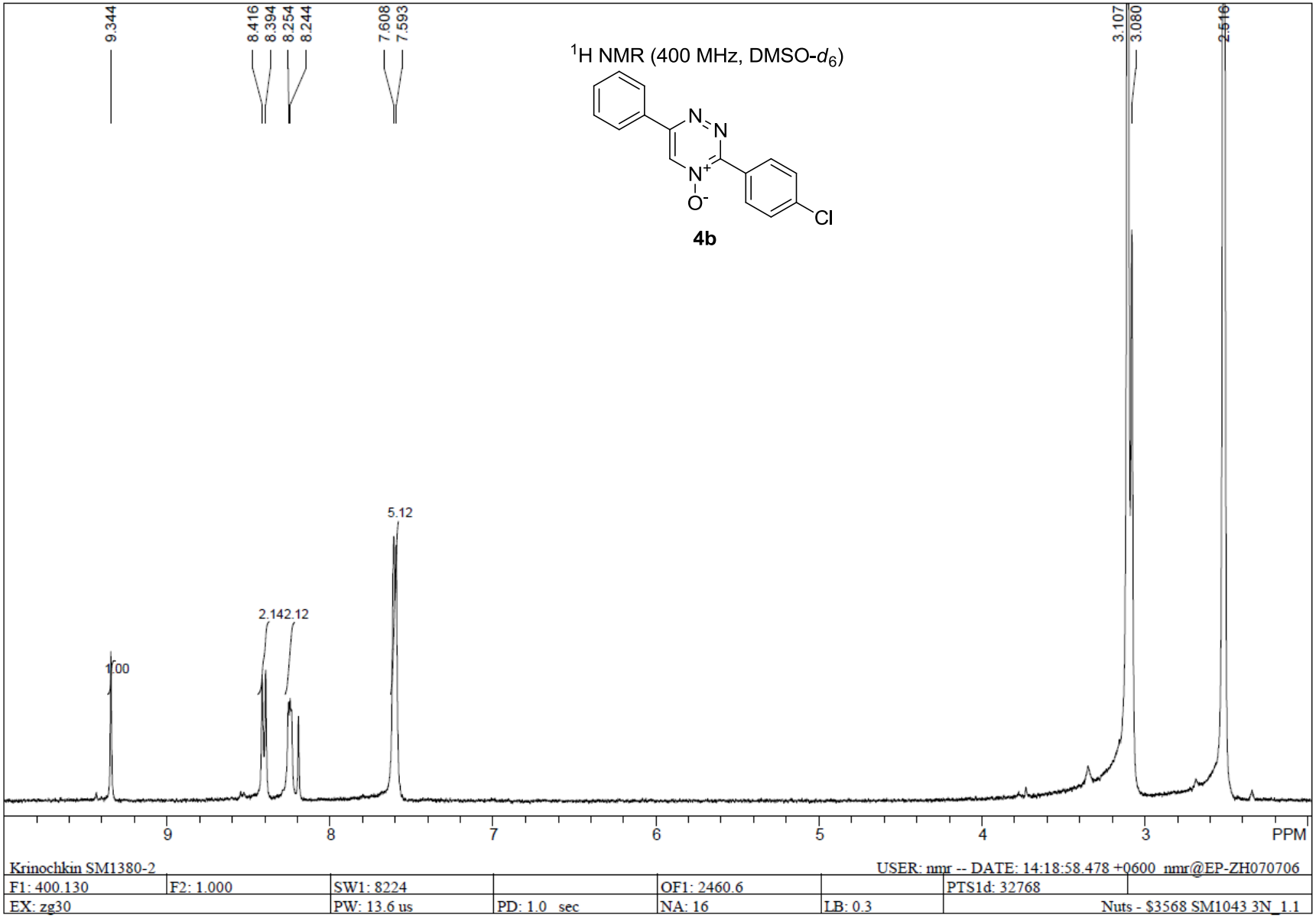
Krinochkin SM1067/1 USER: nmr -- DATE: 12:23:50.307 +0500 nmr@EP-ZH070706

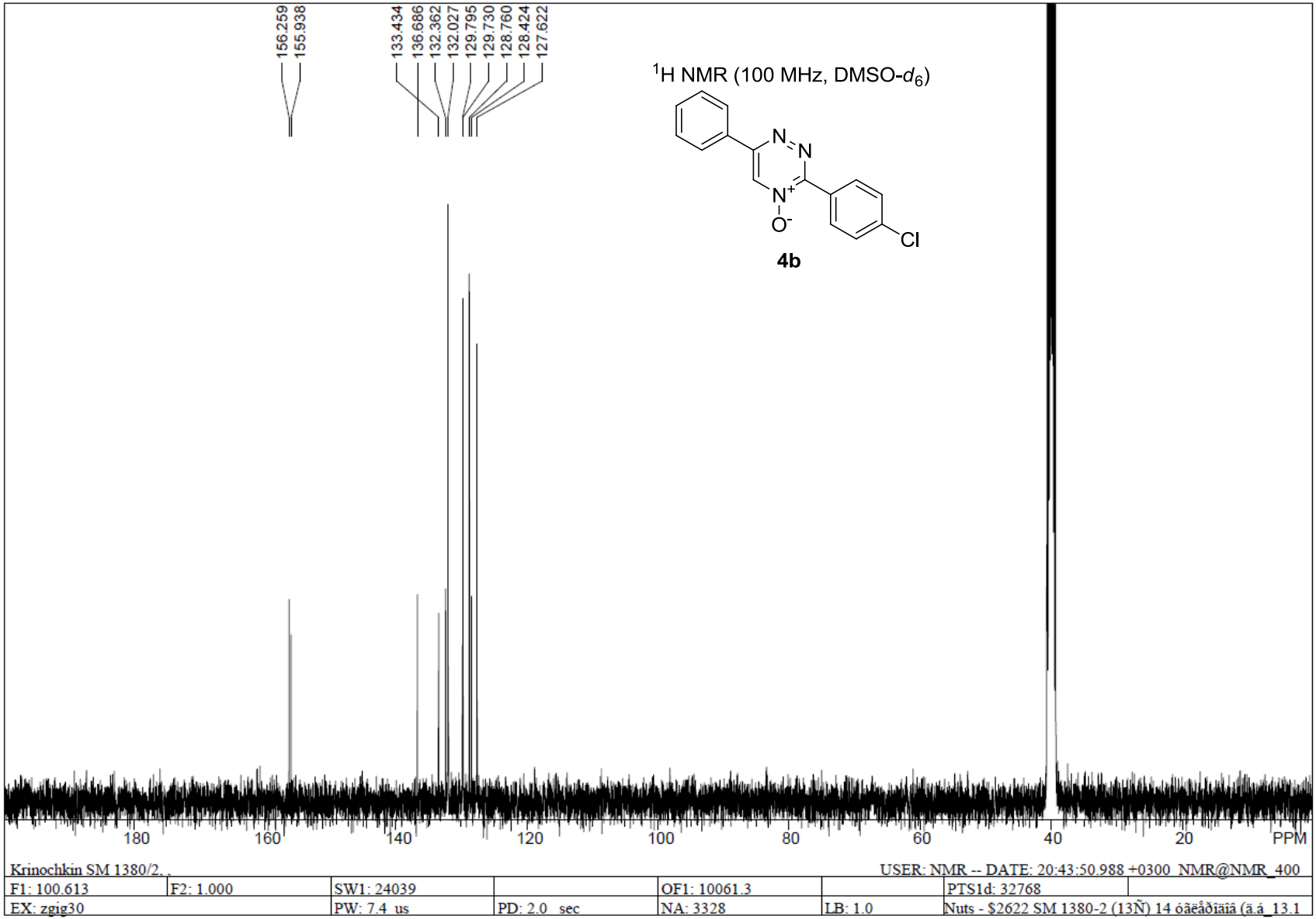
F1: 376.498	F2: 1.000	SW1: 75000		OF1: -52709.8		PTS1d: 65536	
EX: zgfhigqn		PW: 17.0 us	PD: 1.0 sec	NA: 12	LB: 0.3	Nuts - $4055 SM1067(1)_19.1	

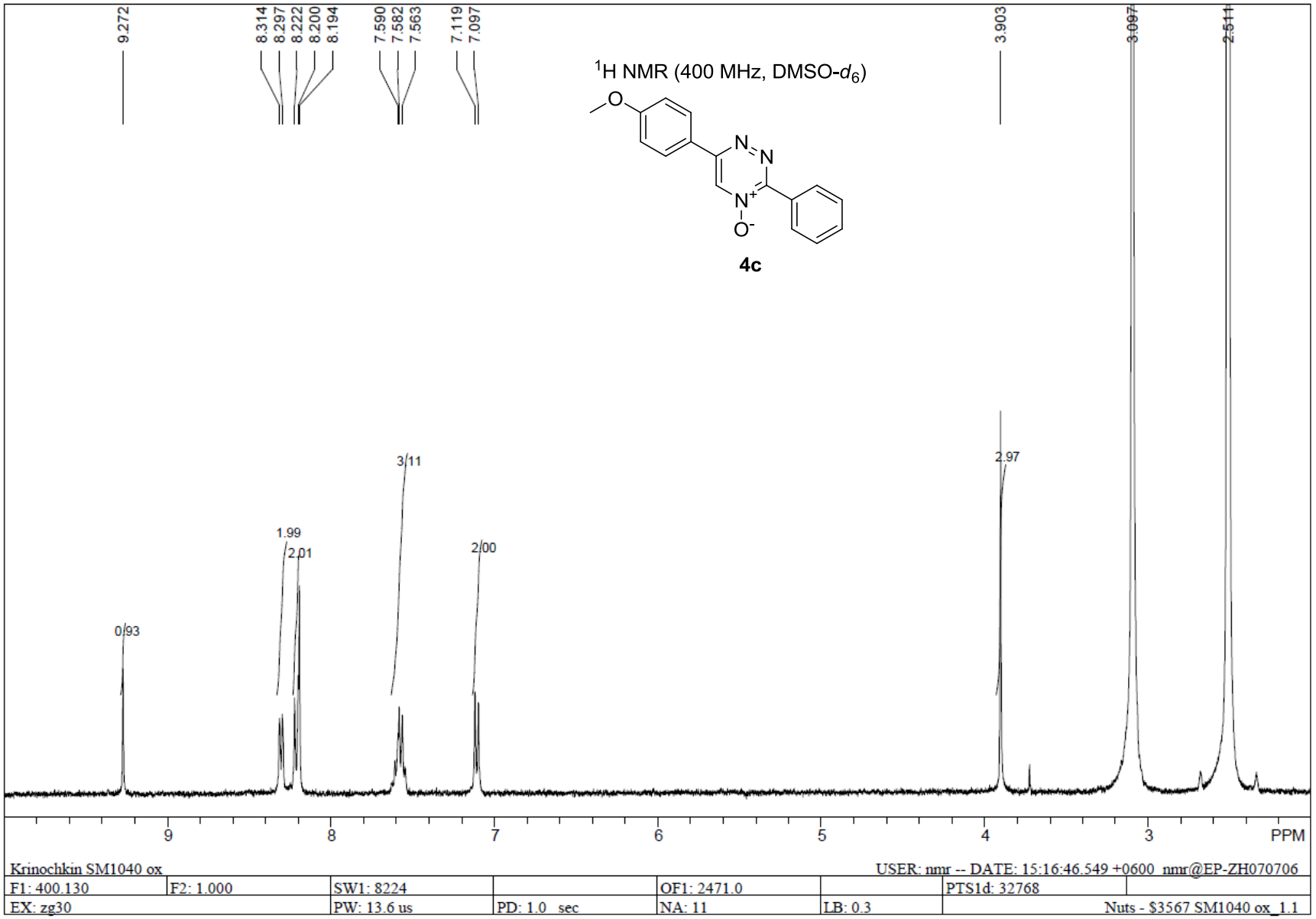

164.368
161.939
159.868
153.685
153.655
148.485
136.008
139.428
135.928
132.967
131.910
131.830
130.758
129.562
123.210
123.181
118.186
117.974
113.869
113.636
40.633
40.429
40.217
40.006
39.802
39.590
39.386
13C NMR (100 MHz, DMSO-d6)
F
N
N
N
S
3j
180
160
140
120
100
80
60
40
20
PPM
Krinochkin GM 566. .
USER: NMR -- DATE: 01:12:55.376 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24039
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 5120
LB: 1.0
Nuts - $3560 GM 566 OK! äîëîæèòü íà 13Ñ!_13.1

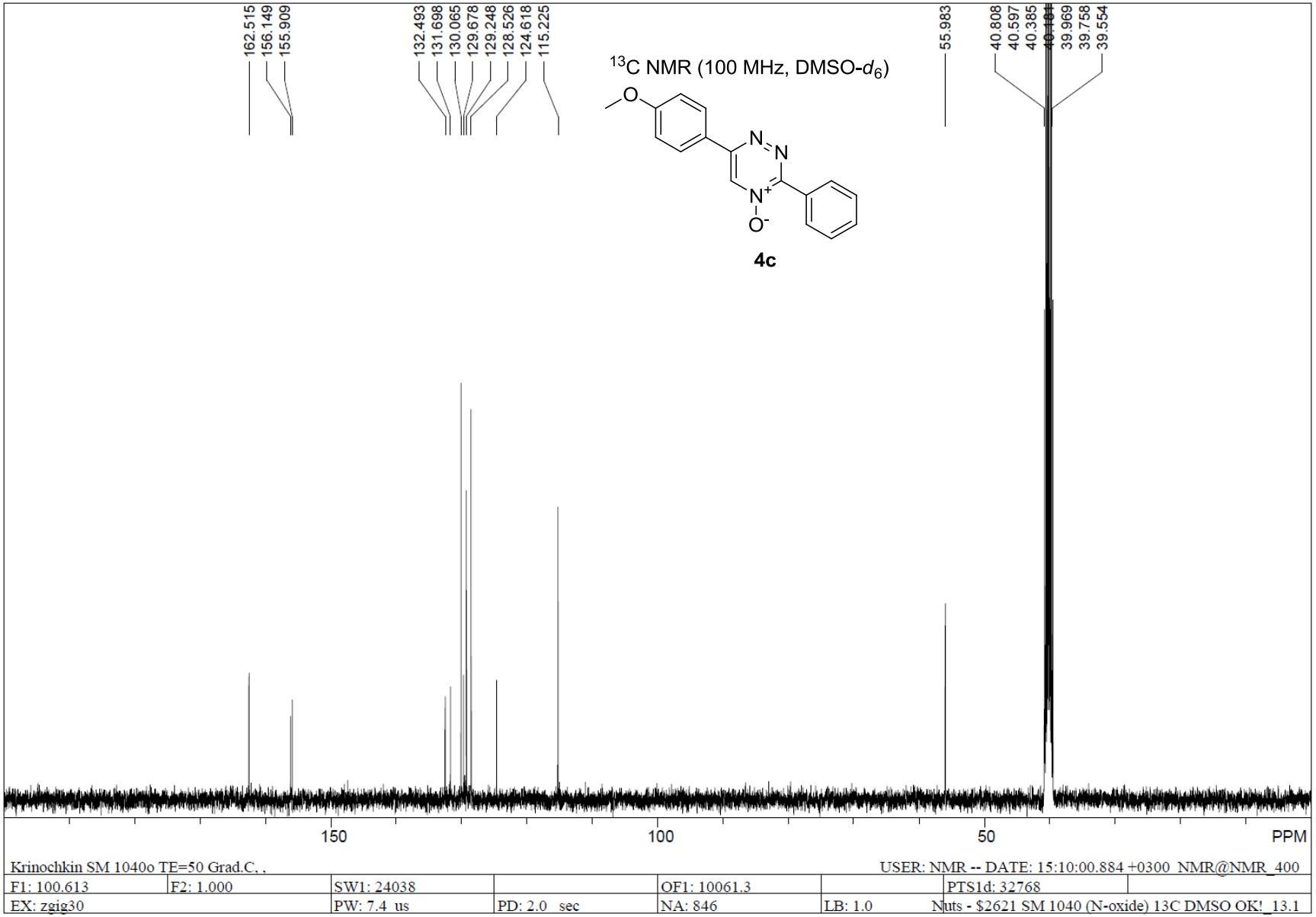

9.203
8.160
8.150
8.141
7.570
7.566
7.558
3.100
2.727
2.511
^{1}H NMR (400 MHz, DMSO-d_6)
4a
2.98
2.02
1.00
2.97
9
8
7
6
5
4
3
2
PPM
Krinochkin SM1068/1
USER: nmr -- DATE: 14:26:55.471 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 8
LB: 0.3
Nuts - $4053 SM1068(1)_1.1

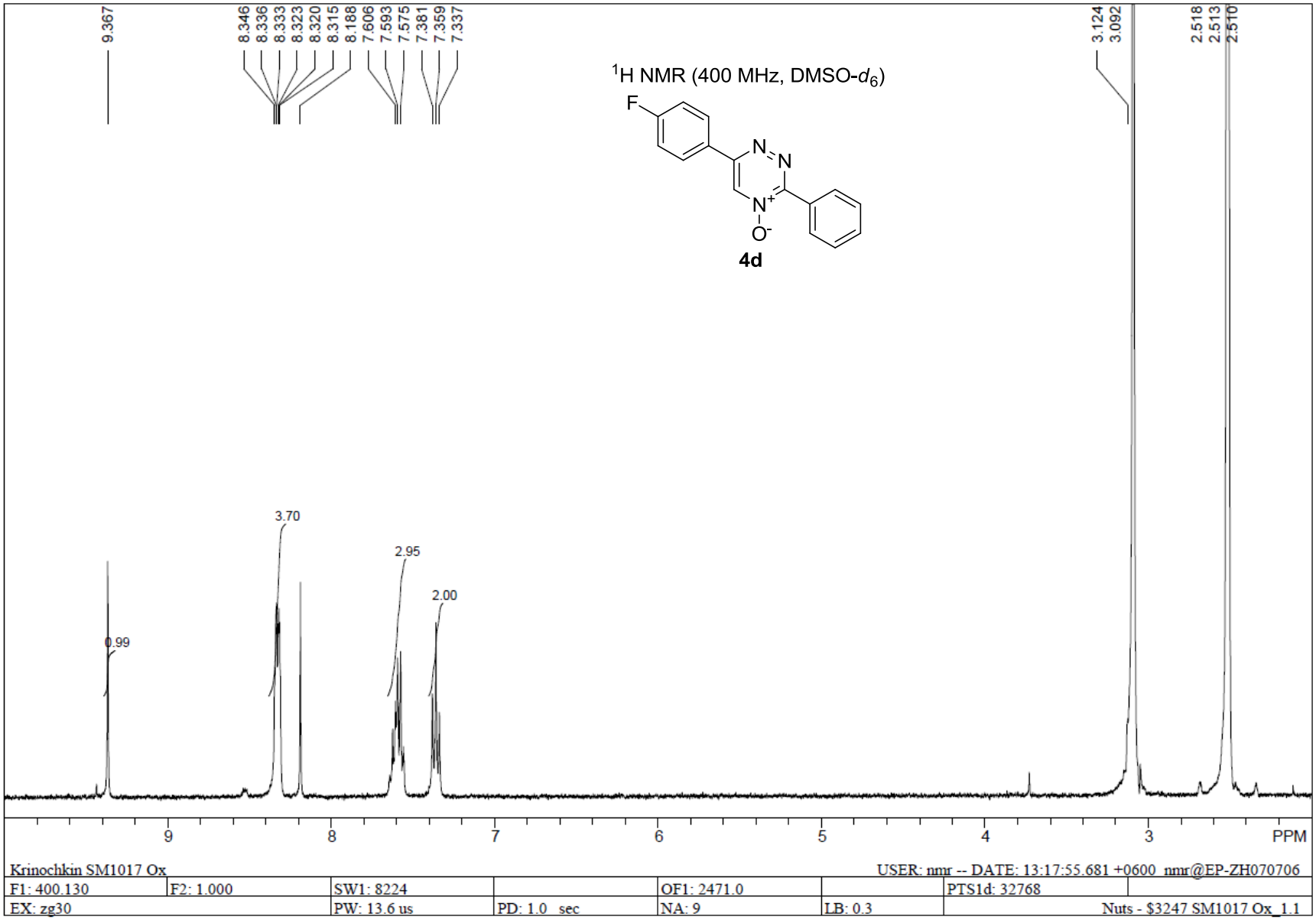

159.511
156.587
132.705
131.611
131.495
129.599
127.426
40.641
40.437
40.225
40.021
39.809
39.598
39.394
17.109
^{13}C NMR (100 MHz, DMSO-d_6)
N
N
N+
O-
4a
150
100
50
PPM
Krinochkin SM 1068. .
USER: NMR -- DATE: 04:43:44.433 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 2560
LB: 1.0
Nuts - $2620 SM 1068 13Ñ â DMSO_13.1

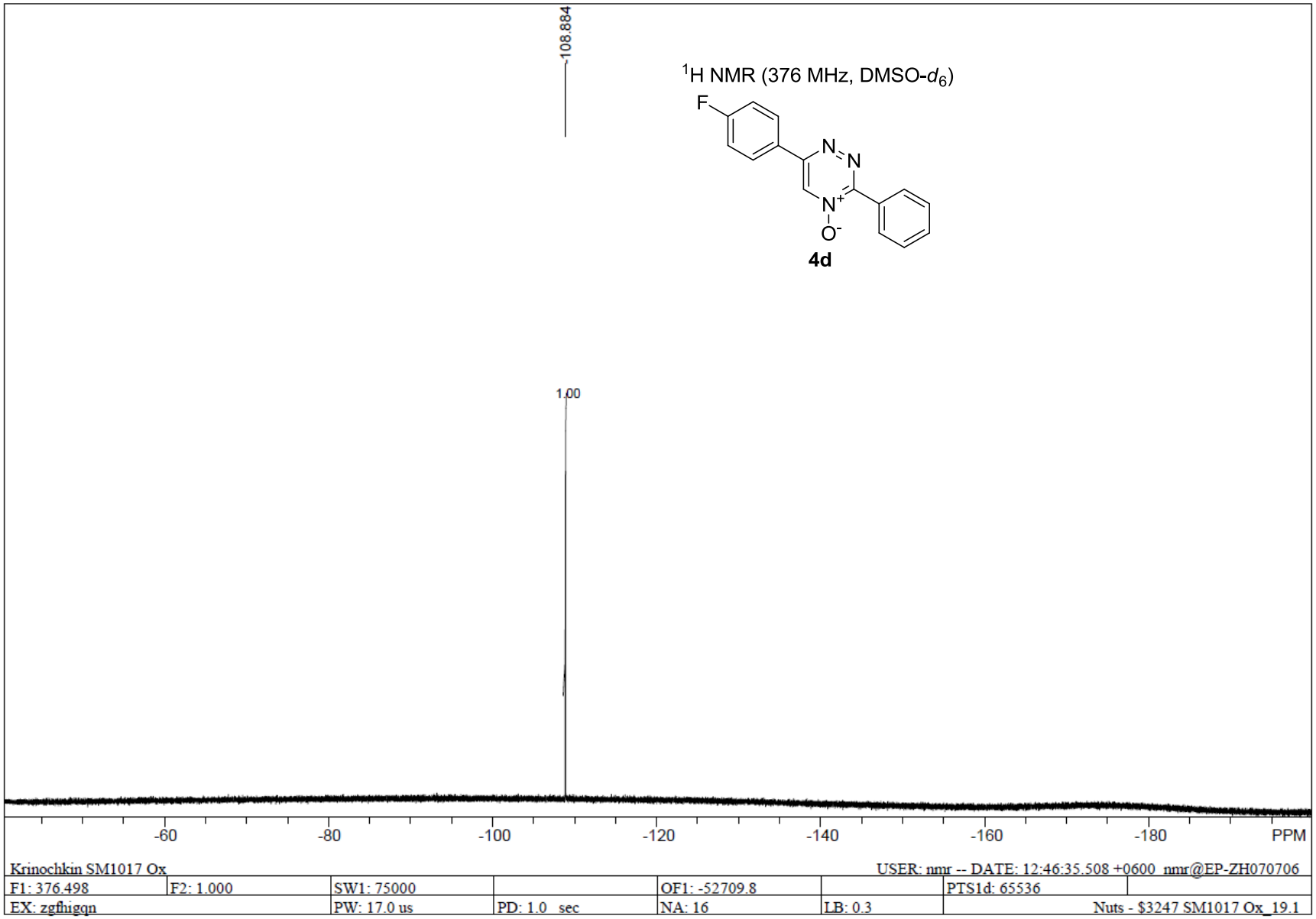

9.344
8.416
8.394
8.254
8.244
7.608
7.593
3.107
3.080
2.516
^{1}H NMR (400 MHz, DMSO-d_6)
N
N
N+
O-
Cl
4b
5.12
2.14
2.12
1.00
9
8
7
6
5
4
3
PPM
Krinochkin SM1380-2
USER: nmr -- DATE: 14:18:58.478 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.6
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3568 SM1043 3N_1.1

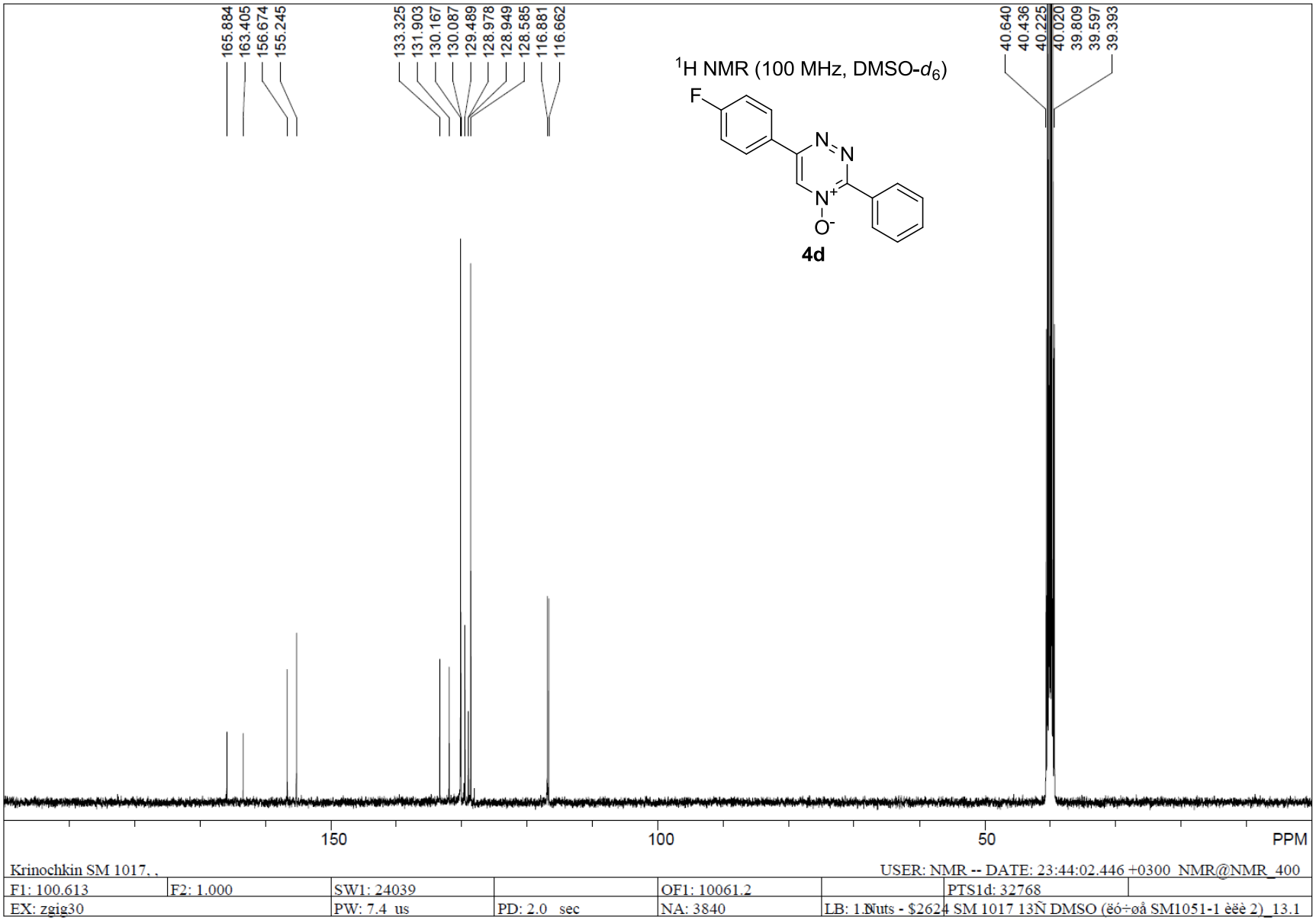

156.259
155.938
133.434
136.686
132.362
132.027
129.795
129.730
128.760
128.424
127.622
^{1}H NMR (100 MHz, DMSO-d_6)
N
N
N+
O-
Cl
4b
180
160
140
120
100
80
60
40
20
PPM
Krinochkin SM 1380/2, ,
USER: NMR -- DATE: 20:43:50.988 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24039
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3328
LB: 1.0
Nuts - $2622 SM 1380-2 (13Ñ) 14 óãëåðîãîâ (ã.á_13.1

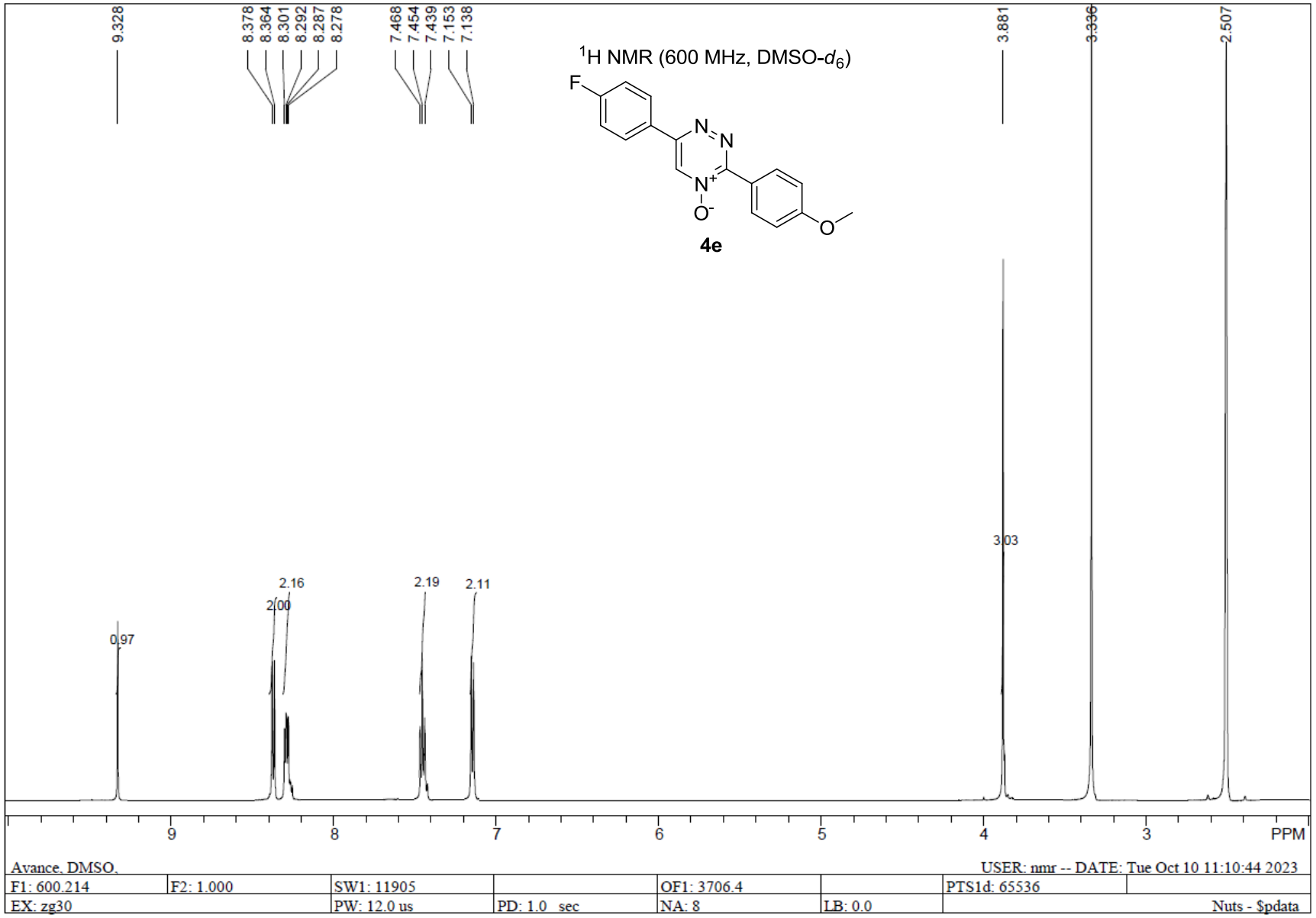

9.272
8.314
8.297
8.222
8.200
8.194
7.590
7.582
7.563
7.119
7.097
3.903
3.097
2.511
^{1}H NMR (400 MHz, DMSO-d_6)
4c
0.93
1.99
2.01
3.11
2.00
2.97
9
8
7
6
5
4
3
PPM
Krinochkin SM1040 ox
USER: nmr -- DATE: 15:16:46.549 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 11
LB: 0.3
Nuts - $3567 SM1040 ox_1.1


162.515
156.149
155.909
132.493
131.698
130.065
129.678
129.248
128.526
124.618
115.225
55.983
40.808
40.597
40.385
40.161
39.969
39.758
39.554
^{13}C NMR (100 MHz, DMSO-d_6)
O
N
N
N+
O-
4c
150
100
50
PPM
Krinochkin SM 1040o TE=50 Grad.C. ,
USER: NMR -- DATE: 15:10:00.884 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 846
LB: 1.0
Nuts - $2621 SM 1040 (N-oxide) 13C DMSO OK!_13.1

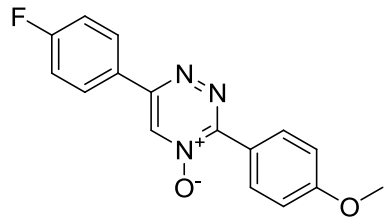

9.367
8.346
8.336
8.333
8.323
8.320
8.315
8.188
7.606
7.593
7.575
7.381
7.359
7.337
3.124
3.092
2.518
2.513
2.510
^{1}H NMR (400 MHz, DMSO-d_6)
F
N
N
N+
O-
4d
3.70
2.95
2.00
0.99
9
8
7
6
5
4
3
PPM
Krinochkin SM1017 Ox
USER: nmr -- DATE: 13:17:55.681 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 9
LB: 0.3
Nuts - $3247 SM1017 Ox_1.1


108.884
^{1}H NMR (376 MHz, DMSO-d_6)
F
N
N
N+
O-
4d
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1017 Ox
USER: nmr -- DATE: 12:46:35.508 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3247 SM1017 Ox_19.1


165.884
163.405
156.674
155.245
133.325
131.903
130.167
130.087
129.489
128.978
128.949
128.585
116.881
116.662
40.640
40.436
40.225
40.020
39.809
39.597
39.393
^{1}H NMR (100 MHz, DMSO-d_6)
F
N
N
N$^+$
O$^-$
4d
150
100
50
PPM
Krinochkin SM 1017, ,
USER: NMR -- DATE: 23:44:02.446 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24039
OF1: 10061.2
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.00
Nuts - $2624 SM 1017 13Ñ DMSO (ëó÷øå SM1051-1 èëè 2)_13.1


9.328
8.378
8.364
8.301
8.292
8.287
8.278
7.468
7.454
7.439
7.153
7.138
3.881
3.336
2.507
^{1}H NMR (600 MHz, DMSO-d_6)
F
N
N
N+
O-
O
4e
3.03
2.16
2.00
2.19
2.11
0.97
9
8
7
6
5
4
3
PPM
Avance, DMSO,
USER: nmr -- DATE: Tue Oct 10 11:10:44 2023
F1: 600.214
F2: 1.000
SW1: 11905
OF1: 3706.4
PTS1d: 65536
EX: zg30
PW: 12.0 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $pdata

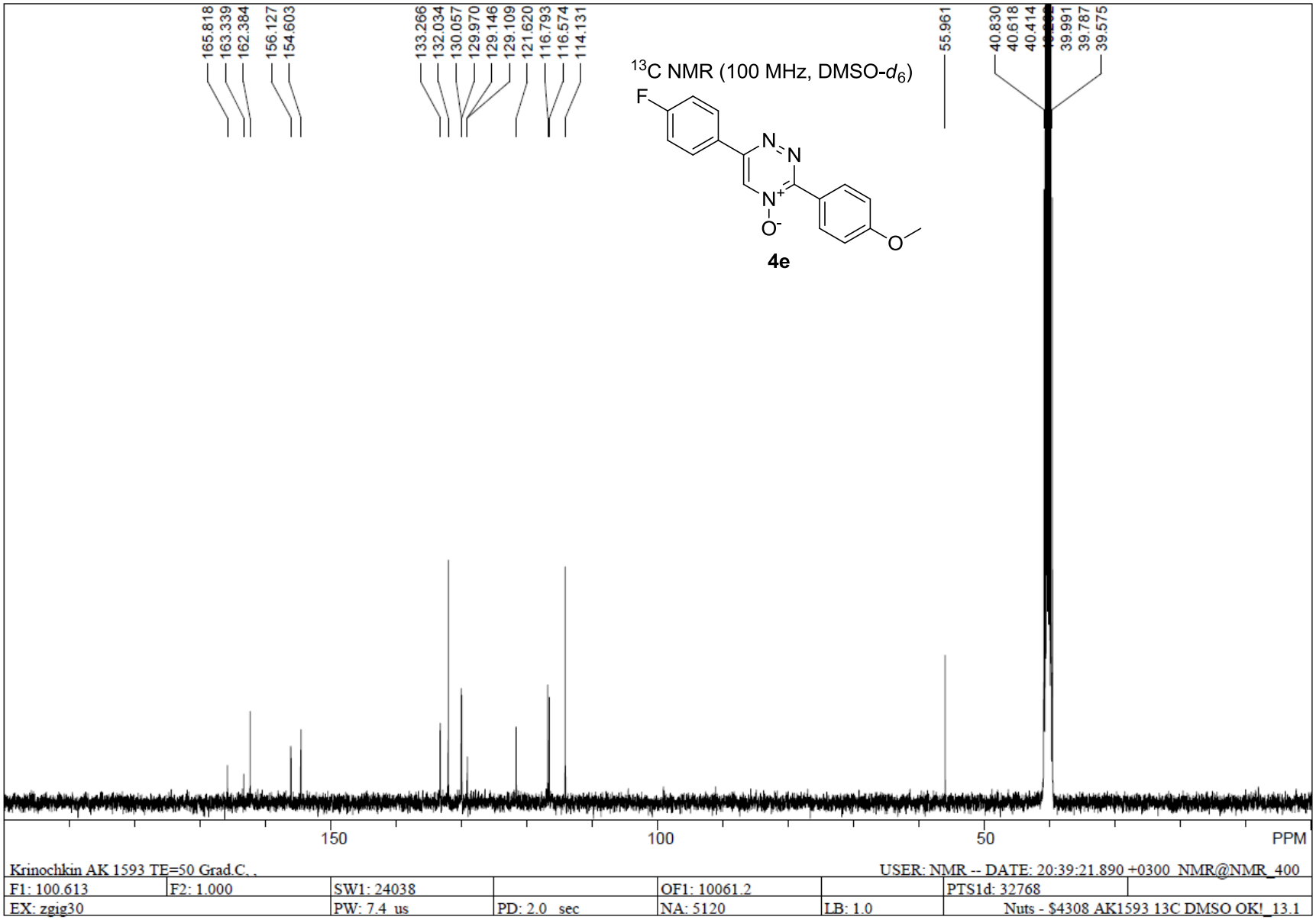
^{19}F NMR (564 MHz, DMSO-d_6)

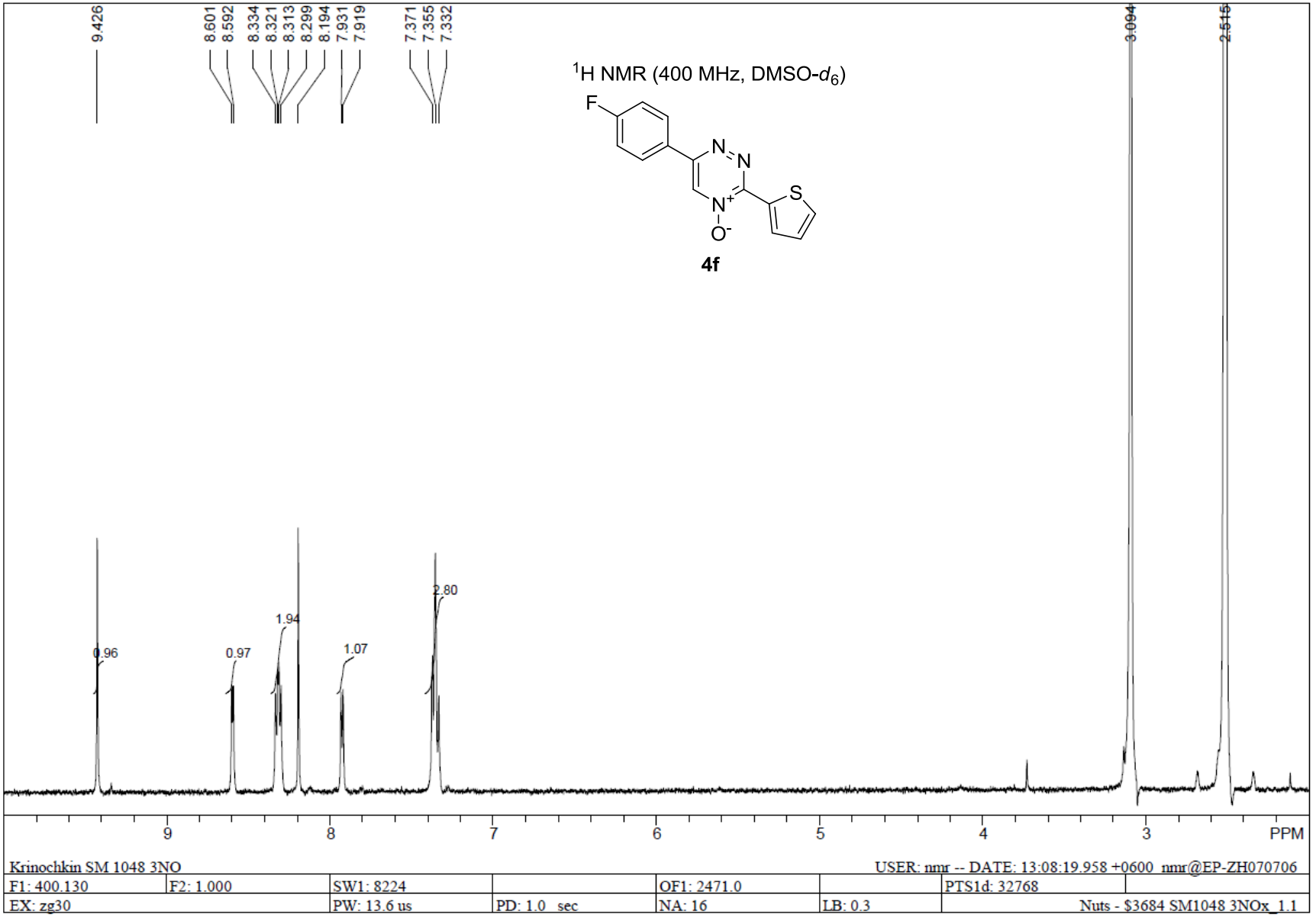


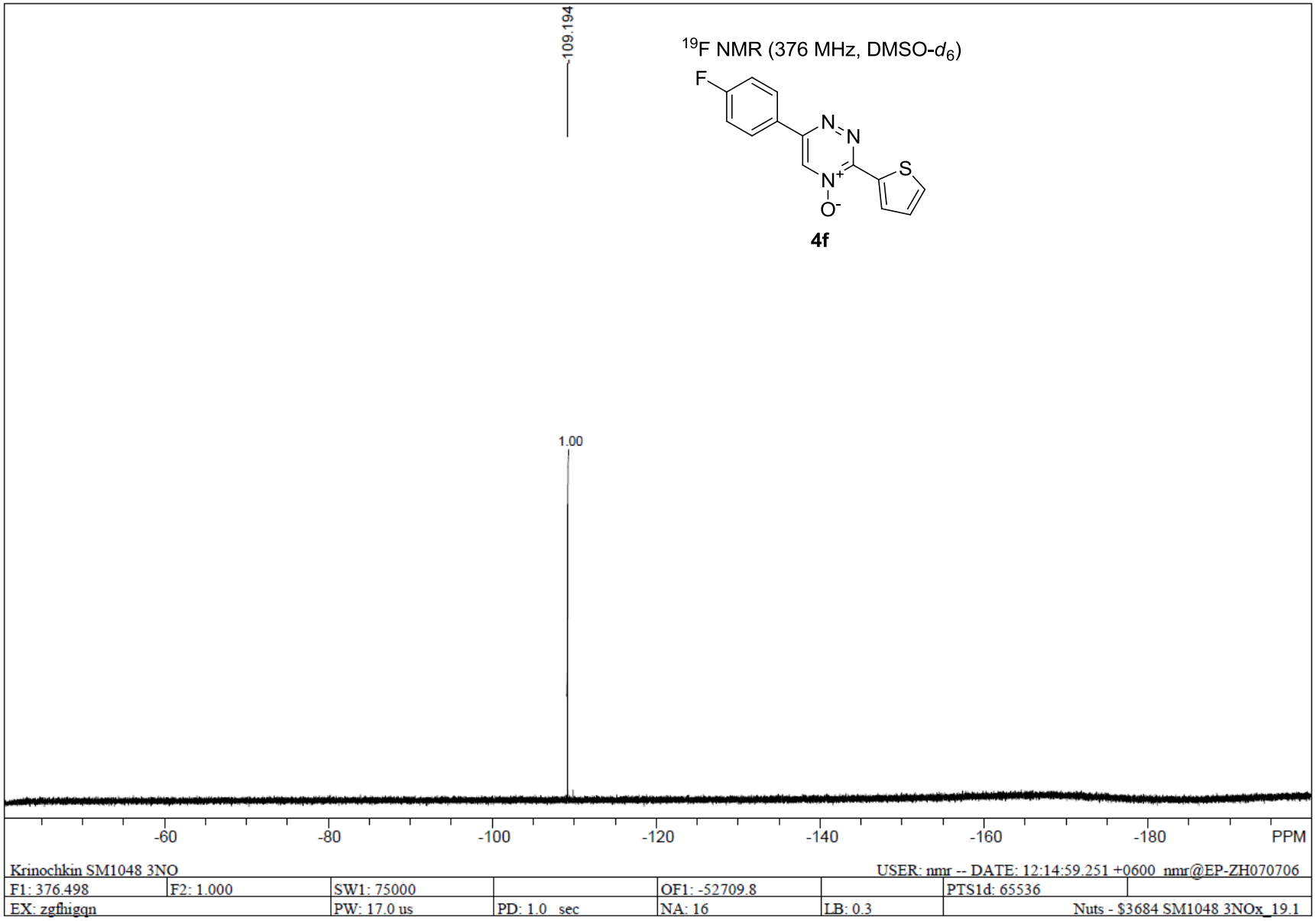
4e

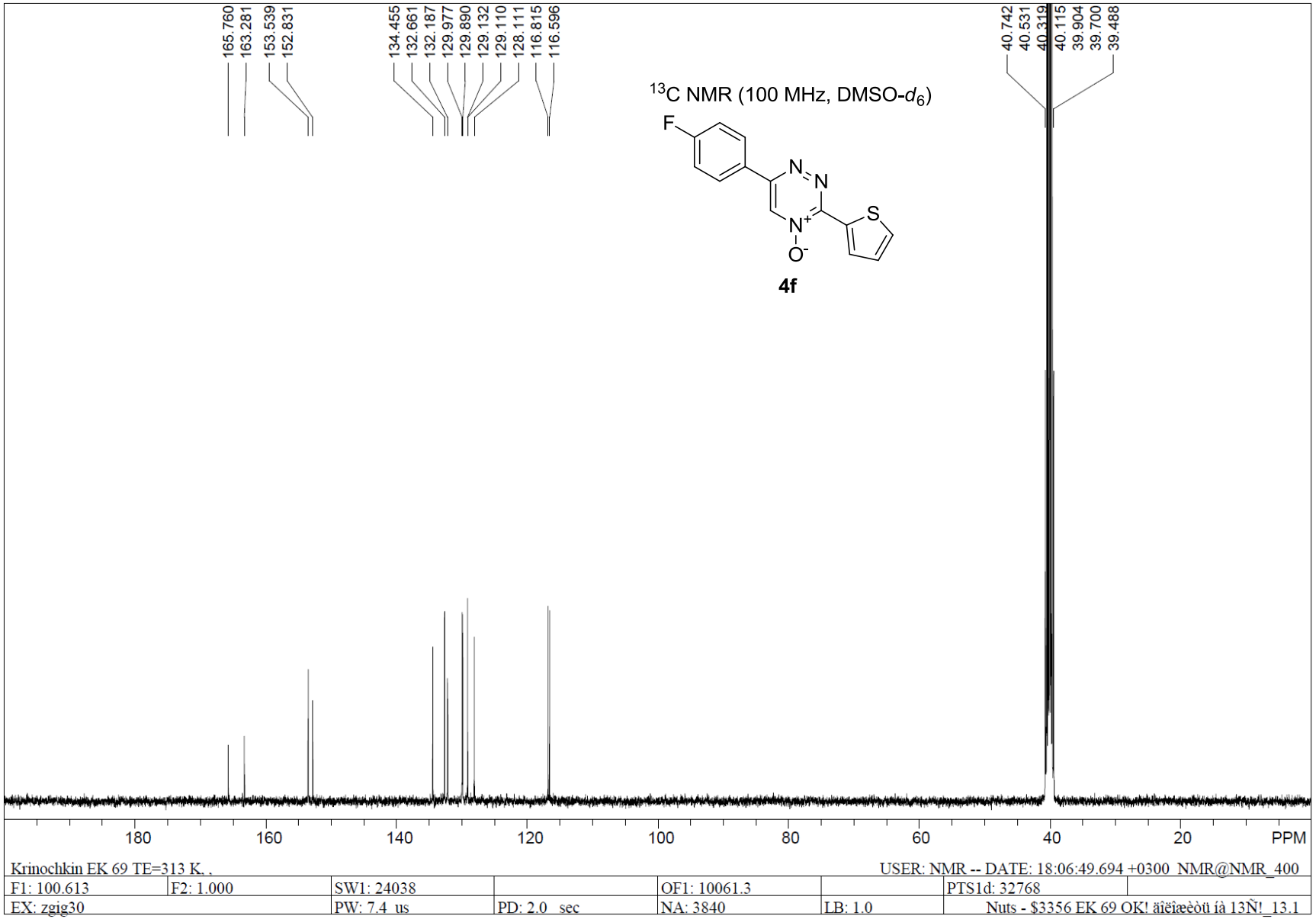
Avance, DMSO, USER: nmr -- DATE: Tue Oct 10 11:12:32 2023

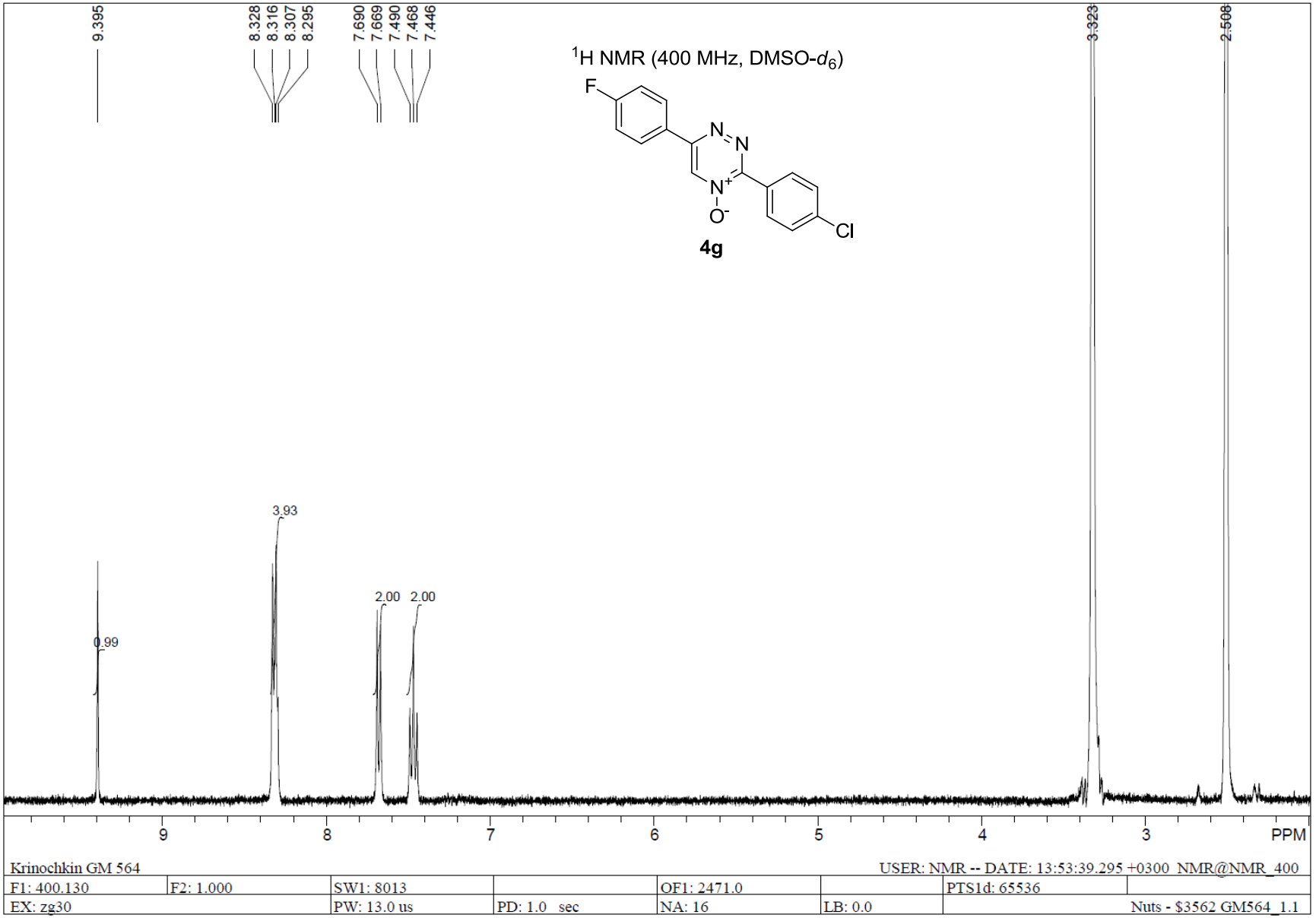
F1: 564.705	F2: 1.000	SW1: 131579		OF1: -56477.1		PTS1d: 65536	
EX: zg		PW: 15.0 us	PD: 1.0 sec	NA: 8	LB: 0.0		Nuts - $pdata


165.818
163.339
162.384
156.127
154.603
133.266
132.034
130.057
129.970
129.146
129.109
121.620
116.793
116.574
114.131
55.961
40.830
40.618
40.414
39.991
39.787
39.575
^{13}C NMR (100 MHz, DMSO-d_6)
F
N
N
N+
O-
O
4e
150
100
50
PPM
Krinochkin AK 1593 TE=50 Grad.C. .
USER: NMR -- DATE: 20:39:21.890 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.2
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 5120
LB: 1.0
Nuts - $4308 AK1593 13C DMSO OK!_13.1

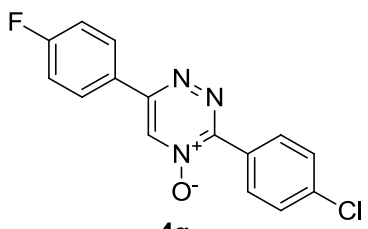

9.426
8.601
8.592
8.334
8.321
8.313
8.299
8.194
7.931
7.919
7.371
7.355
7.332
3.094
2.515
^{1}H NMR (400 MHz, DMSO-d_6)
F
N
N
N+
O-
S
4f
0.96
0.97
1.94
1.07
2.80
9
8
7
6
5
4
3
PPM
Krinochkin SM 1048 3NO
USER: nmr -- DATE: 13:08:19.958 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3684 SM1048 3NOx_1.1


-109.194
^{19}F NMR (376 MHz, DMSO-d_6)
F
N
N
N+
O-
S
4f
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1048 3NO
USER: nmr -- DATE: 12:14:59.251 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3684 SM1048 3NOx_19.1


165.760
163.281
153.539
152.831
134.455
132.661
132.187
129.977
129.890
129.132
129.110
128.111
116.815
116.596
40.742
40.531
40.319
40.115
39.904
39.700
39.488
^{13}C NMR (100 MHz, DMSO-d_6)
F
N
N
S
N+
O-
4f
180
160
140
120
100
80
60
40
20
PPM
Krinochkin EK 69 TE=313 K, ,
USER: NMR -- DATE: 18:06:49.694 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $3356 EK 69 OK! äîëïæèòü íà 13Ñ!_13.1


9.395
8.328
8.316
8.307
8.295
7.690
7.669
7.490
7.468
7.446
3.323
2.508
^{1}H NMR (400 MHz, DMSO-d_6)
F
N
N
N+
O-
Cl
4g
3.93
2.00
2.00
0.99
9
8
7
6
5
4
3
PPM
Krinochkin GM 564
USER: NMR -- DATE: 13:53:39.295 +0300 NMR@NMR_400
F1: 400.130
F2: 1.000
SW1: 8013
OF1: 2471.0
PTS1d: 65536
EX: zg30
PW: 13.0 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $3562 GM564_1.1

^{19}F NMR (376 MHz, DMSO-d_6)

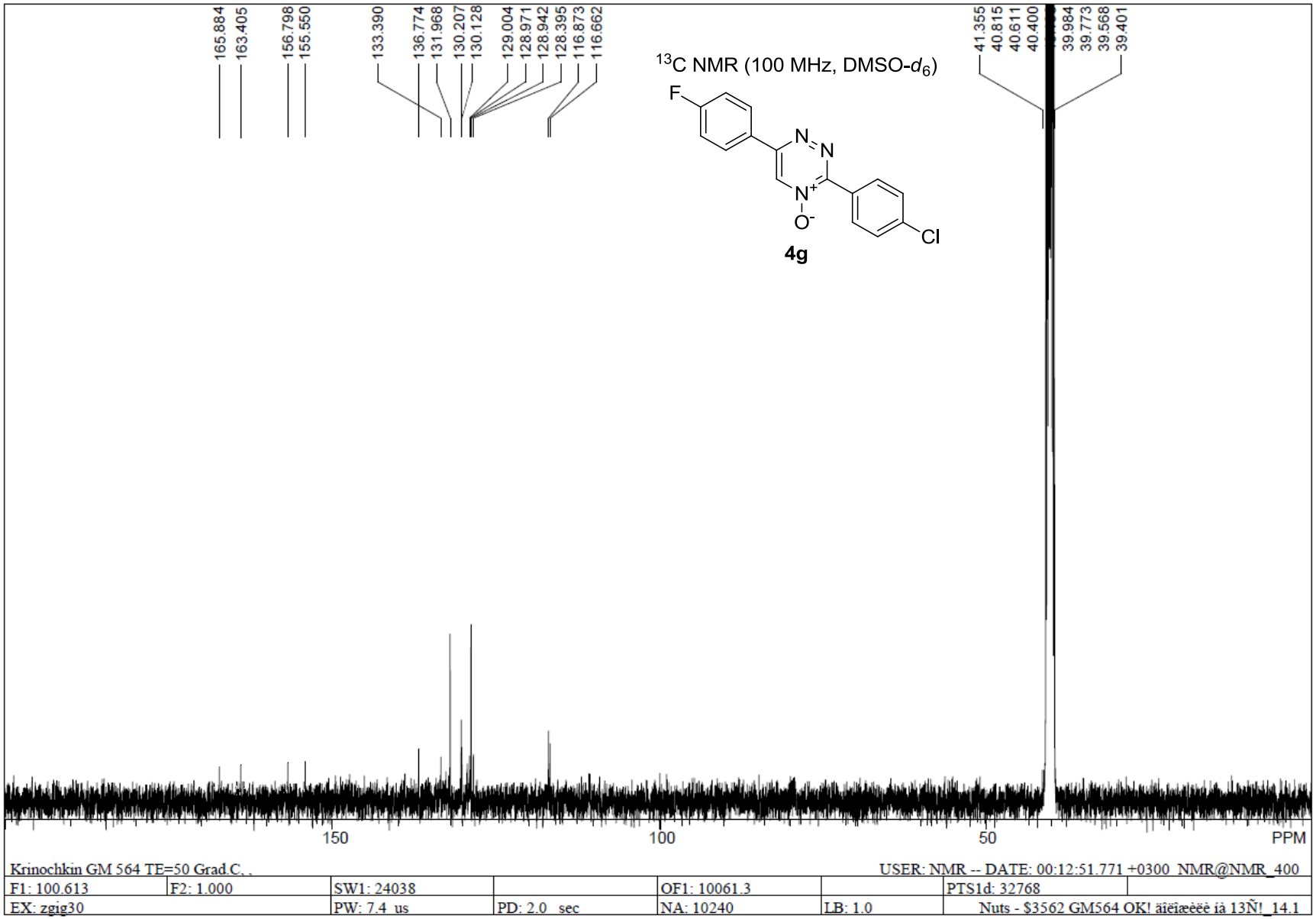


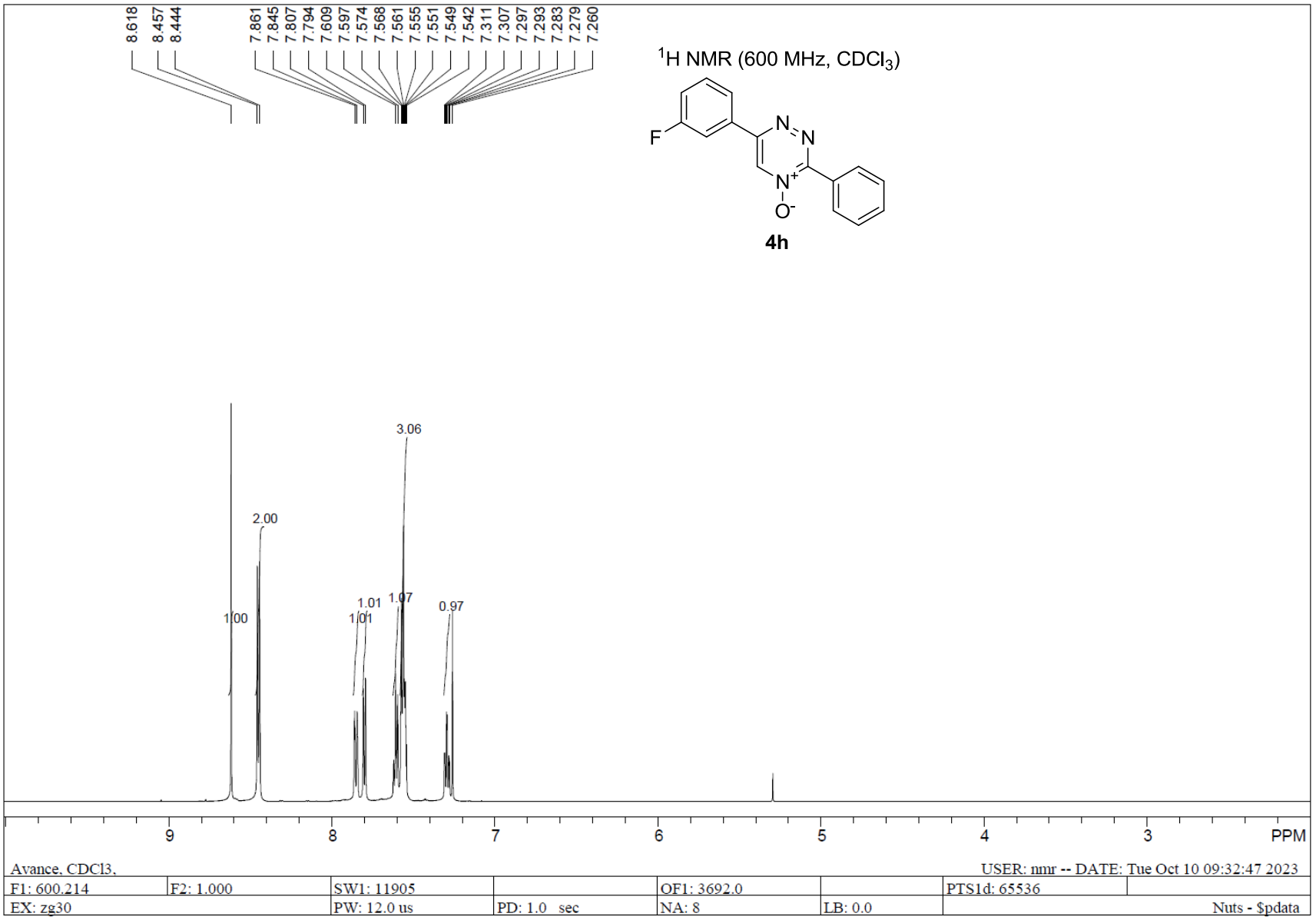
4g

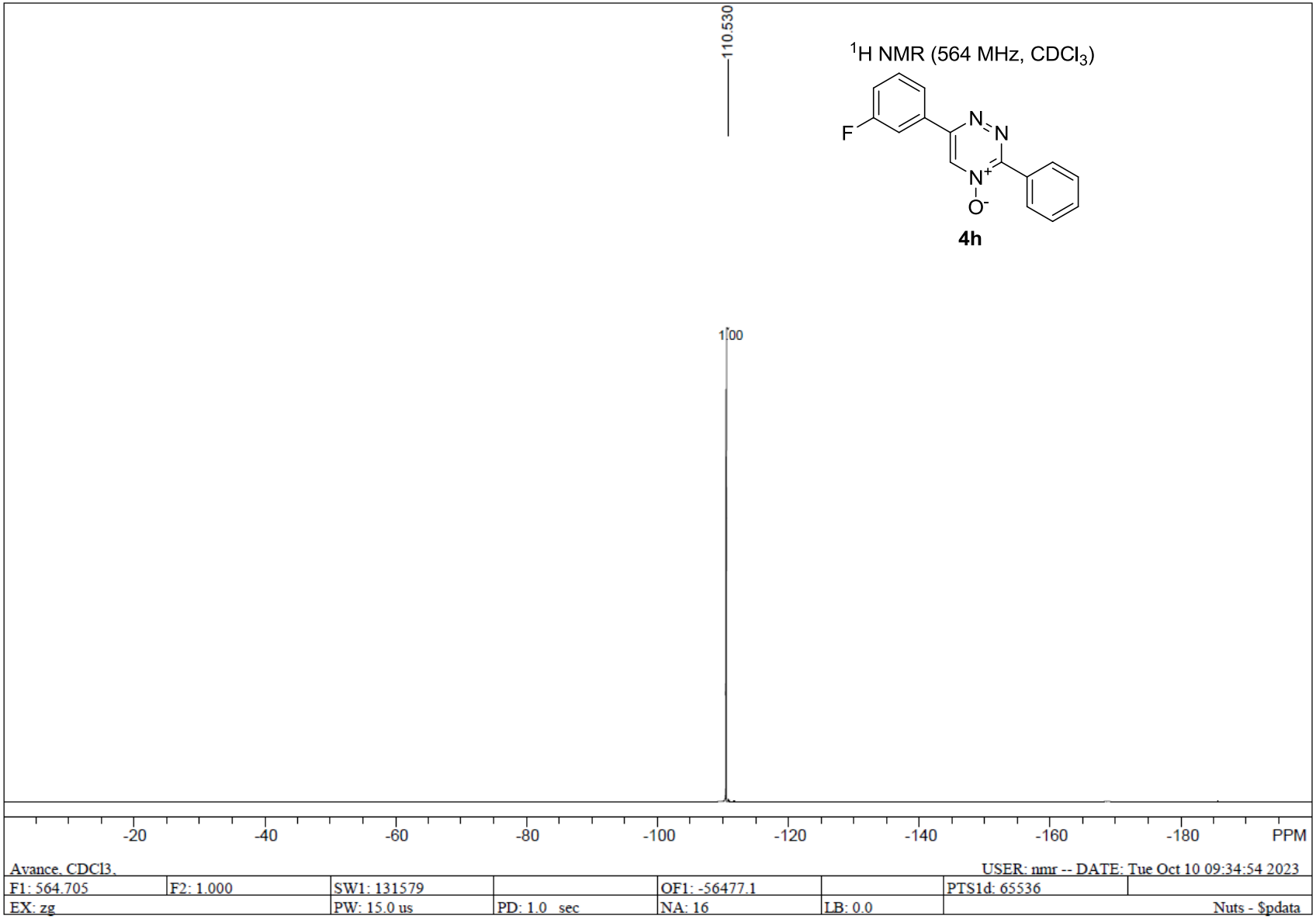
Krinochkin SM1386-2

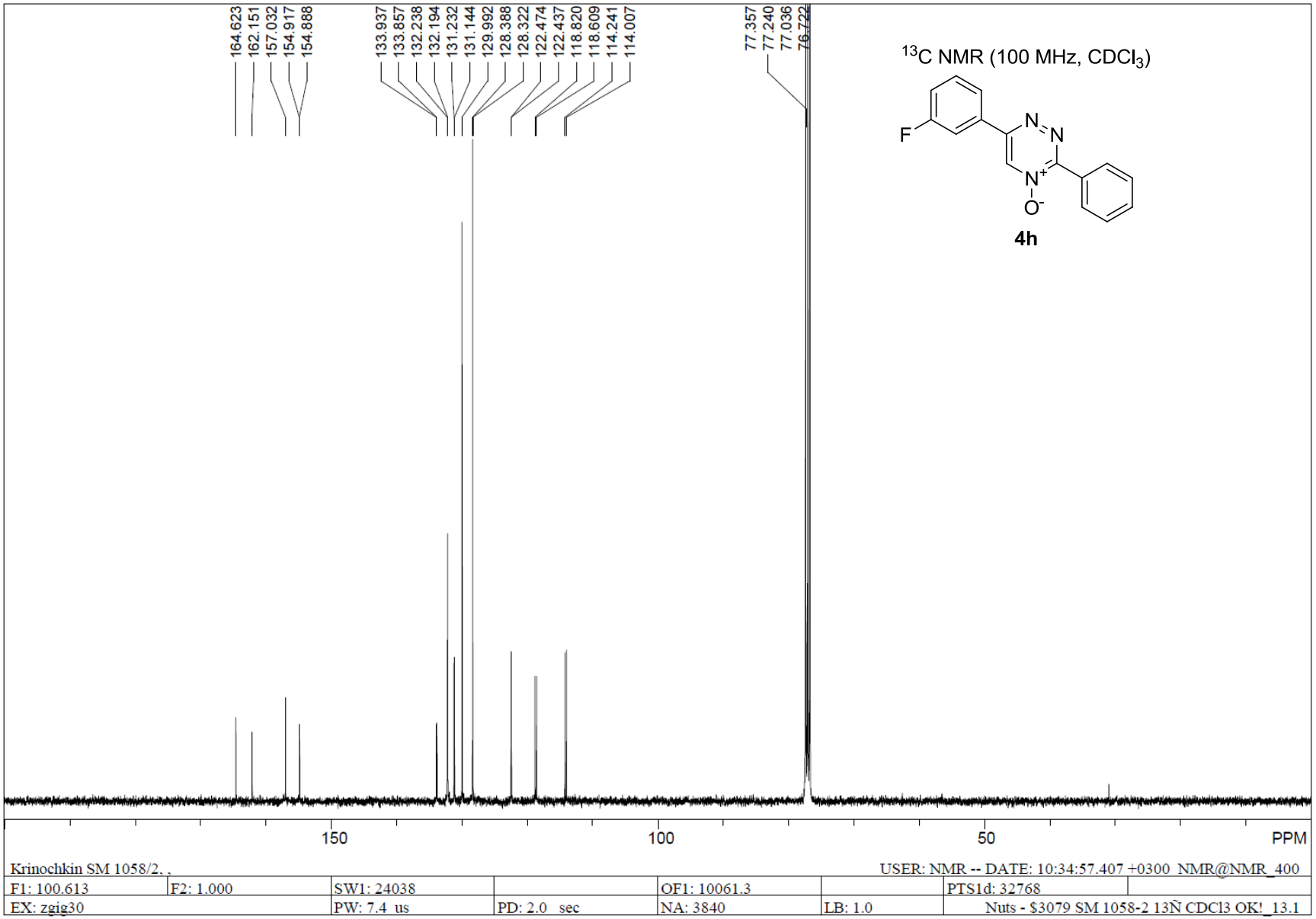
USER: nmr -- DATE: 12:31:21.138 +0600 nmr@EP-ZH070706

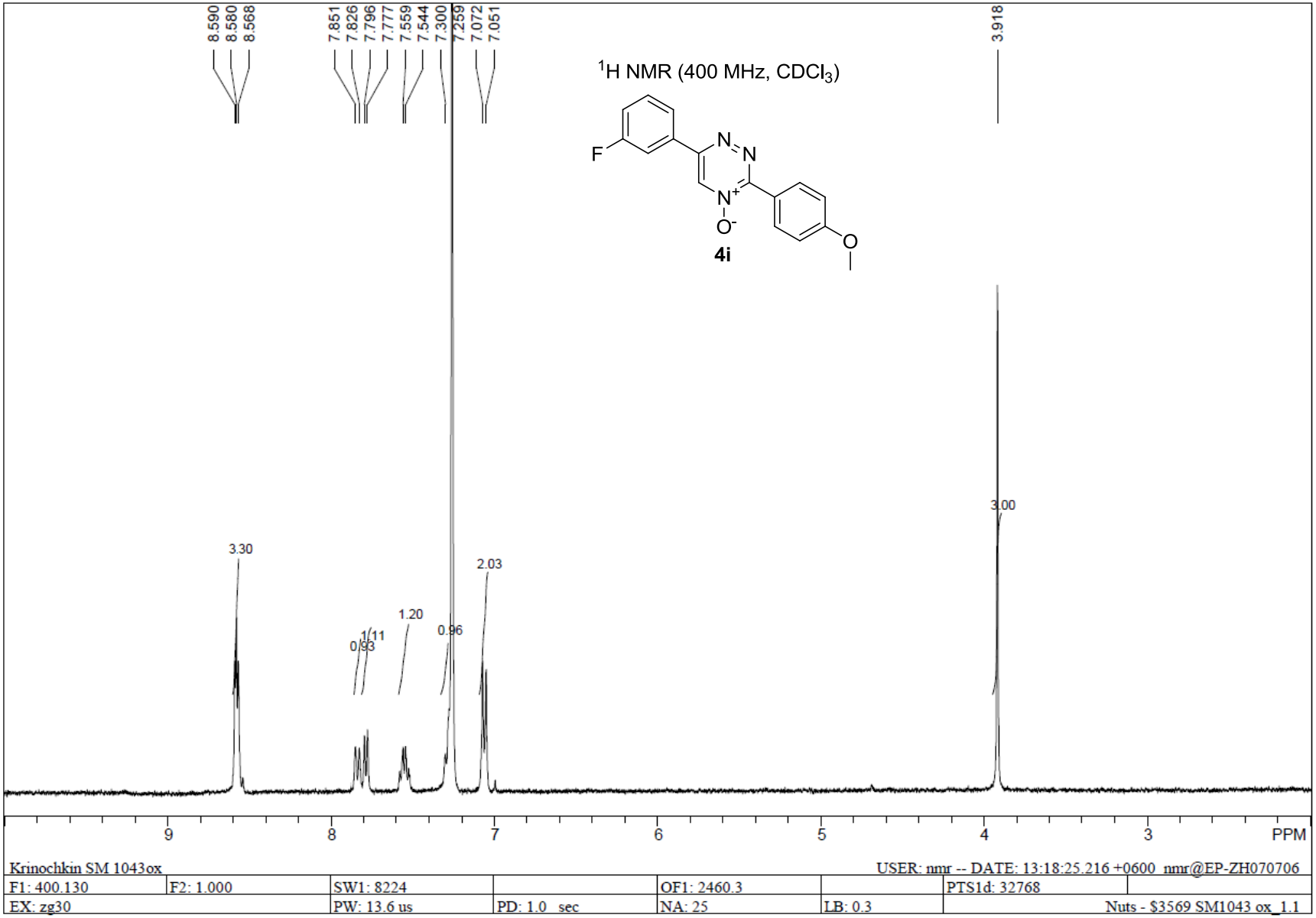
F1: 376.498	F2: 1.000	SW1: 89286		OF1: -37649.6		PTS1d: 65536
EX: zgfhigqn		PW: 17.0 us	PD: 1.0 sec	NA: 12	LB: 0.3	Nuts - $3739 SM1386-2_19.1

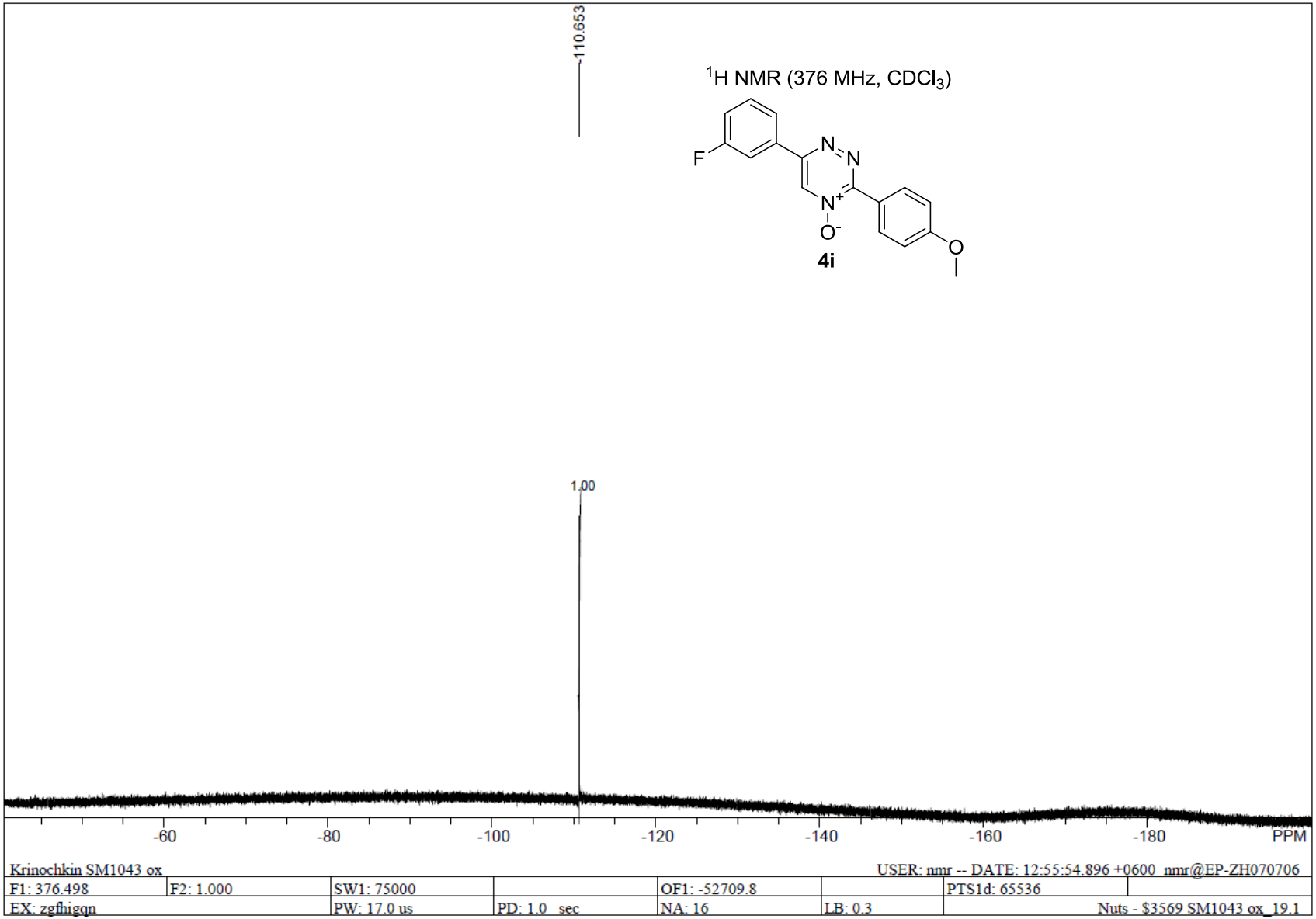

165.884
163.405
156.798
155.550
133.390
136.774
131.968
130.207
130.128
129.004
128.971
128.942
128.395
116.873
116.662
41.355
40.815
40.611
40.400
39.984
39.773
39.568
39.401
^{13}C NMR (100 MHz, DMSO-d_6)
F
N
N
N+
O-
Cl
4g
150
100
50
PPM
Krinochkin GM 564 TE=50 Grad.C. .
USER: NMR -- DATE: 00:12:51.771 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 10240
LB: 1.0
Nuts - $3562 GM564 OK! äîëîæèëè íà 13Ñ!_14.1

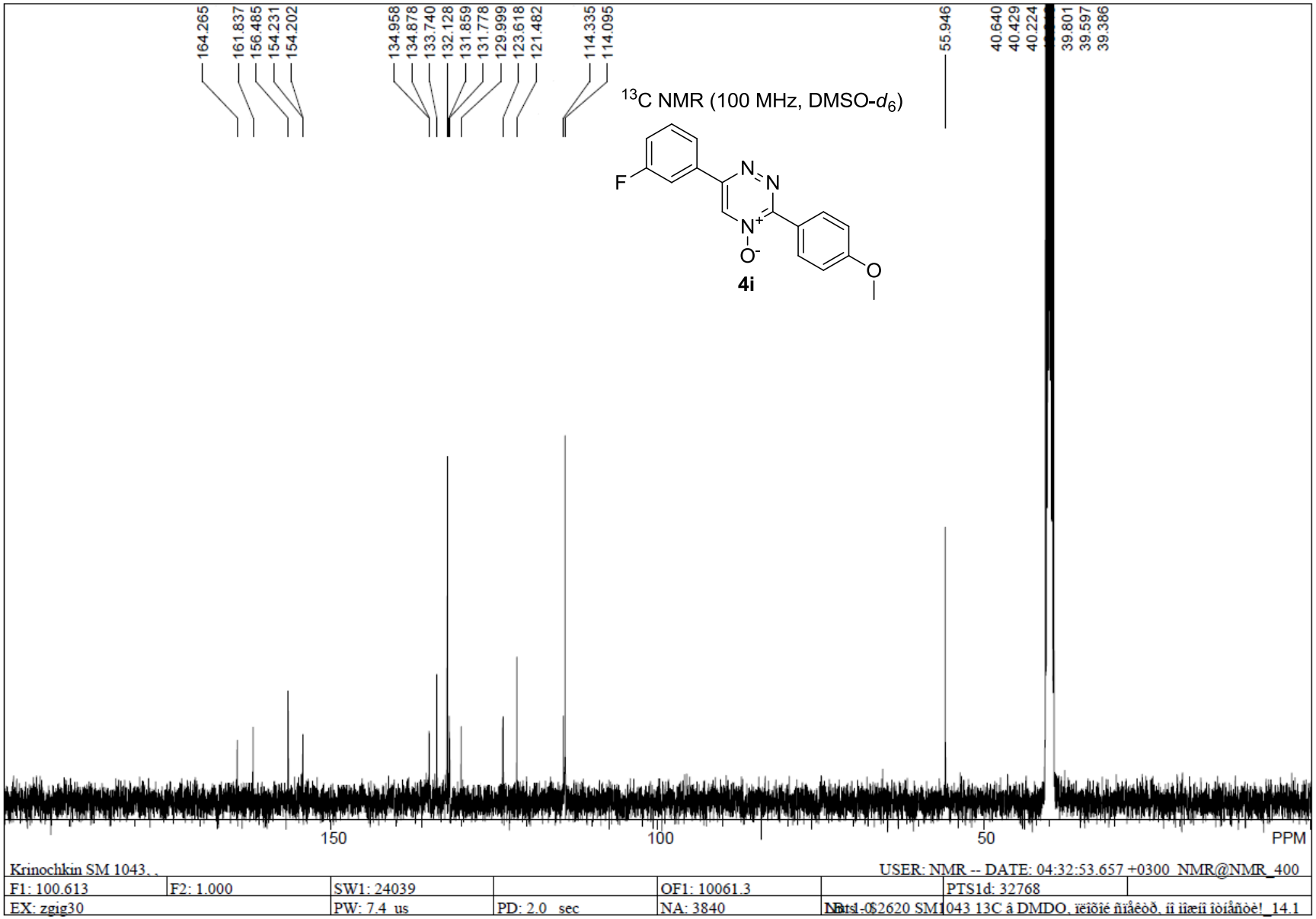

8.618
8.457
8.444
7.861
7.845
7.807
7.794
7.609
7.597
7.574
7.568
7.561
7.555
7.551
7.549
7.542
7.311
7.307
7.297
7.293
7.283
7.279
7.260
^{1}H NMR (600 MHz, CDCl$_3$)
F
N
N
N$^+$
O$^-$
4h
3.06
2.00
1.00
1.01
1.01
1.07
0.97
9
8
7
6
5
4
3
PPM
Avance, CDCl3,
USER: nmr -- DATE: Tue Oct 10 09:32:47 2023
F1: 600.214
F2: 1.000
SW1: 11905
OF1: 3692.0
PTS1d: 65536
EX: zg30
PW: 12.0 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $pdata

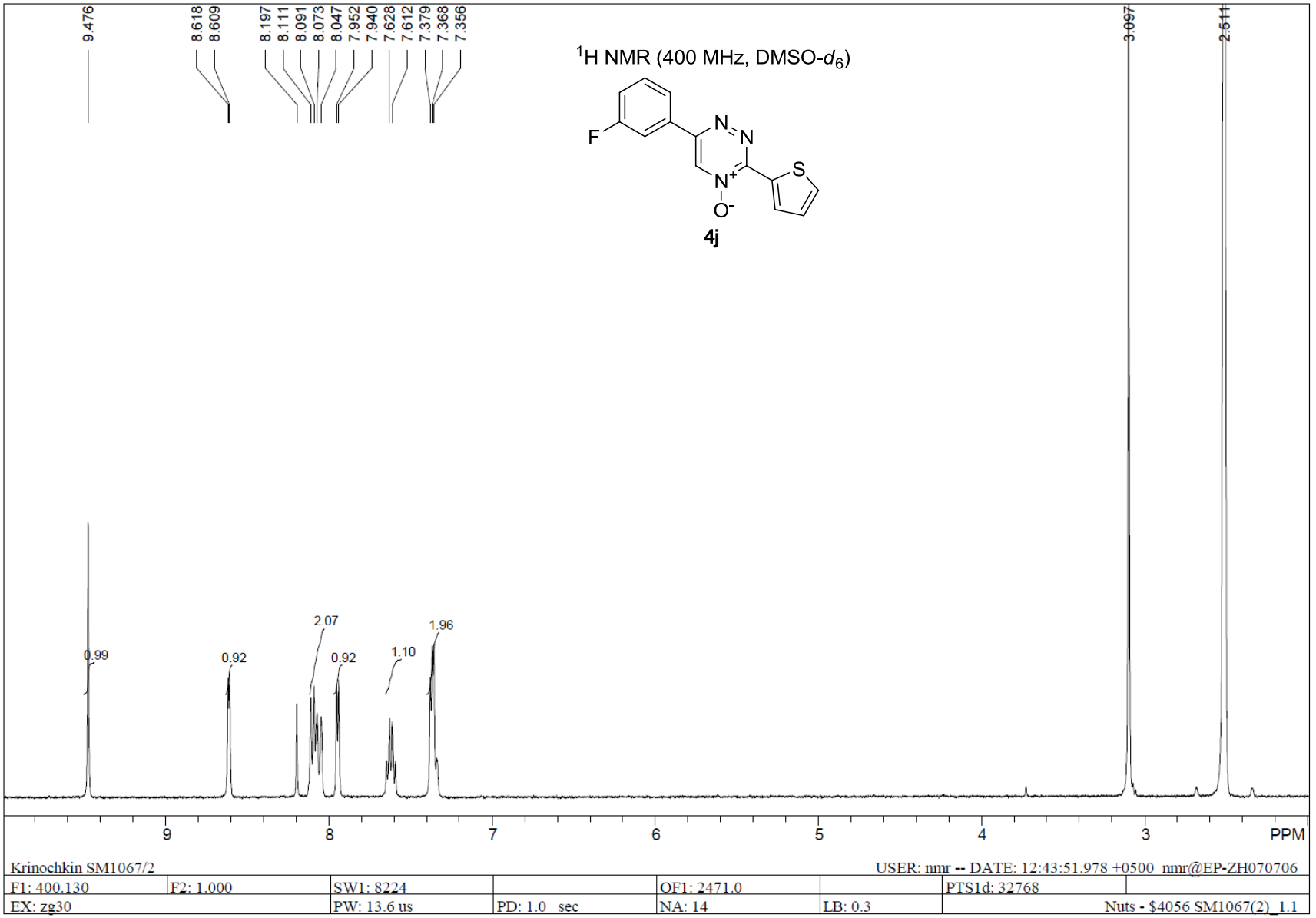

110.530
^{1}H NMR (564 MHz, $CDCl_3$)
F
N
N
N+
O-
4h
1.00
-20
-40
-60
-80
-100
-120
-140
-160
-180
PPM
Avance, CDCl3,
USER: nmr -- DATE: Tue Oct 10 09:34:54 2023
F1: 564.705
F2: 1.000
SW1: 131579
OF1: -56477.1
PTS1d: 65536
EX: zg
PW: 15.0 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $pdata

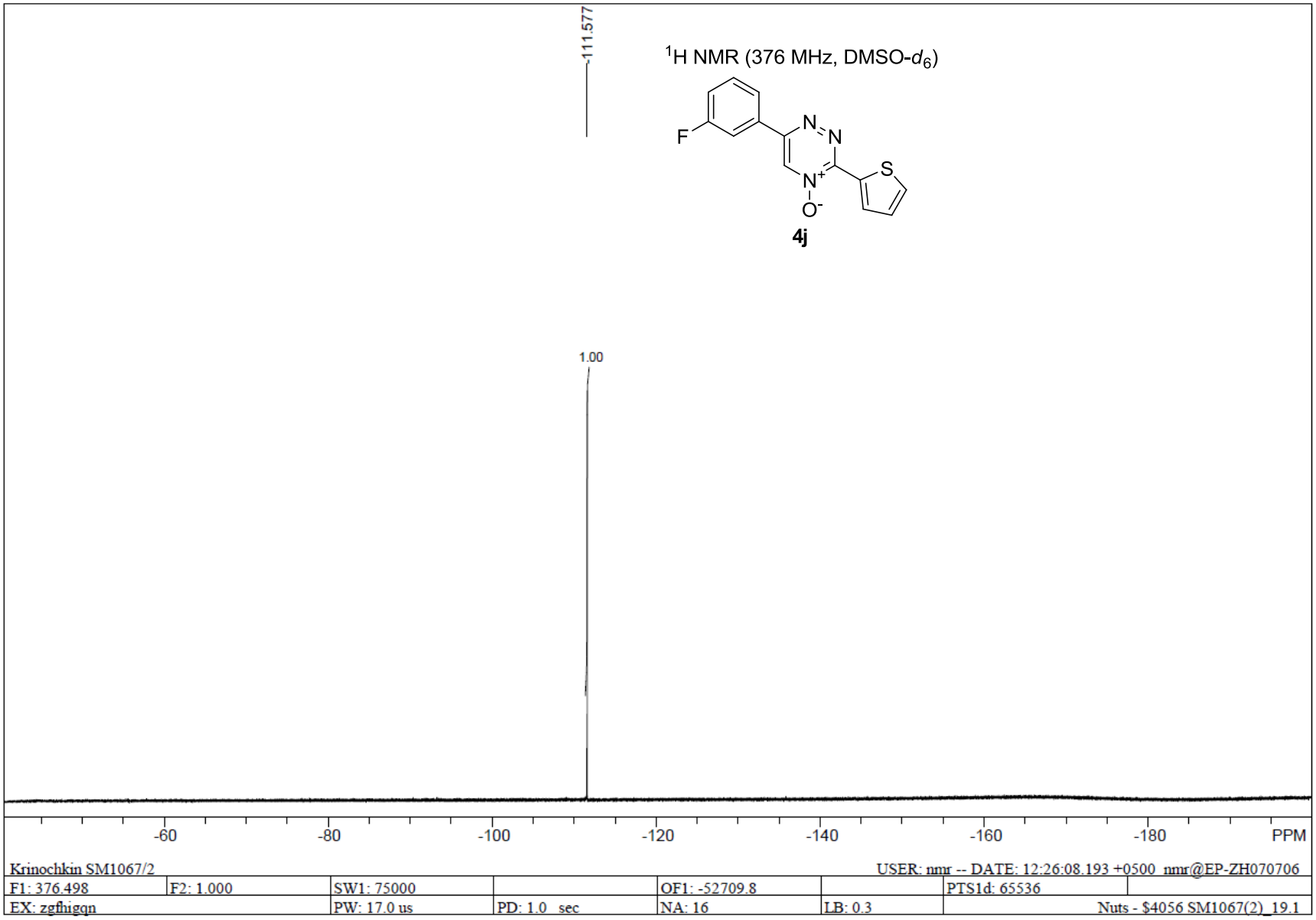

164.623
162.151
157.032
154.917
154.888
133.937
133.857
132.238
132.194
131.232
131.144
129.992
128.388
128.322
122.474
122.437
118.820
118.609
114.241
114.007
77.357
77.240
77.036
76.722
13C NMR (100 MHz, CDCl3)
F
N
N
N+
O-
4h
150
100
50
PPM
Krinochkin SM 1058/2, ,
USER: NMR -- DATE: 10:34:57.407 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $3079 SM 1058-2 13Ñ CDCl3 OK!_13.1

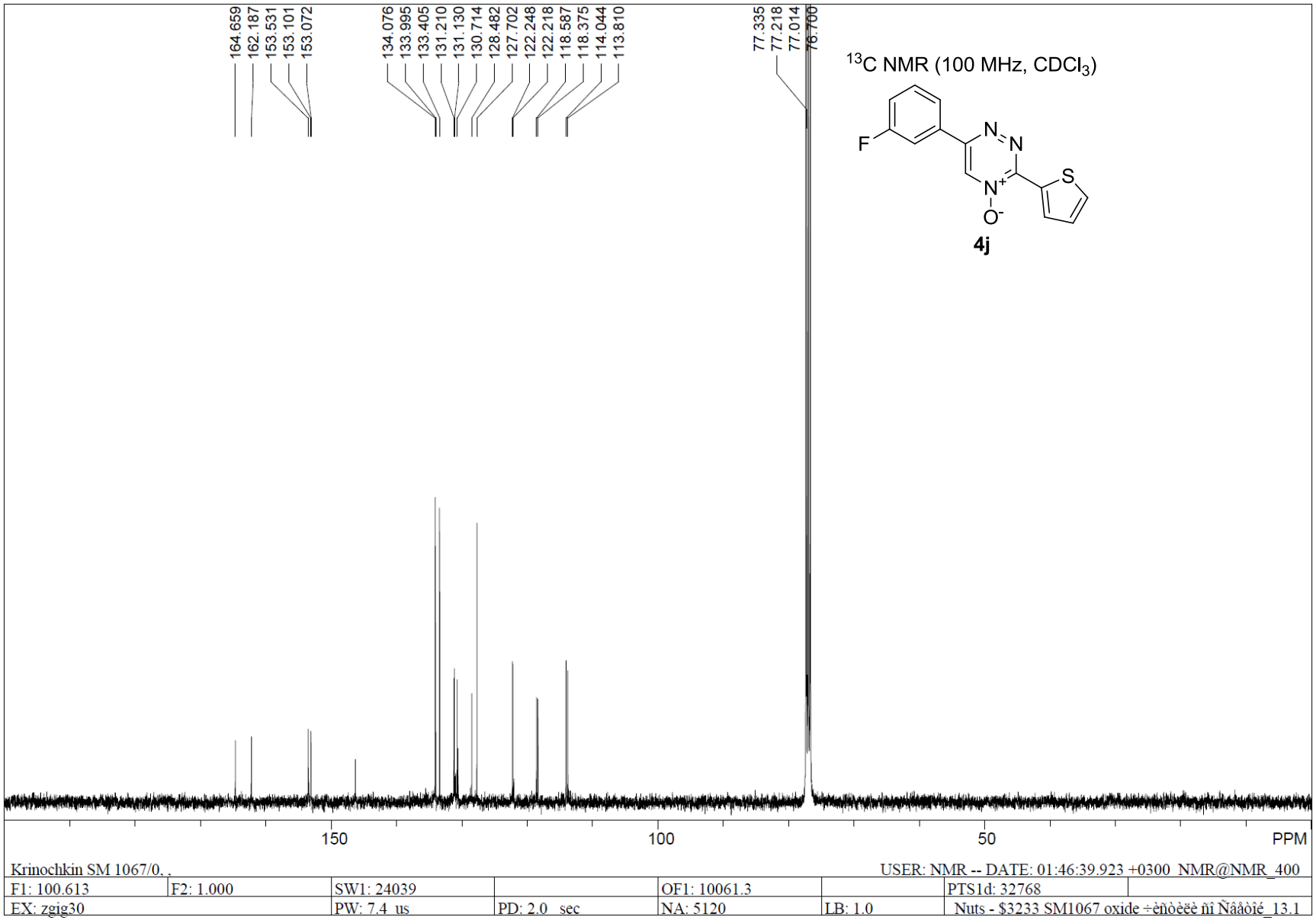

8.590
8.580
8.568
7.851
7.826
7.796
7.777
7.559
7.544
7.300
7.259
7.072
7.051
3.918
^{1}H NMR (400 MHz, $CDCl_3$)
F
N
N
N+
O-
O
4i
3.30
0.93
1.11
1.20
0.96
2.03
3.00
9
8
7
6
5
4
3
PPM
Krinochkin SM 1043ox
USER: nmr -- DATE: 13:18:25.216 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.3
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 25
LB: 0.3
Nuts - $3569 SM1043 ox_1.1

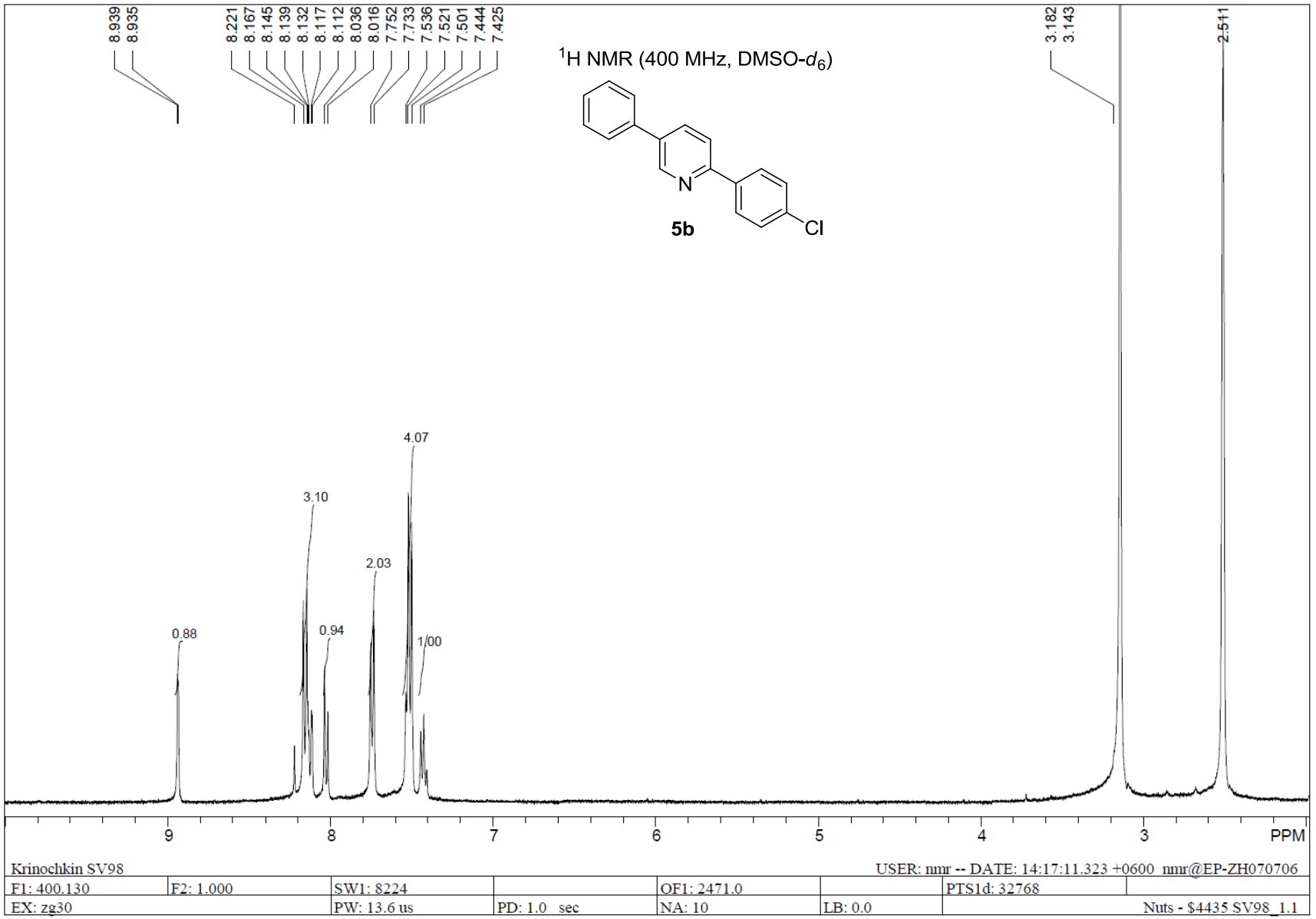

110.653
^{1}H NMR (376 MHz, $CDCl_3$)
F
N
N
N+
O-
O
4i
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1043 ox
USER: nmr -- DATE: 12:55:54.896 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3569 SM1043 ox_19.1

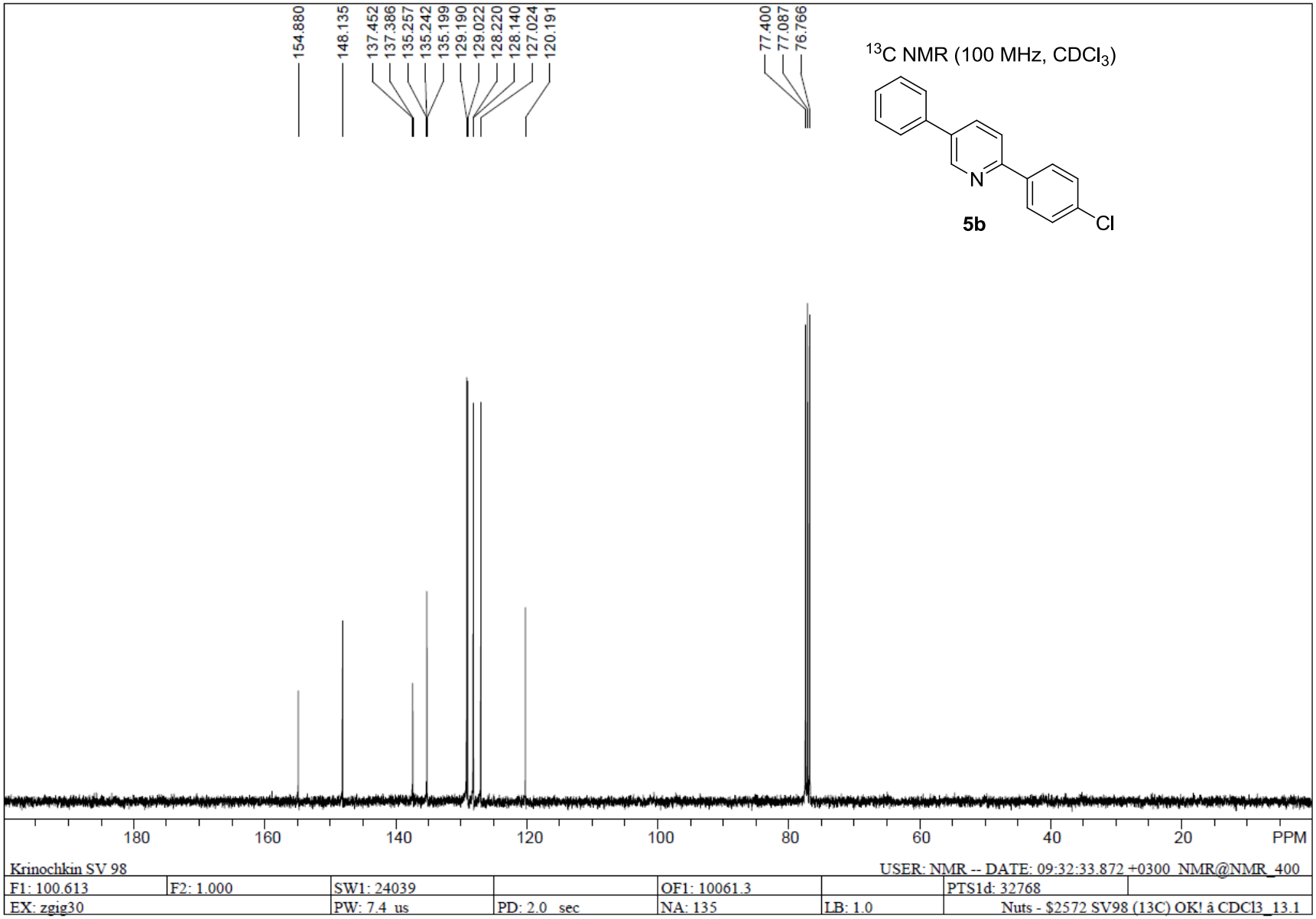

164.265
161.837
156.485
154.231
154.202
134.958
134.878
133.740
132.128
131.859
131.778
129.999
123.618
121.482
114.335
114.095
55.946
40.640
40.429
40.224
39.801
39.597
39.386
^{13}C NMR (100 MHz, DMSO-d_6)
F
N
N
N+
O-
O
4i
150
100
50
PPM
Krinochkin SM 1043, ,
USER: NMR -- DATE: 04:32:53.657 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24039
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
Nuts1-02620 SM1043 13C â DMDO, ïëîõîé ñïåêòð, íî íîæíî îòíåñòè!_14.1

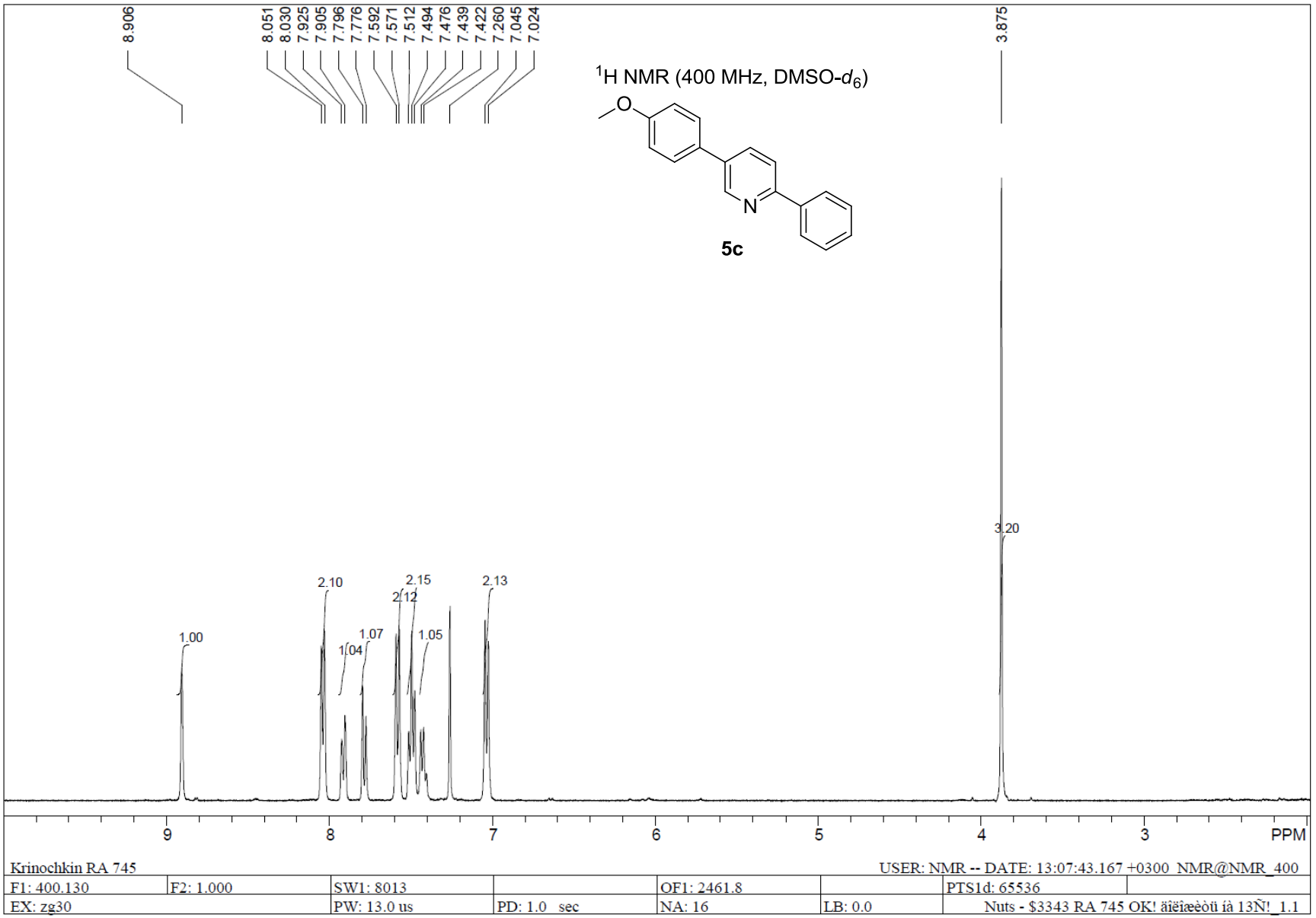

9.476
8.618
8.609
8.197
8.111
8.091
8.073
8.047
7.952
7.940
7.628
7.612
7.379
7.368
7.356
3.097
2.511
^{1}H NMR (400 MHz, DMSO-d_6)
F
N
N
S
N+
O-
4j
0.99
0.92
2.07
0.92
1.10
1.96
9
8
7
6
5
4
3
PPM
Krinochkin SM1067/2
USER: nmr -- DATE: 12:43:51.978 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 14
LB: 0.3
Nuts - $4056 SM1067(2)_1.1

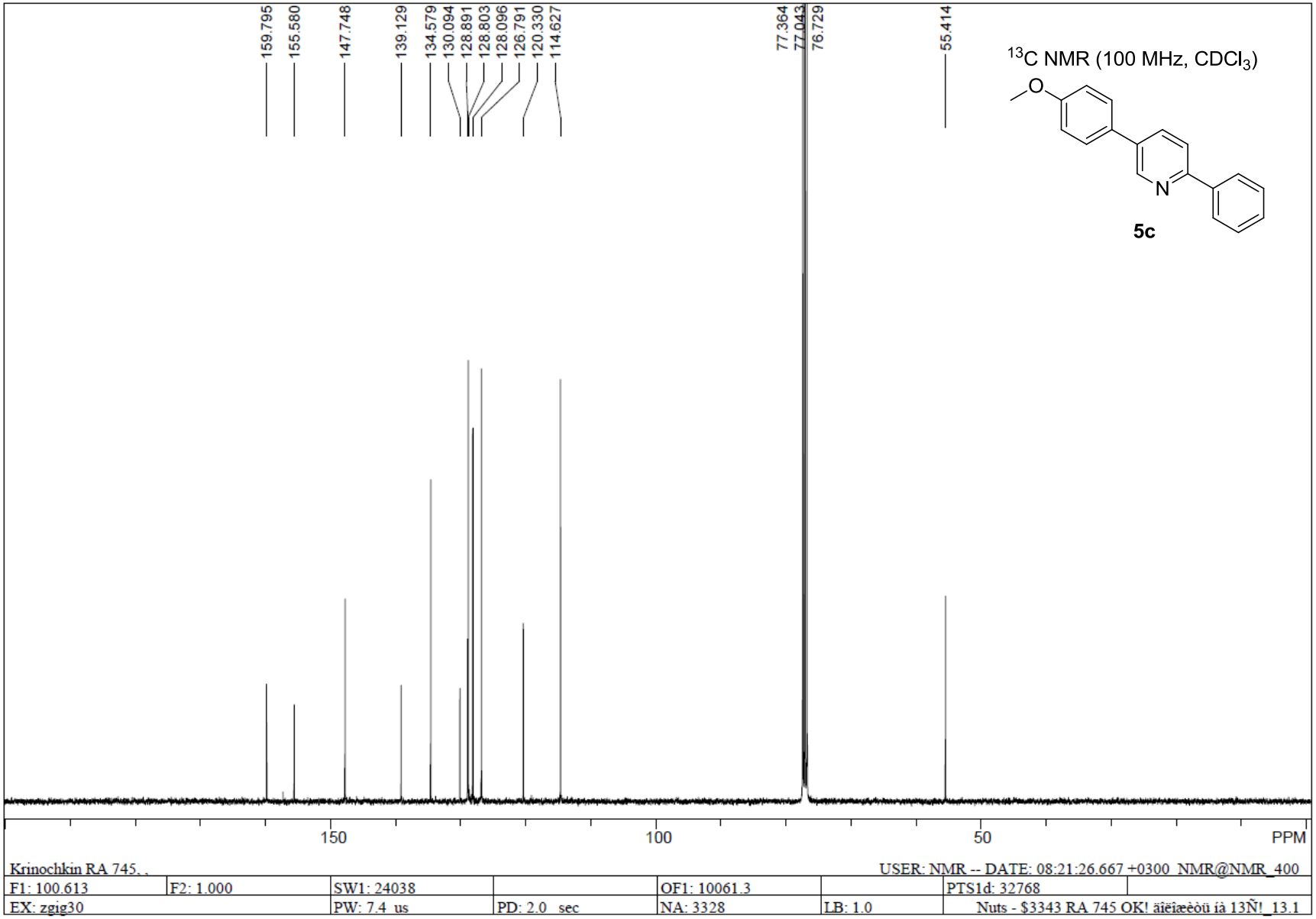

-111.577
^{1}H NMR (376 MHz, DMSO-d_6)
F
N
N
N+
O-
S
4j
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1067/2
USER: nmr -- DATE: 12:26:08.193 +0500 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $4056 SM1067(2)_19.1

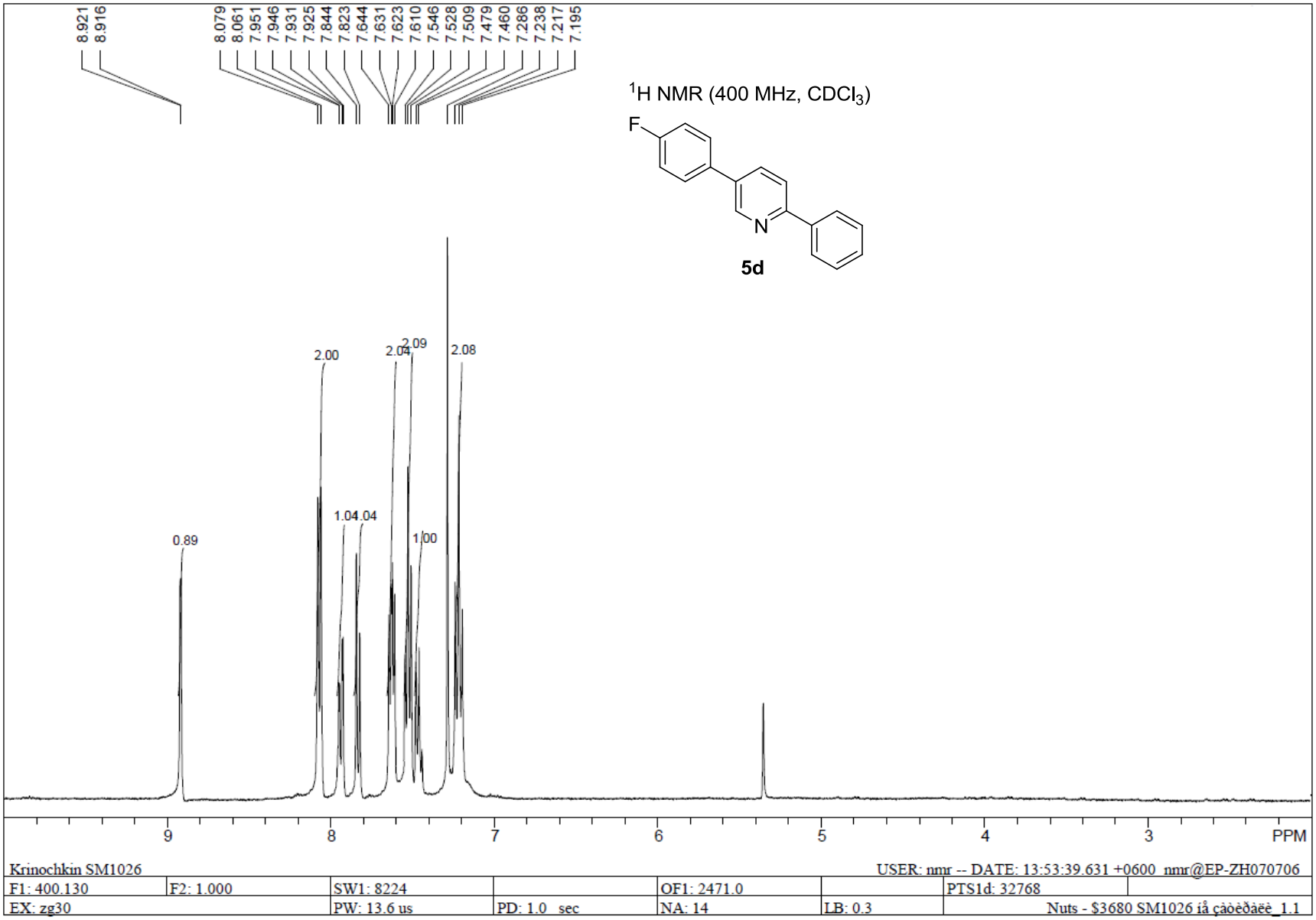

164.659
162.187
153.531
153.101
153.072
134.076
133.995
133.405
131.210
131.130
130.714
128.482
127.702
122.248
122.218
118.587
118.375
114.044
113.810
77.335
77.218
77.014
76.700
^{13}C NMR (100 MHz, CDCl$_3$)
F
N
N
N$^+$
O$^-$
S
4j
150
100
50
PPM
Krinochkin SM 1067/0, ,
USER: NMR -- DATE: 01:46:39.923 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24039
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 5120
LB: 1.0
Nuts - $3233 SM1067 oxide ÷èñòèêè ñî Ñâåòîé_13.1

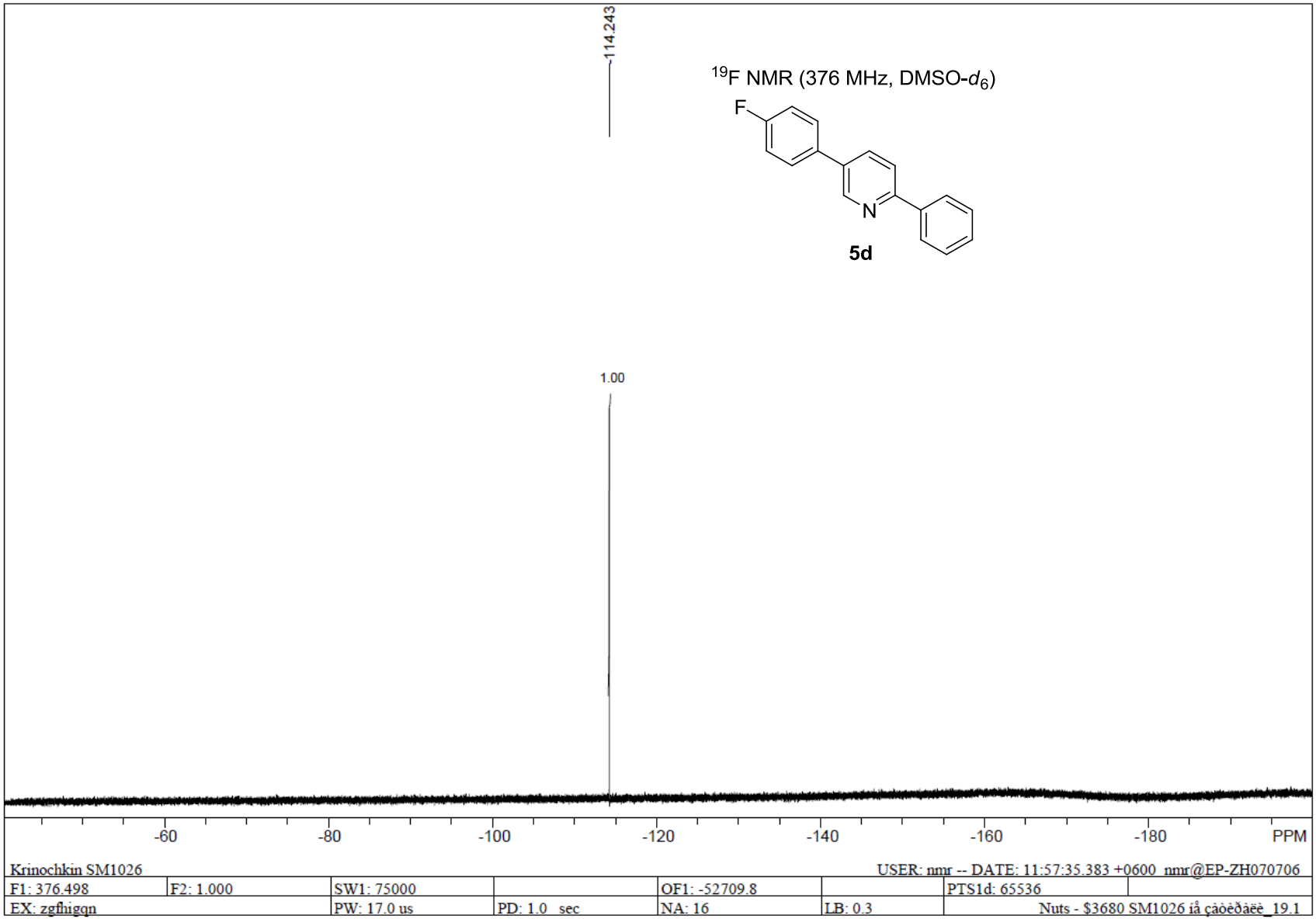

8.939
8.935
8.221
8.167
8.145
8.139
8.132
8.117
8.112
8.036
8.016
7.752
7.733
7.536
7.521
7.501
7.444
7.425
3.182
3.143
2.511
^{1}H NMR (400 MHz, DMSO-d_6)
N
Cl
5b
4.07
3.10
2.03
0.88
0.94
1.00
9
8
7
6
5
4
3
PPM
Krinochkin SV98
USER: nmr -- DATE: 14:17:11.323 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 10
LB: 0.0
Nuts - $4435 SV98_1.1

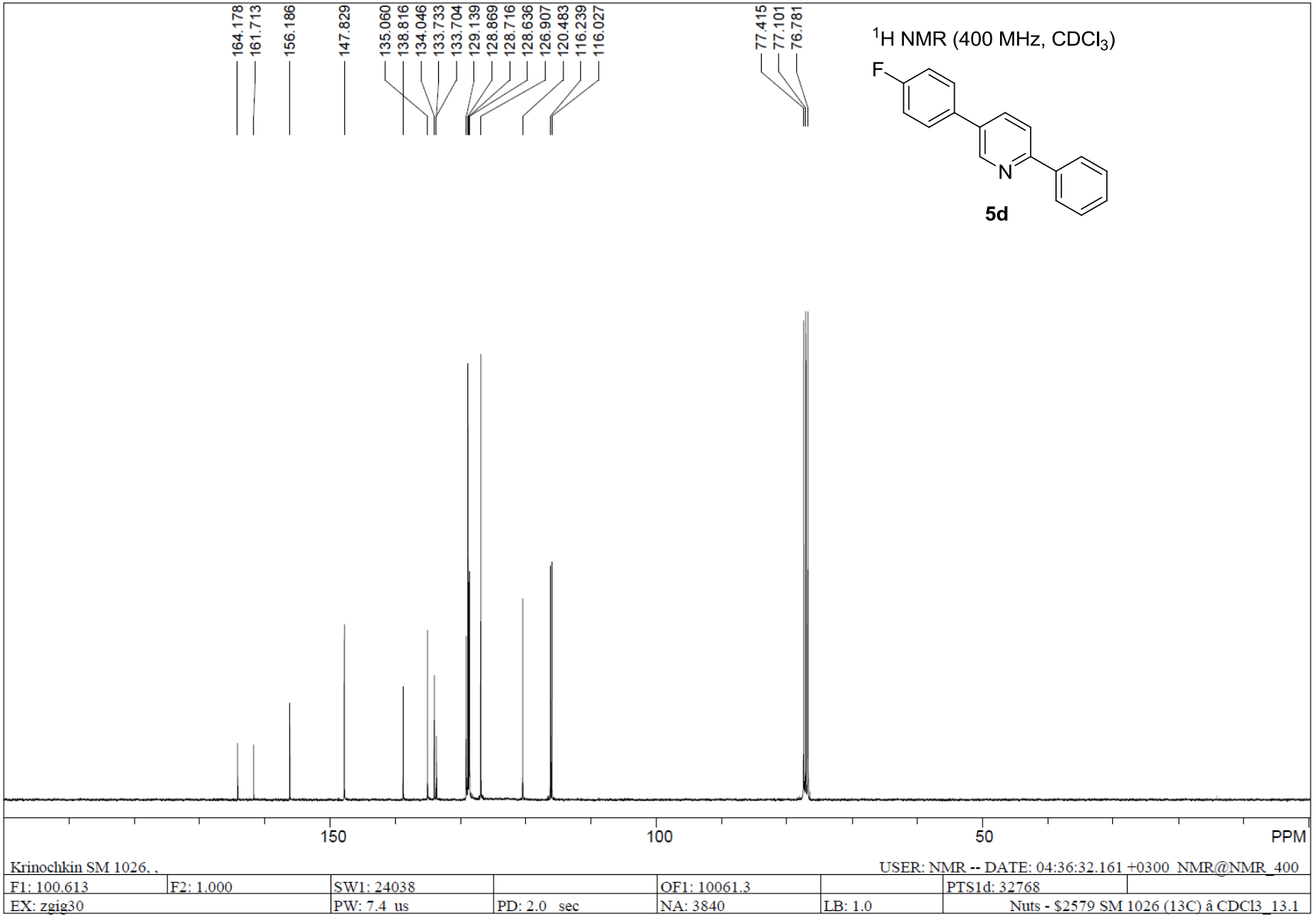

154.880
148.135
137.452
137.386
135.257
135.242
135.199
129.190
129.022
128.220
128.140
127.024
120.191
77.400
77.087
76.766
^{13}C NMR (100 MHz, $CDCl_3$)
N
Cl
5b
180
160
140
120
100
80
60
40
20
PPM
Krinochkin SV 98
USER: NMR -- DATE: 09:32:33.872 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24039
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 135
LB: 1.0
Nuts - $2572 SV98 (13C) OK! â CDCl3_13.1

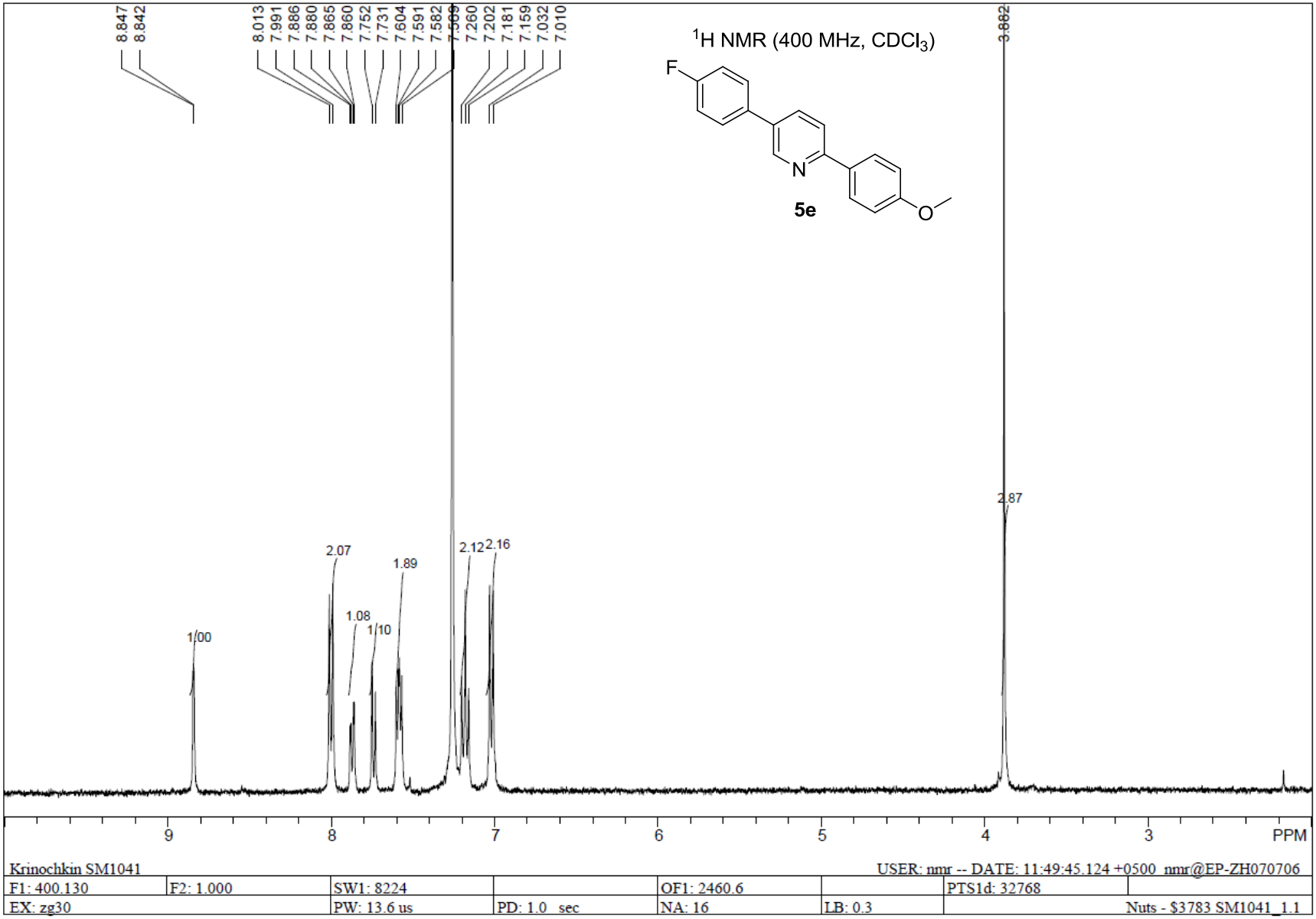

8.906
8.051
8.030
7.925
7.905
7.796
7.776
7.592
7.571
7.512
7.494
7.476
7.439
7.422
7.260
7.045
7.024
3.875
^{1}H NMR (400 MHz, DMSO-d_6)
O
N
5c
3.20
2.10
2.15
2.12
2.13
1.00
1.07
1.04
1.05
9
8
7
6
5
4
3
PPM
Krinochkin RA 745
USER: NMR -- DATE: 13:07:43.167 +0300 NMR@NMR_400
F1: 400.130
F2: 1.000
SW1: 8013
OF1: 2461.8
PTS1d: 65536
EX: zg30
PW: 13.0 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $3343 RA 745 OK! äîëíæèòü íà 13Ñ!_1.1

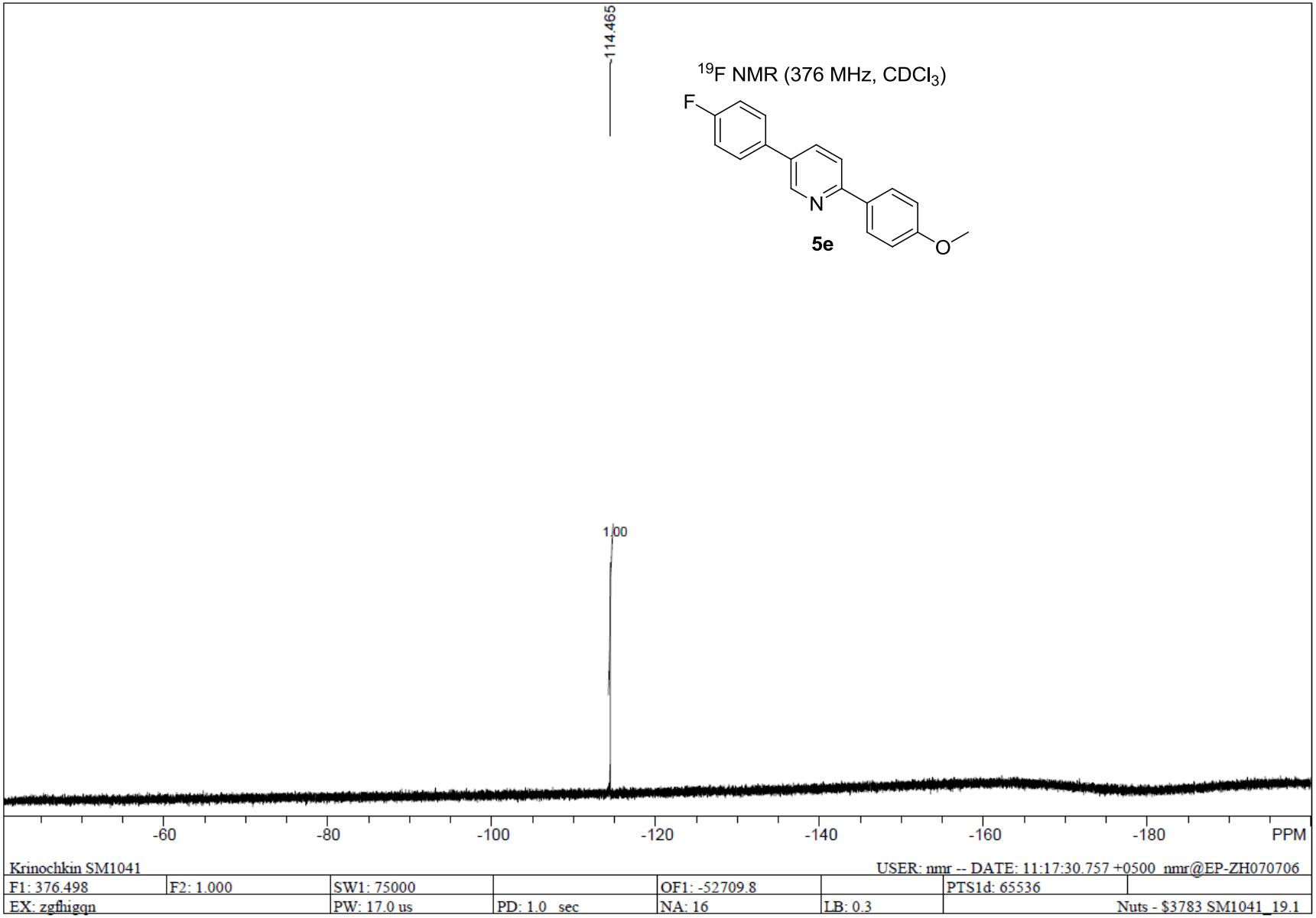

159.795
155.580
147.748
139.129
134.579
130.094
128.891
128.803
128.096
126.791
120.330
114.627
77.364
77.043
76.729
55.414
13C NMR (100 MHz, CDCl3)
O
N
5c
150
100
50
PPM
Krinochkin RA 745, ,
USER: NMR -- DATE: 08:21:26.667 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3328
LB: 1.0
Nuts - $3343 RA 745 OK! äîëîæèòü íà 13Ñ!_13.1

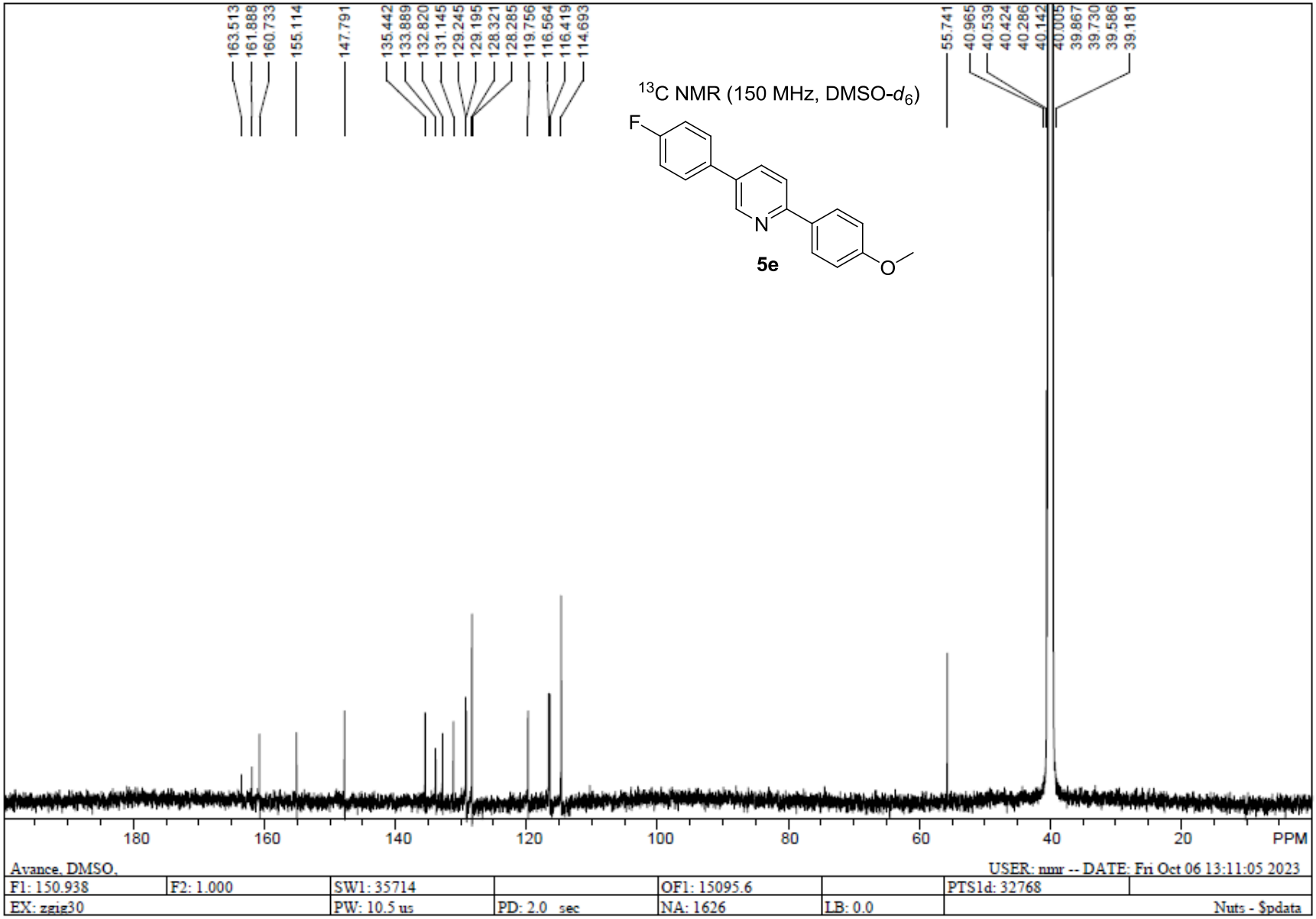

8.921
8.916
8.079
8.061
7.951
7.946
7.931
7.925
7.844
7.823
7.644
7.631
7.623
7.610
7.546
7.528
7.509
7.479
7.460
7.286
7.238
7.217
7.195
1H NMR (400 MHz, CDCl3)
F
N
5d
0.89
2.00
1.04
1.04
2.04
2.09
1.00
2.08
9
8
7
6
5
4
3
PPM
Krinochkin SM1026
USER: nmr -- DATE: 13:53:39.631 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 14
LB: 0.3
Nuts - $3680 SM1026 íå çàòèðàëè_1.1

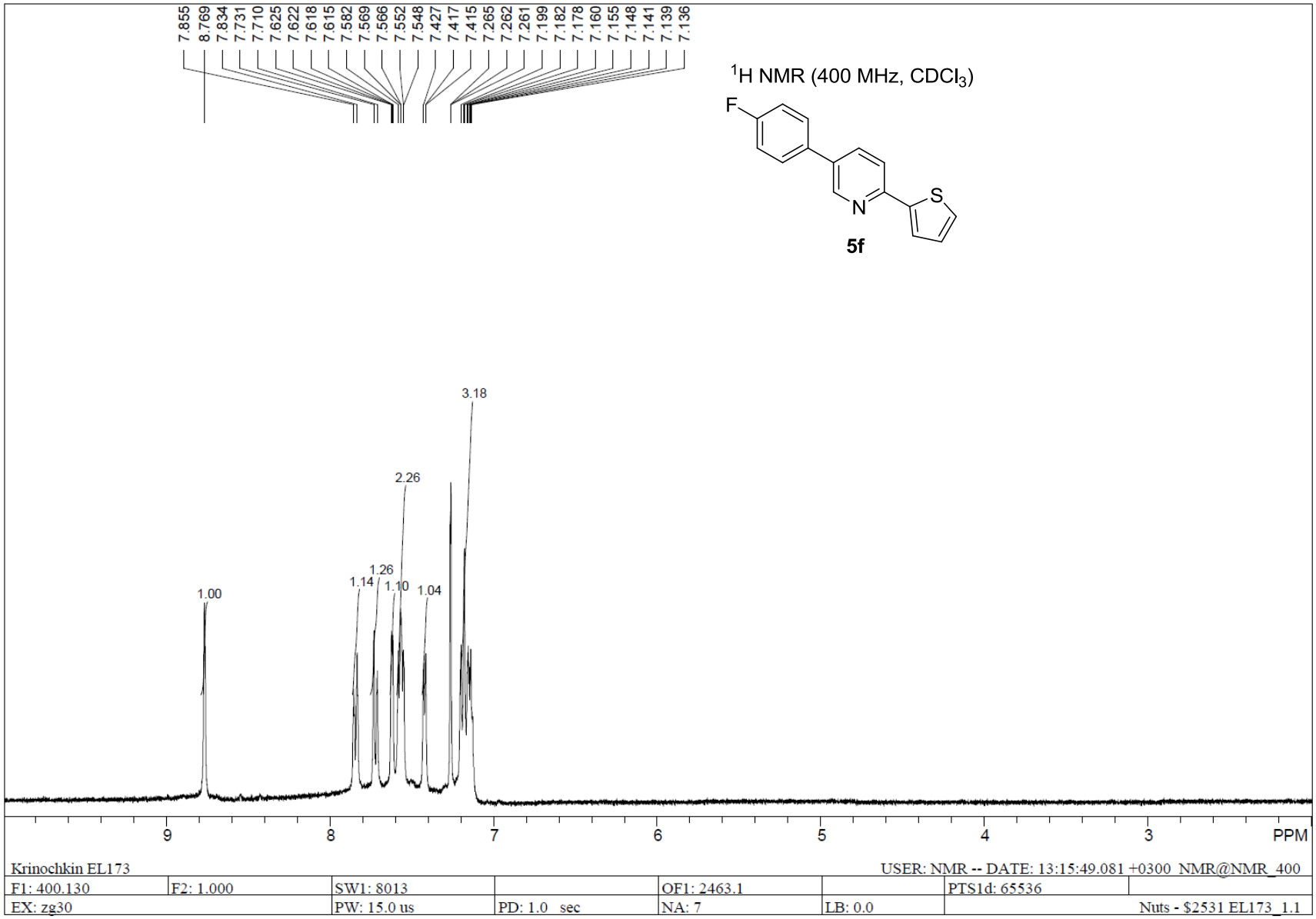

-114.243
^{19}F NMR (376 MHz, DMSO-d_6)
F
N
5d
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1026
USER: nmr -- DATE: 11:57:35.383 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3680 SM1026 íå çàòèðàëè_19.1

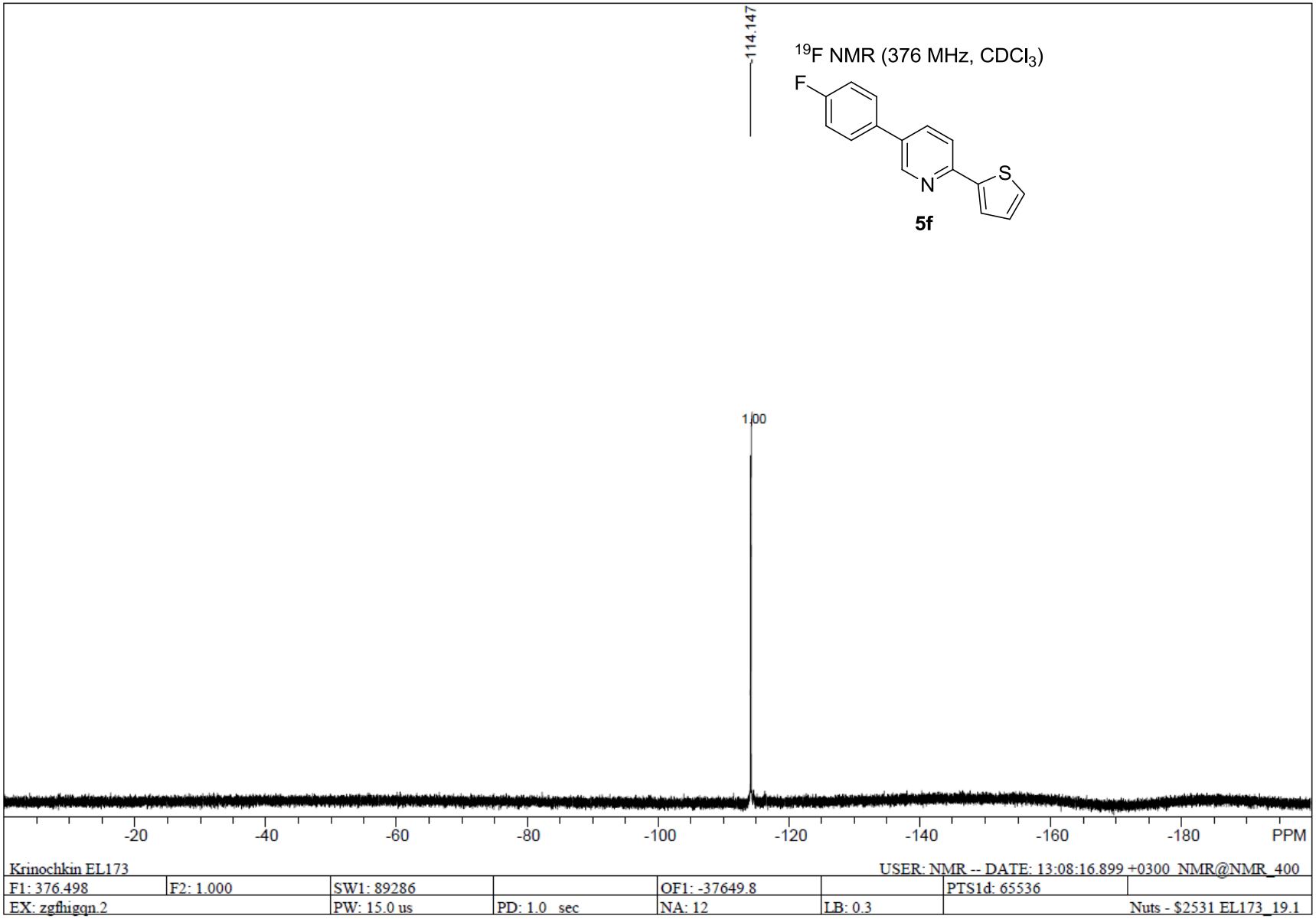

164.178
161.713
156.186
147.829
135.060
138.816
134.046
133.733
133.704
129.139
128.869
128.716
128.636
126.907
120.483
116.239
116.027
77.415
77.101
76.781
^{1}H NMR (400 MHz, $CDCl_3$)
F
N
5d
150
100
50
PPM
Krinochkin SM 1026, ,
USER: NMR -- DATE: 04:36:32.161 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $2579 SM 1026 (13C) â CDCl3_13.1

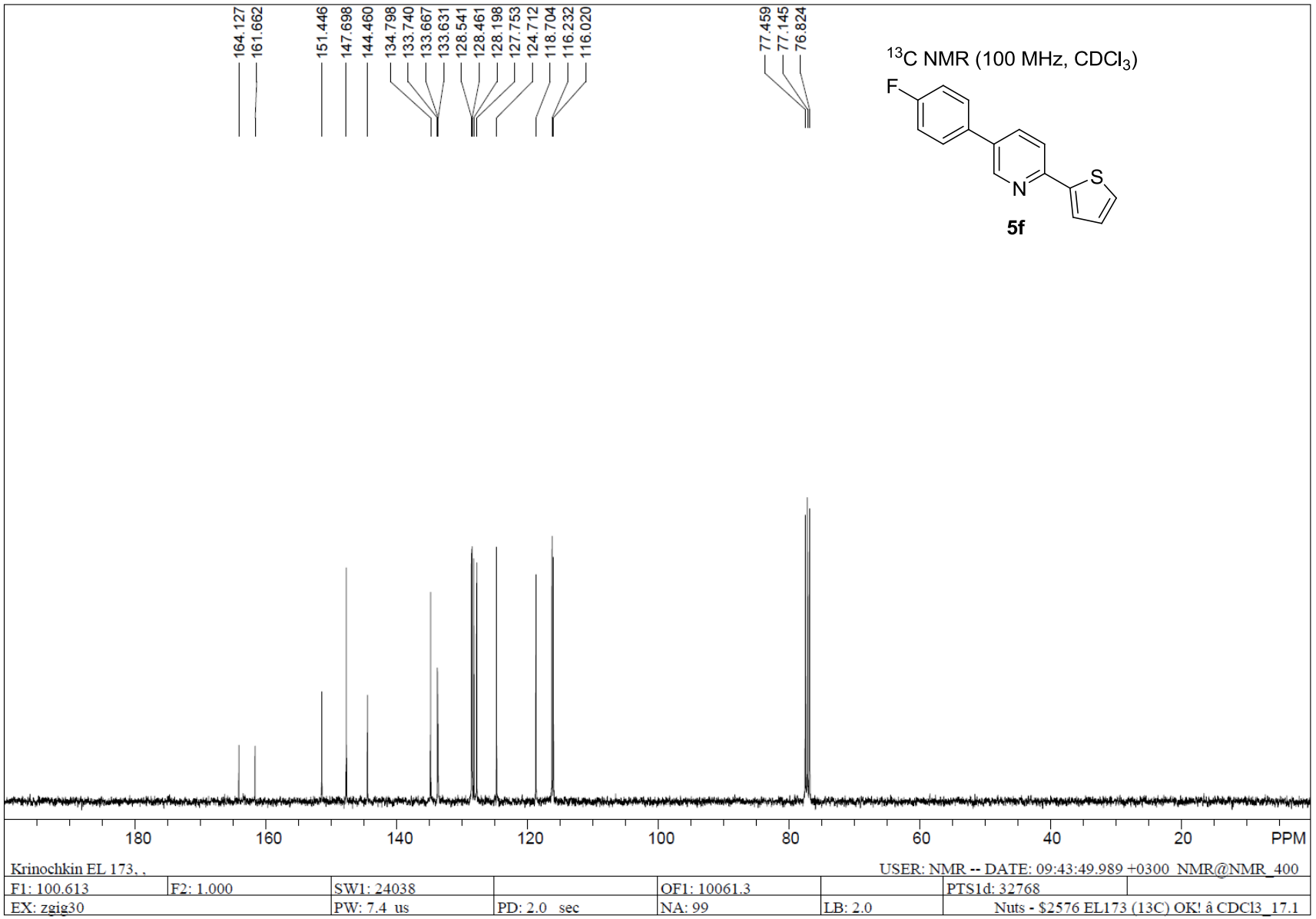

8.847
8.842
8.013
7.991
7.886
7.880
7.865
7.860
7.752
7.731
7.604
7.591
7.582
7.569
7.260
7.202
7.181
7.159
7.032
7.010
3.882
^{1}H NMR (400 MHz, $CDCl_3$)
F
N
O
5e
2.87
2.07
1.89
2.12
2.16
1.08
1.10
1.00
9
8
7
6
5
4
3
PPM
Krinochkin SM1041
USER: nmr -- DATE: 11:49:45.124 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.6
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3783 SM1041_1.1

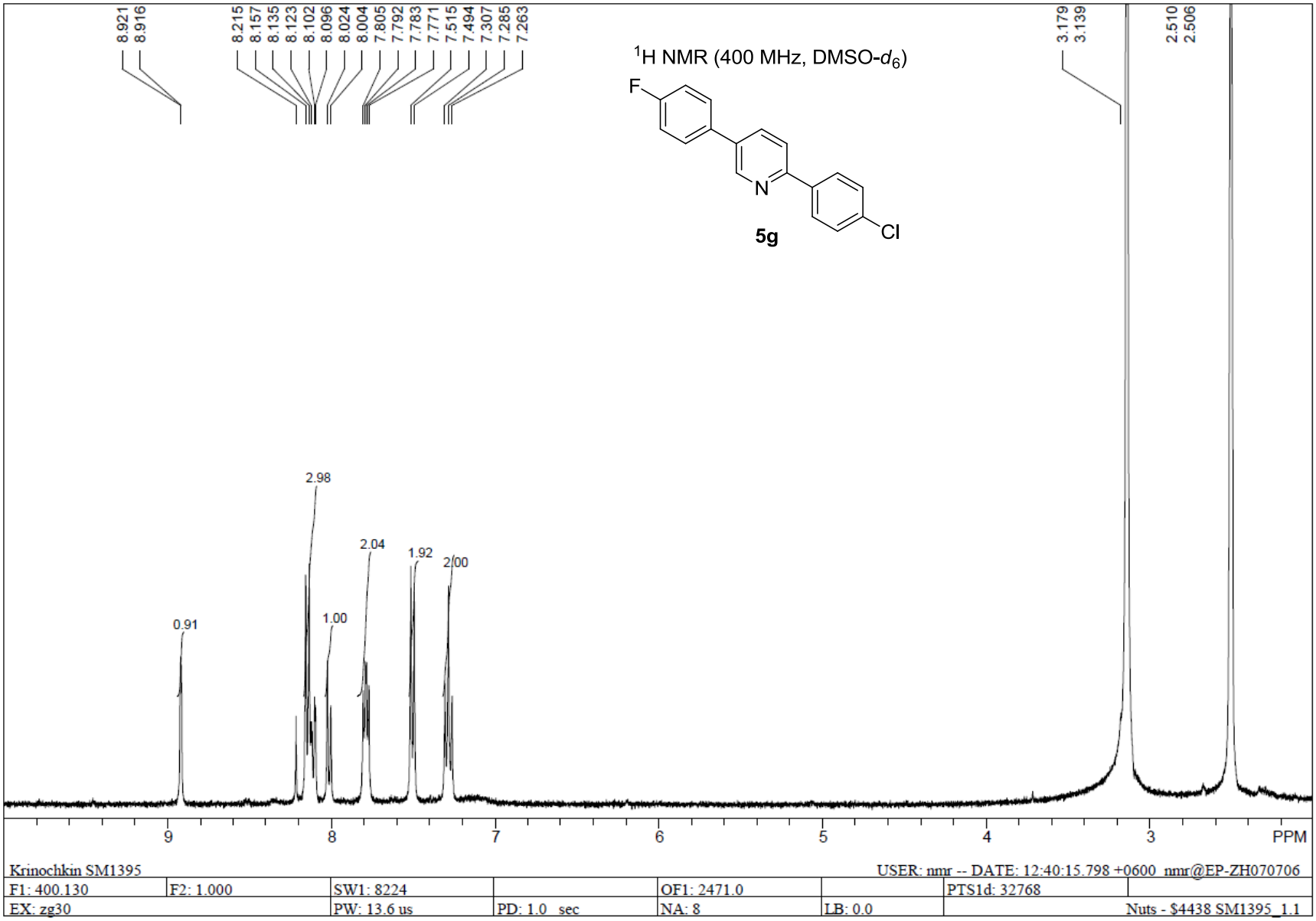

114.465
^{19}F NMR (376 MHz, $CDCl_3$)
F
N
O
5e
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1041
USER: nmr -- DATE: 11:17:30.757 +0500 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 16
LB: 0.3
Nuts - $3783 SM1041_19.1

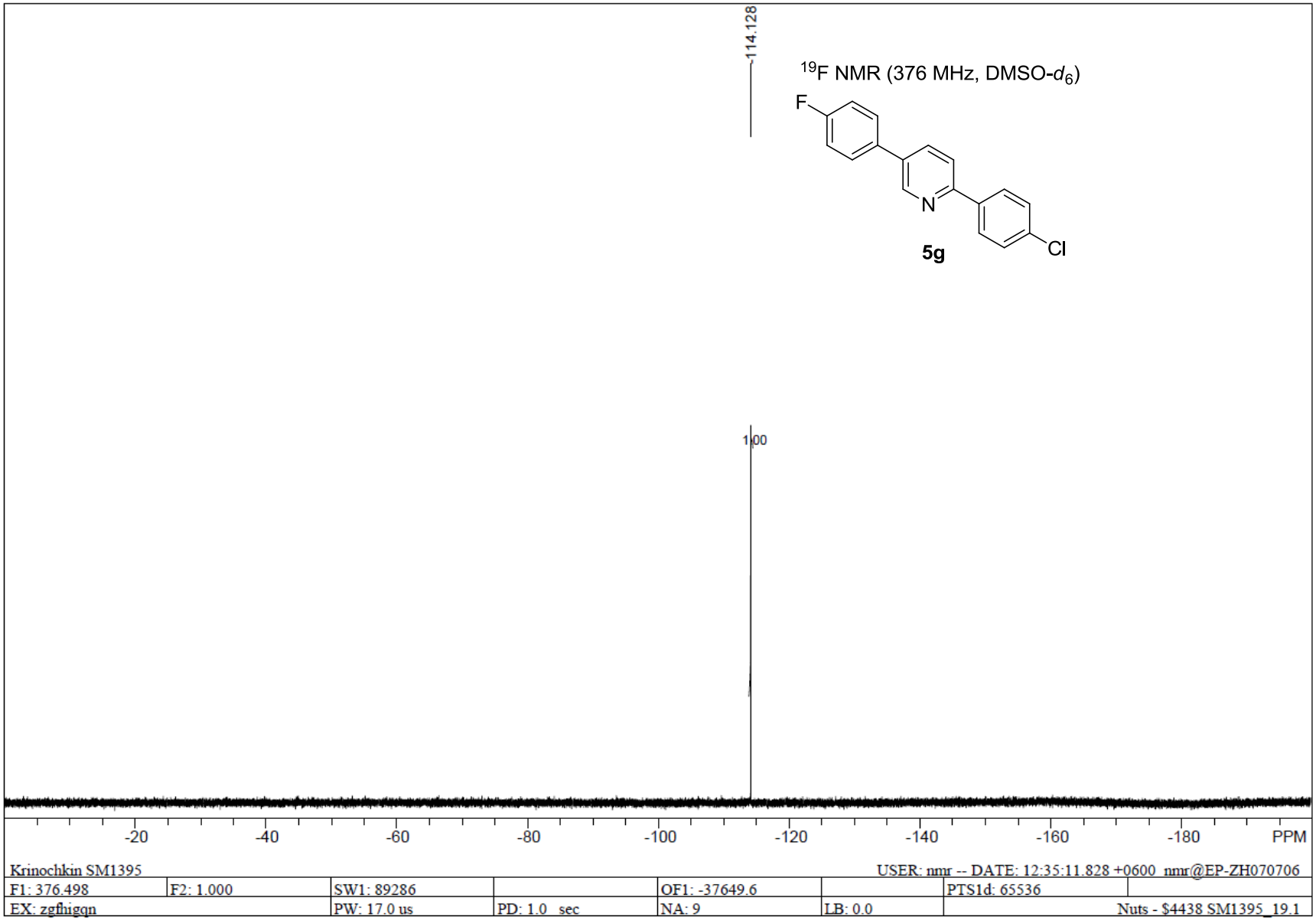

163.513
161.888
160.733
155.114
147.791
135.442
133.889
132.820
131.145
129.245
129.195
128.321
128.285
119.756
116.564
116.419
114.693
55.741
40.965
40.539
40.424
40.286
40.142
40.005
39.867
39.730
39.586
39.181
^{13}C NMR (150 MHz, DMSO-d_6)
F
N
O
5e
180
160
140
120
100
80
60
40
20
PPM
Avance, DMSO,
USER: nmr -- DATE: Fri Oct 06 13:11:05 2023
F1: 150.938
F2: 1.000
SW1: 35714
OF1: 15095.6
PTS1d: 32768
EX: zgig30
PW: 10.5 us
PD: 2.0 sec
NA: 1626
LB: 0.0
Nuts - $pdata

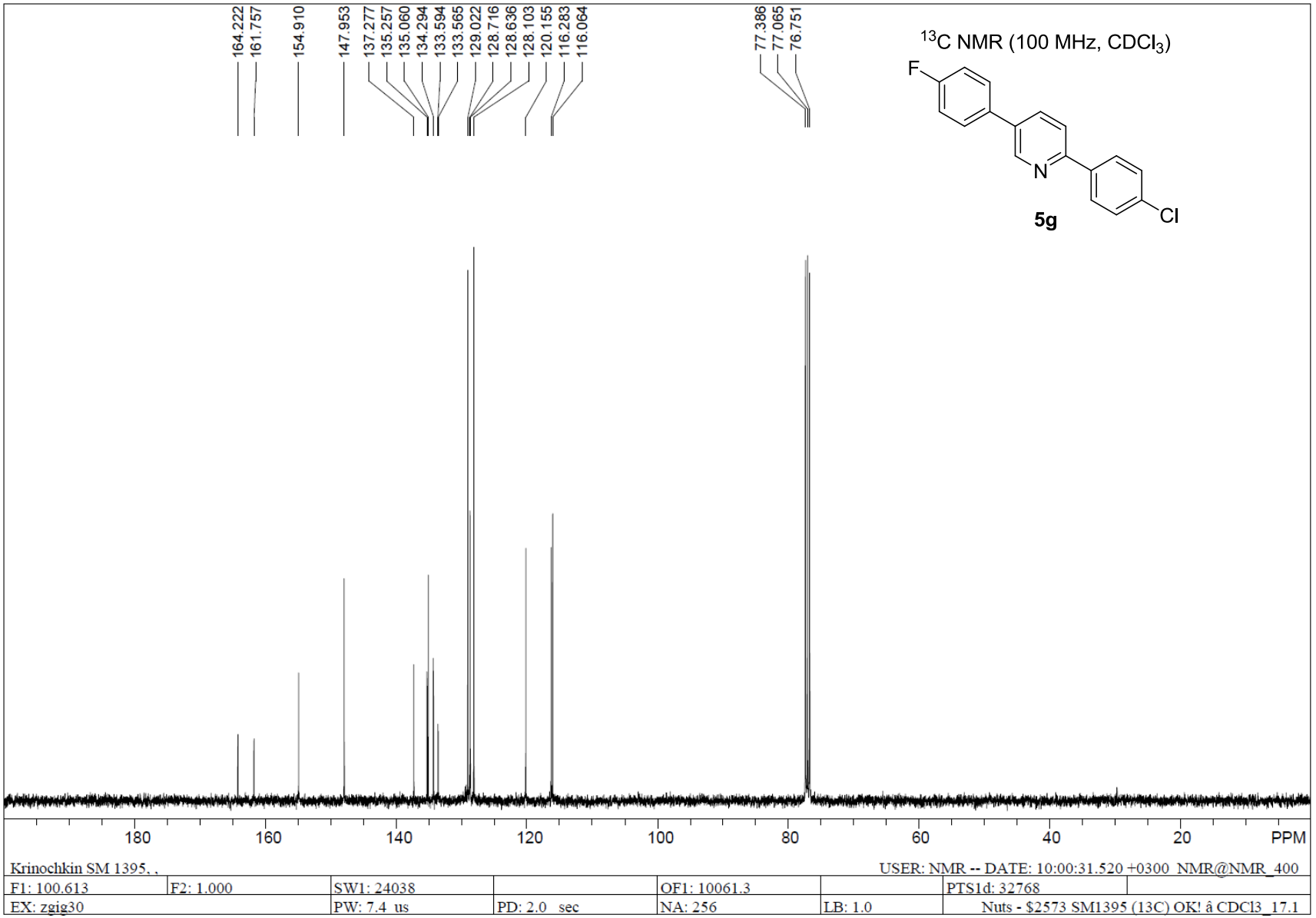

7.855
8.769
7.834
7.731
7.710
7.625
7.622
7.618
7.615
7.582
7.569
7.566
7.552
7.548
7.427
7.417
7.415
7.265
7.262
7.261
7.199
7.182
7.178
7.160
7.155
7.148
7.141
7.139
7.136
1H NMR (400 MHz, CDCl3)
F
N
S
5f
3.18
2.26
1.26
1.14
1.10
1.04
1.00
9
8
7
6
5
4
3
PPM
Krinochkin EL173
USER: NMR -- DATE: 13:15:49.081 +0300 NMR@NMR_400
F1: 400.130
F2: 1.000
SW1: 8013
OF1: 2463.1
PTS1d: 65536
EX: zg30
PW: 15.0 us
PD: 1.0 sec
NA: 7
LB: 0.0
Nuts - $2531 EL173_1.1

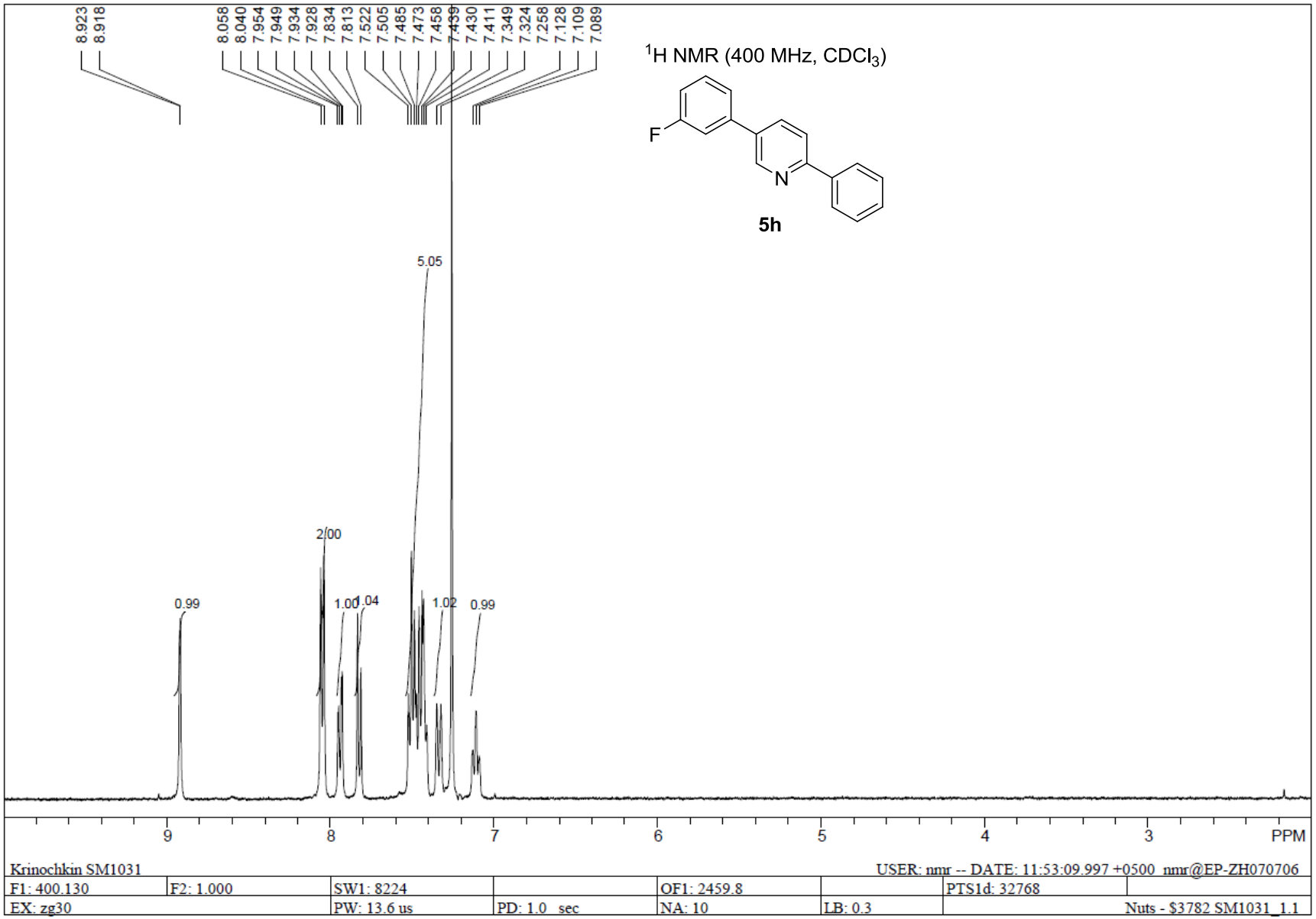

114.147
^{19}F NMR (376 MHz, $CDCl_3$)
F
N
S
5f
1.00
-20
-40
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin EL173
USER: NMR -- DATE: 13:08:16.899 +0300 NMR@NMR_400
F1: 376.498
F2: 1.000
SW1: 89286
OF1: -37649.8
PTS1d: 65536
EX: zgfhigqn.2
PW: 15.0 us
PD: 1.0 sec
NA: 12
LB: 0.3
Nuts - $2531 EL173_19.1

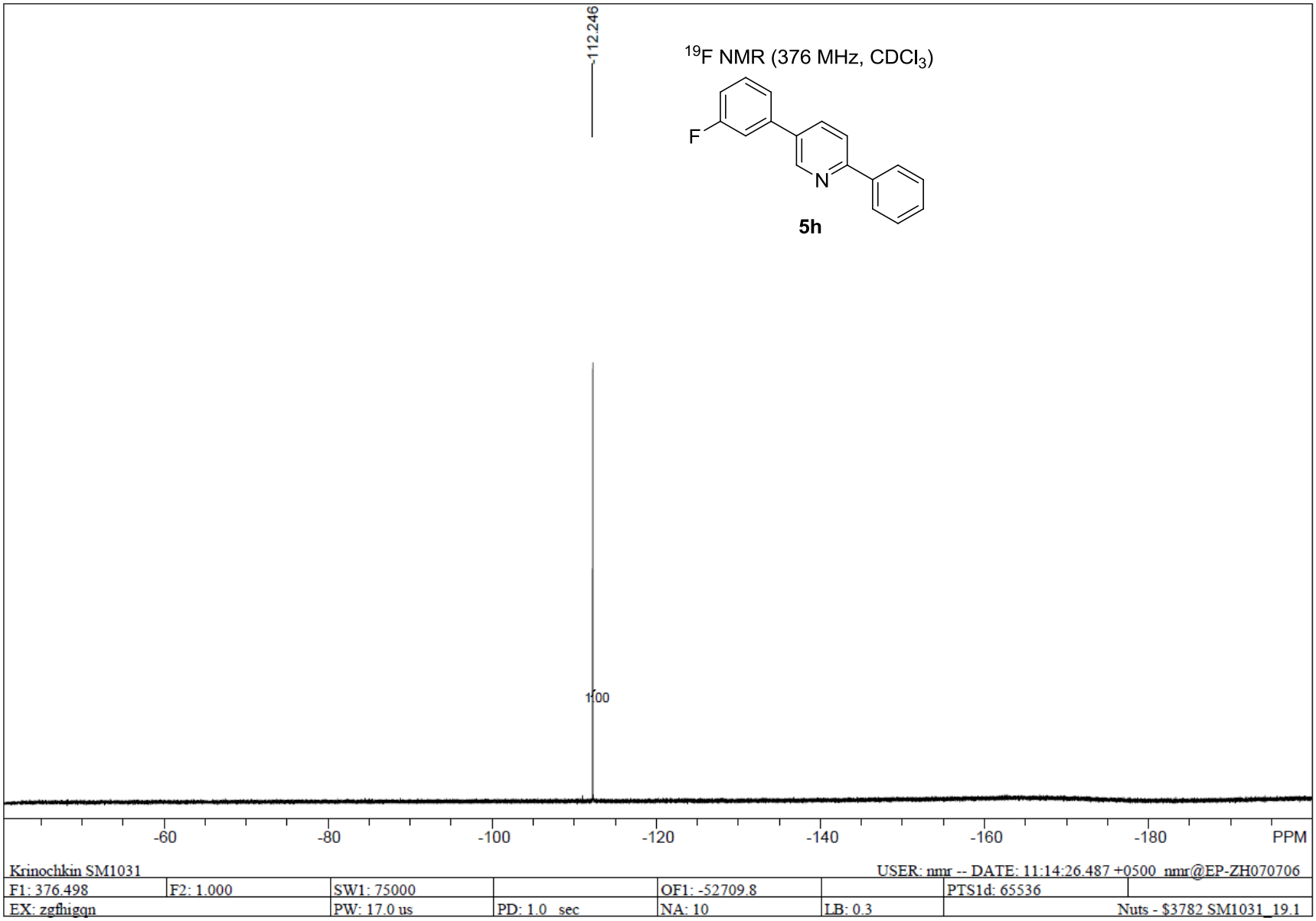

164.127
161.662
151.446
147.698
144.460
134.798
133.740
133.667
133.631
128.541
128.461
128.198
127.753
124.712
118.704
116.232
116.020
77.459
77.145
76.824
13C NMR (100 MHz, CDCl3)
F
N
S
5f
180
160
140
120
100
80
60
40
20
PPM
Krinochkin EL 173, ,
USER: NMR -- DATE: 09:43:49.989 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 99
LB: 2.0
Nuts - $2576 EL173 (13C) OK! â CDCl3_17.1

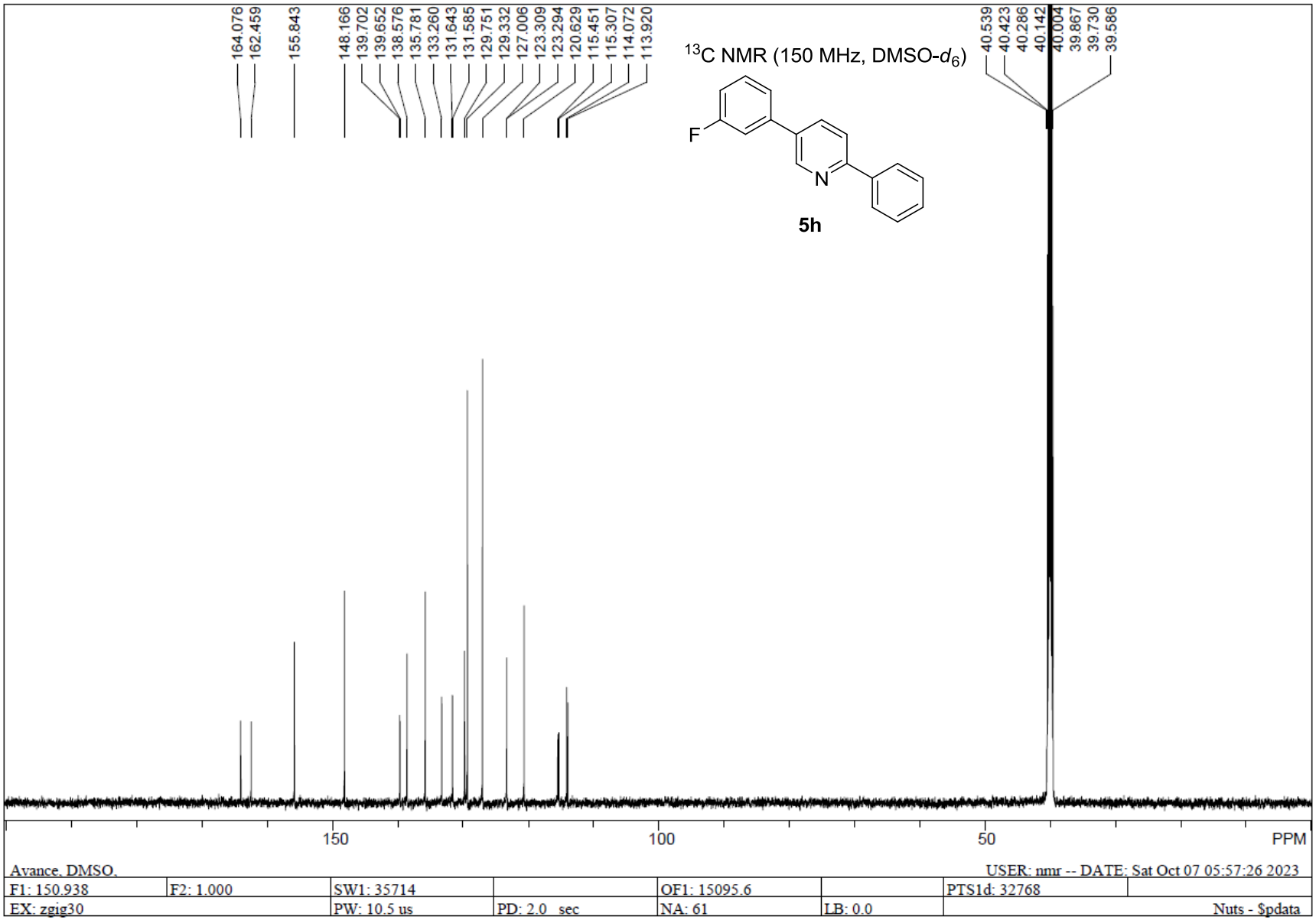

8.921
8.916
8.215
8.157
8.135
8.123
8.102
8.096
8.024
8.004
7.805
7.792
7.783
7.771
7.515
7.494
7.307
7.285
7.263
3.179
3.139
2.510
2.506
^{1}H NMR (400 MHz, DMSO-d_6)
F
N
Cl
5g
0.91
2.98
1.00
2.04
1.92
2.00
9
8
7
6
5
4
3
PPM
Krinochkin SM1395
USER: nmr -- DATE: 12:40:15.798 +0600 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2471.0
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $4438 SM1395_1.1

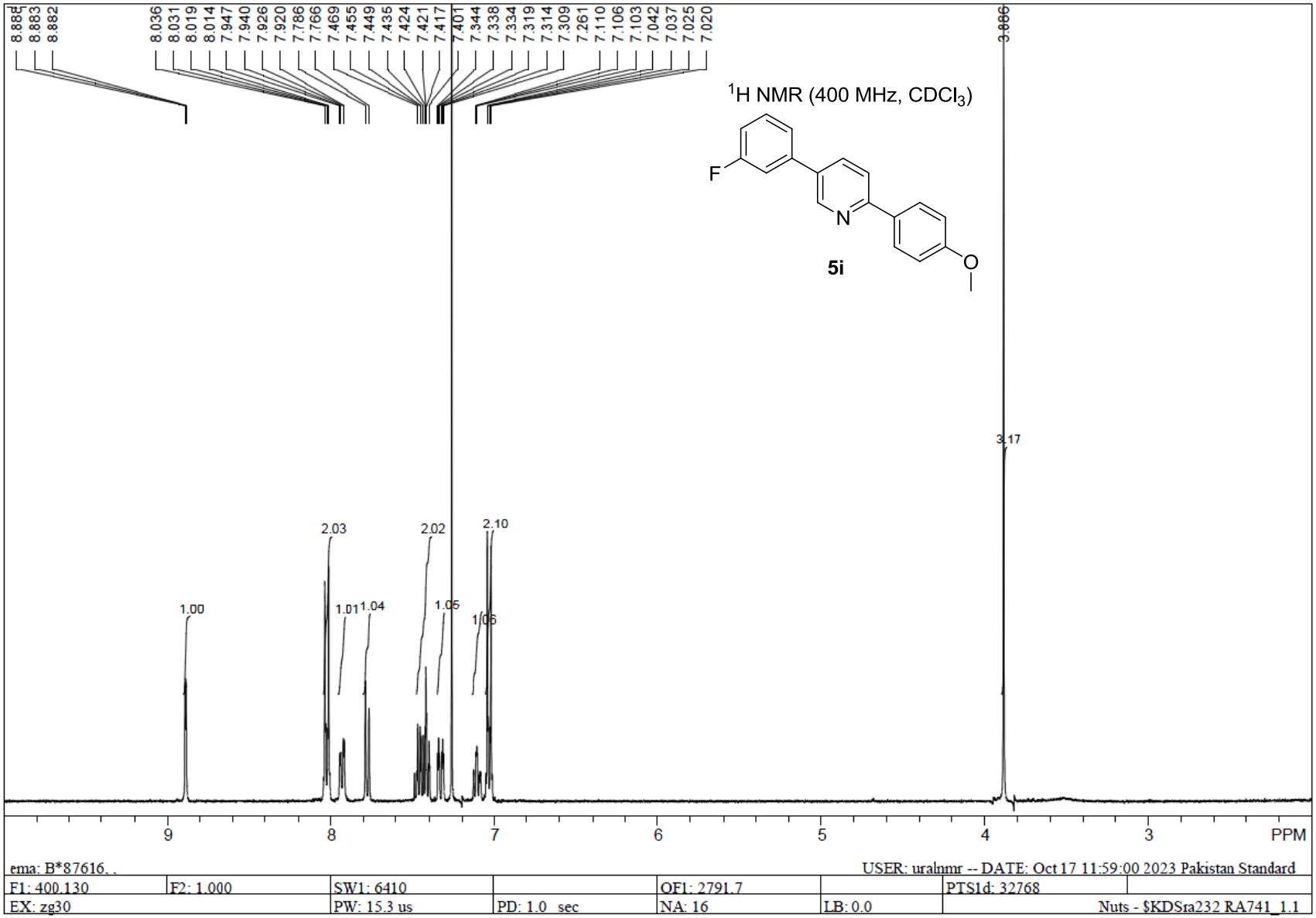

114.128
^{19}F NMR (376 MHz, DMSO-d_6)
F
N
Cl
5g
1.00
-20
-40
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1395
USER: nmr -- DATE: 12:35:11.828 +0600 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 89286
OF1: -37649.6
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 9
LB: 0.0
Nuts - $4438 SM1395_19.1

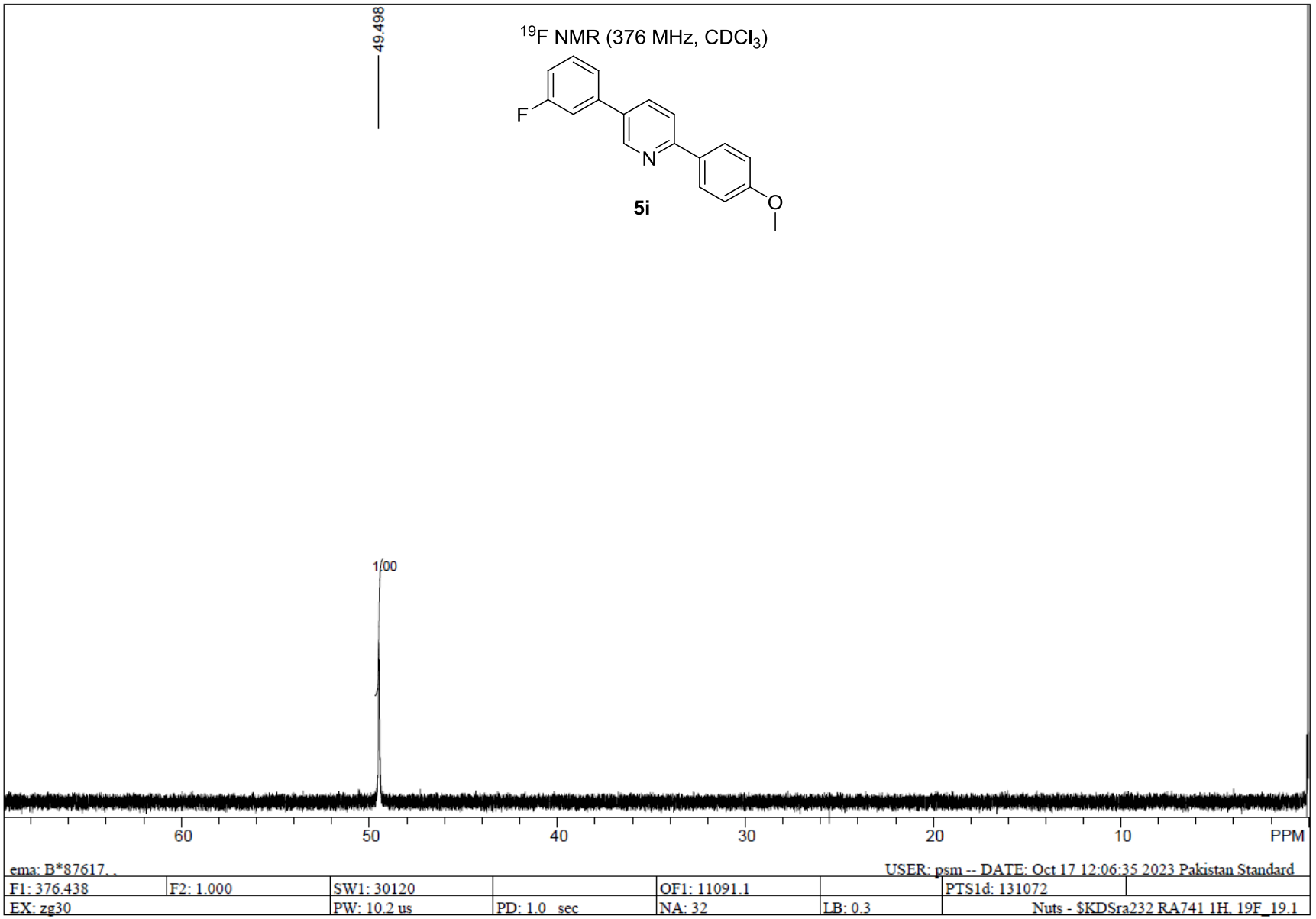

164.222
161.757
154.910
147.953
137.277
135.257
135.060
134.294
133.594
133.565
129.022
128.716
128.636
128.103
120.155
116.283
116.064
77.386
77.065
76.751
^{13}C NMR (100 MHz, CDCl$_3$)
F
N
Cl
5g
180
160
140
120
100
80
60
40
20
PPM
Krinochkin SM 1395, ,
USER: NMR -- DATE: 10:00:31.520 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 256
LB: 1.0
Nuts - $2573 SM1395 (13C) OK! â CDCl3_17.1

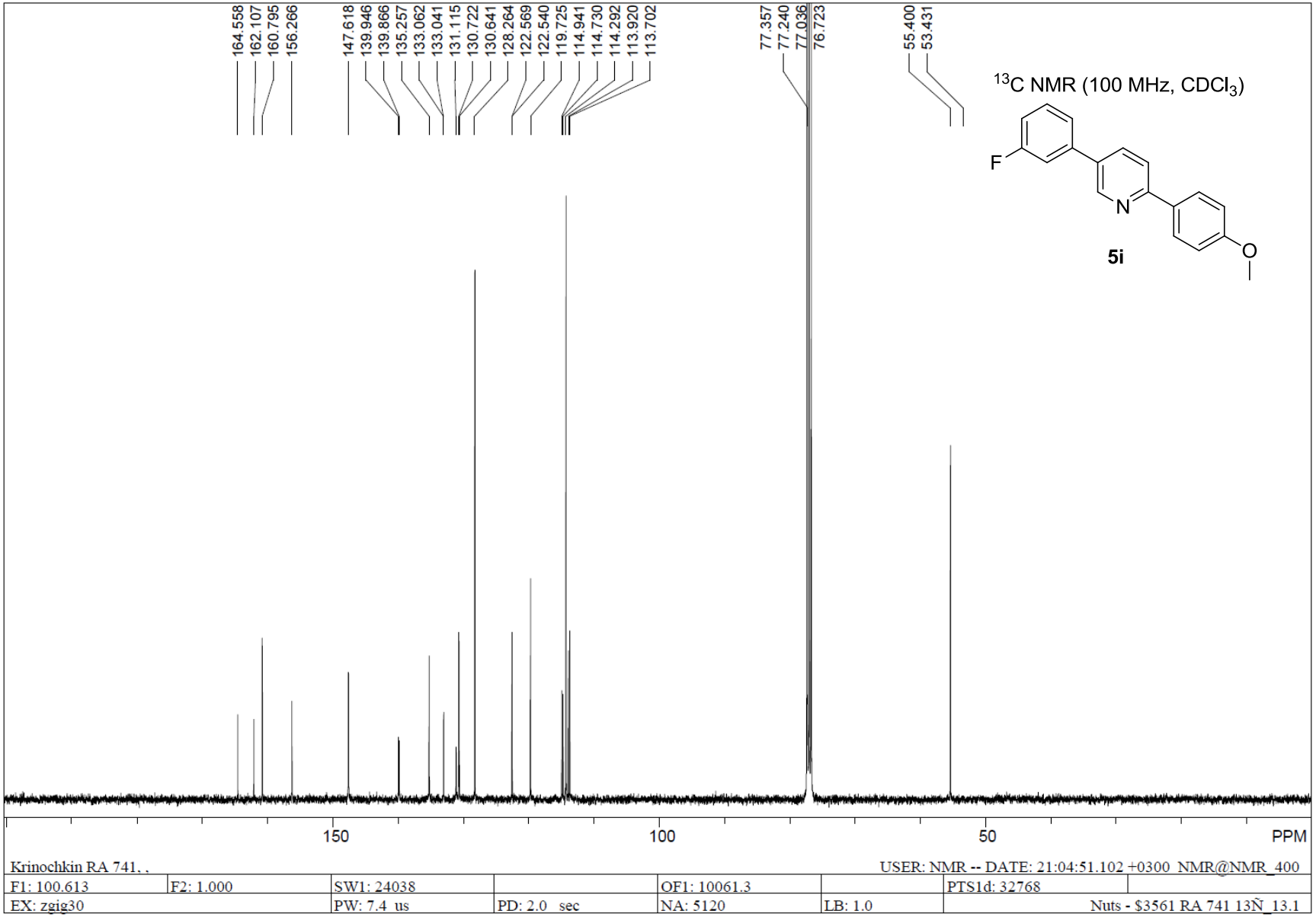

8.923
8.918
8.058
8.040
7.954
7.949
7.934
7.928
7.834
7.813
7.522
7.505
7.485
7.473
7.458
7.439
7.430
7.411
7.349
7.324
7.258
7.128
7.109
7.089
^{1}H NMR (400 MHz, $CDCl_3$)
F
N
5h
5.05
2.00
0.99
1.00
1.04
1.02
0.99
9
8
7
6
5
4
3
PPM
Krinochkin SM1031
USER: nmr -- DATE: 11:53:09.997 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2459.8
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 10
LB: 0.3
Nuts - $3782 SM1031_1.1

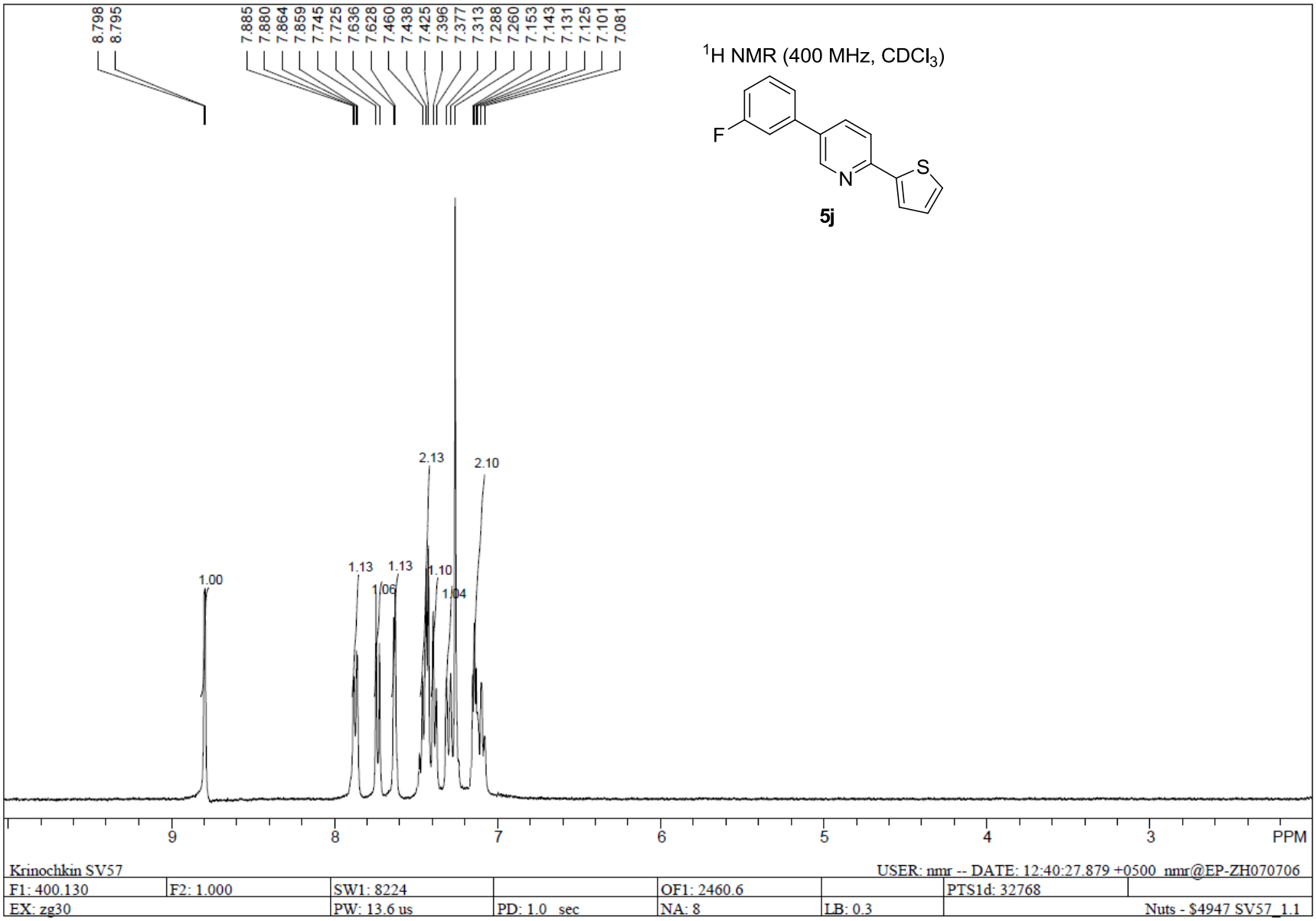

-112.246
^{19}F NMR (376 MHz, $CDCl_3$)
F
N
5h
1.00
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SM1031
USER: nmr -- DATE: 11:14:26.487 +0500 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 10
LB: 0.3
Nuts - $3782 SM1031_19.1

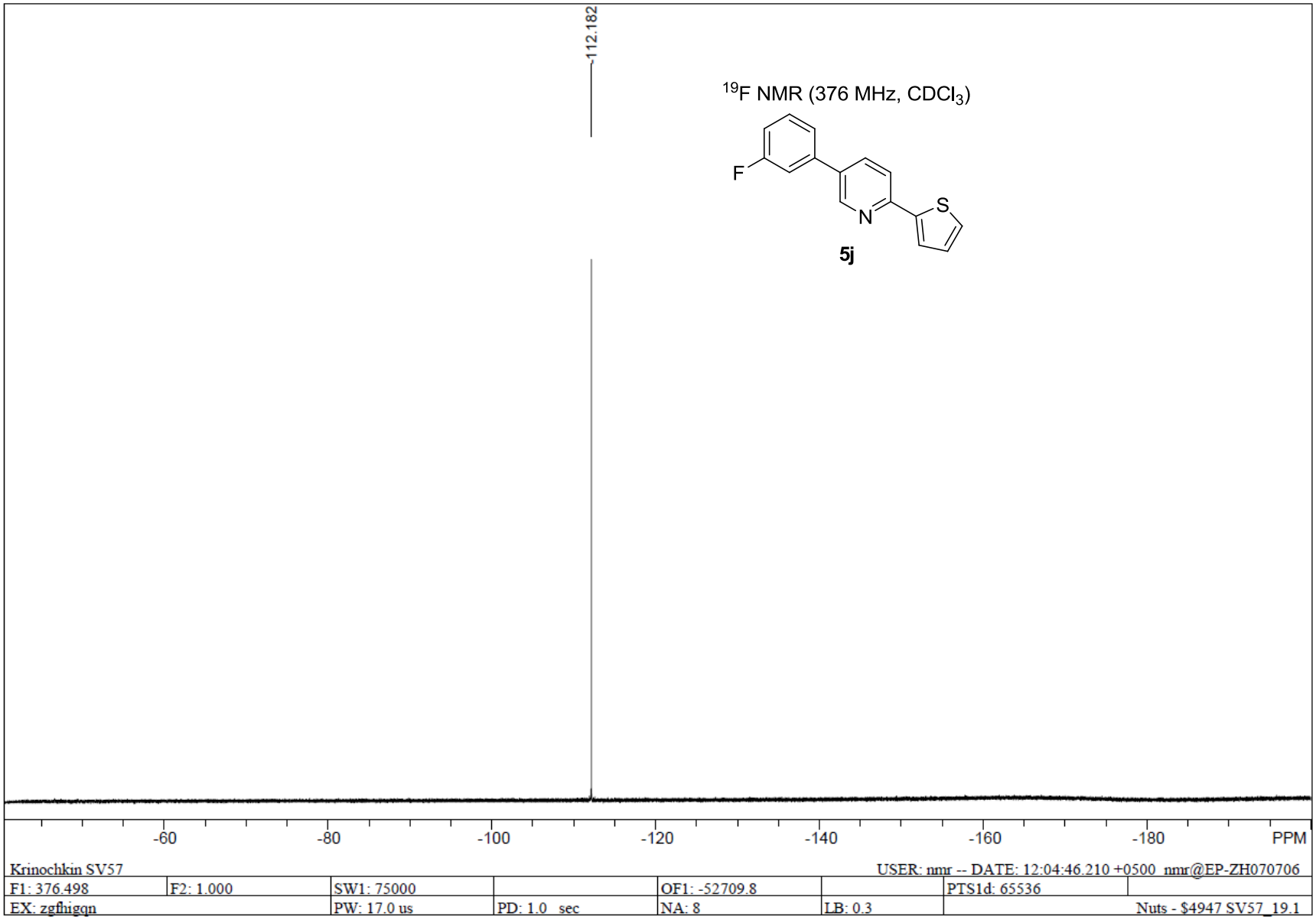

164.076
162.459
155.843
148.166
139.702
139.652
138.576
135.781
133.260
131.643
131.585
129.751
129.332
127.006
123.309
123.294
120.629
115.451
115.307
114.072
113.920
40.539
40.423
40.286
40.142
40.004
39.867
39.730
39.586
13C NMR (150 MHz, DMSO-d6)
F
N
5h
150
100
50
PPM
Avance, DMSO,
USER: nmr -- DATE: Sat Oct 07 05:57:26 2023
F1: 150.938
F2: 1.000
SW1: 35714
OF1: 15095.6
PTS1d: 32768
EX: zgig30
PW: 10.5 us
PD: 2.0 sec
NA: 61
LB: 0.0
Nuts - $pdata

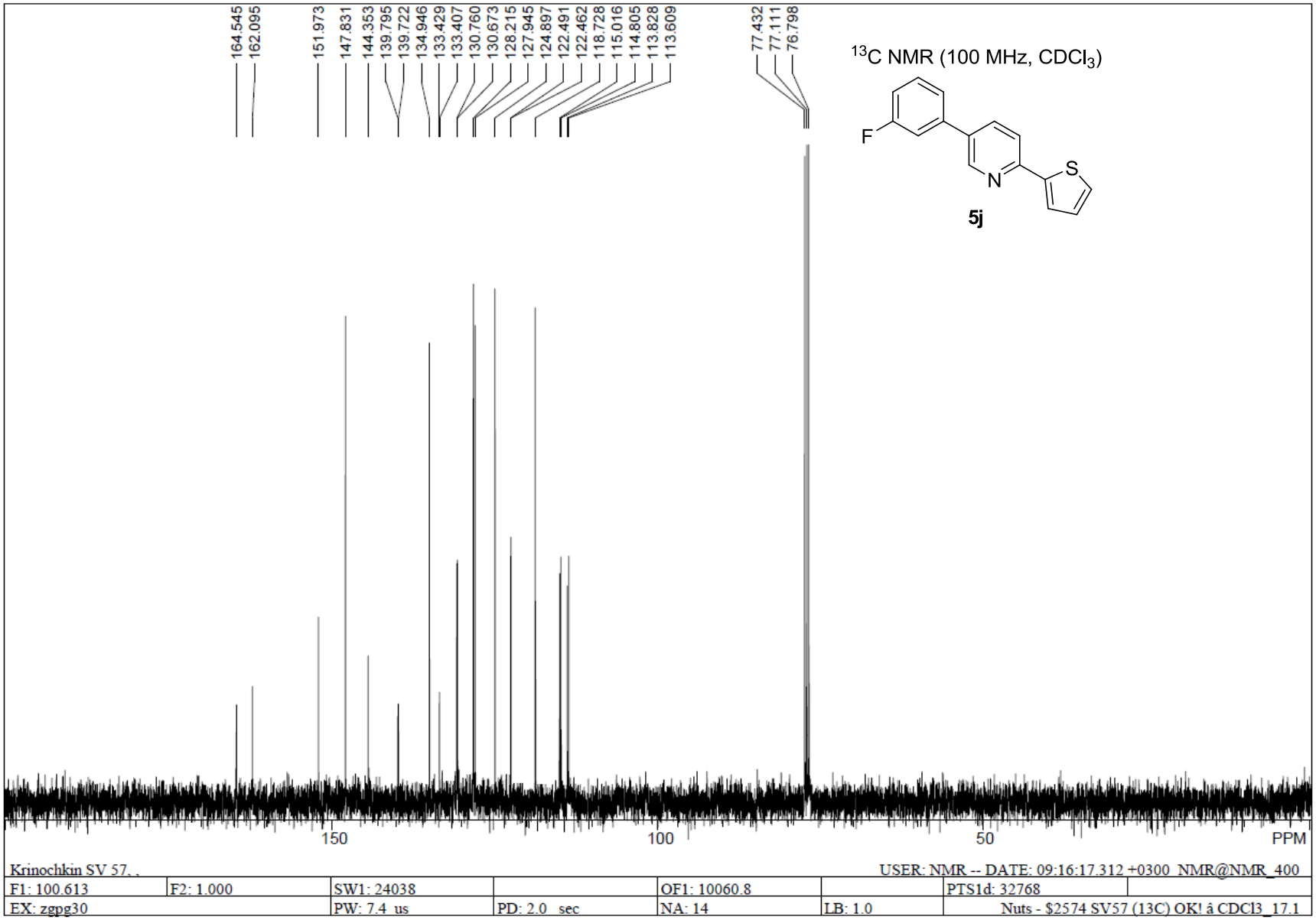

8.885
8.883
8.882
8.036
8.031
8.019
8.014
7.947
7.940
7.926
7.920
7.786
7.766
7.469
7.455
7.449
7.435
7.424
7.421
7.417
7.401
7.344
7.338
7.334
7.319
7.314
7.309
7.261
7.110
7.106
7.103
7.042
7.037
7.025
7.020
3.886
3.17
1H NMR (400 MHz, CDCl3)
F
N
O
5i
1.00
2.03
1.01
1.04
2.02
1.05
1.06
2.10
9
8
7
6
5
4
3
PPM
ema: B*87616, .
USER: uralnmr -- DATE: Oct 17 11:59:00 2023 Pakistan Standard
F1: 400.130
F2: 1.000
SW1: 6410
OF1: 2791.7
PTS1d: 32768
EX: zg30
PW: 15.3 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $KDSra232 RA741_1.1

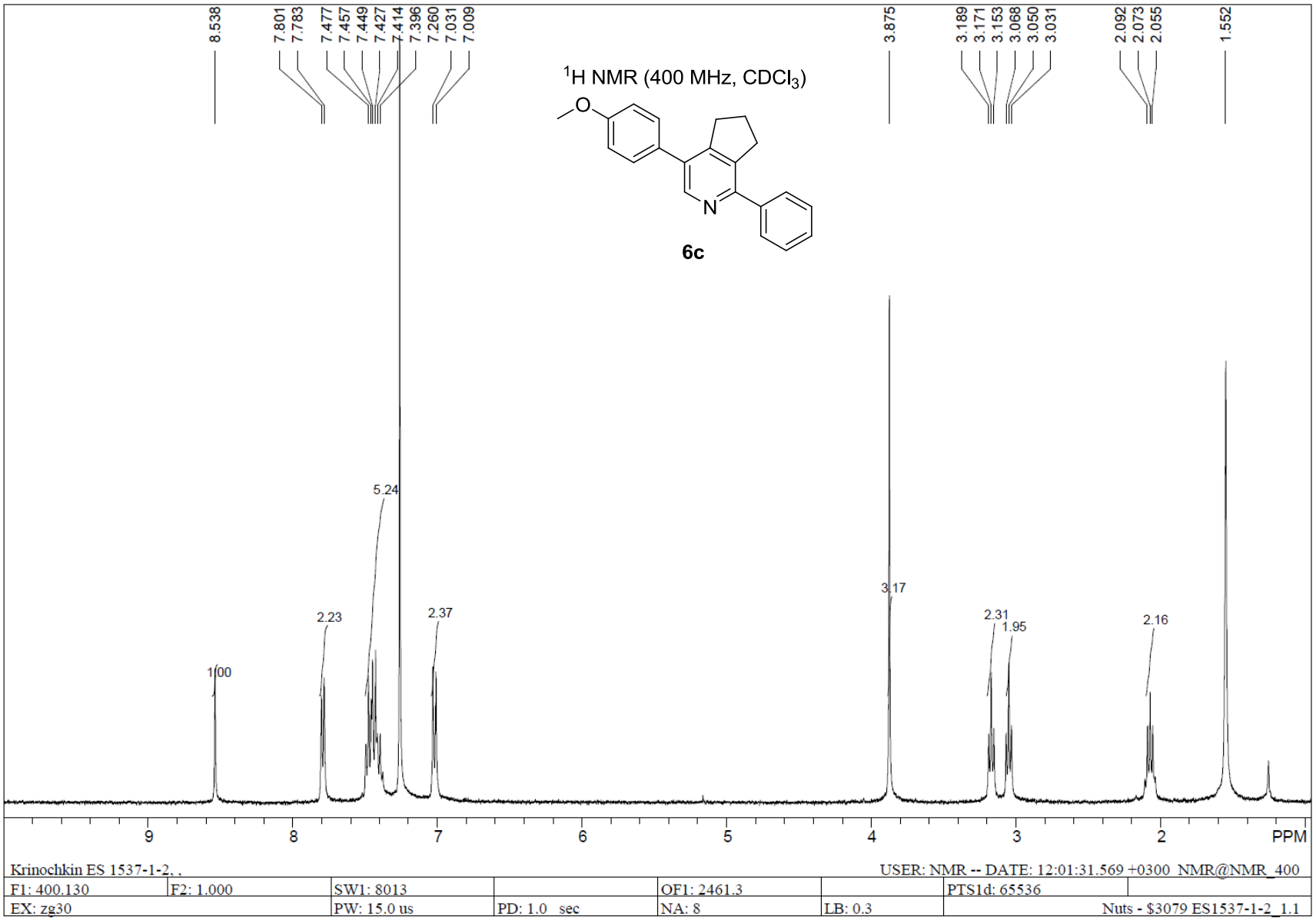

49.498
^{19}F NMR (376 MHz, $CDCl_3$)
F
N
O
5i
1.00
60
50
40
30
20
10
PPM
ema: B*87617, ,
USER: psm -- DATE: Oct 17 12:06:35 2023 Pakistan Standard
F1: 376.438
F2: 1.000
SW1: 30120
OF1: 11091.1
PTS1d: 131072
EX: zg30
PW: 10.2 us
PD: 1.0 sec
NA: 32
LB: 0.3
Nuts - $KDSra232 RA741 1H, 19F_19.1

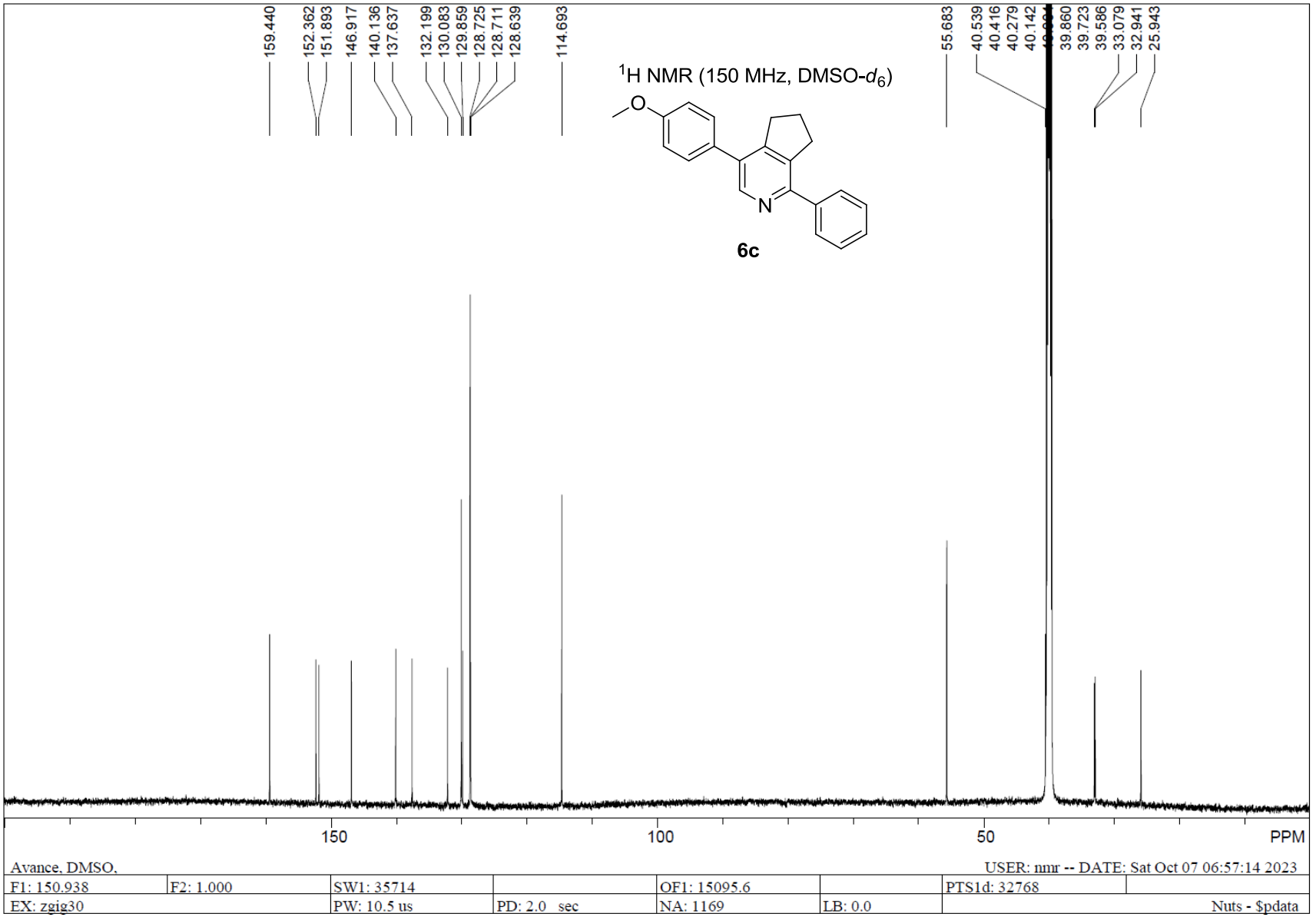

164.558
162.107
160.795
156.266
147.618
139.946
139.866
135.257
133.062
133.041
131.115
130.722
130.641
128.264
122.569
122.540
119.725
114.941
114.730
114.292
113.920
113.702
77.357
77.240
77.036
76.723
55.400
53.431
^{13}C NMR (100 MHz, CDCl$_3$)
F
N
O
5i
150
100
50
PPM
Krinochkin RA 741, ,
USER: NMR -- DATE: 21:04:51.102 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 5120
LB: 1.0
Nuts - $3561 RA 741 13Ñ_13.1

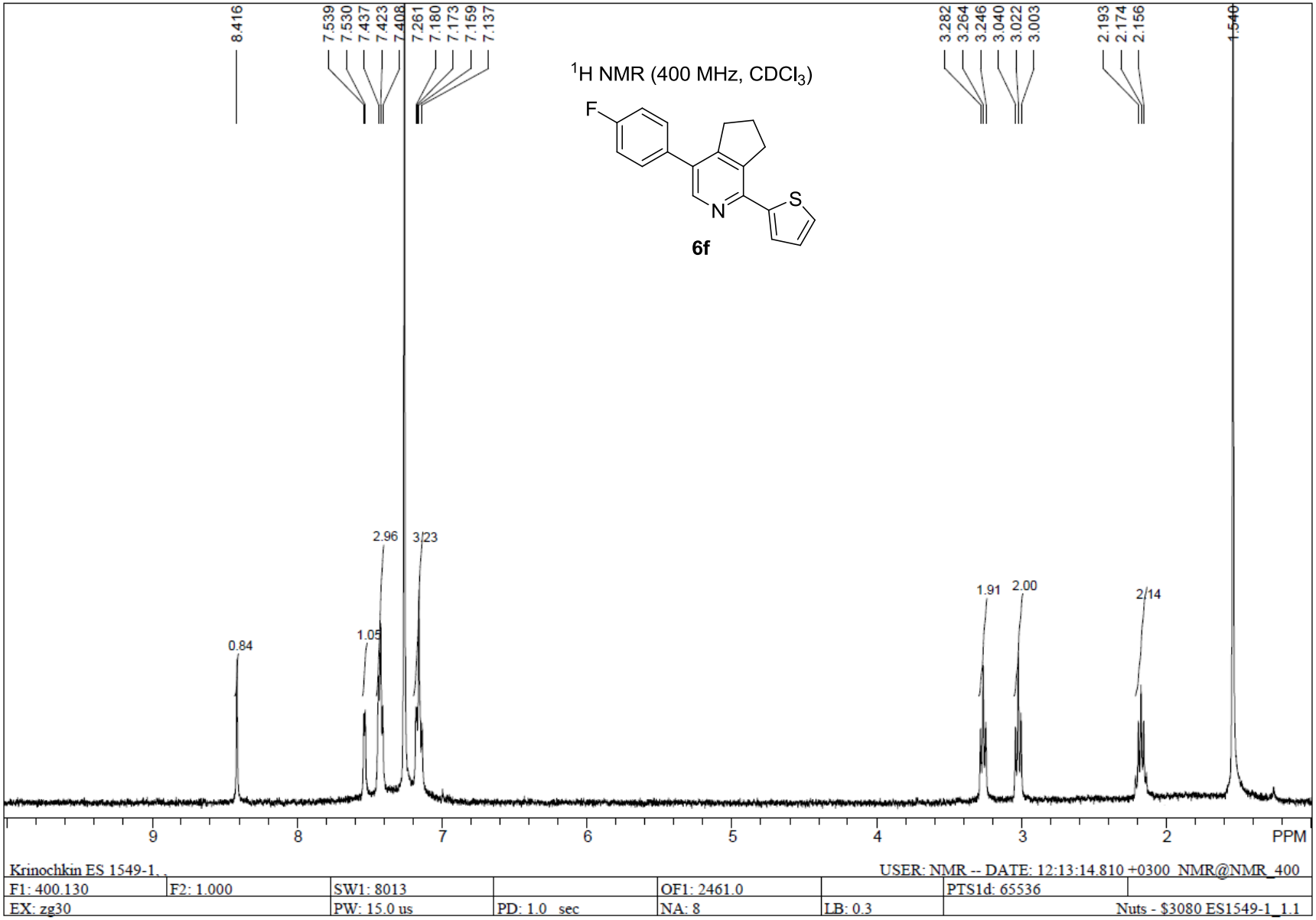

8.798
8.795
7.885
7.880
7.864
7.859
7.745
7.725
7.636
7.628
7.460
7.438
7.425
7.396
7.377
7.313
7.288
7.260
7.153
7.143
7.131
7.125
7.101
7.081
1H NMR (400 MHz, CDCl3)
F
N
S
5j
1.00
1.13
1.06
1.13
2.13
1.10
1.04
2.10
9
8
7
6
5
4
3
PPM
Krinochkin SV57
USER: nmr -- DATE: 12:40:27.879 +0500 nmr@EP-ZH070706
F1: 400.130
F2: 1.000
SW1: 8224
OF1: 2460.6
PTS1d: 32768
EX: zg30
PW: 13.6 us
PD: 1.0 sec
NA: 8
LB: 0.3
Nuts - $4947 SV57_1.1


112.182
^{19}F NMR (376 MHz, $CDCl_3$)
F
N
S
5j
-60
-80
-100
-120
-140
-160
-180
PPM
Krinochkin SV57
USER: nmr -- DATE: 12:04:46.210 +0500 nmr@EP-ZH070706
F1: 376.498
F2: 1.000
SW1: 75000
OF1: -52709.8
PTS1d: 65536
EX: zgfhigqn
PW: 17.0 us
PD: 1.0 sec
NA: 8
LB: 0.3
Nuts - $4947 SV57_19.1

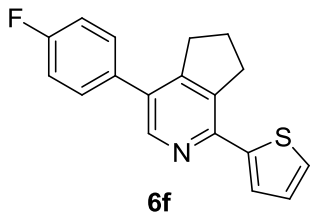

164.545
162.095
151.973
147.831
144.353
139.795
139.722
134.946
133.429
133.407
130.760
130.673
128.215
127.945
124.897
122.491
122.462
118.728
115.016
114.805
113.828
113.609
77.432
77.111
76.798
^{13}C NMR (100 MHz, CDCl$_3$)
F
N
S
5j
150
100
50
PPM
Krinochkin SV 57, ,
USER: NMR -- DATE: 09:16:17.312 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.8
PTS1d: 32768
EX: zgpg30
PW: 7.4 us
PD: 2.0 sec
NA: 14
LB: 1.0
Nuts - $2574 SV57 (13C) OK! â CDCl3_17.1


8.538
7.801
7.783
7.477
7.457
7.449
7.427
7.414
7.396
7.260
7.031
7.009
3.875
3.189
3.171
3.153
3.068
3.050
3.031
2.092
2.073
2.055
1.552
^{1}H NMR (400 MHz, $CDCl_3$)
O
N
6c
5.24
2.23
2.37
1.00
3.17
2.31
1.95
2.16
9
8
7
6
5
4
3
2
PPM
Krinochkin ES 1537-1-2, ,
USER: NMR -- DATE: 12:01:31.569 +0300 NMR@NMR_400
F1: 400.130
F2: 1.000
SW1: 8013
OF1: 2461.3
PTS1d: 65536
EX: zg30
PW: 15.0 us
PD: 1.0 sec
NA: 8
LB: 0.3
Nuts - $3079 ES1537-1-2_1.1


159.440
152.362
151.893
146.917
140.136
137.637
132.199
130.083
129.859
128.725
128.711
128.639
114.693
55.683
40.539
40.416
40.279
40.142
39.860
39.723
39.586
33.079
32.941
25.943
^{1}H NMR (150 MHz, DMSO-d_6)
O
N
6c
150
100
50
PPM
Avance, DMSO,
USER: nmr -- DATE: Sat Oct 07 06:57:14 2023
F1: 150.938
F2: 1.000
SW1: 35714
OF1: 15095.6
PTS1d: 32768
EX: zgig30
PW: 10.5 us
PD: 2.0 sec
NA: 1169
LB: 0.0
Nuts - $pdata


8.416
7.539
7.530
7.437
7.423
7.408
7.261
7.180
7.173
7.159
7.137
3.282
3.264
3.246
3.040
3.022
3.003
2.193
2.174
2.156
1.540
^{1}H NMR (400 MHz, CDCl$_3$)
F
N
S
6f
2.96
3.23
1.05
0.84
1.91
2.00
2.14
9
8
7
6
5
4
3
2
PPM
Krinochkin ES 1549-1, ,
USER: NMR -- DATE: 12:13:14.810 +0300 NMR@NMR_400
F1: 400.130
F2: 1.000
SW1: 8013
OF1: 2461.0
PTS1d: 65536
EX: zg30
PW: 15.0 us
PD: 1.0 sec
NA: 8
LB: 0.3
Nuts - $3080 ES1549-1_1.1

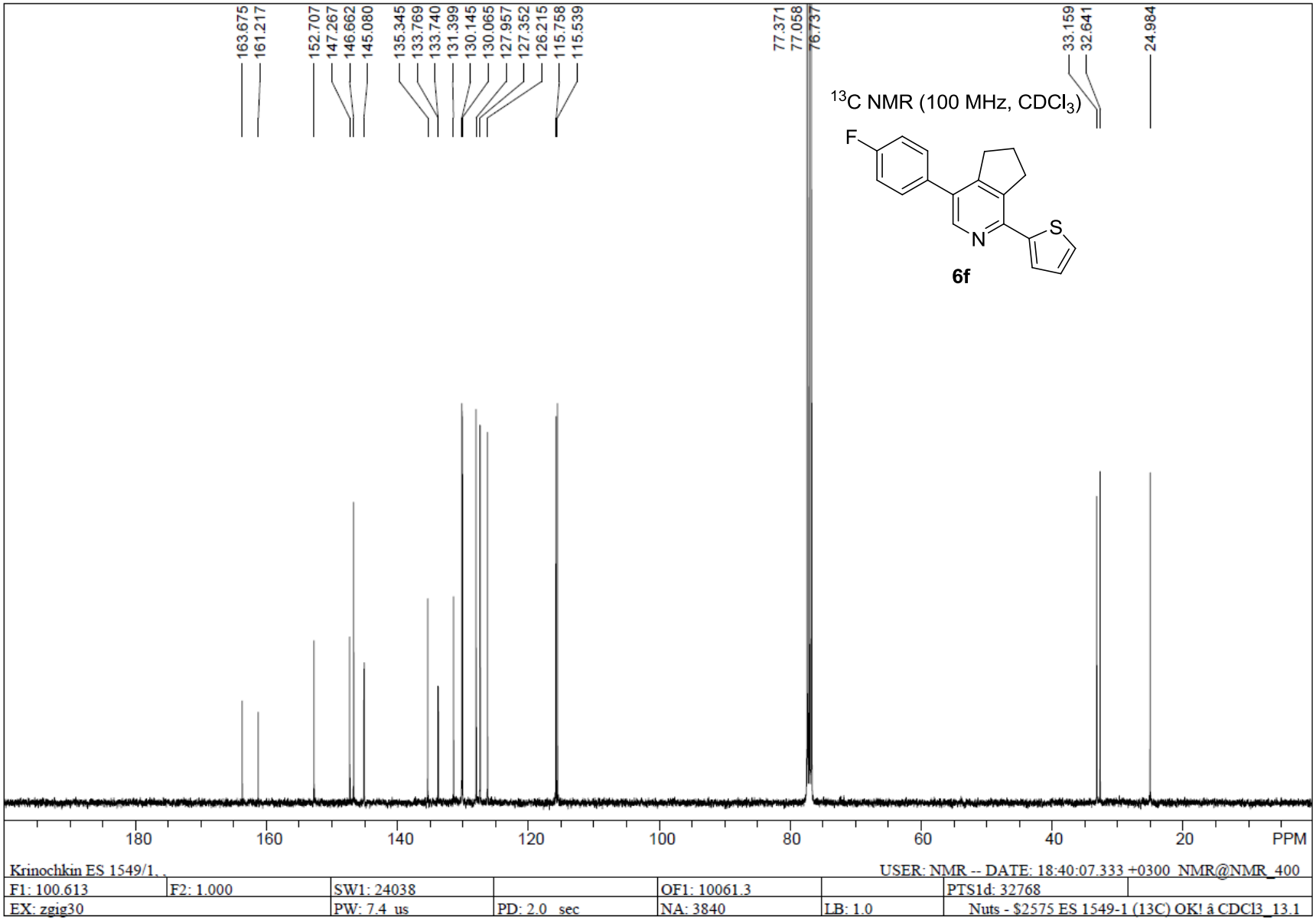
^{19}F NMR (564 MHz, $CDCl_3$)



6f

Avance, CDCl3, USER: nmr -- DATE: Tue Oct 17 09:14:11 2023

F1: 564.705	F2: 1.000	SW1: 131579		OF1: -56477.1		PTS1d: 65536	
EX: zg		PW: 15.0 us	PD: 1.0 sec	NA: 8	LB: 0.0		Nuts - $pdata


163.675
161.217
152.707
147.267
146.662
145.080
135.345
133.769
133.740
131.399
130.145
130.065
127.957
127.352
126.215
115.758
115.539
77.371
77.058
76.737
33.159
32.641
24.984
13C NMR (100 MHz, CDCl3)
F
N
S
6f
180
160
140
120
100
80
60
40
20
PPM
Krinochkin ES 1549/1, ,
USER: NMR -- DATE: 18:40:07.333 +0300 NMR@NMR_400
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10061.3
PTS1d: 32768
EX: zgig30
PW: 7.4 us
PD: 2.0 sec
NA: 3840
LB: 1.0
Nuts - $2575 ES 1549-1 (13C) OK! â CDCl3 13.1