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Supplementary material

SUPPLEMENTARY MATERIAL TO  
**Synthesis, antimycobacterial and antifungal evaluation of new  
4-(furan-2-ylmethyl)-6-methylpyridazin-3(2H)-ones**

BURCU KARAYAVUZ<sup>1</sup>, SIVA KRISHNA VAGOLU<sup>2</sup>, DIDEM KART<sup>3</sup>, TONE TØNJUM<sup>2,4</sup>  
and OYA UNSAL-TAN<sup>1\*</sup>

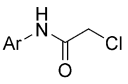
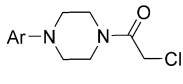

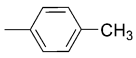
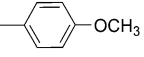
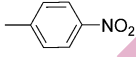


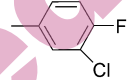
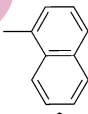
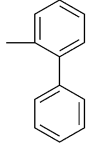


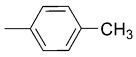
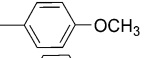
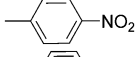
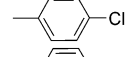
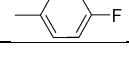
<sup>1</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Hacettepe University, Ankara, Turkey, <sup>2</sup>Unit for Genome Dynamics, Department of Microbiology, University of Oslo, Oslo, Norway, <sup>3</sup>Department of Pharmaceutical Microbiology, Faculty of Pharmacy, Hacettepe University, Ankara, Turkey, and <sup>4</sup>Unit for Genome Dynamics, Department of Microbiology, Oslo University Hospital, Oslo, Norway.

Table S1. Yields, melting points and literature melting points of 2-Chloro-*N*-arylacetamides (**3a-j**) and 2-chloro-1-(4-arylpiperazin-1-yl)ethanones (**4a-f**)  
Page S2-S3

IR, ESI-MS, <sup>1</sup>H and <sup>13</sup>C- NMR Spectra Of The Target Compounds Page S4-S60

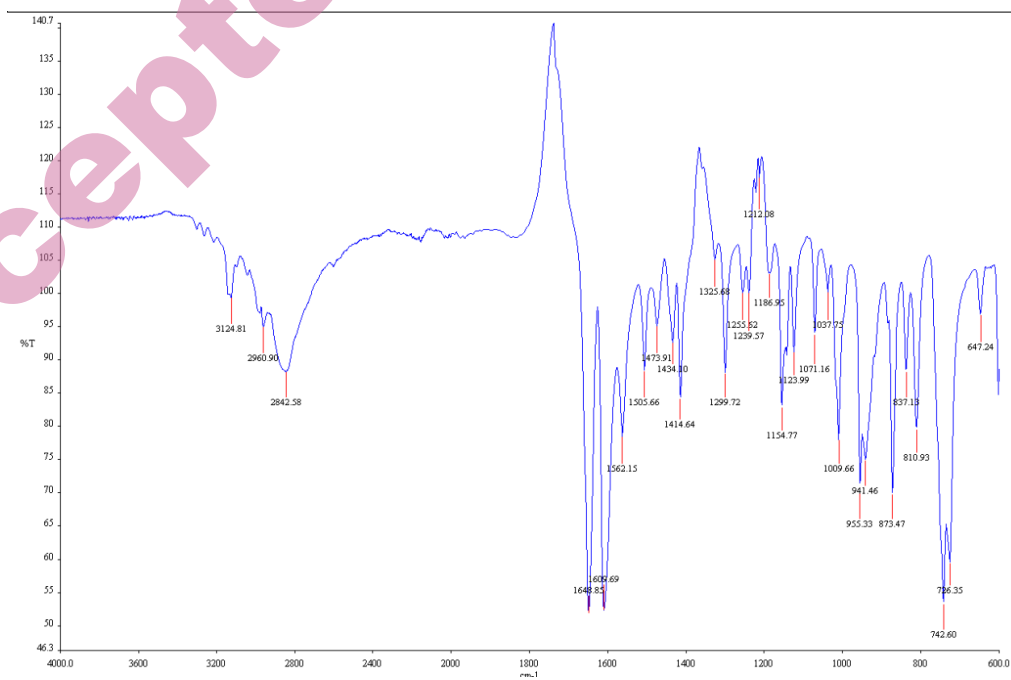
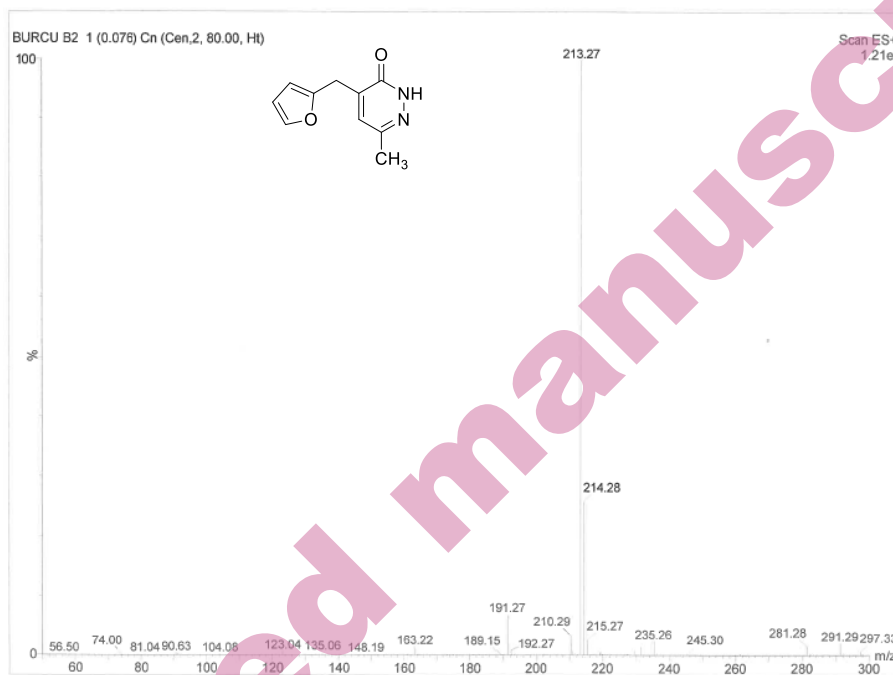
\* Corresponding author. E-mail: oyaunsal@hacettepe.edu.tr; Tel. +90-533-346 20 50

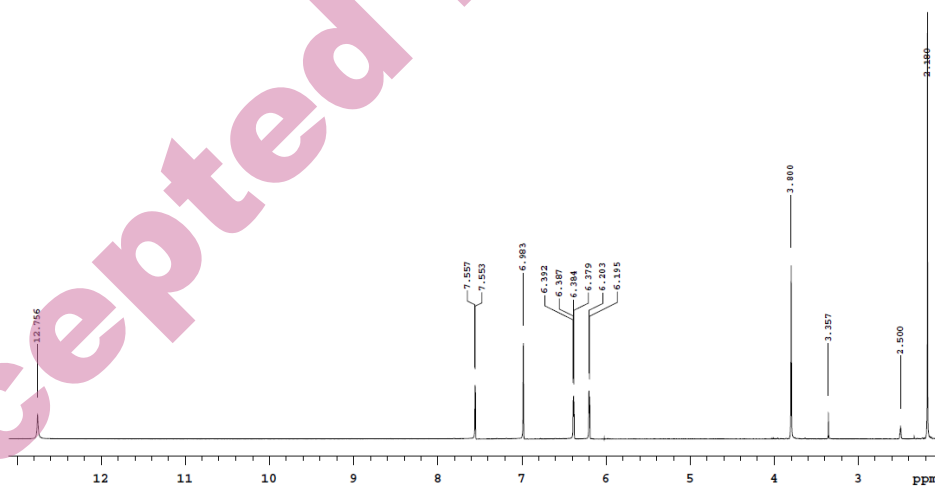
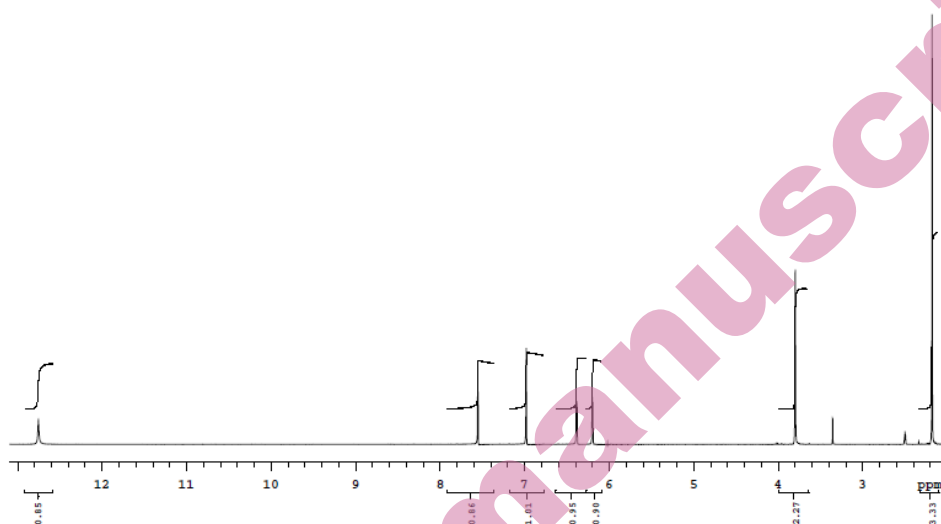
Table S1. Yields, melting points and literature melting points of 2-Chloro-*N*-arylacetamides (**3a-j**) and 2-chloro-1-(4-arylpiperazin-1-yl)ethanones (**4a-f**)

			
		M.p. [Lit M.p.] (° C)	
3a		94.9	133 [132] <sup>1</sup>
3b		96.8	119 [130] <sup>2</sup>
3c		96.0	119 [119-120] <sup>3</sup>
3d		92.0	118 [118] <sup>2</sup>
3e		93.2	148 [150] <sup>2</sup>
3f		94.2	131 [130-131] <sup>4</sup>
3g		92.4	75 [75-77] <sup>5</sup>
3h		90.1	150 [154] <sup>6</sup>
3i		86.2	152 [152-153] <sup>6</sup>
3j		83.4	175 [178-180] <sup>7</sup>
4a		67.6	75 [77] <sup>8</sup>
4b		83.2	75 [60-1] <sup>9</sup>
4c		81.4	106 [109-111] <sup>10</sup>
4d		78.28	104 [100-101] <sup>11</sup>
4e		77.17	81 [84-85] <sup>12</sup>
4f		85.13	104 [95] <sup>13</sup>

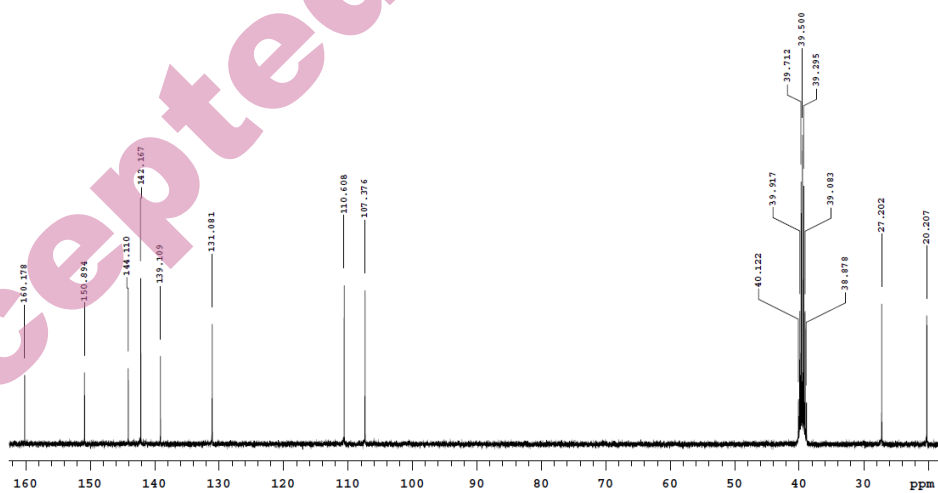
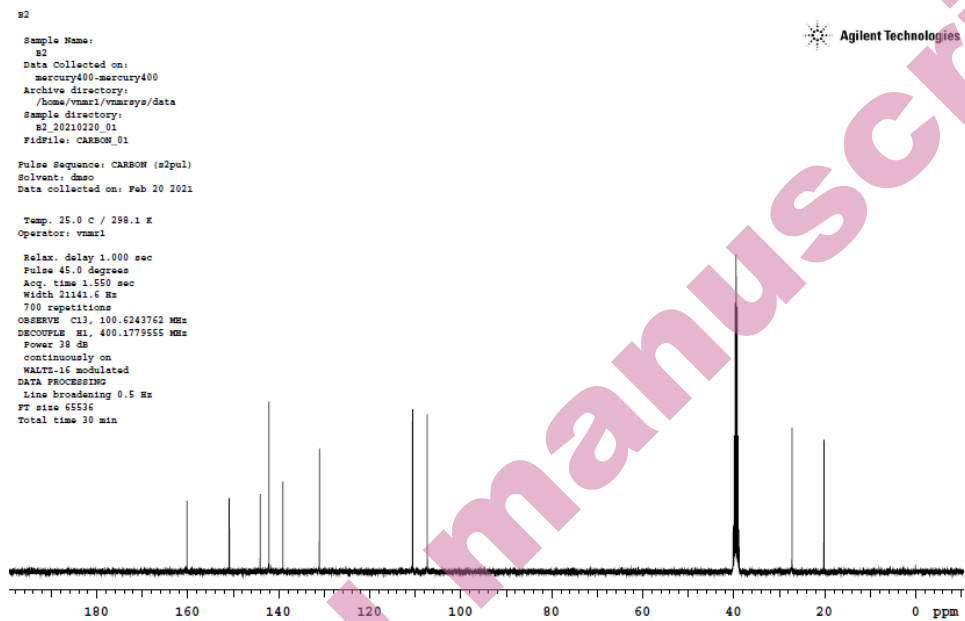
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12. K. Kamiński, B. Wiklik, J. Obniska, *Med. Chem. Res.* **24** (2015) 3047–3061 (<https://doi.org/10.1007/s00044-015-1360-6>)
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## 4-(2-FURYLMETHYL)-6-METHYLPYRIDAZIN-3(2H)-ONE (2)

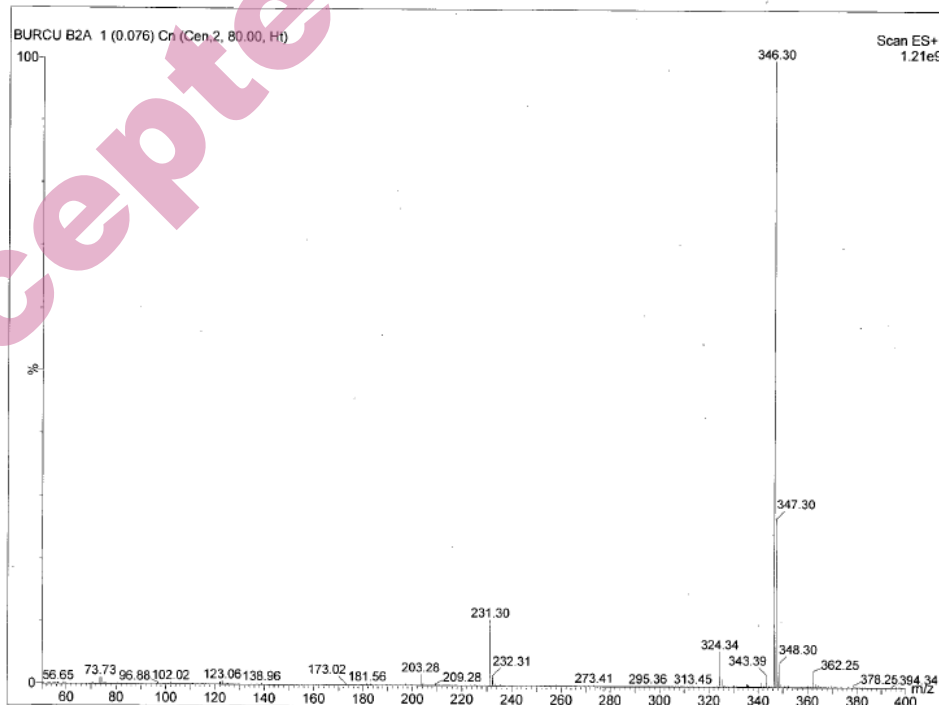
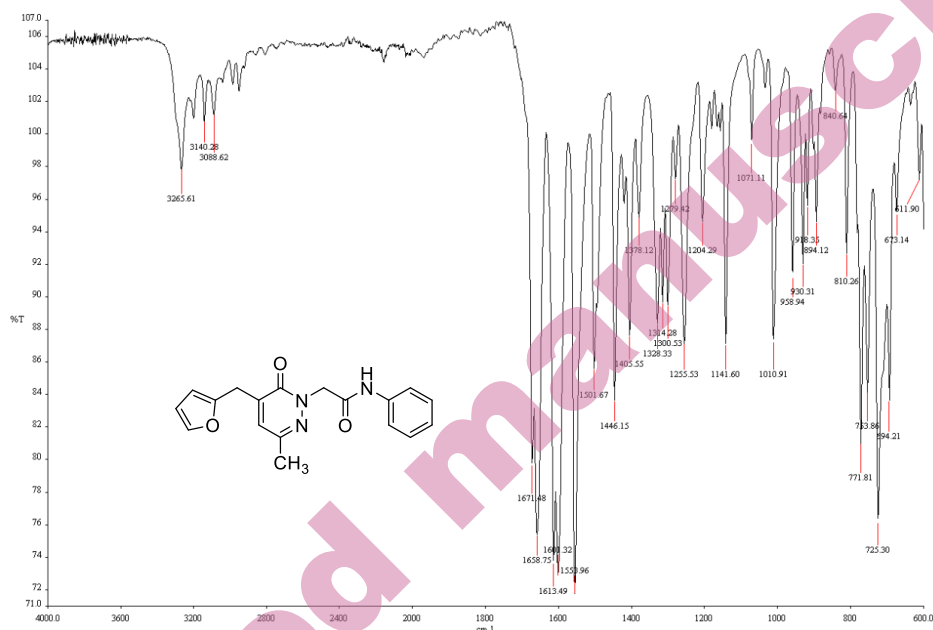


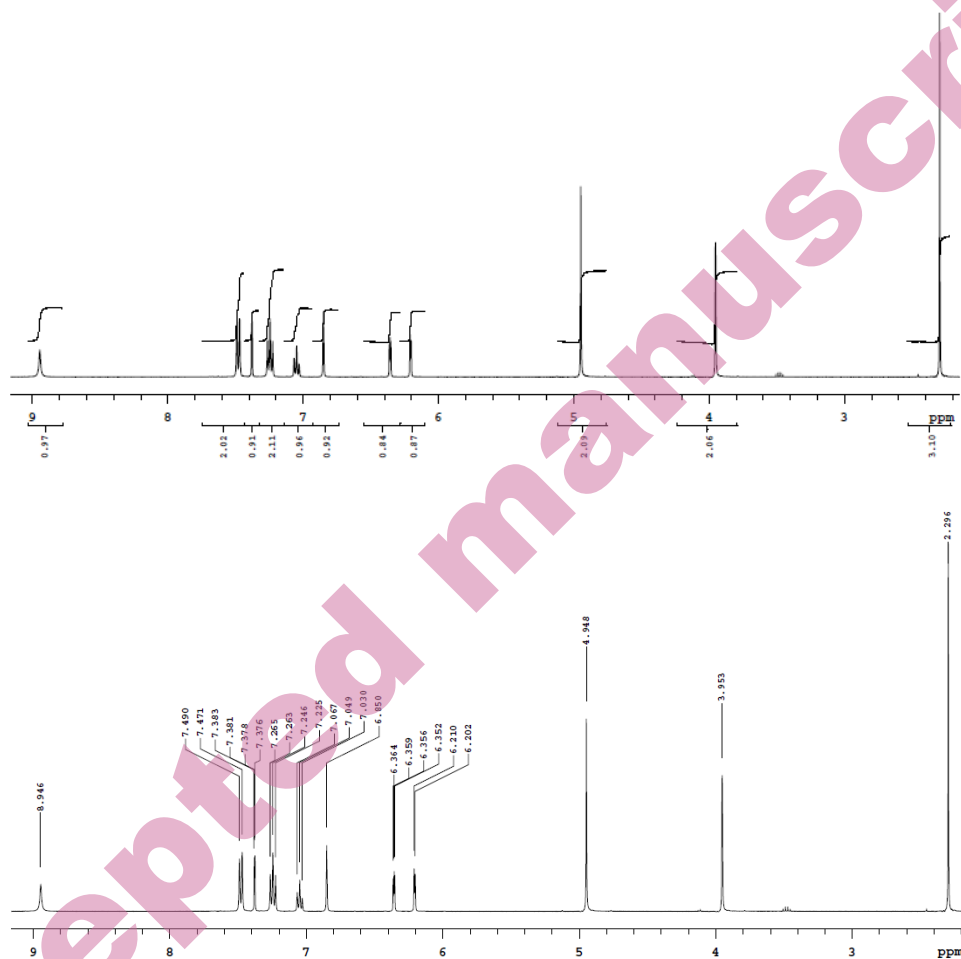


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2-[5-(FURAN-2-YLMETHYL)-3-METHYL-6-OXOPYRIDAZIN-1(6H)-YL]-N-PHENYLACETAMIDE (5A)









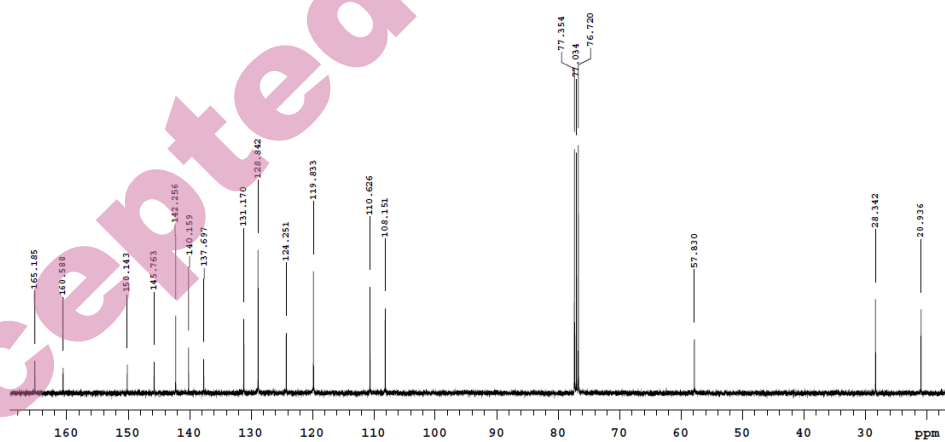
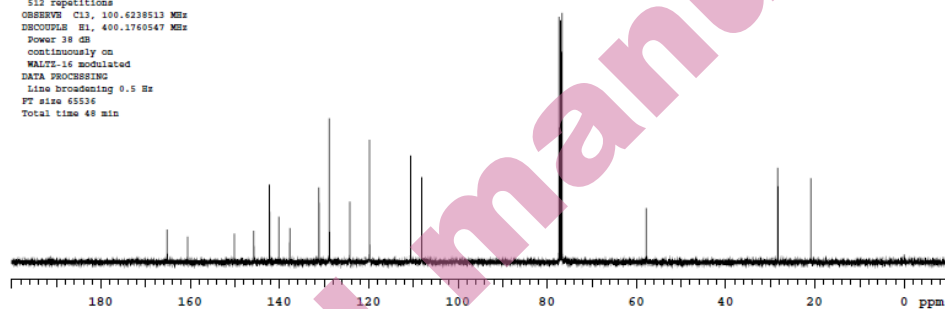
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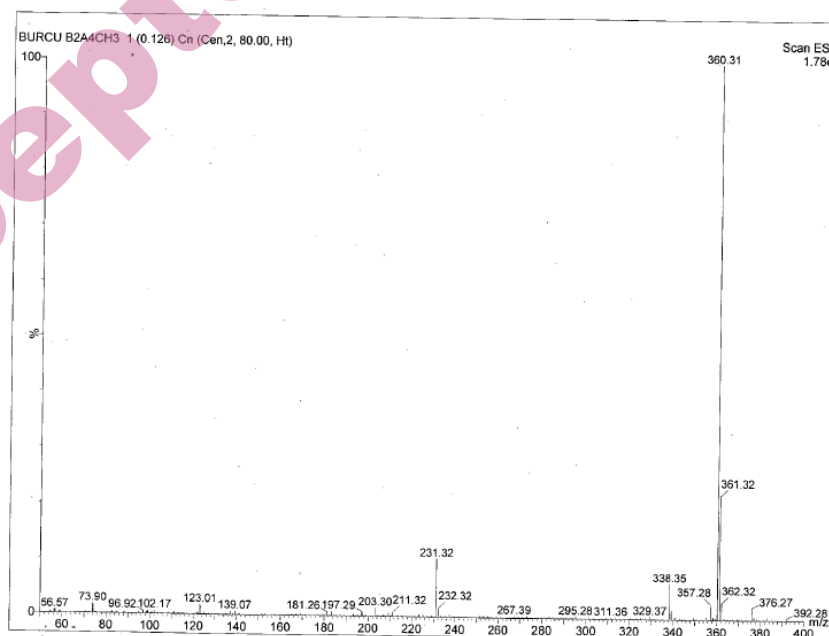
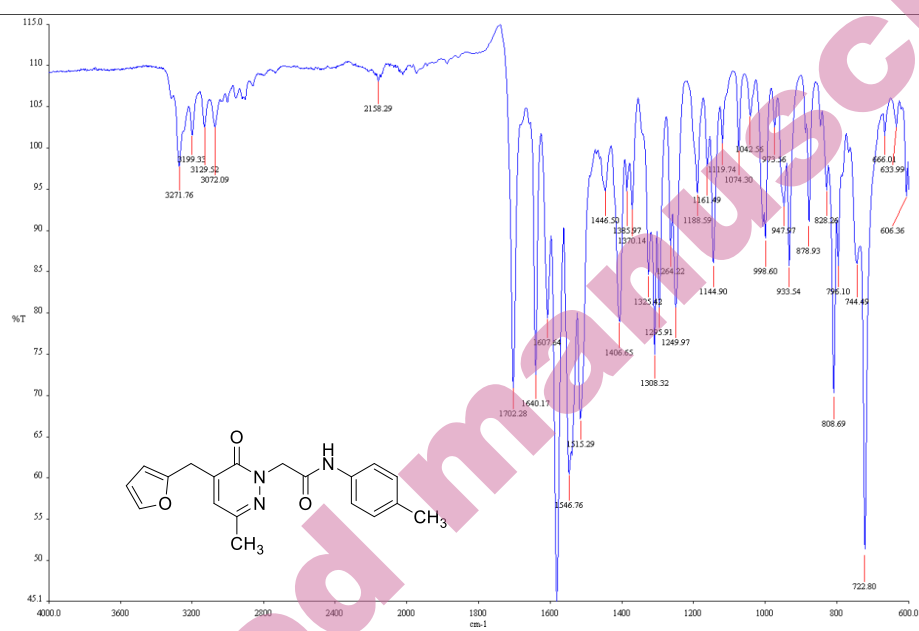
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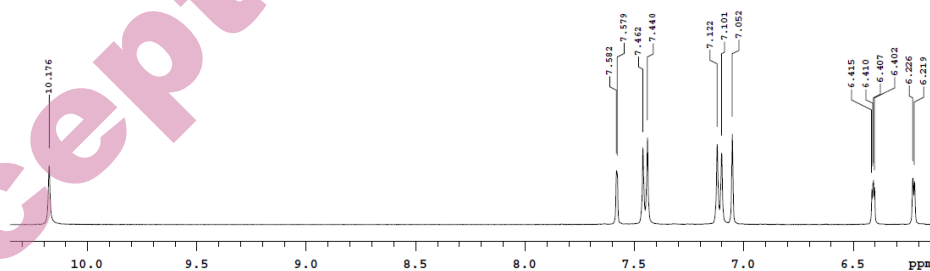
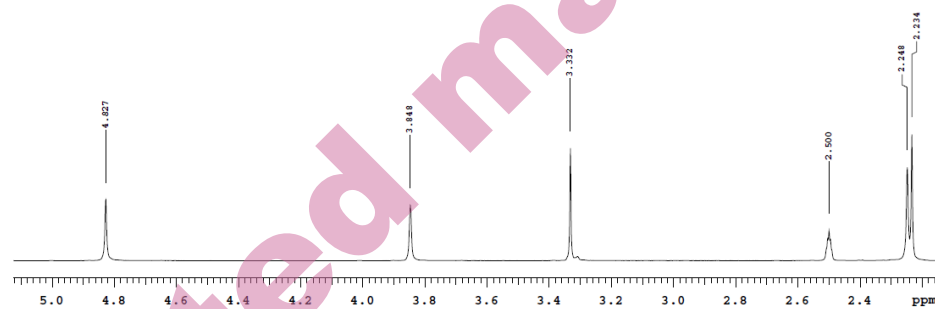
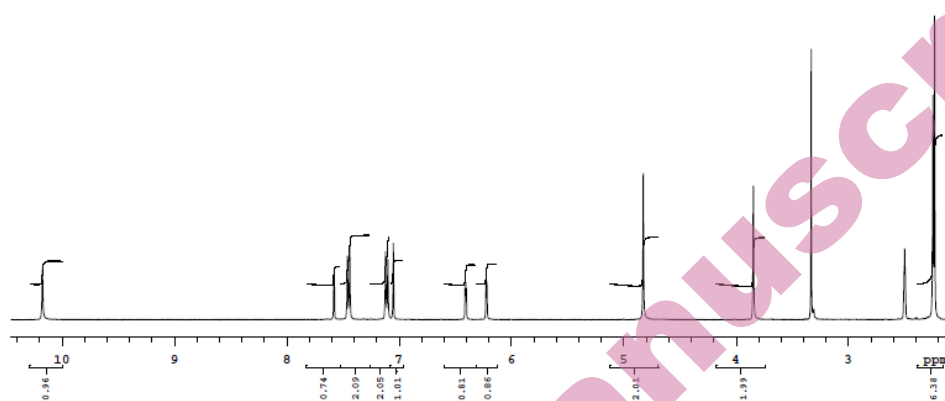
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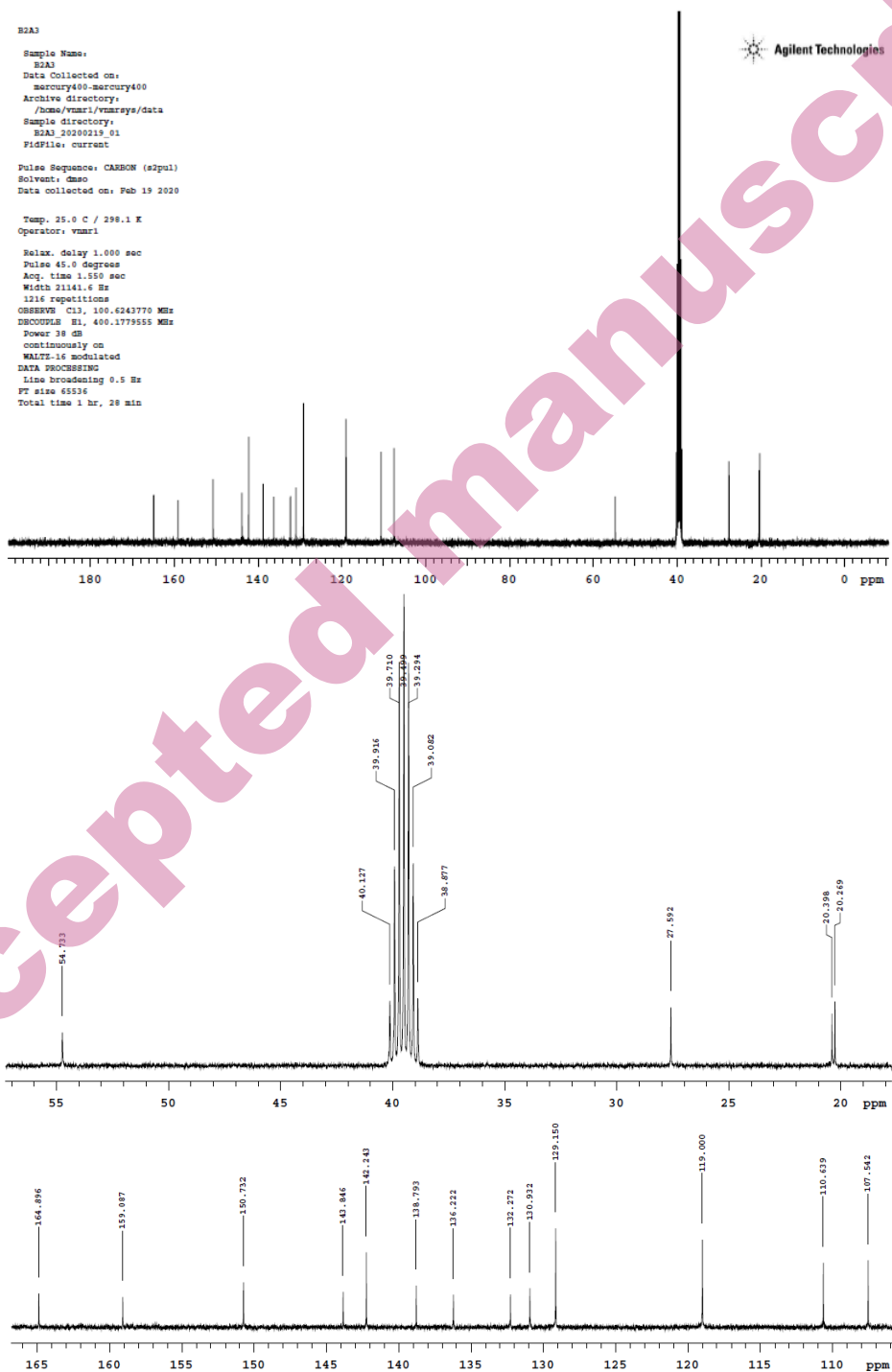


## 2-[5-(FURAN-2-YLMETHYL)-3-METHYL-6-OXOPYRIDAZIN-1(6H)-YL]-N-(4-METHYLPHENYL)ACETAMIDE (5B)

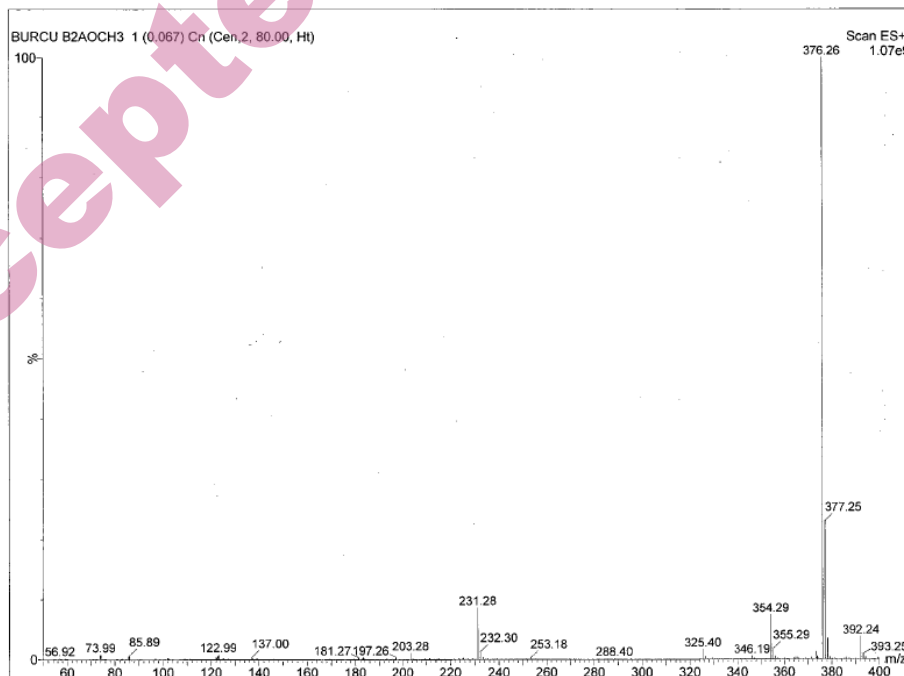
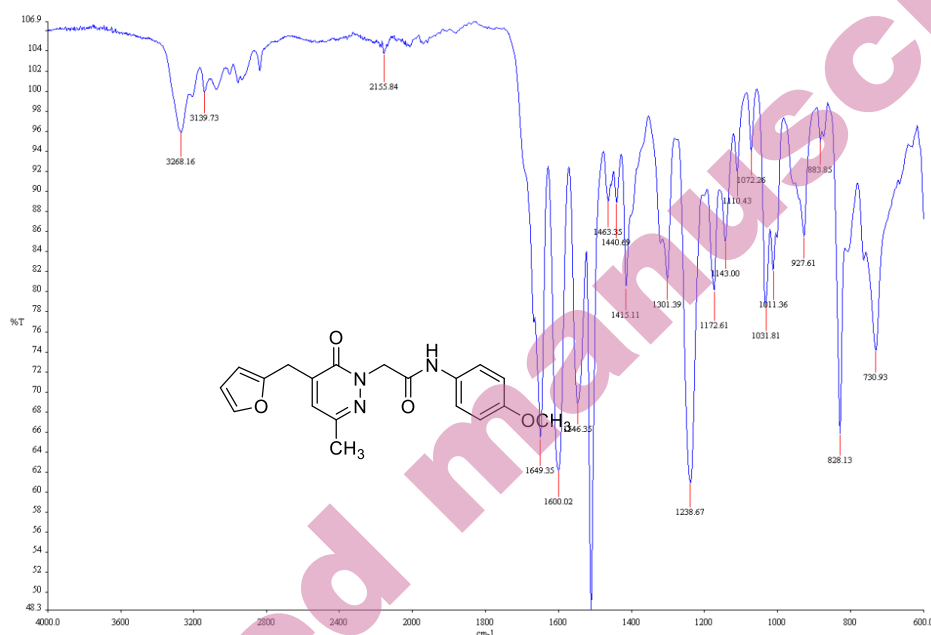


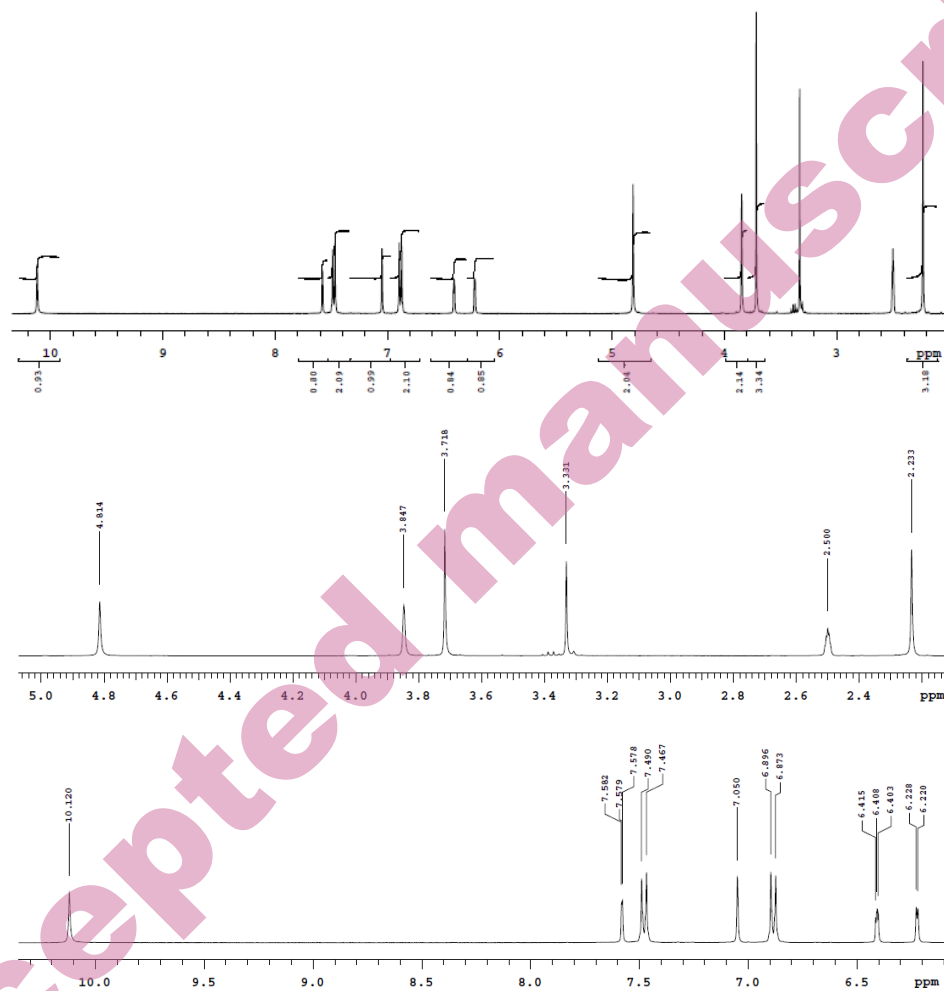


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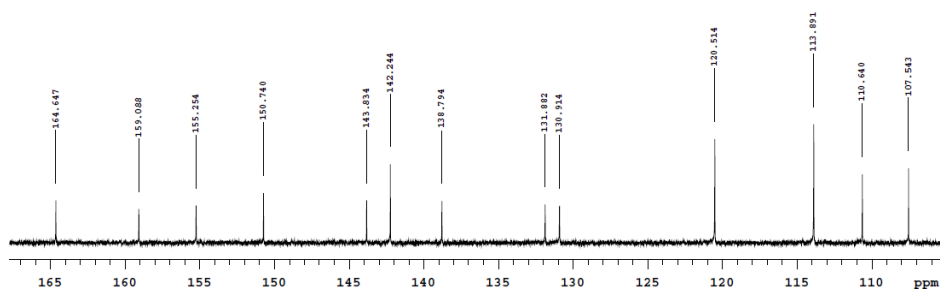
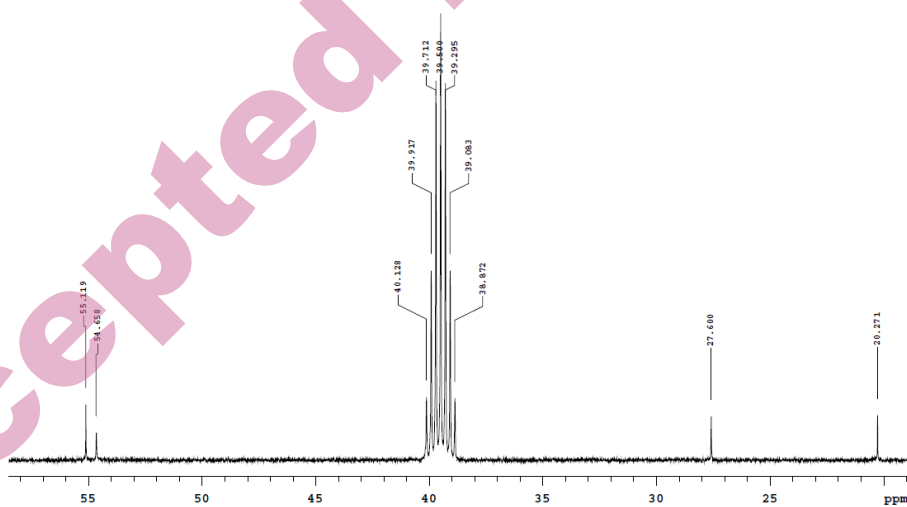
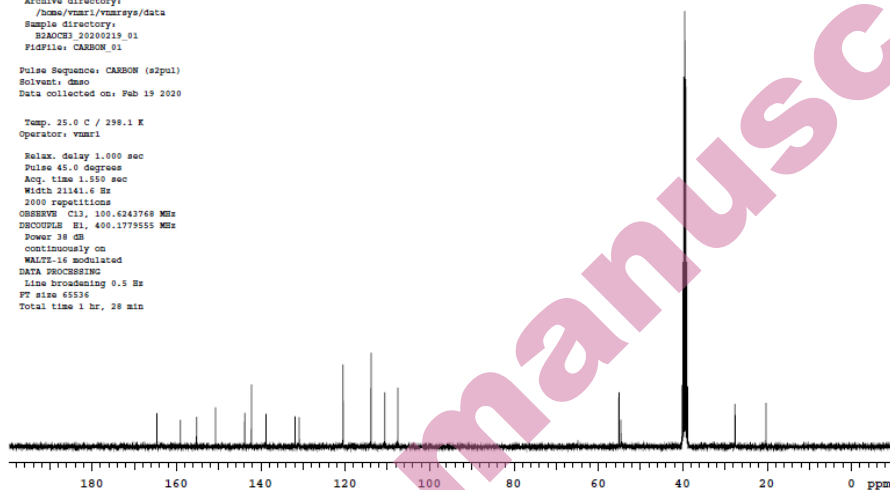
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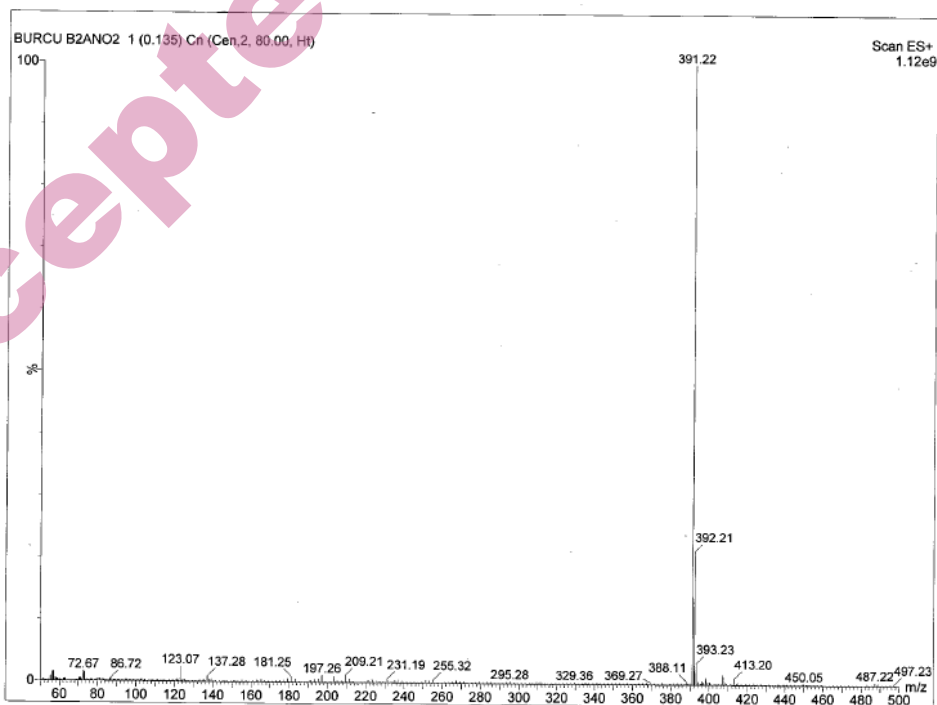
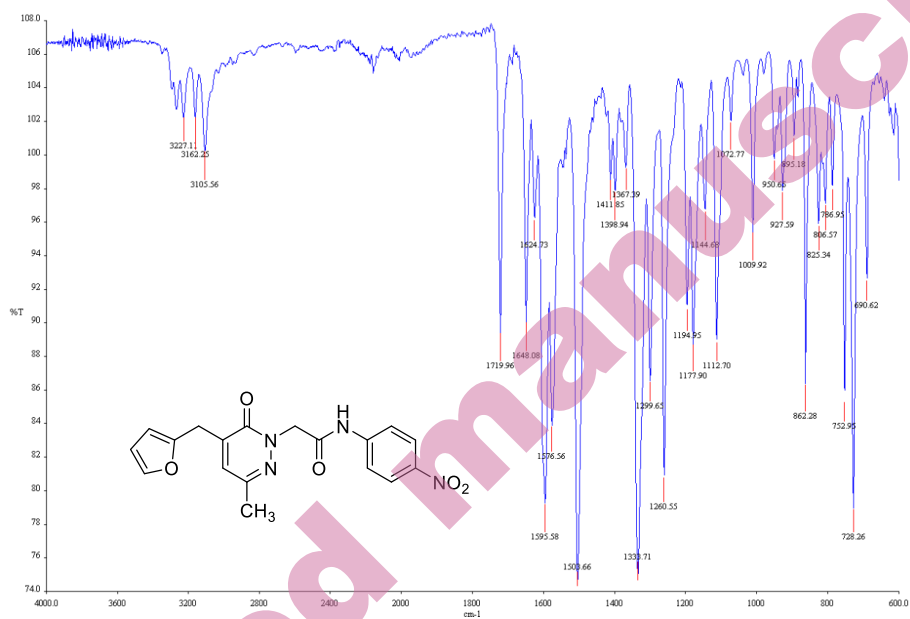




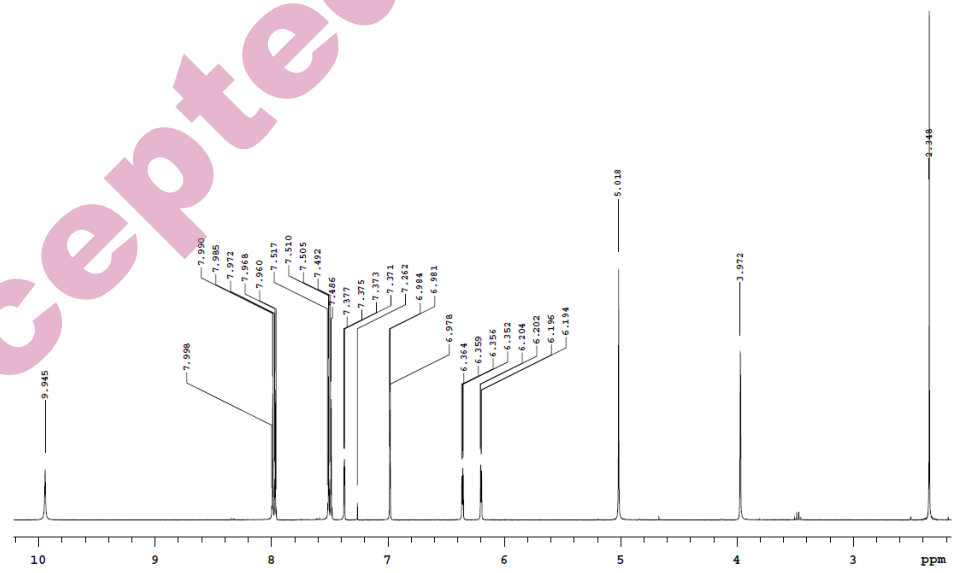
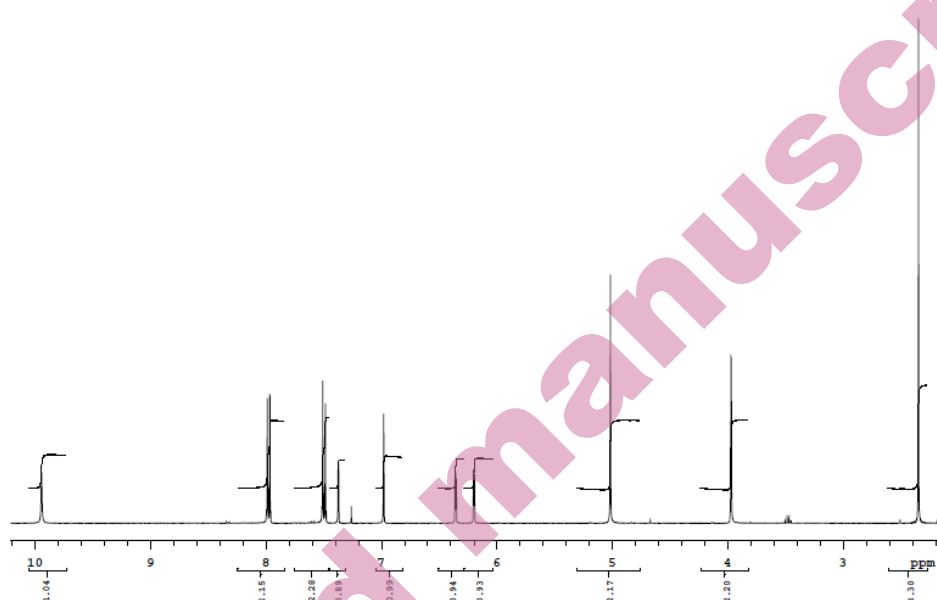
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## 2-[5-(FURAN-2-YLMETHYL)-3-METHYL-6-OXOPYRIDAZIN-1(6H)-YL]-N-(4-NITROPHENYL)ACETAMIDE (5D)







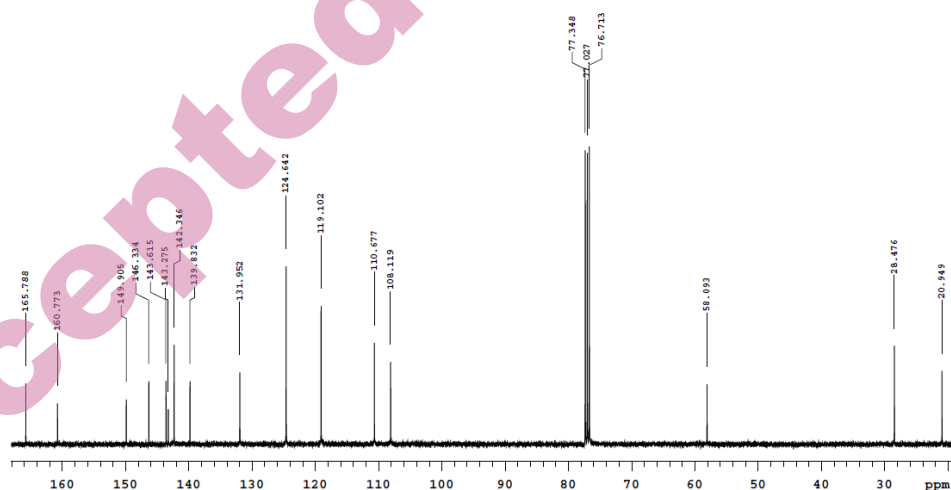
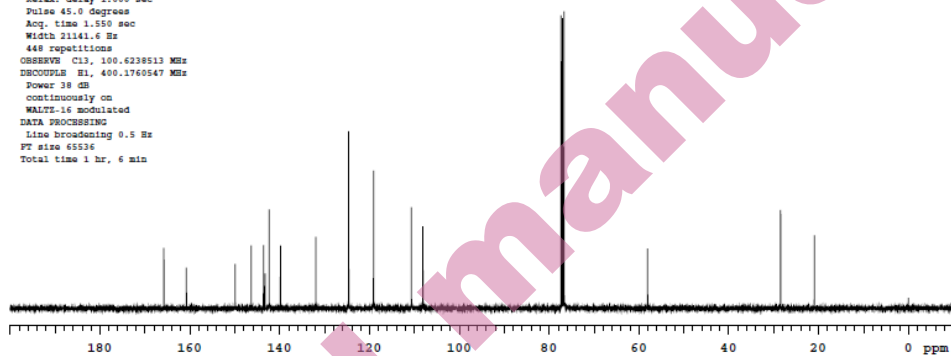


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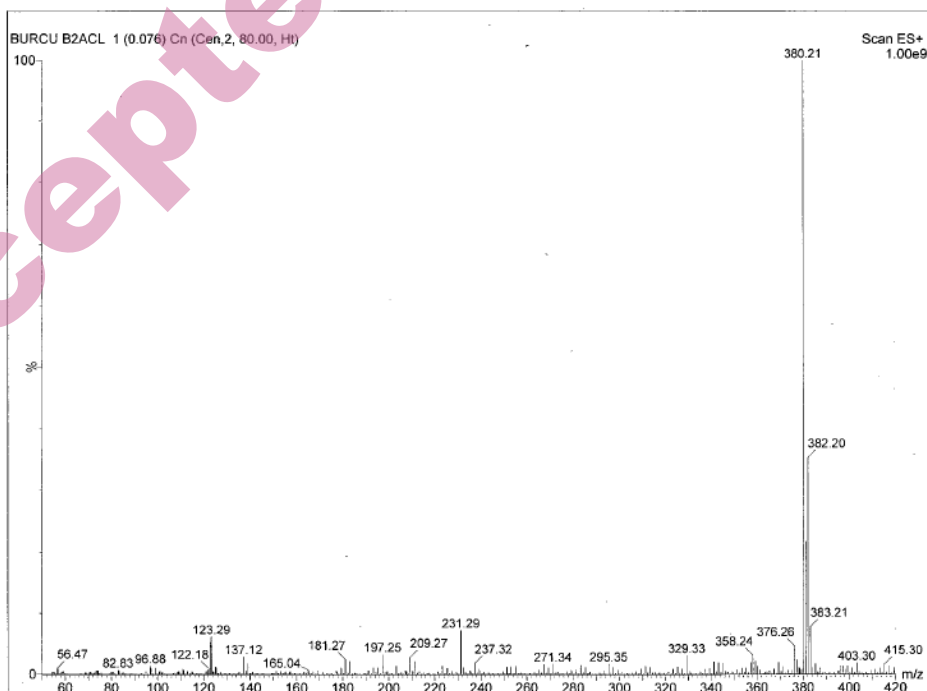
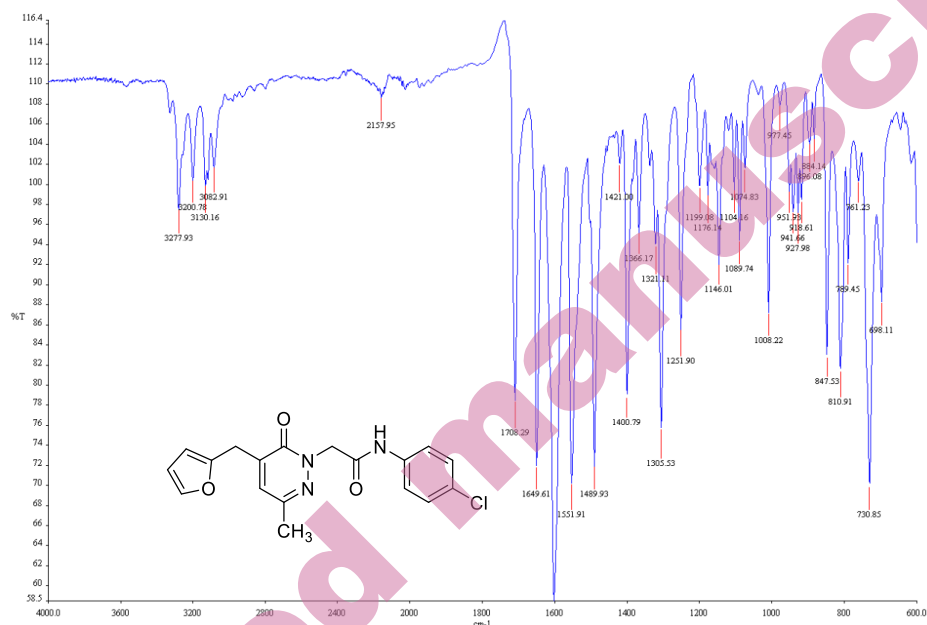
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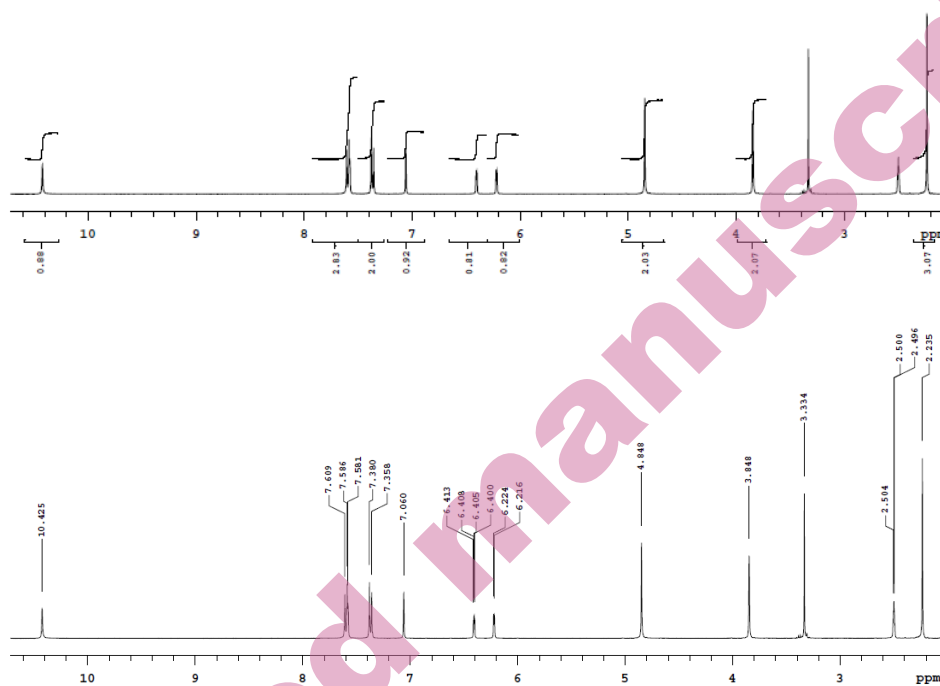
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PROCURSE H1, 400.1760547 MHz  
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Total time 1 hr, 6 min

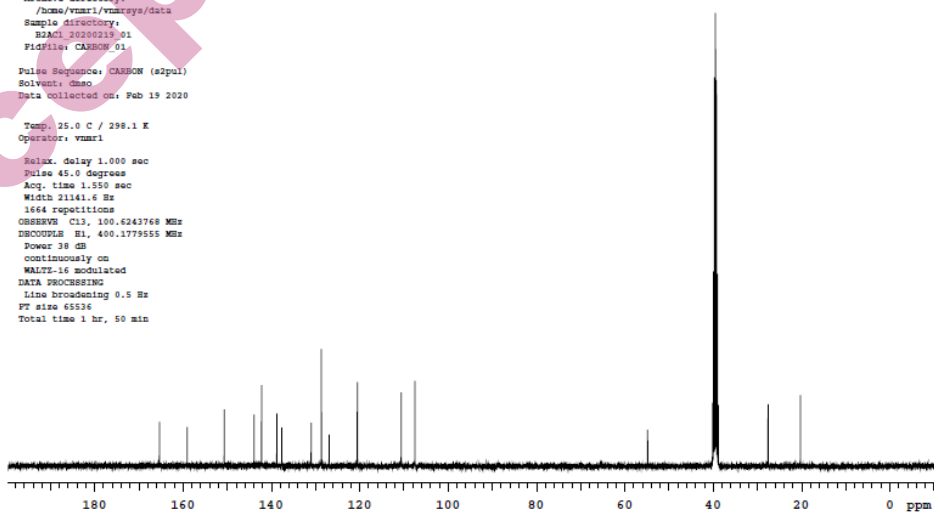


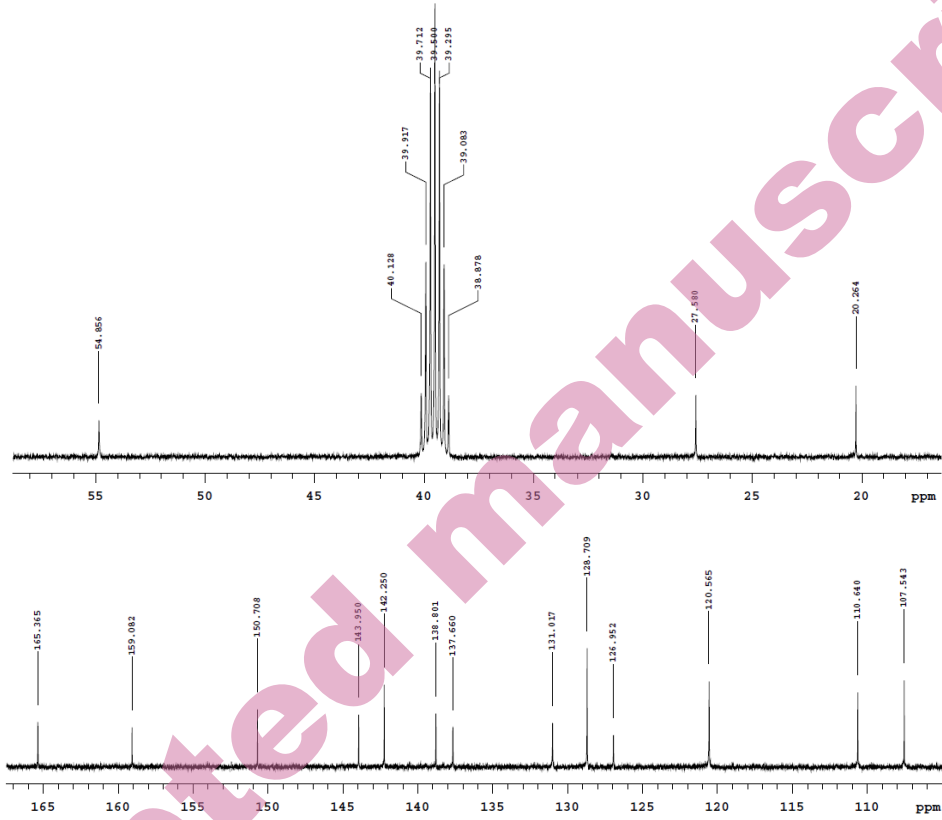
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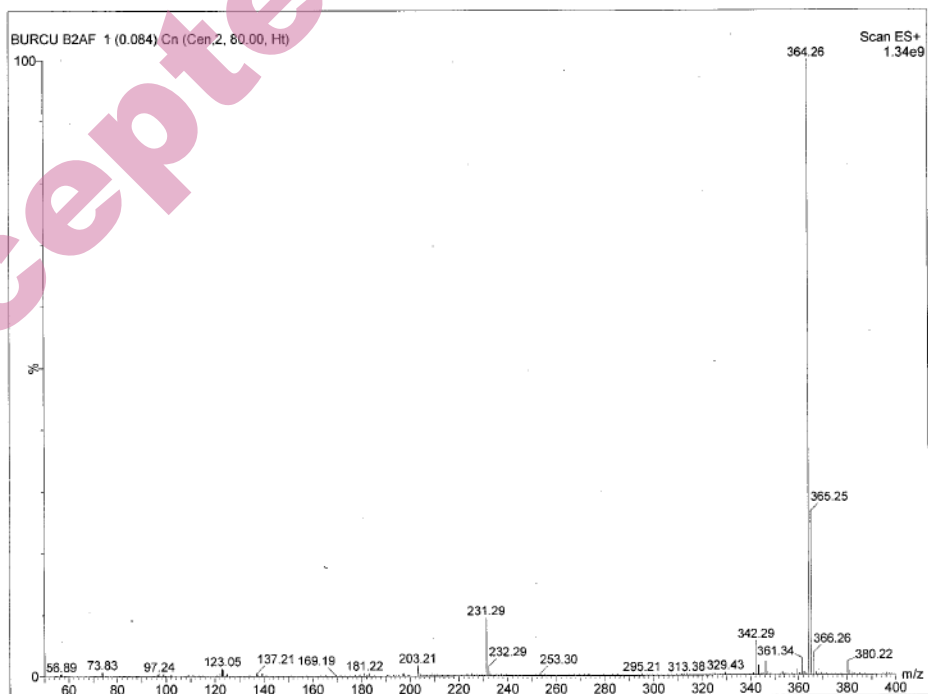
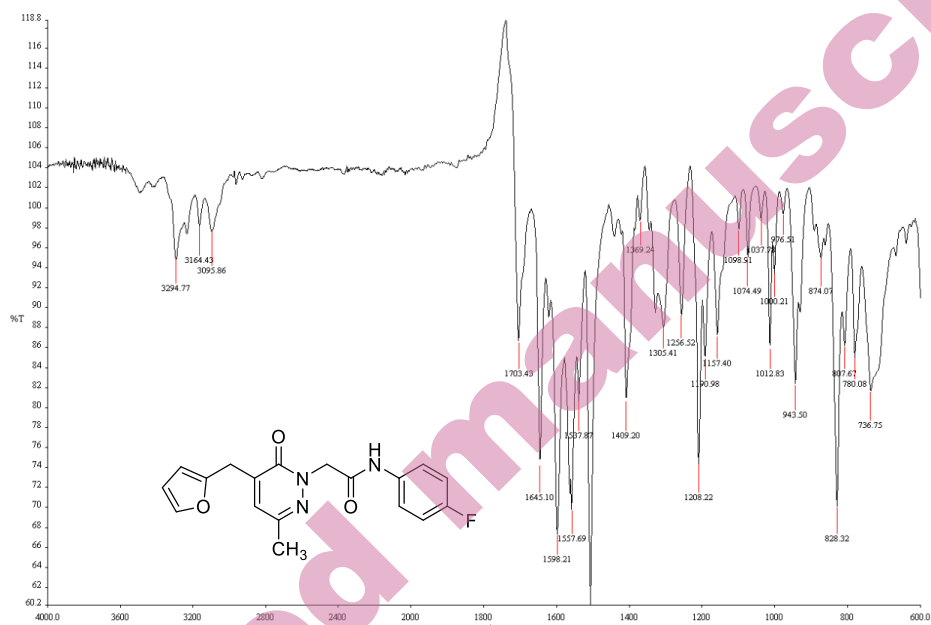


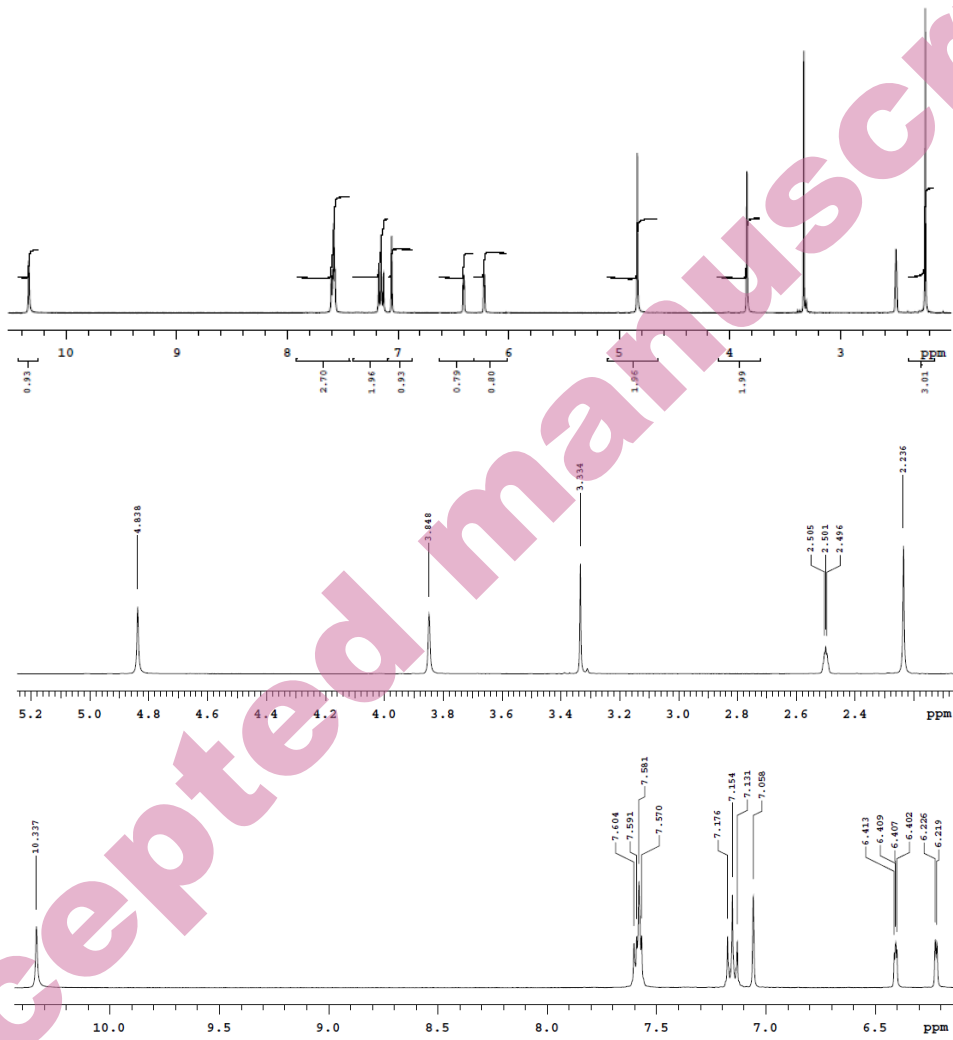
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 Data collected on: Feb 19 2020  
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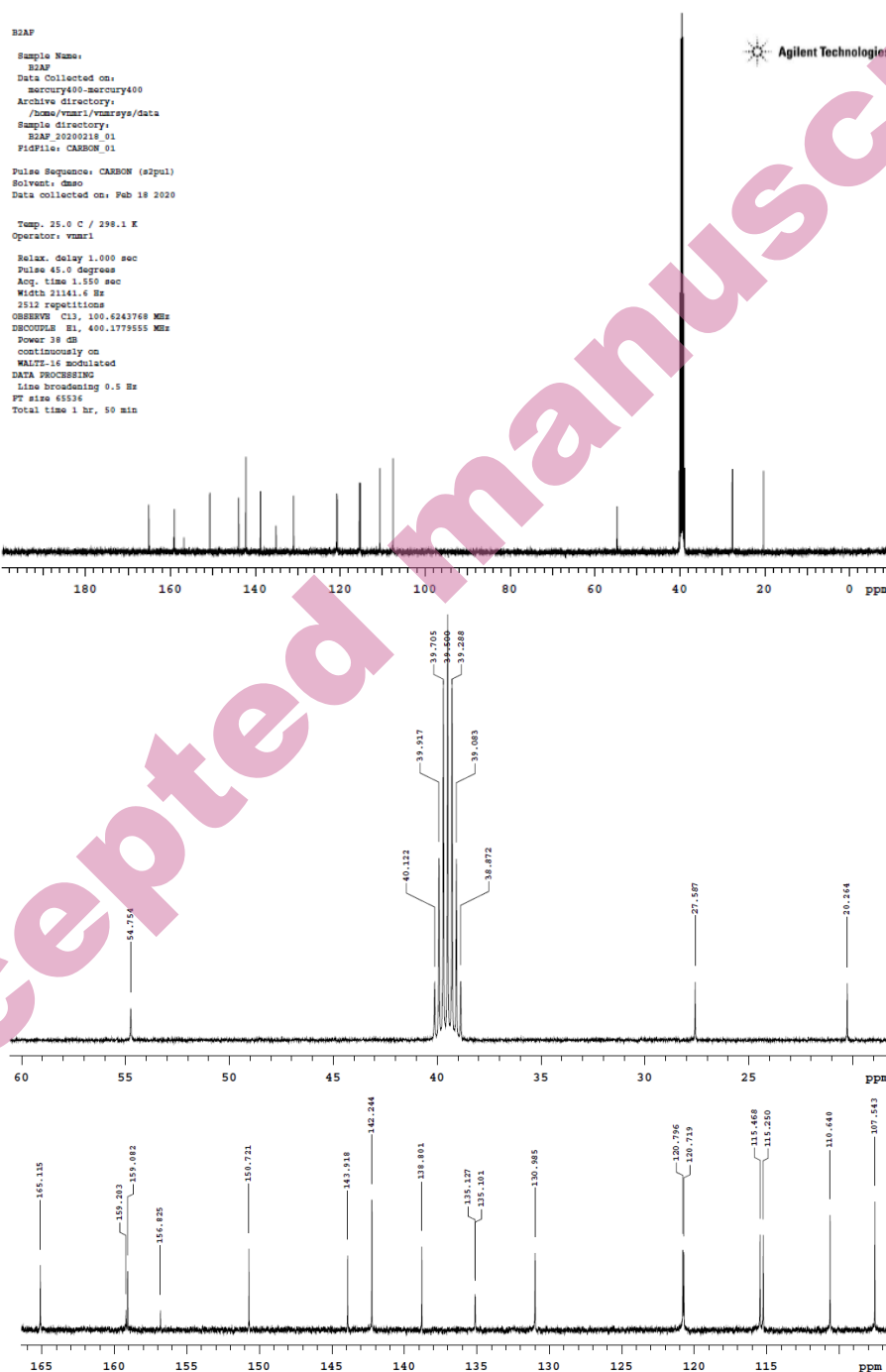




## 2-[5-(FURAN-2-YLMETHYL)-3-METHYL-6-OXOPYRIDAZIN-1(6H)-YL]-N-(4-FLUOROPHENYL)ACETAMIDE (5F)

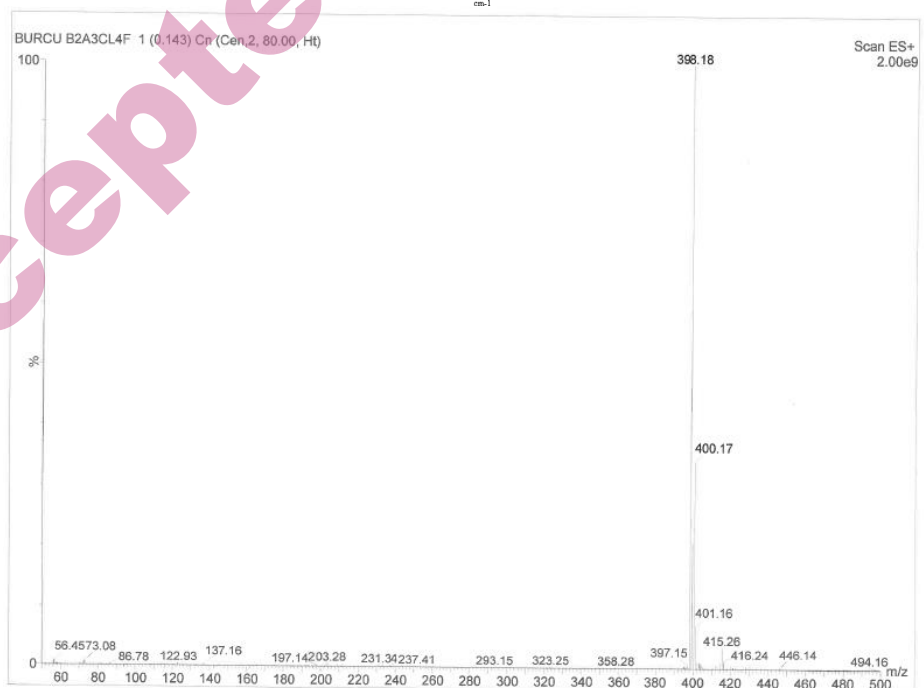
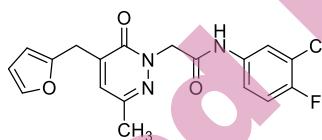
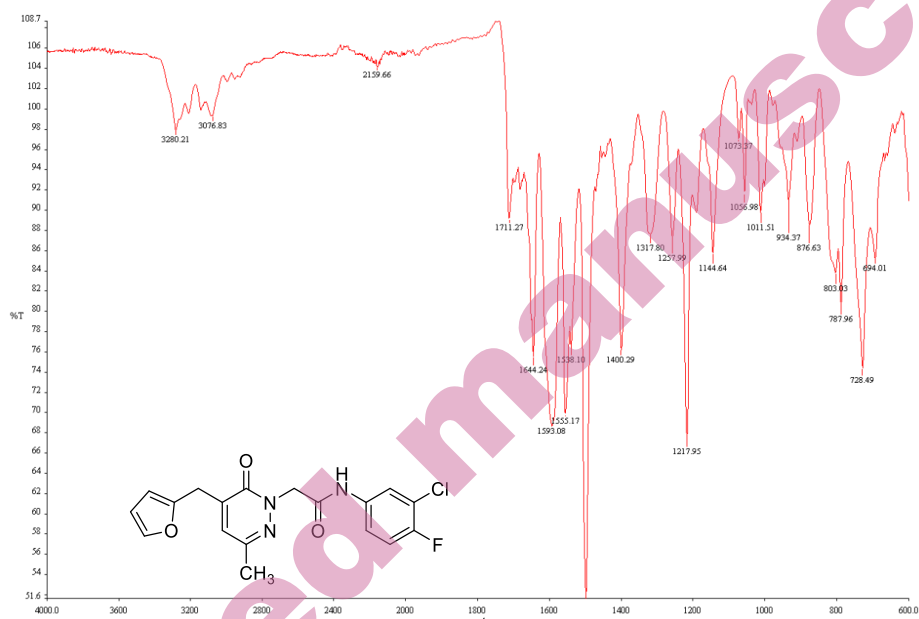


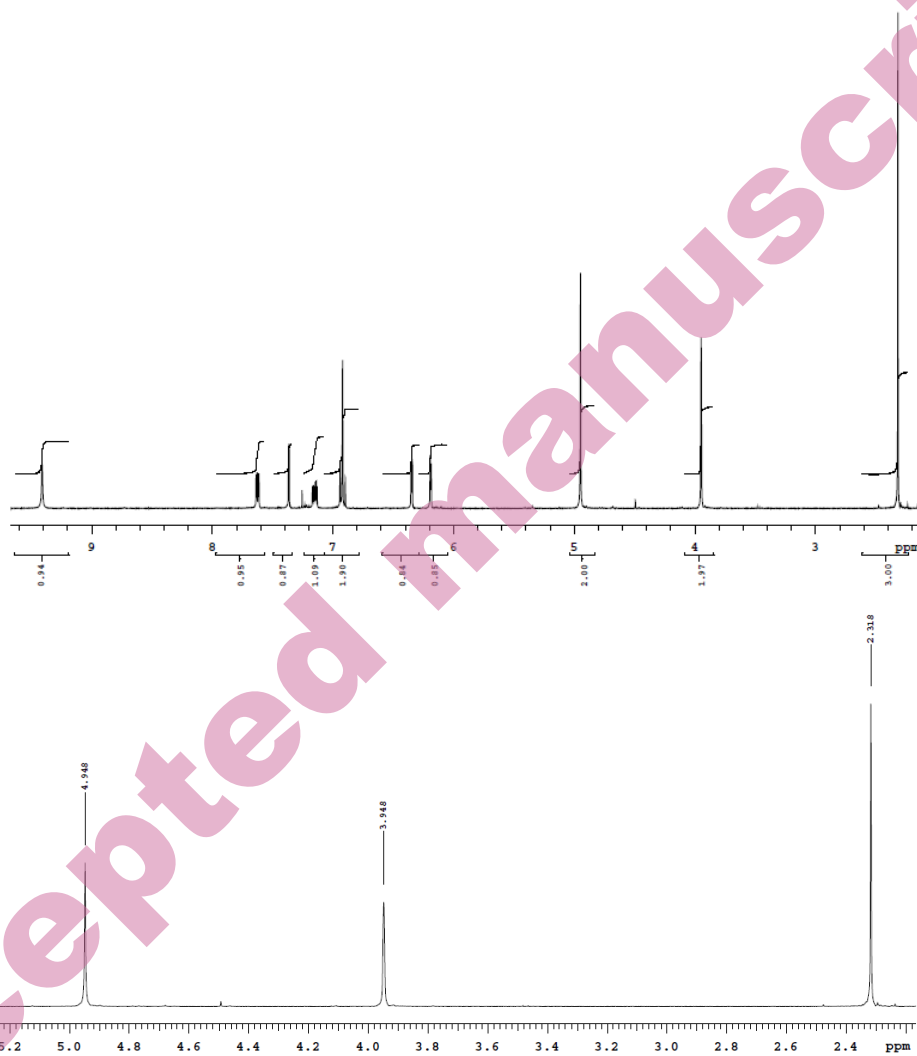


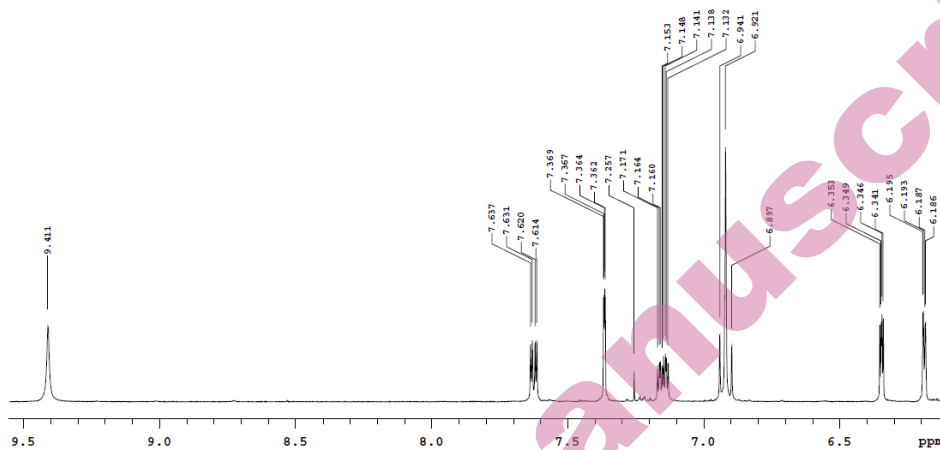




2-[5-(FURAN-2-YLMETHYL)-3-METHYL-6-OXOPYRIDAZIN-1(6H)-YL]-N-(3-CHLORO-4-FLUOROPHENYL)ACETAMIDE (5G)







82A3C14F

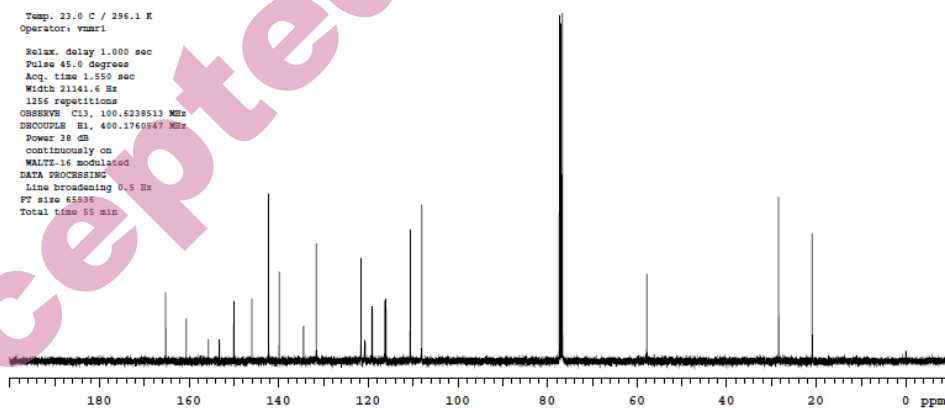
Sample Name:  
82A3C14F  
Data Collected on:  
mercury400-mercury400  
Archive directory:  
/home/vmr1/vmrsys/data  
Sample directory:  
82A3C14F 20210221\_01  
FidFile: CARBON\_01

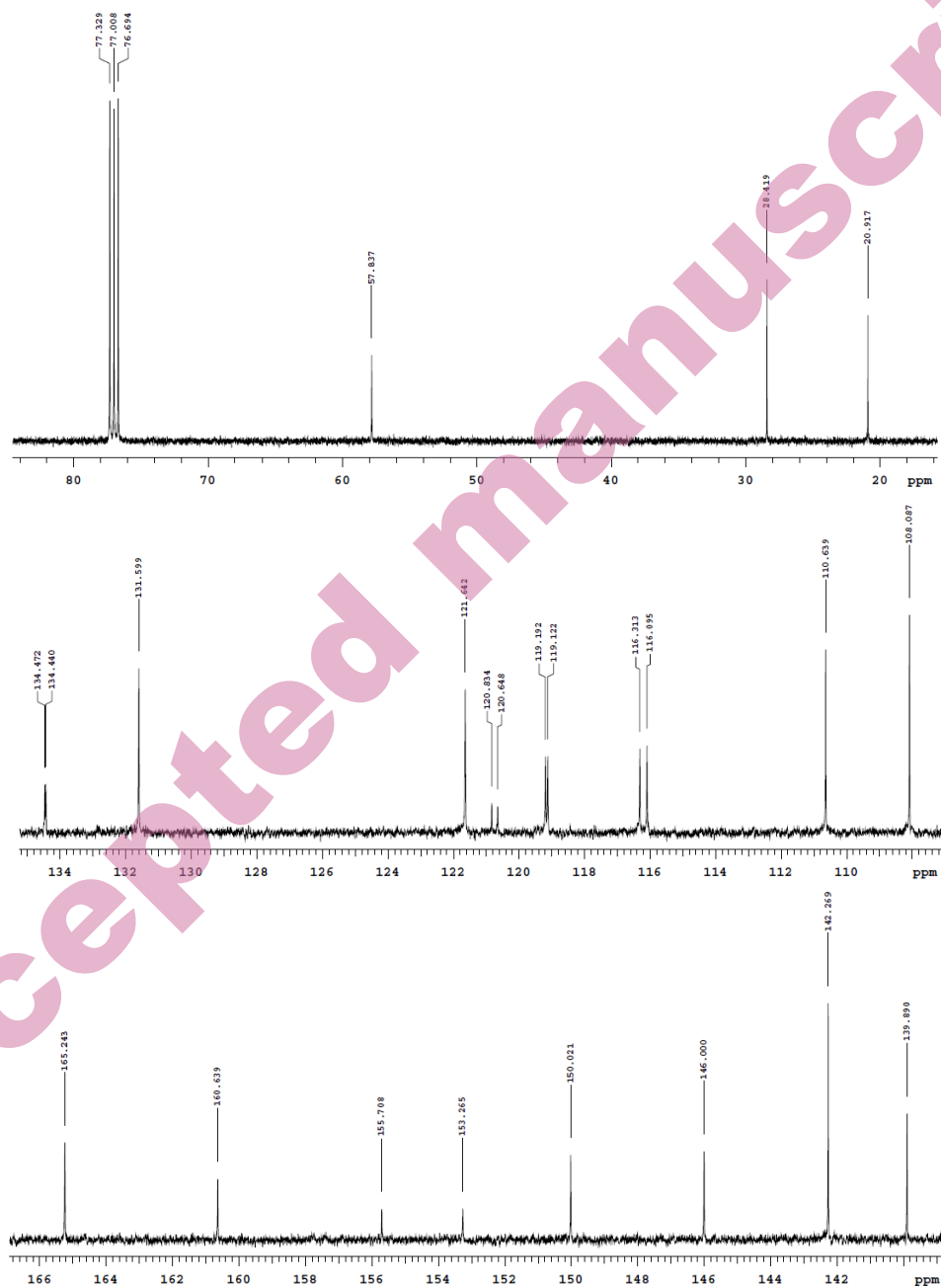


Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 21 2021

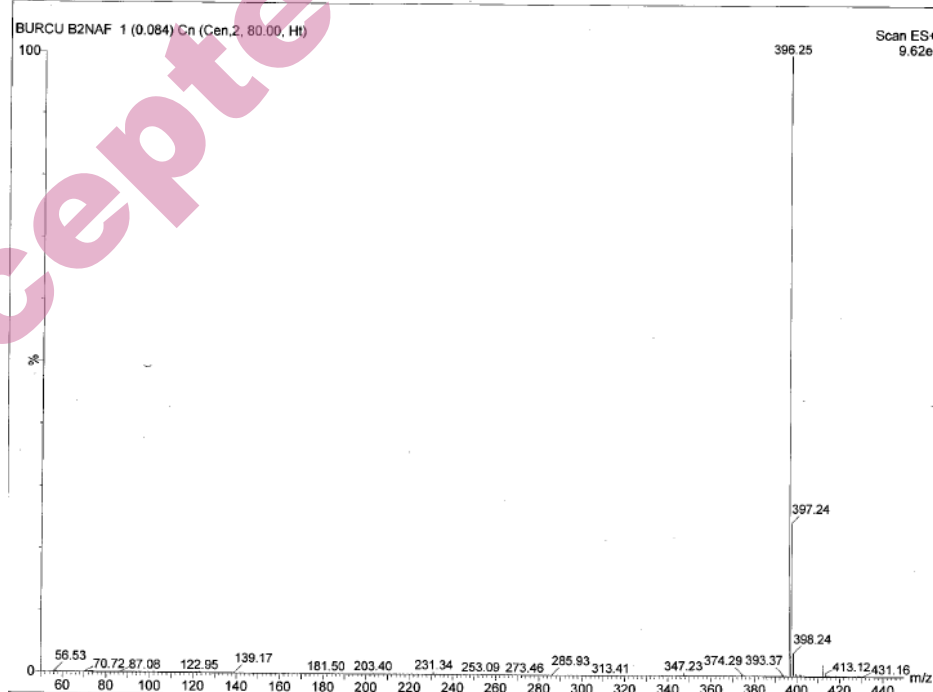
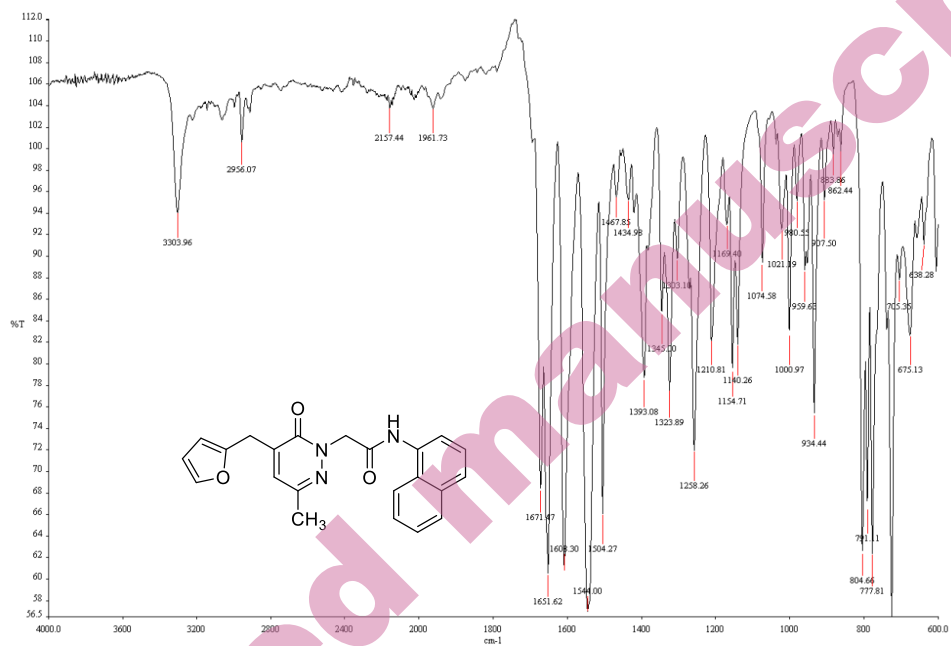
Temp. 23.0 C / 296.1 K  
Operator: vmr1

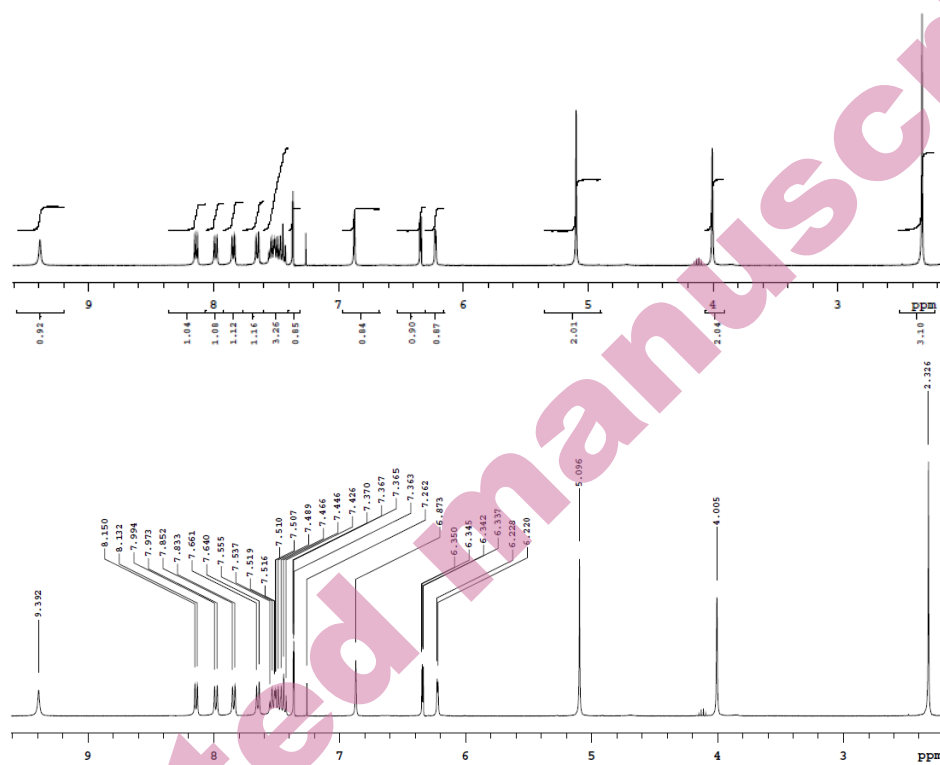
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.950 sec  
Width 21141.6 Hz  
1256 repetitions  
OBSERVE C13, 100.6238513 MHz  
DECOUPLE H1, 400.1760547 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
F2 size 65536  
Total time 55 min



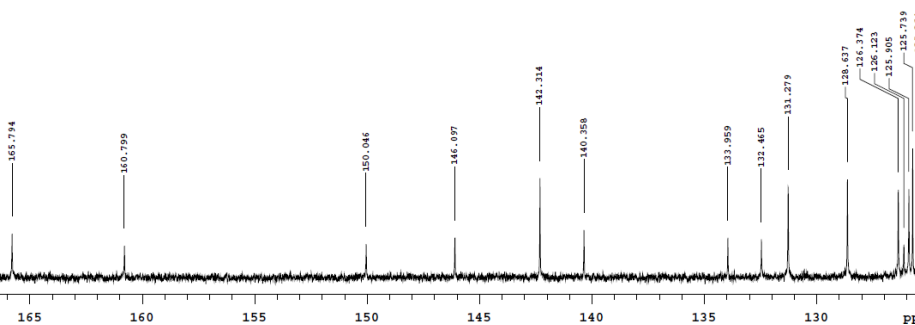
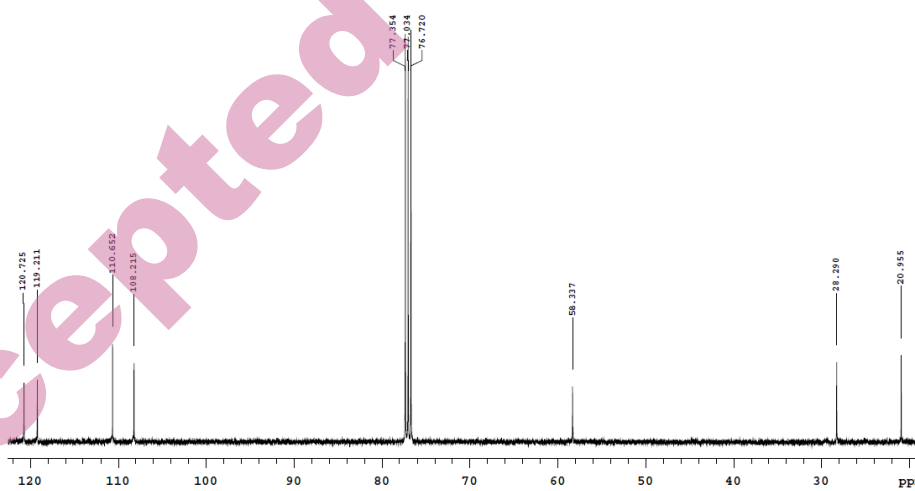
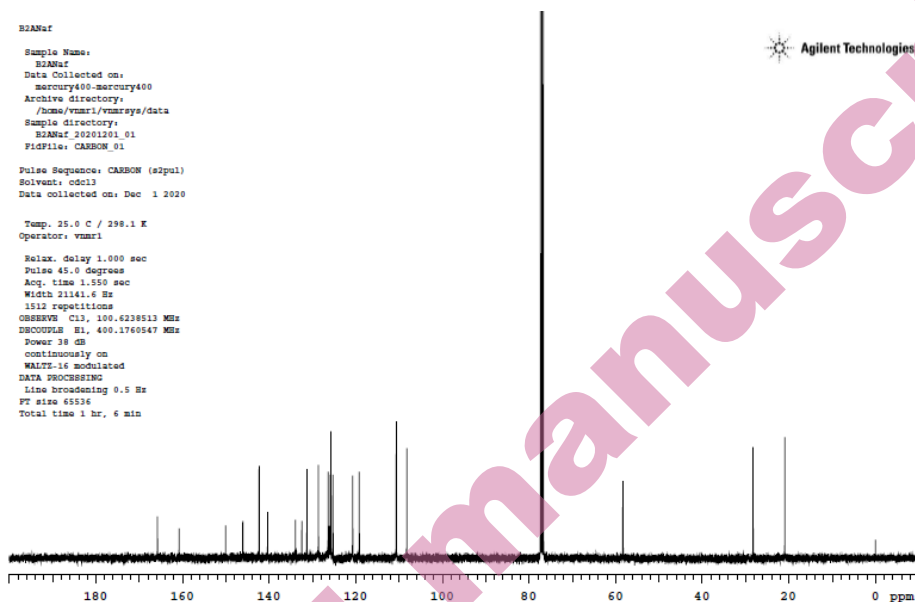


2-[5-(FURAN-2-YLMETHYL)-3-METHYL-6-OXOPYRIDAZIN-1(6H)-YL]-N-(NAPHTHALEN-1-YL)ACETAMIDE (5H)



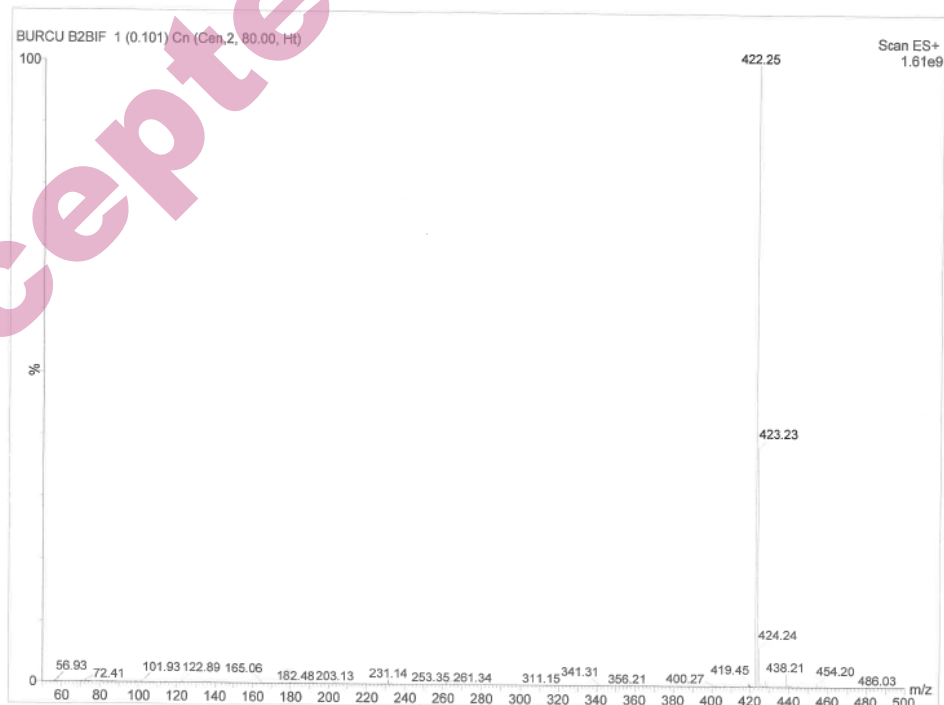
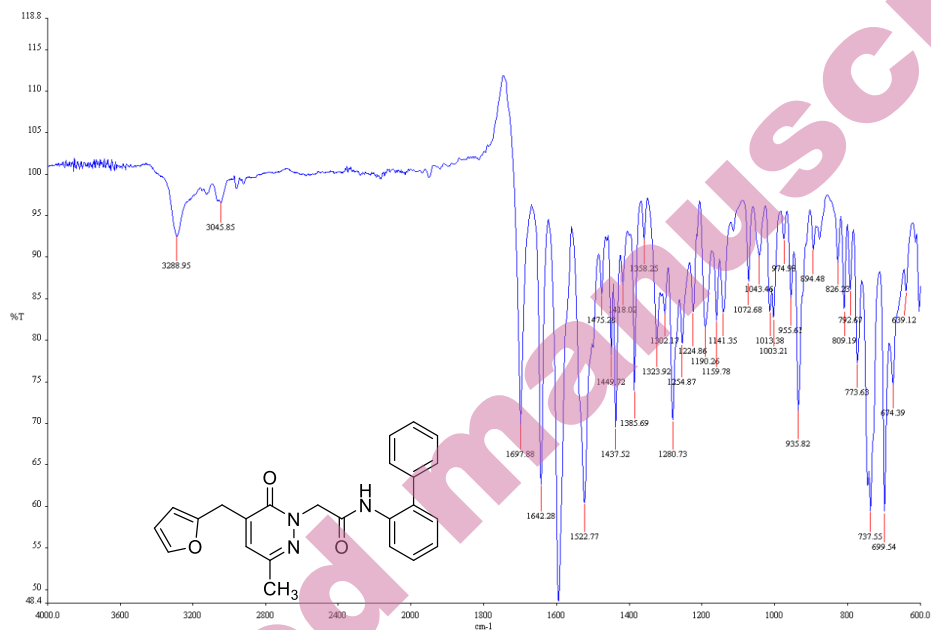


E2ANwf  
 Sample Name:  
 E2ANwf  
 Data Collected on:  
 mercury400-mercury400  
 Archive directory:  
 /home/vmr1/vmrays/data  
 Sample directory:  
 E2ANwf\_20201201\_01  
 File: CARBON\_01  
 Pulse Sequence: CARBON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Dec 1 2020  
 Temp: 25.0 C / 298.1 K  
 Operator: vmr1  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.550 sec  
 Width 21141.6 Hz  
 1512 repetitions  
 OBSERVE Ch3, 100.6238513 MHz  
 DECOUPLE E1, 400.1760547 MHz  
 Power 38 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 1 hr, 6 min

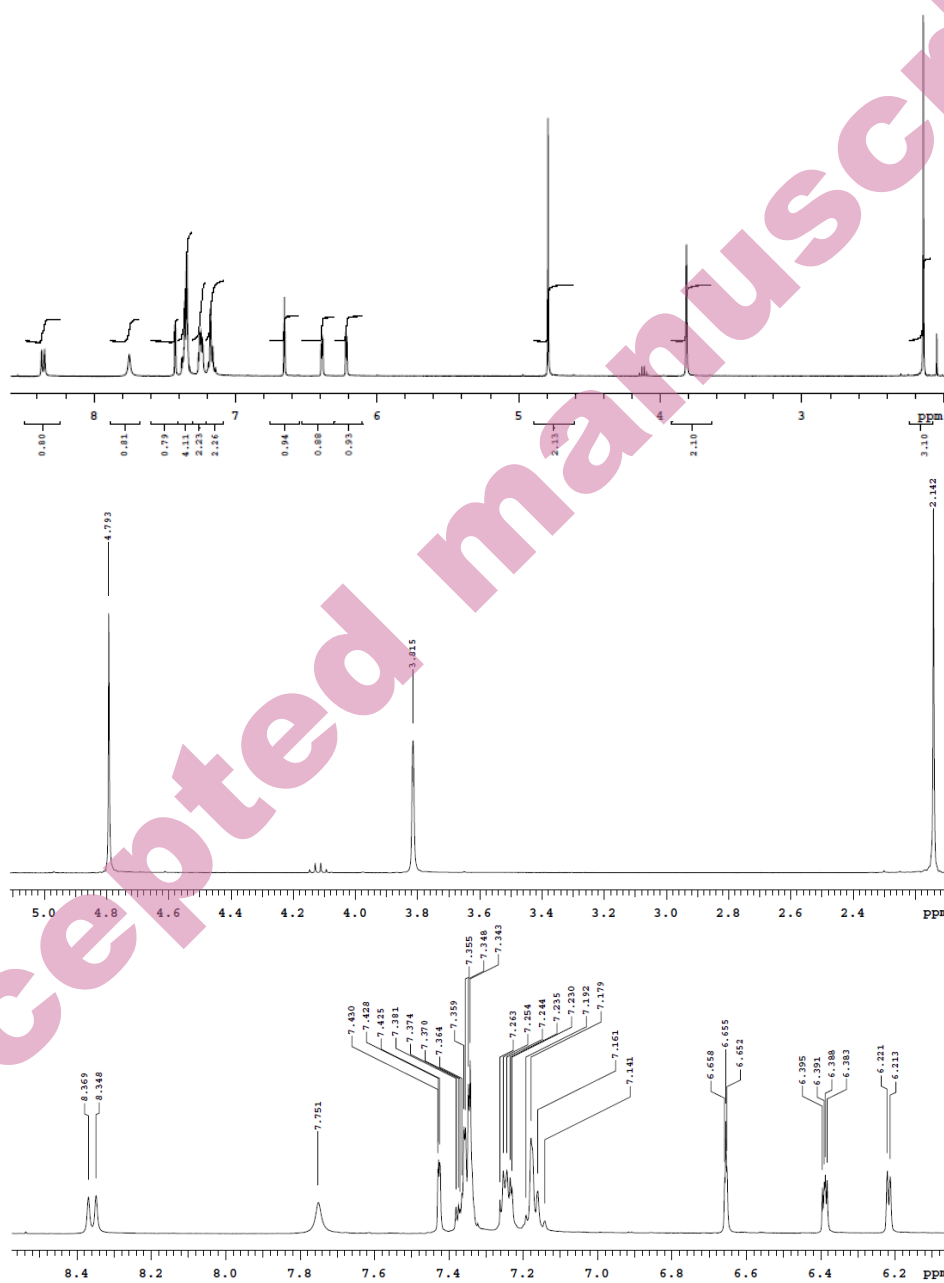


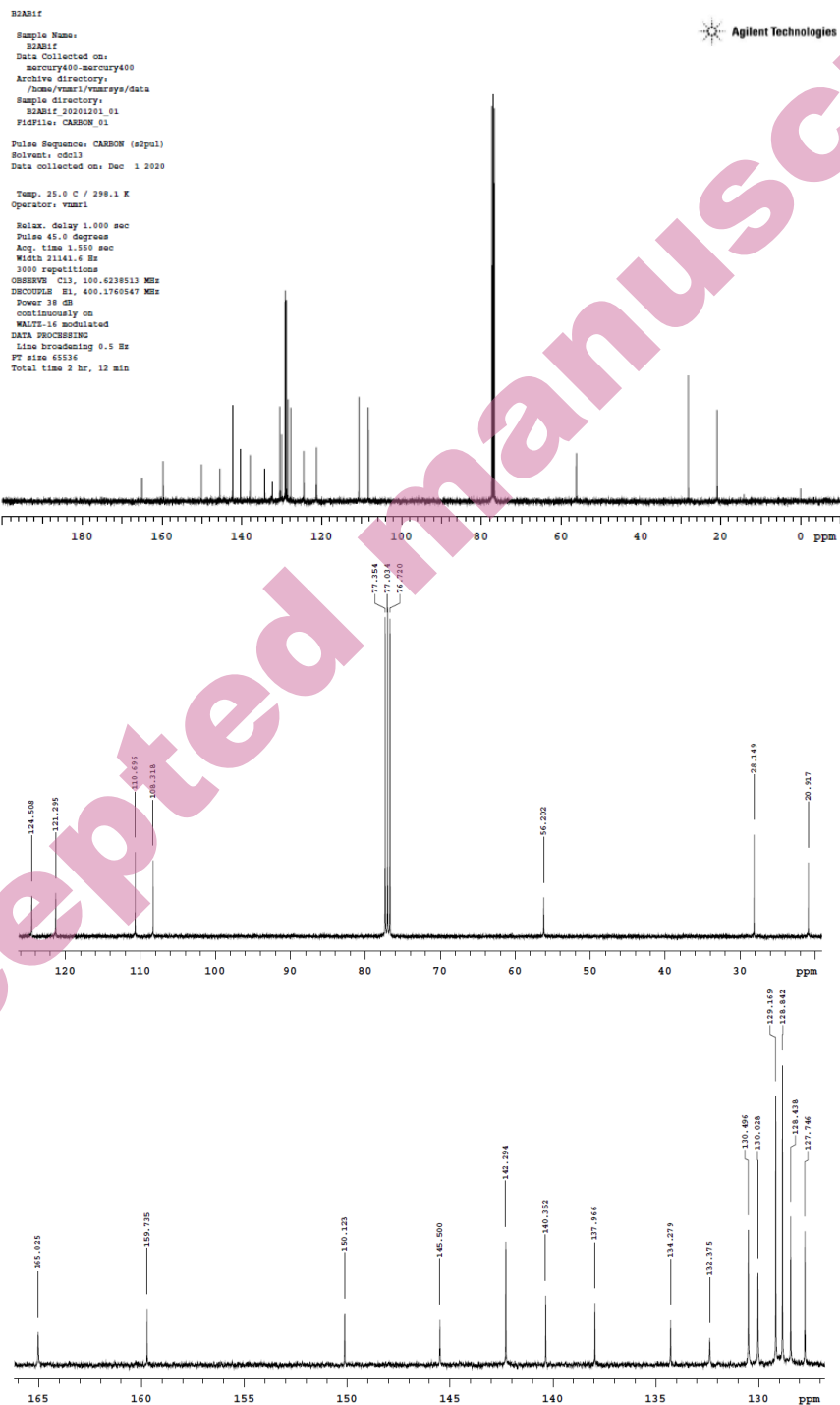
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## 2-[5-(FURAN-2-YLMETHYL)-3-METHYL-6-OXOPYRIDAZIN-1(6H)-YL]-N-((1,1'-BIPHENYL)-2-YL)ACETAMIDE (5I)

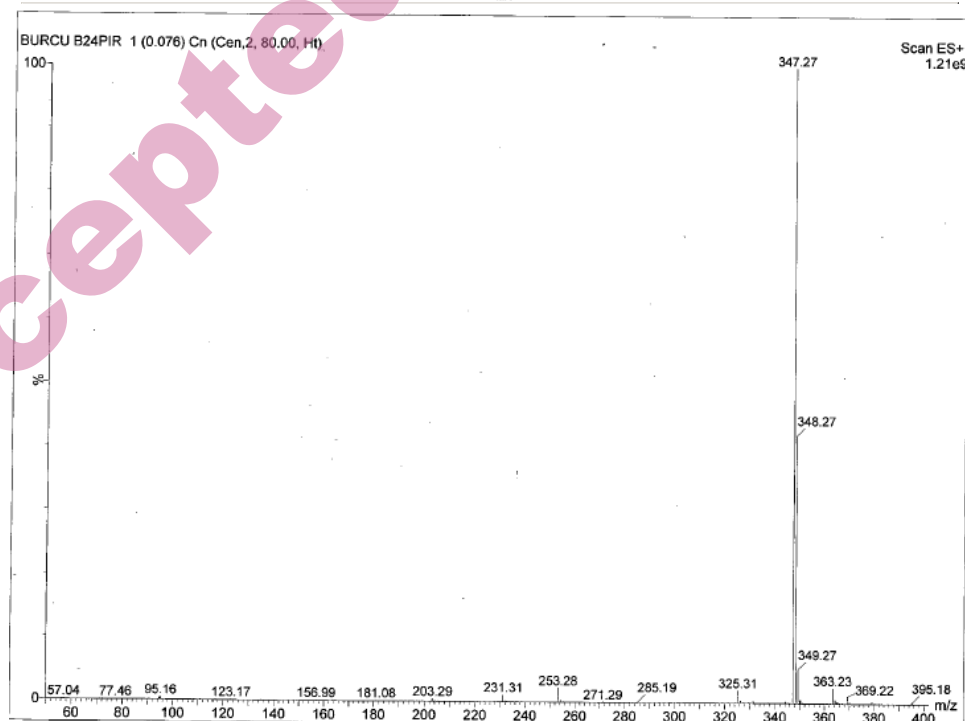
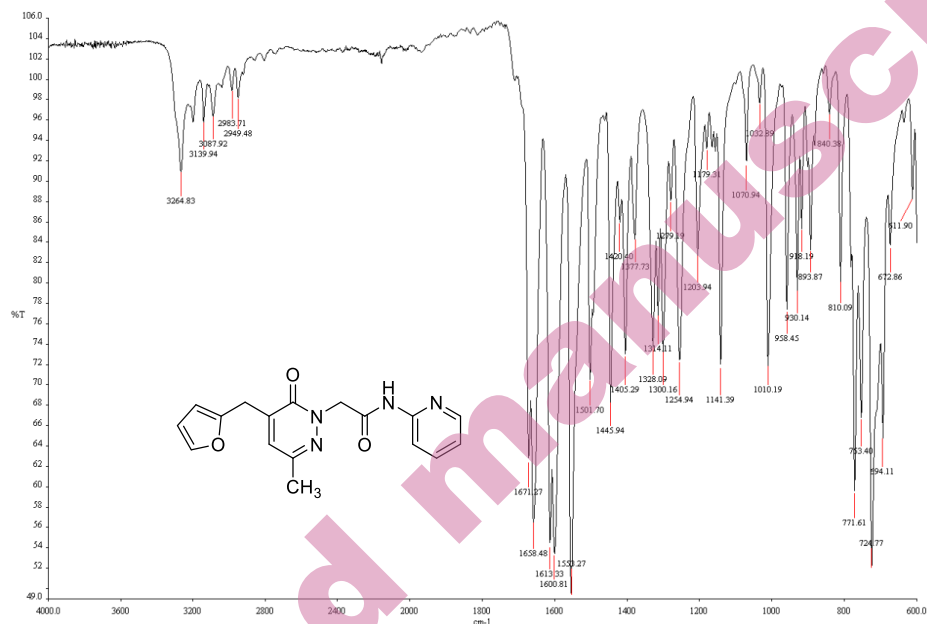


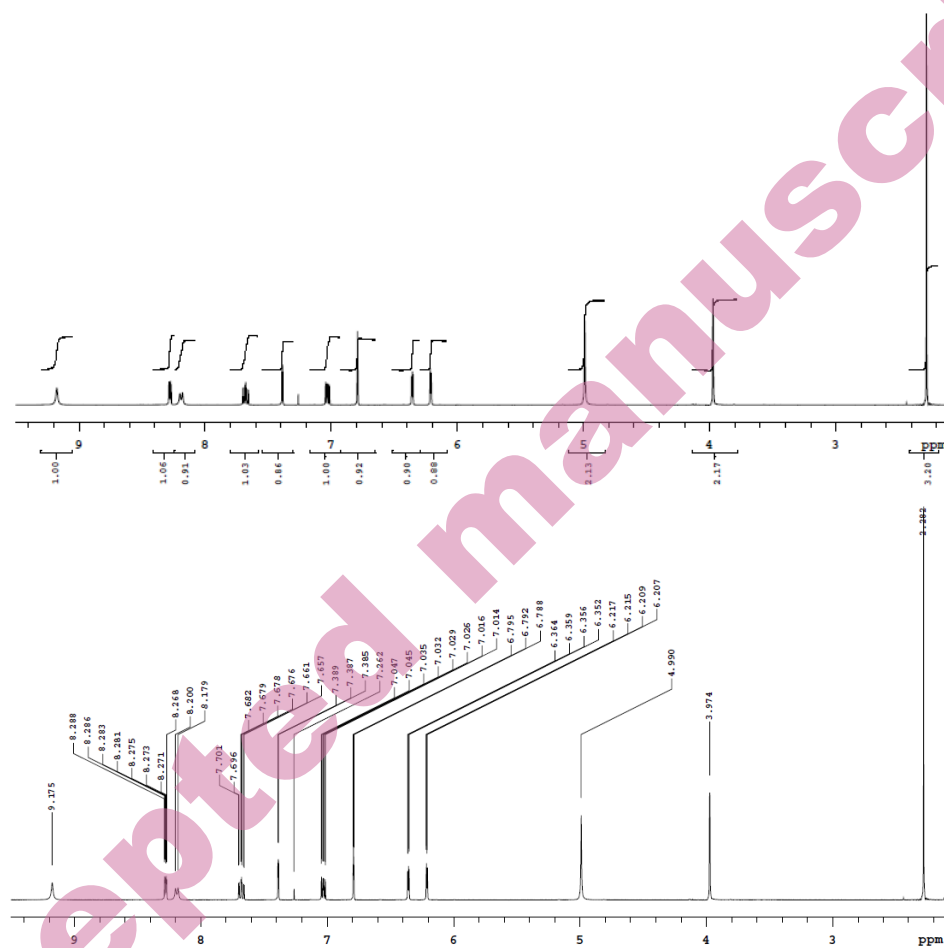






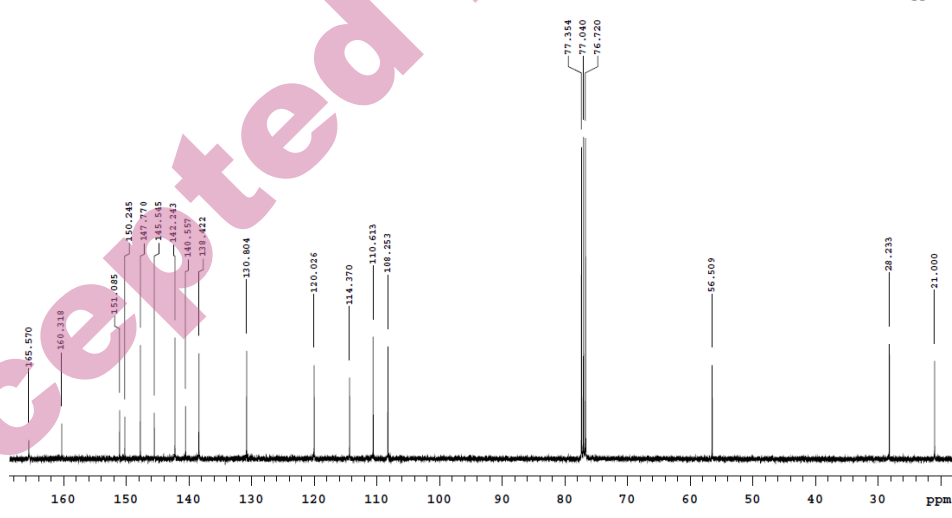
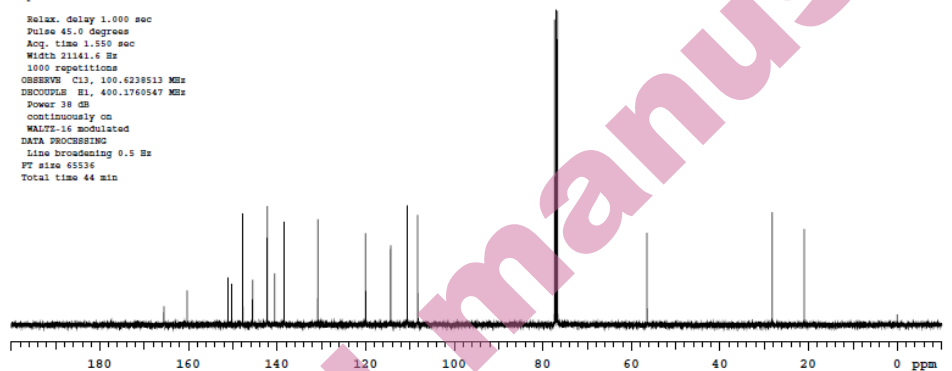
2-[5-(FURAN-2-YLMETHYL)-3-METHYL-6-OXOPYRIDAZIN-1(6H)-YL]-N-(PYRIDIN-2-YL)ACETAMIDE (5J)



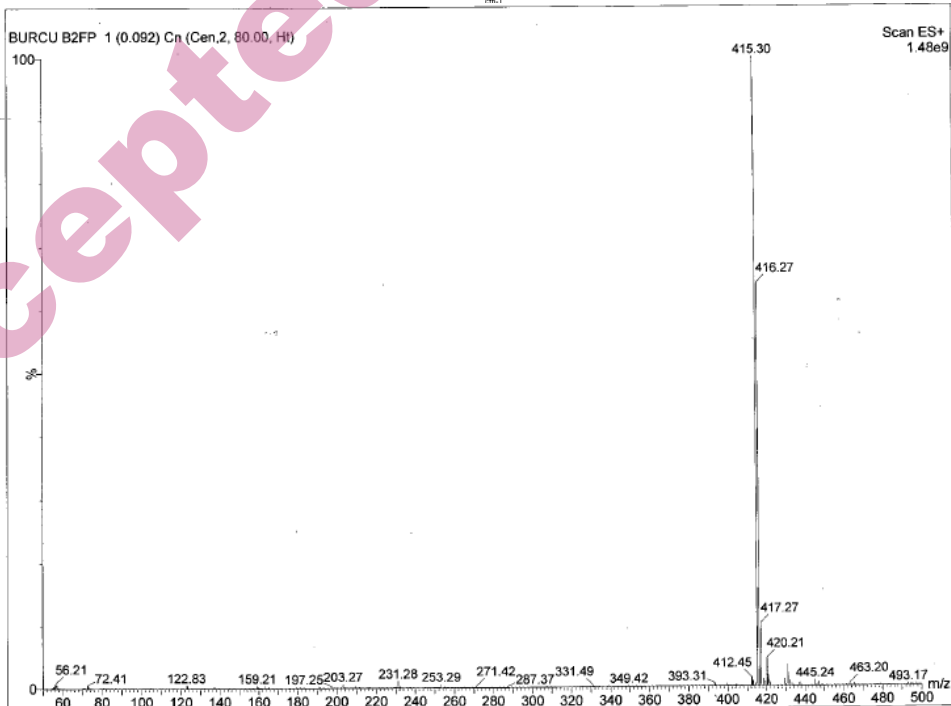
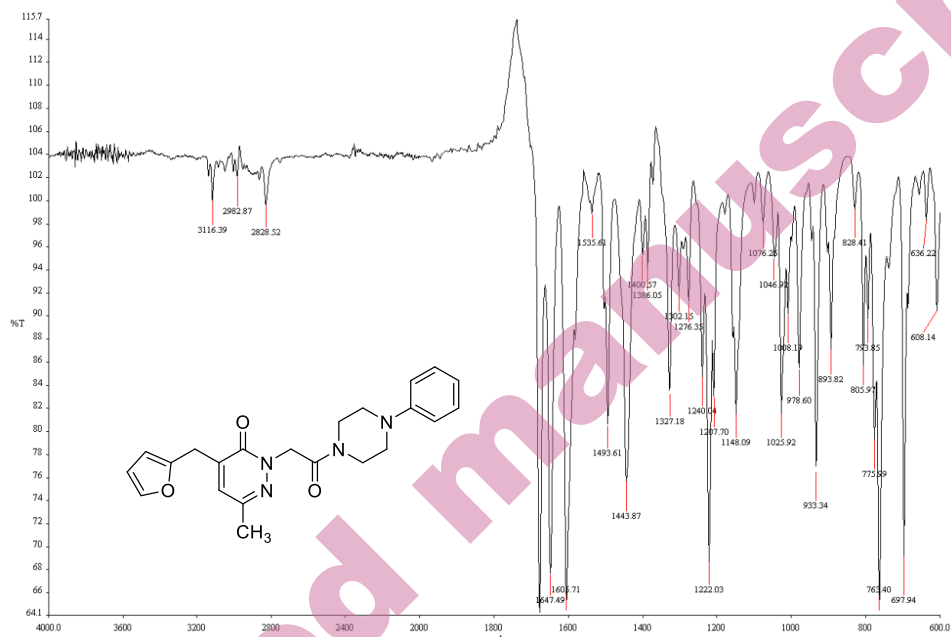


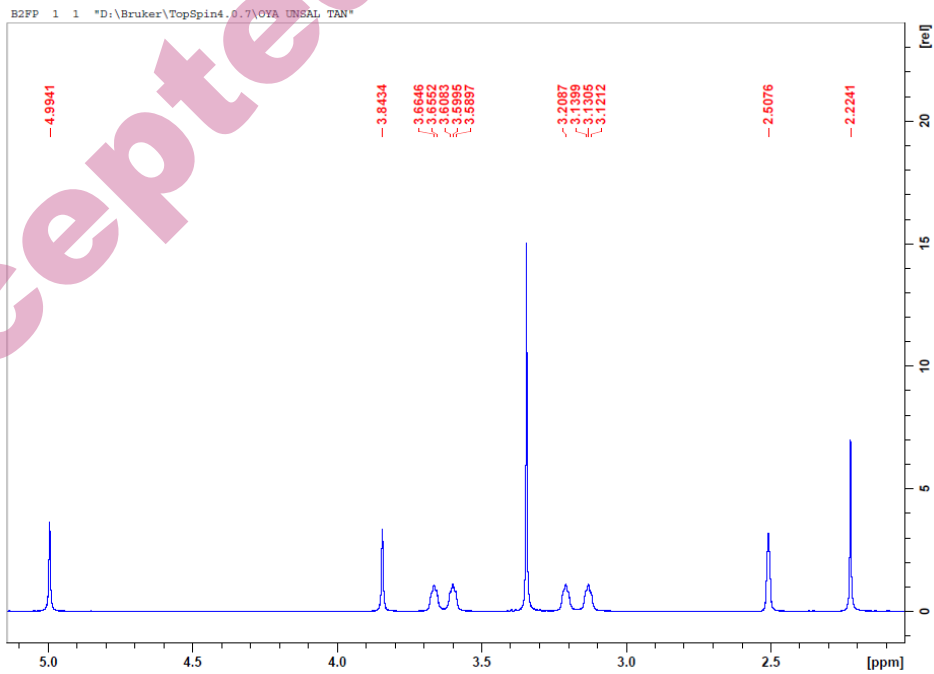
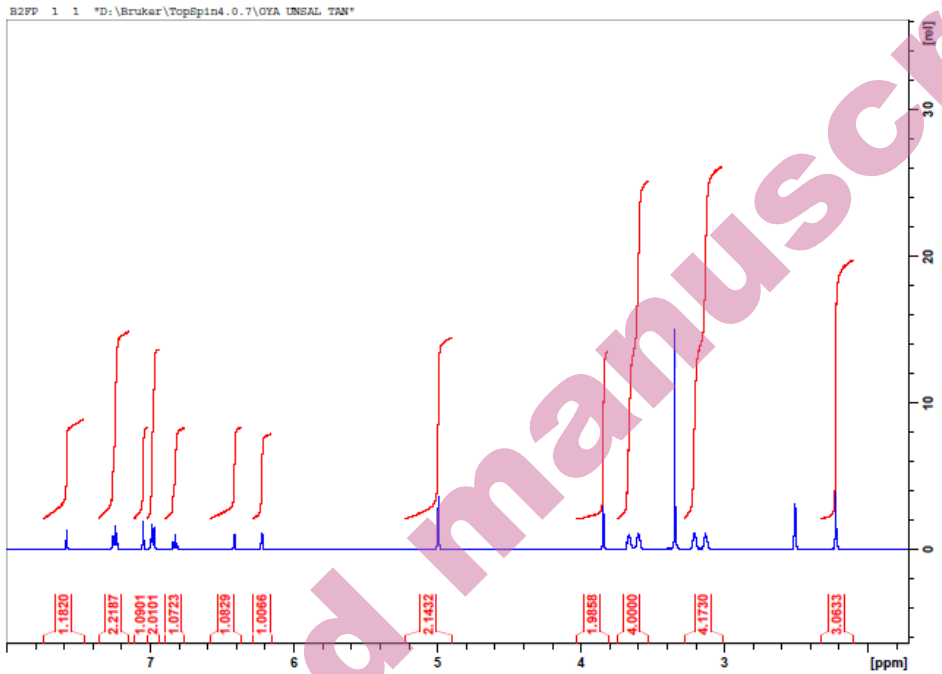


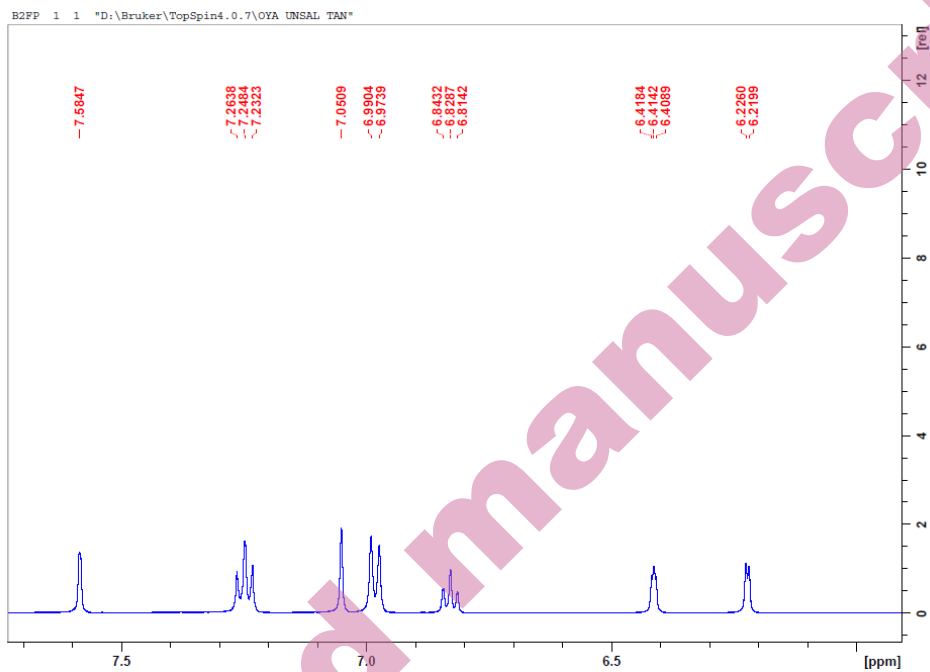
**BJAPir**  
 Sample Name:  
 BJAPir  
 Data Collected on:  
 mercury400-mercury400  
 Archive directory:  
 /home/vmari/vmarrays/data  
 Sample directory:  
 BJAPir\_20201201\_01  
 Fidfile: CARBON\_01  
 Pulse Sequence: CARBON (s2ps1)  
 Solvent: cdcl3  
 Data collected on: Dec 1 2020  
 Temp. 25.0 C / 298.1 K  
 Operator: vmari  
 Relax delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.550 sec  
 Width 21141.6 Hz  
 1000 repetitions  
 OBSERVE C13, 100.6238513 MHz  
 DECOUPLE H1, 400.1760547 MHz  
 Power 38 dB  
 continuously on  
 WALTZ-16 Modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 44 min



## 4-(FURAN-2-YLMETHYL)-6-METHYL-2-[2-OXO-2-(4-PHENYLPIPERAZIN-1-YL)ETHYL]PYRIDAZIN-3(2H)-ONE (6A)



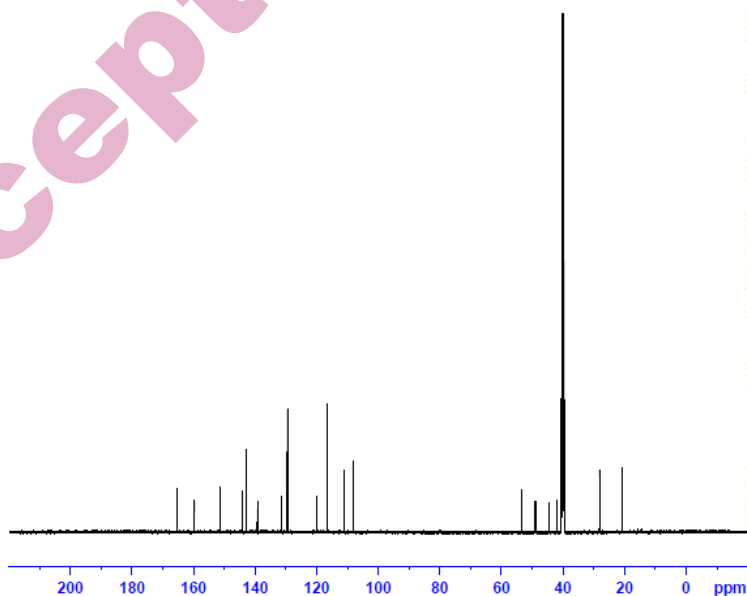




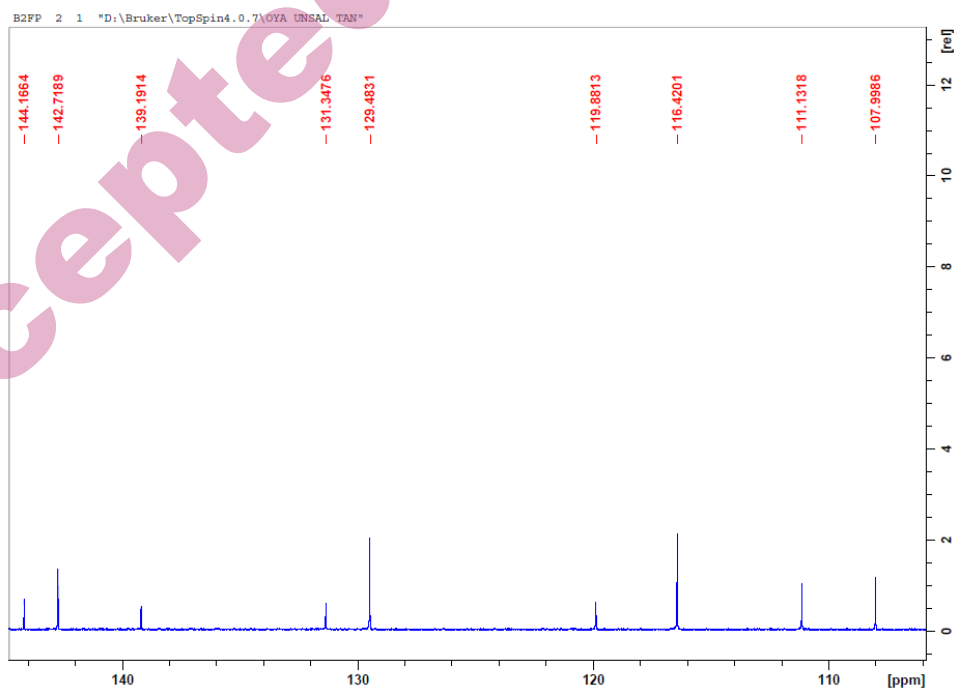
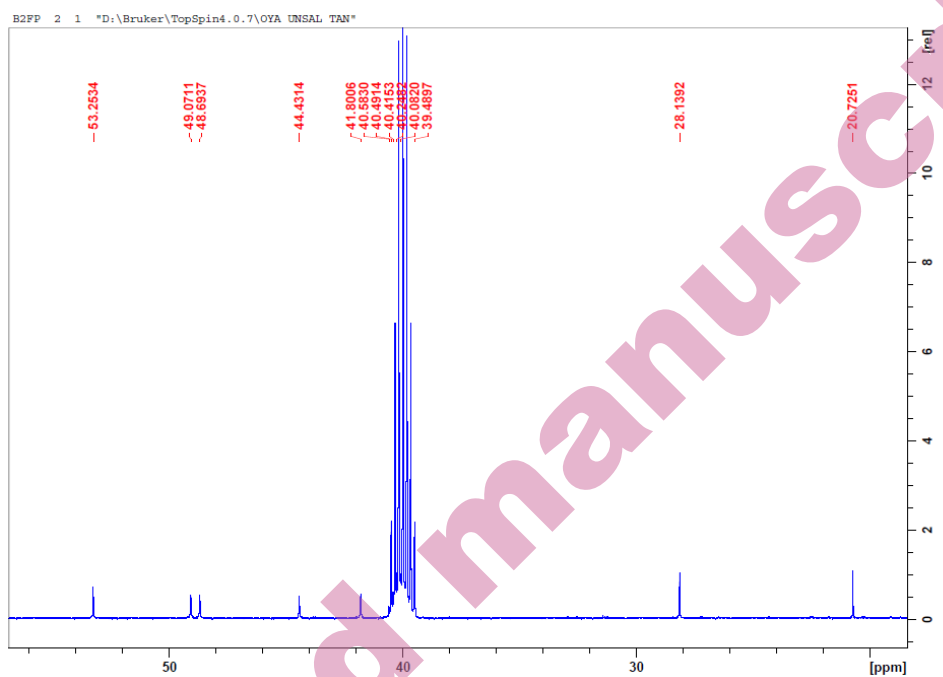
Current Data Parameters  
 NAME B2FP  
 EXPNO 2  
 PROCNO 1

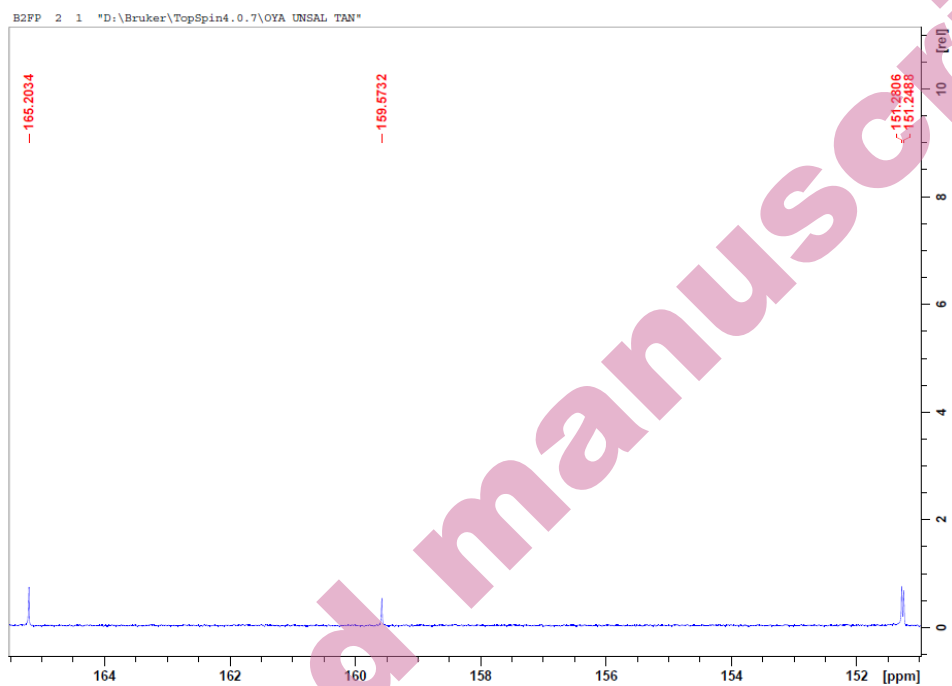
F2 - Acquisition Parameters  
 Date\_ 20201022  
 Time 10.30 h  
 INSTRUM Avance  
 PROBRD Z151574\_0038 (   
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1500  
 DS 4  
 SWH 30120.482 Hz  
 FIDRES 0.919204 Hz  
 AQ 1.0878977 sec  
 RG 101  
 LW 16.600 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 125.7703643 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 85.1809976 W  
 SFO2 500.1320005 MHz  
 NUC2 1H  
 CPDPRG2 waltz65  
 PCPD2 80.00 usec  
 PLW2 24.04299927 W  
 PLW12 0.24043000 W  
 PLW13 0.12093000 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7577885 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

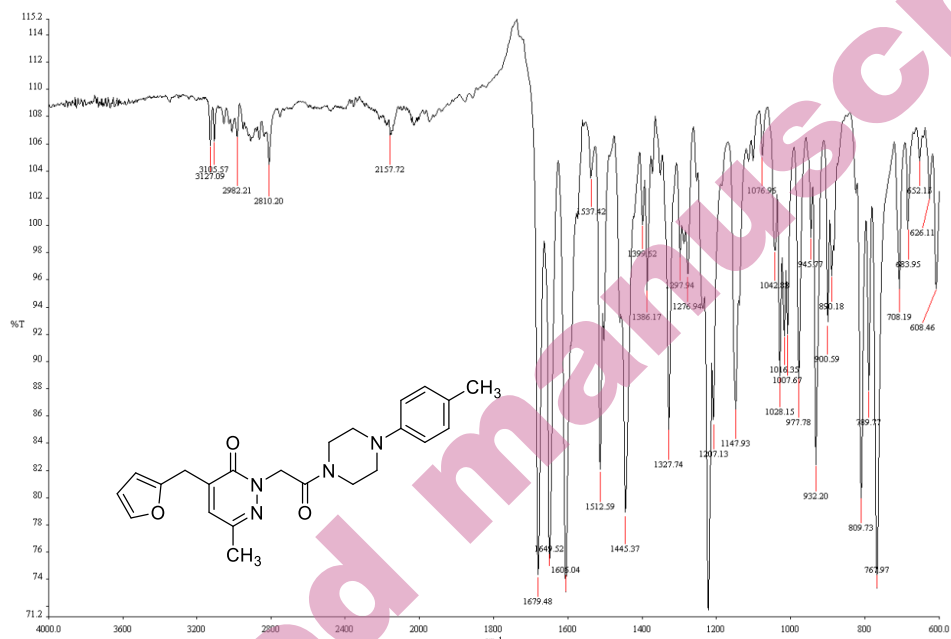


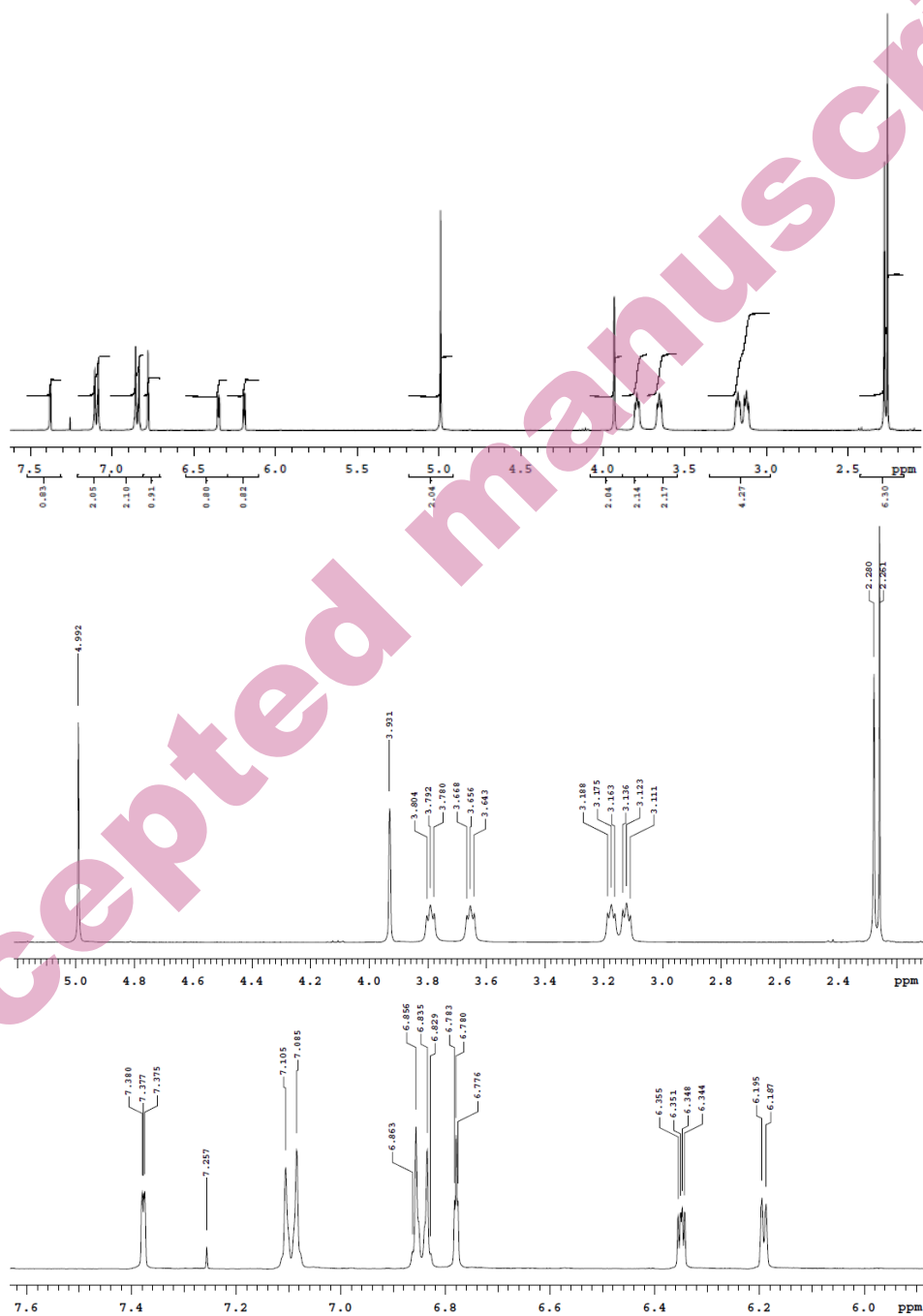






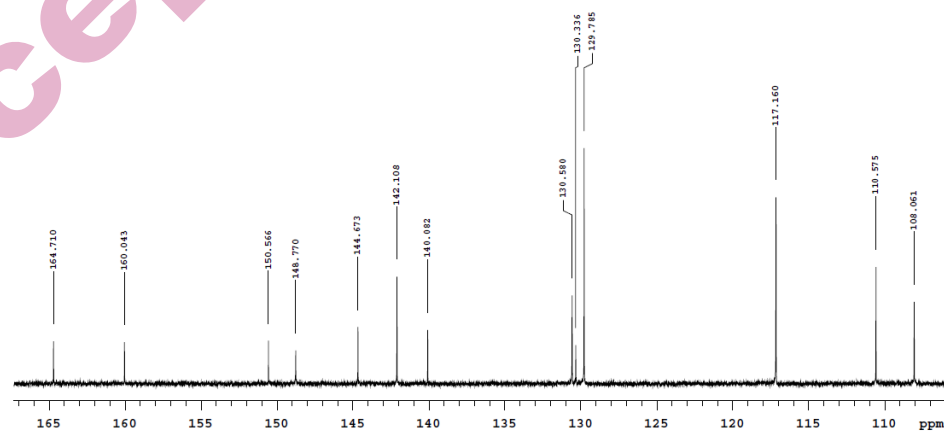
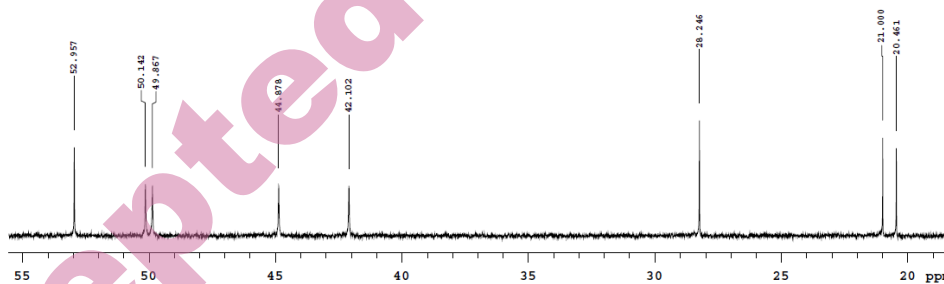
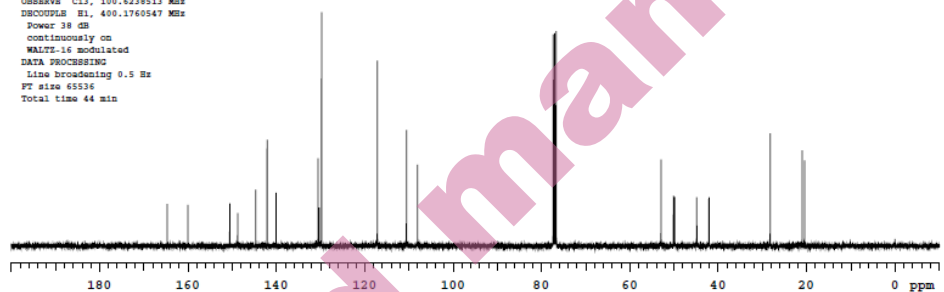
4-(FURAN-2-YLMETHYL)-6-METHYL-2-[2-OXO-2-(4-(4-METHYLPHENYL)PIPERAZIN-1-YL)ETHYL]PYRIDAZIN-3(2H)-ONE (6B)



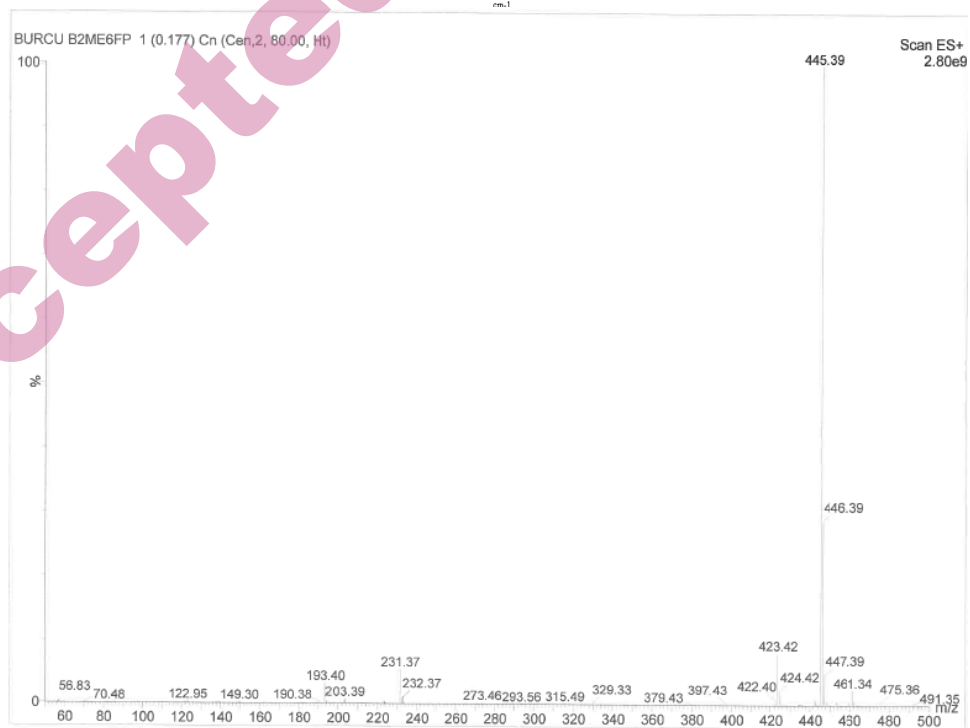
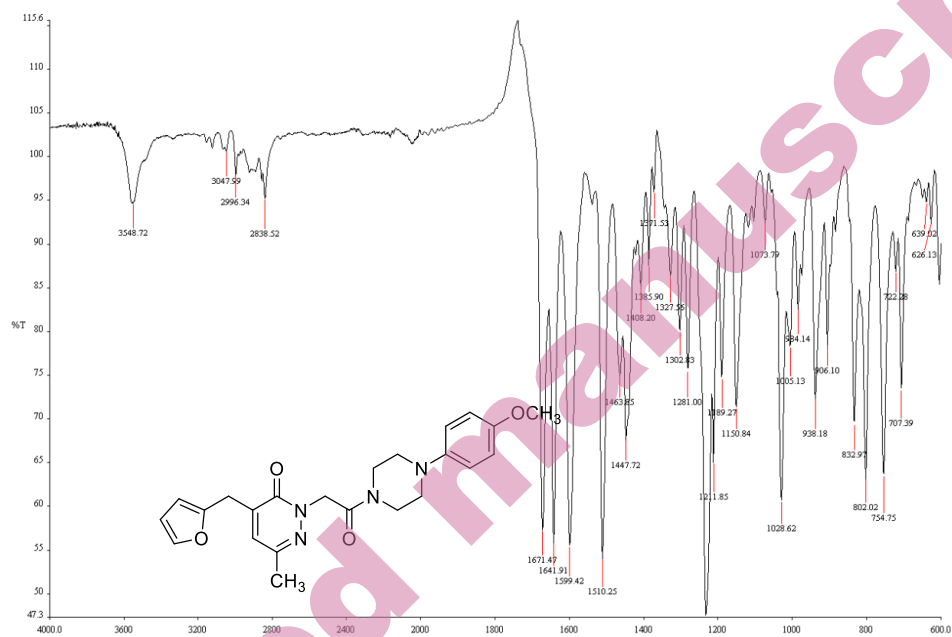


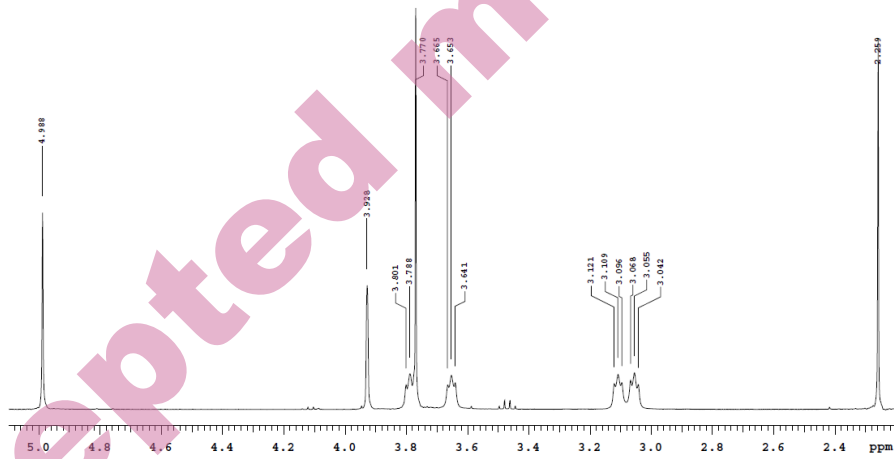
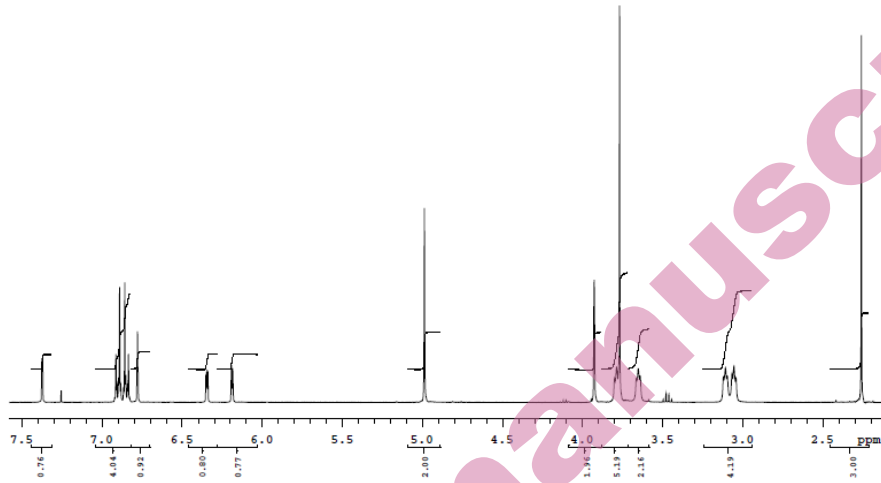


B24MPP  
 Sample Name:  
 B24MPP  
 Data Collected on:  
 mercury400-mercury400  
 Archive directory:  
 /home/vnmr1/vnmrswy/data  
 Sample directory:  
 B24MPP\_20210221\_01  
 FidFile: CARBON\_01  
  
 Pulse Sequence: CARBON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Feb 21 2021  
  
 Temp. 23.0 C / 296.1 K  
 Operator: vnmr1  
  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.550 sec  
 Width 21141.6 Hz  
 1000 repetitions  
 OBSERVE C13, 100.6238513 MHz  
 DECOUPLE H1, 400.1760547 MHz  
 Power 38 dB  
 Continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 44 min

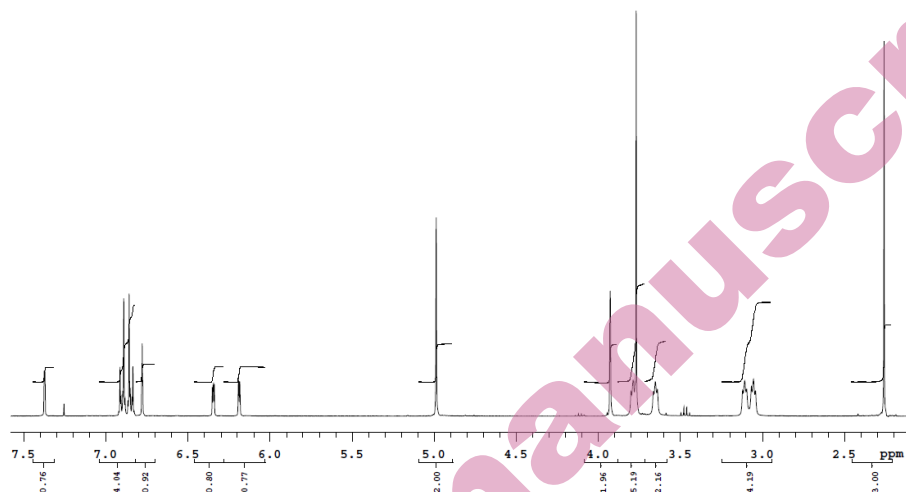


## 4-(FURAN-2-YLMETHYL)-6-METHYL-2-[2-OXO-2-(4-(4-METHOXYPHENYL)PIPERAZIN-1-YL)ETHYL]PYRIDAZIN-3(2H)-ONE (6C)





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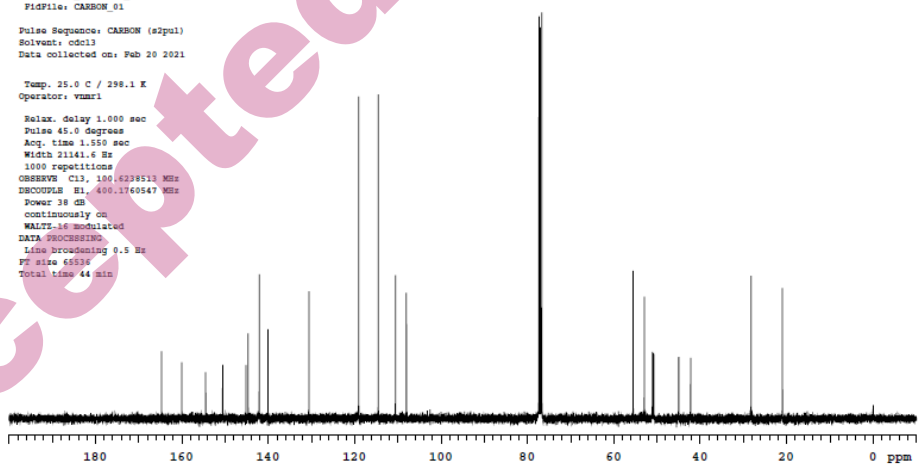
E2Me0FP

Sample Name:  
E2Me0FP  
Data Collected on:  
mercury400-mercury400  
Archive directory:  
/home/vnmr1/vnmrsys/data  
Sample directory:  
E2Me0FP\_20210220\_01  
FidFile: CARBON\_01

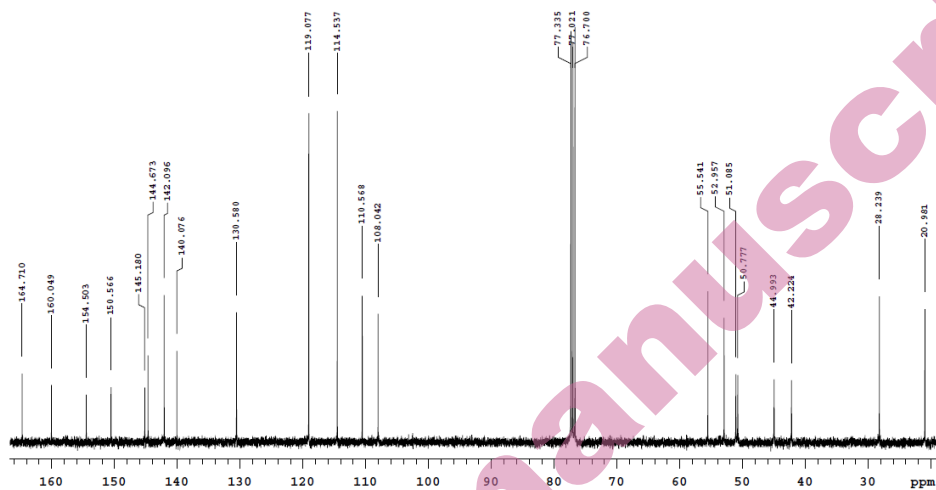
Pulse Sequence: CARBON (e2pul)  
Solvent: cdcl3  
Data collected on: Feb 20 2021

Temp: 25.0 C / 298.1 K  
Operator: vnmr1

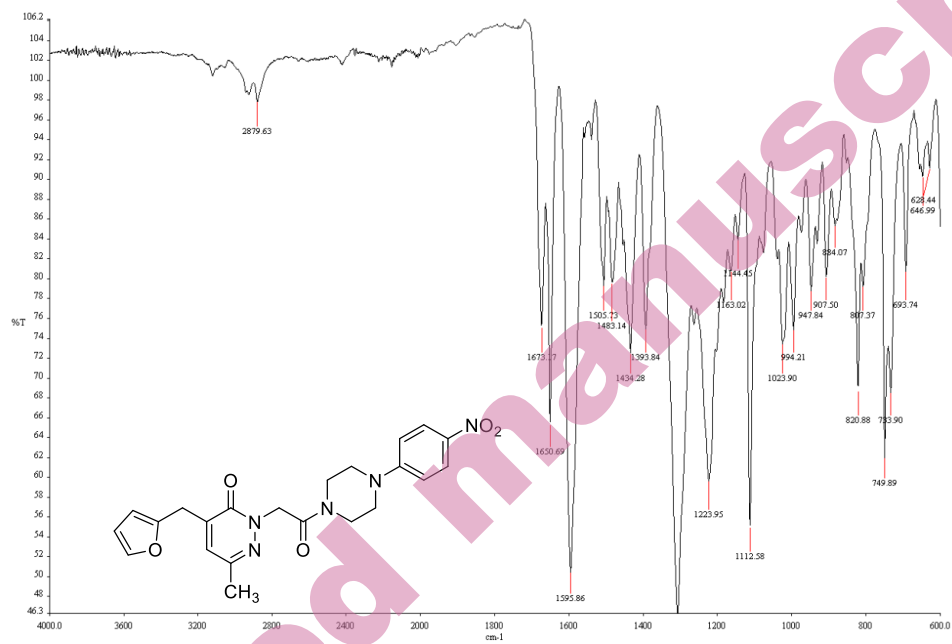
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.550 sec  
Width 21141.6 Hz  
1000 repetitions  
OBSERVE C13, 100.6238513 MHz  
NUC1 C13, 100.6238513 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
PF size 65536  
Total time 44 min

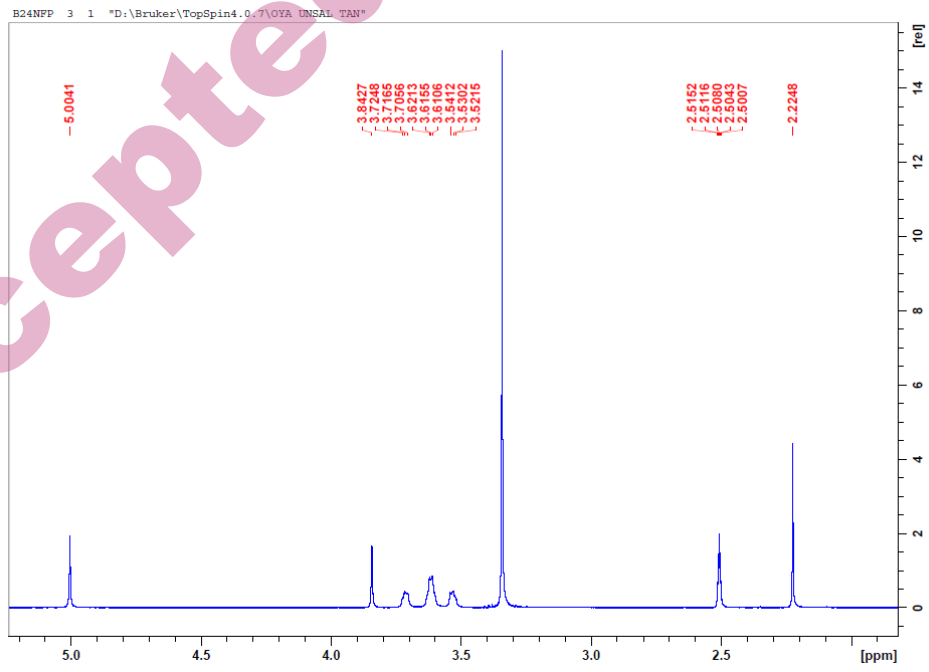
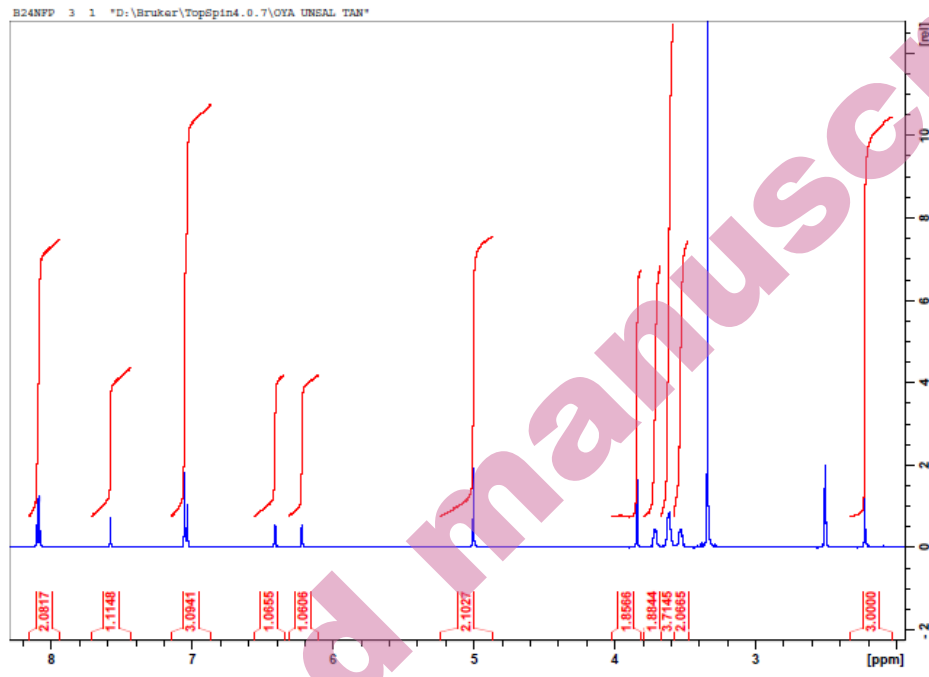


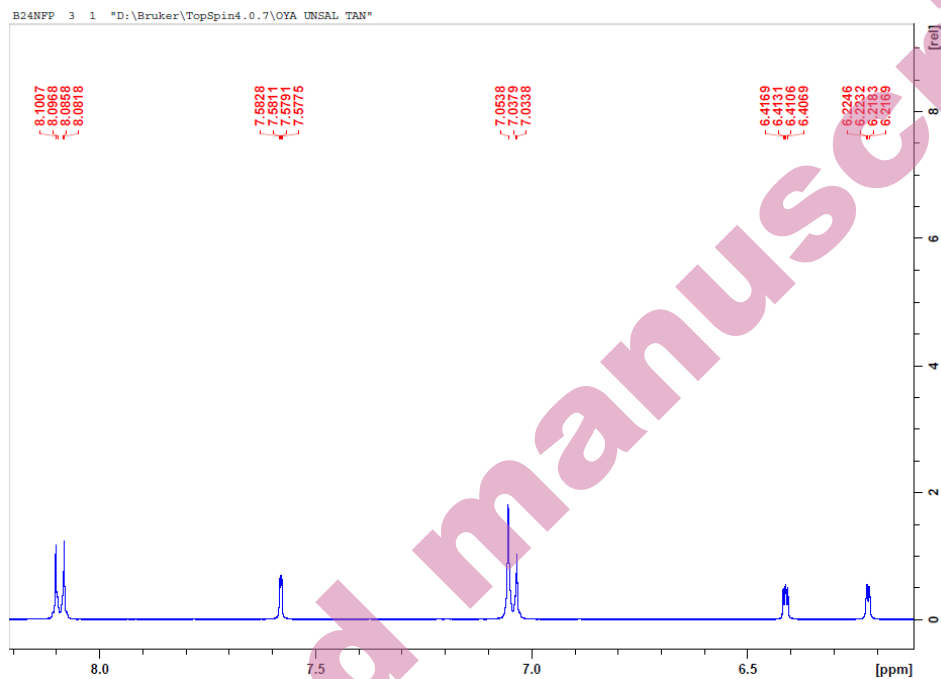




## 4-(FURAN-2-YLMETHYL)-6-METHYL-2-[2-OXO-2-(4-(4-NITROPHENYL)PIPERAZIN-1-YL)ETHYL]PYRIDAZIN-3(2H)-ONE (6D)



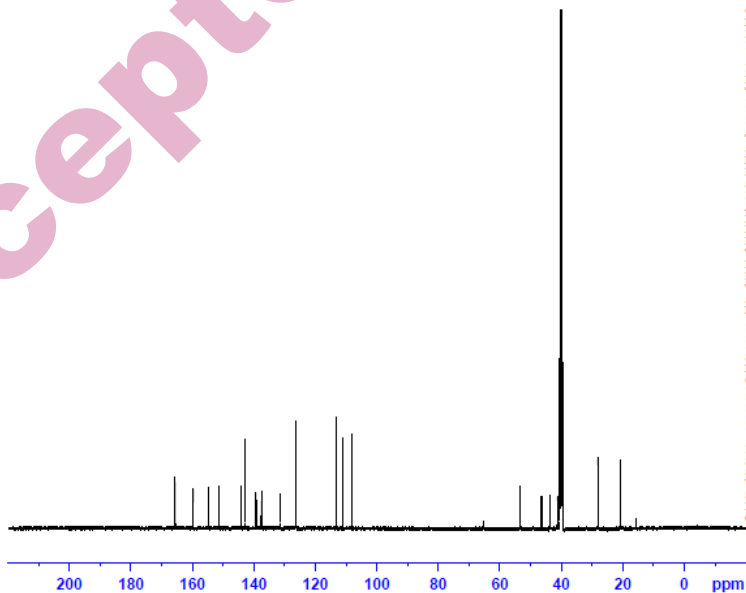


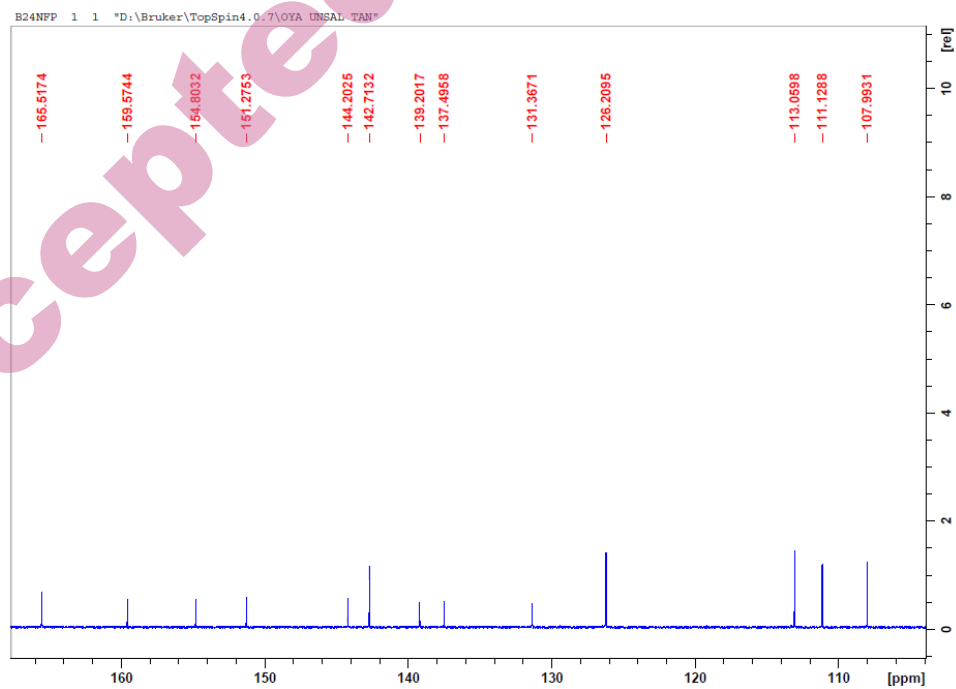
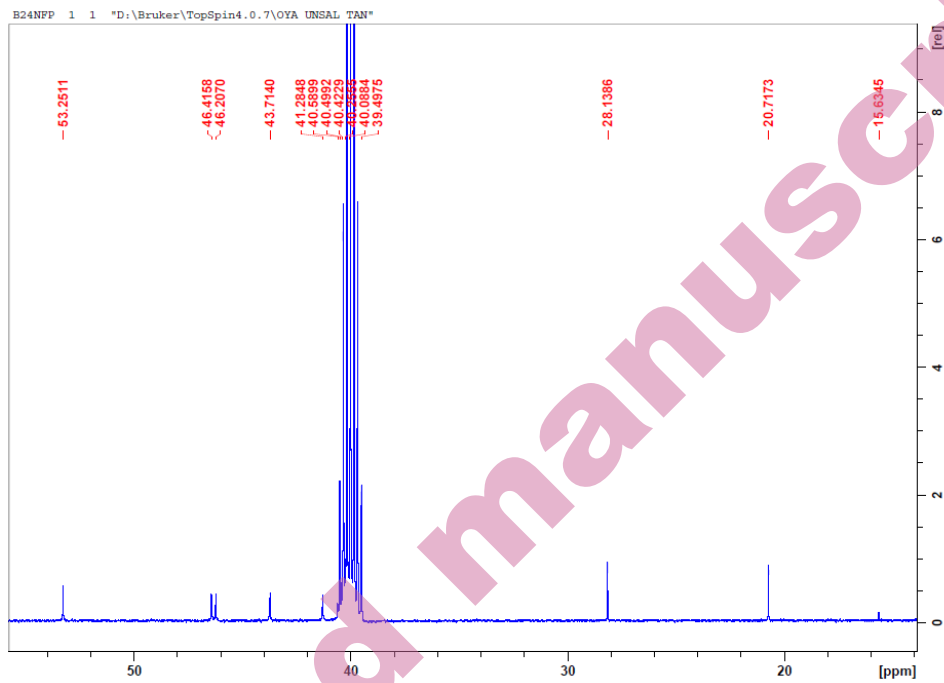


Current Data Parameters  
 NAME B24NFP  
 EXPNO 1  
 PROCNO 1

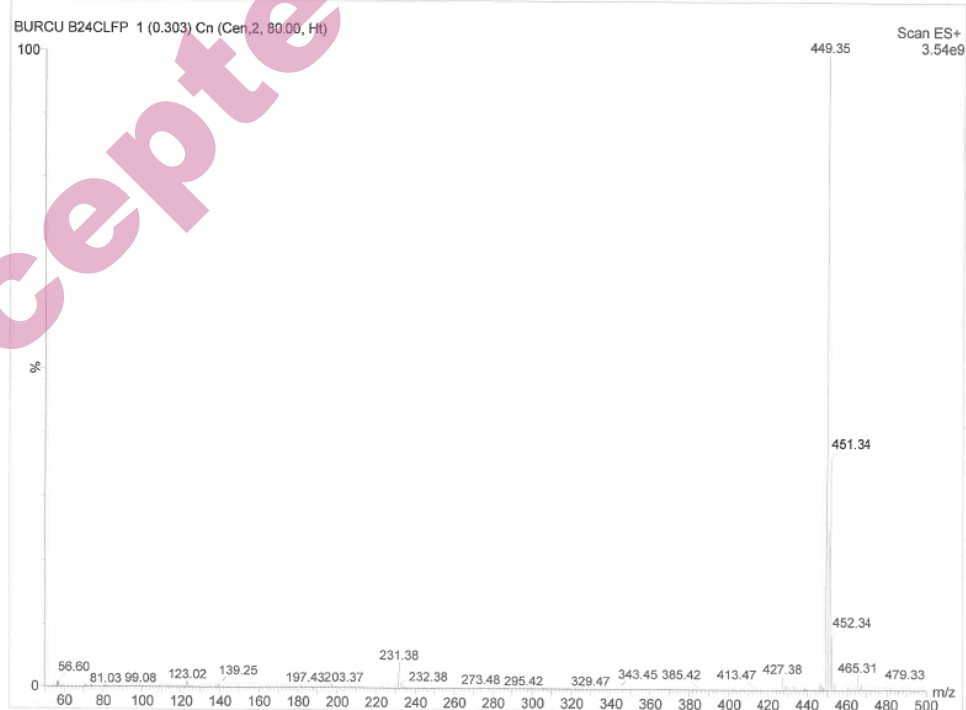
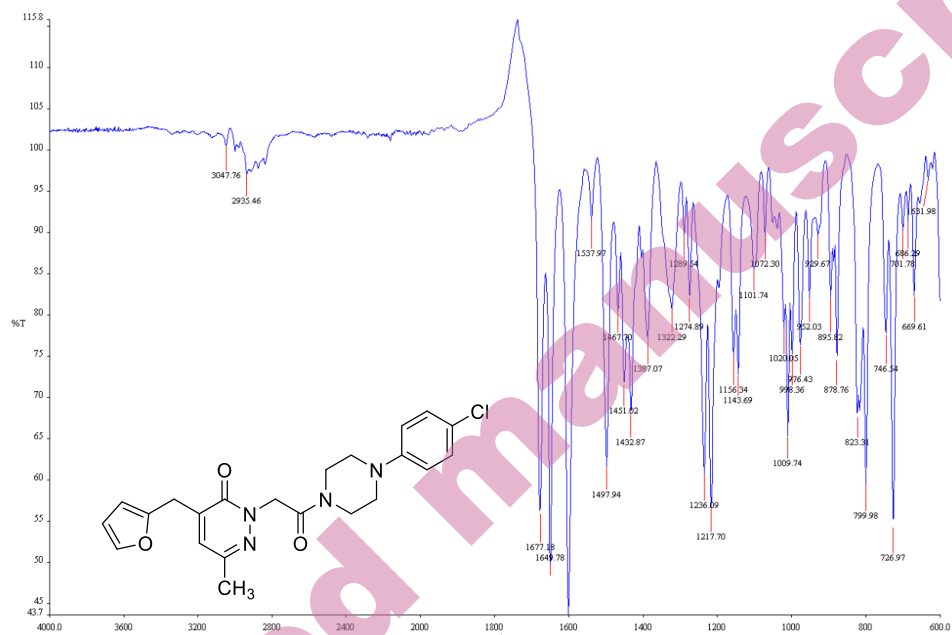
F2 - Acquisition Parameters  
 Date\_ 20201022  
 Time 12.00 h  
 INSTRUM Avance  
 PROBRD Z151574\_0038 ( )  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DM60  
 NS 1600  
 DS 4  
 SWH 30120.482 Hz  
 FIDRES 0.919204 Hz  
 AQ 1.0878977 sec  
 RG 101  
 DW 16.600 usec  
 DE 6.50 usec  
 TR 299.2 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 125.7703643 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLM1 85.18099976 W  
 SFO2 500.1320005 MHz  
 NUC2 1H  
 CPDPRG2 waltz65  
 PCPD2 80.00 usec  
 PLM2 24.04299927 W  
 PLM12 0.24043000 W  
 PLM13 0.12093000 W

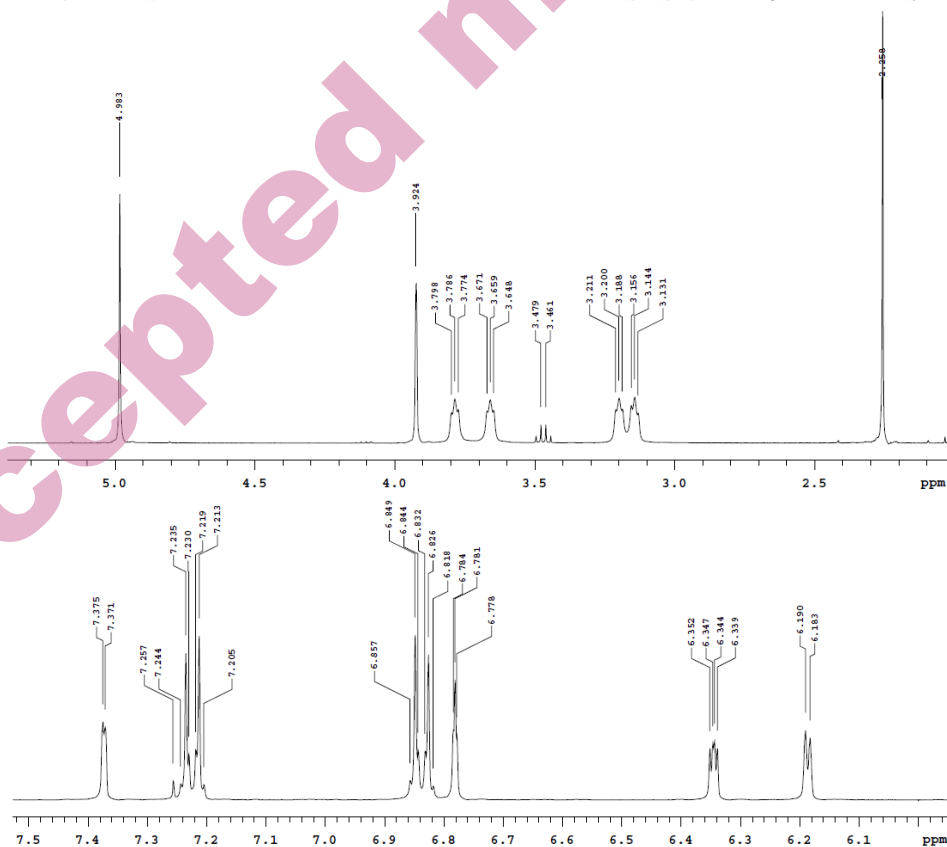
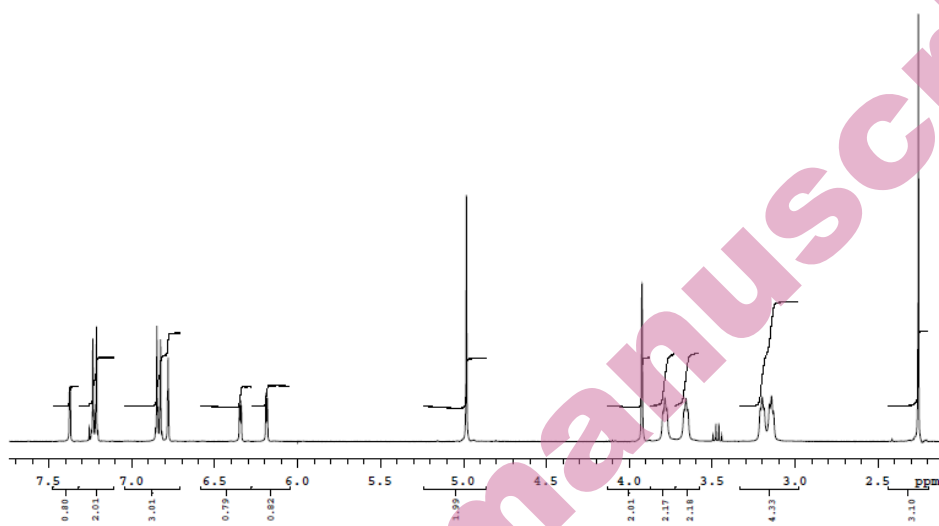
F2 - Processing parameters  
 SI 32768  
 SF 125.7577885 MHz  
 NCM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 CB 1.40





## 4-(FURAN-2-YLMETHYL)-6-METHYL-2-[2-OXO-2-(4-(4-CHLOROPHENYL)PIPERAZIN-1-YL)ETHYL]PYRIDAZIN-3(2H)-ONE (6E)



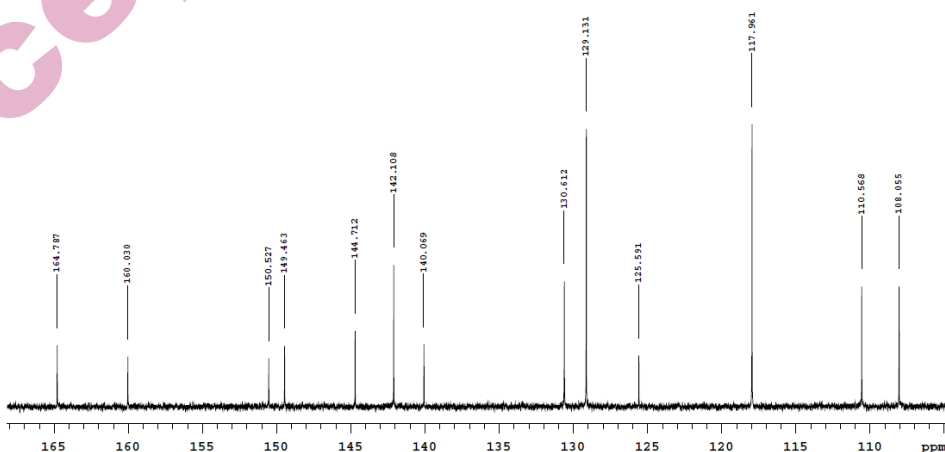
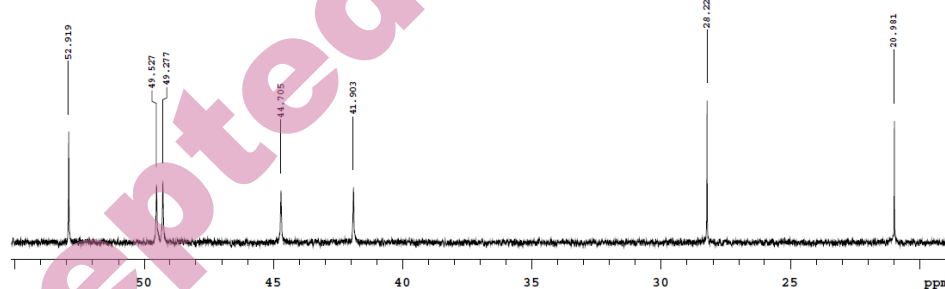
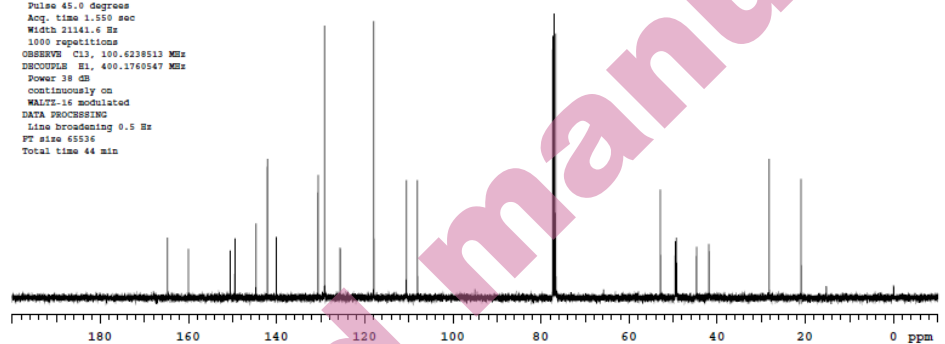




B24CLFP  
Sample Name:  
B24CLFP  
Data Collected on:  
mercury400-mercury400  
Archive directory:  
/home/vmri/vmrays/data  
Sample directory:  
B24CLFP\_20210220\_01  
Filefile: CARBON\_01  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 20 2021

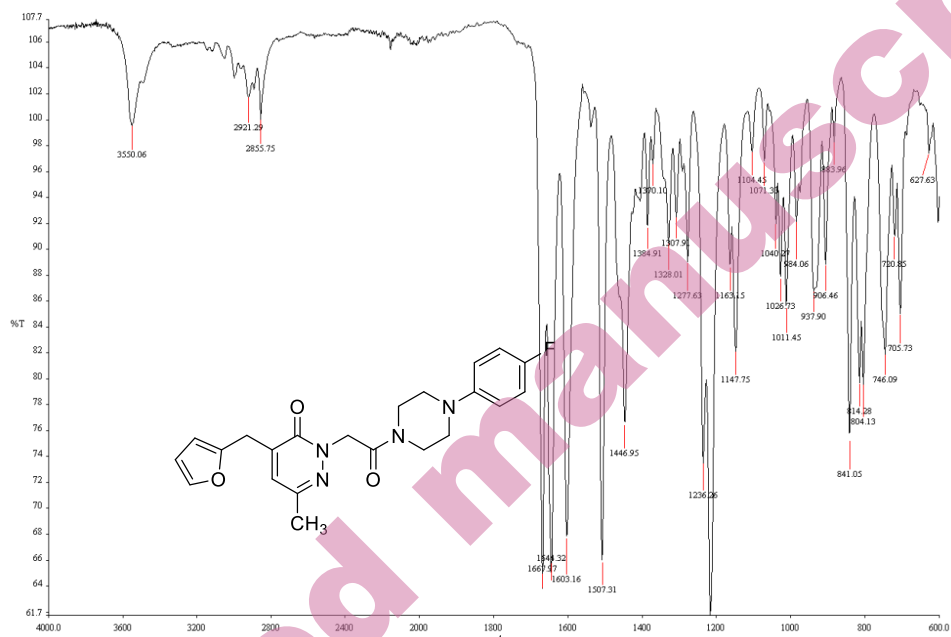
Temp. 25.0 C / 298.1 K  
Operator: vmri

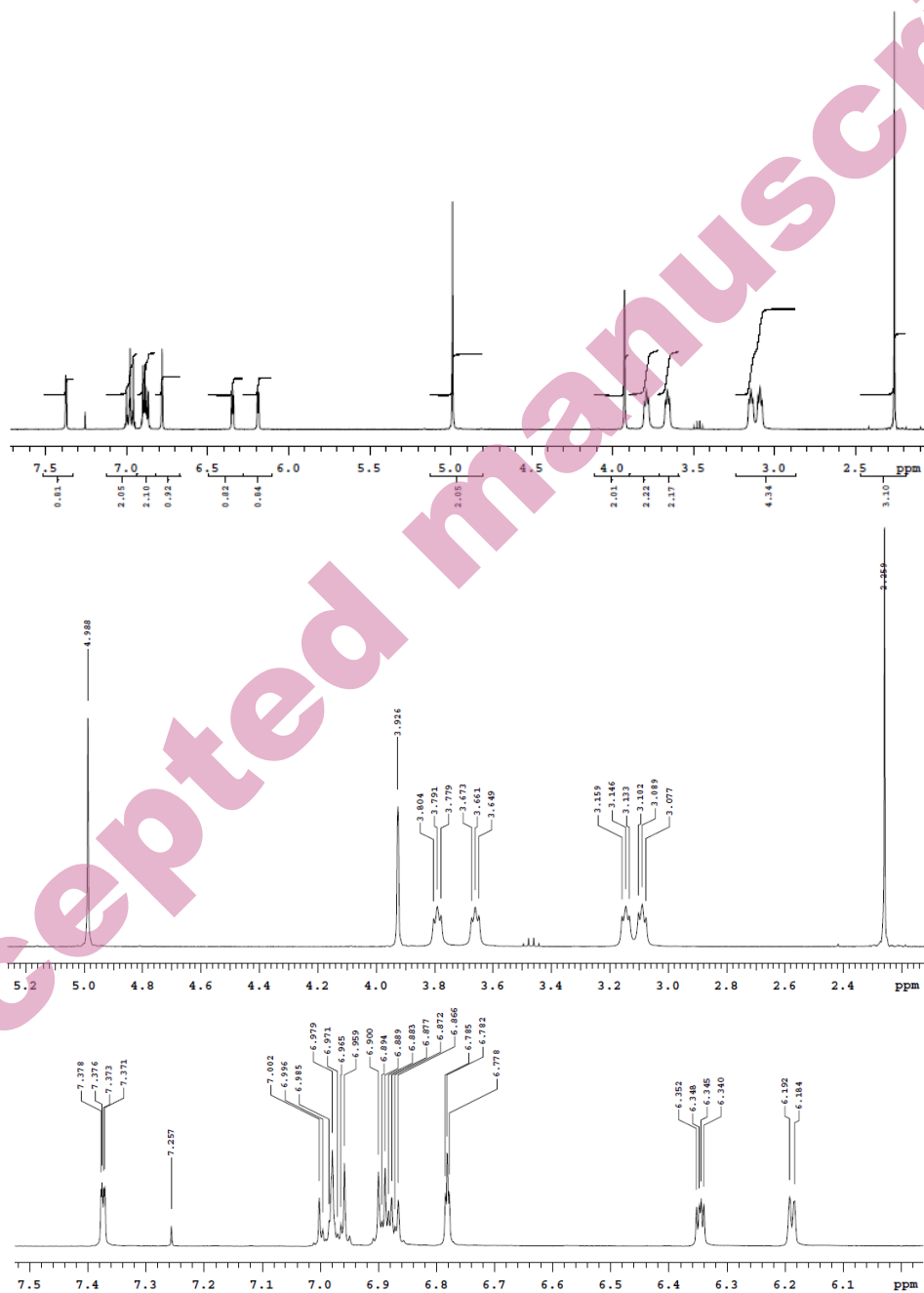
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.550 sec  
Width 21141.6 Hz  
1600 repetitions  
OBSERVE C13, 100.6238513 MHz  
DECOUPLE H1, 400.1760547 MHz  
Power 38 dB  
Continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 44 min





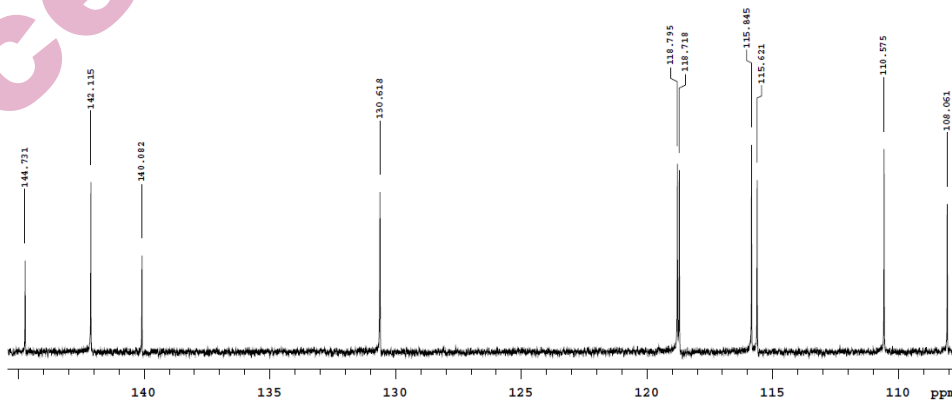
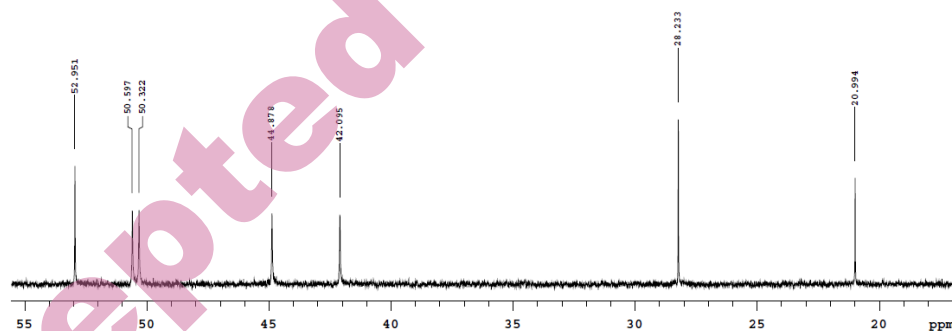
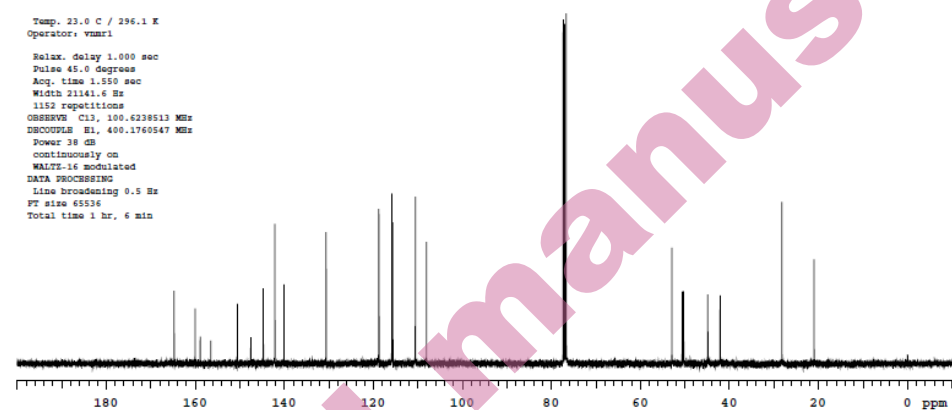
4-(FURAN-2-YLMETHYL)-6-METHYL-2-[2-OXO-2-(4-(4-FLUOROPHENYL)PIPERAZIN-1-YL)ETHYL]PYRIDAZIN-3(2H)-ONE (6F):





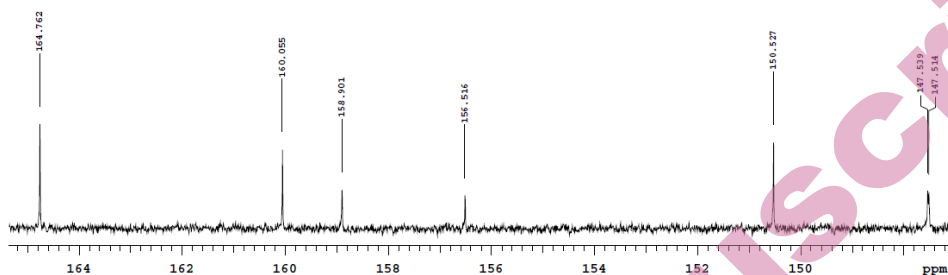


B24FFP  
 Sample Name:  
 B24FFP  
 Data Collected on:  
 Mercury400-Mercury400  
 Archive directory:  
 /home/vmr1/vmraysa/data  
 Sample directory:  
 B24FFP\_20210221\_01  
 Fidfile: current  
 Pulse Sequence: CARBON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Feb 21 2021  
 Temp: 23.0 C / 296.1 K  
 Operator: vmr1  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.550 sec  
 Width 21141.6 Hz  
 1152 repetitions  
 OBSERVE C13, 100.6238513 MHz  
 DECOUPLE H1, 400.1760547 MHz  
 Power 38 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 1 hr, 6 min



S60

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Accepted manuscript