

## Some Pyrimidohexahydroquinoline Candidates: Synthesis, DFT, Cytotoxic Activity Evaluation, Molecular Docking, and *In Silico* Studies

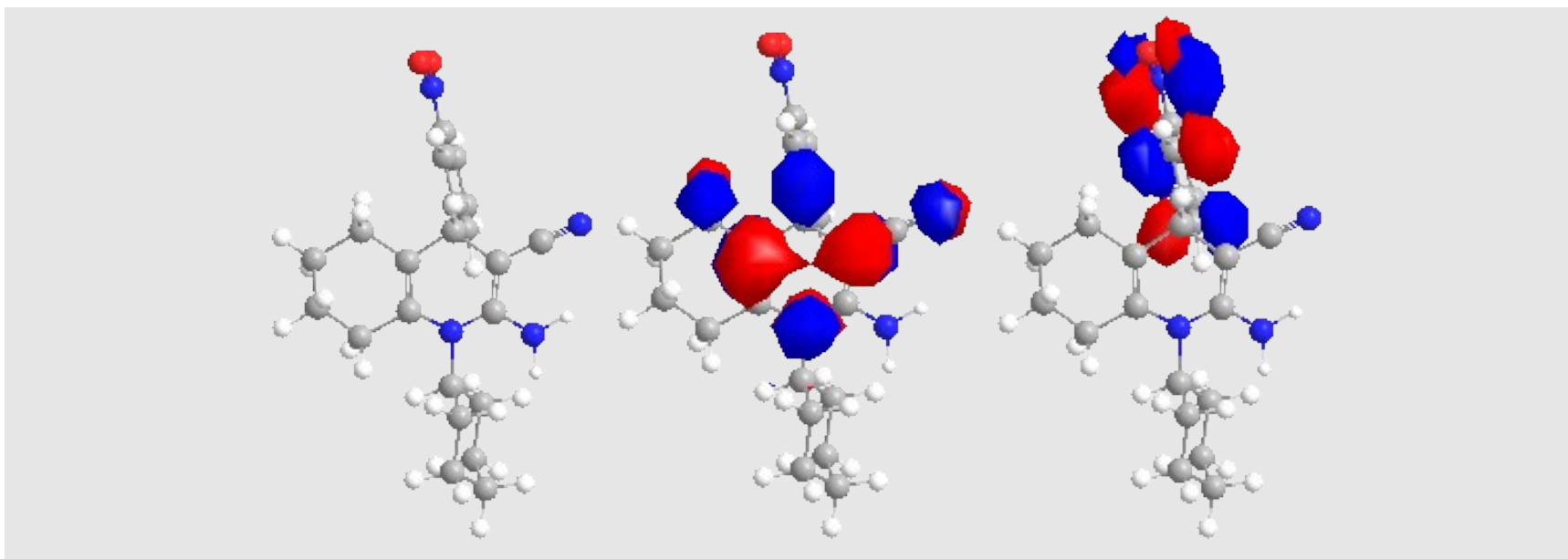
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<sup>a</sup> Chemistry Department, Faculty of Science, Ain Shams University, Cairo 11566, Egypt

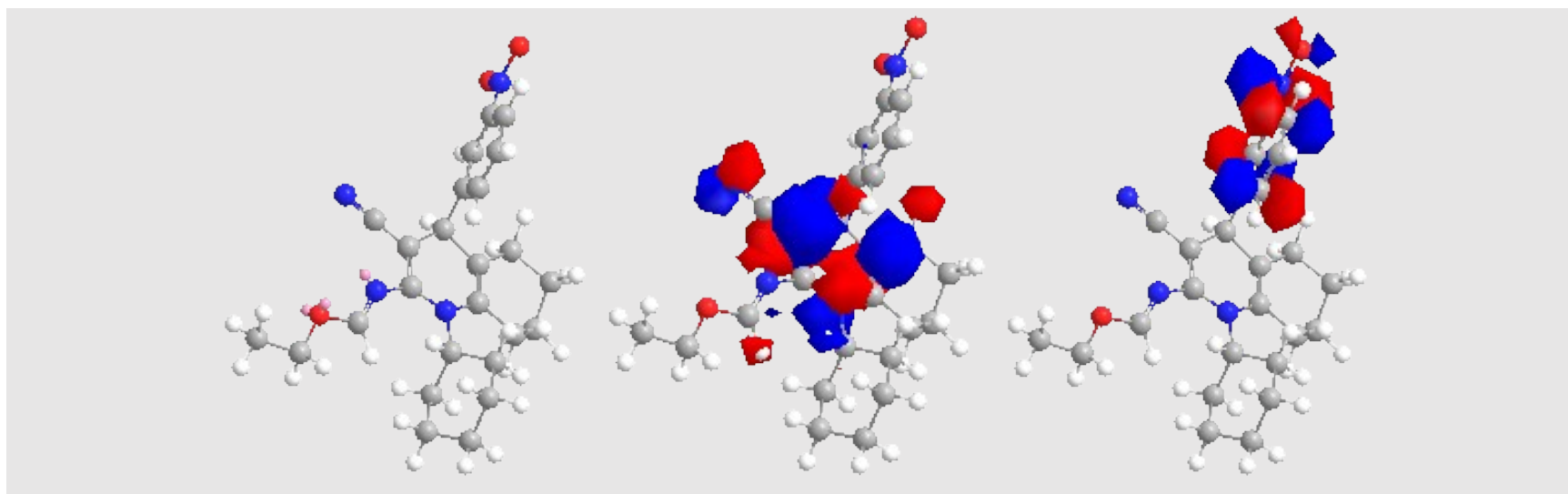
<sup>b</sup> Chemistry Department, College of Science, King Khalid University, P.O. Box 9004, Abha 62223, Saudi Arabia

\*E-mail: [sayed.karam2008@sci.asu.edu.eg](mailto:sayed.karam2008@sci.asu.edu.eg)

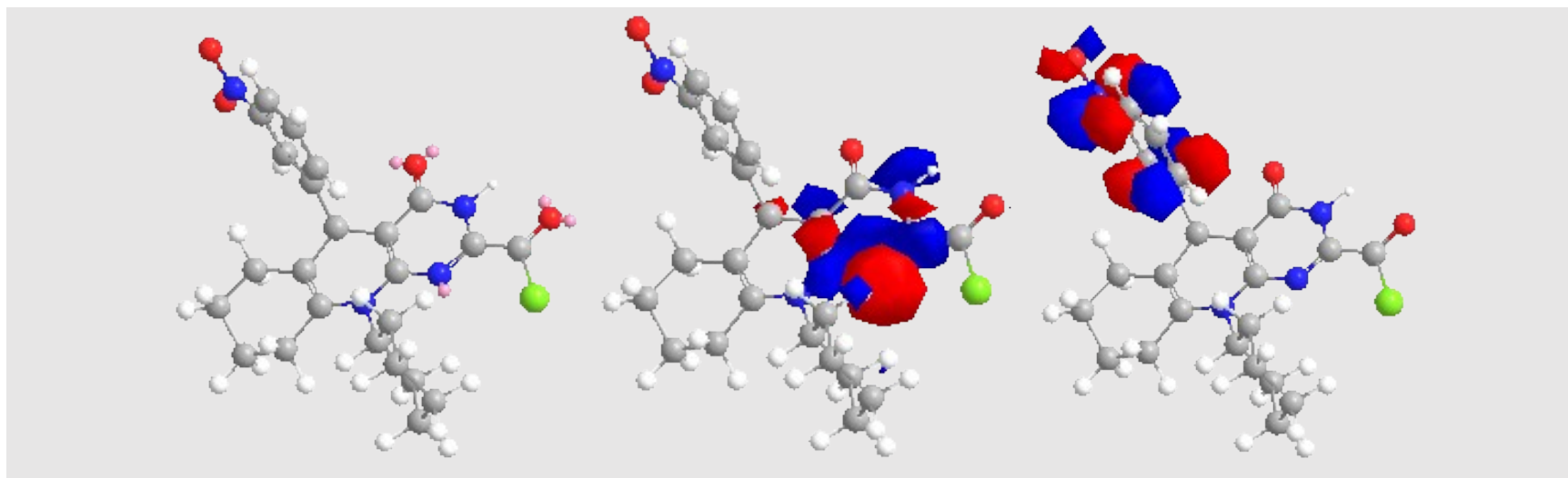
### Supporting information



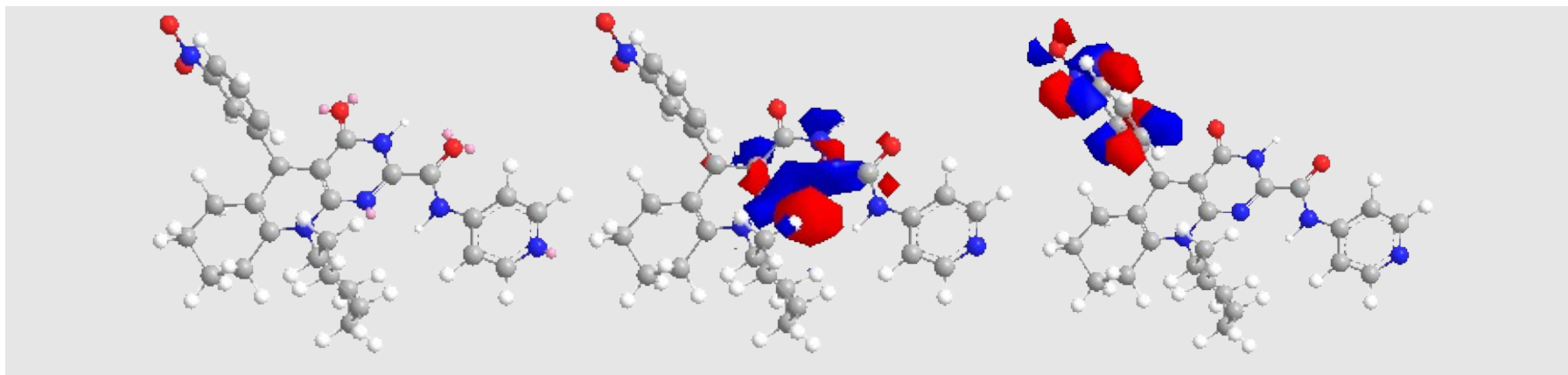
**Compound 4**



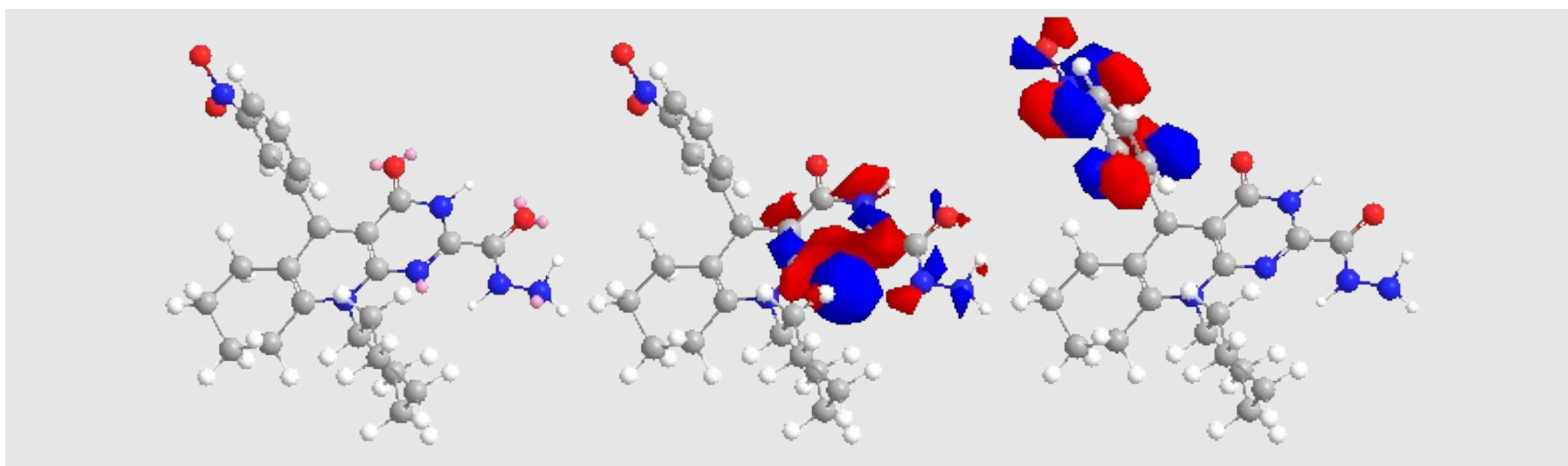
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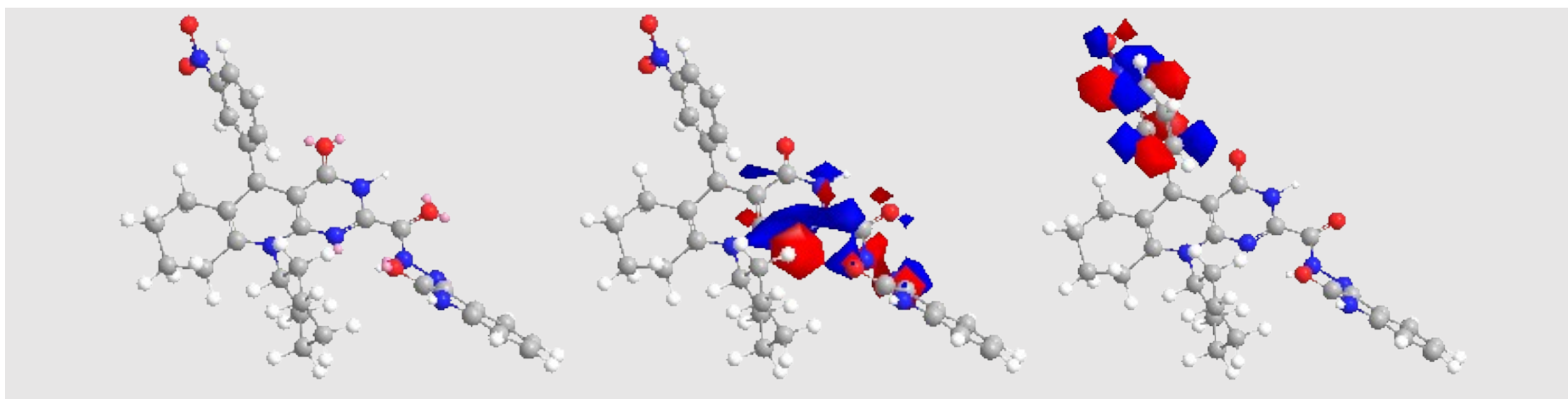
**Compound 6**



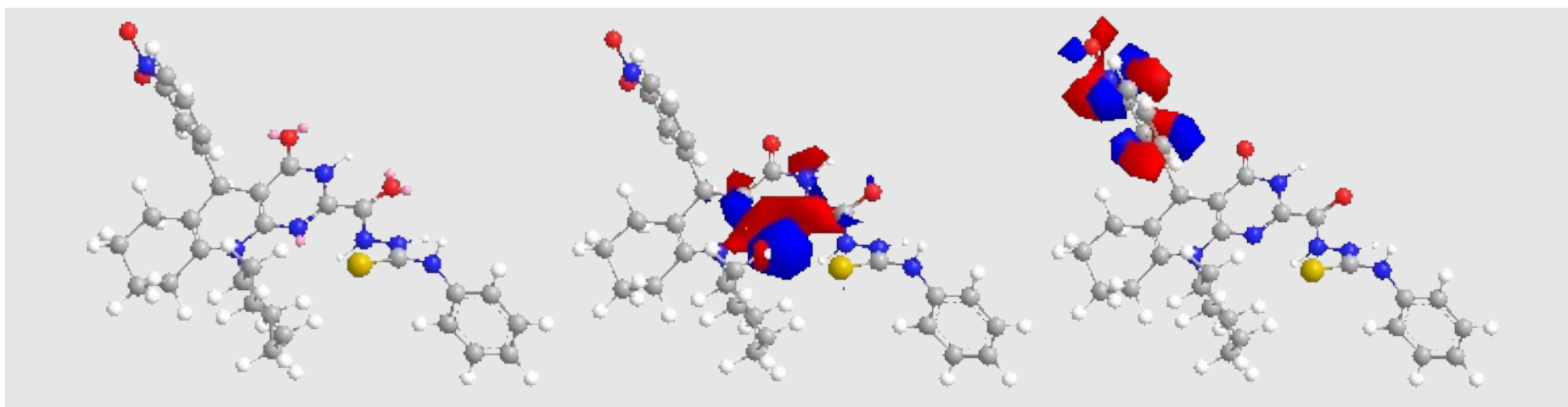
**Compound 7**



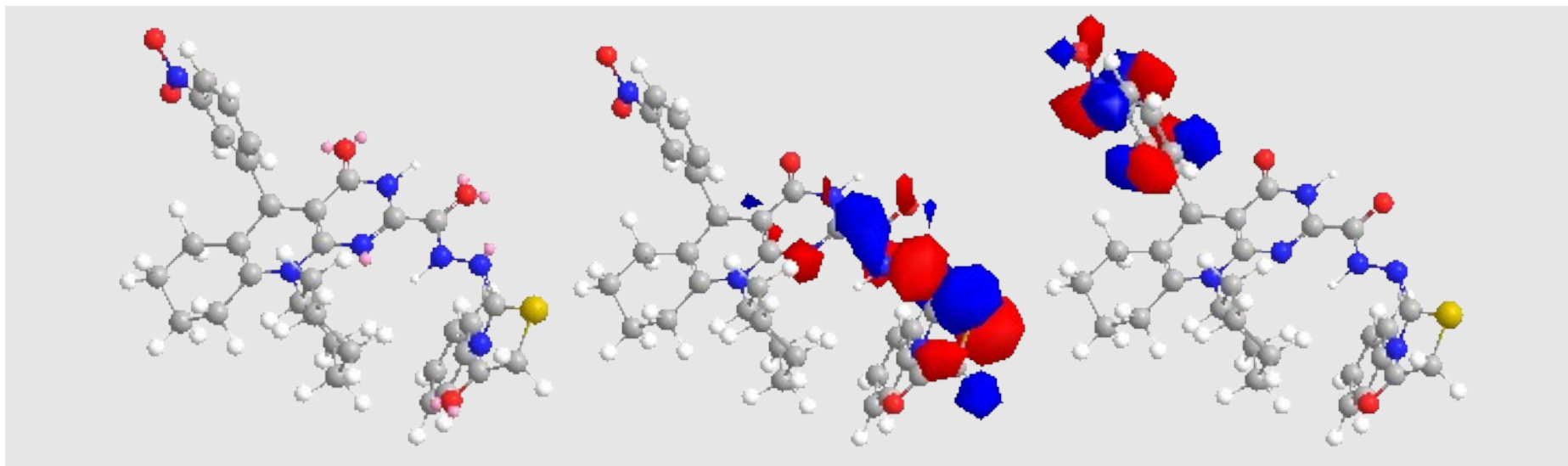
**Compound 8**



**Compound 9**



**Compound 10**



**Compound 11**

**Fig. 5.** Optimized structures (left), HOMO (middle), and LUMO (right) for compounds 4-11. Atom color index: White H, Grey C, Blue N, Red O, and Green Cl.

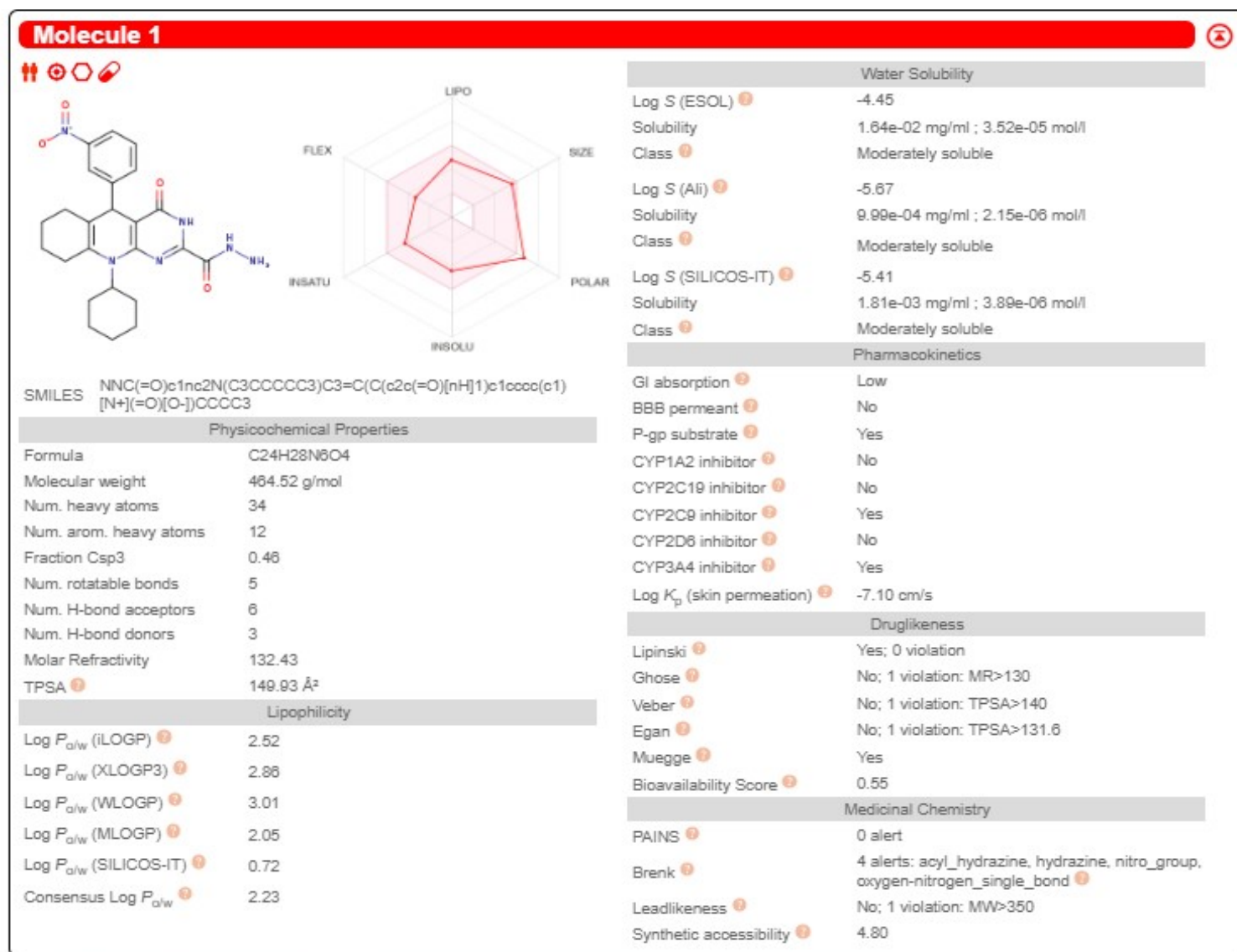


Fig. 7. ADME prediction of compound 8.

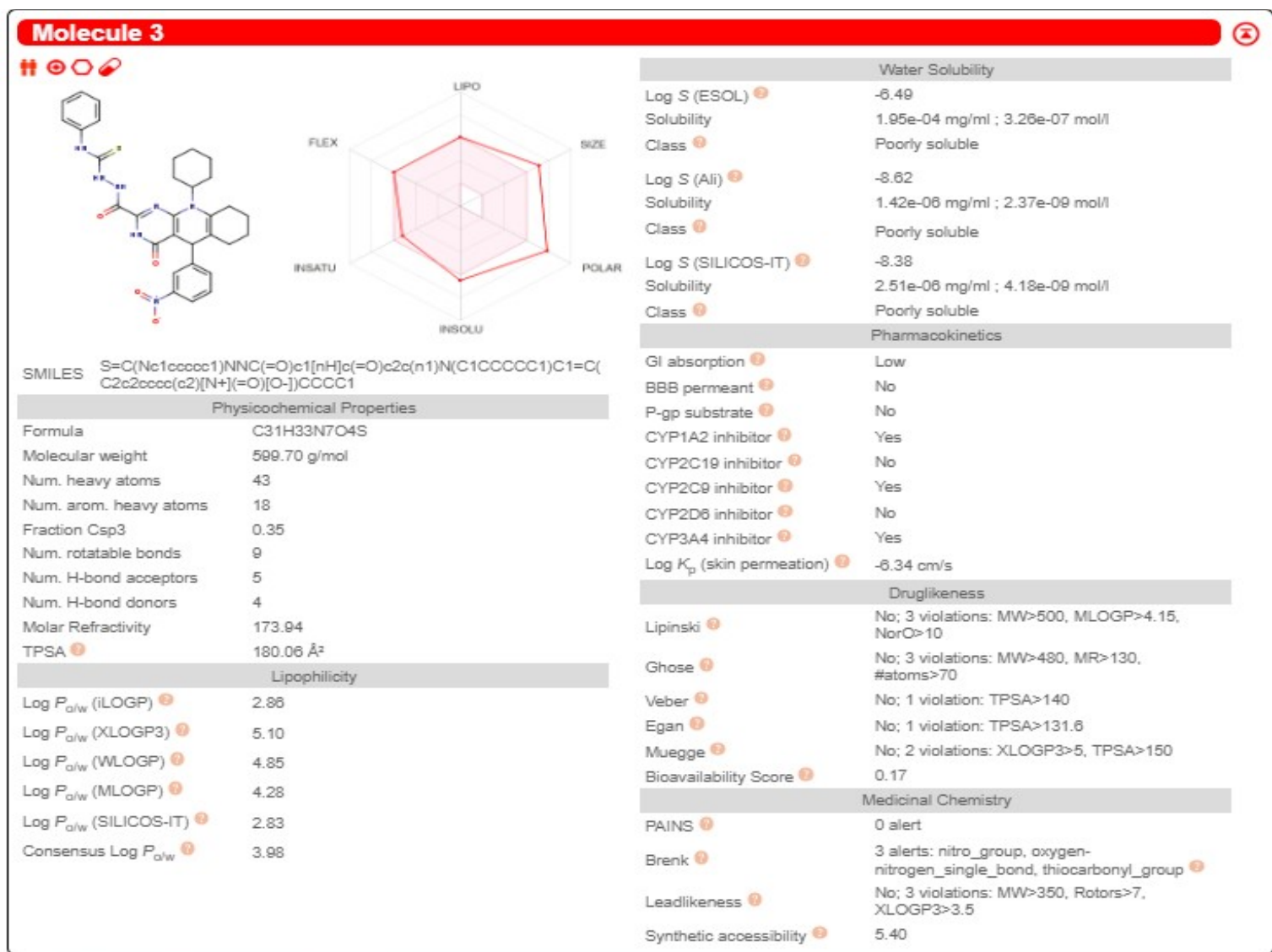


Fig. 8. ADME prediction of compound 10.

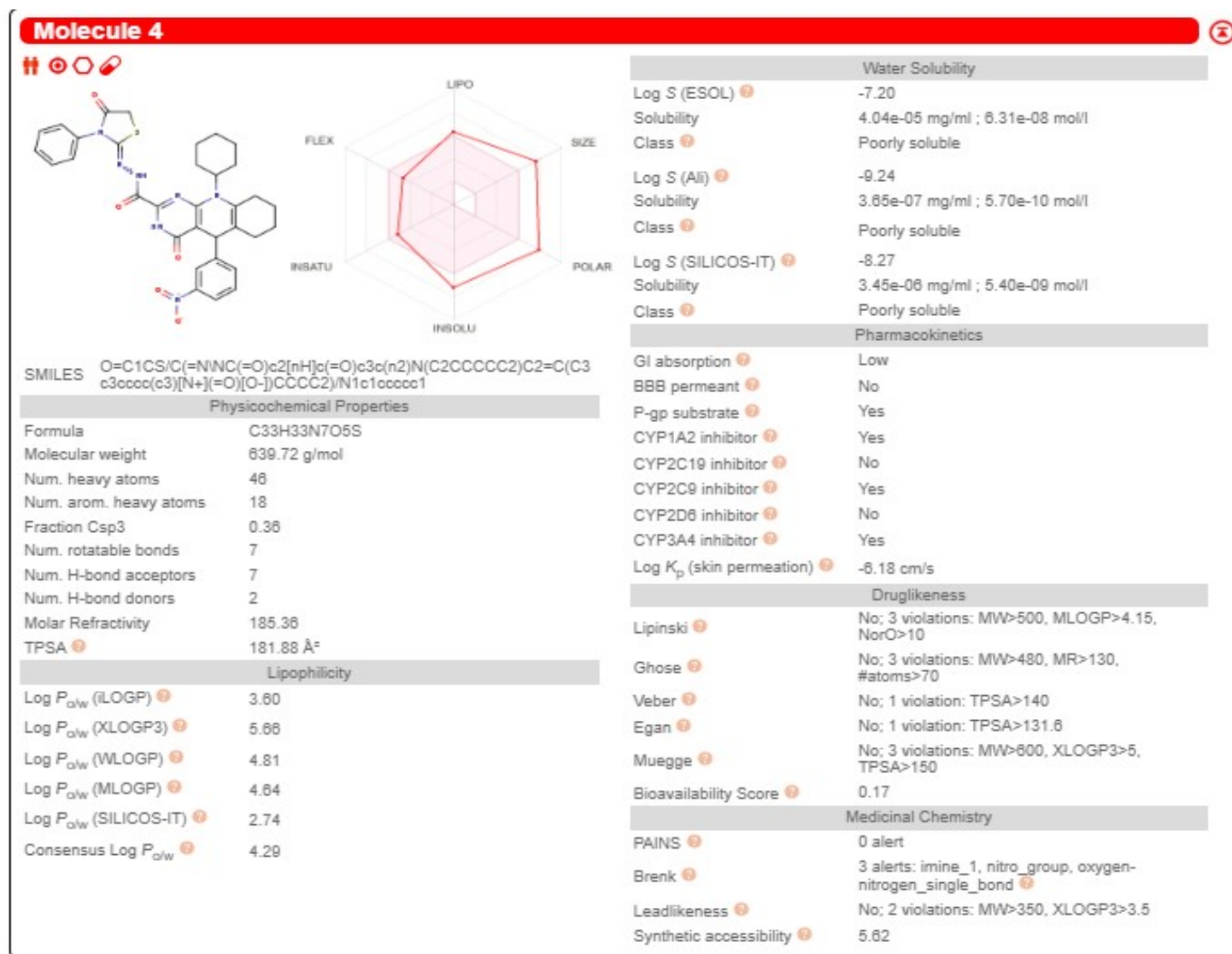
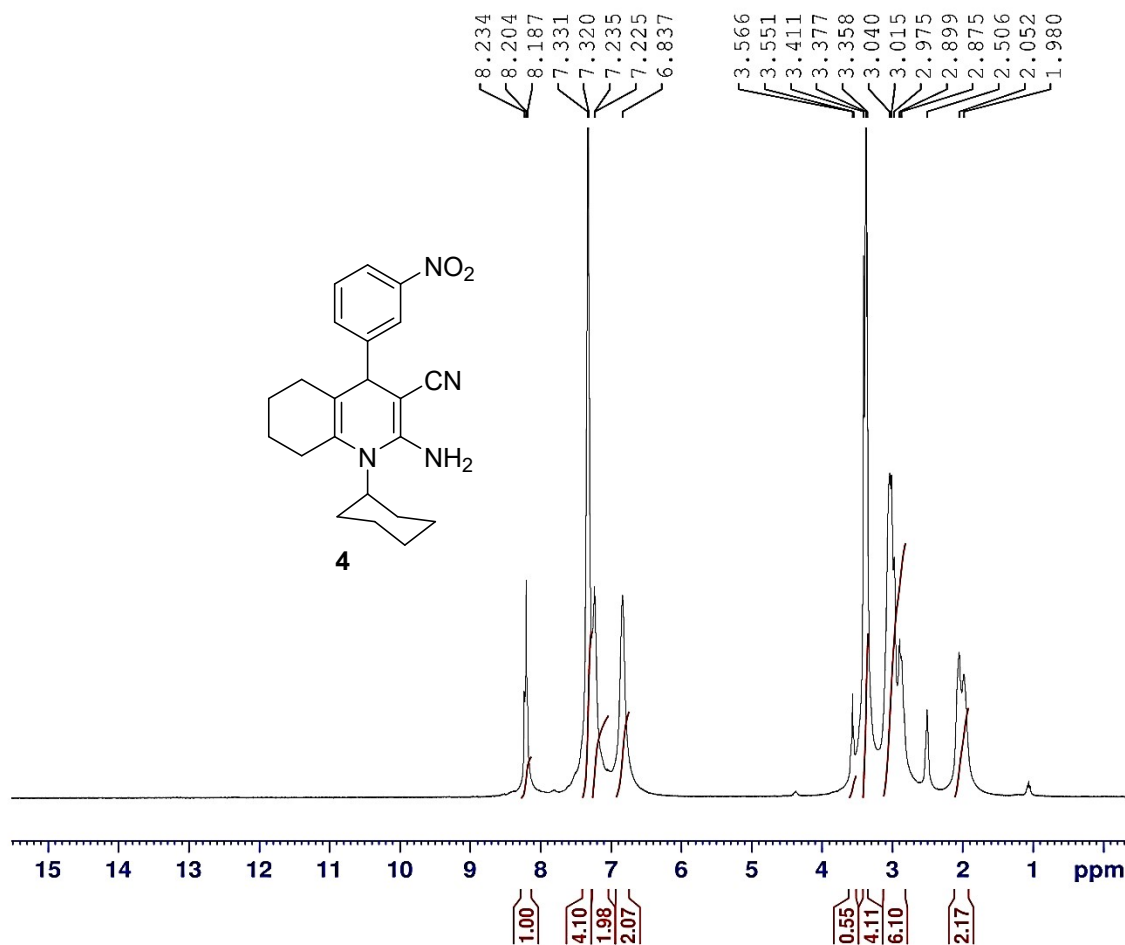


Fig. 9. ADME prediction of compound 11.



# Spectral data



Current Data Parameters  
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 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220918  
 Time 11.15  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 65  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
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 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

7.982  
7.376  
7.355  
7.346  
7.338  
7.307  
7.283  
7.265  
7.250  
7.248  
4.466  
4.448  
4.430  
4.413  
3.730  
3.062  
2.955  
2.915  
2.903  
2.850  
2.813  
2.793  
2.783  
2.769  
2.753  
2.745  
2.731  
2.173  
2.166  
2.009  
1.996  
1.981  
1.978  
1.485  
1.433  
1.415  
1.397  
1.349  
1.331  
1.313  
1.282  
1.264  
1.247

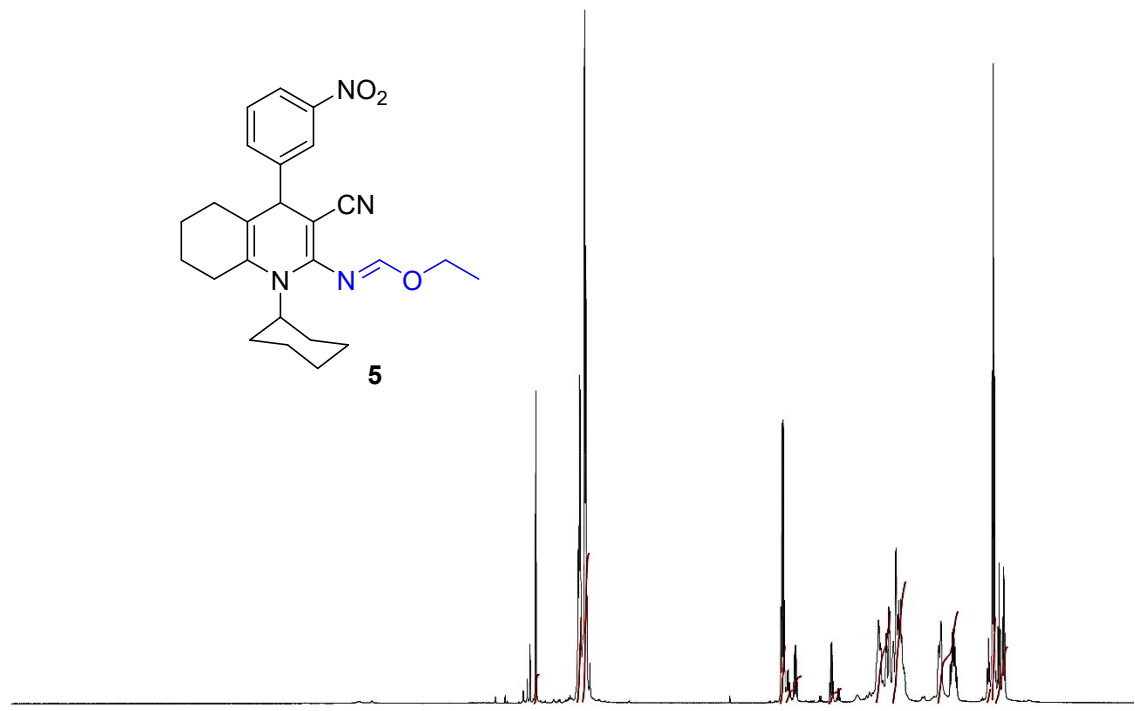
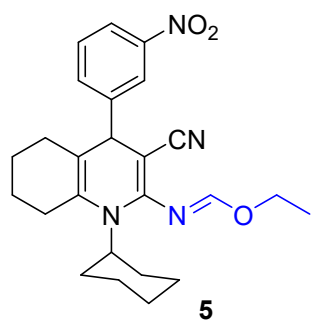


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EXPNO 1  
PROCNO 1

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PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 106  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

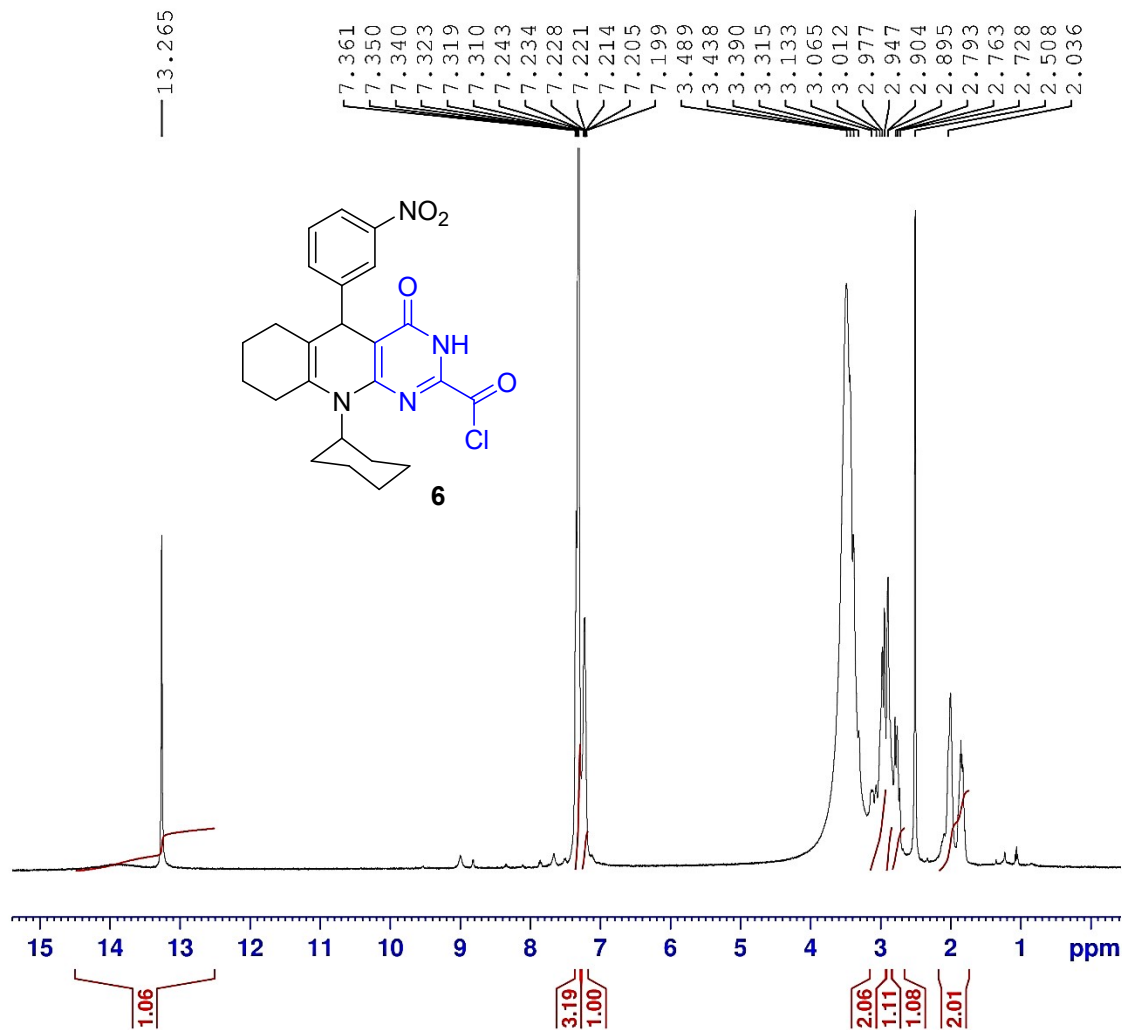
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NUC1 1H  
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PLW1 18.00000000 W

F2 - Processing parameters  
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SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.00 3.14 5.16 2.01 0.94 0.51 3.19 4.19 0.53 3.06 1.95



Current Data Parameters

NAME sayed-karam-CA5  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

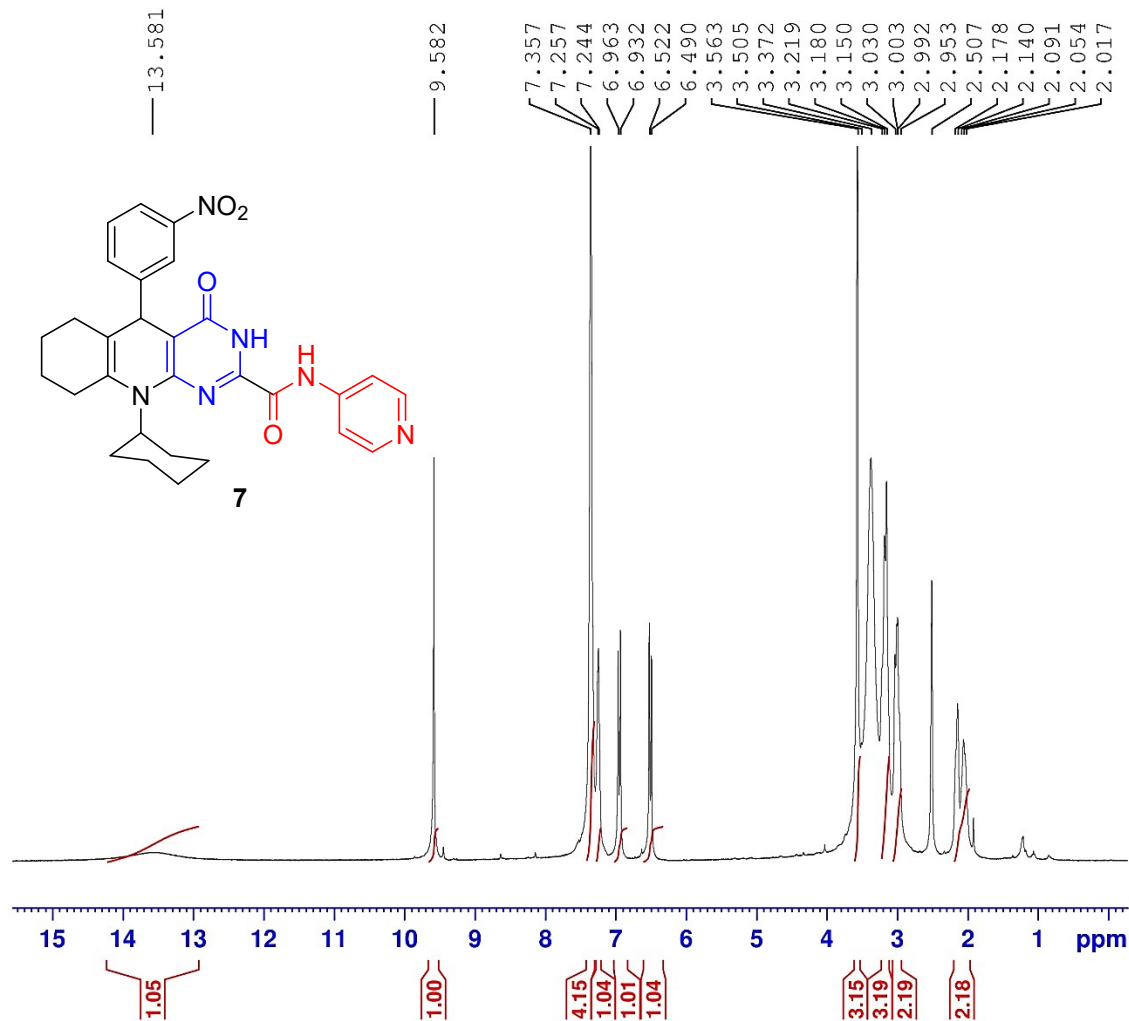
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Time 10.55  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 91  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

==== CHANNEL f1 =====

SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters

SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

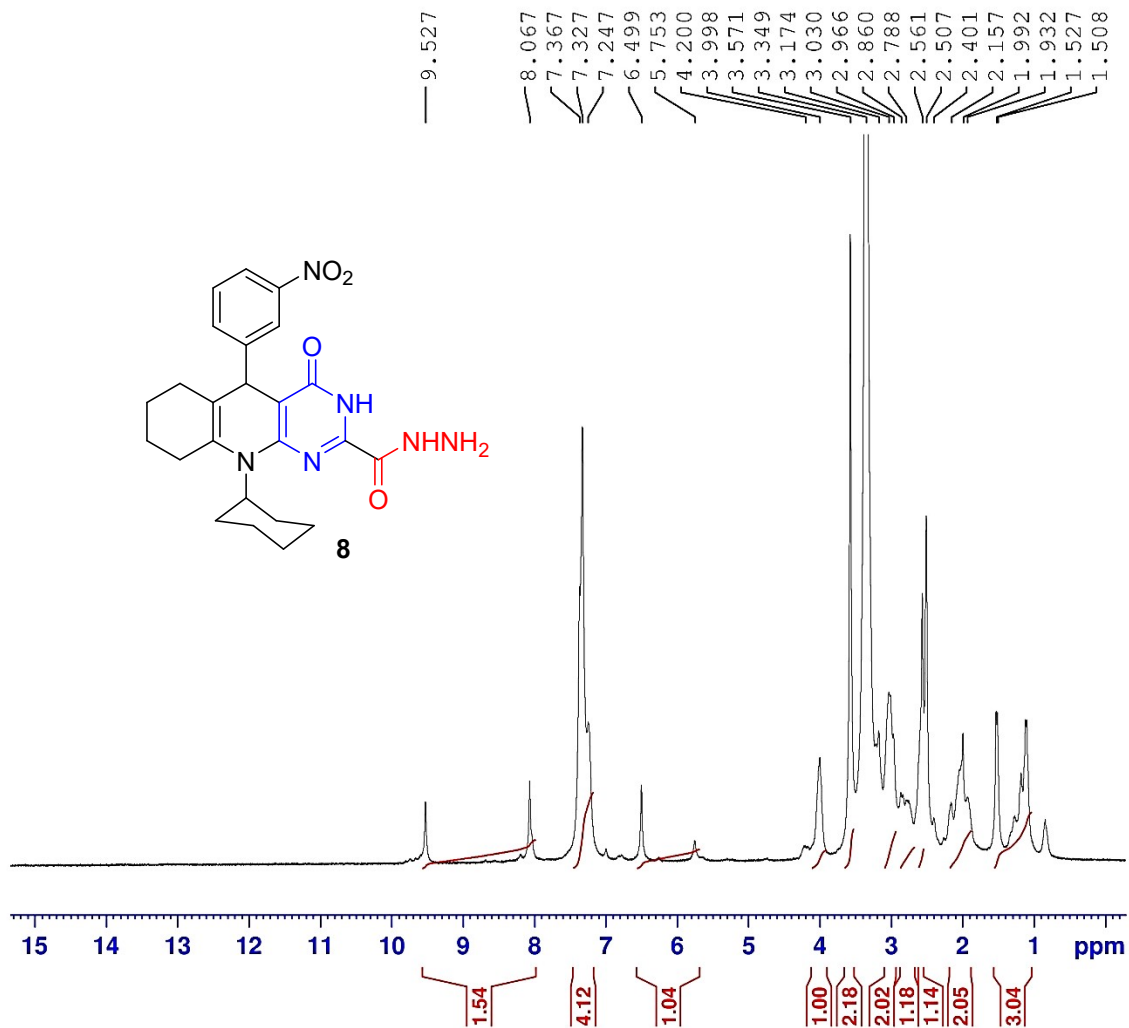
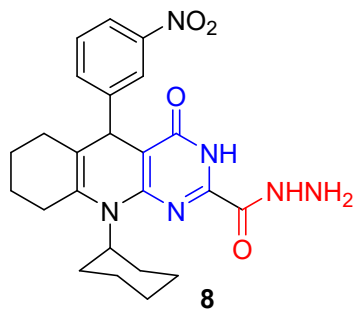


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 EXPNO 1  
 PROCNO 1

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 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 128  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



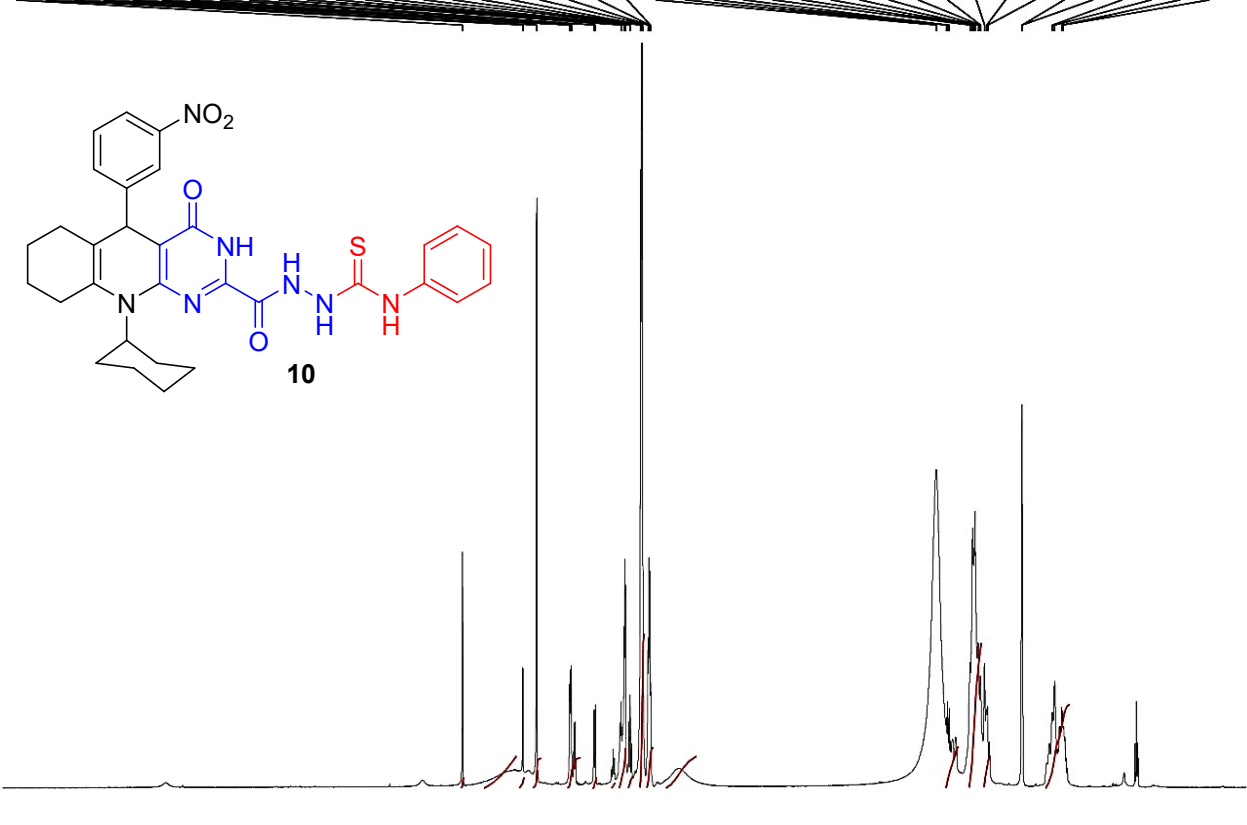
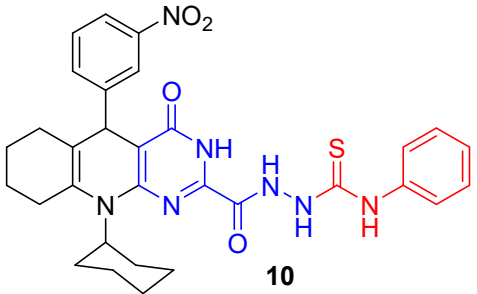
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 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 128  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

9.617  
8.850  
8.675  
8.255  
8.245  
8.236  
8.231  
7.945  
7.927  
7.600  
7.561  
7.553  
7.548  
7.487  
7.356  
7.351  
7.340  
7.329  
7.259  
7.249  
7.238  
7.228  
3.598  
3.468  
3.451  
3.433  
3.168  
3.138  
3.116  
3.103  
3.065  
3.042  
3.035  
2.985  
2.960  
2.945  
2.511  
2.507  
2.122  
2.093  
2.007  
1.992

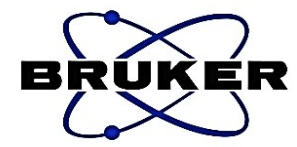


15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.00  
3.18  
1.10  
2.94  
2.97  
1.02  
0.59  
4.20  
1.10  
15.05  
3.93  
3.11

4.06  
14.20  
3.17

8.10



Current Data Parameters  
 NAME sayed-karam-CA19  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220912  
 Time 9.51  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 128  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

7.989  
7.374  
7.355  
7.336  
7.284  
7.273  
7.254  
3.054  
2.917  
2.907  
2.850  
2.809  
2.786  
2.770  
2.745  
2.170  
2.126  
2.092  
2.035  
2.010  
1.980  
1.965  
1.874  
1.864  
1.843  
1.773  
1.760  
1.738  
1.694  
1.685  
1.673  
1.652  
1.501  
1.474  
1.446  
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1.397  
1.378  
1.339  
1.307  
1.263  
1.244

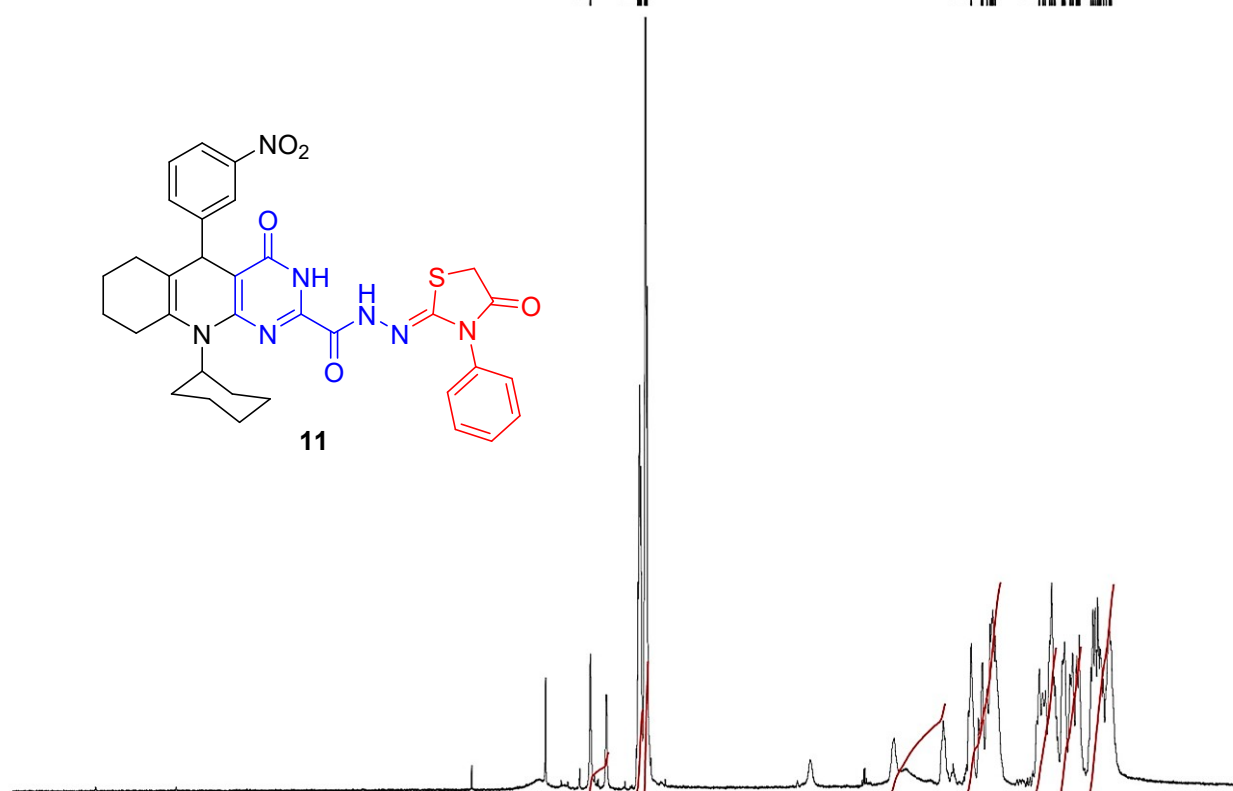
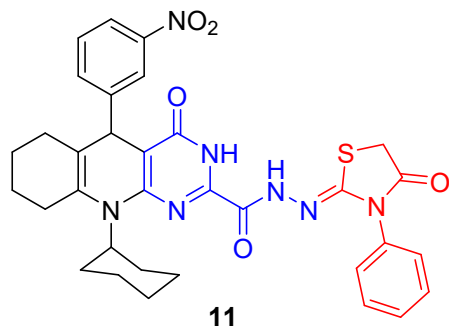


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PROCNO 1

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PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 106  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.00 1.03 1.00 3.03 5.20 1.03 2.19 5.07 3.50 3.52 5.04