

SUPPLEMENTAL MATERIALS

for

Design, Synthesis and Evaluation of Novel 2-Oxoindoline-based Acetohydrazides as Antitumor Agents

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Copy of HRMS, ¹H & ¹³C NMR SPECTRA OF THE COMPOUNDS

Figure S1. HRMS of compound 4a

D:\DATA\Old\TA-MS\200823\109A

08/23/20 17:38:53

109A #17 RT: 0.16 AV: 1 NL: 2.23E9

T: FTMS + p ESI Full ms [100.0000-1500.0000]

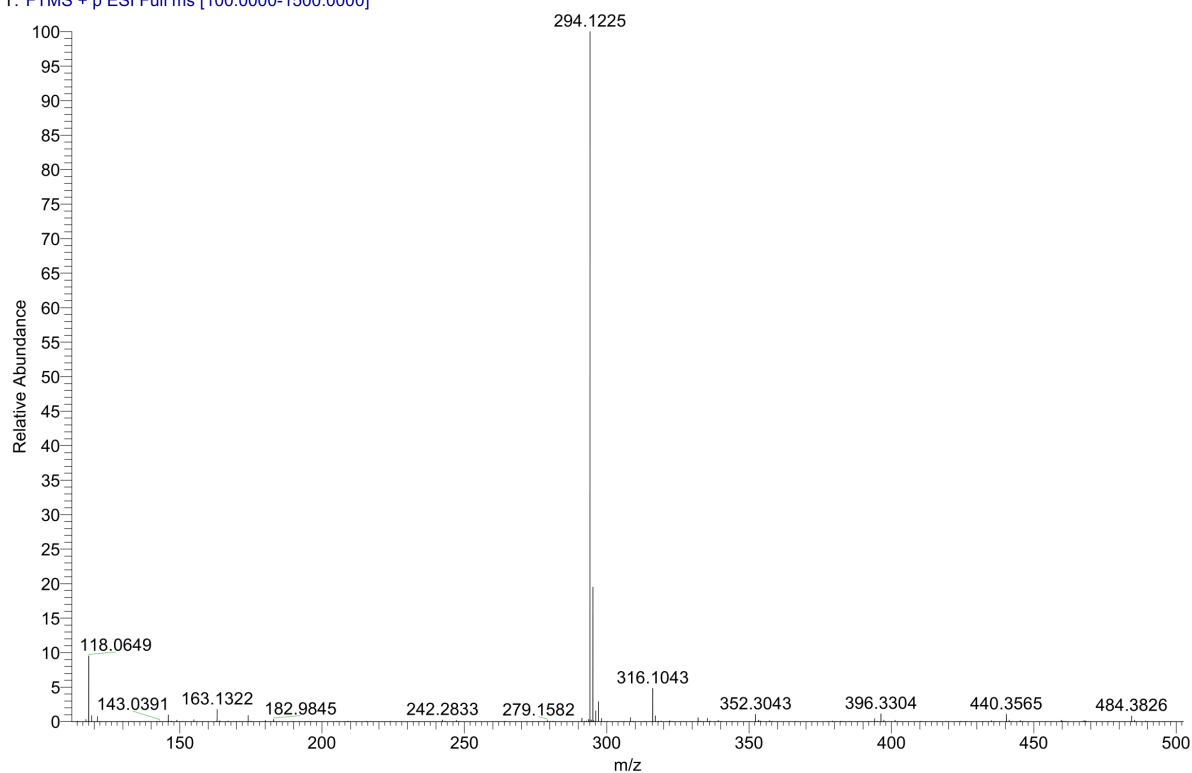
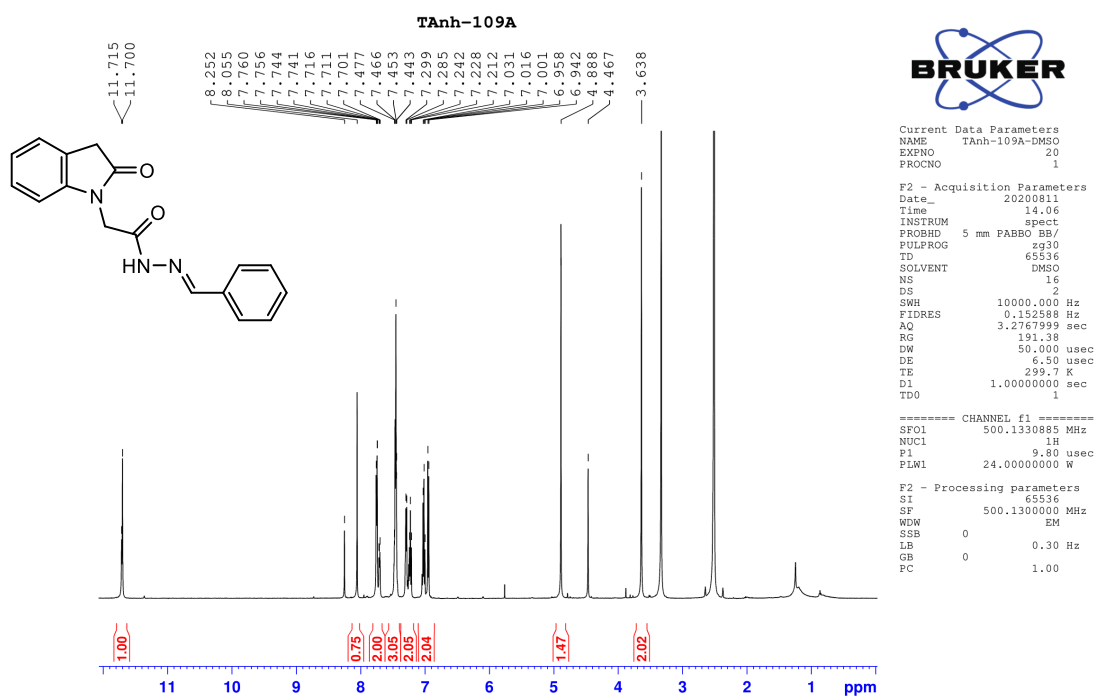


Figure S2. ¹H NMR of compound 4a



Copy of HRMS, ¹H & ¹³C NMR SPECTRA OF THE COMPOUNDS

Figure S1. HRMS of compound 4a

D:\DATA\Old\TA-MS\200823\109A

08/23/20 17:38:53

109A #17 RT: 0.16 AV: 1 NL: 2.23E9

T: FTMS + p ESI Full ms [100.0000-1500.0000]

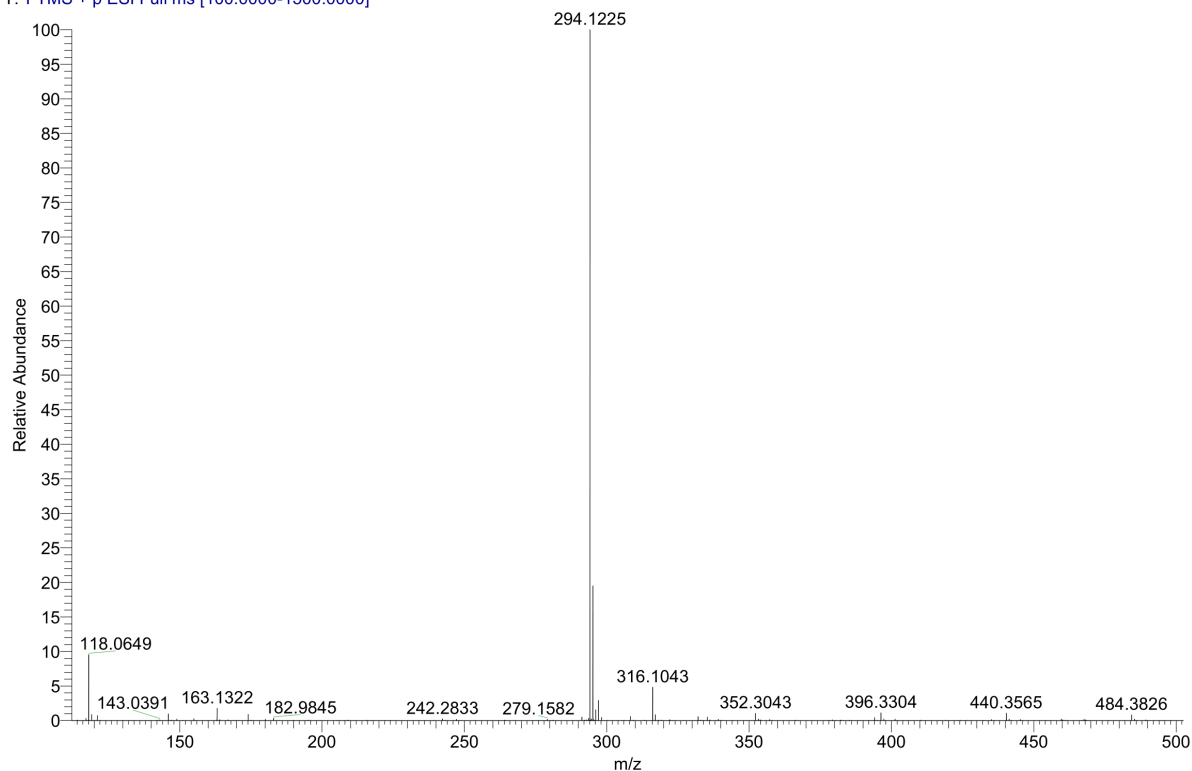


Figure S2. ¹H NMR of compound 4a

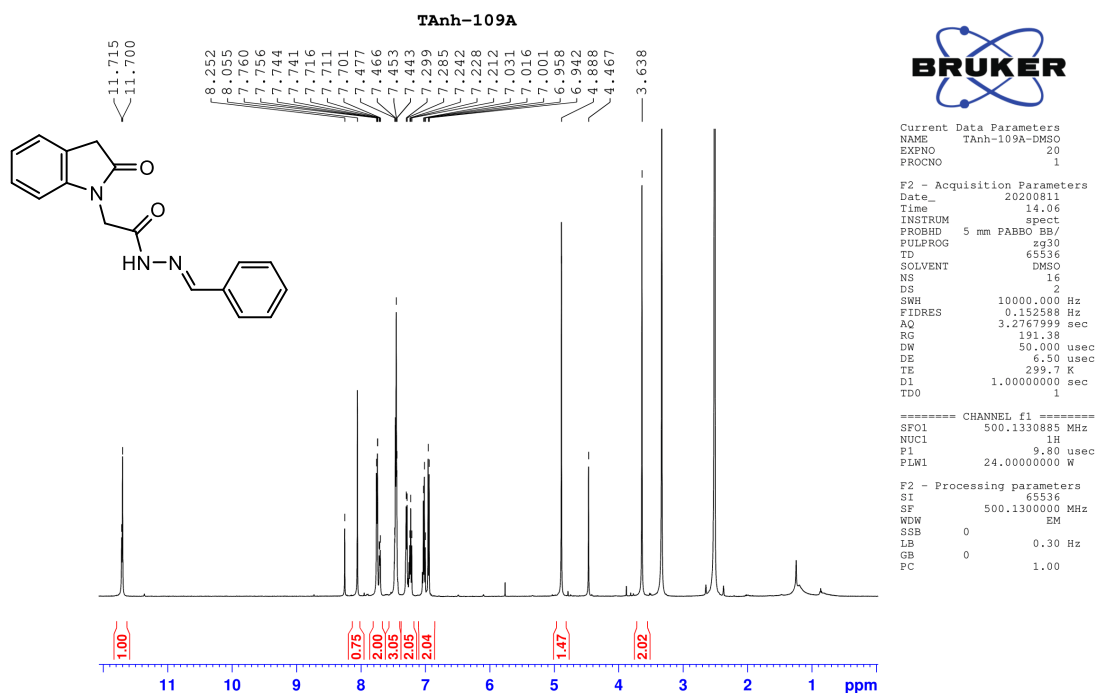


Figure S3. ^{13}C NMR of compound 4a

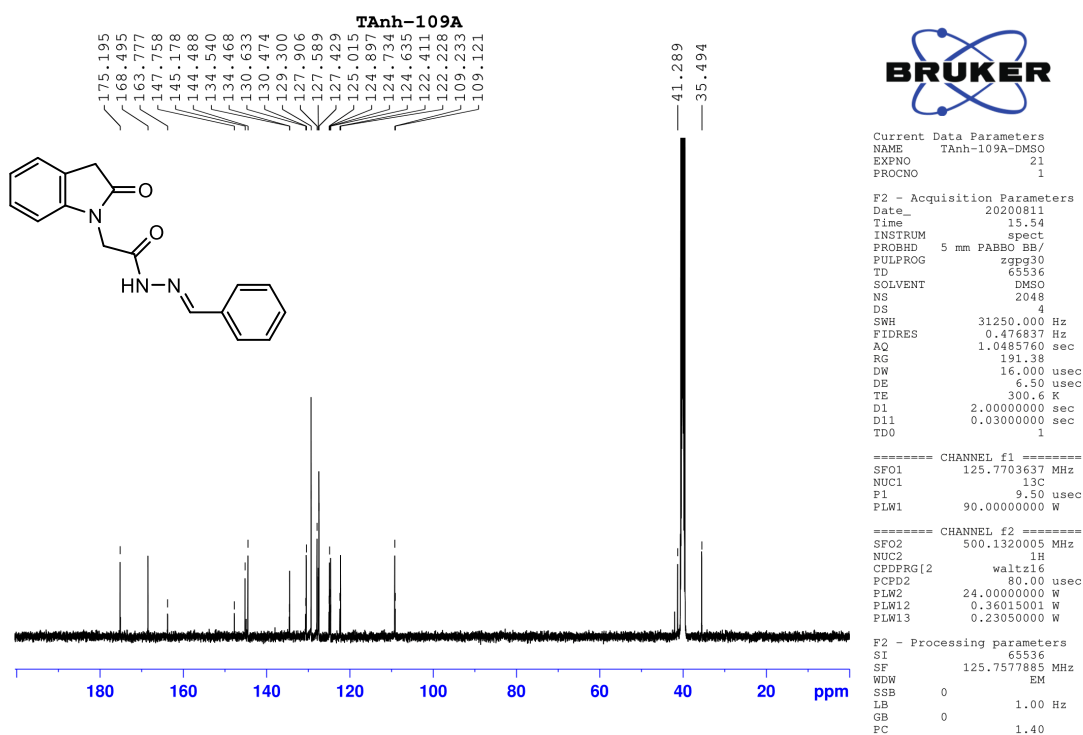


Figure S4. HRMS of compound 4b

D:\DATA\Old\TA-MS\200823\109B

08/23/20 17:44:45

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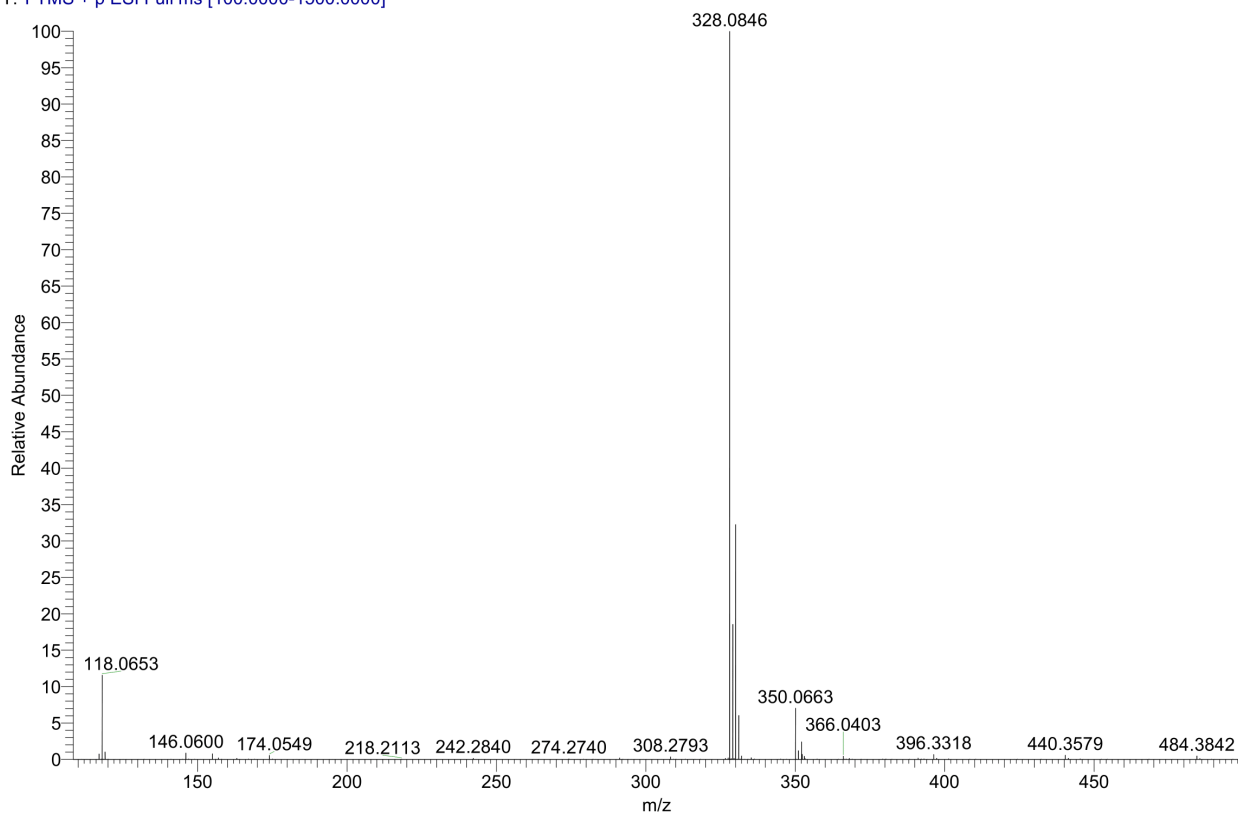


Figure S5. ¹H NMR of compound 4b

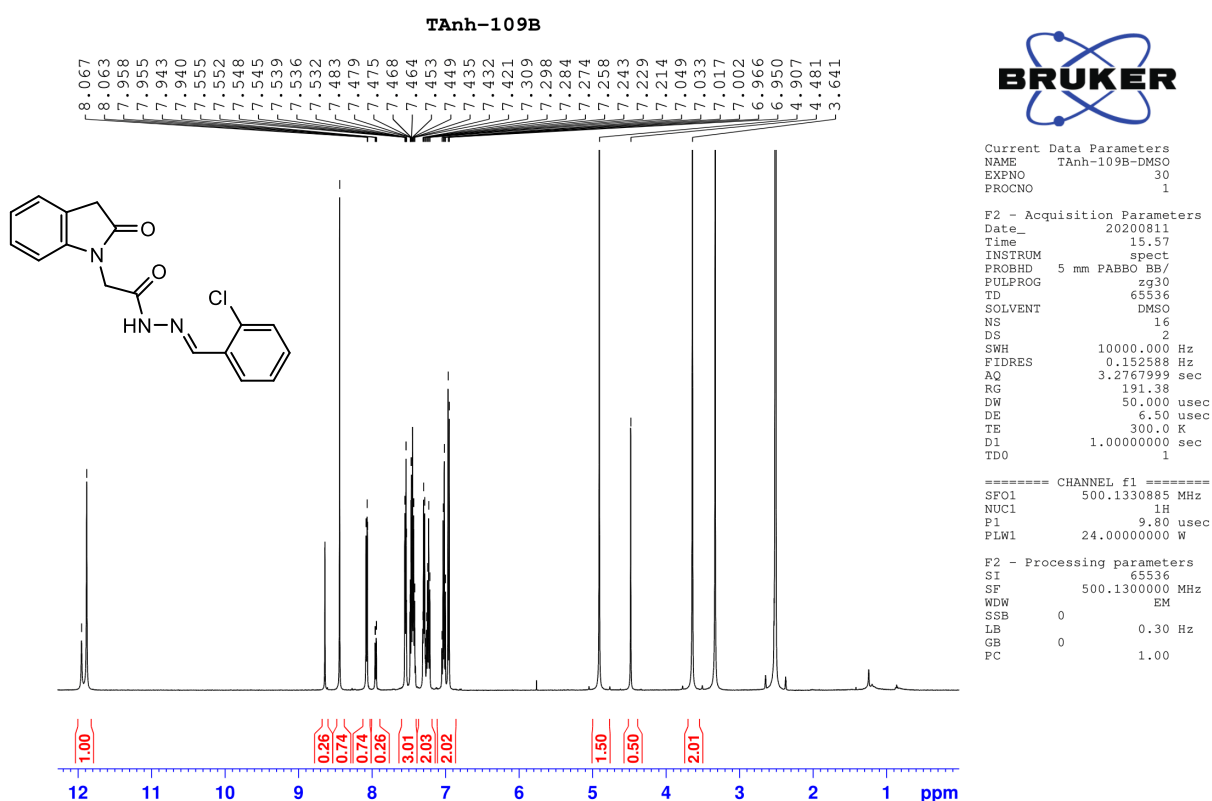


Figure S6. ¹³C NMR of compound 4b

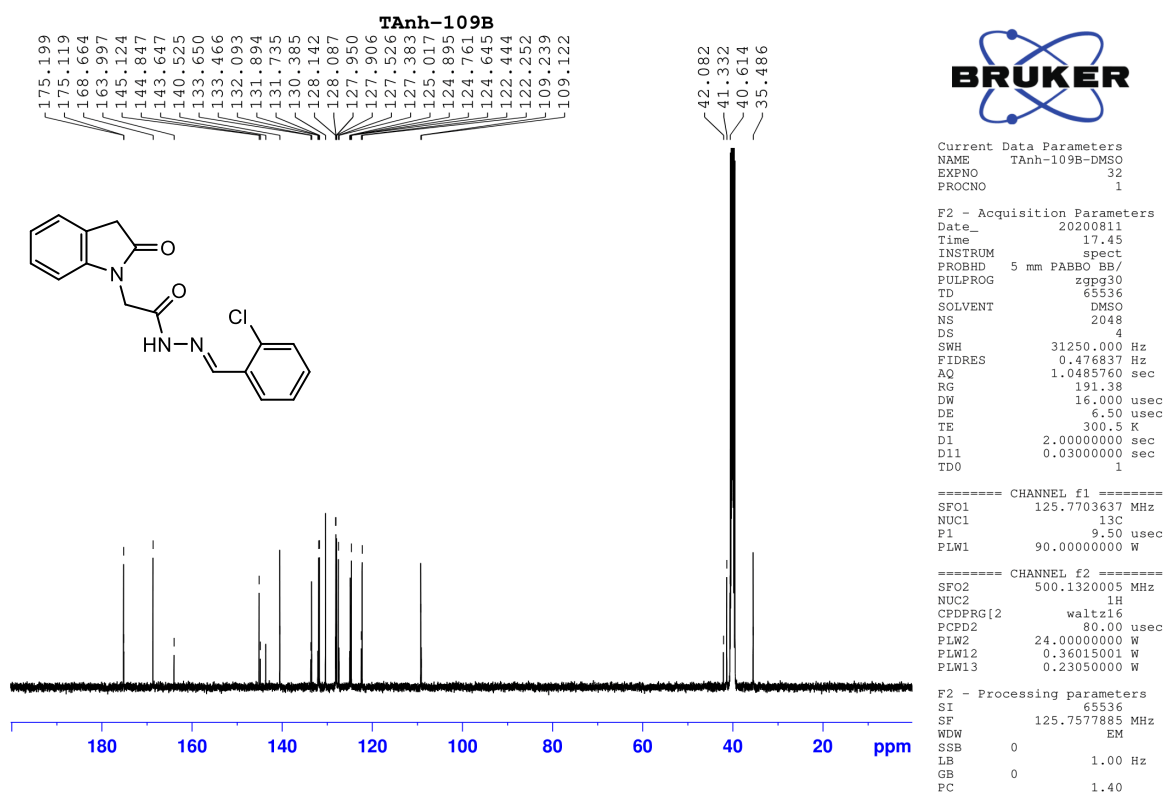


Figure S7. HRMS of compound 4c

D:\DATA\Old\TA-MS\200803\109C

08/03/20 15:19:15

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

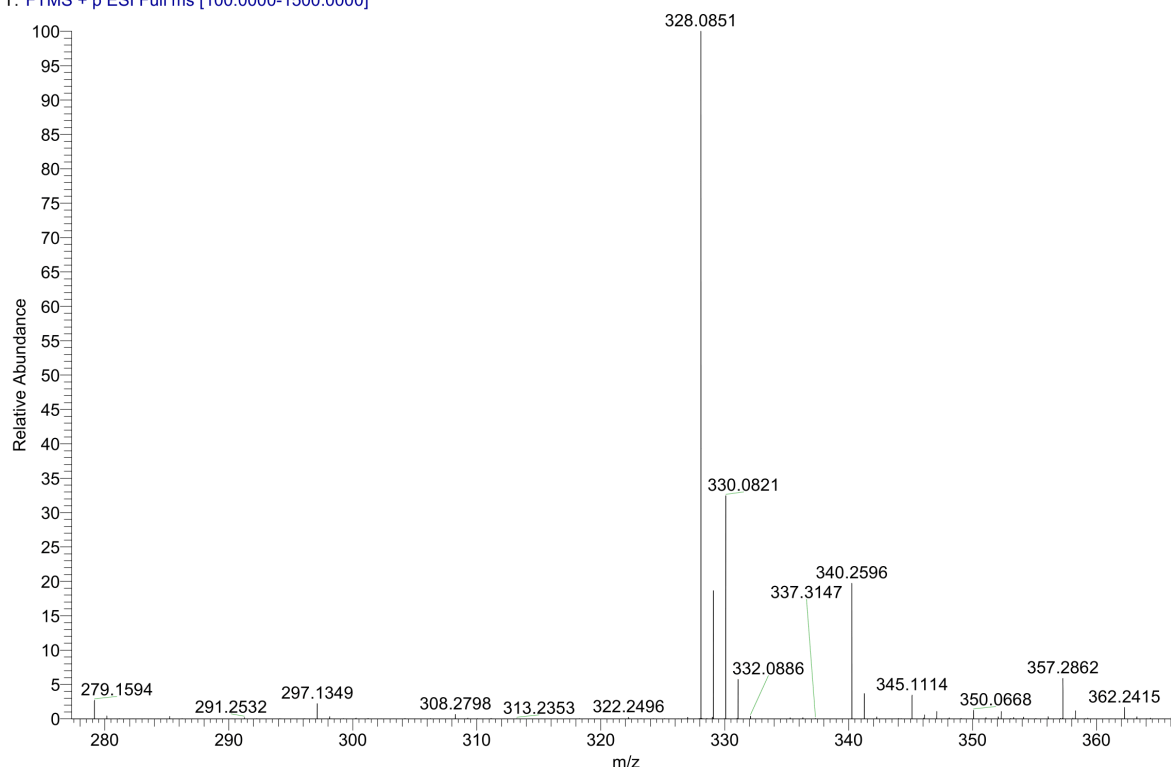


Figure S8. ¹H NMR of compound 4c

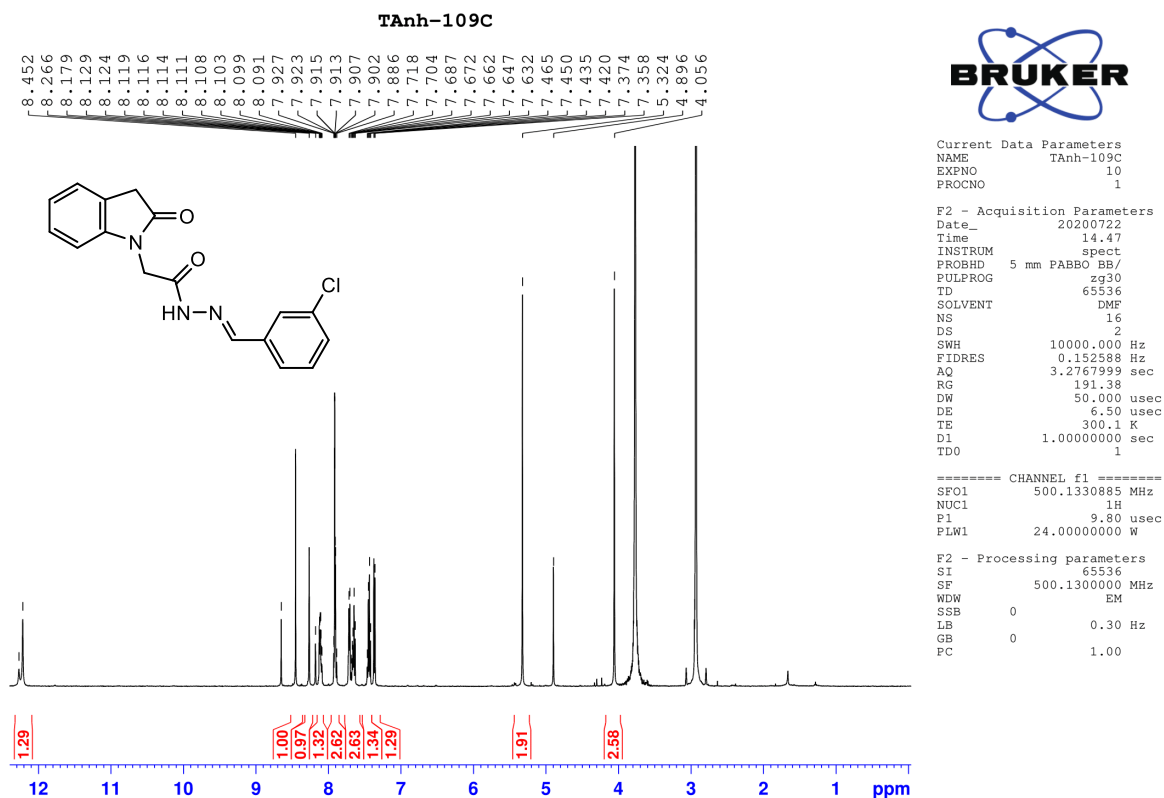


Figure S9. ^{13}C NMR of compound 4c

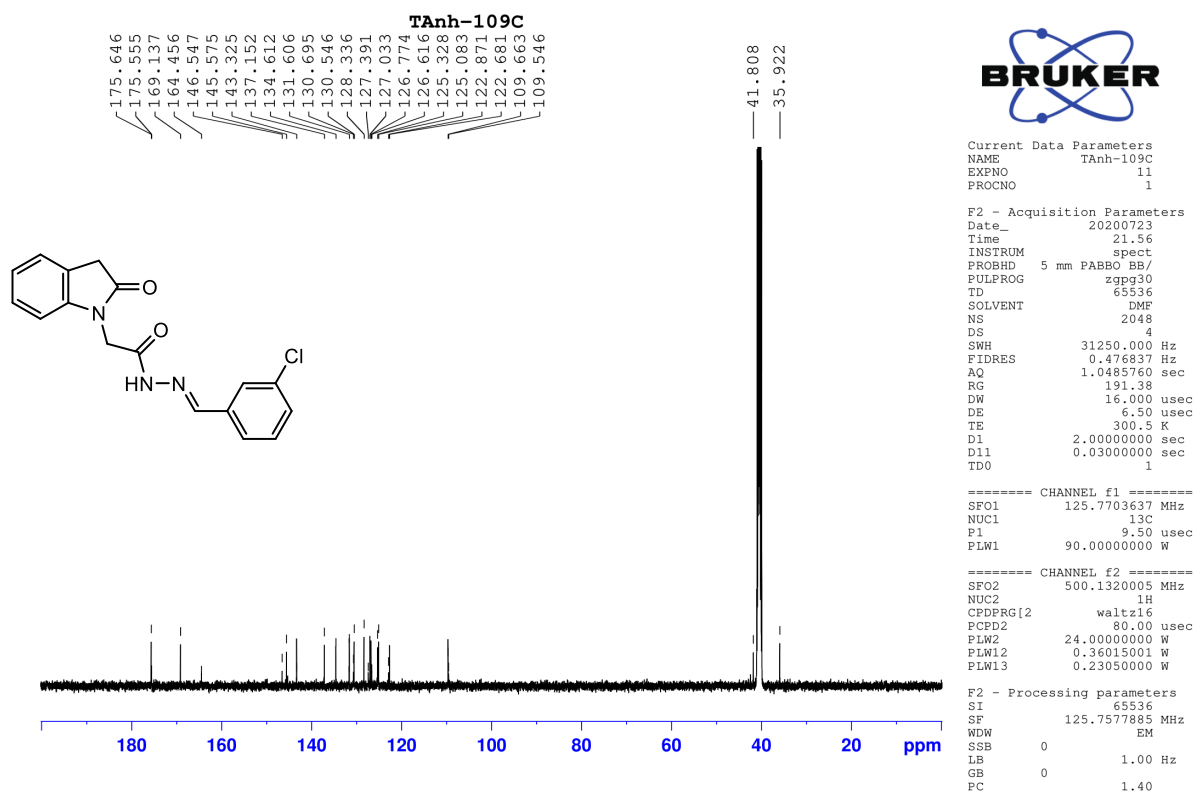


Figure S10. HRMS of compound 4d

D:\DATA\Old\TA-MS\200823\109D

08/23/20 17:56:29

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

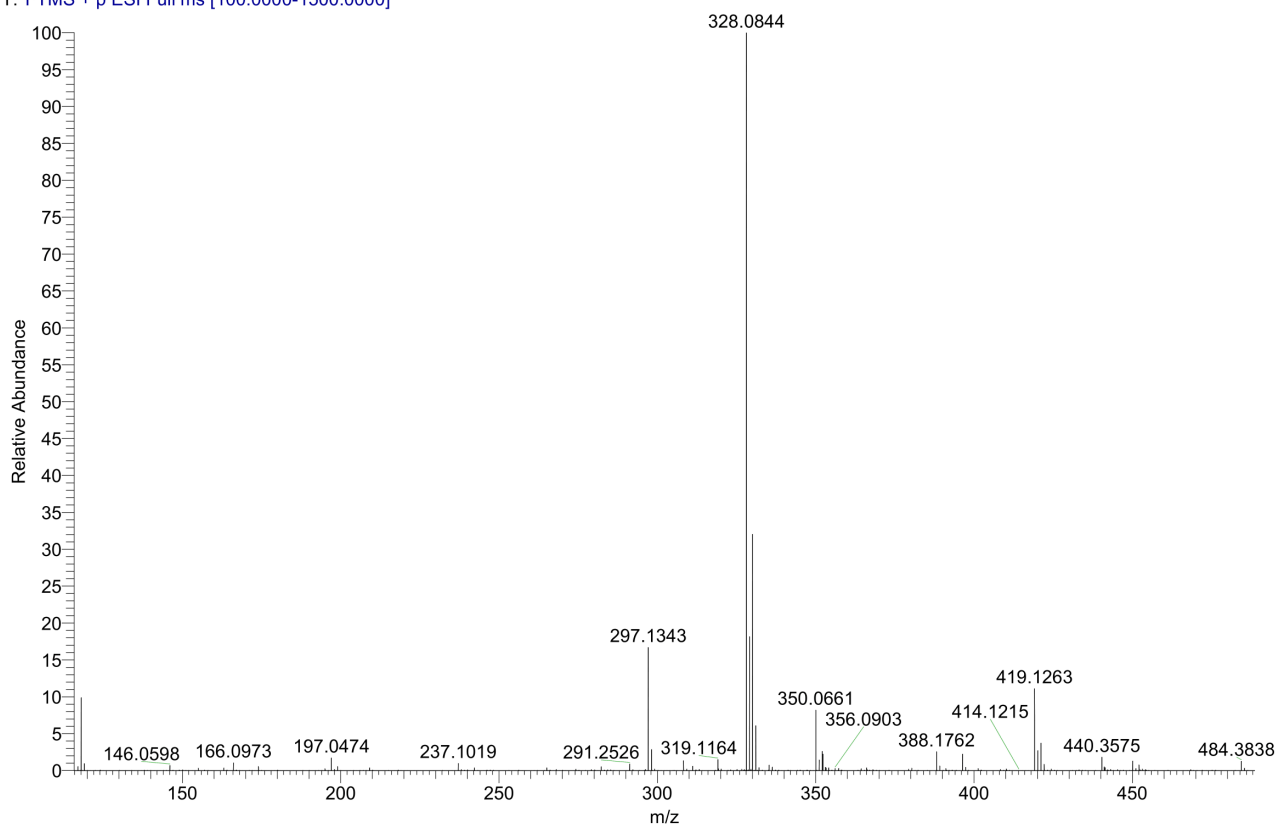


Figure S11. ¹H NMR of compound 4d

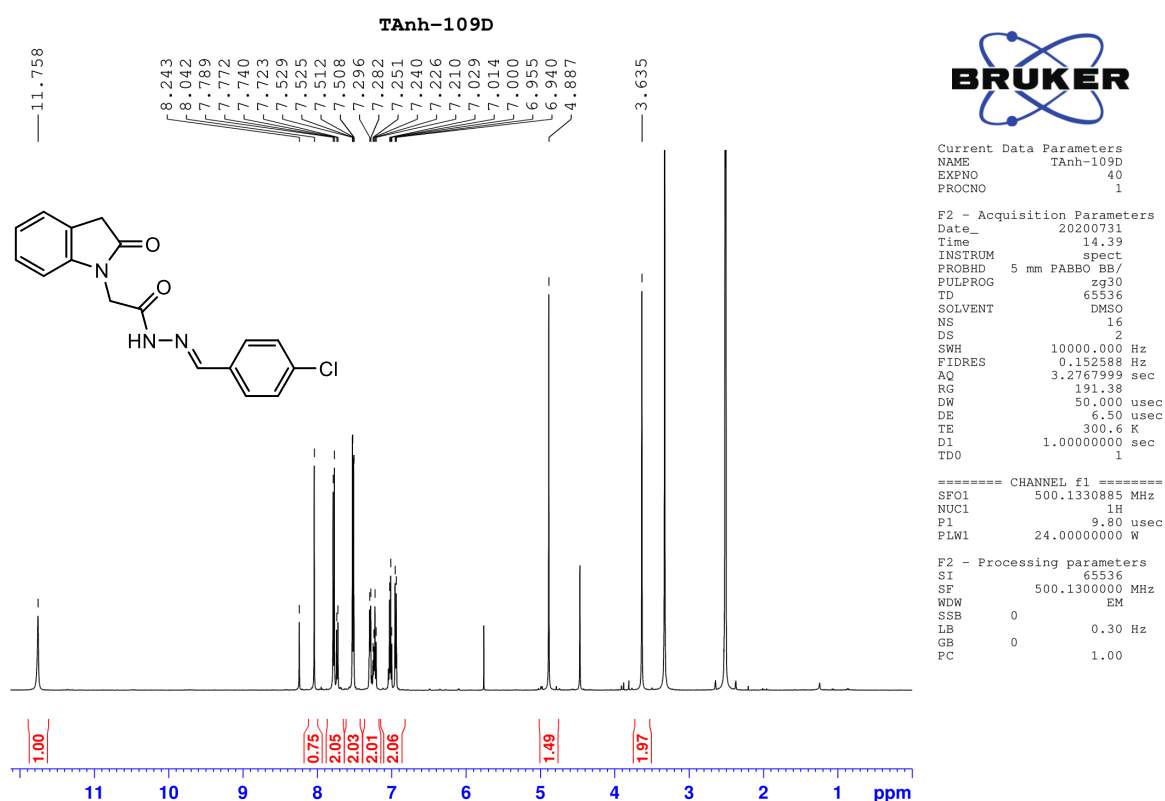


Figure S12. ¹³C NMR of compound 4d

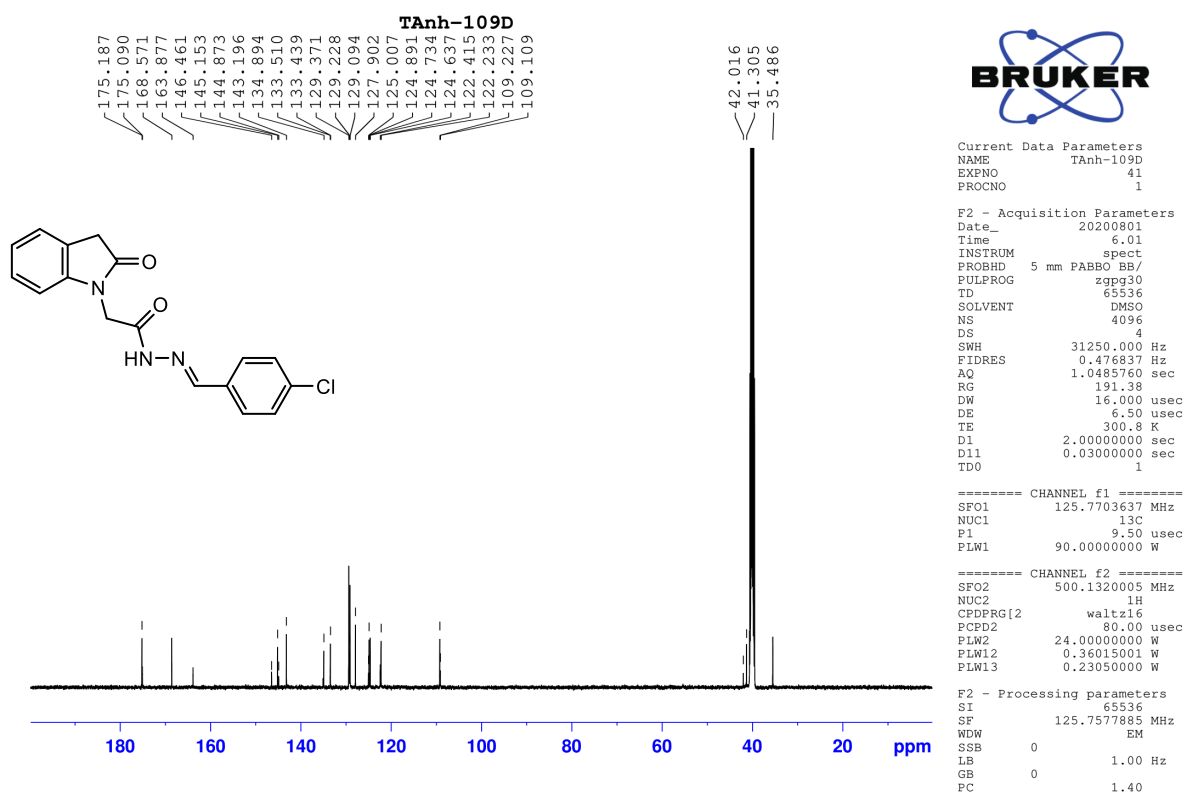


Figure S13. HRMS of compound 4e

D:\DATA\Old\TA-MS\200823\109E

08/23/20 17:50:37

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

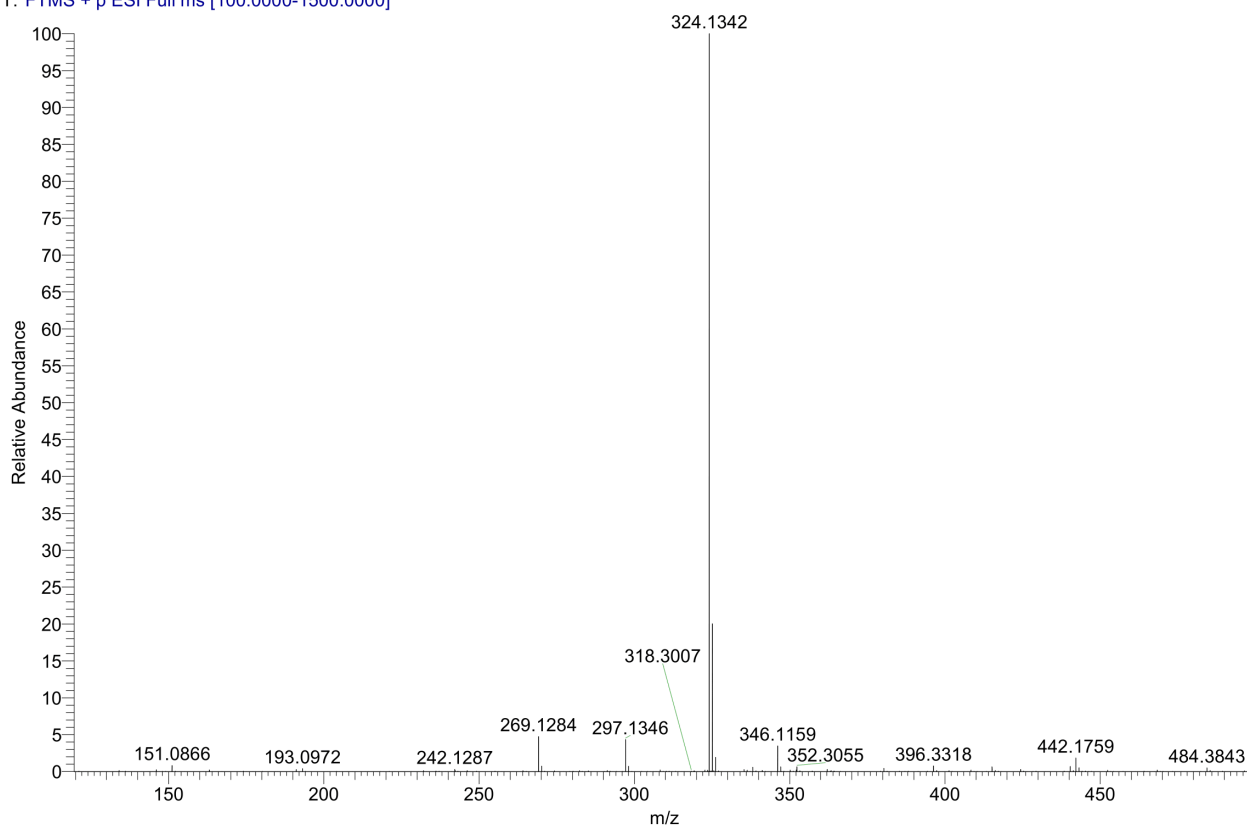


Figure S14. ¹H NMR of compound 4e

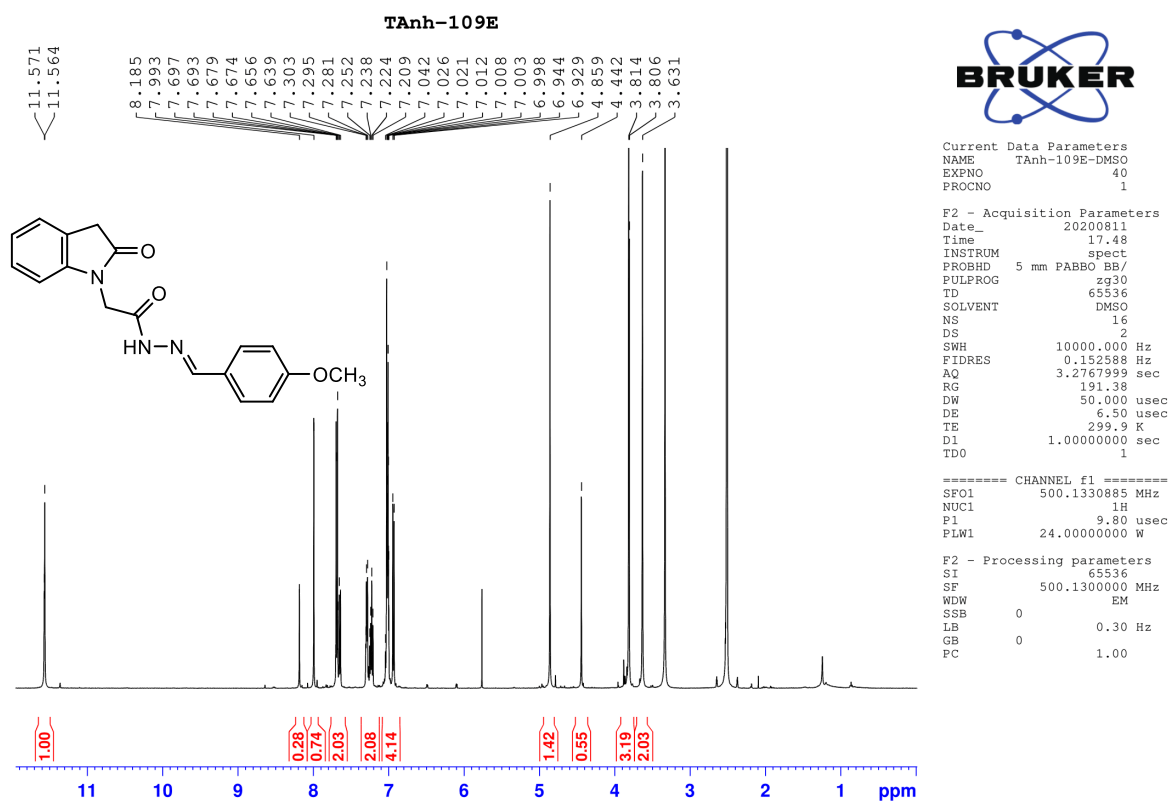


Figure S15. ^{13}C NMR of compound 4e

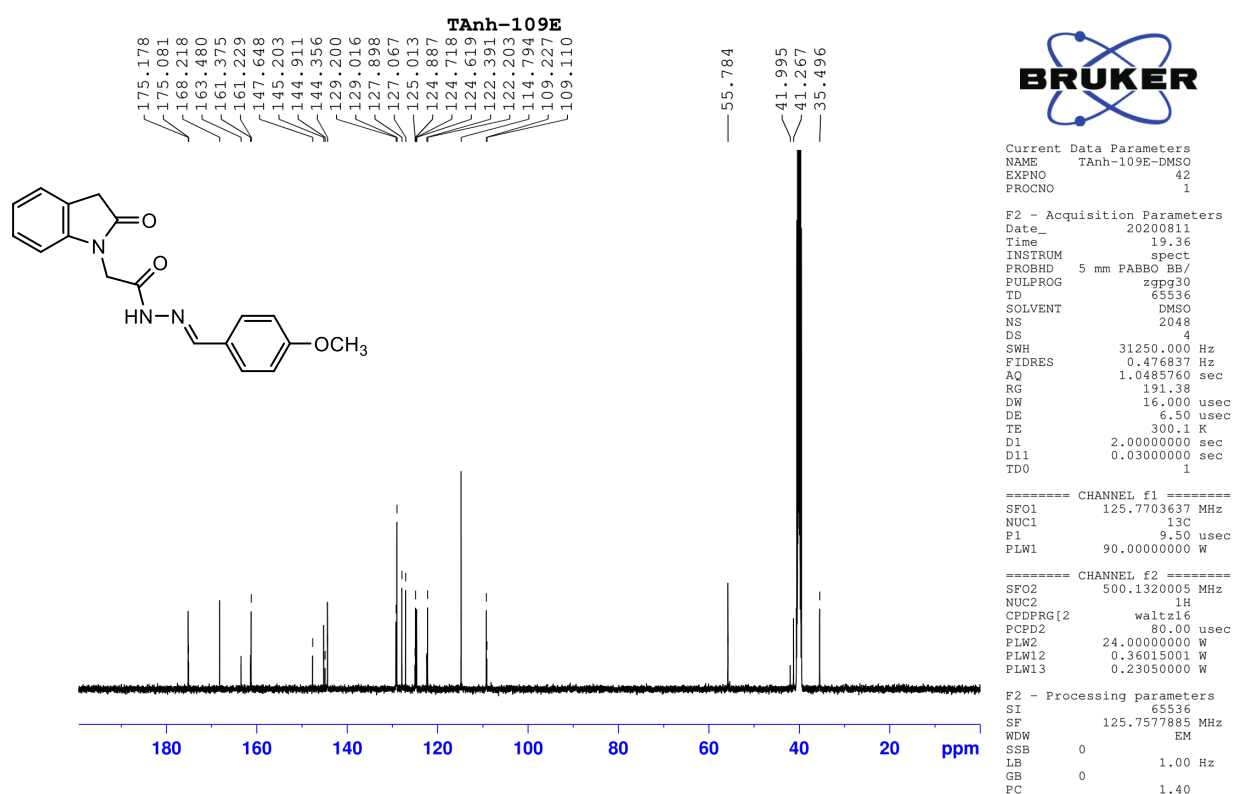


Figure S16. HRMS of compound 4f

D:\DATA\Old\TA-MS\200823\109F

08/23/20 18:02:21

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

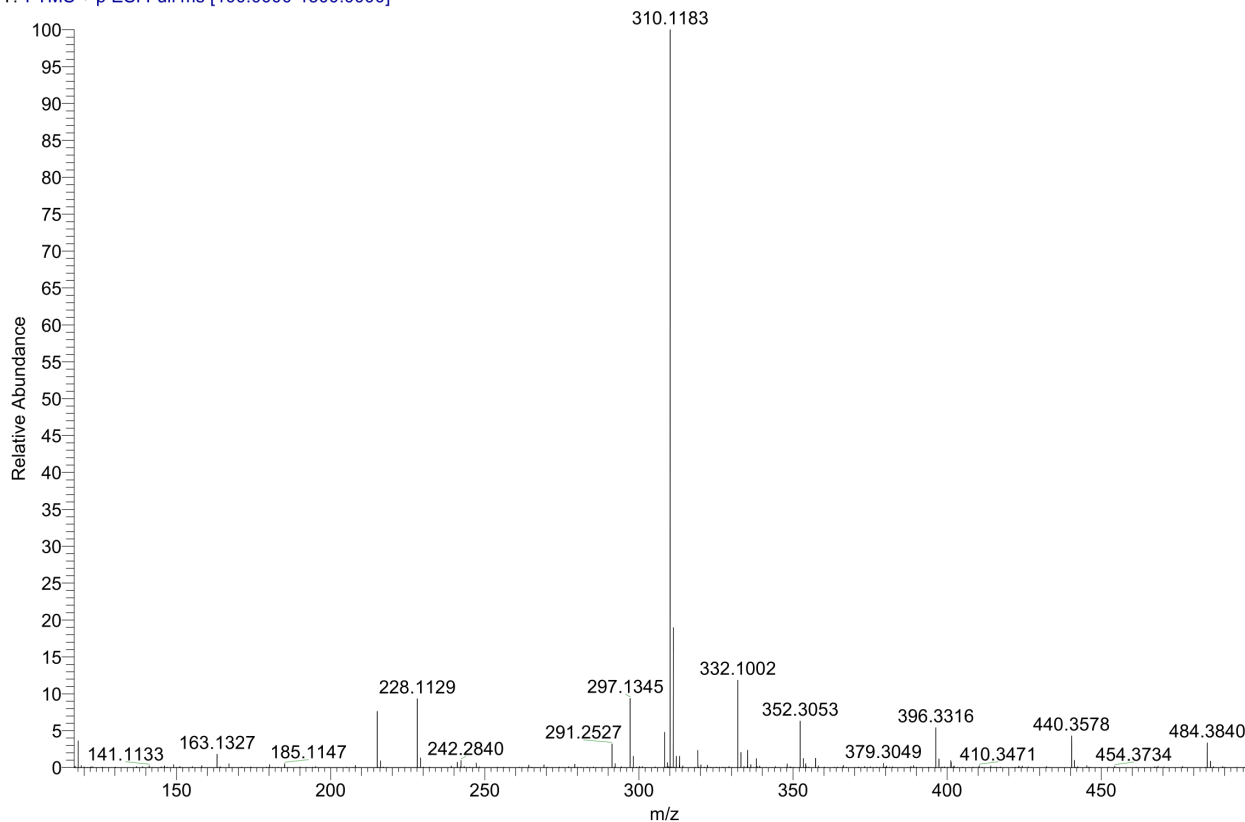
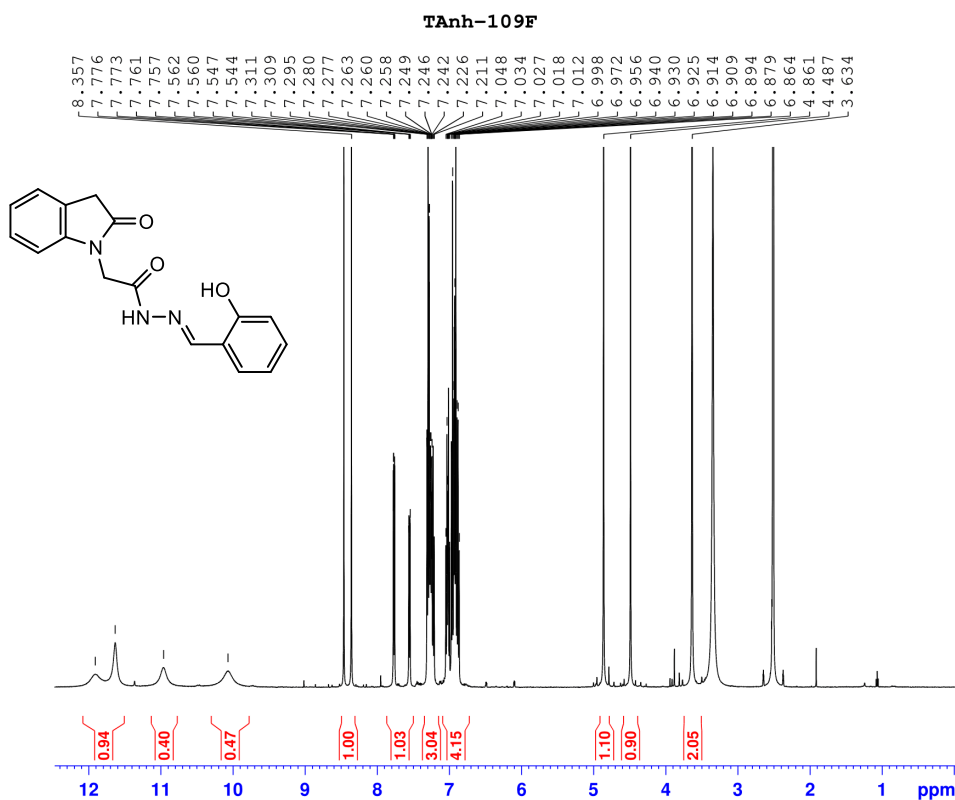


Figure S17. ¹H NMR of compound 4f



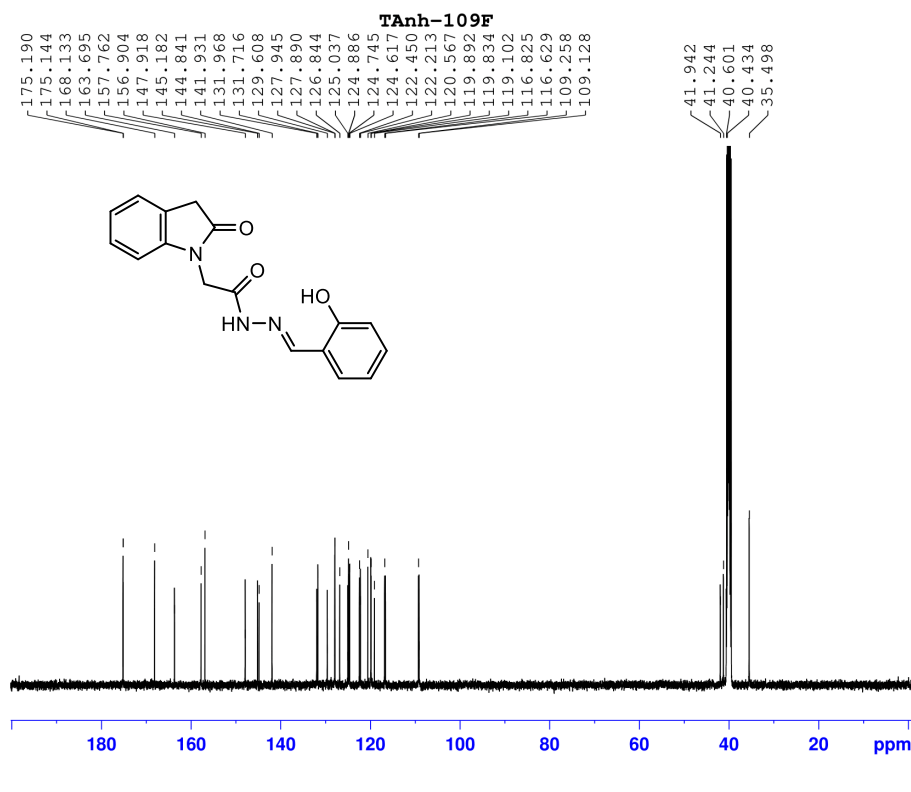
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PROCNO 1

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FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 191.38
DW 50.000 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 500.1330885 MHz
NUC1 1H
P1 9.80 usec
PLW1 24.00000000 W

F2 - Processing parameters
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SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S18. ¹³C NMR of compound 4f



Current Data Parameters
NAME TAnh-109F-DMSO
EXPNO 52
PROCNO 1

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Time 21.27
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 191.38
DW 16.000 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 125.7703637 MHz
NUC1 13C
P1 9.50 usec
PLW1 90.00000000 W

===== CHANNEL f2 =====
SF02 500.1320005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 24.00000000 W
PLW12 0.36015001 W
PLW13 0.23050000 W

F2 - Processing parameters
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SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
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Figure S19. HRMS of compound 4g

D:\DATA\Old\TA-MS\200823\109G

08/23/20 18:08:13

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

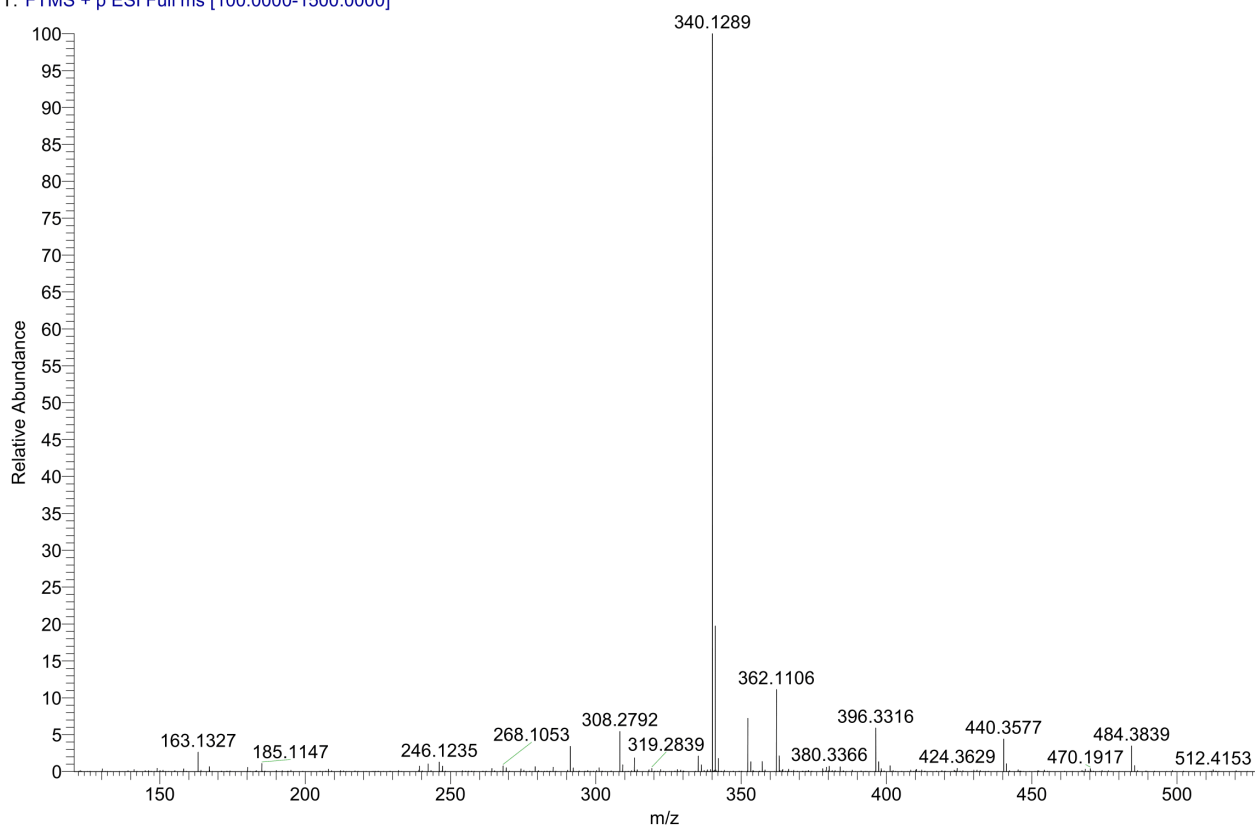


Figure S20. ¹H NMR of compound 4g

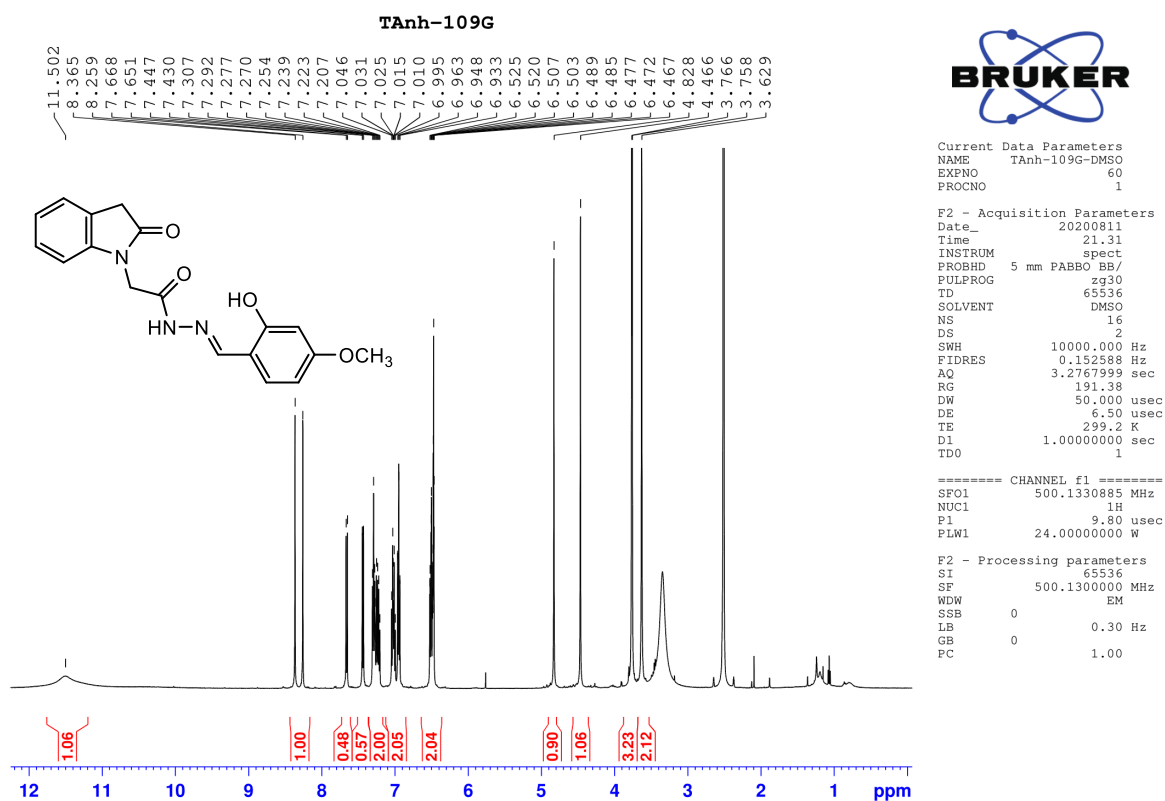


Figure S21. ^{13}C NMR of compound 4g

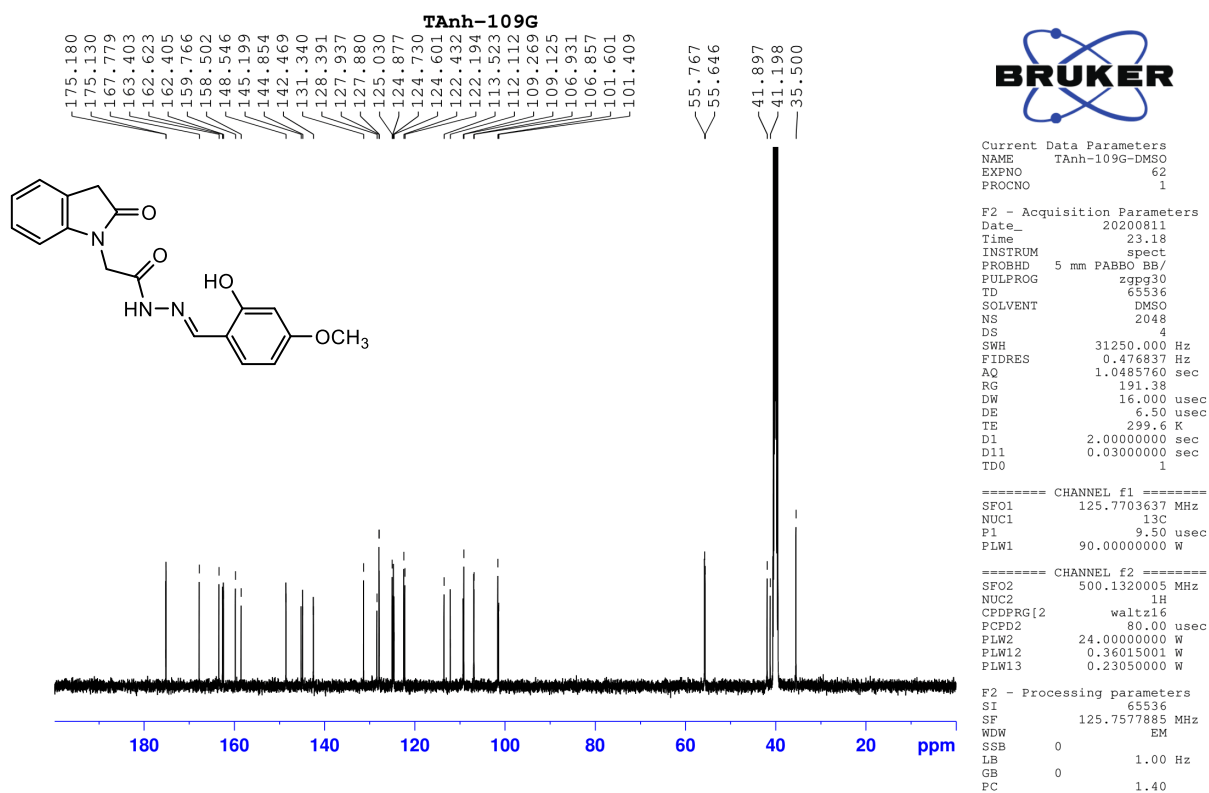


Figure S22. HRMS of compound 4h

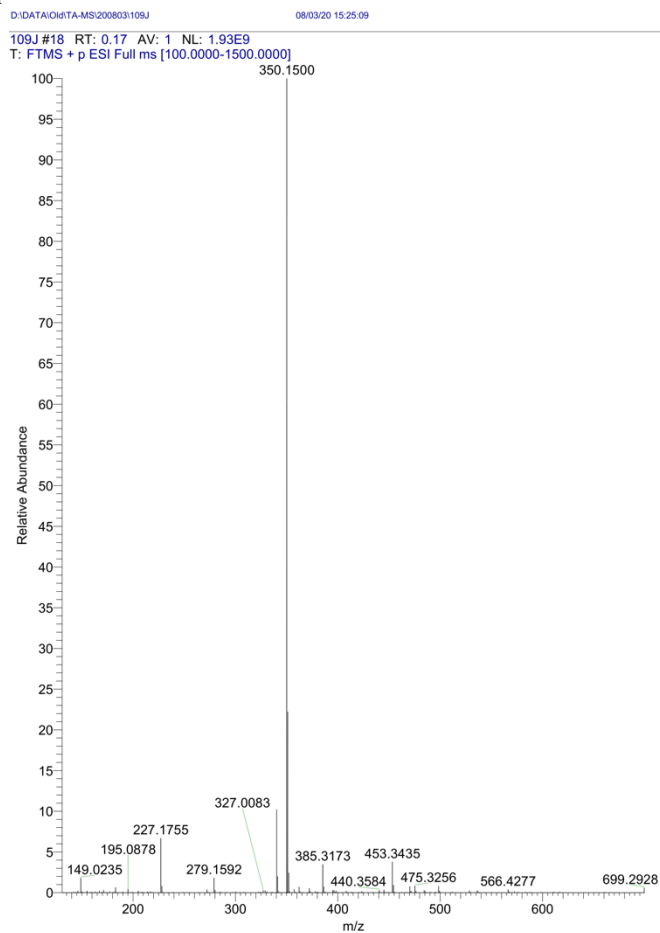


Figure S23. ¹H NMR of compound 4h

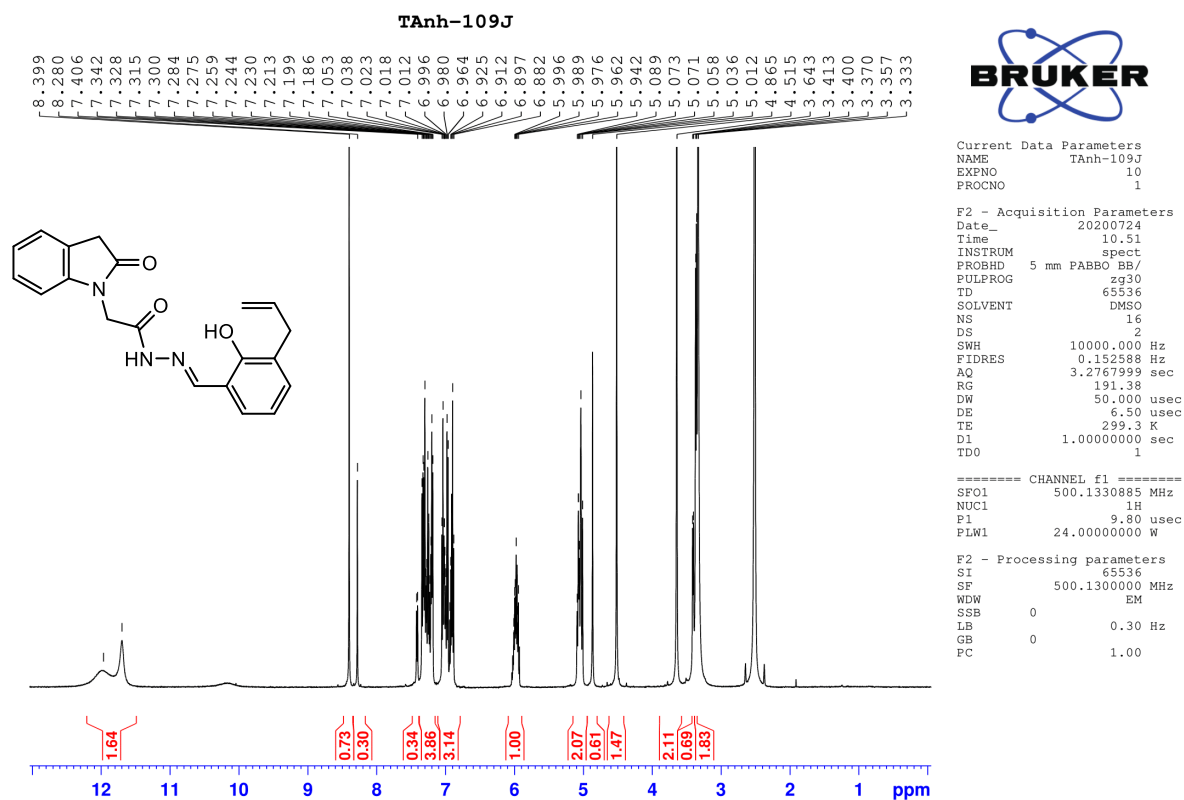


Figure S24. ¹³C NMR of compound 4h

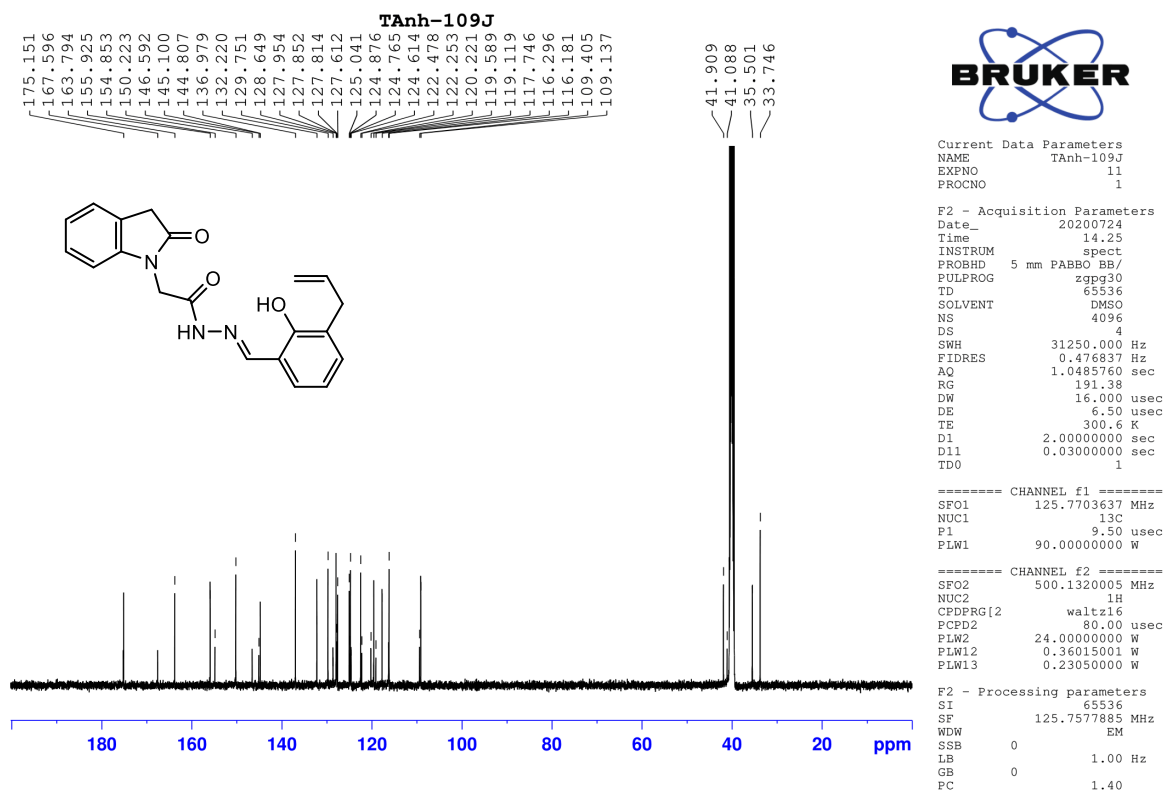


Figure S25. HRMS of compound 4i

D:\DATA\Old\TA-MS\200823\111A

08/23/20 18:14:05

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

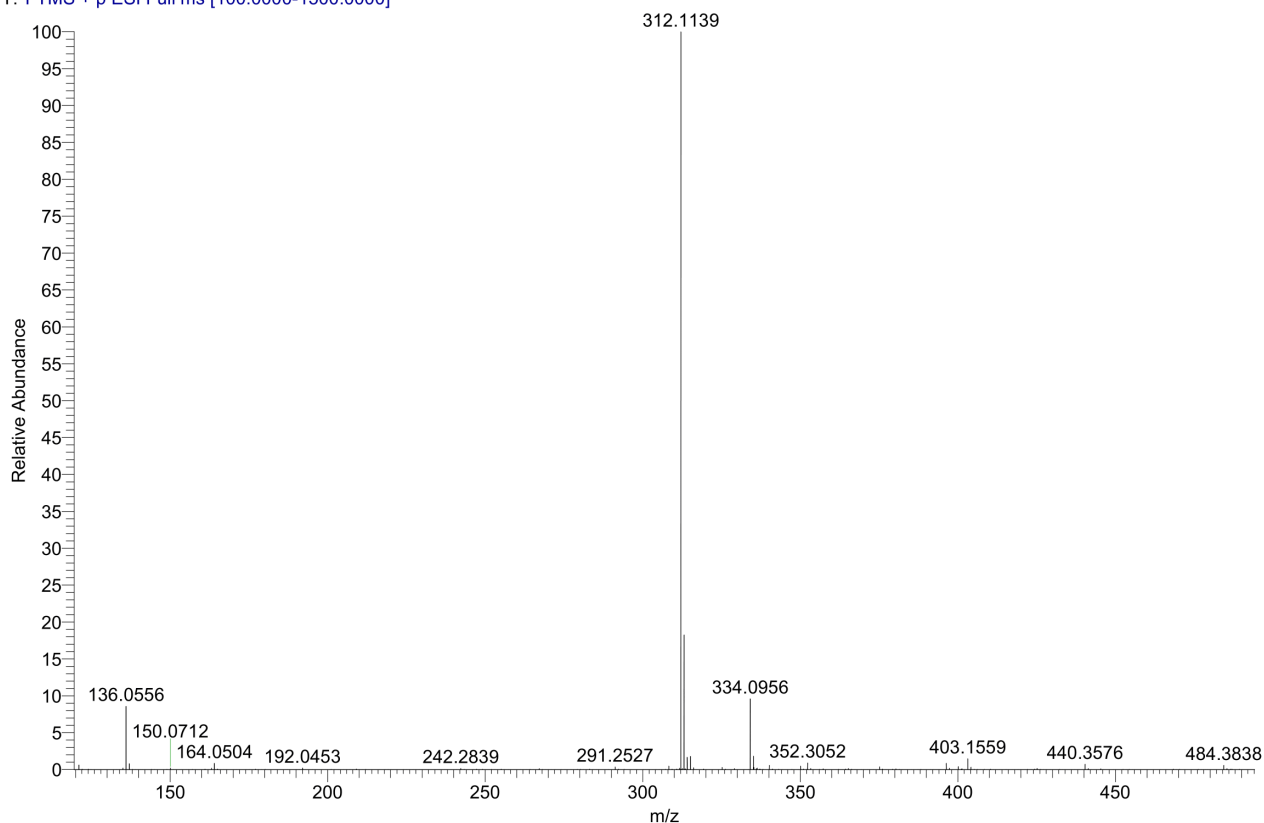


Figure S26. ¹H NMR of compound 4i

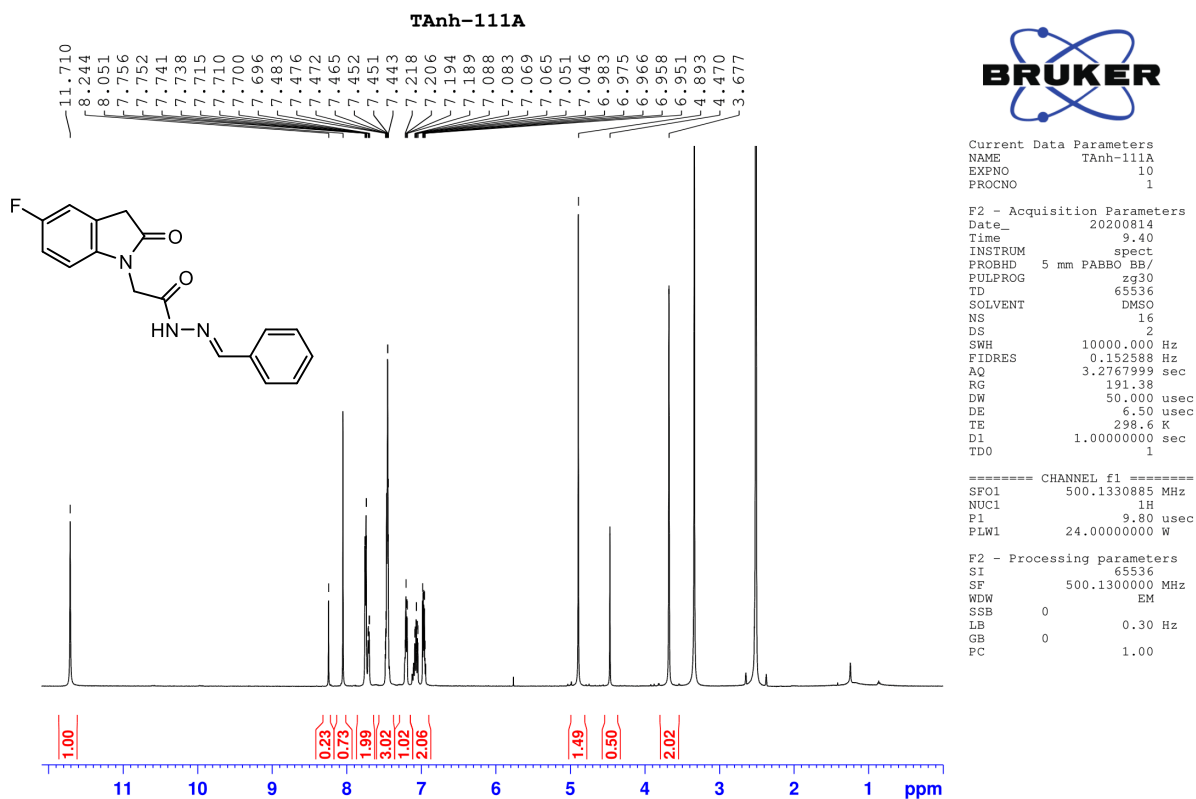


Figure S27. ^{13}C NMR of compound 4i

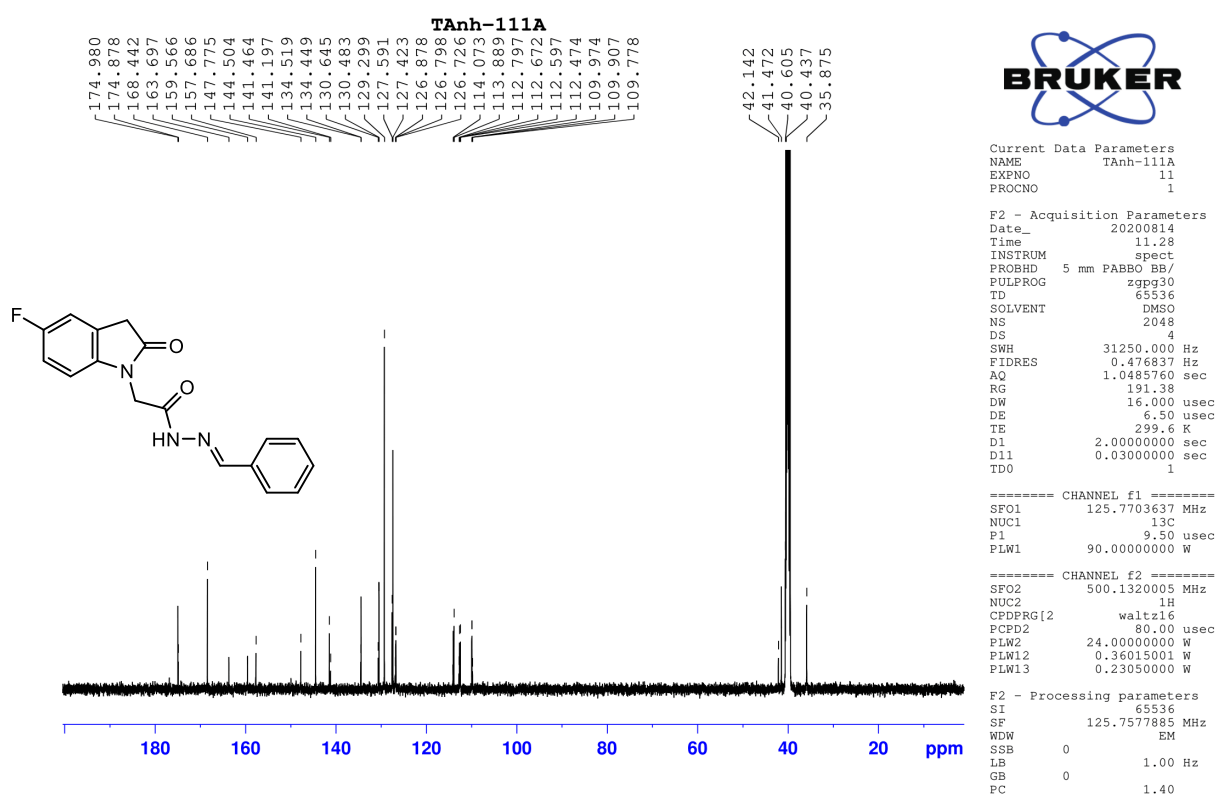


Figure S28. HRMS of compound 4j

D:\DATA\Old\TA-MS\200823\111B

08/23/20 18:19:57

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

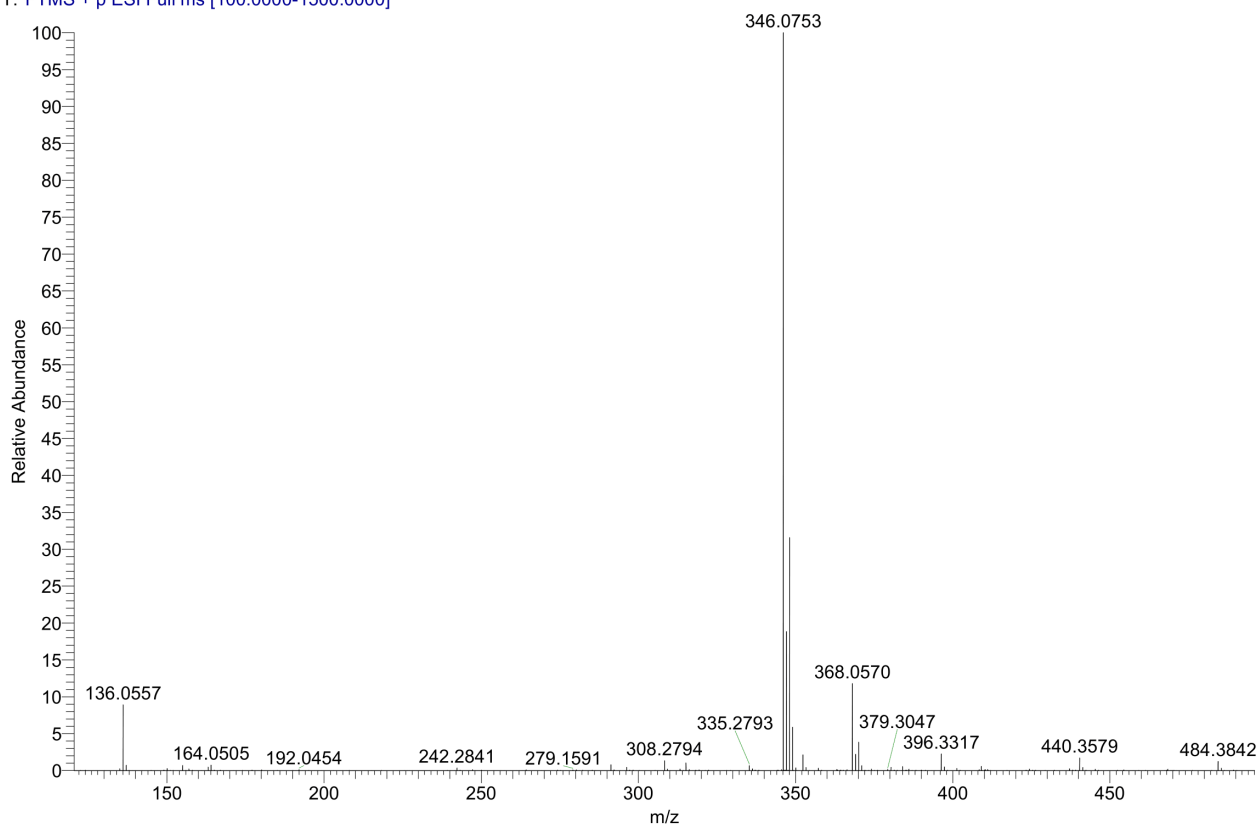


Figure S29. ¹H NMR of compound 4j

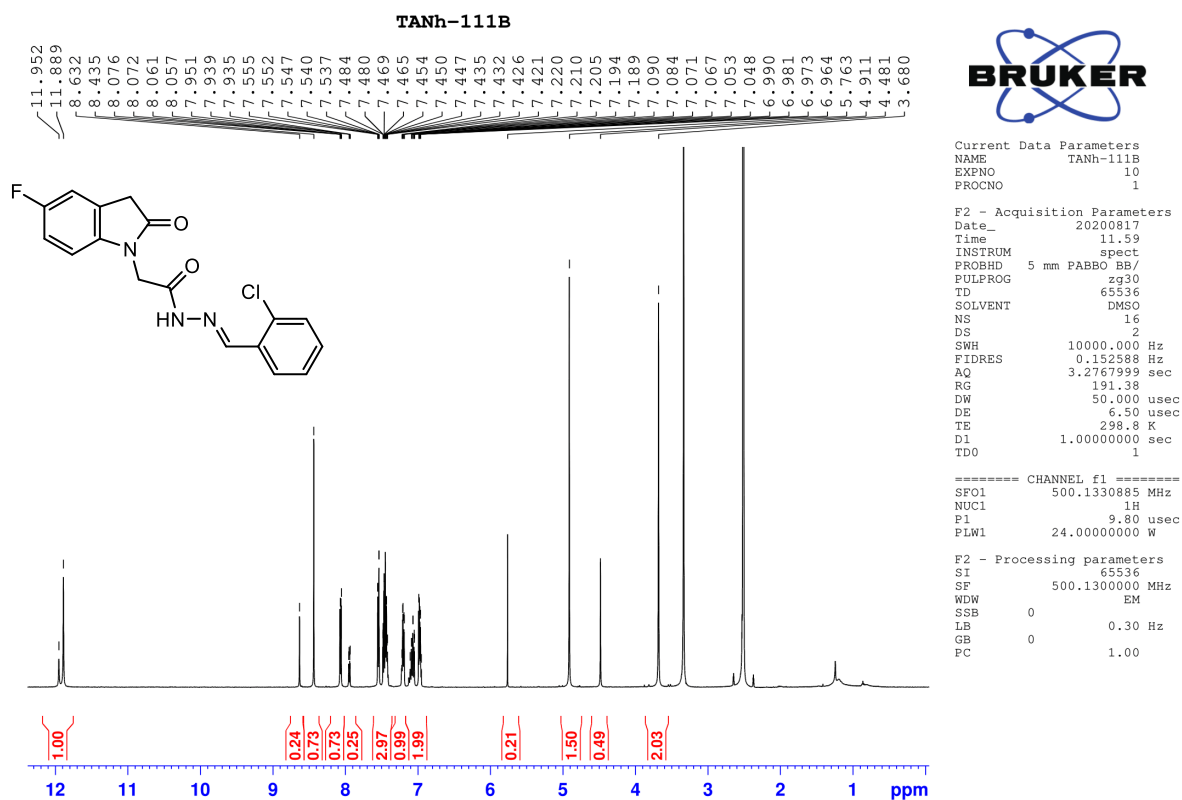


Figure S30. ¹³C NMR of compound 4j

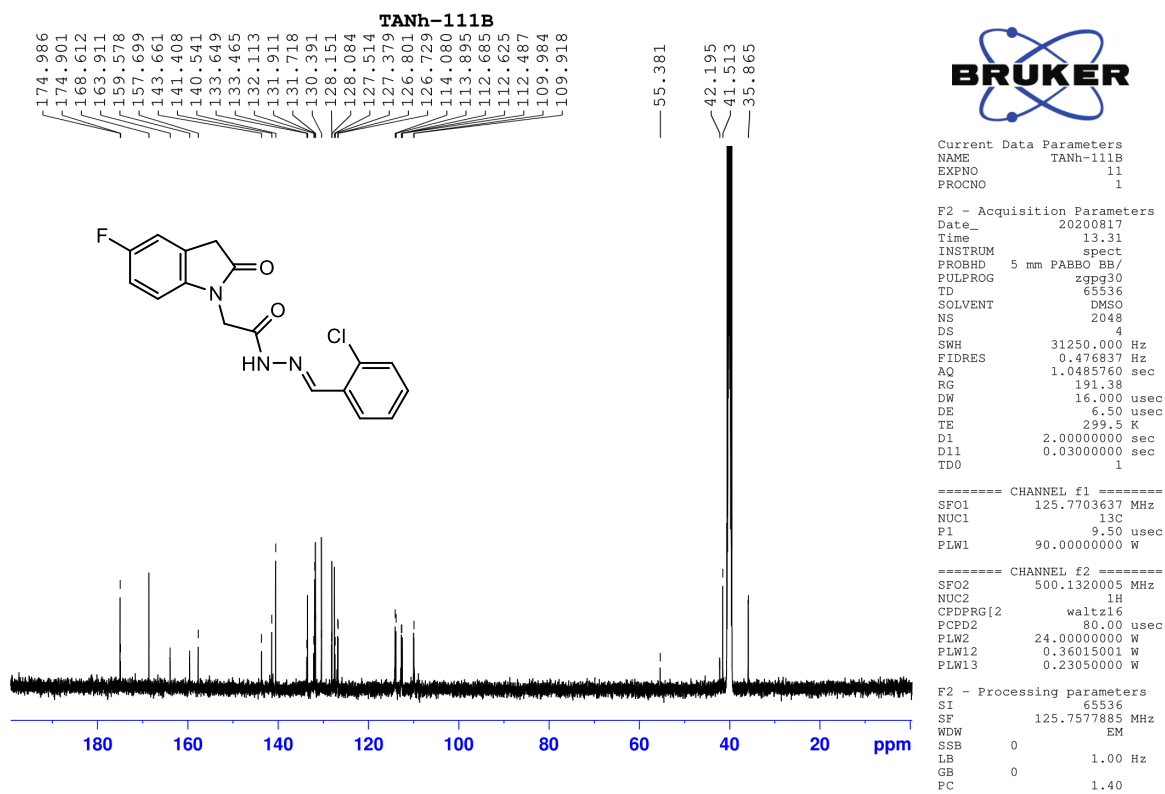


Figure S31. HRMS of compound 4k

D:\DATA\Old\TA-MS\200823\111C

08/23/20 18:25:49

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

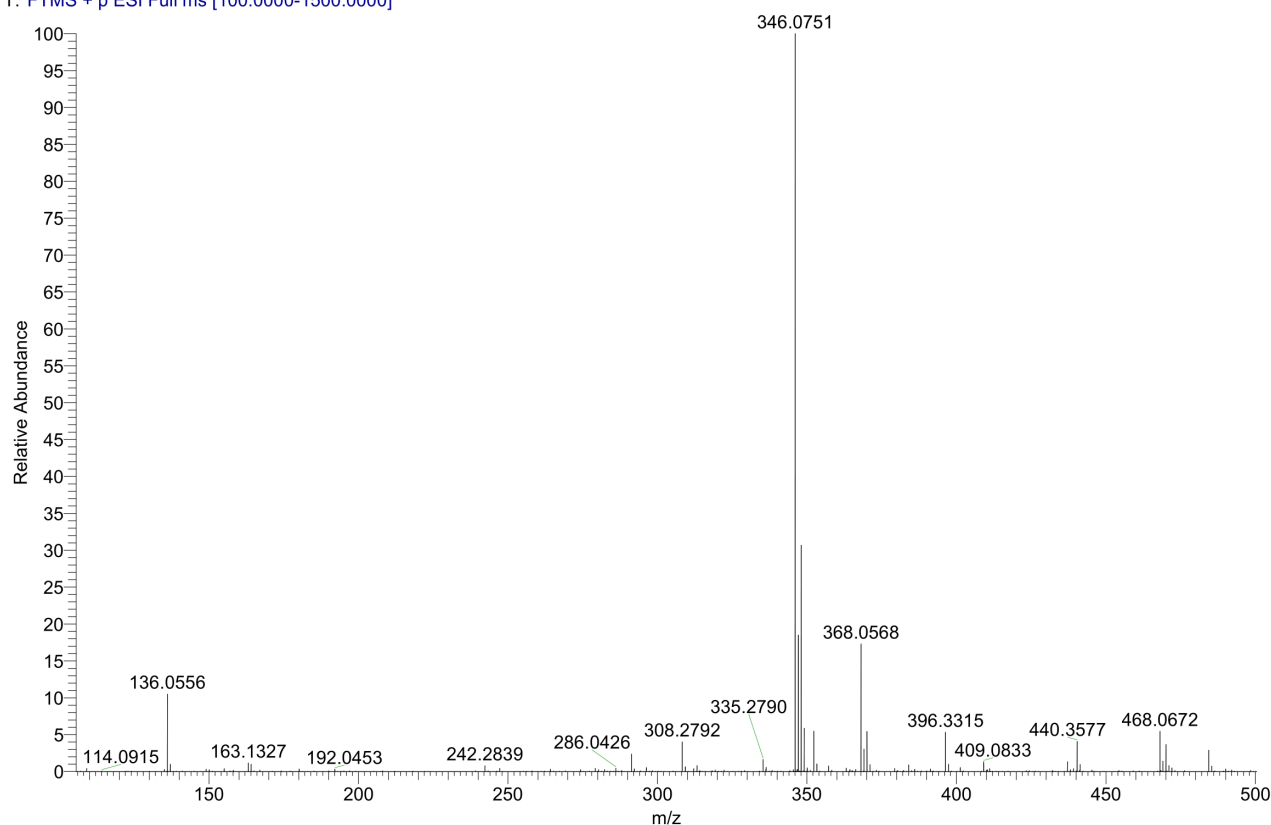


Figure S32. ¹H NMR of compound 4k

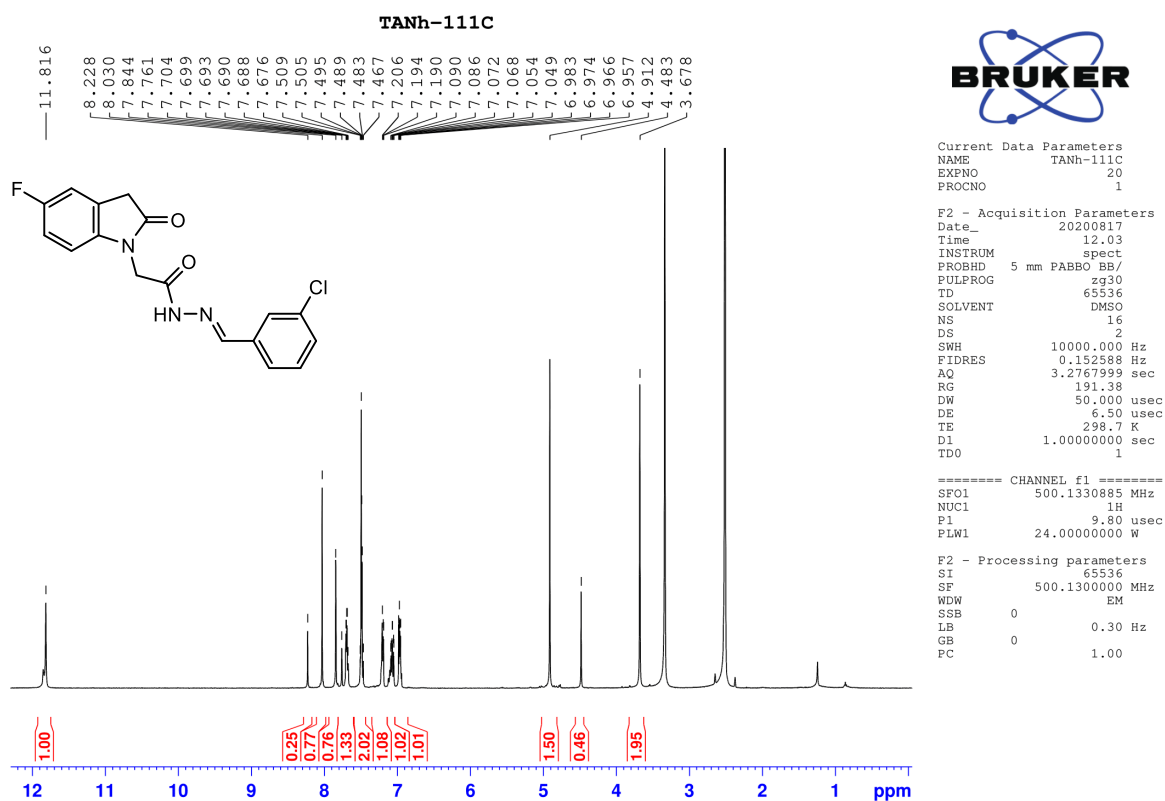


Figure S33. ^{13}C NMR of compound 4k

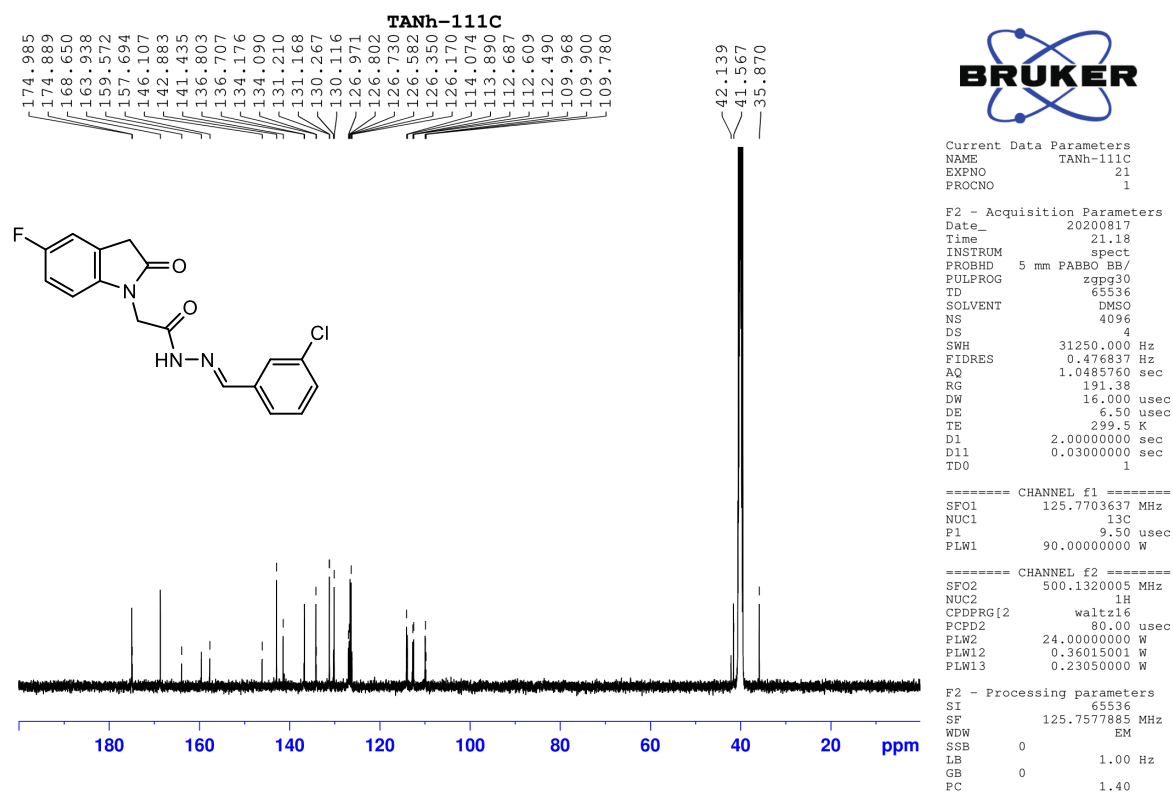


Figure S34. HRMS of compound 4l

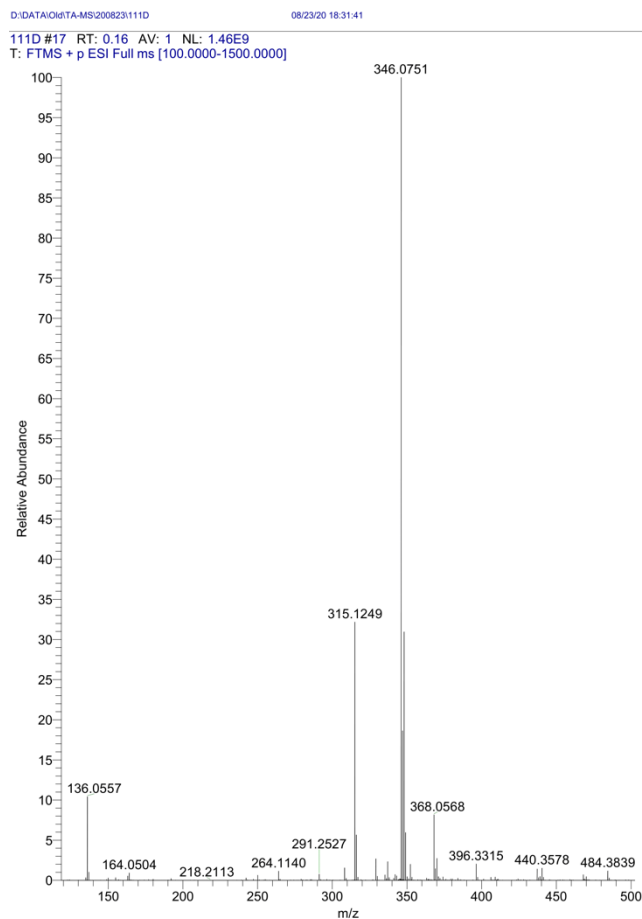
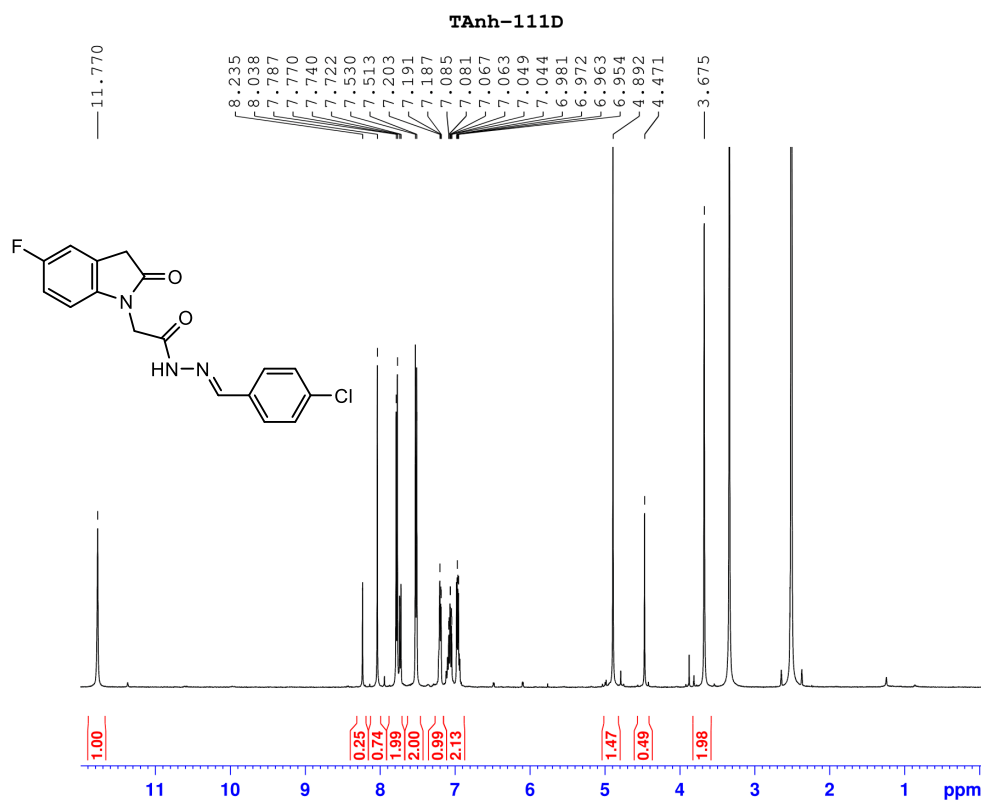


Figure S35. ¹H NMR of compound 4l



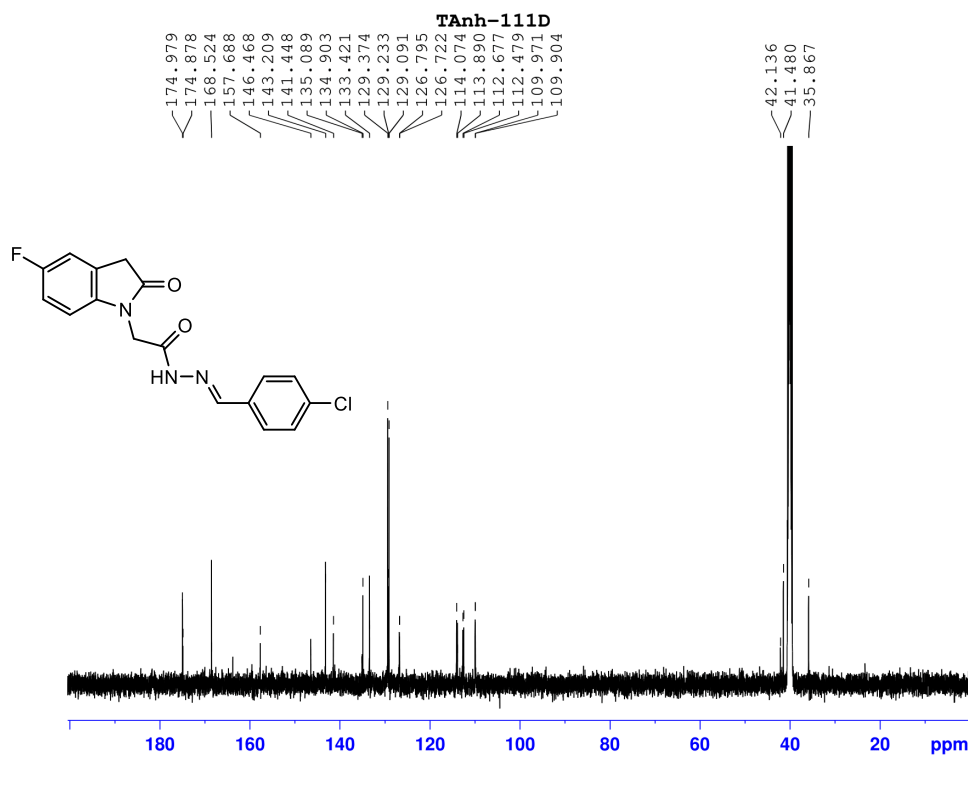
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SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 191.38
DW 50.000 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 9.80 usec
PLW1 24.00000000 W

F2 - Processing parameters
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WDW EM
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LB 0.30 Hz
GB 0
PC 1.00

Figure S36. ¹³C NMR of compound 4l



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EXPNO 11
PROCNO 1

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Time 12.54
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 191.38
DW 16.000 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 9.50 usec
PLW1 90.00000000 W

===== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 24.00000000 W
PLW12 0.36015001 W
PLW13 0.23050000 W

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

Figure S37. HRMS of compound 4m

D:\DATA\Old\TA-MS\200823\111E

08/23/20 18:37:33

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

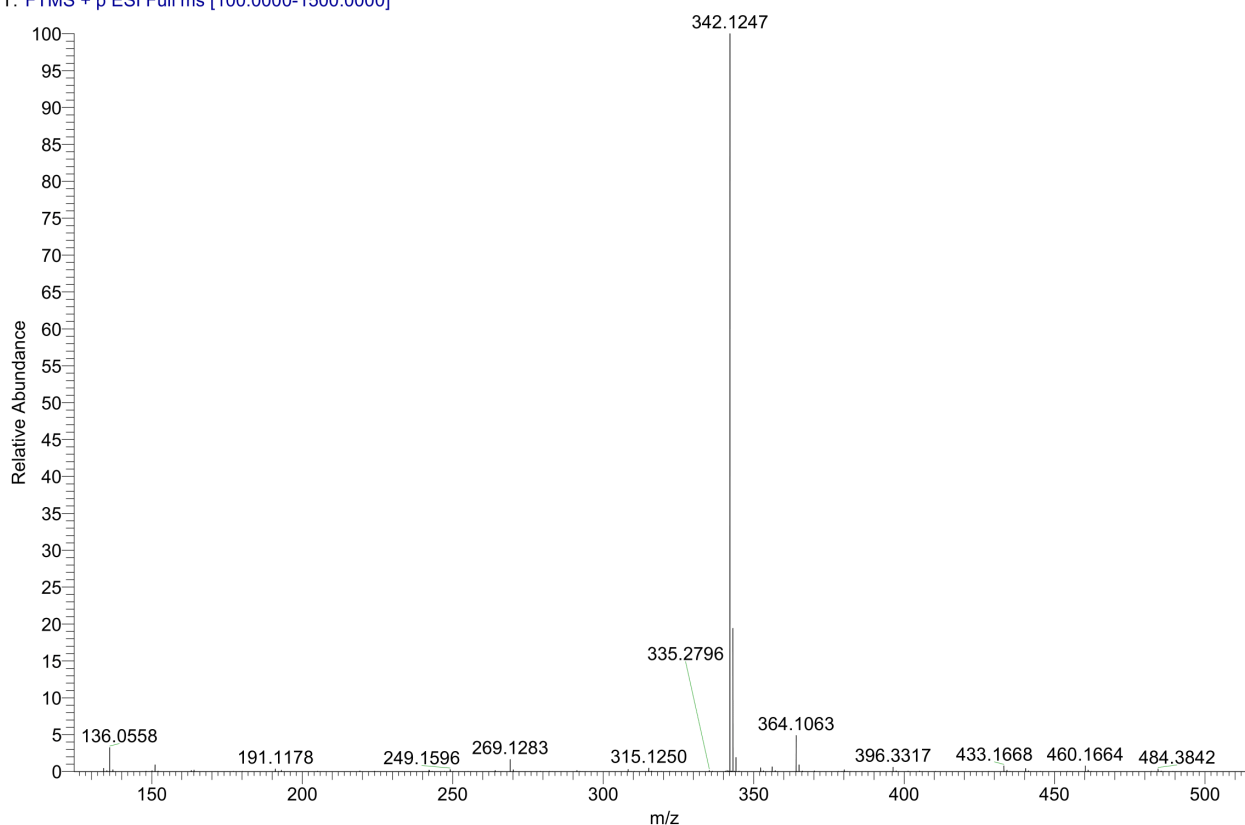


Figure S38. ¹H NMR of compound 4m

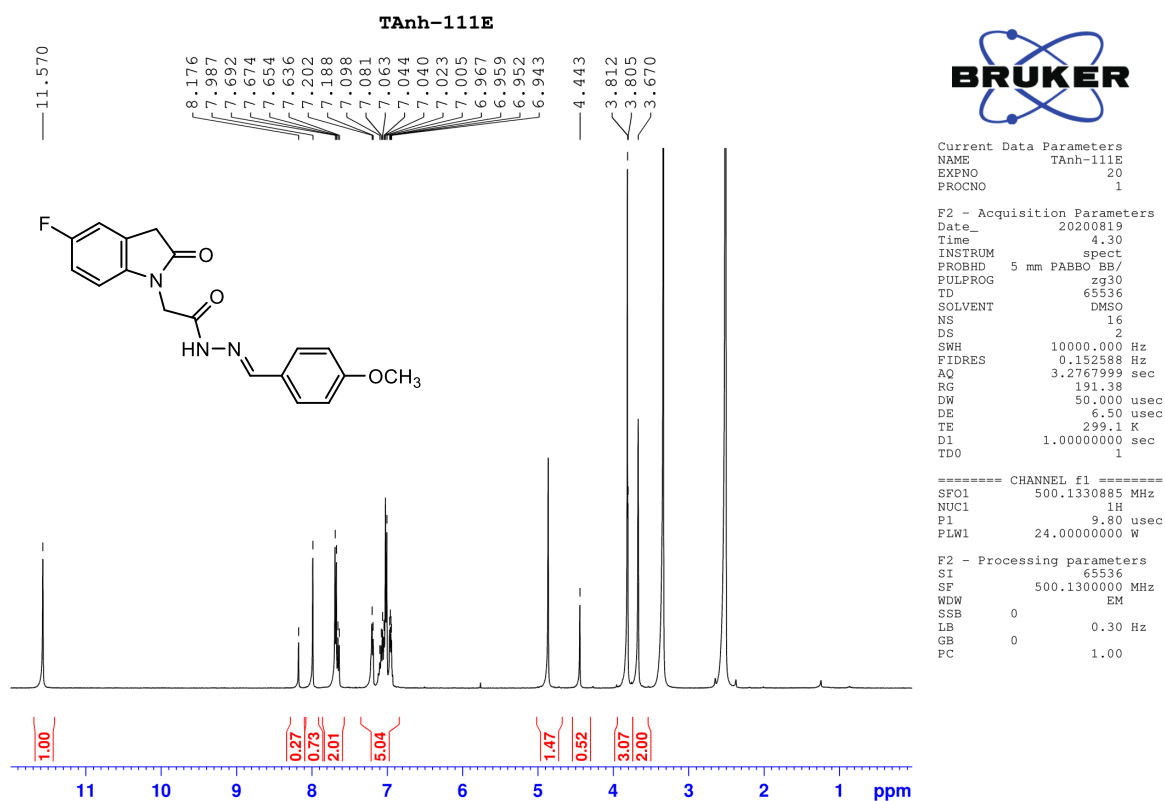


Figure S39. ^{13}C NMR of compound 4m

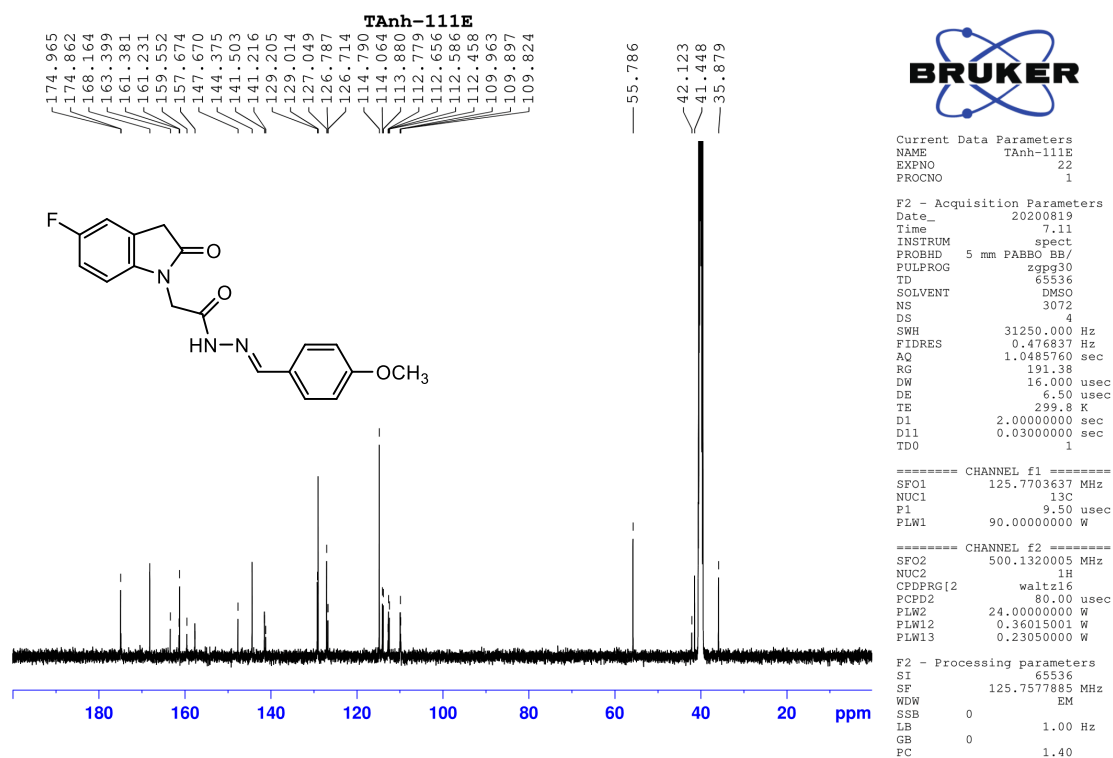


Figure S40. HRMS of compound 4n

D:\DATA\Old\TA-MS\200823\111F

08/23/20 18:43:25

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

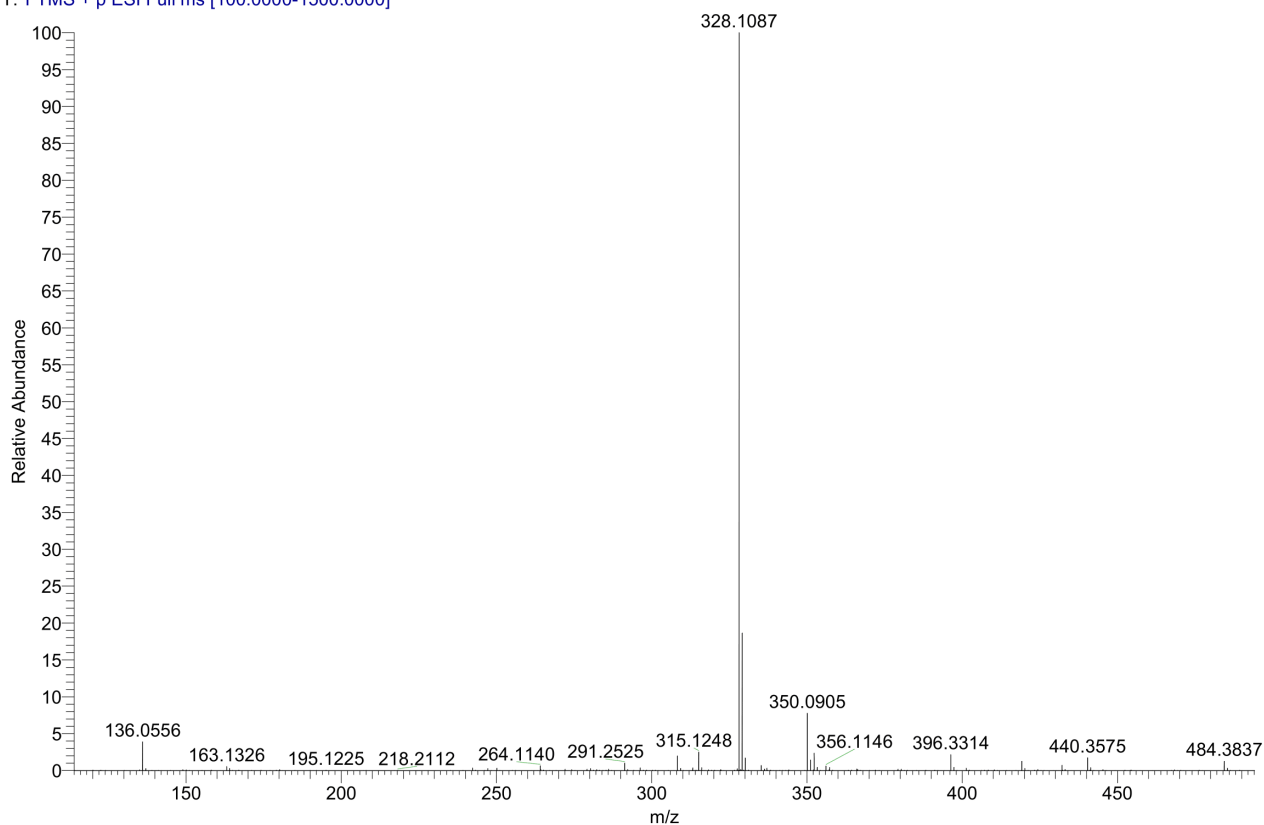


Figure S41. ¹H NMR of compound 4n

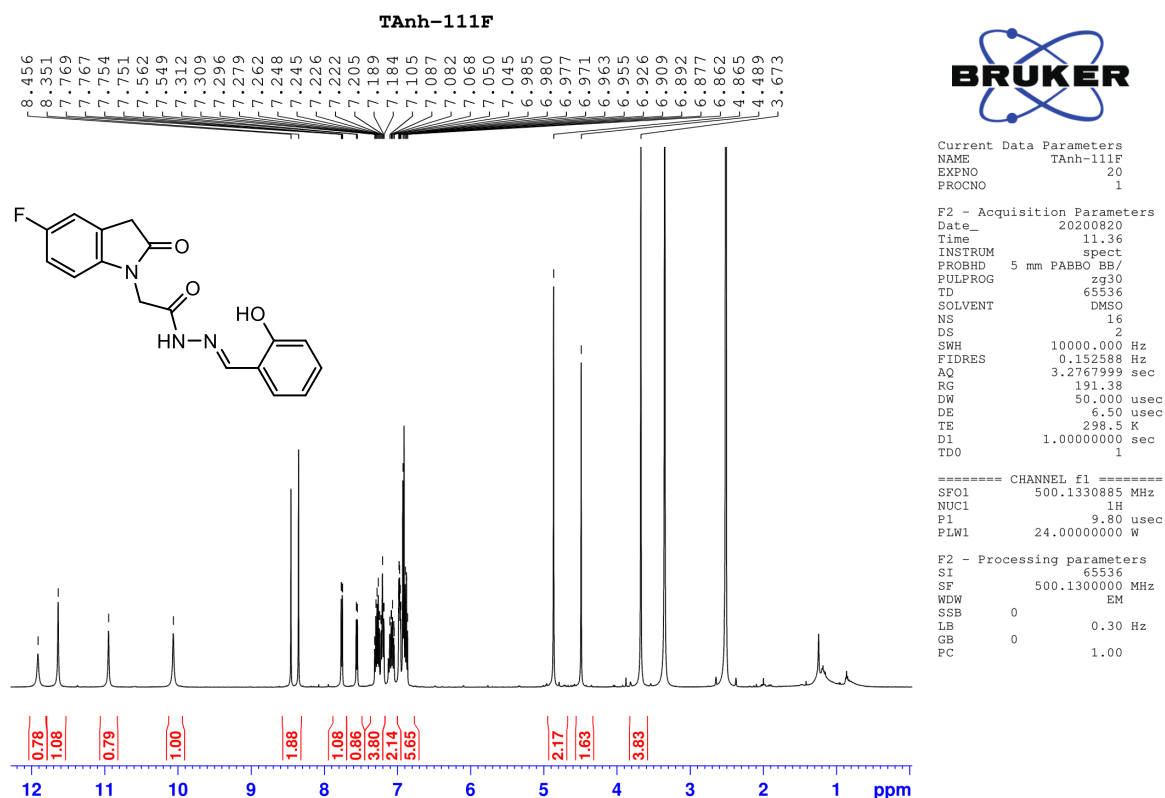


Figure S42. ¹³C NMR of compound 4n

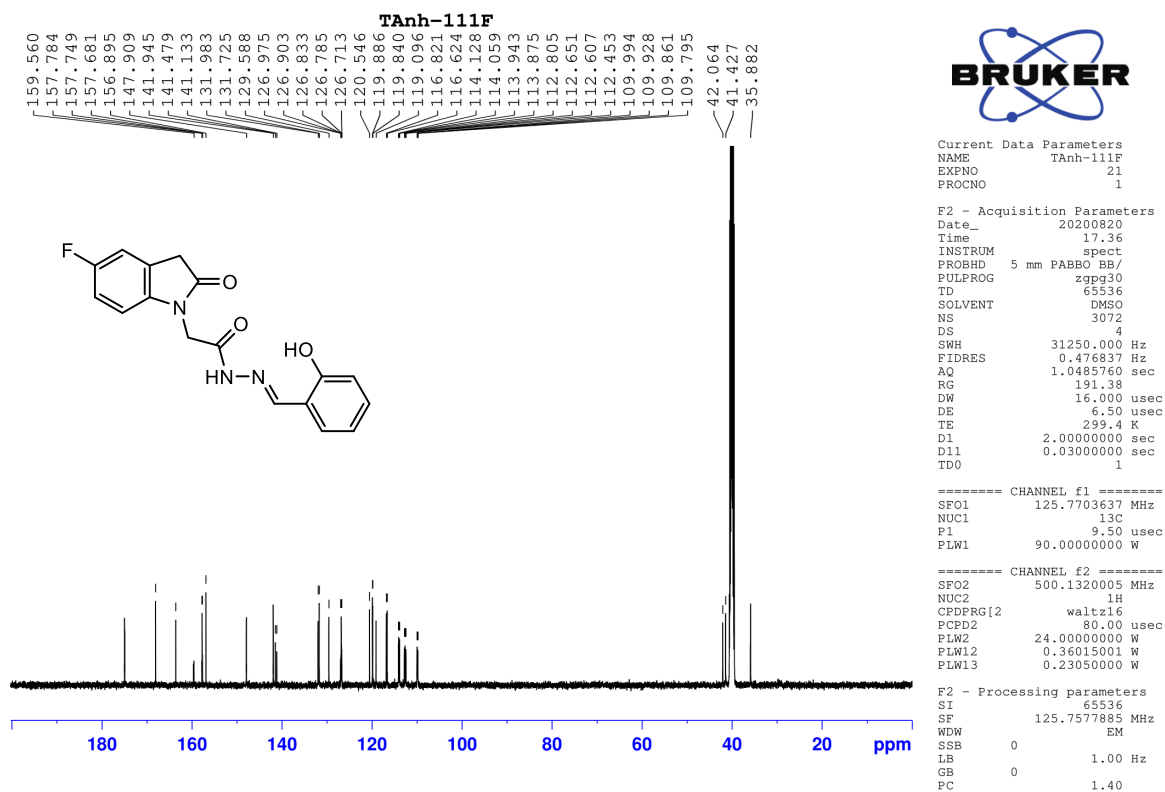


Figure S43. HRMS of compound 4o

D:\DATA\Old\TA-MS\200823\111G

08/23/20 18:49:17

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

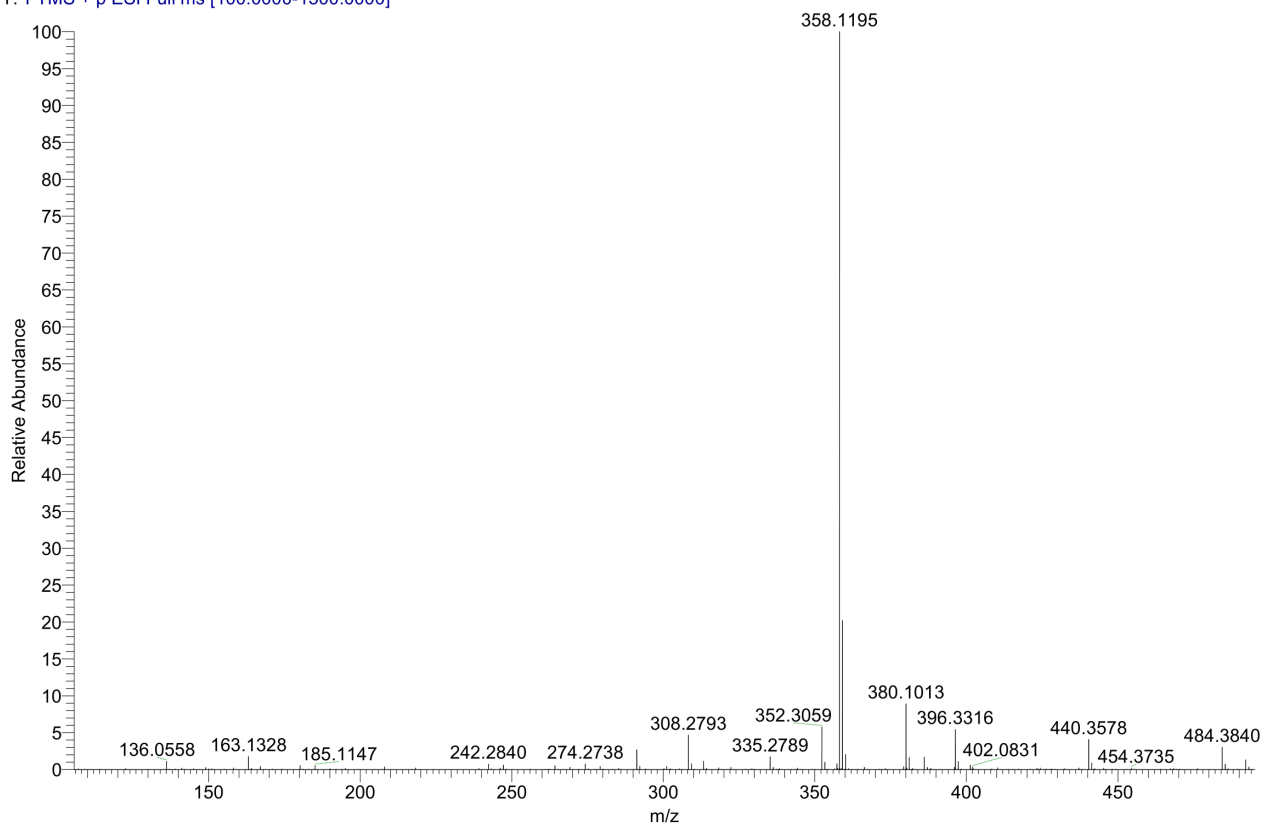


Figure S44. ¹H NMR of compound 4o

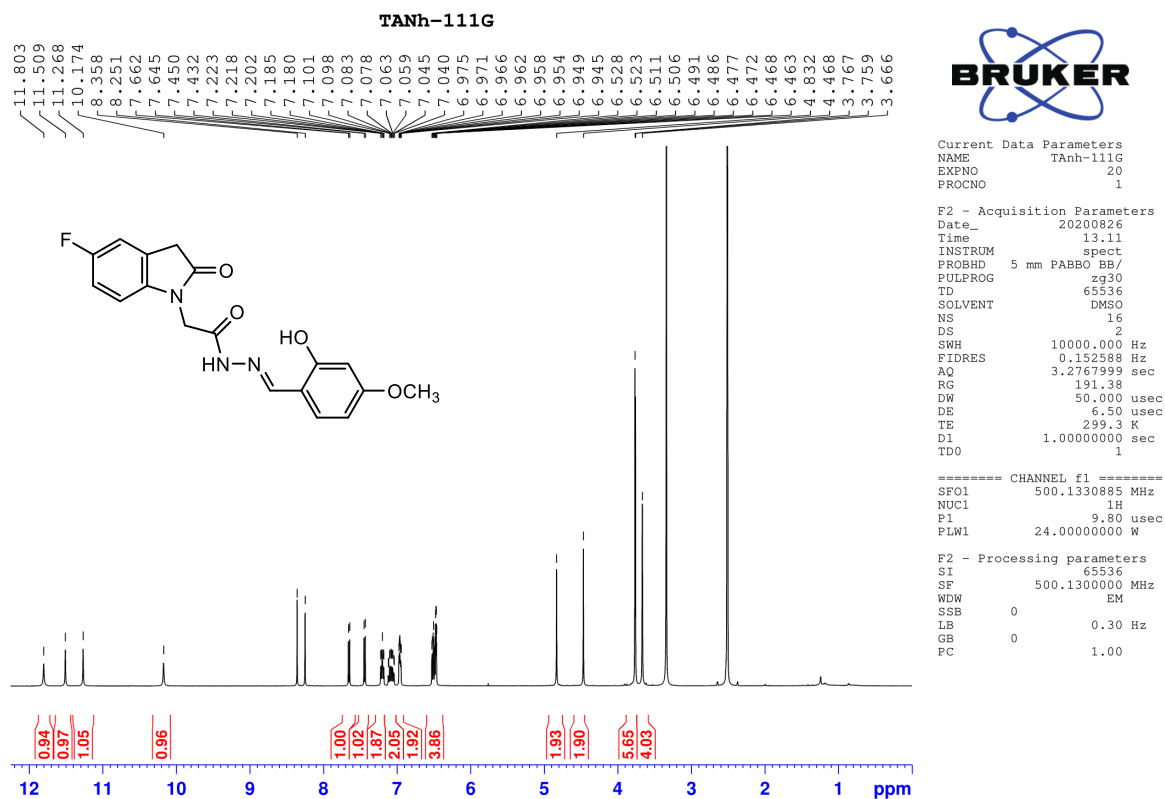


Figure S45. ^{13}C NMR of compound 4o

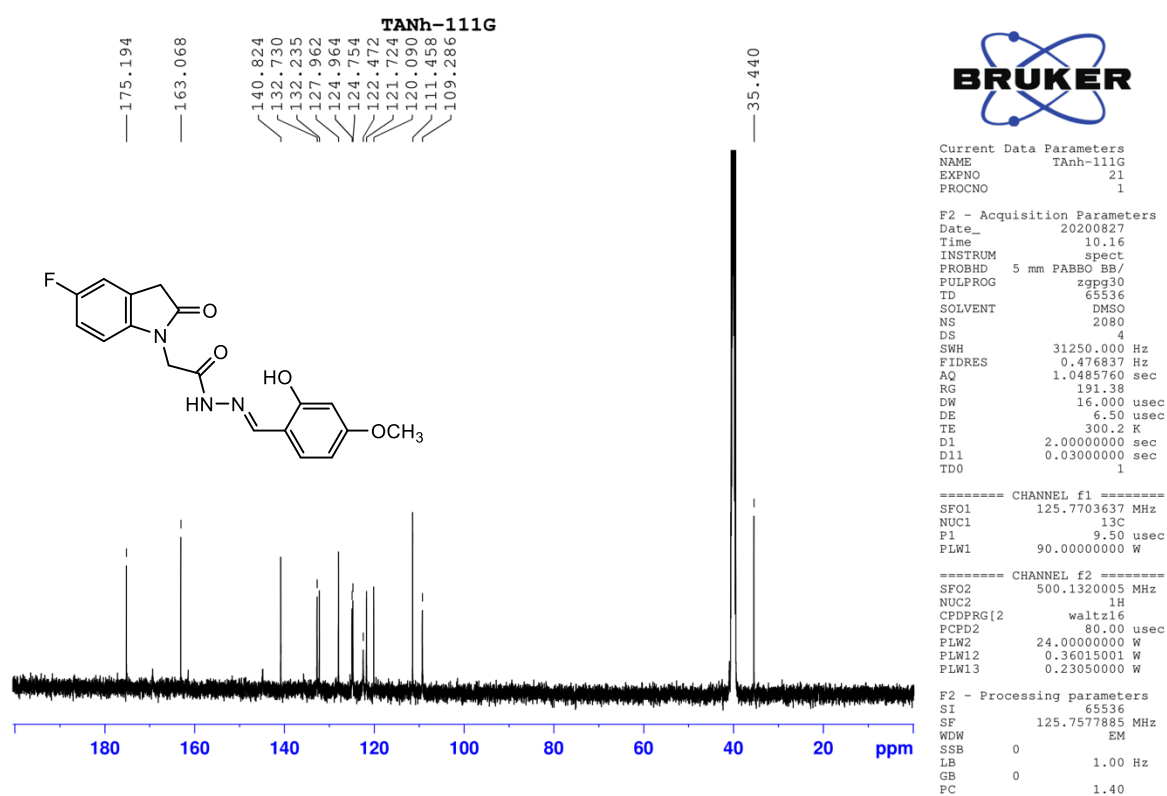


Figure S46. HRMS of compound 4p

D:\DATA\Old\TA-MS\200823\111H

08/23/20 18:55:09

111H #18 RT: 0.17 AV: 1 NL: 1.88E9
 T: FTMS + p ESI Full ms [100.0000-1500.0000]

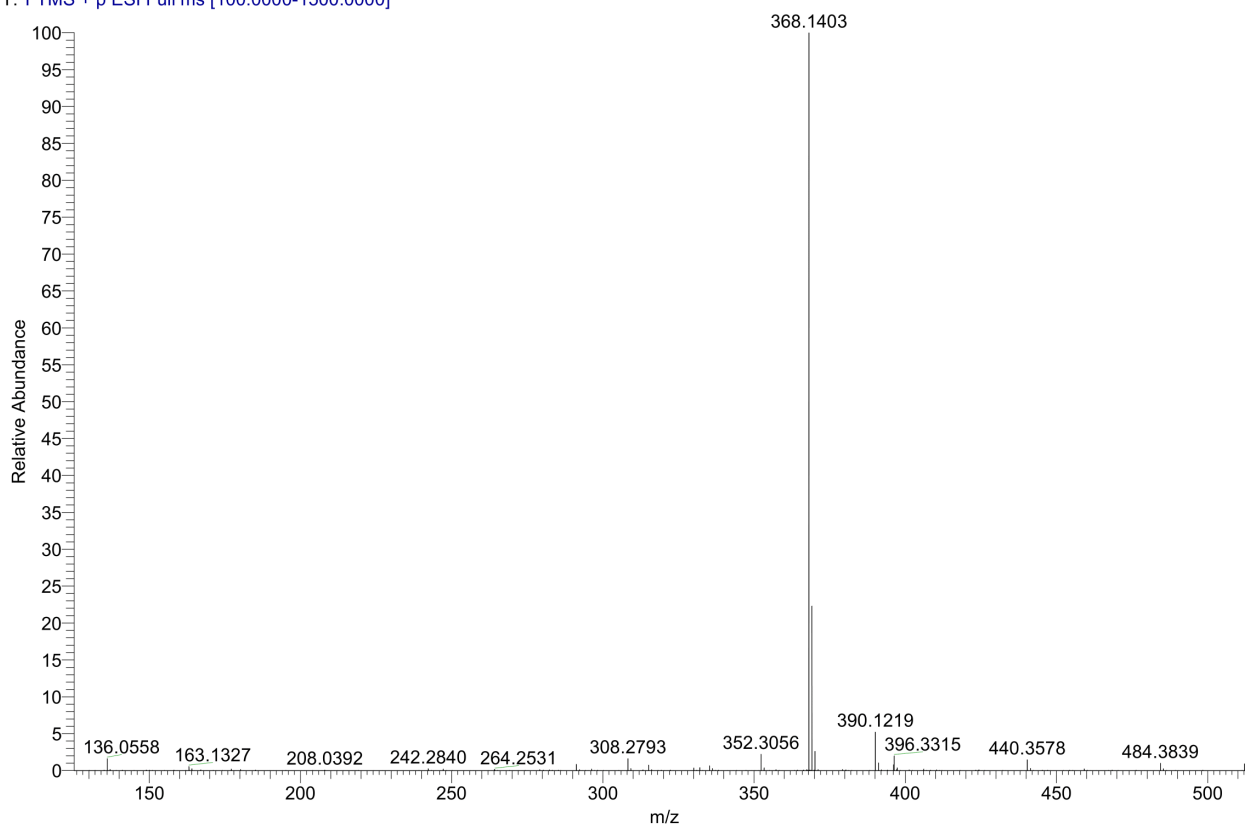


Figure S47. ¹H NMR of compound 4p

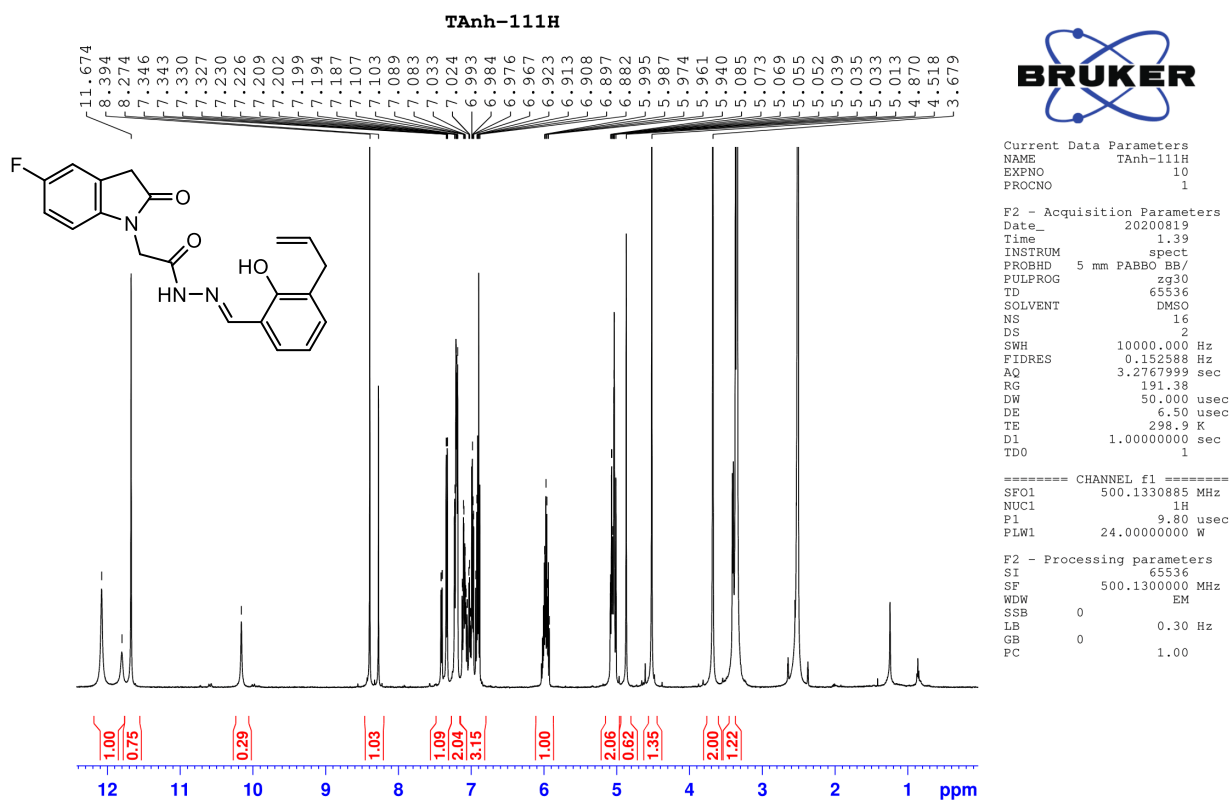


Figure S48. ¹³C NMR of compound 4p

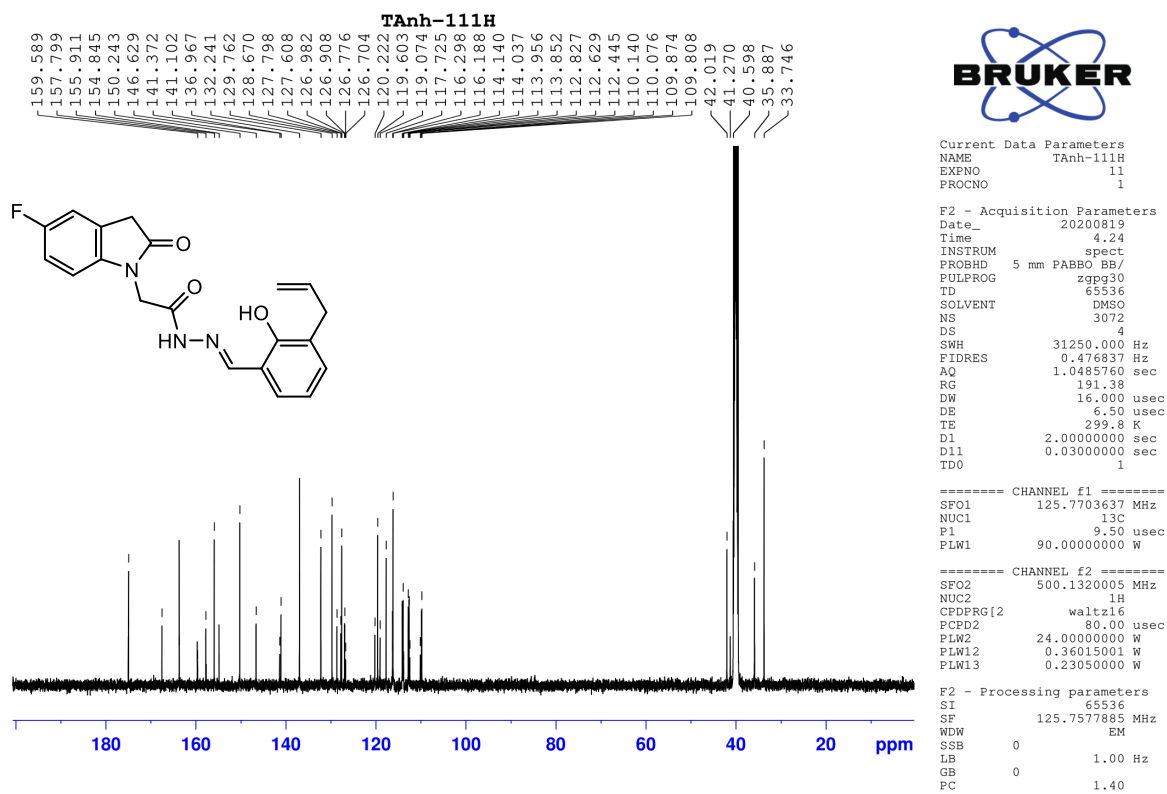


Figure S49. HRMS of compound 5a

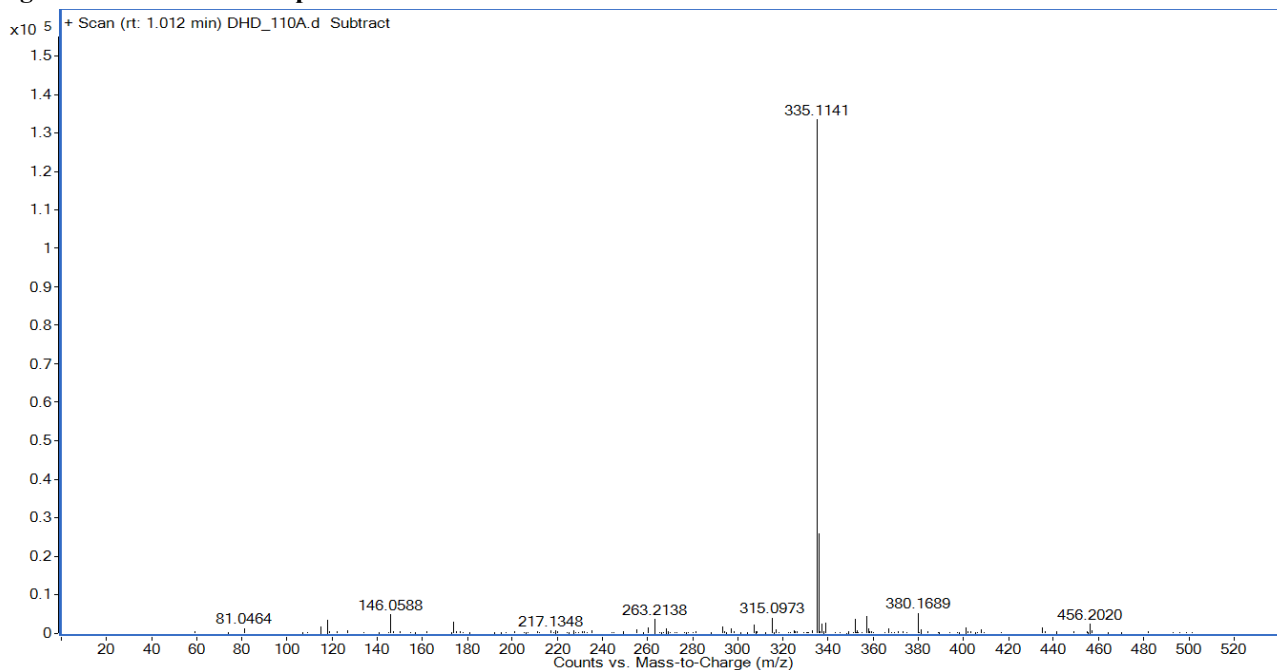


Figure S50. ¹H NMR of compound 5a

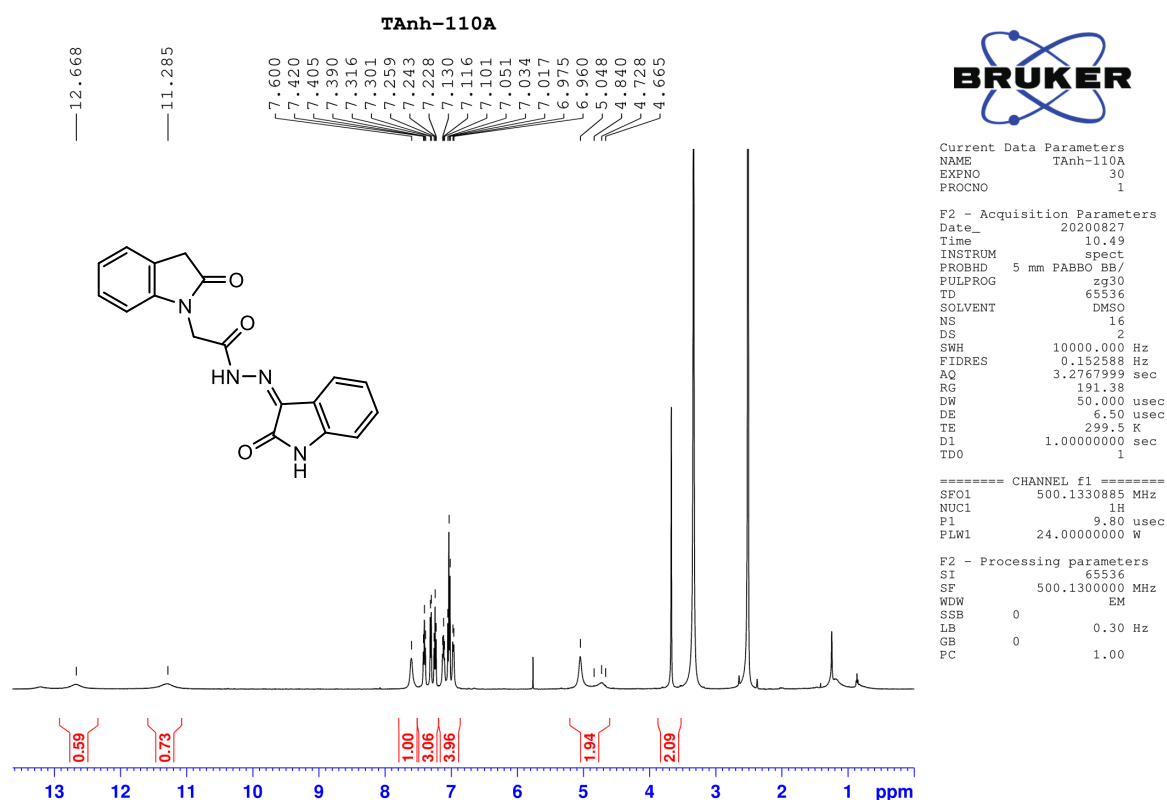


Figure S51. ^{13}C NMR of compound 5a

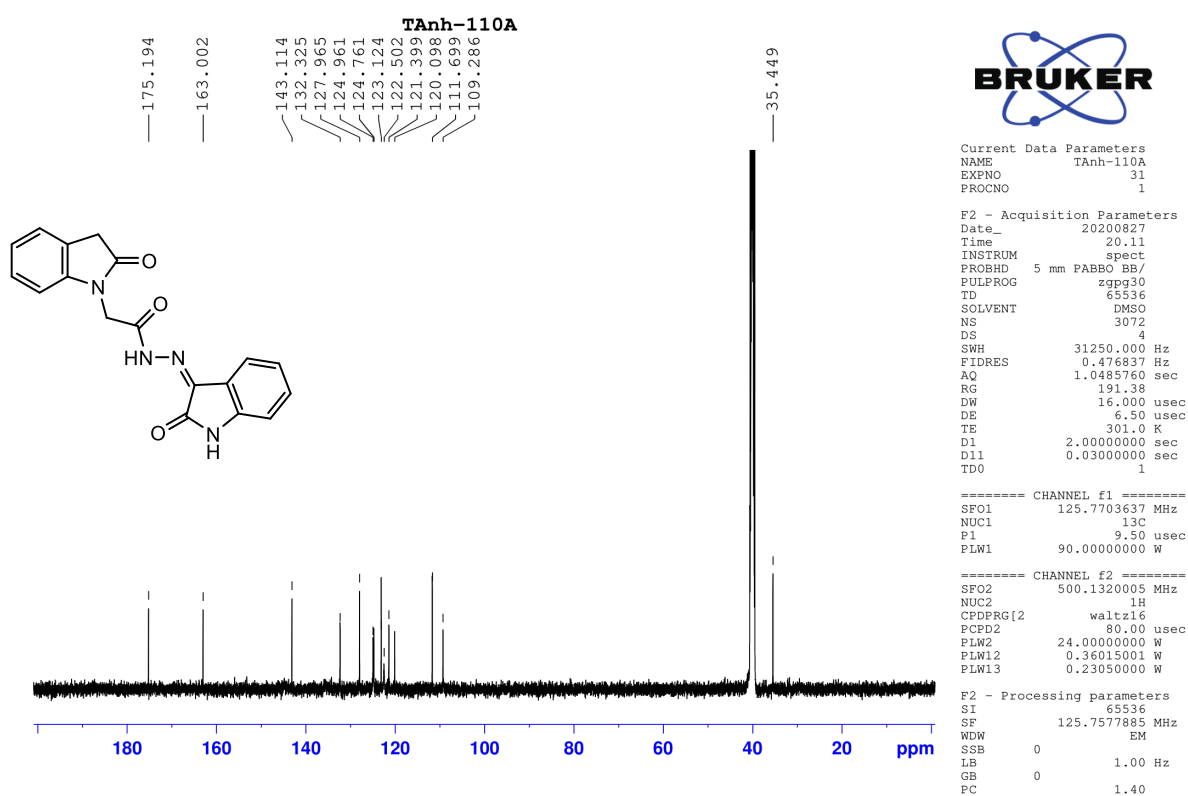


Figure S52. HRMS of compound 5b

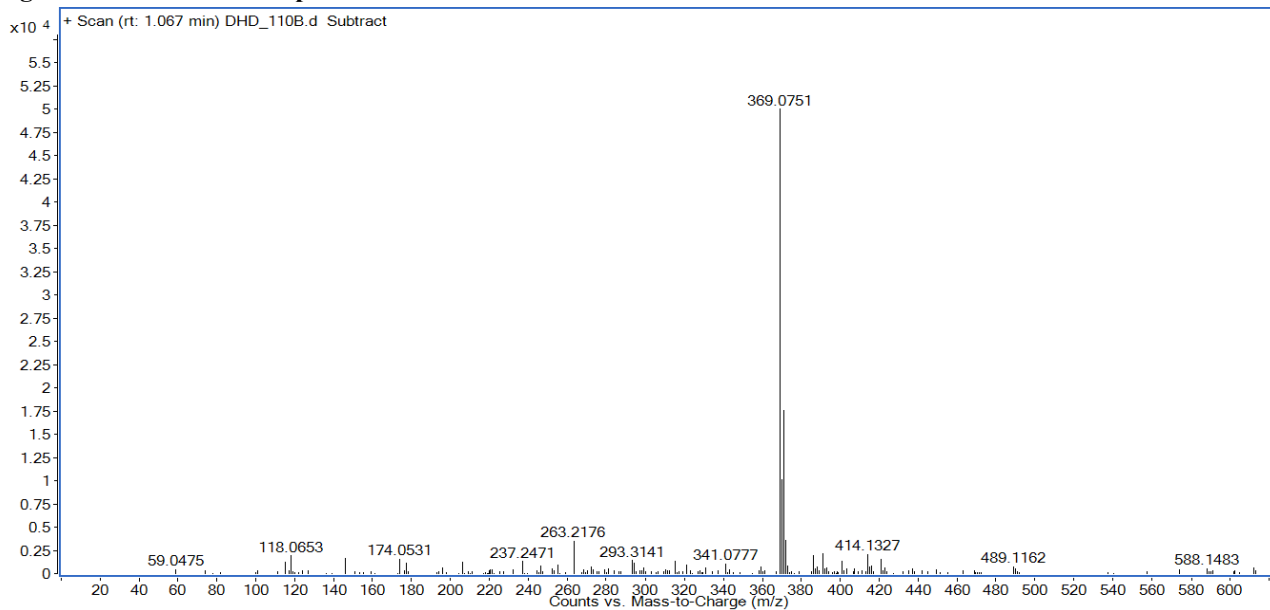


Figure S53. ¹H NMR of compound 5b

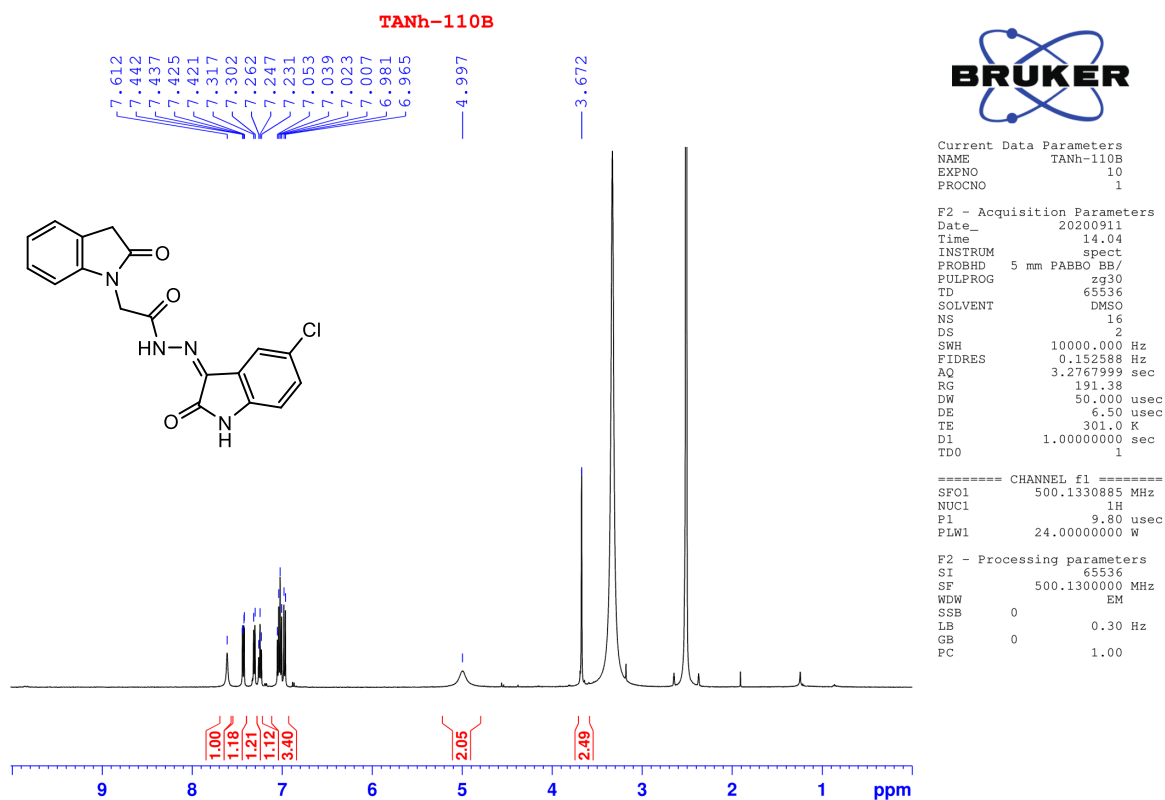


Figure S54. ¹³C NMR of compound 5b

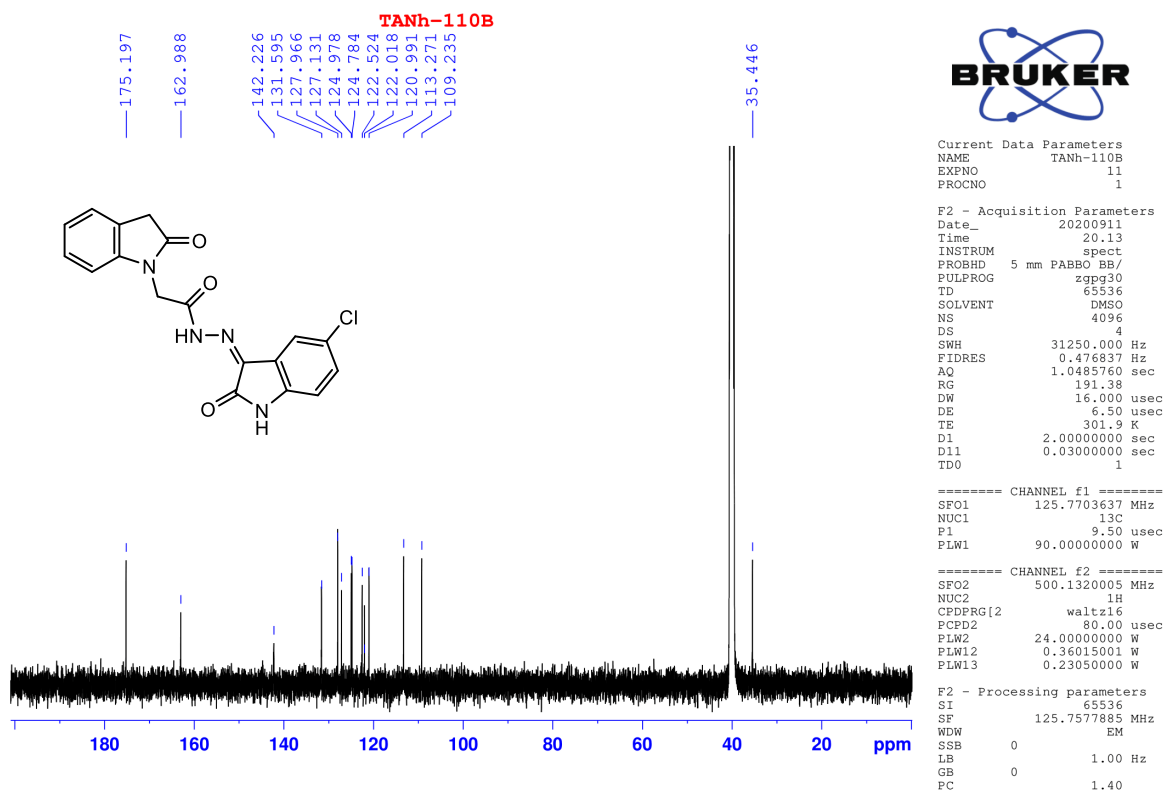


Figure S55. HRMS of compound 5c

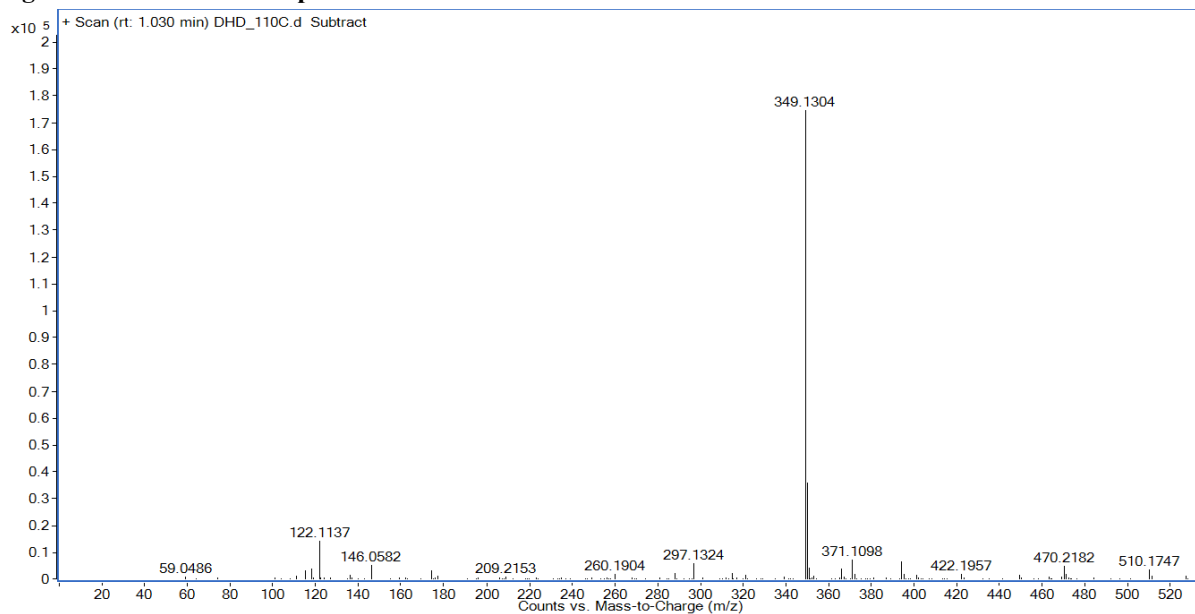


Figure S56. ¹H NMR of compound 5c

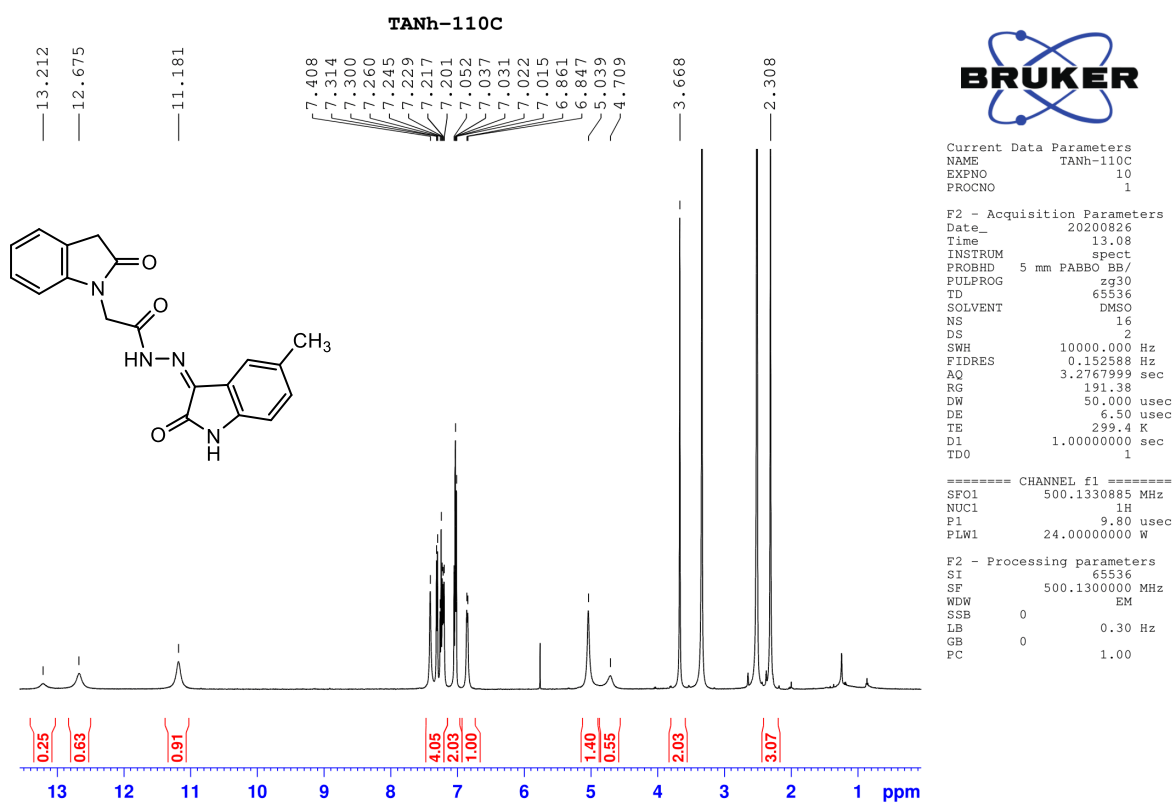


Figure S57. ^{13}C NMR of compound 5c

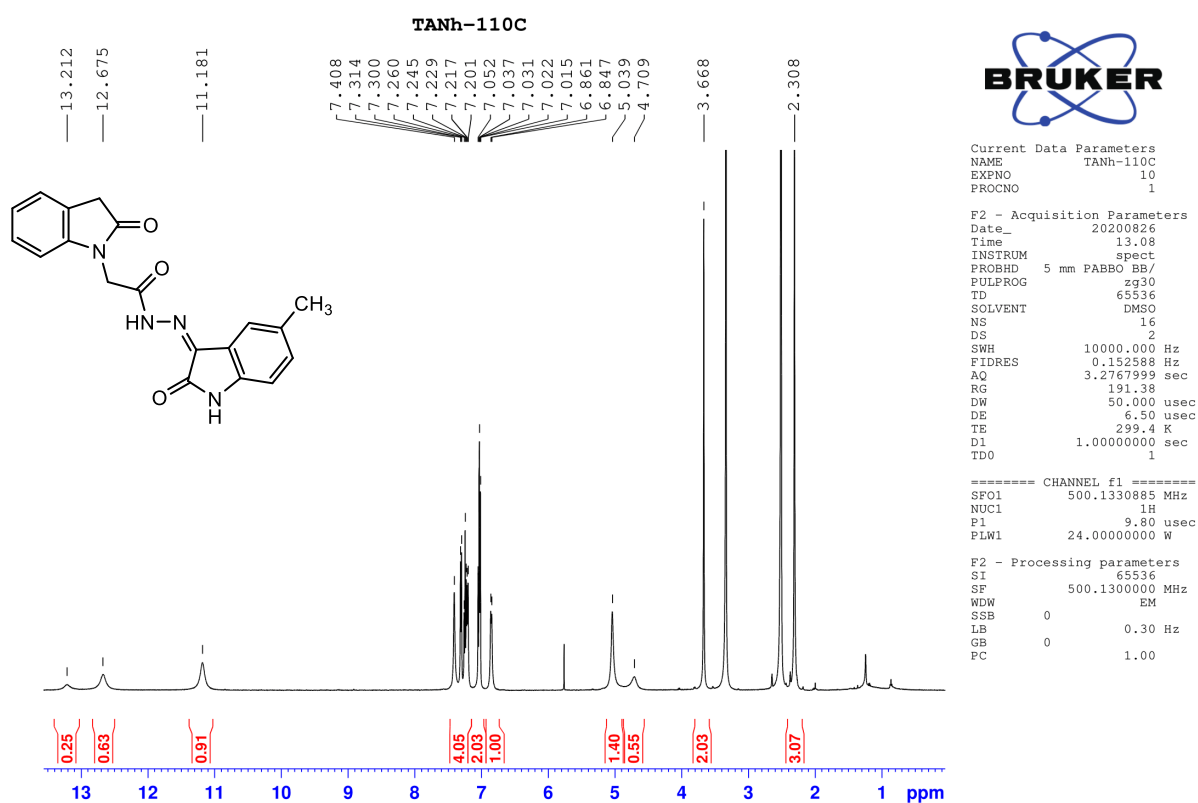


Figure S58. HRMS of compound 5d

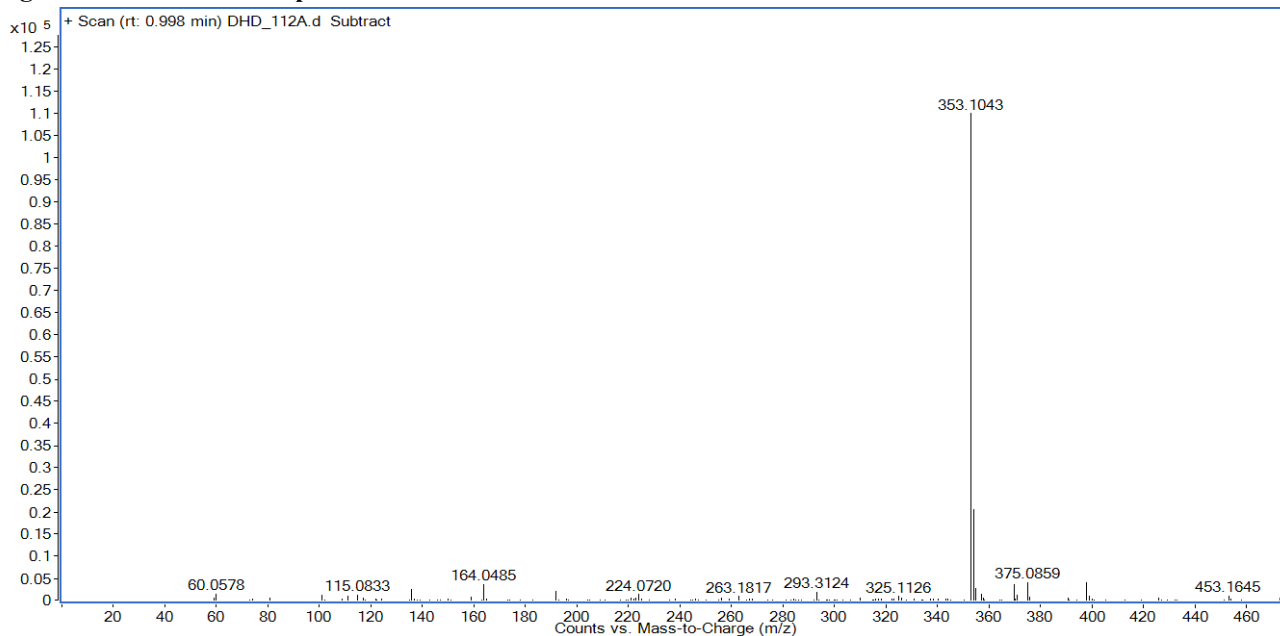


Figure S59. ¹H NMR of compound 5d

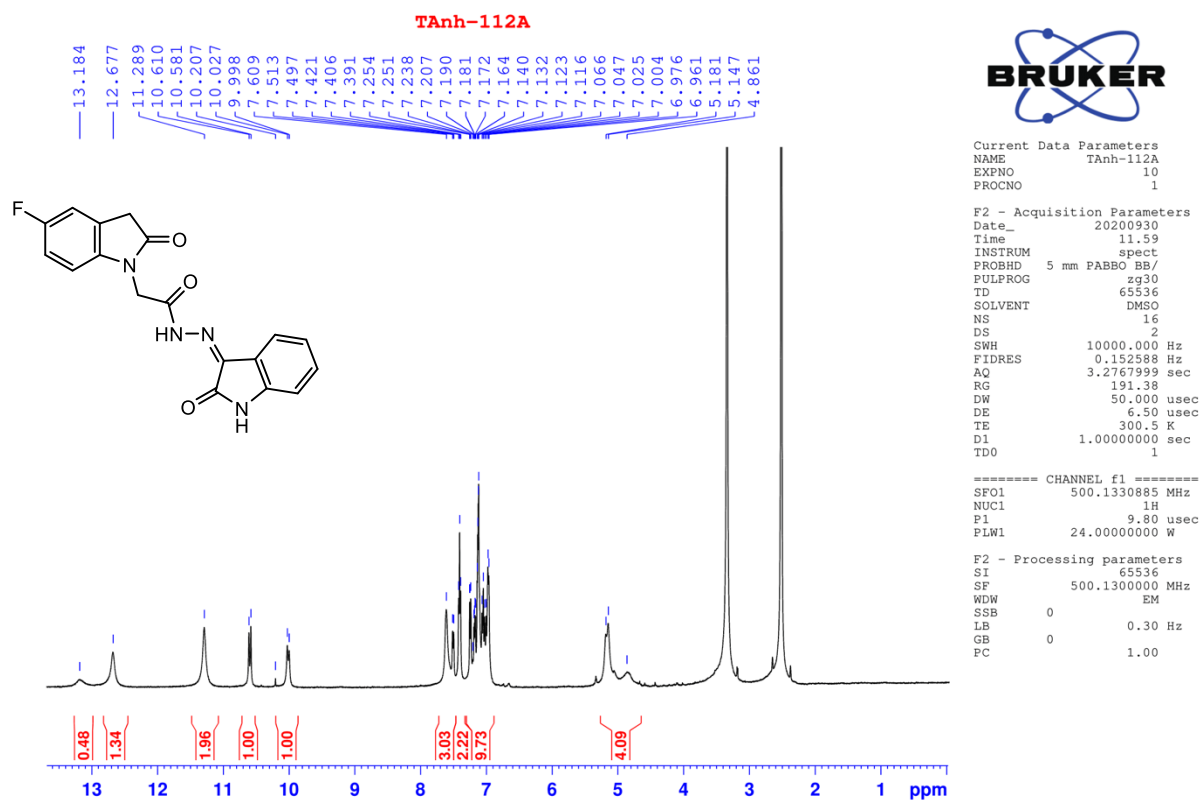


Figure S60. ¹³C NMR of compound 5d

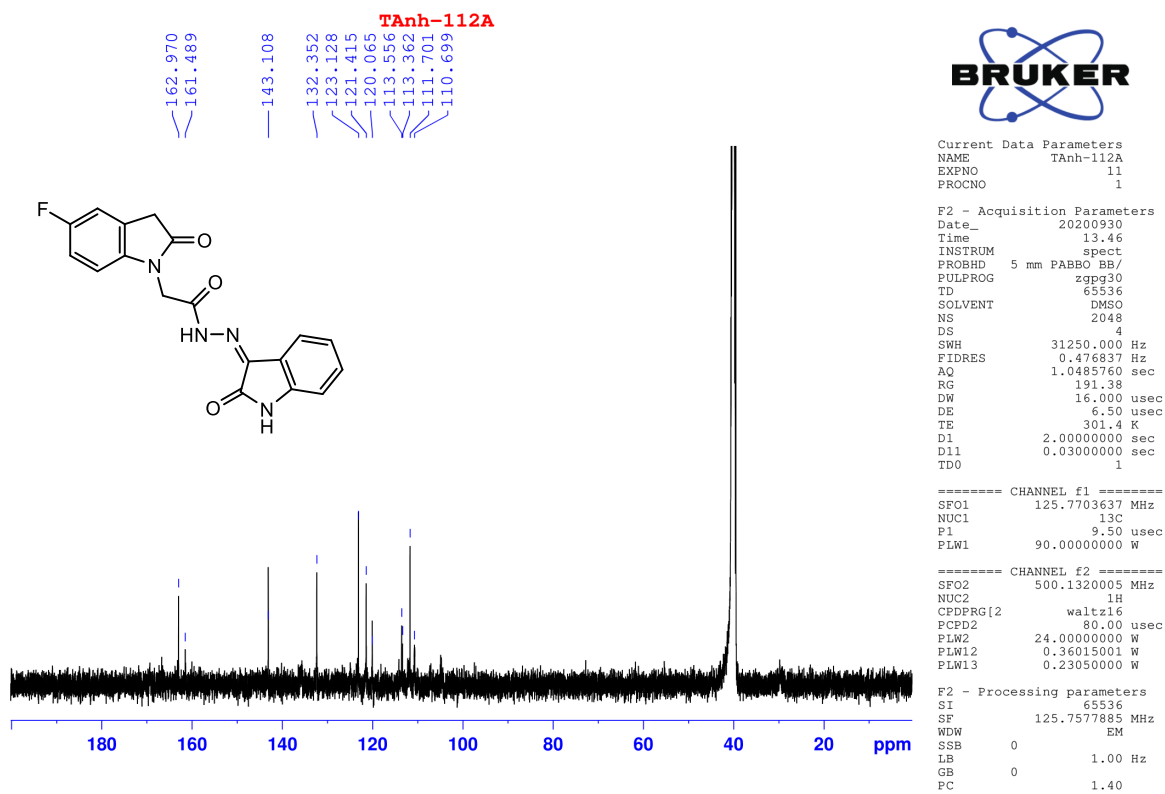


Figure S61. HRMS of compound 5e

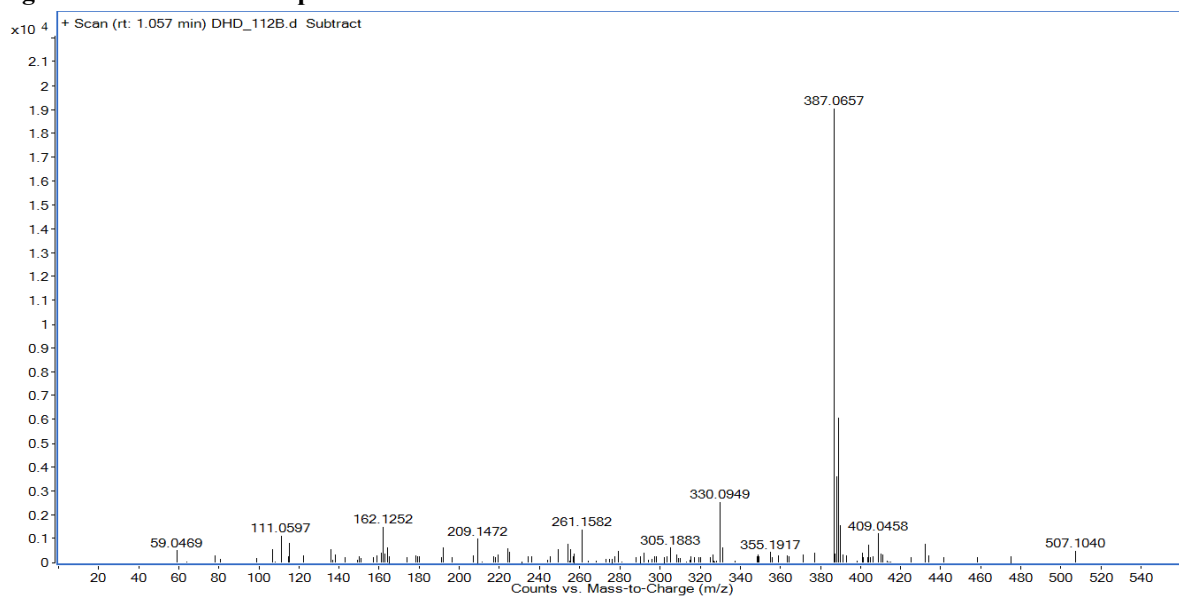


Figure S62. ¹H NMR of compound 5e

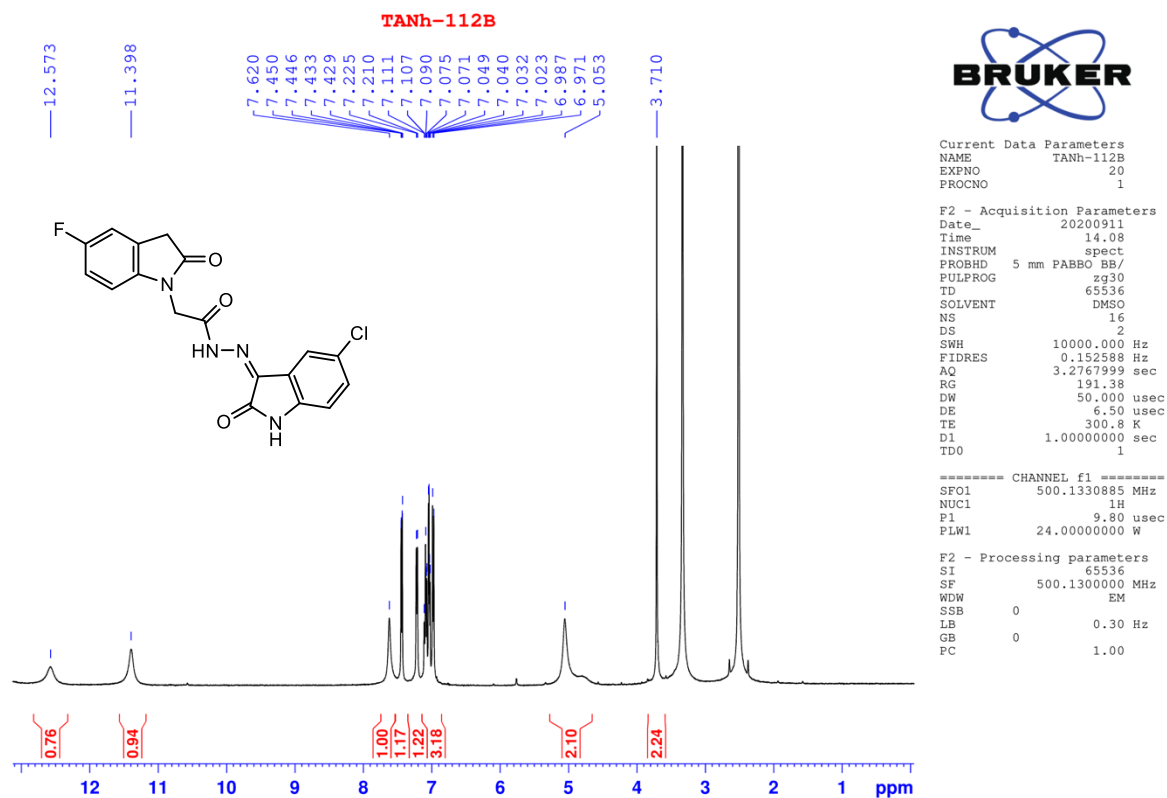


Figure S63. ^{13}C NMR of compound 5e

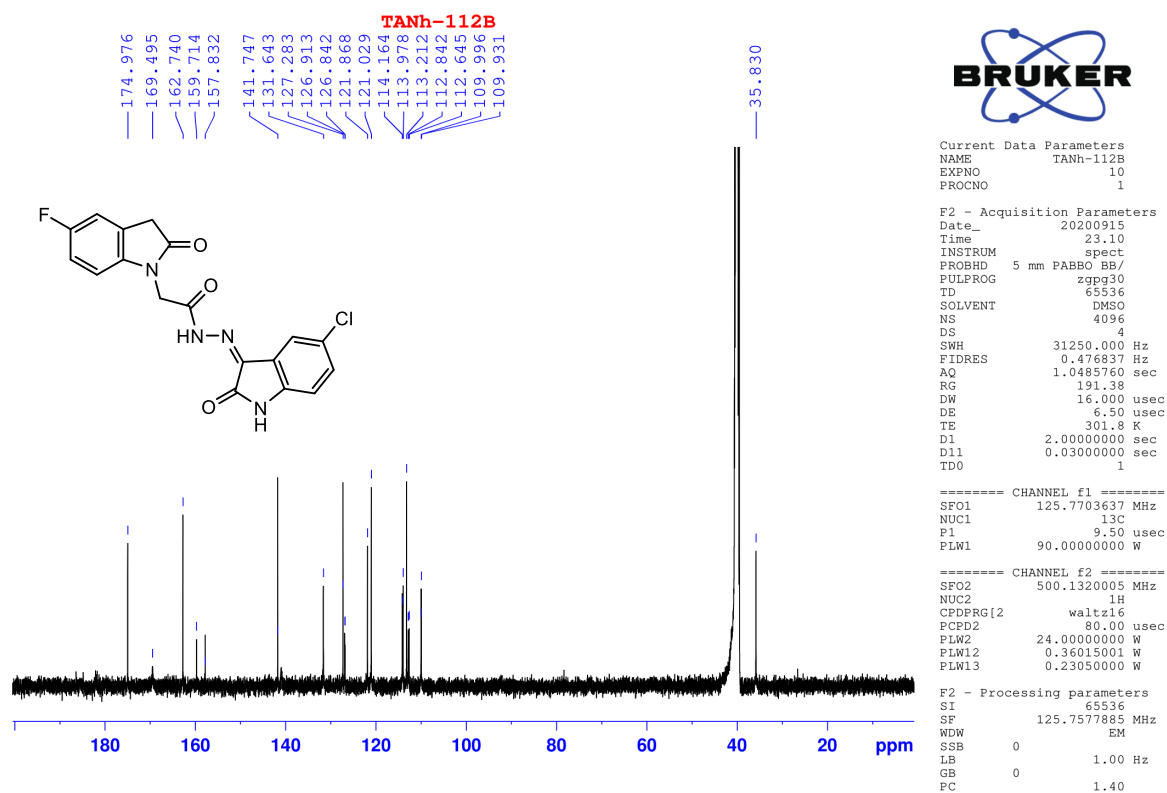


Figure S64. HRMS of compound 5f

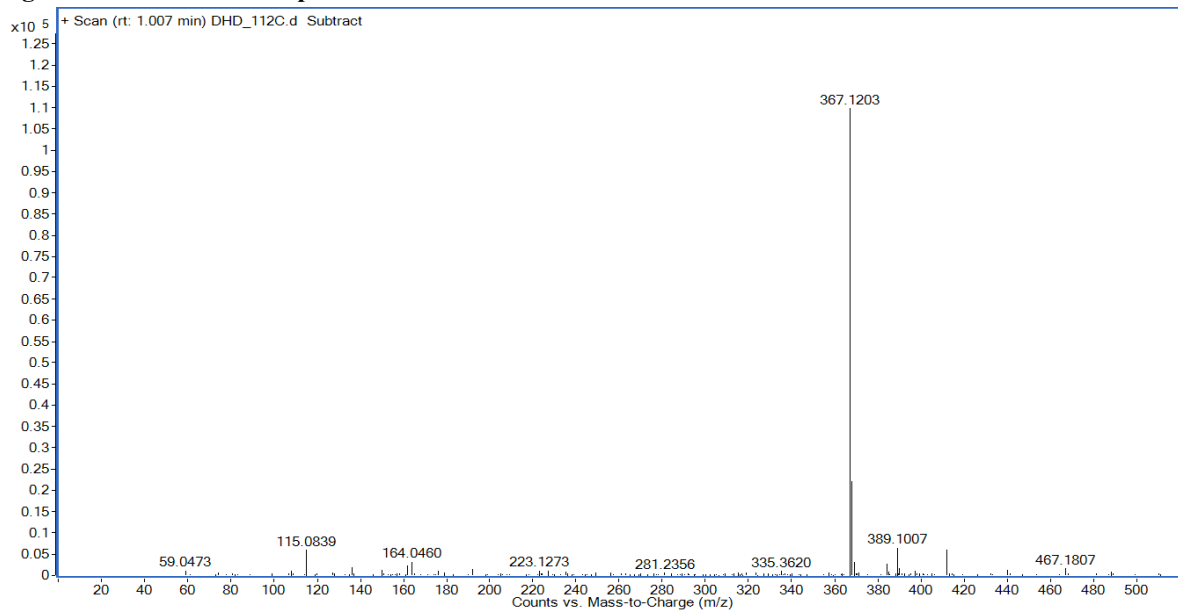


Figure S65. ¹H NMR of compound 5f

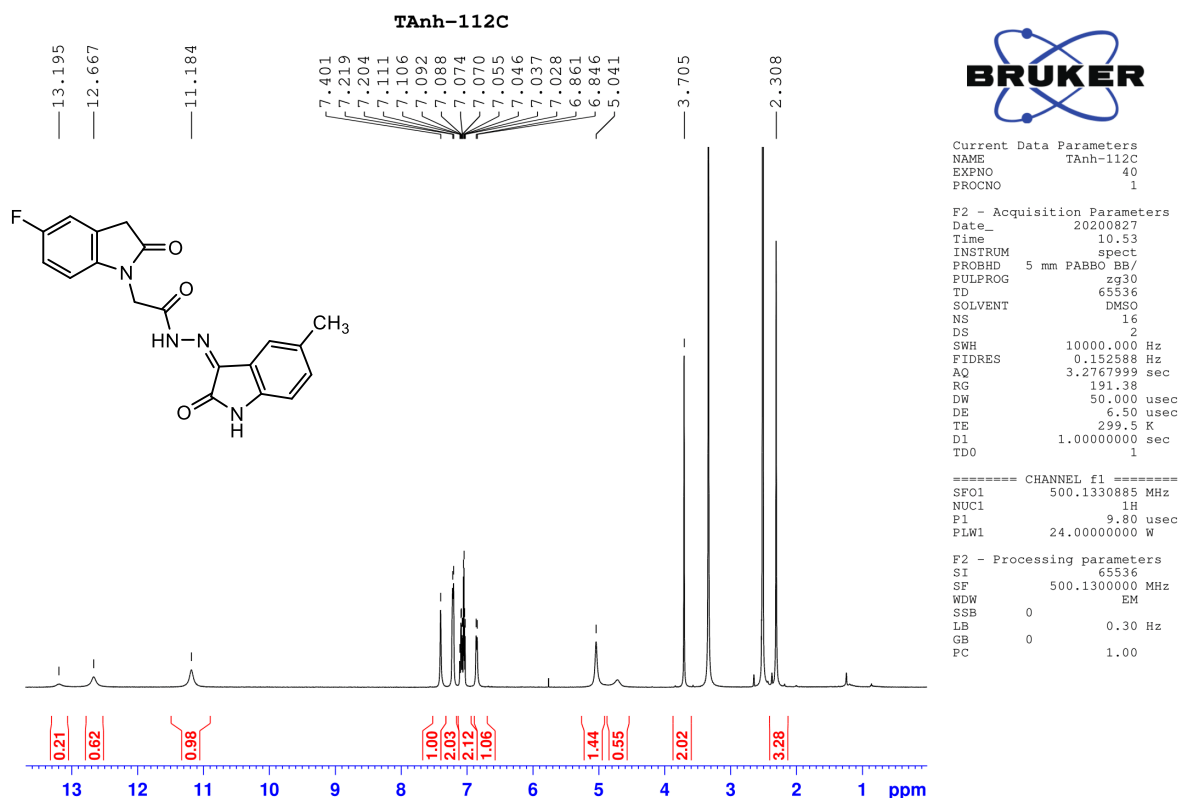


Figure S66. ¹³C NMR of compound 5f

