

Supporting Information

N1-Benzofused Modification of Fluoroquinolones Reduces Activity Against Gram-Negative Bacteria

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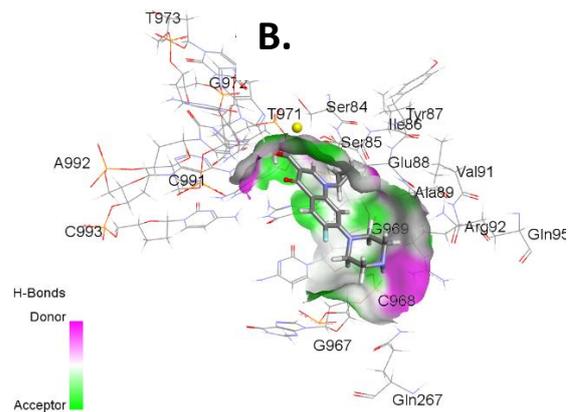
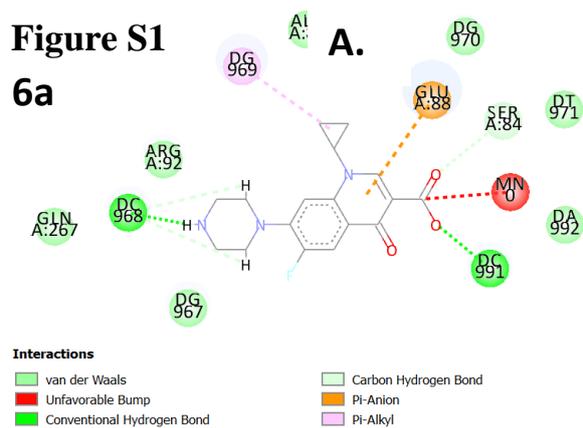
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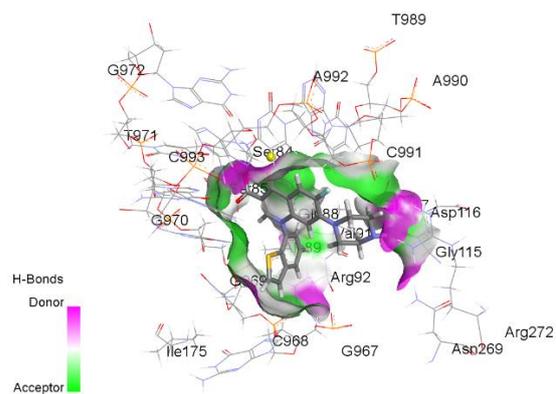
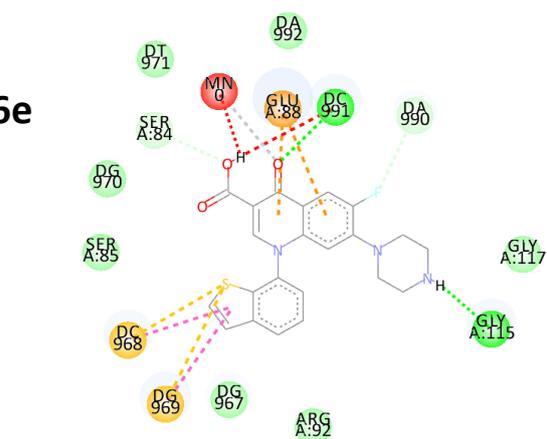
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Figure S1
6a



6e



6g

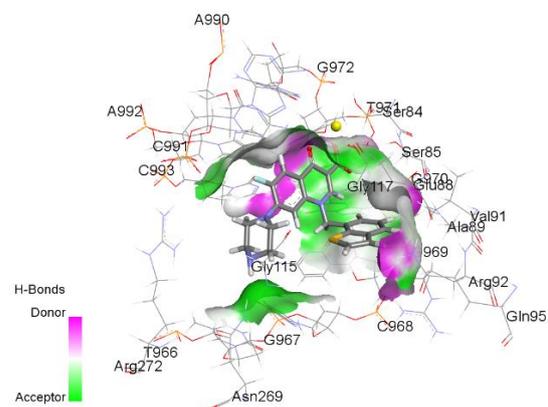
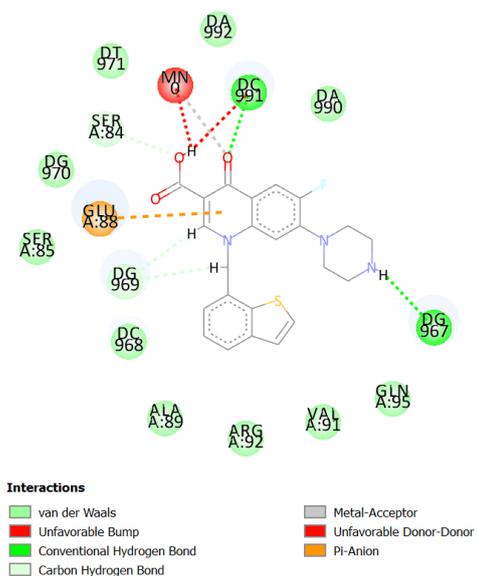


Figure S1. (A,B) Molecular modelling results for ciprofloxacin (**6a**) and N1-benzofused compounds **6e** and **6g** against *S. aureus* DNA gyrase. Binding poses shown in 2D (A) and 3D (B) views.

LC-MS Analysis

Figure S2. LC-MS profile of compound 3a.

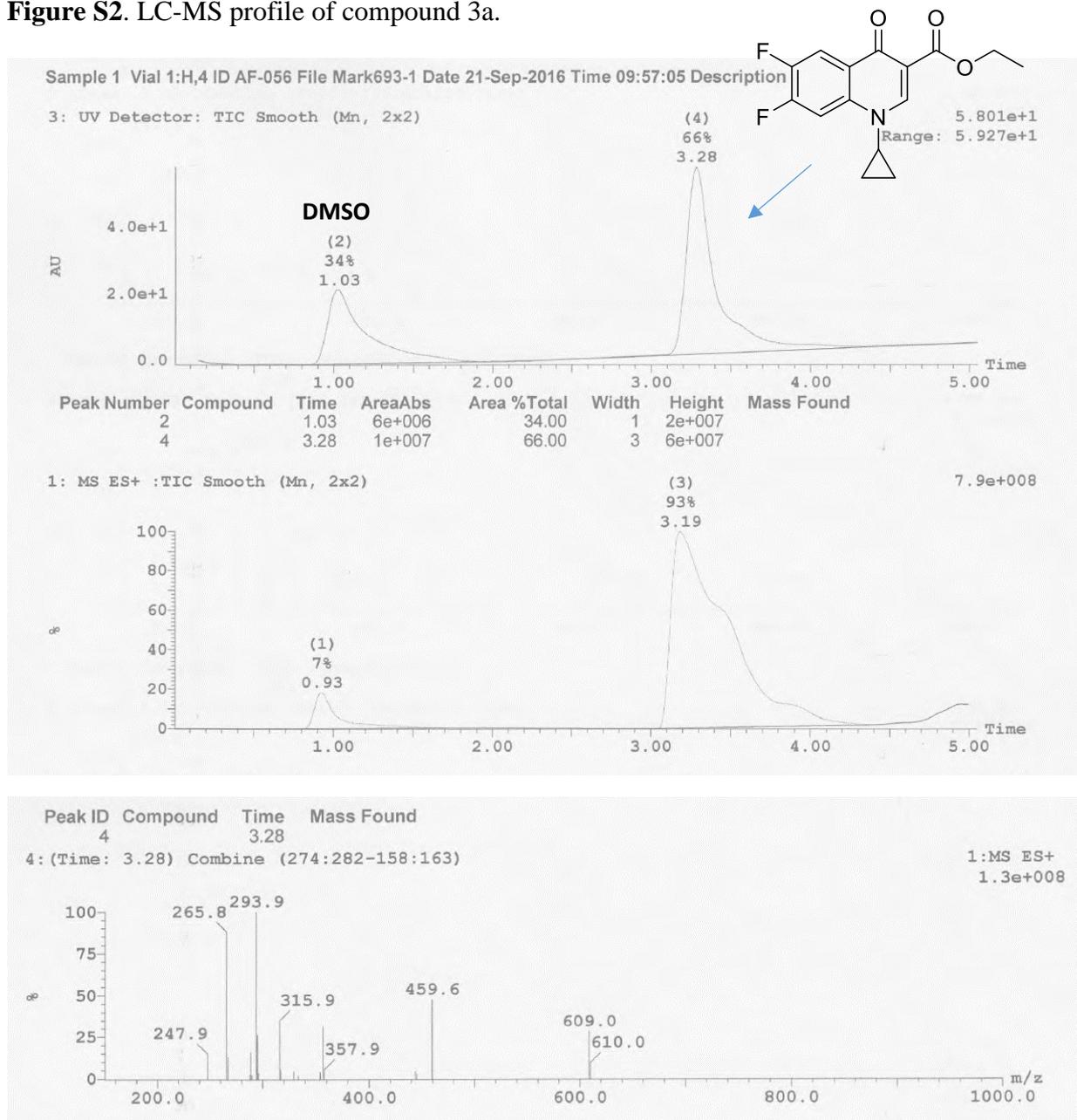


Figure S3. LC-MS profile of compound 3b.

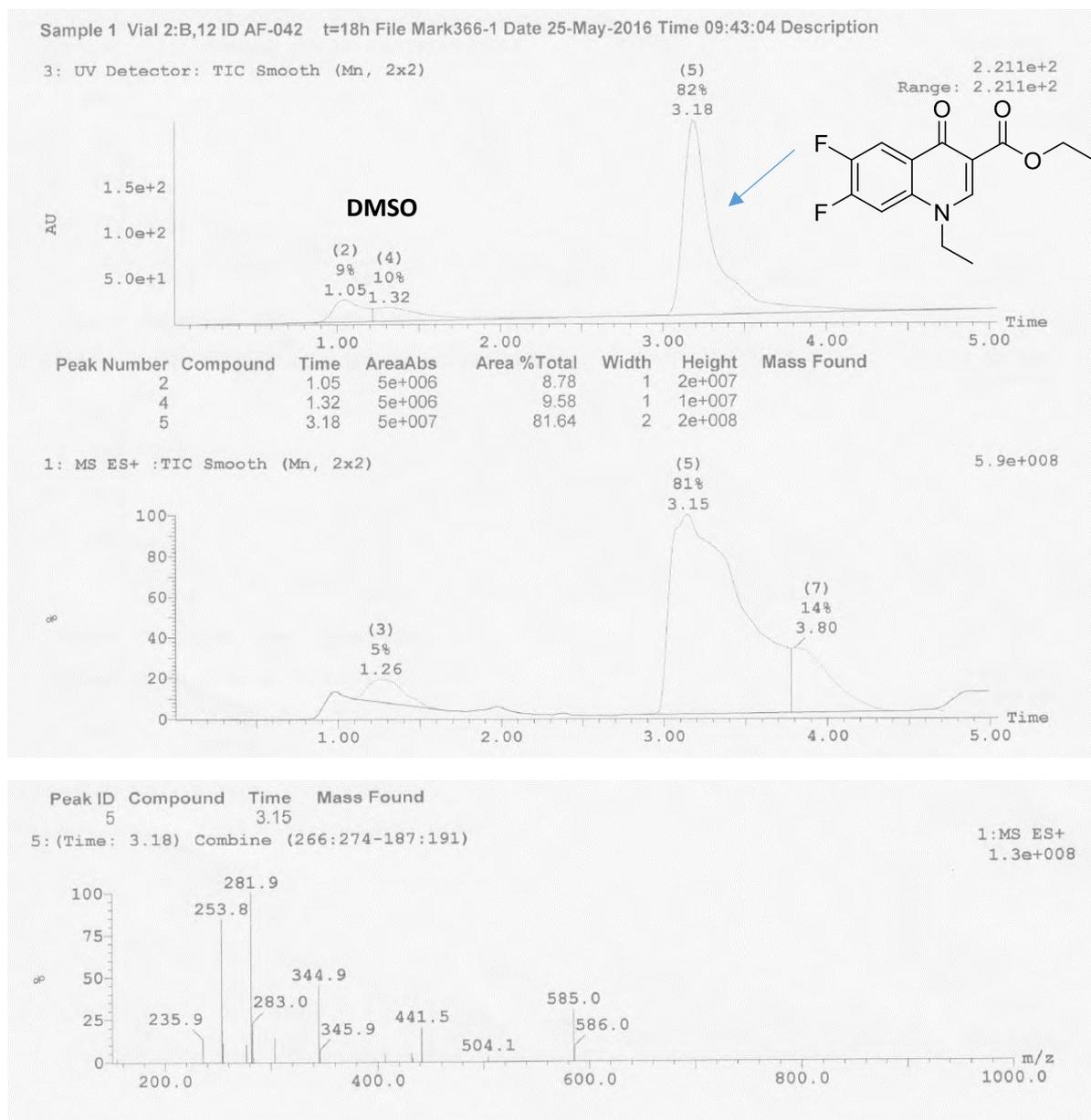


Figure S4. LC-MS profile of compound 3c.

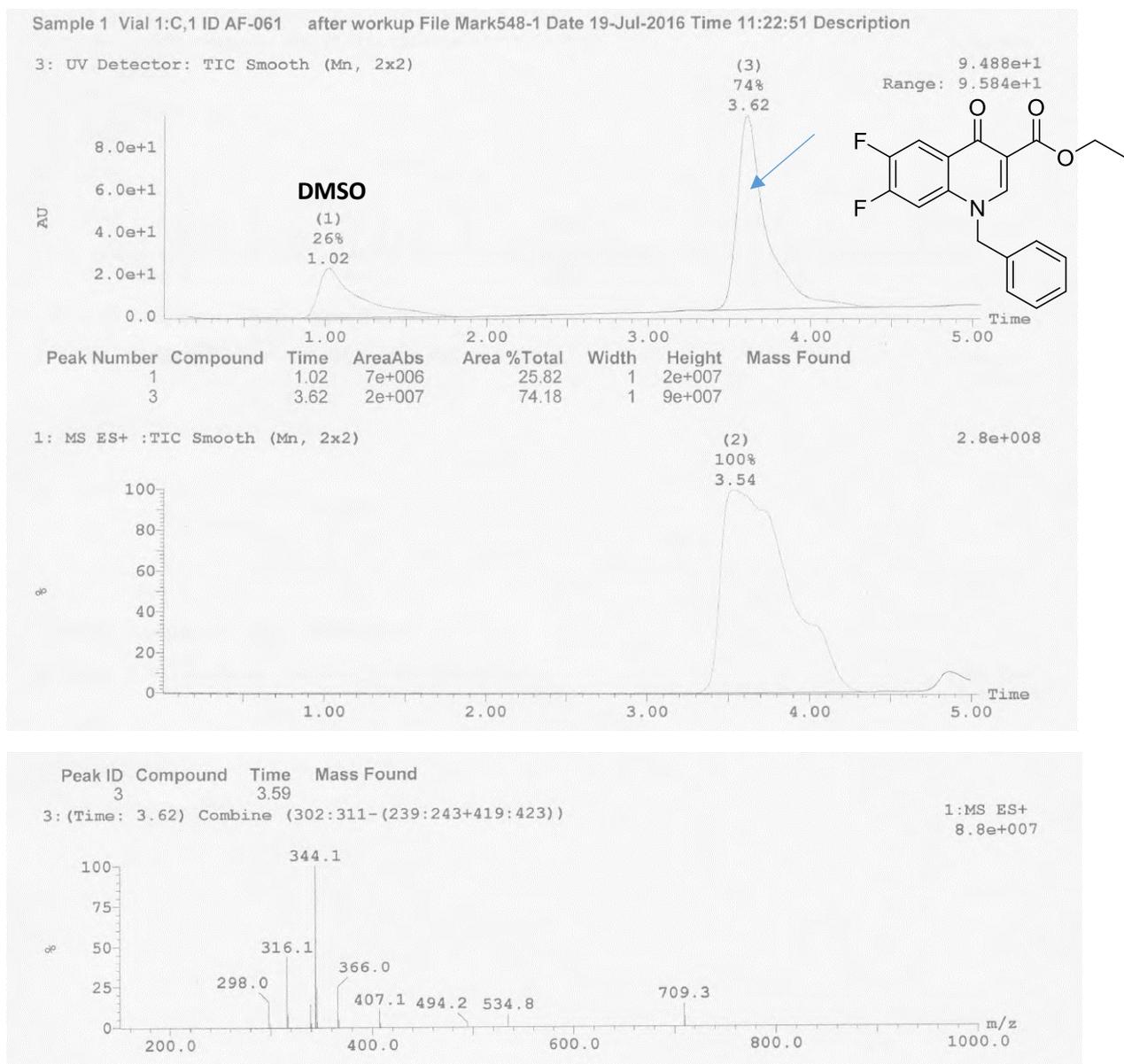


Figure S5. LC-MS profile of compound 3d.

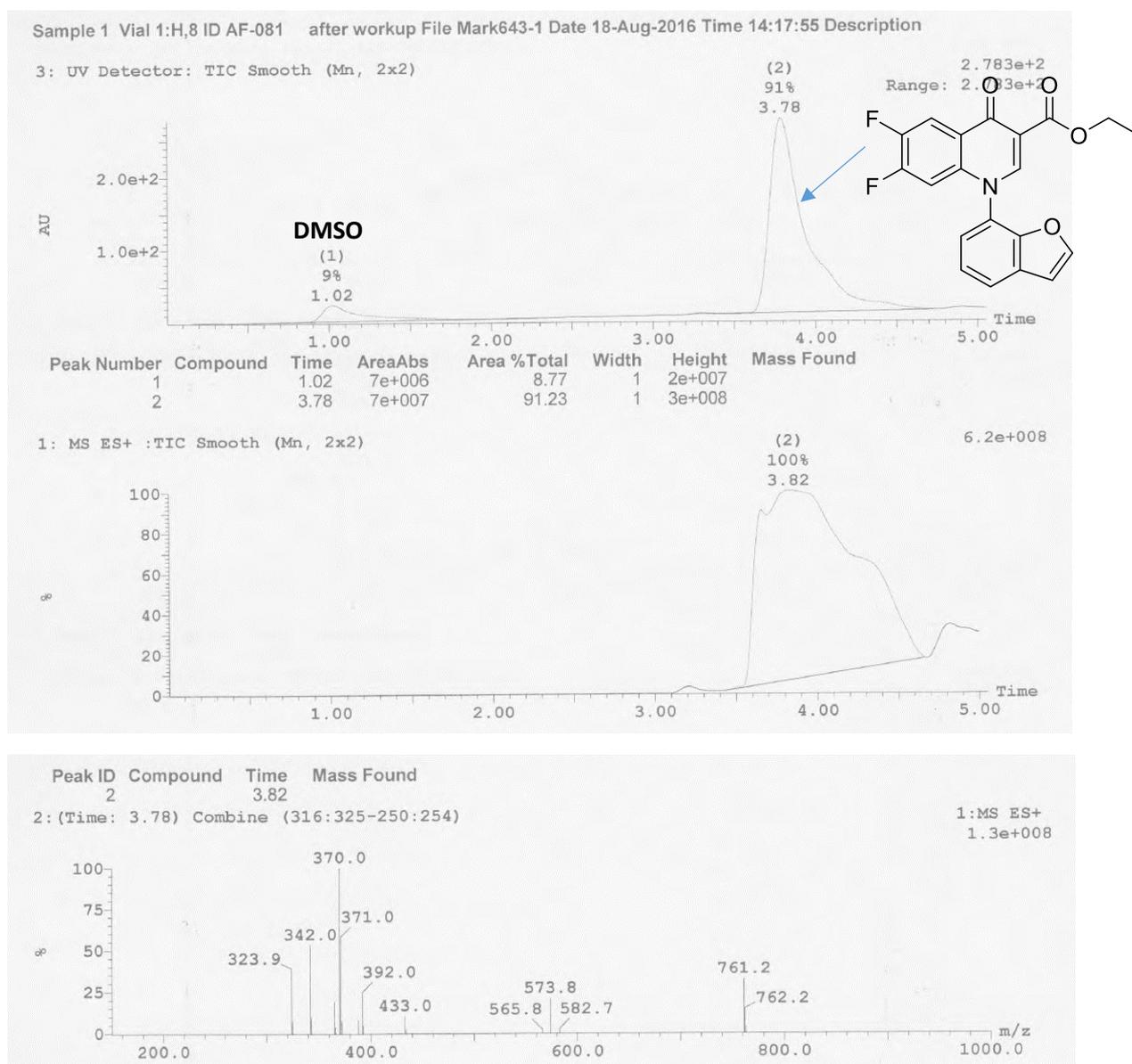


Figure S6. LC-MS profile of compound 3e.

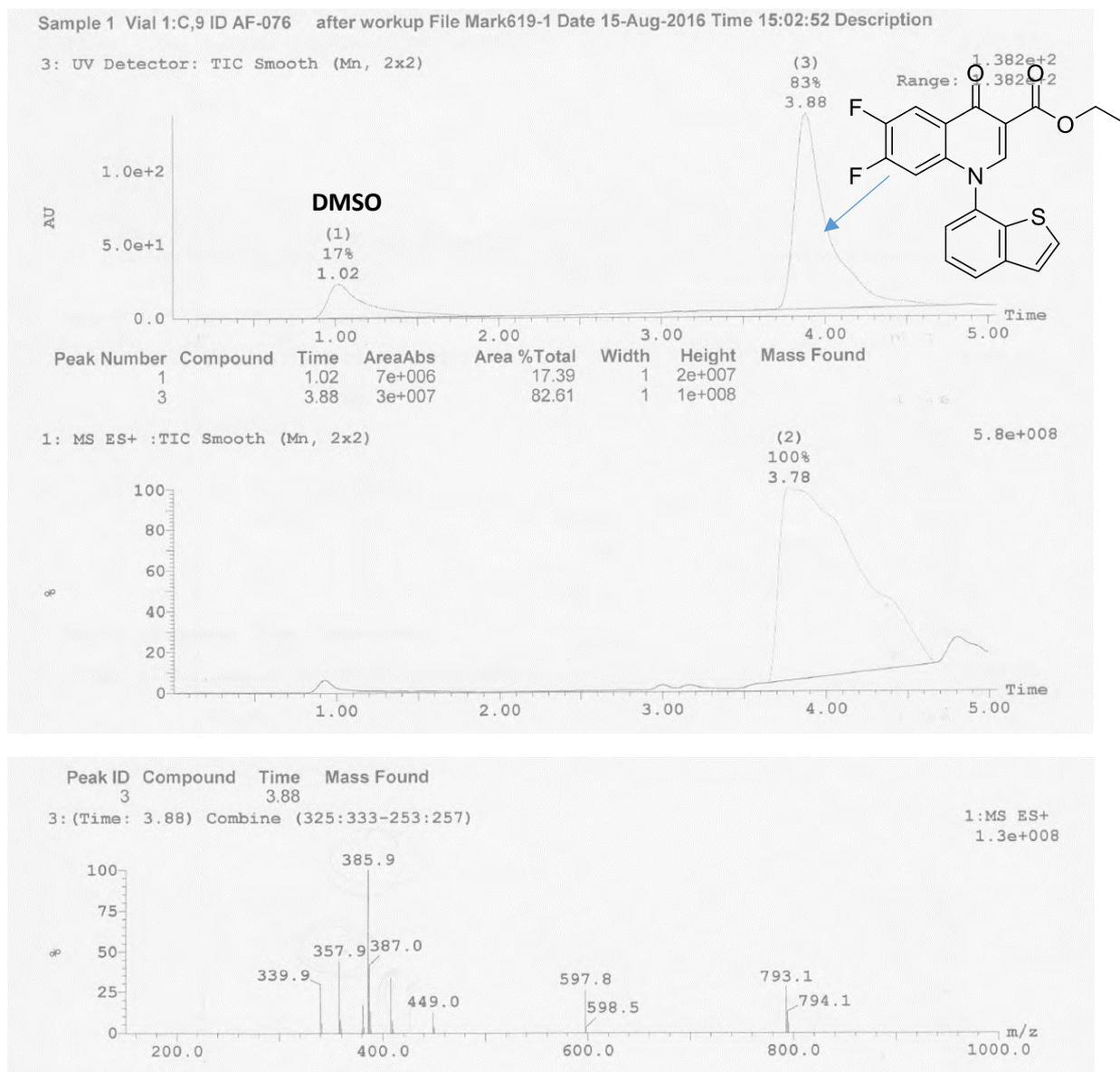


Figure S7. LC-MS profile of compound 3f.

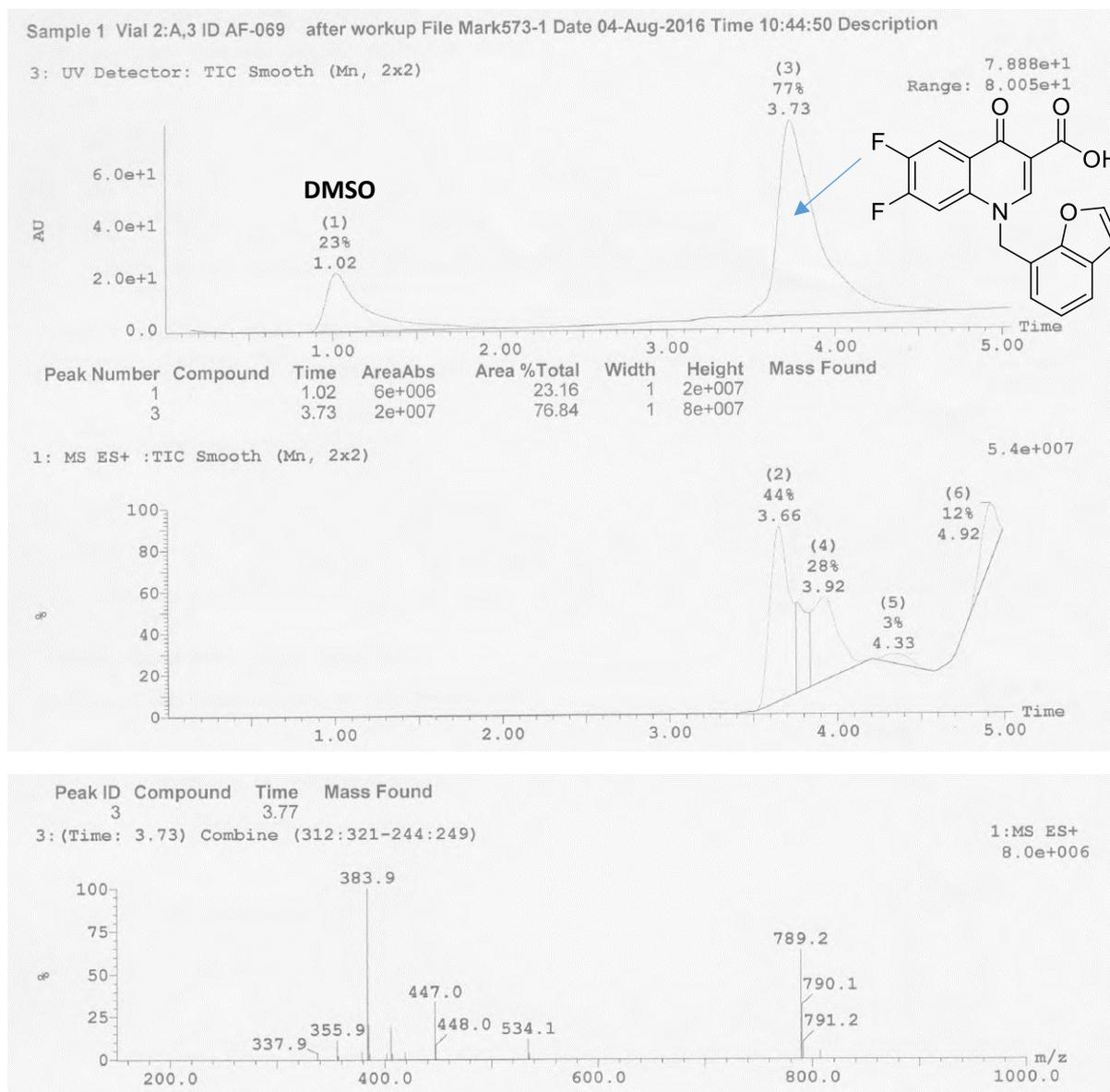


Figure S8. LC-MS profile of compound 3g.

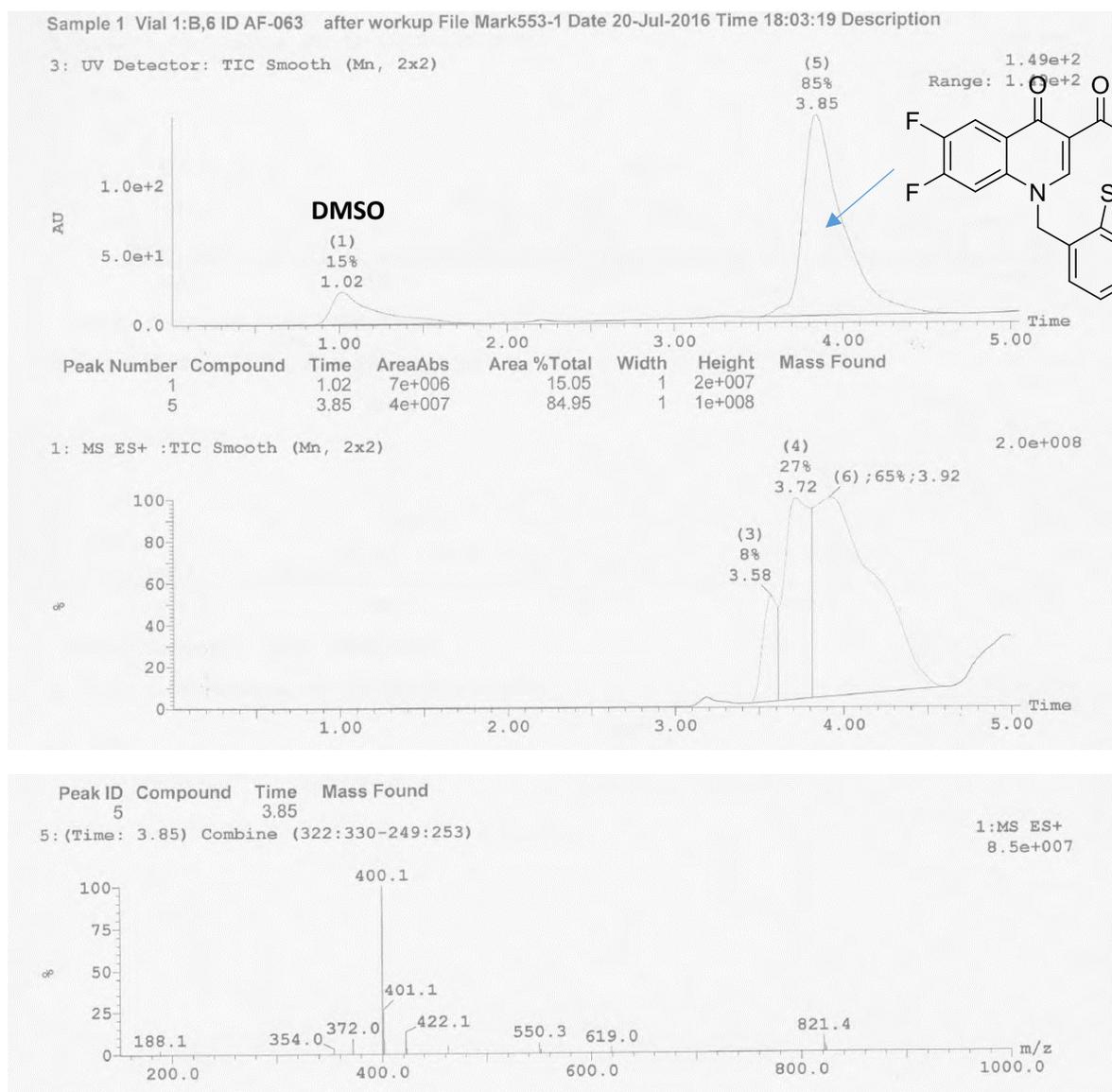


Figure S9. LC-MS profile of compound 4a.

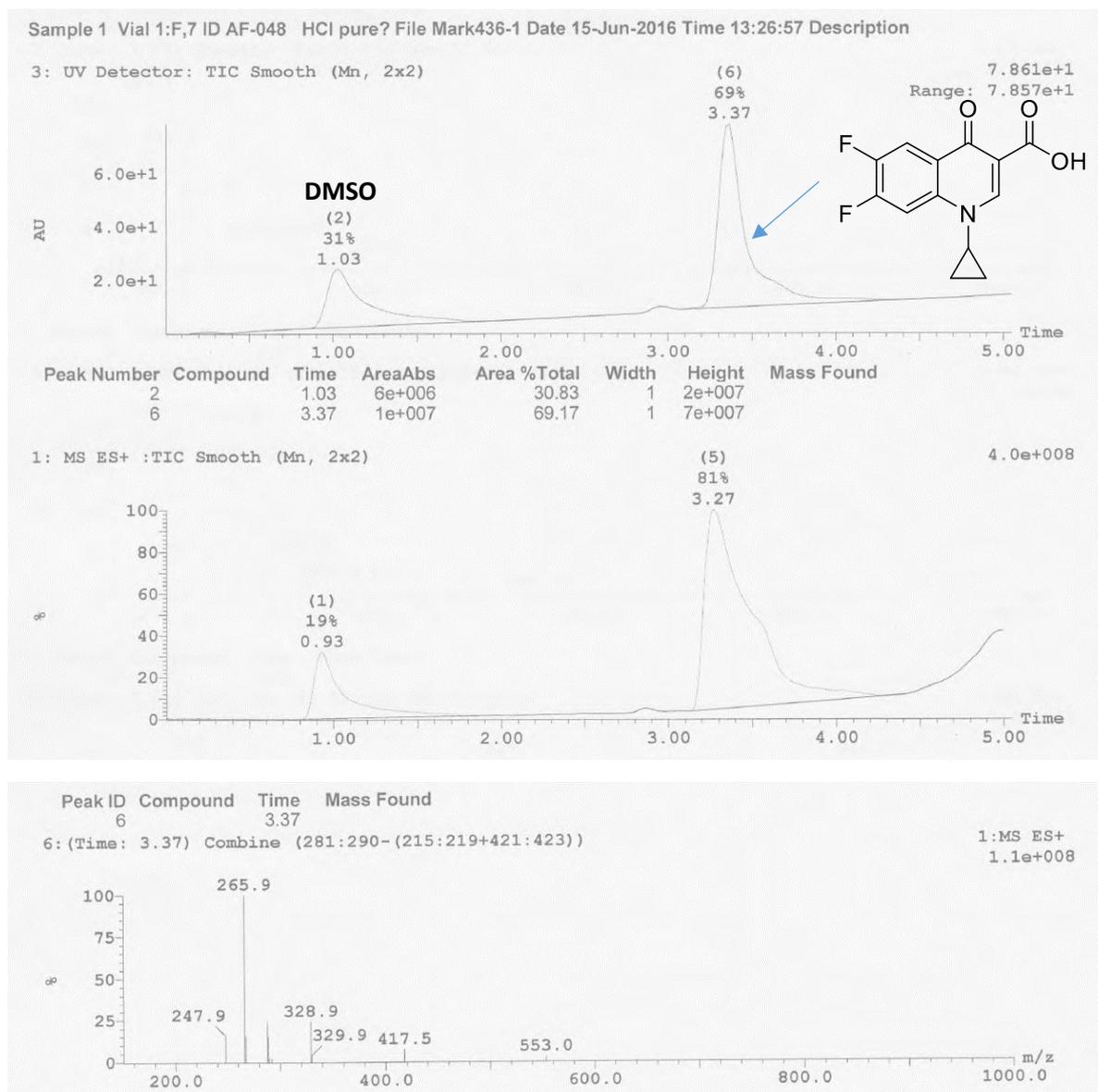


Figure S10. LC-MS profile of compound 4b.

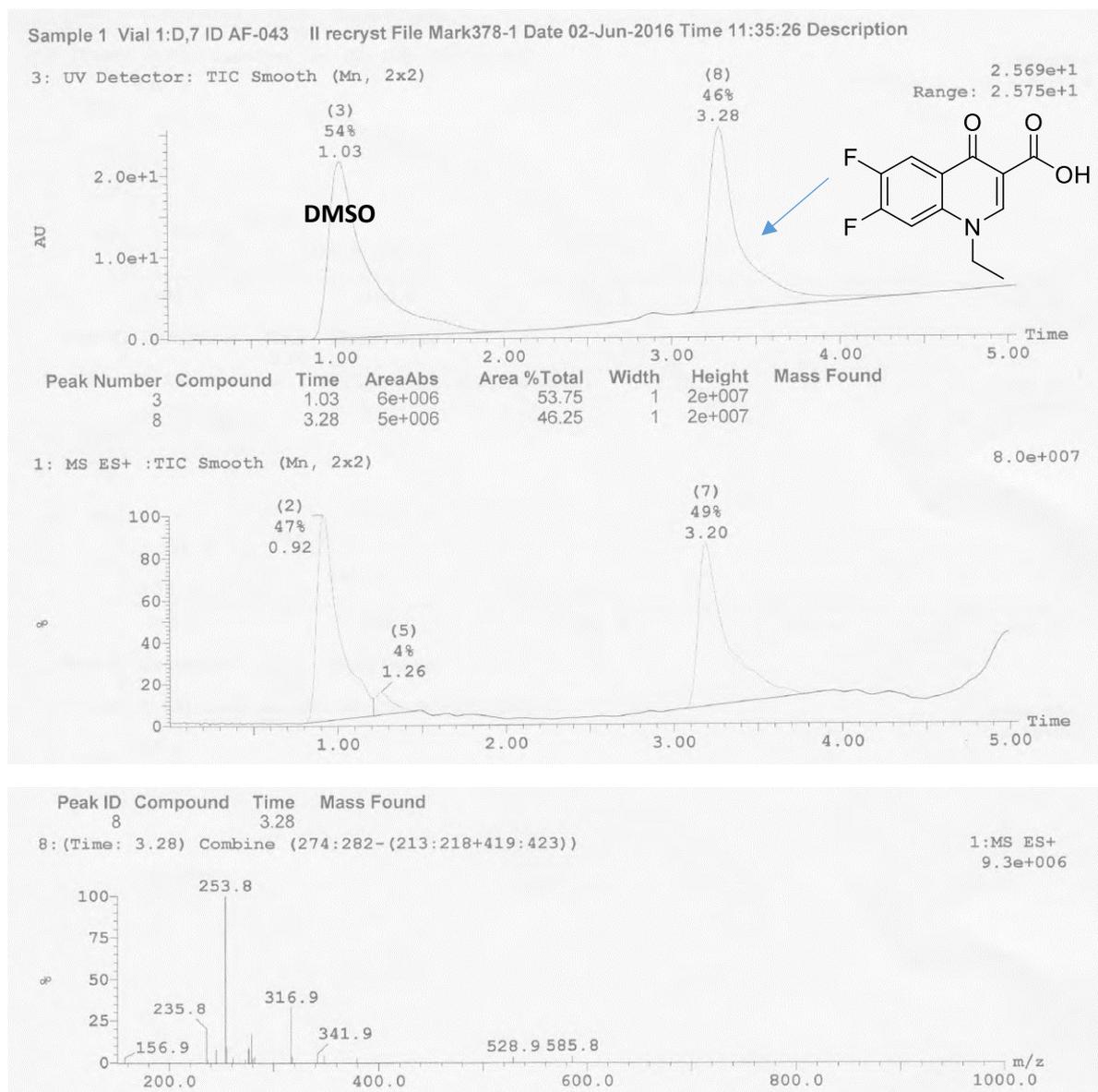


Figure S11. LC-MS profile of compound 4c.

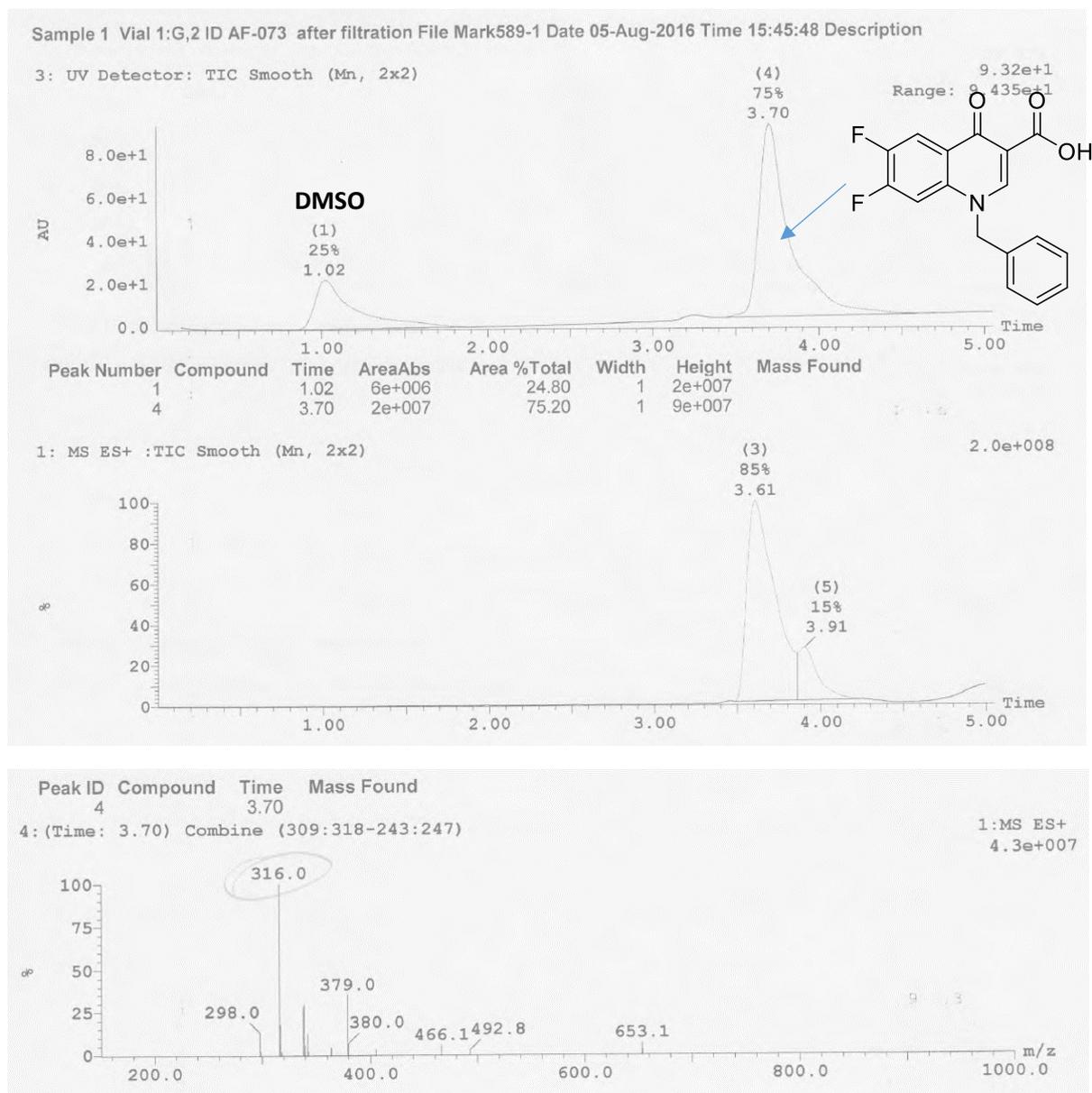


Figure S12. LC-MS profile of compound 4d.

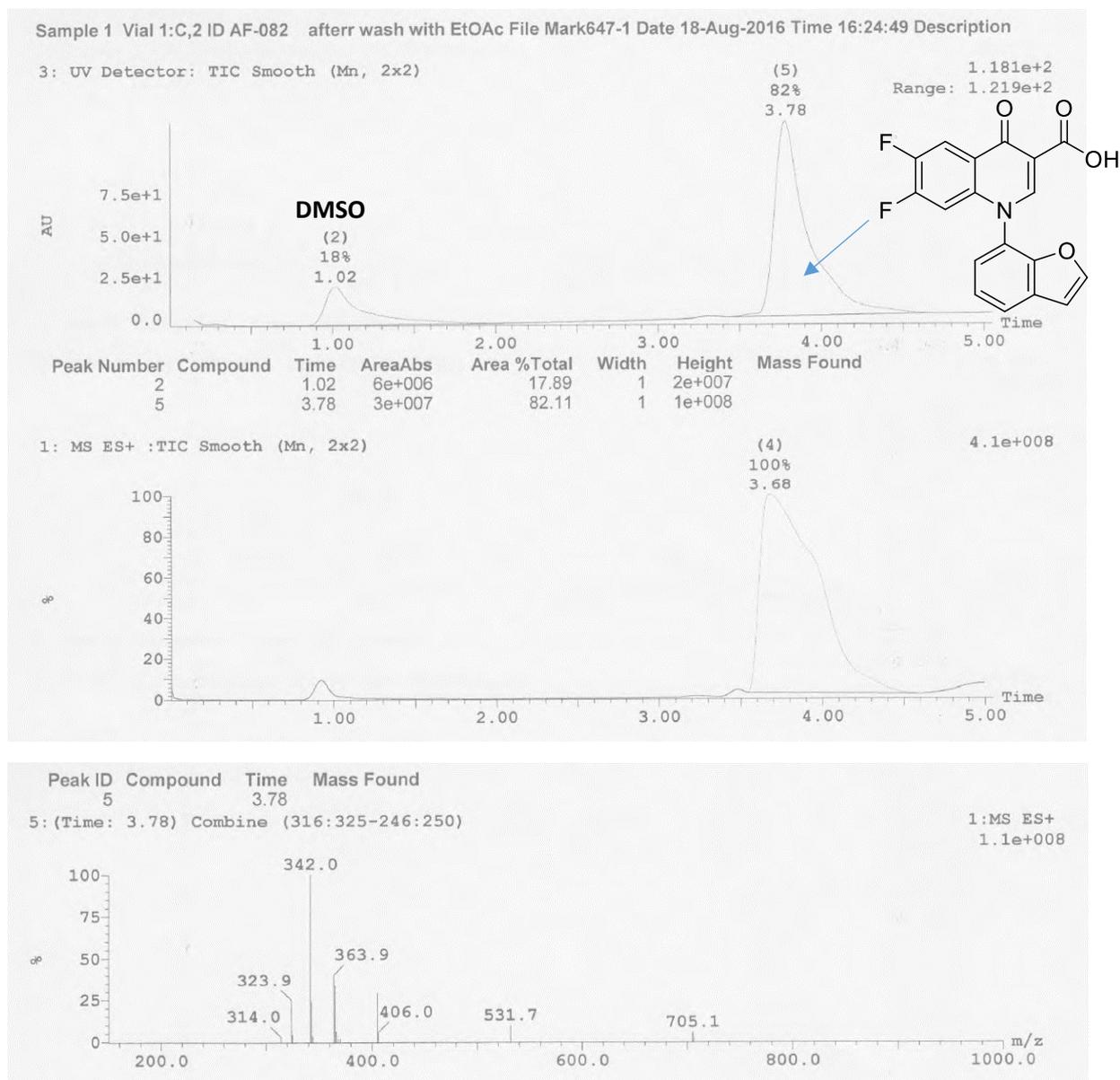


Figure S13. LC-MS profile of compound 4e.

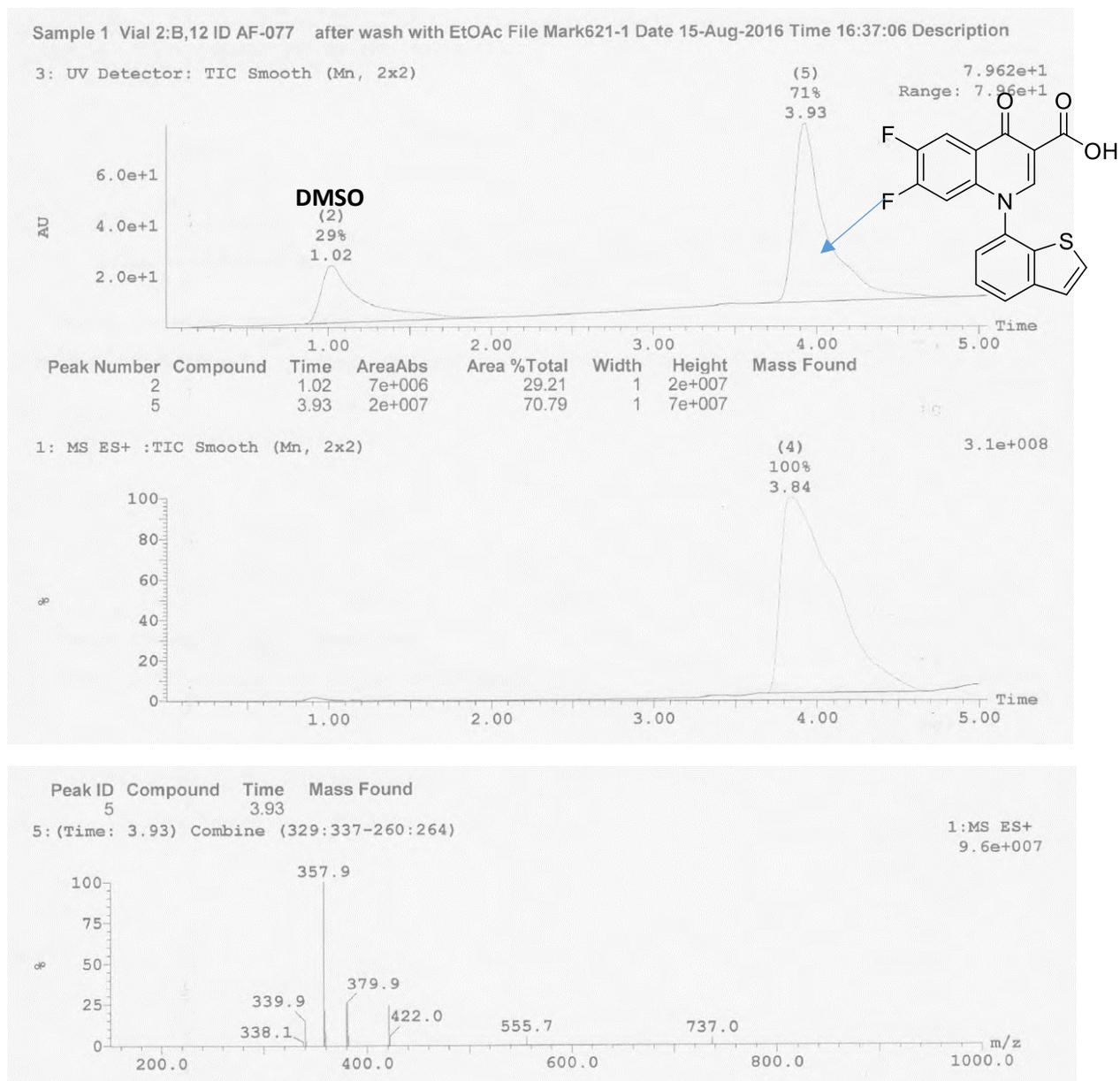


Figure S14. LC-MS profile of compound 4f.

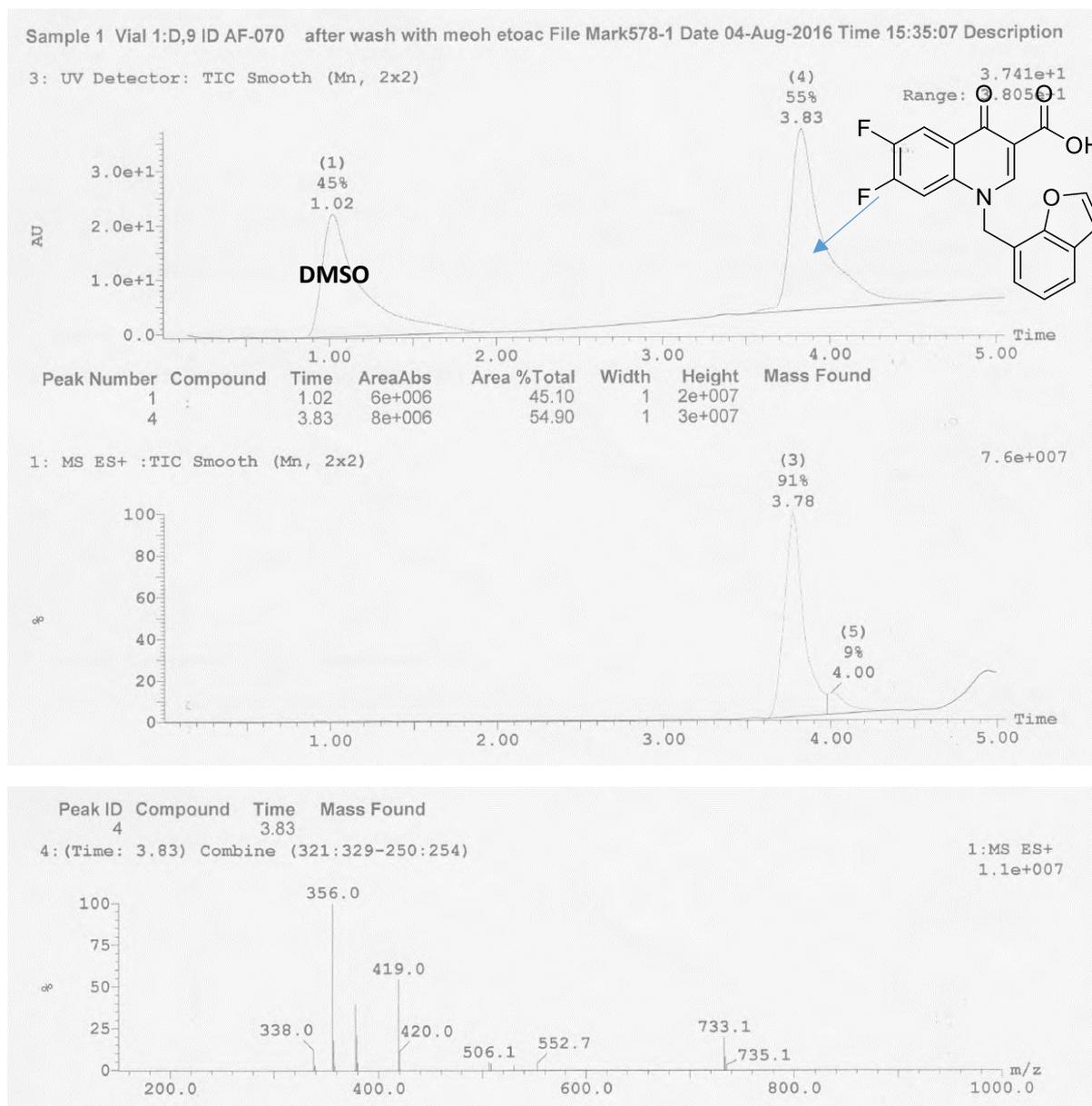


Figure S15. LC-MS profile of compound 4g.

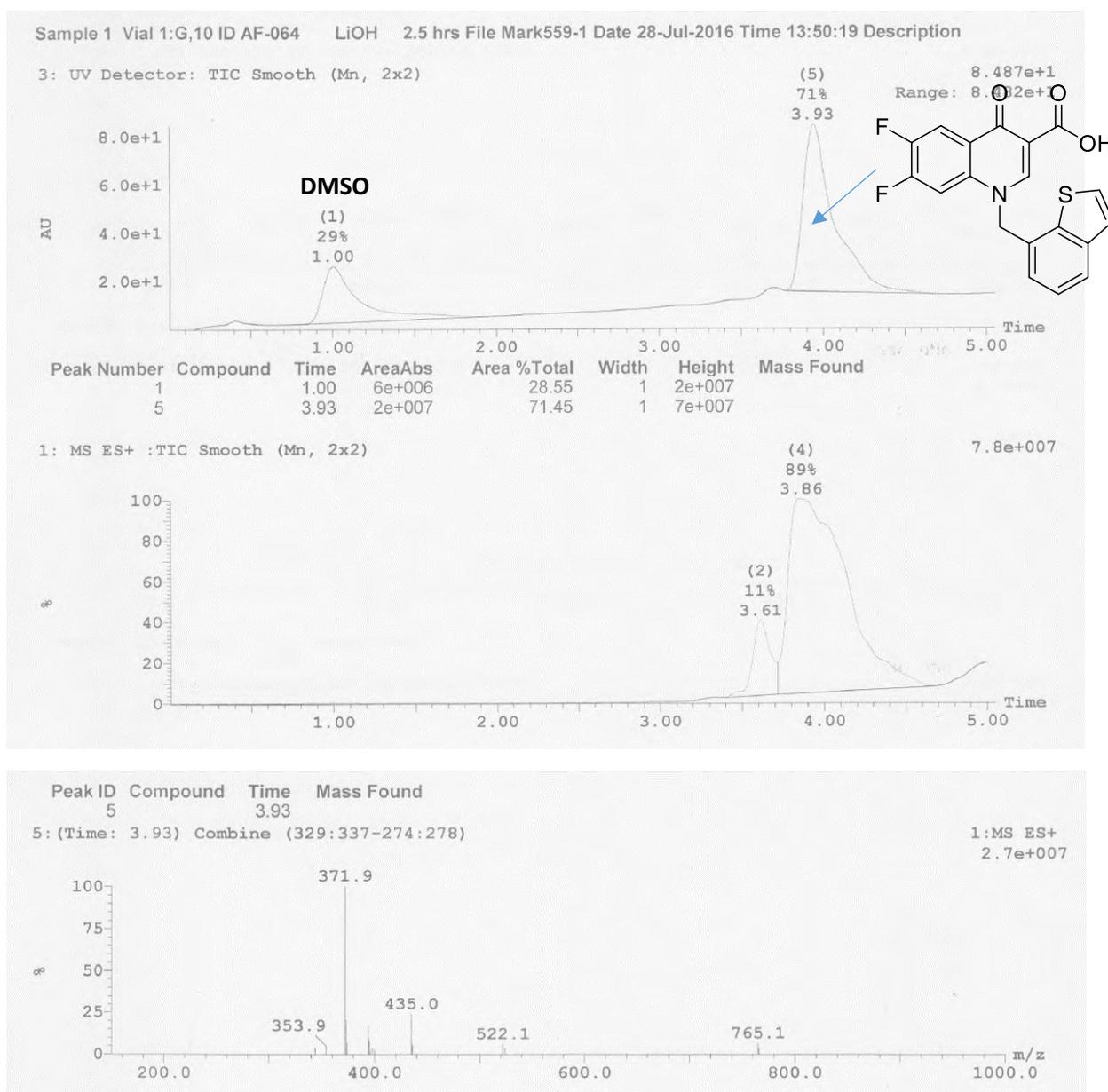


Figure S16. LC-MS profile of compound 5a.

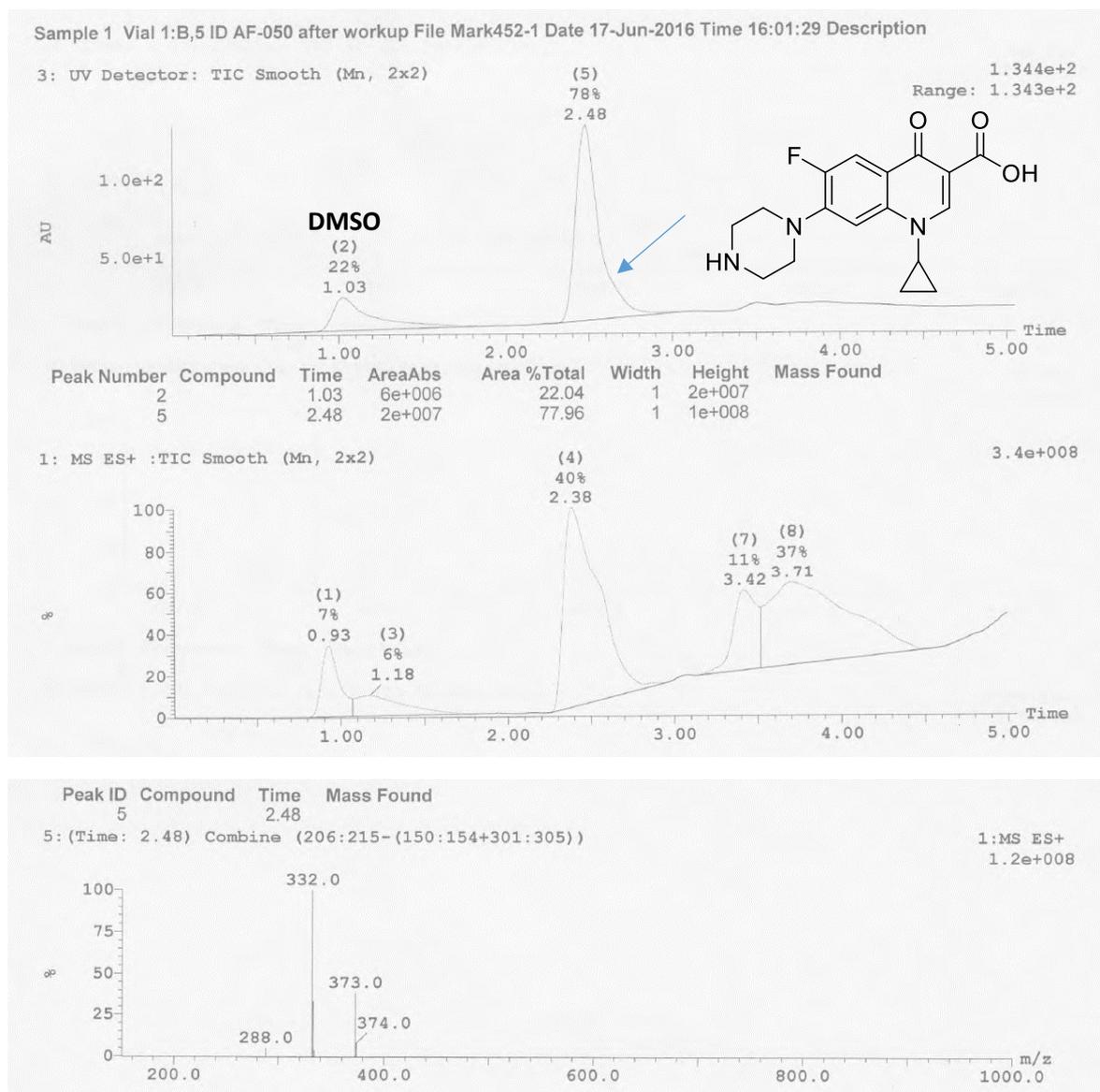


Figure S17. LC-MS profile of compound 5b.

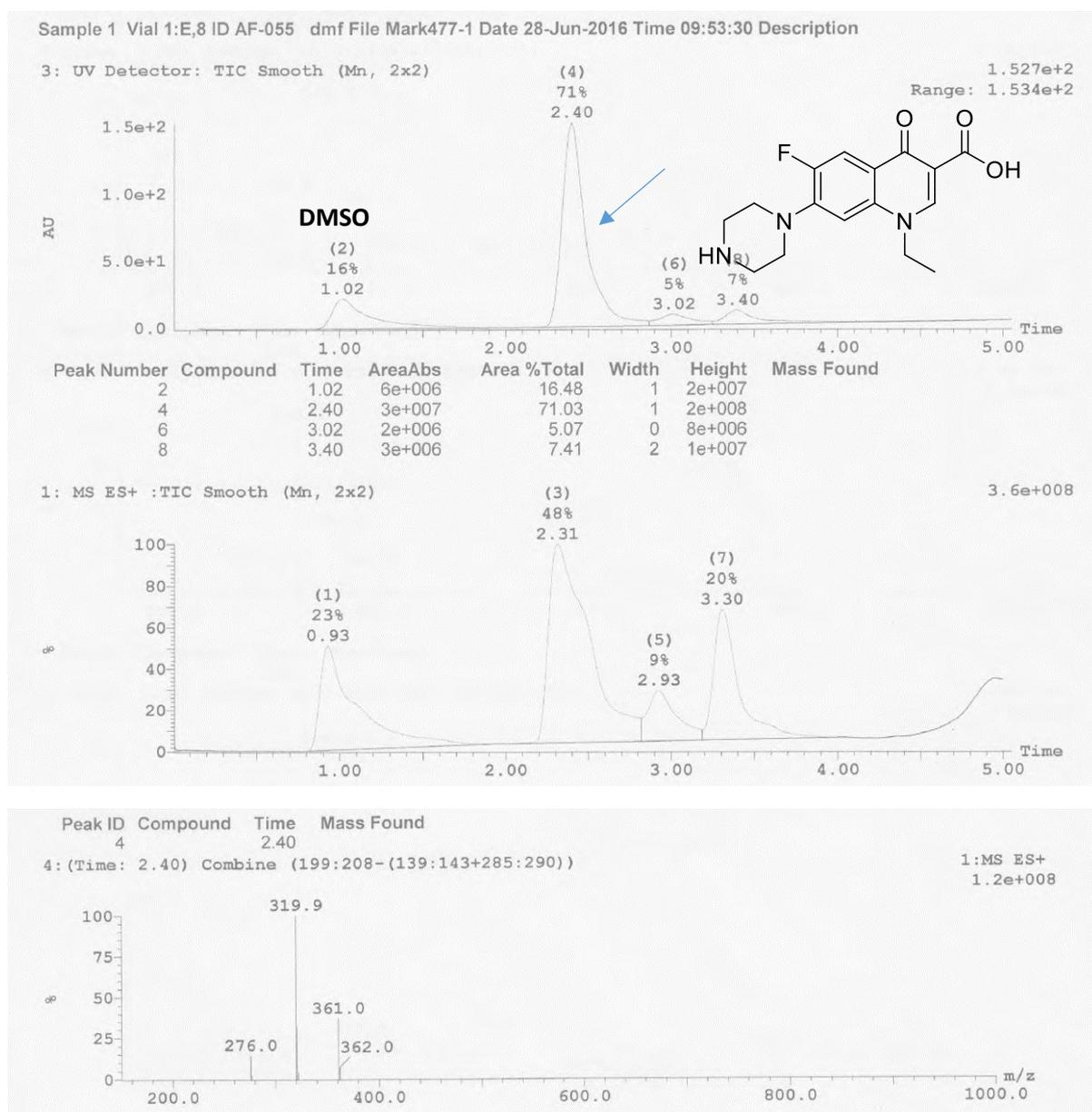


Figure S18. LC-MS profile of compound 5c.

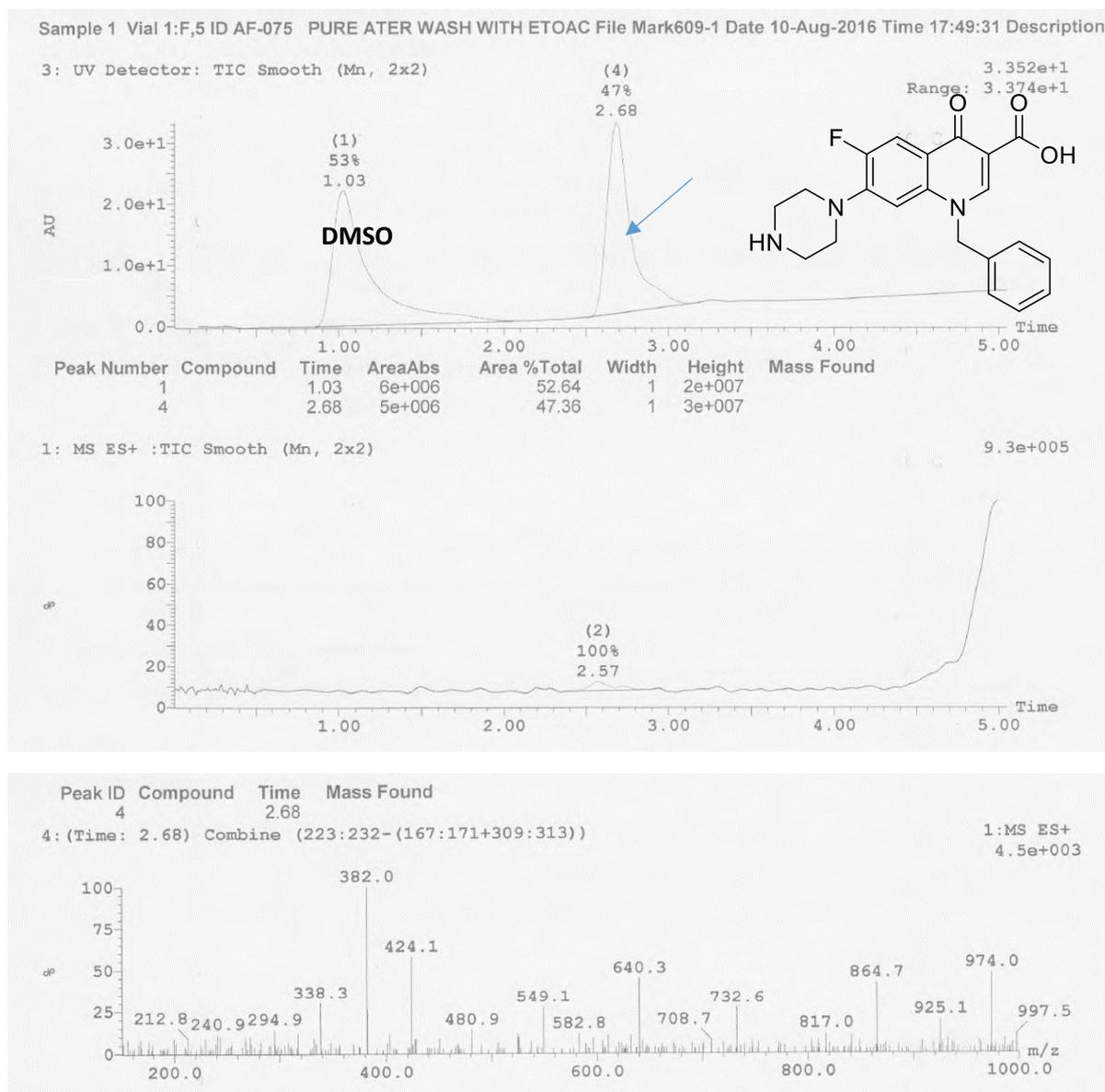


Figure S19. LC-MS profile of compound 5d.

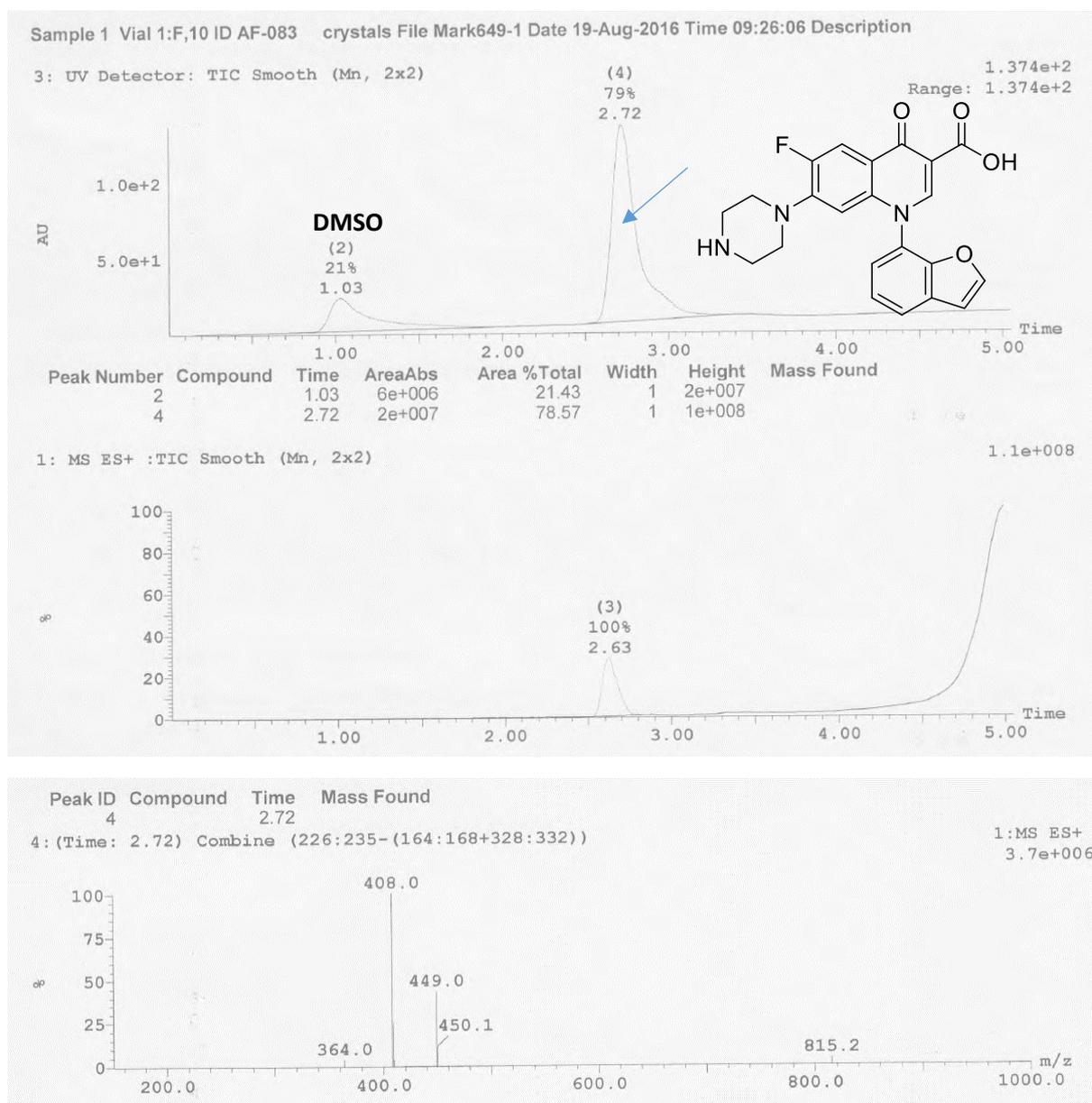


Figure S20. LC-MS profile of compound 5e.

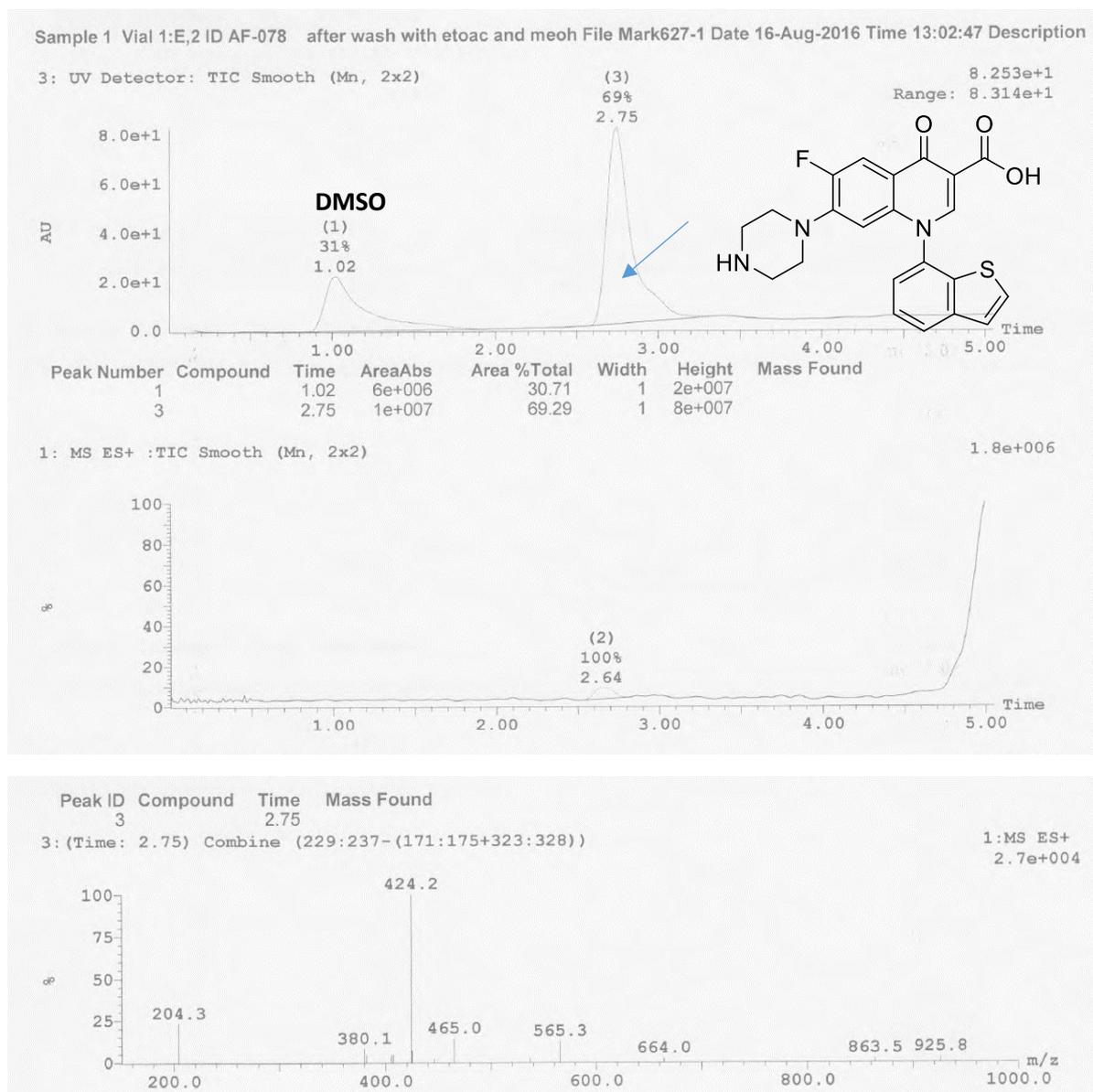


Figure S21. LC-MS profile of compound 5f.

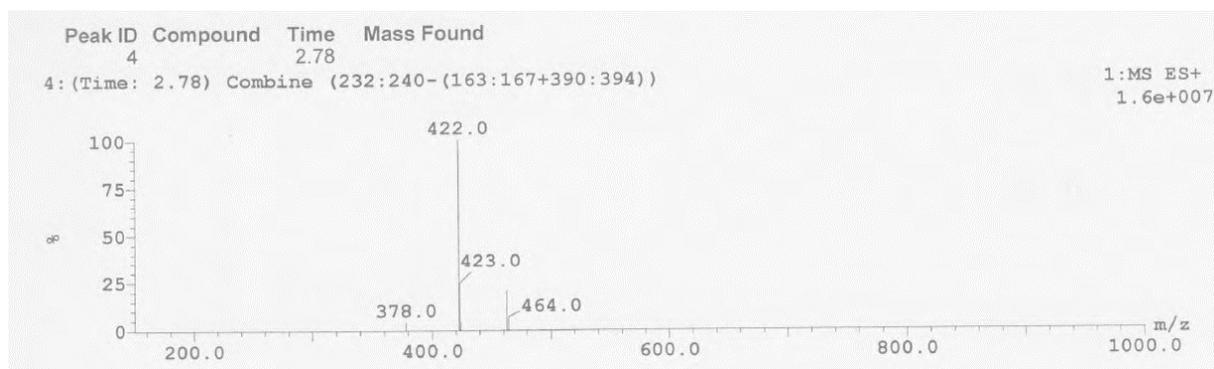
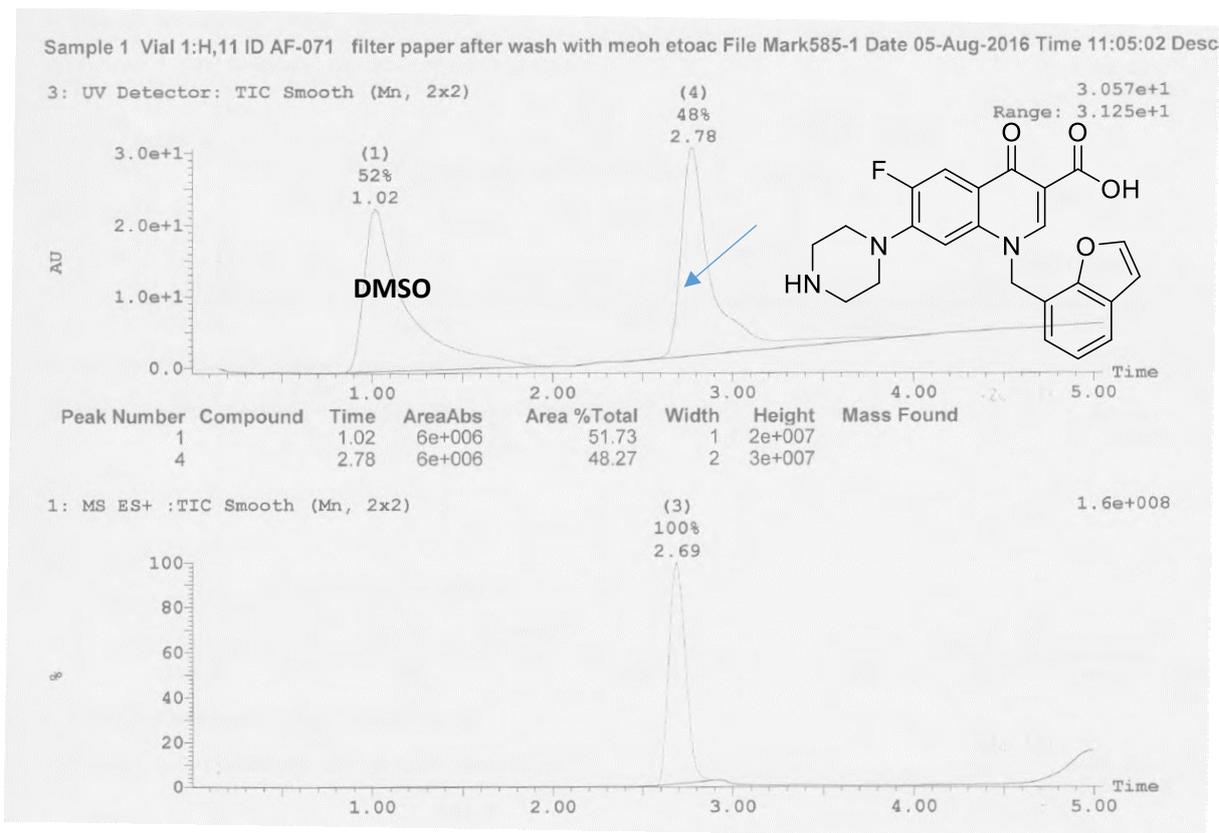


Figure S22. LC-MS profile of compound 5g.

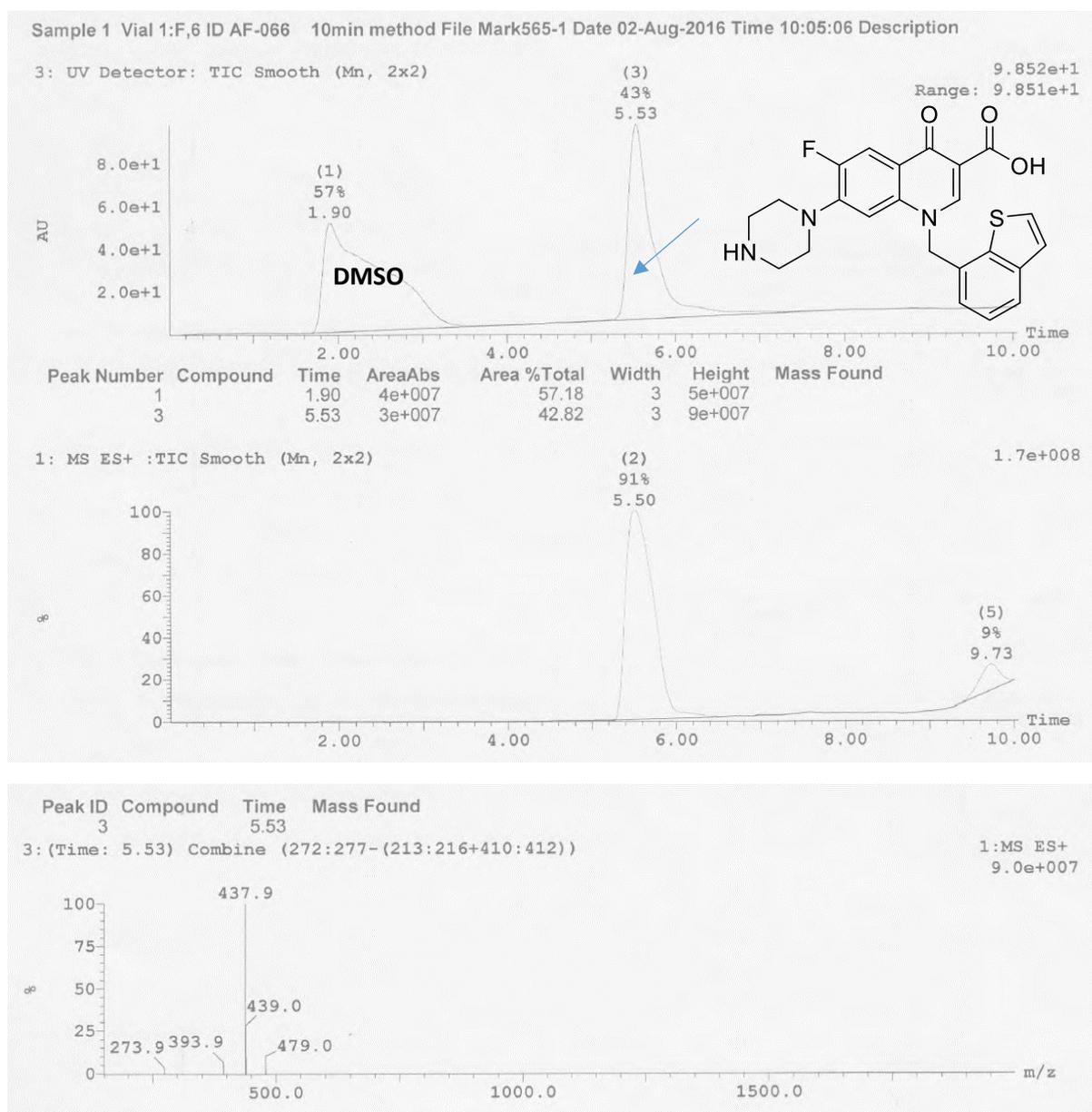


Figure S23A. LC-MS profile of compound 6a, method A (5 minutes).

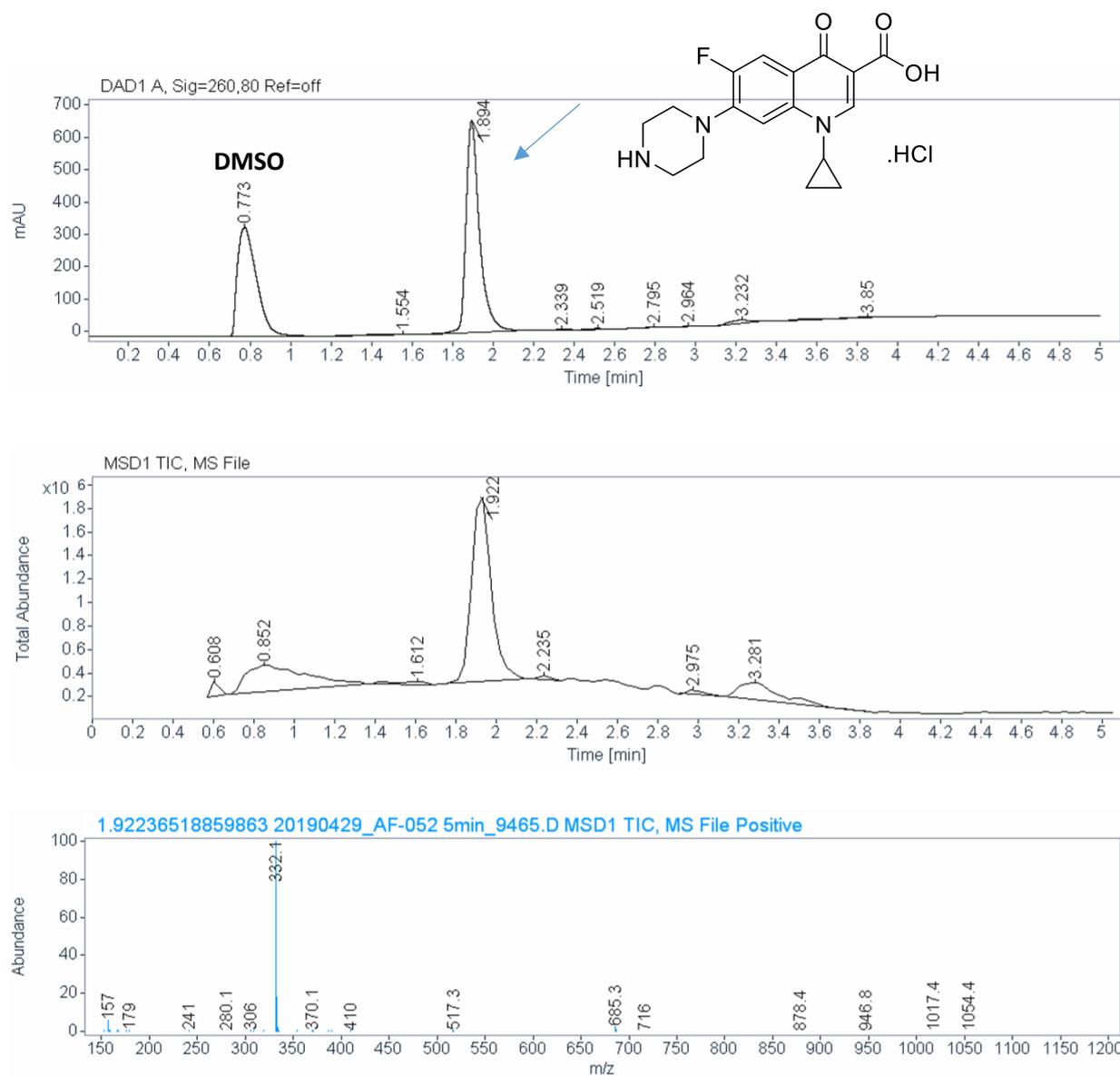


Figure S23B. LC-MS profile of compound 6a, method B (10 minutes).

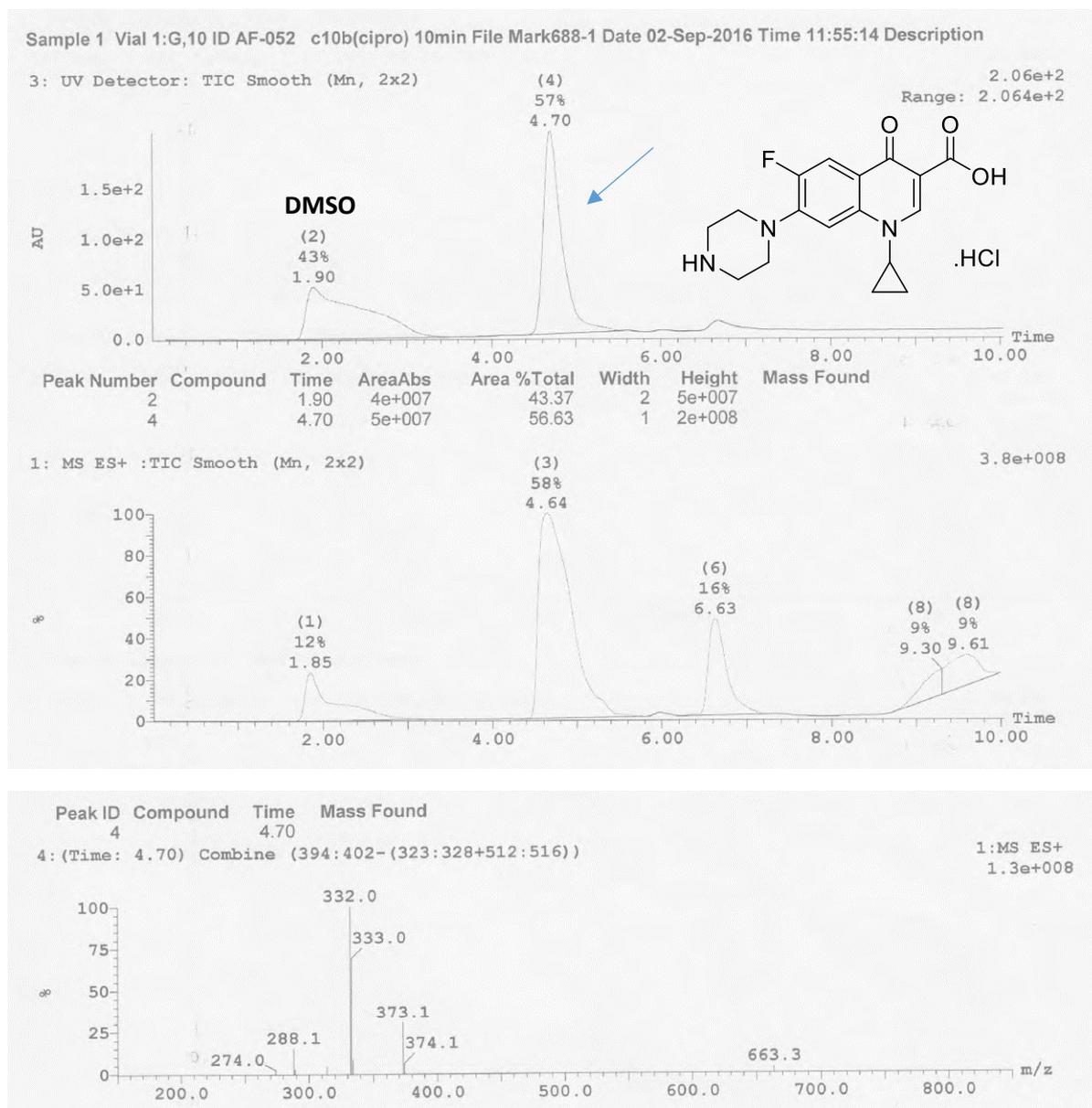


Figure S24A. LC-MS profile of compound 6b, method A (5 minutes).

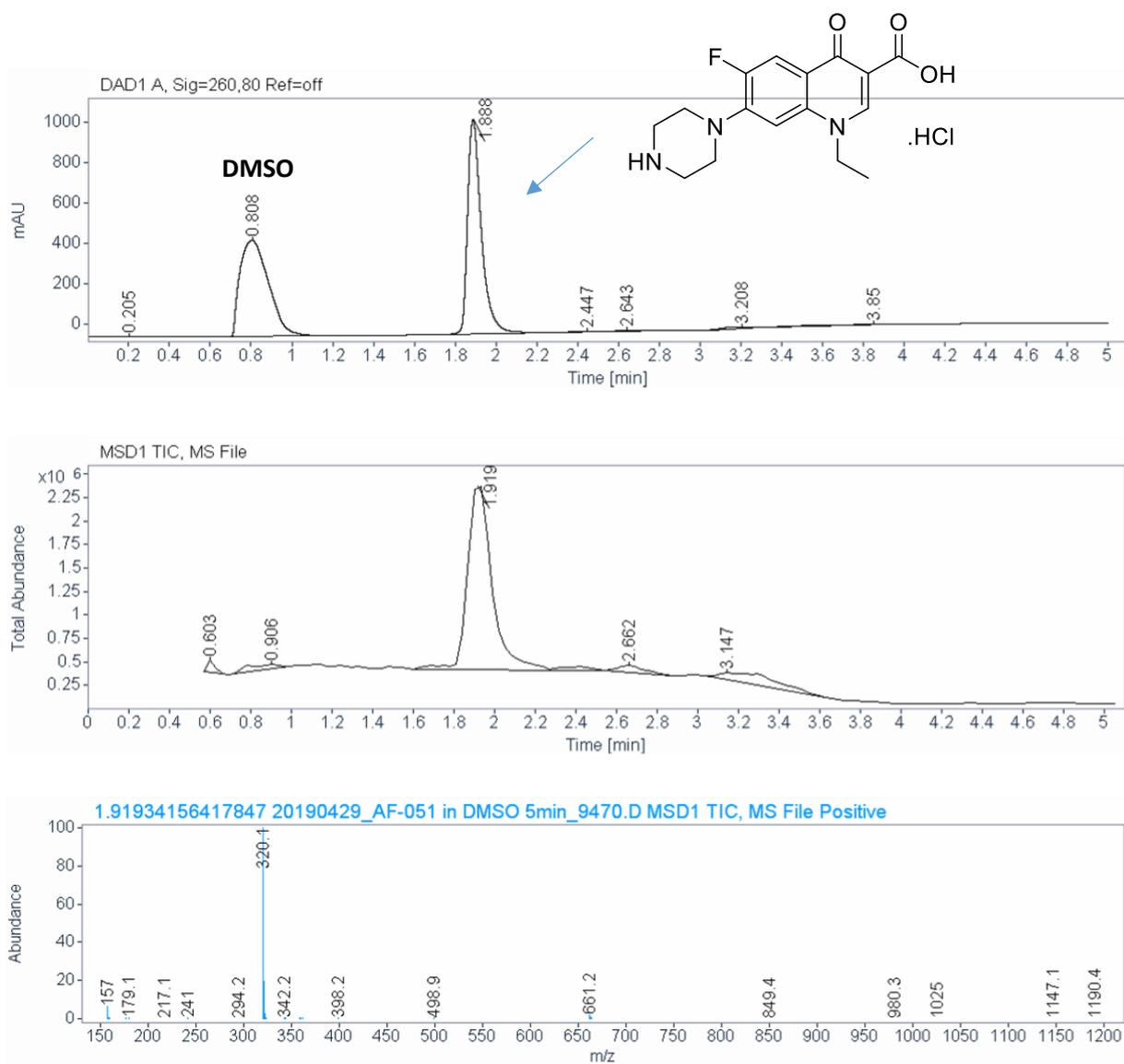


Figure S24B. LC-MS profile of compound 6b, method B (10 minutes).

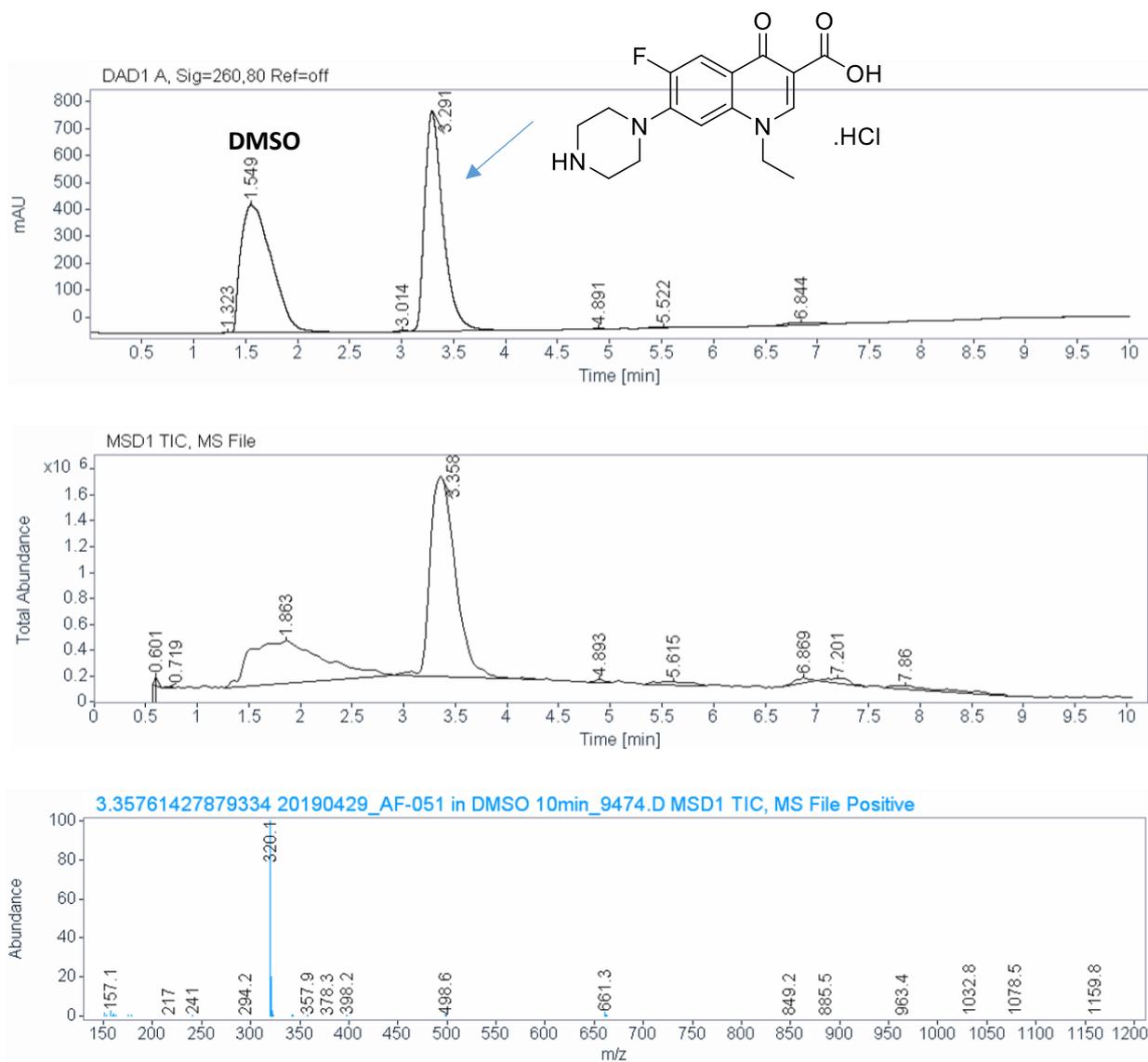


Figure S25A. LC-MS profile of compound 6c, method A (5 minutes).

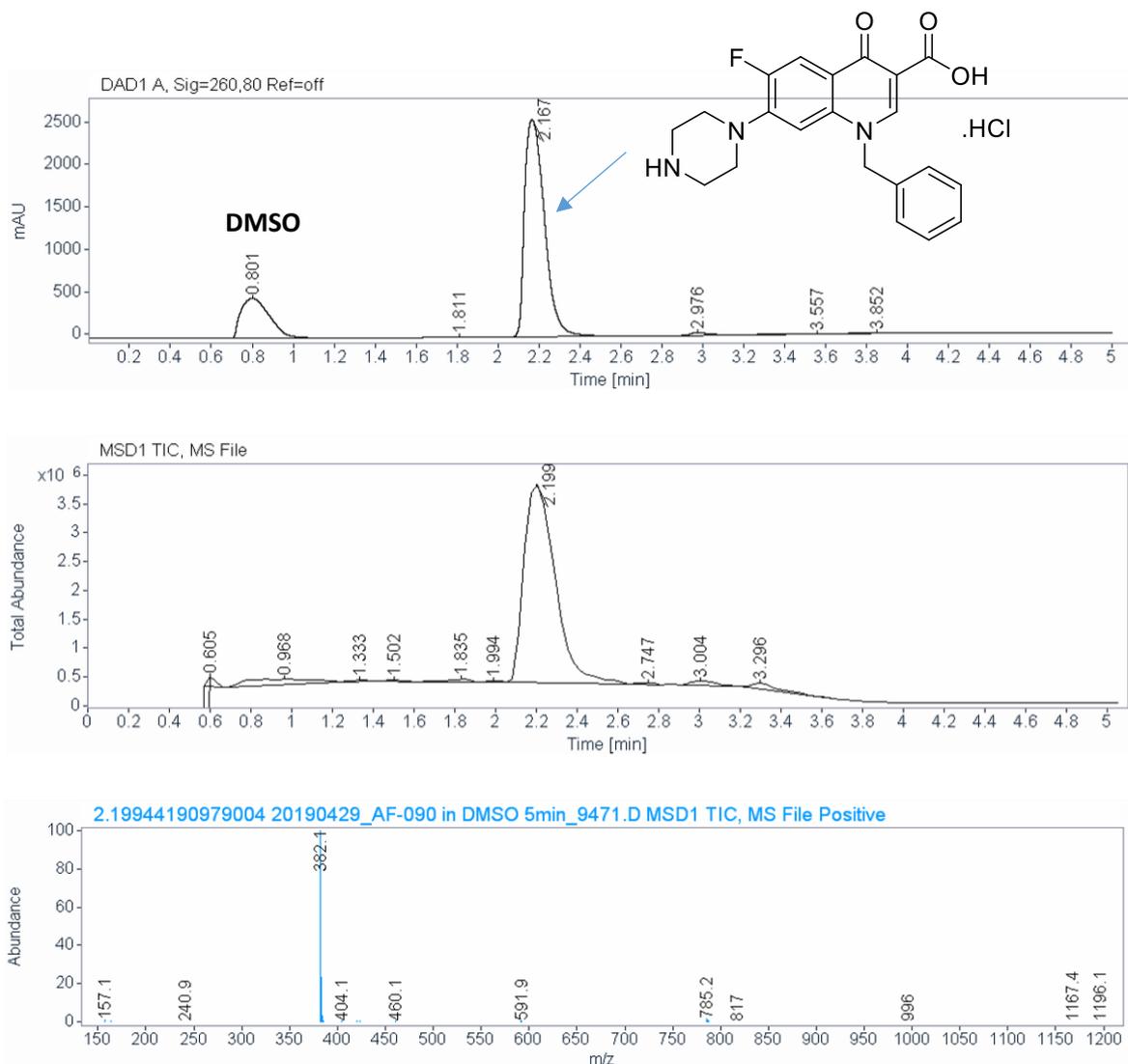


Figure S25B. LC-MS profile of compound 6c, method B (10 minutes).

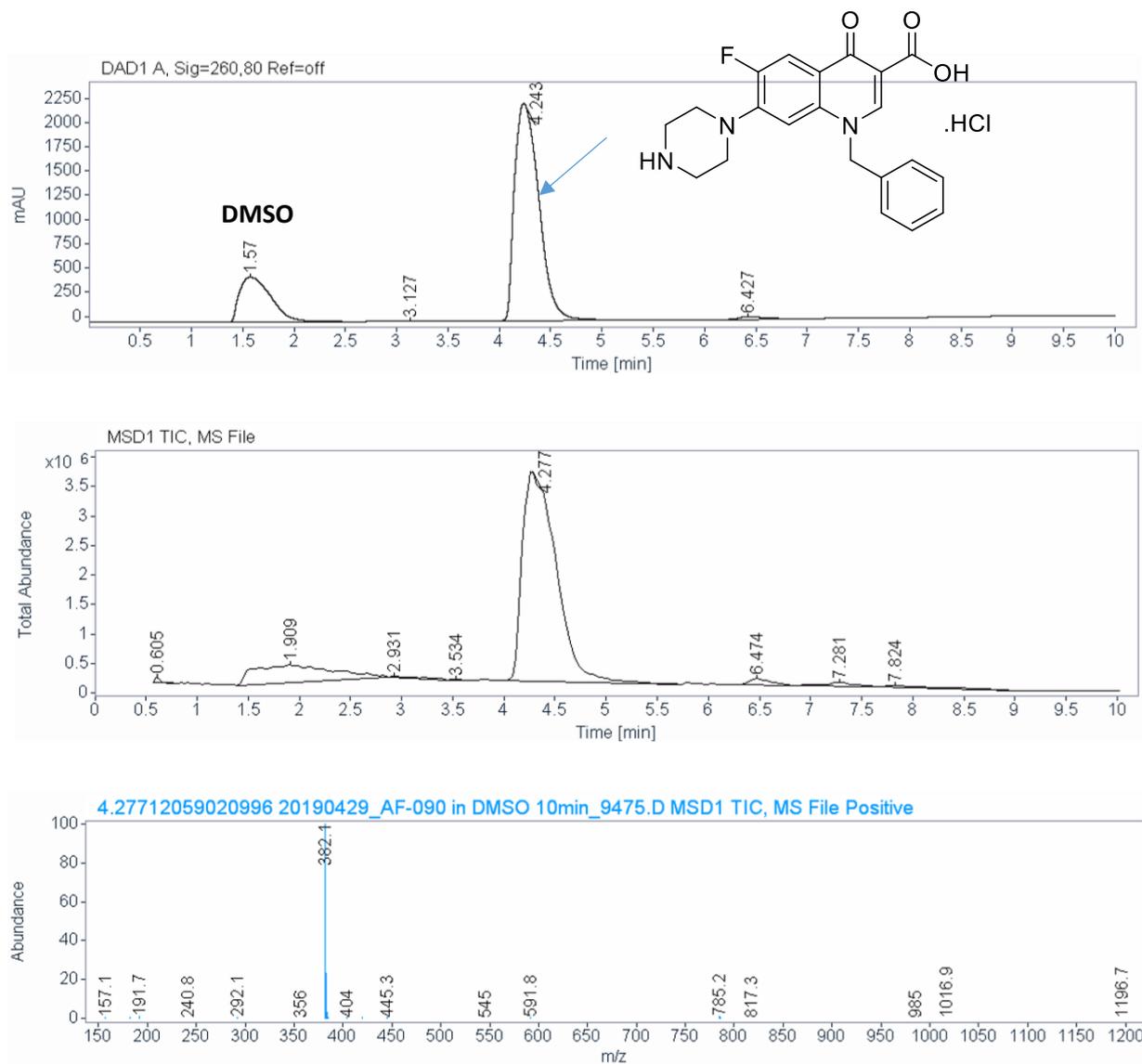


Figure S26A. LC-MS profile of compound 6d, method A (5 minutes).

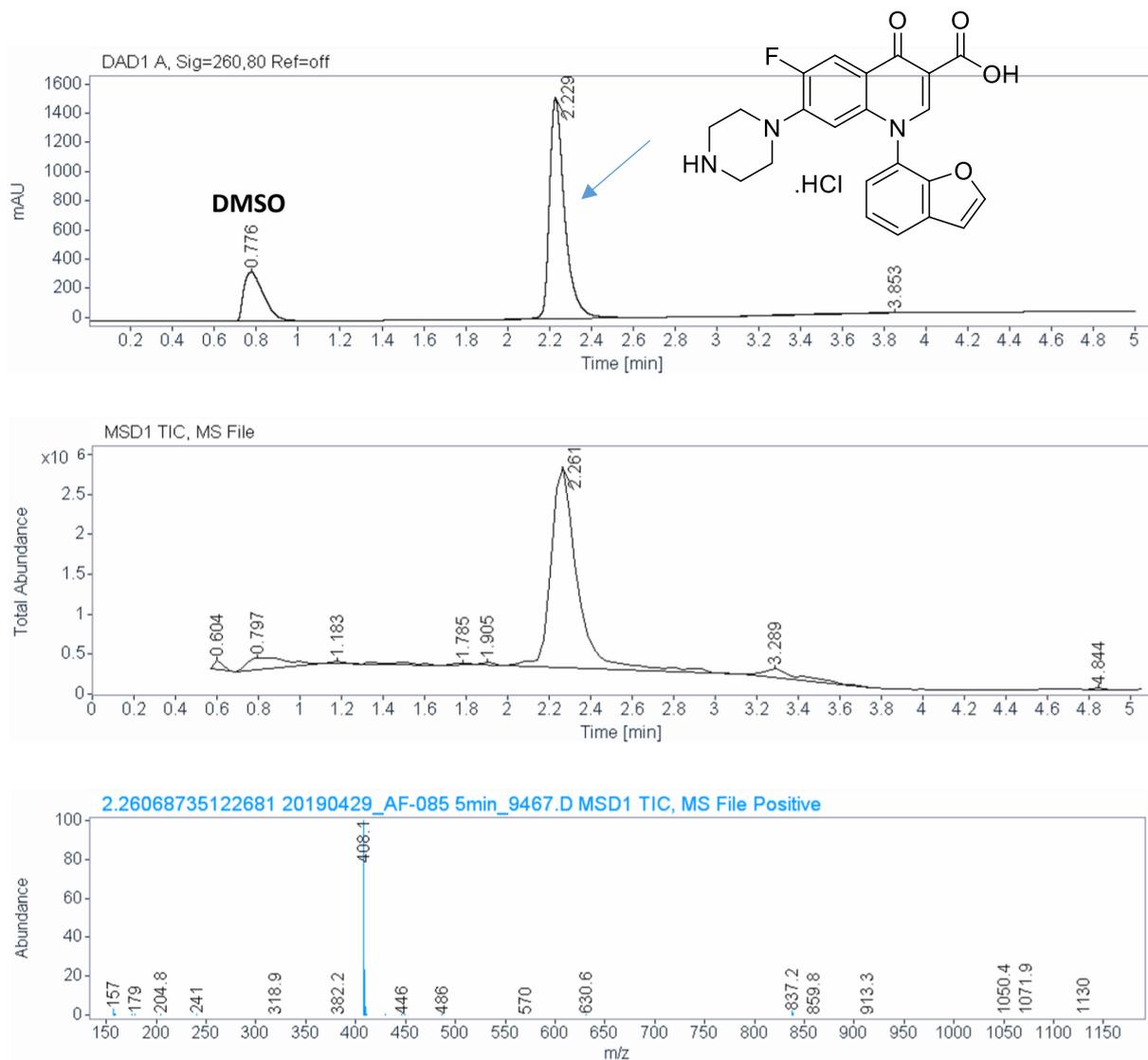


Figure S26B. LC-MS profile of compound 6d, method B (10 minutes).

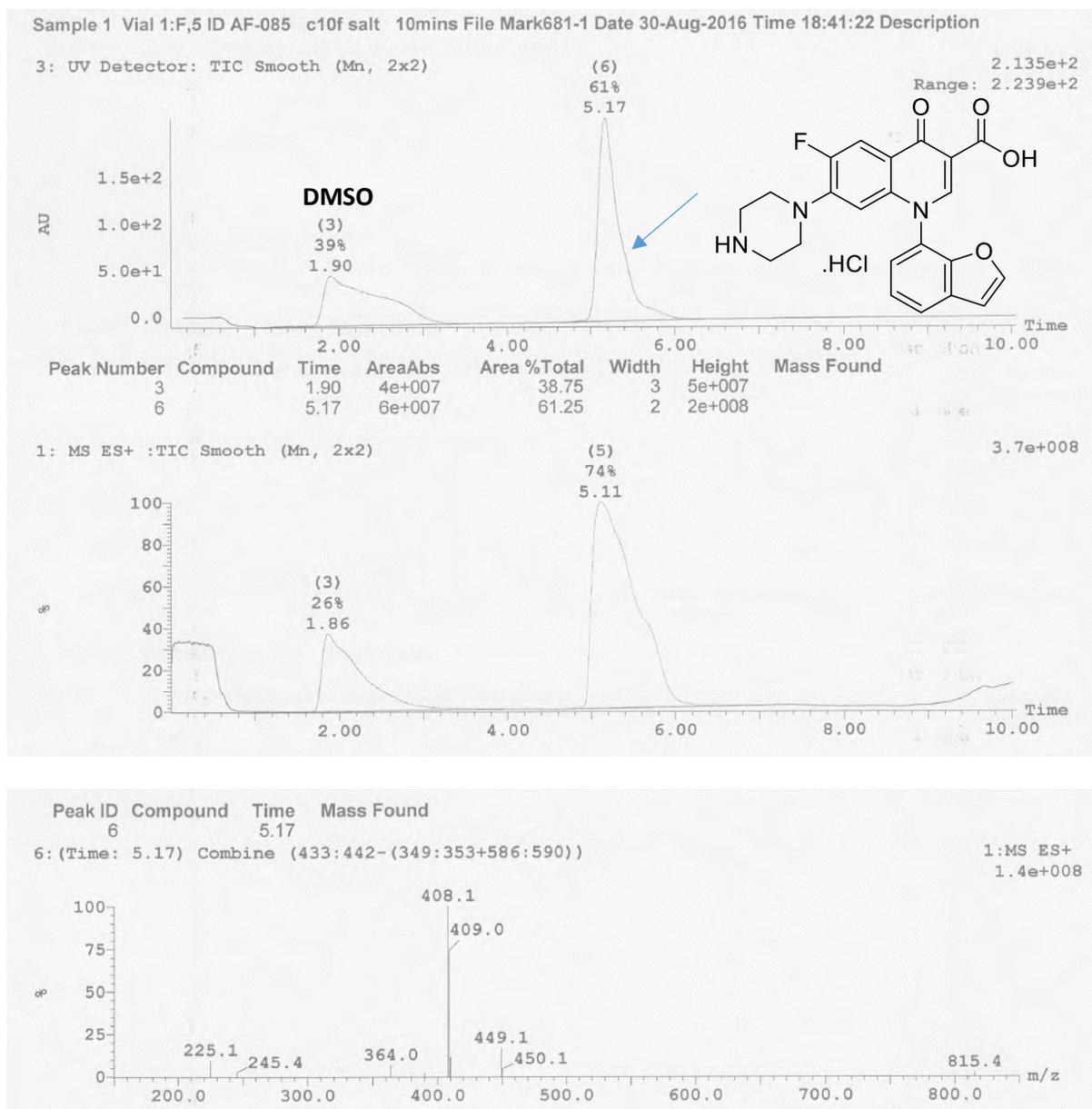


Figure S27A. LC-MS profile of compound 6e, method A (5 minutes).

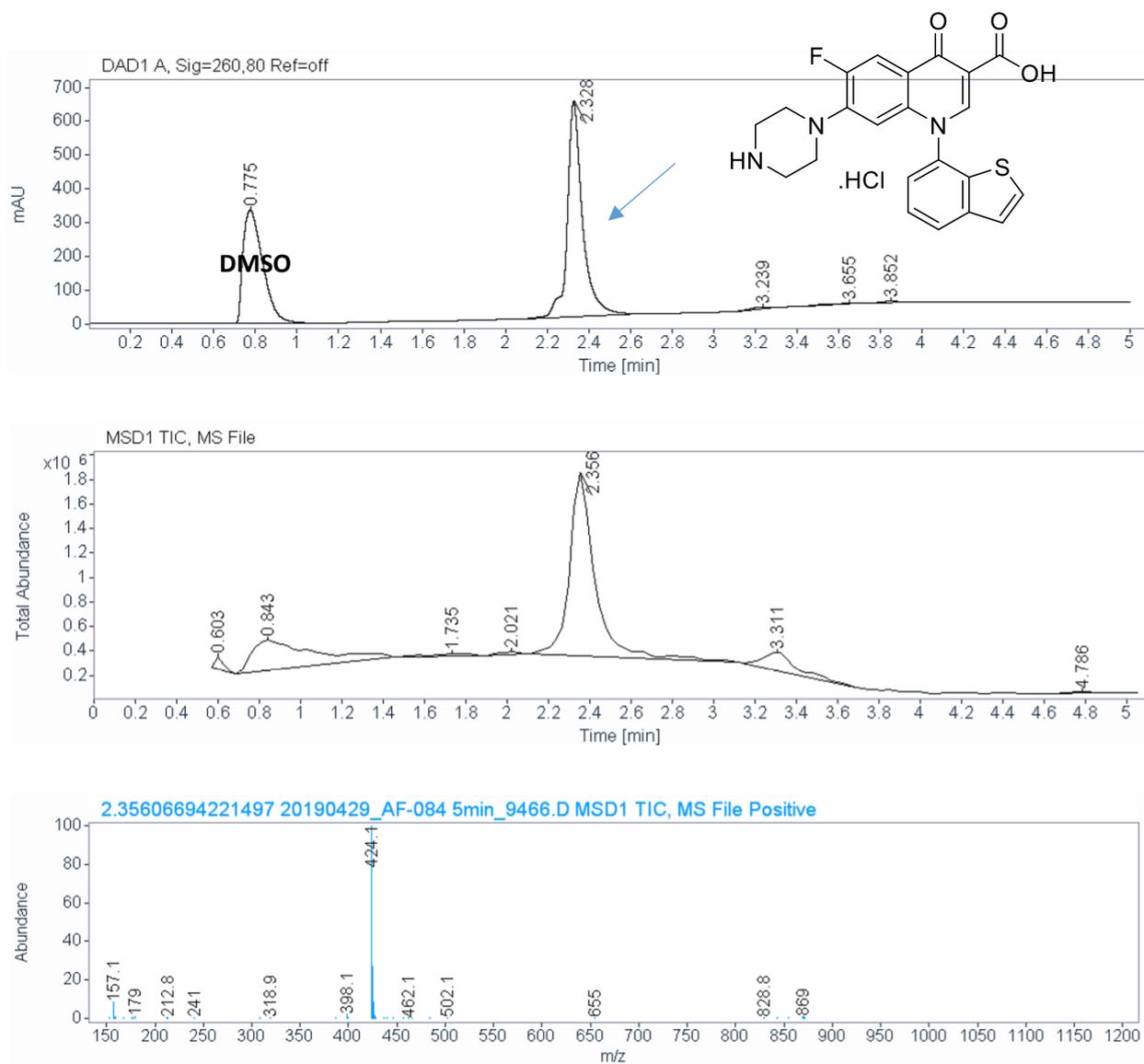


Figure S27B. LC-MS profile of compound 6e, method B (10 minutes).

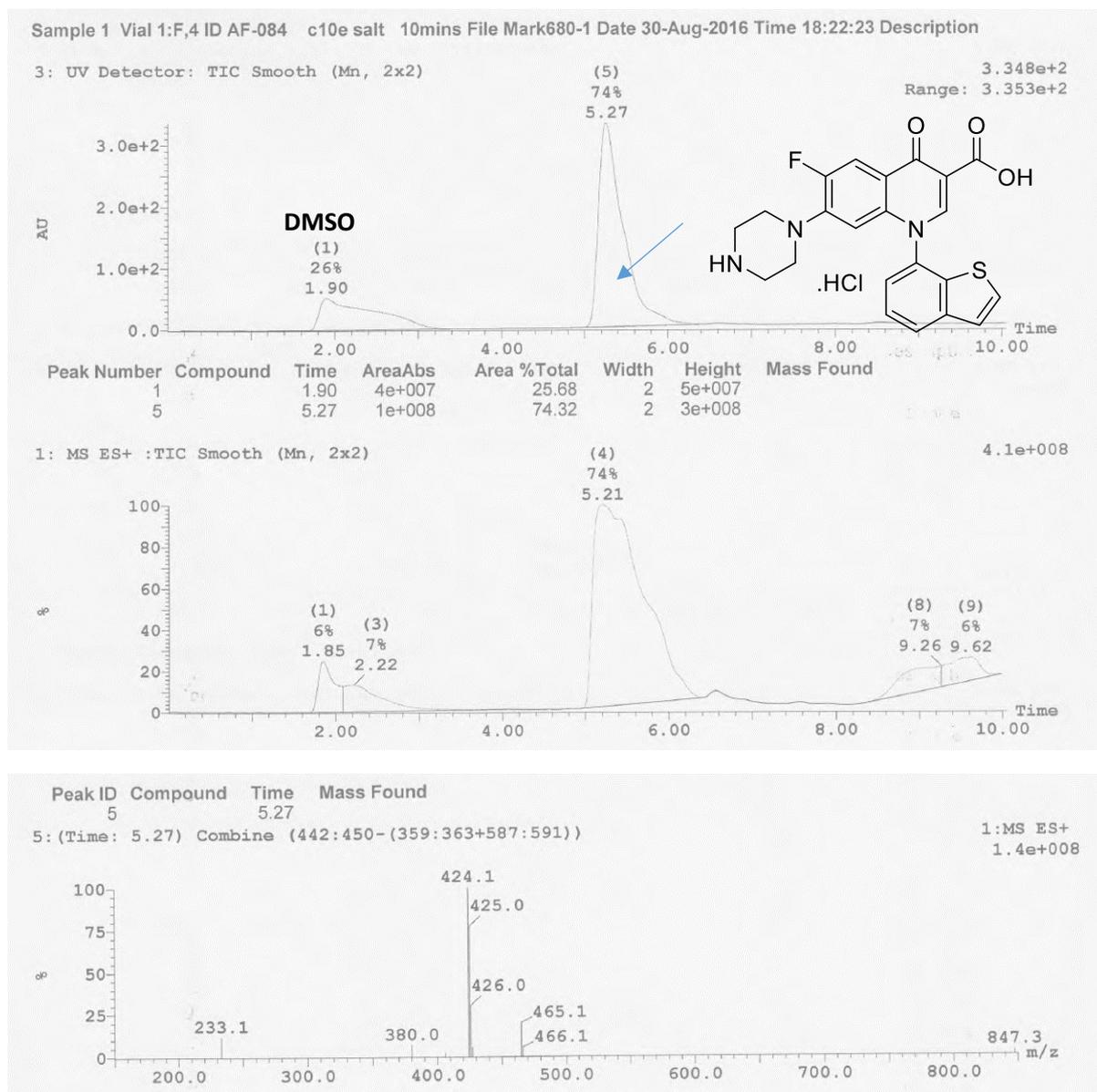


Figure S28A. LC-MS profile of compound 6f, method A (5 minutes).

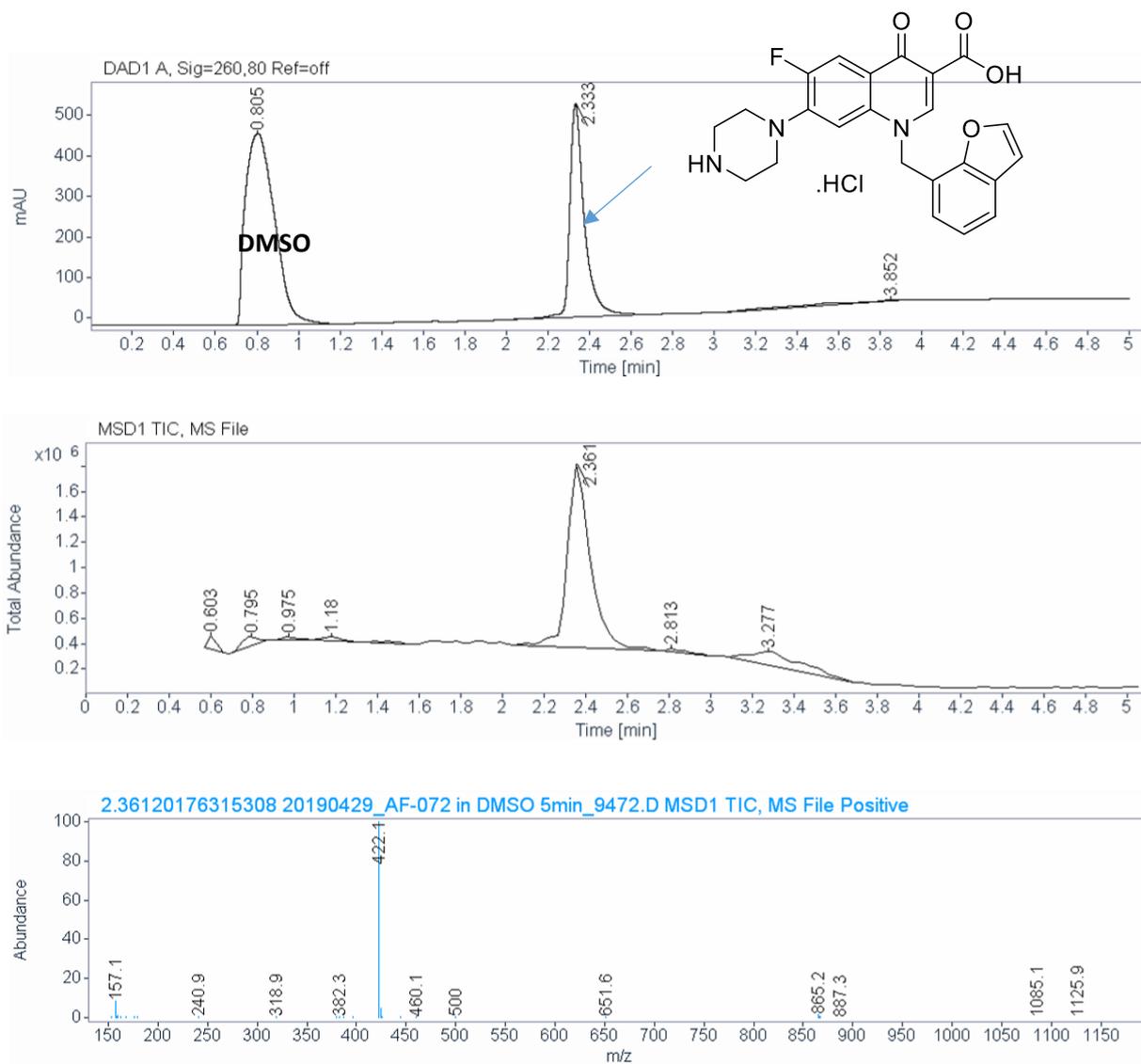


Figure S28B. LC-MS profile of compound 6f, method B (10 minutes).

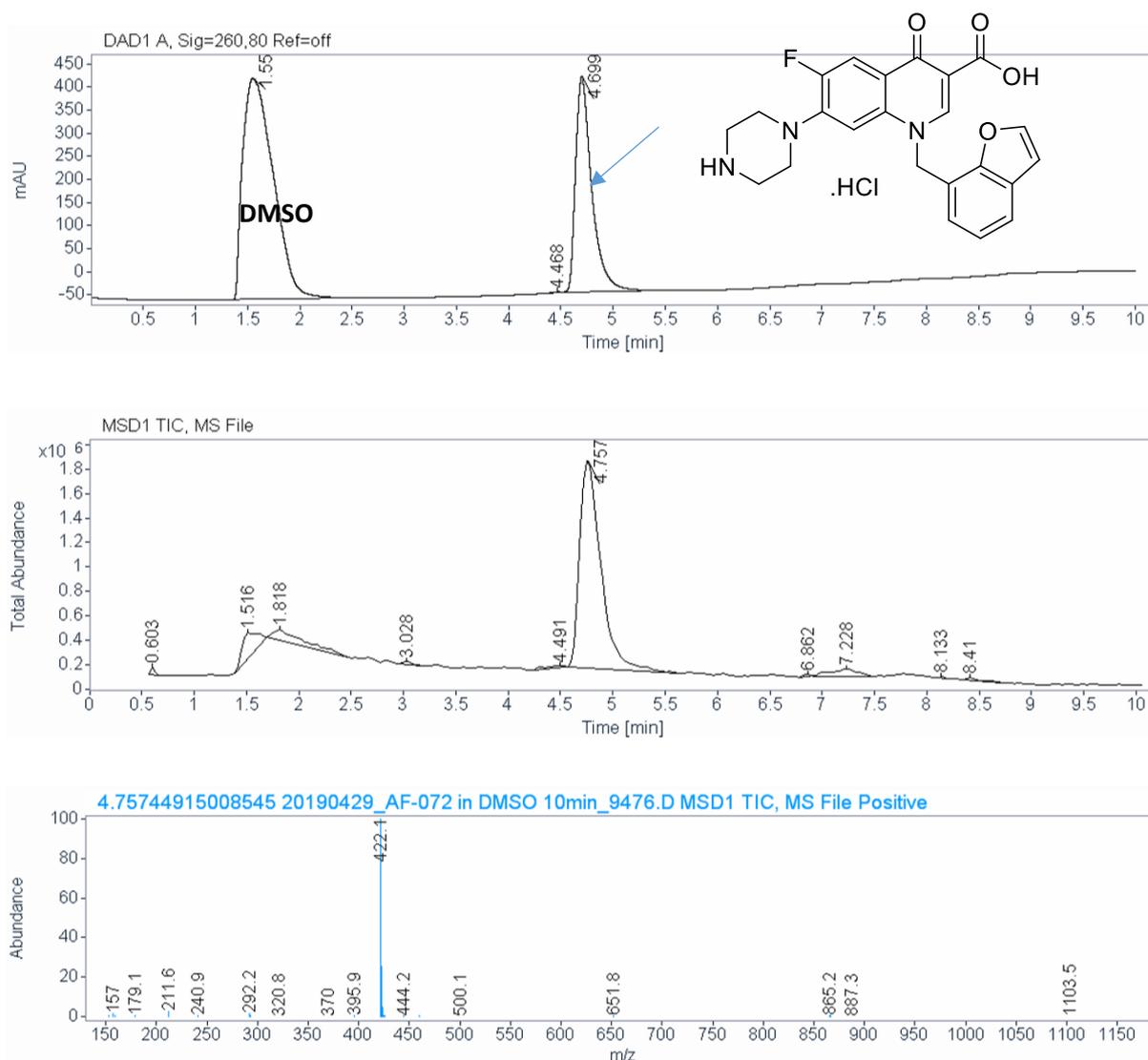


Figure S29A. LC-MS profile of compound 6g, method A (5 minutes).

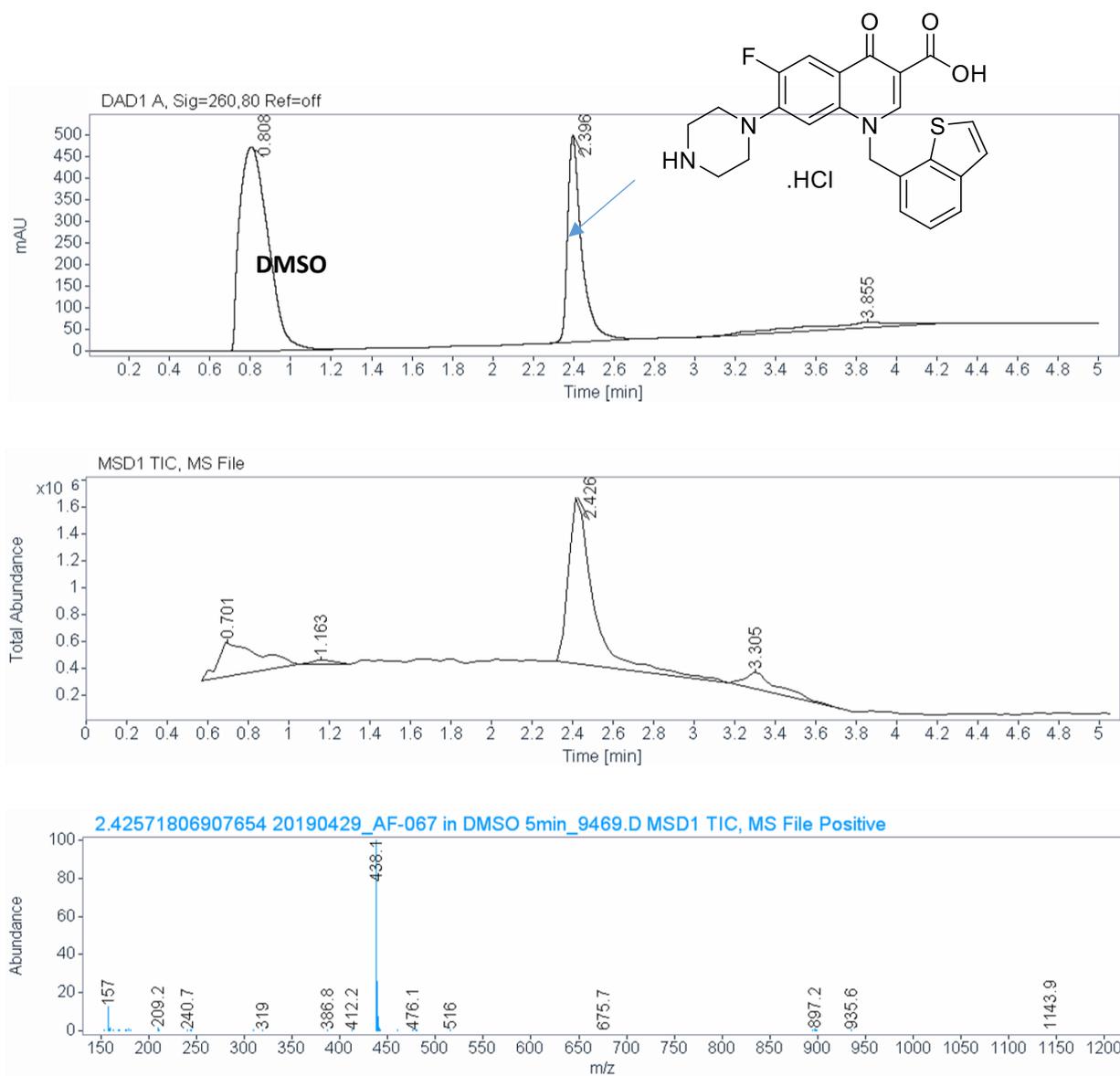
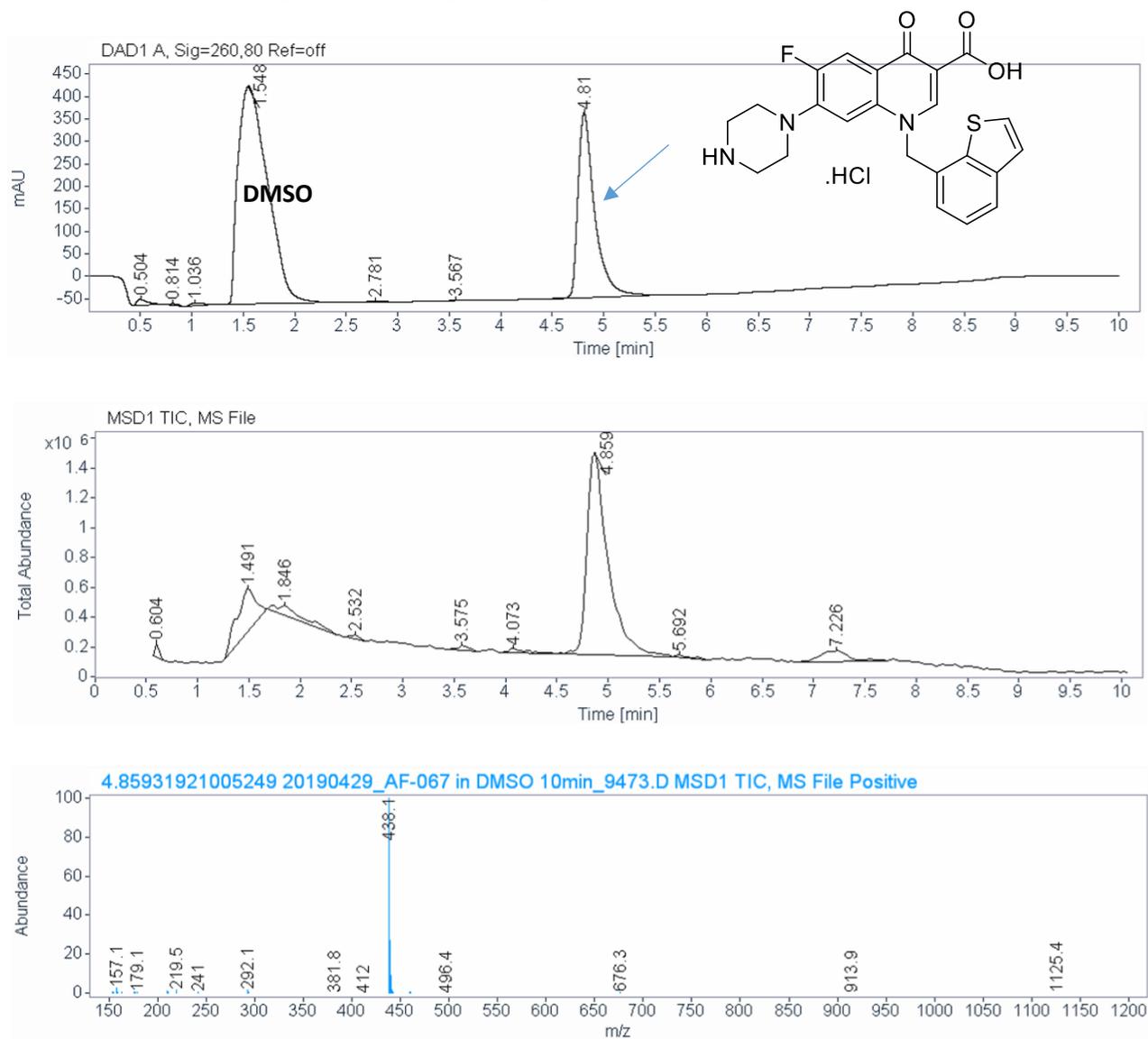


Figure S29B. LC-MS profile of compound 6g, method B (10 minutes).



HRMS Analysis

Figure S30. HRMS spectrum of compound 6a.

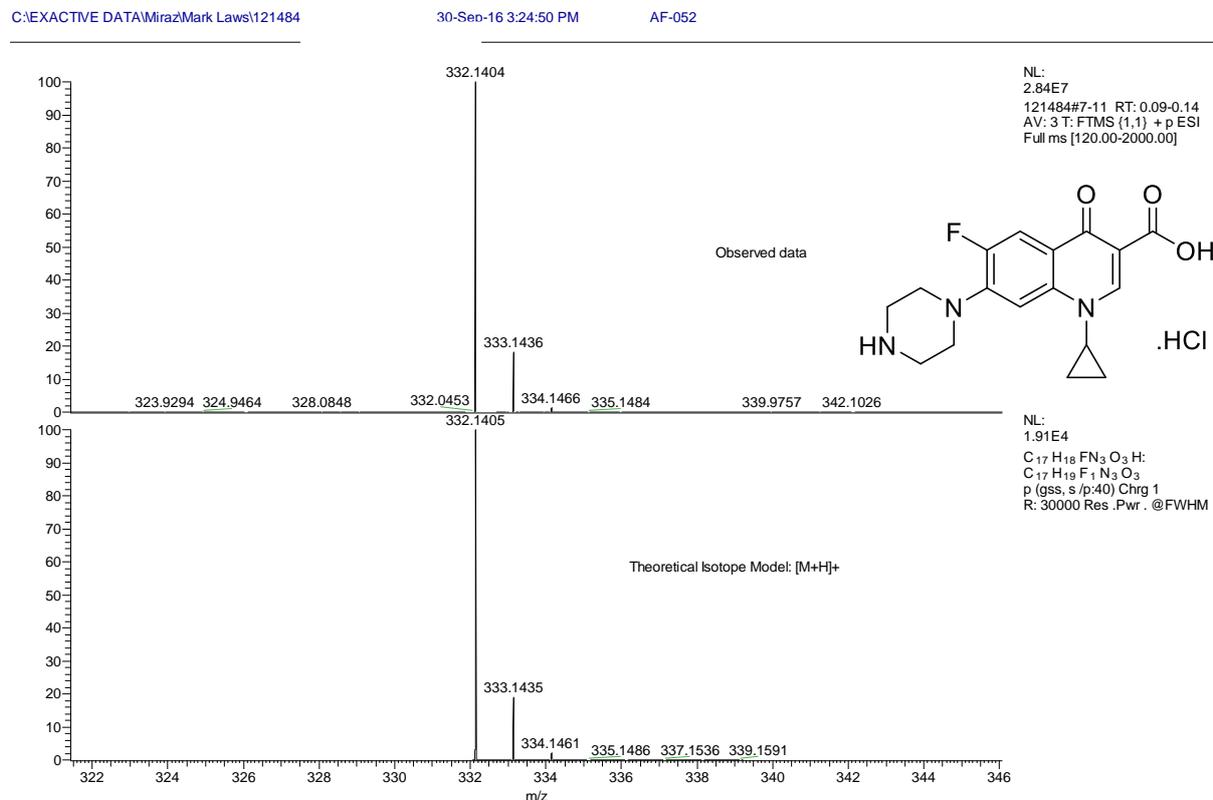


Figure S31. HRMS spectrum of compound 6b.

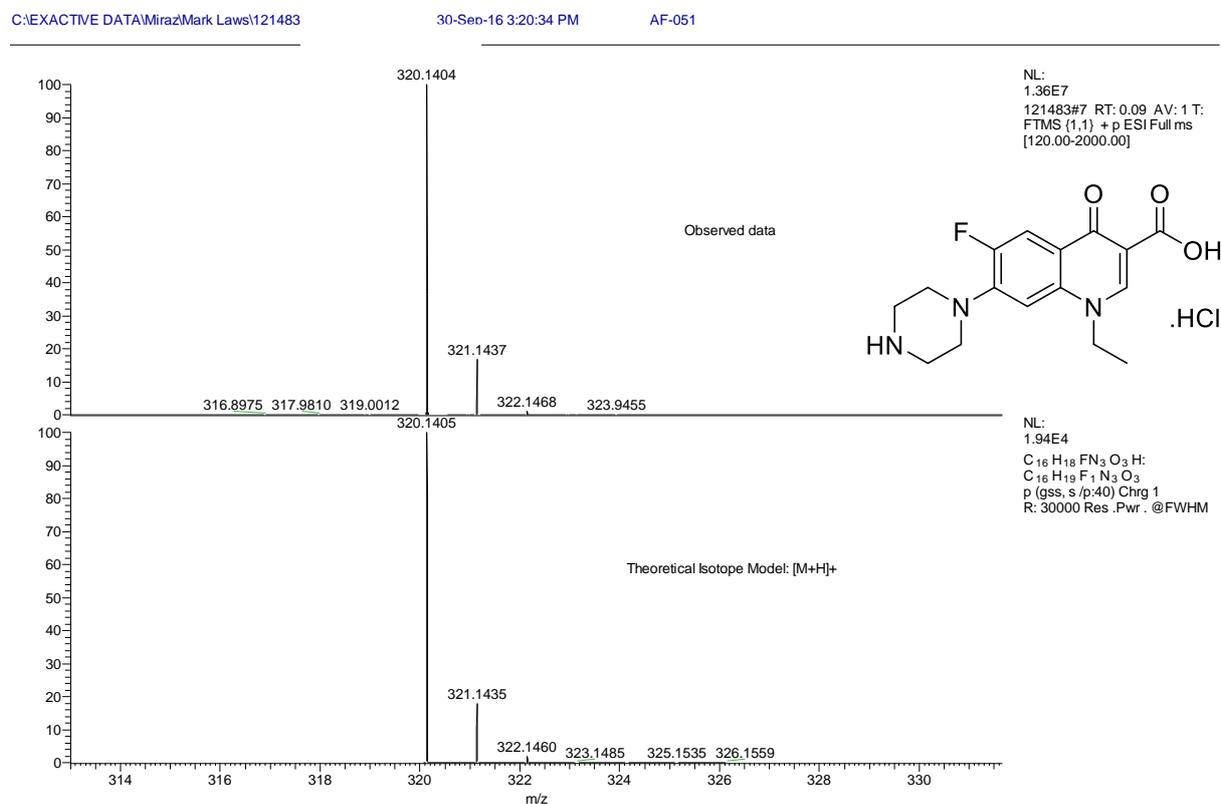


Figure S32. HRMS spectrum of compound 6c.

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AF-090

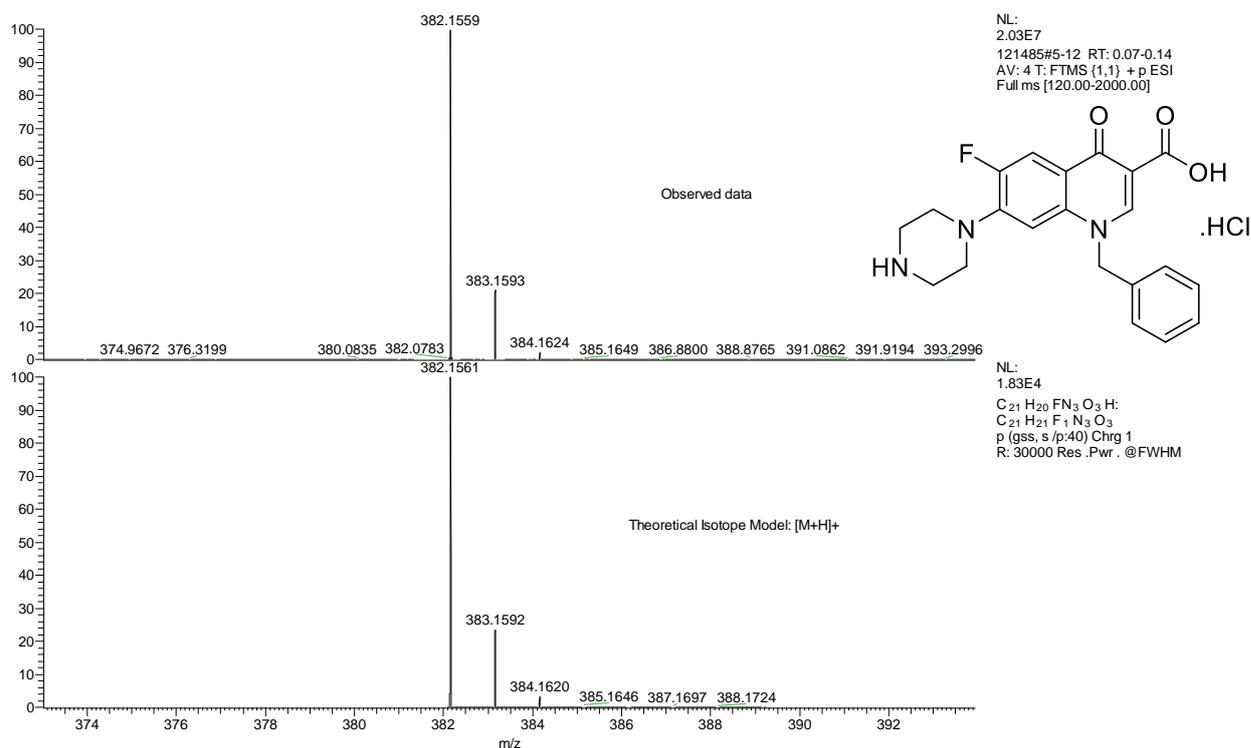


Figure S33. HRMS spectrum of compound 6d.

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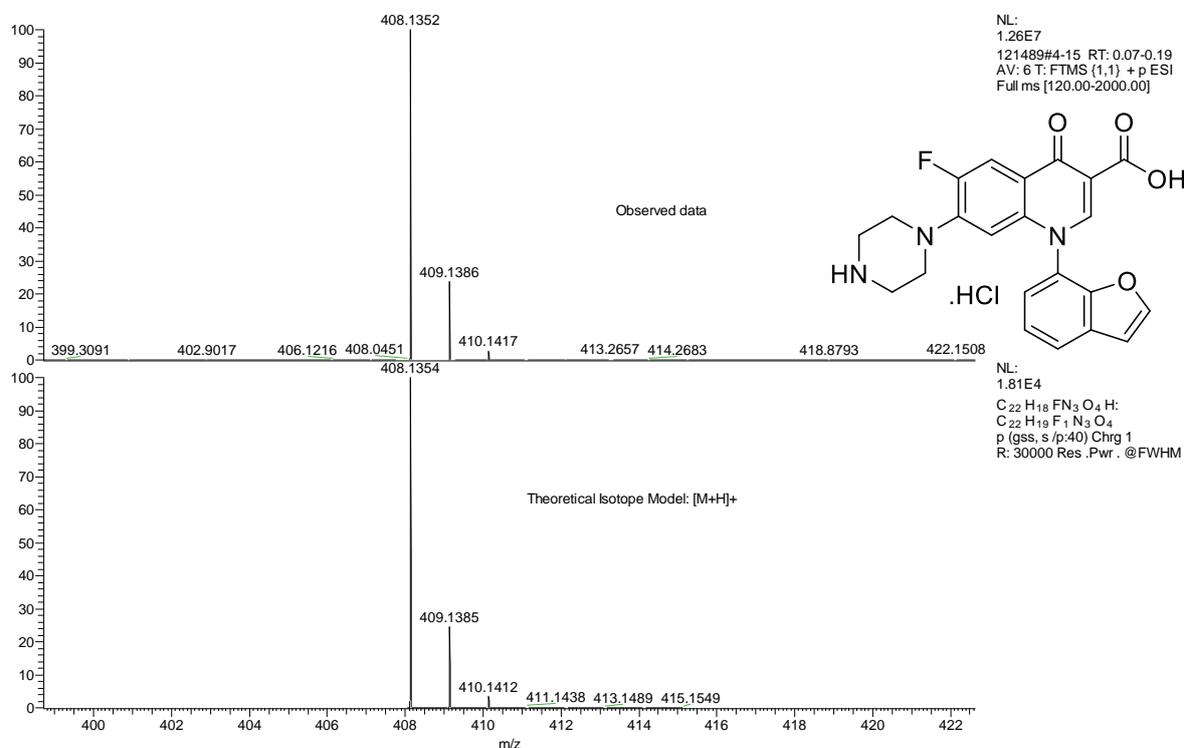


Figure S34. HRMS spectrum of compound 6e.

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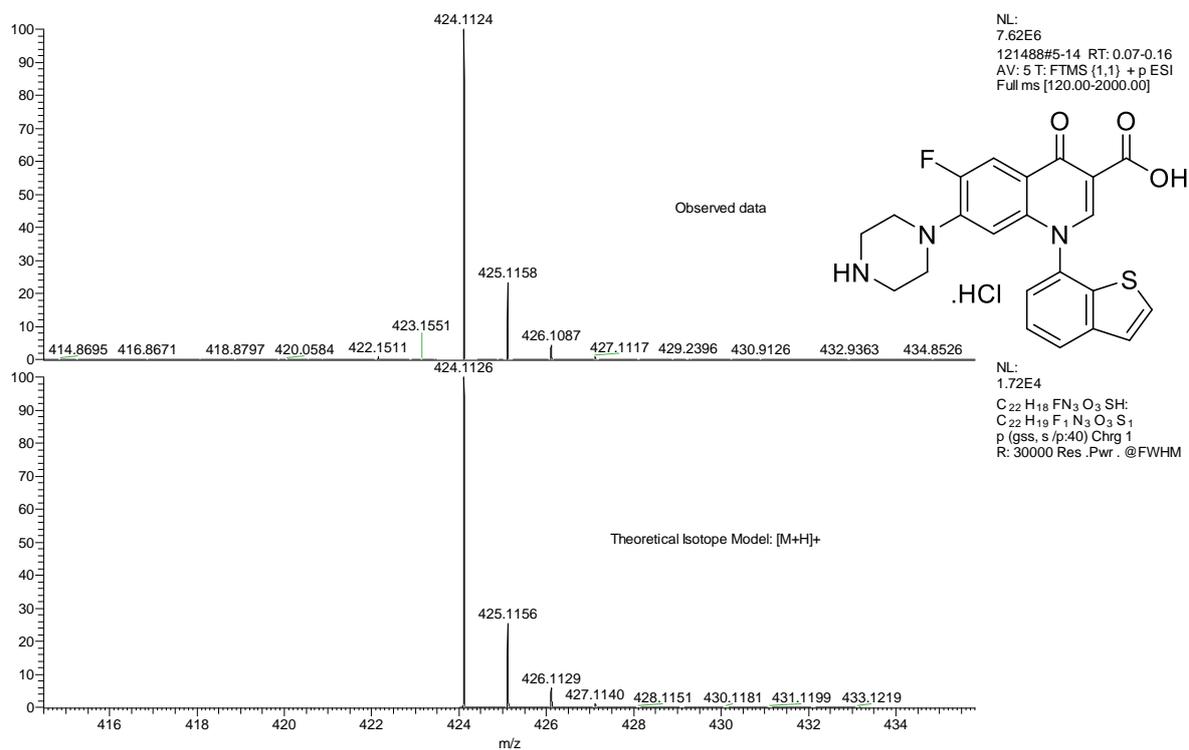


Figure S35. HRMS spectrum of compound 6f.

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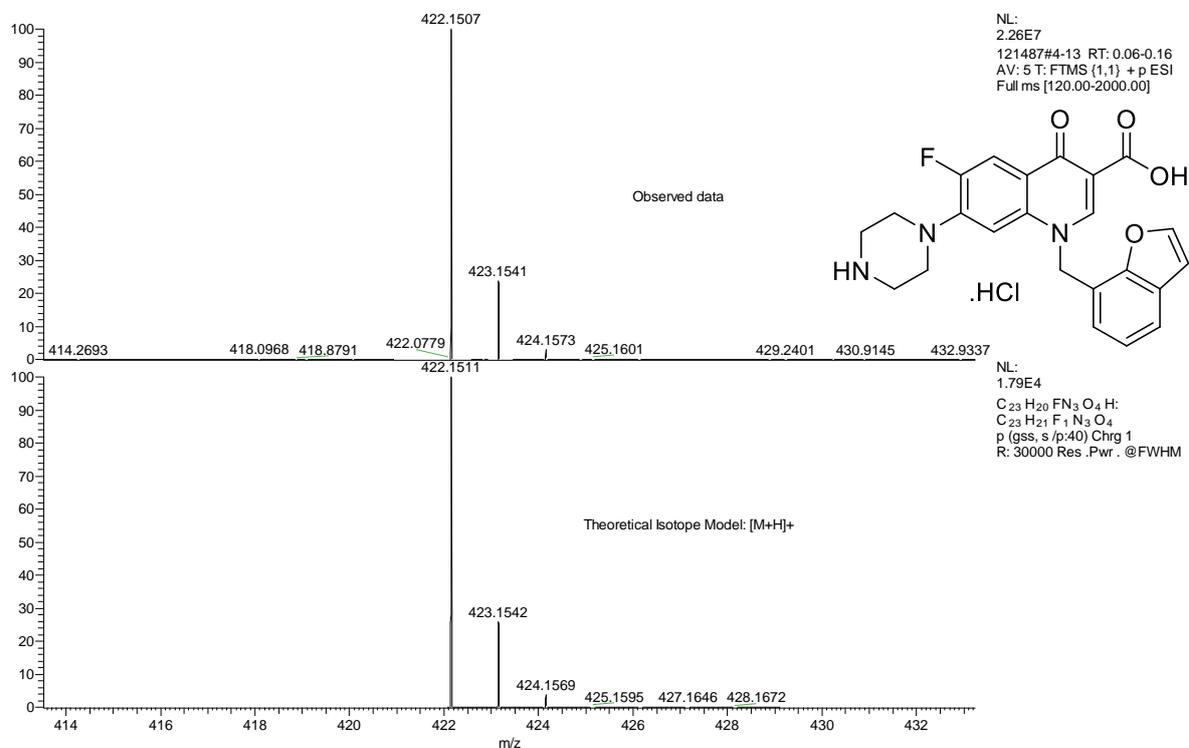
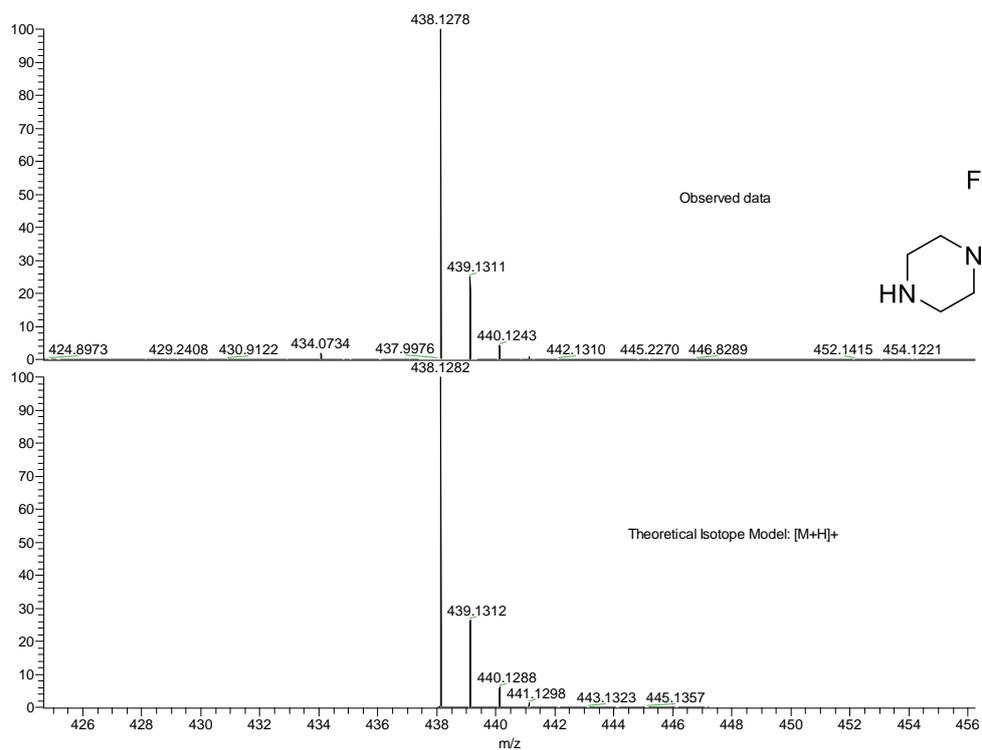


Figure S36. HRMS spectrum of compound 6g.

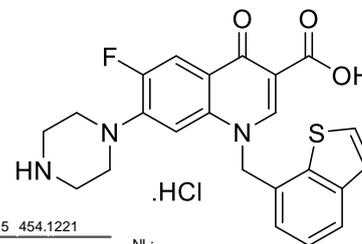
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¹H NMR Spectra

Figure S37. Proton NMR spectrum of compound 2a.

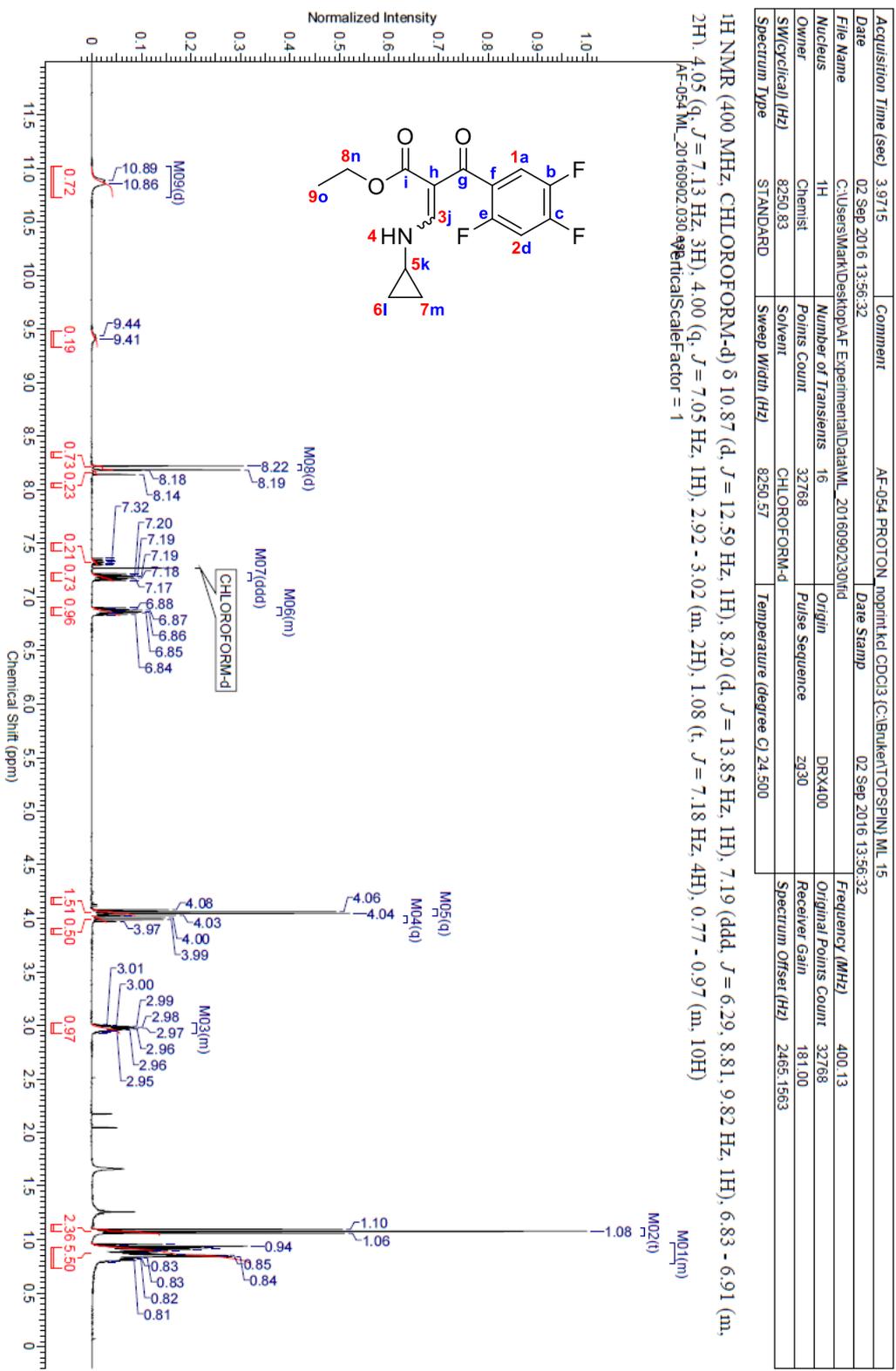


Figure S38. Proton NMR spectrum of compound 2b.

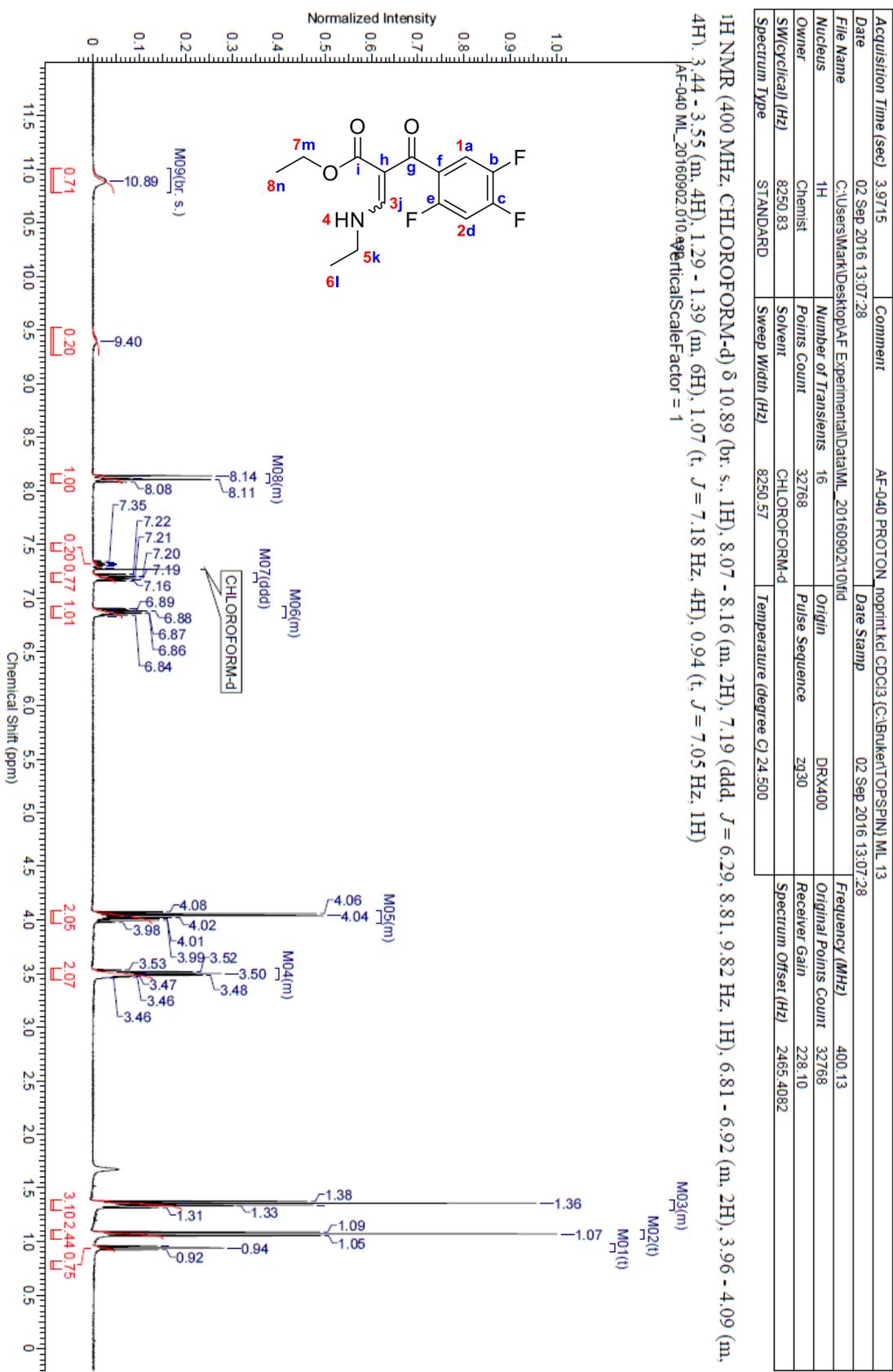
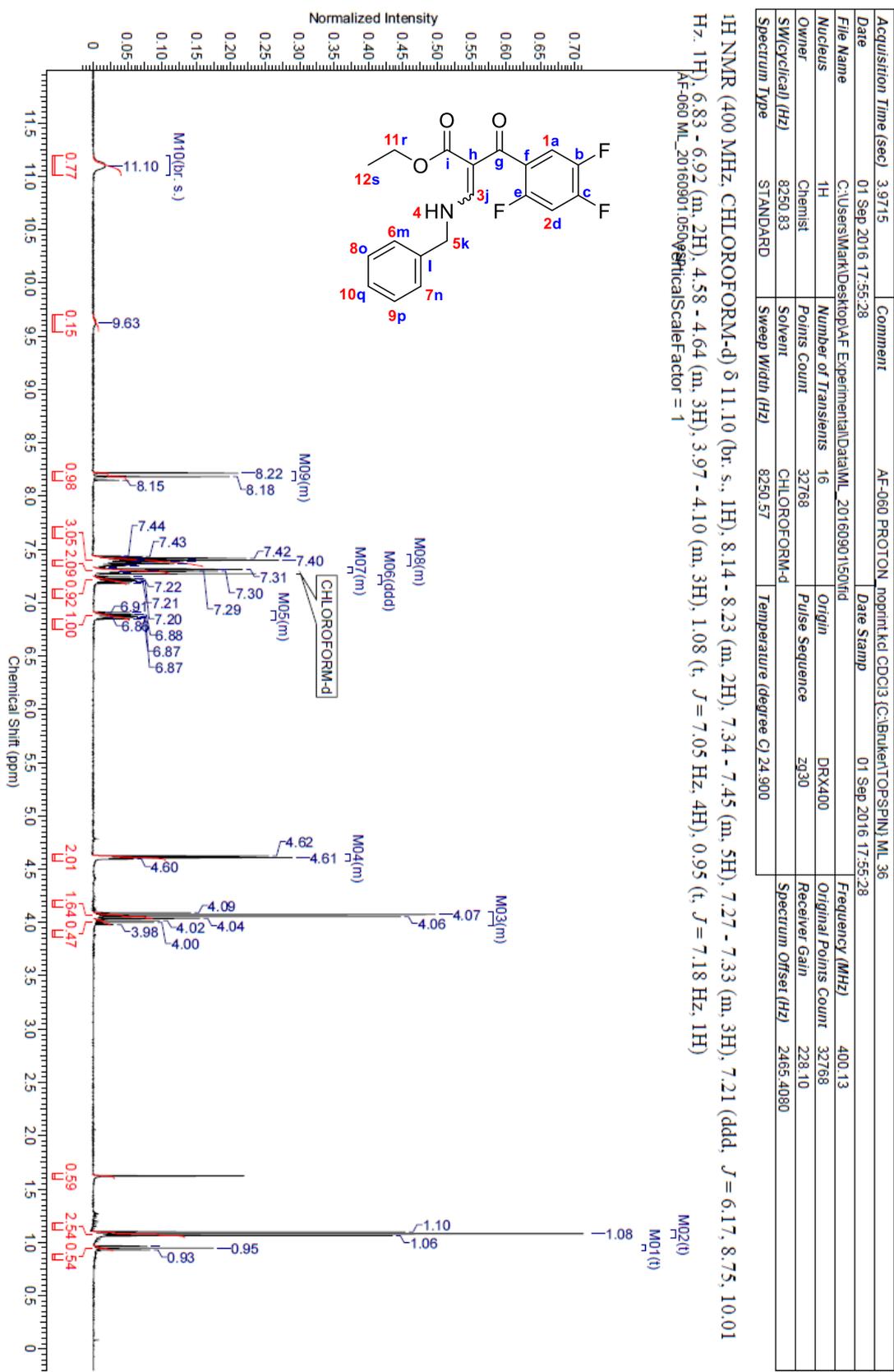
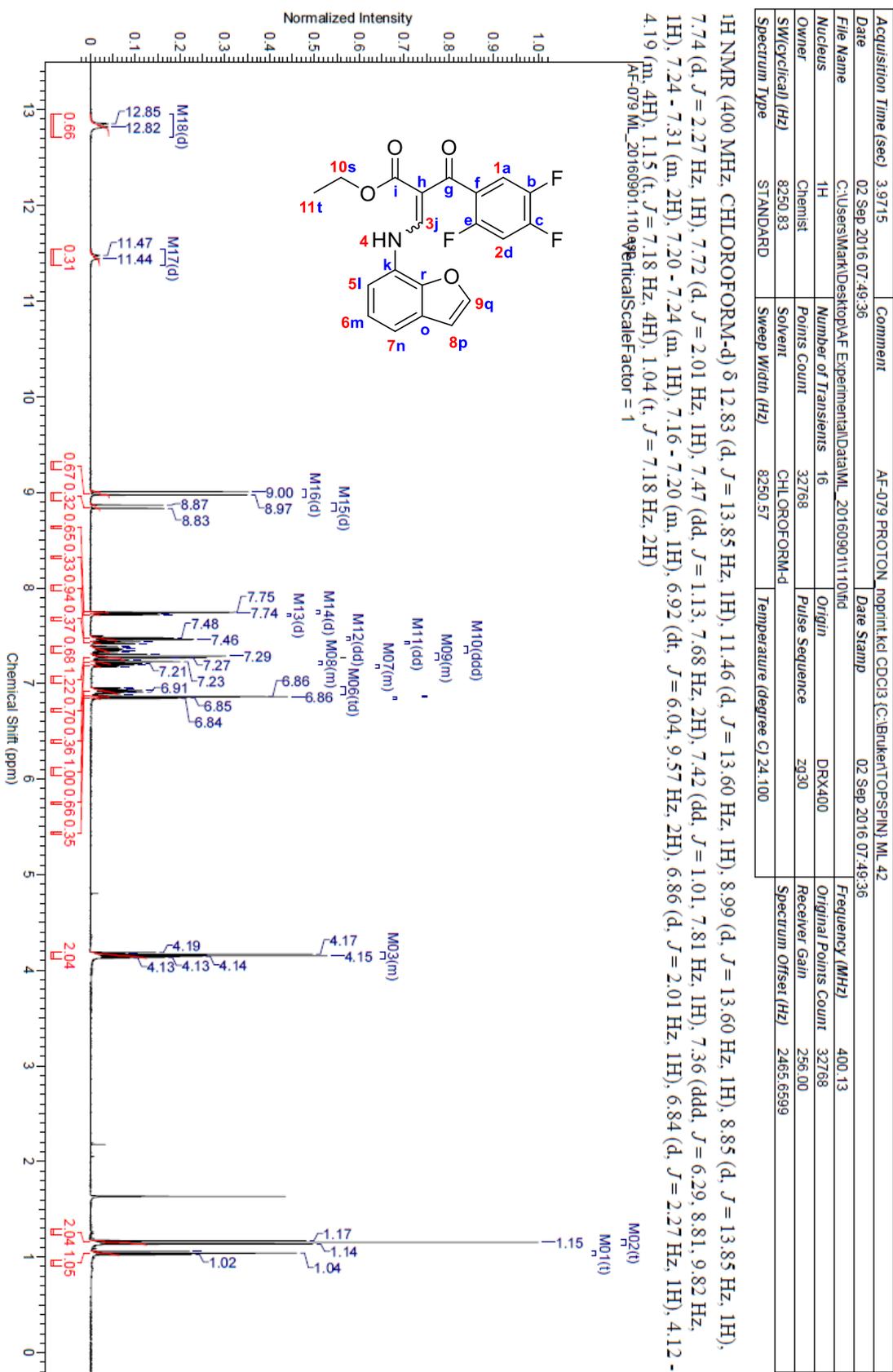


Figure S39. Proton NMR spectrum of compound 2c.



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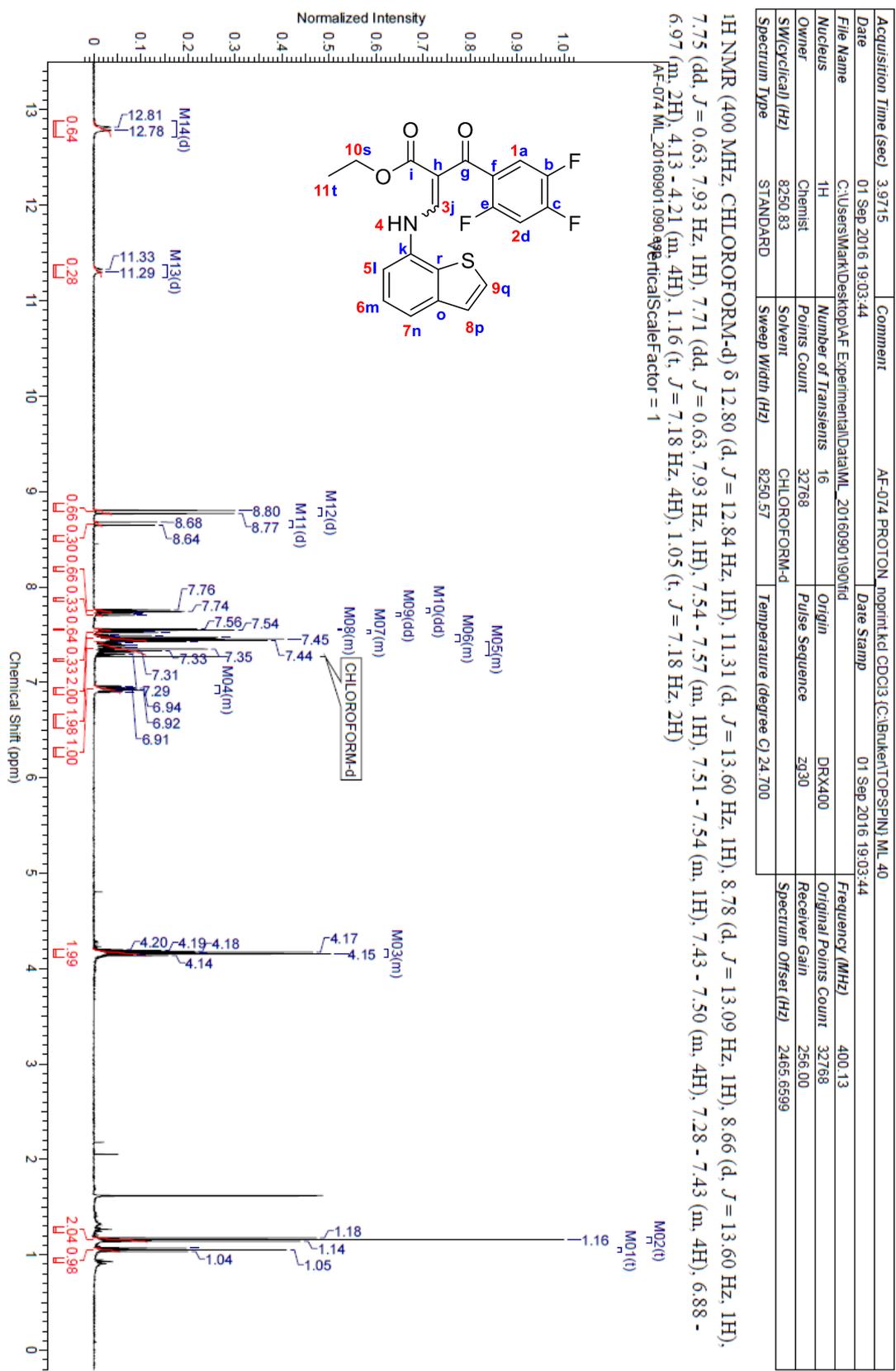
Figure S40. Proton NMR spectrum of compound 2d.



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Figure S41. Proton NMR spectrum of compound 2e.



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Figure S42. Proton NMR spectrum of compound 2f.

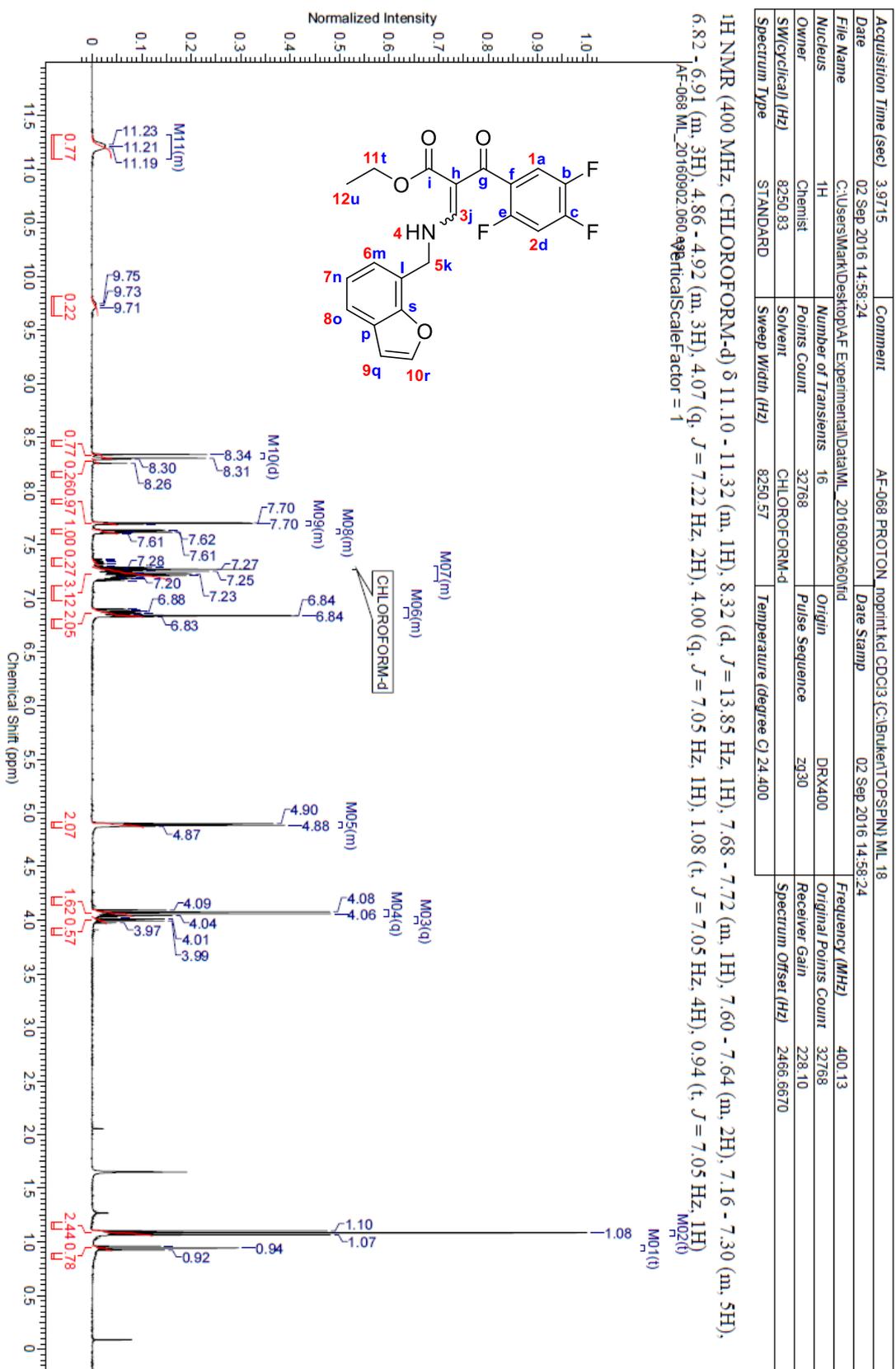
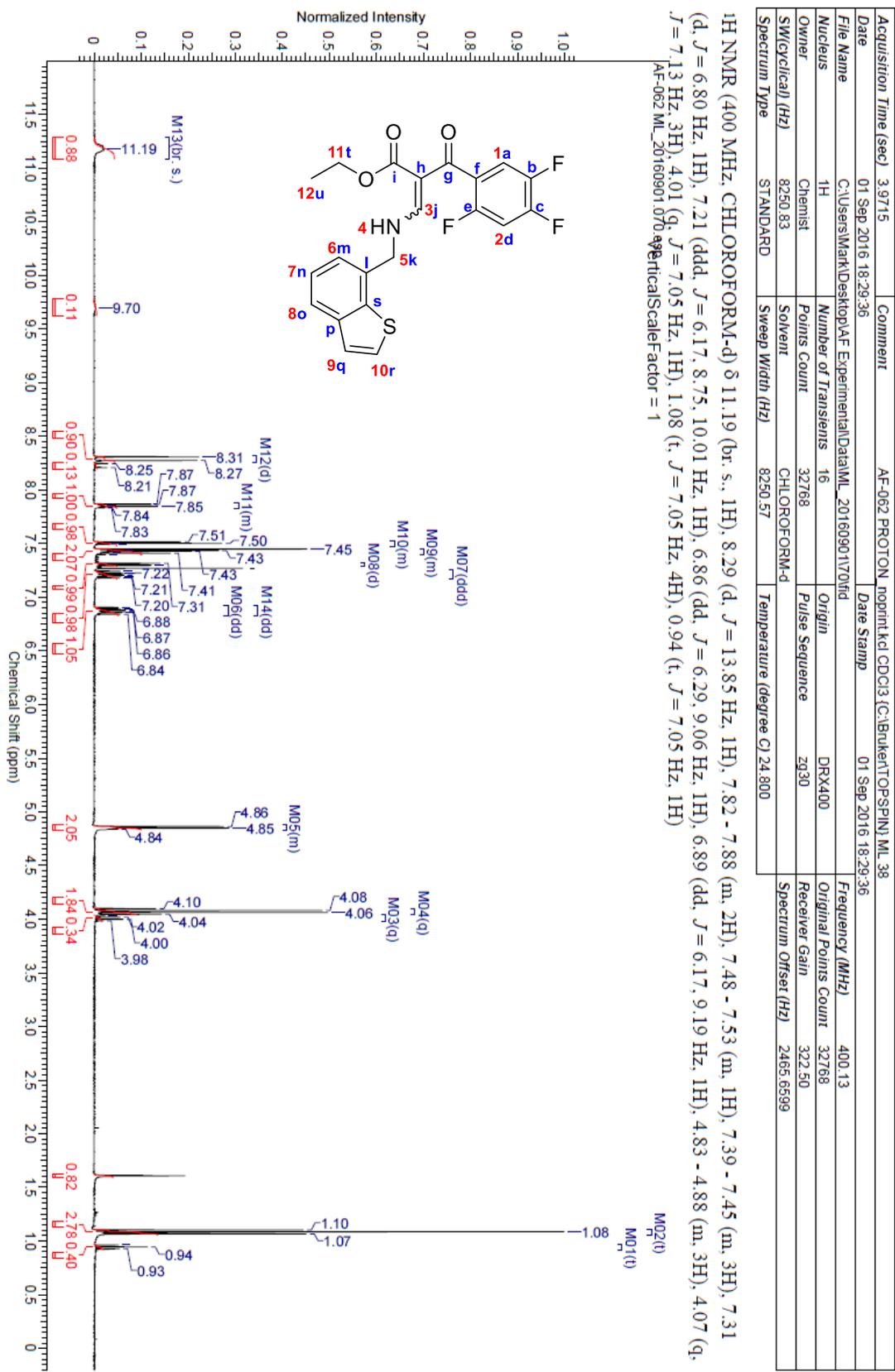


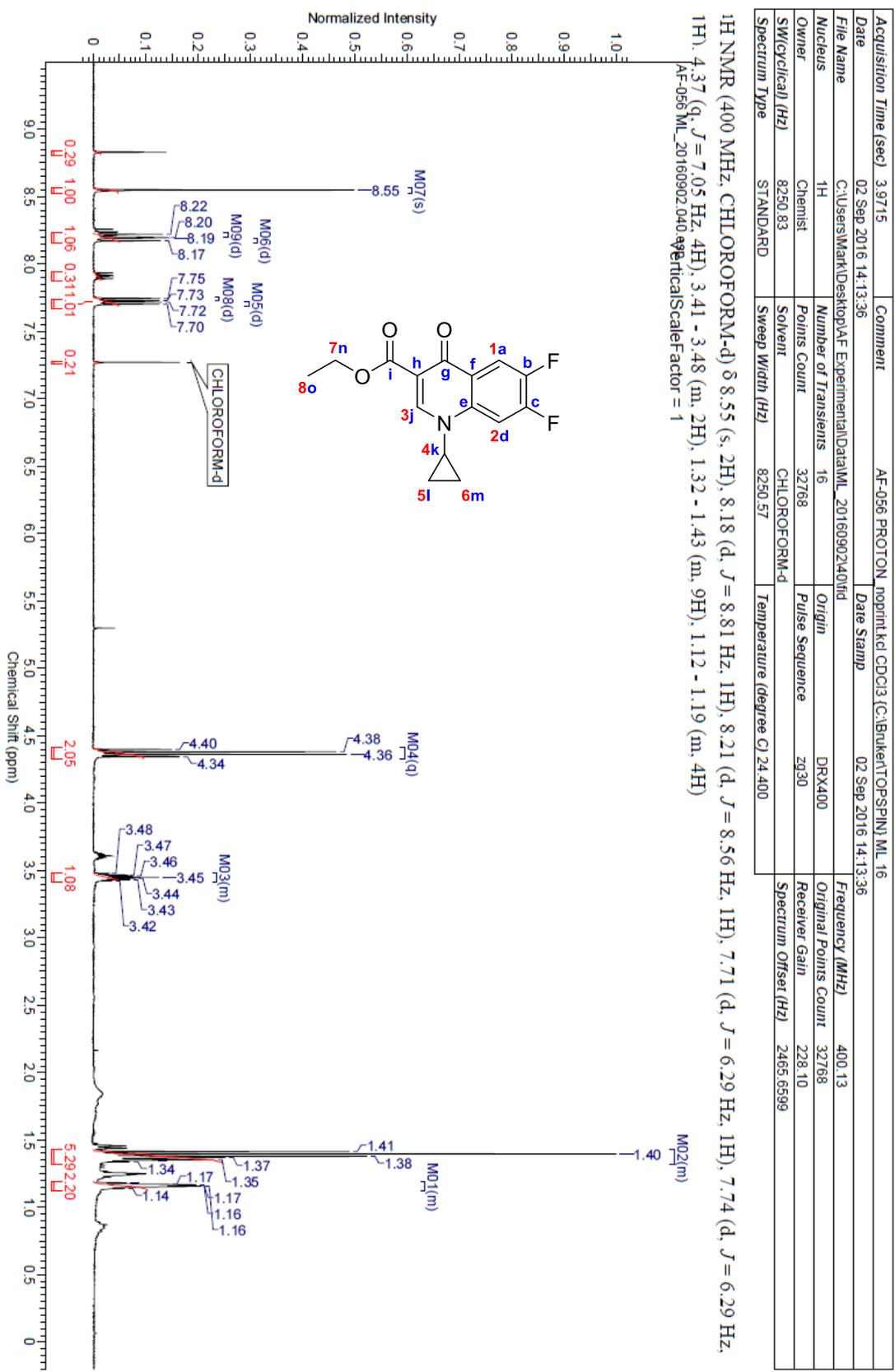
Figure S43. Proton NMR spectrum of compound 2g.



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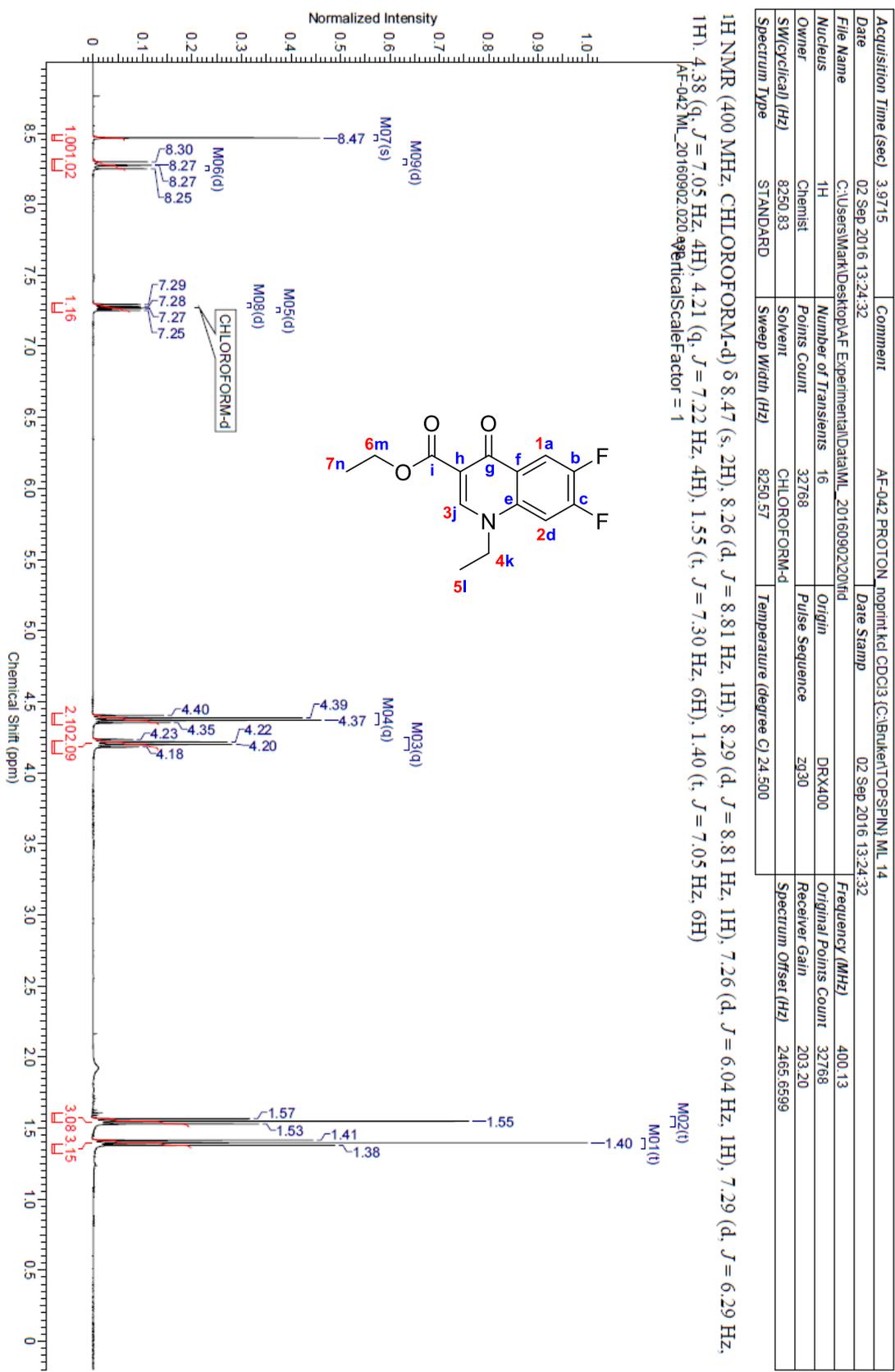
Figure S44. Proton NMR spectrum of compound 3a.



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Figure S45. Proton NMR spectrum of compound 3b.



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Figure S46. Proton NMR spectrum of compound 3c.

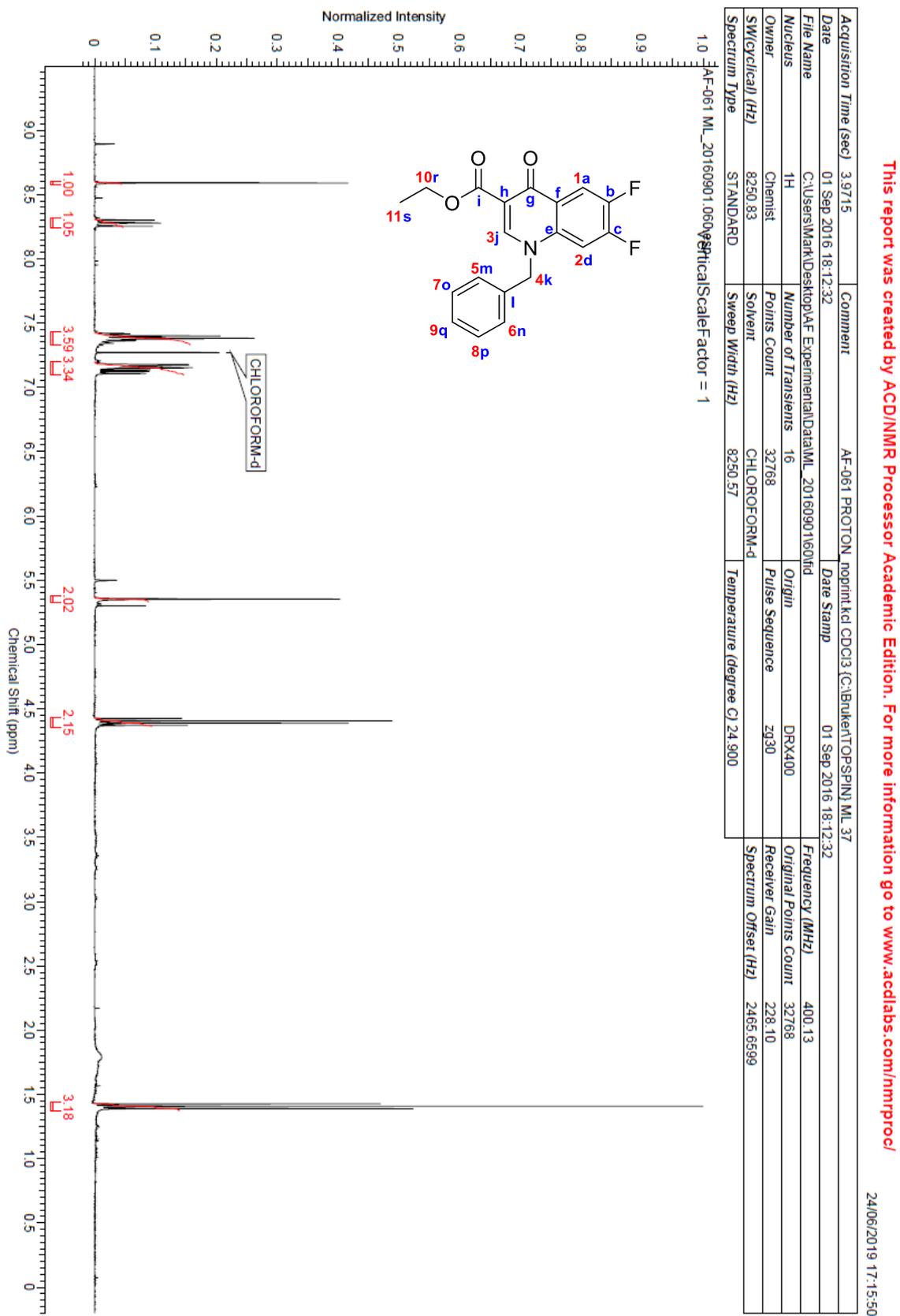
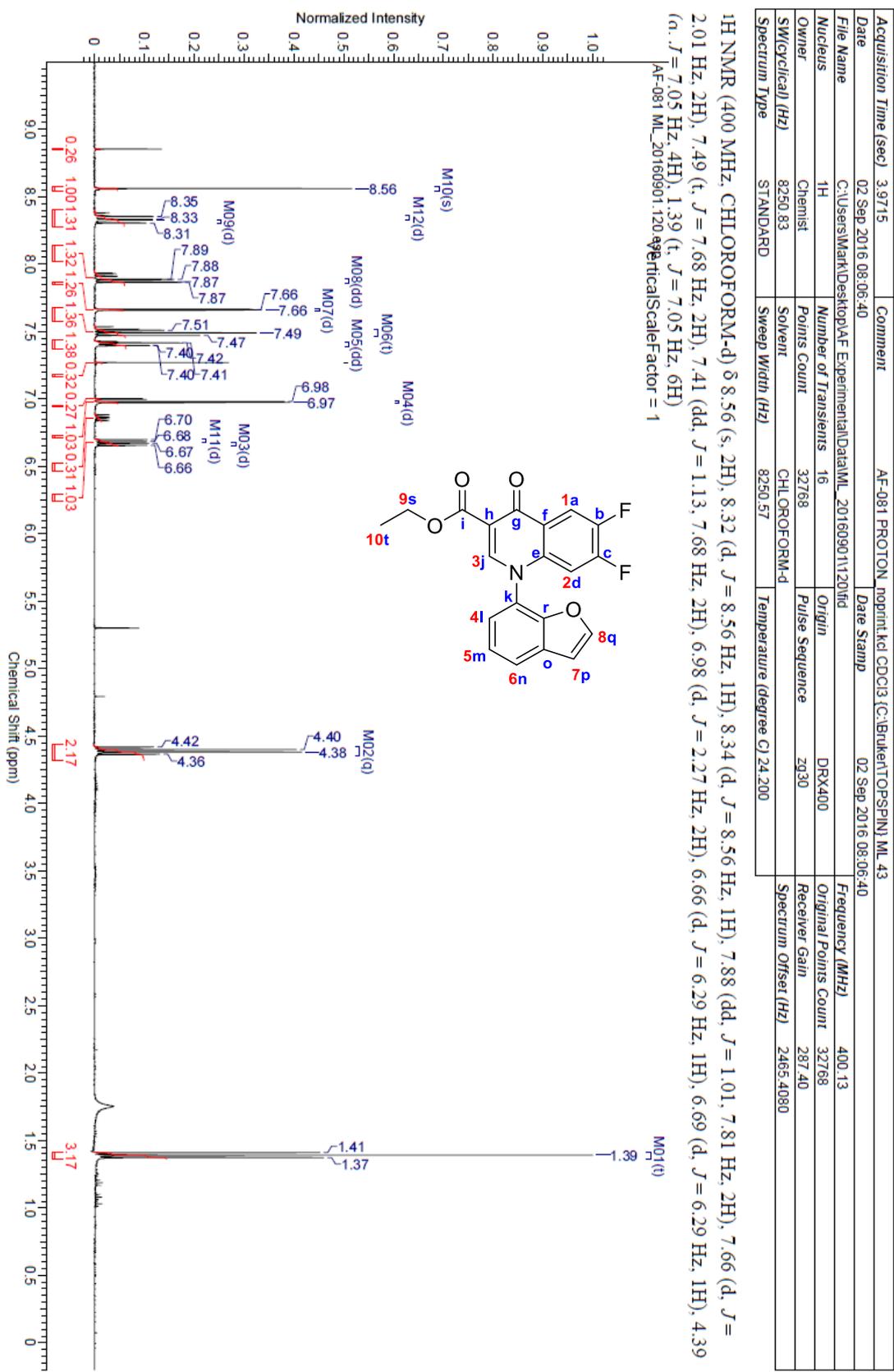


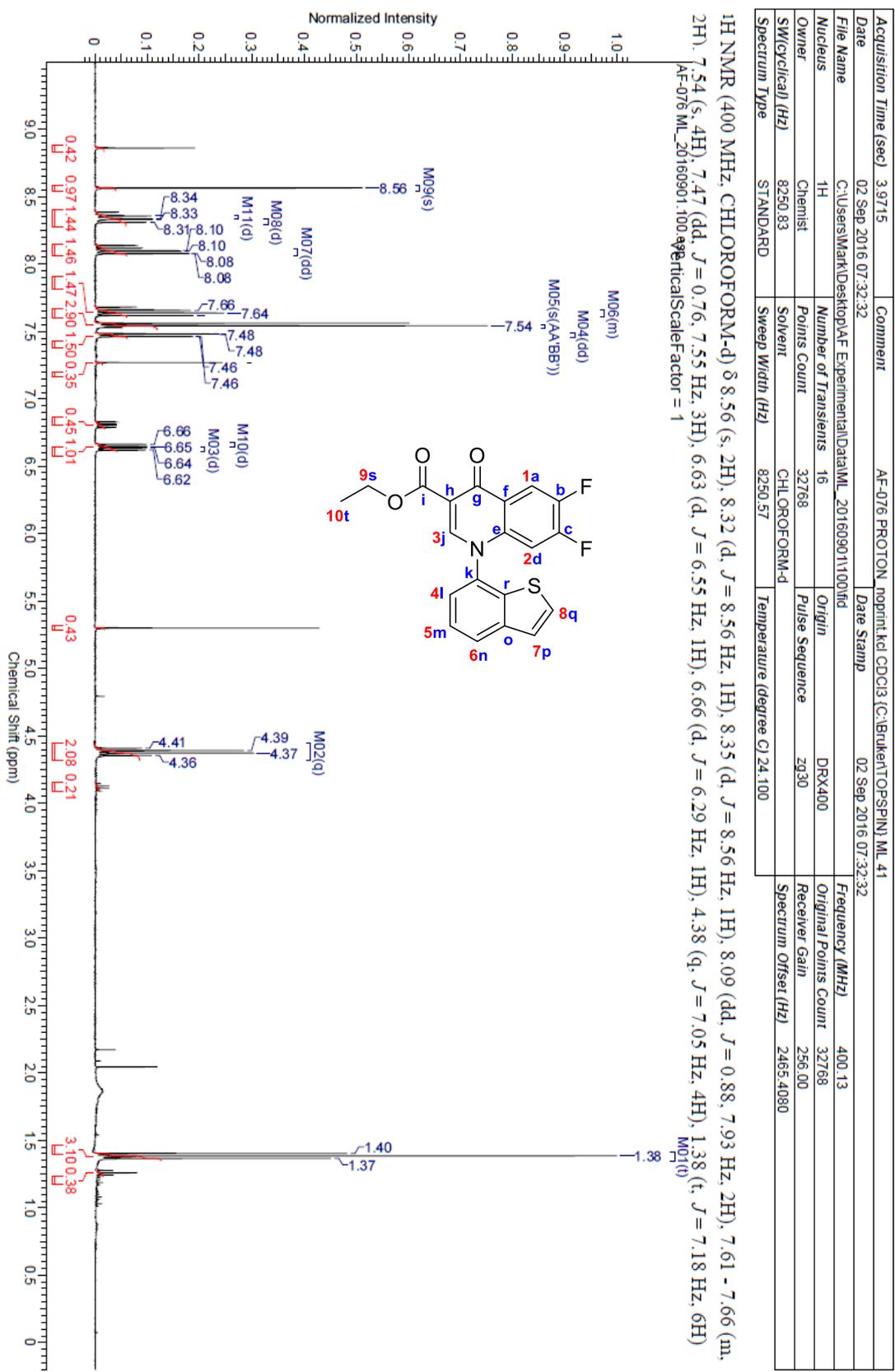
Figure S47. Proton NMR spectrum of compound 3d.



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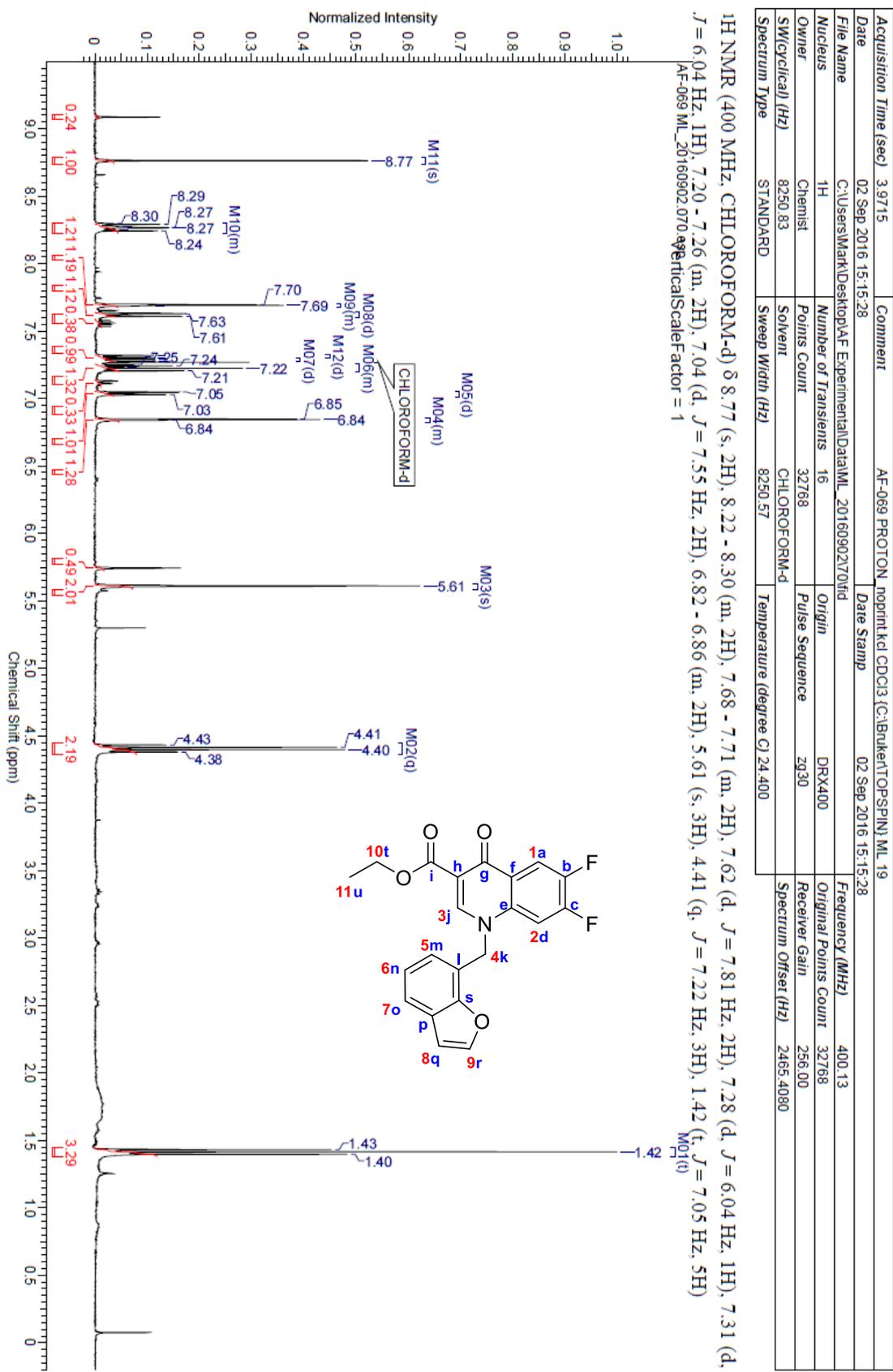
Figure S48. Proton NMR spectrum of compound 3e.



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Figure S49. Proton NMR spectrum of compound 3f.



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Figure S50. Proton NMR spectrum of compound 3g.

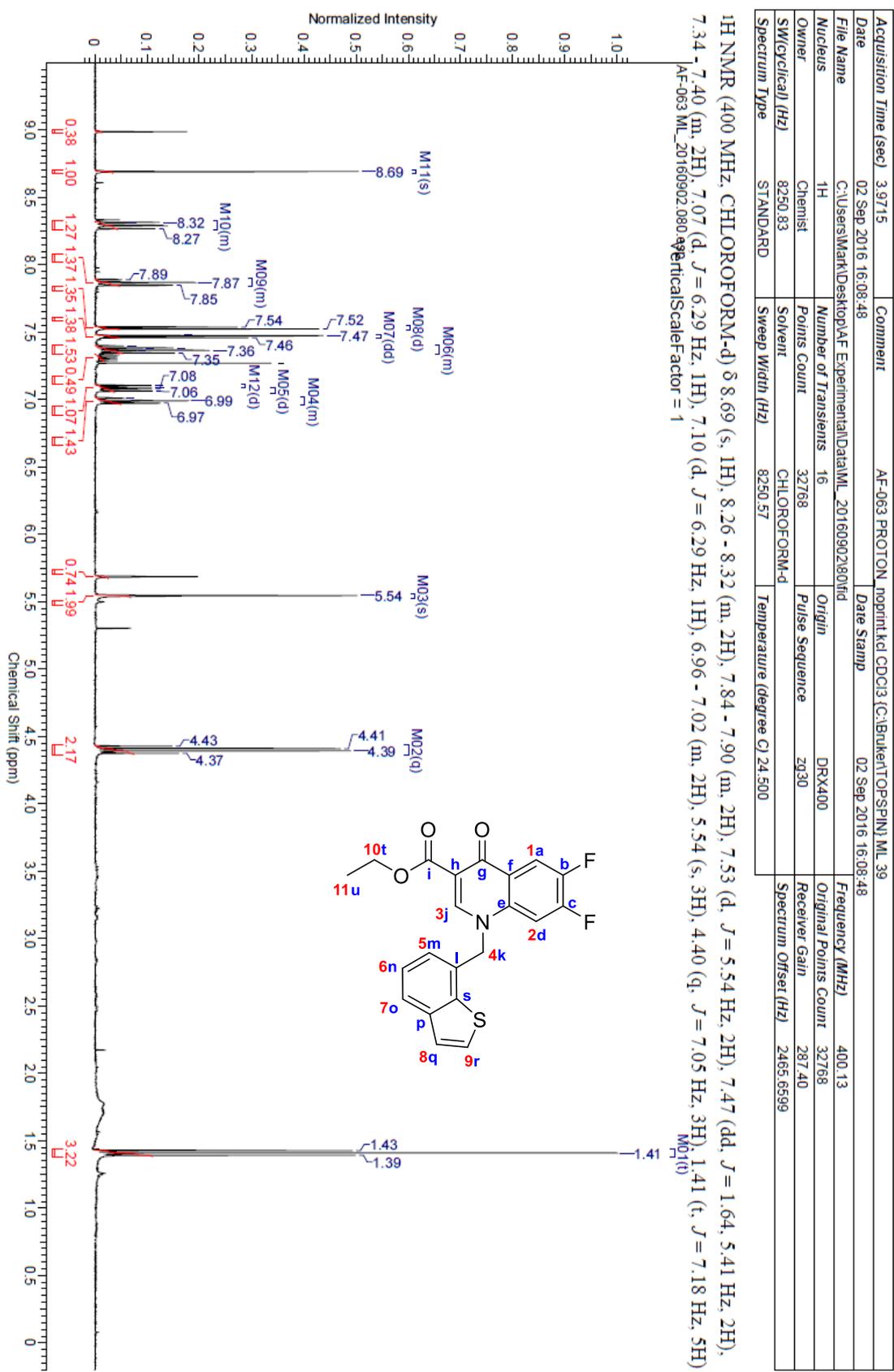
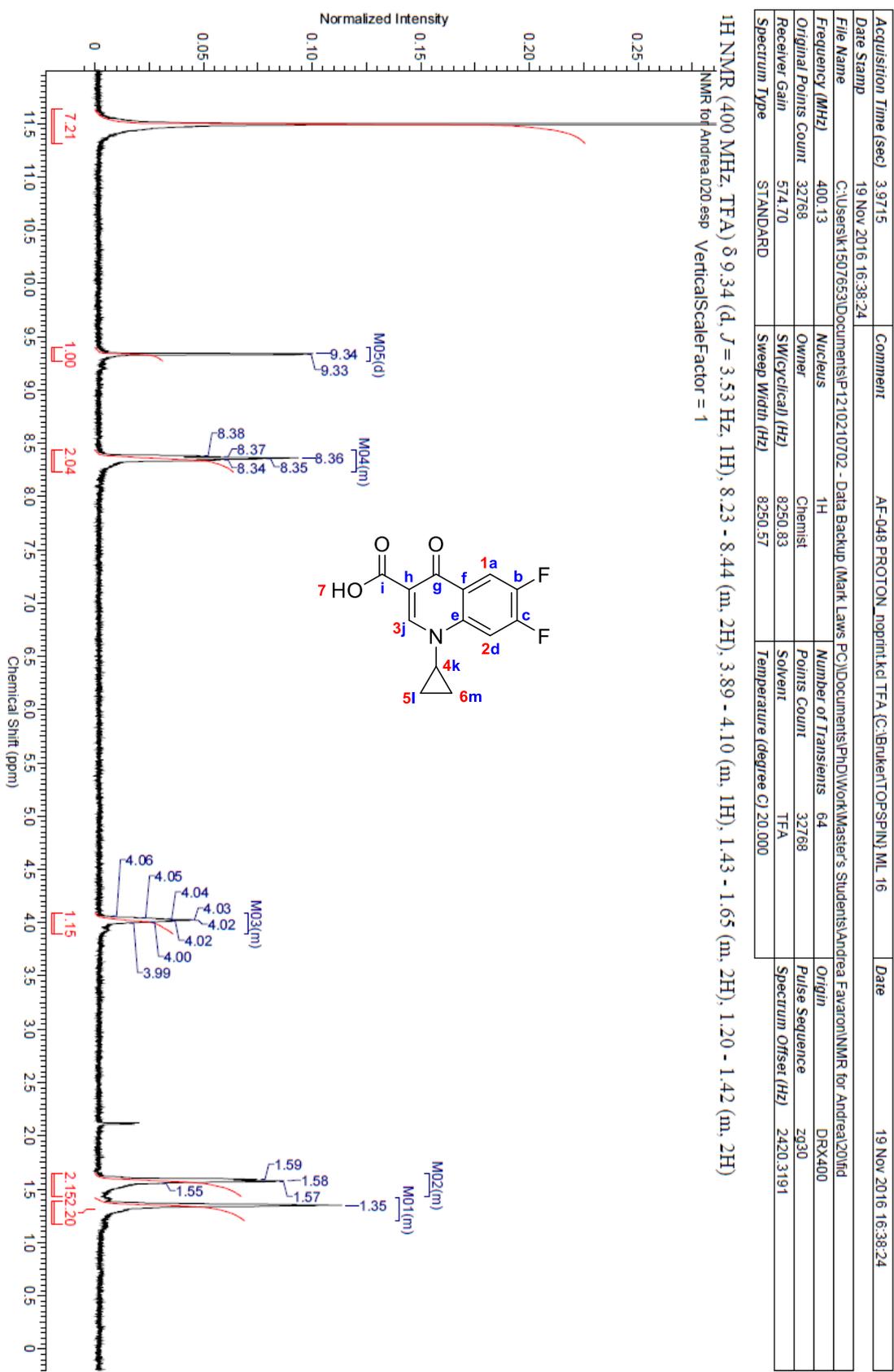


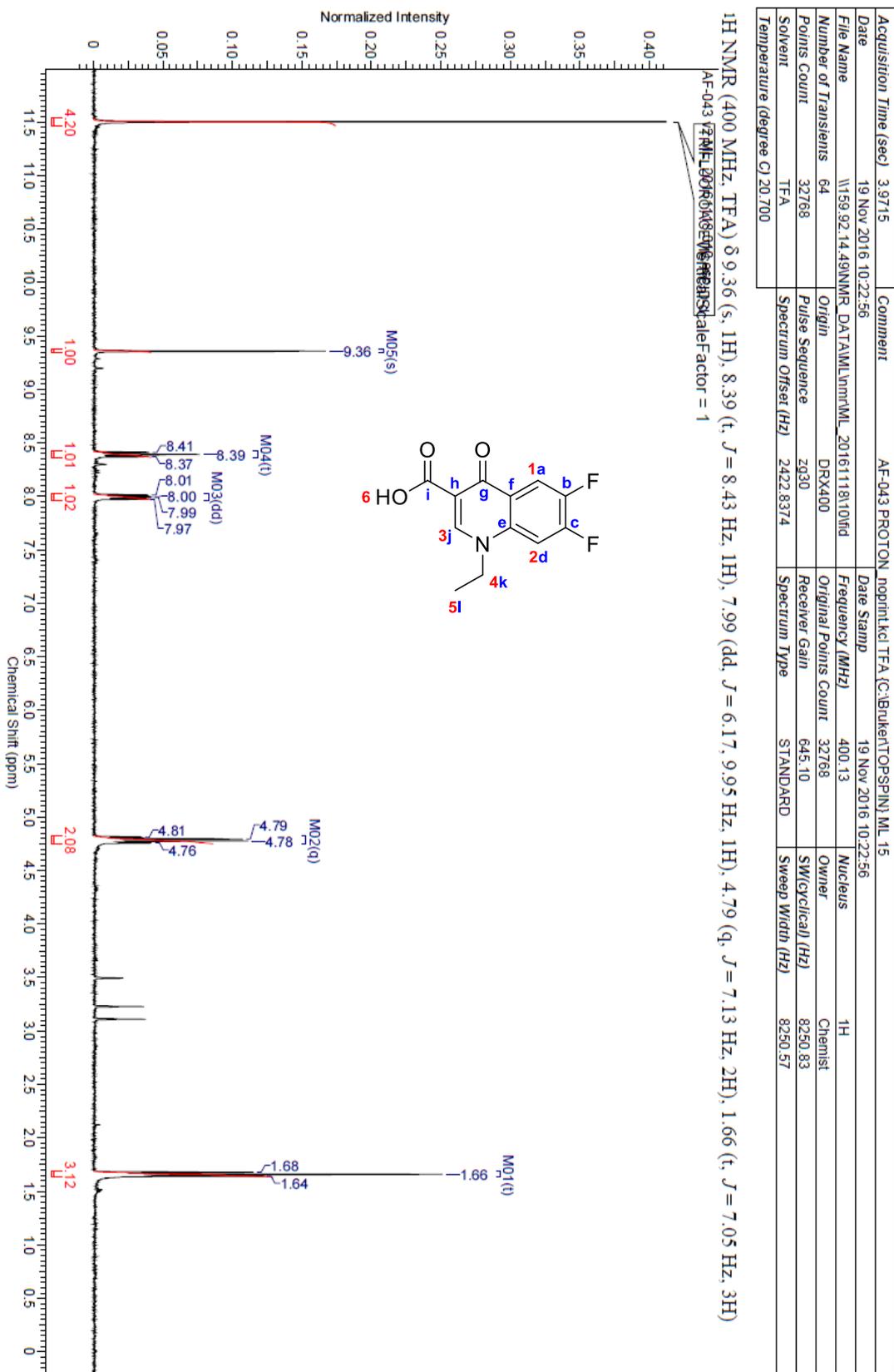
Figure S51. Proton NMR spectrum of compound 4a.



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24/06/2019 17:48:43

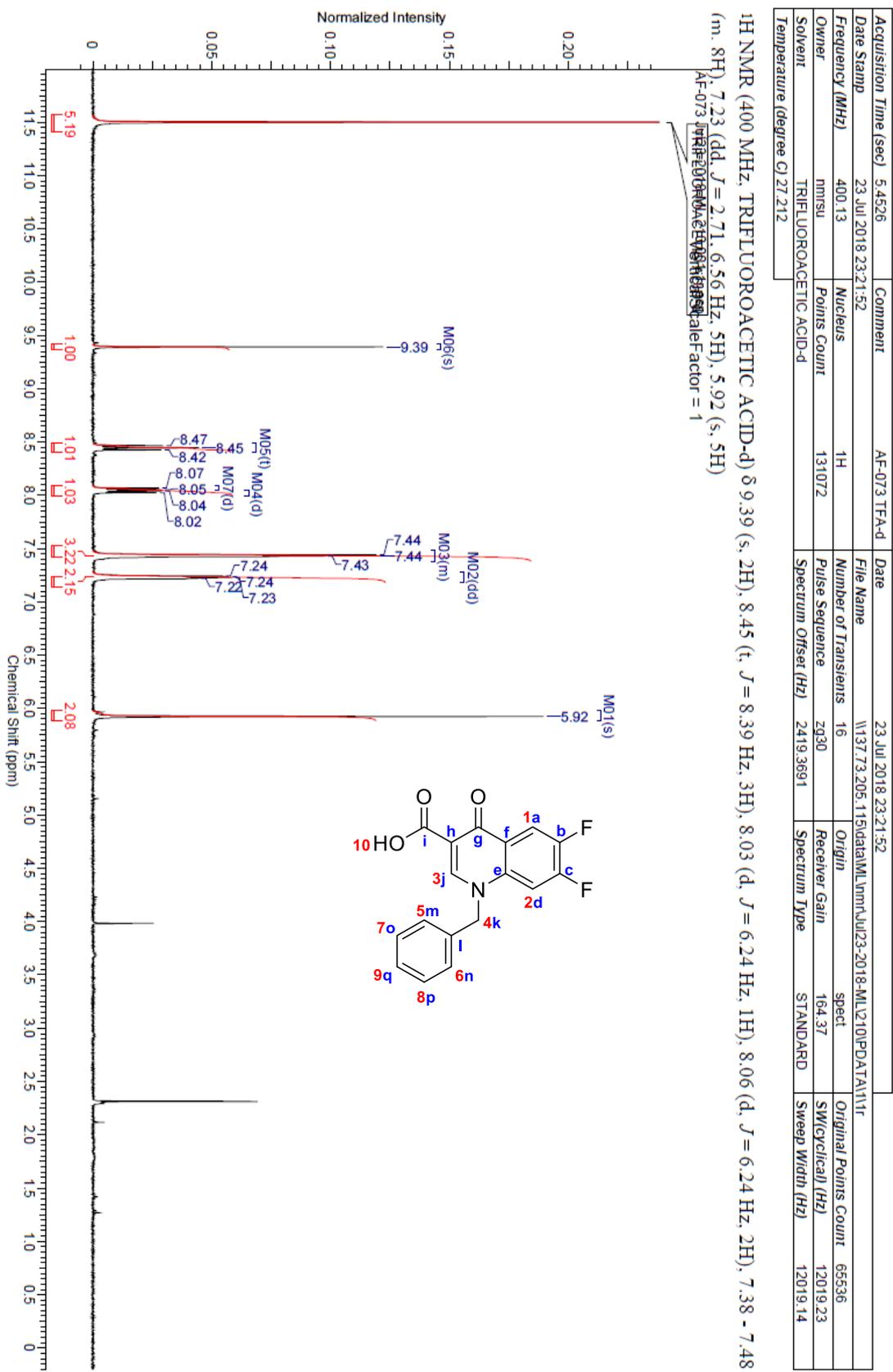
Figure S52. Proton NMR spectrum of compound 4b.



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

24/06/2019 15:33:51

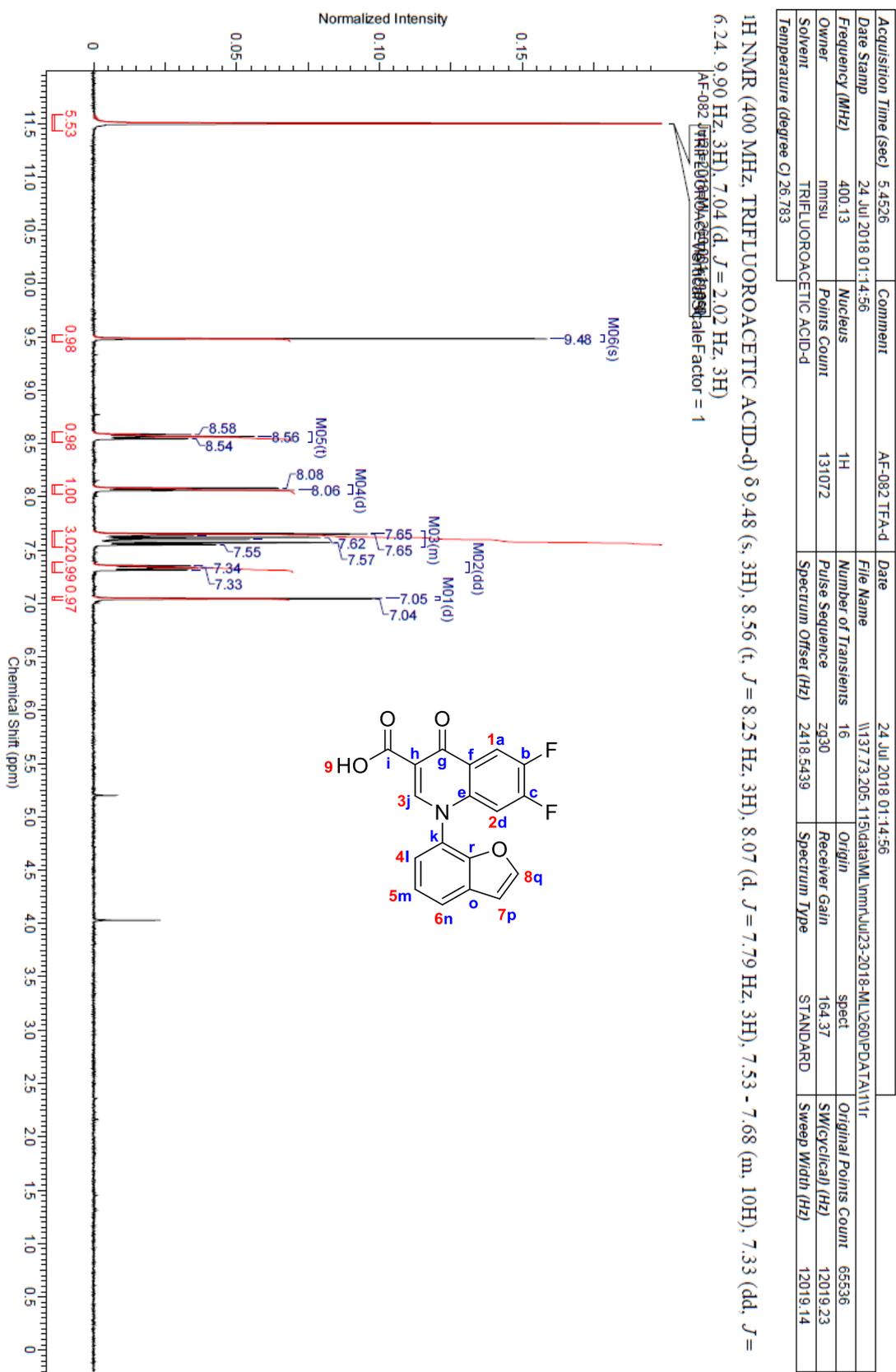
Figure S53. Proton NMR spectrum of compound 4c.



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

24/06/2019 16:17:15

Figure S54. Proton NMR spectrum of compound 4d.



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24/06/2019 16:29:22

Figure S55. Proton NMR spectrum of compound 4e.

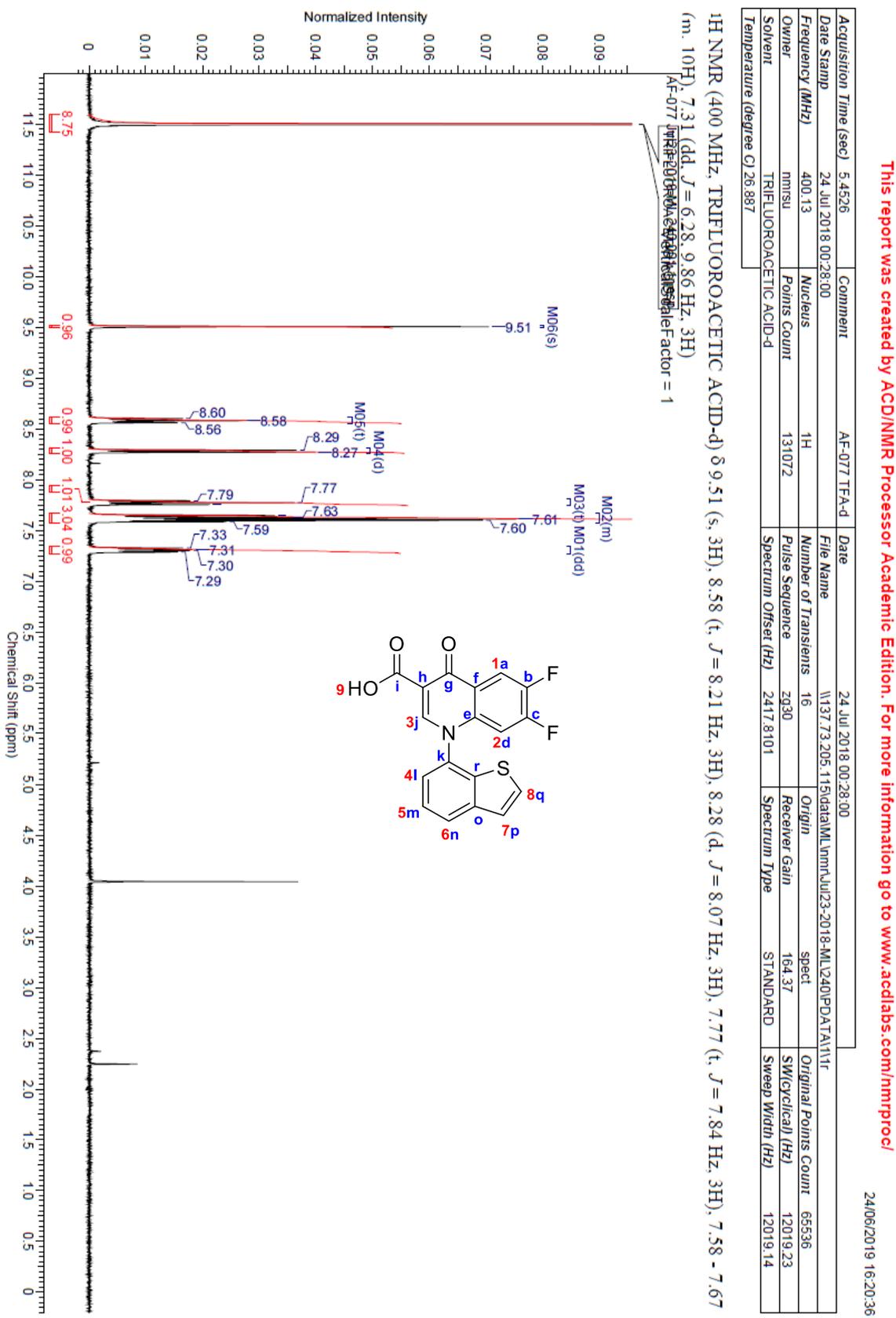
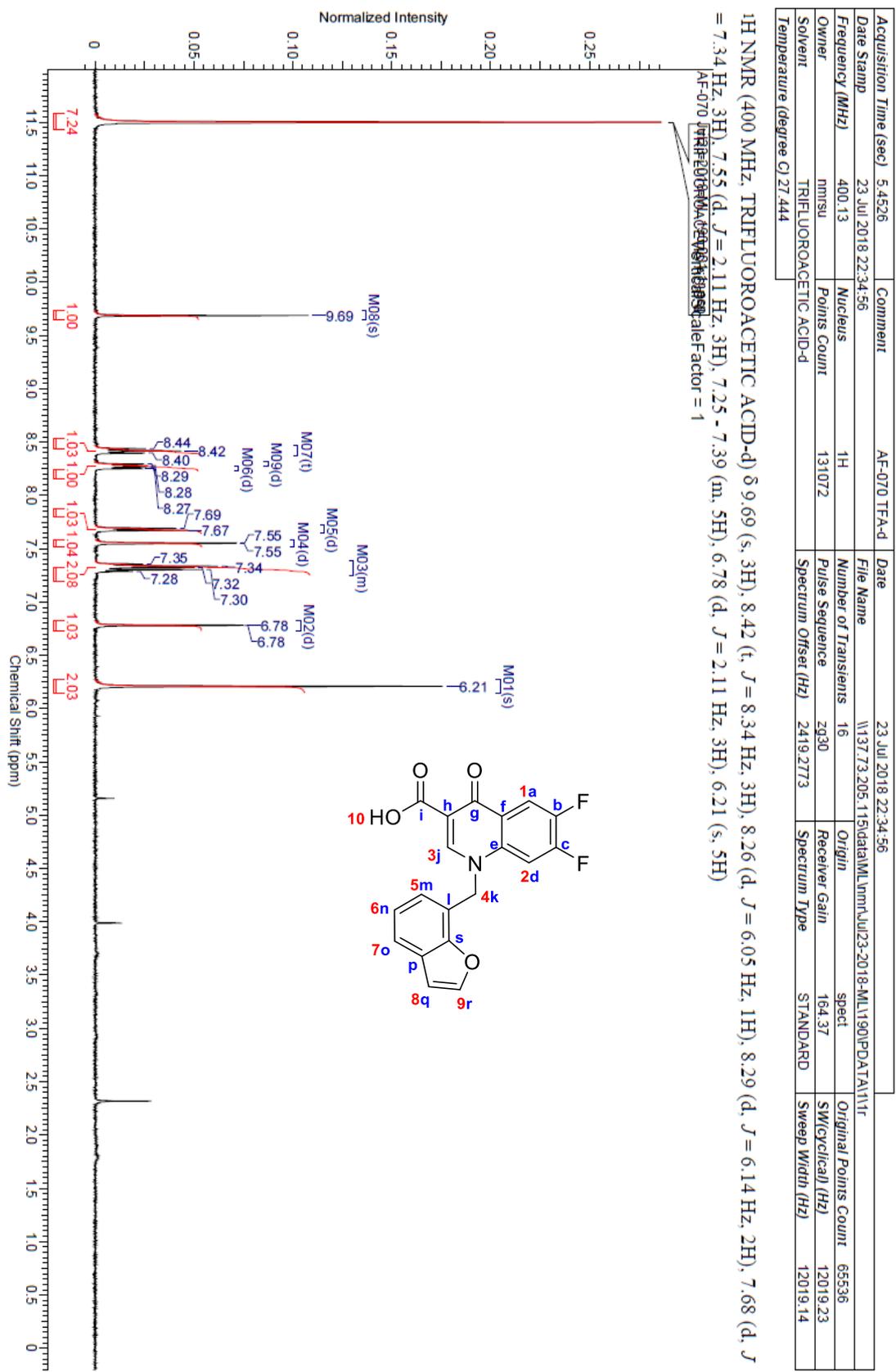


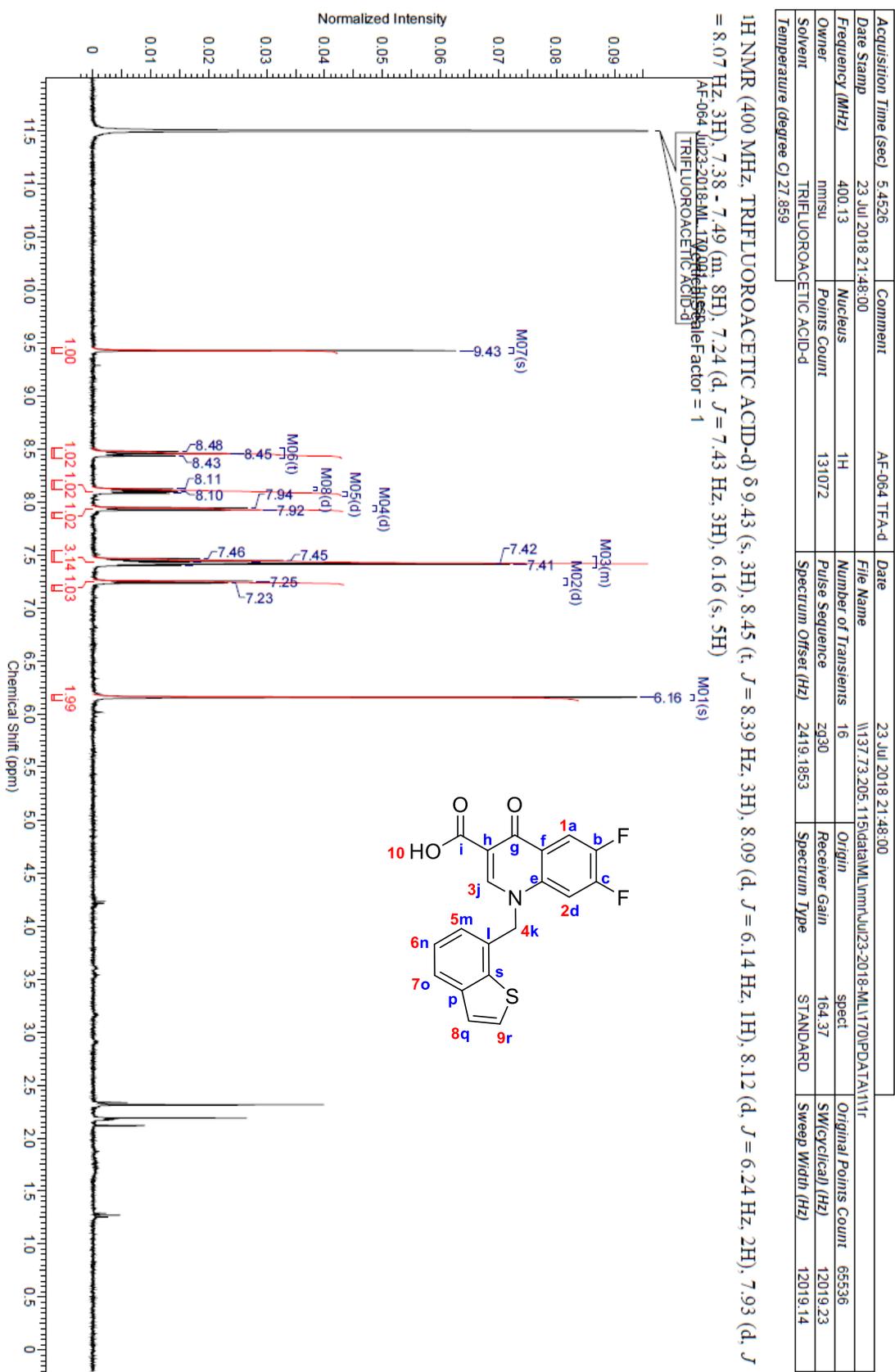
Figure S56. Proton NMR spectrum of compound 4f.



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

24/06/2019 16:07:01

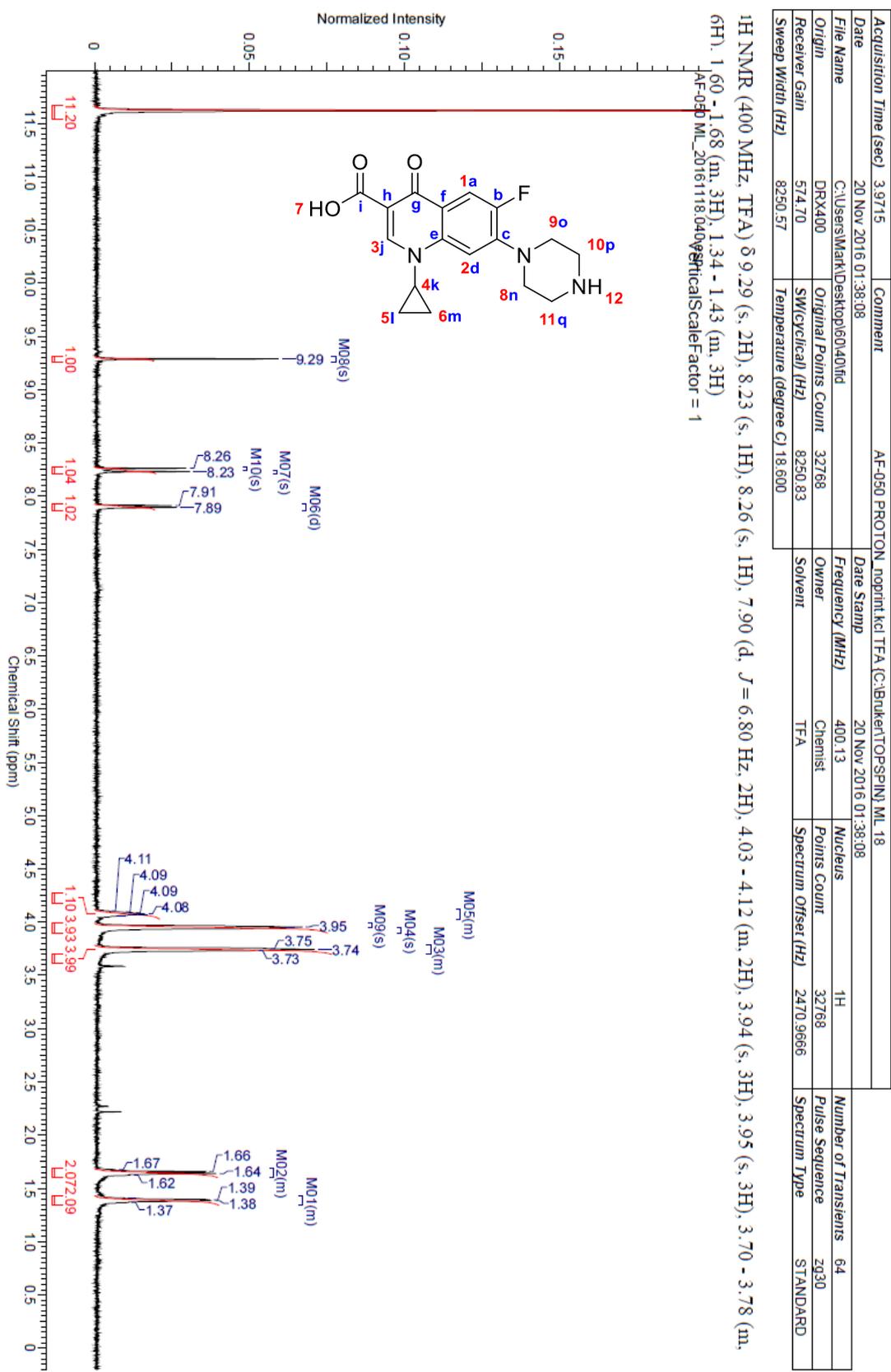
Figure S57. Proton NMR spectrum of compound 4g.



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

24/06/2019 15:56:17

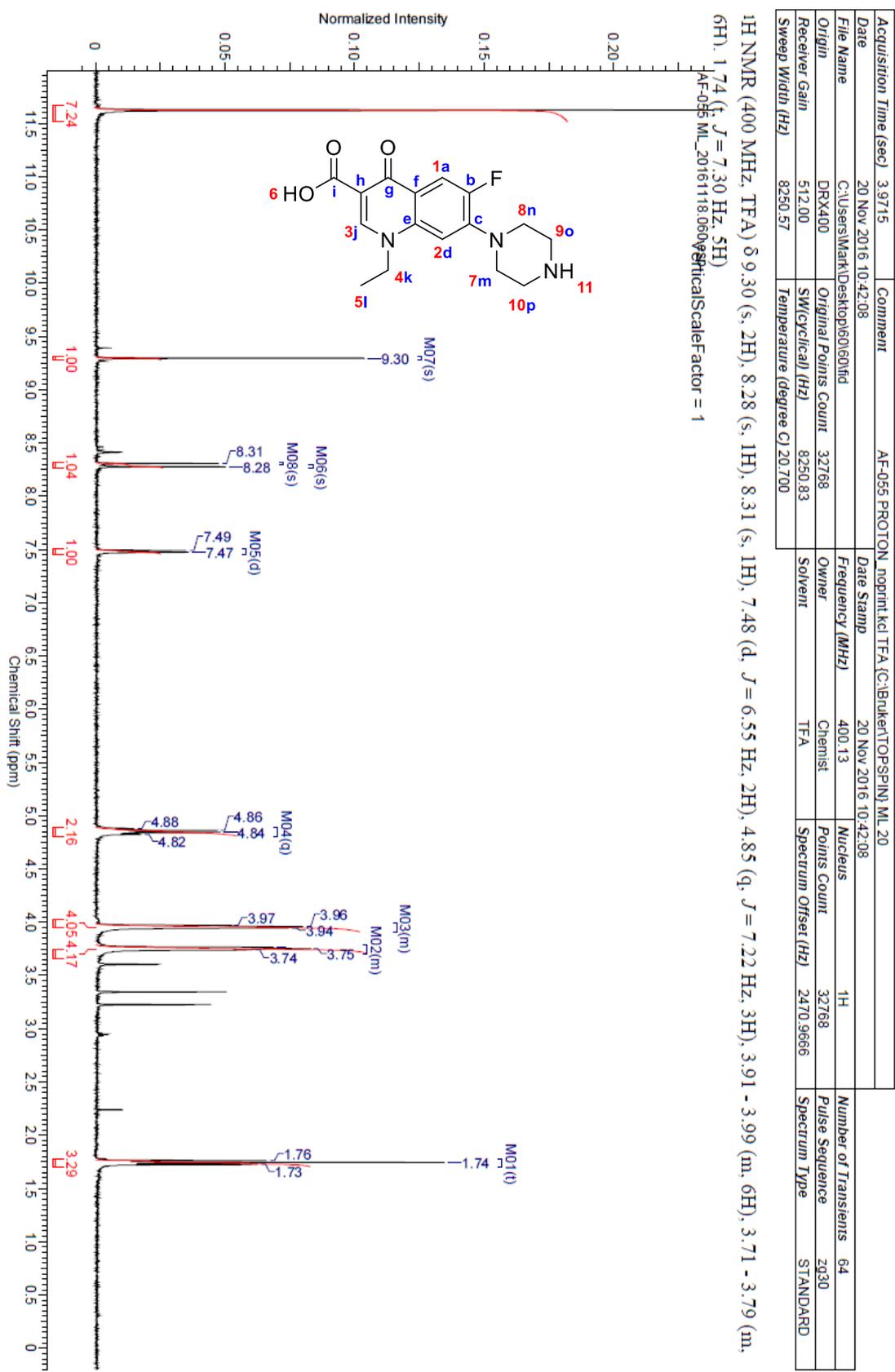
Figure S58. Proton NMR spectrum of compound 5a.



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

24/06/2019 15:37:48

Figure S59. Proton NMR spectrum of compound 5b.



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/inmpro/

24/06/2019 15:47:30

Acquisition Time (sec)	5.4526	Comment	AF-075 TFA-d	Date	23 Jul 2018 23:43:12
Date Stamp	23 Jul 2018 23:43:12	File Name	V137.73.205.115\data\ML\mtr\Jul23-2018-ML\220\FDATA\111r	Origin	
Frequency (MHz)	400.13	Nucleus	¹ H	Number of Transients	16
Owner	nimsu	Points Count	131072	Pulse Sequence	zg30
Solvent	TRIFLUOROACETIC ACID-d	Spectrum Offset (Hz)	2419.1853	Receiver Gain	142.38
Temperature (degree C)	27.109	Spectrum Type	STANDARD	SW(cyclical) (Hz)	12019.23
				Sweep Width (Hz)	12019.14

¹H NMR (400 MHz, TRIFLUOROACETIC ACID-d) δ 9.29 (s, 1H), 8.23 (d, $J = 12.47$ Hz, 1H), 7.41 - 7.47 (m, 4H), 7.39 (d, $J = 6.88$ Hz, 1H), 7.18 - 7.28 (m, 3H), 5.91 (s, 3H), 3.69 - 3.86 (m, 6H), 3.52 - 3.69 (m, 6H)

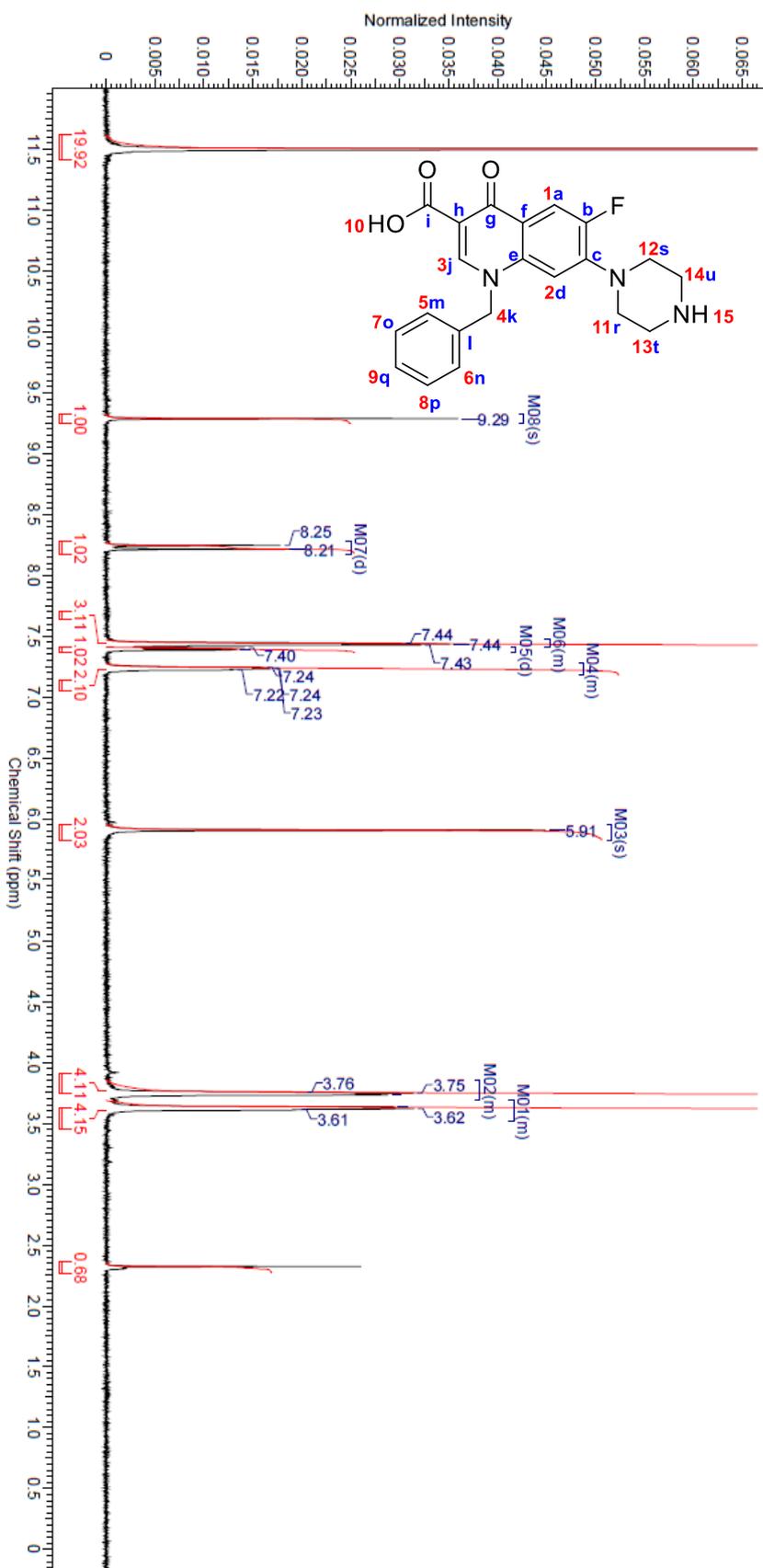
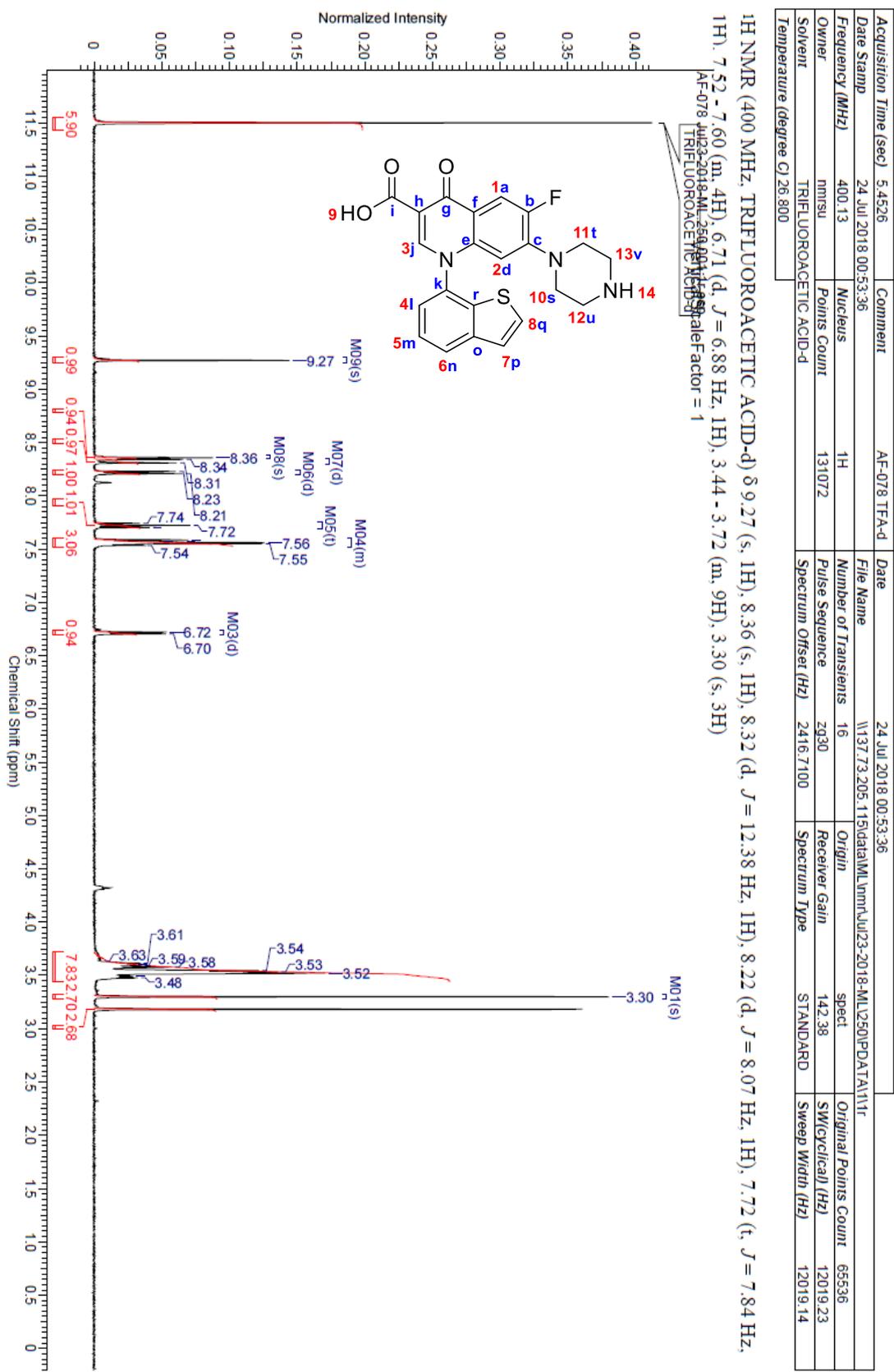


Figure S62. Proton NMR spectrum of compound 5e.



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

24/06/2019 16:27:38

Figure S66. Proton NMR spectrum of compound 6b.

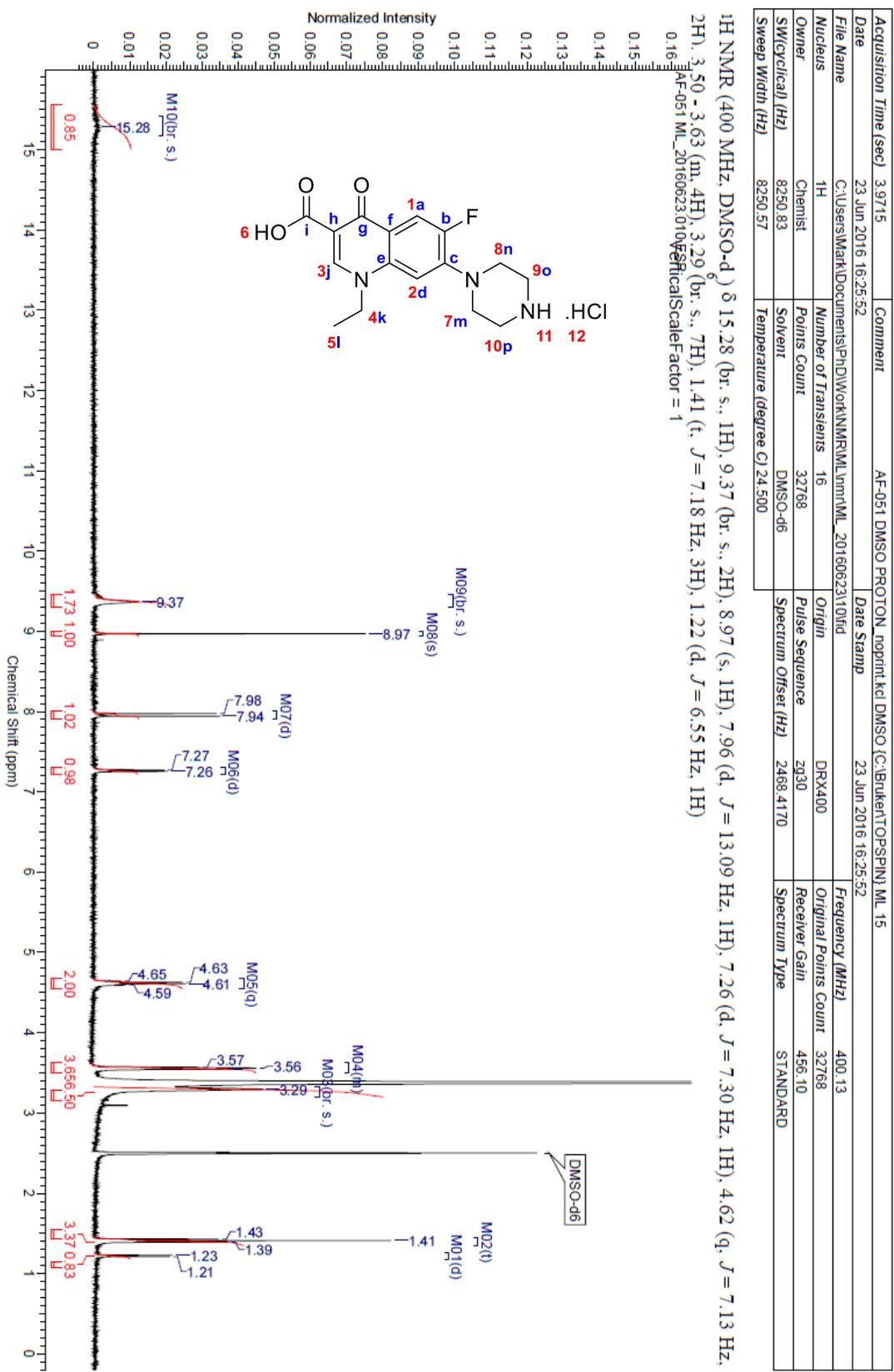


Figure S67. Proton NMR spectrum of compound 6c.

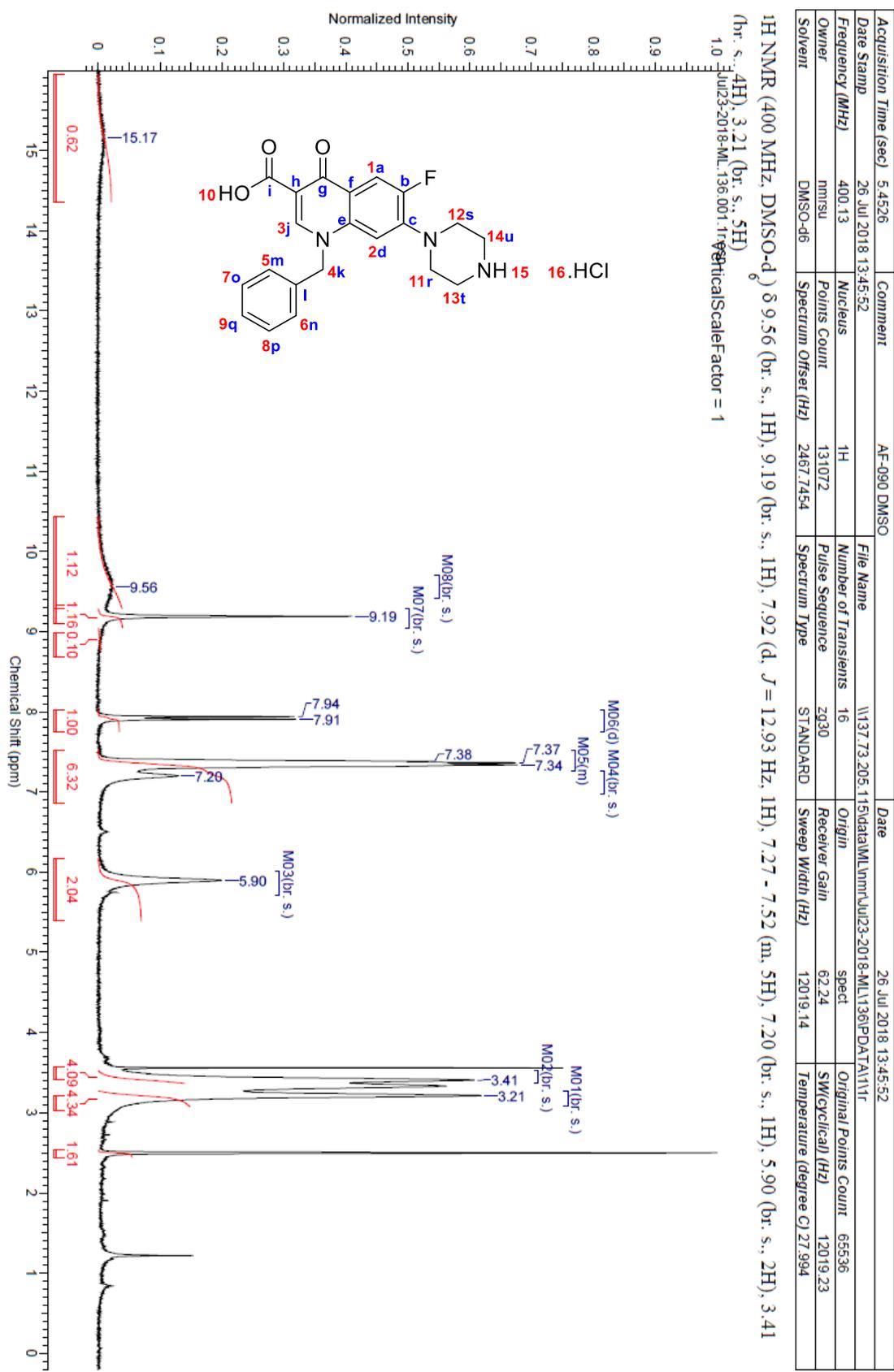


Figure S68. Proton NMR spectrum of compound 6d.

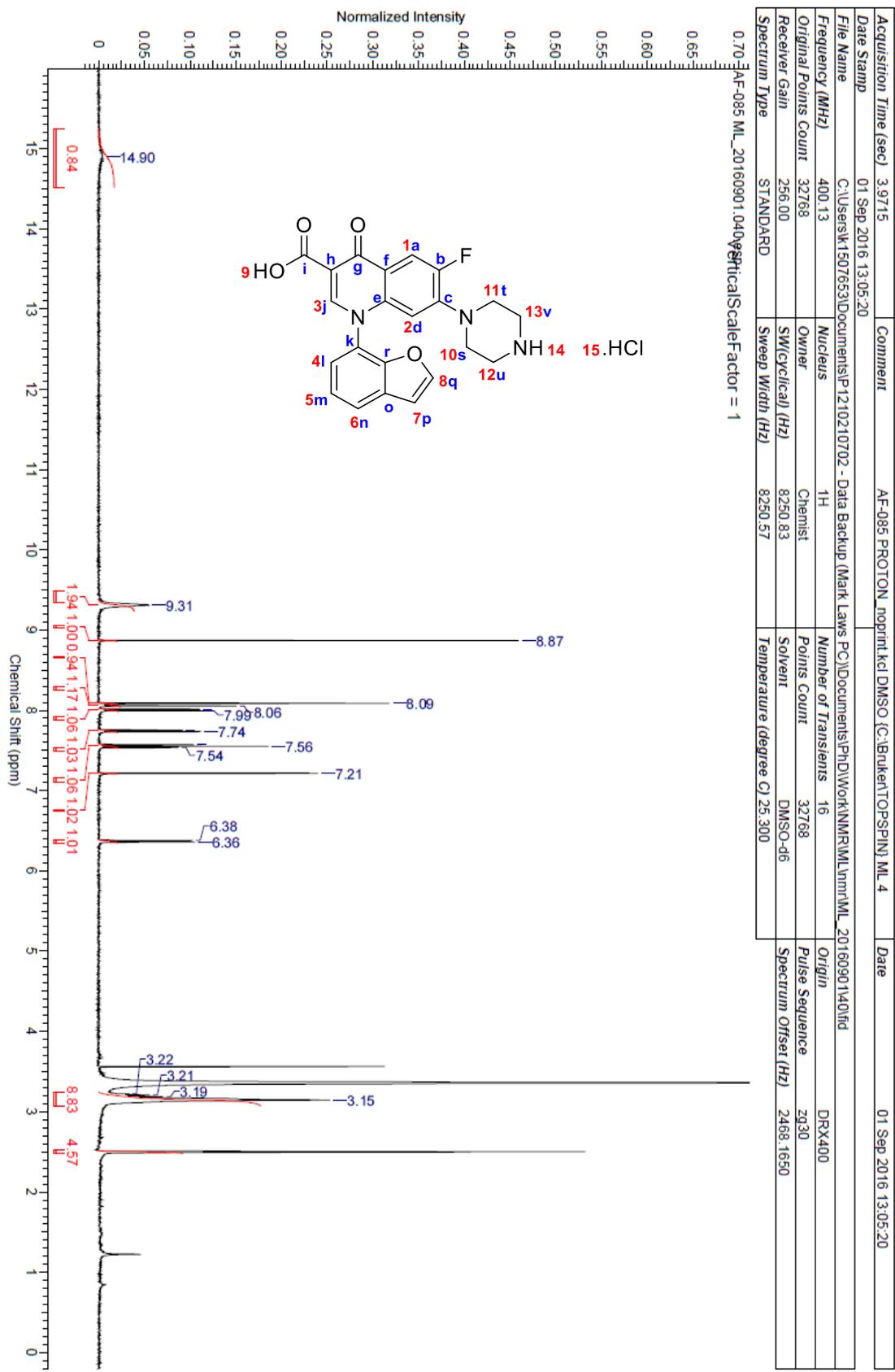


Figure S70. Proton NMR spectrum of compound 6f.

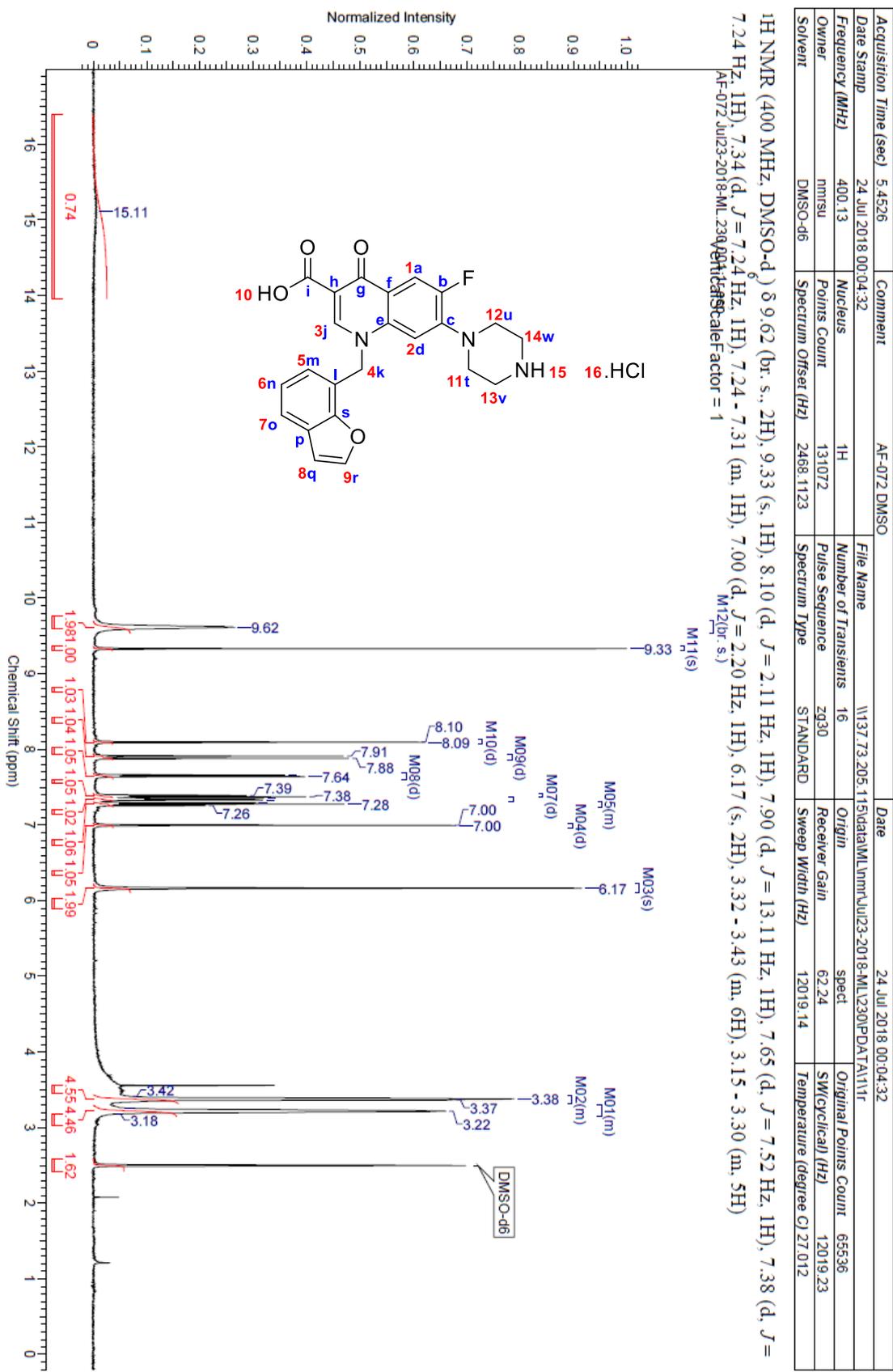
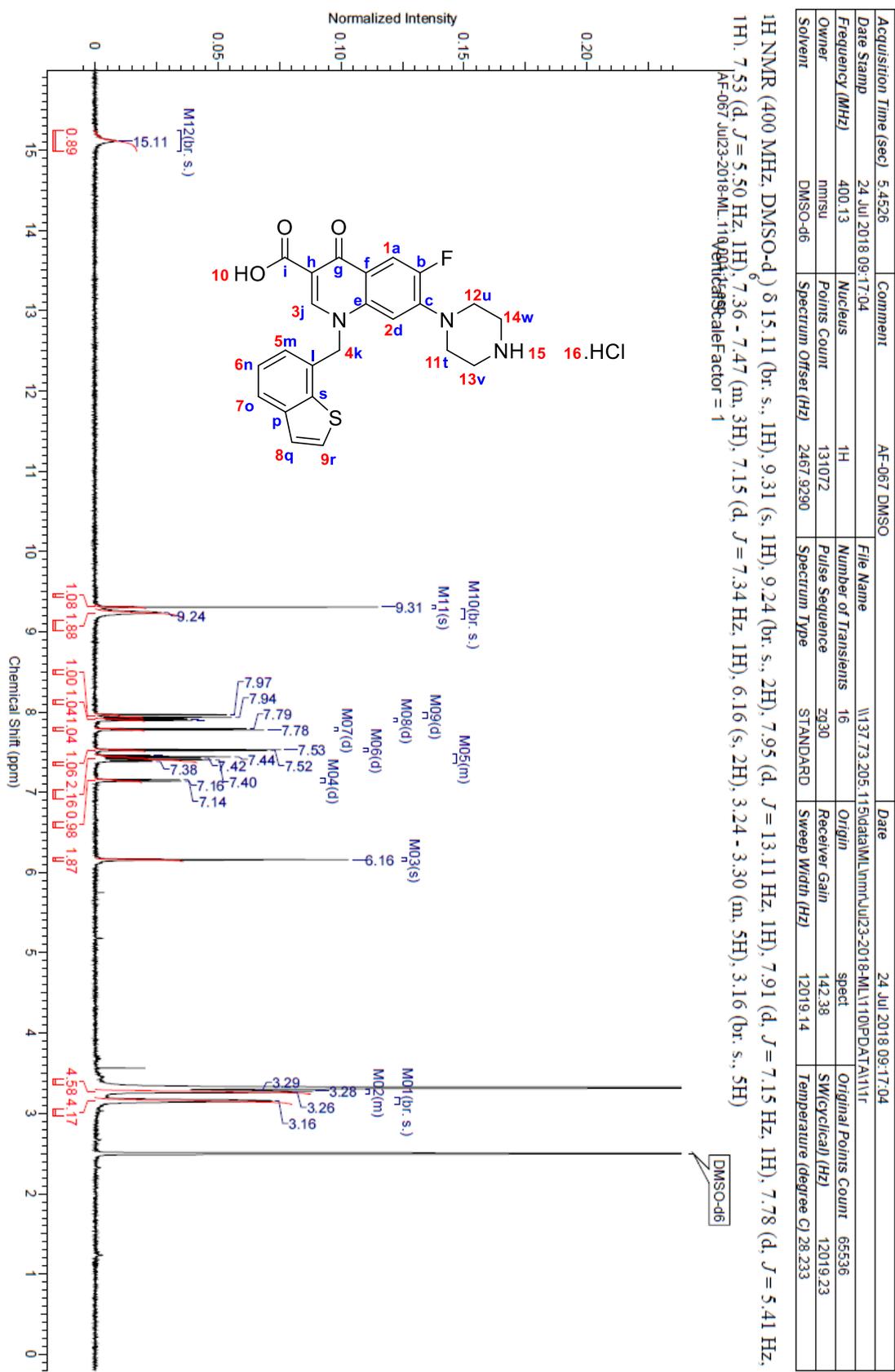


Figure S71. Proton NMR spectrum of compound 6g.

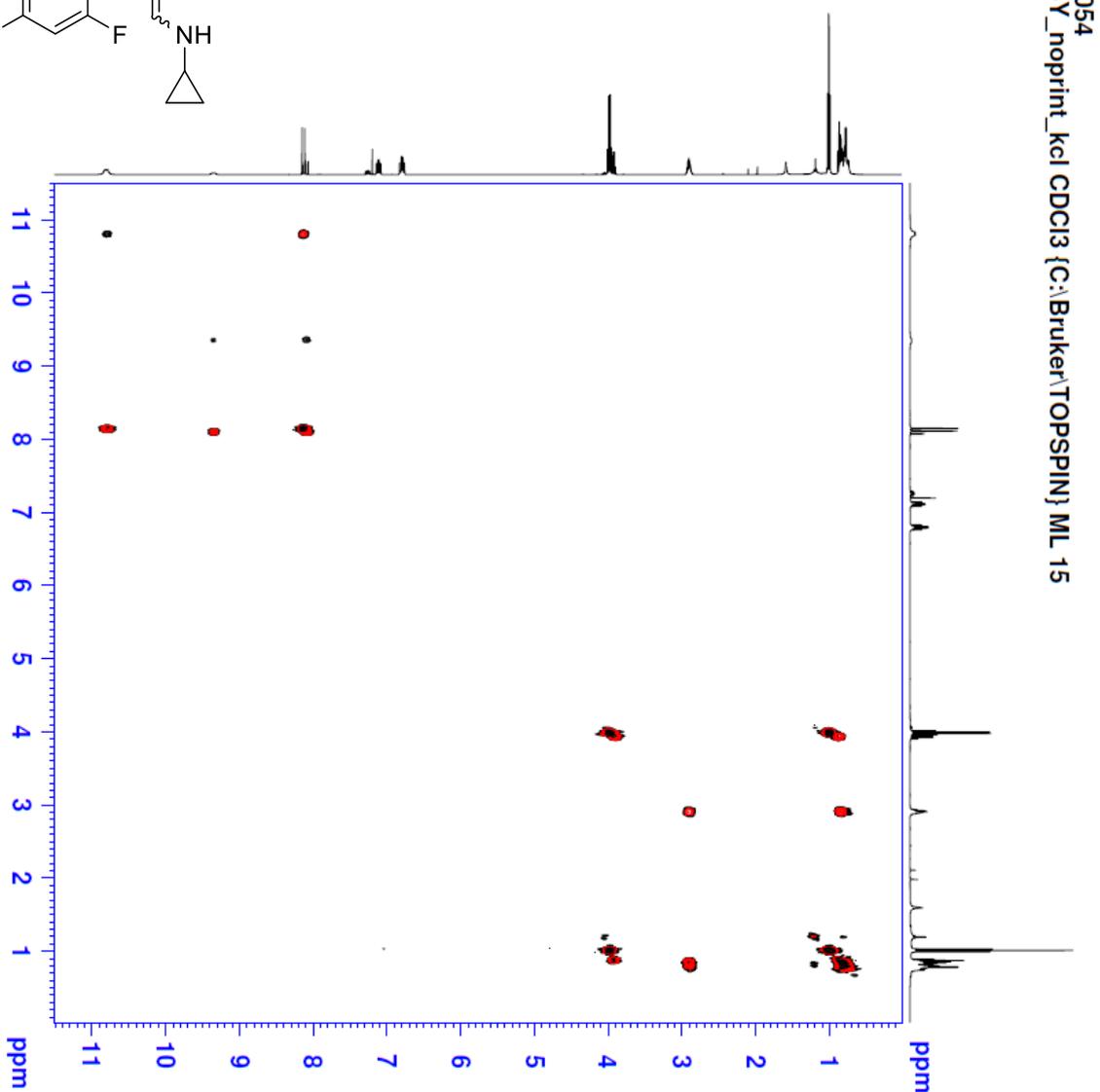
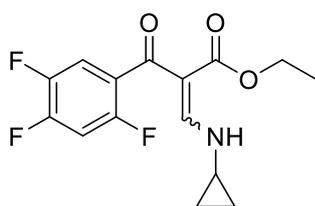


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/improc/

24/06/2019 16:01:39

COSY Spectra

Figure S72. COSY spectrum of compound 2a.



AF-054
 COSY_noprint_kcl CDC13 {C:\Bruker\TOPSPIN} ML 15



```

Current Data Parameters
NAME          ML_20160902
EXPNO        31
PROCNO       1

F2 - Acquisition Parameters
Date_         20160902
Time_        13.58
INSTRUM      DRX400
PROBHD       5 mm QNP 1H/13
PULPROG      zgpg30
TD           2048
SOLVENT      CDCl3
NS           6
DS           2
SWH           4595.588 Hz
FIDRES       2.243940 Hz
AQ           0.2229812 sec
RG           5792.6
DM           108.800 usec
DE           38.00 usec
TE           300.2 K
D1           0.0000100 sec
d13          1.96805096 sec
d16          0.00020000 sec
IN0          0.00021760 sec

----- CHANNEL f1 -----
NUC1          13C
P1           10.00 usec
PL1          -1.00 dB
SFO1         400.1323391 MHz

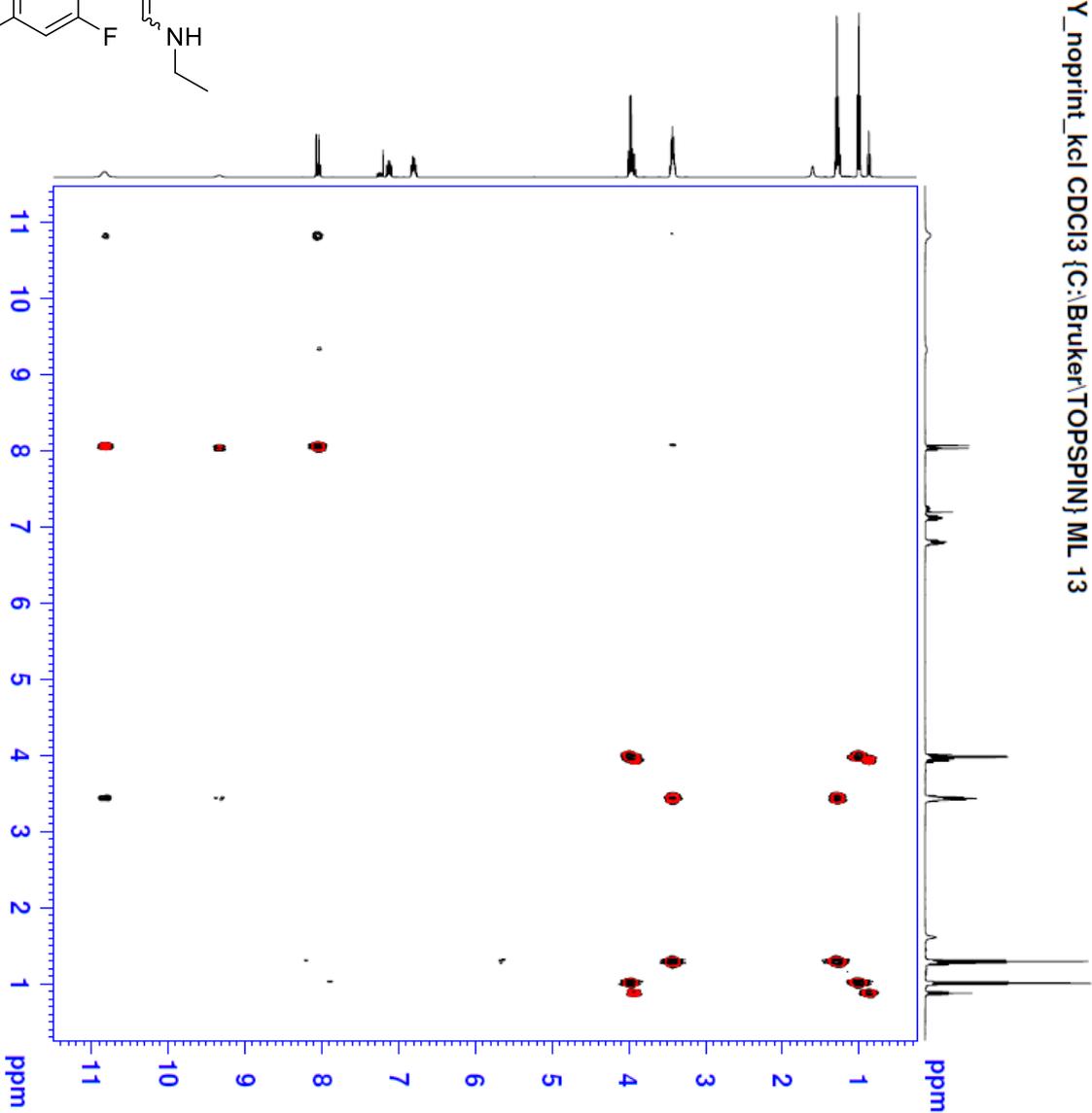
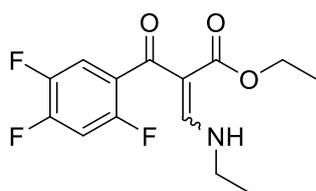
----- GRADIENT CHANNEL -----
GPNAM1       SINE,100
SINE1        SINE,100
GPNAM2       SINE,100
SINE2        SINE,100
GPNAM3       SINE,100
SINE3        SINE,100
GZ1          15.00 %
GZ2          40.00 %
GZ3          40.00 %
PL6          1000.00 usec

F1 - Acquisition parameters
ND0          1
TD           128
SFO1         400.1323391 MHz
SWH          35.91352 Hz
SF           11.485 ppm
FNUC1        13C
FNUC2        1H

F2 - Processing parameters
SI           1024
SF           400.1300344 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
PC           1.40

F1 - Processing parameters
SI           1024
SF           400.1300344 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
  
```

Figure S73. COSY spectrum of compound 2b.



AF-040
 COSY_noprint_kcl CDCl3 {C:\Bruker\TOPSPIN} ML 13



```

Current Data Parameters
NAME      ML_20160902
EXPNO    11
PROCNO   1

F2 - Acquisition Parameters
Date_    20160902
Time     13.08
INSTRUM  DRX400
PROBHD   5 mm QNP
PULPROG  cosyprgf
TD       2048
SOLVENT  CDCl3
NS       2
DS       8
SWH      4496.403 Hz
FIDRES   2.19589 Hz
AQ       0.272898 sec
RG       113.204
DM       113.204
DE       6.00 usec
TE       297.5 K
D0       0.00000300 sec
d1       1.96395504 sec
d13      0.00000400 sec
d16      0.00020000 sec
IN0      0.00022240 sec

===== CHANNEL f1 =====
NUC1     1H
P1       10.50 usec
PL1     -3.00 dB
SFO1    400.1323812 MHz

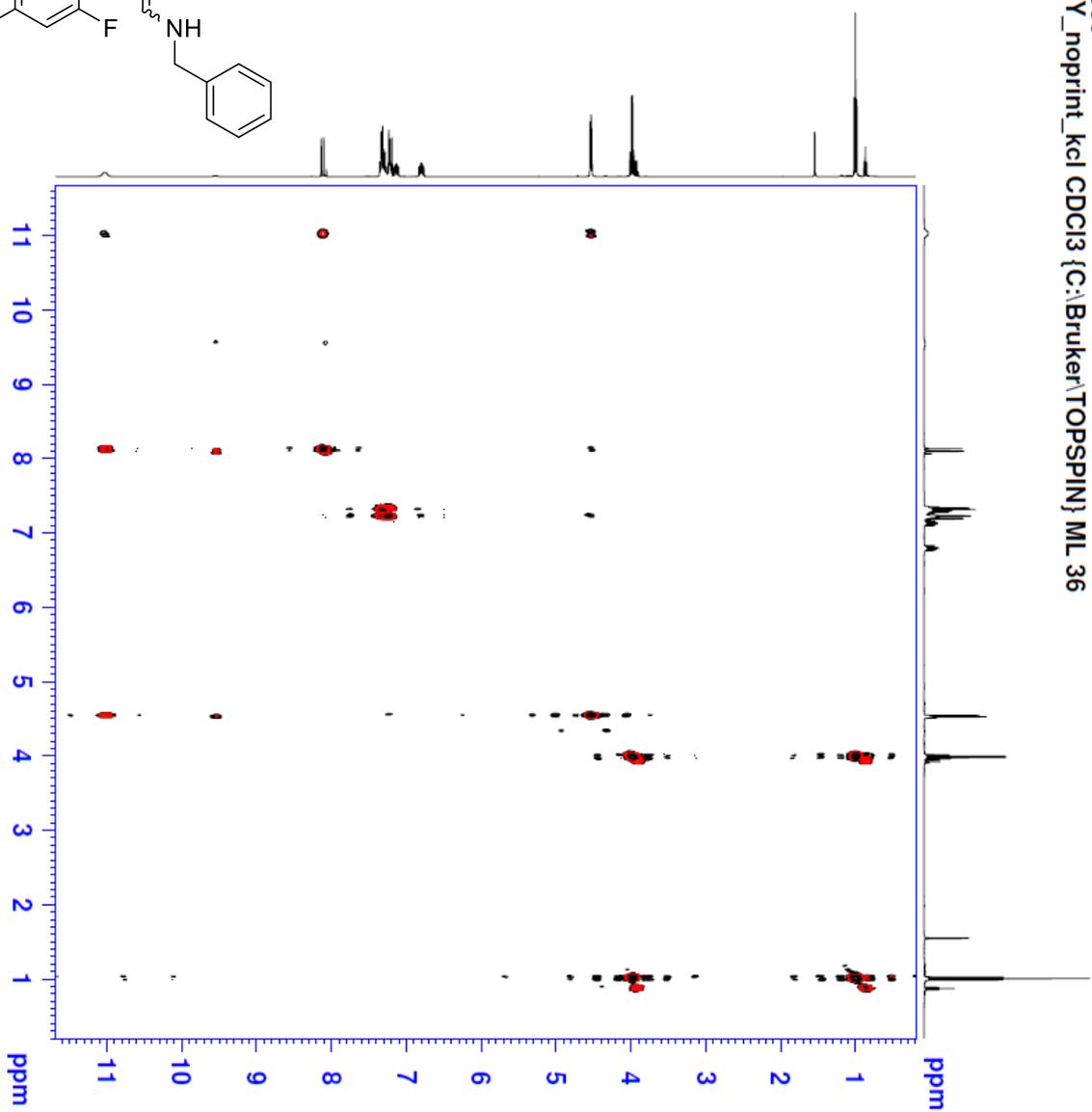
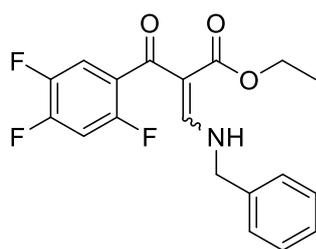
===== GRADIENT CHANNEL =====
GPRAM1  SINE.100
GPRAM2  SINE.100
GPRAM3  SINE.100
GB21    12.00 %
GB22    12.00 %
GB23    40.00 %
p16     1000.00 usec

F1 - Acquisition parameters
ND0     1
TD      128
SFO1    400.1324 MHz
RG       35.128147 Hz
SM       11.231 PPM
FMODE   QF

F2 - Processing parameters
SI      1024
SF      400.1300343 MHz
WDW     SINE
SSB     0
LB      0.00 Hz
GB      0
PC      1.40

F1 - Processing parameters
SI      1024
SF      400.1300343 MHz
WDW     SINE
SSB     0
LB      0.00 Hz
GB      0
  
```

Figure S74. COSY spectrum of compound 2c.



AF-060
 COSY_noprint_kel CDCl3 {C:\Bruker\TOPSPIN} ML 36



```

Current Data Parameters
NAME           ML_20160901
EXPNO         51
PROCNO        1

F2 - Acquisition Parameters
Date_         20160901
Time         17.57
INSTRUM      DRX400
PROBHD       5 mm QNP 1H/13
PULPROG      cosyprmf4f
TD           2048
SOLVENT      CDCl3
NS           2
DS           1
SWH          4595.588 Hz
FIDRES       0.2243940 Hz
AQ           0.2229812 sec
RG           3649.1
DE           108.800 usec
TE           297.9 K
D0           0.00000300 sec
d13          1.968805096 sec
d16          0.00000400 sec
IN0          0.00021780 sec

----- CHANNEL f1 -----
NUC1          1H
P1            10.50 usec
PL1          -3.00 dB
SFO1         400.1324130 MHz

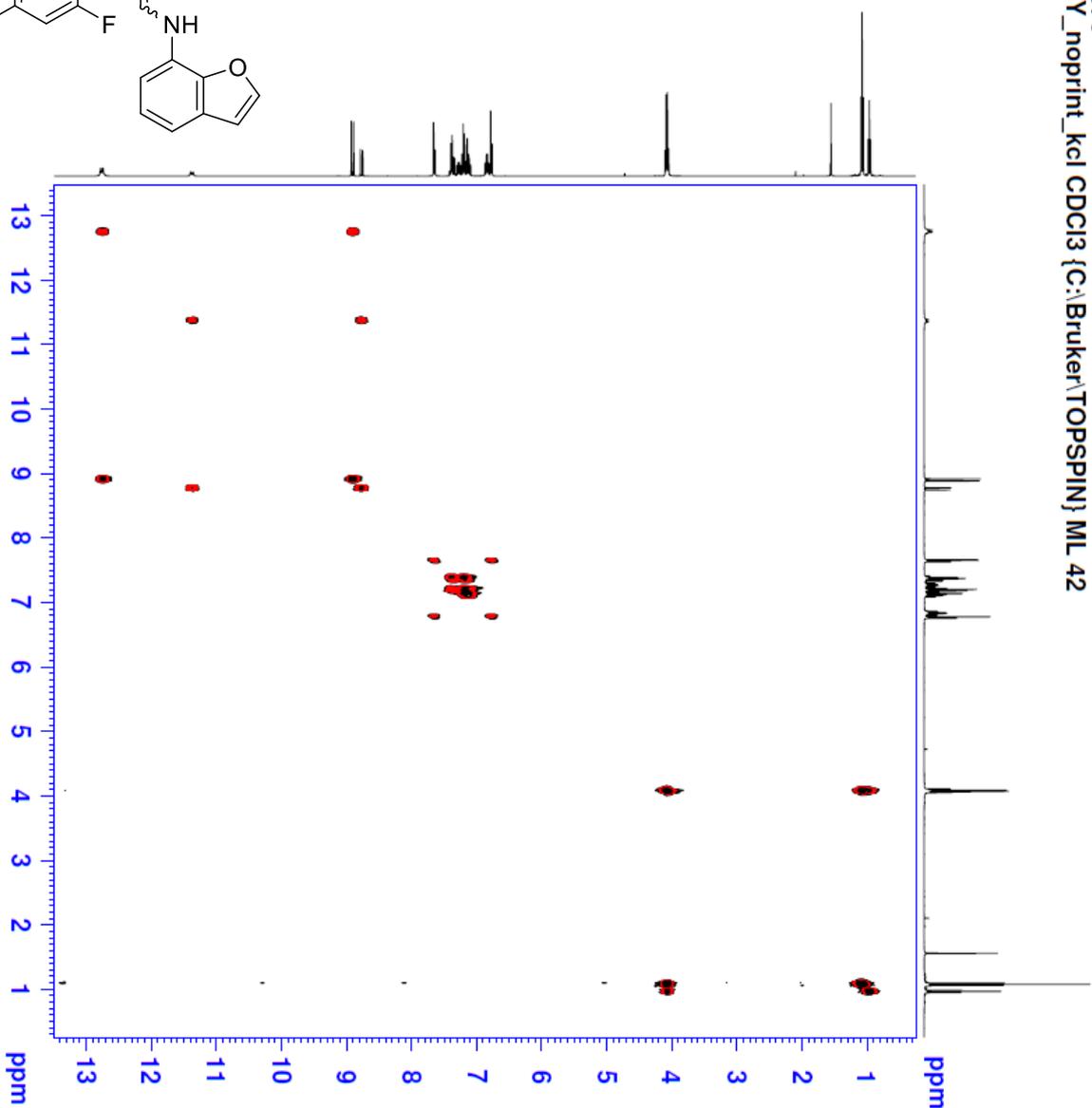
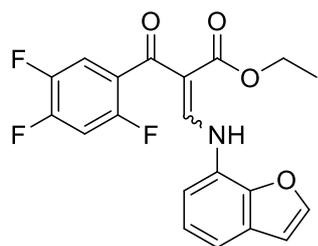
----- GRADIENT CHANNEL -----
GRN1         SINE:100
GRN2         SINE:100
GRN3         SINE:100
GR21         12.00 %
GR22         40.00 %
GR23         40.00 %
P16          1000.00 usec

F1 - Acquisition parameters
ND0           1
ID0           128
SFO1         400.1324 MHz
SF01         35.10324 MHz
SFO2         11.485 MHz
P1MODE       QF

F2 - Processing parameters
SI            1024
SF           400.1300382 MHz
WDW          SINE
SSB          0
GB           0.00 Hz
PC           1.40

F1 - Processing parameters
SI            1024
SF           400.1300382 MHz
WDW          SINE
SSB          0
GB           0.00 Hz
  
```

Figure S75. COSY spectrum of compound 2d.



AF-079
 COSY_noprint_kel CDC13 {C:\Bruker\TOPSPIN} ML 42



```

Current Data Parameters
NAME      ML_20160901
EXPNO     111
PROCNO    1

F2 - Acquisition Parameters
-----
Time          20160901
Date_         7 50
INSTRUM      DRX400
PROBHD       5 mm QNP 1H/13
PULPROG      cosygmrf4f
TD           2048
SOLVENT      CDCl3
NS           2
DS           8
SWH          5296.610 Hz
FIDRES       2.586426 Hz
AQ           0.138426 sec
RG           0.157926
AQ           94.400 usec
DE           6.00 usec
TE           297.1 K
D0           0.00000300 sec
D1           1.99877095 sec
d13          0.00000400 sec
D16         0.00020000 sec
IN0          0.00018880 sec

----- CHANNEL f1 -----
NUC1        13
P1          10.50 usec
PL1         -3.00 dB
SFO1        400.1327656 MHz

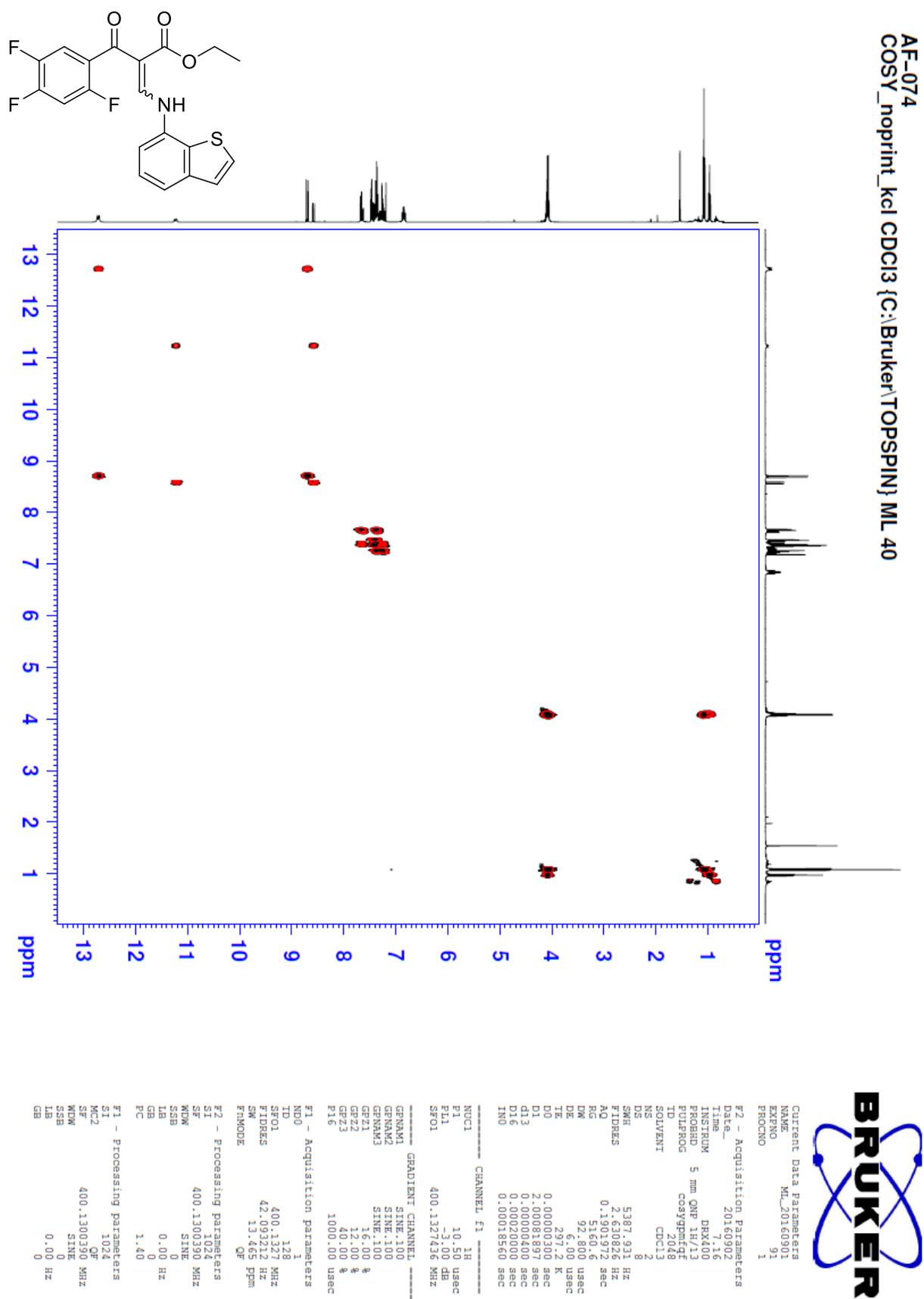
----- GRADIENT CHANNEL -----
GPNAM1      SINE.100
SINE.100
GPNAM2      SINE.100
SINE.100
GPNAM3      SINE.100
SINE.100
GRZ1        16.00 %
GRZ2        12.00 %
GRZ3        40.00 %
F16         1000.00 usec

F1 - Acquisition parameters
-----
TD          128
SFO1        400.1328 MHz
FIDRES      41.379768 Hz
SW          13.237 ppm
FMODE       QF

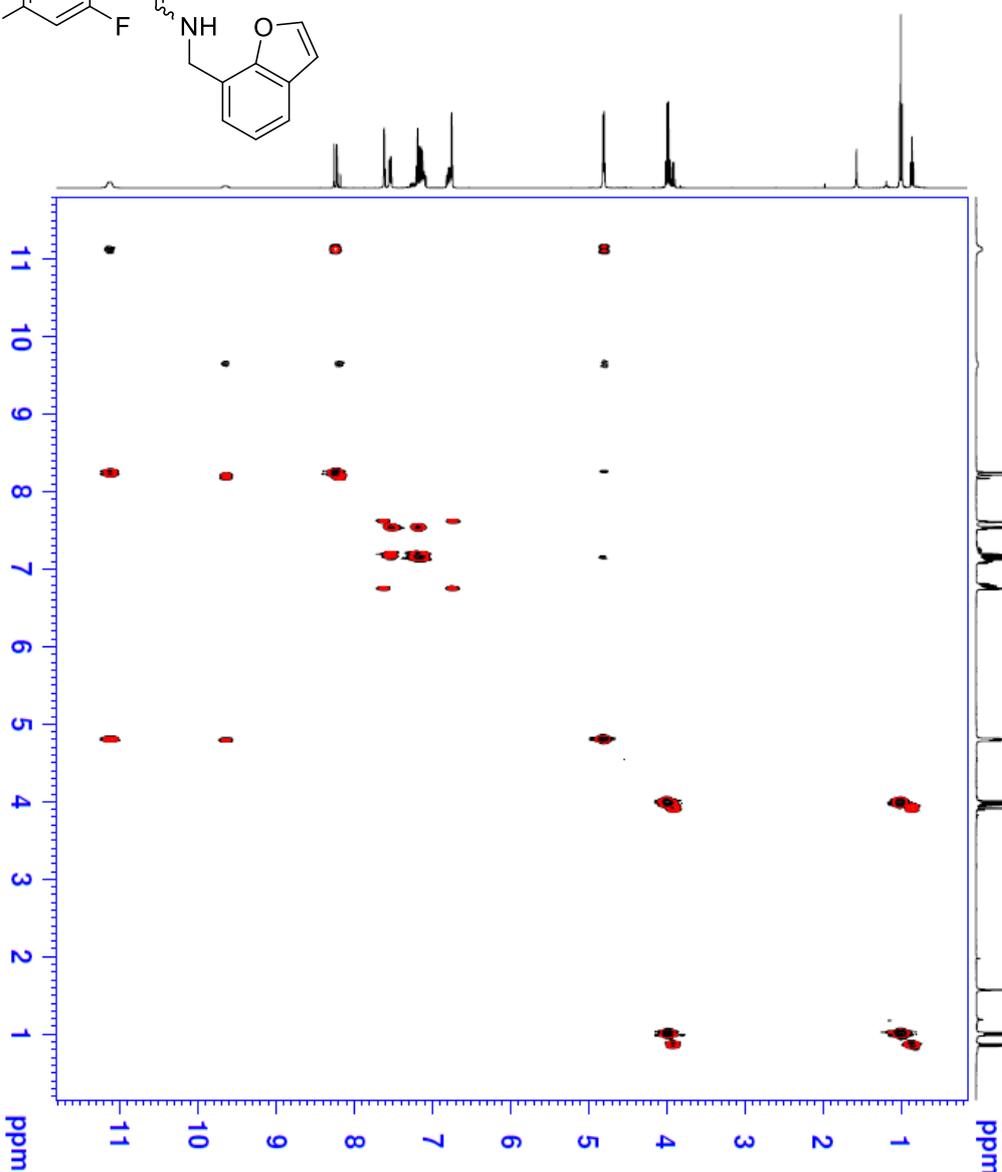
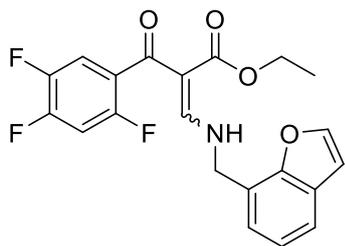
F2 - Processing parameters
-----
SI          1024
SF          400.1300387 MHz
WDW         SINE
SSB         0
GB          0
PC          1.40

F1 - Processing parameters
-----
SI          1024
SF          400.1300387 MHz
WDW         SINE
SSB         0
GB          0
PC          1.40
  
```

Figure S76. COSY spectrum of compound 2e.



AF-068
 COSY_noprint_kcl CDCl3 {C:\Bruker\TOPSPIN} ML 18



```

Current Data Parameters
NAME      ML_20160902
EXPNO    61
PROCNO   1

F2 - Acquisition Parameters
Date_    20160902
Time     15:00
INSTRUM  DRX400
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       2
DS       8
SWH      4664.179 Hz
FIDRES   2.271431 Hz
AQ       0.2197028 sec
RG       3849.1
DW       107.200 usec
DE       2.100 usec
TE       300.2 K
D1       0.000003100 sec
d13      0.000004000 sec
D15      0.000200000 sec
IN0      0.000214400 sec

----- CHANNEL f1 -----
NUC1     1H
P1       10.50 usec
PL1      -1.00 dB
SFO1    400.1324298 MHz

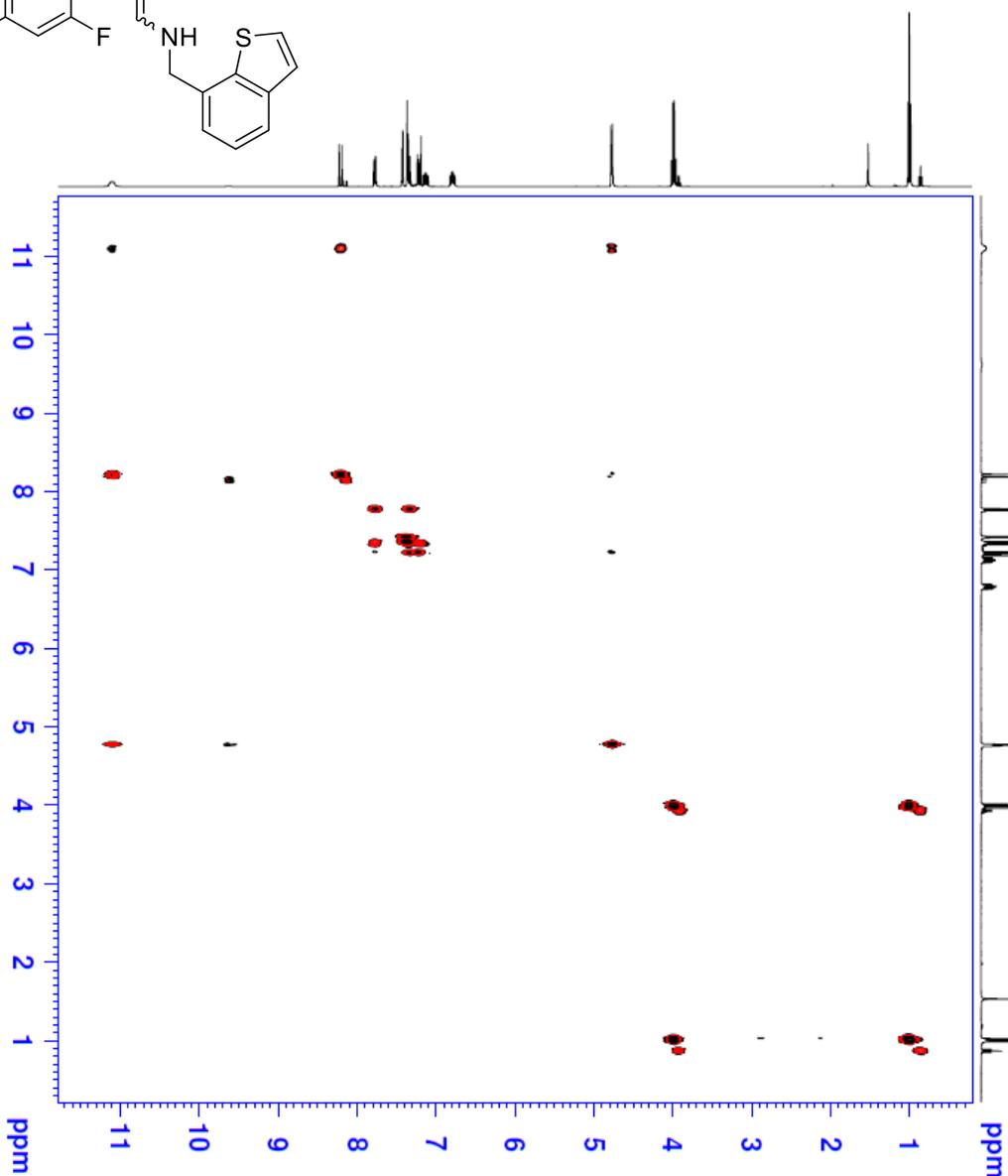
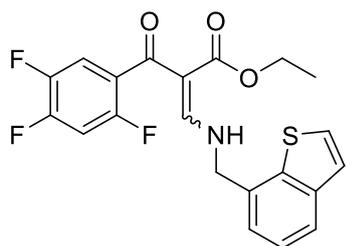
----- GRADIENT CHANNEL -----
GPNAM1   SINE.100
GPNAM2   SINE.100
GPNAM3   SINE.100
GPZ1     16.00 %
GPZ2     12.00 %
GPZ3     40.00 %
P16      1000.00 usec

F1 - Acquisition parameters
ND0      1
TD       128
SFO1    400.1324 MHz
FIDRES   36.438200 Hz
EM       11.000 PPM
FMODE    QF

F2 - Processing parameters
SI       1024
SF       400.1300393 MHz
WDW      SINE
SSB      0
LB       0.00 Hz
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
MC2      OF
SF       400.1300393 MHz
WDW      SINE
SSB      0
LB       0.00 Hz
GB       0
  
```

AF-062
 COSY_noprint_kel CDC13 {C:\Bruker\TOPSPIN} ML 38



```

Current Data Parameters
NAME      ML_20160901
EXPNO    71
PROCNO   1

F2 - Acquisition Parameters
Date_    20160901
Time     18.30
INSTRUM  DRX400
PROBHD   5 mm QNP 1H/13
PULPROG  cosygpf04
TD        65536
SOLVENT  CDCl3
NS        8
DS        8
SWH       4629.629 Hz
FIDRES    2.260561 Hz
AQ         0.2213420 sec
RG         5792.6
DM         108.000 usec
DE         6.00 usec
TE        297.8 K
D0         0.00000000 sec
D1         1.97000000 sec
D12        0.00000000 sec
D13        0.00000000 sec
D16        0.00021600 sec
IN0

----- CHANNEL f1 -----
NUC1      1H
P1        10.50 usec
PL1       -3.00 dB
SFO1     400.1324359 MHz

----- GRADIENT CHANNEL -----
GPNAM1    SINE.100
GPNAM2    SINE.100
GPNAM3    SINE.100
GRZ1      16.00 %
GRZ2      12.00 %
GRZ3      40.00 %
F16       1000.00 usec

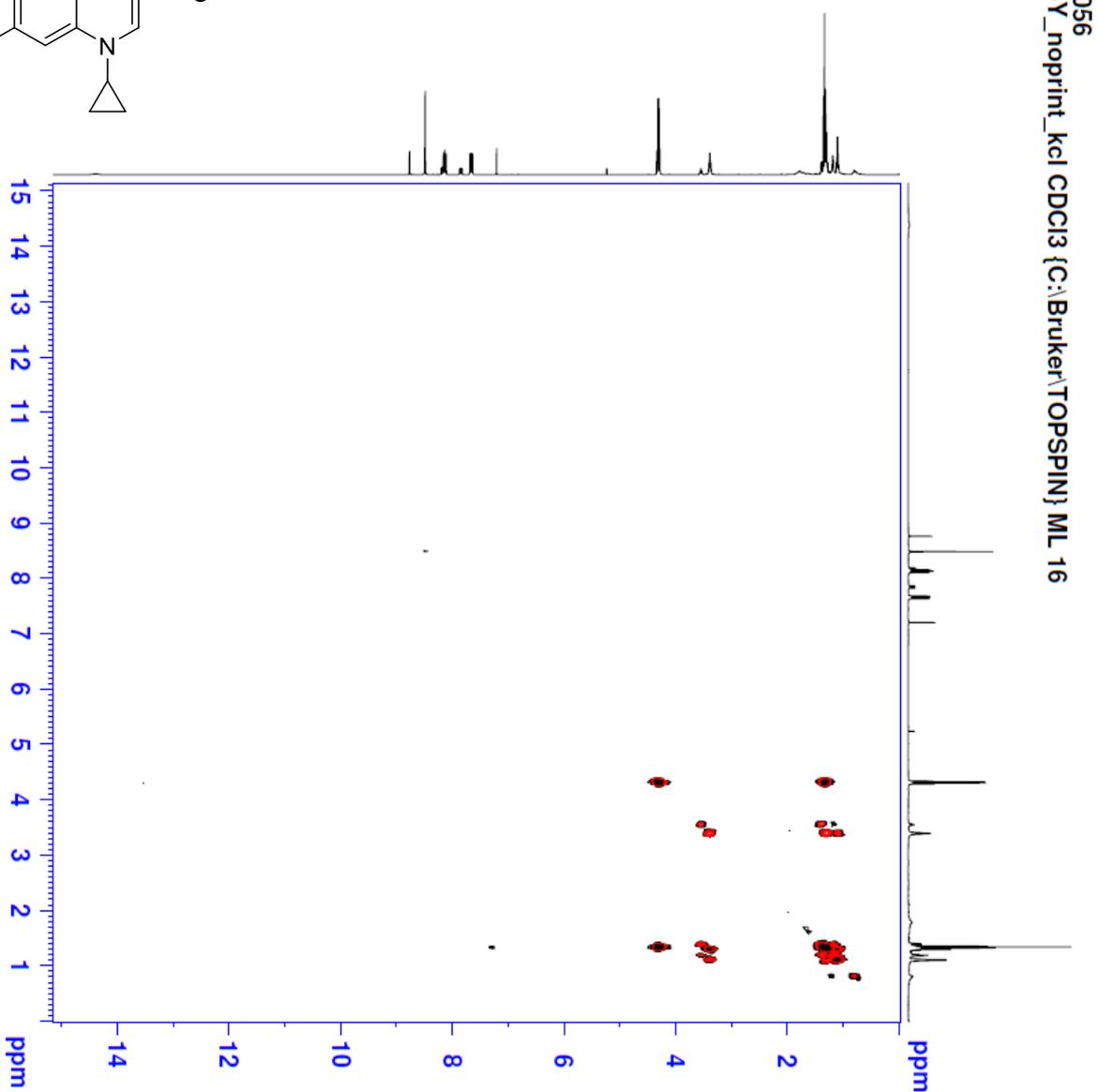
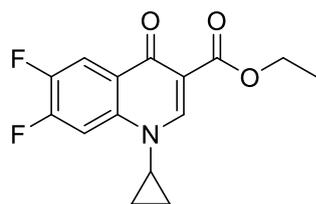
F1 - Acquisition Parameters
ND0        1
TD         128
SFO1     400.1324 MHz
FIDRES    36.168980 Hz
SW        11.570 ppm
FHM000    OF

F2 - Processing parameters
SI         1024
SF        400.1300390 MHz
WDW        SINE
SSB        0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
SF        400.1300390 MHz
WDW        SINE
SSB        0.00 Hz
GB         0
PC         1.40
  
```



Figure S79. COSY spectrum of compound 3a.



AF-056
 COSY_noprint_kci CDC13 {C:\Bruker\TOPSPIN} ML 16



```

Current Data Parameters
NAME      ML_20160902
EXPNO    41
PROCNO   1

F2 - Acquisition Parameters
Date_    20160902
Time     14:14
INSTRUM  DSI400
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       2
DS       8
SWH      6067.961 Hz
FIDRES   2.962872 Hz
AQ       0.1688876 sec
RG       512.46
RW       82.400 ussec
DM       297.5 K
TE       0.00000300 sec
D0       2.02334690 sec
d13      0.00000400 sec
d16      0.00020000 sec
IN0      0.00016480 sec

----- CHANNEL f1 -----
NUC1     1H
P1       10.50 ussec
PL1      0.00 dB
SFO1     400.1330962 MHz

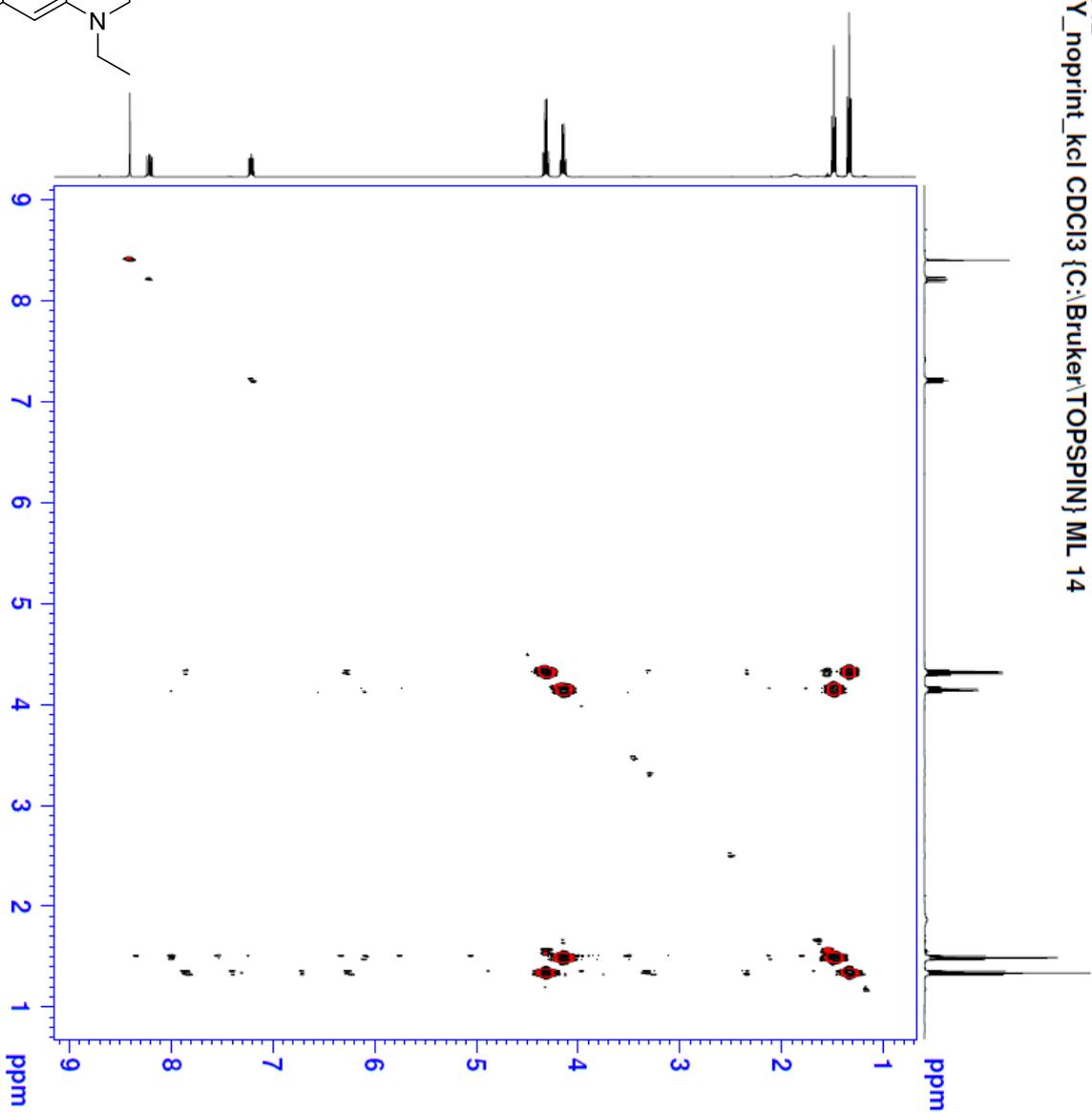
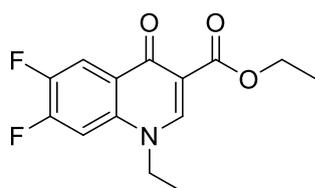
----- GRADIENT CHANNEL -----
GENNAM1 SINE.100
SINE.100
GENNAM2 SINE.100
SINE.100
GENNAM3 SINE.100
SINE.100
GPZ1    16.00 %
GPZ2    12.00 %
GPZ3    40.00 %
P16     1000.00 ussec

F1 - Acquisition parameters
NUC0     13C
TD       65536
SFO1     400.1331 MHz
FIDRES   47.405945 Hz
SW       15.165 ppm
FNUMODE  QF

F2 - Processing parameters
SI       1024
SF       400.1300315 MHz
WDW      SINE
SSB      0
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
MC2      QF
SF       400.1300315 MHz
WDW      SINE
SSB      0
GB       0
PC       0
  
```

Figure S80. COSY spectrum of compound 3b.



AF-042
 COSY_noprint_kcl CDCl3 {C:\Bruker\TOPSPIN} ML 14



```

Current Data Parameters
NAME          ML_20180902
EXPNO        21
PROCNO       1
F2 - Acquisition Parameters
Date_        20160902
Time         13.41
INSTRUM     DRX400
PROBHD      5 mm QNP 1H/13
PULPROG     cosyprf1qt
TD          2048
SOLVENT     CDCl3
DS          8
SMH         3387.534 Hz
FIDRES      1.654069 Hz
AQ          0.3024824 sec
RG          3649.1
DE          147.600 usec
TE          297.2 K
D0          0.0000200 sec
d13         0.8000400 sec
d16         0.0002000 sec
IN0         0.00029520 sec

----- CHANNEL f1 -----
NUC1        1H
P1          10.50 usec
PL1         -3.00 dB
SFO1        400.1319945 MHz

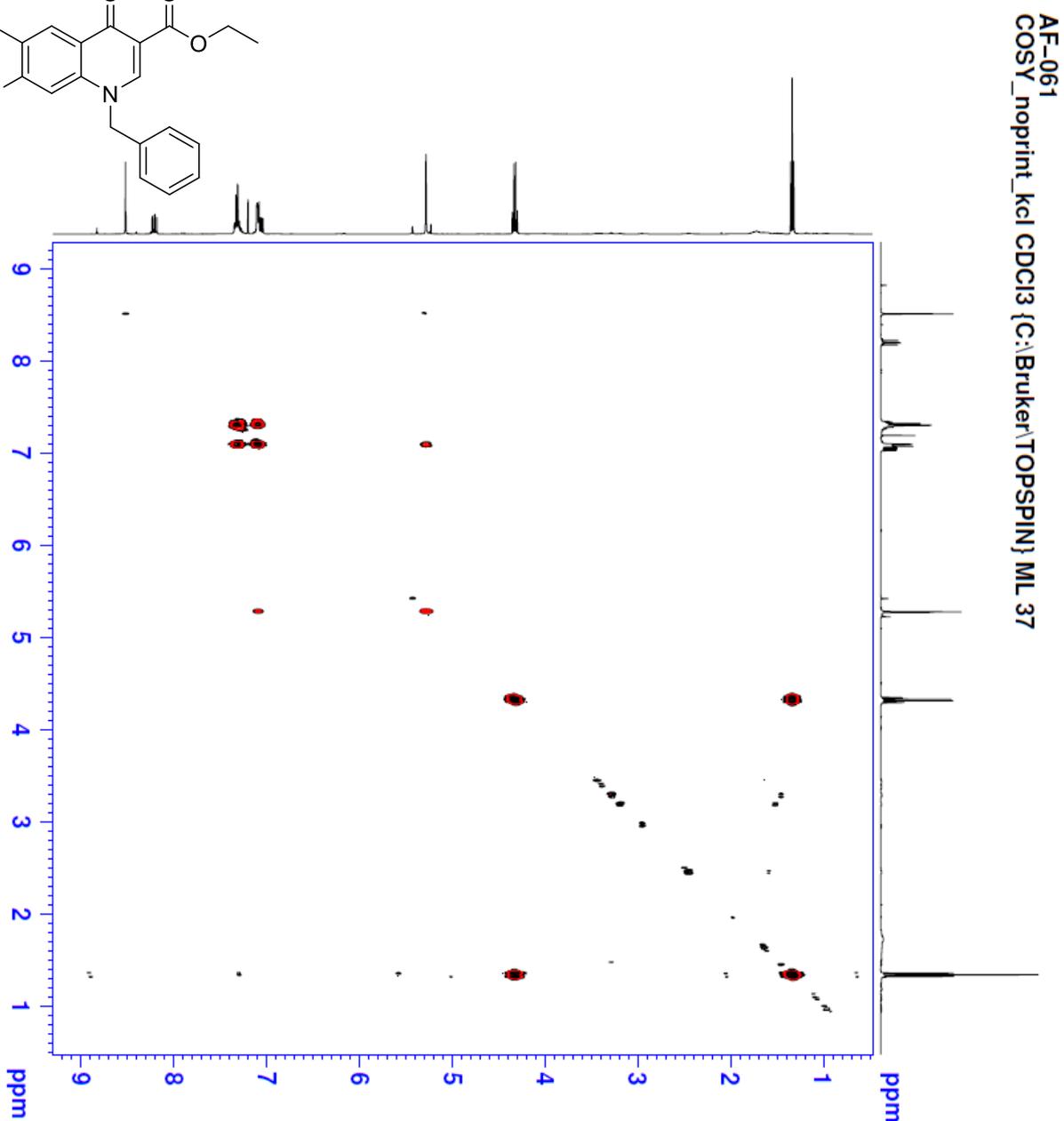
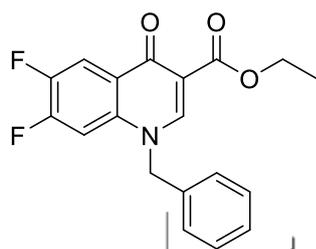
----- GRADIENT CHANNEL -----
GPNAM1      SINE.100
GPNAM2      SINE.100
GPNAM3      SINE.100
GPZ1        16.00 %
GPZ2        12.00 %
GPZ3        40.00 %
P16         1000.00 usec

F1 - Acquisition Parameters
ND0         1
TD          128
SFO1        400.1319945 MHz
SI          26.463142
SI0RES      8.400
FHM0DE     QF

F2 - Processing parameters
SI          1024
SF          400.1300301 MHz
WDW         SINE
SSB         0
LB          0.00 Hz
GB          0
PC          1.40

F1 - Processing parameters
SI          1024
MC2         QF
SF          400.1300301 MHz
WDW         SINE
SSB         0
LB          0.00 Hz
GB          0
  
```

Figure S81. COSY spectrum of compound 3c.



AF-061
 COSY_noprint_kcl CDCl3 {C:\Bruker\TOPSPIN} ML 37



```

Current Data Parameters
NAME      ML_20160901
EXPNO    61
PROCNO   1

F2 - Acquisition Parameters
Date_    20160901
Time     18.14
INSTRUM DRX400
PROBHD  5 mm QNP 1H/13
PULPROG cosygmrgf
TD       2048
SOLVENT CDCl3
NS       8
DS       2
SWH      3531.073 Hz
FIDRES  1.724157 Hz
AQ       0.2901884 sec
RG       3649.1
DE       141.600 usec
TE       297.9 K
D0       0.00000300 sec
D1       1.90046704 sec
d13      0.00000400 sec
D16      0.00020000 sec
IN0      0.00028320 sec

----- CHANNEL f1 -----
NUC1     1H
P1       10.50 usec
PL1      -3.00 dB
SFO1     400.1319877 MHz

----- GRADIENT CHANNEL -----
GPNAM1   SINE.100
GPNAM2   SINE.100
GPNAM3   SINE.100
GP21     16.00 %
GP22     12.00 %
GP23     40.00 %
P16      1000.00 usec

F1 - Acquisition parameters
NUC0      13C
NUC1      1H
SFO0      100.628150 MHz
SFO1      400.132 MHz
FIDRES    27.586513 Hz
SW        8.825 ppm
FMODE    OF

F2 - Processing parameters
SI        1024
SF        400.1300348 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
EC        1.40

F1 - Processing parameters
SI        1024
MC2       OF
SF        400.1300348 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
    
```

AF-081
 COSY_noprint_kel CDCl3 (C:\Bruker\TOPSPIN) ML 43



Current Data Parameters
 NAME ML_20160901
 EXNO 121
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20160902
 Time 8:07
 INSTRUM DRX400
 PROBRD 5 mm QNP 1H/13
 PULPROG cosygprg4
 ID 2048
 SOLVENT CDCl3
 NS 8
 DS 8
 SWH 6009.615 Hz
 FIDRES 2.934382 Hz
 AQ 0.1705268 sec
 RG 3649.1
 DE 83.200 usac
 TE 297.2 K
 D0 0.00000300 sec
 D1 2.02129889 sec
 D12 0.00000400 sec
 D18 0.00020000 sec
 IN0 0.00016640 sec

CHANNEL f1
 NUC1 1H
 P1 10.50 usac
 PL1 -3.00 dB
 SFO1 400.131033 MHz

GRADIENT CHANNEL

GENAM1 SINE,100
 GENAM2 SINE,100
 GENAM3 SINE,100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 usac

F1 - Acquisition Parameters

NUC0 128
 TD 400.1313 MHz
 SFO1 46.950119 Hz
 SW 15.019 ppm
 F1MODE QF

F2 - Processing Parameters

SI 1024
 SF 400.1300349 MHz
 WDM SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 FC 1.40

F1 - Processing Parameters

SI 1024
 SF 400.1300349 MHz
 WDM SINE
 SSB 0
 LB 0.00 Hz
 GB 0

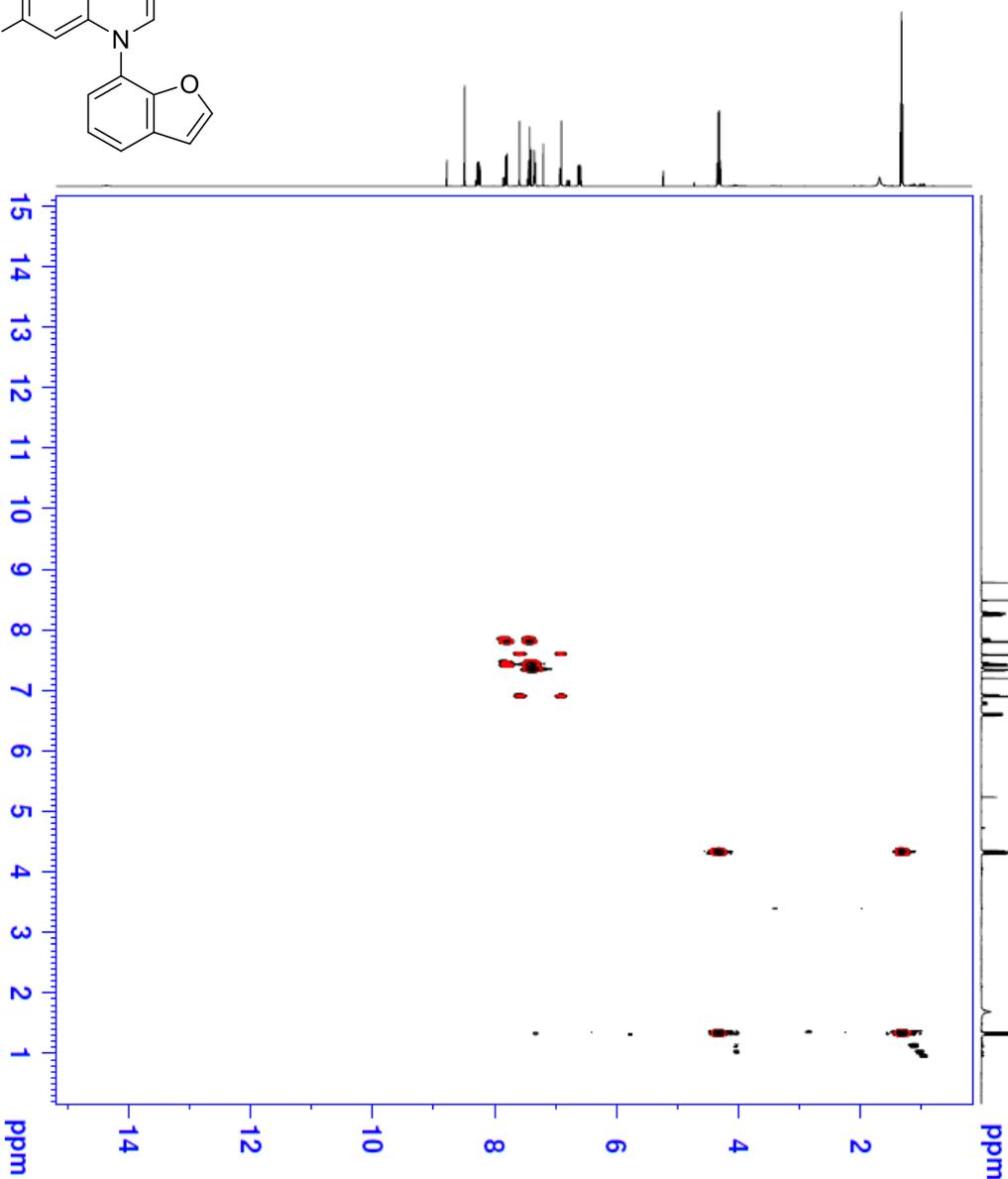
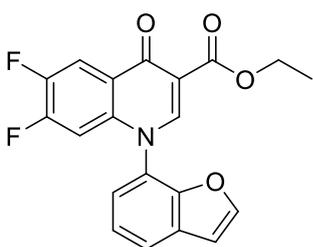
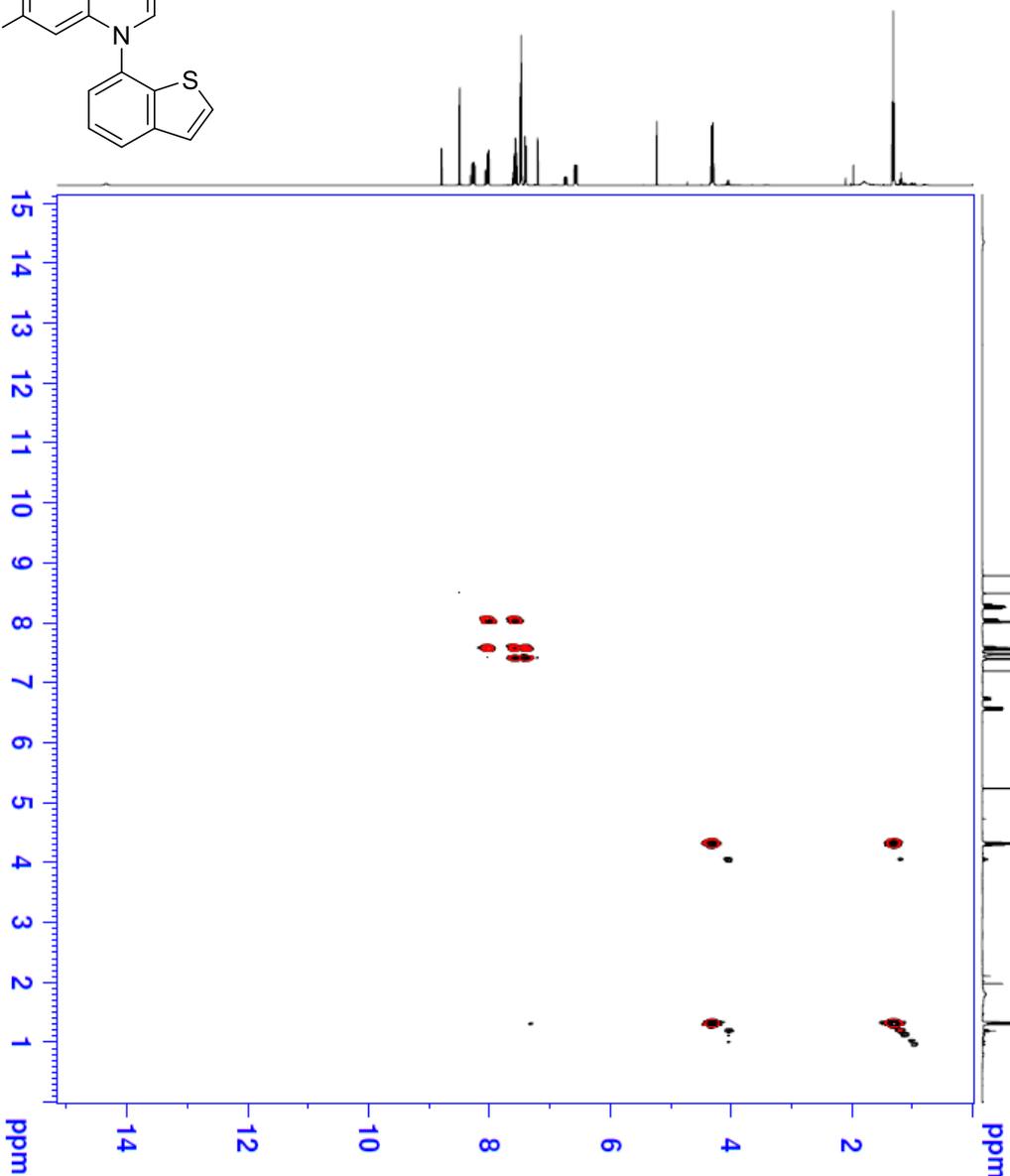
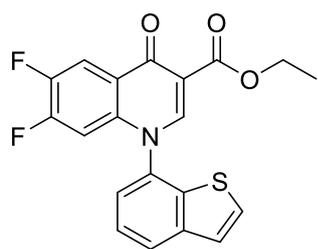


Figure S83. COSY spectrum of compound 3e.



AF-076
COSY_noprint_kci CDCI3 {C:\Bruker\TOPSPIN} ML 41



```

Current Data Parameters
NAME          ML_20160901
EXNO         101
PROCNO       1

F2 - Acquisition Parameters
Date_        20160902
Time         7.33
INSTRUM     DRX400
PROBHD      5 mm QNP 1H/13
PULPROG     cosygprqt
TD          2048
SOLVENT     CDCl3
NS          8
DS          4
SWH         6067.961 Hz
FIDRES     2.962872 Hz
AQ         0.1688876 sec
RG         5160.6
DW         82.400 usec
DE         6.00 usec
TE         297.1 K
D0         0.00000300 sec
D1         2.02334690 sec
D13        0.00000400 sec
D16        0.00020000 sec
IN0        0.00016480 sec

----- CHANNEL f1 -----
NUC1        13C
P1          10.50 usec
PL1         -3.00 dB
SFO1        400.130616 MHz

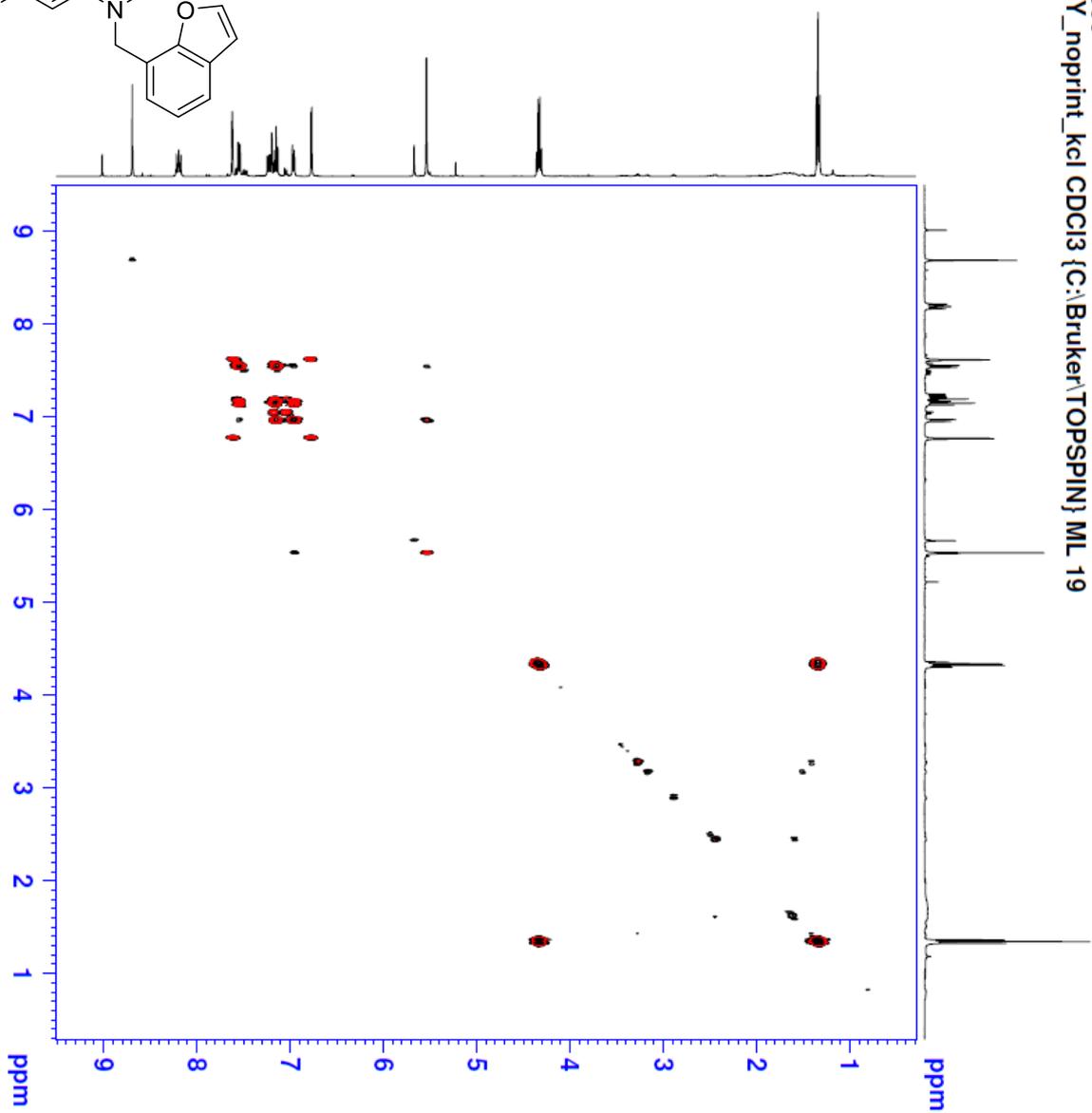
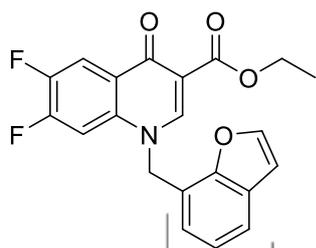
----- GRADIENT CHANNEL -----
GPNAM1     SINE.100
SINE1     SINE.100
GPNAM2     SINE.100
SINE2     SINE.100
GPNAM3     SINE.100
SINE3     SINE.100
GPZ1       16.00 %
GPZ2       12.00 %
GPZ3       40.00 %
F16        1000.00 usec

F1 - Acquisition parameters
NUC0        13C
TD          128
SFO1        400.1331 MHz
FIDRES     47.405945 Hz
SW         15.165 ppm
FNUC0      OF

F2 - Processing parameters
SI          1024
SF          400.1300351 MHz
WDW         SINE
SSB         0
LBB         0.00 Hz
GB          0
PC          1.40

F1 - Processing parameters
SI          1024
MC2         OF
SF          400.1300351 MHz
WDW         SINE
SSB         0
LBB         0.00 Hz
GB          0
    
```

Figure S84. COSY spectrum of compound 3f.



AF-069
 COSY_noprint_kcl CDC13 {C:\Bruker\TOPSPIN} ML 19



```

Current Data Parameters
NAME      ML_20160902
EXPNO    71
PROCNO   1

F2 - Acquisition Parameters
Date_    20160902
Time     15.16
INSTRUM  DRX400
PROBHD   5 mm QNP 1H/13
PULPROG  cosyprmg4
SOLVENT  CDCl3
NS       2
DS       8
SWH      3687.316 Hz
FIDRES   1.800447 Hz
AQ       0.2778944 sec
RG       3649.1
DE       135.600 usec
TE       297.2 K
NUC1     13C
NUC2     1H
P1       10.50 usec
P11      -3.00 dB
SFO1     400.131942 MHz

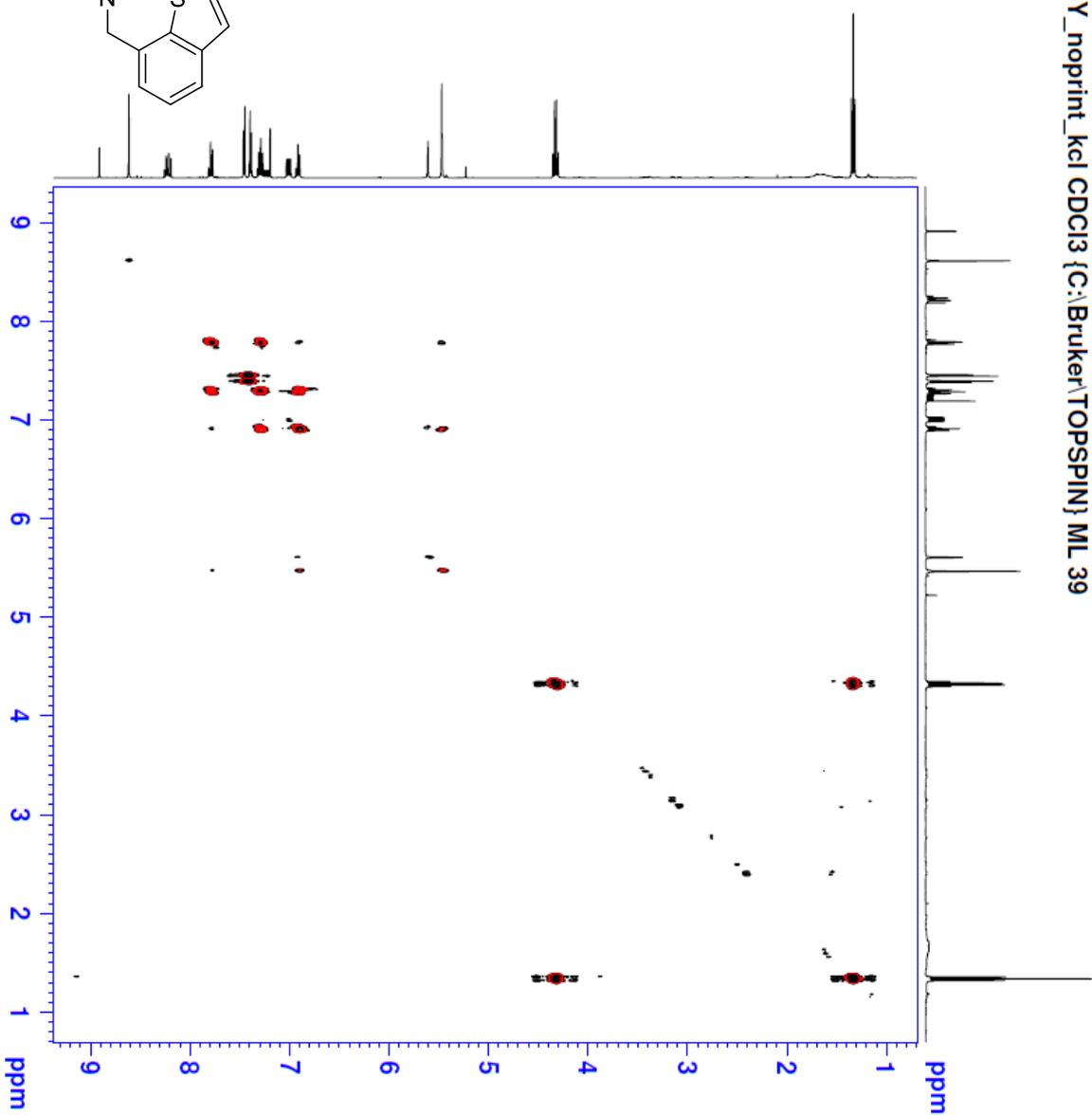
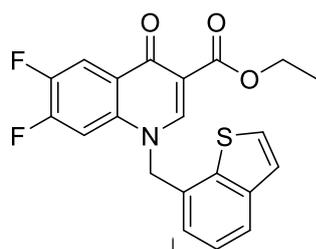
GRADIENT CHANNEL
GRNAM1   G1
GRNAM2   SINE:100
GRNAM3   SINE:100
GPZ1     16.00 %
GPZ2     12.00 %
GPZ3     40.00 %
P16      1000.00 usec

F1 - Acquisition parameters
ND0      1
TD        128
SFO1     400.132 MHz
SI        28.80
SFIDRES  9.740 ppm
FMODE    QP

F2 - Processing parameters
SI        1024
SF        400.1300357 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
FC        1.40

F1 - Processing parameters
SI        1024
MC2       OF
SF        400.1300357 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
  
```

Figure S85. COSY spectrum of compound 3g.



AF-063
 COSY_noprint_kcl CDCl3 {C:\Bruker\TOPSPIN} ML_39



Current Data Parameters
 NAME ML_2016092
 EXPNO 81
 FPROGNO 1

F2 - Acquisition Parameters

Date_ 20160902
 Time 16.09
 INSTRUM DRX400
 PROBRD 5 mm QNP 1H/13
 PULPROG cosygpmrf
 ID 2048
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 3472.222 Hz
 FIDRES 1.656421 Hz
 AQ 0.2951060 sec
 RG 3649.1
 DM 144.000 usec
 DE 6.00 usec
 TE 297.5 K
 D0 0.00000300 sec
 D1 1.89637101 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00028800 sec

CHANNEL F1
 NUC1 1H
 P1 10.50 usec
 PL1 -3.00 dB
 SFO1 400.1320480 MHz

GRADIENT CHANNEL

GNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GRZ1 16.00 %
 GRZ2 42.00 %
 GRZ3 40.00 %
 F16 1000.00 usec

F1 - Acquisition Parameters

ND0 128
 TD 128
 SFO1 400.132 MHz
 FIDRES 27.126736 Hz
 SW 8.678 ppm
 FPMODE QF

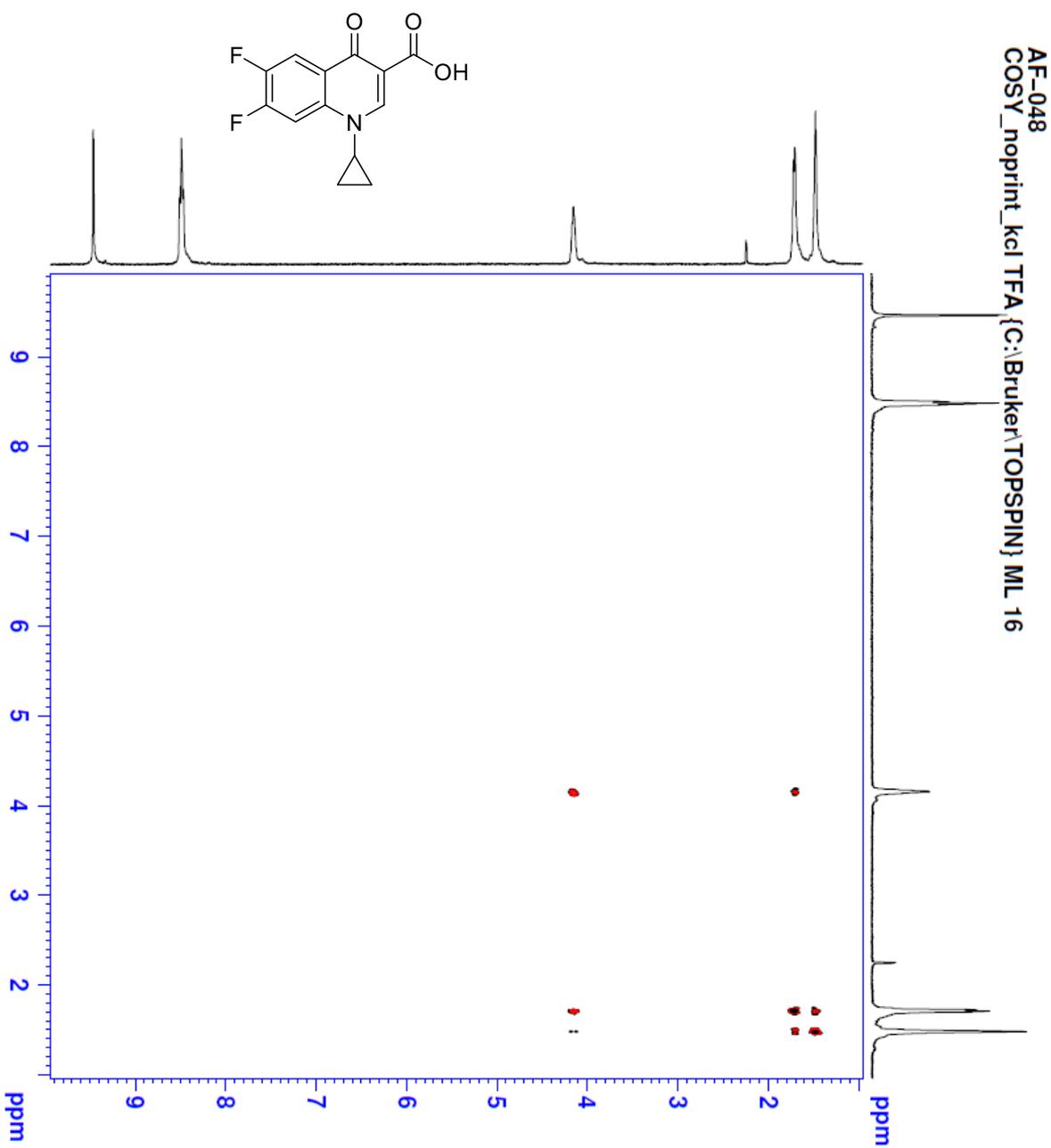
F2 - Processing parameters

SI 400.1301324 MHz
 KW 400.1301324 MHz
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters

SI 1024
 MC2 QF
 SF 400.1300362 MHz
 KW 400.1300362 MHz
 SSB 0
 LB 0.00 Hz
 GB 0

Figure S86. COSY spectrum of compound 4a.



```

Current Data Parameters
NAME      ML_20161118
EXPNO     21
PROCNO    1

F2 - Acquisition Parameters
Date_     20161119
Time      10:41:19
INSTRUM   spect
PROBHD    5 mm QNP 1H/13
PULPROG   cosyprnfdf
TD         2048
SOLVENT   TFA
NS         4
DS         8
SWH        3591.954 Hz
FIDRES     1.753884 Hz
AQ         0.282708 sec
RG         369.21
DM         139.400 usec
DE         293.0 K
TE         0.00000300 sec
D0         1.90661097 sec
d13        0.00000400 sec
d16        0.00020000 sec
INVO       0.00027840 sec

----- CHANNEL f1 -----
NUC1       13C
P1         10.50 usec
PL1        -1.00 dB
SFO1       400.1321719 MHz

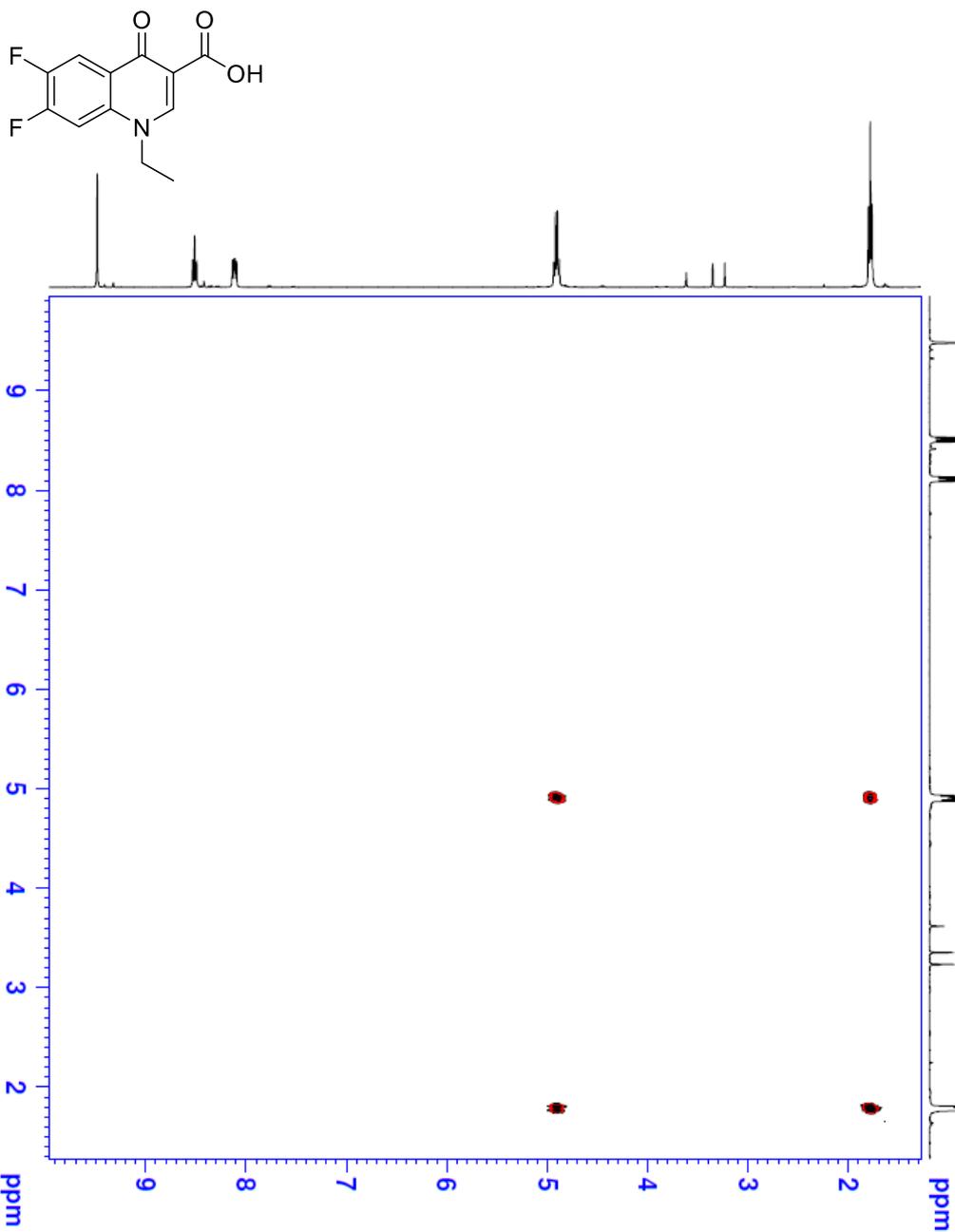
----- GRADIENT CHANNEL -----
GRNAM1     SINE.100
GRNAM2     SINE.100
GRNAM3     SINE.100
GRZ1       16.00 %
GRZ2       12.00 %
GRZ3       40.00 %
P16        1000.00 usec

F1 - Acquisition parameters
NUC1       13C
NUC2       1H
SFO1       400.1321719 MHz
SFO2       400.1321719 MHz
FIDRES     28.062144 Hz
SWH        8.977 ppm
FMODE      QF

F2 - Processing parameters
SI         1024
SF         400.1300000 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         400.1300000 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
  
```

AF-043
 COSY_noprint_kcl TFA {C:\Bruker\TOPSPIN} ML 15



BRUKER

```

Current Data Parameters
NAME      ML_20161118
EXPNO    11
PROCNO   1

F2 - Acquisition Parameters
Date_    20161119
Time     10.23
INSTRUM  DRX400
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  TFA
NS        274
DS        4
SWH       3472.222 Hz
FIDRES    1.695421 Hz
AQ        0.2951060 sec
RG        5792.6
DM        144.000 usec
DE        6.00 usec
TE        293.7 K
D0        0.00000300 sec
d13       1.0000140 sec
d17       0.00020000 sec
d16       0.00028800 sec
IN0       0.00028800 sec

----- CHANNEL f1 -----
NUC1      1H
P1        10.50 usec
PL1       -3.00 dB
SFO1     400.1322468 MHz

----- GRADIENT CHANNEL -----
GGRNAM1  SINE.100
GGRNAM2  SINE.100
GGRNAM3  SINE.100
GCZ1     12.00 %
GCZ2     12.00 %
GCZ3     40.00 %
PL6      1000.00 usec

F1 - Acquisition parameters
ND0      1
TD        128
SFO1     400.1322 MHz
FIDRES    27.126736 Hz
SM        8.678 ppm
FNM0DE   QF

F2 - Processing parameters
SI        32768
SF        400.130000 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
WC2       QF
SF        400.130000 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
  
```

Figure S87. COSY spectrum of compound 4b.

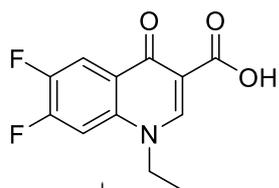


Figure S88. COSY spectrum of compound 4c.

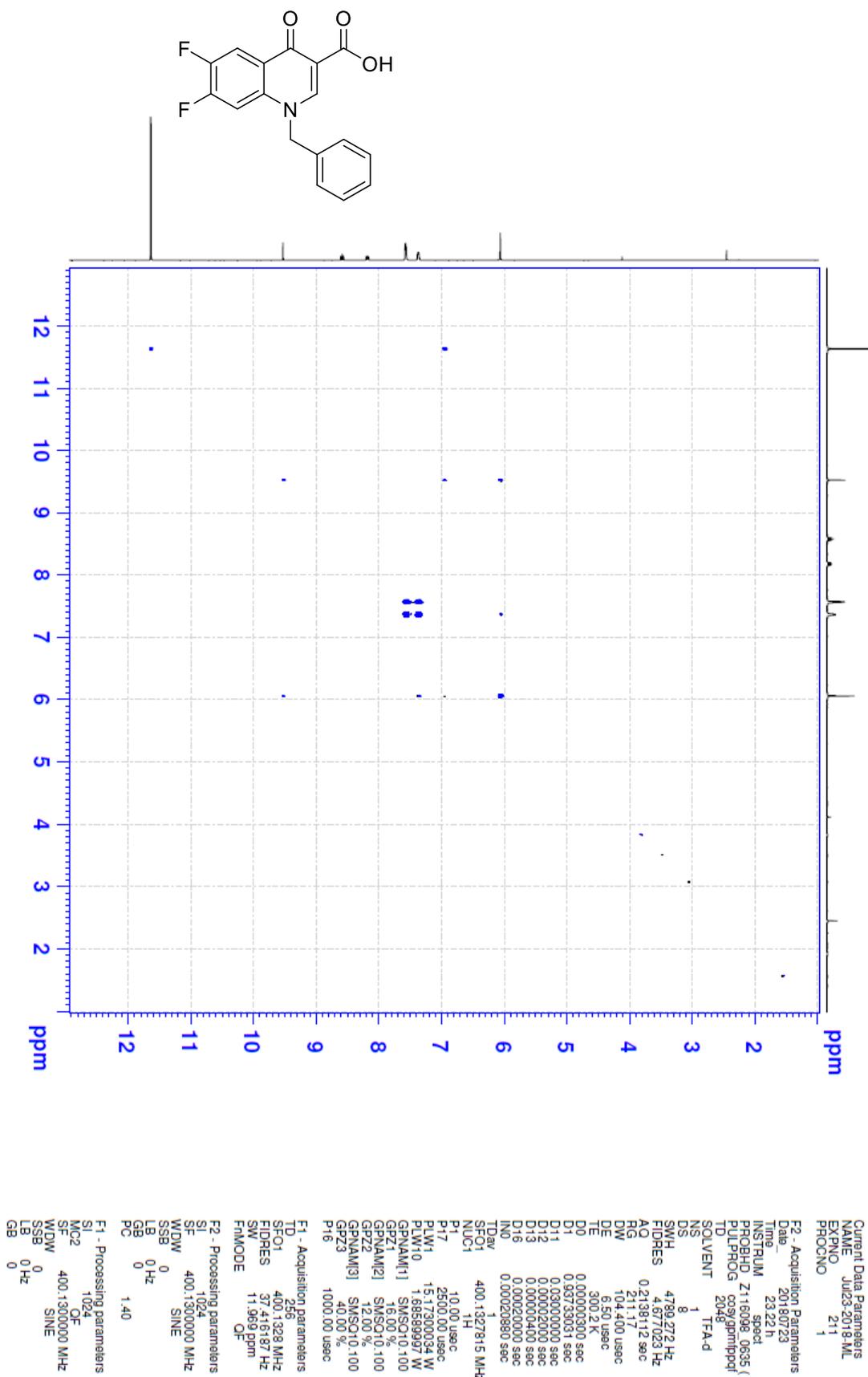


Figure S89. COSY spectrum of compound 4d.

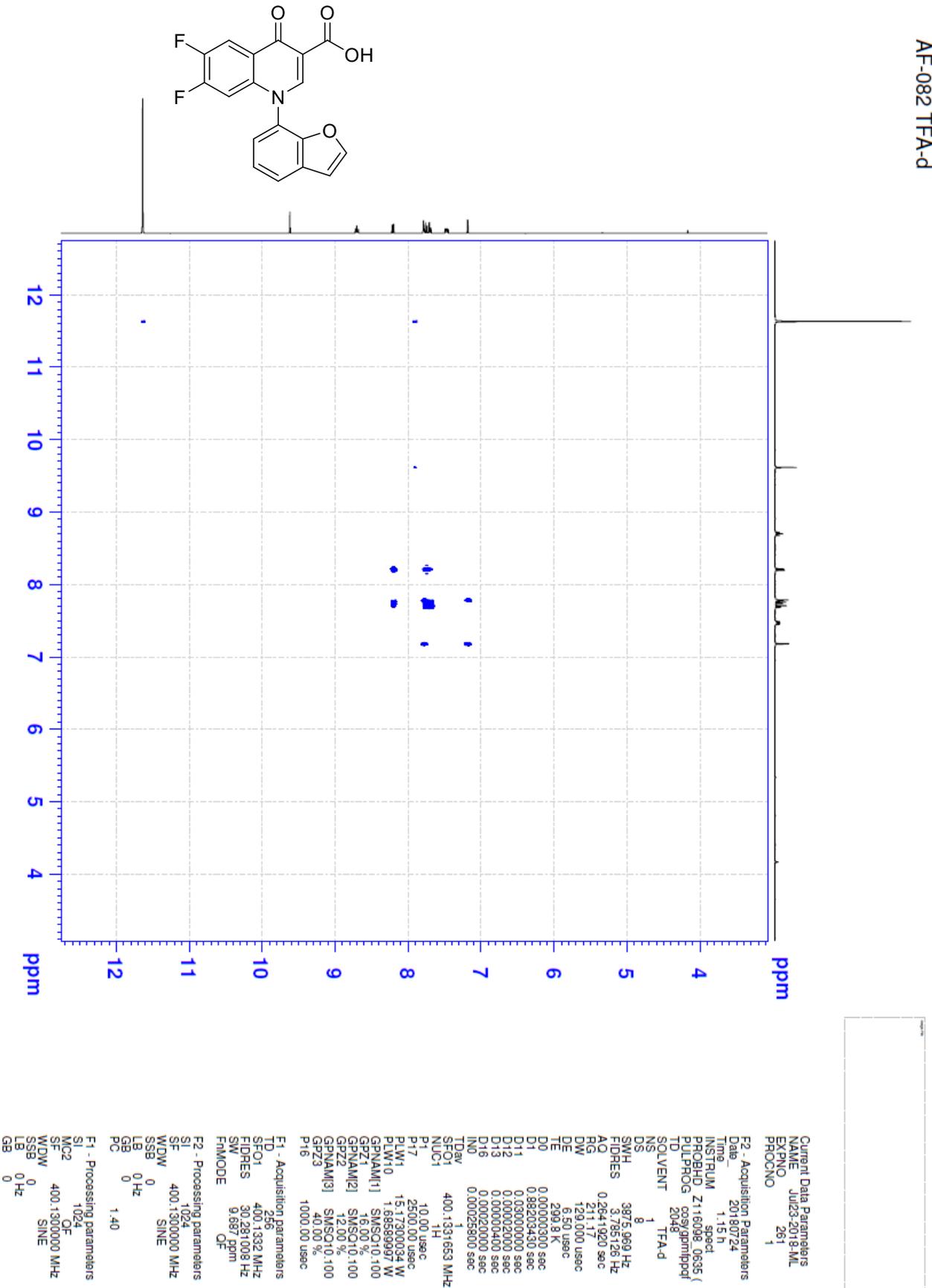


Figure S90. COSY spectrum of compound 4e.

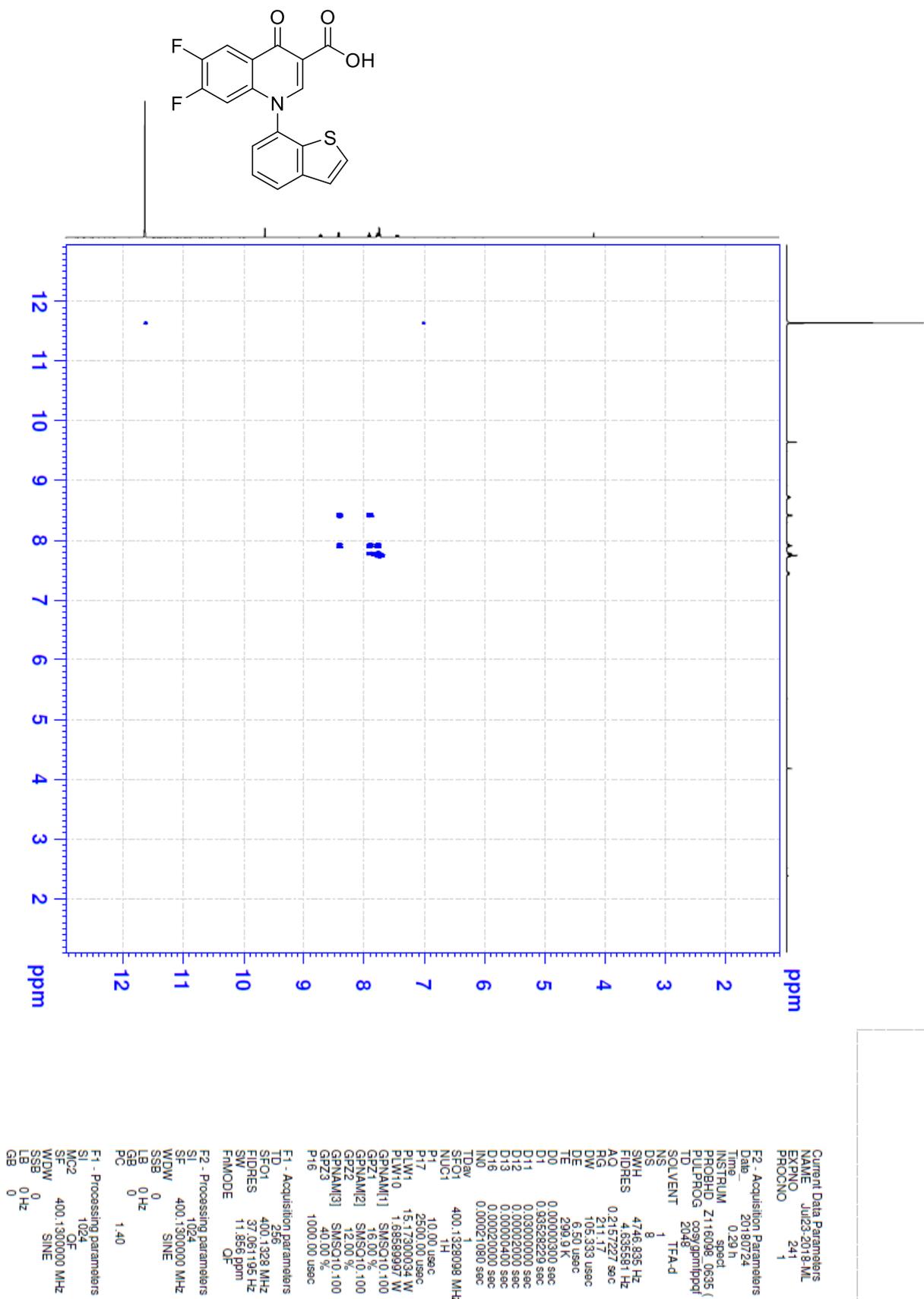


Figure S91. COSY spectrum of compound 4f.

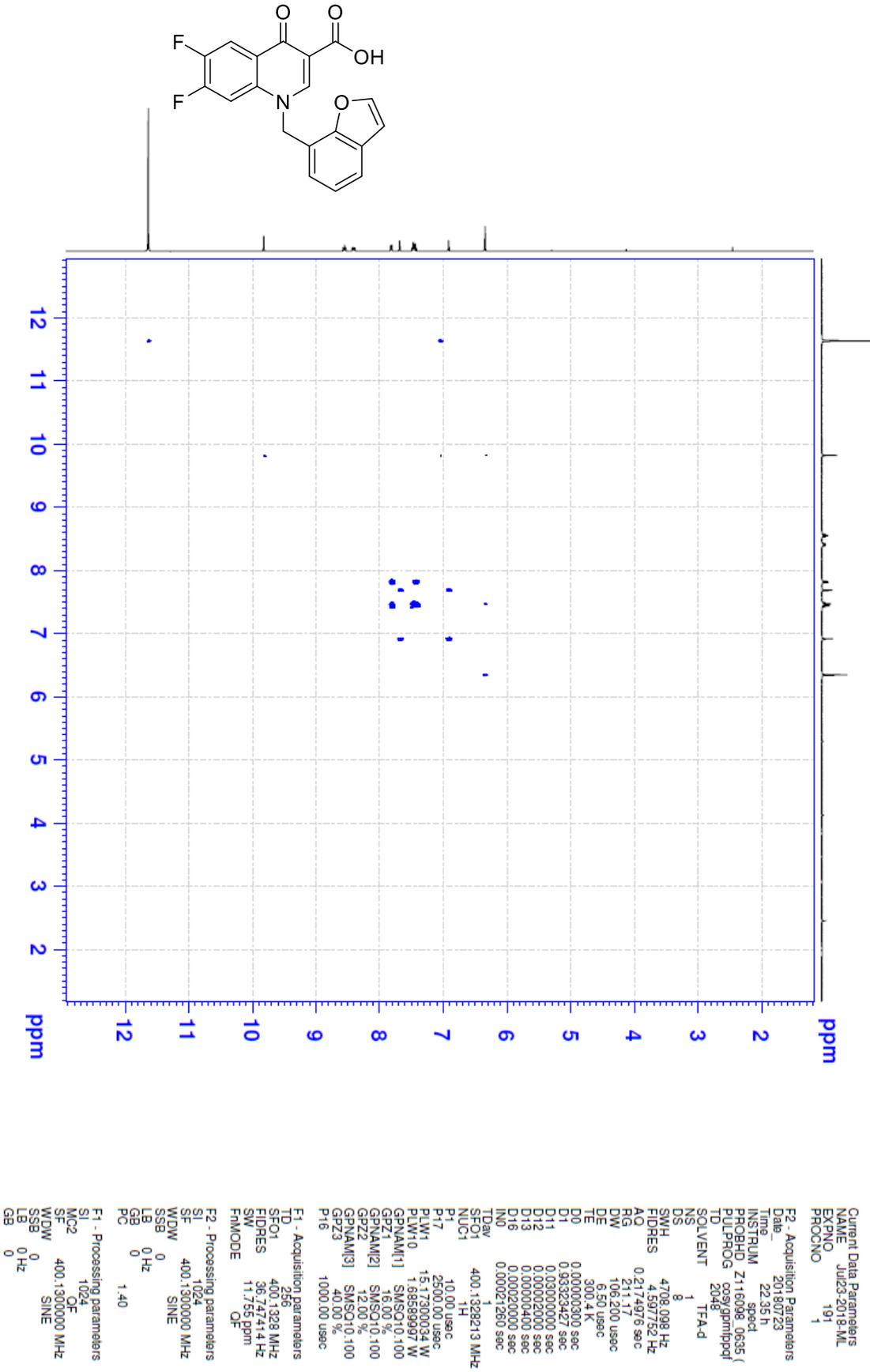
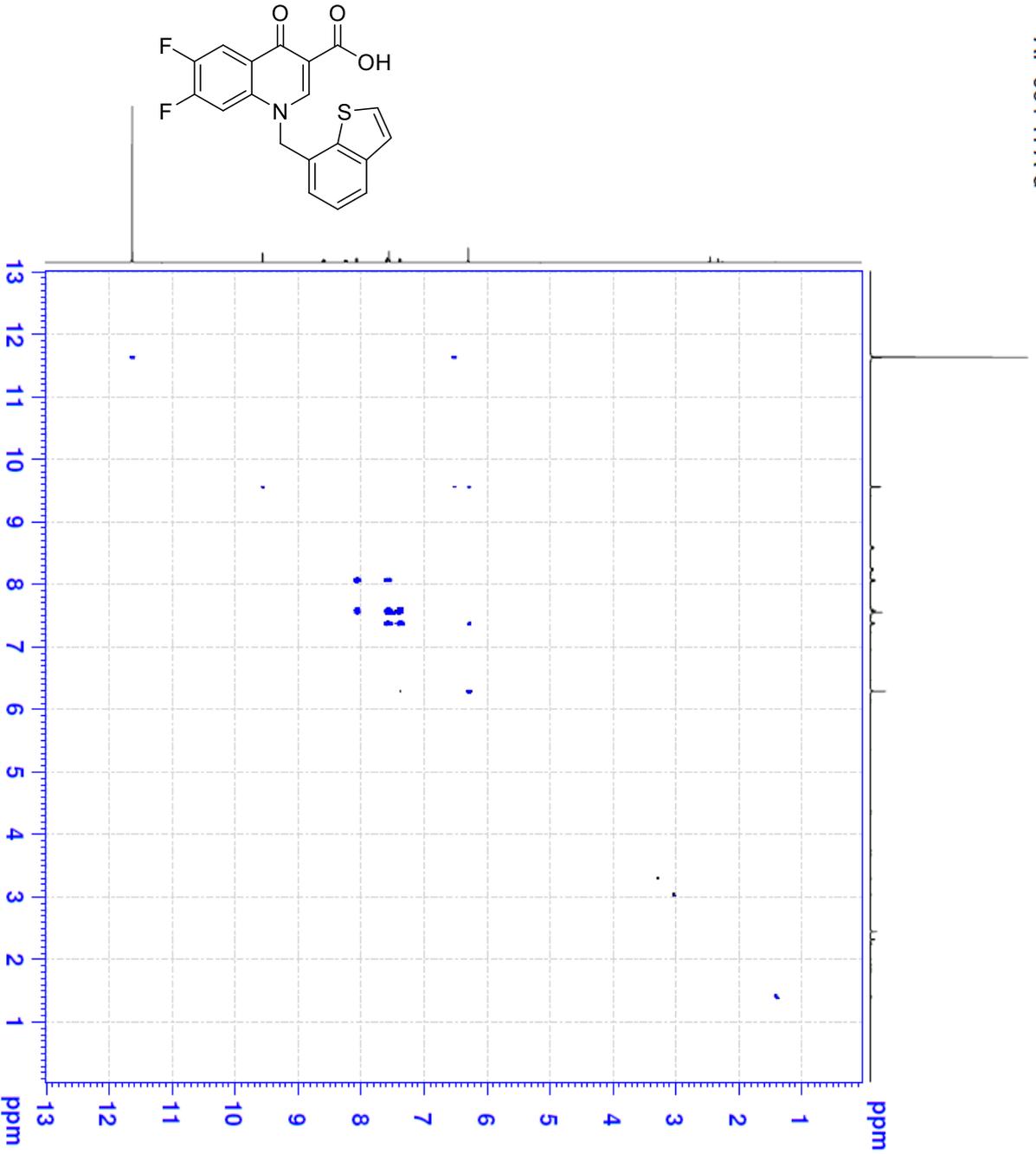


Figure S92. COSY spectrum of compound 4g.



Current Data Parameters
 NAME Jun23-2018-MIL
 EXPNO 171
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180723
 Time 21:48:11
 INSTRUM spect
 PROBRD Z116098_0635 (PILPROG
 PULPROG zgpgm3ppp)
 TD 2048
 SOLVENT 1 TFA-d
 NS 8
 DS 8
 SMH 51.07 505 Hz
 FIDRES 6.0756991 Hz
 AQ 0.1870176 sec
 RG 211.17
 DW 96.200 usec
 DE 6.50 usec
 TE 300.9 K
 D0 0.00000300 sec
 D1 0.03000000 sec
 D12 0.00002000 sec
 D15 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00019240 sec
 TDSW 400.1326110 MHz
 SFO1 400.1326110 MHz
 NUC1 1H
 P1 10.00 usec
 P17 2500.00 usec
 PLW1 15.17300094 W
 PLW10 1.58689907 W
 GPNAM[1] SMSO10:100
 GPNAM[2] SMSO10:100
 GPNAM[3] SMSO10:100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 256
 SFO1 400.1326 MHz
 FIDRES 40.605511 Hz
 SW 12.969 ppm
 FMODE OF

F2 - Processing parameters
 SI 1024
 SF 400.1300000 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 OF SINE
 SF 400.1300000 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0

Figure S93. COSY spectrum of compound 5a.

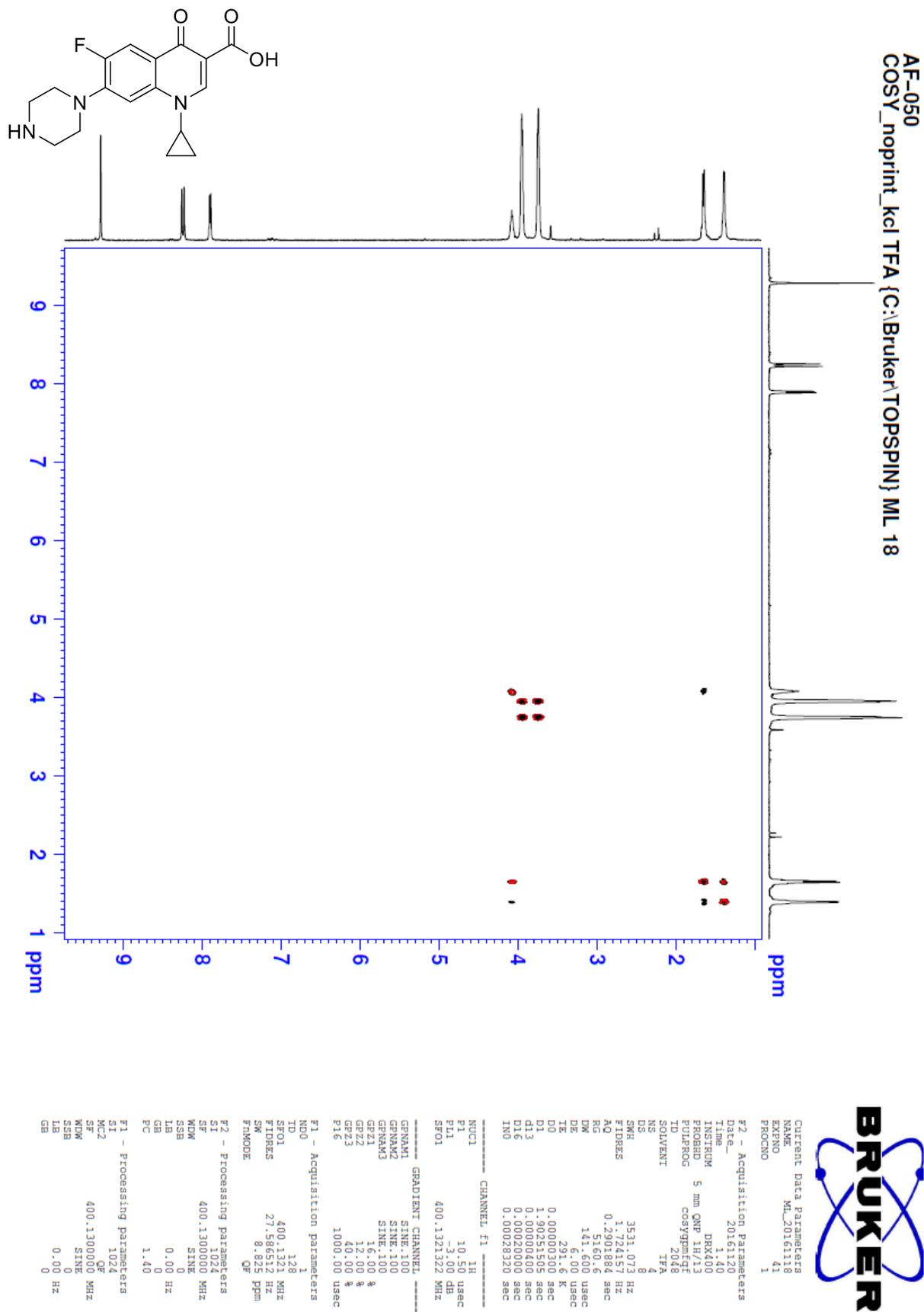
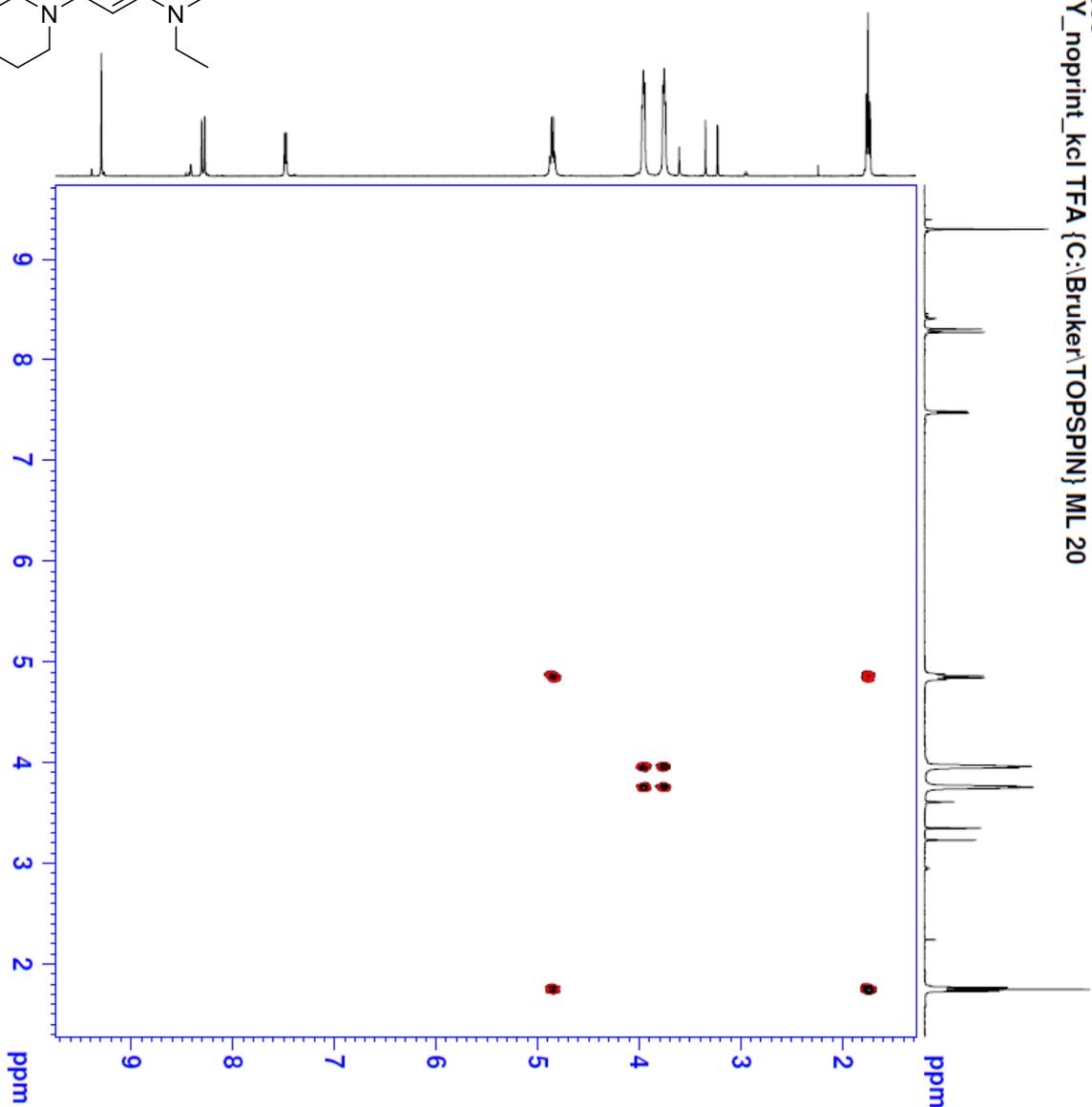
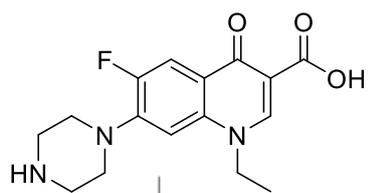


Figure S94. COSY spectrum of compound 5b.



AF-055
COSY_noprint_kcl TFA {C:\Bruker\TOPSPIN} ML 20



Current Data Parameters
NAME ML_20161118
EXNO 61
PROCNO 1

F2 - Acquisition Parameters

Date_ 20161120
Time 10:42
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
ID cosygpmfdrf
SOLVENT TFA
NS 4
DS 8
SWH 3387.534 Hz
FIDRES 1.554069 Hz
AQ 0.3024824 sec
RG 47.9912
RQ 147.600 usec
DM 5.00
TE 293.7 K
D0 0.00000300 sec
D1 1.89022696 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00029520 sec

CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 400.132032 MHz

GRADIENT CHANNEL

GPRAMA1 SINE.100
GPRAMA2 SINE.100
GPRAMA3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
F16 1000.00 usec

F1 - Acquisition parameters

ND0 1
TD 128
SFO1 400.1322 MHz
FIDRES 26.465109 Hz
SW 8.466 ppm
FMODE QF

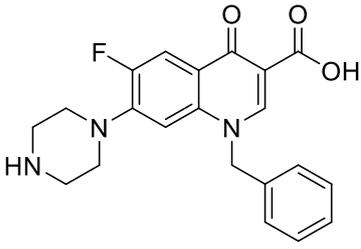
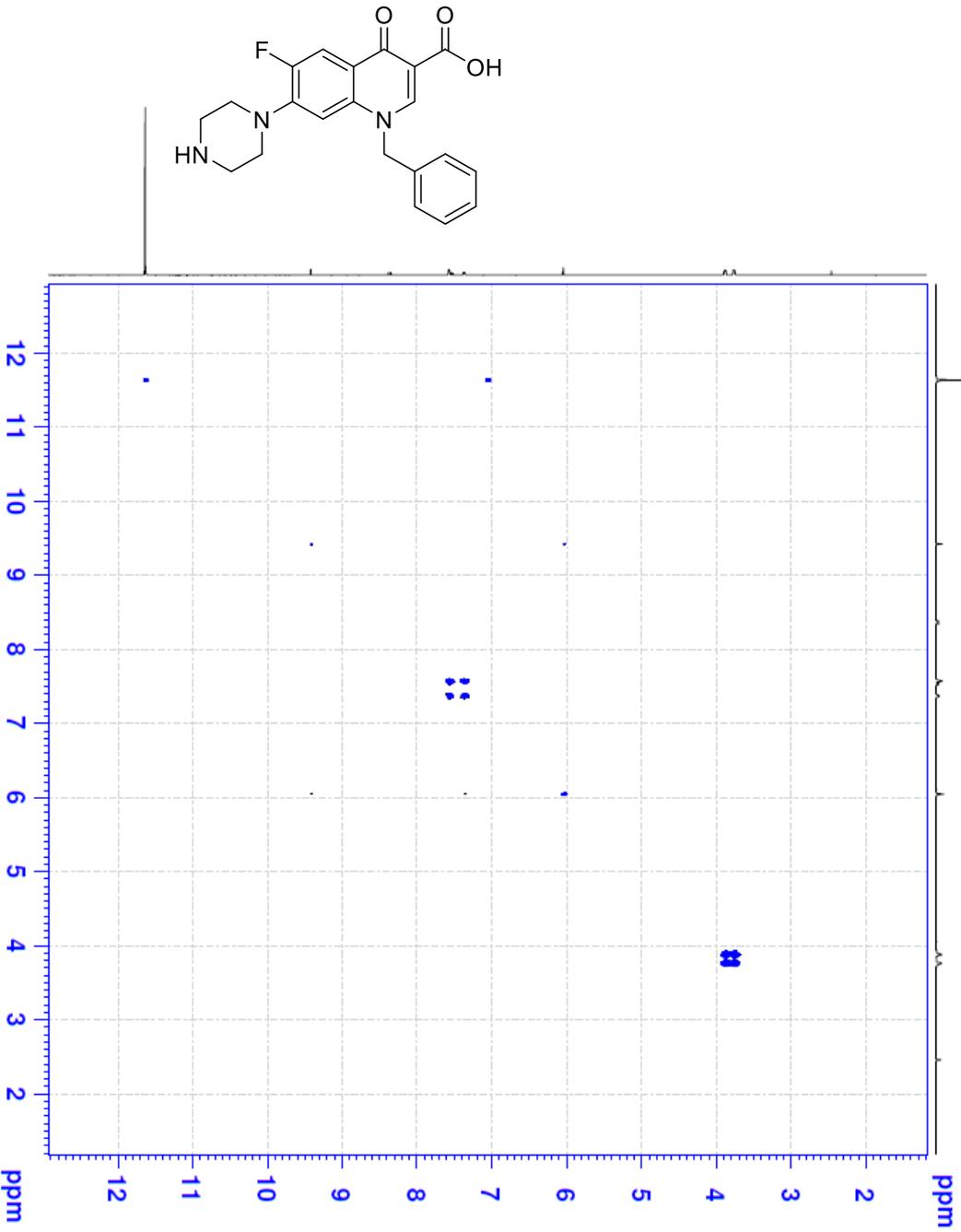
F2 - Processing parameters

SI 400.130000 MHz
MHZ 400.130000 MHz
SINE SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 QF
SF 400.1300000 MHz
KHZ 400.130000 MHz
SINE SINE
LB 0.00 Hz
GB 0

Figure S95. COSY spectrum of compound 5c.



Current Data Parameters
 NAME: J023-2019-ML
 EXPNO: 221
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20180223
 Time: 23:43:11
 INSTRUM: spect
 PROBHD: Z116098_06395 (cosy,gpmi1ppf)
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: TFA-d
 NS: 8
 DS: 4
 SWH: 4708.098 Hz
 FIDRES: 4.597782 Hz
 AQC: 0.2174976 sec
 RG: 327.177
 DW: 108.200 usec
 DE: 6.50 usec
 TE: 300.1 K
 D0: 0.0000390 sec
 DD: 0.0000000 sec
 D1: 0.0300000 sec
 D12: 0.0000200 sec
 D13: 0.0000400 sec
 D16: 0.0002000 sec
 IN0: 0.00021260 sec

TDav: 1
 SFO1: 400.1329214 MHz
 NUC1: ¹H
 P1: 10.00 usec
 P17: 2500.00 usec
 PLW1: 15.17300034 W
 GPNAM1: 1.68589997 W
 SWSO1: 10.100
 GPNAM2: 16.00 %
 SWSO2: 10.100
 GPNAM3: 12.00 %
 SWSO3: 10.100
 GPZ3: 40.00 %
 P16: 1000.00 usec

F1 - Acquisition parameters
 TD: 256
 SFO1: 400.1328 MHz
 FIDRES: 36.74714 Hz
 SW: 11.755 ppm
 FMODE: OF

F2 - Processing parameters
 SI: 1024
 SF: 400.1300000 MHz
 WDW: SINE
 SSB: 0
 LB: 0 Hz
 GB: 0
 PC: 1.40

F1 - Processing parameters
 SI: 1024
 SF: 400.1300000 MHz
 WDW: SINE
 SSB: 0
 LB: 0 Hz
 GB: 0

Figure S96. COSY spectrum of compound 5d.

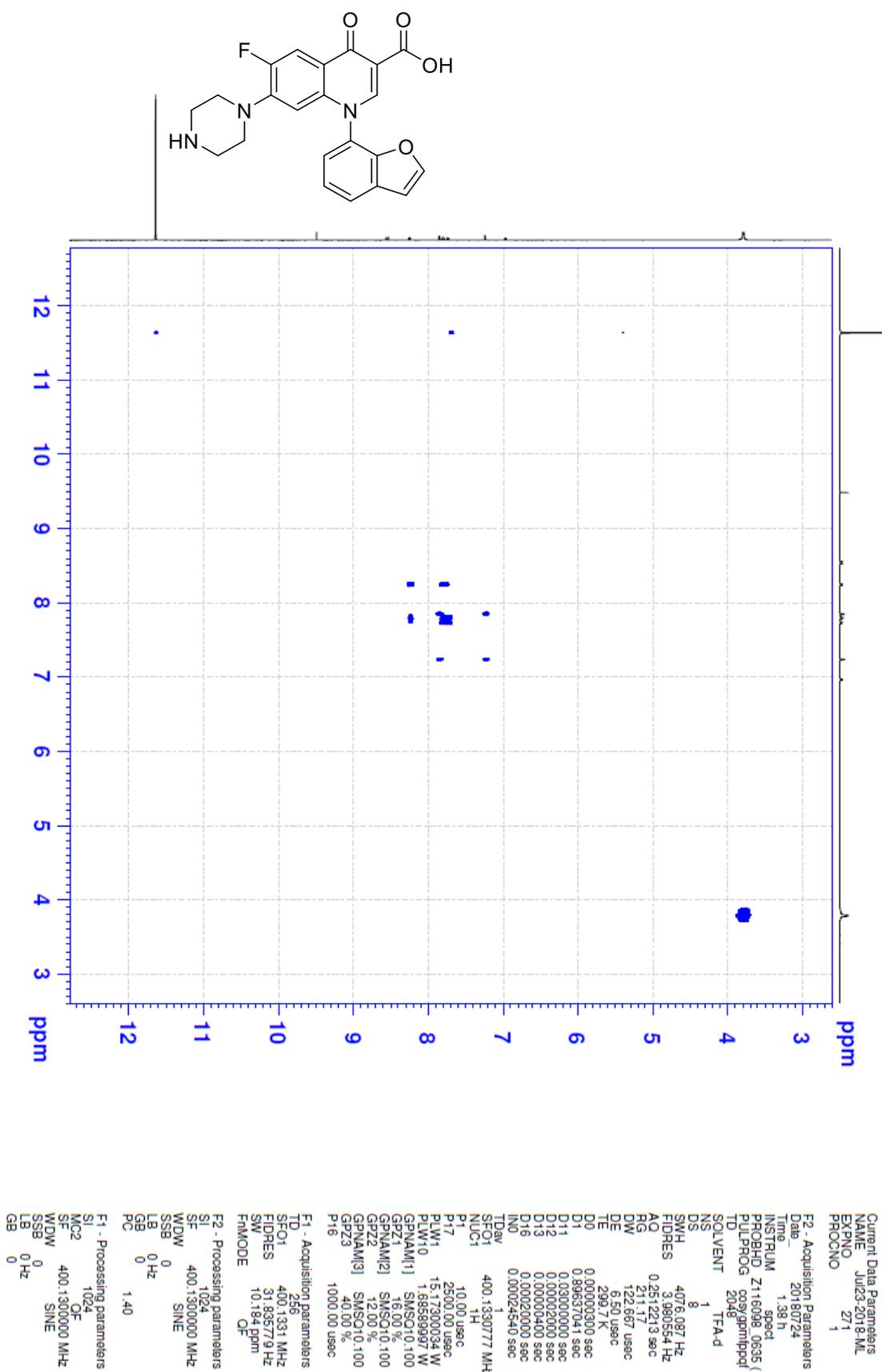


Figure S97. COSY spectrum of compound 5e.

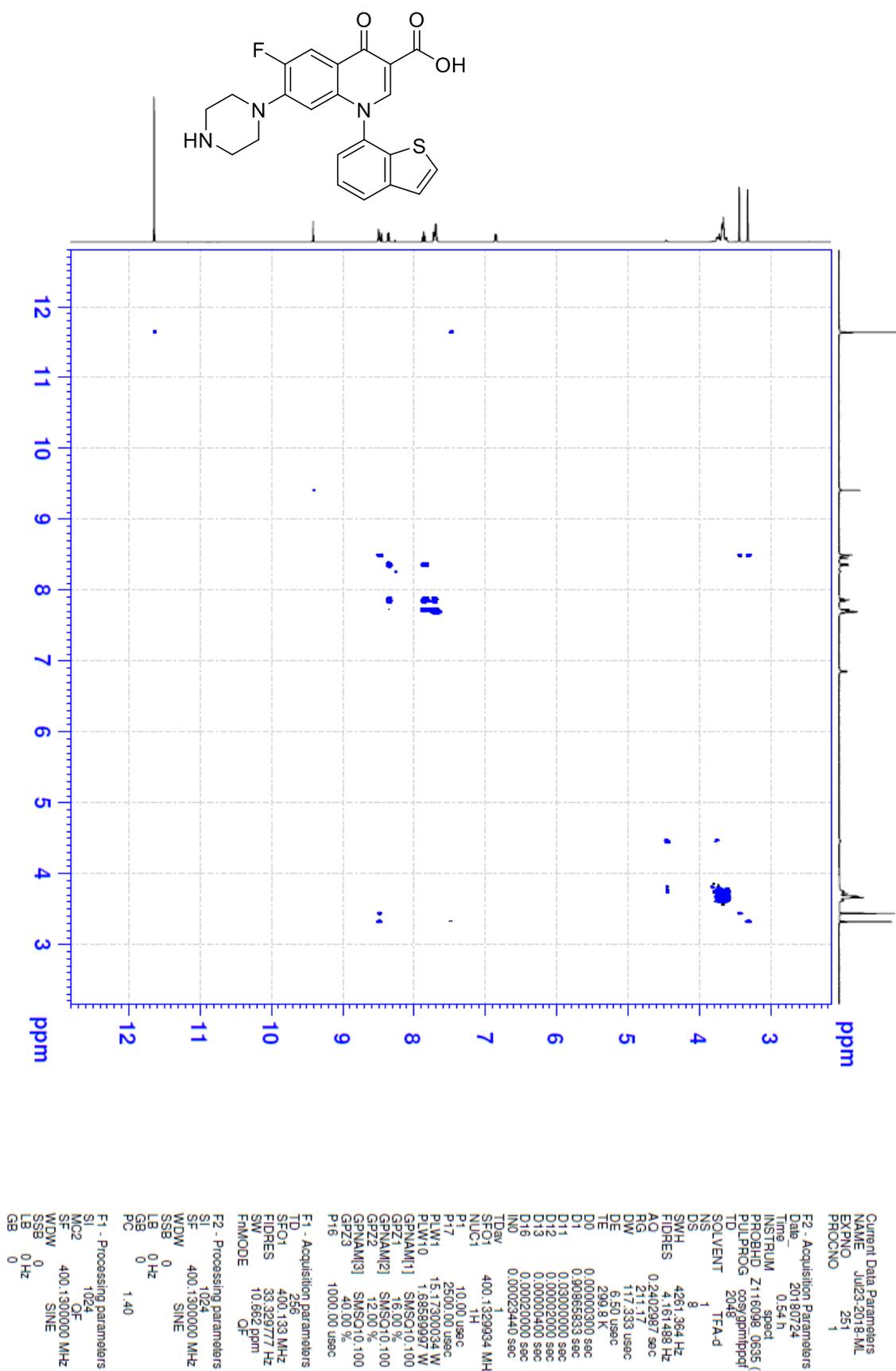


Figure S98. COSY spectrum of compound 5f.

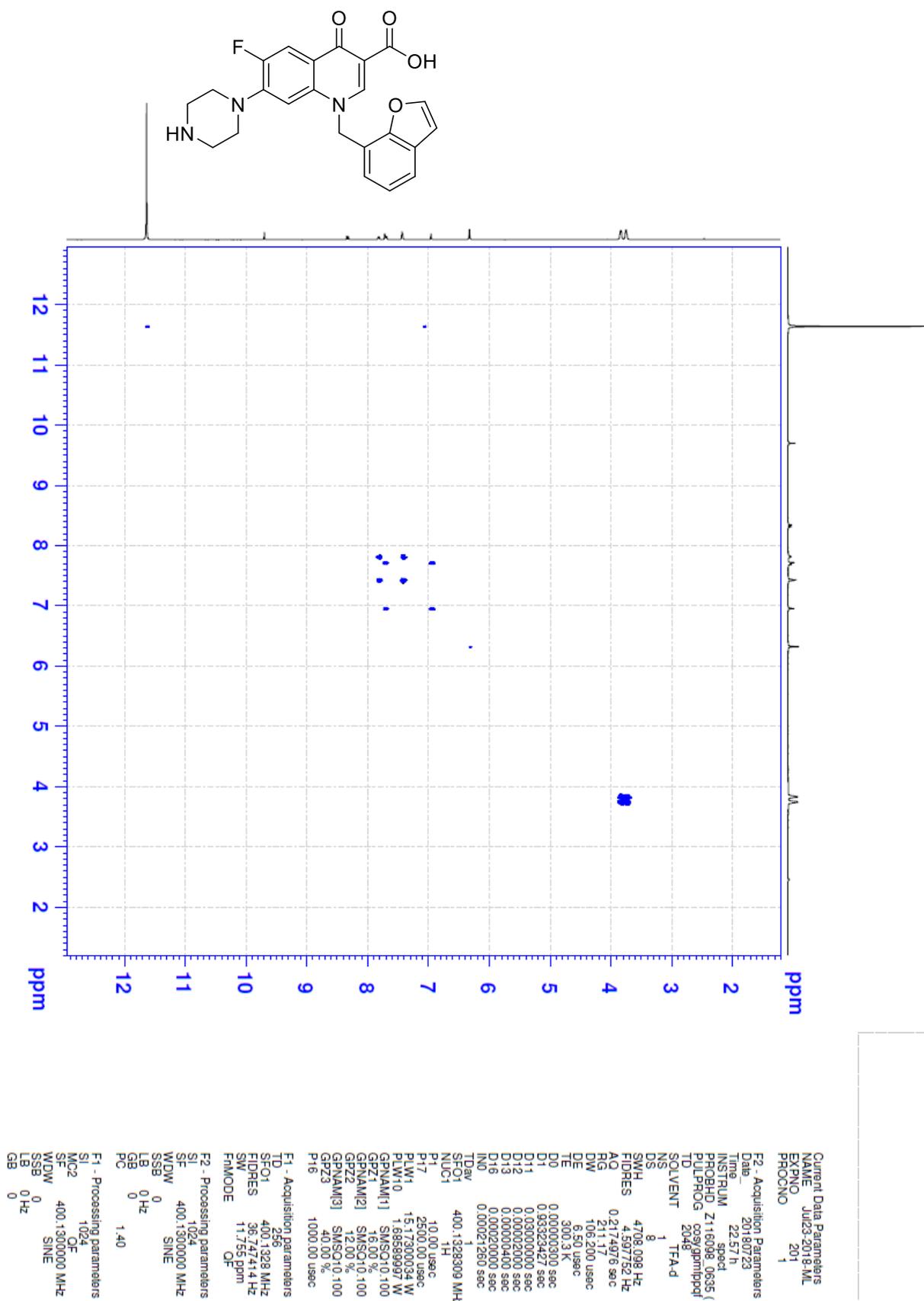


Figure S99. COSY spectrum of compound 5g.

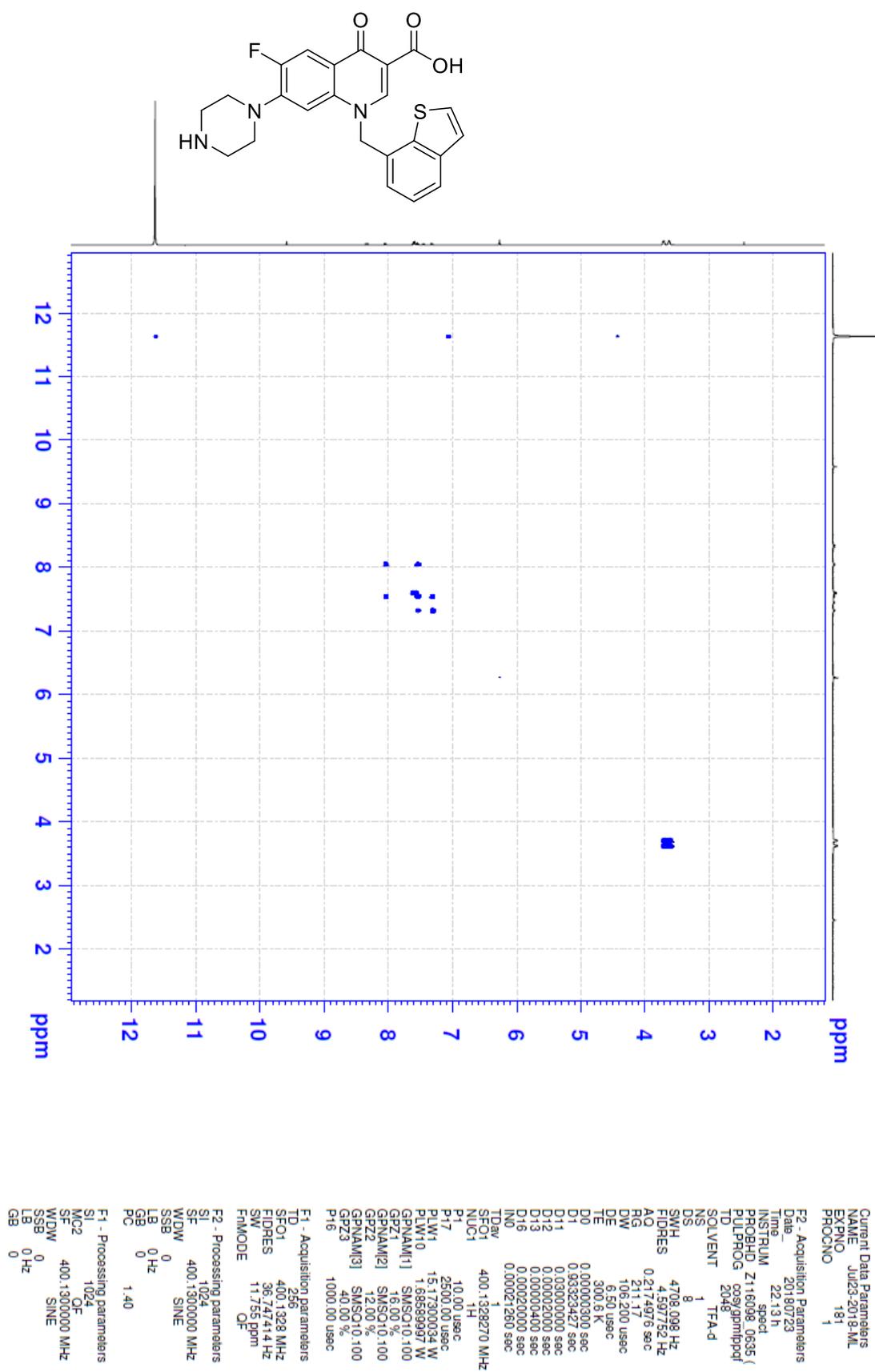


Figure S100. COSY spectrum of compound 6a.

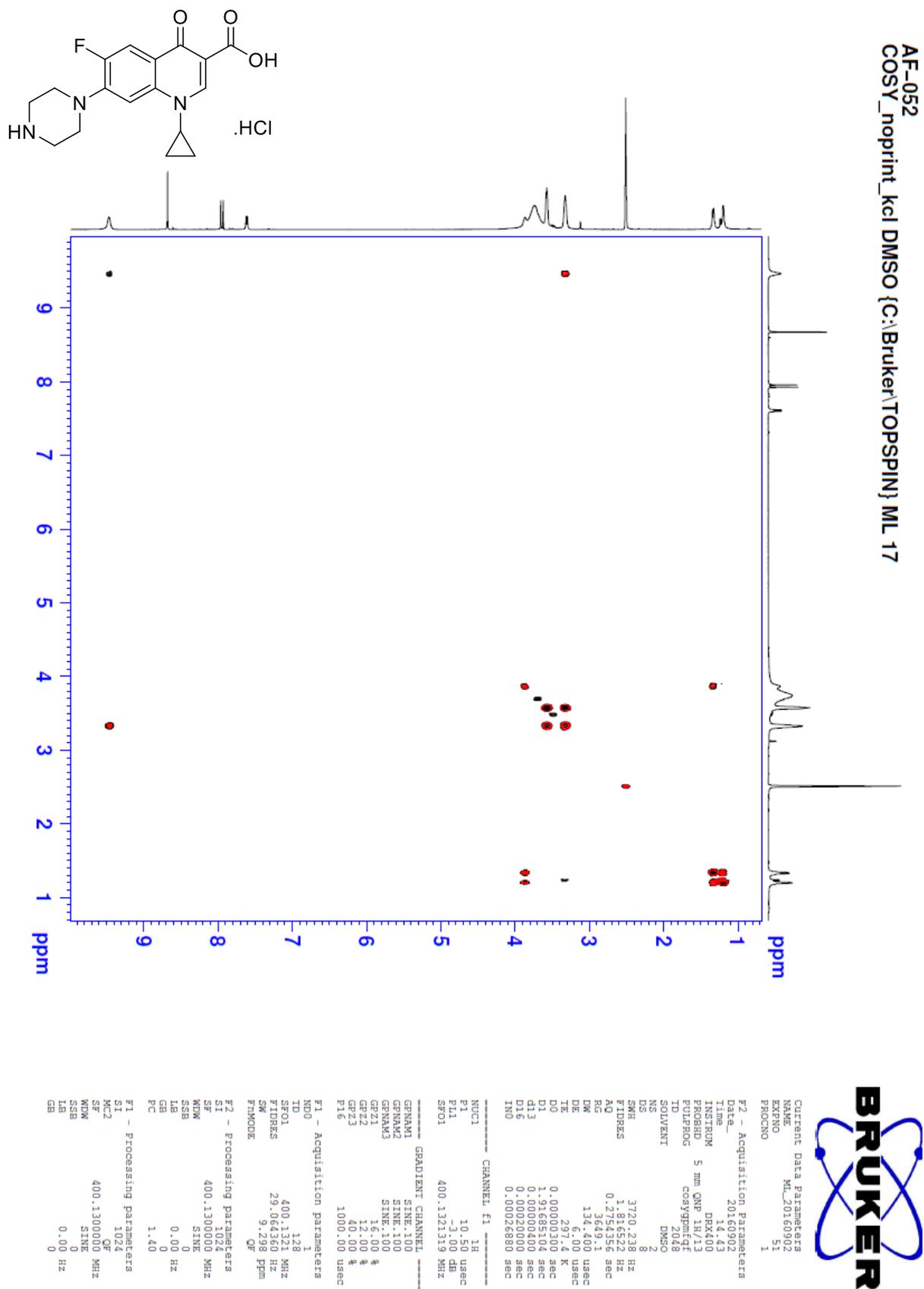
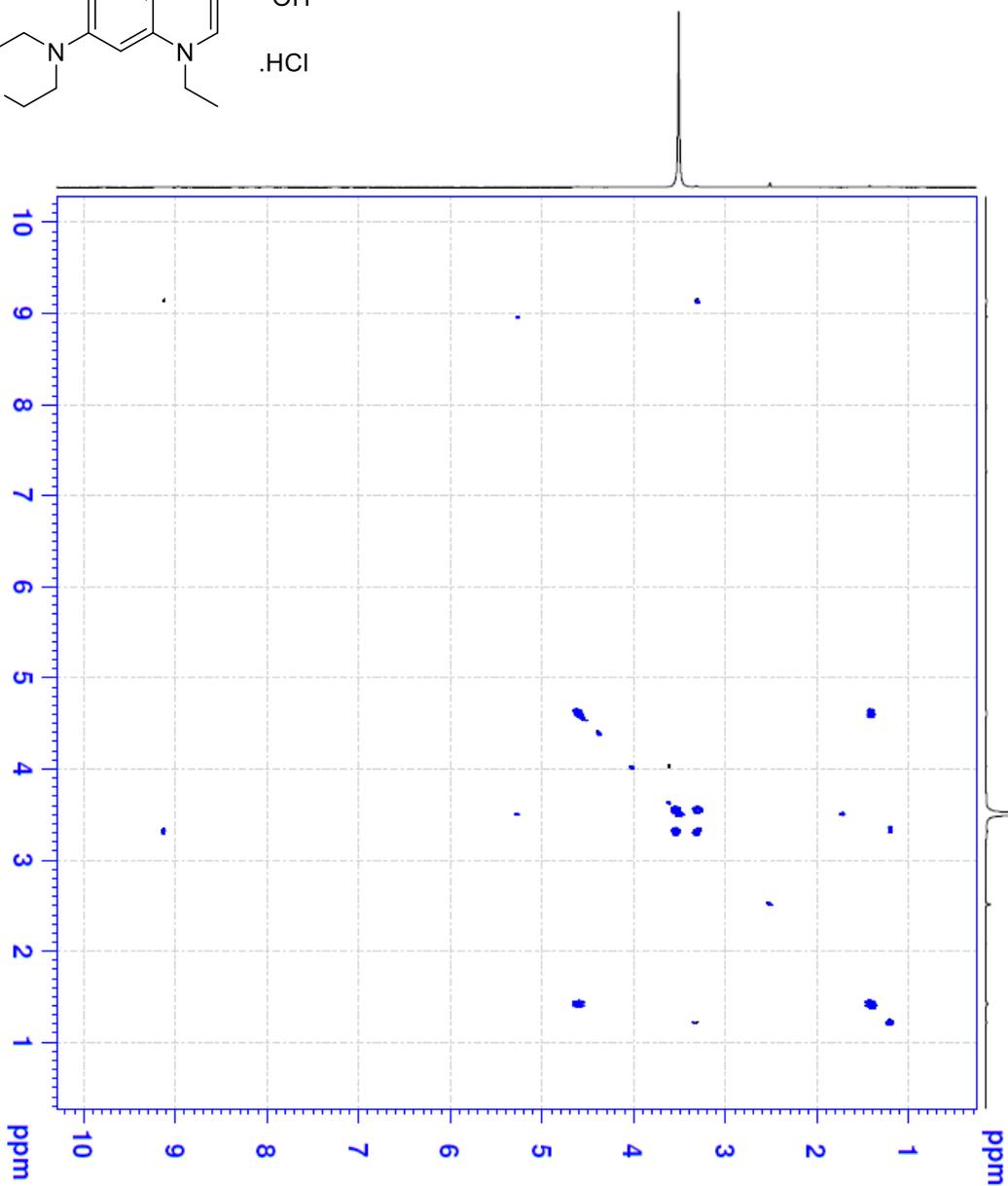
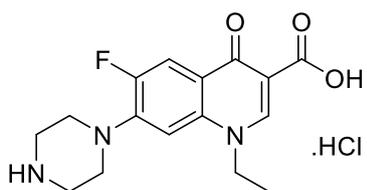


Figure S101. COSY spectrum of compound 6b.



Current Data Parameters
 NAME: AF127-2019-ML
 EXPNO: 21
 PROCNO: 1

F2 - Acquisition Parameters
 Date_ 20190428
 Time 2:27 h
 INSTRUM spect
 PROBHD Z116098_0635 (PULPROG
 PULPROG cosygpmppof
 TD 2048
 SOLVENT 1 DMSO
 NS 8
 DS 1
 SWH 4012.941 Hz
 FIDRES 31.918790 Hz
 AQ 0.2551508 sec
 RG 211.177
 DW 124.600 usec
 DE 6.50 usec
 TE 296.0 K
 D0 0.00000000 sec
 D1 0.89227432 sec
 D11 0.03000000 sec
 D12 0.00020000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00024900 sec

TDav 1
 SFO1 400.1321111 MHz
 NUC1 1H
 P1 10.00 usec
 P17 2500.00 usec
 PLW1 15.17300034 W
 PLW10 1.68889997 W
 GPNAM11 SMC10:100
 GPNAM12 SMC10:100
 GPNAM13 SMC10:100
 GPF2 12.00 %
 GPF3 40.00 %
 P16 1000.00 usec

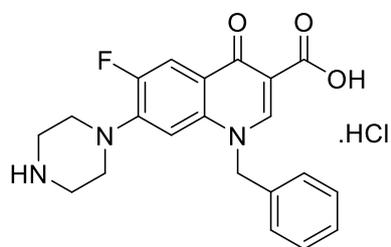
F1 - Acquisition parameters
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 SFO1 400.1321 MHz
 FIDRES 31.375502 Hz
 SW 10.037 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300000 MHz
 WDW 0 SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 SF 400.1300000 MHz
 WDW 0 SINE
 SSB 0
 LB 0 Hz
 GB 0

Figure S102. COSY spectrum of compound 6c.

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Jul23-2018-ML.137.001.2r.esp

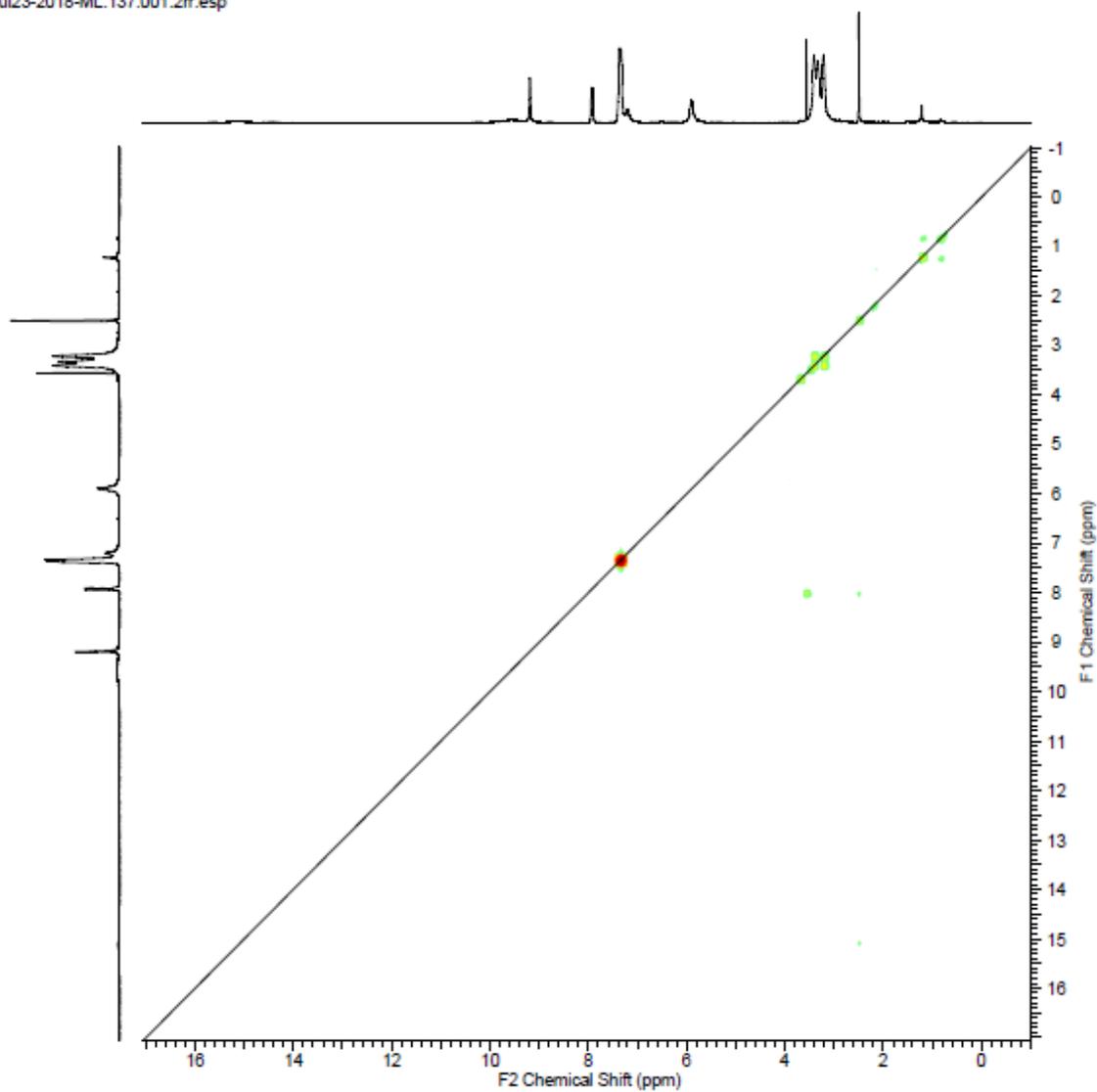
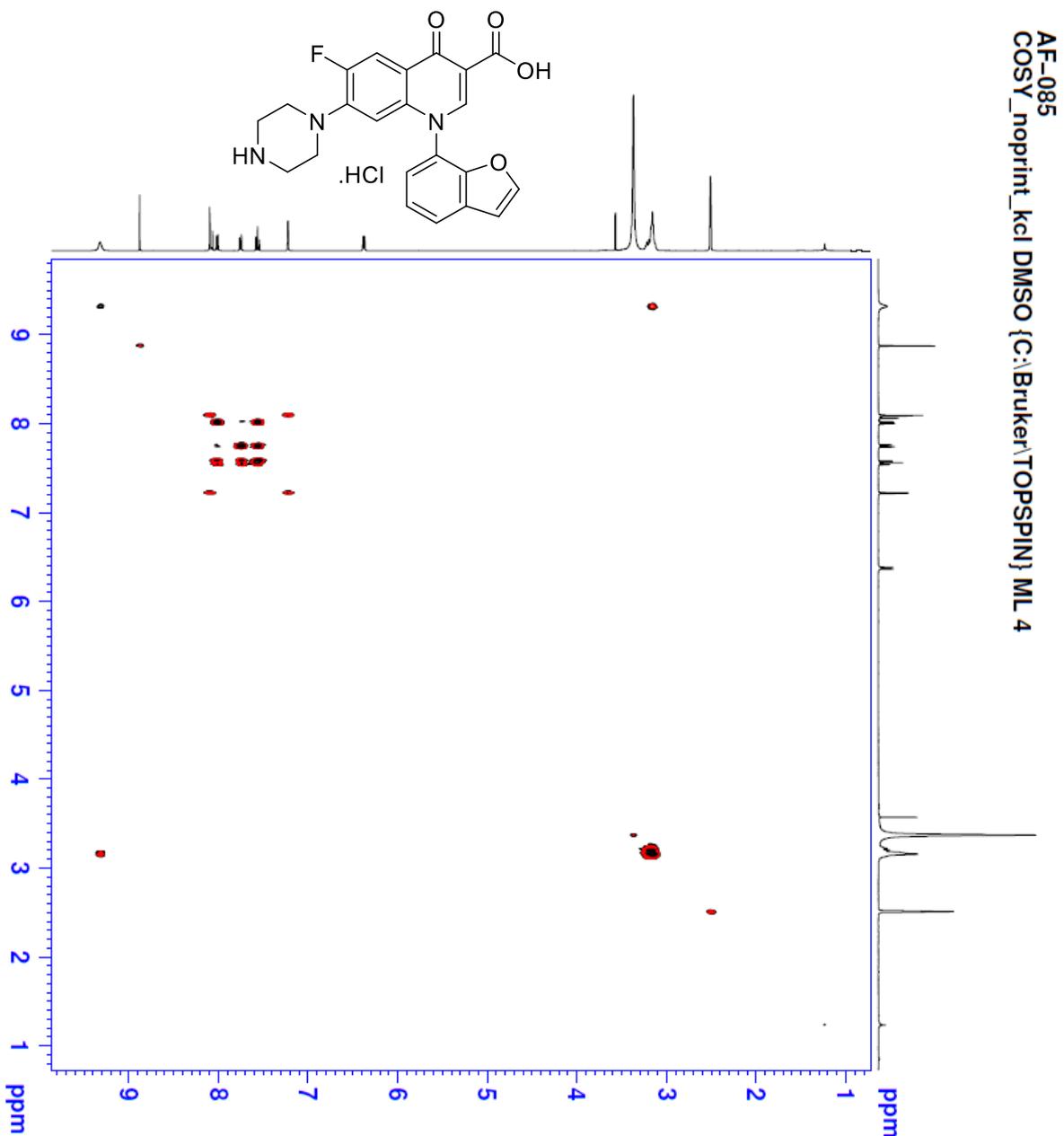


Figure S103. COSY spectrum of compound 6d.



```

Current Data Parameters
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EXPNO        41
PROCNO       1

F2 - Acquisition Parameters
Date_         20160901
Time          13.06
INSTRUM      DRX400
PROBHD       5 mm QNP 1H/13
PULPROG      cosyqpmzg1
TD           2048
SOLVENT      DMSO
NS           2
DS           2
SFR          3654.971 Hz
FIDRES       1.784654 Hz
AQ           0.2803532 sec
RG           3649.1
DE           136.800 usac
TE           298.3 K
D0           0.00000300 sec
D1           1.91070700 sec
d12          0.00000400 sec
D16          0.00020000 sec
IN0          0.00027360 sec

----- CHANNEL f1 -----
NUC1          1H
P1           10.50 usac
PL1          -3.00 dB
SFO1         400.1321162 MHz

----- GRADIENT CHANNEL -----
GPRNA1       SINE,100
GPRNA2       SINE,100
GPRNA3       SINE,100
GRZ1         16.000 $
GRZ2         12.000 $
GRZ3         10.000 $
F16          1000.00 usac

F1 - Acquisition parameters
ND0           1
TD           128
SFO1         400.1321 MHz
FIDRES       28.554459 Hz
SW           9.134 ppm
ENVMODE      QF

F2 - Processing parameters
SI           400.130000 MHz
MWDW        SINE
SSB          0
LB           0.00 Hz
GB           0
PC           1.40

F1 - Processing parameters
SI           1024
MC2          QF
SF           400.1300000 MHz
WDW          SINE
SSB          0.00 Hz
LB           0
GB           0
  
```

Figure S104. COSY spectrum of compound 6e.

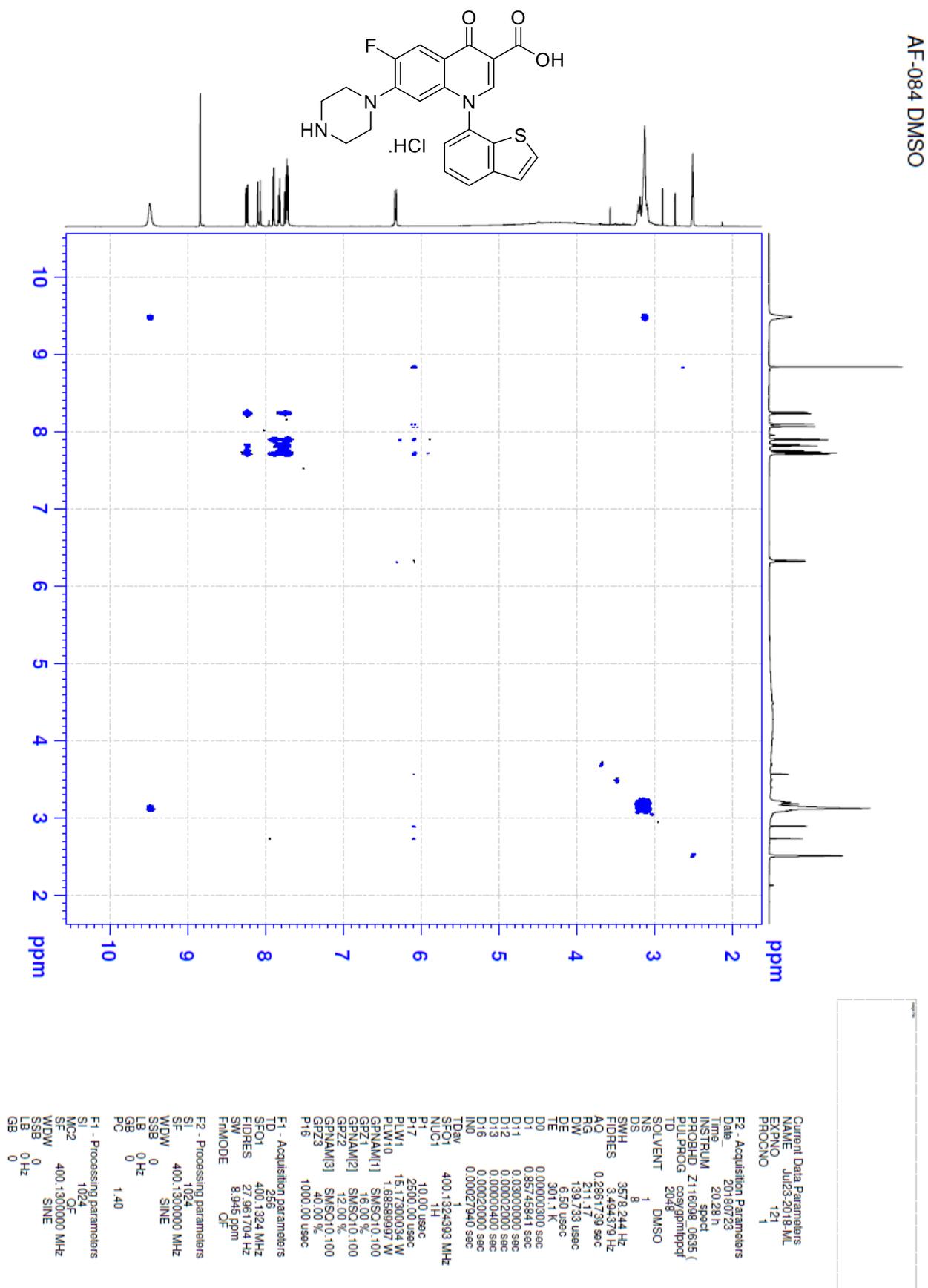


Figure S105. COSY spectrum of compound 6f.

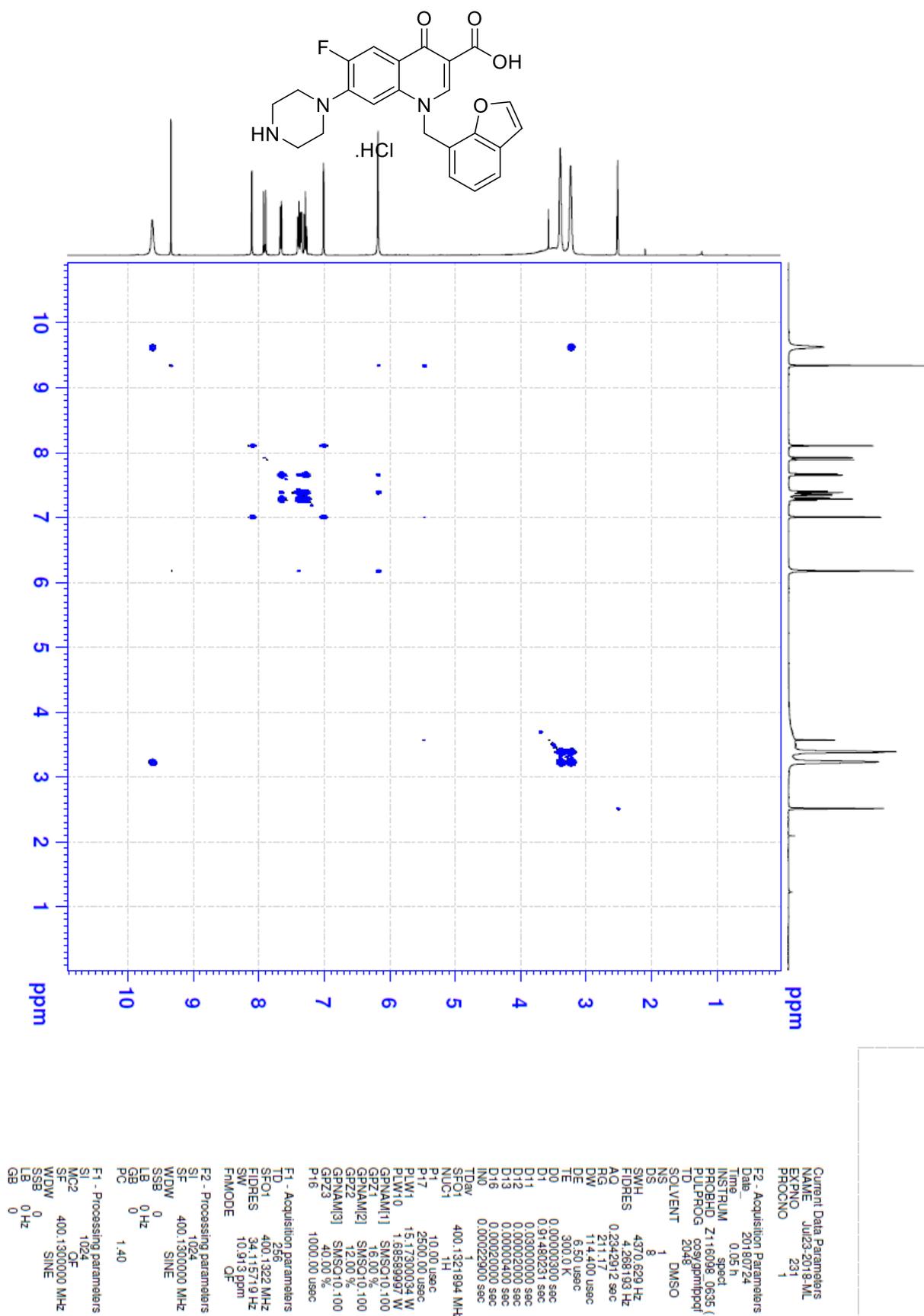
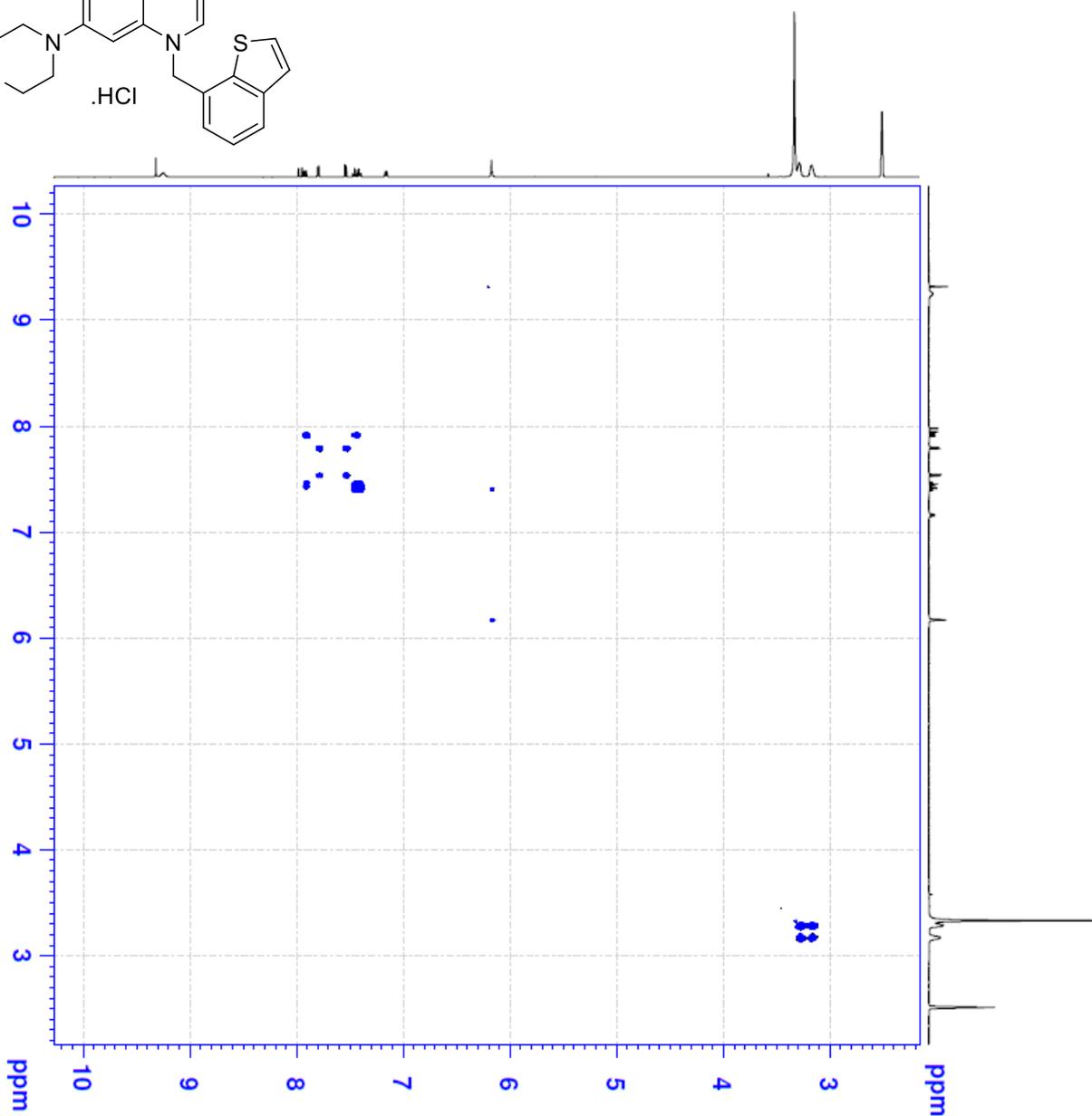
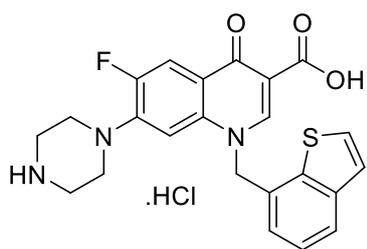


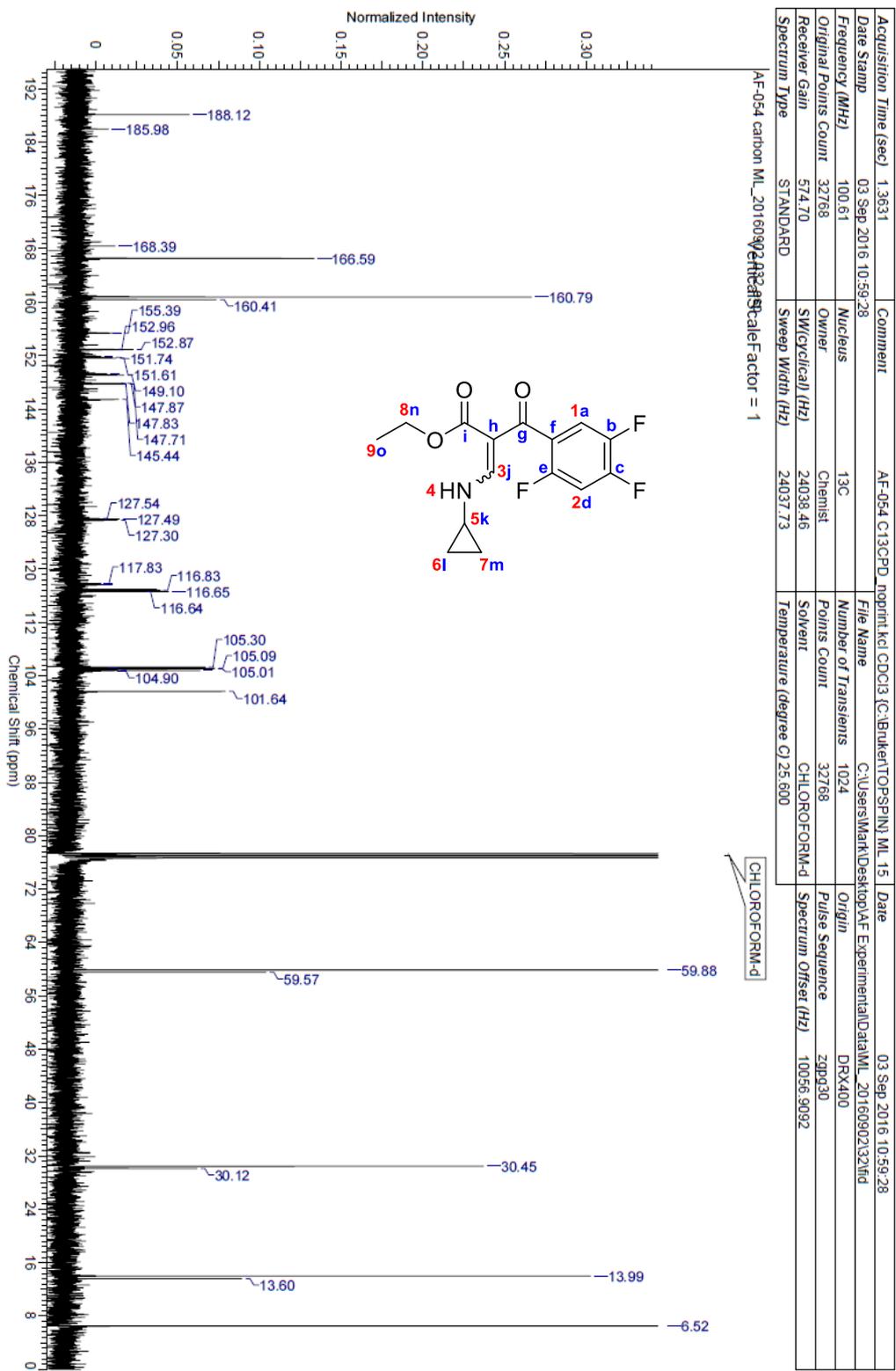
Figure S106. COSY spectrum of compound 6g.



Current Data Parameters
 NAME Jul23-2018-ML
 EXPNO 111
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20180724
 Time 9:17 h
 INSTRUM spect
 PROBHID Z116098_0635 (PULPROG
 PULPROG cosy/gm1ppof
 TD 2048
 SOLVENT DMSO
 NS 1
 DS 8
 SWH 3246.753 Hz
 FIDRES 3.170657 Hz
 AQ 0.3153920 sec
 RG 211.17
 DW 154.000 usec
 DE 6.50 usec
 TE 301.2 K
 D0 0.00000300 sec
 D1 0.82469028 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 D13 0.00004000 sec
 D16 0.00020000 sec
 INU 0.00030790 sec
 TDAV 1
 SFC1 400.1324866 MHz
 NUC1 1H
 P1 10.00 usec
 P17 2500.00 usec
 PLW1 15.17300034 W
 PLW10 1.6868997 W
 GPNAM1) SMC10.100
 GPNAM1) 16.00 %
 GPNAM2) SMC10.100
 GPZ2 12.00 %
 GPNAM3) SMC10.100
 GPZ3 40.00 %
 P16 1000.00 usec
 F1 - Acquisition parameters
 TD 256
 SFC1 400.1325 MHz
 FIDRES 25.391724 Hz
 SW 8.119 ppm
 FMODE QF
 F2 - Processing parameters
 SI 1024
 SF 400.1300000 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40
 F1 - Processing parameters
 SI 1024
 SF 400.1300000 MHz
 WDW SINE
 SSB 0 Hz
 LB 0
 GB 0

¹³C NMR Spectra

Figure S107. Carbon NMR spectrum of compound 2a.



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Figure S108. Carbon NMR spectrum of compound 2b.

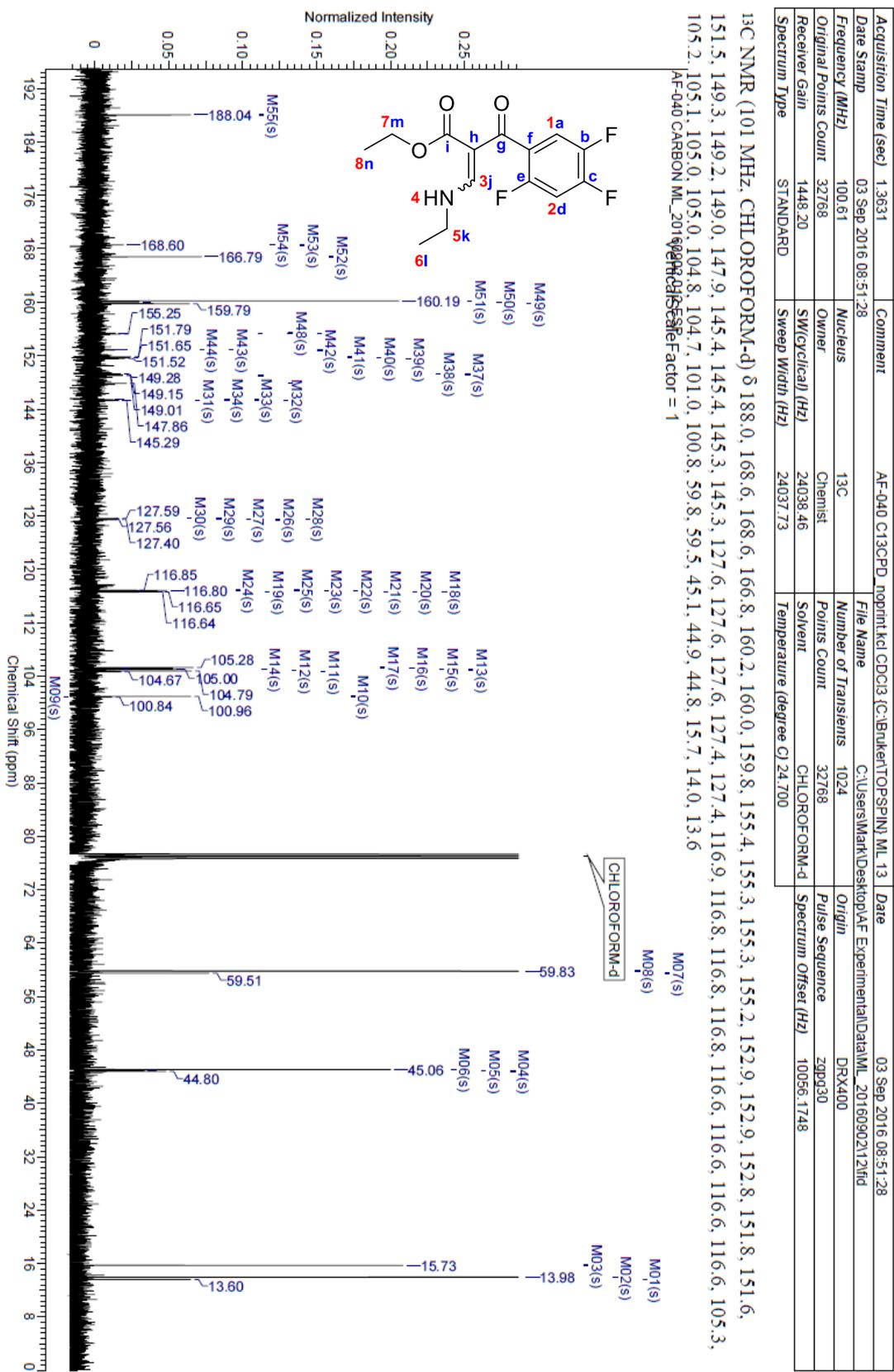
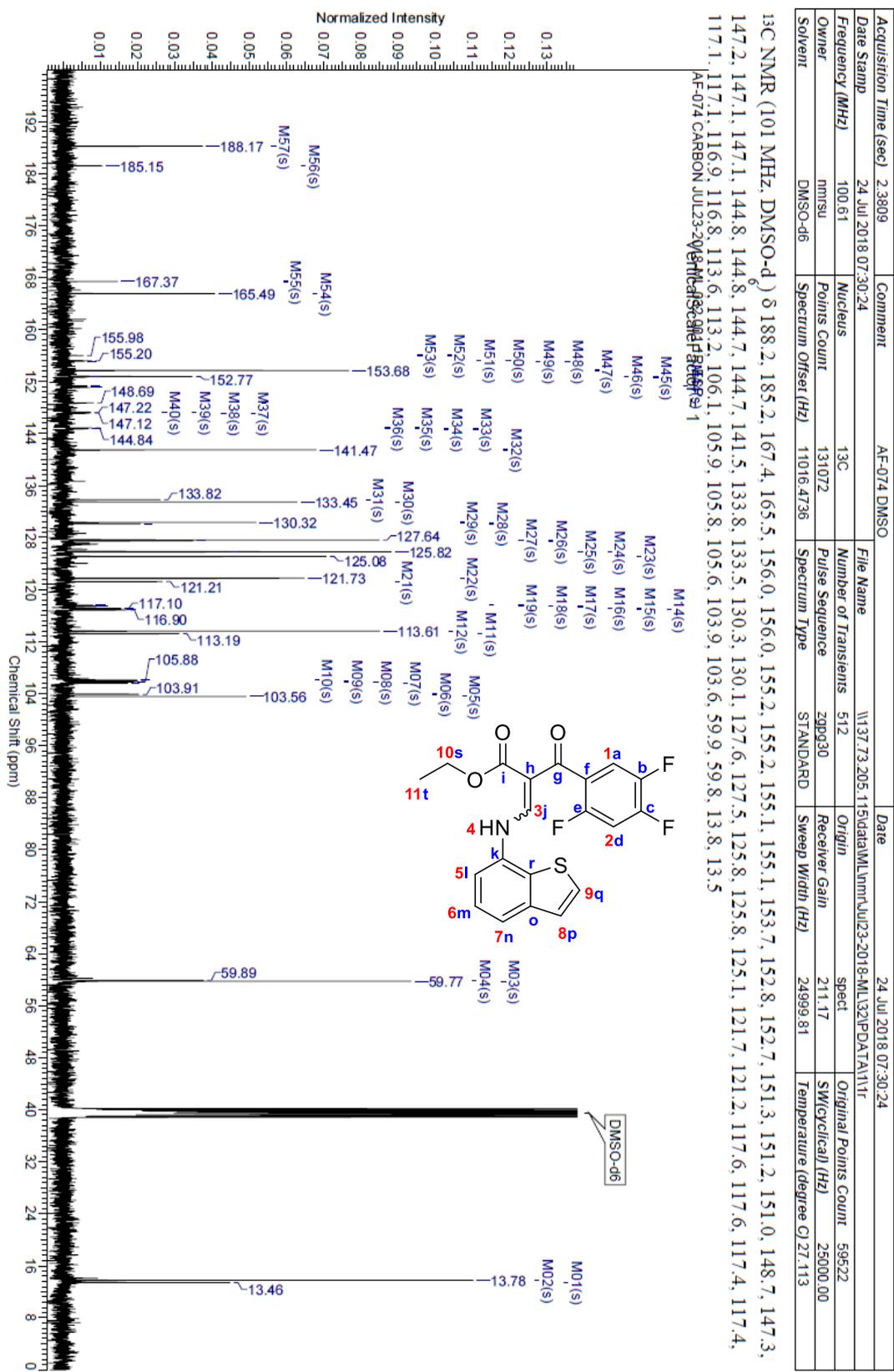


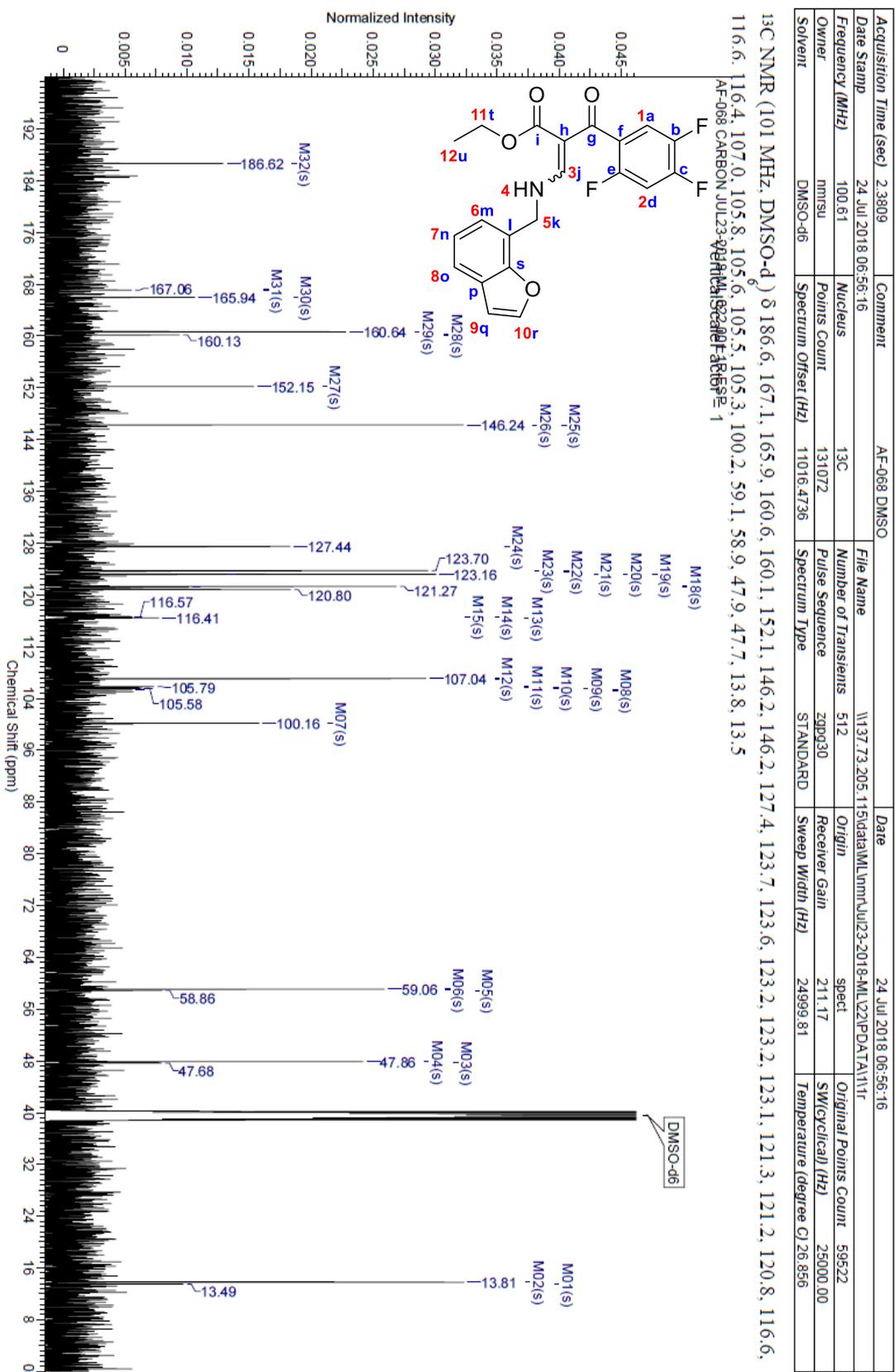
Figure S111. Carbon NMR spectrum of compound 2e.



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25/06/2019 15:46:54

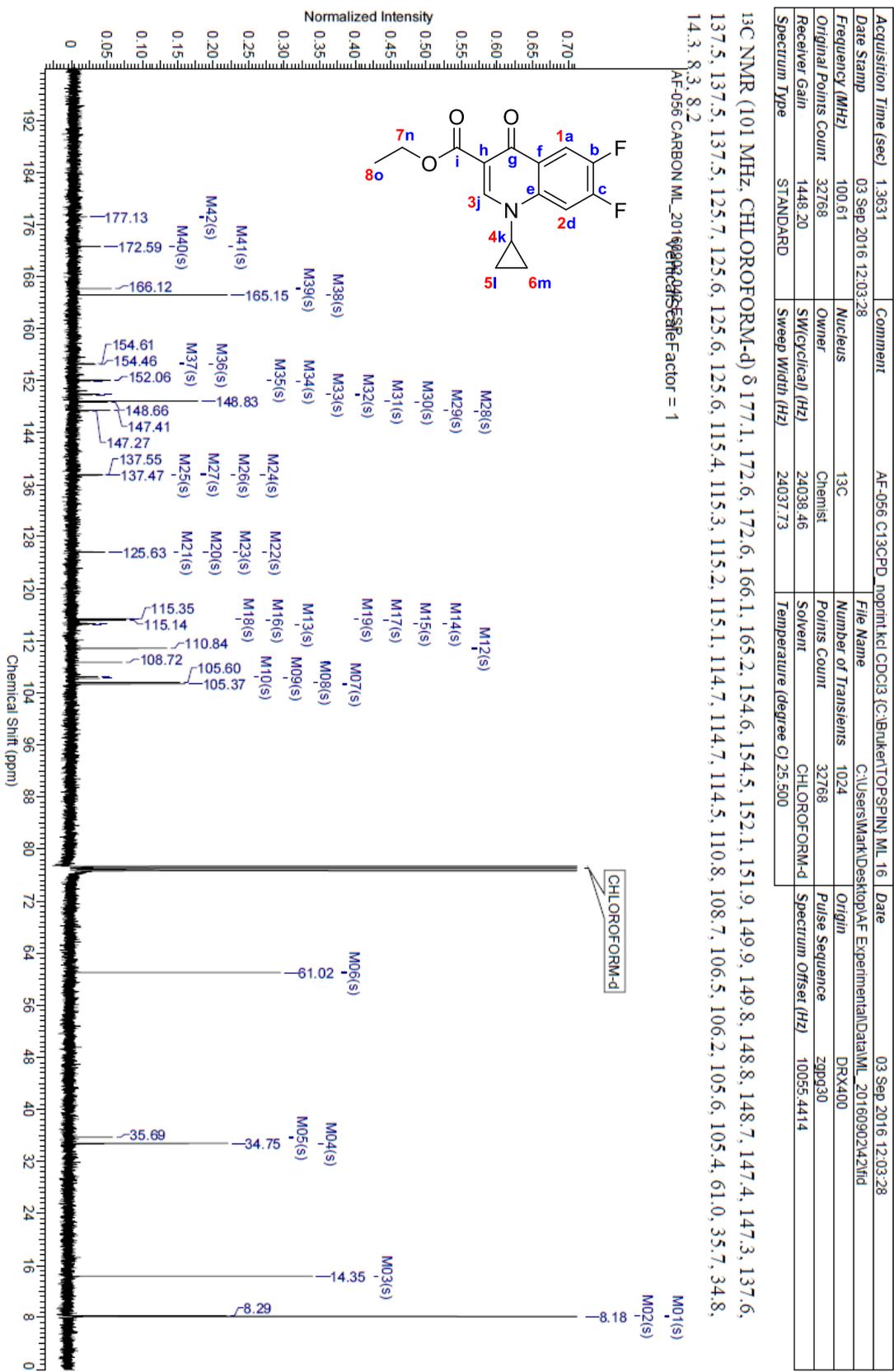
Figure S112. Carbon NMR spectrum of compound 2f.



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25/06/2019 15:45:48

Figure S114. Carbon NMR spectrum of compound 3a.



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25/06/2019 15:49:21

Figure S115. Carbon NMR spectrum of compound 3b.

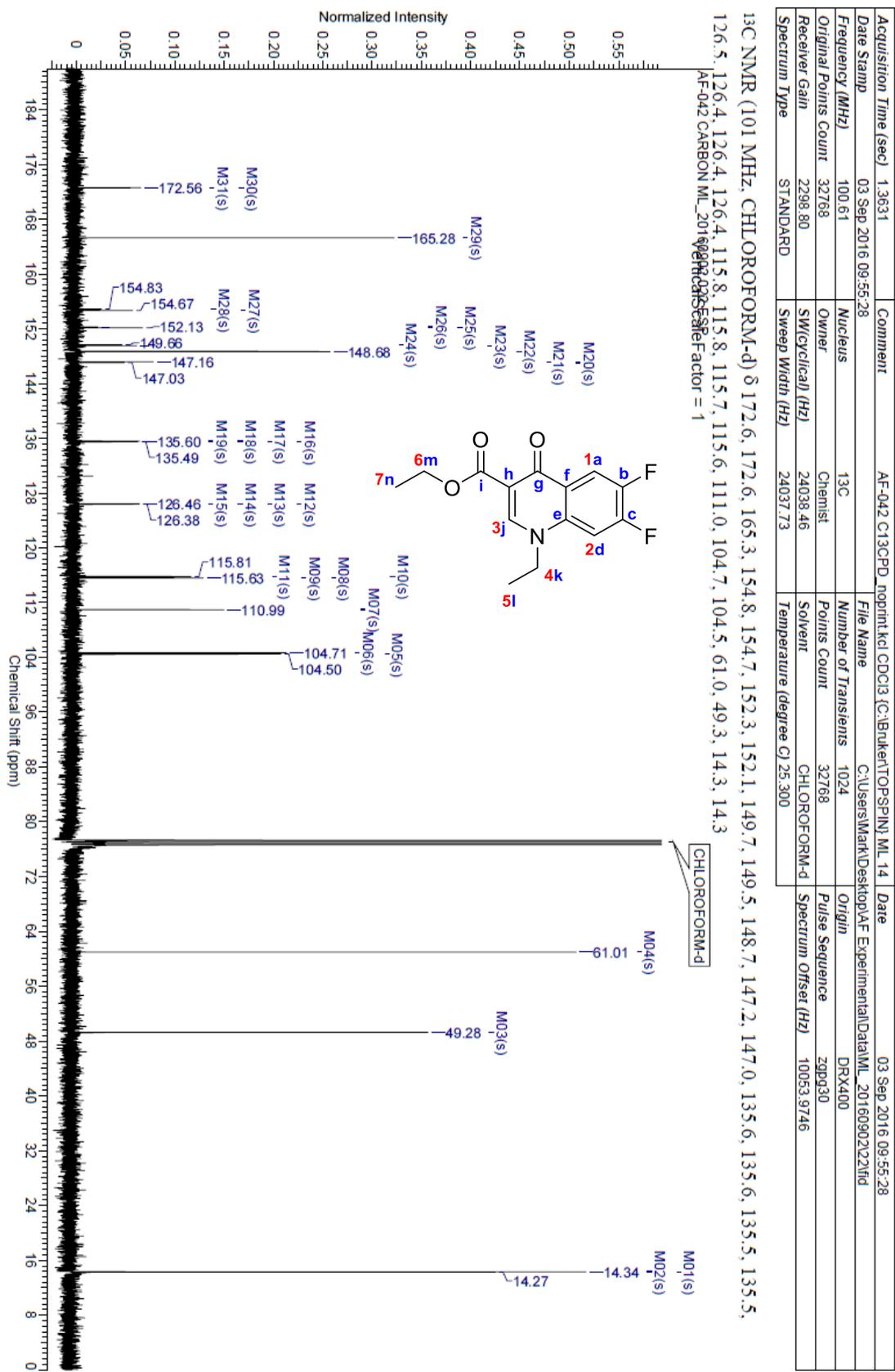
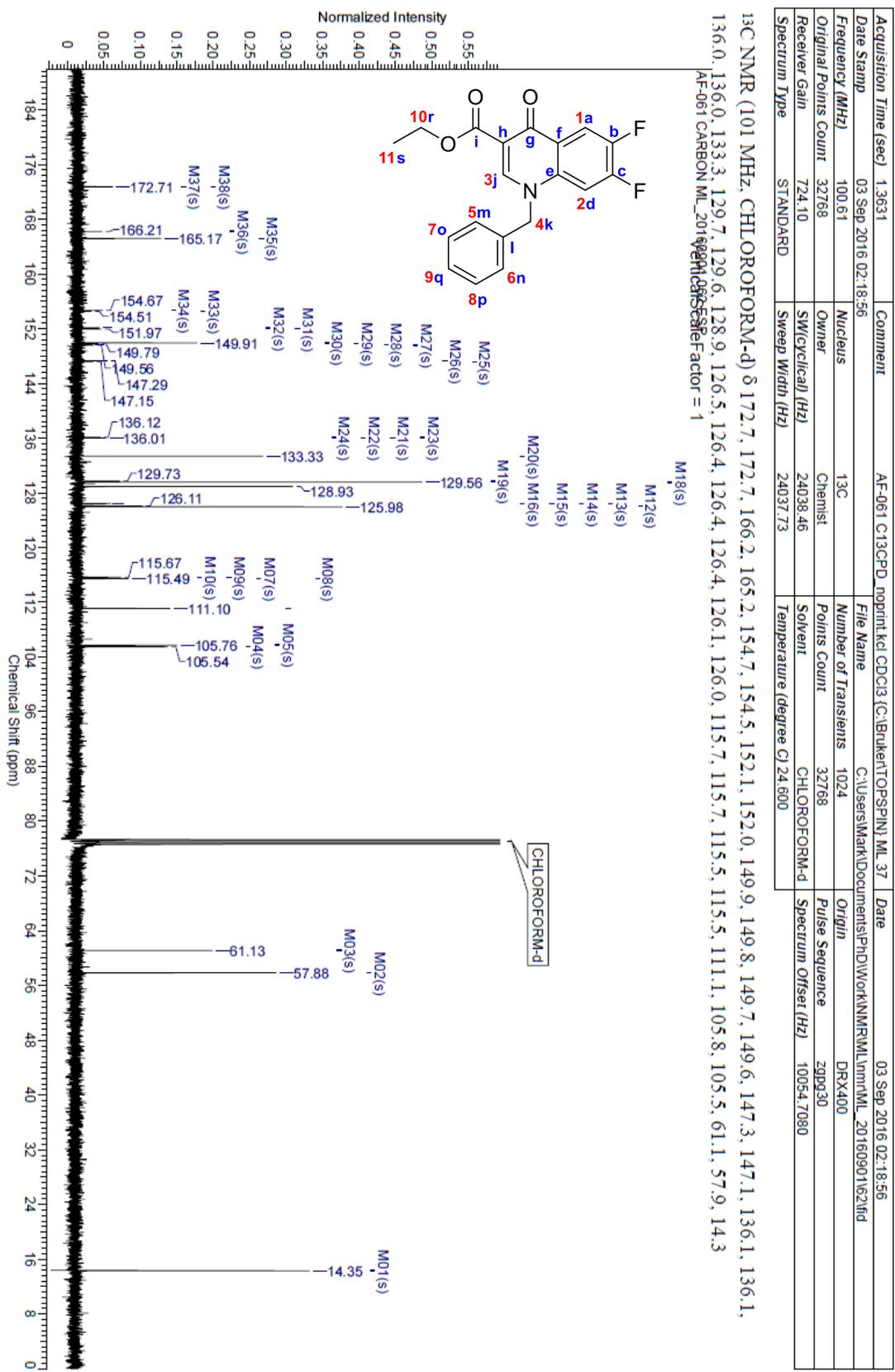


Figure S116. Carbon NMR spectrum of compound 3c.



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Figure S117. Carbon NMR spectrum of compound 3d.

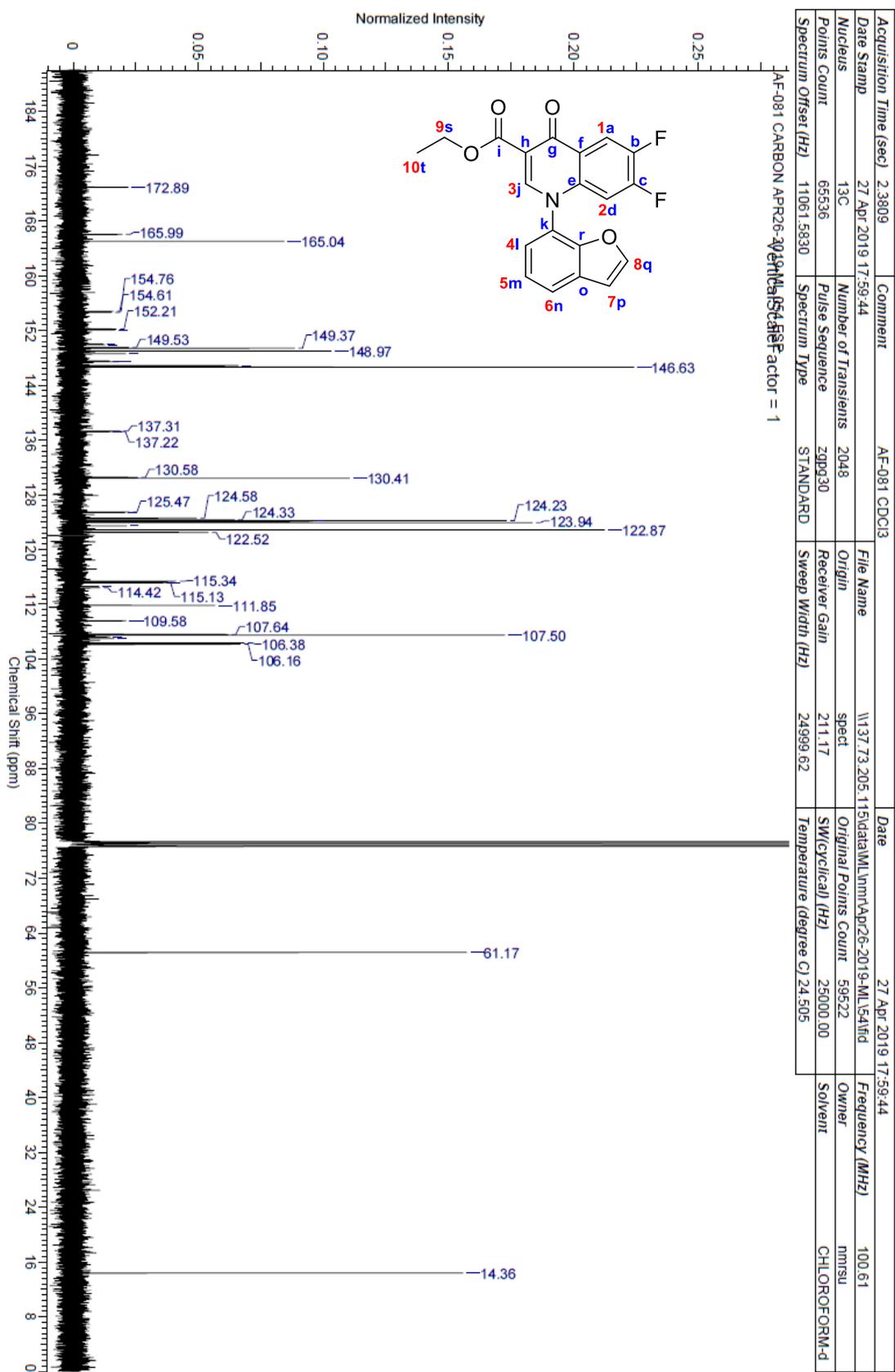
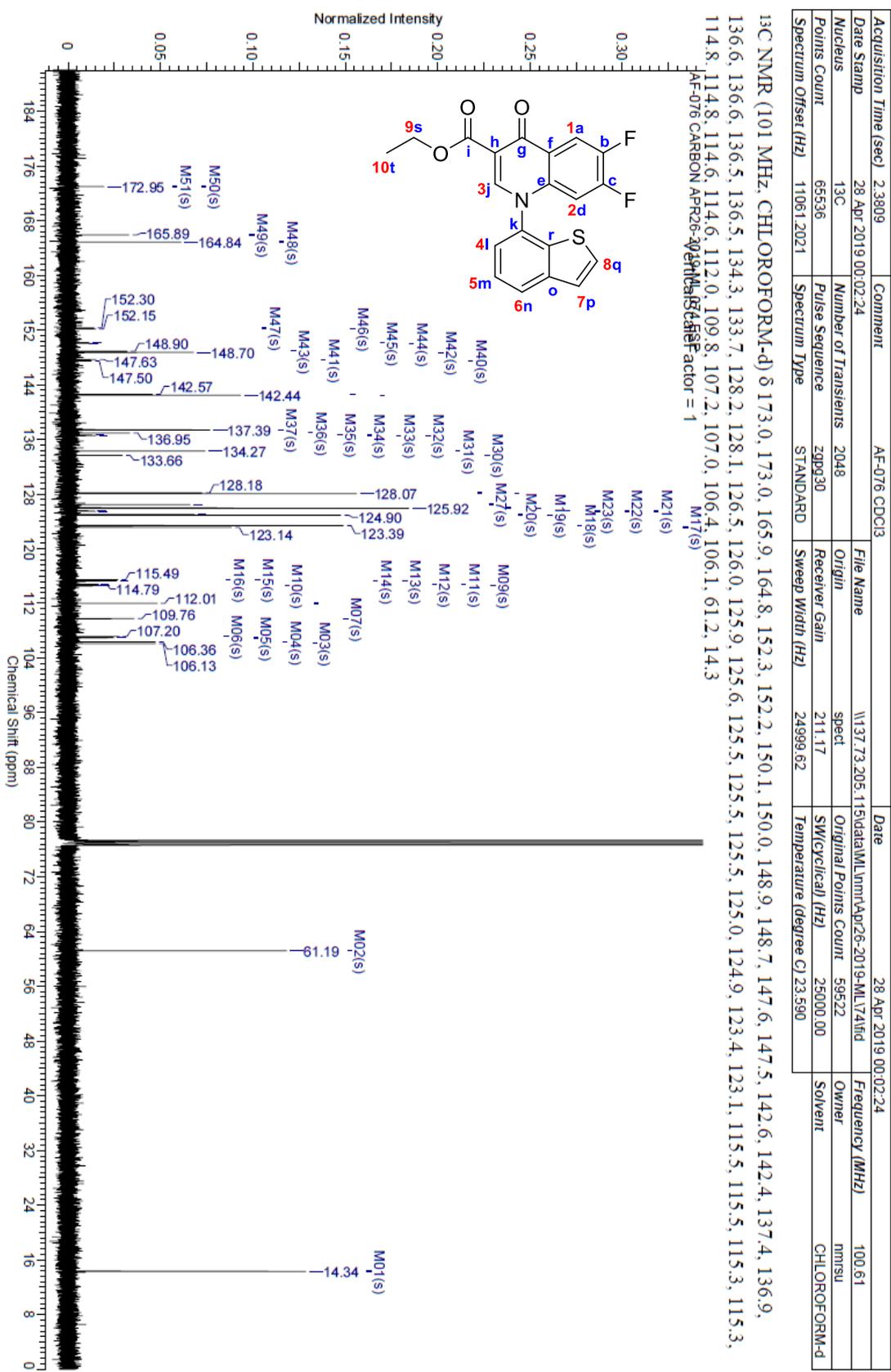


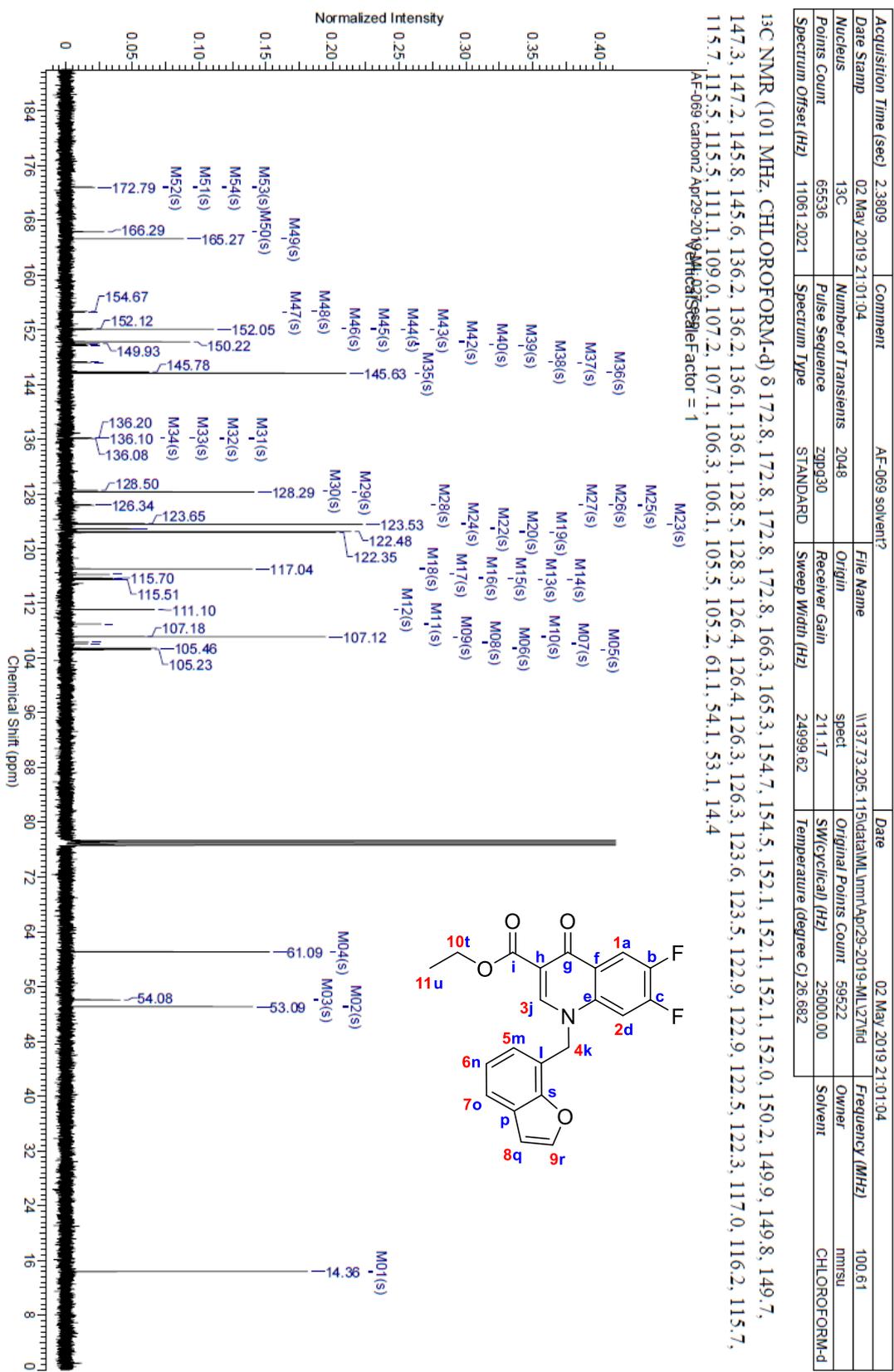
Figure S118. Carbon NMR spectrum of compound 3e.



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25/06/2019 15:38:26

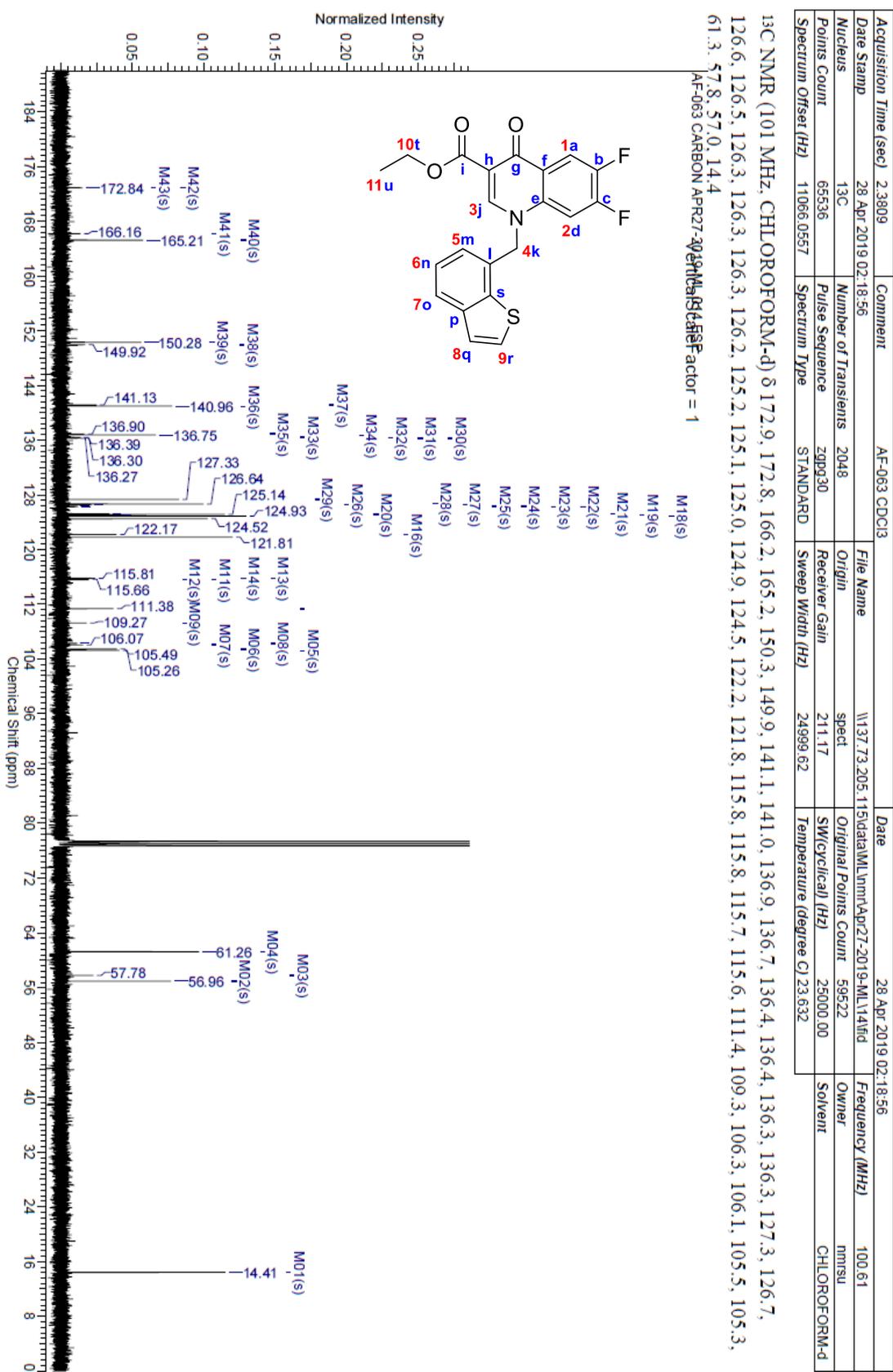
Figure S119. Carbon NMR spectrum of compound 3f.



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25/06/2019 15:29:38

Figure S120. Carbon NMR spectrum of compound 3g.



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25/06/2019 14:00:52

Acquisition Time (sec)	2.3809	Comment	AF-057 TFA-D	Date	24 Jul 2018 11:31:28
Date Stamp	24 Jul 2018 11:31:28	File Name	\\137.73.205.115\data\ML\mnr\Jul23-2018-ML1103\F\DATA111F	Number of Transients	512
Frequency (MHz)	100.61	Nucleus	¹³ C	Points Count	131072
Original Points Count	59522	Owner	nmsu	Pulse Sequence	zgpg30
Receiver Gain	211.17	SW(Cyclical) (Hz)	25000.00	Solvent	TRIFLUOROACETIC ACID-D
Spectrum Offset (Hz)	11317.3691	Spectrum Type	STANDARD	Sweep Width (Hz)	24999.81
				Temperature (degree C)	28.422

¹³C NMR (101 MHz, TRIFLUOROACETIC ACID-D) δ 174.8, 174.8, 171.7, 161.6, 161.4, 158.9, 158.7, 156.0, 155.9, 153.4, 153.3, 152.7, 142.8, 142.6, 120.9, 120.8, 120.8, 115.9, 115.8, 115.8, 115.7, 115.6, 110.6, 110.3, 106.9, 41.5, 10.0

AF-057 CARBON JUL23-2018 TFA-D

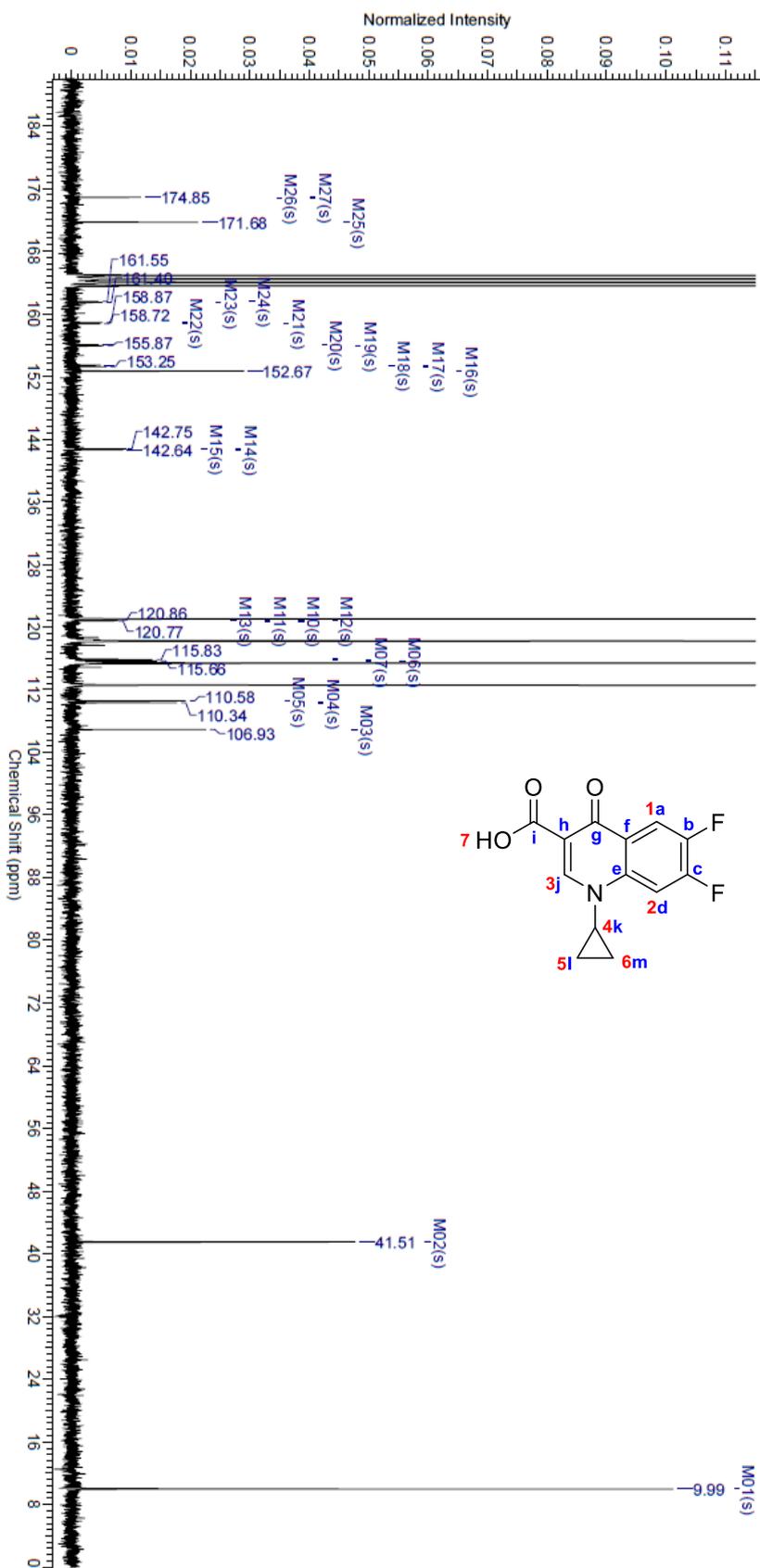


Figure S122. Carbon NMR spectrum of compound 4b.

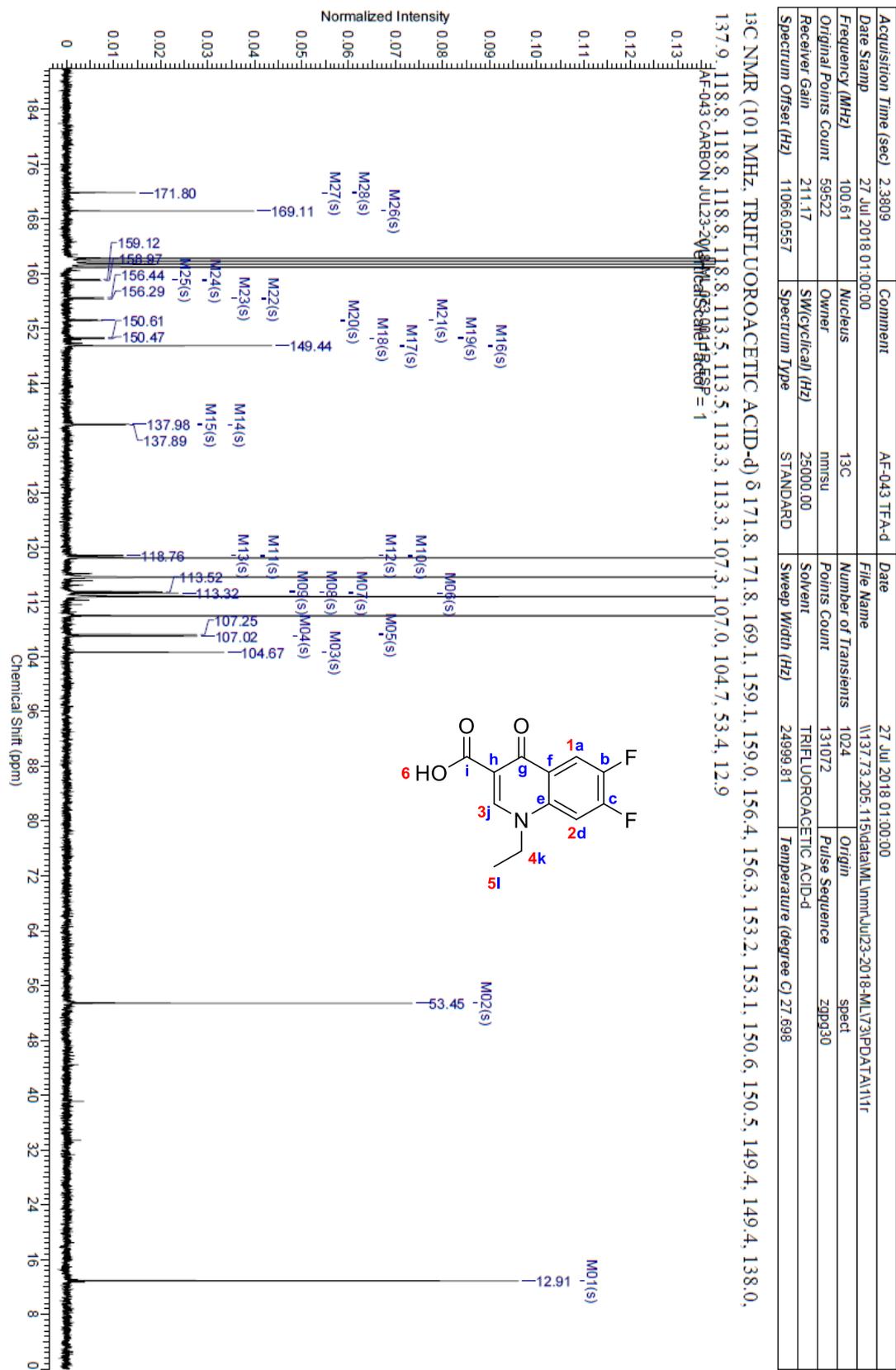
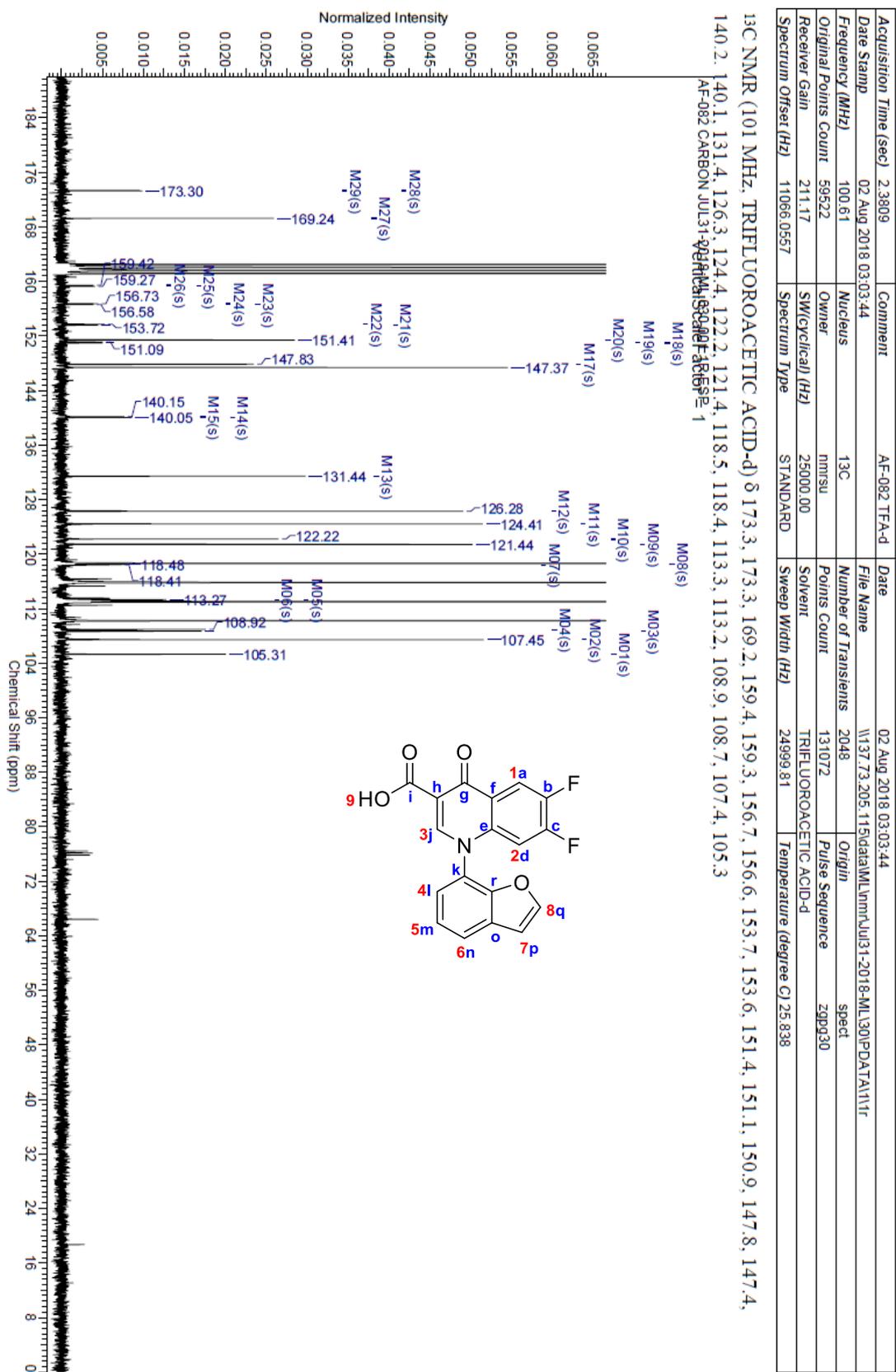


Figure S123. Carbon NMR spectrum of compound 4d.



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25/06/2019 15:58:51

Figure S124. Carbon NMR spectrum of compound 4e.

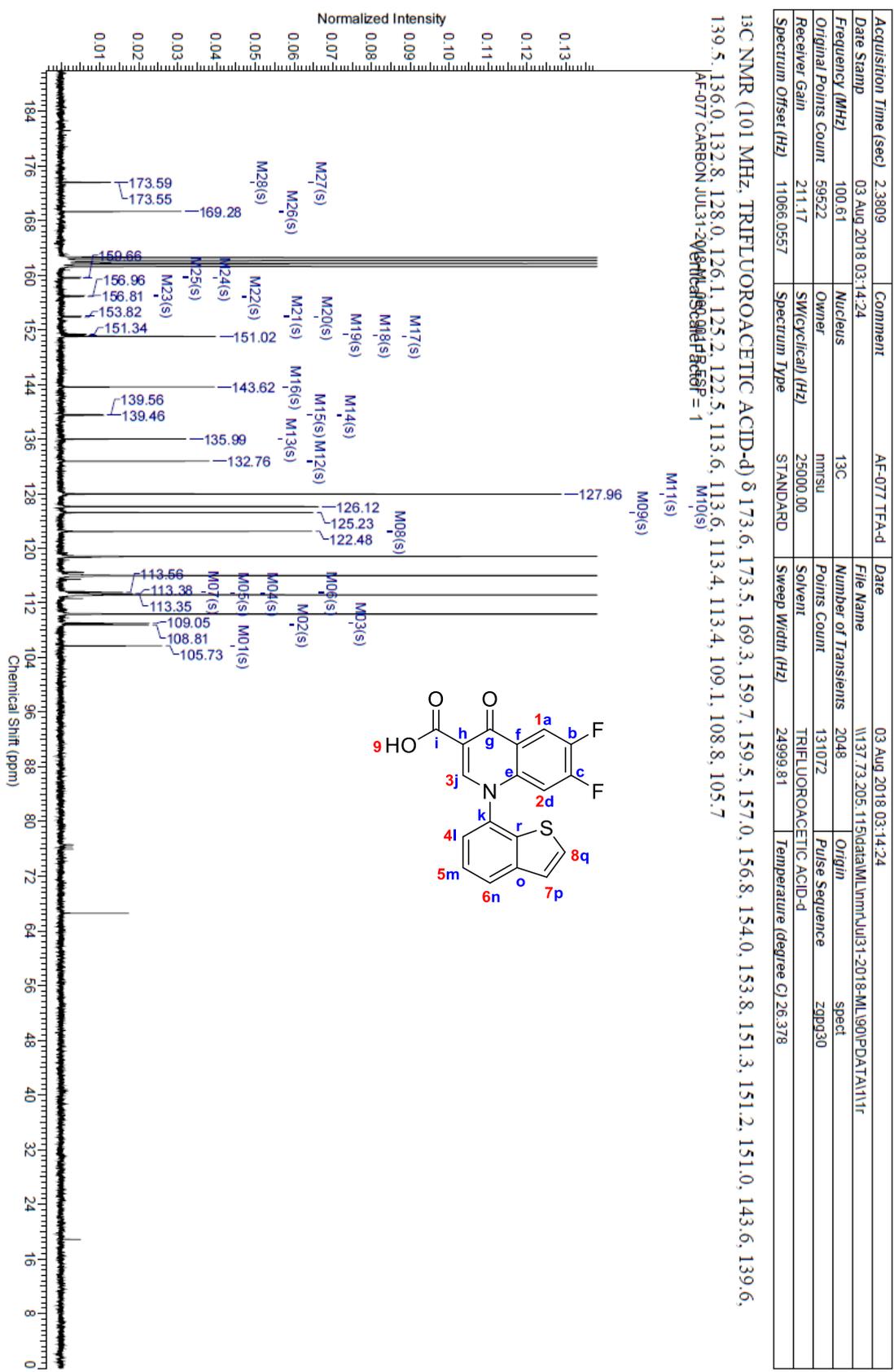
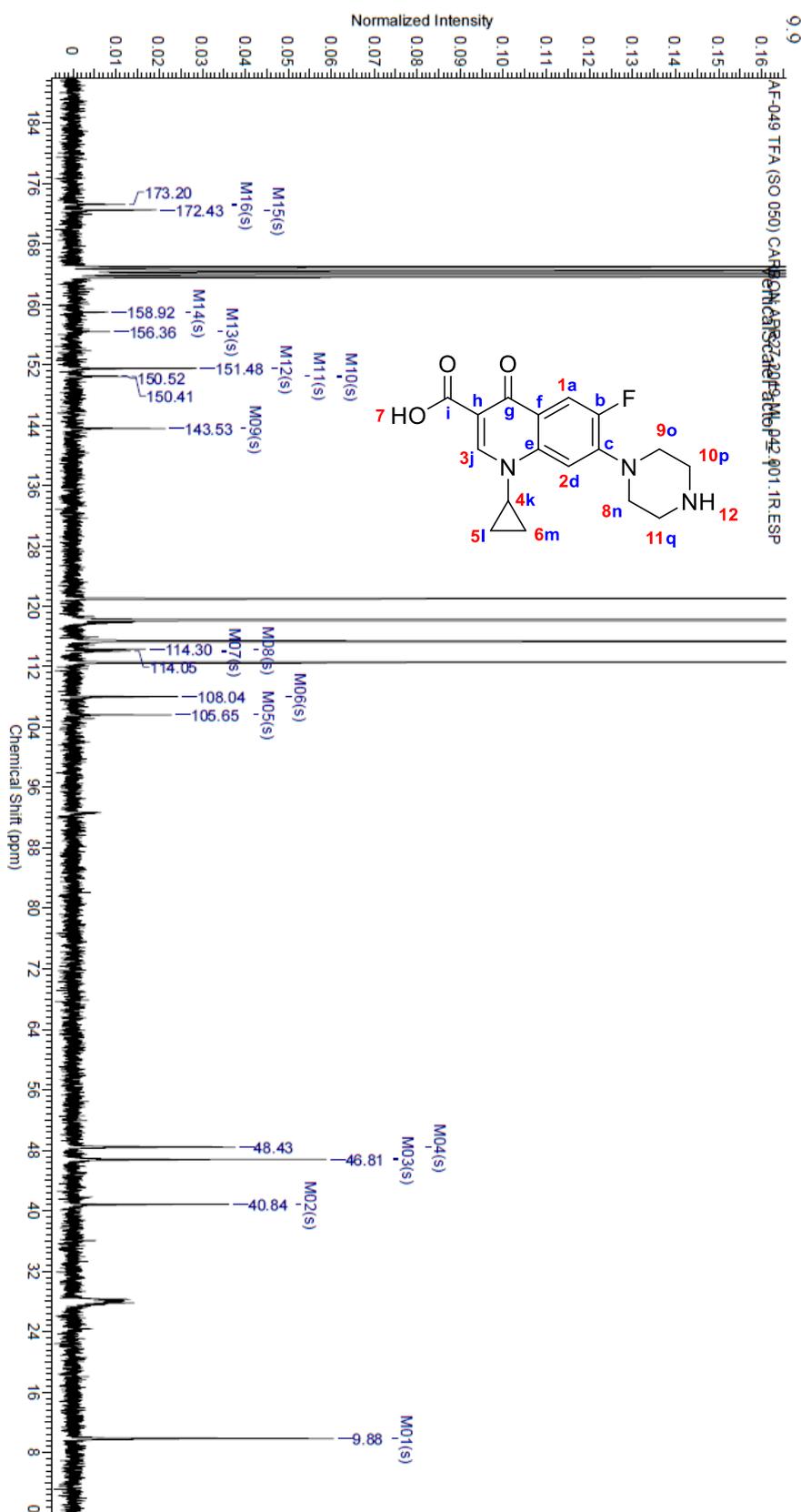


Figure S126. Carbon NMR spectrum of compound 5a.



Acquisition Time (sec)	2.3809	Comment	AF-049 TFA-d	Date	28 Apr 2019 08:02:24
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Frequency (MHz)	100.61	Nucleus	¹³ C	Number of Transients	1024
Original Points Count	59522	Owner	nmsu	Points Count	131072
Receiver Gain	211.17	SW/Cyclical (Hz)	25000.00	Pulse Sequence	zgpg30
Spectrum Offset (Hz)	11328.9102	Spectrum Type	STANDARD	Solvent	TRIFLUOROACETIC ACID-d
		Sweep Width (Hz)	24999.81	Temperature (degree C)	23.488

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25/06/2019 16:00:53

Figure S127. Carbon NMR spectrum of compound 5b.

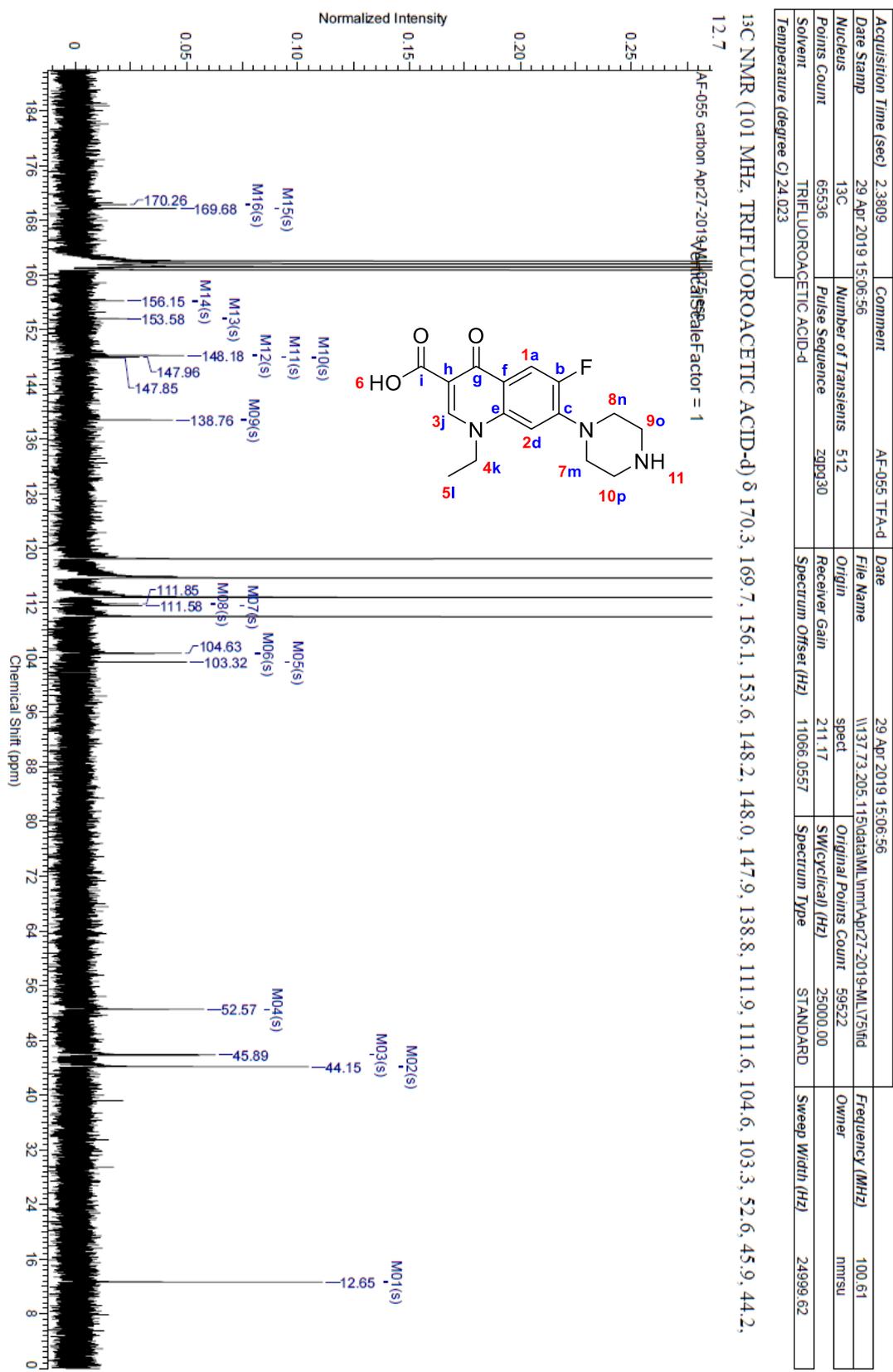
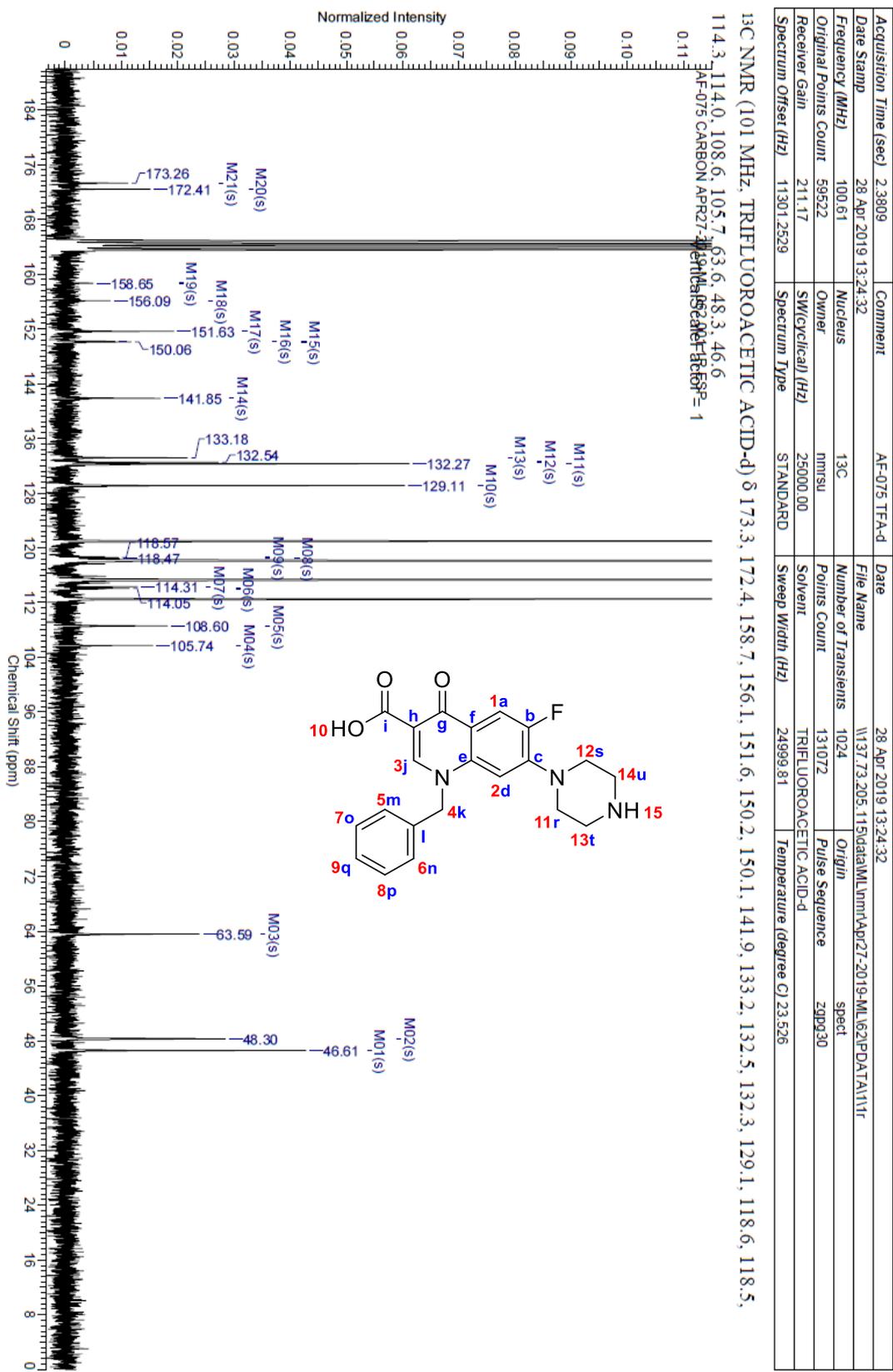


Figure S128. Carbon NMR spectrum of compound 5c.



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25/06/2019 15:37:25

Figure S129. Carbon NMR spectrum of compound 5d.

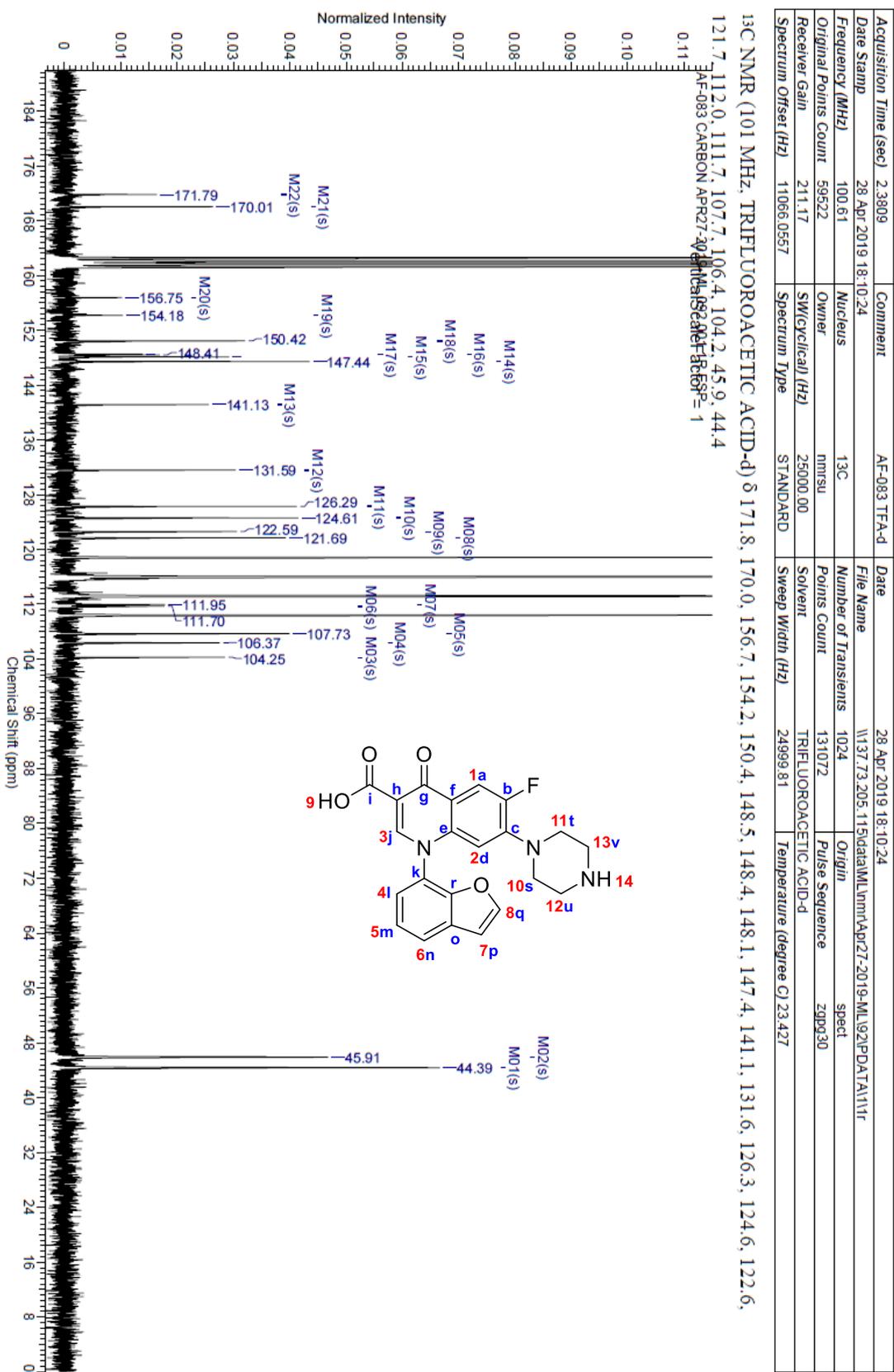
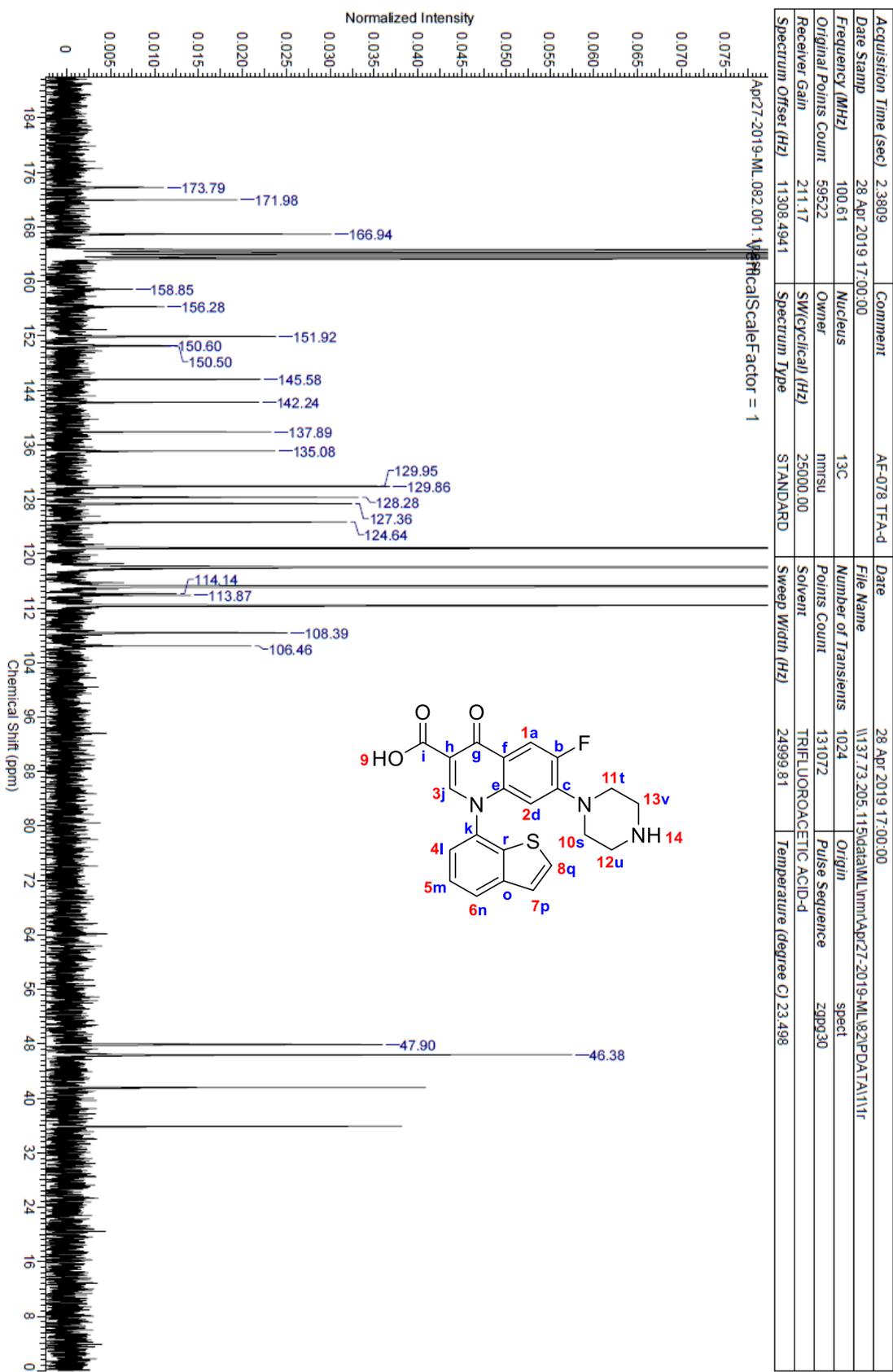


Figure S130. Carbon NMR spectrum of compound 5e.



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25/06/2019 16:26:50

Figure S131. Carbon NMR spectrum of compound 5f.

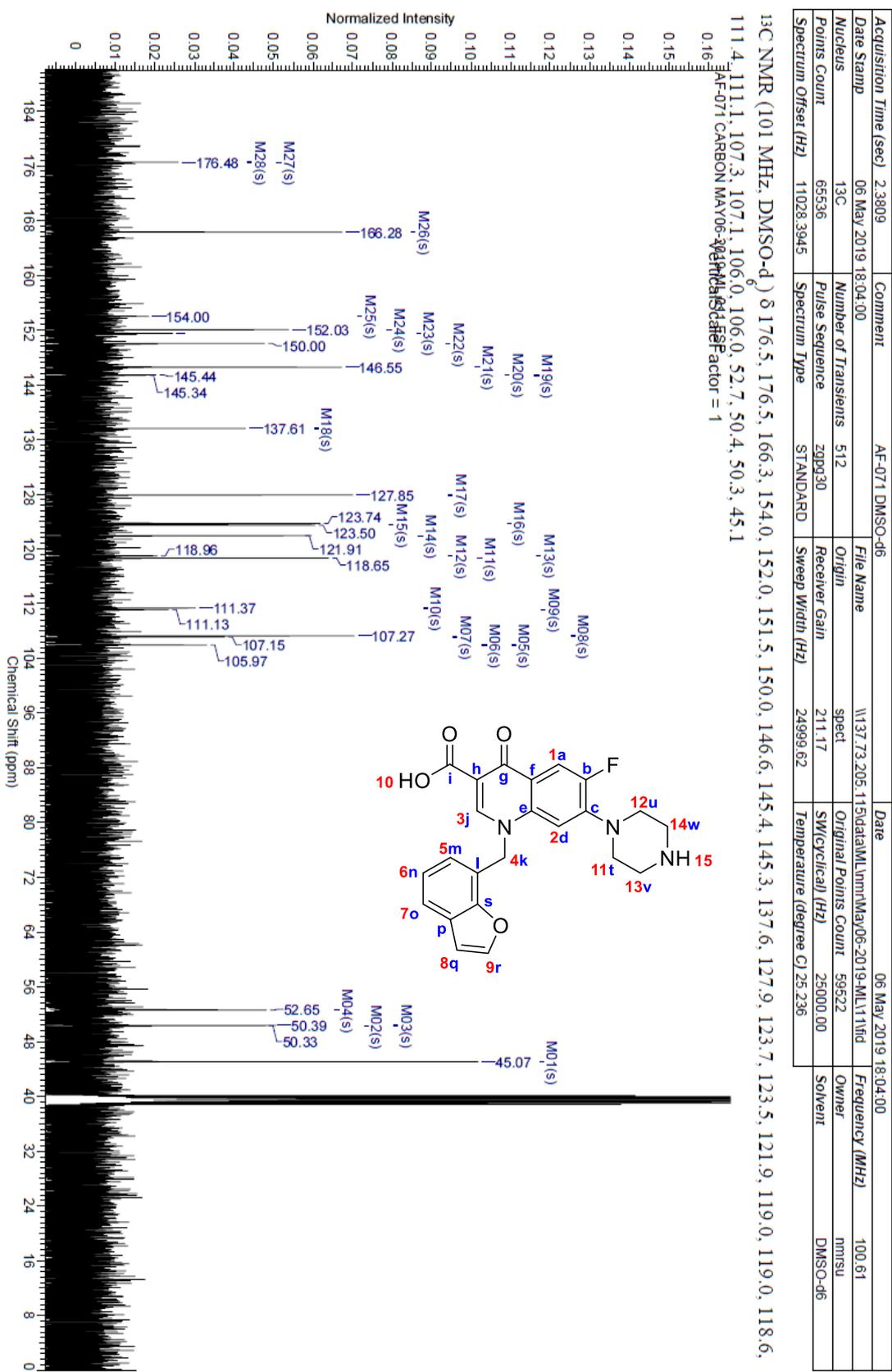


Figure S132. Carbon NMR spectrum of compound 6a.

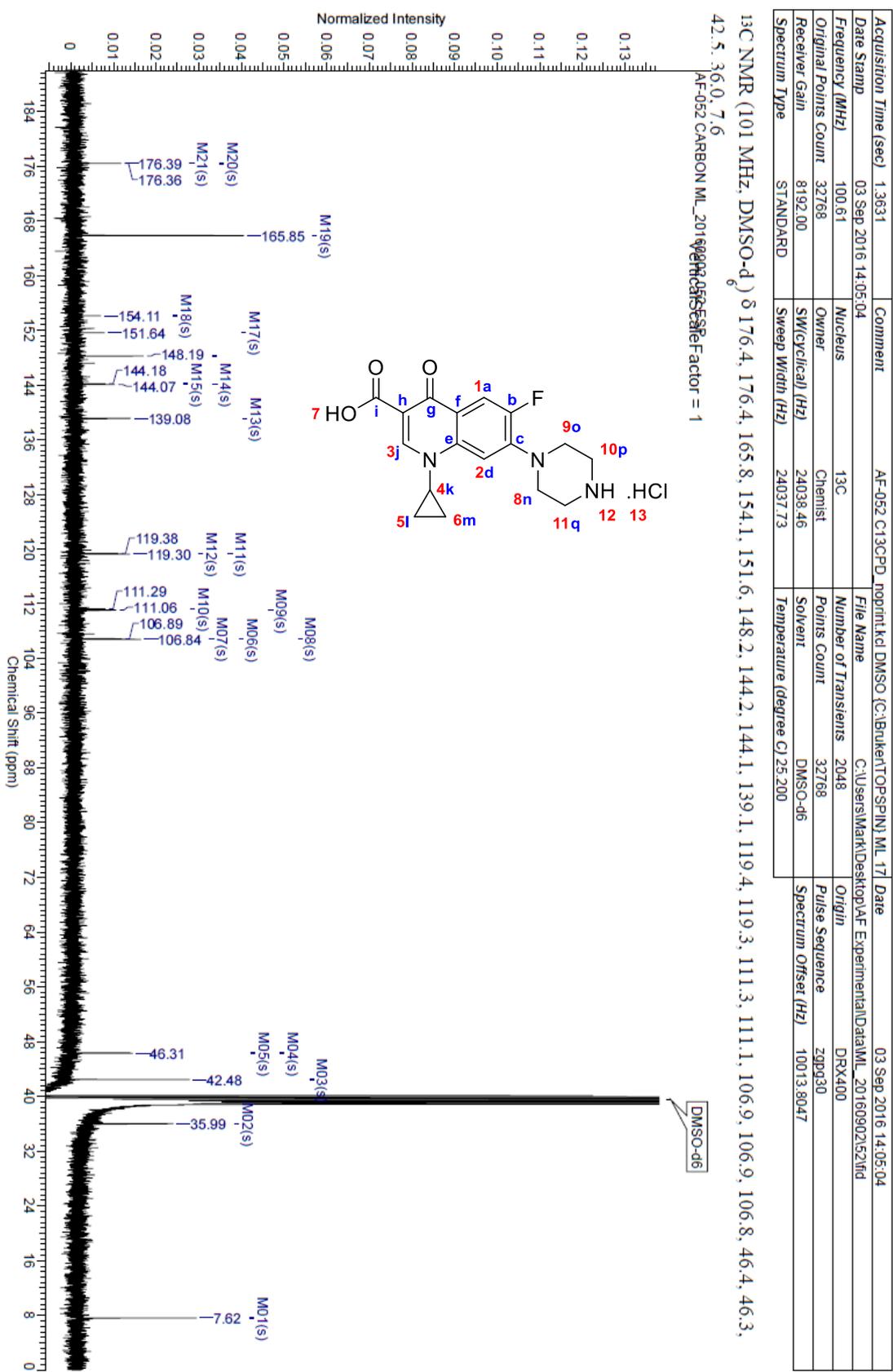


Figure S133. Carbon NMR spectrum of compound 6b.

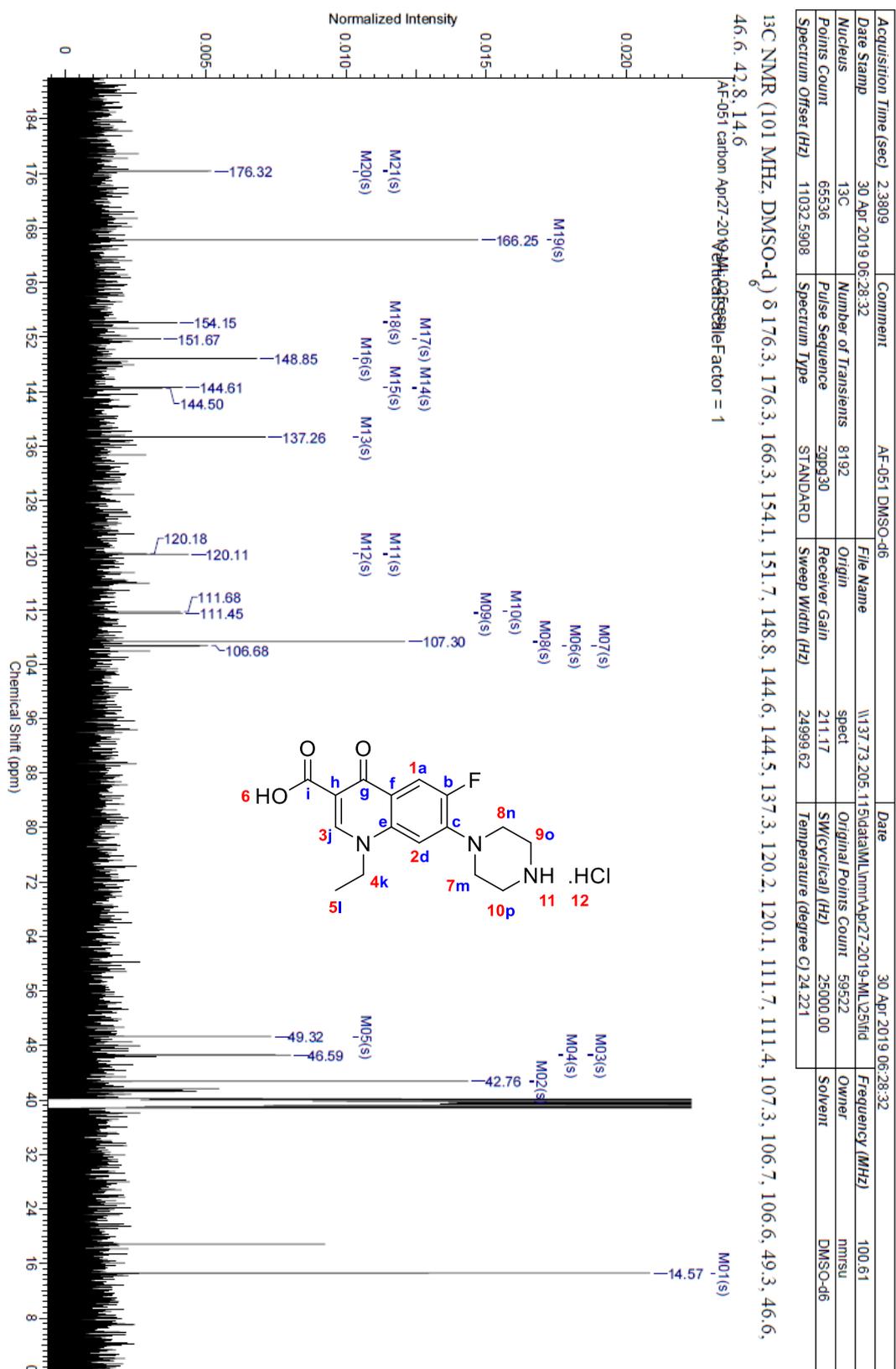
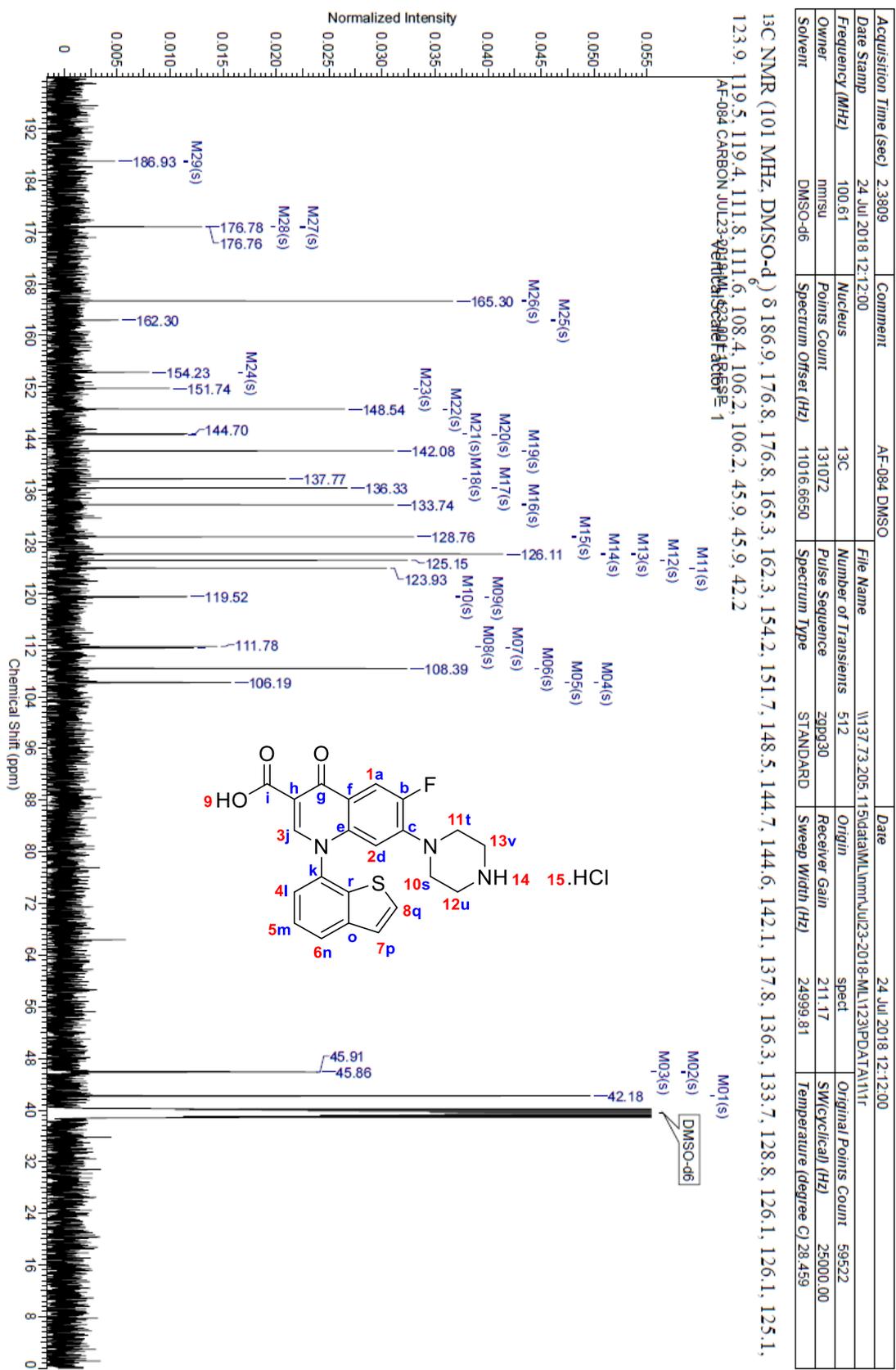


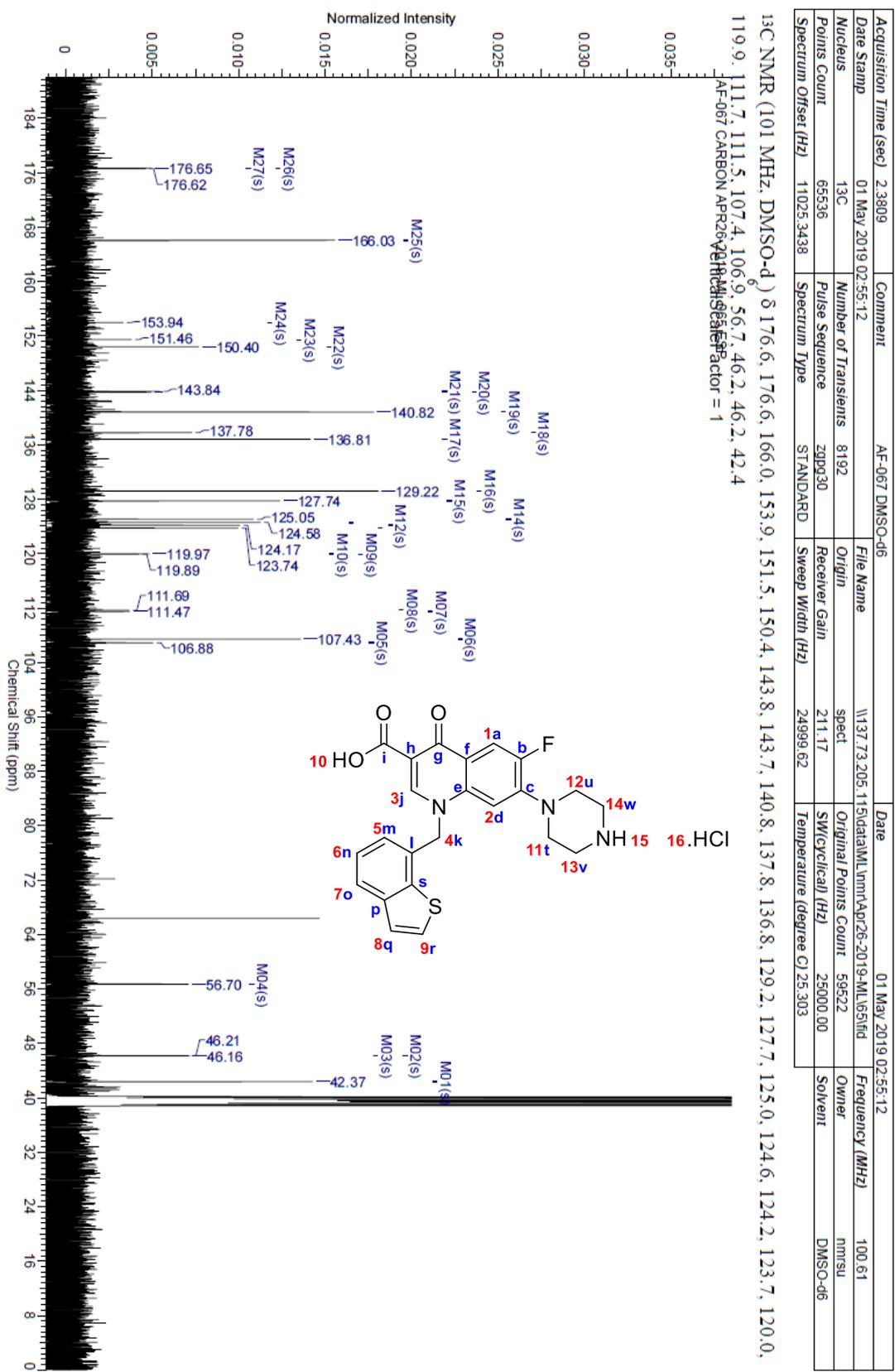
Figure S136. Carbon NMR spectrum of compound 6e.



This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

25/06/2019 16:06:13

Figure S138. Carbon NMR spectrum of compound 6g.

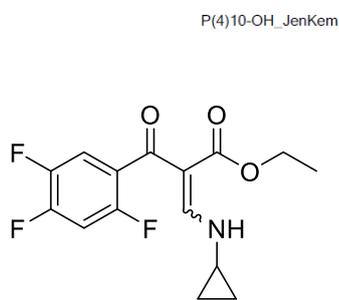
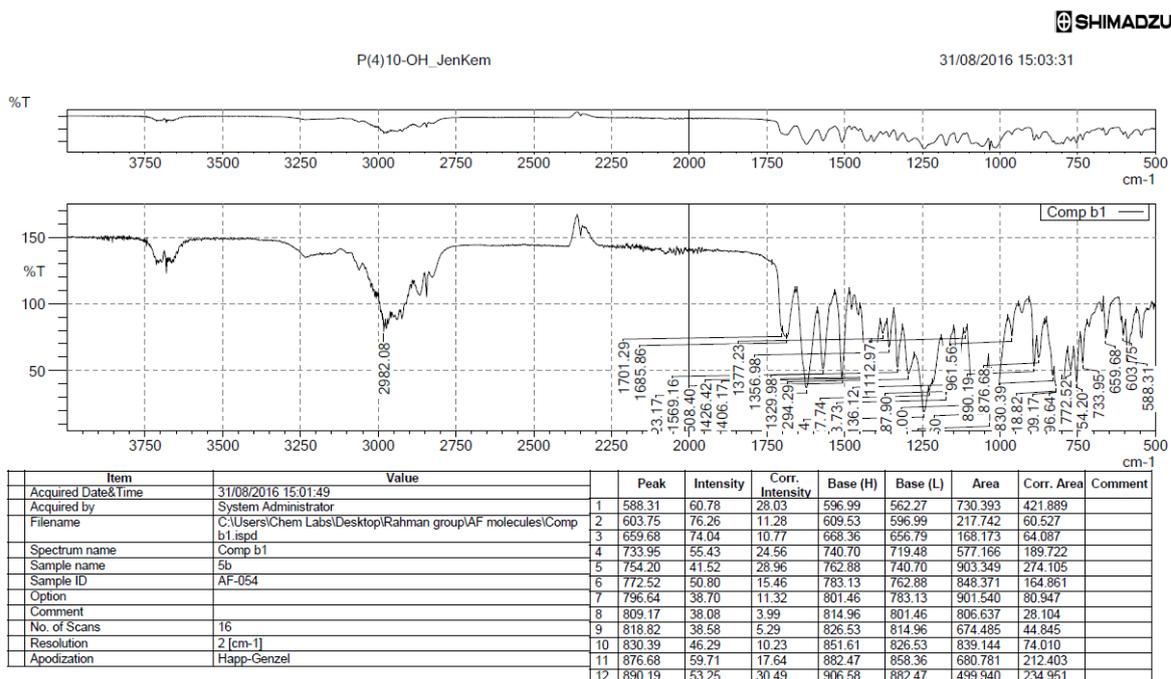


This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmpro/

25/06/2019 16:04:10

IR Spectra

Figure S139. IR spectrum of compound 2a.



SHIMADZU

13	961.56	75.88	18.31	975.06	942.27	346.275	185.153		
14	1014.60	22.03	39.05	1029.07	975.06	2683.904	1076.960		
15	1032.93	12.19	42.72	1037.75	1029.07	529.910	143.282		
16	1058.00	28.21	23.54	1077.29	1037.75	2449.751	549.827		
17	1087.90	38.85	18.56	1107.19	1077.29	1465.950	362.961		
18	1112.97	78.10	2.87	1116.83	1107.19	193.473	12.738		
19	1136.12	43.36	38.01	1148.66	1116.83	1195.379	593.600		
20	1173.73	31.78	46.10	1189.17	1148.66	1592.998	732.152		
21	1227.74	35.09	2.47	1230.64	1218.10	776.406	11.725		
22	1244.14	18.98	25.10	1275.00	1230.64	2715.021	455.885		
23	1294.29	47.41	24.81	1313.58	1275.00	1543.997	472.376		
24	1329.98	52.52	37.18	1342.51	1313.58	795.041	472.726		
25	1356.98	67.51	22.30	1364.70	1342.51	444.433	245.967		
26	1377.23	77.93	9.17	1383.98	1364.70	335.636	86.244		
27	1406.17	48.20	28.31	1414.85	1383.98	1022.220	397.180		
28	1426.42	48.96	32.24	1449.57	1414.85	1164.560	665.982		
29	1508.40	44.46	64.94	1530.58	1485.25	777.226	1203.980		
30	1569.16	51.50	48.44	1587.48	1532.51	954.819	1076.060		
31	1623.17	37.14	66.56	1654.03	1587.48	2084.863	2293.507		
32	1685.86	74.70	4.61	1688.75	1659.82	254.427	57.556		
33	1701.29	79.54	3.14	1734.08	1700.32	-462.630	-249.615		
34	2982.08	79.19	9.58	2984.97	2977.26	119.077	28.300		

Figure S140. IR spectrum of compound 2b.

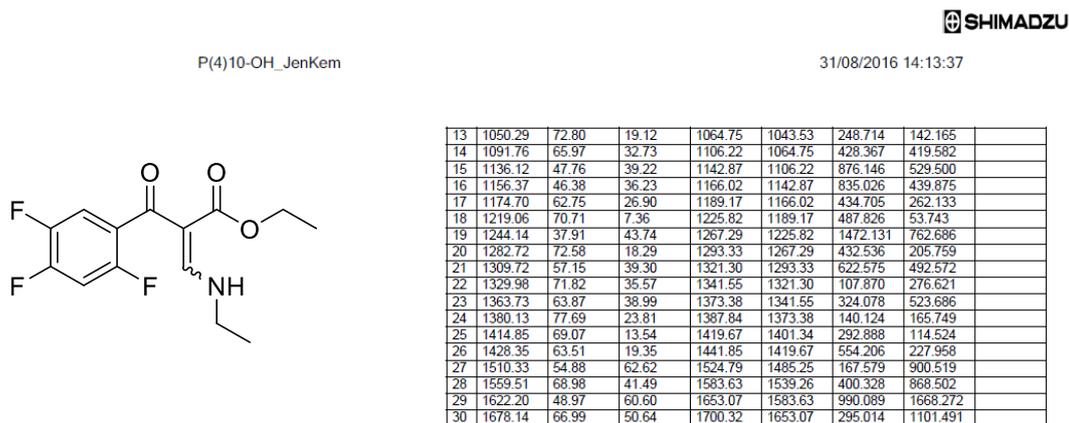
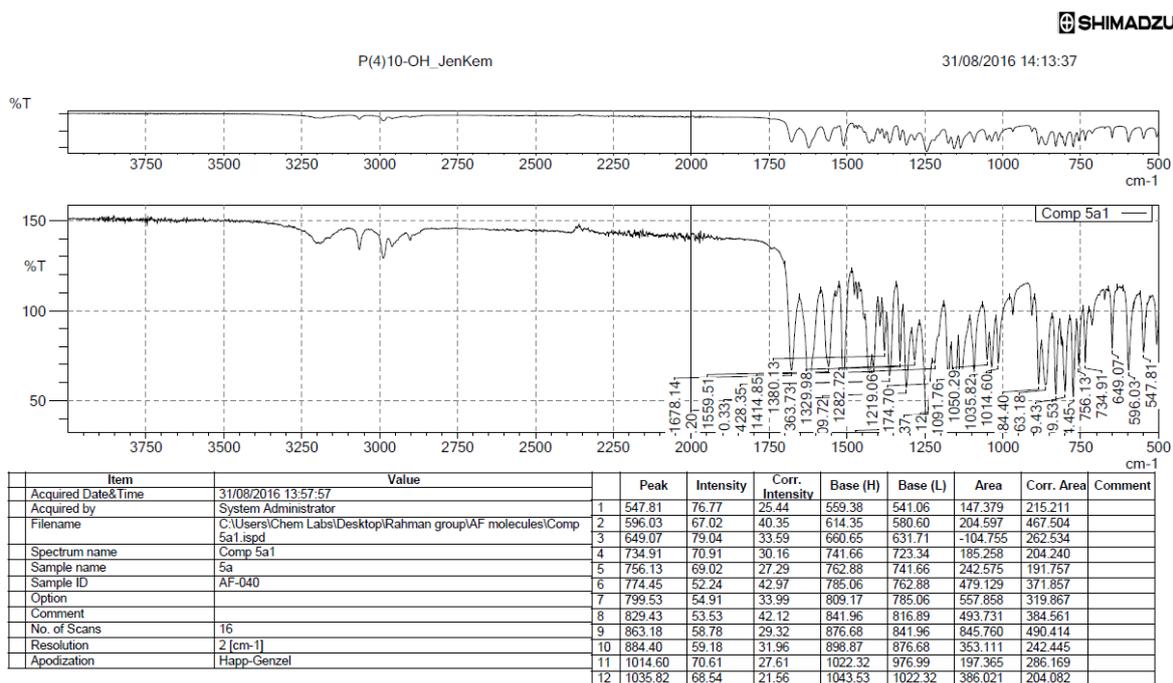


Figure S141. IR spectrum of compound 2c.

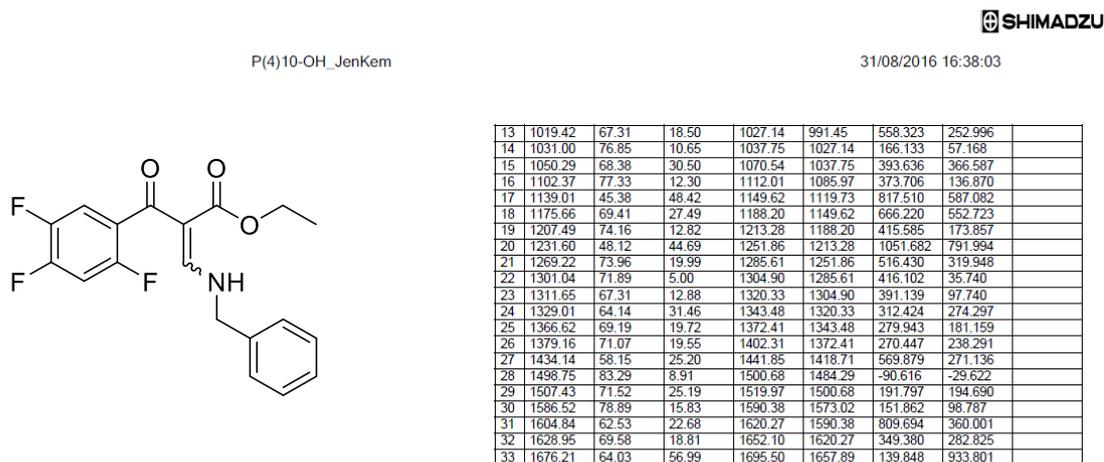
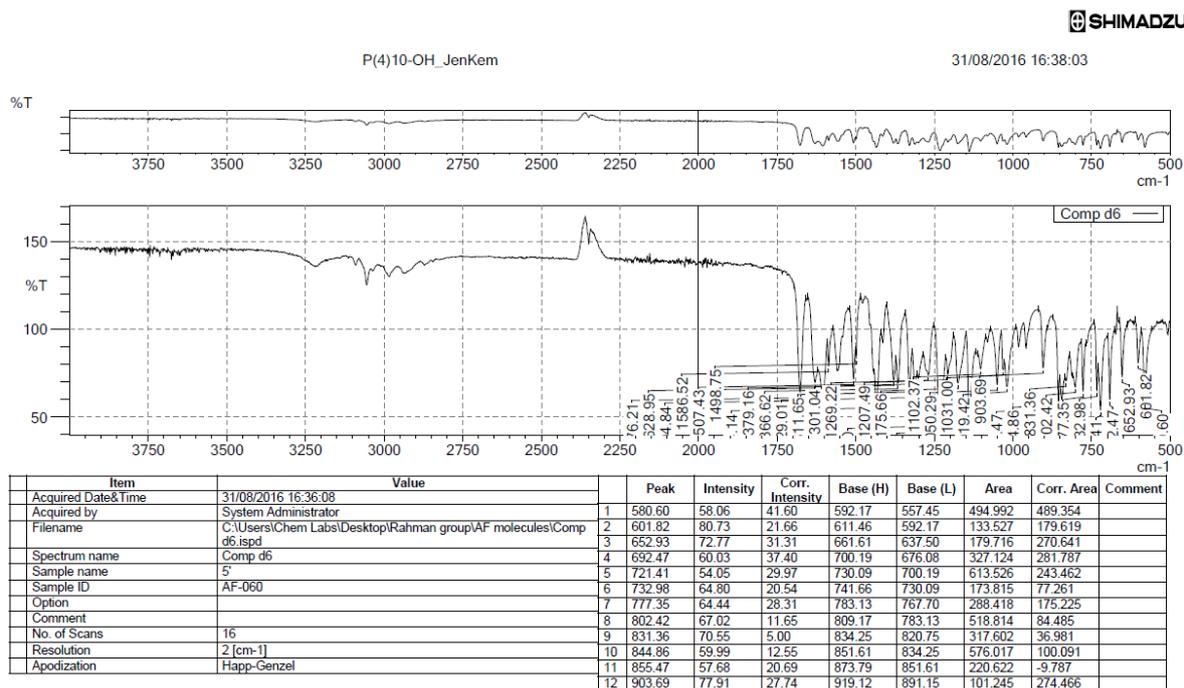


Figure S142. IR spectrum of compound 2d.

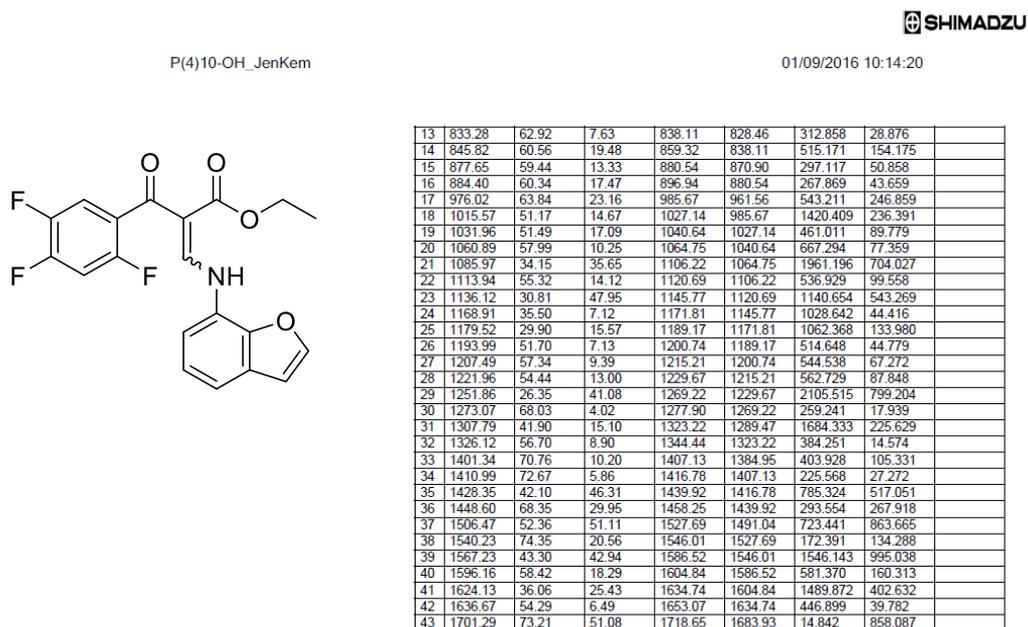
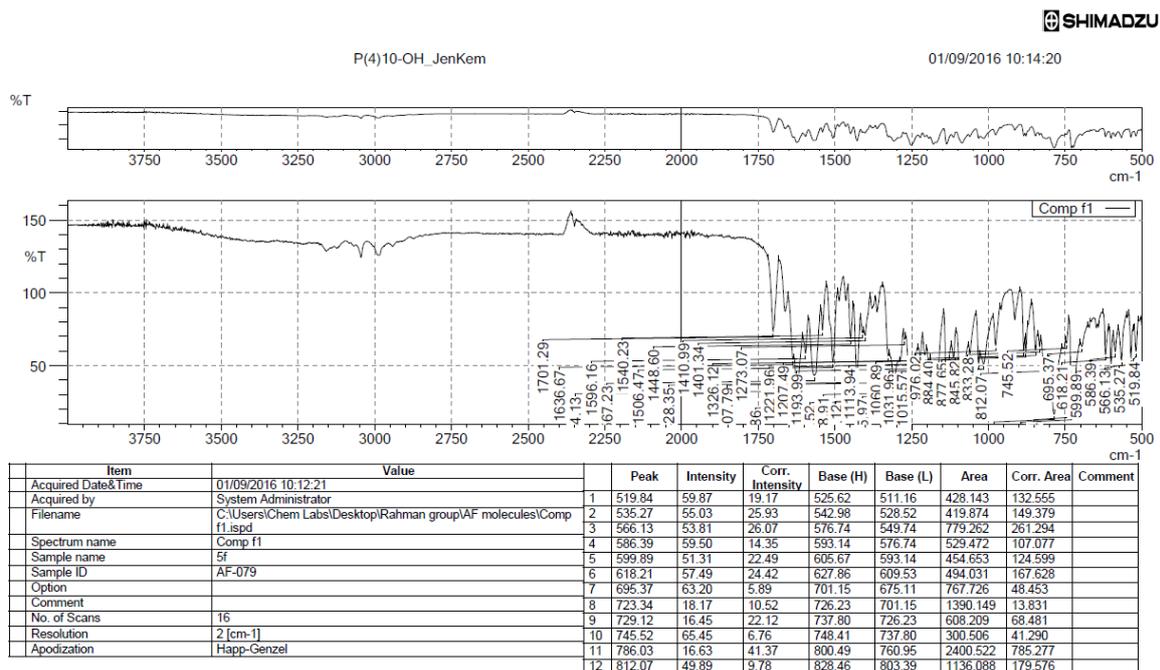
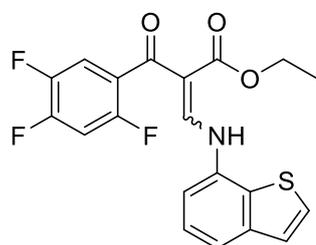
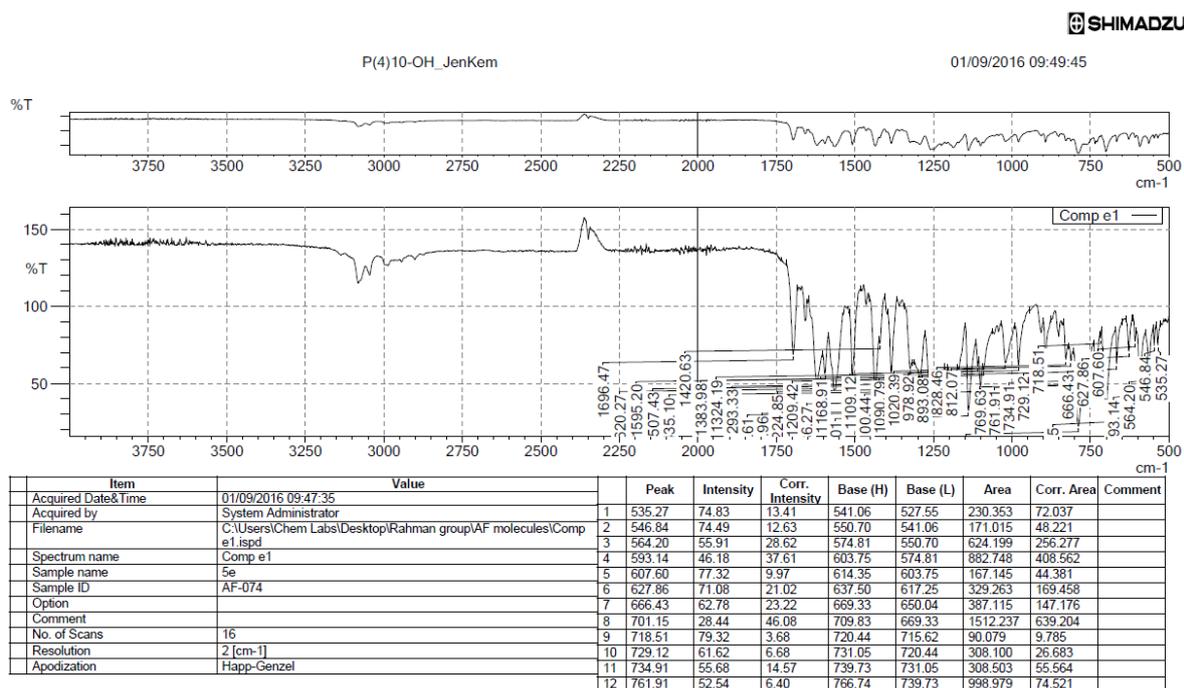


Figure S143. IR spectrum of compound 2e.



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13	769.63	52.87	2.41	772.52	766.74	266.729	7.948		
14	787.96	22.19	40.86	804.35	772.52	1807.454	638.980		
15	812.07	64.63	8.02	820.75	804.35	488.577	41.538		
16	828.46	65.50	16.59	836.18	820.75	387.588	111.065		
17	893.08	60.46	30.31	899.83	874.76	476.568	253.135		
18	978.92	61.80	28.39	991.45	945.16	709.844	363.947		
19	1020.39	63.20	25.28	1033.89	991.45	1025.193	524.630		
20	1090.79	58.68	4.62	1093.69	1061.86	854.291	-17.977		
21	1100.44	48.19	15.27	1106.22	1093.69	554.383	94.254		
22	1109.12	61.45	7.66	1114.90	1106.22	279.634	27.710		
23	1139.01	32.33	51.99	1149.62	1114.90	1382.964	763.354		
24	1168.91	58.95	6.29	1172.77	1149.62	679.222	82.673		
25	1186.27	41.96	13.15	1193.99	1172.77	1071.255	144.349		
26	1209.42	56.58	4.19	1214.24	1203.63	439.434	23.025		
27	1224.85	49.97	7.27	1229.67	1214.24	700.266	56.347		
28	1248.96	35.67	5.58	1253.78	1229.67	1338.506	50.977		
29	1258.61	34.75	12.22	1276.93	1253.78	1063.618	137.717		
30	1293.33	53.22	20.16	1310.69	1276.93	1237.001	329.684		
31	1324.19	59.37	14.91	1340.58	1317.44	526.724	107.061		
32	1383.98	57.02	42.76	1395.56	1365.66	518.765	539.817		
33	1420.63	75.93	6.89	1423.53	1405.20	160.671	20.933		
34	1435.10	47.70	41.30	1452.46	1423.53	813.005	571.265		
35	1507.43	51.71	48.57	1517.08	1481.39	431.927	569.905		
36	1595.20	56.36	17.95	1602.91	1584.59	601.338	148.069		
37	1620.27	49.92	33.27	1647.28	1602.91	1253.079	679.230		
38	1696.47	68.72	49.27	1717.68	1683.93	75.123	753.677		

Figure S144. IR spectrum of compound 2f.

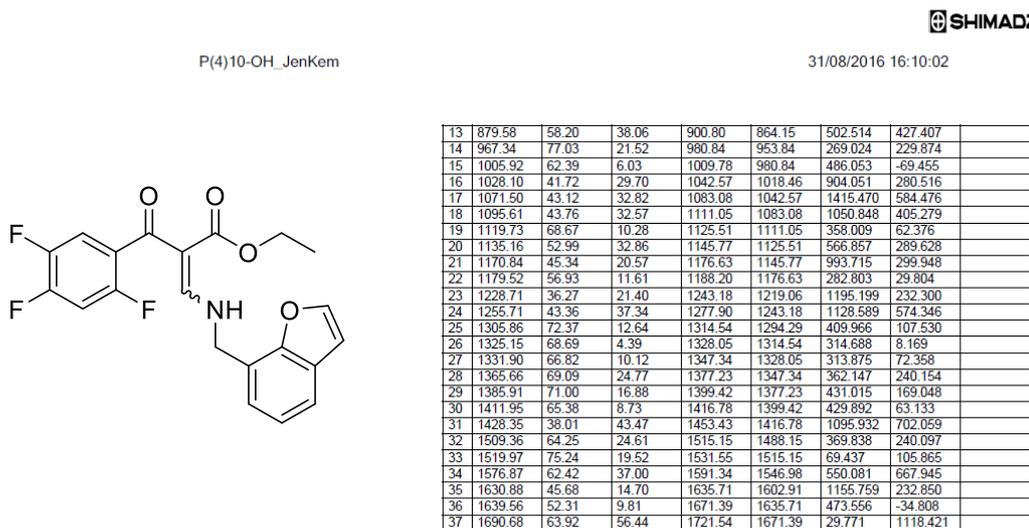
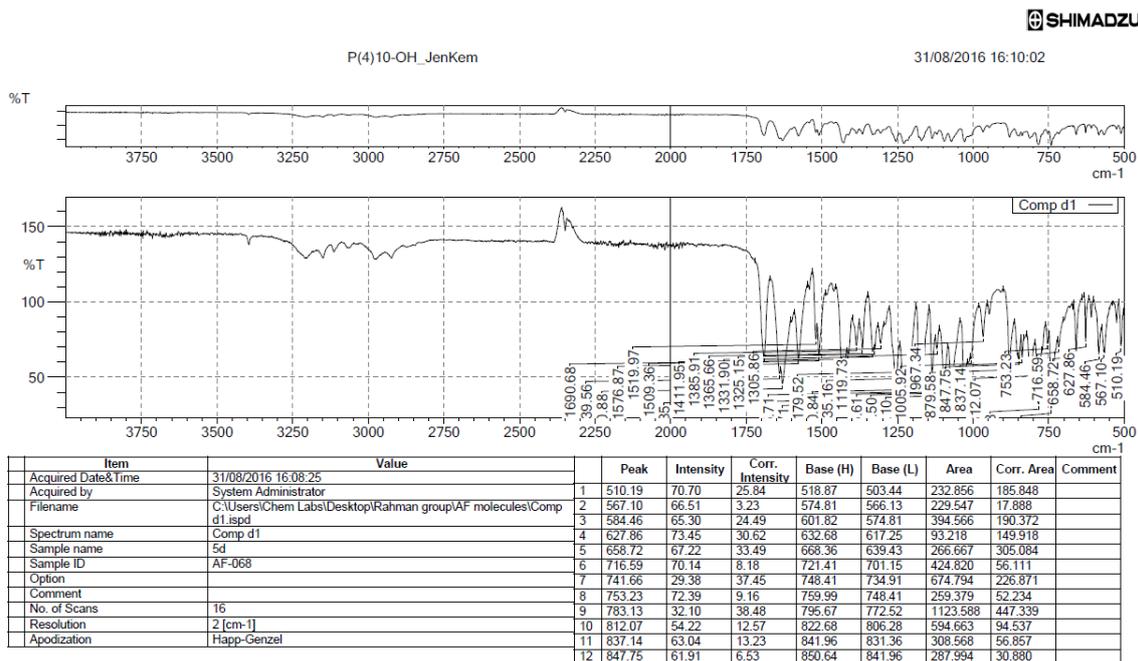


Figure S145. IR spectrum of compound 2g.

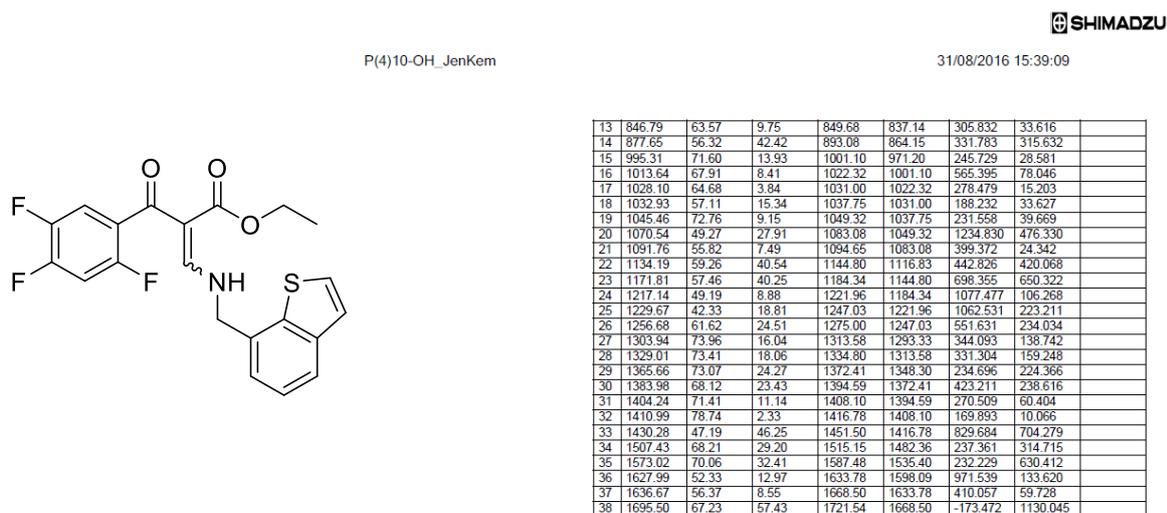
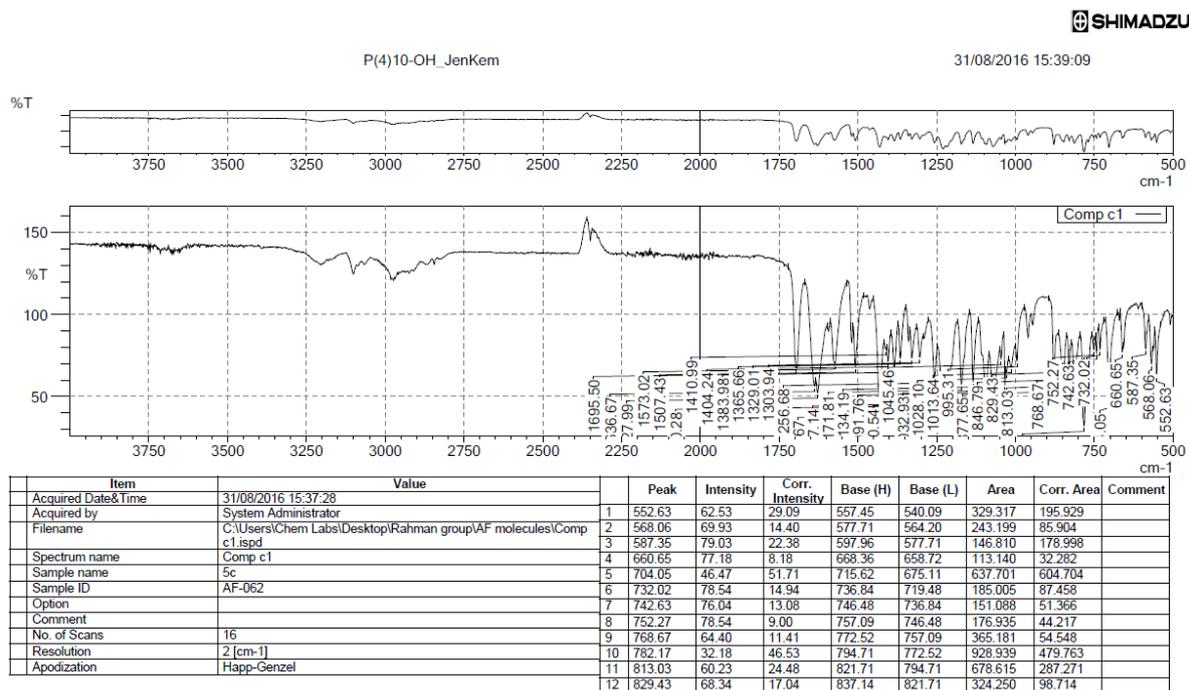


Figure S146. IR spectrum of compound 3a.

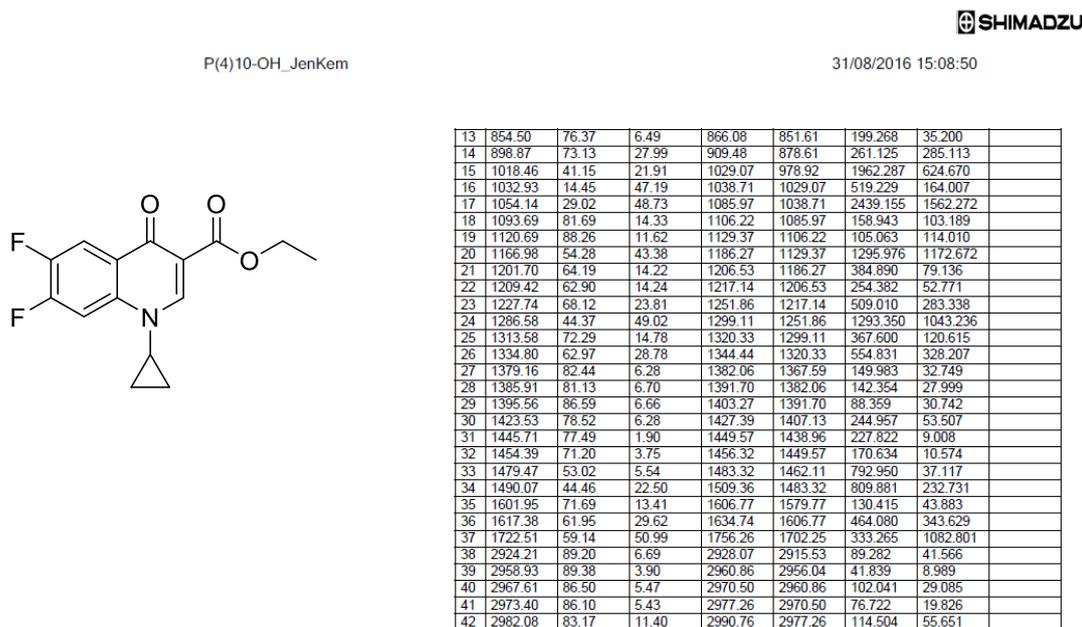
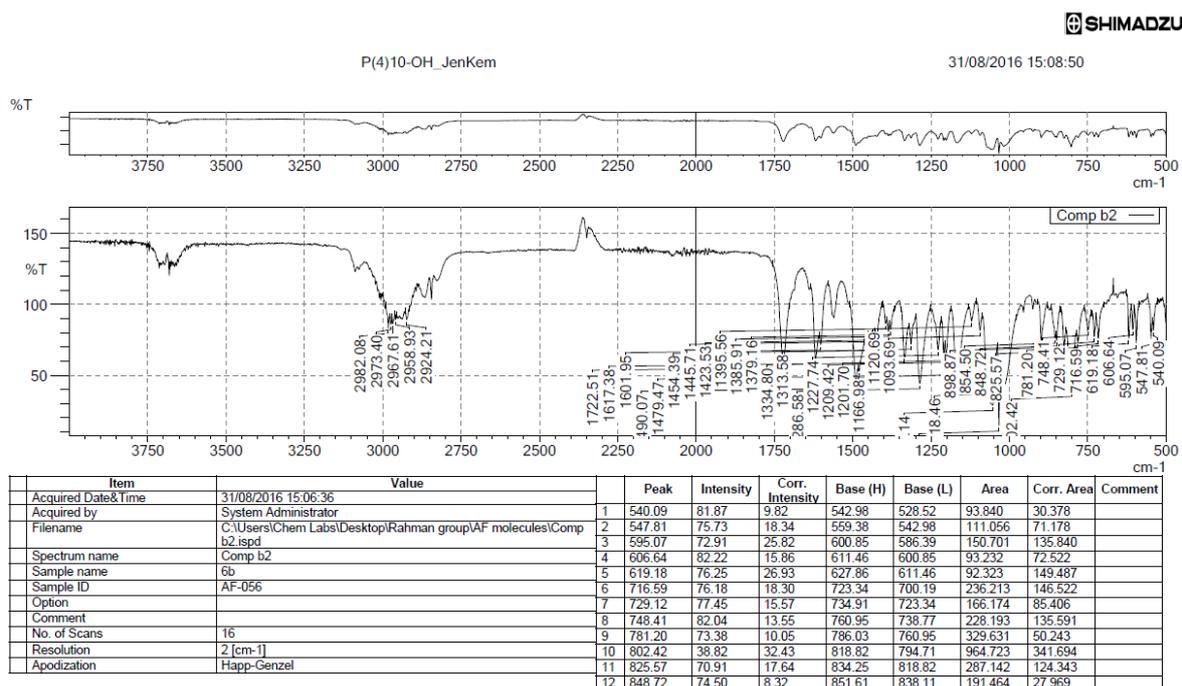


Figure S147. IR spectrum of compound 3b.

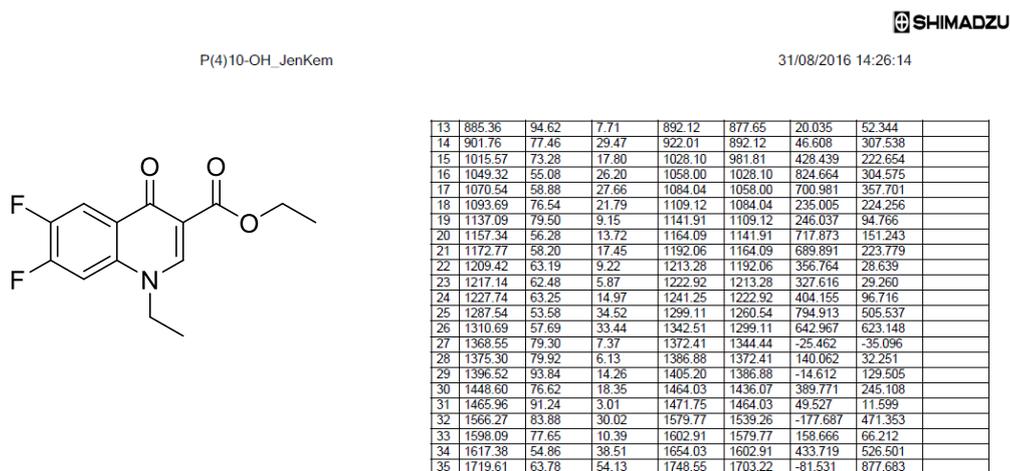
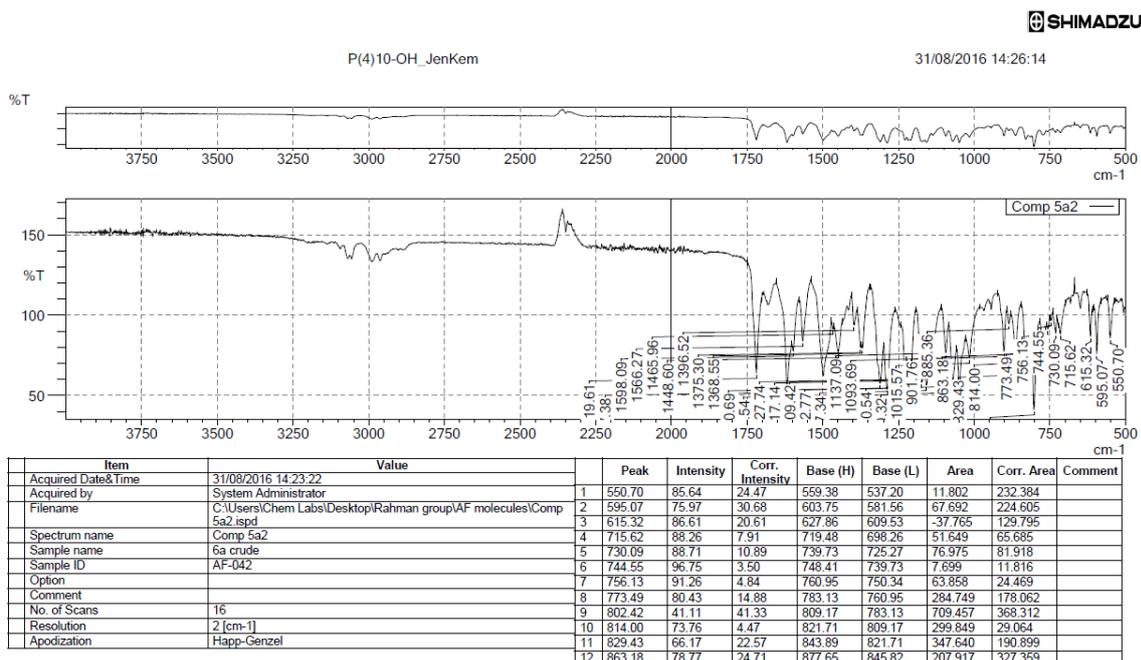
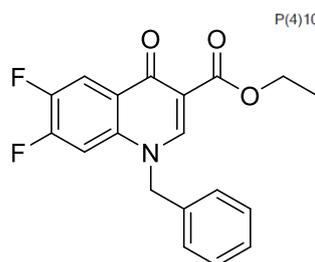
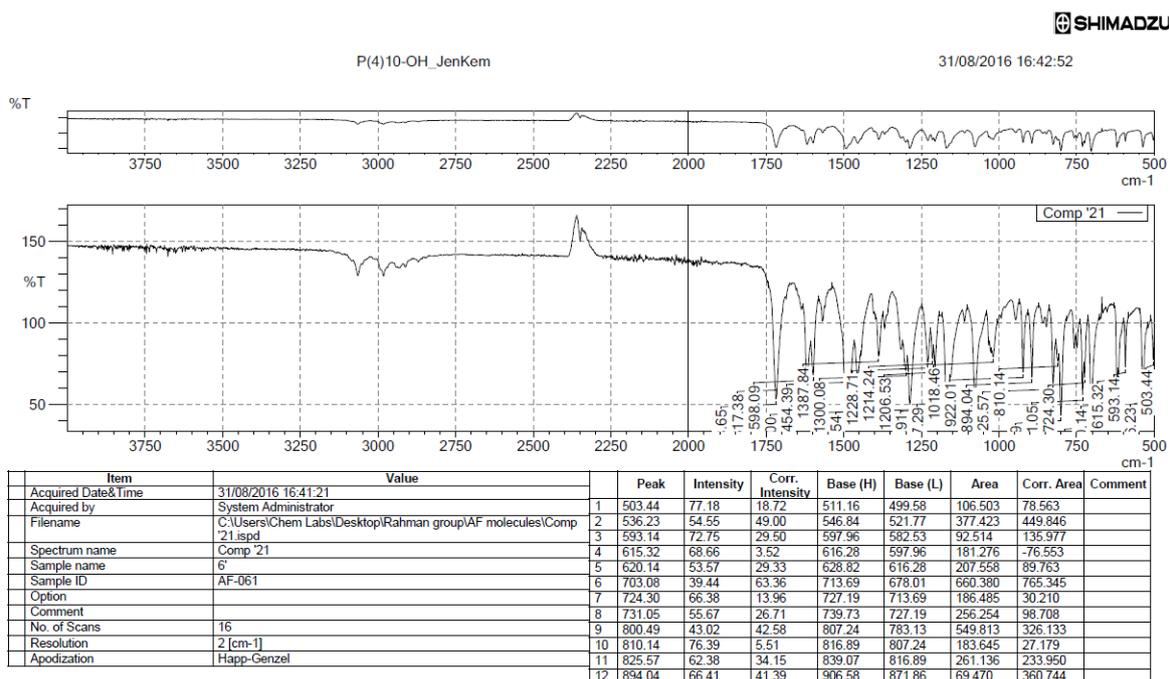
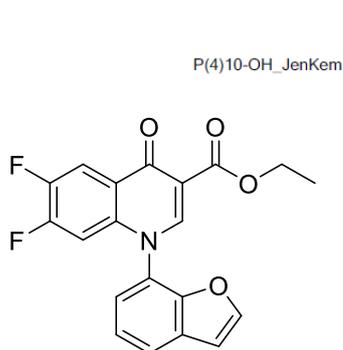
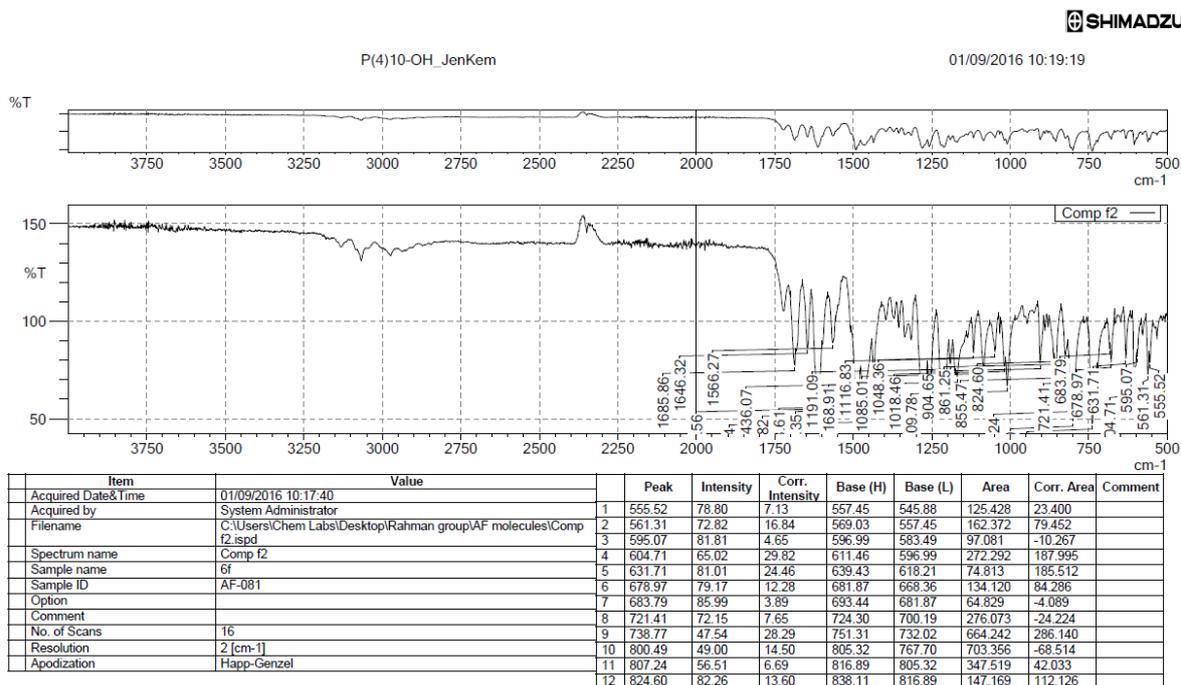


Figure S148. IR spectrum of compound 3c.



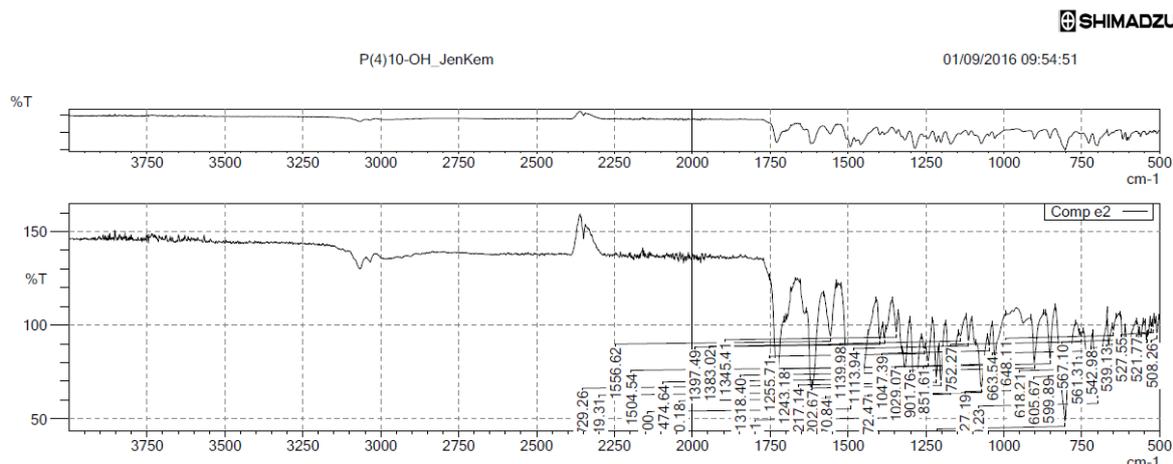
13	922.01	69.59	40.31	935.52	906.58	57.918	337.593	
14	1018.46	78.88	8.78	1023.28	1004.96	213.113	61.527	
15	1077.29	54.82	53.26	1101.40	1040.64	637.688	1107.126	
16	1168.91	50.52	32.50	1184.34	1157.34	753.321	368.462	
17	1206.53	72.77	16.42	1210.38	1193.02	200.812	113.314	
18	1214.24	77.88	10.84	1220.03	1210.38	146.418	47.539	
19	1228.71	75.30	24.23	1248.96	1220.03	201.080	275.915	
20	1287.54	49.75	33.04	1294.29	1248.96	656.202	389.579	
21	1300.08	70.54	11.15	1309.72	1294.29	355.298	91.732	
22	1387.84	79.40	24.83	1396.52	1373.38	149.044	252.802	
23	1454.39	66.86	17.09	1465.96	1445.71	488.912	173.387	
24	1492.00	48.52	26.73	1537.33	1481.39	534.534	167.753	
25	1598.09	67.94	28.36	1606.77	1580.73	217.471	241.163	
26	1617.38	62.61	34.16	1631.85	1606.77	398.900	362.210	
27	1718.65	53.18	54.57	1742.76	1702.25	457.305	871.822	

Figure S149. IR spectrum of compound 3d.



13	855.47	73.69	13.33	859.32	838.11	183.970	77.408	
14	861.25	80.68	4.07	875.72	859.32	126.094	-2.609	
15	904.65	78.41	27.32	913.33	893.08	134.653	239.943	
16	1009.78	66.93	16.99	1014.60	985.67	377.493	119.780	
17	1018.46	77.03	8.39	1030.03	1014.60	196.572	49.975	
18	1048.36	84.37	17.07	1063.79	1036.78	146.988	178.736	
19	1085.01	75.86	26.13	1102.37	1063.79	325.048	392.026	
20	1116.83	83.72	18.16	1125.51	1102.37	74.417	128.669	
21	1168.91	71.55	5.03	1172.77	1139.98	522.624	-1.079	
22	1191.09	78.11	11.15	1195.92	1183.38	204.588	69.808	
23	1211.35	57.83	13.90	1218.10	1195.92	675.986	158.445	
24	1258.61	59.56	23.22	1263.43	1235.46	495.012	254.351	
25	1279.82	55.59	20.02	1302.97	1273.07	622.293	277.522	
26	1436.07	70.51	22.49	1441.85	1410.02	226.209	199.120	
27	1491.04	50.95	22.60	1506.47	1484.29	630.228	183.399	
28	1566.27	89.01	17.07	1580.73	1557.59	-4.708	170.716	
29	1612.56	57.76	40.81	1634.74	1599.06	680.953	745.681	
30	1646.32	86.27	30.78	1662.71	1634.74	-103.971	384.025	
31	1685.86	77.40	12.30	1700.32	1682.96	169.014	157.564	

Figure S150. IR spectrum of compound 3e.

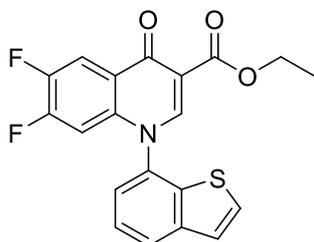


Item	Value	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area	Comment
Acquired Date&Time	01/09/2016 09:53:22	1	508.26	95.97	7.77	513.09	502.48	-1.905	38.483
Acquired by	System Administrator	2	521.77	99.01	4.54	525.62	518.87	-6.993	15.440
Filename	C:\Users\Chem Labs\Desktop\Rahman group\AF molecules\Comp e2.ispd	3	527.55	99.19	3.05	531.41	525.52	-4.926	9.470
Spectrum name	Comp e2	4	539.13	93.83	2.08	541.06	537.20	19.202	3.422
Sample name	6e	5	542.98	92.21	5.53	546.84	541.06	23.399	16.243
Sample ID	AF-076	6	561.31	87.03	11.99	565.17	552.63	58.593	57.150
Option		7	567.10	95.35	3.41	572.88	565.17	9.804	8.983
Comment		8	599.89	77.26	8.35	602.78	596.99	106.987	23.724
No. of Scans	16	9	605.67	76.64	14.16	610.50	602.78	107.756	49.561
Resolution	2 [cm-1]	10	618.21	79.94	22.65	625.93	610.50	114.806	154.794
Apodization	Happ-Genzel	11	648.11	97.25	3.85	651.00	638.47	-12.867	18.453
		12	663.54	89.29	16.68	668.36	651.00	75.656	146.978

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13	699.23	61.05	27.52	715.62	689.58	674.873	416.294		
14	727.19	68.76	27.66	744.55	715.62	465.145	365.841		
15	752.27	93.97	2.73	756.13	744.55	47.613	11.185		
16	803.39	48.84	56.91	834.25	769.63	1241.296	1600.846		
17	851.61	82.23	25.89	866.08	834.25	39.018	302.005		
18	901.76	79.99	24.98	914.30	871.86	108.707	343.907		
19	1029.07	82.18	19.69	1037.75	992.42	173.152	337.966		
20	1047.39	89.19	7.17	1052.21	1037.75	79.398	42.819		
21	1072.47	66.98	25.49	1091.76	1052.21	693.905	397.850		
22	1113.94	91.84	12.23	1122.62	1104.29	23.216	97.221		
23	1139.98	94.37	3.55	1144.80	1122.62	21.622	29.430		
24	1170.84	66.03	33.33	1187.24	1144.80	745.113	692.312		
25	1202.67	70.72	21.99	1209.42	1187.24	310.812	203.680		
26	1217.14	72.34	22.15	1228.71	1209.42	258.731	179.563		
27	1243.18	80.96	13.26	1251.86	1228.71	240.564	147.028		
28	1255.71	87.61	3.02	1264.39	1251.86	121.661	16.878		
29	1285.61	53.62	45.63	1302.01	1264.39	840.423	790.788		
30	1318.40	77.52	14.33	1325.15	1302.01	280.325	168.218		
31	1345.41	96.47	12.64	1358.91	1338.66	-100.428	105.739		
32	1383.02	93.06	5.97	1389.77	1378.20	41.196	32.136		
33	1397.49	92.55	13.12	1409.06	1389.77	-24.746	110.198		
34	1460.18	63.86	17.15	1465.96	1436.07	695.787	301.752		
35	1474.64	73.89	7.44	1481.39	1465.96	344.260	49.381		
36	1492.00	58.13	24.78	1501.65	1481.39	593.610	248.756		
37	1504.54	80.16	6.74	1522.87	1501.65	-4.070	23.081		
38	1556.62	94.20	25.74	1576.87	1539.26	-248.268	493.580		
39	1619.31	66.87	7.96	1634.74	1616.42	206.167	-7.577		
40	1729.26	70.57	44.10	1751.44	1706.11	197.419	851.406		

Figure S151. IR spectrum of compound 3f.

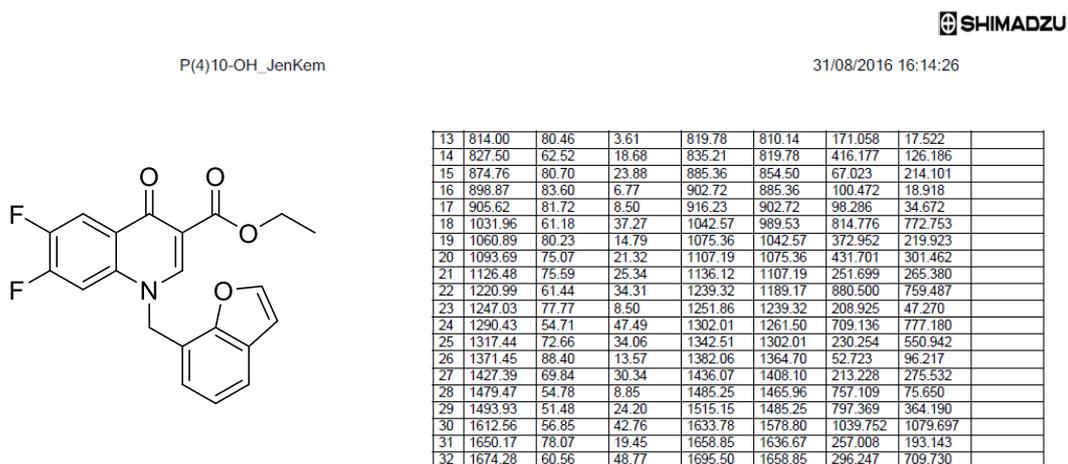
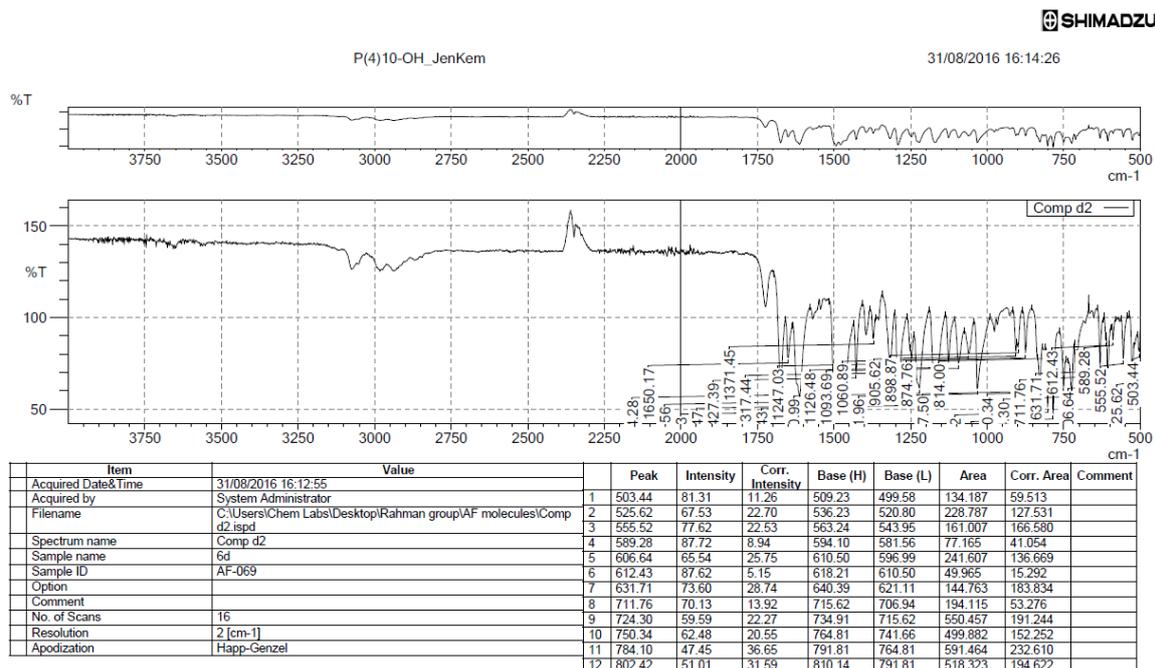


Figure S152. IR spectrum of compound 3g.

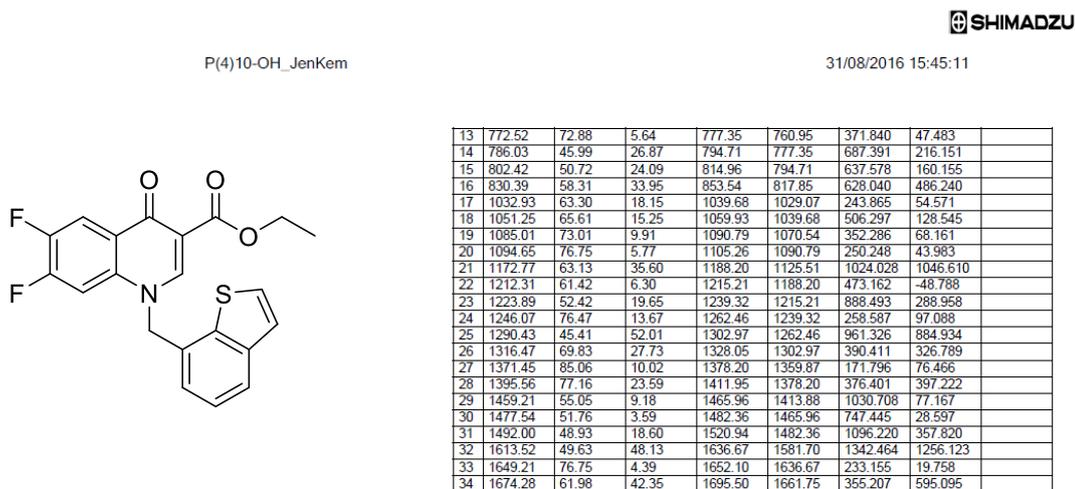
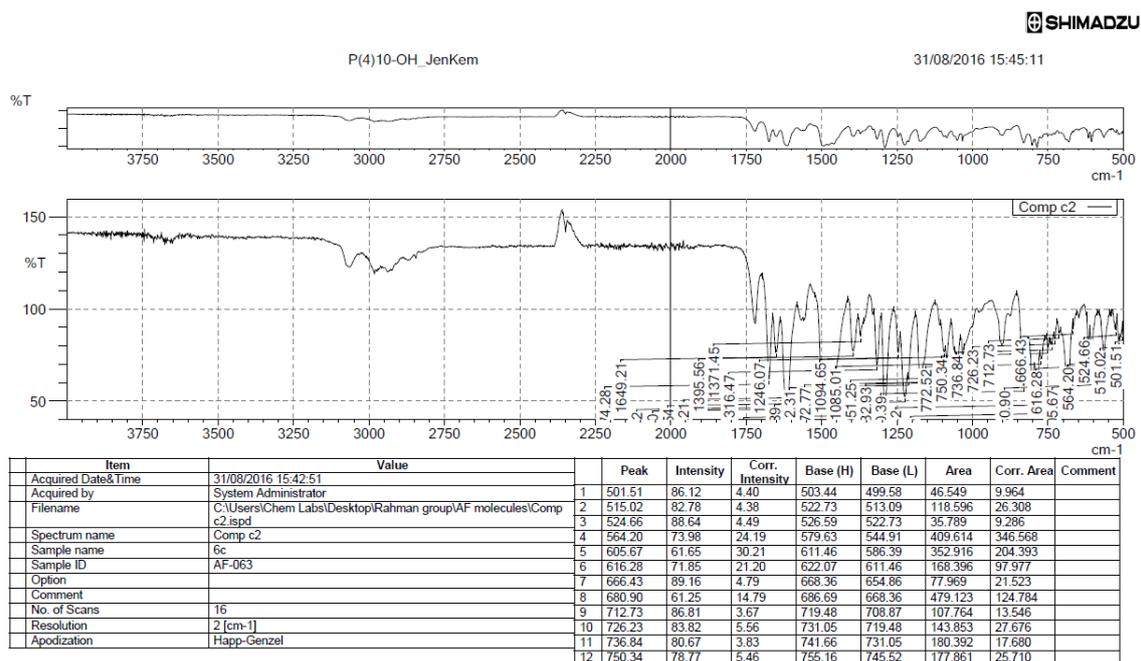


Figure S153. IR spectrum of compound 4a.

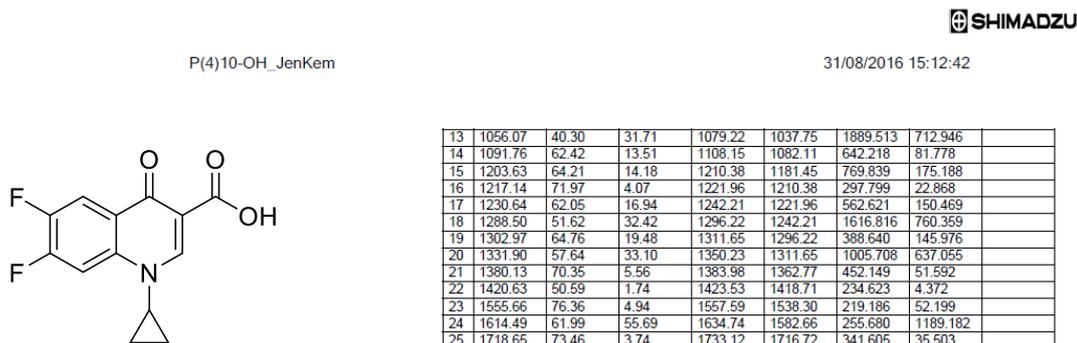
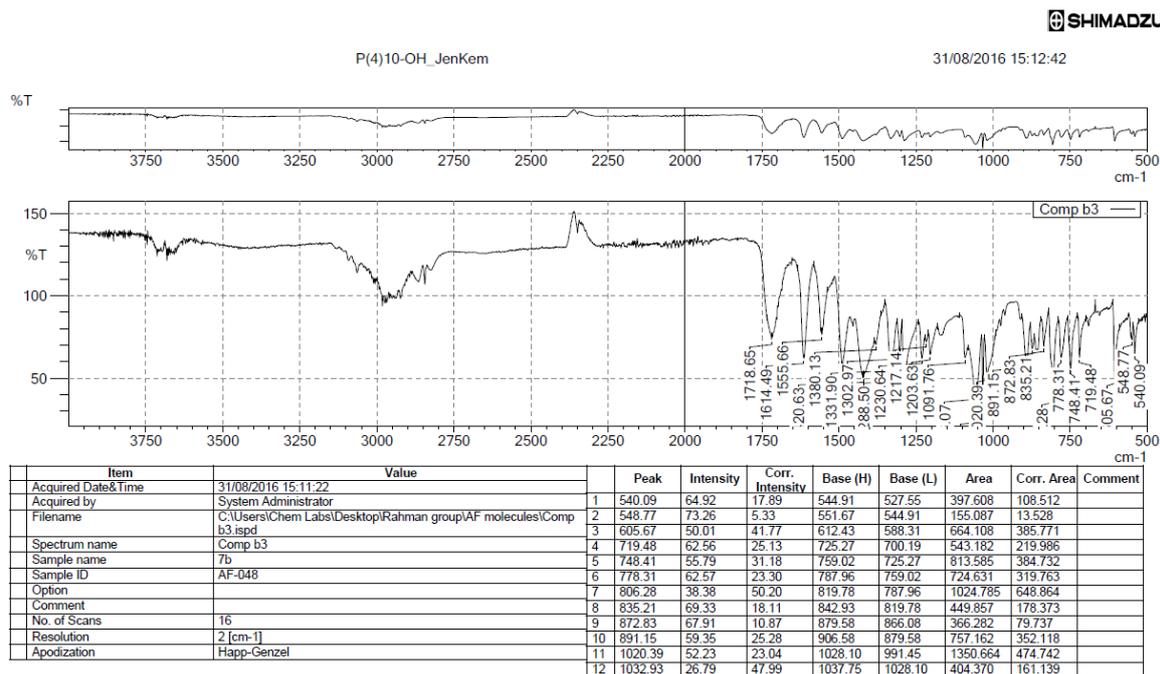


Figure S154. IR spectrum of compound 4b.

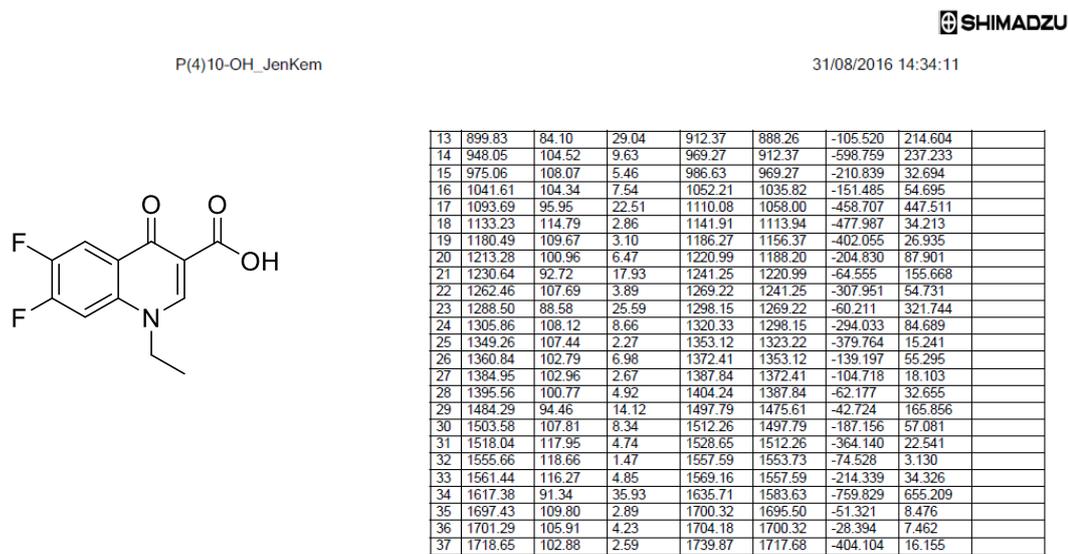
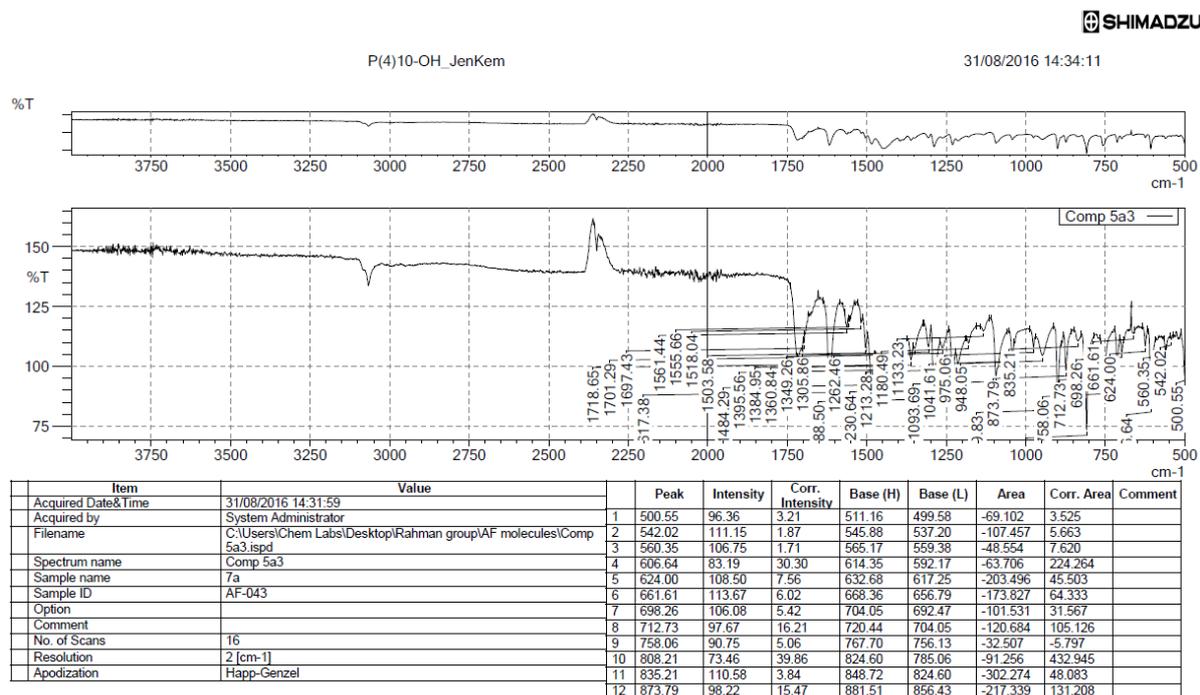


Figure S155. IR spectrum of compound 4c.

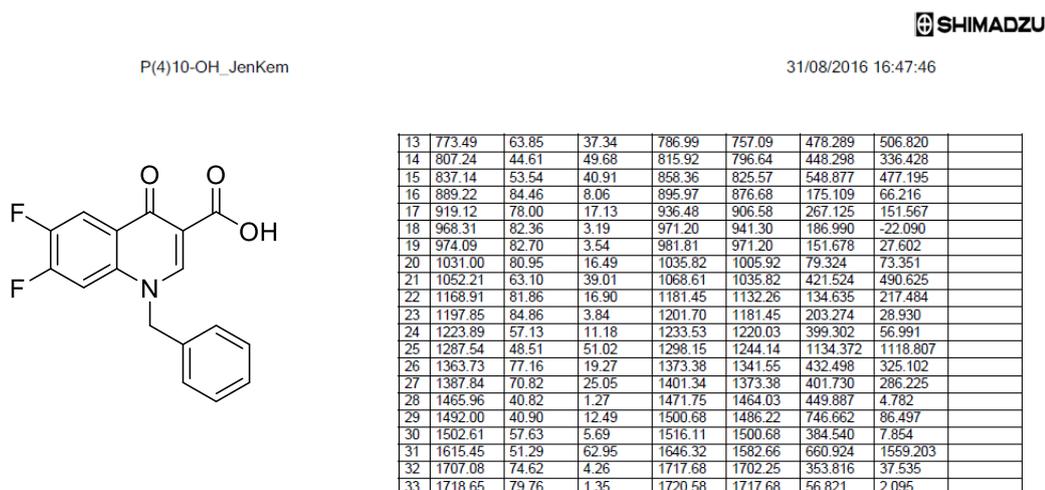
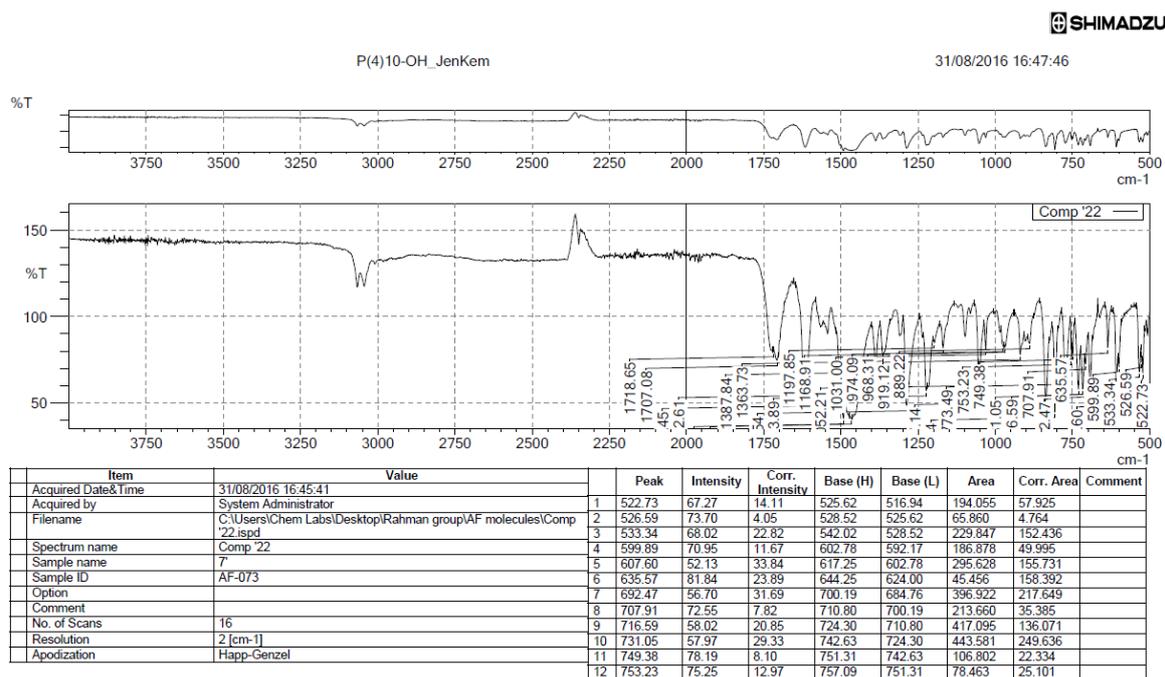


Figure S156. IR spectrum of compound 4d.

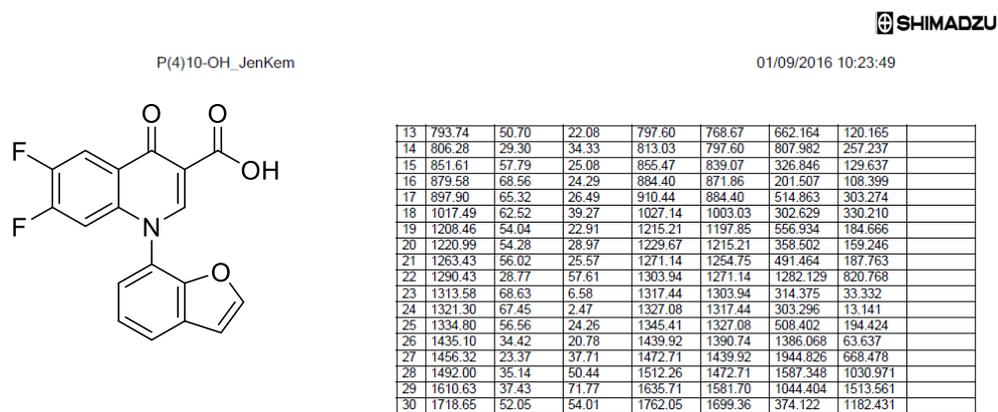
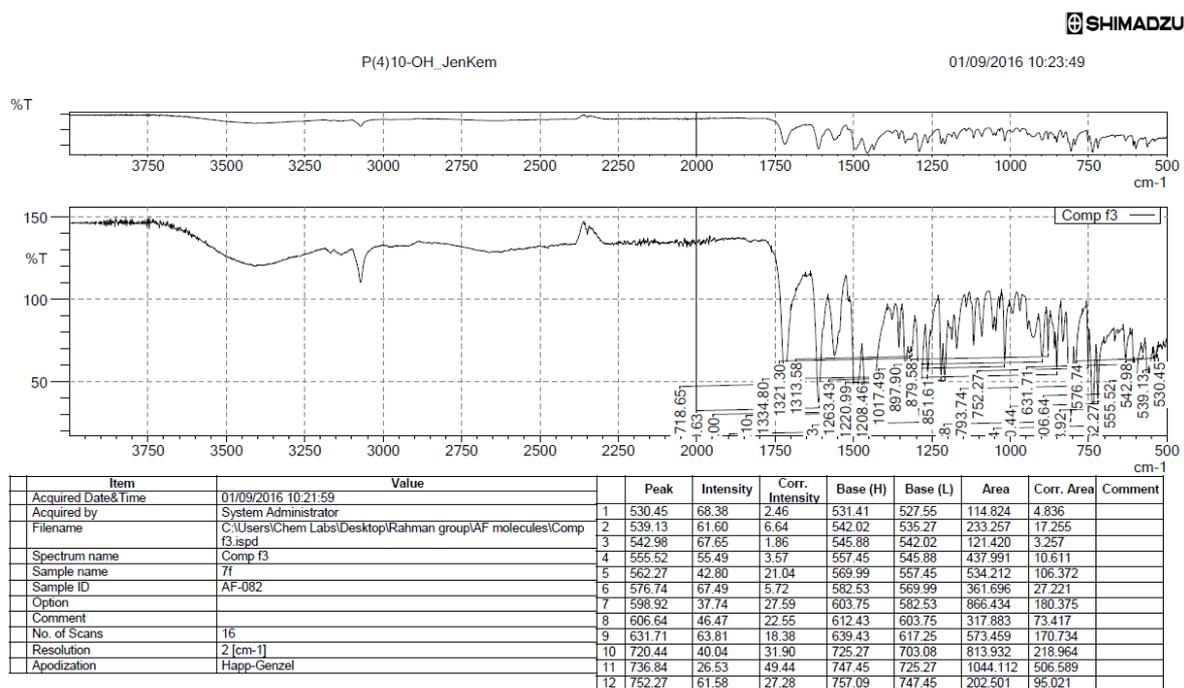


Figure S157. IR spectrum of compound 4e.

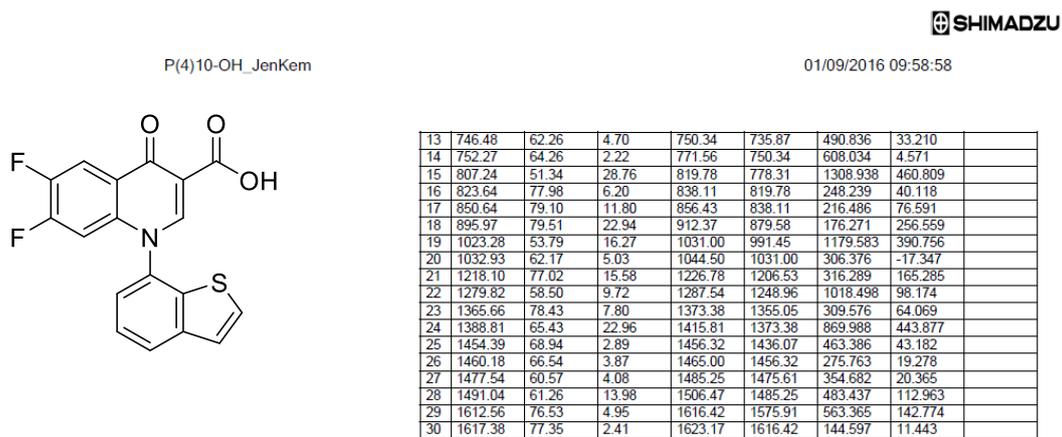
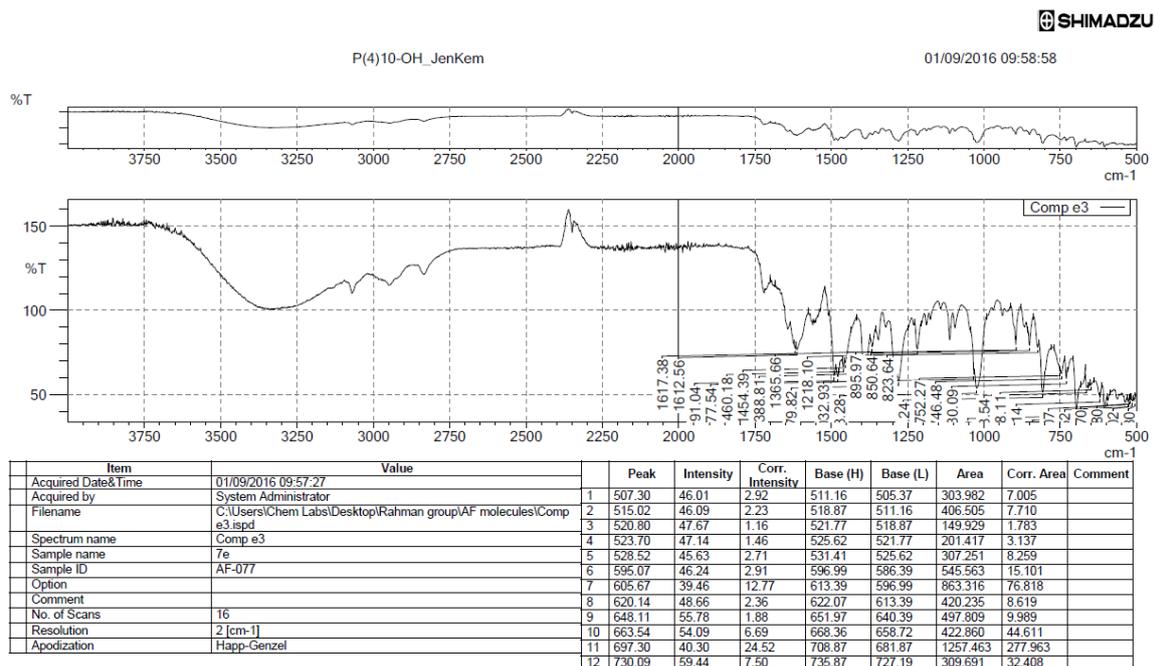


Figure S158. IR spectrum of compound 4f.

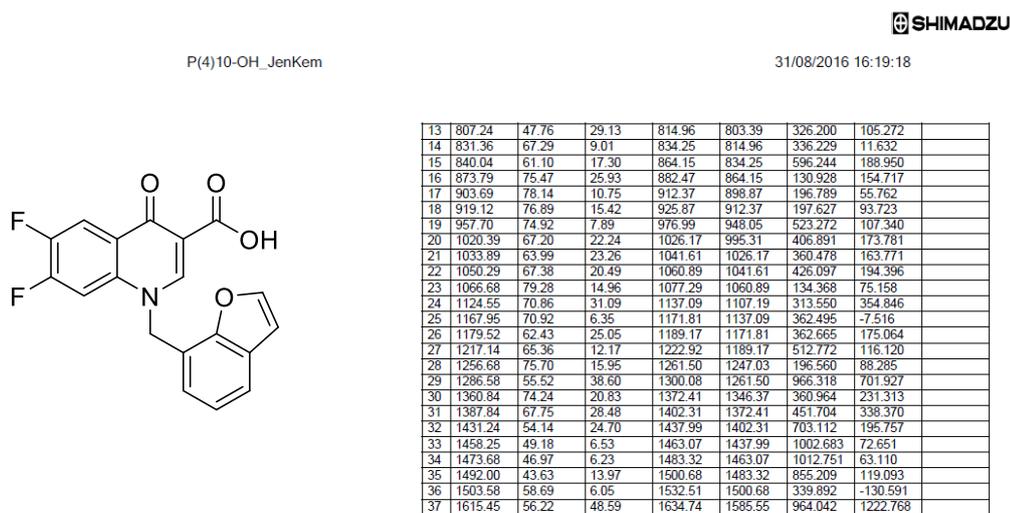
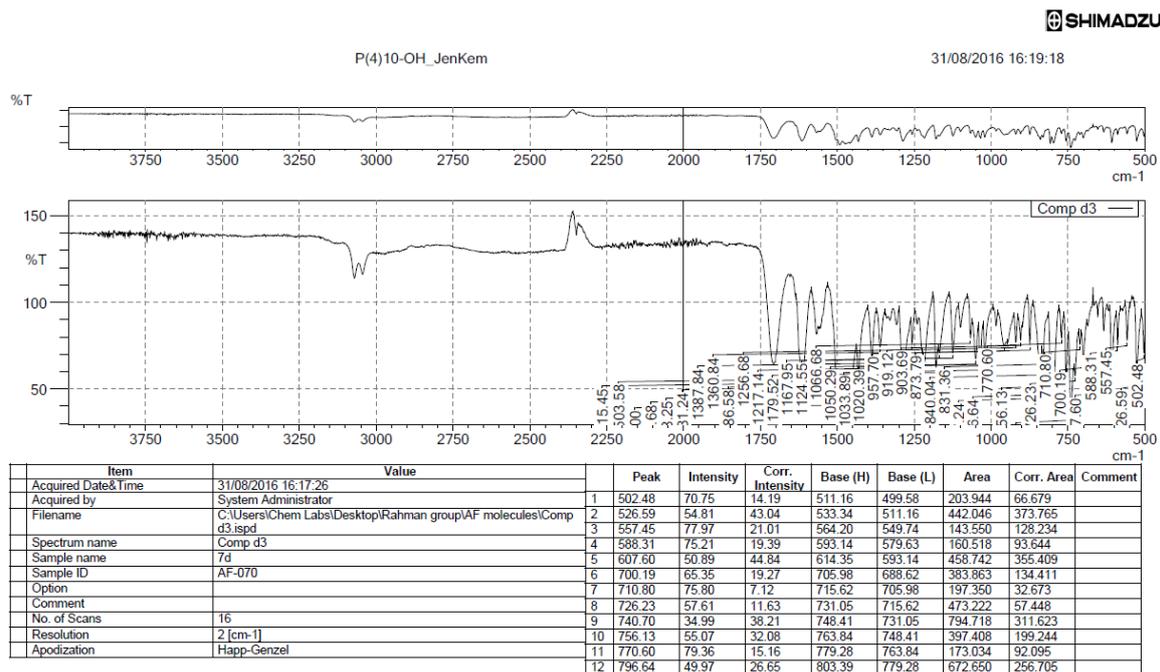
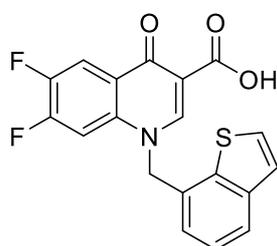
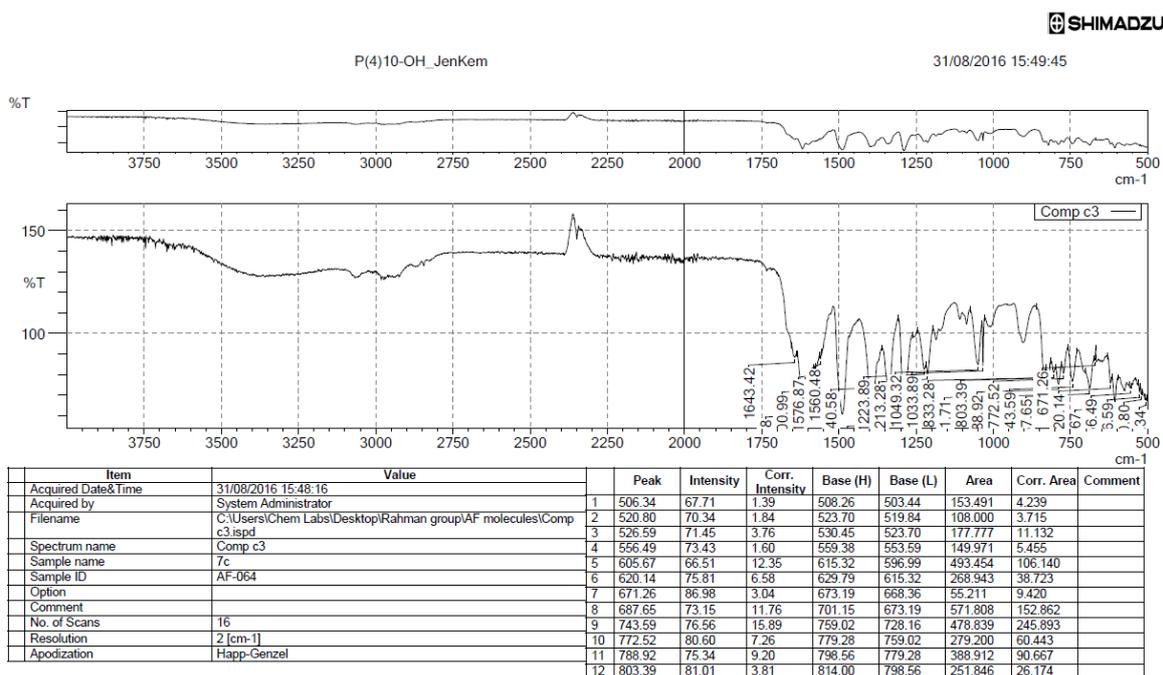


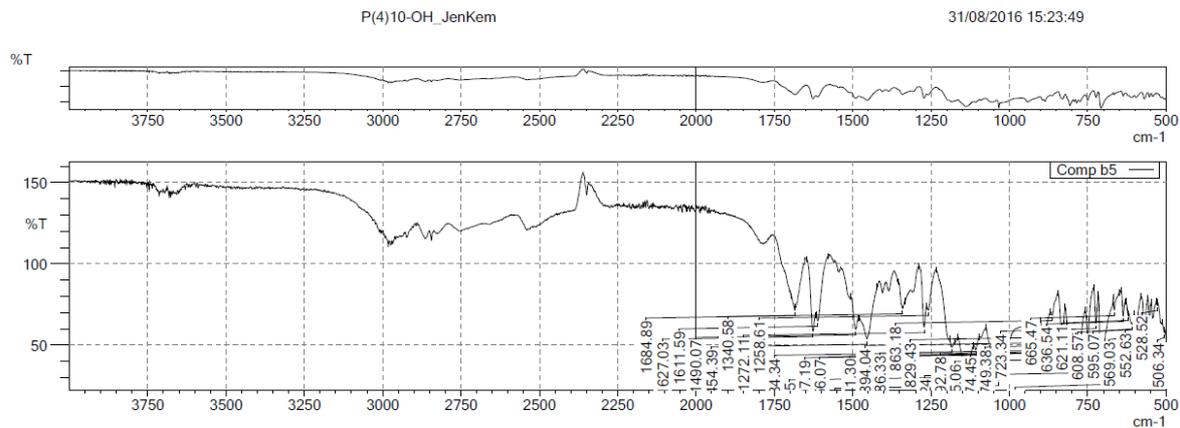
Figure S159. IR spectrum of compound 4g.



13	821.71	72.65	12.58	829.43	814.00	310.304	82.405		
14	833.28	81.00	6.19	861.25	829.43	73.462	23.467		
15	1033.89	84.47	21.54	1036.78	1028.10	9.523	65.356		
16	1049.32	84.91	22.35	1076.33	1036.78	89.253	423.529		
17	1213.28	80.36	8.23	1218.10	1194.95	218.272	72.213		
18	1223.89	82.62	5.88	1245.10	1218.10	226.771	43.539		
19	1289.47	58.73	45.60	1307.79	1262.46	740.575	900.646		
20	1340.58	76.55	21.96	1359.87	1307.79	539.692	560.797		
21	1560.48	87.67	2.46	1562.41	1557.59	54.221	7.313		
22	1576.87	82.52	1.71	1581.70	1574.95	111.177	3.893		
23	1600.99	75.26	3.81	1607.74	1581.70	556.802	52.006		
24	1617.38	63.17	18.78	1634.74	1607.74	678.792	240.341		
25	1643.42	88.45	3.42	1652.10	1637.64	144.437	32.527		

Figure S160. IR spectrum of compound 5a.

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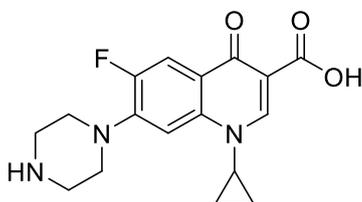


Item	Value	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area	Comment
Acquired Date&Time	31/08/2016 15:22:06	1	506.34	57.95	2.74	512.12	504.41	303.813	9.299
Acquired by	System Administrator	2	528.52	74.69	1.97	531.41	526.59	116.270	4.075
Filename	C:\Users\Administrator\Desktop\Rahman group\AF molecules\Comp b5.ispd	3	552.63	64.04	13.70	557.45	546.84	300.523	63.155
Spectrum name	Comp b5	4	569.03	58.38	21.11	579.63	557.45	647.880	192.358
Sample name	9b	5	595.07	63.38	9.08	601.82	579.63	657.853	94.220
Sample ID	AF-050	6	608.57	62.78	6.54	619.18	601.82	598.235	66.426
Option		7	621.11	68.51	2.73	627.86	619.18	241.034	9.211
Comment		8	636.54	67.90	12.24	643.29	629.79	336.739	68.619
No. of Scans	16	9	665.47	71.47	8.51	668.36	648.11	446.738	62.143
Resolution	2 [cm-1]	10	707.91	28.96	51.93	716.59	668.36	2032.209	1085.711
Apodization	Happ-Genzel	11	723.34	63.50	19.67	731.05	716.59	377.317	136.040
		12	749.38	53.65	22.43	758.06	731.05	786.360	207.127

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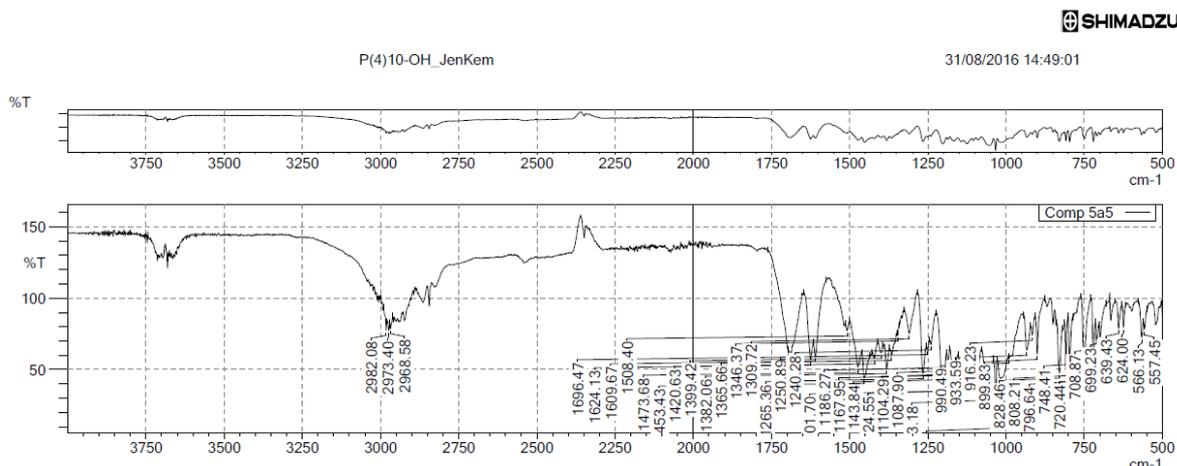
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13	774.45	49.14	9.18	779.28	758.06	854.451	69.736		
14	785.06	44.80	10.52	788.92	779.28	481.014	48.664		
15	792.78	49.54	5.97	796.64	788.92	363.694	20.458		
16	807.24	36.07	26.83	821.71	796.64	1171.357	276.697		
17	829.43	58.18	18.32	843.89	821.71	729.501	236.653		
18	863.18	68.41	4.31	868.00	843.89	600.263	26.381		
19	886.33	50.09	9.16	892.12	868.00	932.165	41.641		
20	894.04	54.68	2.98	901.76	892.12	391.012	10.651		
21	941.30	48.23	14.40	959.63	901.76	2457.635	338.182		
22	1033.89	28.39	20.78	1040.64	1029.07	643.893	64.089		
23	1056.07	47.58	9.69	1074.40	1040.64	1638.923	206.140		
24	1107.19	47.11	4.58	1113.94	1095.61	907.200	35.143		
25	1138.05	33.46	18.80	1164.09	1113.94	2891.928	502.731		
26	1184.34	48.67	4.29	1191.09	1173.73	856.356	36.258		
27	1258.61	71.60	6.82	1264.39	1234.50	492.559	50.324		
28	1272.11	60.96	20.98	1288.50	1264.39	501.686	172.301		
29	1340.58	72.52	8.52	1354.09	1333.83	432.648	89.700		
30	1454.39	53.78	20.98	1478.50	1421.60	1930.032	578.955		
31	1490.07	59.64	11.82	1505.51	1481.39	791.231	148.216		
32	1611.59	64.91	8.35	1616.42	1578.80	534.436	32.115		
33	1627.03	58.56	20.55	1646.32	1618.35	609.210	207.696		
34	1684.89	71.54	3.12	1695.50	1682.96	308.797	20.392		

Figure S161. IR spectrum of compound 5b.

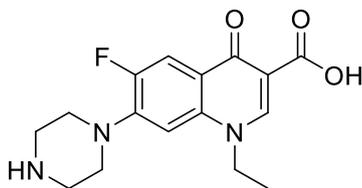


Item	Value	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area	Comment
Acquired Date&Time	31/08/2016 14:46:19	1	557.46	78.08	7.98	560.35	549.74	168.741	41.142
Acquired by	System Administrator	2	566.13	72.30	16.52	576.74	560.35	252.640	103.827
Filename	C:\Users\Chem Labs\Desktop\Rahman group\AF molecules\Comp 5a5.ispd	3	624.00	79.65	15.88	629.79	617.25	133.019	76.755
Spectrum name	Comp 5a5	4	639.43	78.93	17.84	651.00	629.79	192.693	126.623
Sample name	9a	5	699.23	72.58	11.52	703.08	678.97	332.818	68.502
Sample ID	AF-055	6	708.87	68.24	14.46	713.69	703.08	260.689	76.275
Option		7	720.44	47.10	44.22	728.16	713.69	346.742	229.333
Comment		8	748.41	58.10	42.76	761.91	728.16	541.063	567.081
No. of Scans	16	9	796.64	45.28	42.39	801.46	786.03	429.432	236.136
Resolution	2 [cm-1]	10	808.21	49.48	35.41	812.07	801.46	299.727	146.470
Apodization	Happ-Genzel	11	828.46	47.75	33.18	837.14	818.82	646.818	295.407
		12	899.83	60.95	29.50	906.58	876.68	391.199	202.965

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13	916.23	74.11	9.05	921.05	906.58	280.323	53.417
14	933.59	63.71	21.30	943.23	921.05	585.919	242.835
15	990.49	58.33	1.13	991.45	989.53	79.282	1.089
16	1032.93	12.67	44.87	1039.68	1028.10	674.814	183.734
17	1053.18	32.34	27.75	1078.25	1039.68	2145.248	644.326
18	1087.90	53.52	9.29	1096.58	1078.25	760.922	80.780
19	1104.29	50.95	8.48	1110.08	1096.58	599.111	54.531
20	1124.55	39.05	14.98	1137.09	1110.08	1429.952	195.657
21	1143.84	46.91	7.70	1153.48	1137.09	794.130	64.251
22	1167.95	49.77	13.14	1179.52	1153.48	1160.865	188.517
23	1186.27	55.18	7.77	1190.13	1179.52	429.825	41.291
24	1201.70	38.52	32.96	1223.89	1190.13	1317.518	504.353
25	1240.28	67.55	7.00	1244.14	1223.89	443.031	47.190
26	1250.89	64.28	3.93	1254.75	1244.14	351.692	20.578
27	1265.36	47.34	33.09	1283.68	1254.75	793.518	372.017
28	1309.72	75.20	21.28	1325.15	1283.68	491.434	410.542
29	1346.37	73.76	3.92	1349.26	1341.55	180.803	13.877
30	1365.66	60.20	8.28	1373.38	1349.26	810.545	96.054
31	1382.06	50.89	14.87	1387.84	1373.38	608.476	111.587
32	1399.42	61.77	6.29	1410.02	1393.63	574.361	56.543
33	1420.63	57.78	7.23	1427.39	1410.02	644.959	52.229
34	1453.43	44.09	17.55	1461.14	1436.07	1197.394	225.509
35	1473.68	51.71	17.53	1500.68	1461.14	1339.375	281.429
36	1508.40	77.22	5.76	1514.19	1500.68	266.012	38.296
37	1609.67	59.68	16.84	1616.42	1574.95	506.990	140.344
38	1624.13	56.92	21.47	1646.32	1616.42	643.008	247.817
39	1696.47	62.49	2.46	1761.08	1695.50	-287.987	-362.422
40	2968.58	78.89	4.83	2970.50	2960.86	169.327	26.017
41	2973.40	77.24	5.95	2979.18	2970.50	164.900	20.752
42	2982.08	77.57	8.84	2990.76	2979.18	163.050	33.548

Figure S162. IR spectrum of compound 5c.

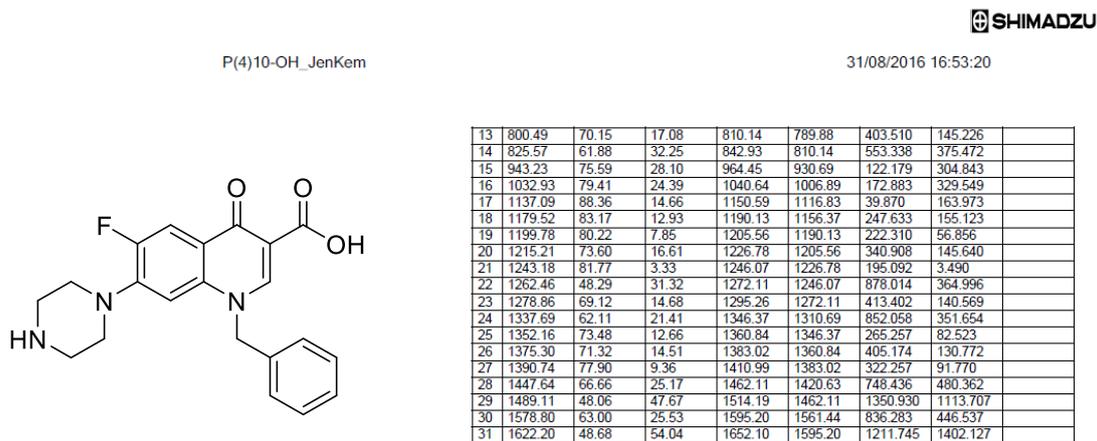
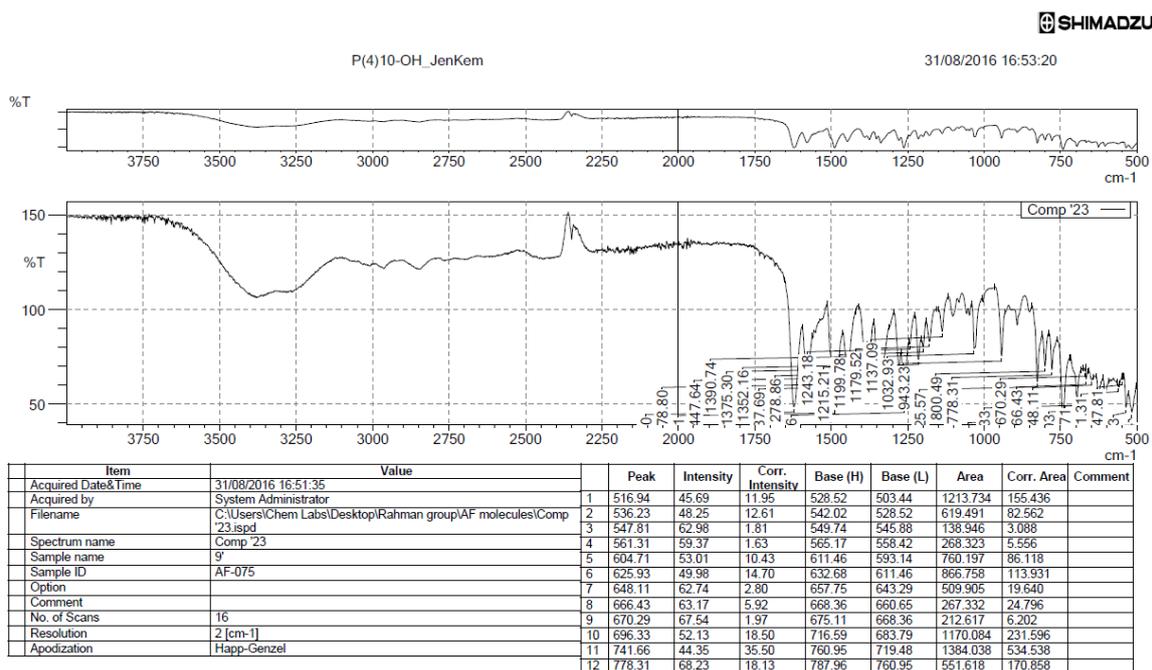


Figure S163. IR spectrum of compound 5d.

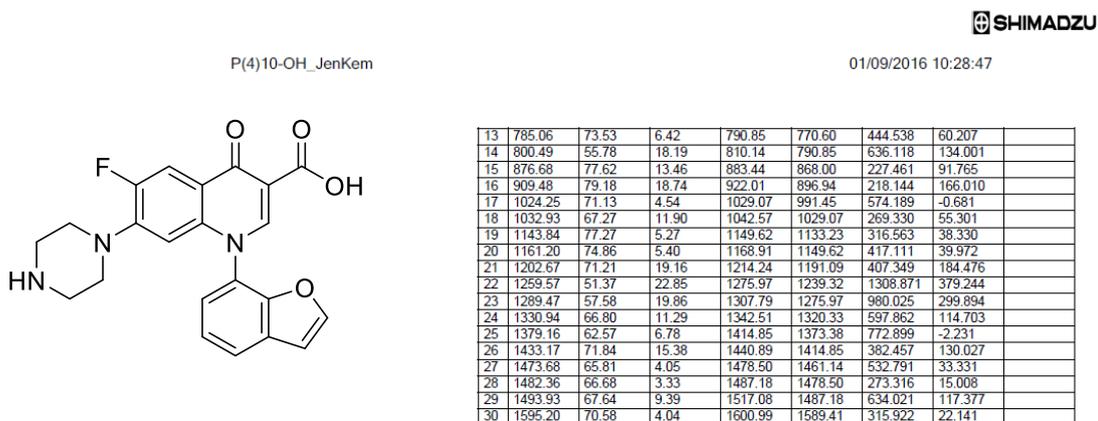
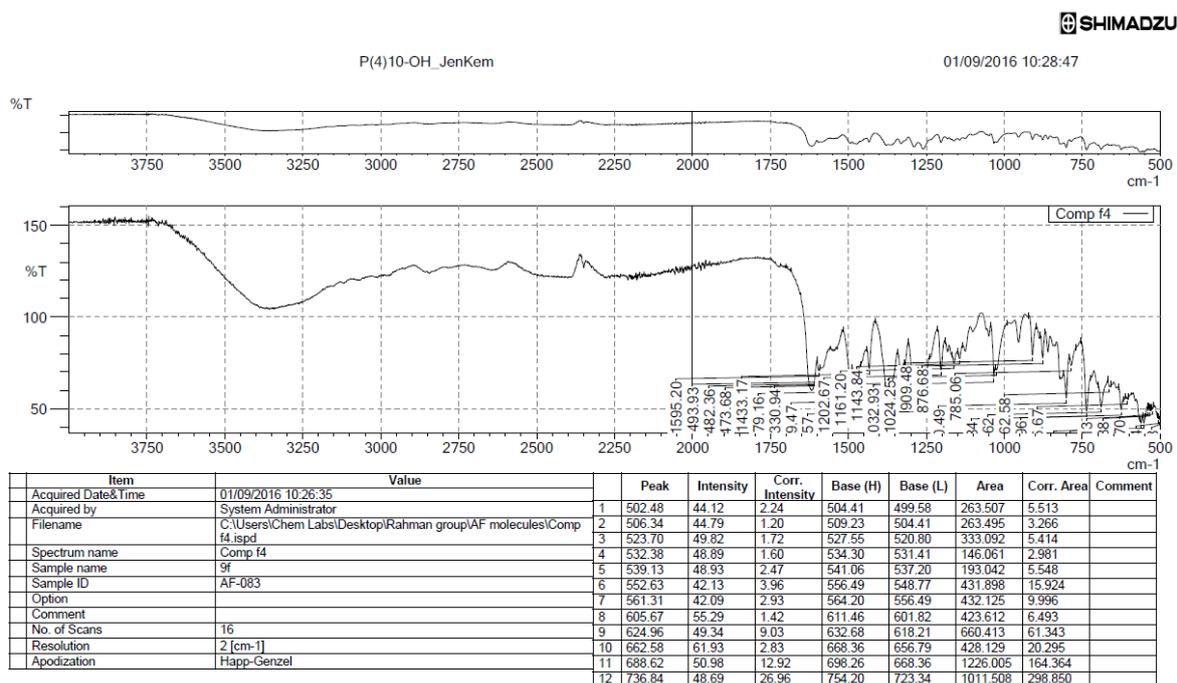


Figure S164. IR spectrum of compound 5e.

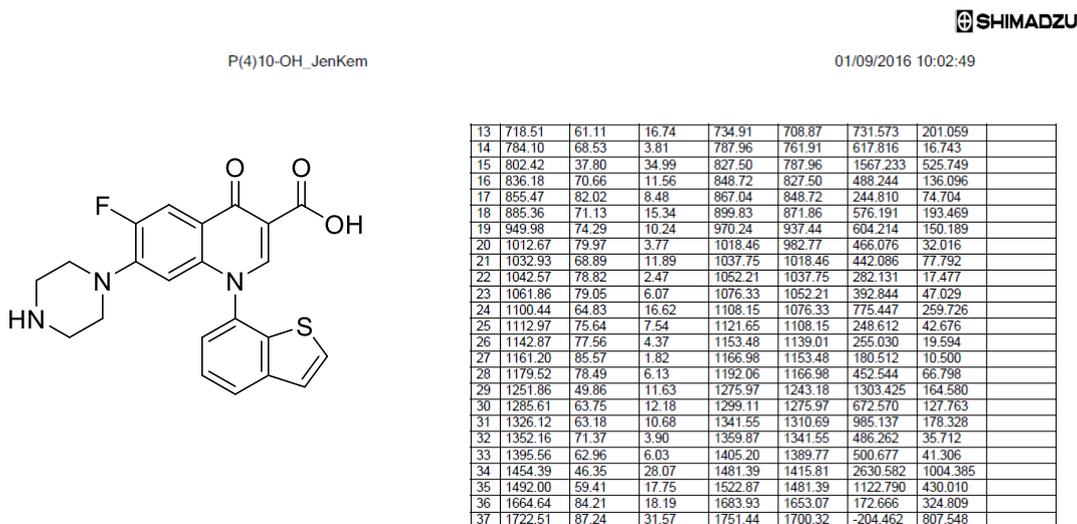
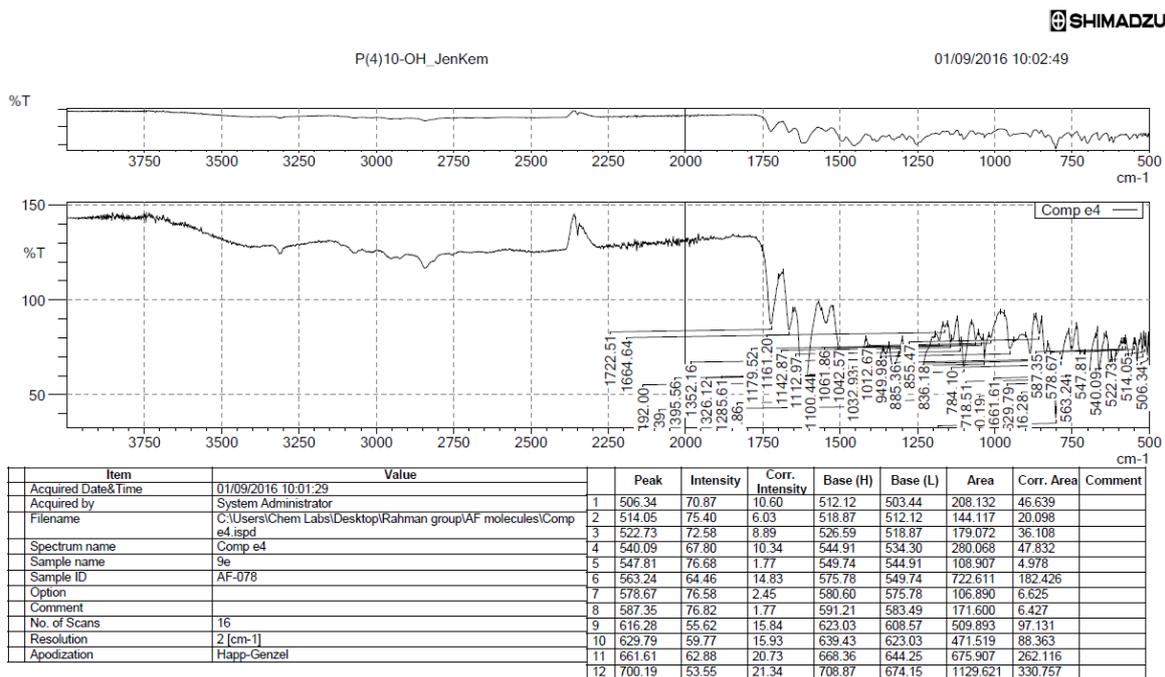


Figure S165. IR spectrum of compound 5f.

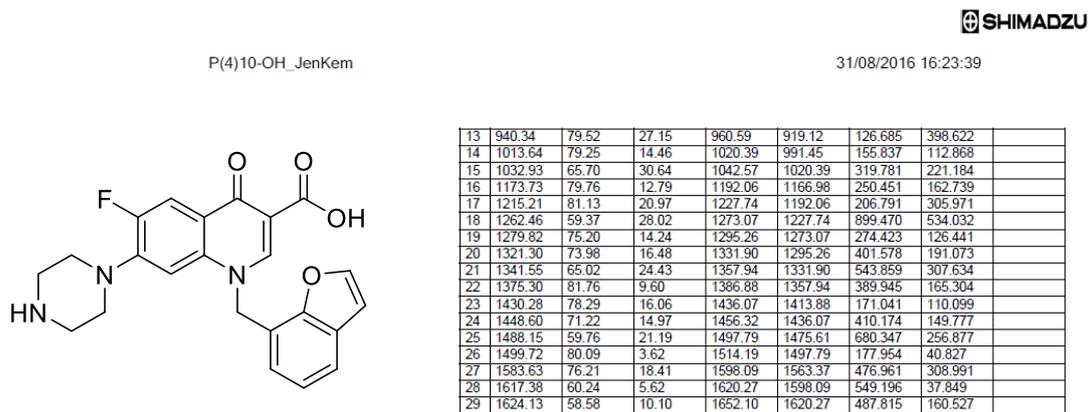
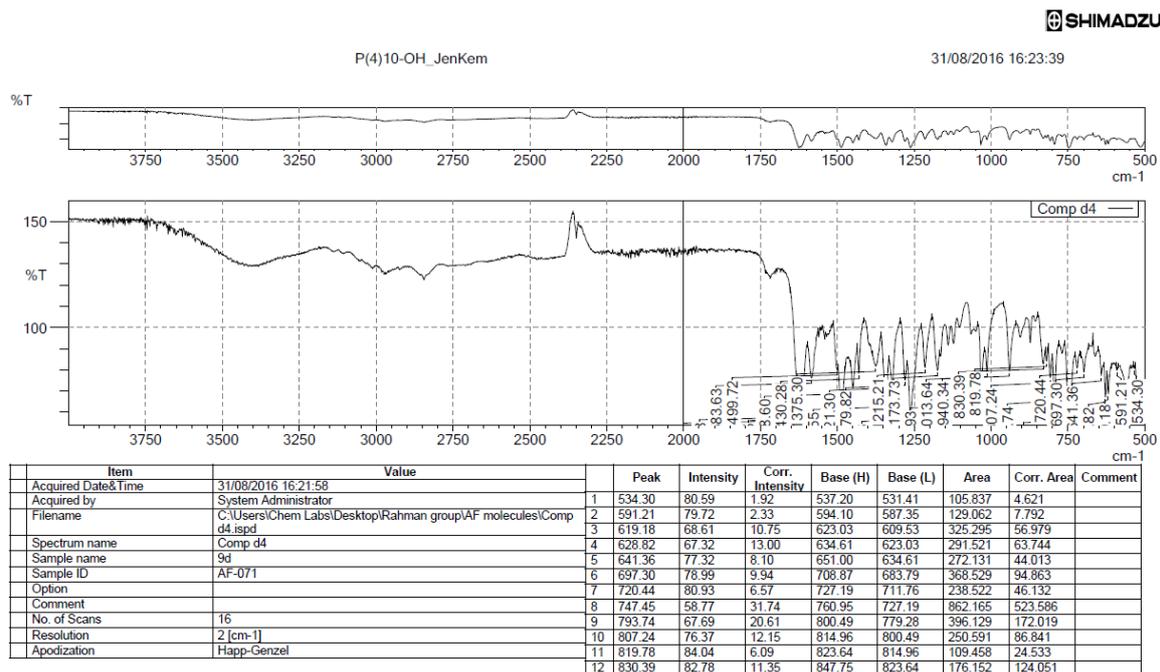


Figure S166. IR spectrum of compound 5g.

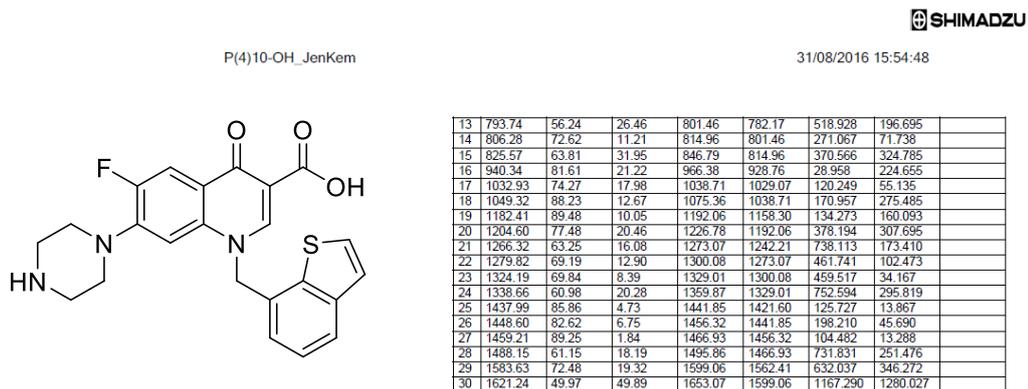
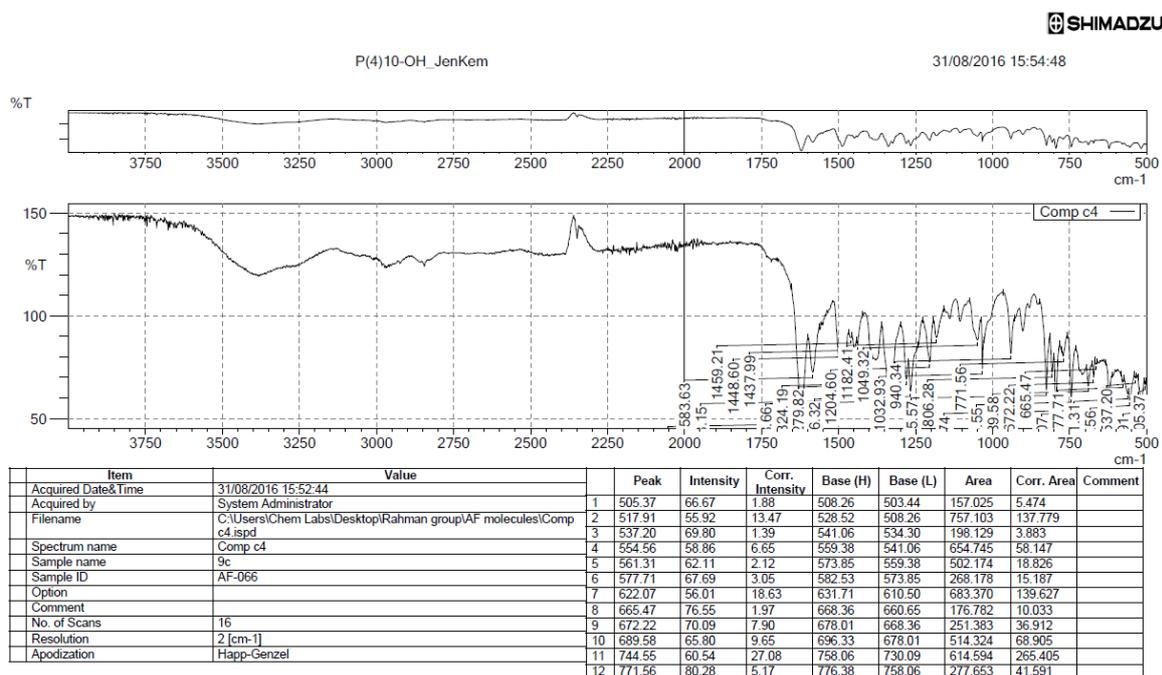


Figure S167. IR spectrum of compound 6a.

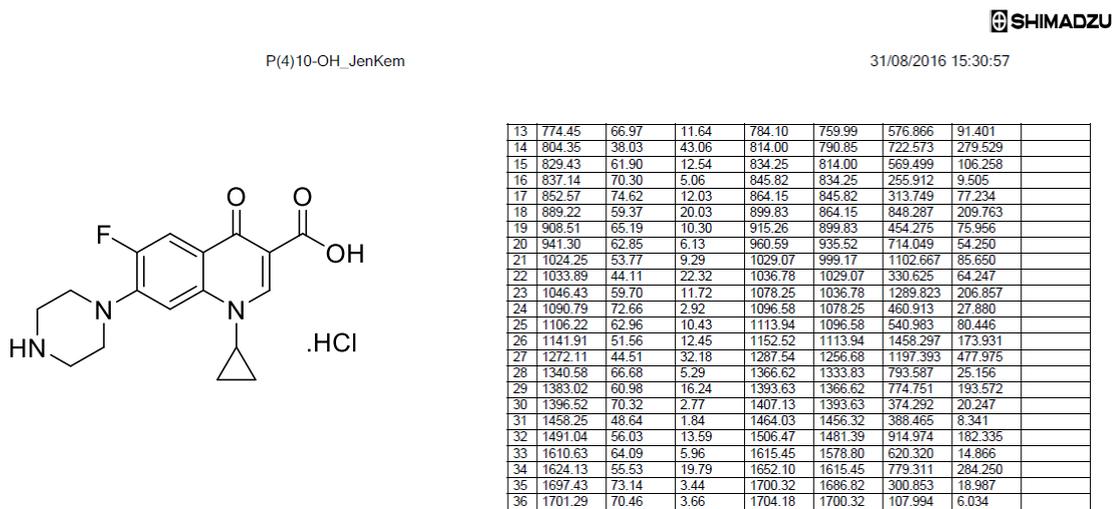
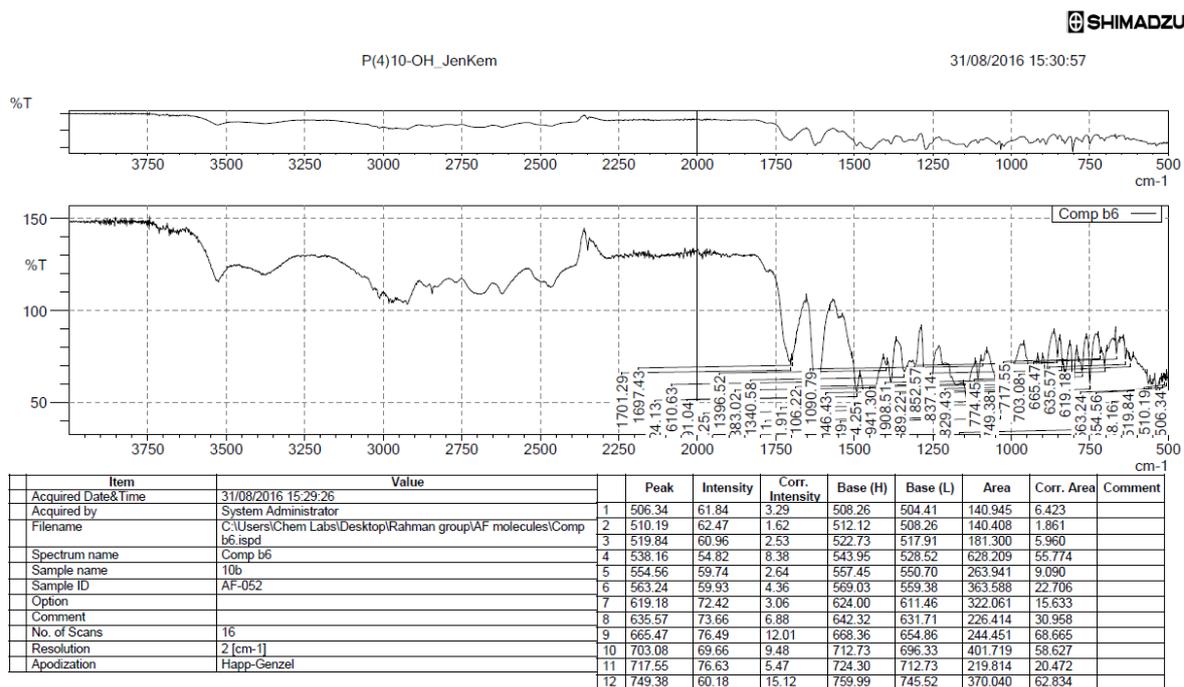


Figure S168. IR spectrum of compound 6b.

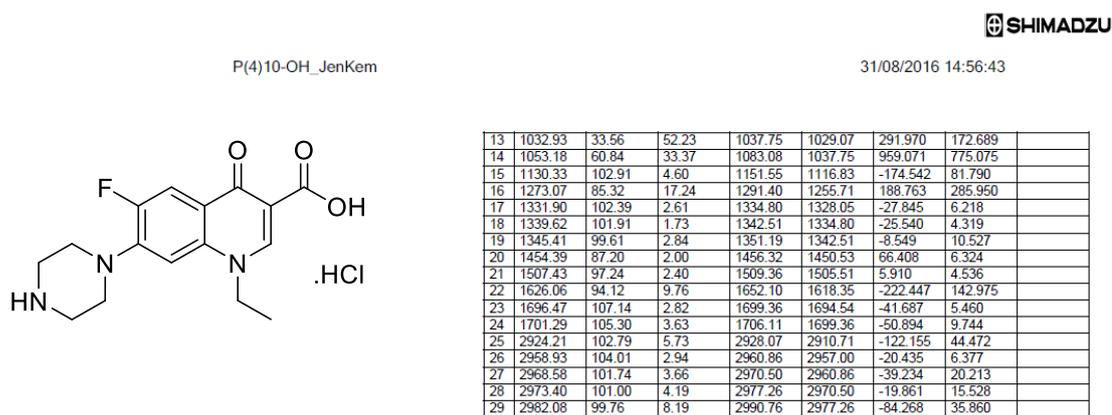
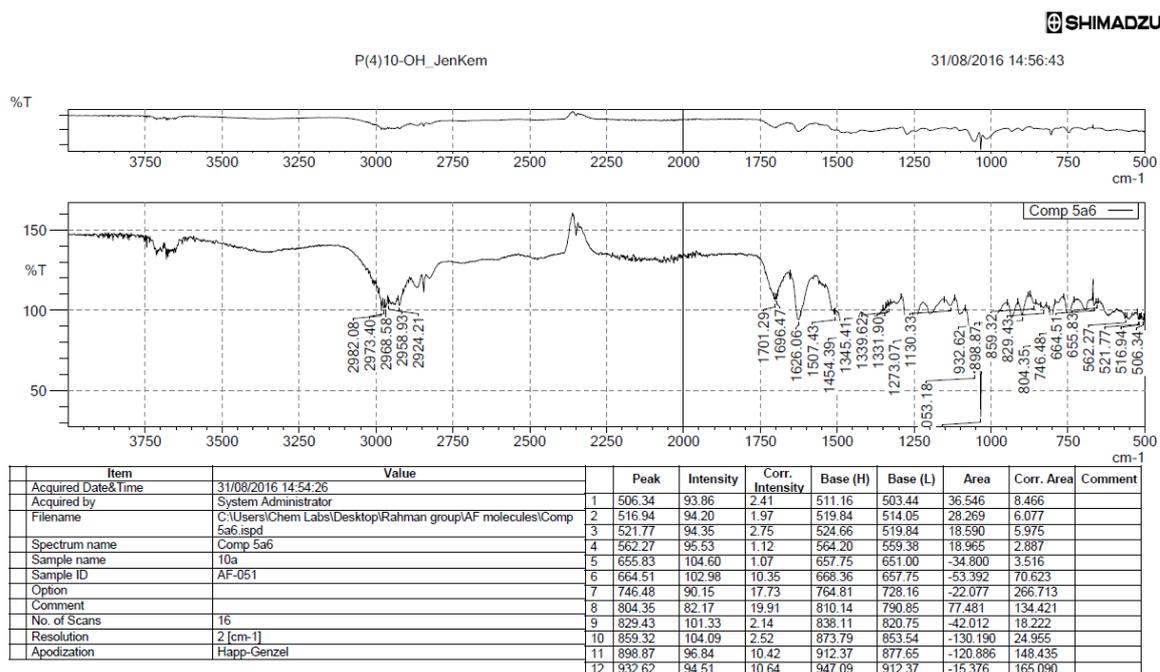
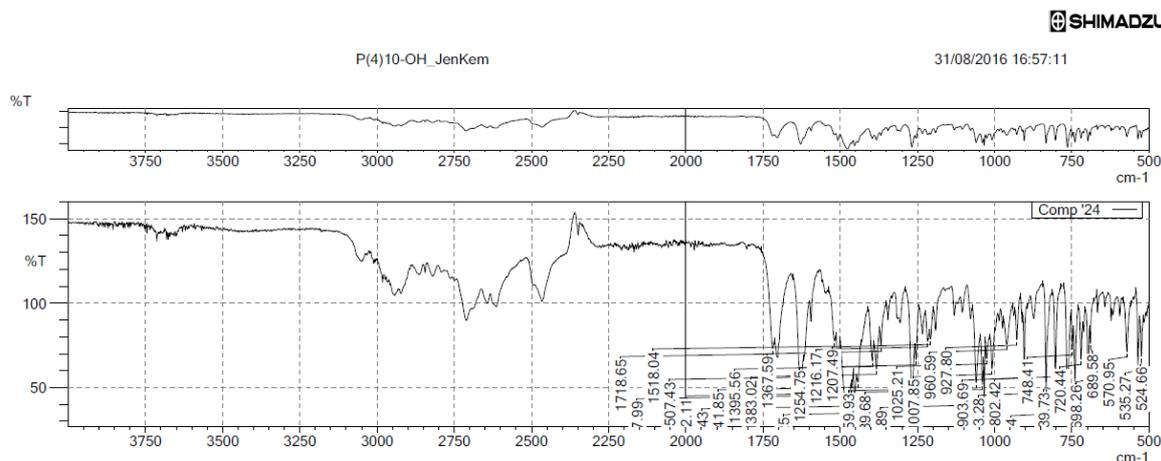
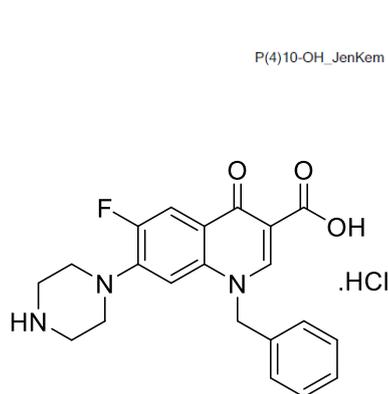


Figure S169. IR spectrum of compound 6c.

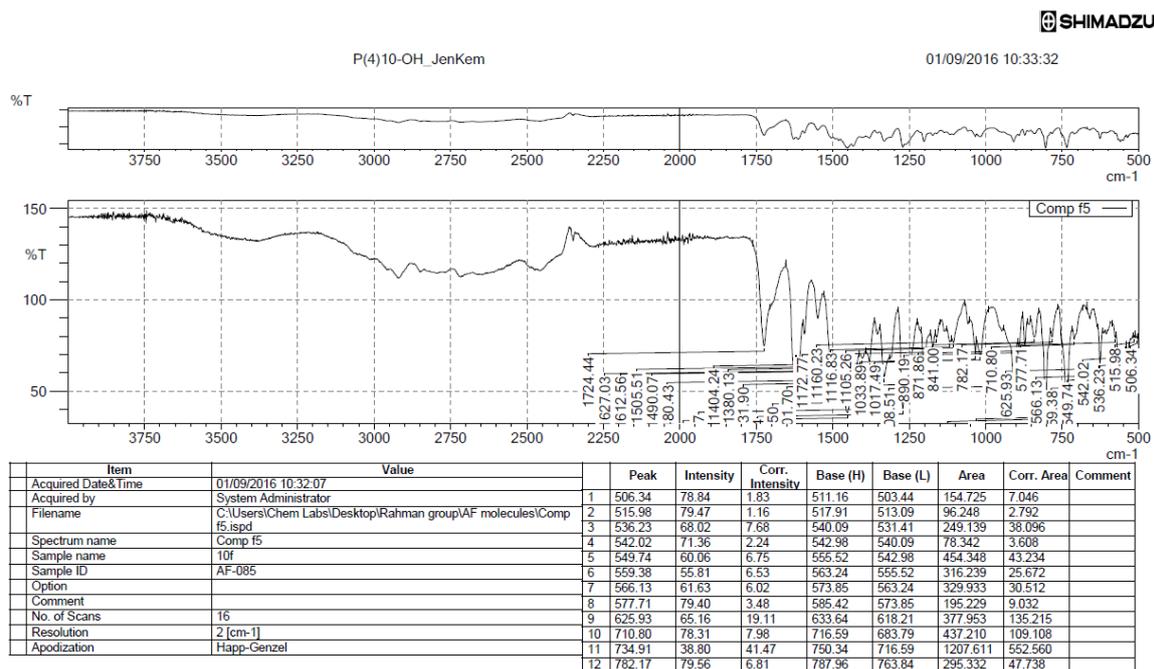


Item	Value	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area	Comment
Acquired Date&Time	31/08/2016 16:55:46	1	524.66	68.39	22.64	530.45	518.87	214.193	110.343
Acquired by	System Administrator	2	535.27	63.27	34.35	542.02	530.45	166.723	155.355
Filename	C:\Users\Chem Label\Desktop\Rahman group\AF molecules\Comp 24.ispd	3	570.95	71.26	29.59	582.53	559.38	250.017	269.573
Spectrum name	Comp_24	4	689.58	76.11	12.61	692.47	678.97	107.801	18.166
Sample name	10'	5	698.26	57.81	32.15	705.98	692.47	277.251	152.344
Sample ID	AF-090	6	720.44	66.84	25.09	728.16	714.66	224.365	125.042
Option		7	739.73	53.69	35.13	744.55	728.16	344.091	203.211
Comment		8	748.41	72.42	17.56	752.27	744.55	135.153	57.876
No. of Scans	16	9	763.84	37.99	64.05	777.35	752.27	502.323	568.673
Resolution	2 [cm-1]	10	802.42	59.64	48.18	814.00	785.06	145.533	382.762
Apodization	Happ-Genzel	11	833.28	50.03	59.58	844.86	814.00	235.400	511.505
		12	903.69	58.99	36.00	908.51	895.97	204.616	149.410



13	927.80	78.29	20.51	933.59	917.19	135.263	135.572		
14	960.59	75.58	17.88	971.20	942.27	390.847	231.090		
15	1007.85	61.00	21.06	1015.57	999.17	437.934	145.706		
16	1025.21	67.14	11.72	1030.03	1015.57	369.028	68.252		
17	1033.89	42.83	27.37	1035.82	1030.03	234.989	74.033		
18	1039.68	51.88	19.29	1046.43	1035.82	379.909	93.688		
19	1059.93	52.89	36.02	1072.47	1046.43	664.765	367.416		
20	1207.49	78.65	8.31	1211.35	1198.81	176.812	46.866		
21	1216.17	77.25	9.60	1224.85	1211.35	215.422	60.330		
22	1264.75	66.56	14.10	1258.61	1244.14	257.218	55.551		
23	1268.25	38.59	46.51	1289.47	1258.61	655.276	391.899		
24	1367.59	74.67	13.14	1372.41	1350.23	237.719	63.834		
25	1383.02	60.97	18.67	1390.74	1372.41	510.840	149.830		
26	1395.56	65.62	15.88	1409.06	1390.74	389.652	139.058		
27	1441.85	53.37	9.73	1446.67	1432.21	540.055	55.870		
28	1453.43	42.18	16.19	1457.28	1446.67	523.479	77.018		
29	1462.11	49.73	5.55	1465.00	1457.28	357.961	19.566		
30	1507.43	59.54	20.05	1514.19	1500.68	398.972	123.337		
31	1518.04	77.55	7.78	1538.30	1514.19	170.737	38.897		
32	1627.99	48.06	32.21	1652.10	1619.31	686.598	411.459		
33	1718.65	72.94	12.00	1756.26	1712.86	-275.593	-72.602		

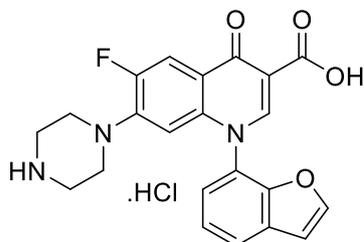
Figure S170. IR spectrum of compound 6g.



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13	804.35	37.51	50.46	825.57	787.96	1070.886	644.748	
14	841.00	79.53	12.09	853.54	825.57	402.380	174.387	
15	871.86	74.92	15.04	879.58	864.15	262.296	107.389	
16	890.19	73.79	7.90	895.01	879.58	288.683	47.901	
17	908.51	55.59	23.71	942.27	895.01	1264.163	361.931	
18	1017.49	69.87	13.73	1030.03	991.45	735.961	214.567	
19	1033.89	70.20	10.02	1051.25	1030.03	396.831	50.489	
20	1105.26	76.36	5.22	1111.05	1069.57	512.423	42.254	
21	1116.83	76.83	3.94	1127.44	1111.05	335.450	33.417	
22	1160.23	79.42	4.18	1165.05	1149.62	264.768	29.365	
23	1172.77	74.24	7.51	1180.49	1165.05	339.247	57.619	
24	1201.70	56.55	26.37	1212.31	1180.49	843.946	291.462	
25	1261.50	47.07	5.46	1265.36	1222.92	1422.506	85.837	
26	1271.14	40.24	20.62	1287.54	1265.36	775.400	148.998	
27	1331.90	57.82	19.74	1346.37	1314.54	1032.793	295.066	
28	1380.13	66.00	13.36	1392.66	1363.73	729.121	164.631	
29	1404.24	67.94	3.08	1411.95	1392.66	587.051	30.982	
30	1433.17	42.64	10.05	1437.99	1411.95	1145.013	91.081	
31	1451.50	38.04	15.44	1474.64	1439.92	1823.456	294.398	
32	1480.43	58.85	5.65	1486.22	1474.64	439.414	28.620	
33	1490.07	63.72	2.92	1496.83	1486.22	370.005	20.295	
34	1505.51	66.19	9.03	1529.62	1499.72	530.238	107.472	
35	1612.56	63.55	9.92	1618.35	1598.09	567.382	115.699	
36	1627.03	63.71	15.07	1653.07	1620.27	309.373	119.444	
37	1724.44	74.71	33.24	1762.05	1705.15	-60.863	712.752	

Figure S171. IR spectrum of compound 6e.

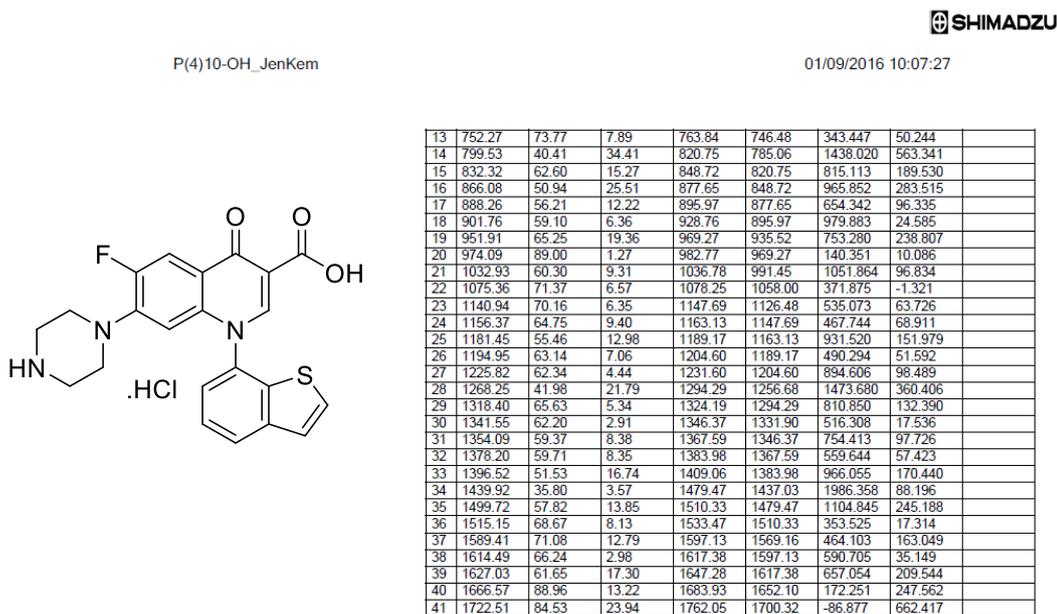
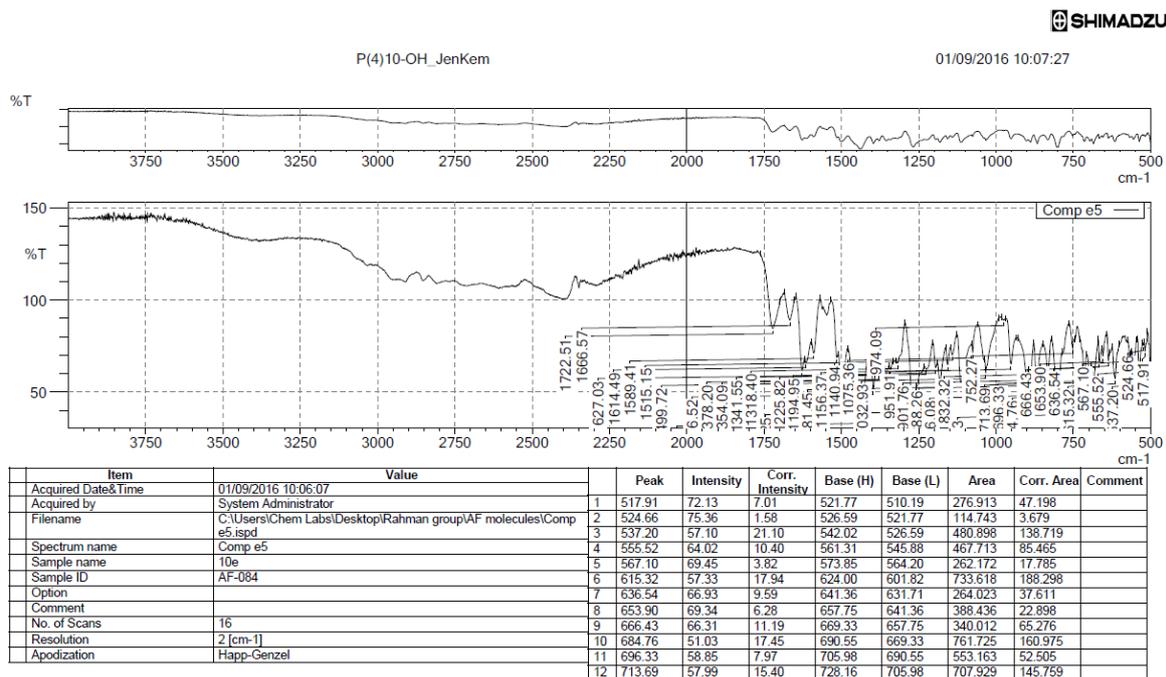
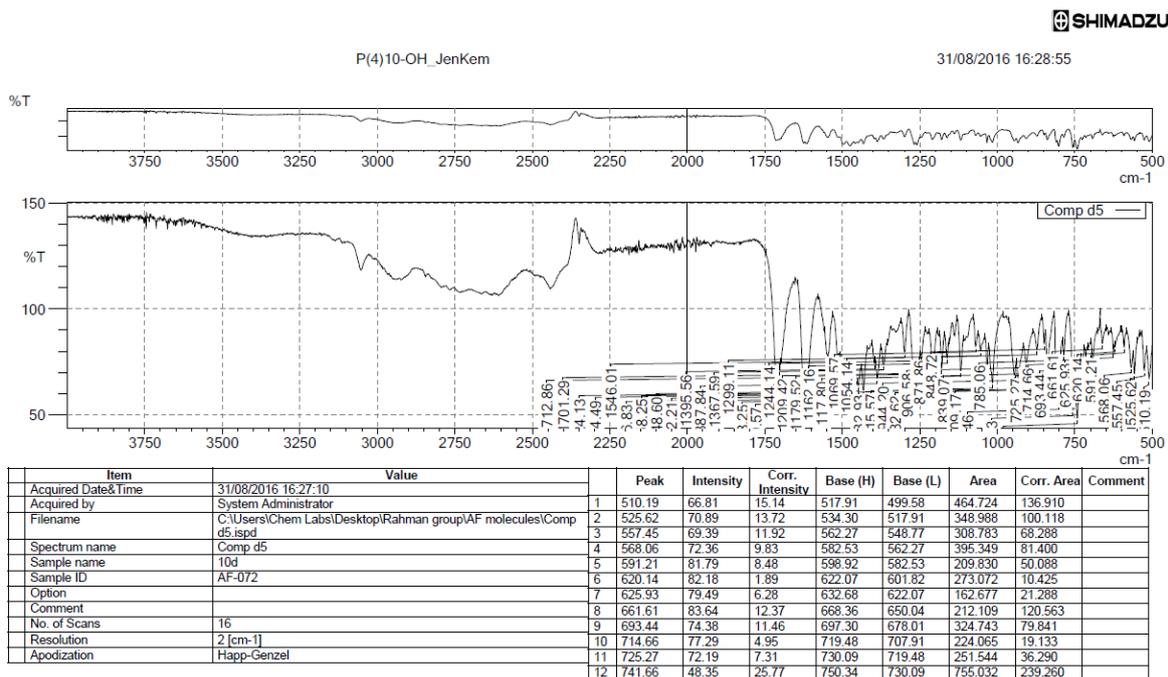


Figure S172. IR spectrum of compound 6f.



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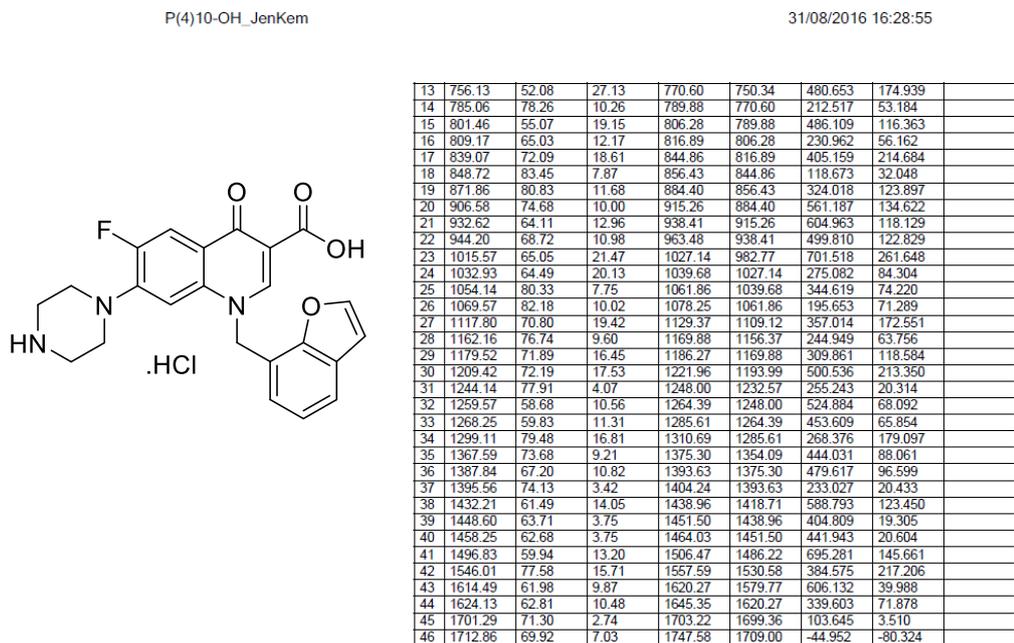
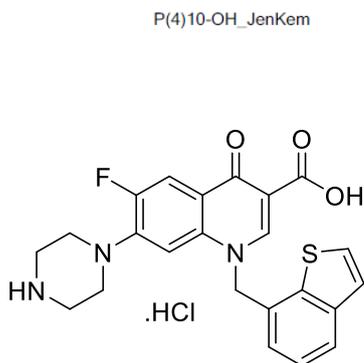
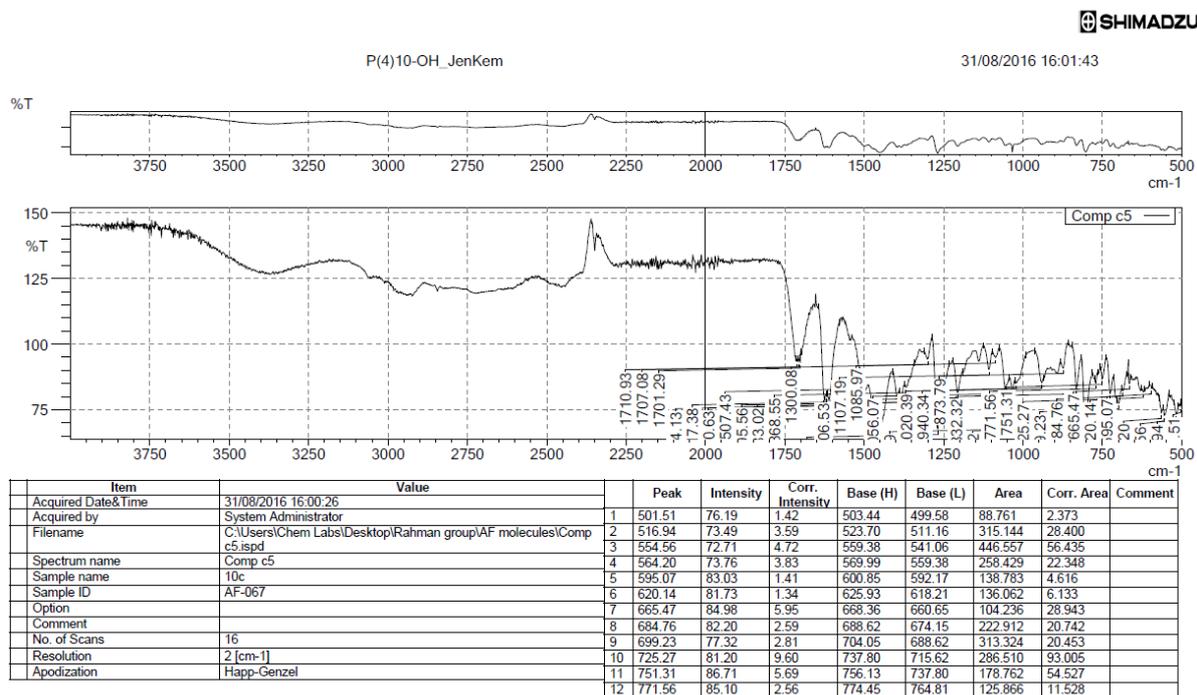


Figure S173. IR spectrum of compound 6g.



13	802.42	70.03	22.72	815.92	781.20	654.159	380.769		
14	832.32	83.14	14.39	845.82	815.92	259.656	178.897		
15	873.79	90.88	4.95	881.51	858.36	120.759	52.212		
16	940.34	85.28	3.80	961.56	935.52	241.650	41.738		
17	1020.39	85.18	2.65	1026.17	991.45	377.116	67.408		
18	1033.89	69.68	17.01	1042.57	1026.17	286.496	68.735		
19	1056.07	83.23	8.84	1074.40	1042.57	341.746	116.882		
20	1085.97	94.92	3.02	1096.58	1074.40	79.924	34.824		
21	1107.19	90.34	7.81	1124.55	1096.58	139.636	95.205		
22	1206.53	81.61	10.12	1221.96	1191.09	396.665	141.713		
23	1268.25	67.67	31.58	1286.58	1231.60	938.107	805.093		
24	1300.08	94.37	5.42	1311.65	1286.58	66.546	66.094		
25	1368.55	83.60	2.59	1373.38	1342.51	397.730	57.307		
26	1383.02	79.88	3.54	1389.77	1373.38	298.211	29.977		
27	1395.56	79.86	4.68	1409.06	1389.77	319.534	49.638		
28	1507.43	85.00	1.75	1512.26	1506.47	73.098	4.271		
29	1610.63	78.82	6.62	1616.42	1578.80	251.269	55.881		
30	1617.38	79.95	1.29	1619.31	1616.42	56.253	1.915		
31	1624.13	78.55	8.77	1645.35	1619.31	146.489	89.018		
32	1701.29	93.00	3.55	1704.18	1700.32	21.406	5.900		
33	1707.08	93.38	1.32	1709.00	1704.18	28.773	3.321		
34	1710.93	93.36	1.21	1713.83	1709.00	29.103	2.909		

Table S1

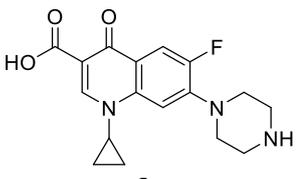
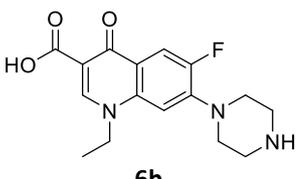
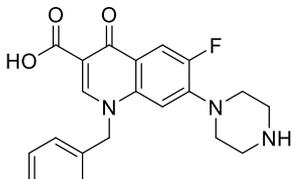
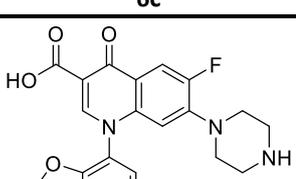
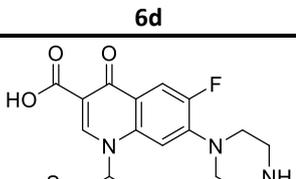
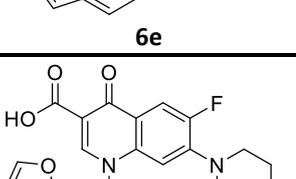
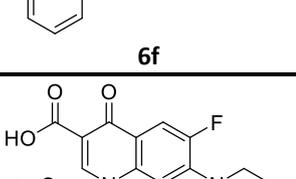
Compound	Pose	<i>S. aureus</i> GyraseA with DNA				<i>K. pneumoniae</i> GyraseA with DNA			
		Subunit I (GyrA1)		Subunit II (GyrA2)		Subunit I (GyrA1)		Subunit II (GyrA2)	
		ChemScore	ΔG (kcal/mol)	ChemScore	ΔG (kcal/mol)	ChemScore	ΔG (kcal/mol)	ChemScore	ΔG (kcal/mol)
	1	19.015	-23.5912	17.9679	-20.812	19.5618	-21.7873	14.437	-17.2497
	2	18.6785	-22.3179	17.4624	-19.3749	18.9911	-22.3009	14.4264	-17.2631
	3	18.4116	-22.6901	17.4176	-19.5767	18.9659	-21.4667	14.2923	-17.259
	4	18.3579	-20.8162	17.4053	-19.9609	18.8762	-21.7556	13.9285	-21.2718
	5	18.2934	-20.5248	17.3675	-21.7069	18.6456	-21.6769	13.8058	-17.4839
	6	18.2452	-20.3763	16.9389	-18.8812	18.5986	-22.3718	13.7849	-16.8172
	7	17.9322	-20.3626	16.8043	-21.077	18.4412	-22.1318	13.6828	-16.919
	8	17.8748	-20.576	16.5406	-19.9763	18.0295	-20.1253	13.4749	-17.9284
	9	17.7158	-20.4671	16.3727	-18.4667	18.0148	-21.4708	13.2012	-16.4885
	10	15.9372	-18.578	15.4572	-17.2486	17.4271	-21.458	13.0517	-18.5486
	1	19.8667	-21.5395	18.288	-21.7767	18.7201	-21.2675	14.6246	-18.3252
	2	18.0233	-22.4758	18.1771	-21.3961	18.5004	-20.6171	14.265	-16.5579
	3	17.9643	-19.784	17.9041	-20.9702	18.4374	-21.7994	14.0222	-18.9375
	4	17.6878	-19.5941	17.5853	-22.4999	18.0984	-21.3281	13.9448	-16.4876
	5	17.6428	-21.3247	17.5717	-19.2494	17.8982	-21.6551	13.8709	-18.1633
	6	17.0688	-20.5237	17.3923	-19.164	17.8932	-19.7203	13.3791	-16.9902
	7	16.7168	-19.8492	17.2979	-22.3496	17.6474	-20.6776	13.0782	-16.6124
	8	16.1811	-19.7817	16.9364	-23.2768	17.6064	-21.2443	12.8941	-15.2309
	9	15.8422	-18.1975	16.6093	-18.8153	17.6033	-20.736	12.7003	-14.7561
	10	15.4482	-18.5583	16.2631	-19.4697	17.4824	-20.0576	12.2694	-16.7888
	1	21.0028	-22.8366	21.2817	-24.0464	21.4557	-23.8936	19.5191	-23.1904
	2	20.7241	-25.3622	20.7575	-22.9127	20.7475	-22.9921	17.6006	-19.7543
	3	20.3784	-22.9843	20.7125	-23.1097	20.2582	-23.7218	17.0698	-24.3173
	4	20.2414	-27.0529	20.6623	-23.5423	19.9449	-23.233	16.9657	-19.8946
	5	20.0564	-22.5644	20.6113	-23.275	19.7408	-23.585	16.755	-19.8839
	6	19.8613	-22.9684	20.1788	-22.4355	19.7034	-23.6423	16.712	-18.6538
	7	19.6996	-23.3613	19.4286	-21.3365	19.3027	-23.8576	16.632	-20.2258
	8	19.3211	-21.6361	19.4266	-21.9081	19.2159	-23.8039	16.278	-20.1084
	9	19.2689	-21.7208	18.2177	-20.5938	19.1216	-23.1827	16.0657	-24.2871
	10	17.9111	-21.9367	18.0494	-23.4122	18.7828	-20.9026	15.4169	-20.0502
	1	21.9327	-25.7391	19.6446	-25.1047	23.293	-27.6932	18.1307	-22.7802
	2	21.4631	-25.3351	19.3691	-23.7173	23.1027	-27.8039	17.8454	-22.3851
	3	21.4525	-25.1178	19.1292	-24.7031	23.0932	-26.7071	17.8339	-21.7959
	4	20.9933	-24.7591	19.1235	-23.4604	22.7861	-26.474	17.7402	-22.5159
	5	20.8088	-24.4527	19.1076	-22.9216	22.7497	-28.6988	17.4623	-21.1548
	6	20.4933	-26.3817	18.8404	-24.495	22.7345	-26.8916	16.6164	-20.5651
	7	20.17	-25.5802	18.768	-23.8146	22.7099	-26.2972	16.1586	-20.9985
	8	19.1537	-28.6353	17.8378	-21.2861	22.6665	-26.1774	15.0048	-20.147
	9	18.9	-26.2366	17.8195	-21.7924	22.5627	-27.0266	14.6204	-17.7354
	10	18.1598	-22.9399	17.4906	-22.4833	21.9163	-25.8775	14.3136	-20.3627
	1	22.7264	-28.2025	20.2349	-23.52	23.3059	-27.7591	17.9659	-24.2013
	2	22.4539	-26.5328	20.0599	-26.3648	22.8447	-27.2144	17.2422	-23.2938
	3	22.379	-27.5564	19.8426	-23.2674	22.3977	-26.1046	17.2267	-22.2034
	4	22.3721	-29.4673	19.4867	-25.6941	22.3257	-25.9407	16.2817	-20.5823
	5	22.1723	-25.7923	19.4388	-24.9892	22.2999	-27.0945	16.067	-19.9703
	6	21.7199	-25.5481	19.377	-27.4029	22.2581	-25.8221	15.9869	-21.2619
	7	21.7158	-25.3829	19.0838	-25.4816	21.9756	-27.1476	15.9448	-21.1802
	8	21.2266	-27.1813	18.9775	-23.3966	21.3329	-25.6246	15.4755	-20.2775
	9	20.6962	-27.5057	18.4125	-21.9597	21.0572	-27.1539	15.01	-21.4326
	10	20.6649	-27.8474	17.8826	-22.6384	20.9572	-25.7359	14.7313	-20.338
	1	23.1522	-25.5482	22.0146	-24.3903	22.4313	-25.3748	18.8167	-23.2206
	2	22.8932	-26.4973	21.3729	-23.7541	21.3942	-24.9152	18.8093	-22.4623
	3	22.2973	-24.4731	21.1813	-26.308	21.2883	-26.3852	18.5314	-22.4095
	4	21.8529	-24.2695	20.9503	-23.3308	21.2784	-24.7633	18.5104	-21.7027
	5	21.8042	-24.7147	20.7564	-23.3031	20.8111	-22.9127	18.4162	-21.9581
	6	21.3619	-23.5706	20.6387	-22.947	20.5504	-23.8177	17.6598	-21.3662
	7	20.6388	-24.5721	20.0784	-22.3253	20.4313	-24.3793	16.1005	-18.5159
	8	20.1401	-22.4174	19.8064	-22.8983	20.1437	-23.7156	15.3344	-19.2586
	9	19.5261	-22.382	19.7332	-22.3956	19.9679	-24.1996	15.0544	-19.6293
	10	19.3666	-22.8497	19.2319	-24.5302	18.1112	-20.5118	14.8832	-17.0829
	1	23.4943	-28.602	22.3227	-24.8709	23.7909	-27.1988	20.1066	-23.9475
	2	22.5529	-26.69	22.2542	-25.2095	23.338	-26.7974	19.3969	-22.7357
	3	22.0029	-25.6426	21.6142	-24.549	22.8833	-26.4776	19.1681	-22.4697
	4	21.5357	-23.9133	21.4723	-24.3895	21.9563	-25.5088	19.038	-23.4453
	5	21.3201	-27.81	21.345	-23.7118	21.8306	-26.0423	18.9794	-22.4162
	6	21.1582	-24.7549	21.1972	-23.5954	21.7848	-26.3824	18.7465	-22.4579
	7	20.9505	-23.6745	21.1511	-23.8016	21.6403	-25.8628	17.5725	-22.2551
	8	20.1898	-23.0974	21.1397	-24.6914	21.5924	-24.1509	17.1012	-20.6497
	9	19.2848	-21.3876	21.0387	-23.1754	21.5313	-24.4966	16.0953	-23.6243
	10	18.7351	-23.9732	20.6707	-22.7675	21.2156	-24.9092	16.0269	-19.1232

Table S1. Binding affinities of compounds **6a-g** against DNA gyrase from *S. aureus*, *K. pneumoniae*.