

## Supporting Information

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### Synthesis and biological assessment of novel acylhydrazone derivatives of 2-methyl-1,4-naphthoquinone

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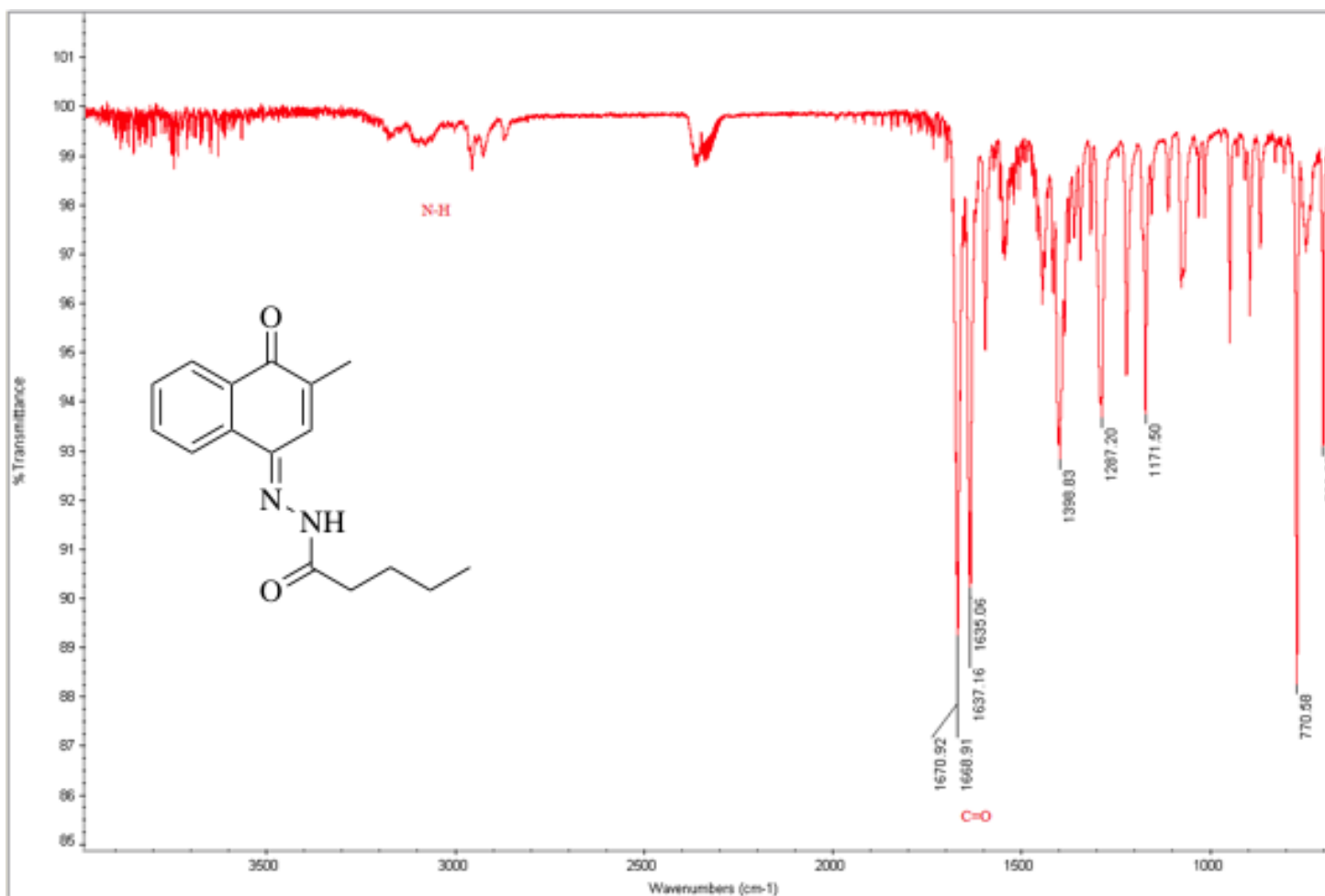


Figure S1. IR spectrum of compound 6a

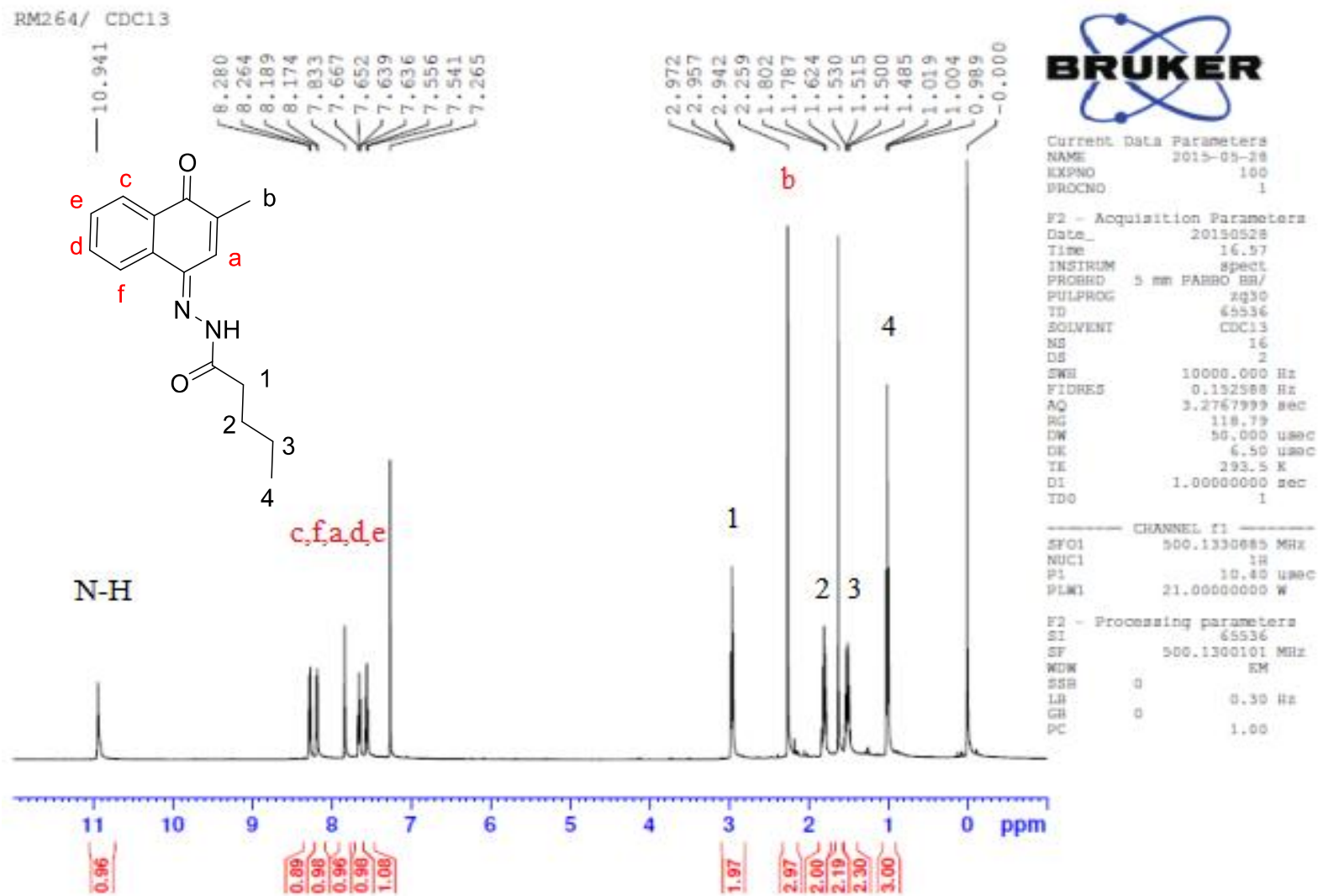


Figure S2. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz) spectrum of compound **6a**

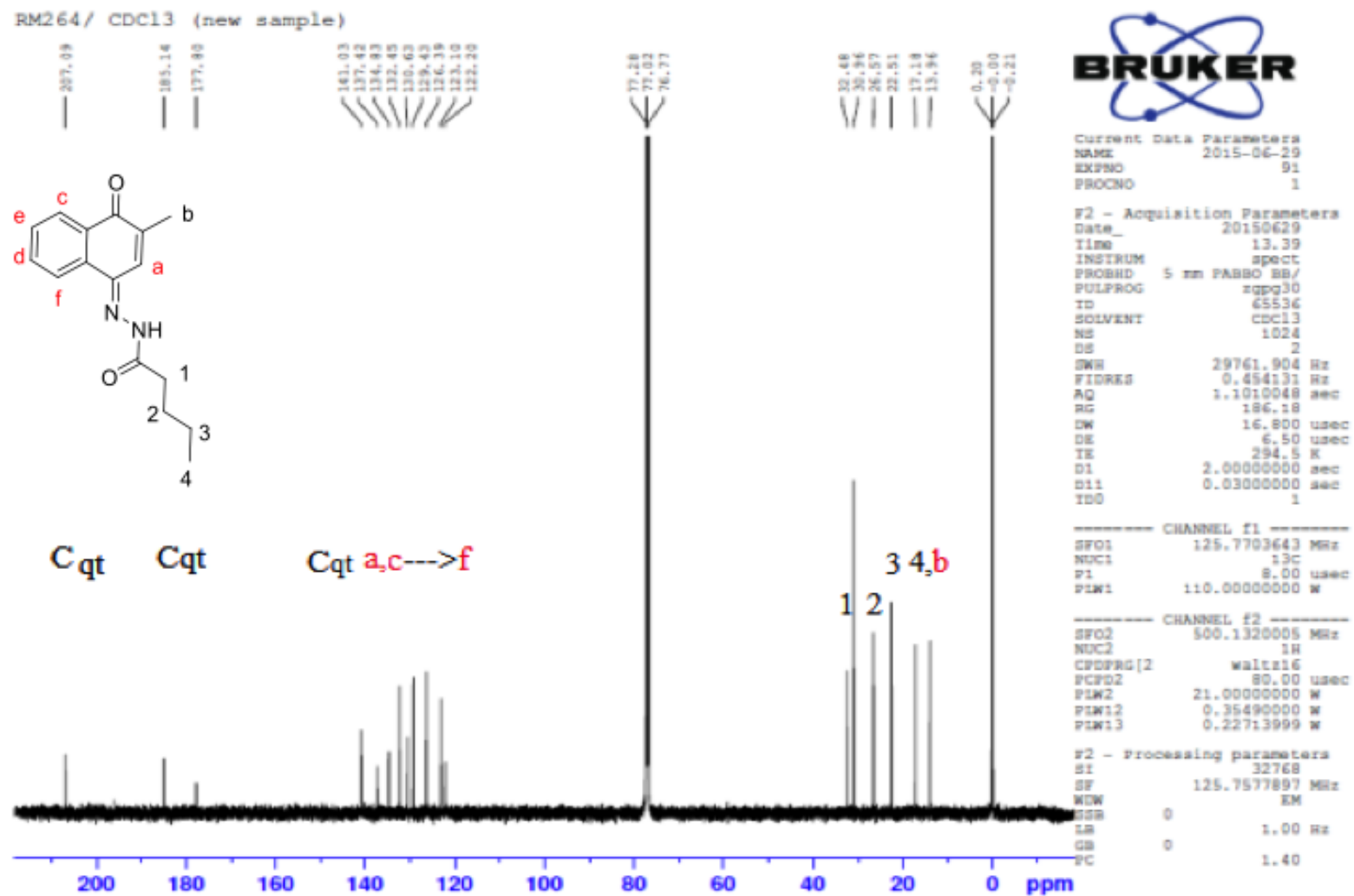


Figure S3. <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) spectrum of compound **6a**

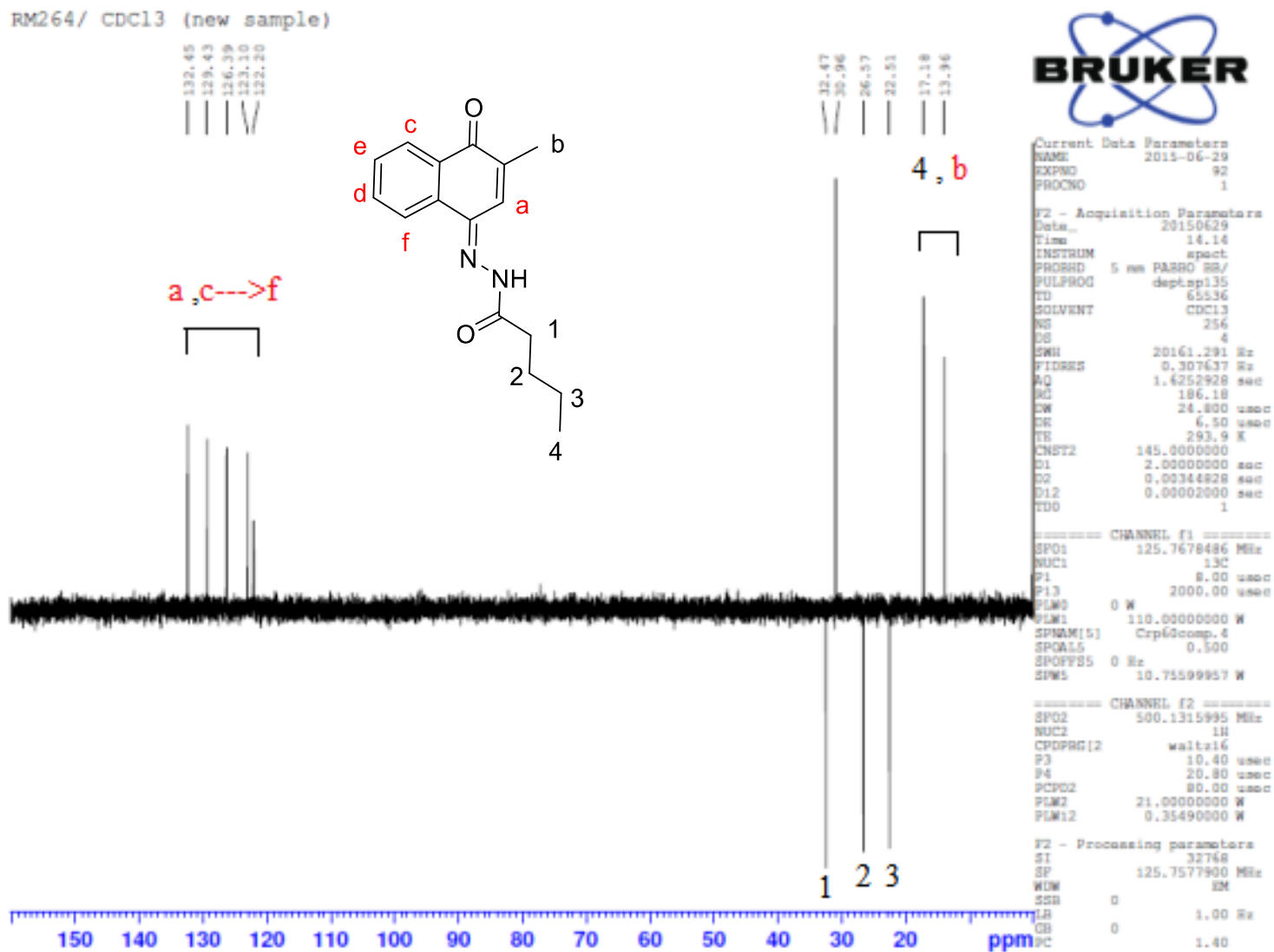
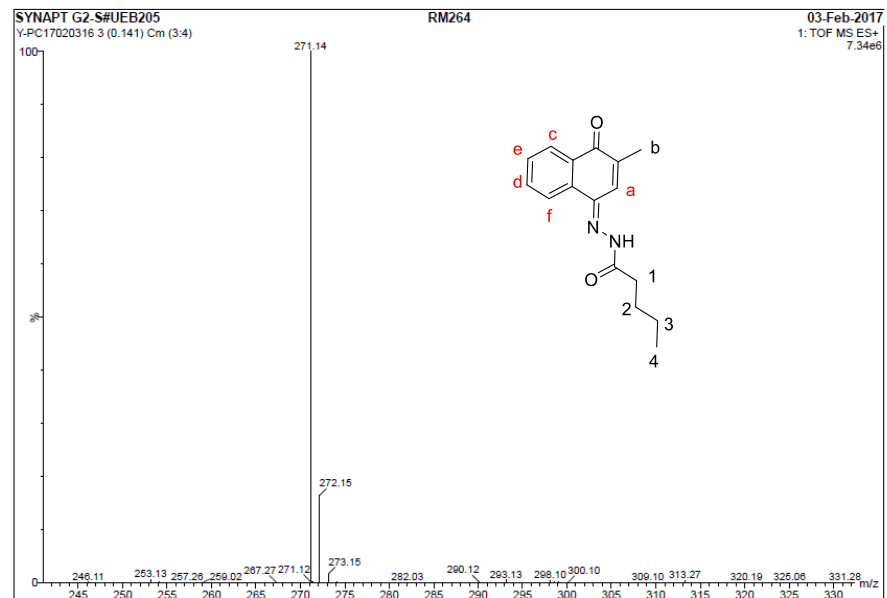


Figure S4. DEPT NMR ( $\text{CDCl}_3$ , 100 MHz) spectrum of compound **6a**



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

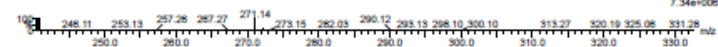
Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions  
 457 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)  
 Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

SYNAPT G2.S#UEB205 RM264 03-Feb-2017  
 Y-PC17020316 3 (0.141) Cm (3:4) 1: TOF MS ES+  
 7.34e6



Minimum: -1.5  
 Maximum: 1.0 1.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
271.1445	271.1447	-0.2	-0.7	8.5	2414.2	0.000	100.00	C16 H19 N2 O2
	271.1452	-0.7	-2.6	1.5	2430.0	15.760	0.00	C H15 N14 O3

Figure S5. HRMS spectrum of compound 6a



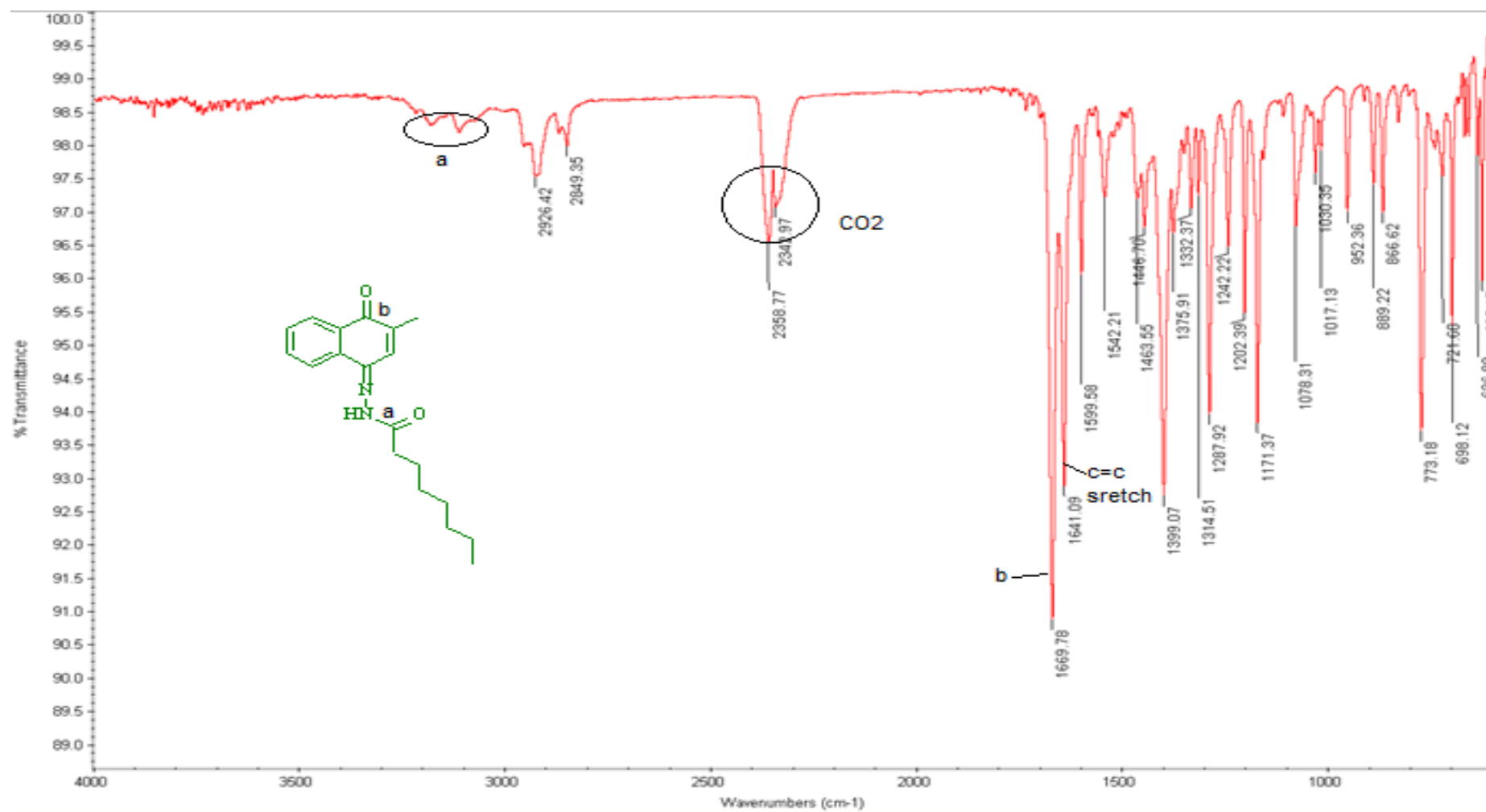


Figure S6. IR spectrum of compound 6b

RM176/CDC13



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 PROCNO 1

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 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 2  
 SWH 10000.000 Hz  
 FIDRES 0.152588 Hz  
 AQ 3.2767999 sec  
 RG 84.41  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 300.8 K  
 D1 1.00000000 sec  
 TDO 1

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 NUC1 1H  
 P1 9.80 usec  
 PLW1 21.00000000 W

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 SF 500.1300106 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

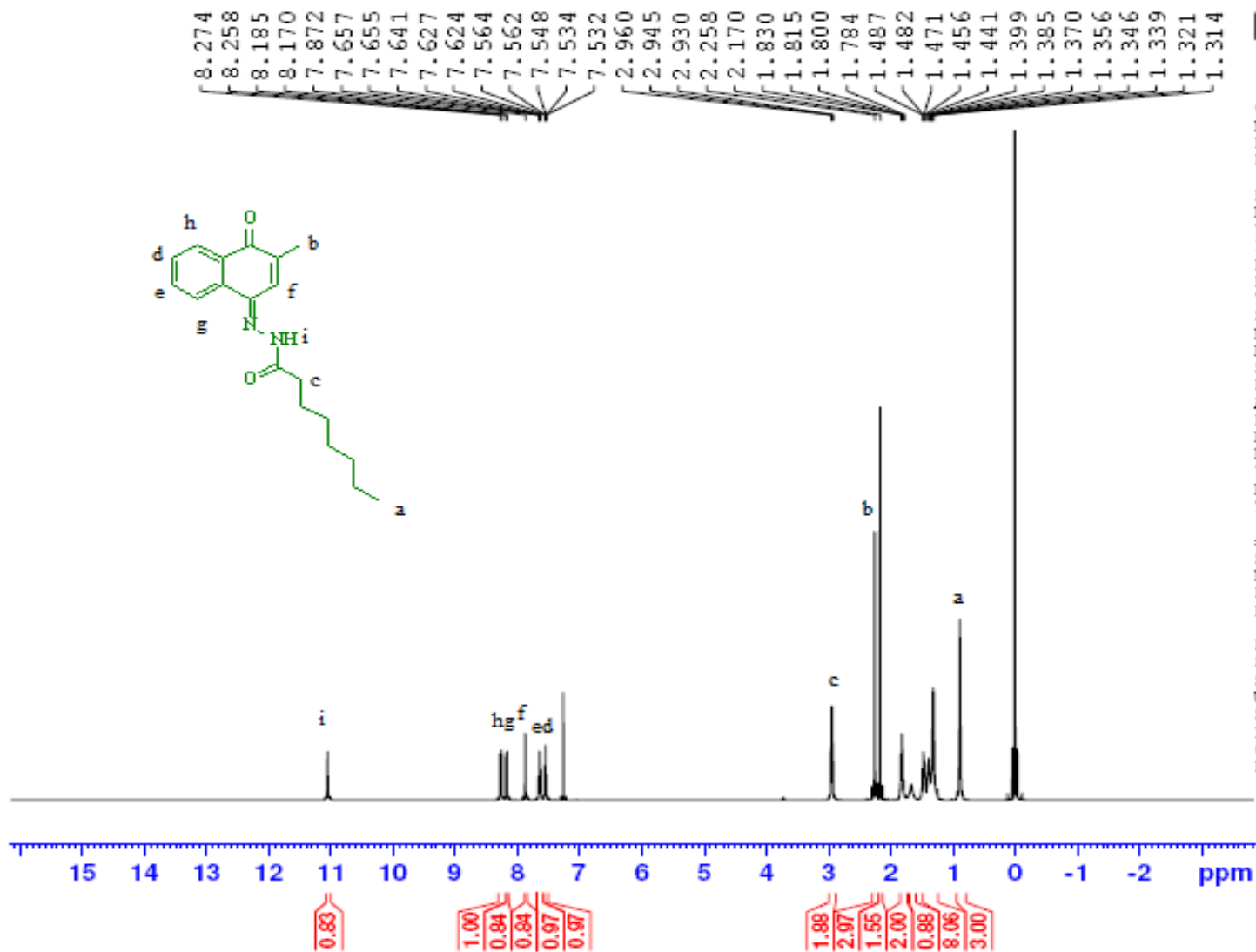


Figure S7. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz) spectrum of compound **6b**

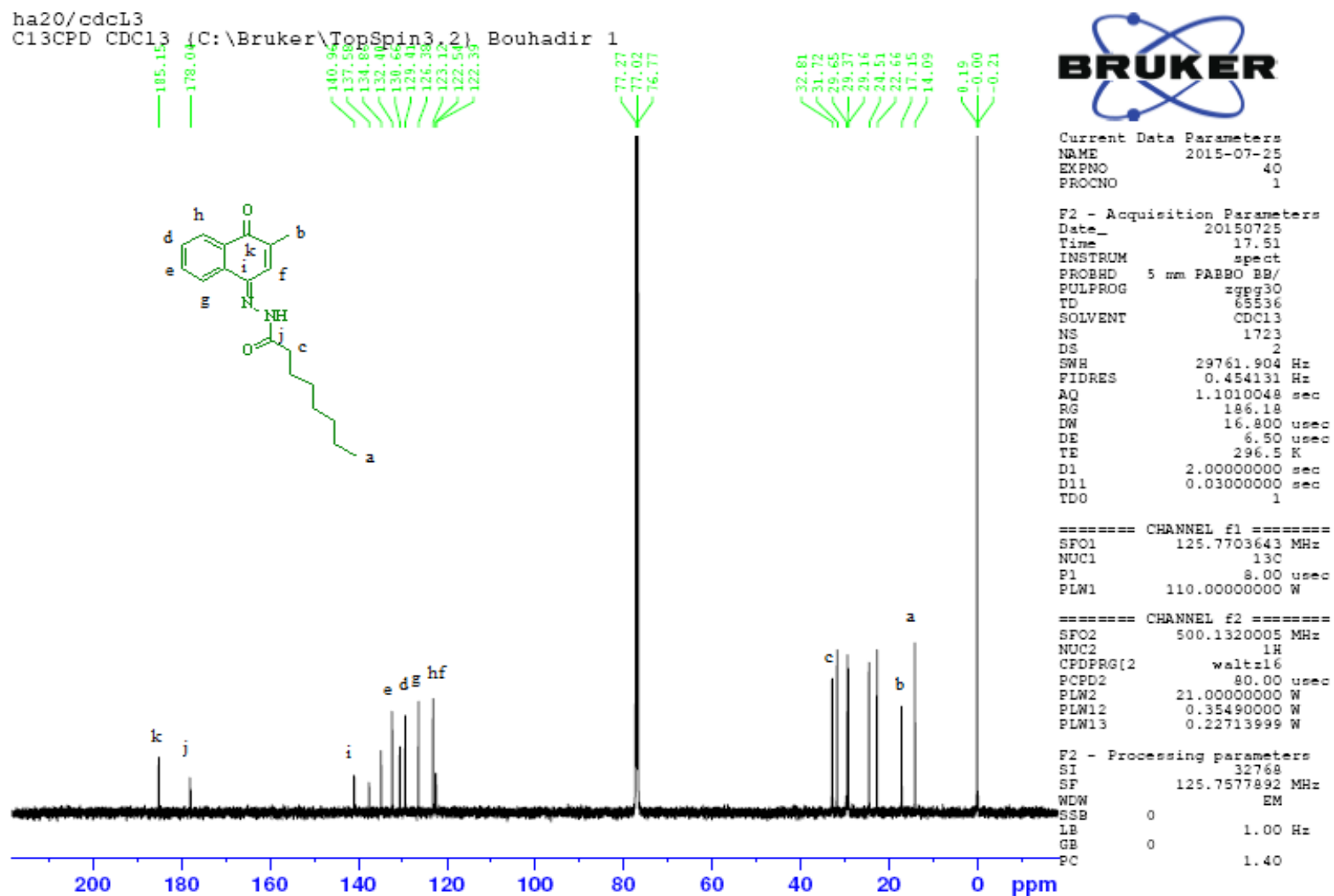


Figure S8.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectrum of compound **6b**

HA 20/CDC13  
DEPT

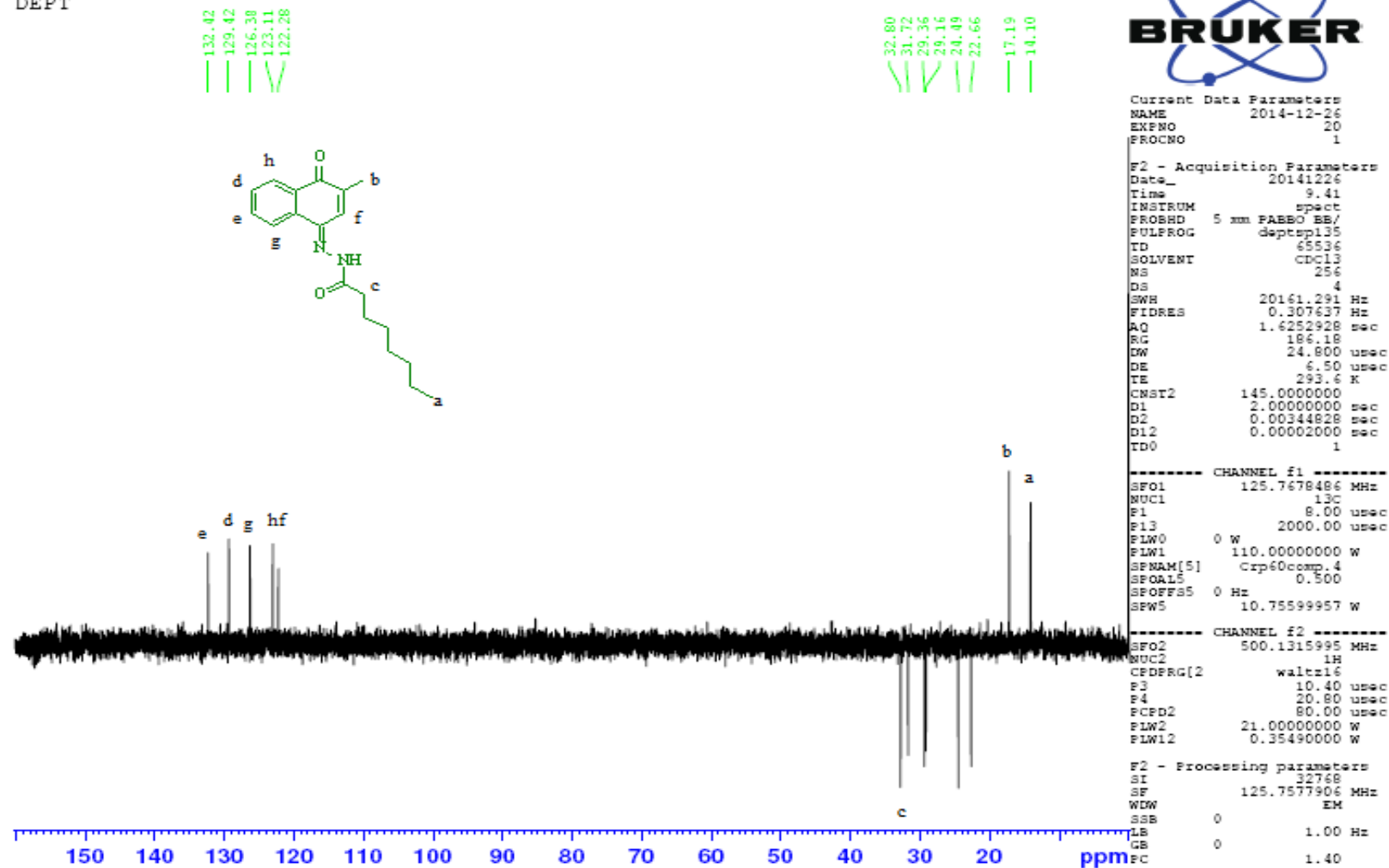


Figure S9. DEPT NMR (CDCl<sub>3</sub>, 100 MHz) spectrum of compound **6b**

2

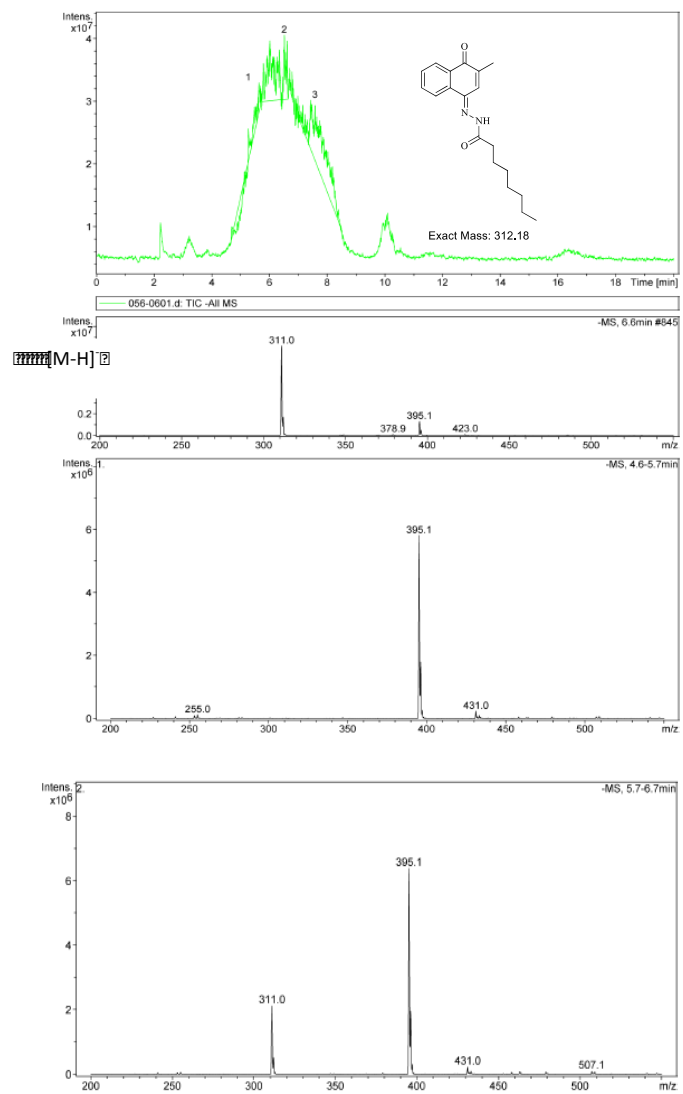
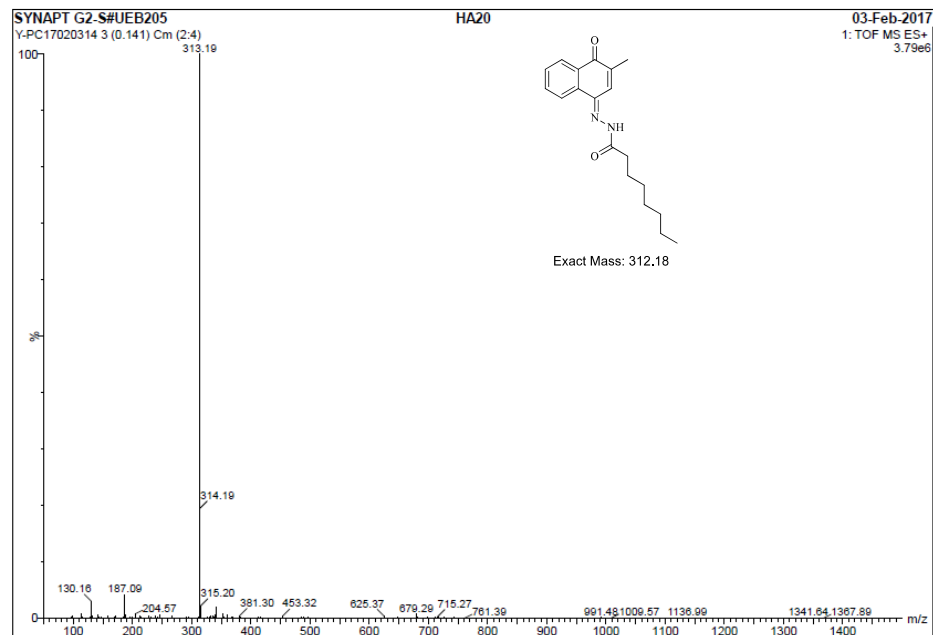


Figure S10. LC-MS spectrum of compound 6b



### Elemental Composition Report

Page 1

#### Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

664 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

SYNAPT G2-S#UEB205

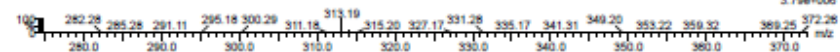
Y-PC17020314 3 (0.141) Cm (2-4)

HA20

03-Feb-2017

1: TOF MS ES+

3.79e6



Minimum: -1.5  
Maximum: 1.0 1.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
313.1915	313.1916	-0.1	-0.3	8.5	2014.2	0.000	100.00	C19 H25 N2 O2
	313.1921	-0.6	-1.9	1.5	2028.7	14.547	0.00	C4 H21 N14 O3

Figure S11. HRMS spectrum of compound 6b

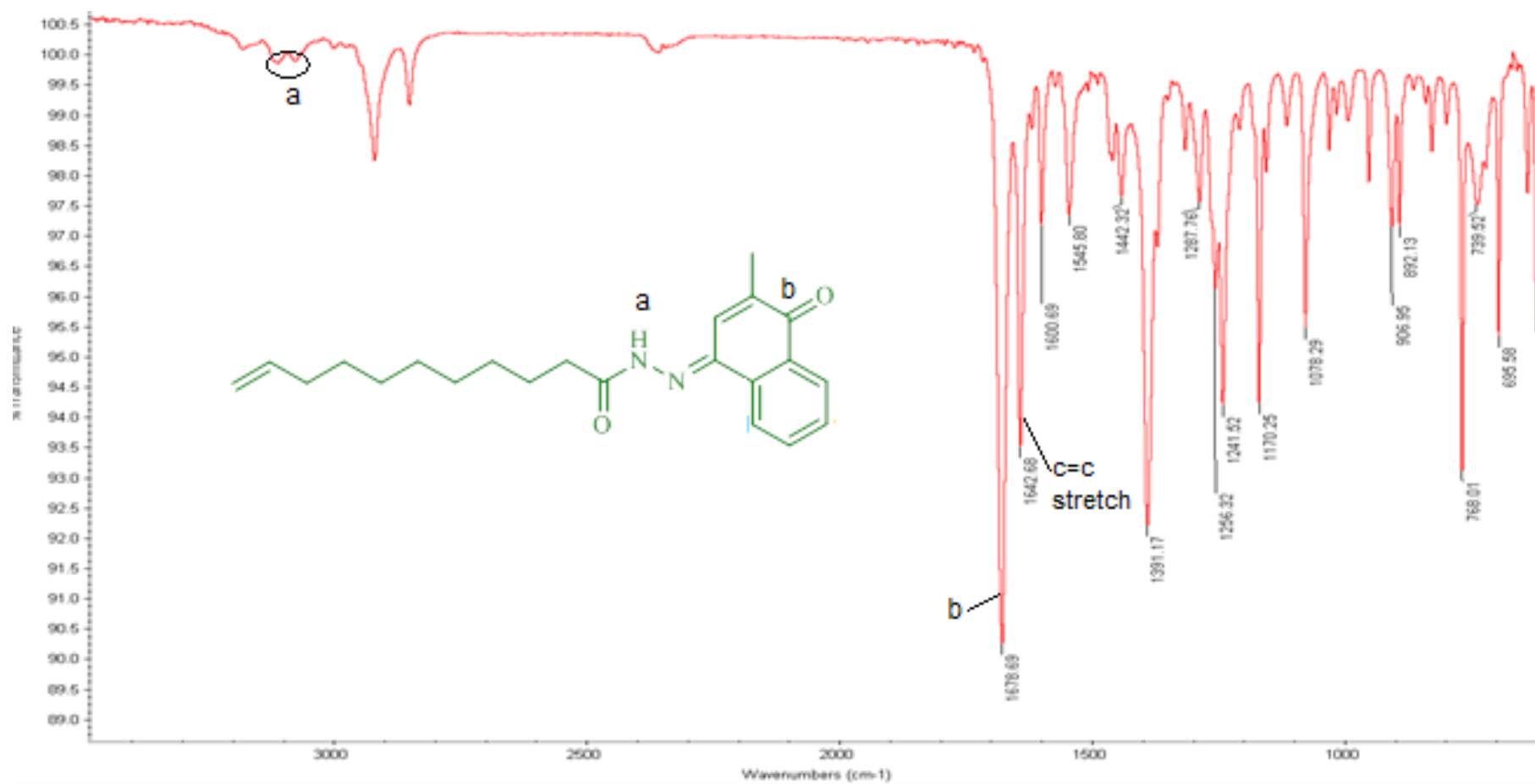
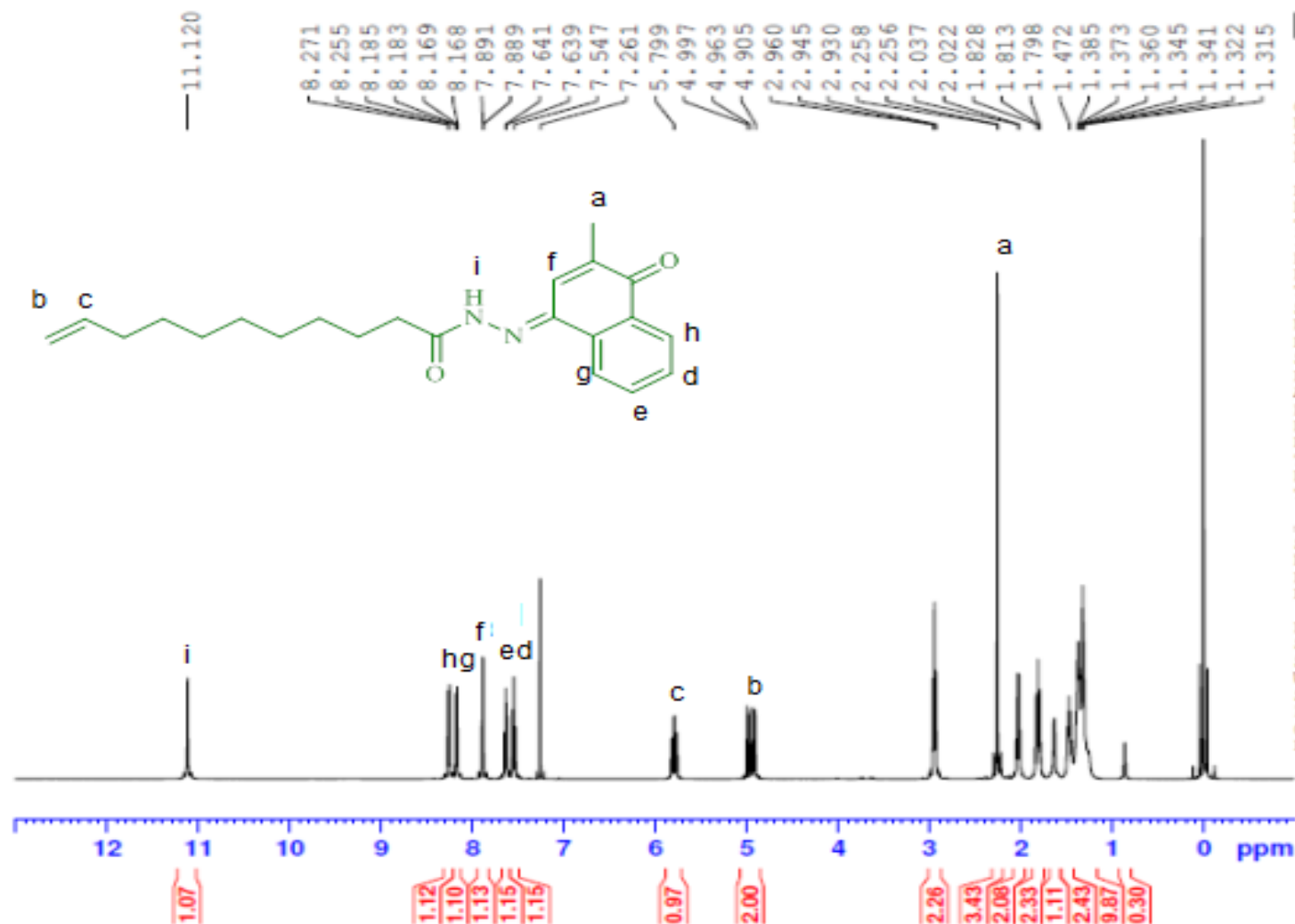


Figure S12. IR spectrum of compound 6c

RM170/ CDC13



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PROCNO 1

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PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 79.05  
DW 50.000 usec  
DE 6.50 usec  
TE 300.7 K  
D1 1.00000000 sec  
TDO 1

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NUC1 1H  
P1 9.80 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
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SF 500.1300111 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S13. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz) spectrum of compound **6c**



RM170 13C/CDC13

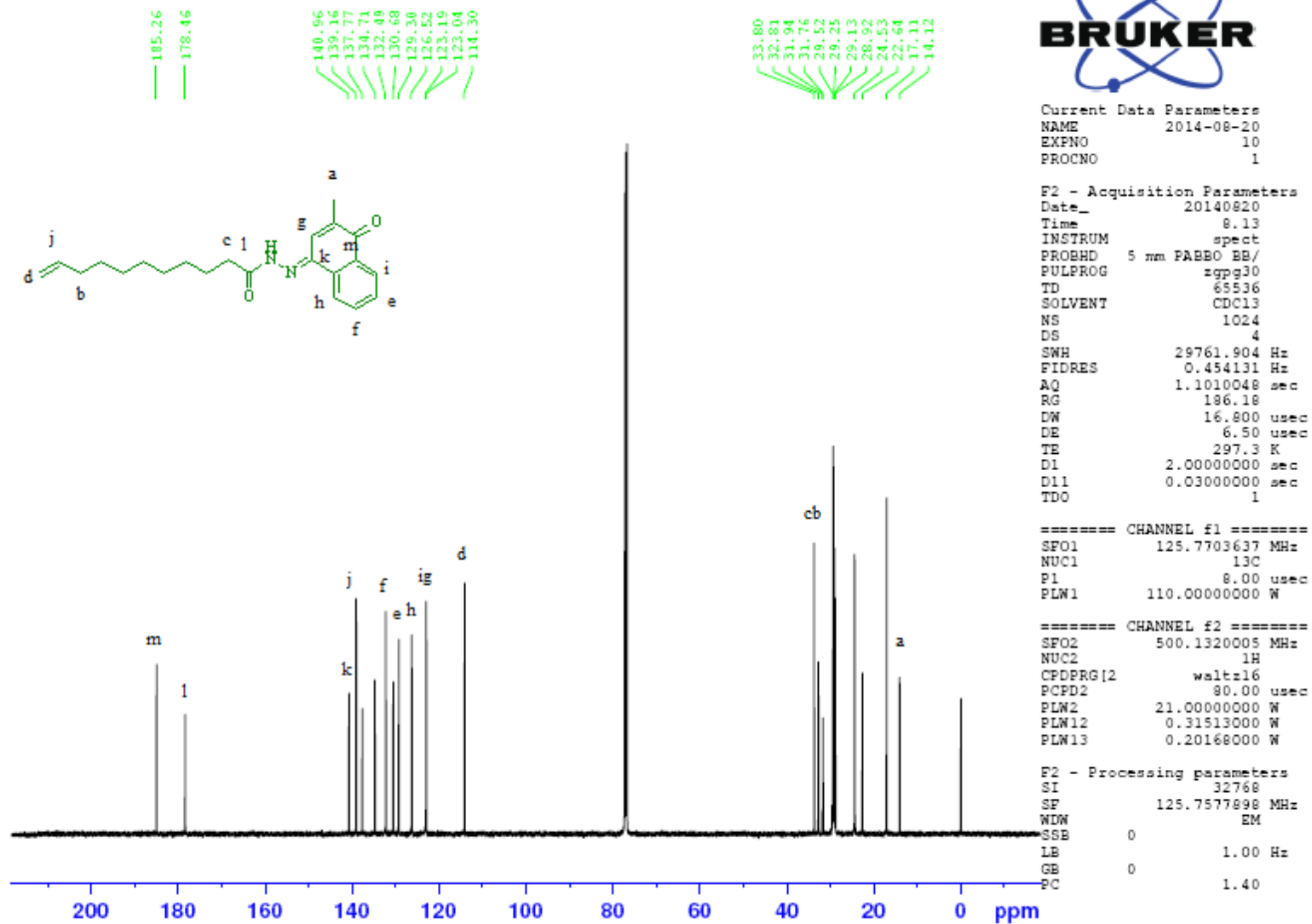
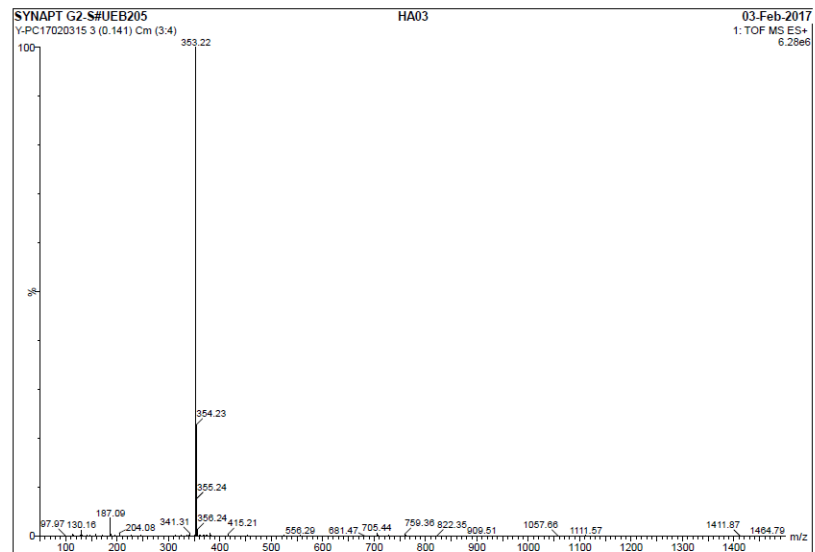


Figure S14.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectrum of compound **6c**



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

883 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

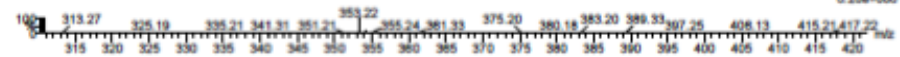
SYNAPT G2-S#UEB205

HA03

03-Feb-2017

1: TOF MS ES+

6.28e+006



Minimum:

Maximum: 1.0 1.0 -1.5

Mass

Calc. Mass mDa ppm DBE i-FIT Norm Conf(%) Formula

353.2230 353.2229 0.1 0.3 9.5 2033.0 0.022 97.78 C22 H29 N2 O2

353.2234 -0.4 -1.1 2.5 2036.8 3.809 2.22 C7 H25 N14 O3

Figure S15. HRMS spectrum of compound 6b

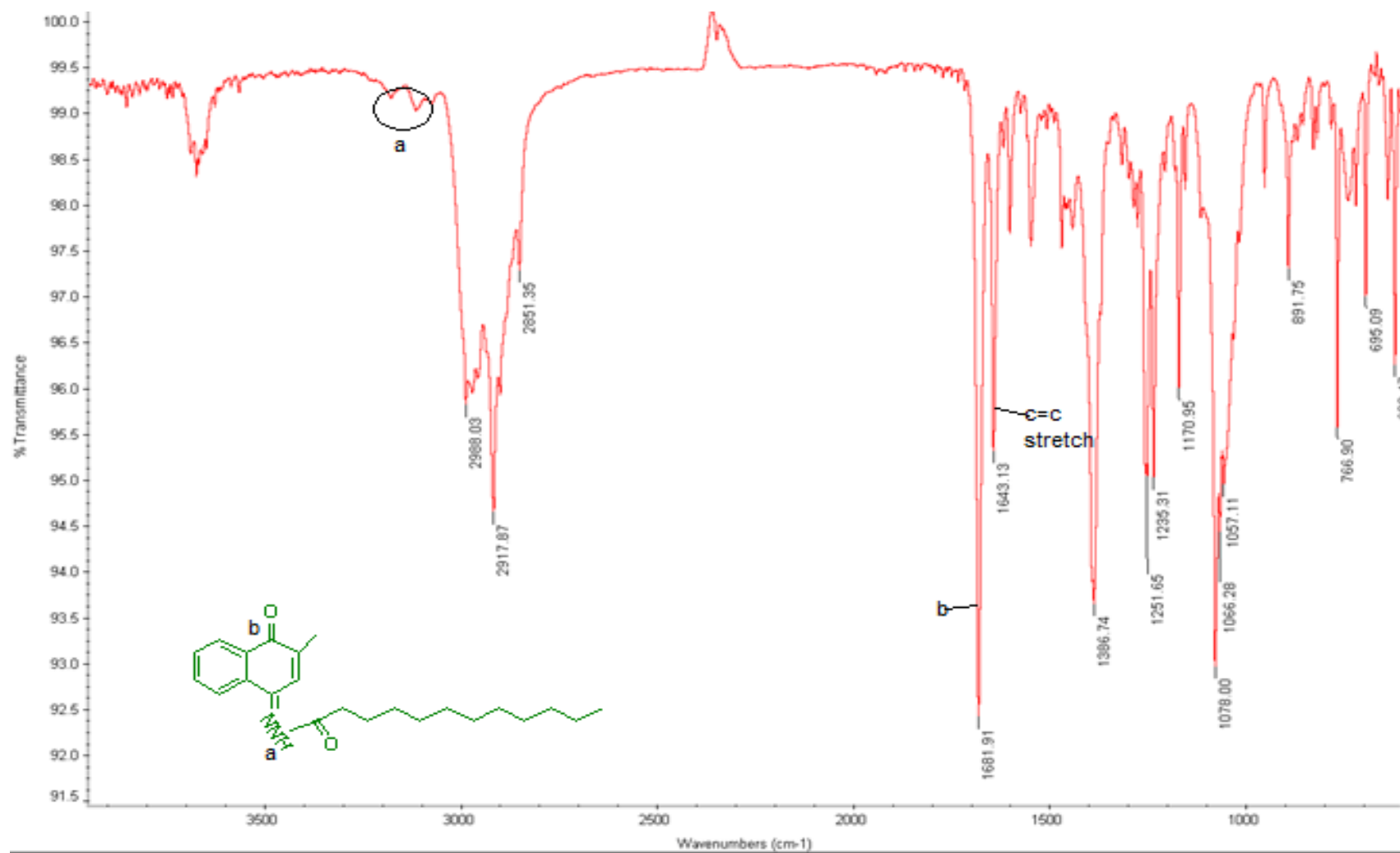


Figure S16. IR spectrum of compound 6d

HA04/CDC13

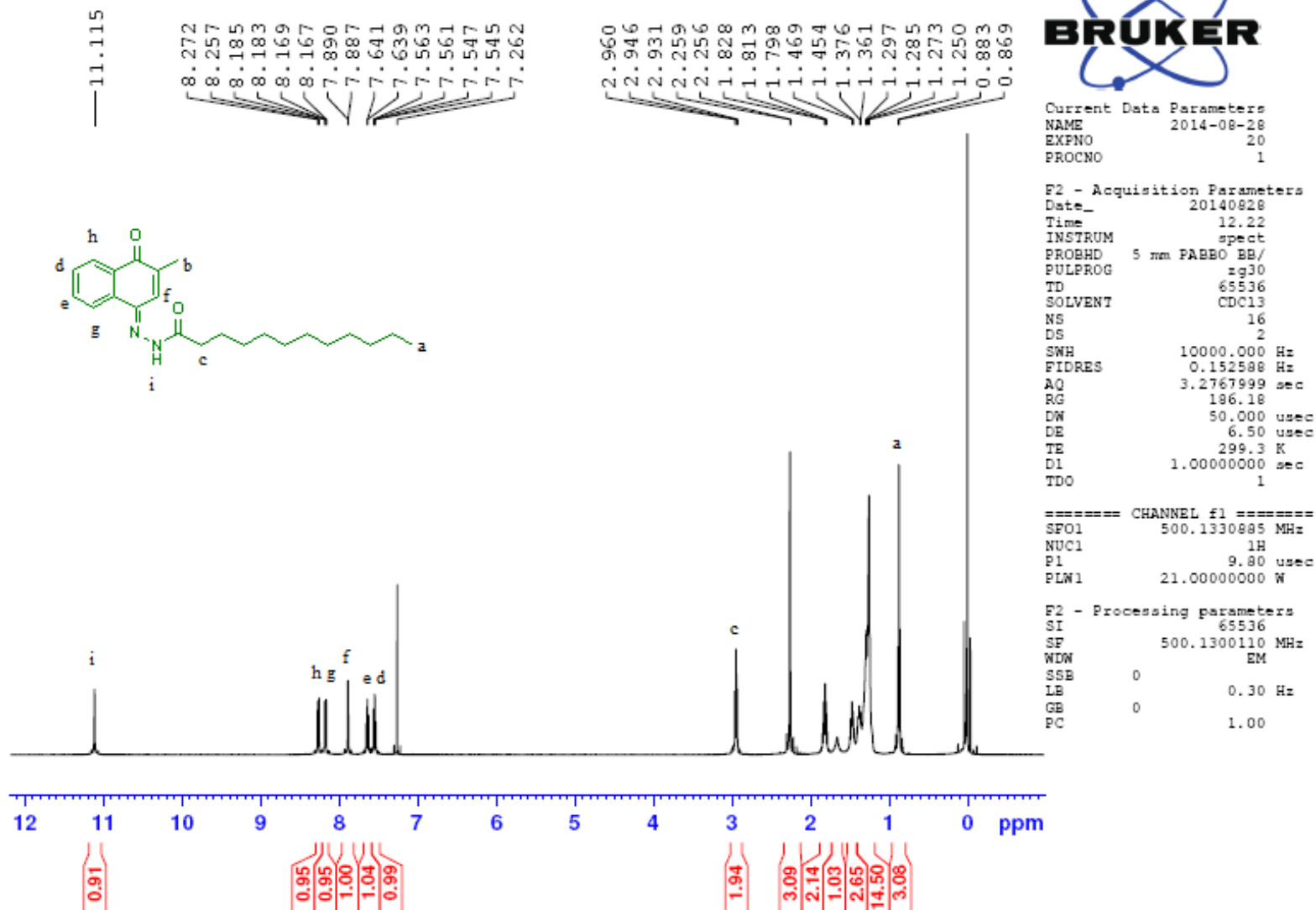


Figure S17. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz) spectrum of compound **6d**

HA14  
C13CPD

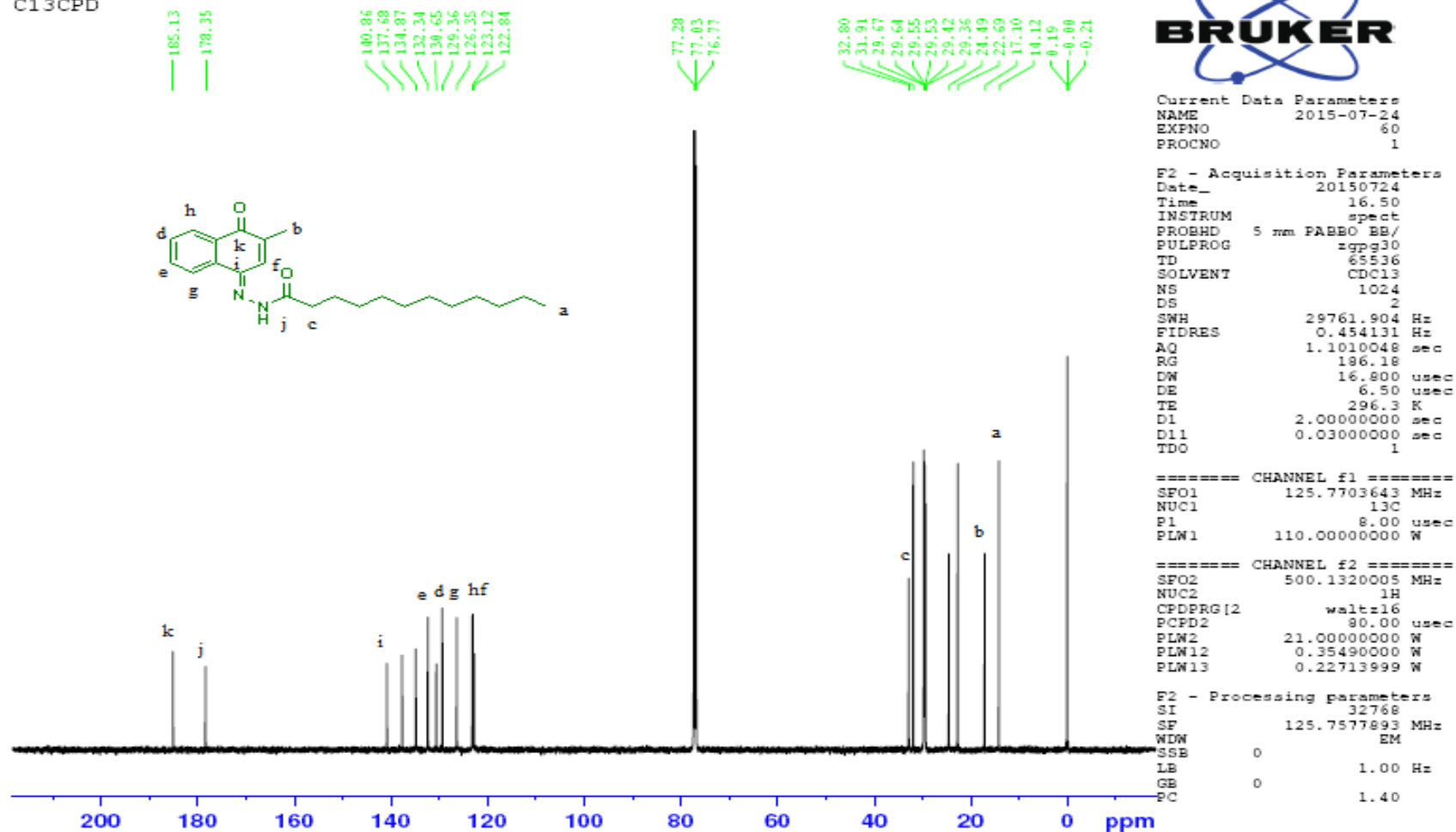


Figure S18.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectrum of compound **6d**

Display Report - All Windows All Analyses

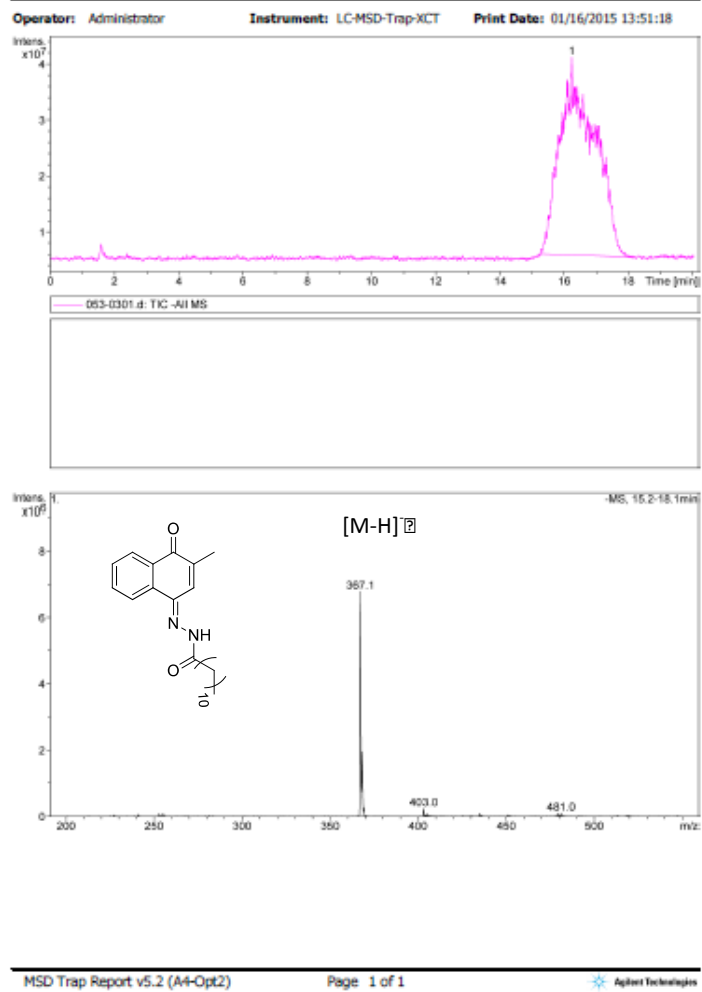
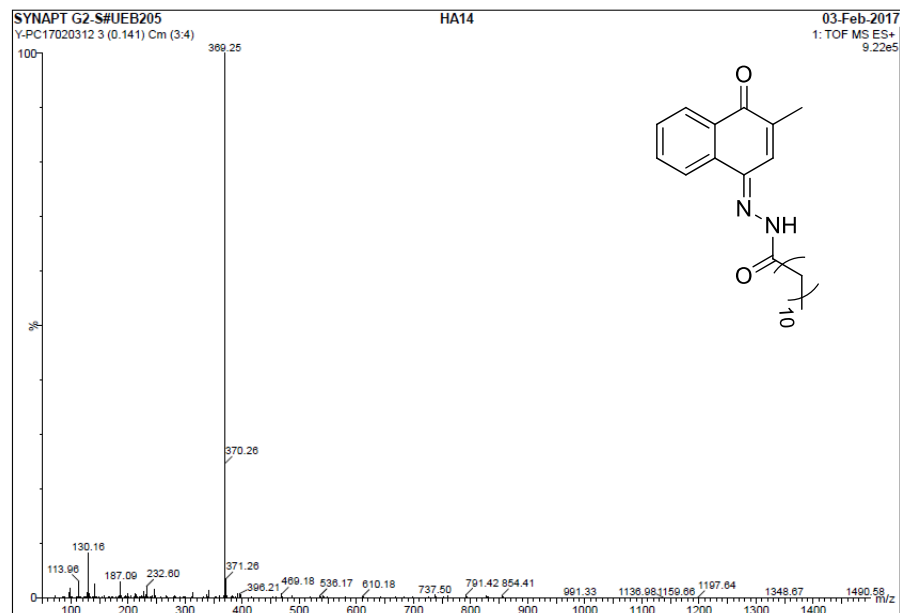


Figure S19. LC-MS spectrum of compound 6d



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0  
 Element prediction: Off  
 Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

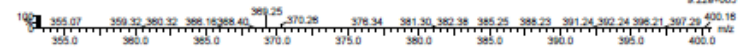
963 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

SYNAPT G2-S#UEB205 HA14  
 Y-PC17020312 3 (0.141) Cm (3:4)

03-Feb-2017  
 1: TOF MS ES+  
 9.22e+05



Minimum: 1.0 1.0 -1.5  
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
369.2540	369.2542	-0.2	-0.5	8.5	1499.3	0.000	100.00	C23 H23 N2 O2
	369.2547	-0.7	-1.9	1.5	1514.1	14.875	0.00	C8 H29 N14 O3

Figure S20. HRMS spectrum of compound 6d

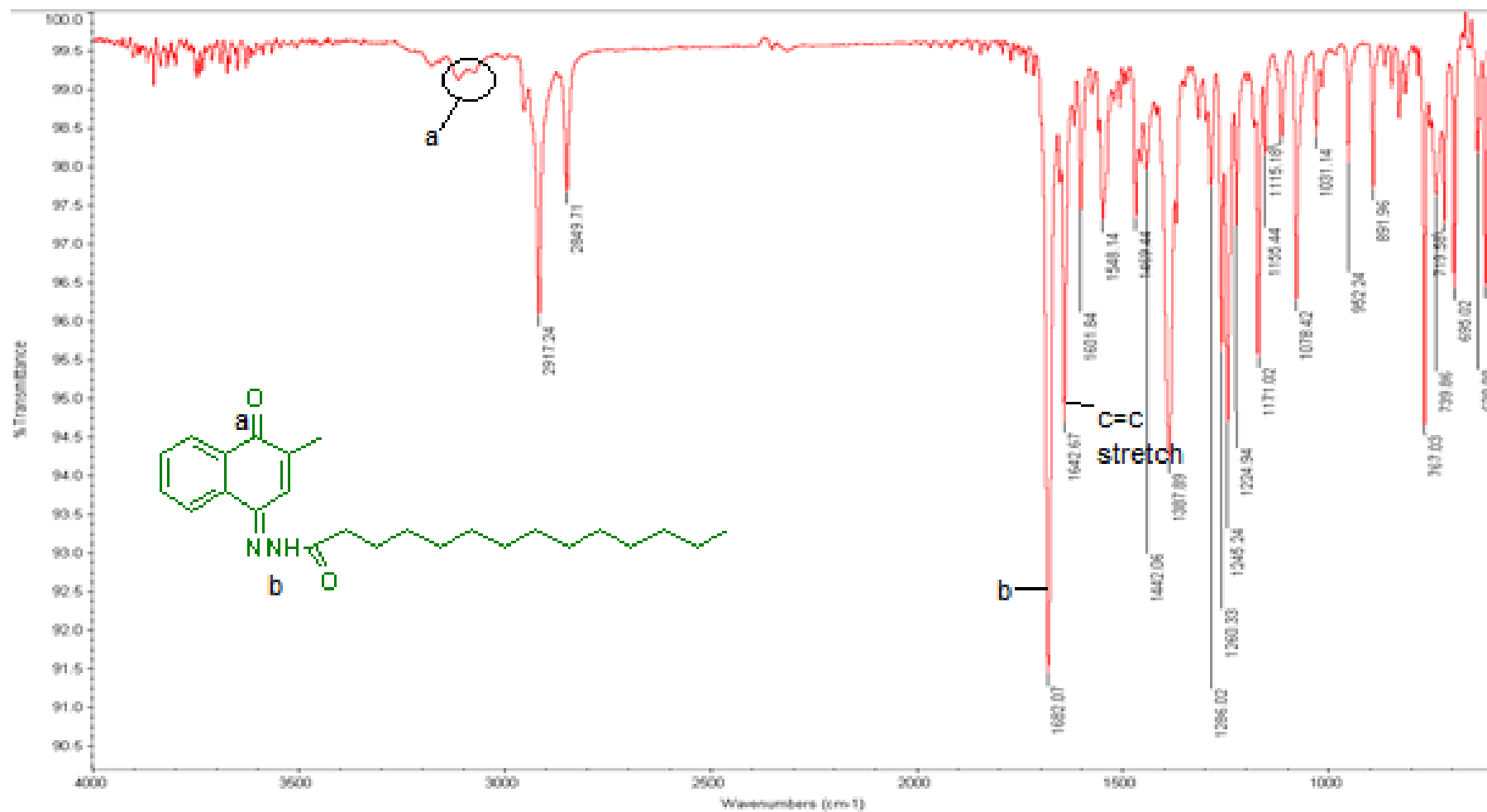


Figure S21. IR spectrum of compound 6e



HA05/CDCl3

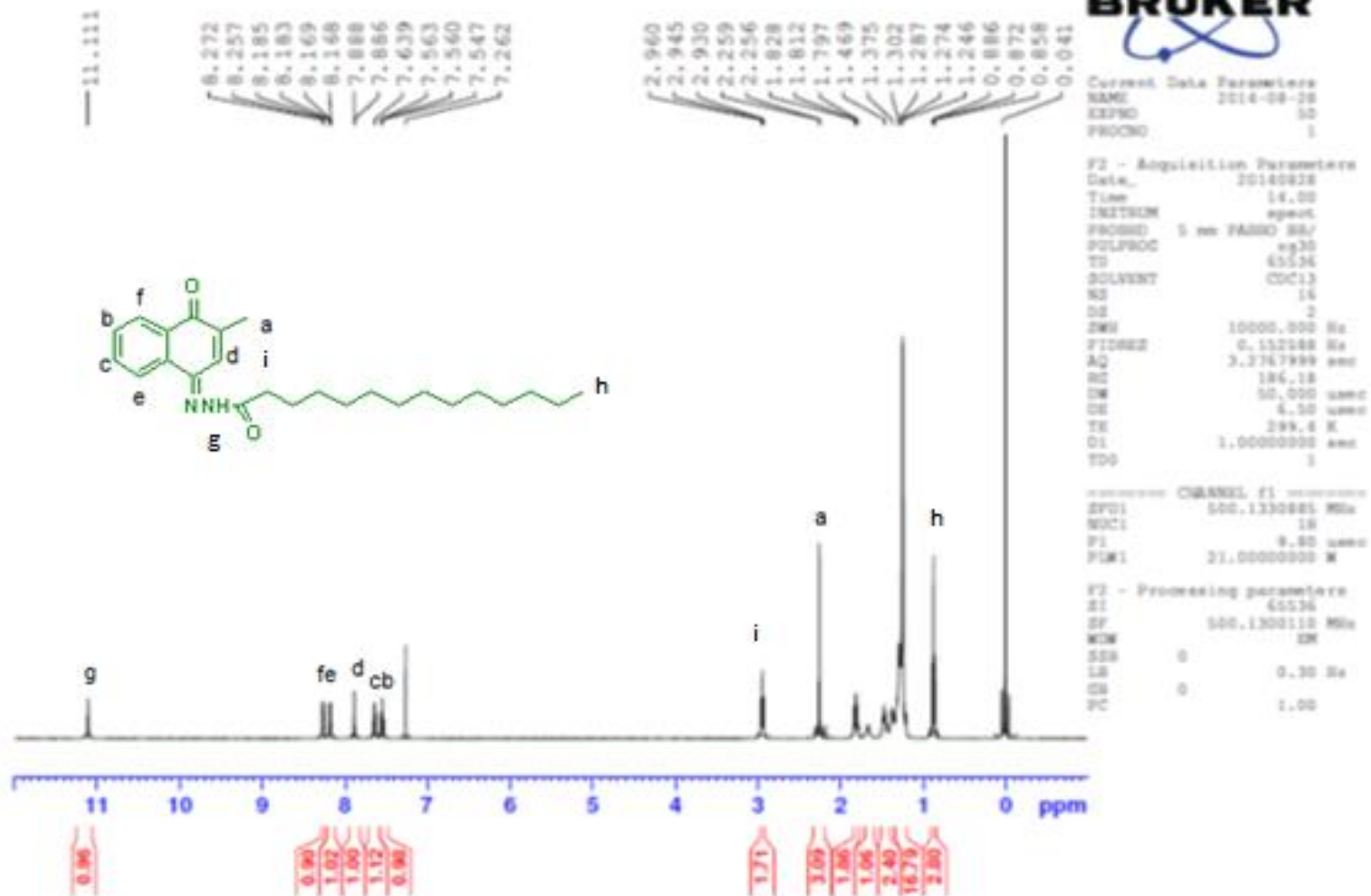
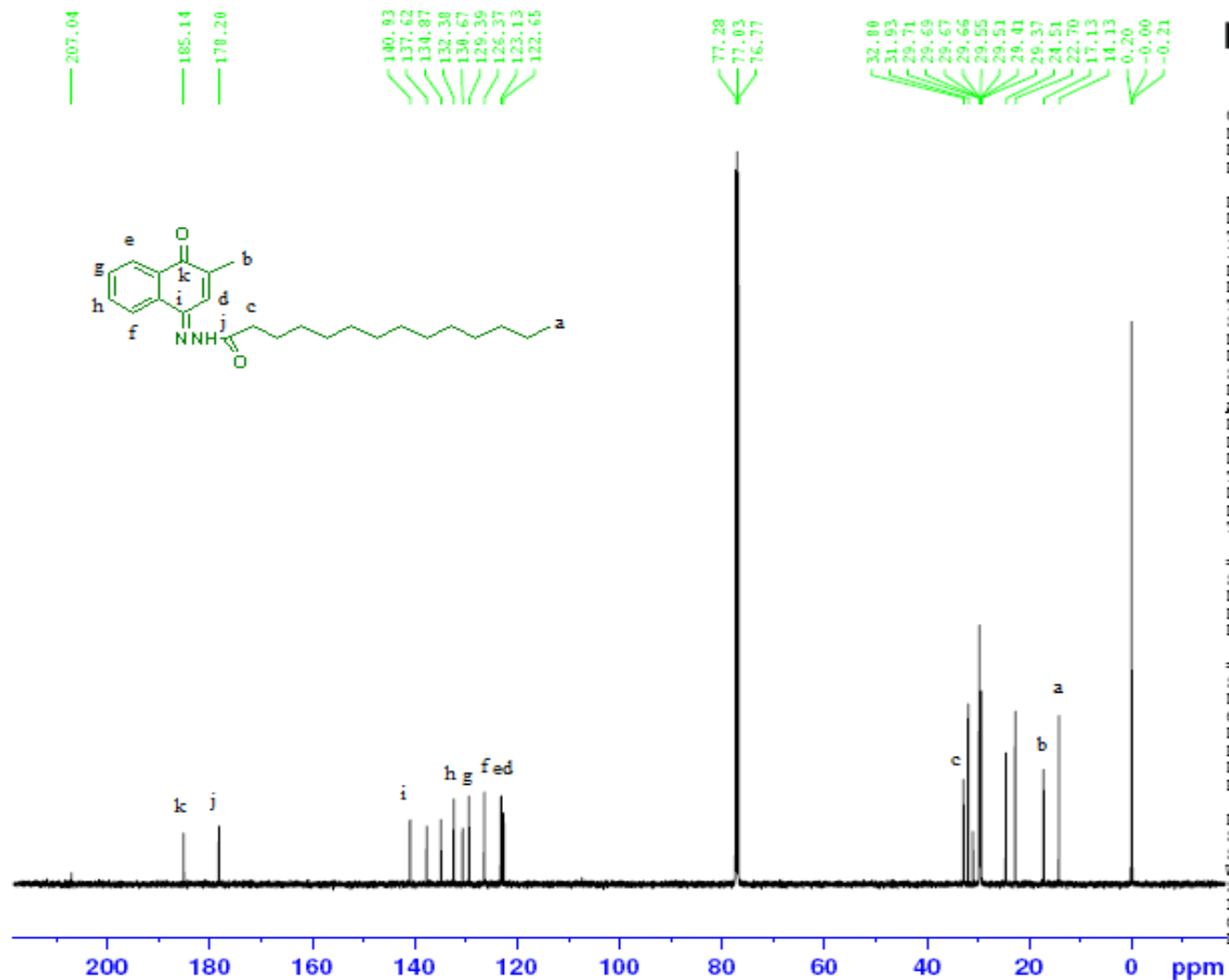


Figure S22. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz) spectrum of compound 6e

HA15/CDC13



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EXPNO 190  
PROCNO 1

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SOLVENT CDC13  
NS 1024  
DS 2  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010048 sec  
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DE 6.50 usec  
TE 296.5 K  
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D11 0.03000000 sec  
TDO 1

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NUC1 13C  
P1 8.00 usec  
PLW1 110.00000000 W

==== CHANNEL f2 =====  
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NUC2 1H  
CPDPRG2 waltz16  
PCPD2 90.00 usec  
PLW2 21.00000000 W  
PLW12 0.35490000 W  
PLW13 0.22713999 W

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

Figure S23.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz) spectrum of compound **6e**

HA05/CDC13  
C13DEPT135

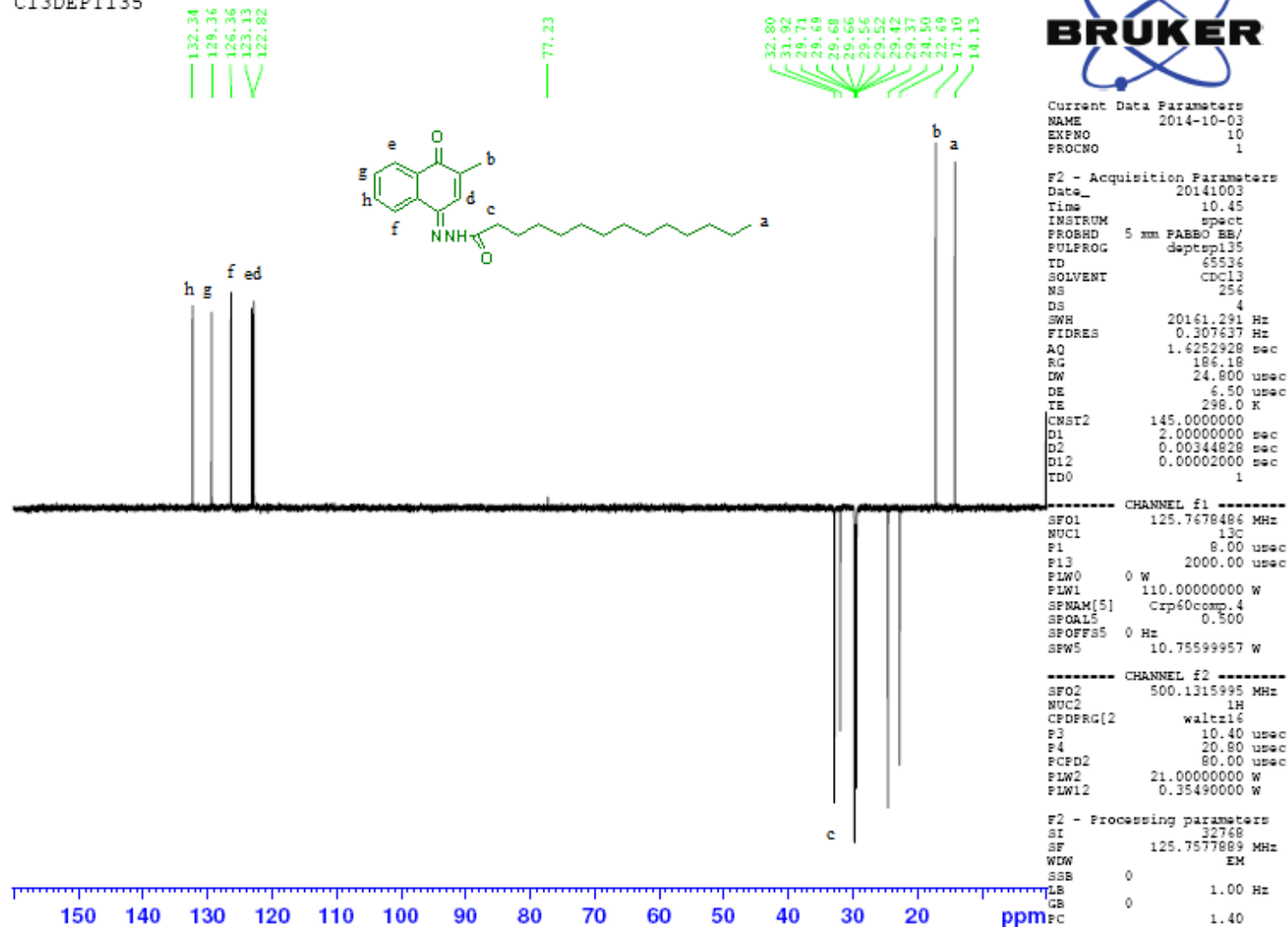
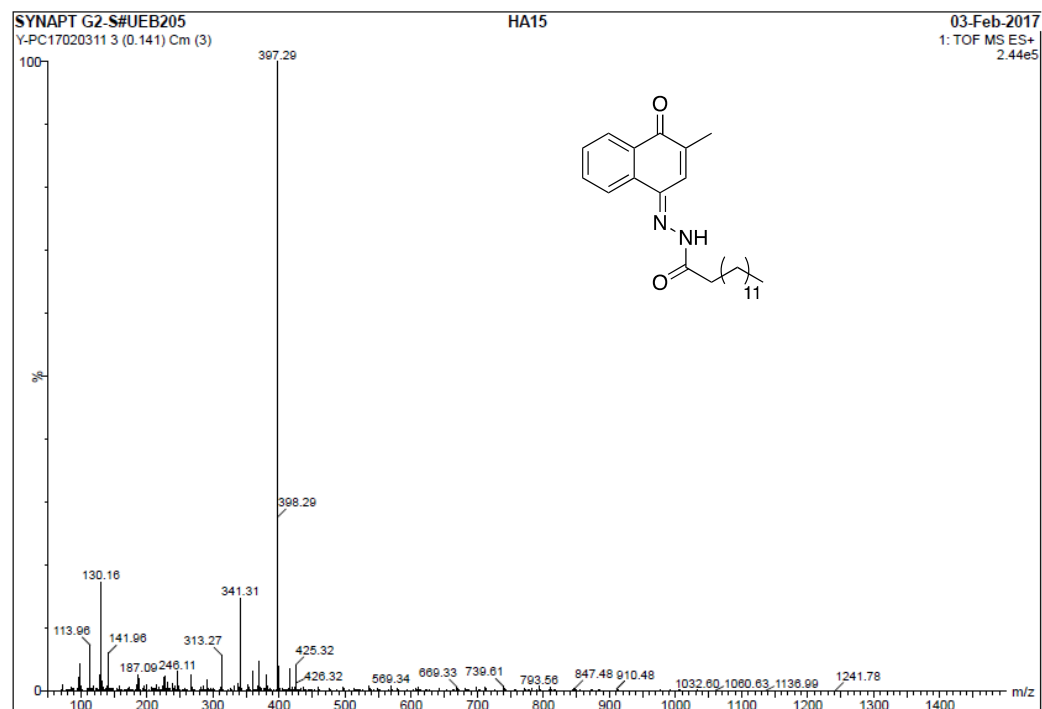


Figure S24. DEPT NMR (CDCl<sub>3</sub>, 100 MHz) spectrum of compound **6e**



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

1130 formulae evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

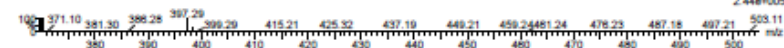
SYNAPT G2-S#UEB205

HA15

03-Feb-2017

1: TOF MS ES+

2.44e005



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(k)	Formula
397.2852	397.2855	-0.3	-0.8	8.5	1021.8	0.000	100.00	C25 H37 N2 O2
	397.2860	-0.8	-2.0	1.5	1026.6	14.744	0.00	C10 H23 N14 O3

Figure S25. HRMS spectrum of compound 6e

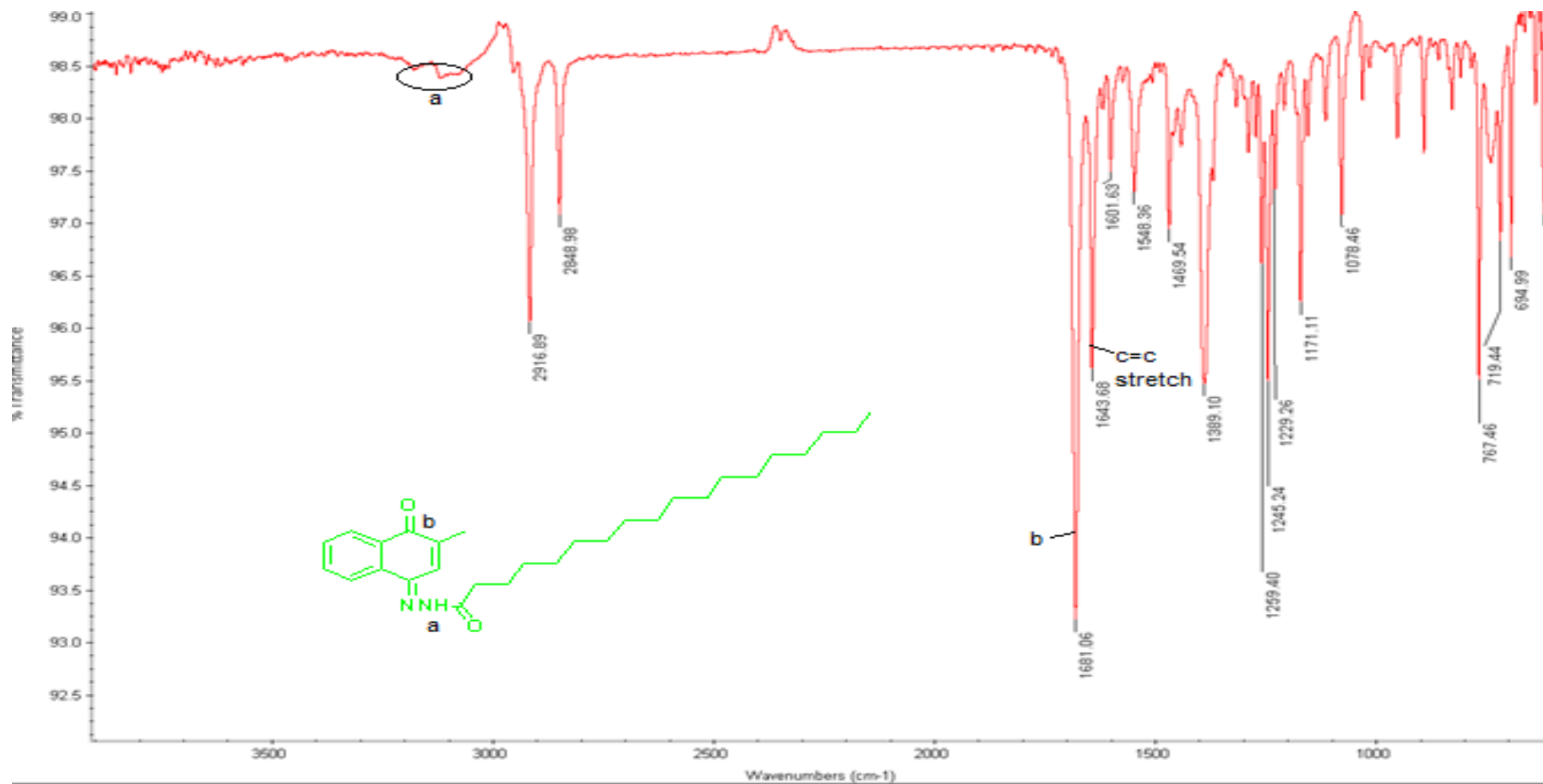


Figure S26. IR spectrum of compound 6f

RM185/CDC13

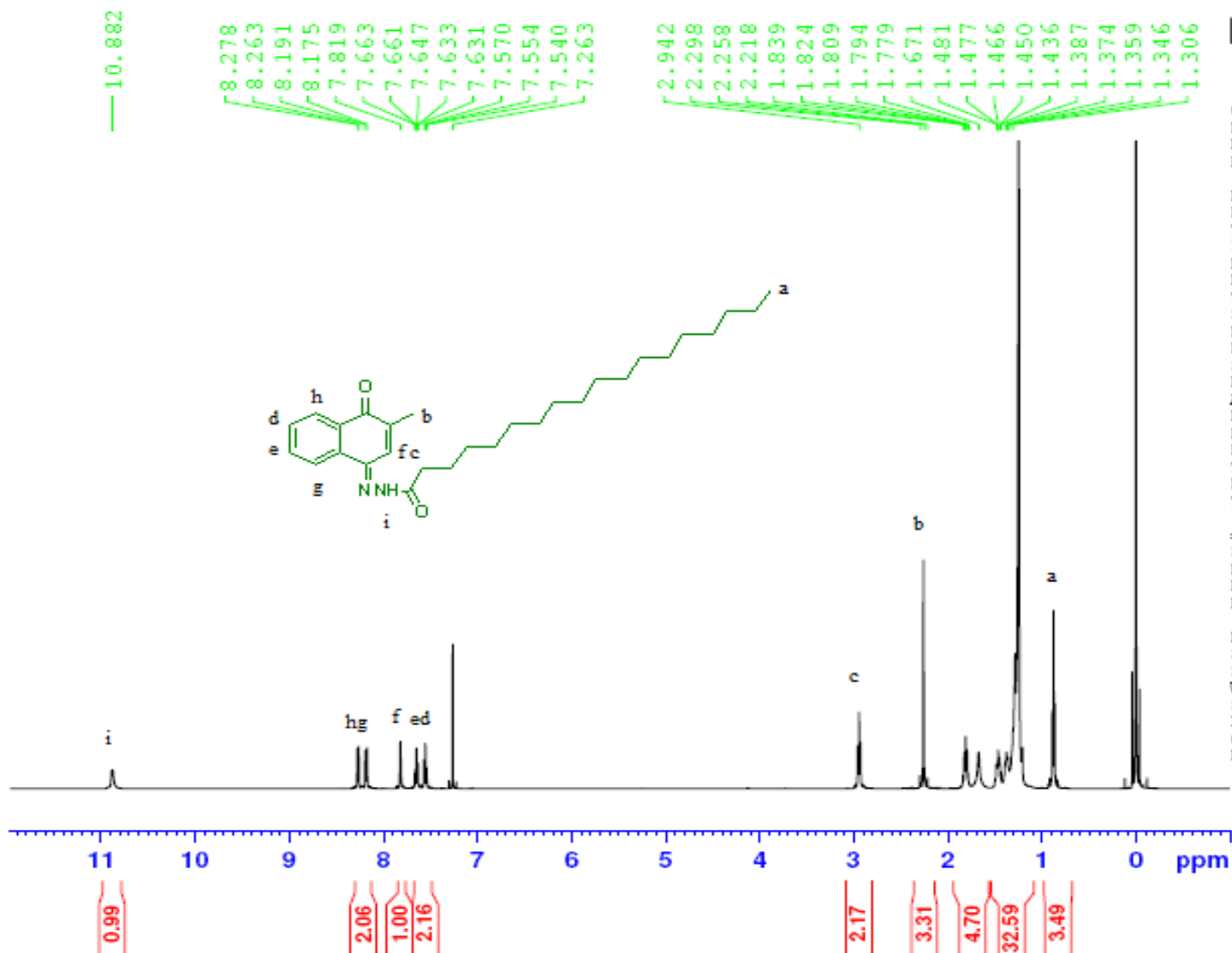
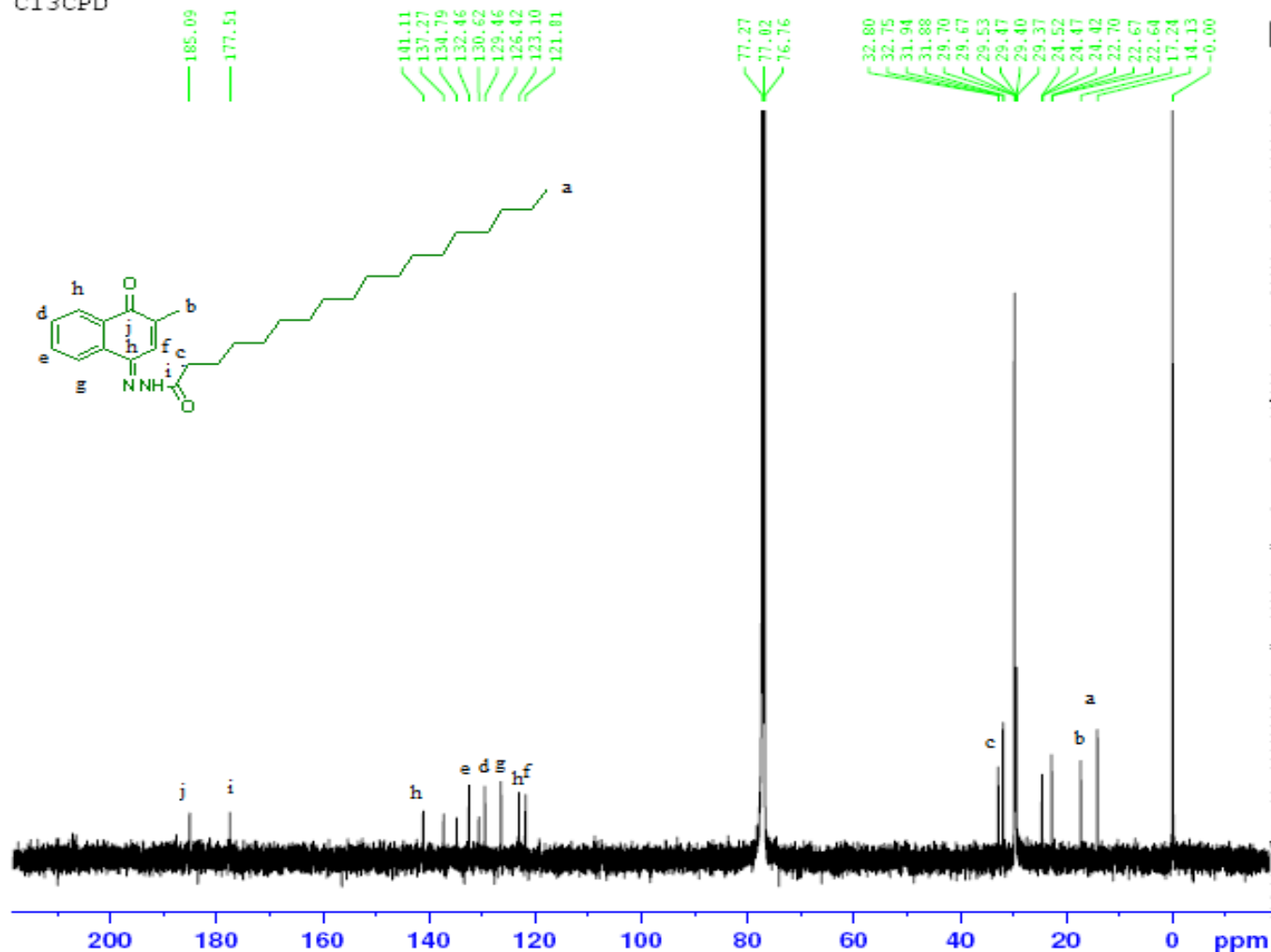


Figure S27. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz) spectrum of compound **6f**

HA17/CDC13  
C13CPD



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PROCNO 1

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SOLVENT CDC13  
NS 2100  
DS 2  
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FIDRES 0.454131 Hz  
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RG 196.18  
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TE 295.8 K  
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D11 0.03000000 sec  
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NUC1 13C  
P1 8.00 usec  
PLW1 110.00000000 W  
  
==== CHANNEL f2 =====  
SFO2 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 21.00000000 W  
PLW12 0.35490000 W  
PLW13 0.22713999 W

F2 - Processing parameters  
SI 32768  
SF 125.7577894 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Figure S28. <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) spectrum of compound 6f





# Display Report - All windows All Analyses

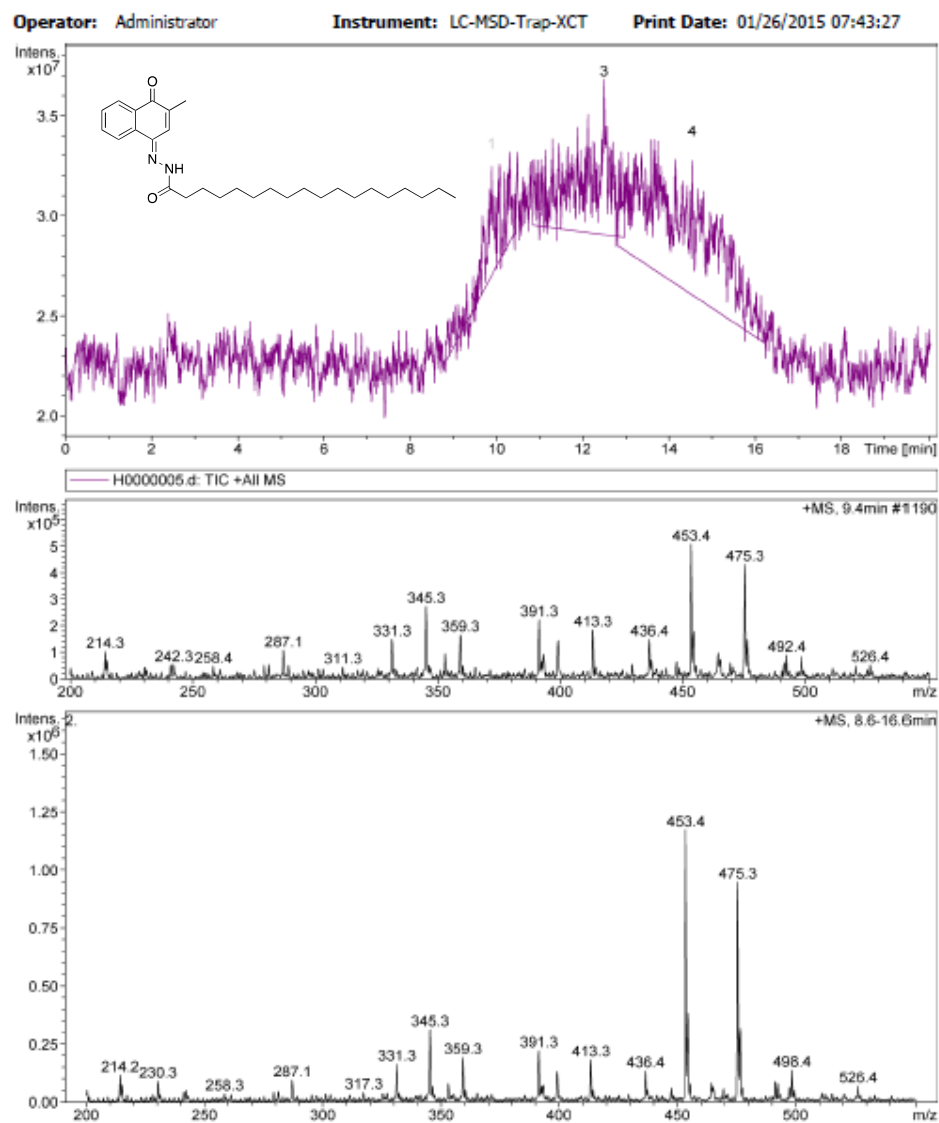
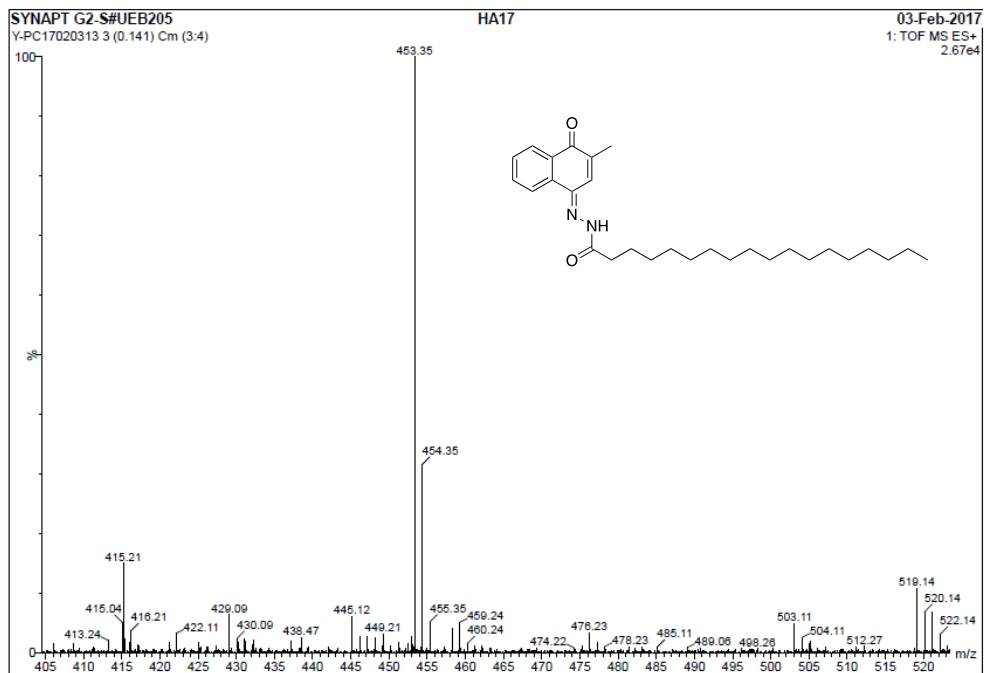


Figure S30. LC-MS spectrum of compound 6f



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

1455 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

SYNAPT G2-S#UEB205

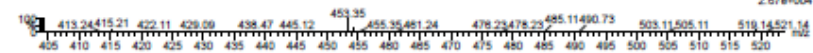
Y-PC17020313 3 (0.141) Cm (3:4)

HA17

03-Feb-2017

1: TOF MS ES+

2.67e+004

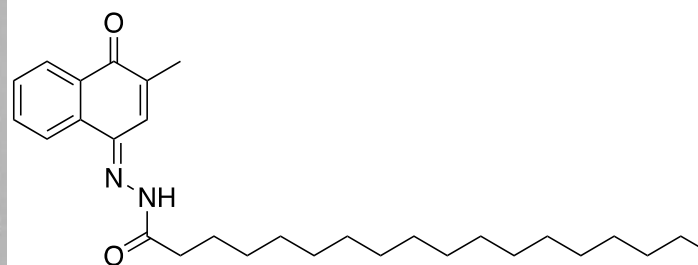


Minimum: -1.5  
Maximum: 1.0 1.0 50.0

Mass	Calc. Mass	Mass mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
453.3480	453.3481	-0.1	-0.2	8.5	592.6	0.000	99.98	C29 H45 N2 O2
	453.3486	-0.6	-1.3	1.5	600.9	8.348	0.02	C14 H41 N14 O3

Figure S31. HRMS spectrum of compound 6f

71 HA17	76.521	9.791	6.193
72 HA17	76.934	9.761	6.207
Valeur moyenne	76.728	9.776	6.200
Déviati�n (abs.)	0.292	0.021	0.010
Delta [%]	0.414	0.029	0.014



**Figure S32.** Elemental analysis of compound **6f**

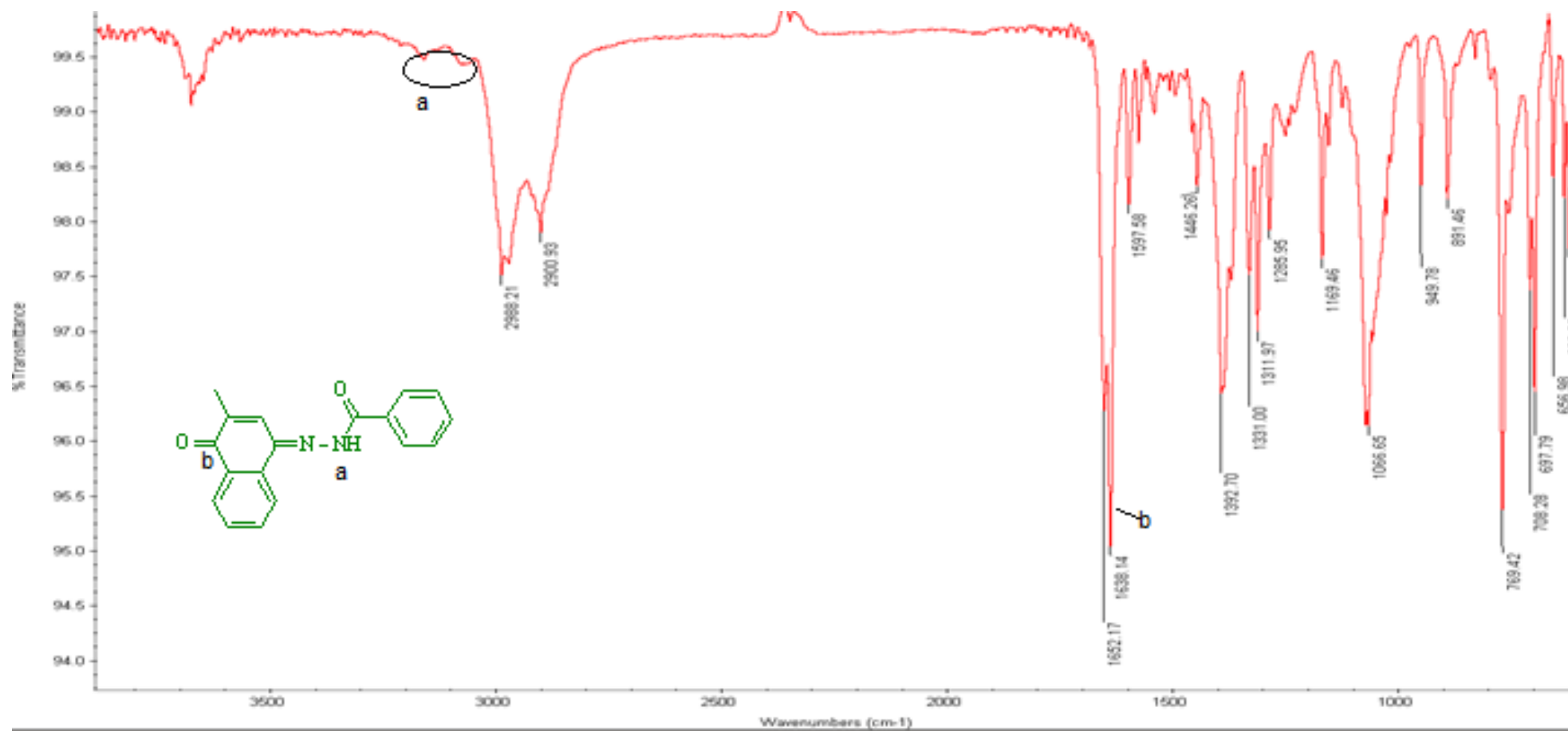
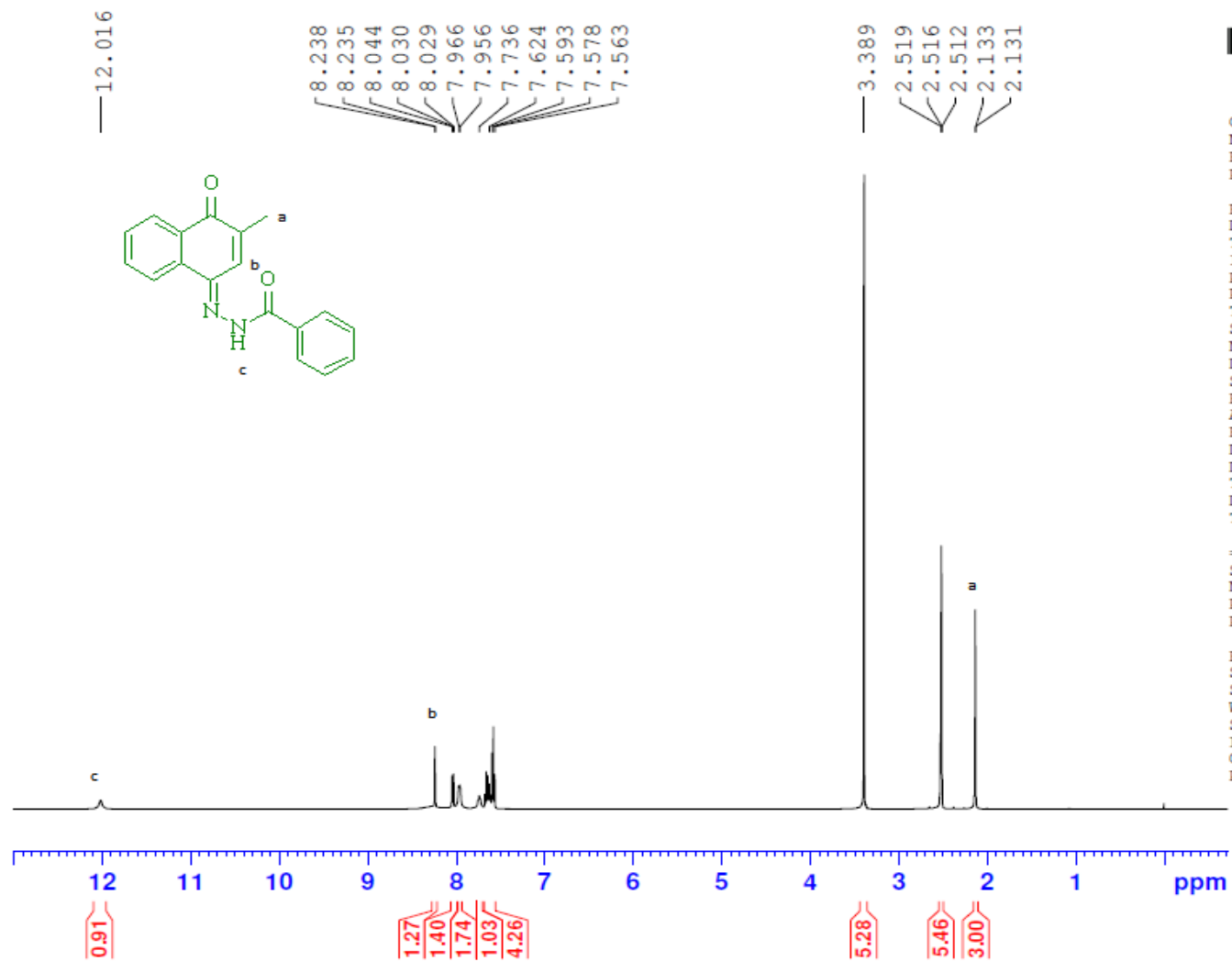


Figure S33. IR spectrum of compound 6g

HA18/dms0



Current Data Parameters  
NAME 2015-08-06  
EXPNO 40  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150806  
Time 14.04  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 54.99  
DW 50.000 usec  
DE 6.50 usec  
TE 295.4 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.40 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1299954 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S34. <sup>1</sup>H NMR (DMSO, 500 MHz) spectrum of compound **6g**

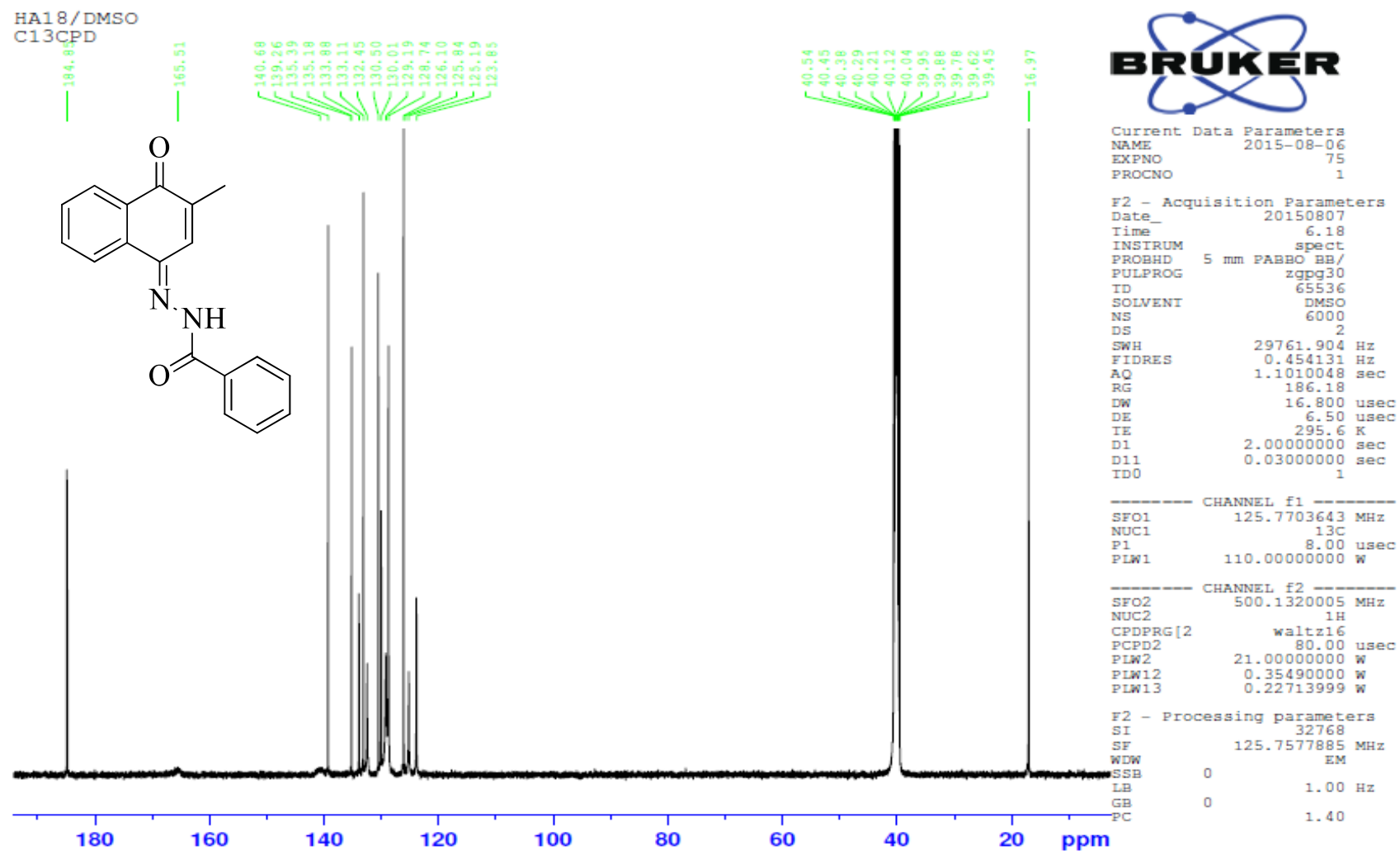


Figure S35. <sup>13</sup>C NMR (DMSO, 100 MHz) spectrum of compound **6g**

HA18/DMSO

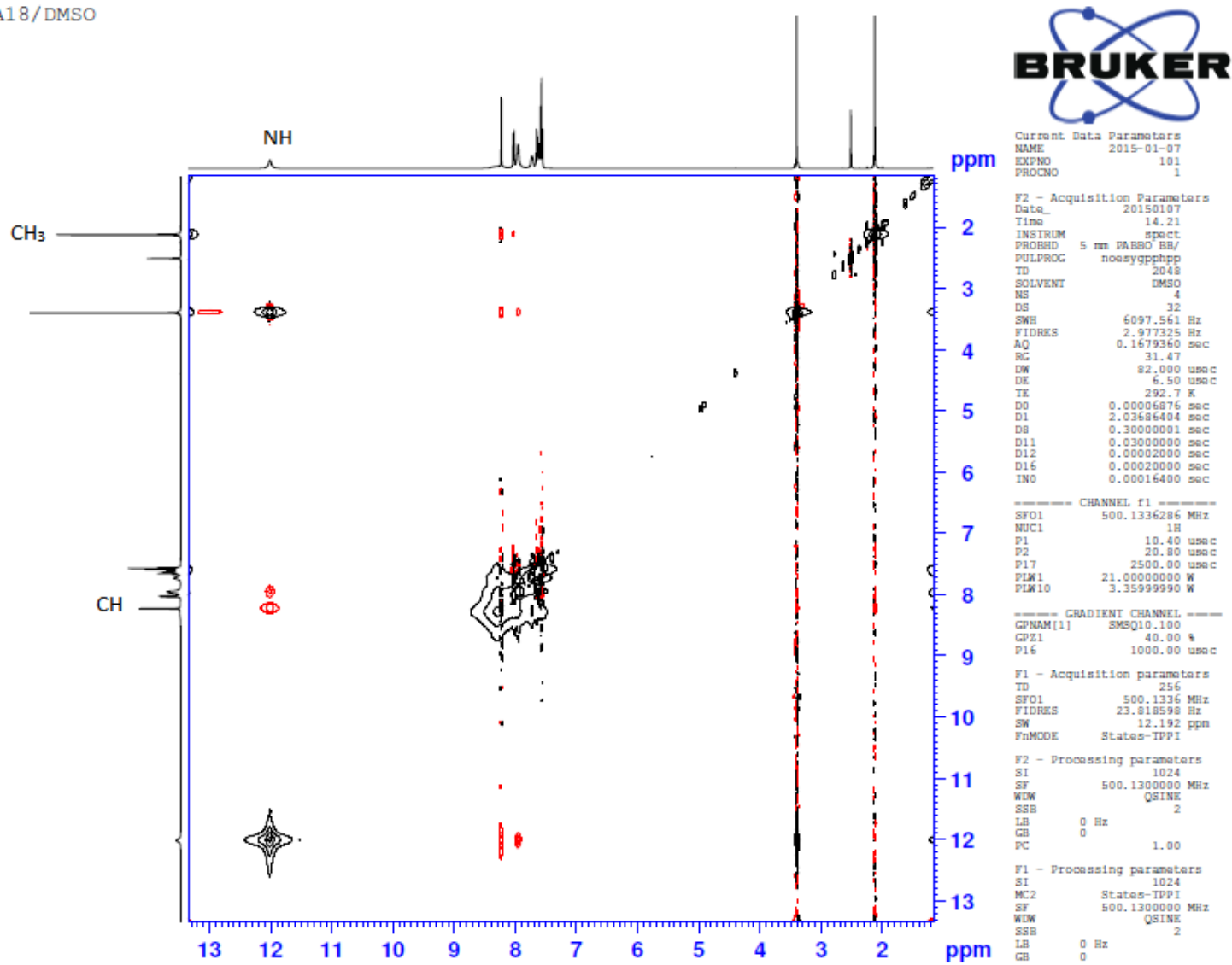


Figure S36. NOESY 2D-NMR spectrum of compound 6g

Display Report - All Windows All Analyses

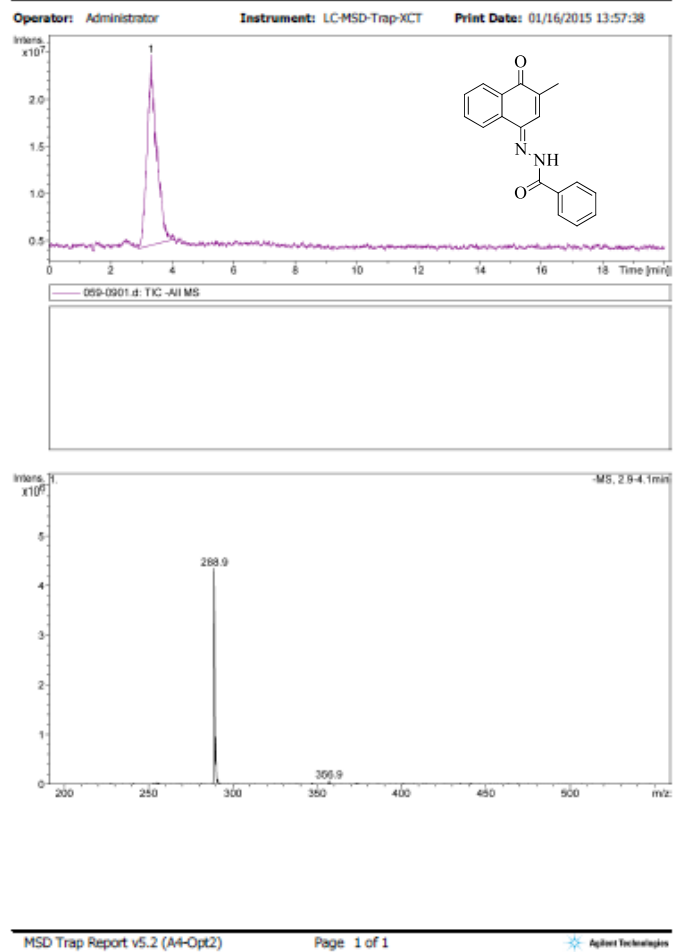
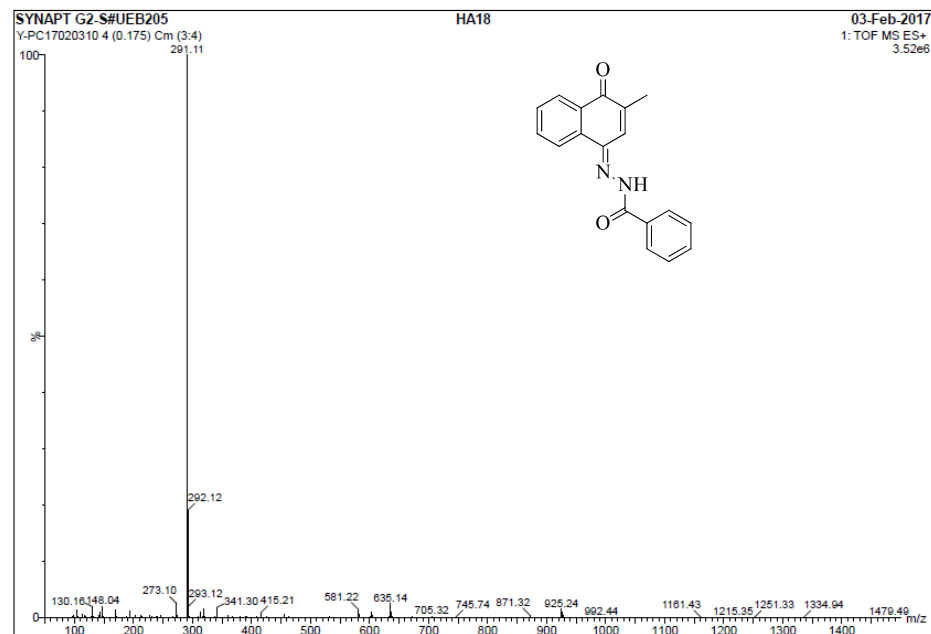


Figure S37. LC-MS spectrum of compound 6g





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

S61 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-20 N: 0-20 O: 0-20

SYNAPT G2-S#UEB205

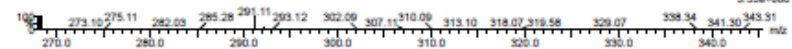
Y-PC17020310 4 (0.175) Cm (3:4)

HA18

03-Feb-2017

1: TOF MS ES+

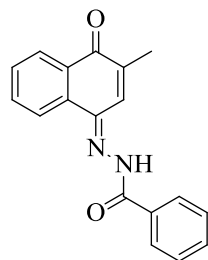
3.52e6



Minimum: -1.5  
 Maximum: 50.0

Mass	Calc. Mass	Mass mDa	FFM	DBE	i-FIT	Norm	Conf (%)	Formula
291.1132	291.1134	-0.2	-0.7	12.5	2039.8	0.000	100.00	C18 H15 N2 O2
	291.1139	-0.7	-2.4	5.5	2051.4	11.518	0.00	C3 H11 N14 O3
	291.1125	0.7	2.4	0.5	2052.3	12.426	0.00	C2 H15 N10 O7

Figure S38. HRMS spectrum of compound 6g



N° Nom	C [%]	H [%]	N [%]
65 HA18	74.266	4.879	9.707
66 HA18	74.421	4.876	9.661
Valeur moyenne	74.343	4.878	9.684
Déviaton (abs.)	0.110	0.002	0.033
Delta [%]	0.155	0.003	0.046

**Figure S39.** Elemental analysis of compound **6g**

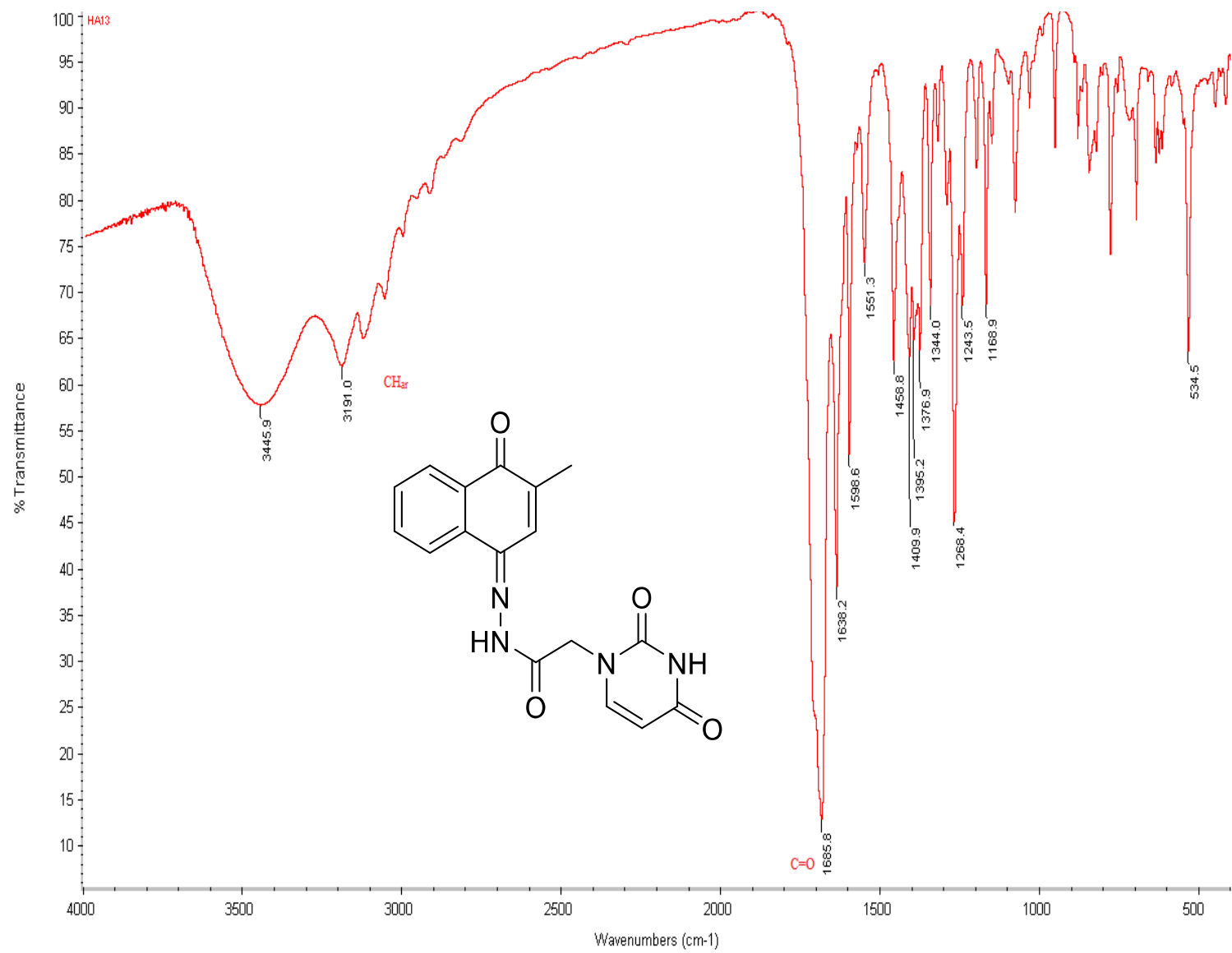


Figure S40. IR spectrum of compound 6h

HA13/DMSO

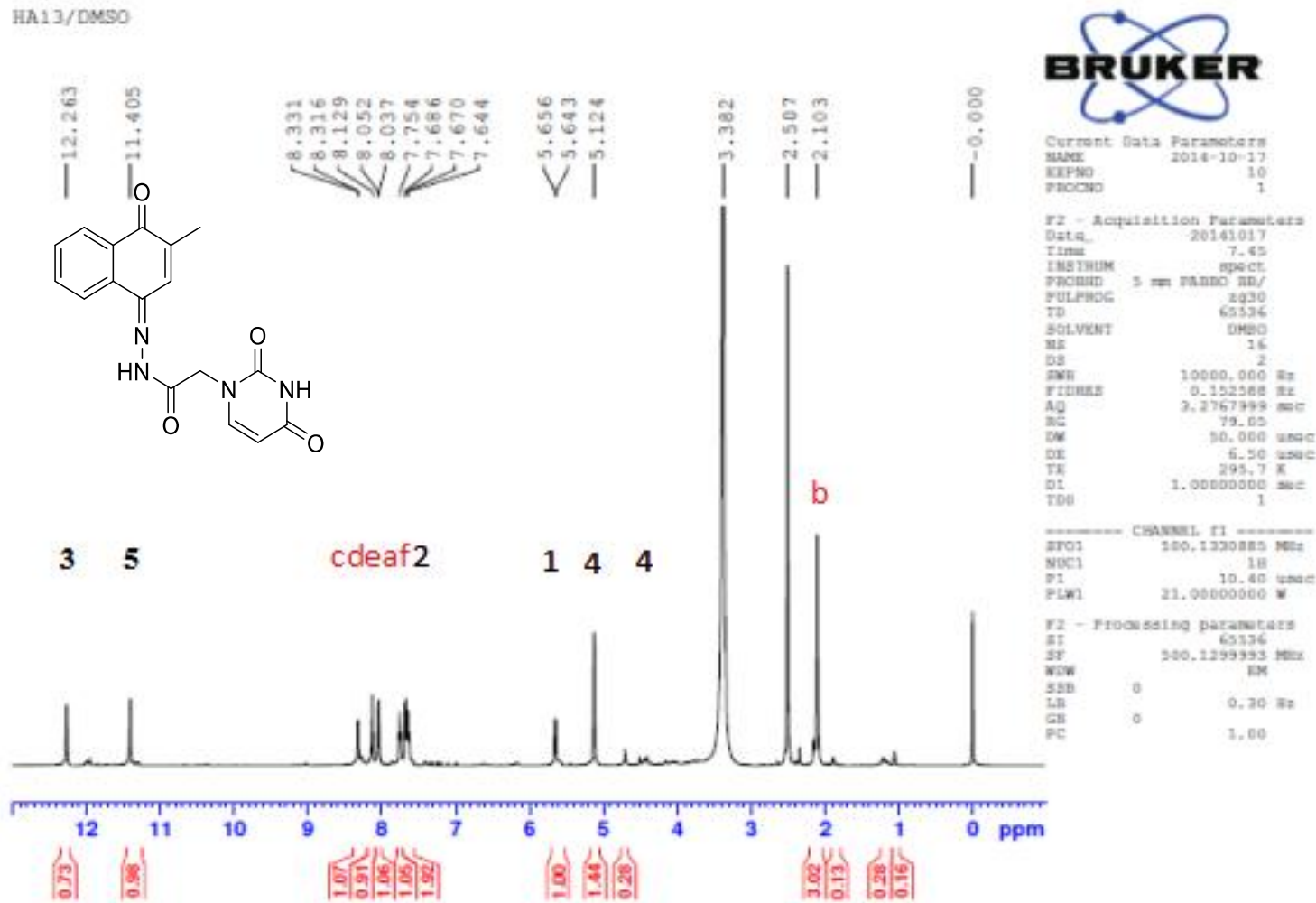


Figure S41. <sup>1</sup>H NMR (DMSO, 500 MHz) spectrum of compound 6h

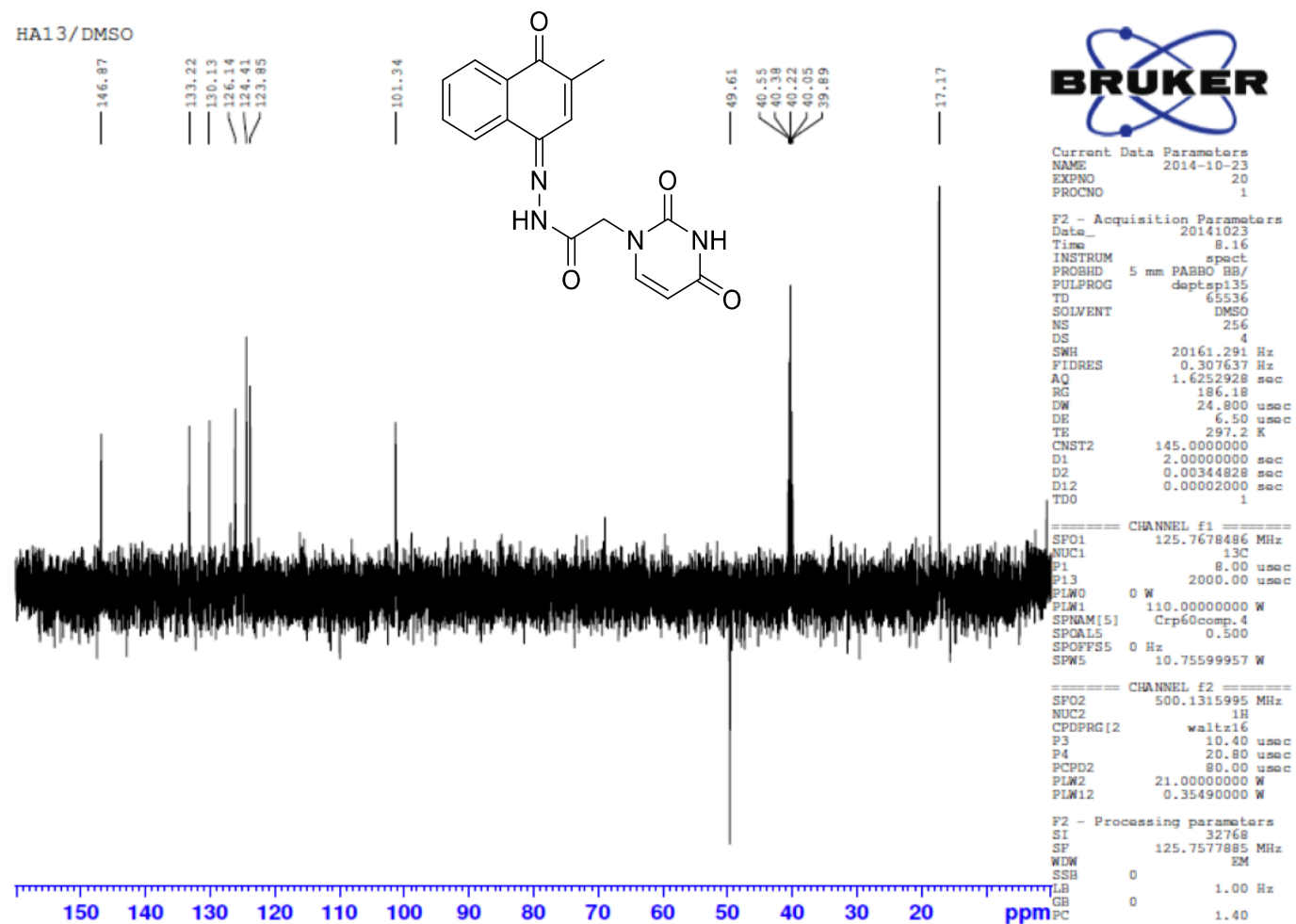


Figure S42. DEPT NMR (DMSO, 100 MHz) spectrum of compound **6h**

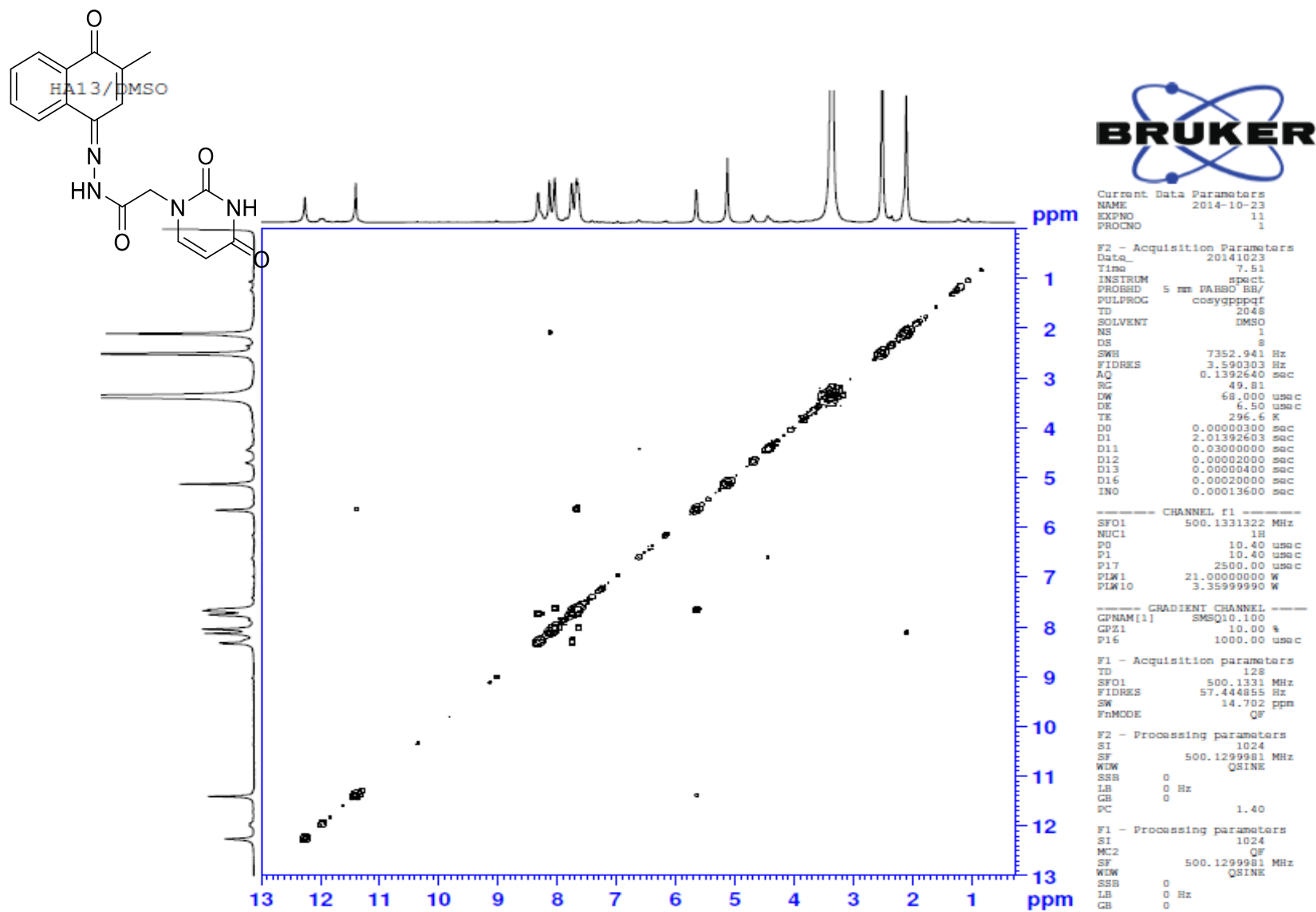
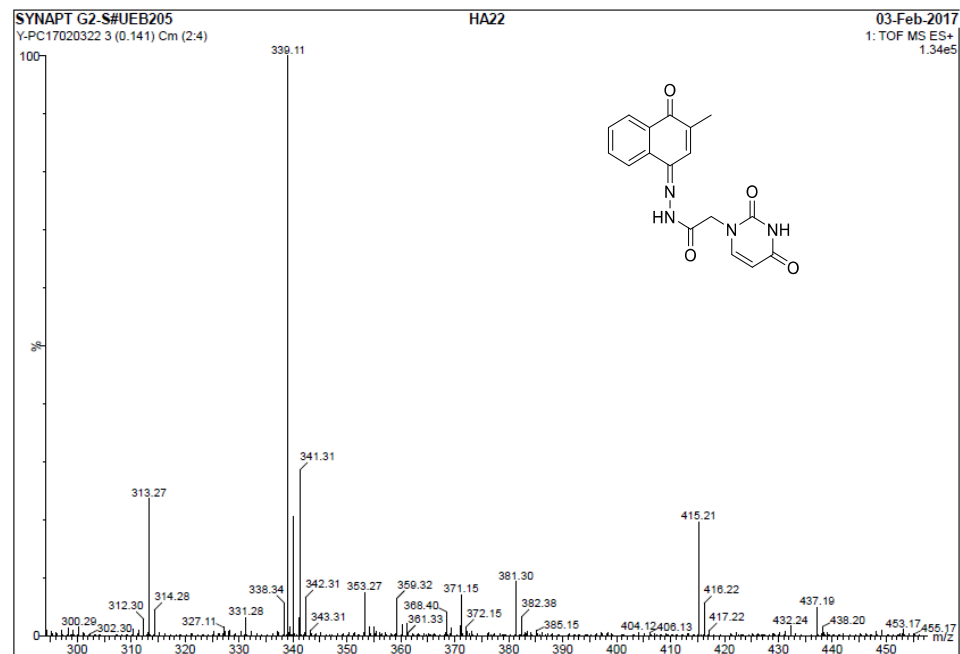


Figure S43. COSY 2D-NMR spectrum of compound **6h**



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: C#H#N#O#S

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

810 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

SYNAPT G2-S#UEB205

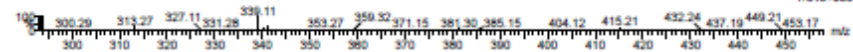
HA22

03-Feb-2017

Y-PC17020322 3 (0.141) Cm (2:4)

1: TOF MS ES+

1.34e+005



Minimum:

Maximum: 1.0 1.0 -1.5

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(k) Formula

339.1094	339.1093	0.1	0.3	12.5	1191.2	0.000	100.00	C17 H15 N4 O4
	339.1098	-0.4	-1.2	5.5	1207.8	16.603	0.00	C2 H11 N16 O5
	339.1085	0.9	2.7	0.5	1208.7	17.521	0.00	C H15 N12 O9

Figure S44. HRMS spectrum of compound 6h

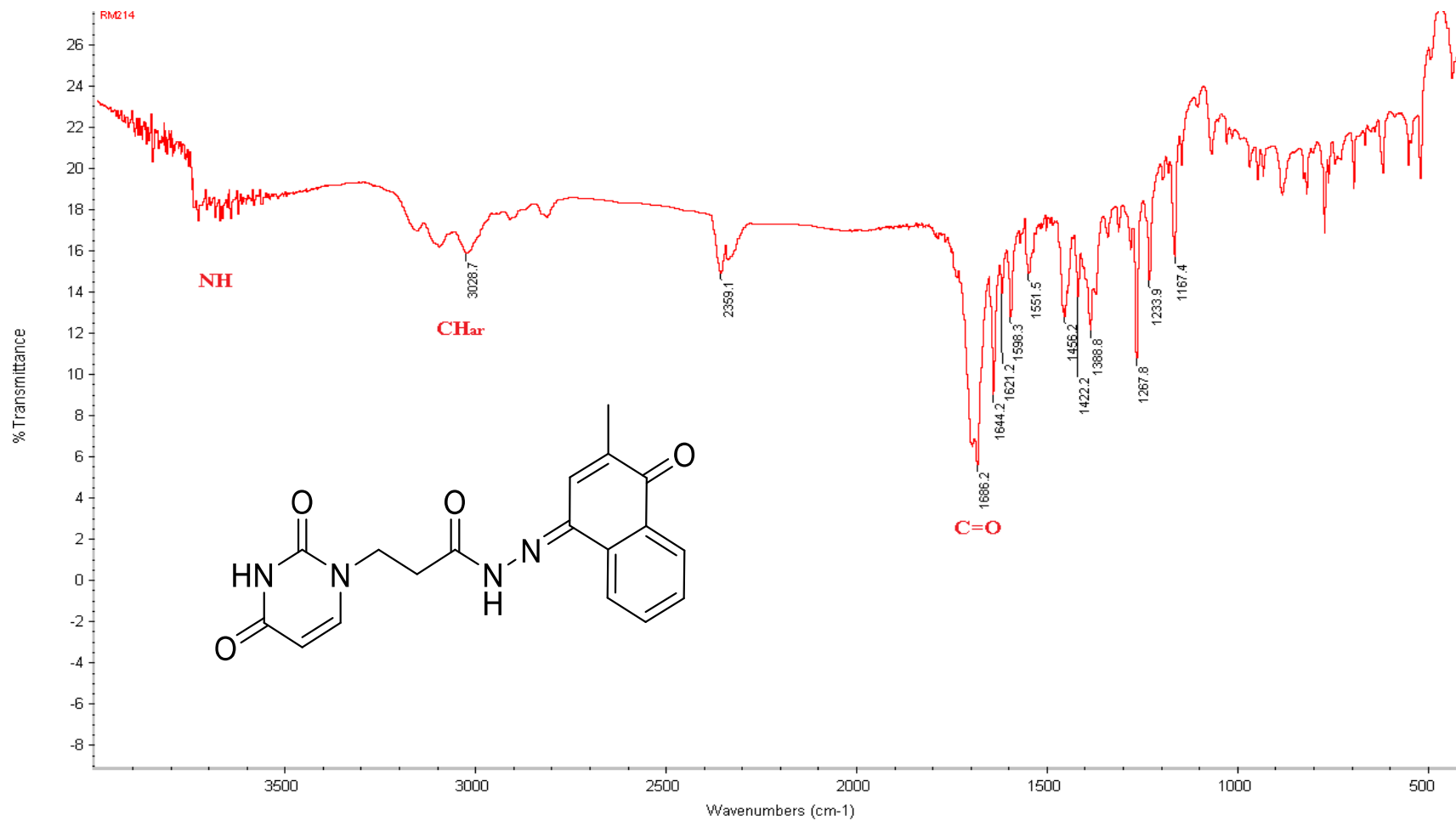
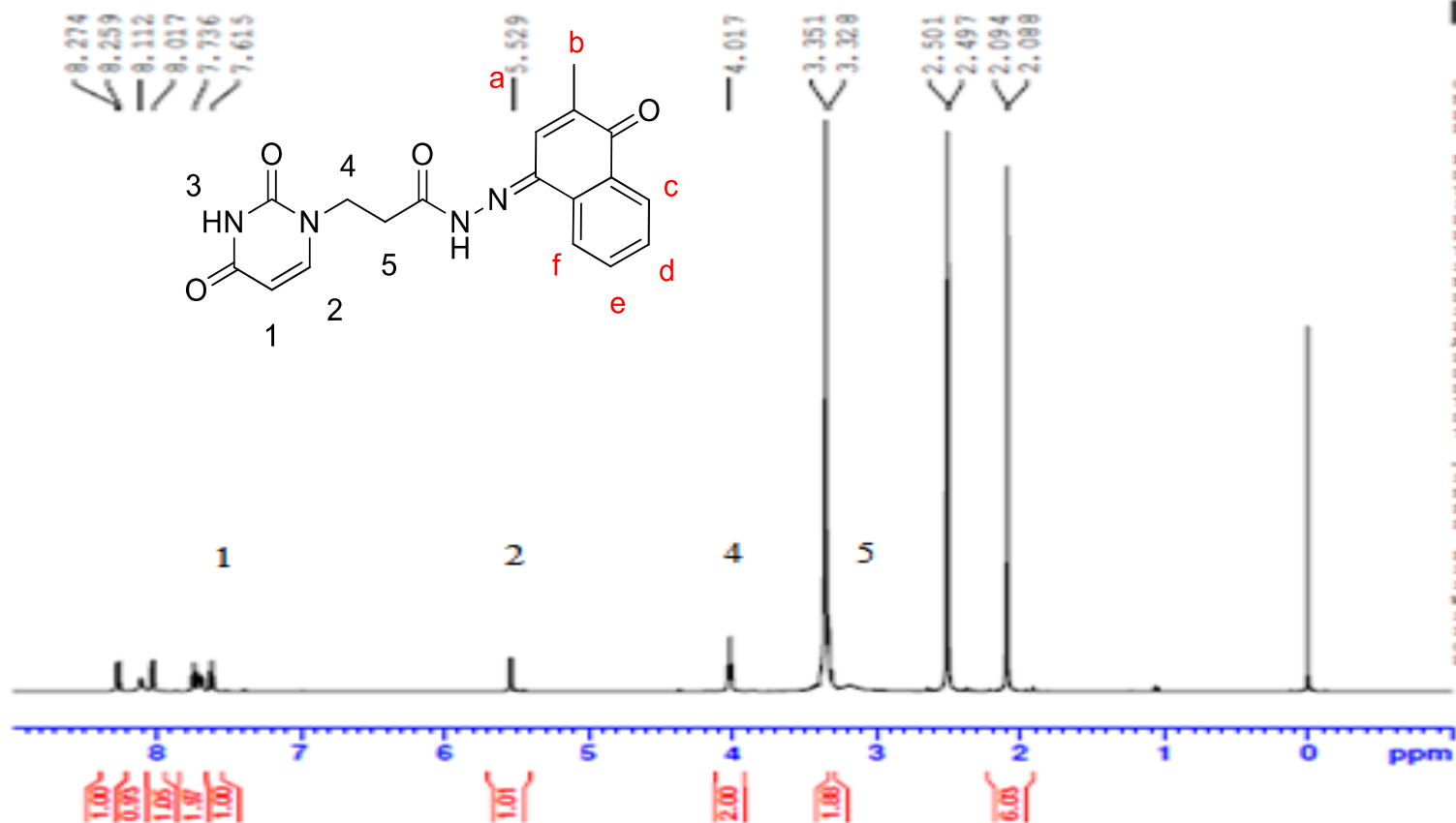


Figure S45. IR spectrum of compound 6i



RM214/ DMSO



Current Data Parameters  
NAME 2014-10-22  
EXPNO 214  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20141022  
Time 14.29  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 92.59  
DW 50.000 usec  
DE 6.50 usec  
TE 296.1 K  
D1 1.0000000 sec  
TD0 1

CHANNEL f1  
SFO1 500.1330885 MHz  
NUC1 1H  
P1 10.40 usec  
PLA1 21.0000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300010 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S46. <sup>1</sup>H NMR (DMSO, 500 MHz) spectrum of compound **6i**

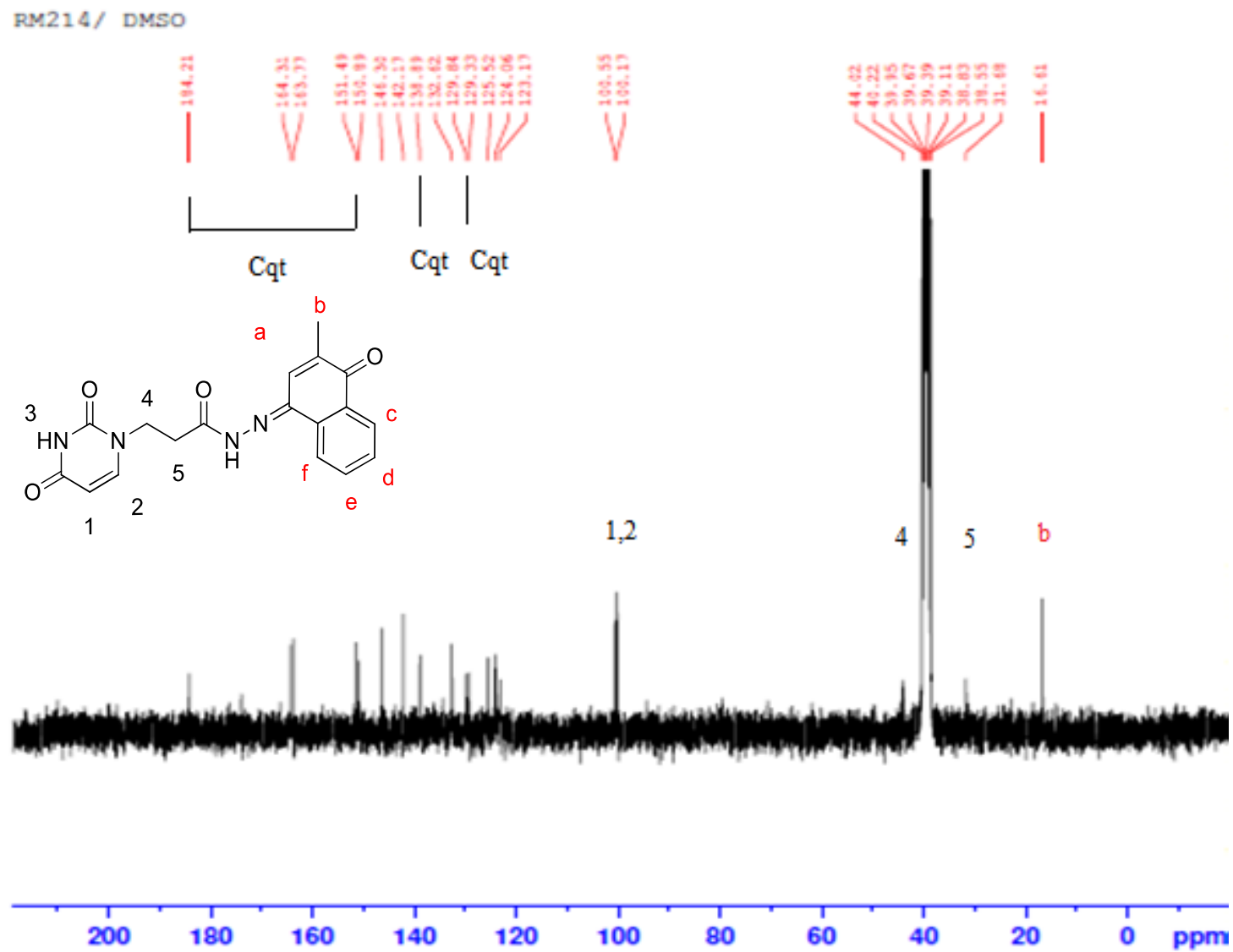
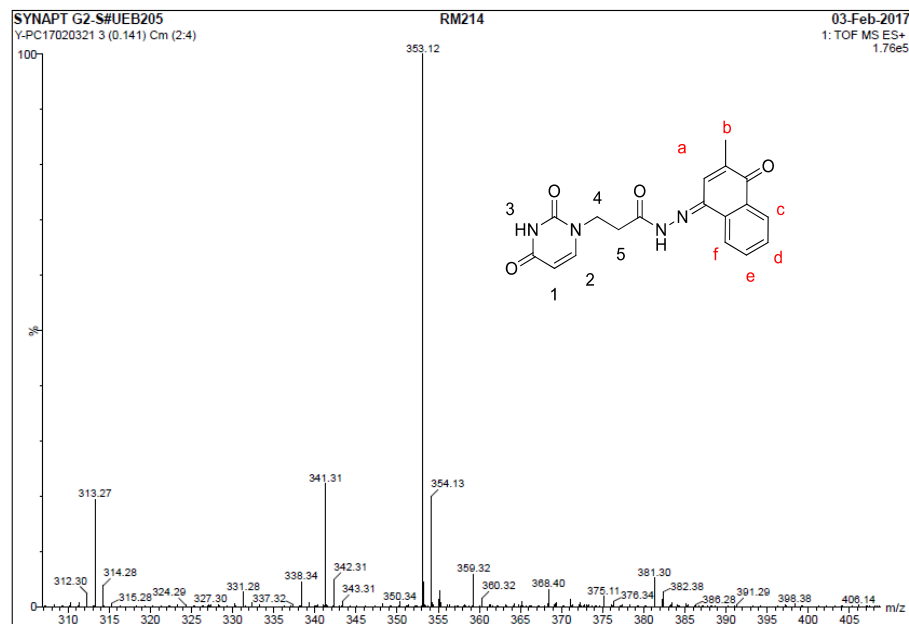


Figure S47.  $^{13}\text{C}$  NMR (DMSO, 100 MHz) spectrum of compound **6i**



#### Elemental Composition Report

Page 1

#### Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

884 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

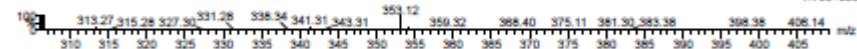
Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

SYNAPT G2-S#UEB205  
Y-PC17020321 3 (0.141) Cm (2:4)

RM214

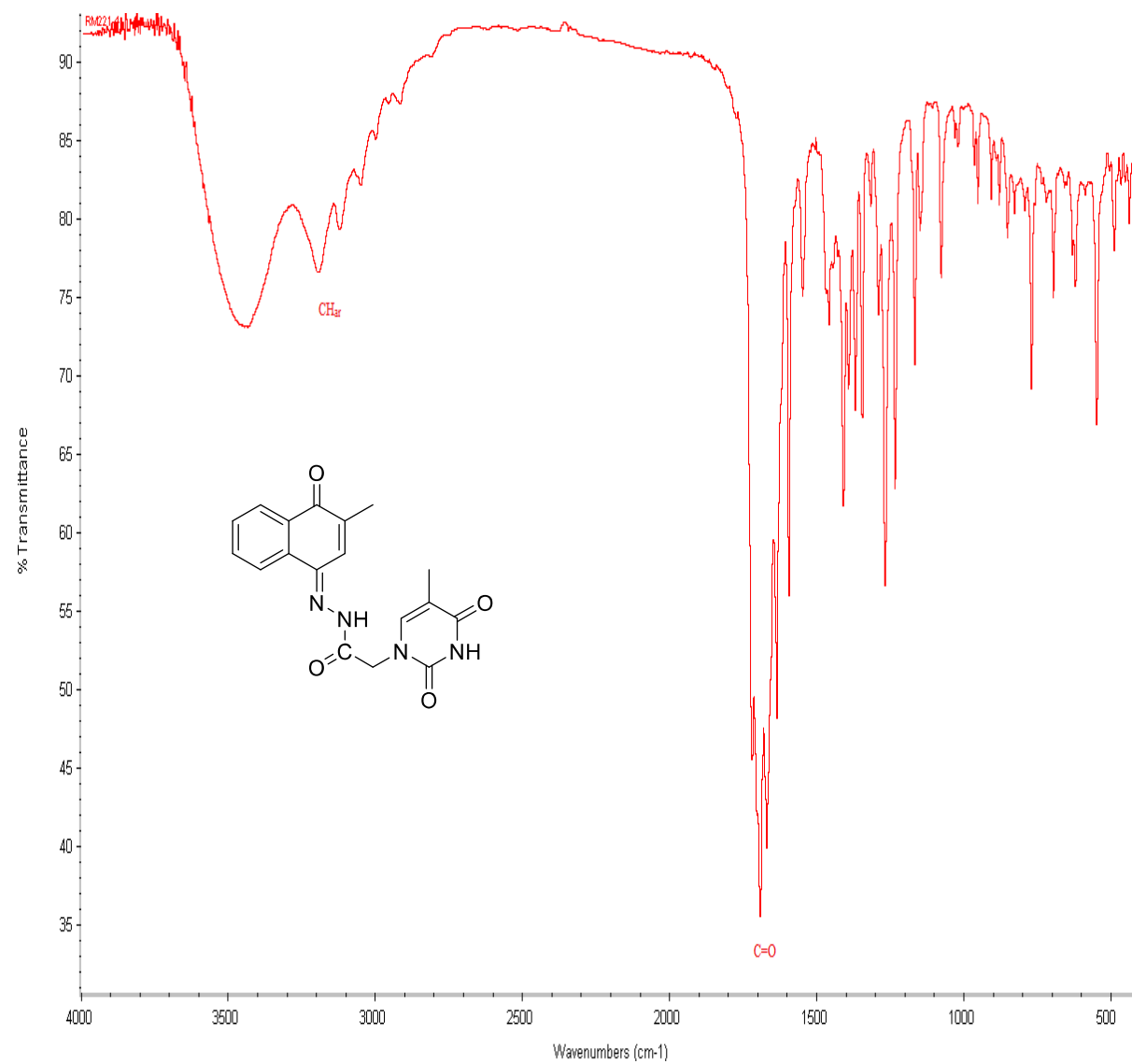
03-Feb-2017  
1: TOF MS ES+  
1.76e+005



Minimum: -1.5  
Maximum: 1.0 1.0 50.0

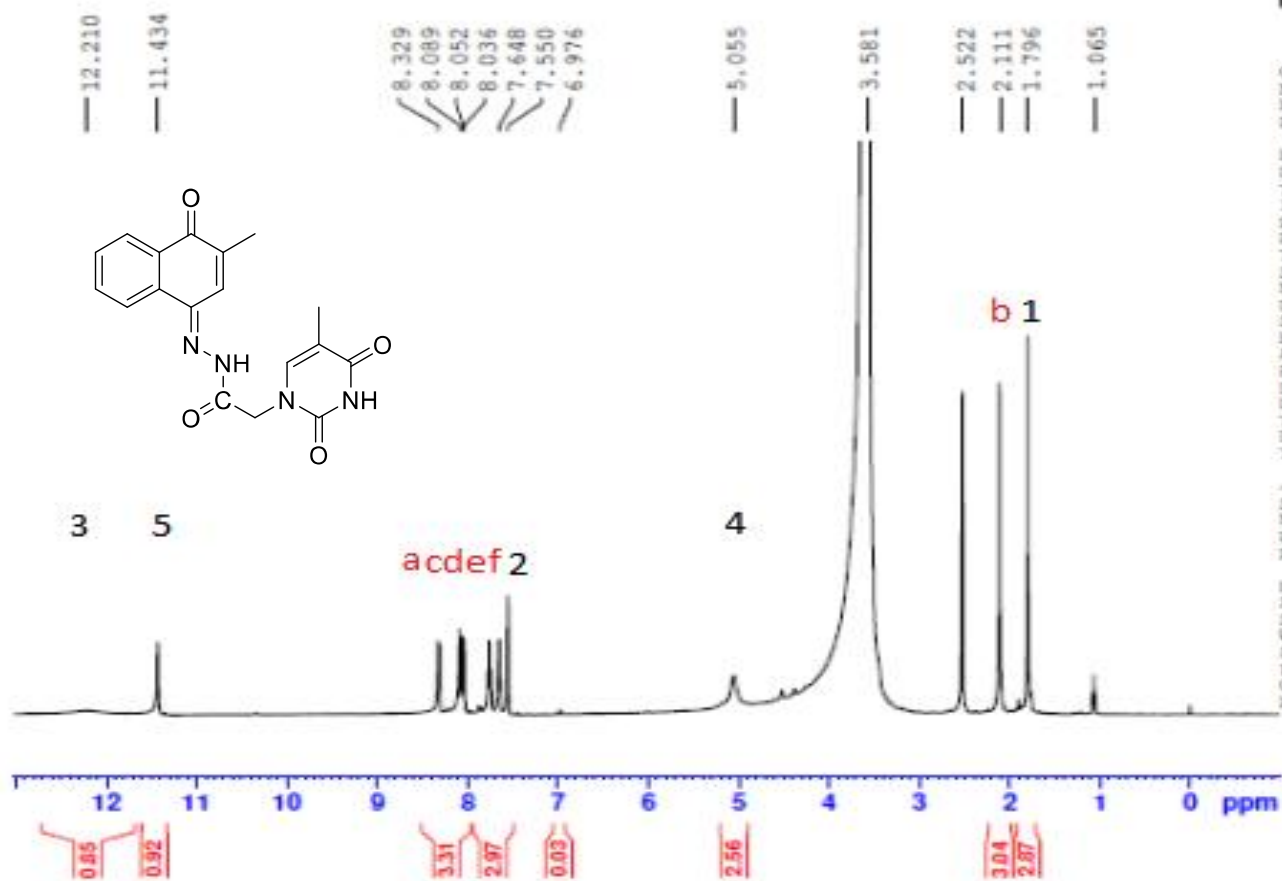
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
353.1249	353.1250	-0.1	-0.3	12.5	1123.2	0.000	100.00	C18 H17 N4 O4
	353.1255	-0.6	-1.7	5.5	1137.1	13.978	0.00	C3 H13 N16 O5
	353.1241	0.8	2.3	0.5	1137.9	14.793	0.00	C2 H17 N12 O9

Figure S48. HRMS spectrum of compound **6i**



**Figure S49.** IR spectrum of compound **6j**

RM221/ DMSO



Current Data Parameters  
NAME 2014-11-07  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20141107  
Time 12.56  
INSTRUM spect  
PROBHD 1 mm ZBBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 31.47  
DM 50.000 usec  
DE 6.50 usec  
TE 294.4 K  
D1 1.0000000 sec  
TD0 1

----- CHANNEL f1 -----

SFO1 500.133885 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters

SI 65536  
SF 500.1299916 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
CB 0  
PC 1.00

Figure S50. <sup>1</sup>H NMR (DMSO, 500 MHz) spectrum of compound **6j**

RM221/ DMSO

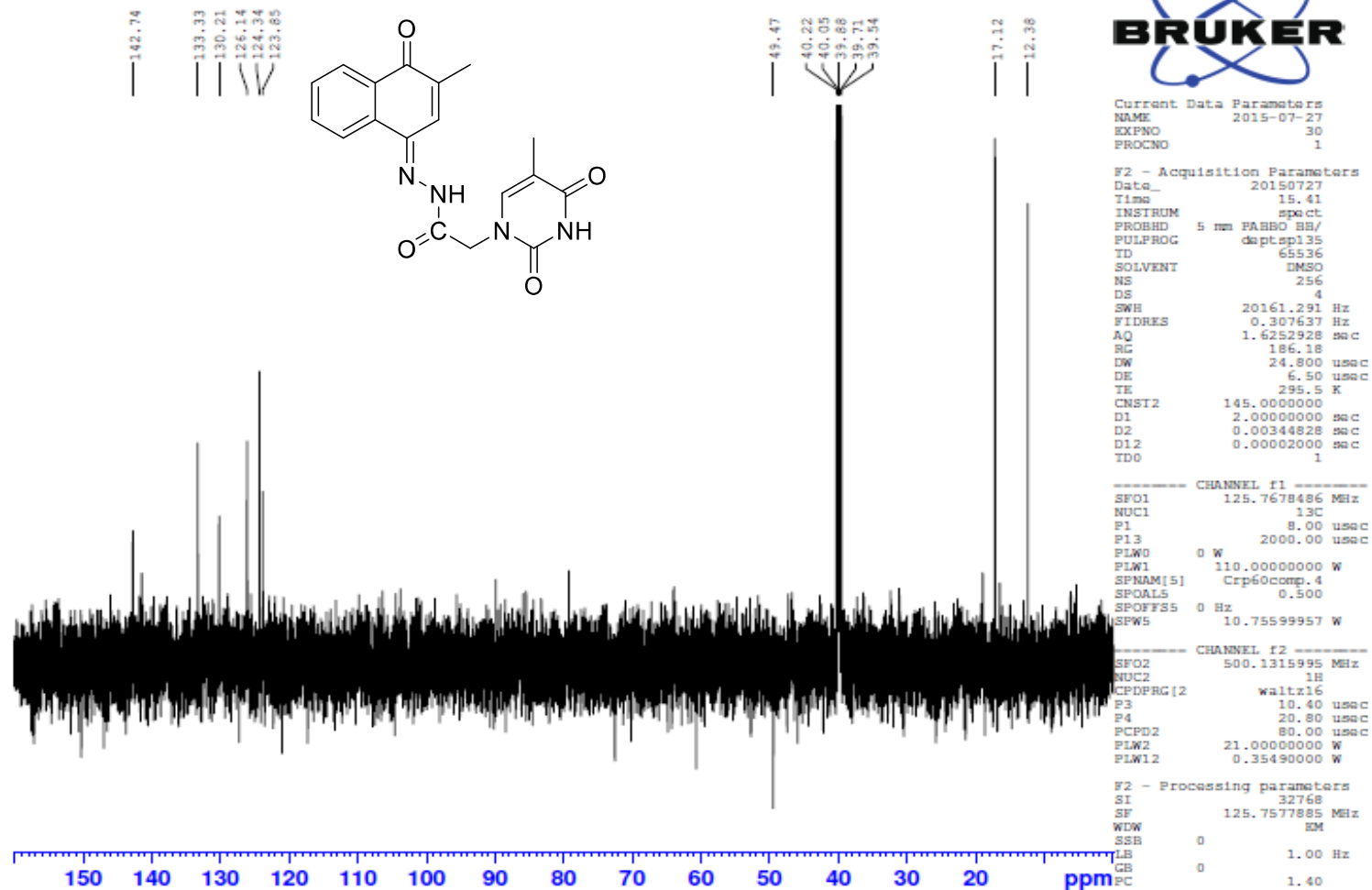


Figure S51. DEPT NMR (DMSO, 100 MHz) spectrum of compound 6j

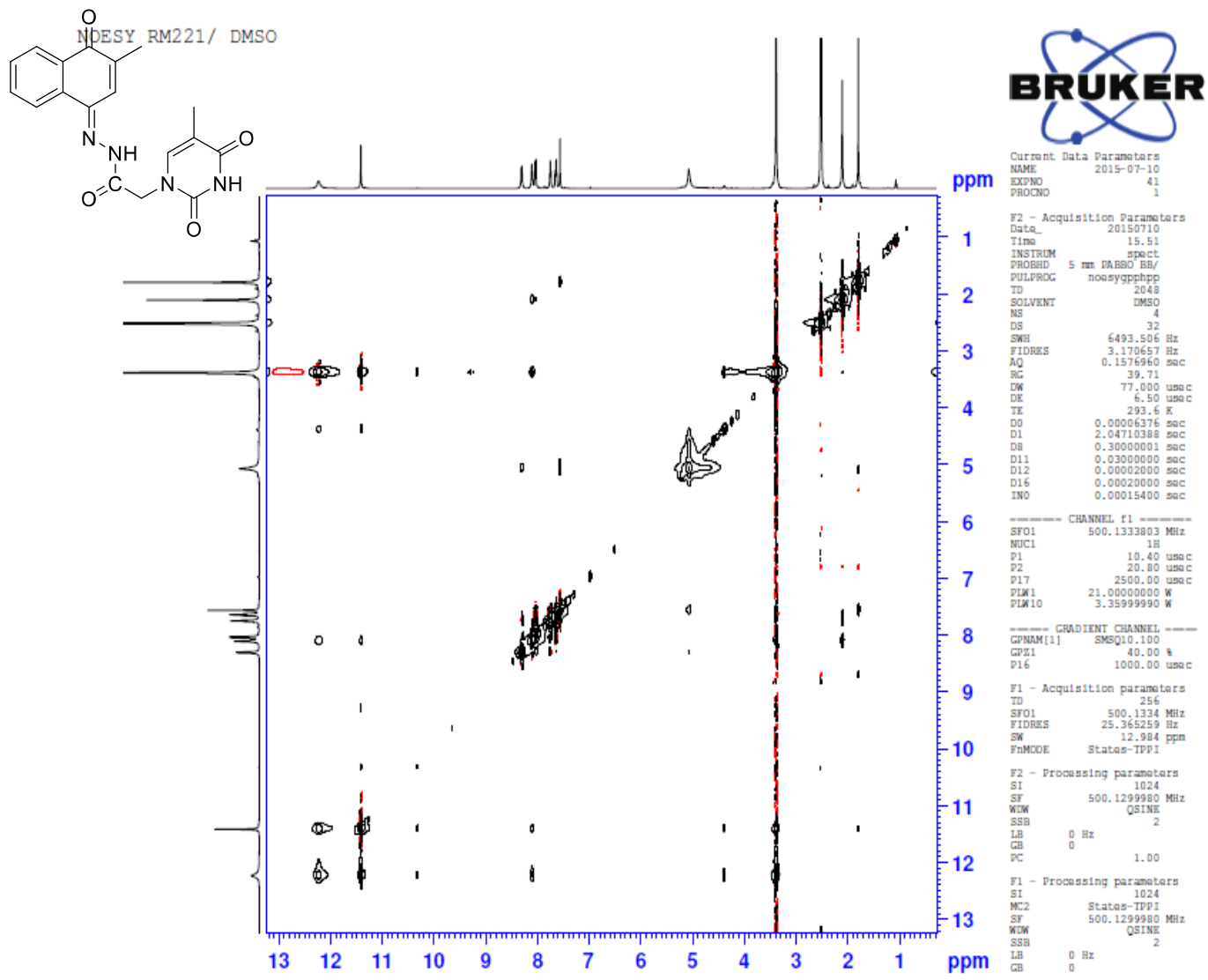
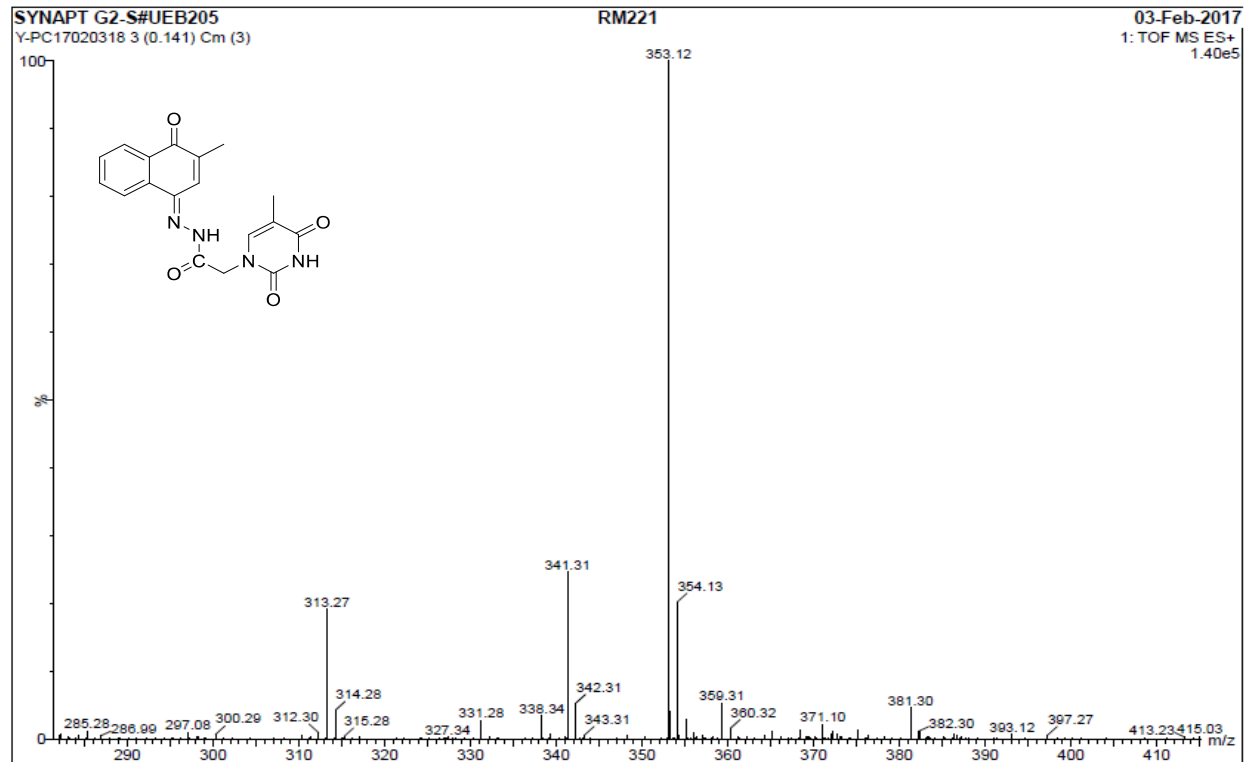


Figure S52. NOESY 2D-NMR spectrum of compound 6j





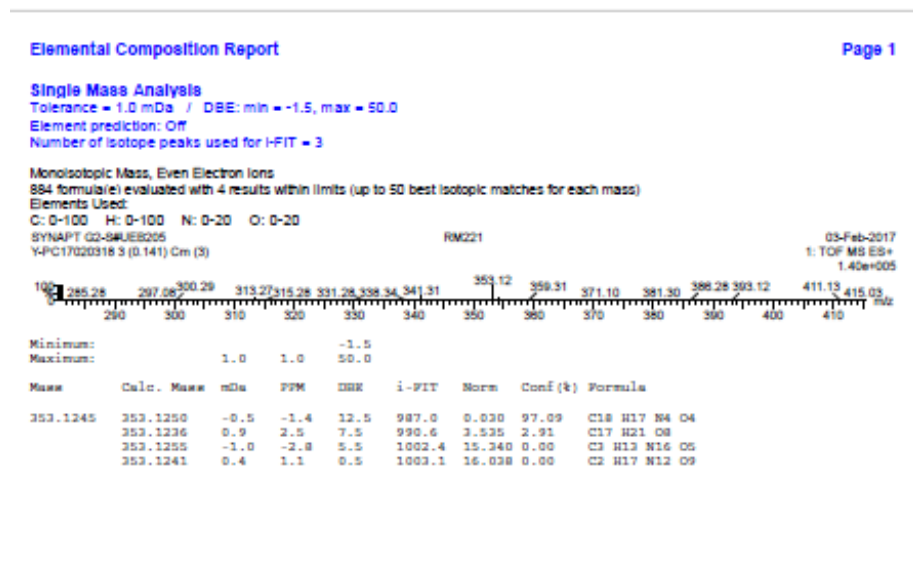
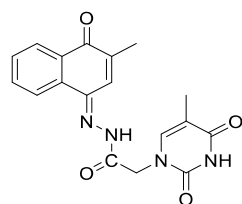


Figure S53. HRMS spectrum of compound 6j



N° Nom	C [%]	H [%]	N [%]
53 RM221	61.464	4.579	15.775
54 RM221	61.021	4.690	15.618
Valeur moyenne	61.242	4.634	15.697
Déviatiion (abs.)	0.313	0.078	0.111
Delta [%]	0.442	0.111	0.157

Figure S54. Elemental analysis of compound 6j

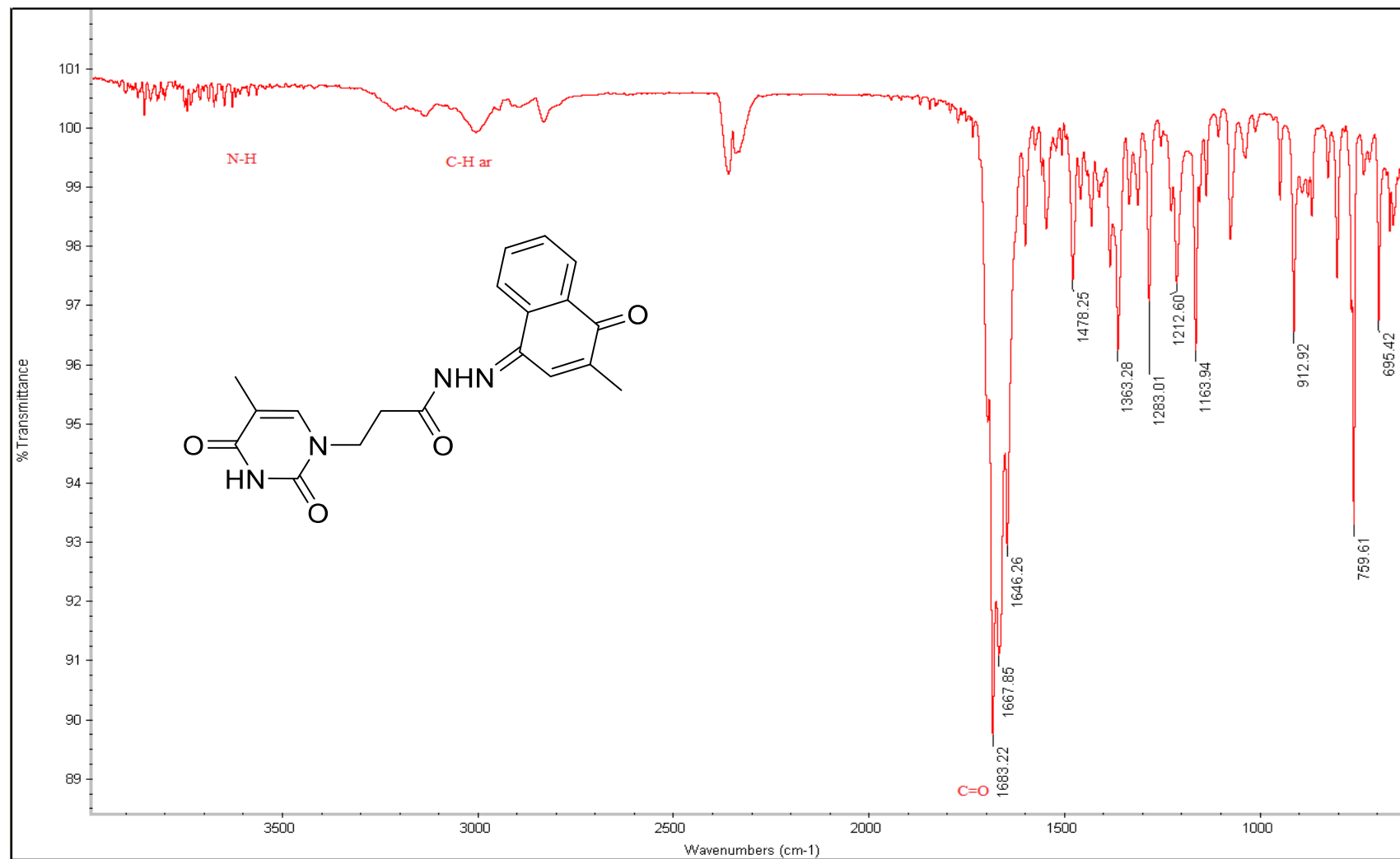


Figure S55. IR spectrum of compound 6k

RM217/ DMSO

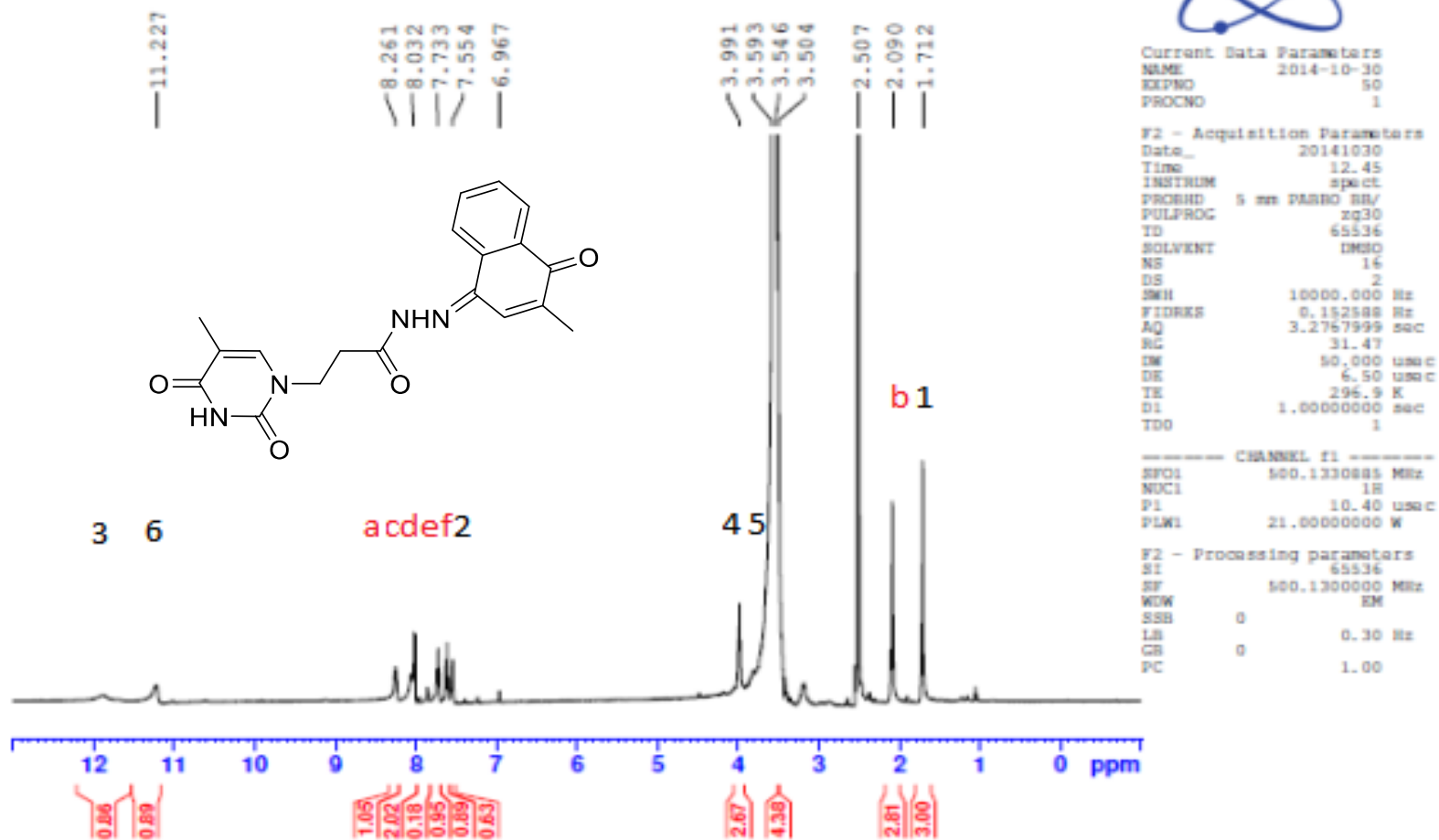


Figure S56. <sup>1</sup>H NMR (DMSO, 500 MHz) spectrum of compound 6k

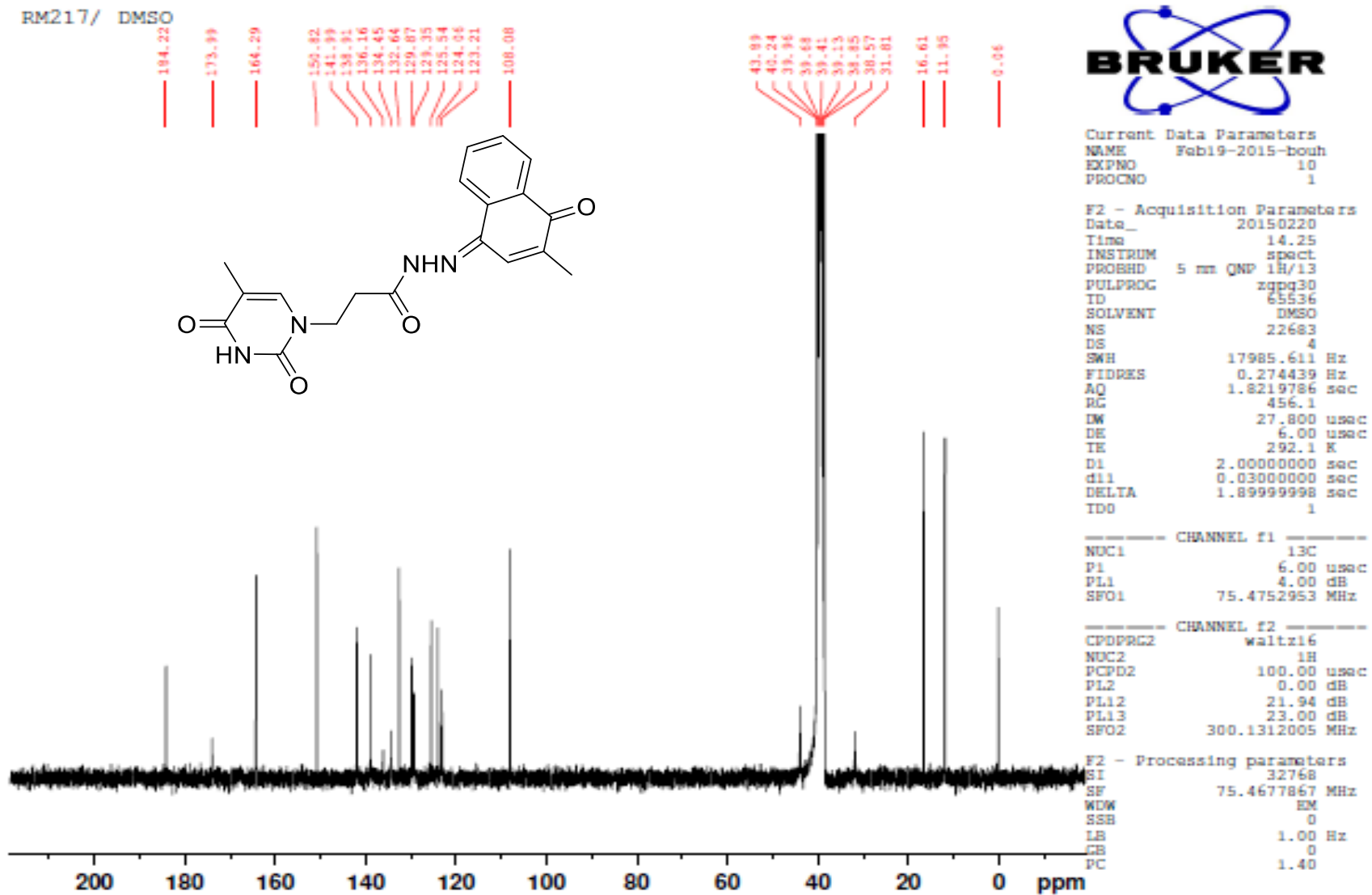


Figure S57. <sup>13</sup>C NMR (DMSO, 100 MHz) spectrum of compound **6k**

RM217/ DMSO

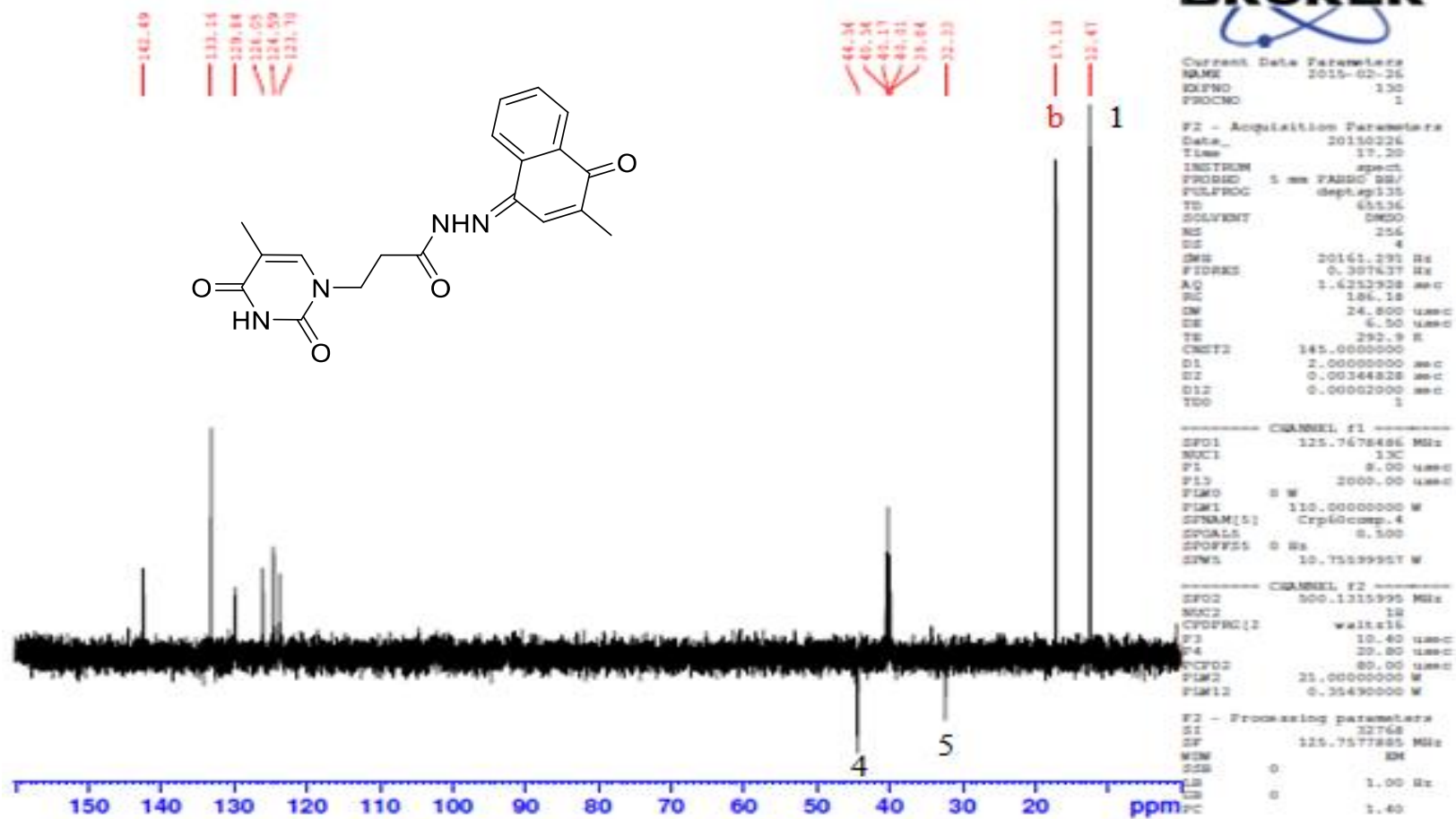


Figure S58. DEPT NMR (DMSO, 100 MHz) spectrum of compound **6k**

# Display Report - All Windows All Analyses

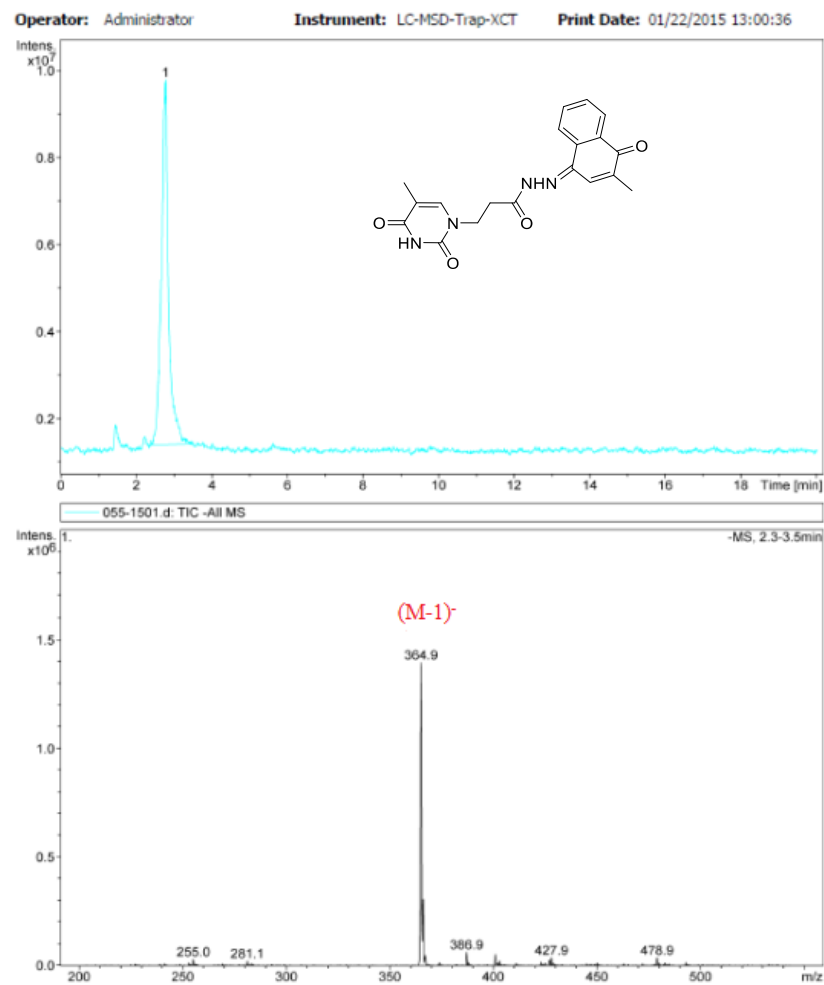
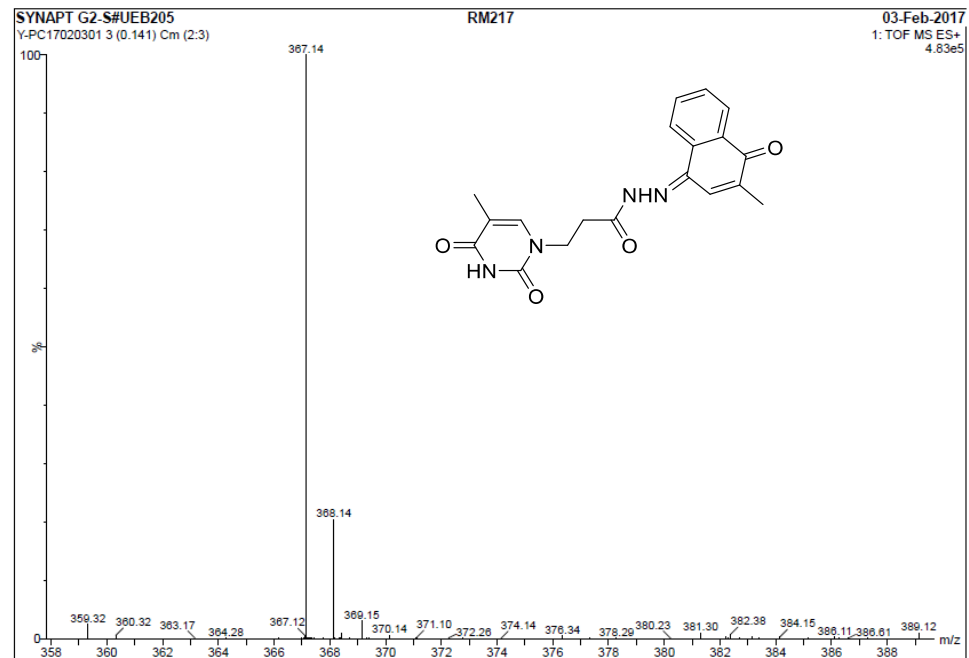


Figure S59. LC-MS spectrum of compound 6k



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

354 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

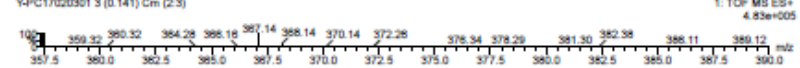
SYNAPT G2-S#UEB205

RM217

03-Feb-2017

Y-PC17020301 3 (0.141) Cm (2:3)

1: TOF MS ES+



Minimum: -1.5  
 Maximum: 50.0

Mass	Calc. Mass	Mass mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
367.1407	367.1406	0.1	0.3	12.5	1317.2	0.000	100.00	C19 H19 N4 O4
	367.1411	-0.4	-1.1	5.5	1329.2	12.047	0.00	C4 H15 N16 O6
	367.1398	0.9	2.5	0.5	1330.0	12.797	0.00	C3 H19 N12 O9

Figure S60. HRMS spectrum of compound 6k

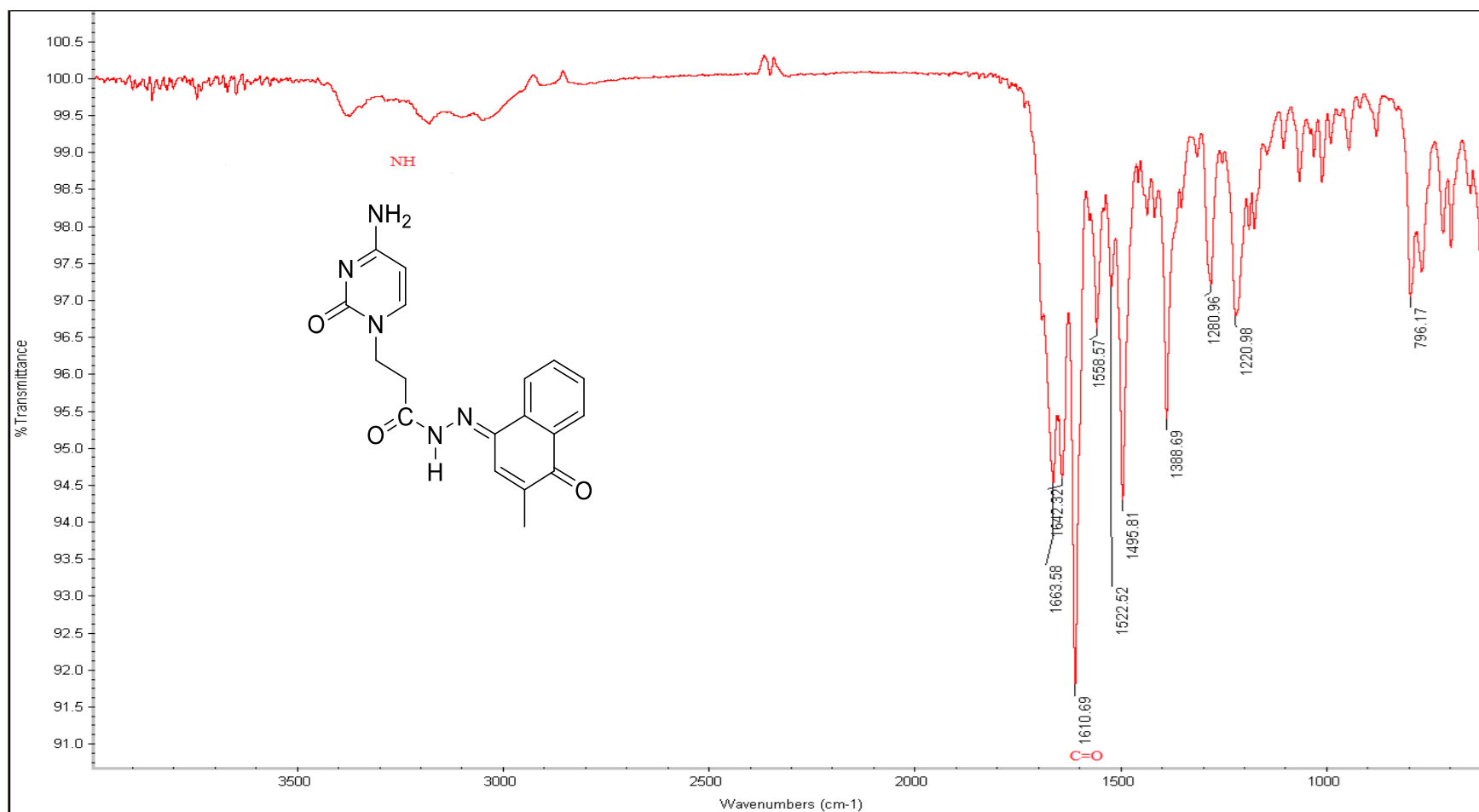


Figure S61. IR spectrum of compound **6l**



RM222/ DMSO

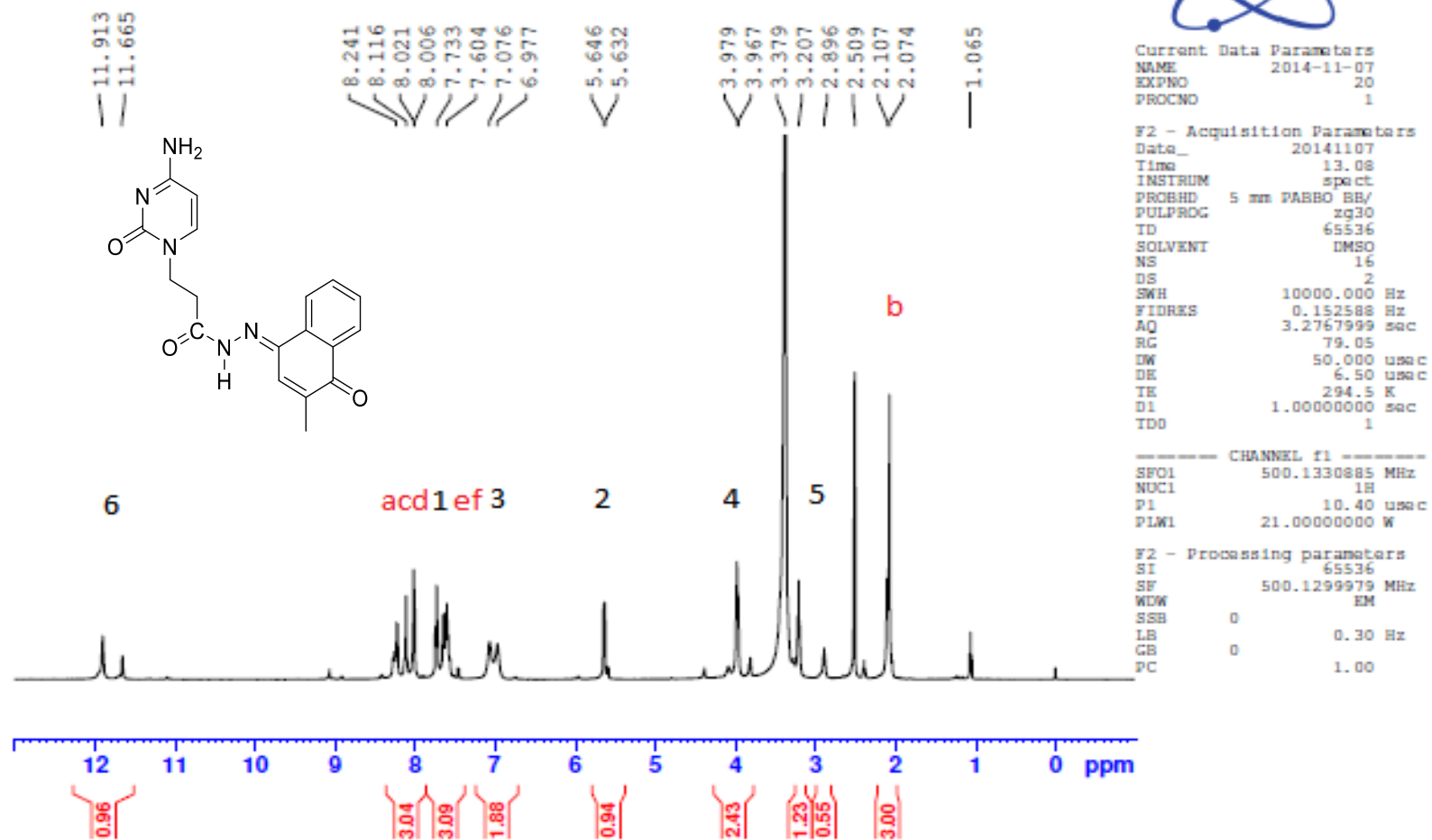


Figure S62. <sup>1</sup>H NMR (DMSO, 500 MHz) spectrum of compound **6l**

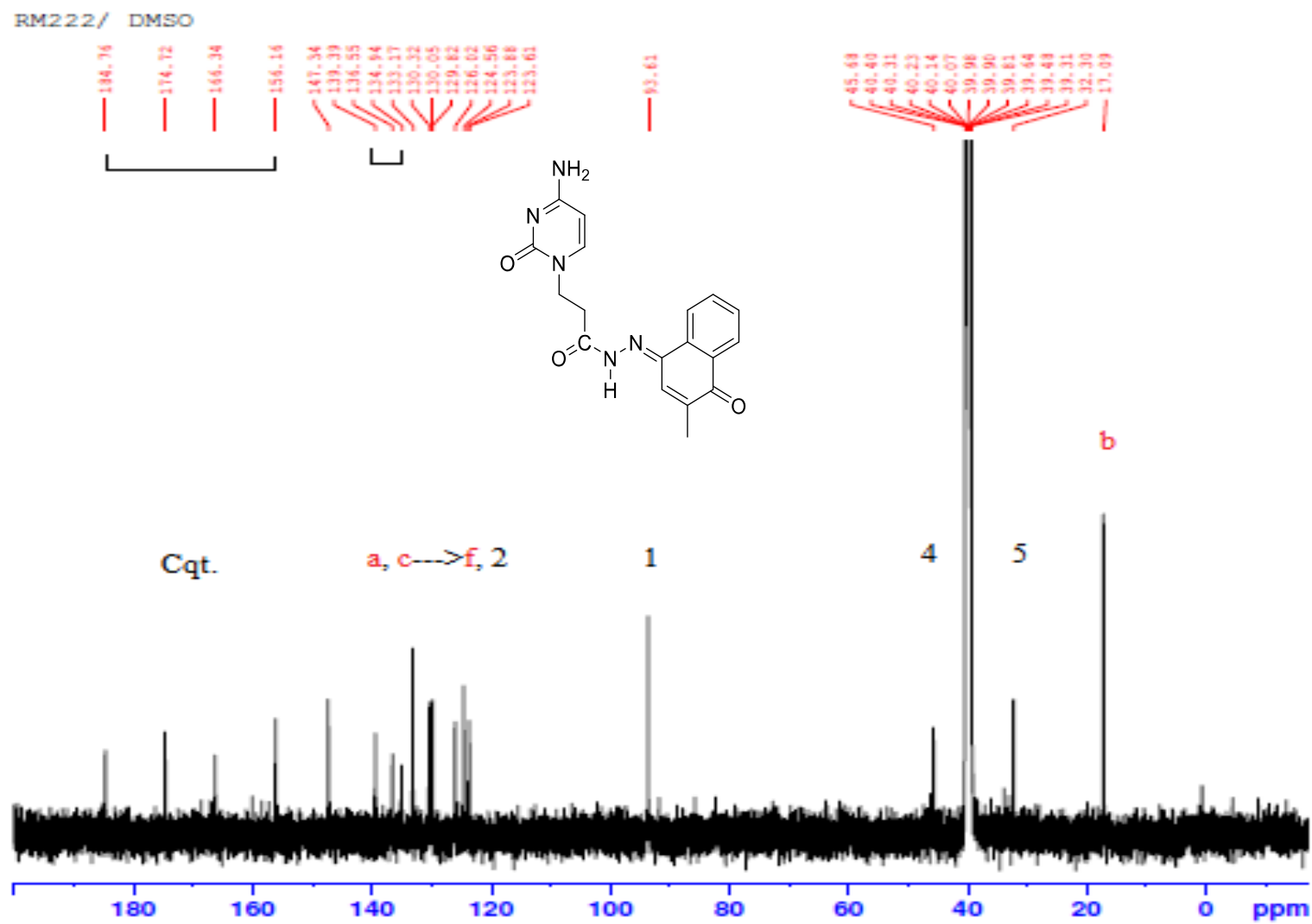


Figure S63.  $^{13}\text{C}$  NMR (DMSO, 100 MHz) spectrum of compound 6l

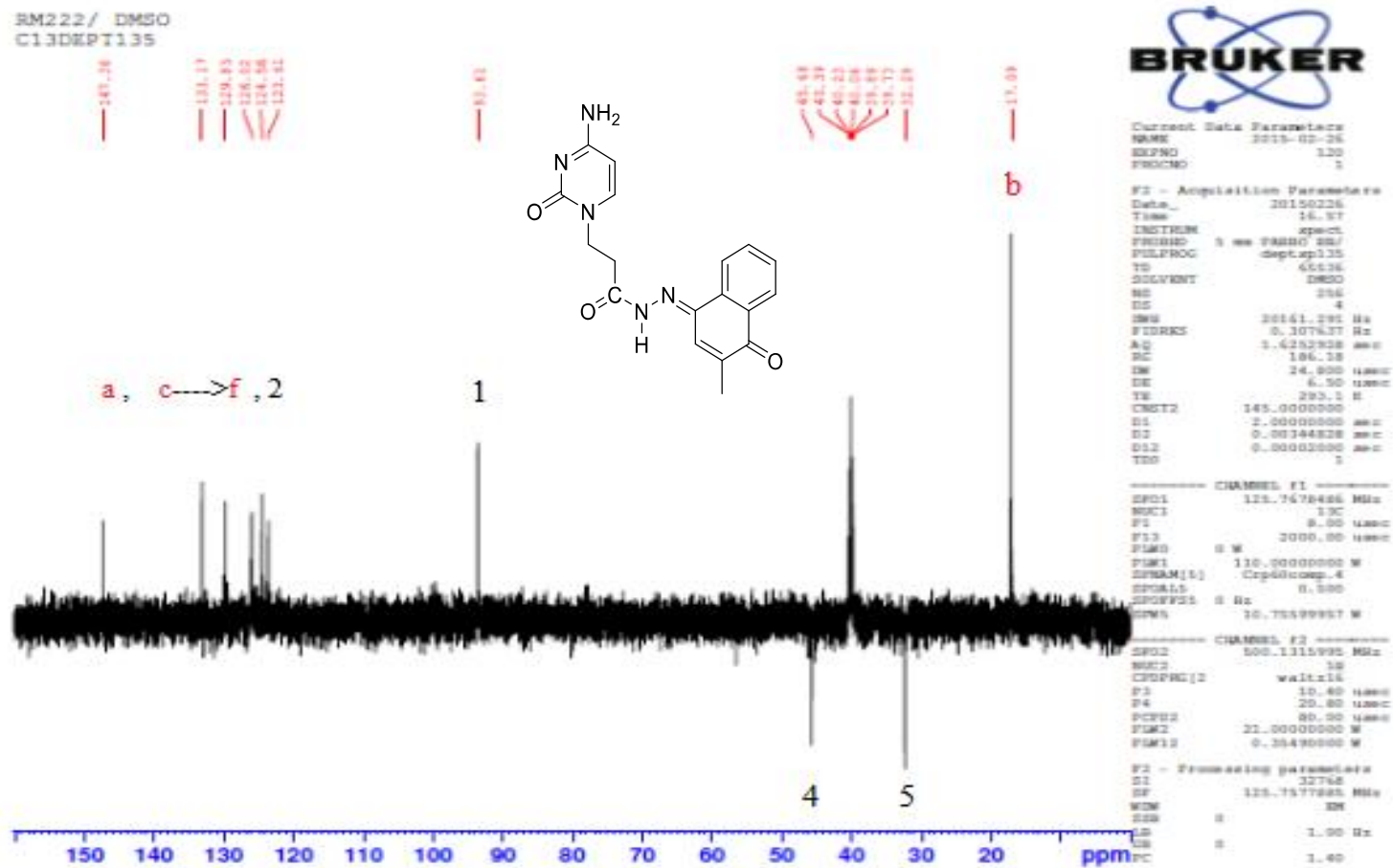


Figure S64. DEPT NMR (DMSO, 100 MHz) spectrum of compound **6l**

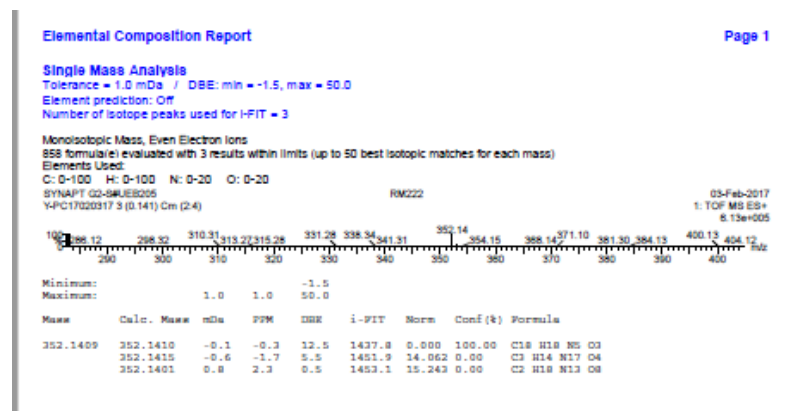
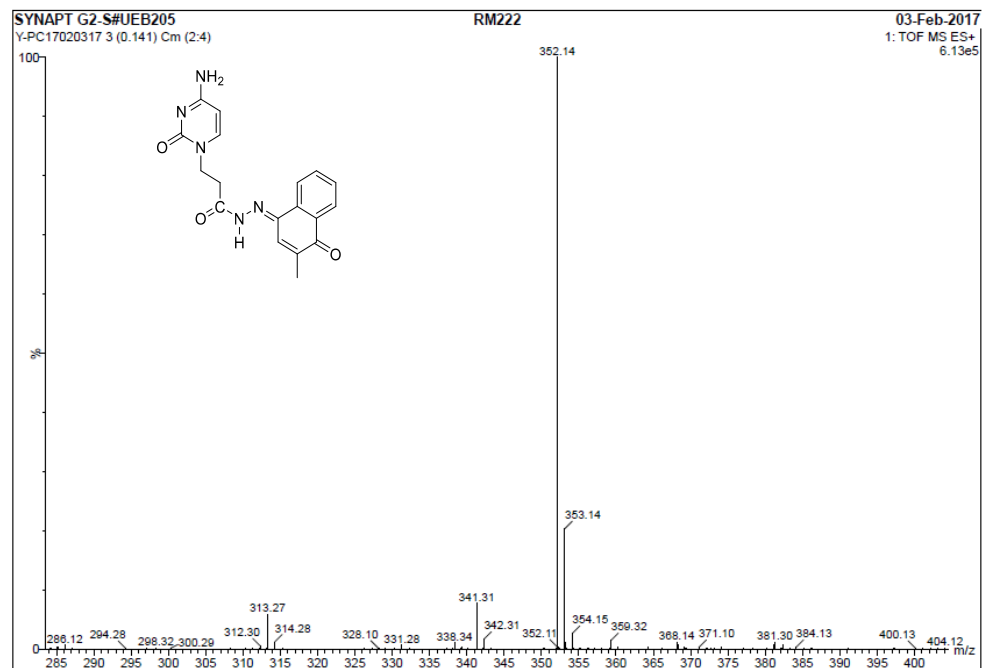


Figure S65. HRMS spectrum of compound 61

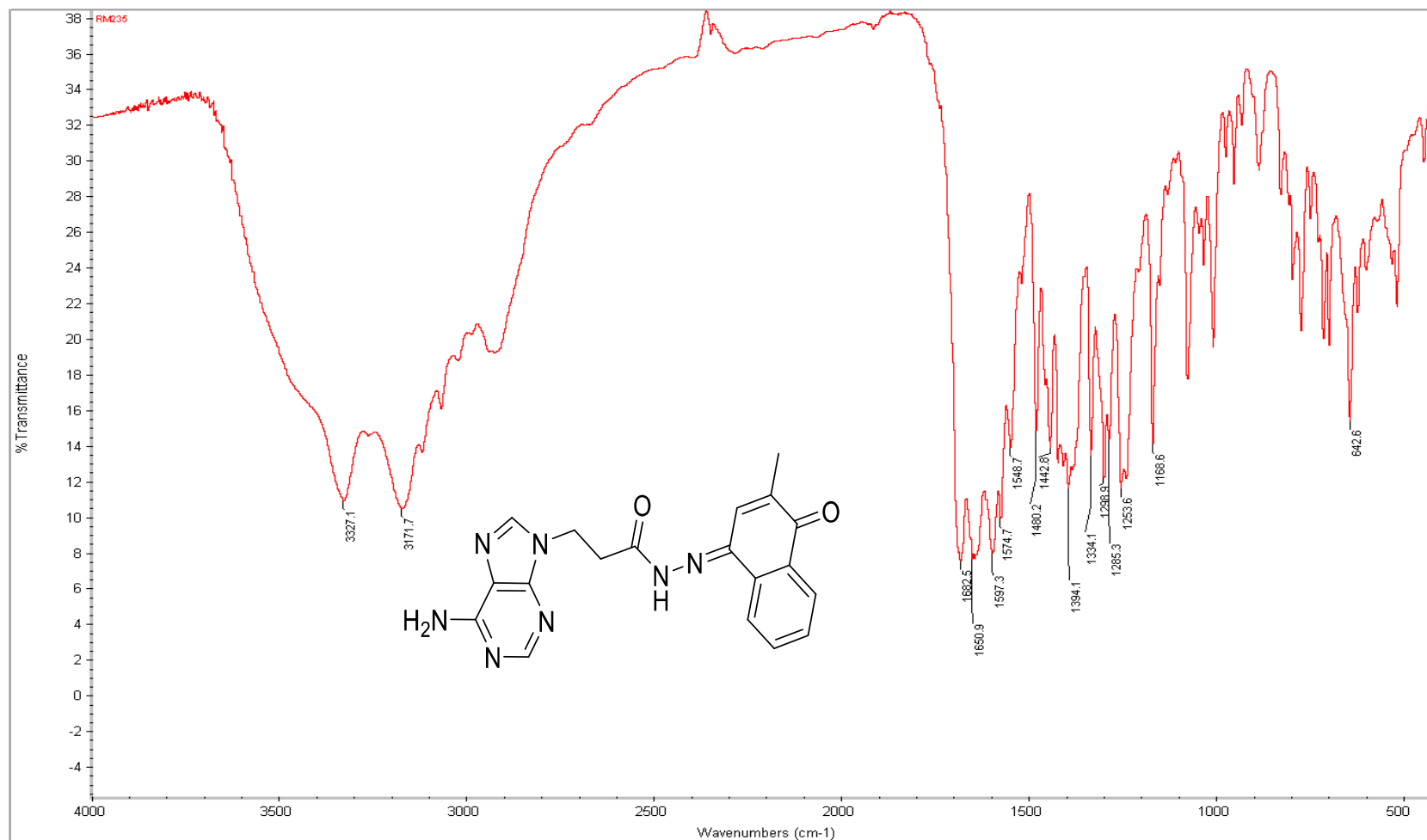


Figure S66. IR spectrum of compound 6m

RM235/ DMSO

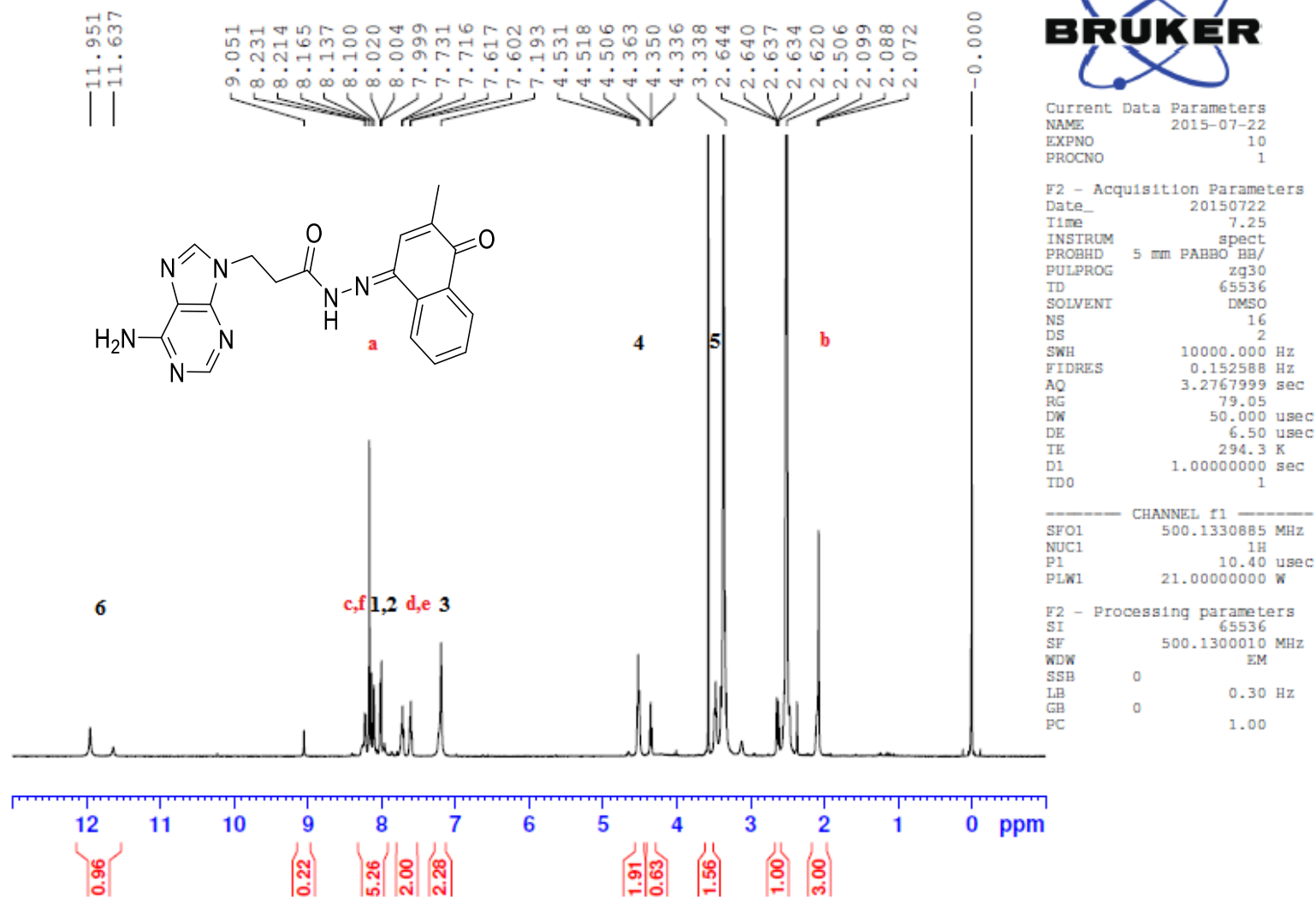


Figure S67.  $^1\text{H}$  NMR (DMSO, 500 MHz) spectrum of compound **6m**

RM235/ DMSO

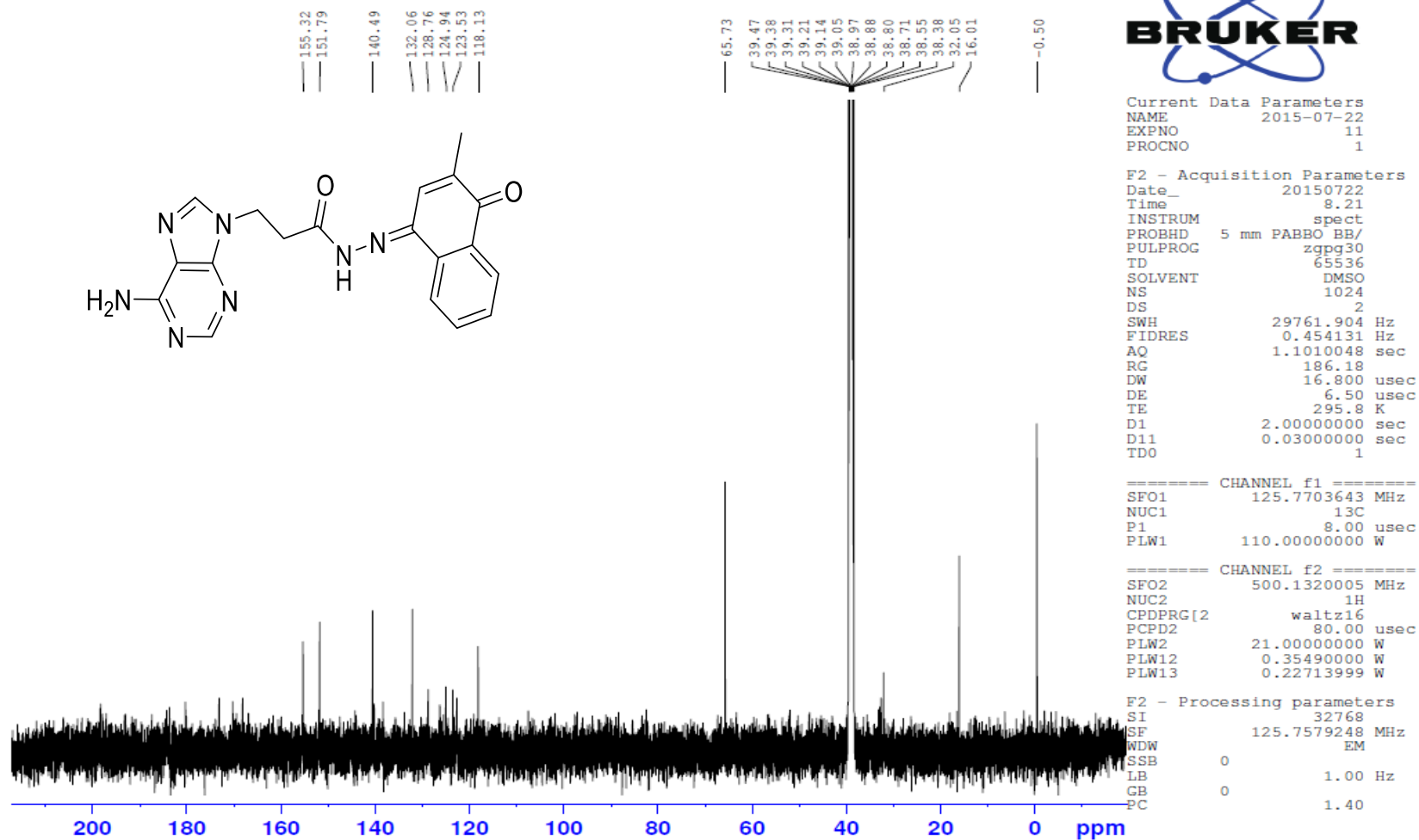
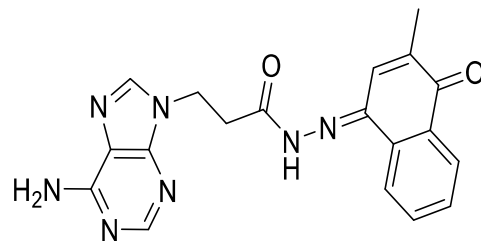


Figure S68. <sup>13</sup>C NMR (DMSO, 100 MHz) spectrum of compound 6m

RM235/ DMSO

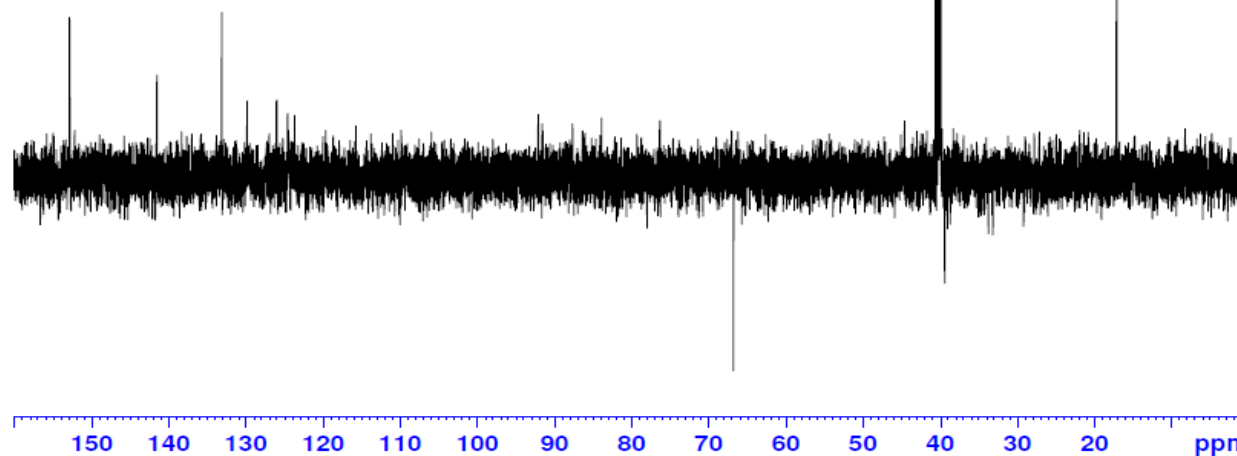
152.88  
141.57  
133.15  
129.84  
126.02



66.82

40.55  
40.38  
40.22  
40.05  
39.88  
39.39

17.10



Current Data Parameters  
NAME 2015-07-22  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150722  
Time 8.37  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG deptsp135  
TD 65536  
SOLVENT DMSO  
NS 256  
DS 4  
SWH 20161.291 Hz  
FIDRES 0.307637 Hz  
AQ 1.6252928 sec  
RG 186.18  
DW 24.800 usec  
DE 6.50 usec  
TE 295.3 K  
CNST2 145.0000000  
D1 2.00000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TDO 1

----- CHANNEL f1 -----  
SFO1 125.7678486 MHz  
NUC1 13C  
P1 8.00 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 110.00000000 W  
SPNAM[5] Crp60comp.4  
SPOAL5 0.500  
SPOFFS5 0 Hz  
SPW5 10.75599957 W

----- CHANNEL f2 -----  
SFO2 500.1315995 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
P3 10.40 usec  
P4 20.80 usec  
PCPD2 80.00 usec  
PLW2 21.00000000 W  
PLW12 0.35490000 W

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

Figure S69. DEPT NMR (DMSO, 100 MHz) spectrum of compound 6m



# Display Report - All Windows All Analyses

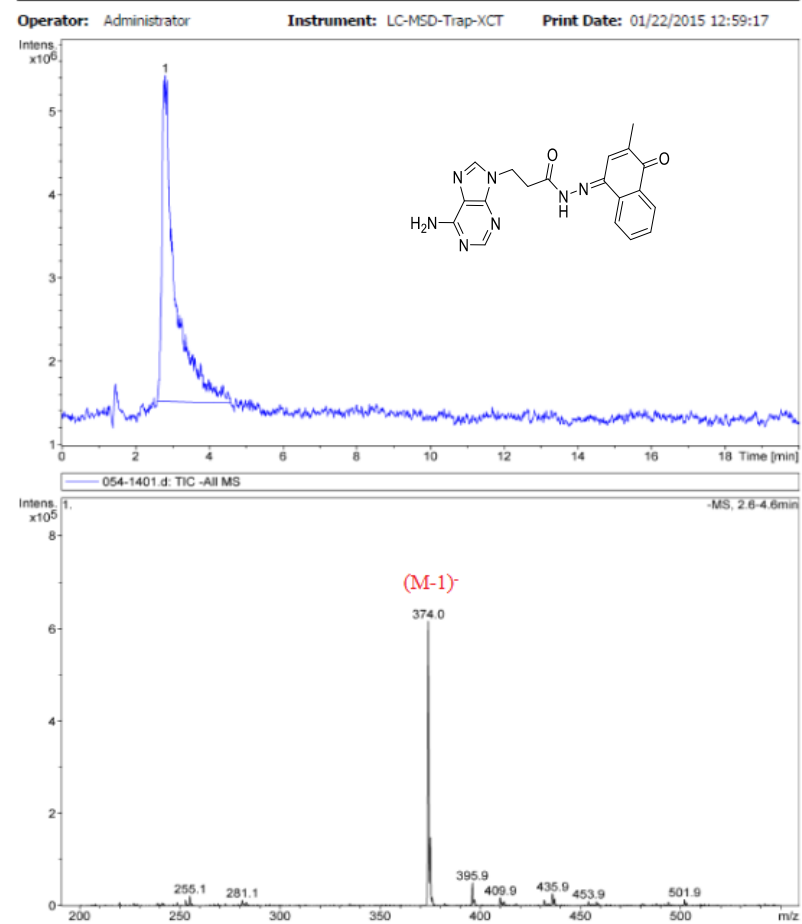
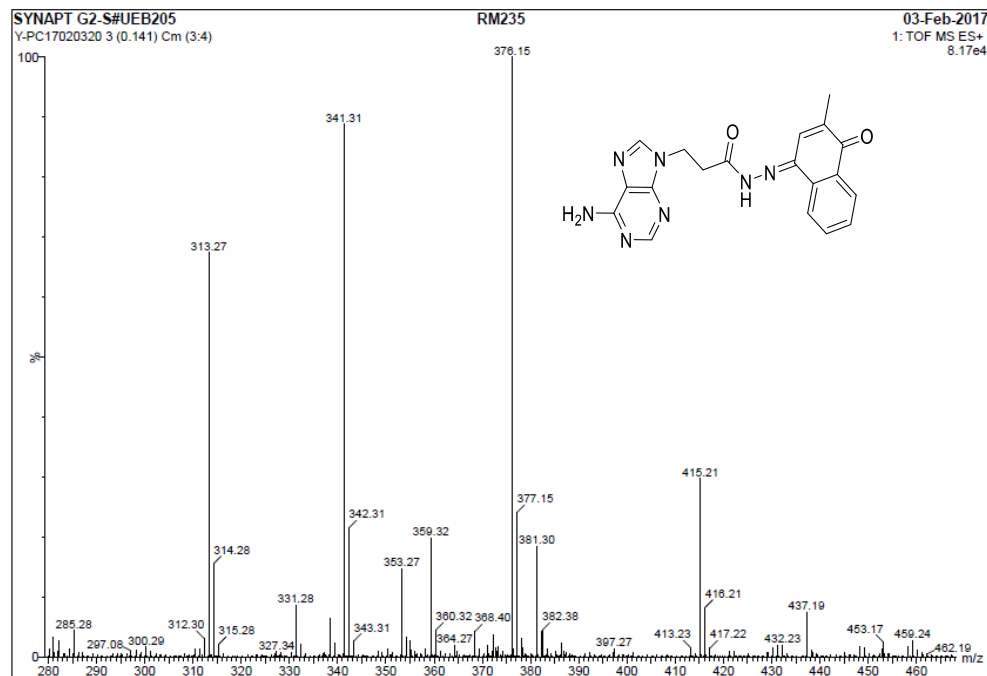


Figure S70. LC-MS spectrum of compound 6m



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

593 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20

SYNAPT G2-S#UEB205

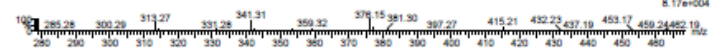
Y-PC17020320 3 (0.141) Cm (3:4)

RM235

03-Feb-2017

1: TOF MS ES+

8.17e+04



Minimum: -1.5

Maximum: 1.0 1.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (R)	Formula
376.1523	376.1522	0.1	0.3	14.5	919.4	0.000	100.00	C19 H18 N7 O2
	376.1527	-0.4	-1.1	7.5	936.6	17.273	0.00	C4 H14 N19 O3
	376.1514	0.9	2.4	2.5	936.9	17.526	0.00	C3 H18 N15 O7

Figure S71. HRMS spectrum of compound 6m