Electronic Supplementary Information for

Rhodium-catalyzed iminoiodane-mediated oxyamidation studies of 5-vinyluracil derivatives using aryl and alkyl sulfamates

Zhaoxin Wang,[§,a] Zongxin Jin,[§,a] Quanxing Zhong,[a] Yinan Zhang,[a] Yan Wu,[a] Yujiao Ma,[a] Hua Sun,[a,*] Peng Yu[a,*] and Robert H. Dodd[a,b,*]

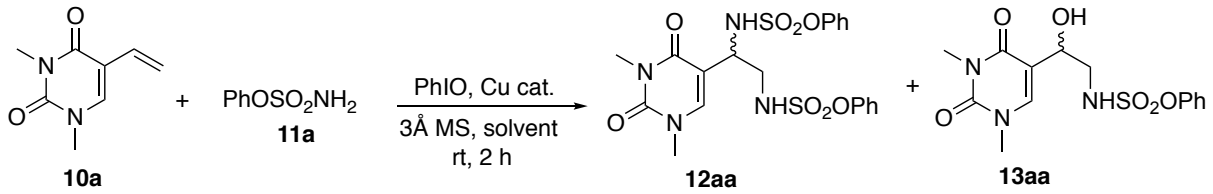
[a]*China International Science and Technology Cooperation Base of Food Nutrition/Safety and Medicinal Chemistry, College of Biotechnology, Tianjin University of Science & Technology, Tianjin, 300457, China.*[b] *Université Paris-Saclay, Centre National de la Recherche Scientifique (CNRS), Institut de Chimie des Substances Naturelles, UPR 2301, 91198, Gif-sur-Yvette, France*

robert.dodd@cnrs.fr

Table of contents

Table of contents

General procedure for optimization study of Cu-catalyzed reaction of 10a with 11a



10a 12aa 13aa

Diphenyl (1-(1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)ethane-1,2-diyl)bis(sulfamate) (12aa) and phenyl (2-(1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)-2-hydroxyethyl)sulfamate (13aa). A mixture of 5-vinyluracil derivative **10a** (1 equiv), phenylsulfamate **11a** (1.5 equiv), iodosylbenzene (1.5 equiv), copper catalyst (0.2 – 0.4 equiv) and 3Å molecular sieves (250 mg) in the indicated solvent (3 mL) was stirred for 2 h at room temperature unless indicated otherwise. The reaction mixture was then poured into saturated aqueous sodium chloride solution (20 mL) and extracted with dichloromethane (2 x 20 mL). The organic extracts were combined, dried over sodium sulfate and the solvent was removed under vacuum. The residue was purified by column chromatography on silica gel (dichloromethane / methanol = 50: 1) (petroleum ether/ethyl acetate 3: 1) affording compound **12aa**: white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, *J* = 8 Hz, 1H), 8.52 (t, *J* = 6 Hz, 1H), 7.56 (s, 1H), 7.47 – 7.17 (m, 10H), 4.44 (m, 1H), 3.52 – 3.45 (m, 1H), 3.24 (s, 3H), 3.12 (s, 3H); ^{13}C NMR(100 MHz, $CDCl_3$) δ 162.2, 151.4, 150.4, 150.3, 143.9, 130.4, 130.1, 129.9, 127.3, 126.8, 122.2, 121.6, 115.7, 108.4, 52.7, 45.8, 37.1, 27.9; HRMS (ESI), m/z: calcd for $C_{20}H_{22}N_4O_8S_2Na^+$ 533.0777; found: 533.0749.

Continued elution of the chromatography column using dichloromethane/methanol (50:1) provided compound **13aa**:white solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31 (t, *J* = 5.6 Hz, 1H), 7.58 (s, 1H), 7.44 (m, 2H), 7.33 (m, 1H), 7.29 (m, 2H), 5.47 (d, *J* = 4.4 Hz, 1H), 4.61 (m, 1H), 3.41 – 3.33 (m, 1H), 3.32 (s, 3H), 3.27 (s, 1H), 3.16 – 3.10 (m, 1H); ^{13}C NMR (100

MHz, DMSO-d_6) δ 162.5, 151.7, 150.5, 142.2, 130.3, 127.1, 122.4, 112.4, 65.6, 48.7, 37.0, 27.8; HRMS (ESI) m/z: calcd for $C_{14}H_{17}N_3O_6SNa^+$ 378.0736, found 378.0746.

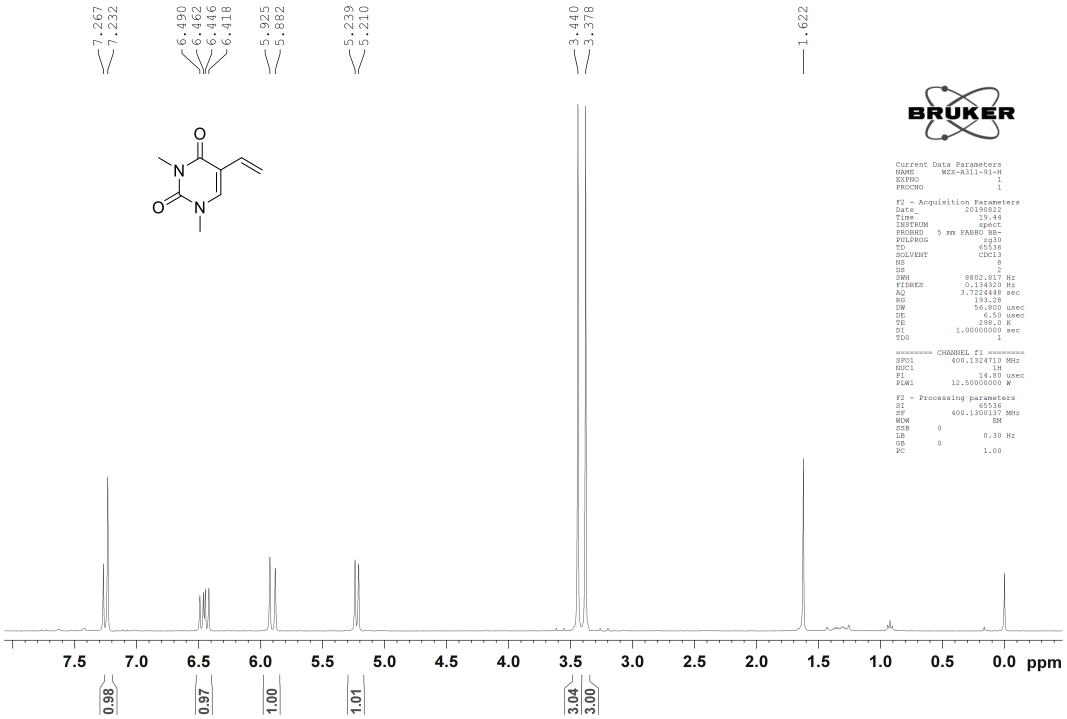
See Table below for conditions and yields.

Table Optimization of copper-catalyzed formation of 12aa and 13aa[a]

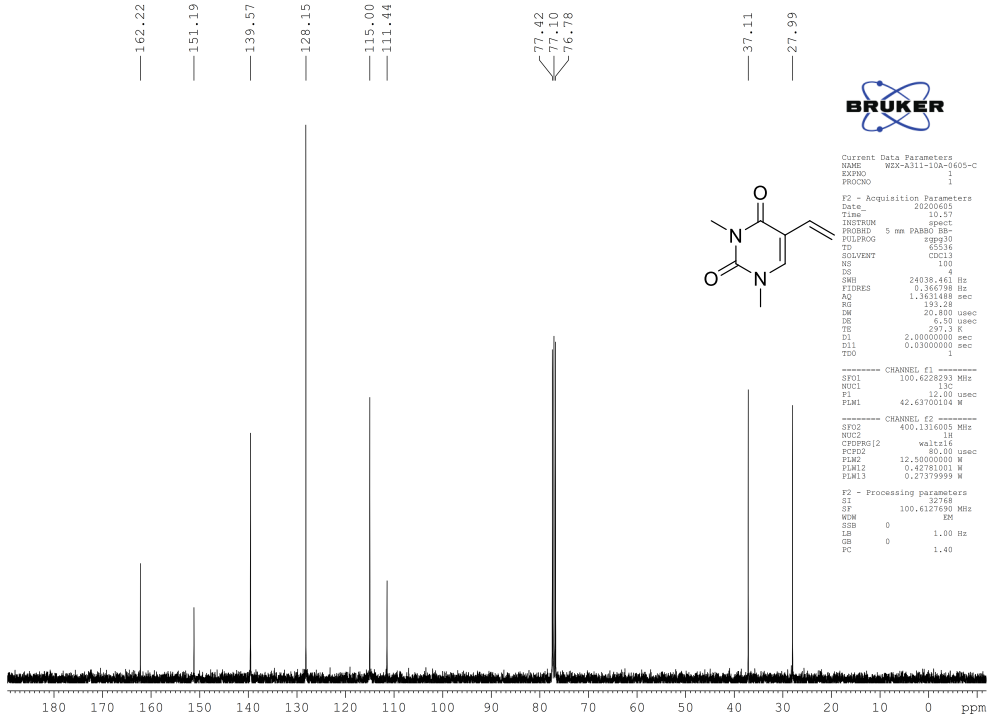
Entry	Catalyst	Equiv	Solvent	Yield (%)[b]	
				12aa	**13aa**
1	$Cu(CH_3CN)_4PF_6$	0.2	DCM	22	35
2	CuBr	0.2	DCM	4	0
3	CuBr	0.2	DCM[c]	4	0
4	$Cu(acac)_2$	0.2	DCM	33	29
5	CuOTf	0.2	DCM	29	45
6	$Cu(OTf)_2$	0.2	DCM	36	31
7	$Cu(OTf)_2$	0.2	DCM[c]	37	33
8	$Cu(OTf)_2$	0.3	DCM	45	30
9	$Cu(OTf)_2$	0.4	DCM	49	28
10	$Cu(OTf)_2$	0.3	MeCN	10	29
11	$Cu(OTf)_2$	0.3	Dioxane	10	14
12	$Cu(OTf)_2$	0.3	Toluene	0	0
13	$Cu(OTf)_2$	0.3	DCE	37	31
14	$Cu(OTf)_2$	0.3	THF	12	15

[a] General conditions : **10a** (5 mmol), **11a** (7.5 mmol), PhIO (7.5 mmol), 3Å molecular sieves (2.5 g) in solvent (25 mL) and catalyst were stirred for 2 h under argon in a sealed tube. [b] Isolated yield. [c] Reaction conducted at reflux.

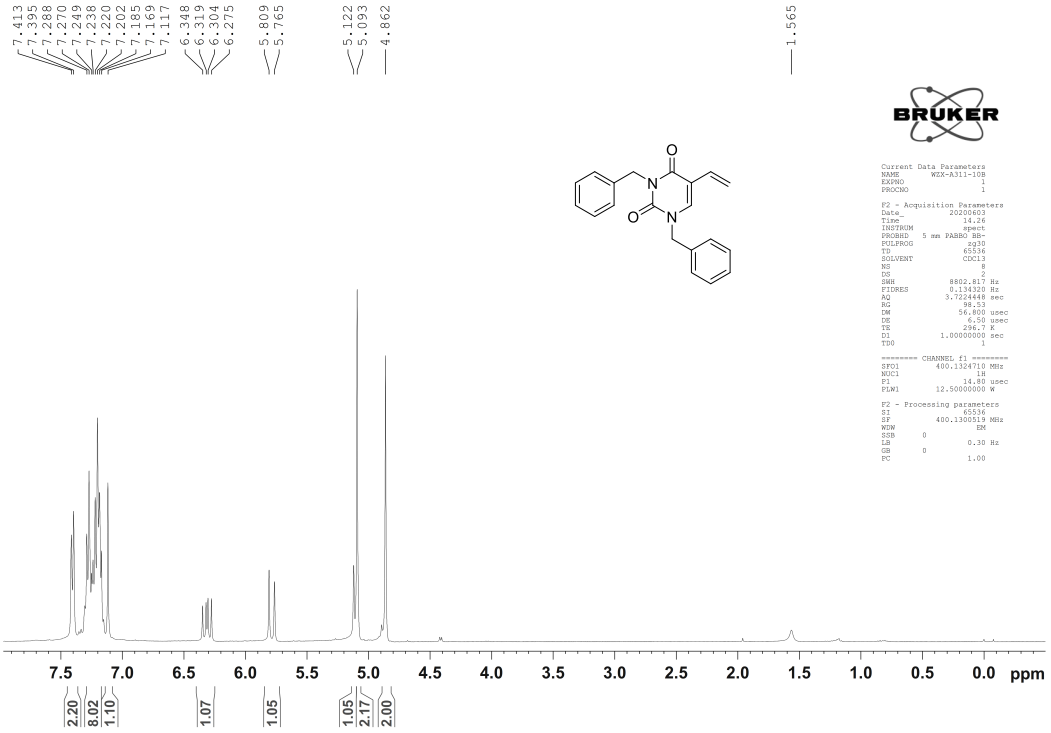
^{1}H NMR spectrum of **10a** (400 MHz, $CDCl_3$)



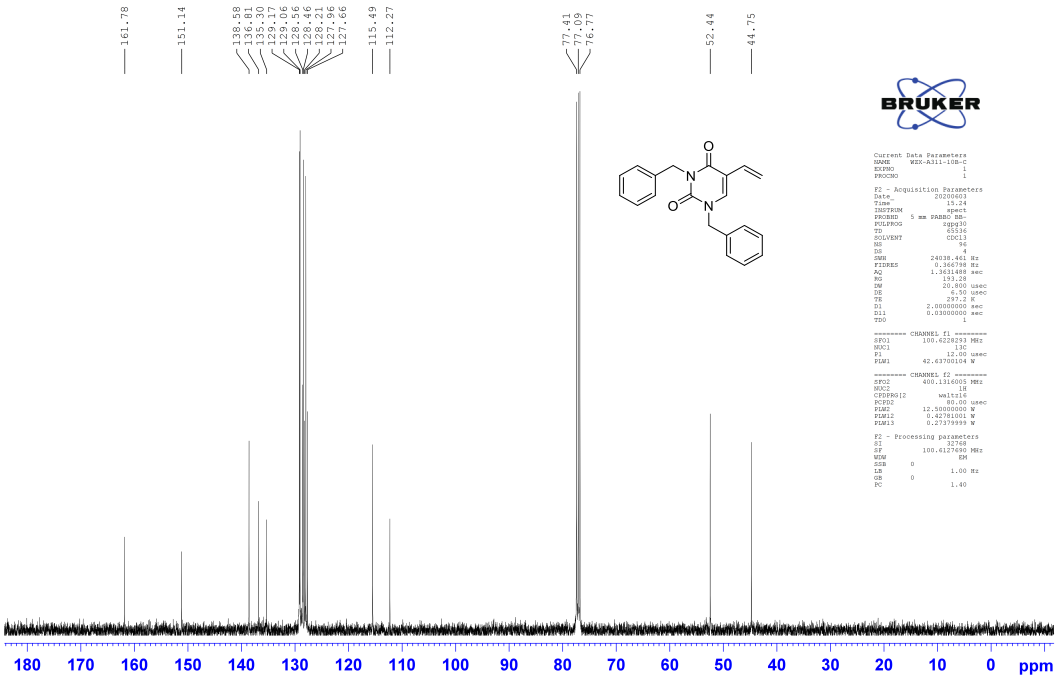
^{13}C NMR spectrum of **10a** (100 MHz, $CDCl_3$)



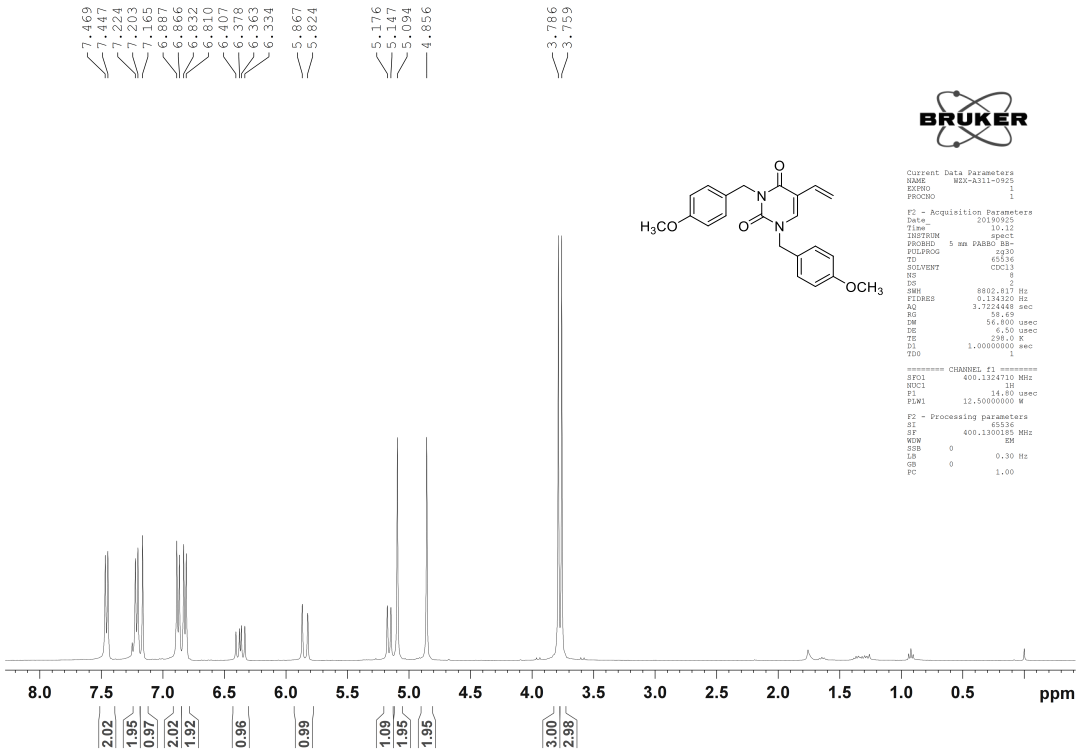
^{1}H NMR spectrum of **10b** (400 MHz, $CDCl_3$)



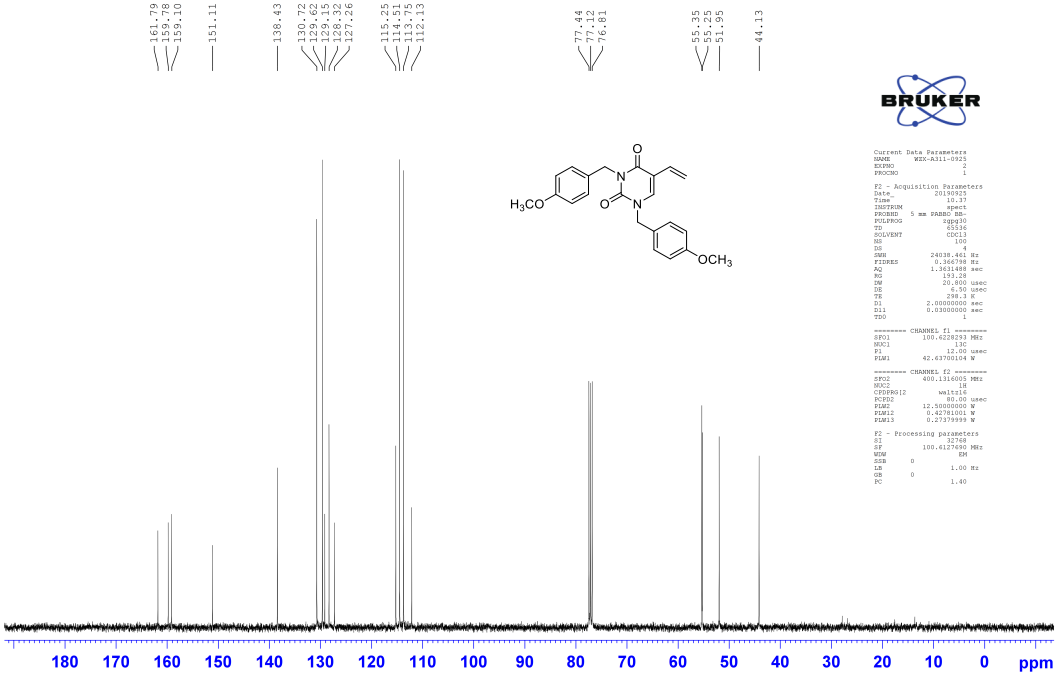
^{13}C NMR spectrum of **10b** (100 MHz, $CDCl_3$)



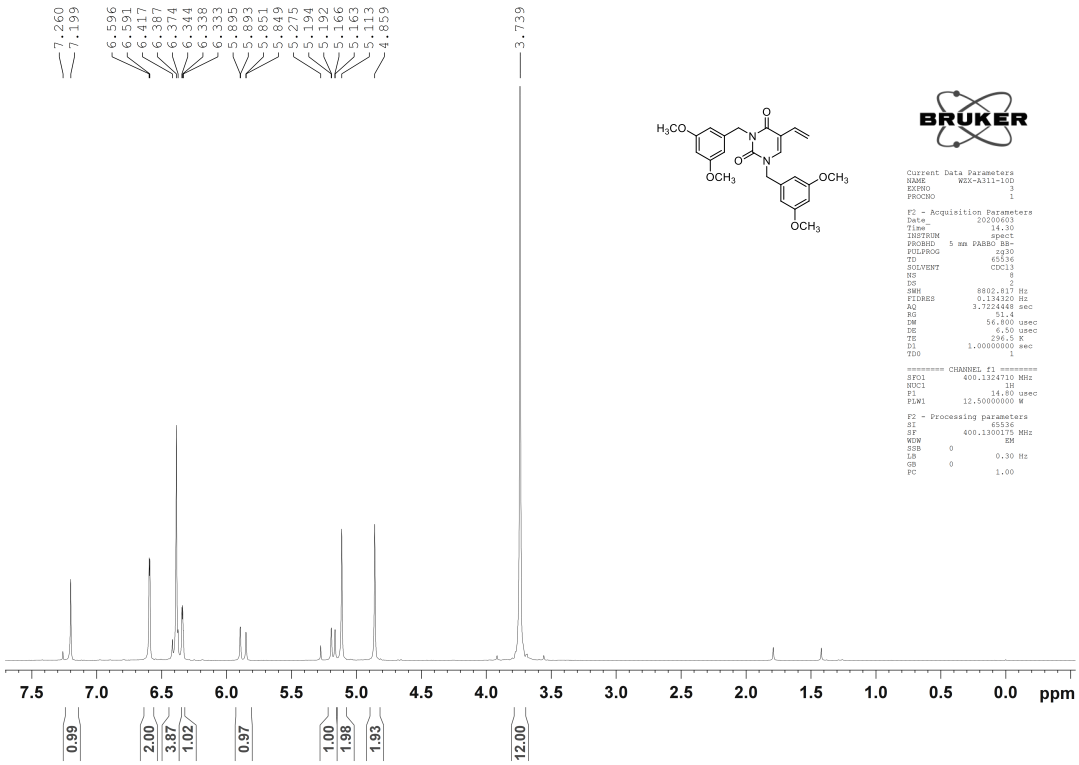
^{1}H NMR spectrum of **10c** (400 MHz, $CDCl_3$)



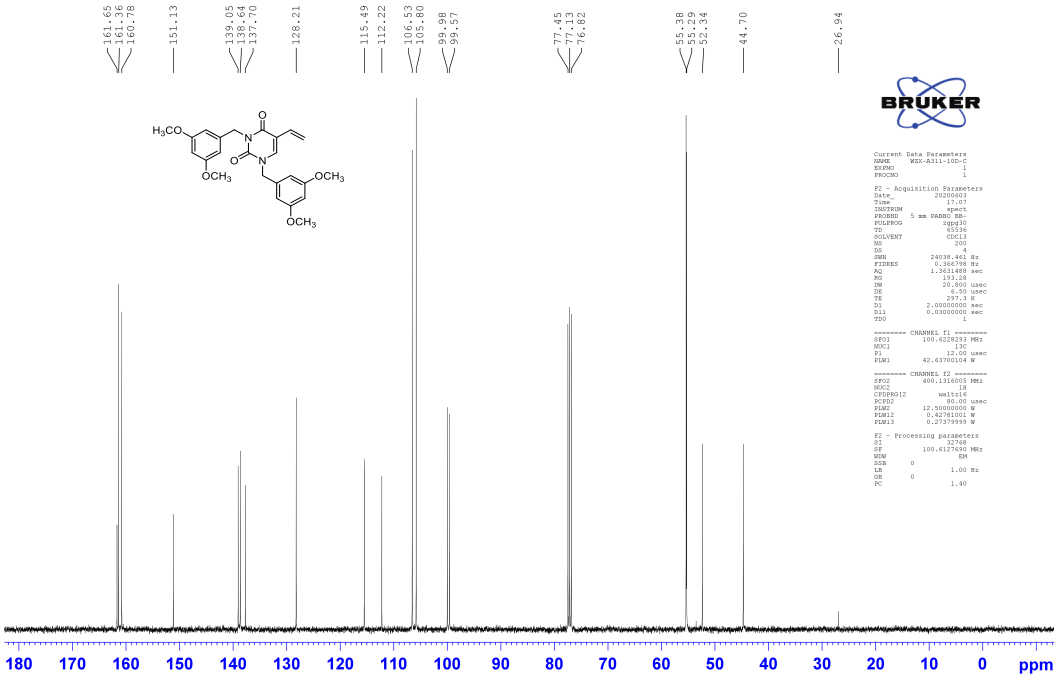
^{13}C NMR spectrum of **10c** (100 MHz, $CDCl_3$)



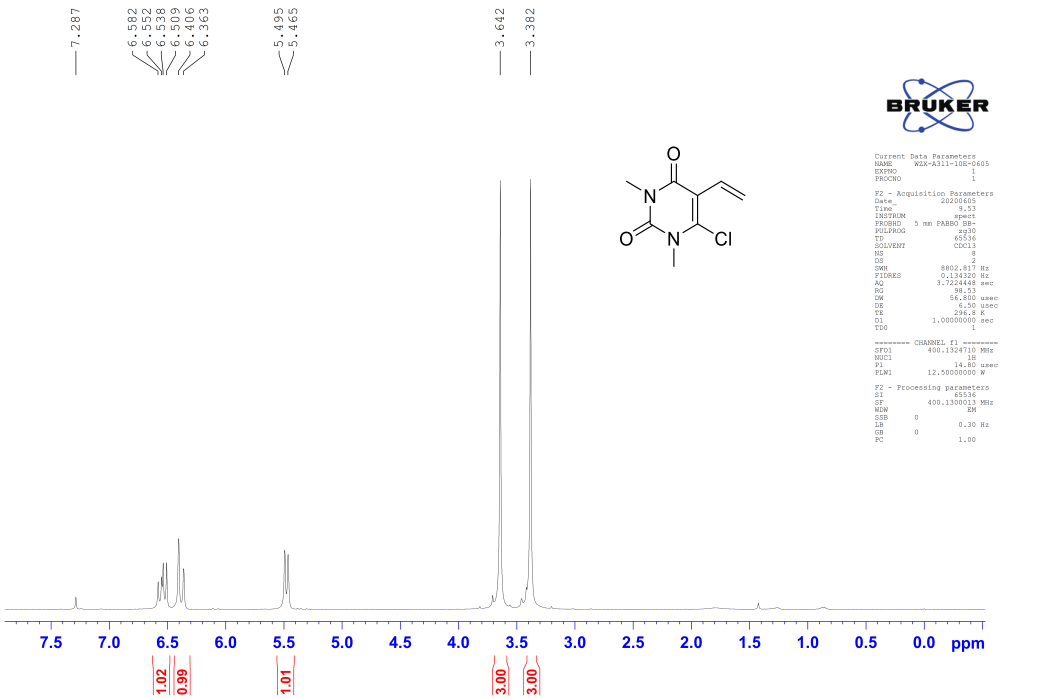
^{1}H NMR spectrum of **10d** (400 MHz, $CDCl_3$)



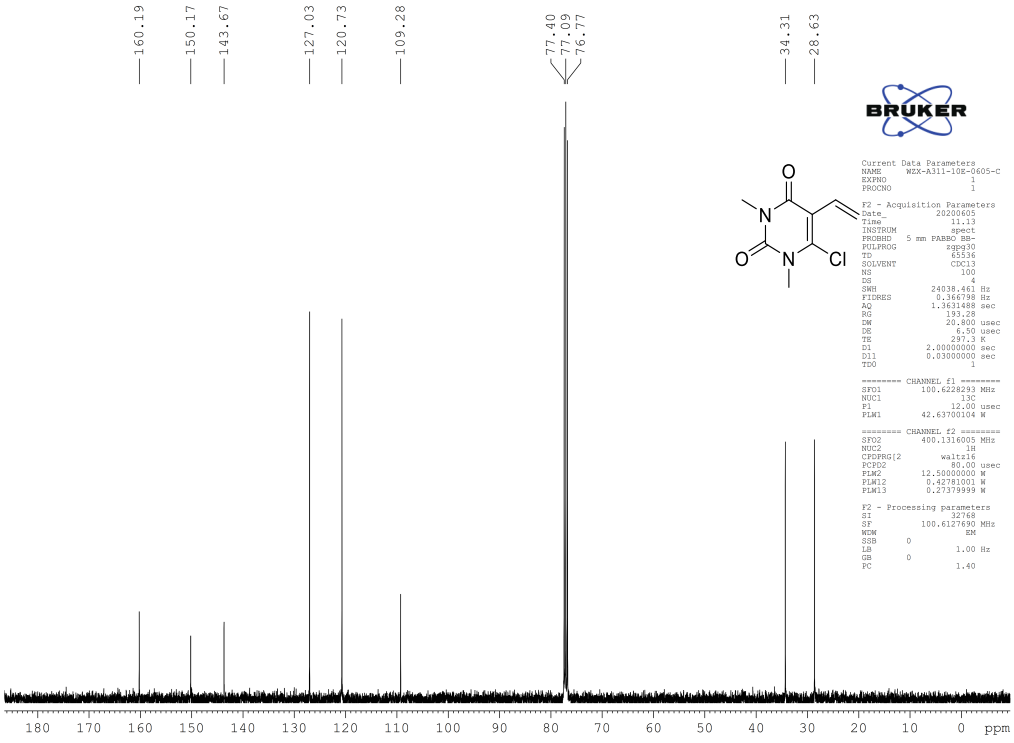
^{13}C NMR spectrum of **10d** (100 MHz, $CDCl_3$)



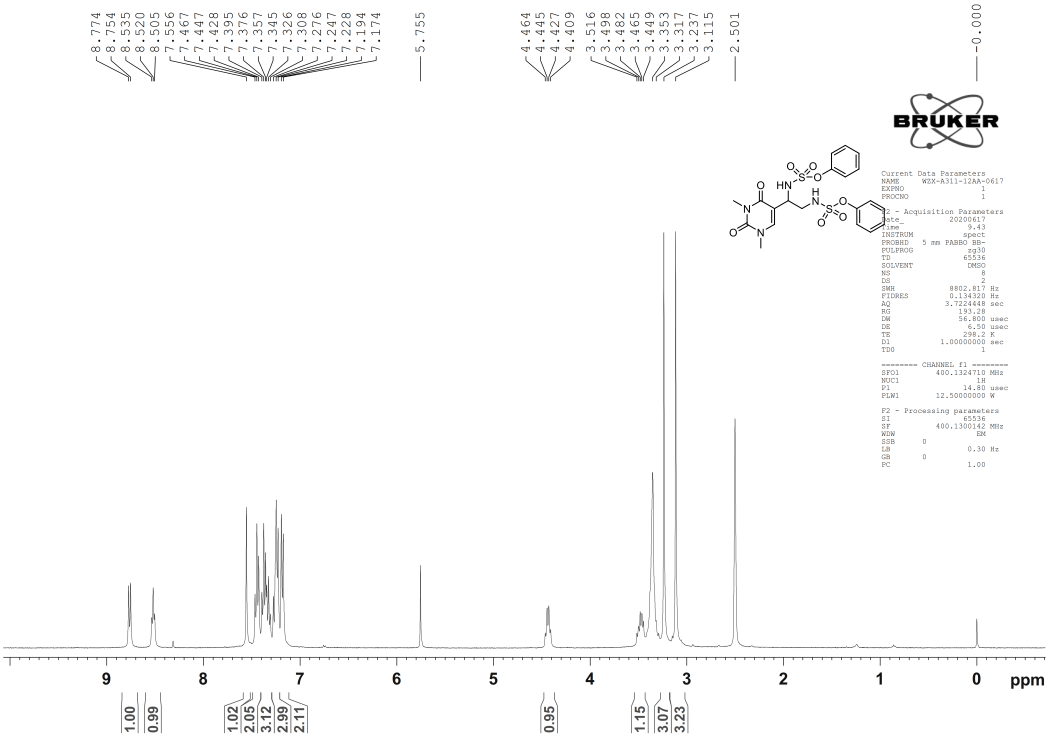
^{1}H NMR spectrum of **10e** (400 MHz, $CDCl_3$)



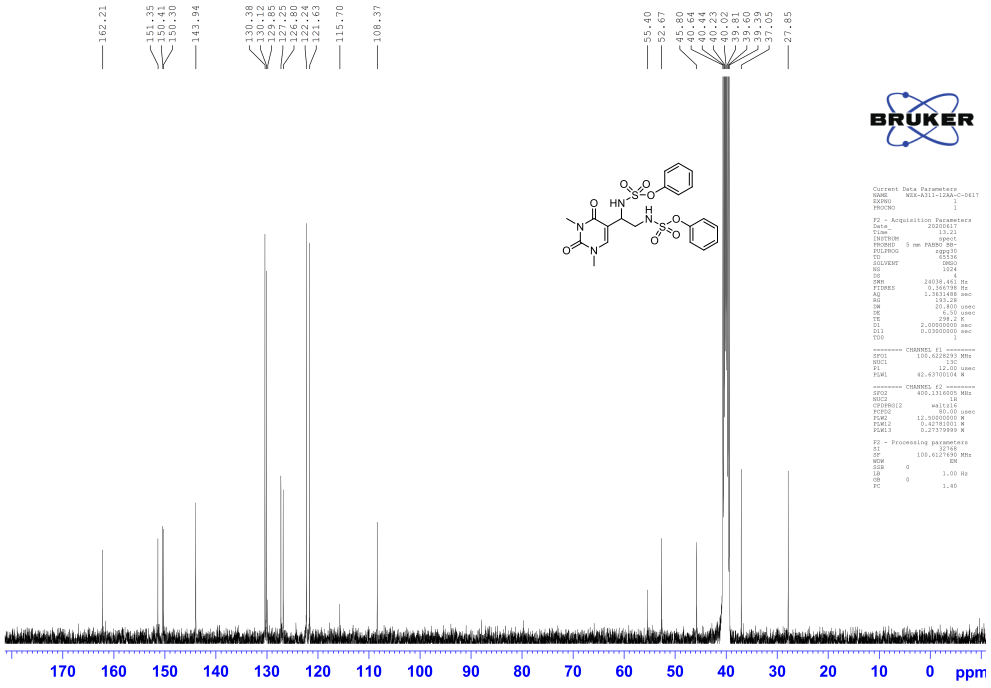
^{13}C NMR spectrum of **10e** (100 MHz, $CDCl_3$)



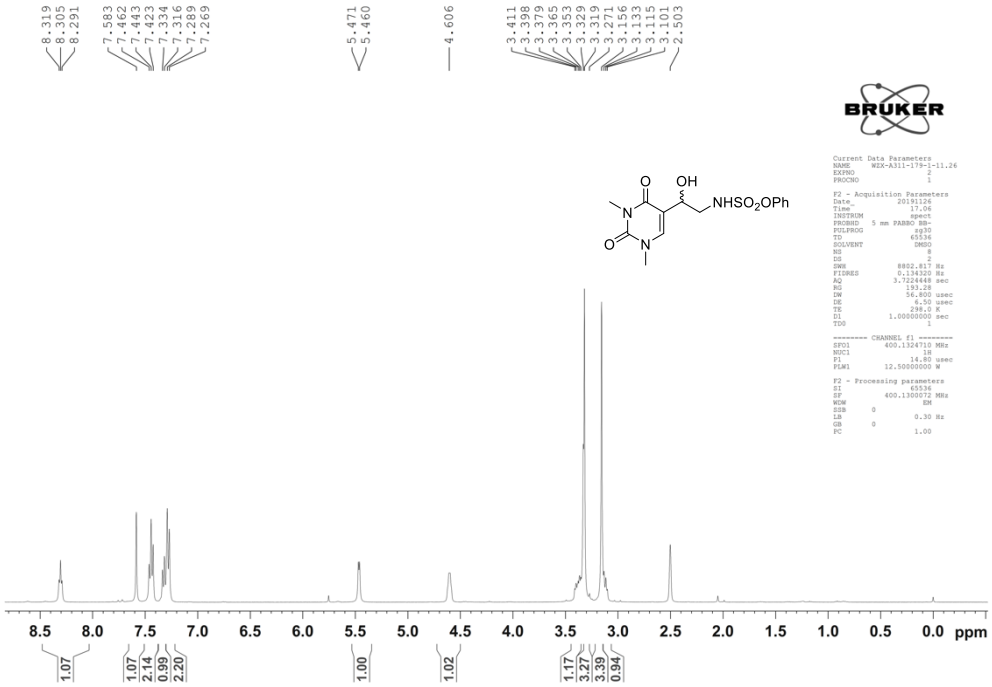
^{1}H NMR spectrum of **12aa** (400 MHz, $CDCl_3$)



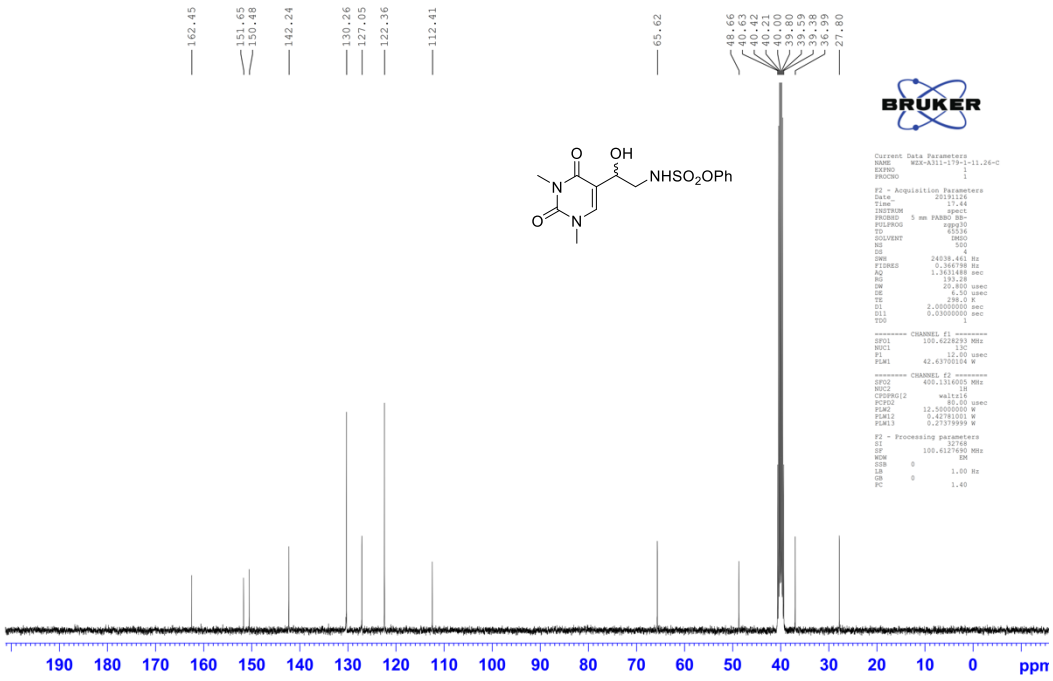
^{13}C NMR spectrum of **12aa** (100 MHz, $CDCl_3$)



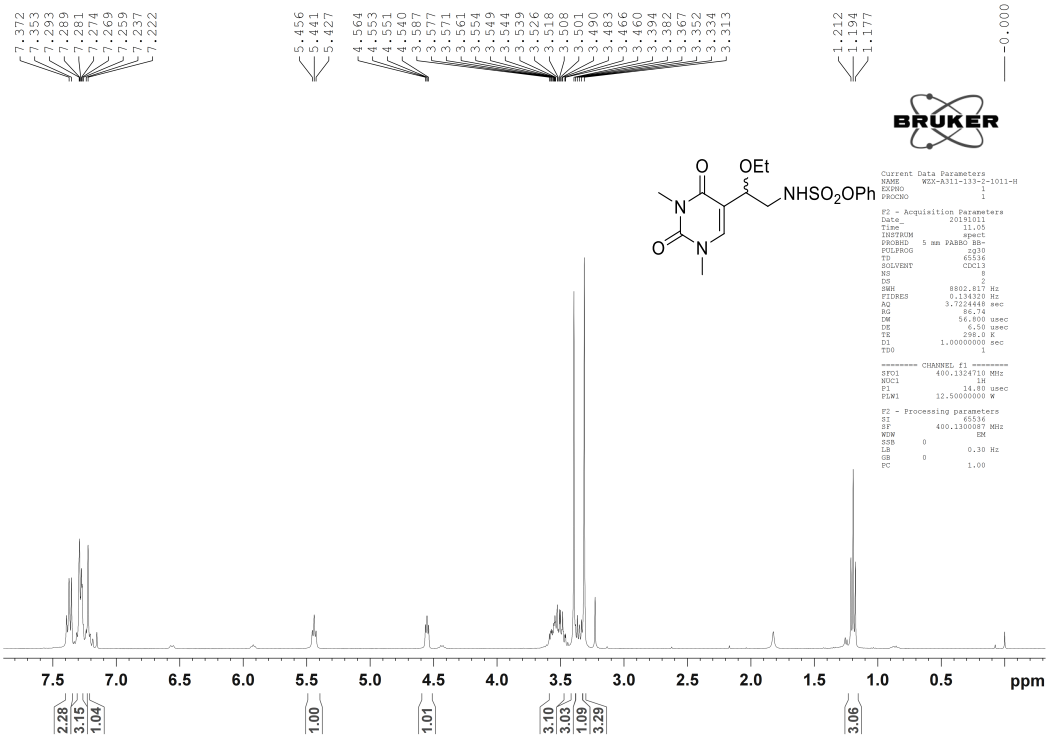
NMR spectrum of **13aa** (400 MHz, $CDCl_3$)



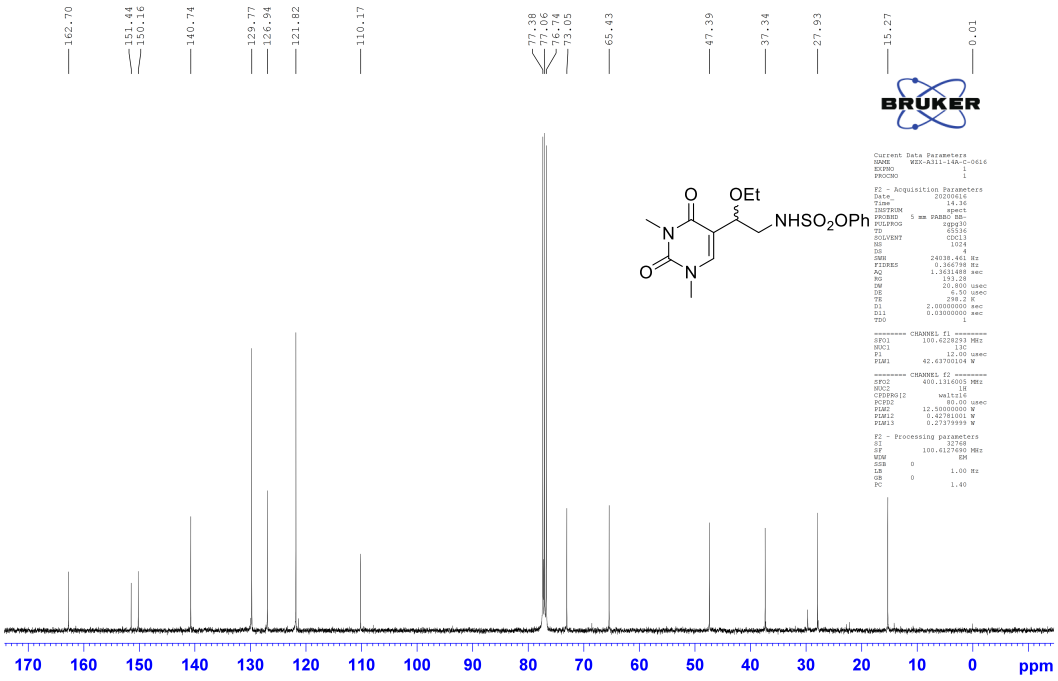
^{13}C NMR spectrum of **13aa** (100 MHz, $CDCl_3$)



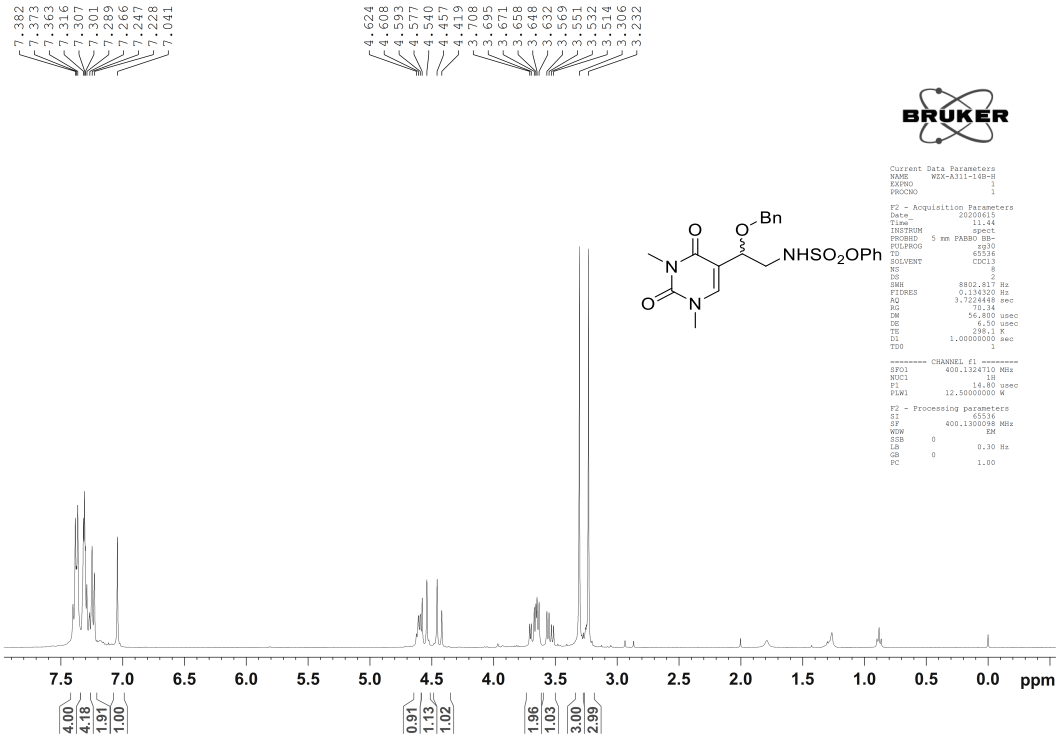
^{1}H NMR spectrum of **14a** (400 MHz, $CDCl_3$)



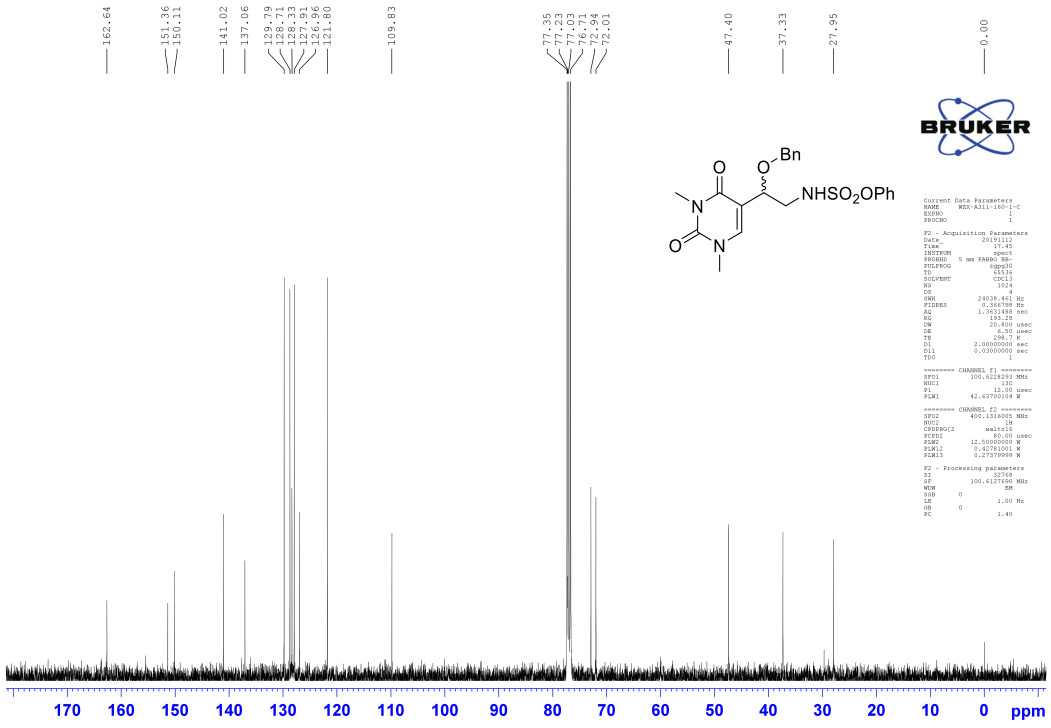
^{13}C NMR spectrum of **14a** (100 MHz, $CDCl_3$)



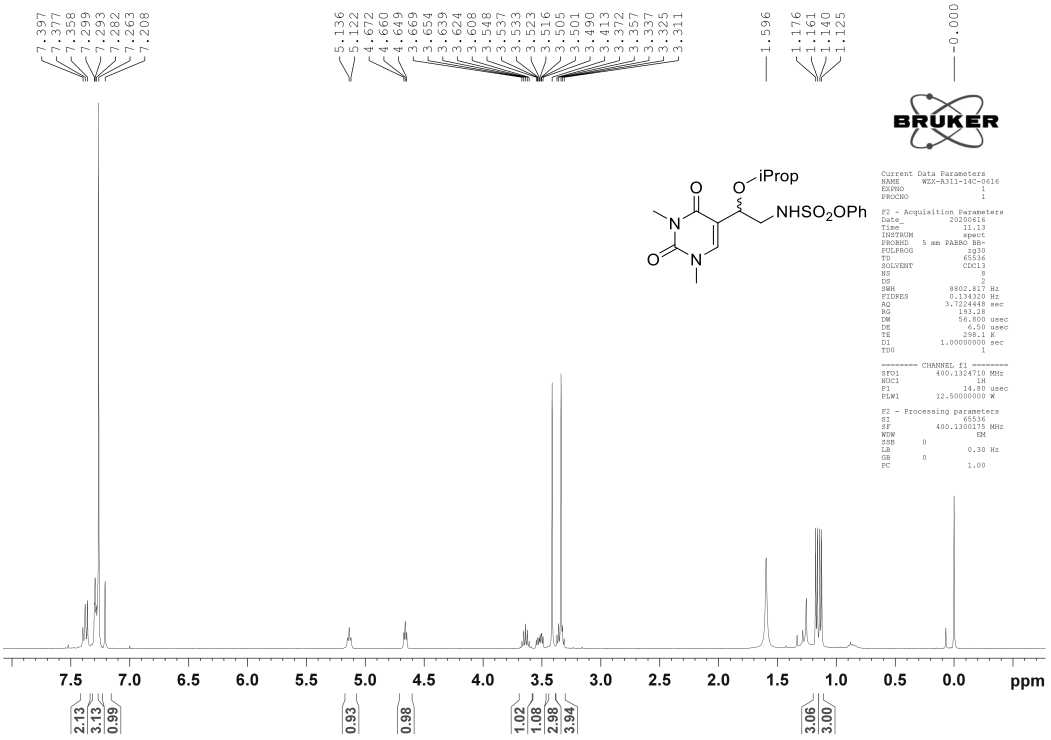
^{1}H NMR spectrum of **14b** (400 MHz, $CDCl_3$)



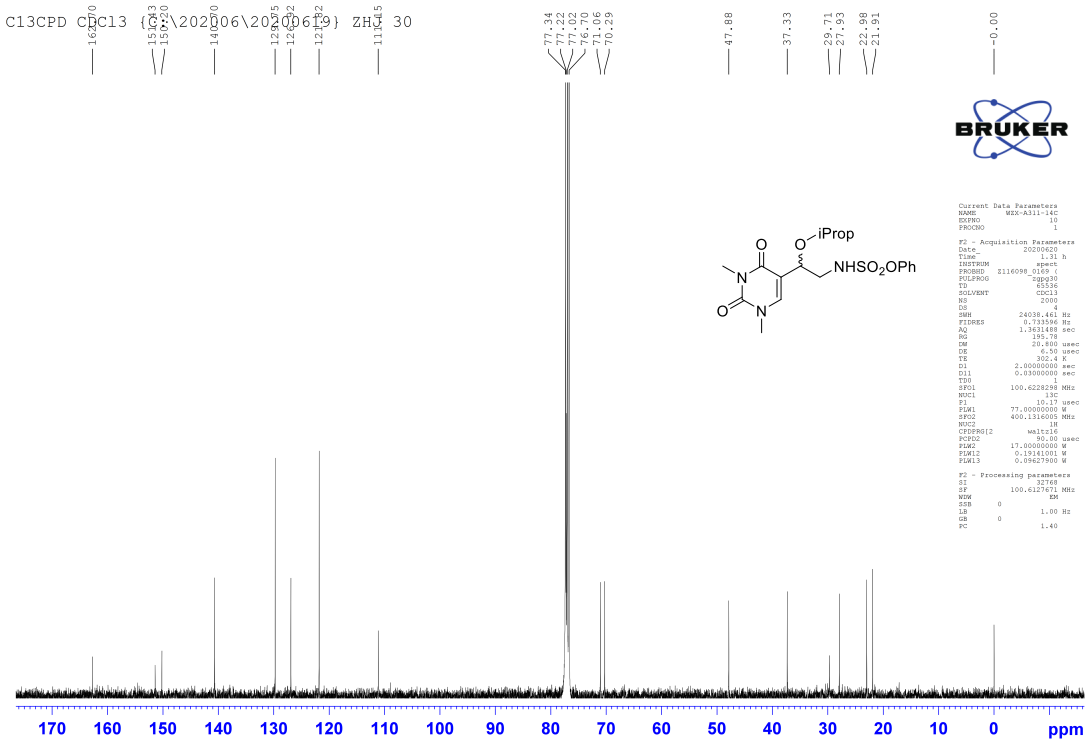
^{13}C NMR spectrum of **14b** (100 MHz, $CDCl_3$)



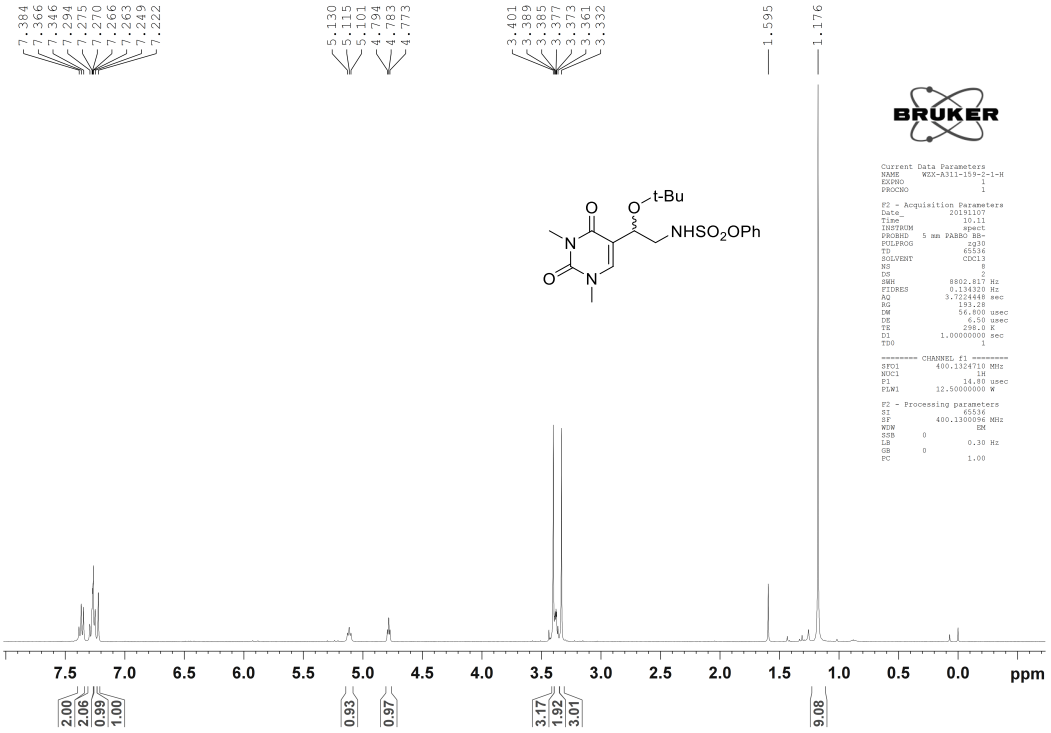
^{1}H NMR spectrum of **14c** (400 MHz, $CDCl_3$)



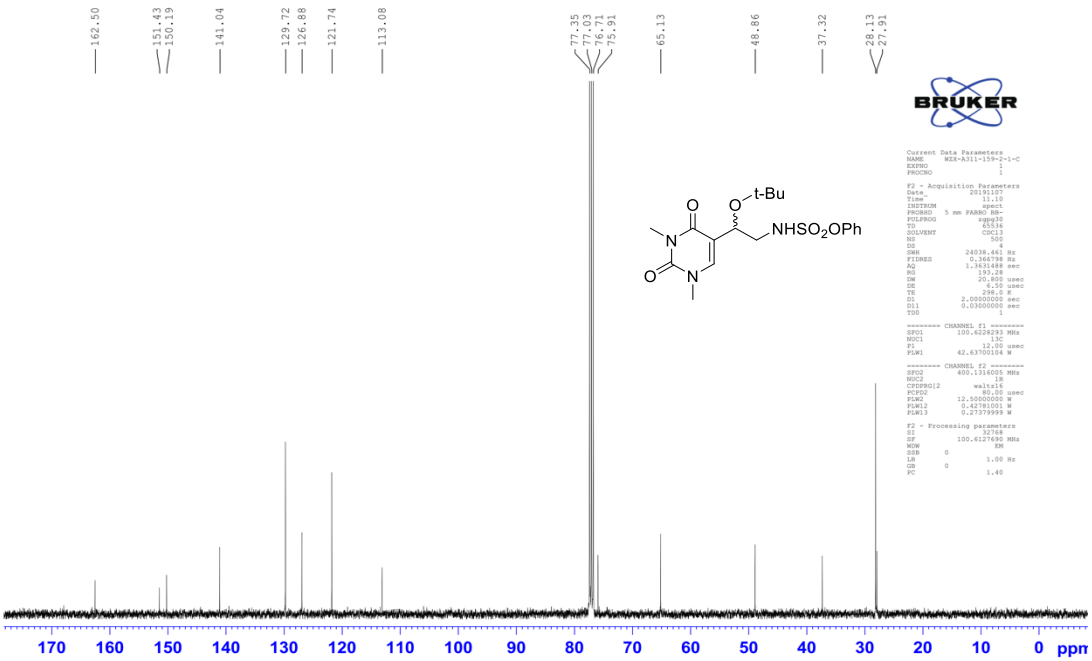
^{13}C NMR spectrum of **14c** (100 MHz, $CDCl_3$)



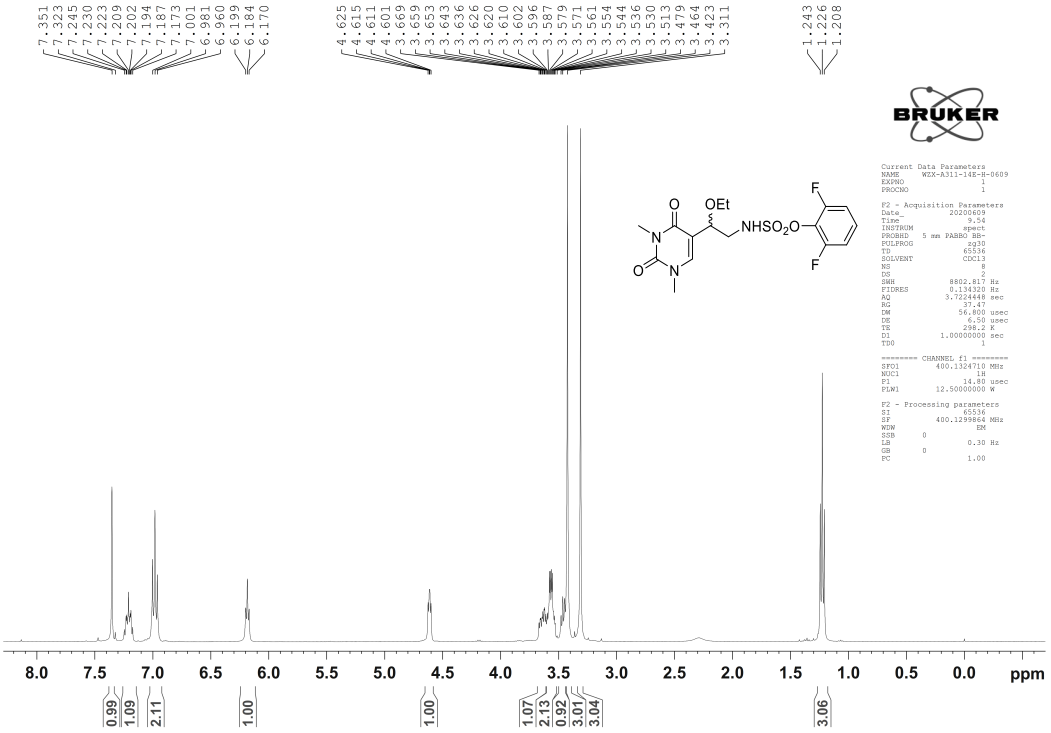
^{1}H NMR spectrum of **14d** (400 MHz, $CDCl_3$)



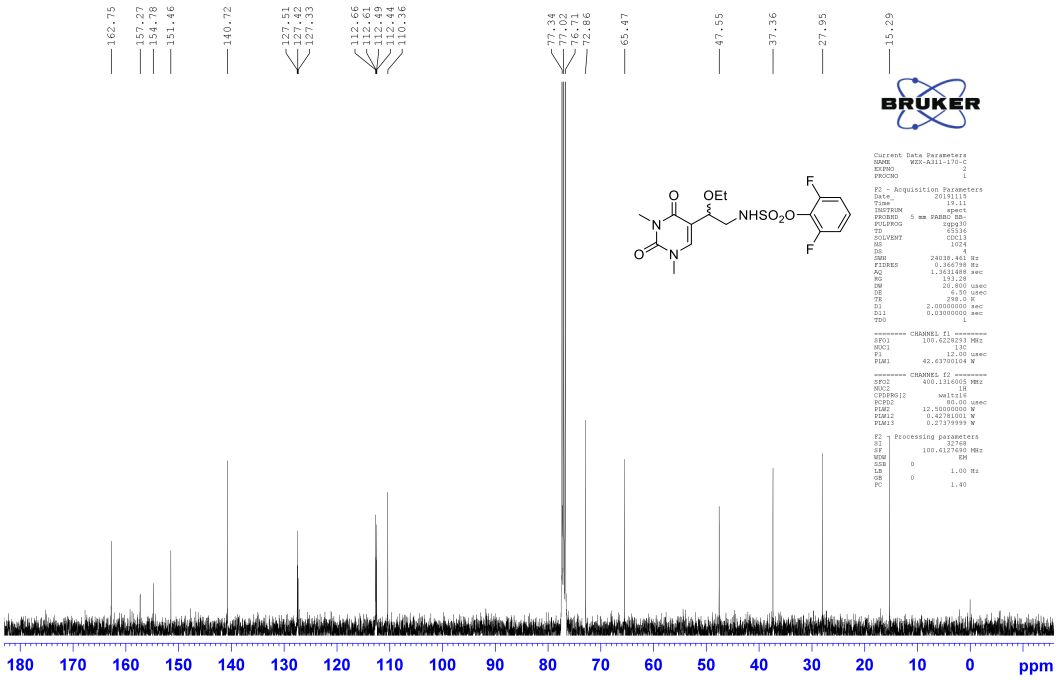
^{13}C NMR spectrum of **14d** (100 MHz, $CDCl_3$)



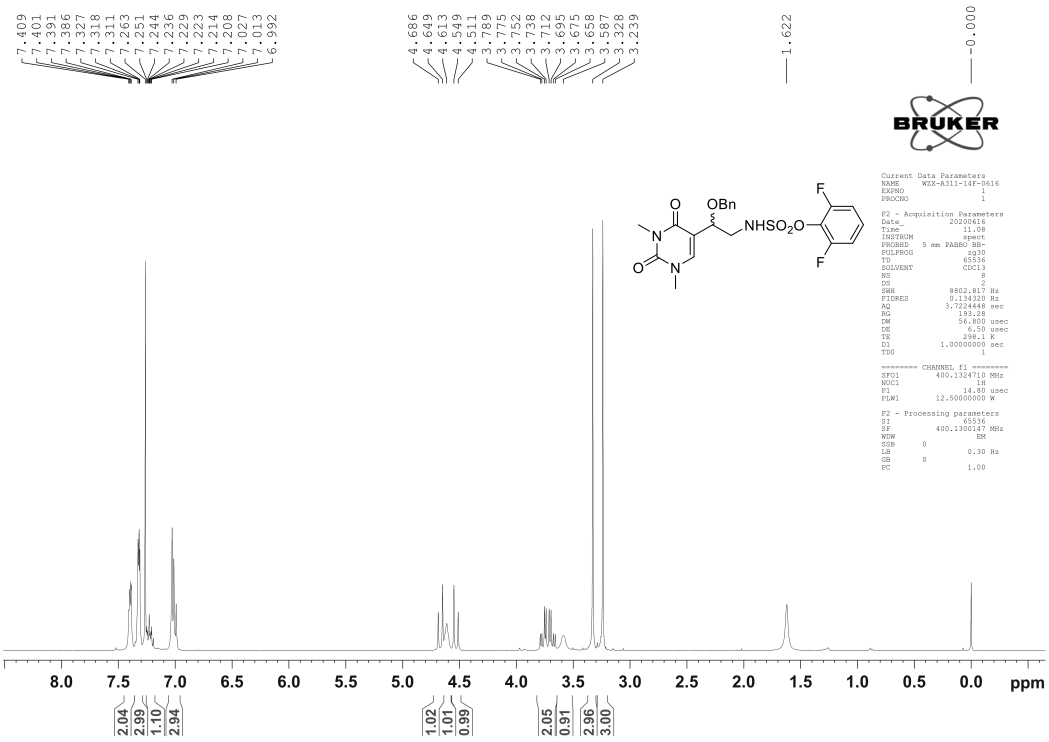
^{1}H NMR spectrum of **14e** (400 MHz, $CDCl_3$)



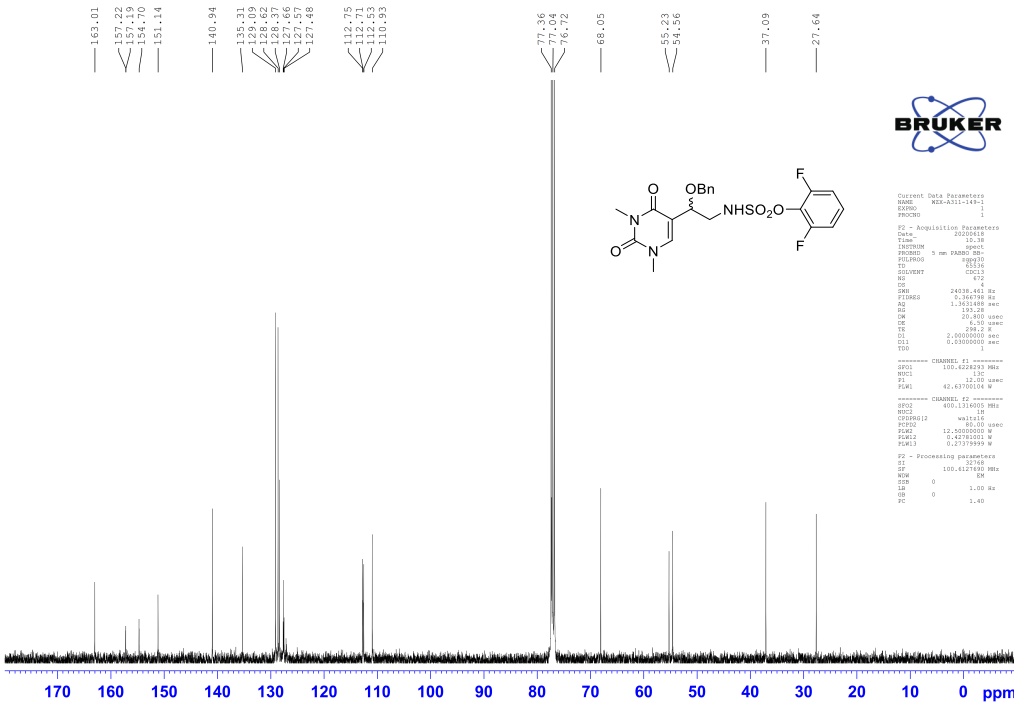
^{13}C NMR spectrum of **14e** (100 MHz, $CDCl_3$)



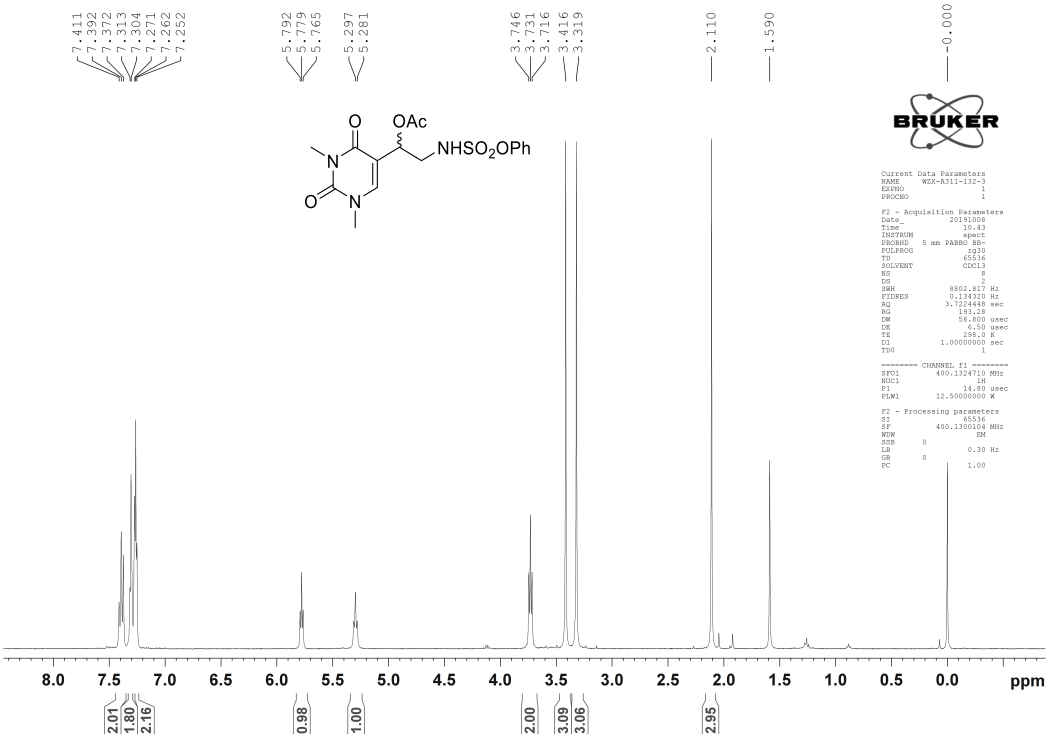
^{1}H NMR spectrum of **14f** (400 MHz, $CDCl_3$)



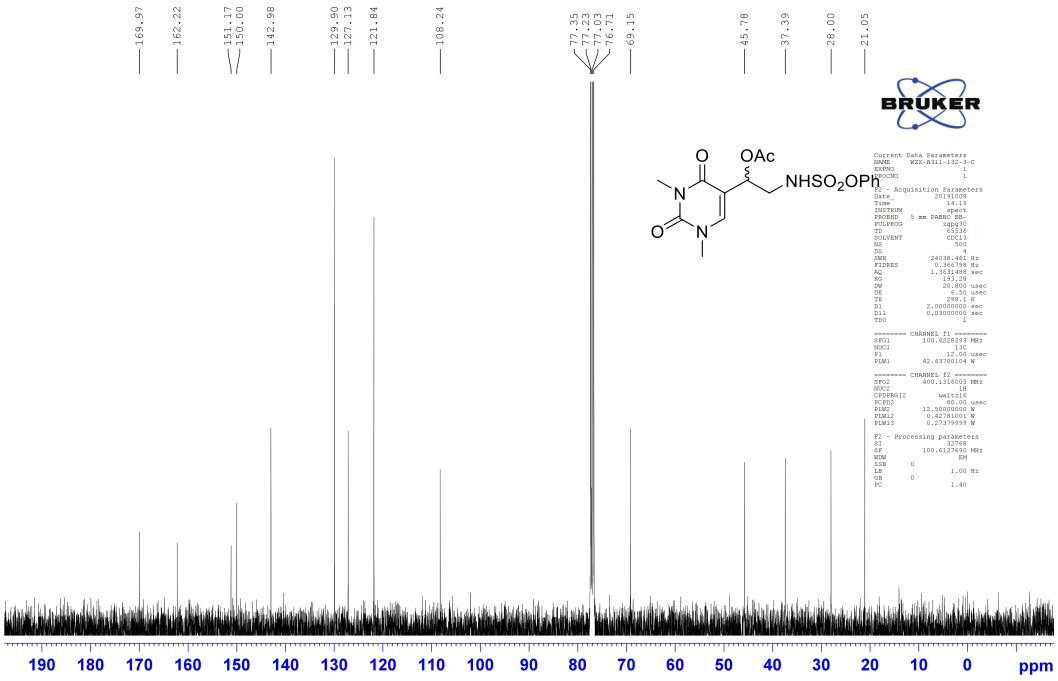
^{13}C NMR spectrum of **14f** (100 MHz, $CDCl_3$)



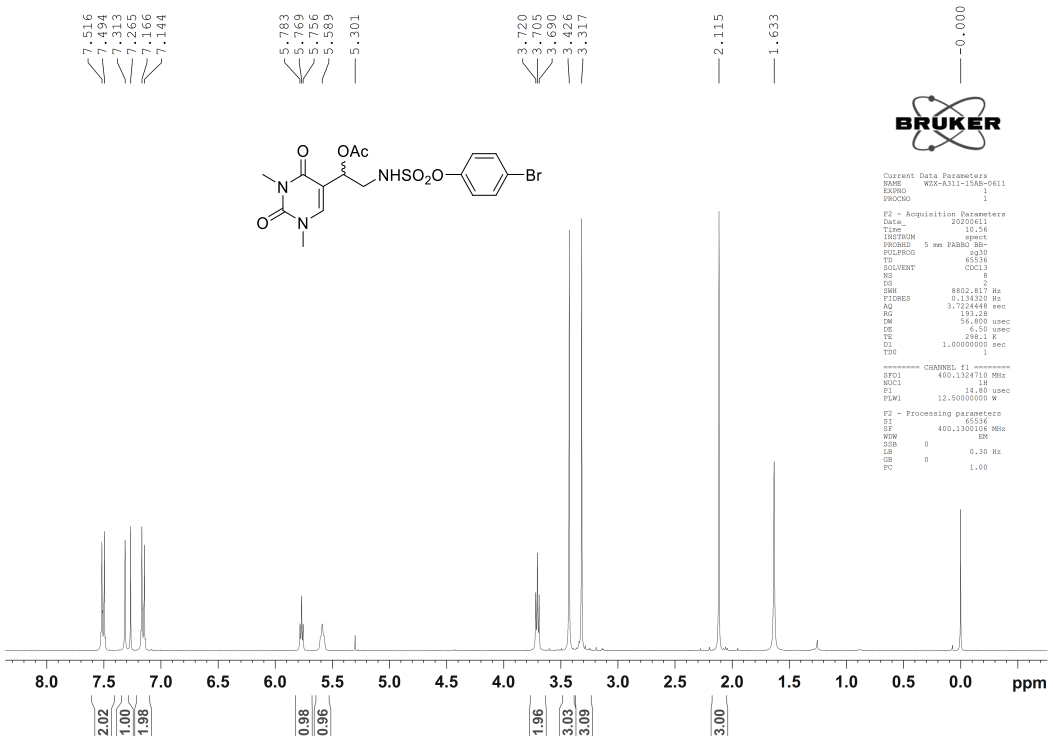
^{1}H NMR spectrum of **15aa** (400 MHz, $CDCl_3$)



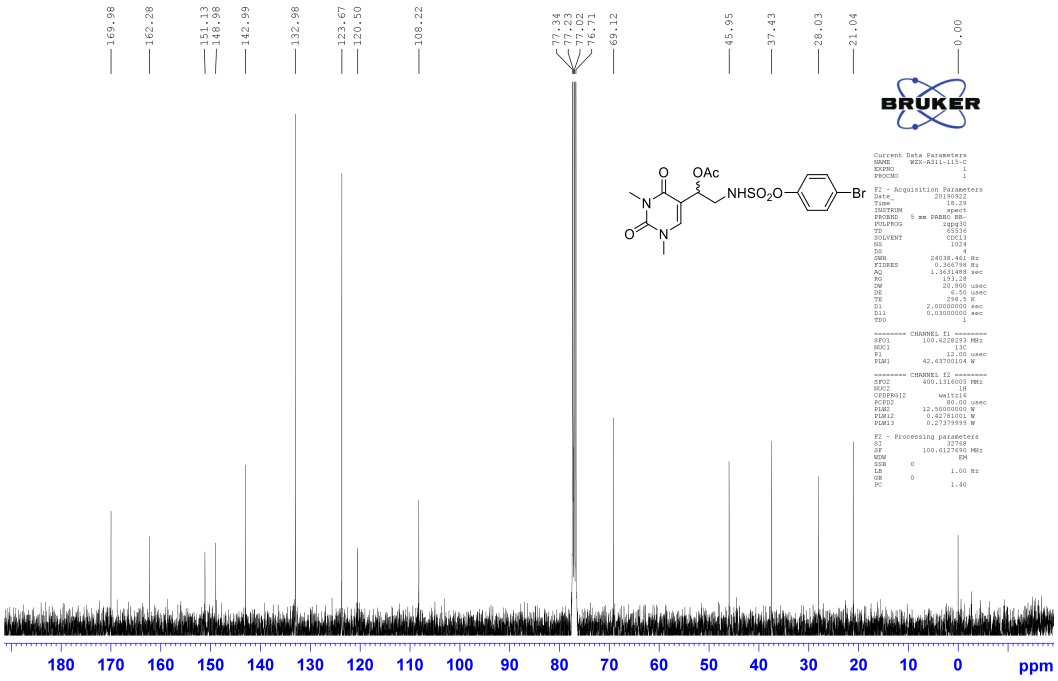
^{13}C NMR spectrum of **15aa** (100 MHz, $CDCl_3$)



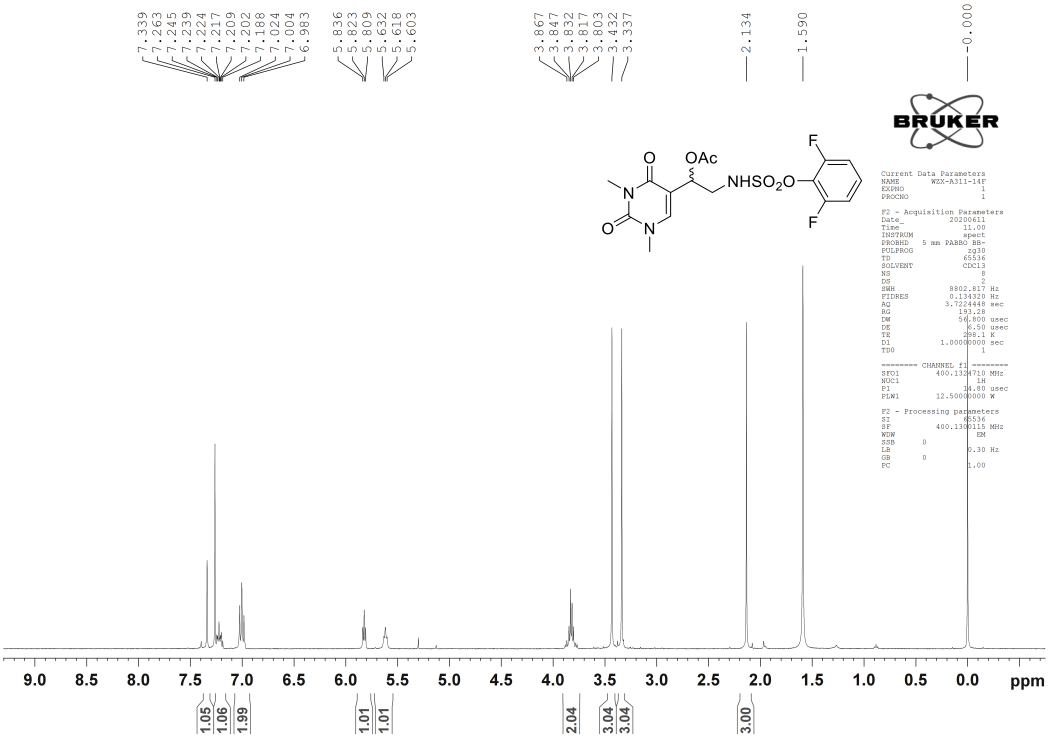
H NMR spectrum of **15ab** (400 MHz, $CDCl_3$)



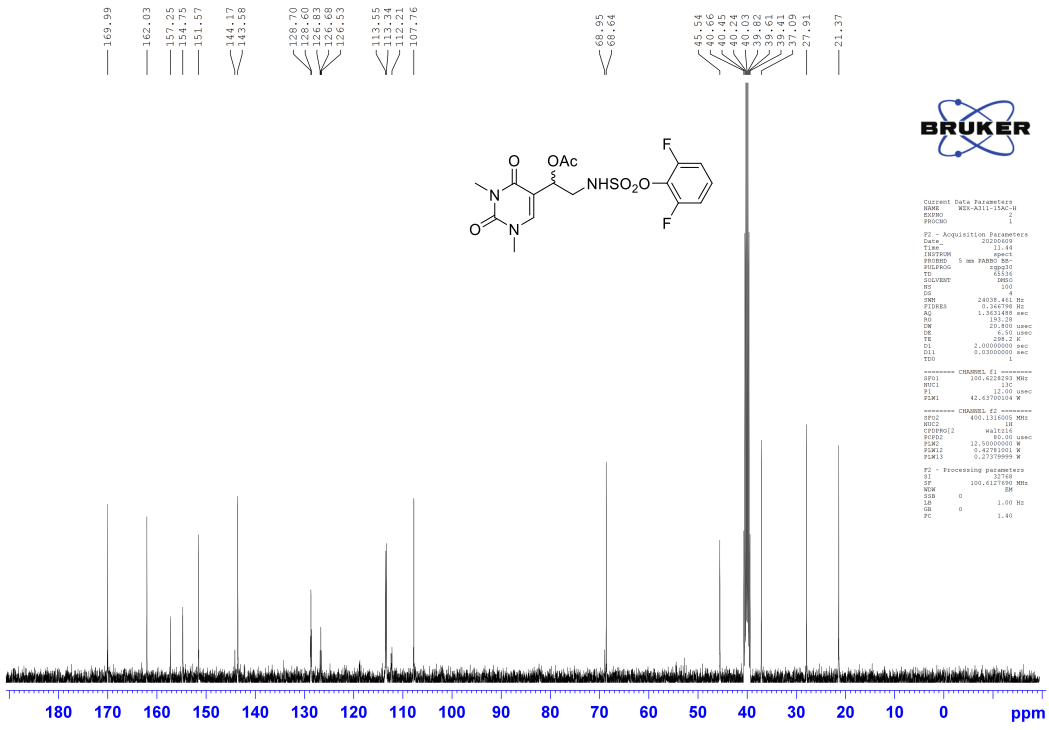
^{13}C NMR spectrum of **15ab** (100 MHz, $CDCl_3$)



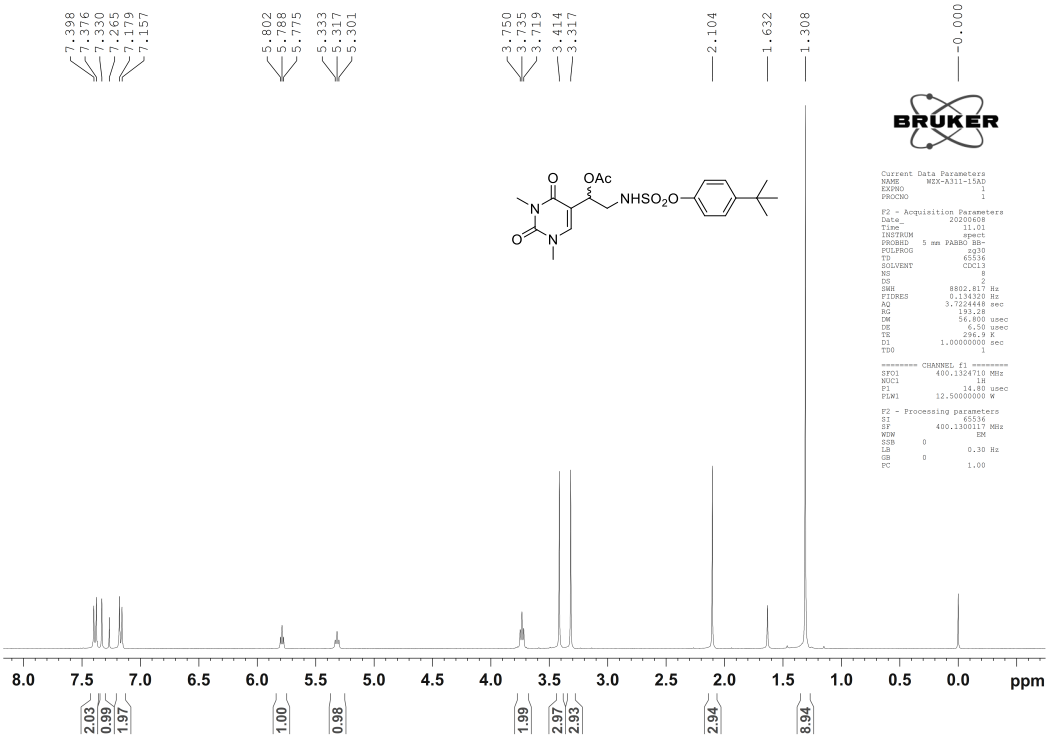
^{1}H NMR spectrum of **15ac** (400 MHz, $CDCl_3$)



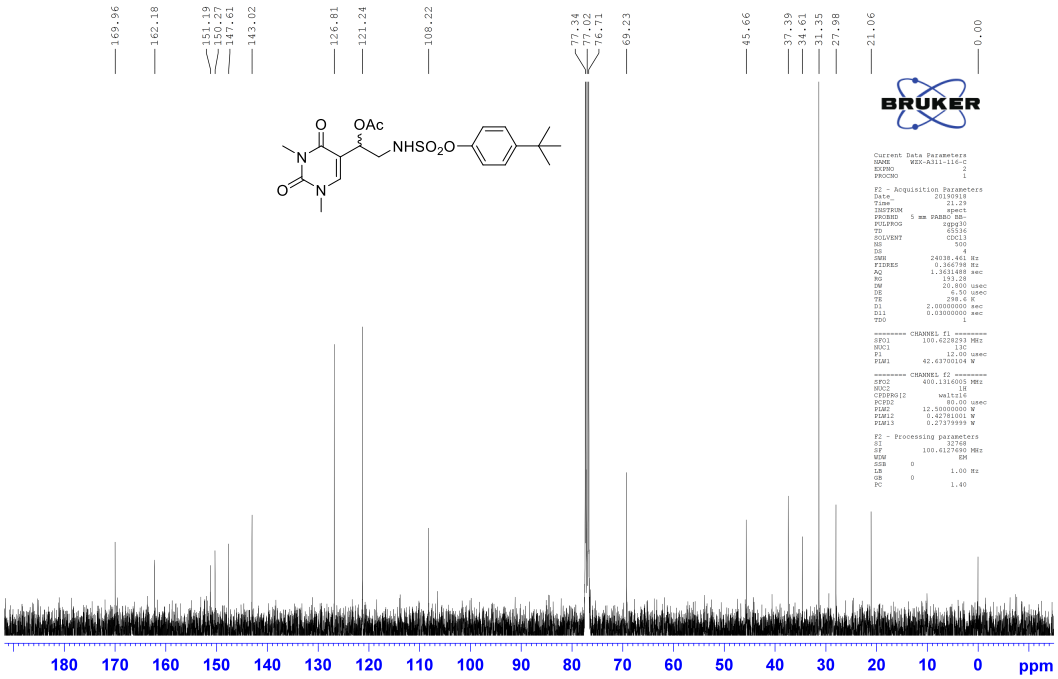
^{13}C NMR spectrum of **15ac** (100 MHz, DMSO-d_6)



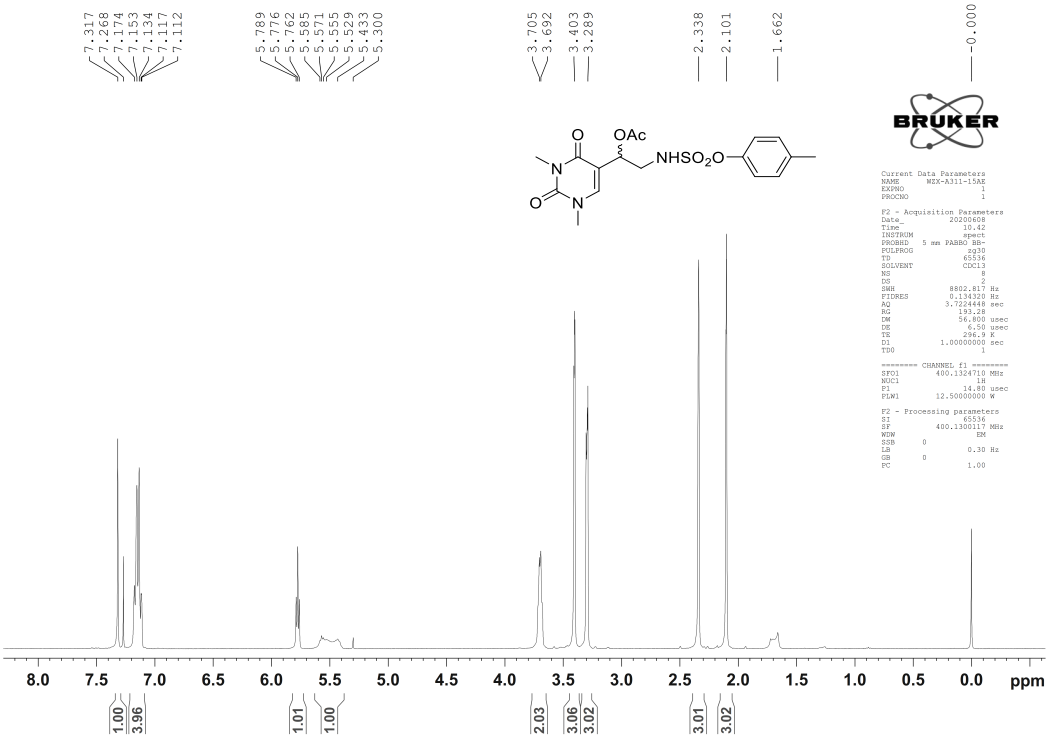
^{1}H NMR spectrum of **15ad** (400 MHz, $CDCl_3$)



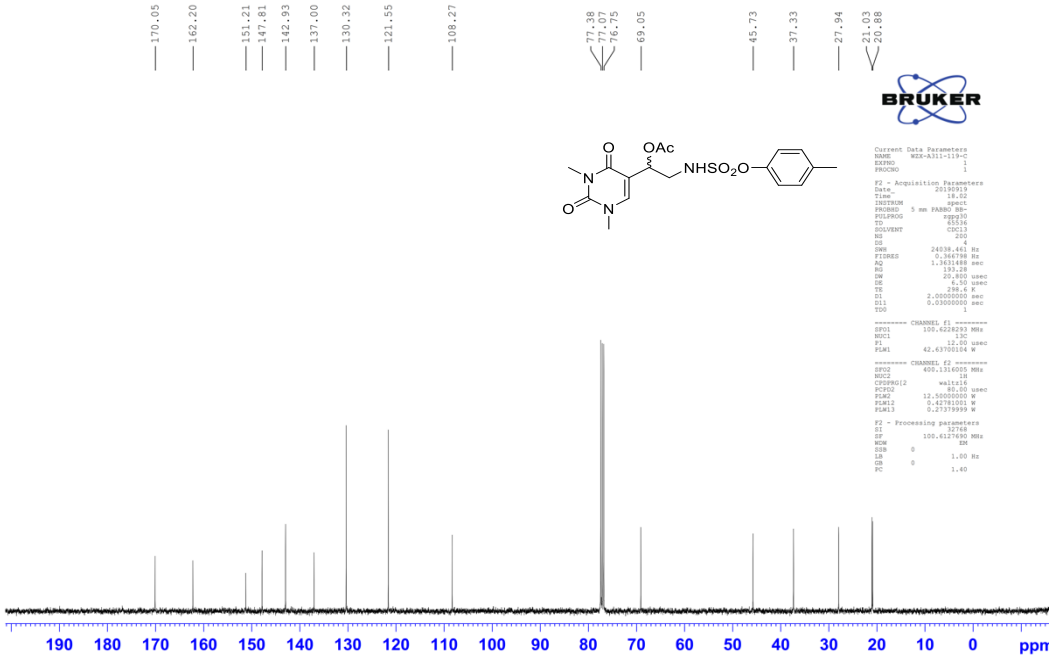
^{13}C NMR spectrum of **15ad** (100 MHz, $CDCl_3$)



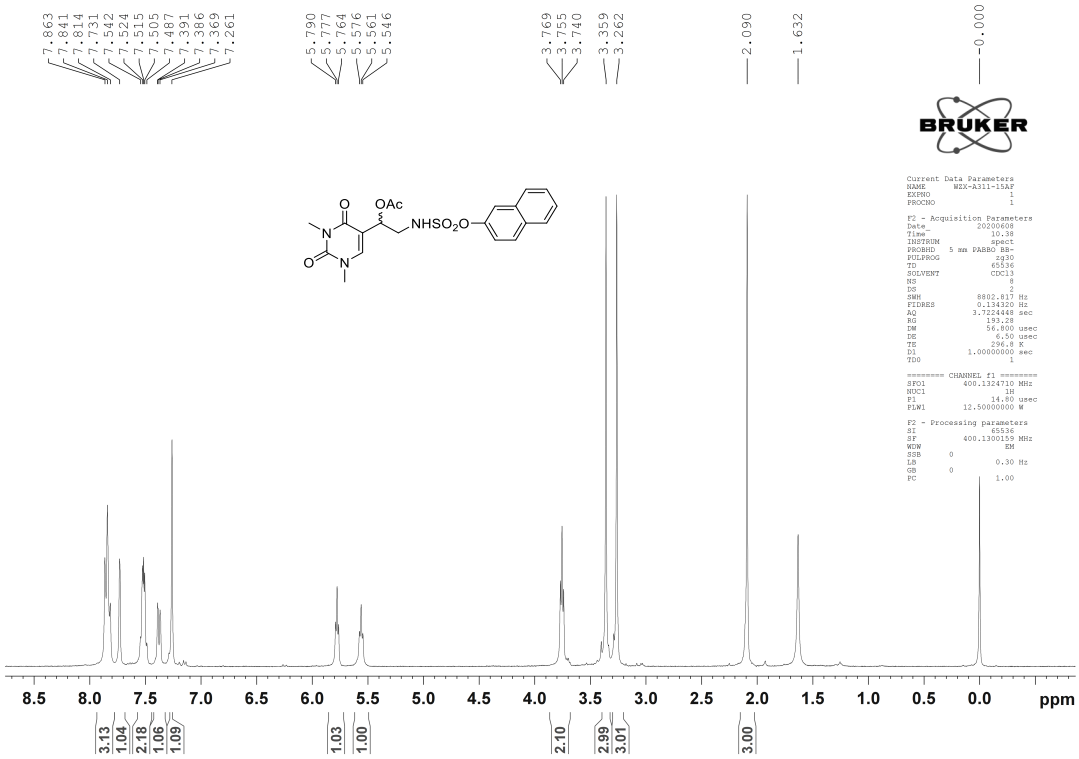
^{1}H NMR spectrum of **15ae** (400 MHz, $CDCl_3$)



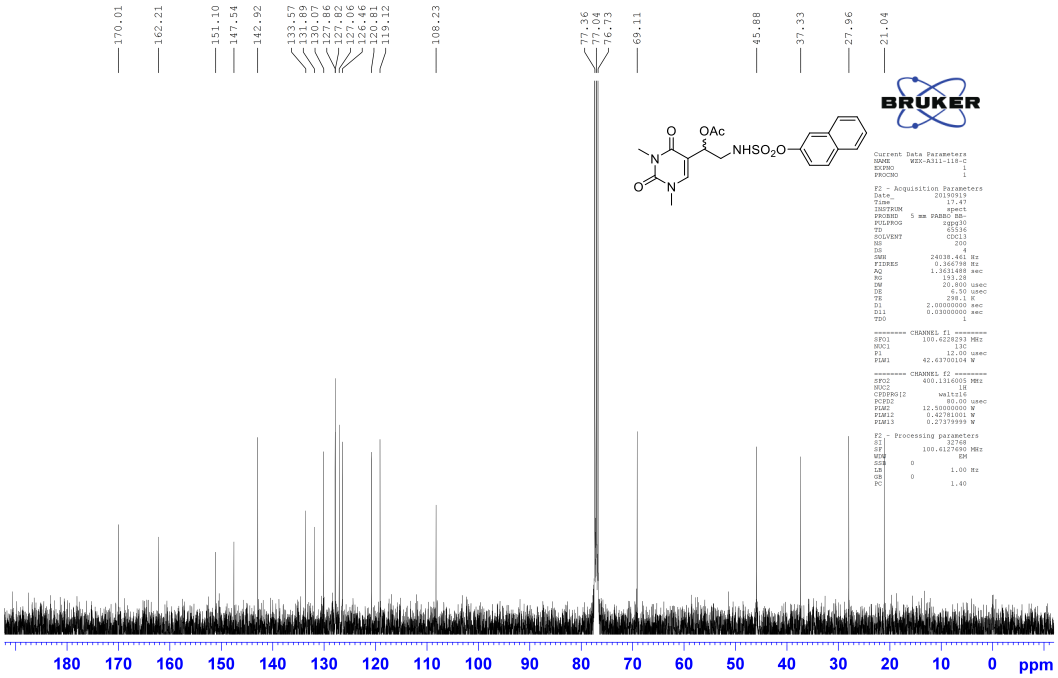
^{13}C NMR spectrum of **15ae** (100 MHz, $CDCl_3$)



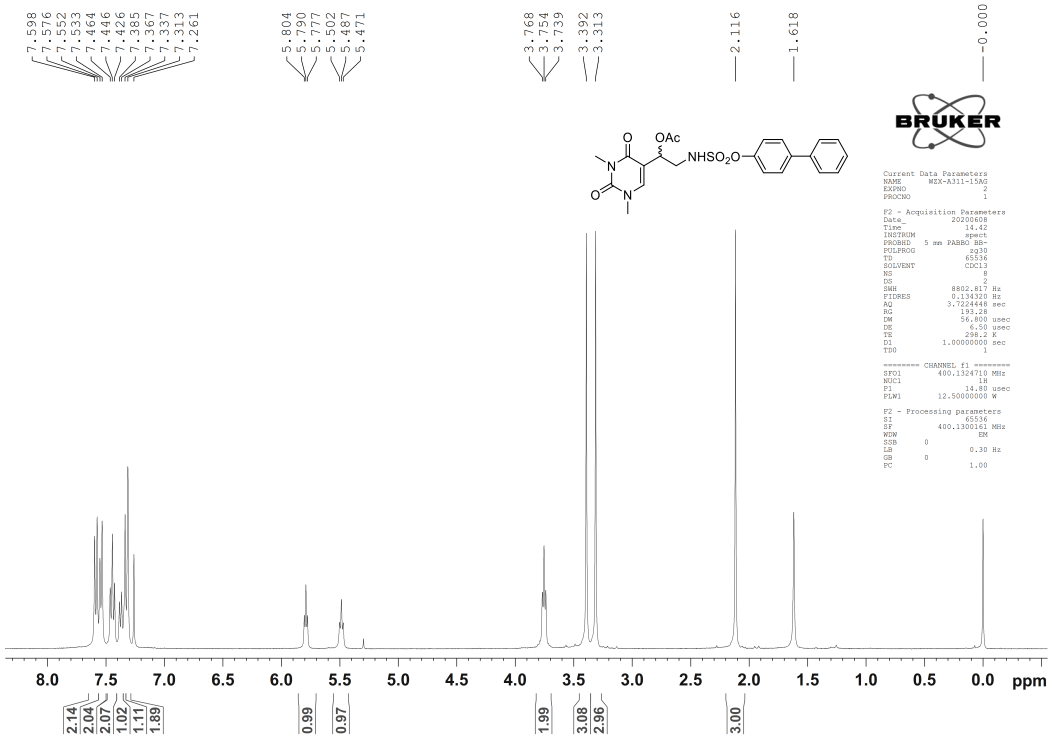
^{1}H NMR spectrum of **15af** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **15af** (100 MHz, $CDCl_3$)

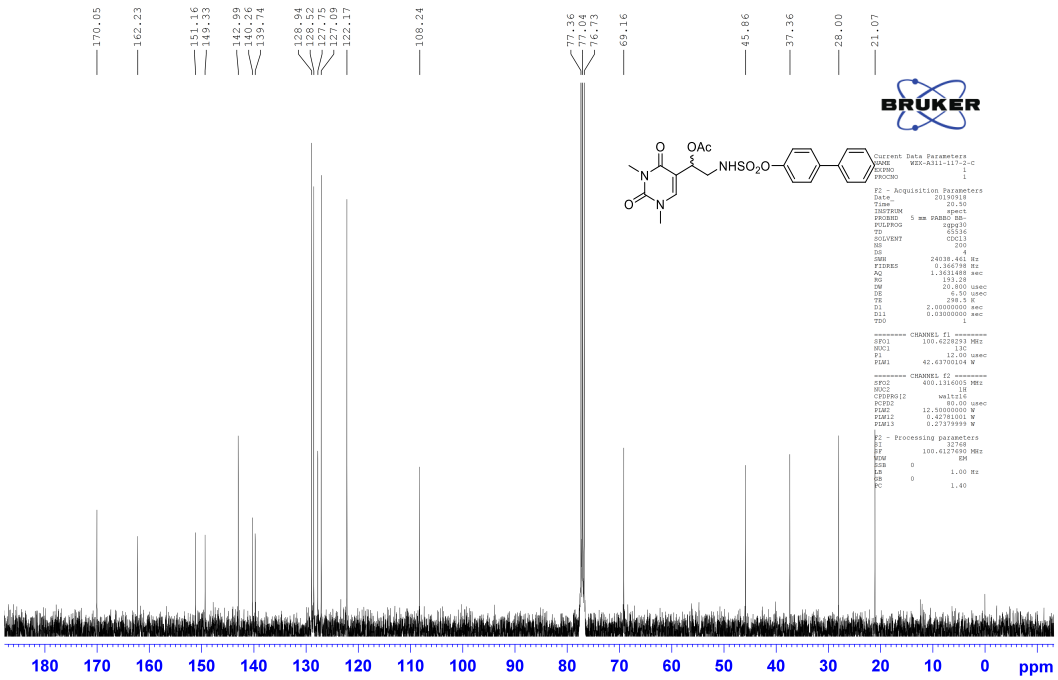


^{1}H NMR spectrum of **15ag** (400 MHz, $CDCl_3$)

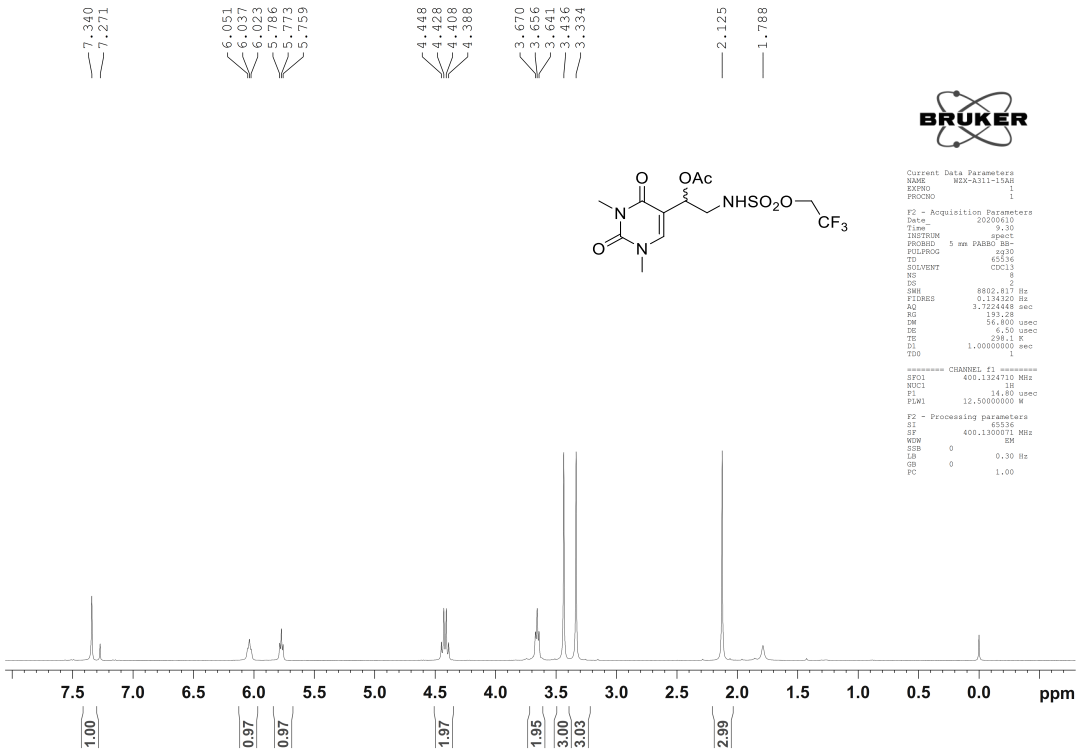


13

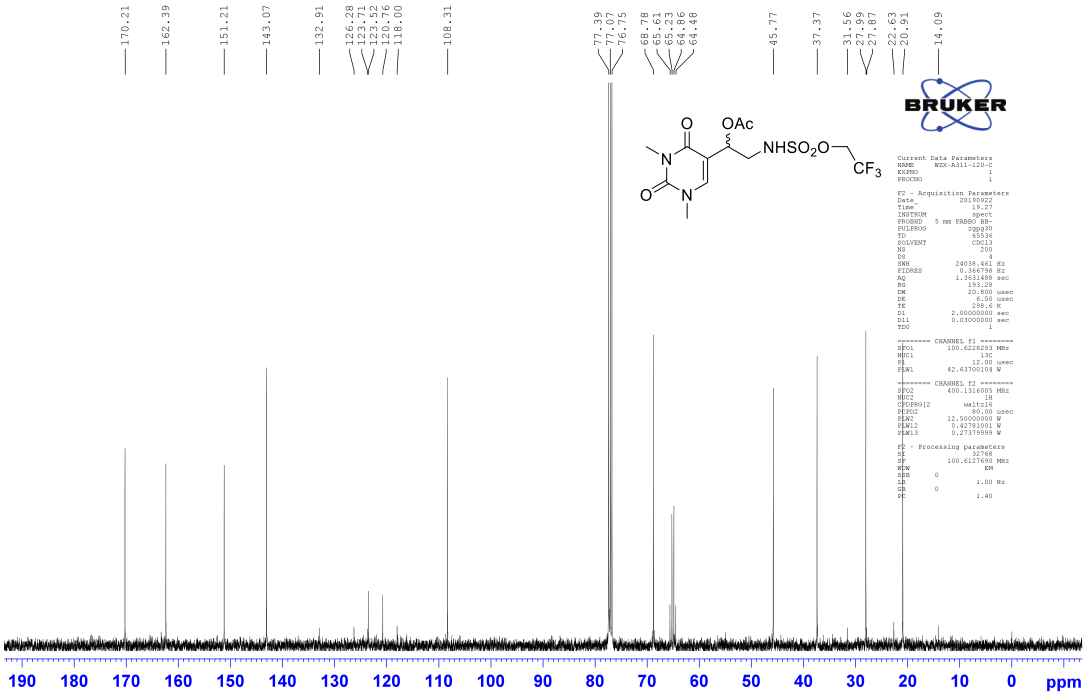
C NMR spectrum of **15ag** (100 MHz, $CDCl_3$)



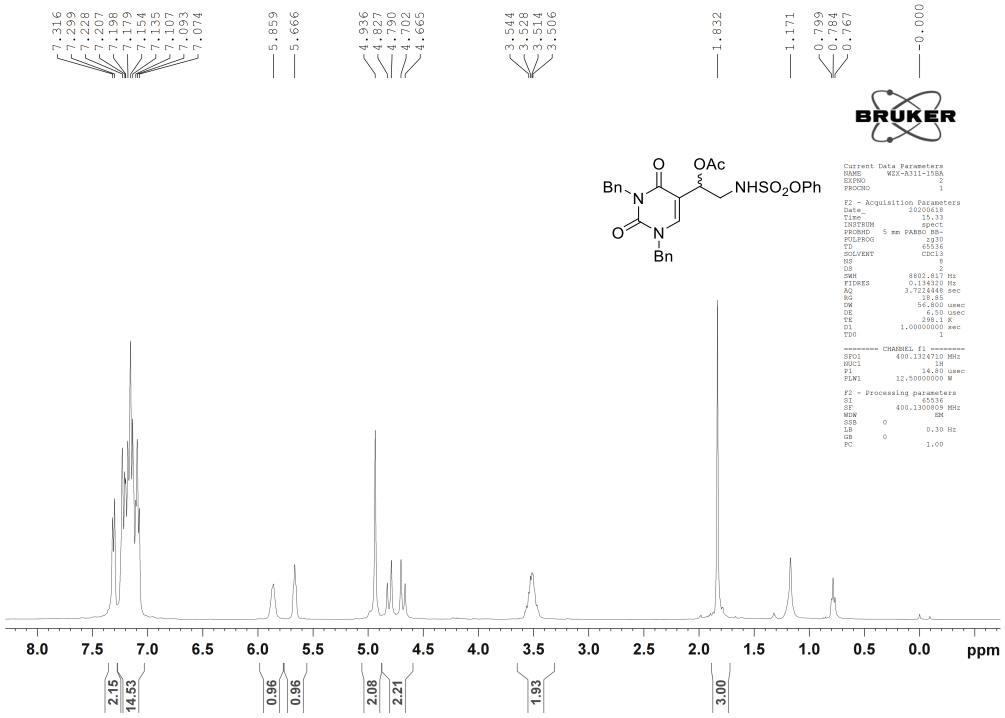
^{1}H NMR spectrum of **15ah** (400 MHz, $CDCl_3$)



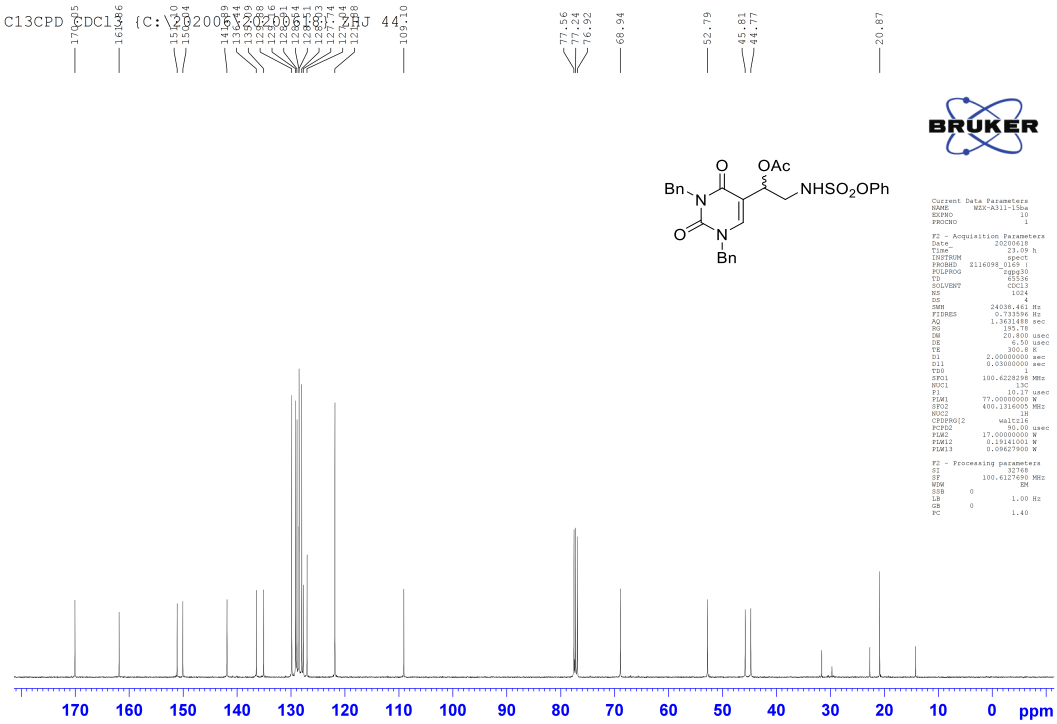
^{13}C NMR spectrum of **15ah** (100 MHz, $CDCl_3$)



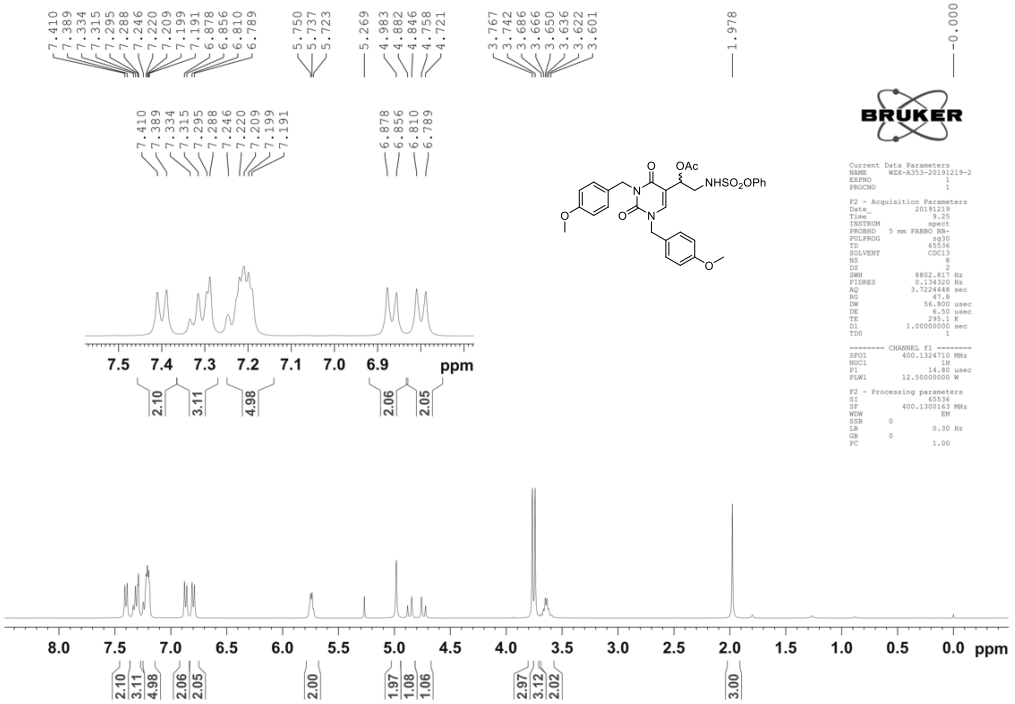
^{1}H NMR spectrum of **15ba** (400 MHz, $CDCl_3$)



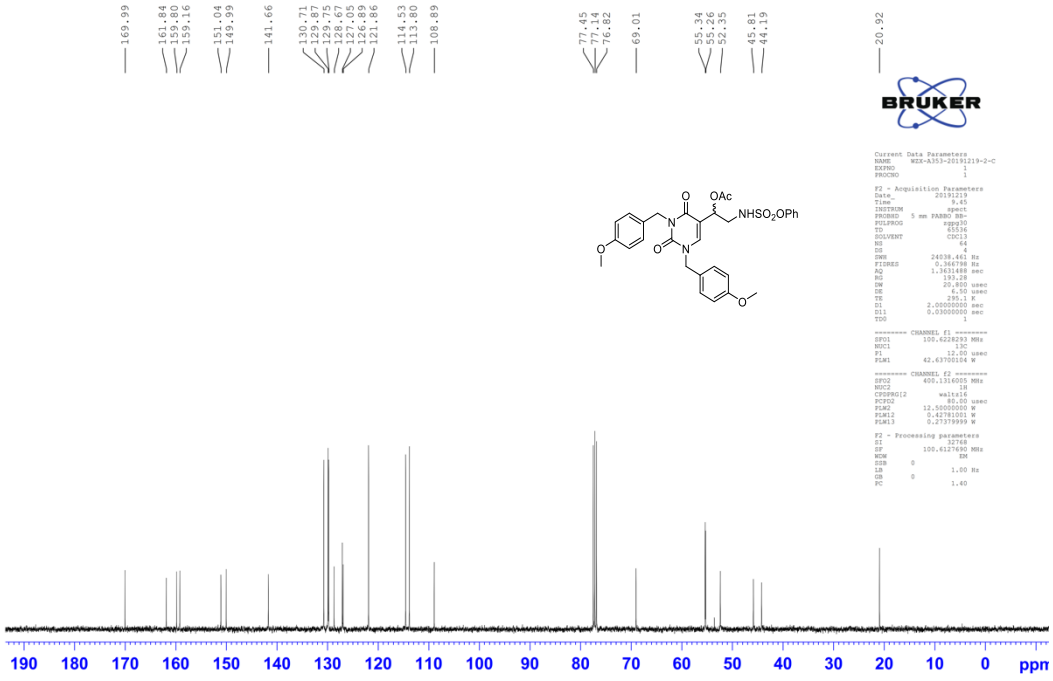
^{13}C NMR spectrum of **15ba** (100 MHz, $CDCl_3$)



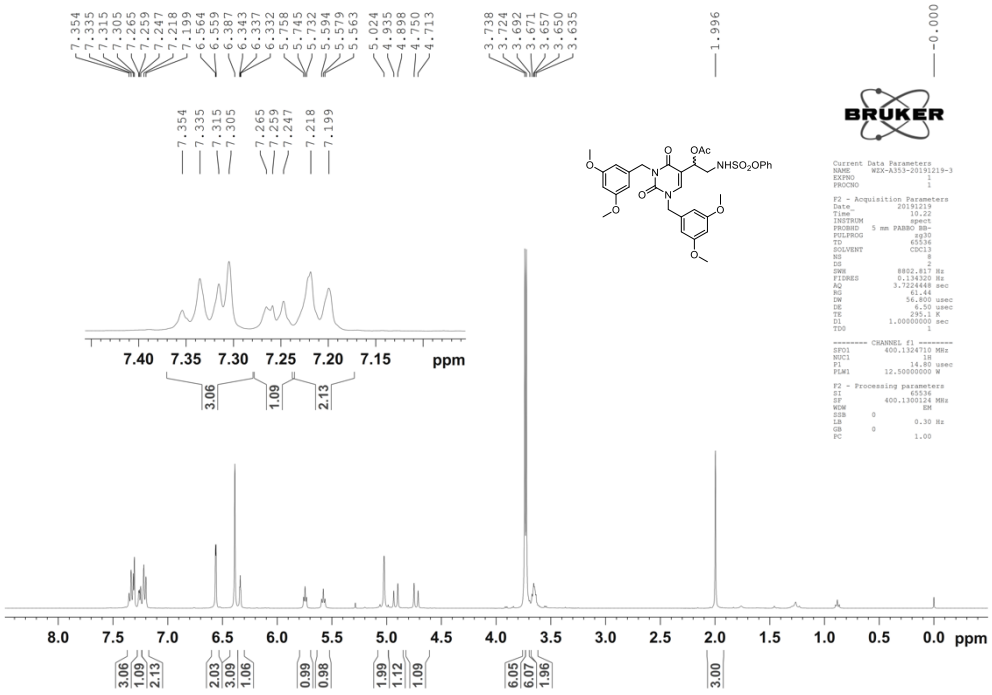
^{1}H NMR spectrum of **15ca** (400 MHz, $CDCl_3$)



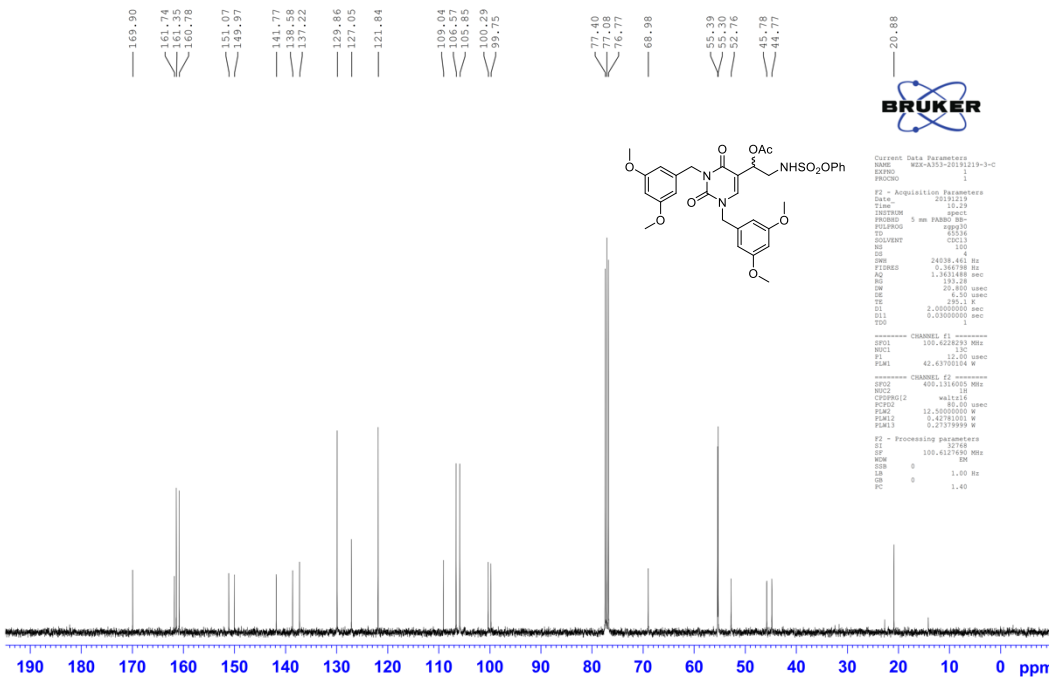
^{13}C NMR spectrum of **15ca** (100 MHz, $CDCl_3$)



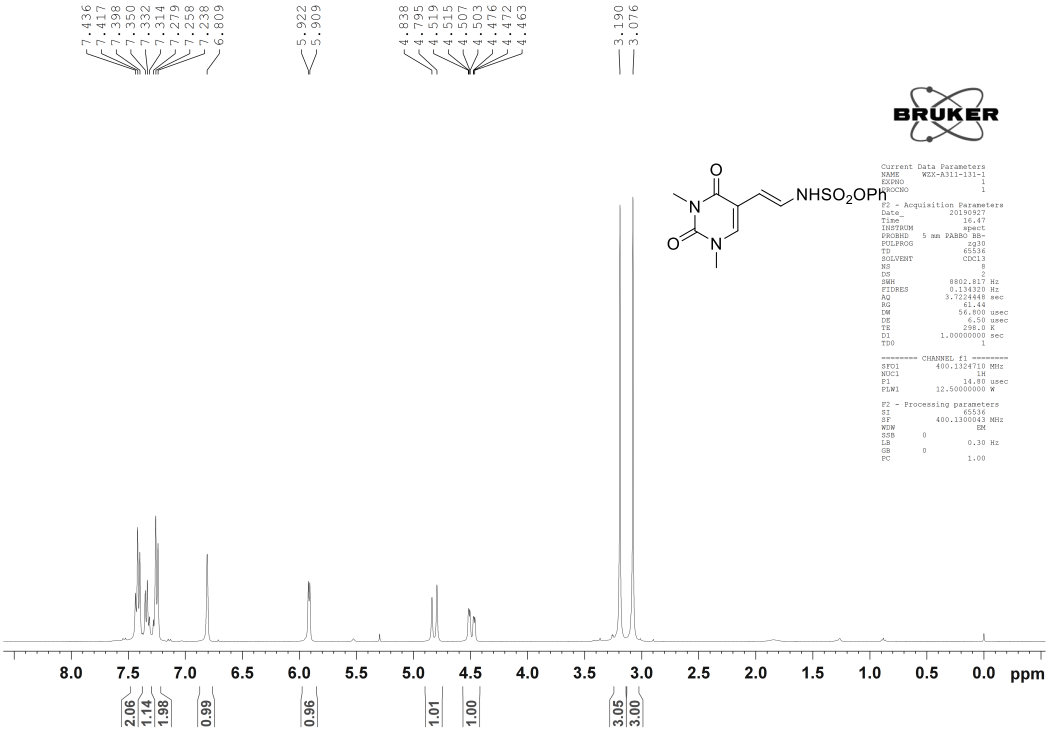
^{1}H NMR spectrum of **15da** (400 MHz, $CDCl_3$)



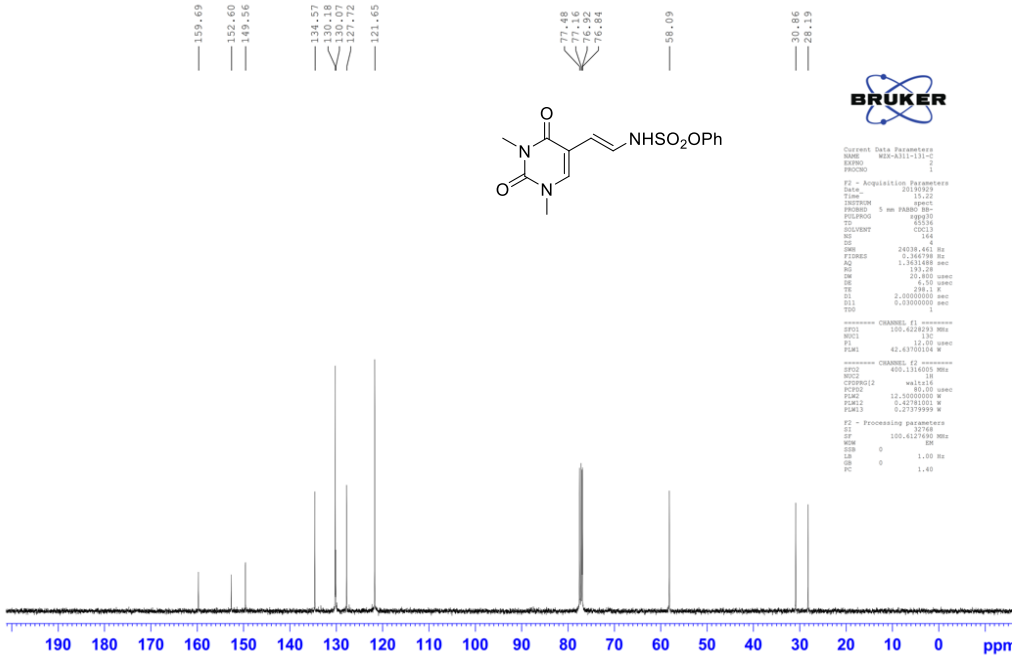
^{13}C NMR spectrum of **15da** (100 MHz, $CDCl_3$)



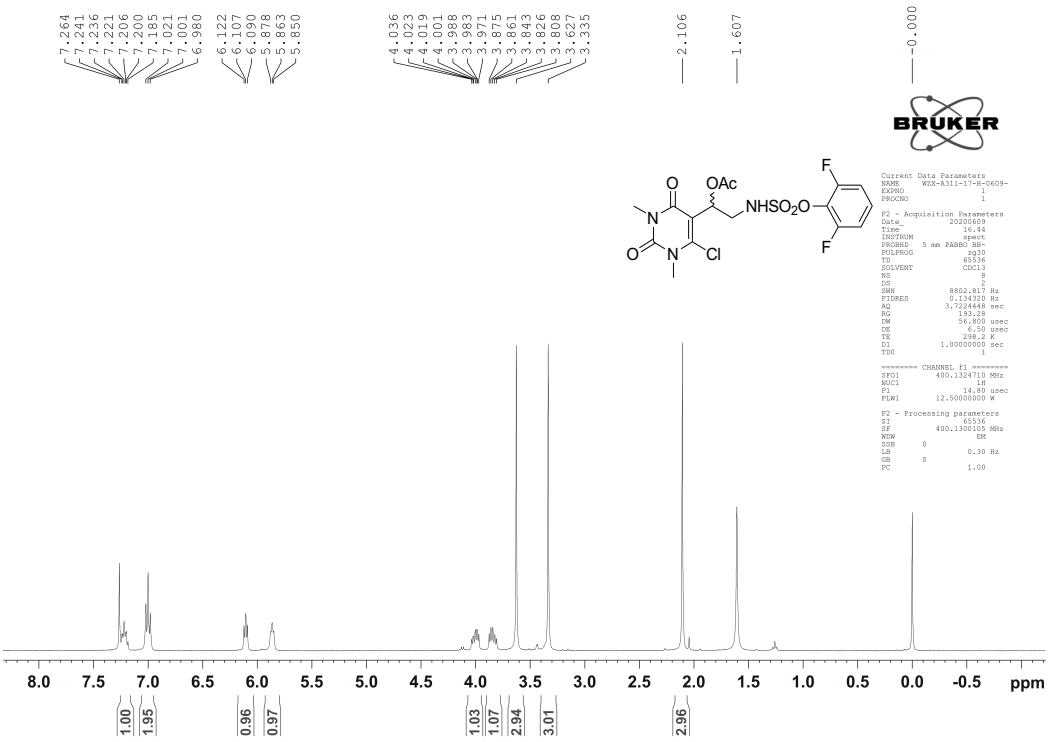
^{1}H NMR spectrum of **16** (400 MHz, $CDCl_3$)



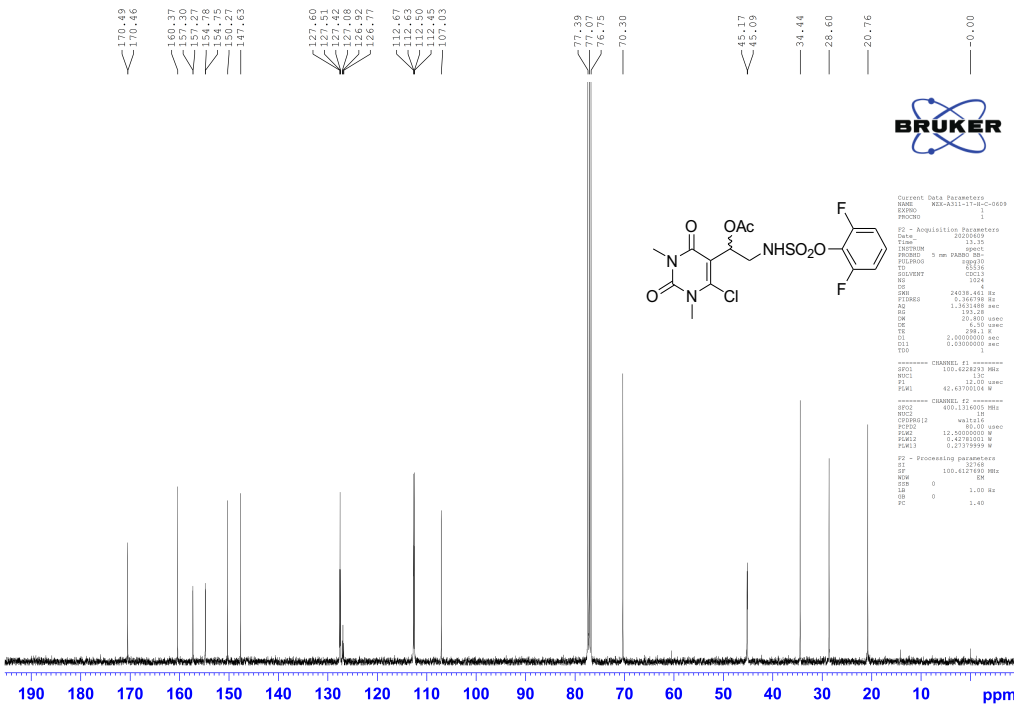
^{13}C NMR spectrum of **16** (100 MHz, $CDCl_3$)



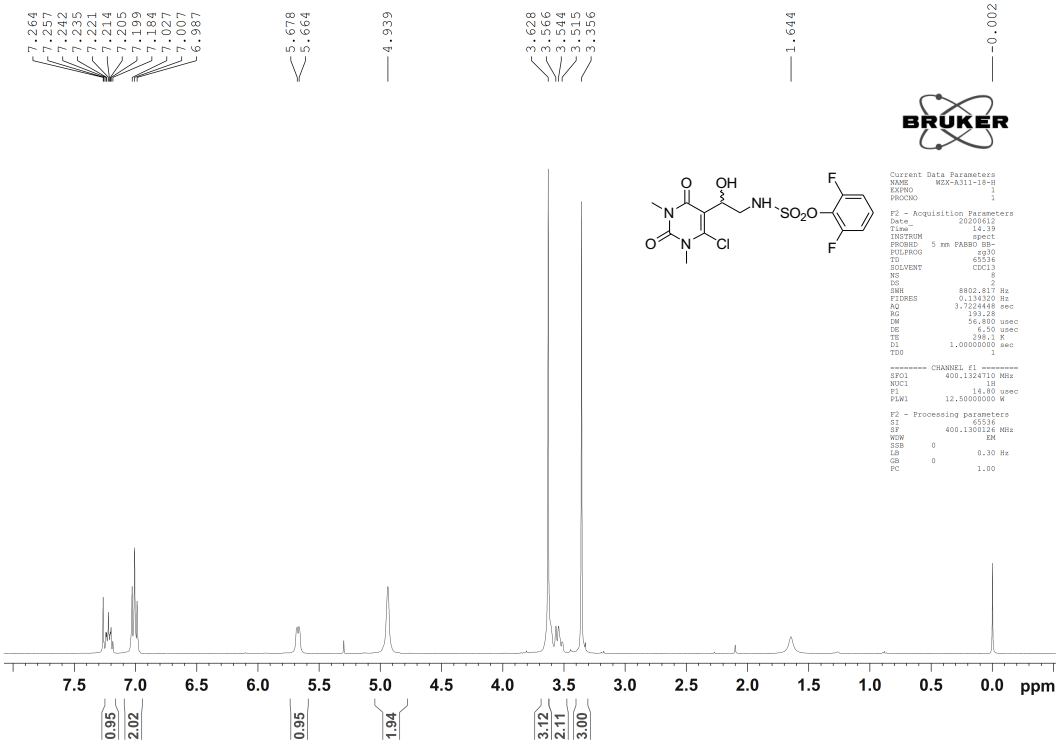
^{1}H NMR spectrum of **17** (400 MHz, $CDCl_3$)



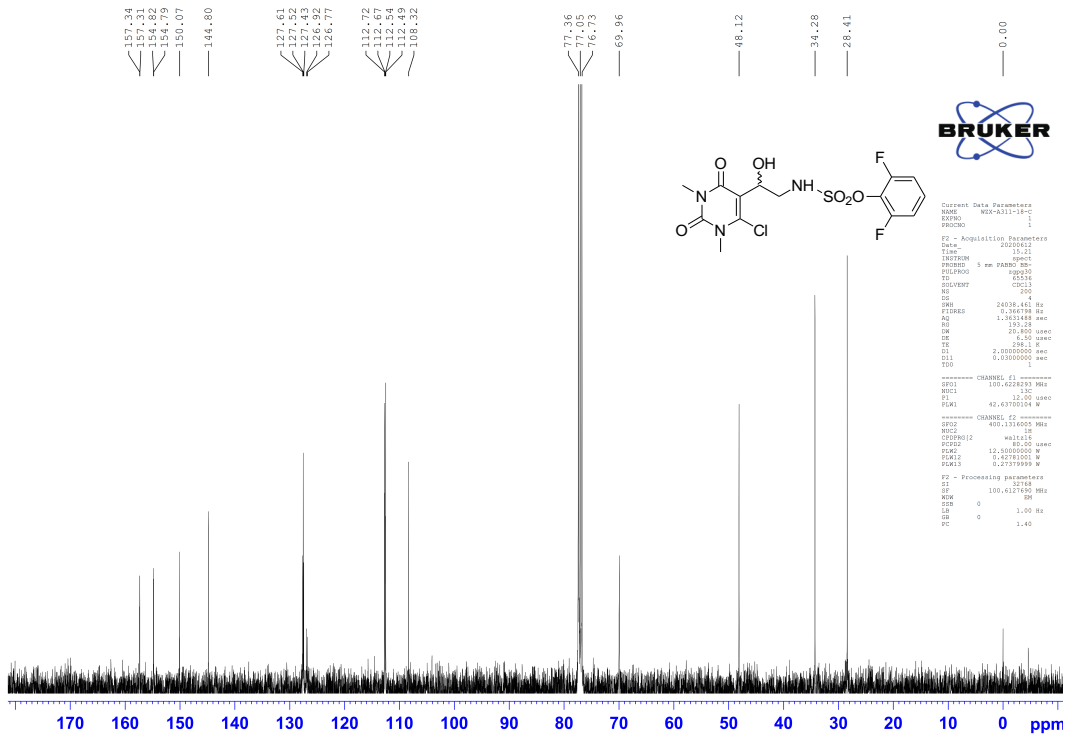
^{13}C NMR spectrum of **17** (100 MHz, $CDCl_3$



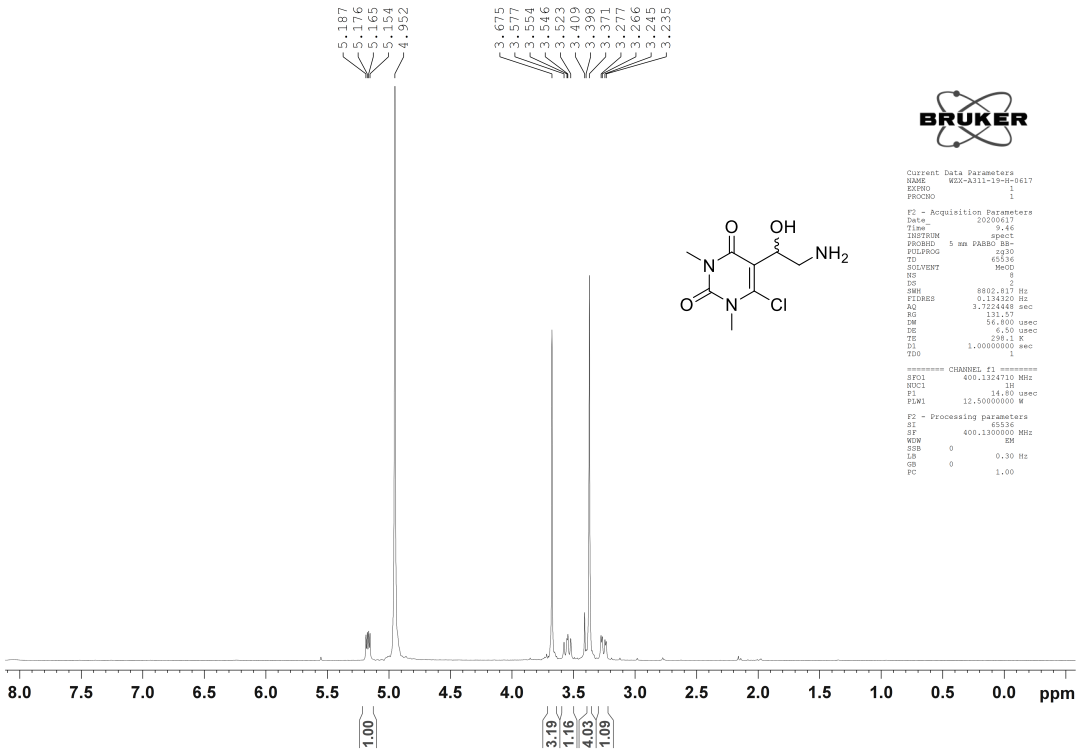
^{1}H NMR spectrum of **18** (400 MHz, $CDCl_3$)



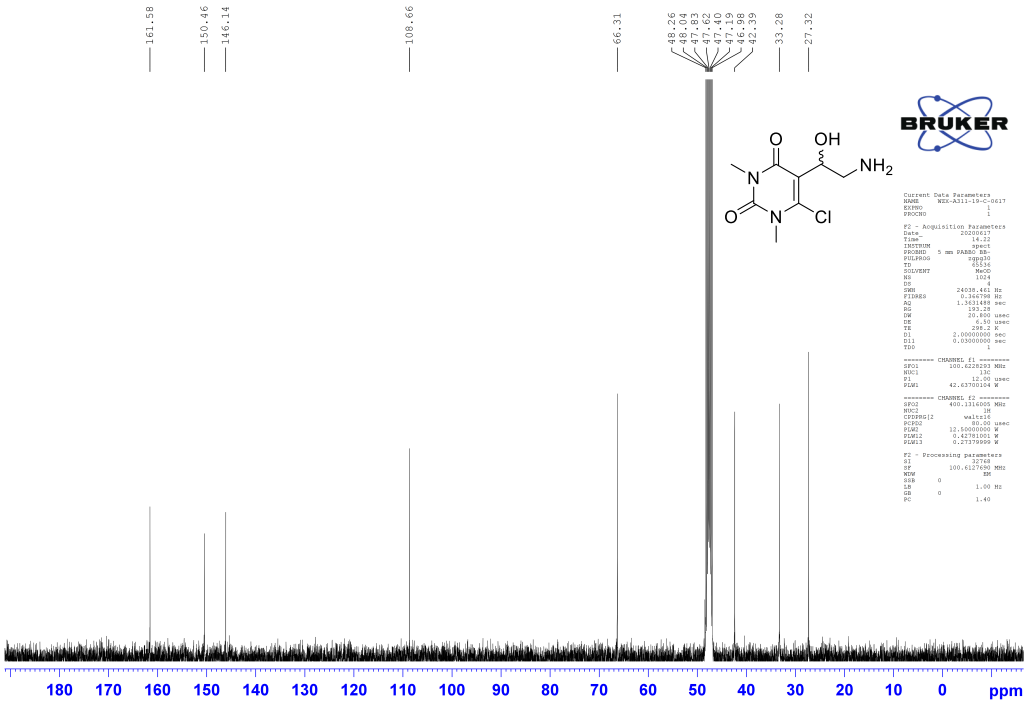
^{13}C NMR spectrum of **18** (100 MHz, $CDCl_3$)



1H NMR spectrum of **19** (400 MHz, CD_3OD-d_4)



^{13}C NMR spectrum of **19** (100 MHz, CD_3OD -d_4)



HRMS spectrum of **12aa**

Formula Predictor Report - JZX-A195-83.lcd Page 1 of 1

Data File: D:\DATA\郁鹏\王栋\20171031\JZX-A195-83.lcd

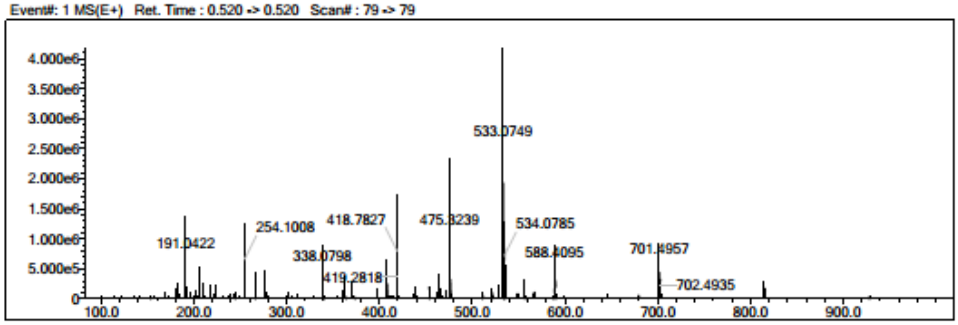
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	11	15	18O	2	0	0	S	2	0	1	I	3	0	0	H
B	3	0	0	F	1	0	0	Cl	1	0	0					Na
C	4	10	14	Na	1	0	0	Ti	2	0	0					K
N	3	0	3	Si	4	0	0	Fe	2	0	0					NH4
O	2	0	5	P	3	0	0	Br	1	0	0					Br

Error Margin (mDa): 100.0
HC Ratio: 0.0 - 3.0
Max Isotopes: all
MSn Iso RI (%): 75.00

DBE Range: 0.0 - 50.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

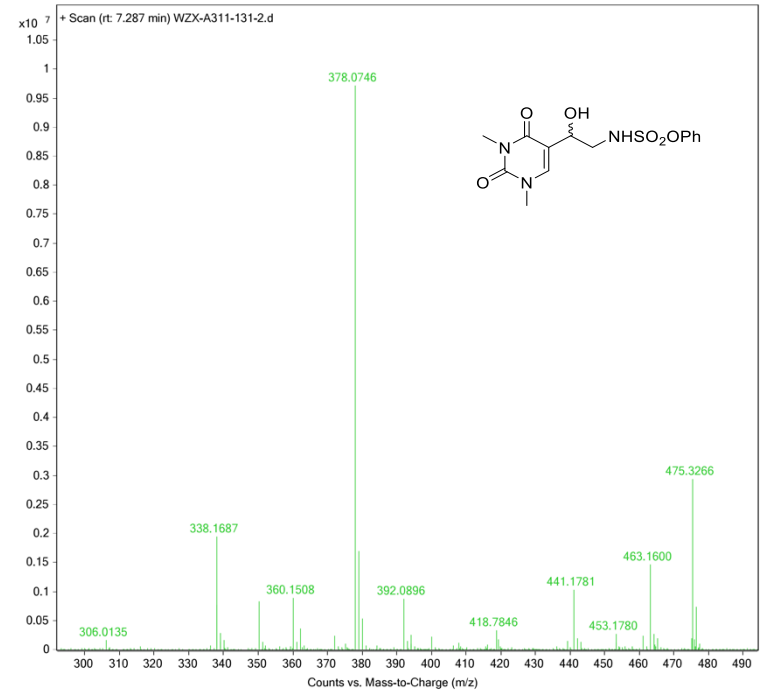
Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 50

Event#: 1 MS(E+) Ret. Time : 0.520 -> 0.520 Scan# : 79 -> 79



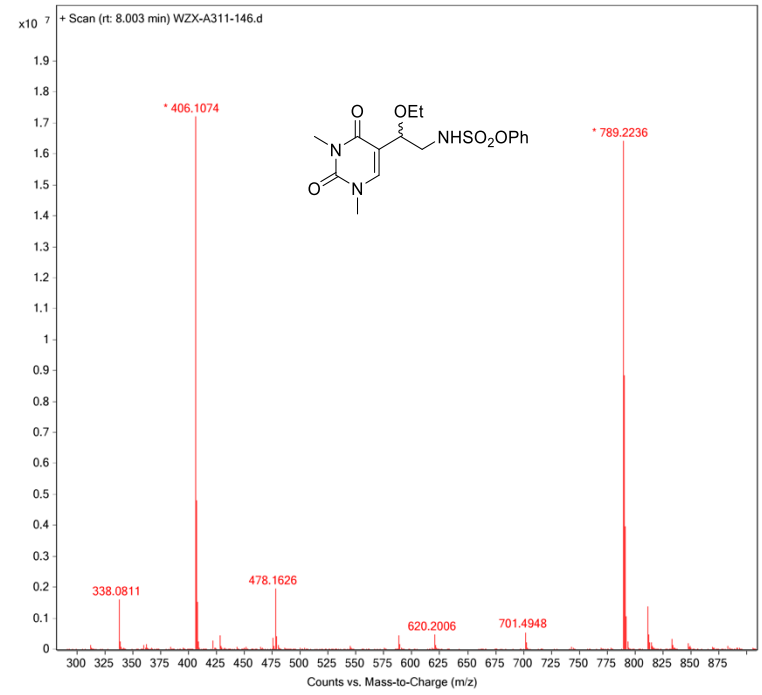
HRMS spectrum of **13aa**

Sample Name	WZX-A311-131-2	**Position**	P1-B1	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-131-2.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/25/2019 10:58:37 PM (UTC+08:00)



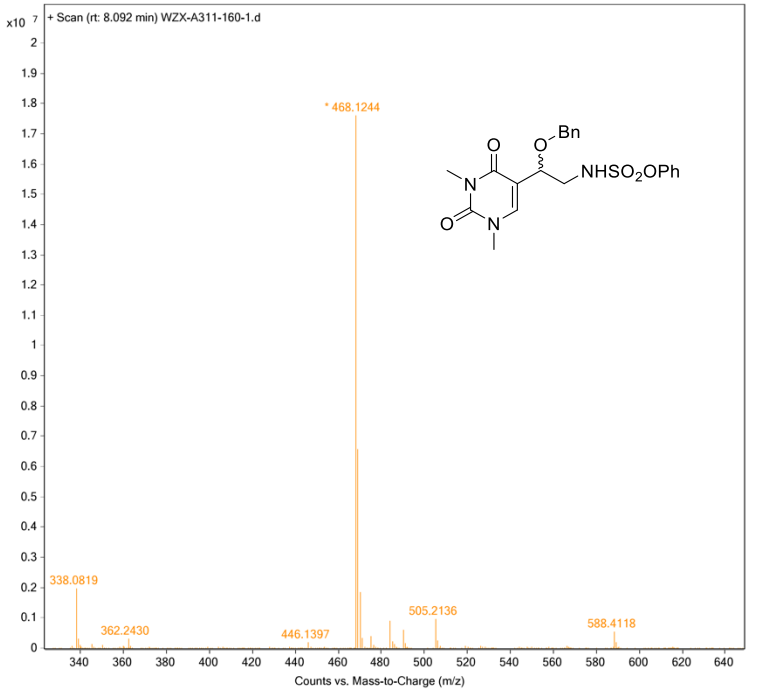
HRMS spectrum of **14a**

Sample Name	WZX-A311-146	**Position**	P1-A5	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-146.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/25/2019 9:08:18 PM (UTC+08:00)



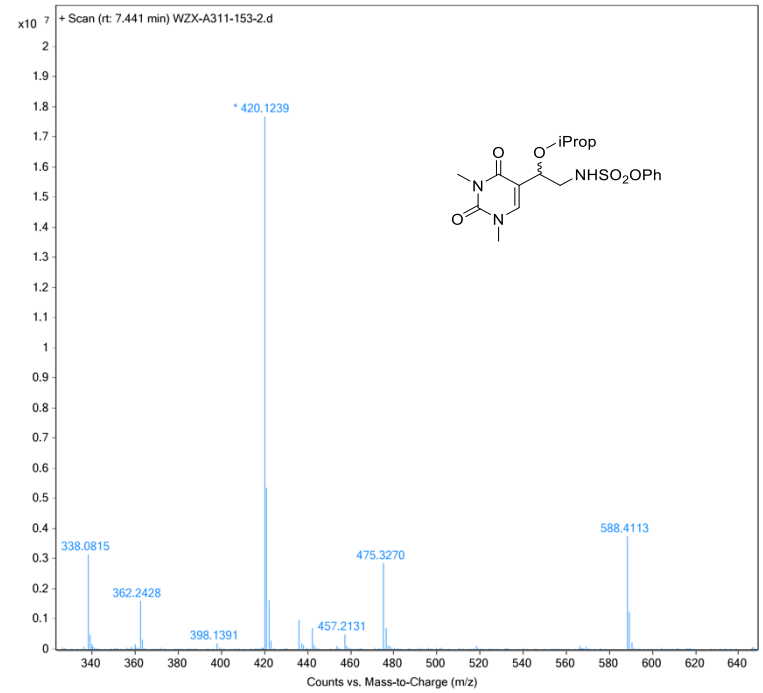
HRMS spectrum of **14b**

Sample Name	WZX-A311-160-1	**Position**	P1-C2	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-160-1.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 2:36:11 AM (UTC+08:00)



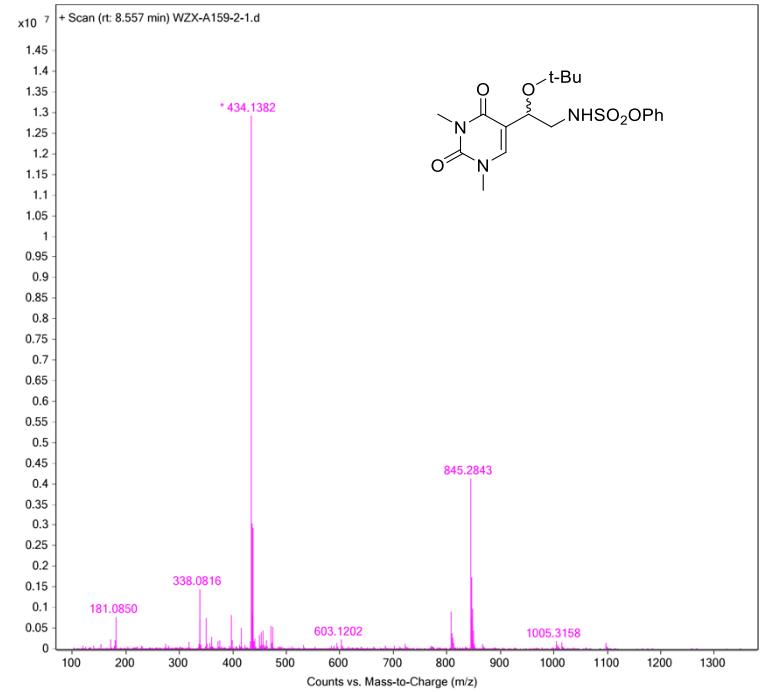
HRMS spectrum of **14c**

Sample Name	WZX-A311-153-2	**Position**	P1-C1	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-153-2.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 2:20:25 AM (UTC+08:00)



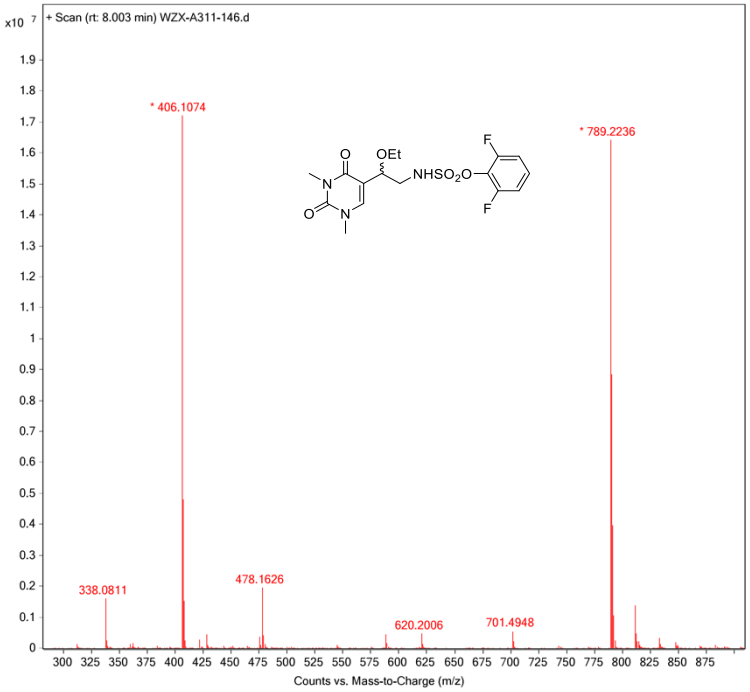
HRMS spectrum of **14d**

Sample Name	WZX-A159-2-1	**Position**	P1-B4	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A159-2-1.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/25/2019 11:48:31 PM (UTC+08:00)



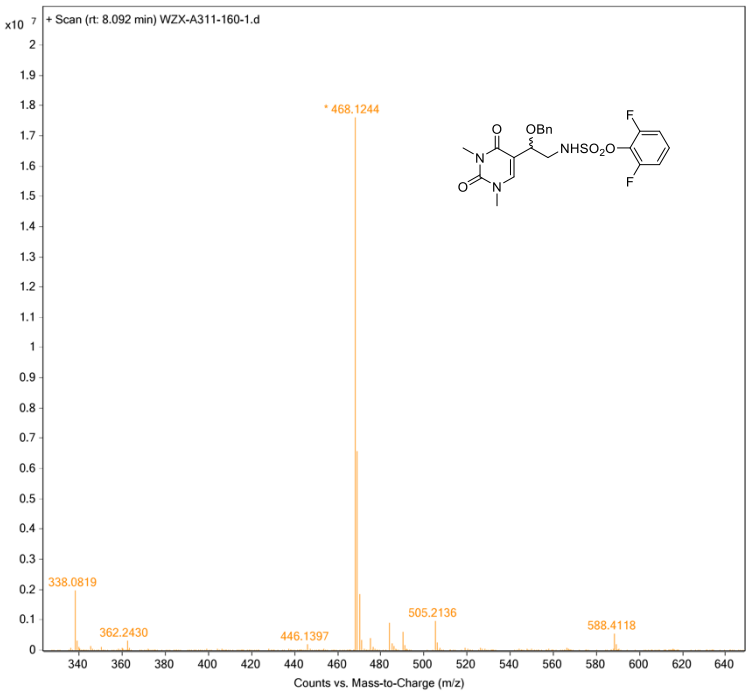
HRMS spectrum of **14e**

Sample Name	WZX-A311-146	**Position**	P1-A5	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-146.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/25/2019 9:08:18 PM (UTC+08:00)



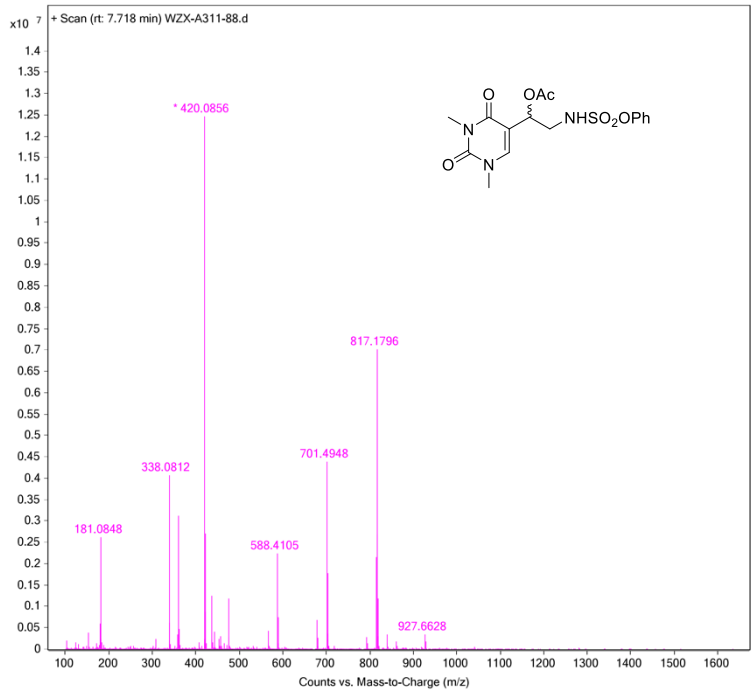
HRMS spectrum of **14f**

Sample Name	WZX-A311-160-1	**Position**	P1-C2	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-160-1.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 2:36:11 AM (UTC+08:00)



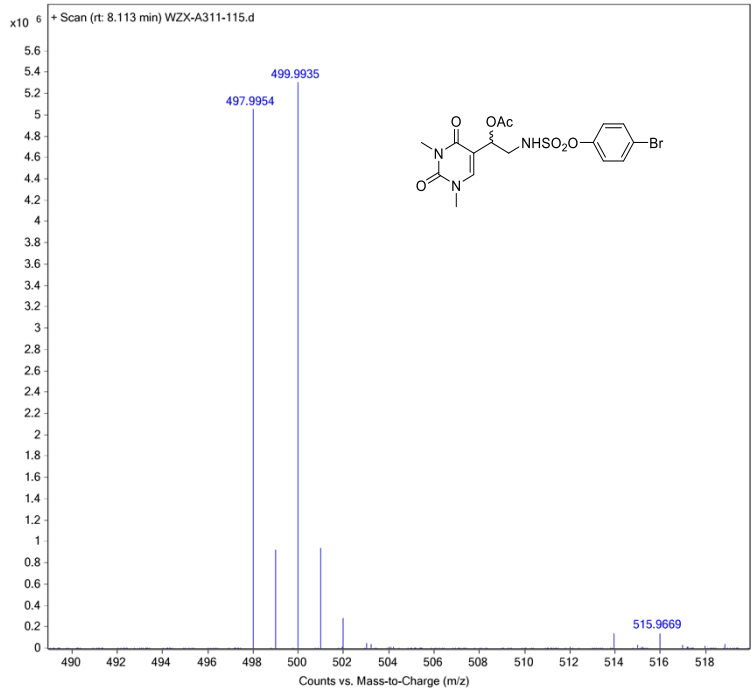
HRMS spectrum of **15aa**

Sample Name	WZX-A311-88-1	**Position**	P1-A3	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-88.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/25/2019 8:24:17 PM (UTC+08:00)



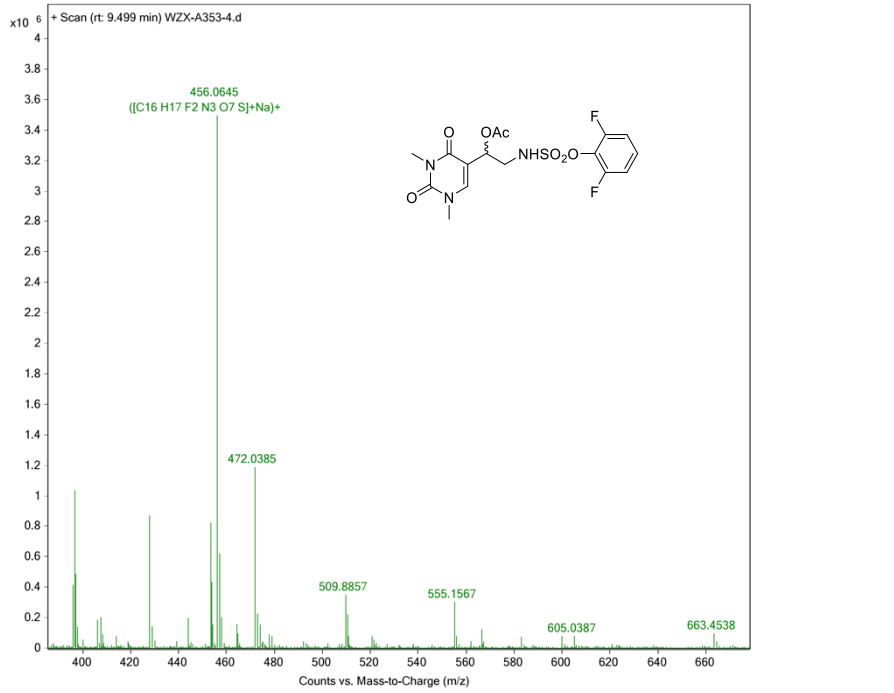
HRMS spectrum of **15ab**

Sample Name	WZX-A311-115	**Position**	P1-A7	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-115.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/25/2019 9:39:48 PM (UTC+08:00)



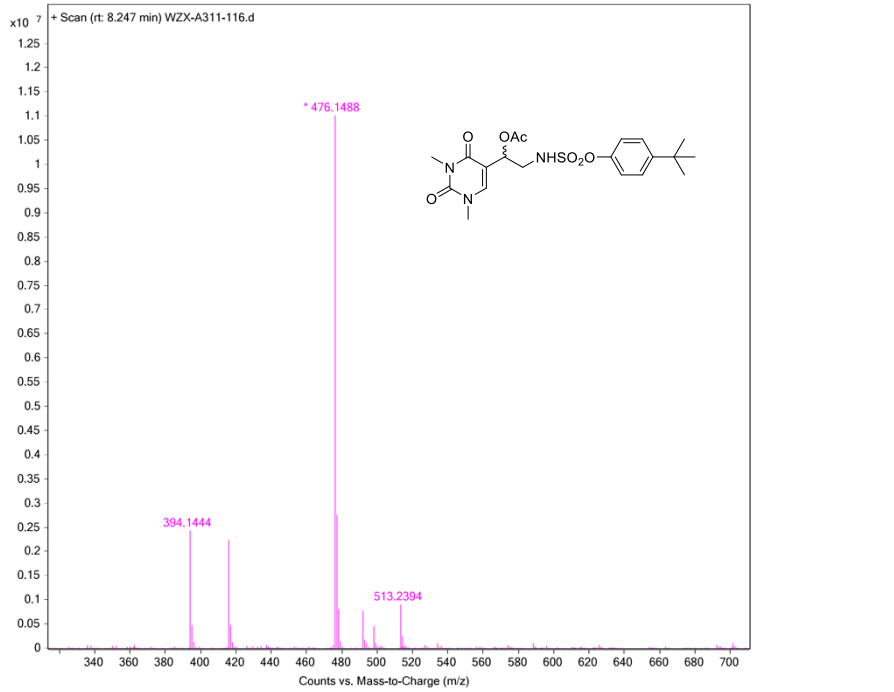
HRMS spectrum of **15ac**

Sample Name	WZX-A353-4	**Position**	P1-A1	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A353-4.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	12/22/2019 3:33:29 PM (UTC+08:00)



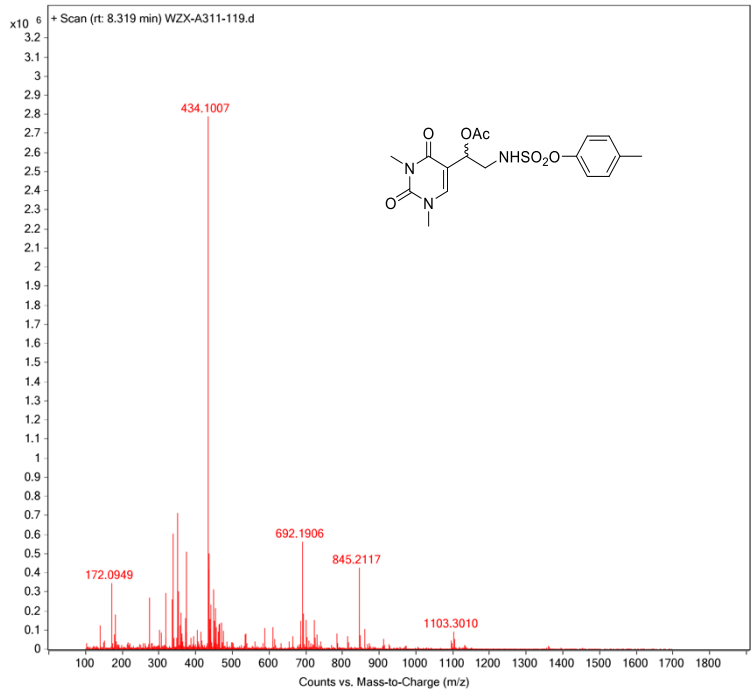
HRMS spectrum of **15ad**

Sample Name	WZX-A311-116	**Position**	P1-C3	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-116.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 2:51:56 AM (UTC+08:00)



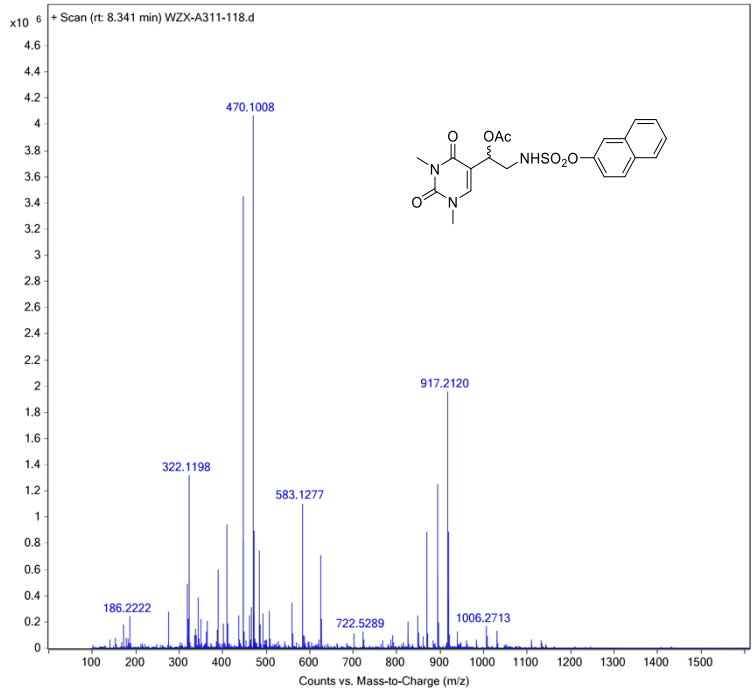
HRMS spectrum of **15ae**

Sample Name	WZX-A311-119	**Position**	P1-B6	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-119.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 12:20:03 AM (UTC+08:00)



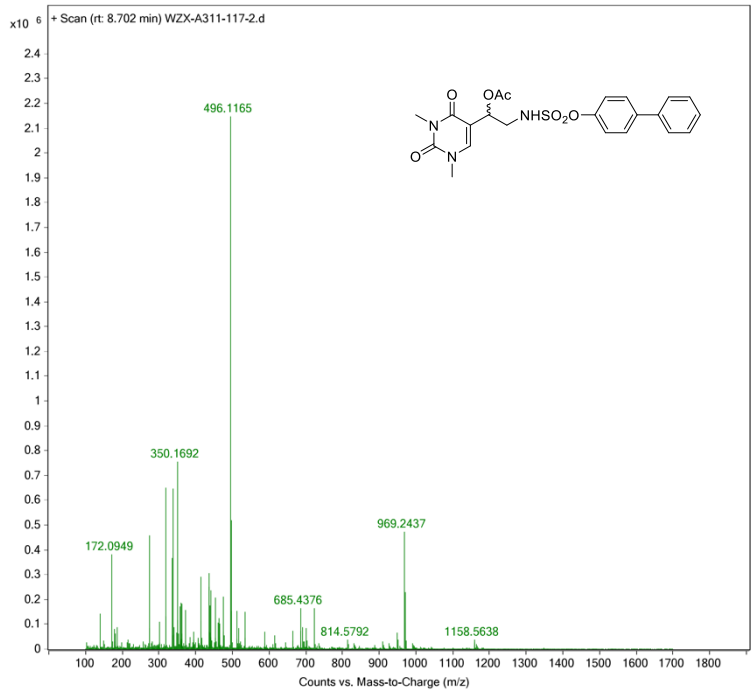
HRMS spectrum of **15af**

Sample Name	WZX-A311-118	**Position**	P1-B8	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-118.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 12:51:35 AM (UTC+08:00)



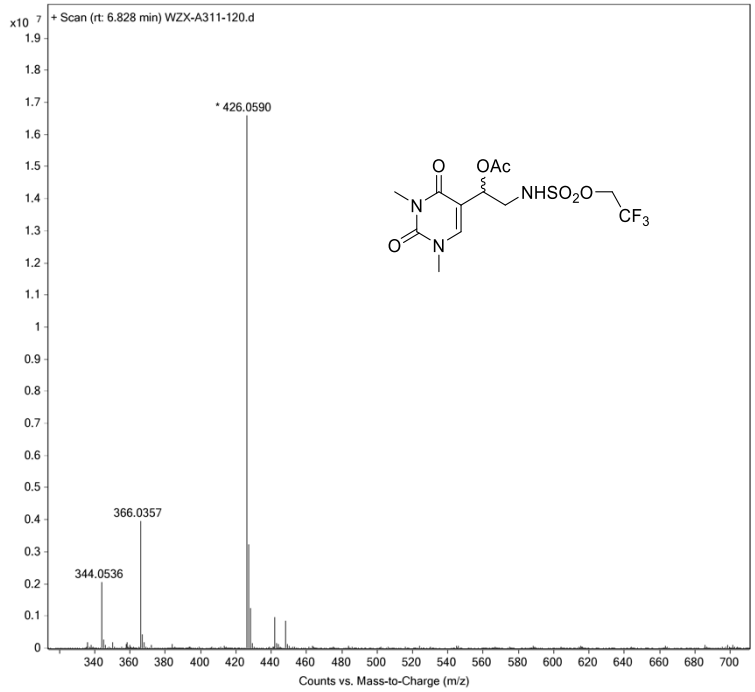
HRMS spectrum of **15ag**

Sample Name	WZX-A311-117-2	**Position**	P1-B7	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-117-2.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 12:35:49 AM (UTC+08:00)



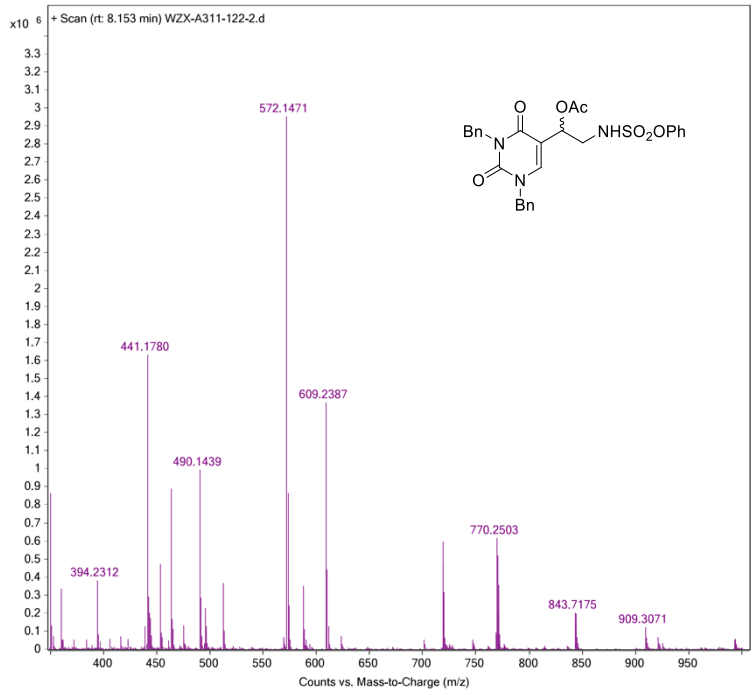
HRMS spectrum of **15ah**

Sample Name	WZX-A311-120	**Position**	P1-C4	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-120.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 3:07:43 AM (UTC+08:00)



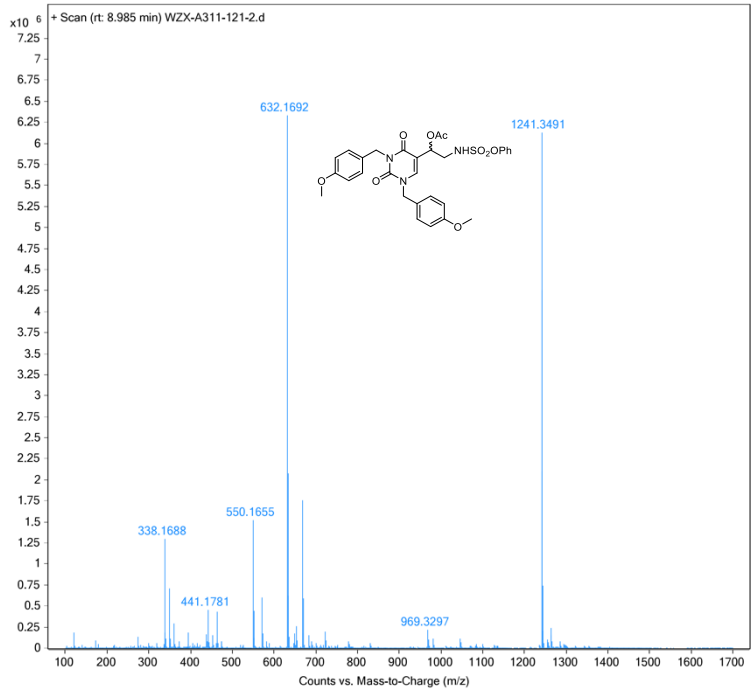
HRMS spectrum of **15ba**

Sample Name	WZX-A311-122-2	**Position**	P1-A10	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-122-2.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/25/2019 10:27:03 PM (UTC+08:00)



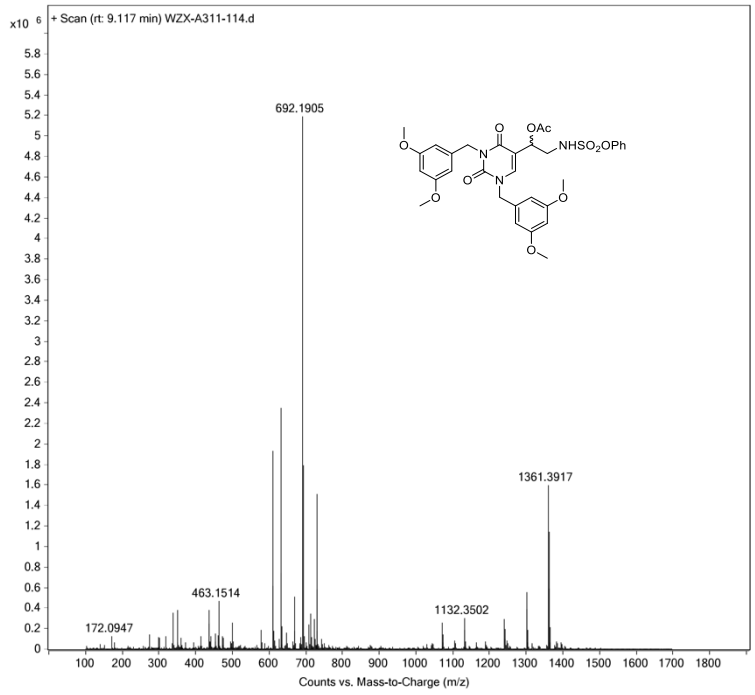
HRMS spectrum of **15ca**

Sample Name	WZX-A311-121-2	**Position**	P1-B2	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-121-2.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/25/2019 11:14:23 PM (UTC+08:00)



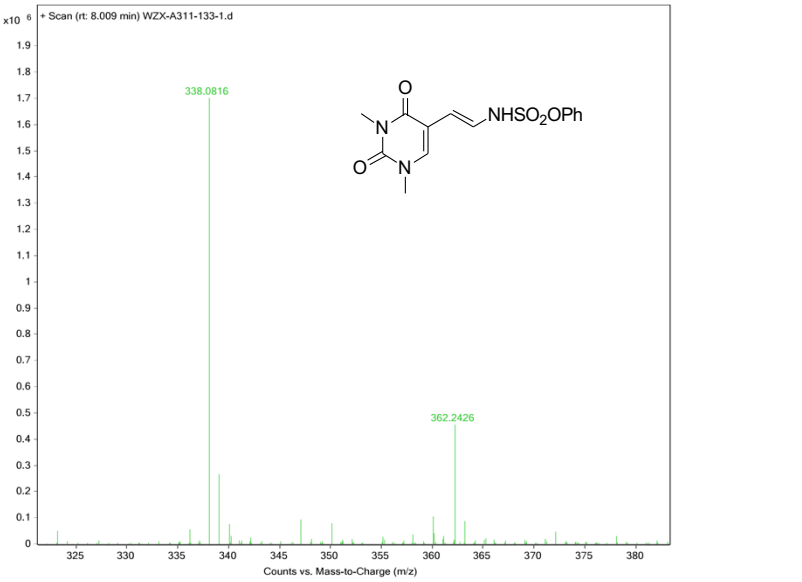
HRMS spectrum of **15da**

Sample Name	WZX-A311-114	**Position**	P1-B5	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-114.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 12:04:17 AM (UTC+08:00)



HRMS spectrum of **16**

Sample Name	WZX-A311-133-1	**Position**	P1-B11	**Instrument Name**	Instrument 1
User Name	WZX	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	WZX-A311-133-1.d
ACQ Method	20191125.m	**Comment**		**Acquired Time**	11/26/2019 1:38:48 AM (UTC+08:00)



HRMS spectrum of **17**

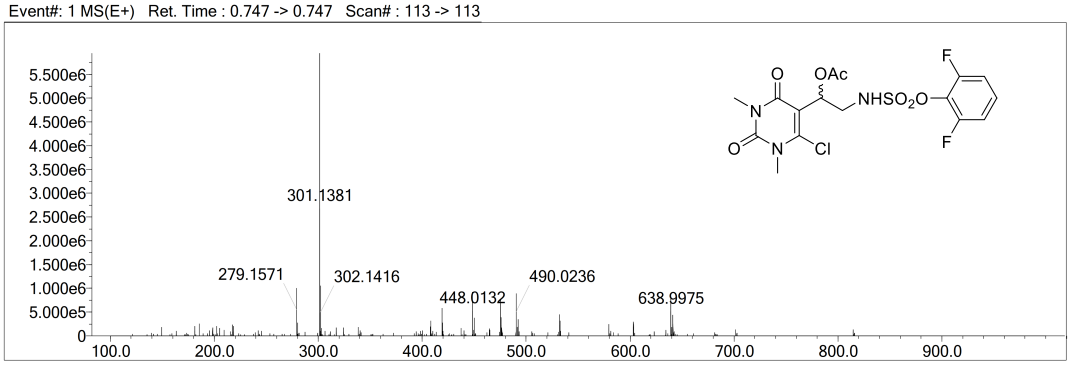
Formula Predictor Report - JZX-A262-50.lcd

Data File: D:\DATA\郁鹏\孙华\2018.10.30\JZX-A262-50.lcd

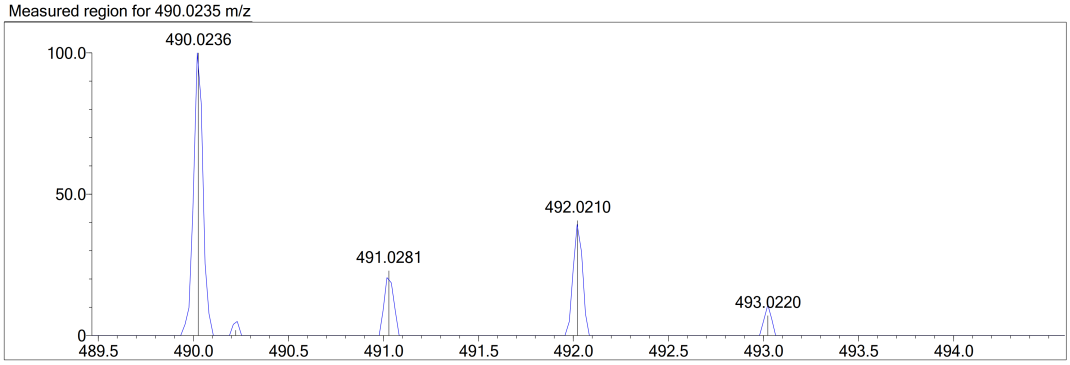
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	16	16	18O	2	0	0	S	2	0	1	Br	1	0	0	H
2H	1	0	0	F	1	0	2	Cl	1	0	1	I	3	0	0	Na
C	4	16	16	Na	1	0	0	K	1	0	0					K
N	3	0	3	Si	4	0	0	Cr	2	0	0					NH4
O	2	7	7	P	3	0	0	Se	2	0	0					Br

Error Margin (ppm):	100	DBE Range:	0.0 - 50.0	Electron Ions:	both
HC Ratio:	0.0 - 5.0	Apply N Rule:	yes	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	50

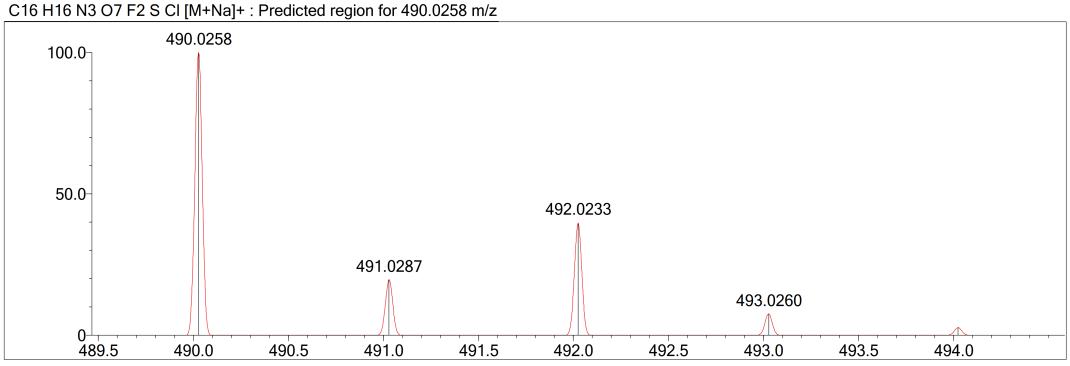
Event#: 1 MS(E+) Ret. Time : 0.747 -> 0.747 Scan# : 113 -> 113



Measured region for 490.0235 m/z



C16 H16 N3 O7 F2 S Cl [M+Na]+ : Predicted region for 490.0258 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	72.58	C16 H16 N3 O7 F2 S Cl	[M+Na]+	490.0235	490.0258	-2.3	-4.69	79.95	9.0

HRMS spectrum of **18**

Data File: D:\DATA\郁鹏\孙华\2018.10.30\JZX-A262-63.lcd

Elmt	Val.	Min	Max
H	1	13	17
B	3	0	0
C	4	10	14
N	3	1	3
O	2	3	6

Elmt	Val.	Min	Max
18O	2	0	0
F	1	0	2
Na	1	0	0
Mg	2	0	0
Si	4	0	0

Elmt	Val.	Min	Max
P	3	0	0
S	2	1	1
Cl	1	0	1
Ti	2	0	0
Fe	2	0	0

Elmt	Val.	Min	Max
Se	2	0	0
Br	1	0	0
I	3	0	0

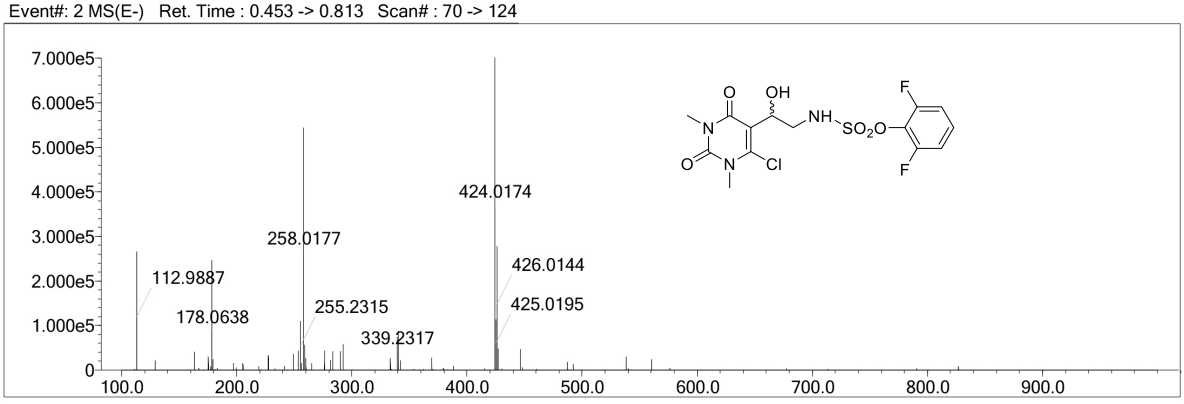
Use Adduct
H
HCOO
CH3COO
Cl

Error Margin (mDa): 1000.0
HC Ratio: 0.0 - 3.0
Max Isotopes: all
MSn Iso RI (%): 75.00

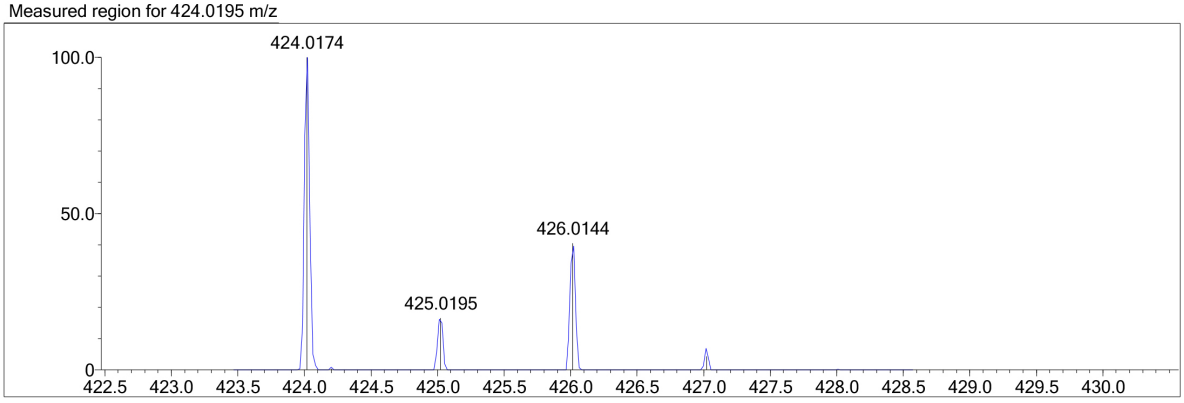
DBE Range: 0.0 - 50.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 50

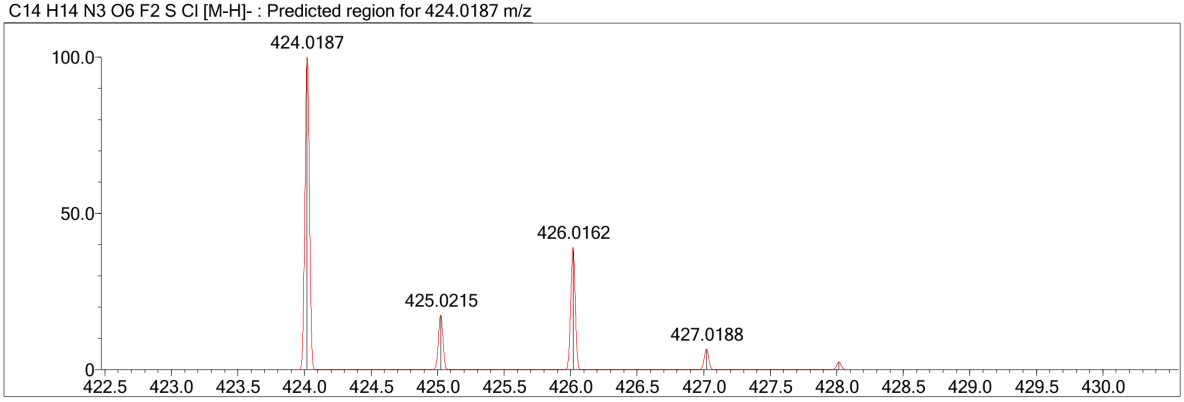
Event#: 2 MS(E-) Ret. Time : 0.453 -> 0.813 Scan# : 70 -> 124



Measured region for 424.0195 m/z



C14 H14 N3 O6 F2 S Cl [M-H]- : Predicted region for 424.0187 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	76.02	C14 H14 N3 O6 F2 S Cl	[M-H]-	424.0195	424.0187	0.8	1.89	77.75	8.0

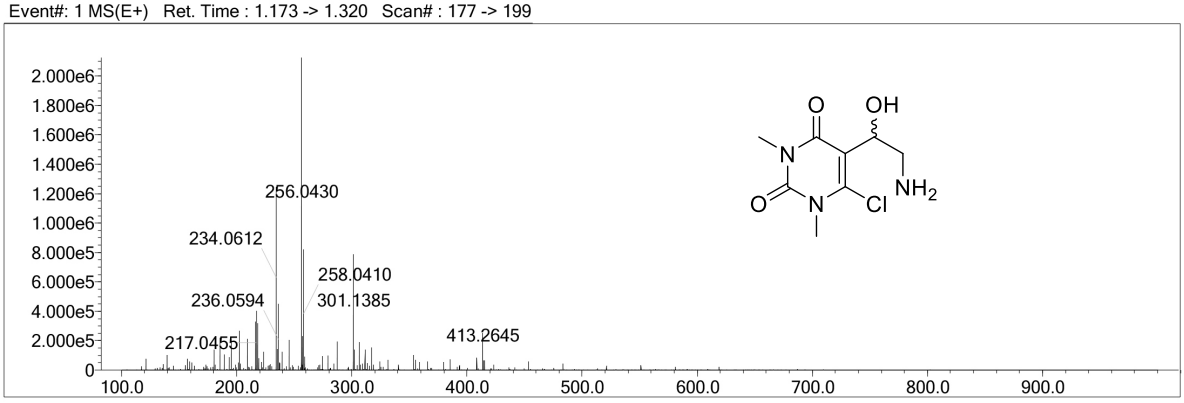
HRMS spectrum of **19**

Data File: D:\DATA\郁鹏\孙华\2018.10.30\JZX-A262-41.lcd

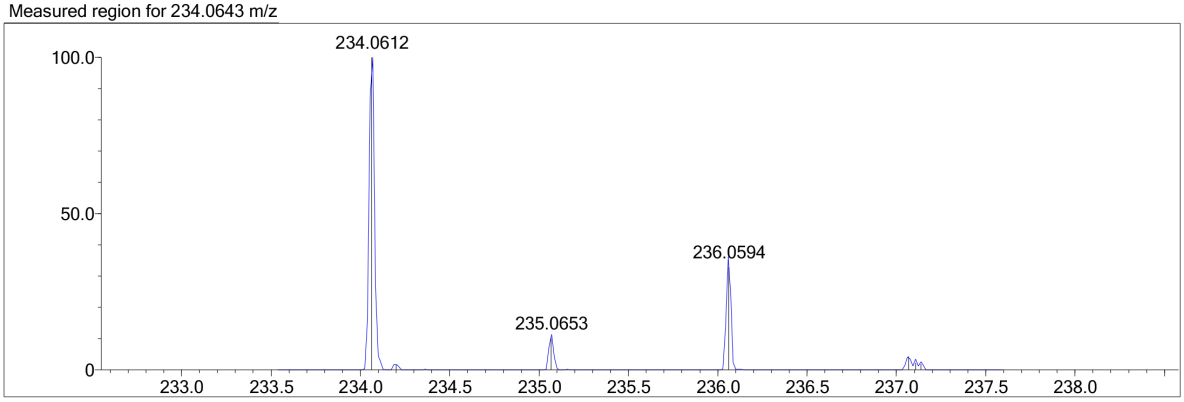
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	12	18O	2	0	0	P	3	0	0	Se	2	0	0	H
B	3	0	0	F	1	0	0	S	2	0	0	Br	1	0	0	Na
C	4	6	8	Na	1	0	0	Cl	1	0	1	I	3	0	0	K
N	3	1	3	Mg	2	0	0	Ti	2	0	0					NH4
O	2	3	6	Si	4	0	0	Fe	2	0	0					Br

Error Margin (mDa):	1000.0	DBE Range:	0.0 - 50.0	Electron Ions:	both
HC Ratio:	0.0 - 3.0	Apply N Rule:	yes	Use MSn Info:	yes
Max Isotopes:	all	Isotope RI (%):	1.00	Isotope Res:	10000
MSn Iso RI (%):	75.00	MSn Logic Mode:	AND	Max Results:	50

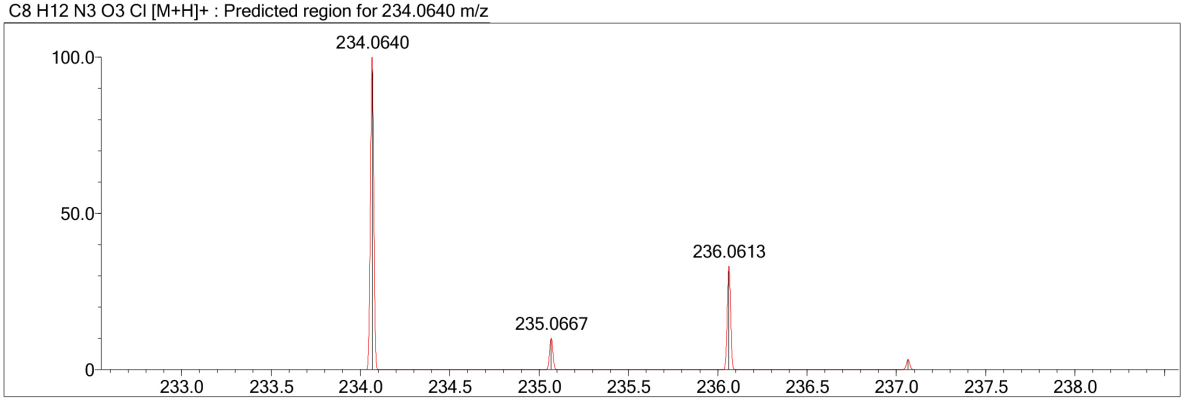
Event#: 1 MS(E+) Ret. Time : 1.173 -> 1.320 Scan# : 177 -> 199



Measured region for 234.0643 m/z



C8 H12 N3 O3 Cl [M+H]+ : Predicted region for 234.0640 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	93.08	C8 H12 N3 O3 Cl	[M+H]+	234.0643	234.0640	0.3	1.28	93.73	4.0