

Supplementary Information

Copper complexes and carbon nanotube-copper ferrite-catalyzed benzenoid A-ring selenation of quinones: An efficient method for the synthesis of trypanocidal agents

Guilherme A. M. Jardim,^{a,b} Icaro A. O. Bozzi,^a Willian X. C. Oliveira,^a Camila Mesquita-Rodrigues,^c Rubem F. S. Menna-Barreto,^c Ramar A. Kumar,^{d,e} Edmond Gravel,^d Eric Doris,^{d*} Antonio L. Braga^b and Eufrânio N. da Silva Júnior^{a*}

^aInstitute of Exact Sciences, Department of Chemistry, Federal University of Minas Gerais, Belo Horizonte, MG, 31270-901, Brazil. E-mail: eufranio@ufmg.br;

^bDepartment of Chemistry, Federal University of Santa Catarina, 88040-900 Florianópolis, Brazil;

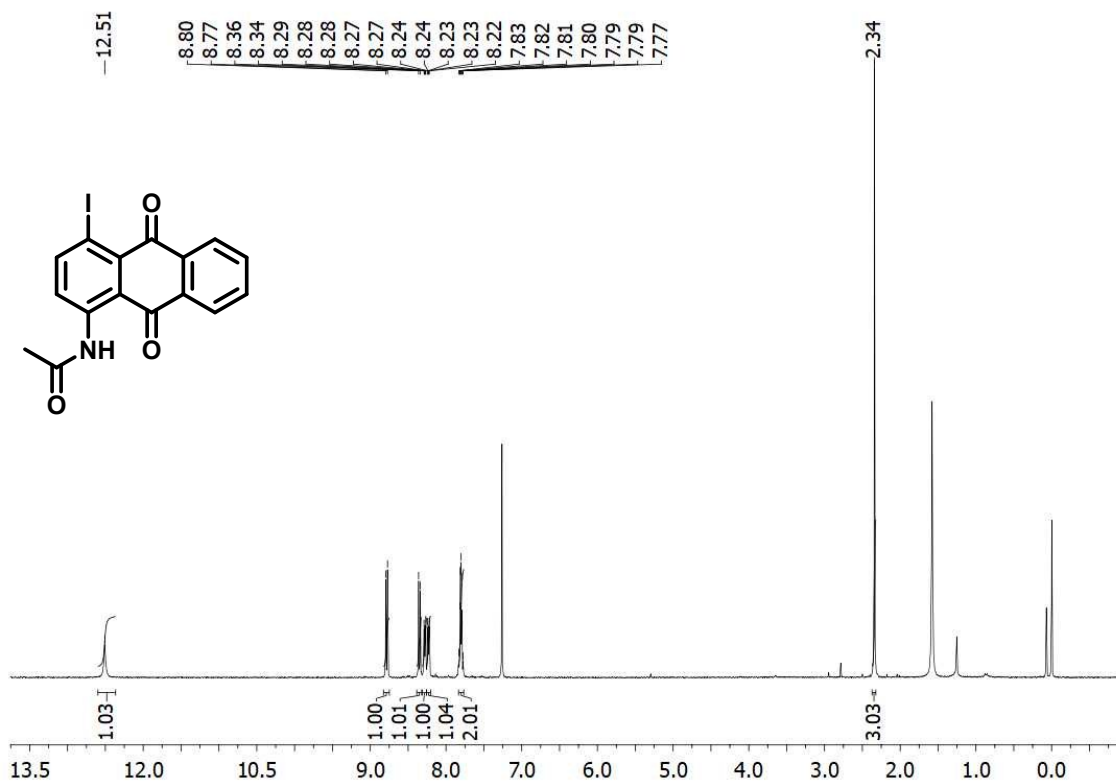
^cOswaldo Cruz Institute, FIOCRUZ, Rio de Janeiro, RJ, 21045-900, Brazil;

^dService de Chimie Bioorganique et de Marquage (SCBM) CEA, Université Paris-Saclay 91191 Gif-sur-Yvette (France), E-mail: eric.doris@cea.fr;

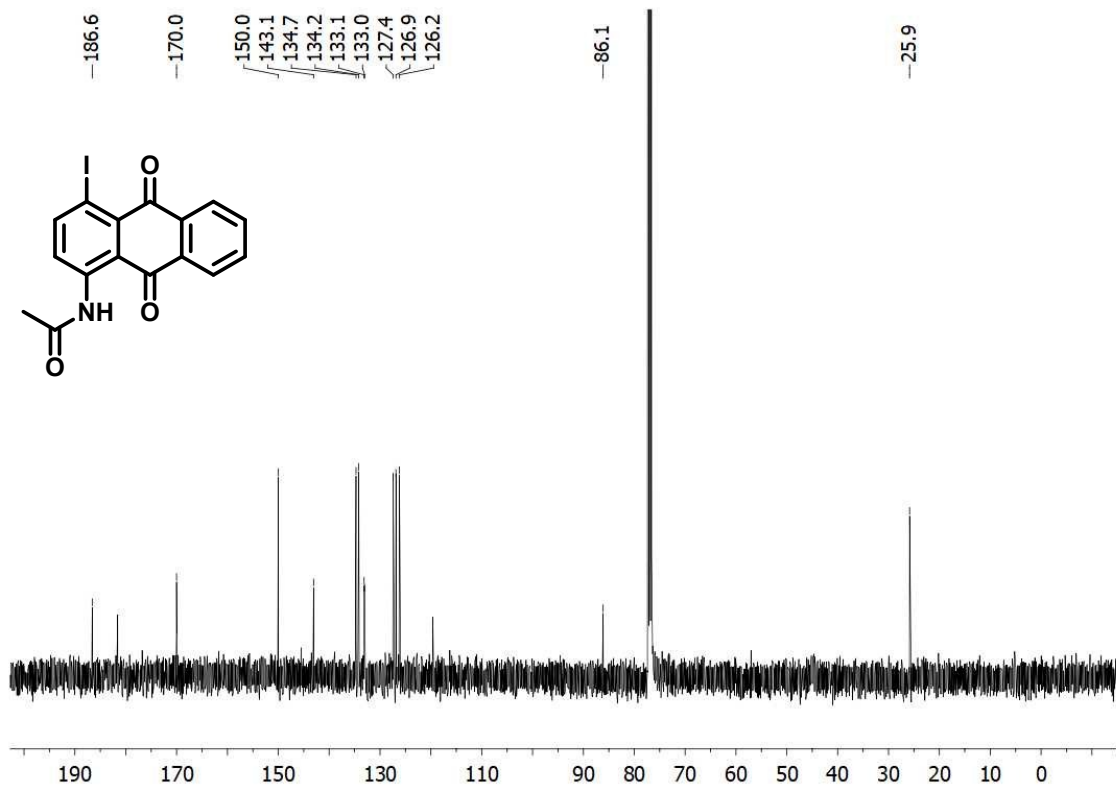
^eSRM Research Institute, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, 603203 Chennai, India.

Contents

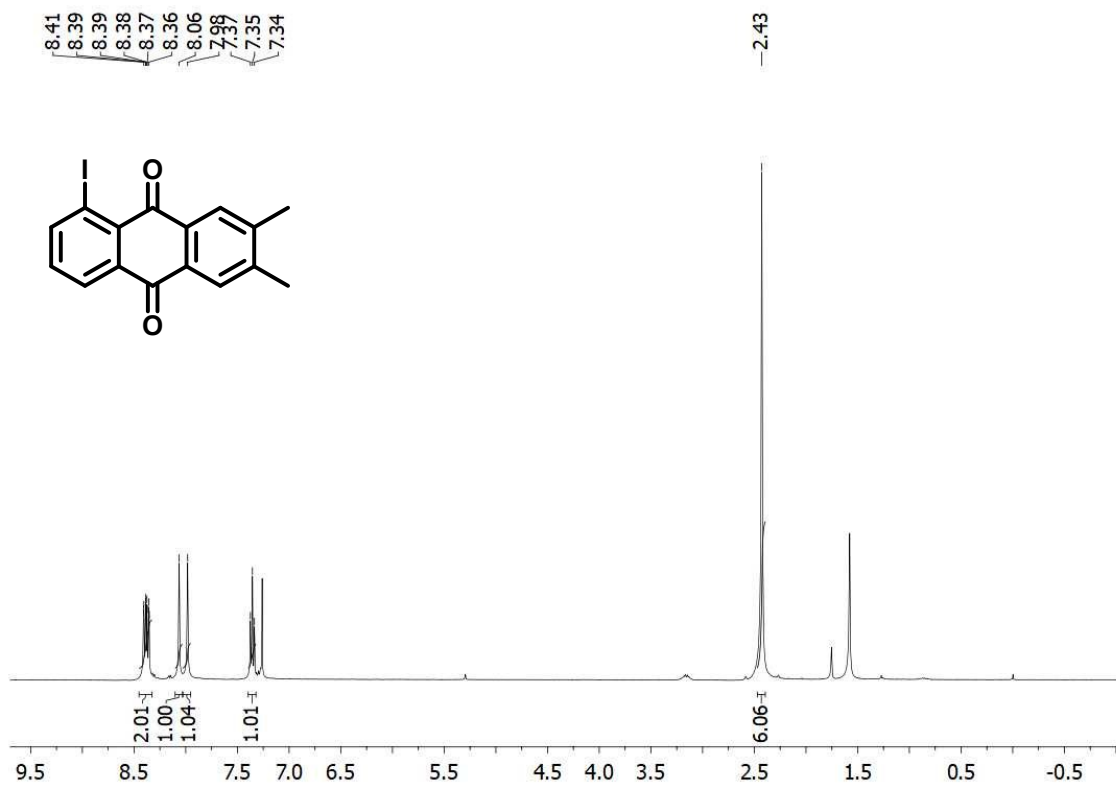
A) Copies of NMR spectra of novel compounds	S02
B) Copies of HRMS spectra of novel compounds	S27



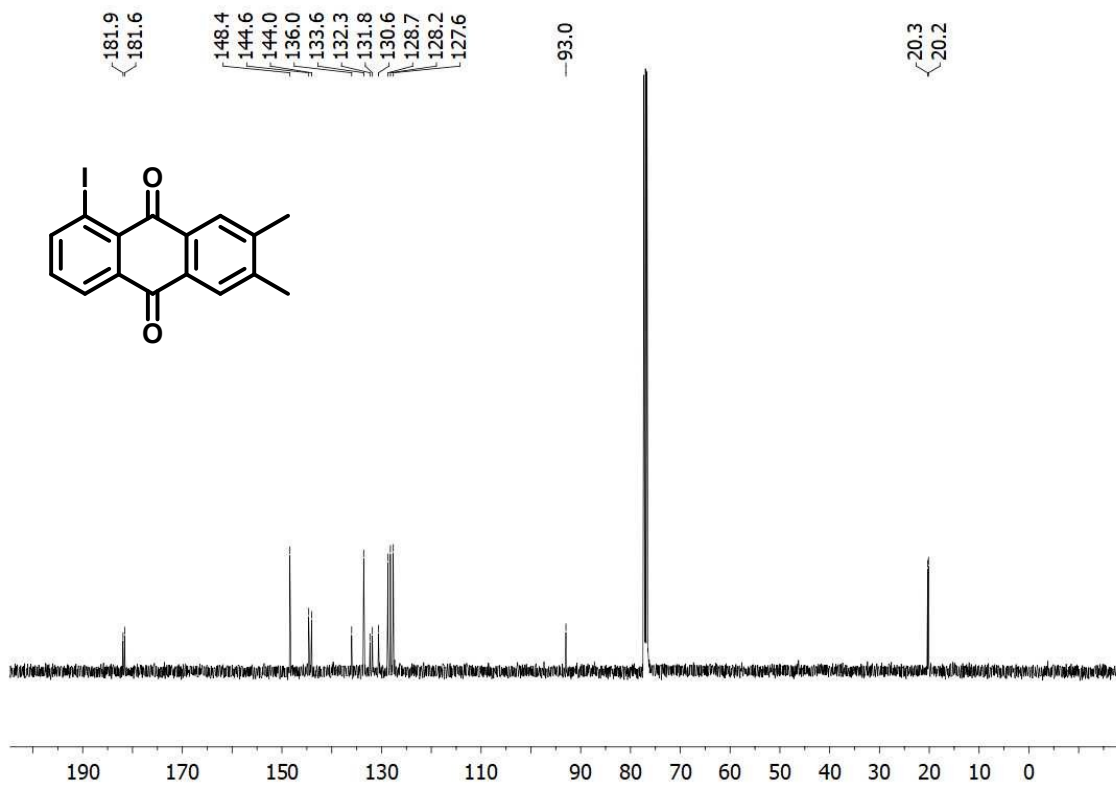
¹H NMR spectrum (400 MHz, CDCl₃) of compound **1p**



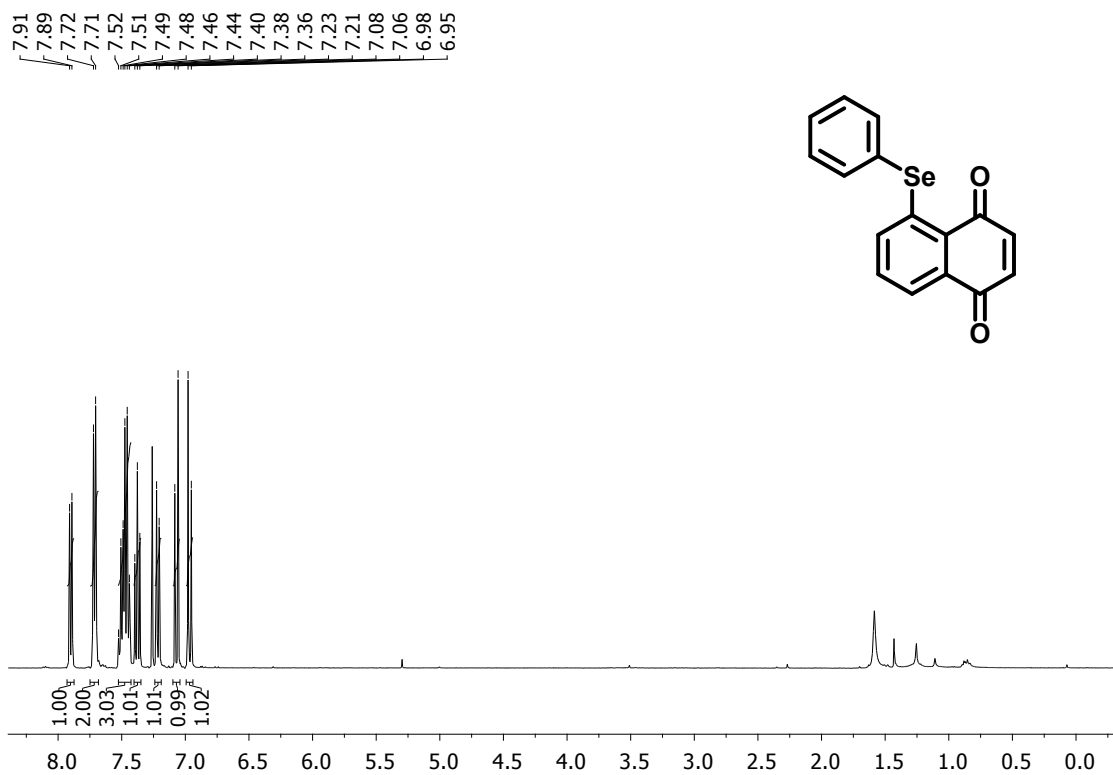
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **1p**



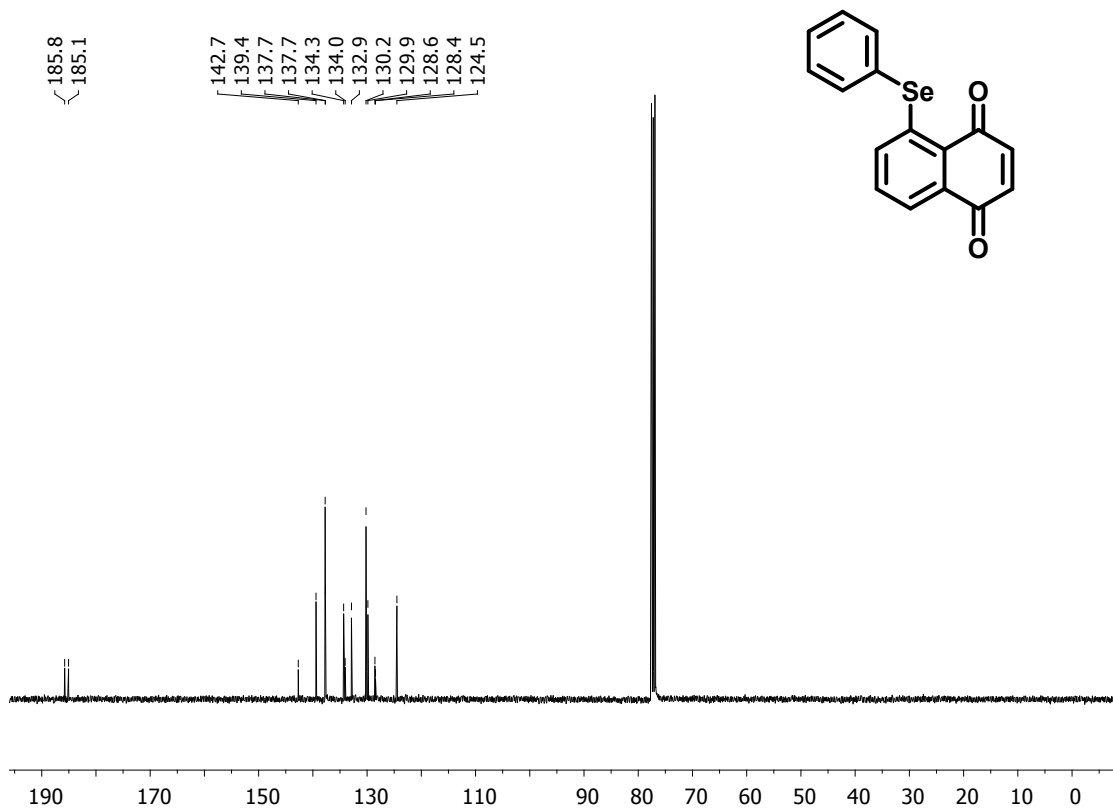
^1H NMR spectrum (400 MHz, CDCl_3) of compound **1r**



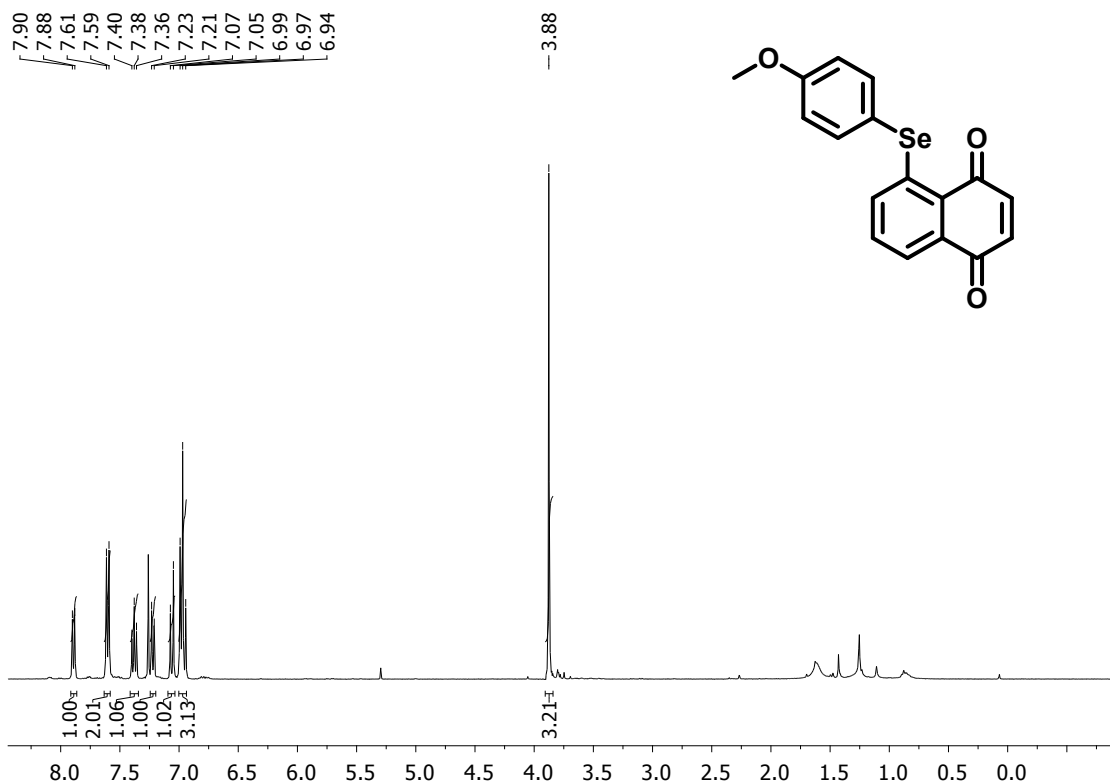
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **1r**



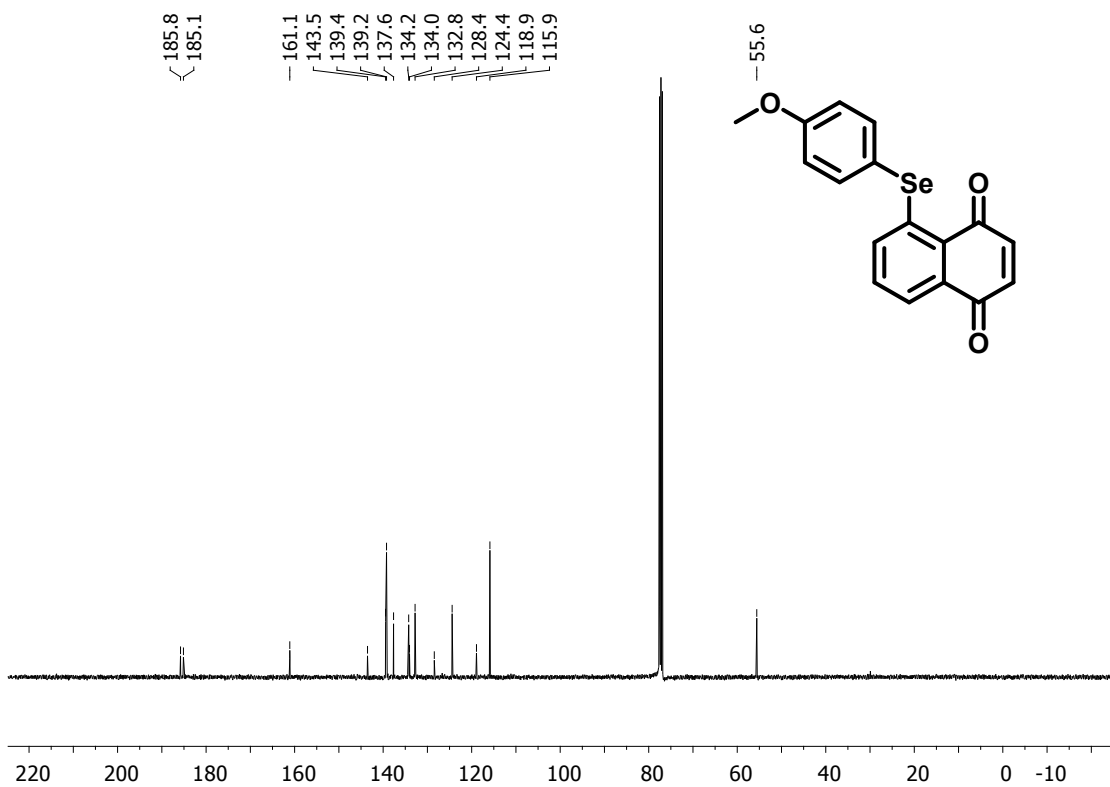
¹H NMR spectrum (400 MHz, CDCl₃) of compound 2a



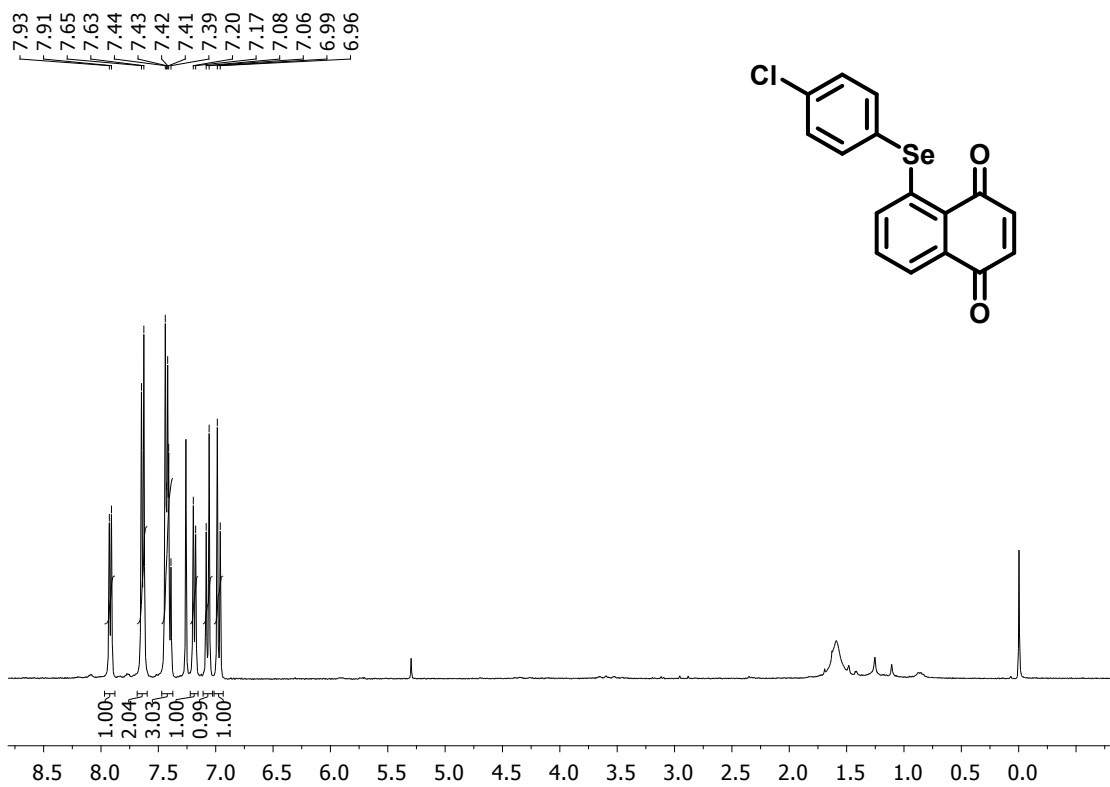
¹³C NMR spectrum (100 MHz, CDCl₃) of compound 2a



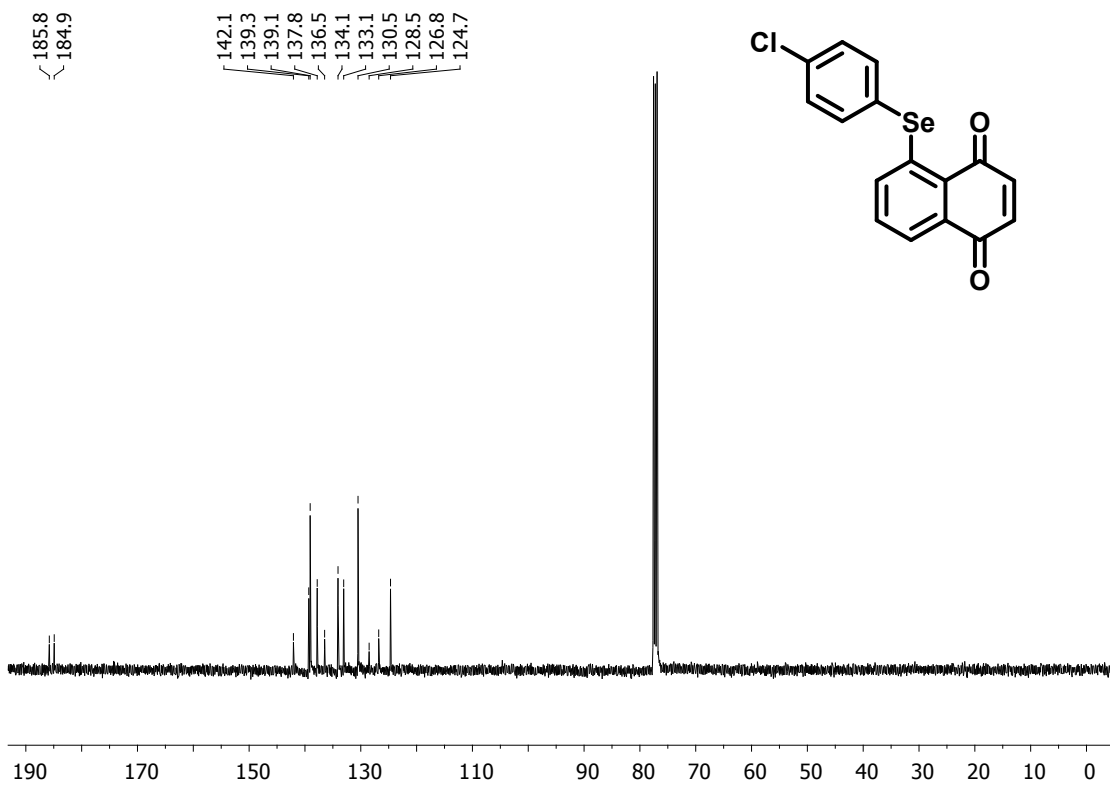
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2b**



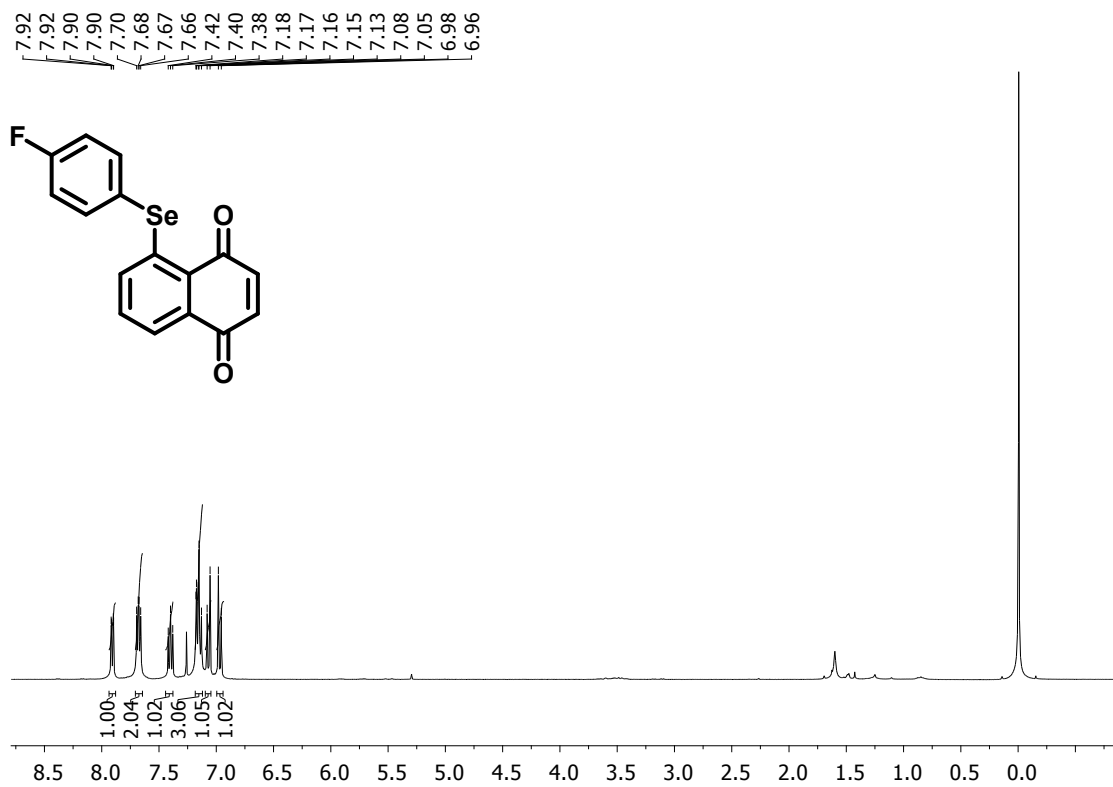
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2b**



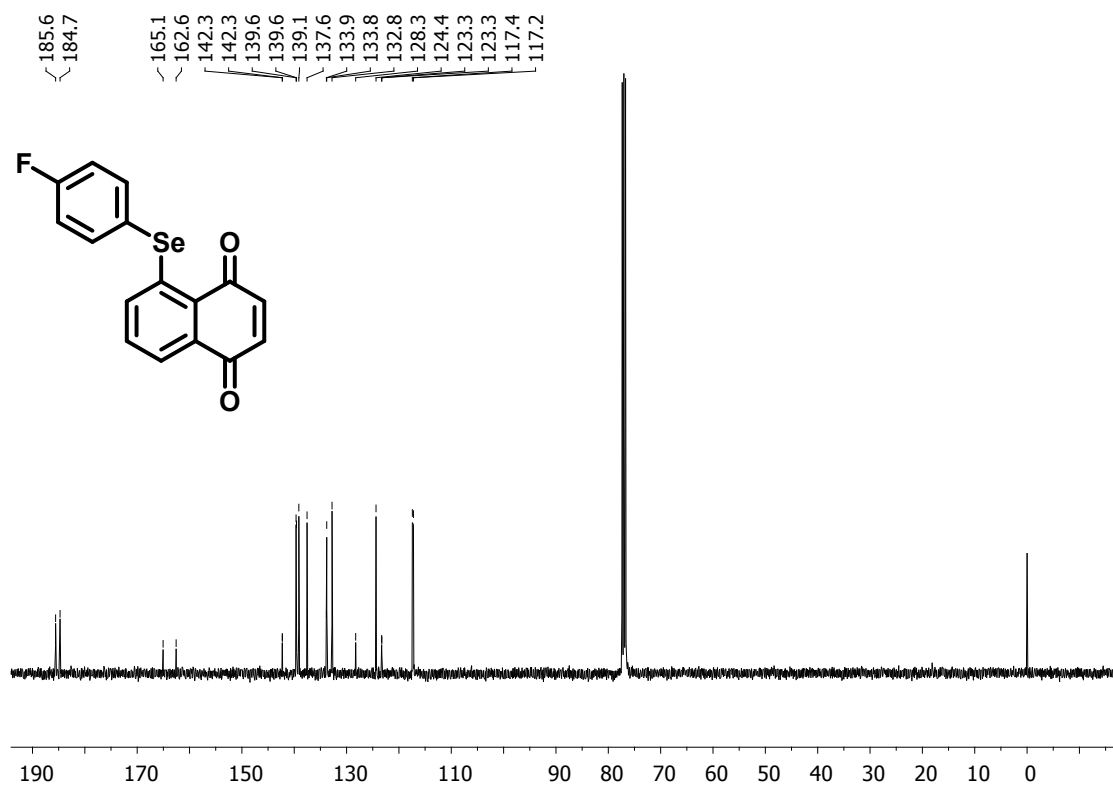
$^1\text{H NMR}$ spectrum (400 MHz, CDCl_3) of compound **2c**



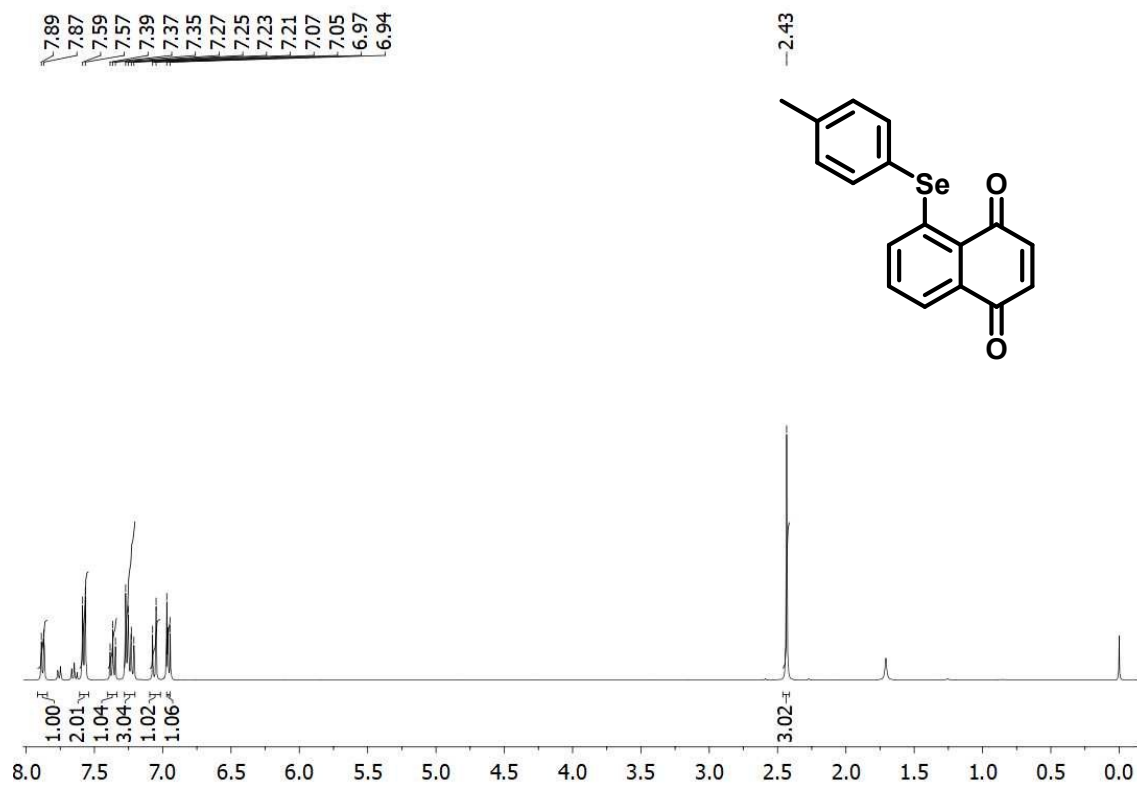
$^{13}\text{C NMR}$ spectrum (100 MHz, CDCl_3) of compound **2c**



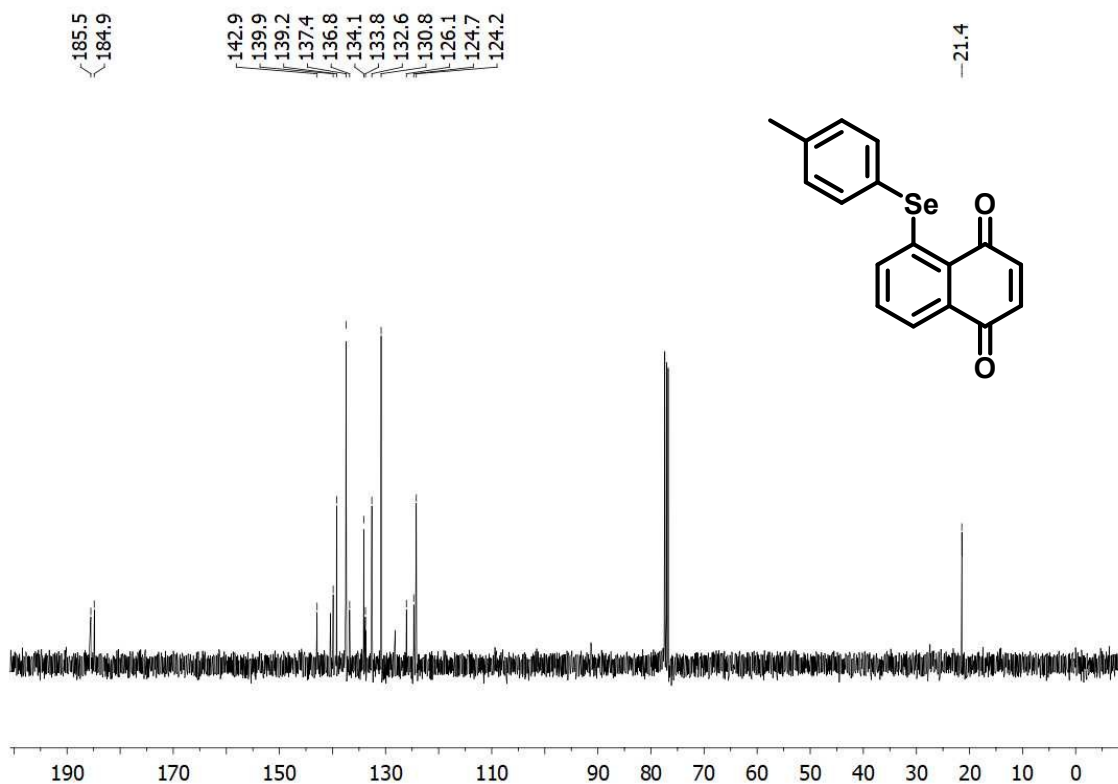
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2d**



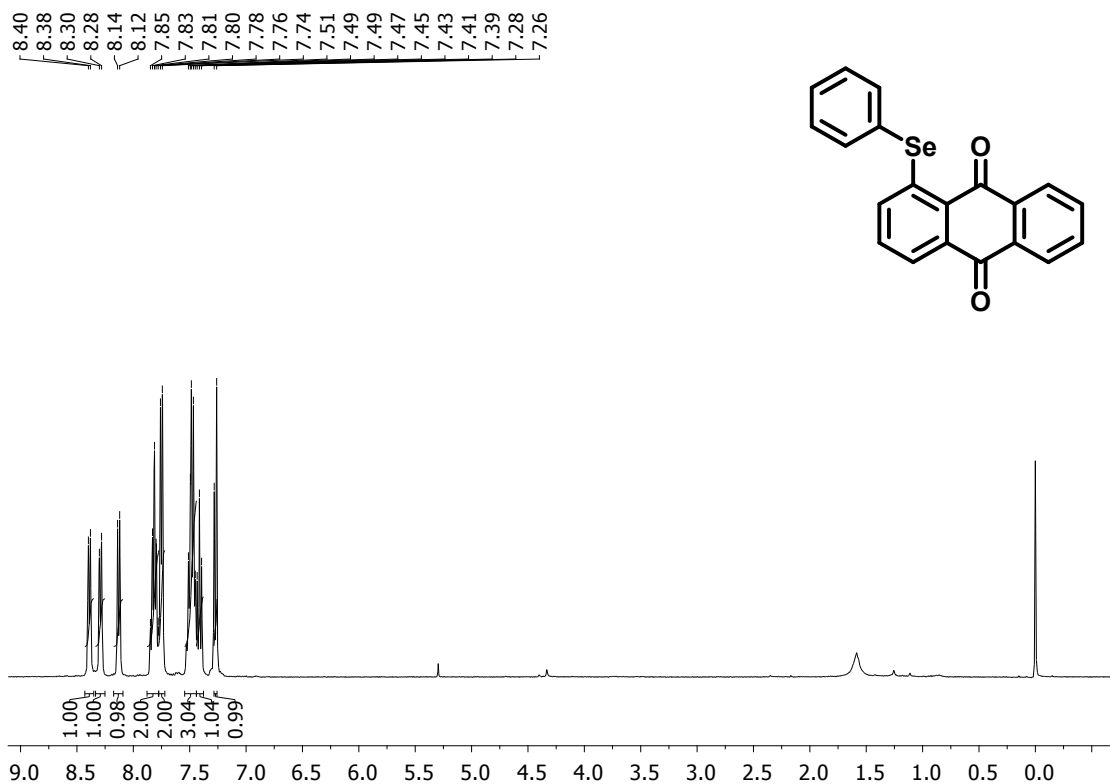
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2d**



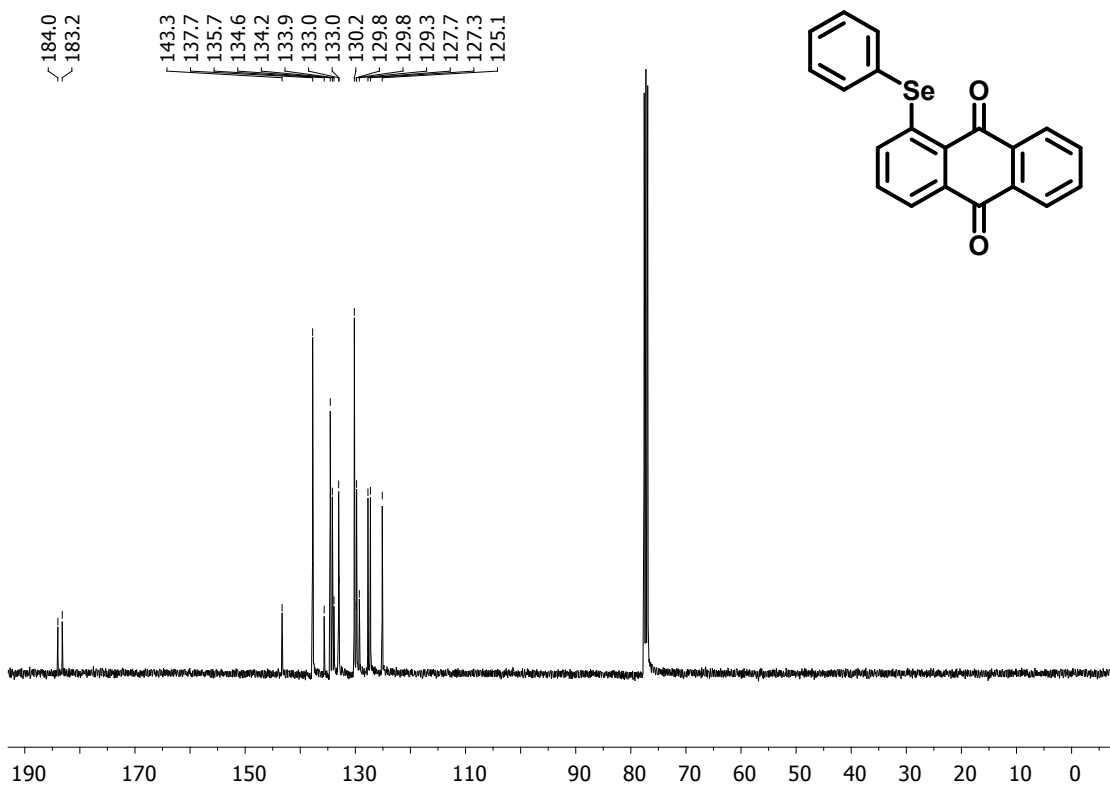
^1H NMR spectrum (400 MHz, CDCl_3) of compound **2e**



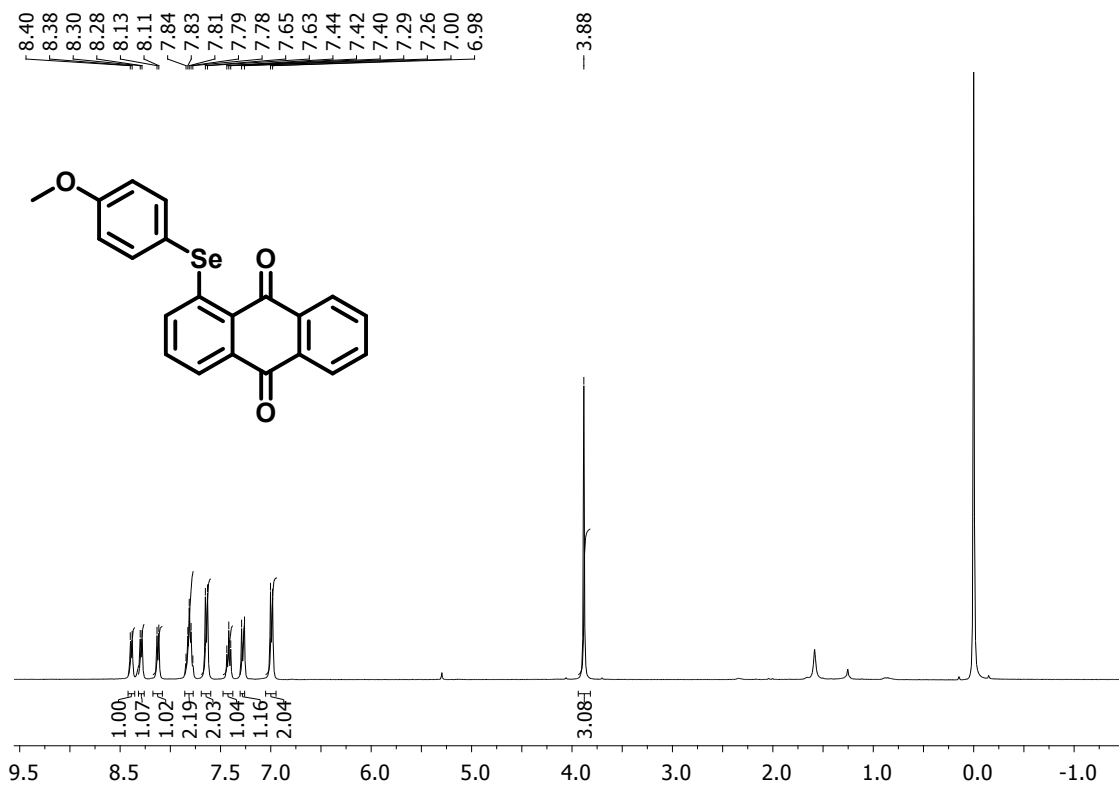
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **2e**



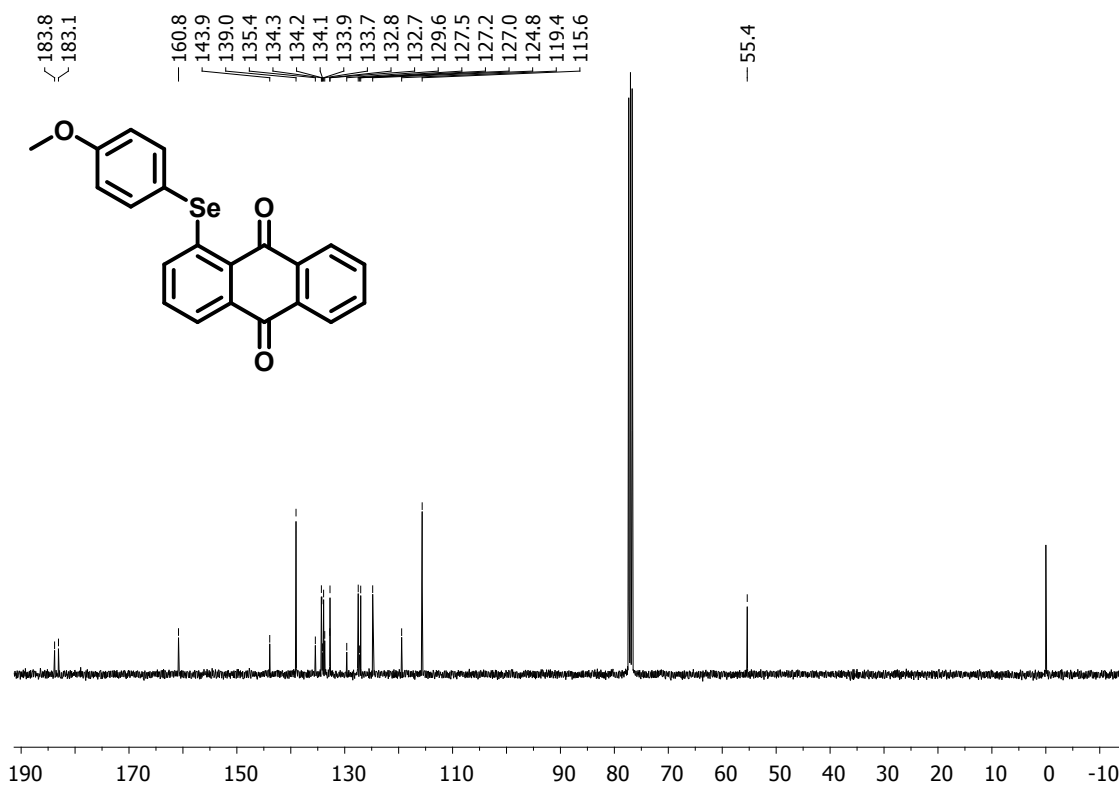
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2f**



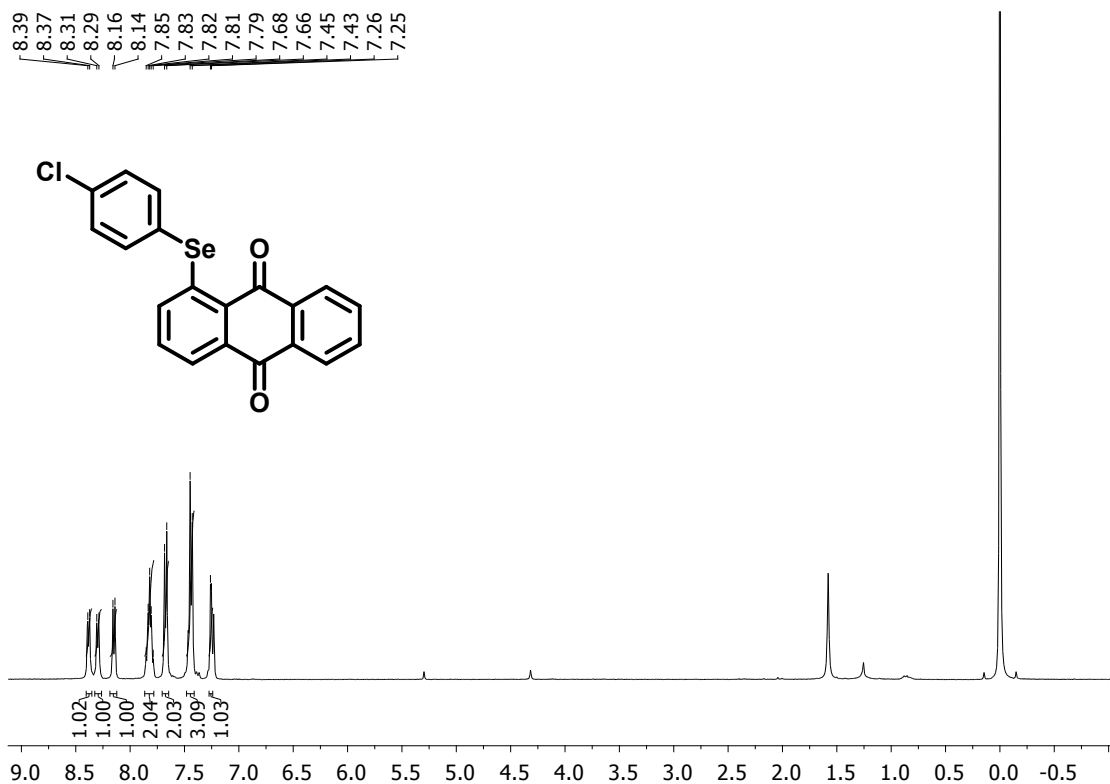
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2f**



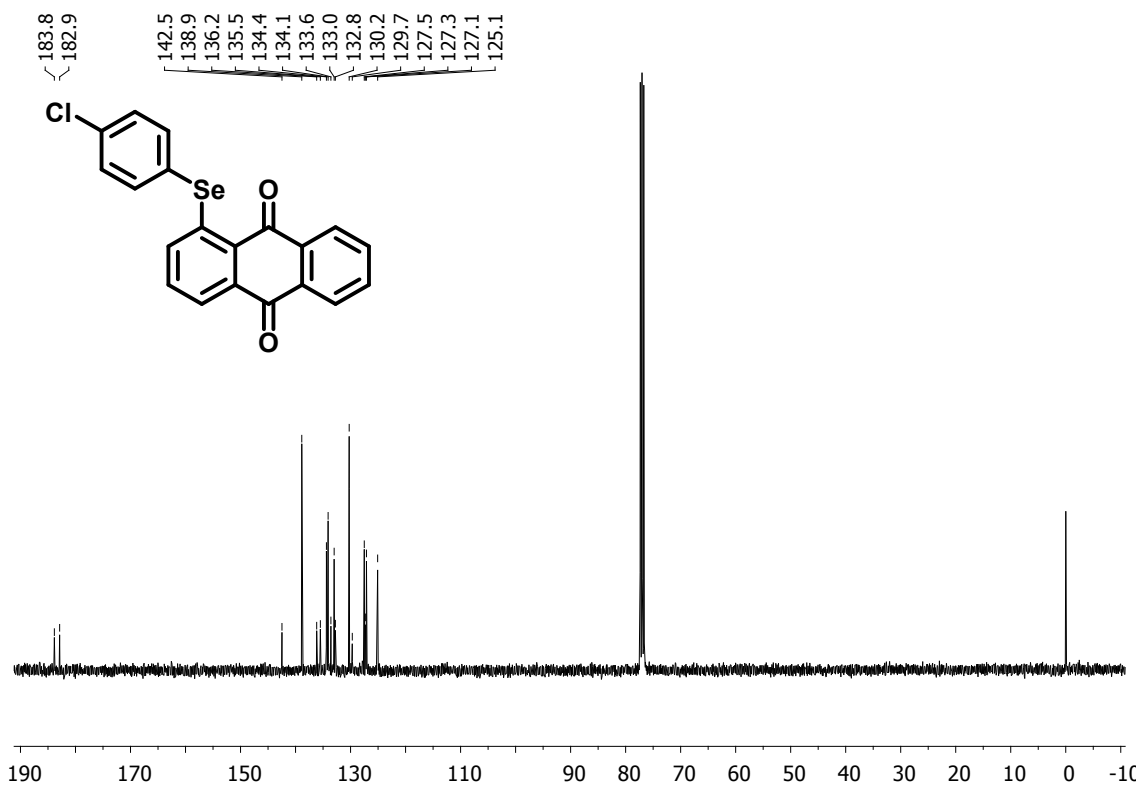
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2g**



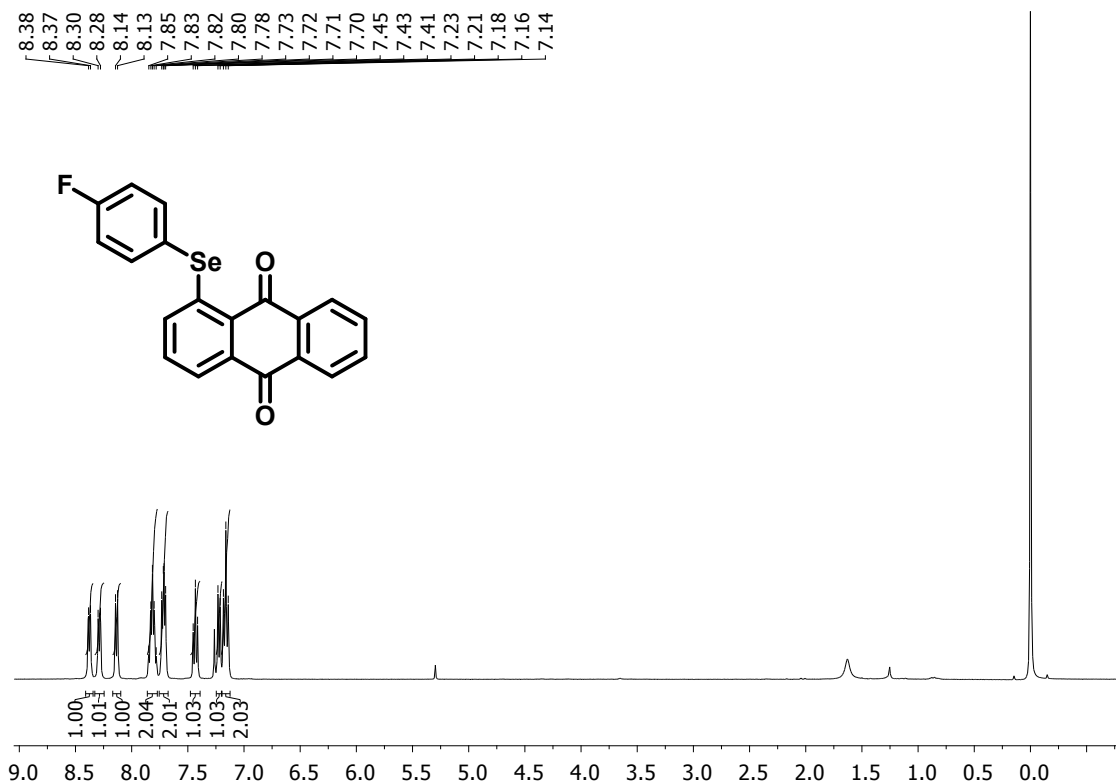
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2g**



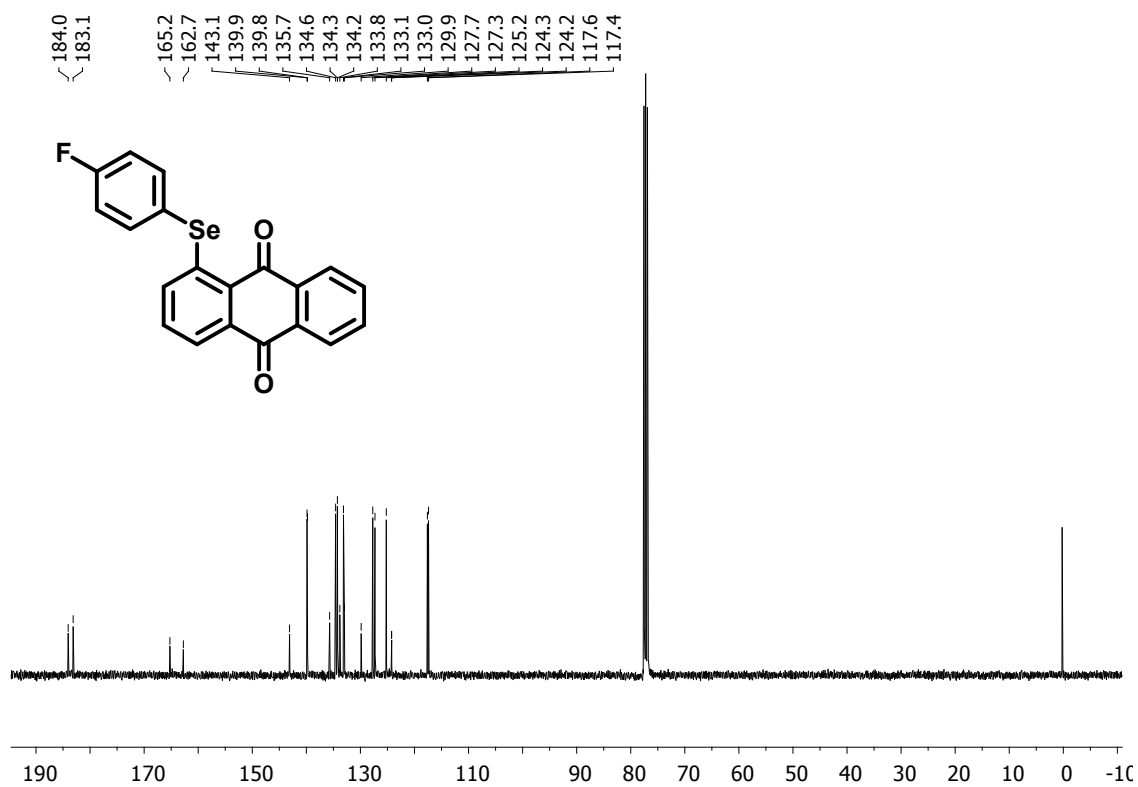
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2h**



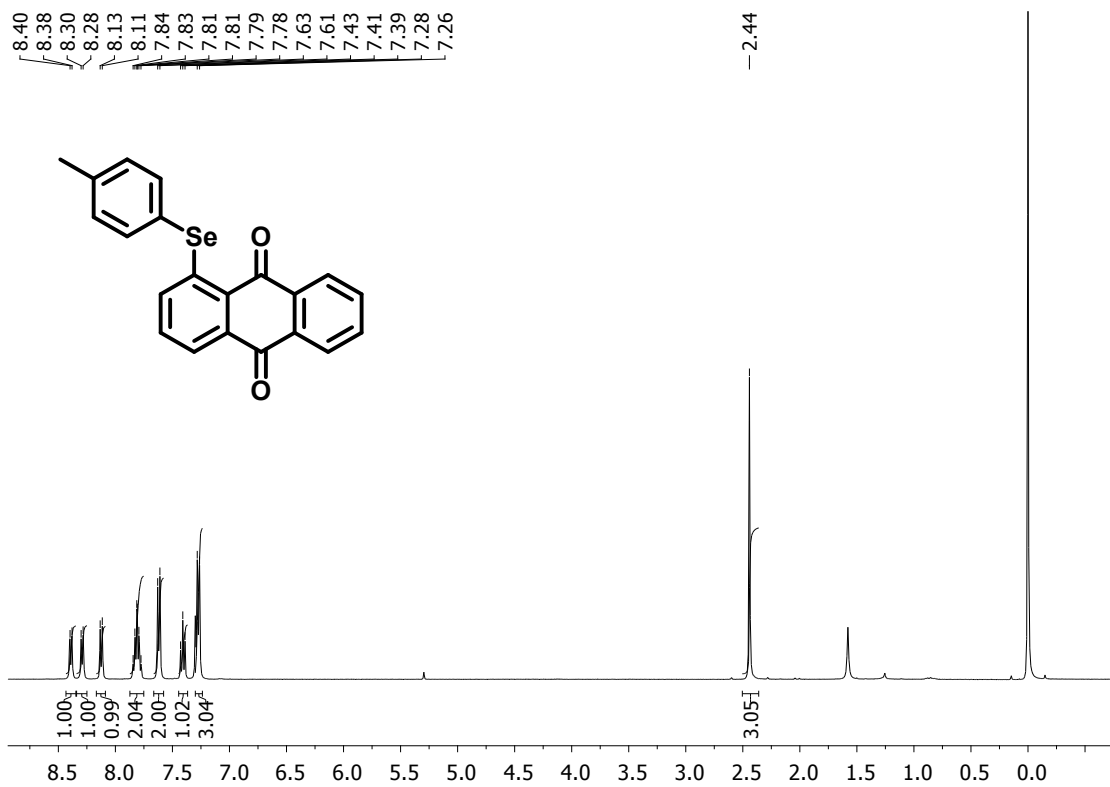
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2h**



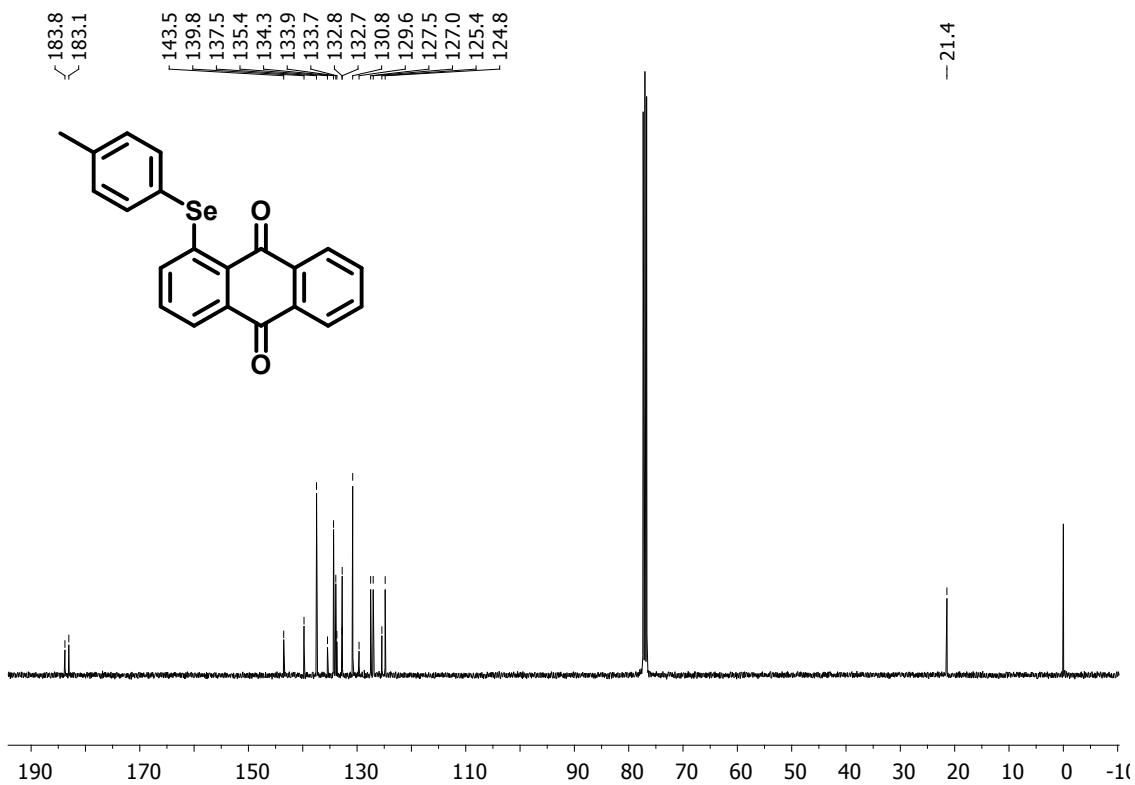
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2i**



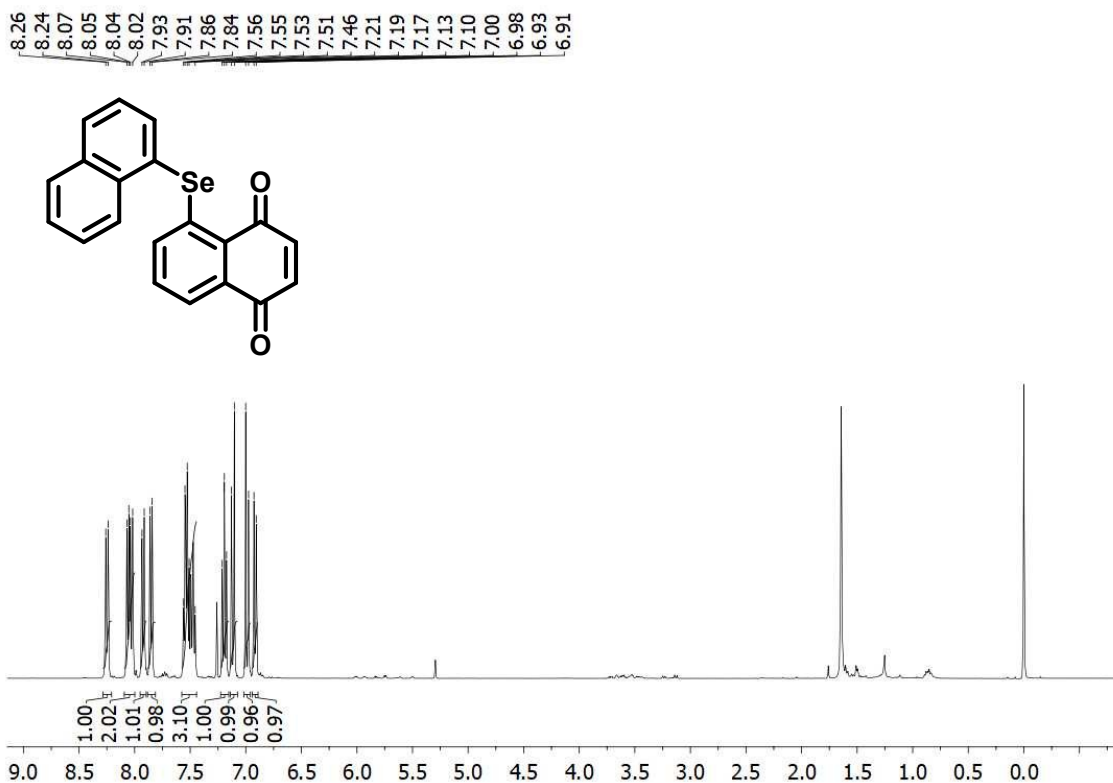
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2i**



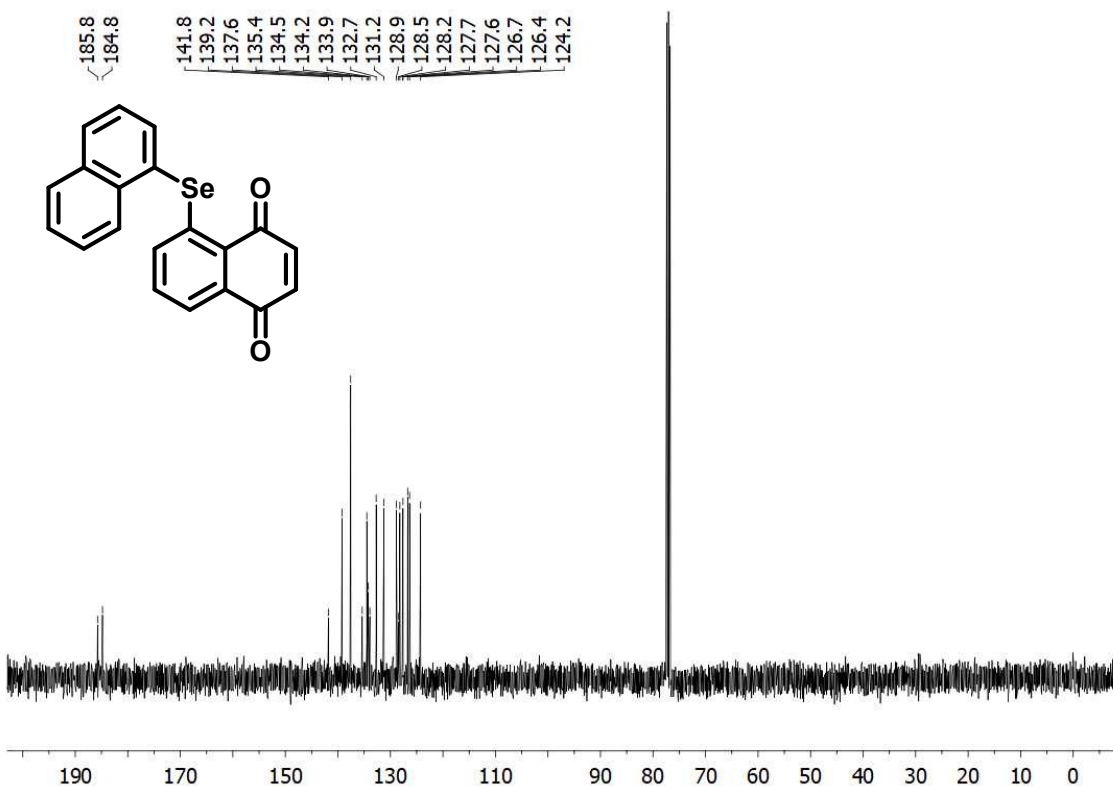
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2j**



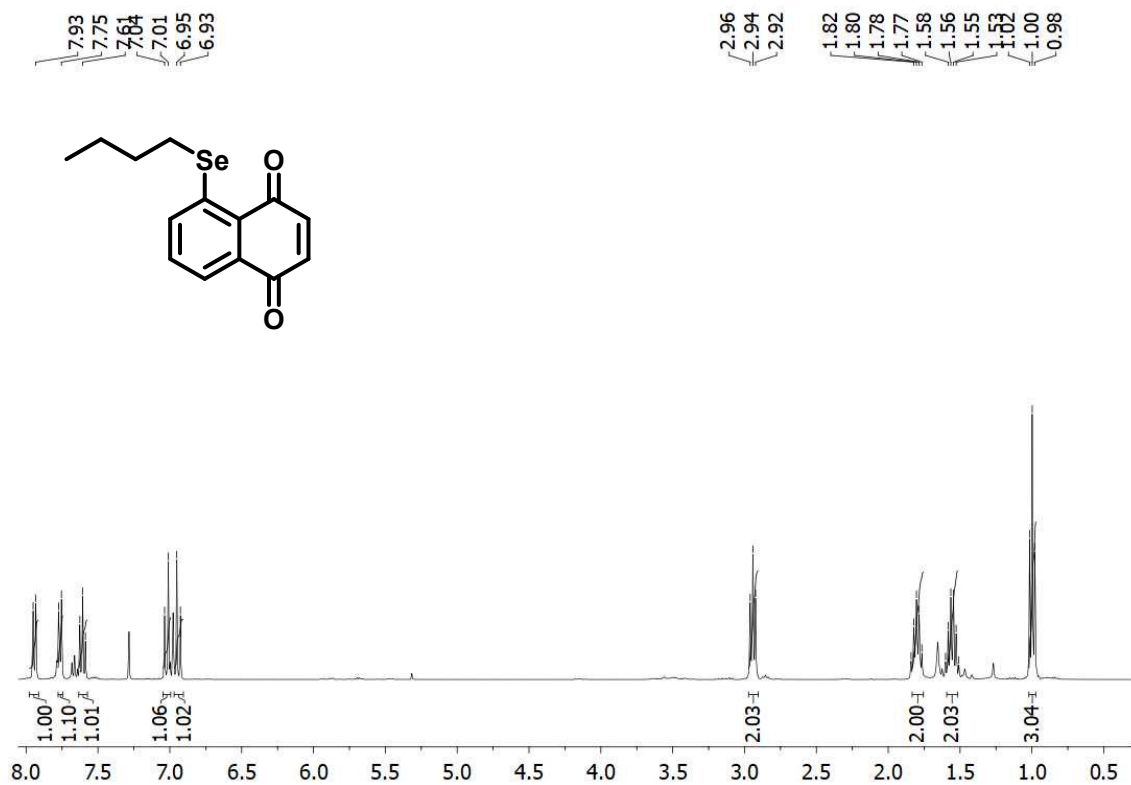
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2j**



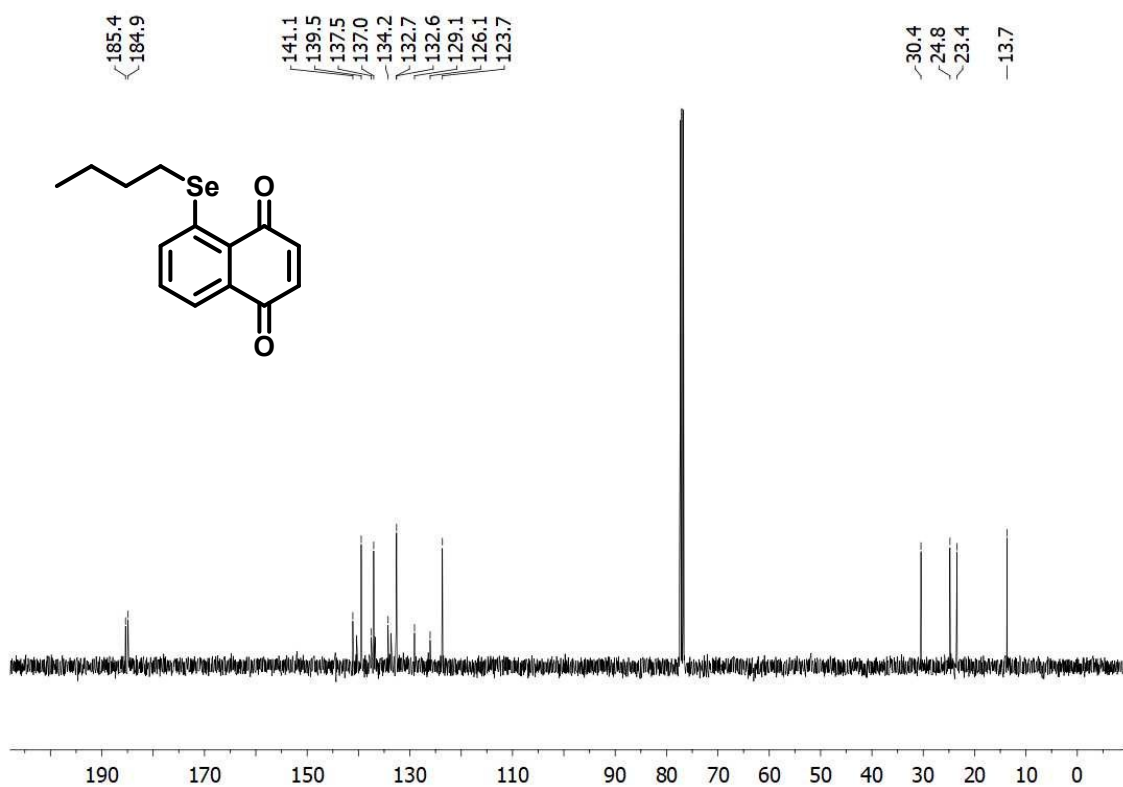
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2k**



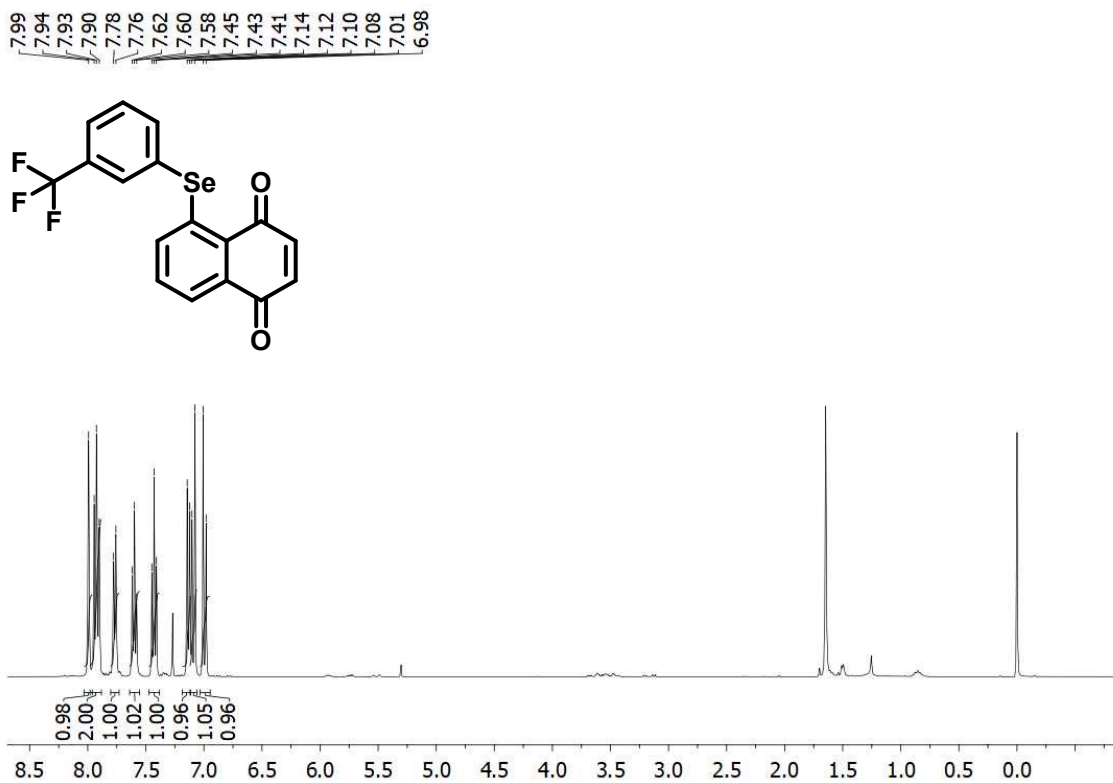
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2k**



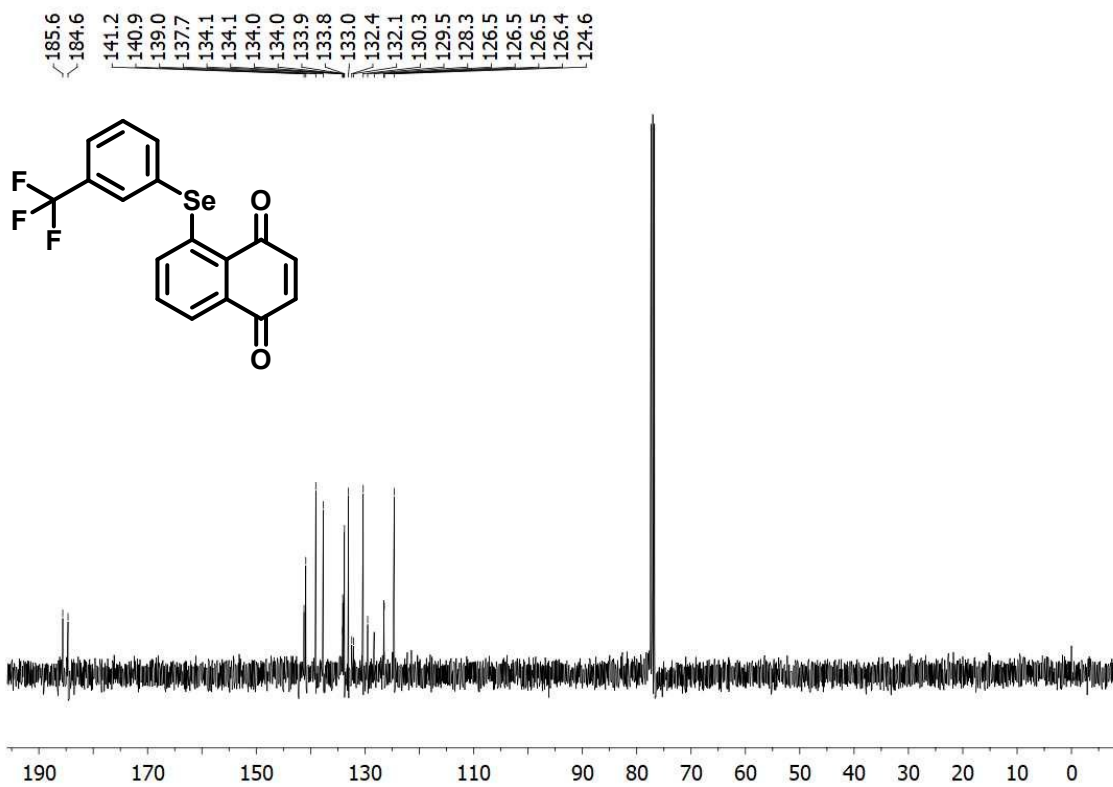
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2l**



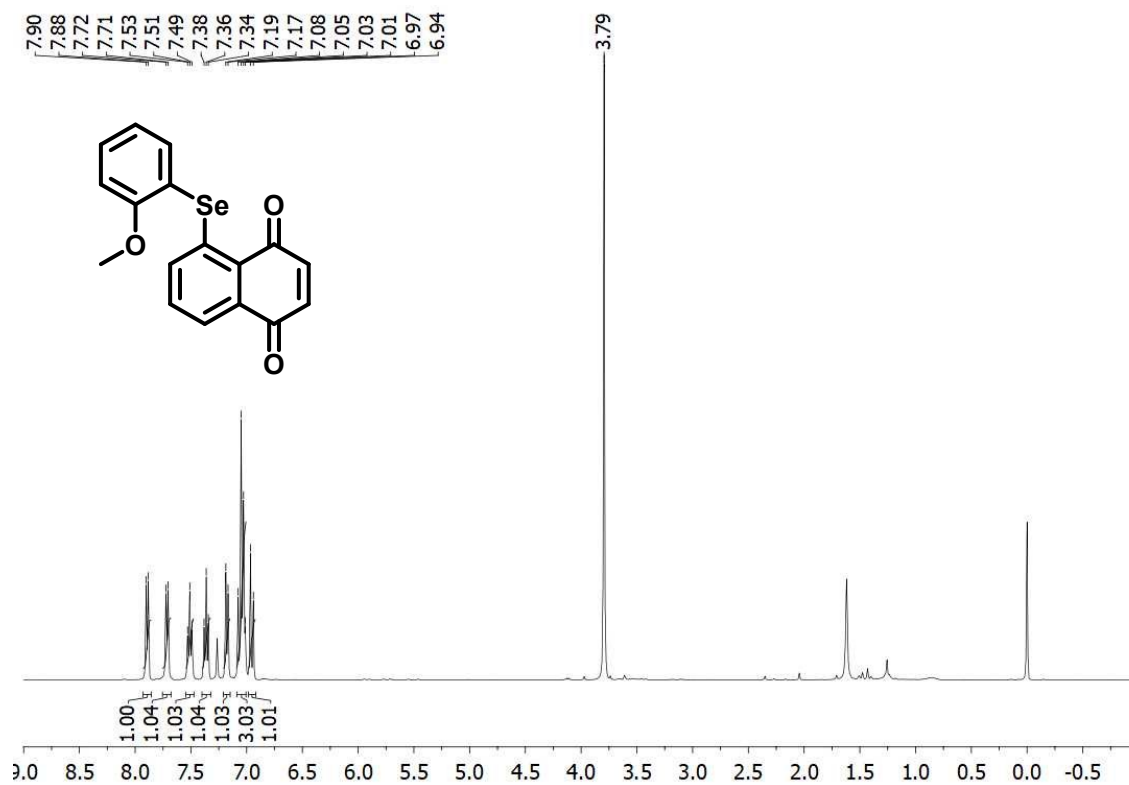
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2l**



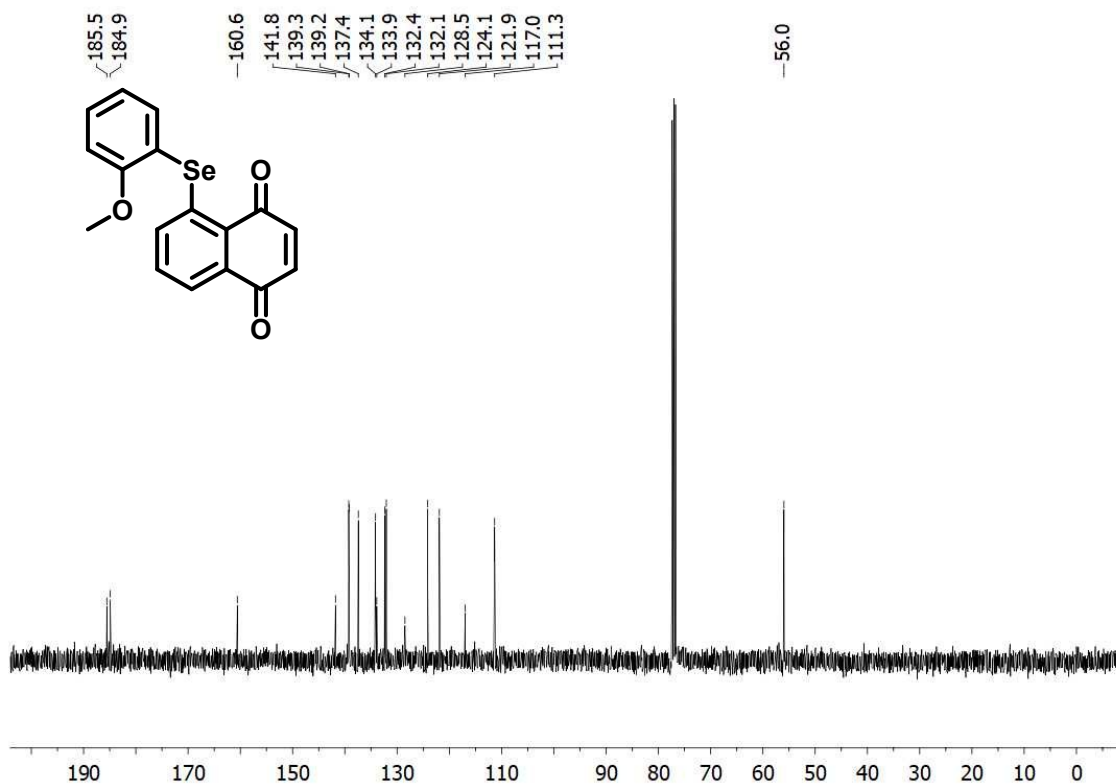
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2m**



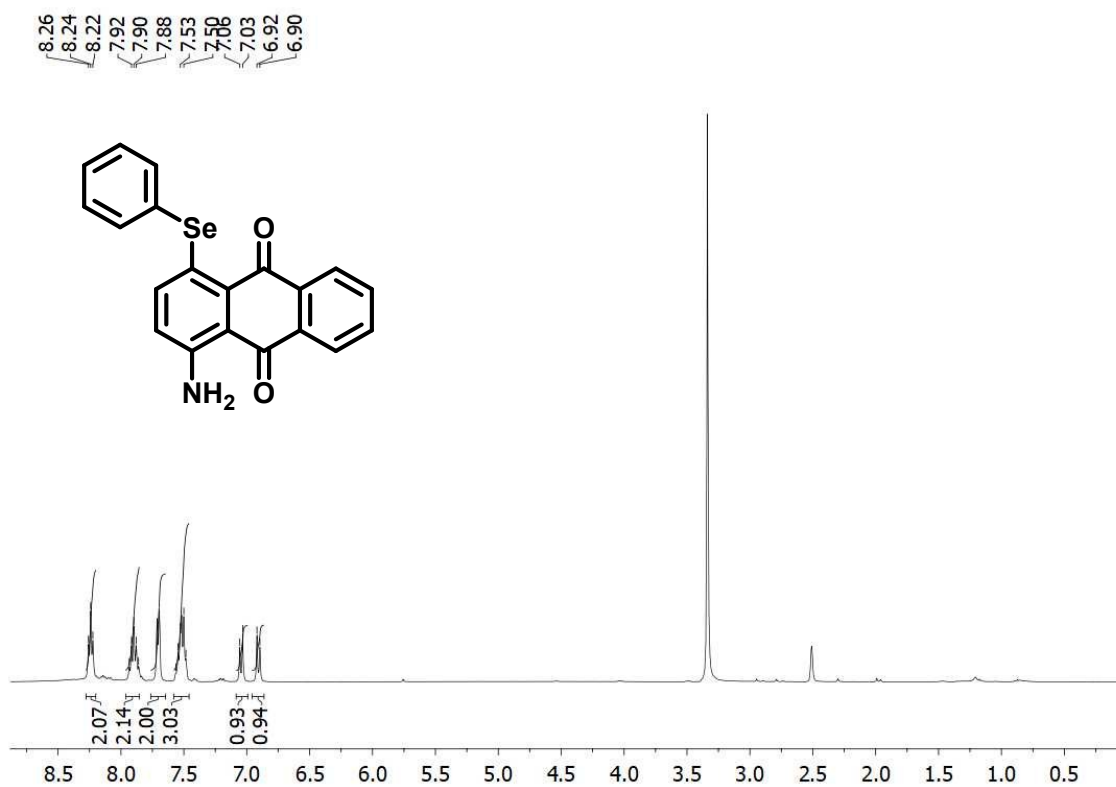
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2m**



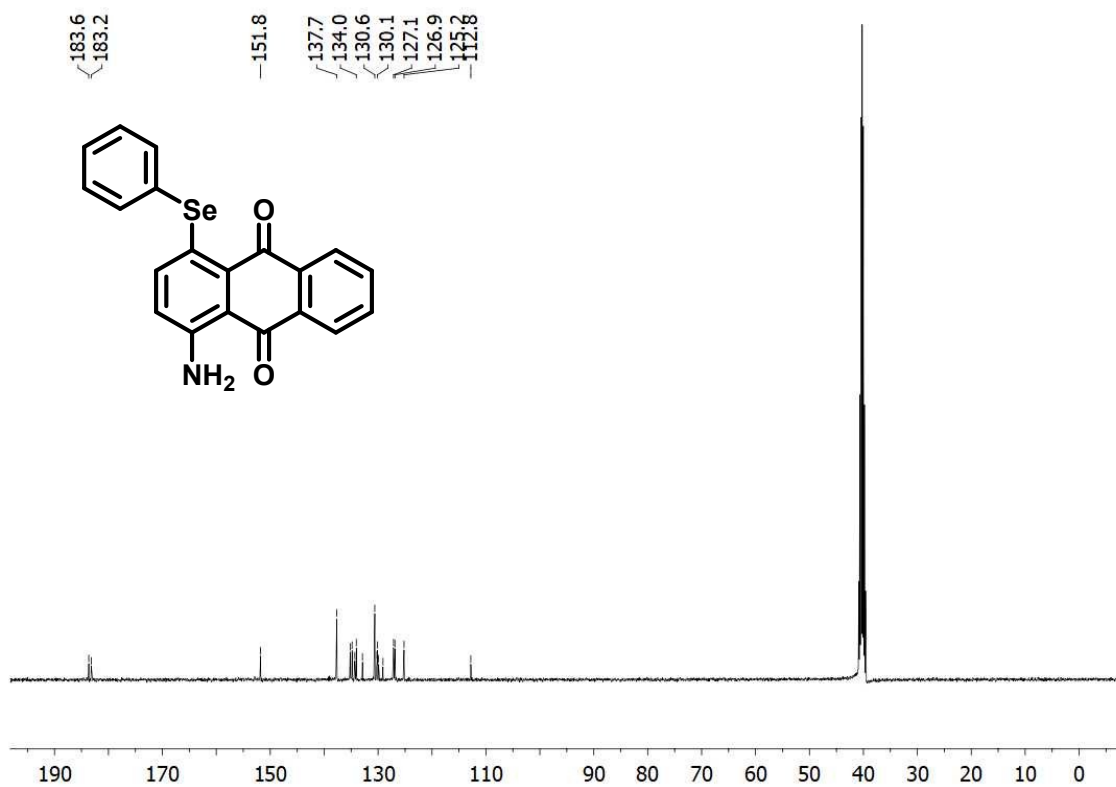
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2n**



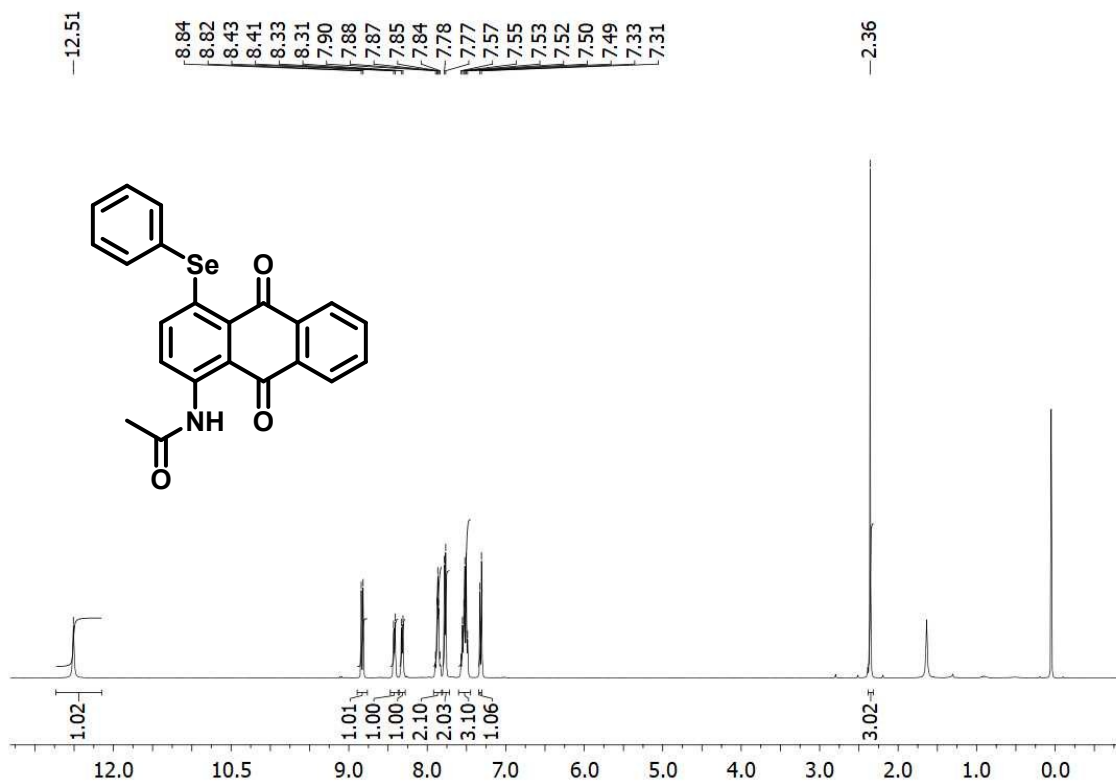
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2n**



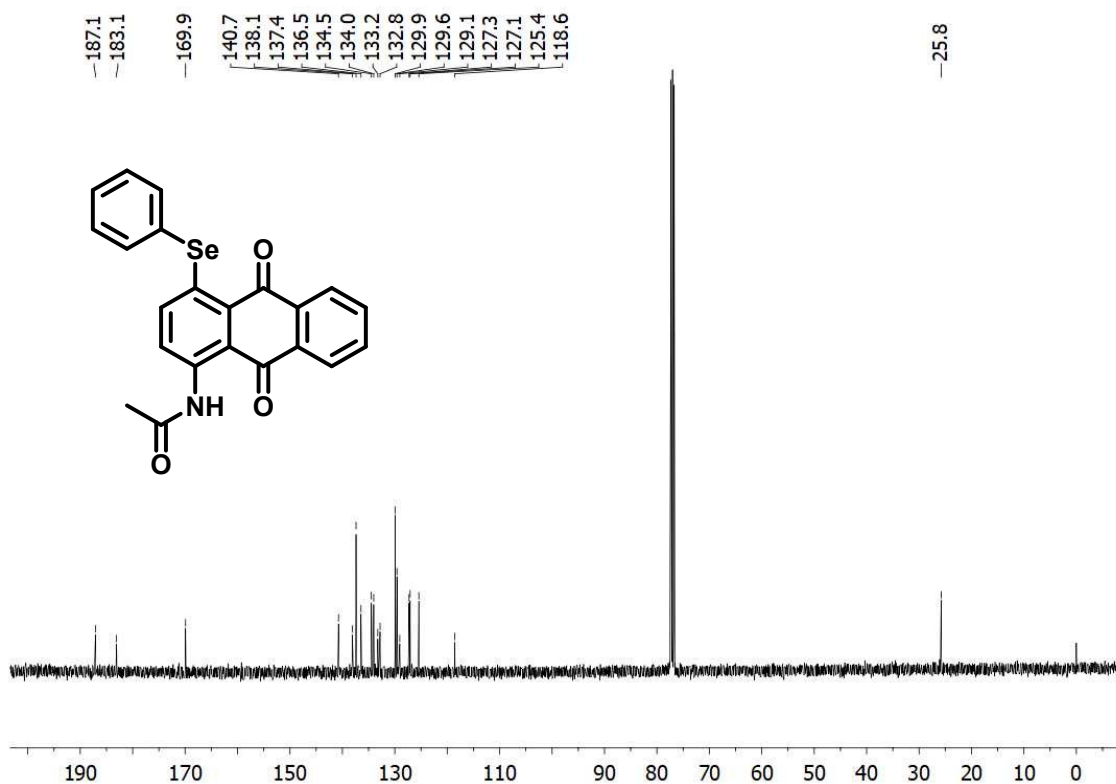
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound **2o**



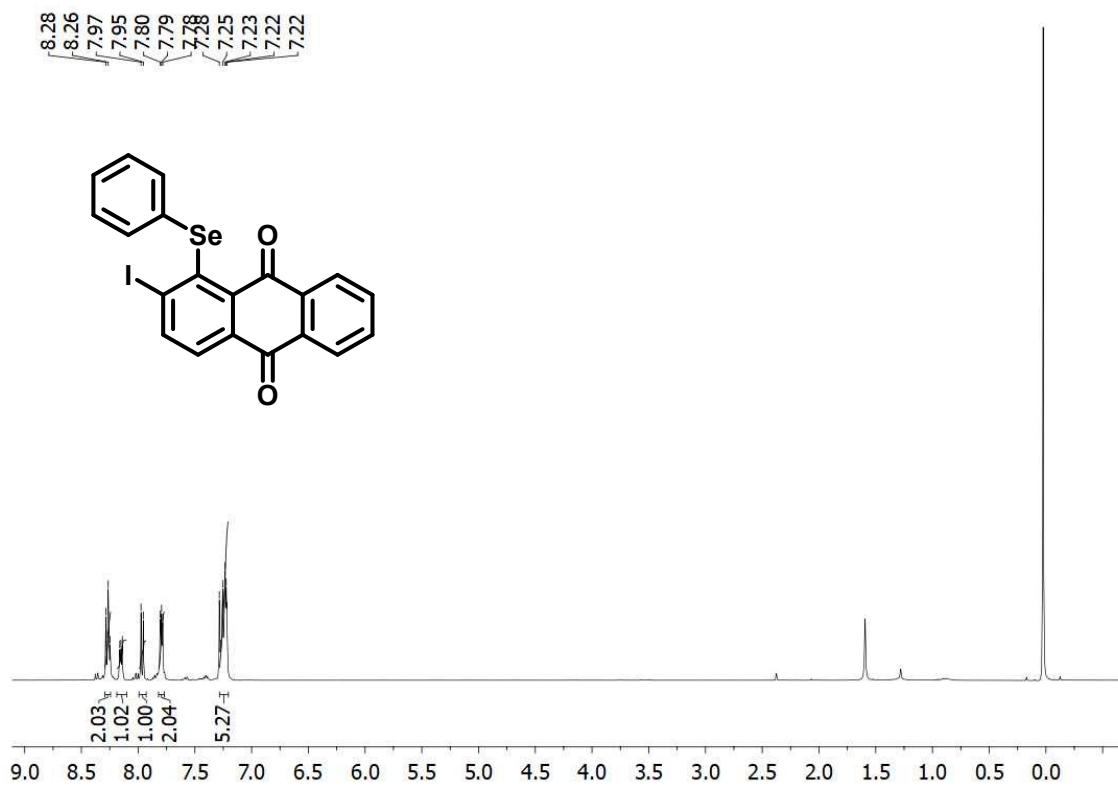
¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of compound **2o**



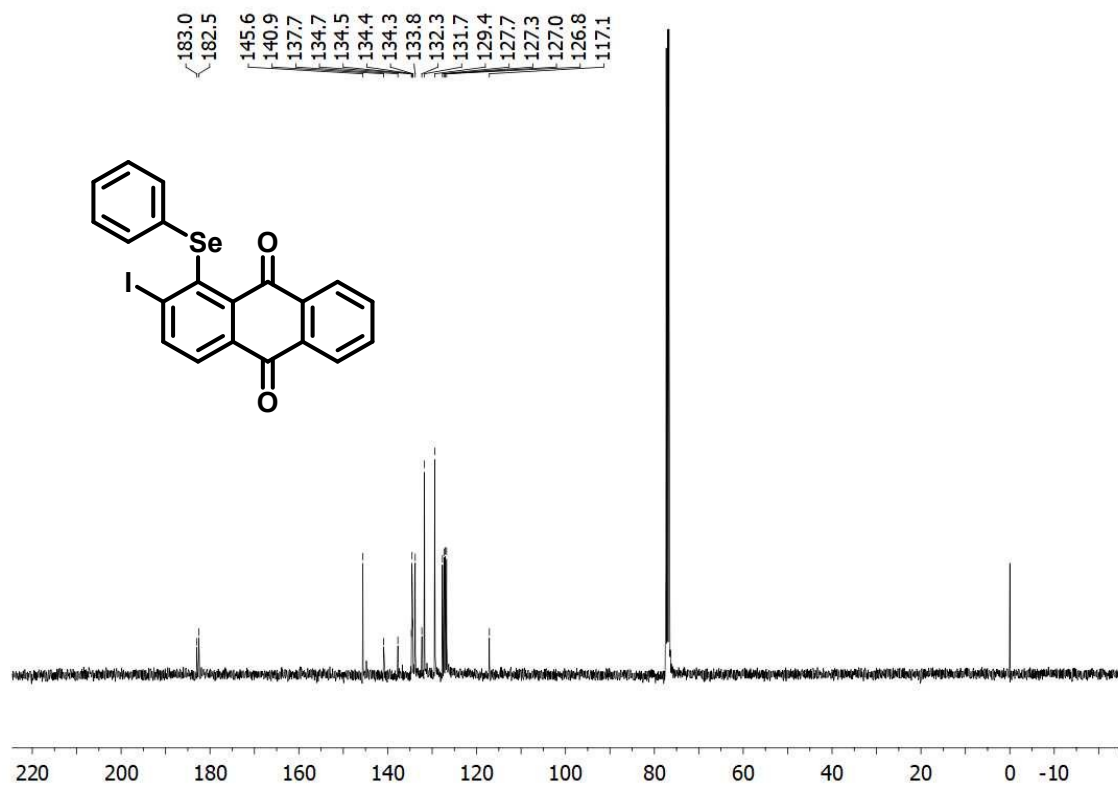
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2p**



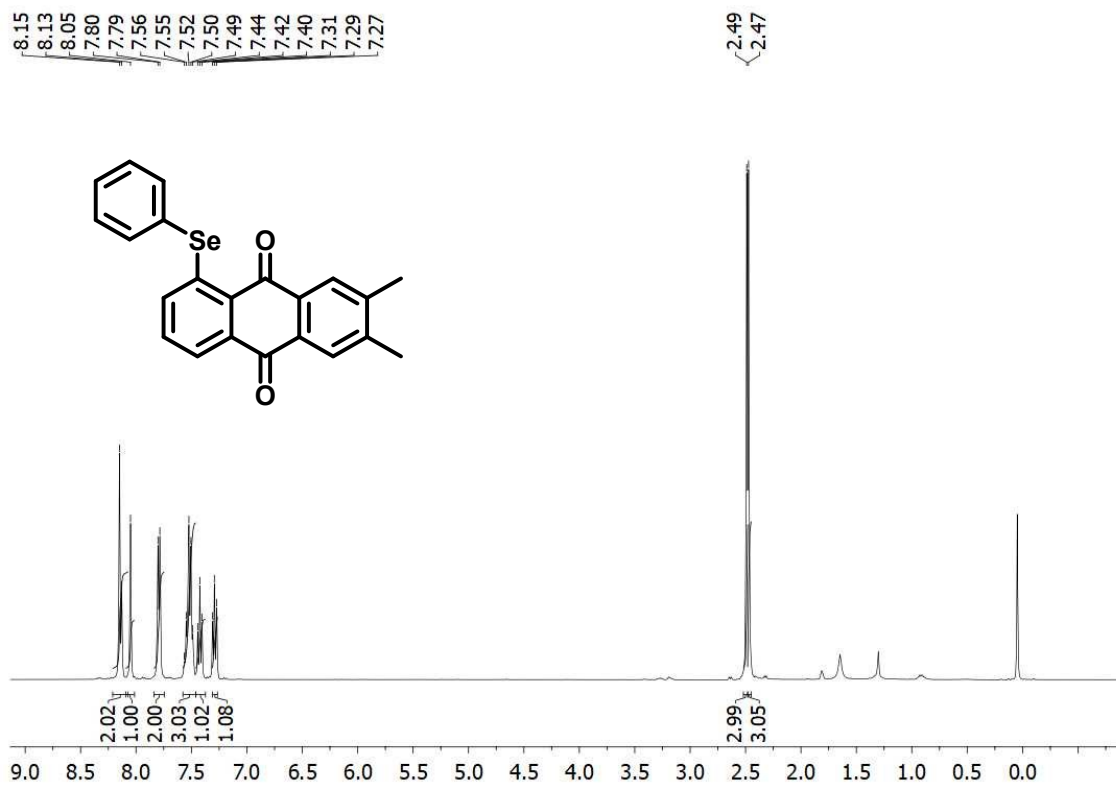
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2p**



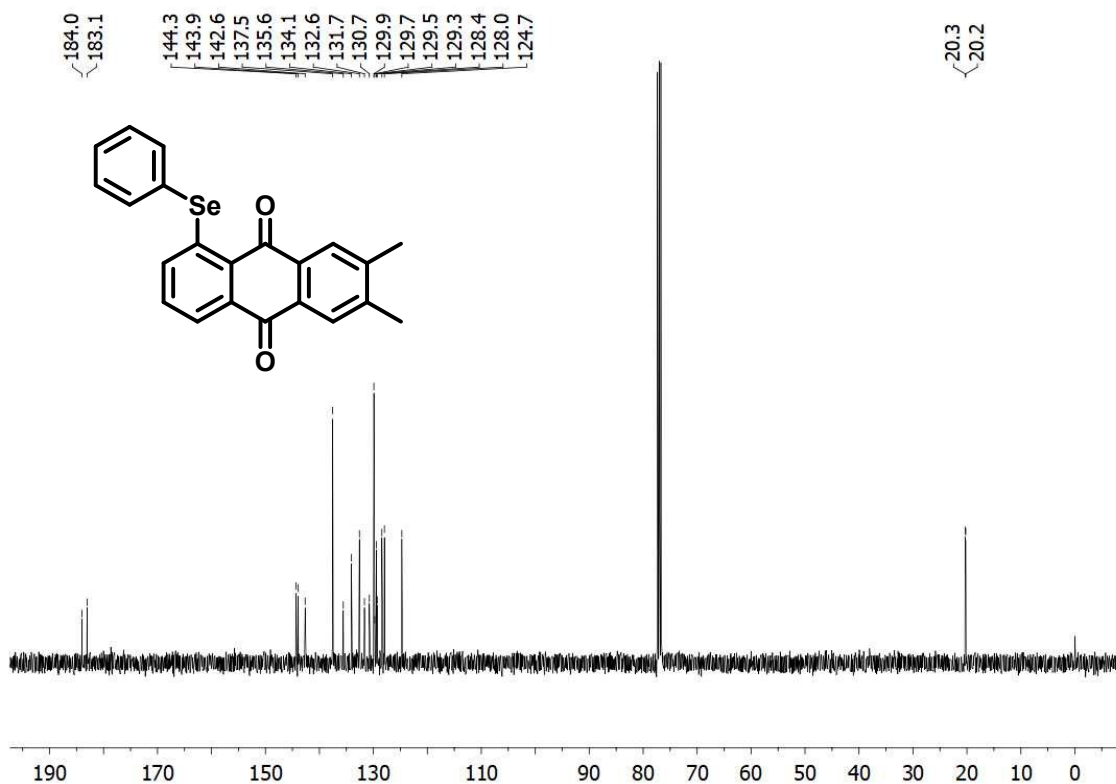
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2q**



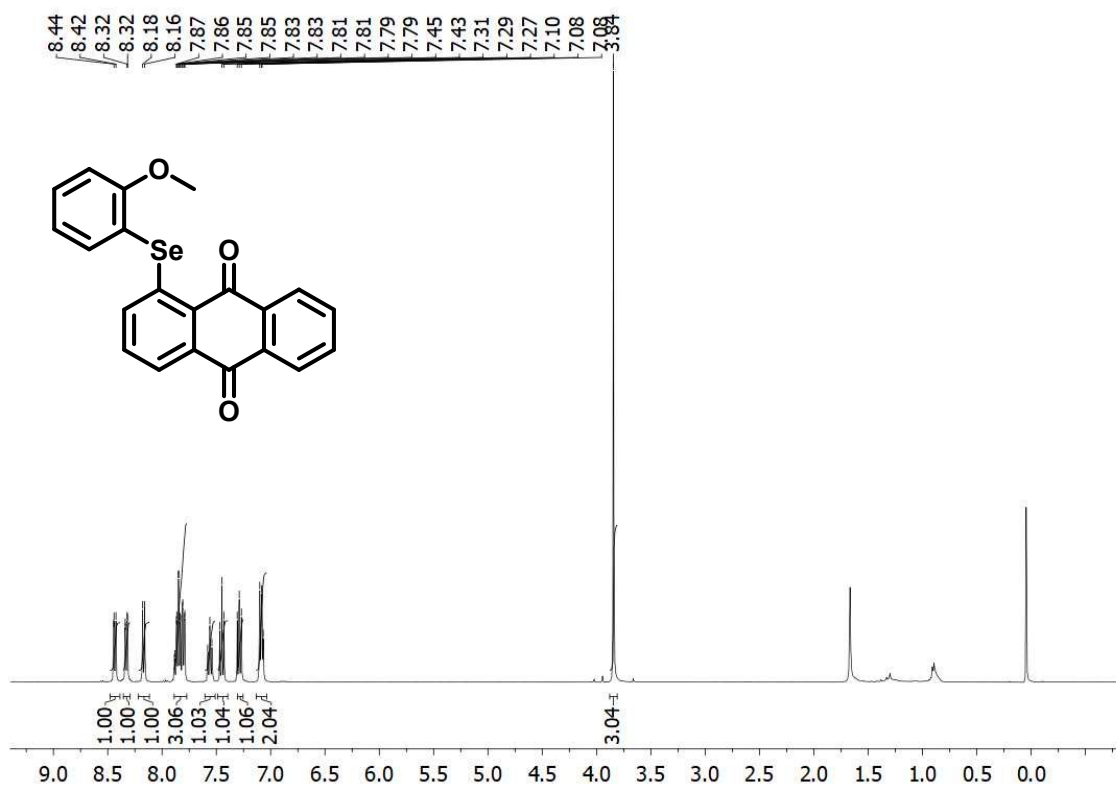
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2q**



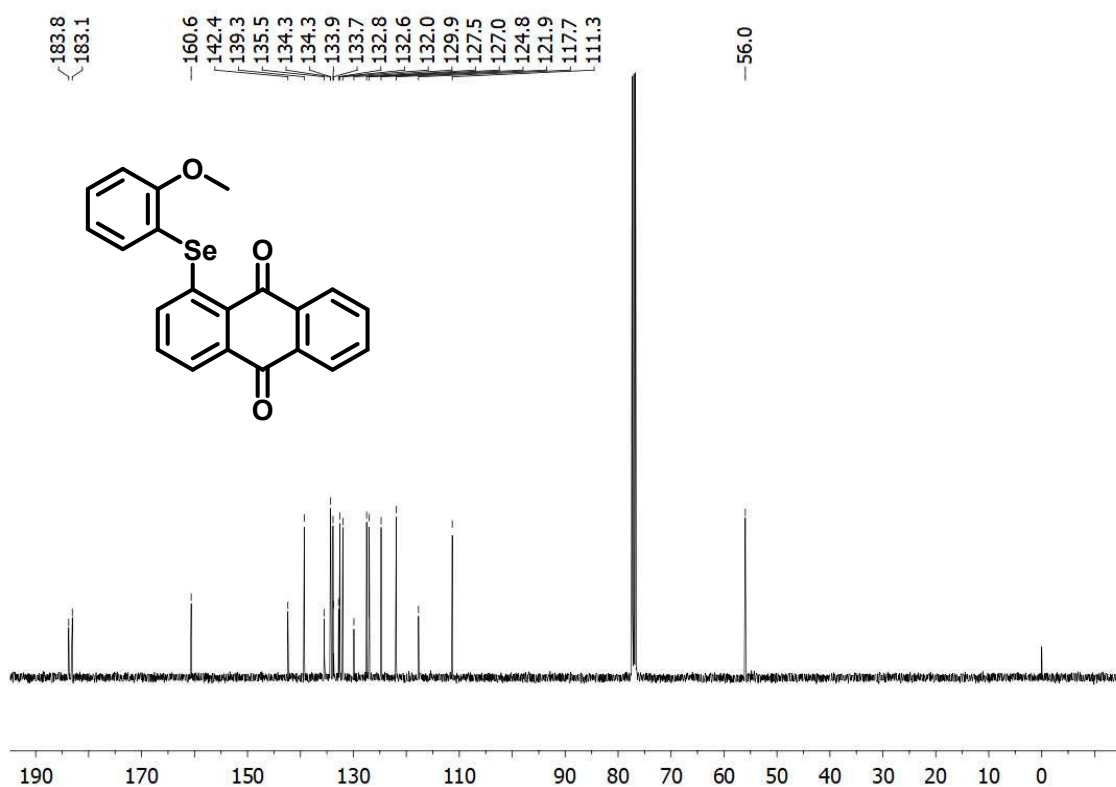
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2r**



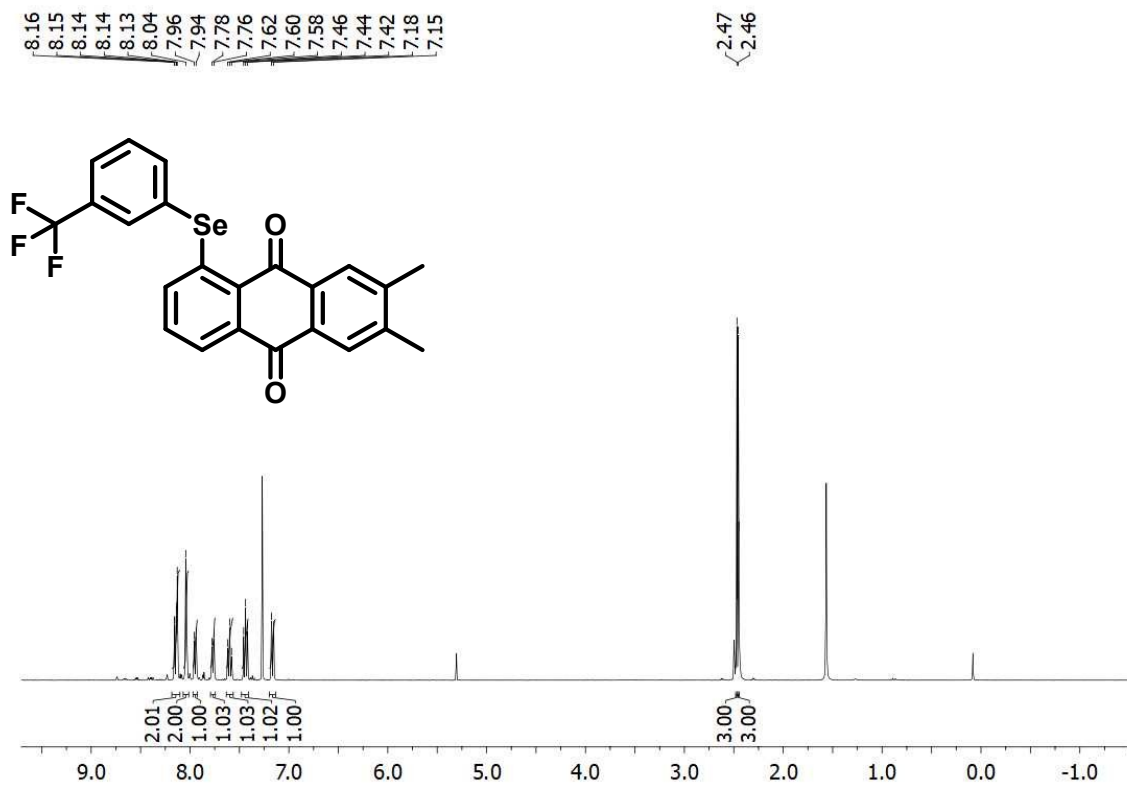
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2r**



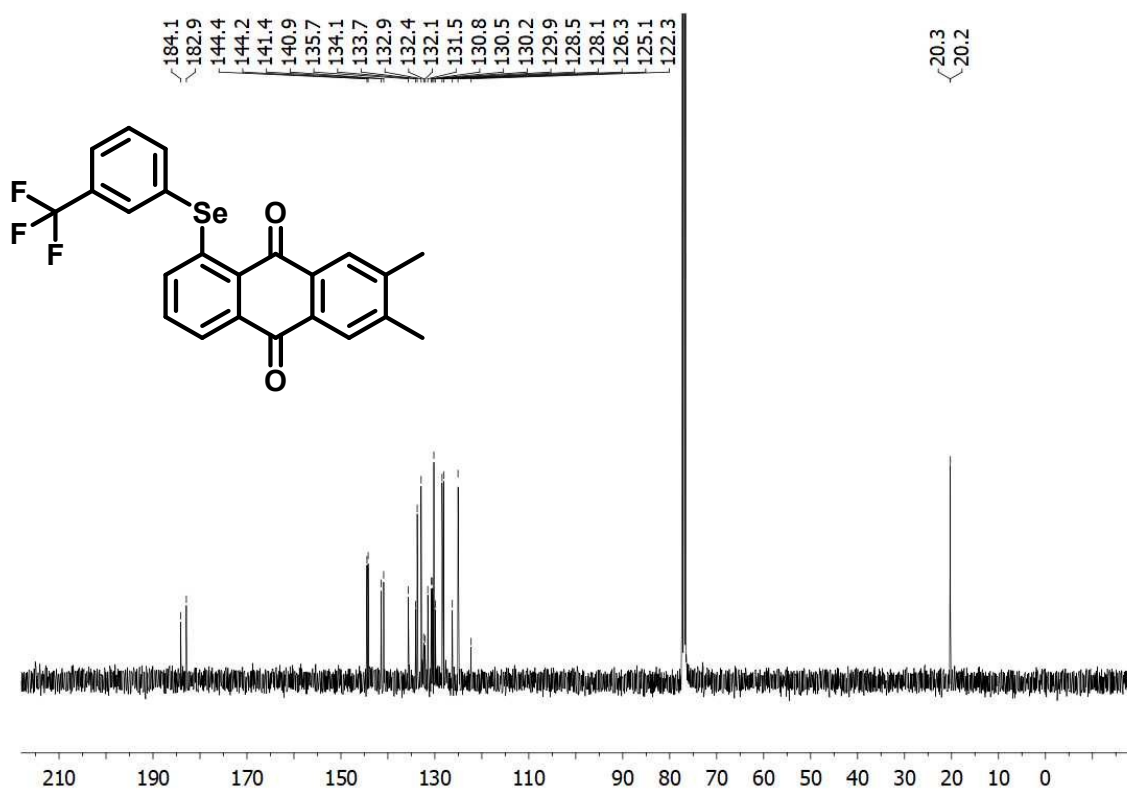
^1H NMR spectrum (400 MHz, CDCl_3) of compound **2s**



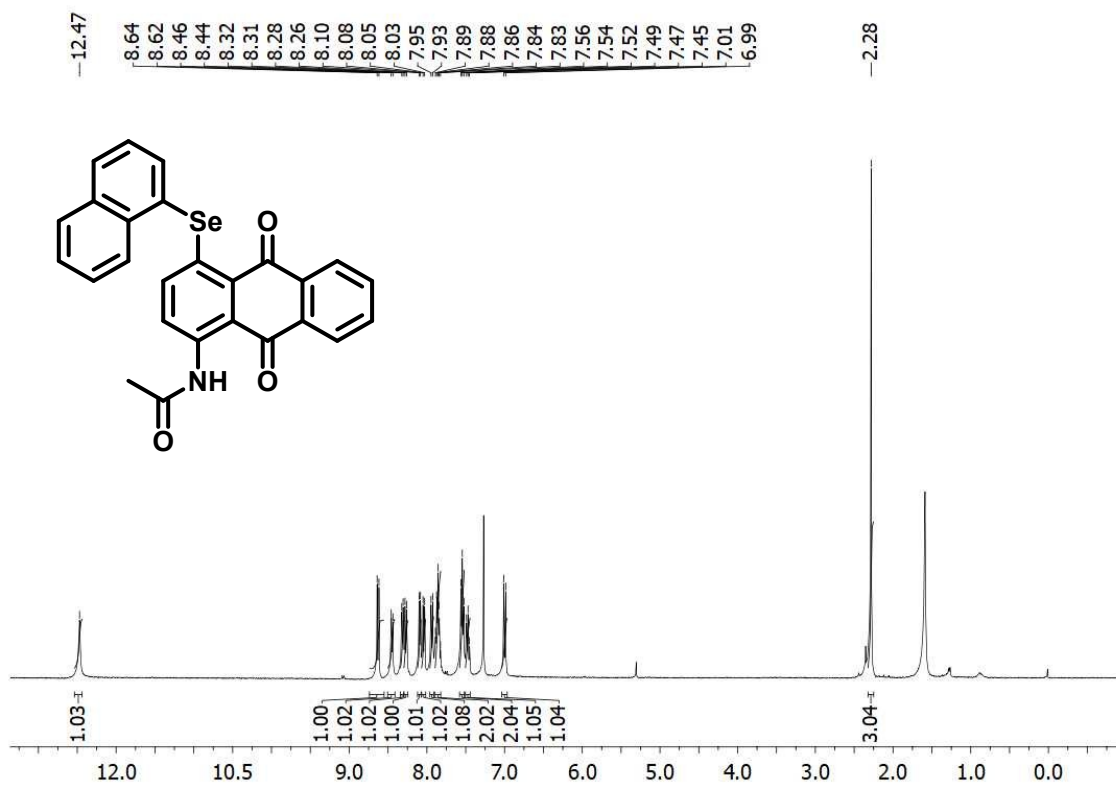
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **2s**



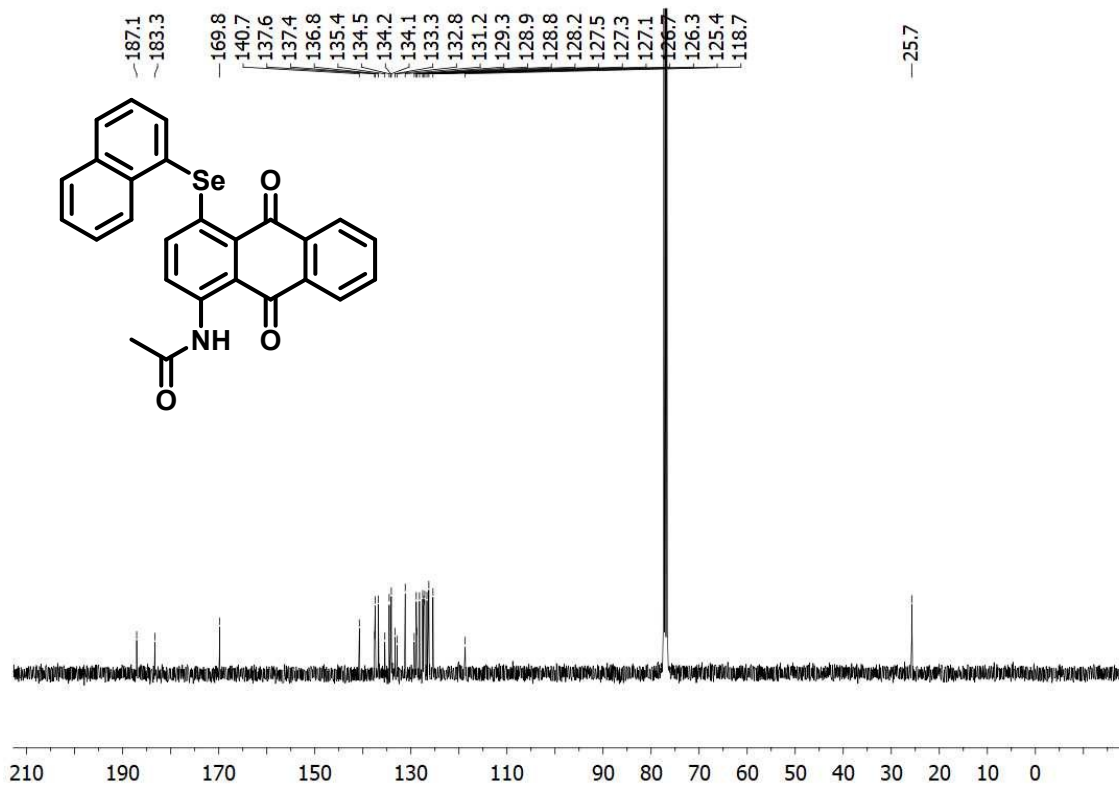
^1H NMR spectrum (400 MHz, CDCl_3) of compound **2t**



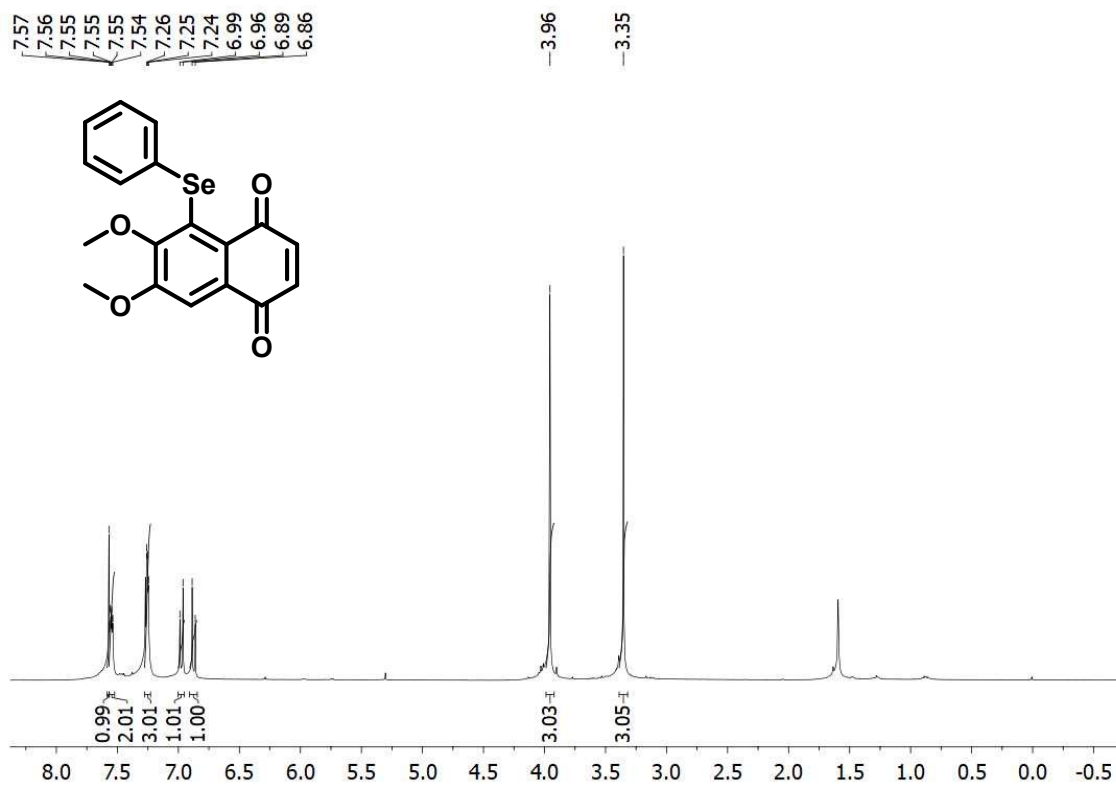
^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **2t**



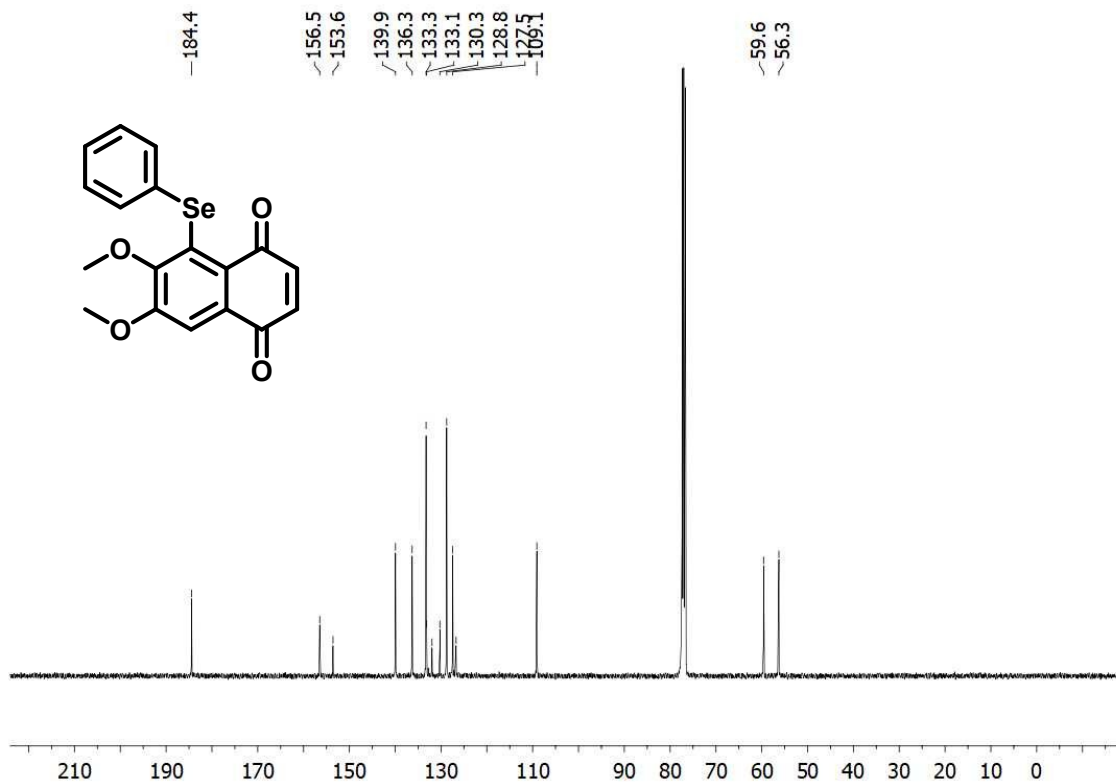
¹H NMR spectrum (400 MHz, CDCl₃) of compound **2u**



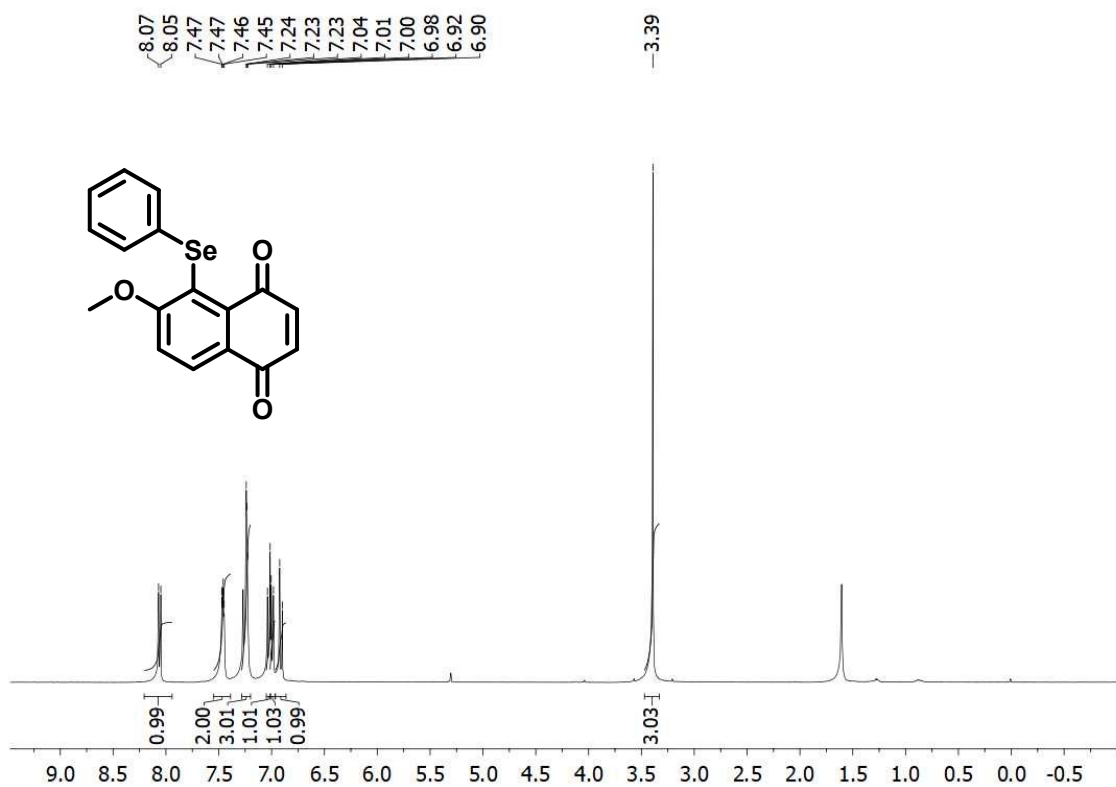
¹³C NMR spectrum (100 MHz, CDCl₃) of compound **2u**



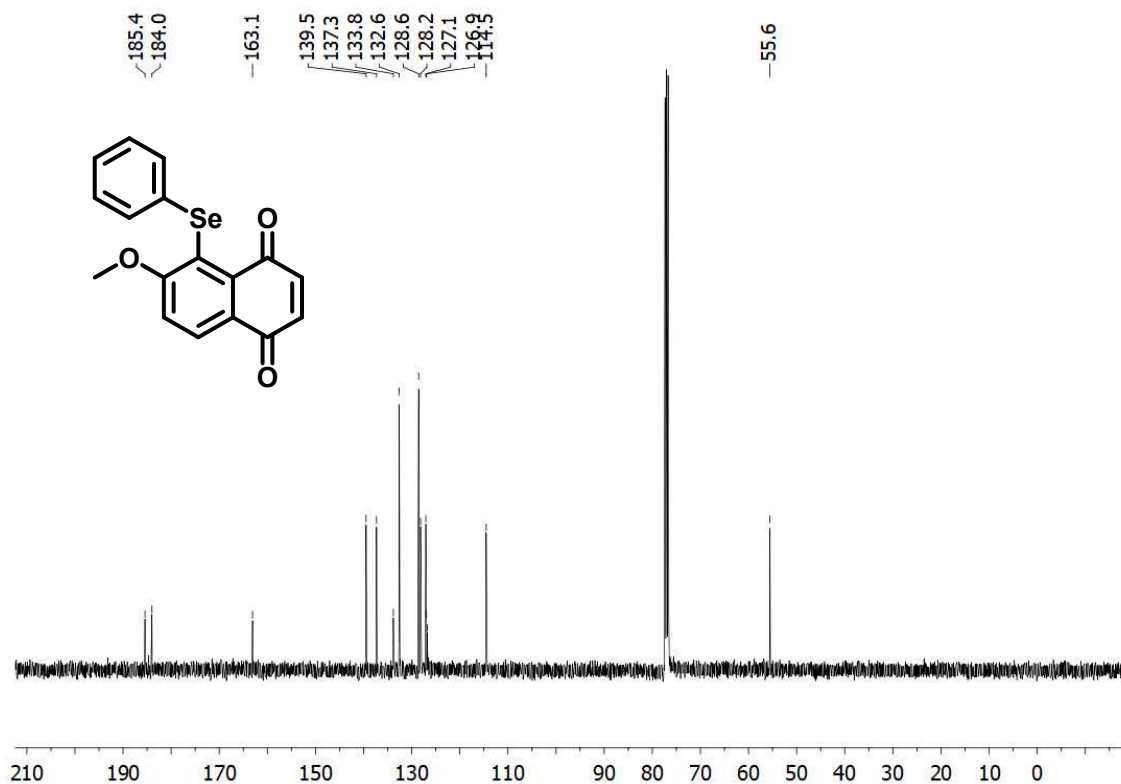
^1H NMR spectrum (400 MHz, CDCl_3) of compound **2v**



^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **2v**



$^1\text{H NMR}$ spectrum (400 MHz, CDCl_3) of compound **2x**



$^{13}\text{C NMR}$ spectrum (100 MHz, CDCl_3) of compound **2x**

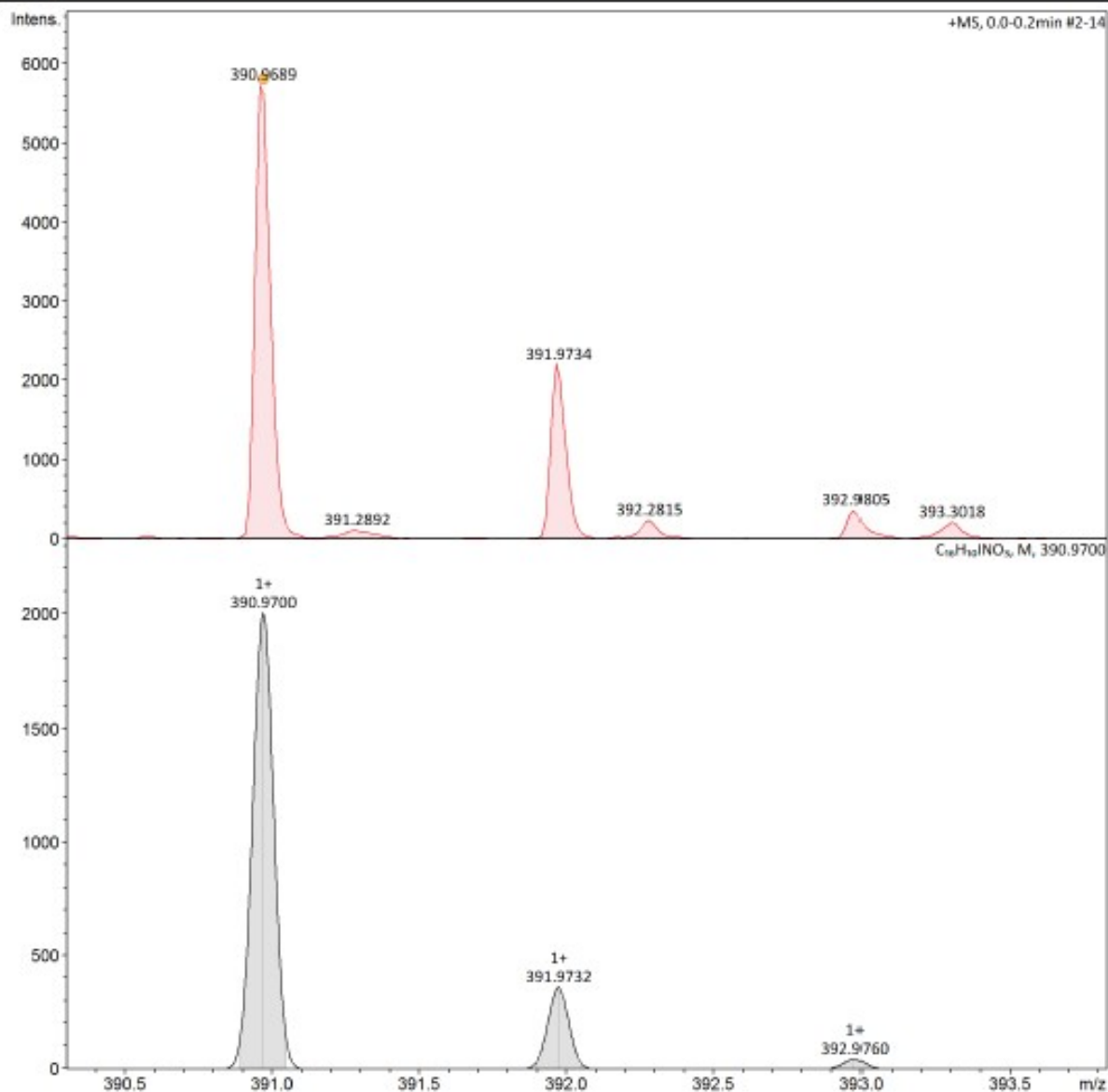
HRMS (APPI⁺) of compound **1p**

Display Report

Analysis Info		Acquisition Date	4/17/2019 12:06:14 PM	
Analysis Name	D:\Data\LabSELEN Marcelo QMC CFM 17-04-2019\ENSJ 875000002.d		Operator	tofq
Method	DEFAULT_adptado 27 03 2019 APPI até limpeza.m		Instrument	micrOTOF-Q 228888.10243
Sample Name	LabSELEN Marcelo QMC CFM 17-04-2019			
Comment				

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

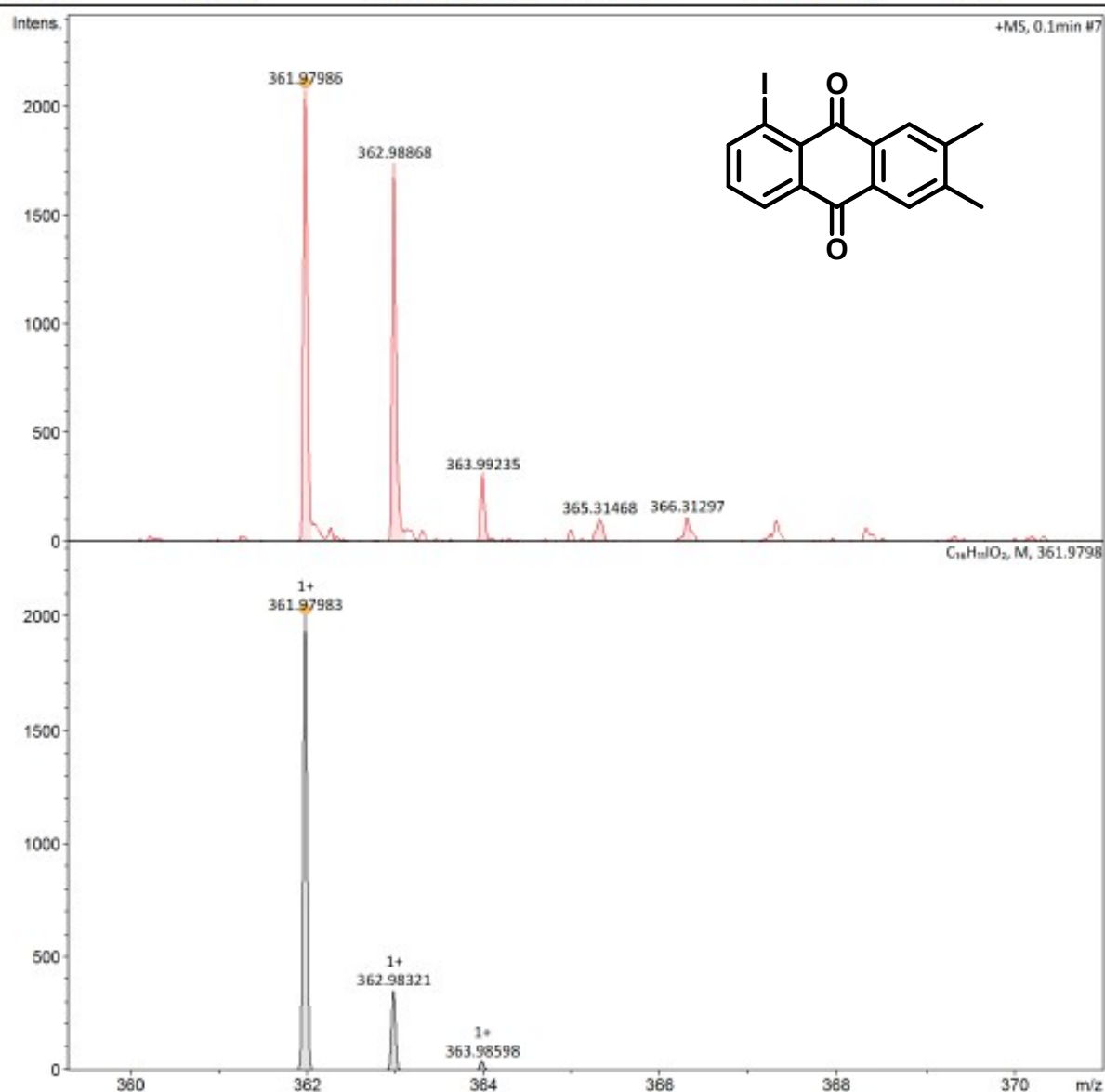


HRMS (APPI⁺) of compound **1q**

Display Report

Analysis Info		Acquisition Date	6/10/2019 2:33:23 PM
Analysis Name	D:\Data\2019\Q-TOF\LabSELEN\LabSELEN Marcelo QMC CFM 10-06-2019\889000001.d	Operator	micrOTOF-QII
Method	appi 10 06 19.m	Instrument	micrOTOF-Q 228888.10243
Sample Name	889		
Comment			

Acquisition Parameter					
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

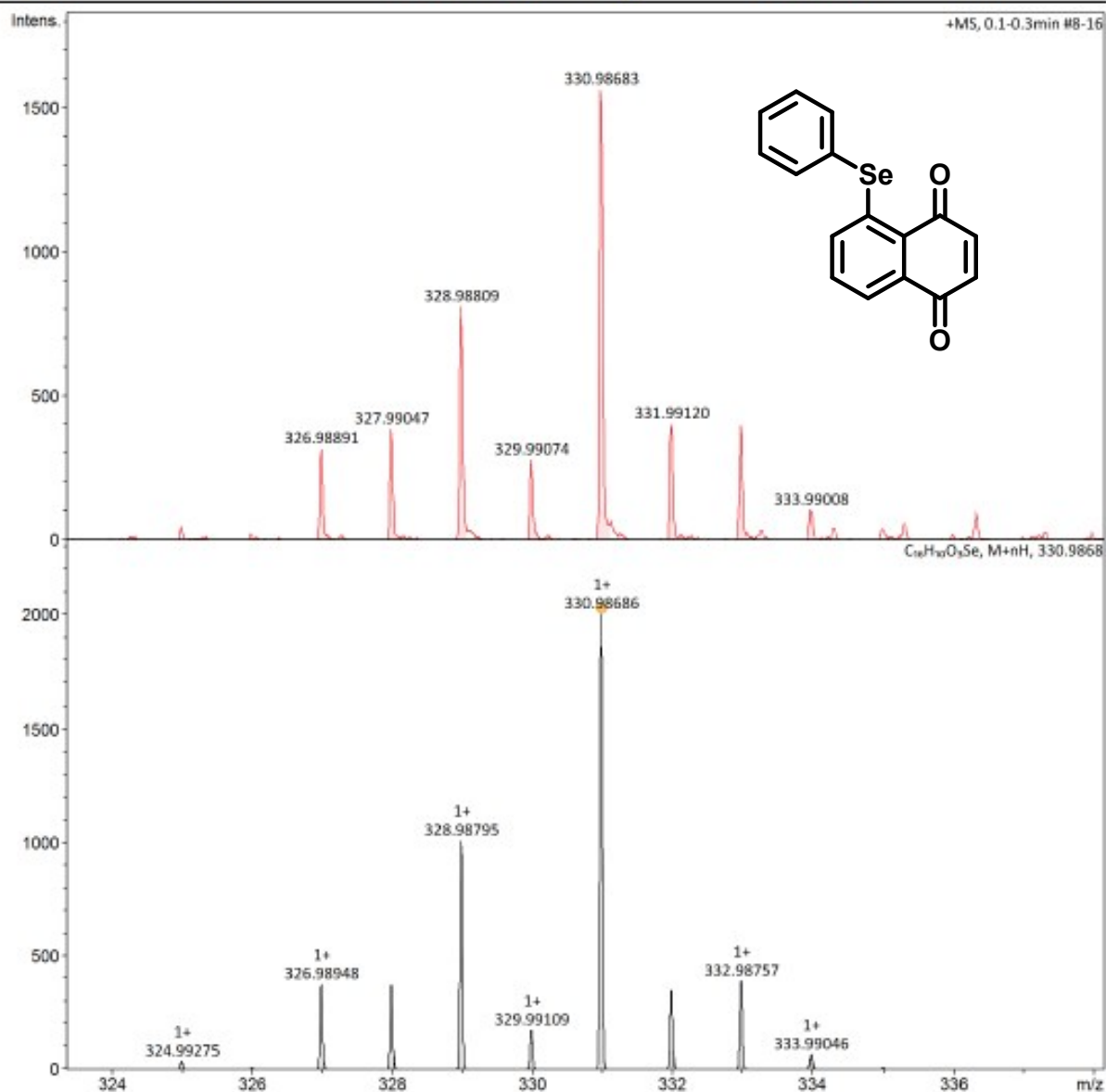


HRMS (APPI⁺) of compound **2a**

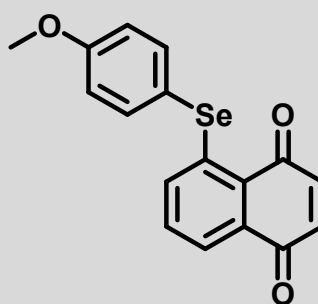
Display Report

Analysis Info		Acquisition Date 6/10/2019 3:55:17 PM
Analysis Name	D:\Data\2019\Q-TOF\LabSELEN\LabSELEN Marcelo QMC CFM 10-06-2019\820000001.d	Operator micrOTOF-QII
Method	tune low appi 10 06 19.m	Instrument micrOTOF-Q 228888.10243
Sample Name	820	
Comment		

Acquisition Parameter					
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



HRMS (APPI⁺) of compound **2b**



HRMS (APPI⁺) of compound **2c**

Display Report

Analysis Info

Analysis Name	D:\Data\2019\Q-TOF\LabSELEN\LabSELEN Marcelo QMC CFM 10-06-2019\821000001.d
Method	tune low appi 10 06 19.m
Sample Name	821
Comment	

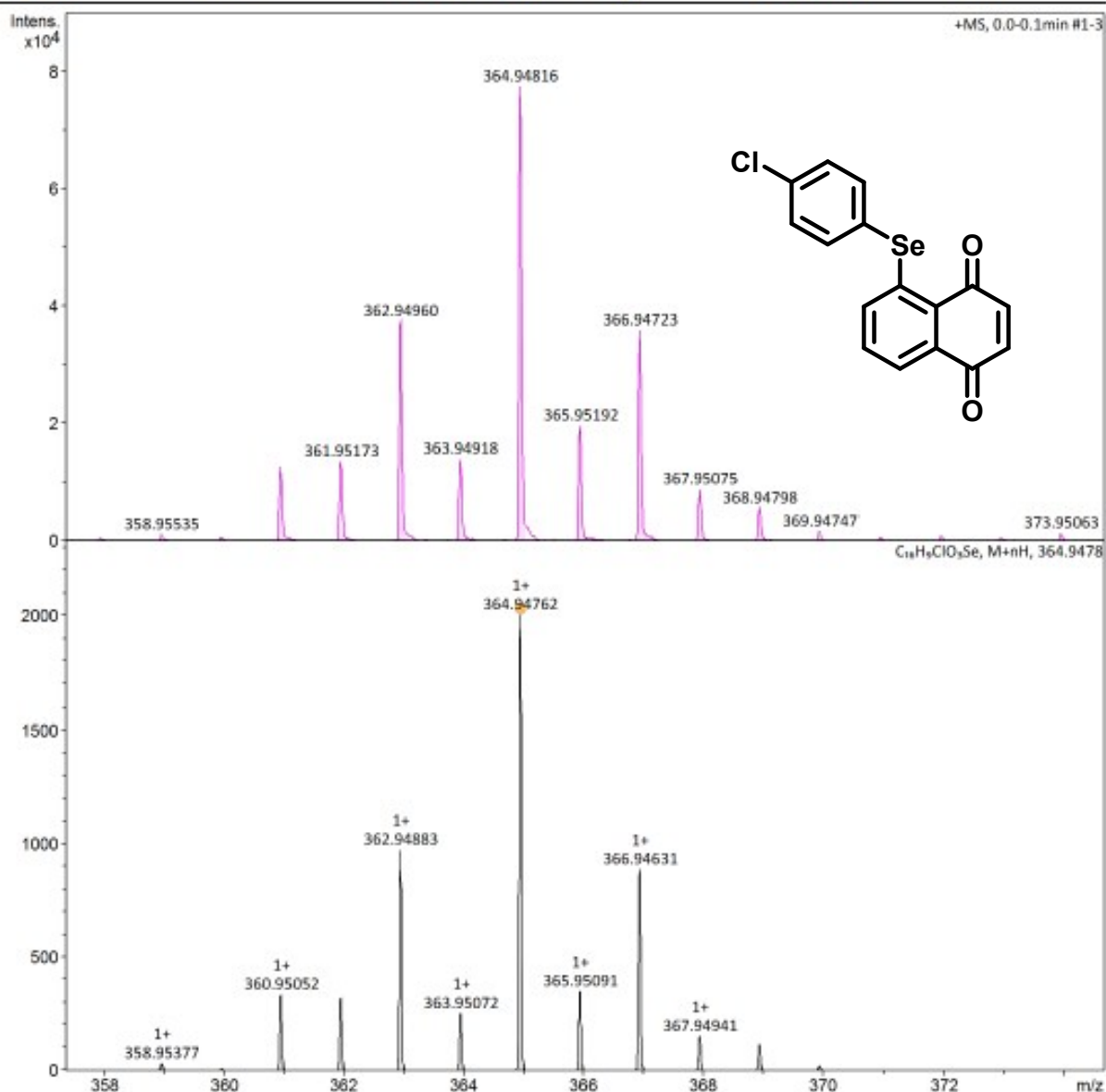
Acquisition Date 6/10/2019 4:11:13 PM

Operator micrOTOF-QII

Instrument micrOTOF-Q 228888.10243

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

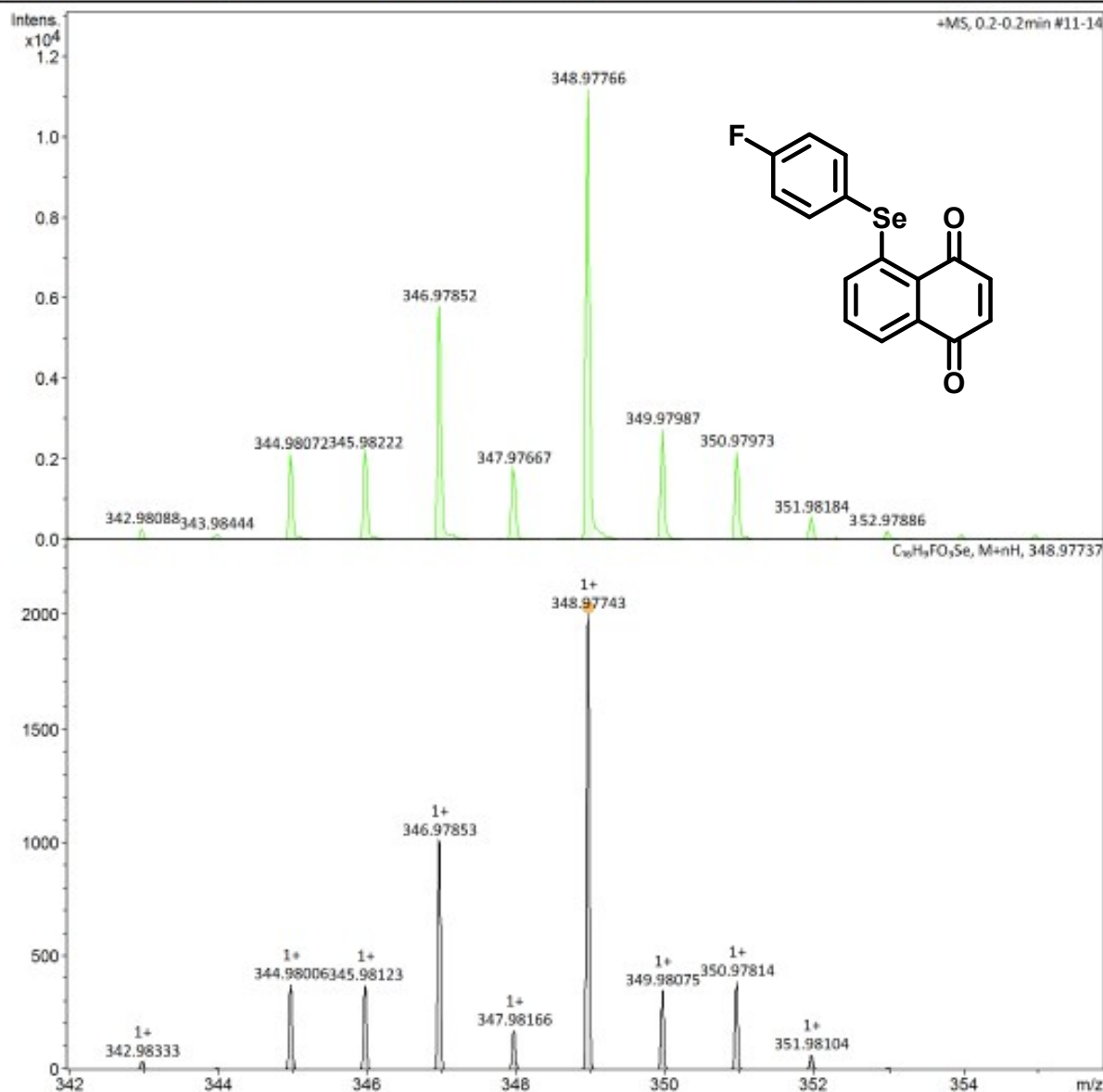


HRMS (APPI⁺) of compound **2d**

Display Report

Analysis Info		Acquisition Date 6/10/2019 4:51:24 PM
Analysis Name	D:\Data\2019\Q-TOF\LabSELEN\LabSELEN Marcelo QMC CFM 10-06-2019\823000002.d	Operator micrOTOF-QII
Method	tune low appi 10 06 19 Vanessa.m	Instrument micrOTOF-Q 228888.10243
Sample Name	823	
Comment		

Acquisition Parameter					
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

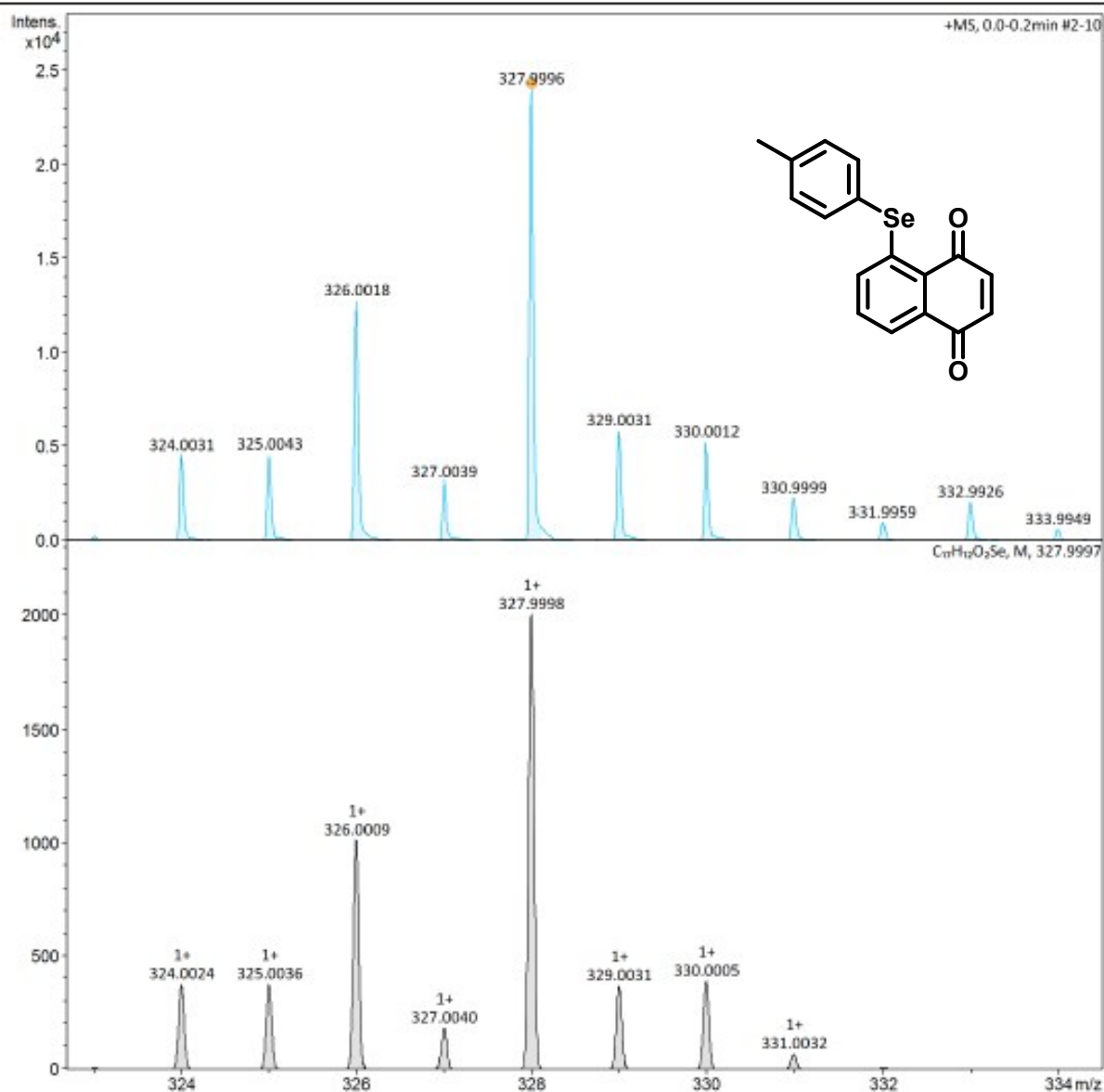


HRMS (APPI⁺) of compound **2e**

Display Report

Analysis Info		Acquisition Date	4/17/2019 10:13:27 AM	
Analysis Name	D:\Data\LabSELEN Marcelo QMC CFM 17-04-2019\ENSJ 822000004.d	Operator	tofq	
Method	DEFAULT_adptado 27 03 2019 APPI até limpeza.m	Instrument	micrOTOF-Q 228888.10243	
Sample Name	LabSELEN Marcelo QMC CFM 17-04-2019	Comment		

Acquisition Parameter					
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS (APPI⁺) of compound **2k**

Display Report

Analysis Info

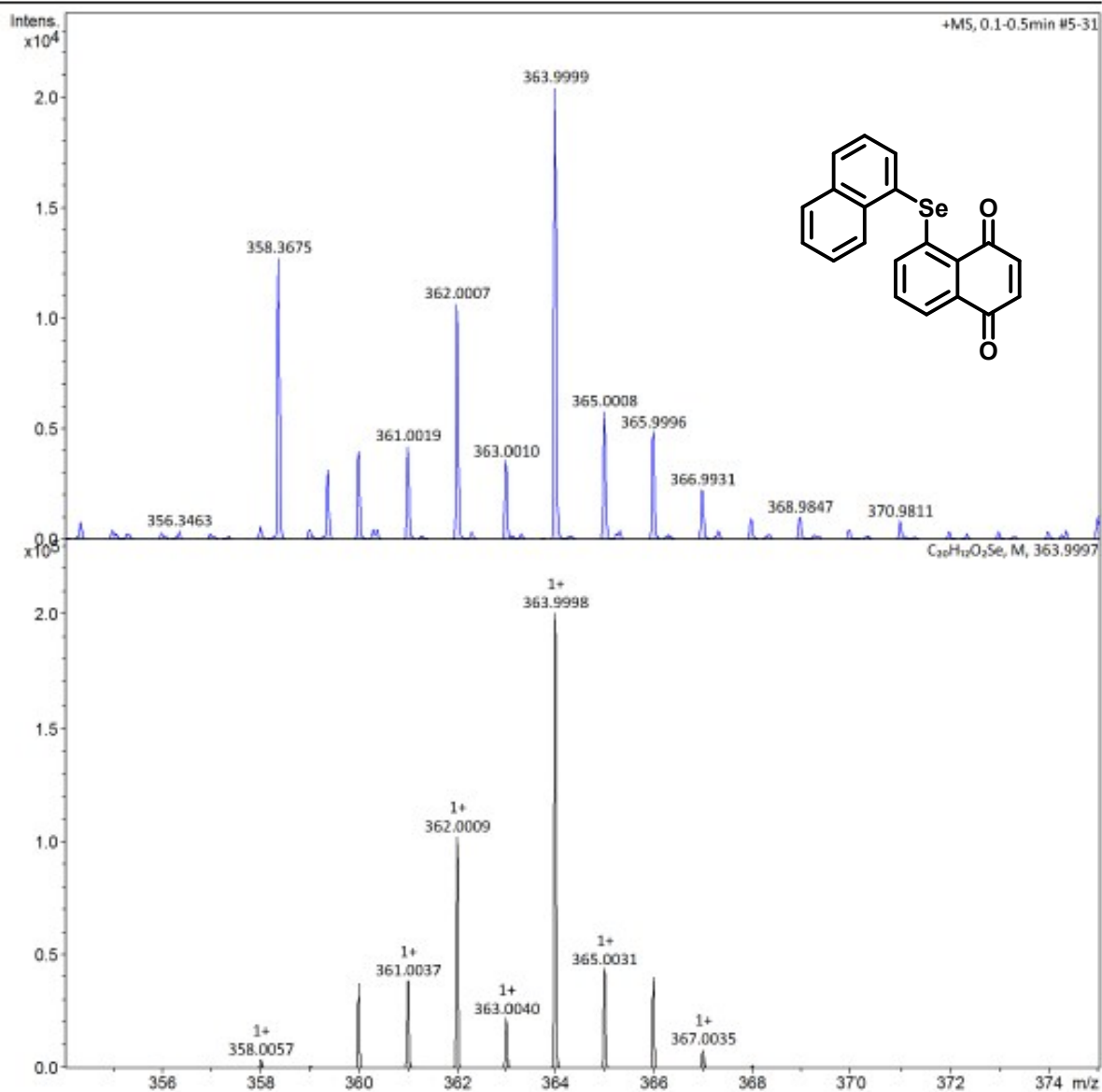
Analysis Name D:\Data\LabSelen 11.01.19\GJSC060000004.d
 Method DEFAULT_adptado Elis APPI.m
 Sample Name GJSC060
 Comment

Acquisition Date 1/11/2019 10:03:09 AM

Operator tofq
 Instrument micrOTOF-Q 228888.10243

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1200 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS (APPI⁺) of compound **21**

Display Report

Analysis Info

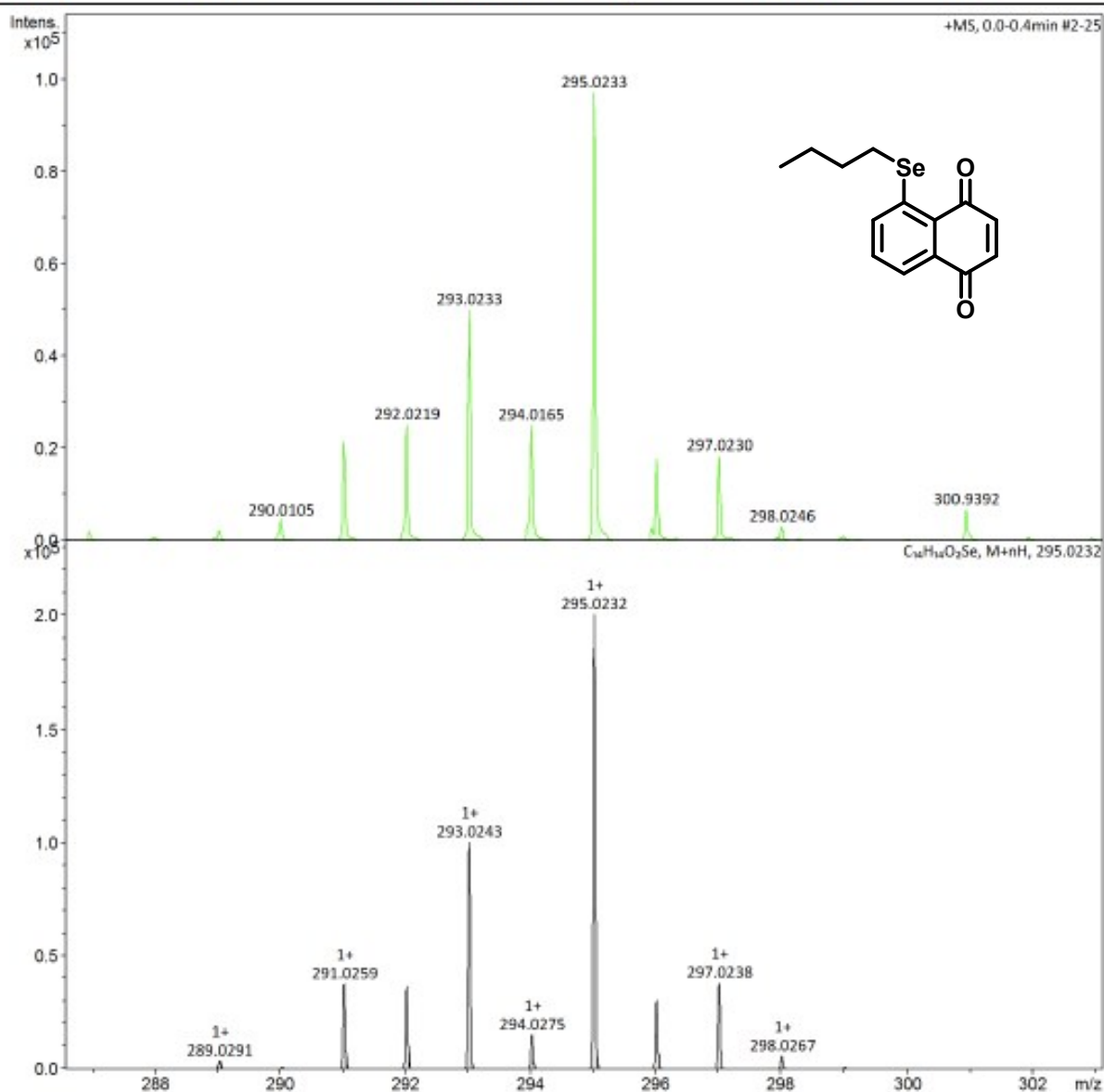
Analysis Name D:\Data\LabSelen 11.01.19\GJSC056000002.d
 Method tune_low_2018.m
 Sample Name GJSC056
 Comment

Acquisition Date 1/11/2019 11:34:01 AM

Operator tofq
 Instrument micrOTOF-Q 228888.10243

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



HRMS (APPI⁺) of compound **2m**

Display Report

Analysis Info

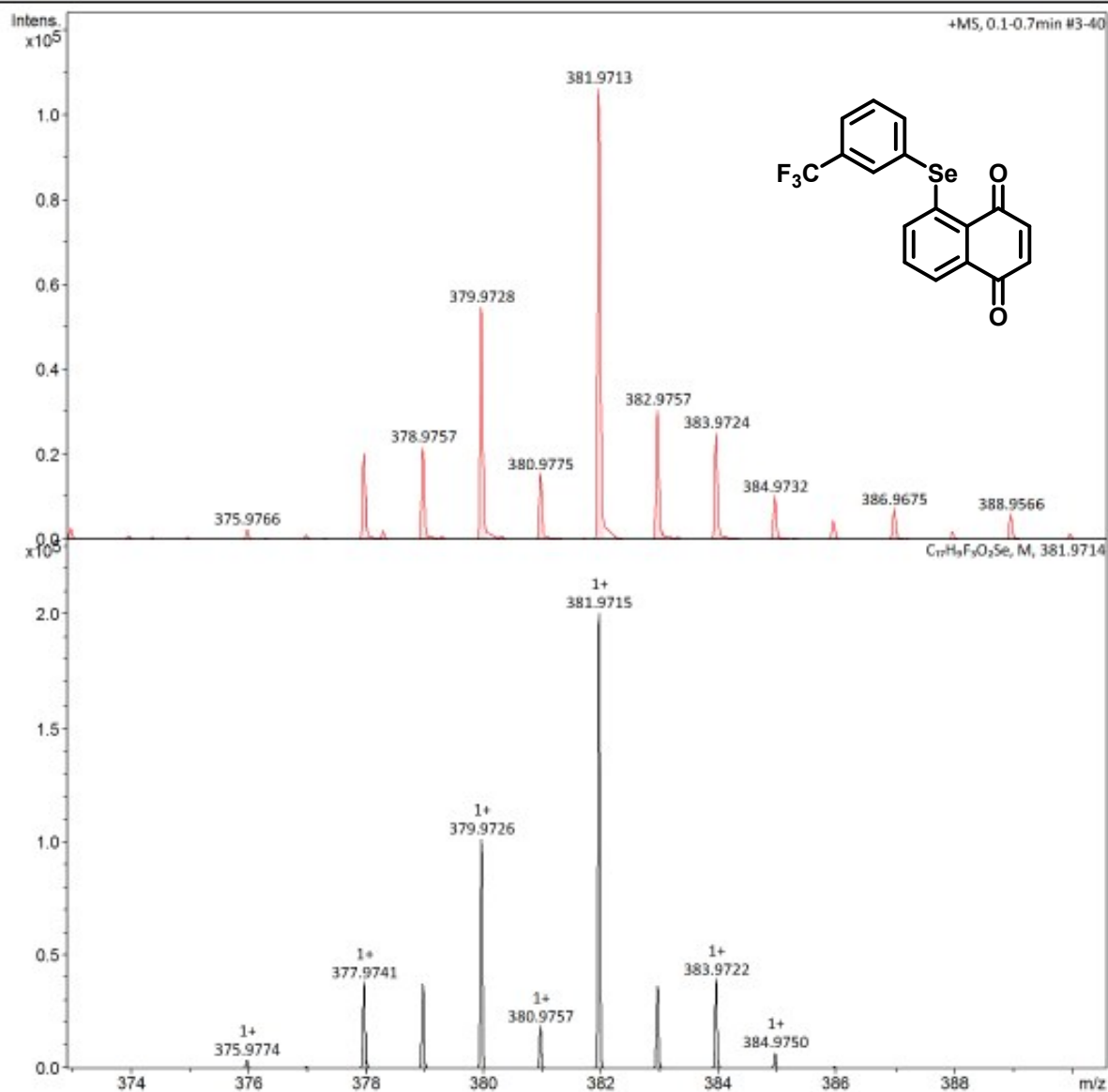
Analysis Name D:\Data\LabSelen 11.01.19\GJSC061000001.d
 Method DEFAULT_adptado Elis APPI.m
 Sample Name GJSC061
 Comment

Acquisition Date 1/11/2019 10:11:40 AM

Operator tofq
 Instrument micrOTOF-Q 228888.10243

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1200 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS (APPI⁺) of compound **2n**

Display Report

Analysis Info

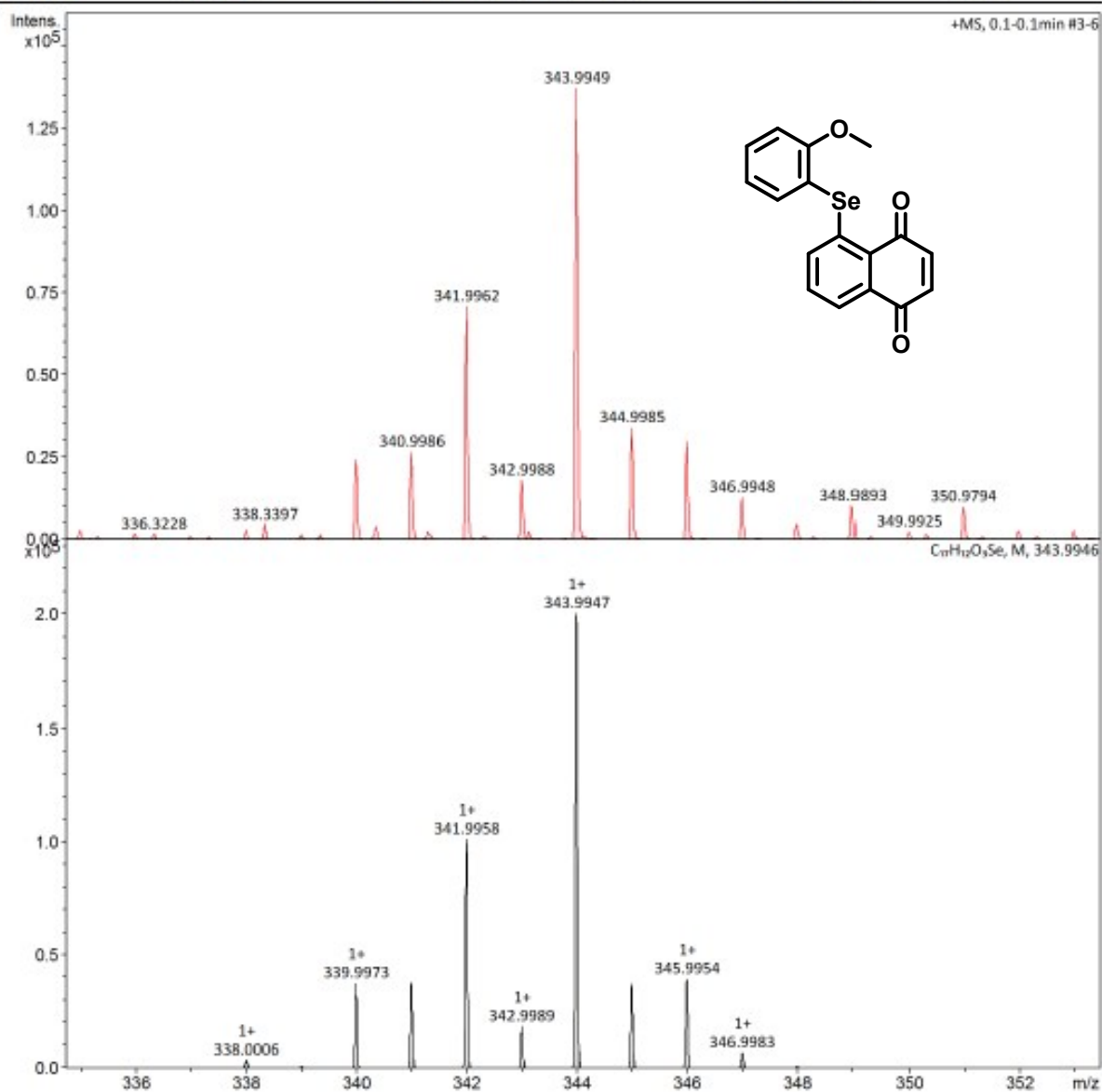
Analysis Name D:\Data\LabSelen 11.01.19\GJSC088000001.d
 Method testeinical APPI_Elis.m
 Sample Name GJSC088
 Comment

Acquisition Date 1/11/2019 10:30:12 AM

Operator tofq
 Instrument micrOTOF-Q 228888.10243

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulzer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



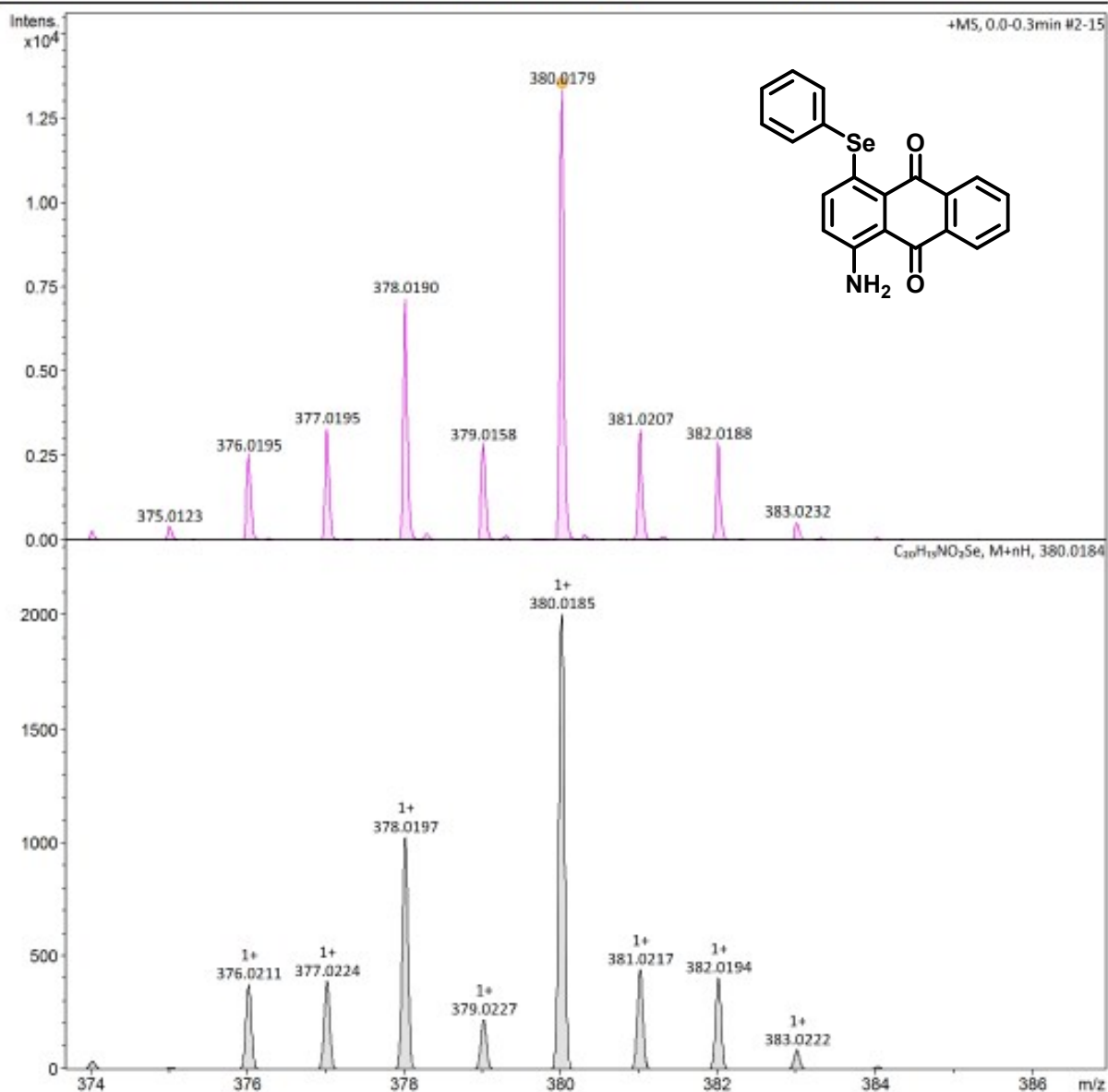
HRMS (APPI⁺) of compound **2o**

Display Report

Analysis Info		Acquisition Date	4/17/2019 11:48:37 AM	
Analysis Name	D:\Data\LabSELEN Marcelo QMC CFM 17-04-2019\ENSJ 874000003.d		Operator	tofq
Method	DEFAULT_adptado 27 03 2019 APPI até limpeza.m		Instrument	micrOTOF-Q 228888.10243
Sample Name	LabSELEN Marcelo QMC CFM 17-04-2019		Comment	

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS (APPI⁺) of compound 2p

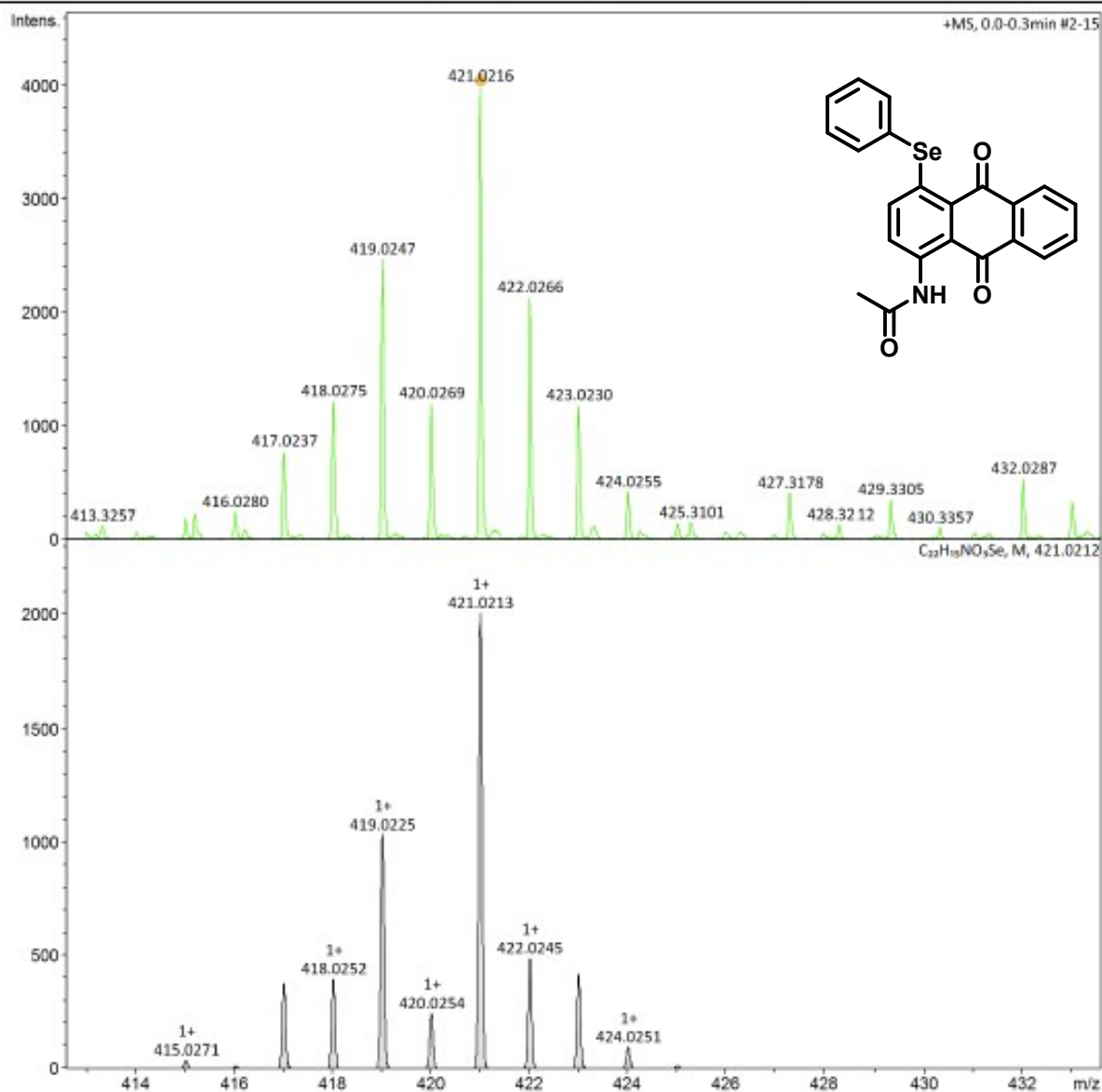
Display Report

Analysis Info

Analysis Name	D:\Data\LabSELEN Marcelo QMC CFM 17-04-2019\ENSJ 871000007.d	Acquisition Date	4/17/2019 12:51:22 PM
Method	DEFAULT_adptado 27 03 2019 APPI até limpeza.m	Operator	tofq
Sample Name	LabSELEN Marcelo QMC CFM 17-04-2019	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



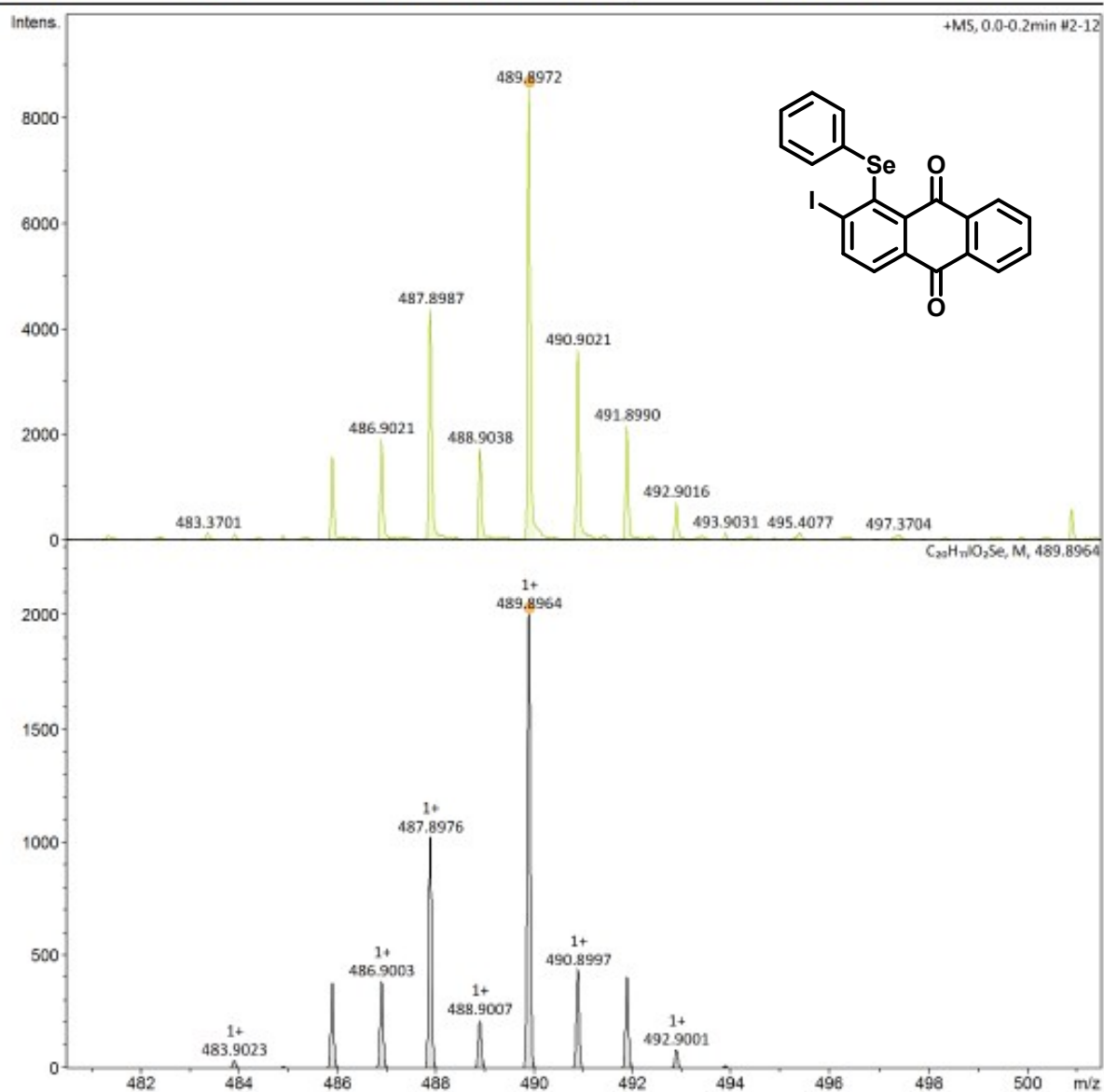
HRMS (APPI⁺) of compound 2q

Display Report

Analysis Info		Acquisition Date	4/17/2019 9:58:05 AM	
Analysis Name	D:\Data\LabSELEN Marcelo QMC CFM 17-04-2019\ENSJ 870000007.d		Operator	tofq
Method	DEFAULT_adptado 27 03 2019 APPI até limpeza.m		Instrument	micrOTOF-Q 228888.10243
Sample Name	LabSELEN Marcelo QMC CFM 17-04-2019			
Comment				

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



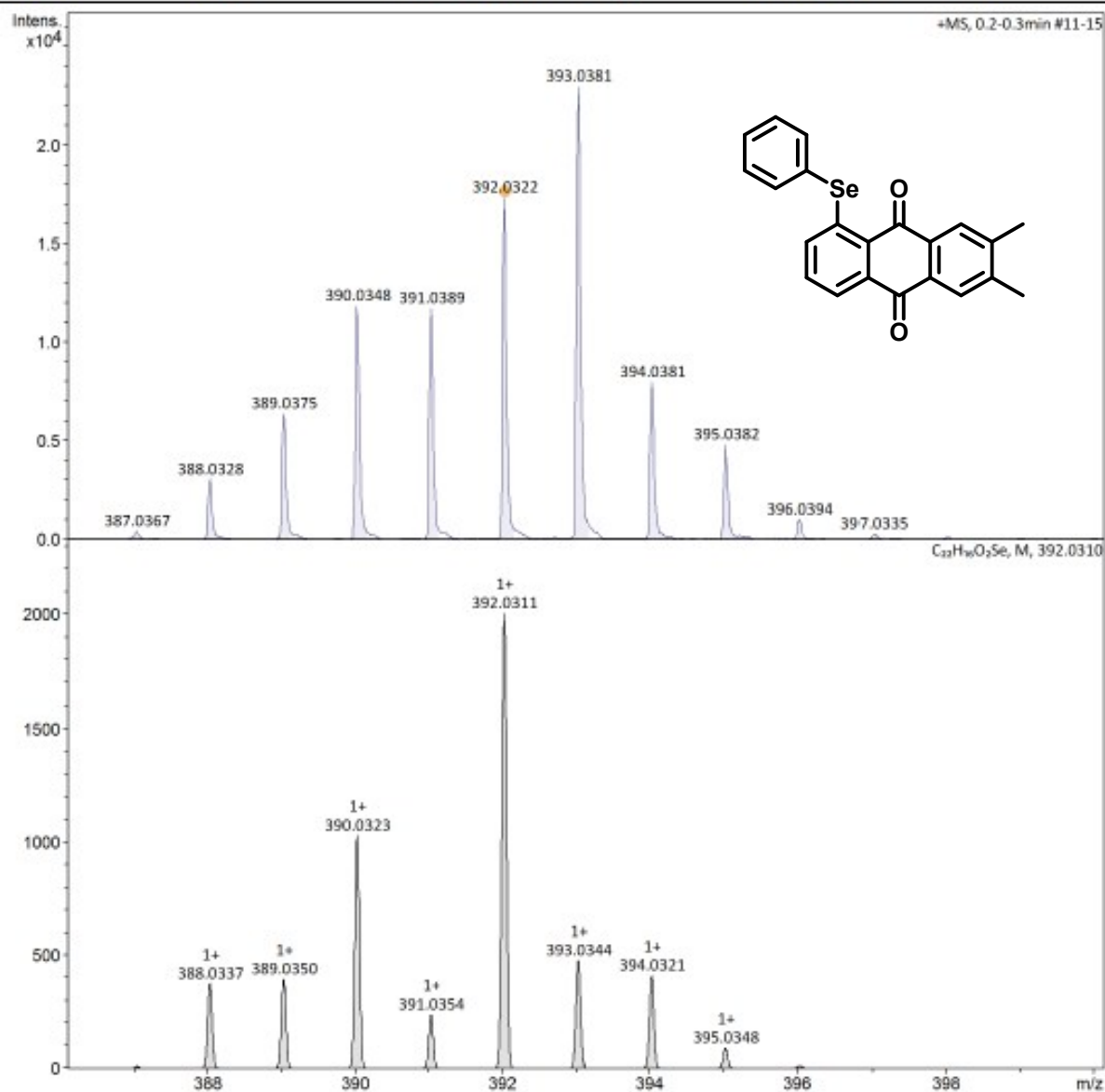
HRMS (APPI⁺) of compound **2r**

Display Report

Analysis Info		Acquisition Date 4/17/2019 10:42:34 AM
Analysis Name	D:\Data\LabSELEN Marcelo QMC CFM 17-04-2019\ENSJ 872000004.d	
Method	DEFAULT_adptado 27 03 2019 APPI até limpeza.m	Operator tofq
Sample Name	LabSELEN Marcelo QMC CFM 17-04-2019	Instrument microTOF-Q 228888.10243
Comment		

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

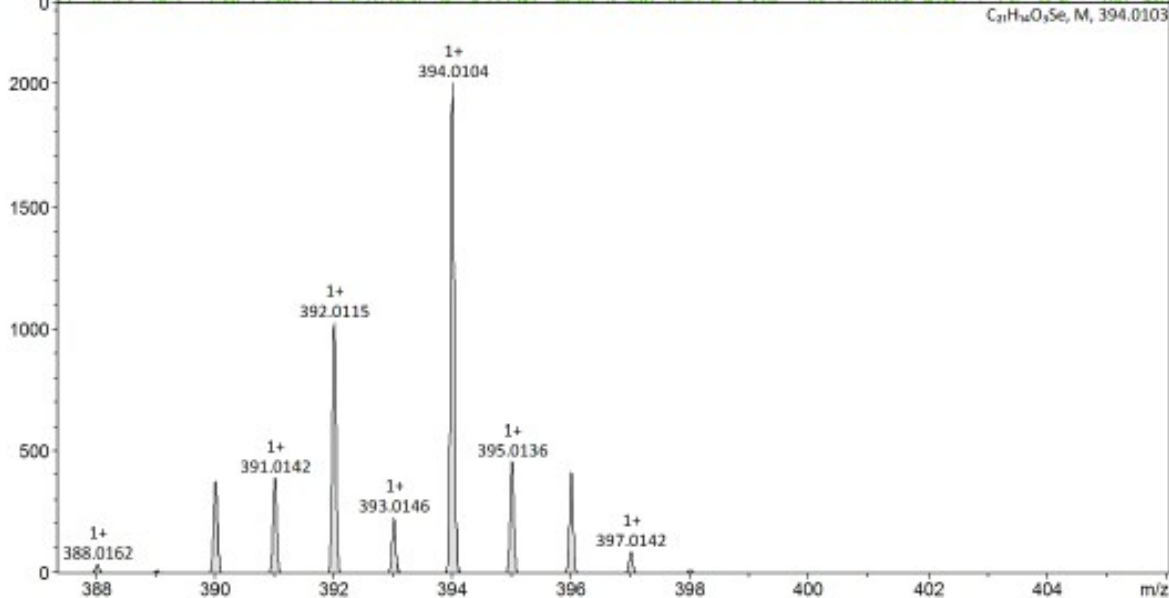
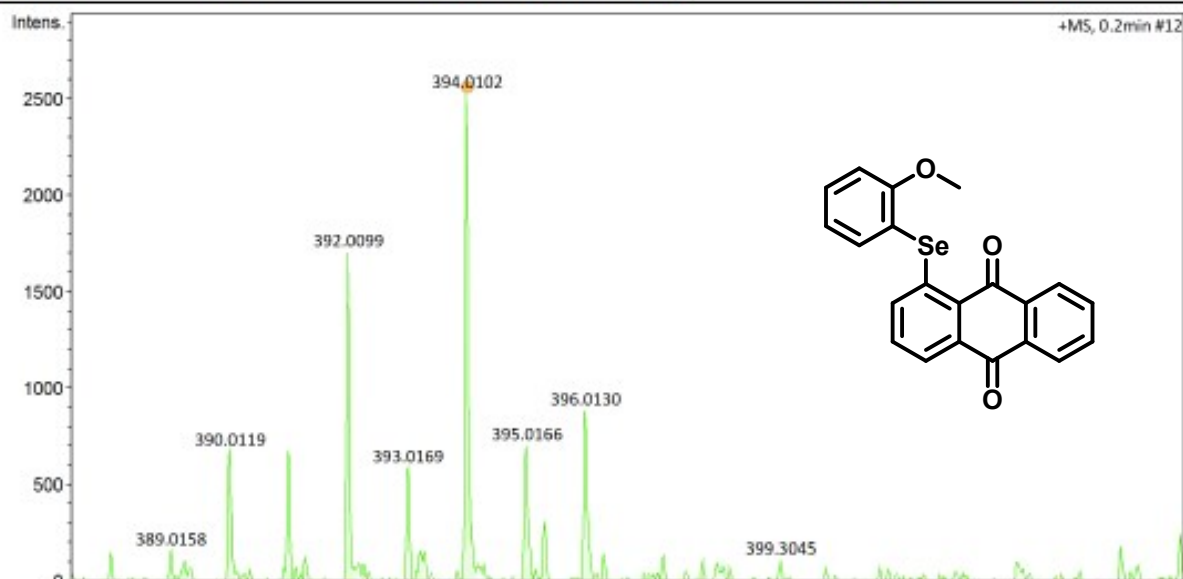


HRMS (APPI⁺) of compound **2s**

Display Report

Analysis Info		Acquisition Date 4/17/2019 11:29:18 AM	
Analysis Name	D:\Data\LabSELEN Marcelo QMC CFM 17-04-2019\ENSJ 873000002.d	Operator	tofq
Method	DEFAULT_adptado 27 03 2019 APPI até limpeza.m	Instrument	micrOTOF-Q 228888.10243
Sample Name	LabSELEN Marcelo QMC CFM 17-04-2019		
Comment			

Acquisition Parameter					
Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



HRMS (APPI+) of compound 2t

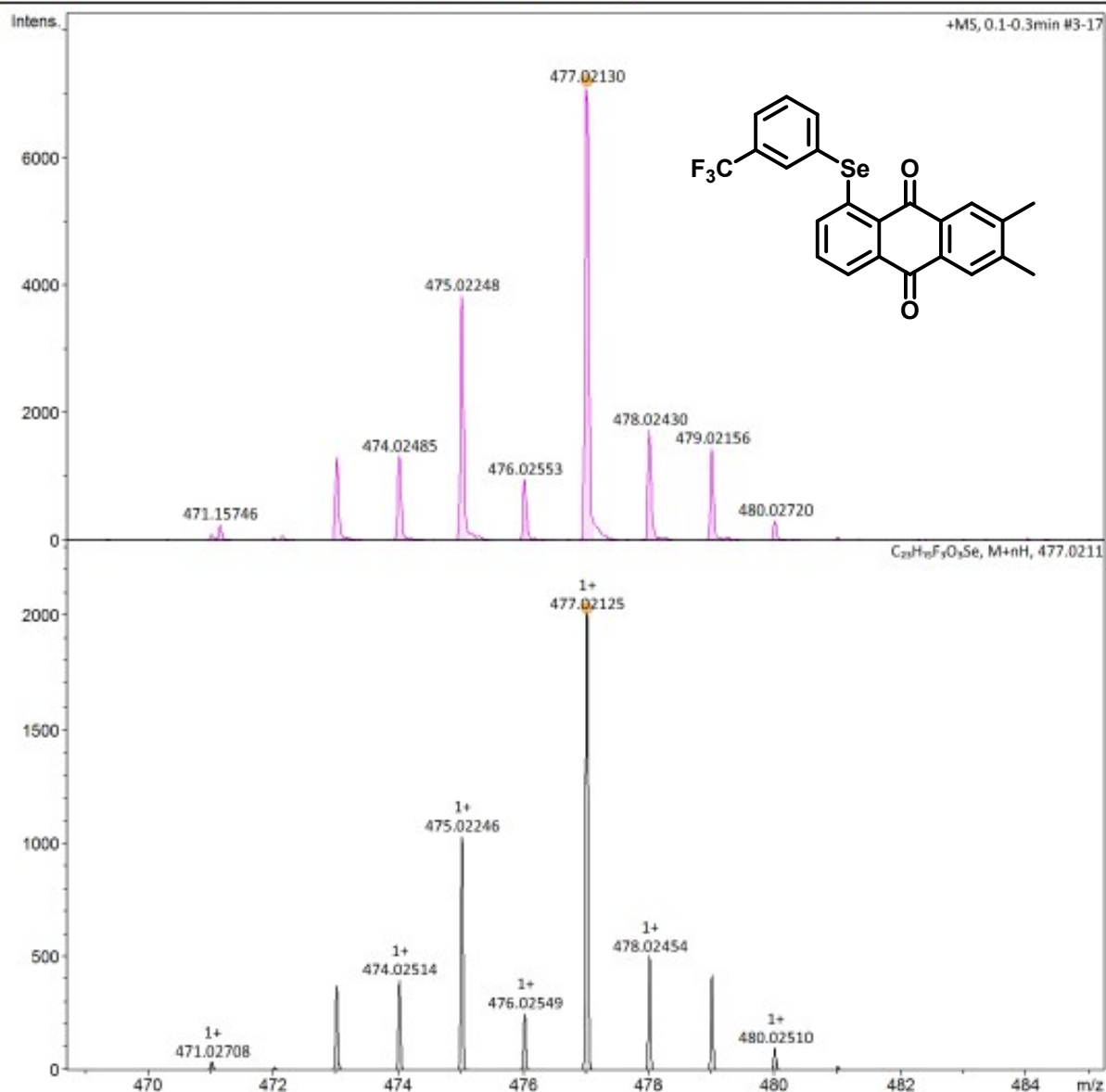
Display Report

Analysis Info

Analysis Name	D:\Data\2019\Q-TOF\LabSELEN\LabSELEN Marcelo QMC CFM 10-06-2019\8900000001.d	Acquisition Date	8/10/2019 2:46:43 PM
Method	appi 10 06 19.m	Operator	micrOTOF-QII
Sample Name	890	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



HRMS (APPI⁺) of compound **2u**

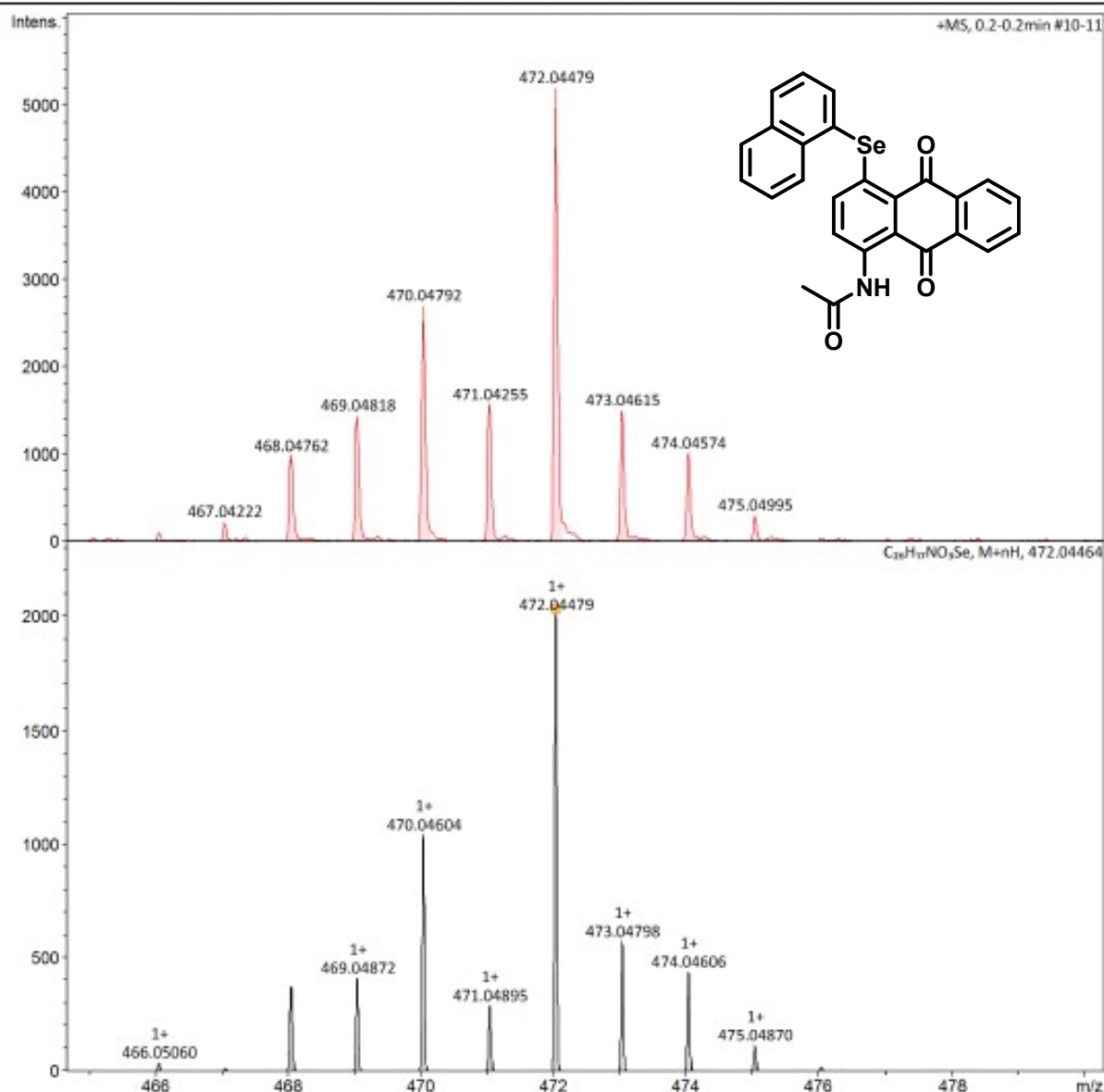
Display Report

Analysis Info

Analysis Name	D:\Data\2019\Q-TOF\LabSELEN\LabSELEN Marcelo QMC CFM 10-06-2019\891000002.d	Acquisition Date	6/10/2019 3:42:11 PM
Method	appi 10 06 19.m	Operator	micrOTOF-QII
Sample Name	891	Instrument	micrOTOF-Q 228888.10243
Comment			

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



HRMS (APPI⁺) of compound 2v

Display Report

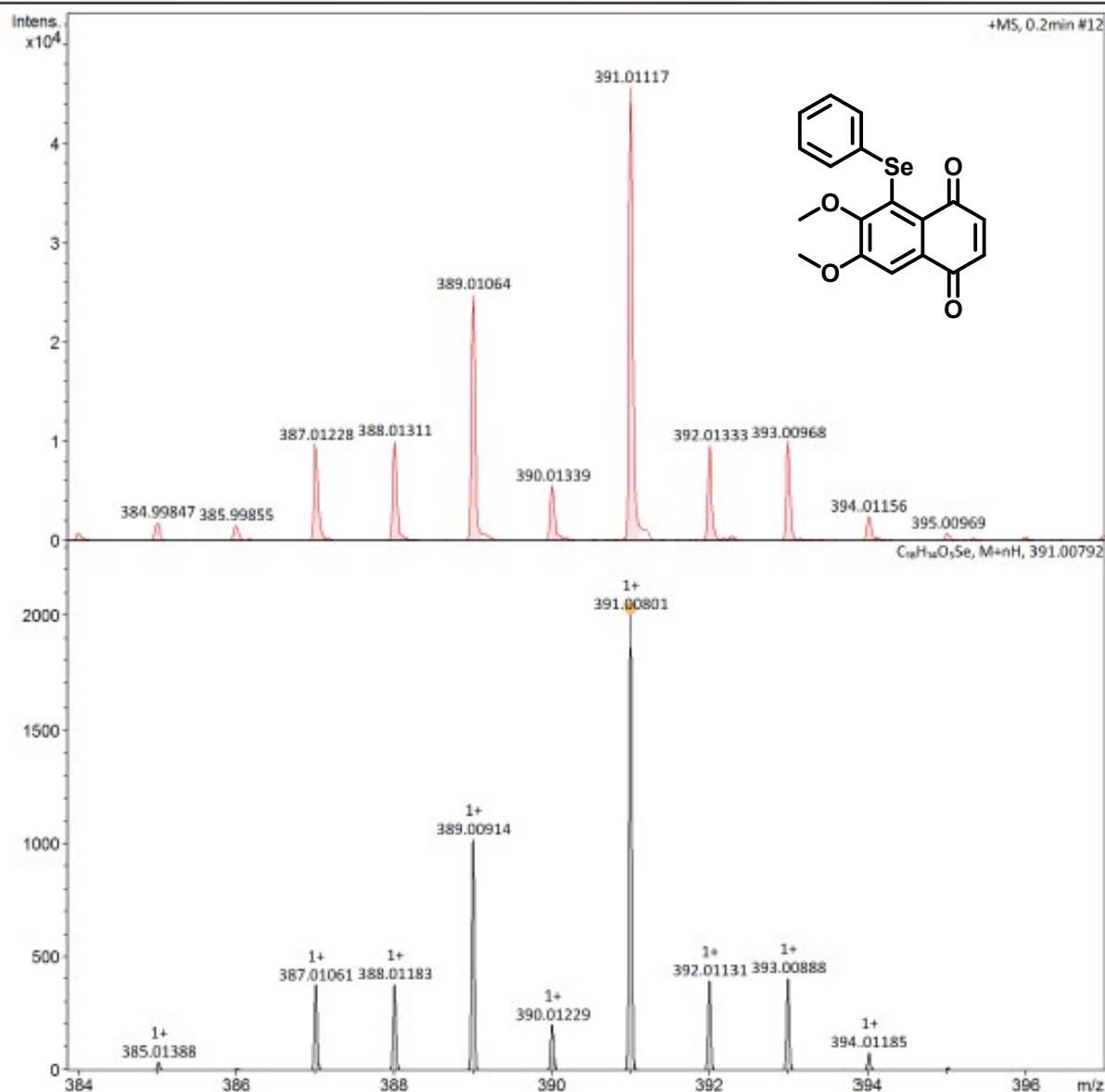
Analysis Info

Analysis Name D:\Data\2019\Q-TOF\LabSELEN\LabSELEN Marcelo QMC CFM 10-06-2019\892000004.d
 Method appi 10 06 19.m
 Sample Name 892
 Comment

Acquisition Date 6/10/2019 3:03:19 PM
 Operator micrOTOF-QII
 Instrument micrOTOF-Q 228888.10243

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



HRMS (APPI⁺) of compound 2x

Display Report

Analysis Info

Analysis Name	D:\Data\2019\Q-TOF\LabSELEN\LabSELEN Marcelo QMC CFM 10-06-2019\893000002.d
Method	appi 10 06 19.m
Sample Name	893
Comment	
Acquisition Date	8/10/2019 3:24:06 PM
Operator	micrOTOF-QII
Instrument	micrOTOF-Q 228888.10243

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulzer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

