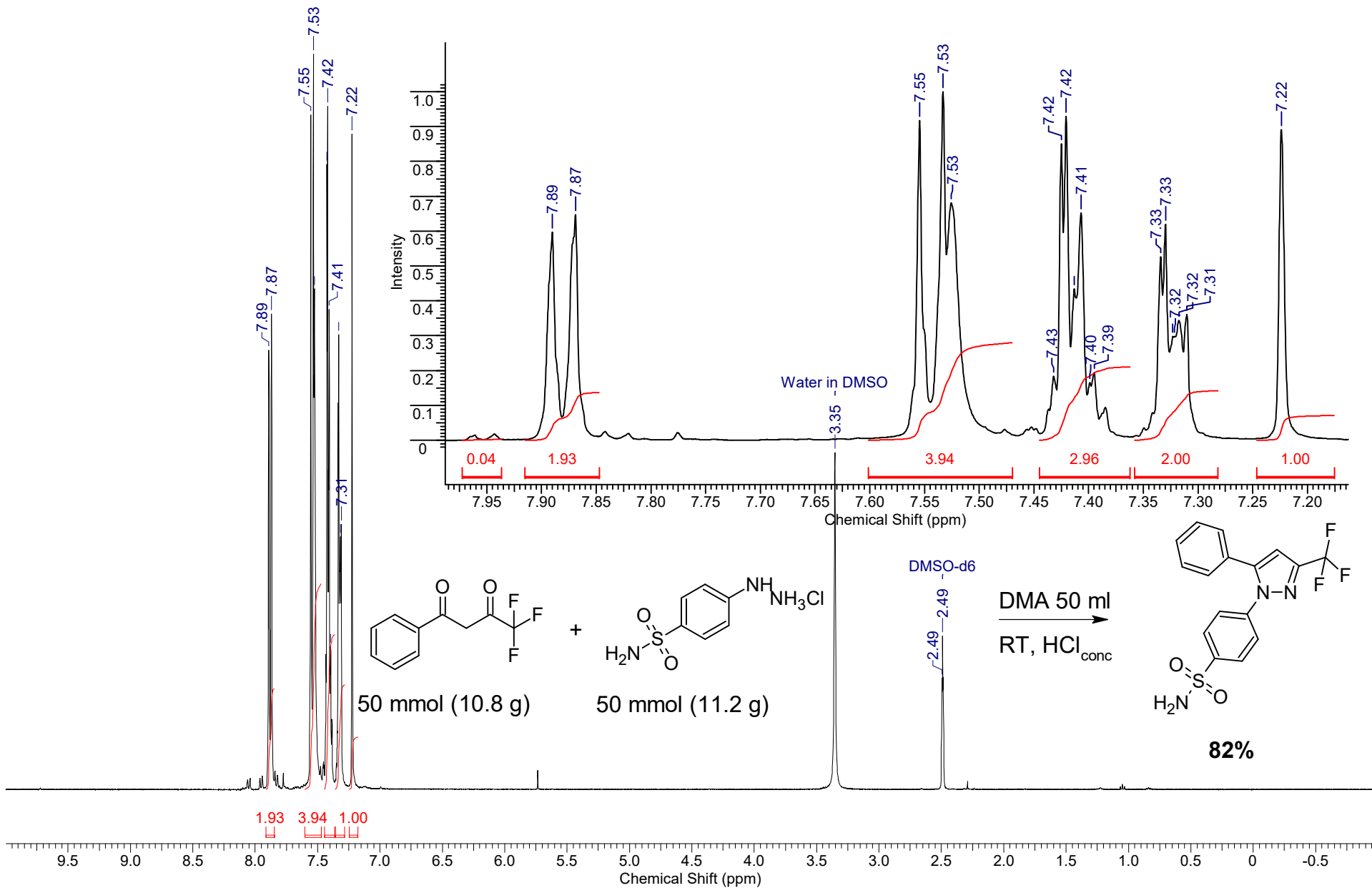


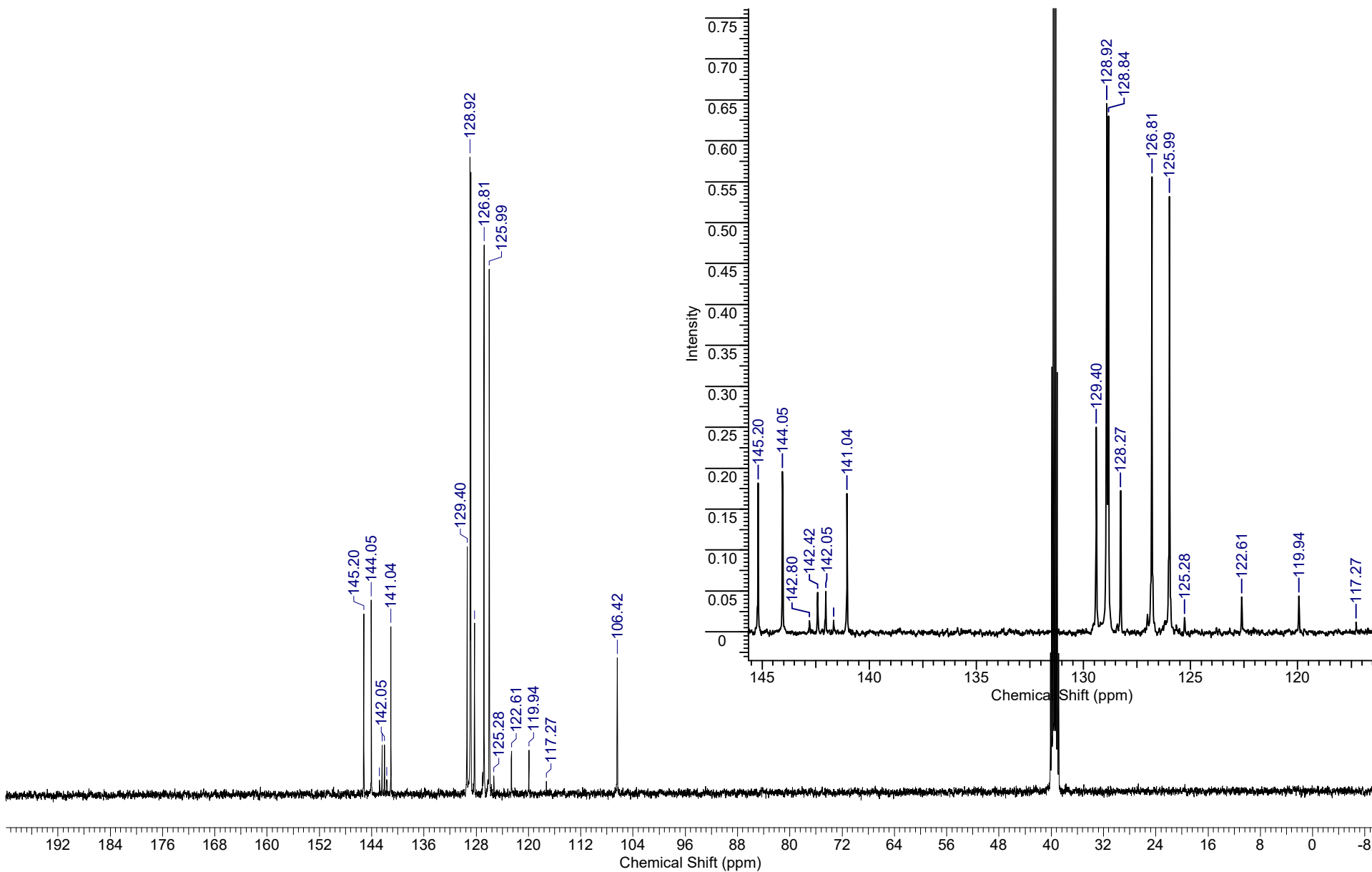
# 4-[5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide: <sup>1</sup>H NMR

<b>Acquisition Time (sec)</b>	3.2998	<b>Comment</b>	Account No. YYZ002 H2NO2S proton		<b>Date</b>	21 Feb 2014 23:06:40	
<b>File Name</b>	D:\Google Drive\UCLA\My Data\2014 02 19\NMR\Proton\Proton_fid			<b>Frequency (MHz)</b>	400.13		
<b>Nucleus</b>	1H	<b>Number of Transients</b>	8	<b>Original Points Count</b>	26441	<b>Points Count</b>	131072
<b>Pulse Sequence</b>	zg30	<b>Solvent</b>	DMSO-D6	<b>Sweep Width (Hz)</b>	8012.82	<b>Temperature (degree C)</b>	26.001



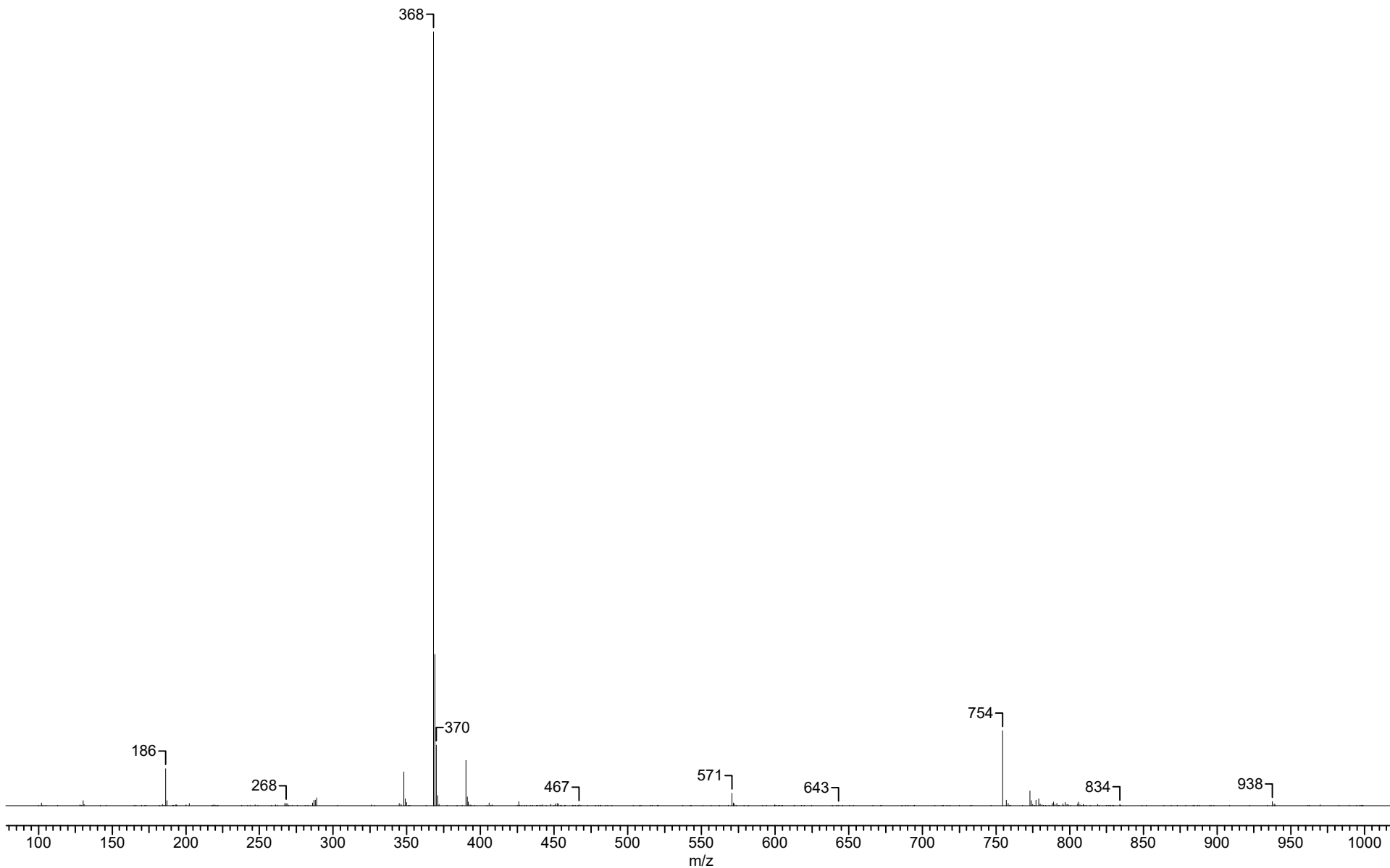
### 4-[5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide: <sup>13</sup>C NMR

<b>Acquisition Time (sec)</b>	1.2976	<b>Comment</b>	Account No. YYZ002 H2NO2S carbon		<b>Date</b>	21 Feb 2014 23:21:36	
<b>File Name</b>	D:\Google Drive\UCLA\My Data\2014 02 19\NMR\Carbon\Carbon_fid				<b>Frequency (MHz)</b>	100.62	
<b>Nucleus</b>	13C	<b>Number of Transients</b>	256	<b>Original Points Count</b>	32768	<b>Points Count</b>	131072
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	DMSO-D6	<b>Sweep Width (Hz)</b>	25252.53	<b>Temperature (degree C)</b>	26.425



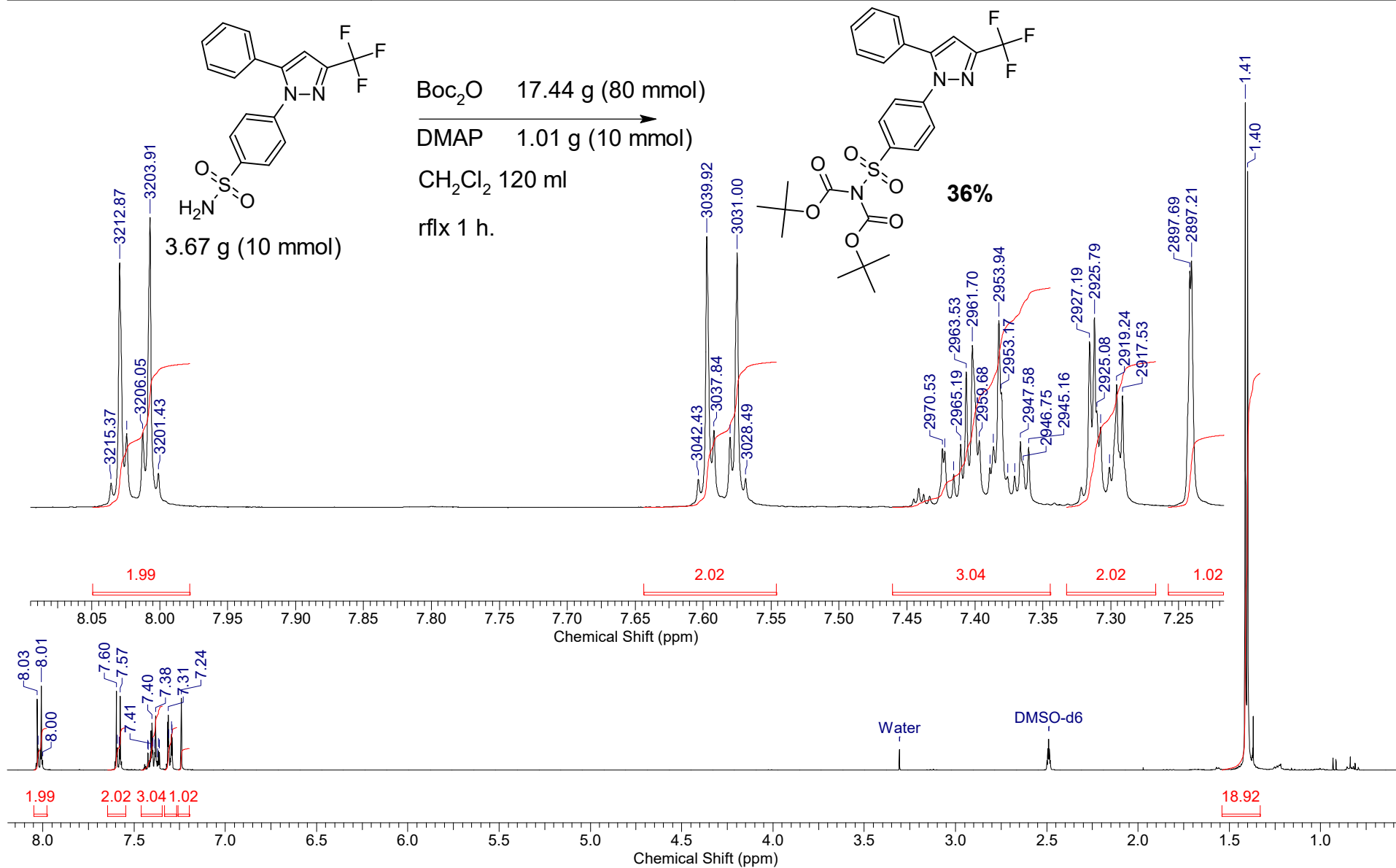
### 4-[5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide: ESI MS

<b>Count</b>	253	<b>Data Type</b>	Centroided Mass Spectrum		<b>Date Stamp</b>	09:00:00	
<b>File Name</b>	C:\GDRIVE\PUBLISHING\2015 COX-2\COMPOUNDS\PH, H2NO2S-PH, CF3 PYRAZOLE\LCMS\SULPHMSV.AIA\MSSIG01.CDF						
<b>Inlet Model</b>	Electrospray Inlet	<b>Instrument</b>	Agilent Technologies / 1946A /		<b>Ion Mode</b>	ES+	
<b>Operator</b>	EN	<b>Owner</b>	EN	<b>Retention Time</b>	17.052	<b>Scan</b>	1303
<b>Separation Type</b>	Other Chromatography	<b>Spectrum Title</b>	Results	<b>TIC</b>	190.70	<b>Total Signal</b>	705157



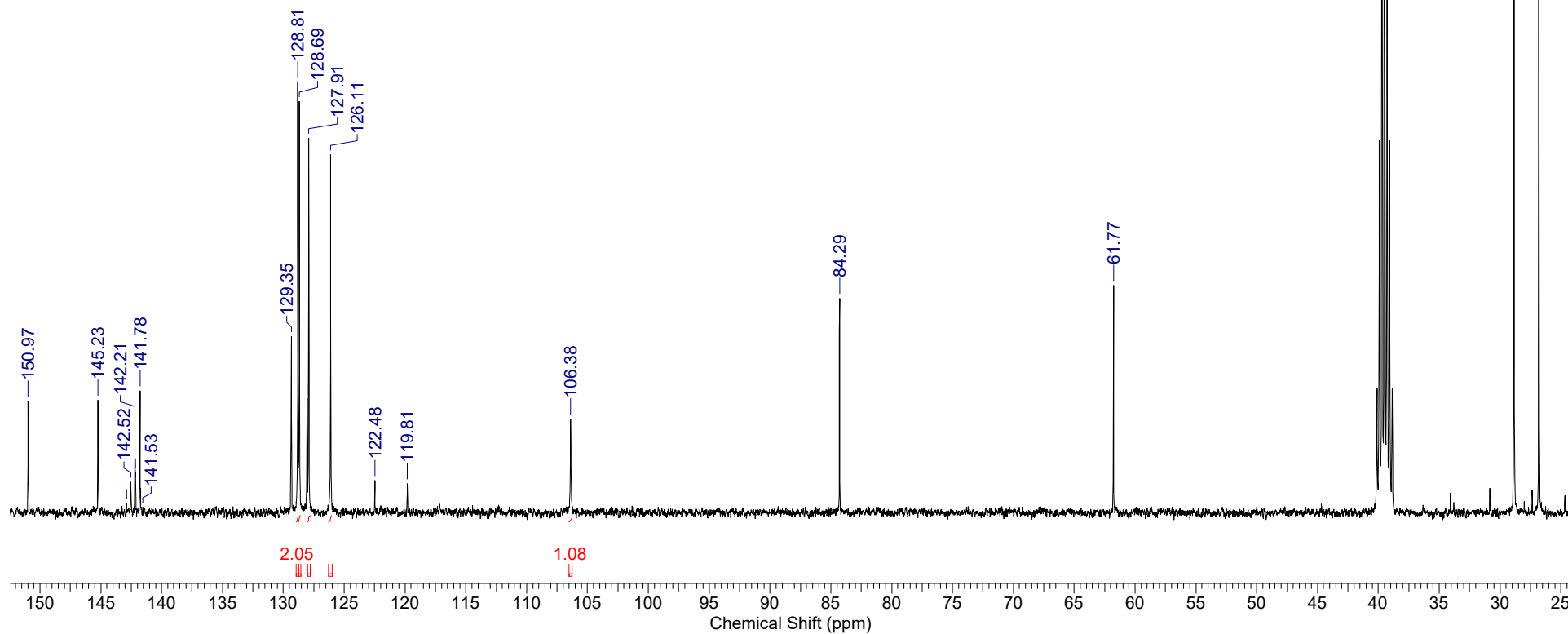
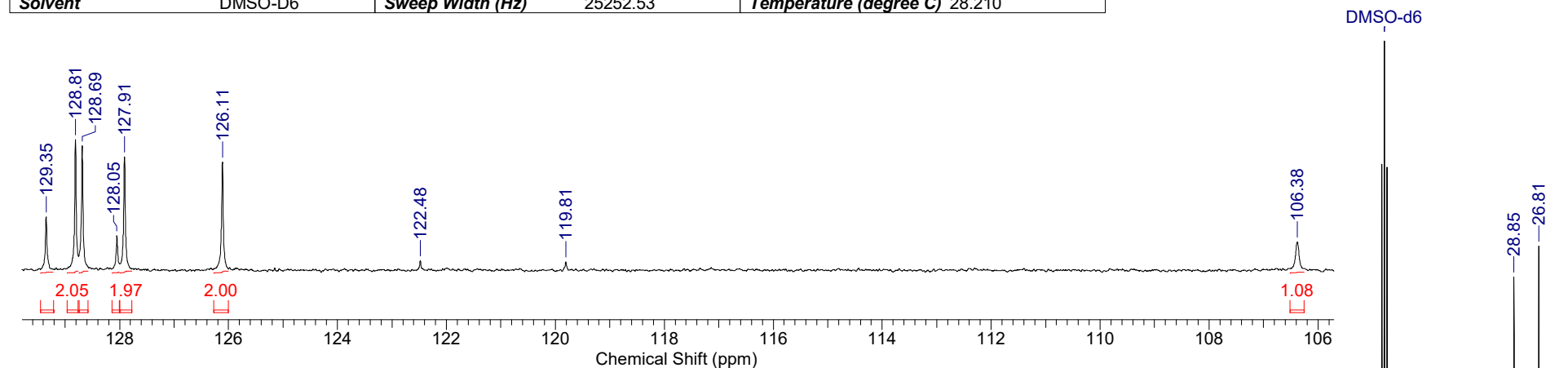
# di-tert-butyl ({4-[5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl}sulfonyl)imidodicarbonate: <sup>1</sup>H NMR

Acquisition Time (sec)	3.2998	Comment	Account No. YYZ002 Boc2NO2SPh, Ph, CF3 proton		
Date	03 May 2014 00:27:44				
File Name	D:\Google Drive\UCLA\My Data\2014 04 15 Ph, Boc2NO2S-Ph, CF3 pyrazole\2014 04 15 Ph, Boc2NO2S-Ph, CF3 pyrazole_590000fid				
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	8
Original Points Count	26441	Points Count	262144	Pulse Sequence	zg30
Solvent	DMSO-D6	Sweep Width (Hz)	8012.82	Temperature (degree C)	26.535



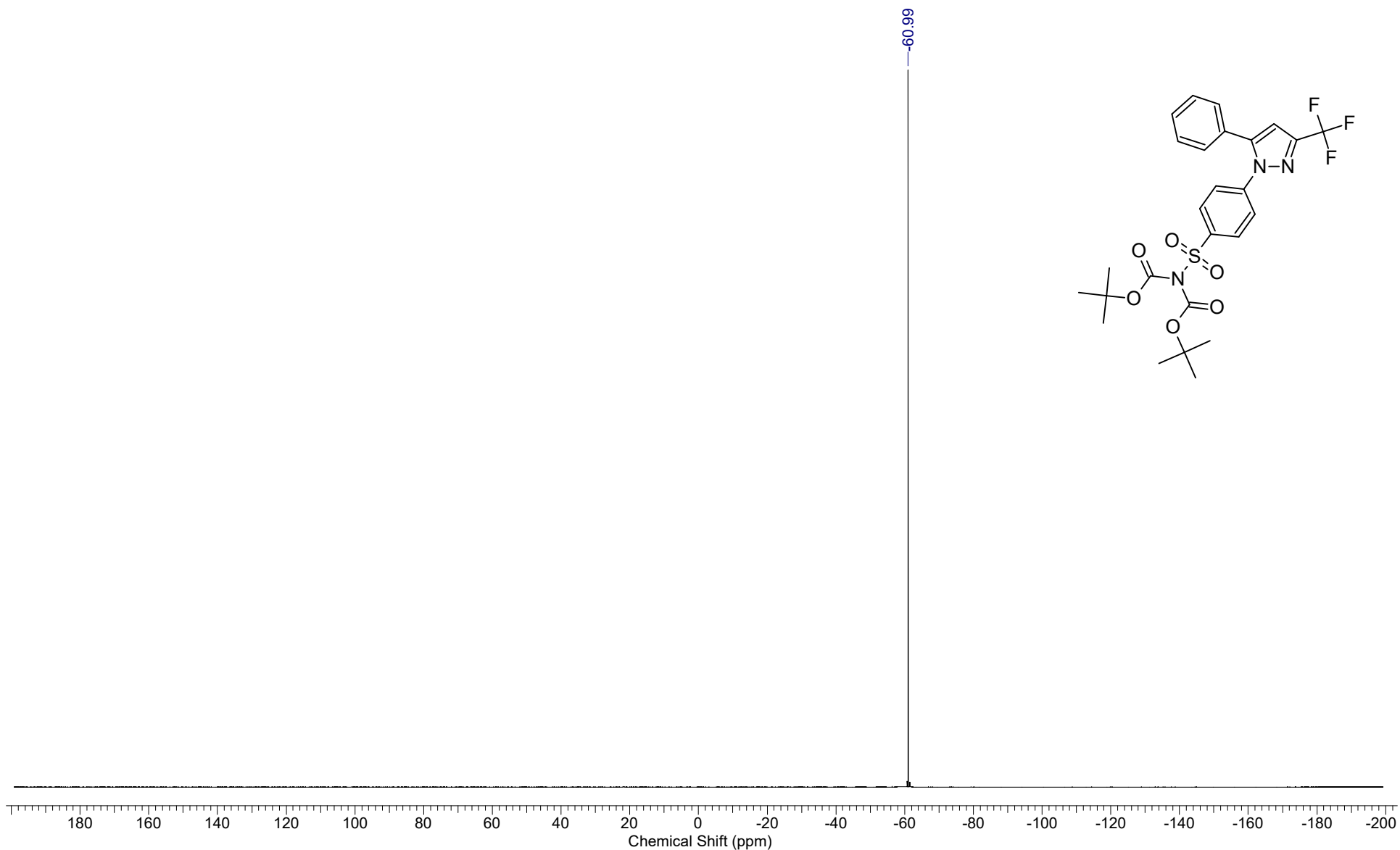
di-tert-butyl ({4-[5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl)sulfonyl)imidodicarbonate: <sup>13</sup>C NMR

<b>Acquisition Time (sec)</b>	1.2976	<b>Comment</b>	Account No. YYZ002 Boc2NO2SPh, Ph, CF3 carbon	<b>Date</b>	03 May 2014 00:44:48
<b>File Name</b>	D:\Google Drive\UCLA\My Data\2014 04 15\2014 04 15_591000fid	<b>Frequency (MHz)</b>	100.62	<b>Nucleus</b>	<sup>13</sup> C
<b>Number of Transients</b>	256	<b>Original Points Count</b>	32768	<b>Points Count</b>	262144
<b>Solvent</b>	DMSO-D6	<b>Sweep Width (Hz)</b>	25252.53	<b>Temperature (degree C)</b>	28.210
				<b>Pulse Sequence</b>	zgpg30



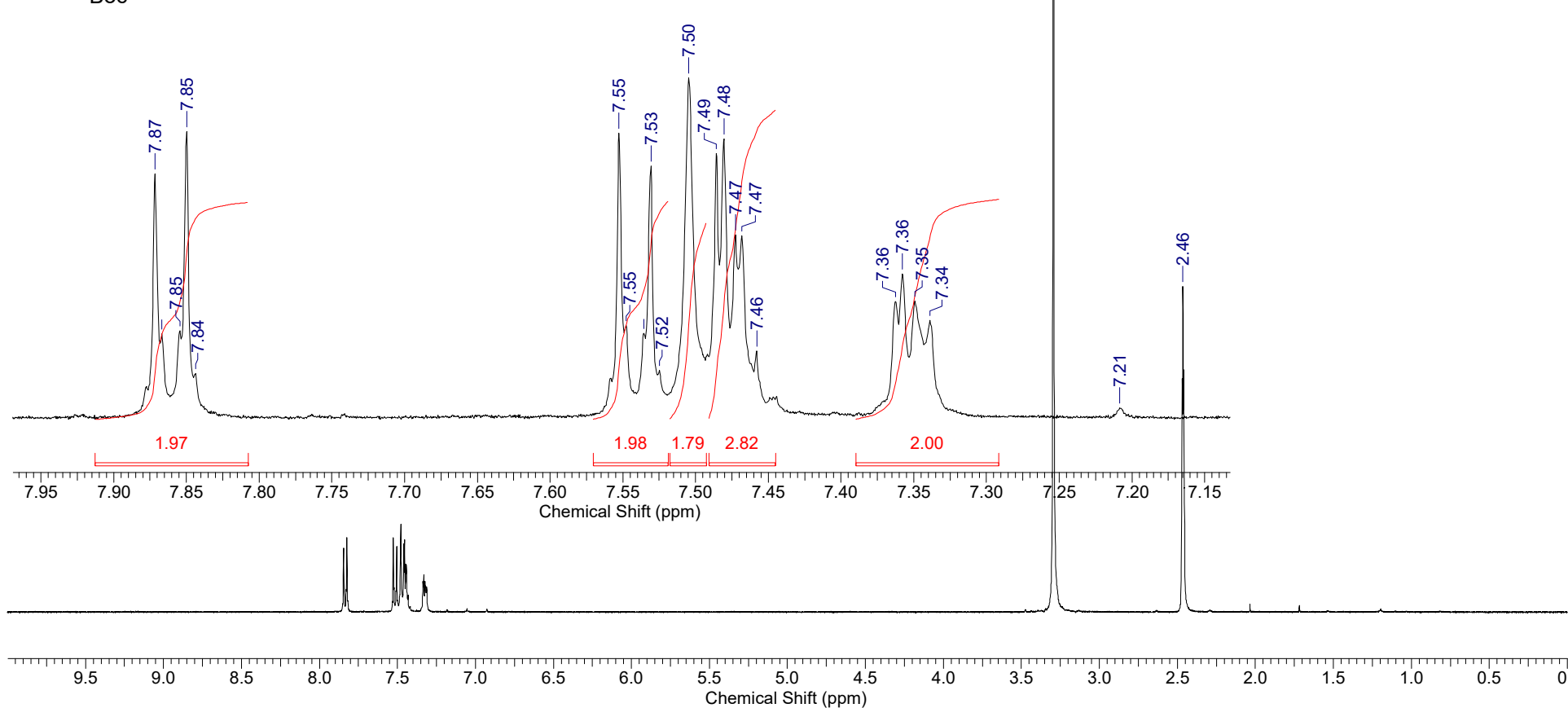
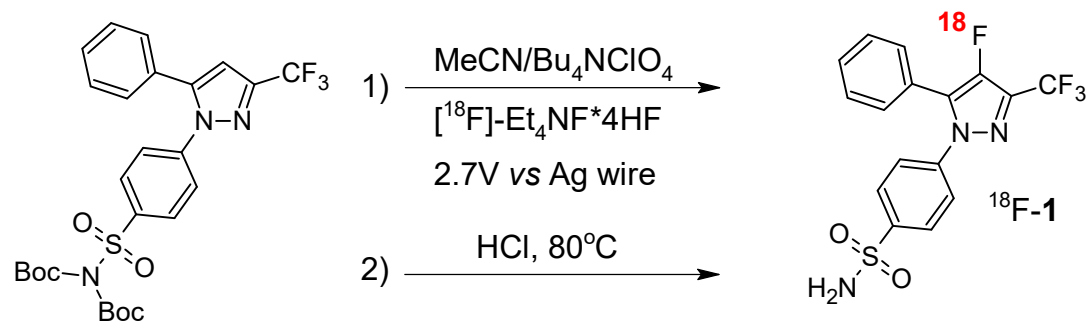
di-tert-butyl ({4-[5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl}sulfonyl)imidodicarbonate: <sup>19</sup>F NMR

<b>Acquisition Time (sec)</b>	0.8738	<b>Comment</b>	Account No. YYZ002 Boc2NO2SPh, Ph, CF3 fluorine		<b>Date</b>	03 May 2014 00:46:56
<b>File Name</b>	D:\Google Drive\UCLA\My Data\2014 04 15\2014 04 15_592000fid	<b>Frequency (MHz)</b>	376.50	<b>Nucleus</b>	19F	
<b>Number of Transients</b>	32	<b>Original Points Count</b>	131072	<b>Points Count</b>	131072	
<b>Solvent</b>	DMSO-D6	<b>Sweep Width (Hz)</b>	150000.00	<b>Temperature (degree C)</b>	27.744	
				<b>Pulse Sequence</b>	zgfhiqqn.2	



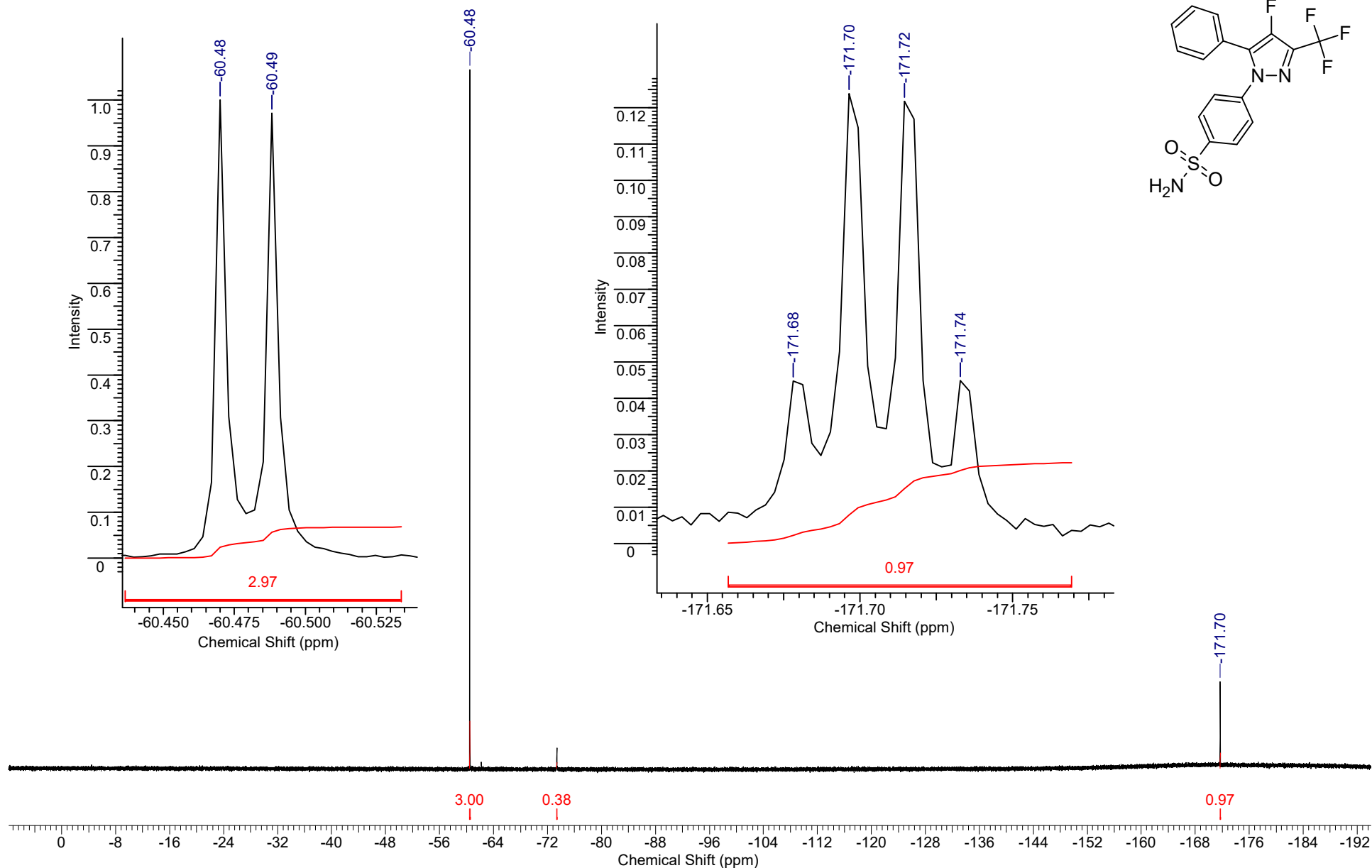
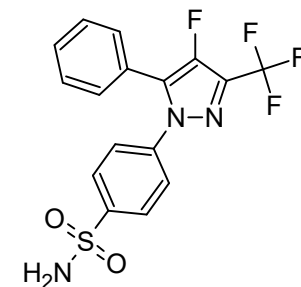
# 4-[4-fluoro-5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]-benzenesulfonamide (<sup>19</sup>F-1): <sup>1</sup>H-NMR

Acquisition Time (sec)	3.2998	Comment	Account No. YYZ002 F-positron proton	Date	09 Jul 2014 22:43:12
File Name	D:\GDrive\Publishing\2015 COX-2\Compounds\Compound 1\NMR\Proton AV400\Proton AV400_fid	Frequency (MHz)	400.13		
Nucleus	1H	Number of Transients	8	Original Points Count	26441
Pulse Sequence	zg30	Solvent	DMSO-D6	Sweep Width (Hz)	8012.82
		Points Count	65536	Temperature (degree C)	26.045



# 4-[4-fluoro-5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]-benzenesulfonamide (<sup>19</sup>F-1): <sup>19</sup>F NMR

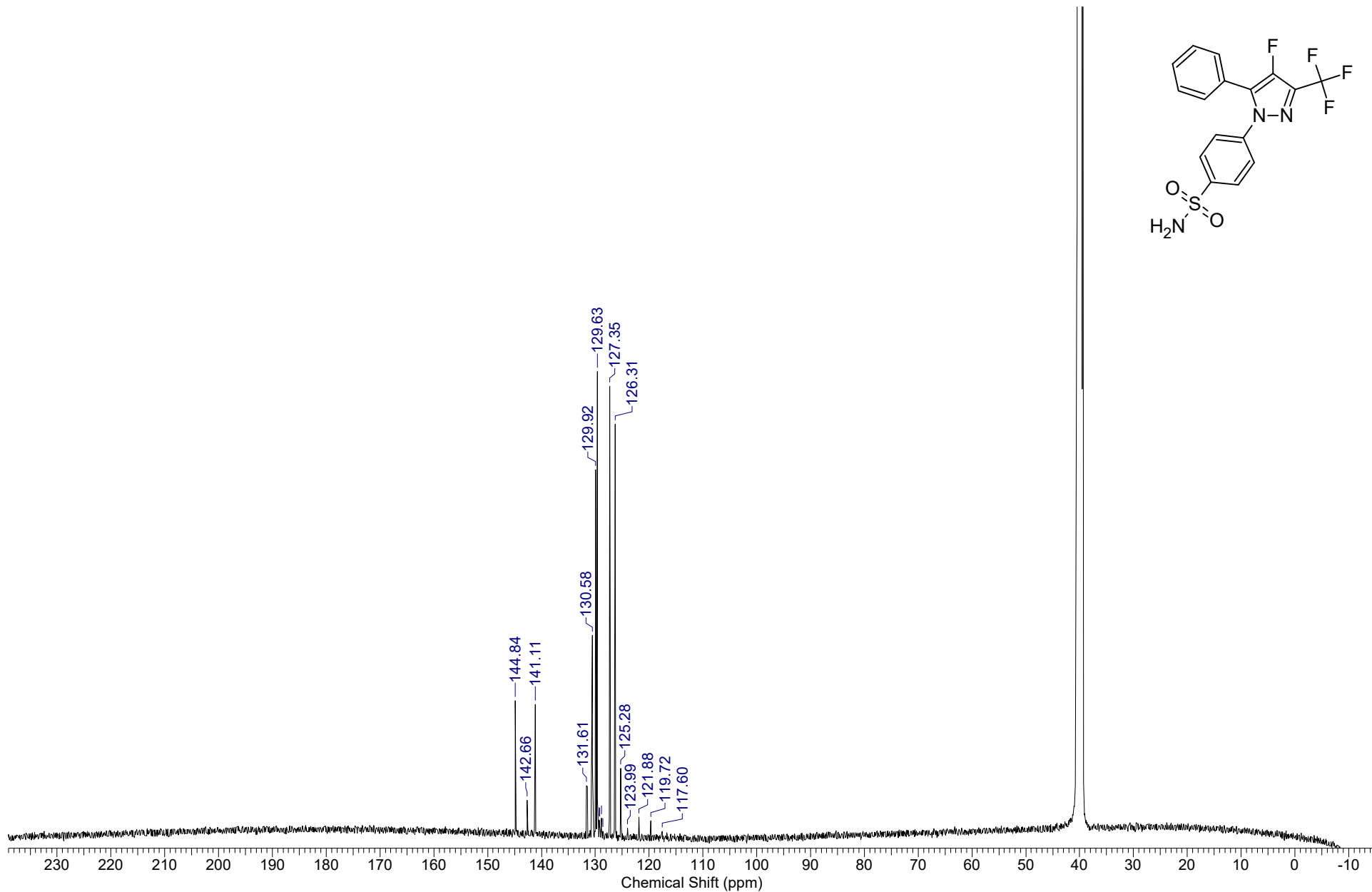
Acquisition Time (sec)	0.8738	Comment	Account No. YYZ002 Posicoxib fluorine	Date	09 Jul 2014 22:51:44
File Name	D:\GDrive\Publishing\2015 COX-2\Compounds\Compound 1\NMR\Fluorine AV400\Fluorine AV400_fid		Frequency (MHz)	376.50	
Nucleus	19F	Number of Transients	8	Original Points Count	131072
Pulse Sequence	zgf1qn30	Solvent	DMSO-D6	Sweep Width (Hz)	150000.00
				Points Count	131072
				Temperature (degree C)	26.036



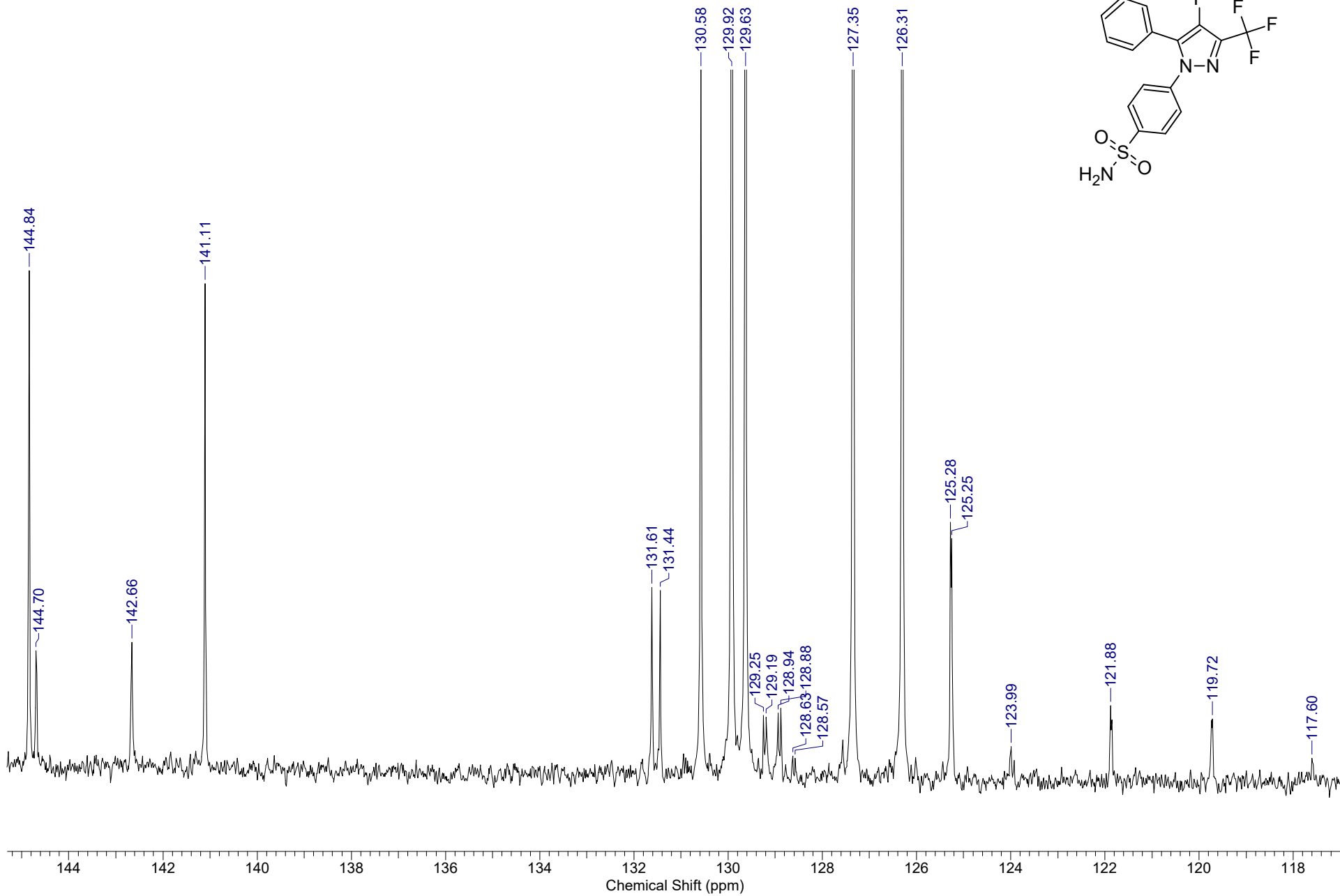
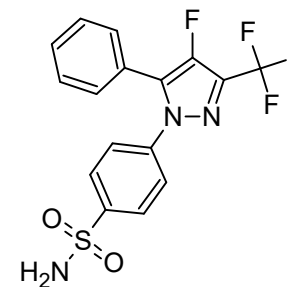


# 4-[4-fluoro-5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]-benzenesulfonamide (<sup>19</sup>F-1): <sup>13</sup>C NMR

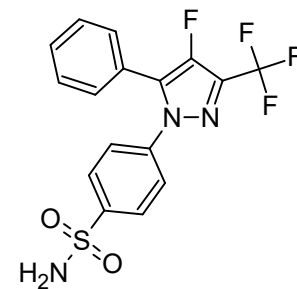
<b>Acquisition Time (sec)</b>	1.0486	<b>Date</b>	11 Jul 2014 18:50:40				
<b>File Name</b>	D:\GDrive\Publishing\2015 COX-2\Compounds\Compound 1\NMR\Carbon AV500\Carbon AV500_fid				<b>Frequency (MHz)</b>	125.77	
<b>Nucleus</b>	13C	<b>Number of Transients</b>	840	<b>Original Points Count</b>	32768	<b>Points Count</b>	32768
<b>Pulse Sequence</b>	zgpg30	<b>Solvent</b>	DMSO-D6	<b>Sweep Width (Hz)</b>	31250.00	<b>Temperature (degree C)</b>	25.001



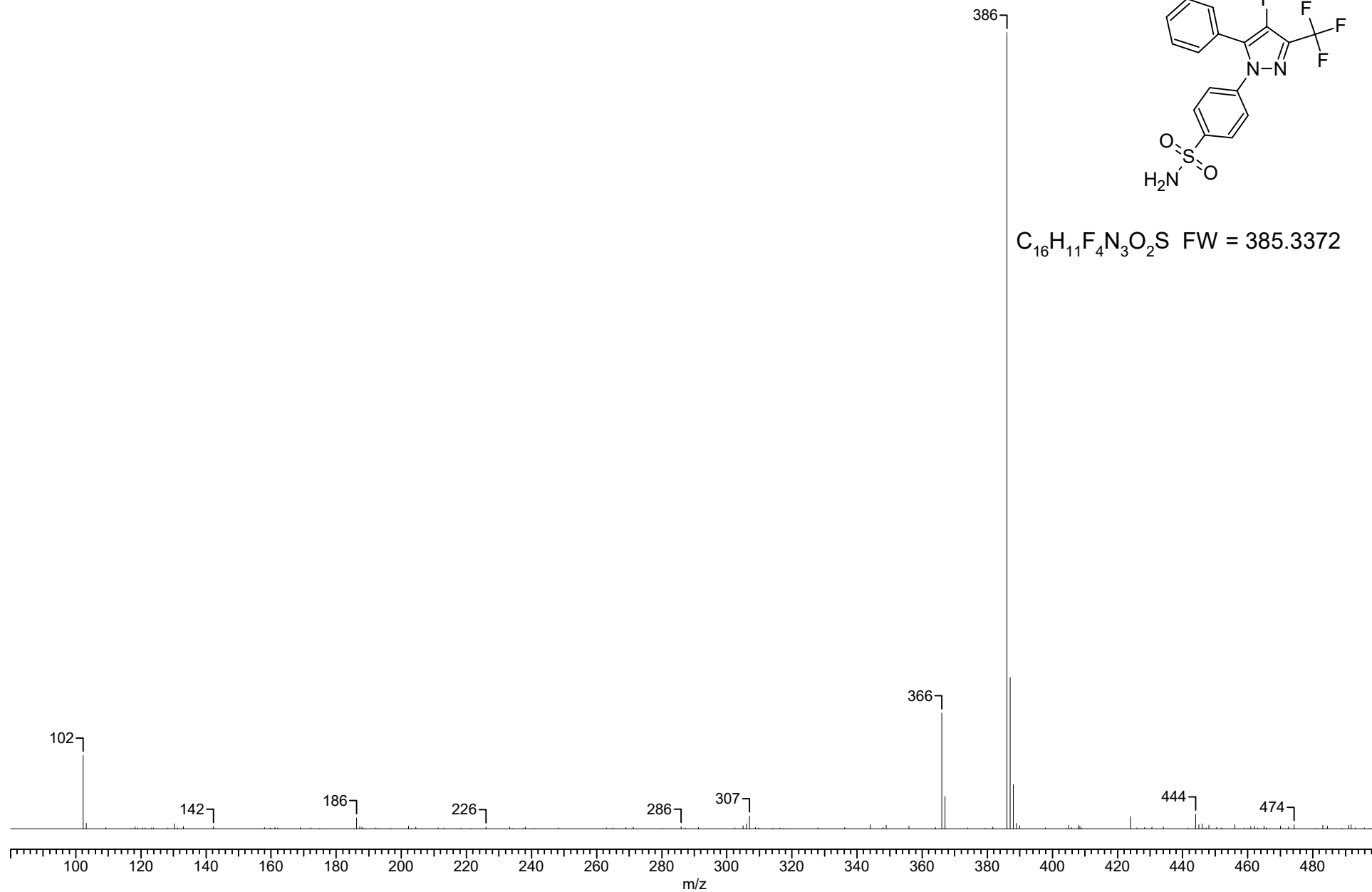
# 4-[4-fluoro-5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]-benzenesulfonamide (<sup>19</sup>F-1): <sup>13</sup>C NMR



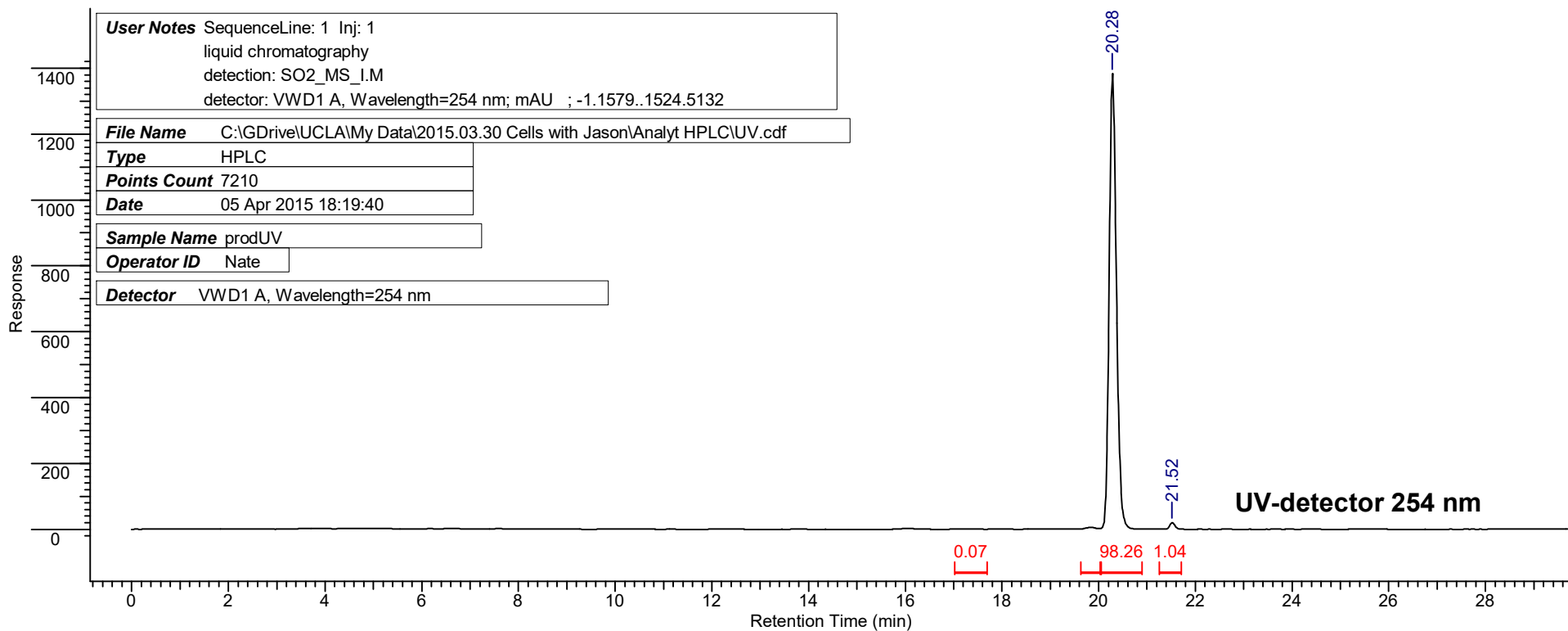
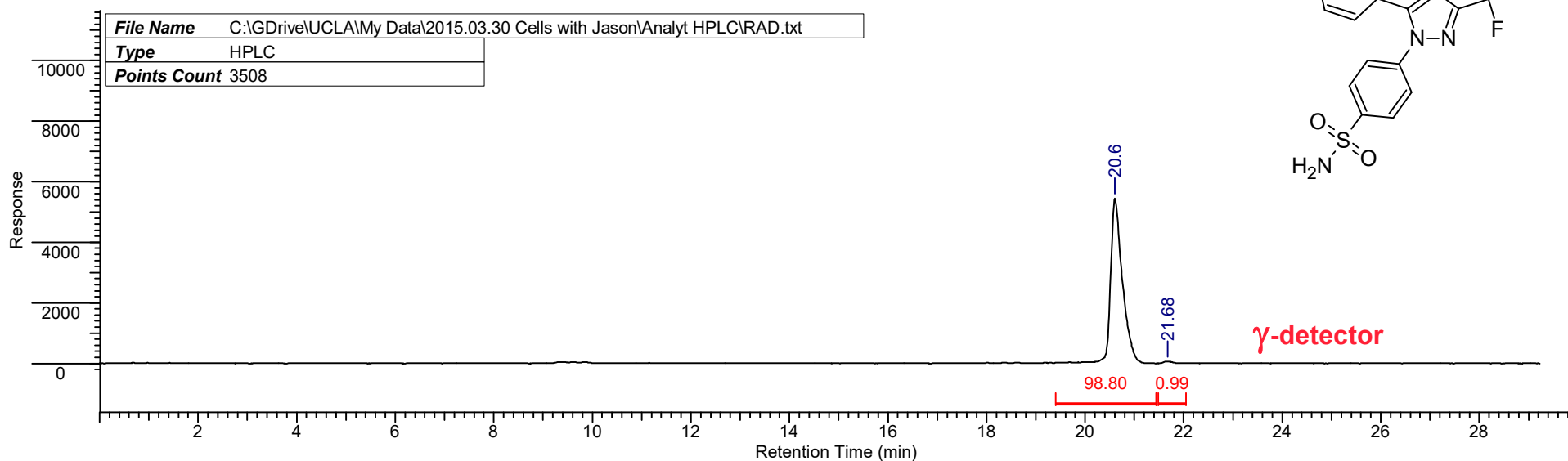
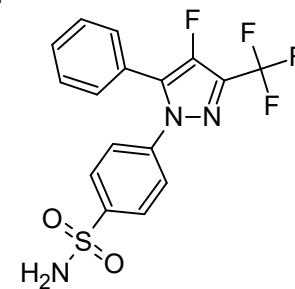
4-[4-fluoro-5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]-benzenesulfonamide (<sup>19</sup>F-1): ESI MS



C<sub>16</sub>H<sub>11</sub>F<sub>4</sub>N<sub>3</sub>O<sub>2</sub>S FW = 385.3372



# 4-[4-fluoro-5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]-benzenesulfonamide (<sup>19</sup>F-1): Analytical HPLC



# Compound S3: UV-254, Total ion chromatograms and ESI MS spectrum

