1-[2,6-dimethyl-4-(pent-4-yn-1-yloxy)phenyl]-4-phenyl-1,2,4-triazolidine-3,5-dione

Gary W. Breton*

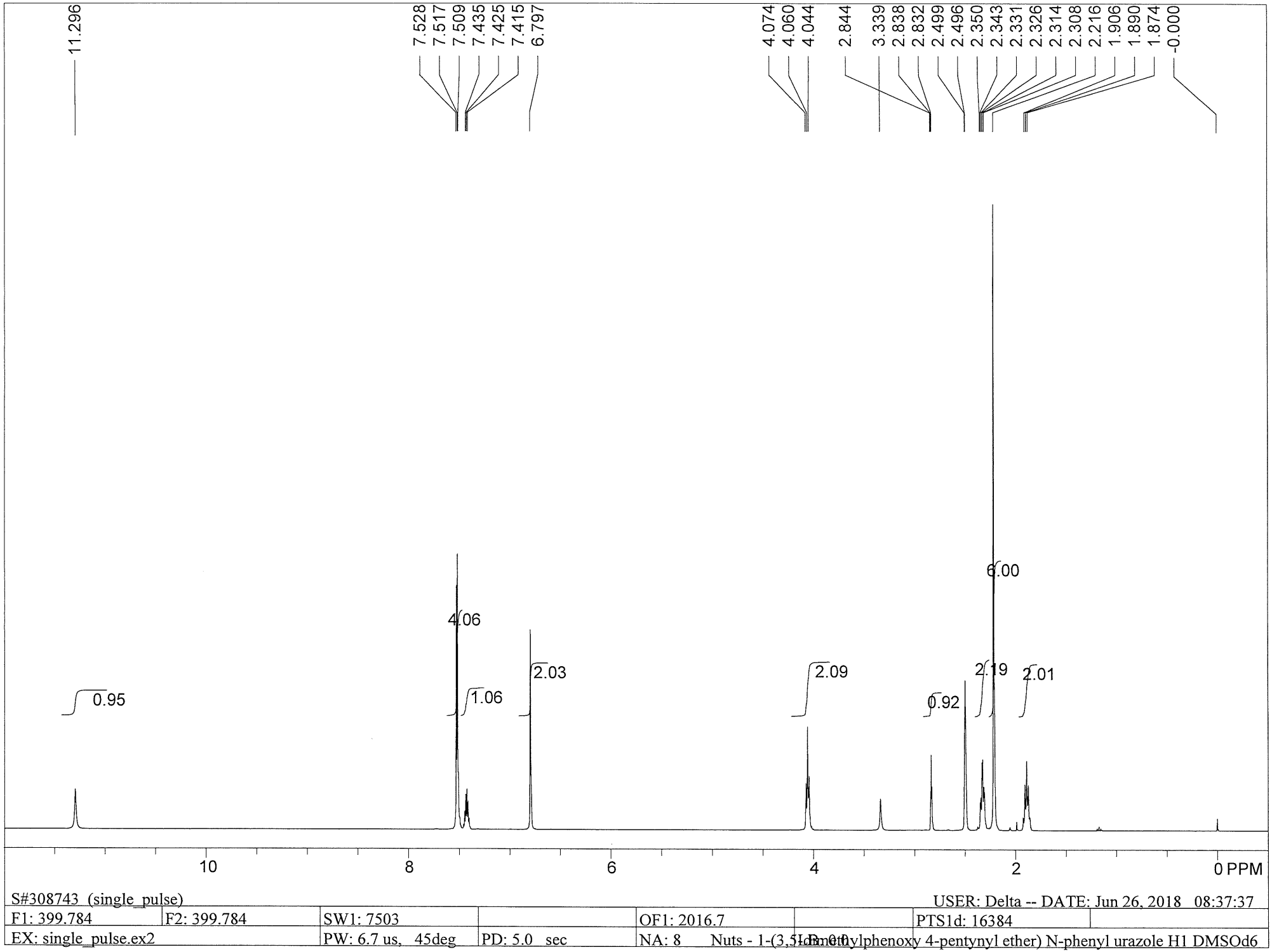
Department of Chemistry, Berry College, 2277 Martha Berry HWY,
Mount Berry GA 30149 USA
gbreton@berry.edu

Supplementary Materials

Data for Compound 3

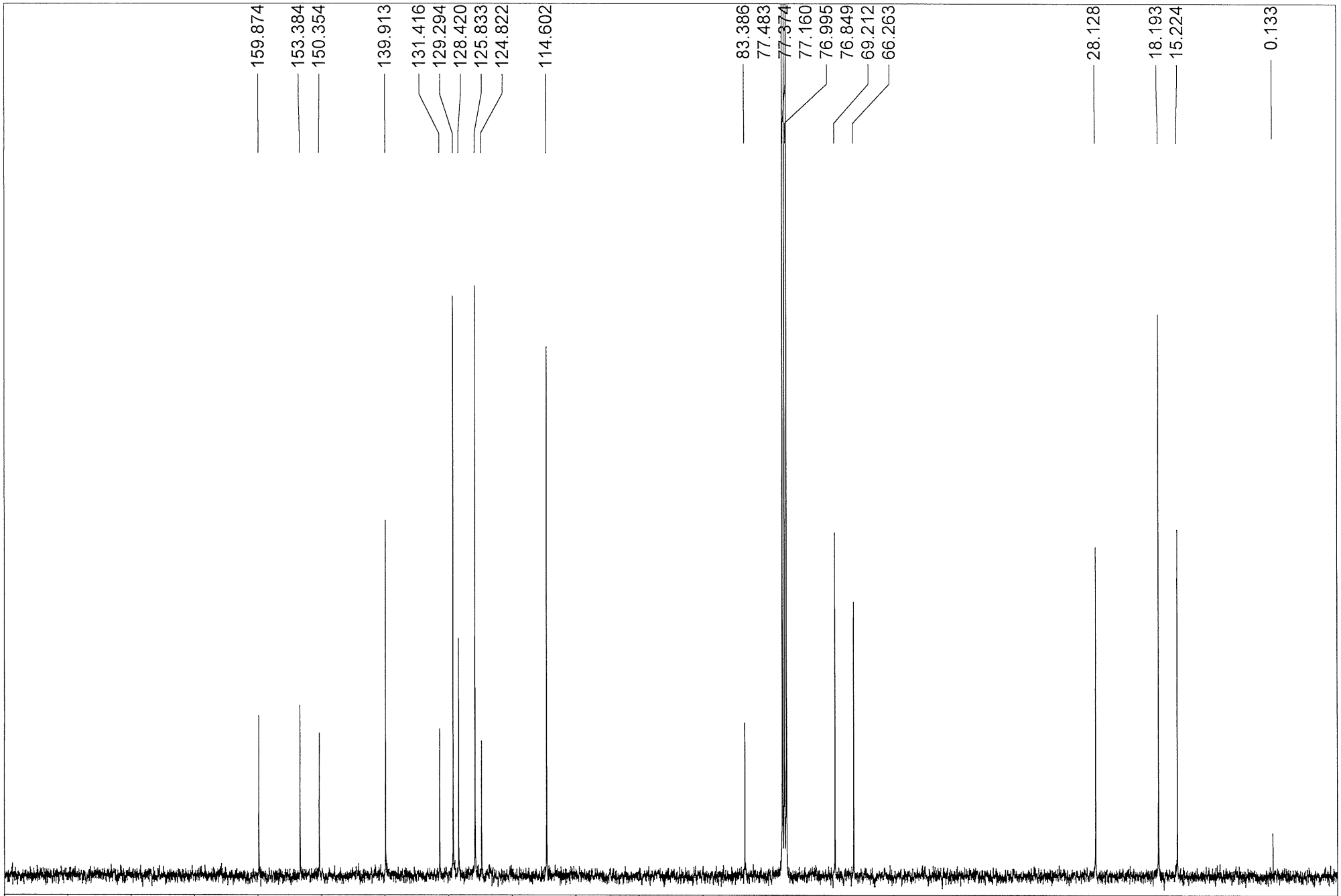
1-[2,6-dimethyl-4-(pent-4-yn-1-yloxy)phenyl]-4-phenyl-1,2,4-triazolidine-3,5-dione

- ^{1}H NMR spectrum
- ^{13}C NMR spectrum
- HETCOR spectrum
- IR spectrum
- HRMS spectra



S#308743 (single_pulse) USER: Delta -- DATE: Jun 26, 2018 08:37:37

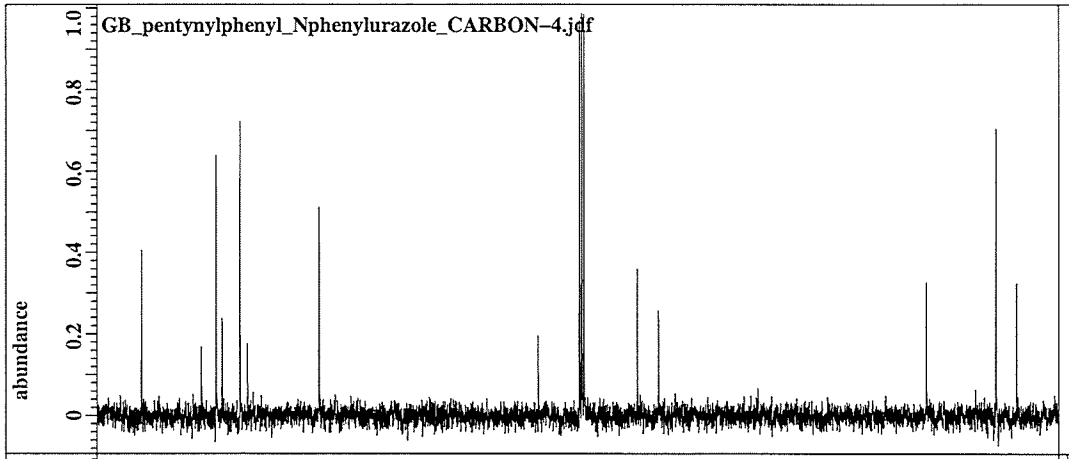
F1: 399.784	F2: 399.784	SW1: 7503		OF1: 2016.7		PTS1d: 16384
EX: single_pulse.ex2		PW: 6.7 us, 45deg	PD: 5.0 sec	NA: 8	Nuts - 1-(3,5-dimethylphenoxy 4-pentynyl ether) N-phenyl urazole H1 DMSOd6	

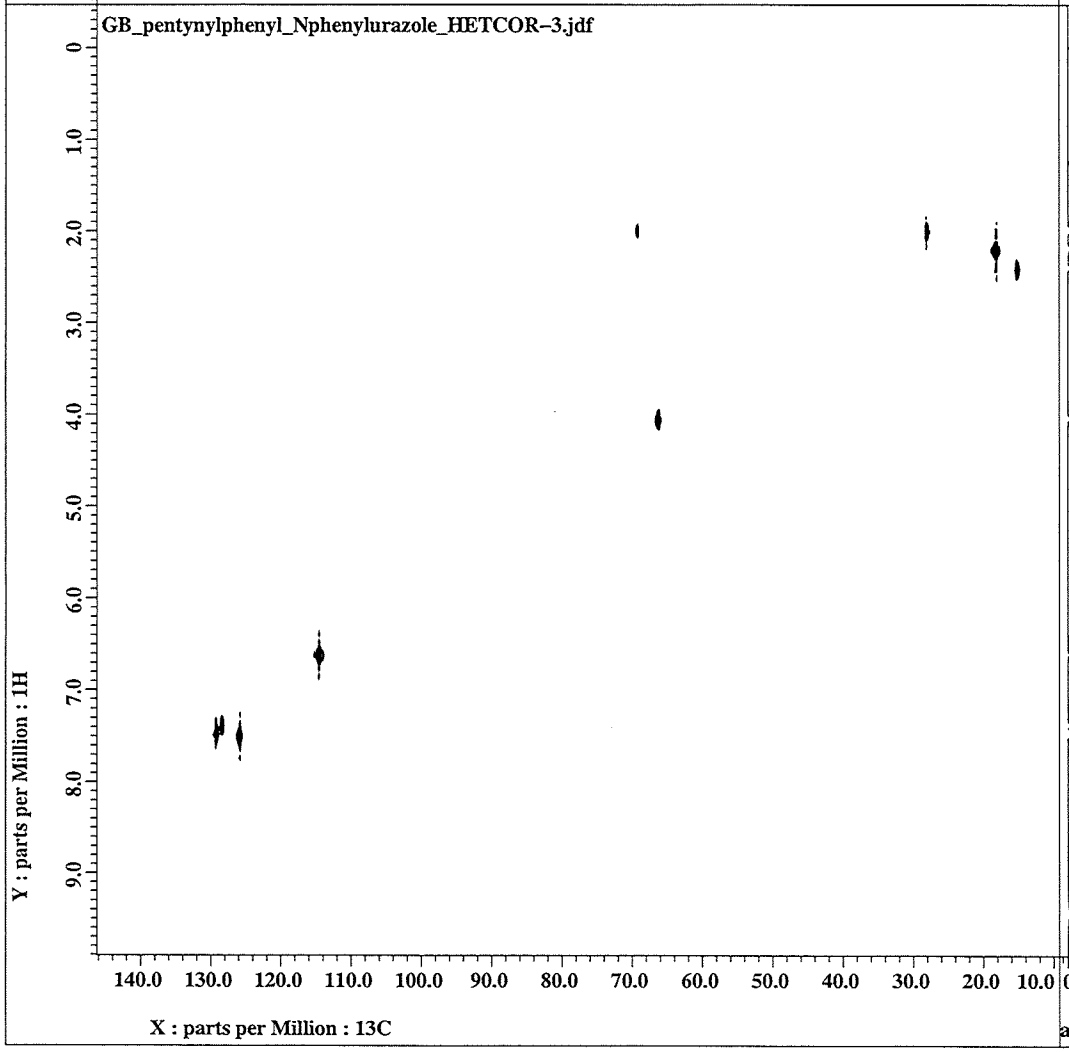


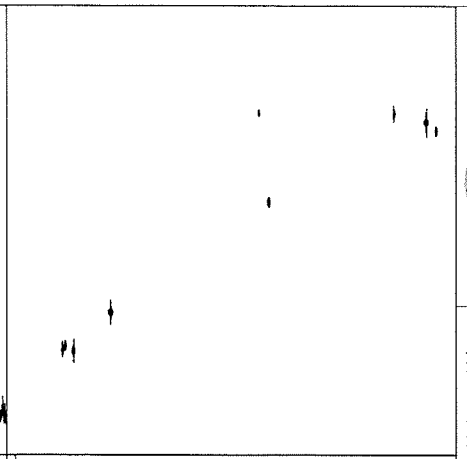
S#466614 (single pulse decoupled gated NOE)

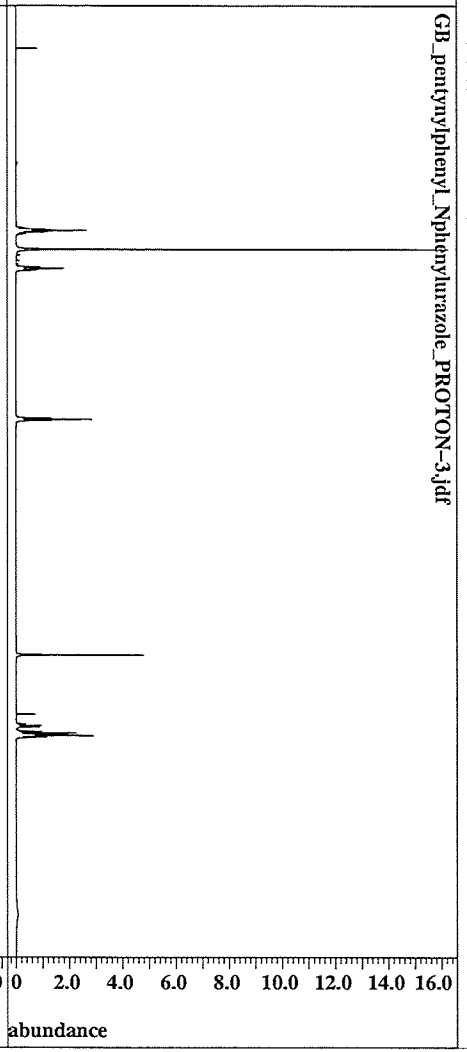
USER: Delta -- DATE: Jun 25, 2018 13:24:40

F1: 100.535	F2: 399.784	SW1: 31407		OF1: 10057.1		PTS1d: 32768
EX: single_pulse_dec		PW: 3.6 us, 30deg	PD: 2.0 sec	NA: 499		Nuts B10 (3,5-dimethylphenoxy 4-pentynyl ether) N-phenyl urazole C13









Filename	= GB_pentynylphenyl_Np
Author	= chemlab
Experiment	= hetcor.ex2
Sample_id	= GB_pentynylphenyl_Np
Solvent	= CHLOROFORM-D
Creation_time	= 12-JAN-2023 12:17:13
Revision_time	= 12-JAN-2023 13:06:12
Current_time	= 12-JAN-2023 13:06:12
Data_format	= 2D REAL REAL
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Dim_title	= 13C 1H
Dim_units	= [ppm] [ppm]
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Spectrometer	= JNM-ECS400
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X_acq_duration	= 59.392[ms]
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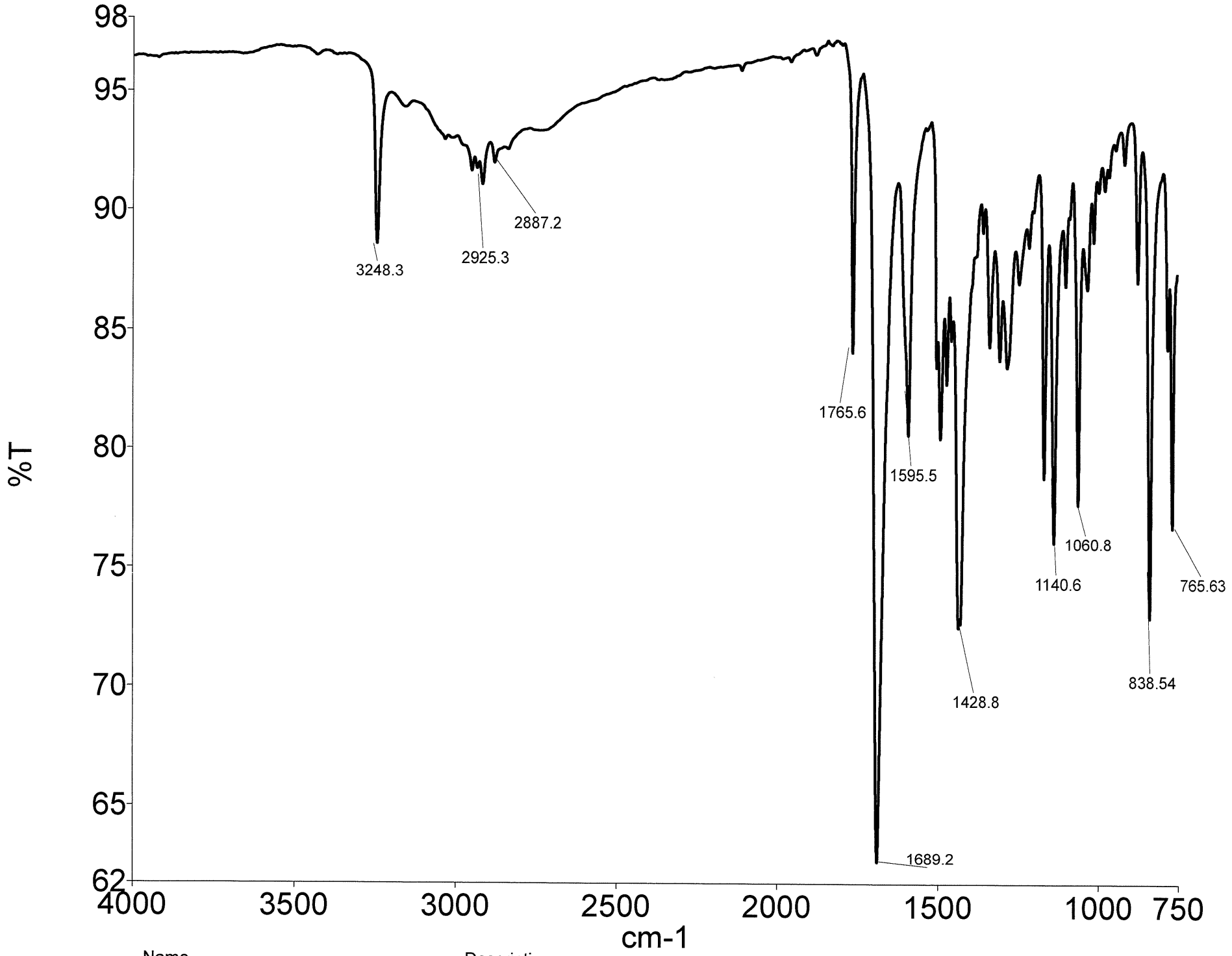
X_freq	= 100.52530333[MHz]
X_offset	= 77.54129439[ppm]
X_points	= 1024
X_prescans	= 4
X_resolution	= 16.83728448[Hz]
X_sweep	= 17.24137931[kHz]
Y_domain	= 1H
Y_freq	= 399.78219838[MHz]
Y_offset	= 4.71190905[ppm]
Y_points	= 128
Y_prescans	= 0
Y_resolution	= 32.46550864[Hz]
Y_sweep	= 4.15558511[kHz]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 1024
X_acq_time	= 59.392[ms]
X_atn	= 5.2[dB]
X_pulse	= 10[us]
Y_acq_time	= 30.80192[ms]
Y_atn	= 3[dB]
Y_pulse	= 13.5[us]
Irr_atn_dec	= 20.8[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
J_constant	= 140[Hz]
Recvr_gain	= 60
Relaxation_delay	= 1[s]
T1	= 1[us]
Temp_get	= 19[dC]



Name — Description

22X Lab User 5916 — Sample 5916 By 22X Lab User Date Thursday, January 12 2023

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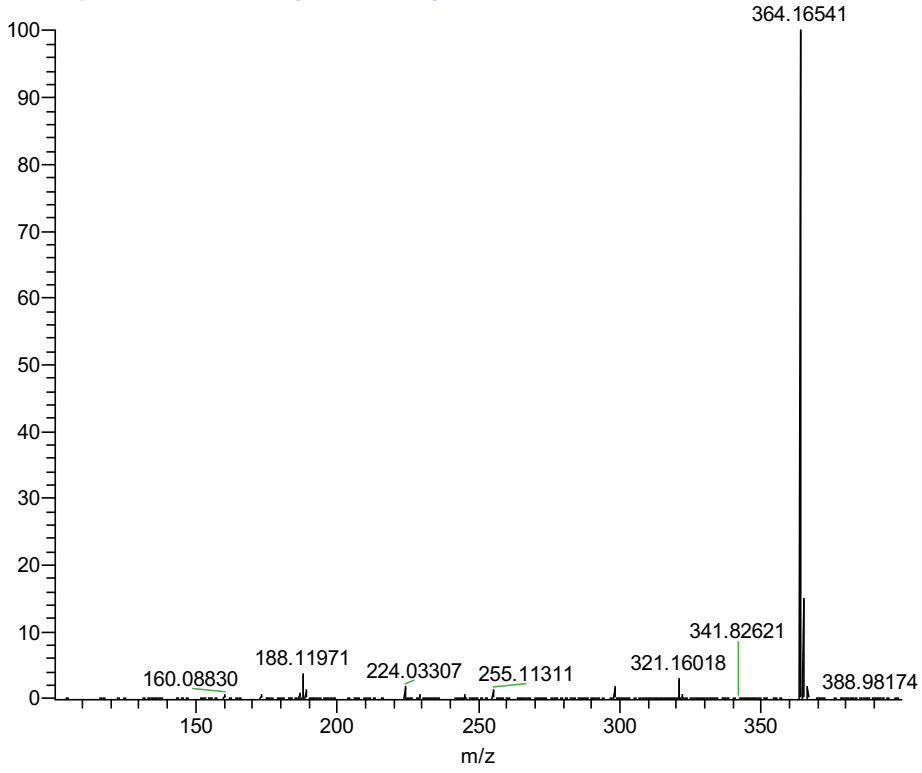
T: FTMS + p APCI corona Full ms [100.00-400.00]



m/z	Intensity	
187.11188	1983210.8	0.95
188.11814	1601015.9	0.77
188.11883	3373668.5	1.62
188.11971	7834584.0	3.75
189.12307	1449726.6	0.69
189.12752	2731794.8	1.31
224.03189	2725828.8	1.31
224.03307	3919032.8	1.88
255.11147	1413567.5	0.68
255.11311	2894534.5	1.39
298.11903	3911099.8	1.87

GB2019B

Elemental composition search on mass 364.16541

m/z= 359.16541-369.16541

m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
364.16541	364.16557	-0.16	12.5	$C_{21}H_{22}O_3N_3$

Elemental composition search on mass 364.16541

m/z= 359.16541-369.16541

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
364.16541	364.16557	-0.43	12.5	$C_{21}H_{22}O_3N_3$

321.16018	6255346.5	3.00
364.15203	1448505.5	0.69
364.16156	22516060.0	10.79
364.16541	208685312.0	100.00
364.17093	5115780.5	2.45
364.17423	1481466.8	0.71
365.16630	11301020.0	5.42
365.16934	30929358.0	14.82
366.17258	3540352.5	1.70