Supplementary Information

Discovery, optimization, and cellular activities of 2-(aroylamino)cinnamamide derivatives against colon cancer

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S1. Cellular mechanisms of compound 1512

S1-A. Induction of apoptosis and apoptotic changes in HCT-116 cancer cell lines upon treatment with 4112.

Method.

See Main test section 4.2.8. Nuclear fragmentation by DAPI staining.

Result.

1512 caused extensive changes in the nuclear matter as illustrated in Figure S1-A.

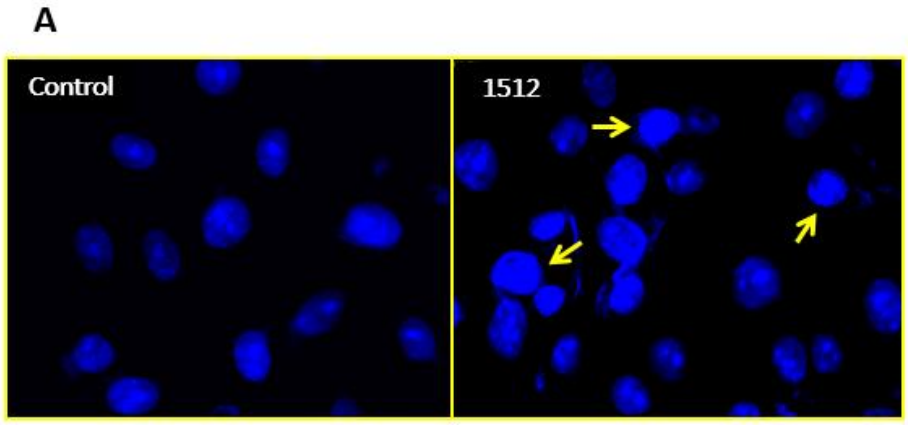


Figure S1-A. Effect of 1512 at 32 µM (IC_{50} concentration) for 48 h on the nuclear structures of HCT-116 cells. Treated cells show nuclear condensation and fragmentation along with the condensed blue fluorescence of DAPI.

S1-B. Cell cycle distribution upon treatment with 1512

Method:

To analyze the DNA content by flow cytometry, HCT-116 cells were seeded at a density of $3x10^6$ cell/ T 75 flask for 24 h and then exposed to different compounds at their IC_{50} values for 24 h. The cells were collected by trypsinization, washed with phosphate buffered saline (PBS) and fixed in ice-cold absolute alcohol. Thereafter, cells were stained using Cycletest^{TM} Plus DNA Reagent Kit (BD Biosciences, San Jose, CA) according to the manufacturer's instructions. Cell cycle distribution was determined using a FACS Calibur flow cytometer (BD Biosciences, San Jose, CA).

Result:

The exposure of the cells to **1512** led to a significant increase in the proportion of cells in pre-G1 phase (Up to 9-fold compared to the control) (Figure S1-B). Accumulation of cells in pre-G1 phase, likely as a result of degradation or fragmentation of genetic material indicates a possible role for apoptosis through compound-induced growth inhibition.

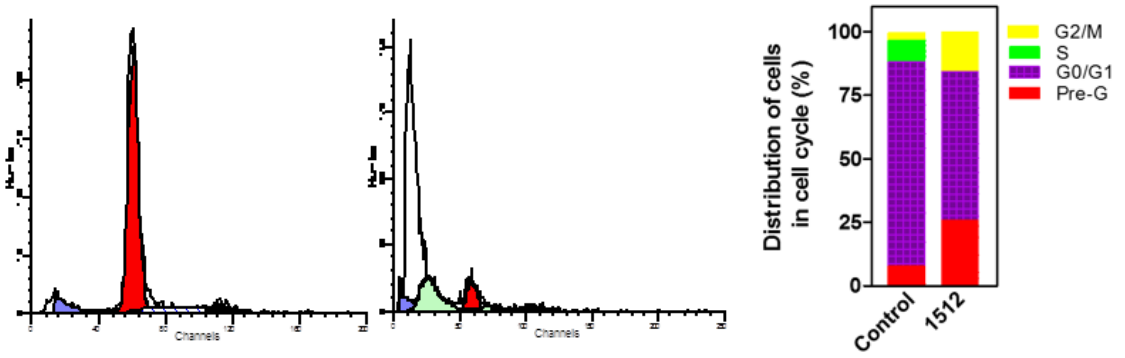


Figure S1-B. Representative DNA histograms of HCT-116 cells following treatment with 1512 at 32 µM (IC_{50} concentration) for 24 h.

S1-C. Changes in marker proteins cyclin B1 cyclin D1, Phospho-histone3 and cleaved caspase3 in apoptotic cells upon treatment with 1512.

Method:

Cells were cultured on sterile 22 mm^2 cover slips (Harvard Apparatus, MA, USA) in sterile six well plates at a density of 2×10^5 cells/well. 24 h after seeding, cells were exposed to IC_{50} of the tested compound in fresh medium for 24 h. At the end of the exposure, cells attached to cover slips were washed with PBS and fixed with 3.7% paraformaldhyde for 10 min, permeabilized with 0.25% Triton X-100 in TBST containing 0.01% Tween 20 for 10 min, and blocked for 1 hr with 5% goat serum in TBST. The fixed and permeabilized cells were incubated with rabbit mAb Cyclin B1, rabbit mAb Cyclin D1, mouse mAB Phosphohistone-H3 or mouse cleaved caspase-3 rabbit mAb (Cell signaling technology, MA, USA) at a dilution of 1:500 in blocking solution overnight at 4ºC, followed by secondary anti-mouse Alexa fluor-488- (Invitrogen, Carlsbad, CA) and Cy3-goat anti-Rabbit antibody (Jackson Immuno Research, West Grove, PA, USA) in 1:1000 dilution in the blocking solution for 1 hr at room temperature in the dark. 4',6'-Diamidino-2-Phenylindole, dihydrochloride (DAPI) (Sigma– Aldrich, St. Louis, MO, USA) was used as counter stain to stain the DNA. The cover slips were then mounted on a glass slide with anti-fade mounting medium and viewed with an epifluorescence microscope, Leica, DM 5500 B (Leica, Buffalo Grove, IL, USA) at a magnification of 60×, and data were captured digitally and quantified using the microscope provided software.

Result:

Accumulation of the apoptotic markers of cyclin B1, cyclin D1, phosphor-histone3 and cleaved caspase3 further confirmed the apoptotic changes upon exposure to compound **1512** (Figure S1-C).

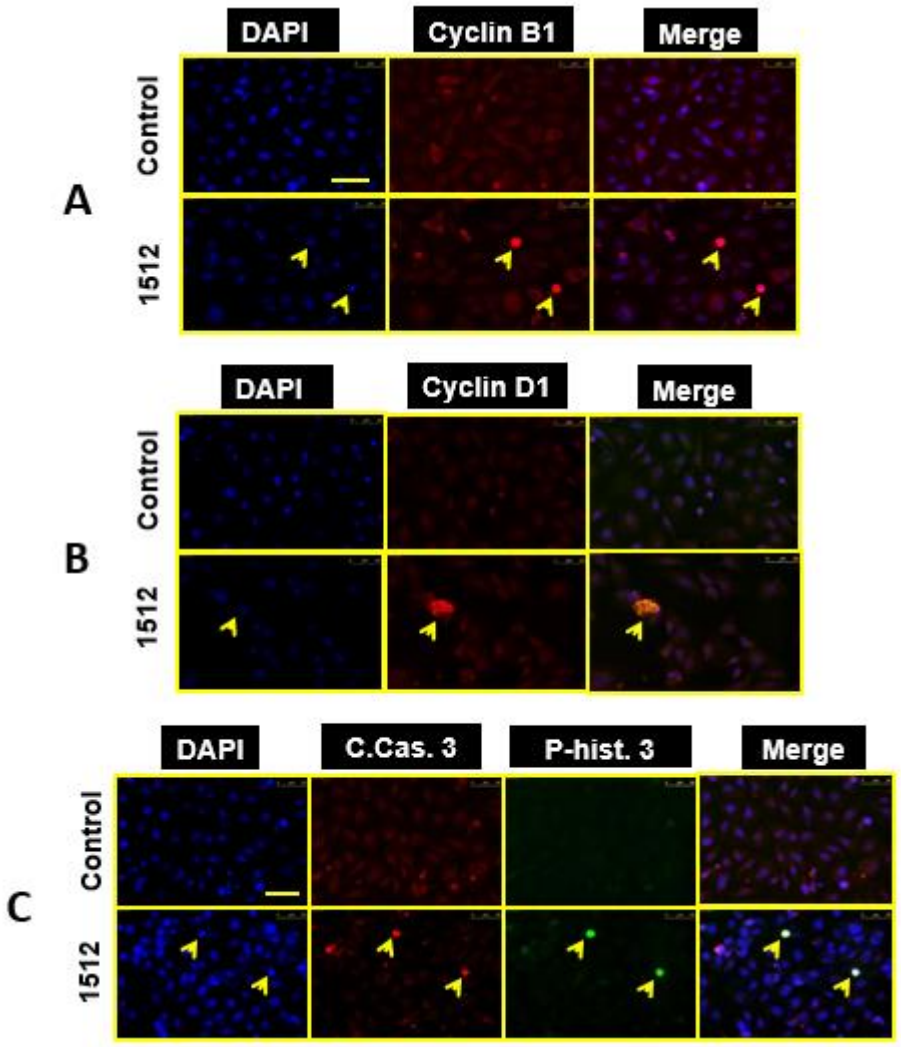


Figure S1-C. Effects of 1512 and on cellular expression of cyclin B1 (A) cyclin D1 (B) in HCT-116 after treatment for 24 h compared to control. Cells were stained with DAPI and incubated with a Cy3-coupled secondary antibody to visualize the distribution of cyclin B1 and cyclin D1 (red) proteins. Treatment of HCT-116 with 1512 increased the nuclear expression of cyclin B1 and cyclin D1 (arrow head) compared with the untreated cells. Scale bar, 50 µm. (C) Effect of 1512 on the cellular expression of caspase-3 (C.Cas. 3) and phospho-histone 3 (P-hist. 3) in human colon cancer cells (HCT-116). The cells were stained with DAPI to visualize nuclei (blue) and with Alexa Fluor 488- and Cy3-coupled secondary antibodies to visualize the distribution of caspase-3 (red) and phospho-histone-3 (green) proteins using immunofluorescence microscopy. The nuclear expression of the pro-apoptotic proteins, activated caspase 3 and phospho-histone 3 (yellow arrows) compared to the untreated cells. Scale bar, 50 µm.

S1-D. Elevation of oxidative stress indicators within HCT-116 cells upon treatment with 1512.

The underlying mechanism by which **1512** induced cancer cells to undergo apoptotic cell death was investigated by measuring changes in redox indicators within HCT-116 CRC cell lines. In this study, we first checked the influence of **1512** on cellular activities of the peroxide scavenging enzymes catalase and superoxide dismutase (SOD) (**Figure 8A**).

Method:

For DHE and DCFDA, cells were cultured on sterile 22 mm2 cover slips (Harvard Apparatus, MA, USA) in sterile six well plates at a density of 2×105 cells/well. 24 h after seeding, cells were exposed to IC_{50} of the tested compounds in fresh medium for 24 h. At the end of the exposure, cells attached to cover slips were washed thrice with PBS and incubated with DHE 10µM or DCFDA 10 µM for 30 min at 37 ºC in the dark. Thereafter, cells were washed thrice

with PBS and the cover slips were then mounted on a glass slide with anti-fade mounting medium containing 4',6'-Diamidino-2-Phenylindole, dihydrochloride (DAPI) (Sigma–Aldrich, St. Louis, MO, USA), which was used as counter stain and viewed with an epifluorescence microscope, Leica, DM 5500 B (Leica, Buffalo Grove, IL, USA) at a magnification of 60×. Data were captured digitally and quantified using the microscope provided software.

For assessment of SOD and CAT activities as well as SOD and MDA levels, 4 x10^6 cell/ T 75 flask were exposed to the IC_{50} of tested compound for 24 h. The cells were collected by trypsinization and washed twice with PBS. Cells were directly homogenized in PBS on ice with a Dounce homogenizer 3 times (each 25 strokes) at 10-min intervals, then centrifuged at 15000 rpm for 15 min at 4 ºC. An aliquot was kept to determine the protein concentration using a BioRad protein assay DC kit (Bio Rad Laboratories, CA). Different parameters were then assessed using equal protein amounts in all samples and employing the specified kit according to the manufacturer's instructions. (3, 4, 5 and 6).

Results:

Activities of both enzymes significantly diminished to 34.7% and 25.1% respectively, compared to untreated cells (control). However, the cellular contents of the non-enzymatic SH containing redox markers, such as reduced glutathione (GSH) and malondialdehyde (MDA, a lipid oxidation marker) were only slightly affected (95.2% and 103.4% respectively, compared to control).

To confirm the increased intracellular ROS production, we performed dihydroethidium (DHE) staining test at which untreated HCT cancer cells were compared to **1512**-treated cells (at 32 µM, the IC_{50} value). As seen in figure 8B, the cells treated with **1512** attained more red fluorescence than the untreated cells indicating higher cellular peroxide content, which resulted from increased ROS production within the drug-treated cancer cells [1].

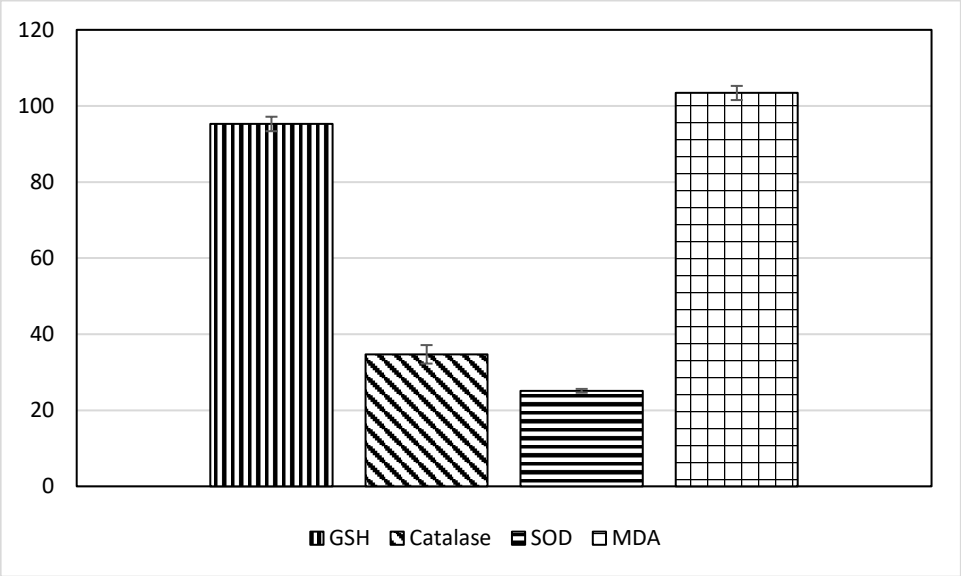


Figure 8. (A) Effect of 1512 (32 µM, 48 h) on redox indicators with HCT-116. The values are expressed as percentage of controls and calculated from the means of three independent experiments. (B) Effect of compound 1512 on superoxide anion generation in HCT-116 cells using DHE staining method. Red fluorescence represents DHE staining and DAPI was used as counter nuclear stain.

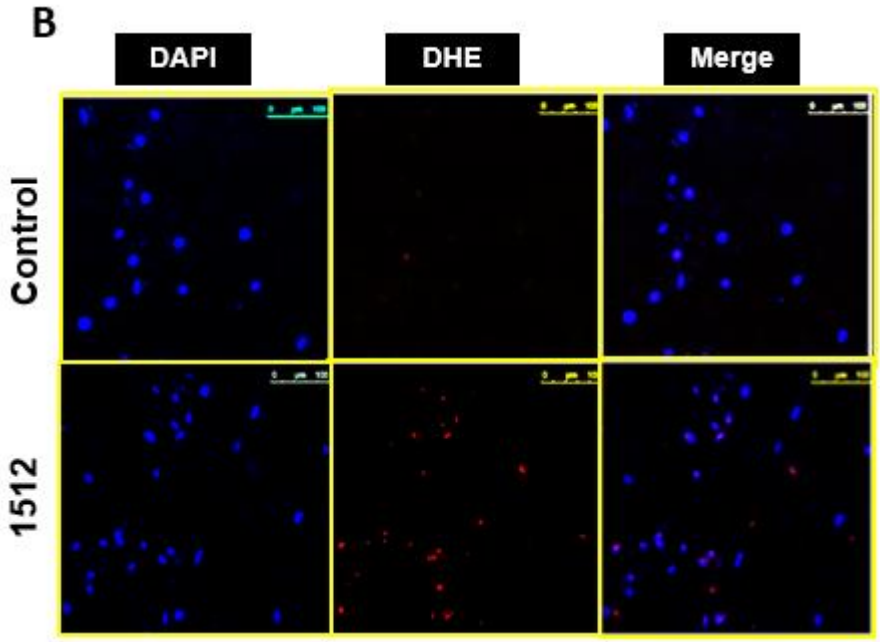
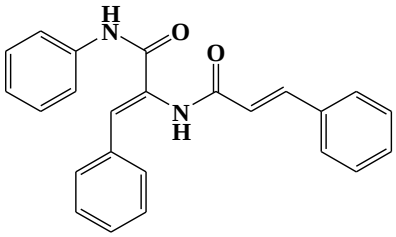


Figure S1-D. (A) Effect of 1512 (32 uM, 48 h) on redox indicators with HCT-116. The values are expressed as percentage of controls and calculated from the means of three independent experiments. (B) Effect of compound 1512 on superoxide anion generation in HCT-116 cells using DHE staining method. Red fluorescence represents DHE staining and DAPI was used as counter nuclear stain.

S2. Spectra of Compounds

Spectra of (1501)[2-3]



^{1}H NMR

1501A

4/23/2017 10:06:13 PM

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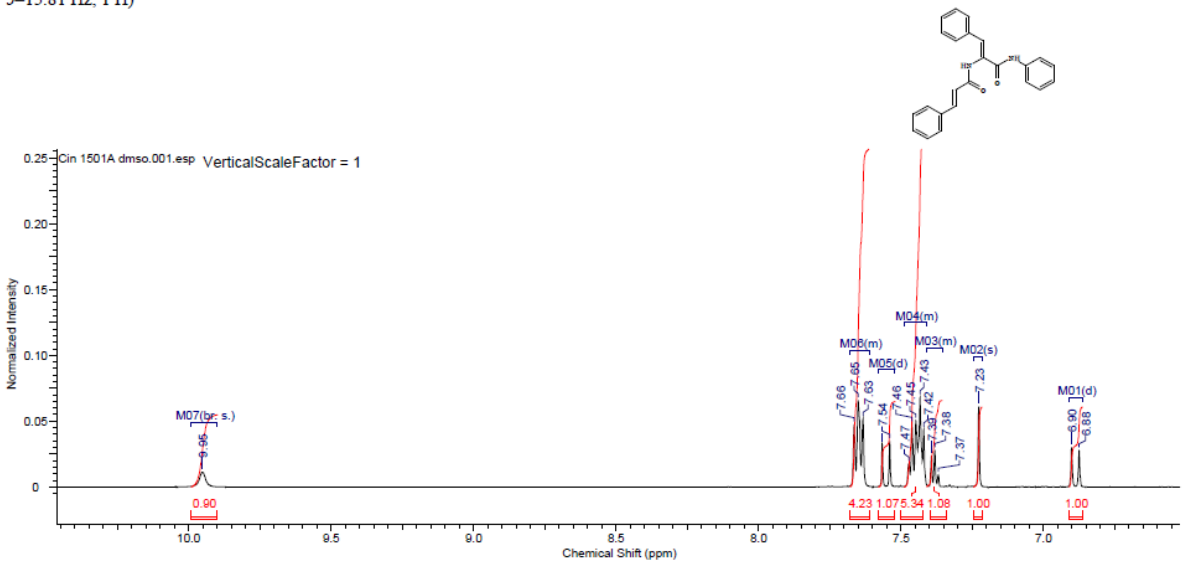
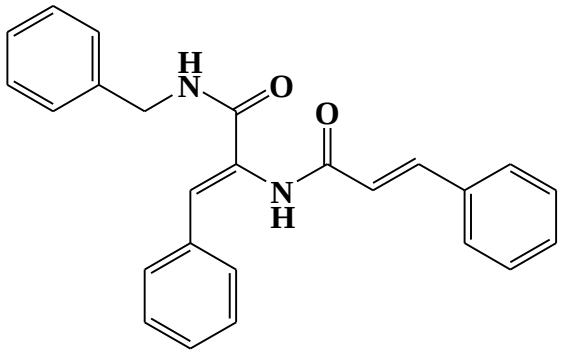
Spectrum Type	STANDARD	***Sweep Width (Hz)***	12335.15	***Temperature (degree C)***	25.014		

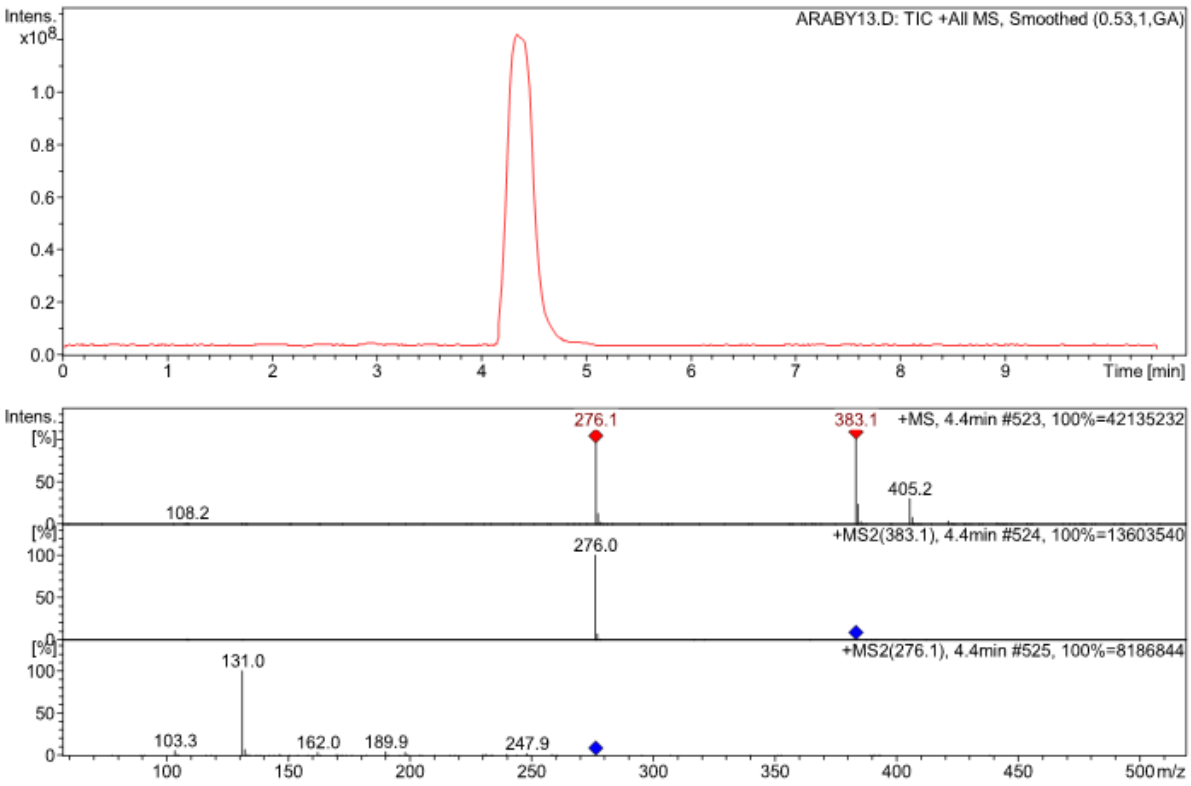
^{1}H NMR (DMSO-d_6) δ ppm 9.95 (br. s., 1 H), 7.61 - 7.68 (m, 5 H), 7.55 (d, *J*=15.81 Hz, 1 H), 7.41 - 7.49 (m, 7 H), 7.36 - 7.41 (m, 1 H), 7.23 (s, 1 H), 6.89 (d, *J*=15.81 Hz, 1 H)



Spectra of (1502)[2, 4]



LC/MS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405.2
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m/z

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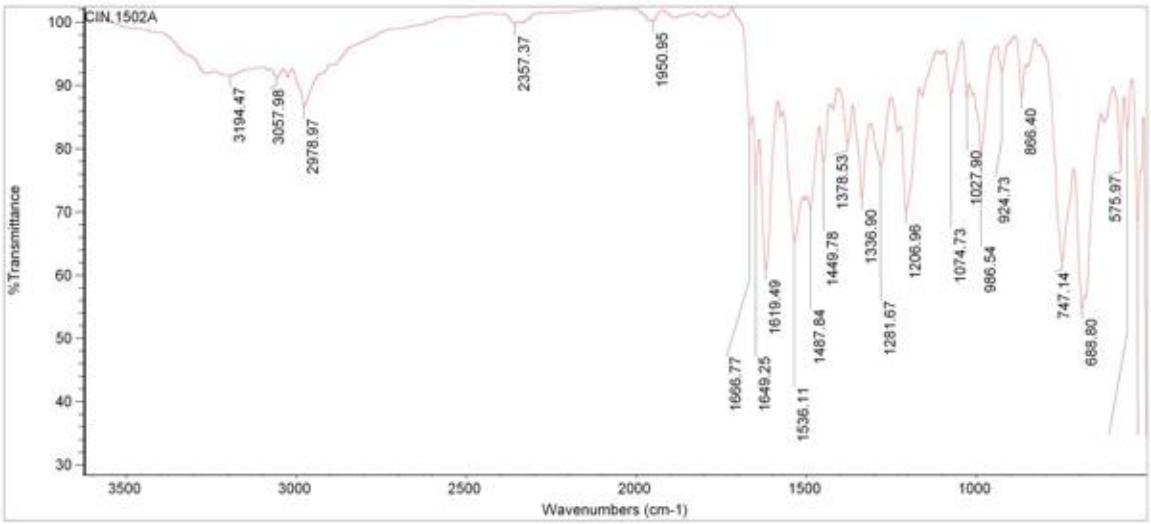

^{1}H NMR

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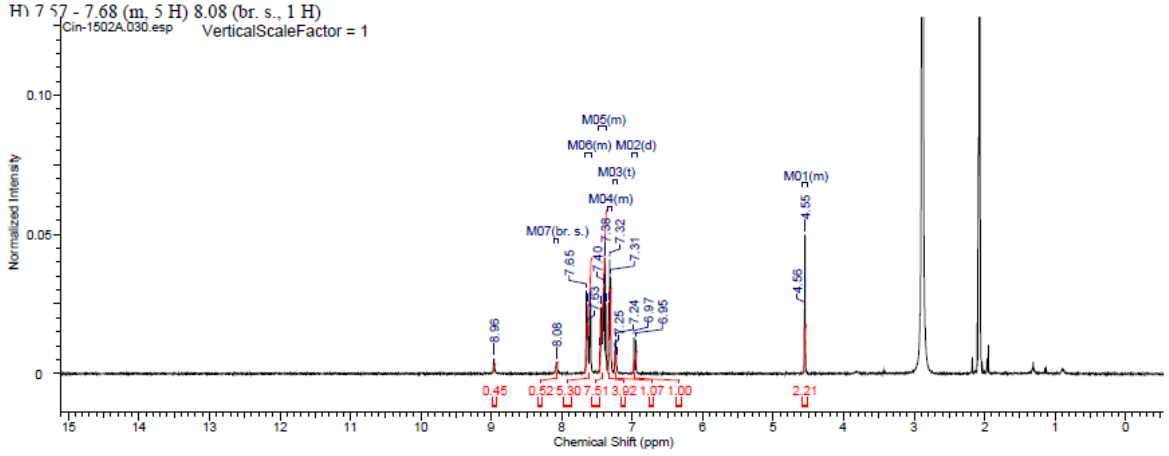

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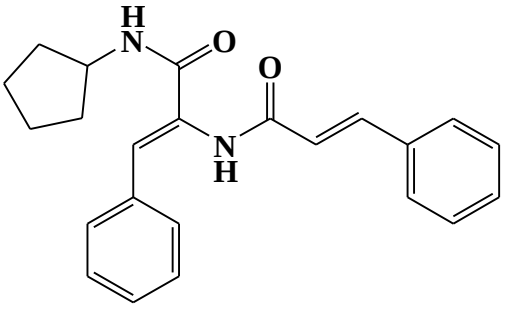

^{1}H NMR

1503

2018-10-01 7:54:52 AM

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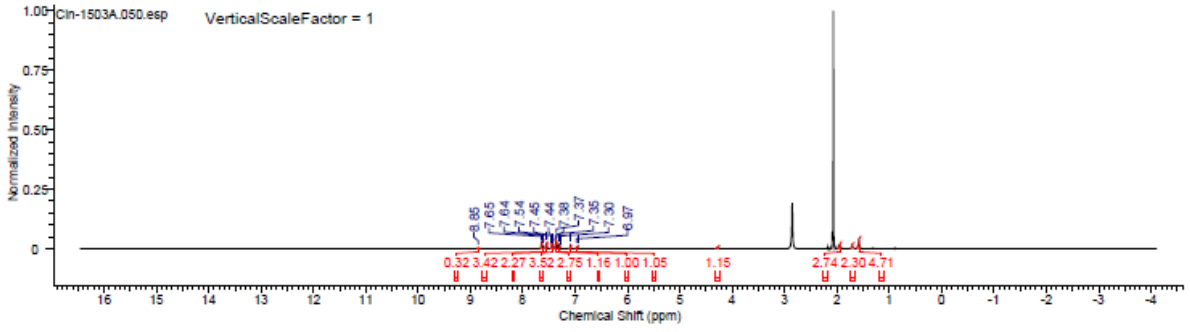

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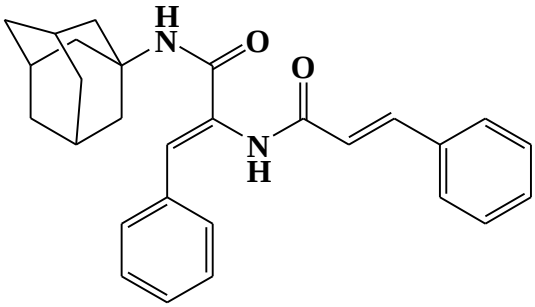

CIN-1505A-4m

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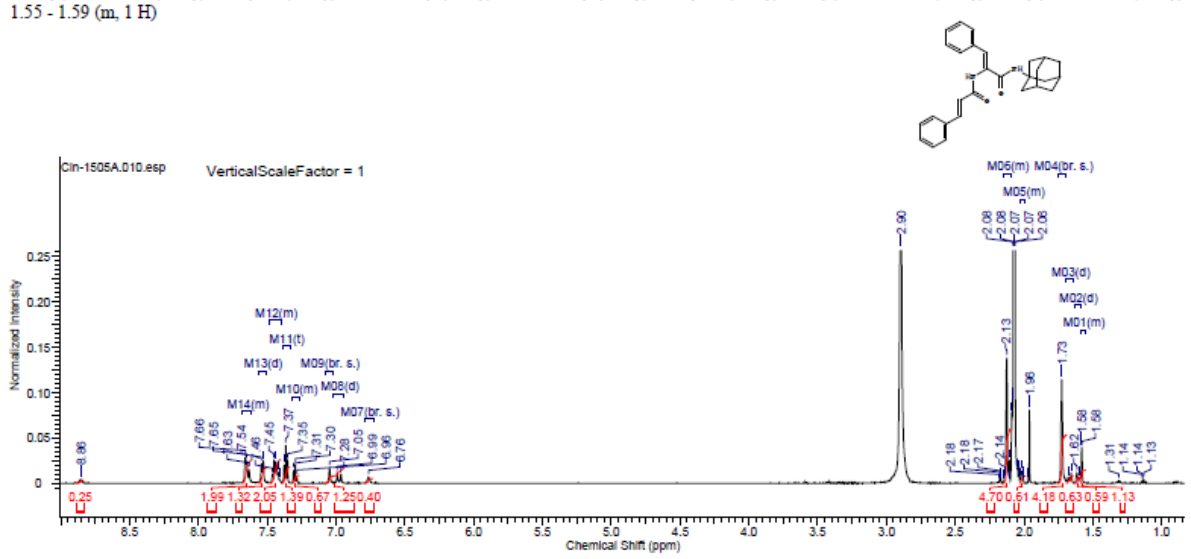

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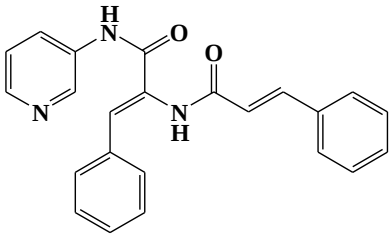
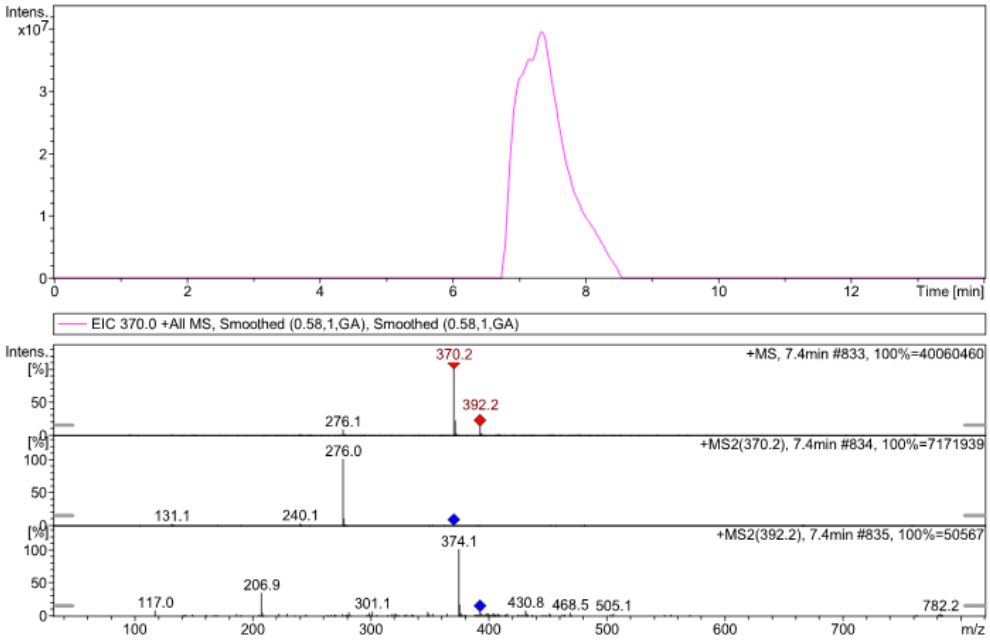
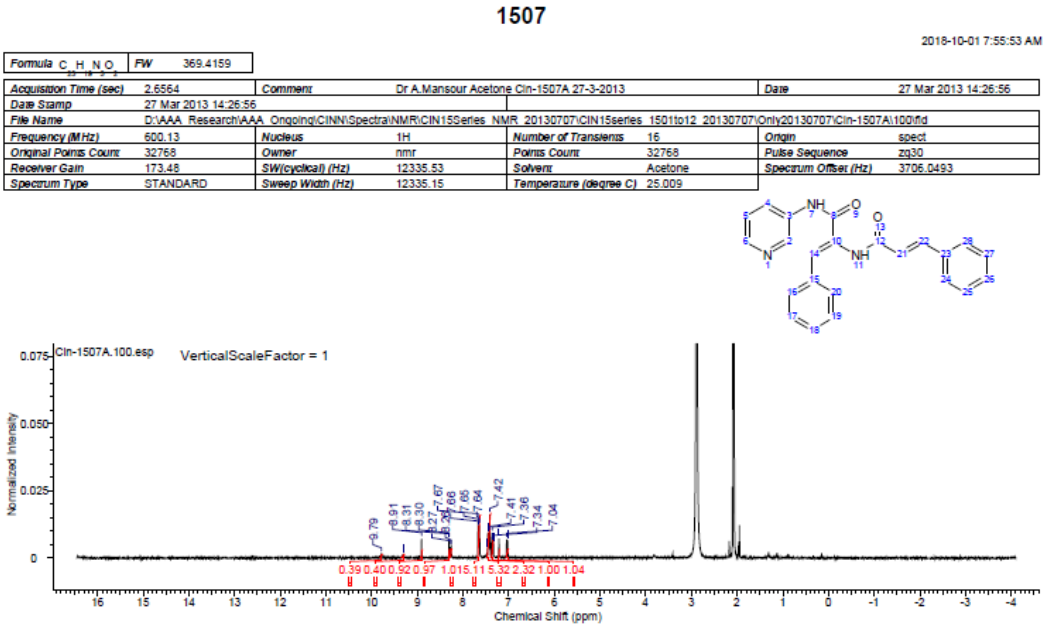


LC/MS



^{1}H NMR



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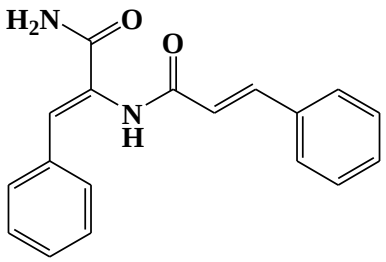

^{1}H NMR

1508

10/6/2018 12:11:26 AM
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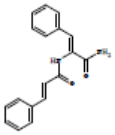

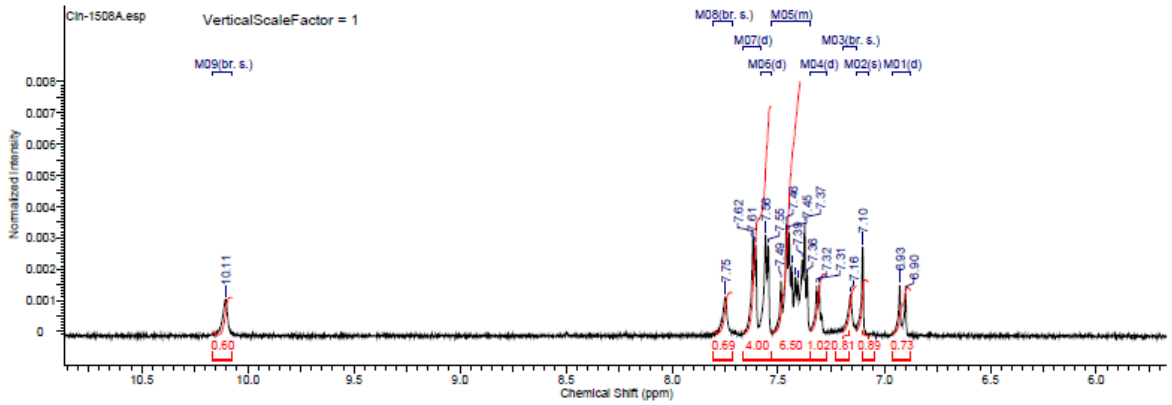

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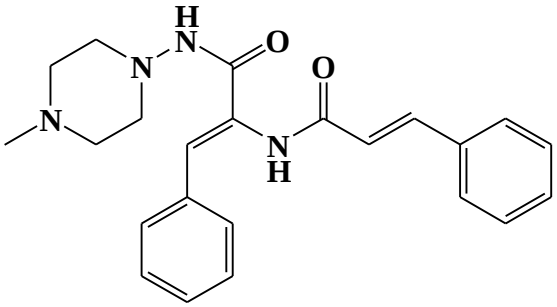

^{1}H NMR

Cin-1511A

4/7/2015 04:15:42

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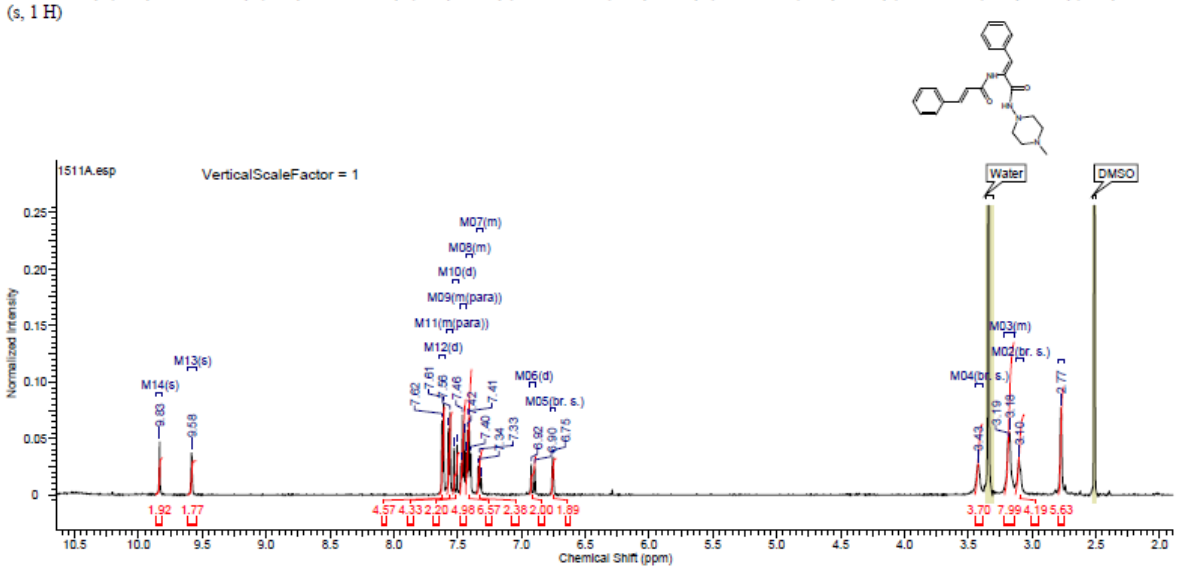
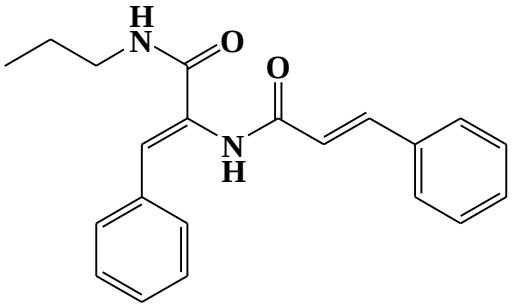
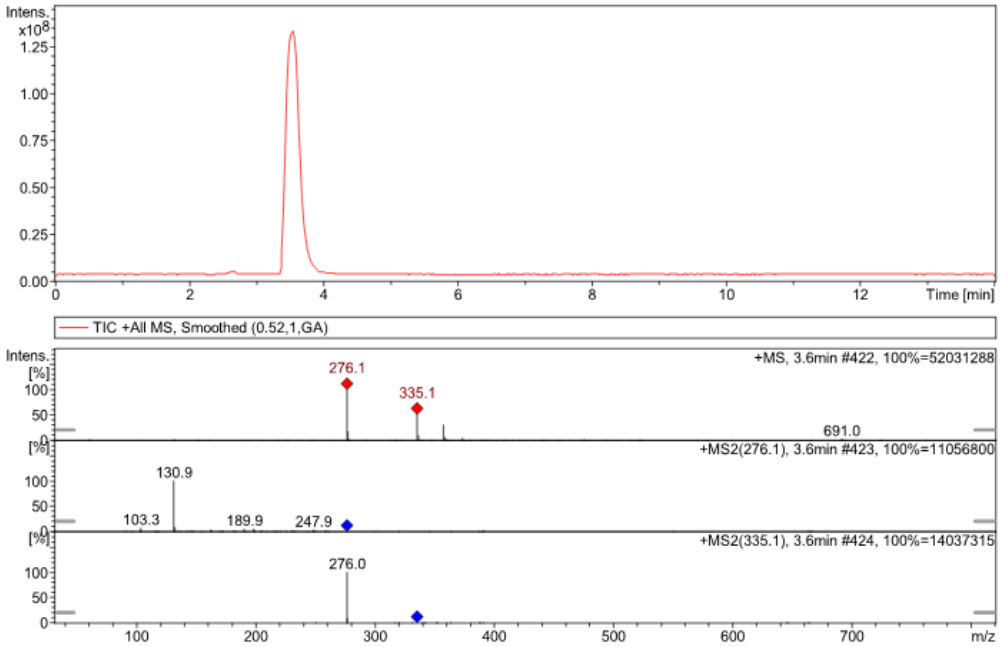


Spectra of (1512)



LC/MS



^{1}H NMR

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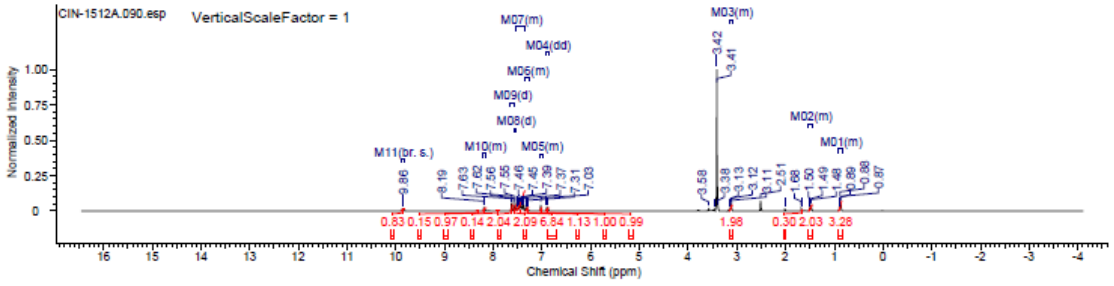
1512

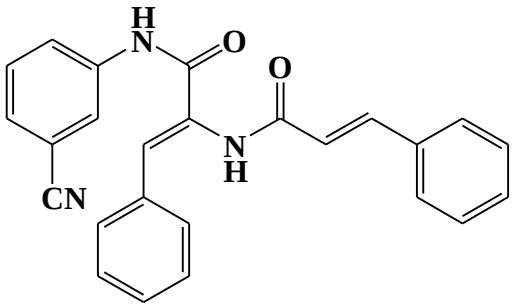
2018-10-01 7:58:31 AM

Formula $C_{21}H_{22}N_2O_2$	FW	334.4116					
Acquisition Time (sec)	2.6564	Comment	Dr.Mansour DMSO CIN-1512A			Date	07 Jul 2013 14:22:40
Date Stamp	07 Jul 2013 14:22:40						
File Name	D:\AAA_Research\AAA_Ongoing\CINN\Spectra\NMR\CIN15Series_NMR_20130707\CIN15series_1501to12_20130707\Garbage\CIN-1512A\90\fid						
Frequency (MHz)	600.13	Nucleus	1H	Number of Transients	16	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	34.94	SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.0483
Spectrum Type	STANDARD	Sweep Width (Hz)	12335.15	Temperature (degree C)	25.001		

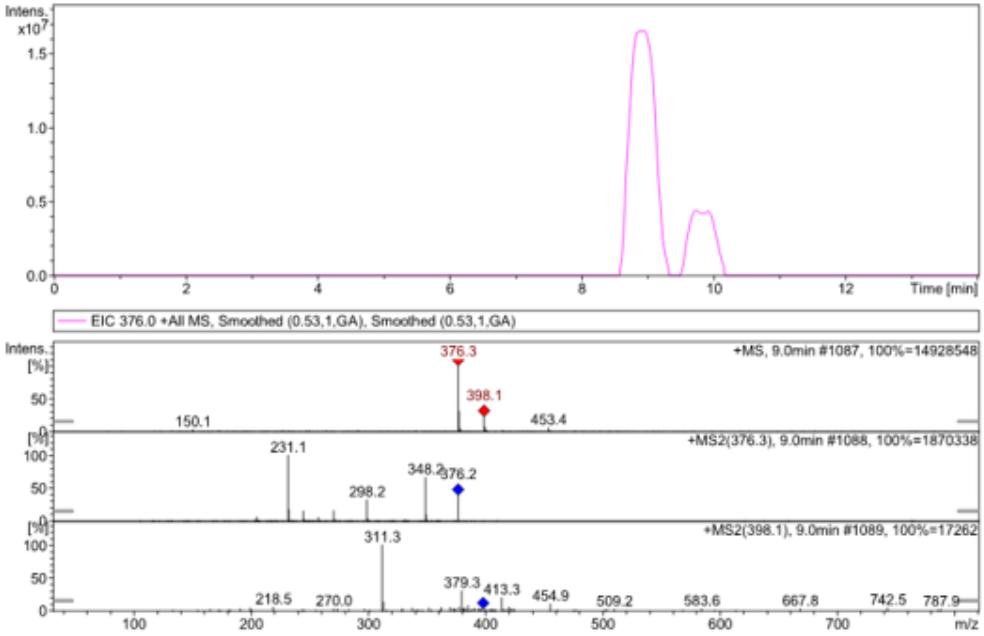
^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 0.84 - 0.91 (m, 3 H) 1.44 - 1.53 (m, 2 H) 3.09 - 3.16 (m, 2 H) 6.90 (dd, *J*=15.81, 2.64 Hz, 1 H) 6.99 - 7.04 (m, 1 H) 7.28 - 7.34 (m, 1 H) 7.34 - 7.52 (m, 7 H) 7.56 (d, *J*=6.78 Hz, 2 H) 7.62 (d, *J*=7.15 Hz, 2 H) 8.15 - 8.22 (m, 1 H) 9.86 (br. s., 1 H)



Spectra of (1513)



LC/MS



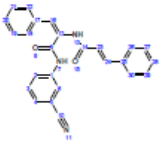
^{1}H NMR

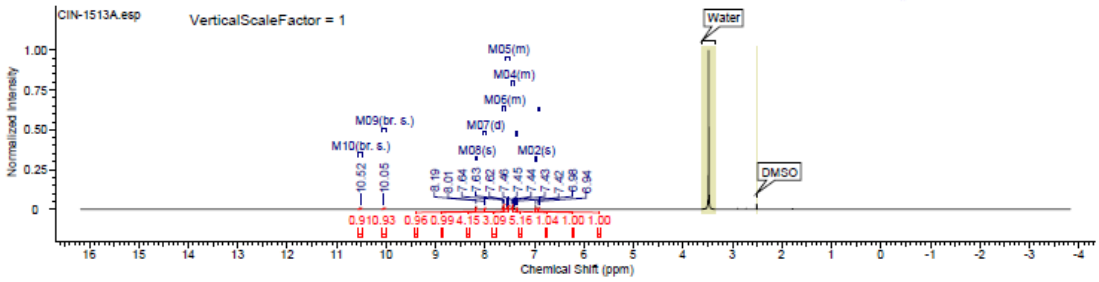
1513

2018-10-06 5:28:54 PM

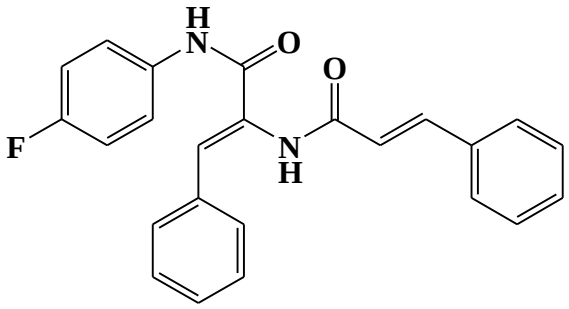
Formula $C_{25}H_{19}N_3O_2$	*FW* 393.4373				
Acquisition Time (sec)	1.9268	*Comment*	Dr.Abdelsattar Omar Sample: CINB-12A DMSO	*Date*	22 Dec 2014 14:18:24
Date Stamp	22 Dec 2014 14:18:24				
File Name	E:\AAA Research\Spectra Reservoir\NMR 20141223\Dr.Omar CIN-13A 22-12-2014\20\fid			*Frequency (MHz)*	850.15
Nucleus	1H	*Number of Transients*	16	*Origin* spect	*Original Points Count* 32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence* zg30	*Receiver Gain* 7.13
SW(cyclical) (Hz)	17006.80	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)* 5250.0283	*Spectrum Type* STANDARD
Sweep Width (Hz)	17006.28	*Temperature (degree C)*	25.000		

^{1}H NMR (850 MHz, DMSO-d_6) δ ppm 10.52 (br. s., 1 H) 10.05 (br. s., 1 H) 8.19 (s, 1 H) 8.01 (d, *J*=7.78 Hz, 1 H) 7.60 - 7.66 (m, 4 H) 7.50 - 7.58 (m, 3 H) 7.40 - 7.48 (m, 5 H) 7.34 - 7.39 (m, 1 H) 6.98 (s, 1 H) 6.93 (d, *J*=16.09 Hz, 1 H)

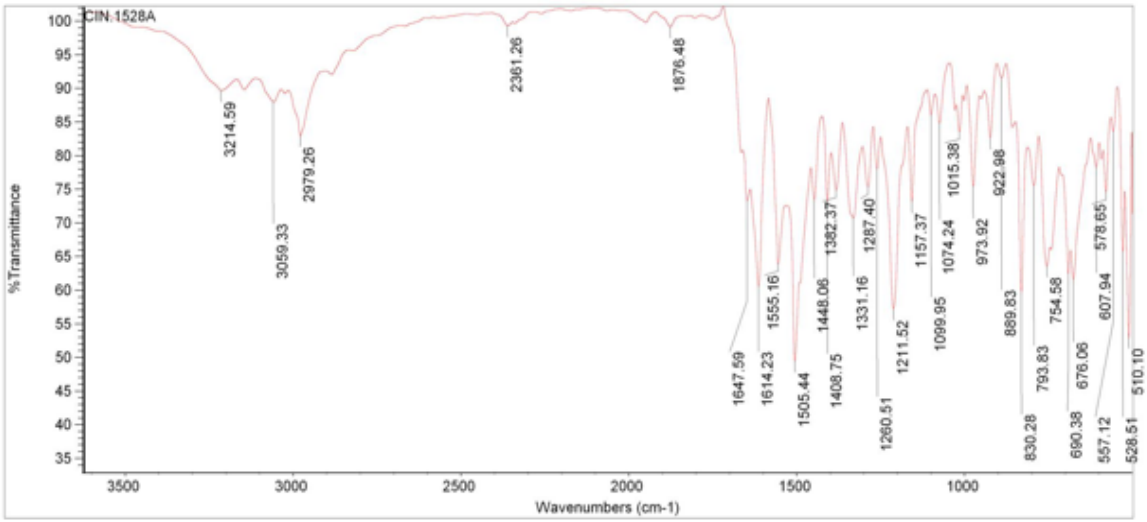




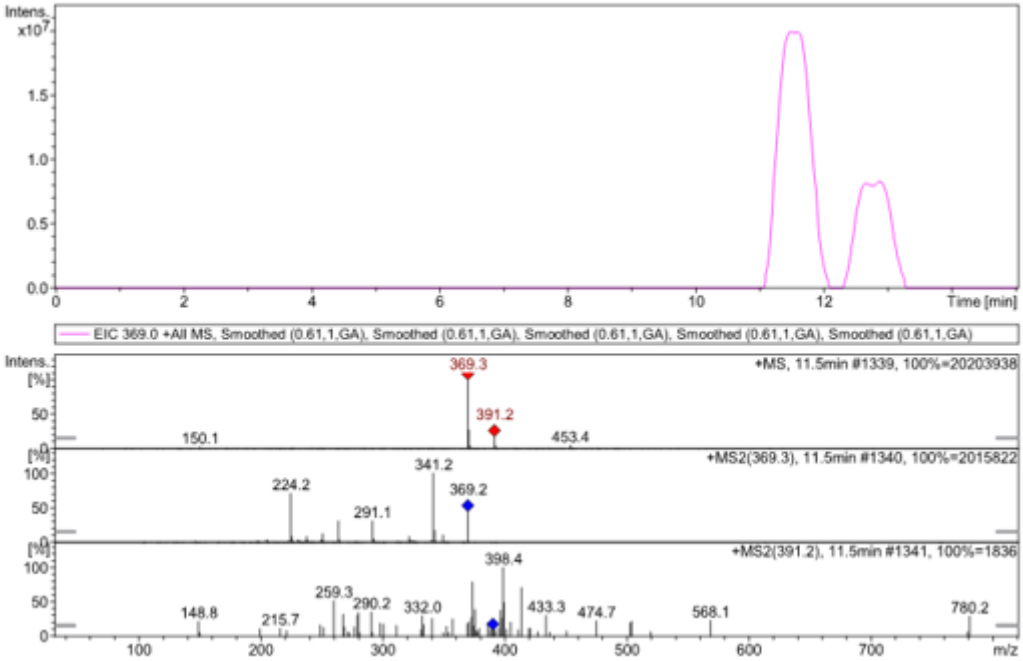
Spectra of (1528)



FT-IR



LC/MS



^{1}H NMR

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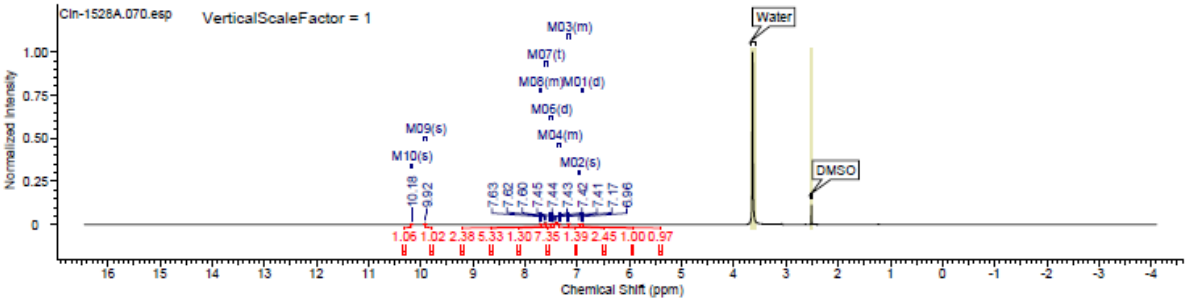
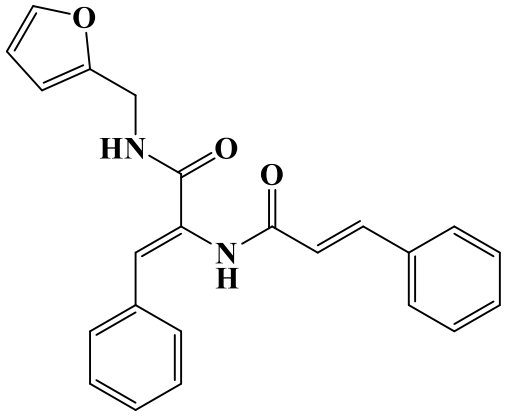
1528

2018-10-01 8:02:14 AM

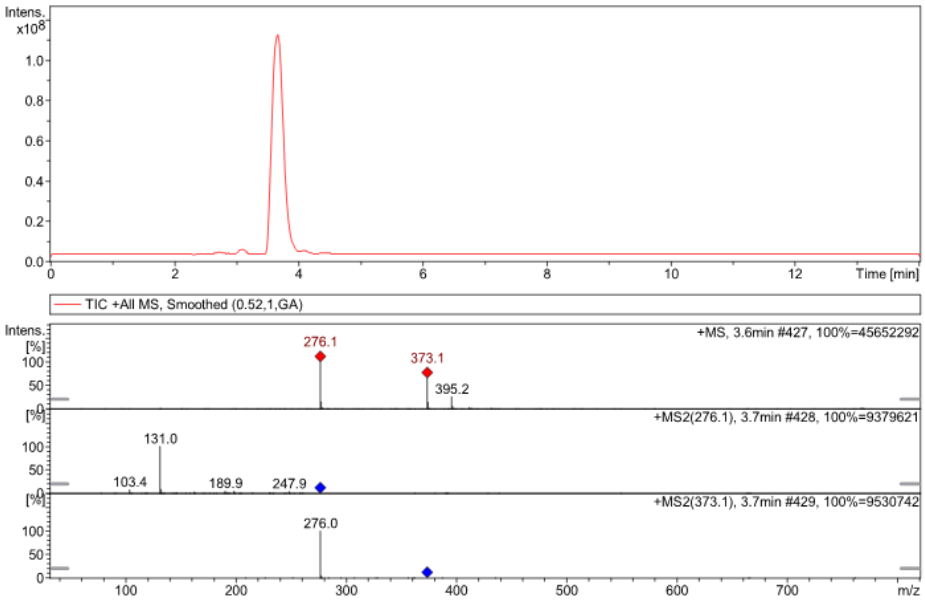
Formula $C_{24}H_{19}FN_2O_2$	FW 386.4183				
Acquisition Time (sec)	2.6564	Comment	Dr A Mansour DMSO CIN-1528A	Date	09 Jun 2013 12:06:08
Date Stamp	09 Jun 2013 12:06:08				
File Name	D:\AAA_Research\AAA_Ongoing\CINN\Spectra\NMR\CIN15Series_NMR_20130707\CIN15series_1513to31_20130707\Cin-1528A\70\fid				
Frequency (MHz)	600.13	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	15.76	SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6
Spectrum Type	STANDARD	Sweep Width (Hz)	12335.15	Temperature (degree C)	25.008

^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ ppm 6.91 (d, *J*=15.81 Hz, 1 H) 6.96 (s, 1 H) 7.13 - 7.20 (m, 3 H) 7.33 - 7.37 (m, 1 H) 7.39 - 7.48 (m, 8 H) 7.51 (d, *J*=15.81 Hz, 1 H) 7.62 (t, *J*=6.96 Hz, 5 H) 7.68 - 7.74 (m, 2 H) 9.92 (s, 1 H) 10.18 (s, 1 H)

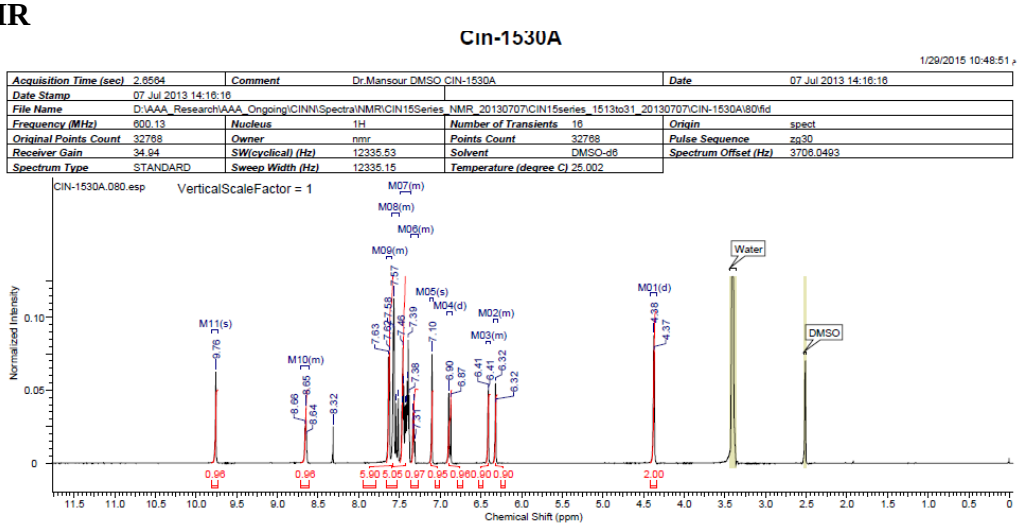




LC/MS



^{1}H NMR



No.	(ppm)	(Hz)	Height
1	4.37	2620.9	0.0761
2	4.38	2626.6	0.0877
3	6.32	3790.6	0.0401
4	6.32	3792.8	0.0547
5	6.32	3793.6	0.0547
6	6.41	3845.5	0.0484
7	6.41	3846.7	0.0502
8	6.41	3848.5	0.0496

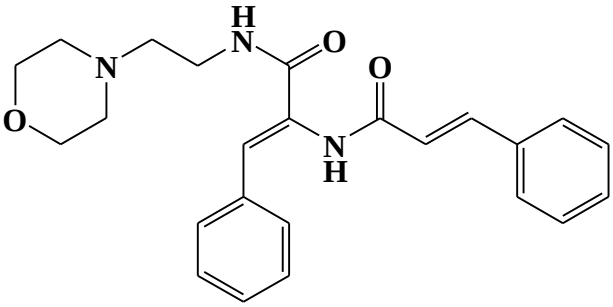
No.	(ppm)	(Hz)	Height
9	6.87	4122.6	0.0436
10	6.90	4138.4	0.0481
11	7.10	4262.3	0.0748
12	7.31	4387.6	0.0148
13	7.31	4388.7	0.0135
14	7.32	4395.1	0.0414
15	7.34	4402.3	0.0348
16	7.34	4403.4	0.0308

No.	(ppm)	(Hz)	Height
17	7.38	4429.4	0.0465
18	7.39	4437.3	0.0846
19	7.41	4444.8	0.0565
20	7.42	4452.4	0.0406
21	7.43	4459.9	0.0399
22	7.45	4469.7	0.0533
23	7.46	4477.2	0.0790
24	7.47	4484.0	0.0399

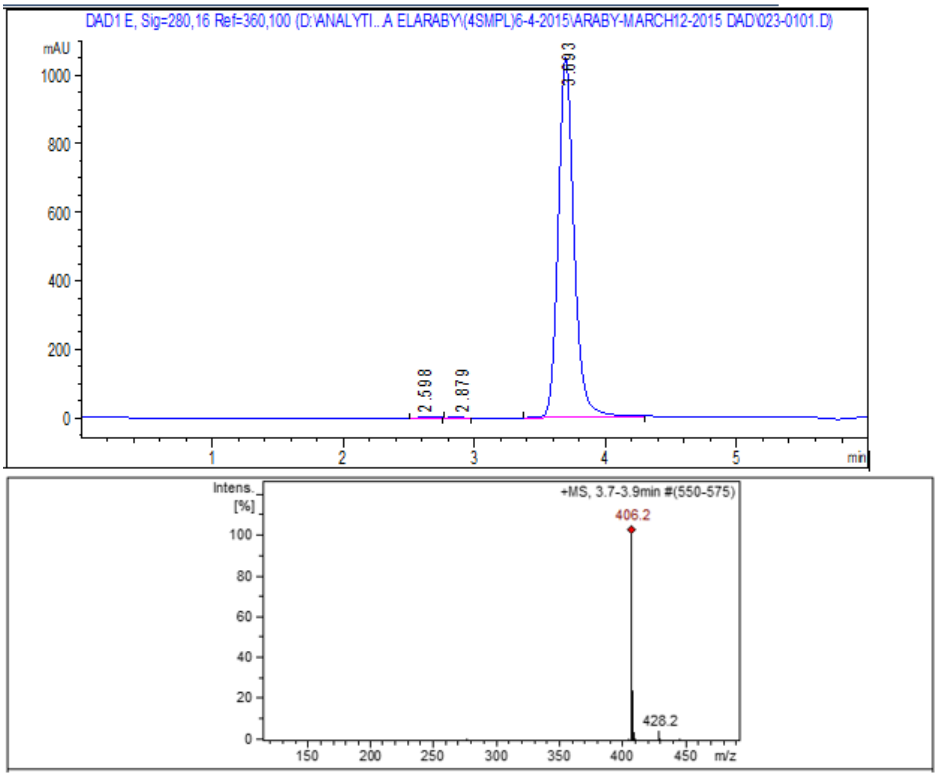
No.	(ppm)	(Hz)	Height
25	7.51	4510.0	0.0444
26	7.54	4525.8	0.0412
27	7.57	4542.3	0.1130
28	7.57	4543.1	0.1103
29	7.58	4547.6	0.0913
30	7.62	4574.7	0.0756
31	7.63	4581.9	0.0728
32	7.64	4582.6	0.0726

No.	(ppm)	(Hz)	Height
33	8.32	4991.8	0.0249
34	8.64	5186.4	0.0177
35	8.65	5192.1	0.0376
36	8.66	5197.7	0.0252
37	9.76	5856.5	0.0626

Spectra of (1531)



LC/MS



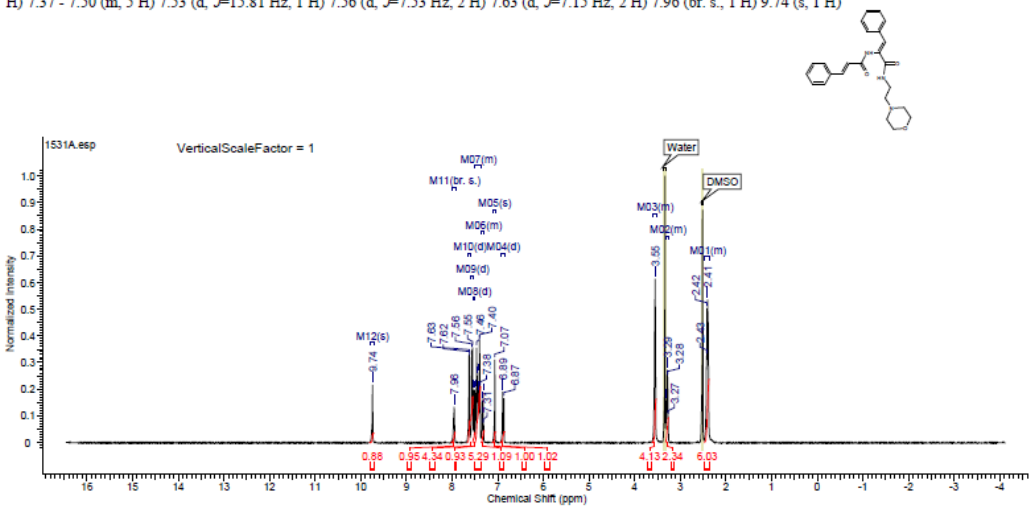
^{1}H NMR

Cin-1531A

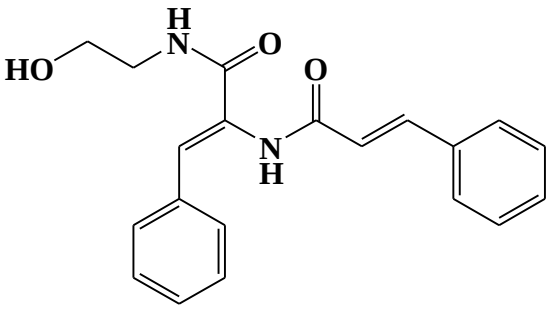
4/6/2015 02:51:29

Acquisition Time (sec)	2.6564	*Comment*	Dr.A.Mansour DMSO RAKAN 51A			*Date*	25 Feb 2015 14:29:04
Date Stamp	25 Feb 2015 14:29:04			*File Name*	E:\Google Drive\Projects\CIN-Extension\Spectra\Rakan\RAKAN 51A\1\fid		
Frequency (MHz)	600.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	99.00	*SW(cyclical) (Hz)*	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.0500
Spectrum Type	STANDARD	*Sweep Width (Hz)*	12335.15	*Temperature (degree C)*	25.021		

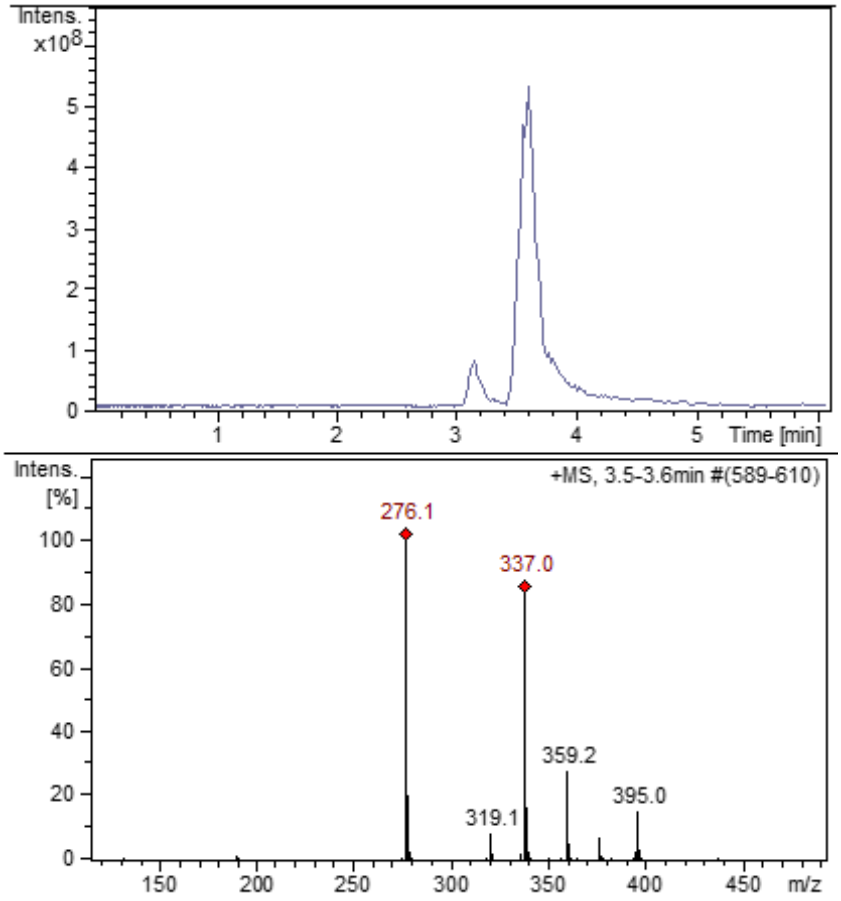
^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ ppm 2.37 - 2.47 (m, 6 H) 3.25 - 3.32 (m, 2 H) 3.52 - 3.61 (m, 4 H) 6.88 (d, *J*=16.19 Hz, 1 H) 7.07 (s, 1 H) 7.29 - 7.36 (m, 1 H) 7.37 - 7.50 (m, 5 H) 7.53 (d, *J*=15.81 Hz, 1 H) 7.56 (d, *J*=7.53 Hz, 2 H) 7.63 (d, *J*=7.15 Hz, 2 H) 7.96 (br. s., 1 H) 9.74 (s, 1 H)



Spectra of (1532)



LC/MS



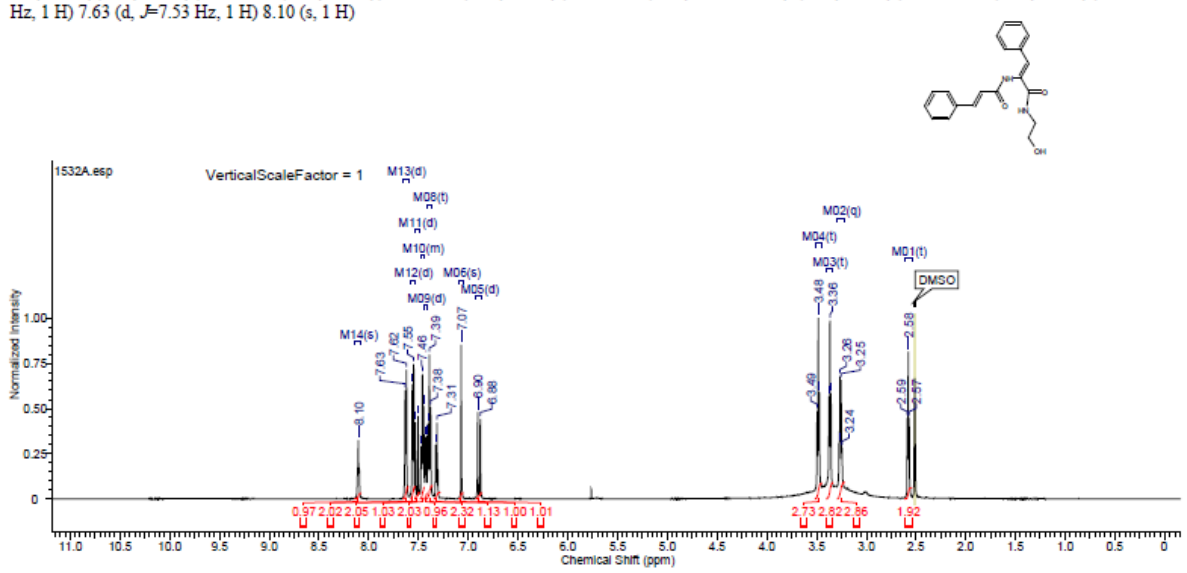
^{1}H NMR

Cin-1532A

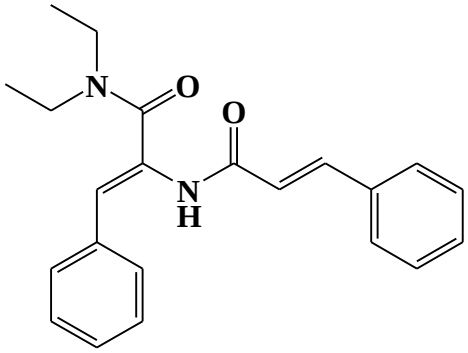
4/7/2015 05:03:02

Acquisition Time (sec)	2.6564	*Comment*	Dr.A.Mansour DMSO RAKAN 1532A	*Date*	25 Feb 2015 14:41:52
Date Stamp	25 Feb 2015 14:41:52			*File Name*	E:\Google Drive\Projects\CIN-Extension\Spectra\Rakan\RAKAN 1532A\1\fid
Frequency (MHz)	600.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	34.94	*SW(cyclical) (Hz)*	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.0500
Spectrum Type	STANDARD	*Sweep Width (Hz)*	12335.15	*Temperature (degree C)*	25.000		

^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 2.58 (t, J=5.65 Hz, 1 H) 3.26 (q, J=6.02 Hz, 2 H) 3.36 (t, J=5.83 Hz, 2 H) 3.48 (t, J=6.21 Hz, 2 H) 6.89 (d, J=15.81 Hz, 1 H) 7.07 (s, 1 H) 7.32 (d, J=7.53 Hz, 1 H) 7.39 (t, J=7.53 Hz, 2 H) 7.43 (d, J=7.15 Hz, 1 H) 7.44 - 7.48 (m, 1 H) 7.52 (d, J=15.81 Hz, 1 H) 7.56 (d, J=7.91 Hz, 1 H) 7.63 (d, J=7.53 Hz, 1 H) 8.10 (s, 1 H)



Spectra of (1535)



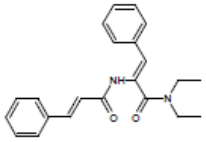
^{1}H NMR

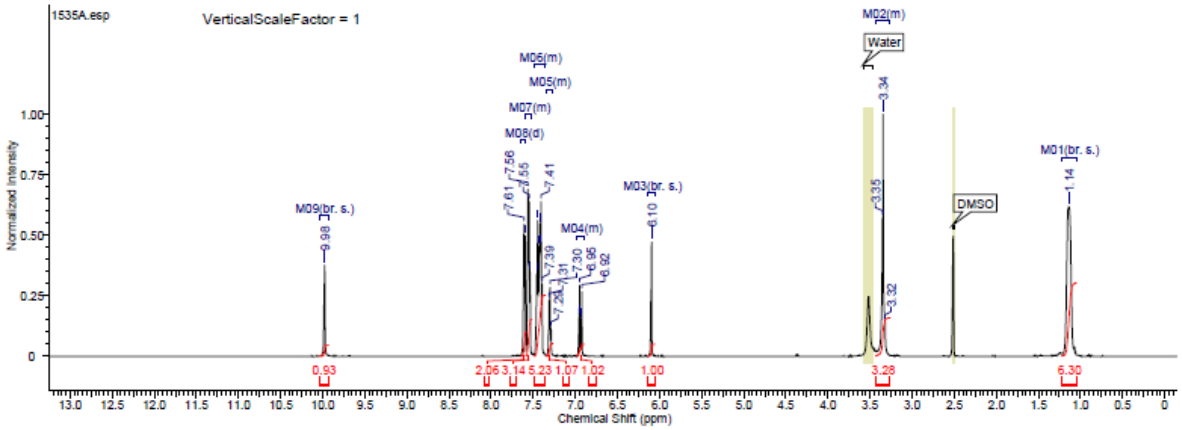
Cin-1535A

4/7/2015 05:00:33

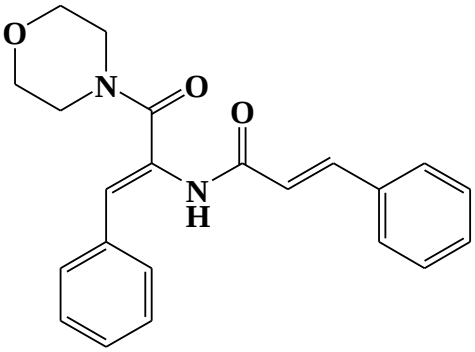
Acquisition Time (sec)	2.6564	*Comment*	Dr.A.Mansour DMSO RAKAN 1535A			*Date*	25 Feb 2015 14:20:32
Date Stamp	25 Feb 2015 14:20:32			*File Name*	E:\Google Drive\Projects\CIN-Extension\Spectra\Rakan\RAKAN 1535A\1\fid		
Frequency (MHz)	600.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	37.66	*SW(cyclical) (Hz)*	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.0493
Spectrum Type	STANDARD	*Sweep Width (Hz)*	12335.15	*Temperature (degree C)*	24.993		

^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 1.14 (br. s., 6 H) 3.26 - 3.43 (m, 3 H) 6.10 (br. s., 1 H) 6.89 - 6.98 (m, 1 H) 7.27 - 7.35 (m, 1 H) 7.36 - 7.49 (m, 5 H) 7.52 - 7.59 (m, 3 H) 7.60 (d, J=7.15 Hz, 2 H) 9.98 (br. s., 1 H)





Spectra of (1536)



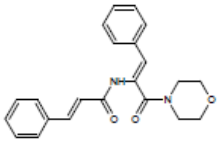
^{1}H NMR

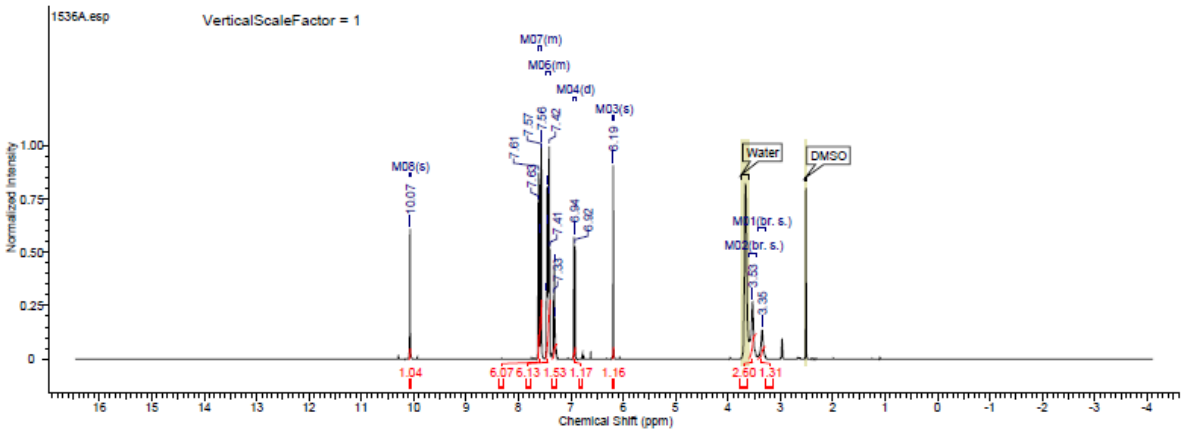
Cin-1536A

4/7/2015 05:06:29

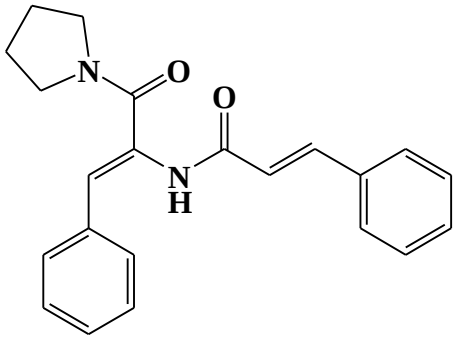
Acquisition Time (sec)	2.6564	*Comment*	Dr.A.Mansour DMSO RAKAN 1536A			*Date*	25 Feb 2015 14:22:40
Date Stamp	25 Feb 2015 14:22:40			*File Name*	E:\Google Drive\Projects\CIN-Extension\Spectra\Rakan\RAKAN 1536A\1\fid		
Frequency (MHz)	600.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	37.66	*SW(cyclical) (Hz)*	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.0500
Spectrum Type	STANDARD	*Sweep Width (Hz)*	12335.15	*Temperature (degree C)*	25.000		

^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 3.35 (br. s., 1 H) 3.53 (br. s., 3 H) 6.19 (s, 1 H) 6.93 (d, *J*=15.81 Hz, 1 H) 7.27 - 7.36 (m, 2 H) 7.40 - 7.48 (m, 6 H) 7.56 - 7.63 (m, 6 H) 10.07 (s, 1 H)





Spectra of (1555)



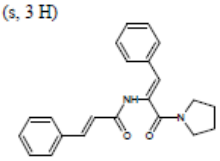
^{1}H NMR

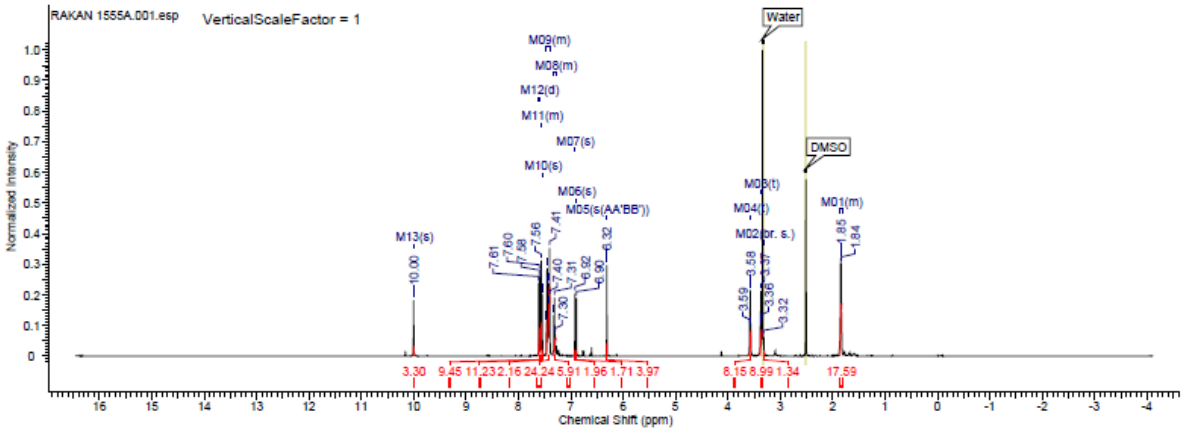
Cin-1555A

4/7/2015 05:09:42

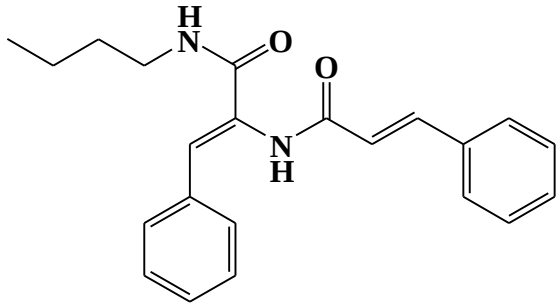
Acquisition Time (sec)	2.6564	*Comment*	Dr.A.Mansour DMSO RAKAN 1555A			*Date*	25 Feb 2015 14:58:56
Date Stamp	25 Feb 2015 14:58:56			*File Name*	E:\Google Drive\Projects\CIN-Extension\Spectra\Rakan\RAKAN 1555A\1\fid		
Frequency (MHz)	600.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	87.48	*SW(cyclical) (Hz)*	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.0500
Spectrum Type	STANDARD	*Sweep Width (Hz)*	12335.15	*Temperature (degree C)*	24.992		

^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 1.83 - 1.87 (m, 18 H) 3.32 (br. s., 1 H) 3.37 (t, *J*=6.59 Hz, 9 H) 3.58 (t, *J*=6.02 Hz, 8 H) 6.32 (s, 4 H) 6.90 (s, 2 H) 6.92 (s, 2 H) 7.28 - 7.33 (m, 6 H) 7.40 - 7.47 (m, 24 H) 7.54 (s, 2 H) 7.56 - 7.58 (m, 11 H) 7.61 (d, *J*=6.78 Hz, 9 H) 10.00 (s, 3 H)





Spectra of (1556)



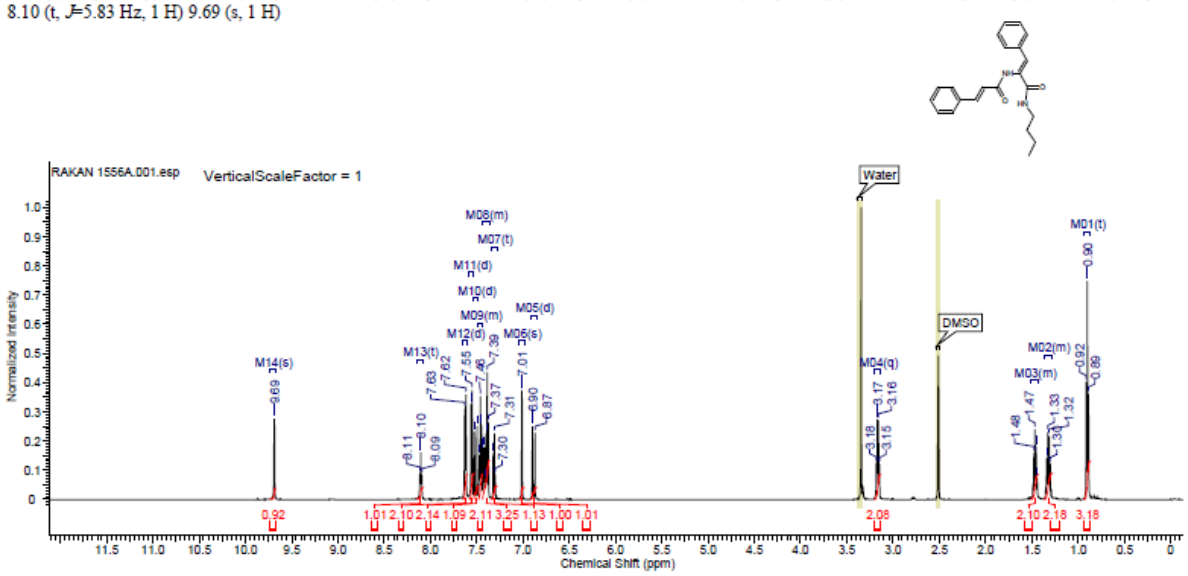
^{1}H NMR

Cin-1556A

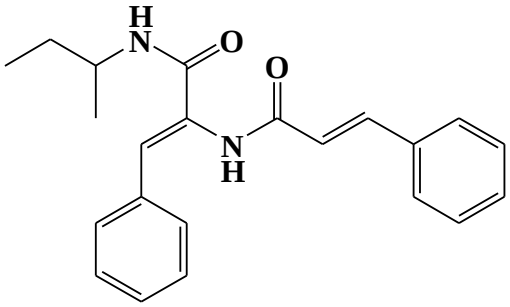
4/7/2015 05:40:40

Acquisition Time (sec)	2.6564	*Comment*	Dr.A.Mansour DMSO RAKAN 1556A			*Date*	25 Feb 2015 14:33:20
Date Stamp	25 Feb 2015 14:33:20			*File Name*	E:\Google Drive\Projects\CIN-Extension\Spectra\Rakan\RAKAN 1556A\1\fid		
Frequency (MHz)	600.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	43.27	*SW(cyclical) (Hz)*	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.0500
Spectrum Type	STANDARD	*Sweep Width (Hz)*	12335.15	*Temperature (degree C)*	24.996		

^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 0.90 (t, *J*=7.34 Hz, 3 H) 1.28 - 1.37 (m, 2 H) 1.43 - 1.51 (m, 2 H) 3.17 (q, *J*=6.78 Hz, 2 H) 6.88 (d, *J*=16.19 Hz, 1 H) 7.01 (s, 1 H) 7.31 (t, *J*=7.34 Hz, 1 H) 7.36 - 7.44 (m, 3 H) 7.44 - 7.48 (m, 2 H) 7.51 (d, *J*=15.81 Hz, 1 H) 7.56 (d, *J*=7.53 Hz, 2 H) 7.62 (d, *J*=7.15 Hz, 2 H) 8.10 (t, *J*=5.83 Hz, 1 H) 9.69 (s, 1 H)



Spectra of (1557)



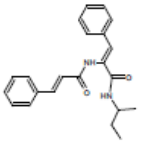
^{1}H NMR

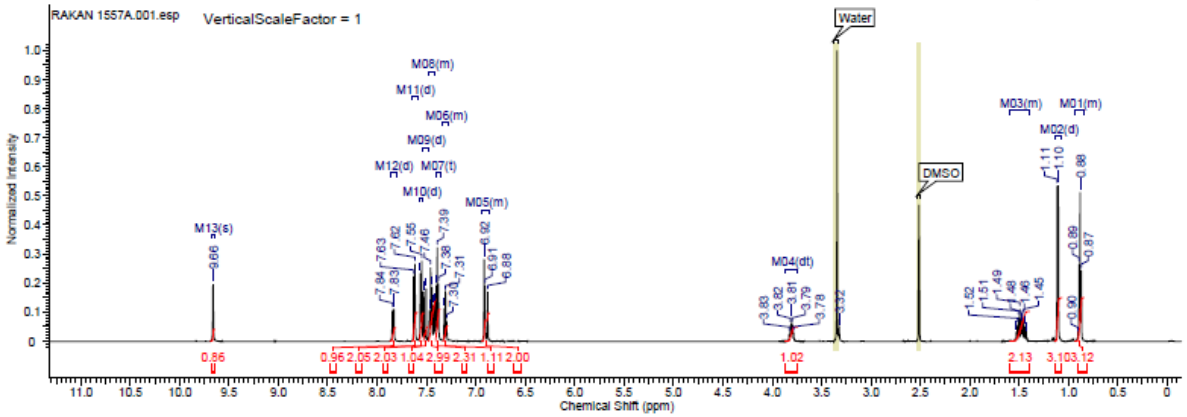
Cin-1557A

4/7/2015 05:47:10

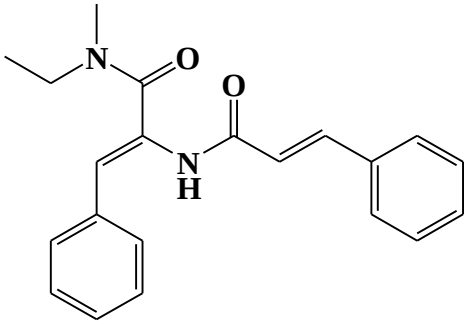
Acquisition Time (sec)	2.6564	*Comment*	Dr.A.Mansour DMSO RAKAN 1557A			*Date*	25 Feb 2015 15:03:12
Date Stamp	25 Feb 2015 15:03:12			*File Name*	E:\Google Drive\Projects\CIN-Extension\Spectra\Rakan\RAKAN 1557A\1\fid		
Frequency (MHz)	600.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	83.44	*SW(cyclical) (Hz)*	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.0500
Spectrum Type	STANDARD	*Sweep Width (Hz)*	12335.15	*Temperature (degree C)*	24.996		

^{1}H NMR (600 MHz, DMSO-d_6) δ ppm 0.84 - 0.93 (m, 3 H) 1.11 (d, *J*=6.78 Hz, 3 H) 1.39 - 1.59 (m, 2 H) 3.81 (dt, *J*=13.93, 7.34 Hz, 1 H) 6.86 - 6.94 (m, 2 H) 7.28 - 7.34 (m, 1 H) 7.39 (t, *J*=7.72 Hz, 2 H) 7.41 - 7.49 (m, 3 H) 7.52 (d, *J*=15.81 Hz, 1 H) 7.56 (d, *J*=7.91 Hz, 2 H) 7.62 (d, *J*=7.15 Hz, 2 H) 7.84 (d, *J*=8.66 Hz, 1 H) 9.66 (s, 1 H)





Spectra of (1559)



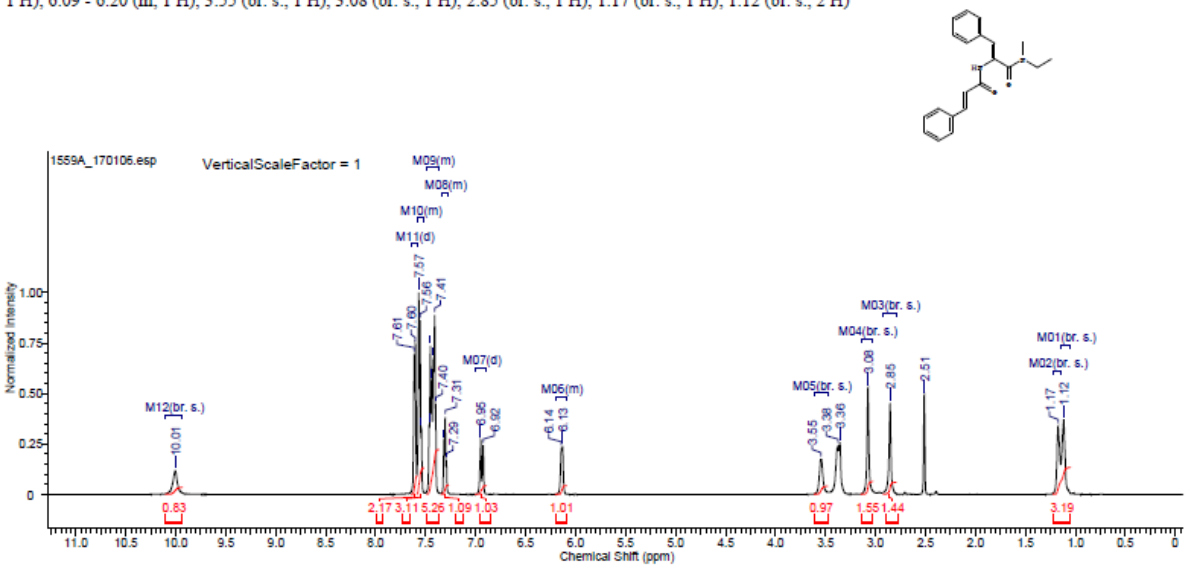
^{1}H NMR

CIN-1559A-4m

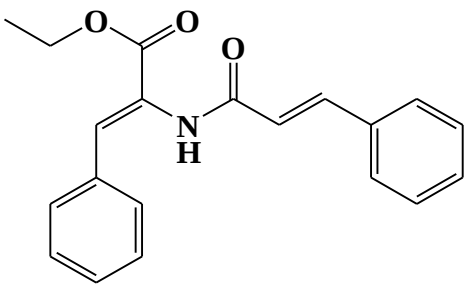
1/6/2017 05:26:08 PM

Acquisition Time (sec)	2.6564	Comment	Dr.A.Mansour DMSO RAKAN 1559A	Date	25 Feb 2015 14:50:24
Date Stamp	25 Feb 2015 14:50:24				
File Name	E:\Google Drive\Projects\CIN\Safo-Cinnamamide\Spectra Bis-Cinnamamide\1H NMR\SecondBatch-Table4I-4f\ConfirmedCpdsNMR\RAKAN 1559A\1\fid				
Frequency (MHz)	600.13	Nucleus	1H	Number of Transients	16	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	30.24	SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.0500
Spectrum Type	STANDARD	Sweep Width (Hz)	12335.15	Temperature (degree C)	24.997		

^{1}H NMR (DMSO-d_6) δ ppm 10.01 (br. s., 1 H), 7.61 (d, *J*=7.15 Hz, 2 H), 7.52 - 7.59 (m, 3 H), 7.37 - 7.49 (m, 5 H), 7.27 - 7.34 (m, 1 H), 6.94 (d, *J*=15.81 Hz, 1 H), 6.09 - 6.20 (m, 1 H), 3.55 (br. s., 1 H), 3.08 (br. s., 1 H), 2.85 (br. s., 1 H), 1.17 (br. s., 1 H), 1.12 (br. s., 2 H)



Spectra of (15EE)[5]



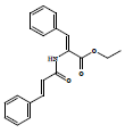
^{1}H NMR

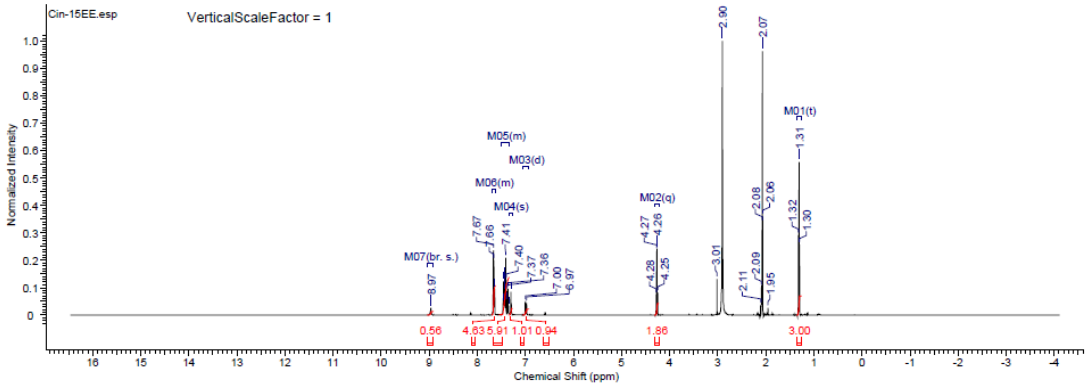
CIN-15EE, 5

12/17/2016 07:09:34 PM

Acquisition Time (sec)	2.6564	*Comment*	Dr.A.Mansour Acetone Cin-1522B 27-3-2012			*Date*	27 Mar 2013 13:46:24
Date Stamp	27 Mar 2013 13:46:24						
File Name	E:\AAA_Research\AAA_Ongoing\CINN\Spectra\NMR\CIN15Series_NMR_20130707\CIN15series_1513to31_20130707\Cin-1522B\1\fid						
Frequency (MHz)	600.13	*Nucleus*	1H	*Number of Transients*	16	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zg30
Receiver Gain	106.17	*SW(cyclical) (Hz)*	12335.53	*Solvent*	Acetone	*Spectrum Offset (Hz)*	3706.0493
Spectrum Type	STANDARD	*Sweep Width (Hz)*	12335.15	*Temperature (degree C)*	25.009		

^{1}H NMR (Acetone) δ ppm 8.97 (br. s., 1 H), 7.62 - 7.69 (m, 5 H), 7.34 - 7.50 (m, 6 H), 7.30 (s, 1 H), 6.99 (d, *J*=15.81 Hz, 1 H), 4.27 (q, *J*=7.03 Hz, 2 H), 1.31 (t, *J*=7.15 Hz, 3 H)



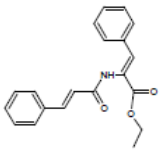


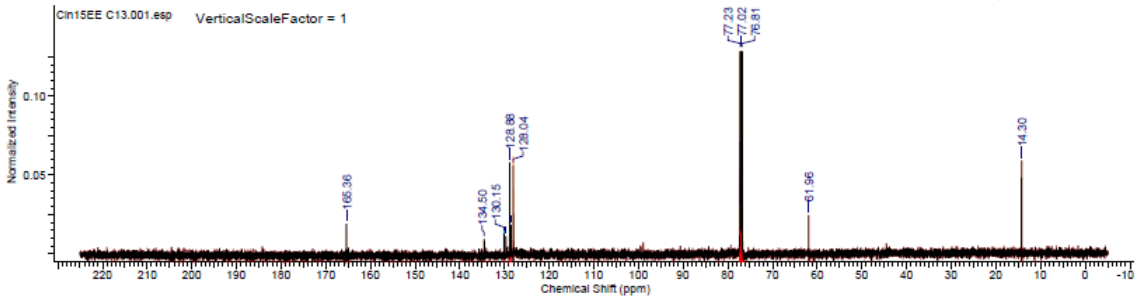
^{13}C NMR

CIN-15EE

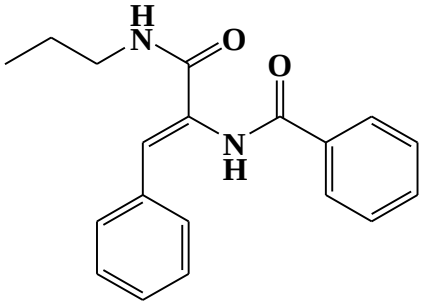
11/20/2014 01:27:01

Acquisition Time (sec)	0.4719	*Comment*	Dr.Mansour CDCl3 CIn15EE C13			*Date*	14 Nov 2014 07:24:32
Date Stamp	14 Nov 2014 07:24:32			*File Name*	E:\AAA_Research\Spectra Reservoir\CIN_13C_20-11-14\CIn15EE C13\1\fid		
Frequency (MHz)	150.92	*Nucleus*	13C	*Number of Transients*	4096	*Origin*	spect
Original Points Count	16384	*Owner*	nmr	*Points Count*	16384	*Pulse Sequence*	zgpg30
Receiver Gain	173.48	*SW(cyclical) (Hz)*	34722.22	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	16599.3105	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	34720.10	*Temperature (degree C)*	25.001

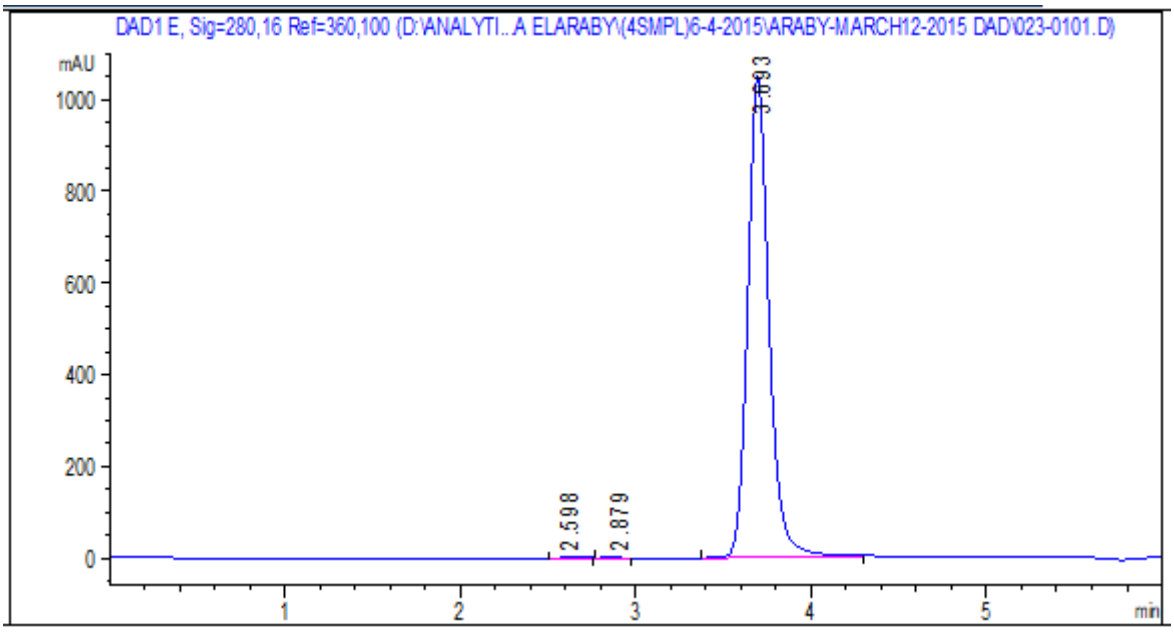


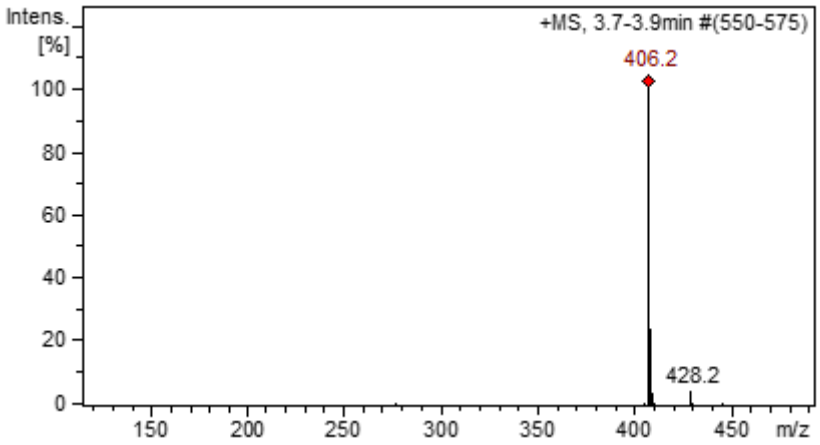


Spectra of (1612)



LC/MS





^{1}H NMR

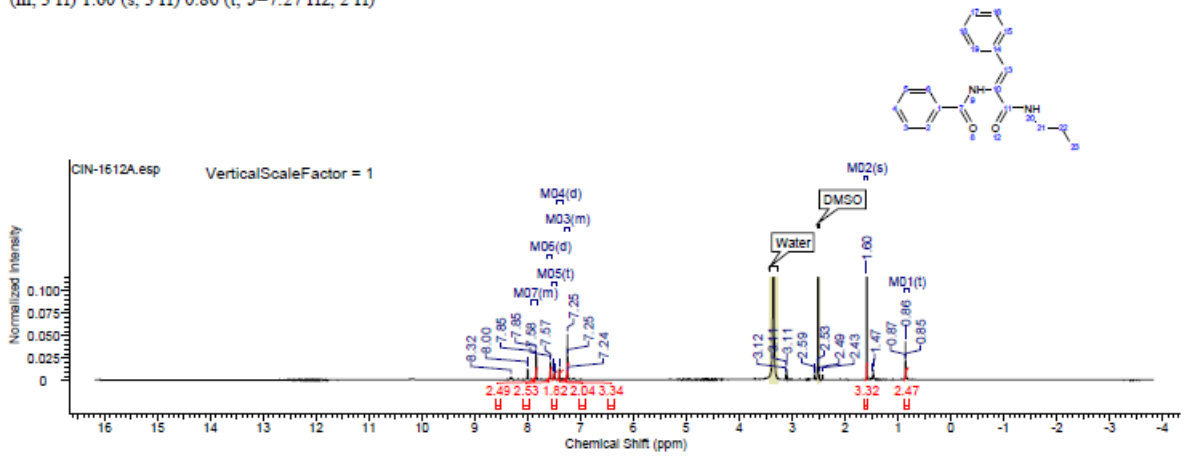
1612

2018-10-06 5:34:48 PM

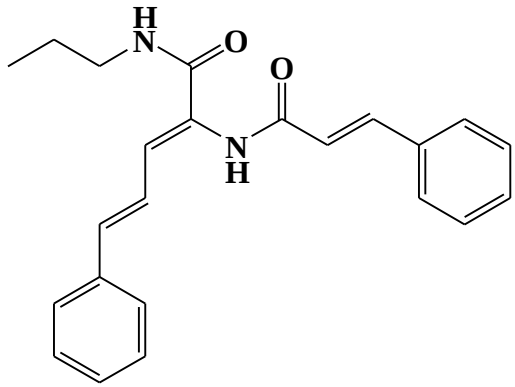
Formula $C_{18}H_{20}N_2O_2$	FW	308.3743

Acquisition Time (sec)	1.9268	Comment	Dr.Mustafa El-Araby Sample : CIN-1612 DMSO			Date	06 Apr 2015 10:15:12
Date Stamp	06 Apr 2015 10:15:12						
File Name	E:\AAA Research\Spectra Reservoir\April2015\Cln 1612 1712 1532\MUSTAFA CIN-1612 08-04-2015\20\fid					Frequency (MHz)	850.15
Nucleus	1H	Number of Transients	20	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	10.55
SW(cyclical) (Hz)	17006.80	Solvent	DMSO-d6	Spectrum Offset (Hz)	5250.0283	Spectrum Type	STANDARD
Sweep Width (Hz)	17006.28	Temperature (degree C)	25.001				

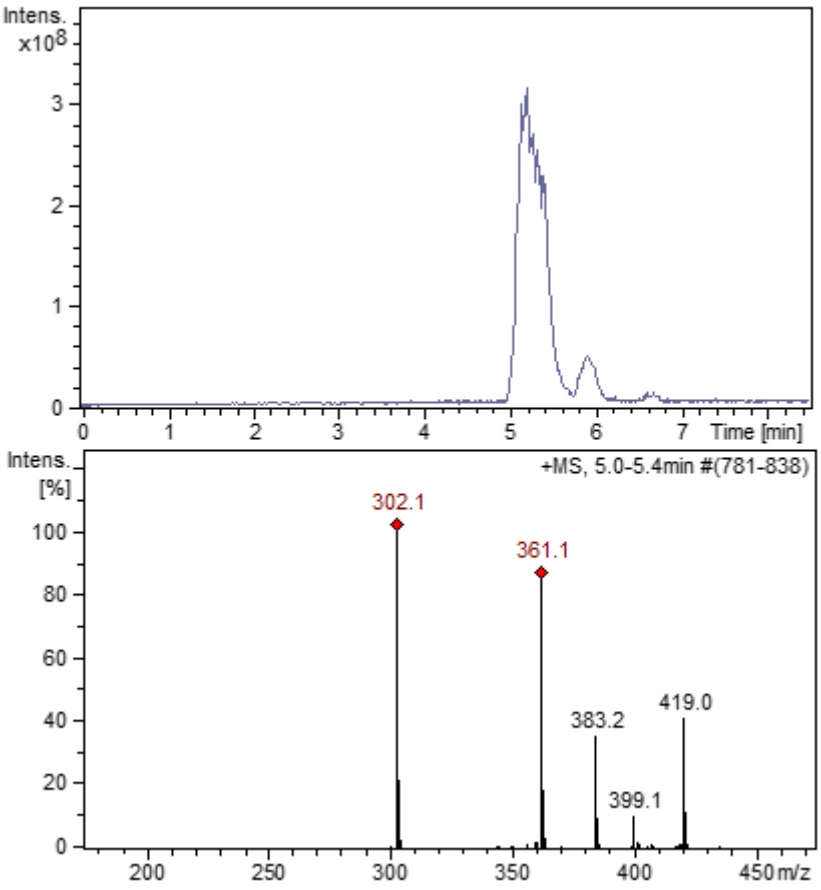
^{1}H NMR (850 MHz, DMSO-d_6) δ ppm 7.82 - 7.92 (m, 2 H) 7.57 (d, *J*=8.30 Hz, 3 H) 7.50 (t, *J*=7.53 Hz, 2 H) 7.40 (d, *J*=8.30 Hz, 2 H) 7.22 - 7.32 (m, 3 H) 1.60 (s, 3 H) 0.86 (t, *J*=7.27 Hz, 2 H)



Spectra of (1712)



LC/MS



^{1}H NMR

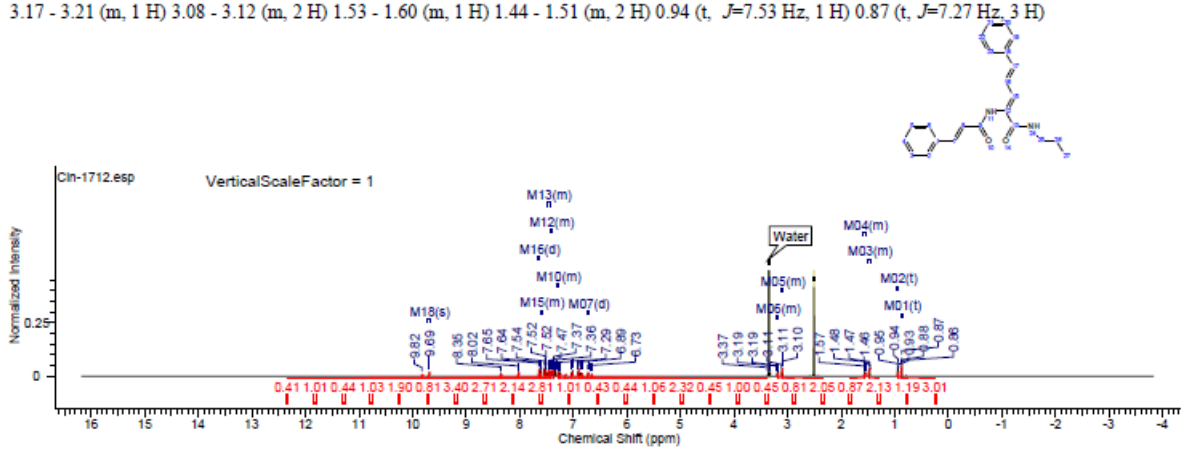
1712

2018-10-06 5:35:14 PM

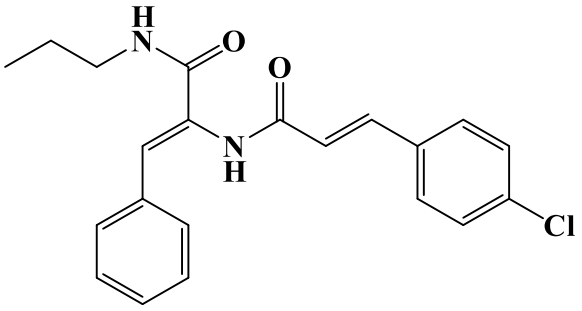
Formula $C_{22}H_{24}N_4O_2$	FW	360.4489

Acquisition Time (sec)	1.9268	Comment	Dr.Mustafa El-Araby Sample : CUR-1712 DMSO			Date	08 Apr 2015 10:19:28
Date Stamp	08 Apr 2015 10:19:28						
File Name	E:\AAA Research\Spectra Reservoir\April2015\Cln 1612 1712 1532\MUSTAFA CUR-1712 08-04-2015\30\fid					Frequency (MHz)	850.15
Nucleus	1H	Number of Transients	20	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	9.04
SW(cyclical) (Hz)	17006.80	Solvent	DMSO-d6	Spectrum Offset (Hz)	5250.0283	Spectrum Type	STANDARD
Sweep Width (Hz)	17006.28	Temperature (degree C)	24.999				

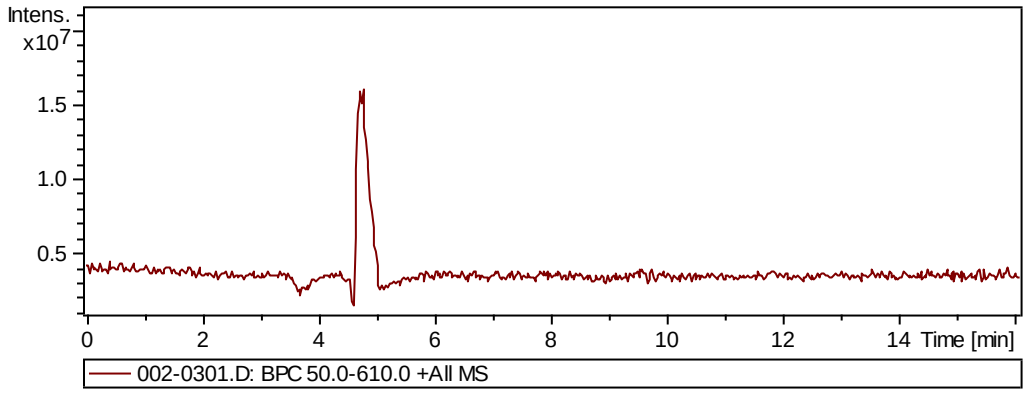
^{1}H NMR (850 MHz, DMSO-d_6) δ ppm 9.69 (s, 1 H) 8.02 (t, *J*=5.71 Hz, 1 H) 7.64 (d, *J*=7.27 Hz, 2 H) 7.59 - 7.62 (m, 1 H) 7.50 - 7.55 (m, 3 H) 7.44 - 7.48 (m, 3 H) 7.40 - 7.44 (m, 2 H) 7.34 - 7.39 (m, 3 H) 7.28 - 7.31 (m, 1 H) 7.00 - 7.05 (m, 1 H) 6.87 - 6.92 (m, 2 H) 6.73 (d, *J*=10.90 Hz, 1 H) 3.17 - 3.21 (m, 1 H) 3.08 - 3.12 (m, 2 H) 1.53 - 1.60 (m, 1 H) 1.44 - 1.51 (m, 2 H) 0.94 (t, *J*=7.53 Hz, 1 H) 0.87 (t, *J*=7.27 Hz, 3 H)

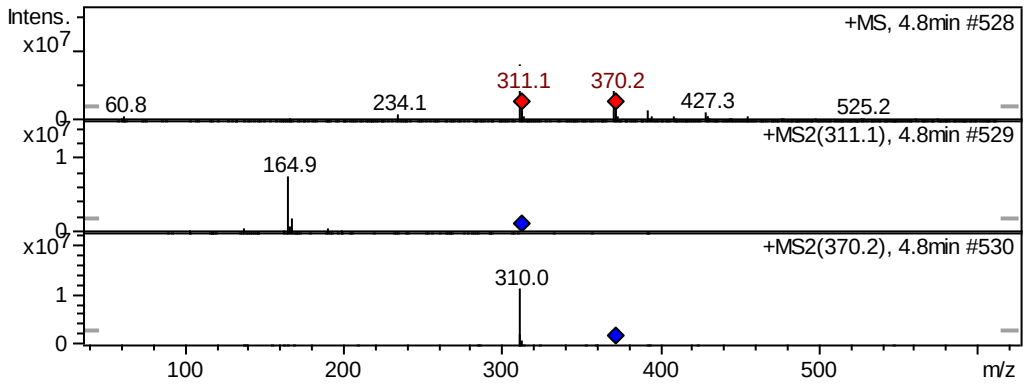


Spectra of (1812)

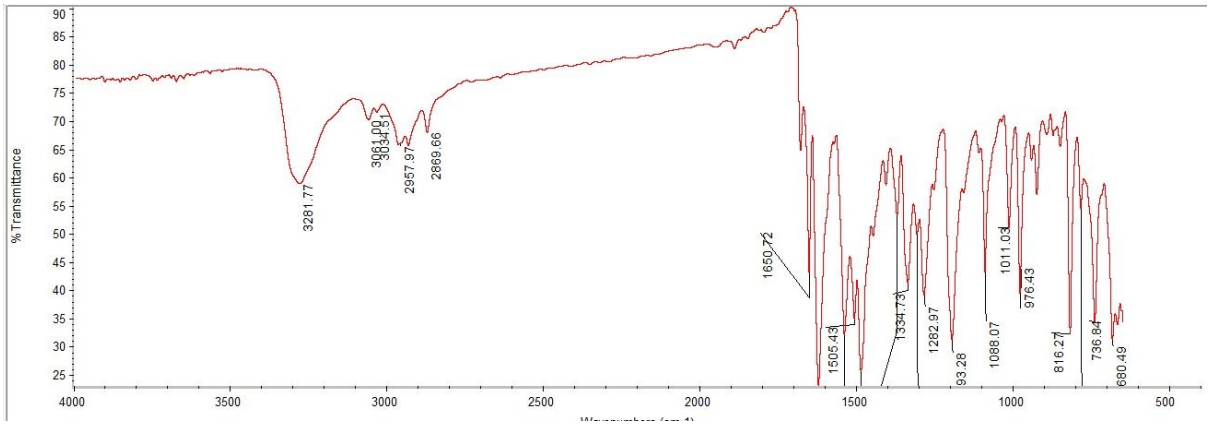


LC/MS





FT-IR



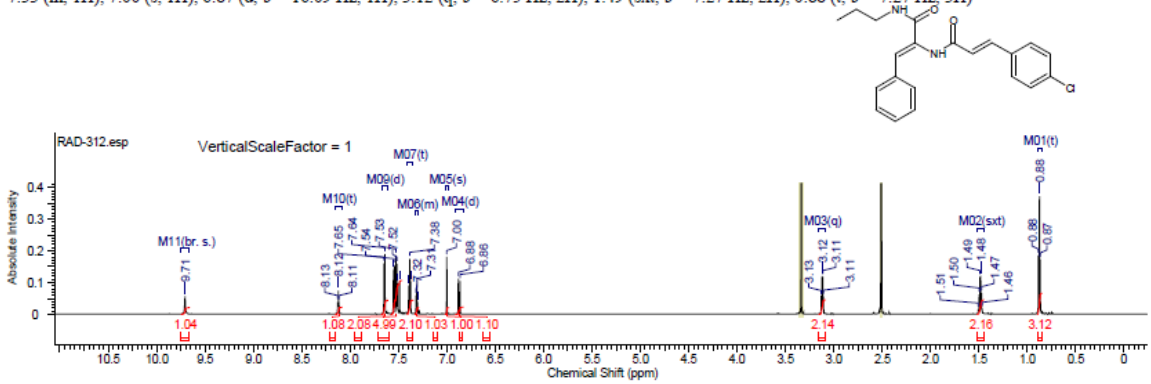
^{1}H NMR

RAD-312

05/11/2016 9:57:37 AM
Dr.Mustafa El-Araby Sample : RAD-312 DMSO

Formula $C_{21}H_{21}ClN_2O_2$		FW	368.8566				
Acquisition Time (sec)	1.9268	Comment	Dr.Mustafa El-Araby Sample : RAD-312 DMSO			Date	08 Apr 2015 11:25:36
Date Stamp	08 Apr 2015 11:25:36						
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-312 08-04-2015\180\fid					Frequency (MHz)	850.15
Nucleus	1H	Number of Transients	20	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	10.55
SW(cyclical) (Hz)	17006.80	Solvent	DMSO-d6	Spectrum Offset (Hz)	5250.0283	Spectrum Type	STANDARD
Sweep Width (Hz)	17006.28	Temperature (degree C)	25.001				

^{1}H NMR (850 MHz, DMSO-d_6) δ 9.71 (br. s., 1H), 8.12 (t, J = 5.71 Hz, 1H), 7.64 (d, J = 8.30 Hz, 2H), 7.46 - 7.58 (m, 4H), 7.38 (t, J = 7.79 Hz, 2H), 7.29 - 7.33 (m, 1H), 7.00 (s, 1H), 6.87 (d, J = 16.09 Hz, 1H), 3.12 (q, J = 6.75 Hz, 2H), 1.49 (sxt, J = 7.27 Hz, 2H), 0.88 (t, J = 7.27 Hz, 3H)



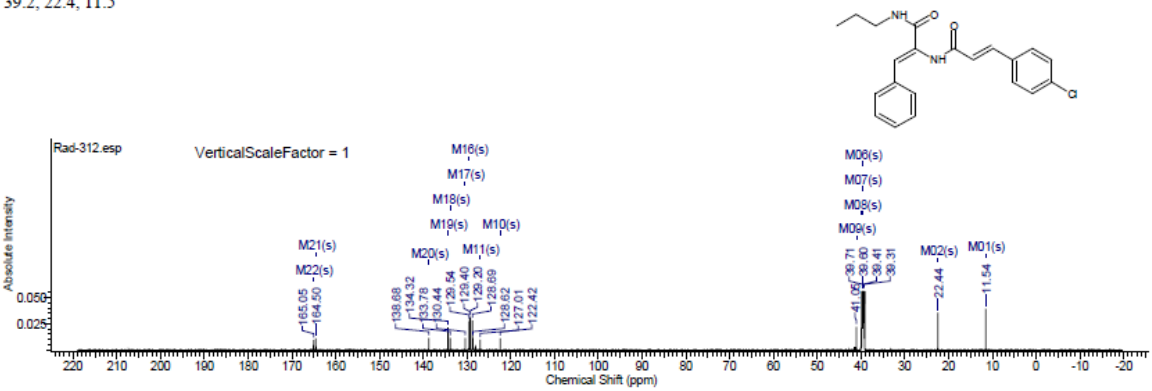
^{13}C NMR

RAD-312

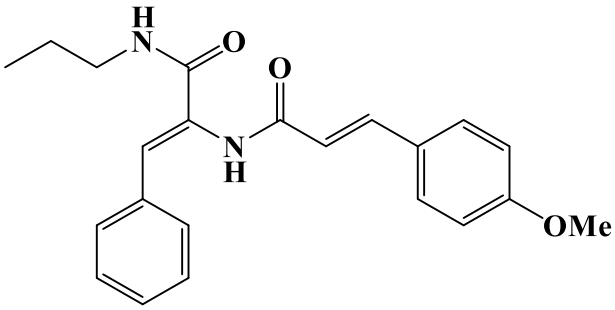
20/09/2016 8:33:47 AM
Dr.Mostafa Sample ; RAD-312 DMSO

Formula $C_{21}H_{21}ClN_2O_2$		FW	368.8566				
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-312 DMSO			Date	20 Apr 2016 09:04:48
Date Stamp	20 Apr 2016 09:04:48						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-312 19-04-2016\80\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	2396	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21301.5977
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

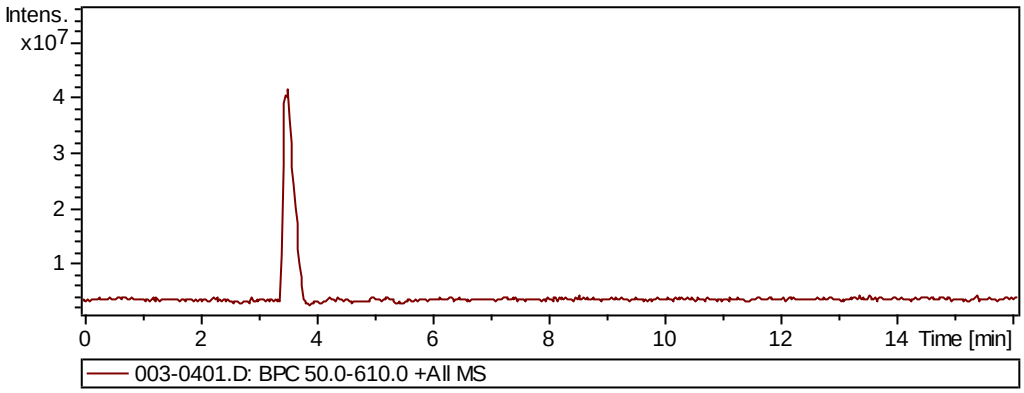
^{13}C NMR (214 MHz, DMSO-d_6) δ 165.1, 164.5, 138.7, 134.3, 133.8, 130.4, 129.5, 129.4, 129.2, 128.7, 128.6, 127.0, 122.4, 41.1, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 11.5

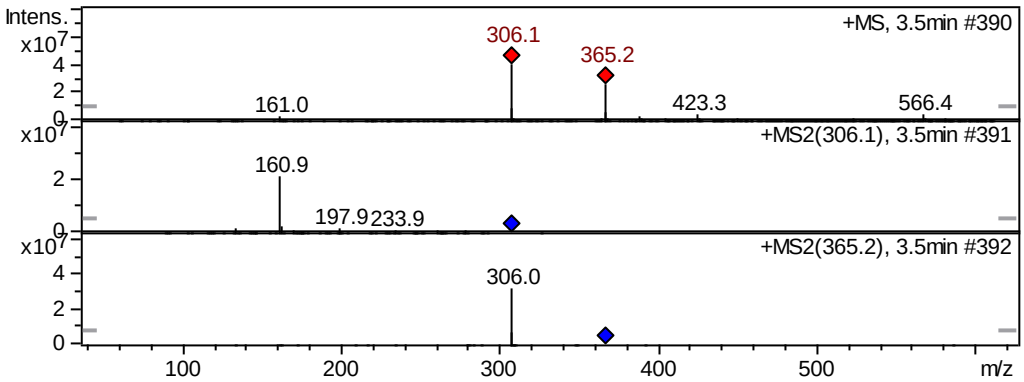


Spectra of (1912)

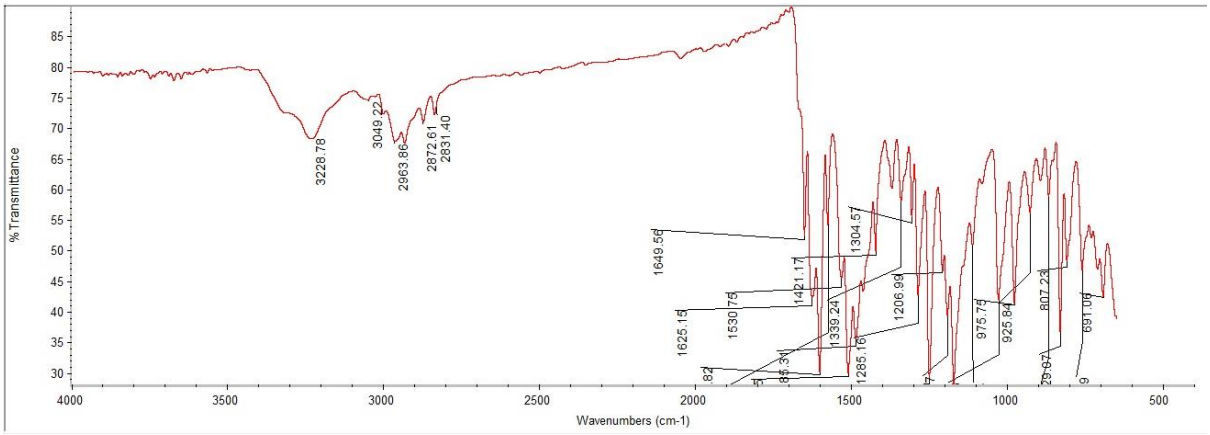


LC/MS





FT-IR



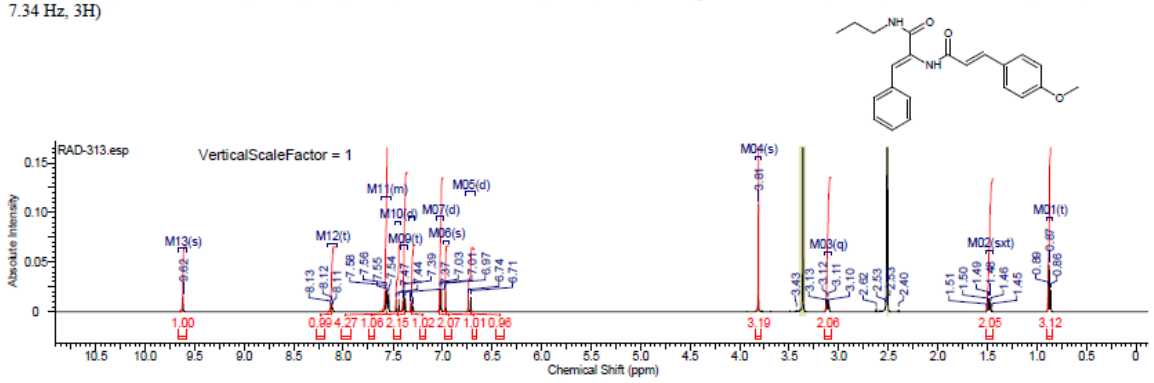
^{1}H NMR

RAD-313

05/11/2016 10:04:00 AM
Dr.Mustafa Sample : RAD-313 DMSO PROTON DMSO (D:\Magdy) nmr 32

Formula $C_{22}H_{24}N_2O_3$	FW	364.4376					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-313 DMSO PROTON DMSO (D:\Magdy) nmr 32				
Date	18 Jun 2015 16:19:44			Date Stamp	18 Jun 2015 16:19:44		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-313 18-06-2015\10\fid						
Nucleus	1H	Number of Transients	32	Origin	spect	Frequency (MHz)	600.15
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	144.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.62 (s, 1H), 8.12 (t, J = 5.65 Hz, 1H), 7.51 - 7.62 (m, 4H), 7.45 (d, J = 15.43 Hz, 1H), 7.38 (t, J = 7.72 Hz, 2H), 7.28 - 7.33 (m, 1H), 7.02 (d, J = 8.66 Hz, 2H), 6.97 (s, 1H), 6.72 (d, J = 15.81 Hz, 1H), 3.81 (s, 3H), 3.11 (q, J = 6.40 Hz, 2H), 1.48 (sxt, J = 7.30 Hz, 2H), 0.87 (t, J = 7.34 Hz, 3H)



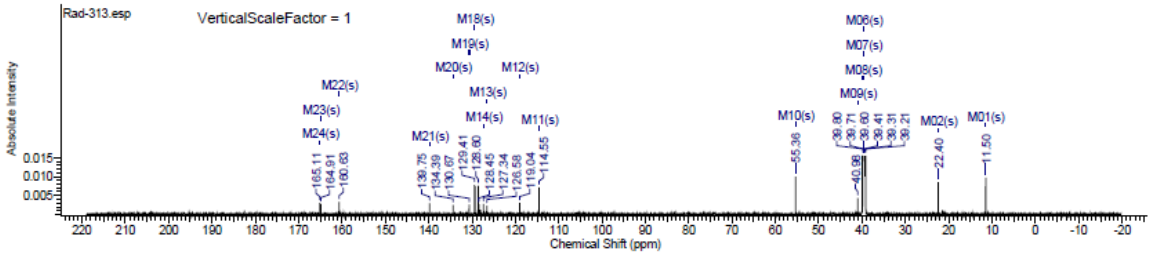
^{13}C NMR

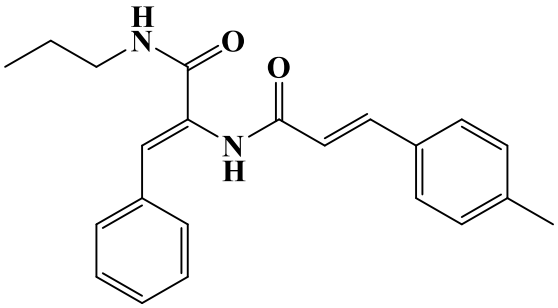
RAD-313

20/09/2016 8:34:14 AM
Dr.Mostafa Sample ; RAD-313 DMSO

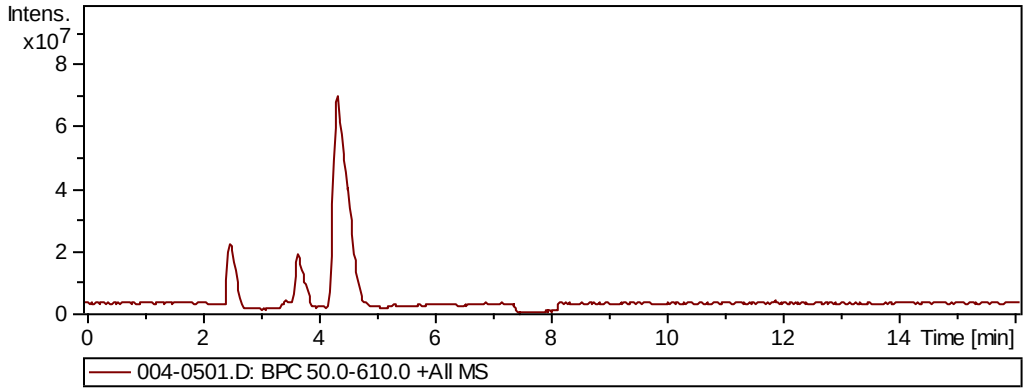
Formula $C_{22}H_{24}N_2O_3$	FW	364.4375					
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-313 DMSO			Date	19 Apr 2016 20:25:20
Date Stamp	19 Apr 2016 20:25:20						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-313 19-04-2016\30\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3500	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21289.1406
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

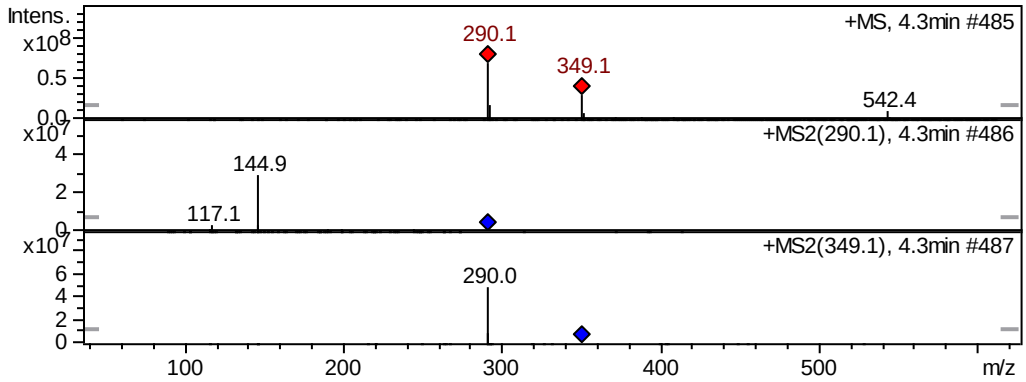
^{13}C NMR (214 MHz, DMSO-d$_6$) δ 165.1, 164.9, 160.6, 139.7, 134.4, 130.7, 129.4, 129.3, 128.6, 128.5, 127.3, 126.6, 119.0, 114.5, 55.4, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 11.5




H
N
O
O
N
H

LC/MS


Intens.
x10^7
8
6
4
2
0
0
2
4
6
8
10
12
14 Time [min]
004-0501.D: BPC 50.0-610.0 +All MS


Intens.
x10^8
0.5
0.0
290.1
349.1
542.4
+MS, 4.3min #485
x10^7
4
2
0
144.9
117.1
+MS2(290.1), 4.3min #486
x10^7
6
4
2
0
290.0
+MS2(349.1), 4.3min #487
100
200
300
400
500
m/z

^{1}H NMR

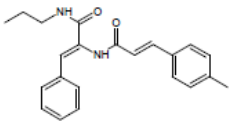
RAD-314

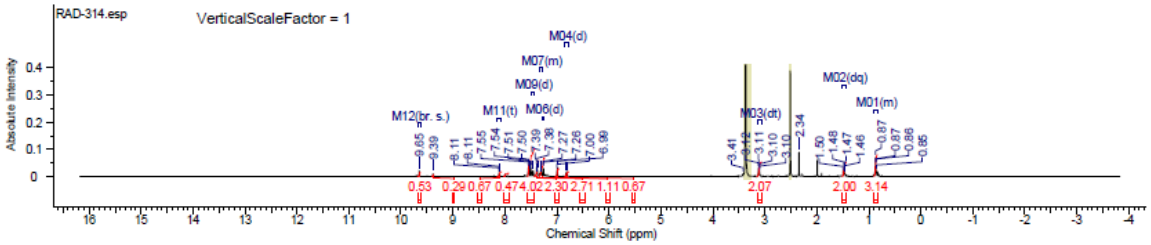
02/10/2016 6:30:24 AM
Dr.Mustafa El-Araby Sample : RAD-314 DMSO

Formula $C_{20}H_{24}N_2O_3$	FW	348.4382

Acquisition Time (sec)	1.9268	Comment	Dr.Mustafa El-Araby Sample : RAD-314 DMSO			Date	08 Apr 2015 10:23:44
Date Stamp	08 Apr 2015 10:23:44						
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-314_08-04-2015\40\fid					Frequency (MHz)	850.15
Nucleus	1H	Number of Transients	20	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	9.04
SW(cyclical) (Hz)	17006.80	Solvent	DMSO-d6	Spectrum Offset (Hz)	5250.0283	Spectrum Type	STANDARD
Sweep Width (Hz)	17006.28	Temperature (degree C)	25.000				

^{1}H NMR (850 MHz, DMSO-d$_6$) δ 9.65 (br. s., 1H), 8.11 (t, *J* = 5.45 Hz, 1H), 7.49 - 7.57 (m, 3H), 7.46 (d, *J* = 15.57 Hz, 1H), 7.34 - 7.43 (m, 3H), 7.28 - 7.34 (m, 2H), 7.26 (d, *J* = 7.78 Hz, 1H), 6.95 - 7.03 (m, 1H), 6.82 (d, *J* = 15.57 Hz, 1H), 3.11 (td, *J* = 6.68, 13.10 Hz, 2H), 1.48 (qd, *J* = 7.07, 14.08 Hz, 2H), 0.84 - 0.90 (m, 3H)





^{13}C NMR

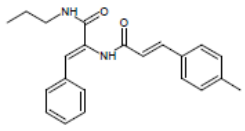
RAD-314

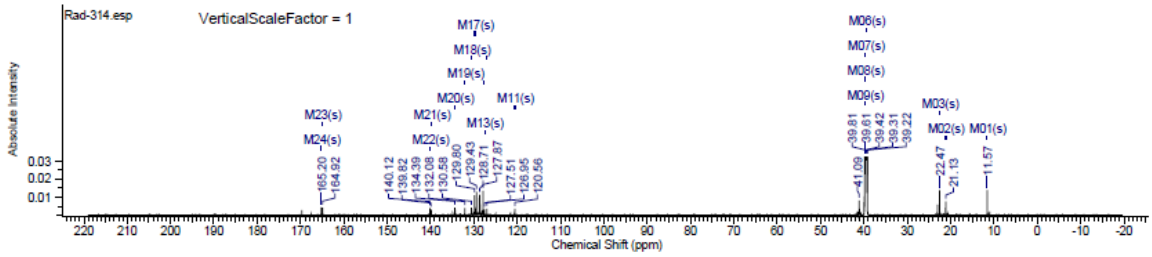
20/09/2016 8:34:47 AM
Dr.Mostafa Sample ; RAD-314 DMSO

Formula $C_{20}H_{24}N_2O_3$	FW	348.4382

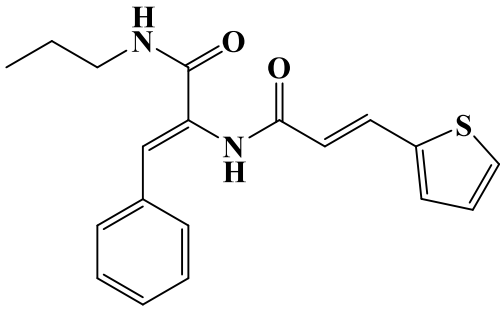
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-314 DMSO			Date	19 Apr 2016 23:07:28
Date Stamp	19 Apr 2016 23:07:28						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-314_19-04-2016\40\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3500	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21309.3809
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.006		

^{13}C NMR (214 MHz, DMSO-d$_6$) δ 165.2, 164.9, 140.1, 139.8, 134.4, 132.1, 130.6, 129.8, 129.4, 128.7, 127.9, 127.5, 126.9, 120.6, 41.1, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.5, 21.1, 11.6

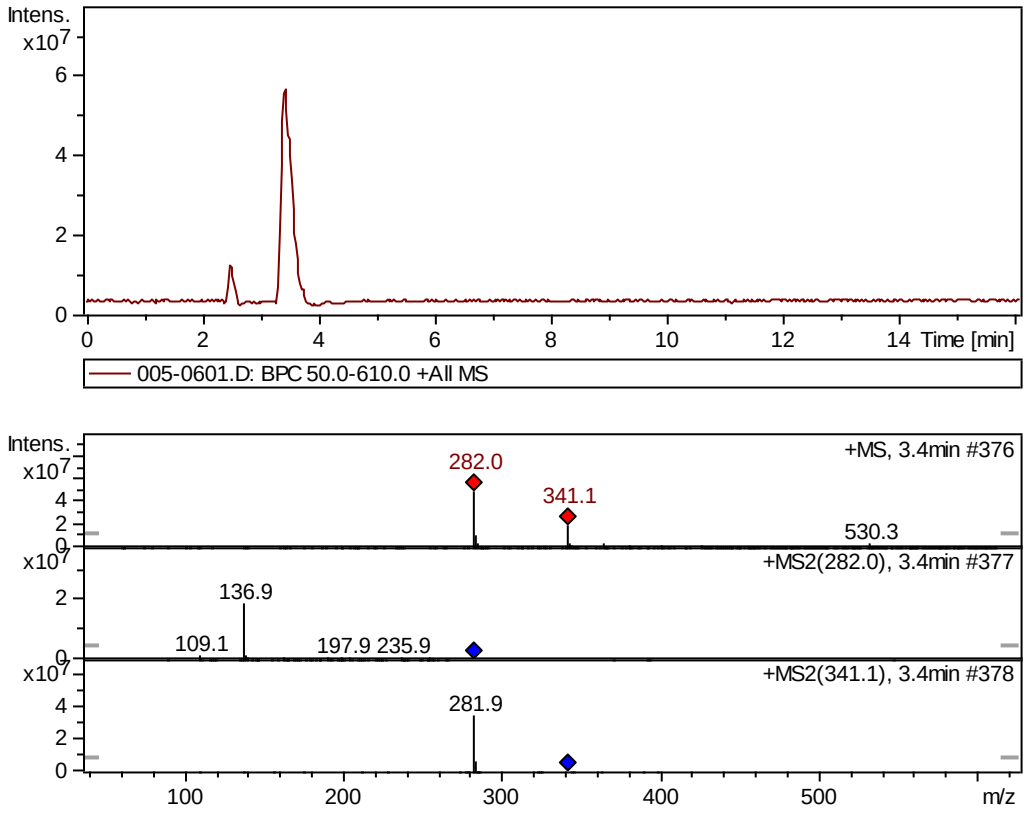




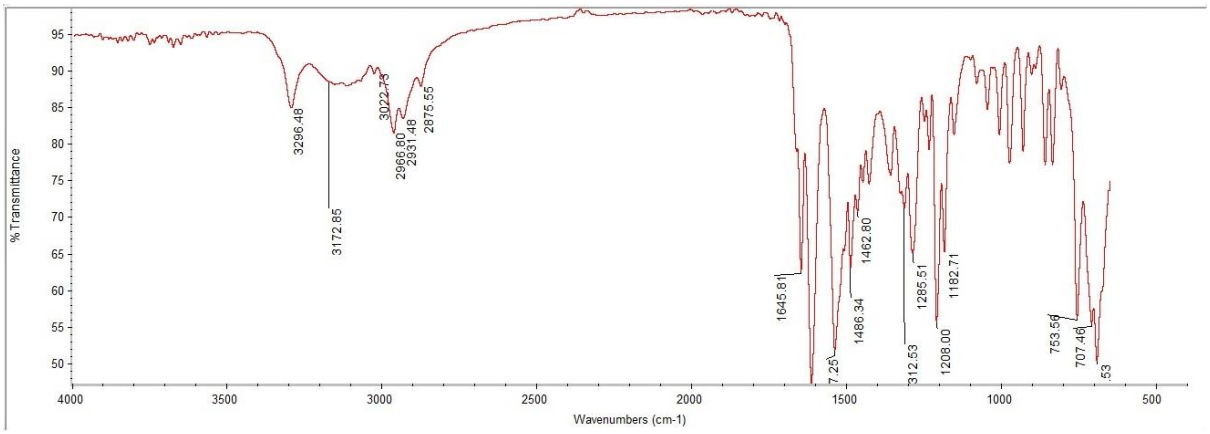
Spectra of (2112)



LC/MS



FT-IR



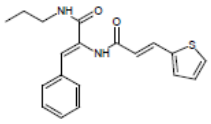
^{1}H NMR

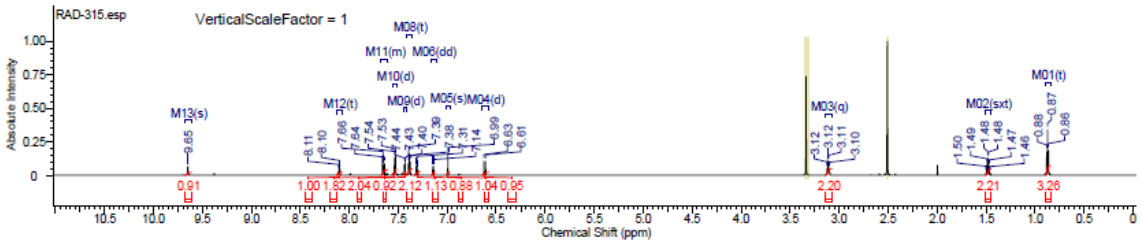
RAD-315

08/11/2016 7:51:58 AM
Dr.Mustafa El-Araby Sample : RAD-315 DMSO

Formula $C_{10}H_{20}N_2O_3S$	FW	340.4393					
Acquisition Time (sec)	1.9268	Comment	Dr.Mustafa El-Araby Sample : RAD-315 DMSO			Date	08 Apr 2015 10:53:36
Date Stamp	08 Apr 2015 10:53:36						
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-315 08-04-2015\110\fid					Frequency (MHz)	850.15
Nucleus	1H	Number of Transients	20	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	10.55
SW(cyclical) (Hz)	17006.80	Solvent	DMSO-d6	Spectrum Offset (Hz)	5250.0283	Spectrum Type	STANDARD
Sweep Width (Hz)	17006.28	Temperature (degree C)	25.001				

^{1}H NMR (850 MHz, DMSO-d_6) δ 9.65 (s, 1H), 8.10 (t, J = 5.71 Hz, 1H), 7.61 - 7.68 (m, 2H), 7.53 (d, J = 7.79 Hz, 2H), 7.43 (d, J = 3.11 Hz, 1H), 7.39 (t, J = 7.79 Hz, 2H), 7.28 - 7.33 (m, 1H), 7.14 (dd, J = 3.37, 4.93 Hz, 1H), 6.99 (s, 1H), 6.62 (d, J = 15.57 Hz, 1H), 3.11 (q, J = 6.75 Hz, 2H), 1.48 (sxt, J = 7.27 Hz, 2H), 0.87 (t, J = 7.53 Hz, 3H)





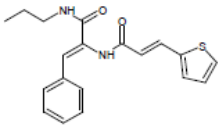
^{13}C NMR

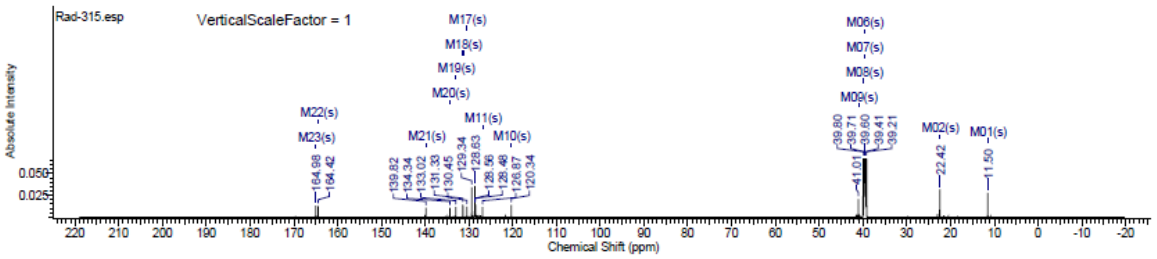
RAD-315

20/09/2016 8:35:12 AM
Dr.Mostafa Sample ; RAD-315 DMSO

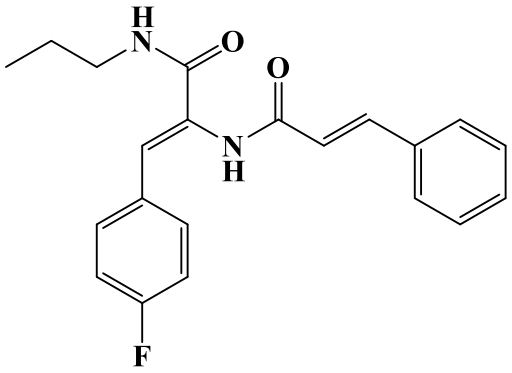
Formula $C_{10}H_{20}N_2O_3S$	FW	340.4393					
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-315 DMSO			Date	20 Apr 2016 01:49:36
Date Stamp	20 Apr 2016 01:49:36						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-315 19-04-2016\50\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3500	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21293.8125
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

^{13}C NMR (214 MHz, DMSO-d_6) δ 165.0, 164.4, 139.8, 134.3, 133.0, 131.3, 130.5, 129.3, 128.6, 128.6, 128.5, 128.5, 126.9, 120.3, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 11.5

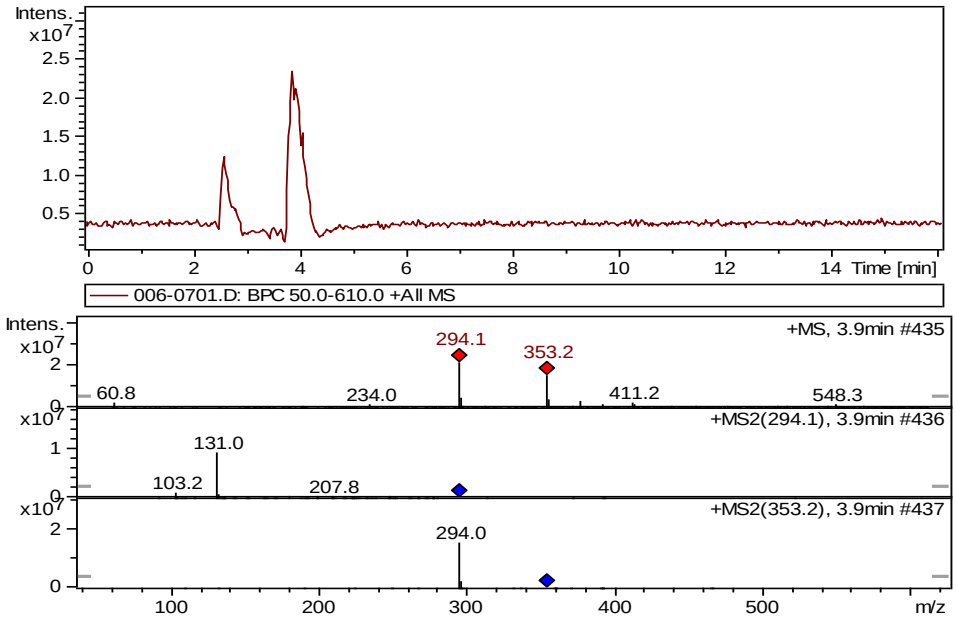




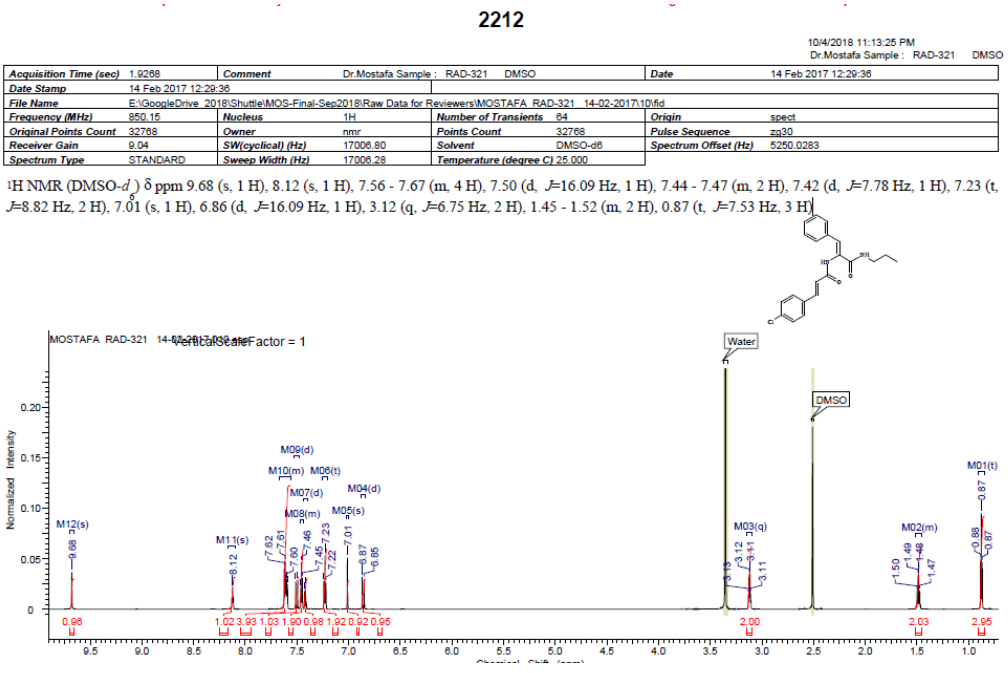
Spectra of (2212)



LC/MS


Intens.
x10^7
2.5
2.0
1.5
1.0
0.5
0
2
4
6
8
10
12
14 Time [min]
006-0701.D: BPC 50.0-610.0 +All MS
+MS, 3.9min #435
294.1
353.2
60.8
234.0
411.2
548.3
+MS2(294.1), 3.9min #436
131.0
103.2
207.8
+MS2(353.2), 3.9min #437
294.0
100
200
300
400
500
m/z

^{1}H NMR


2212
10/4/2018 11:13:25 PM
Dr.Mostafa Sample : RAD-321 DMSO
Acquisition Time (sec) 1.9268
Comment Dr.Mostafa Sample : RAD-321 DMSO
Date 14 Feb 2017 12:29:36
Date Stamp 14 Feb 2017 12:29:36
File Name E:\GoogleDrive_2018\Shuttle\MOS-Final-Sep2018\Raw Data for Reviewers\MOSTAFA_RAD-321_14-02-2017\10\fid
Frequency (MHz) 850.15
Nucleus 1H
Number of Transients 64
Origin spect
Original Points Count 32768
Owner nmr
Points Count 32768
Pulse Sequence zg30
Receiver Gain 9.04
SW(cyclical) (Hz) 17006.80
Solvent DMSO-d6
Spectrum Offset (Hz) 5250.0283
Spectrum Type STANDARD
Sweep Width (Hz) 17006.28
Temperature (degree C) 25.000
¹H NMR (DMSO-d6) δ ppm 9.68 (s, 1 H), 8.12 (s, 1 H), 7.56 - 7.67 (m, 4 H), 7.50 (d, J=16.09 Hz, 1 H), 7.44 - 7.47 (m, 2 H), 7.42 (d, J=7.78 Hz, 1 H), 7.23 (t, J=8.82 Hz, 2 H), 7.01 (s, 1 H), 6.86 (d, J=16.09 Hz, 1 H), 3.12 (q, J=6.75 Hz, 2 H), 1.45 - 1.52 (m, 2 H), 0.87 (t, J=7.53 Hz, 3 H)
MOSTAFA RAD-321
VerticalScaleFactor = 1
Water
DMSO
M01(t)
M02(m)
M03(q)
M04(d)
M05(s)
M06(t)
M07(d)
M08(m)
M09(d)
M10(m)
M11(s)
M12(s)
Normalized Intensity
0.20
0.15
0.10
0.05
0
0.96
1.02
3.93
1.03
1.90
0.98
1.92
0.92
0.95
2.00
2.03
2.95
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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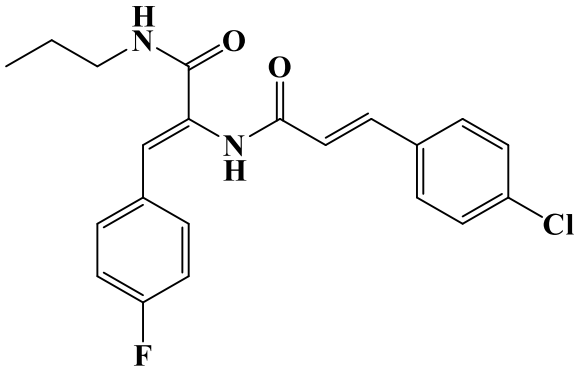
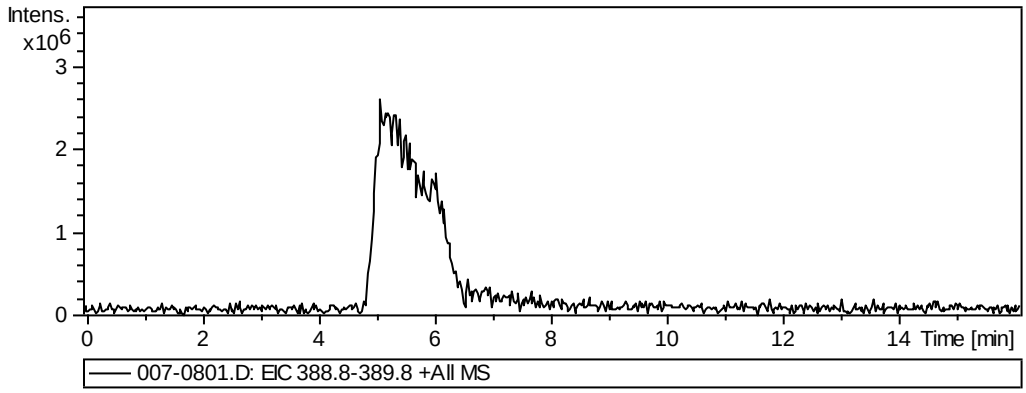
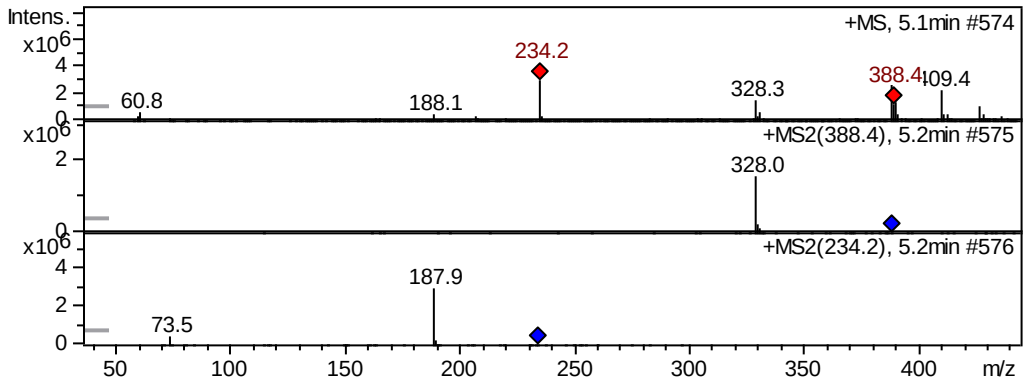
2.5
2.0
1.5
1.0

Spectra of (2312)

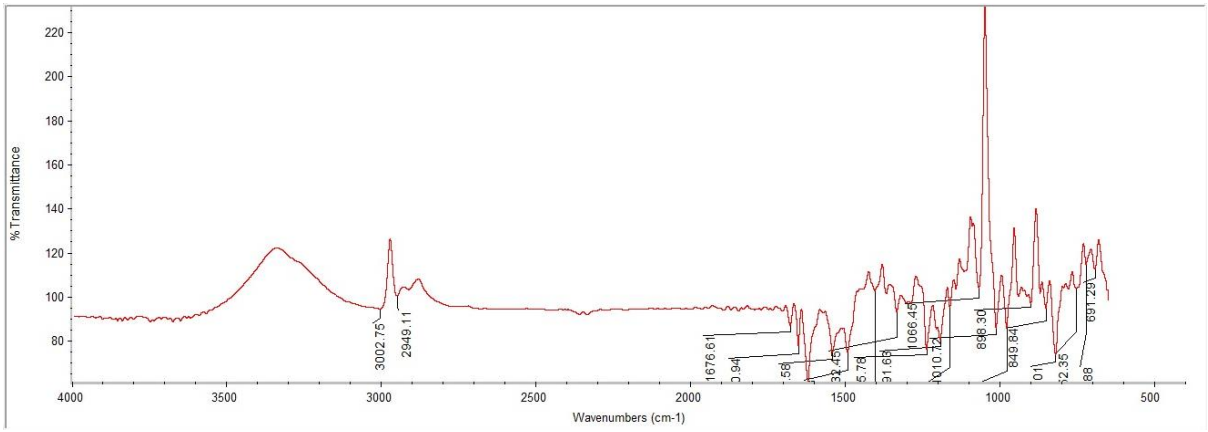


LC/MS





FT-IR



^{1}H NMR

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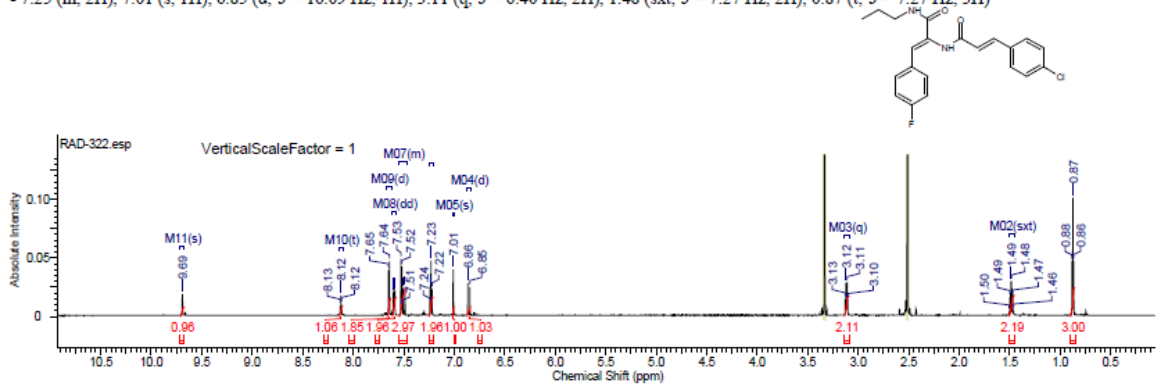
RAD-322

08/11/2016 7:58:08 AM
Dr.Mustafa El-Araby Sample : RAD-322 DMSO

Formula $C_{21}H_{20}ClFN_2O_2$		*FW*	386.8471				
Acquisition Time (sec)	1.9268	*Comment*	Dr.Mustafa El-Araby Sample : RAD-322 DMSO			*Date*	08 Apr 2015 10:45:04
Date Stamp	08 Apr 2015 10:45:04						
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-322_08-04-2015\90\fid					*Frequency (MHz)*	850.15
Nucleus	1H	*Number of Transients*	20	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	10.55
SW(cyclical) (Hz)	17006.80	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	5250.0283	*Spectrum Type*	STANDARD
Sweep Width (Hz)	17006.28	*Temperature (degree C)*	25.000				

^{1}H NMR (850 MHz, DMSO-d_6) δ 9.69 (s, 1H), 8.12 (t, *J* = 5.71 Hz, 1H), 7.64 (d, *J* = 8.30 Hz, 2H), 7.60 (dd, *J* = 5.71, 8.82 Hz, 2H), 7.46 - 7.55 (m, 3H), 7.21 - 7.25 (m, 2H), 7.01 (s, 1H), 6.85 (d, *J* = 16.09 Hz, 1H), 3.11 (q, *J* = 6.40 Hz, 2H), 1.48 (sxt, *J* = 7.27 Hz, 2H), 0.87 (t, *J* = 7.27 Hz, 3H)



^{13}C NMR

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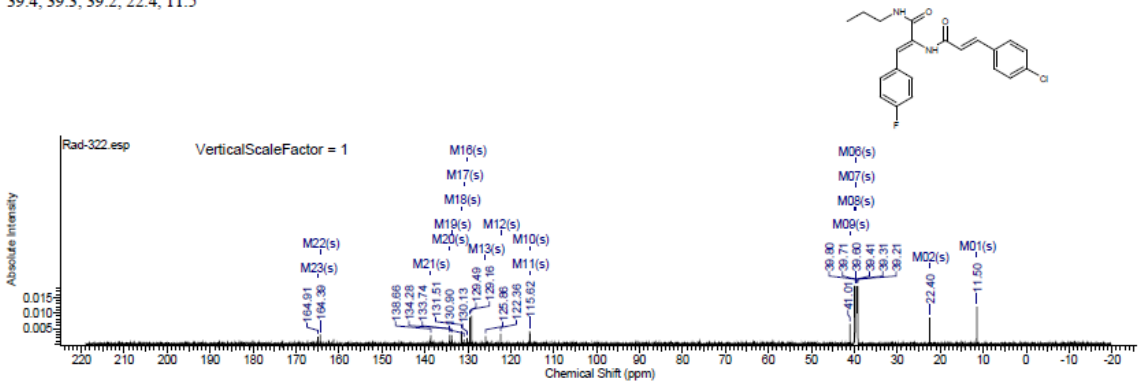
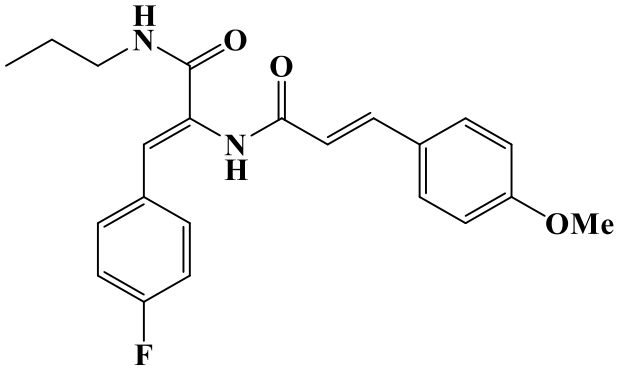
RAD-322

20/09/2016 8:35:42 AM
Dr.Mostafa Sample : RAD-322 DMSO

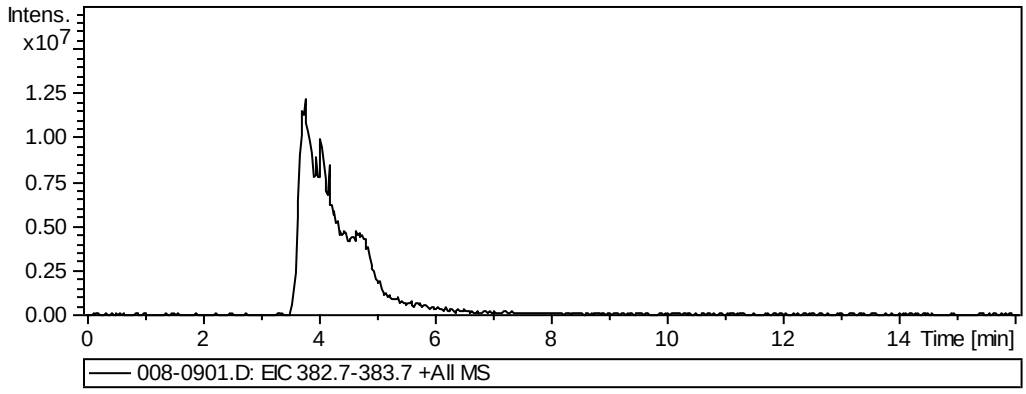
Formula $C_{21}H_{20}ClFN_2O_2$		*FW*	386.8471				
Acquisition Time (sec)	0.6423	*Comment*	Dr.Mostafa Sample : RAD-322 DMSO			*Date*	19 Apr 2016 12:53:04
Date Stamp	19 Apr 2016 12:53:04						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-322_18-04-2016\150\fid						
Frequency (MHz)	213.77	*Nucleus*	13C	*Number of Transients*	2384	*Origin*	spect
Original Points Count	32768	*Owner*	nmr	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	186.93	*SW(cyclical) (Hz)*	51020.41	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	21292.2539
Spectrum Type	STANDARD	*Sweep Width (Hz)*	51018.85	*Temperature (degree C)*	25.000		

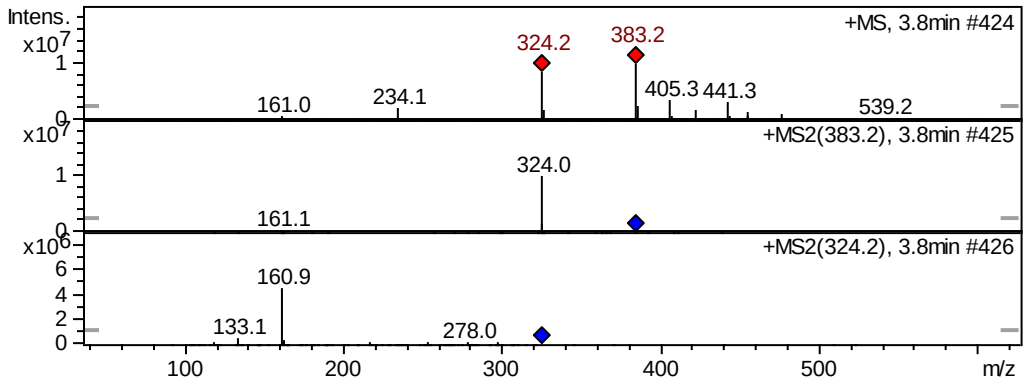
^{13}C NMR (214 MHz, DMSO-d_6) δ 164.9, 164.4, 138.7, 134.3, 133.7, 131.5, 130.9, 130.1, 129.5, 129.2, 125.9, 122.4, 115.6, 115.5, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 11.5



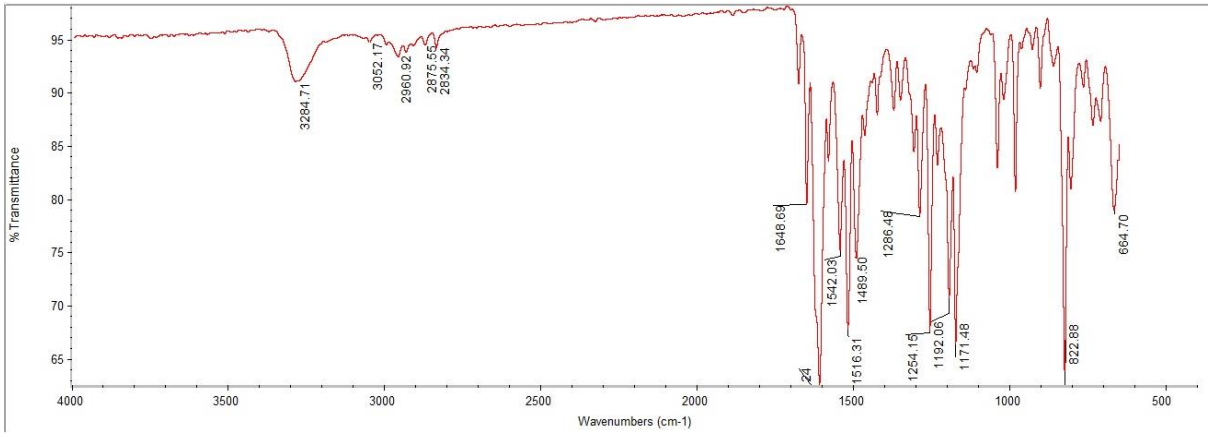


LC/MS





FT-IR



^{1}H NMR

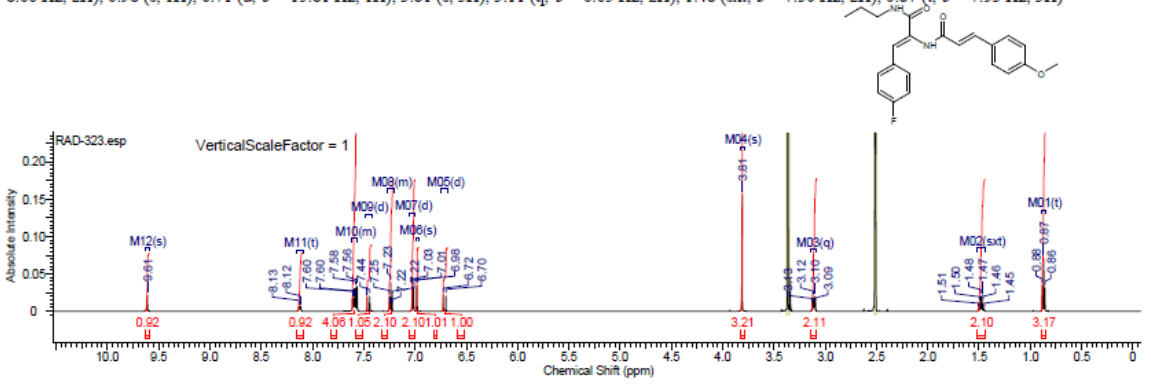
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

RAD-323

08/11/2016 8:02:57 AM
Dr.Mustafa Sample : RAD-323 DMSO PROTON DMSO {D:\Magdy} nmr 26

Formula $C_{20}H_{18}FNO_3$	FW	382.4280					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-323 DMSO PROTON DMSO {D:\Magdy} nmr 26				
Date	18 Jun 2015 15:47:44			Date Stamp	18 Jun 2015 15:47:44		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-323_18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	128.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.61 (s, 1H), 8.12 (t, *J* = 5.65 Hz, 1H), 7.56 - 7.61 (m, 4H), 7.45 (d, *J* = 15.81 Hz, 1H), 7.20 - 7.26 (m, 2H), 7.02 (d, *J* = 8.66 Hz, 2H), 6.98 (s, 1H), 6.71 (d, *J* = 15.81 Hz, 1H), 3.81 (s, 3H), 3.11 (q, *J* = 6.65 Hz, 2H), 1.48 (sxt, *J* = 7.30 Hz, 2H), 0.87 (t, *J* = 7.53 Hz, 3H)



^{13}C NMR

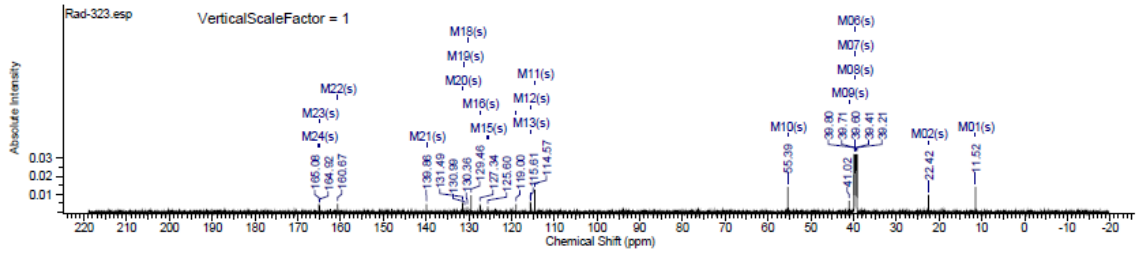
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

RAD-323

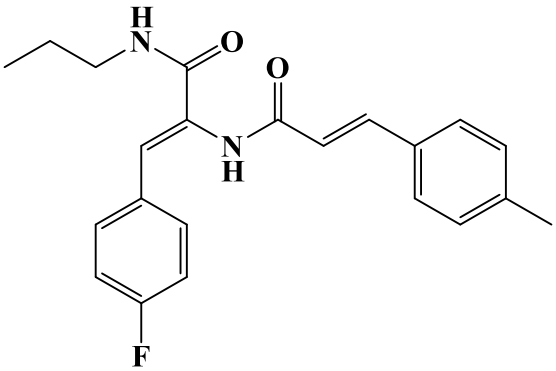
20/09/2016 8:36:09 AM
Dr.Mostafa Sample : RAD-323 DMSO

Formula $C_{20}H_{18}FNO_3$	FW	382.4280					
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample : RAD-323 DMSO			Date	19 Apr 2016 10:15:12
Date Stamp	19 Apr 2016 10:15:12						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-323_18-04-2016\110\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	604	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21295.3691
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	24.999		

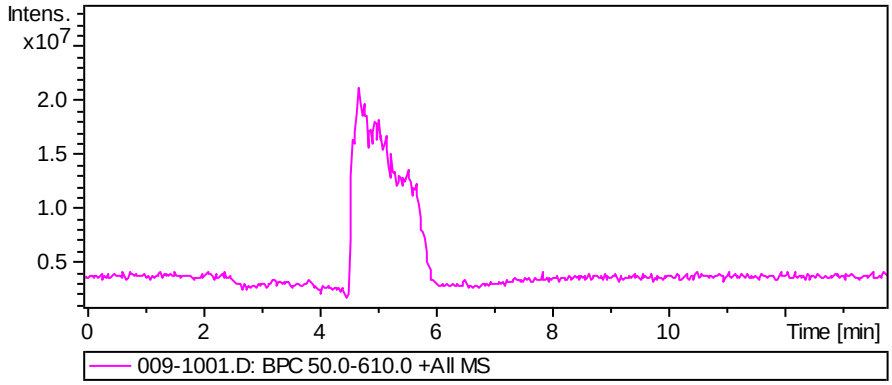
^{13}C NMR (214 MHz, DMSO-d$_6$) δ 165.1, 164.9, 160.7, 139.9, 131.5, 131.0, 130.4, 129.5, 127.3, 125.6, 119.0, 115.6, 115.5, 114.6, 55.4, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 11.5

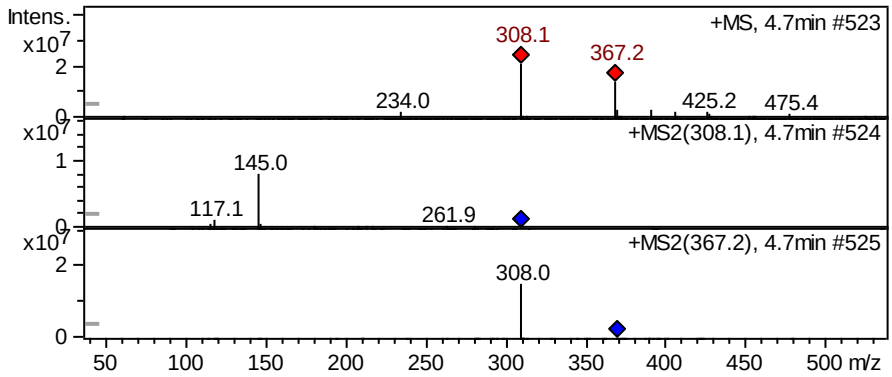


Spectra of (2512)

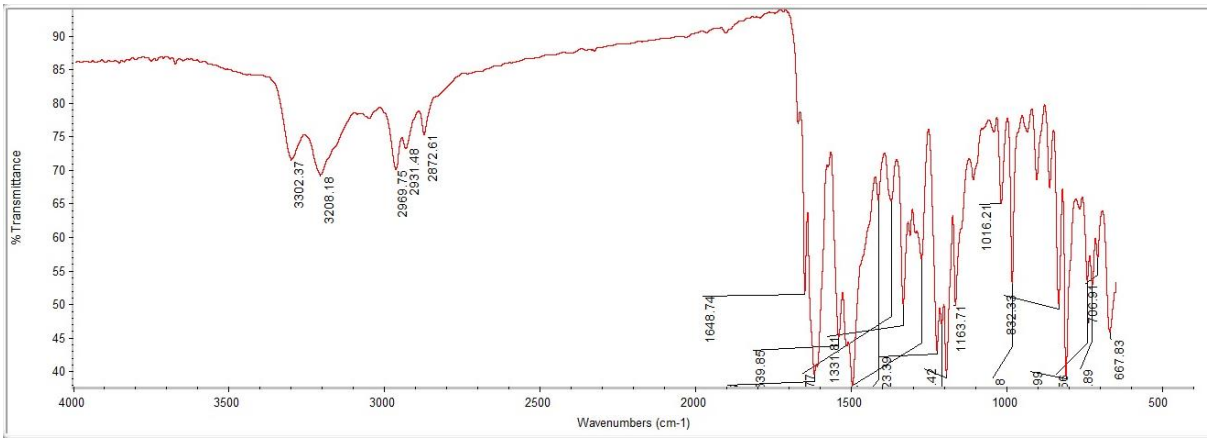


LC/MS





FT-IR



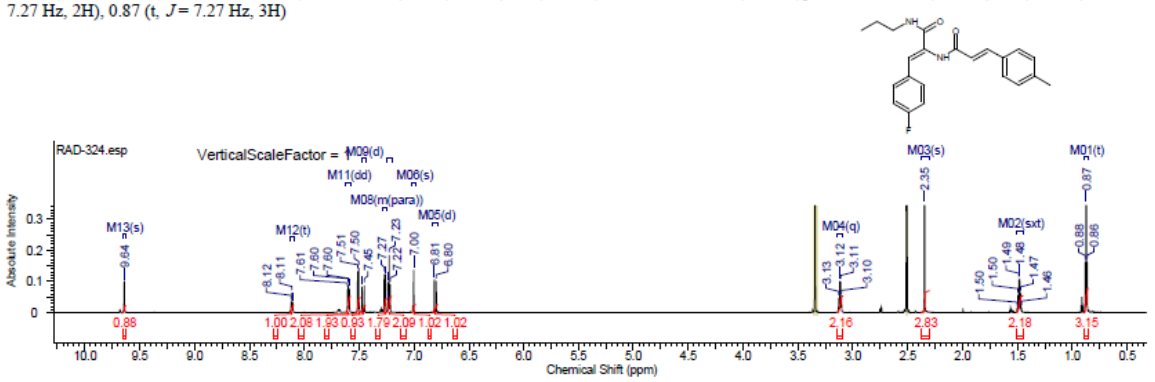
^{1}H NMR

RAD-324

08/11/2016 8:11:51 AM
Dr.Mustafa El-Araby Sample : RAD-324 DMSO

Formula $C_{20}H_{23}FN_2O_2$	FW 366.4286				
Acquisition Time (sec)	1.9268	Comment	Dr.Mustafa El-Araby Sample : RAD-324 DMSO	Date	08 Apr 2015 11:21:20
Date Stamp	08 Apr 2015 11:21:20				
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-324_08-04-2015\170\fid			Frequency (MHz)	850.15
Nucleus	1H	Number of Transients	20	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	9.04
SW(cyclical) (Hz)	17006.80	Solvent	DMSO-d6	Spectrum Offset (Hz)	5250.0283	Spectrum Type	STANDARD
Sweep Width (Hz)	17006.28	Temperature (degree C)	25.001				

^{1}H NMR (850 MHz, DMSO-d_6) δ 9.64 (s, 1H), 8.11 (t, J = 5.71 Hz, 1H), 7.60 (dd, J = 5.71, 8.82 Hz, 2H), 7.48 - 7.53 (m, J = 7.78 Hz, 2H), 7.46 (d, J = 16.09 Hz, 1H), 7.25 - 7.28 (m, J = 8.30 Hz, 2H), 7.20 - 7.25 (m, 2H), 7.00 (s, 1H), 6.81 (d, J = 15.57 Hz, 1H), 3.12 (q, J = 6.75 Hz, 2H), 2.35 (s, 3H), 1.48 (sxt, J = 7.27 Hz, 2H), 0.87 (t, J = 7.27 Hz, 3H)



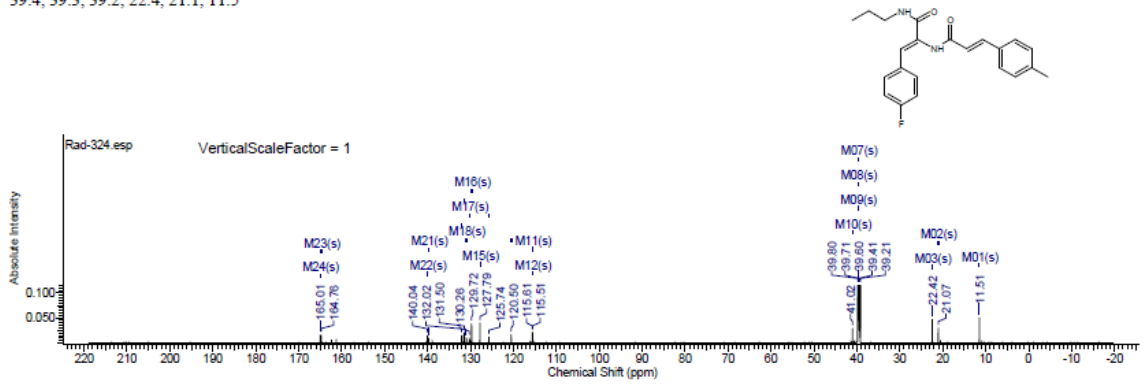
^{13}C NMR

RAD-324

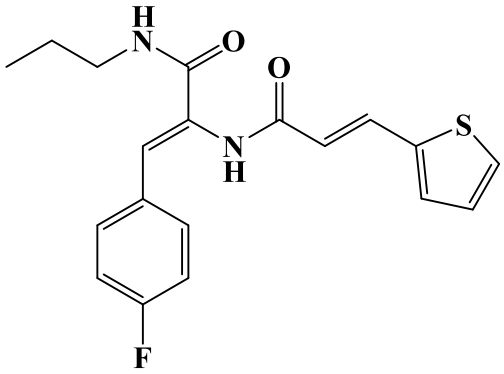
20/09/2016 8:36:44 AM
Dr.Mostafa Sample : RAD-324 DMSO

Formula $C_{20}H_{23}FN_2O_2$	FW 366.4286						
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample : RAD-324 DMSO			Date	18 Apr 2016 12:12:32
Date Stamp	18 Apr 2016 12:12:32						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-324_18-04-2016\10\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	1464	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21293.8125
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.002		

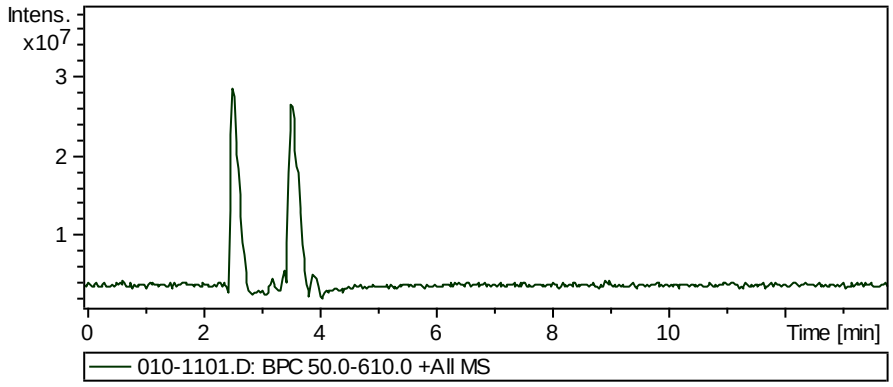
^{13}C NMR (214 MHz, DMSO-d_6) δ 165.0, 164.8, 140.0, 139.7, 132.0, 131.5, 131.0, 130.3, 129.7, 127.8, 125.7, 120.5, 115.6, 115.5, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 21.1, 11.5

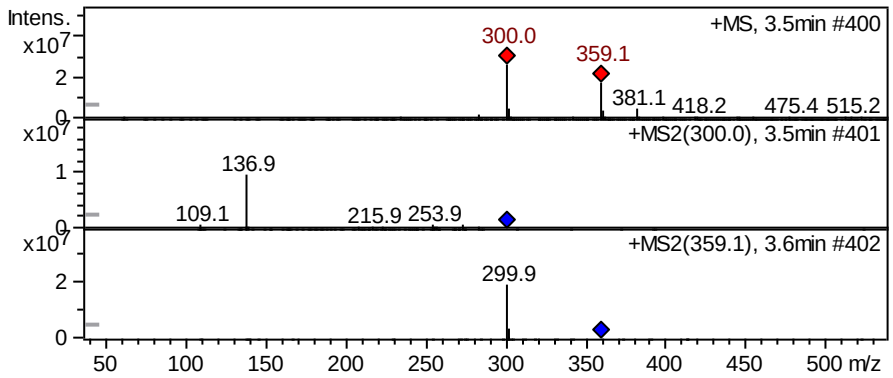


Spectra of (2612)

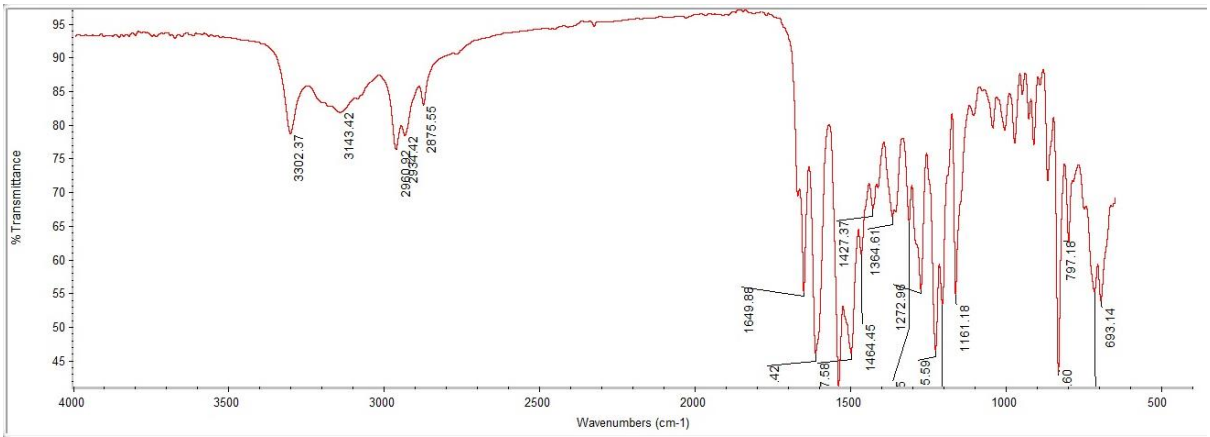


LC/MS





FT-IR



^{1}H NMR

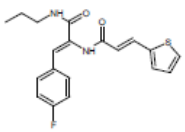
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

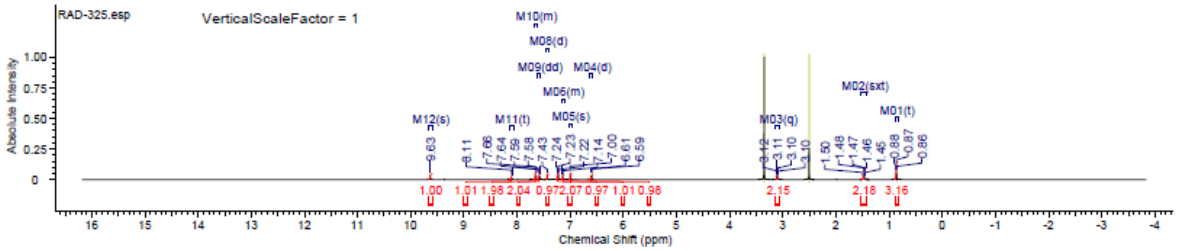
RAD-325

18/02/2017 10:53:56 AM
Dr.Mostafa Sample : RAD-325 DMSO

Formula $C_{18}H_{16}FN_3O_2S$		FW	358.4298				
Acquisition Time (sec)	1.9268	Comment	Dr.Mostafa Sample : RAD-325 DMSO			Date	14 Feb 2017 12:38:08
Date Stamp	14 Feb 2017 12:38:08						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Rad 355 new amines\MOSTAFA_RAD-325_14-02-2017\20\fid					Frequency (MHz)	850.15
Nucleus	1H	Number of Transients	64	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	10.55
SW(cyclical) (Hz)	17006.80	Solvent	DMSO-d6	Spectrum Offset (Hz)	5250.0283	Spectrum Type	STANDARD
Sweep Width (Hz)	17006.28	Temperature (degree C)	25.001				

^{1}H NMR (850 MHz, DMSO-d_6) δ 9.63 (s, 1H), 8.11 (t, J = 5.71 Hz, 1H), 7.61 - 7.68 (m, 2H), 7.58 (dd, J = 5.97, 8.04 Hz, 2H), 7.43 (d, J = 3.11 Hz, 1H), 7.23 (t, J = 8.56 Hz, 2H), 7.11 - 7.16 (m, 1H), 7.00 (s, 1H), 6.60 (d, J = 15.57 Hz, 1H), 3.11 (q, J = 6.40 Hz, 2H), 1.48 (sxt, J = 7.27 Hz, 2H), 0.87 (t, J = 7.53 Hz, 3H)





^{13}C NMR

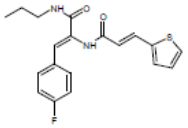
This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

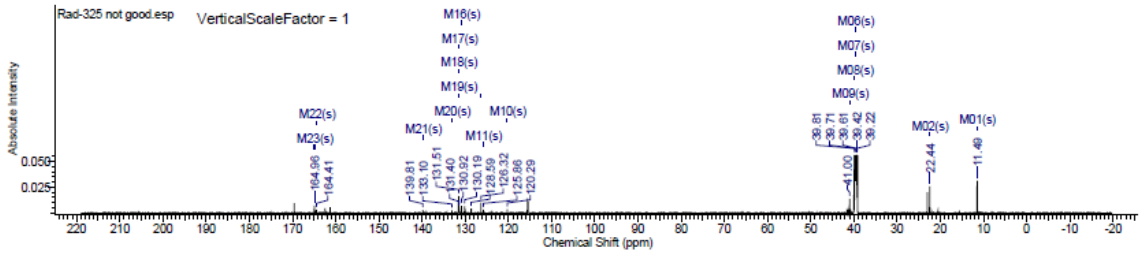
RAD-325

25/09/2016 2:04:21 PM
Dr.Mostafa Sample : RAD-325 DMSO

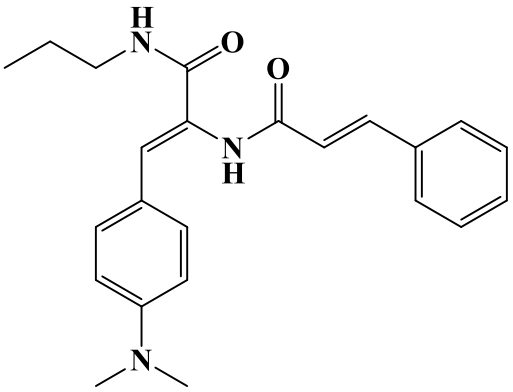
Formula $C_{18}H_{16}FN_3O_2S$		FW	358.4298				
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample : RAD-325 DMSO			Date	19 Apr 2016 09:47:28
Date Stamp	19 Apr 2016 09:47:28						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-325_18-04-2016\100\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	1930	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21298.4824
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

^{13}C NMR (214 MHz, DMSO-d_6) δ 165.0, 164.4, 139.8, 133.1, 131.6, 131.5, 131.4, 130.9, 130.2, 128.6, 128.5, 126.3, 125.9, 120.3, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 11.5

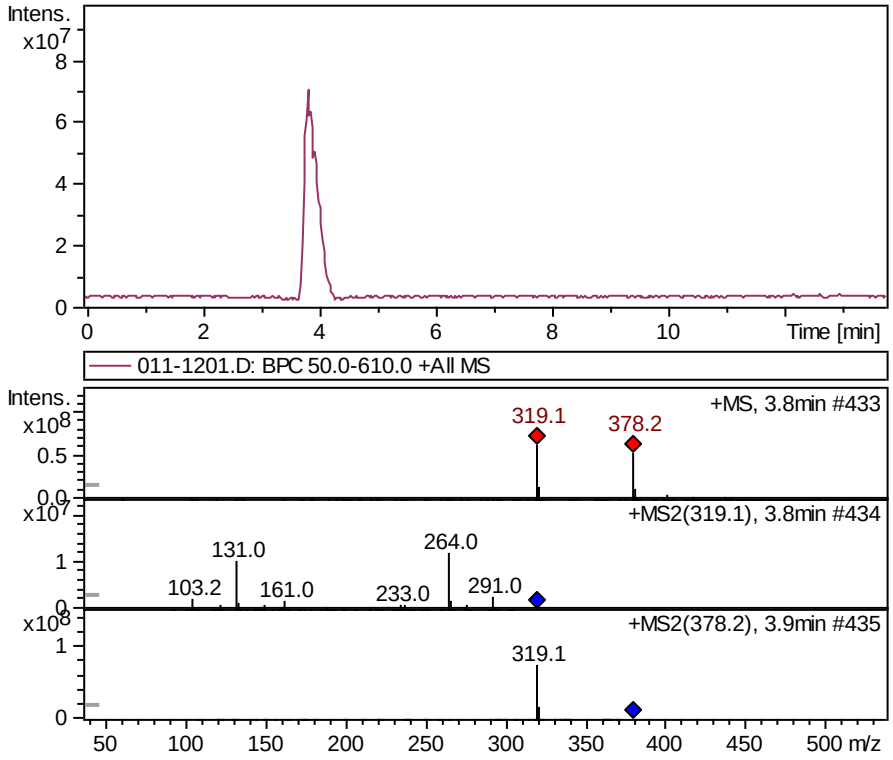




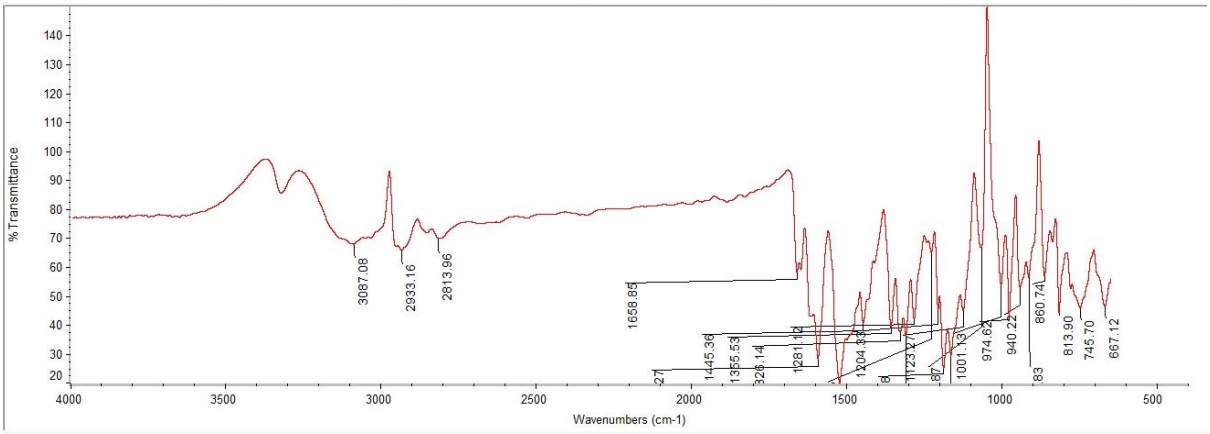
Spectra of (2712)



LC/MS



FT-IR



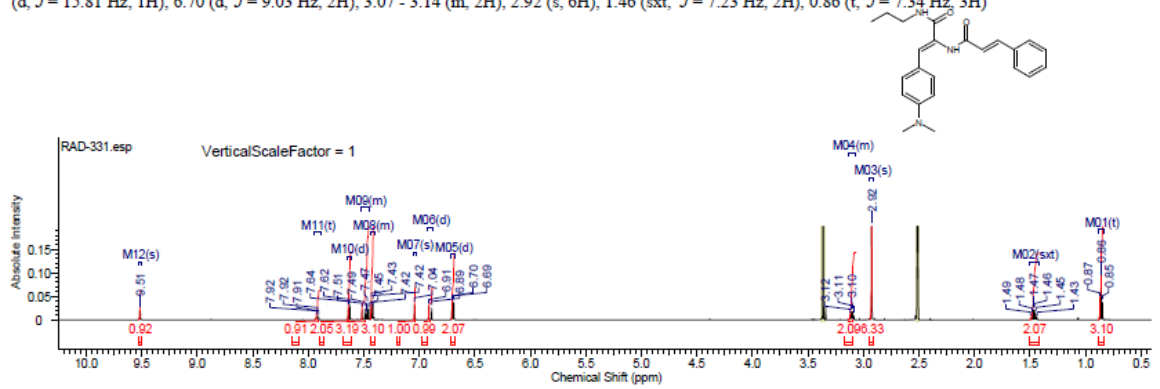
^{1}H NMR

RAD-331

08/11/2016 8:20:31 AM
Dr.Mustafa Sample : RAD-331 DMSO PROTON DMSO {D:\Magdy} nmr 34

Formula $C_{22}H_{27}N_3O_2$	FW	377.4794					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-331 DMSO PROTON DMSO {D:\Magdy} nmr 34				
Date	18 Jun 2015 16:30:24			Date Stamp	18 Jun 2015 16:30:24		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-331_18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	128.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.51 (s, 1H), 7.91 (t, J = 5.84 Hz, 1H), 7.63 (d, J = 7.15 Hz, 2H), 7.45 - 7.52 (m, 3H), 7.40 - 7.44 (m, 3H), 7.04 (s, 1H), 6.90 (d, J = 15.81 Hz, 1H), 6.70 (d, J = 9.03 Hz, 2H), 3.07 - 3.14 (m, 2H), 2.92 (s, 6H), 1.46 (sxt, J = 7.23 Hz, 2H), 0.86 (t, J = 7.34 Hz, 3H)



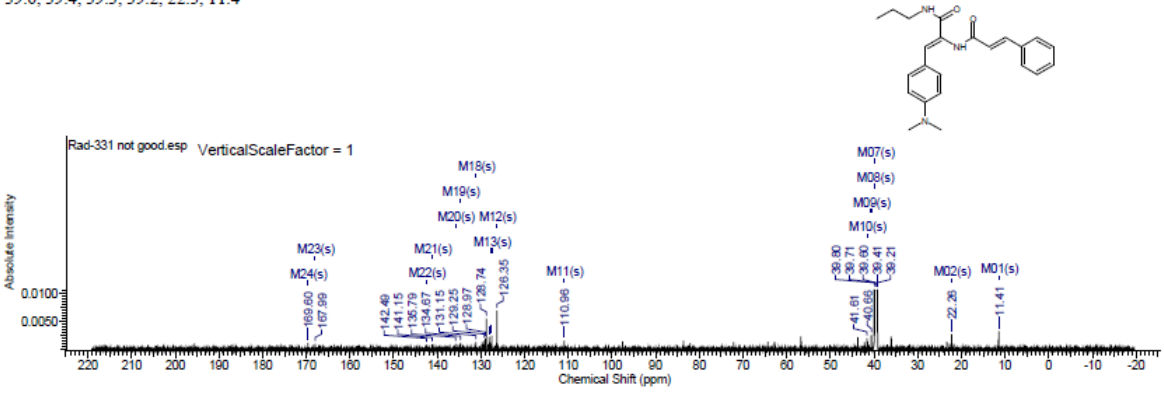
^{13}C NMR

RAD-331

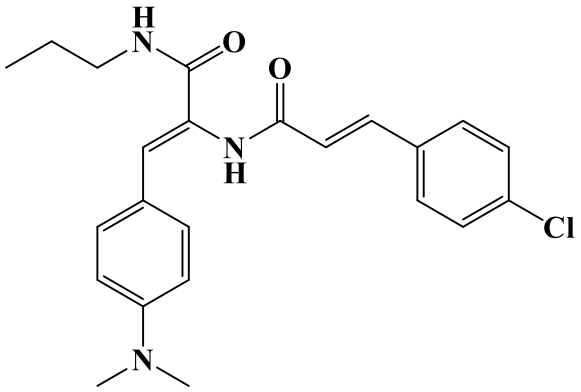
25/09/2016 2:12:54 PM
Dr.Mostafa Sample ; RAD-331 DMSO

Formula $C_{22}H_{27}N_3O_2$	FW	377.4794					
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-331 DMSO			Date	20 Apr 2016 10:49:20
Date Stamp	20 Apr 2016 10:49:20						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-331_19-04-2016\100\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3007	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21320.2813
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	24.999		

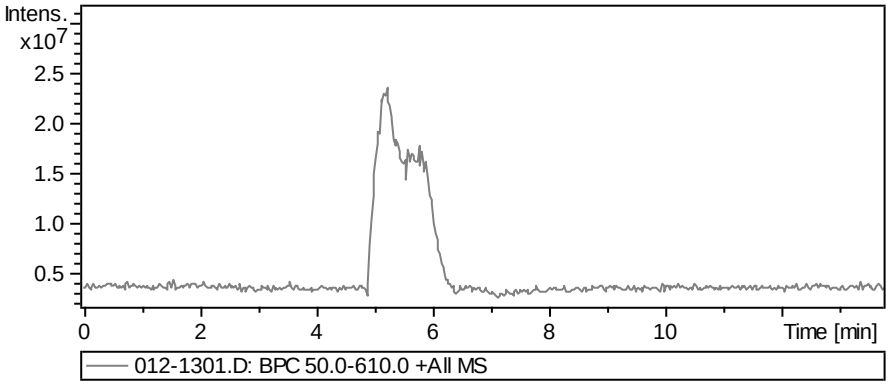
^{13}C NMR (214 MHz, DMSO-d$_6$) δ 169.6, 168.0, 142.5, 141.1, 135.8, 134.7, 131.2, 129.3, 129.0, 128.7, 128.1, 127.5, 126.3, 111.0, 41.6, 40.7, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.3, 11.4

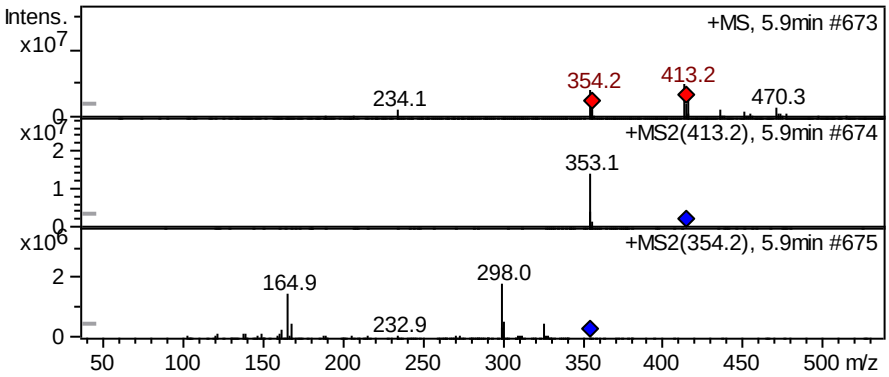


Spectra of (2812)

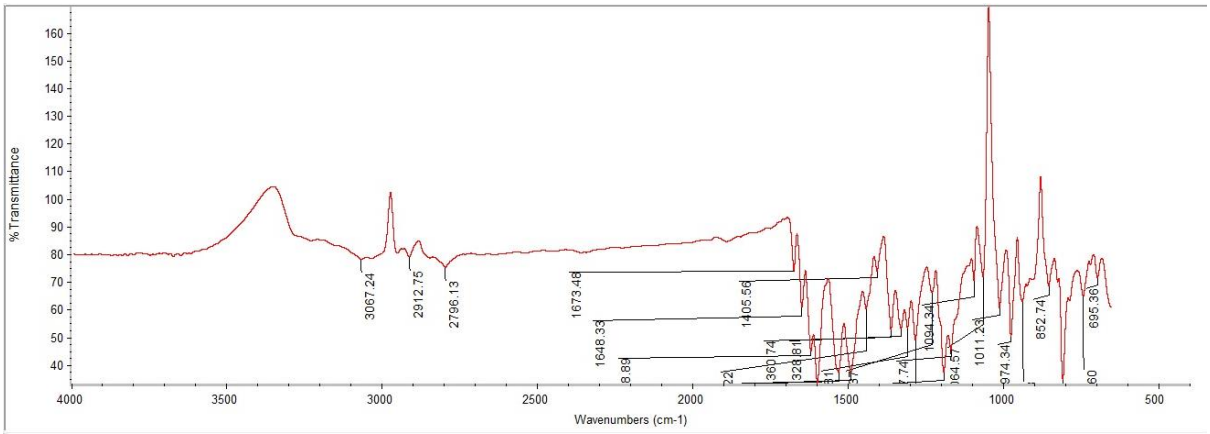


LC/MS





FT-IR



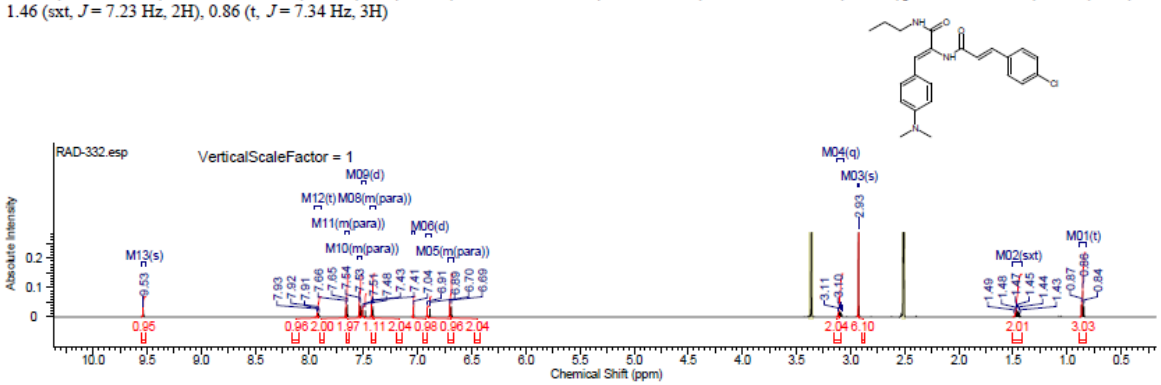
^{1}H NMR

RAD-332

08/11/2016 8:27:20 AM
Dr.Mustafa Sample : RAD-332 DMSO PROTON DMSO (D:\Magdy) nmr 15

Formula $C_{25}H_{26}ClN_3O_2$		FW 411.9244					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-332 DMSO PROTON DMSO (D:\Magdy) nmr 15				
Date	18 Jun 2015 14:52:16			Date Stamp	18 Jun 2015 14:52:16		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-332_18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	128.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.53 (s, 1H), 7.92 (t, J = 6.02 Hz, 1H), 7.63 - 7.68 (m, J = 8.66 Hz, 2H), 7.52 - 7.55 (m, J = 8.28 Hz, 2H), 7.50 (d, J = 15.81 Hz, 1H), 7.39 - 7.44 (m, J = 9.03 Hz, 2H), 7.04 (s, 1H), 6.90 (d, J = 15.81 Hz, 1H), 6.67 - 6.72 (m, J = 9.03 Hz, 2H), 3.10 (q, J = 6.40 Hz, 2H), 2.93 (s, 6H), 1.46 (sxt, J = 7.23 Hz, 2H), 0.86 (t, J = 7.34 Hz, 3H)



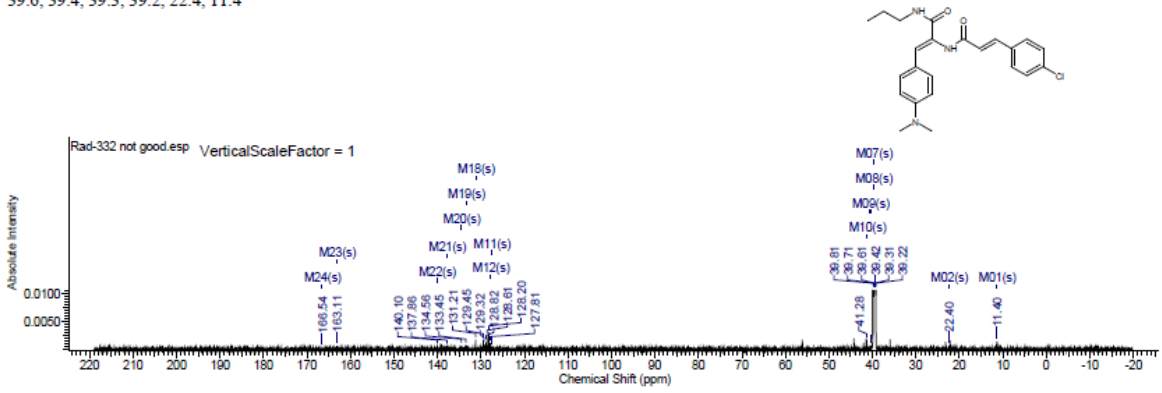
^{13}C NMR

RAD-332

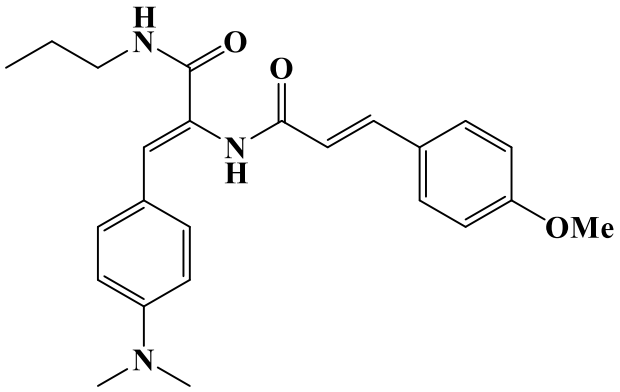
25/09/2016 3:09:37 PM
Dr.Mostafa Sample ; RAD-332 DMSO

Formula $C_{25}H_{26}ClN_3O_2$		FW 411.9244					
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-332 DMSO			Date	20 Apr 2016 07:13:52
Date Stamp	20 Apr 2016 07:13:52						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-332_19-04-2016\70\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3500	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21286.0273
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.001		

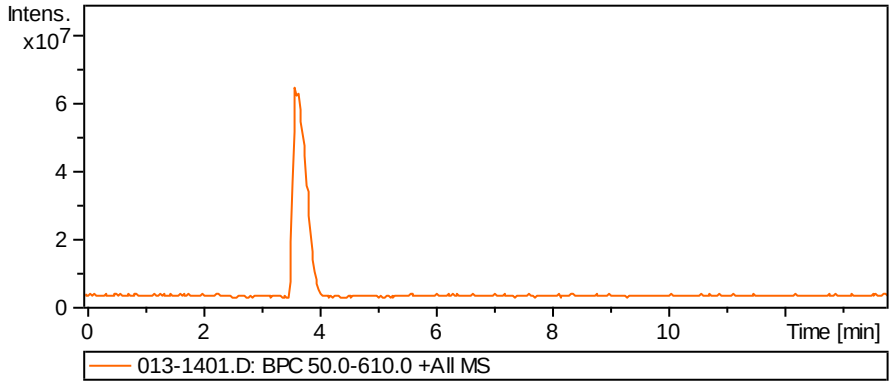
^{13}C NMR (214 MHz, DMSO-d$_6$) δ 166.5, 163.1, 140.1, 137.9, 134.6, 133.4, 131.2, 129.4, 129.3, 128.8, 128.6, 128.2, 127.8, 127.5, 41.3, 40.5, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 11.4

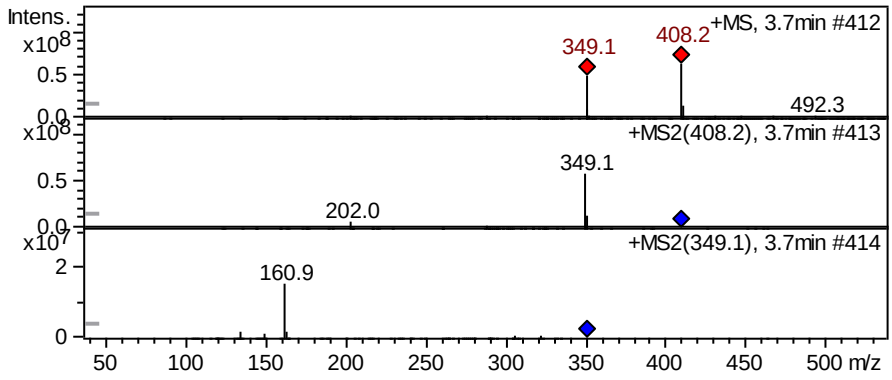


Spectra of (2912)

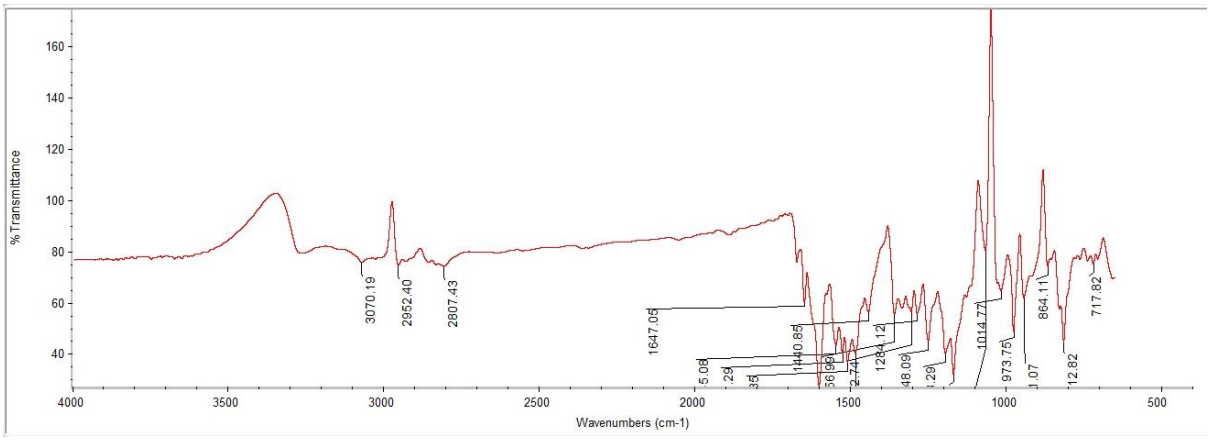


LC/MS





FT-IR



^{1}H NMR

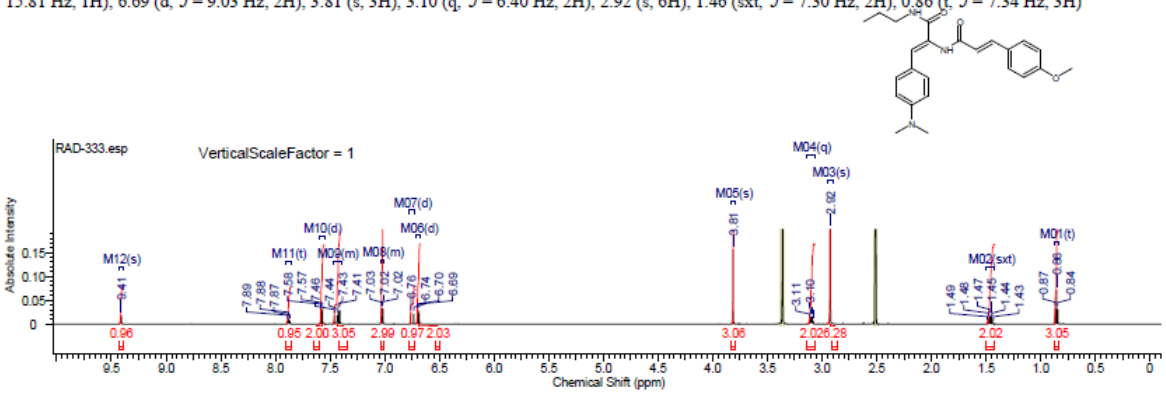
RAD-333

08/11/2016 8:30:41 AM
Dr.Mustafa Sample : RAD-333 DMSO PROTON DMSO (D:\Magdy) nmr 18

Formula $C_{24}H_{26}N_2O_4$	FW	407.5054

Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-333 DMSO PROTON DMSO (D:\Magdy) nmr 18				
Date	18 Jun 2015 15:07:12			Date Stamp	18 Jun 2015 15:07:12		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-333 18-06-2015\10\fid						
Nucleus	1H	Number of Transients	32	Origin	spect	Frequency (MHz)	600.15
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Original Points Count	32768
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Receiver Gain	128.00
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000			Spectrum Type	STANDARD

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.41 (s, 1H), 7.88 (t, J = 5.83 Hz, 1H), 7.58 (d, J = 9.04 Hz, 2H), 7.40 - 7.47 (m, 3H), 7.01 - 7.04 (m, 3H), 6.75 (d, J = 15.81 Hz, 1H), 6.69 (d, J = 9.03 Hz, 2H), 3.81 (s, 3H), 3.10 (q, J = 6.40 Hz, 2H), 2.92 (s, 6H), 1.46 (sxt, J = 7.30 Hz, 2H), 0.86 (t, J = 7.34 Hz, 3H)



^{13}C NMR

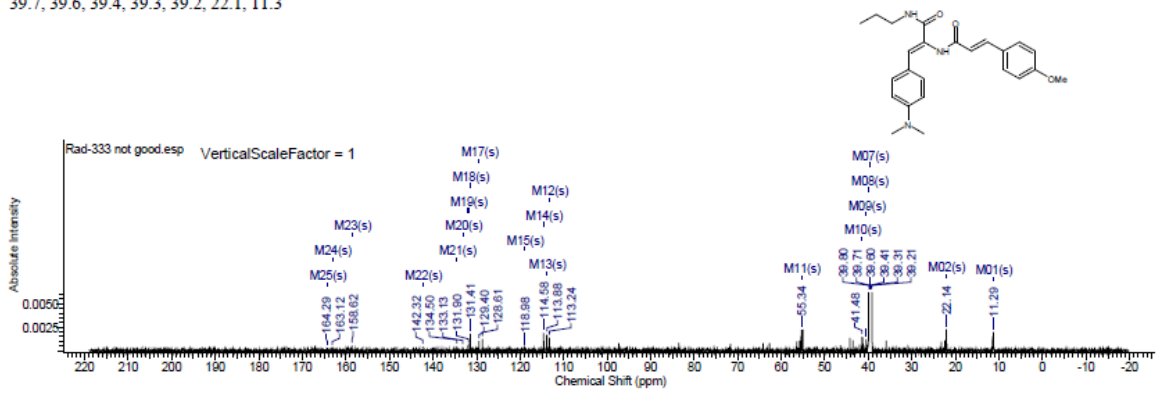
RAD-333

25/09/2016 3:18:33 PM
Dr.Moustafa Sample : RAD-333 DMSO

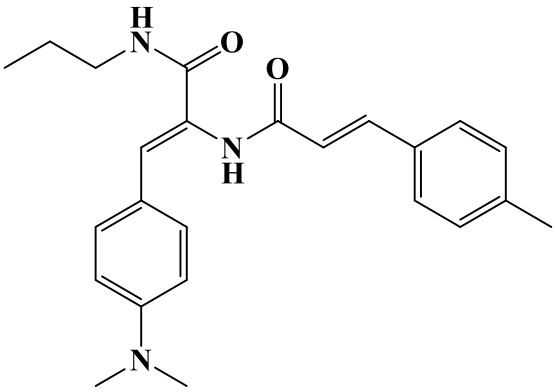
Formula $C_{24}H_{26}N_2O_4$	FW	407.5053

Acquisition Time (sec)	0.6423	Comment	Dr.Moustafa Sample : RAD-333 DMSO			Date	22 Apr 2016 05:48:32
Date Stamp	22 Apr 2016 05:48:32						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-333 21-04-2016\20\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	12288	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21286.0273
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	24.999		

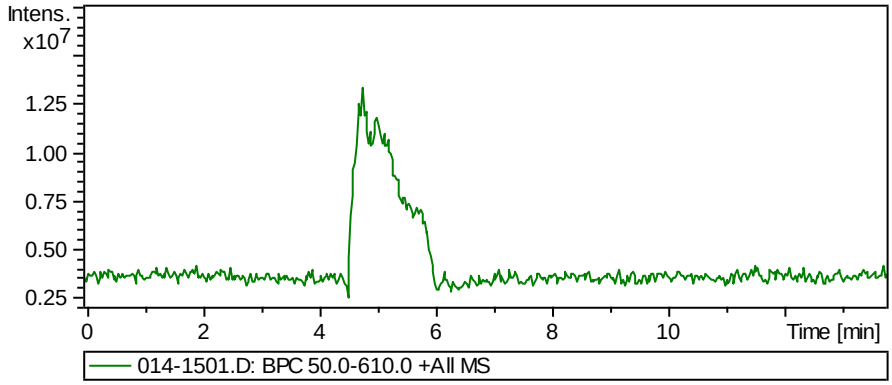
^{13}C NMR (214 MHz, DMSO-d_6) δ 164.3, 163.1, 158.6, 142.3, 134.5, 133.1, 131.9, 131.4, 129.4, 128.6, 119.0, 114.6, 113.9, 113.2, 55.3, 41.5, 40.5, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.1, 11.3

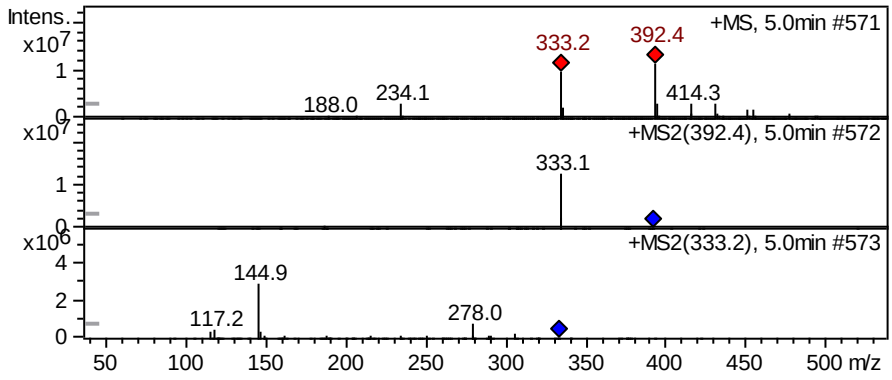


Spectra of (3012)

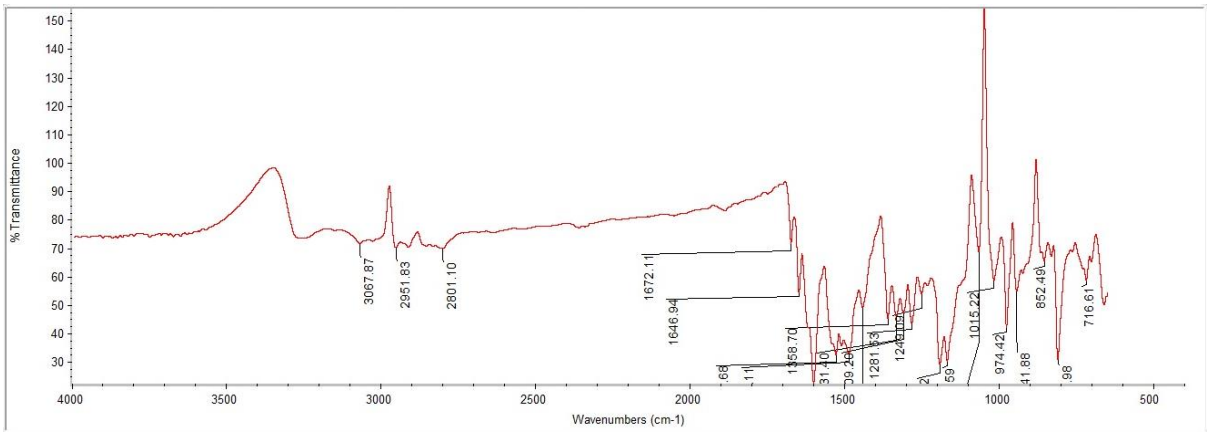


LC/MS





FT-IR



^{1}H NMR

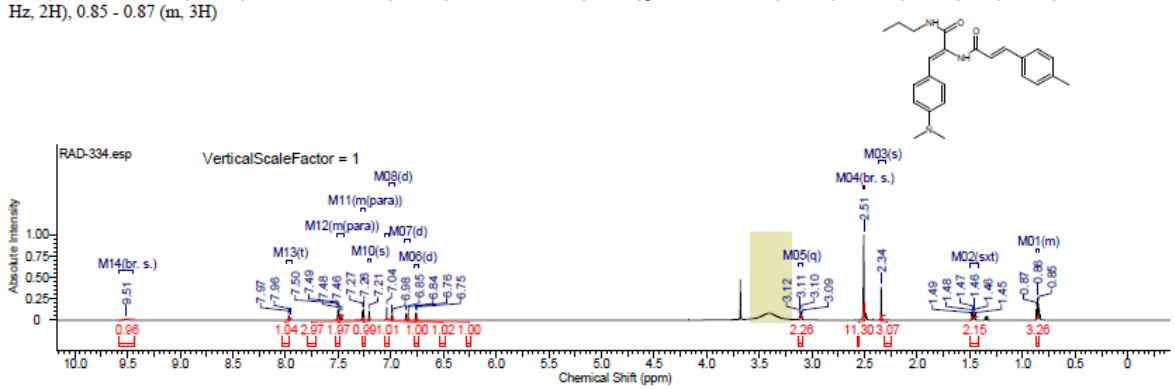
RAD-334

18/02/2017 10:53:27 AM
Dr.Mostafa Sample : RAD-334 DMSO

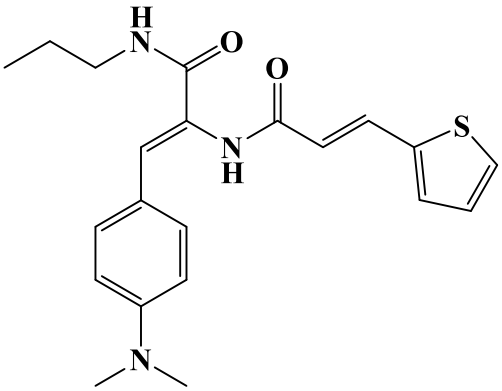
Formula $C_{24}H_{20}N_4O_3$	FW	391.5060

Acquisition Time (sec)	1.9268	*Comment*	Dr.Mostafa Sample : RAD-334 DMSO			*Date*	14 Feb 2017 12:44:32
Date Stamp	14 Feb 2017 12:44:32						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Rad 355 new amines\MOSTAFA_RAD-334_14-02-2017\30\fid					*Frequency (MHz)*	850.15
Nucleus	1H	*Number of Transients*	64	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	10.55
SW(cyclical) (Hz)	17006.80	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	5250.0283	*Spectrum Type*	STANDARD
Sweep Width (Hz)	17006.28	*Temperature (degree C)*	25.000				

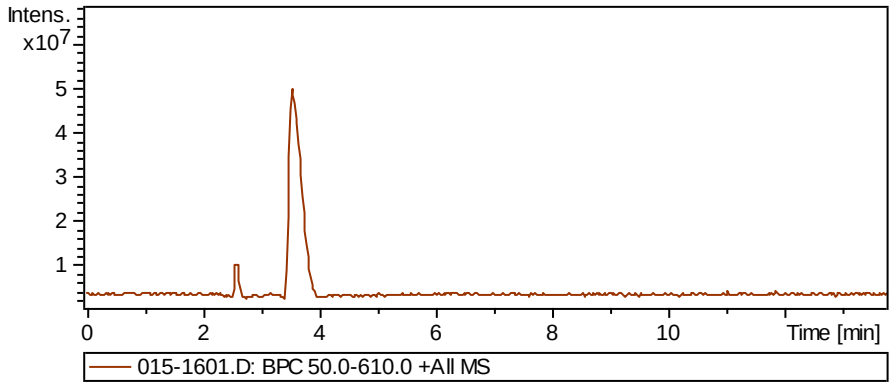
^{1}H NMR (850 MHz, DMSO-d$_6$) δ 9.51 (br. s., 1H), 7.96 (t, *J* = 5.97 Hz, 1H), 7.45 - 7.52 (m, 2H), 7.24 - 7.28 (m, *J* = 7.78 Hz, 2H), 7.21 (s, 1H), 7.04 (s, 1H), 6.99 (d, *J* = 8.30 Hz, 1H), 6.84 (d, *J* = 15.57 Hz, 1H), 6.76 (d, *J* = 8.30 Hz, 1H), 3.11 (q, *J* = 6.57 Hz, 2H), 2.51 (br. s., 9H), 2.34 (s, 2H), 1.47 (sxt, *J* = 7.16 Hz, 2H), 0.85 - 0.87 (m, 3H)

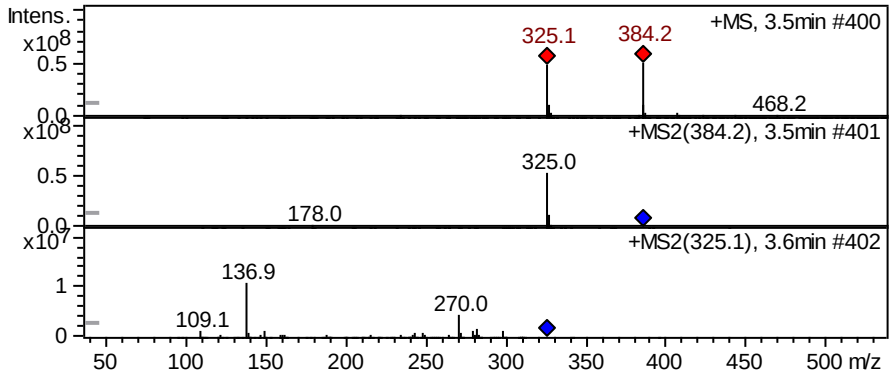


Spectra of (3112)

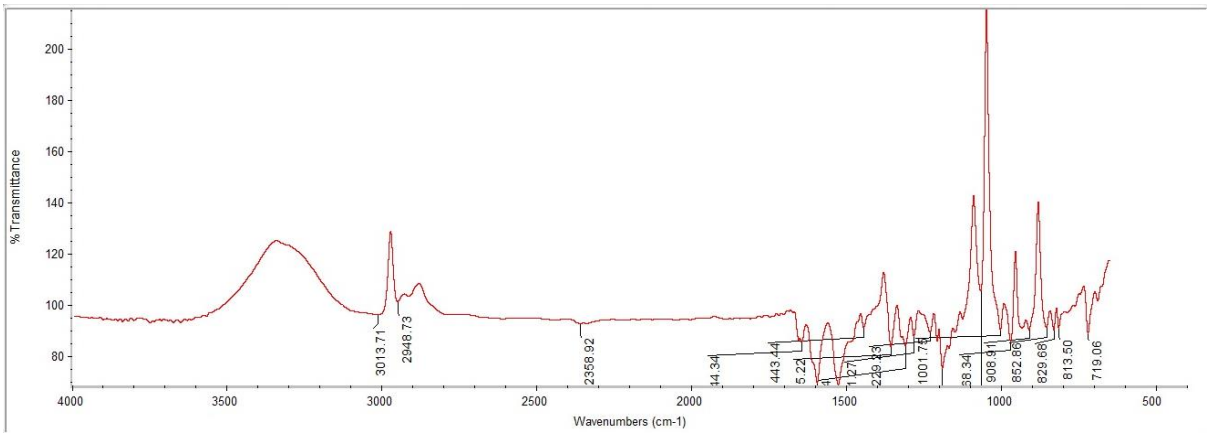


LC/MS





FT-IR



^{1}H NMR

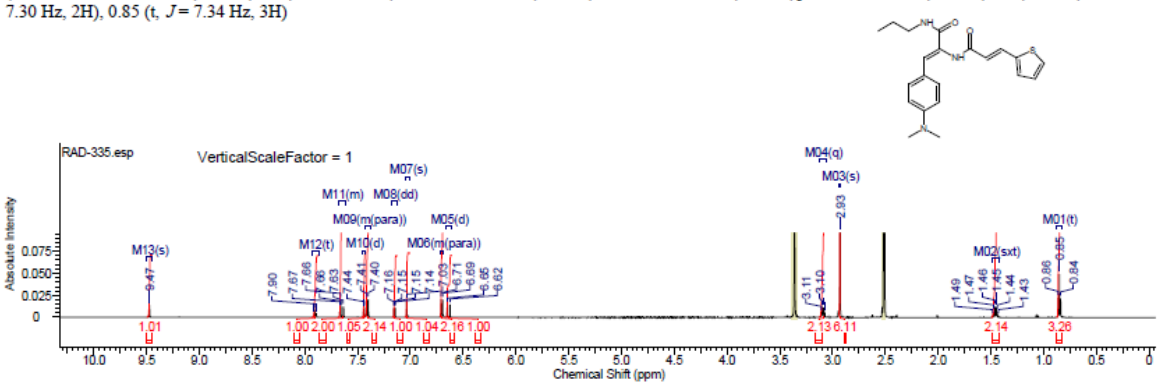
RAD-335

08/11/2016 8:37:35 AM
Dr.Mustafa Sample : RAD-335 DMSO PROTON DMSO (D:\Magdy) nmr 16

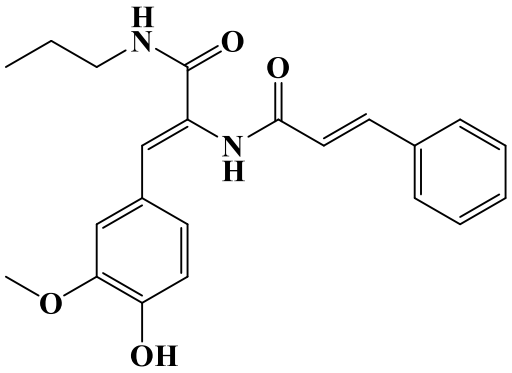
Formula $C_{21}H_{21}N_3O_2S$	FW	383.5071

Acquisition Time (sec)	2.6564	*Comment*	Dr.Mustafa Sample : RAD-335 DMSO PROTON DMSO (D:\Magdy) nmr 16				
Date	18 Jun 2015 14:56:32			*Date Stamp*	18 Jun 2015 14:56:32		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-335 18-06-2015\10\fid					*Frequency (MHz)*	600.15
Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	161.00
SW(cyclical) (Hz)	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.1750	*Spectrum Type*	STANDARD
Sweep Width (Hz)	12335.15	*Temperature (degree C)*	25.000				

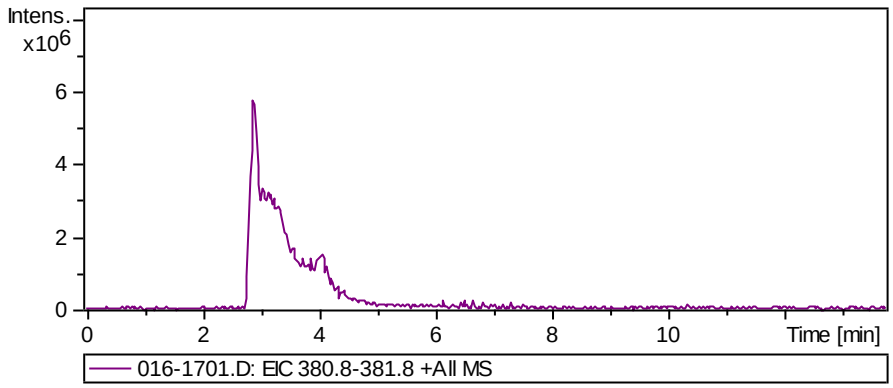
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.47 (s, 1H), 7.90 (t, *J* = 5.83 Hz, 1H), 7.61 - 7.68 (m, 2H), 7.44 (d, *J* = 3.39 Hz, 1H), 7.38 - 7.42 (m, *J* = 9.04 Hz, 2H), 7.15 (dd, *J* = 3.58, 5.08 Hz, 1H), 7.03 (s, 1H), 6.68 - 6.72 (m, *J* = 9.03 Hz, 2H), 6.64 (d, *J* = 15.81 Hz, 1H), 3.09 (q, *J* = 6.40 Hz, 2H), 2.93 (s, 5H), 1.46 (sxt, *J* = 7.30 Hz, 2H), 0.85 (t, *J* = 7.34 Hz, 3H)

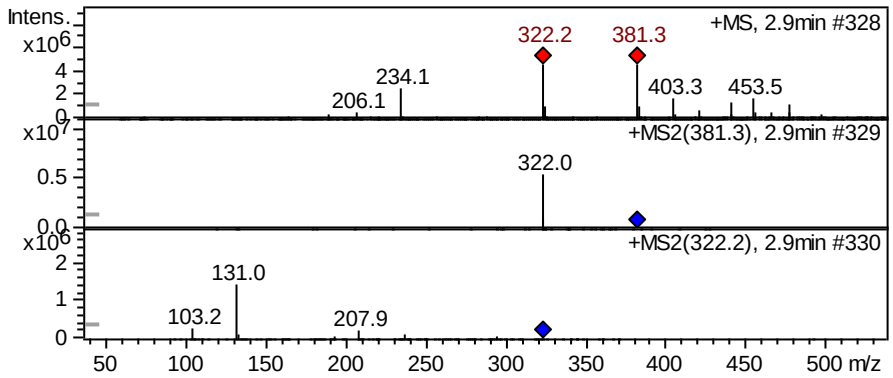


Spectra of (3212)

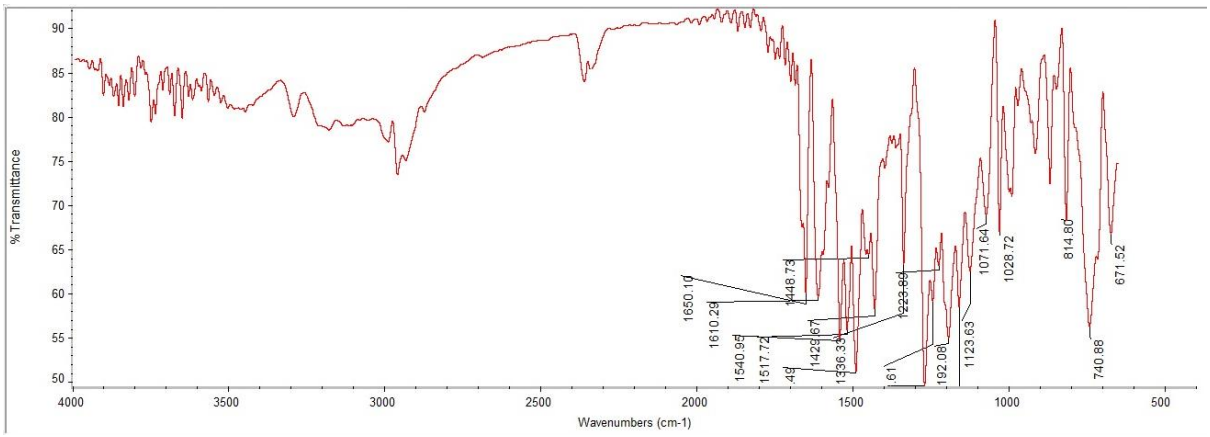


LC/MS





FT-IR



^{1}H NMR

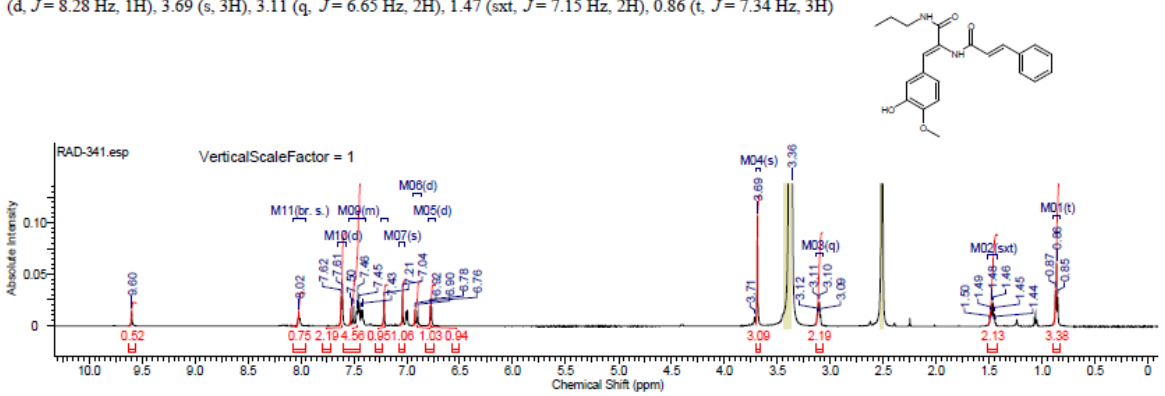
RAD-341

08/11/2016 8:41:07 AM
Dr.Mustafa Sample : RAD-341 DMSO PROTON DMSO (D:\Magdy) nmr 23

Formula $C_{22}H_{24}N_2O_4$	FW	380.4370

Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-341 DMSO PROTON DMSO (D:\Magdy) nmr 23				
Date	18 Jun 2015 15:32:48			Date Stamp	18 Jun 2015 15:32:48		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-341 18-06-2015\10\fid						
Nucleus	1H	Number of Transients	32	Origin	spect	Frequency (MHz)	600.15
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Original Points Count	32768
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Receiver Gain	114.00
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000			Spectrum Type	STANDARD

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 8.02 (br. s., 1H), 7.61 (d, *J* = 7.15 Hz, 2H), 7.39 - 7.55 (m, 4H), 7.21 (s, 1H), 7.04 (s, 1H), 6.91 (d, *J* = 16.19 Hz, 1H), 6.77 (d, *J* = 8.28 Hz, 1H), 3.69 (s, 3H), 3.11 (q, *J* = 6.65 Hz, 2H), 1.47 (sxt, *J* = 7.15 Hz, 2H), 0.86 (t, *J* = 7.34 Hz, 3H)



^{13}C NMR

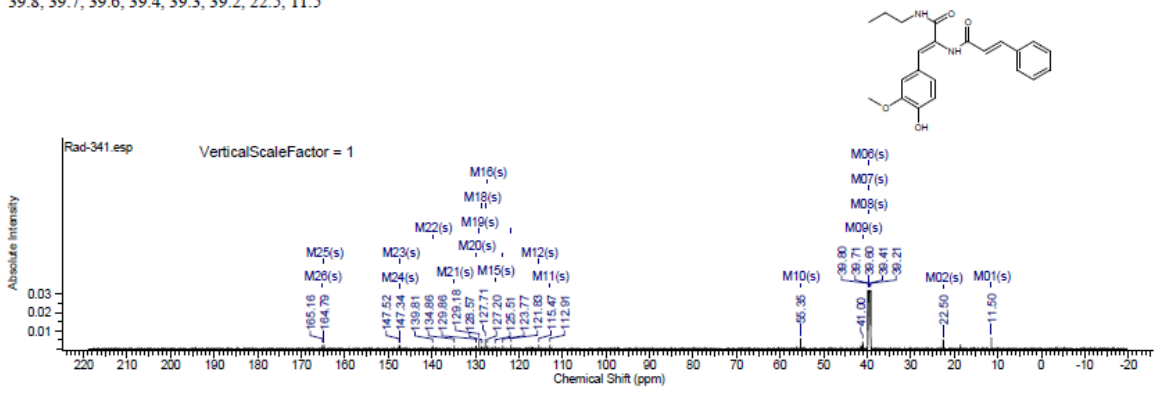
RAD-341

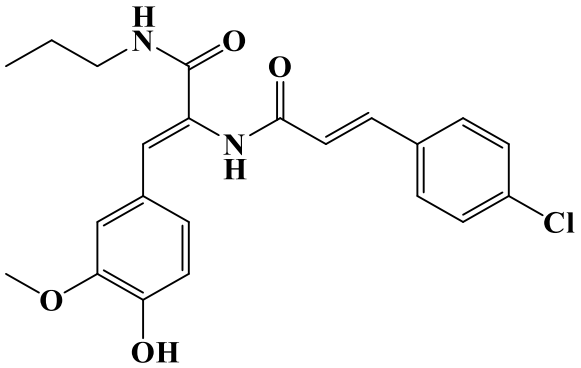
20/09/2016 9:24:57 AM
Dr.Mostafa Sample : RAD-341 DMSO

Formula $C_{22}H_{24}N_2O_4$	FW	380.4370

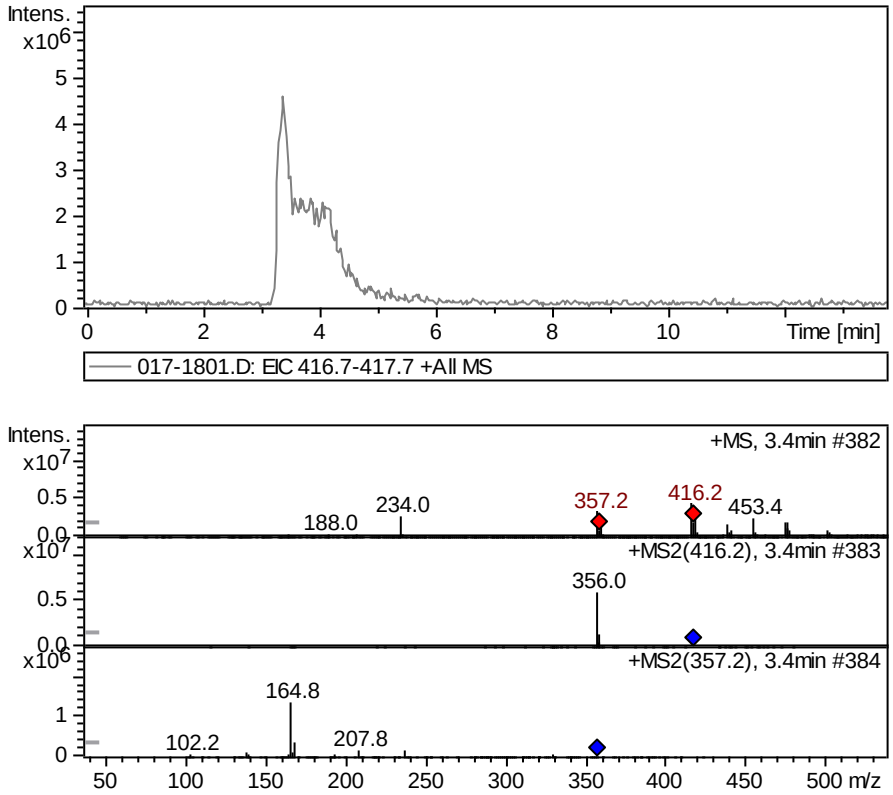
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample : RAD-341 DMSO			Date	19 Apr 2016 05:54:56
Date Stamp	19 Apr 2016 05:54:56						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-341 18-04-2016\80\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3072	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21296.9258
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

^{13}C NMR (214 MHz, DMSO-d$_6$) δ 165.2, 164.8, 147.5, 147.3, 139.8, 134.9, 129.9, 129.2, 128.6, 127.7, 127.2, 125.5, 123.8, 121.8, 115.5, 112.9, 55.4, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.5, 11.5

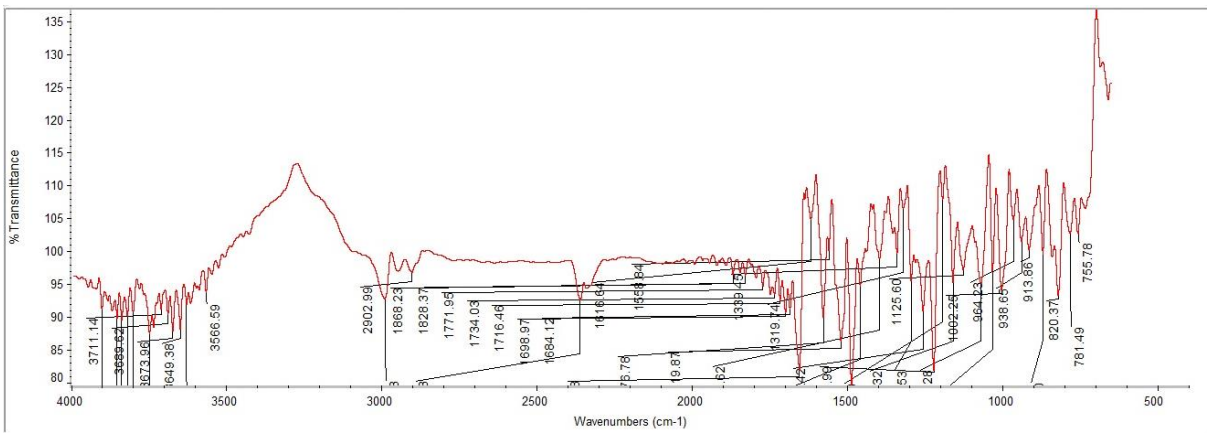




LC/MS



FT-IR



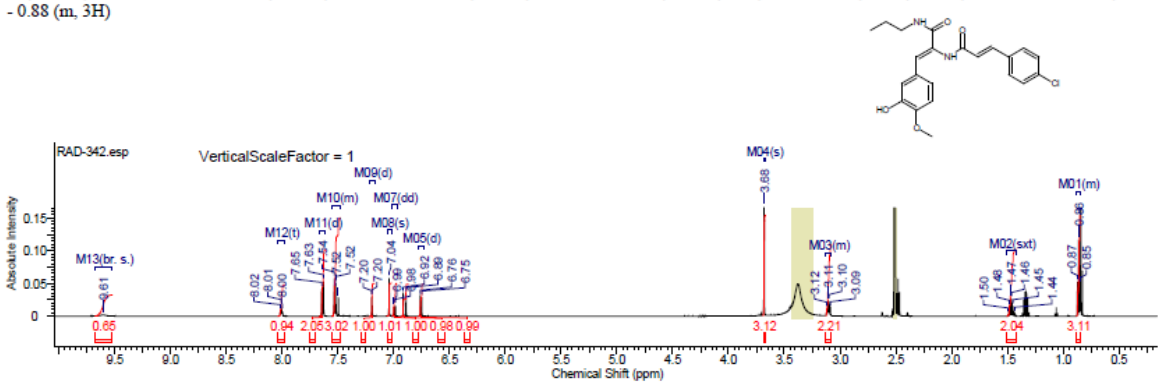
^{1}H NMR

RAD-342

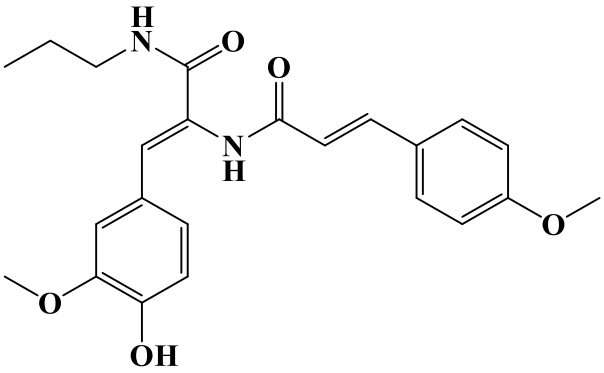
08/11/2016 8:51:48 AM
Dr.Mustafa Sample : RAD-342 DMSO PROTON DMSO (D:\Magdy) nmr 33

Formula $C_{20}H_{19}ClN_2O_4$		*FW* 414.8820					
Acquisition Time (sec)	2.6564	*Comment*	Dr.Mustafa Sample : RAD-342 DMSO PROTON DMSO (D:\Magdy) nmr 33				
Date	18 Jun 2015 16:24:00			*Date Stamp*	18 Jun 2015 16:24:00		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-342 18-06-2015\10\fid					*Frequency (MHz)*	600.15
Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	144.00
SW(cyclical) (Hz)	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.1750	*Spectrum Type*	STANDARD
Sweep Width (Hz)	12335.15	*Temperature (degree C)*	25.000				

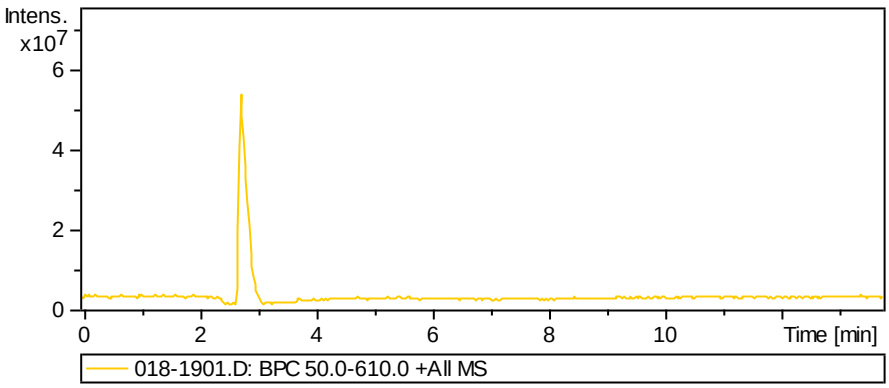
^{1}H NMR (600 MHz, DMSO-d_6) δ 9.61 (br. s., 1H), 8.01 (t, J = 5.83 Hz, 1H), 7.64 (d, J = 8.28 Hz, 2H), 7.48 - 7.56 (m, 3H), 7.20 (d, J = 2.26 Hz, 1H), 7.04 (s, 1H), 6.99 (dd, J = 1.88, 8.28 Hz, 1H), 6.90 (d, J = 16.19 Hz, 1H), 6.76 (d, J = 8.28 Hz, 1H), 3.68 (s, 3H), 3.08 - 3.13 (m, 2H), 1.47 (sxt, J = 7.23 Hz, 2H), 0.85 - 0.88 (m, 3H)

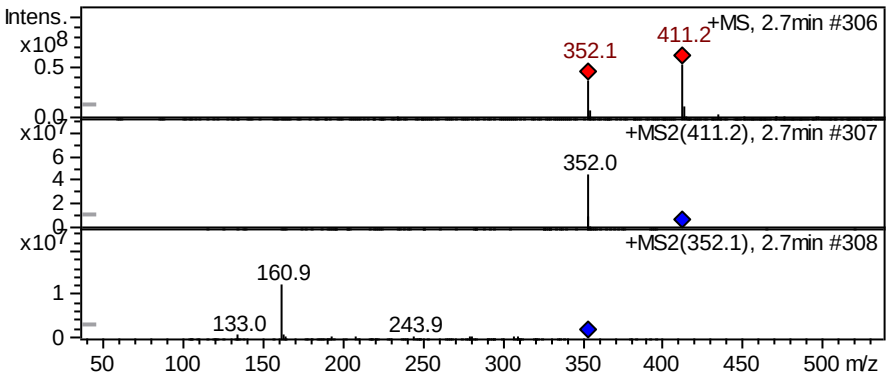


Spectra of (3412)

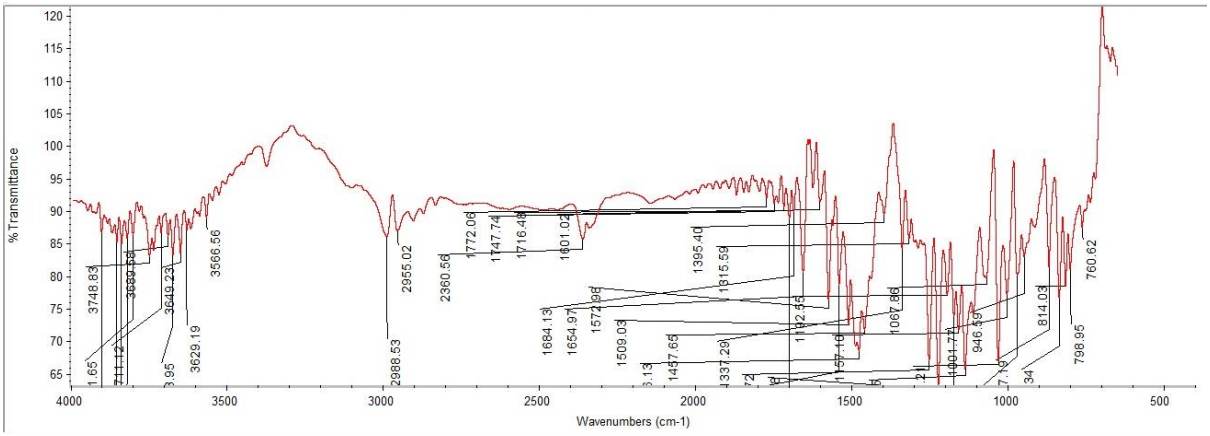


LC/MS





FT-IR



^{1}H NMR

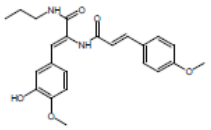
RAD-343

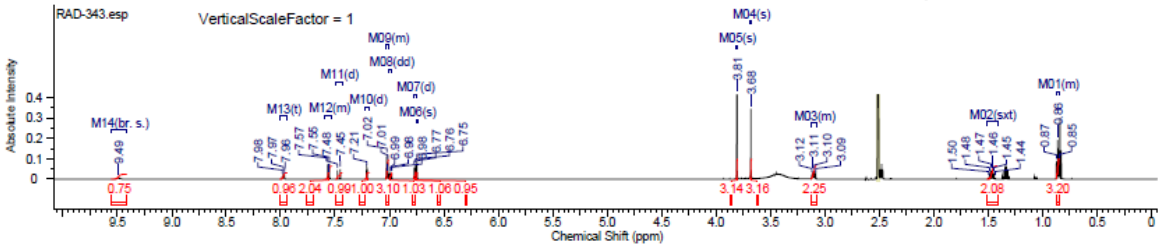
11/10/2016 8:44:34 AM
Dr.Mustafa Sample : RAD-343 DMSO PROTON DMSO (D:\Magdy) nmr 19

Formula $C_{25}H_{26}N_2O_4$	FW	410.4629

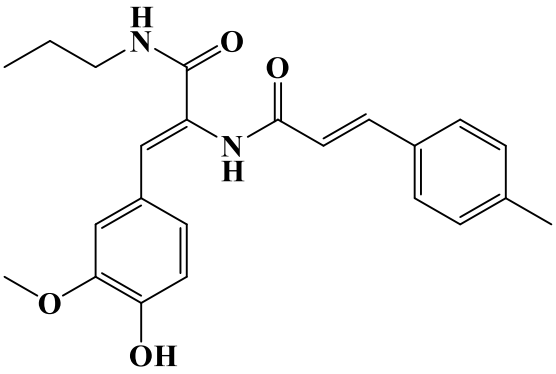
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-343 DMSO PROTON DMSO (D:\Magdy) nmr 19				
Date	18 Jun 2015 15:11:28			Date Stamp	18 Jun 2015 15:11:28		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-343 18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	128.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.49 (br. s., 1H), 7.97 (t, J = 6.02 Hz, 1H), 7.53 - 7.59 (m, 2H), 7.46 (d, J = 15.81 Hz, 1H), 7.21 (d, J = 1.88 Hz, 1H), 7.00 - 7.03 (m, 3H), 6.99 (dd, J = 1.88, 8.28 Hz, 1H), 6.77 (d, J = 6.78 Hz, 1H), 6.75 (s, 1H), 3.81 (s, 3H), 3.68 (s, 3H), 3.08 - 3.13 (m, 2H), 1.47 (sxt, J = 7.30 Hz, 2H), 0.85 - 0.88 (m, 3H)

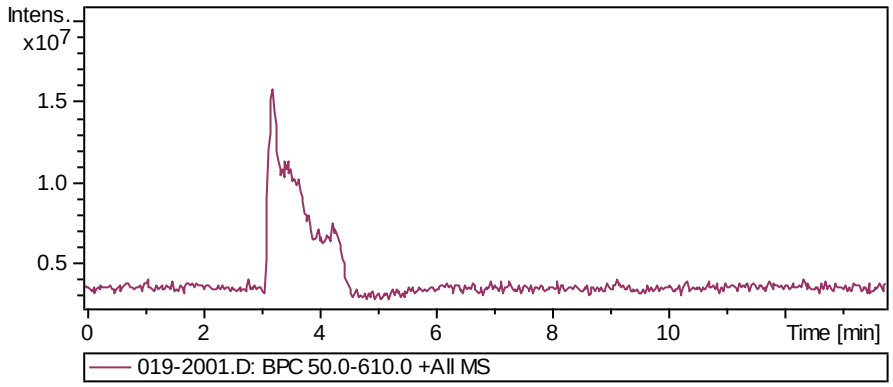


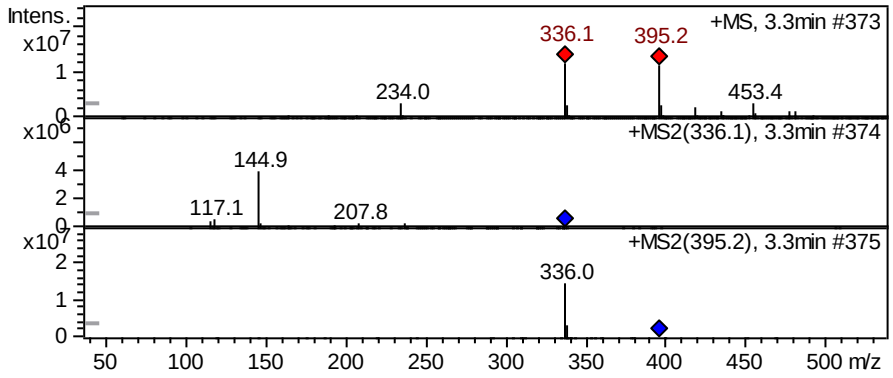


Spectra of (3512)

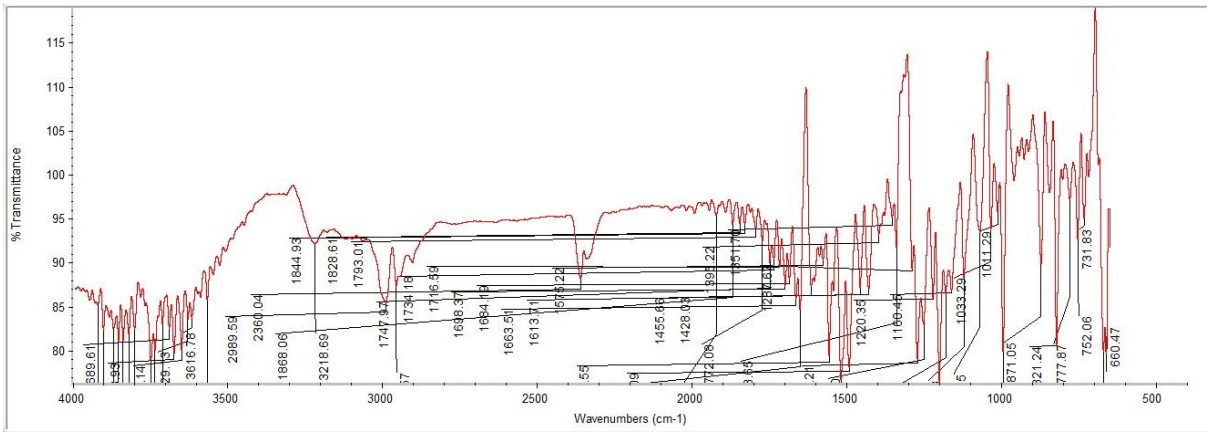


LC/MS





FT-IR



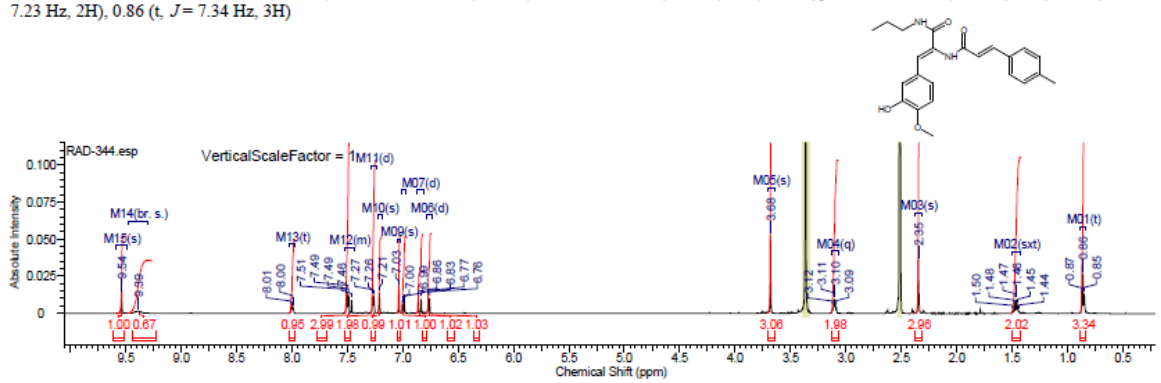
^{1}H NMR

RAD-344

08/11/2016 9:06:10 AM
Dr.Mustafa Sample : RAD-344 DMSO PROTON DMSO (D:\Magdy) nmr 10

Formula $C_{22}H_{26}N_2O_4$	FW	394.4635					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-344 DMSO PROTON DMSO (D:\Magdy) nmr 10				
Date	18 Jun 2015 14:24:32			Date Stamp	18 Jun 2015 14:24:32		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-344 18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	144.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.54 (s, 1H), 9.39 (br. s., 1H), 8.00 (t, J = 5.65 Hz, 1H), 7.44 - 7.53 (m, 3H), 7.27 (d, J = 7.91 Hz, 2H), 7.21 (s, 1H), 7.03 (s, 1H), 6.99 (dd, J = 1.88, 8.28 Hz, 1H), 6.85 (d, J = 15.81 Hz, 1H), 6.76 (d, J = 8.28 Hz, 1H), 3.68 (s, 3H), 3.10 (q, J = 6.65 Hz, 2H), 2.35 (s, 3H), 1.47 (sxt, J = 7.23 Hz, 2H), 0.86 (t, J = 7.34 Hz, 3H)



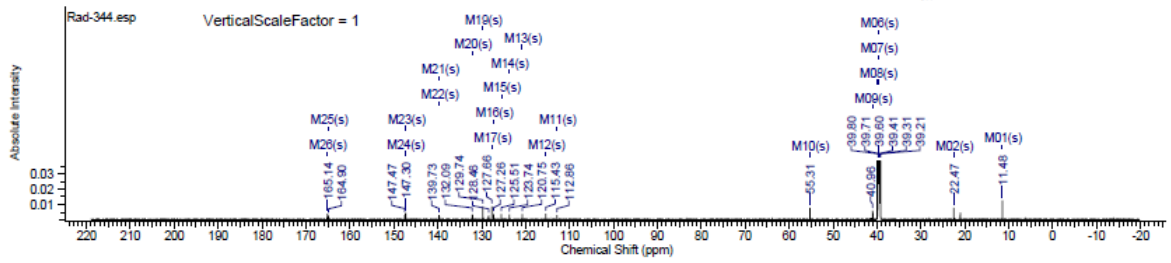
^{13}C NMR

RAD-344

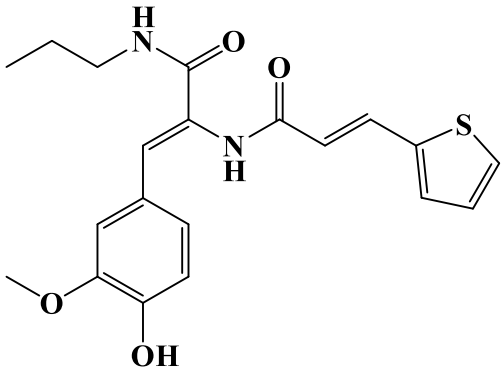
20/09/2016 9:31:55 AM
Dr.Mustafa Sample ; RAD-344 DMSO

Formula $C_{22}H_{26}N_2O_4$	FW	394.4635					
Acquisition Time (sec)	0.8423	Comment	Dr.Mustafa Sample ; RAD-344 DMSO			Date	20 Apr 2016 20:06:08
Date Stamp	20 Apr 2016 20:06:08						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-344 19-04-2016\140\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3500	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21290.6973
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

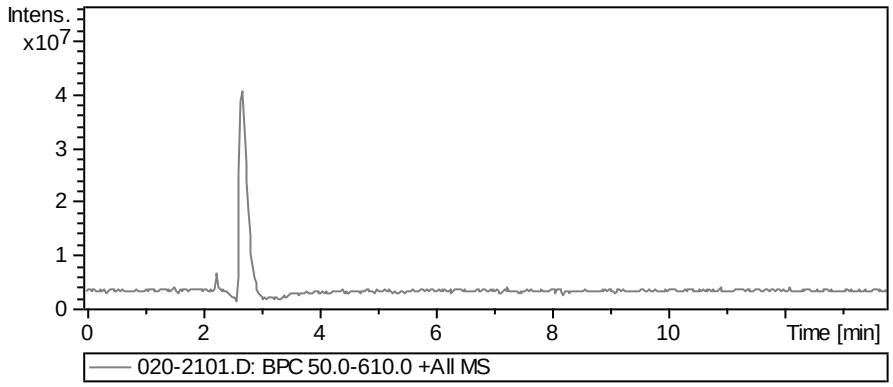
^{13}C NMR (214 MHz, DMSO-d_6) δ 165.1, 164.9, 147.5, 147.3, 139.7, 139.6, 132.1, 129.7, 128.5, 127.7, 127.3, 125.5, 123.7, 120.8, 115.4, 112.9, 55.3, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.5, 11.5

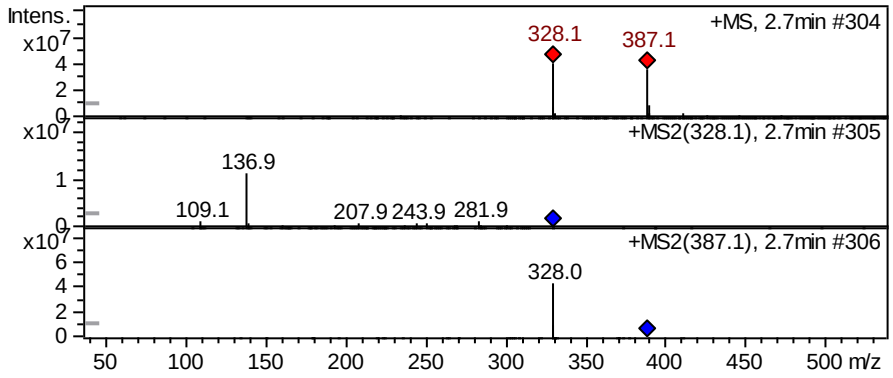


Spectra of (3612)

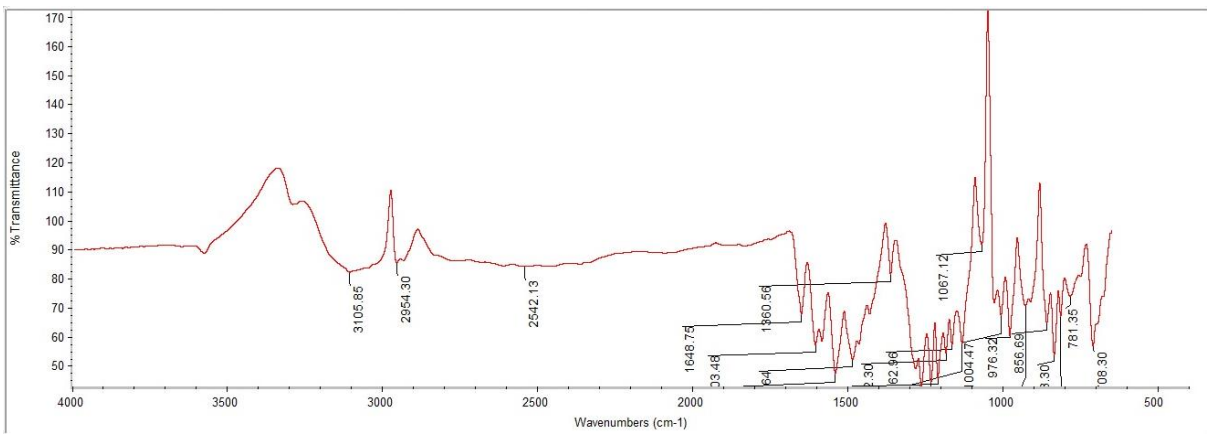


LC/MS





FT-IR



^{1}H NMR

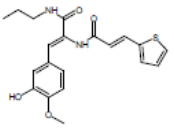
RAD-345

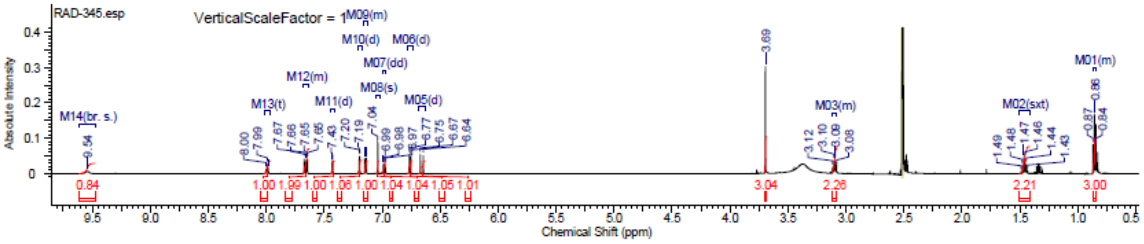
11/10/2016 8:53:39 AM
Dr.Mustafa Sample : RAD-345 DMSO PROTON DMSO (D:\Magdy) nmr 14

Formula $C_{22}H_{22}N_2O_4S$	FW	386.4647

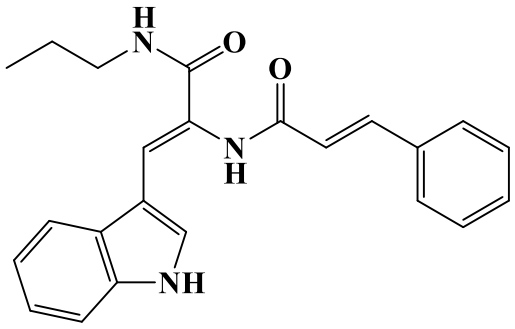
Acquisition Time (sec)	2.6564	*Comment*	Dr.Mustafa Sample : RAD-345 DMSO PROTON DMSO (D:\Magdy) nmr 14				
Date	18 Jun 2015 14:45:52			*Date Stamp*	18 Jun 2015 14:45:52		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-345 18-06-2015\10\fid					*Frequency (MHz)*	600.15
Nucleus	1H	*Number of Transients*	32	*Origin*	spect	*Original Points Count*	32768
Owner	nmr	*Points Count*	32768	*Pulse Sequence*	zg30	*Receiver Gain*	144.00
SW(cyclical) (Hz)	12335.53	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	3706.1750	*Spectrum Type*	STANDARD
Sweep Width (Hz)	12335.15	*Temperature (degree C)*	25.000				

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.54 (br. s., 1H), 7.99 (t, J = 5.83 Hz, 1H), 7.63 - 7.68 (m, 2H), 7.43 (d, J = 3.39 Hz, 1H), 7.19 (d, J = 1.88 Hz, 1H), 7.13 - 7.16 (m, 1H), 7.04 (s, 1H), 6.98 (dd, J = 1.88, 8.28 Hz, 1H), 6.76 (d, J = 7.91 Hz, 1H), 6.66 (d, J = 15.81 Hz, 1H), 3.69 (s, 3H), 3.08 - 3.12 (m, 2H), 1.46 (sxt, J = 7.23 Hz, 2H), 0.84 - 0.87 (m, 3H)

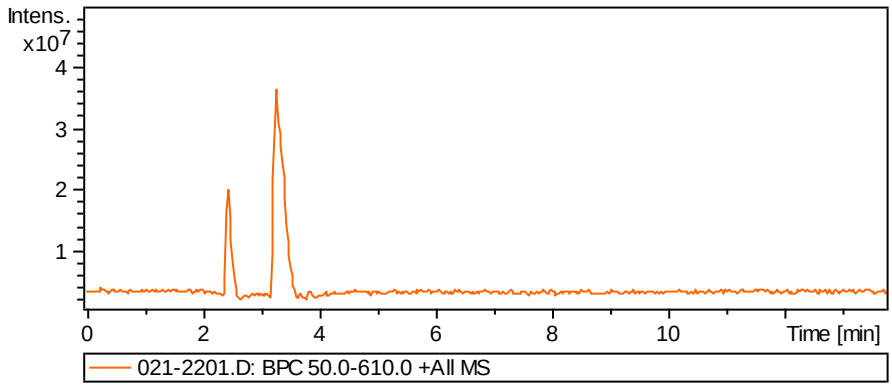


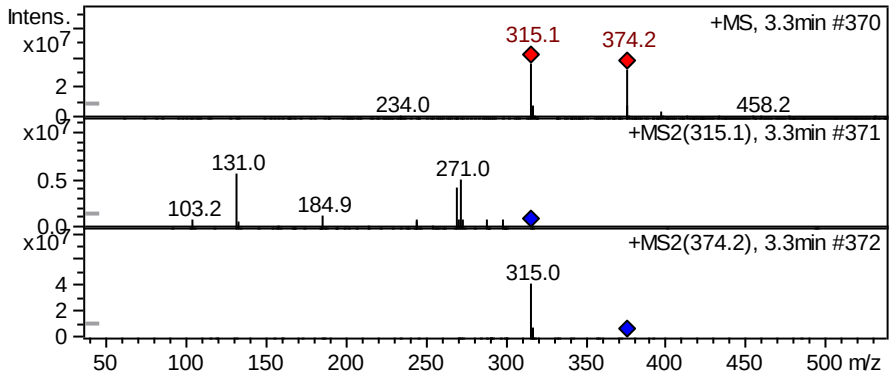


Spectra of (3712)

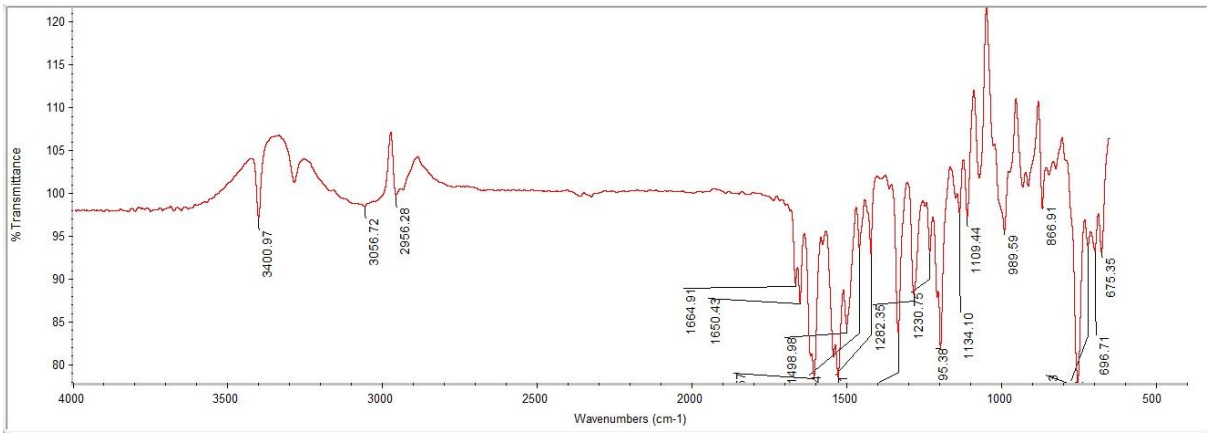


LC/MS





FT-IR



^{1}H NMR

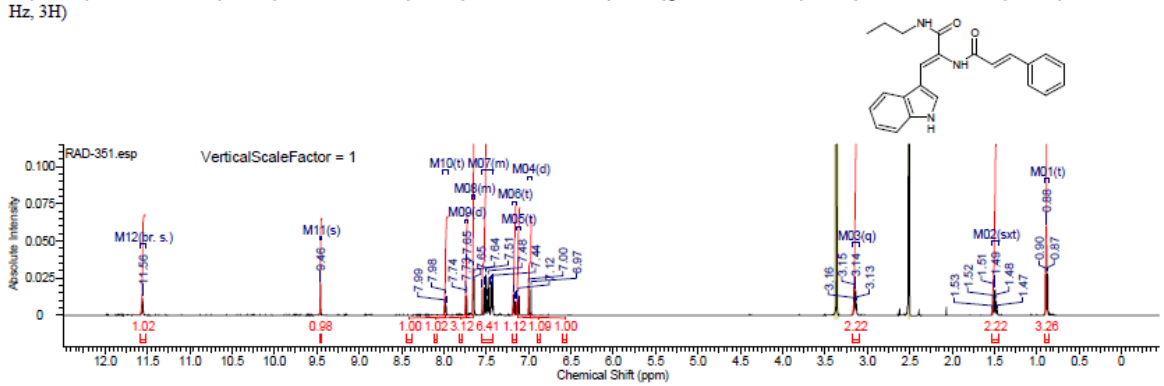
RAD-351

08/11/2016 11:46:25 AM
Dr.Mustafa Sample : RAD-351 DMSO PROTON DMSO (D:\Magdy) nmr 30

Formula $C_{23}H_{23}N_3O_2$	FW	373.4476

Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-351 DMSO PROTON DMSO (D:\Magdy) nmr 30				
Date	18 Jun 2015 16:09:04			Date Stamp	18 Jun 2015 16:09:04		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-351 18-06-2015\10\fid						
Nucleus	1H	Number of Transients	32	Origin	spect	Frequency (MHz)	600.15
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Original Points Count	32768
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Receiver Gain	144.00
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000			Spectrum Type	STANDARD

^{1}H NMR (600 MHz, DMSO-d_6) δ 11.56 (br. s., 1H), 9.46 (s, 1H), 7.98 (t, J = 5.83 Hz, 1H), 7.74 (d, J = 7.91 Hz, 1H), 7.63 - 7.67 (m, 3H), 7.42 - 7.55 (m, 5H), 7.17 (t, J = 7.53 Hz, 1H), 7.12 (t, J = 7.53 Hz, 1H), 6.98 (d, J = 15.81 Hz, 1H), 3.14 (q, J = 6.53 Hz, 2H), 1.50 (sxt, J = 7.23 Hz, 2H), 0.88 (t, J = 7.34 Hz, 3H)



^{13}C NMR

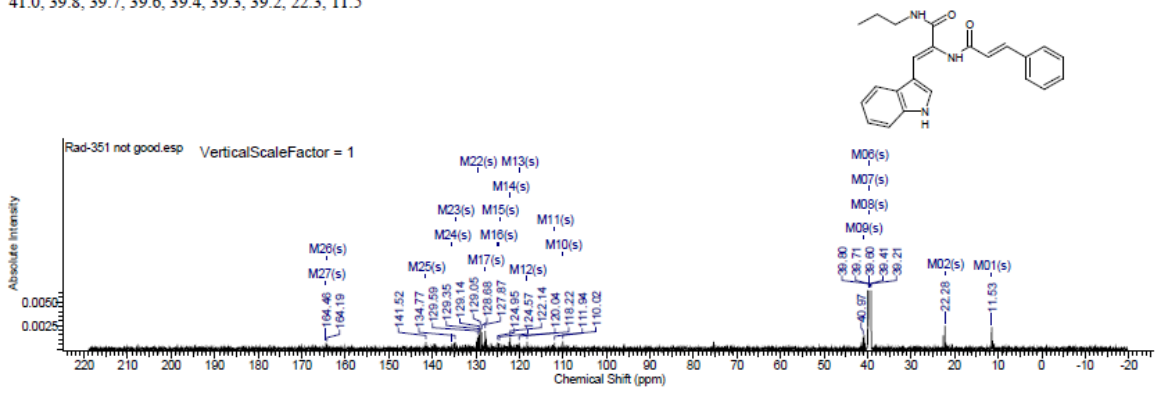
RAD-351

25/09/2016 3:26:58 PM
Dr.Moustafa Sample : RAD-351 DMSO

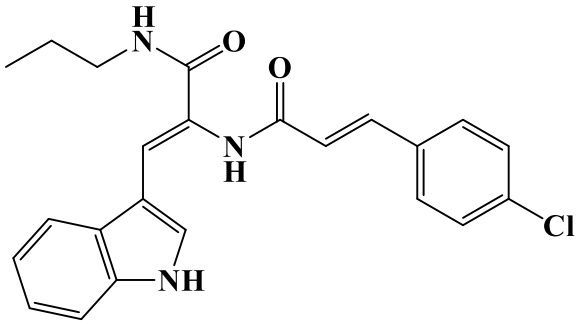
Formula $C_{23}H_{23}N_3O_2$	FW	373.4476

Acquisition Time (sec)	0.6423	Comment	Dr.Moustafa Sample : RAD-351 DMSO			Date	22 Apr 2016 15:05:20
Date Stamp	22 Apr 2016 15:05:20						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-351 21-04-2016\30\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	12288	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21293.8125
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

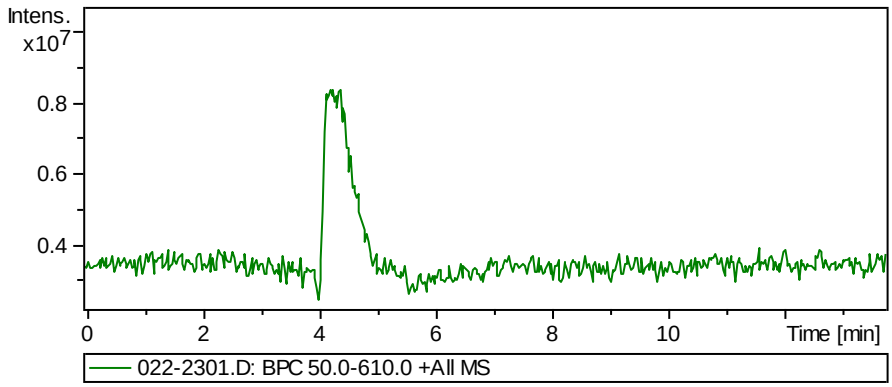
^{13}C NMR (214 MHz, DMSO-d_6) δ 164.5, 164.2, 141.5, 135.5, 134.8, 129.6, 129.3, 129.1, 129.0, 128.7, 127.9, 124.9, 124.6, 122.1, 120.0, 118.2, 111.9, 110.0, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.3, 11.5

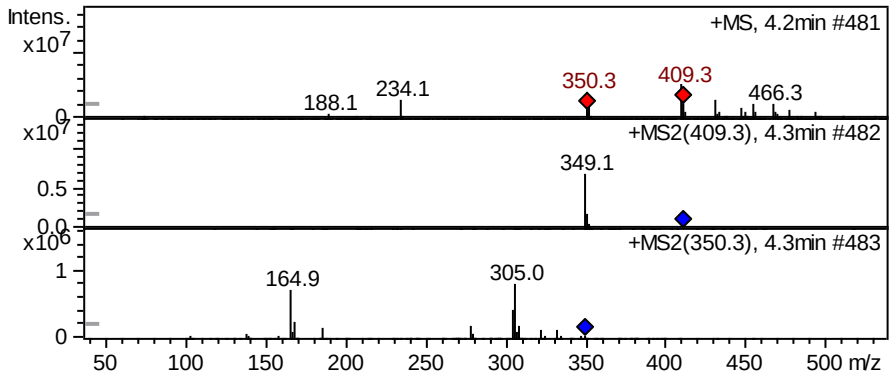


Spectra of (3812)

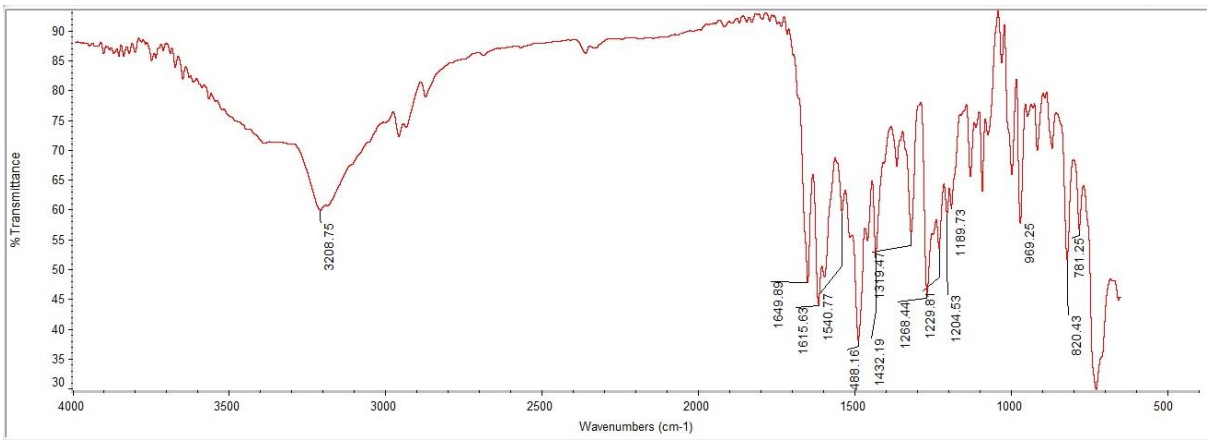


LC/MS





FT-IR



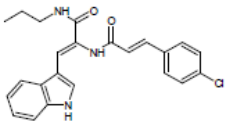
^{1}H NMR

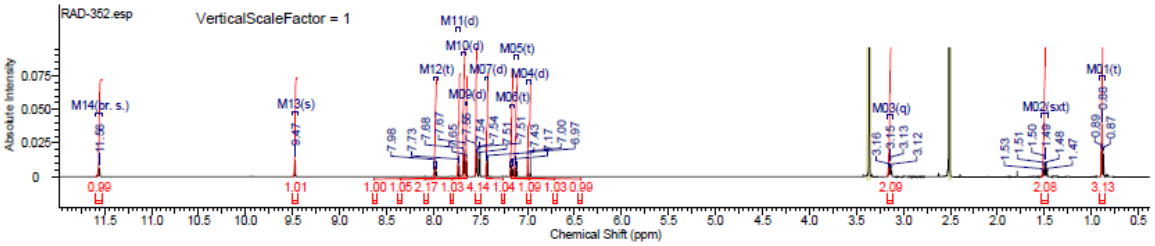
RAD-352

08/11/2016 11:51:59 AM
Dr.Mustafa Sample : RAD-352 DMSO PROTON DMSO (D:\Magdy) nmr 35

Formula $C_{22}H_{20}ClN_3O_2$		FW 407.8927			
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-352 DMSO PROTON DMSO (D:\Magdy) nmr 35		
Date	18 Jun 2015 16:34:40	Date Stamp	18 Jun 2015 16:34:40		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-352 18-06-2015\10\fid			Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Original Points Count	32768
Owner	nmr	Points Count	32768	Receiver Gain	144.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000		

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 11.56 (br. s., 1H), 9.47 (s, 1H), 7.98 (t, J = 5.83 Hz, 1H), 7.73 (d, J = 7.91 Hz, 1H), 7.68 (d, J = 8.66 Hz, 2H), 7.65 (d, J = 2.63 Hz, 1H), 7.50 - 7.56 (m, 3H), 7.43 (d, J = 7.91 Hz, 1H), 7.17 (t, J = 7.15 Hz, 1H), 7.12 (t, J = 7.34 Hz, 1H), 6.98 (d, J = 15.81 Hz, 1H), 3.14 (q, J = 6.53 Hz, 2H), 1.50 (sxt, J = 7.30 Hz, 2H), 0.88 (t, J = 7.53 Hz, 3H)





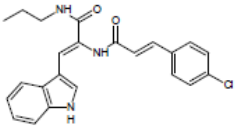
^{13}C NMR

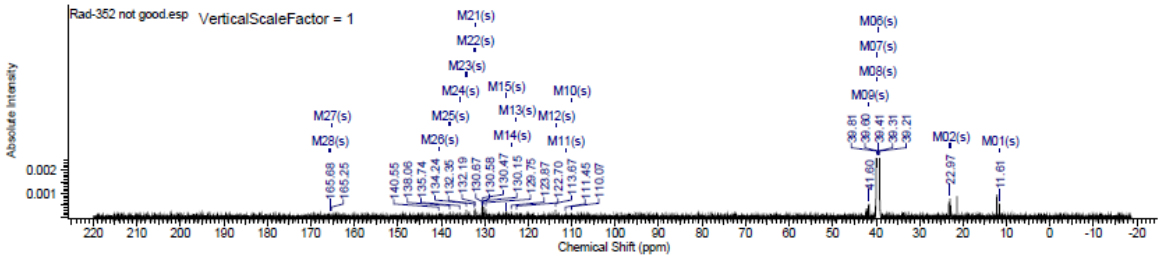
RAD-352

25/09/2016 3:33:14 PM
Dr.Moustafa Sample : RAD-352 DMSO

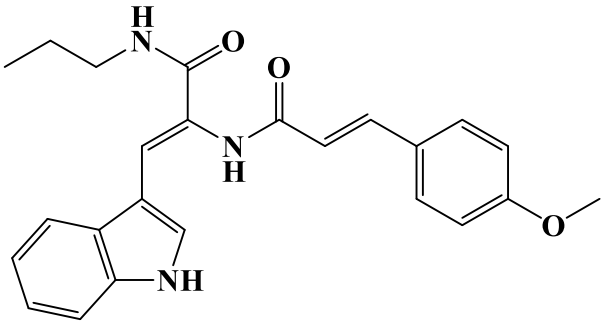
Formula $C_{22}H_{20}ClN_3O_2$		FW 407.8927					
Acquisition Time (sec)	0.6423	Comment	Dr.Moustafa Sample : RAD-352 DMSO			Date	21 Apr 2016 11:25:36
Date Stamp	21 Apr 2016 11:25:36						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-352 21-04-2016\10\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	12288	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21516.4648
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	24.999		

^{13}C NMR (214 MHz, DMSO-d$_6$) δ 165.7, 165.3, 140.5, 138.1, 135.7, 134.2, 132.3, 132.2, 130.7, 130.6, 130.5, 130.1, 129.8, 125.1, 123.9, 122.7, 113.7, 111.5, 110.1, 41.6, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 23.0, 11.6

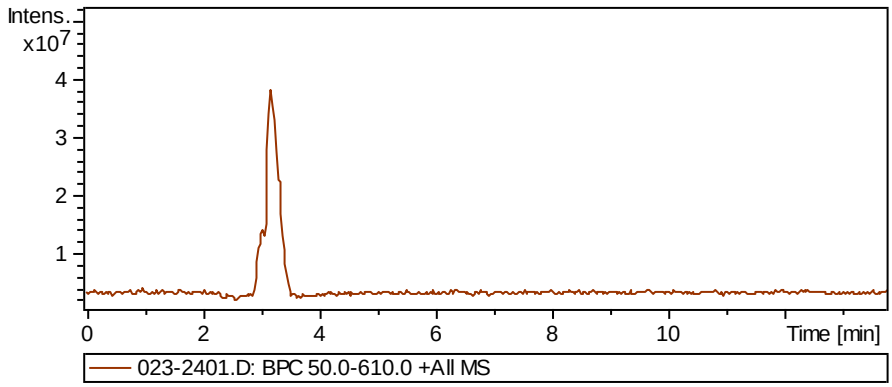


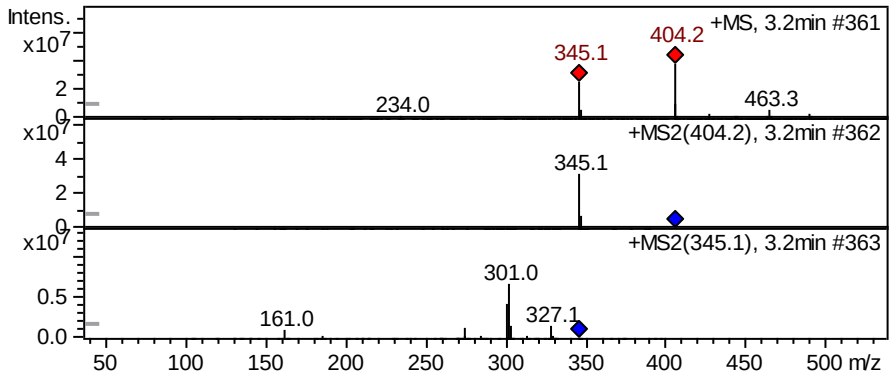


Spectra of (3912)

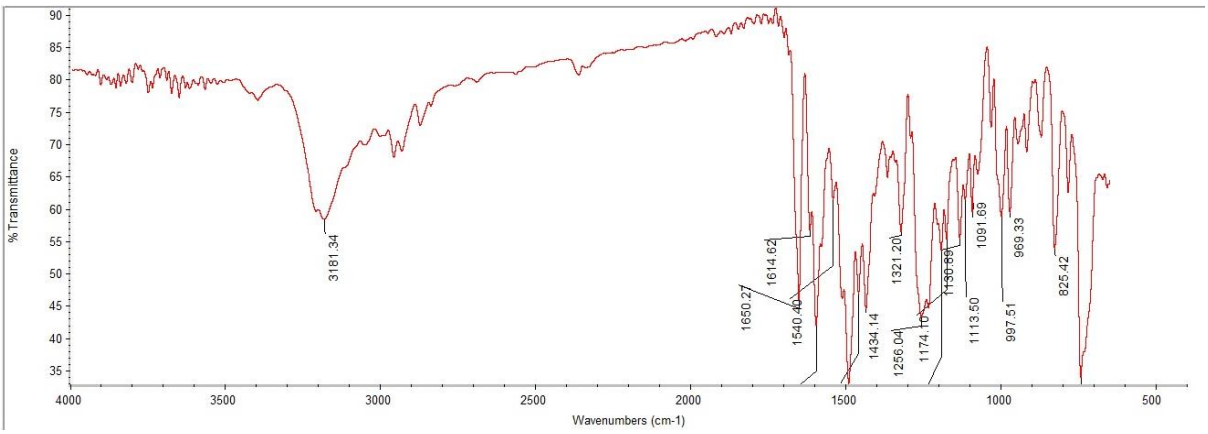


LC/MS





FT-IR



^{1}H NMR

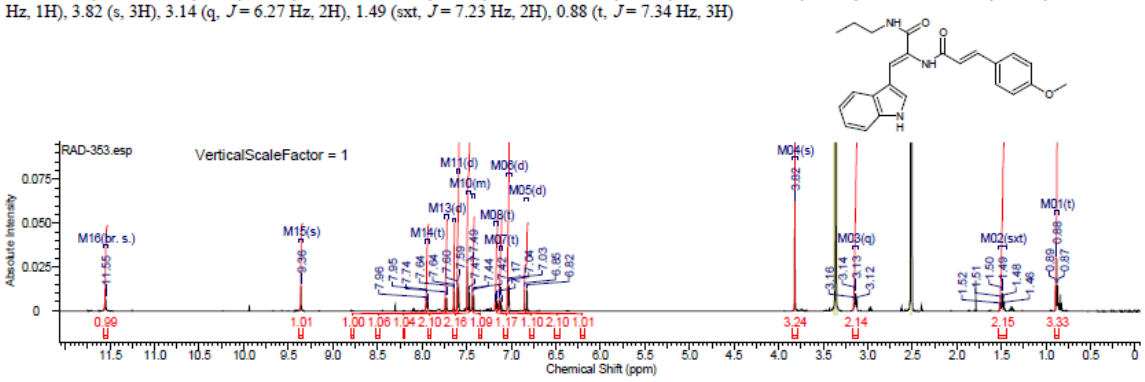
RAD-353

09/11/2016 7:58:16 AM
Dr.Mustafa Sample : RAD-353 DMSO PROTON DMSO {D:\Magdy} nmr 28

Formula $C_{21}H_{16}N_2O_3$	FW	403.4736

Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-353 DMSO PROTON DMSO {D:\Magdy} nmr 28				
Date	18 Jun 2015 15:58:24			Date Stamp	18 Jun 2015 15:58:24		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-353 18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	144.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d_6) δ 11.55 (br. s., 1H), 9.36 (s, 1H), 7.95 (t, J = 5.83 Hz, 1H), 7.73 (d, J = 7.91 Hz, 1H), 7.64 (d, J = 2.26 Hz, 1H), 7.60 (d, J = 8.66 Hz, 2H), 7.46 - 7.50 (m, 2H), 7.43 (d, J = 7.91 Hz, 1H), 7.17 (t, J = 7.53 Hz, 1H), 7.12 (t, J = 7.53 Hz, 1H), 7.03 (d, J = 8.66 Hz, 2H), 6.84 (d, J = 15.81 Hz, 1H), 3.82 (s, 3H), 3.14 (q, J = 6.27 Hz, 2H), 1.49 (sxt, J = 7.23 Hz, 2H), 0.88 (t, J = 7.34 Hz, 3H)



^{13}C NMR

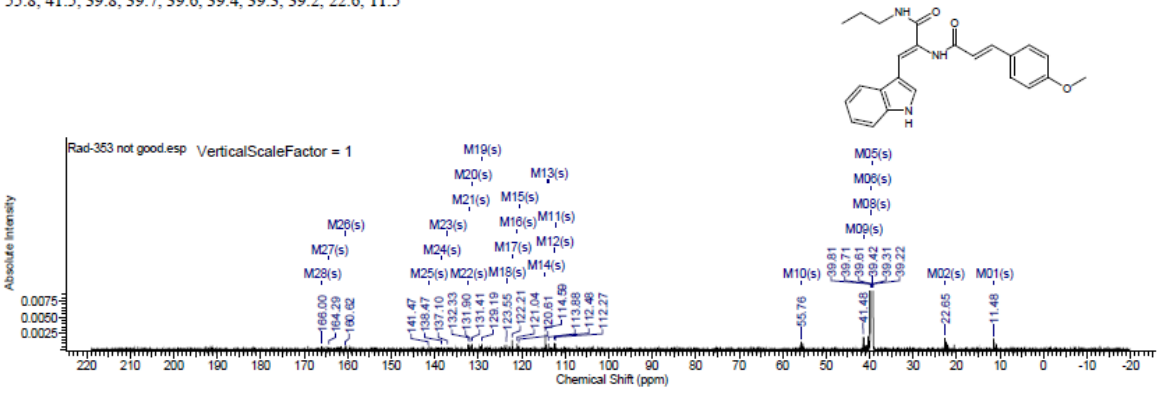
RAD-353

25/09/2016 3:40:24 PM
Dr.Moustafa Sample : RAD-353 DMSO

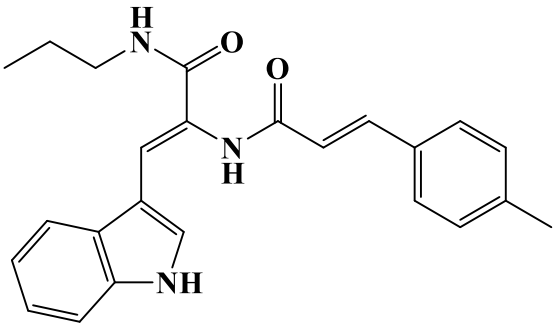
Formula $C_{21}H_{16}N_2O_3$	FW	403.4736

Acquisition Time (sec)	0.6423	Comment	Dr.Moustafa Sample : RAD-353 DMSO			Date	23 Apr 2016 09:43:12
Date Stamp	23 Apr 2016 09:43:12						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-353 21-04-2016\50\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	12288	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21287.5840
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.002		

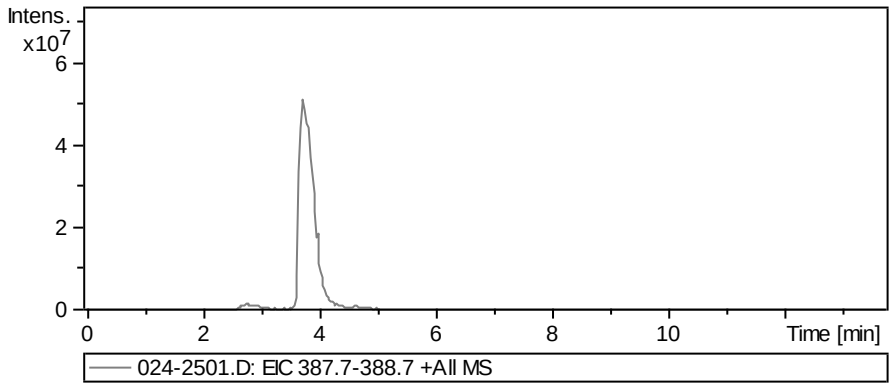
^{13}C NMR (214 MHz, DMSO-d_6) δ 166.0, 164.3, 160.6, 141.5, 138.5, 137.1, 132.3, 131.9, 131.4, 129.2, 123.5, 122.2, 121.0, 120.6, 114.6, 113.9, 112.5, 112.3, 55.8, 41.5, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.6, 11.5

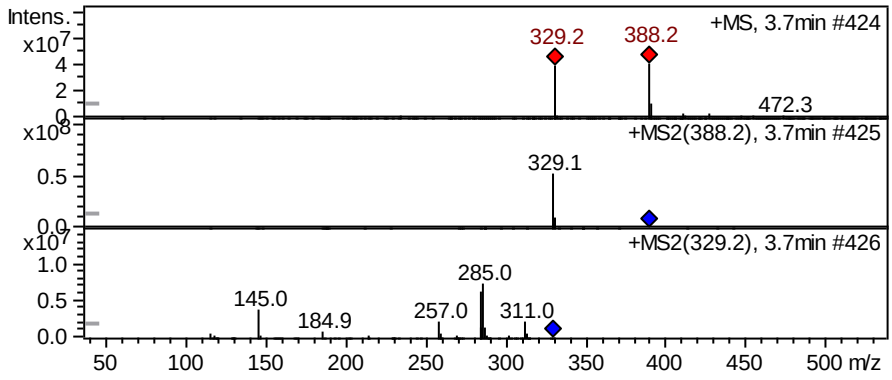


Spectra of (4012)

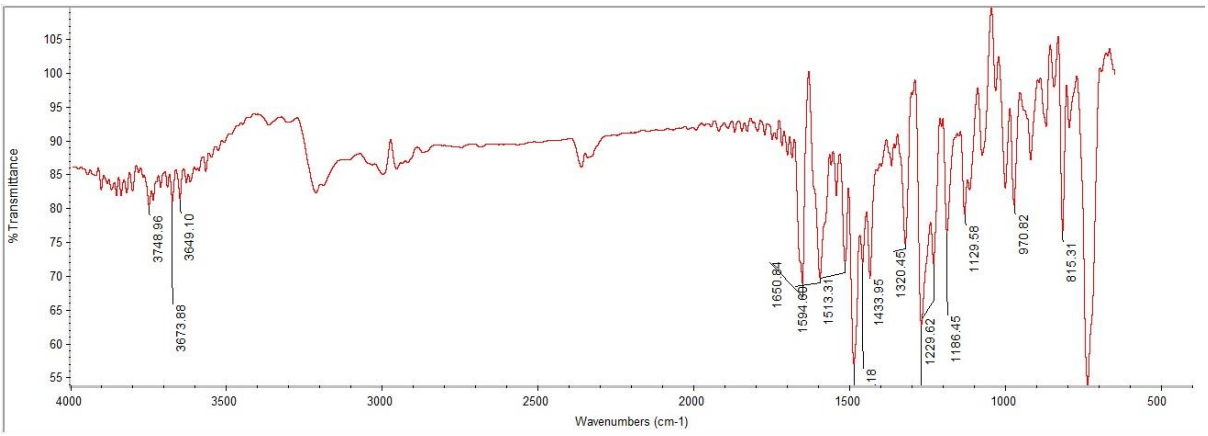


LC/MS





FT-IR



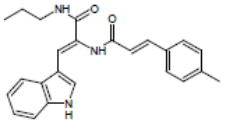
^{1}H NMR

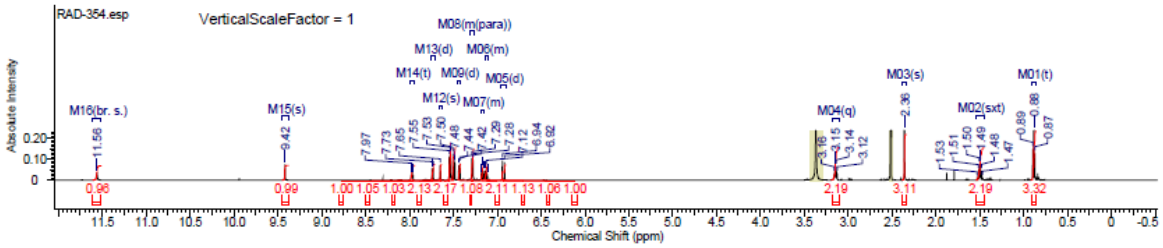
RAD-354

09/11/2016 8:10:30 AM
Dr.Mustafa Sample : RAD-354 DMSO PROTON DMSO (D:\Magdy) nmr 29

Formula $C_{21}H_{21}N_3O_2$	FW	387.4742					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-354 DMSO PROTON DMSO (D:\Magdy) nmr 29				
Date	18 Jun 2015 16:04:48			Date Stamp	18 Jun 2015 16:04:48		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-354_18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	114.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 11.56 (br. s., 1H), 9.42 (s, 1H), 7.97 (t, J = 5.83 Hz, 1H), 7.73 (d, J = 7.91 Hz, 1H), 7.65 (s, 1H), 7.52 - 7.56 (m, J = 7.91 Hz, 2H), 7.47 - 7.52 (m, 2H), 7.43 (d, J = 7.91 Hz, 1H), 7.26 - 7.30 (m, J = 7.91 Hz, 2H), 7.15 - 7.18 (m, 1H), 7.11 - 7.14 (m, 1H), 6.93 (d, J = 15.81 Hz, 1H), 3.14 (q, J = 6.40 Hz, 2H), 2.36 (s, 3H), 1.50 (sxt, J = 7.30 Hz, 2H), 0.88 (t, J = 7.53 Hz, 3H)





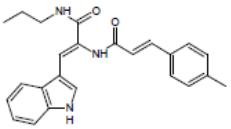
^{13}C NMR

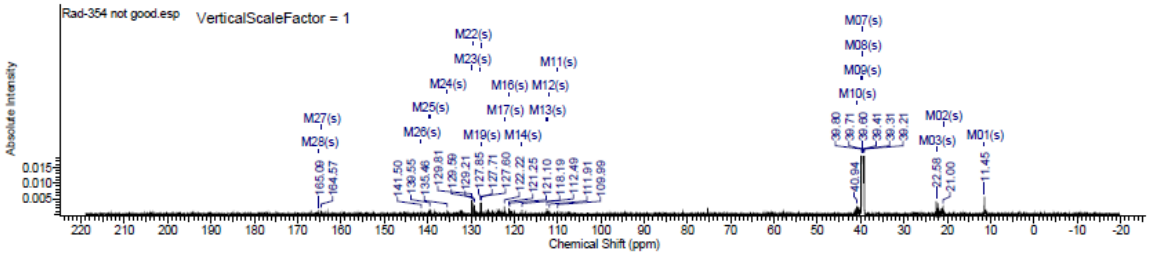
RAD-354

25/09/2016 3:51:57 PM
Dr.Mostafa Sample ; RAD-354 DMSO

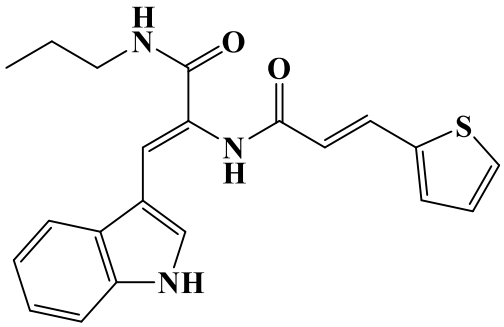
Formula $C_{21}H_{21}N_3O_2$	FW	387.4742					
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-354 DMSO			Date	19 Apr 2016 17:45:20
Date Stamp	19 Apr 2016 17:45:20						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-354_19-04-2016\20\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3500	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21289.1406
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

^{13}C NMR (214 MHz, DMSO-d$_6$) δ 165.1, 164.6, 141.5, 139.6, 135.5, 129.8, 129.6, 129.2, 127.9, 127.7, 127.6, 122.2, 121.3, 121.1, 118.2, 112.5, 111.9, 110.0, 40.9, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.6, 21.0, 11.5

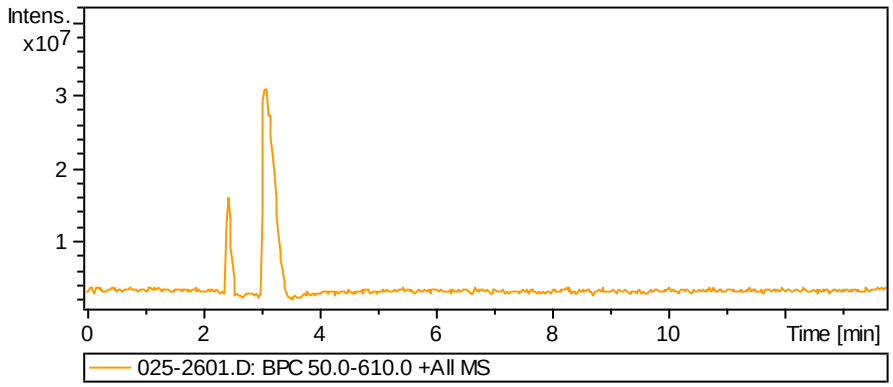


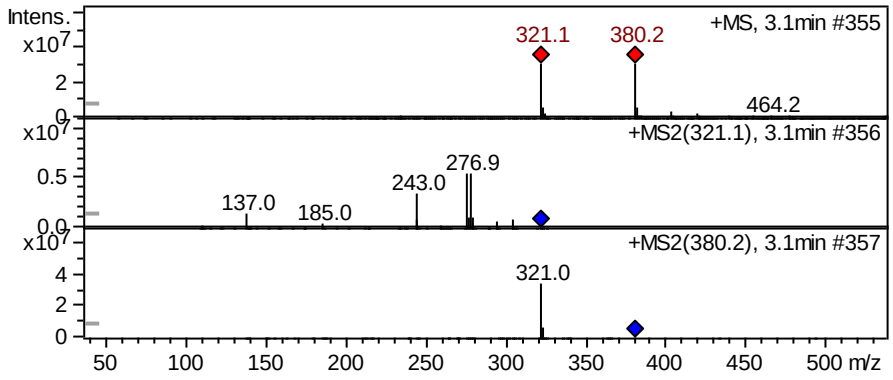


Spectra of (4112)

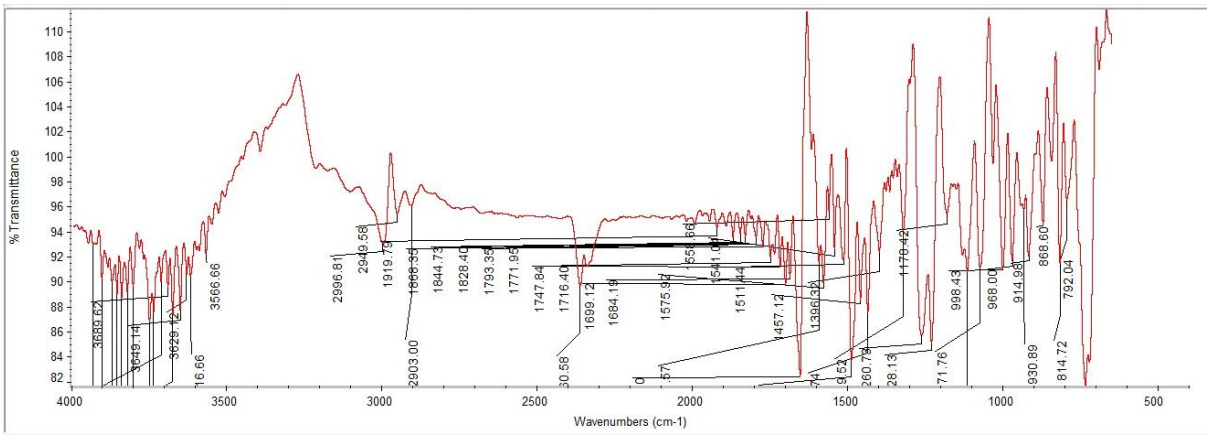


LC/MS





FT-IR



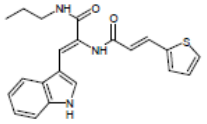
^{1}H NMR

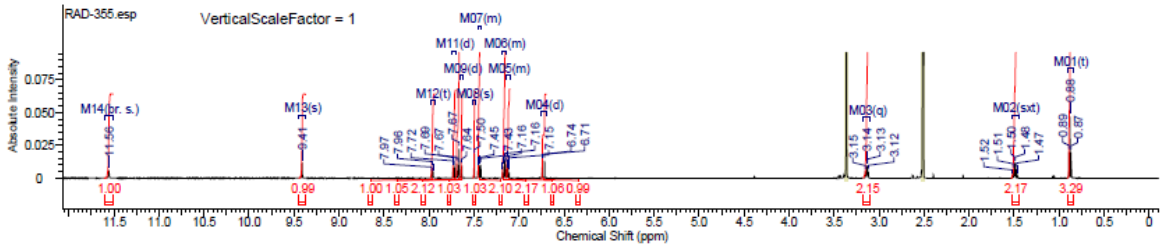
RAD-355

09/11/2016 8:15:32 AM
Dr.Mustafa Sample : RAD-355 DMSO PROTON DMSO (D:\Magdy) nmr 27

Formula $C_{24}H_{24}N_2O_3S$	FW	379.4753					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-355 DMSO PROTON DMSO (D:\Magdy) nmr 27				
Date	18 Jun 2015 15:54:08			Date Stamp	18 Jun 2015 15:54:08		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-355_18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	161.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 11.56 (br. s., 1H), 9.41 (s, 1H), 7.96 (t, J = 5.83 Hz, 1H), 7.72 (d, J = 7.91 Hz, 1H), 7.65 - 7.70 (m, 2H), 7.64 (d, J = 1.88 Hz, 1H), 7.50 (s, 1H), 7.42 - 7.46 (m, 2H), 7.14 - 7.19 (m, 2H), 7.10 - 7.14 (m, 1H), 6.73 (d, J = 15.43 Hz, 1H), 3.13 (q, J = 6.40 Hz, 2H), 1.49 (sxt, J = 7.23 Hz, 2H), 0.88 (t, J = 7.53 Hz, 3H)





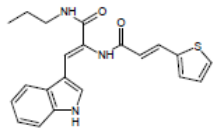
^{13}C NMR

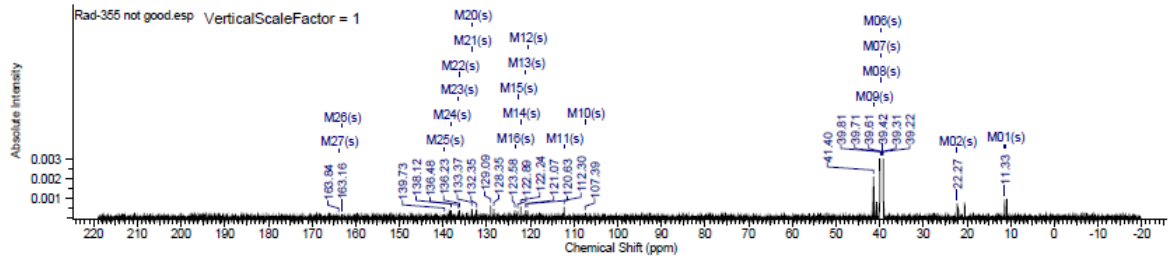
RAD-355

25/09/2016 3:57:30 PM
Dr.Moustafa Sample : RAD-355 DMSO

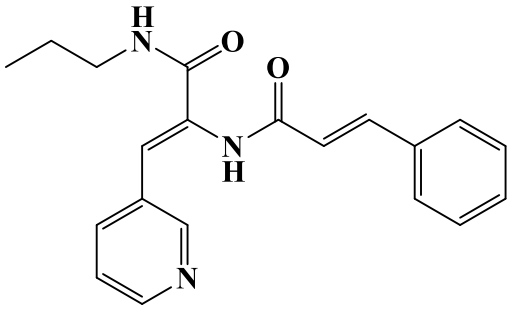
Formula $C_{24}H_{24}N_2O_3S$	FW	379.4753					
Acquisition Time (sec)	0.6423	Comment	Dr.Moustafa Sample : RAD-355 DMSO			Date	23 Apr 2016 00:24:16
Date Stamp	23 Apr 2016 00:24:16						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-355_21-04-2016\40\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	12288	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21292.2539
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

^{13}C NMR (214 MHz, DMSO-d$_6$) δ 163.8, 163.2, 139.7, 138.1, 136.5, 136.2, 133.4, 133.3, 132.4, 129.1, 128.3, 123.6, 122.9, 122.2, 121.1, 120.6, 112.3, 107.4, 41.4, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.3, 11.3

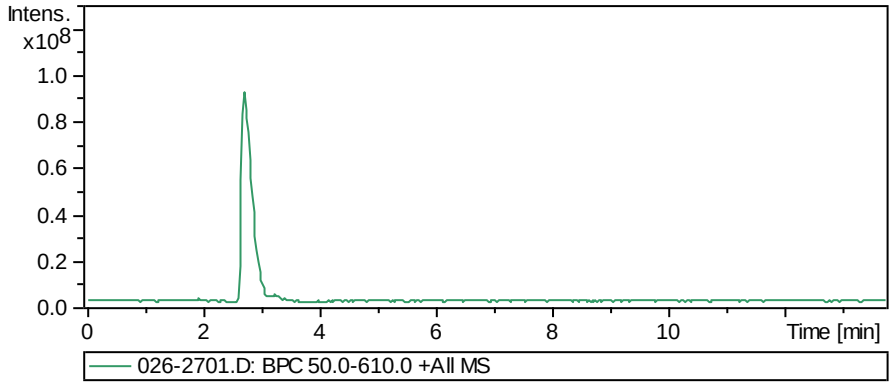


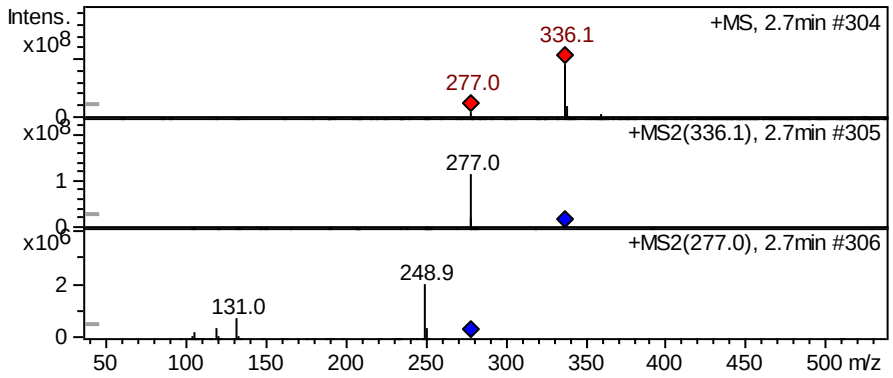


Spectra of (4212)

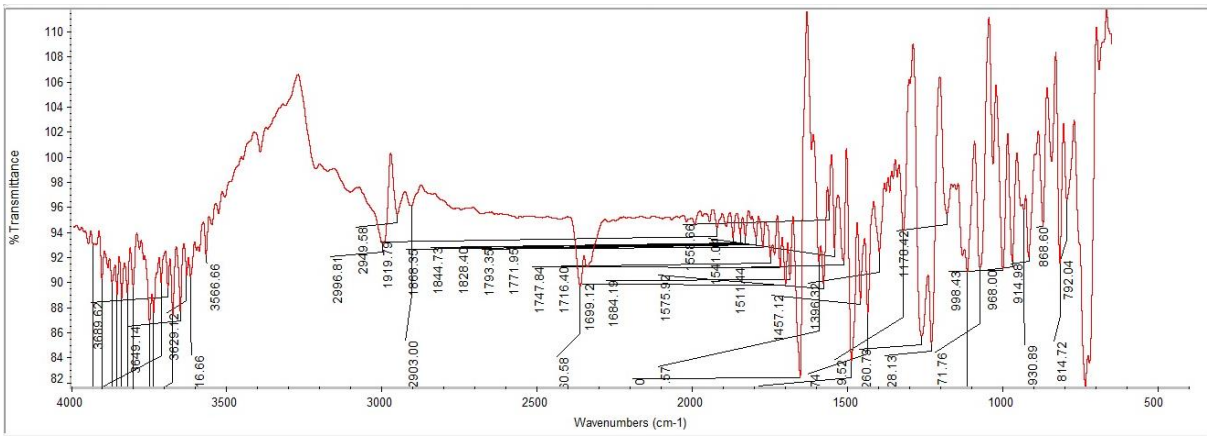


LC/MS





FT-IR



^{1}H NMR

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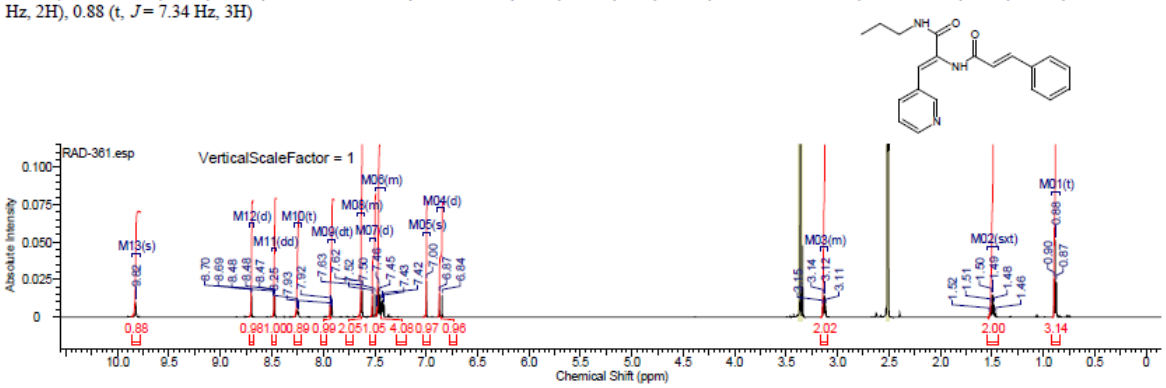
RAD-361

09/11/2016 8:21:08 AM
Dr.Mustafa Sample : RAD-361 DMSO PROTON DMSO {D:\Magdy} nmr 31

Formula $C_{20}H_{17}N_3O_3$	FW	335.3996

Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-361 DMSO PROTON DMSO {D:\Magdy} nmr 31				
Date	18 Jun 2015 16:15:28			Date Stamp	18 Jun 2015 16:15:28		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-361_18-06-2015\10\fid						
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	144.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.82 (s, 1H), 8.70 (d, *J* = 2.26 Hz, 1H), 8.47 (dd, *J* = 1.69, 4.71 Hz, 1H), 8.25 (t, *J* = 5.65 Hz, 1H), 7.92 (td, *J* = 1.74, 8.19 Hz, 1H), 7.60 - 7.66 (m, 2H), 7.51 (d, *J* = 15.81 Hz, 1H), 7.39 - 7.49 (m, 4H), 7.00 (s, 1H), 6.86 (d, *J* = 16.19 Hz, 1H), 3.09 - 3.17 (m, 2H), 1.49 (sxt, *J* = 7.30 Hz, 2H), 0.88 (t, *J* = 7.34 Hz, 3H)



^{13}C NMR

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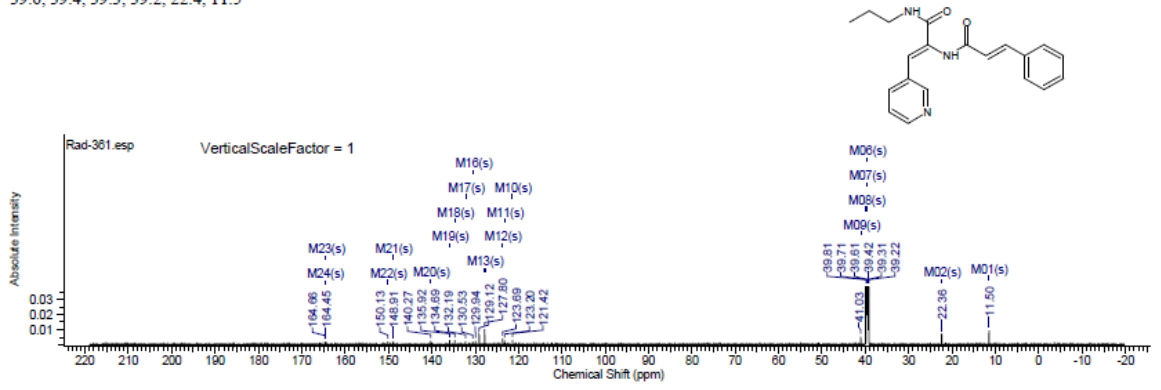
RAD-361

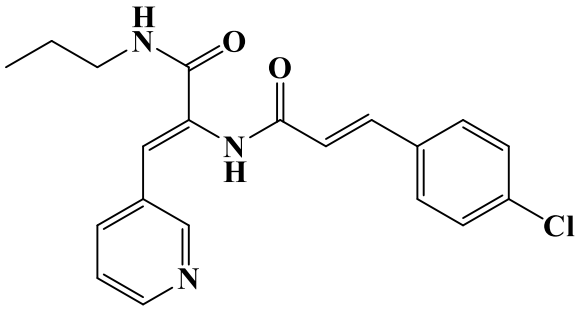
20/09/2016 9:41:55 AM
Dr.Mostafa Sample : RAD-361 DMSO

Formula $C_{20}H_{17}N_3O_3$	FW	335.3996

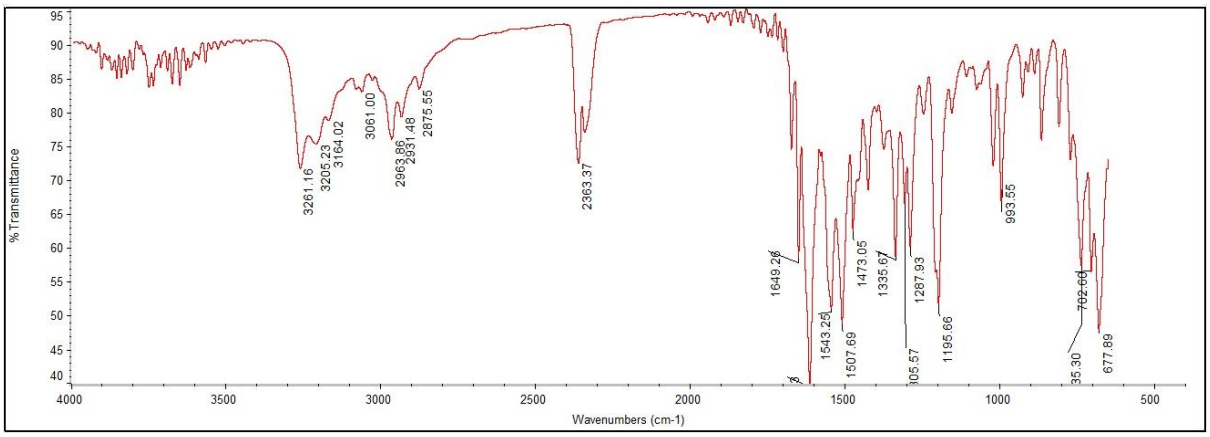
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample : RAD-361 DMSO			Date	19 Apr 2016 11:08:32
Date Stamp	19 Apr 2016 11:08:32						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-361_18-04-2016\130\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	1320	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21289.1406
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.002		

^{13}C NMR (214 MHz, DMSO-d$_6$) δ 164.7, 164.5, 150.1, 148.9, 140.3, 135.9, 134.7, 132.2, 130.5, 129.9, 129.1, 127.8, 123.7, 123.2, 121.4, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 11.5





FT-IR



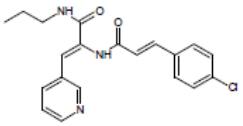
^{1}H NMR

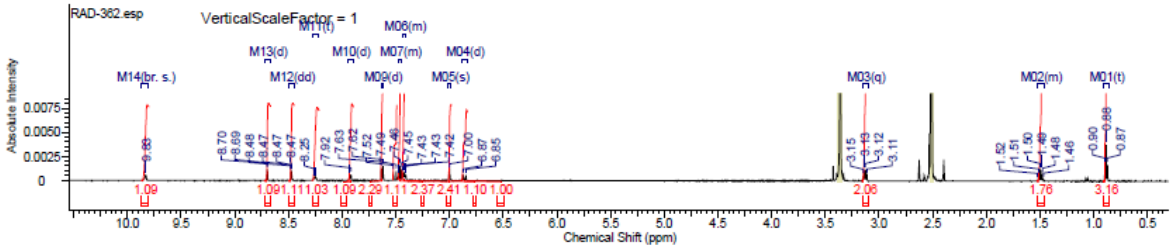
RAD-362

09/11/2016 8:30:38 AM
Dr.Mustafa Sample : RAD-362 DMSO PROTON DMSO (D:\Magdy) nmr 12

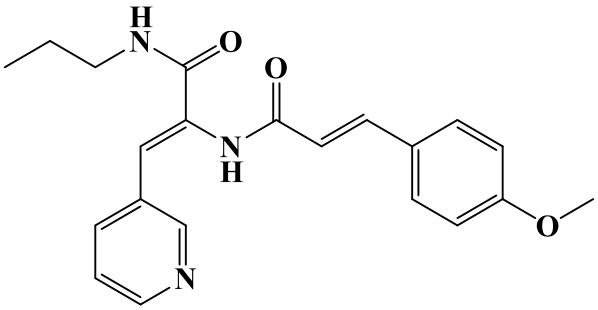
Formula $C_{20}H_{16}ClN_3O_2$		*FW* 369.8447			
Acquisition Time (sec) 2.6564	*Comment* Dr.Mustafa Sample : RAD-362 DMSO PROTON DMSO (D:\Magdy) nmr 12				
Date 18 Jun 2015 14:35:12	*Date Stamp* 18 Jun 2015 14:35:12				
File Name E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-362 18-06-2015\10\fid				*Frequency (MHz)*	600.15
Nucleus 1H	*Number of Transients* 32	*Origin* spect		*Original Points Count*	32768
Owner nmr	*Points Count* 32768	*Pulse Sequence* zg30		*Receiver Gain*	181.00
SW(cyclical) (Hz) 12335.53	*Solvent* DMSO-d6	*Spectrum Offset (Hz)*	3706.1750	*Spectrum Type*	STANDARD
Sweep Width (Hz) 12335.15	*Temperature (degree C)* 25.000				

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.83 (br. s., 1H), 8.70 (d, J = 2.26 Hz, 1H), 8.47 (dd, J = 1.69, 4.71 Hz, 1H), 8.25 (t, J = 5.46 Hz, 1H), 7.92 (d, J = 7.91 Hz, 1H), 7.63 (d, J = 7.15 Hz, 2H), 7.51 (d, J = 15.81 Hz, 1H), 7.44 - 7.48 (m, 2H), 7.40 - 7.44 (m, 2H), 7.00 (s, 1H), 6.86 (d, J = 15.81 Hz, 1H), 3.13 (q, J = 6.53 Hz, 2H), 1.46 - 1.53 (m, 1H), 0.88 (t, J = 7.34 Hz, 3H)

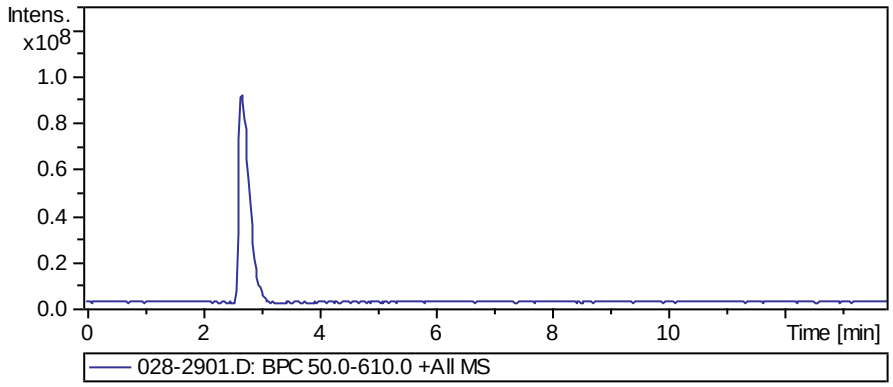


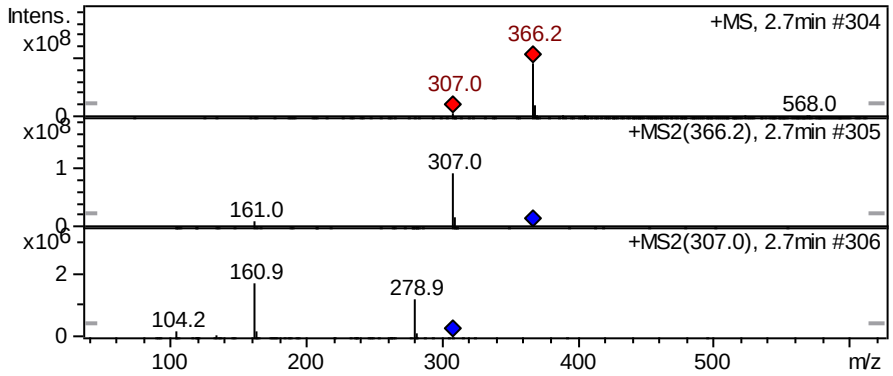


Spectra of (4412)

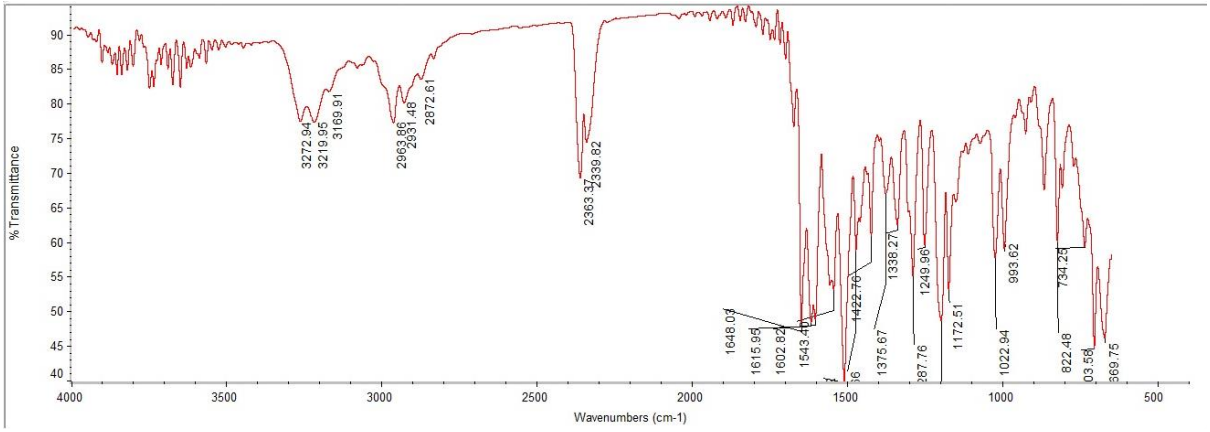


LC/MS





FT-IR



^{1}H NMR

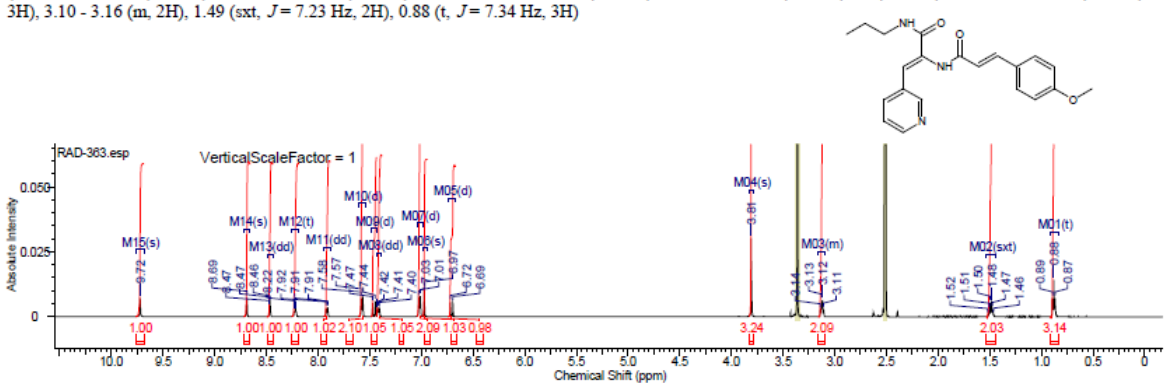
RAD-363

09/11/2016 8:34:26 AM
Dr.Mustafa Sample : RAD-363 DMSO PROTON DMSO (D:\Magdy) nmr 13

Formula $C_{21}H_{23}N_3O_3$	FW	365.4256

Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-363 DMSO PROTON DMSO (D:\Magdy) nmr 13				
Date	18 Jun 2015 14:41:36			Date Stamp	18 Jun 2015 14:41:36		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-363_18-06-2015\10\fid						
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	144.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.72 (s, 1H), 8.69 (s, 1H), 8.47 (dd, J = 1.69, 4.71 Hz, 1H), 8.22 (t, J = 5.27 Hz, 1H), 7.91 (dd, J = 1.32, 8.09 Hz, 1H), 7.57 (d, J = 8.66 Hz, 2H), 7.46 (d, J = 15.43 Hz, 1H), 7.41 (dd, J = 4.71, 8.09 Hz, 1H), 7.02 (d, J = 8.66 Hz, 2H), 6.97 (s, 1H), 6.71 (d, J = 15.81 Hz, 1H), 3.81 (s, 3H), 3.10 - 3.16 (m, 2H), 1.49 (sxt, J = 7.23 Hz, 2H), 0.88 (t, J = 7.34 Hz, 3H)



^{13}C NMR

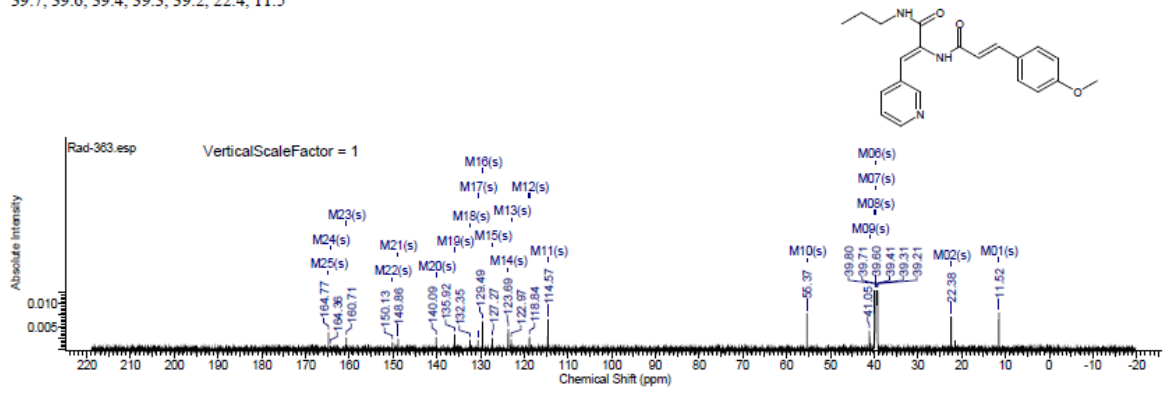
RAD-363

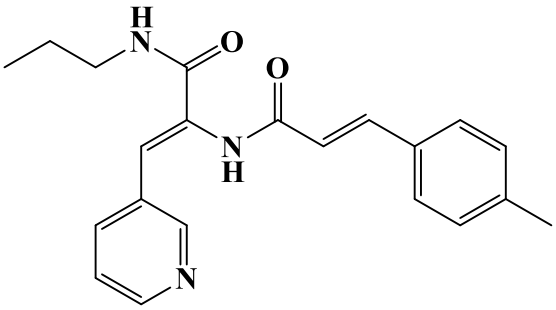
20/09/2016 10:17:55 AM
Dr.Mostafa Sample ; RAD-363 DMSO

Formula $C_{21}H_{23}N_3O_3$	FW	365.4256

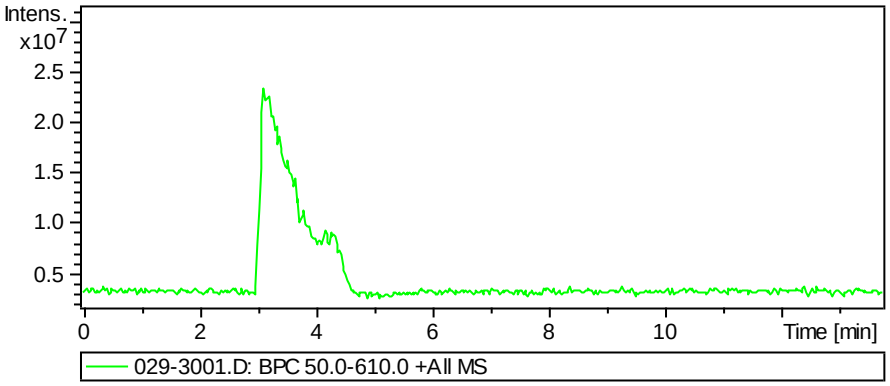
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-363 DMSO			Date	19 Apr 2016 14:22:40
Date Stamp	19 Apr 2016 14:22:40						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-363_19-04-2016\10\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	979	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21292.2539
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.001		

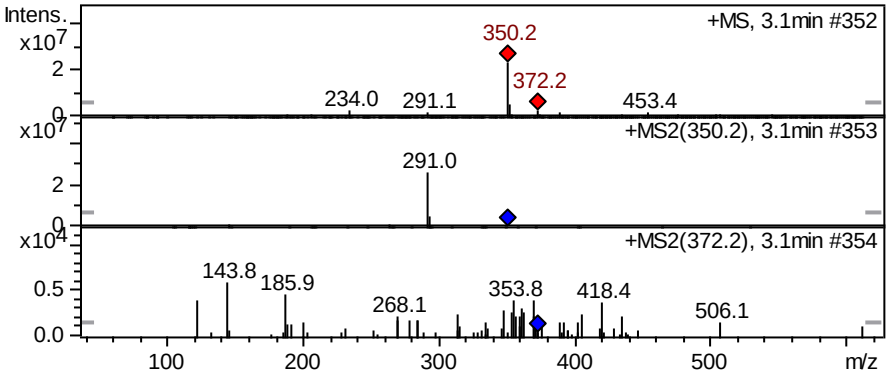
^{13}C NMR (214 MHz, DMSO-d$_6$) δ 164.8, 164.4, 160.7, 150.1, 148.9, 140.1, 135.9, 132.3, 130.6, 129.5, 127.3, 123.7, 123.0, 118.8, 114.6, 55.4, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 11.5





LC/MS


Intens.
x10^7
2.5
2.0
1.5
1.0
0.5
0
2
4
6
8
10
Time [min]
029-3001.D: BPC 50.0-610.0 +All MS


Intens.
x10^7
2
0
+MS, 3.1min #352
350.2
372.2
234.0
291.1
453.4
x10^7
2
0
+MS2(350.2), 3.1min #353
291.0
x10^4
0.5
0.0
+MS2(372.2), 3.1min #354
143.8
185.9
268.1
353.8
418.4
506.1
100
200
300
400
500
m/z

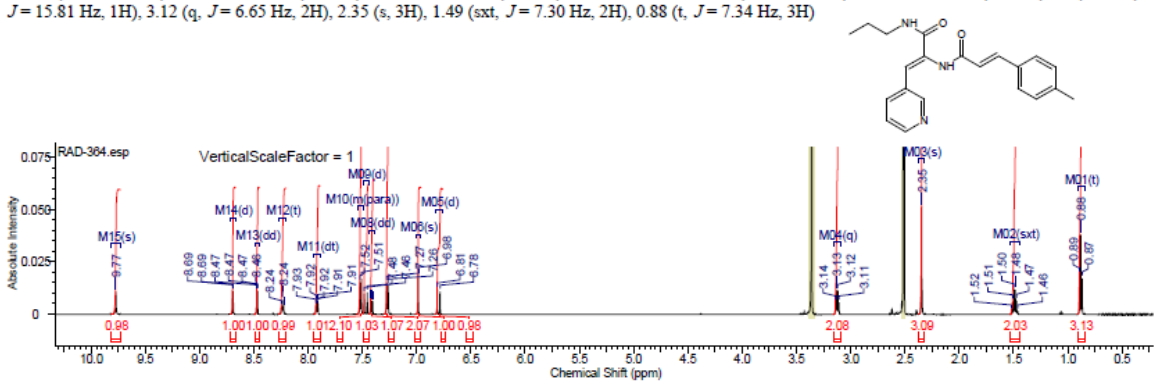
^{1}H NMR

RAD-364

09/11/2016 8:37:59 AM
Dr.Mustafa Sample : RAD-364 DMSO PROTON DMSO (D:\Magdy) nmr 21

Formula $C_{21}H_{19}N_3O_2$	FW	349.4262					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-364 DMSO PROTON DMSO (D:\Magdy) nmr 21				
Date	18 Jun 2015 15:22:08			Date Stamp	18 Jun 2015 15:22:08		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-364_18-06-2015\10\fid						
Nucleus	1H	Number of Transients	32	Origin	spect	Frequency (MHz)	600.15
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Original Points Count	32768
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Receiver Gain	161.00
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000			Spectrum Type	STANDARD

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.77 (s, 1H), 8.69 (d, J = 1.88 Hz, 1H), 8.47 (dd, J = 1.69, 4.71 Hz, 1H), 8.23 (t, J = 5.83 Hz, 1H), 7.92 (td, J = 1.60, 8.09 Hz, 1H), 7.49 - 7.54 (m, J = 7.91 Hz, 2H), 7.47 (d, J = 15.81 Hz, 1H), 7.41 (dd, J = 4.33, 8.09 Hz, 1H), 7.24 - 7.30 (m, J = 7.91 Hz, 2H), 6.98 (s, 1H), 6.80 (d, J = 15.81 Hz, 1H), 3.12 (q, J = 6.65 Hz, 2H), 2.35 (s, 3H), 1.49 (sxt, J = 7.30 Hz, 2H), 0.88 (t, J = 7.34 Hz, 3H)



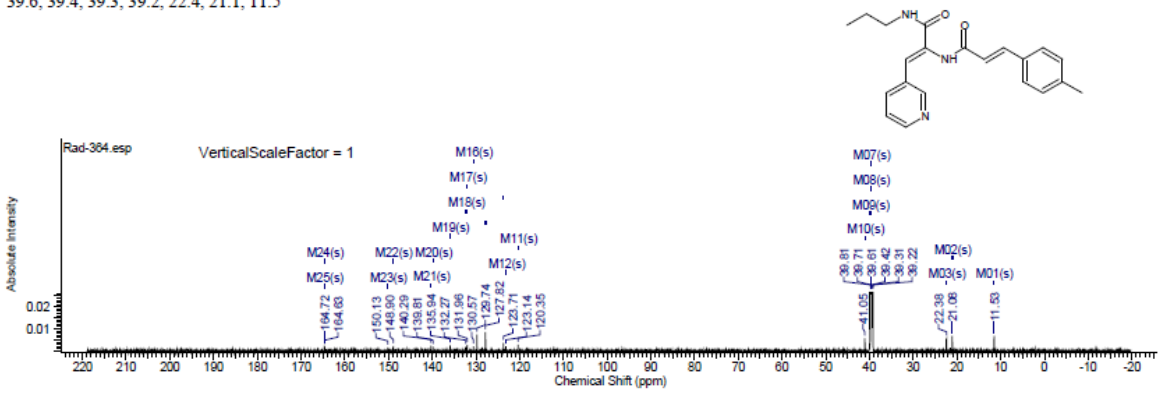
^{13}C NMR

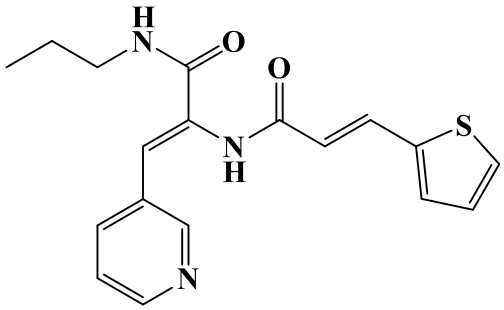
RAD-364

20/09/2016 9:50:37 AM
Dr.Mostafa Sample ; RAD-364 DMSO

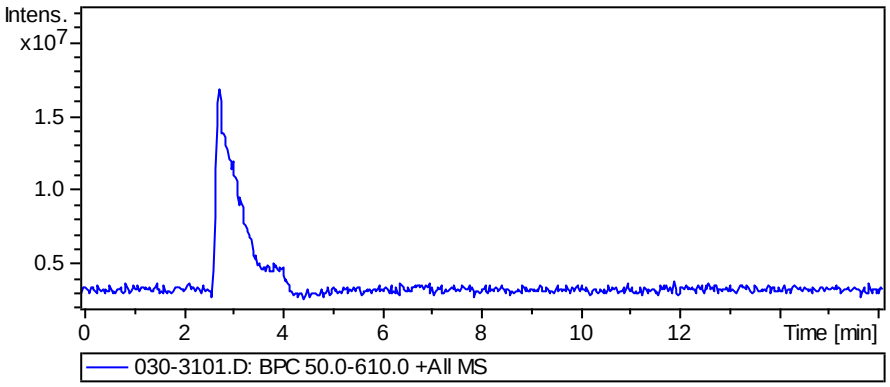
Formula $C_{21}H_{19}N_3O_2$	FW	349.4262					
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-364 DMSO			Date	20 Apr 2016 13:08:00
Date Stamp	20 Apr 2016 13:08:00						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-364_19-04-2016\110\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	1147	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21293.8125
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	24.999		

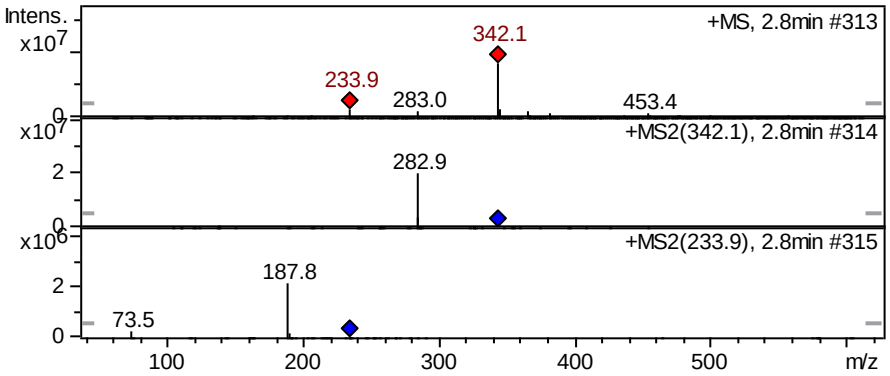
^{13}C NMR (214 MHz, DMSO-d$_6$) δ 164.7, 164.6, 150.1, 148.9, 140.3, 139.8, 135.9, 132.3, 132.0, 130.6, 129.7, 127.8, 123.7, 123.1, 120.4, 41.1, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.4, 21.1, 11.5



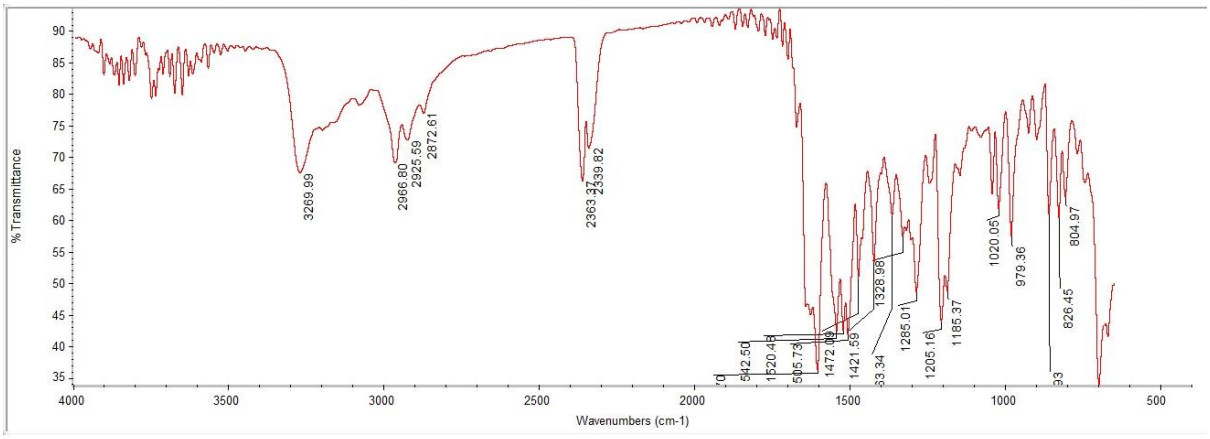


LC/MS





FT-IR



^{1}H NMR

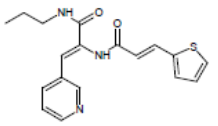
RAD-365

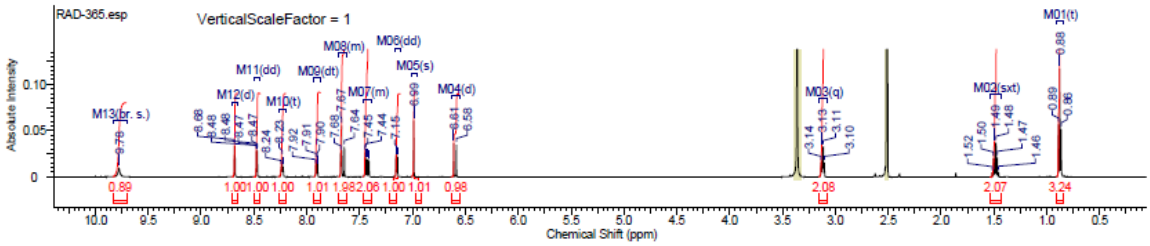
09/11/2016 8:39:53 AM
Dr.Mustafa Sample : RAD-365 DMSO PROTON DMSO (D:\Magdy) nmr 22

Formula $C_{15}H_{16}N_4O_2S$	FW	341.4274

Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-365 DMSO PROTON DMSO (D:\Magdy) nmr 22				
Date	18 Jun 2015 15:28:32			Date Stamp	18 Jun 2015 15:28:32		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-365_18-06-2015\10\fid						
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	144.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.78 (br. s., 1H), 8.68 (d, J = 1.88 Hz, 1H), 8.47 (dd, J = 1.51, 4.89 Hz, 1H), 8.23 (t, J = 5.84 Hz, 1H), 7.91 (td, J = 1.79, 8.09 Hz, 1H), 7.62 - 7.70 (m, 2H), 7.39 - 7.47 (m, 2H), 7.15 (dd, J = 3.58, 5.08 Hz, 1H), 6.99 (s, 1H), 6.60 (d, J = 15.81 Hz, 1H), 3.12 (q, J = 6.65 Hz, 2H), 1.49 (sxt, J = 7.23 Hz, 2H), 0.88 (t, J = 7.53 Hz, 3H)





^{13}C NMR

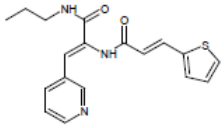
RAD-365

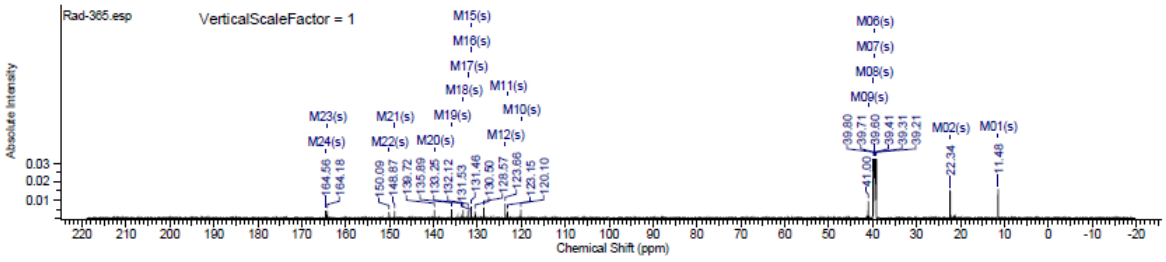
20/09/2016 9:54:23 AM
Dr.Mostafa Sample ; RAD-365 DMSO

Formula $C_{15}H_{16}N_4O_2S$	FW	341.4274

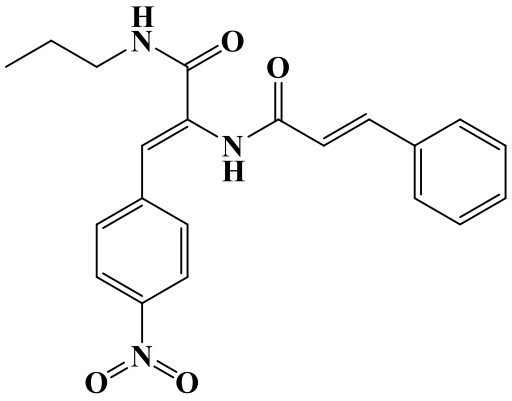
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-365 DMSO			Date	20 Apr 2016 17:24:00
Date Stamp	20 Apr 2016 17:24:00						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-365_19-04-2016\130\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3500	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21284.4688
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.000		

^{13}C NMR (214 MHz, DMSO-d$_6$) δ 164.6, 164.2, 150.1, 148.9, 139.7, 135.9, 133.3, 132.1, 131.5, 131.5, 130.5, 128.6, 123.7, 123.2, 120.1, 41.0, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.3, 11.5

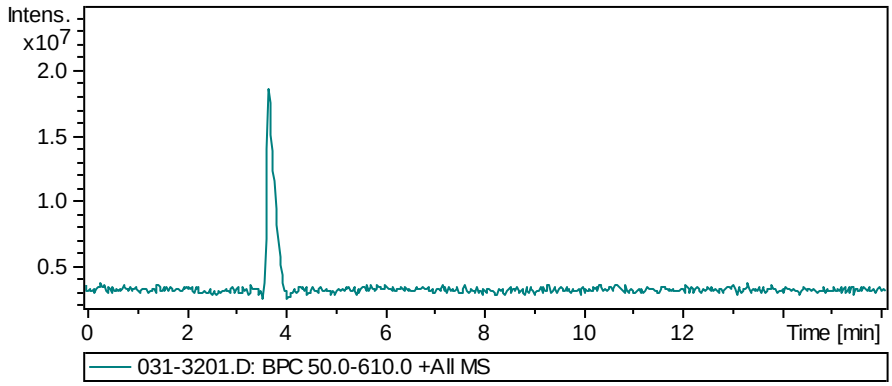


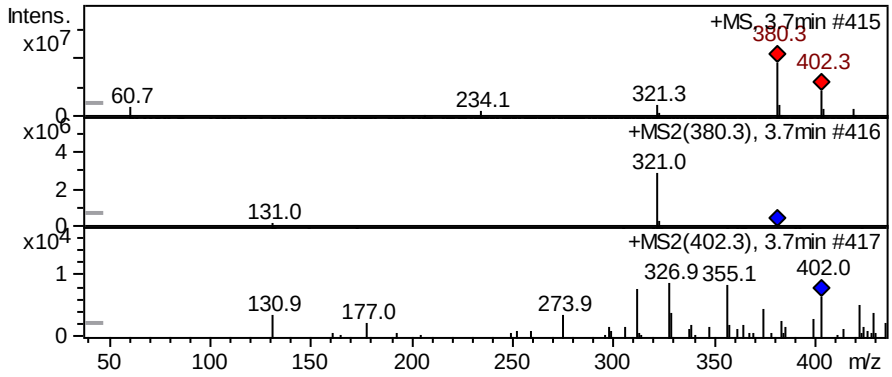


Spectra of (4712)

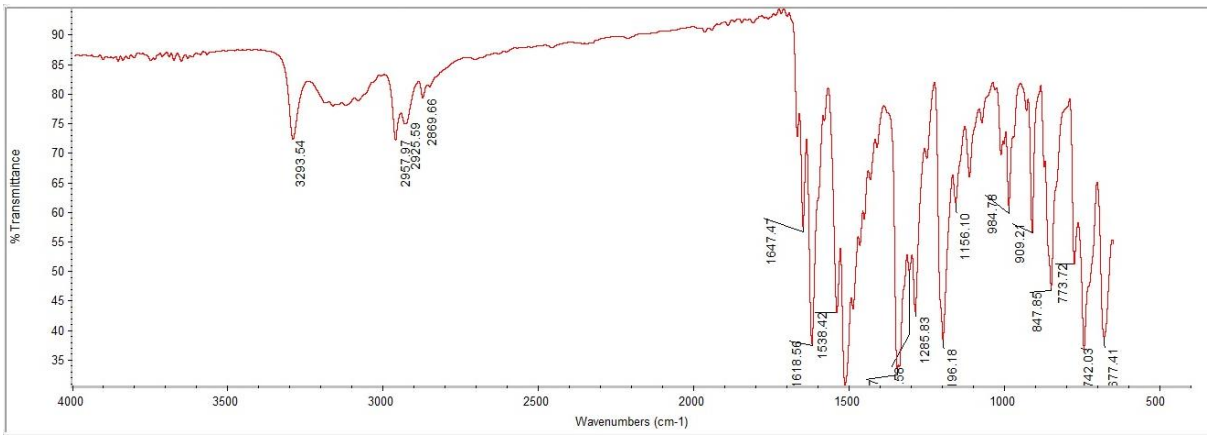


LC/MS





FT-IR



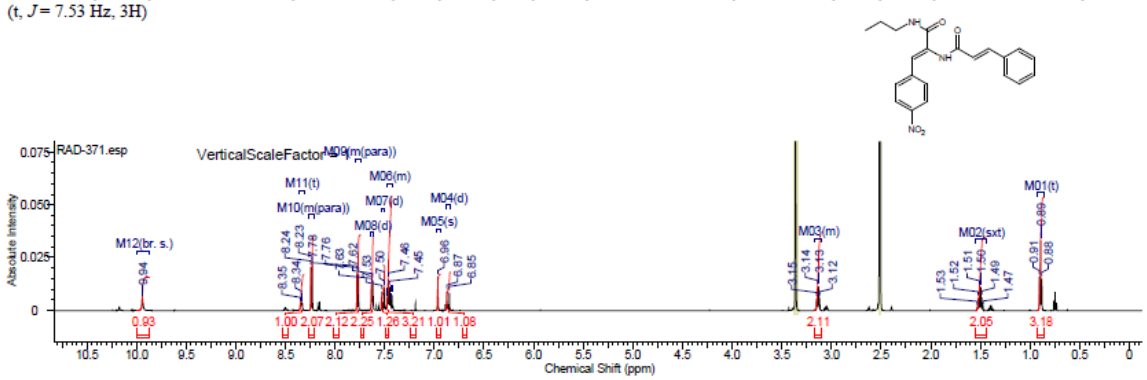
^{1}H NMR

RAD-371

11/10/2016 9:01:33 AM
Dr.Mustafa Sample : RAD-371 DMSO PROTON DMSO {D:\Magdy} nmr 17

Formula $C_{20}H_{17}N_3O_4$	FW	379.4091					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-371 DMSO PROTON DMSO {D:\Magdy} nmr 17				
Date	18 Jun 2015 15:00:48			Date Stamp	18 Jun 2015 15:00:48		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-371 18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	144.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.94 (br. s., 1H), 8.34 (t, J = 5.84 Hz, 1H), 8.21 - 8.26 (m, J = 8.66 Hz, 2H), 7.74 - 7.79 (m, J = 9.03 Hz, 2H), 7.62 (d, J = 7.15 Hz, 2H), 7.51 (d, J = 15.81 Hz, 1H), 7.43 - 7.48 (m, 3H), 6.96 (s, 1H), 6.86 (d, J = 16.19 Hz, 1H), 3.10 - 3.17 (m, 2H), 1.50 (sxt, J = 7.30 Hz, 2H), 0.89 (t, J = 7.53 Hz, 3H)



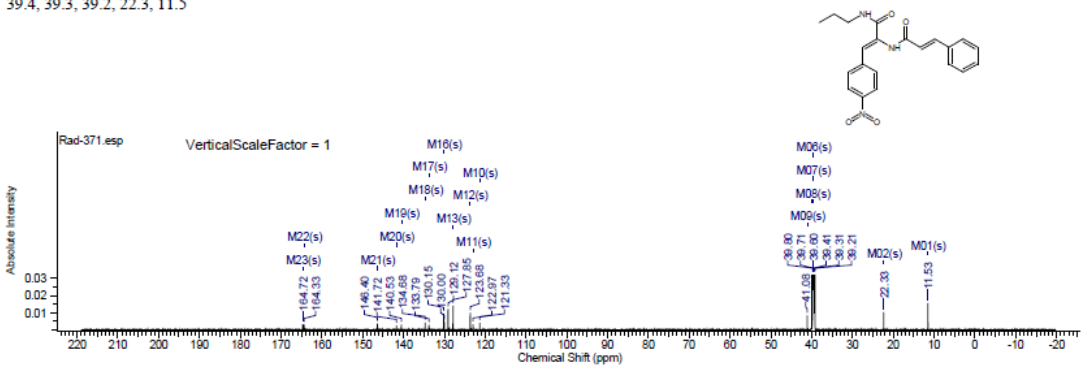
^{13}C NMR

RAD-371

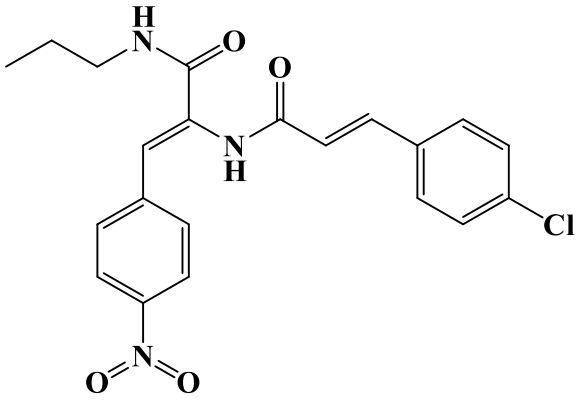
20/09/2016 9:58:56 AM
Dr.Mustafa Sample ; RAD-371 DMSO

Formula $C_{20}H_{17}N_3O_4$	FW	379.4091					
Acquisition Time (sec)	0.6423	Comment	Dr.Mustafa Sample ; RAD-371 DMSO			Date	21 Apr 2016 01:30:24
Date Stamp	21 Apr 2016 01:30:24						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-371 19-04-2016\160\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3500	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21290.6973
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	24.998		

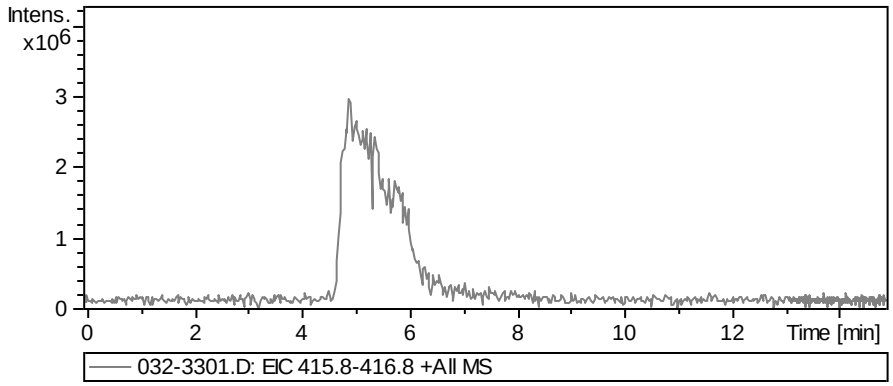
^{13}C NMR (214 MHz, DMSO-d_6) δ 164.7, 164.3, 146.4, 141.7, 140.5, 134.7, 133.8, 130.2, 130.0, 129.1, 127.8, 123.7, 123.0, 121.3, 41.1, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.3, 11.5

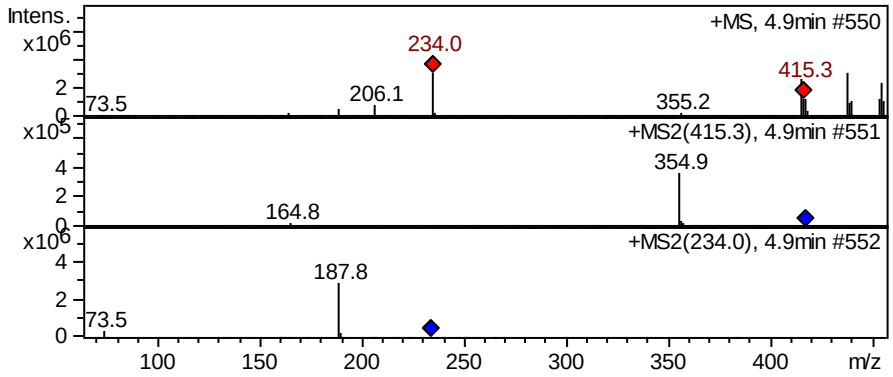


Spectra of (4812)

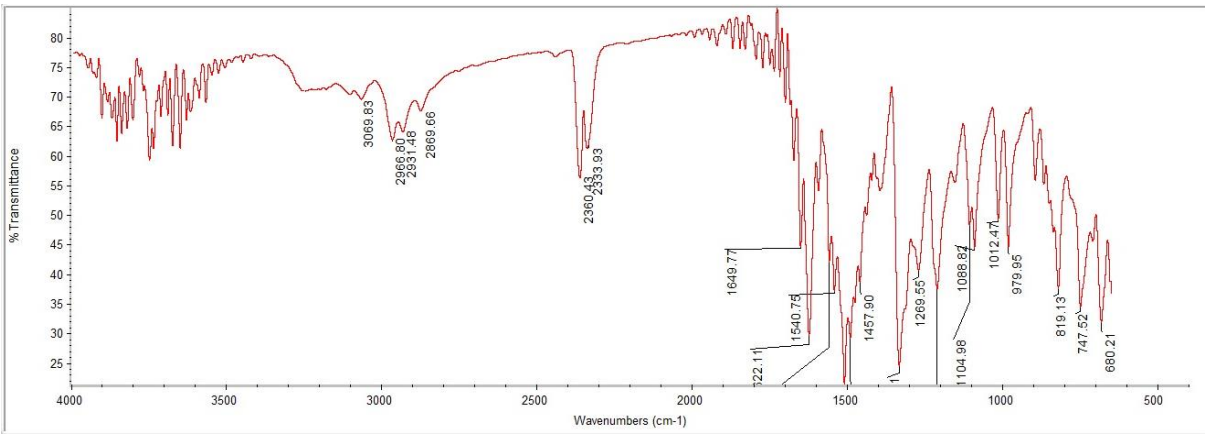


LC/MS





FT-IR



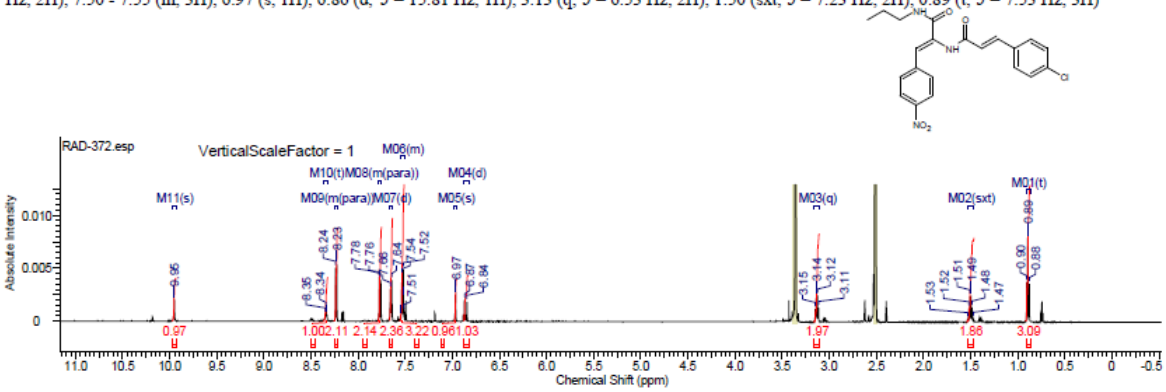
^{1}H NMR

RAD-372

11/10/2016 9:08:12 AM
Dr.Mustafa Sample : RAD-372 DMSO PROTON DMSO {D:\Magdy} nmr 20

Formula $C_{20}H_{20}ClN_3O_4$		FW 413.8542			
Acquisition Time (sec) 2.6564	Comment Dr.Mustafa Sample : RAD-372 DMSO PROTON DMSO {D:\Magdy} nmr 20				
Date 18 Jun 2015 15:17:52		Date Stamp 18 Jun 2015 15:17:52			
File Name E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-372 18-06-2015\10\fid				Frequency (MHz) 600.15	
Nucleus 1H	Number of Transients 32	Origin spect		Original Points Count 32768	
Owner nmr	Points Count 32768	Pulse Sequence zg30		Receiver Gain 161.00	
SW(cyclical) (Hz) 12335.53	Solvent DMSO-d6	Spectrum Offset (Hz) 3706.1750		Spectrum Type STANDARD	
Sweep Width (Hz) 12335.15	Temperature (degree C) 25.000				

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.95 (s, 1H), 8.34 (t, J = 5.46 Hz, 1H), 8.21 - 8.25 (m, J = 9.04 Hz, 2H), 7.75 - 7.79 (m, J = 9.04 Hz, 2H), 7.65 (d, J = 8.66 Hz, 2H), 7.50 - 7.55 (m, 3H), 6.97 (s, 1H), 6.86 (d, J = 15.81 Hz, 1H), 3.13 (q, J = 6.53 Hz, 2H), 1.50 (sxt, J = 7.23 Hz, 2H), 0.89 (t, J = 7.53 Hz, 3H)



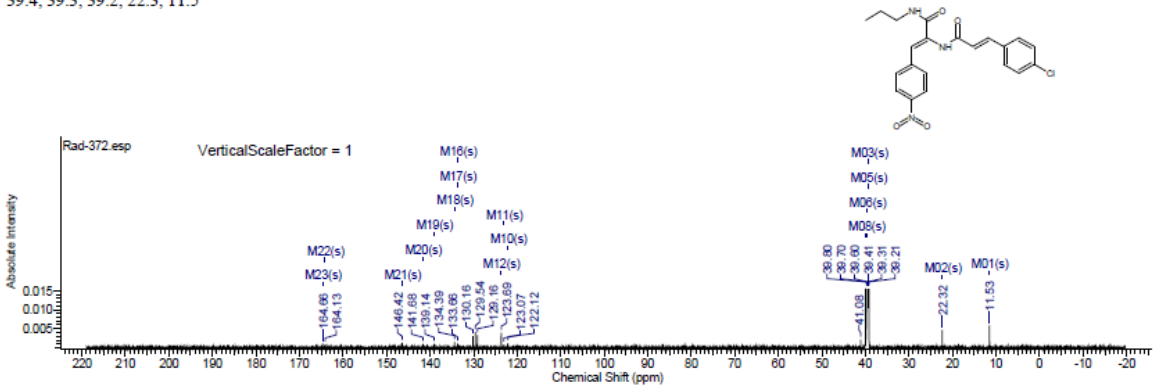
^{13}C NMR

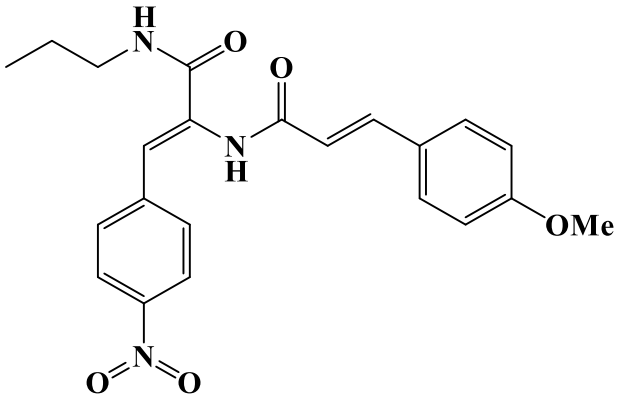
RAD-372

20/09/2016 10:02:49 AM
Dr.Mostafa Sample : RAD-372 DMSO

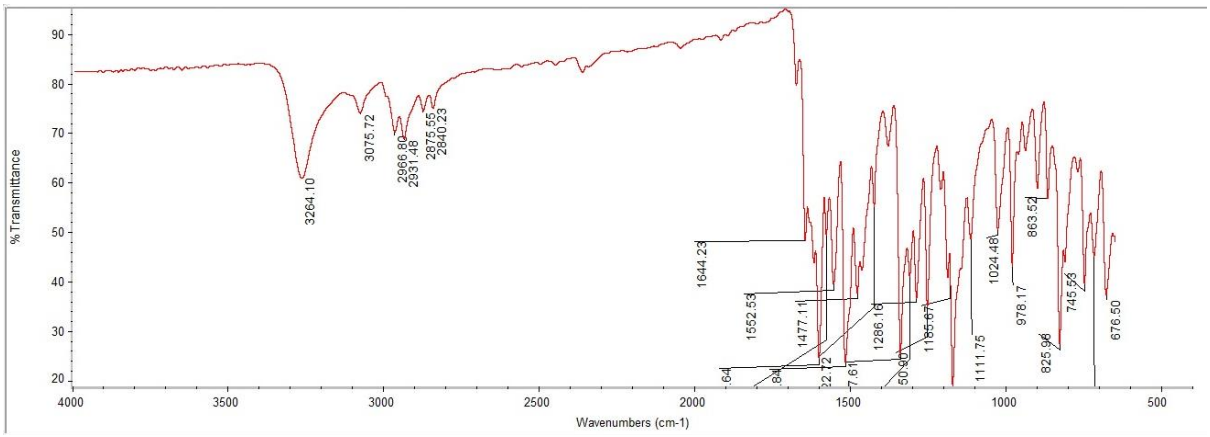
Formula $C_{20}H_{20}ClN_3O_4$		FW 413.8542			
Acquisition Time (sec) 0.6423	Comment Dr.Mostafa Sample : RAD-372 DMSO			Date 19 Apr 2016 08:17:52	
Date Stamp 19 Apr 2016 08:17:52					
File Name E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-372 18-04-2016\90\fid					
Frequency (MHz) 213.77	Nucleus 13C	Number of Transients 3072		Origin spect	
Original Points Count 32768	Owner nmr	Points Count 32768		Pulse Sequence zgpg30	
Receiver Gain 186.93	SW(cyclical) (Hz) 51020.41	Solvent DMSO-d6		Spectrum Offset (Hz) 21290.6973	
Spectrum Type STANDARD	Sweep Width (Hz) 51018.85	Temperature (degree C) 24.999			

^{13}C NMR (214 MHz, DMSO-d_6) δ 164.7, 164.1, 146.4, 141.7, 139.1, 134.4, 133.7, 133.7, 130.2, 129.5, 129.2, 123.7, 123.1, 122.1, 41.1, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.3, 11.5




H
N
O
O
N
H
OMe
N
O
O

FT-IR


% Transmittance
Wavenumbers (cm-1)
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3075.72
2966.80
2931.48
2875.55
2840.23
1644.23
1552.53
1477.11
1286.16
1165.67
1111.75
1024.48
978.17
863.52
825.96
745.53
676.50

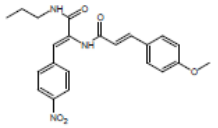
^{1}H NMR

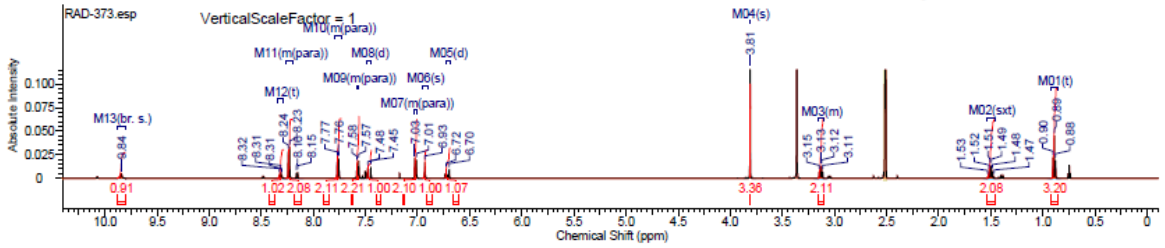
RAD-373

09/11/2016 9:23:51 AM
Dr.Mustafa Sample : RAD-373 DMSO PROTON DMSO (D:\Magdy) nmr 25

Formula $C_{20}H_{20}N_2O_6$	FW	409.4351					
Acquisition Time (sec)	2.6564	Comment	Dr.Mustafa Sample : RAD-373 DMSO PROTON DMSO (D:\Magdy) nmr 25				
Date	18 Jun 2015 15:43:28			Date Stamp	18 Jun 2015 15:43:28		
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA RAD-373 18-06-2015\10\fid					Frequency (MHz)	600.15
Nucleus	1H	Number of Transients	32	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	128.00
SW(cyclical) (Hz)	12335.53	Solvent	DMSO-d6	Spectrum Offset (Hz)	3706.1750	Spectrum Type	STANDARD
Sweep Width (Hz)	12335.15	Temperature (degree C)	25.000				

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.84 (br. s., 1H), 8.31 (t, J = 5.65 Hz, 1H), 8.20 - 8.26 (m, J = 9.04 Hz, 2H), 7.73 - 7.79 (m, J = 8.66 Hz, 2H), 7.56 - 7.58 (m, J = 8.66 Hz, 2H), 7.46 (d, J = 15.81 Hz, 1H), 7.01 - 7.03 (m, J = 8.66 Hz, 2H), 6.93 (s, 1H), 6.71 (d, J = 15.81 Hz, 1H), 3.81 (s, 3H), 3.10 - 3.16 (m, 2H), 1.50 (sxt, J = 7.23 Hz, 2H), 0.89 (t, J = 7.53 Hz, 3H)





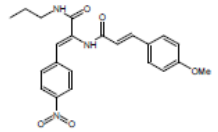
^{13}C NMR

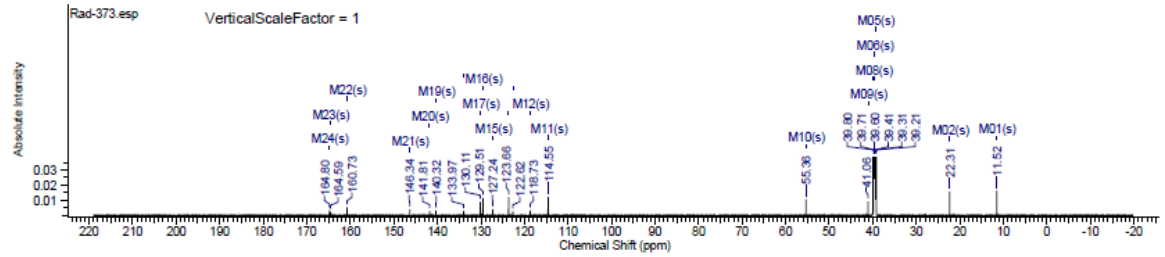
RAD-373

20/09/2016 10:06:57 AM
Dr.Mostafa Sample : RAD-373 DMSO

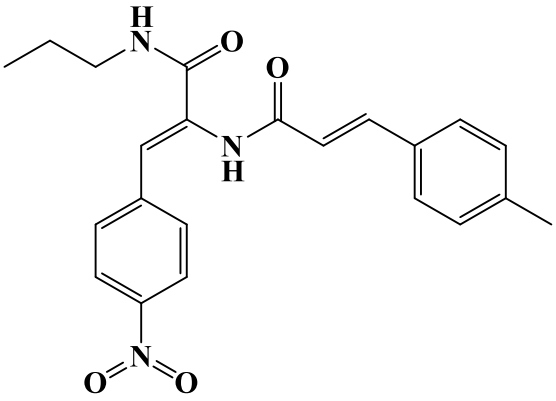
Formula $C_{20}H_{20}N_2O_6$	FW	409.4351					
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample : RAD-373 DMSO			Date	19 Apr 2016 01:11:12
Date Stamp	19 Apr 2016 01:11:12						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA RAD-373 18-04-2016\60\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	3072	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21287.5840
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	24.999		

^{13}C NMR (214 MHz, DMSO-d_6) δ 164.8, 164.6, 160.7, 146.3, 141.8, 140.3, 134.0, 130.1, 129.5, 127.2, 123.7, 122.6, 118.7, 114.5, 55.4, 41.1, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.3, 11.5

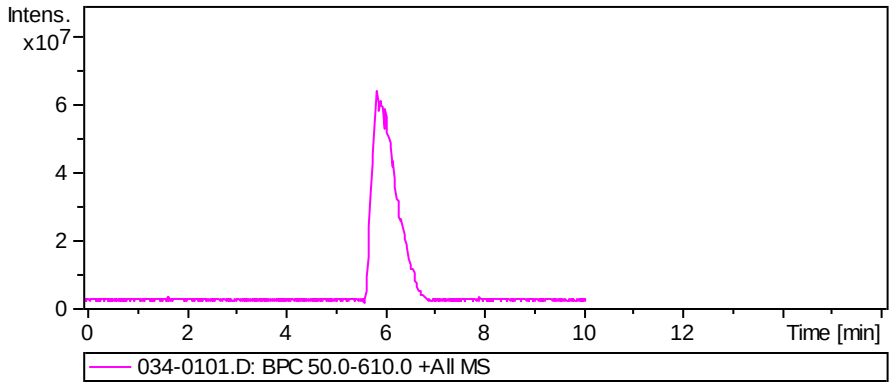


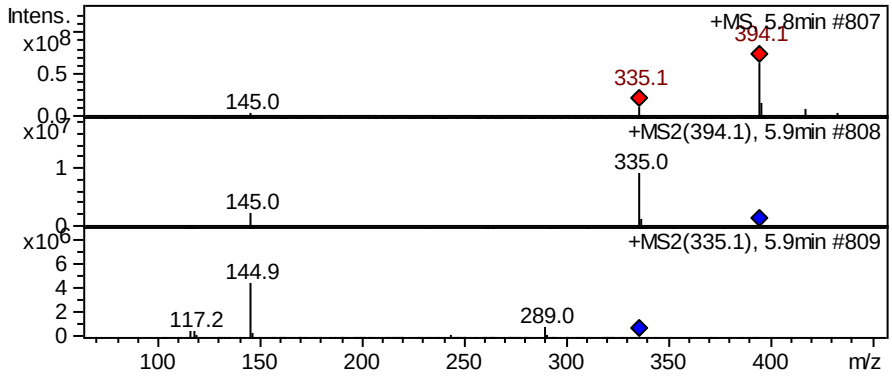


Spectra of (5012)

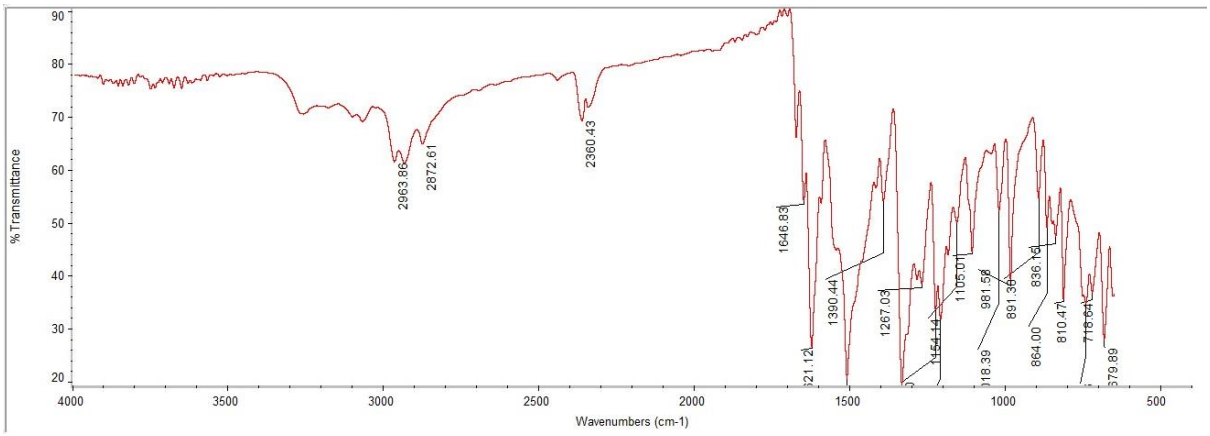


LC/MS





FT-IR



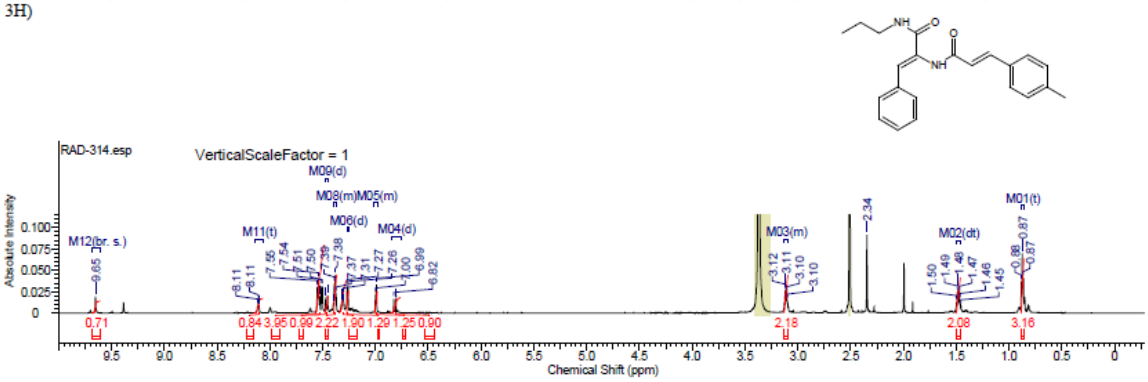
^{1}H NMR

RAD-374

09/11/2016 9:46:47 AM
Dr.Mustafa El-Araby Sample : RAD-314 DMSO

Formula $C_{20}H_{24}N_2O_3$	FW	348.4382					
Acquisition Time (sec)	1.9268	Comment	Dr.Mustafa El-Araby Sample : RAD-314 DMSO			Date	08 Apr 2015 10:23:44
Date Stamp	08 Apr 2015 10:23:44						
File Name	E:\Mostafa Alaraby Project\Oxazolone NMR\NMR final oxazolone\MUSTAFA_RAD-314_08-04-2015\40\fid					Frequency (MHz)	850.15
Nucleus	1H	Number of Transients	20	Origin	spect	Original Points Count	32768
Owner	nmr	Points Count	32768	Pulse Sequence	zg30	Receiver Gain	9.04
SW(cyclical) (Hz)	17006.80	Solvent	DMSO-d6	Spectrum Offset (Hz)	5250.0283	Spectrum Type	STANDARD
Sweep Width (Hz)	17006.28	Temperature (degree C)	25.000				

^{1}H NMR (850 MHz, DMSO-d$_6$) δ 9.65 (br. s., 1H), 8.11 (t, J = 5.45 Hz, 1H), 7.48 - 7.57 (m, 4H), 7.46 (d, J = 15.57 Hz, 1H), 7.37 - 7.40 (m, 2H), 7.27 - 7.34 (m, 2H), 7.26 (d, J = 7.78 Hz, 1H), 6.98 - 7.01 (m, 1H), 6.82 (d, J = 15.57 Hz, 1H), 3.09 - 3.13 (m, 2H), 1.48 (td, J = 7.20, 14.14 Hz, 2H), 0.87 (t, J = 7.27 Hz, 3H)



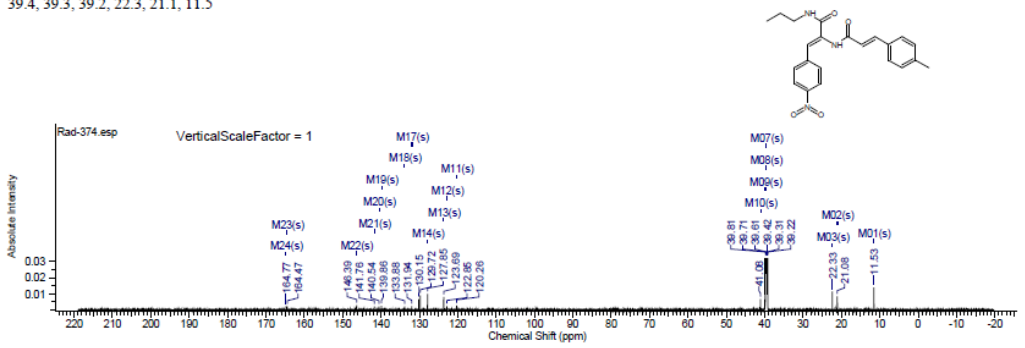
^{13}C NMR

RAD-374

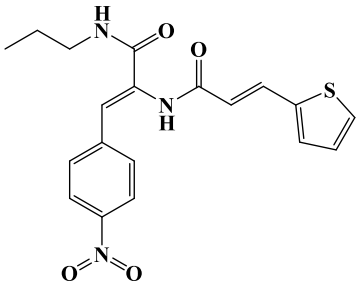
20/09/2016 10:09:40 AM
Dr.Mostafa Sample ; RAD-374 DMSO

Formula $C_{20}H_{24}N_2O_3$	FW	393.4357					
Acquisition Time (sec)	0.6423	Comment	Dr.Mostafa Sample ; RAD-374 DMSO			Date	20 Apr 2016 14:09:52
Date Stamp	20 Apr 2016 14:09:52						
File Name	E:\Projects\Mostafa Alaraby Project\Oxazolone\Oxazolone NMR\NMR final oxazolone\13 CNMR New 18-4-2016\MUSTAFA_RAD-374_19-04-2016\120\fid						
Frequency (MHz)	213.77	Nucleus	13C	Number of Transients	963	Origin	spect
Original Points Count	32768	Owner	nmr	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	186.93	SW(cyclical) (Hz)	51020.41	Solvent	DMSO-d6	Spectrum Offset (Hz)	21292.2539
Spectrum Type	STANDARD	Sweep Width (Hz)	51018.85	Temperature (degree C)	25.001		

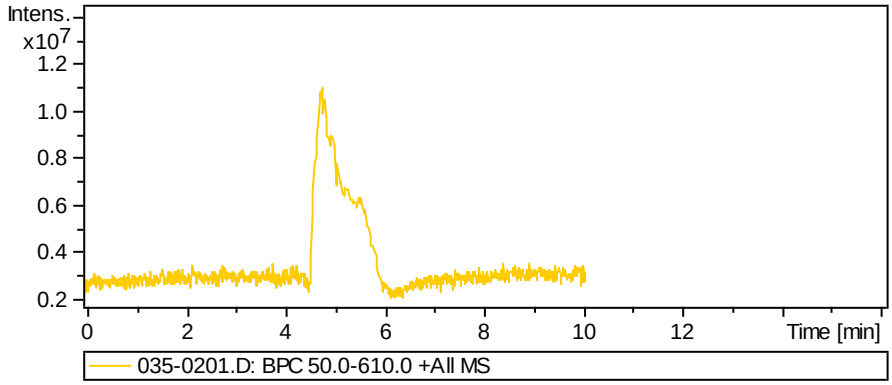
^{13}C NMR (214 MHz, DMSO-d$_6$) δ 164.8, 164.5, 146.4, 141.8, 140.5, 139.9, 133.9, 131.9, 130.1, 129.7, 127.9, 123.7, 122.8, 120.3, 41.1, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.3, 21.1, 11.5

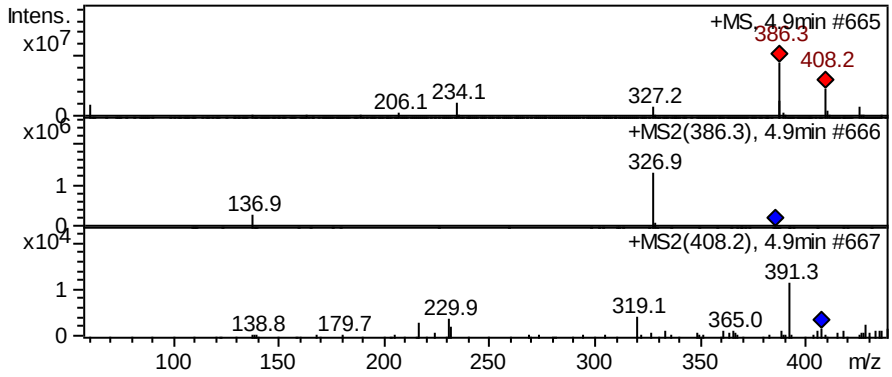


Spectra of (5112)

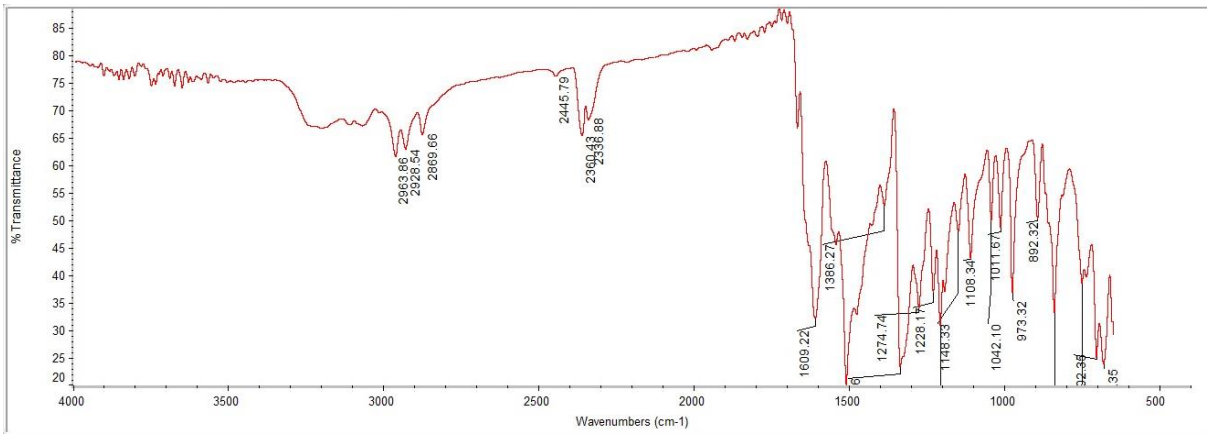


LC/MS

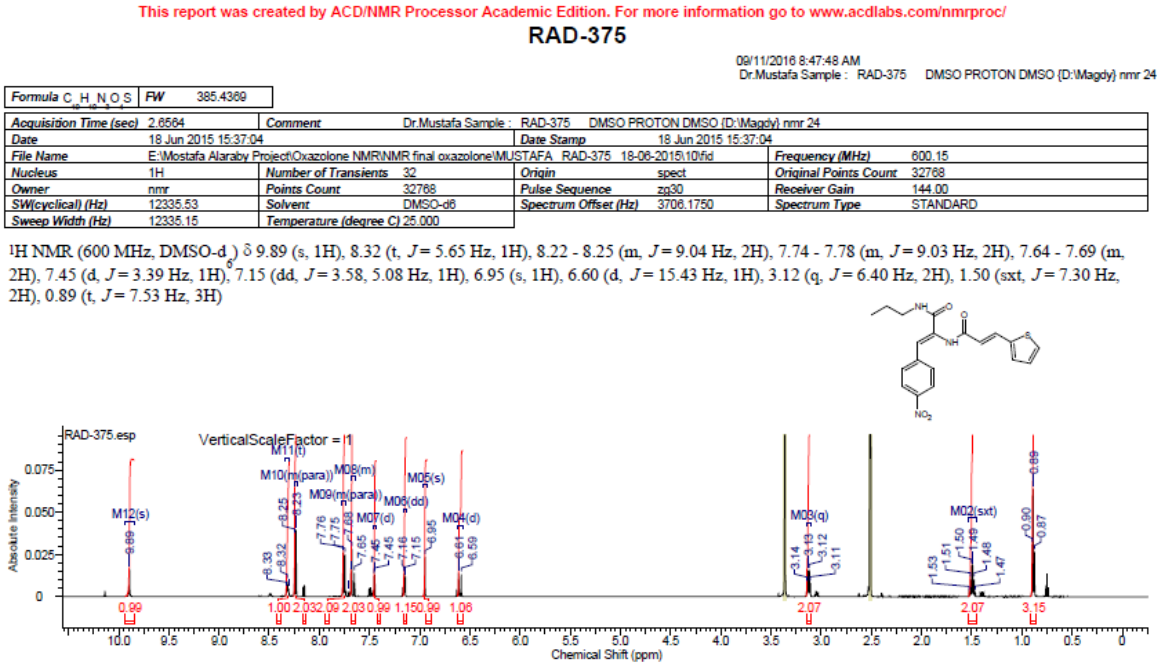




FT-IR

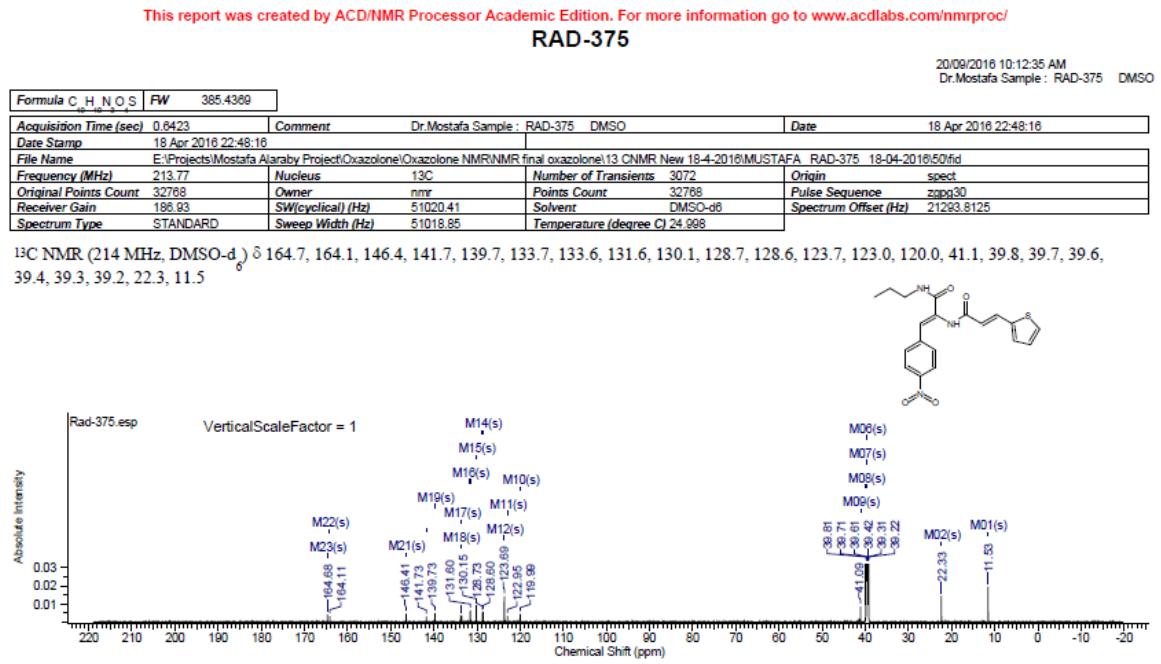


^{1}H NMR



^{1}H NMR (600 MHz, DMSO-d_6) δ 9.89 (s, 1H), 8.32 (t, J = 5.65 Hz, 1H), 8.22 - 8.25 (m, J = 9.04 Hz, 2H), 7.74 - 7.78 (m, J = 9.03 Hz, 2H), 7.64 - 7.69 (m, 2H), 7.45 (d, J = 3.39 Hz, 1H), 7.15 (dd, J = 3.58, 5.08 Hz, 1H), 6.95 (s, 1H), 6.60 (d, J = 15.43 Hz, 1H), 3.12 (q, J = 6.40 Hz, 2H), 1.50 (sxt, J = 7.30 Hz, 2H), 0.89 (t, J = 7.53 Hz, 3H)

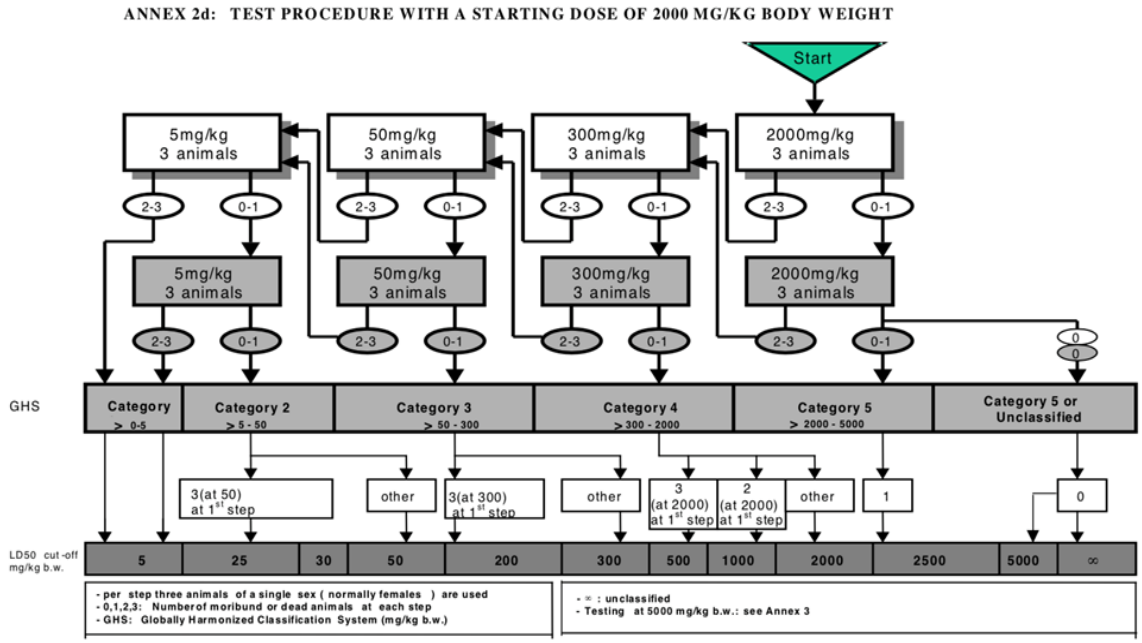
^{13}C NMR



^{13}C NMR (214 MHz, DMSO-d_6) δ 164.7, 164.1, 146.4, 141.7, 139.7, 133.7, 133.6, 131.6, 130.1, 128.7, 128.6, 123.7, 123.0, 120.0, 41.1, 39.8, 39.7, 39.6, 39.4, 39.3, 39.2, 22.3, 11.5

II. Further Data on LD50 determination

Chart of the OECD protocol, Guideline 423
OECD Guideline for testing of chemicals
Acute Oral Toxicity – Acute Toxic Class Method
https://ntp.niehs.nih.gov/iccvam/suppdocs/feddocs/oecd/oecd_gl423.pdf



III. References for Reported Compounds

1. Heiss, E. H.; Schilder, Y. D.; Dirsch, V. M., Chronic treatment with resveratrol induces redox stress- and ataxia telangiectasia-mutated (ATM)-dependent senescence in p53-positive cancer cells. *J Biol Chem* **2007,** *282* (37), 26759-66.
2. Fahmy, A.; Orabi, M., REACTIONS OF 4-ARYLIDENE-2-STYRYL-5 (4)-OXAZOLONES AND RELATED COMPOUNDS. *INDIAN JOURNAL OF CHEMISTRY* **1972,** *10* (10), 961-964.
3. Tripathy, P. K.; Mukerjee, A. K., A facile synthesis of N-substituted 2-acylamino-2-alkenamides. *Synthesis* **1985,** *1985* (03), 285-288.
4. Mustafa, A.; Asker, W.; Harhash, A. H.; Abdin, T.; Zayed, E. M., Reaktionen mit 2.4-disubstituierten Δ2-Oxazolinonen-(5). *Justus Liebigs Annalen der Chemie* **1968,** *714* (1), 146-154.
5. Mustafa, A.; Asker, W.; Harhash, A. H.; Abdin, T. M. S.; Zayed, E. M., Reaktionen mit 2.4-disubstituierten Δ2-Oxazolinonen-(5). *Justus Liebigs Annalen der Chemie* **1968,** *714* (1), 146-154.