

SUPPLEMENTARY DATA

Discovery of Imeglimin-inspired novel 1,3,5-triazine derivatives as an antidiabetic agent in Streptozotocin-induced Diabetes in Wistar rats via inhibition of DPP-4

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PRELIMINARY DATA OF THE INTERMEDIATES

4,6-Dichloro-[1,3,5]triazin-2-ylamine (2): Yield: 82%; *M.P.*: 157 °C; *R_f*: 0.87, Mobile phase; toluene: acetone (7:3)

4-Chloro-6-morpholin-4-yl-[1,3,5]triazin-2-ylamine (3): Yield: 78%; *M.P.*: 172-173 °C; *R_f*: 0.93, Mobile phase; toluene: acetone (7:3)

4,6-diphenyl-6H-1,3-oxazin-2-amine (7a): Yield: 84%; *M.P.*: 220 °C; *R_f*: 0.83, Mobile phase; ethyl acetate: toluene (7:3)

6-(2-nitrophenyl)-4-phenyl-6H-1,3-oxazin-2-amine (7b): Yield: 88%; *M.P.*: 226 °C; *R_f*: 0.87, Mobile phase; ethyl acetate: toluene (7:3)

6-(3-nitrophenyl)-4-phenyl-6H-1,3-oxazin-2-amine (**7c**): Yield: 78%; *M.P.*: 210 °C; *R_f*: 0.76, Mobile phase; ethyl acetate: toluene (7:3)

6-(4-nitrophenyl)-4-phenyl-6H-1,3-oxazin-2-amine (**7d**): Yield: 75%; *M.P.*: 225 °C; *R_f*: 0.84, Mobile phase; ethyl acetate: toluene (7:3)

2-(2-amino-4-phenyl-6H-1,3-oxazin-6-yl)phenol (**7e**): Yield: 86%; *M.P.*: 228 °C; *R_f*: 0.88, Mobile phase; ethyl acetate: toluene (7:3)

3-(2-amino-4-phenyl-6H-1,3-oxazin-6-yl)phenol (**7f**): Yield: 80%; *M.P.*: 210 °C; *R_f*: 0.86, Mobile phase; ethyl acetate: toluene (7:3)

4-(2-amino-4-phenyl-6H-1,3-oxazin-6-yl)phenol (**7g**): Yield: 85%; *M.P.*: 225 °C; *R_f*: 0.78, Mobile phase; ethyl acetate: toluene (7:3)

6-(2-chlorophenyl)-4-phenyl-6H-1,3-oxazin-2-amine (**7h**): Yield: 82%; *M.P.*: 226 °C; *R_f*: 0.89, Mobile phase; ethyl acetate: toluene (7:3)

6-(3-chlorophenyl)-4-phenyl-6H-1,3-oxazin-2-amine (**7i**): Yield: 76%; *M.P.*: 210 °C; *R_f*: 0.73, Mobile phase; ethyl acetate: toluene (7:3)

6-(4-chlorophenyl)-4-phenyl-6H-1,3-oxazin-2-amine (**7j**): Yield: 89%; *M.P.*: 218 °C; *R_f*: 0.78, Mobile phase; ethyl acetate: toluene (7:3)

4-phenyl-6-(*o*-tolyl)-6H-1,3-oxazin-2-amine (**7k**): Yield: 84%; *M.P.*: 228 °C; *R_f*: 0.87, Mobile phase; ethyl acetate: toluene (7:3)

4-phenyl-6-(*m*-tolyl)-6H-1,3-oxazin-2-amine (**7l**): Yield: 92%; *M.P.*: 230 °C; *R_f*: 0.88, Mobile phase; ethyl acetate: toluene (7:3)

4-phenyl-6-(p-tolyl)-6H-1,3-oxazin-2-amine (7m): Yield: 90%; *M.P.*: 225 °C; *R_f*: 0.87, Mobile phase; ethyl acetate: toluene (7:3)

CPCSEA certificate for animal ethical approval

UNITED INSTITUTE OF PHARMACY, UCER

A-31/1, UPSIDC Industrial Area, Naini, Allahabad - 211010
Ph. : 0532 - 2101568, 2101569



INSTITUTIONAL ANIMAL ETHICS COMMITTEE (IAEC)


REG. No. - 1451/PO/Re/S/11/CPCSEA Dated 16/06//2017 UNDER RULE 13 OF THE
"BREEDING OF AND EXPERIMENTS ON ANIMALS (CONTROL AND
SUPERVISION) RULES 1998"

UIP/IAEC/Nov.-2021/10

DATE: 05/12/2021

CERTIFICATE

This is to certify that Ms. Akanksha Gupta, a research scholar (I. D. No. 15PHPS102) is permitted to carry out experiments for the thesis work entitled "Synthesis, characterization and biological screening of novel nitrogen containing heterocyclic compounds." as per the details mentioned and after observing the usual formalities laid down by IAEC as per the provisions made by CPCSEA.


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e-mail : info@united.ac.in web : http://www.united.ac.in

DOCKING RESULT ANALYSIS OF COMPOUND 8 (a-m)

Entry Name	docking score	glide_gscore	glide energy
8a	-7.032	-7.032	-65.324
8b	-8.213	-8.213	-76.776
8c	-8.956	-8.956	-78.546
8d	-8.814	-8.814	-77.457
8e	-8.012	-8.012	-75.654
8f	-8.112	-8.112	-76.453
8g	-8.083	-8.083	-76.342
8h	-7.213	-7.213	-70.568
8i	-7.876	-7.876	-71.244
8j	-7.657	-7.657	-71.189
8k	-7.011	-7.011	-68.982
8l	-7.113	-7.113	-69.749
8m	-7.098	-7.098	-69.457
Alogliptin (Reference ligand)	-9.447	-9.447	-56.191

DRUG-INTERACTION DIAGRAM

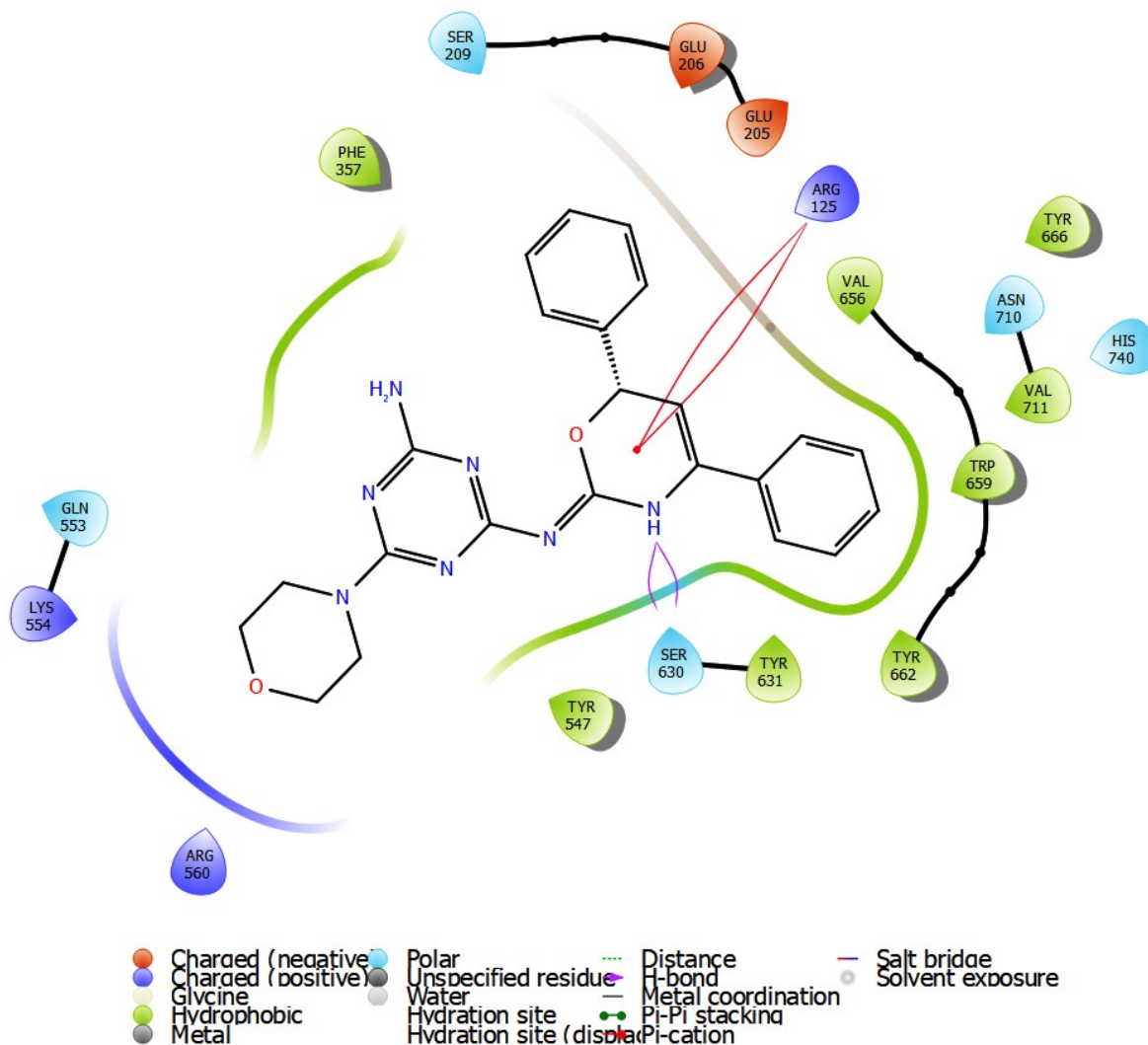


Figure SI 1: Drug-interaction diagram of compound 8(a)

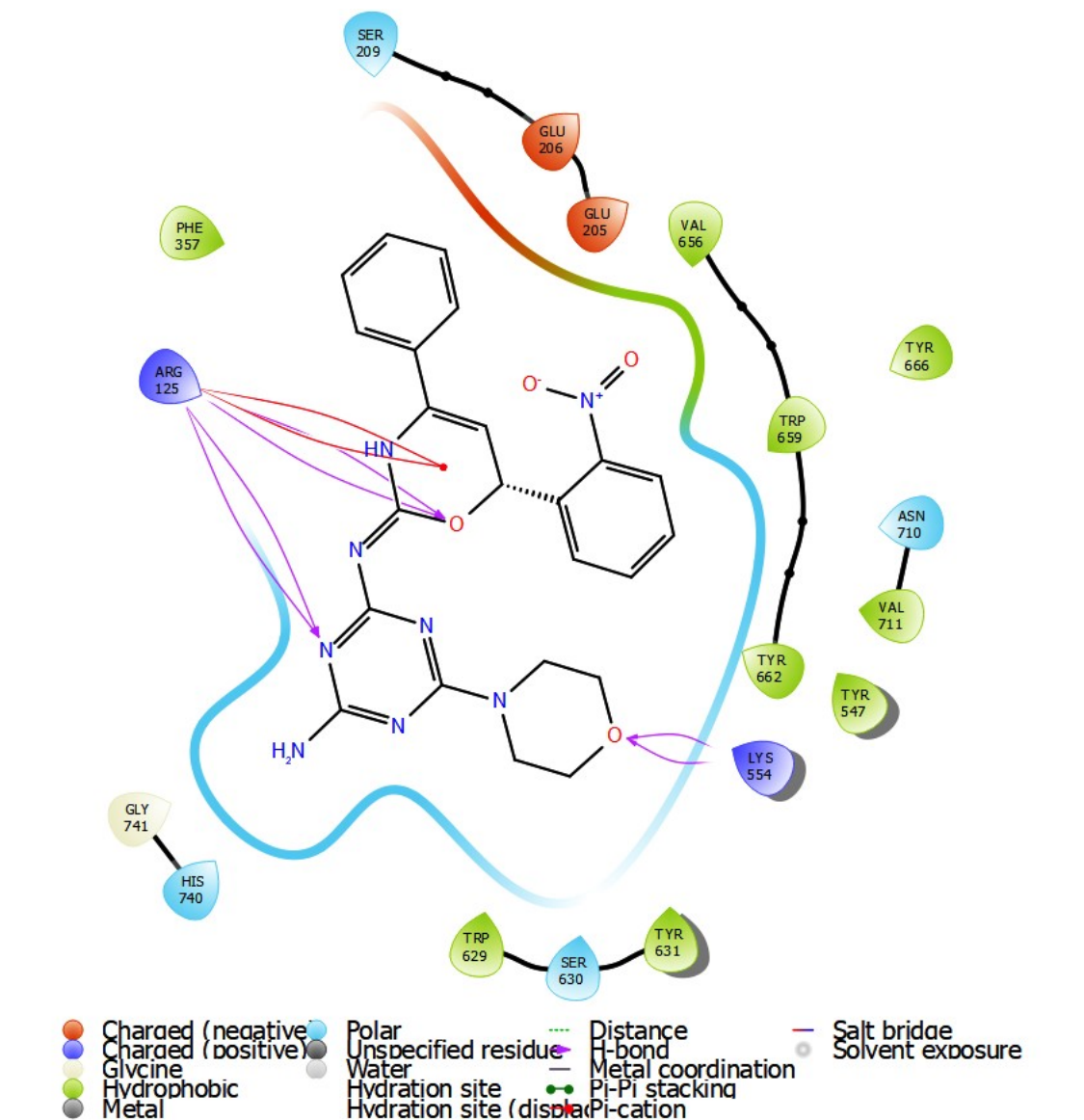


Figure SI 2: Drug-interaction diagram of compound 8(b)

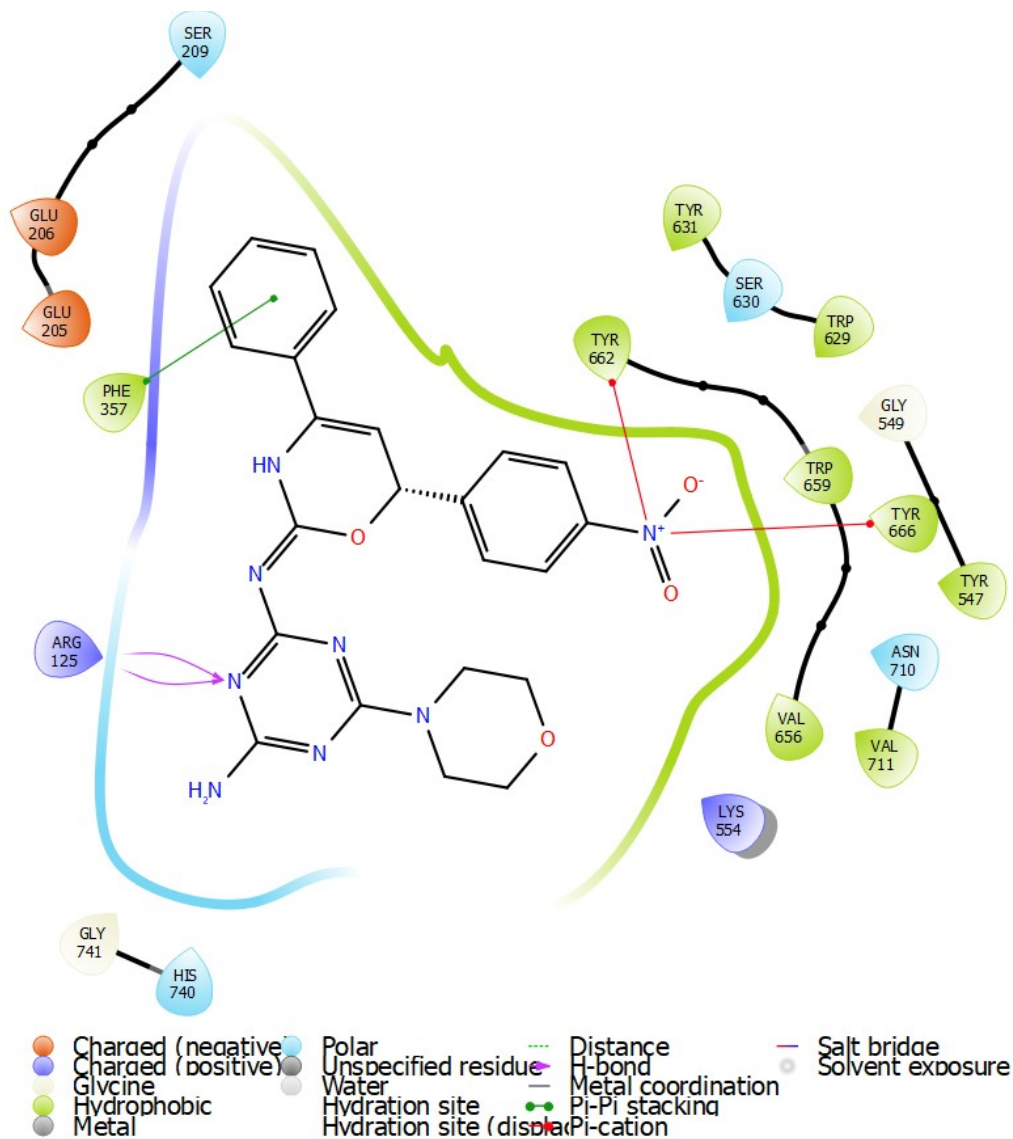


Figure SI 3: Drug-interaction diagram of compound 8(d)

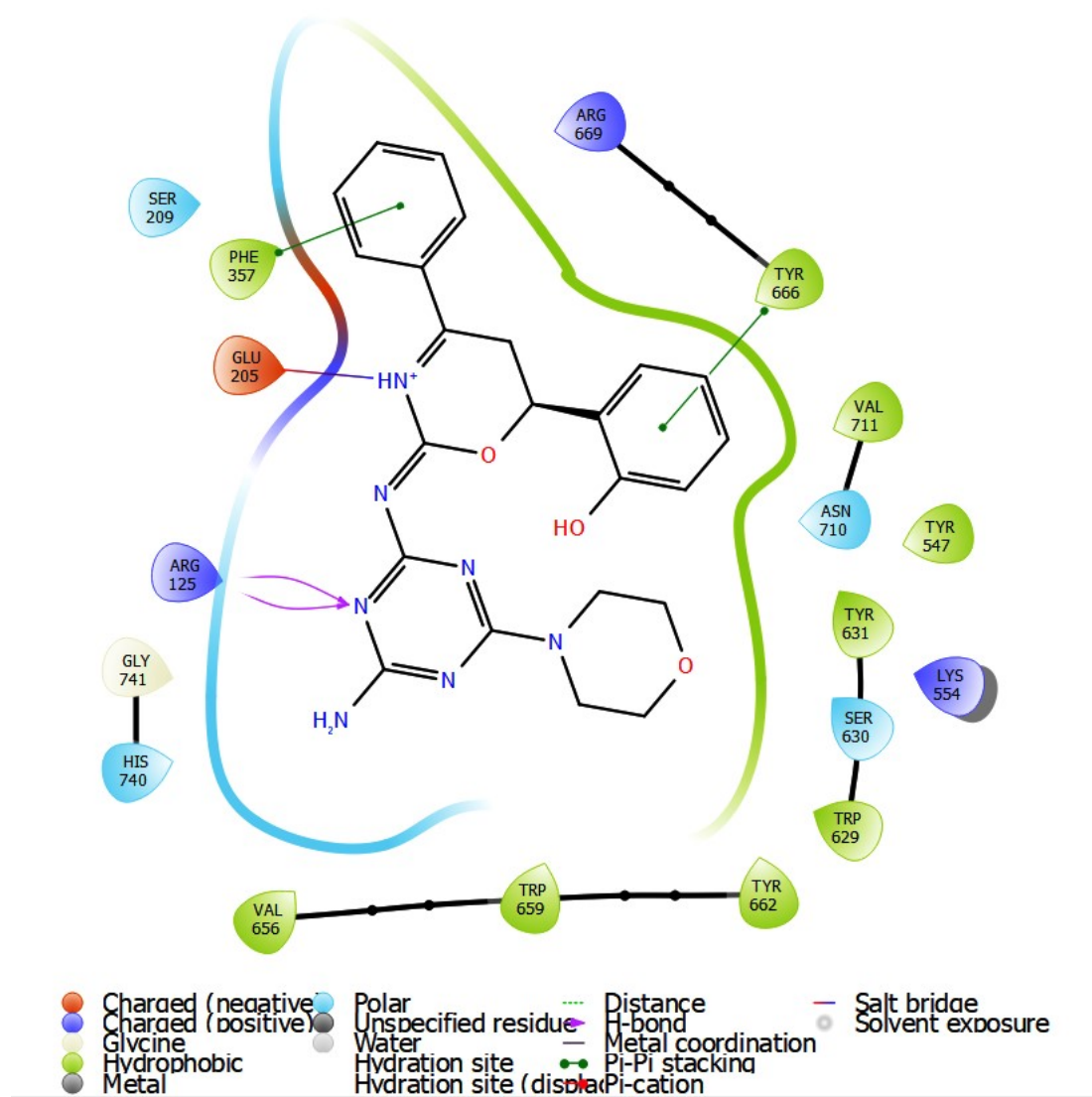


Figure SI 4: Drug-interaction diagram of compound 8(e)

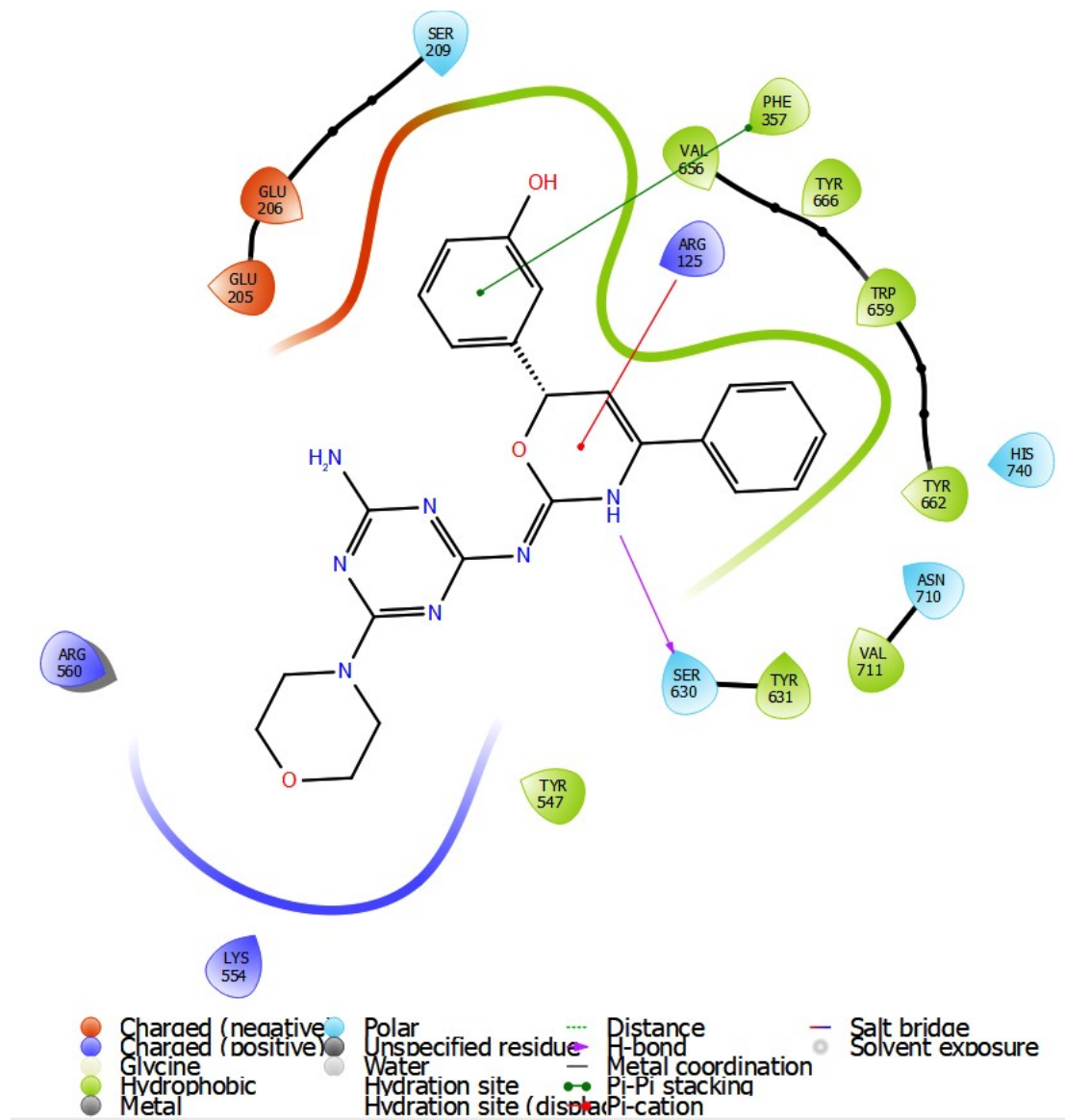


Figure SI 5: Drug-interaction diagram of compound 8(f)

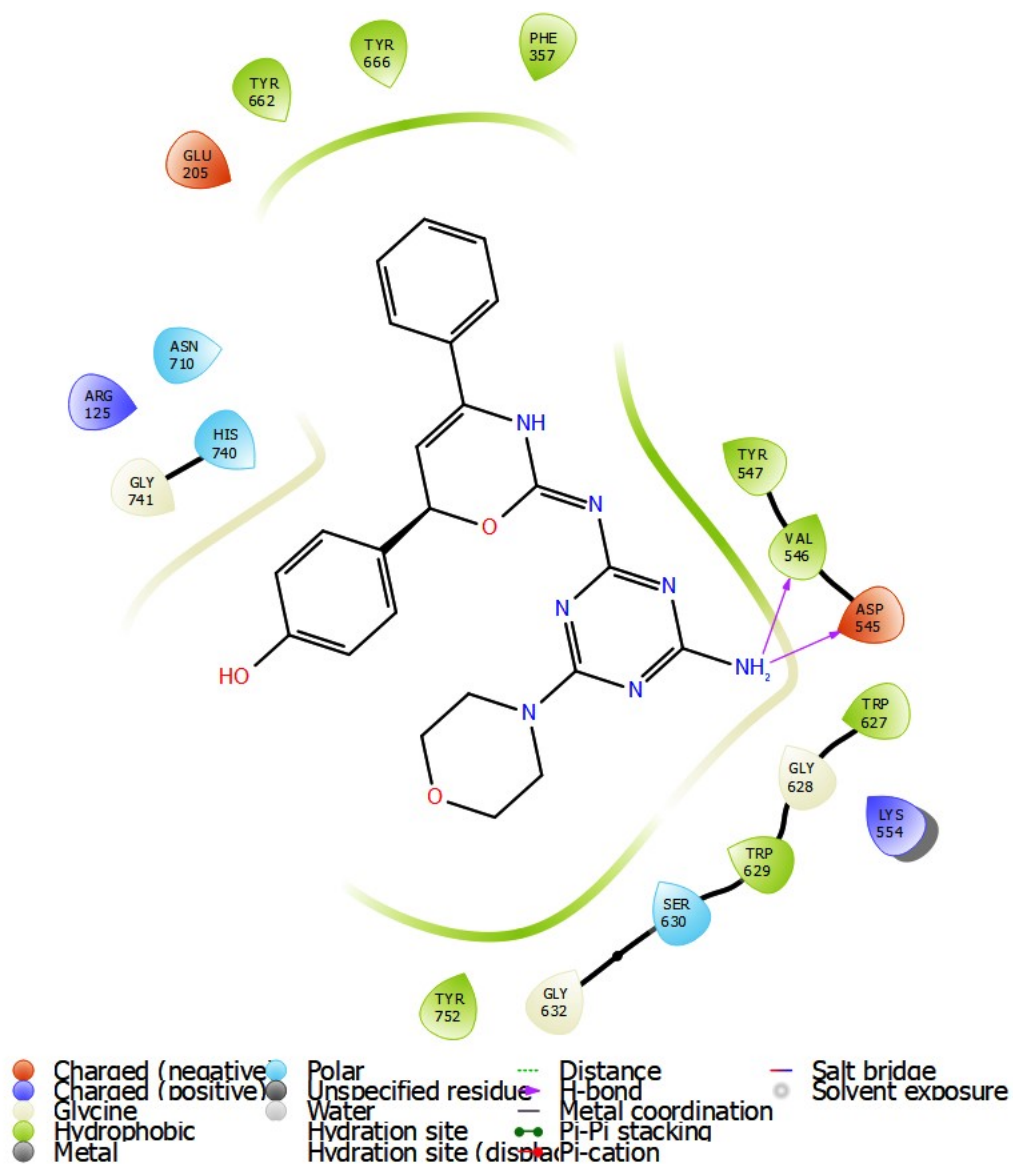


Figure SI 6: Drug-interaction diagram of compound 8(g)

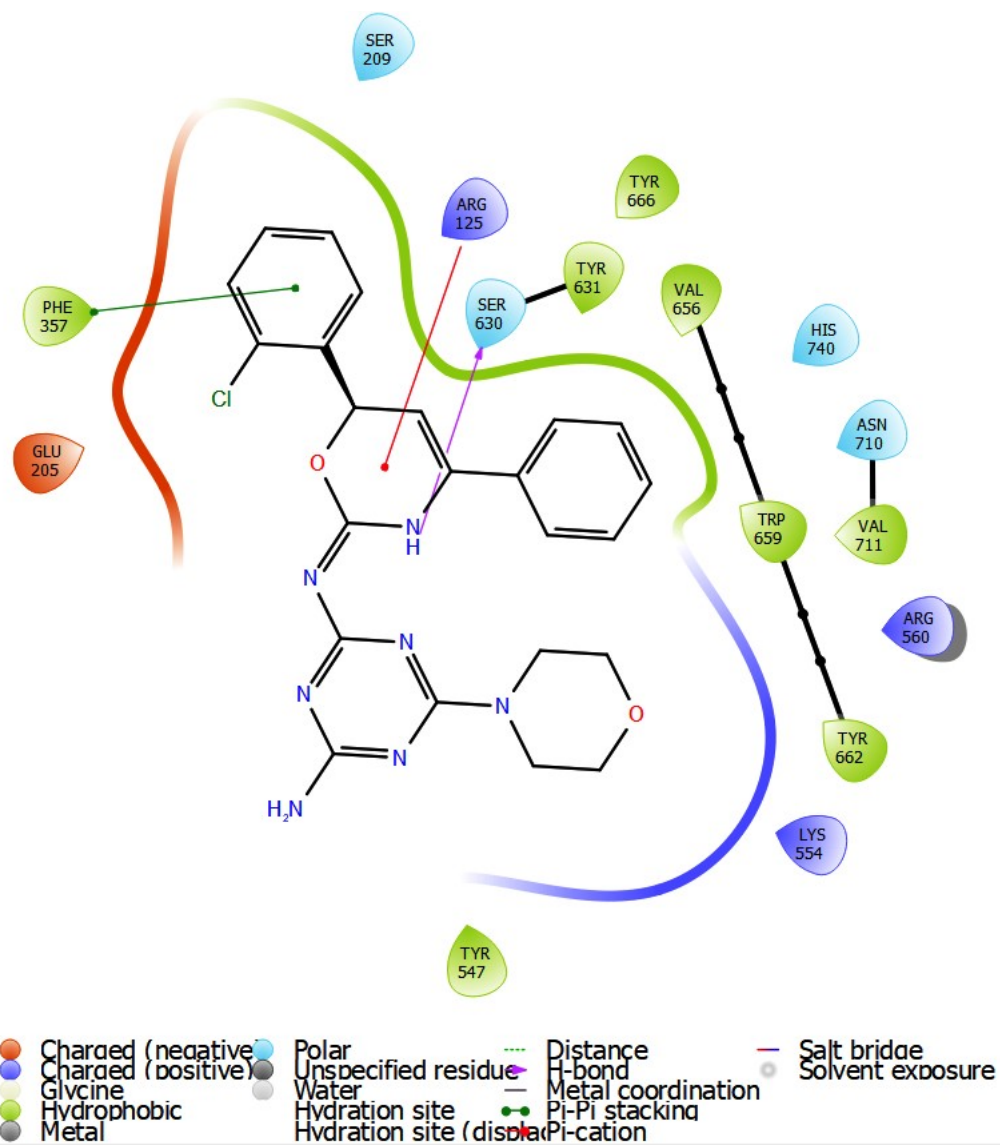


Figure SI 7: Drug-interaction diagram of compound 8(h)

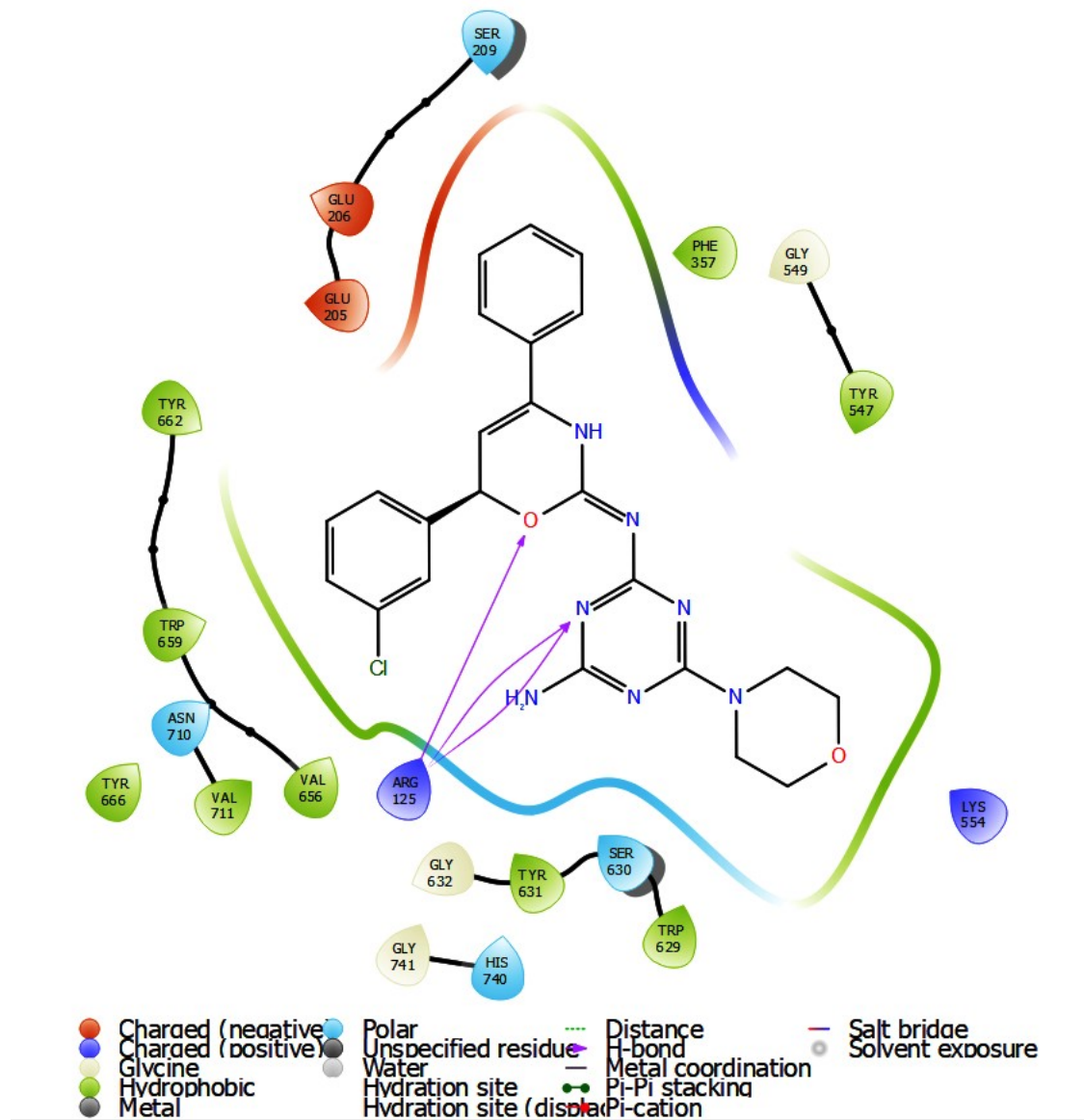


Figure SI 8: Drug-interaction diagram of compound 8(i)

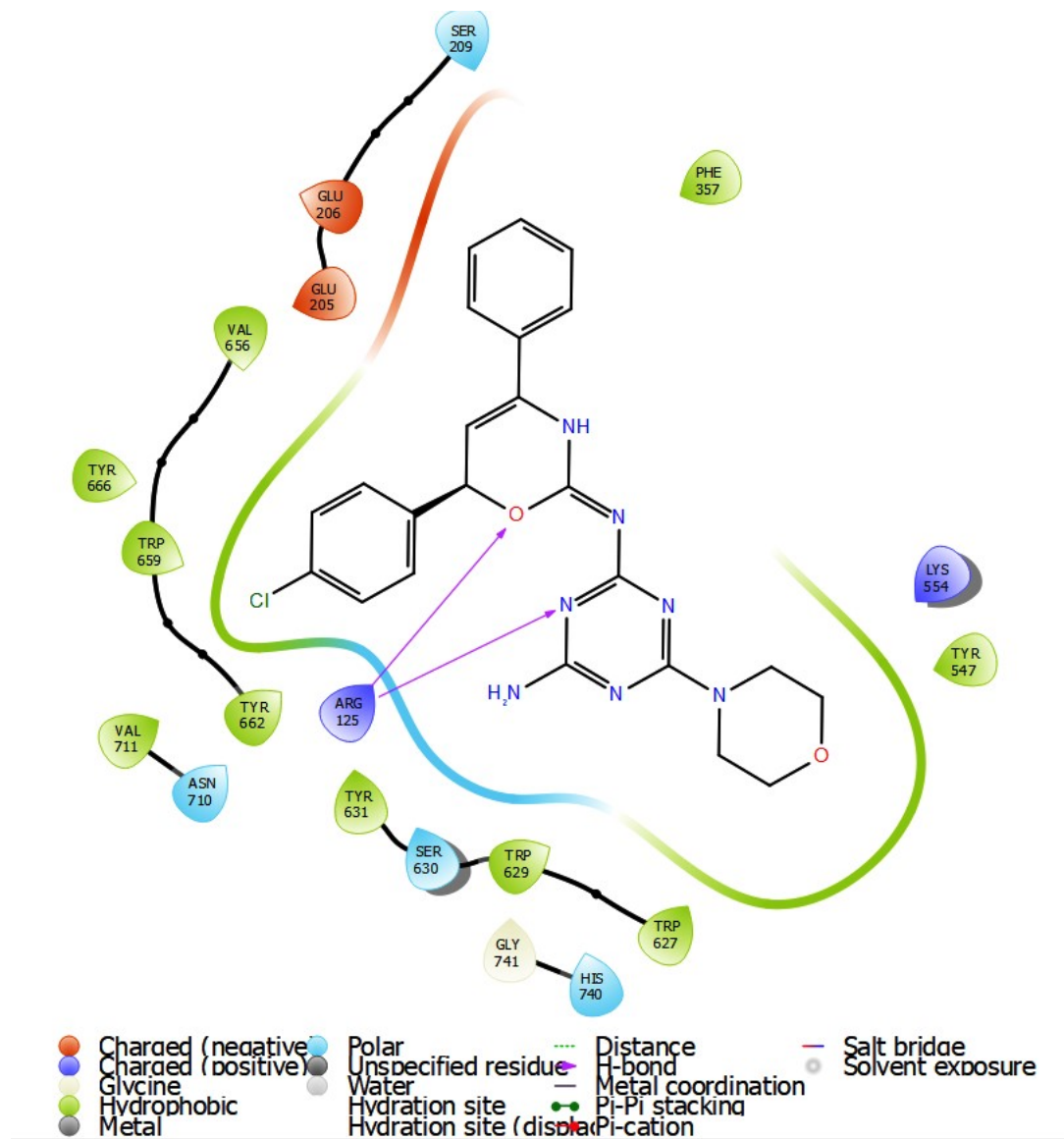


Figure SI 9: Drug-interaction diagram of compound 8(j)

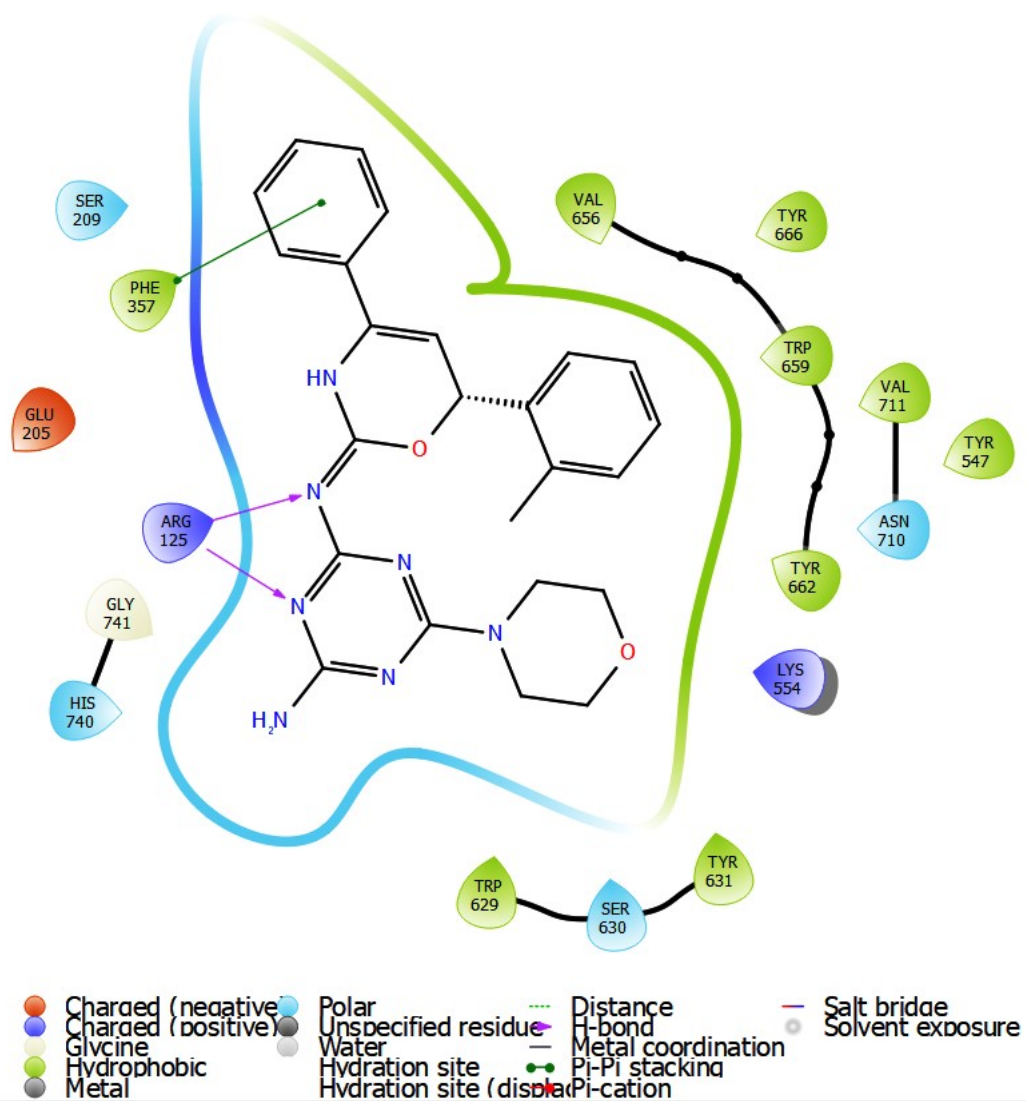


Figure SI 10: Drug-interaction diagram of compound 8(k)

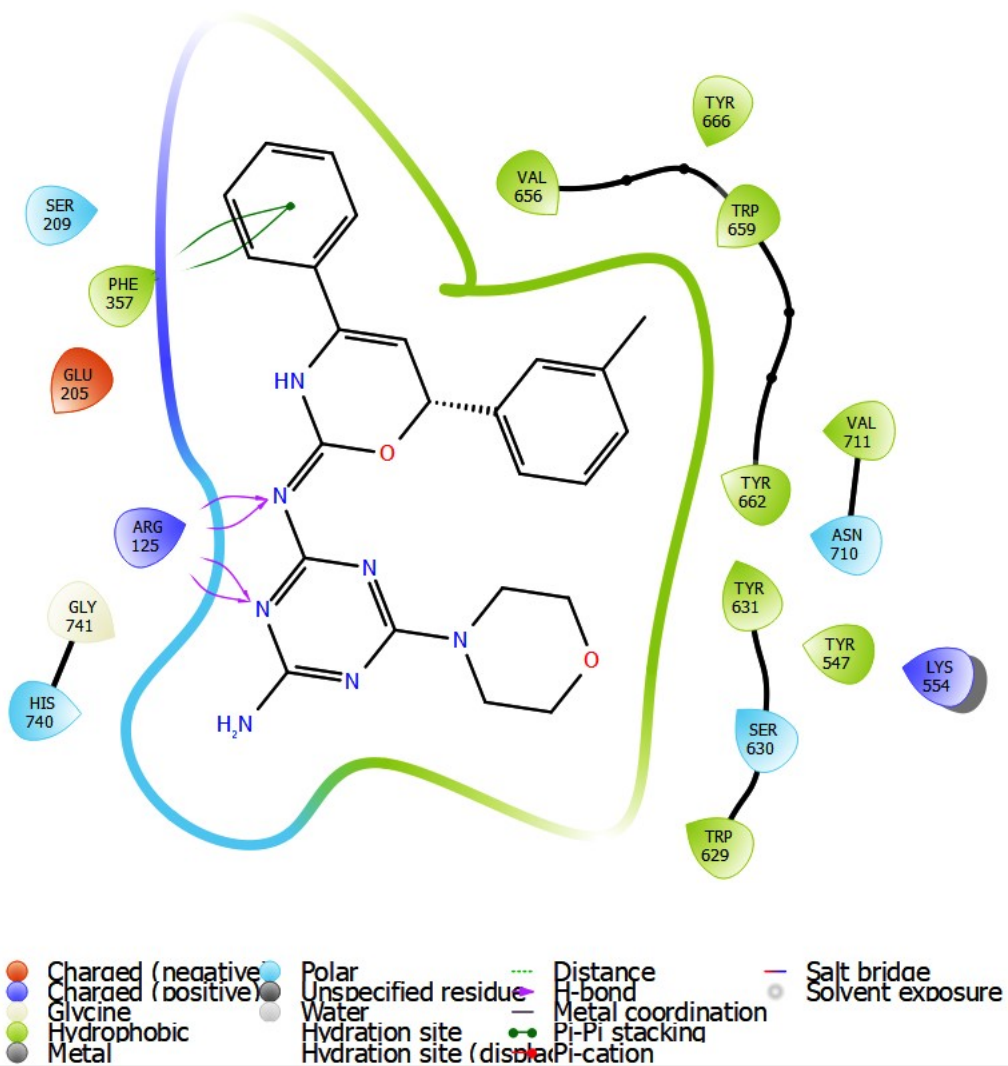


Figure SI 11: Drug-interaction diagram of compound 8(l)

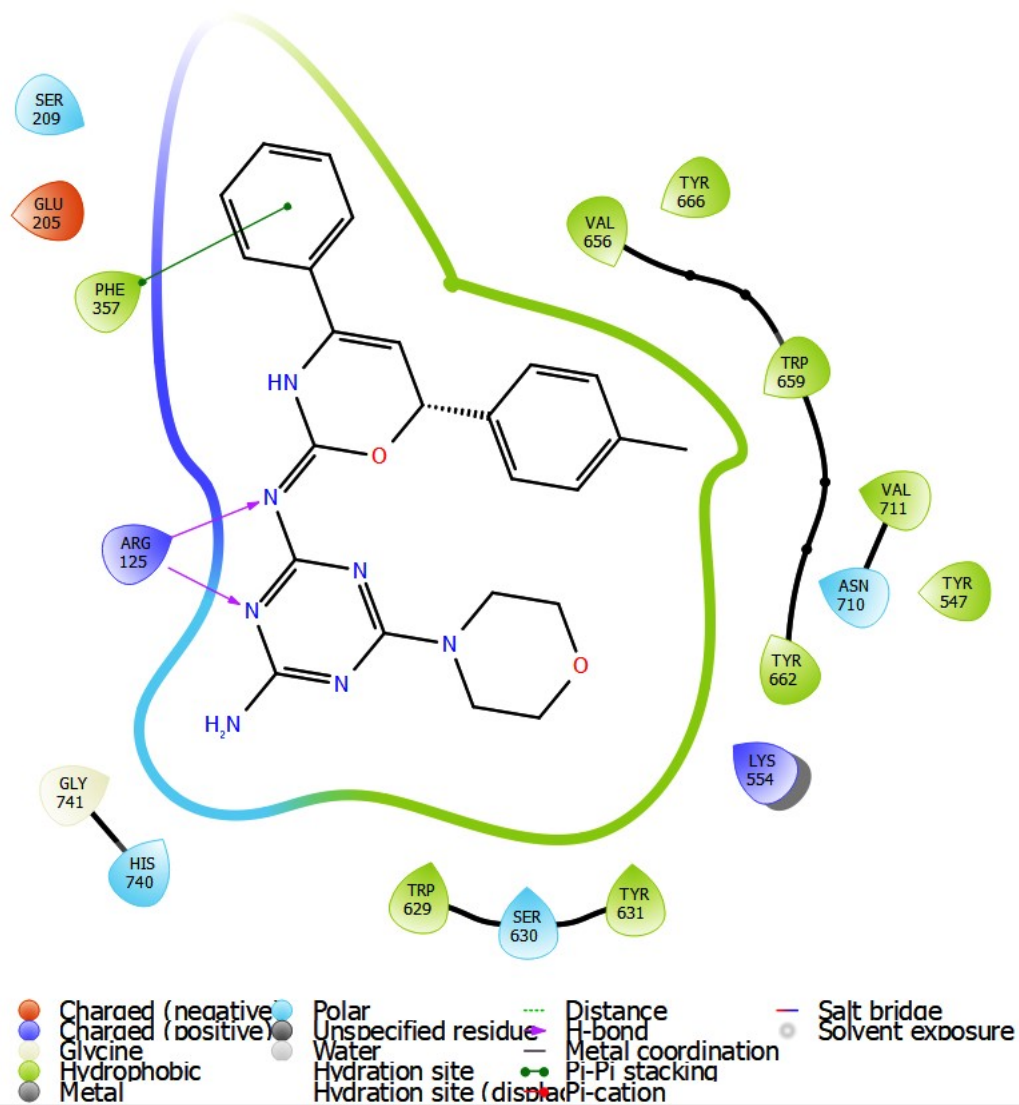


Figure SI 12: Drug-interaction diagram of compound 8(m)

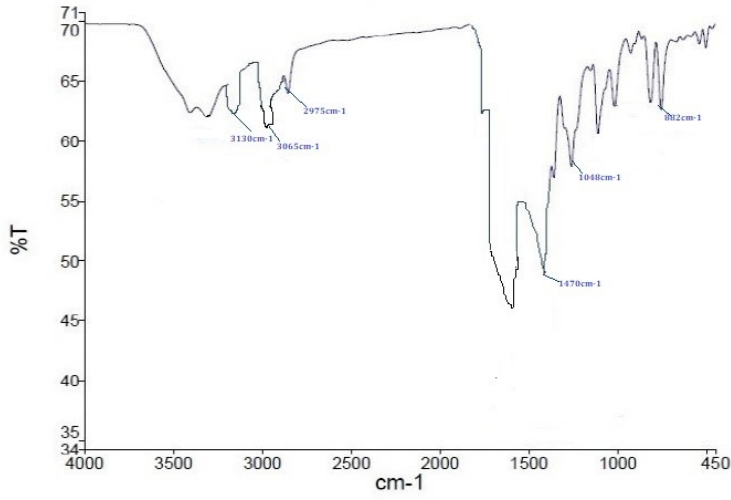
SPECTROSCOPICAL DATA

Compound 8 (a)

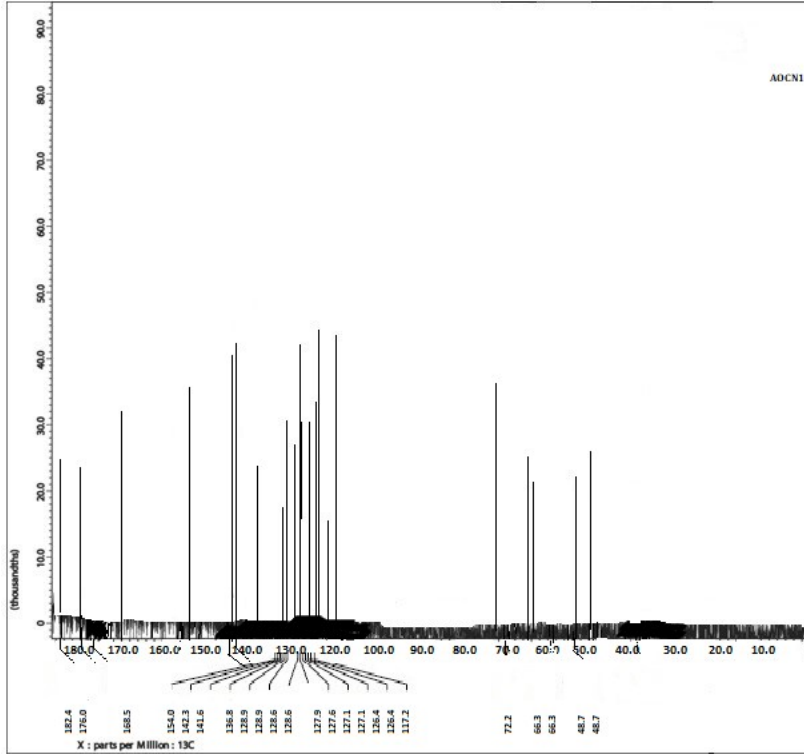
Analyst
Date

SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 10:86 AM

PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 10:86 AM



dharmesh 256.- Sample
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2010476 A011 By
dharmesh Date
Monday
December 06 2021



AOCN1

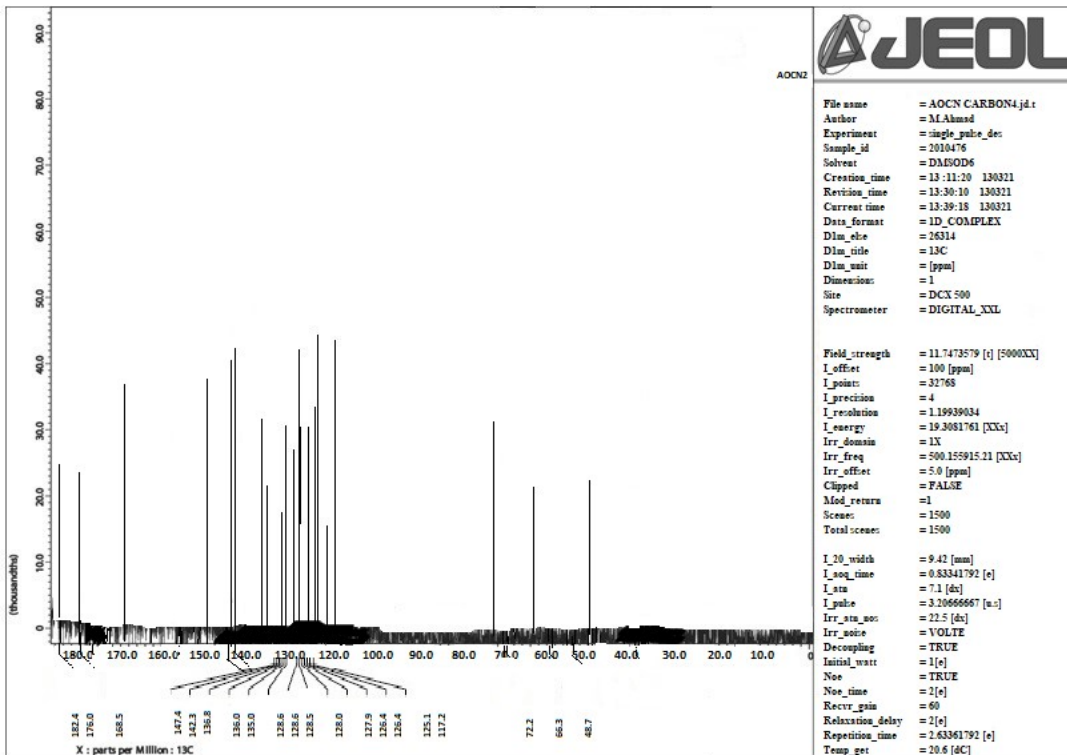
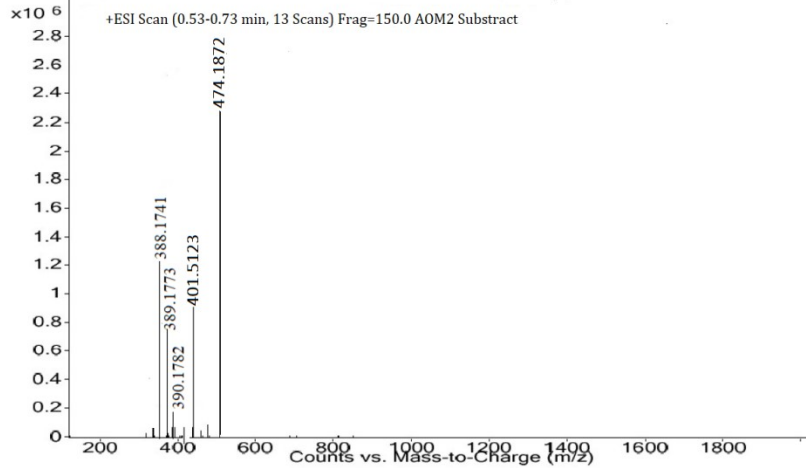
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Revision time = 12:20:18 130321
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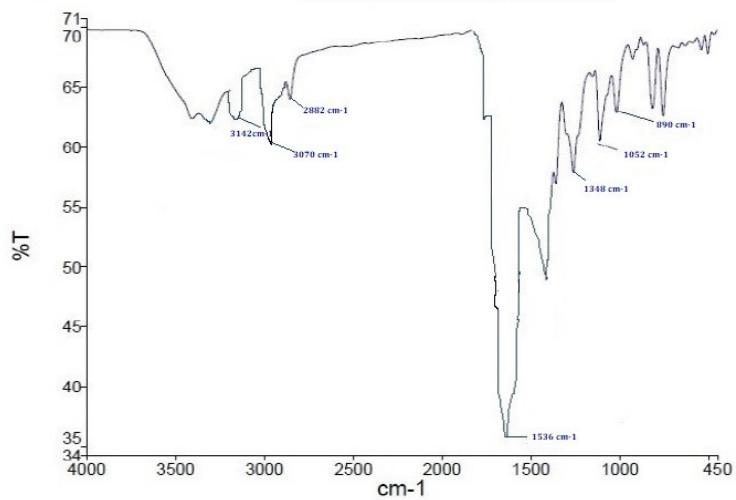
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Compound 8 (c)

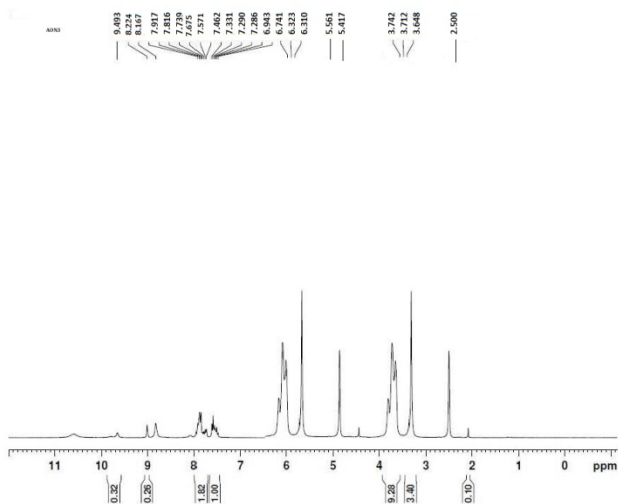
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December 06 2021

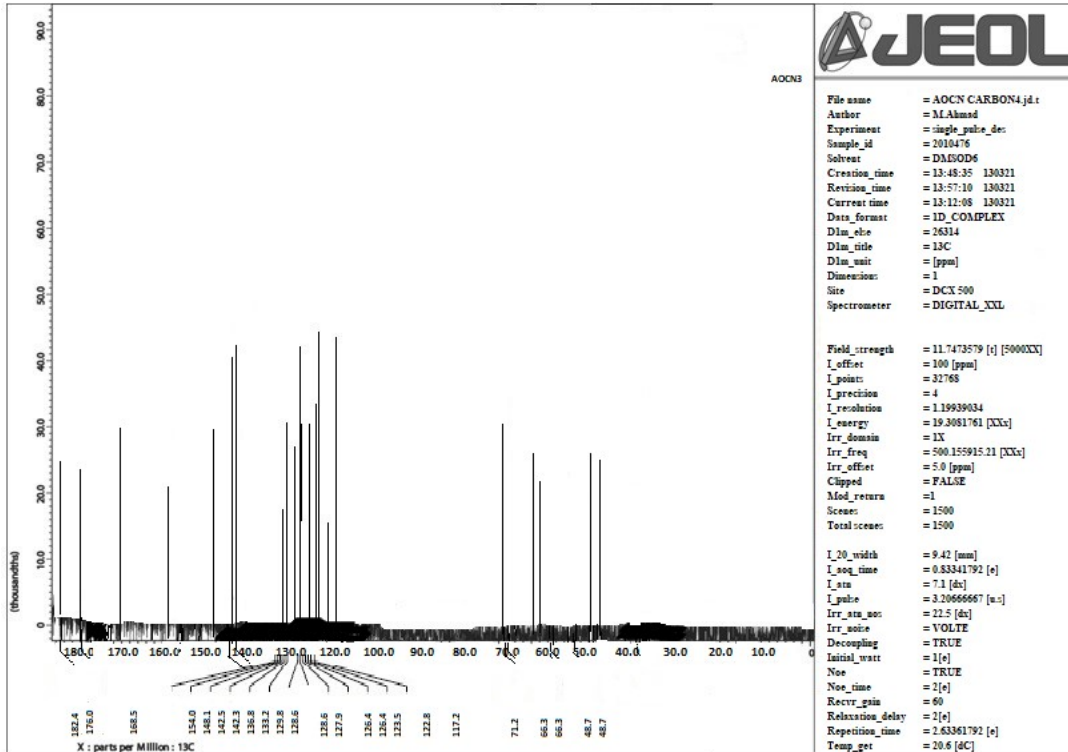
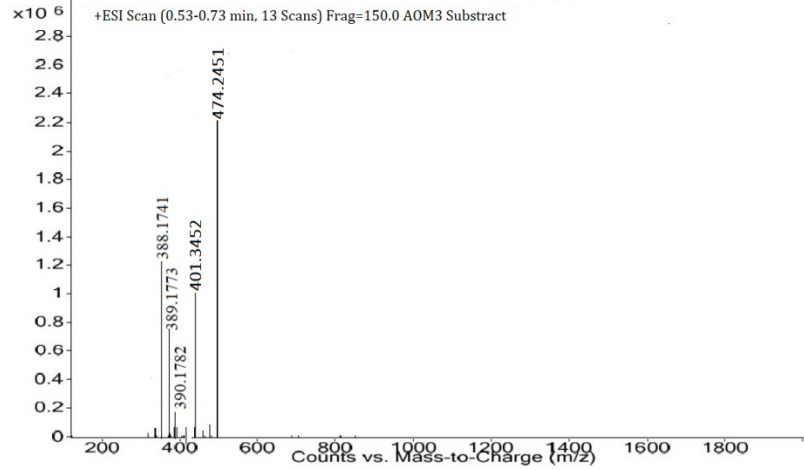


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```

Sample Name	Alanksha (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	3	Inj Position		Sample Type	Sample	IRH Calibration Status	Success
Data Filename	AOM3	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	10/12/2021 11:22:13 AM



AOCN3

File name = AOCN CARBON4.jdt
 Author = M.Ahmad
 Experiment = single_pulse_de
 Sample_id = 2010476
 Solvent = DMSOD6
 Creation_time = 13:48:35 130321
 Revision_time = 13:57:10 130321
 Current_time = 13:12:08 130321
 Data_format = 1D_COMPLEX
 Dia_she = 36314
 Dia_tite = 13C
 Dia_unit = [ppm]
 Dimension = 1
 Site = DCX 500
 Spectrometer = DIGITAL XXL

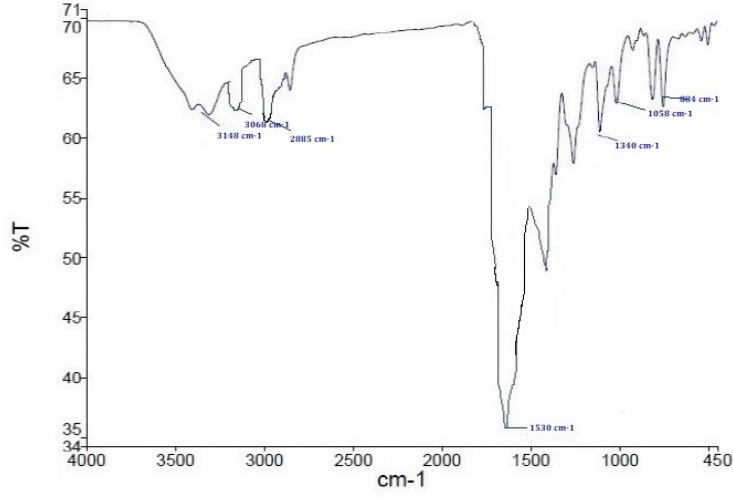
Field_strength = 11.7473579 [t] [5000XX]
 L_offset = 100 [ppm]
 L_point = -32768
 L_precision = 4
 L_resolution = 1.19939034
 L_energy = 19.3081761 [XXs]
 Irr_domain = 1X
 Irr_freq = 500.15591521 [XXs]
 Irr_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scales = 1500
 Total_scales = 1500
 L_20_width = 9.42 [mm]
 L_sog_time = 0.83341792 [e]
 L_tau = -7.1 [ds]
 L_pulse = 3.20666667 [u-]
 Irr_tau_sog = 22.5 [ds]
 Irr_noise = VOLTE
 Decoupling = TRUE
 Initial_watr = 1[e]
 Noe = TRUE
 Noe_time = 2[e]
 Recvr_gain = 60
 Relaxation_delay = 2[e]
 Repetition_time = 2.63361792 [e]
 Temp_get = 20.6 [dC]

Compound 8 (d)

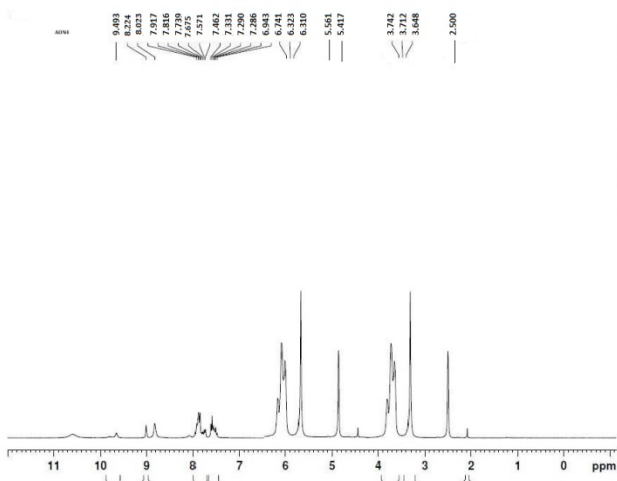
Analyst
Date

SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 11:15 AM

PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 11:15 AM



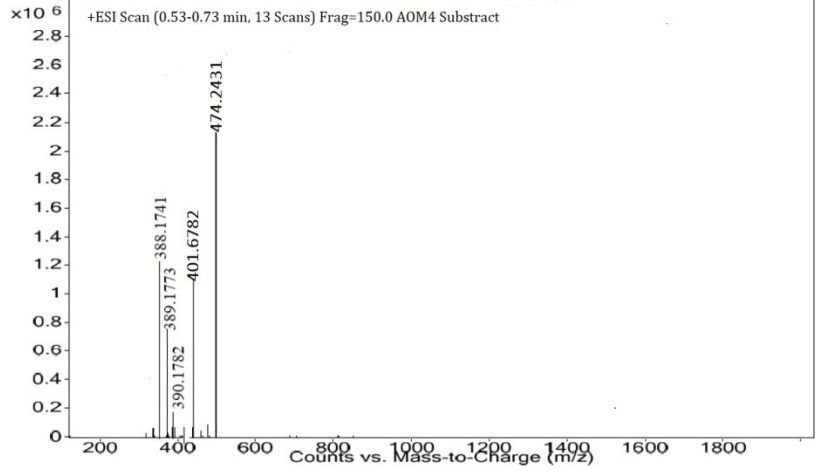
dharmesh 256 - Sample
IR20E09DEC02
2010476.A014 By
dharmesh Date
Monday
December 06 2021



```

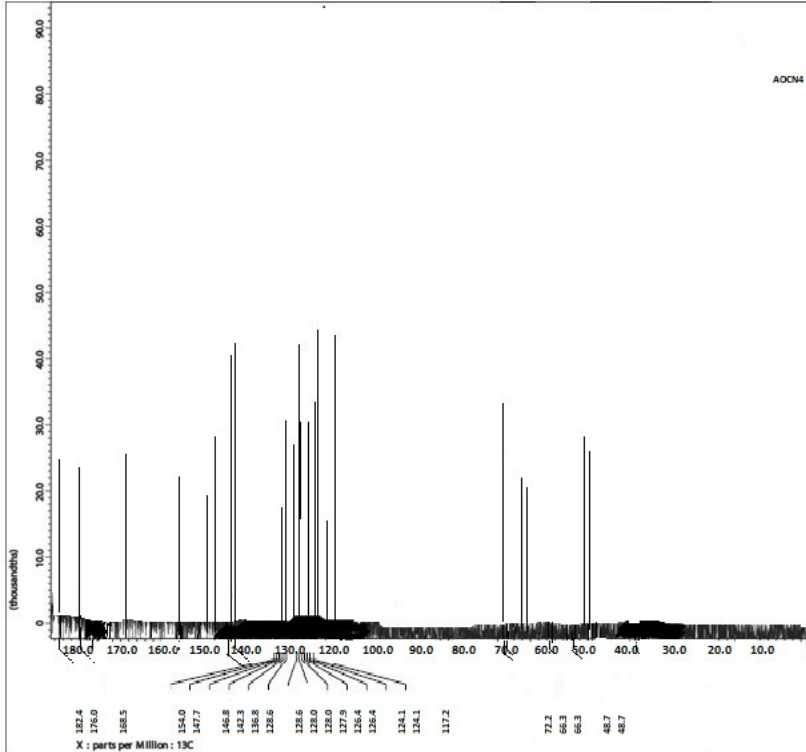
NAME      1274.A04
EXPNO     2
PROCNO    2
Date_     20220308
Time      15.00
INSTRUM   spect
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         512
DS         4
AQ         0.12631930
RG         655.3333333
AQ         0.202228700
RG         655.3333333
F2         100.6261500
F1         125.7613600
SFO       298.15
AQ         0.12631930
RG         655.3333333
F2         100.6261500
F1         125.7613600
SFO       298.15
AQ         0.12631930
RG         655.3333333
F2         100.6261500
F1         125.7613600
SFO       298.15
  
```

Sample Name	Akanisha (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	3	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	AOM4	ACQ Method	ISOGRATIC.m	Comment		Acquired Time	10/12/2021 11:27:23 AM





AOCN4

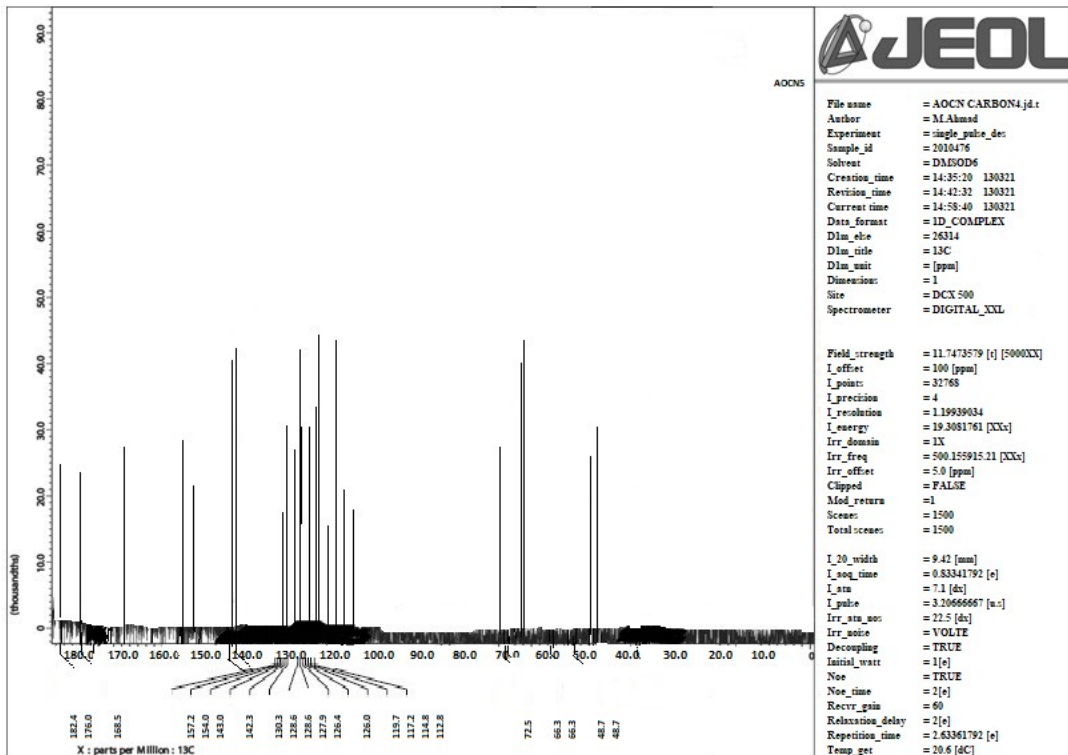
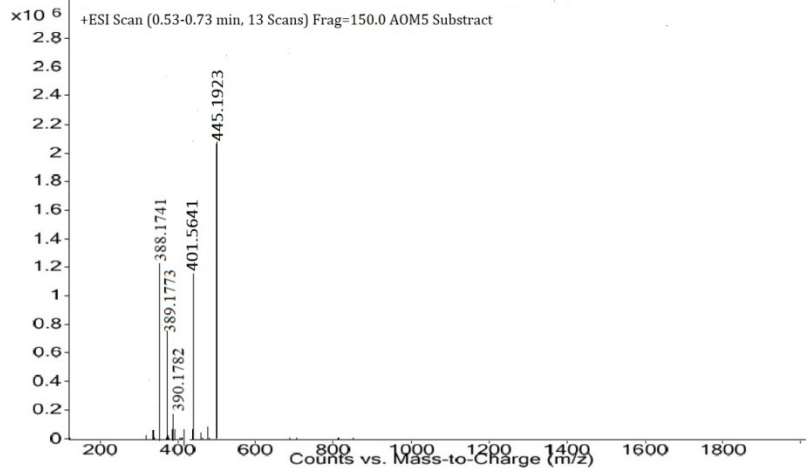


File name = AOCN CARBON4.jd.r
Author = M.Akmal
Experiment = single_pulse_de
Sample_id = 2010476
Solvent = DMSOD6
Creation_time = 14:14:40 130321
Revision_time = 14:22:10 130321
Current_time = 14:32:30 130321
Data_format = ID_COMPLEX
Dim_ebe = 16314
Dim_tide = 13C
Dim_unit = [ppm]
Dimension = 1
Site = DCX 500
Spectrometer = DIGITAL XXL

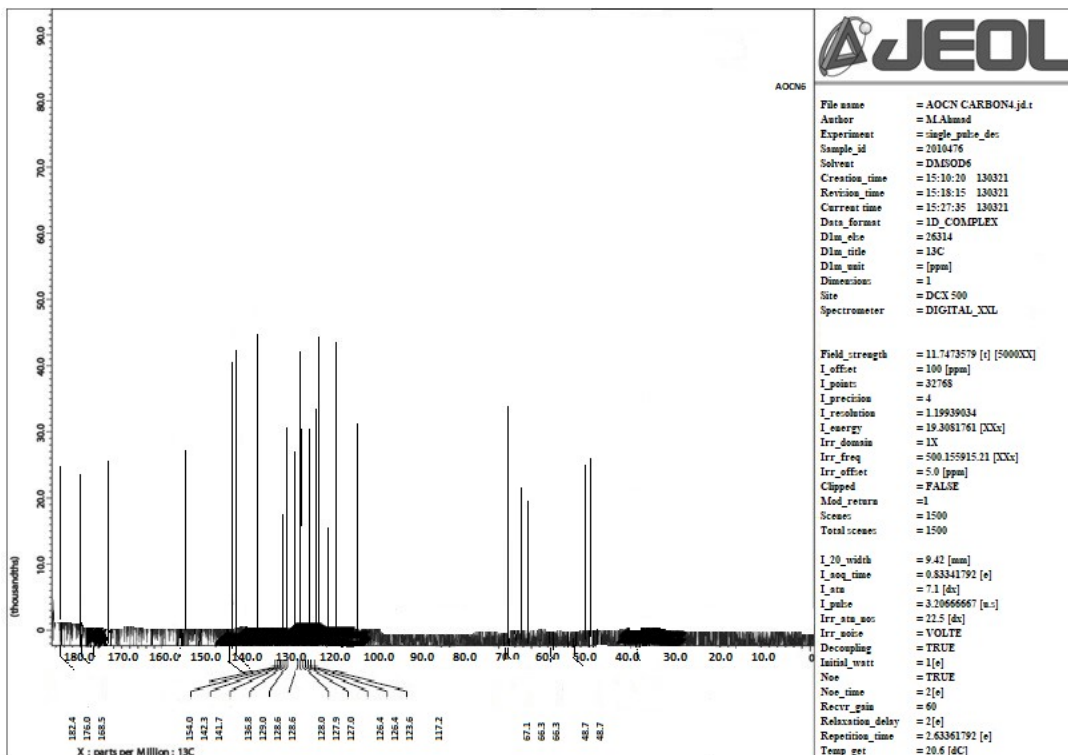
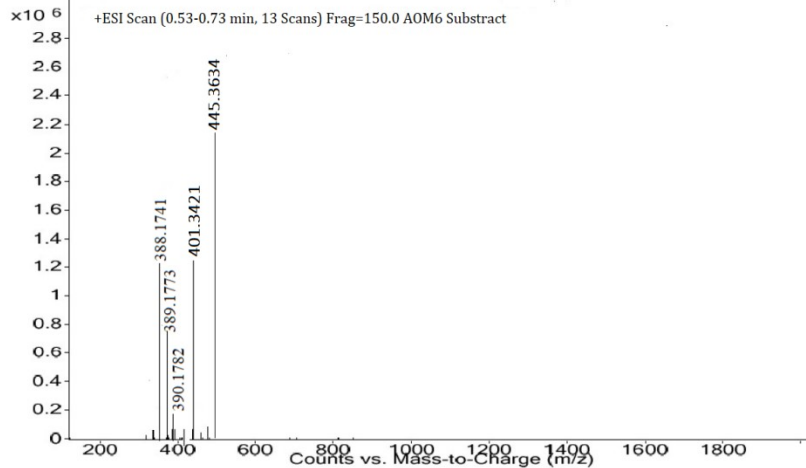
Field_strength = 11.7473579 [t] [50000XX]
F_offset = 100 [ppm]
F_point = 32768
F_precision = 4
F_resolution = 1.19939034
F_energy = 19.3081761 [XXs]
Fv_domain = 1X
Fv_freq = 500.15591511 [XXs]
Fv_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1500
Total_scans = 1500

I_20_width = 9.42 [mm]
I_acq_time = 0.83341792 [s]
I_sns = 7.1 [ds]
I_pulse = 3.20666667 [a.s]
Iv_sns_pos = 22.5 [ds]
Iv_sns = VOLTE
Decoupling = TRUE
Initial_walt = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.63361792 [s]
Temp_get = 20.6 [dC]

Sample Name	Alanksha (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	3	InjPosition		Sample Type	Sample	IRH Calibration Status	Success
Data Filename	AOMS	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	10/12/2021 11:32:11 AM



Sample Name	Alanksha (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	3	Inj Position		Sample Type	Sample	IMM Calibration Status	Success
Data Filename	AOM6	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	10/12/2021 11:37:49 AM



AOCN6

File name	= AOCN CARBON4.jdt
Author	= M.Akmod
Experiment	= single_pulse_de
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 15:10:20 130321
Revision_time	= 15:18:15 130321
Current_time	= 15:27:35 130321
Data_format	= ID_COMPLEX
Dlm_cde	= 26314
Dlm_tide	= 13C
Dlm_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL XXL

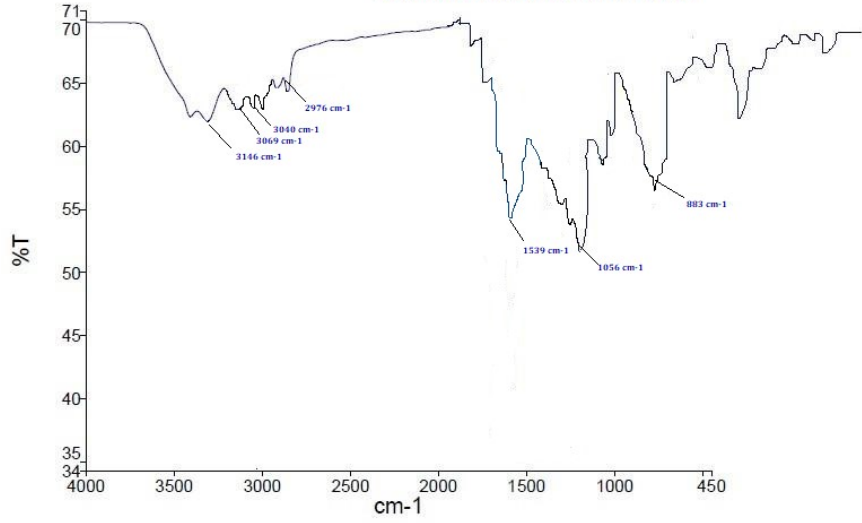
Field_strength	= 11.747879 [t] [5000XX]
L_offset	= 100 [ppm]
L_point	= 32768
L_precision	= 4
L_resolution	= 1.19839034
L_energy	= 19.3061741 [XXs]
Irr_domain	= 1X
Irr_freq	= 500.15591521 [XXs]
Irr_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	= 1
Scenes	= 1500
Total_scenes	= 1500
L20_width	= 9.42 [mm]
L20q_time	= 0.83341792 [e]
L20s	= 7.1 [dc]
L20pbe	= 3.20666667 [u-s]
Irr_sqr_sqr	= 22.5 [db]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_wat	= 1[e]
Noe	= TRUE
Noe_time	= 2[e]
Recvr_gain	= 60
Relaxation_delay	= 2[e]
Repetition_time	= 2.63361792 [e]
Temp_get	= 20.6 [dC]

Compound 8 (g)

Analyst
Date

SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 11:38 AM

PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 11:38 AM



dharmesh 256_ Sample
IR20E09DEC02
2010476 A017 By
dharmesh Date
Monday
December 06 2021

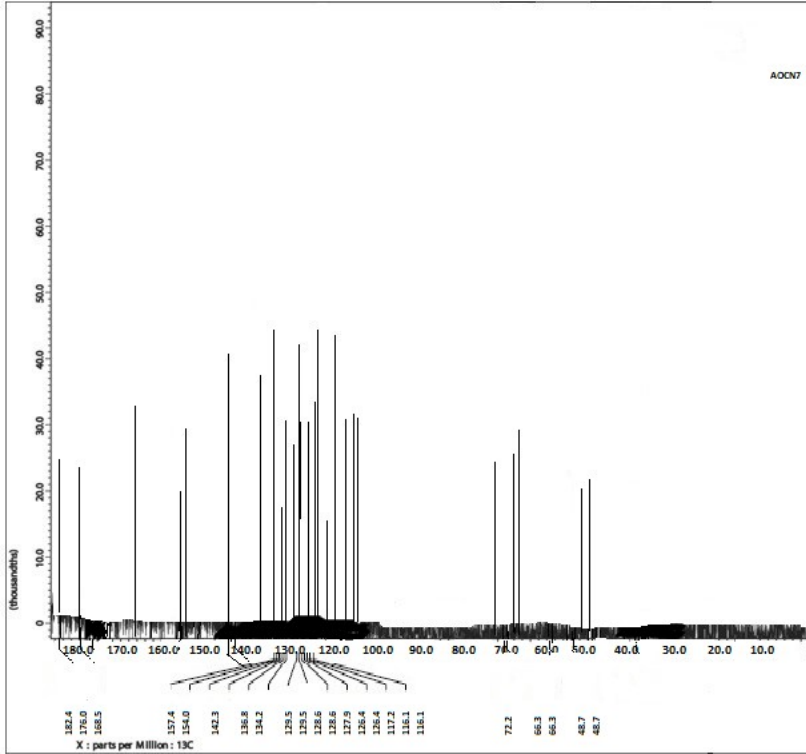


AOCN7

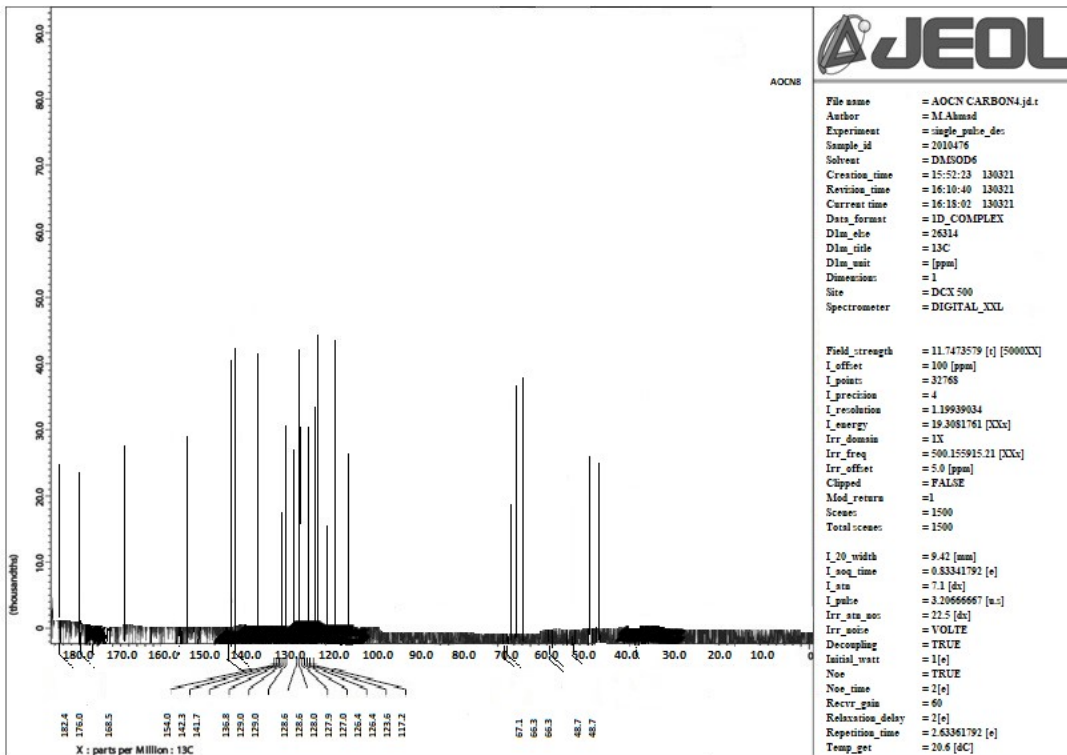
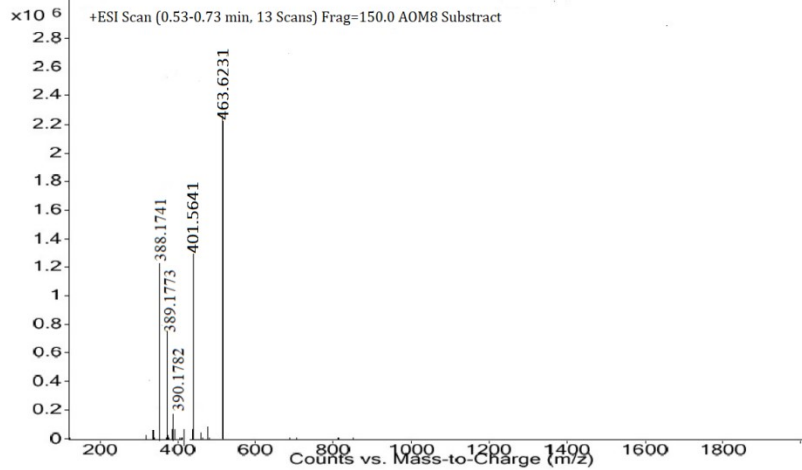
File name = AOCN CARBON4.jdt
Author = M.Ahmad
Experiment = single_pulse_det
Sample_id = 2010476
Solvent = DMSOD6
Creation_time = 15:29:20 130311
Revision_time = 15:38:12 130311
Current_time = 15:46:20 130311
Data_format = 1D_COMPLEX
Dia_eht = 26314
Dia_tilt = 13C
Dia_unit = [ppm]
Dimension = 1
Site = DCX 500
Spectrometer = DIGITAL XXL

Field_strength = 11.7473579 [t] [5000XX]
L_offset = 100 [ppm]
L_point = 32768
L_precision = 4
L_resolution = 1.19939034
L_energy = 19.3081761 [XXs]
Irr_domain = 1X
Irr_freq = 500.155915.21 [XXs]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1500
Total_scans = 1500

I_20_width = 9.42 [mm]
I_sac_time = 0.83341792 [s]
I_sta = 7.1 [ds]
I_pabe = 3.20666667 [m.s]
Irr_sta_sos = 22.5 [ds]
Irr_noise = VOLTE
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recv_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.63361792 [s]
Temp_set = 29.6 [dC]



Sample Name	Alarika (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	3	InjPosition		SampleType	Sample	IRH Calibration Status	Success
Data Filename	AOM8	Acq Method	ISOCRATIC.m	Comment		Acquired Time	10/12/2021 11:54:19 AM



AOCN8

File name	= AOCN CARBON4.jdt
Author	= M.Ahmad
Experiment	= single_pulse_de
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 15:52:23 130321
Revision_time	= 16:10:40 130321
Current time	= 16:18:02 130321
Data_format	= 1D_COMPLEX
Dlm_ole	= 26314
Dlm_title	= 13C
Dlm_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL XXL

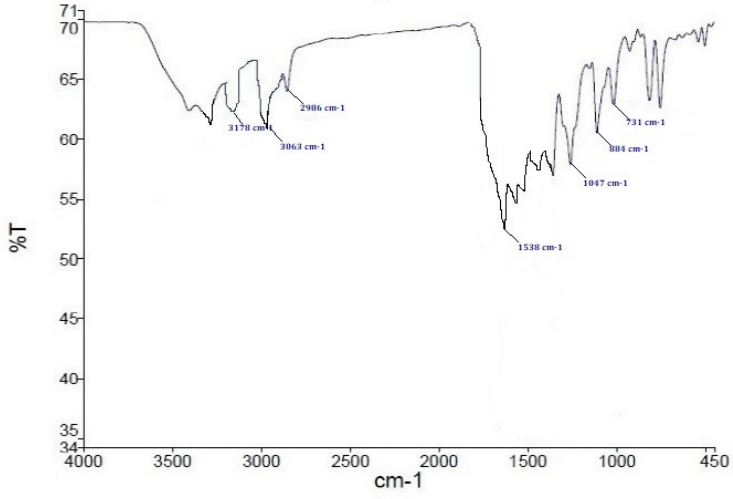
Field_strength	= 11.7473579 [t] [5000XX]
L_offset	= 100 [ppm]
L_p0	= 21765
L_precision	= 4
L_resolution	= 1.19939034
L_energy	= 19.3081761 [XXz]
Irr_domain	= 1X
Irr_freq	= 500.15591521 [XXz]
Irr_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 1500
Total_scans	= 1500
L_20_width	= 9.42 [mm]
L_acq_time	= 0.83341792 [e]
L_sra	= 7.1 [dt]
L_pulse	= 3.20666667 [u:]
Irr_sra_pos	= 22.5 [dt]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watr	= 1[e]
Noe	= TRUE
Noe_time	= 2[e]
Recvr_gain	= 60
Relaxation_delay	= 2[e]
Repetition_time	= 2.63361792 [e]
Temp_get	= 20.6 [dC]

Compound 8 (i)

Analyst
Date

SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 11:52 AM

PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 11:52 AM



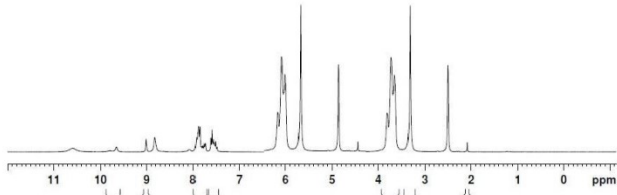
dharmesh 256 - Sample
IR20E09DEC02
2010476 A019 By
dharmesh Date
Monday
December 06 2021



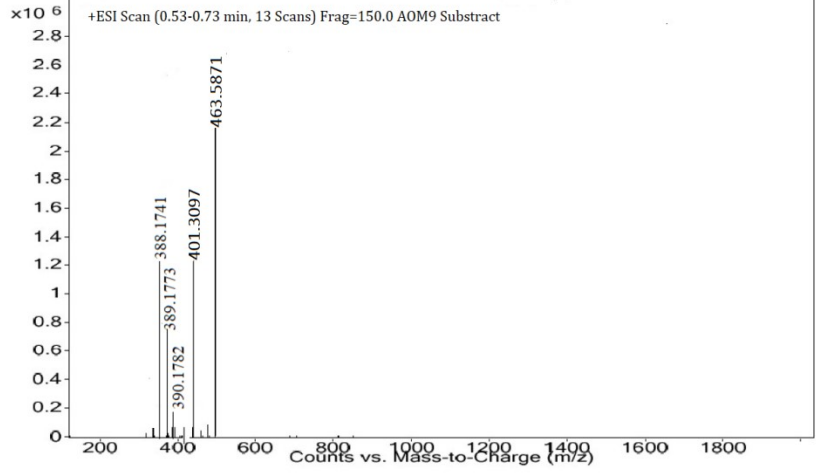
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NAME 1274.A.MS
EXPNO 1
PROCNO 1
Date_ 20201208
Time 15:08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SFO 400
AQ 0.500
RG 327.5
DE 0.150
TE 300.2
F2 -
F3 -
F4 -
F5 -
F6 -
F7 -
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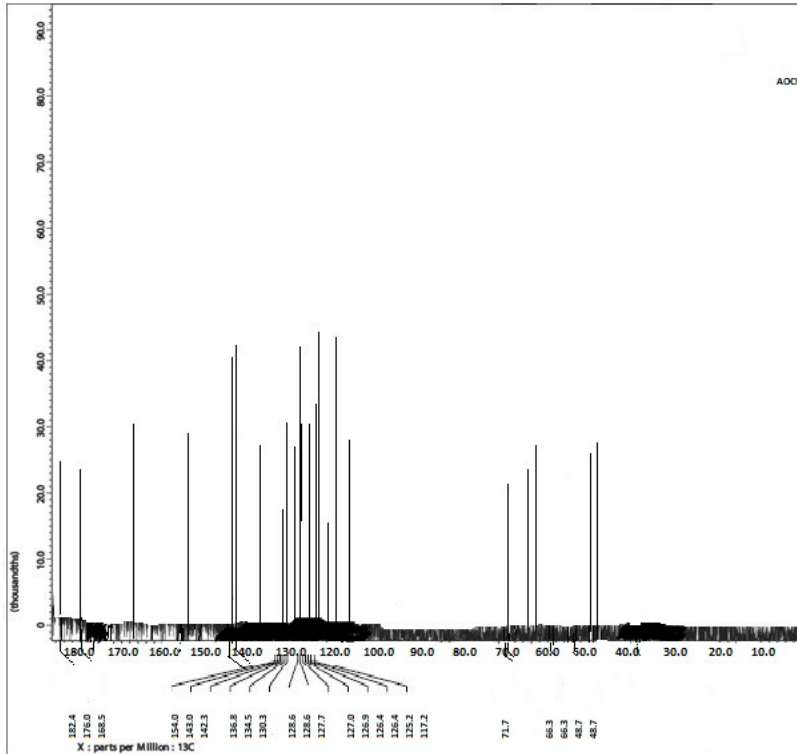


Sample Name	Akanisha (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	IRM Calibration Status	Success
Inj Vol	3	Inj Position		Sample Type	Sample	IRM Calibration Status		
Data Filename	AOM9	ACQ Method	ISOCRATIC.m	Comment		Acquired Time		10/12/2021 11:53:57 AM





AOCN9

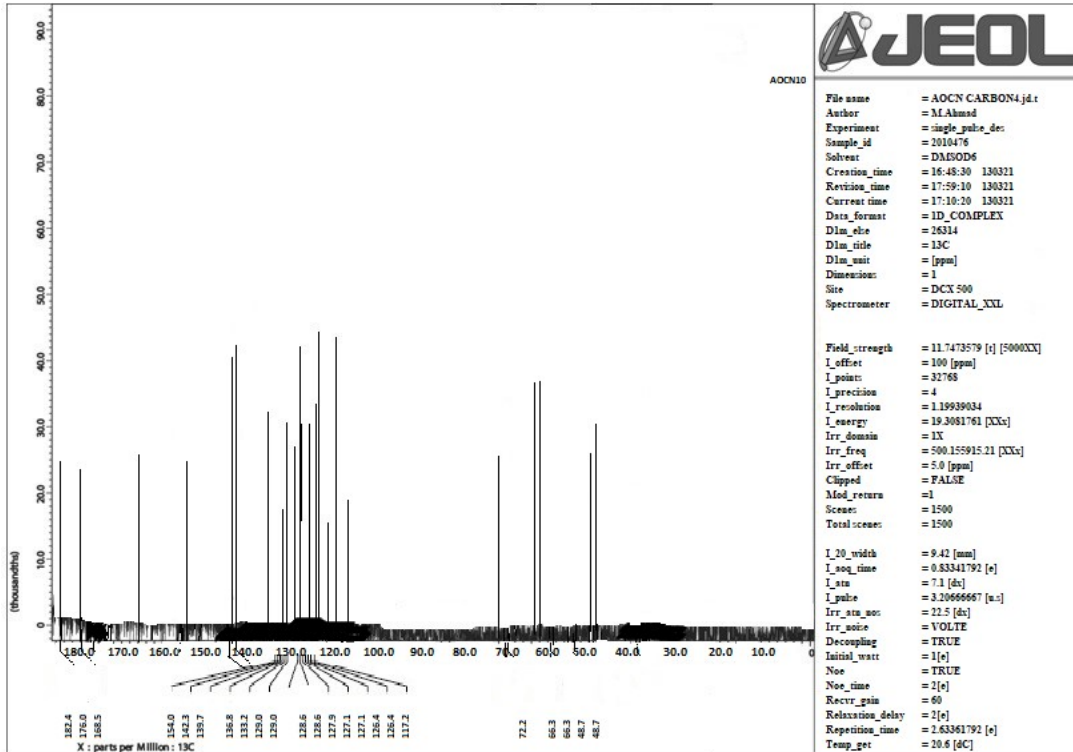
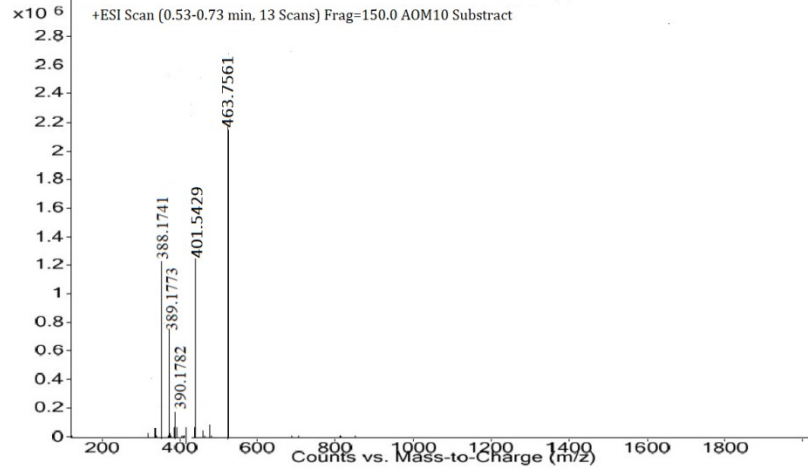


File name = AOCN CARBON4.jd.r
Author = M.Akmal
Experiment = single_pulse_dec
Sample_id = 2010476
Solvent = DMSOD6
Creation_time = 16:13:10 130321
Revision_time = 16:31:16 130321
Current_time = 16:42:40 130321
Data_format = 1D_COMPLEX
Dia_ehe = 26314
Dia_title = 13C
Dia_unit = [ppm]
Dimension = 1
Site = DCX 500
Spectrometer = DIGITAL XXL

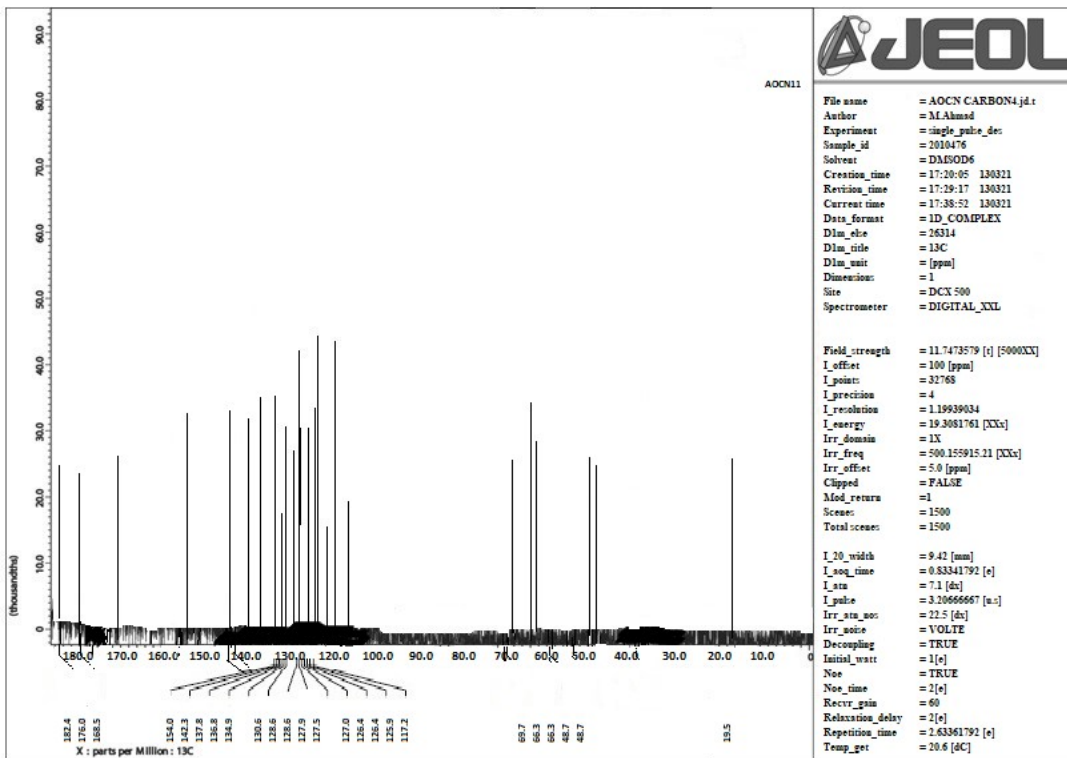
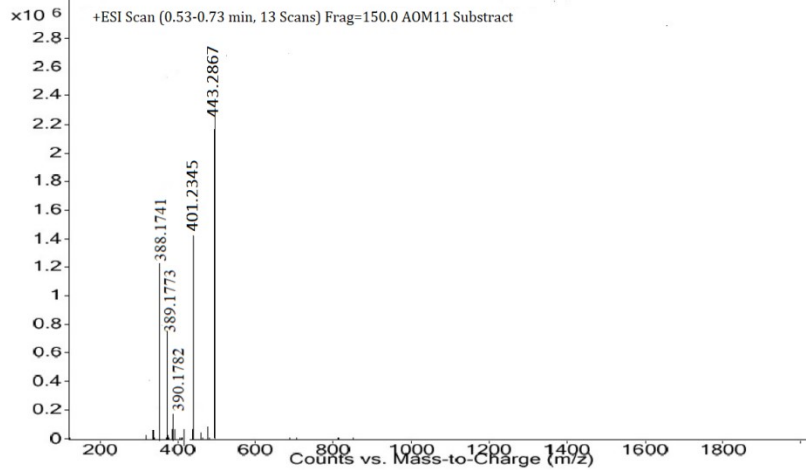
Field_strength = 11.7473579 [t] [5000XX]
F_offset = 100 [ppm]
F_point = 32765
F_precision = 4
F_resolution = 1.19939034
F_energy = 19.3061761 [XXs]
Irr_domain = 1X
Irr_freq = 500.155915.21 [XXs]
Irr_offset = 5.0 [ppm]
Cropped = FALSE
Mod_return = 1
Scans = 1500
Total_scans = 1500

I_20_width = 9.42 [mm]
I_ssq_time = 0.83341792 [e]
I_sta = 7.1 [ds]
I_pulse = 3.20666667 [u.s]
Irr_sta_soc = 22.5 [ds]
Irr_socie = VOLTE
Decoupling = TRUE
Initial_wact = 1[e]
Noe = TRUE
Noe_time = 2[e]
Recvr_gain = 60
Relaxation_delay = 2[e]
Repetition_time = 2.63361792 [e]
Temp_get = 20.6 [dC]

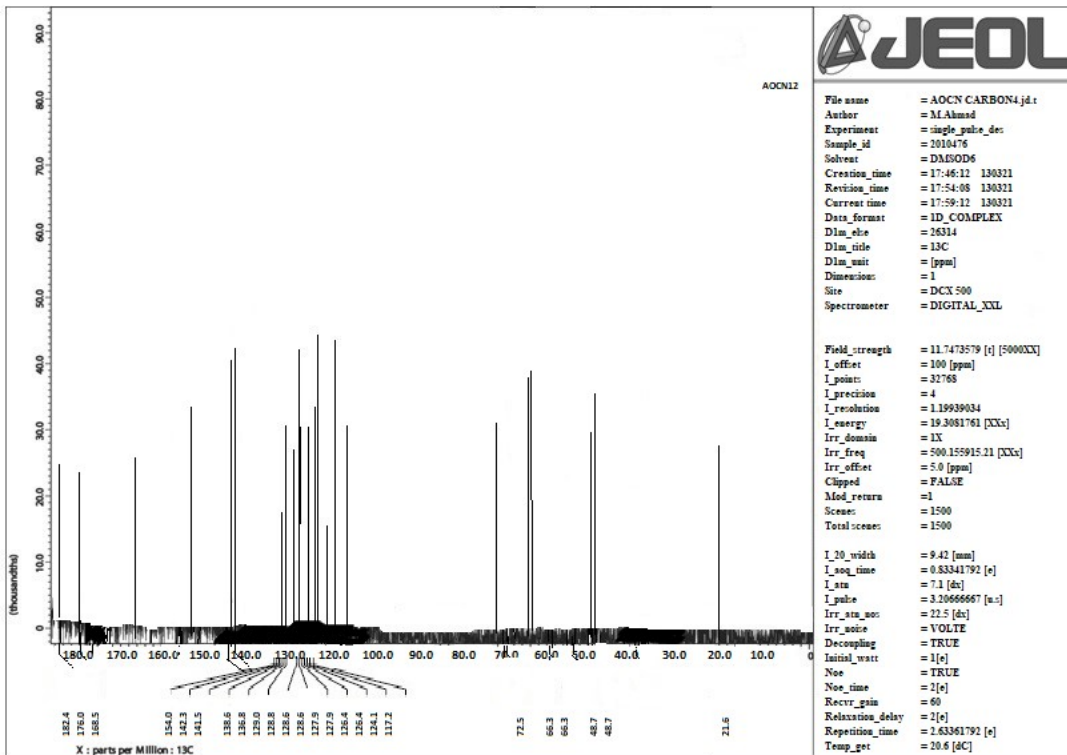
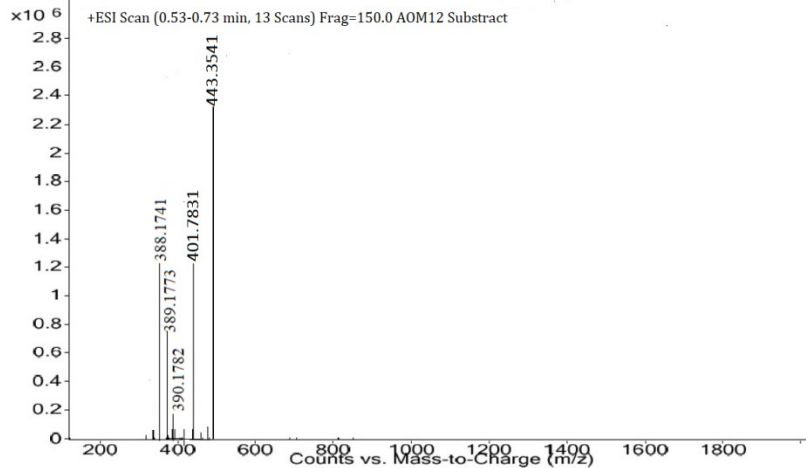
Sample Name	Alarika (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	3	Inj Position		Sample Type	Sample	IRH Calibration Status	Success
Data Filename	AOM10	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	10/12/2021 11:46:12 AM



Sample Name	Alankaha (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	3	InjPosition		Sample Type	Sample	IRM Calibration Status	Success
Data Filename	AOM11	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	10/12/2021 11:15:57AM



Sample Name	Alarika (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	3	Inj Position		Sample Type	Sample	IRH Calibration Status	Success
Data Filename	AOM12	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	10/12/2021 11:42:15 AM

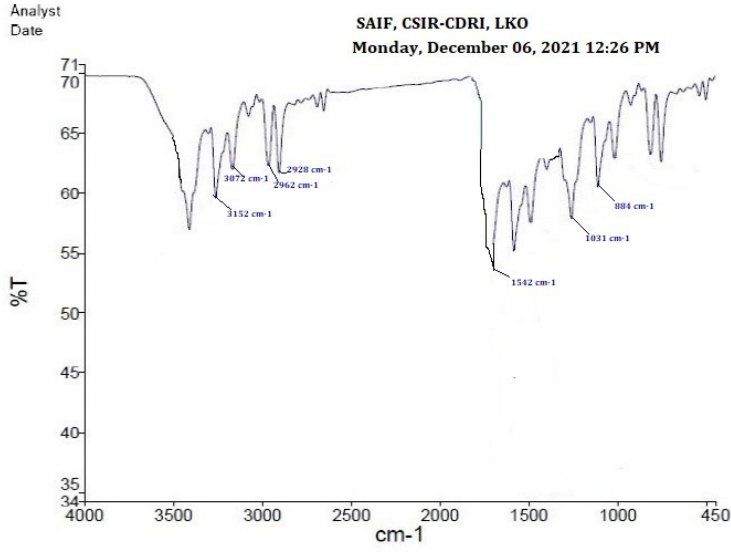


AOCN12

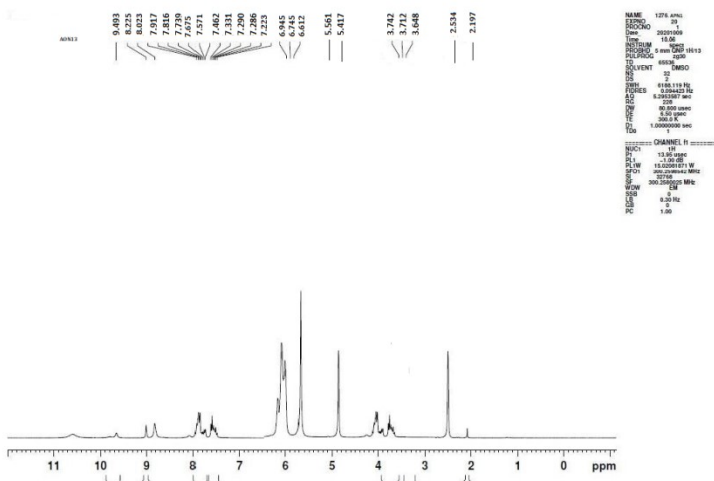
File name = AOCN CARBON4.jd.t
 Author = M.Akmsd
 Experiment = single_pulse_de
 Sample_id = 2010476
 Solvent = DMSO-D6
 Creation_time = 17:46:12 130321
 Revision_time = 17:54:08 130321
 Current_time = 17:59:12 130321
 Data_format = 1D_COMPLEX
 Dia_eht = 26314
 Dia_title = 13C
 Dia_unit = [ppm]
 Dimensions = 1
 Site = DCX 500
 Spectrometer = DIGITAL XXL

Field_strength = 11.743579 [e] (500MHz)
 L_offset = 100 [ppm]
 L_point = 32768
 L_precision = 4
 L_resolution = 1.19939034
 L_energy = 19.3081761 [XXe]
 Irr_domain = 1X
 Irr_freq = 500.15591521 [XXe]
 Irr_offset = 5.0 [ppm]
 Clipped = FALSE
 Mod_return = 1
 Scenes = 1500
 Total_scenes = 1500
 L_20_width = 9.42 [mm]
 L_sqr_time = 0.83341792 [e]
 L_atn = 7.1 [db]
 L_pulse = 3.20666667 [u.s]
 Irr_atn_pos = 22.5 [db]
 Irr_noise = VOLTE
 Decoupling = TRUE
 Initial_watr = 1[e]
 Noe = TRUE
 Noe_time = 2[e]
 Recvr_gain = 60
 Relaxation_delay = 2[e]
 Repetition_time = 1.63361792 [e]
 Temp_get = 20.6 [dC]

Compound 8 (m)



dharmesh 256 - Sample
IR20E09DEC02
2010476 A0113 By
dharmesh Date
Monday
December 06 2021

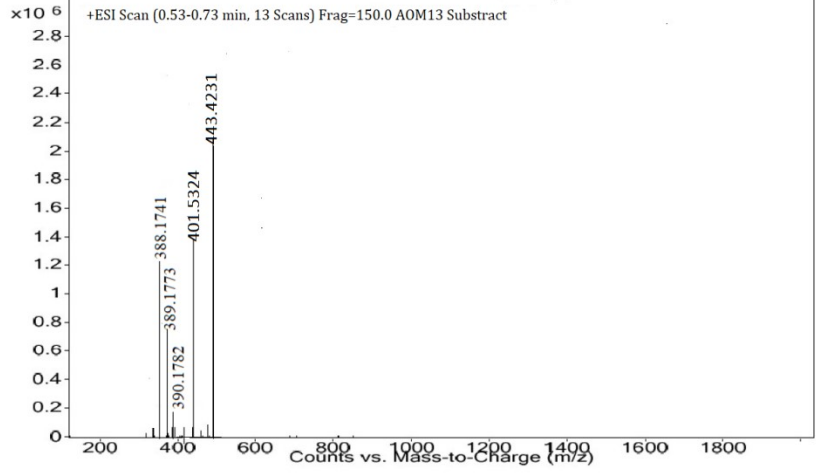


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NAME 1274.A.MU
EXPNO 1
PROCNO 1
PROCDS 20207008
Date_ 15.08
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SFO 400
AQ 0.50000000
RG 1024
DS 4
F2 -
F3 -
F4 -
F5 -
F6 -
F7 -
F8 -
F9 -
F10 -
F11 -
F12 -
F13 -
F14 -
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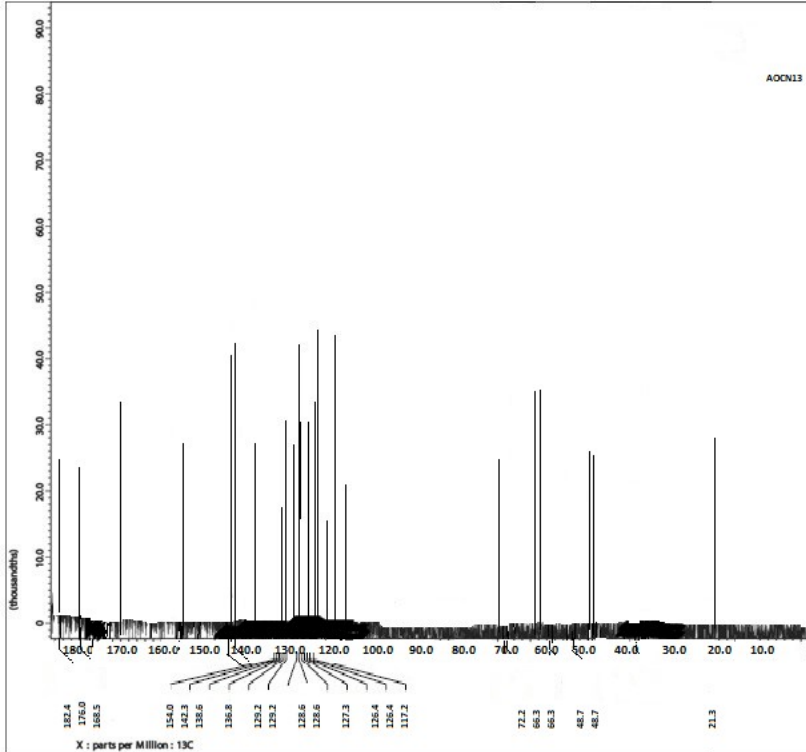
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Sample Name	Akanisha (2010476)	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	3	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	AOM13	ACQ Method	ESOCRATIC.m	Comment		Acquired Time	10/12/2021 11:58:45 AM





AOCN13



File name = AOCN CARBON4.jd.
Author = M.Ahmed
Experiment = single_pulse_dec
Sample_id = 2010476
Solvent = DMSOD6
Creation_time = 18:12:20 130321
Revision_time = 18:22:06 130321
Current_time = 18:29:12 130321
Data_format = 1D_COMPLEX
Dim_elec = 26314
Dim_nucl = 13C
Dim_unit = [ppm]
Dimension = 1
Site = DCX-500
Spectrometer = DIGITAL_XXL

Field_strength = 11.7473579 [e] [500MHz]
L_offset = 100 [ppm]
L_point = 32768
L_precision = 4
L_resolution = 1.19939034
L_energy = 19.3081761 [XXe]
Irr_domain = 1X
Irr_freq = 500.15591511 [XXe]
Irr_offset = 5.0 [ppm]
Clipped = FALSE
Mod_return = 1
Scenes = 1500
Total_scenes = 1500

L_20_width = 9.42 [mm]
L_soc_time = 0.83341792 [e]
L_sca = 7.1 [dx]
L_pulse = 3.20666667 [u.s]
Irr_pwr_wgt = 22.5 [dc]
Irr_pwr = VOLTE
Decoupling = TRUE
Initial_watr = 1[e]
Noe = TRUE
Noe_time = 2[e]
Recvr_gain = 60
Relaxation_delay = 2[e]
Repetition_time = 2.63361792 [e]
Temp_get = 20.6 [dC]