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

Akanksha Gupta[1,2], Hans Raj Bhat[3], Udaya Pratap Singh[1*]

[1] Drug Design and Discovery Laboratory, Department of Pharmaceutical Sciences, Shalom Institute of Health Sciences, Sam Higginbottom University of Agriculture, Technology and Sciences, Prayagraj, Uttar Pradesh, India 211007

[2] United Institute of Pharmacy, Prayagraj, Uttar Pradesh, India 211008

[3] Department of Pharmaceutical Sciences, Dibrugarh University, Dibrugarh Assam, India 786004

Corresponding Author
Udaya Pratap Singh
Email: udaya.singh@shiats.edu.in; udaysingh98@gmail.com

PRELIMINARY DATA OF THE INTERMEDIATES

4-6-Dichloro-[1,3,5]triazin-2-ylamine **(2)**: Yield: 82%; *M.P: 157* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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* ºC; 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. 15PHPSC102)** 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.

MEMBER SECRETARY **CHAIRMAN**

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

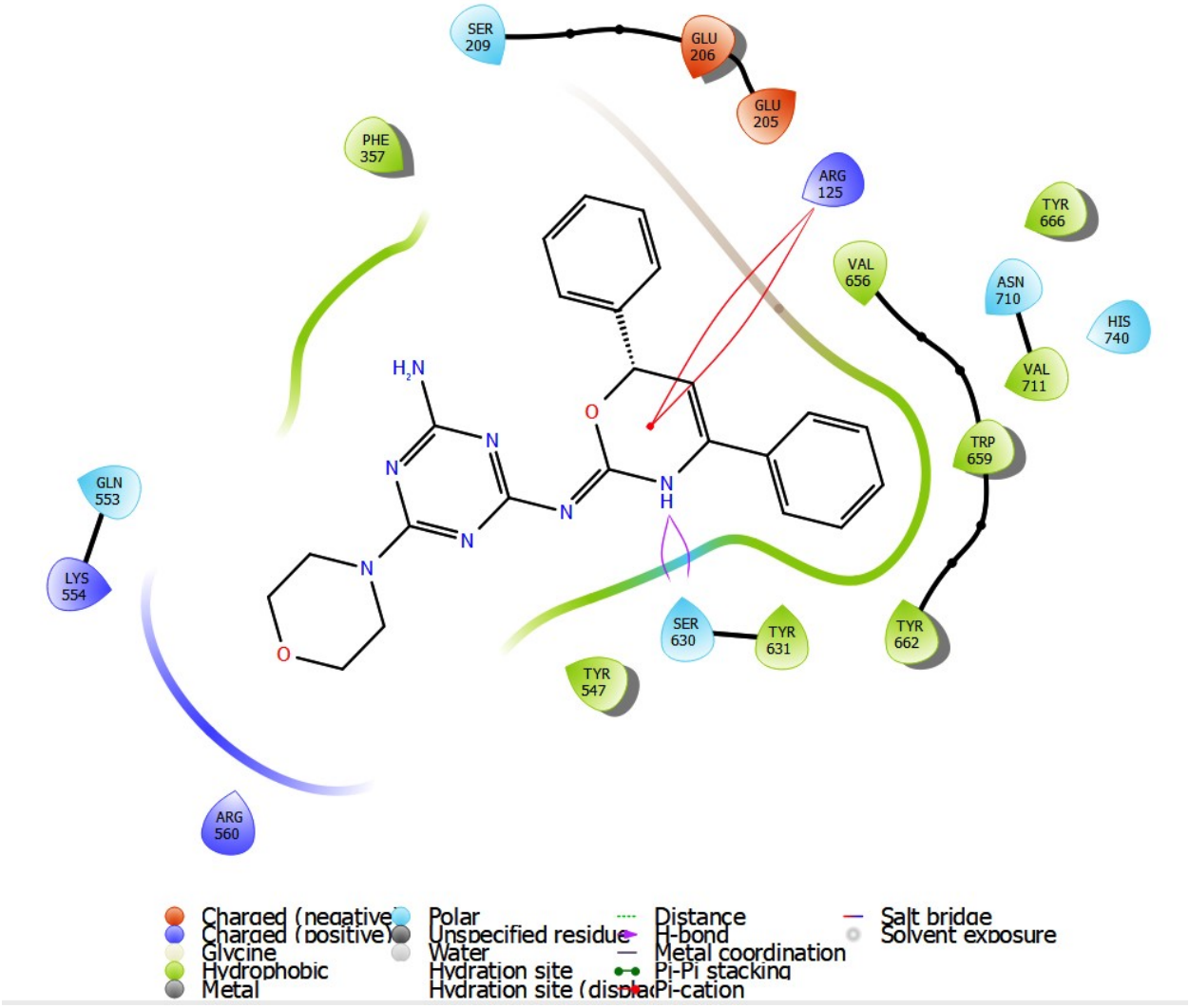


Figure SI 1: Drug-interaction diagram of compound 8(a)

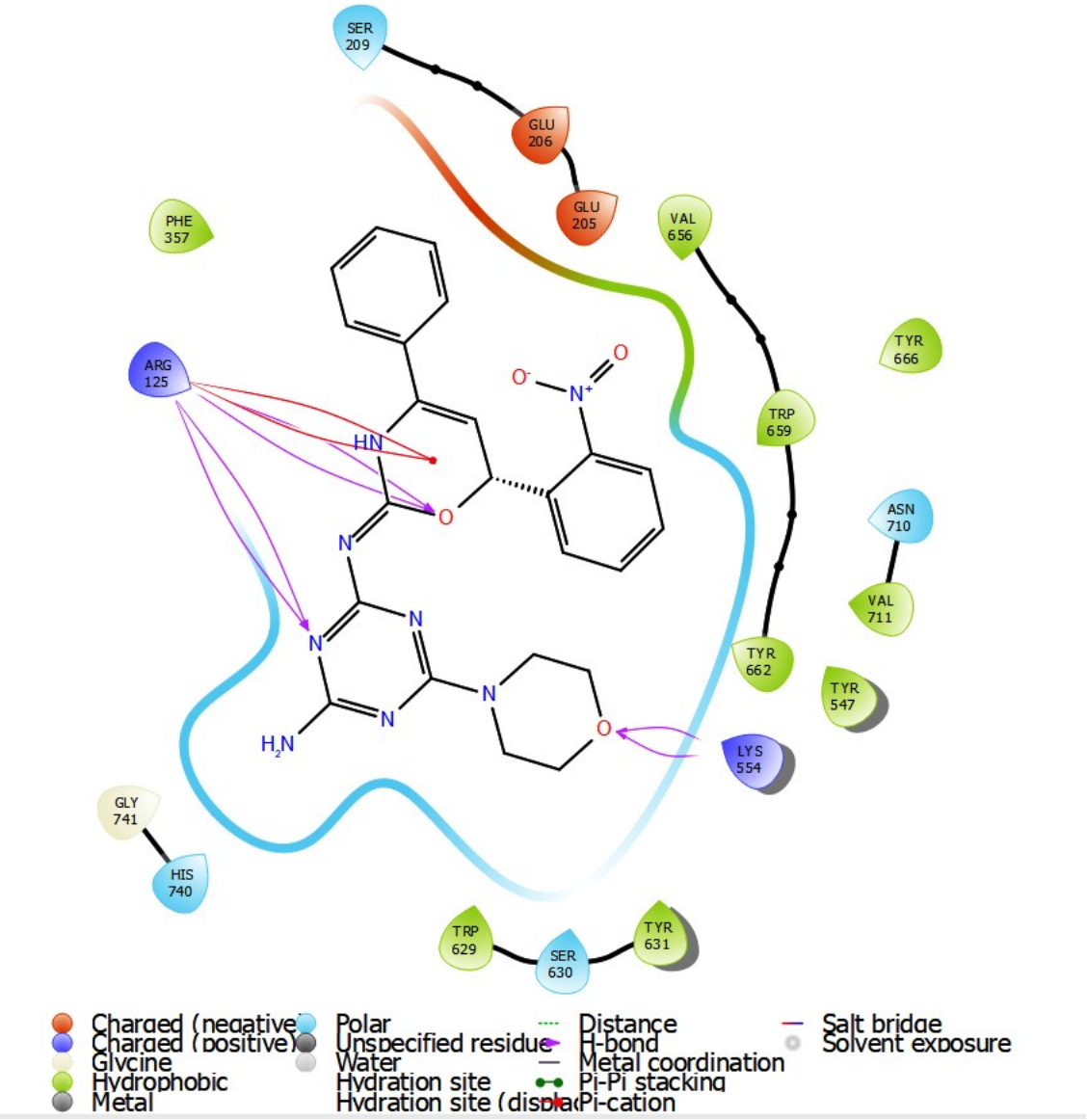


Figure SI 2: Drug-interaction diagram of compound 8(b)

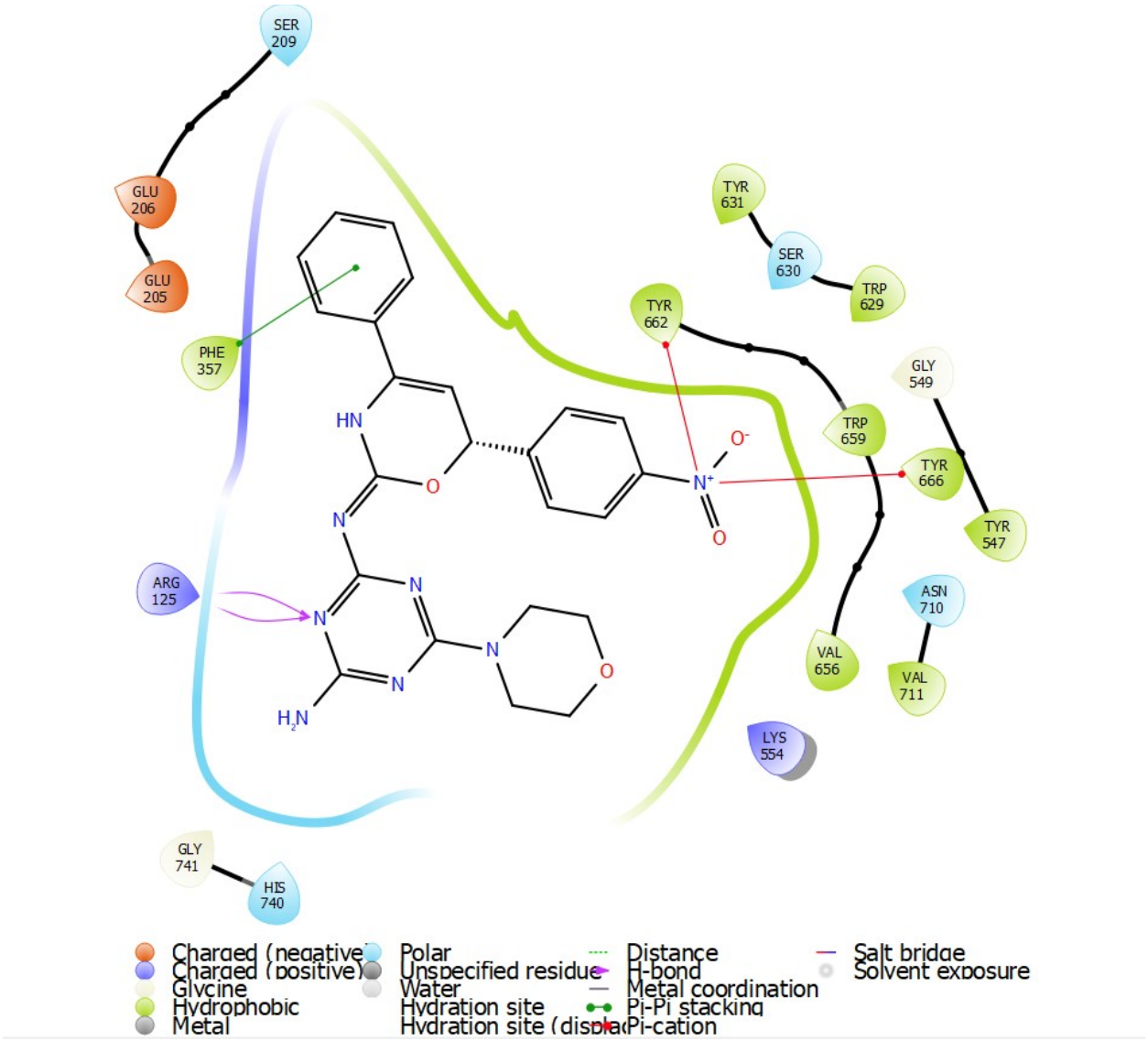


Figure SI 3: Drug-interaction diagram of compound 8(d)

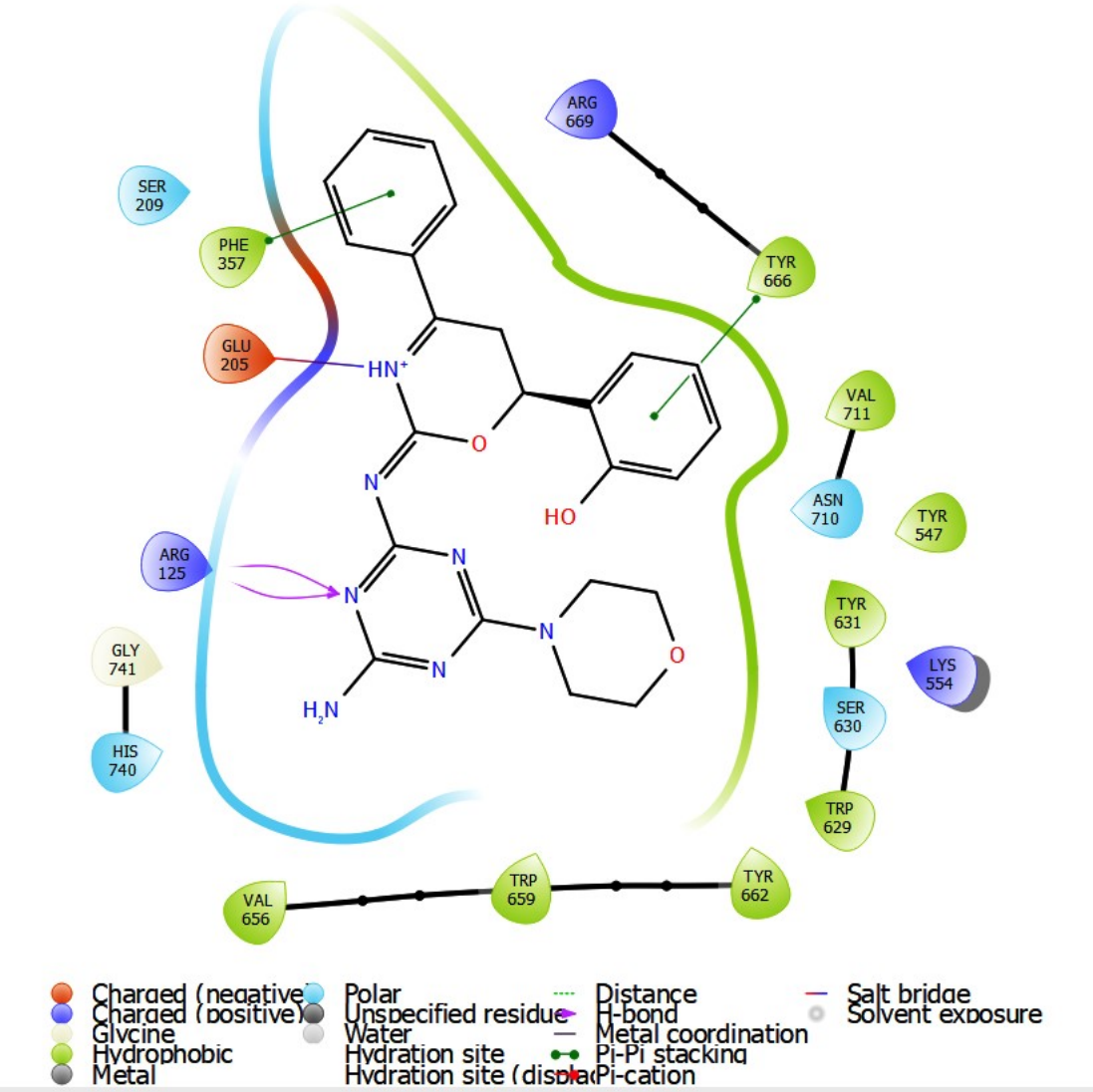


Figure SI 4: Drug-interaction diagram of compound 8(e)

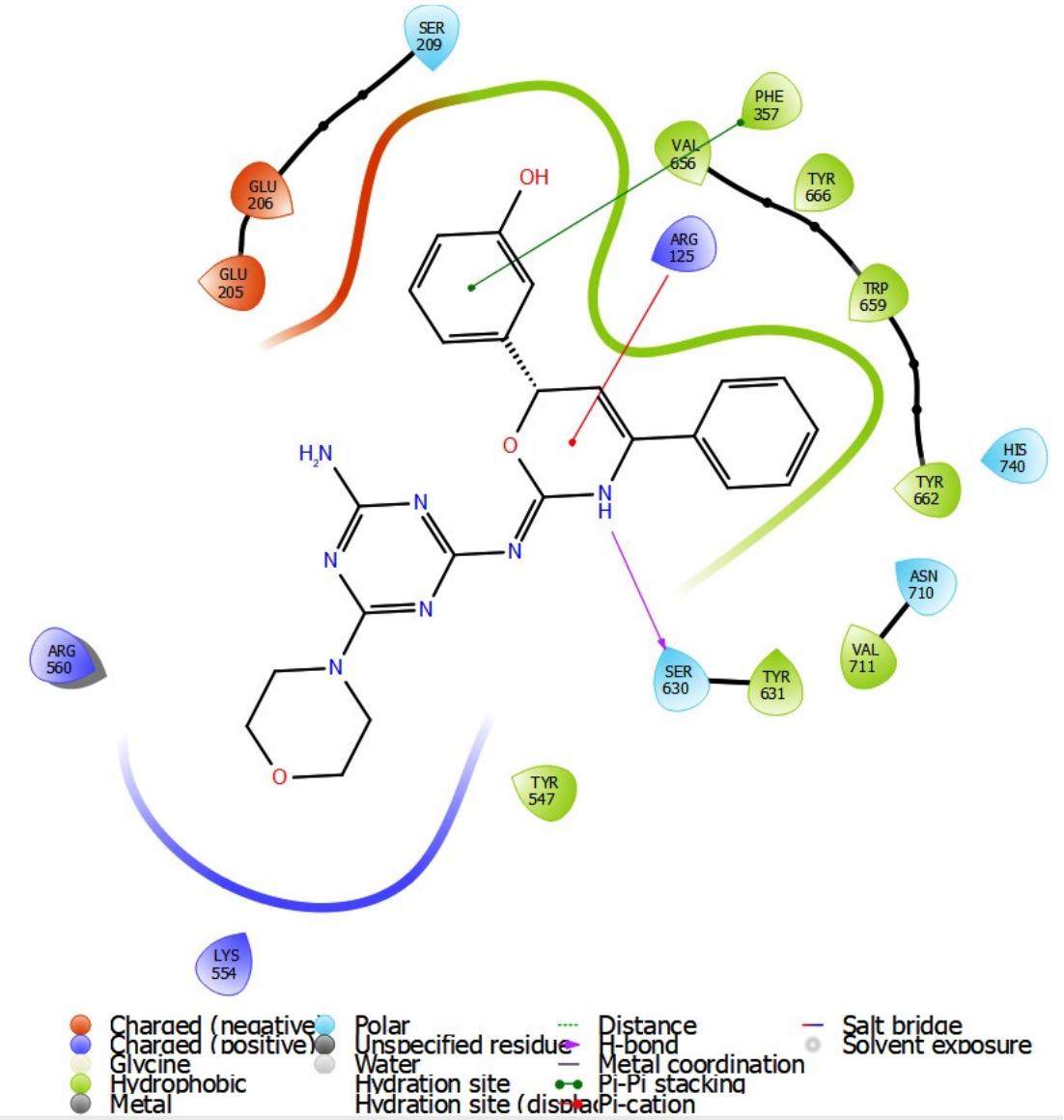


Figure SI 5: Drug-interaction diagram of compound 8(f)

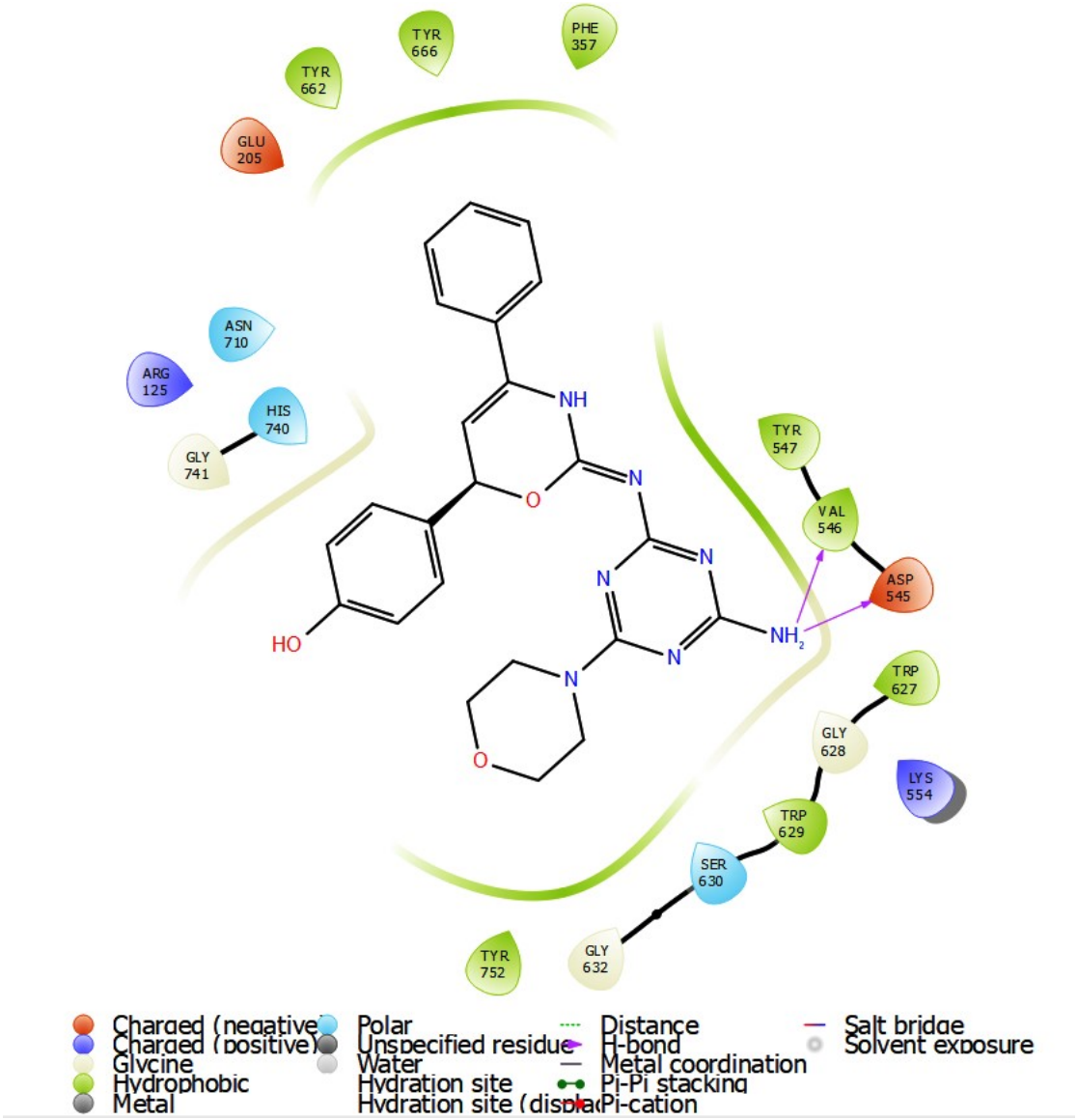


Figure SI 6: Drug-interaction diagram of compound 8(g)

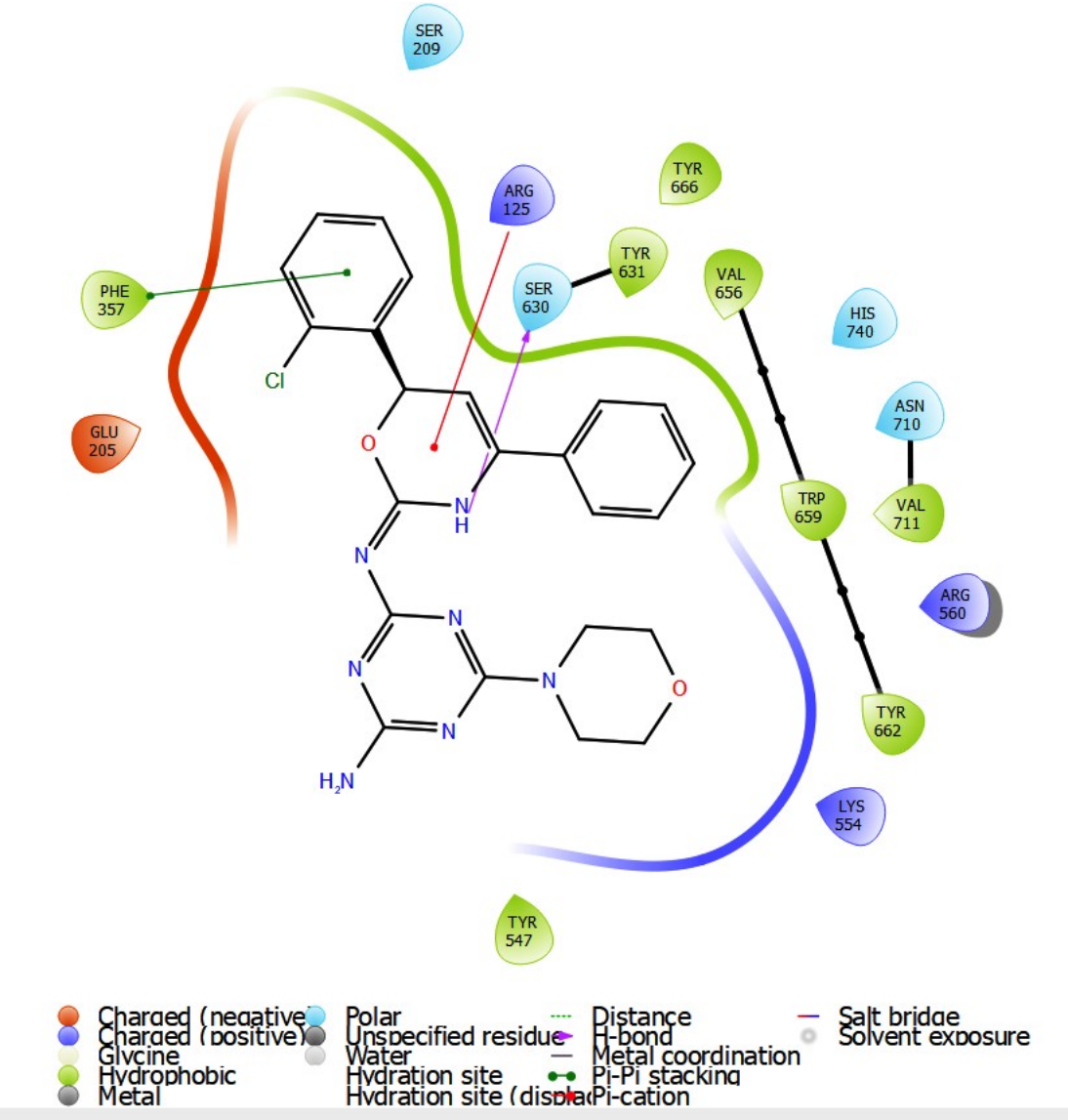


Figure SI 7: Drug-interaction diagram of compound 8(h)

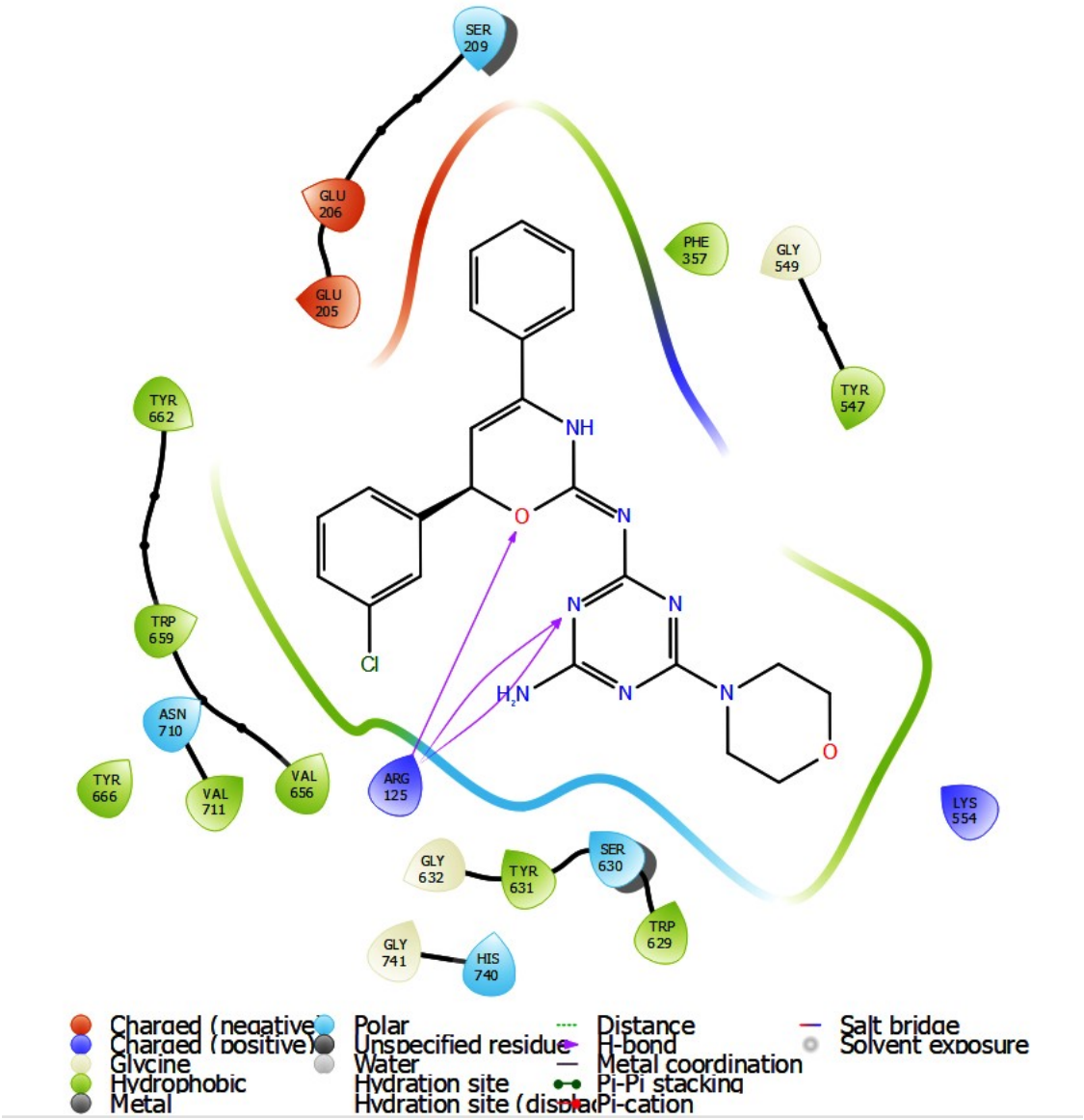


Figure SI 8: Drug-interaction diagram of compound 8(i)

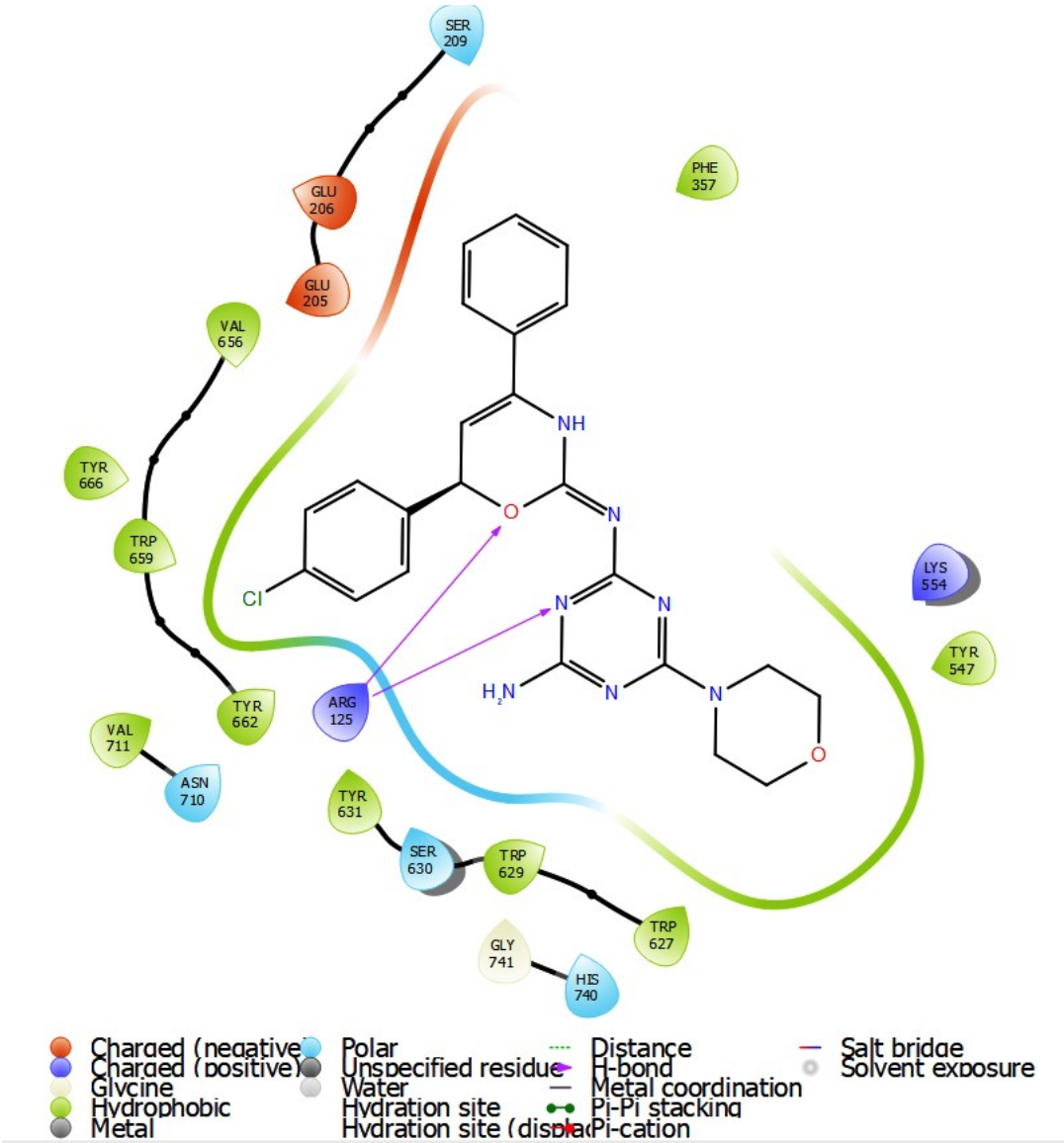


Figure SI 9: Drug-interaction diagram of compound 8(j)

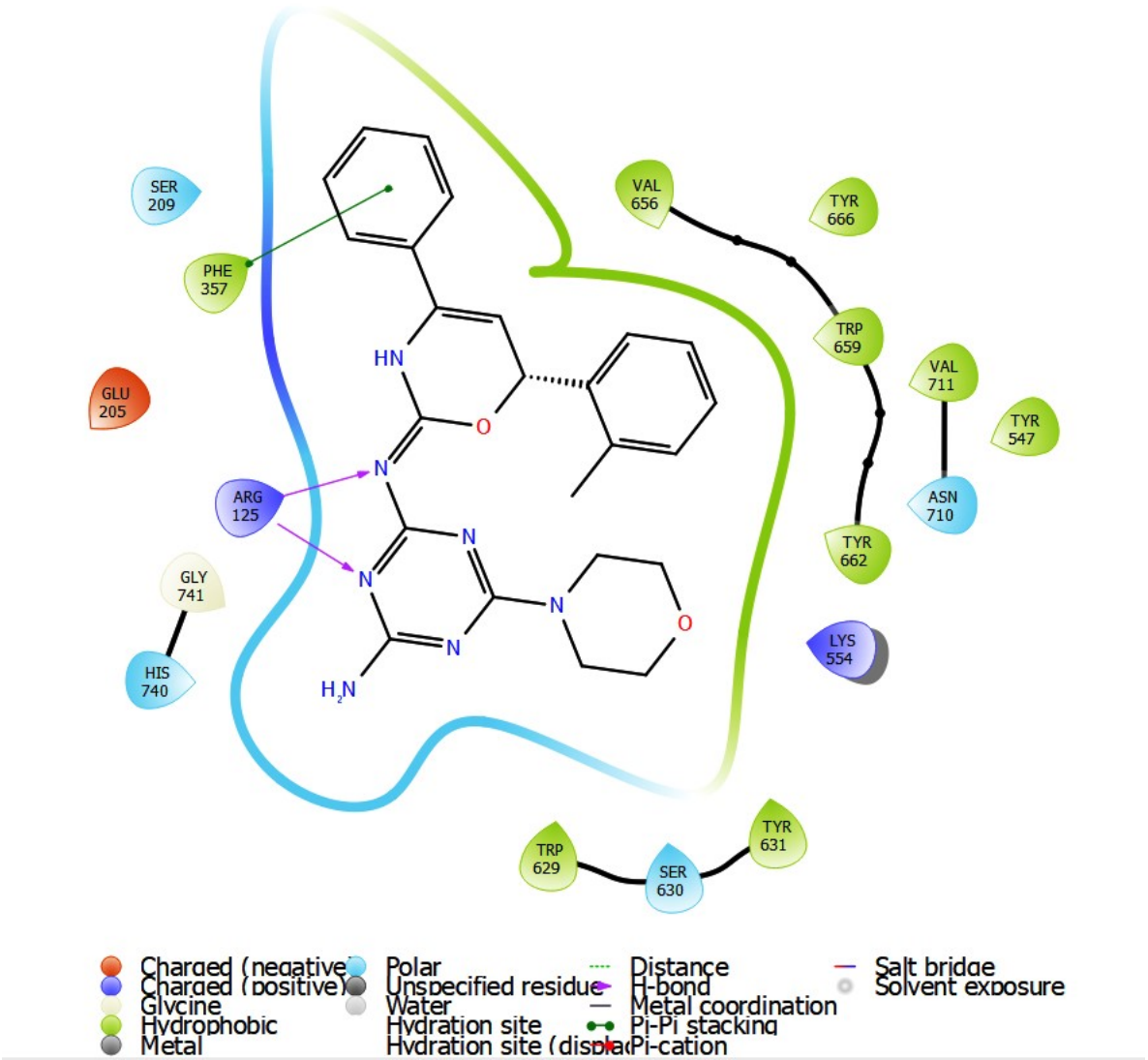


Figure SI 10: Drug-interaction diagram of compound 8(k)

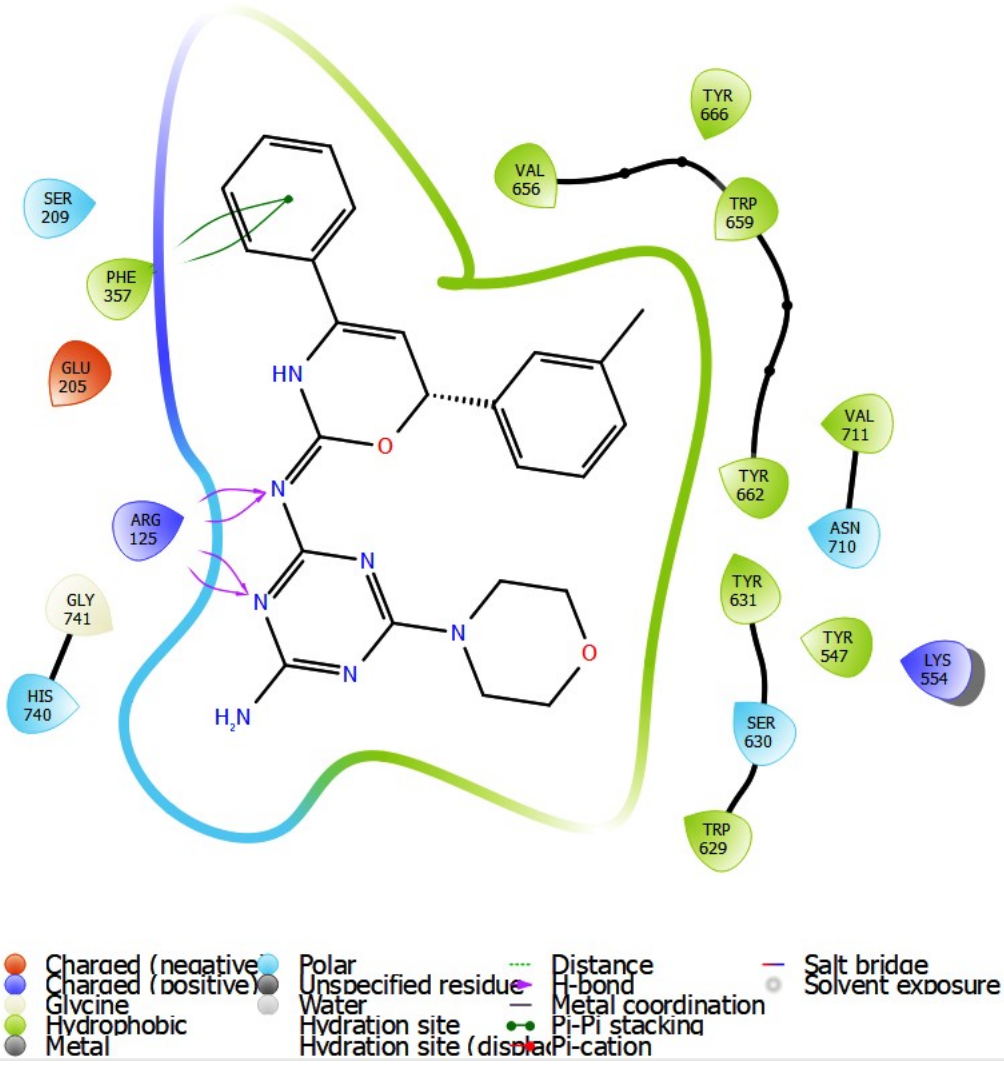


Figure SI 11: Drug-interaction diagram of compound 8(l)

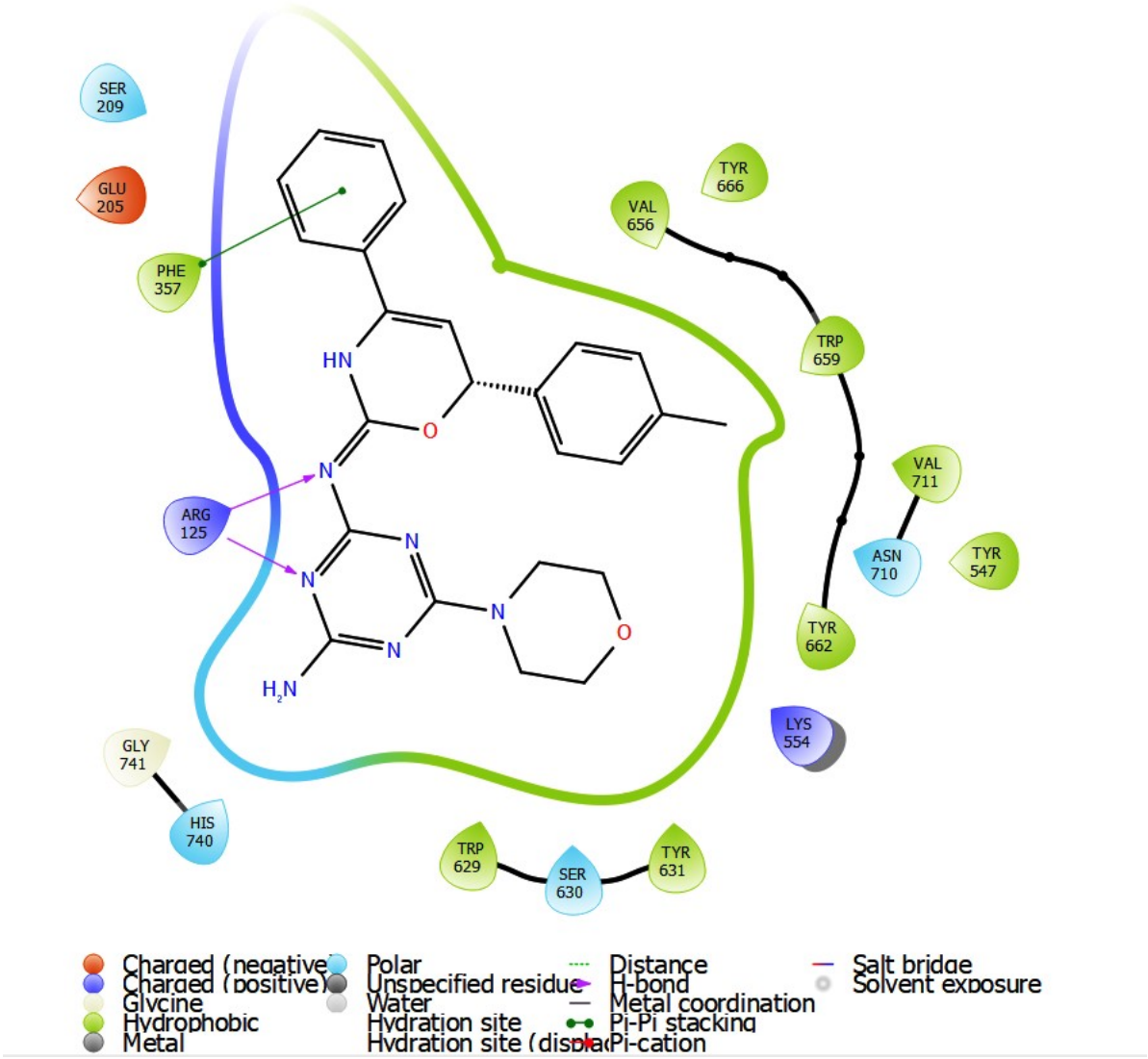
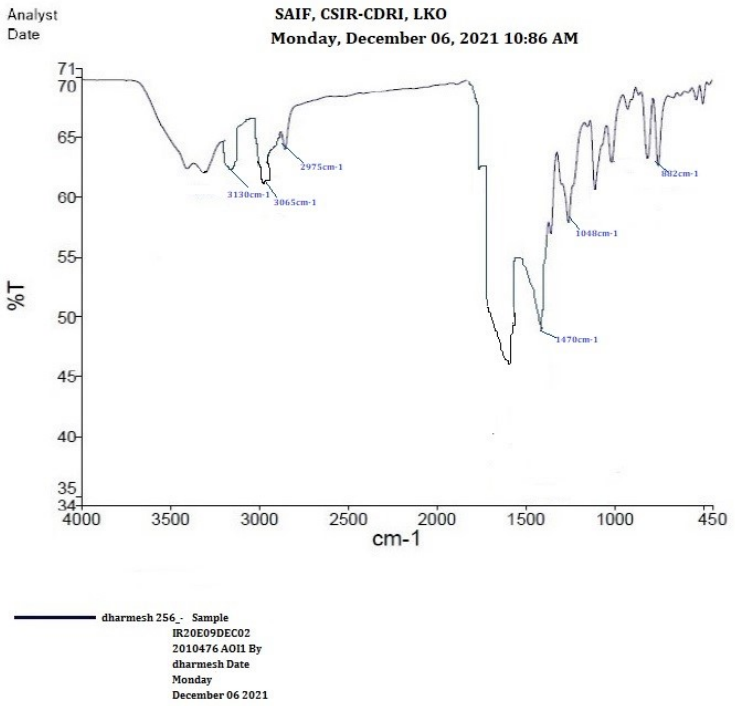
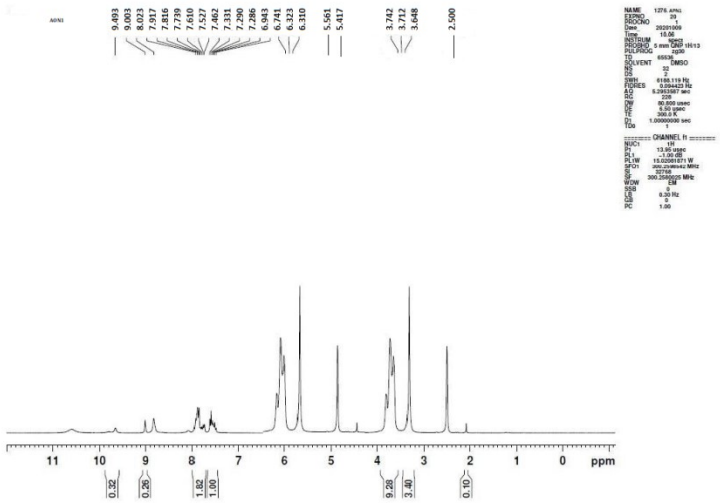


Figure SI 12: Drug-interaction diagram of compound 8(m)

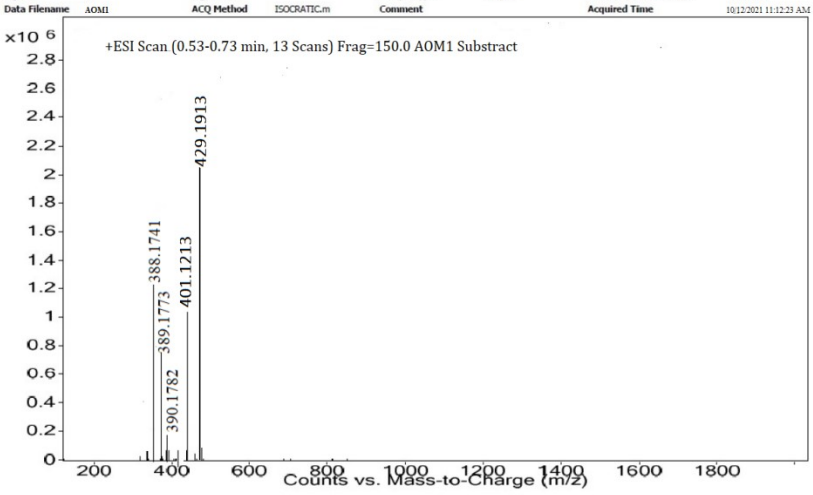
SPECTROSCOPICAL DATA

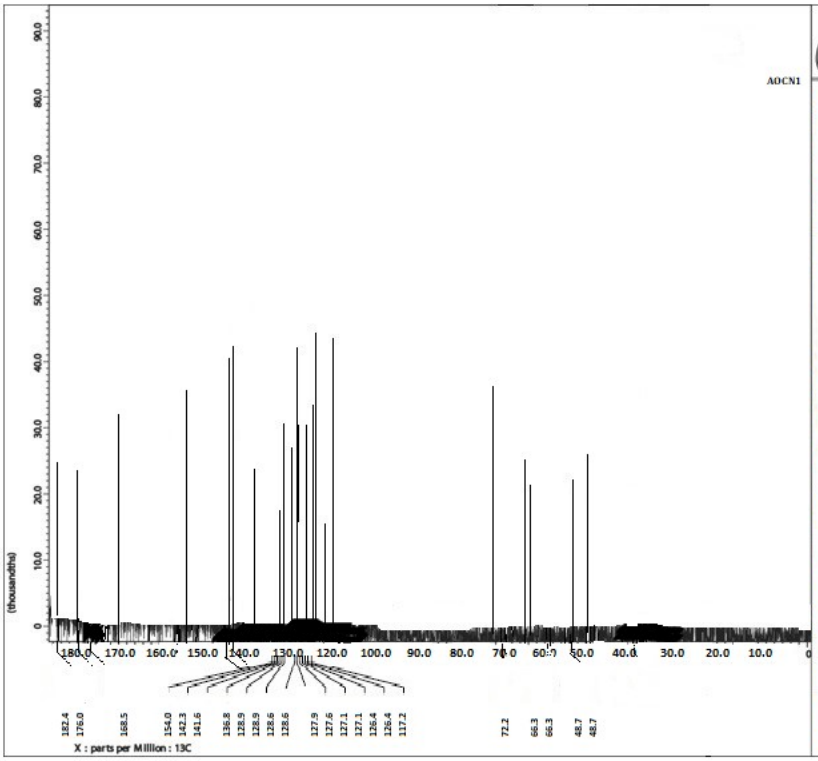
Compound 8 (a)





Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleTypc**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM1	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:12:23 AM

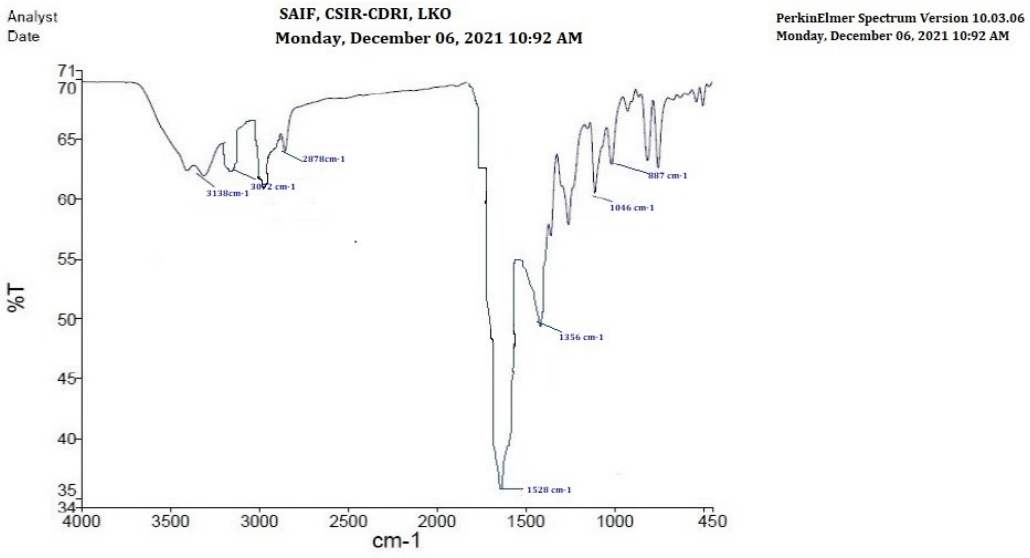


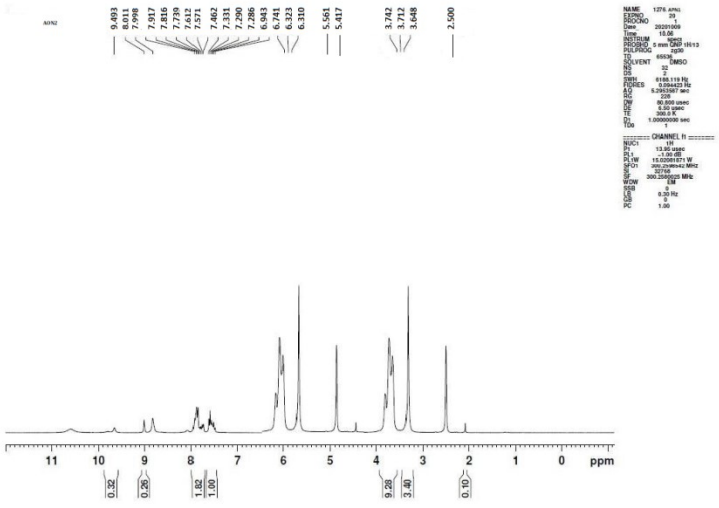


JEOL

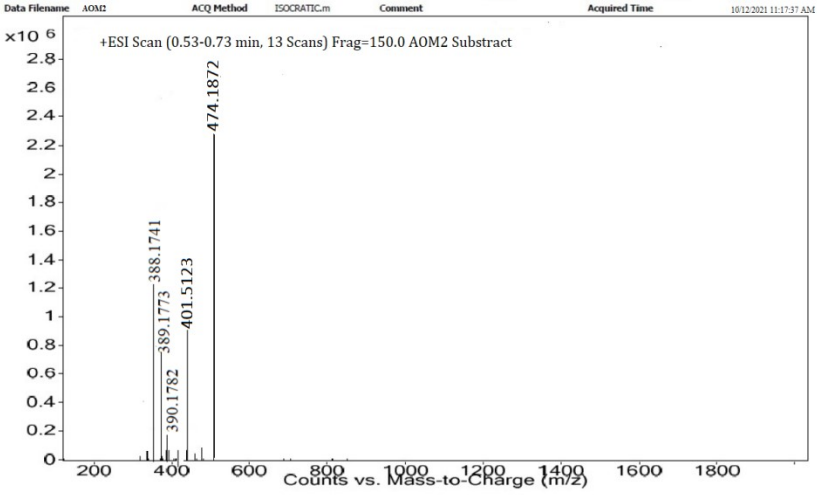
File name	= AOCN CARBON4.jd.t
Author	= M.Ahmad
Experiment	= single_pulse_dec
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 12:10:22 130321
Revision_time	= 12:20:18 130321
Current time	= 12:25:30 130321
Data_format	= 1D_COMPLEX
Dim_ebe	= 26314
Dim_title	= 13C
Dim_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_strength	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	=1
Scanes	= 1500
Total scanes	= 1500
I_20_width	= 9.42 [mm]
I_acq_time	= 0.83341792 [s]
I_atn	= 7.1 [dx]
I_pulse	= 3.20666667 [u.s]
Irr_atn_noe	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 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]

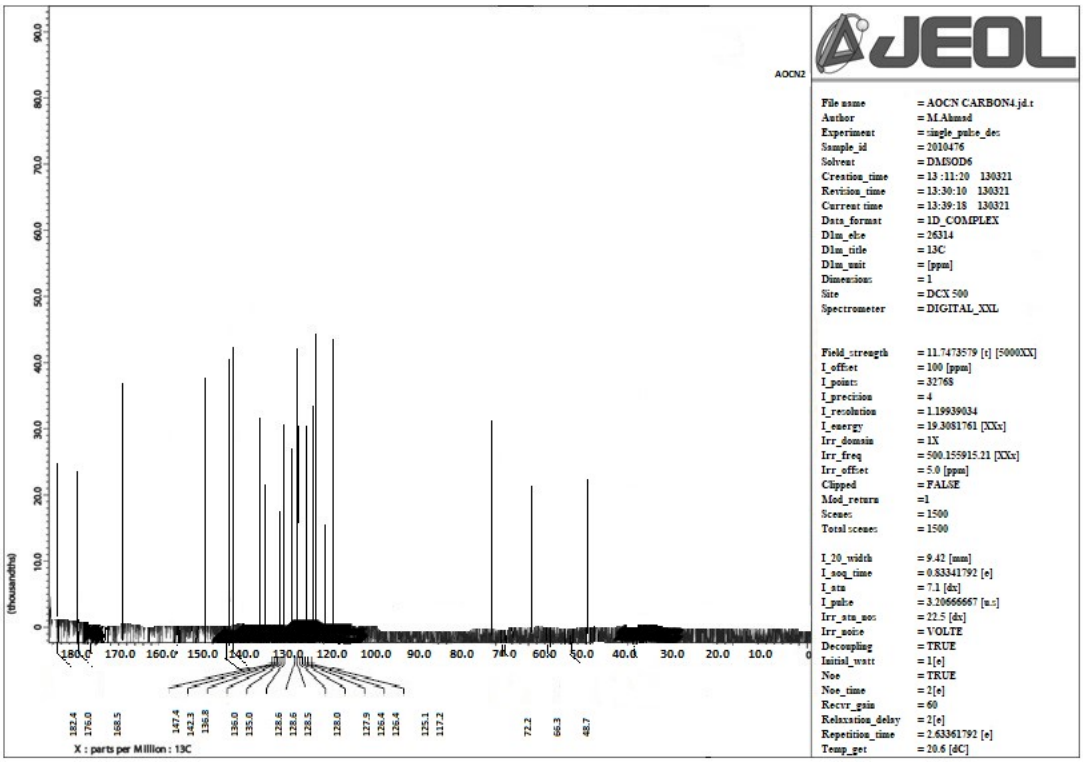
Compound 8 (b)


Analyst
Date
SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 10:92 AM
PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 10:92 AM
%T
cm-1
3138cm-1
3072 cm-1
2878cm-1
1528 cm-1
1356 cm-1
1046 cm-1
887 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI2 By
dharmesh Date
Monday
December 06 2021


9.493
8.031
7.998
7.917
7.816
7.739
7.612
7.571
7.462
7.331
7.290
7.286
6.643
6.741
6.323
6.310
5.561
5.417
3.742
3.712
3.648
2.500
ppm
0.92
0.28
1.82
1.00
9.28
3.40
0.10

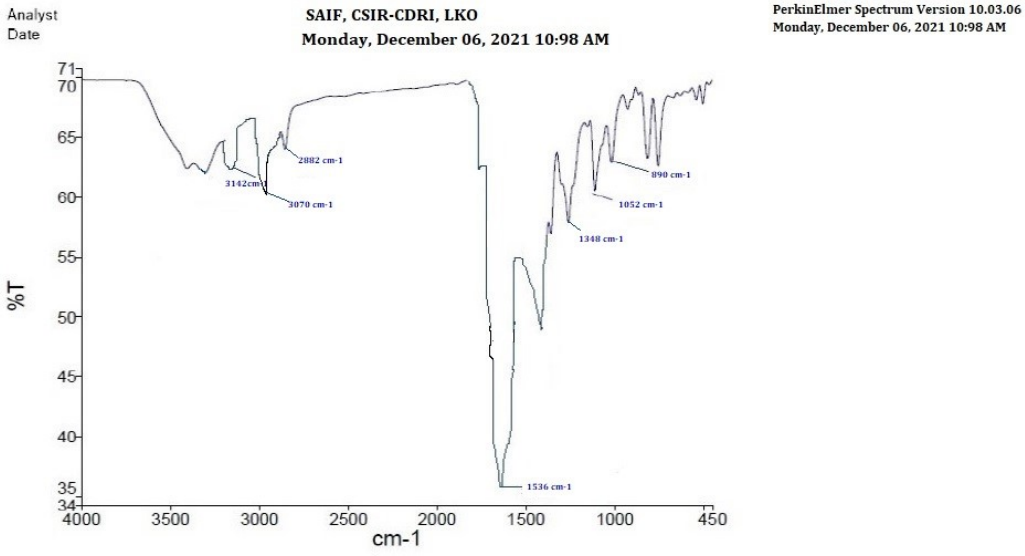
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleTypc**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM2	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:17:37 AM

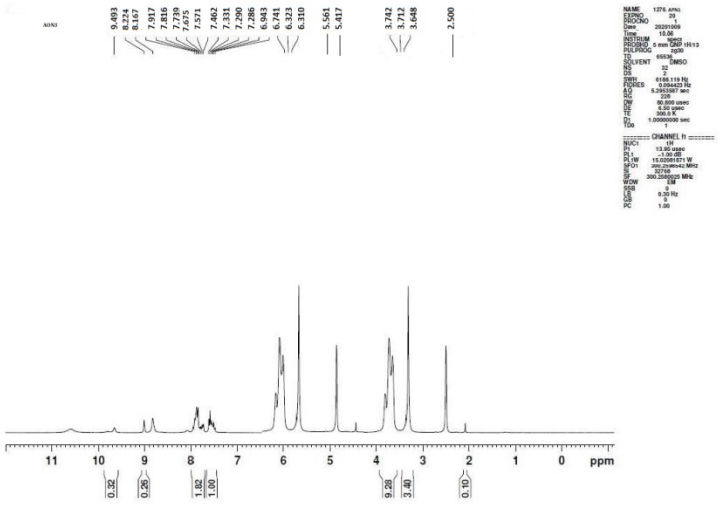




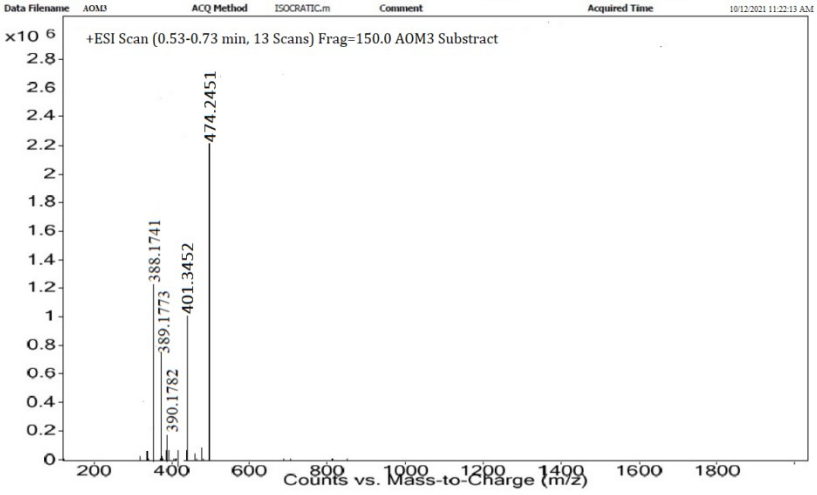
File name	= AOCN CARBON4.jd.t
Author	= MAhmad
Experiment	= single_pulse_dec
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 13 :11:20 130321
Revision_time	= 13:30:10 130321
Current time	= 13:39:18 130321
Data_format	= 1D_COMPLEX
Dim_ele	= 26314
Dim_title	= 13C
Dim_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_strength	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	=1
Scenes	= 1500
Total scenes	= 1500
I_20_width	= 9.42 [mm]
I_acq_time	= 0.83341792 [e]
I_ata	= 7.1 [dx]
I_pulse	= 3.20666667 [u.s]
Irr_ata_acc	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 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]

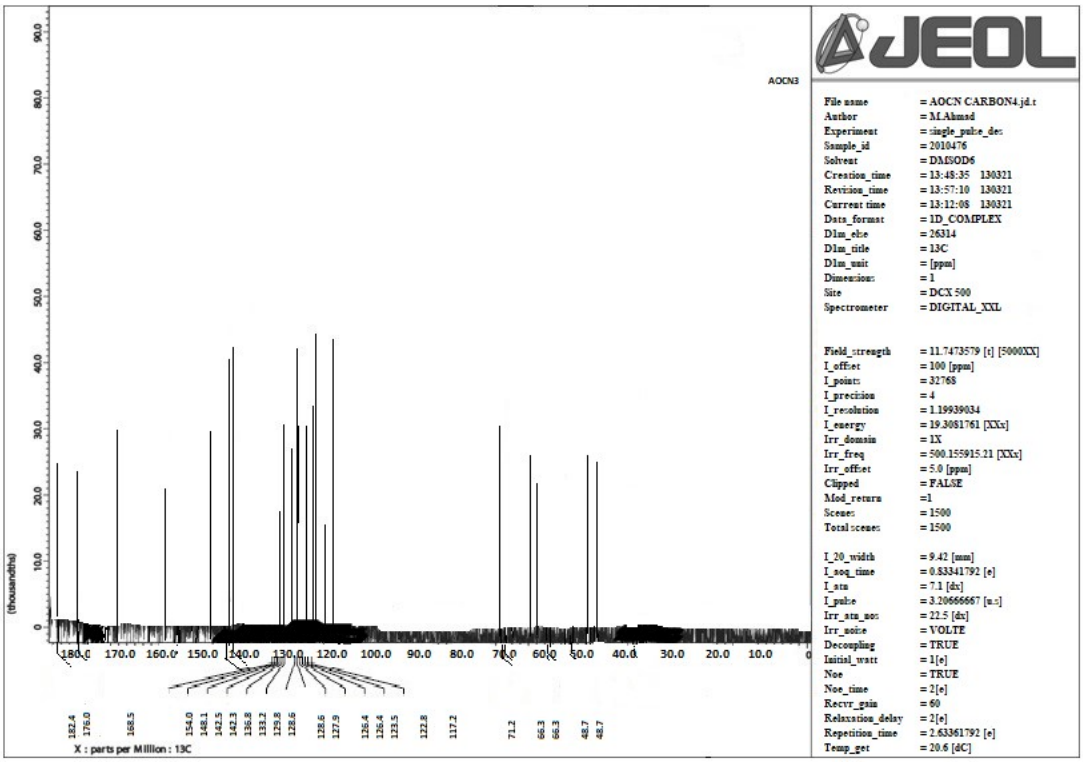
Compound 8 (c)


Analyst
Date
SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 10:98 AM
PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 10:98 AM
%T
cm-1
2882 cm-1
3142cm-1
3070 cm-1
890 cm-1
1052 cm-1
1348 cm-1
1536 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI3 By
dharmesh Date
Monday
December 06 2021

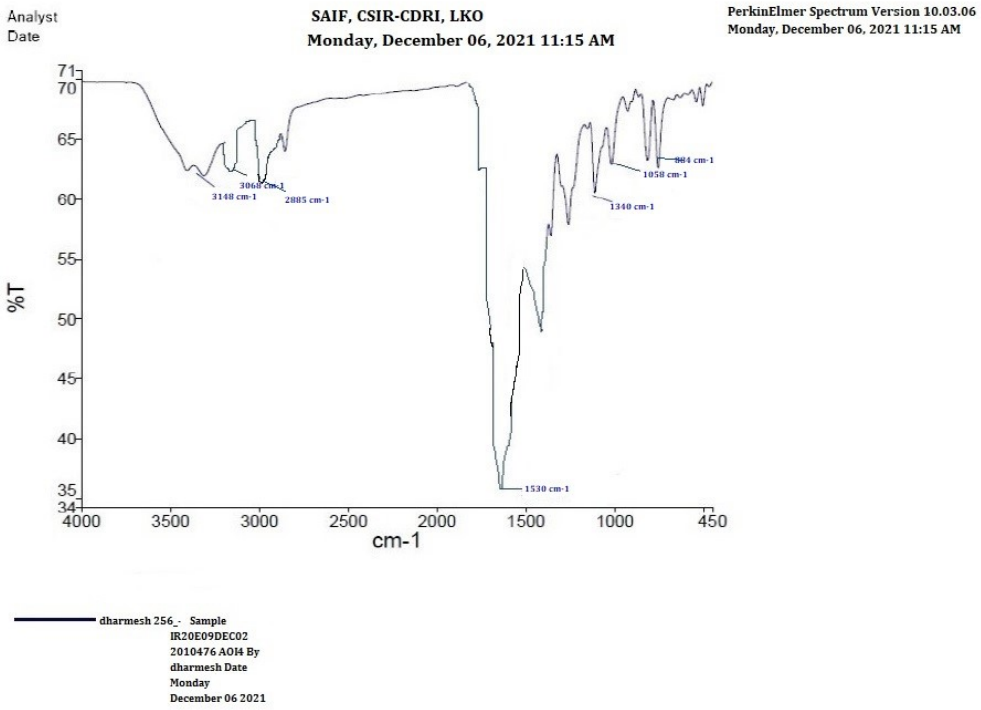

9.493
8.124
8.107
7.917
7.816
7.739
7.675
7.571
7.462
7.331
7.290
7.286
6.643
6.741
6.323
6.310
5.561
5.417
3.742
3.712
3.648
2.500
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.92
0.29
1.82
1.00
9.28
3.40
0.10

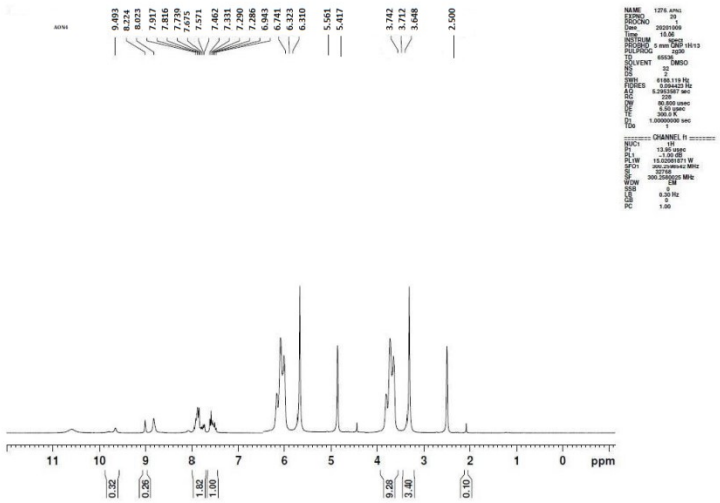
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleTypc**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM3	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:22:13 AM



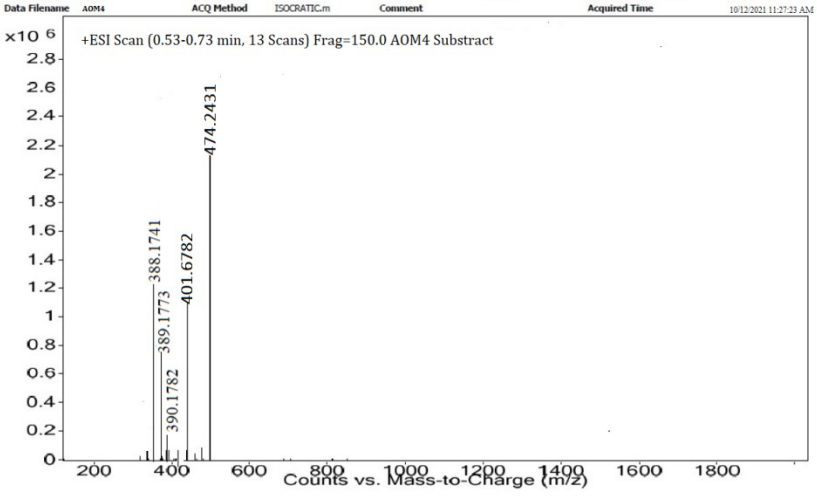


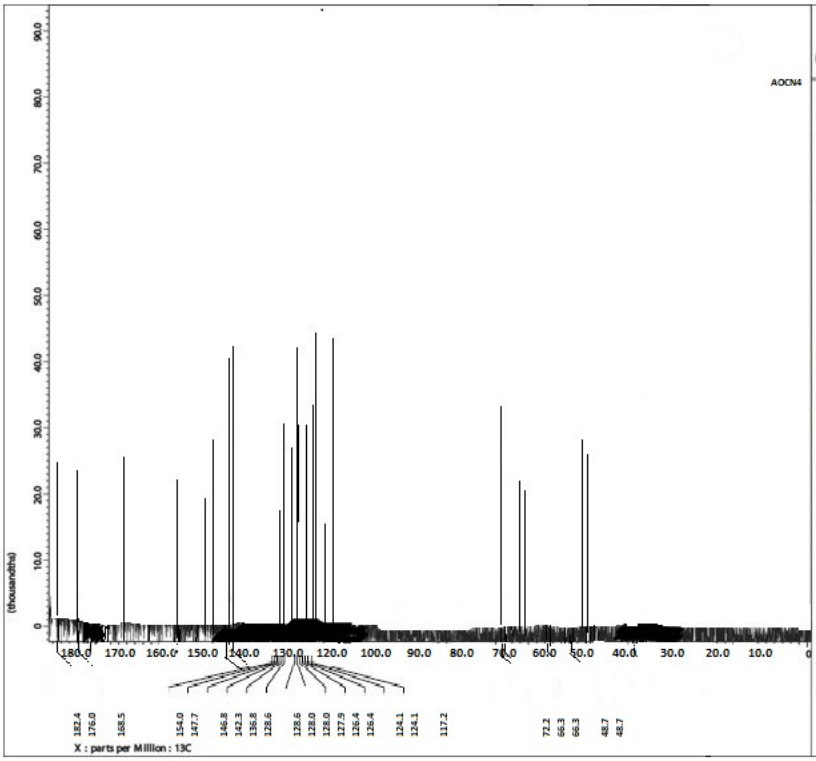
Compound 8 (d)


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
%T
cm-1
3148 cm-1
3060 cm-1
2885 cm-1
1530 cm-1
1340 cm-1
1058 cm-1
884 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI4 By
dharmesh Date
Monday
December 06 2021



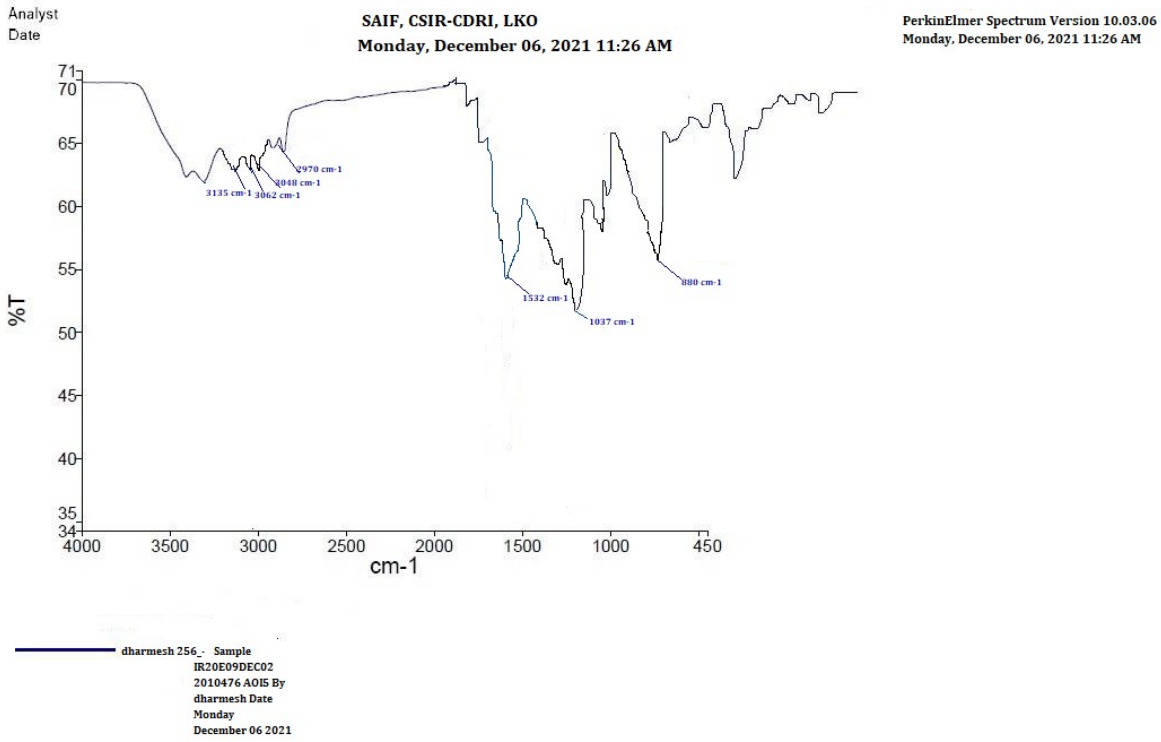
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM4	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:27:23 AM

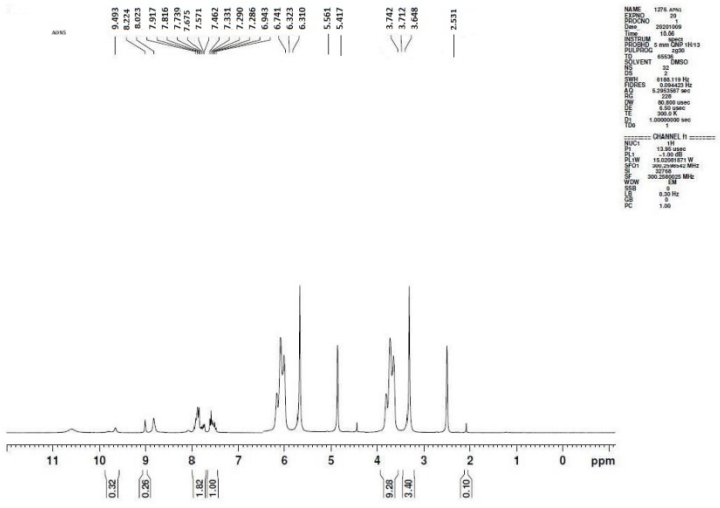




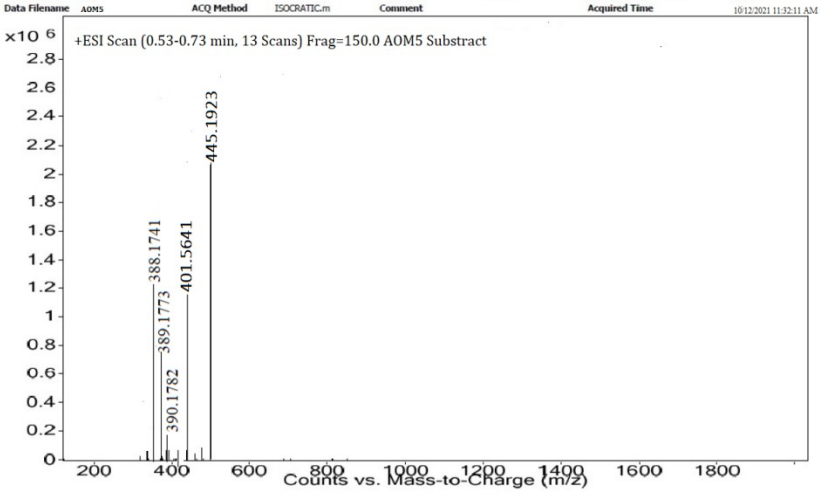
File name	= AOCN CARBON4.jd.t
Author	= M.Ahmad
Experiment	= single_pulse_de
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 14:14:40 130321
Revision_time	= 14:22:10 130321
Current time	= 14:32:30 130321
Data_format	= 1D_COMPLEX
Dim_ele	= 26314
Dim_title	= 13C
Dim_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_strength	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_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_atn	= 7.1 [dx]
I_pulse	= 3.20666667 [u.s]
Irr_atn_acc	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 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]

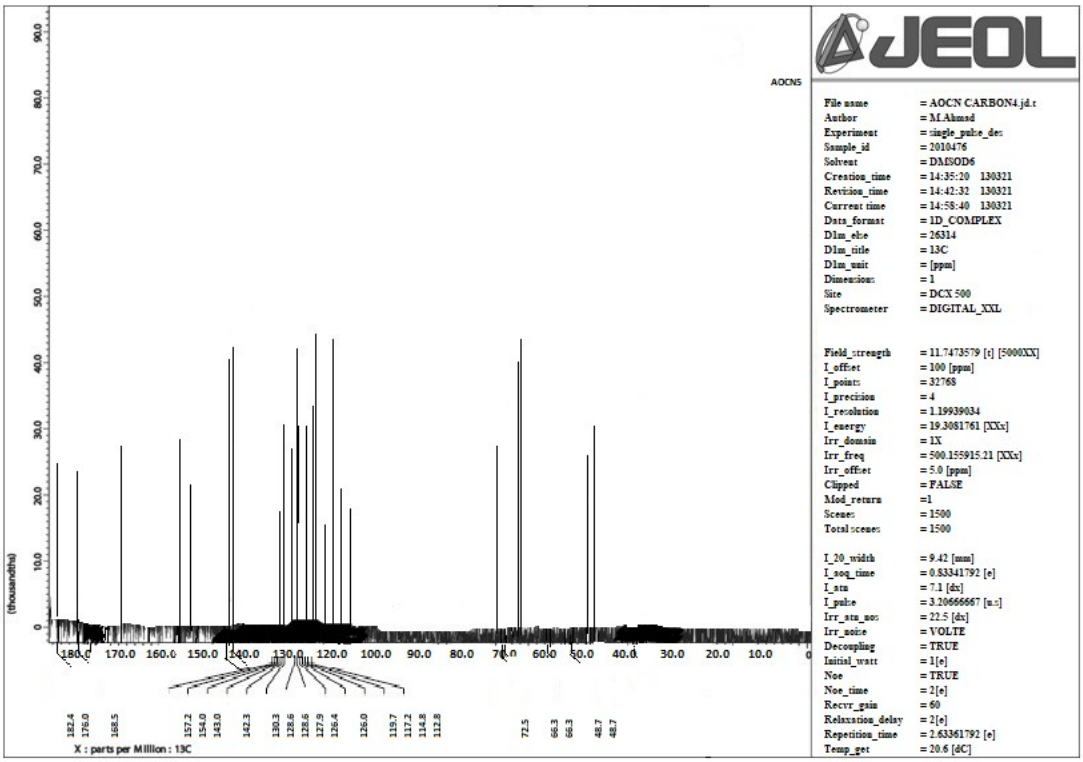
Compound 8 (e)


Analyst
Date
SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 11:26 AM
PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 11:26 AM
%T
cm-1
3135 cm-1
3062 cm-1
3048 cm-1
2970 cm-1
1532 cm-1
1037 cm-1
880 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOIS By
dharmesh Date
Monday
December 06 2021


9.493
8.224
8.033
7.917
7.816
7.739
7.675
7.571
7.462
7.331
7.290
7.286
6.843
6.741
6.323
6.310
5.561
5.417
3.742
3.712
3.648
2.531
ppm
0.92
0.26
1.82
1.00
9.29
3.40
0.10

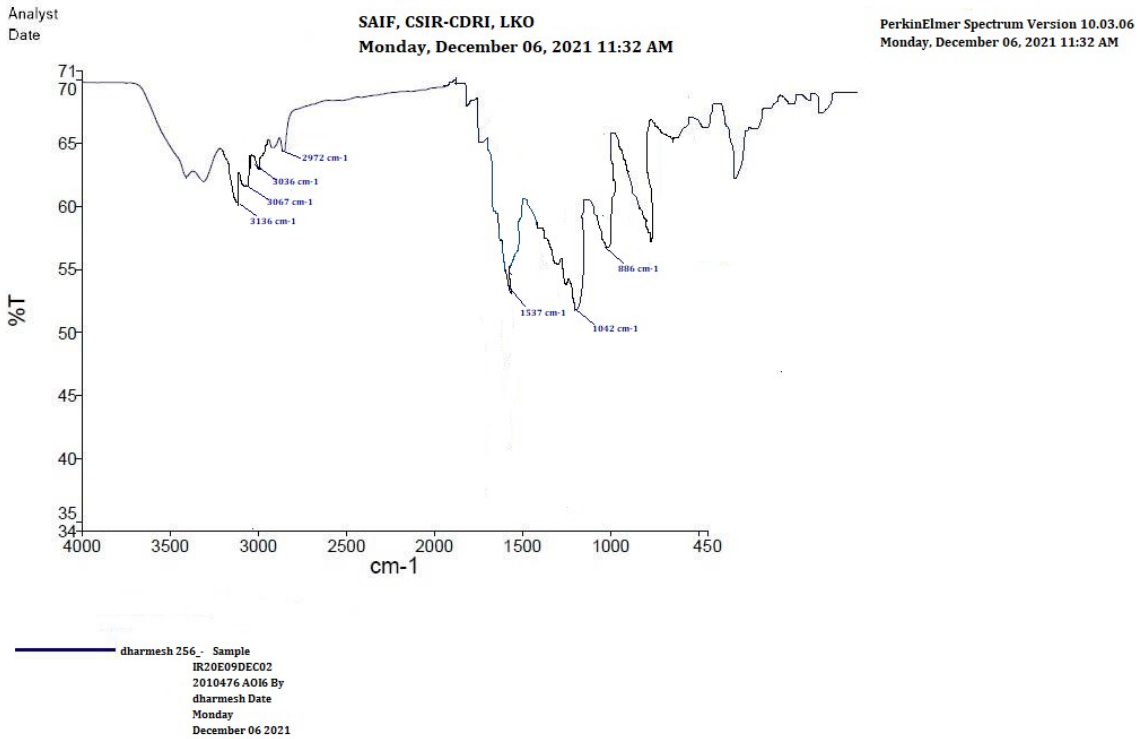
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleTypc**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM5	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:32:11 AM

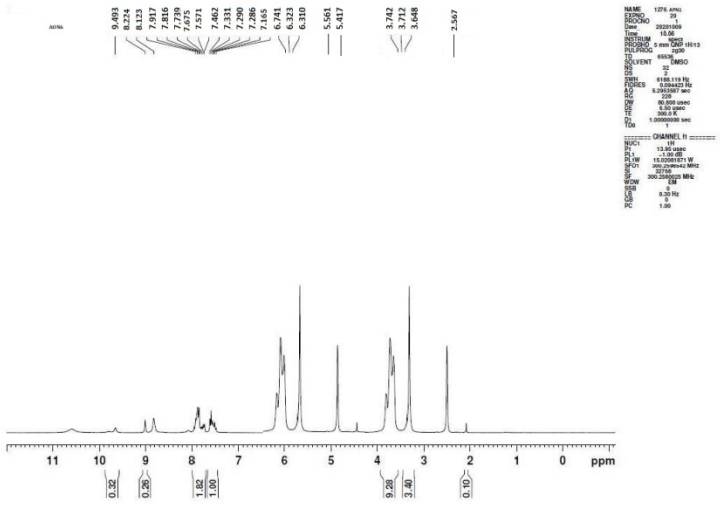




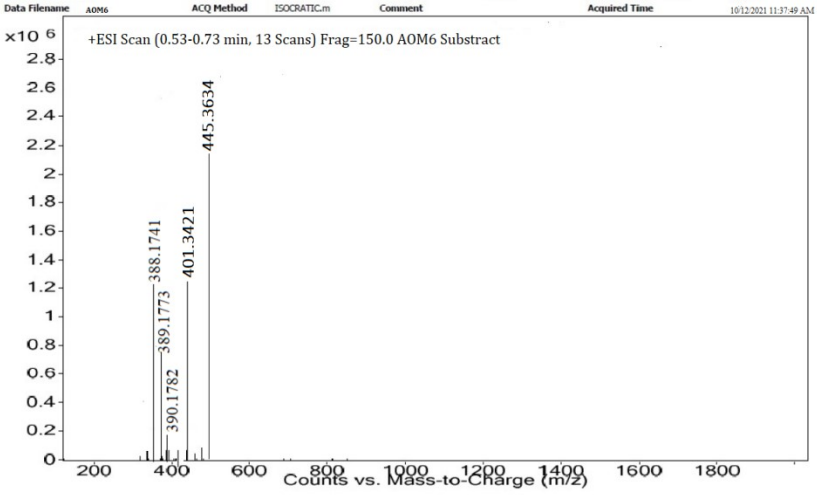
File name	= AOCN CARBON4.jd.t
Author	= M.Ahmad
Experiment	= single_pulse_dec
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 14:35:20 130321
Revision_time	= 14:42:32 130321
Current time	= 14:58:40 130321
Data_format	= 1D_COMPLEX
D1m_ehe	= 26314
D1m_title	= 13C
D1m_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_strength	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	=1
Scenes	= 1500
Total scenes	= 1500
I_20_width	= 9.42 [mm]
I_acq_time	= 0.83341792 [e]
I_atn	= 7.1 [dx]
I_pulse	= 3.20666667 [u.s]
Irr_atn_acc	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 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]

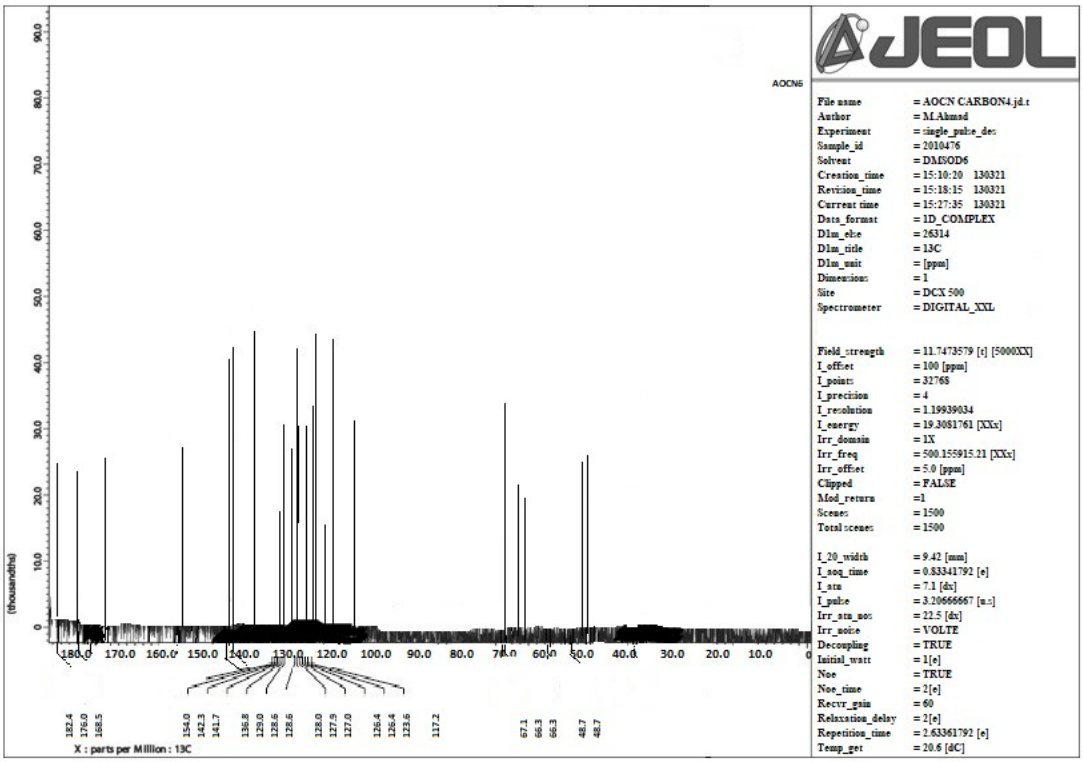
Compound 8 (f)


Analyst
Date
SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 11:32 AM
PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 11:32 AM
%T
cm-1
2972 cm-1
3036 cm-1
3067 cm-1
3136 cm-1
886 cm-1
1537 cm-1
1042 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI6 By
dharmesh Date
Monday
December 06 2021

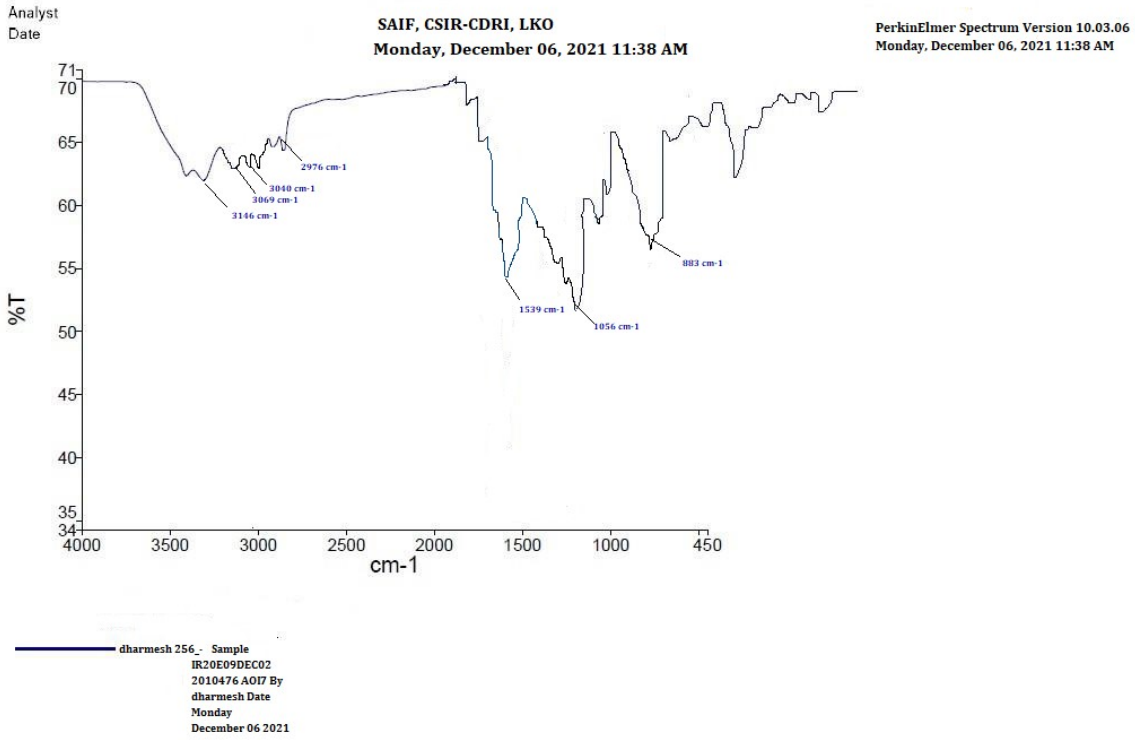

9.493
8.224
8.133
7.917
7.816
7.739
7.675
7.571
7.462
7.331
7.290
7.286
7.145
6.741
6.323
6.310
5.561
5.417
3.742
3.712
3.648
2.567
ppm
0.92
0.26
1.82
1.00
9.29
3.40
0.10

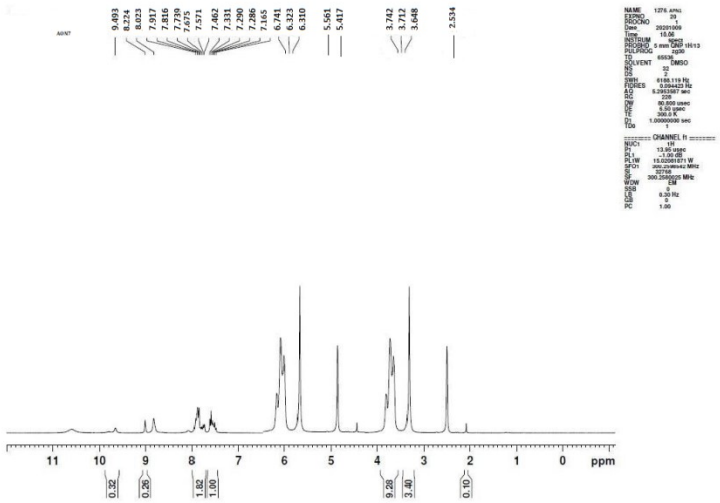
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleTypc**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM6	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:37:49 AM



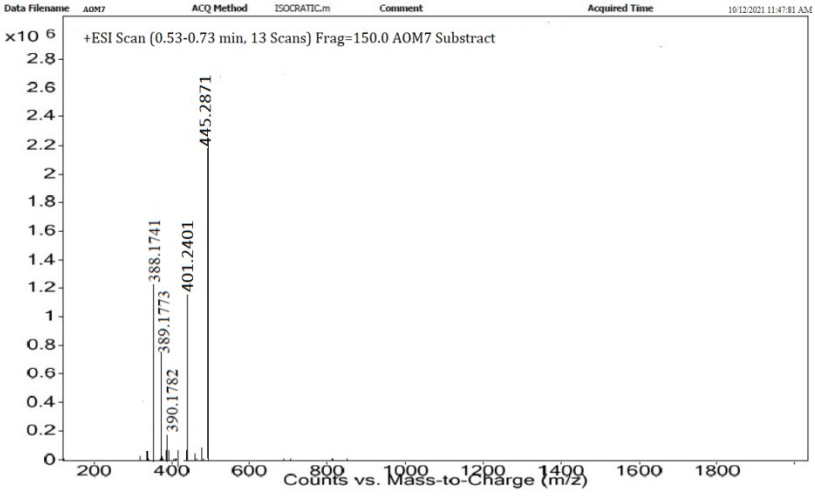


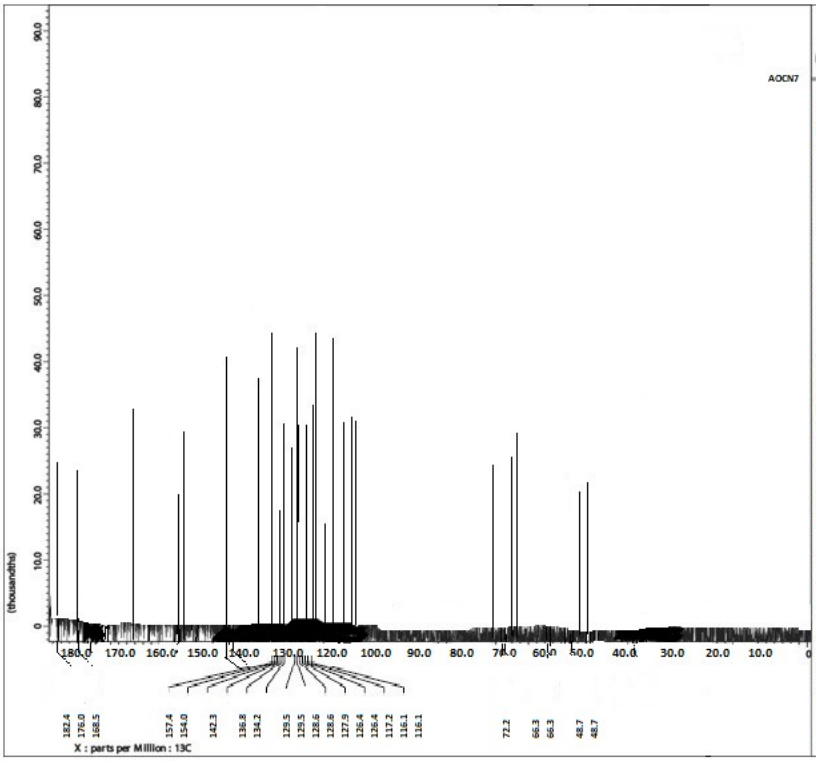
Compound 8 (g)


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
%T
cm-1
2976 cm-1
3040 cm-1
3069 cm-1
3146 cm-1
883 cm-1
1539 cm-1
1056 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI7 By
dharmesh Date
Monday
December 06 2021



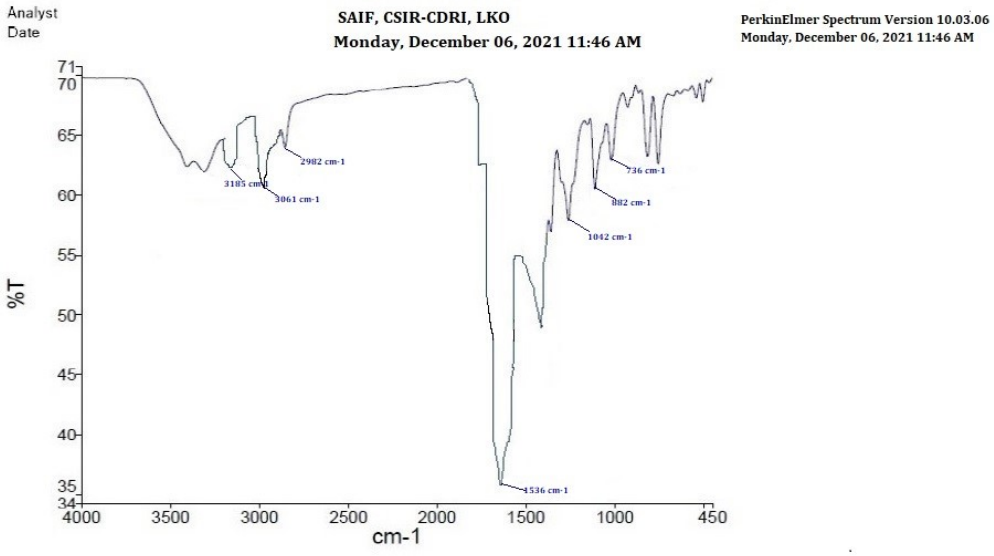
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM7	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:47:81 AM

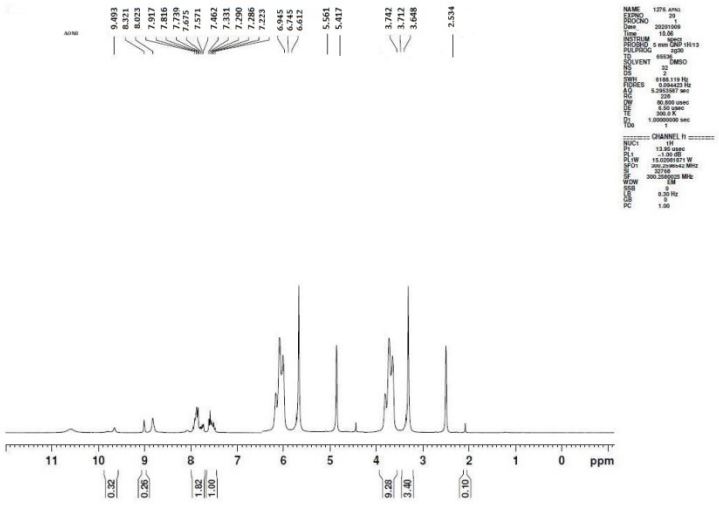




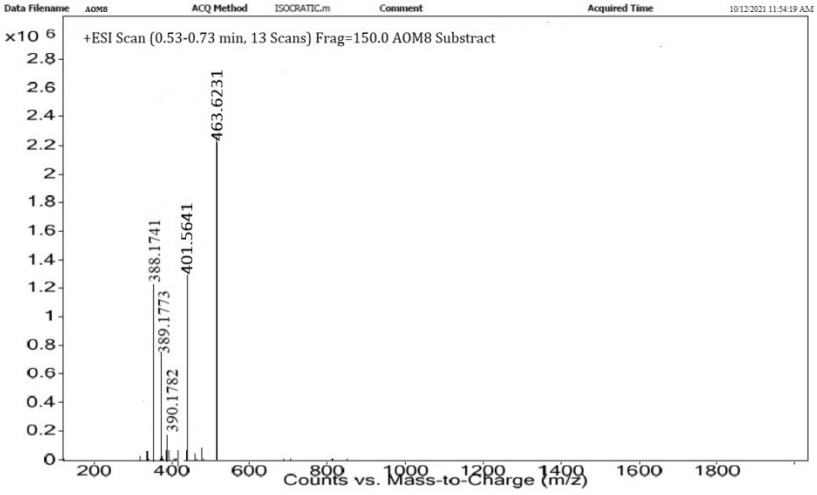
File name	= AOCN CARBON4.jd.t
Author	= M.Ahmed
Experiment	= single_pulse_dec
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 15:29:20 130321
Revision_time	= 15:38:12 130321
Current time	= 15:46:20 130321
Data_format	= 1D_COMPLEX
Dim_ebe	= 26314
Dim_title	= 13C
Dim_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_strength	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_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_atn	= 7.1 [dx]
I_pulse	= 3.20666667 [u.s]
Irr_atn_acc	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 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]

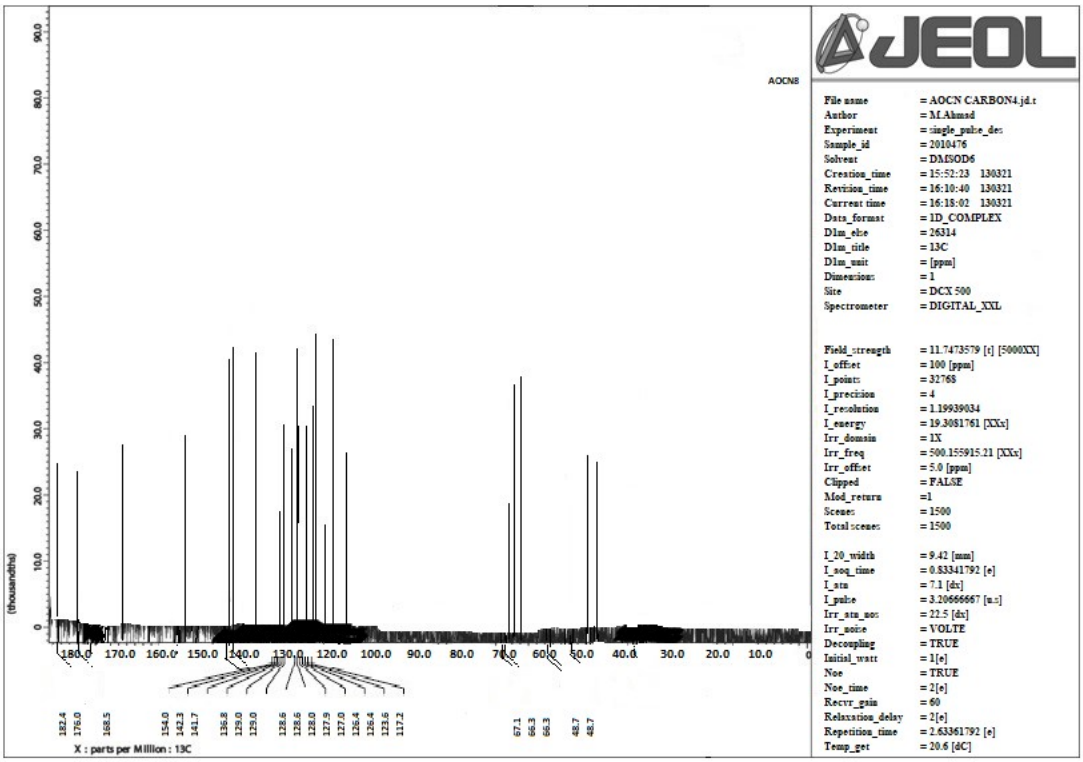
Compound 8 (h)


Analyst
Date
SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 11:46 AM
PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 11:46 AM
%T
cm-1
3105 cm-1
3061 cm-1
2982 cm-1
1536 cm-1
1042 cm-1
882 cm-1
736 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI8 By
dharmesh Date
Monday
December 06 2021


9.493
8.321
8.033
7.857
7.816
7.739
7.675
7.571
7.462
7.331
7.290
7.286
7.223
6.545
6.454
6.432
5.561
5.417
3.742
3.712
3.648
2.534
ppm
0.92
0.29
1.82
1.00
9.28
3.40
0.10

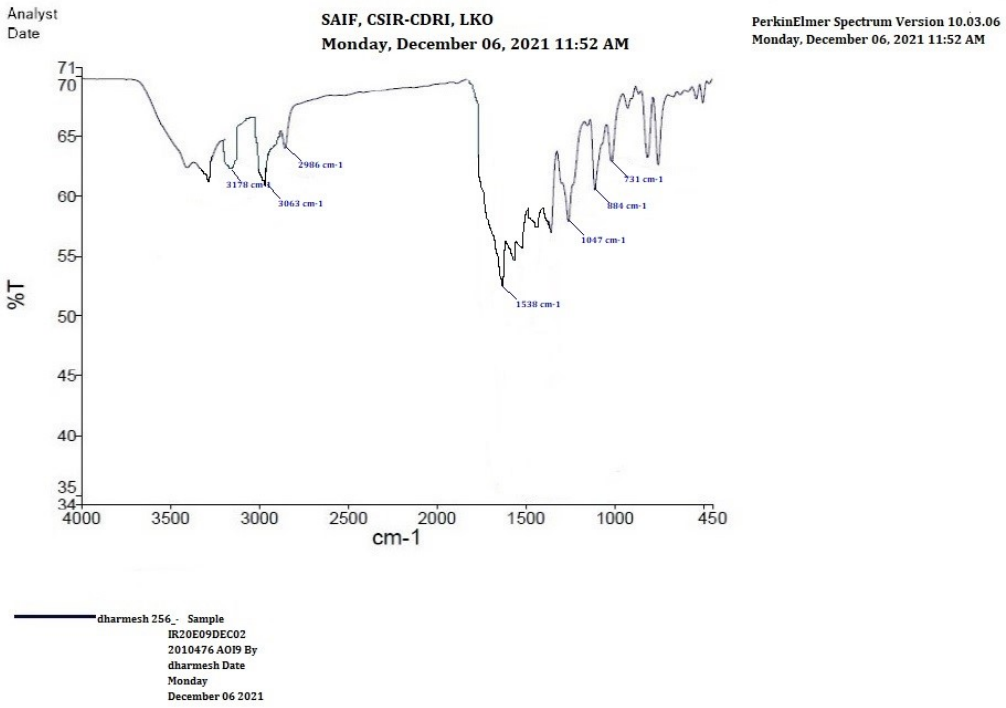
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleTypc**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM8	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:54:19 AM

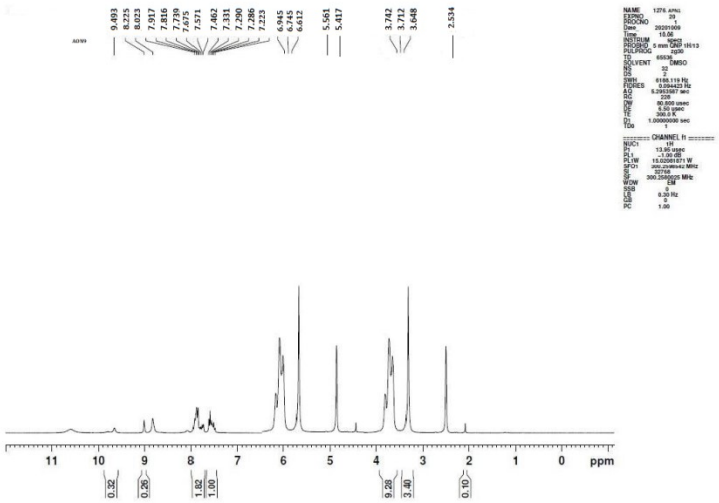




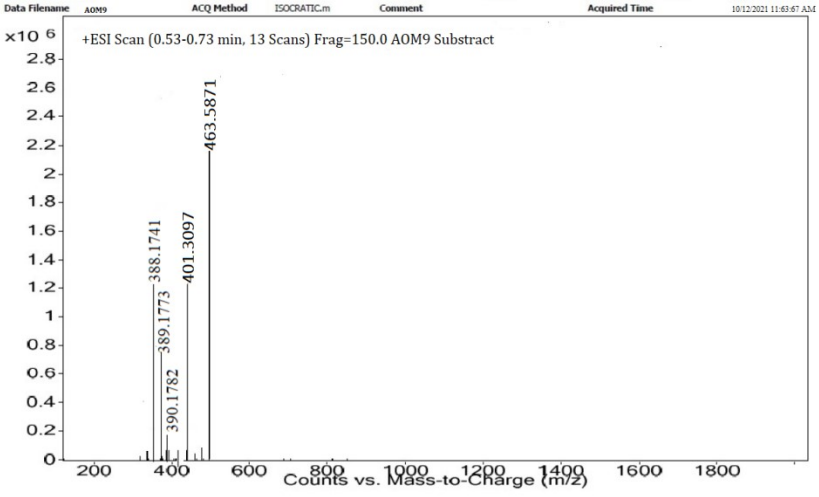
File name	= AOCN CARBON4.jd.t
Author	= M.Ahmad
Experiment	= single_pulse_de
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 15:52:23 130321
Revision_time	= 16:10:40 130321
Current time	= 16:18:02 130321
Data_format	= 1D_COMPLEX
D1m_ele	= 26314
D1m_title	= 13C
D1m_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_strength	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	=1
Scenes	= 1500
Total scenes	= 1500
I_20_width	= 9.42 [mm]
I_acq_time	= 0.83341792 [e]
I_stn	= 7.1 [dx]
I_pulse	= 3.20666667 [u.]
Irr_stn_nos	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 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]

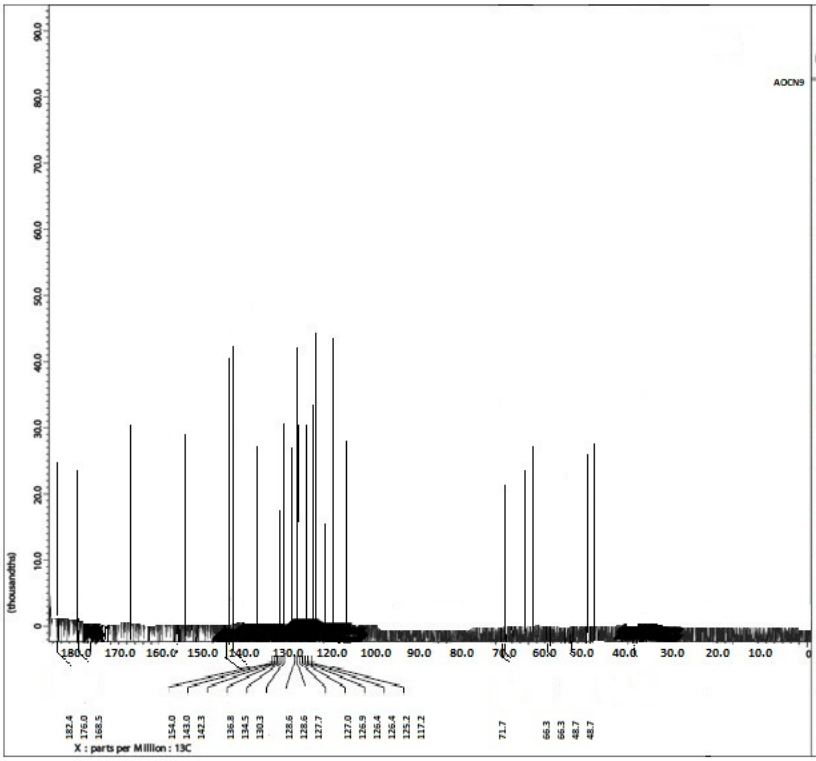
Compound 8 (i)


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
%T
cm-1
2986 cm-1
3178 cm-1
3063 cm-1
731 cm-1
804 cm-1
1047 cm-1
1538 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI9 By
dharmesh Date
Monday
December 06 2021



Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM9	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:63:67 AM

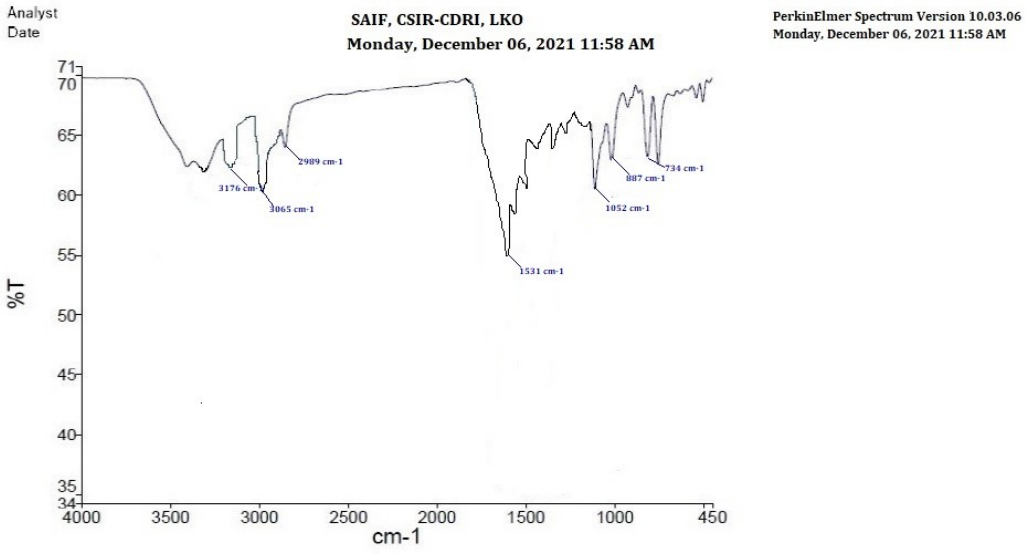


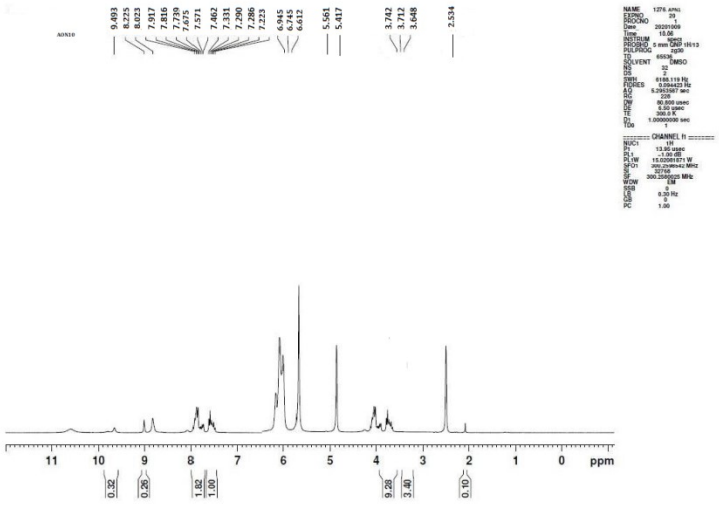


JEOL

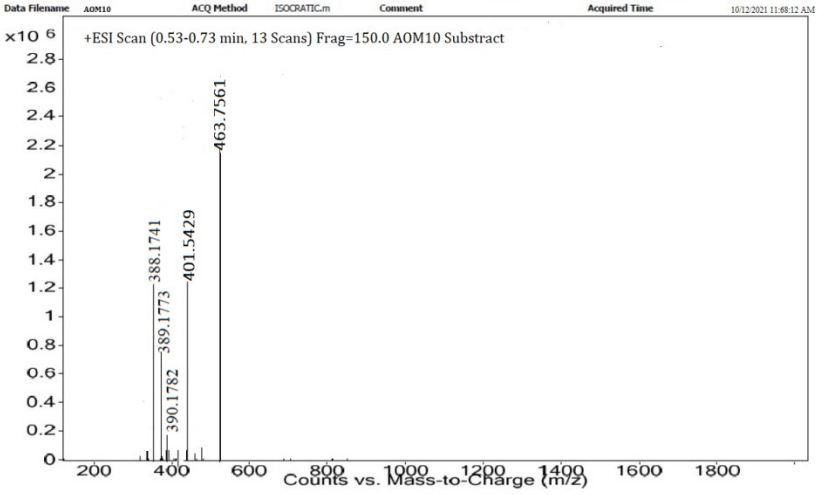
File name	= AOCN CARBON4.jd.t
Author	= M.Ahmad
Experiment	= single_pulse_de
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 16:23:10 130321
Revision_time	= 16:31:16 130321
Current time	= 16:42:40 130321
Data_format	= 1D_COMPLEX
Dim_ele	= 26314
Dim_title	= 13C
Dim_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_strength	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	=1
Scenes	= 1500
Total scenes	= 1500
I_20_width	= 9.42 [mm]
I_noq_time	= 0.83341792 [e]
I_stn	= 7.1 [dx]
I_pulse	= 3.20666667 [u.s]
Irr_stn_nos	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 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]

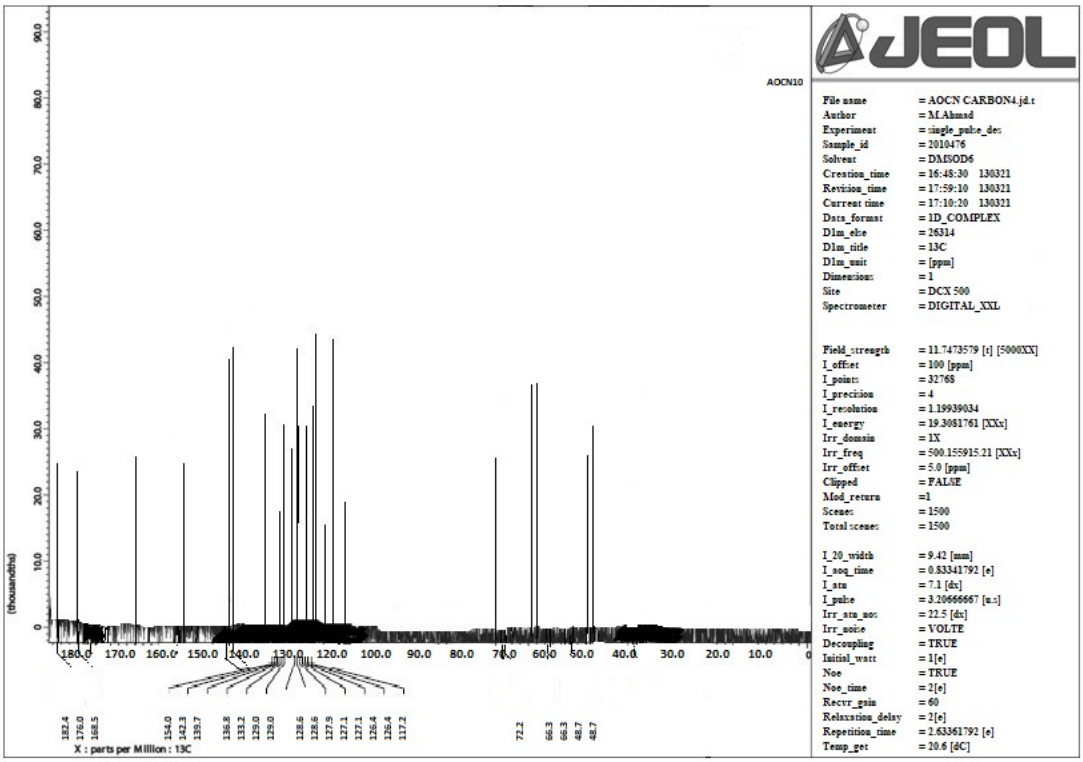
Compound 8 (j)


Analyst
Date
SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 11:58 AM
PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 11:58 AM
%T
cm-1
3176 cm-1
3065 cm-1
2989 cm-1
1531 cm-1
1052 cm-1
887 cm-1
734 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI10 By
dharmesh Date
Monday
December 06 2021


9.493
8.225
8.033
7.917
7.816
7.739
7.675
7.571
7.462
7.331
7.290
7.286
7.221
6.945
6.745
6.612
5.561
5.417
3.742
3.712
3.648
2.534
ppm
0.92
0.98
1.82
1.00
9.28
3.40
0.10

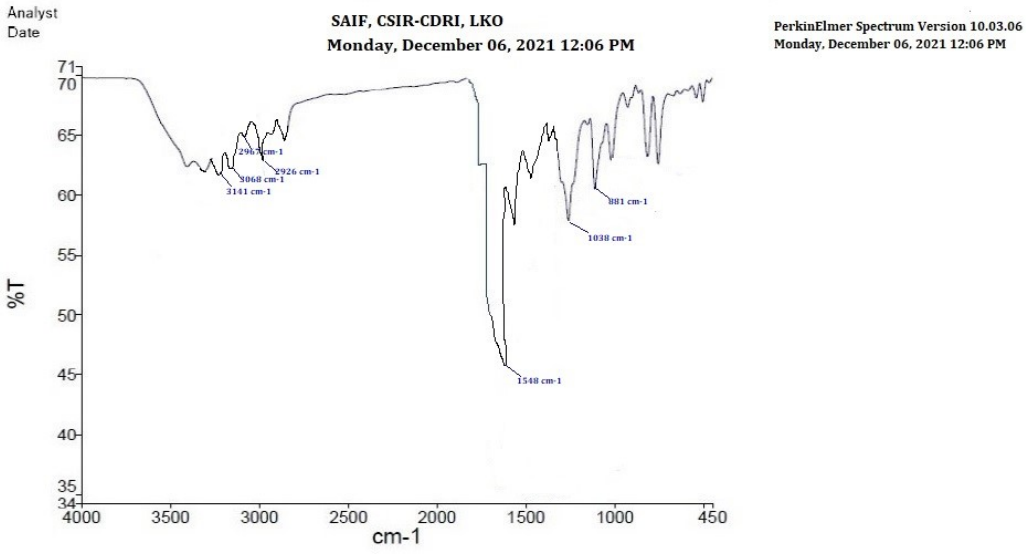
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleTypc**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM10	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:68:12 AM

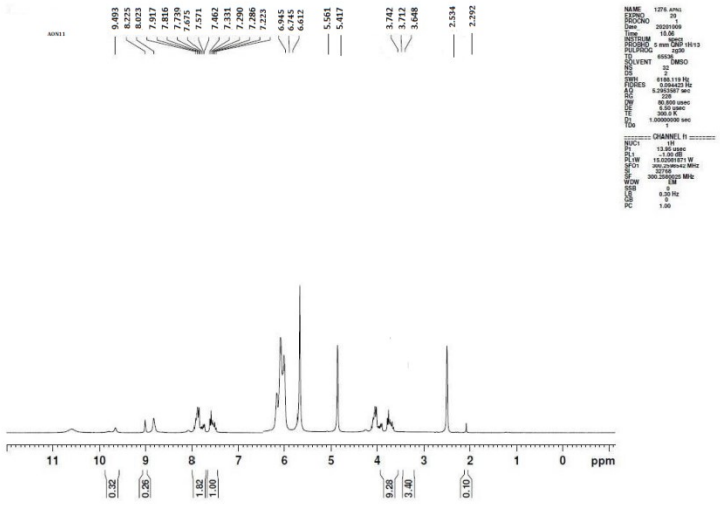




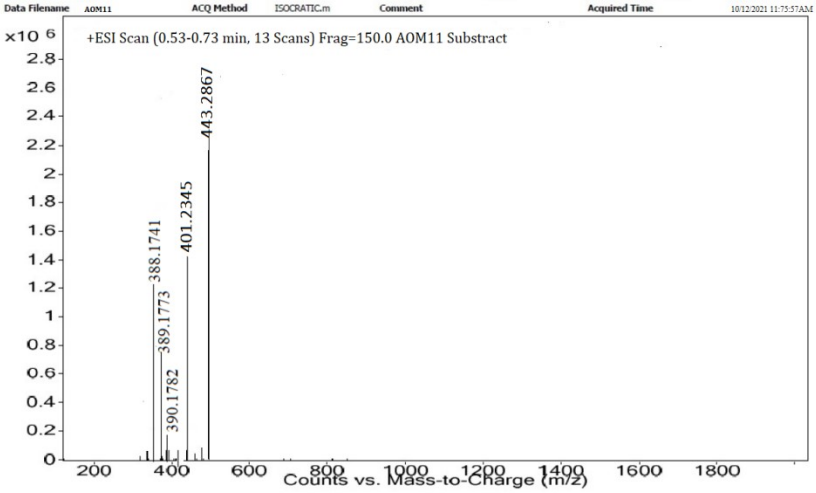
File name	= AOCN CARBON4.jd.t
Author	= M.Ahmad
Experiment	= single_pulse_dec
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 16:48:30 130321
Revision_time	= 17:59:10 130321
Current time	= 17:10:20 130321
Data_format	= 1D_COMPLEX
D1m_ebe	= 26314
D1m_title	= 13C
D1m_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_streagth	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_offset	= 5.0 [ppm]
Clipped	= FALSE
Mod_return	=1
Scanes	= 1500
Total scanes	= 1500
I_20_width	= 9.42 [mm]
I_acq_time	= 0.83341792 [e]
I_atn	= 7.1 [dx]
I_pulse	= 3.20666667 [u.s]
Irr_atn_nos	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 1[e]
Noe	= TRUE
Noe_time	= 2[e]
Recvr_gain	= 60
Relaxation_delay	= 2[e]
Repetition_time	= 2.53361792 [e]
Temp_get	= 20.6 [dC]

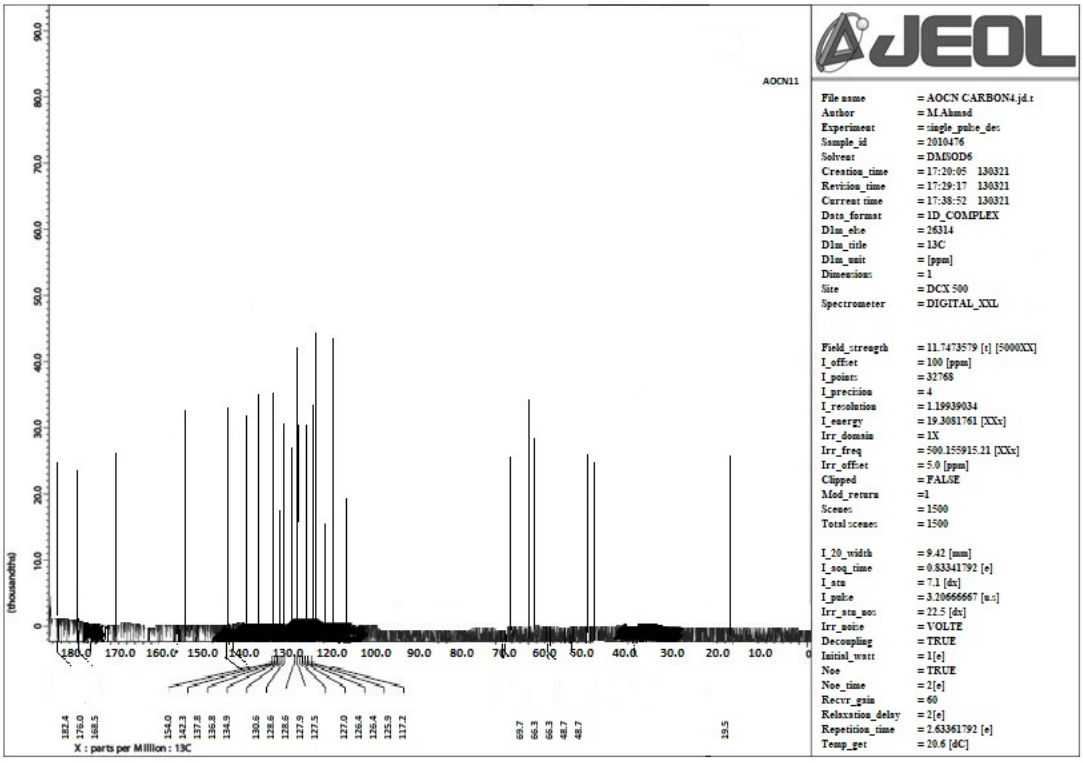
Compound 8 (k)


Analyst
Date
SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 12:06 PM
PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 12:06 PM
%T
cm-1
2963 cm-1
2926 cm-1
3068 cm-1
3141 cm-1
881 cm-1
1038 cm-1
1548 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI11 By
dharmesh Date
Monday
December 06 2021

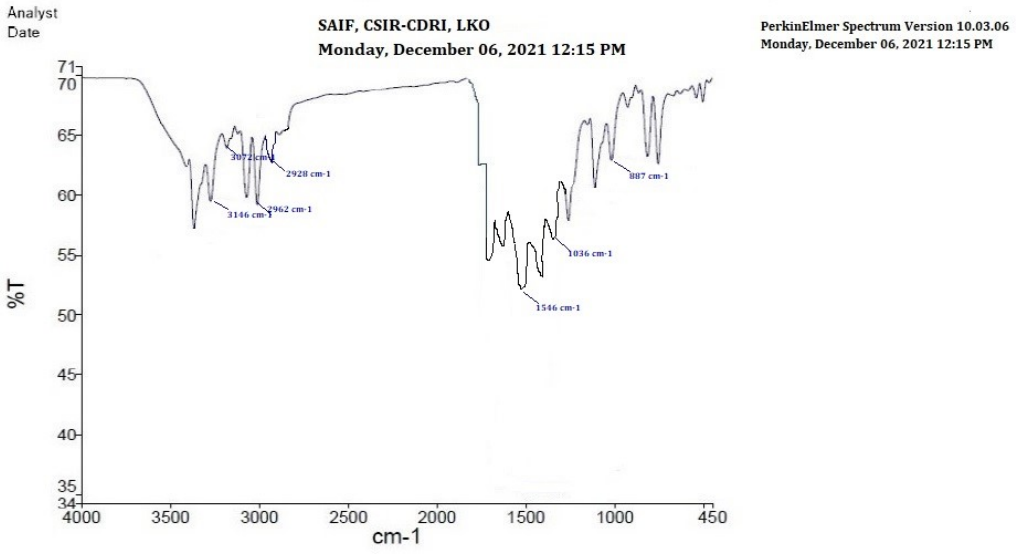

9.493
8.225
8.073
7.857
7.816
7.739
7.675
7.571
7.462
7.331
7.290
7.286
7.223
6.545
6.454
6.432
5.561
5.417
3.742
3.712
3.648
2.534
2.292
ppm
0.92
0.28
1.82
1.00
9.28
3.40
0.10

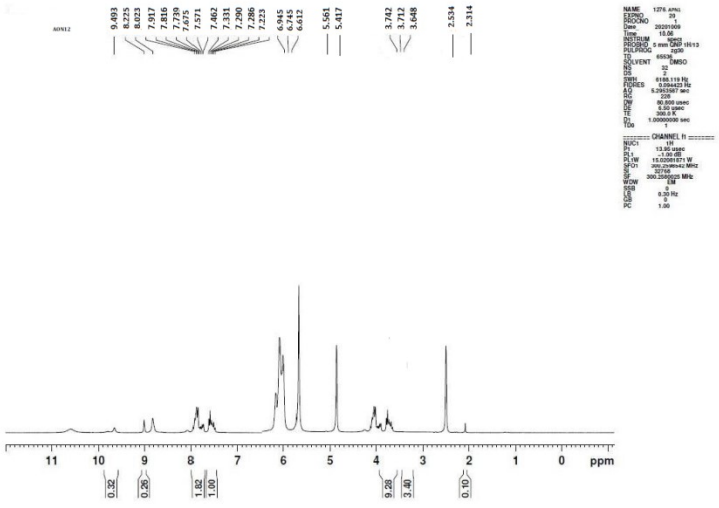
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleTypc**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM11	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:75:57AM



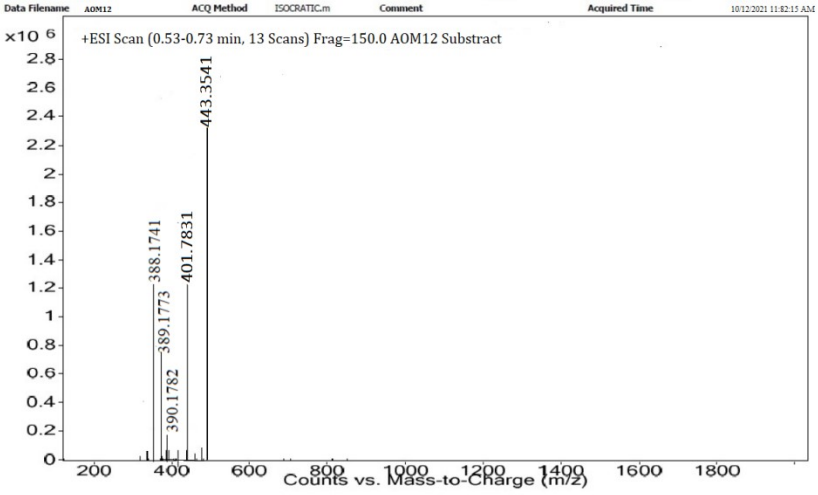


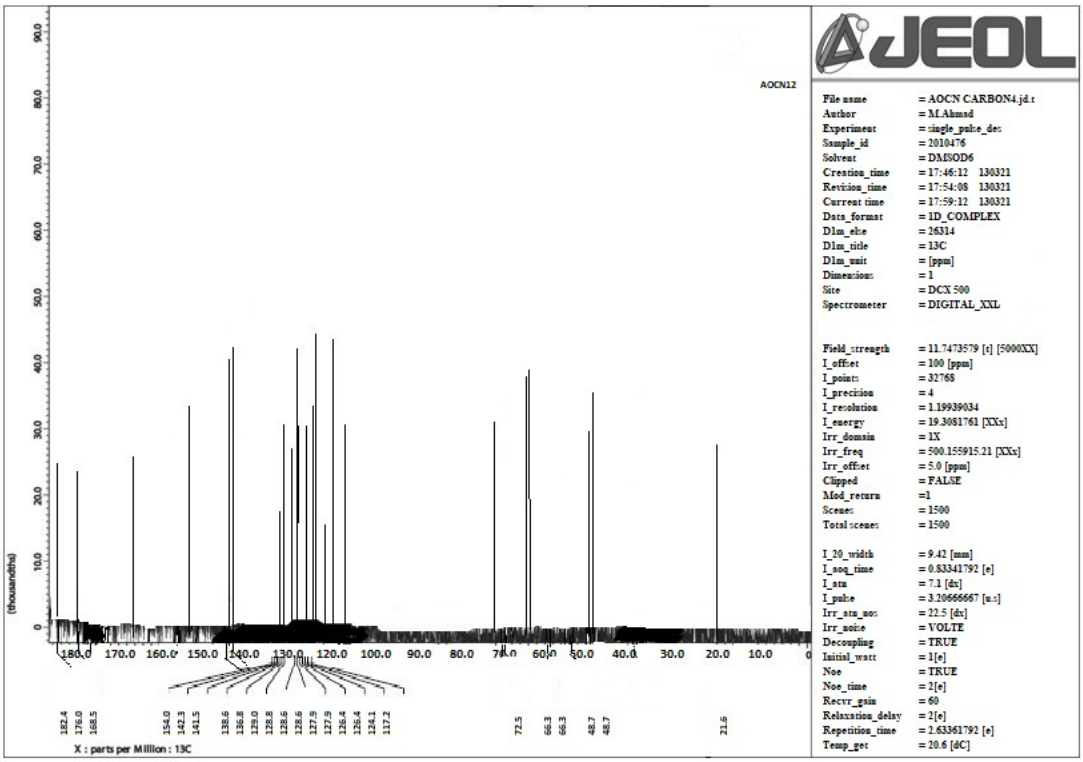
Compound 8 (l)


Analyst
Date
SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 12:15 PM
PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 12:15 PM
%T
cm-1
3072 cm-1
2928 cm-1
3146 cm-1
2962 cm-1
887 cm-1
1036 cm-1
1546 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI12 By
dharmesh Date
Monday
December 06 2021


9.493
8.225
8.033
7.857
7.816
7.739
7.675
7.571
7.462
7.331
7.290
7.286
7.233
6.645
6.454
6.632
5.561
5.417
3.742
3.712
3.648
2.534
2.314
ppm
0.92
0.28
1.82
1.00
9.28
3.40
0.10

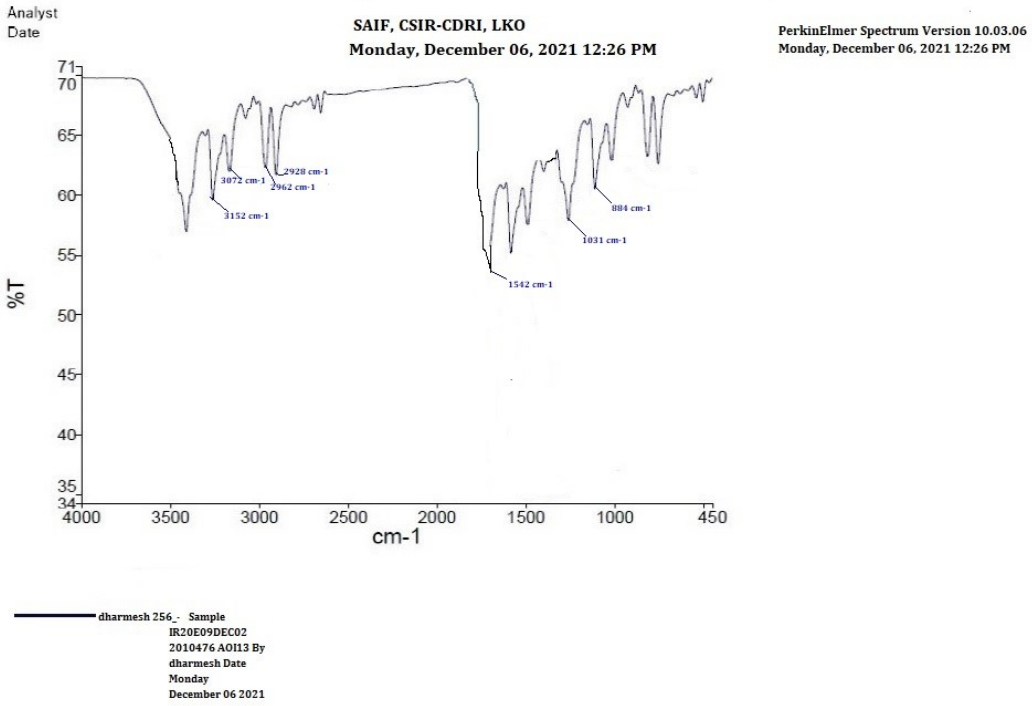
Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleTypc**	Sample	**IRM Calibration Status**	Success
Data Filename	AOM12	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:02:15 AM

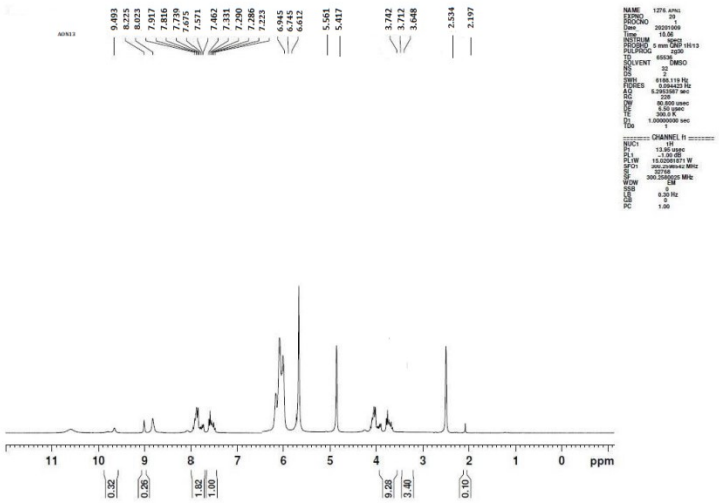




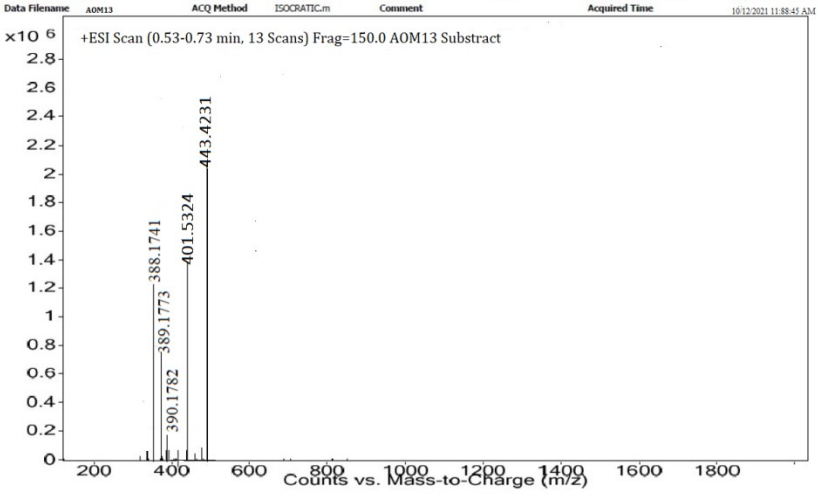
File name	= AOCN CARBON4.jd.t
Author	= M.Ahmad
Experiment	= single_pulse_dec
Sample_id	= 2010476
Solvent	= DMSOD6
Creation_time	= 17:46:12 130321
Revision_time	= 17:54:08 130321
Current time	= 17:59:12 130321
Data_format	= 1D_COMPLEX
D1m_obs	= 26314
D1m_title	= 13C
D1m_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_strength	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_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 [e]
I_atn	= 7.1 [dx]
I_pulse	= 3.20666667 [u.s]
Irr_atn_acc	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 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]

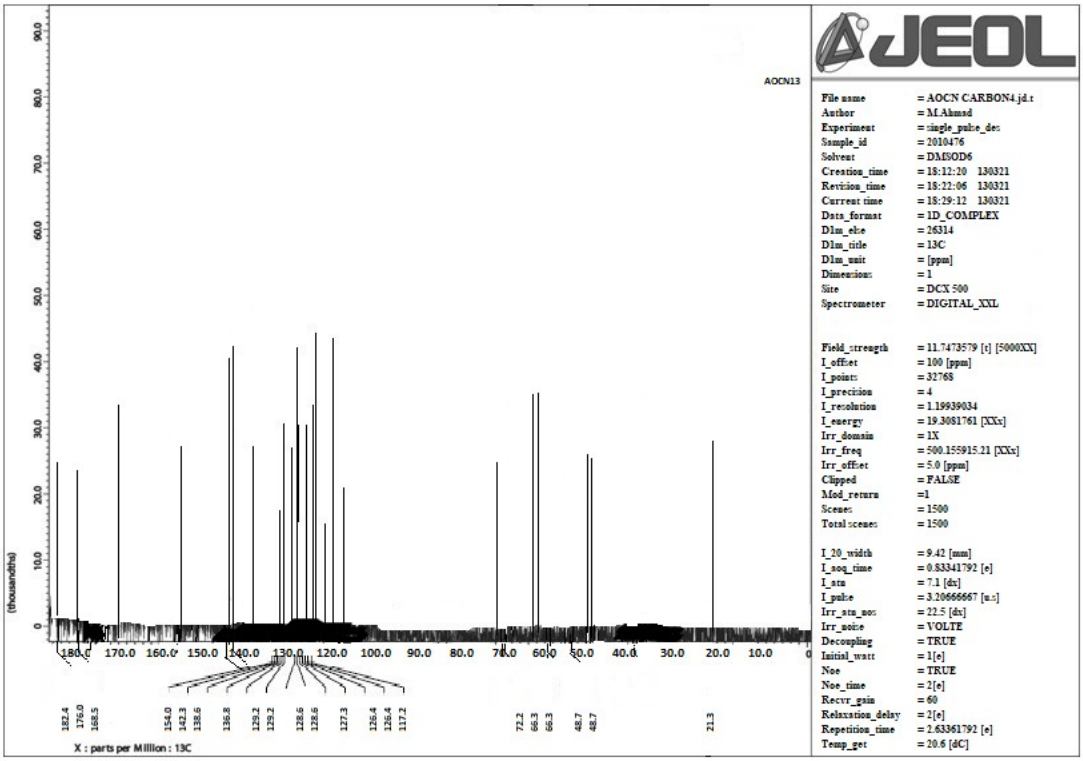
Compound 8 (m)


Analyst
Date
SAIF, CSIR-CDRI, LKO
Monday, December 06, 2021 12:26 PM
PerkinElmer Spectrum Version 10.03.06
Monday, December 06, 2021 12:26 PM
%T
cm-1
3072 cm-1
2928 cm-1
2962 cm-1
3152 cm-1
884 cm-1
1031 cm-1
1542 cm-1
dharmesh 256_- Sample
IR20E09DEC02
2010476 AOI13 By
dharmesh Date
Monday
December 06 2021



Sample Name	Akanksha (2010476)	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	A0M13	**ACQ Method**	ISOCRATIC.m	**Comment**		**Acquired Time**	10/12/2021 11:88:45 AM





File name	= AOCN CARBON4.jd.t
Author	= M.Ahmad
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
D1m_ehe	= 26314
D1m_title	= 13C
D1m_unit	= [ppm]
Dimension	= 1
Site	= DCX 500
Spectrometer	= DIGITAL_XXL
Field_strength	= 11.7473579 [t] [5000XX]
I_offset	= 100 [ppm]
I_points	= 32768
I_precision	= 4
I_resolution	= 1.19939034
I_energy	= 19.3081761 [XXx]
Irr_domain	= 1X
Irr_freq	= 500.155915.21 [XXx]
Irr_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_atn	= 7.1 [dx]
I_pulse	= 3.20666667 [u.s]
Irr_atn_noe	= 22.5 [dx]
Irr_noise	= VOLTE
Decoupling	= TRUE
Initial_watt	= 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]