

Supplementary Data

Synthesis and antifungal screening of tetramethyl hexahydro-1H-xanthene-1,8(2H)-dione derivatives as potential inhibitors of morphogenesis and biofilm in *Candida albicans*

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Savitribai Phule Pune University)

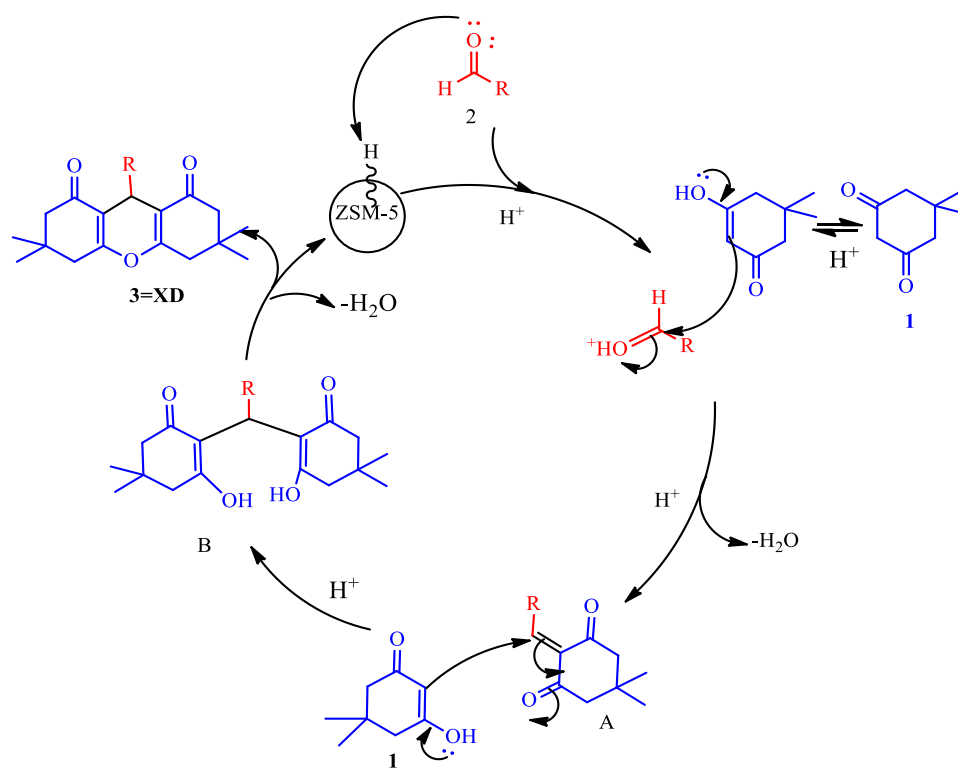
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Savitribai Phule Pune University)

^f Dean, Science and technology, Savitribai Phule Pune University, Pune-411007, India

Chemistry



Scheme S1 The plausible reaction mechanism

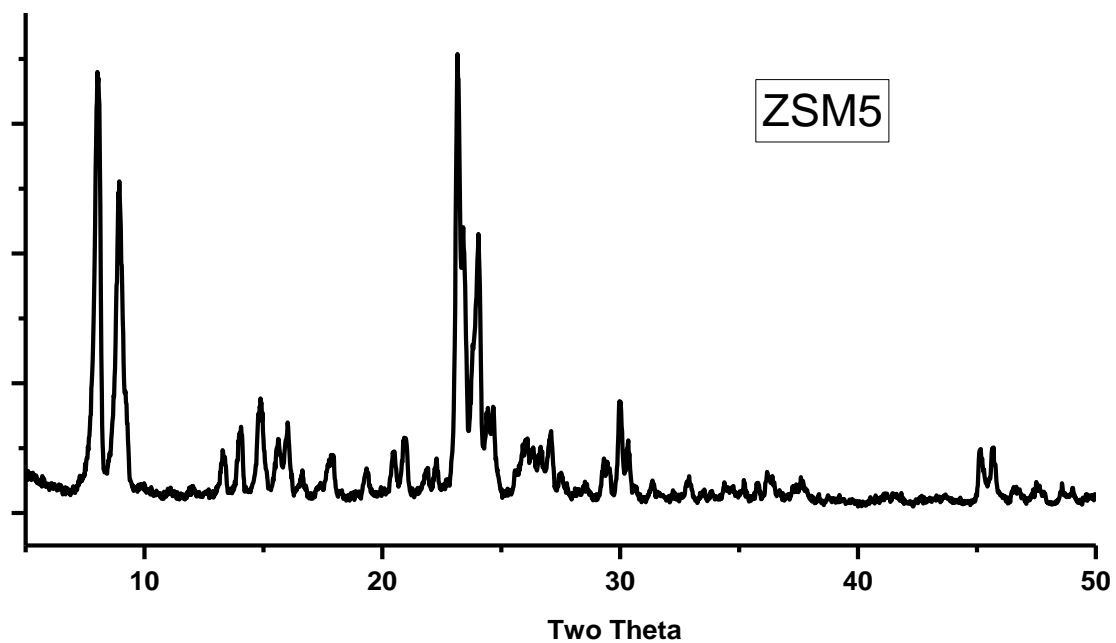


Fig. S1 Powder XRD spectrum of ZSM-5 zeolite

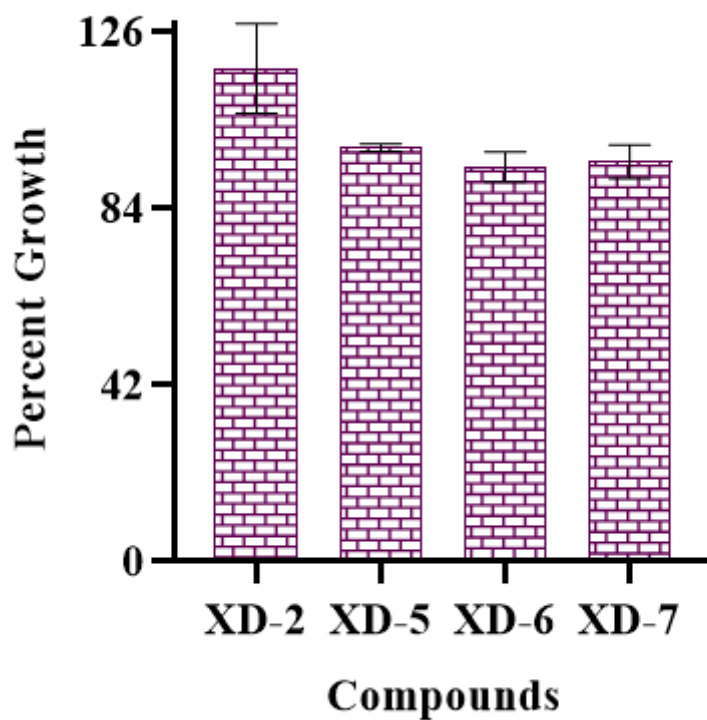
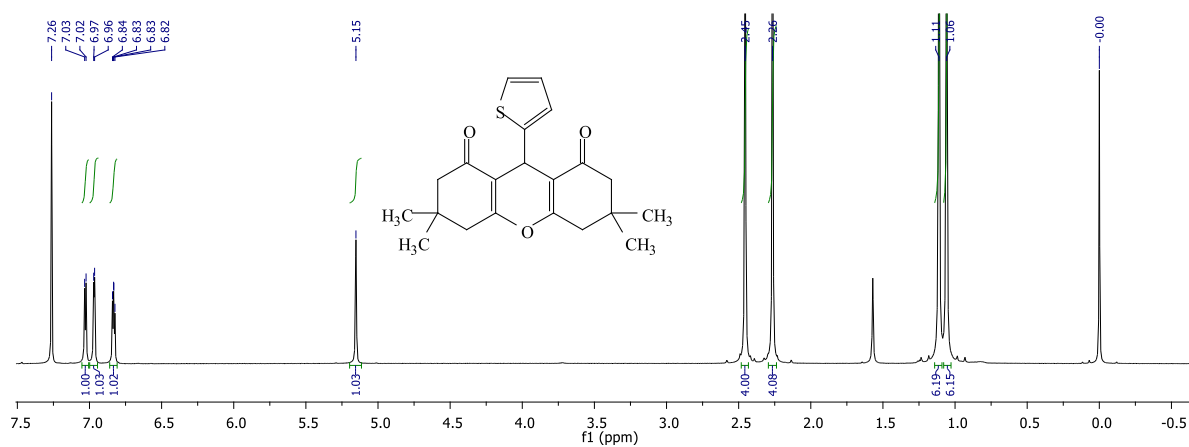
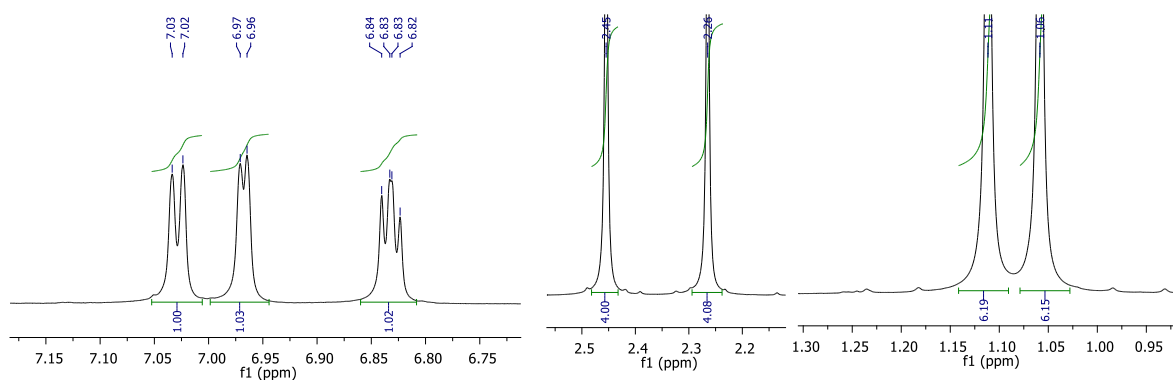
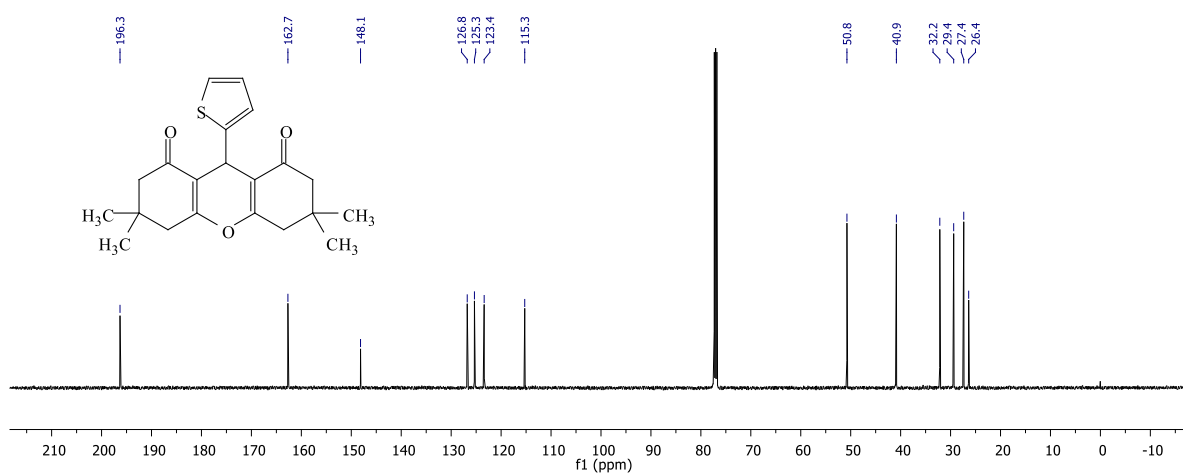


Fig. S2 Cytotoxic study of XD-2, XD-4, XD-5 and XD-6 on HEK 293 cell line: XD derivatives 2, 4, 5 and 6 have shown very less cytotoxicity (8 to 11%).

Spectral and HPLC Analysis of synthesized compounds



¹H NMR (500 MHz, CDCl₃) of XD-1



¹³C NMR (125 MHz, CDCl₃) of XD-1

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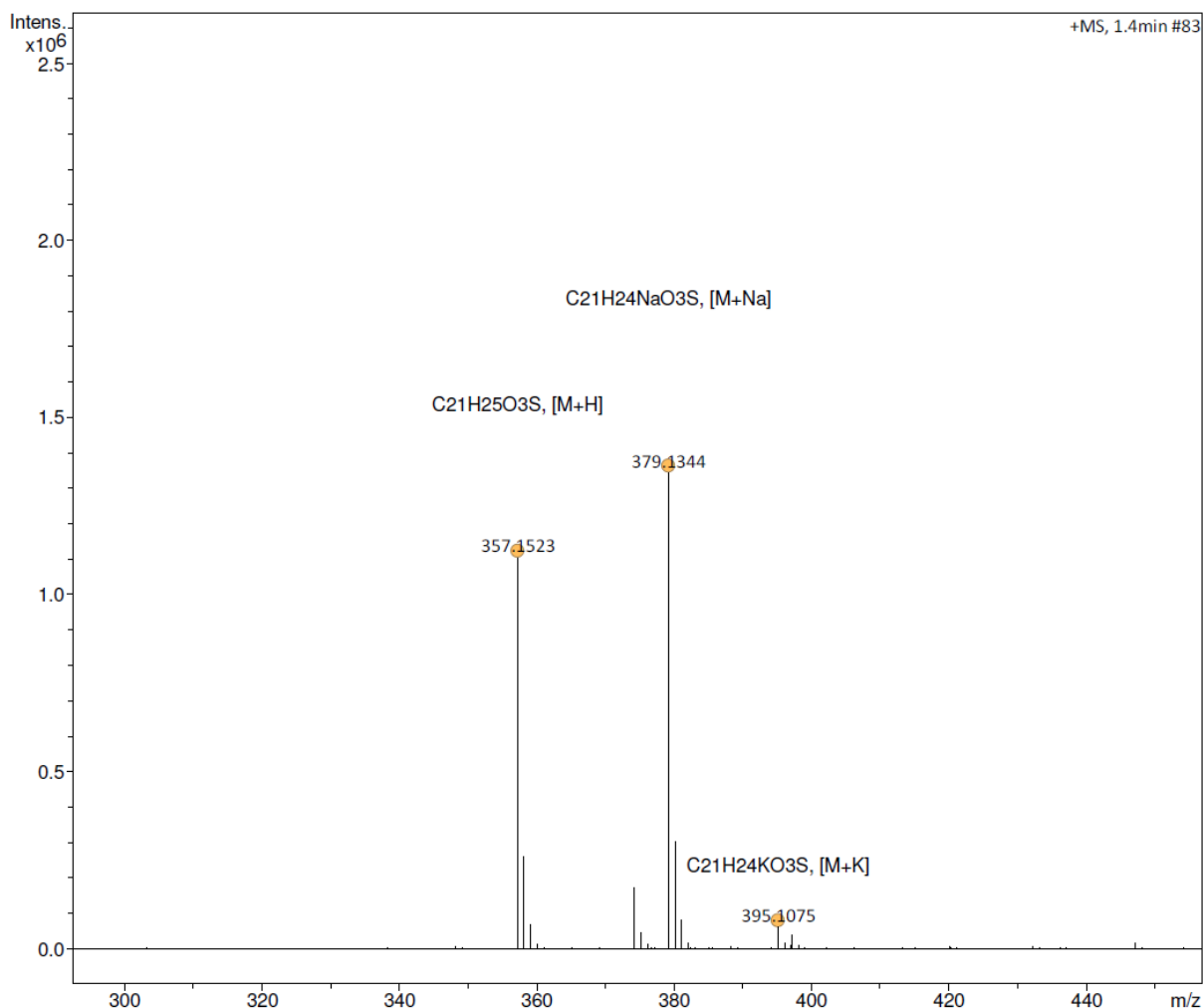
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 Operator CIF
 Instrument impact HD 1819696.00184

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Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
357.152256	1	C21H25O3S	100.00	357.151892	-0.4	-1.0	7.6	9.5	even		ok	M+H
379.134364	1	C21H24NaO3S	100.00	379.133836	-0.5	-1.4	11.9	9.5	even		ok	M+Na
395.107486	1	C21H24KO3S	100.00	395.107774	0.3	0.7	21.1	9.5	even		ok	M+K

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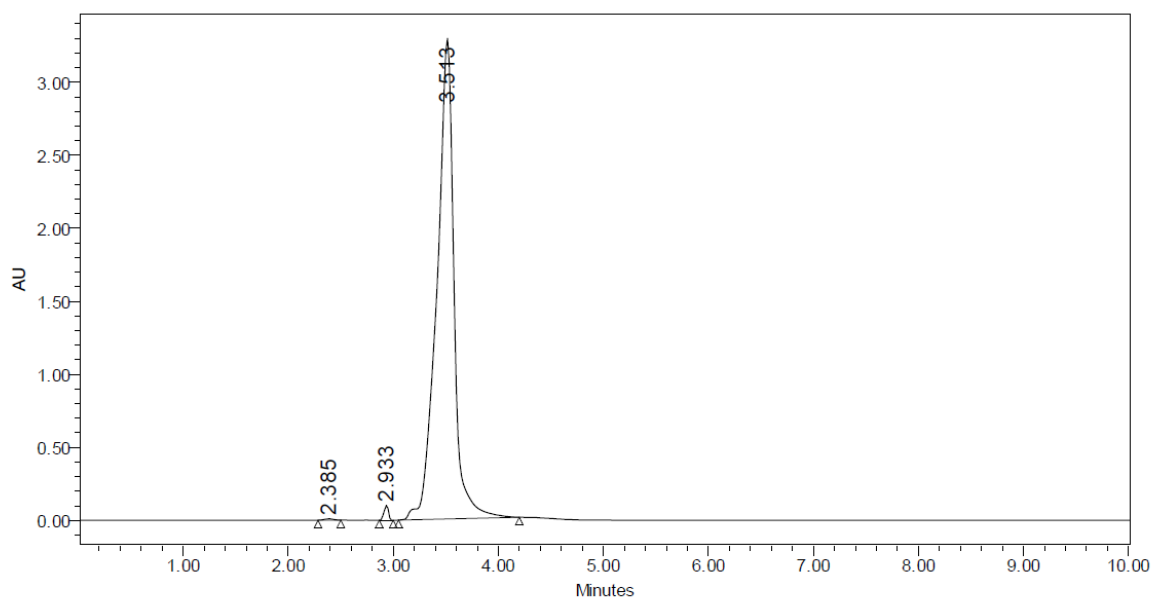
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Page 1 of 1

HR-MS spectrum of XD-1

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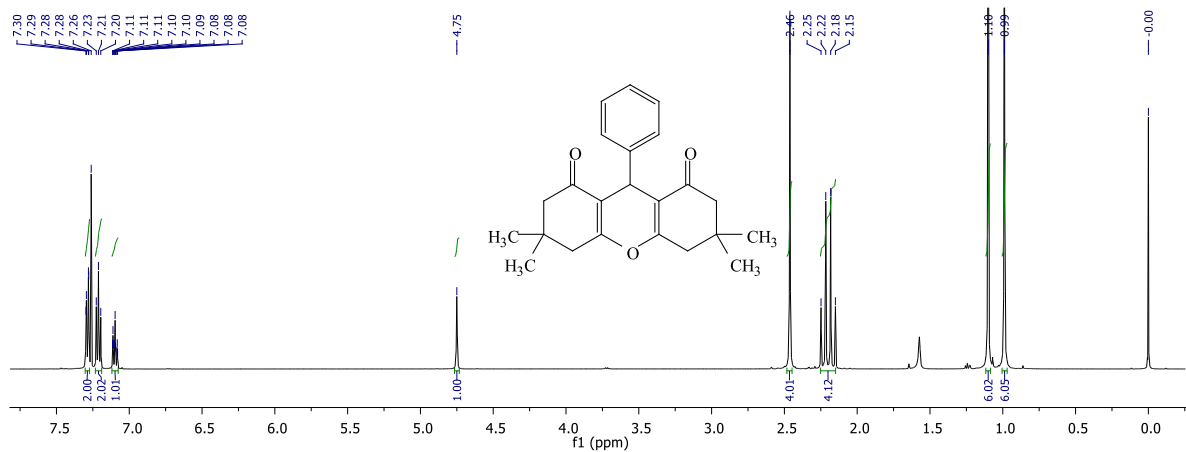
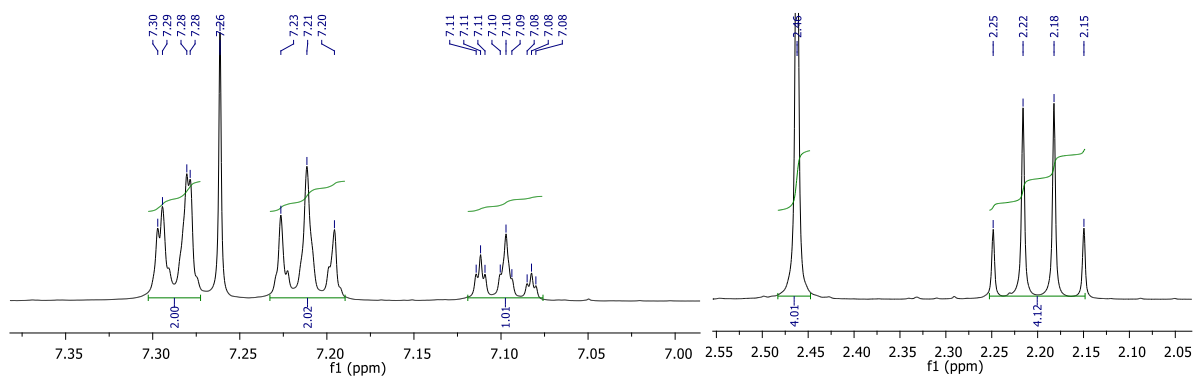


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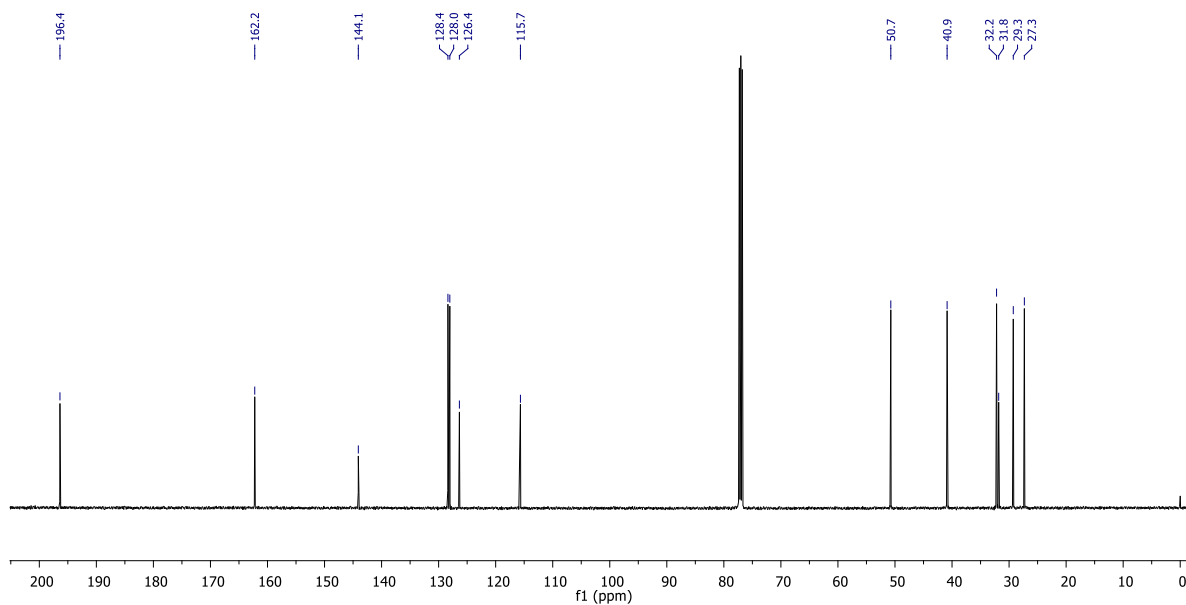
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HPLC spectrum of XD-1



^1H NMR (500 MHz, CDCl_3) of XD-2



^{13}C NMR (125 MHz, CDCl_3) of XD-2

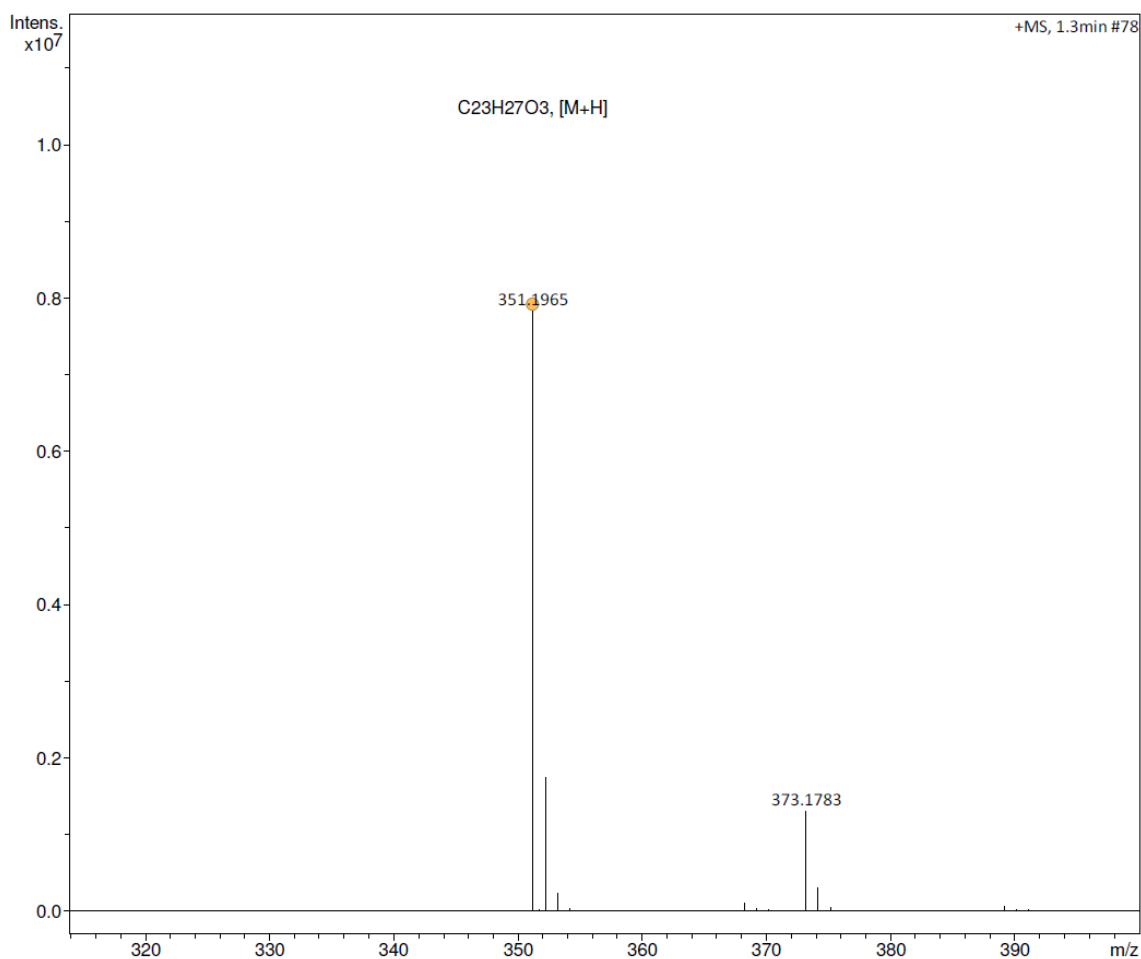
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Comment			

Acquisition Parameter

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Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
351.196540	1	C23H27O3	100.00	351.195471	-1.1	-3.0	18.3	10.5	even	ok		M+H

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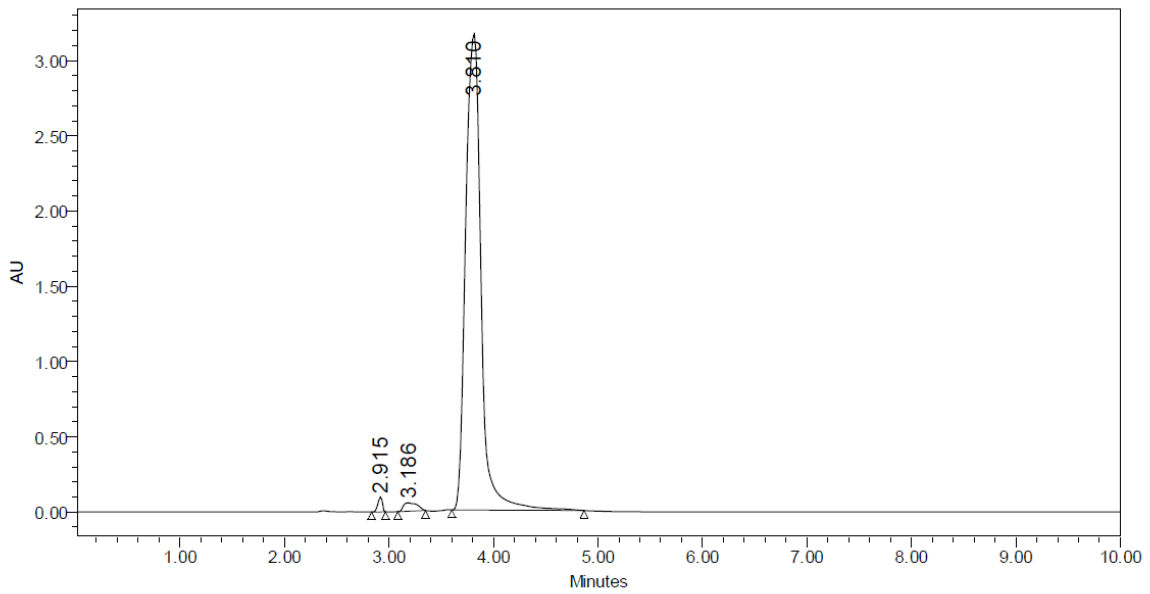
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Page 1 of 1

HR-MS spectrum of XD-2

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Vial:	16	Acq. Method Set:	CIF
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Injection Volume:	10.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA MaxPlot (190.0 nm to
Date Acquired:	09-04-2021 17:27:25 IST		
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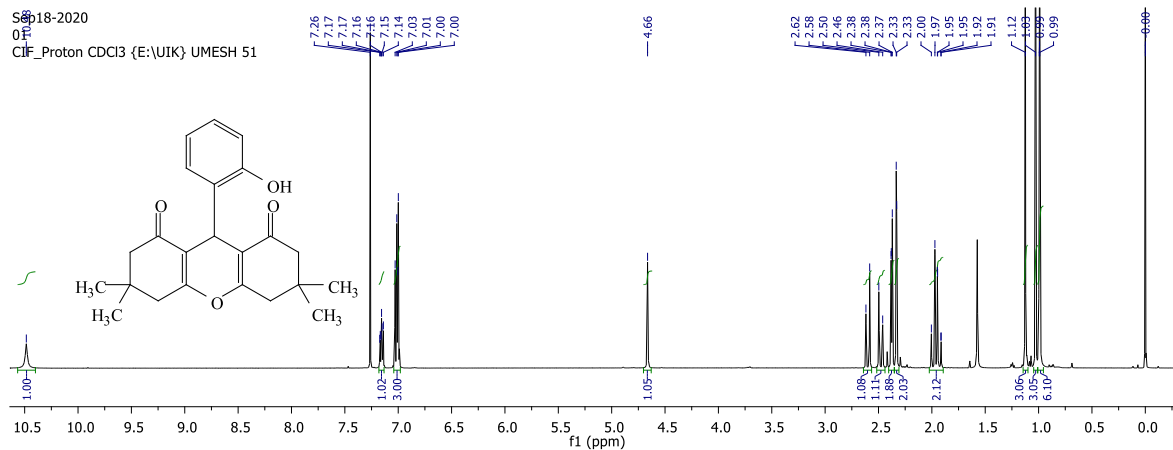
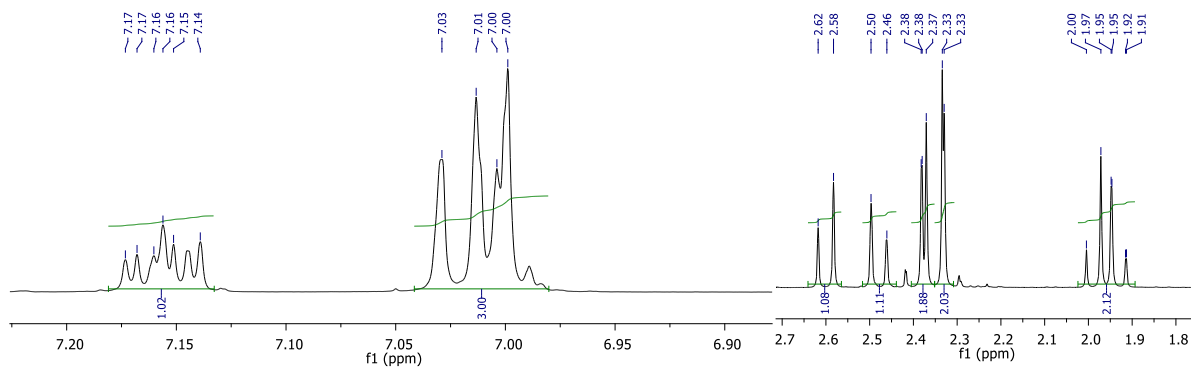


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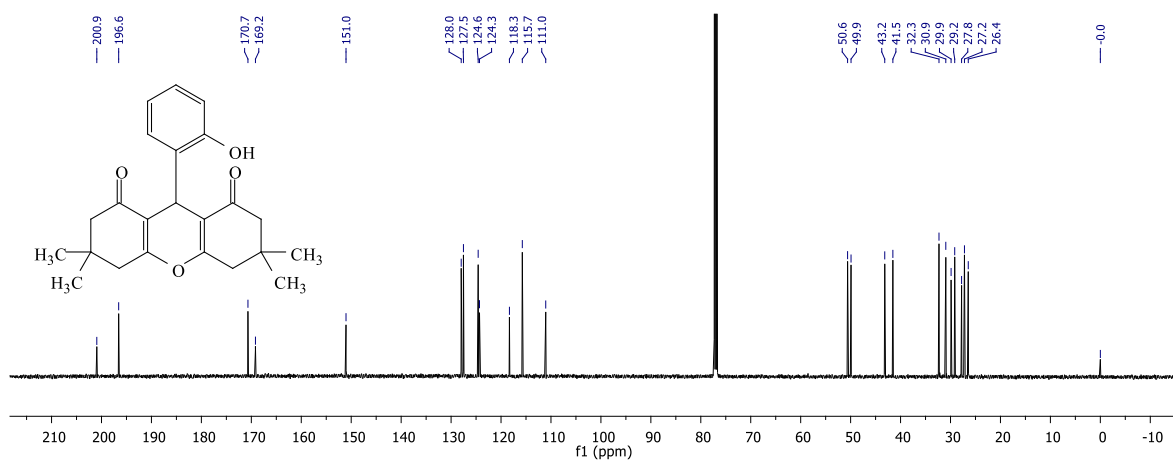
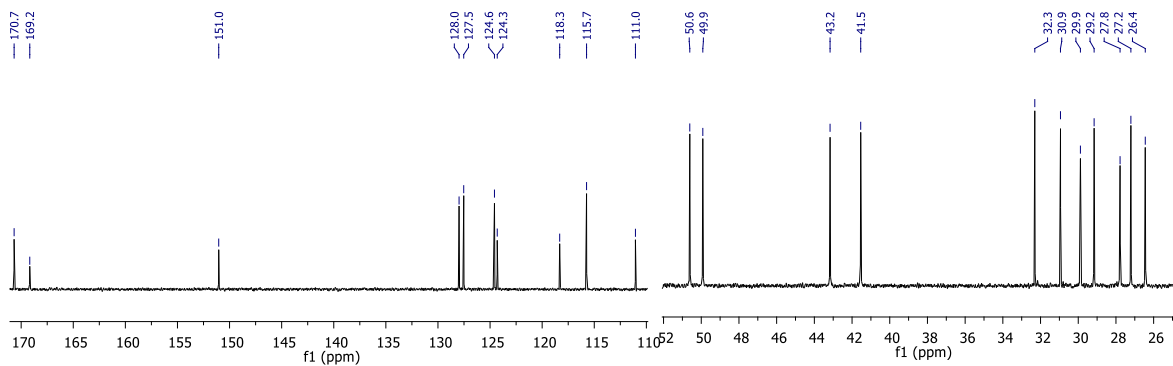
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HPLC spectrum of XD-2



¹H NMR (500 MHz, CDCl₃) of XD-3



¹³C NMR (125 MHz, CDCl₃) of XD-3

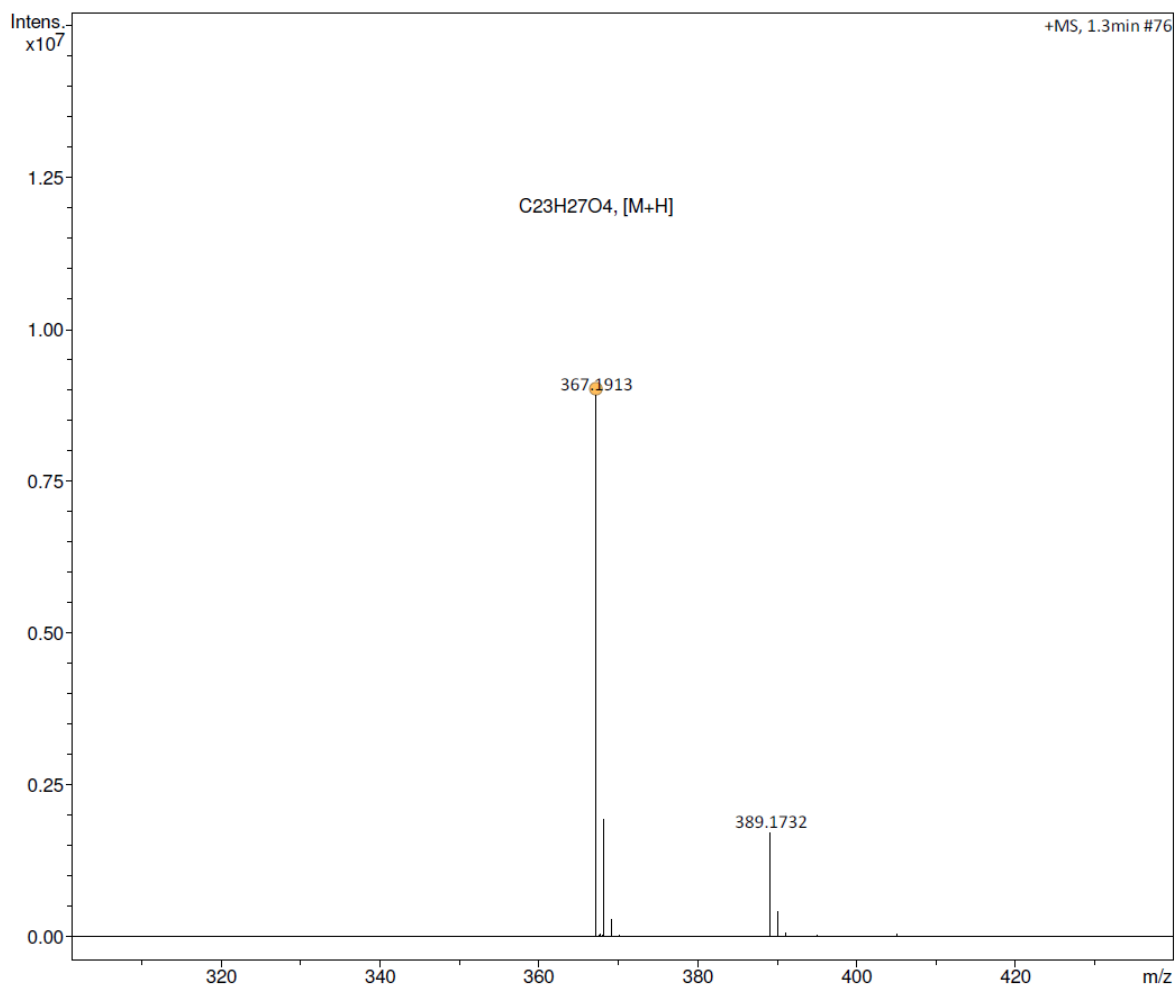
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Comment				

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Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
367.191282	1	C ₂₃ H ₂₇ O ₄	100.00	367.190386	-0.9	-2.4	22.2	10.5	even		ok	M+H

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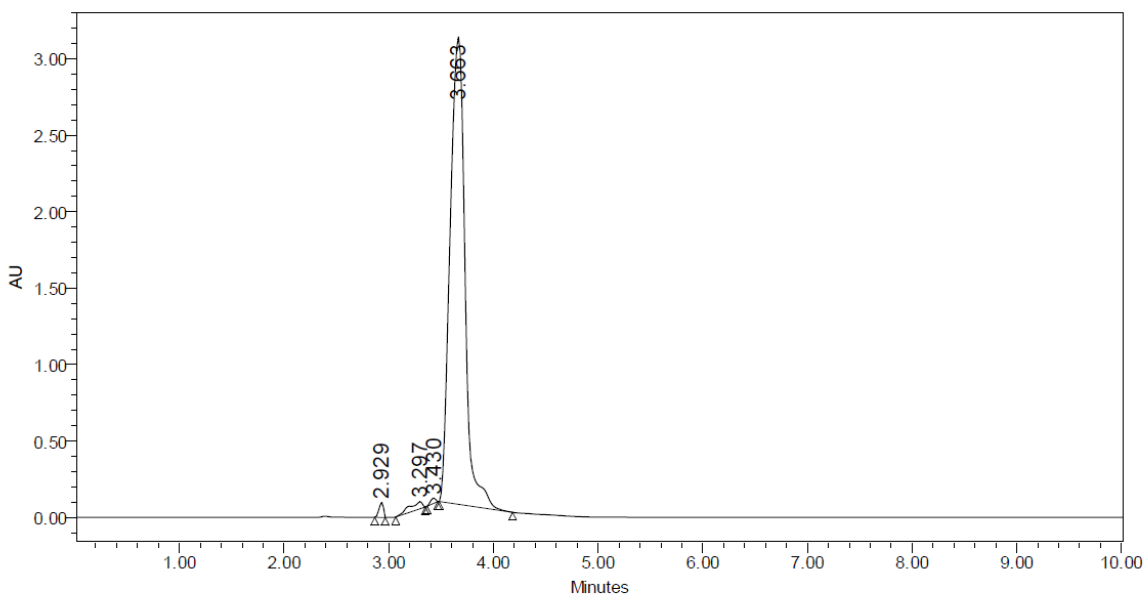
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Page 1 of 1

HR-MS spectrum of XD-3

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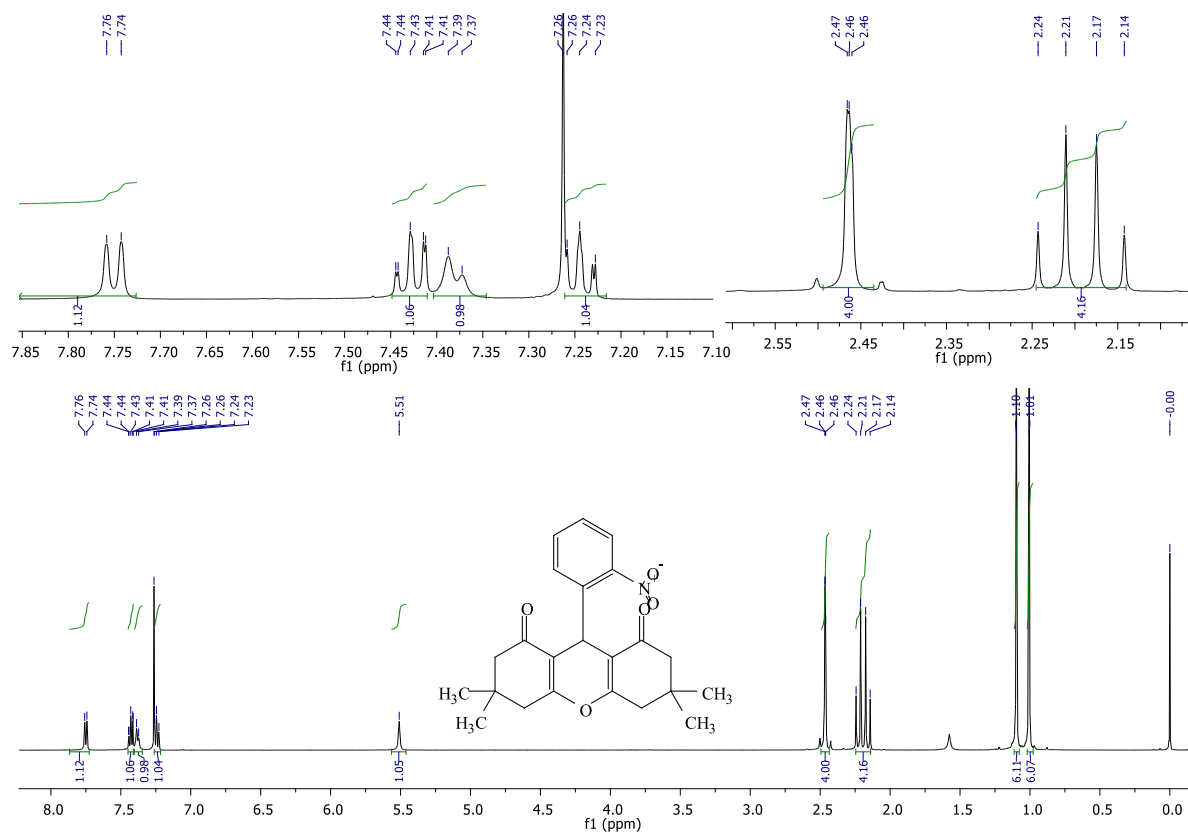


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3	3.430	118620	0.38	32701
4	3.663	30080625	97.26	3061717

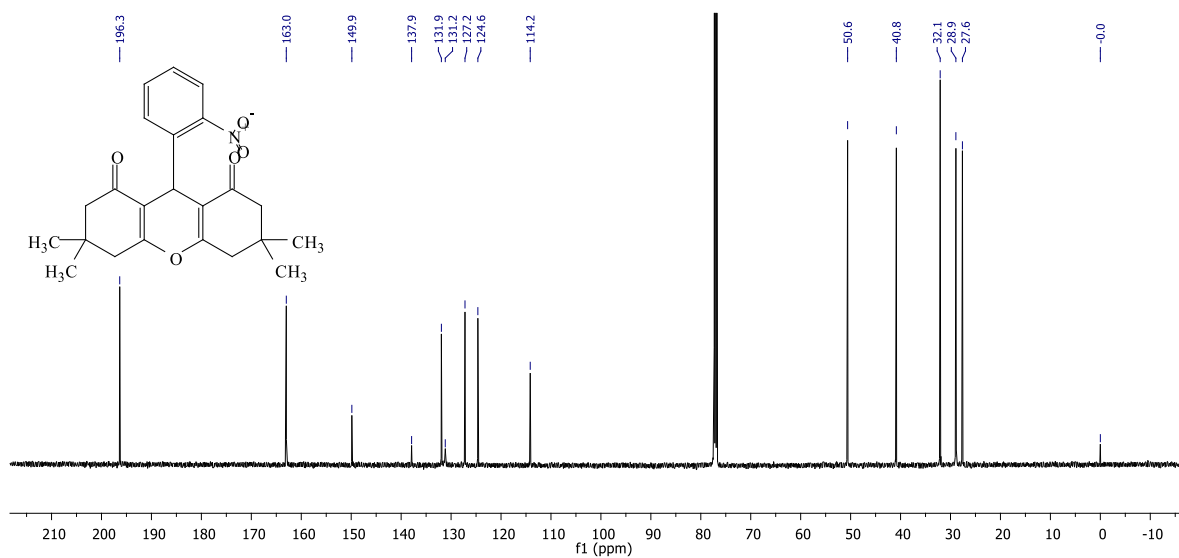
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HPLC spectrum of XD-3



¹H NMR (500 MHz, CDCl₃) of XD-4



¹³C NMR (125 MHz, CDCl₃) of XD-4

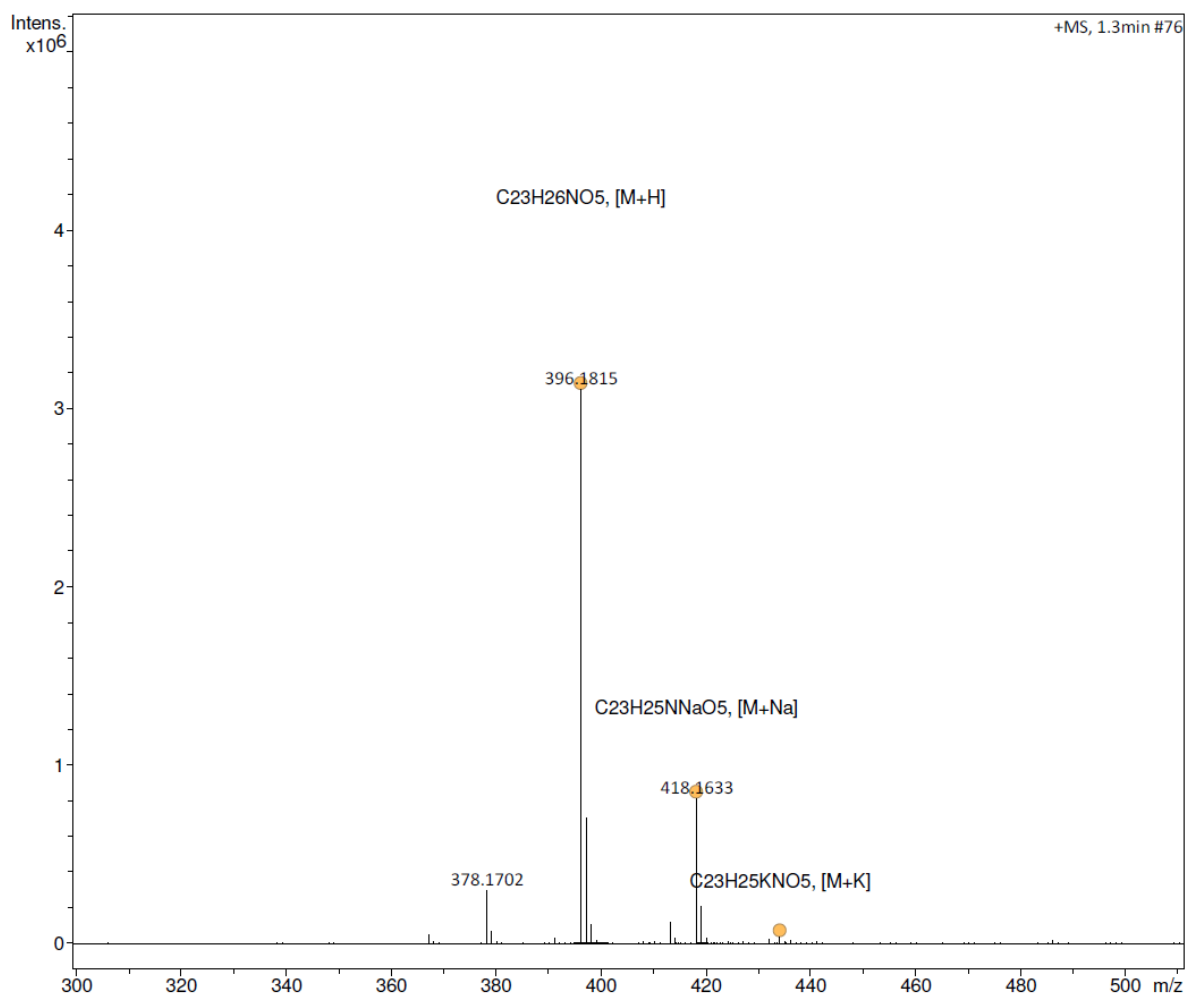
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Sample Name	07	Instrument	impact HD 1819696.00184
Comment			

Acquisition Parameter

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Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



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396.181544	1	C23H26NO5	100.00	396.180549	-1.0	-2.5	18.7	11.5	even		ok	M+H
418.163276	1	C23H25NNO5	100.00	418.162494	-0.8	-1.9	2.7	11.5	even		ok	M+Na
434.136929	1	C23H25KNO5	100.00	434.136431	-0.5	-1.1	58.5	11.5	even		ok	M+K

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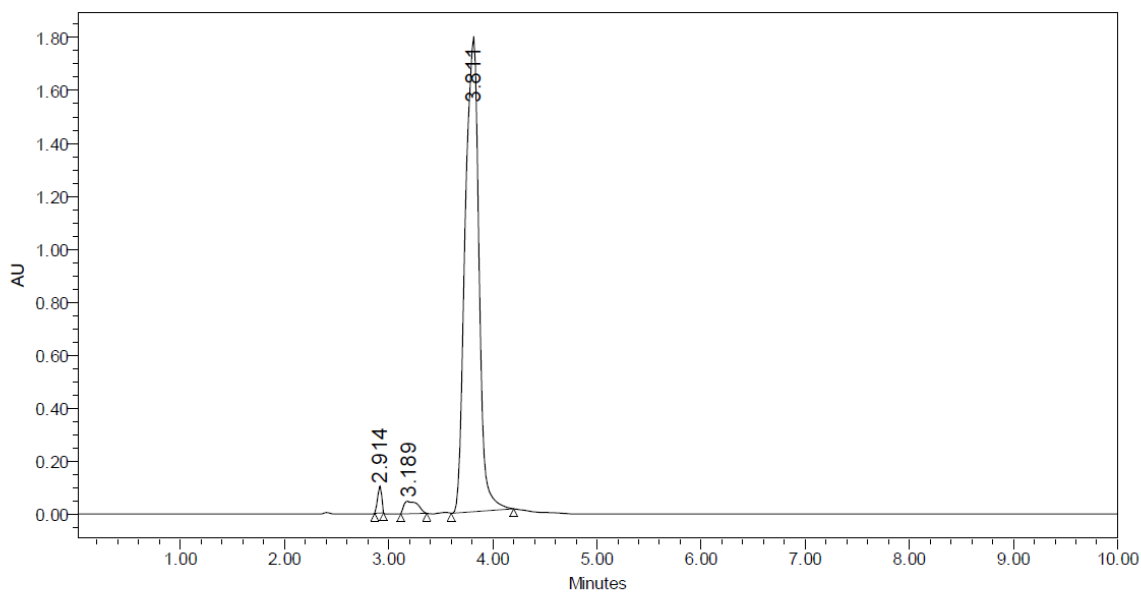
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Page 1 of 1

HR-MS spectrum of XD-4

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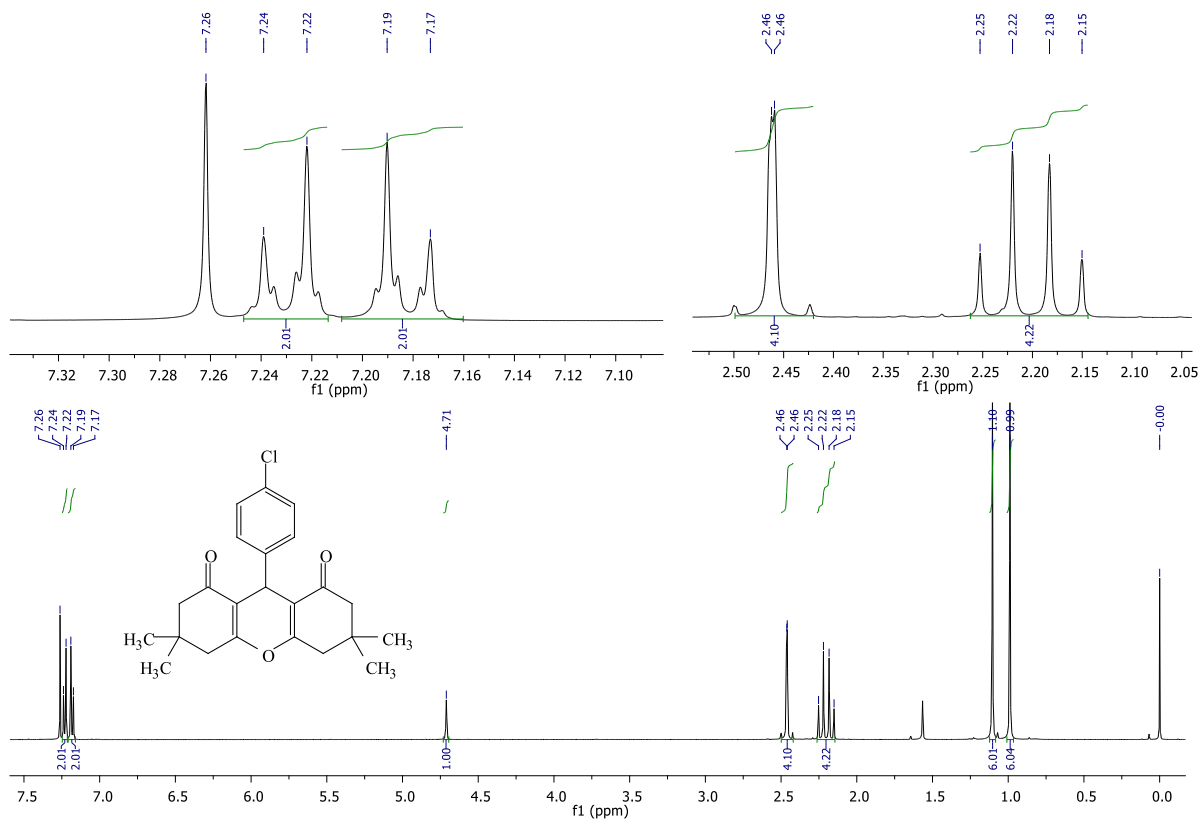


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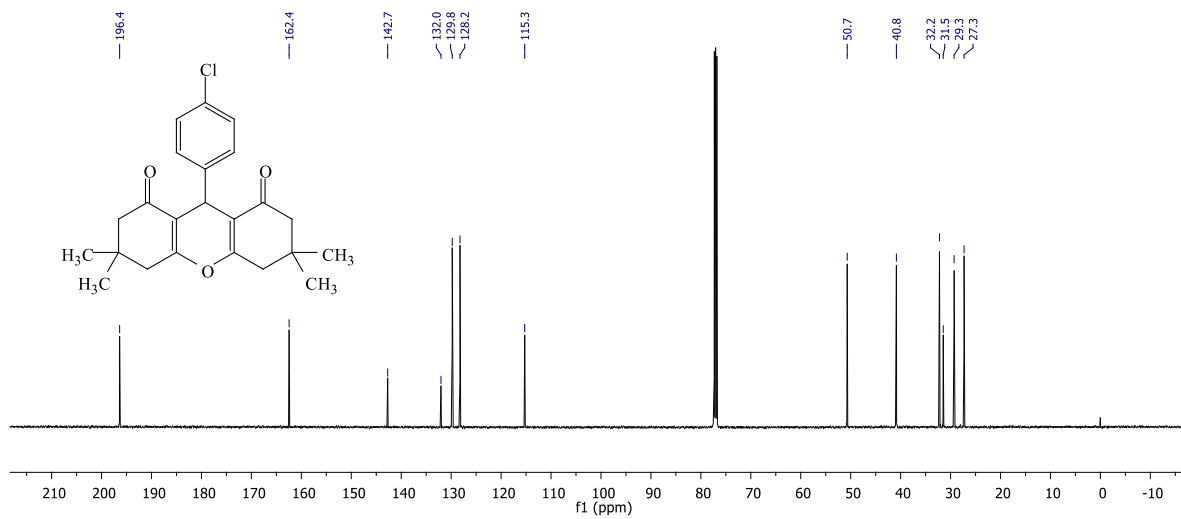
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HPLC spectrum of XD-4



¹H NMR (500 MHz, CDCl₃) of XD-5



¹³C NMR (125 MHz, CDCl₃) of XD-5

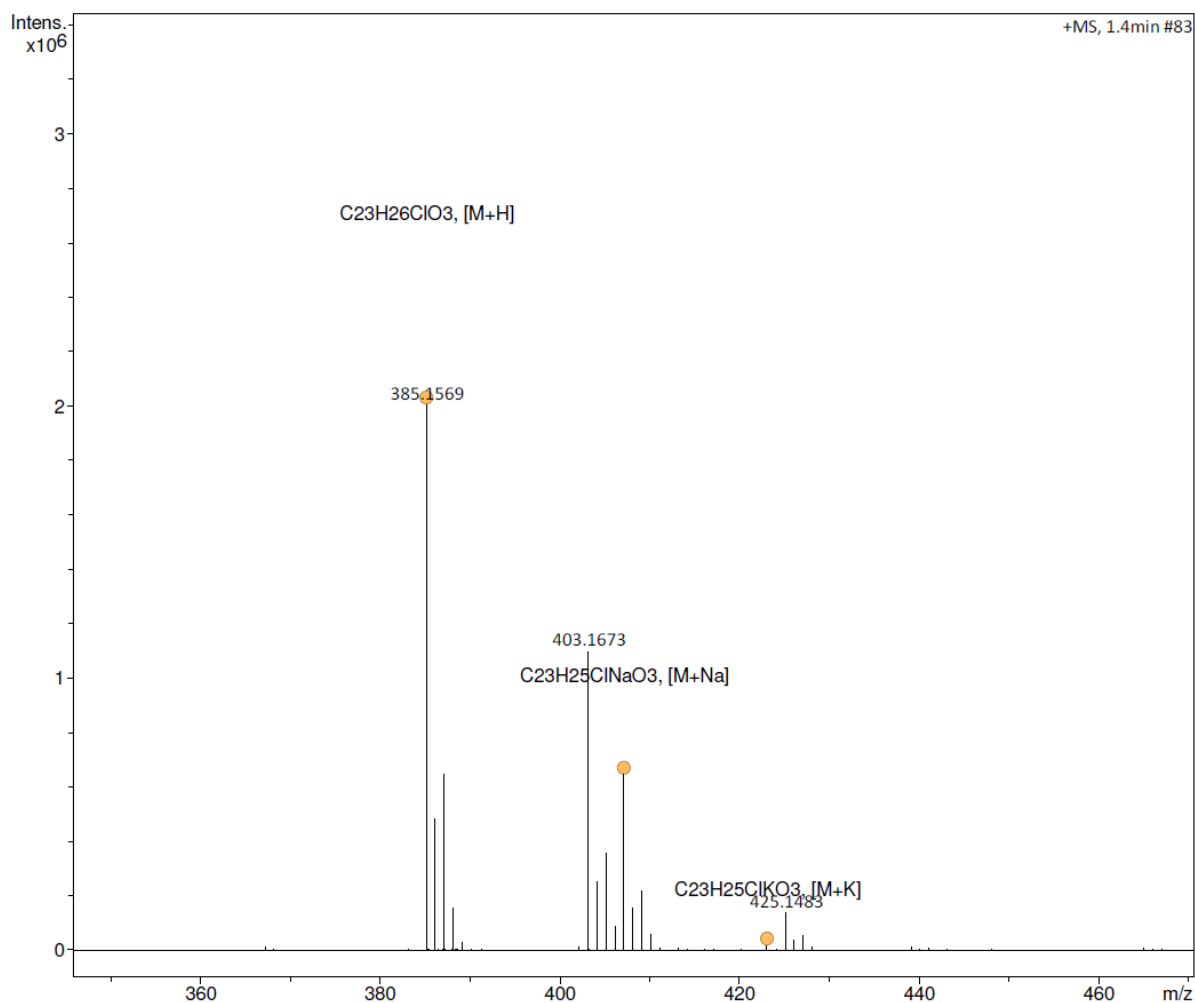
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Acquisition Parameter

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Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
385.156857	1	C ₂₃ H ₂₆ ClO ₃	100.00	385.156499	-0.4	-0.9	16.2	10.5	even		ok	M+H
407.138539	1	C ₂₃ H ₂₅ ClNaO ₃	100.00	407.138443	-0.1	-0.2	10.1	10.5	even		ok	M+Na
423.112565	1	C ₂₃ H ₂₅ ClKO ₃	100.00	423.112380	-0.2	-0.4	199.0	10.5	even		ok	M+K

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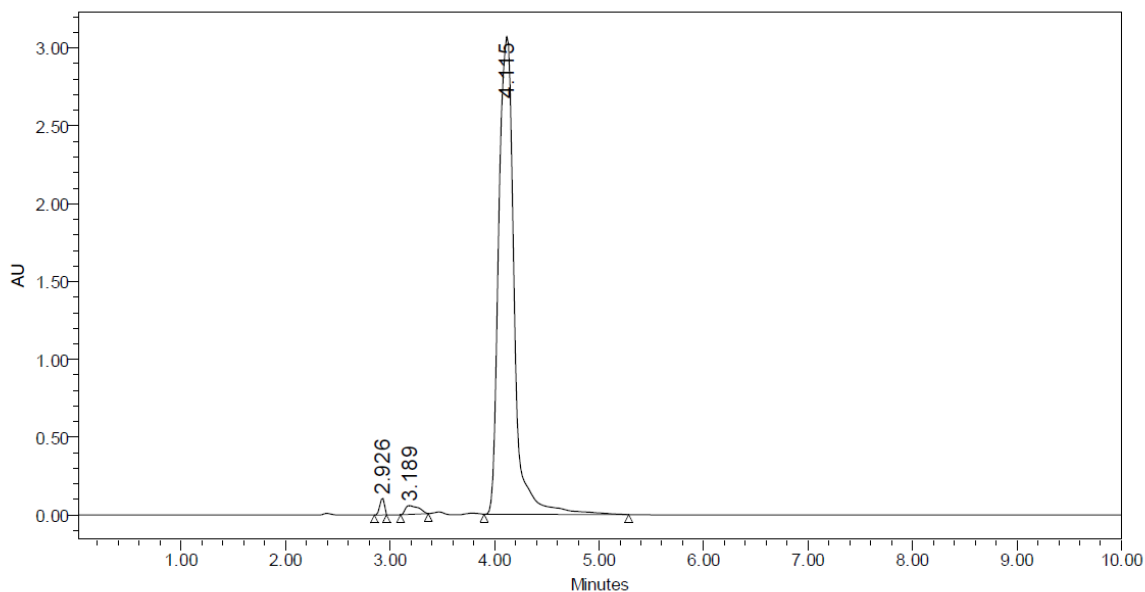
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Page 1 of 1

HR-MS spectrum of XD-5

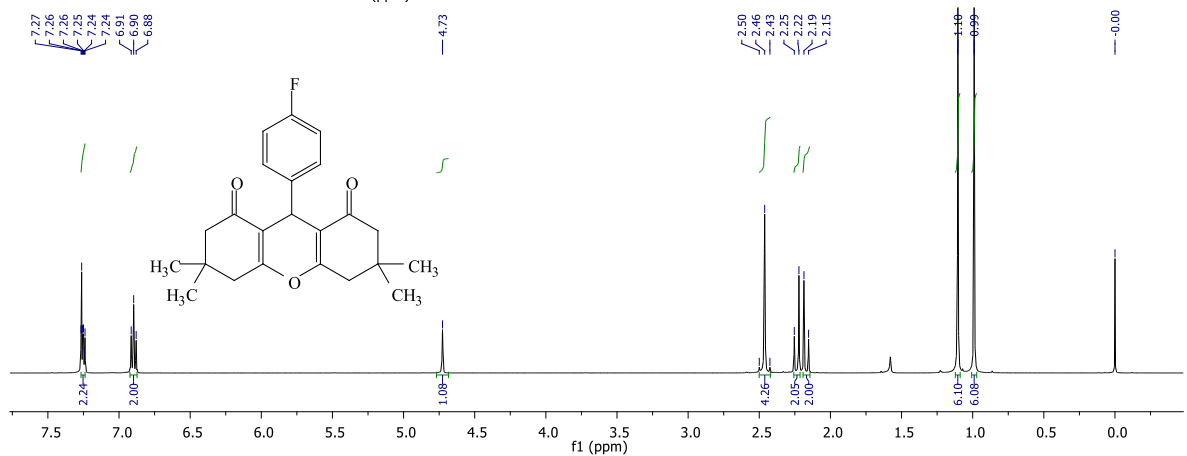
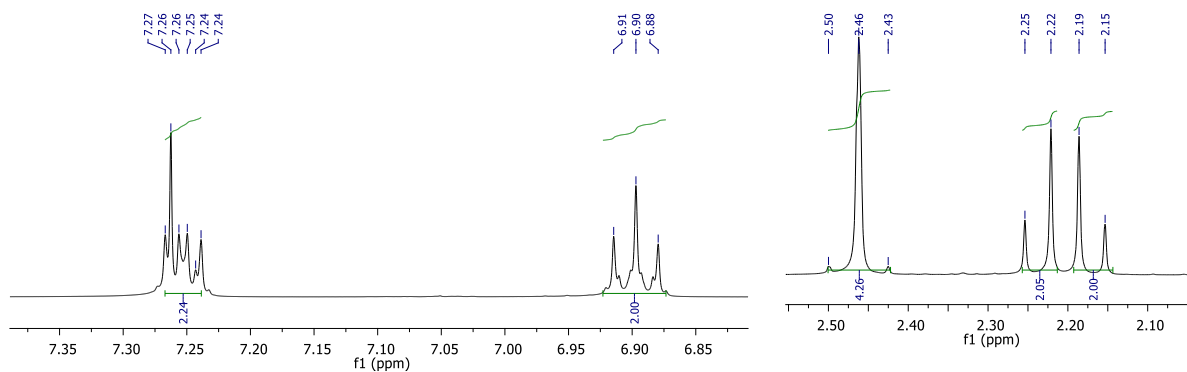
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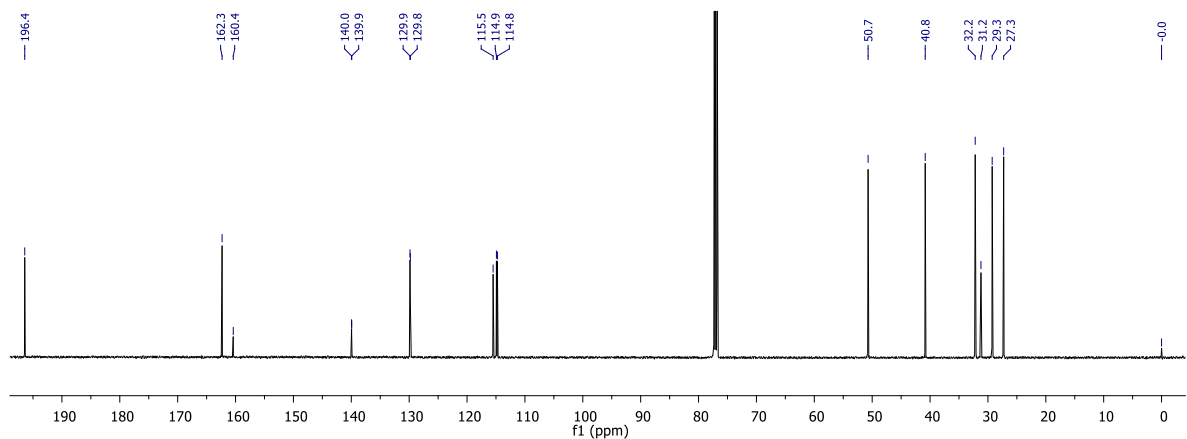
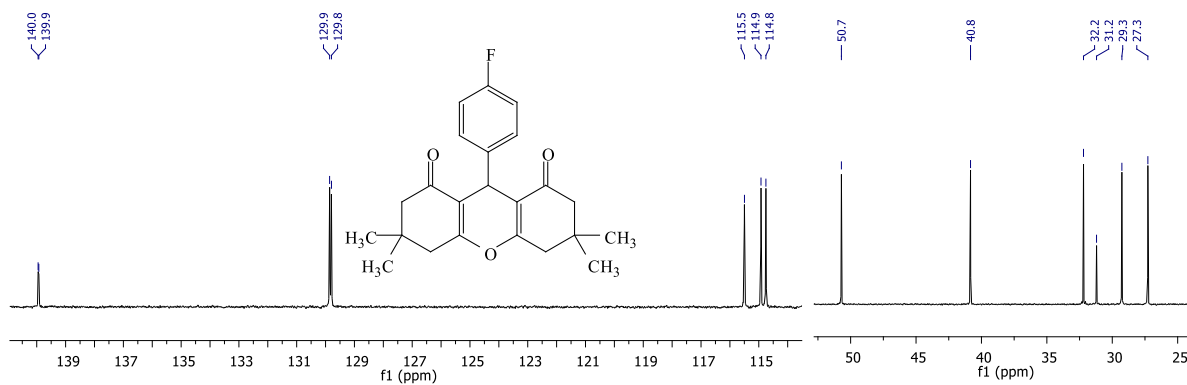


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2	3.189	505331	1.56	57002
3	4.115	31622817	97.41	3074388

HPLC spectrum of XD-5



¹H NMR (500 MHz, CDCl₃) of XD-6



¹³C NMR (125 MHz, CDCl₃) of XD-6

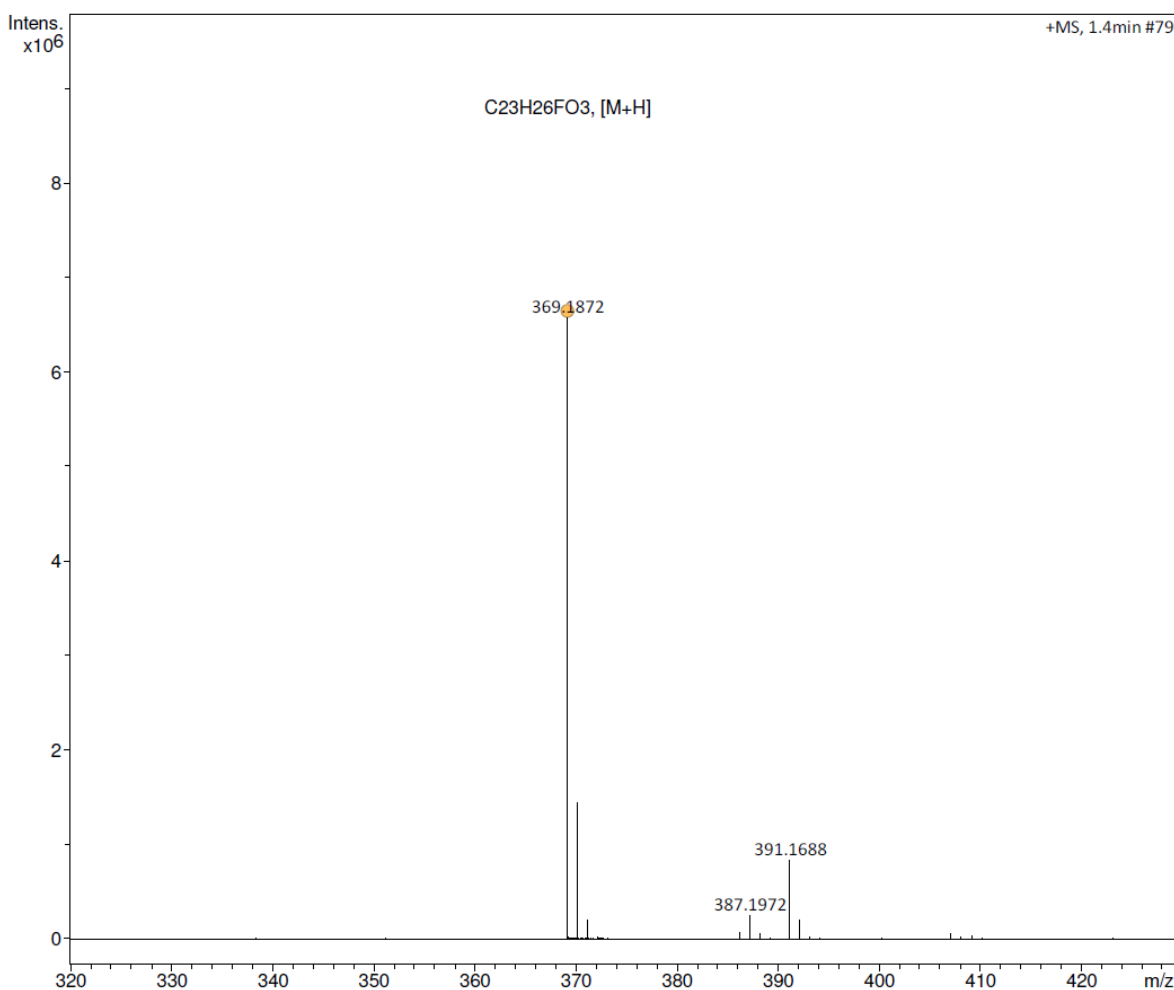
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Sample Name	02	Instrument	impact HD	1819696.00184
Comment				

Acquisition Parameter

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Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
369.187167	1	C ₂₃ H ₂₆ FO ₃	100.00	369.186049	-1.1	-3.0	19.4	10.5	even		ok	M+H

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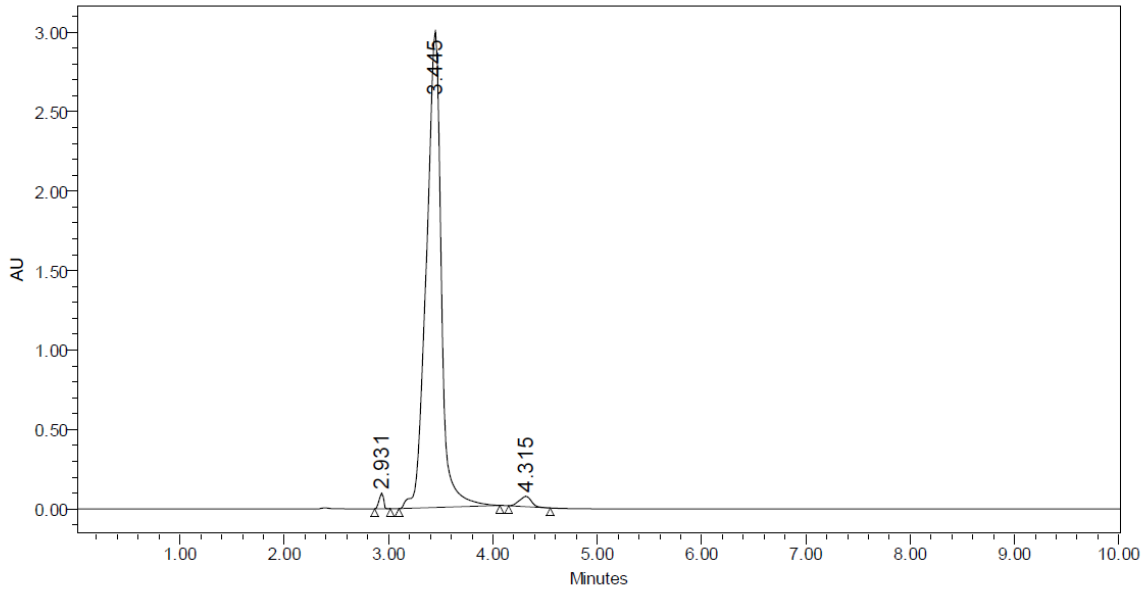
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Page 1 of 1

HR-MS spectrum of XD-6

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Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA MaxPlot (190.0 nm to
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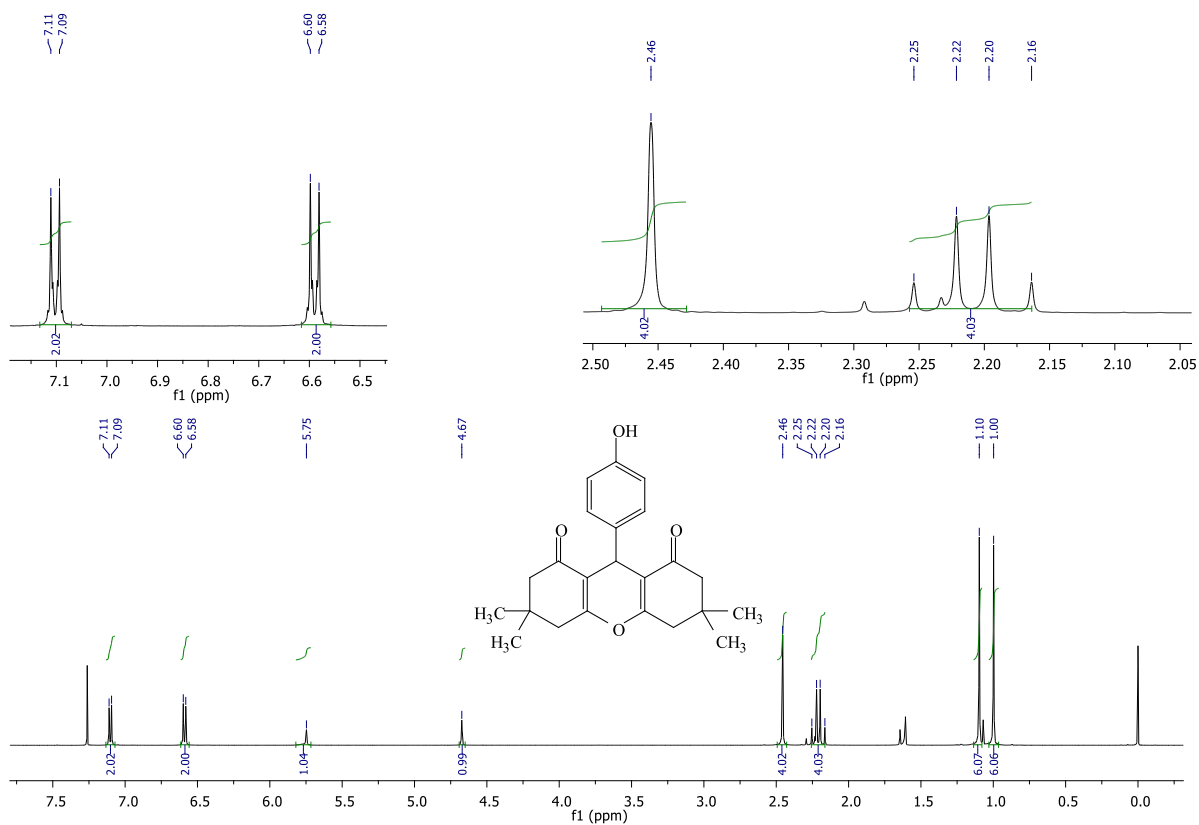


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3	4.315	517376	1.70	64591

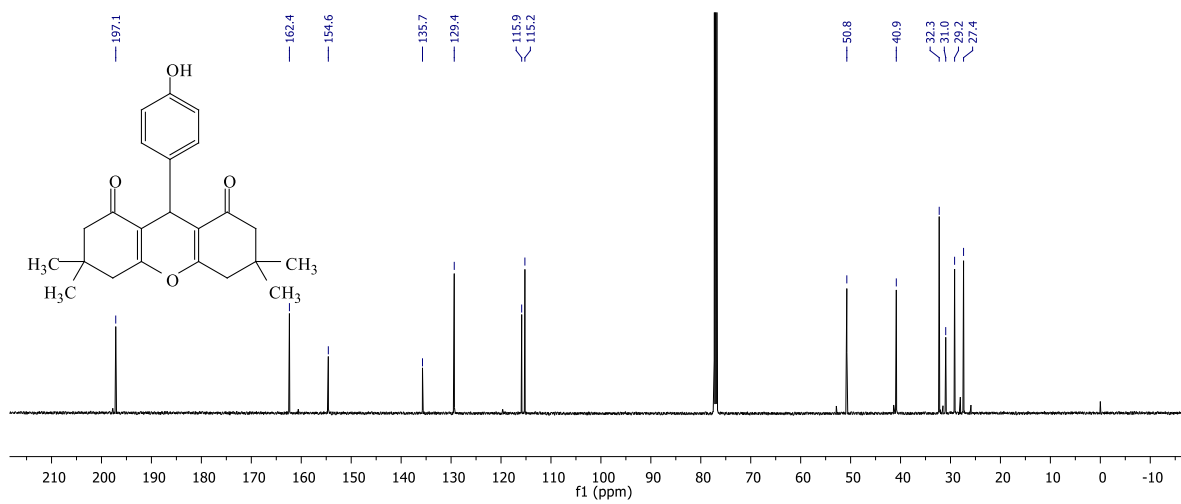
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 Report Method ID 2116
 Page: 1 of 1

Project Name: Defaults\1.8
 Date Printed:
 09-04-2021
 18:02:29 Asia/Kolkata

HPLC spectrum of XD-6



¹H NMR (500 MHz, CDCl₃) of XD-7



¹³C NMR (125 MHz, CDCl₃) of XD-7

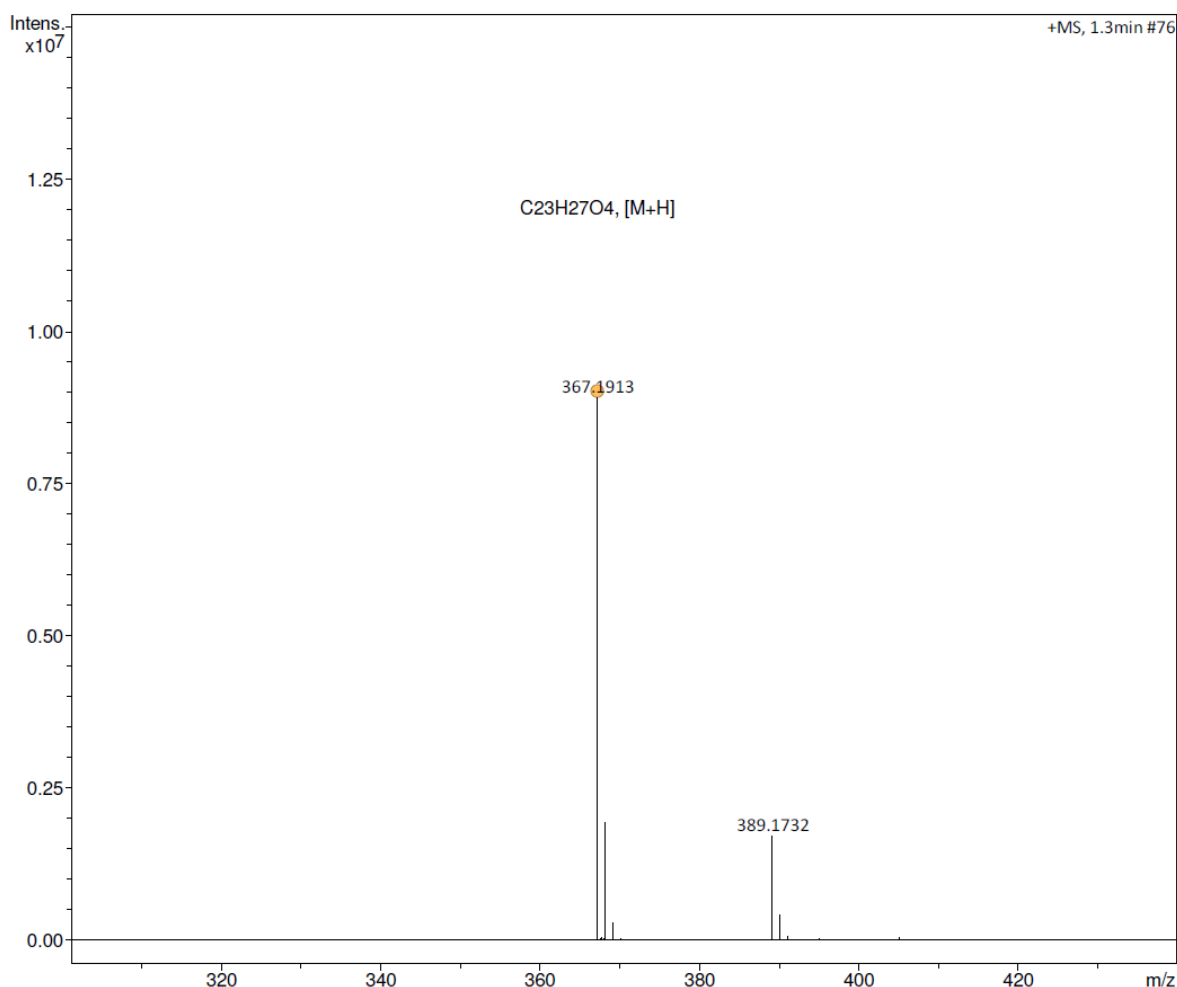
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Analysis Info

Analysis Name	D:\Data\2021\SPPU\CIF\Umesh\06022021\01_GD1_01_2324.d	Acquisition Date	2/6/2021 8:27:50 PM
Method	dlc_ms50-800mz_10min_0.120mlflow_90b.m	Operator	CIF
Sample Name	01	Instrument	impact HD
Comment			1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.7 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
367.191282	1	C23H27O4	100.00	367.190386	-0.9	-2.4	22.2	10.5	even		ok	M+H

GD1_01_2324.d

Bruker Compass DataAnalysis 4.2

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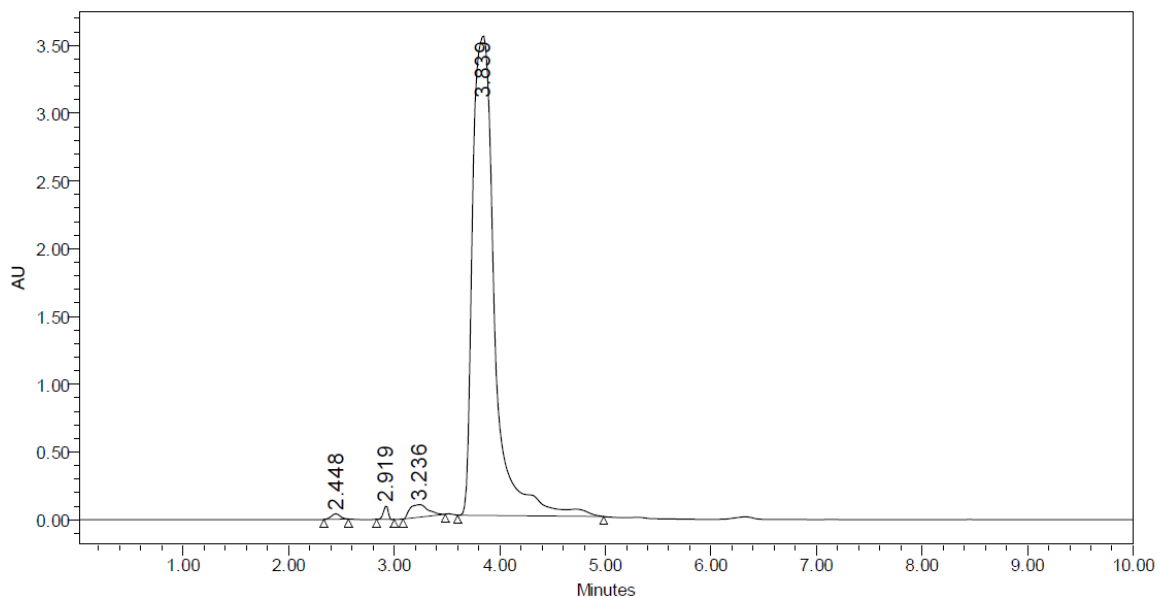
by: CIF

Page 1 of 1

HR-MS spectrum of XD-7

SAMPLE INFORMATION

Sample Name:	7	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	09042021
Vial:	17	Acq. Method Set:	CIF
Injection #:	1	Processing Method:	7
Injection Volume:	10.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA MaxPlot (190.0 nm to
Date Acquired:	09-04-2021 17:51:33 IST		
Date Processed:	09-04-2021 18:11:44 IST		

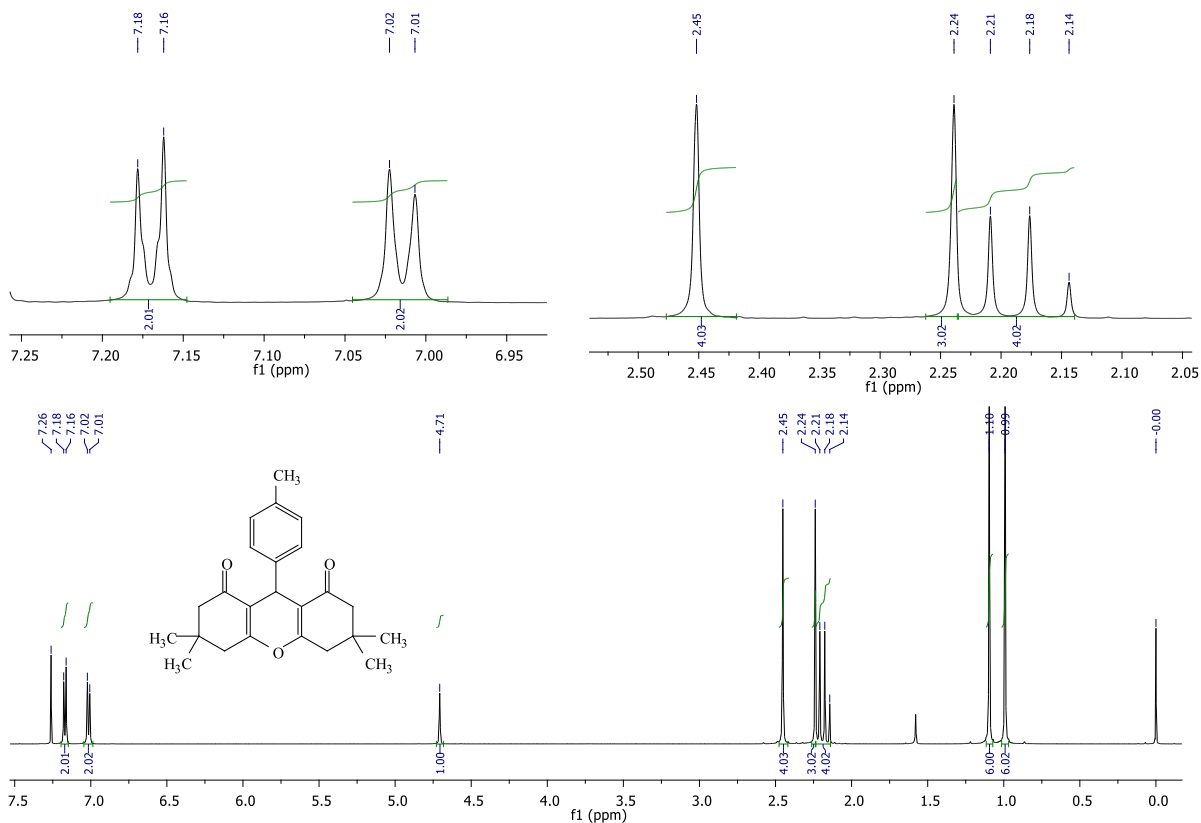


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1	2.448	236370	0.44	39914
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3	3.236	1117550	2.10	92193
4	3.839	51456214	96.87	3553339

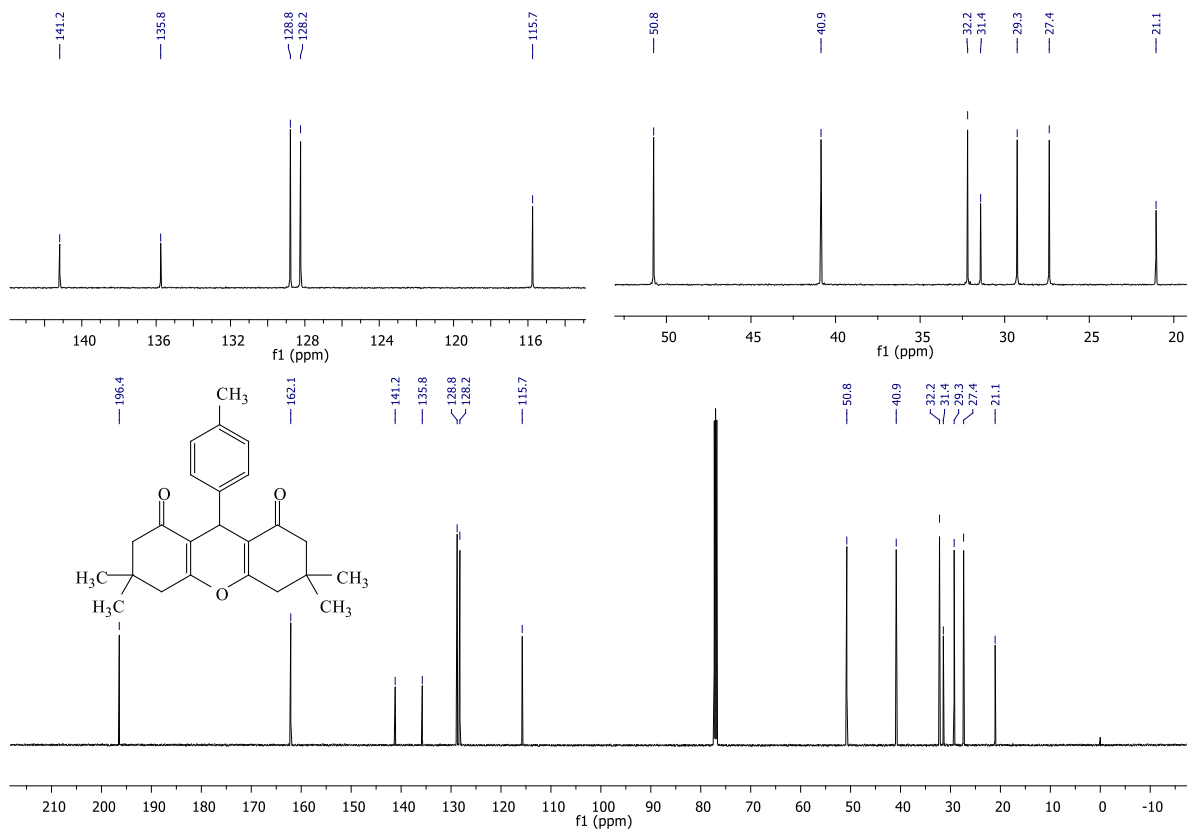
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 Report Method ID2116
 Page: 1 of 1

Project Name: Defaults\1.8
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 09-04-2021
 18:11:56 Asia/Kolkata

HPLC spectrum of XD-7



¹H NMR (500 MHz, CDCl₃) of XD-8



¹³C NMR (125 MHz, CDCl₃) of XD-8

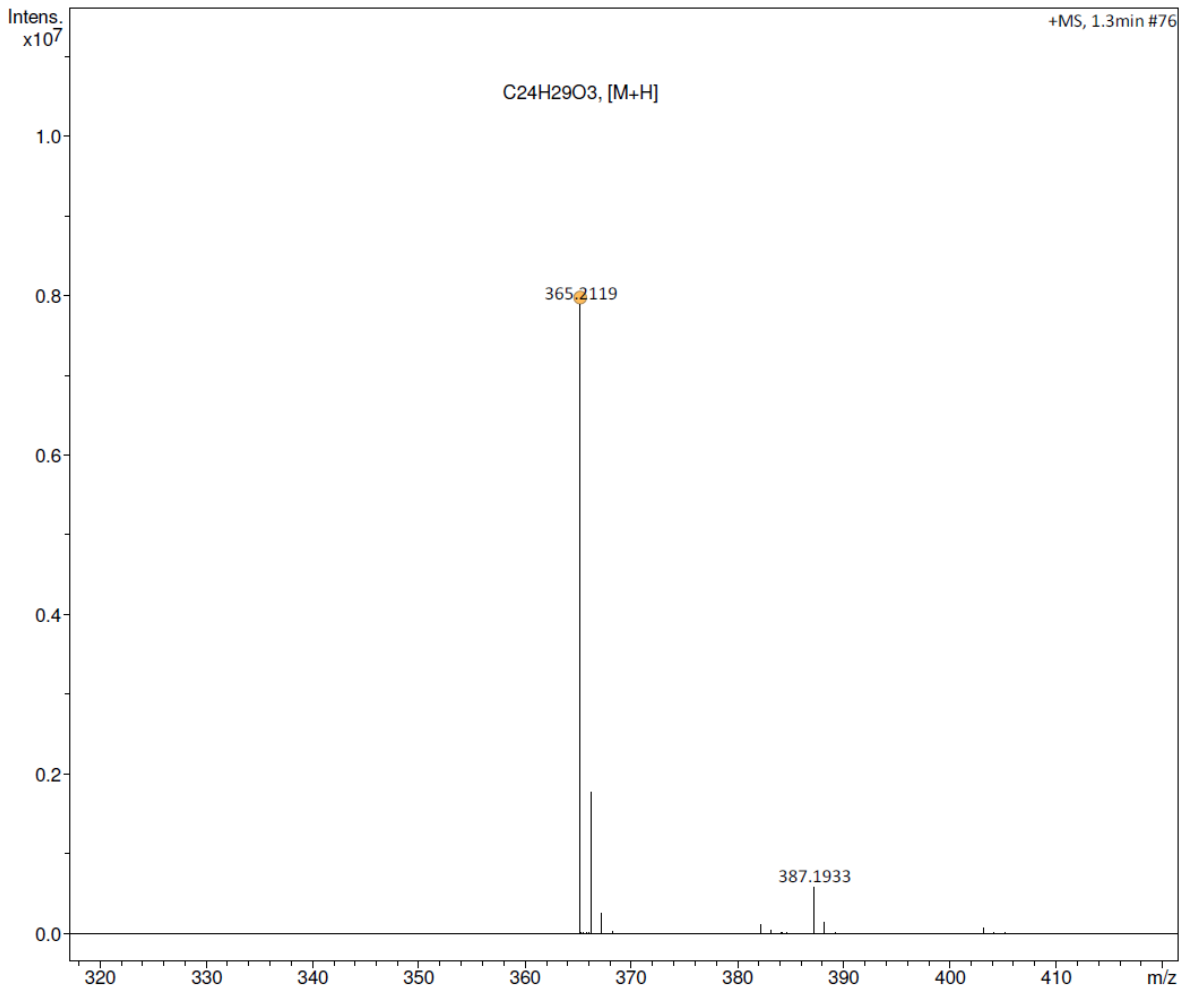
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Analysis Info

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Method	dlc_ms50-800mz_10min_0.120mlflow_90b.m	Operator	CIF
Sample Name	03	Instrument	impact HD 1819696.00184
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.7 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
365.211932	1	C ₂₄ H ₂₉ O ₃	100.00	365.211121	-0.8	-2.2	23.6	10.5	even		ok	M+H

GA4_01_2317.d

Bruker Compass DataAnalysis 4.2

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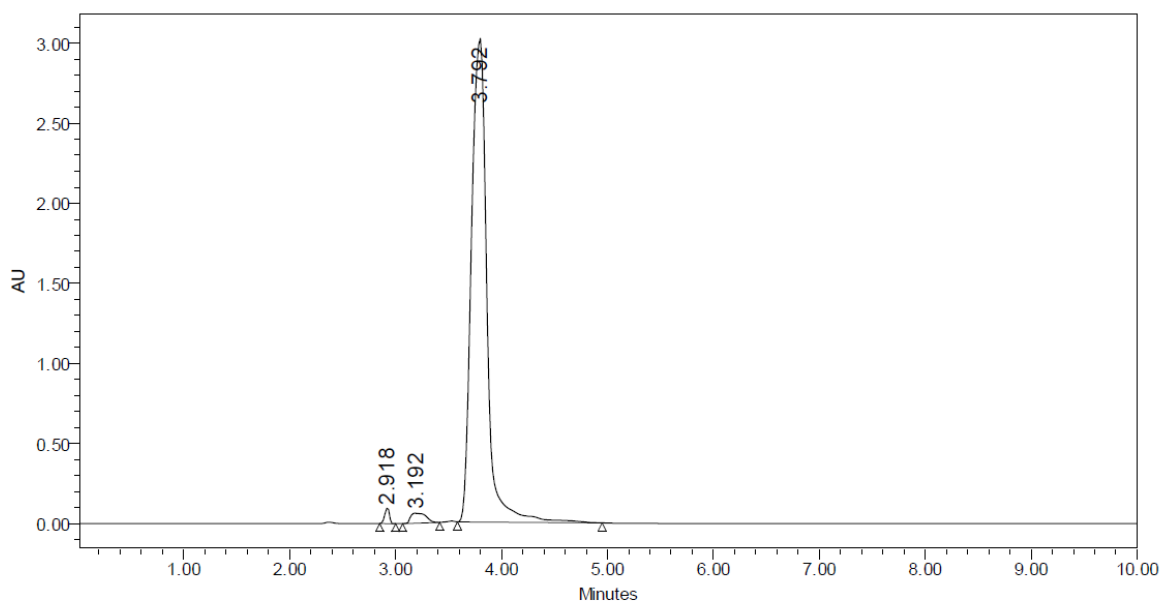
by: CIF

Page 1 of 1

HR-MS spectrum of XD-8

SAMPLE INFORMATION

Sample Name:	8	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	09042021
Vial:	9	Acq. Method Set:	CIF
Injection #:	1	Processing Method:	8
Injection Volume:	10.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA MaxPlot (190.0 nm to
Date Acquired:	09-04-2021 16:11:37 IST		
Date Processed:	09-04-2021 17:59:07 IST		

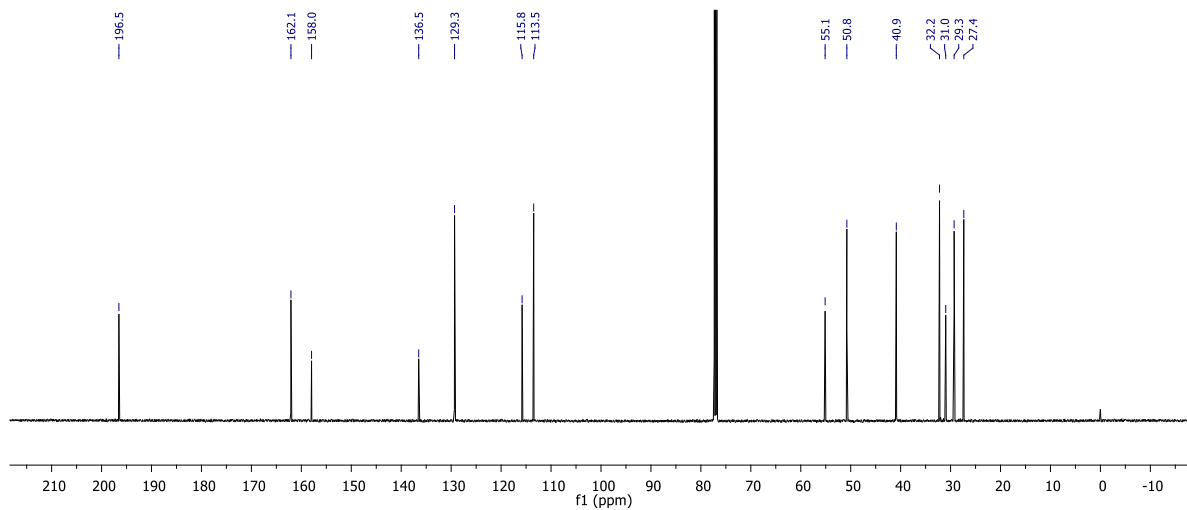
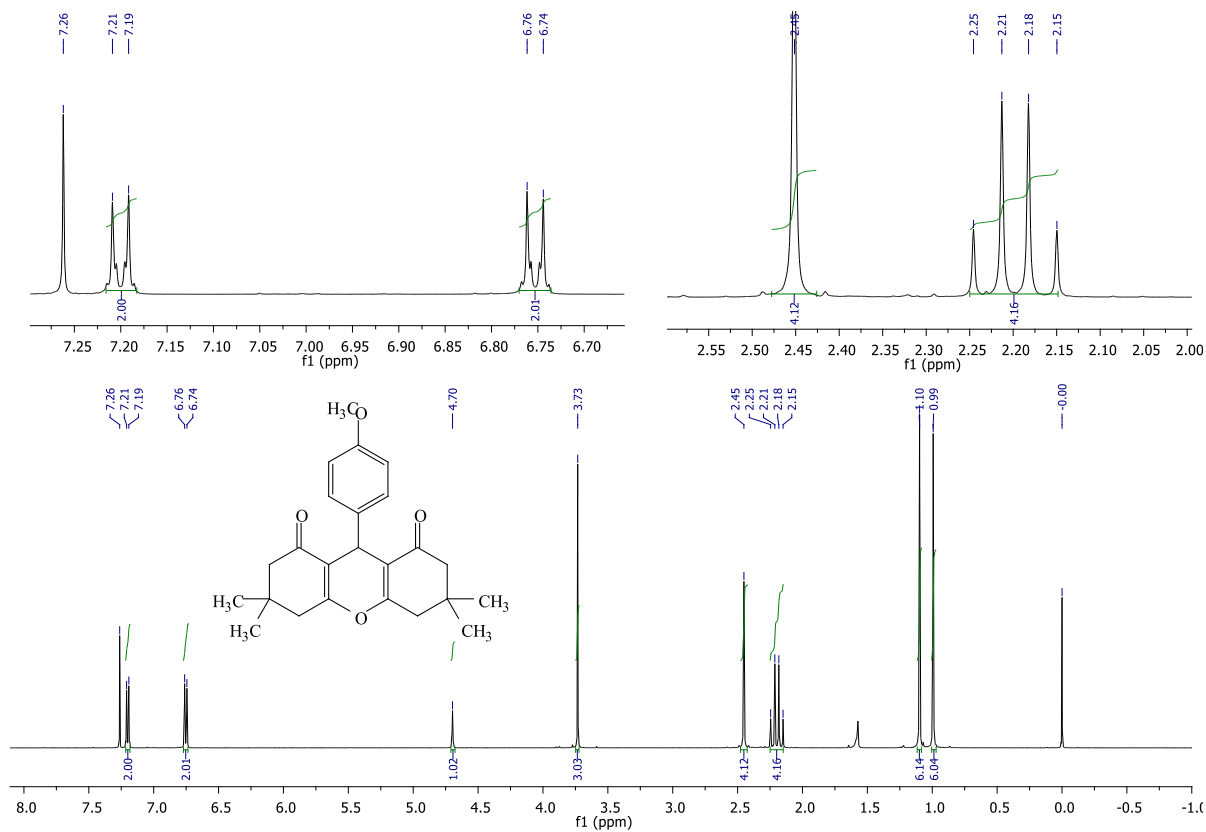


	RT	Area	% Area	Height
1	2.918	299708	0.95	94347
2	3.192	623926	1.97	63364
3	3.792	30745238	97.08	3032285

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Report Method: S P PUNE UNIVERSITY
Report Method ID 2116
Page: 1 of 1

Project Name: Defaults\1.8
Date Printed:
09-04-2021
17:59:21 Asia/Kolkata

HPLC spectrum of XD-8



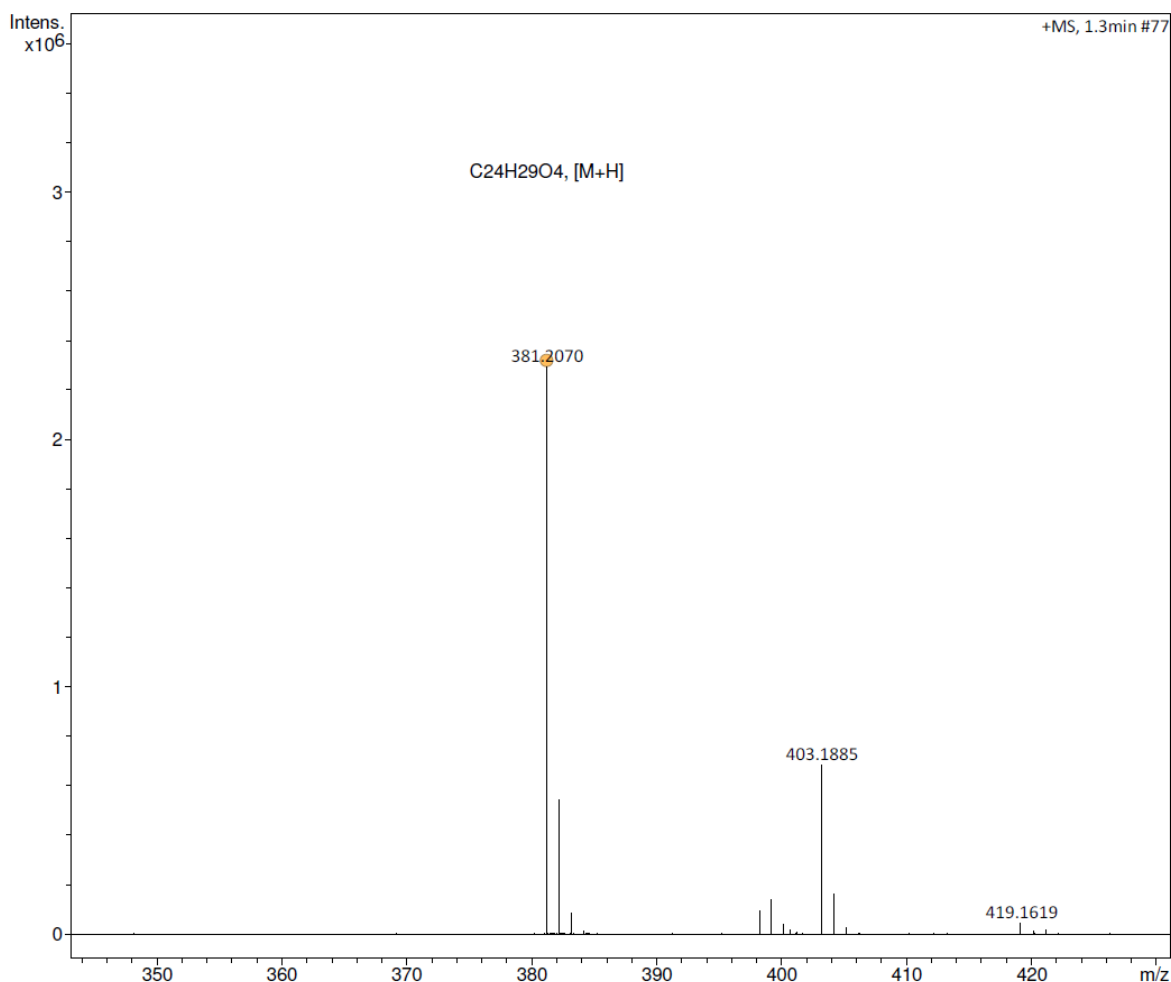
Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info

Analysis Name	D:\Data\2021\SPPU\CIF\Umesh\06022021\04_GC1_01_2323.d	Acquisition Date	2/6/2021 8:15:09 PM
Method	dlc_ms50-800mz_10min_0.120mlflow_90b.m	Operator	CIF
Sample Name	04	Instrument	impact HD 1819696.00184
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.7 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
381.206983	1	C24H29O4	100.00	381.206036	-0.9	-2.5	15.4	10.5	even		ok	M+H

GC1_01_2323.d

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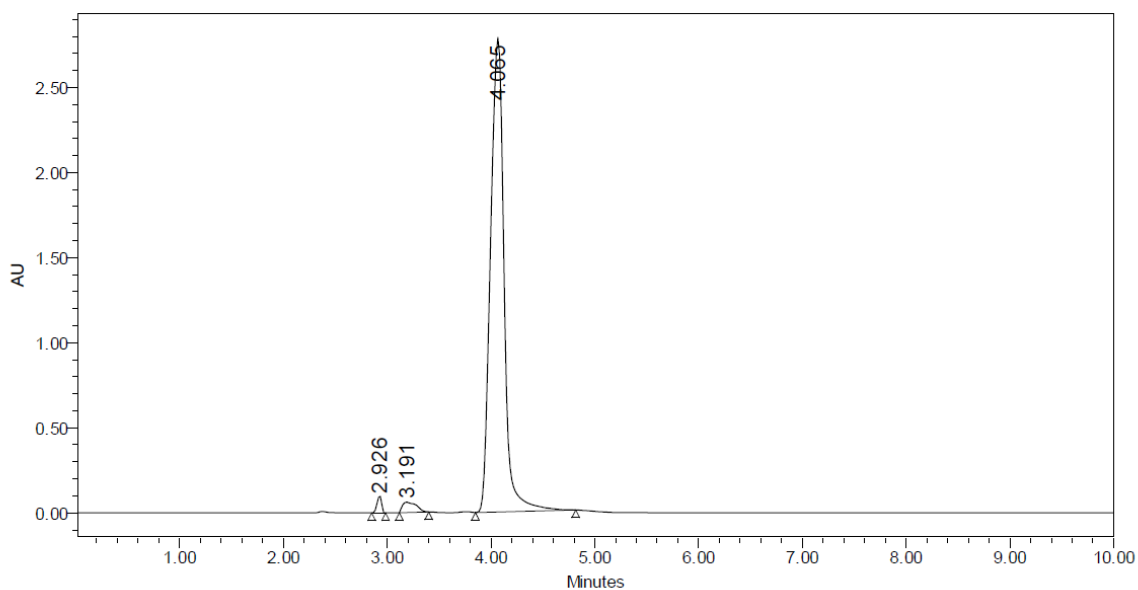
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Page 1 of 1

HR-MS spectrum of XD-9

SAMPLE INFORMATION

Sample Name:	9	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	09042021
Vial:	8	Acq. Method Set:	CIF
Injection #:	1	Processing Method:	9
Injection Volume:	10.00 ul	Channel Name:	PDA MaxPlot 190.0 - 800.0
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA MaxPlot (190.0 nm to
Date Acquired:	09-04-2021 16:00:47 IST		
Date Processed:	09-04-2021 17:57:56 IST		

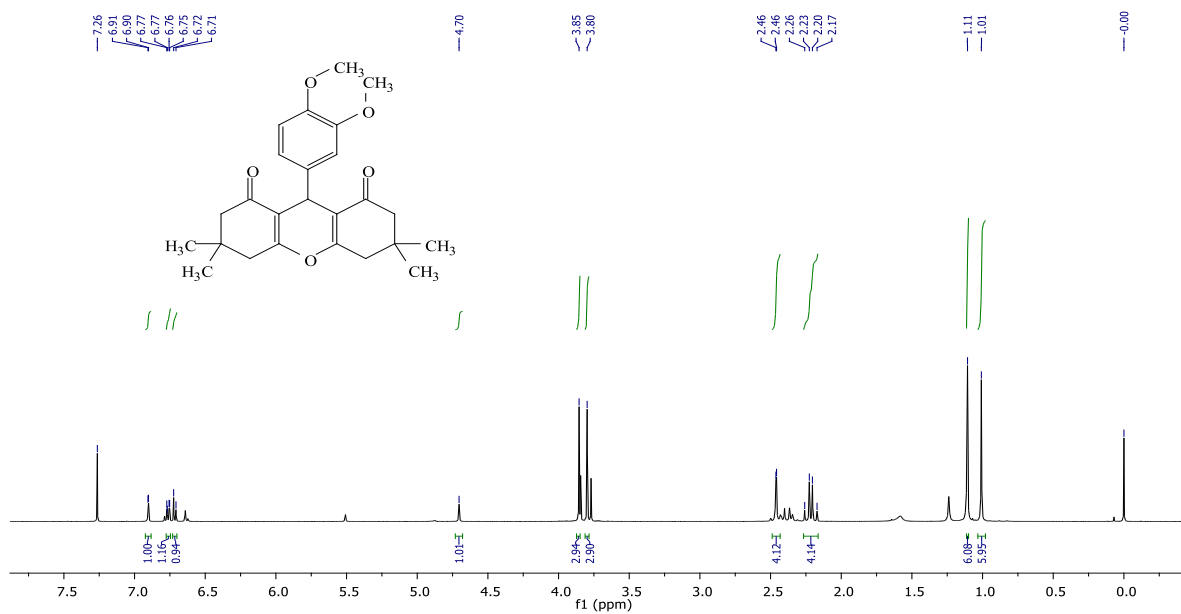


	RT	Area	% Area	Height
1	2.926	302273	1.16	92758
2	3.191	571596	2.19	61259
3	4.065	25241069	96.65	2786120

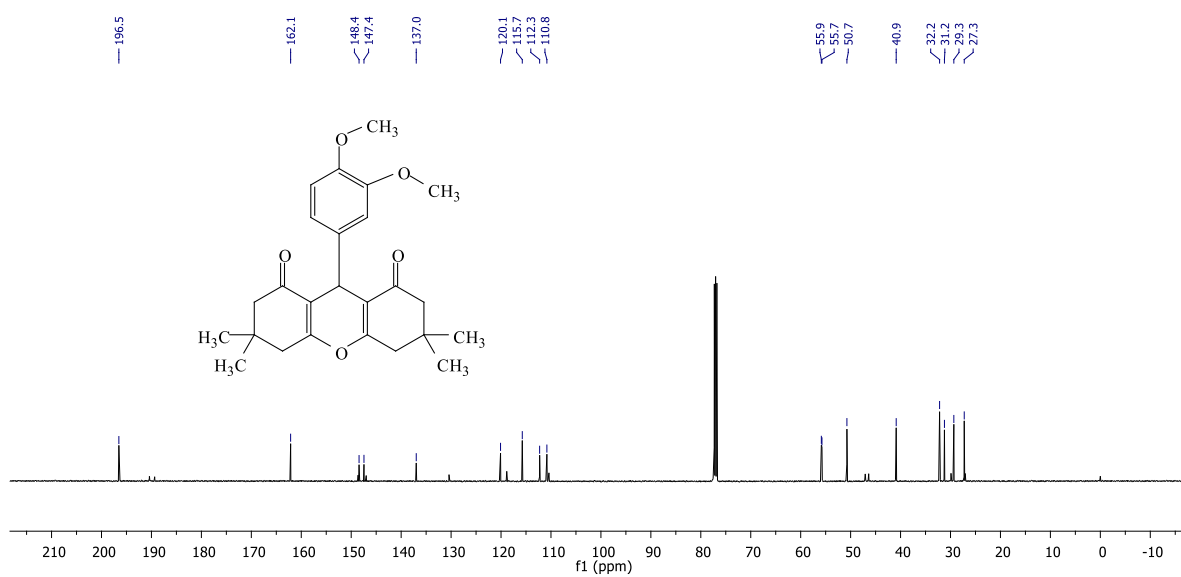
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 Report Method ID2116
 Page: 1 of 1

Project Name: Defaults\1.8
 Date Printed:
 09-04-2021
 17:58:11 Asia/Kolkata

HPLC spectrum of XD-9



¹H NMR (500 MHz, CDCl₃) of XD-10



¹³C NMR (125 MHz, CDCl₃) of XD-10

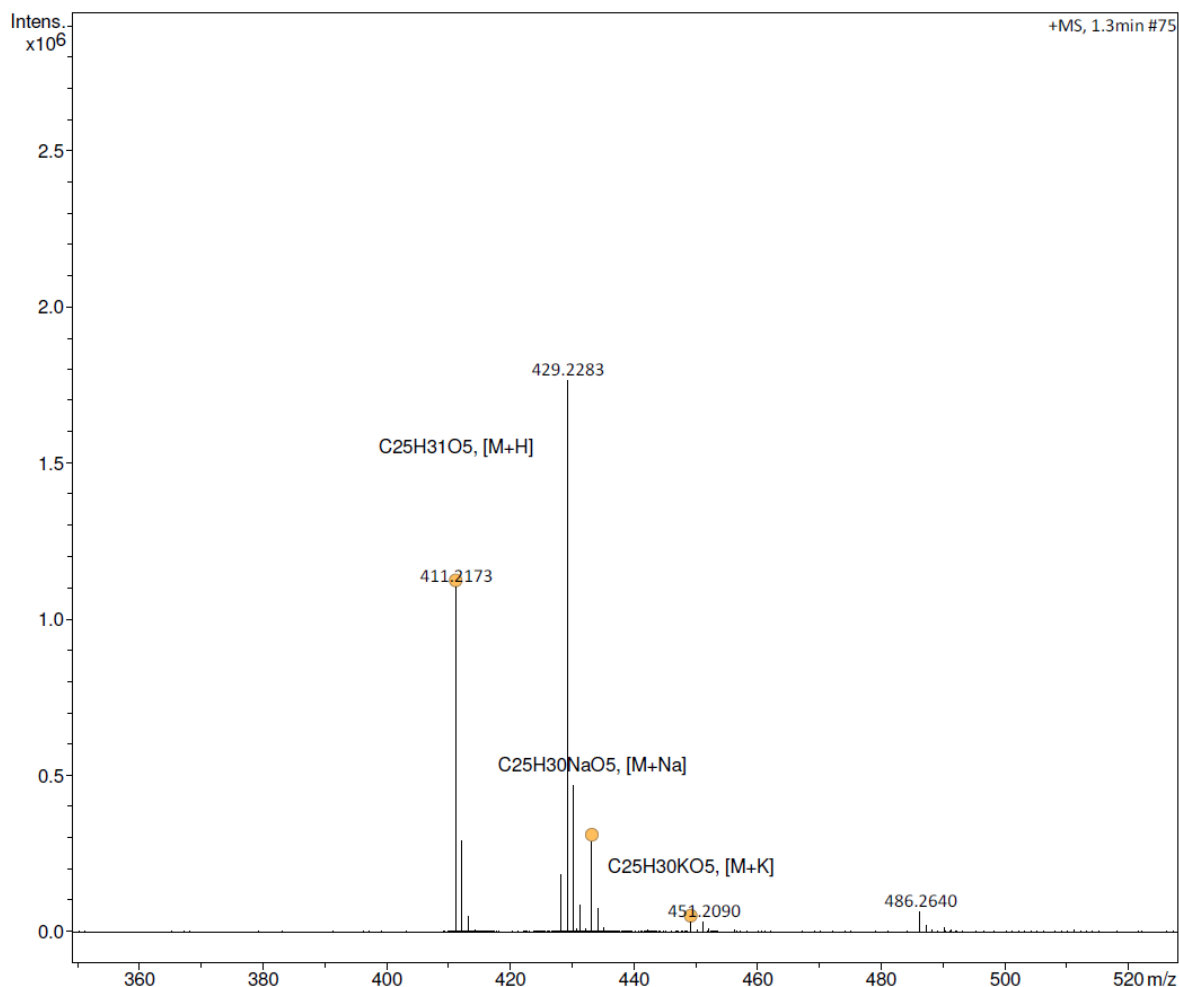
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Analysis Info

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Method	dlc_ms50-800mz_10min_0.120mlflow_90b.m	Operator	CIF	
Sample Name	09	Instrument	impact HD	1819696.00184
Comment				

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.7 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
411.217319	1	C25H31O5	100.00	411.216601	-0.7	-1.7	7.9	10.5	even		ok	M+H
433.198897	1	C25H30NaO5	100.00	433.198545	-0.4	-0.8	14.2	10.5	even		ok	M+Na
449.172708	1	C25H30KO5	100.00	449.172482	-0.2	-0.5	62.9	10.5	even		ok	M+K

GA2_01_2315.d

Bruker Compass DataAnalysis 4.2

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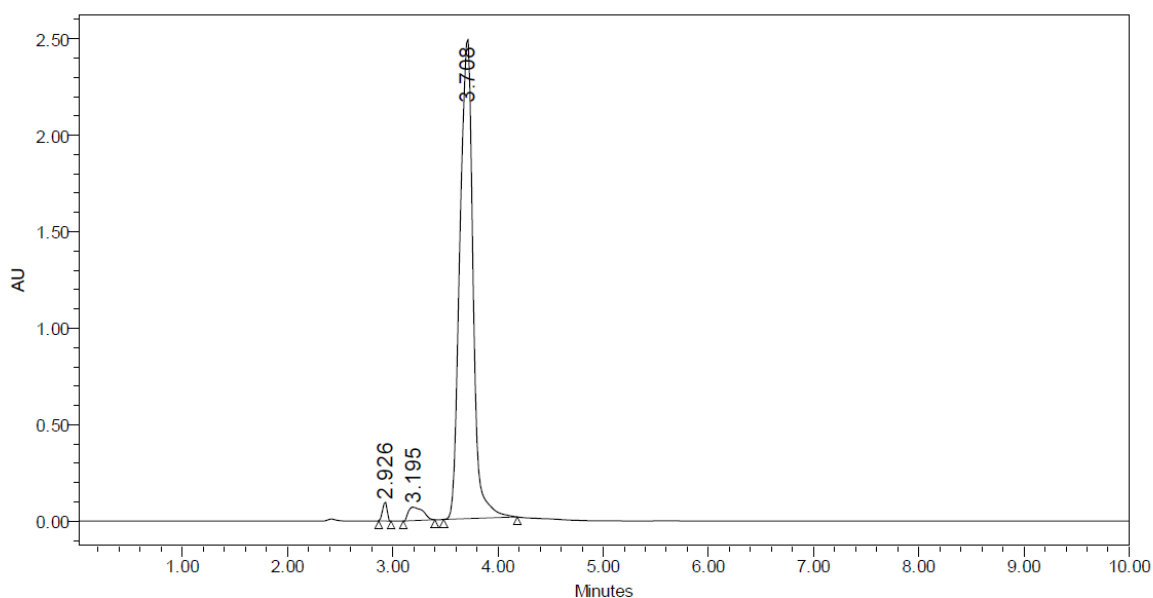
by: CIF

Page 1 of 1

HR-MS spectrum of XD-10

SAMPLE INFORMATION

Sample Name:	10	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	09042021
Vial:	20	Acq. Method Set:	CIF
Injection #:	1	Processing Method:	10
Injection Volume:	10.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA MaxPlot (190.0 nm to
Date Acquired:	09-04-2021 13:49:07 IST		
Date Processed:	09-04-2021 17:54:47 IST		



	RT	Area	% Area	Height
1	2.926	297103	1.32	92538
2	3.195	667762	2.96	70726
3	3.708	21587550	95.72	2508969

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 Page: 1 of 1

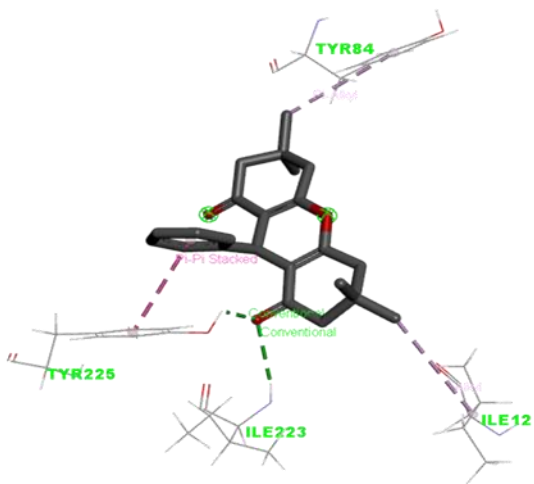
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HPLC spectrum of XD-10

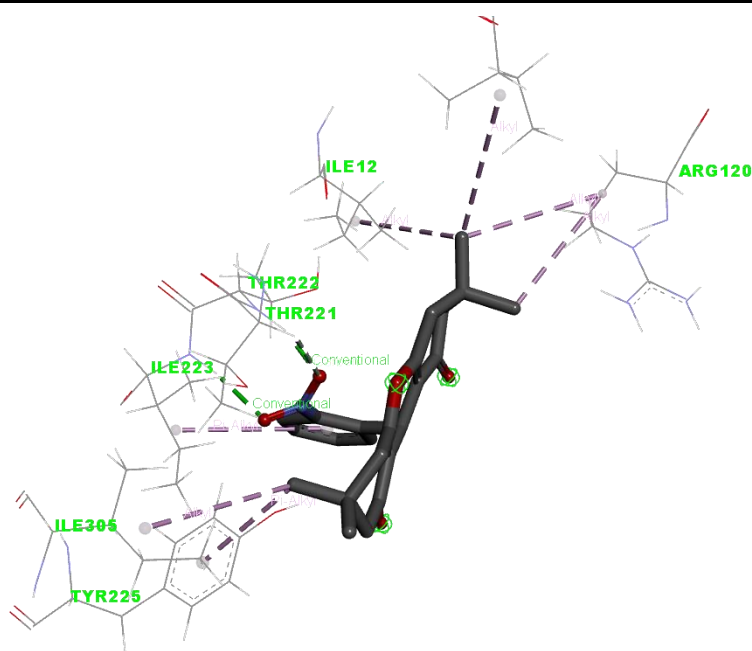
Molecular Docking Study

The important non-bonded interactions between protein and ligands, derived from molecular docking studies. [A = Protein chain, B = Ligand atoms]

XD-2			
Atom1	Atom2	Category	Types
A:ILE223:HN	B:XDE1:O	Hydrogen Bond	Conventional Hydrogen
A:TYR225:HH	B:XDE1:O	Hydrogen Bond	Conventional Hydrogen
A:TYR225	B:XDE1	Hydrophobic	Pi-Pi Stacked
B:XDE1:C	A:ILE12	Hydrophobic	Alkyl
A:TYR84	B:XDE1:C	Hydrophobic	Pi-Alkyl



XD-4			
Atom1	Atom2	Category	Types
A:THR222:HN	B:XDG1:O	Hydrogen Bond	Conventional Hydrogen Bond
A:ILE223:HN	B:XDG1:O	Hydrogen Bond	Conventional Hydrogen Bond
A:THR221:HA	B:XDG1:O	Hydrogen Bond	Carbon Hydrogen Bond
B:XDG1:C	A:ARG120	Hydrophobic	Alkyl
B:XDG1:C	A:ILE12	Hydrophobic	Alkyl
B:XDG1:C	A:ILE30	Hydrophobic	Alkyl
B:XDG1:C	A:ARG120	Hydrophobic	Alkyl
B:XDG1:C	A:ILE305	Hydrophobic	Alkyl
A:TYR225	B:XDG1:C	Hydrophobic	Pi-Alkyl
B:XDG1	A:ILE223	Hydrophobic	Pi-Alkyl



XD-5			
Atom1	Atom2	Category	Types
A:TYR225:HH	B:XDF1:O	Hydrogen Bond	Conventional Hydrogen Bond
A:TYR225	B:XDF1	Hydrophobic	Pi-Pi Stacked
B:XDF1:C	A:ILE12	Hydrophobic	Alkyl
A:TRP51	B:XDF1:C	Hydrophobic	Pi-Alkyl
A:TYR84	B:XDF1:C	Hydrophobic	Pi-Alkyl
A:TYR225	B:XDF1:CL	Hydrophobic	Pi-Alkyl

The 3D molecular model illustrates the binding of the XD-5 ligand to a protein. The ligand is shown in a stick representation with a semi-transparent surface. Key interactions are highlighted with dashed lines: a green dashed line represents a conventional hydrogen bond between the hydroxyl group of TYR225 and the carbonyl oxygen of XDF1. Purple dashed lines indicate hydrophobic interactions: pink lines for Pi-Pi stacked interactions between the aromatic rings of TYR225 and XDF1; magenta lines for Pi-Alkyl interactions between the aromatic rings of TYR225, TYR84, and TRP51 and the aliphatic chains of XDF1; and green lines for Alkyl interactions between the aliphatic chains of XDF1 and the side chains of ILE12 and TYR225.

XD-6			
Atom1	Atom2	Category	Types
A:TYR225:HH	B:XDB1:O	Hydrogen Bond	Conventional Hydrogen Bond
A:TYR225	B:XDB1	Hydrophobic	Pi-Pi Stacked
B:XDB1:C	A:ILE12	Hydrophobic	Alkyl
A:TRP51	B:XDB1:C	Hydrophobic	Pi-Alkyl
A:TYR84	B:XDB1:C	Hydrophobic	Pi-Alkyl

Molecular Dynamics Simulation

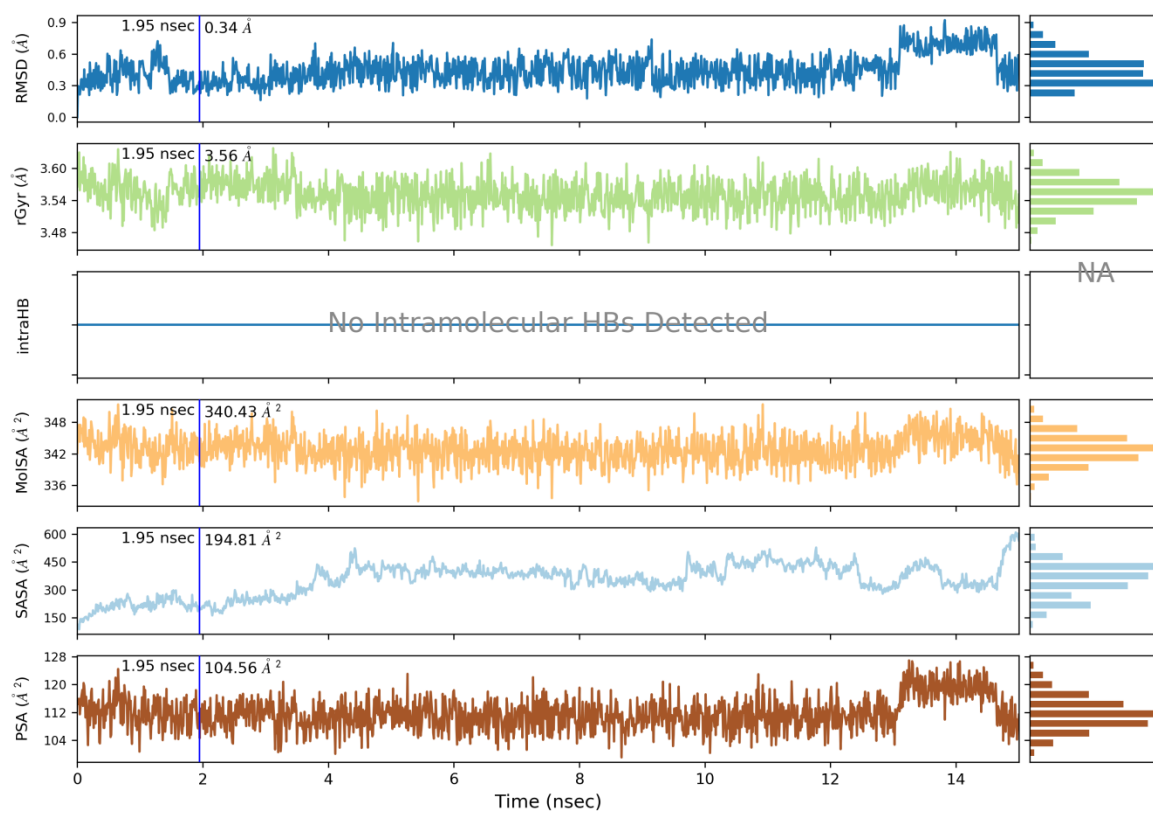


Fig. S3 Different properties of **XD-4** ligand

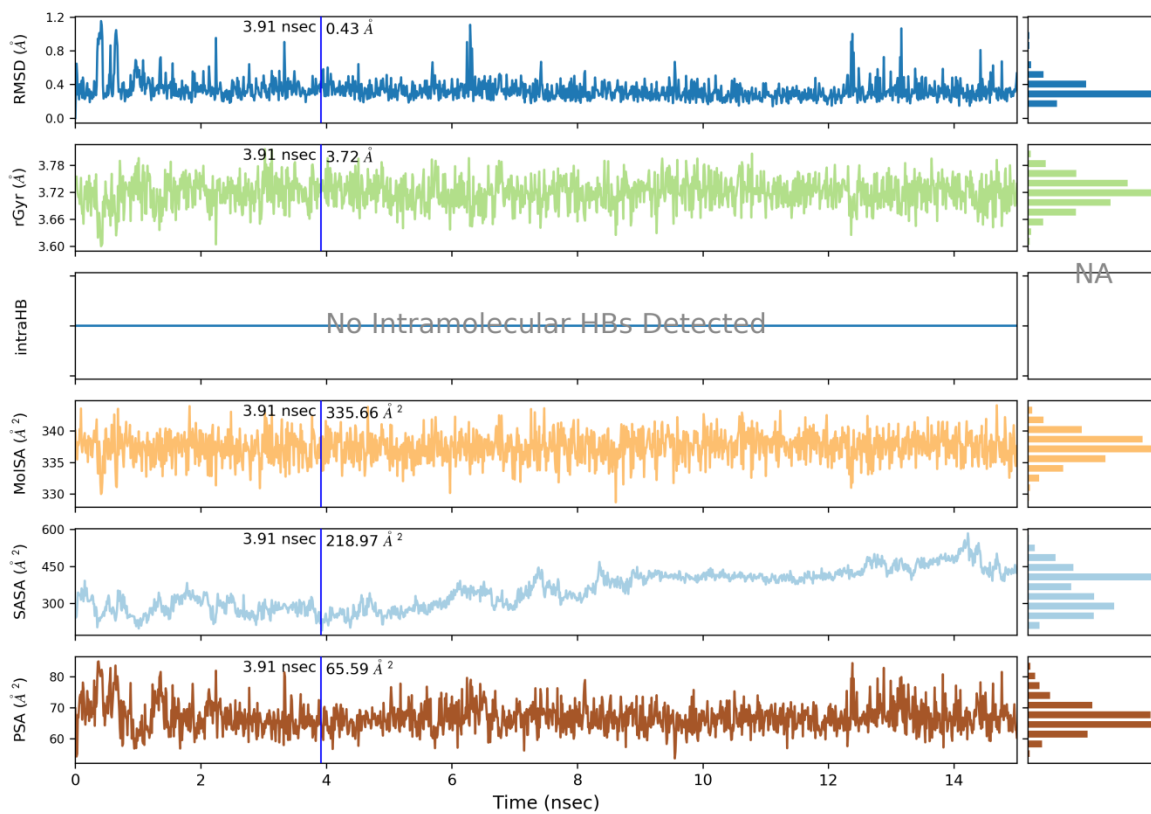


Fig. S4 Different properties of XD-6 ligand