

Supplementary material

Optimal synthesis conditions for NBF-modified 8,13-dihydroberberine derivatives

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UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(pyridin-4-yl)ethan-1-one (**11a**) dissolved in DMF (Absorbance (A), a. u.), at a concentration of $1 \cdot 10^{-4}$ mol/L62

UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(pyridin-4-yl)ethan-1-one (**11a**) dissolved in DMF (Transmittance (T), %), at a concentration of $1 \cdot 10^{-4}$ mol/L.....63

Table S1. Optimization process table for batch synthesis, using derivative **9a** as an example.

Solvent	Acetone**	Benzene	CH ₃ CN	DMF	CHCl ₃
Temperature*, °C			5		
Yield of the target product, %	32	42	45	63	-
Temperature*, °C			25		
Yield of the target product, %	24	55	55	66	15
Temperature*, °C			50		
Yield of the target product, %	<10	34	-	30	Degradation of reaction mixture

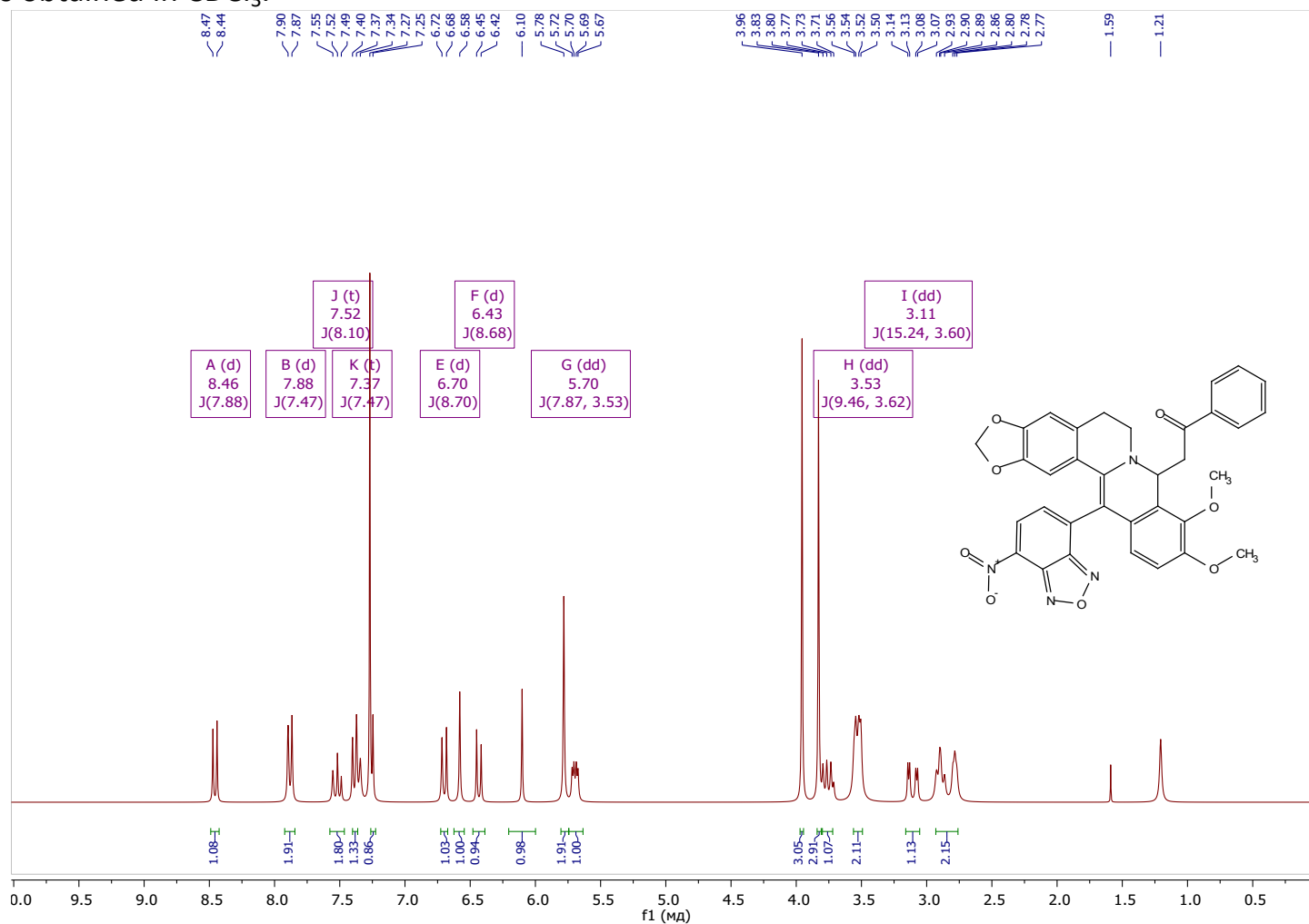
*With further increases in reaction temperature, there is a consistent decrease in the yield of the reaction product. When the temperature exceeds 70°C in any solvent, the reaction mixture goes through complete degradation.

** In the synthesis conditions, acetone acts as a competing reagent and has the potential to substitute the functional group at position C-8. This substitution results in reduced yields of the desired products when the temperature is increased.

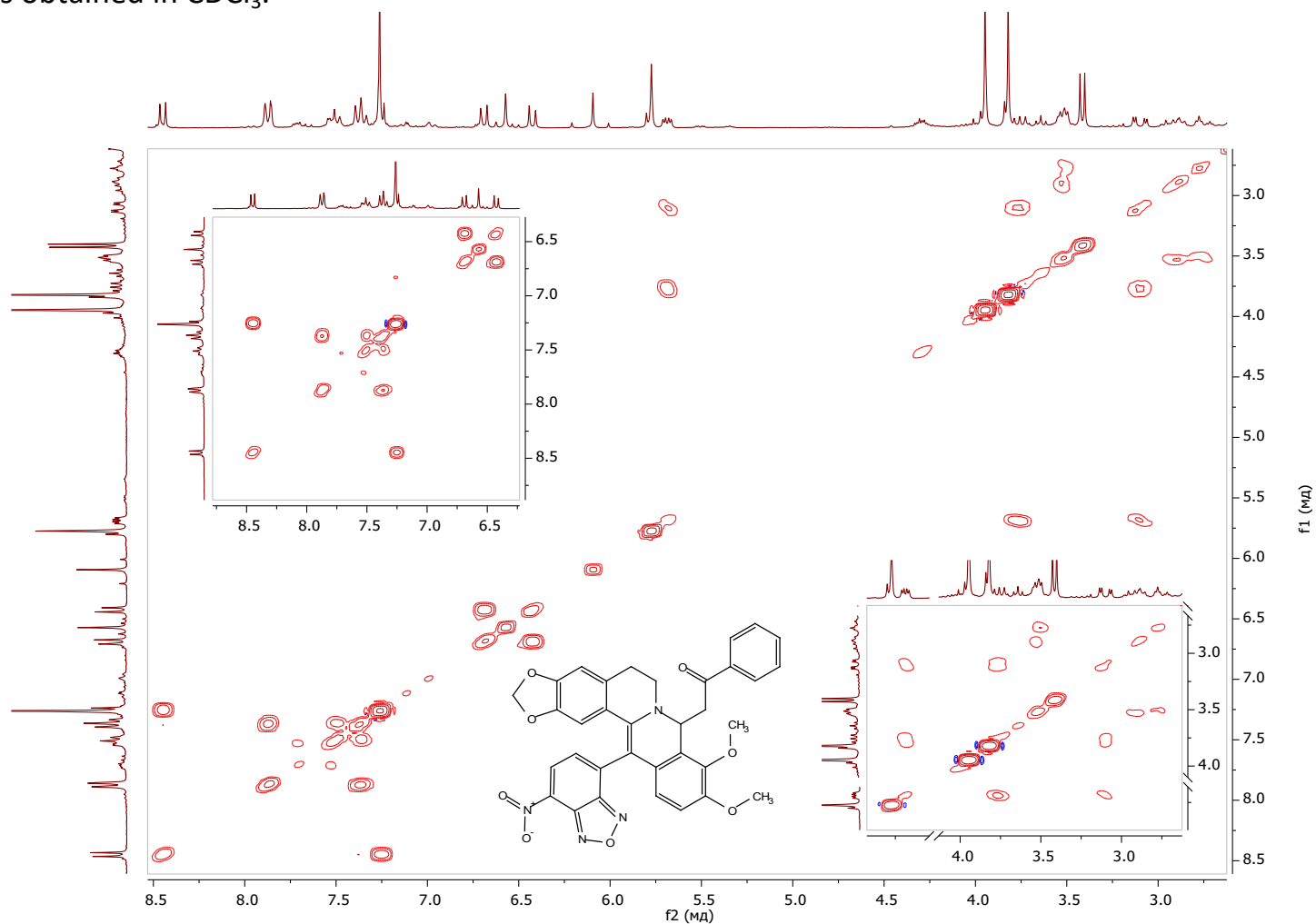
The determination of temperature and solvation effects (Table S1) was conducted under batch conditions. Low-temperature conditions were achieved using a refrigeration chamber, and reaction temperature was controlled using a thermocouple. Room temperature conditions and heating were controlled using an oil bath with a thermocouple.

A measured amount of reduced form berberine (DHB) (1 mmol) was dissolved in 15 mL of the appropriate solvent (in the case of benzene, the solution needed to be heated to accelerate the dissolution process) with stirring. To this solution, 1 mmol of triethylamine (TEA) was added. Separately, 1 mmol of chloronitrobenzofurazane (NBF-Cl) was dissolved in 15 mL of chilled appropriate solvent and slowly added to the solution of activated form berberine (DHB) while continuously stirring. The reaction mixture was stirred in the dark for 2 hours. Then, the solution was separated, analyzed by ¹H spectroscopy, and the product yield was evaluated based on the results of weighing.

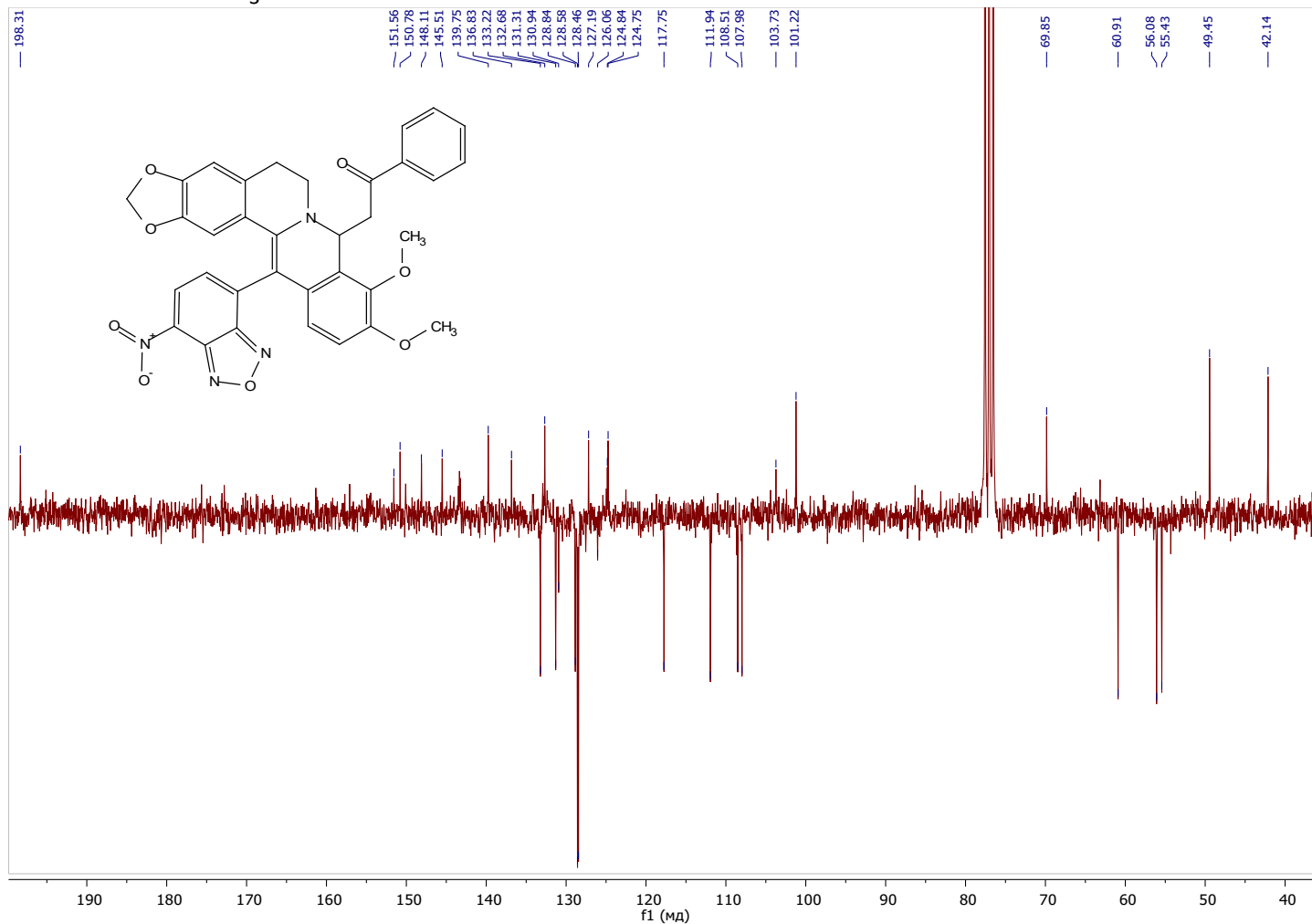
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COSY NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-phenylethan-1-one (**4a**) was obtained in CDCl₃.



^{13}C NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-phenylethan-1-one (**4a**) was obtained in CDCl_3 .



The high-resolution mass spectrum (HRMS) of 2-(9,10-dimethoxy-13-(7-nitrobenzo[*c*][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-*g*]isoquinolino[3,2-*a*]isoquinolin-8-yl)-1-phenylethan-1-one (**4a**).

Display Report

Analysis Info

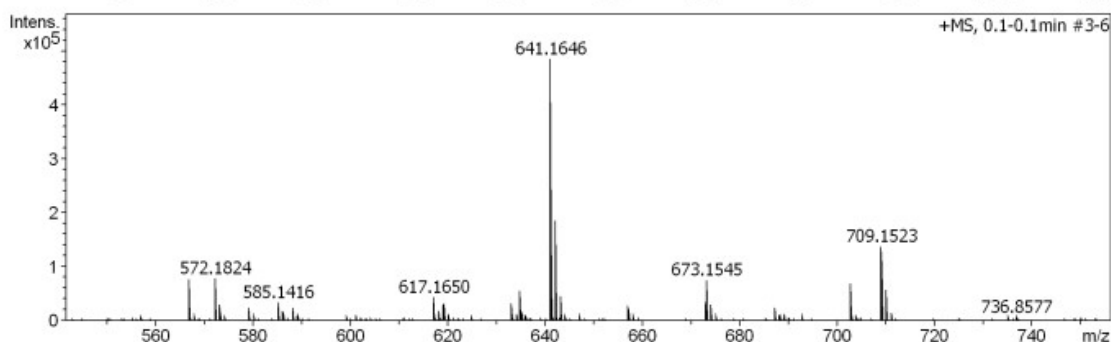
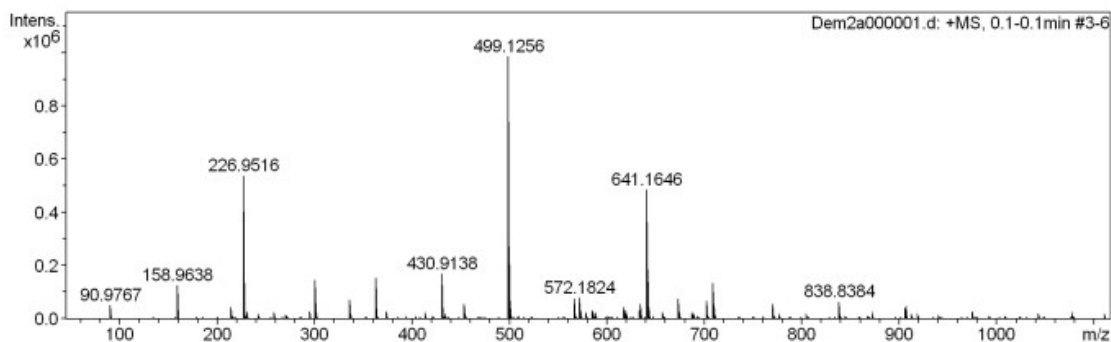
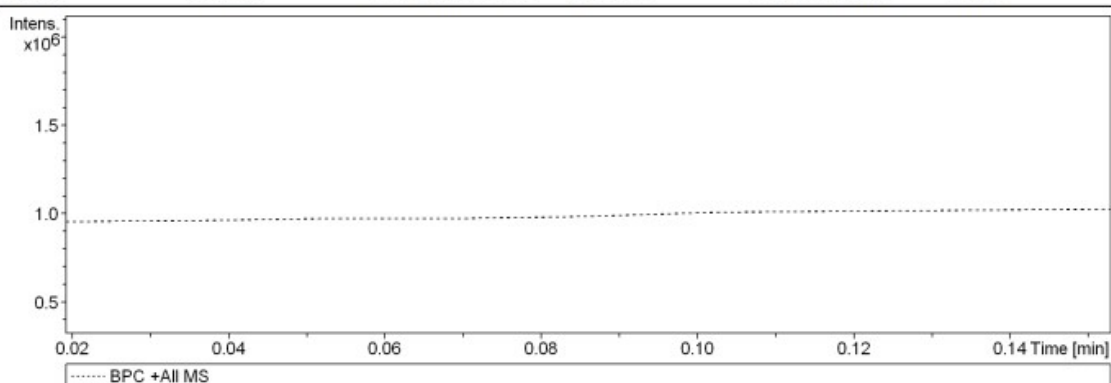
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 Sample Name 1
 Comment

Acquisition Date 7/18/2023 1:33:48 PM

Operator Demidov
 Instrument maXis impact 282001.00109

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source

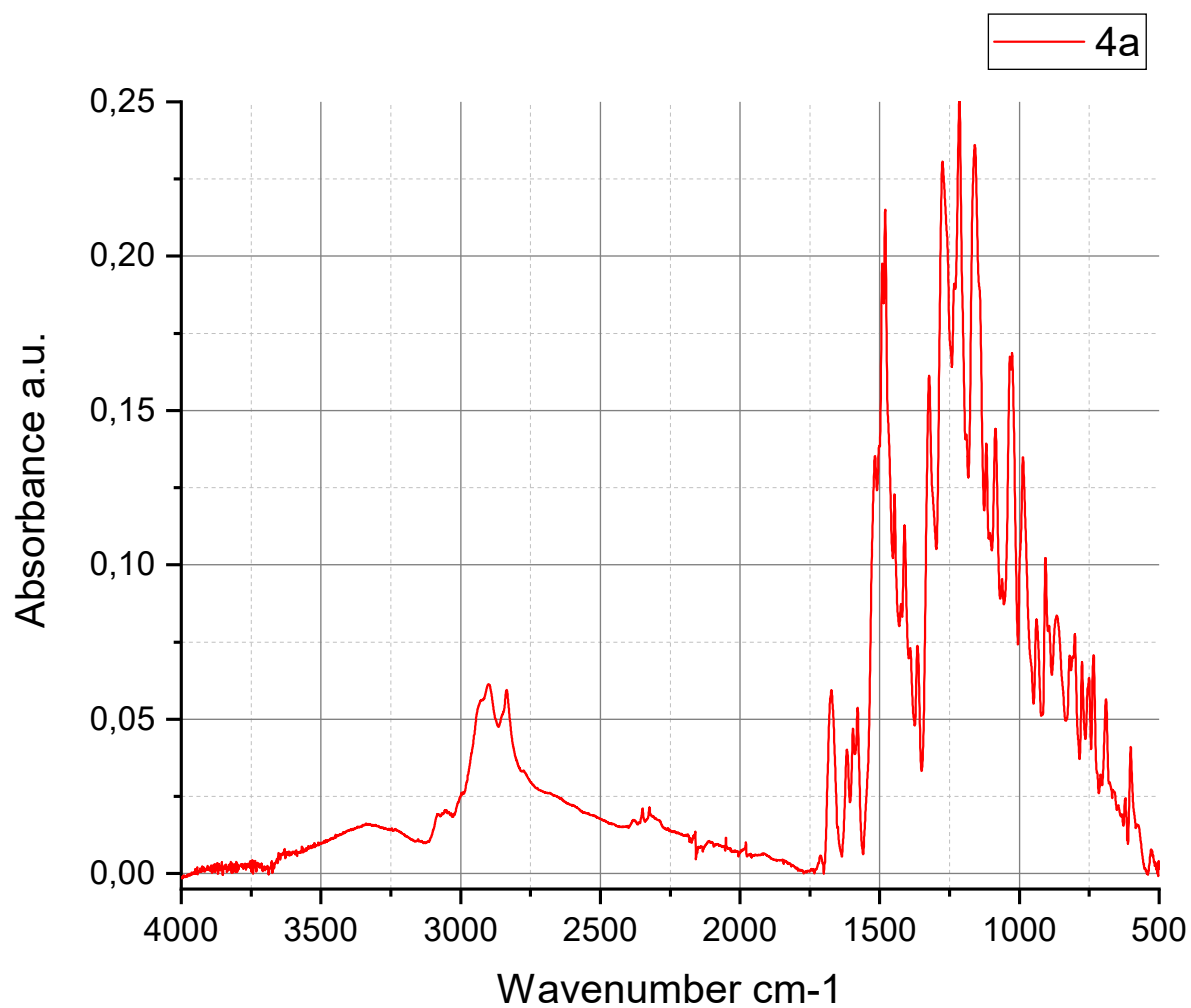


Display Report

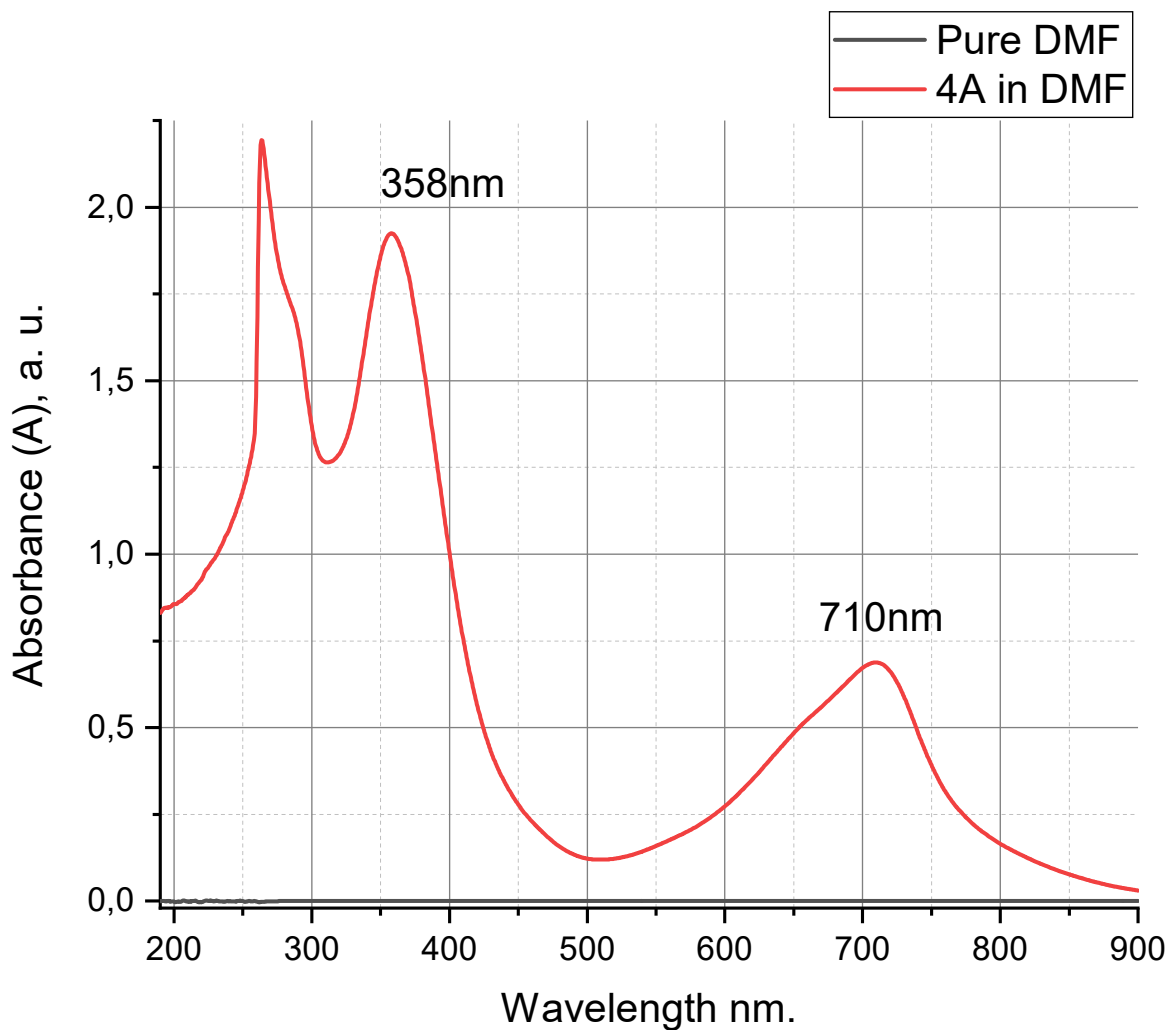
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	2	C26H19N4O7	499.1248	-1.6	11.6	1	100.00	19.5	even	ok
	1	C29H20N2NaO5	499.1264	1.6	23.9	2	100.00	20.5	even	ok
	2	C25H16N8NaO3	499.1238	-3.8	12.4	1	64.58	21.5	even	ok
	1	C23H16KN12	499.1252	-0.8	32.6	2	100.00	21.5	even	ok
	2	C26H24KN2O6	499.1266	1.9	34.5	3	88.64	15.5	even	ok
	3	C22H20KN8O4	499.1239	-3.5	29.0	1	62.61	16.5	even	ok
	1	C27H15N8O3	499.1262	1.1	23.1	2	90.76	24.5	even	ok
	2	C26H19N4O7	499.1248	-1.6	11.6	1	100.00	19.5	even	ok
	641.1646	1	C34H26N4NaO8	641.1643	-0.6	4.0	1	100.00	23.5	even
2		C35H22N8NaO4	641.1656	1.5	15.5	2	58.88	28.5	even	ok

+MS, 0.1-0.1min #3-6

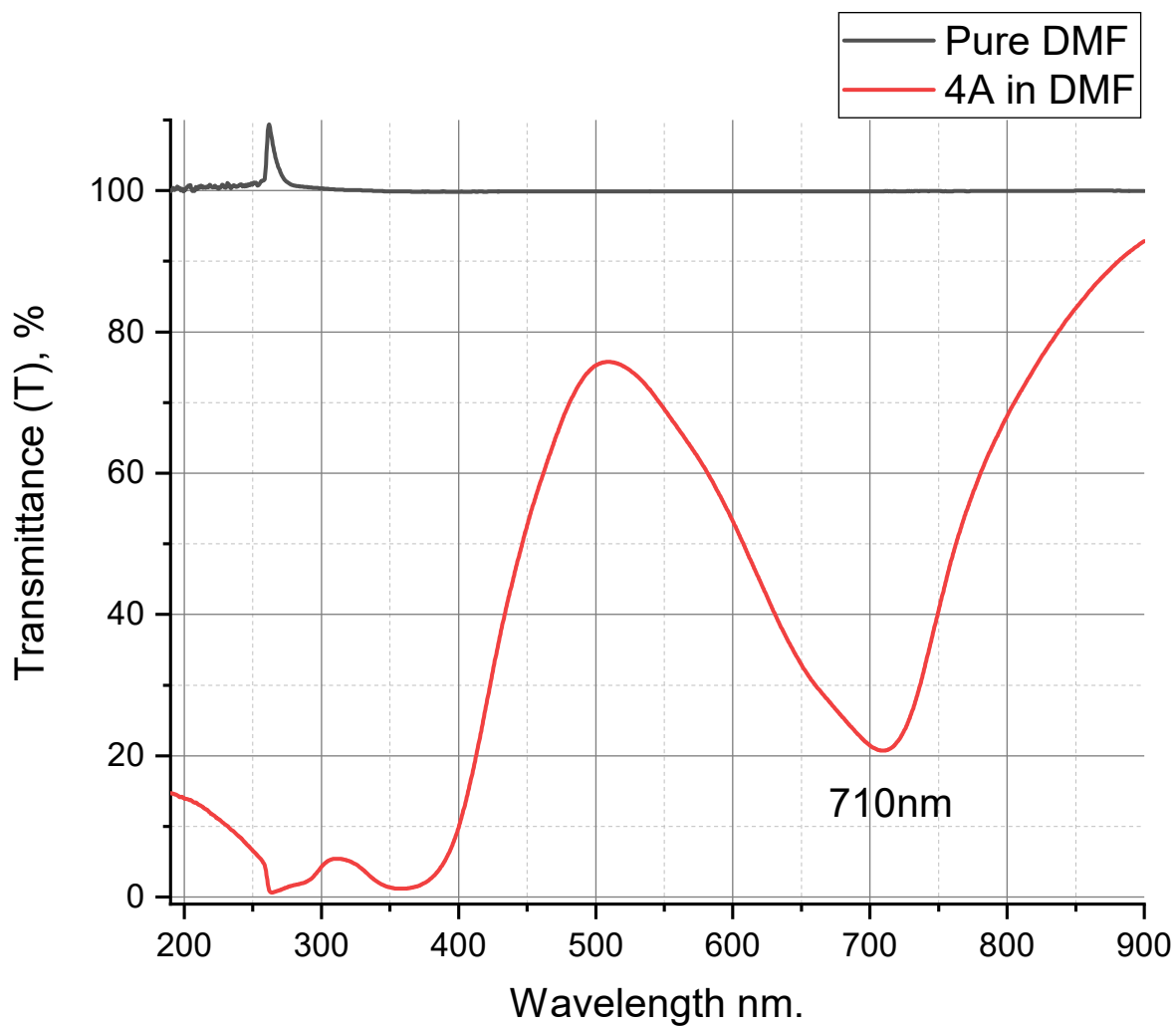
ATR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-phenylethan-1-one (**4a**).



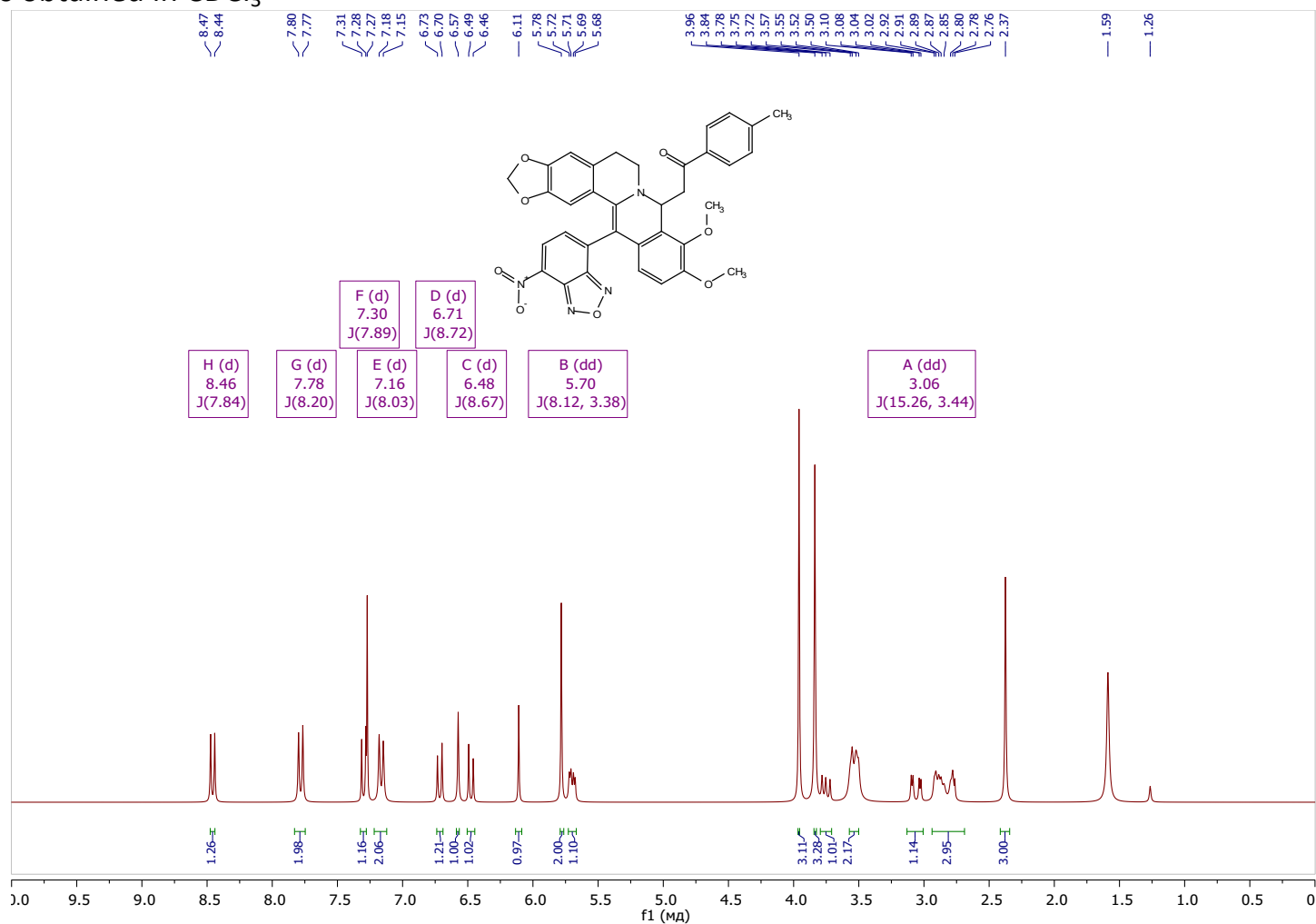
UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-phenylethan-1-one (4a) dissolved in DMF (Absorbance (A), a. u.), at a concentration of $1 \cdot 10^{-4}$ mol/L.



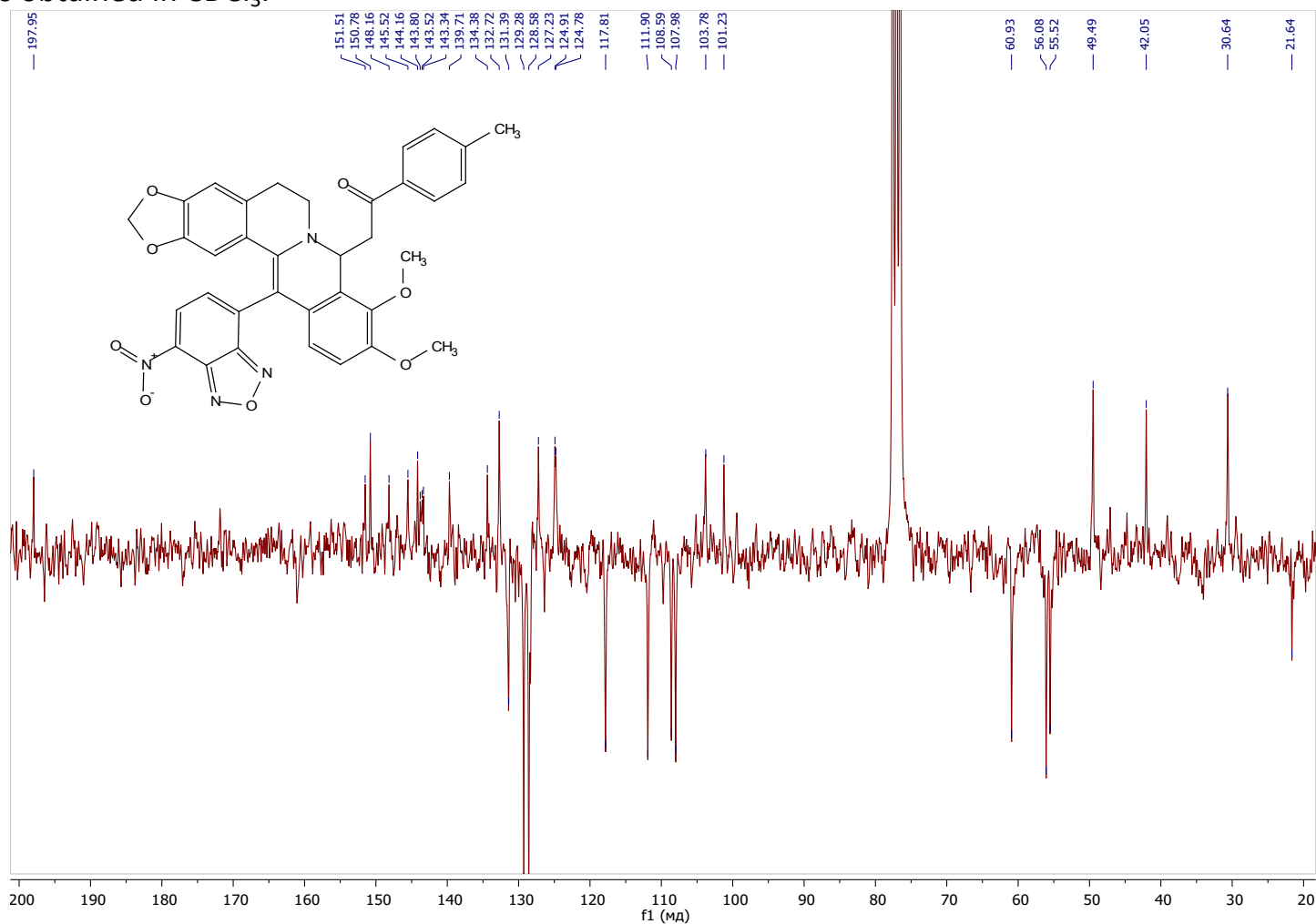
UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-phenylethan-1-one (4a) dissolved in DMF (Transmittance (T), %), at a concentration of 1×10^{-4} mol/L.



^1H NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[*c*][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-*g*]isoquinolino[3,2-*a*]isoquinolin-8-yl)-1-(*p*-tolyl)ethan-1-one (**5a**) was obtained in CDCl_3



^{13}C NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(p-tolyl)ethan-1-one (**5a**) was obtained in CDCl_3 .



The high-resolution mass spectrum (HRMS) of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(p-tolyl)ethan-1-one (**5a**).

Display Report

Analysis Info

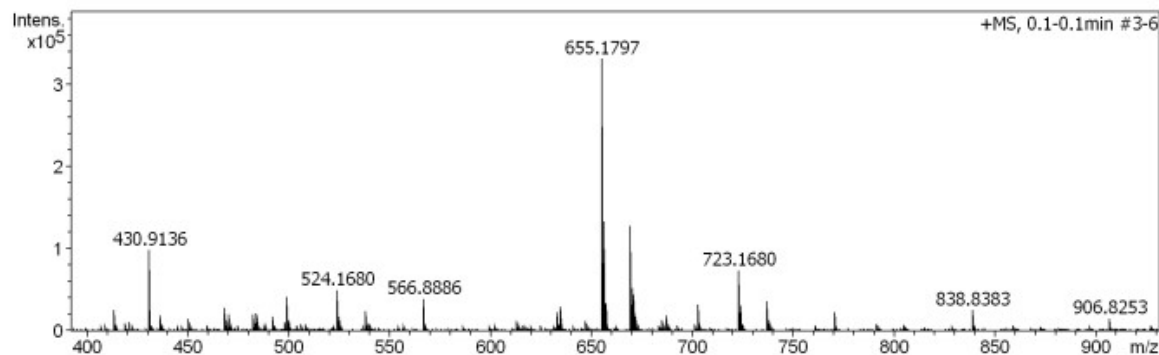
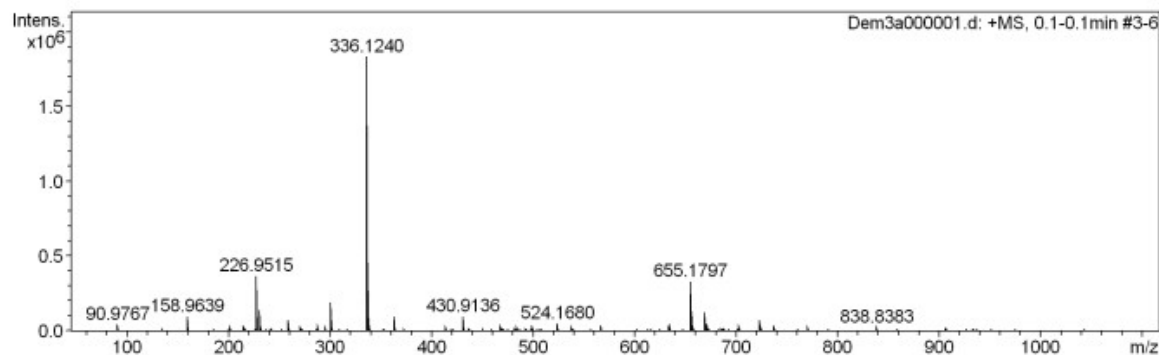
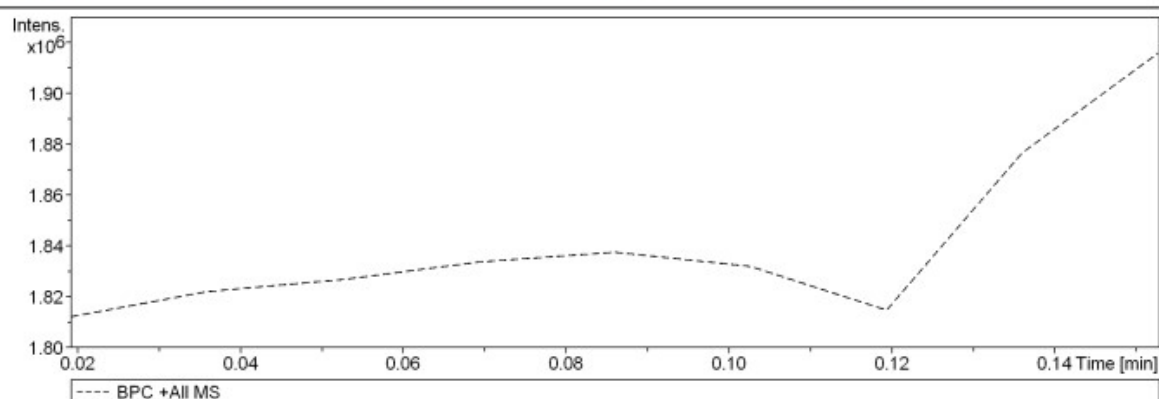
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Acquisition Date 7/18/2023 12:52:04 PM

Operator Demidov
 Instrument maXis impact 282001.00109

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source

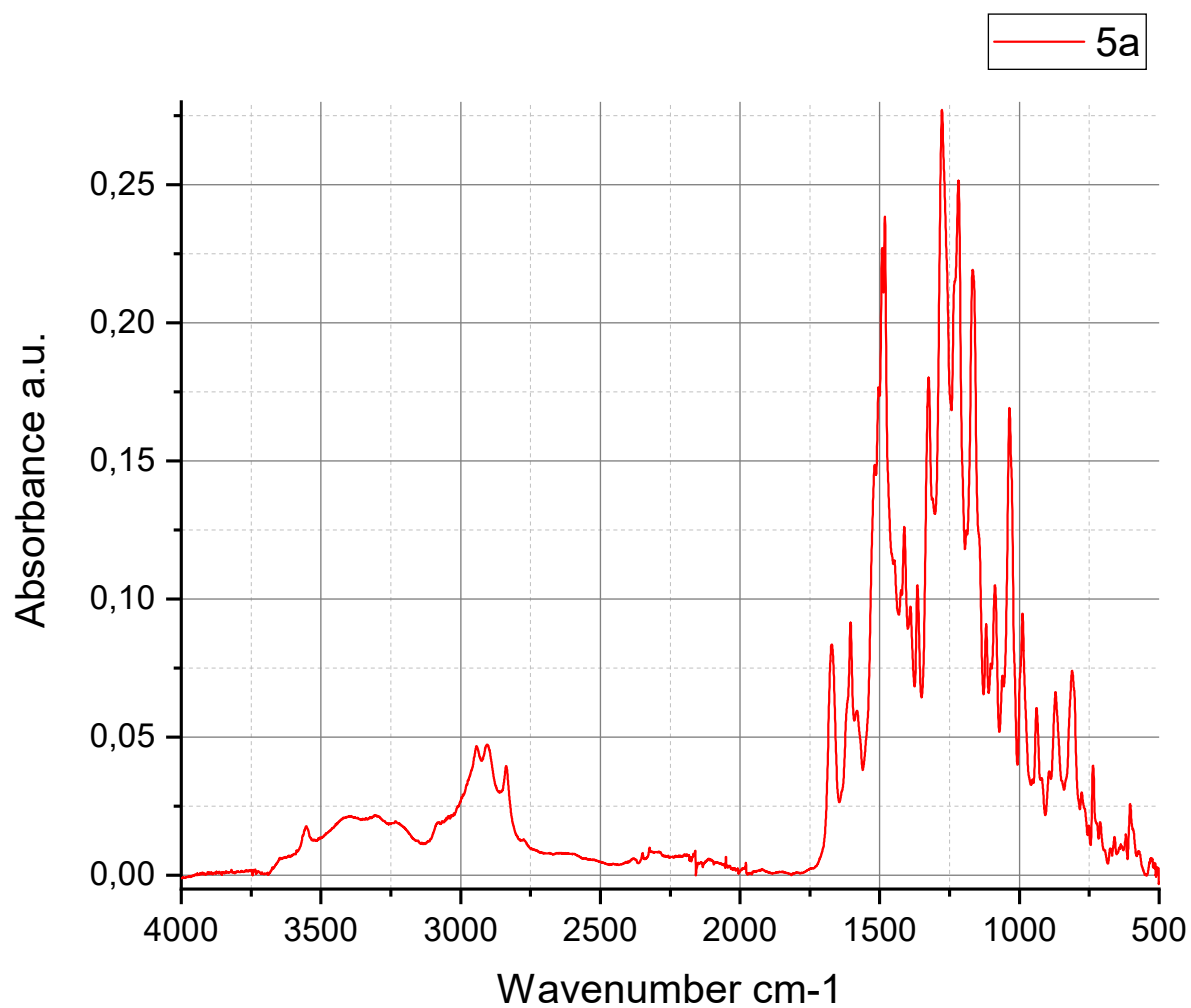


Display Report

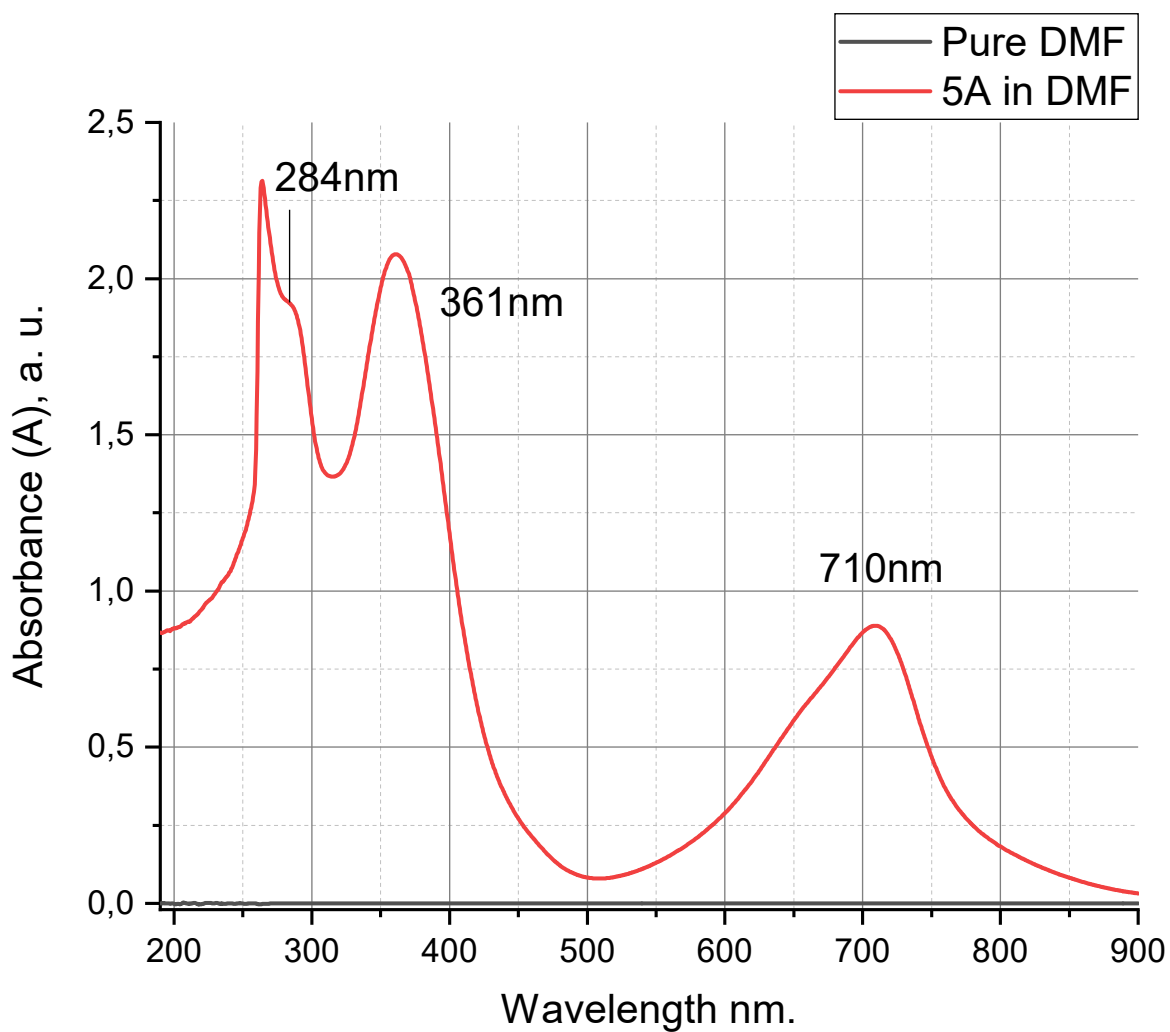
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule
655.1797	1	C36H31O12	655.1810	2.0	1.8	1	100.00	21.5 even	ok
	1	C35H28N4NaO8	655.1799	0.4	4.6	1	100.00	23.5 even	ok
	1	C44H28KN2O2	655.1782	-2.2	58.2	1	100.00	31.5 even	ok

+MS, 0.1-0.1min #3-6

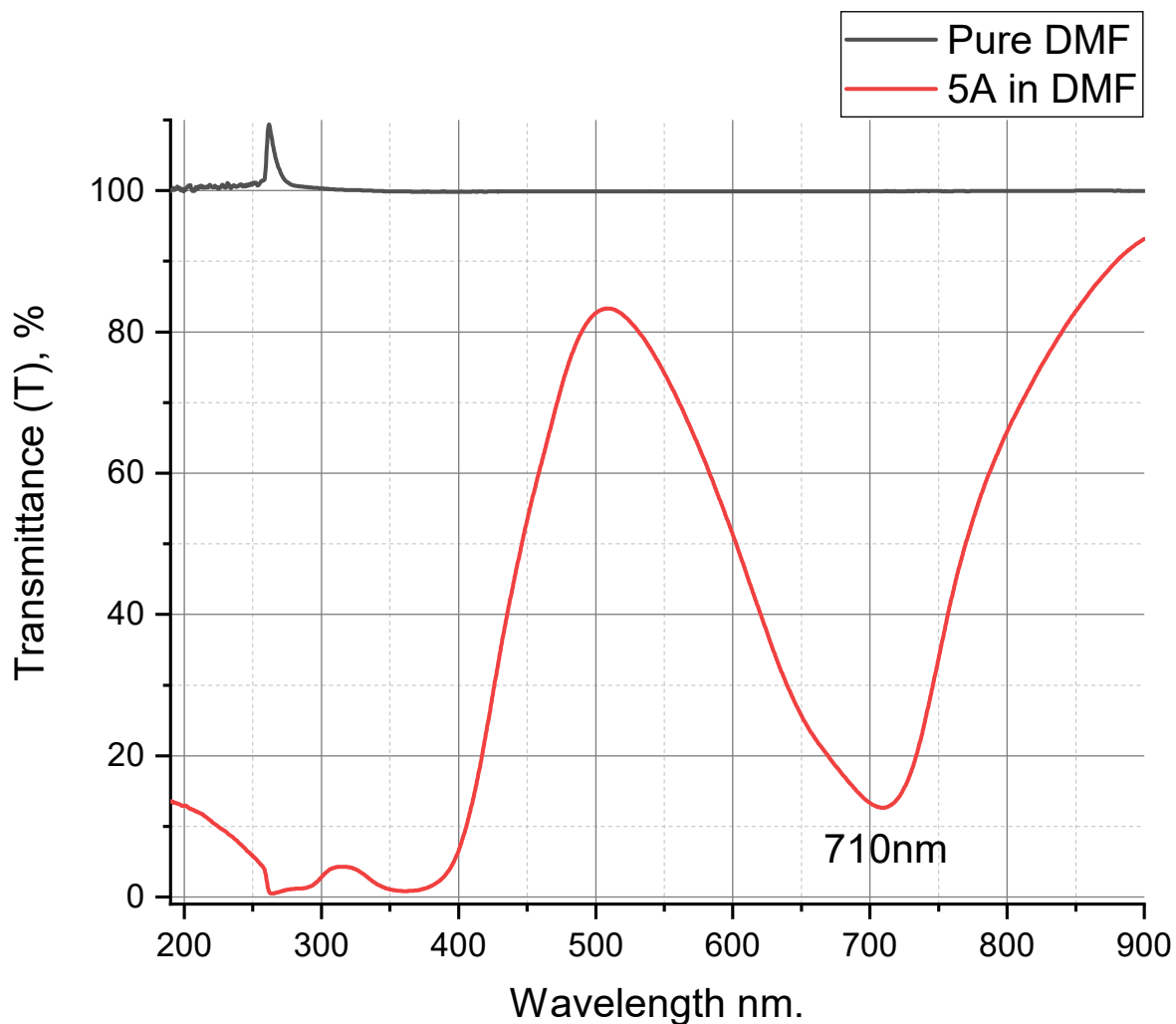
ATR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(p-tolyl)ethan-1-one (**5a**).



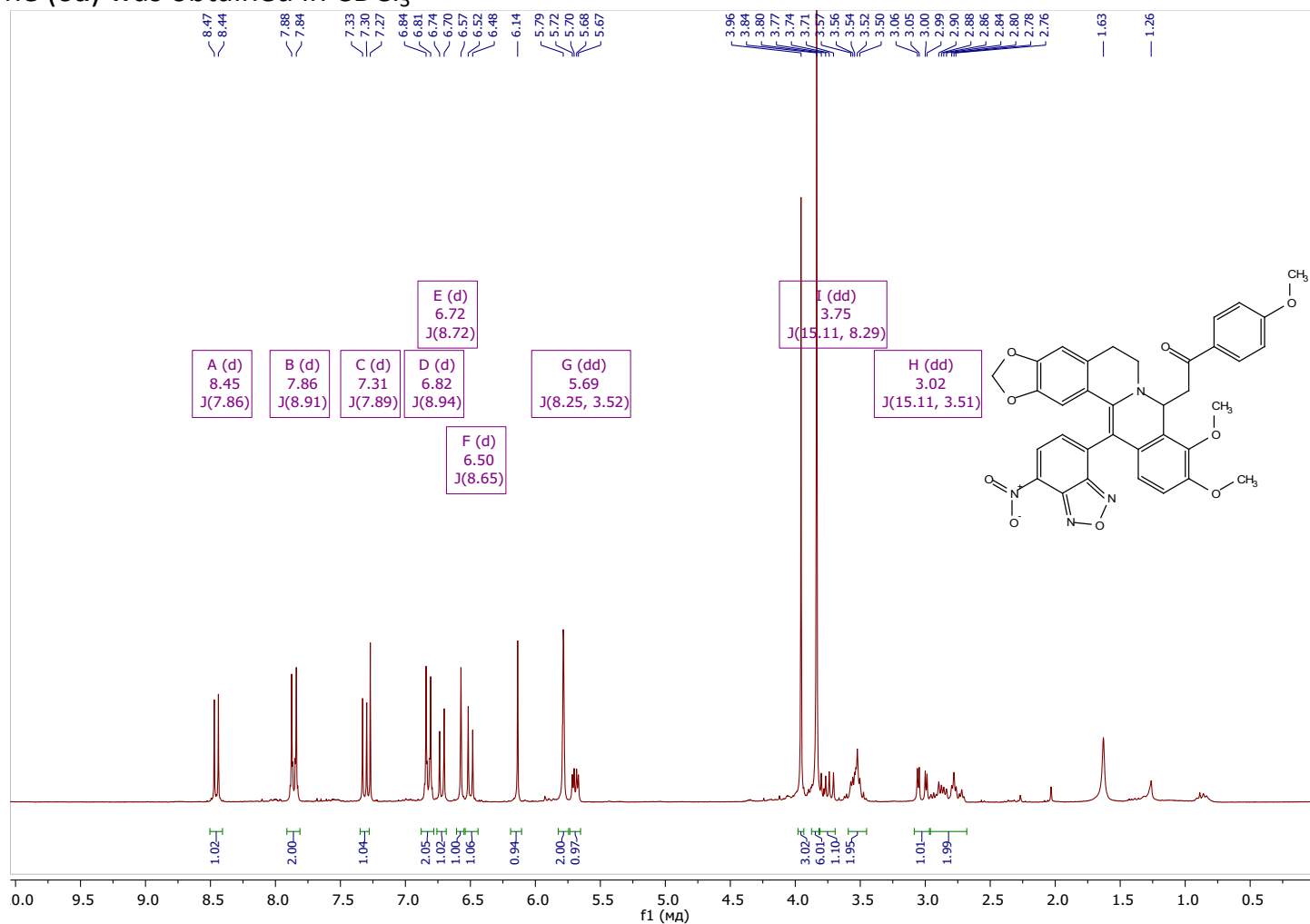
UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(p-tolyl)ethan-1-one (5a) dissolved in DMF (Absorbance (A), a. u.), at a concentration of $1 \cdot 10^{-4}$ mol/L.



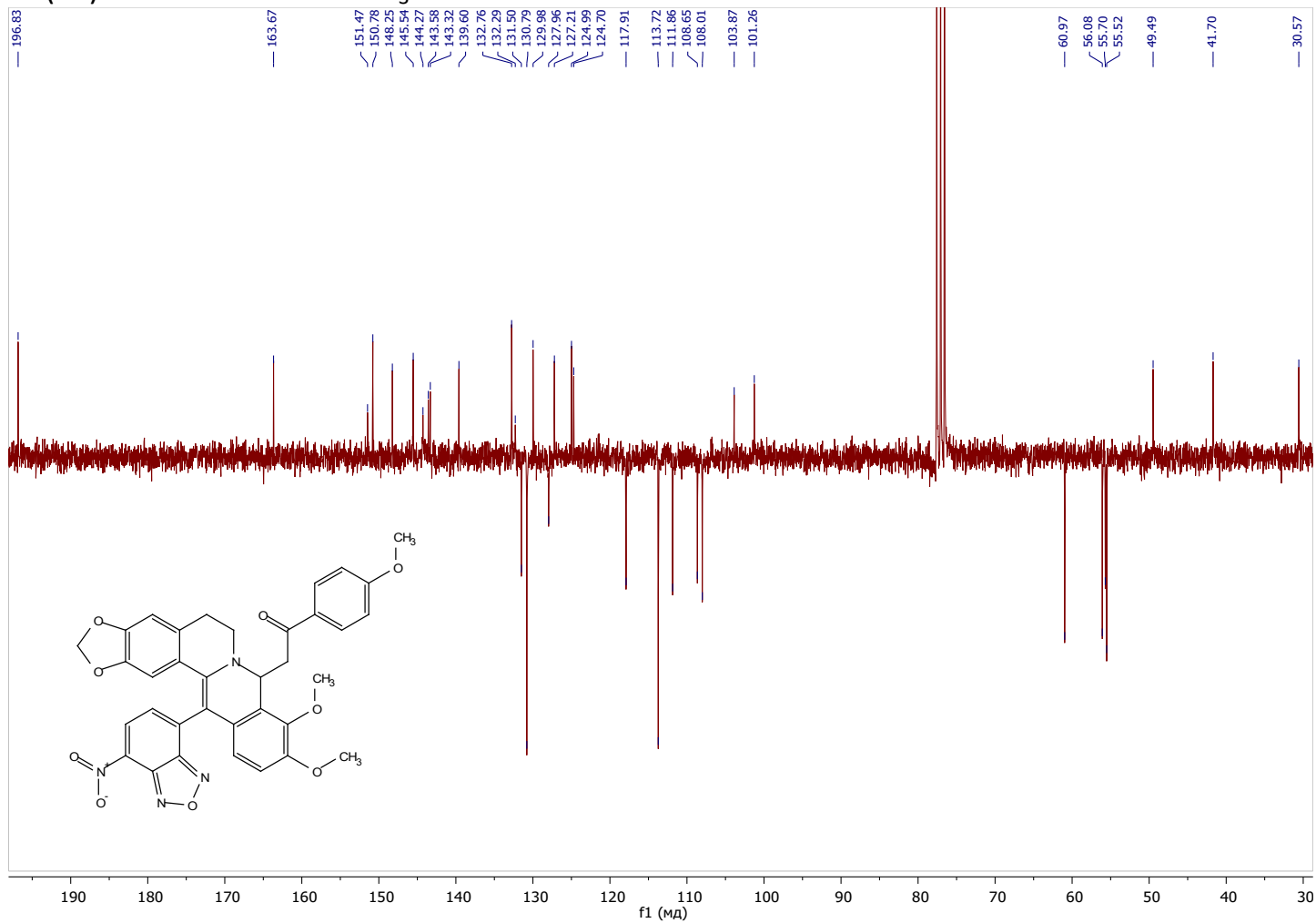
UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(p-tolyl)ethan-1-one (5a) dissolved in DMF (Transmittance (T), %), at a concentration of 1×10^{-4} mol/L.



¹H NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-methoxyphenyl)ethan-1-one (**6a**) was obtained in CDCl₃



C^{13} NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-methoxyphenyl)ethan-1-one (**6a**) was obtained in $CDCl_3$.



The high-resolution mass spectrum (HRMS) of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-methoxyphenyl)ethan-1-one (**6a**).

Display Report

Analysis Info

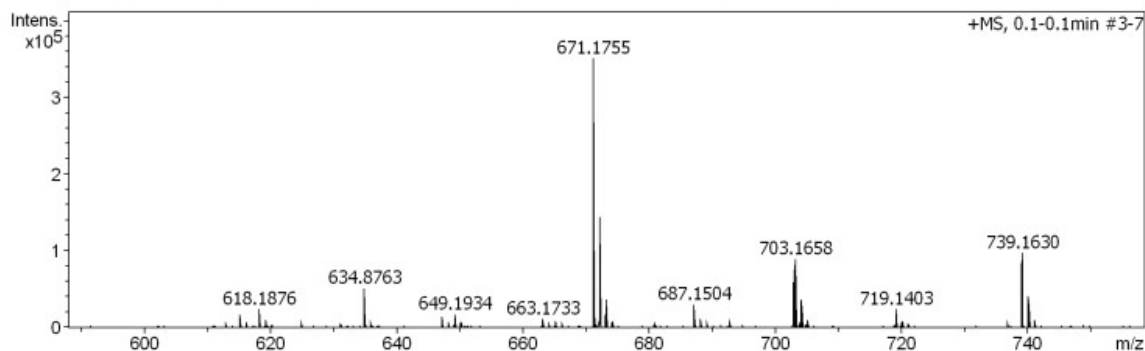
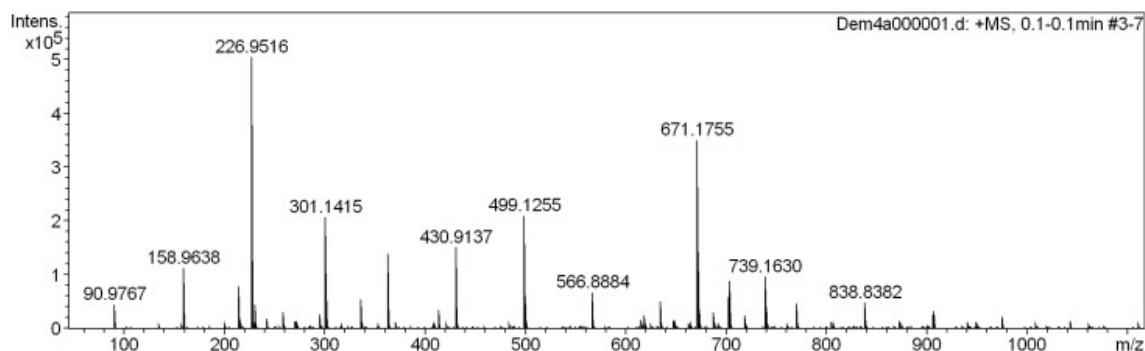
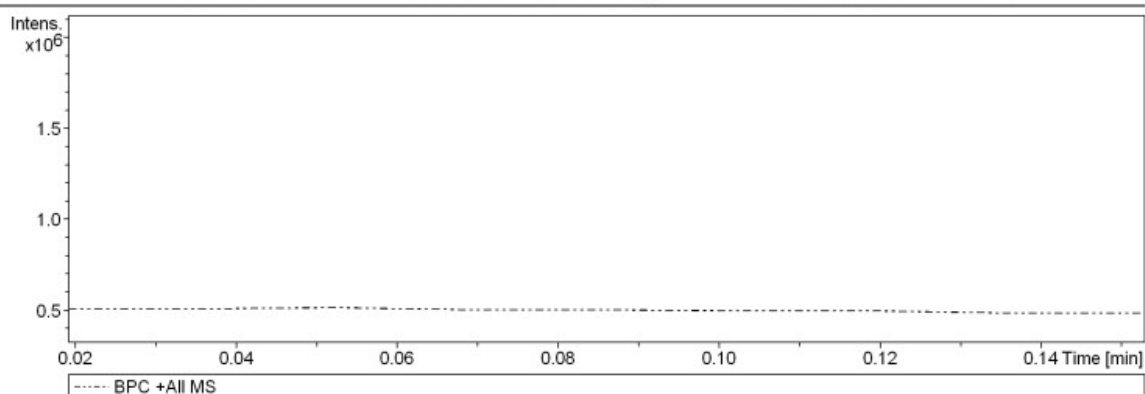
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Acquisition Date 7/18/2023 1:47:49 PM

Operator Demidov
 Instrument maXis impact 282001.00109

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source

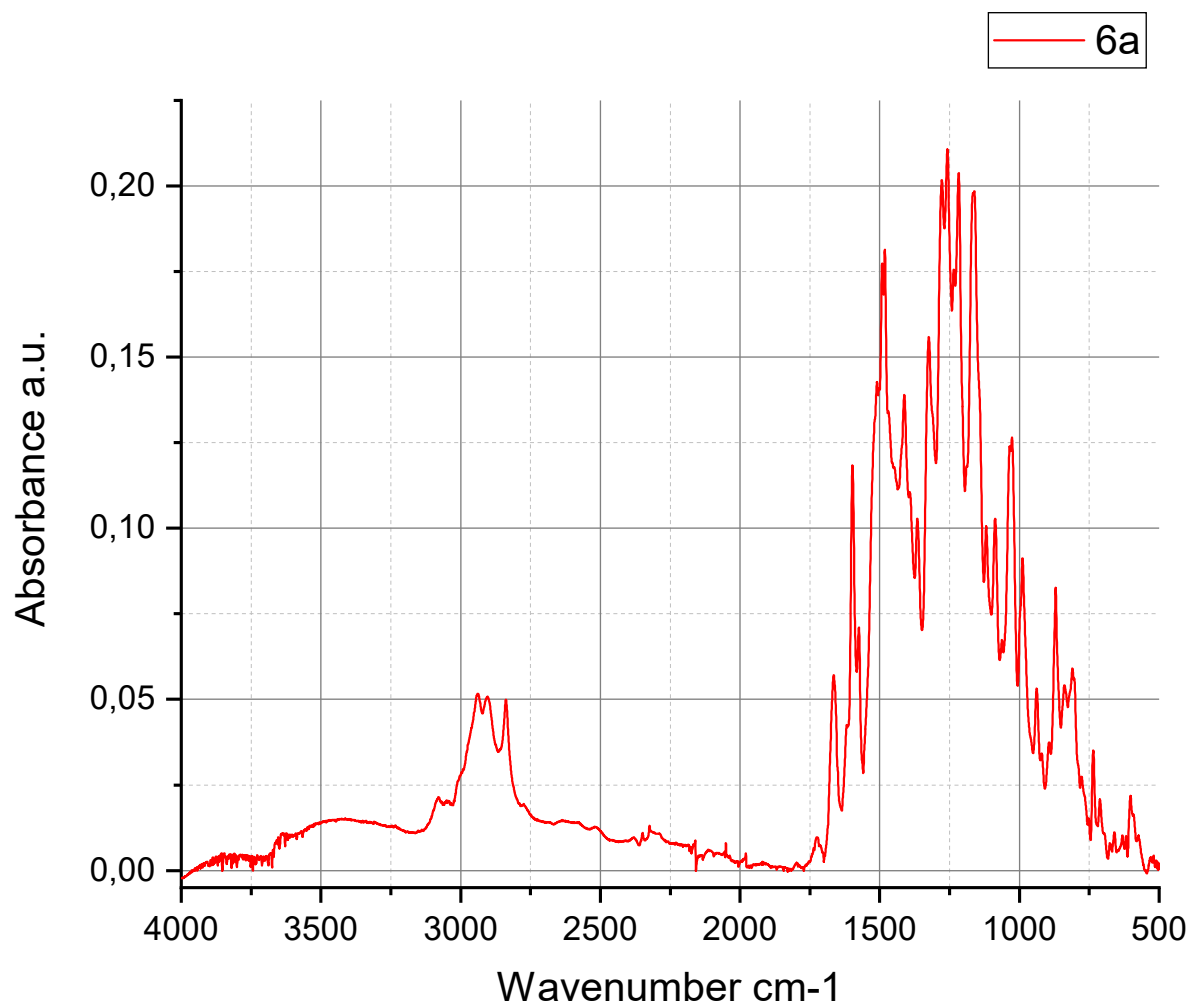


Display Report

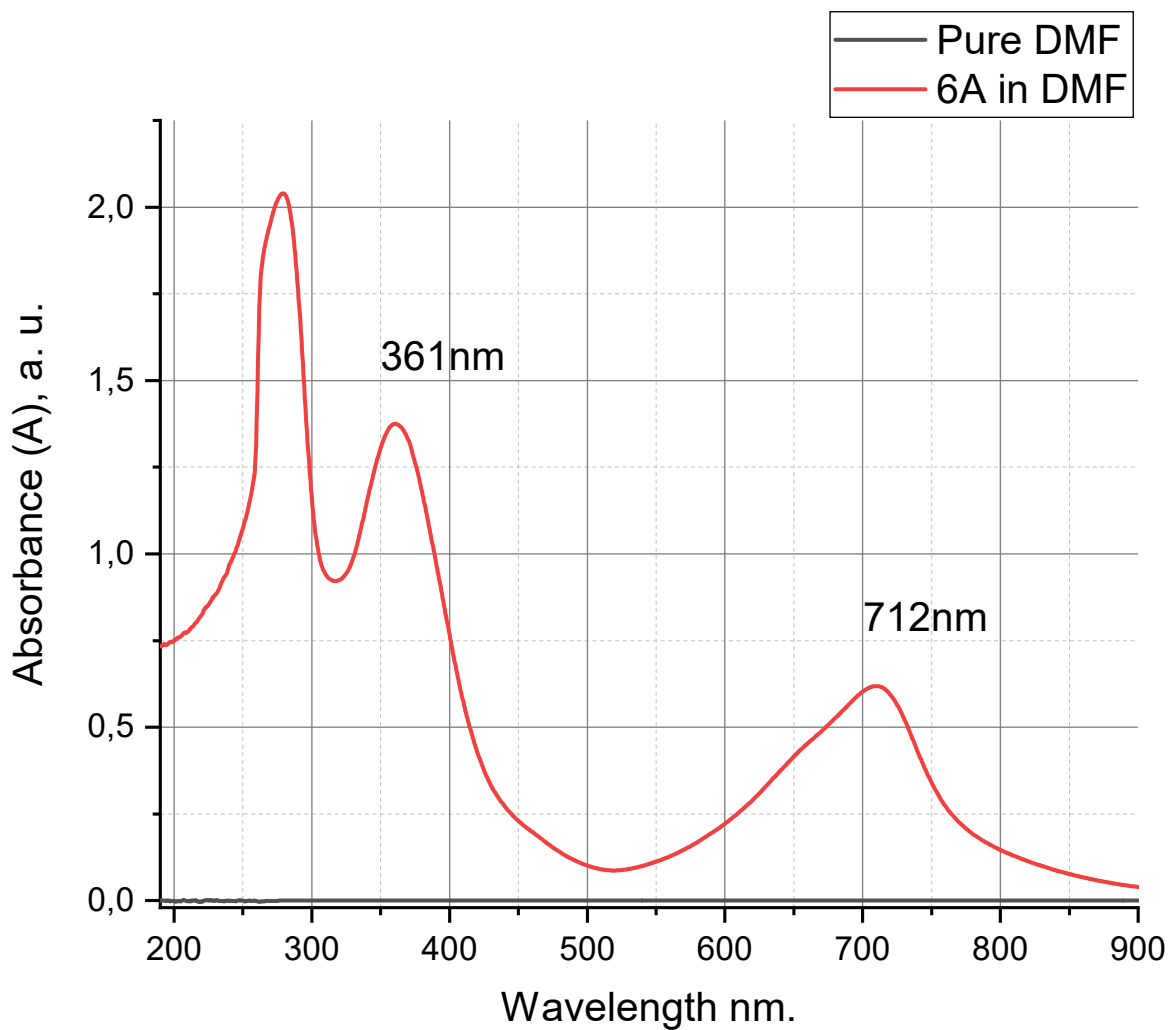
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule
671.1755	1	C37H27N4O9	671.1773	2.6	5.4	100.00	26.5	even	ok
	1	C35H28N4NaO9	671.1748	-0.9	7.4	100.00	23.5	even	ok
	2	C36H24N8NaO5	671.1762	1.1	7.8	95.42	28.5	even	ok

+MS, 0.1-0.1min #3-7

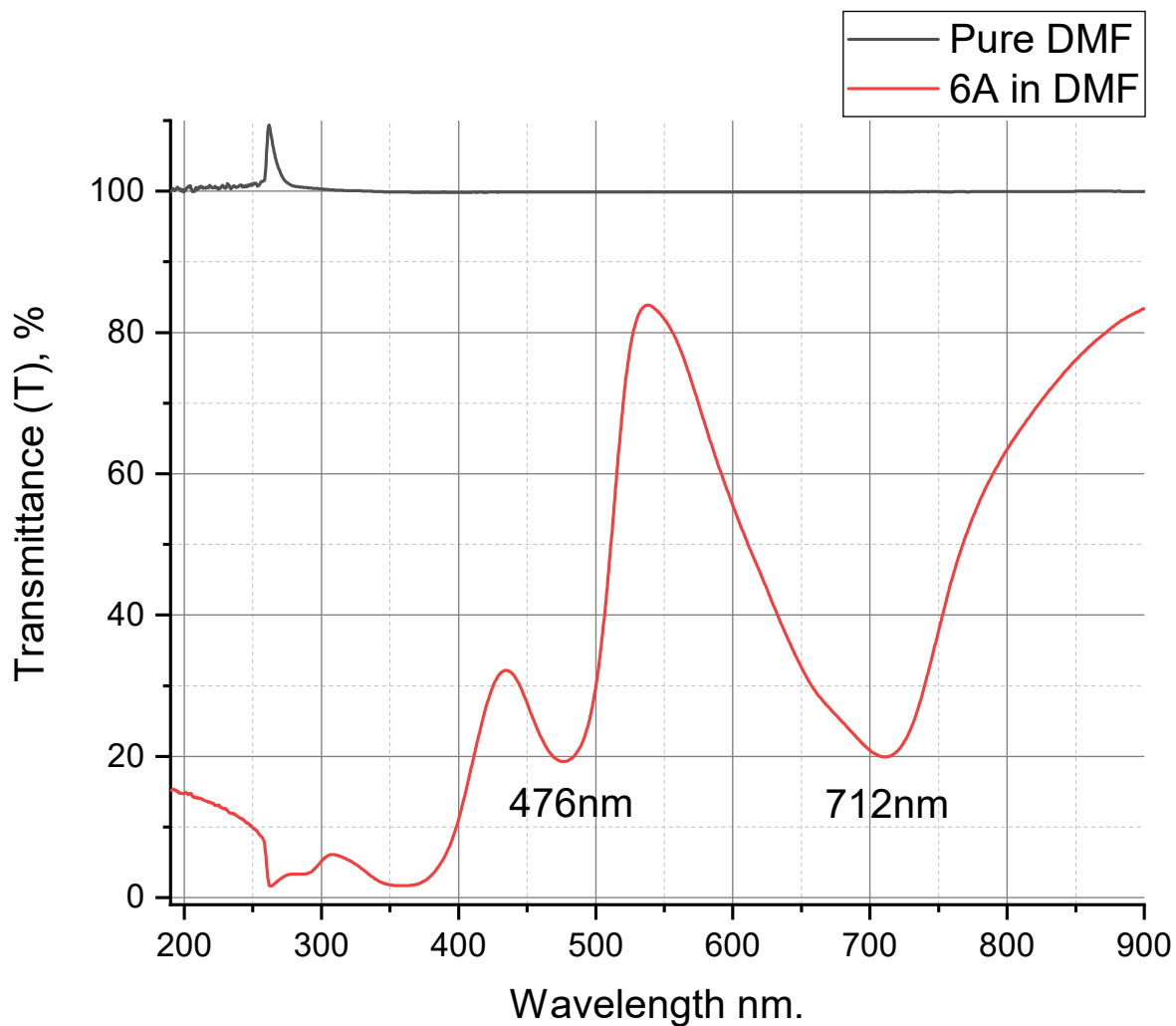
ATR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-methoxyphenyl)ethan-1-one (6a).



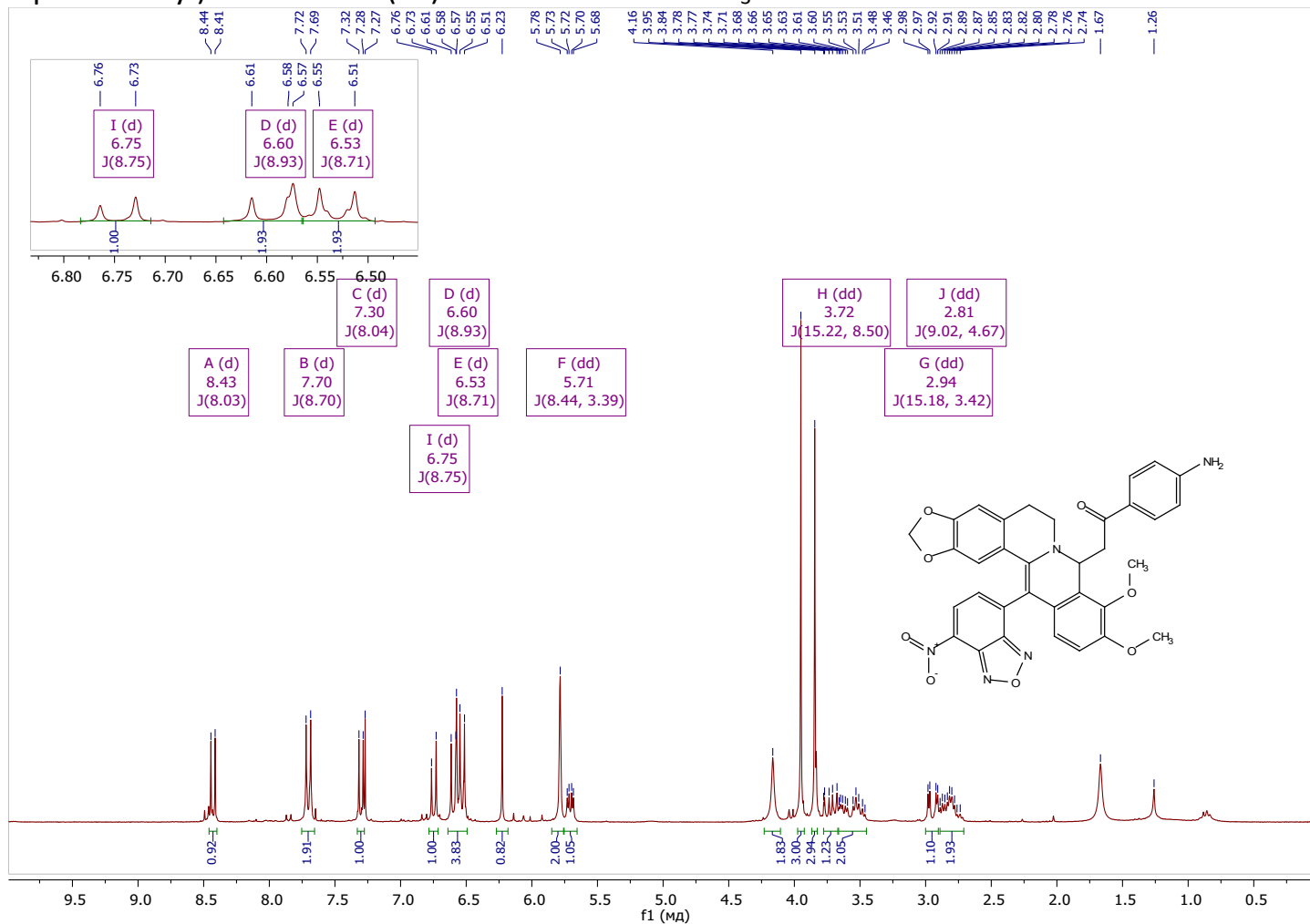
UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-methoxyphenyl)ethan-1-one (6a) dissolved in DMF (Absorbance (A), a. u.), at a concentration of $1 \cdot 10^{-4}$ mol/L.



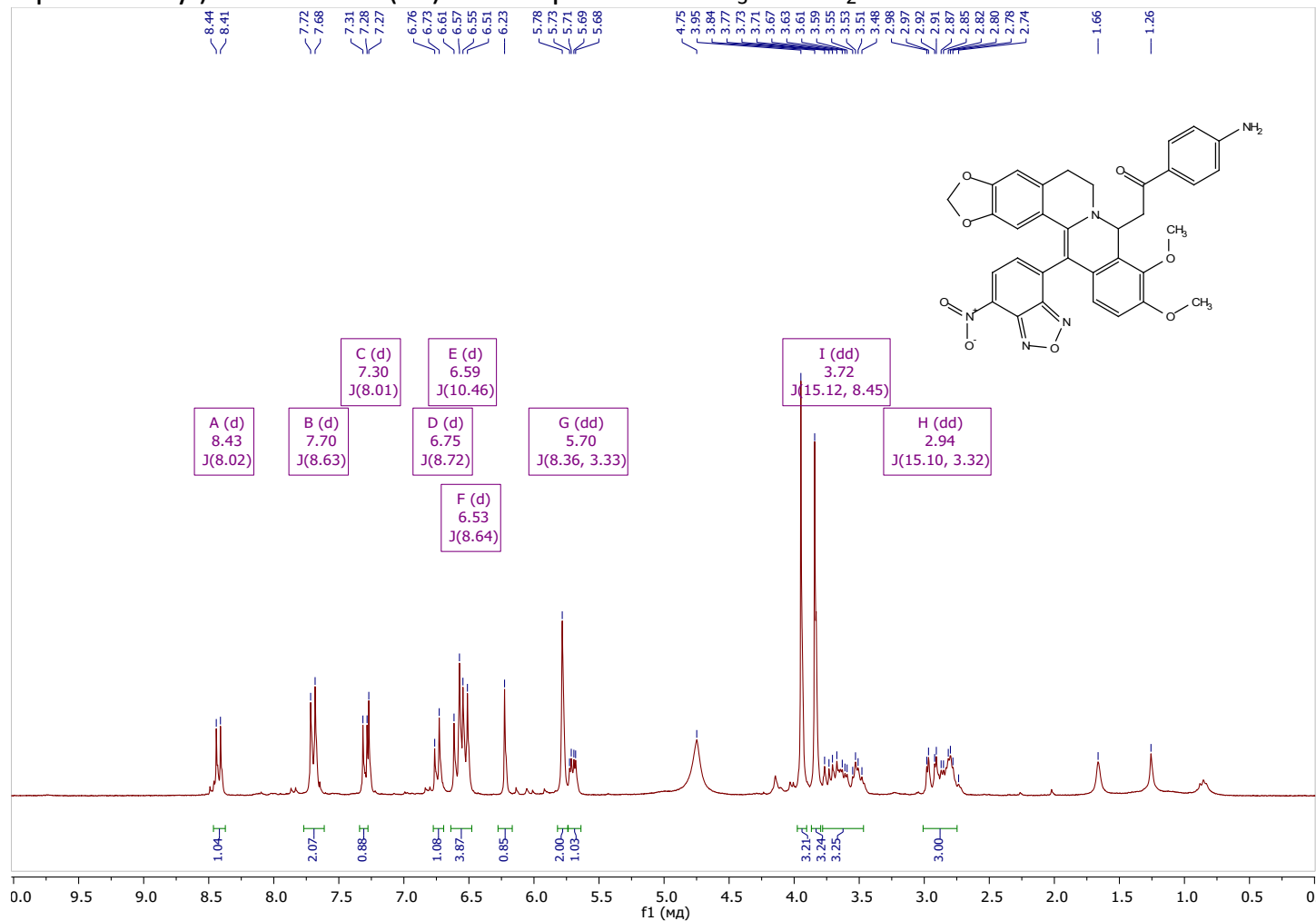
UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-methoxyphenyl)ethan-1-one (6a) dissolved in DMF (Transmittance (T), %), at a concentration of 1×10^{-4} mol/L.



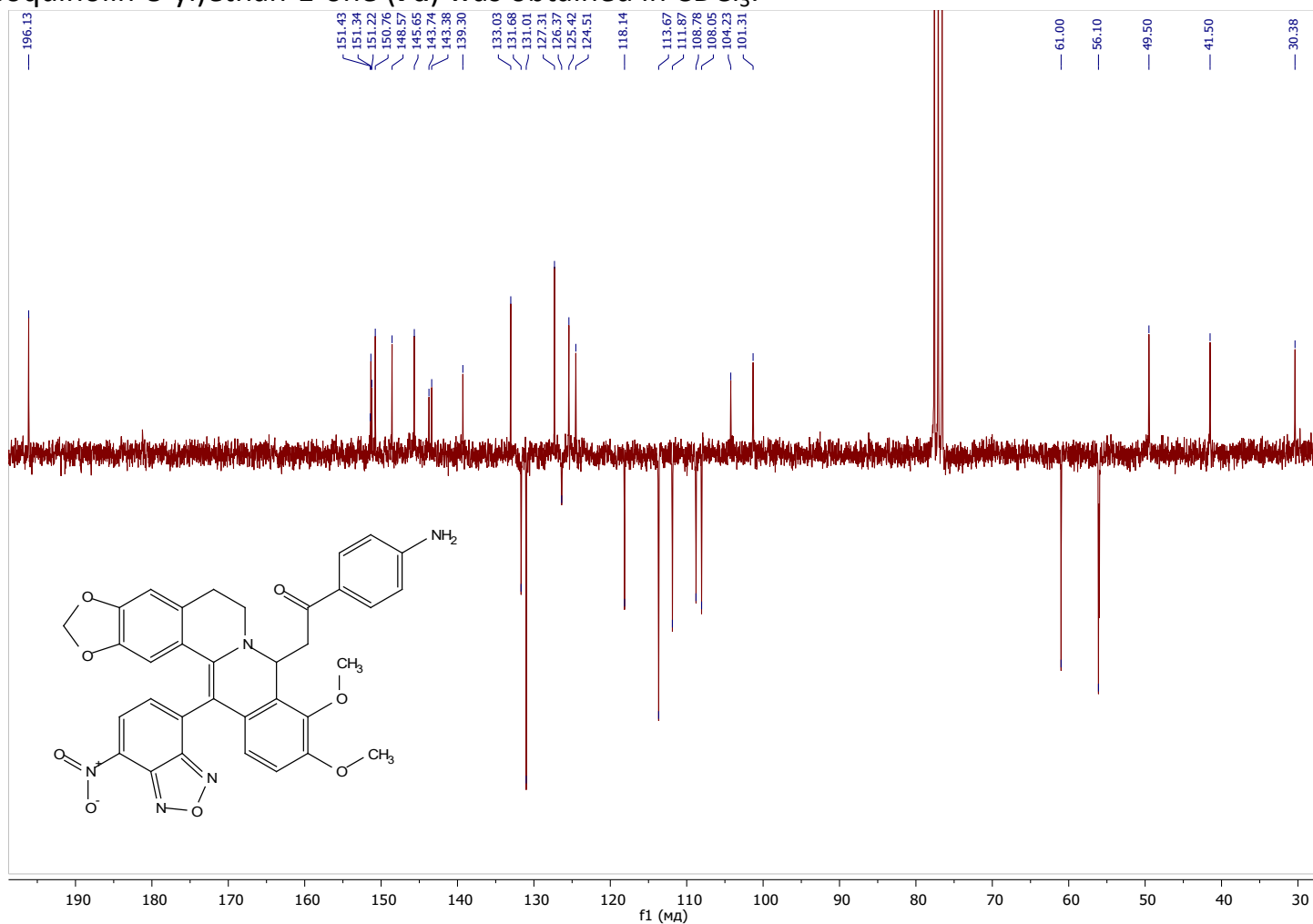
¹H NMR spectrum of 1-(4-aminophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**7a**) was obtained in CDCl₃



^1H NMR spectrum of 1-(4-aminophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**7a**) was acquired in CDCl_3 with D_2O .



^{13}C NMR spectrum of 1-(4-aminophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**7a**) was obtained in CDCl_3 .



The high-resolution mass spectrum (HRMS) of 1-(4-aminophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**7a**).

Display Report

Analysis Info

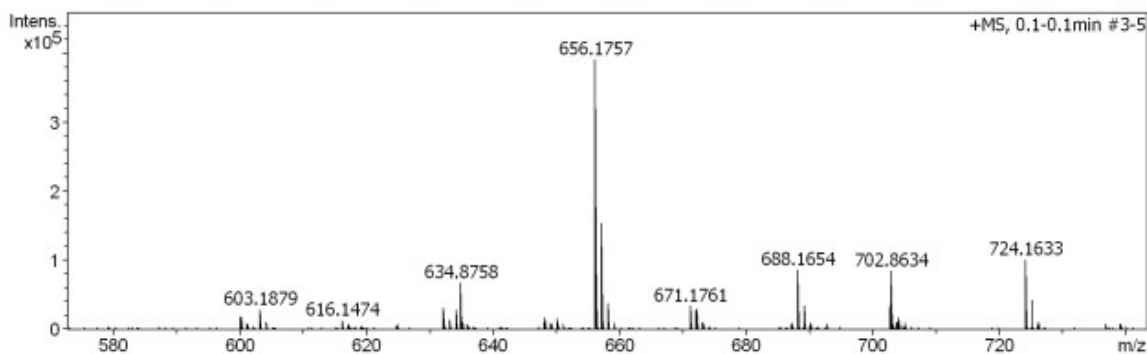
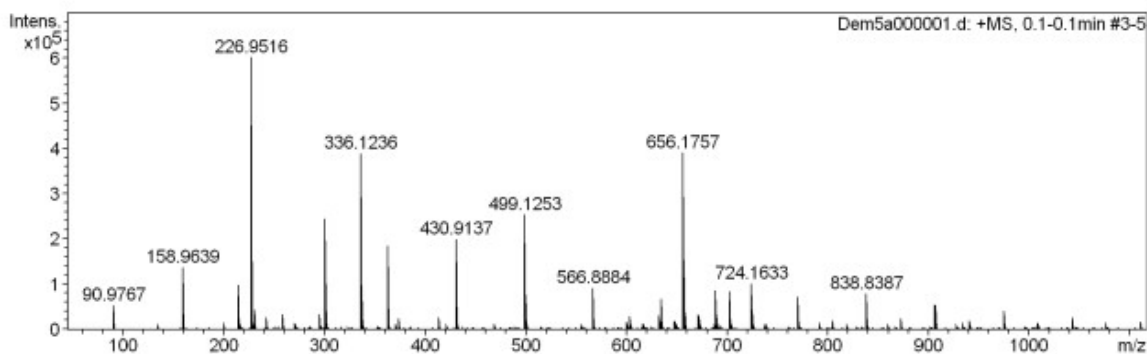
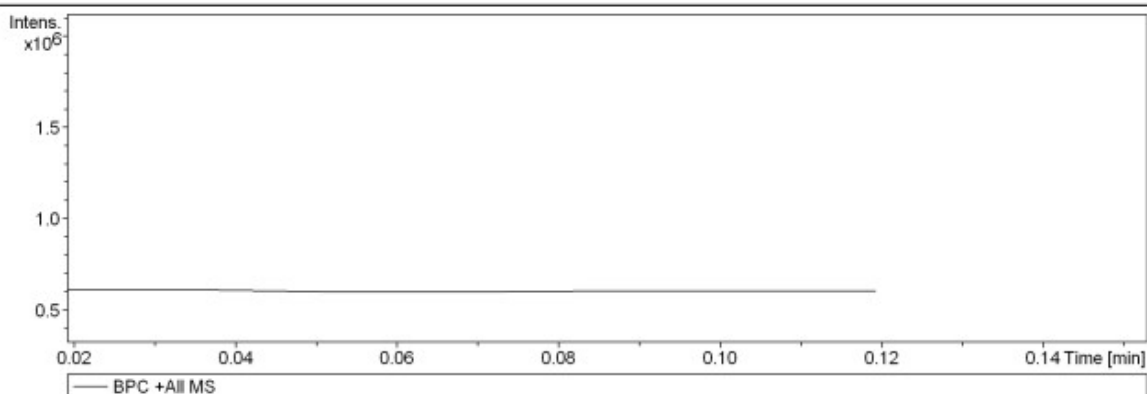
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Sample Name 1
Comment

Acquisition Date 7/18/2023 1:16:52 PM

Operator Demidov
Instrument maXis impact 282001.00109

Acquisition Parameter

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Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source

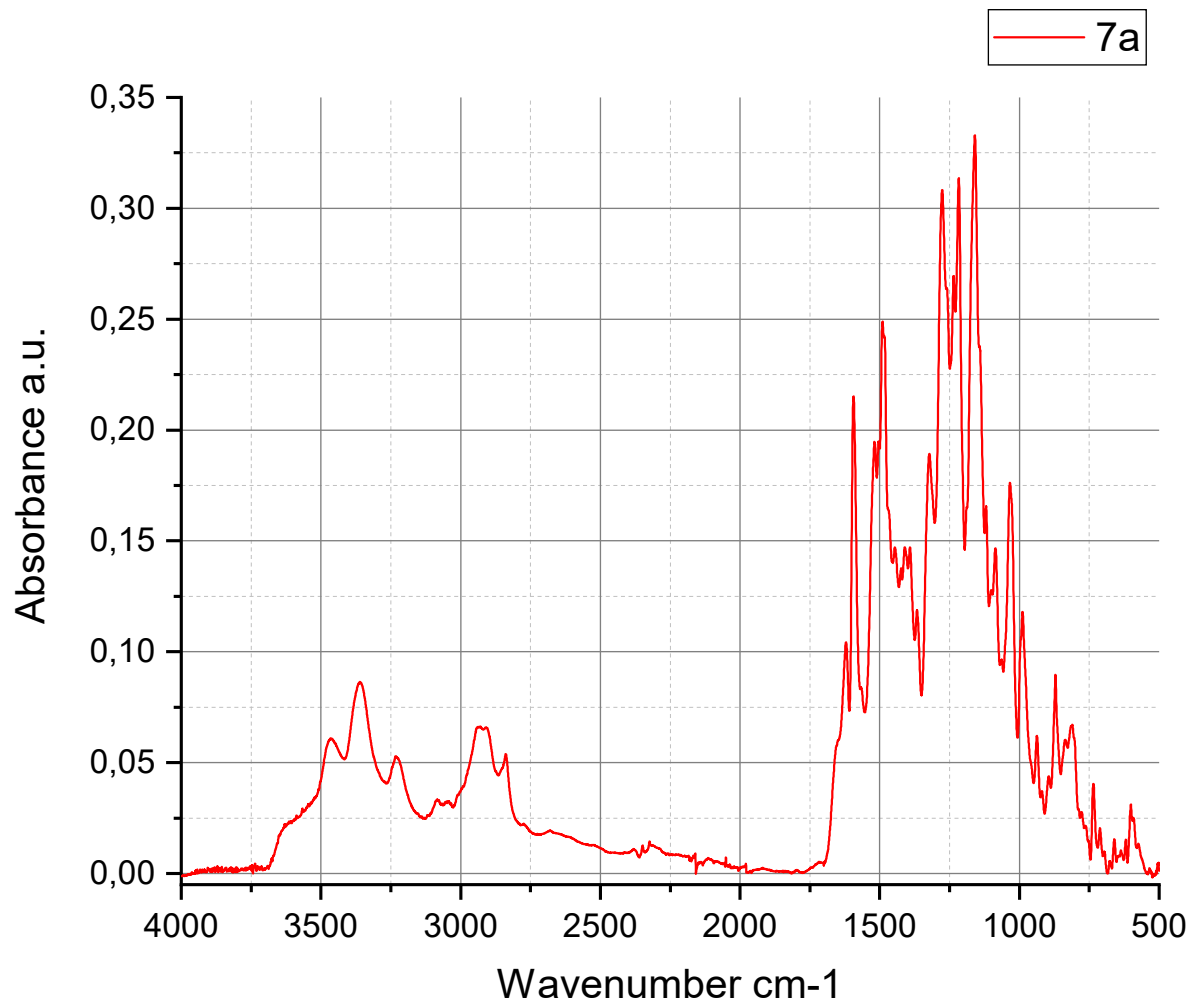


Display Report

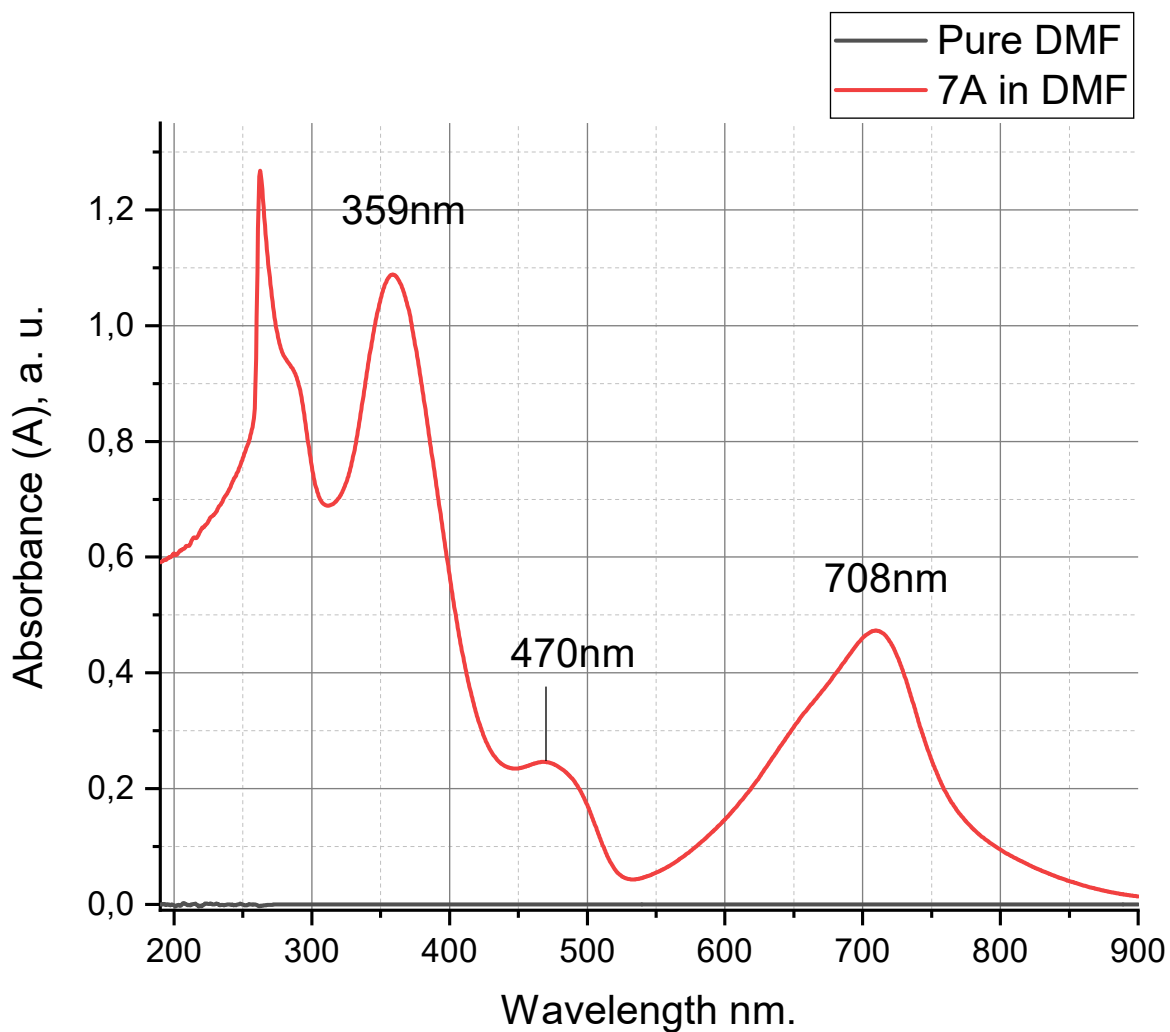
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule	
656.1757	1	C35H30NO12	656.1763	0.9	2.4	1	100.00	21.5	even	ok
	1	C34H27N5NaO8	656.1752	-0.7	2.9	1	100.00	23.5	even	ok
	1	C48H27KN	656.1775	2.8	79.7	1	100.00	35.5	even	ok

+MS, 0.1-0.1min #3-5

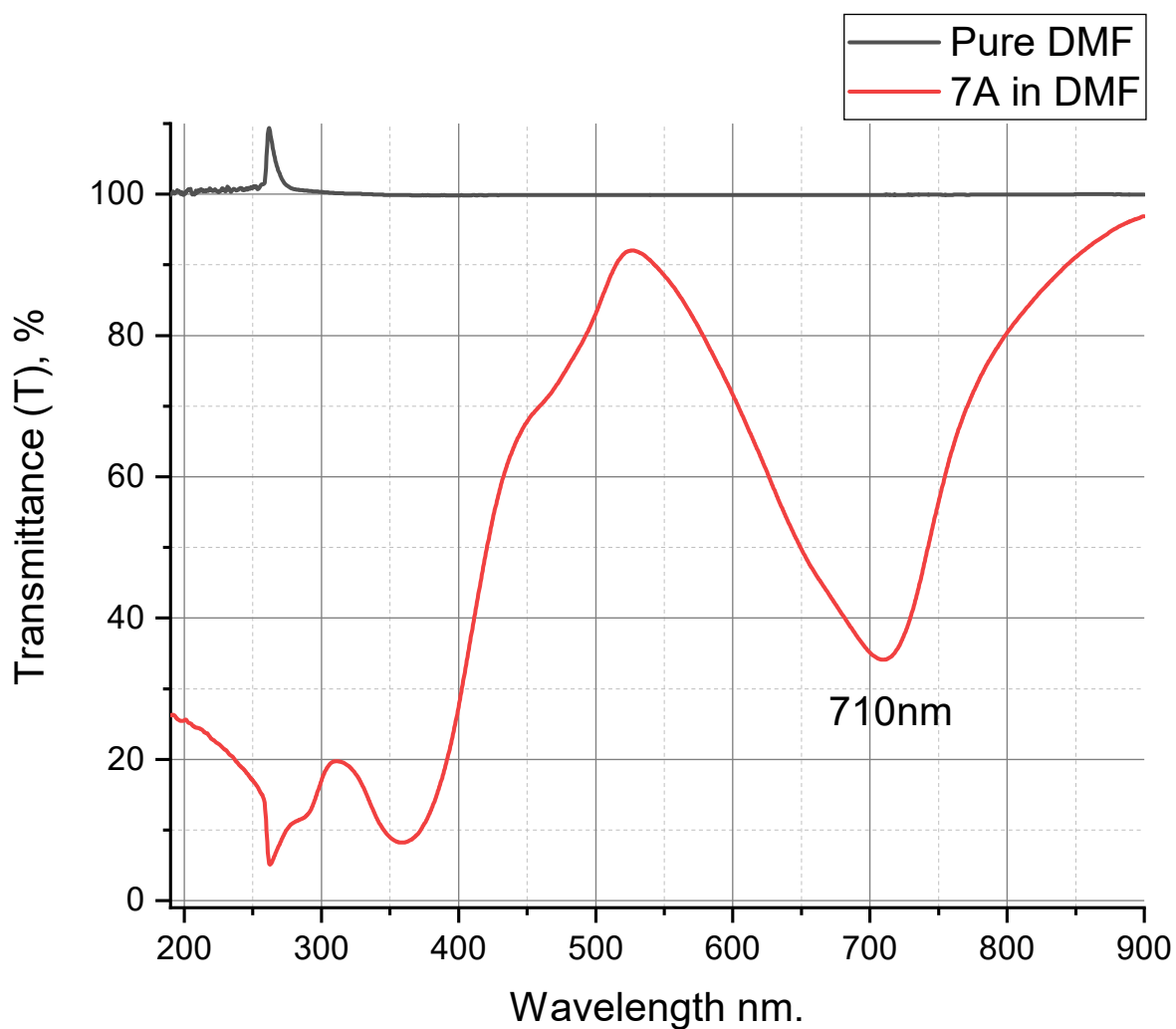
ATR spectrum of 1-(4-aminophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**7a**).



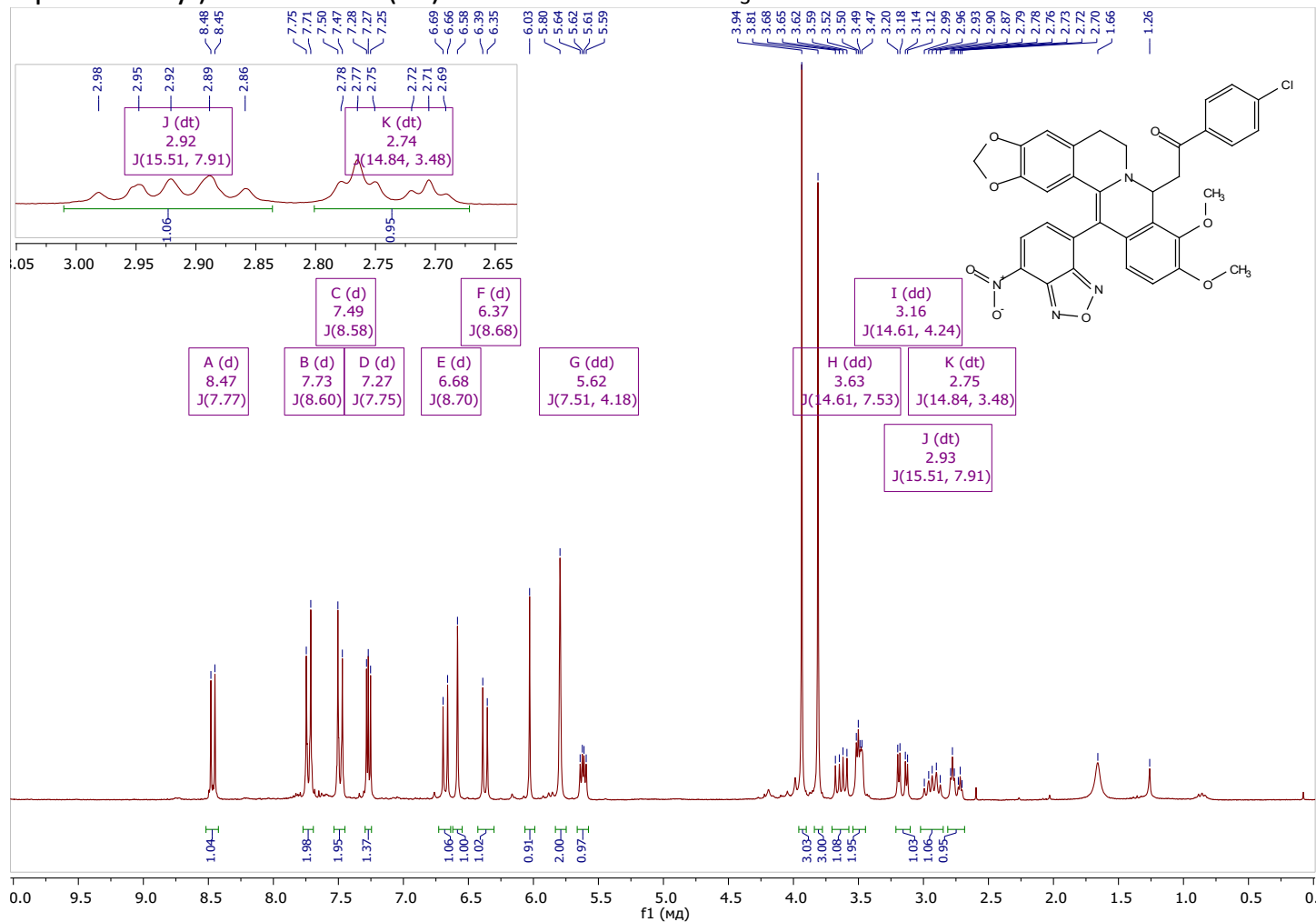
UV-Vis spectrum of 1-(4-aminophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (7a) dissolved in DMF (Absorbance (A), a. u.), at a concentration of $1 \cdot 10^{-4}$ mol/L.



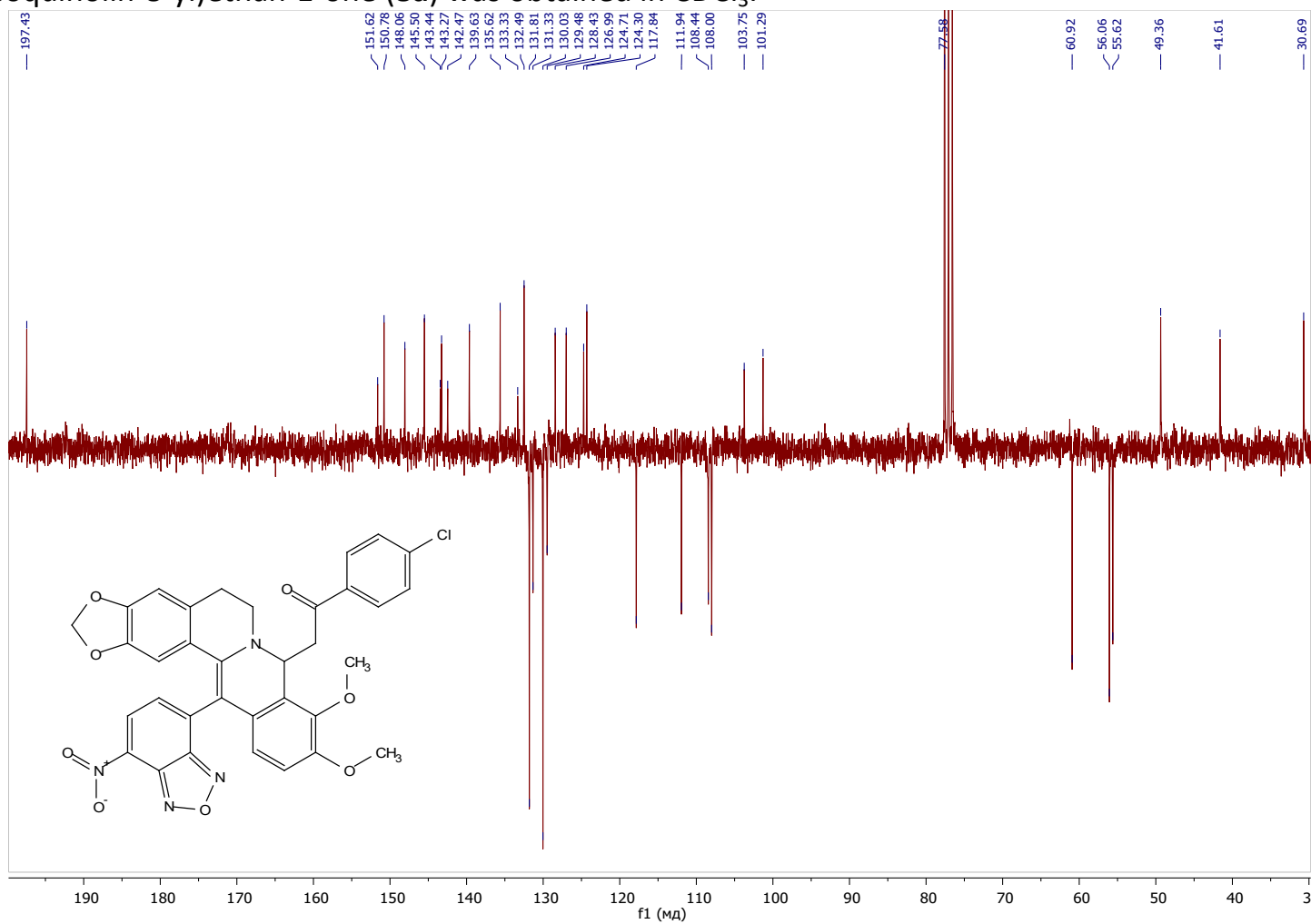
UV-Vis spectrum of 1-(4-aminophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (7a) dissolved in DMF (Transmittance (T), %), at a concentration of 1×10^{-4} mol/L.



^1H NMR spectrum of 1-(4-chlorophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**8a**) was obtained in CDCl_3



^{13}C NMR spectrum of 1-(4-chlorophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**8a**) was obtained in CDCl_3 .



The high-resolution mass spectrum (HRMS) of 1-(4-chlorophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**8a**).

Display Report

Analysis Info

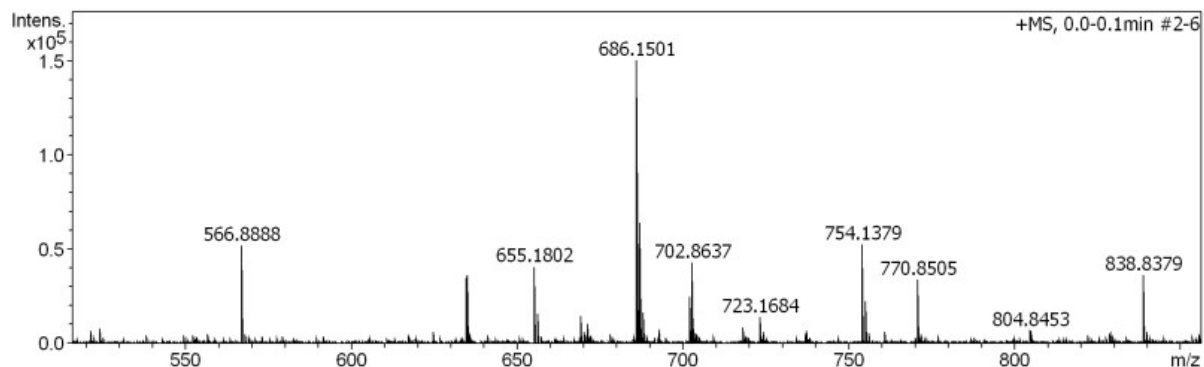
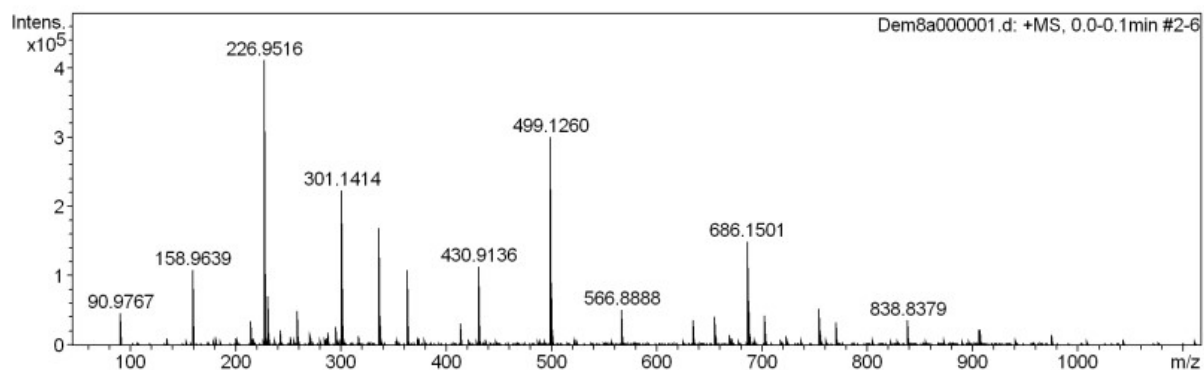
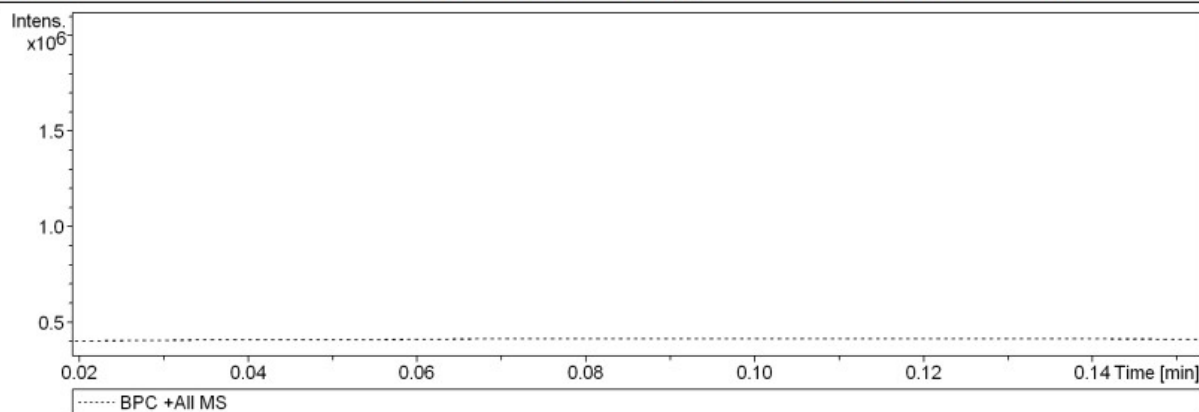
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 Method Tune_pos_Standard23.m
 Sample Name 1
 Comment

Acquisition Date 7/18/2023 1:00:00 PM

Operator Demidov
 Instrument maXis impact 282001.00109

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source

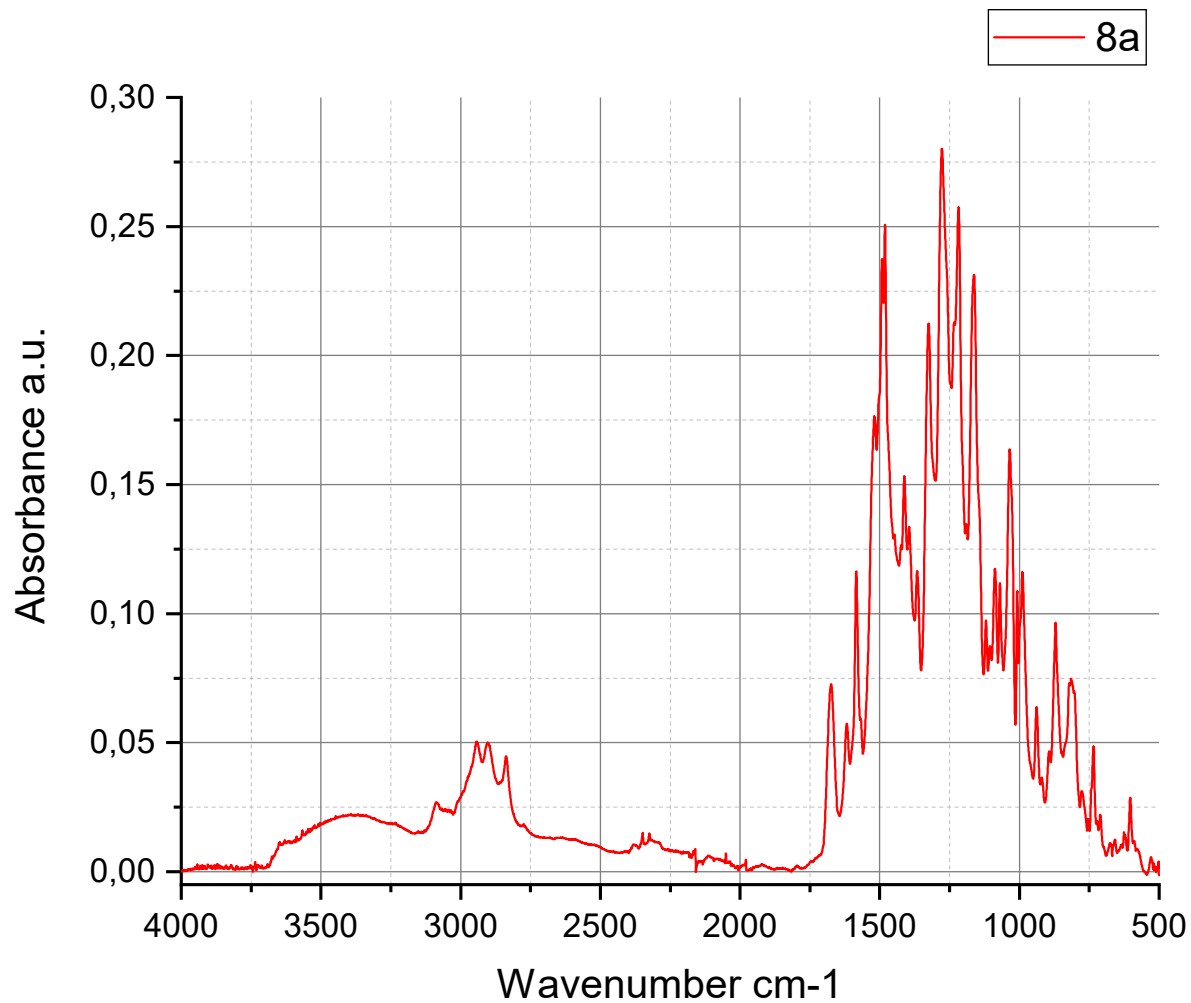


Display Report

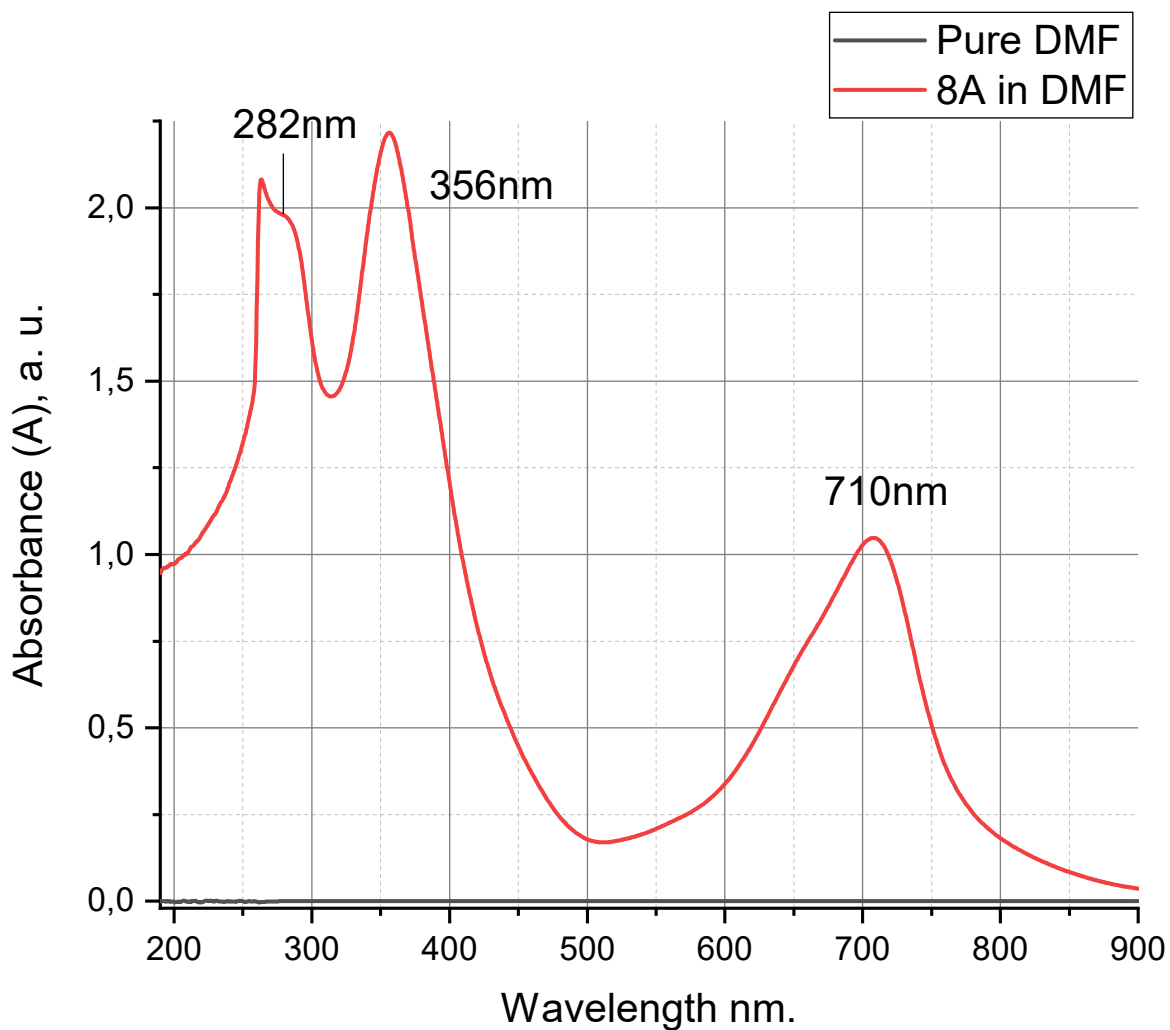
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	1	C34H25N5NaO10	686.1494	-1.1	18.9	1 100.00	24.5	even	ok
	1	C48H25KNO2	686.1517	2.3	66.1	1 100.00	36.5	even	ok

+MS, 0.0-0.1min #2-6

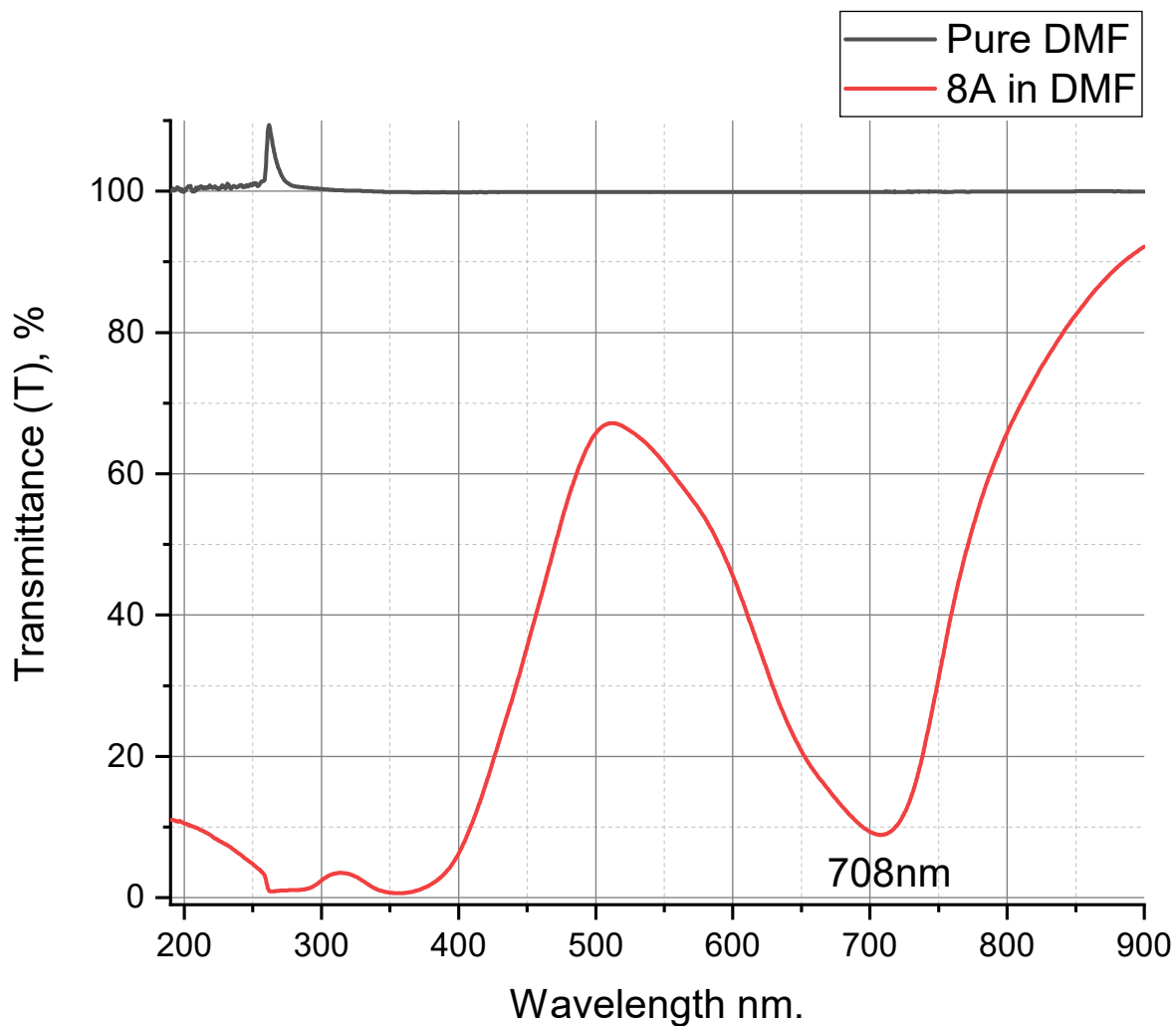
ATR spectrum of 1-(4-chlorophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**8a**).



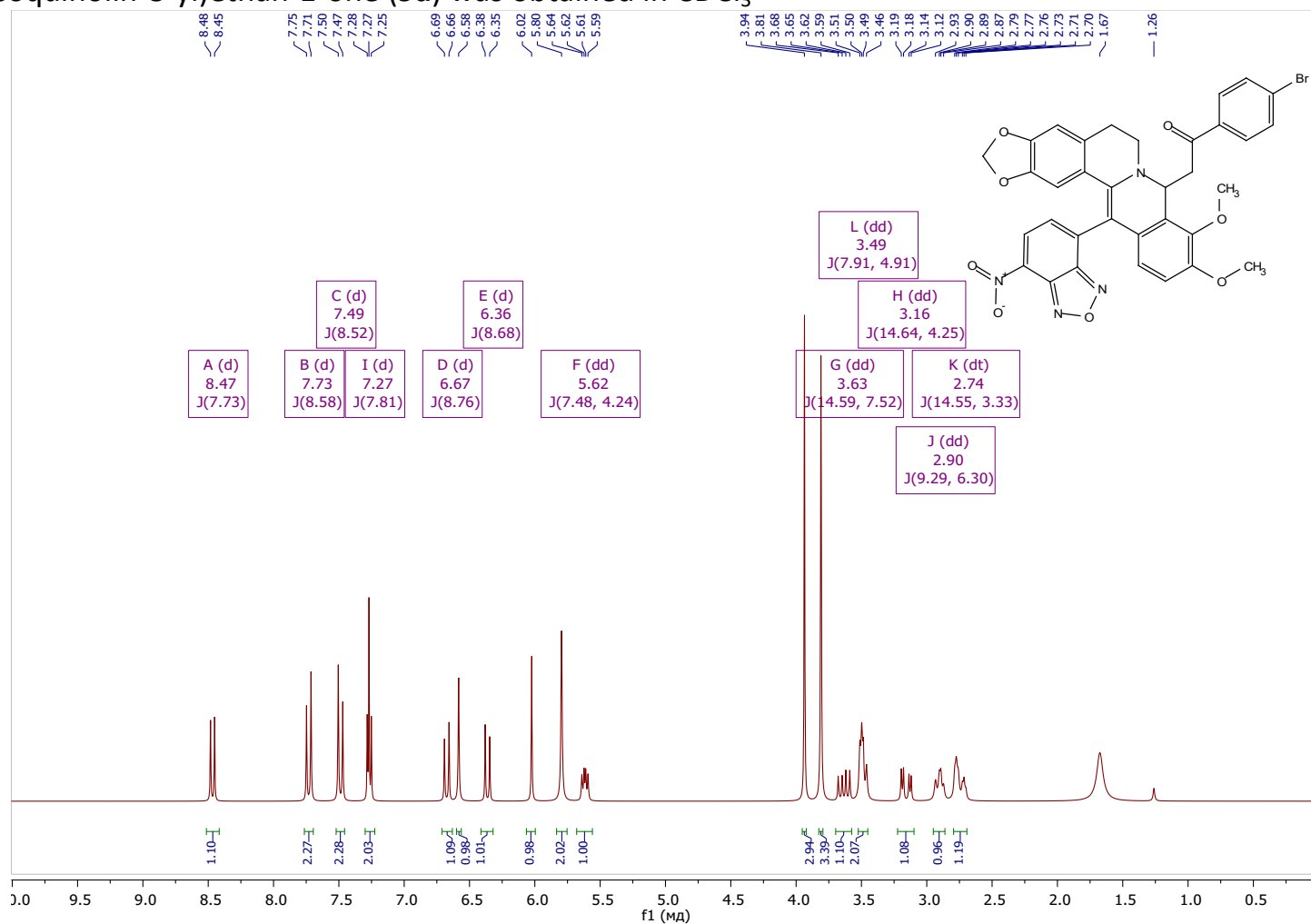
UV-Vis spectrum of 1-(4-chlorophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl) ethan-1-one (8a) dissolved in DMF (Absorbance (A), a. u.), at a concentration of $1 \cdot 10^{-4}$ mol/L.



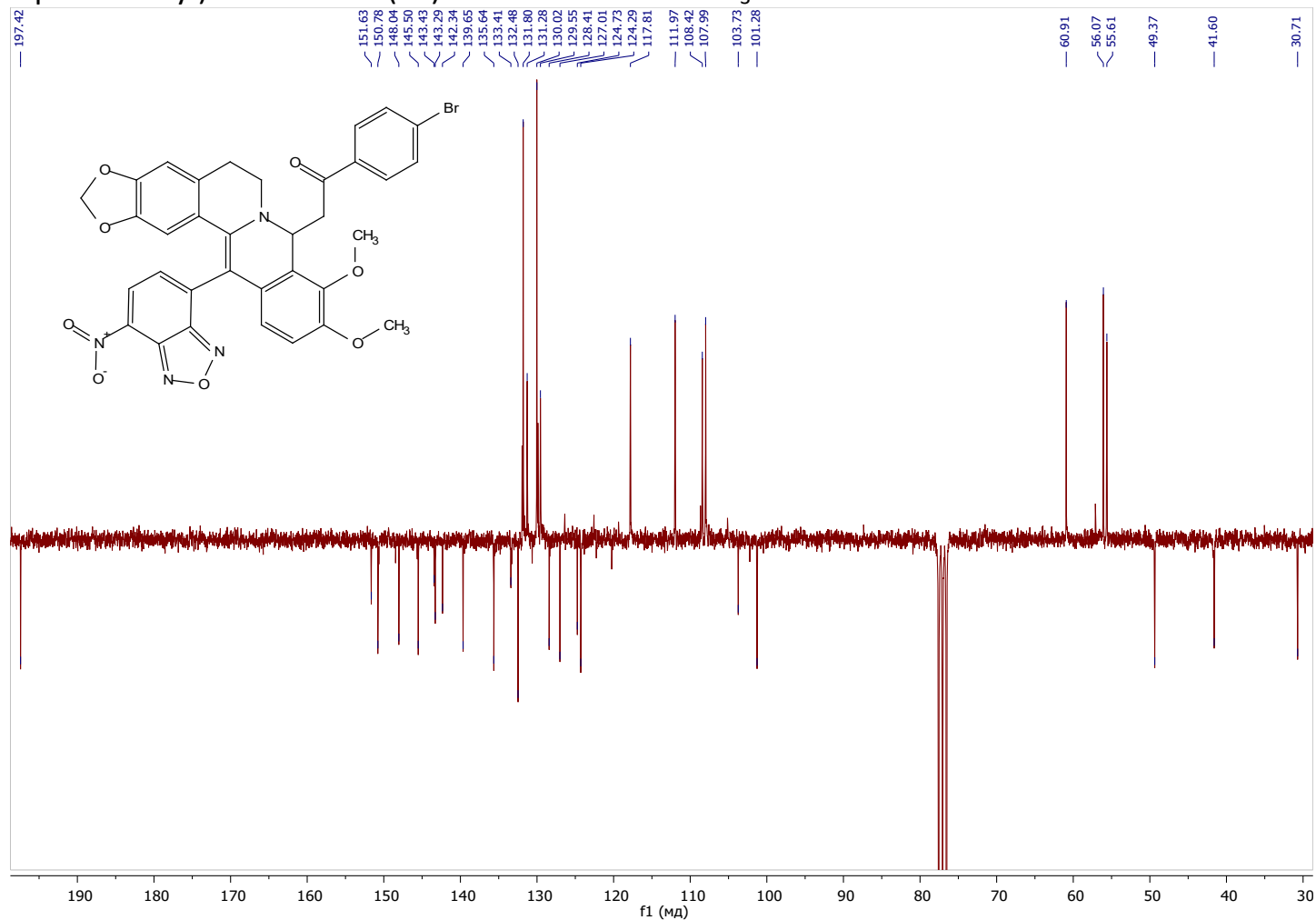
UV-Vis spectrum of 1-(4-chlorophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (8a) dissolved in DMF (Transmittance (T), %), at a concentration of 1×10^{-4} mol/L.



^1H NMR spectrum of 1-(4-bromophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**9a**) was obtained in CDCl_3



^{13}C NMR spectrum of 1-(4-bromophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**9a**) was obtained in CDCl_3 .



The high-resolution mass spectrum (HRMS) of 1-(4-bromophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (**9a**).

Display Report

Analysis Info

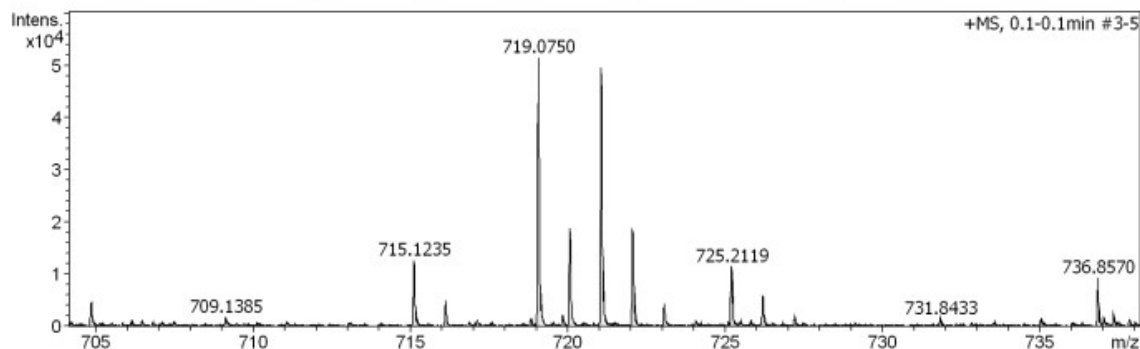
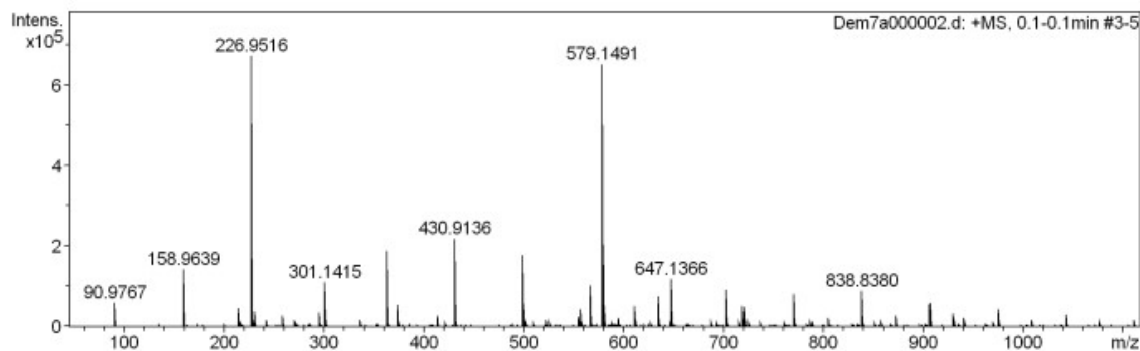
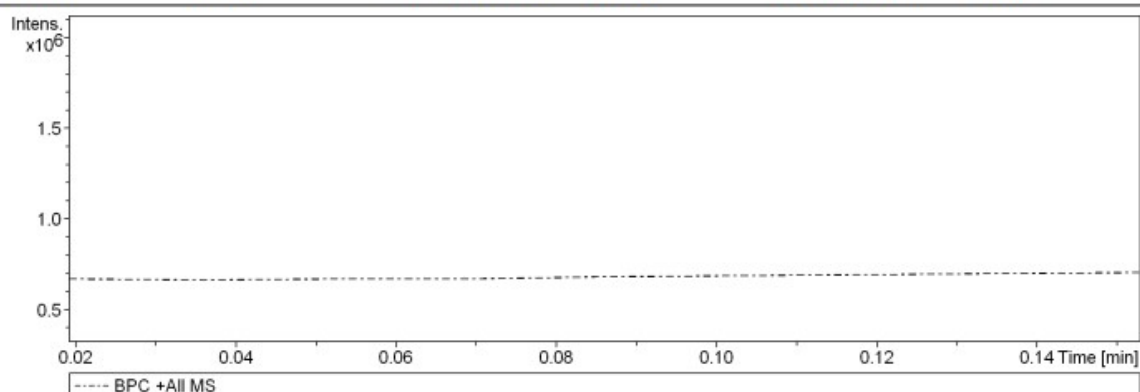
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 Sample Name 1
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Acquisition Date 7/18/2023 1:25:35 PM

Operator Demidov
 Instrument maXis impact 282001.00109

Acquisition Parameter

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Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source

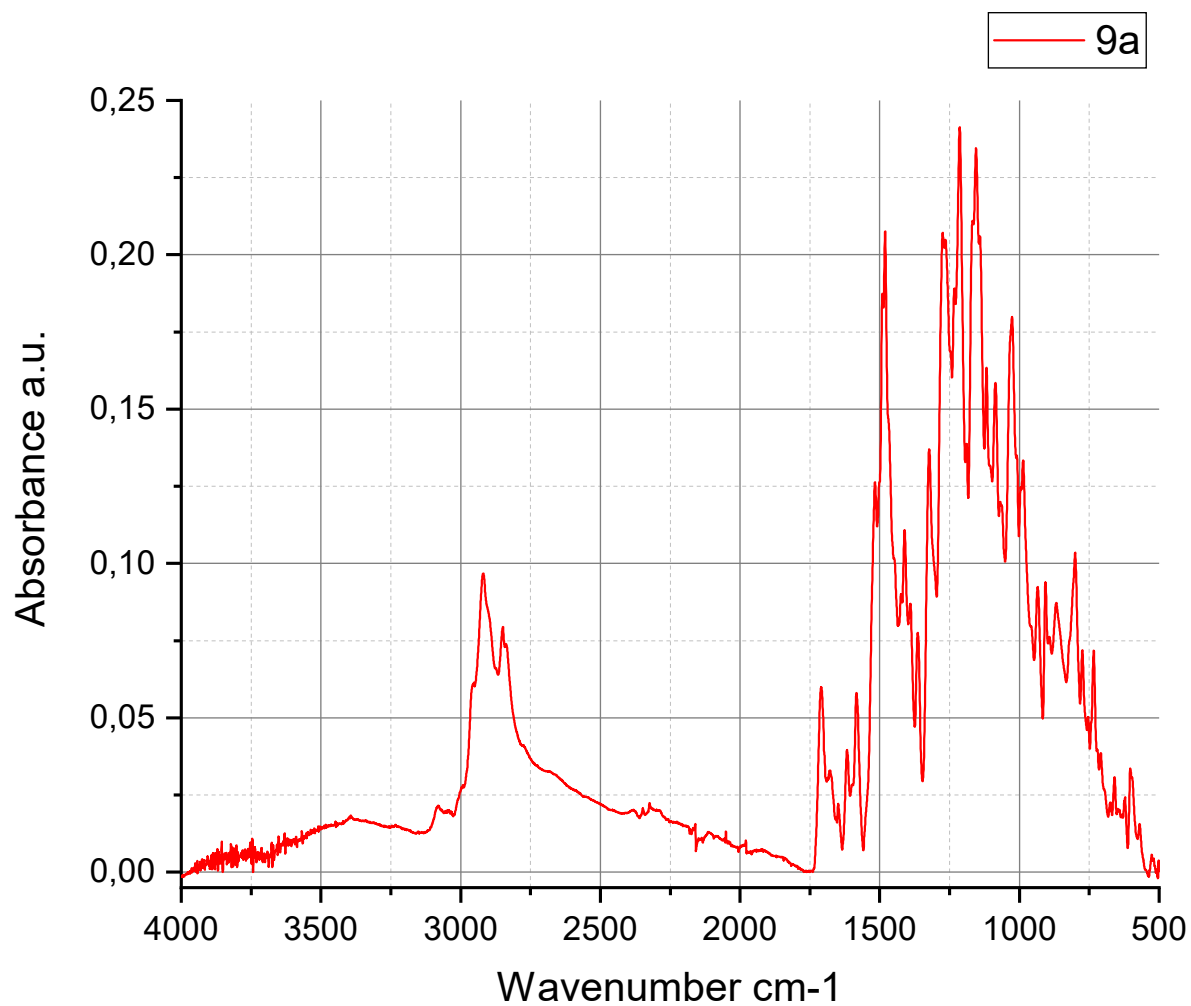


Display Report

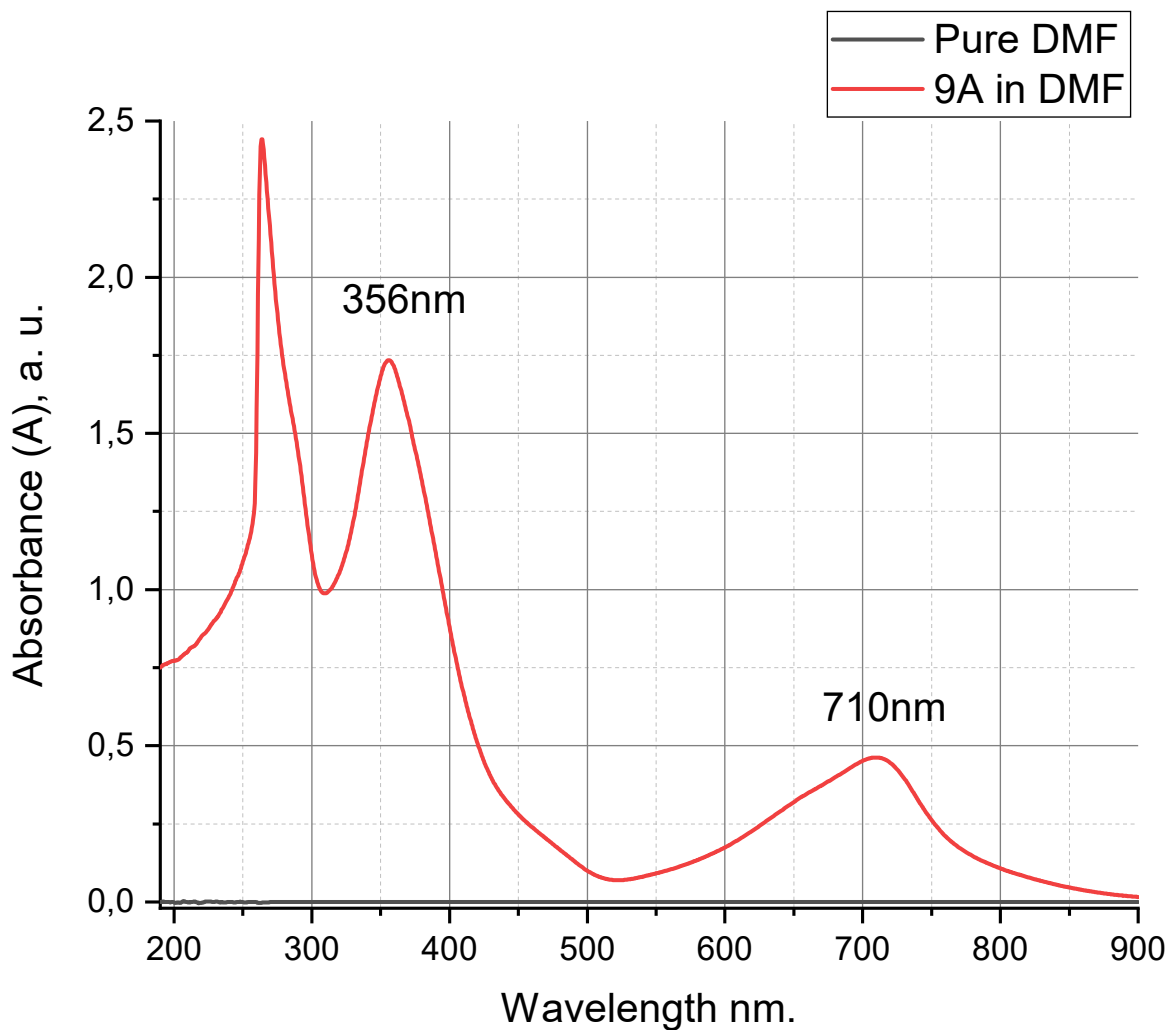
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	1	C34H25BrN4NaO8	719.0748	-0.3	29.7	1	100.00	23.5	even	ok
720.0783	1	C40H28BrKNO5	720.0782	-0.1	406.5	1	100.00	26.5	even	ok
721.0735	1	C43H31Br2O	721.0736	0.1	457.6	4	0.00	27.5	even	ok
	2	C30H44Br3O5	721.0733	-0.3	543.3	5	0.00	7.5	even	ok
	3	C27H31Br2N8O6	721.0728	-1.0	436.8	2	0.06	15.5	even	ok
	4	C31H40Br3N4O	721.0747	1.6	545.8	6	0.00	12.5	even	ok
	5	C26H30BrN2O17	721.0722	-1.8	391.2	1	100.00	12.5	even	ok
	6	C31H35Br2N2O8	721.0755	2.7	440.5	3	0.02	14.5	even	ok
	1	C29H31BrNaO15	721.0739	0.4	393.4	1	100.00	13.5	even	ok
	2	C29H36Br2N2NaO8	721.0731	-0.6	437.6	3	0.05	11.5	even	ok
	3	C30H32Br2N6NaO4	721.0744	1.2	439.3	4	0.03	16.5	even	ok
	4	C29H41Br3N4NaO	721.0723	-1.7	543.7	6	0.00	9.5	even	ok
	5	C30H27BrN4NaO11	721.0752	2.3	395.6	2	32.72	18.5	even	ok
	6	C26H28Br2N12NaO2	721.0717	-2.5	465.8	5	0.00	17.5	even	ok
	1	C39H27BrKN2O5	721.0735	-0.1	382.9	3	10.28	26.5	even	ok
	2	C26H40Br2KN2O9	721.0732	-0.4	446.3	4	0.00	6.5	even	ok
	3	C26H35BrKO16	721.0740	0.7	366.7	1	100.00	8.5	even	ok
4	C27H36Br2KN6O5	721.0746	1.4	447.8	5	0.00	11.5	even	ok	
5	C26H45Br3KN4O2	721.0724	-1.5	511.6	6	0.00	4.5	even	ok	
6	C27H31BrKN4O12	721.0753	2.5	368.2	2	36.21	13.5	even	ok	
1	C27H31Br2N8O6	721.0728	-1.0	436.8	1	100.00	15.5	even	ok	
2	C31H40Br3N4O	721.0747	1.6	545.8	3	0.00	12.5	even	ok	
3	C31H35Br2N2O8	721.0755	2.7	440.5	2	24.48	14.5	even	ok	

+MS, 0.1-0.1min #3-5

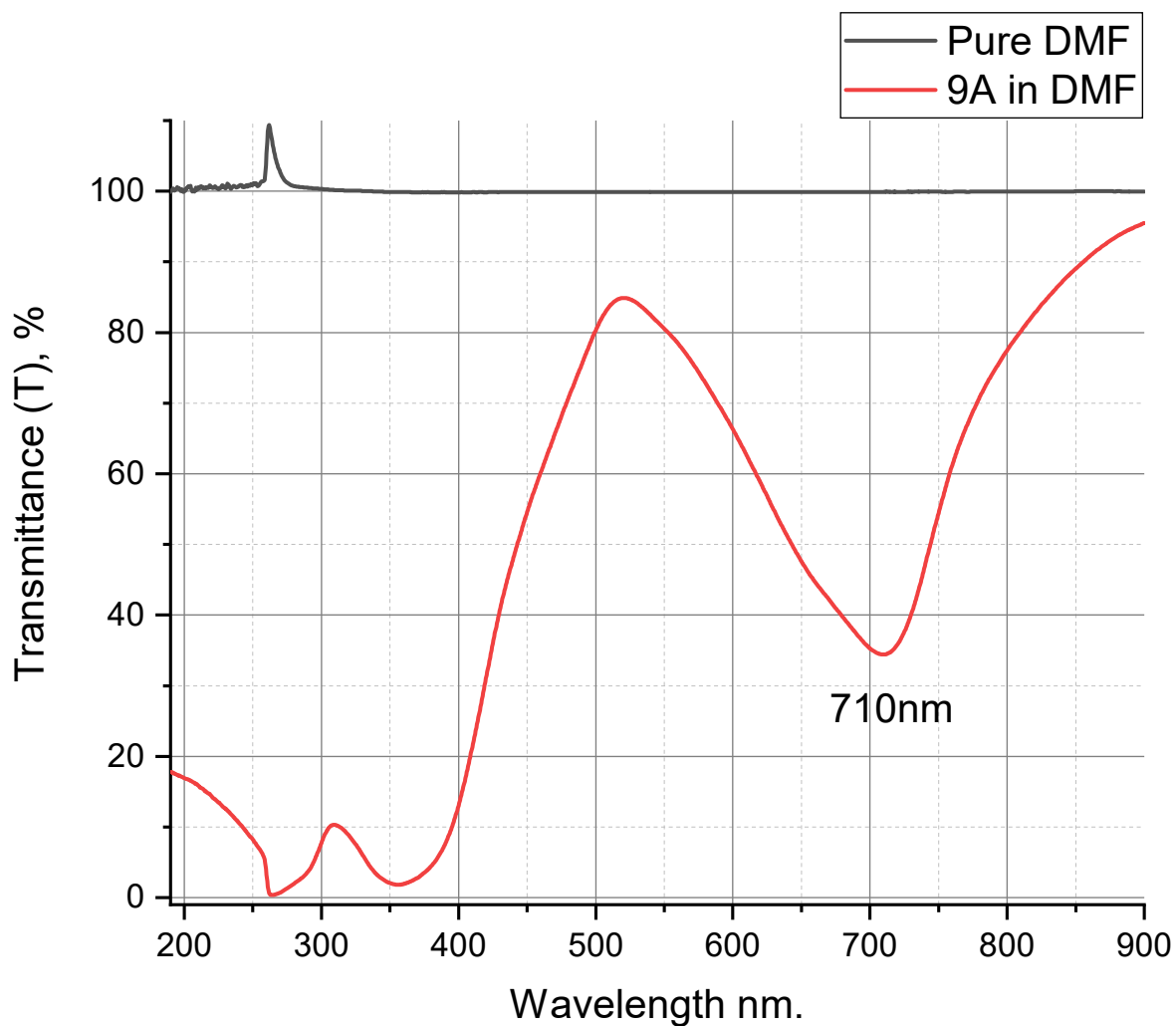
ATR spectrum of 1-(4-bromophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (9a).



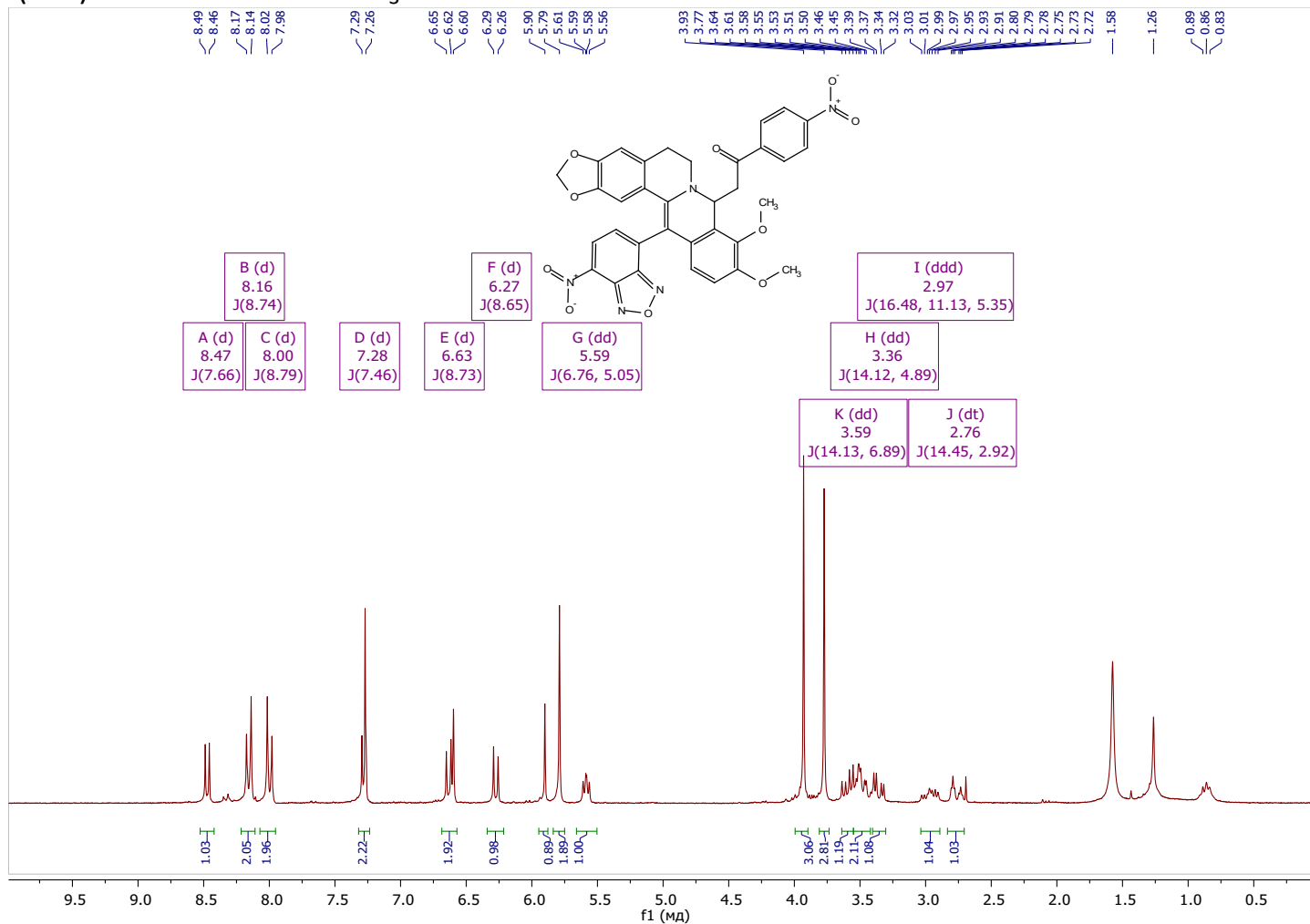
UV-Vis spectrum of 1-(4-bromophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (9a) dissolved in DMF (Absorbance (A), a. u.), at a concentration of $1 \cdot 10^{-4}$ mol/L.



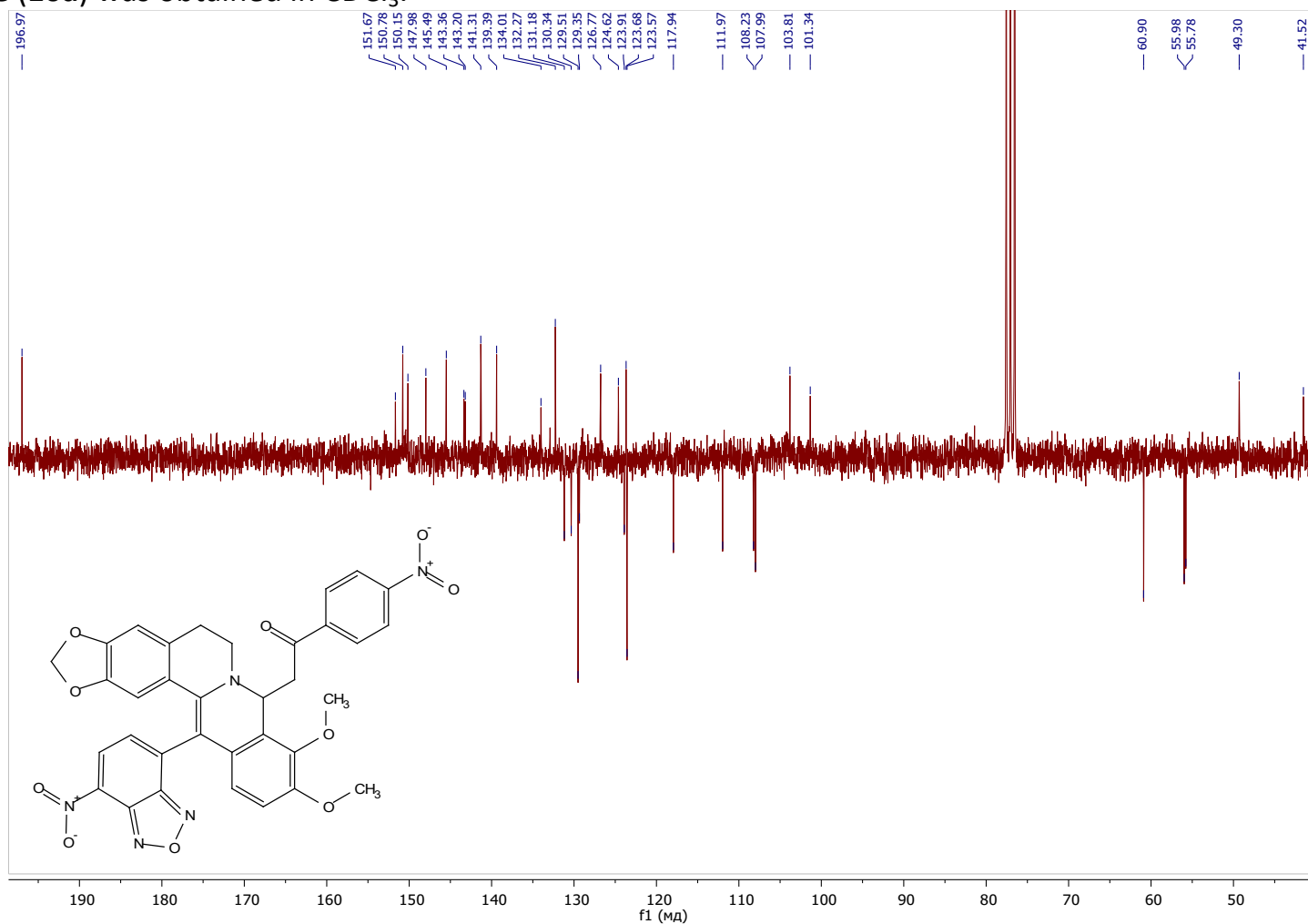
UV-Vis spectrum of 1-(4-bromophenyl)-2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)ethan-1-one (9a) dissolved in DMF (Transmittance (T), %), at a concentration of 1×10^{-4} mol/L.



^1H NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[*c*][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-*g*]isoquinolino[3,2-*a*]isoquinolin-8-yl)-1-(4-nitrophenyl)ethan-1-one (**10a**) was obtained in CDCl_3



^{13}C NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[*c*][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-*g*]isoquinolino[3,2-*a*]isoquinolin-8-yl)-1-(4-nitrophenyl)ethan-1-one (**10a**) was obtained in CDCl_3 .



The high-resolution mass spectrum (HRMS) of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-nitrophenyl)ethan-1-one (**10a**).

Display Report

Analysis Info

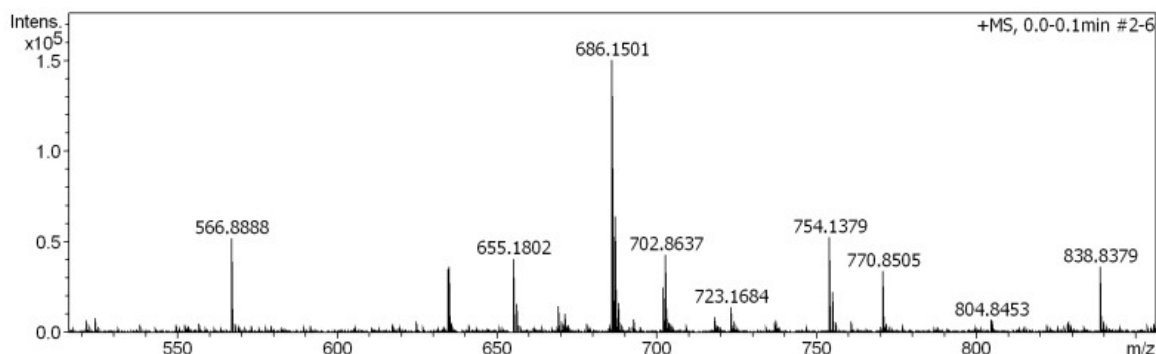
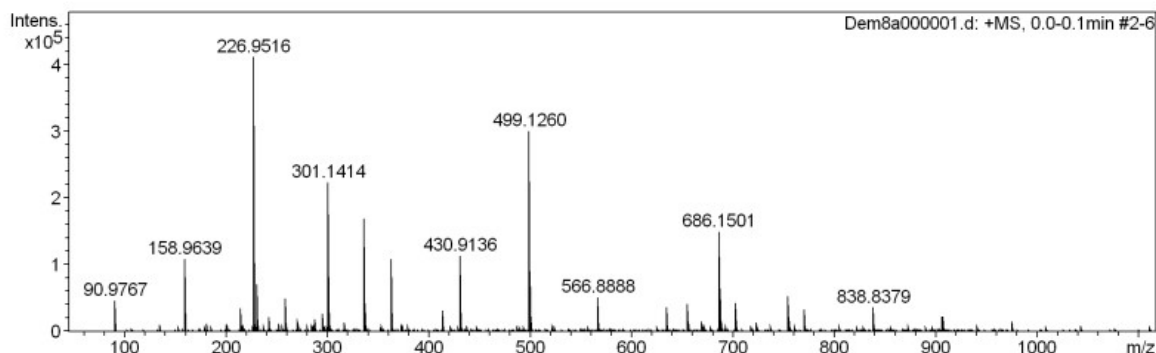
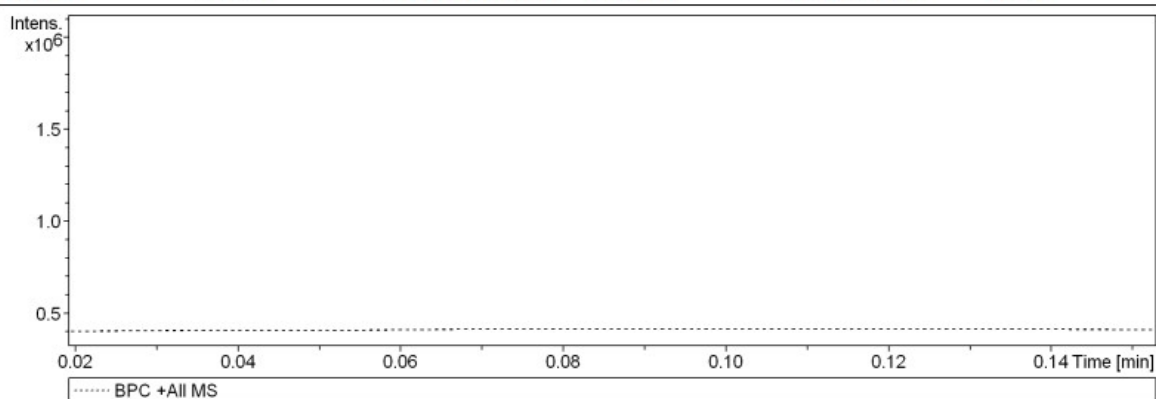
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Acquisition Date 7/18/2023 1:00:00 PM

Operator Demidov
 Instrument maXis impact 282001.00109

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source

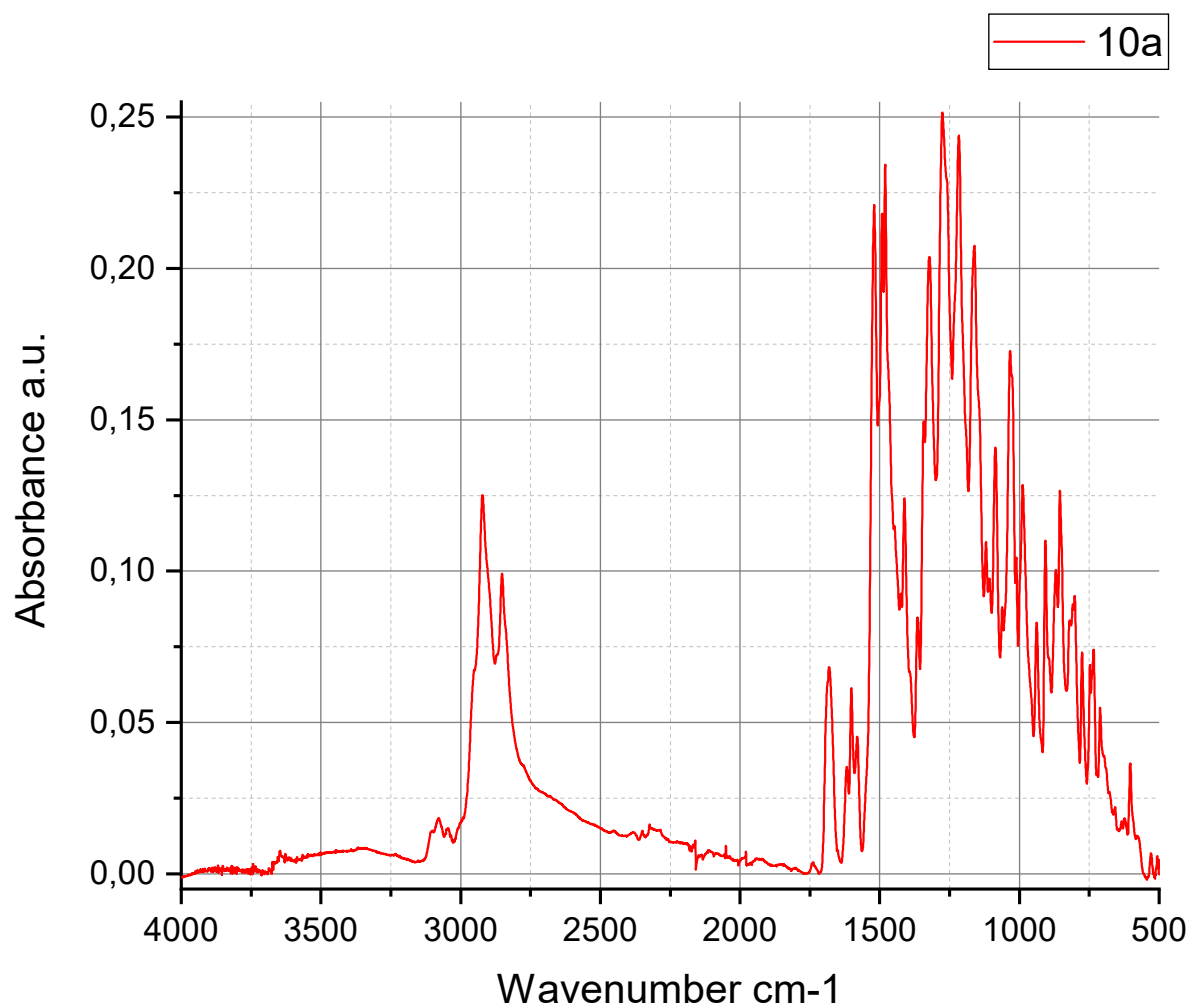


Display Report

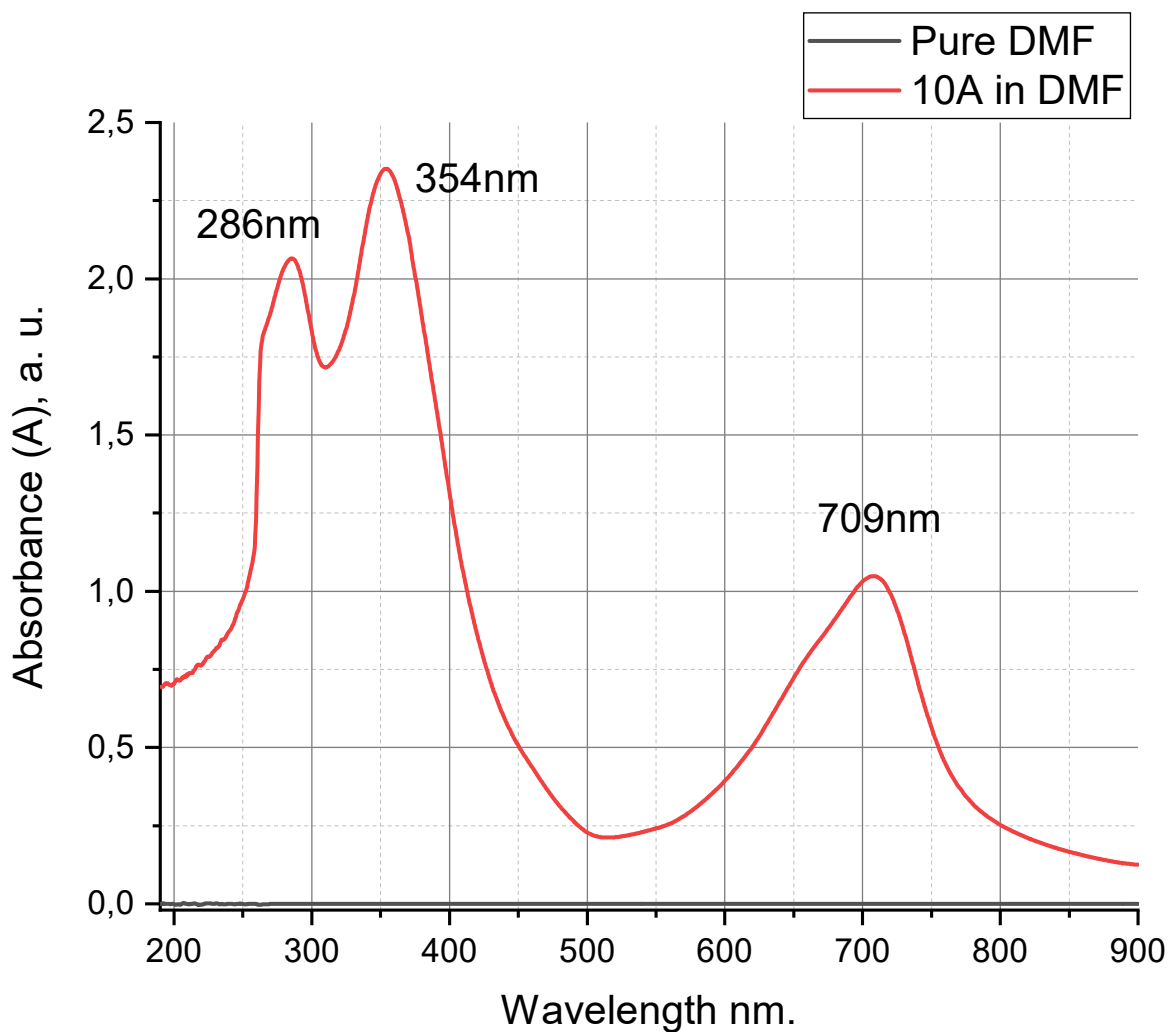
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	1	C34H25N5NaO10	686.1494	-1.1	18.9	1	100.00	24.5	even	ok
	1	C48H25KNO2	686.1517	2.3	66.1	1	100.00	36.5	even	ok

+MS, 0.0-0.1min #2-6

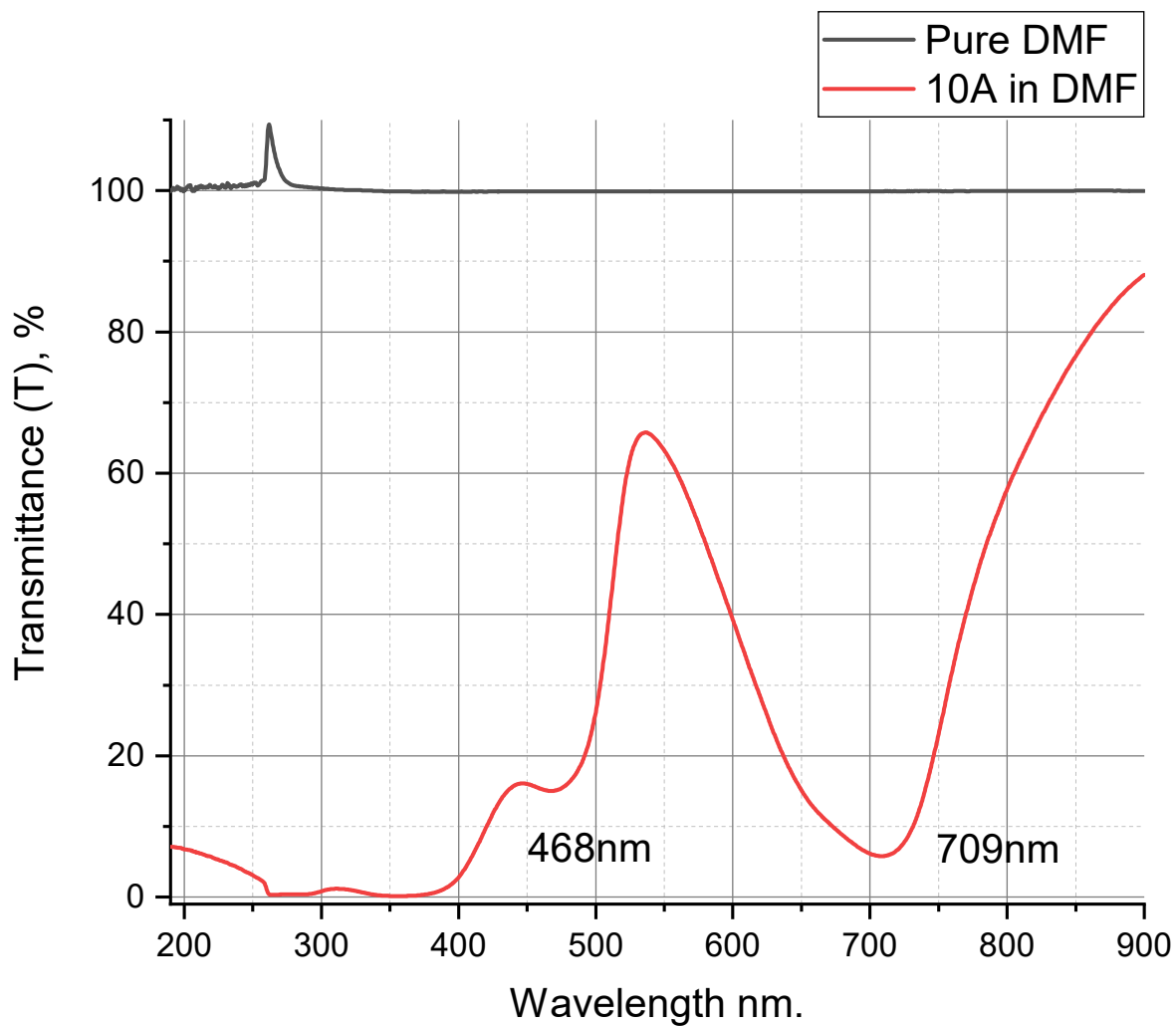
ATR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-nitrophenyl)ethan-1-one (**10a**).



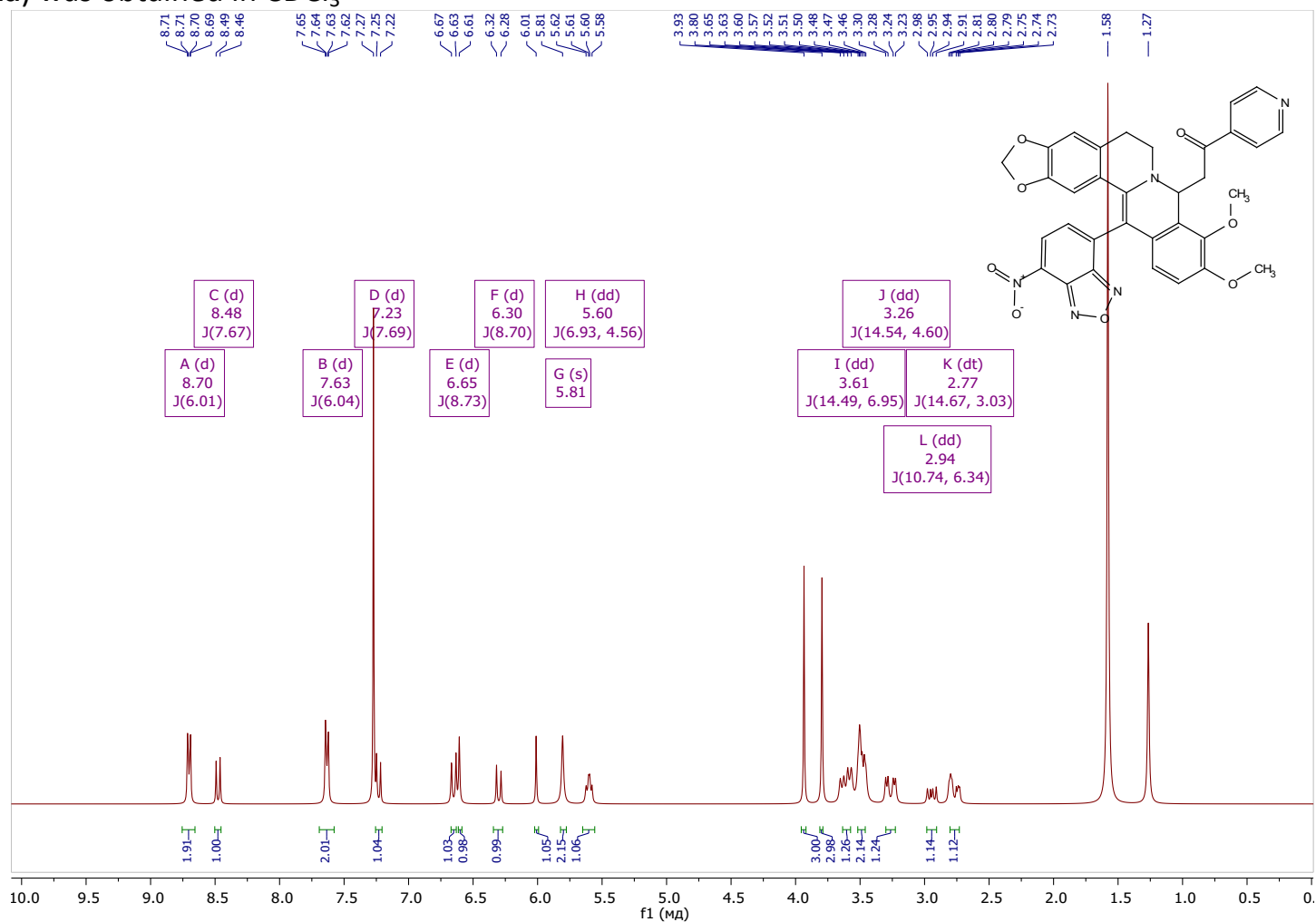
UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-nitrophenyl)ethan-1-one (10a) dissolved in DMF (Absorbance (A), a. u.), at a concentration of $1 \cdot 10^{-4}$ mol/L.



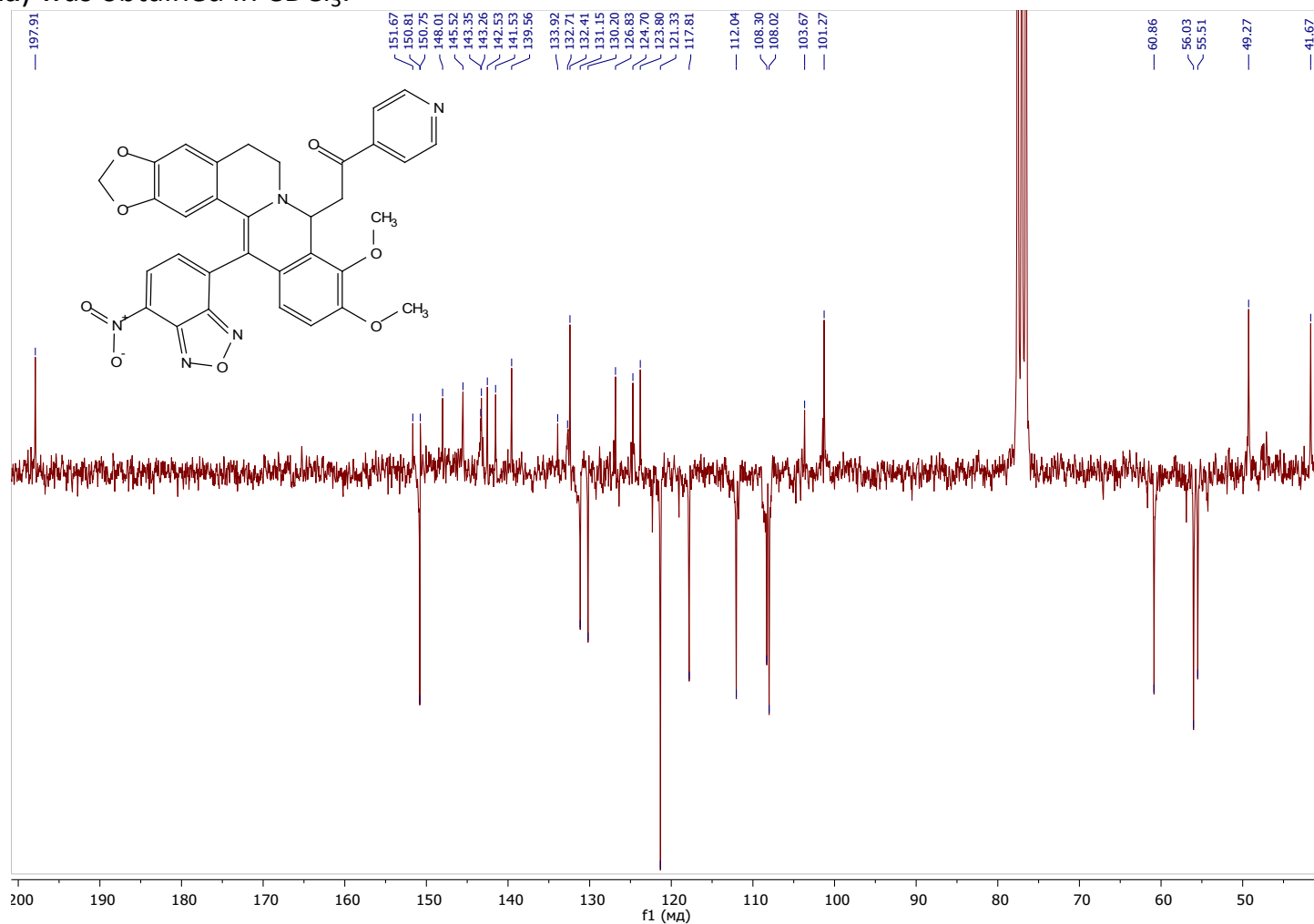
UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(4-nitrophenyl)ethan-1-one (10a) dissolved in DMF (Transmittance (T), %), at a concentration of 1×10^{-4} mol/L.



^1H NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(pyridin-4-yl)ethan-1-one (**11a**) was obtained in CDCl_3



^{13}C NMR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(pyridin-4-yl)ethan-1-one (**11a**) was obtained in CDCl_3 .



The high-resolution mass spectrum (HRMS) of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(pyridin-4-yl)ethan-1-one (**11a**).

Display Report

Analysis Info

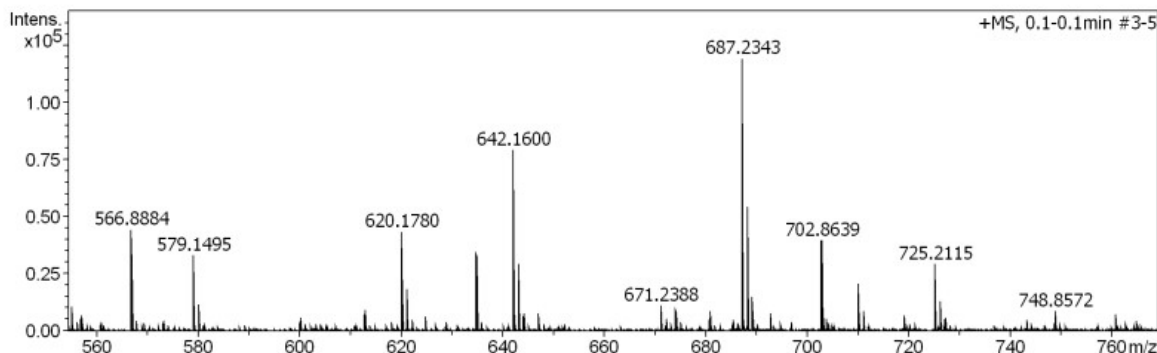
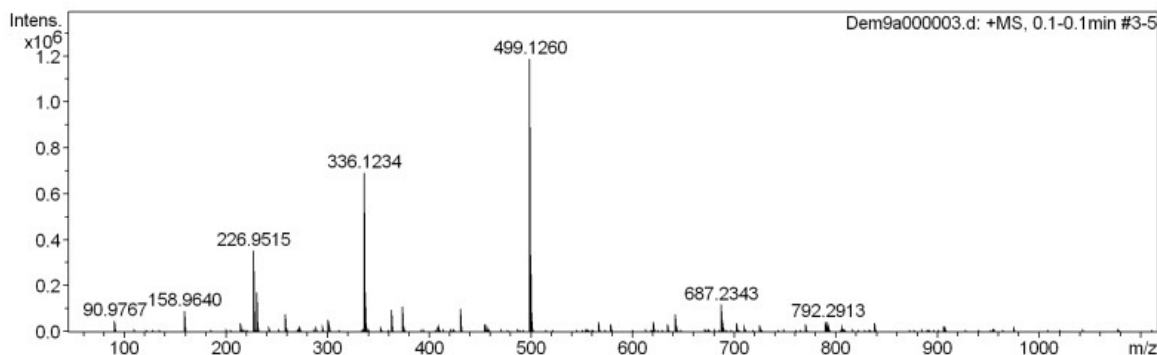
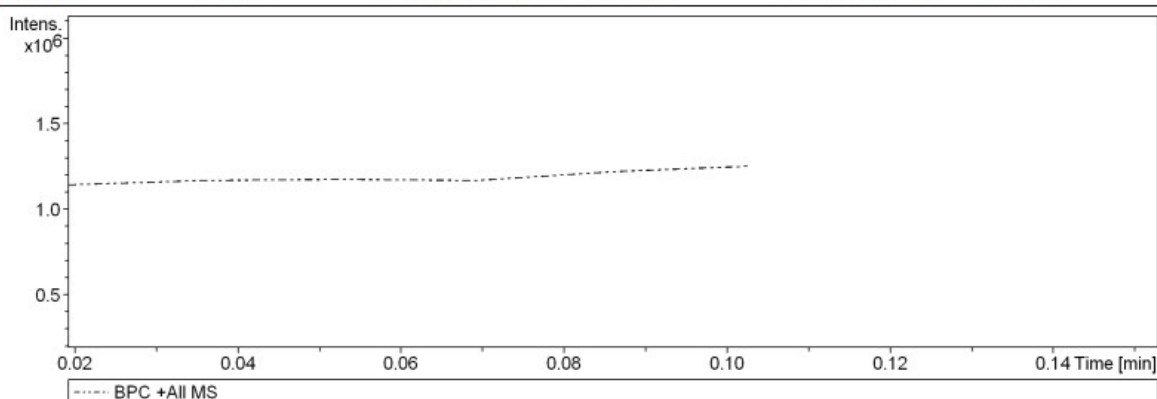
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 Sample Name 1
 Comment

Acquisition Date 7/18/2023 1:53:44 PM

Operator Demidov
 Instrument maXis impact 282001.00109

Acquisition Parameter

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Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source

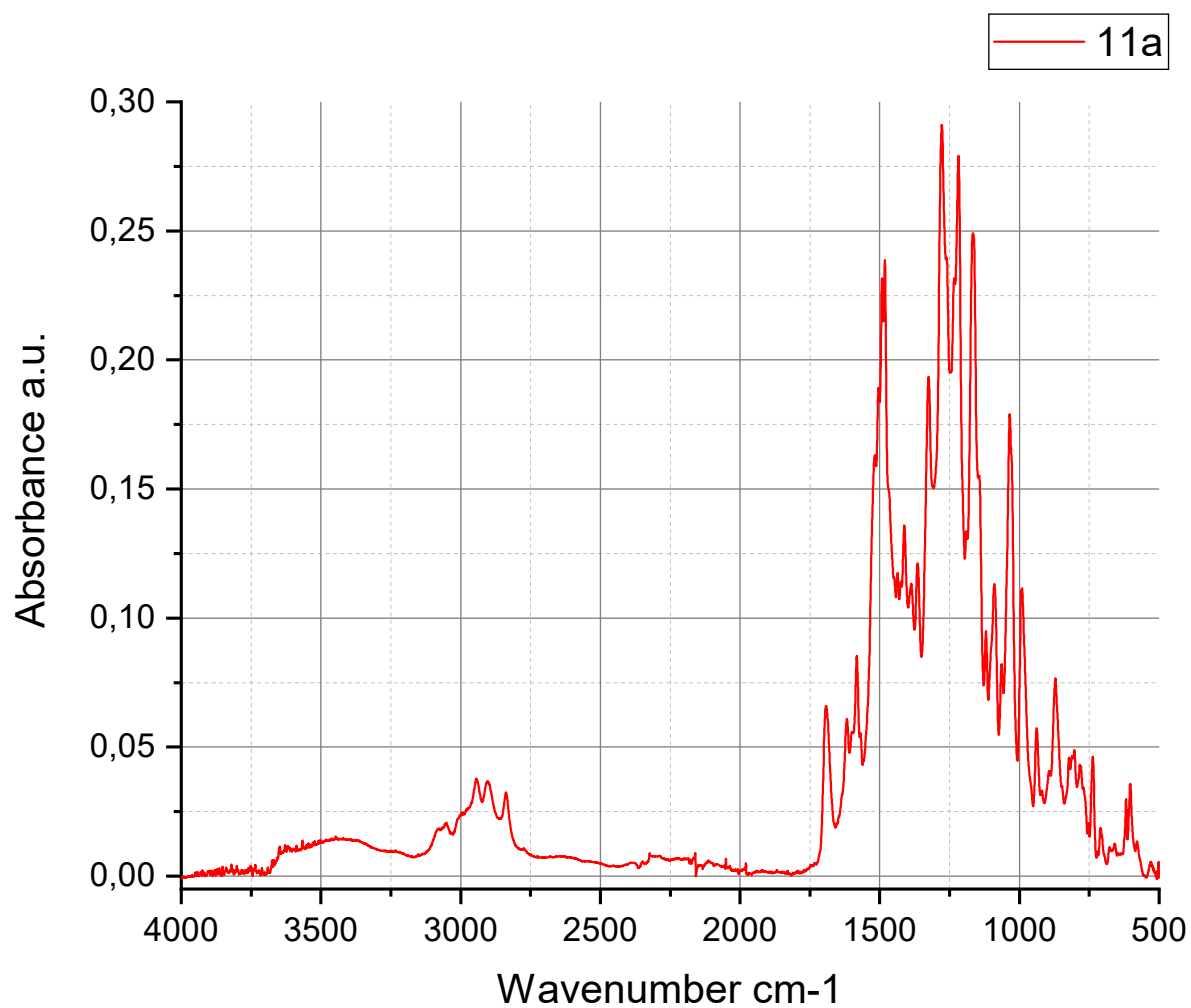


Display Report

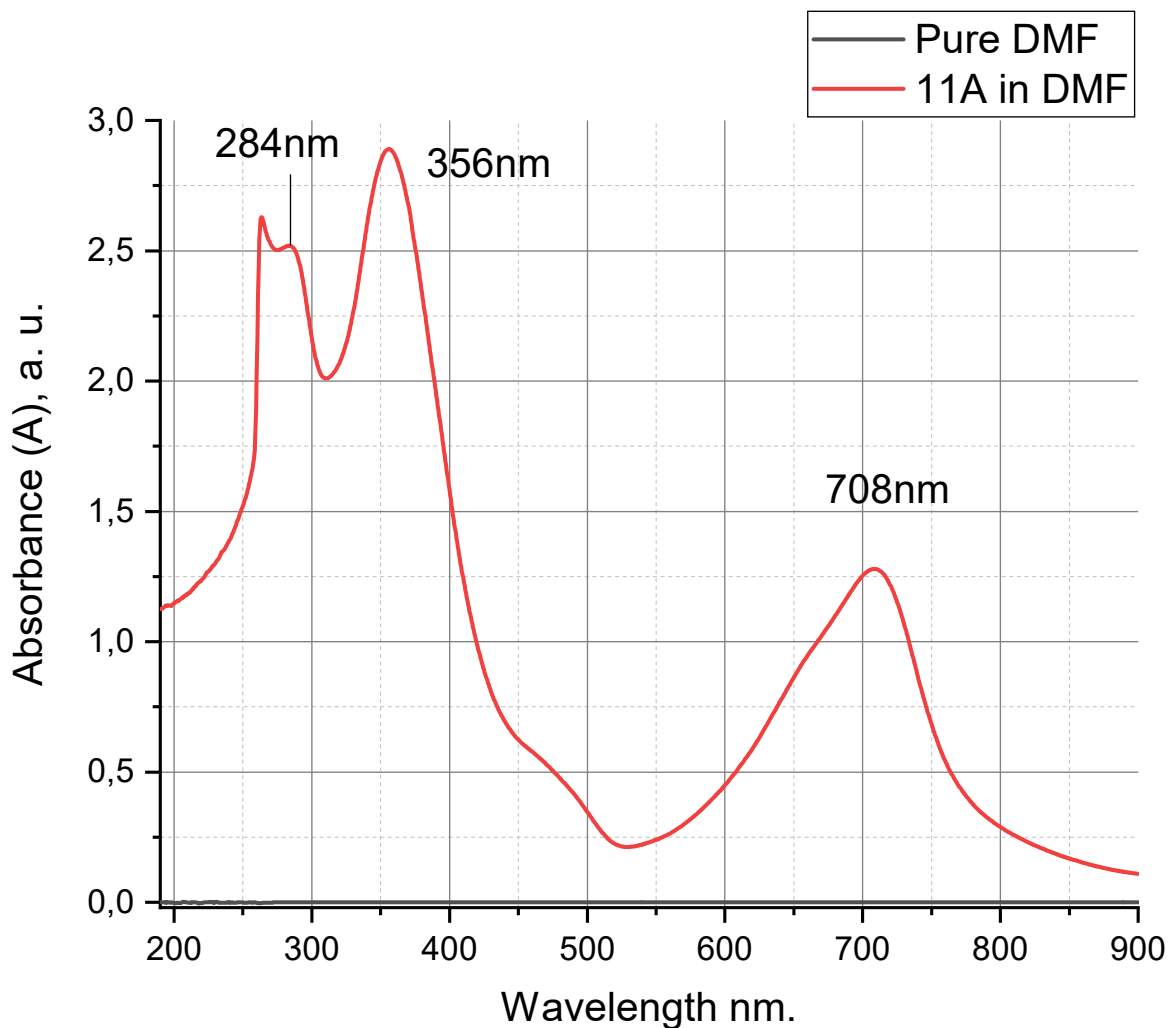
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	1	C33H25N5NaO8	642.1595	-0.8	8.6	1	100.00	23.5	even	ok
	2	C34H21N9NaO4	642.1609	1.3	18.1	2	69.38	28.5	even	ok

+MS, 0.1-0.1min #3-5

ATR spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(pyridin-4-yl)ethan-1-one (**11a**).



UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(pyridin-4-yl)ethan-1-one (11a) dissolved in DMF (Absorbance (A), a. u.), at a concentration of $1 \cdot 10^{-4}$ mol/L.



UV-Vis spectrum of 2-(9,10-dimethoxy-13-(7-nitrobenzo[c][1,2,5]oxadiazol-4-yl)-5,8-dihydro-6H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-8-yl)-1-(pyridin-4-yl)ethan-1-one (11a) dissolved in DMF (Transmittance (T), %), at a concentration of 1×10^{-4} mol/L.

