

Supplementary Data

Synthesis and Chemopreventive Potential of 5-FU/Genistein Hybrids on Colorectal Cancer Cells

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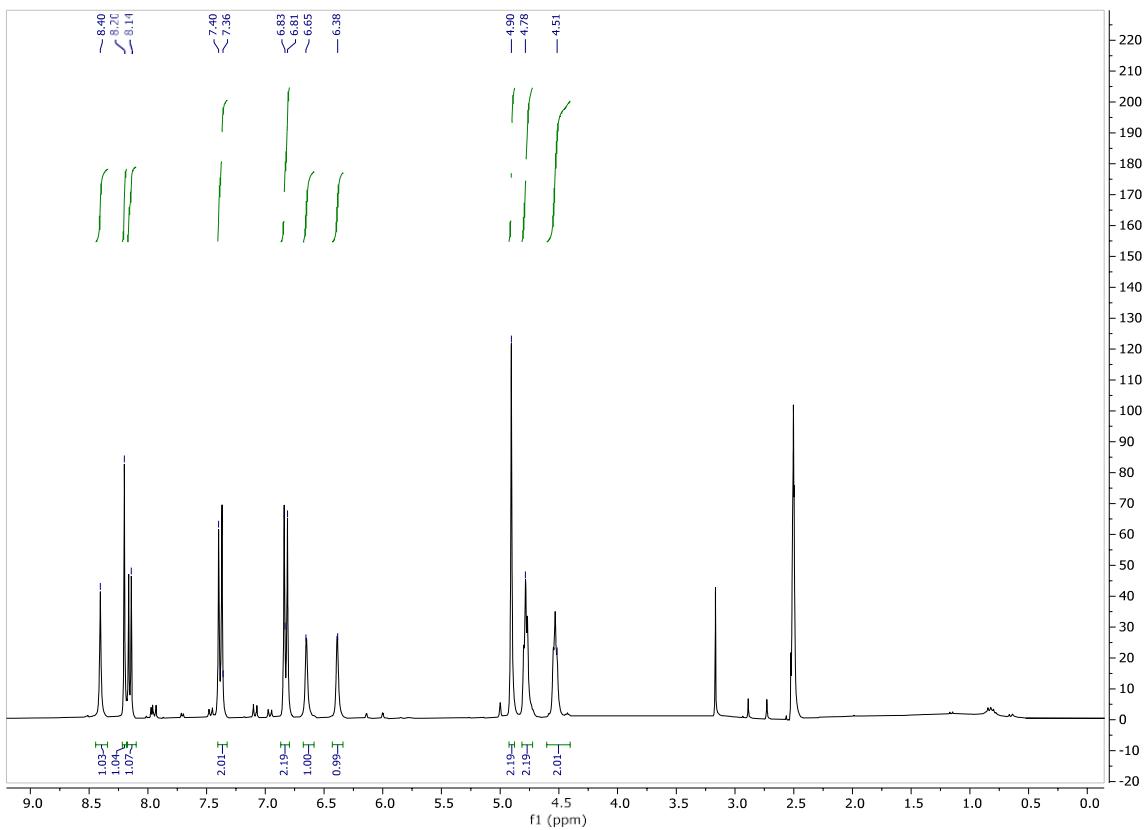
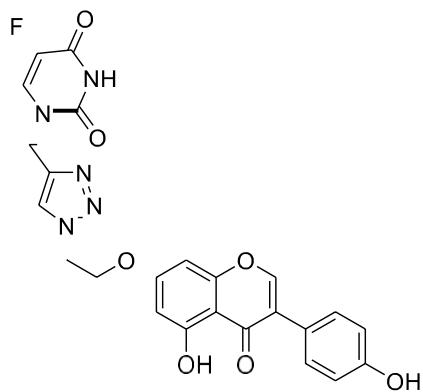
² Medical and Experimental Mycology Group, Corporación para Investigaciones Biológicas, 050034, Medellín, Colombia;

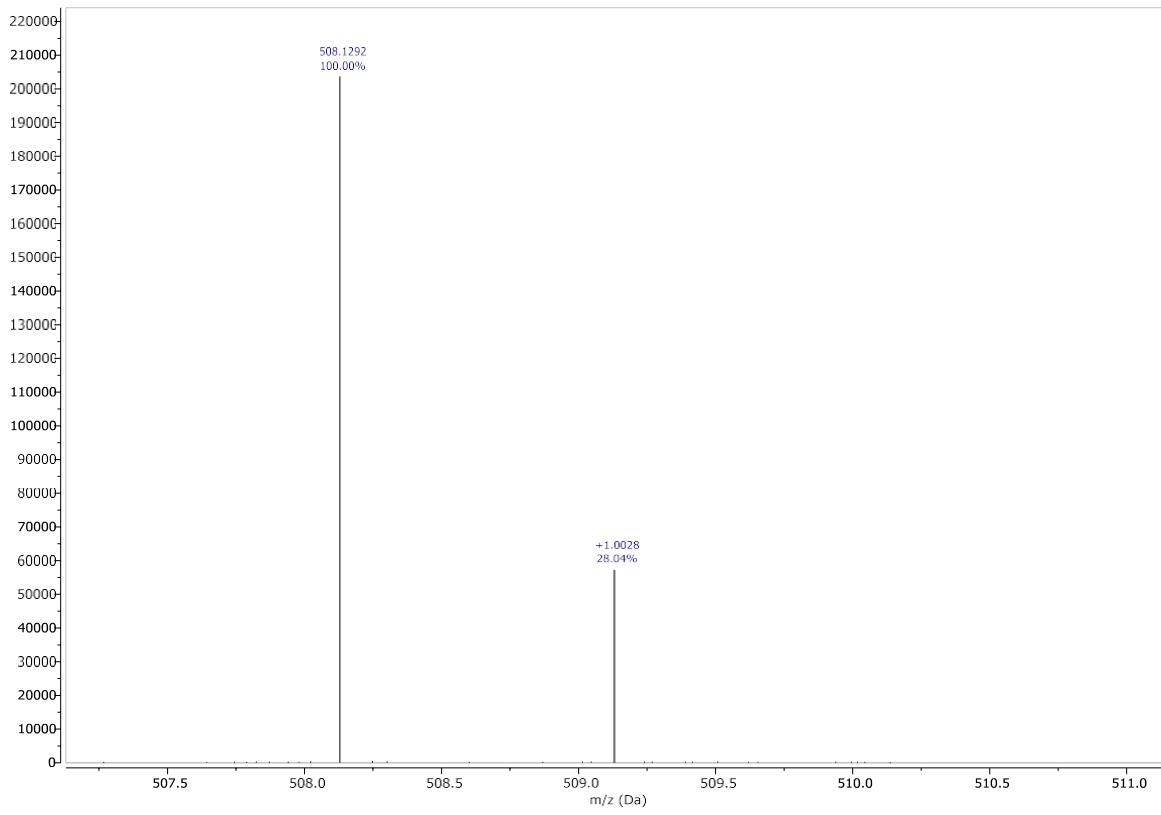
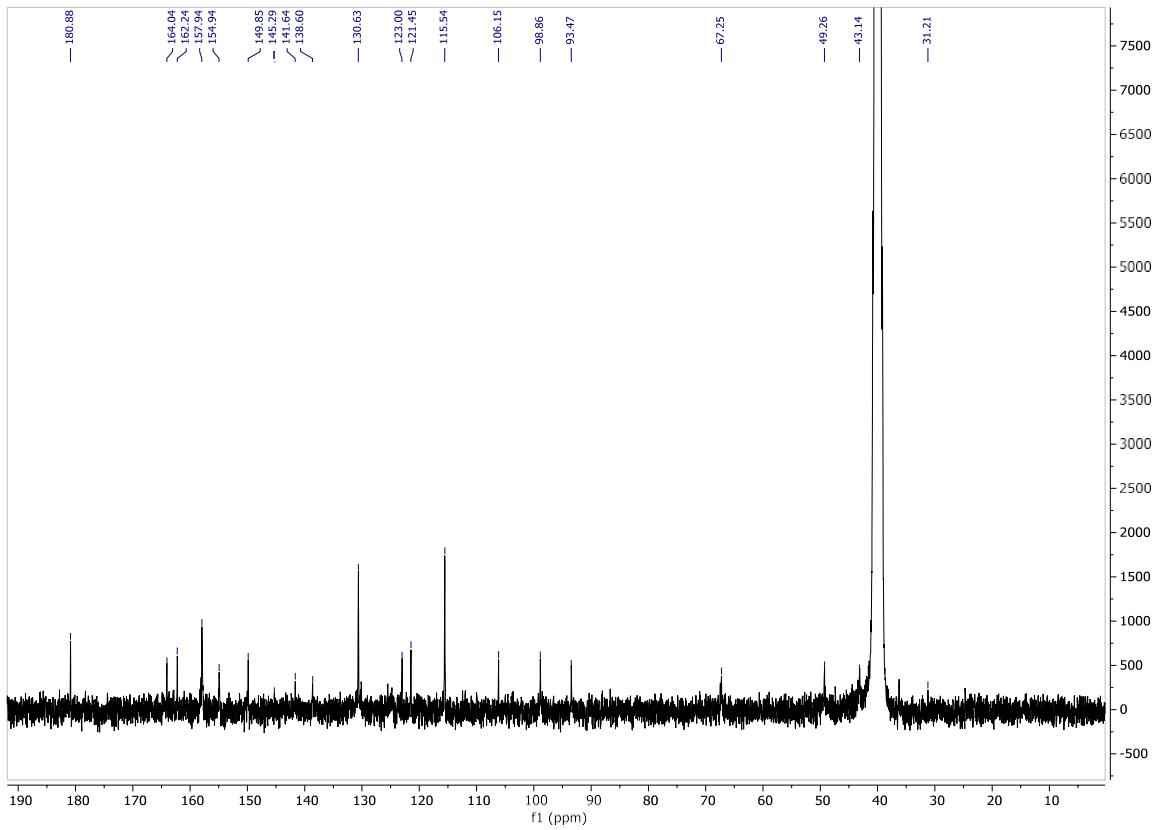
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(W.C.-G.)

¹ H, ¹³ C NMR and MS spectra	Figure S1
HPLC analysis	Figure S2

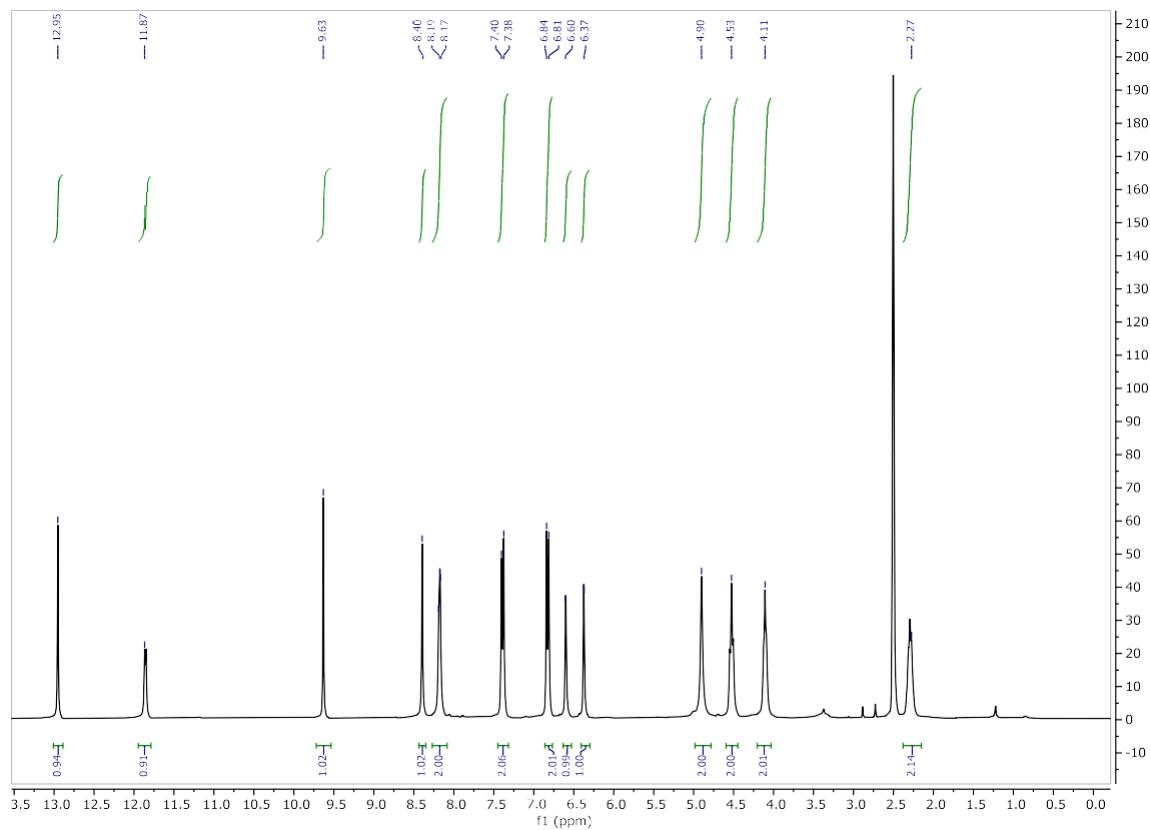
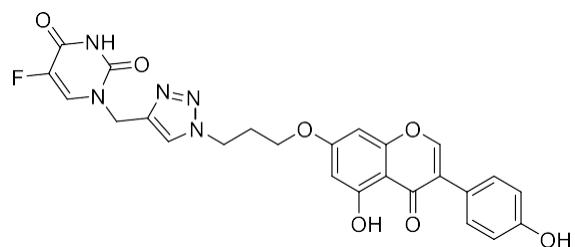
Figure S1. ¹H, ¹³C NMR and MS spectra

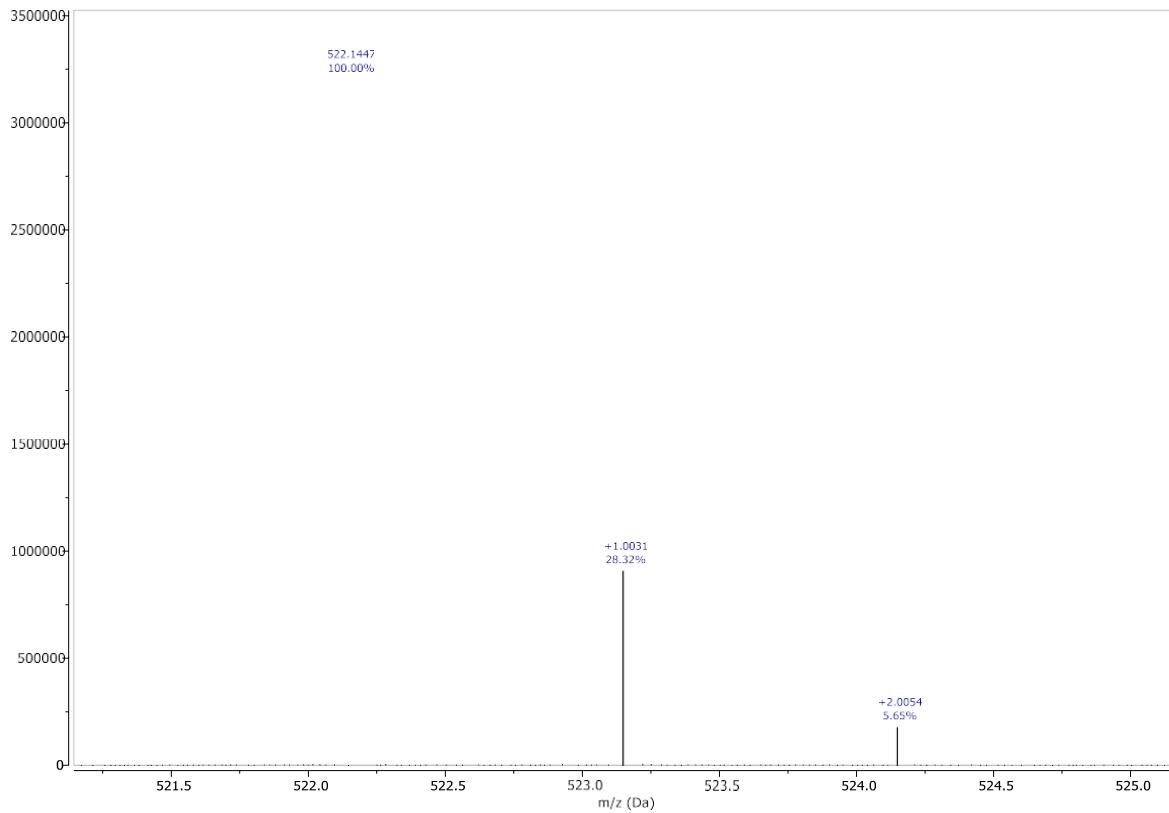
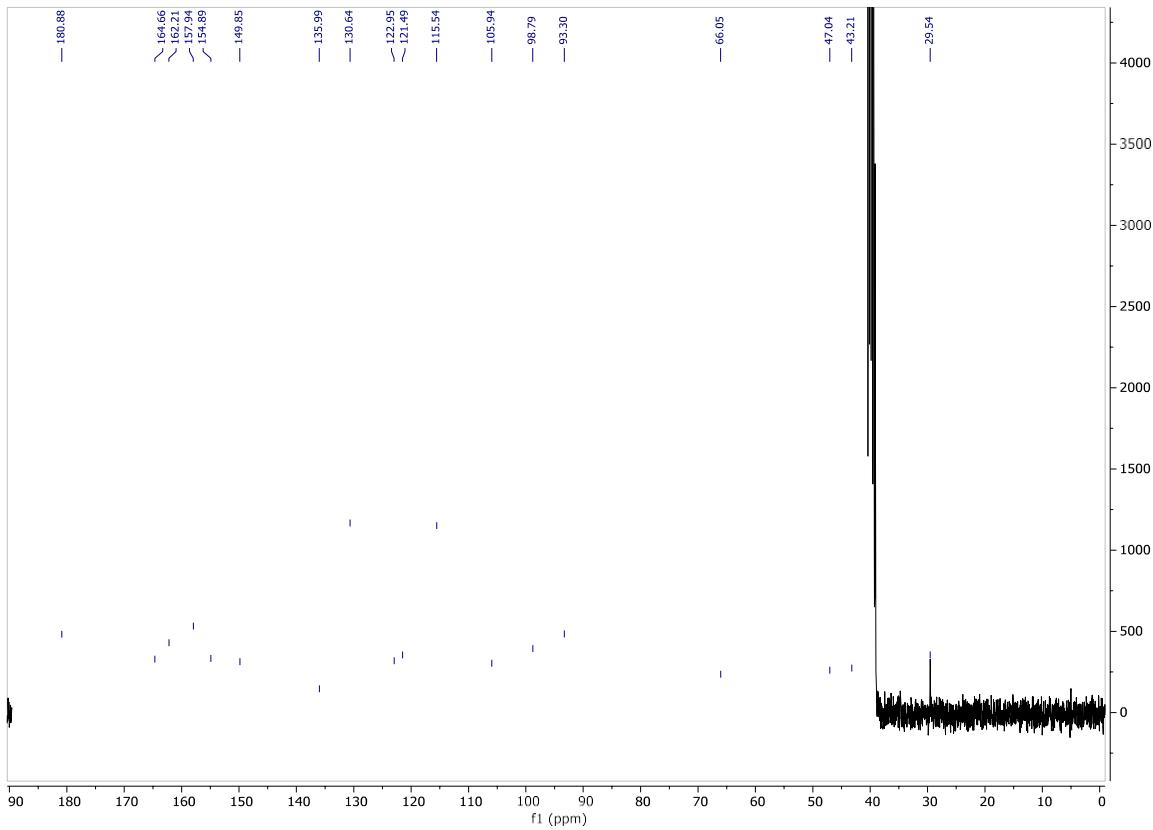
5-fluoro-1-((1-(3-((5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl)oxy)ethyl)-1H-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1H,3H)-dione (4a)



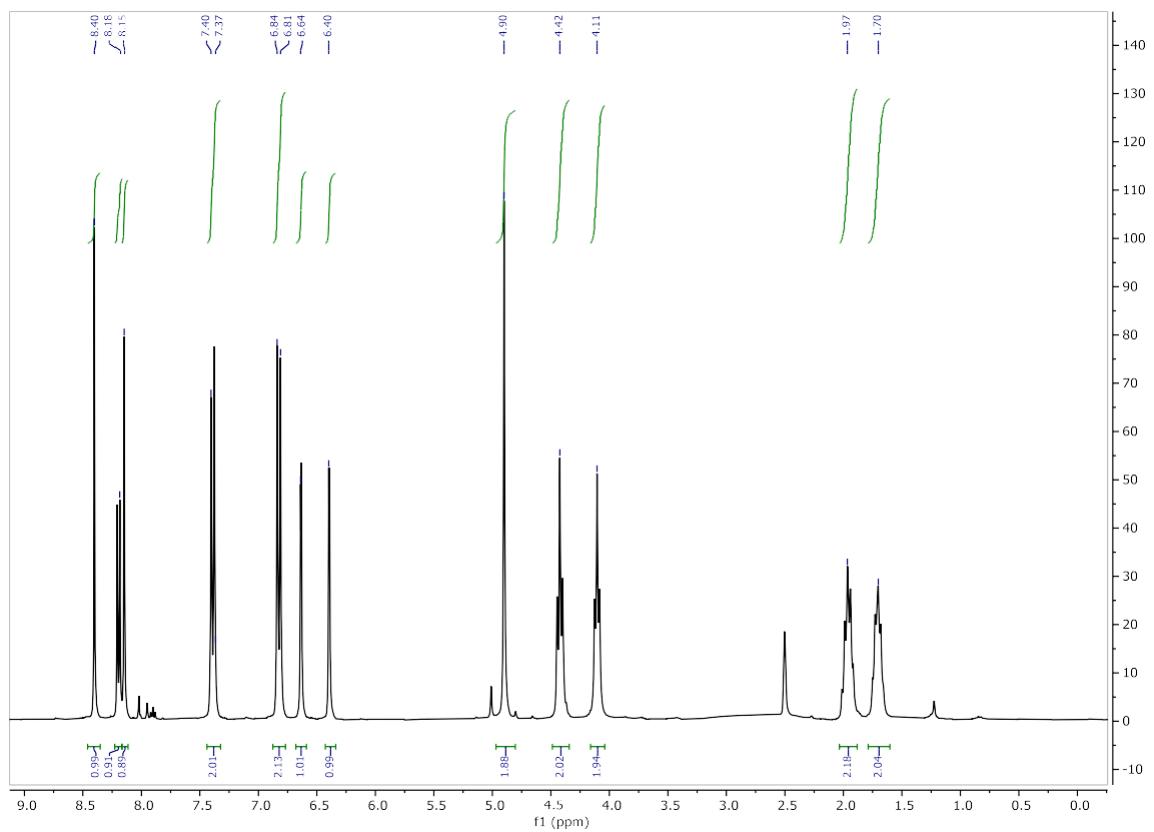
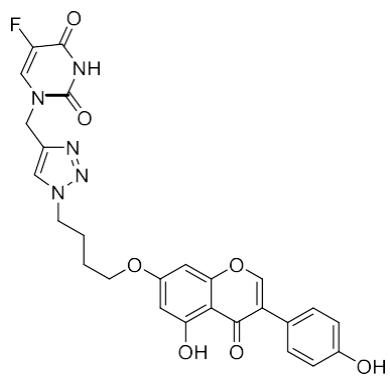


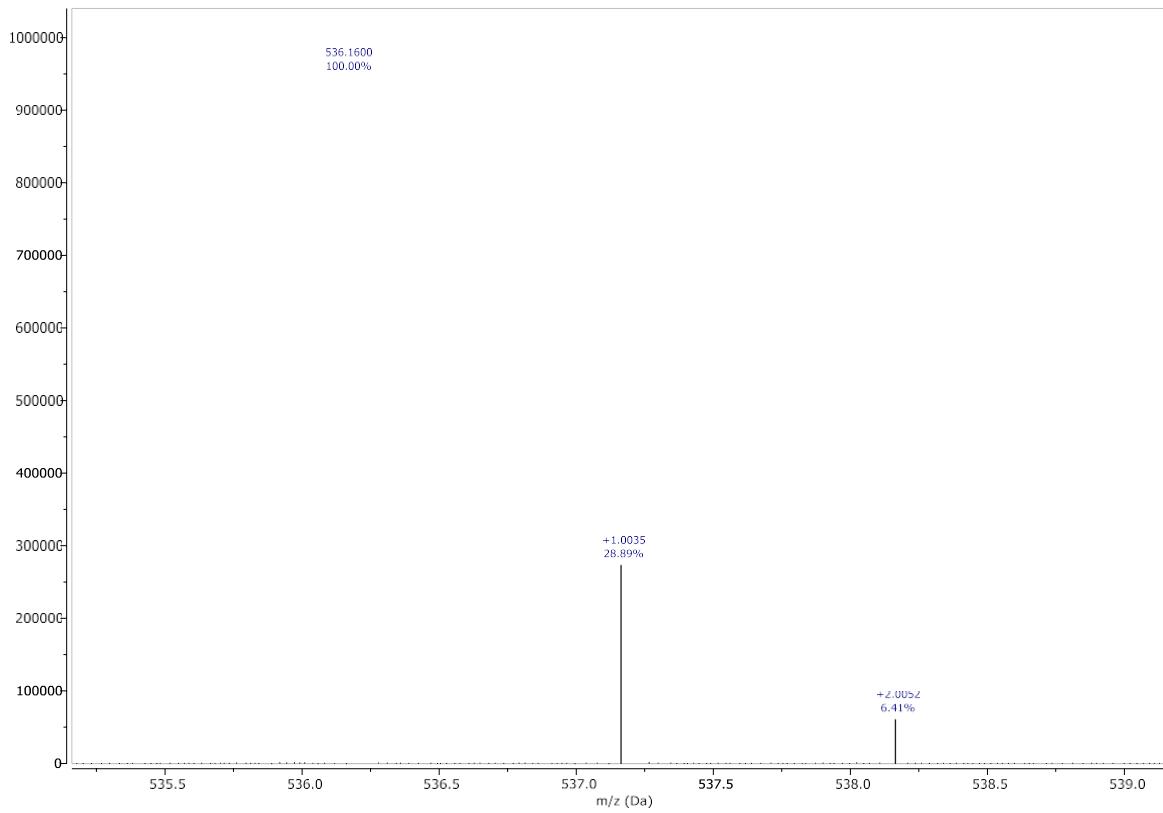
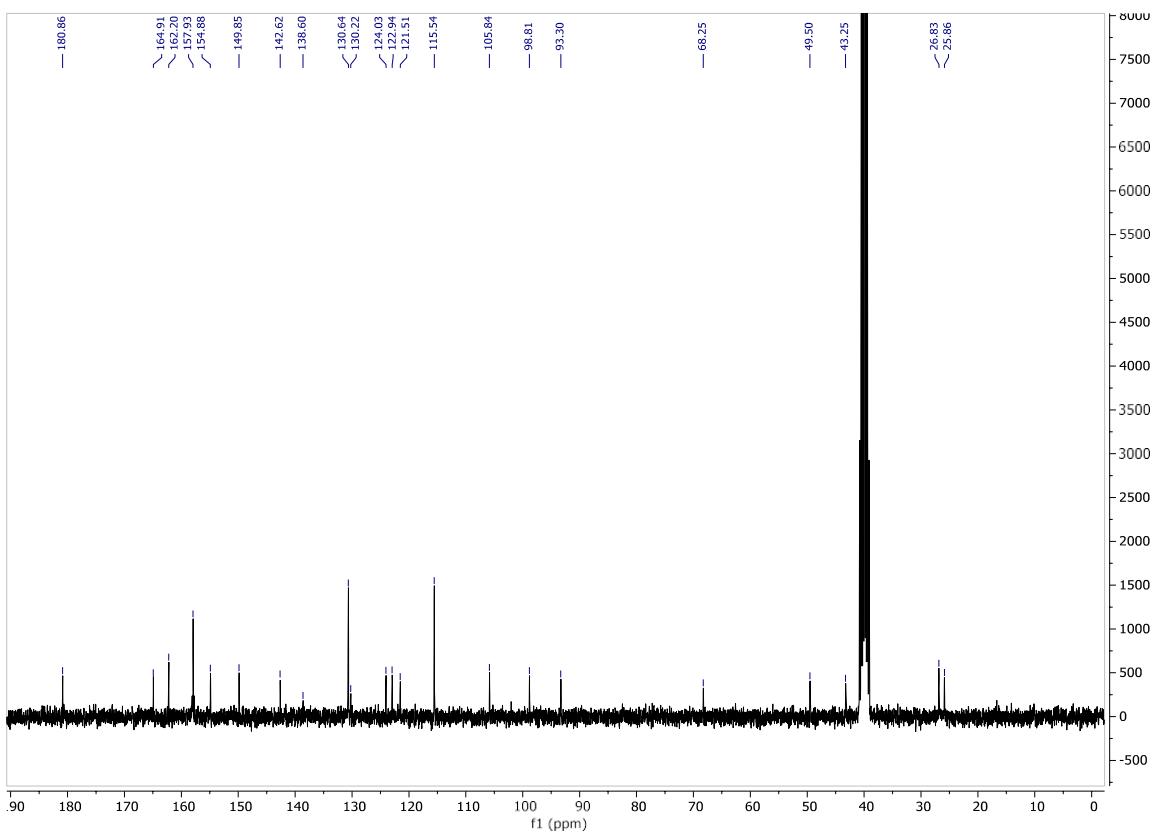
5-fluoro-1-((1-(3-((5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl)oxy)propyl)-1H-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1H,3H)-dione (4b)



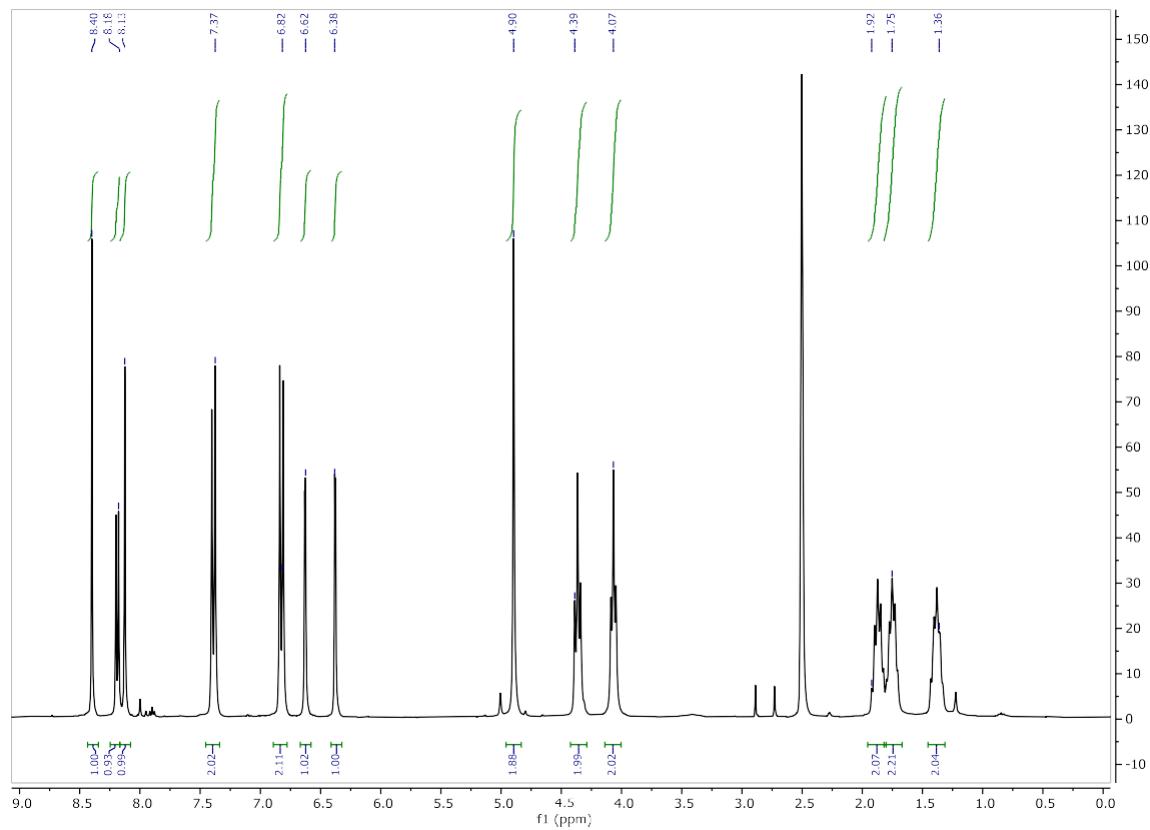
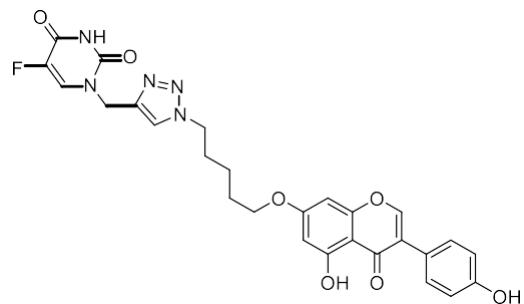


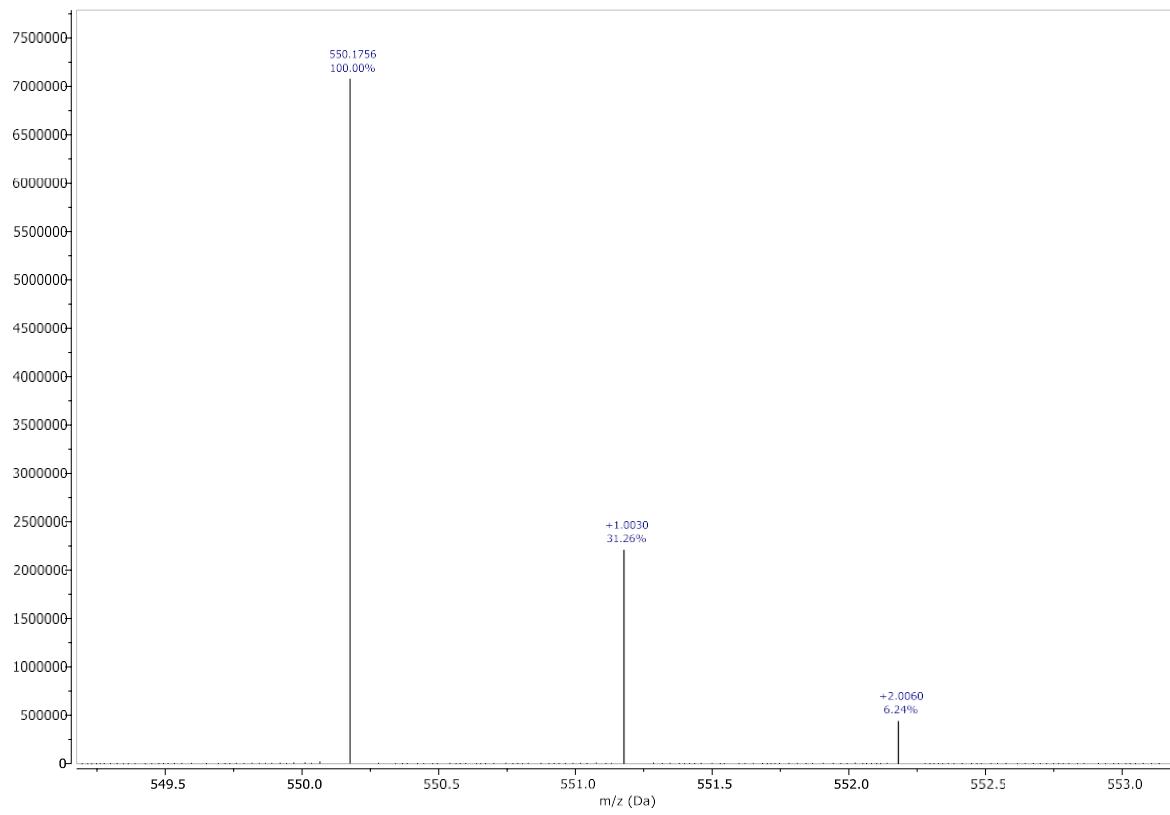
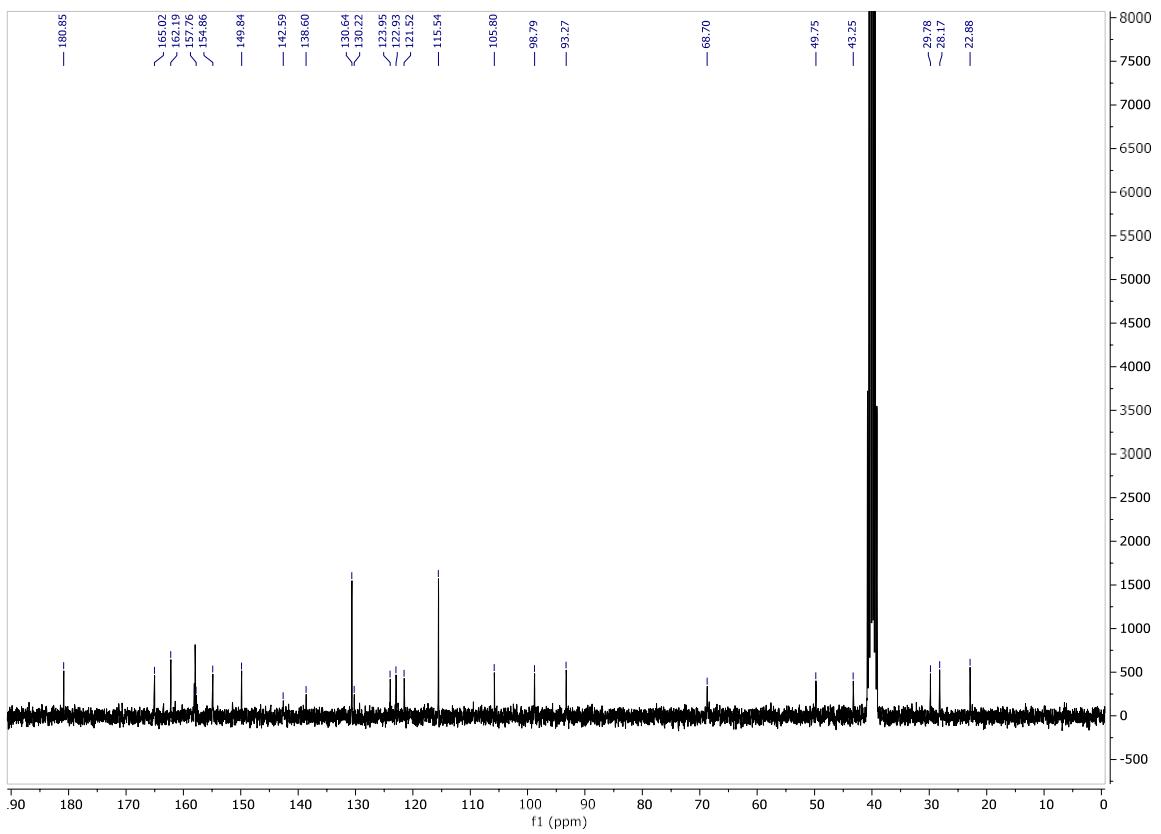
5-fluoro-1-((1-(3-((5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl)oxy)butyl)-1H-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1H,3H)-dione (4c)



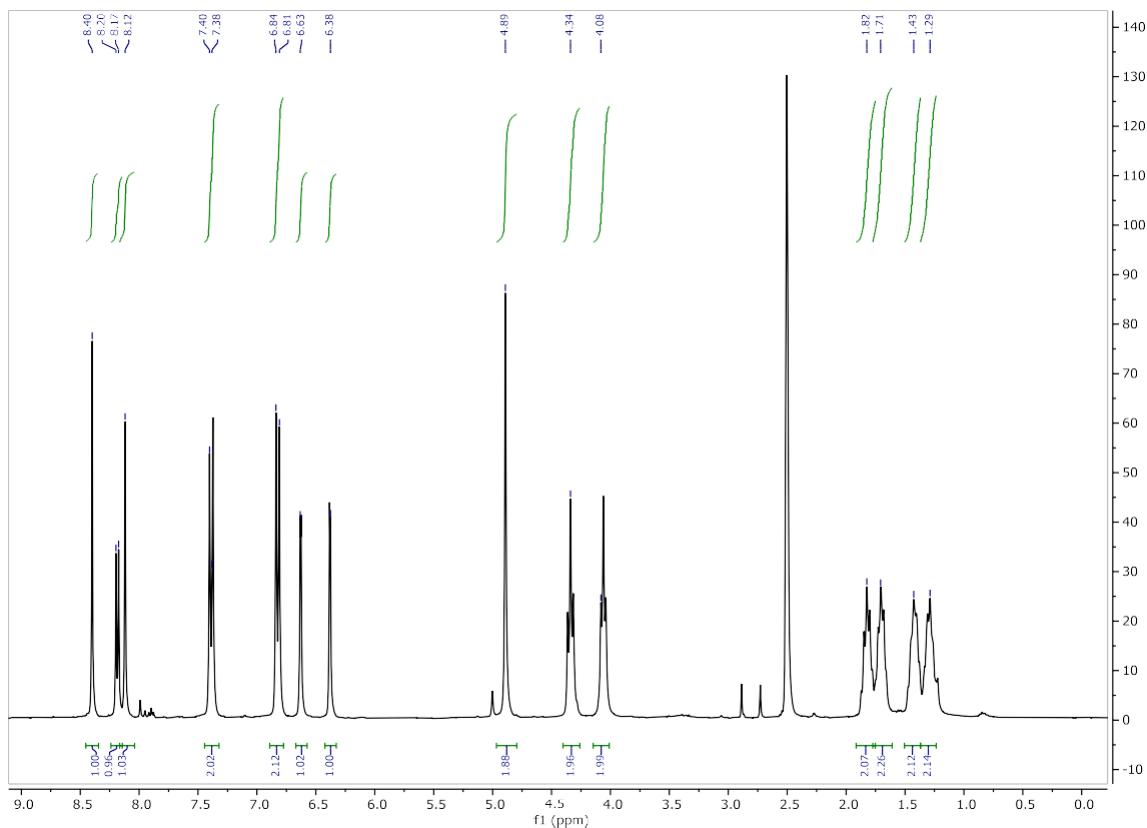
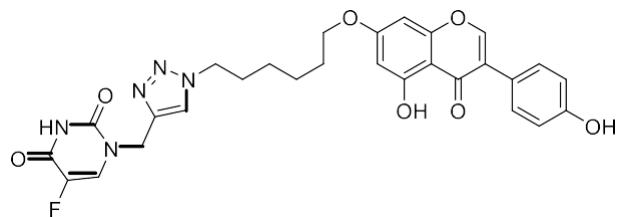


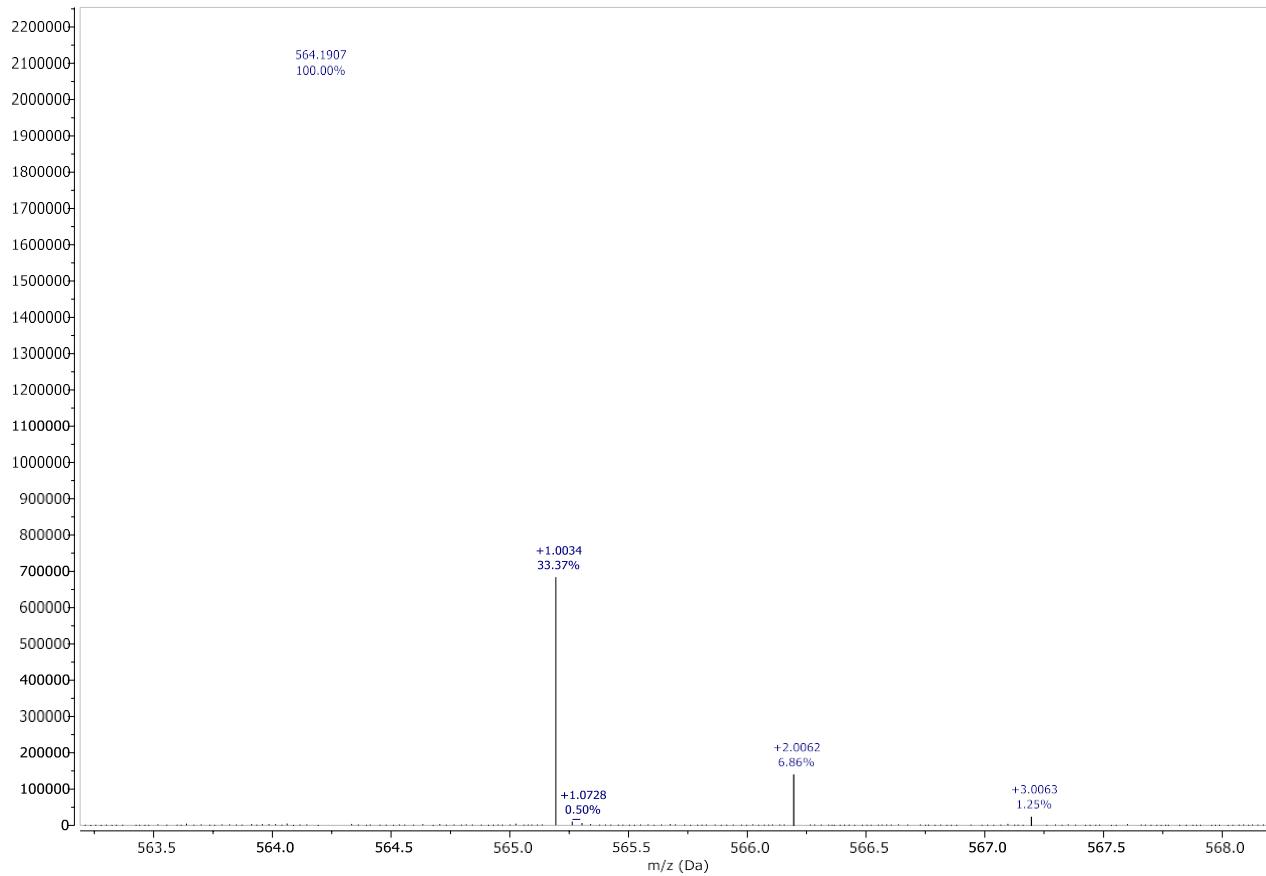
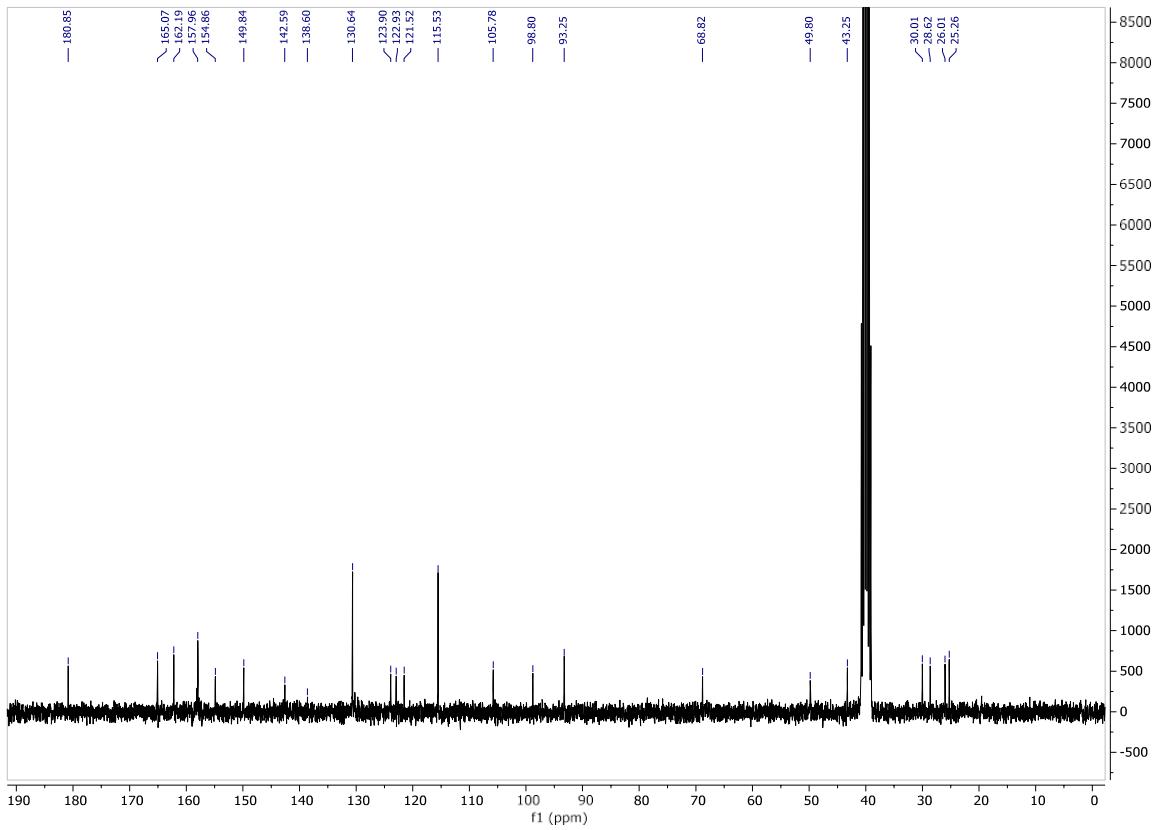
5-fluoro-1-((1-(3-((5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl)oxy)pentyl)-1H-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1H,3H)-dione (4d)



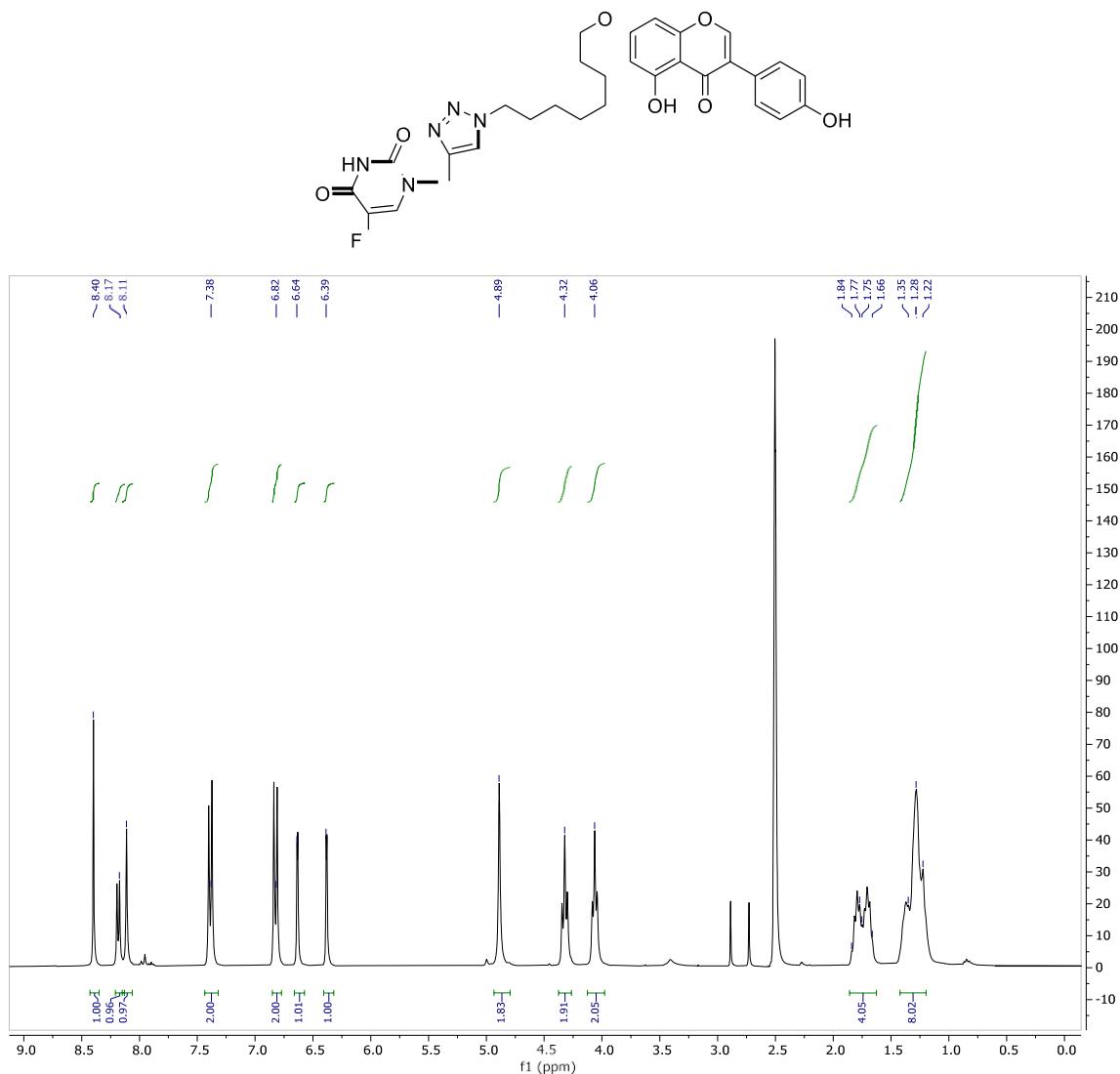


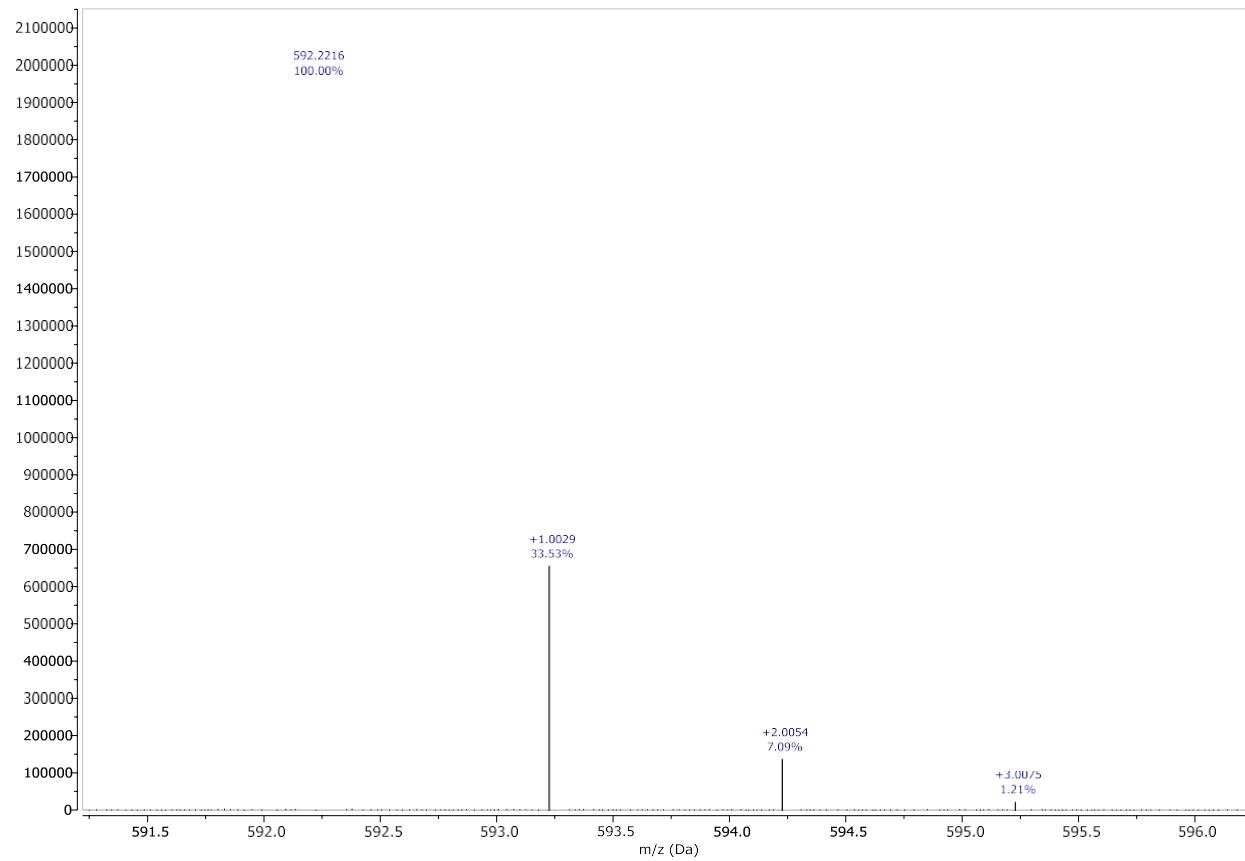
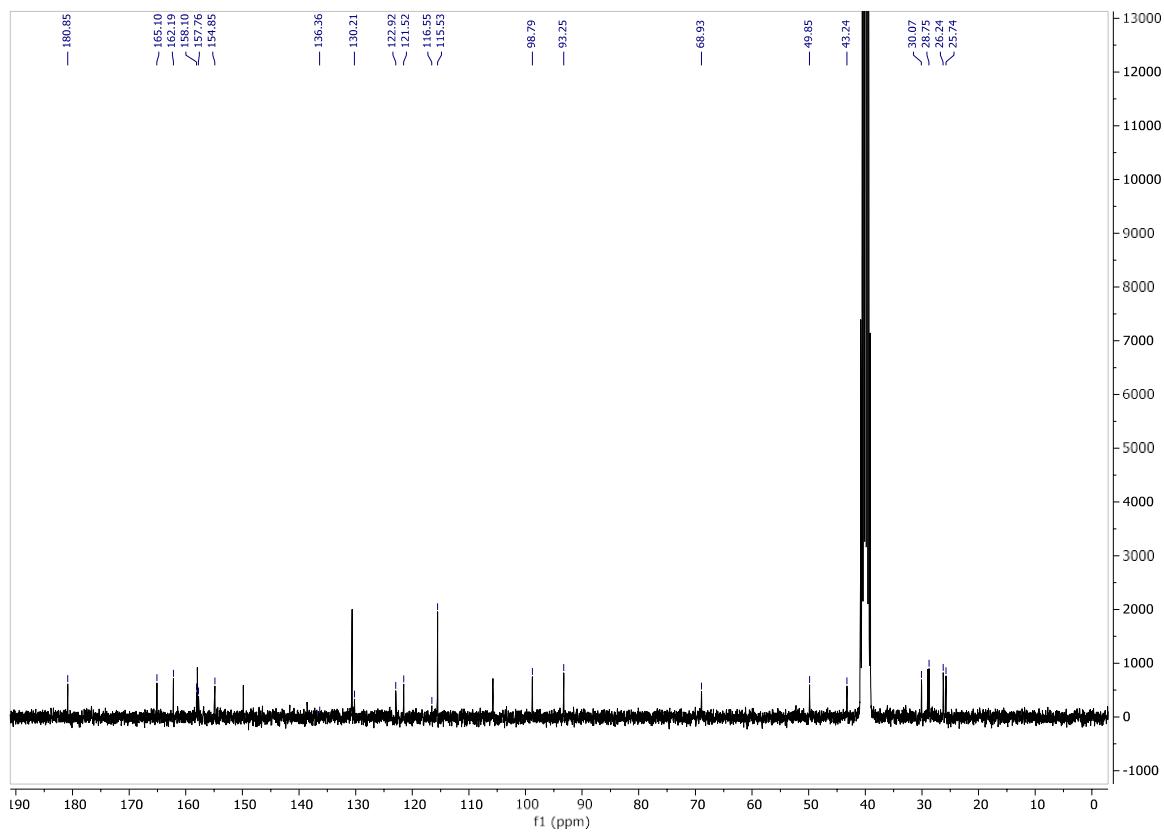
5-fluoro-1-((1-(3-((5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl)oxy)hexyl)-1H-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1H,3H)-dione (4e)



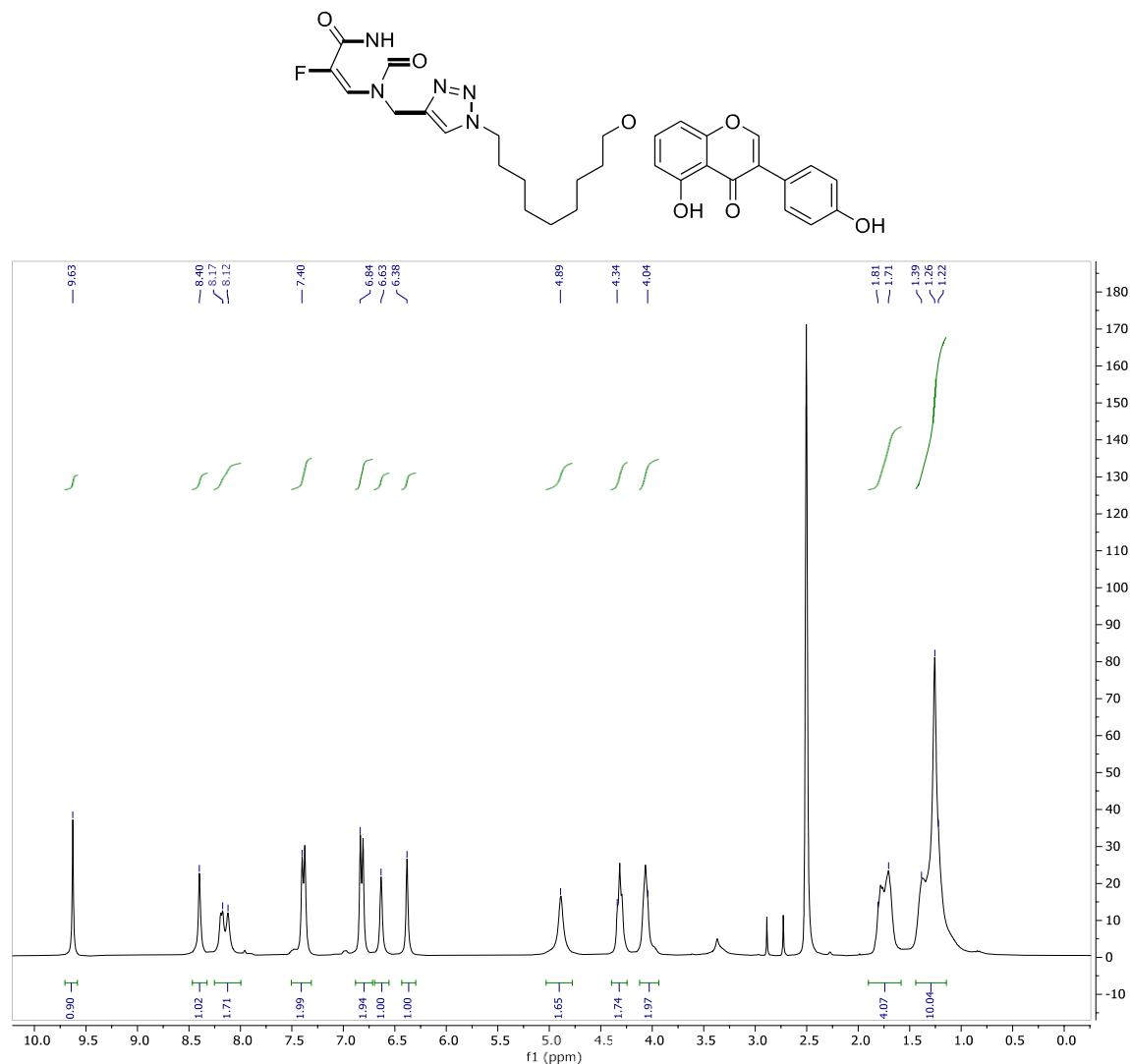


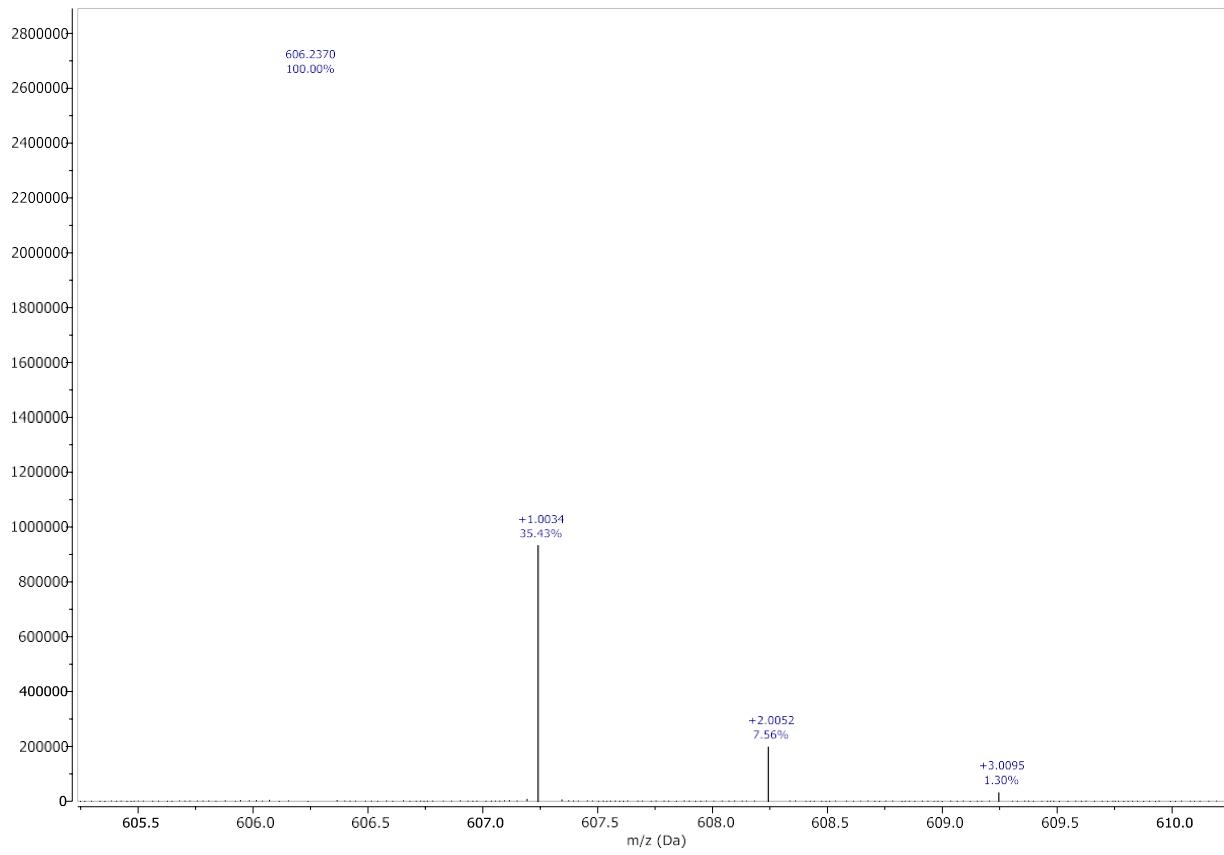
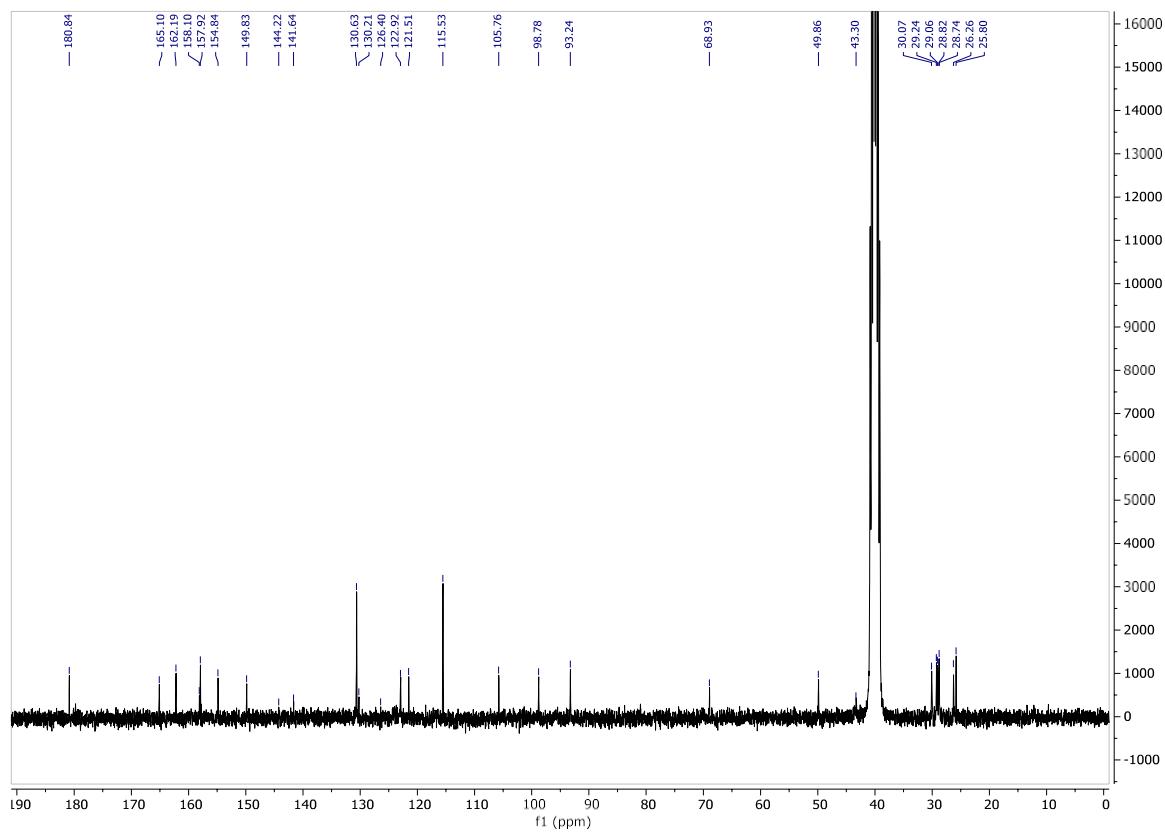
5-fluoro-1-((1-(3-((5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl)oxy)octyl)-1H-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1H,3H)-dione (4f)



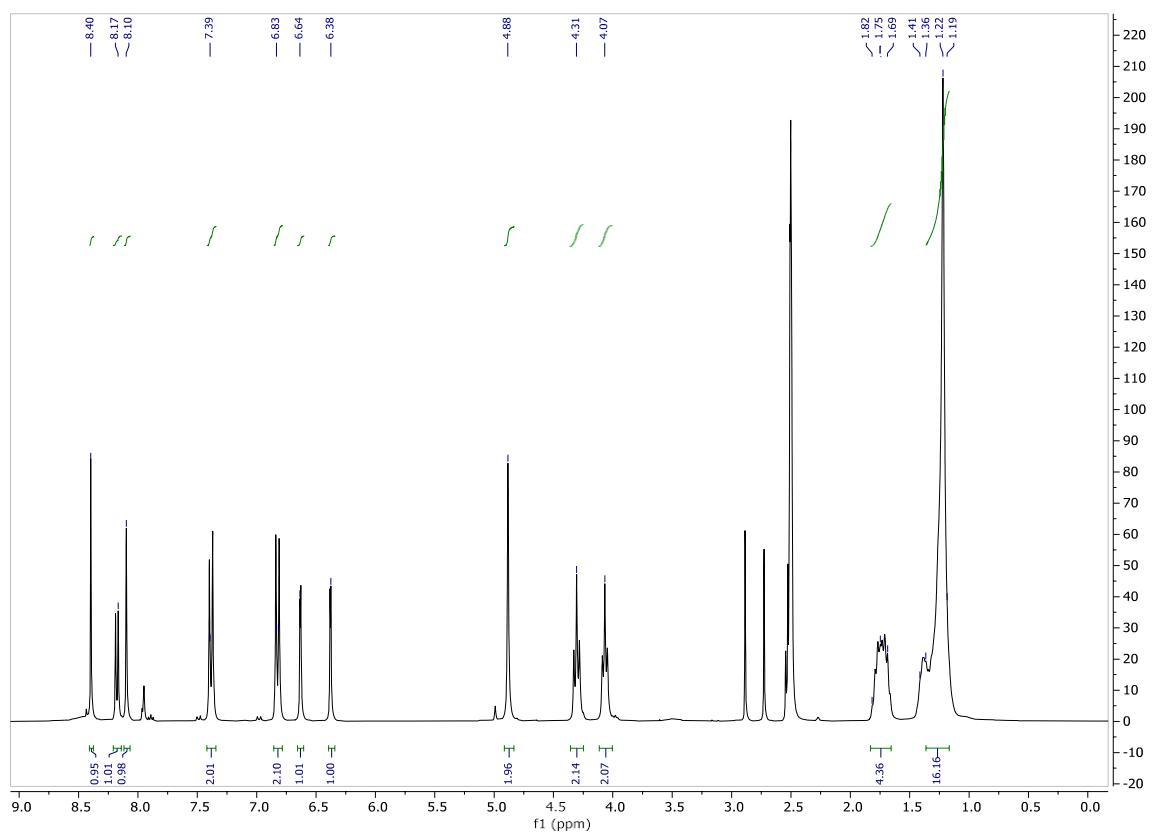
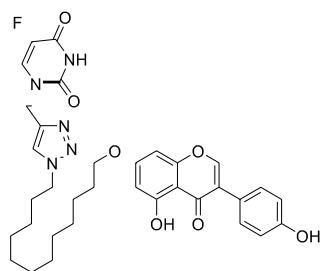


5-fluoro-1-((1-(3-((5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl)oxy)nonyl)-1H-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1H,3H)-dione (4g)





5-fluoro-1-((1-(3-((5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl)oxy)dodecyl)-1H-1,2,3-triazol-4-yl)methyl)pyrimidine-2,4(1H,3H)-dione (4h)



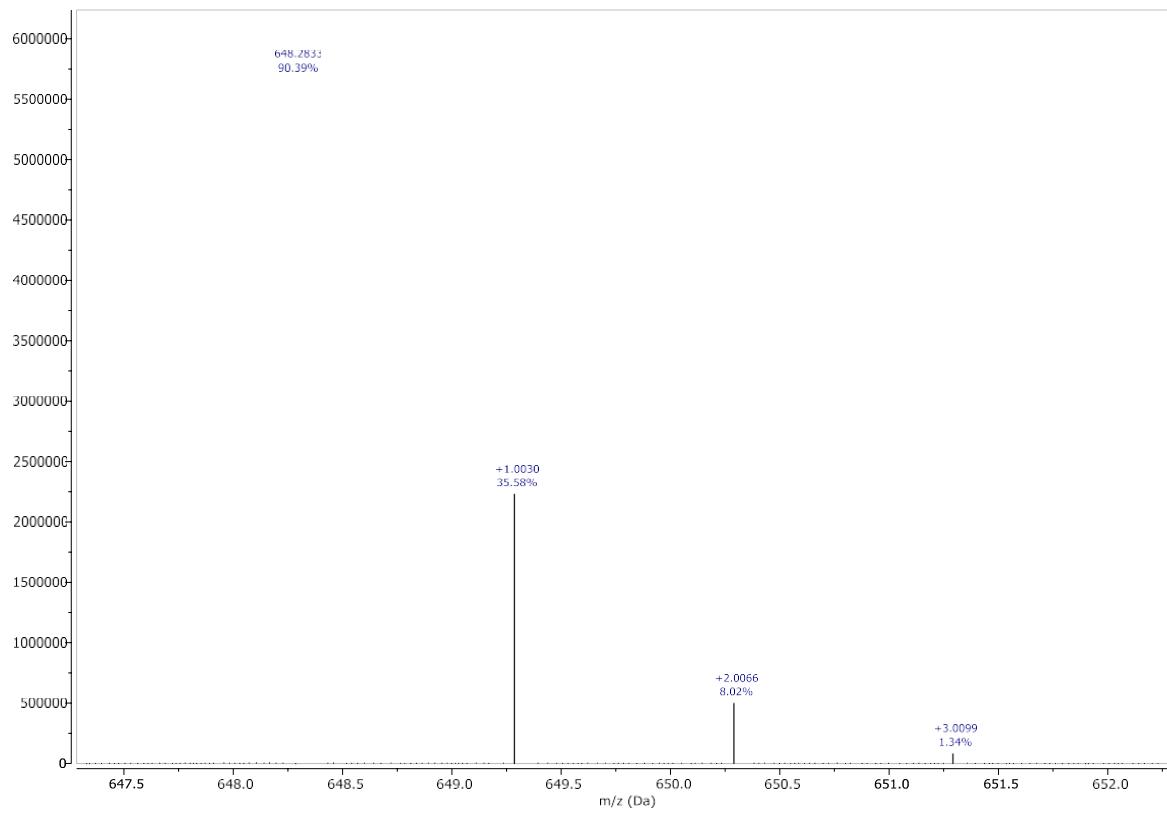
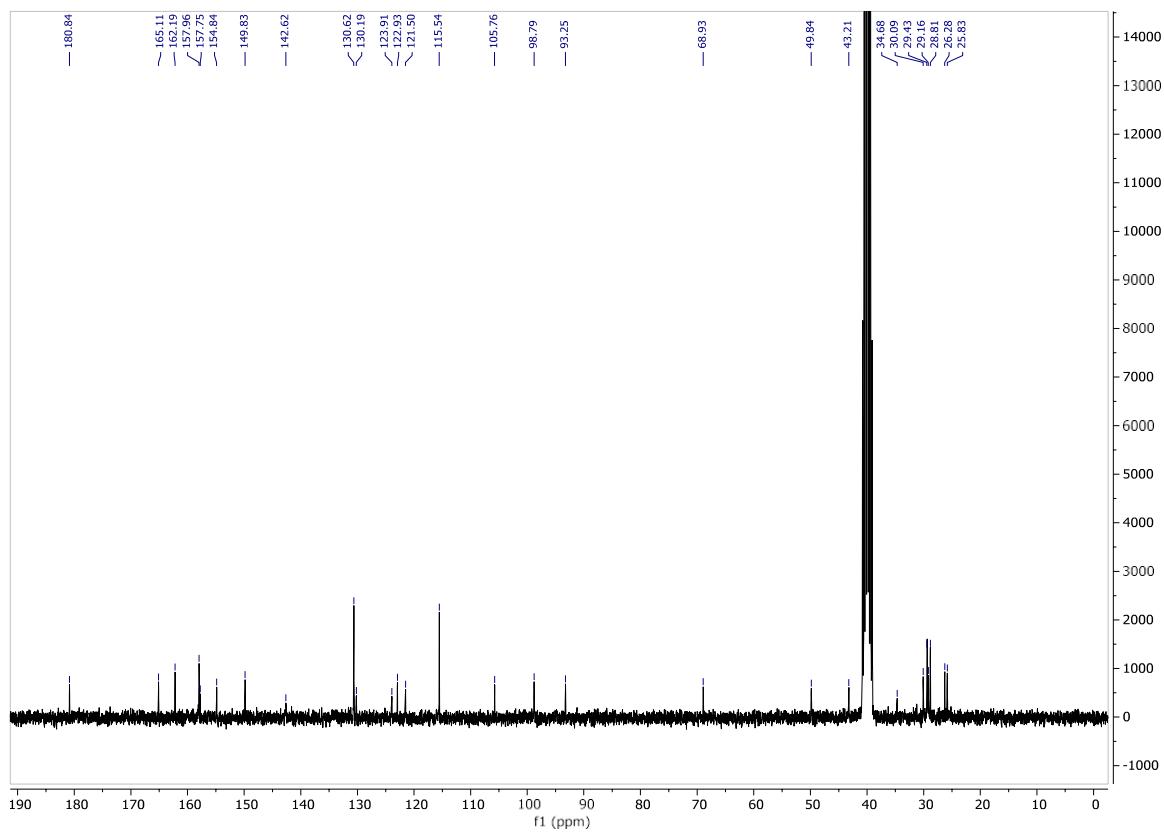
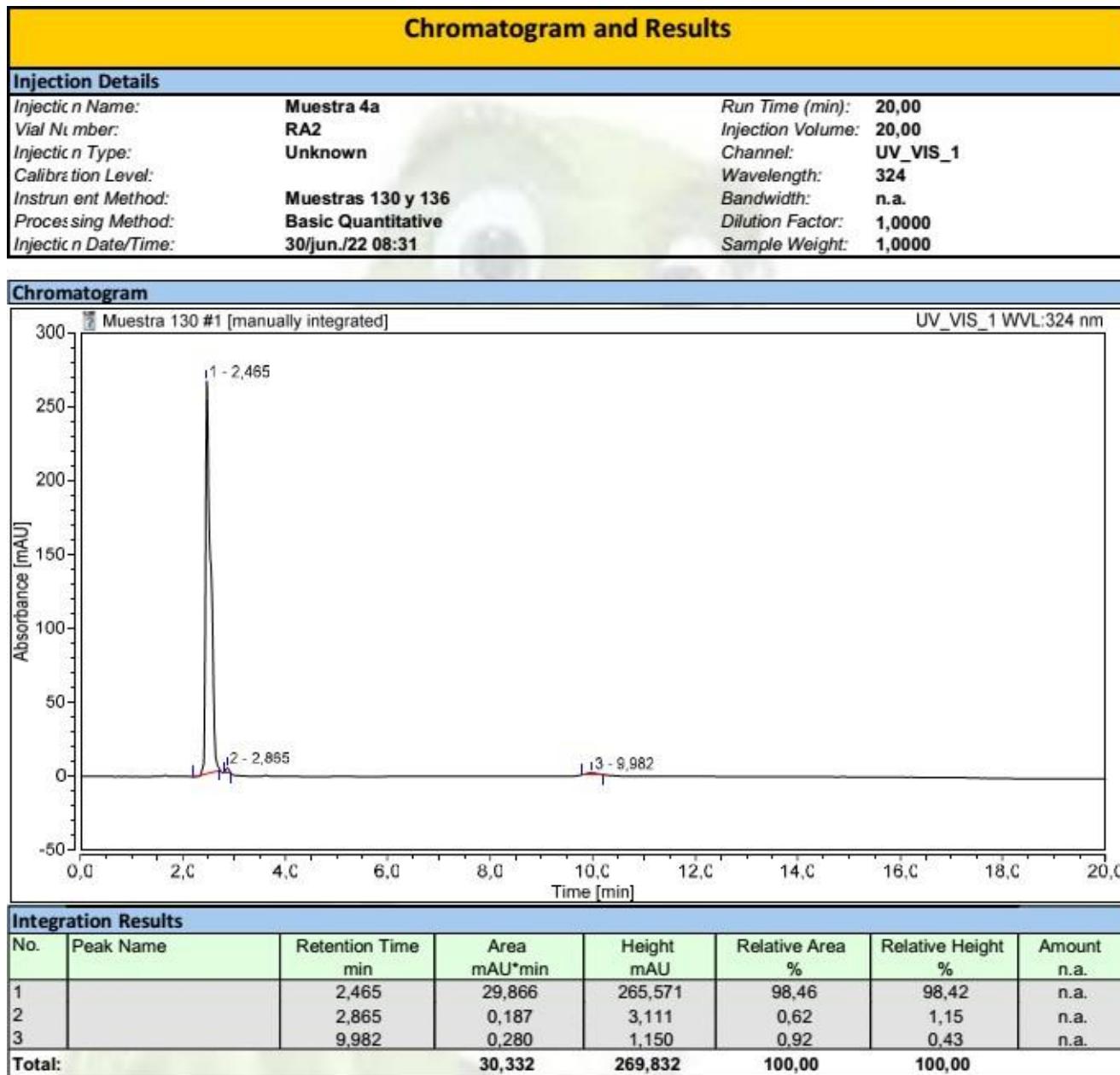


Figure S2. HPLC analysis

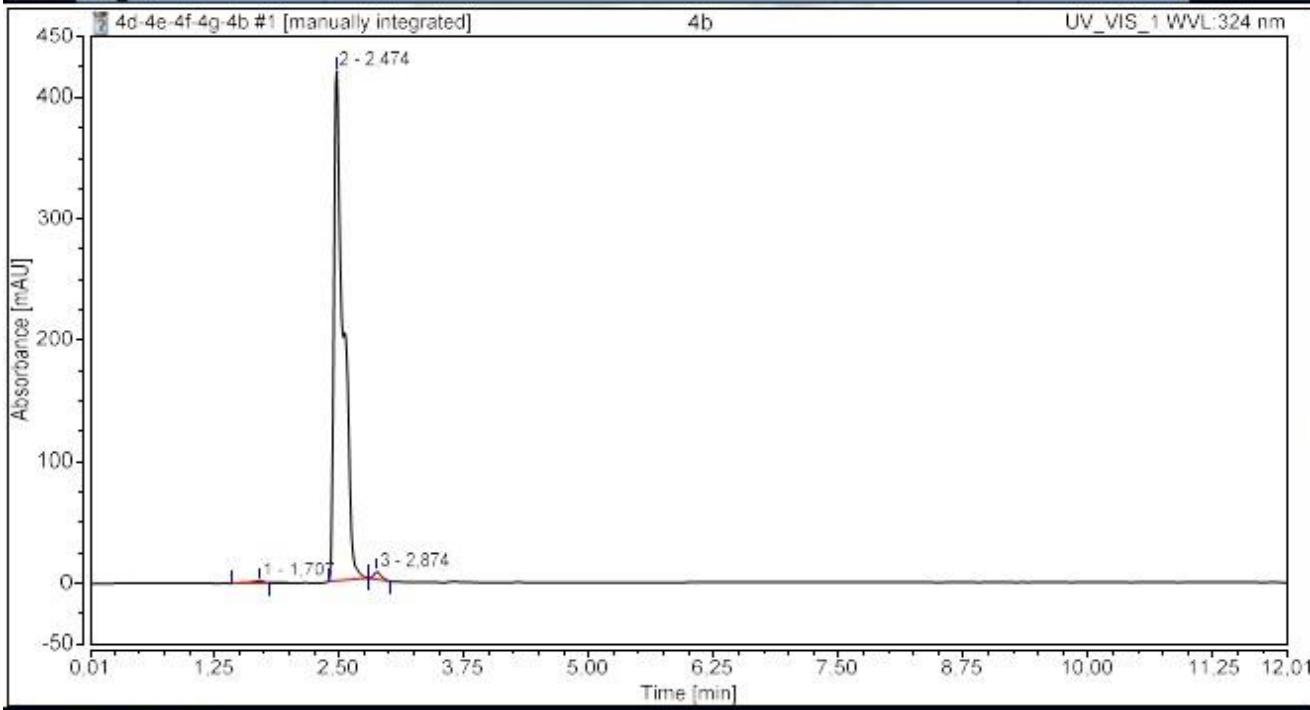


Chromatogram and Results

Injection Details

Injection Name:	4b	Run Time (min):	12,00
Vial Number:	RE3	Injection Volume:	20,00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	324
Instrument Method:	Muestras 130 y 136	Bandwidth:	n.a.
Processing Method:	Pureza muestras 130 y 136	Dilution Factor:	1,0000
Injection Date/Time:	30/jun./22 8:49	Sample Weight:	1,0000

Chromatogram



Integration Results

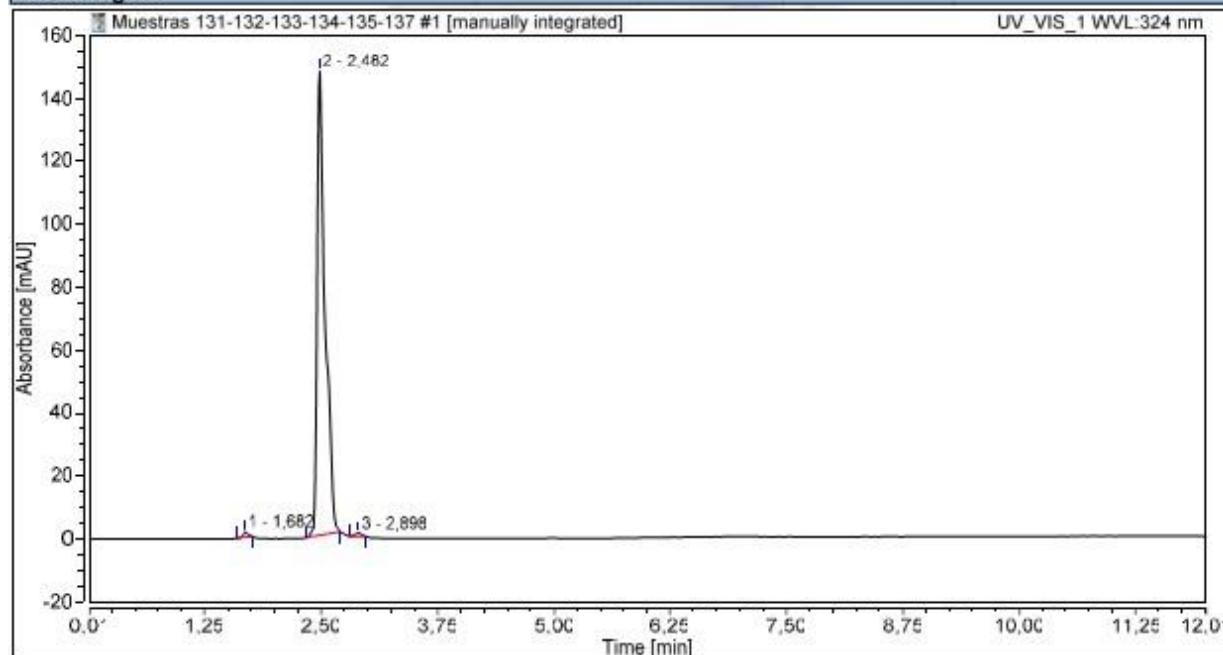
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		1,707	0,306	2,368	0,65	0,55	n.a.
2		2,474	45,910	420,057	98,19	97,96	n.a.
3		2,874	0,543	6,400	1,16	1,49	n.a.
Total:			46,758	428,825	100,00	100,00	

Chromatogram and Results

Injection Details

Injection Name:	4c	Run Time (min):	12,00
Vial Number:	RB2	Injection Volume:	20,00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	324
Instrument Method:	Muestras 130 y 136	Bandwidth:	n.a.
Processing Method:	Pureza muestras 130 y 136	Dilution Factor:	1,0000
Injection Date/Time:	30/jun/22 09:16	Sample Weight:	1,0000

Chromatogram



Integration Results

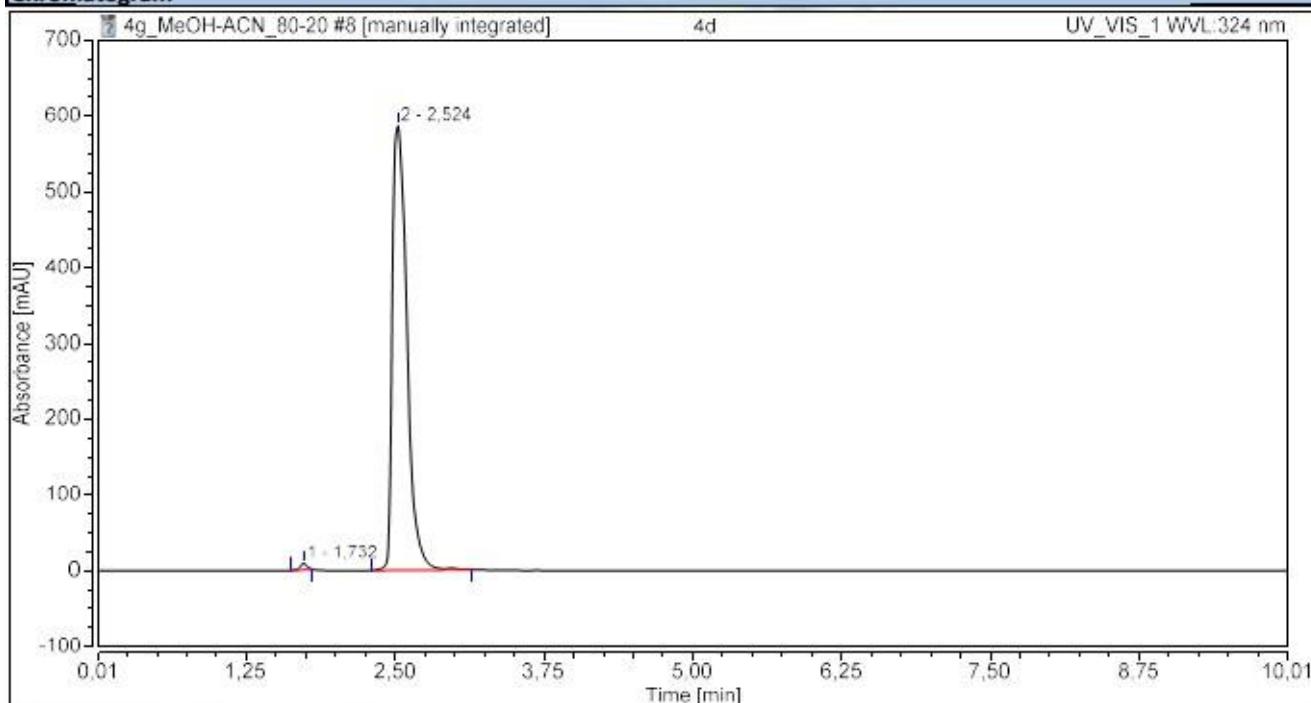
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		1,682	0,096	1,756	0,65	1,17	n.a.
2		2,482	14,533	147,499	98,77	98,15	n.a.
3		2,898	0,084	1,031	0,57	0,69	n.a.
Total:			14,714	150,285	100,00	100,00	

Chromatogram and Results

Injection Details

Injection Name:	4d	Run Time (min):	10,00
Vial Number:	RC1	Injection Volume:	40,00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	324
Instrument Method:	Serie 4a-4h_Isocratico_MeOH-ACN_80-20	Bandwidth:	n.a.
Processing Method:	Pureza muestras 130 y 136	Dilution Factor:	1,0000
Injection Date/Time:	06/oct/22 10:01	Sample Weight:	1,0000

Chromatogram



Integration Results

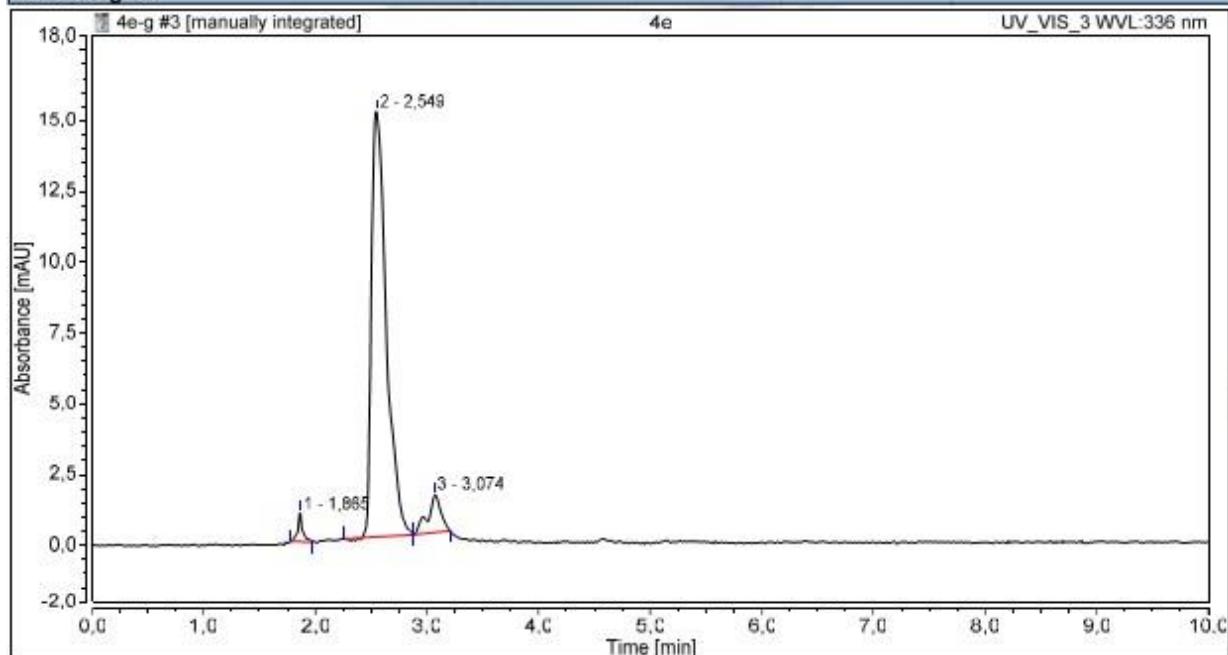
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		1,732	0,549	8,595	0,65	1,44	n.a.
2		2,524	83,316	586,753	99,35	98,56	n.a.
Total:			83,865	595,347	100,00	100,00	

Chromatogram and Results

Injection Details

Injection Name:	4e	Run Time (min):	10,00
Vial Number:	RC2	Injection Volume:	40,00
Injection Type:	Unknown	Channel:	UV_VIS_3
Calibration Level:		Wavelength:	336
Instrument Method:	Serie 4a-4h_Isocratico_MeOH-ACN_80-20	Bandwidth:	n.a.
Processing Method:	Pureza muestras 130 y 136	Dilution Factor:	1,0000
Injection Date/Time:	06/oct/22 12:46	Sample Weight:	1,0000

Chromatogram



Integration Results

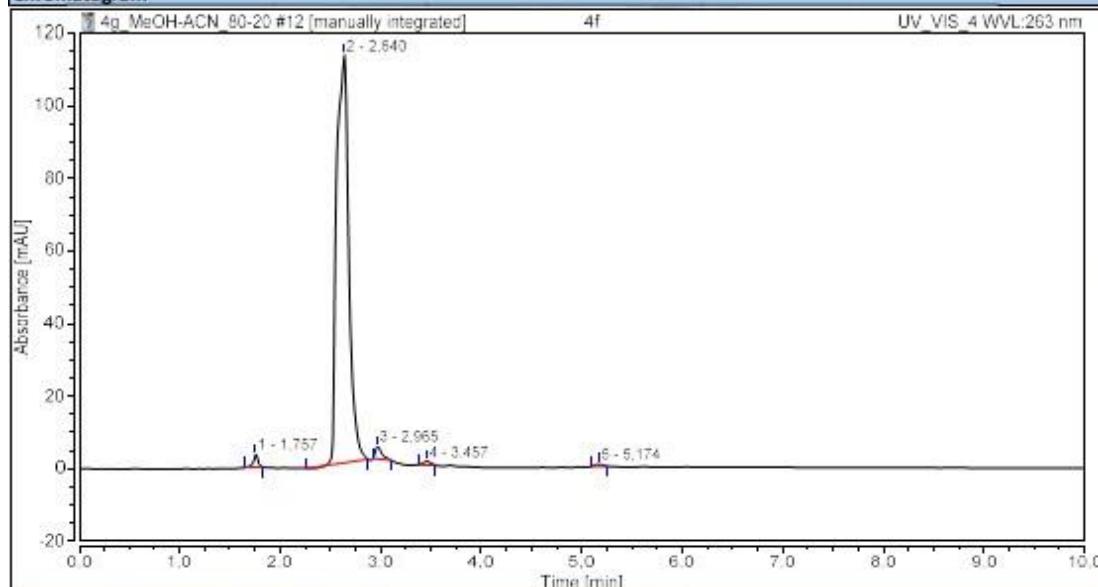
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		1,865	0,021	0,721	0,86	4,34	n.a.
2		2,549	2,319	15,040	95,85	90,50	n.a.
3		3,074	0,080	0,858	3,29	5,16	n.a.
Total:			2,419	16,619	100,00	100,00	

Chromatogram and Results

Injection Details

Injection Name:	4f	Run Time (min):	10,00
Vial Number:	RC3	Injection Volume:	40,00
Injection Type:	Unknown	Channel:	UV_VIS_4
Calibration Level:		Wavelength:	263
Instrument Method:	Serie 4a-4h_Isocratico_MeOH-ACN_80-20	Bandwidth:	n.a.
Processing Method:	Pureza muestras 130 y 136	Dilution Factor:	1,0000
Injection Date/Time:	06/oct/22 10:45	Sample Weight:	1,0000

Chromatogram



Integration Results

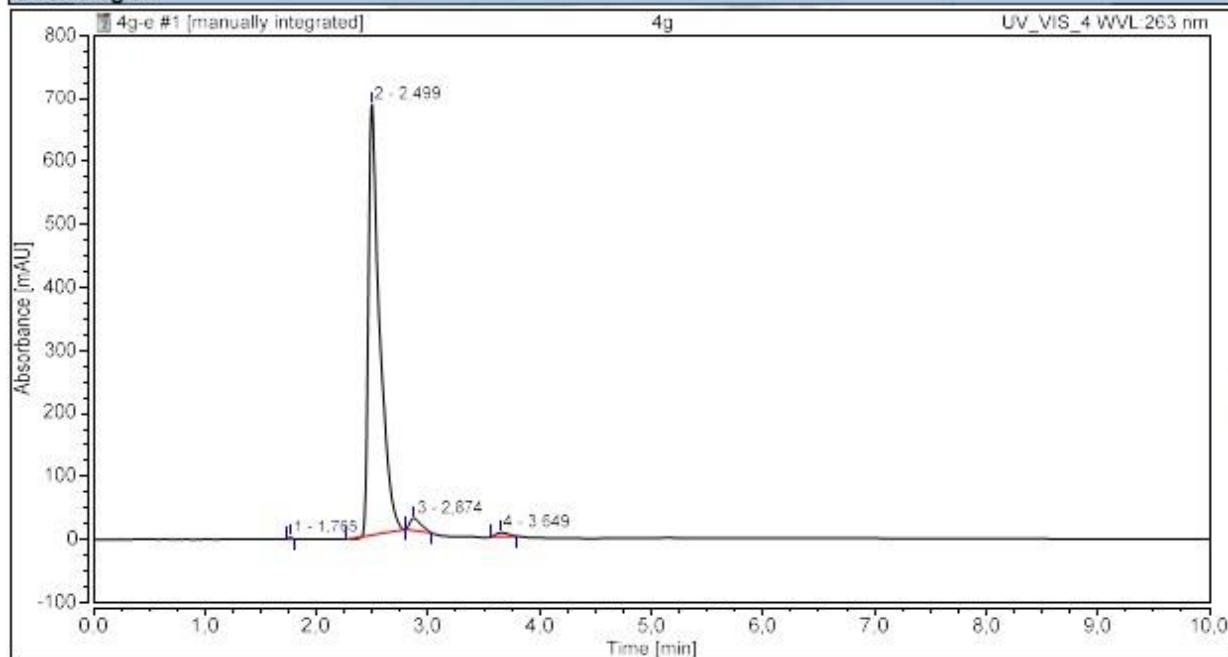
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		1,757	0,174	3,460	1,07	2,87	n.a.
2		2,640	15,736	112,341	96,62	93,17	n.a.
3		2,965	0,248	3,287	1,53	2,73	n.a.
4		3,457	0,086	0,993	0,53	0,82	n.a.
5		5,174	0,042	0,493	0,26	0,41	n.a.
Total:			16,287	120,575	100,00	100,00	

Chromatogram and Results

Injection Details

Injection Name:	4g	Run Time (min):	10,00
Vial Number:	RE3	Injection Volume:	40,00
Injection Type:	Unknown	Channel:	UV_VIS_4
Calibration Level:		Wavelength:	263
Instrument Method:	Serie 4a-4h_Isocratico_MeOH-ACN_80-20	Bandwidth:	n.a.
Processing Method:	Pureza muestras 130 y 136	Dilution Factor:	1,0000
Injection Date/Time:	06/oct/22 14:17	Sample Weight:	1,0000

Chromatogram



Integration Results

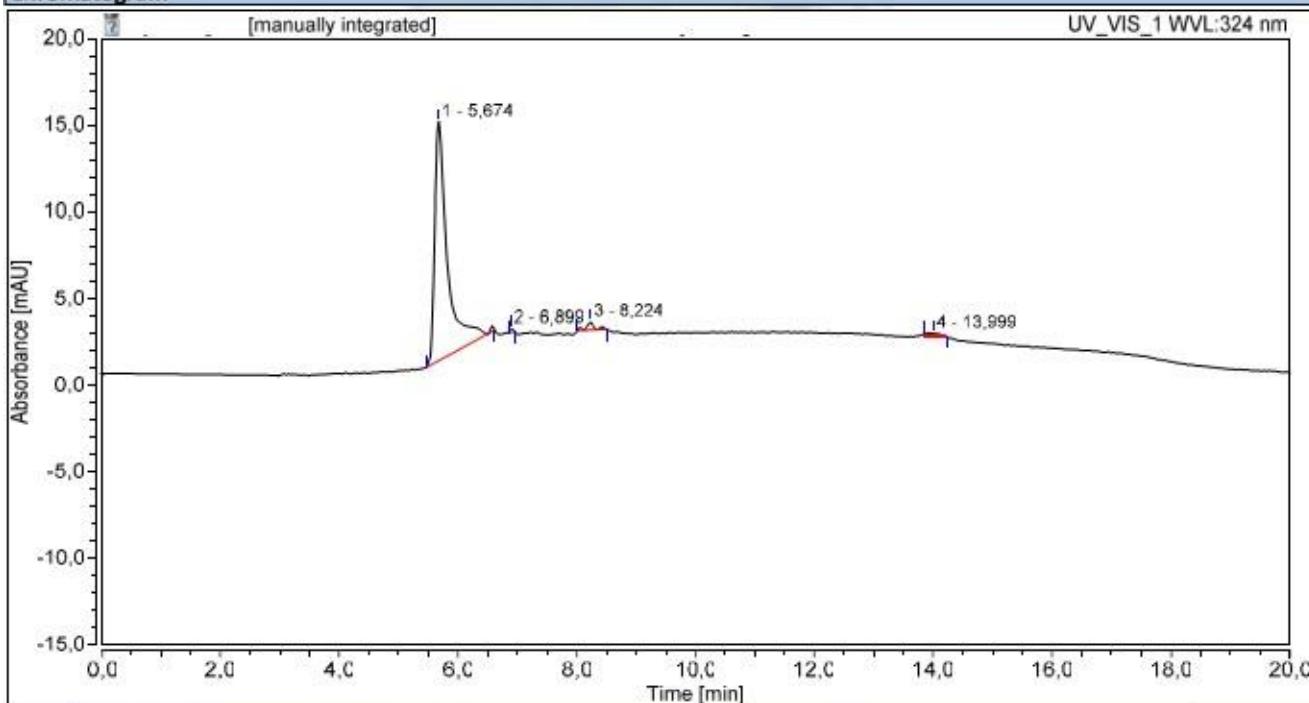
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		1,765	0,104	3,151	0,13	0,44	n.a.
2		2,499	79,204	685,067	96,10	95,87	n.a.
3		2,874	2,320	20,139	2,81	2,82	n.a.
4		3,649	0,794	6,232	0,96	0,87	n.a.
Total:			82,421	714,589	100,00	100,00	

Chromatogram and Results

Injection Details

Injection Name:	Muestra 4h	Run Time (min):	20,00
Vial Number:	RA3	Injection Volume:	20,00
Injection Type:	Unknown	Channel:	UV_VIS_1
Calibration Level:		Wavelength:	324
Instrument Method:	Muestras 130 y 136	Bandwidth:	n.a.
Processing Method:	Pureza muestras 130 y 136	Dilution Factor:	1,0000
Injection Date/Time:	30/jun./22 11:01	Sample Weight:	1,0000

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5,674	3,433	13,811	96,79	93,93	n.a.
2		6,899	0,013	0,235	0,36	1,60	n.a.
3		8,224	0,072	0,496	2,02	3,37	n.a.
4		13,999	0,029	0,162	0,83	1,10	n.a.
Total:			3,547	14,704	100,00	100,00	