

## SUPPORTING INFORMATION

### **Characterization of Dye Extracts from Historical Cultural-Heritage Objects using State-of-the-Art Comprehensive Two-Dimensional Liquid Chromatography and Mass Spectrometry with Active Modulation and Optimized Shifting Gradients**

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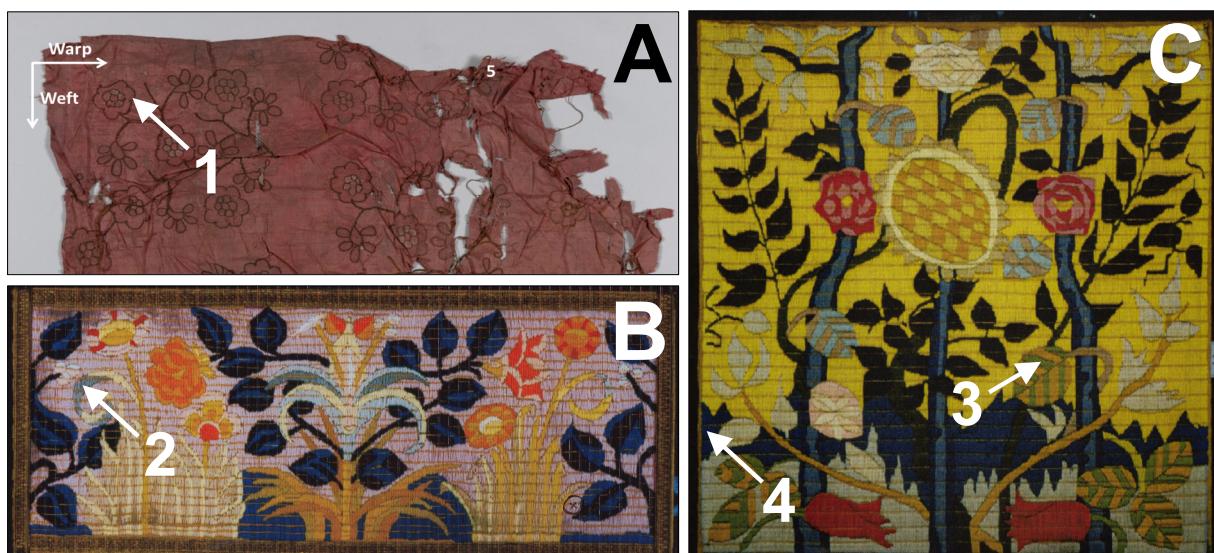
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## S-1 Historical samples and extraction procedure

Figure S-1 below shows the relevant historical objects from which the extract samples were obtained. The first sample (1) investigated is an extract from an embroidery fragment part of a collection of unique textiles found in 17th century shipwreck in the Waddenzee (Figure S-1A), in the northern part of The Netherlands. The collection is special since it was found (possibly stored in a chest), untouched for almost 400 years and most fragments were remarkably well preserved as a result of the archaeological environment. In total, about 250 fragments were found which could be related to about 25 different object groups. Among them, an eastern carpet, a bodice, several sleeves, a purse embroidered with silver yarn and, most preciously, a complete 17<sup>th</sup> century gown. Research is being conducted to understand the function and creation of the objects, as part of that research material analysis will be done.

The other samples represent a different dates and functions. The objects selected are owned by the Van Gogh museum (Amsterdam, the Netherlands) and are embroideries designed by Emile Bernard. Known as a painter and as a good friend of Vincent van Gogh, he designed several embroideries as well. The first investigated item is entitled *Plant and flowers on grey fond* and dates from 1892-1904 (Figure S-1B), the second is entitled *Plant and flowers on yellow fond* and is dated 1891-1892 (Figure S-1C). Both objects are very colourful; 21 samples were taken from the different colours found on the object. In this publication, only results on a limited number of extracts are presented. The arrows shown in Figure S-1 indicate the approximate sampled colour.



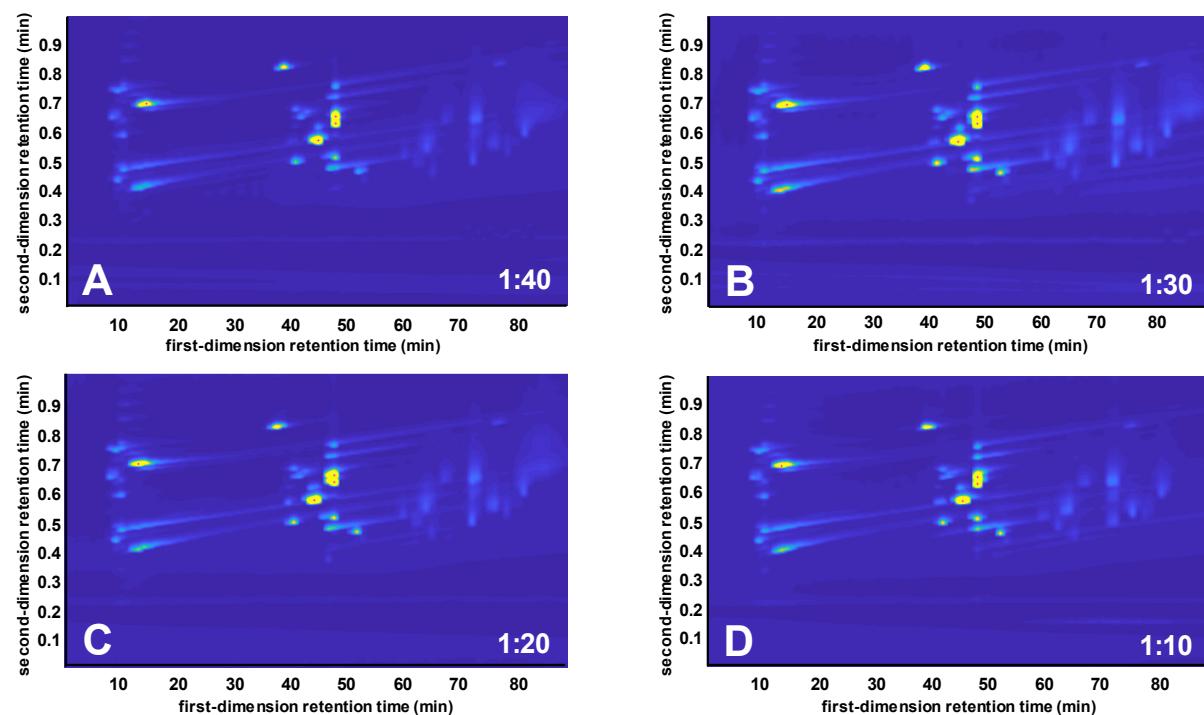
**Figure S-1** Photographs of sampled historical objects presented in this paper. Arrow depicts sampling location. Numbers refer to sample number. A) an embroidery fragment part of a collection of unique textiles found in 17th century shipwreck in the Waddenzee (Photograph: Museum Kaap Skil), B) *Plant and flowers on grey fond* by Emile Bernard, dating from 1892-1904 and C) *Plant and flowers on yellow fond* also by Emile Bernard and is dated 1891-1892. Photographs from B and C: Van Gogh Museum, Amsterdam.

The mild extraction procedure used for these samples is routinely applied in conservation science. It is known as the “oxalic-acid extraction method” and it is based on a published procedure<sup>1</sup>. Briefly, the procedure was as follows:

Approximately 1 mg of textile sample were admixed with 150 µL DMSO and heated at 80 °C for 10 min. After centrifugation, the supernatant was transferred to another vial. The residue was admixed with 100 µL of a solution of methanol/acetone/water/0.5 M oxalic acid 30:30:40:1 (v/v/v/v) and kept at 80 °C for 15 min. The DMSO extract was combined with the oxalic acid extract and the solution was centrifuged for 10 min. The supernatant was transferred to a clean 250 µL insert and 20 µL of the solution were injected into the LC×LC-DAD/ESI-ToF system. Where necessary, some of the samples were diluted 1:1 using MeOH/H<sub>2</sub>O (v/v).

## S-2 Dilution Ratio

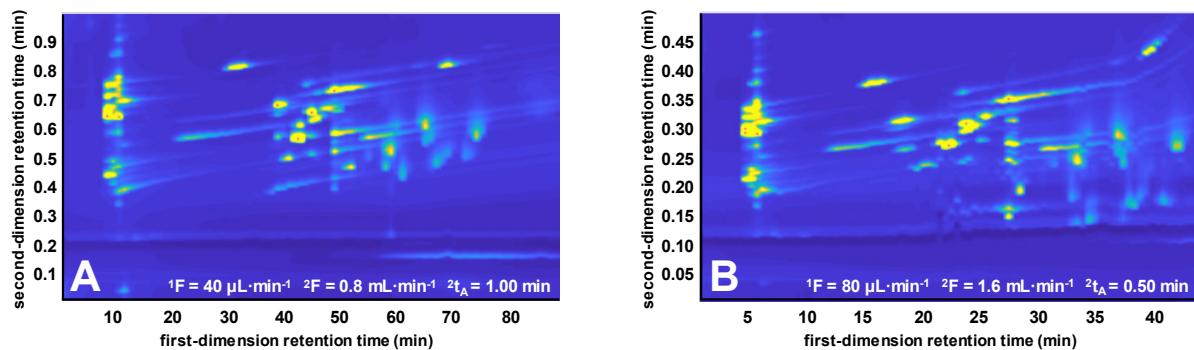
To achieve sufficient retention on the trap columns used in stationary-phase-assisted modulation, dilution flows are typically employed which decrease the solvation strength of the first-dimension effluent. The figure below showcases the application of different dilution ratios.



**Figure S-2** LC $\times$ LC chromatograms of a mixture of 80 natural and synthetic dyes using a dilution flow of A) 1:40, B) 1:30, C) 1:20 and D) 1:10 first-dimension effluent/formate buffer (v/v).

### S-3 Comparison of Modulation Times

The figure below shows the separation of a mixture of 80 synthetic and natural dyes using a modulation time of A) 1.0 and B) 0.5 minutes.



**Figure S-3** LC $\times$ LC separation of a mixture of 80 synthetic and natural dyes using a modulation time of A) 1.0 and B) 0.5 minutes.

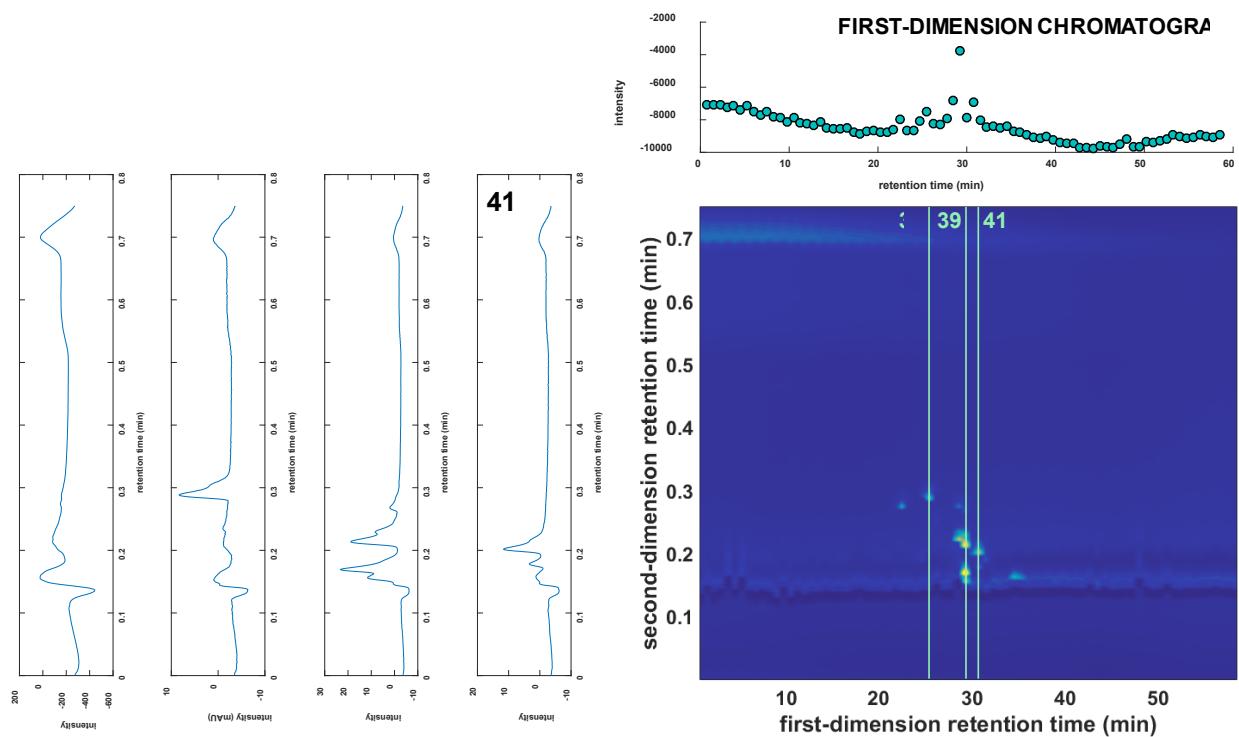
## S-4 LC $\times$ LC chromatograms: Clarification of appearance and guidelines for interpretation.

Figure S-4 below displays an LC $\times$ LC chromatogram of sample 2 as also shown in Figure 5B of the manuscript. To the left, the second-dimension chromatogram (indicated with SUM), and a number of highlighted modulations (indicated by their modulation number) are shown.

The SUM  $^2$ D chromatogram shows not much useful information as it represents the sum of all datapoints across all modulations. To learn more about the individual species, an analyst can make use of data-analysis software to extract the  $^2$ D chromatograms of modulations of interest through selection of specific modulations of interest. As shown by the  $^2$ D chromatograms of modulations 34, 39 and 41, a large number of peaks can be distinguished.

For the first-dimension chromatogram shown above the LC $\times$ LC chromatogram, this exercise is rather complicated. As can be seen, it is even less informative, since the number of datapoints is equal to the number of modulations. While one should be able to discern the peak shapes from this chromatogram, it is good to realize that on the  $^1$ D chromatogram, the peaks are no longer separated, and each modulation data-point represents the sum of all intensities in that modulation.

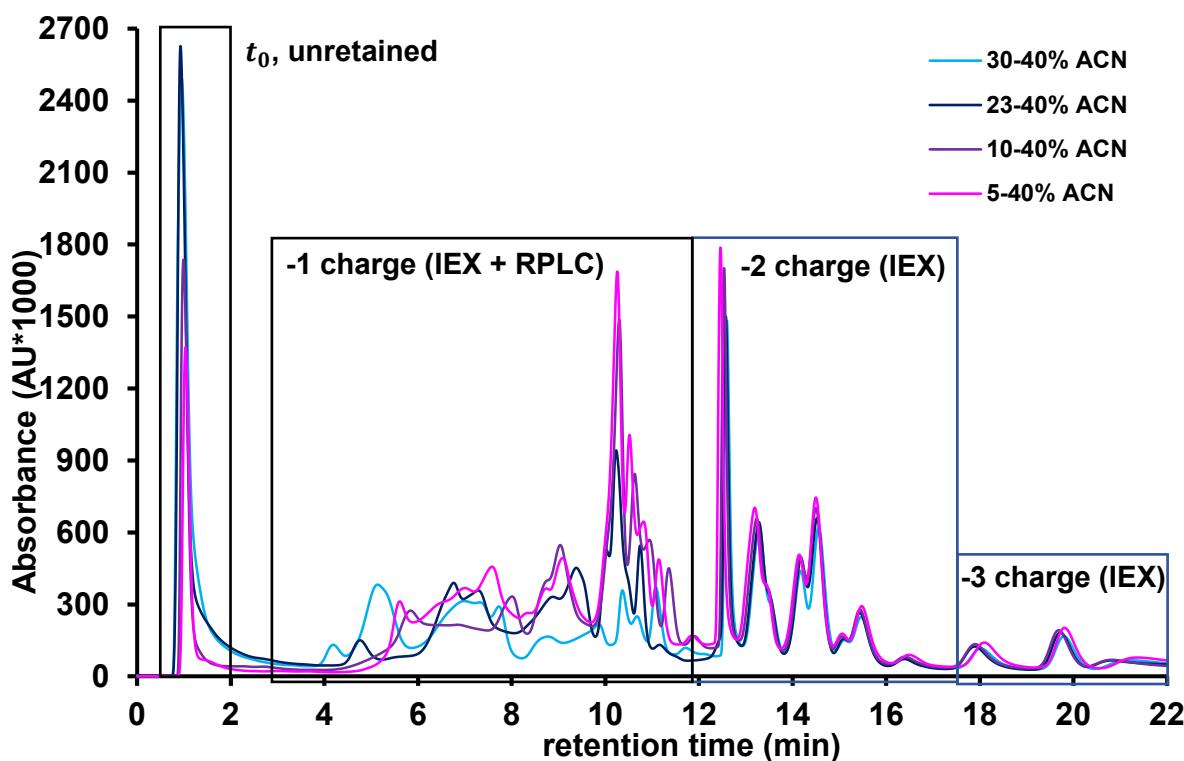
This explains why typically LC $\times$ LC data is shown using colour plots. Readers interested in learning more about LC $\times$ LC are referred elsewhere<sup>2,3</sup>.



**Figure S-4** LC $\times$ LC chromatogram of sample 2 as also shown in the manuscript in Figure 5B. Top: first-dimension chromatogram, left: second-dimension chromatogram of modulation 34, 39 and 41, and the sum of all modulations (full second-dimension chromatogram). See text for discussion.

## S-5 Strong Anion-Exchange Chromatography (First dimension)

Below, strong anion-exchange separations are shown of the mixture of 80 dyes. For all separations an identical salt concentration gradient was applied in combination with a different organic-modifier gradient program preceding it. While the retention of the strong anions is unchanged, the organic modifier appears to have a dramatic effect on the retention of neutral analytes and weaker anions.



**Figure S-5** Overlay of LC-UV chromatograms of the strong anion-exchange separation of a mixture of 80 natural and synthetic dyes using an organic modifier gradient of 30 to 40% (light blue), 23 to 40% (dark blue), 10 to 40% (dark purple) and 5 to 40% (light purple) acetonitrile as gradient preceding the 0 to 50 mM salt gradient used for the ion-exchange.

## S-6 Orthogonality

This section clarifies the calculation of the orthogonality using the Asterisk metric by Camenzuli and Schoenmakers<sup>4</sup> for the separation shown in Figure S-8. First the retention times ( $t_R$ ) of all detected peaks are extracted from the chromatogram (Table S-1).

**Table S-1** Overview of retention times in min.

<sup>1</sup> D time	<sup>2</sup> D time						
6.235	0.397	23.398	0.406	32.250	0.400	40.500	0.157
6.674	0.278	23.250	0.416	32.493	0.148	40.500	0.199
6.373	0.440	22.500	0.413	32.250	0.187	44.396	0.572
6.986	0.465	22.800	0.377	35.604	0.105	44.744	0.199
8.586	0.249	22.973	0.328	35.886	0.394	42.750	0.408
7.113	0.307	27.210	0.452	36.000	0.157	45.139	0.376
7.110	0.366	24.750	0.420	37.981	0.342	45.065	0.325
7.423	0.222	25.184	0.411	37.399	0.288	45.249	0.223
6.506	0.332	24.000	0.417	37.500	0.315	45.000	0.357
7.500	0.397	26.813	0.176	36.750	0.308	45.879	0.341
8.066	0.431	26.570	0.291	36.476	0.275	46.575	0.395
6.750	0.406	27.853	0.345	36.750	0.119	44.250	0.361
6.750	0.416	25.692	0.342	36.750	0.170	44.250	0.346
7.742	0.294	26.427	0.438	36.000	0.258	45.122	0.524
7.289	0.482	25.500	0.421	37.716	0.537	45.000	0.284
7.752	0.455	27.075	0.429	36.337	0.462	45.000	0.497
6.750	0.260	26.474	0.417	36.485	0.384	45.000	0.488
7.090	0.528	28.228	0.383	37.500	0.106	48.191	0.583
7.502	0.558	27.000	0.314	37.500	0.155	47.023	0.270
8.601	0.422	29.572	0.410	36.750	0.204	46.500	0.379
9.271	0.267	29.739	0.395	40.079	0.306	46.500	0.312
7.500	0.382	29.574	0.299	39.306	0.242	47.535	0.314
7.822	0.339	29.702	0.358	39.750	0.166	47.250	0.383
8.366	0.407	29.655	0.495	40.097	0.378	50.527	0.325
7.500	0.586	29.559	0.437	39.750	0.277	49.111	0.230
6.750	0.350	29.573	0.186	41.282	0.508	51.074	0.402
7.784	0.144	27.750	0.422	39.000	0.155	50.142	0.293
9.074	0.150	31.670	0.428	40.728	0.553	49.500	0.364
10.289	0.379	33.099	0.474	39.000	0.148	49.500	0.384
15.671	0.351	33.612	0.357	40.547	0.480	51.750	0.372
14.169	0.389	32.719	0.303	38.250	0.178	51.750	0.354
11.571	0.161	30.000	0.286	38.250	0.124	51.750	0.392
19.753	0.158	31.957	0.197	41.205	0.174	54.607	0.410
18.490	0.402	32.984	0.513	41.870	0.383	54.000	0.400
19.815	0.520	32.270	0.419	42.071	0.355	56.414	0.419
21.814	0.434	33.633	0.242	42.000	0.207	54.750	0.375
20.736	0.273	32.869	0.331	41.250	0.239	55.426	0.389
19.166	0.229	33.868	0.443	41.250	0.263	58.998	0.113
24.361	0.429	32.836	0.385	40.757	0.475		
24.160	0.342	32.250	0.263	40.500	0.409		

Note that the number of detected components is higher than the number of identified compounds. Indeed, unknown species, sometimes at trace concentrations, may be found through the separation power of 2D-LC. Next, the retention times are normalized (Table S-2).

**Table S-2** Overview of normalized retention times.

<b><sup>1</sup>D time</b>	<b><sup>2</sup>D time</b>						
0.000	0.606	0.325	0.625	0.493	0.613	0.649	0.107
0.008	0.360	0.322	0.645	0.498	0.088	0.649	0.195
0.003	0.696	0.308	0.639	0.493	0.169	0.723	0.970
0.014	0.749	0.314	0.566	0.557	0.000	0.730	0.195
0.045	0.299	0.317	0.463	0.562	0.601	0.692	0.630
0.017	0.420	0.398	0.721	0.564	0.106	0.737	0.564
0.017	0.543	0.351	0.654	0.602	0.493	0.736	0.457
0.023	0.244	0.359	0.635	0.591	0.381	0.739	0.244
0.005	0.472	0.337	0.648	0.593	0.436	0.735	0.524
0.024	0.607	0.390	0.146	0.578	0.422	0.751	0.489
0.035	0.678	0.385	0.386	0.573	0.352	0.765	0.602
0.010	0.626	0.410	0.498	0.578	0.029	0.720	0.532
0.010	0.645	0.369	0.493	0.578	0.134	0.720	0.500
0.029	0.393	0.383	0.693	0.564	0.318	0.737	0.871
0.020	0.783	0.365	0.657	0.597	0.898	0.735	0.371
0.029	0.726	0.395	0.673	0.571	0.743	0.735	0.814
0.010	0.321	0.384	0.649	0.573	0.580	0.735	0.796
0.016	0.879	0.417	0.578	0.593	0.000	0.795	0.993
0.024	0.943	0.394	0.433	0.593	0.103	0.773	0.342
0.045	0.659	0.442	0.634	0.578	0.206	0.763	0.570
0.058	0.336	0.445	0.603	0.641	0.416	0.763	0.429
0.024	0.576	0.442	0.402	0.627	0.285	0.783	0.434
0.030	0.486	0.445	0.526	0.635	0.127	0.777	0.579
0.040	0.627	0.444	0.811	0.642	0.566	0.839	0.457
0.024	1.000	0.442	0.690	0.635	0.358	0.813	0.258
0.010	0.509	0.442	0.168	0.664	0.837	0.850	0.618
0.029	0.081	0.408	0.659	0.621	0.104	0.832	0.391
0.054	0.093	0.482	0.671	0.654	0.930	0.820	0.539
0.077	0.570	0.509	0.768	0.621	0.088	0.820	0.580
0.179	0.511	0.519	0.523	0.650	0.780	0.863	0.554
0.150	0.591	0.502	0.411	0.607	0.151	0.863	0.517
0.101	0.115	0.450	0.376	0.607	0.038	0.863	0.597
0.256	0.109	0.488	0.190	0.663	0.144	0.917	0.633
0.232	0.616	0.507	0.848	0.675	0.578	0.905	0.612
0.257	0.862	0.493	0.652	0.679	0.520	0.951	0.653
0.295	0.683	0.519	0.285	0.678	0.212	0.919	0.560
0.275	0.349	0.505	0.470	0.664	0.277	0.932	0.591
0.245	0.257	0.524	0.704	0.664	0.328	1.000	0.016
0.344	0.673	0.504	0.583	0.654	0.769		
0.340	0.492	0.493	0.329	0.649	0.631		

For each retention time  $t_R(i)$ , the normalized retention time is calculated by

$$t_{R,norm}(i) = \frac{t_R(i) - \min(t_R)}{\max(t_R) - \min(t_R)} \quad (\text{S-1})$$

The resulting vectors of values are plotted against each other in Figure S-8. The asterisk method provides information on the spread of the peaks along a number of axes within the separation space to calculate the orthogonality. The spread for each axis is calculated by equations S-2-5, where  $\sigma$  is the standard deviation of the resulting vectors.

$$S_{Z_-} = \sigma([{}^1 t_{R,norm}] - [{}^2 t_{R,norm}]) \quad (\text{S-2})$$

$$S_{Z_+} = \sigma([{}^2 t_{R,norm}] - [1 - {}^1 t_{R,norm}]) \quad (\text{S-3})$$

$$S_{Z_1} = \sigma([{}^1 t_{R,norm}] - 0.5) \quad (\text{S-4})$$

$$S_{Z_2} = \sigma([{}^1 t_{R,norm}] - 0.5) \quad (\text{S-5})$$

Using the obtained spread parameters, the  $Z$  parameters may be calculated according to equations S-6-9. In this case, the  $Z$  parameters were  $Z_- = 0.940$ ,  $Z_+ = 0.965$ ,  $Z_1 = 0.852$ ,  $Z_2 = 0.824$ .

$$Z_- = |1 - 2.5|S_{Z_-} - 0.4|| \quad (\text{S-6})$$

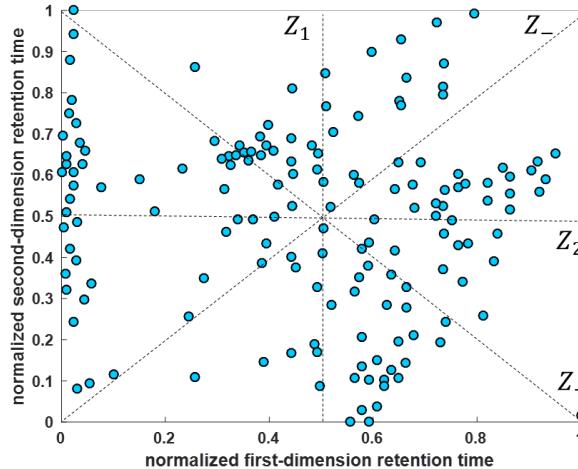
$$Z_+ = |1 - 2.5|S_{Z_+} - 0.4|| \quad (\text{S-7})$$

$$Z_1 = 1 - |2.5 \cdot S_{Z_1} \cdot \sqrt{2} - 1| \quad (\text{S-8})$$

$$Z_2 = 1 - |2.5 \cdot S_{Z_2} \cdot \sqrt{2} - 1| \quad (\text{S-9})$$

Finally, the orthogonality value may be calculated by taking the square root of the product of all  $Z$  parameters (Equation S-10). In this case the value was 0.798.

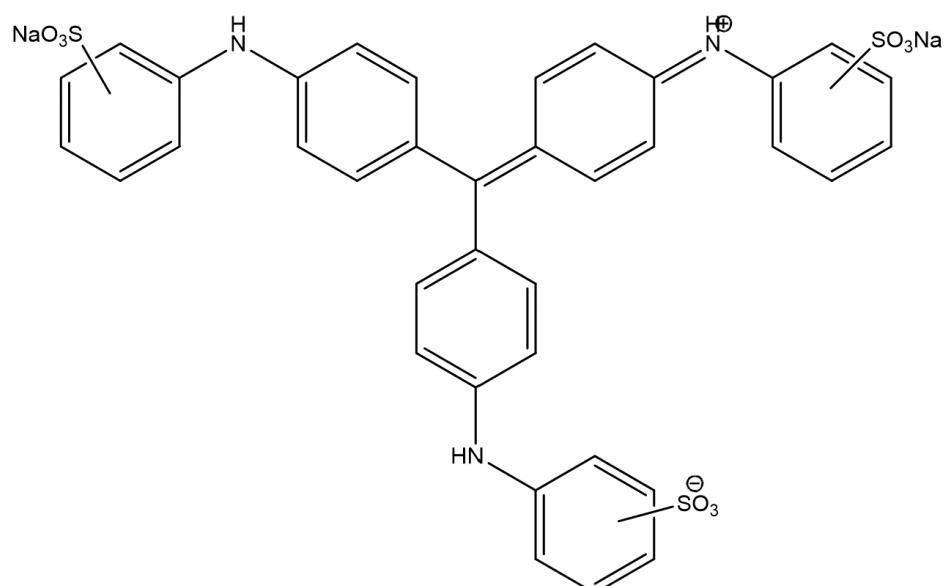
$$A_O = \sqrt{Z_- \cdot Z_+ \cdot Z_1 \cdot Z_2} \quad (\text{S-10})$$



**Figure S-6** Plot of normalized retention times of the first dimension against those of the second dimension. In overlay, the four asterisk axes  $Z_1$ ,  $Z_-$ ,  $Z_2$  and  $Z_+$  have been plotted.

S-7 Water Blue IN

The generic molecular structure of Water Blue IN is shown below.



**Figure S-7** Generic molecular structure of Water Blue IN. Note that the dyestuff Water Blue IN is known to contain a large number of variations of the structure above.

## S-8 Reference database

This section contains a full overview of the reference database recorded for this study using the 1D-LC methods shown below.

### ION-EXCHANGE

Column: Agilent PL-SAX 1000Å 8µm particles, 150×2.1mm. Flow rate: 0.5 mL·min<sup>-1</sup>. Injection volume 20 µL. Four mobile phases were used: A) 60% water (Tris buffer, 5mM, pH=7.5) and 40% acetonitrile, B) 60% water (Tris buffer, 5mM, pH=7.5) with 50 mM ammonium sulfate and 40% acetonitrile, C) 100% water with 1M NaCl, D) 95% water (Tris buffer, 5mM, pH=7.5) and 5% acetonitrile.

Gradient program: 0-0.5 min: isocratic, 100% D; 0.5-4.5 min: linear gradient from 100% D to 100% A; 4.5-5 min: isocratic, 100% A; 5-15 min: linear gradient from 100% A to 100% B; 15-19 min: isocratic at 100% B; 19-19.5 min: linear gradient from 100% B to 100% C; 19.5-27 min: isocratic at 100% C; 27-27.5 min: linear gradient from 100% C to 100% D.

### ION-PAIR REVERSED-PHASE

Column: Agilent ZORBAX Eclipse Plus C18 Rapid Resolution HT (959941-902, 50×4.6mm, 1.8µm particles). Flow rate: 1.85 mL·min<sup>-1</sup>. Injection volume: 5 µL. Two mobile phases are used: A) 95% water TEA (5 mM) buffer pH=3; 5% acetonitrile, B) 5% water, TEA (5 mM) buffer pH=3; 95% acetonitrile

The TEA buffer is prepared dissolving triethylamine (TEA) in a concentration of 5 mM in water and adding formic acid until pH 3.0 is reached.

Gradient program: 0-0.25 min: isocratic, 100% A; 0.25-8.25 min: linear gradient from 100% A to 100% B; 6.25-8.75 min: isocratic, 100% B; 8.75-9.50 min: linear gradient from 100% B to 100% A; 9.50-11 min: isocratic at 100% A.

The flow leaving the column was split through a T-junction: 500×0.254mm tubing towards the DAD detector and 500×0.127mm tubing towards the MS. This means that the section of the blue tubing is 4 times higher, therefore approximately 20% of the flow (0.37 mL/min) reached the MS instrument and 80% (1.48 mL/min) reached the DAD detector.

### GENERAL INFORMATION DYE DATABASE

The UV-VIS spectra have been recorded separately from the MS spectra. Consequently, the reported retention times of chromatographic bands do not match. In some cases, the corrected retention times are reported. The aim of the database is to provide additional data related to the investigated compounds. It is not designed for identification purposes and identification of all observed species within a sample was not within the scope. In some cases, full identification is provided. [M] indicates either the main component found in the sample.

## S-8.1. Alizarin

### GENERAL INFORMATION

**Alternative names:** Turkey Red; 1,2-Dihydroxyanthraquinone

**Color Index Name:** Mordant Red 11

**Color Index Number:** 58000

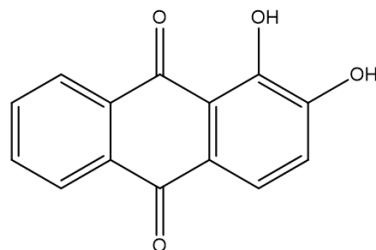
**Type of dye:** Anthraquinone

**Charge:** 0

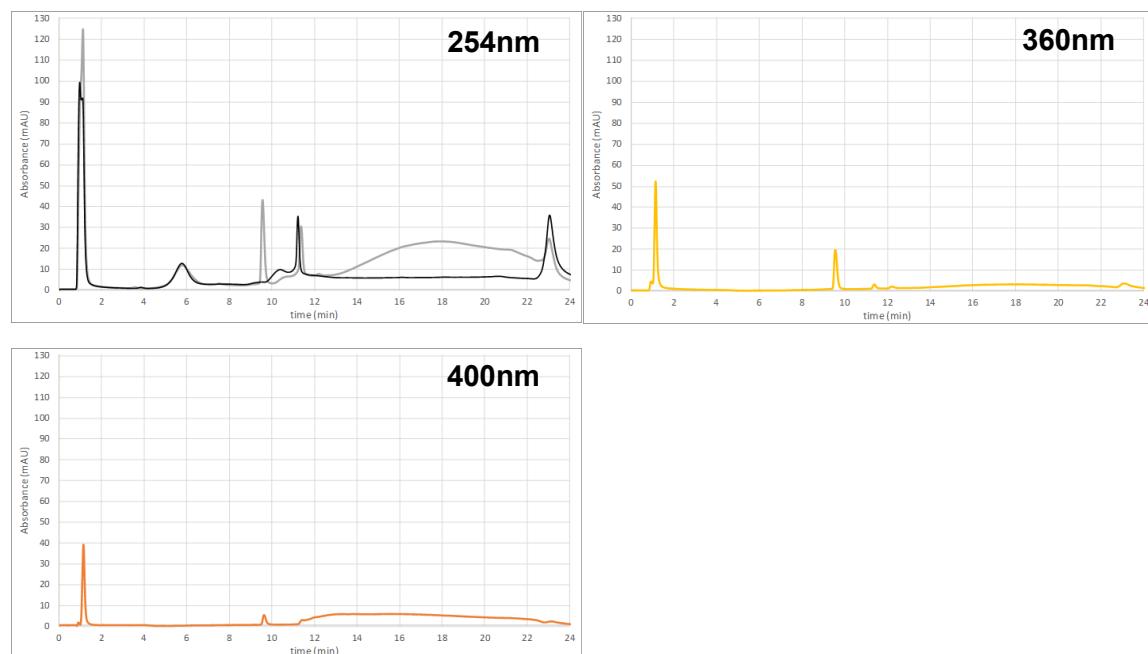
**Molecular Formula:** C<sub>14</sub>H<sub>8</sub>O<sub>4</sub>

**Molecular Weight**

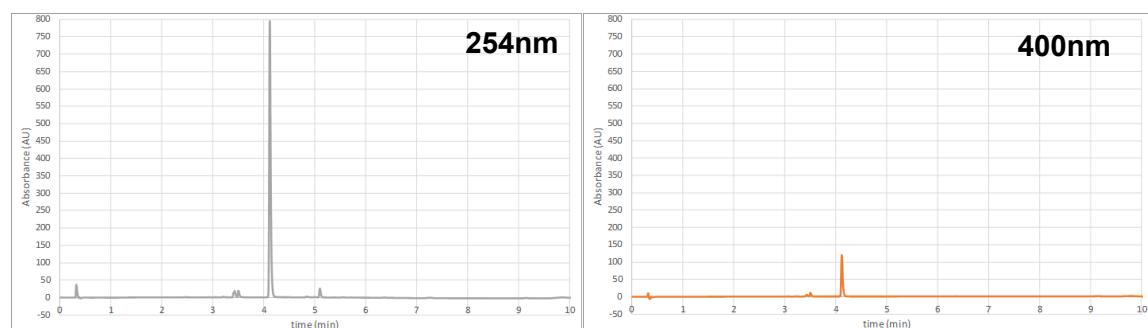
Full molecule:	240.21
Monoisotopic	240.04



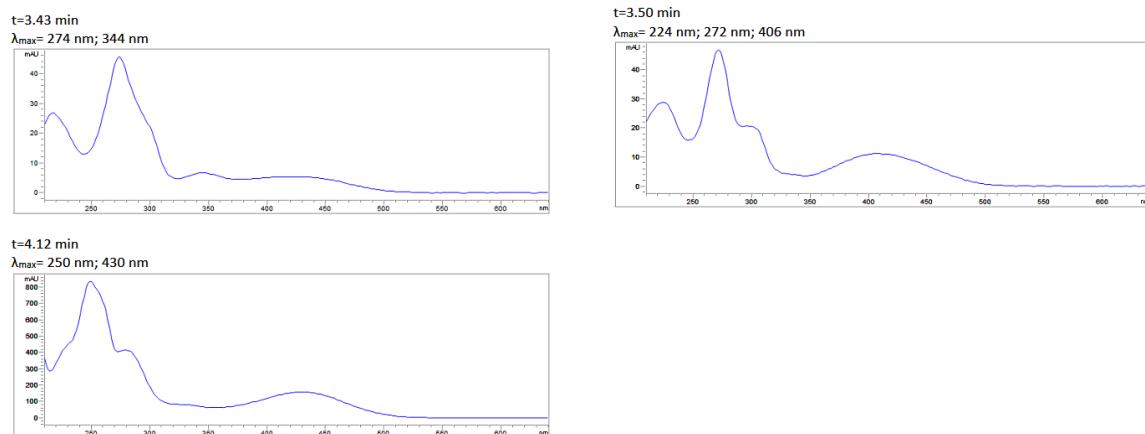
### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

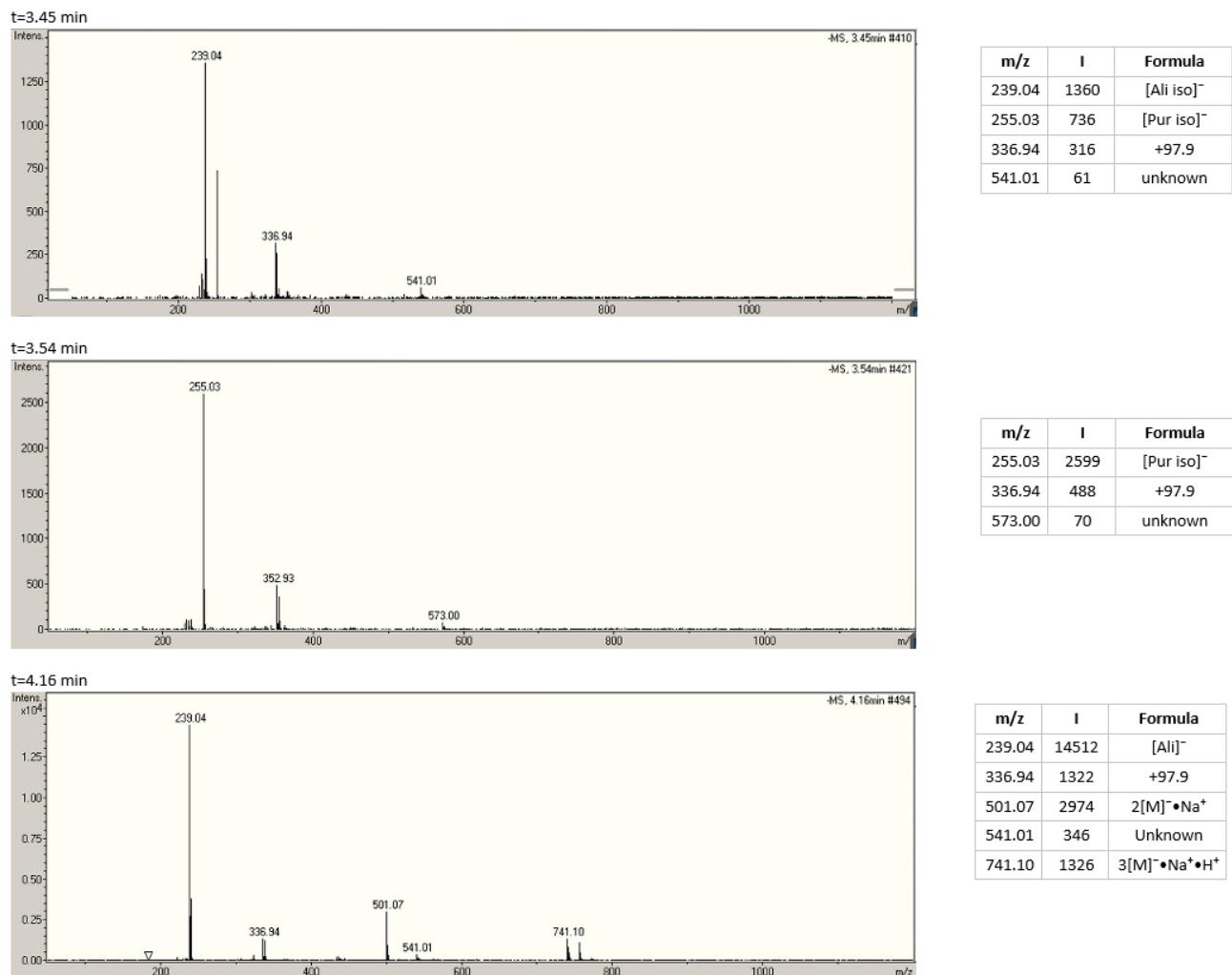


## UV-VIS SPECTRA



## MASS SPECTRA

MS (negative mode)

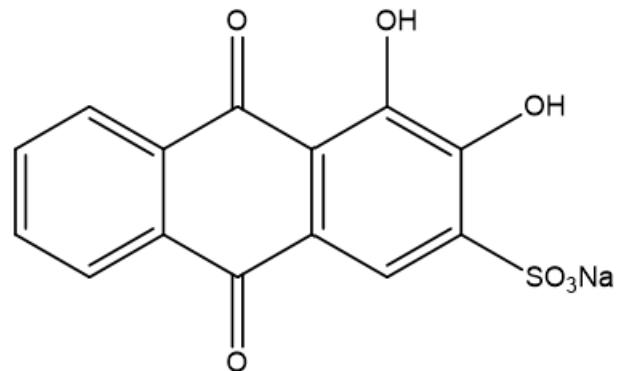


## S-8.2. Alizarin Red S

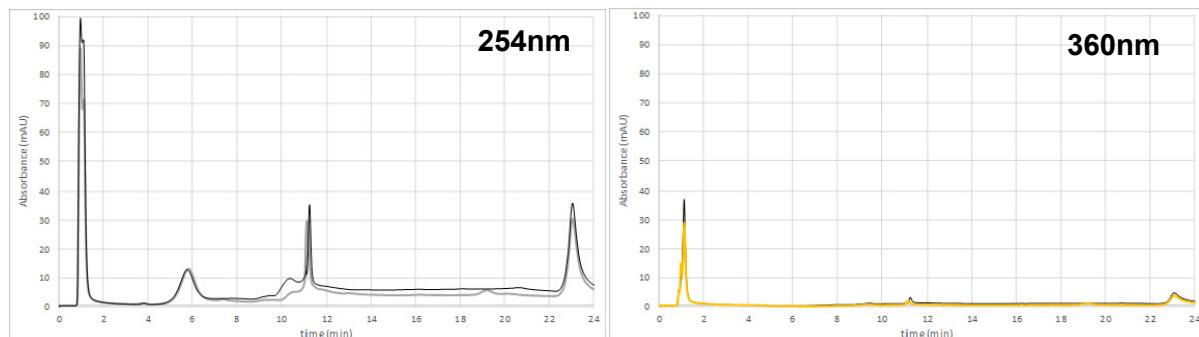
### GENERAL INFORMATION

**Alternative Name:** Diamond Red W  
**Color Index Name:** Mordant Red 3  
**Color Index Number:** 58005  
**Type of dye:** Anthraquinone  
**Charge:** -1  
**Molecular Formula:** C<sub>14</sub>H<sub>7</sub>O<sub>7</sub>S (ion, -1)  
**Molecular Weight**

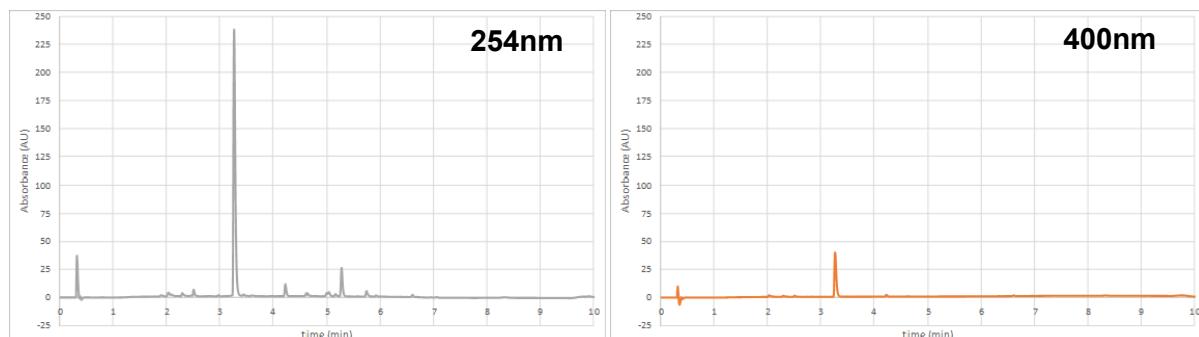
Full molecule:	342.26
Ion (-1)	319.27
Ion (-1), monoisotopic	318.99



### CHROMATOGRAMS: ION-EXCHANGE

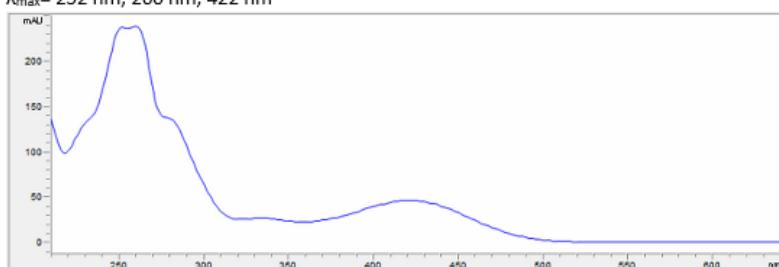


### CHROMATOGRAMS: REVERSED-PHASE



### UV-VIS SPECTRA

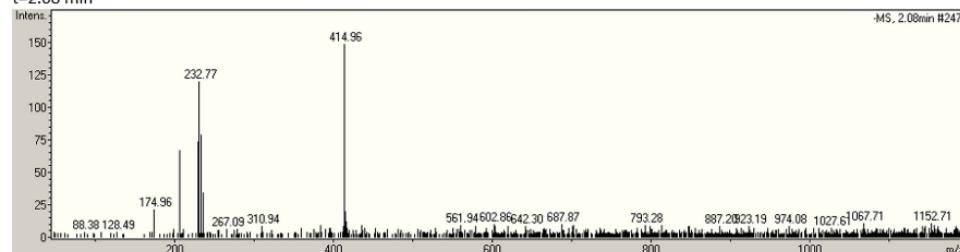
t=3.27 min  
 $\lambda_{\text{max}} = 252 \text{ nm; } 260 \text{ nm; } 422 \text{ nm}$



## MASS SPECTRA

MS (negative mode)

t=2.08 min



m/z	I	Formula
414.96	149	unknown

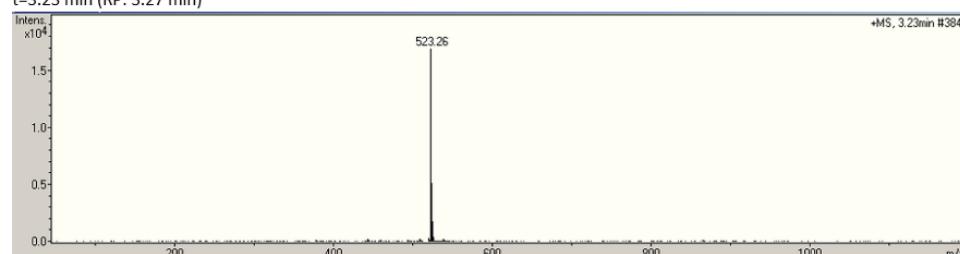
t=3.31 min



m/z	I	Formula
319.00	14106	[M] <sup>-</sup>

MS (positive mode)

t=3.23 min (RP: 3.27 min)



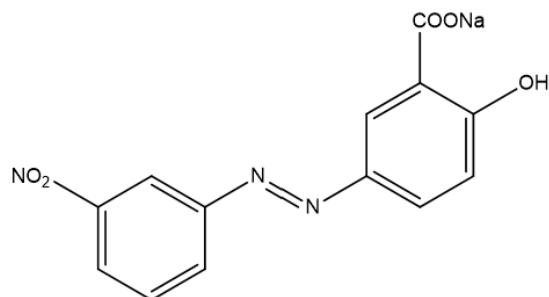
m/z	I	Formula
523.26	16938	[M] <sup>-</sup> •2[TEAH] <sup>+</sup>

### S-8.3. Alizarin Yellow

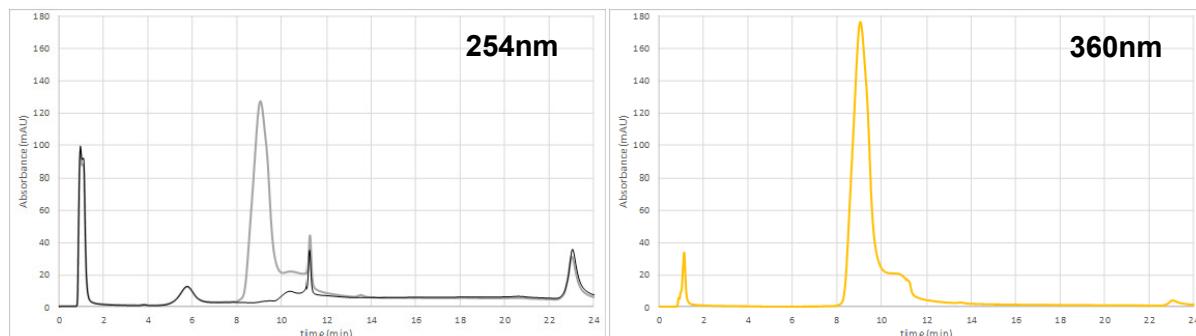
#### GENERAL INFORMATION

**Alternative Name:** Alizarin Yellow GG  
**Color Index Name:** Mordant Yellow 1  
**Color Index Number:** 14025  
**Type of dye:** Monoazo  
**Charge:** -1  
**Molecular Formula:** C<sub>13</sub>H<sub>8</sub>N<sub>3</sub>O<sub>5</sub> (ion, -1)  
**Molecular Weight**

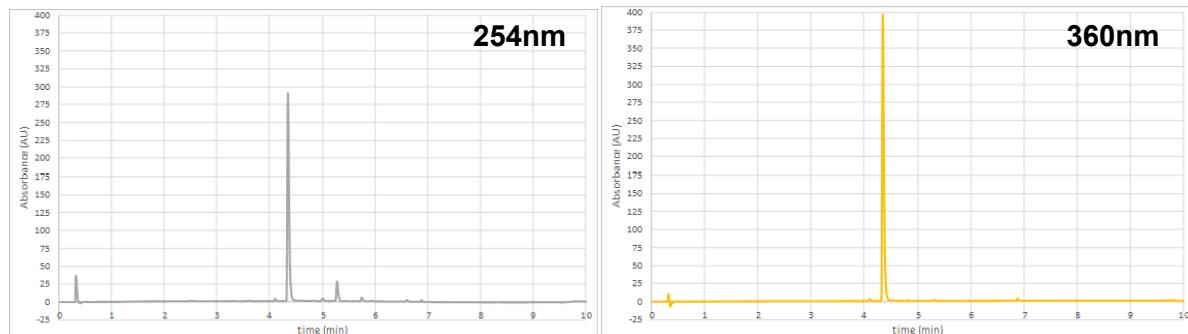
Full molecule:	309.21
Ion (-1)	286.22
Ion (-1), monoisotopic	286.05



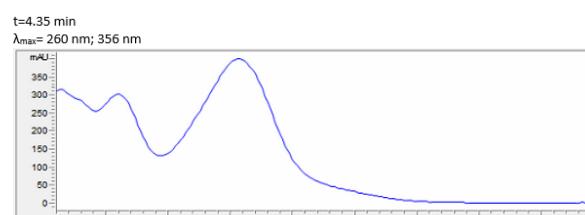
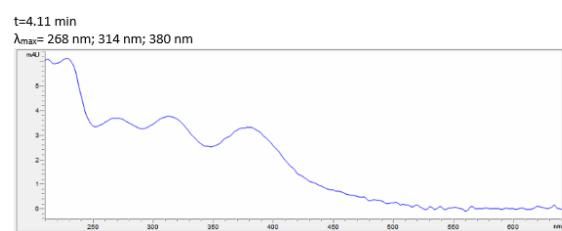
#### CHROMATOGRAMS: ION-EXCHANGE



#### CHROMATOGRAMS: REVERSED-PHASE



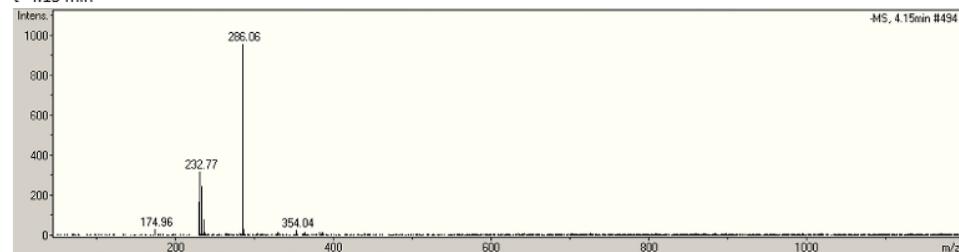
#### UV-VIS SPECTRA



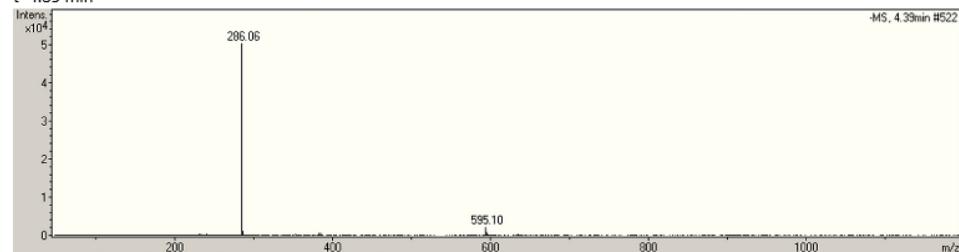
## MASS SPECTRA

MS (negative mode)

t=4.15 min



t=4.39 min



## S-8.4. Amaranth

### GENERAL INFORMATION

**Color Index Name:** Acid Red 27

**Color Index Number:** 16185

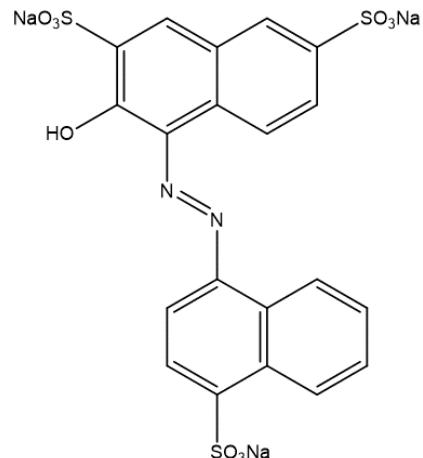
**Type of dye:** Monoazo

**Charge:** -3

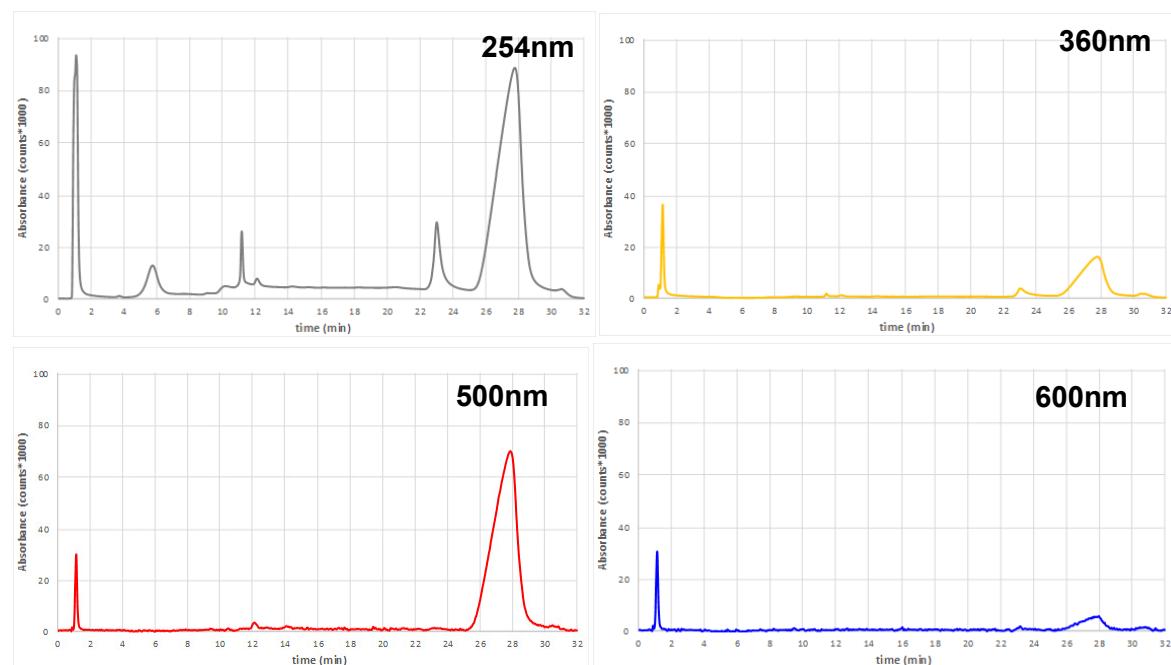
**Molecular Formula:** C<sub>20</sub>H<sub>11</sub>N<sub>2</sub>O<sub>10</sub>S<sub>3</sub> (ion, -3)

**Molecular Weight**

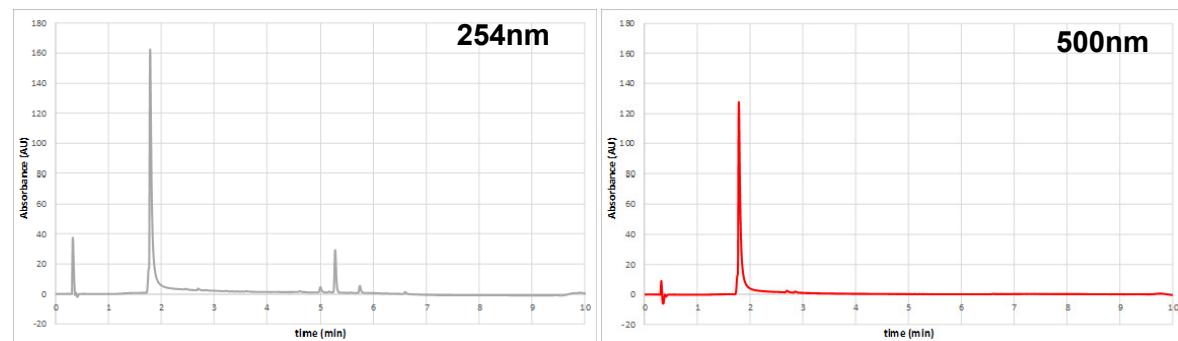
Full molecule:	604.47
Ion (-3)	535.51
Ion (-3), monoisotopic	534.96



### CHROMATOGRAMS: ION-EXCHANGE



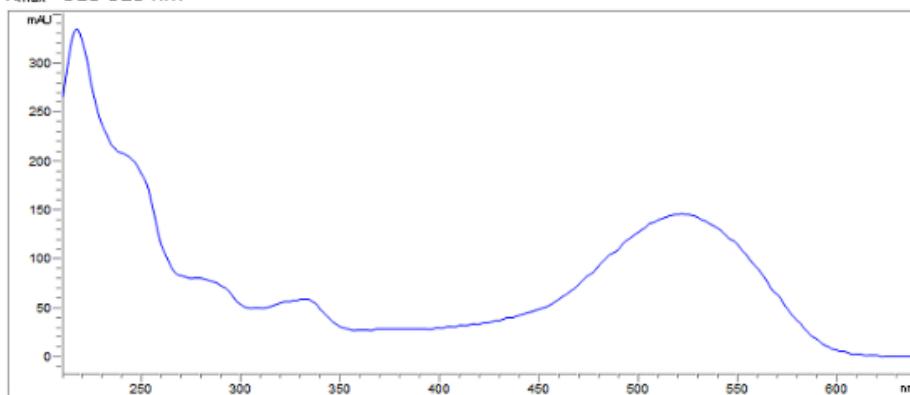
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

t=1.78 min

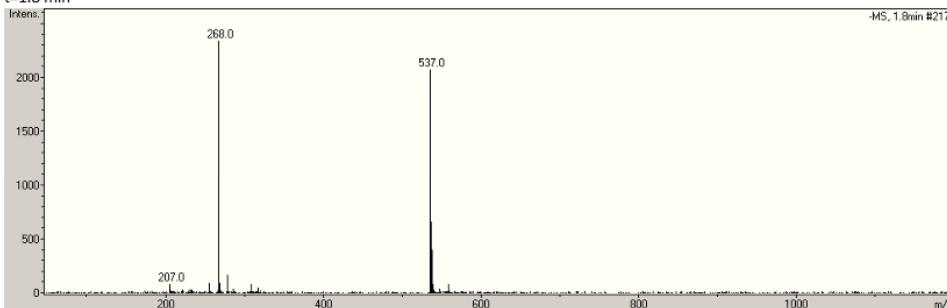
$\lambda_{\text{max}} = 518-523 \text{ nm}$



## MASS SPECTRA

MS (negative mode)

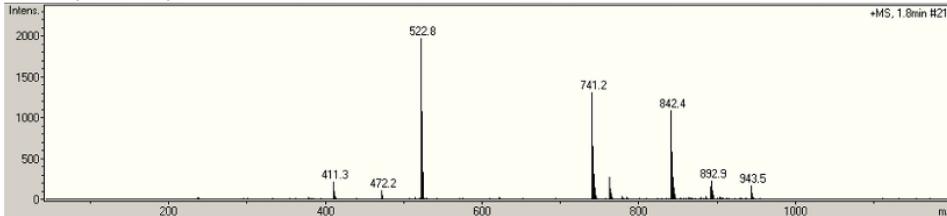
t=1.8 min



m/z	I	Formula
537.0	2075	$[\text{MH}_2]^-$
268.0	2347	$[\text{MH}]^2 \bullet \text{H}^+$

MS (positive mode)

t=1.8 min (RP: 1.78 min)



m/z	I	Formula
411.3	219	unknown
472.2	103	$[\text{MH}]^{2-} \bullet 4[\text{TEAH}]^+$
522.8	1984	$[\text{M}]^{3-} \bullet 5[\text{TEAH}]^+$
741.2	1256	$[\text{MH}_2]^- \bullet 2[\text{TEAH}]^+$
763.2	267	$[\text{MH}]^2 \bullet \text{Na}^+ \bullet 2[\text{TEAH}]^+$
842.4	1093	$[\text{MH}]^{2-} \bullet 3[\text{TEAH}]^+$
892.9	224	unknown
943.5	165	$[\text{M}]^{3-} \bullet 4[\text{TEAH}]^+$

### S-8.5. Amido Black 10B

#### GENERAL INFORMATION

**Color Index Name:** Acid Black 1

**Color Index Number:** 20470

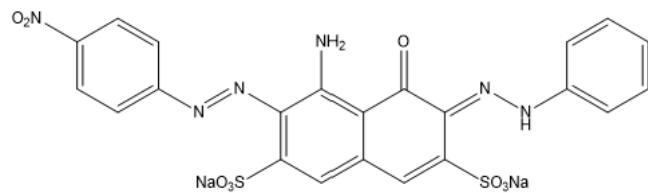
**Type of dye:** Diazo

**Charge:** -2

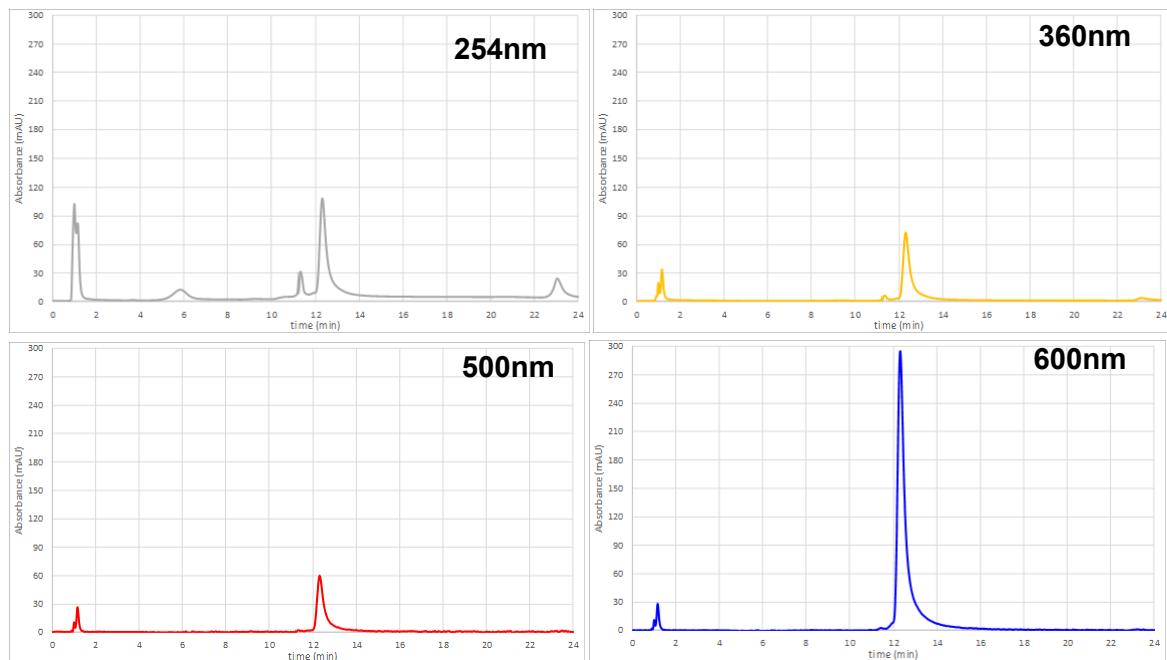
**Molecular Formula:** C<sub>22</sub>H<sub>14</sub>N<sub>6</sub>O<sub>9</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

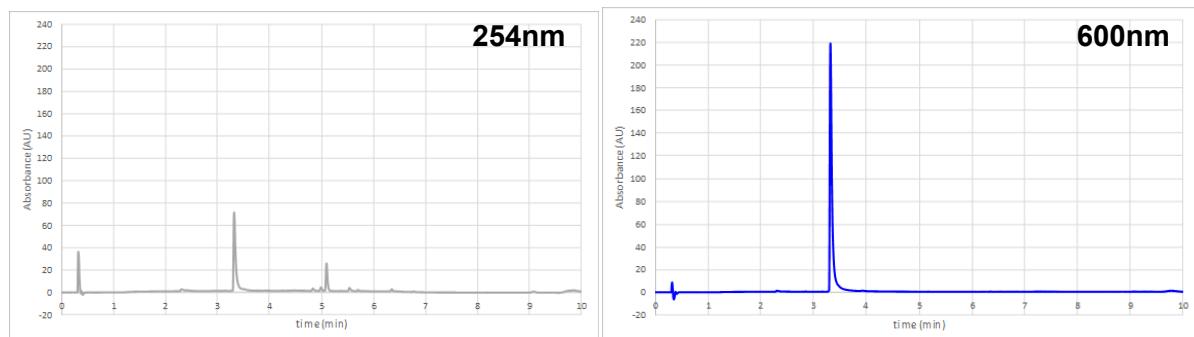
Full molecule:	616.49
Ion (-2)	570.51
Ion (-2), monoisotopic	570.03



#### CHROMATOGRAMS: ION-EXCHANGE

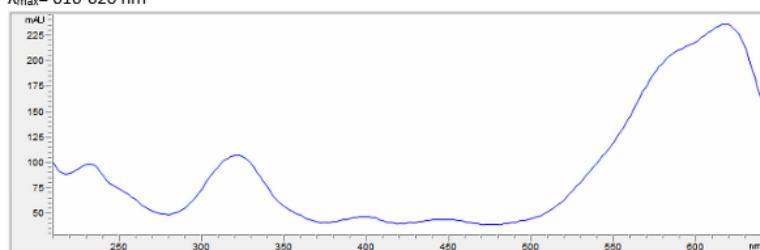


#### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

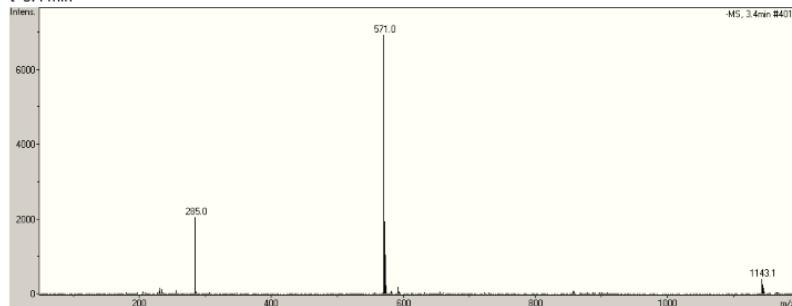
$t=3.32$  min  
 $\lambda_{\text{max}}= 616\text{-}620 \text{ nm}$



## MASS SPECTRA

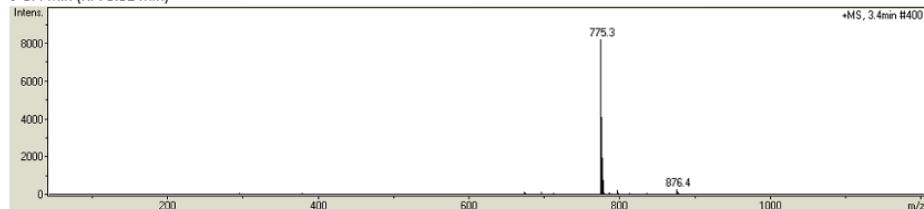
MS (negative mode)

$t=3.4$  min



MS (positive mode)

$t=3.4$  min (RP: 3.32 min)



## S-8.6. Amido Naphthol Red G

### GENERAL INFORMATION

**Alternative names:** Fast Crimson G

**Color Index Name:** Acid Red 1

**Color Index Number:** 18050

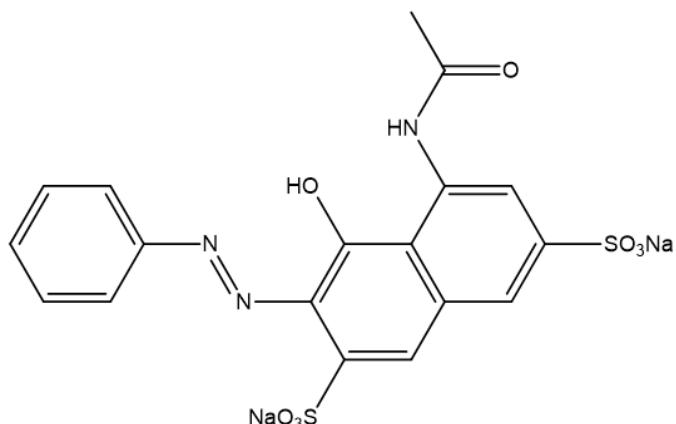
**Type of dye:** Monoazo

**Charge:** -2

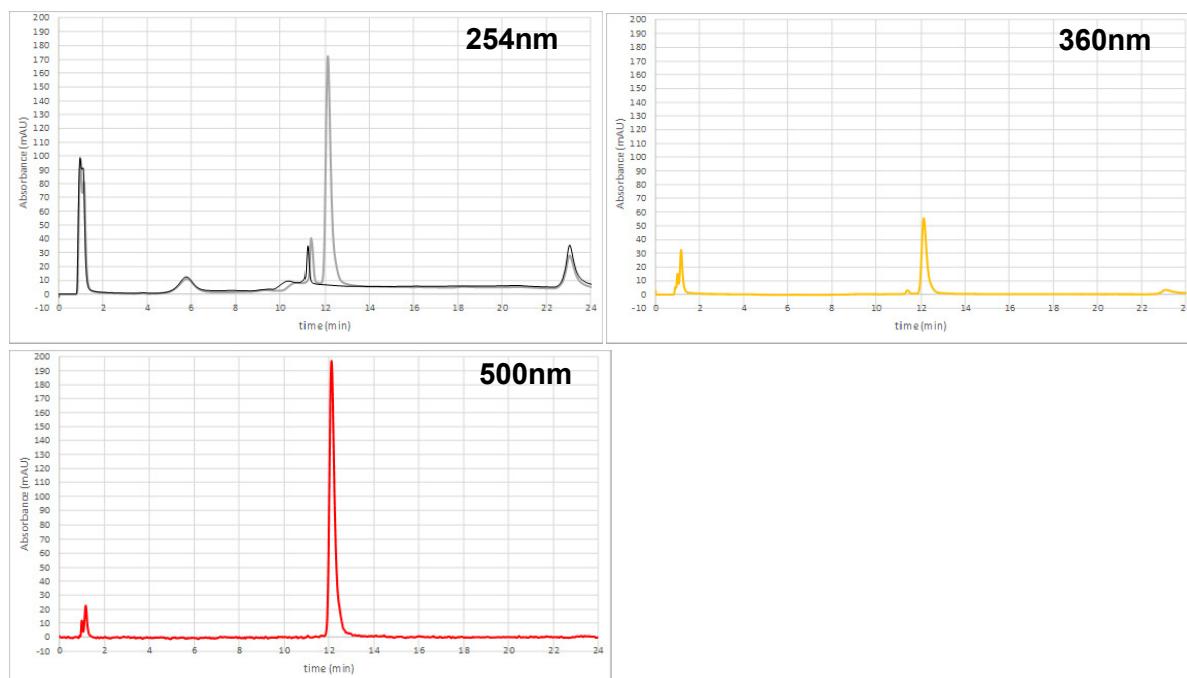
**Molecular Formula:** C<sub>18</sub>H<sub>13</sub>N<sub>3</sub>O<sub>8</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

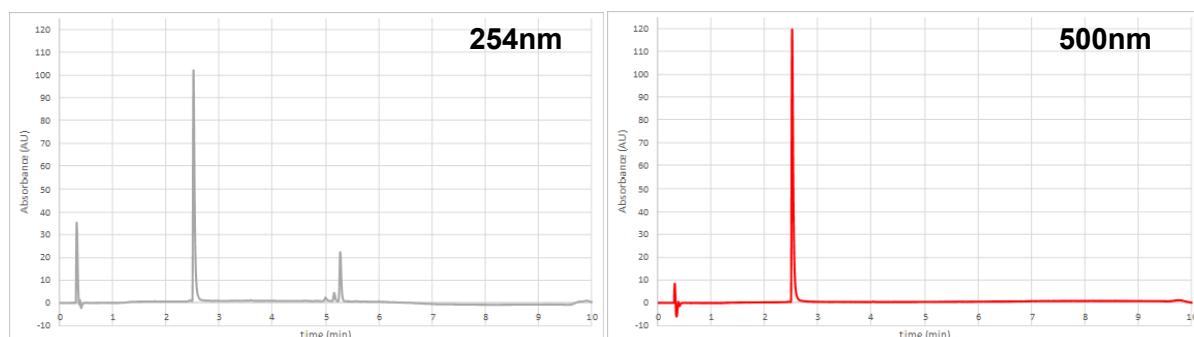
Full molecule:	509.42
Ion (-2)	463.44
Ion (-2), monoisotopic	463.02



### CHROMATOGRAMS: ION-EXCHANGE



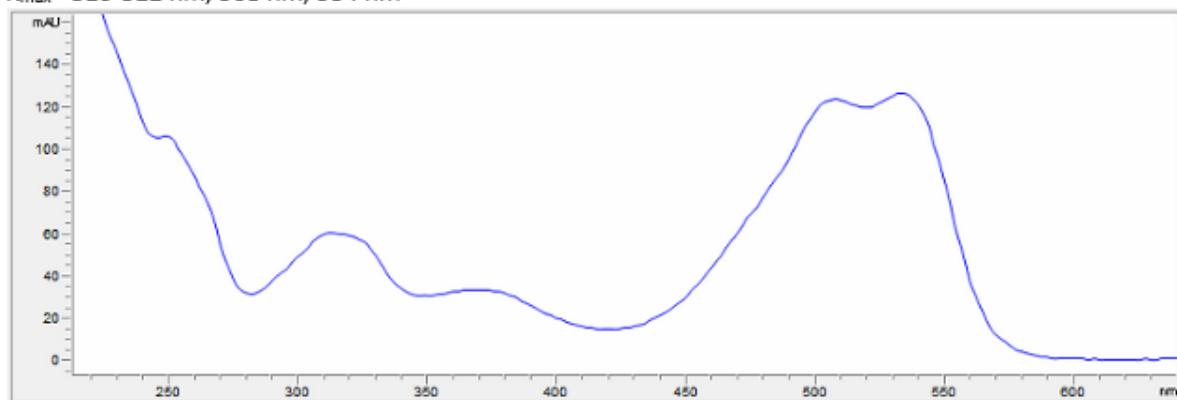
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

t=2.52 min

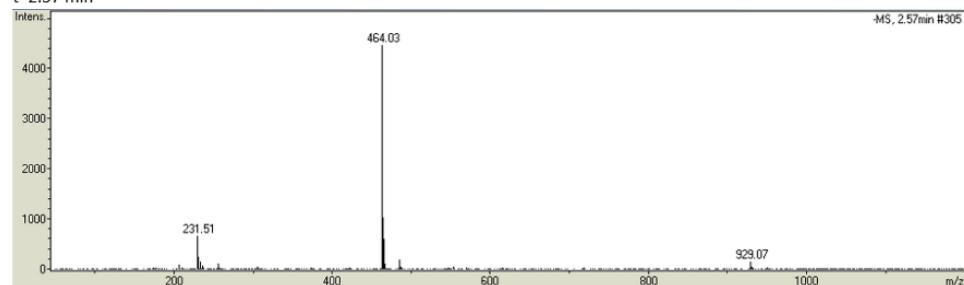
$\lambda_{\text{max}} = 310-312 \text{ nm}; 508 \text{ nm}; 534 \text{ nm}$



## MASS SPECTRA

### MS (negative mode)

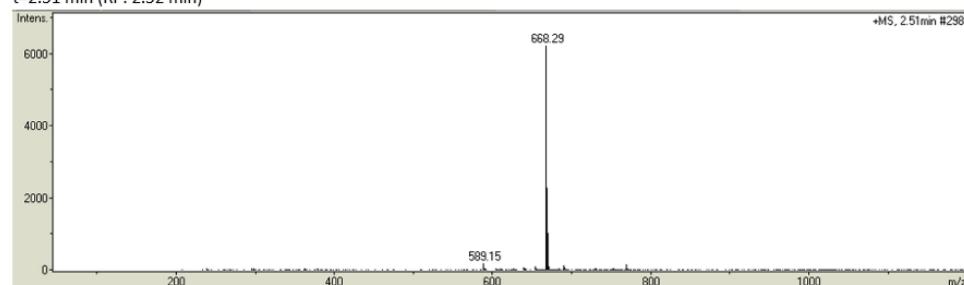
t=2.57 min



m/z	I	Formula
231.51	650	[M] <sup>2-</sup>
464.03	4488	[MH] <sup>-</sup>
929.07	133	[2MH] <sup>-•</sup> H <sup>+</sup>

### MS (positive mode)

t=2.51 min (RP: 2.52 min)



m/z	I	Formula
589.15	167	[MH] <sup>-•</sup> Na <sup>+</sup> •[TEAH] <sup>+</sup>
668.29	6223	[MH] <sup>-•</sup> 2[TEAH] <sup>+</sup>

## S-8.7. Auramine

### GENERAL INFORMATION

**Alternative names:** Auramine O

**Color Index Name:** Basic Yellow 2

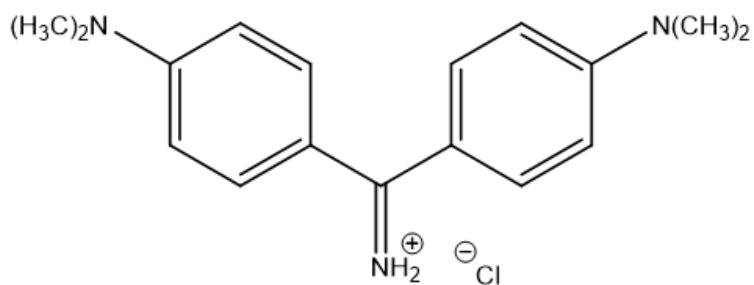
**Color Index Number:** 41000

**Type of dye:** Diarylmethane

**Charge:** +1

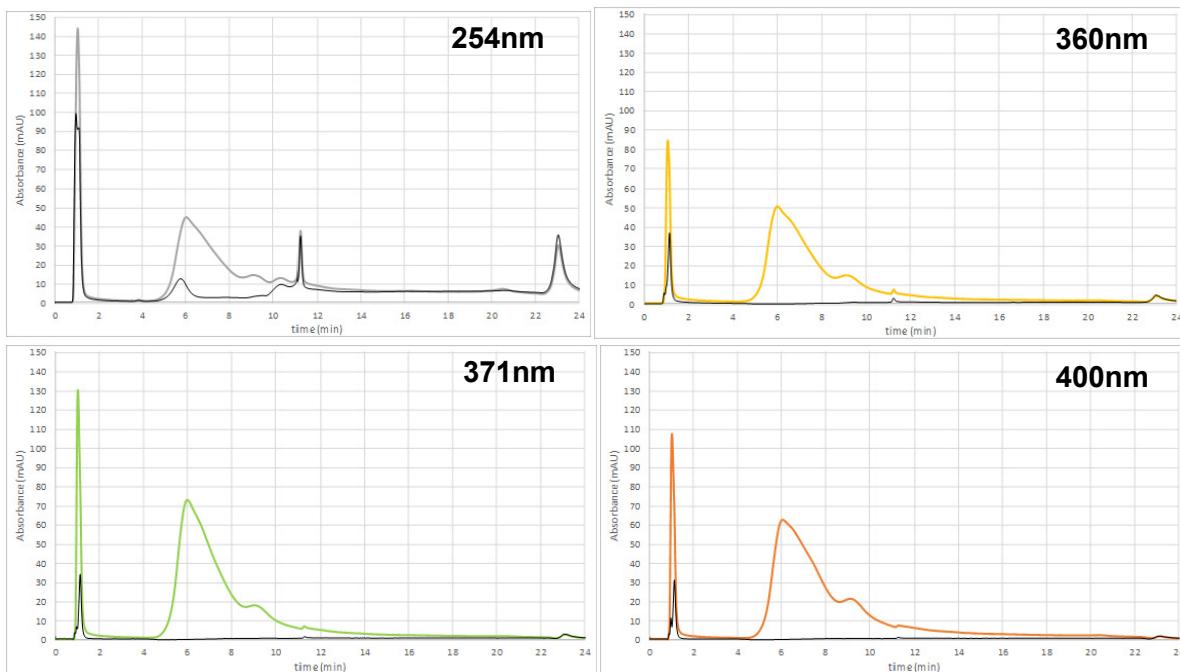
**Molecular Formula:** C<sub>17</sub>H<sub>22</sub>N<sub>3</sub> (ion, +1)

**Molecular Weight**

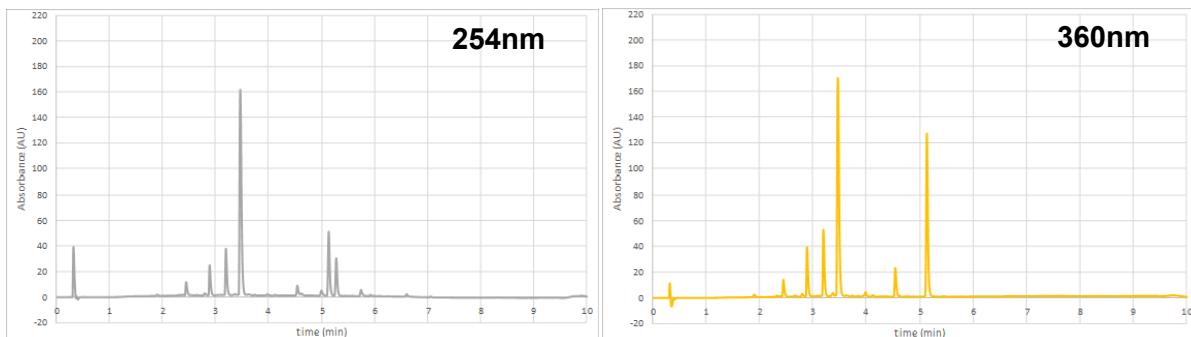


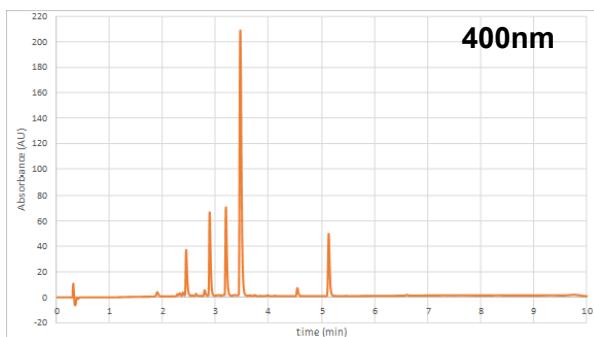
Full molecule:	303.83
Ion (+1)	268.38
Ion (+1), monoisotopic	268.18

### CHROMATOGRAMS: ION-EXCHANGE

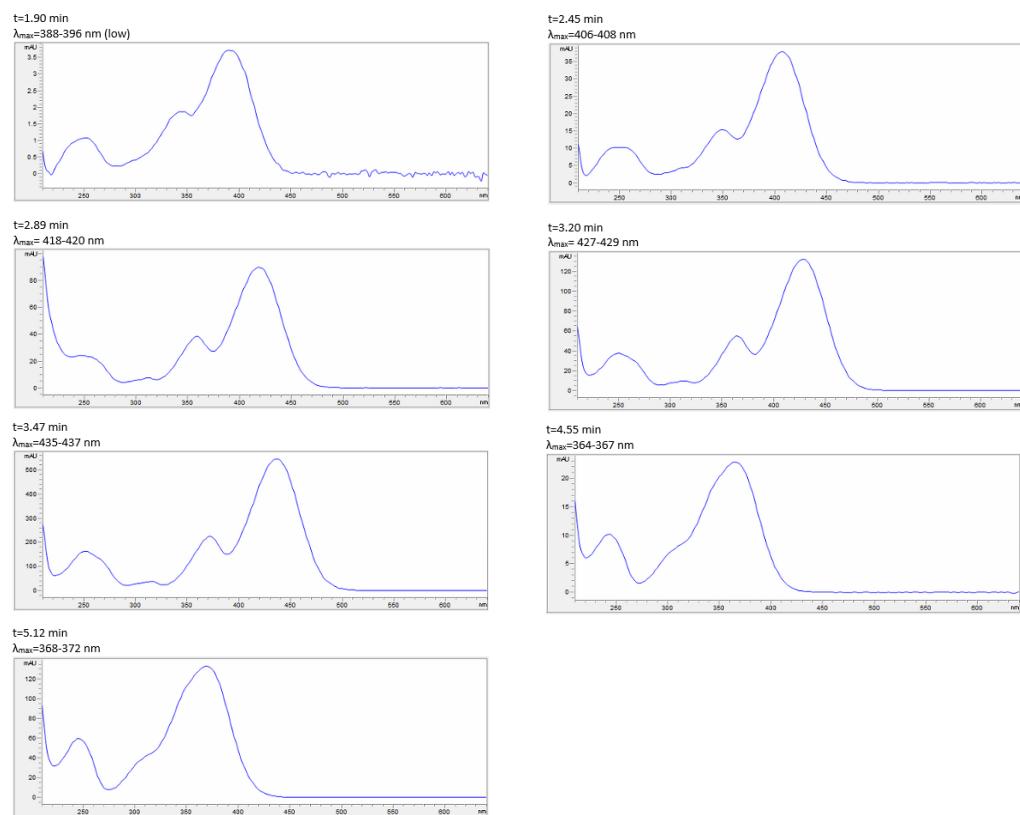


### CHROMATOGRAMS: REVERSED-PHASE

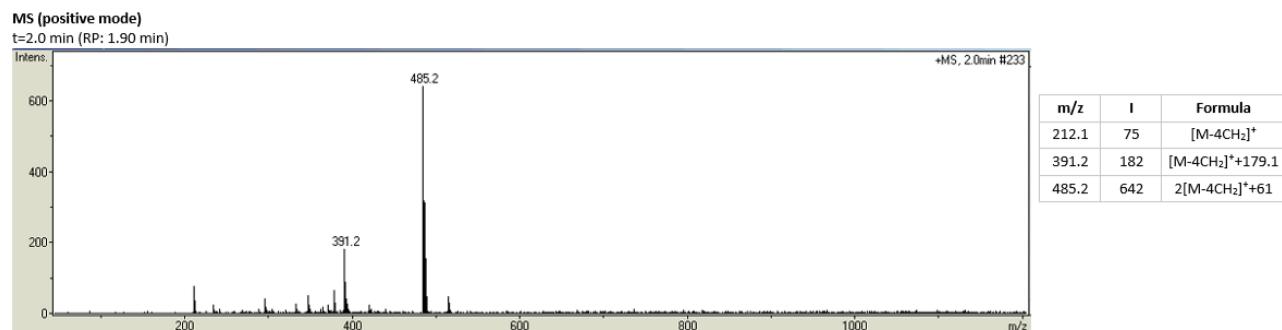


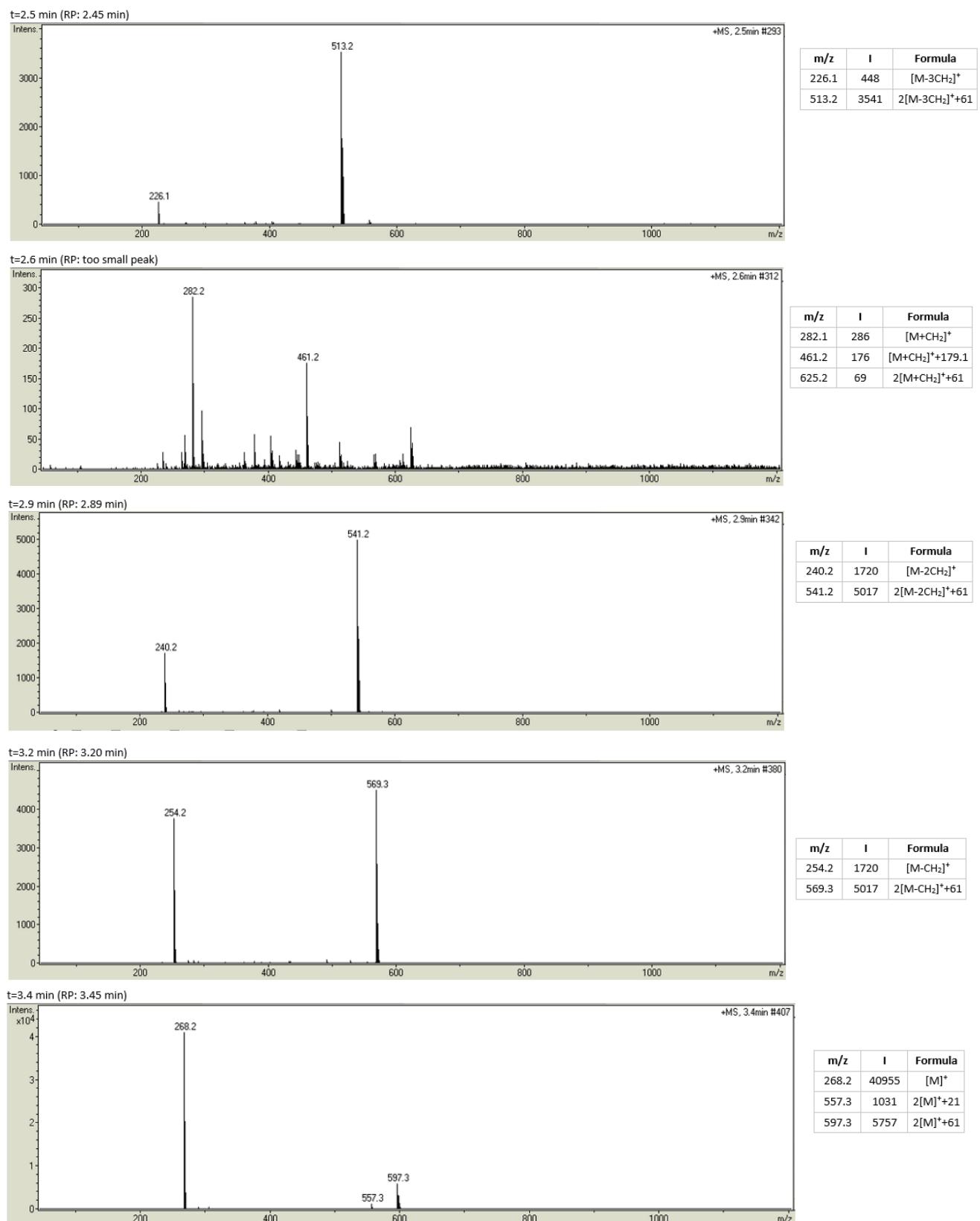


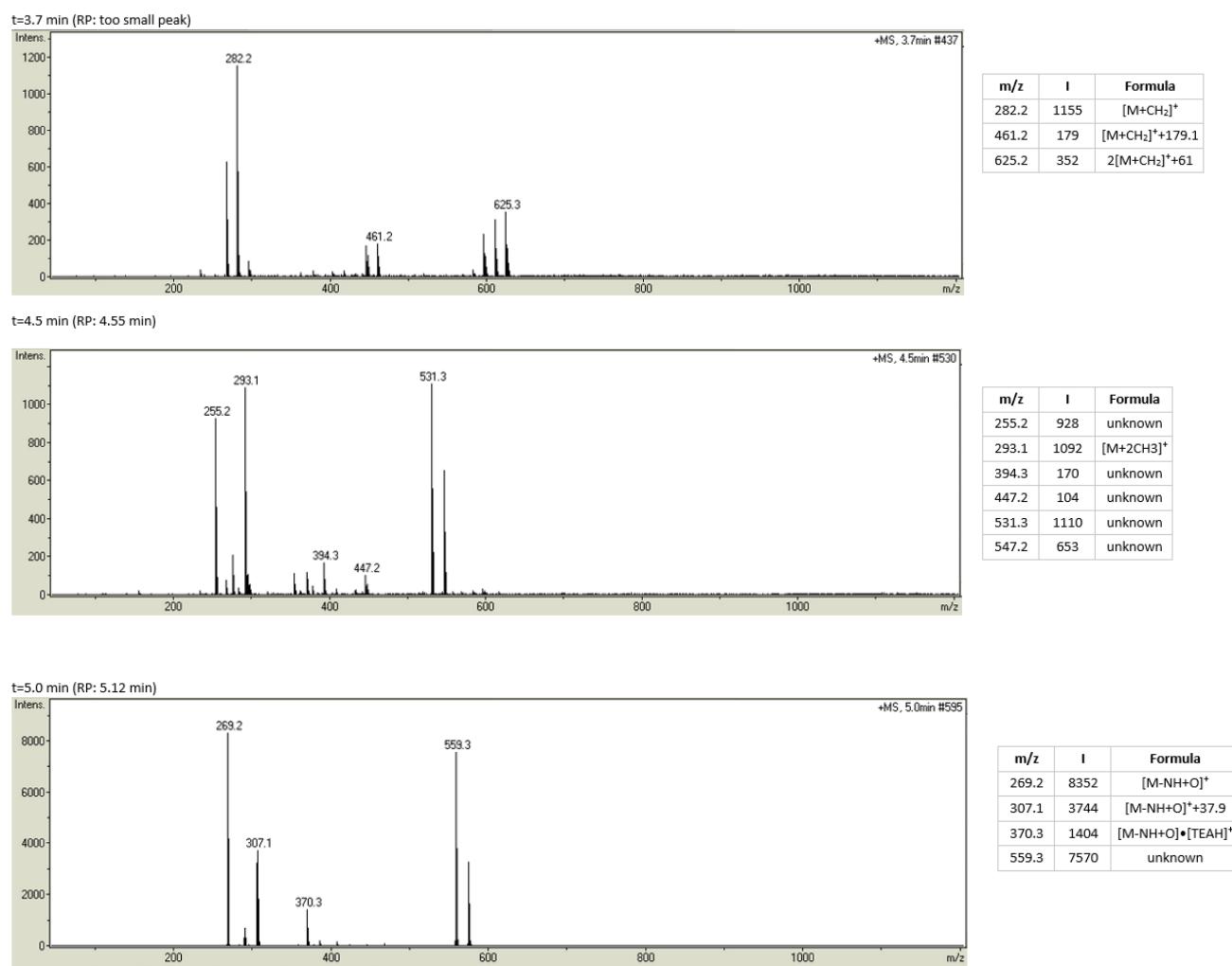
## UV-VIS SPECTRA



## MASS SPECTRA







### S-8.8. Azo Flavine 3R

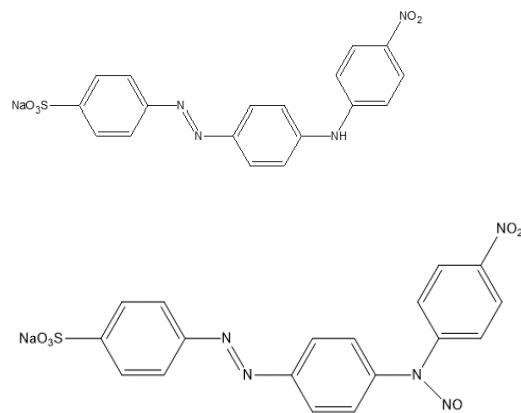
#### GENERAL INFORMATION

**Color Index Name:** Acid Orange 1

**Color Index Number:** 13090

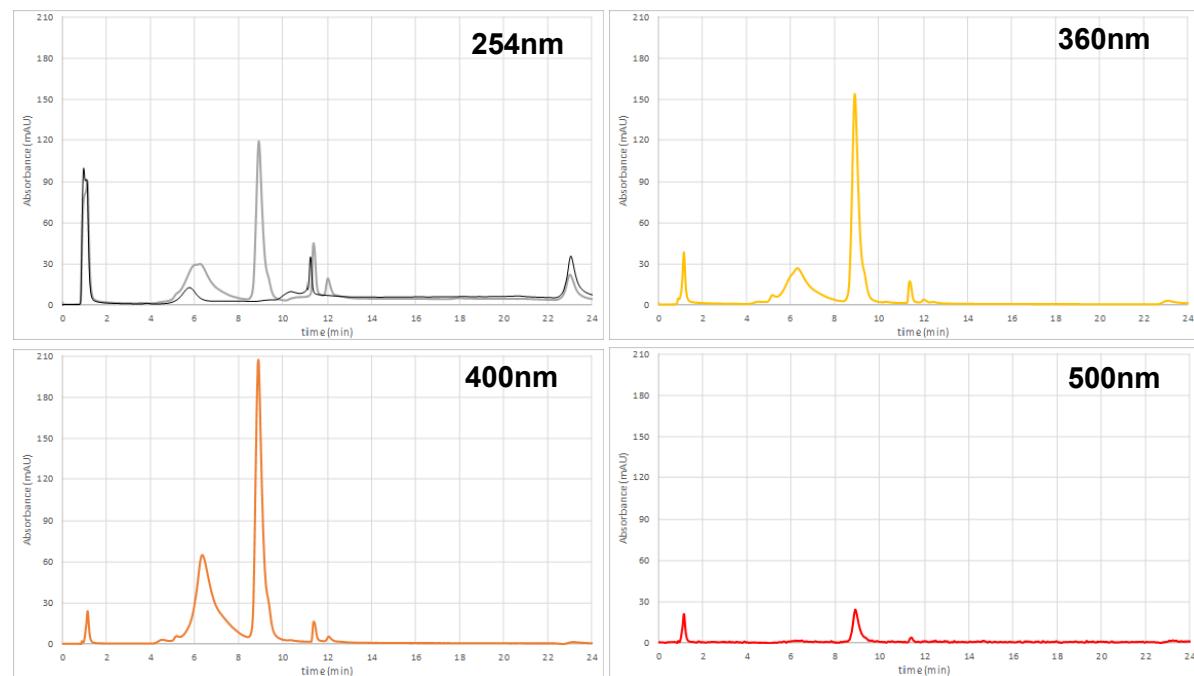
**Type of dye:** Monoazo

**Charge:** -1

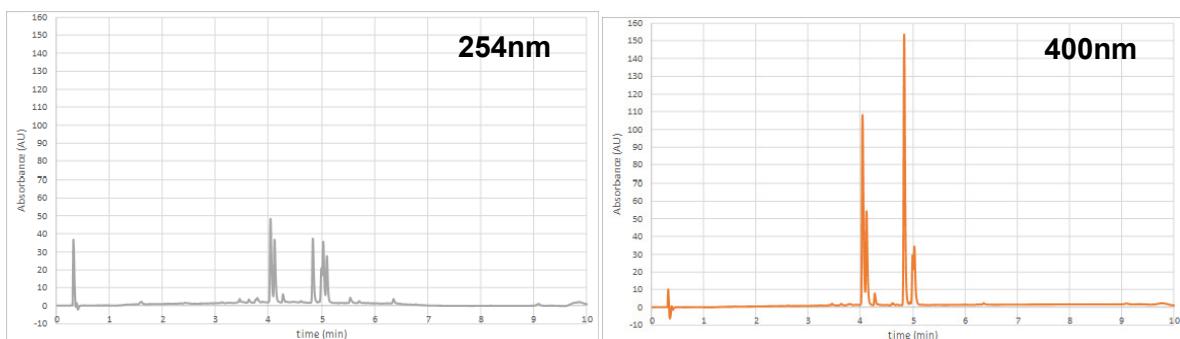


Molecule	Short	Formula (ion)	Full	Ion	Monoisotopic
Normal	[M]	C <sub>18</sub> H <sub>13</sub> N <sub>4</sub> O <sub>5</sub> S	420.37	397.39	397.06
Nitroso	[M+NO]	C <sub>18</sub> H <sub>12</sub> N <sub>5</sub> O <sub>6</sub> S	449.37	426.38	426.05
Di-nitro	[M+NO <sub>2</sub> ]	C <sub>18</sub> H <sub>12</sub> N <sub>5</sub> O <sub>7</sub> S	465.39	442.38	442.05
Tri-nitro	[M+2NO <sub>2</sub> ]	C <sub>18</sub> H <sub>11</sub> N <sub>6</sub> O <sub>9</sub> S	510.37	487.38	487.03

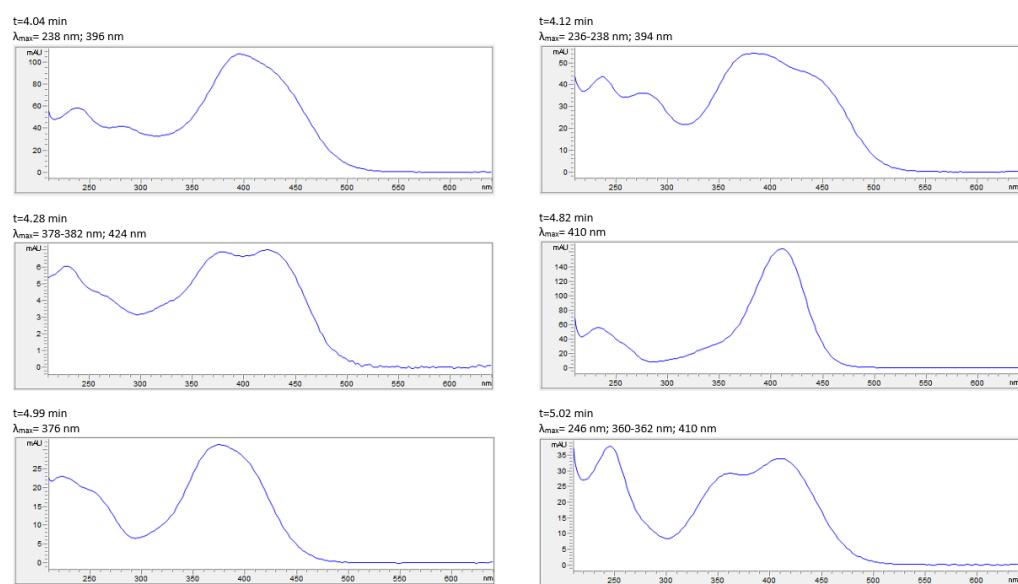
#### CHROMATOGRAMS: ION-EXCHANGE



## CHROMATOGRAMS: REVERSED-PHASE



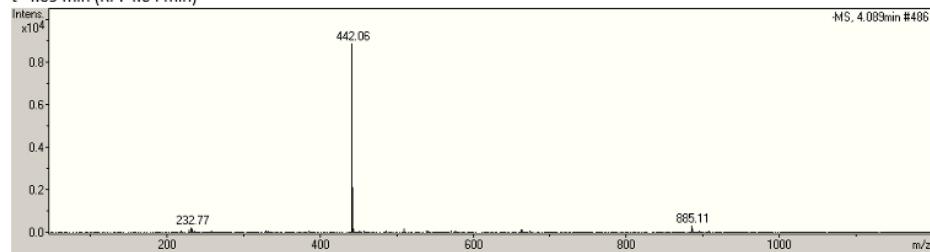
## UV-VIS SPECTRA



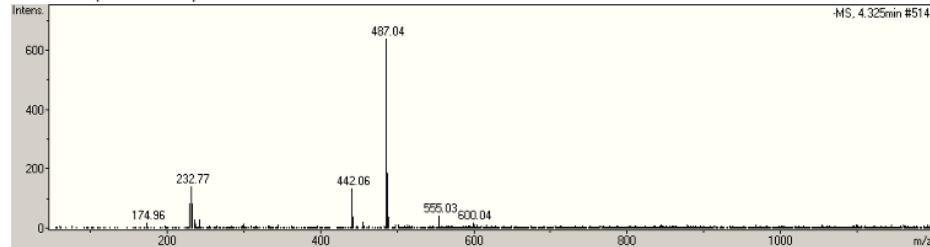
## MASS SPECTRA

### MS (negative mode)

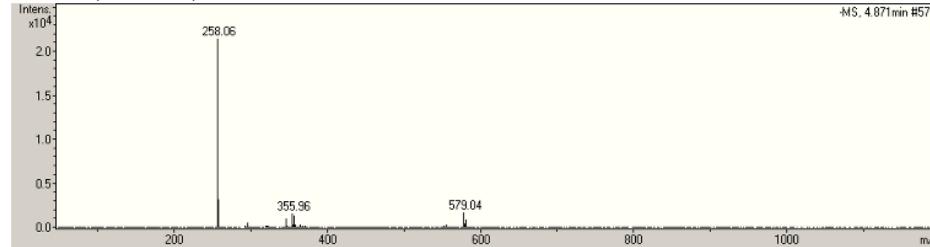
t=4.09 min (RP: 4.04 min)



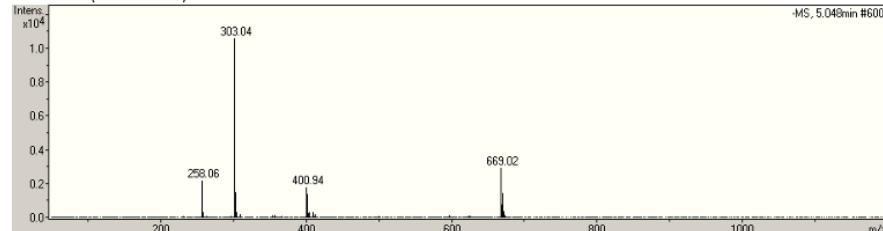
t=4.32 min (RP: 4.28 min)



t=4.87 min (RP: 4.83 min)

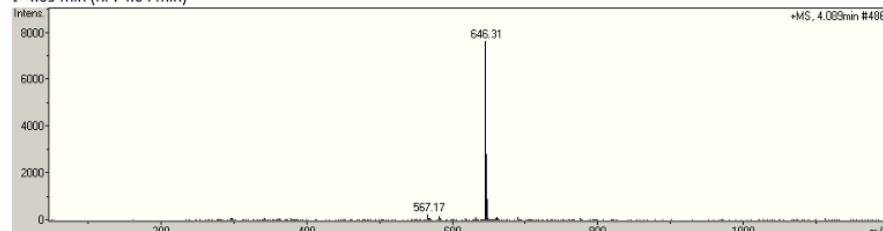


t=5.05 min (RP: 4.99 min)



### MS (positive mode)

t=4.09 min (RP: 4.04 min)



## S-8.9. Azo Fuchsine

### GENERAL INFORMATION

**Color Index Name:** Acid Violet 7

**Color Index Number:** 18055

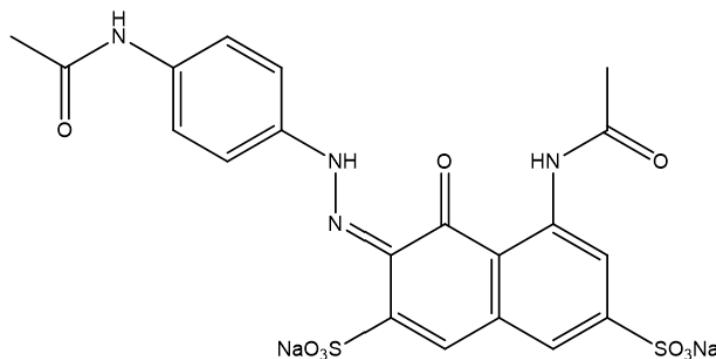
**Type of dye:** Monoazo; Thiazine

**Charge:** -2

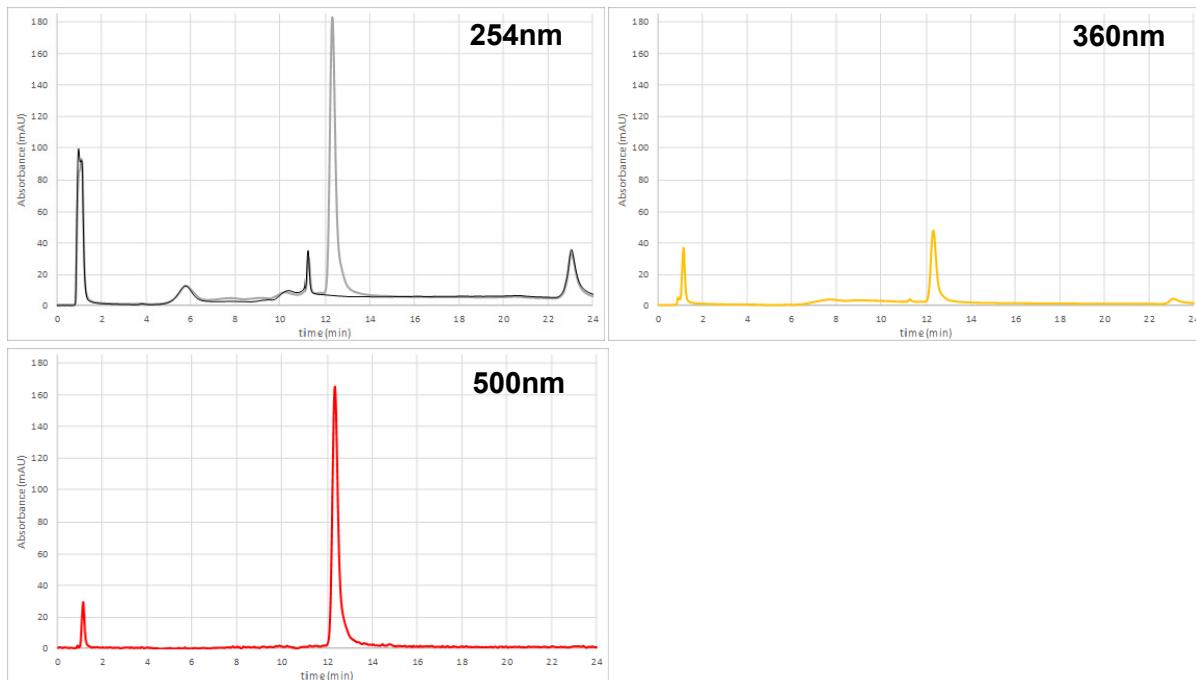
**Molecular Formula:** C<sub>20</sub>H<sub>16</sub>N<sub>4</sub>O<sub>9</sub>S<sub>2</sub> (ion, -2)

### Molecular Weight

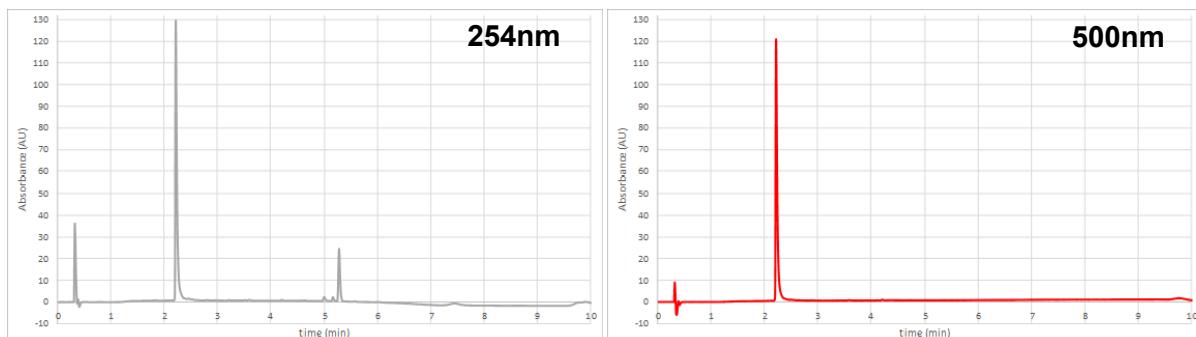
Full molecule:	566.47
Ion (-2)	520.49
Ion (-2), monoisotopic	520.04



### CHROMATOGRAMS: ION-EXCHANGE

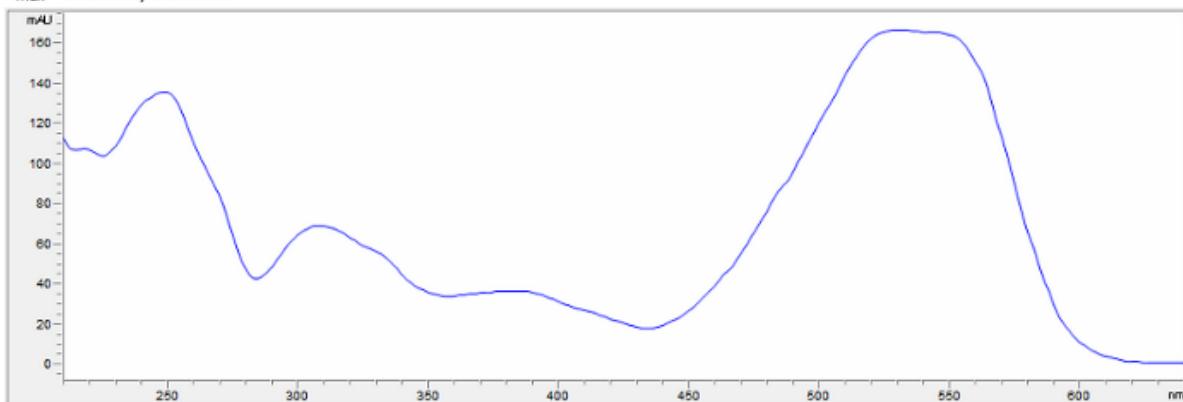


### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

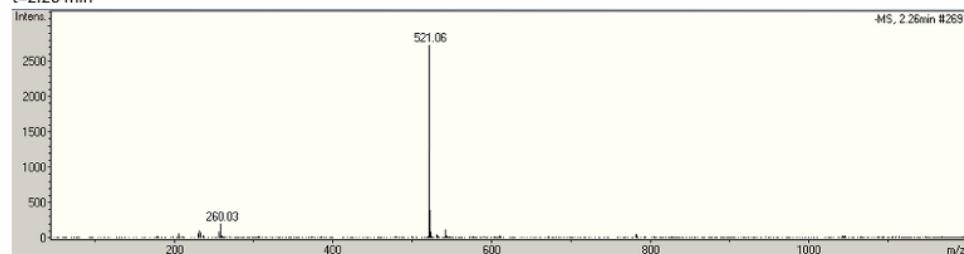
t=2.21 min  
 $\lambda_{\text{max}} = 248 \text{ nm; } 530 \text{ nm}$



## MASS SPECTRA

MS (negative mode)

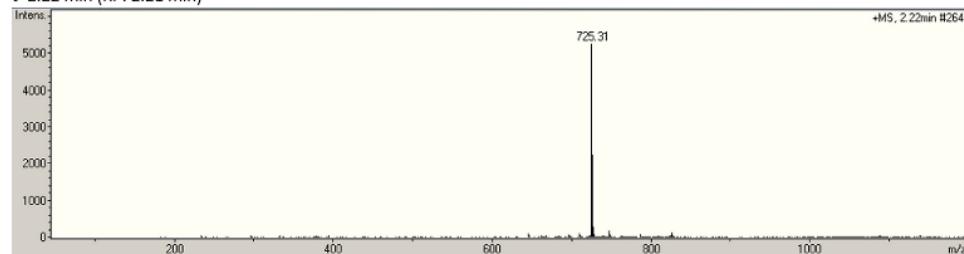
t=2.26 min



m/z	I	Formula
521.06	2739	[MH] <sup>-</sup>
260.03	197	2[MH] <sup>-</sup> •H <sup>+</sup>

MS (positive mode)

t=2.22 min (RP: 2.21 min)



m/z	I	Formula
725.31	5281	[MH] <sup>+</sup> •2[TEAH] <sup>+</sup>

## S-8.10. Berberine

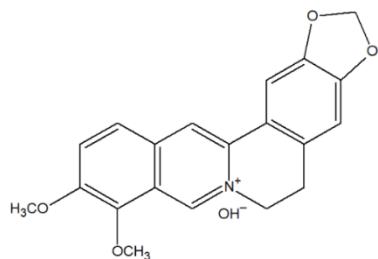
### GENERAL INFORMATION

**Color Index Name:** Natural Yellow 18

**Color Index Number:** 75160

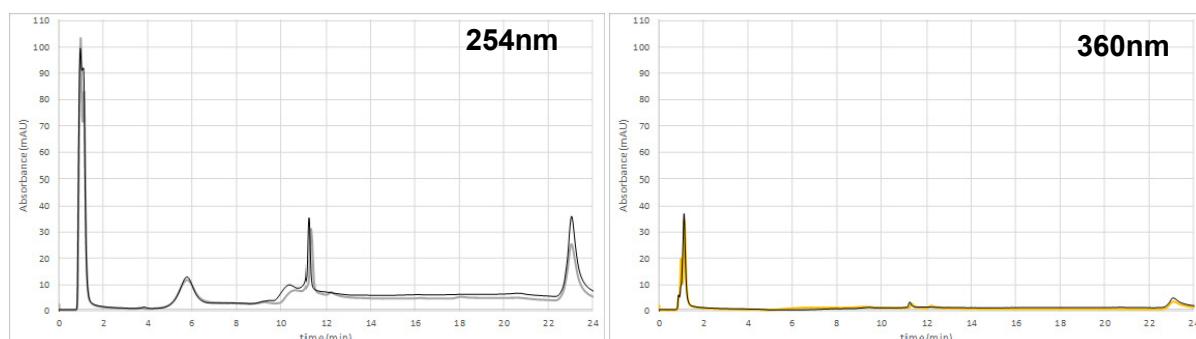
**Type of dye:** Natural, Direct dye

**Scientific name of biological source:** *Berberis Vulgaris L.*

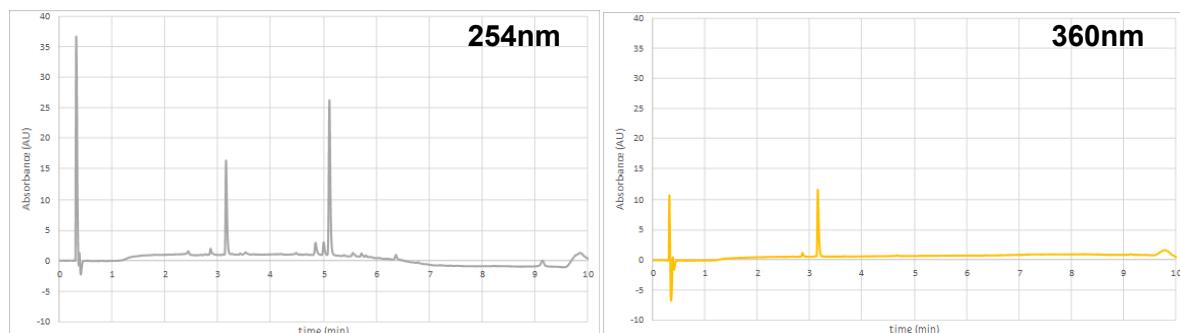


Name	Short	Mw	monoisotopic	Formula
Berberine (ion, +1)	[B]	336.36	336.12	C <sub>20</sub> H <sub>18</sub> NO <sub>4</sub>
Dihydro-Berberine (ion, +1)	[DHB]	338.38	336.12	C <sub>20</sub> H <sub>20</sub> NO <sub>4</sub>

### CHROMATOGRAMS: ION-EXCHANGE



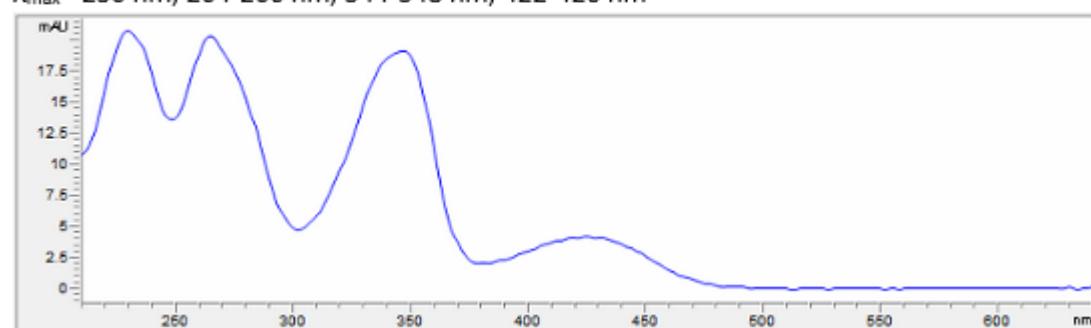
### CHROMATOGRAMS: REVERSED-PHASE



### UV-VIS SPECTRA

t=3.16 min

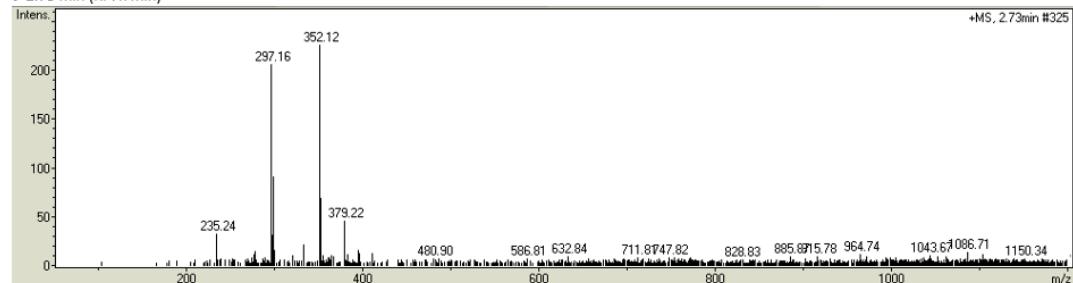
$\lambda_{\text{max}} = 230 \text{ nm}; 264-266 \text{ nm}; 344-348 \text{ nm}; 422-426 \text{ nm}$



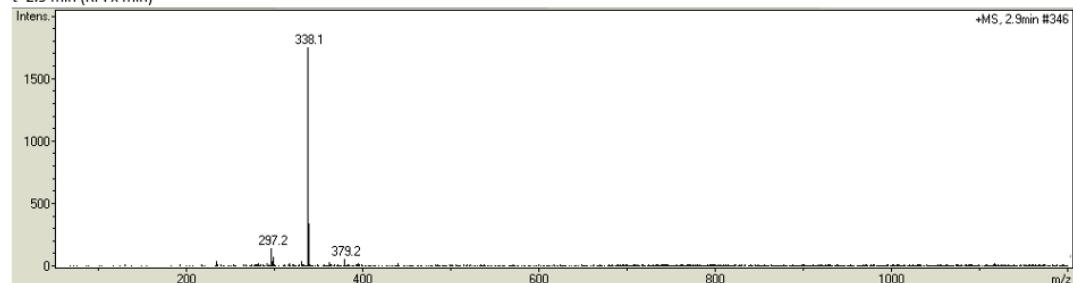
## MASS SPECTRA

MS (positive mode)

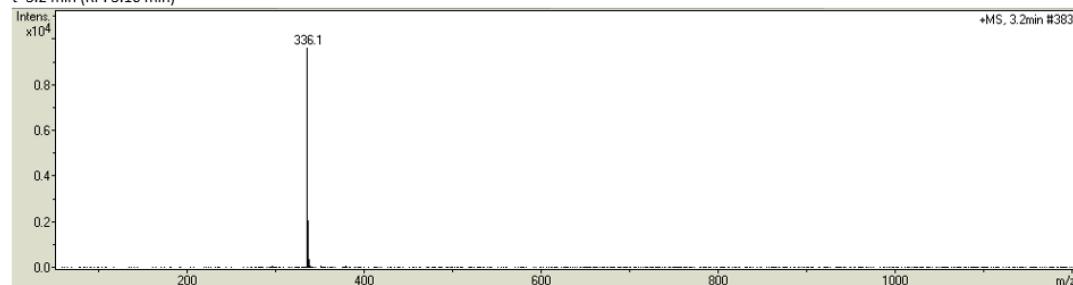
t=2.73 min (RP: x min)



t=2.9 min (RP: x min)



t=3.2 min (RP: 3.16 min)



### S-8.11. Brazilin

#### GENERAL INFORMATION

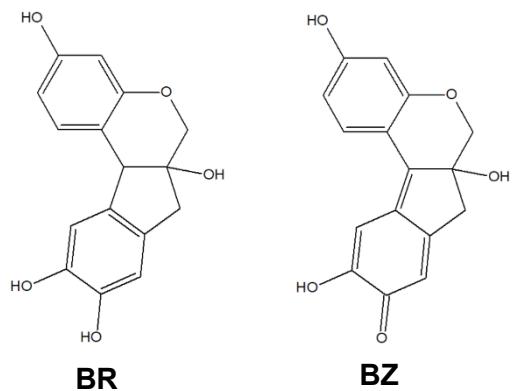
**Color Index Name:** Natural Red 24

**Color Index Number:** 75280

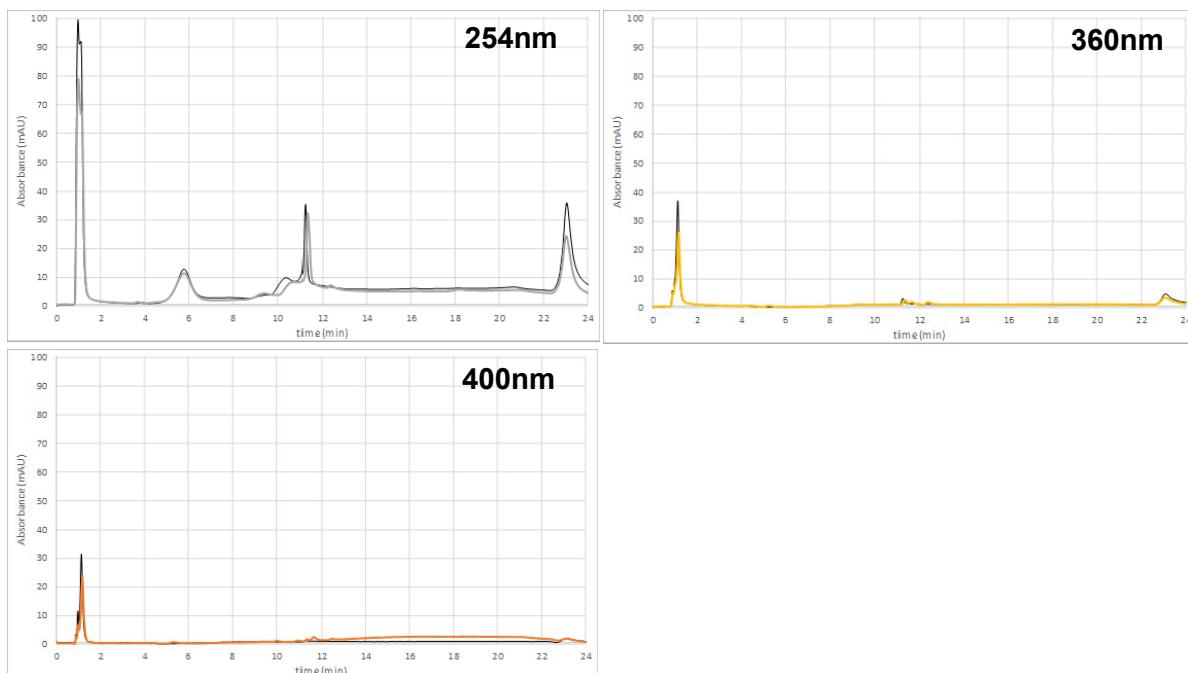
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Caesalpinia sappan L.*

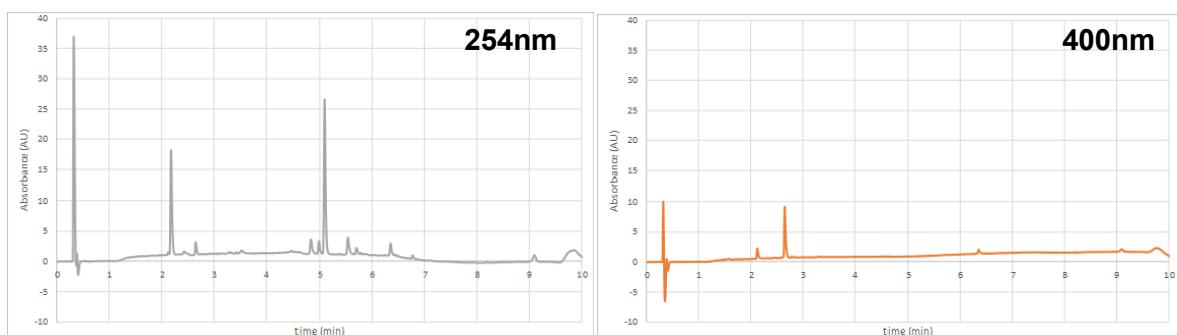
Name	Short	Mw	monoisotopic	Formula
Brazilin	[BR]	286.28	286.08	C <sub>16</sub> H <sub>14</sub> O <sub>5</sub>
Brazilein	[BZ]	284.26	284.07	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>



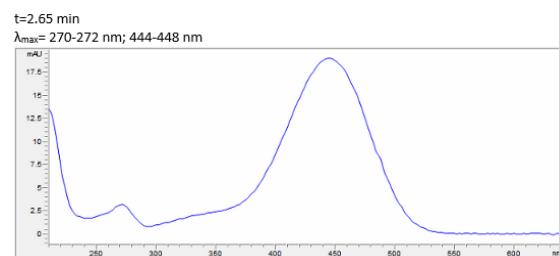
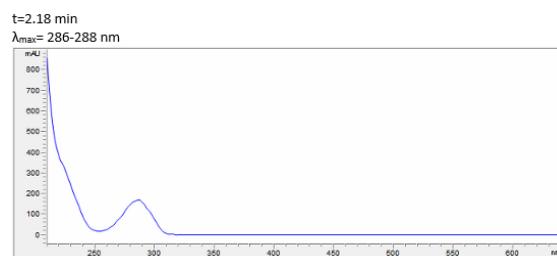
#### CHROMATOGRAMS: ION-EXCHANGE



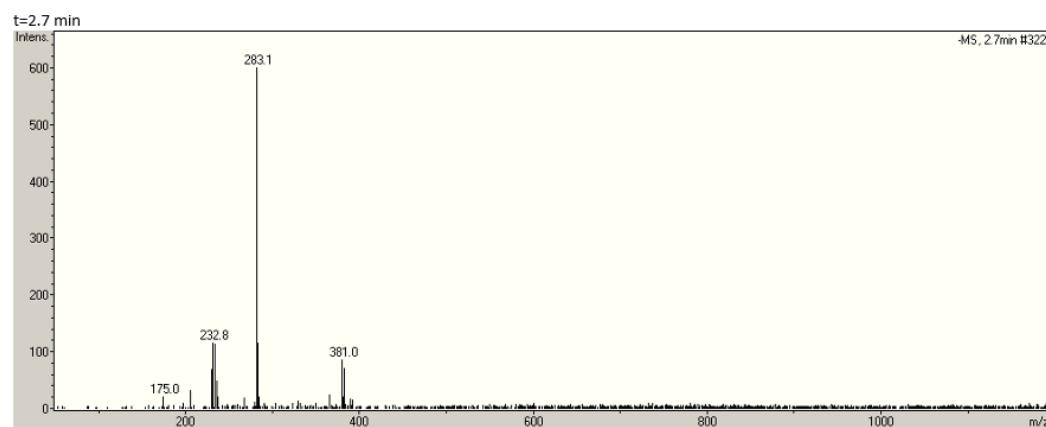
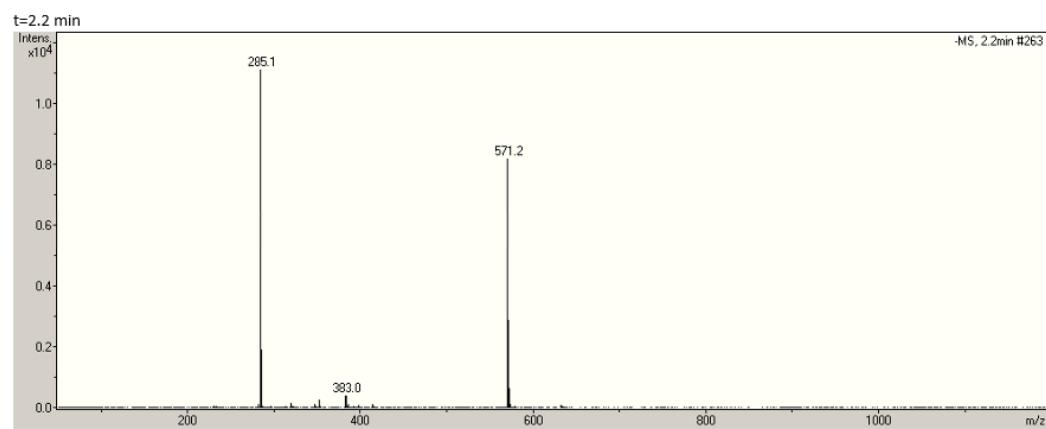
#### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA



## MASS SPECTRA



## S-8.12. Brilliant Yellow

### GENERAL INFORMATION

**Color Index Name:** Direct Yellow 4

**Color Index Number:** 24890

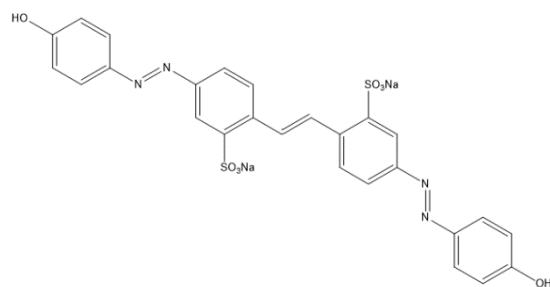
**Type of dye:** Diazo

**Charge:** -2

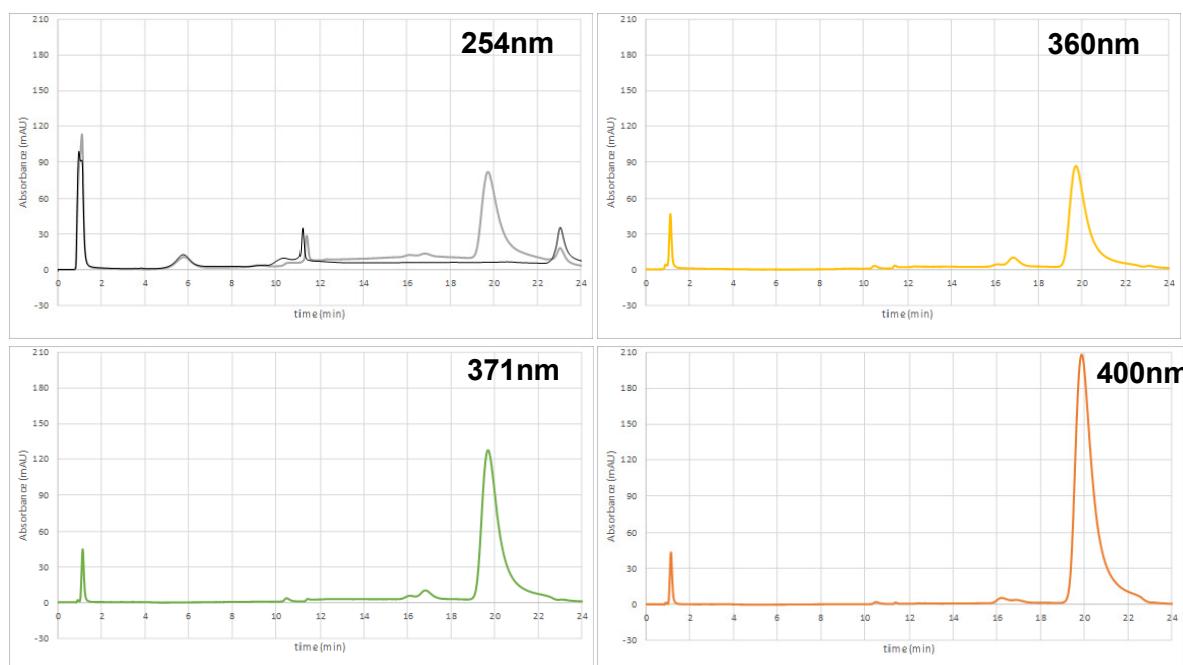
**Molecular Formula:** C<sub>26</sub>H<sub>18</sub>N<sub>4</sub>O<sub>8</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

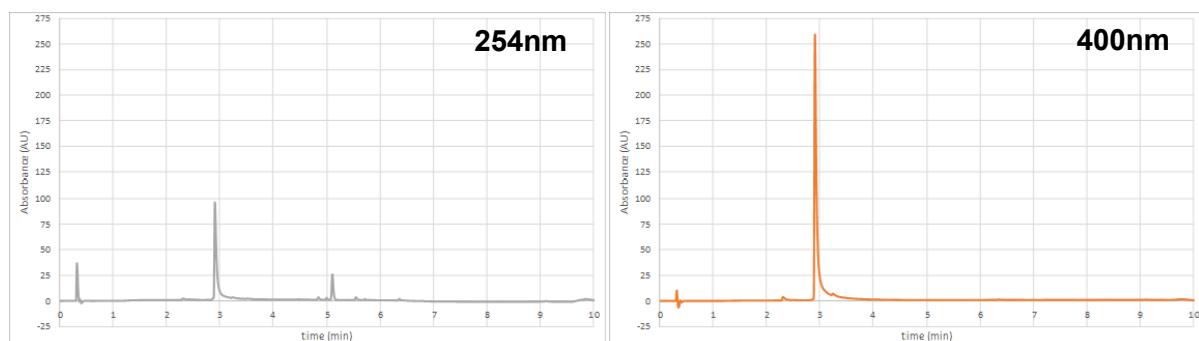
Full molecule:	624.55
Ion (-2)	578.57
Ion (-2), monoisotopic	578.06



### CHROMATOGRAMS: ION-EXCHANGE



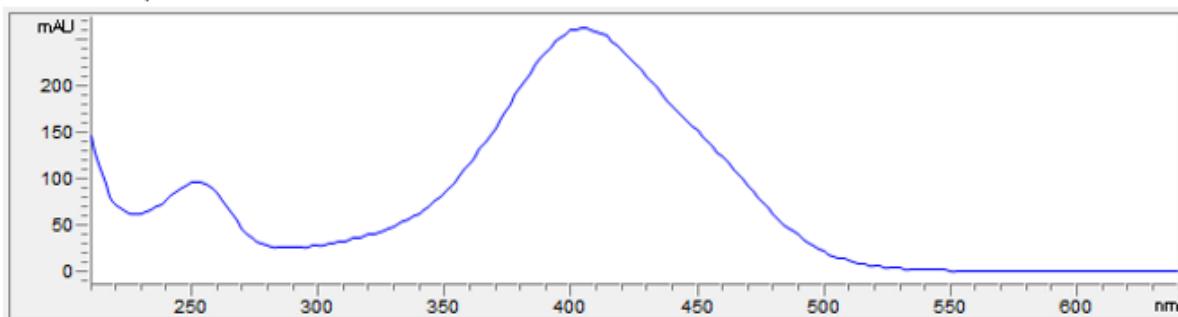
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

t=2.91 min

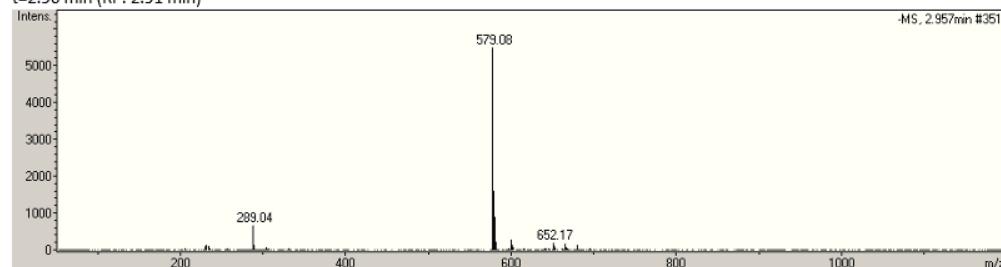
$\lambda_{\text{max}} = 252 \text{ nm}$ ; 404-406 nm



## MASS SPECTRA

### MS (negative mode)

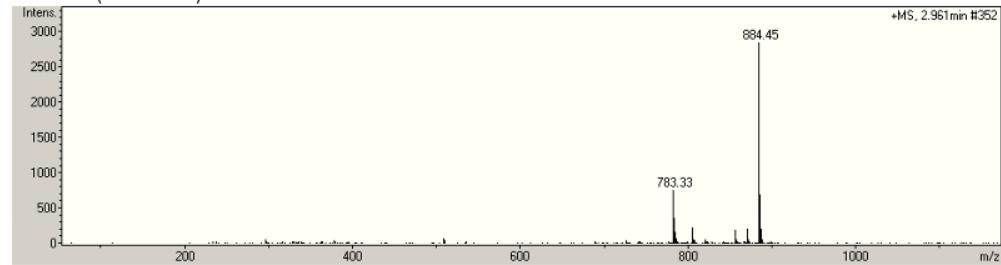
t=2.96 min (RP: 2.91 min)



m/z	I	Formula
289.04	641	[M] <sup>2-</sup>
579.08	5515	[MH] <sup>-</sup>

### MS (positive mode)

t=2.96 min (RP: 2.91 min)



m/z	I	Formula
783.33	743	[MH] <sup>-</sup> •2[TEAH] <sup>+</sup>
884.45	2845	[M] <sup>2-</sup> •3[TEAH] <sup>+</sup>

### S-8.13. Campeche Wood

#### GENERAL INFORMATION

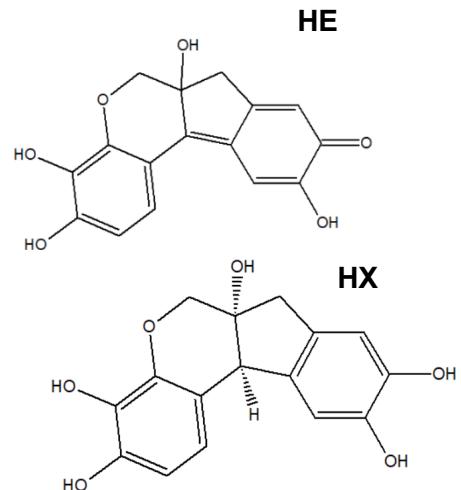
**Alternative names:** Logwood (extract)

**Color Index Name:** Natural Black 1

**Color Index Number:** 75290

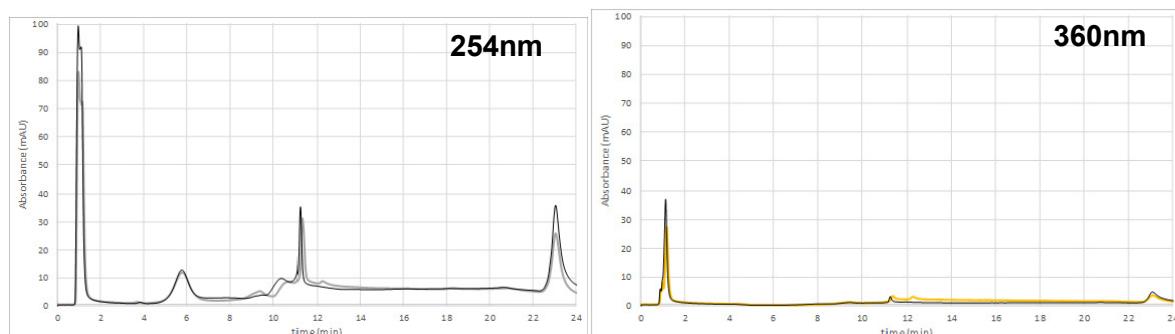
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Haematoxylum campechianum L.*

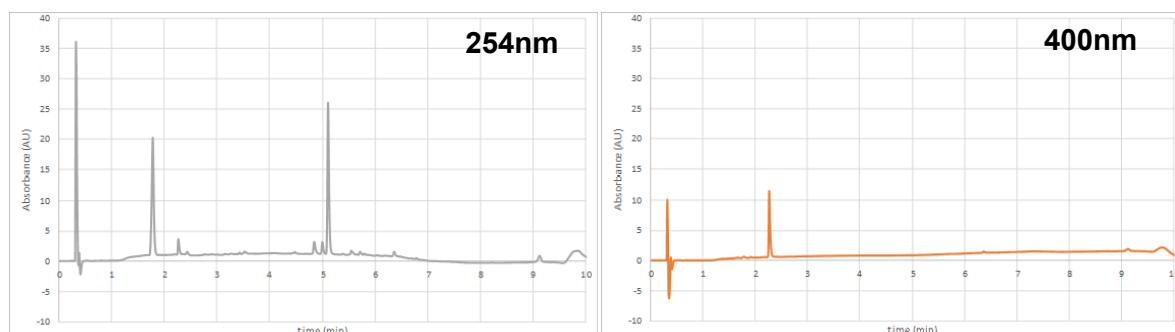


Name	Short	Mw	monoisotopic	Formula
Haematein	[HE]	300.26	300.06	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>
Haematoxylin	[HX]	302.28	302.08	C <sub>16</sub> H <sub>14</sub> O <sub>6</sub>

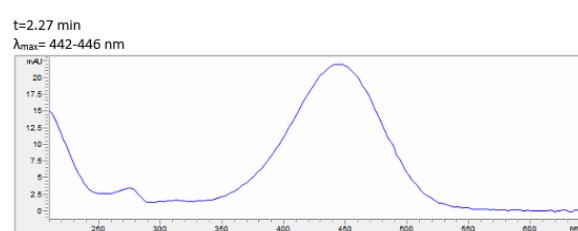
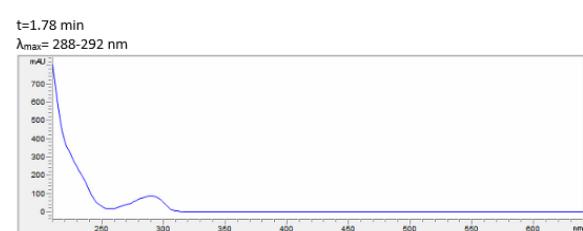
#### CHROMATOGRAMS: ION-EXCHANGE



#### CHROMATOGRAMS: REVERSED-PHASE



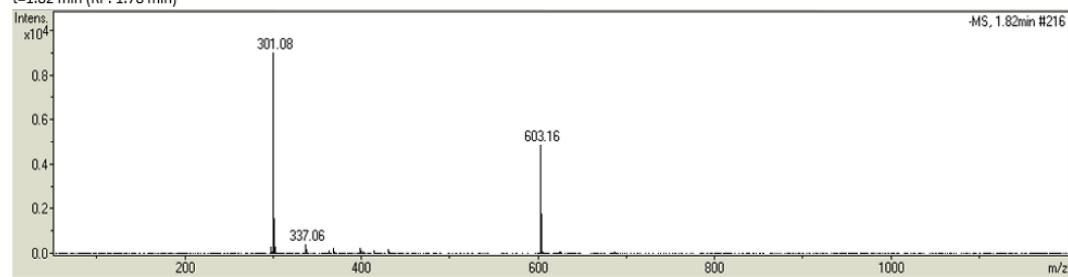
#### UV-VIS SPECTRA



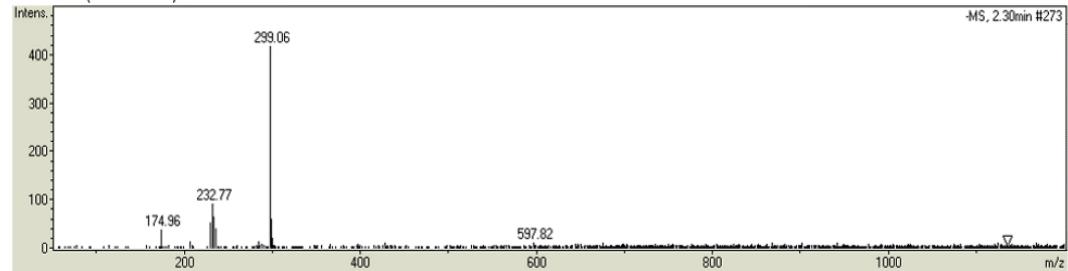
## MASS SPECTRA

MS (negative mode)

t=1.82 min (RP: 1.78 min)



t=2.30 min (RP: 2.27 min)



## S-8.14. Carminic Acid

### GENERAL INFORMATION

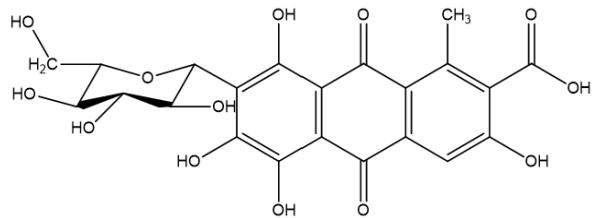
**Alternative names:** Carmine (aluminum salt)

**Color Index Name:** Natural Red 4

**Color Index Number:** 75470

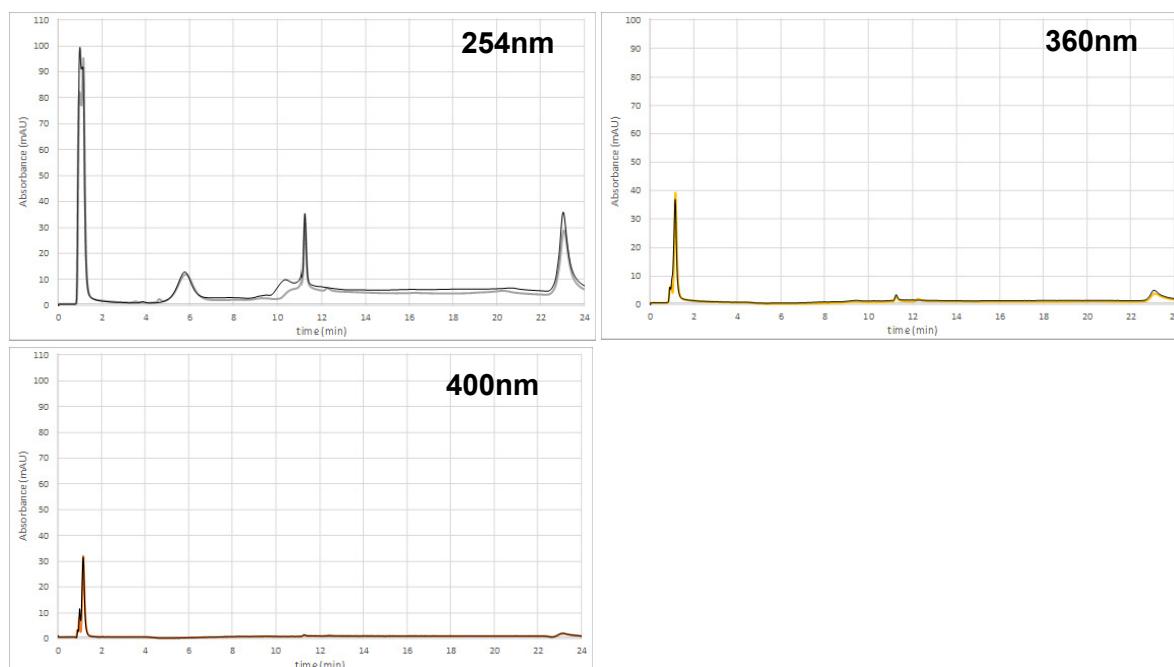
**Type of dye:** Natural, Anthraquinone

**Scientific name of biological source:** *Dactulopius coccus Costa*

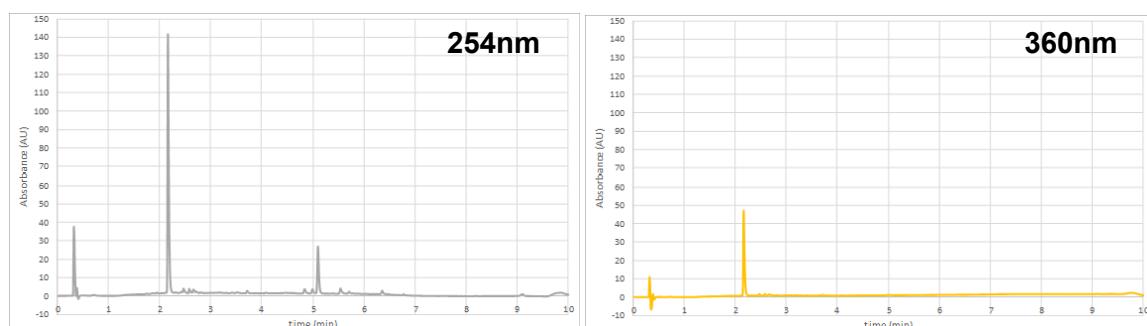


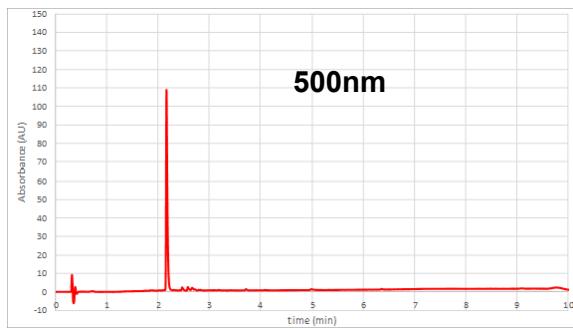
Name	Short	Mw	monoisotopic	Formula
Carminic Acid	[CA]	492.39	492.09	C <sub>22</sub> H <sub>20</sub> O <sub>13</sub>

### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

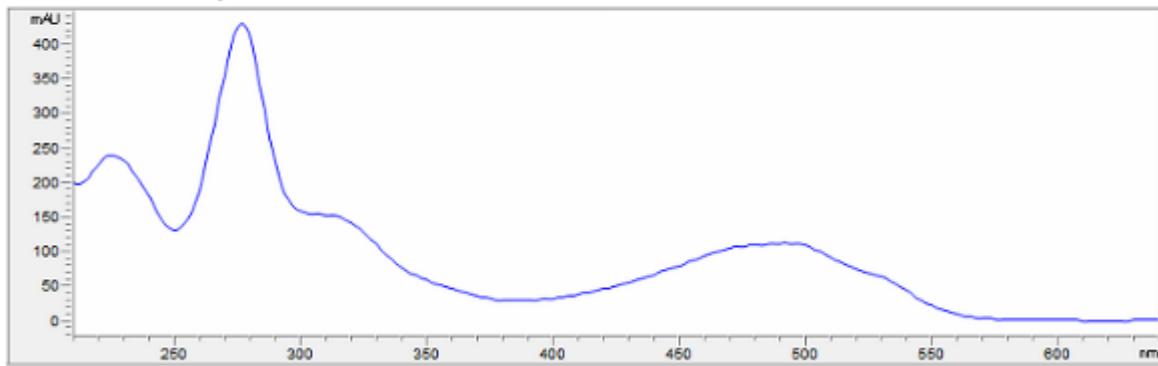




## UV-VIS SPECTRA

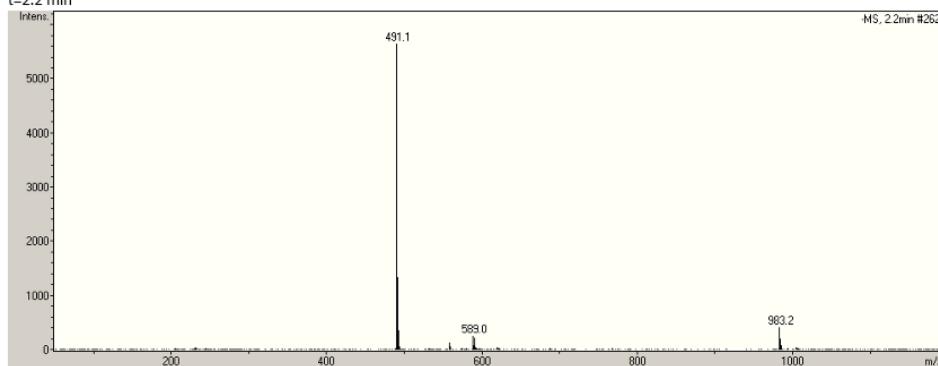
$t=2.16$  min

$\lambda_{\text{max}} = 276\text{-}278 \text{ nm}; 492\text{-}494 \text{ nm}$



## MASS SPECTRA

$t=2.2$  min



$m/z$	I	Formula
491.1	5655	$[\text{CA}]^-$
589.0	238	$+97.9$
983.2	411	$2[\text{CA}]^- \bullet \text{H}^+$

### S-8.15. (+) Catechin Hydrate

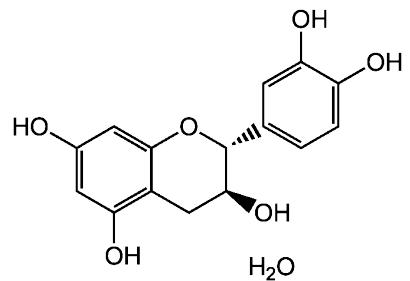
#### GENERAL INFORMATION

**Color Index Name:** Natural Brown 3

**Color Index Number:** n.a.

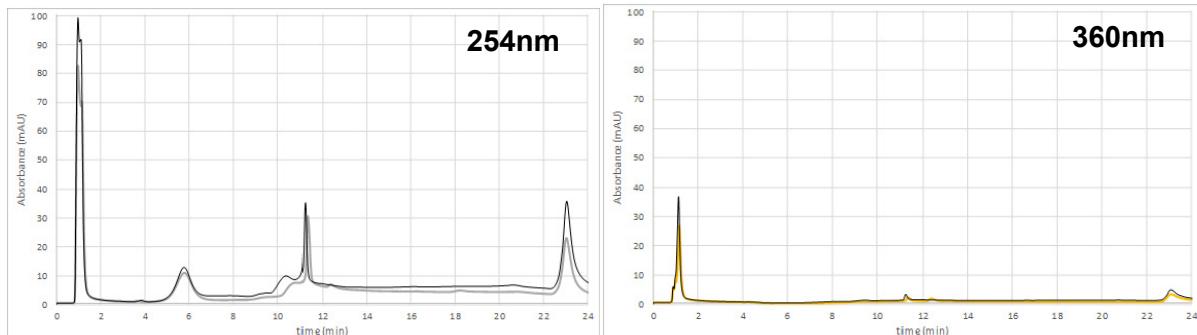
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Rhus coriaria L.* ; *Rhus cotinus L.*

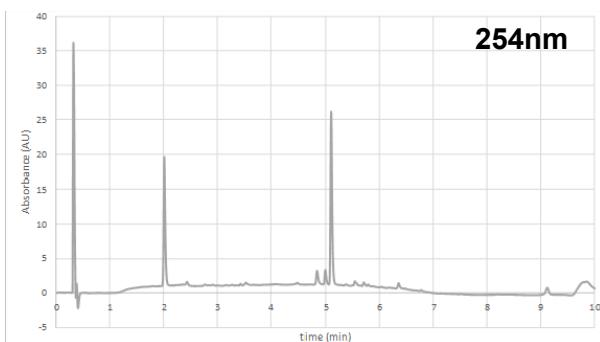


Name	Short	Mw	monoisotopic	Formula
(+) Catechin Hydrate	[CH]	290.27	290.08	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>

#### CHROMATOGRAMS: ION-EXCHANGE



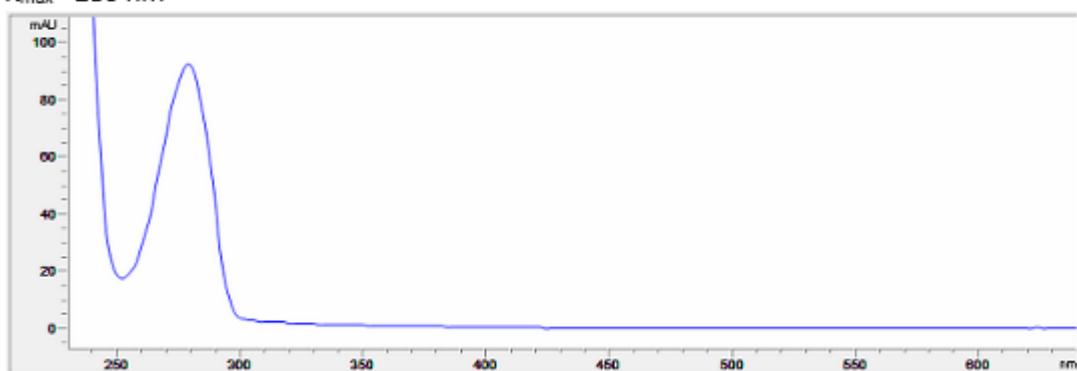
#### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

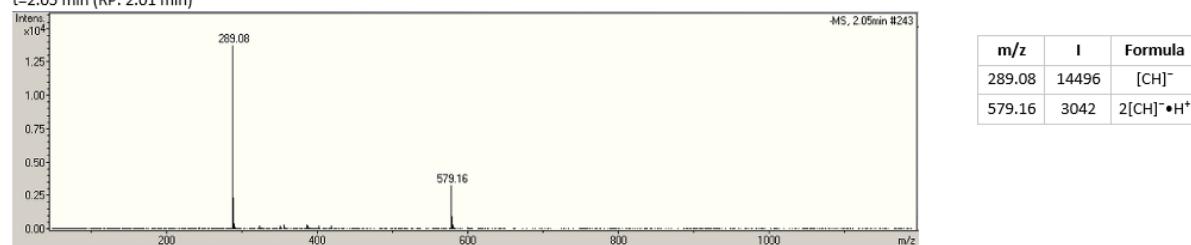
t=2.01 min

$\lambda_{\text{max}} = 280 \text{ nm}$



## MASS SPECTRA

t=2.05 min (RP: 2.01 min)

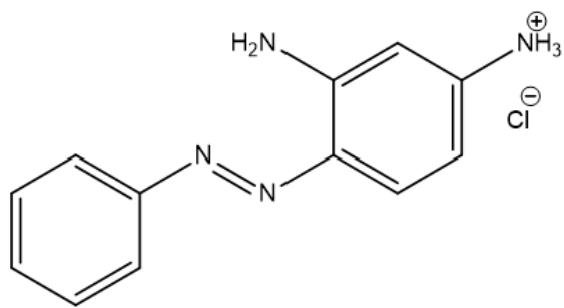


## S-8.16. Chrysoidin

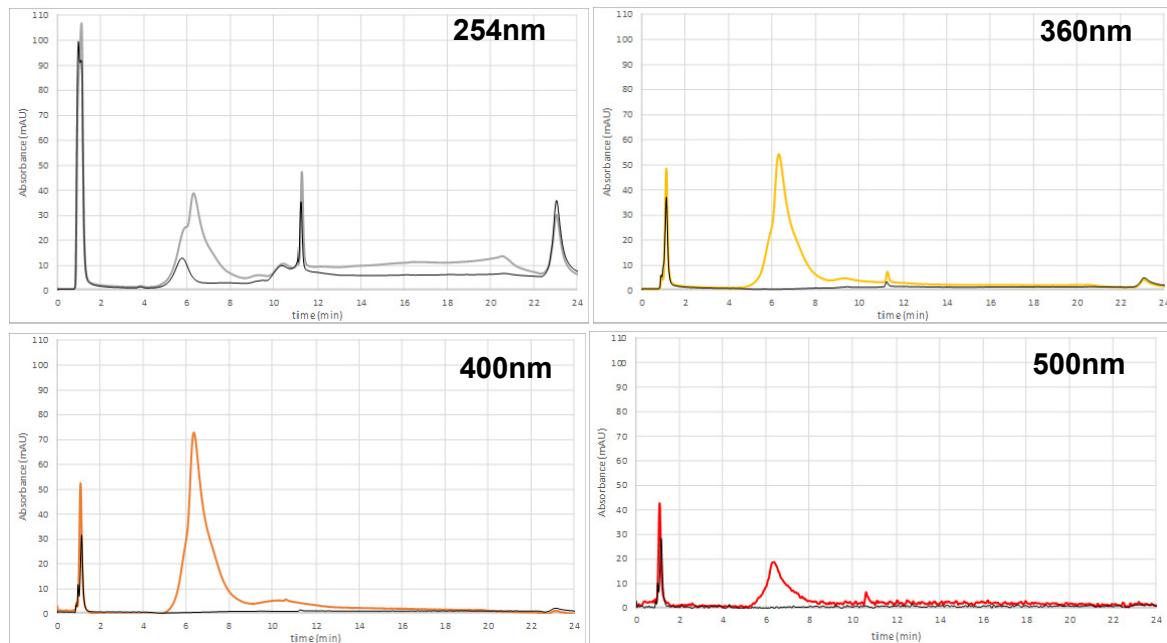
### GENERAL INFORMATION

**Alternative names:** Chrysoidine Y  
**Color Index Name:** Basic Orange 2  
**Color Index Number:** 11270  
**Type of dye:** Monoazo  
**Charge:** +1  
**Molecular Formula:** C<sub>12</sub>H<sub>13</sub>N<sub>4</sub> (ion, +1)  
**Molecular Weight**

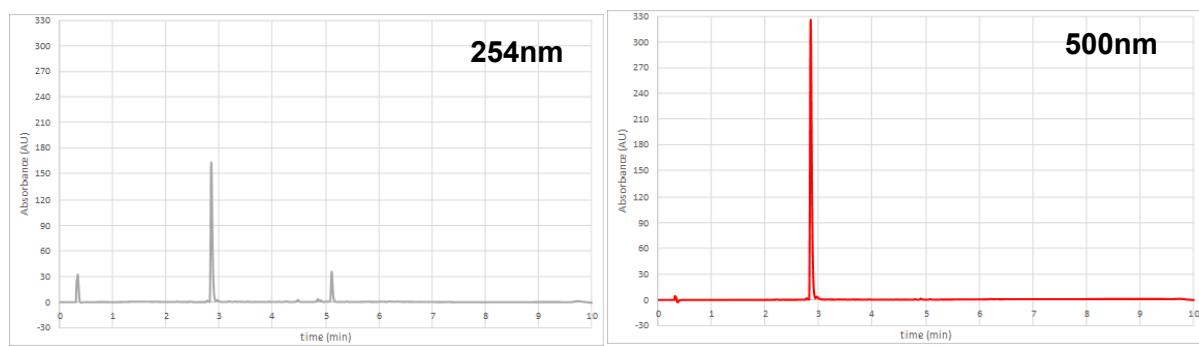
Full molecule:	248.71
Ion (+1)	213.26
Ion (+1), monoisotopic	213.11

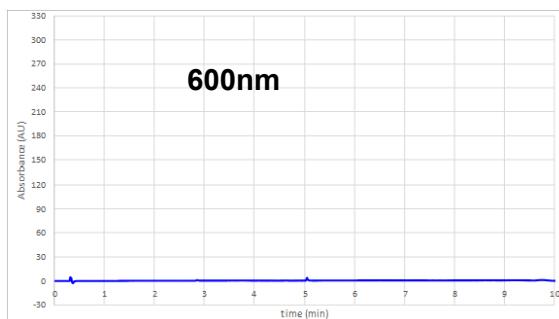


### CHROMATOGRAMS: ION-EXCHANGE



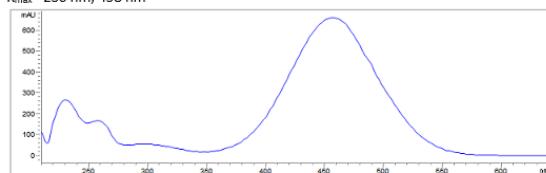
### CHROMATOGRAMS: REVERSED-PHASE



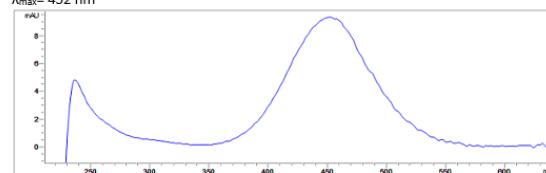


## UV-VIS SPECTRA

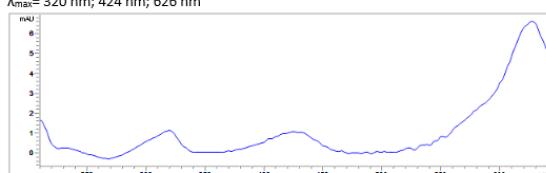
$t=2.86$  min  
 $\lambda_{\max}=230$  nm; 458 nm



$t=2.97$  min  
 $\lambda_{\max}=452$  nm

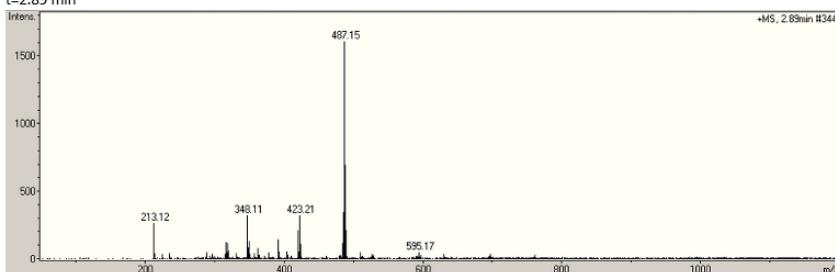


$t=5.04$  min  
 $\lambda_{\max}=320$  nm; 424 nm; 626 nm



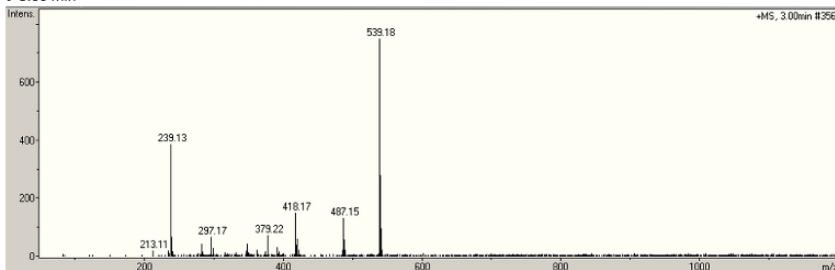
## MASS SPECTRA

$t=2.89$  min



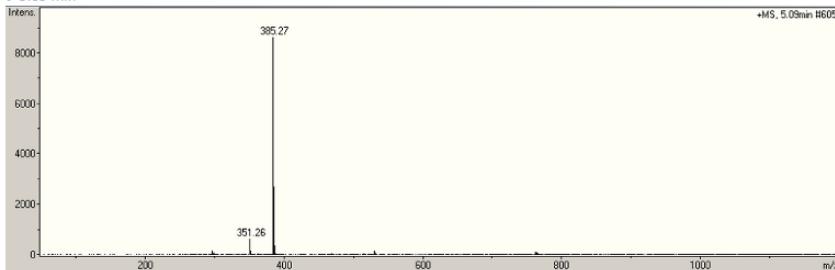
m/z	I	Formula
213.12	259	[M] <sup>+</sup>
487.15	1610	2[M+CH <sub>2</sub> ] <sup>++</sup> 61

$t=3.00$  min



m/z	I	Formula
239.12	386	[unknown] <sup>+</sup>
539.18	752	2[unknown] <sup>++</sup> 61

$t=5.09$  min



m/z	I	Formula
351.26	615	unknown
385.27	8658	[DG] <sup>+</sup>

## S-8.17. Chrysoin

### GENERAL INFORMATION

**Alternative names:** Chrysoine Resorcinol, Tropaeolin O

**Color Index Name:** Acid Orange 6

**Color Index Number:** 14270

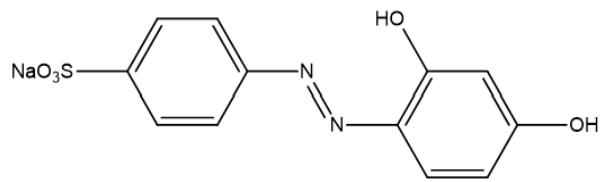
**Type of dye:** Monoazo

**Charge:** -1

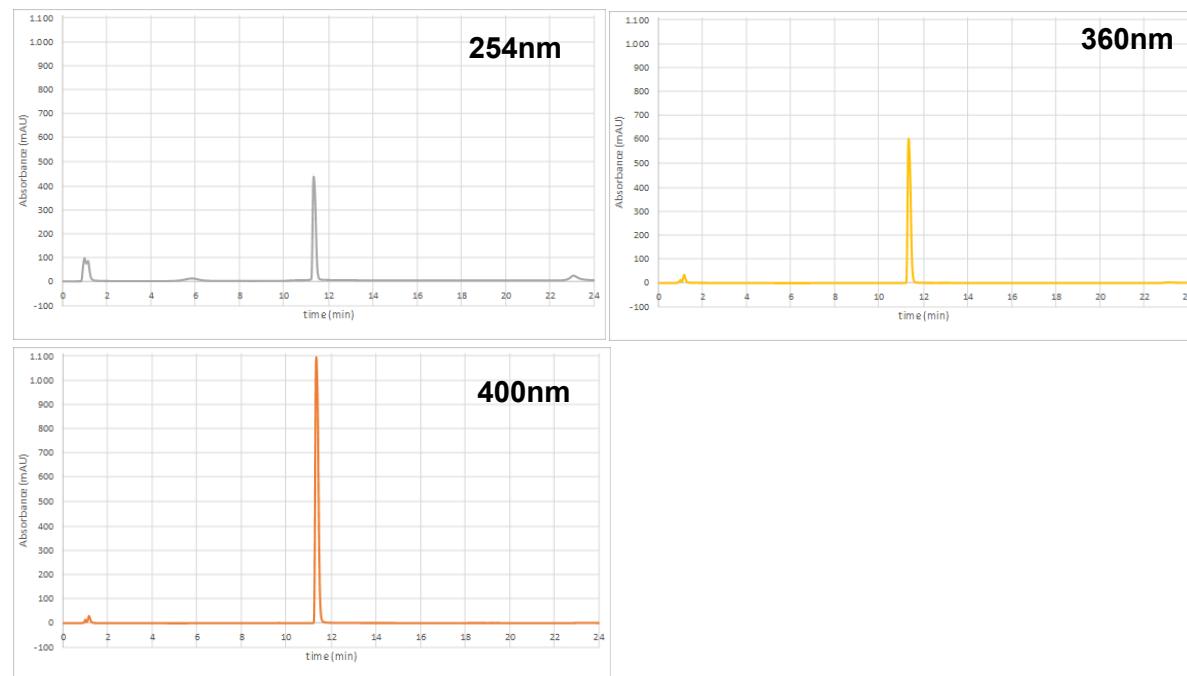
**Molecular Formula:** C<sub>12</sub>H<sub>9</sub>N<sub>2</sub>O<sub>5</sub>S (ion, -1, ONa replaced with OH)

**Molecular Weight**

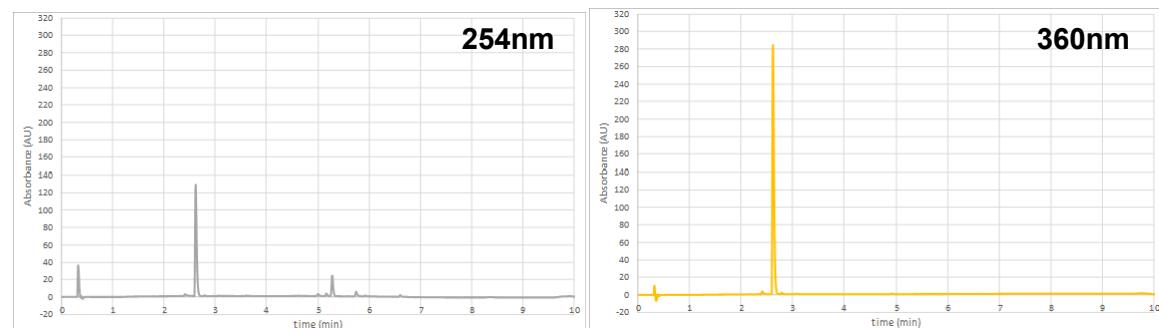
Full molecule:	316.27
Ion (-1)	293.28
Ion (-1), monoisotopic	293.02

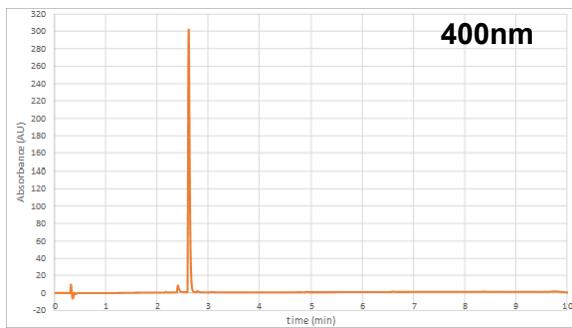


### CHROMATOGRAMS: ION-EXCHANGE

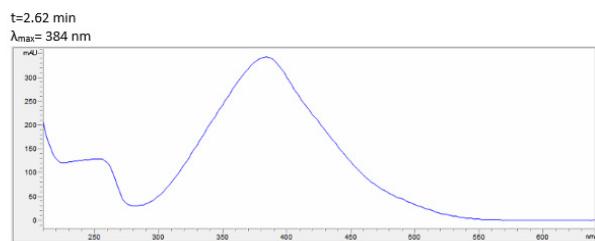
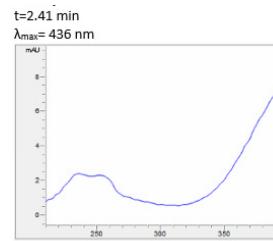


### CHROMATOGRAMS: REVERSED-PHASE





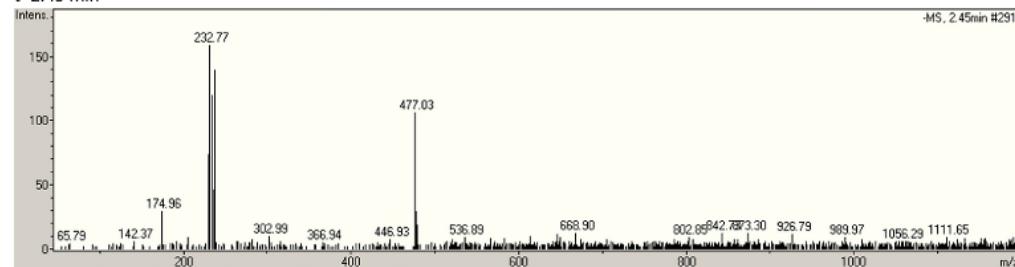
## UV-VIS SPECTRA



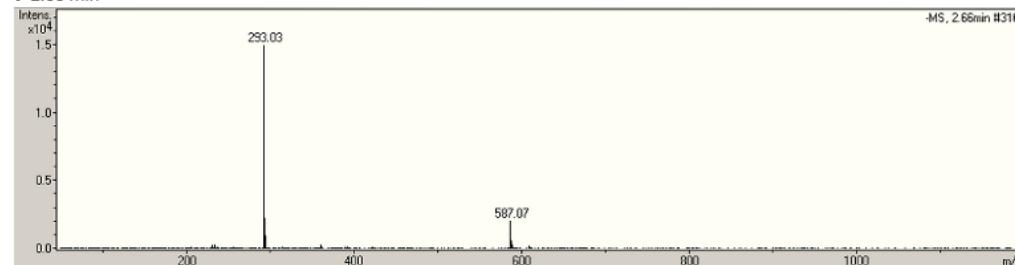
## MASS SPECTRA

### MS (negative mode)

t=2.45 min

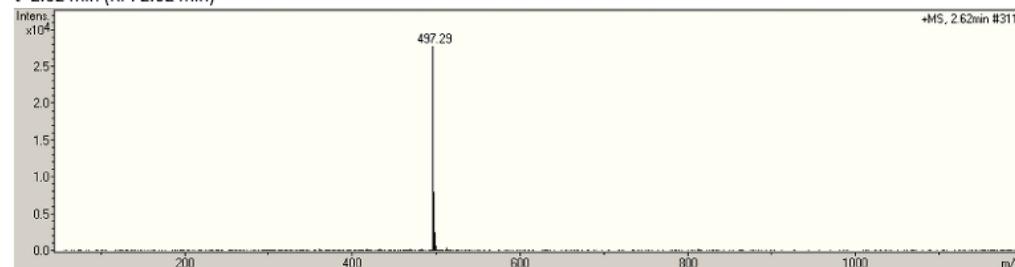


t=2.66 min



### MS (positive mode)

t=2.62 min (RP: 2.62 min)



### S-8.18. Cochineal Red A

#### GENERAL INFORMATION

**Alternative names:** Ponceau 4R; New Coccine

**Color Index Name:** Acid Red 18

**Color Index Number:** 16255

**Type of dye:** Monoazo

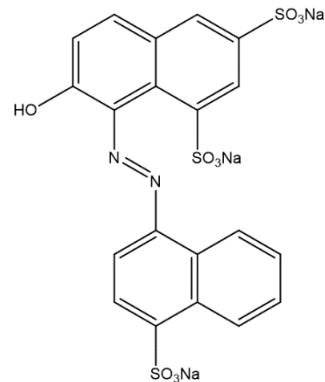
**Charge:** -3

**Related dyes:** 5347 Amaranth (isomer)

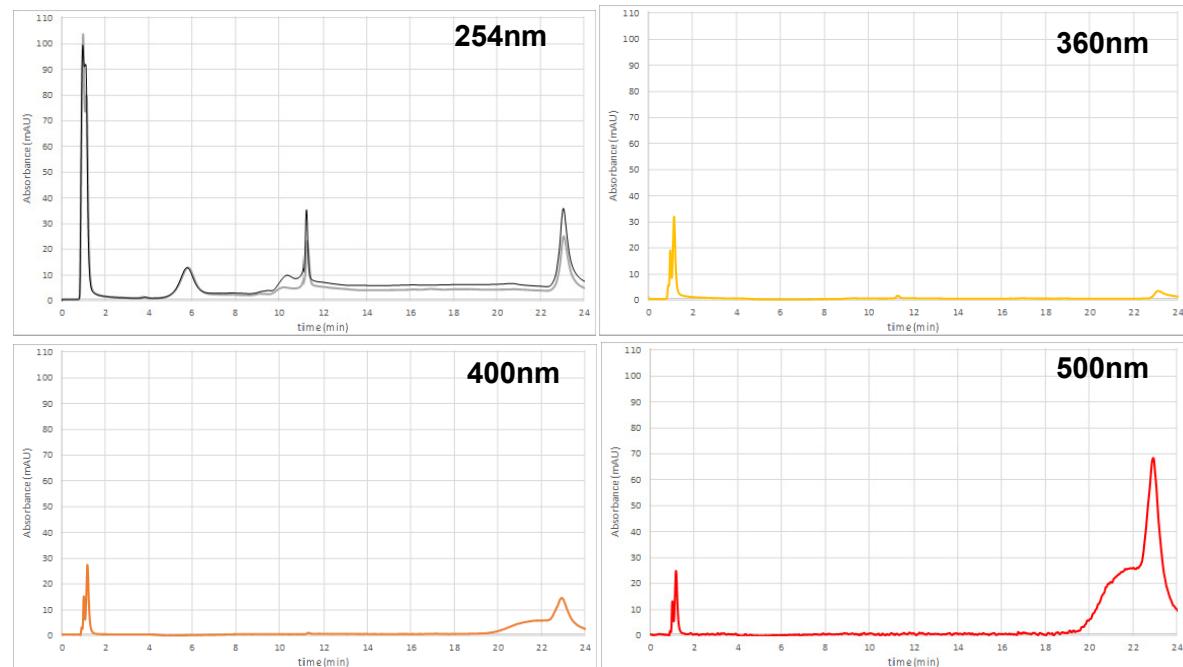
**Molecular Formula:**  $C_{20}H_{11}N_2O_{10}S_3$  (ion, -3)

**Molecular Weight:**

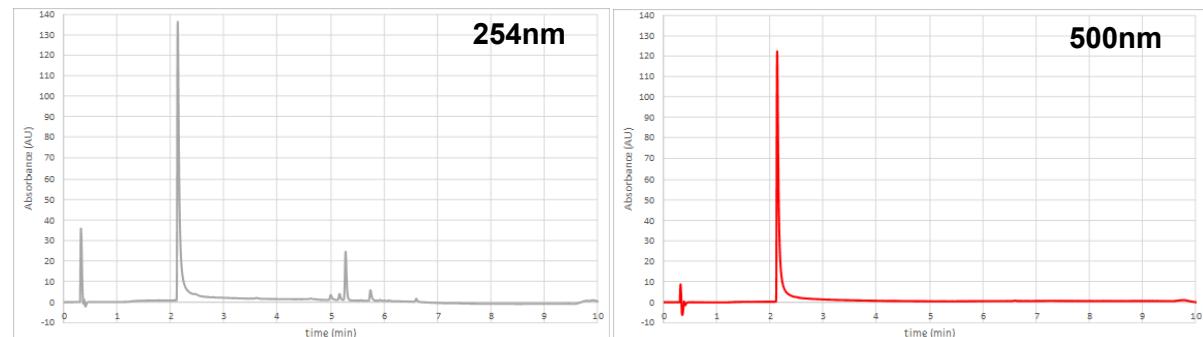
Full molecule:	604.47
Ion (-3)	535.51
Ion (-3), monoisotopic	534.96



#### CHROMATOGRAMS: ION-EXCHANGE



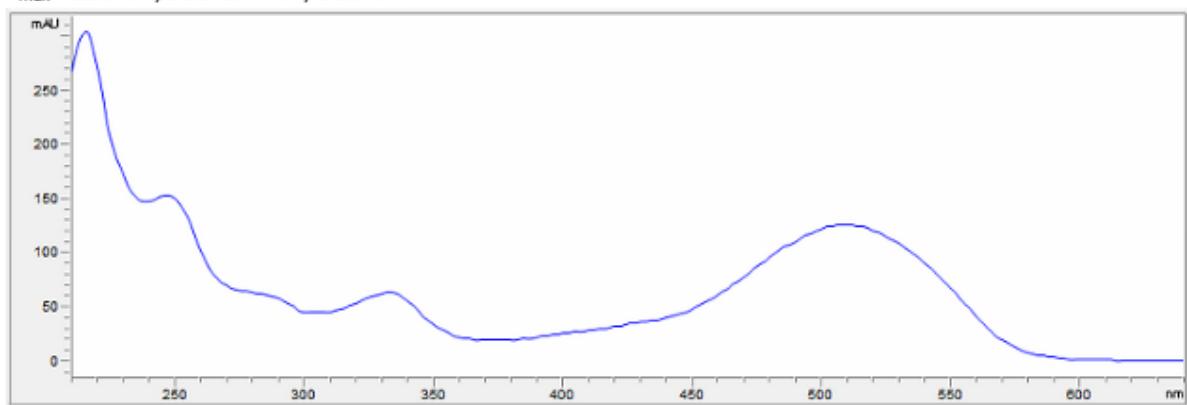
#### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

t=2.14 min

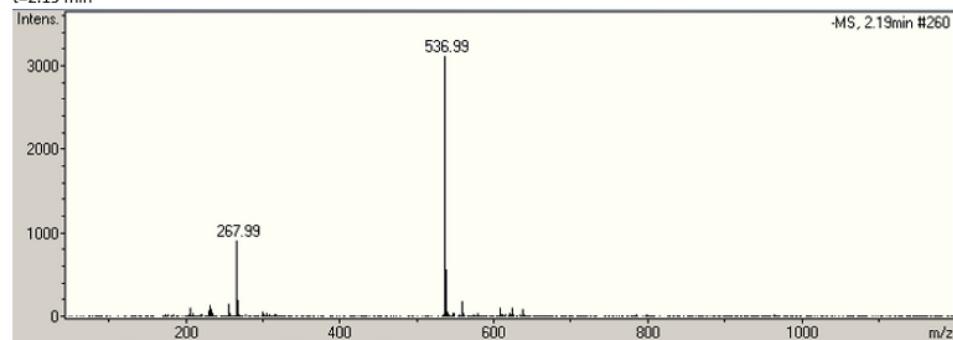
$\lambda_{\text{max}} = 216 \text{ nm}; 332-334 \text{ nm}; 508 \text{ nm}$



## MASS SPECTRA

MS (negative mode)

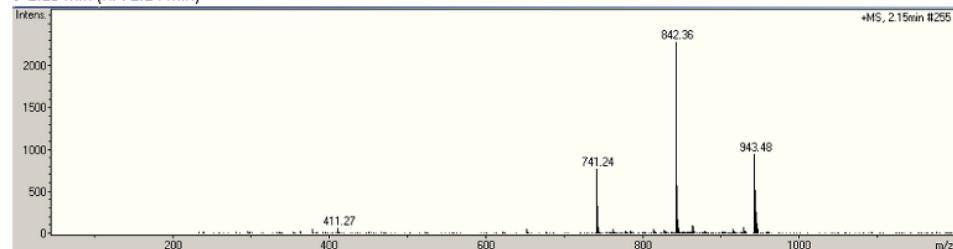
t=2.19 min



m/z	I	Formula
536.99	3115	[MH <sub>2</sub> ] <sup>-</sup>
267.99	907	[MH] <sup>2-</sup>

MS (positive mode)

t=2.15 min (RP: 2.14 min)



m/z	I	Formula
411.27	60	unknown
741.24	765	[MH <sub>2</sub> ] <sup>-</sup> •2[TEAH] <sup>+</sup>
842.36	2283	[MH] <sup>2-</sup> •3[TEAH] <sup>+</sup>
943.48	944	[M] <sup>3-</sup> •4[TEAH] <sup>+</sup>

## S-8.19. Congo Red

### GENERAL INFORMATION

**Color Index Name:** Direct Red 28

**Color Index Number:** 22120

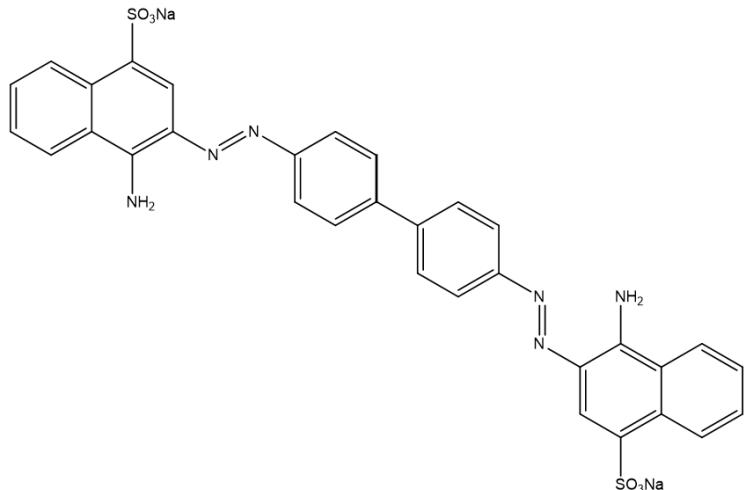
**Type of dye:** Diazo

**Charge:** -2

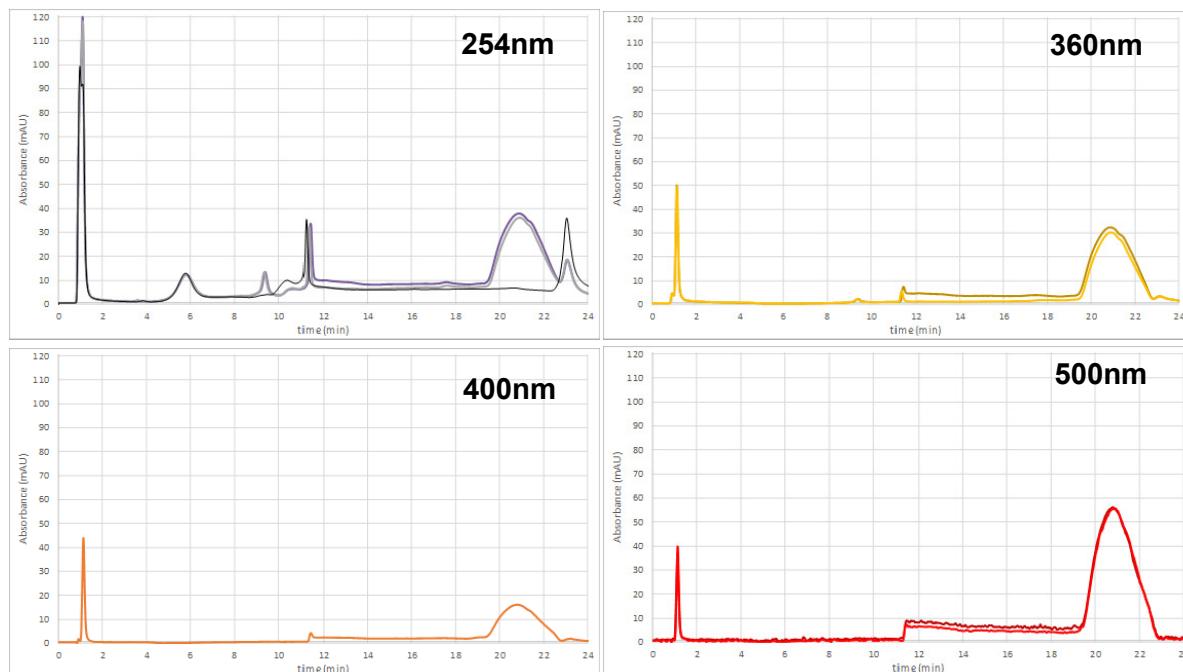
**Molecular Formula:** C<sub>32</sub>H<sub>22</sub>N<sub>6</sub>O<sub>6</sub>S<sub>2</sub> (ion, -2)

### Molecular Weight

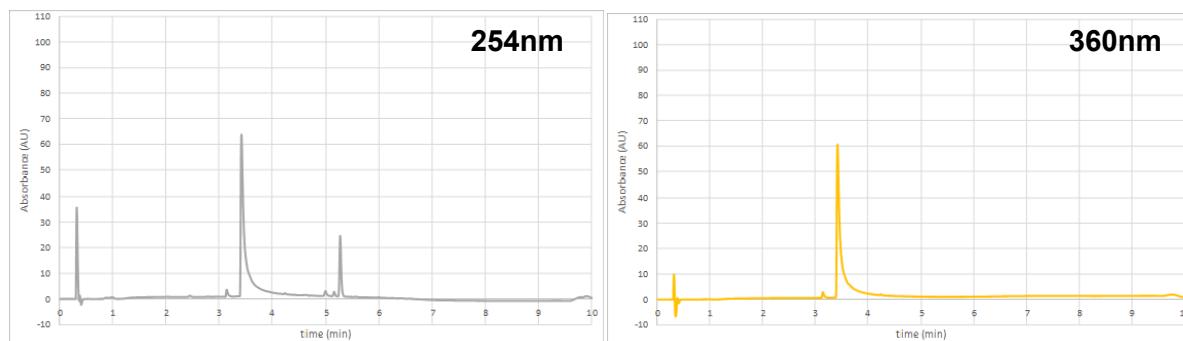
Full molecule:	696.08
Ion (-2)	650.68
Ion (-2), monoisotopic	650.11

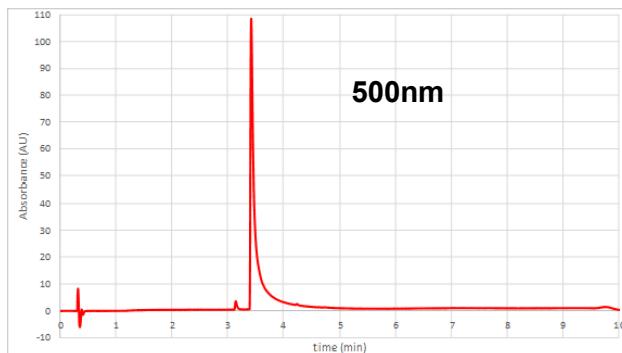


### CHROMATOGRAMS: ION-EXCHANGE



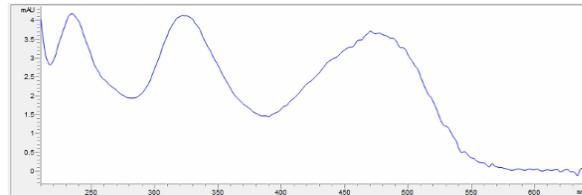
### CHROMATOGRAMS: REVERSED-PHASE



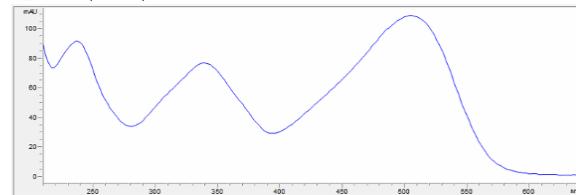


## UV-VIS SPECTRA

t=3.15 min  
 $\lambda_{\text{max}} = 234 \text{ nm}; 322 \text{ nm}; 470 \text{ nm}$



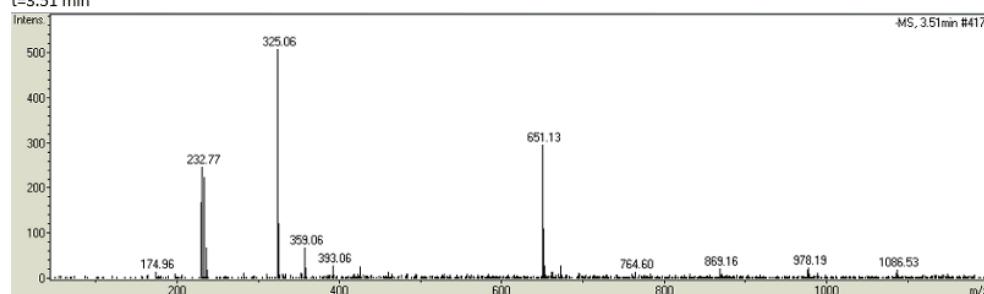
t=3.42 min  
 $\lambda_{\text{max}} = 238 \text{ nm}; 340 \text{ nm}; 506 \text{ nm}$



## MASS SPECTRA

### MS (negative mode)

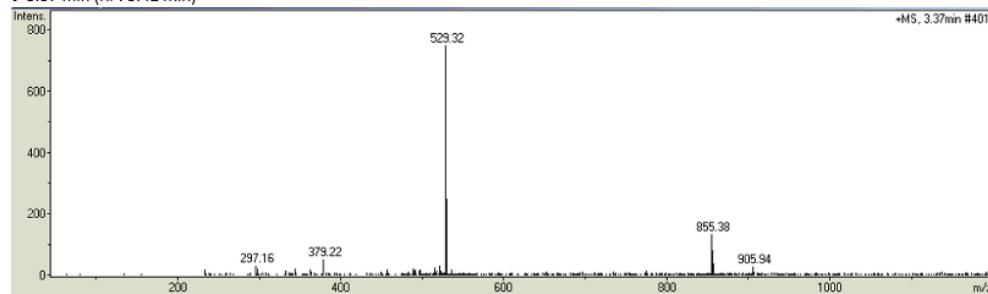
t=3.51 min



m/z	I	Formula
325.06	510	[M] <sup>2-</sup>
651.13	296	[MH] <sup>-</sup>

### MS (positive mode)

t=3.37 min (RP: 3.42 min)



m/z	I	Formula
529.32	753	[M] <sup>2-</sup> •4[TEAH] <sup>+</sup>
855.38	132	[MH] <sup>-</sup> •2[TEAH] <sup>+</sup>

## S-8.20. Cotton Scarlet

### GENERAL INFORMATION

**Alternative names:** Brilliant Crocein MOO, Crocein Scarlet MOO

**Color Index Name:** Acid Red 73

**Color Index Number:** 27290

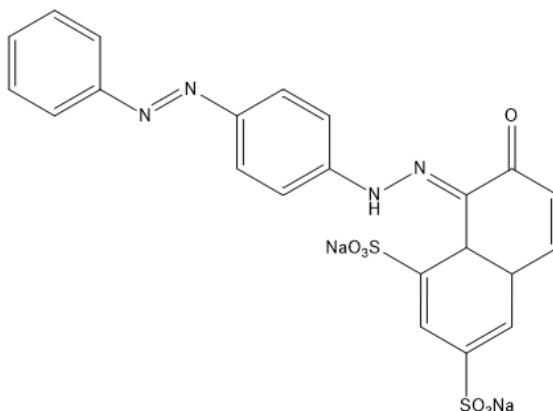
**Type of dye:** Diazo

**Charge:** -2

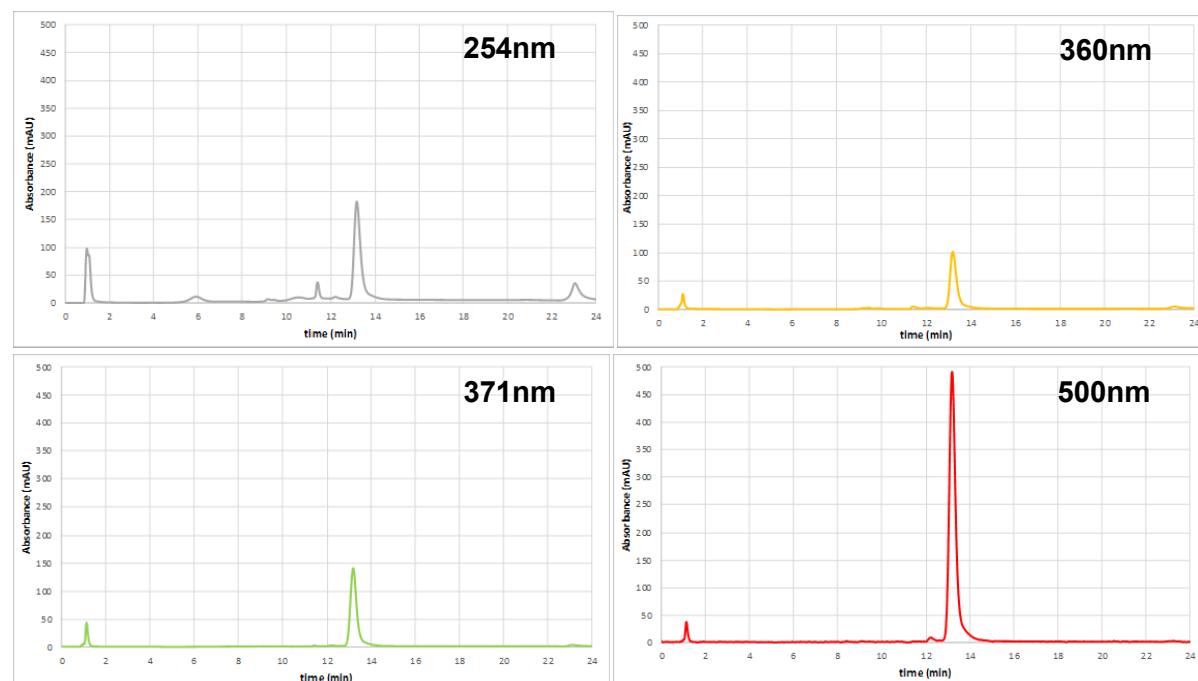
**Molecular Formula:** C<sub>22</sub>H<sub>16</sub>N<sub>4</sub>O<sub>7</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

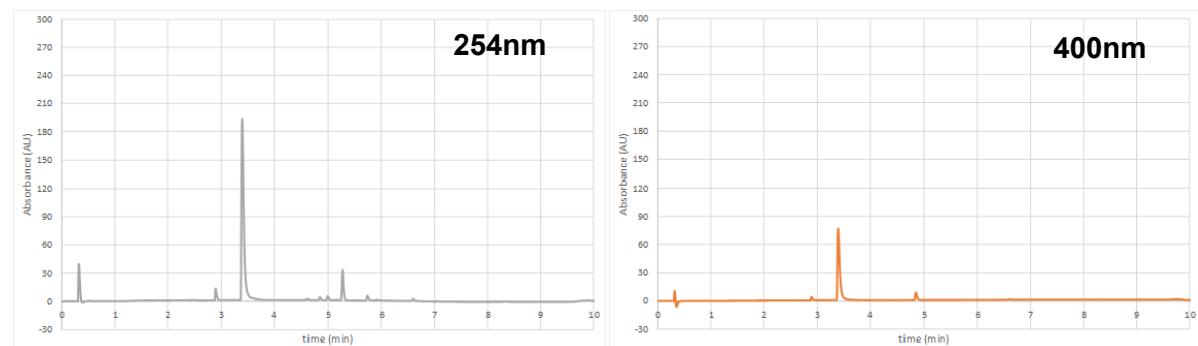
Full molecule:	558.49
Ion (-2)	512.52
Ion (-2), monoisotopic	512.05

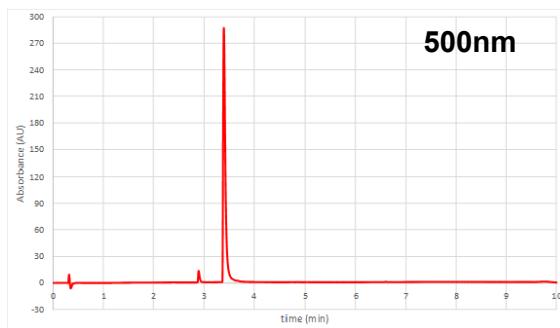


### CHROMATOGRAMS: ION-EXCHANGE



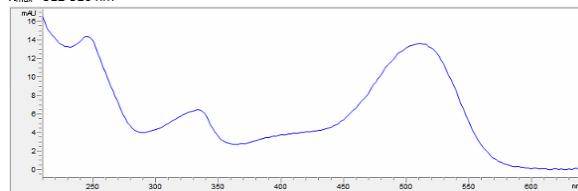
### CHROMATOGRAMS: REVERSED-PHASE



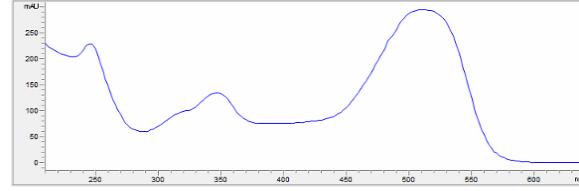


## UV-VIS SPECTRA

$t=2.90$  min  
 $\lambda_{\text{max}}=512-516$  nm



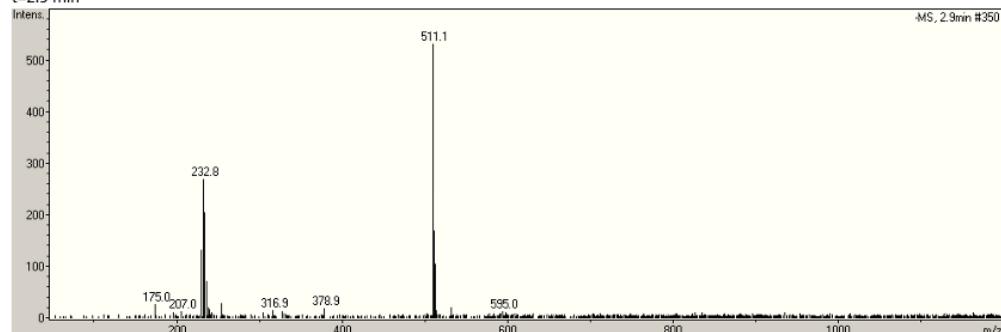
$t=3.40$  min  
 $\lambda_{\text{max}}=508-514$  nm



## MASS SPECTRA

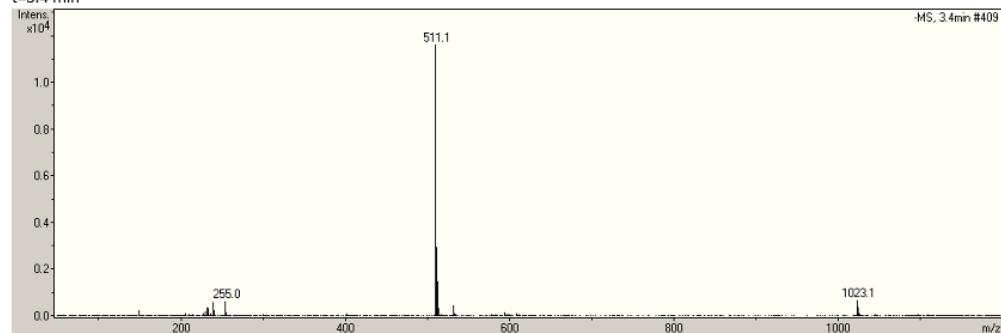
### MS (negative mode)

$t=2.9$  min



m/z	I	Formula
511.1	533	$[\text{MH}]^-$

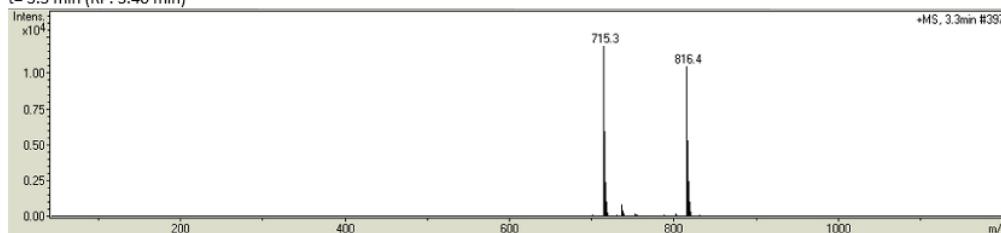
$t=3.4$  min



m/z	I	Formula
511.1	11626	$[\text{MH}]^-$
255.0	590	$[\text{M}]^{2-}$
1023.1	629	$2[\text{MH}]^- \bullet \text{H}^+$

### MS (positive mode)

$t=3.3$  min (RP: 3.40 min)



m/z	I	Formula
715.3	11959	$[\text{MH}]^- \bullet 2[\text{TEAH}]^+$
737.3	756	$[\text{M}]^{2-} \bullet \text{Na}^+ \bullet 2[\text{TEAH}]^+$
816.4	10518	$[\text{M}]^{2-} \bullet 3[\text{TEAH}]^+$

## S-8.21. Crocein Orange G

### GENERAL INFORMATION

**Color Index Name:** Acid Orange 12

**Color Index Number:** 15970

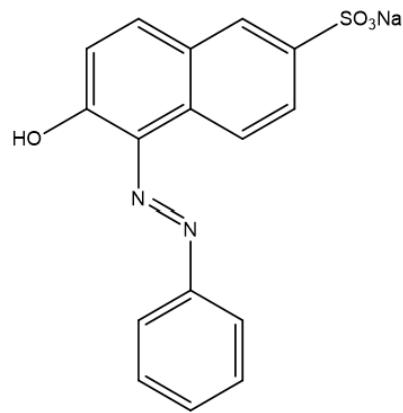
**Type of dye:** Monoazo

**Charge:** -1

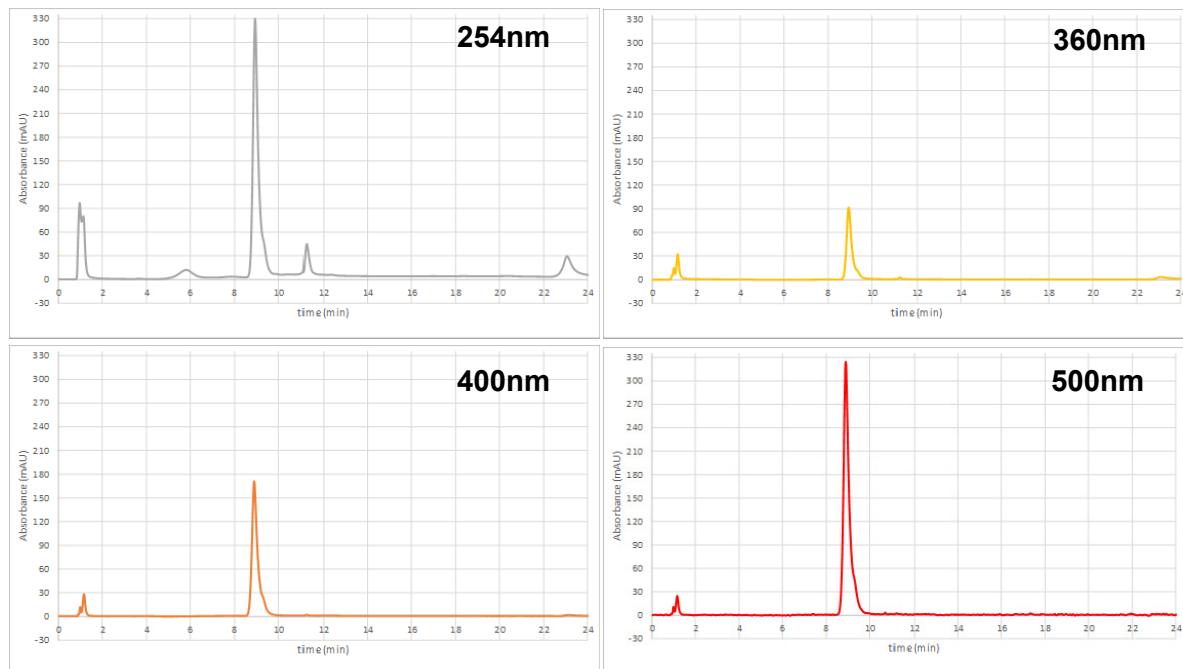
**Molecular Formula:** C<sub>16</sub>H<sub>11</sub>N<sub>2</sub>O<sub>4</sub>S (ion, -1)

**Molecular Weight**

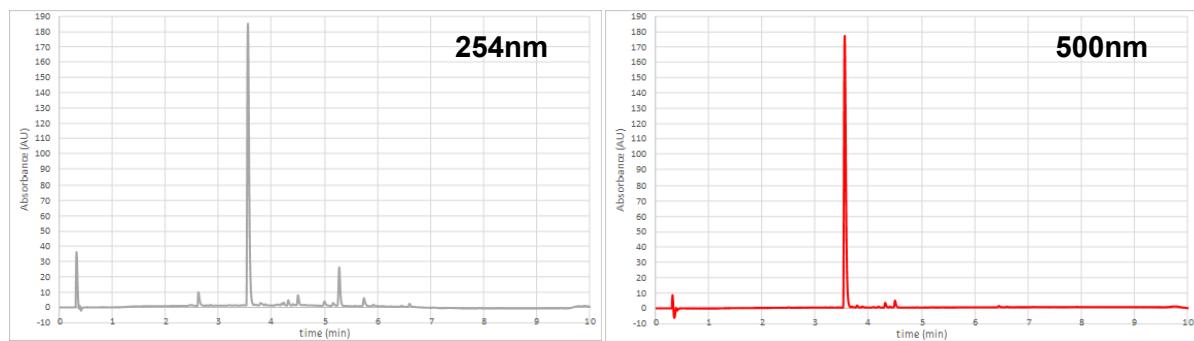
Full molecule:	350.32
Ion (-1)	327.34
Ion (-1), monoisotopic	327.04



### CHROMATOGRAMS: ION-EXCHANGE

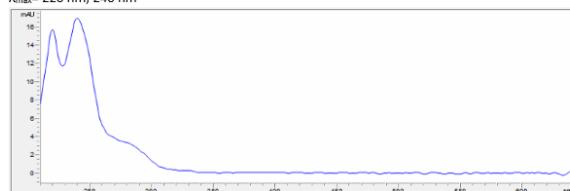


### CHROMATOGRAMS: REVERSED-PHASE



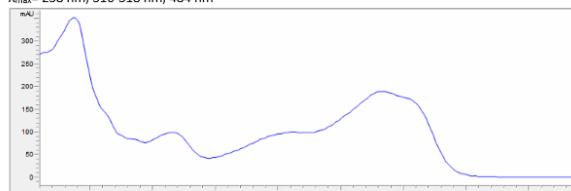
## UV-VIS SPECTRA

t=2.62 min  
 $\lambda_{\text{max}} = 220 \text{ nm; } 240 \text{ nm}$

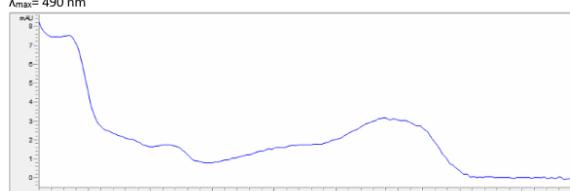


t=3.56 min  
 $\lambda_{\text{max}} = 238 \text{ nm; } 316-318 \text{ nm; } 484 \text{ nm}$

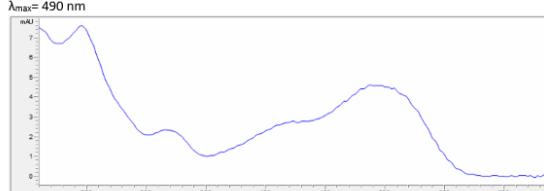
t=3.56 min  
 $\lambda_{\text{max}} = 238 \text{ nm; } 316-318 \text{ nm; } 484 \text{ nm}$



t=4.32 min  
 $\lambda_{\text{max}} = 490 \text{ nm}$



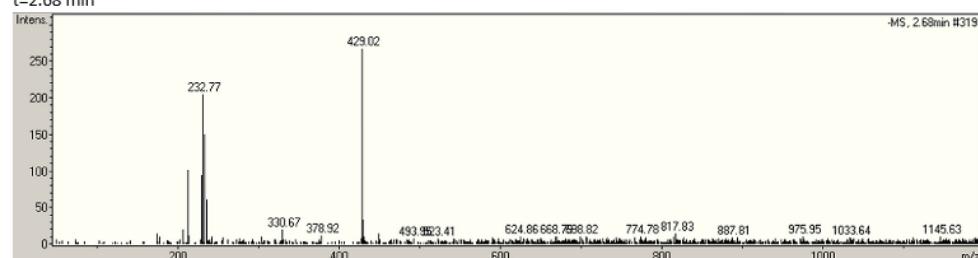
t=4.51 min  
 $\lambda_{\text{max}} = 490 \text{ nm}$



## MASS SPECTRA

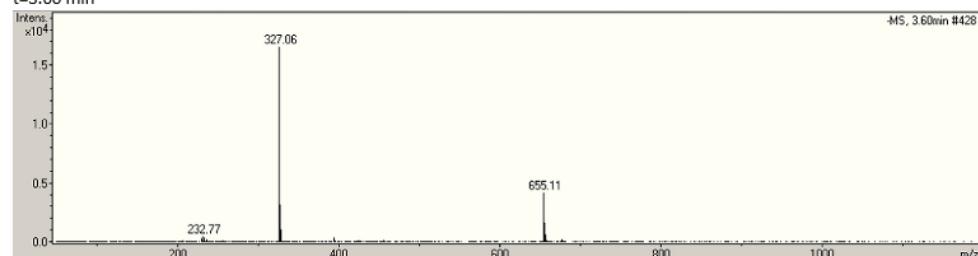
### MS (negative mode)

t=2.68 min



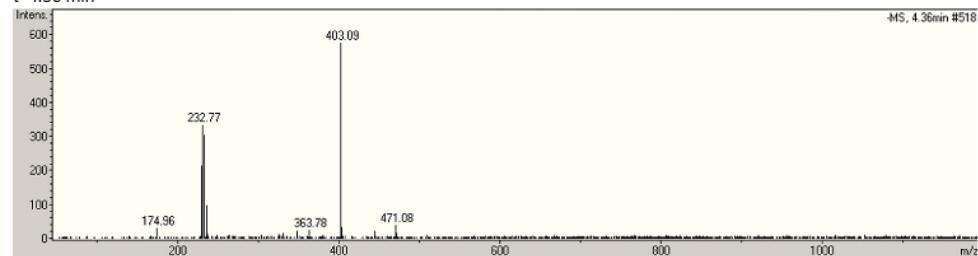
m/z	I	Formula
429.02	268	unknown

t=3.60 min



m/z	I	Formula
327.06	16572	[M] <sup>-</sup>
655.11	4168	2[M] <sup>-</sup> •H <sup>+</sup>

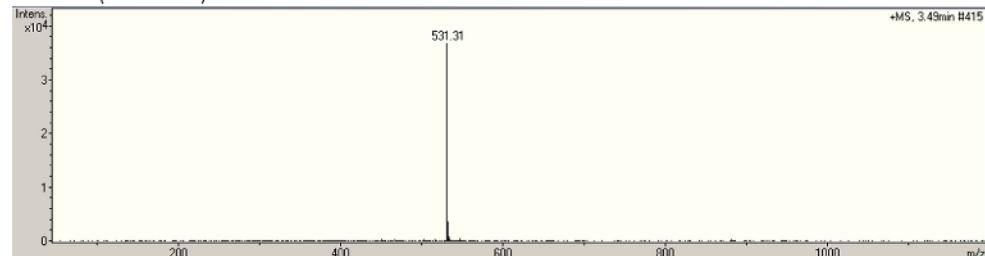
t=4.36 min



m/z	I	Formula
403.09	576	unknown

### MS (positive mode)

t=3.49 min (RP: 3.56 min)



m/z	I	Formula
531.31	36969	[M] <sup>-</sup> •2[TEAH] <sup>+</sup>

## S-8.22. Crystal Ponceau 6R

### GENERAL INFORMATION

**Color Index Name:** Acid Red 44

**Color Index Number:** 16250

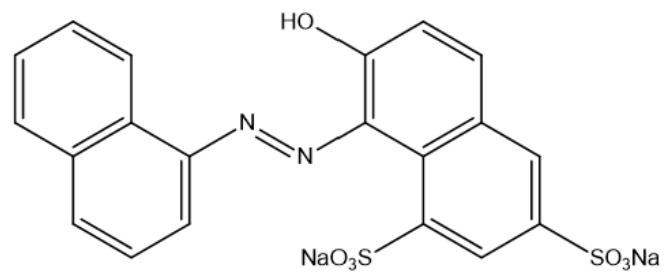
**Type of dye:** Monoazo

**Charge:** -2

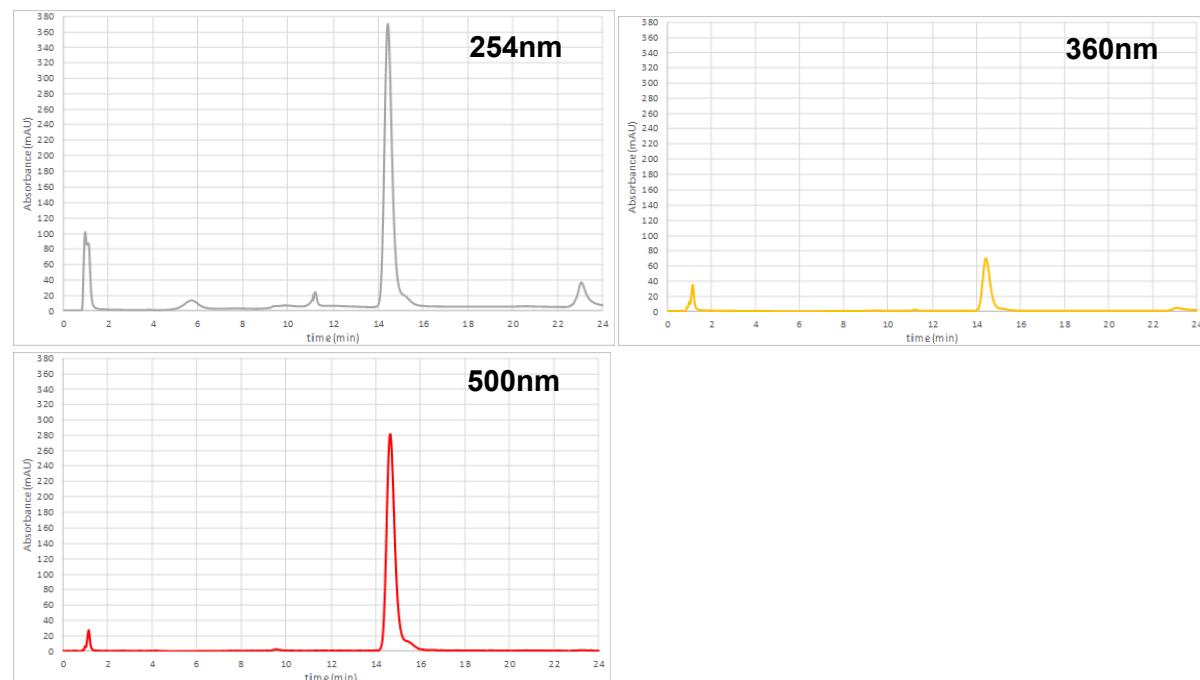
**Molecular Formula:** C<sub>20</sub>H<sub>12</sub>N<sub>2</sub>O<sub>7</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

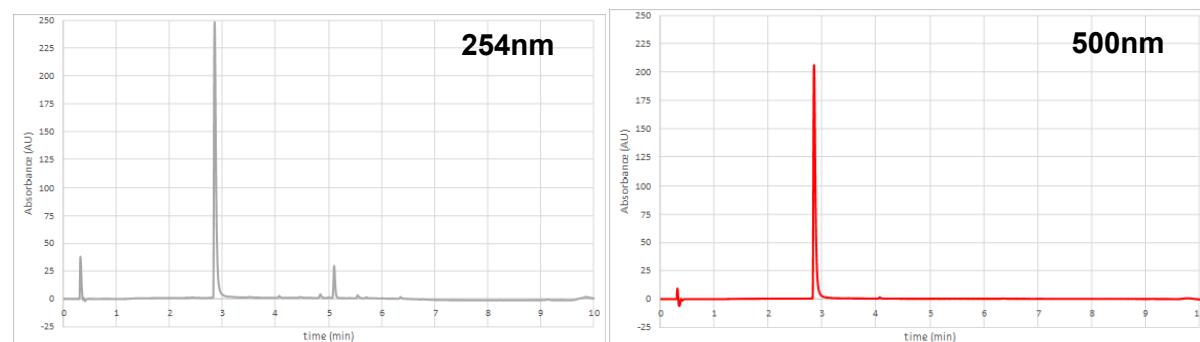
Full molecule:	502.43
Ion (-2)	456.45
Ion (-2), monoisotopic	456.01



### CHROMATOGRAMS: ION-EXCHANGE

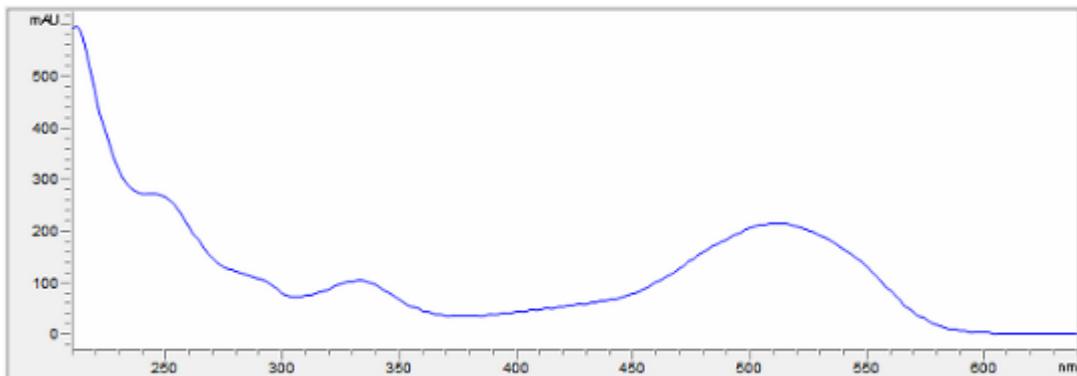


### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

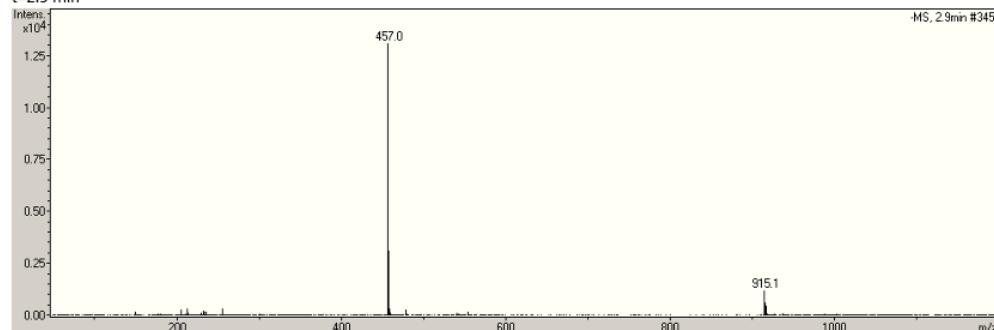
$t=2.85\text{ min}$   
 $\lambda_{\max}=510\text{-}513\text{ nm}$



## MASS SPECTRA

MS (negative mode)

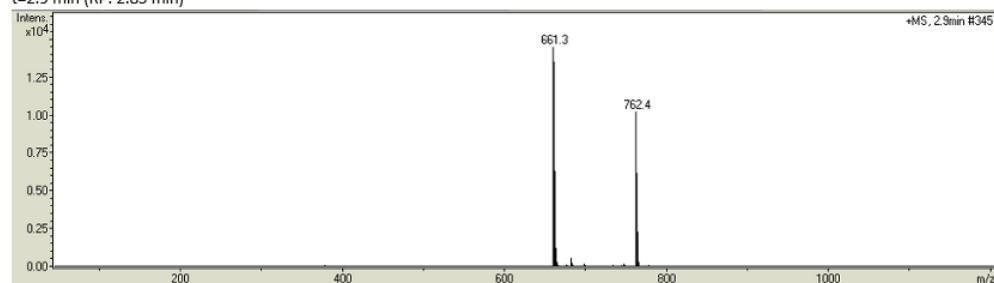
$t=2.9\text{ min}$



m/z	I	Formula
457.0	13110	$[\text{MH}]^-$
915.1	1170	$2[\text{MH}]^- \bullet \text{H}^+$

MS (positive mode)

$t=2.9\text{ min (RP: 2.85 min)}$



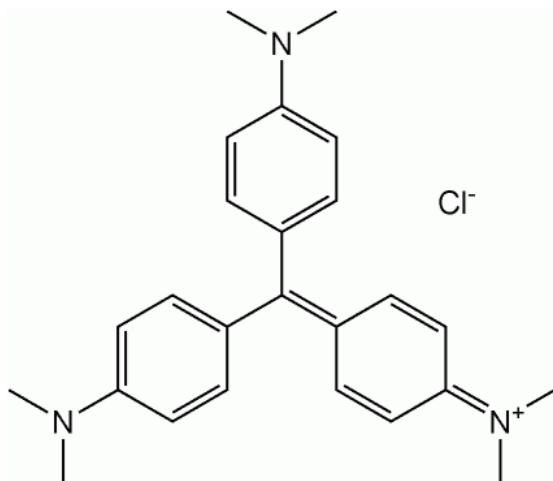
m/z	I	Formula
661.3	14514	$[\text{MH}]^- \bullet 2[\text{TEAH}]^+$
762.4	10226	$[\text{M}]^{2-} \bullet 3[\text{TEAH}]^+$

### S-8.23. Crystal Violet

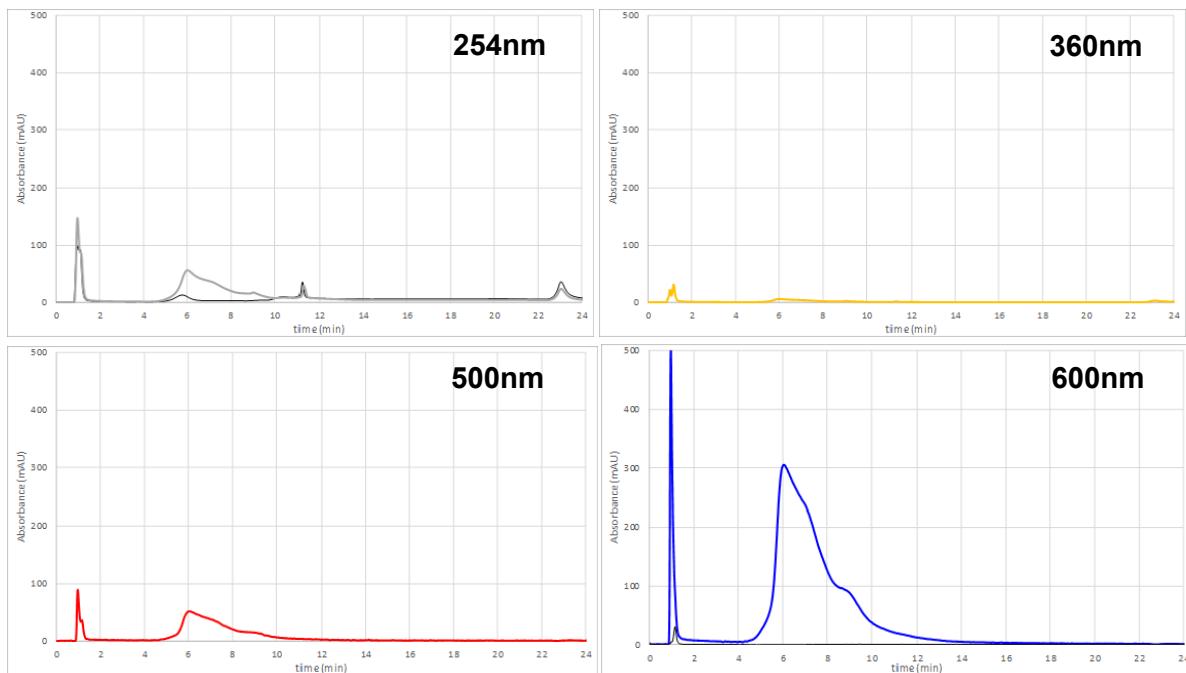
#### GENERAL INFORMATION

**Color Index Name:** Basic Violet 3  
**Color Index Number:** 42555  
**Type of dye:** Triarylmethane  
**Charge:** +1  
**Molecular Formula:** C<sub>25</sub>H<sub>30</sub>N<sub>3</sub> (ion, +1)  
**Molecular Weight**

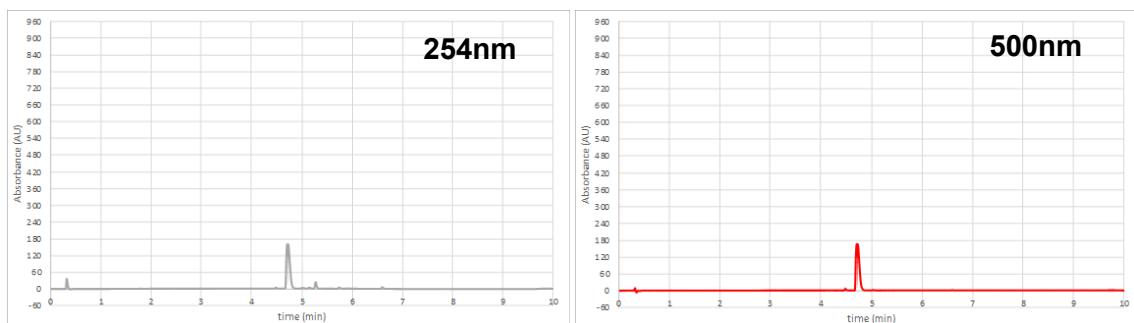
Full molecule:	407.98
Ion (+1)	372.53
Ion (+1), monoisotopic	372.24

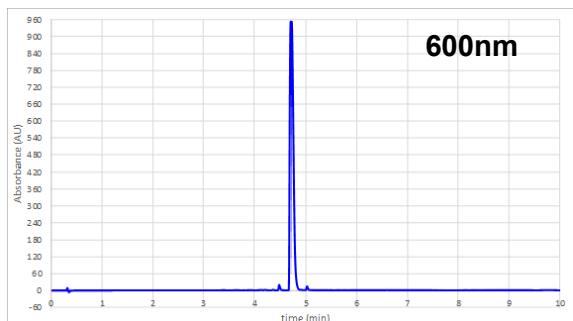


#### CHROMATOGRAMS: ION-EXCHANGE



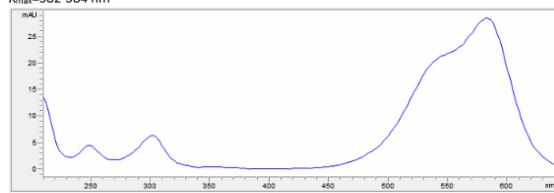
#### CHROMATOGRAMS: REVERSED-PHASE





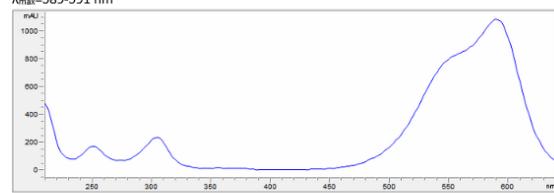
## UV-VIS SPECTRA

t=4.49 min  
 $\lambda_{\text{max}}=582-584 \text{ nm}$

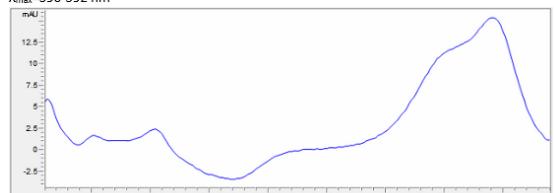


t=4.71 min  
 $\lambda_{\text{max}}=589-591 \text{ nm}$

t=4.71 min  
 $\lambda_{\text{max}}=589-591 \text{ nm}$

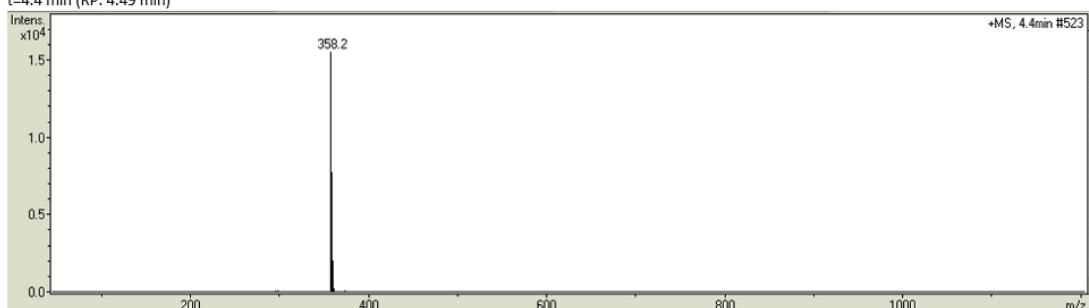


t=5.02 min  
 $\lambda_{\text{max}}=590-592 \text{ nm}$

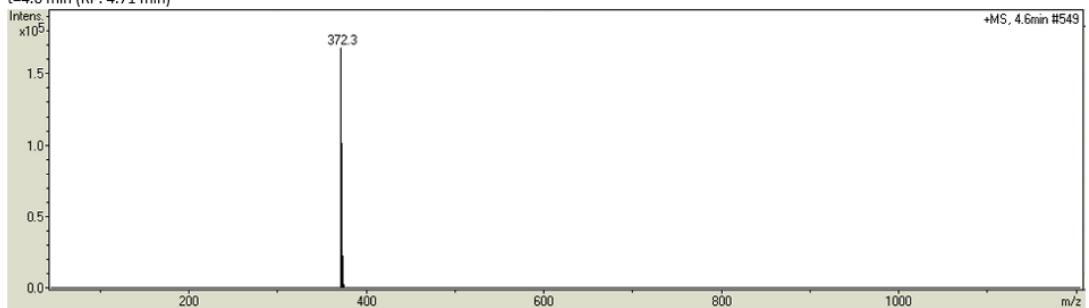


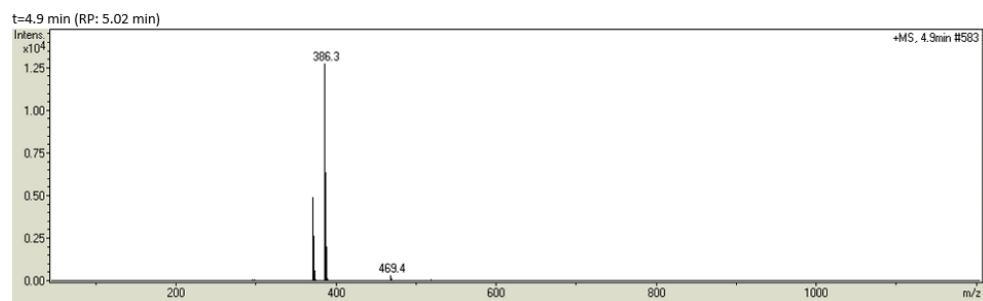
## MASS SPECTRA

MS (positive mode)  
t=4.4 min (RP: 4.49 min)



t=4.6 min (RP: 4.71 min)





## S-8.24. Diamond Green B

### GENERAL INFORMATION

**Alternative names:** Malachite Green

**Color Index Name:** Basic Green 4

**Color Index Number:** 42000

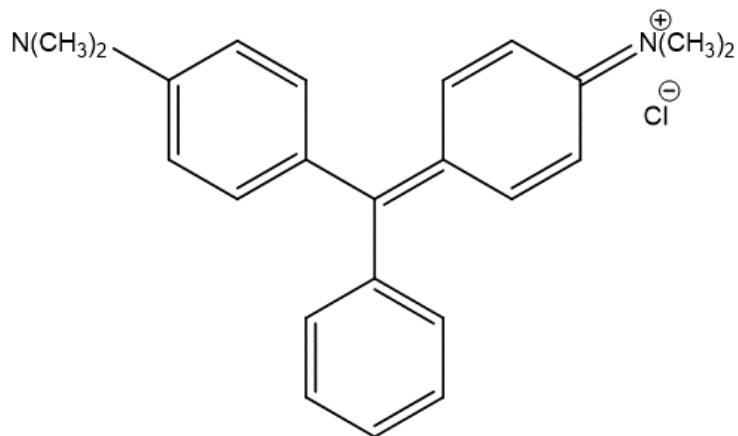
**Type of dye:** Triarylmethane

**Charge:** +1

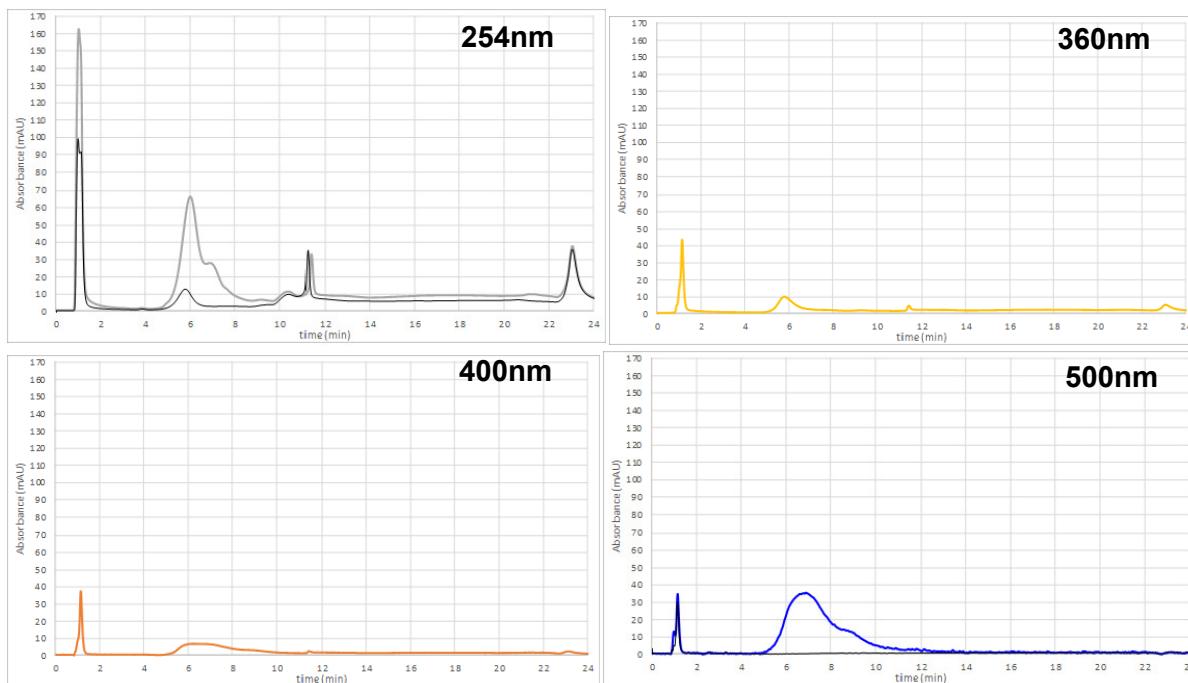
**Molecular Formula:** C<sub>27</sub>H<sub>33</sub>N<sub>2</sub> (ion, +1)

**Molecular Weight**

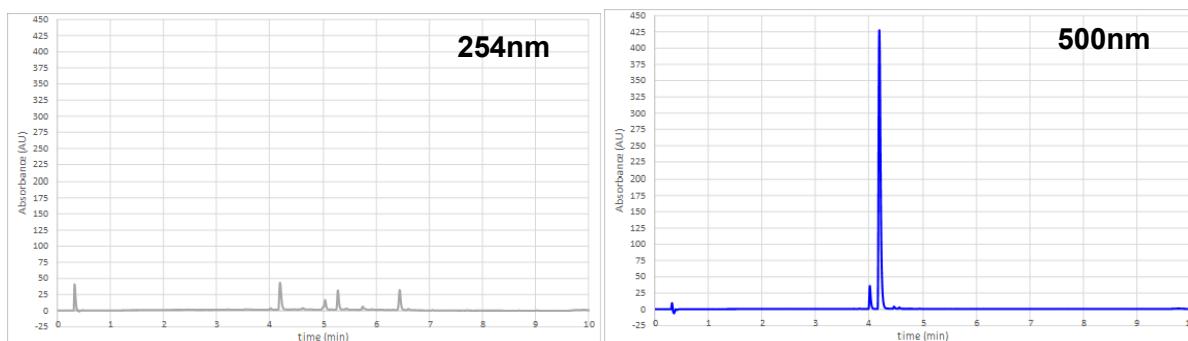
Full molecule:	364.91
Ion (+1)	329.46
Ion (+1), monoisotopic	329.20



### CHROMATOGRAMS: ION-EXCHANGE

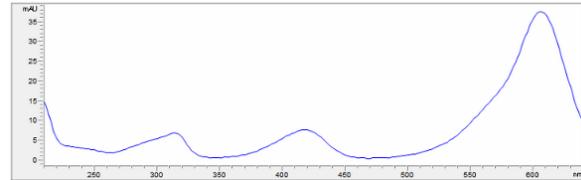


### CHROMATOGRAMS: REVERSED-PHASE

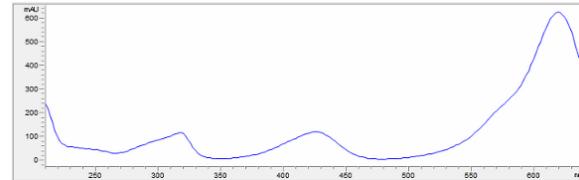


## UV-VIS SPECTRA

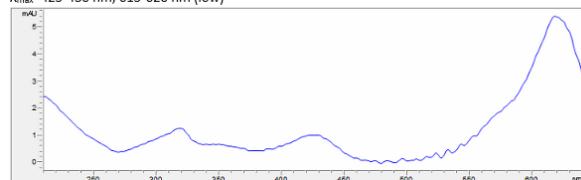
t=4.02 min  
 $\lambda_{\text{max}}=418 \text{ nm; } 606 \text{ nm}$



t=4.20 min  
 $\lambda_{\text{max}}=426 \text{ nm; } 620 \text{ nm}$

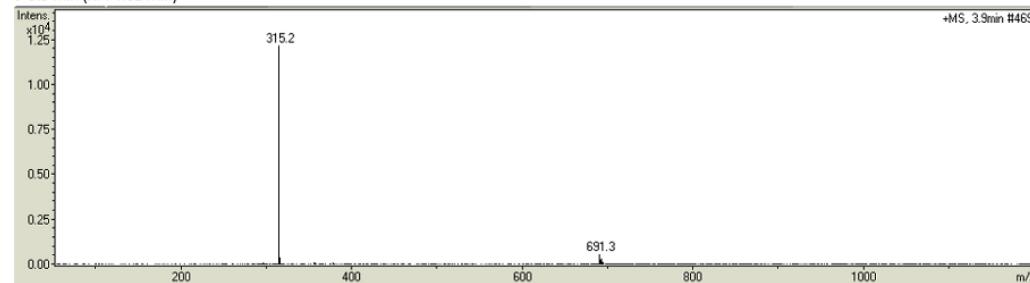


t=4.77 min  
 $\lambda_{\text{max}}=425-430 \text{ nm; } 615-620 \text{ nm (low)}$



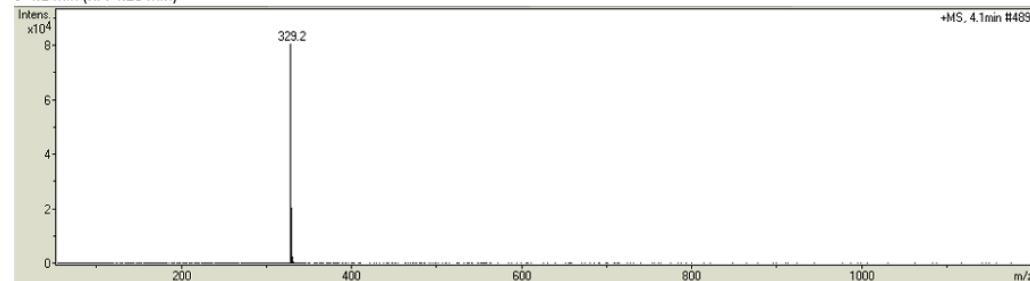
## MASS SPECTRA

t=3.9 min (RP: 4.02 min)



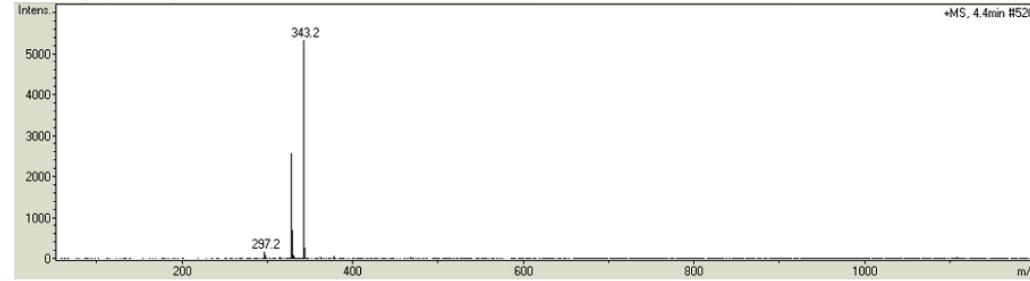
m/z	I	Formula
315.2	12159	$[\text{M}-\text{CH}_2]^+$

t=4.1 min (RP: 4.20 min)



m/z	I	Formula
329.2	80585	$[\text{M}]^+$

t=4.4 min (RP: 4.47 min)



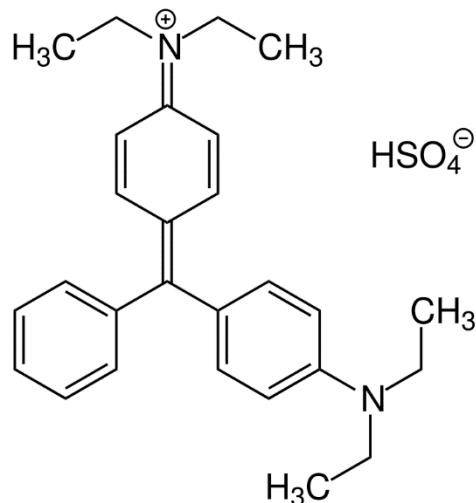
m/z	I	Formula
343.2	5352	$[\text{M}+\text{CH}_2]^+$

### S-8.25. Diamond Green G

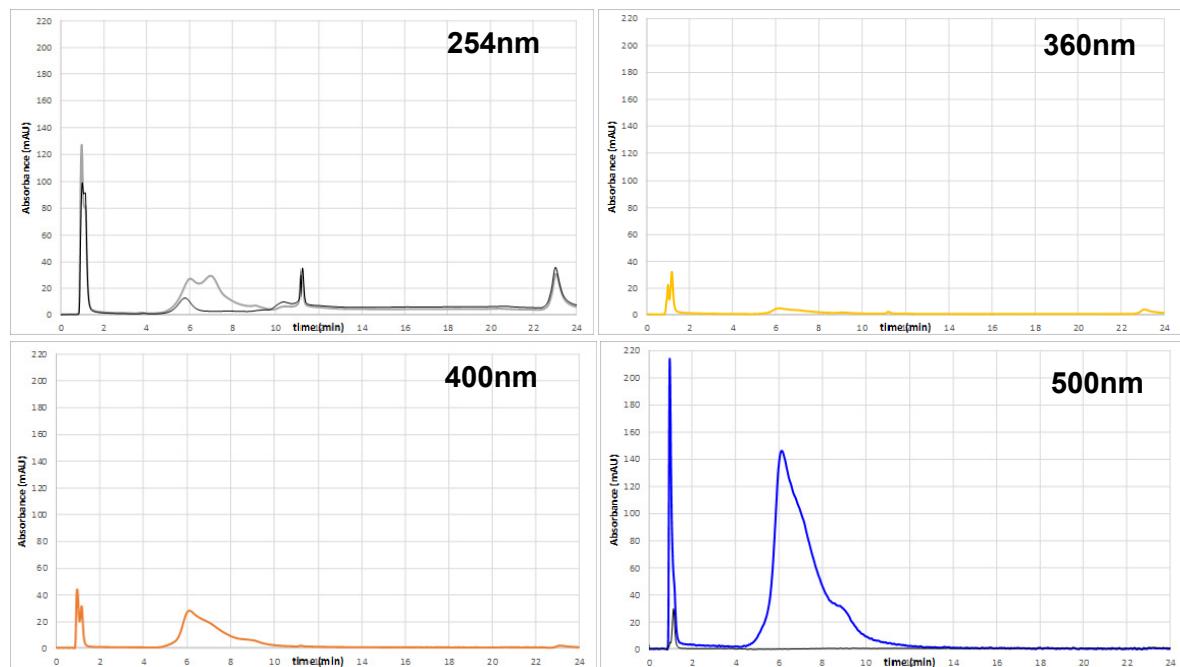
#### GENERAL INFORMATION

**Alternative names:** Brilliant Green  
**Color Index Name:** Basic Green 1  
**Color Index Number:** 42040  
**Type of dye:** Triarylmethane  
**Charge:** +1  
**Molecular Formula:** C<sub>27</sub>H<sub>33</sub>N<sub>2</sub> (ion, +1)  
**Molecular Weight**

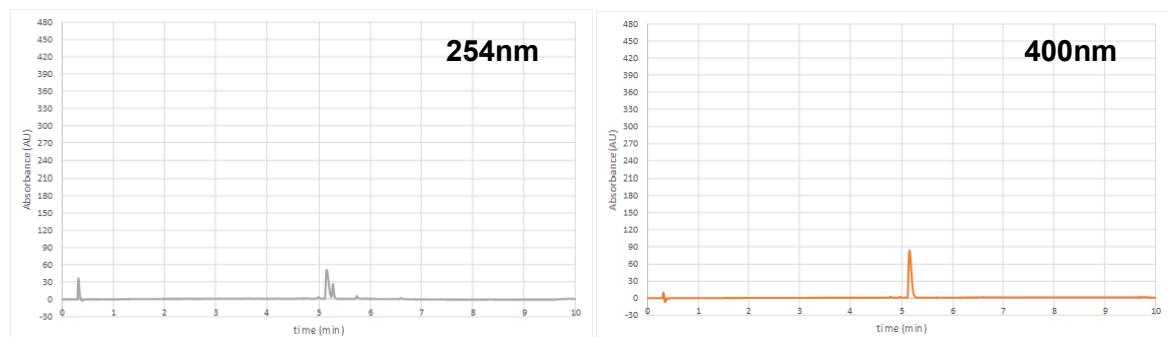
Full molecule:	482.63
Ion (+1)	385.56
Ion (+1), monoisotopic	385.26

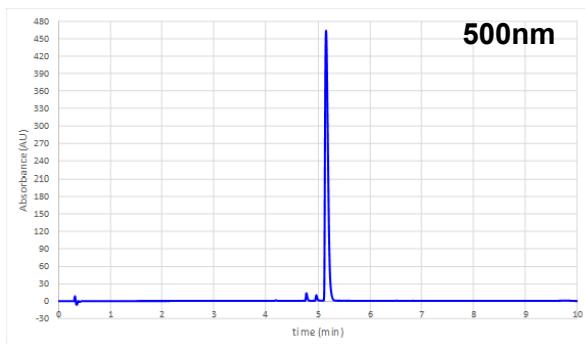


#### CHROMATOGRAMS: ION-EXCHANGE



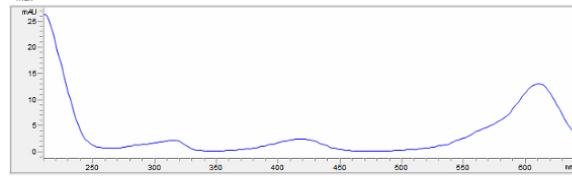
#### CHROMATOGRAMS: REVERSED-PHASE



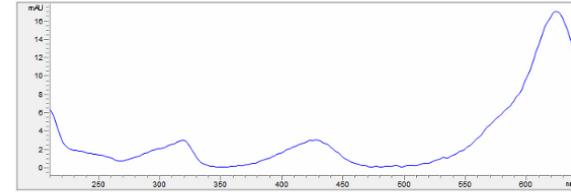


## UV-VIS SPECTRA

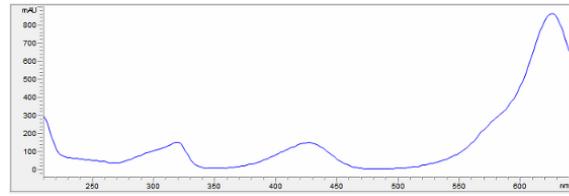
$t=4.77$  min  
 $\lambda_{\max}=609-614$  nm



$t=4.96$  min  
 $\lambda_{\max}=622-626$  nm

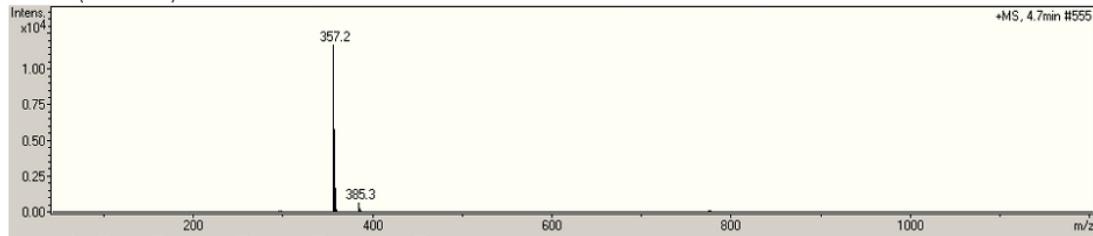


$t=5.15$  min  
 $\lambda_{\max}=320$  nm; 426 nm; 626 nm

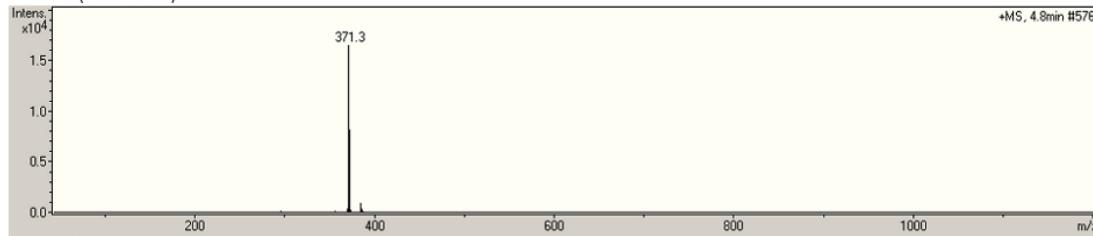


## MASS SPECTRA

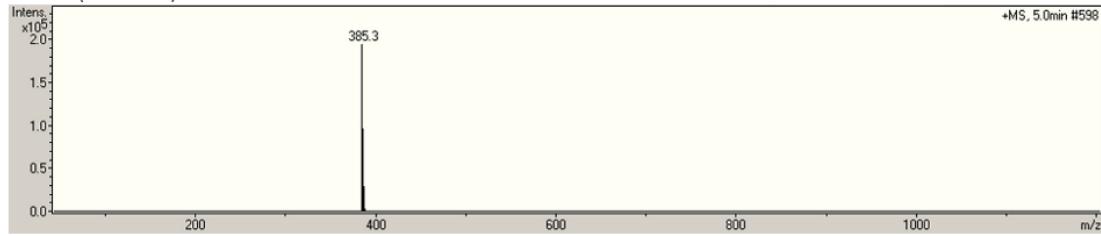
$t=4.7$  min (RP: 4.77 min)



$t=4.8$  min (RP: 4.96 min)



$t=5.0$  min (RP: 5.15 min)



## S-8.26. Emodin

### GENERAL INFORMATION

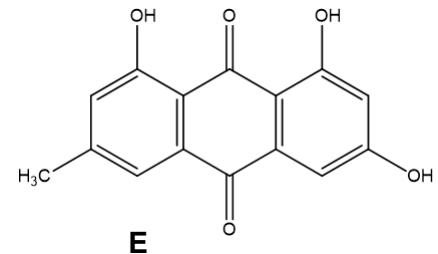
**Color Index Name:** n.a.

**Color Index Number:** n.a.

**Type of dye:** Natural, Mordant dye

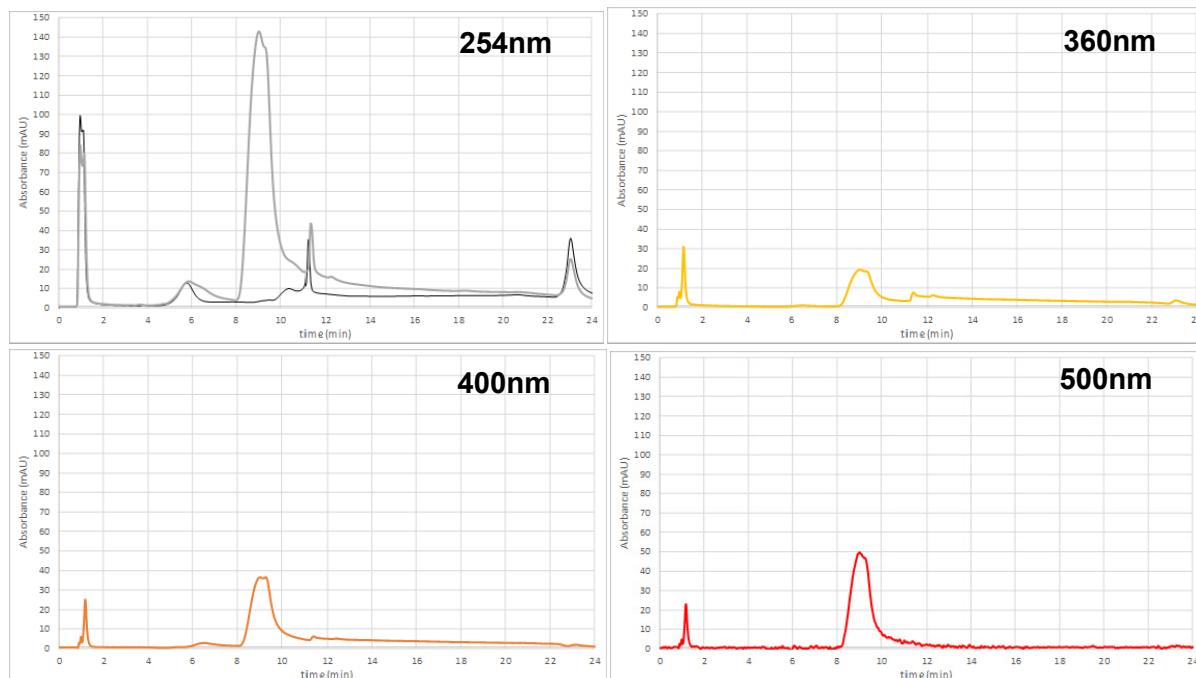
**Related dyes:** Quercetin (302.24), Gallic Acid (170.12)

**Scientific name of biological source:** Many species

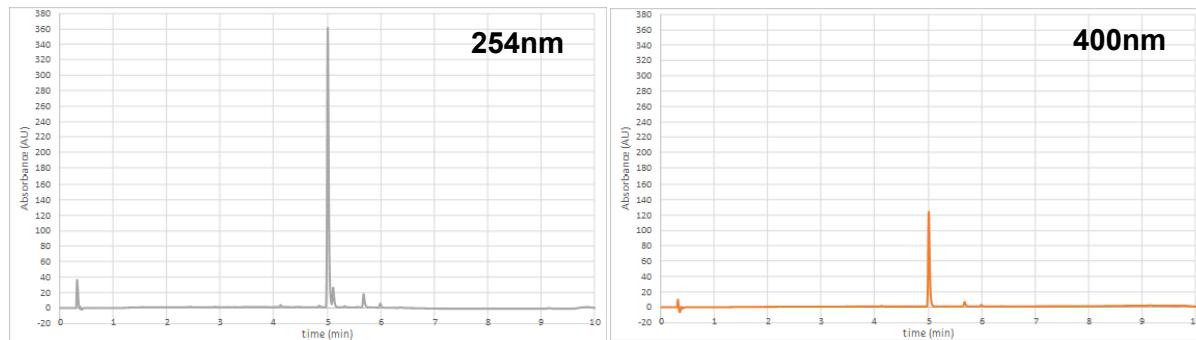


Name	Short	Mw	monoisotopic	Formula
Emodin	[E]	270.24	270.05	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>

### CHROMATOGRAMS: ION-EXCHANGE

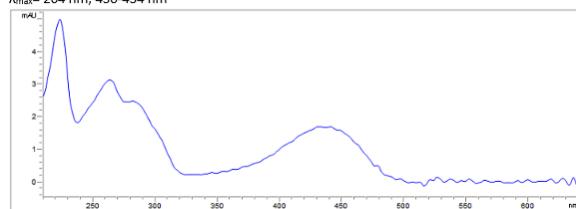


### CHROMATOGRAMS: REVERSED-PHASE

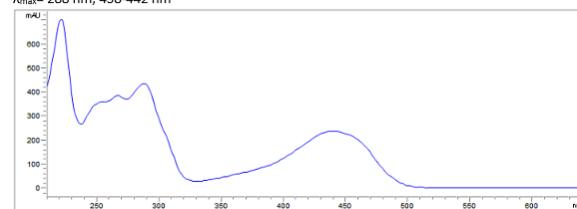


## UV-VIS SPECTRA

t=4.13 min  
 $\lambda_{\text{max}} = 264 \text{ nm}; 430-434 \text{ nm}$

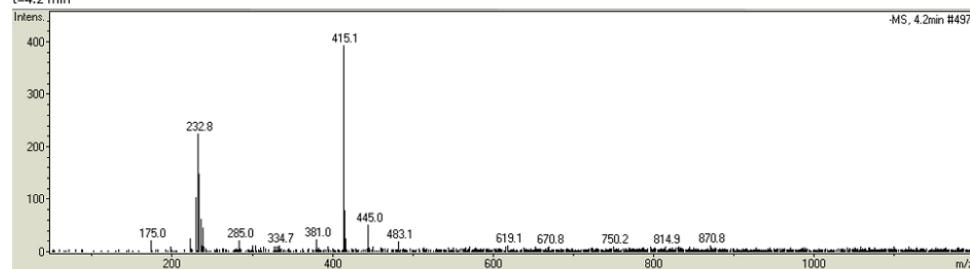


t=5.00 min  
 $\lambda_{\text{max}} = 288 \text{ nm}; 438-442 \text{ nm}$



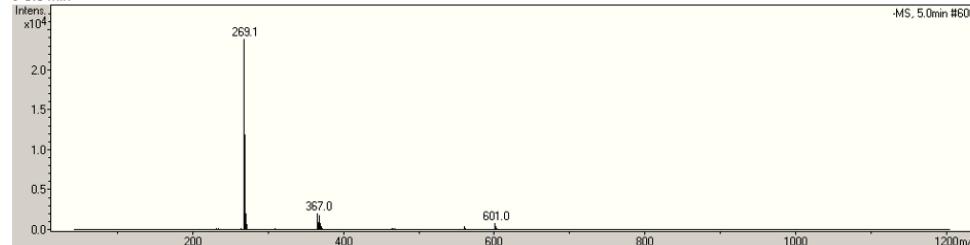
## MASS SPECTRA

t=4.2 min



m/z	I	Formula
431.1	395	[E+Gly] <sup>+</sup>

t=5.0 min



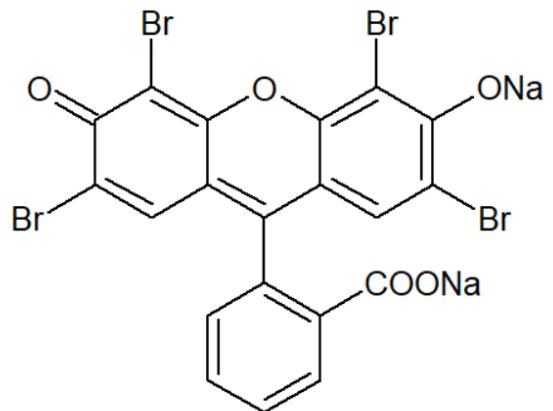
m/z	I	Formula
269.1	23945	[E] <sup>+</sup>
367.0	1931	+97.9
601.0	747	unknown

## S-8.27. Eosin A

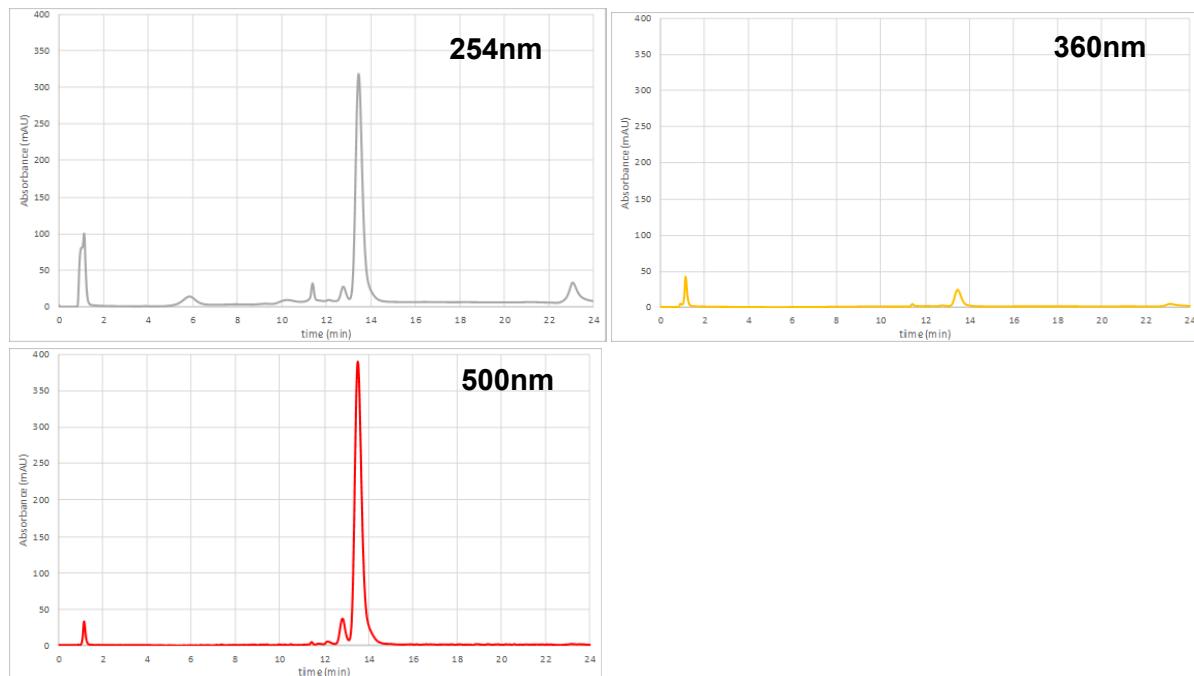
### GENERAL INFORMATION

**Alternative names:** Eosine Y  
**Color Index Name:** Acid Red 87  
**Color Index Number:** 45380  
**Type of dye:** Xanthene  
**Charge:** -1  
**Molecular Formula:** C<sub>20</sub>H<sub>7</sub>Br<sub>4</sub>O<sub>5</sub> (ion, -1, ONa replaced with OH)  
**Molecular Weight**

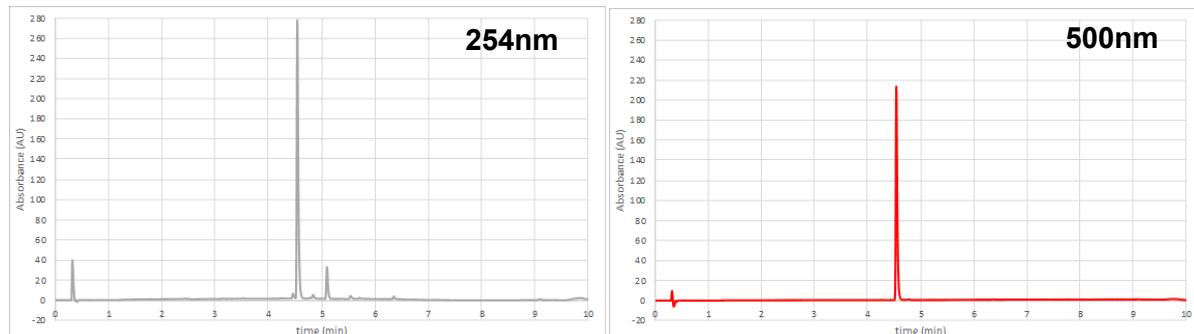
Full molecule:	691.85
Ion (-1)	646.88
Ion (-1), monoisotopic	642.70
<sup>79</sup> Bromine	78.92
<sup>81</sup> Bromine	80.92



### CHROMATOGRAMS: ION-EXCHANGE

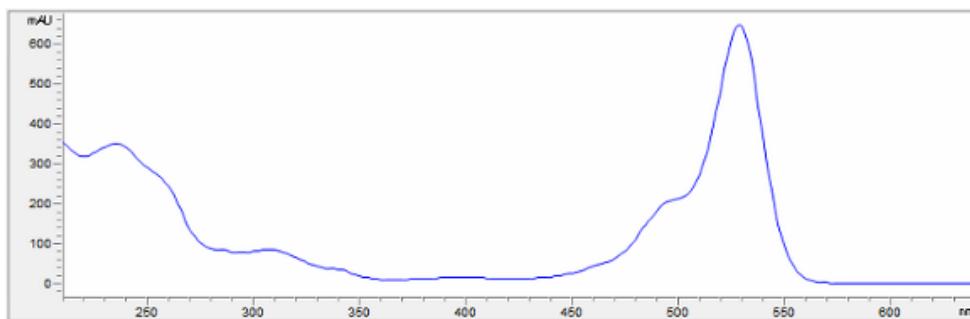


### CHROMATOGRAMS: REVERSED-PHASE



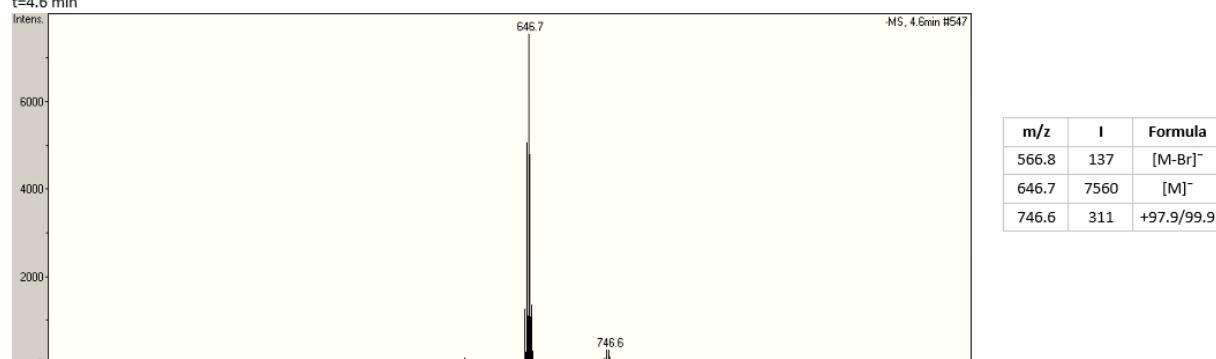
## UV-VIS SPECTRA

t=4.55 min  
 $\lambda_{\text{max}} = 528-530 \text{ nm}$

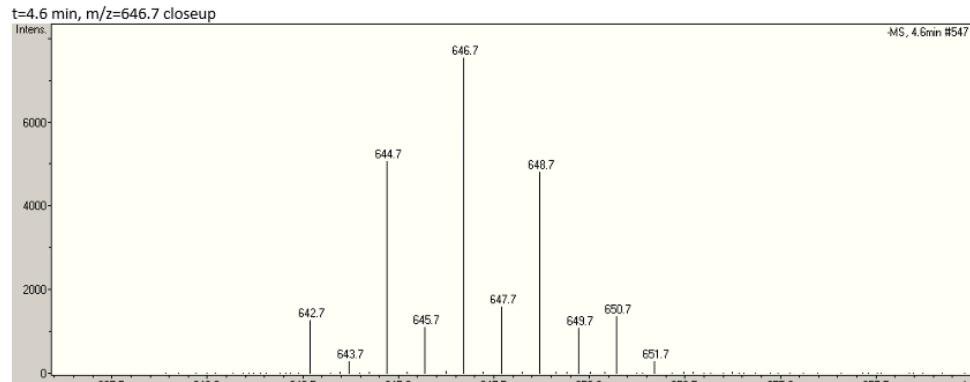


## MASS SPECTRA

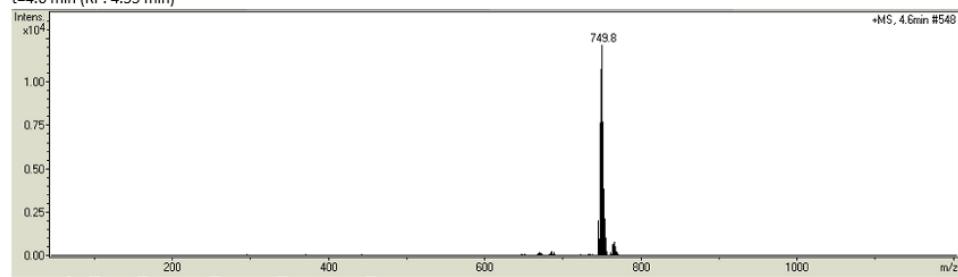
t=4.6 min



t=4.6 min, m/z=646.7 closeup

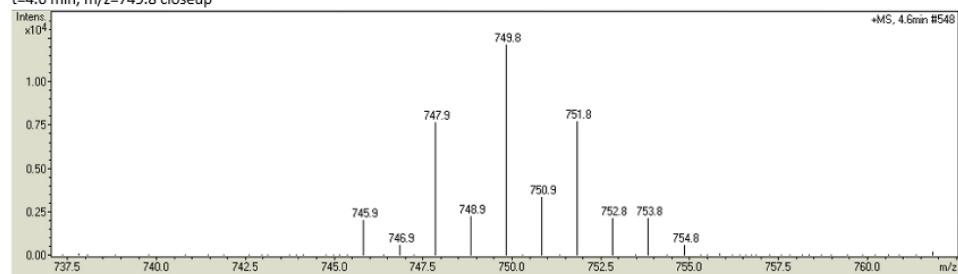


t=4.6 min (RP: 4.55 min)



m/z	I	Formula
749.8	12194	$[M]^- \bullet H^+ \bullet [TEAH]^+$

t=4.6 min,  $m/z$ =749.8 closeup



### S-8.28. (+) Epi Catechin

#### GENERAL INFORMATION

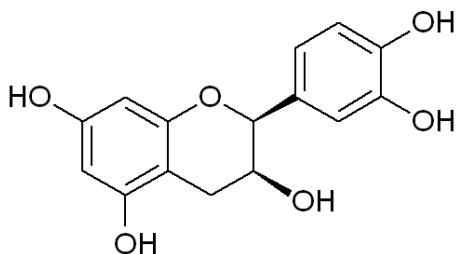
Alternative names: Catechu (extract)

Color Index Name: n.a.

Color Index Number: n.a.

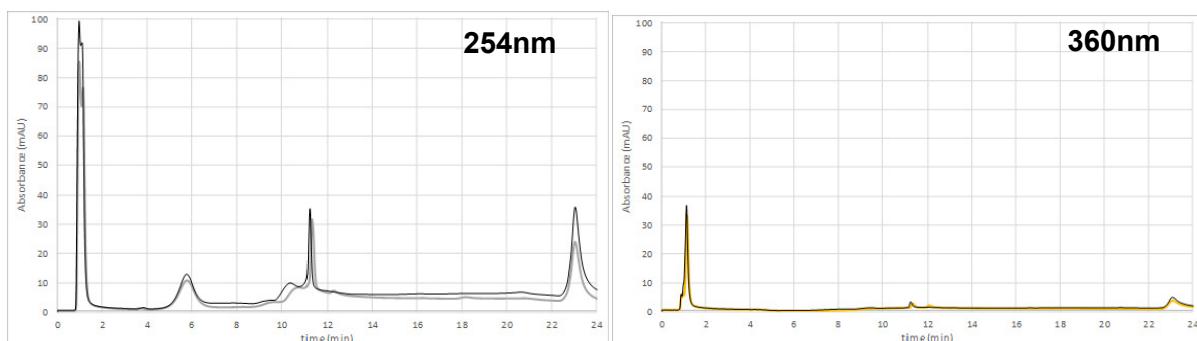
Type of dye: Natural, Mordant dye

Scientific name of biological source: *Rhus coriaria L.* ; *Rhus cotinus L.*

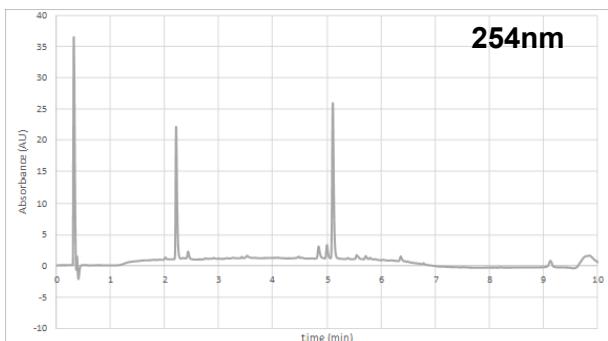


Name	Short	Mw	monoisotopic	Formula
(+) Epi Catechin	[EC]	290.27	290.08	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>

#### CHROMATOGRAMS: ION-EXCHANGE



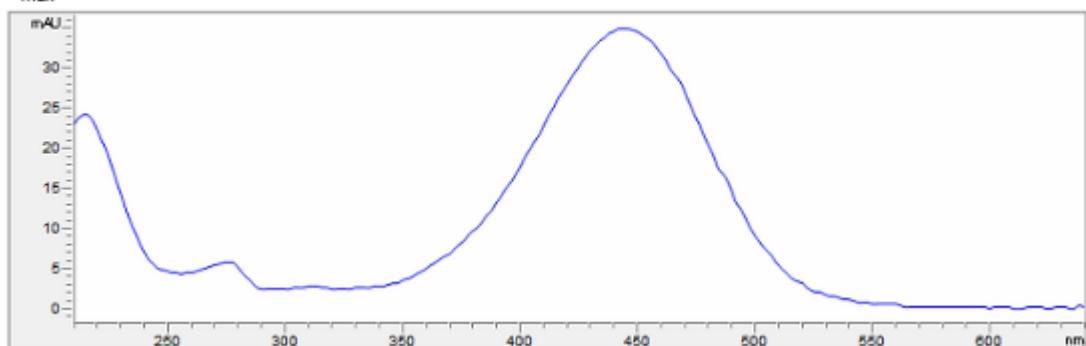
#### CHROMATOGRAMS: REVERSED-PHASE



#### UV-VIS SPECTRA

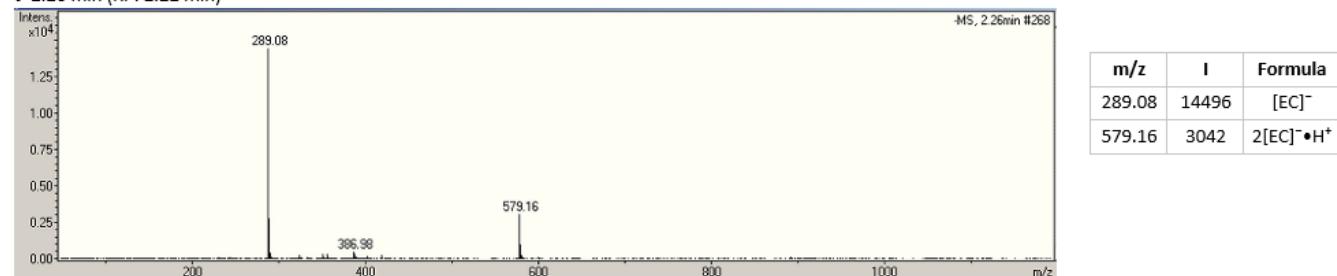
t=2.27 min

$\lambda_{\text{max}} = 444-446 \text{ nm}$



## MASS SPECTRA

t=2.26 min (RP: 2.22 min)



## S-8.29. Erythrosine

### GENERAL INFORMATION

**Color Index Name:** Acid Red 51

**Color Index Number:** 45430

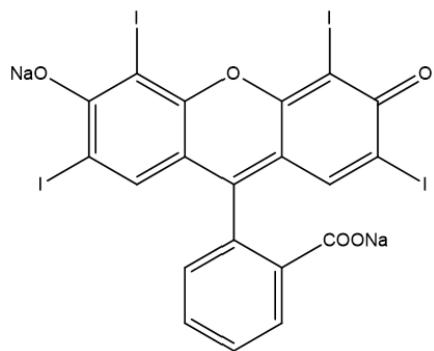
**Type of dye:** Xanthene

**Charge:** -1

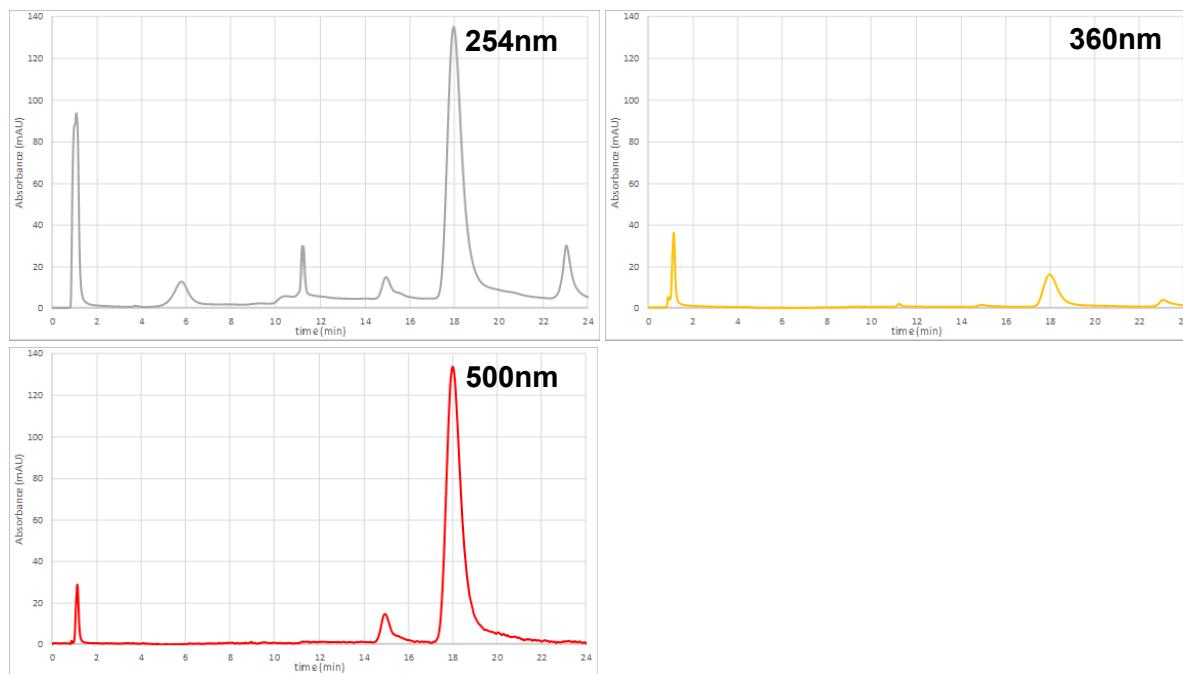
**Molecular Formula:** C<sub>20</sub>H<sub>7</sub>I<sub>4</sub>O<sub>5</sub> (ion, -1, ONa replaced with OH)

**Molecular Weight**

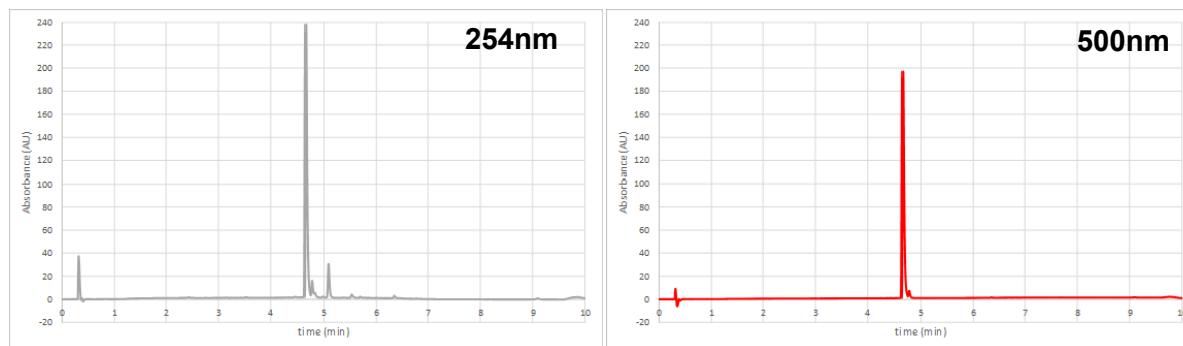
Full molecule:	879.86
Ion (-1)	834.89
Ion (-1), monoisotopic	834.65
<sup>127</sup> Iodine	126.90



### CHROMATOGRAMS: ION-EXCHANGE

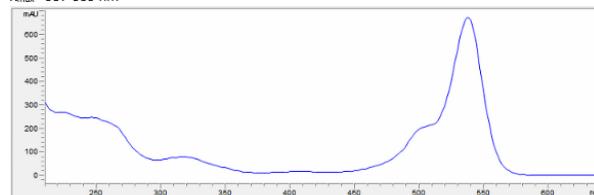


### CHROMATOGRAMS: REVERSED-PHASE

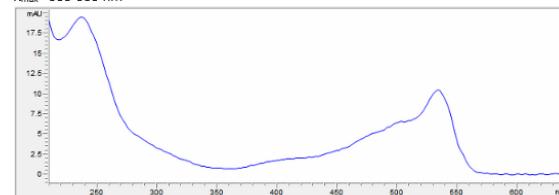


## UV-VIS SPECTRA

t=4.66 min  
 $\lambda_{\text{max}} = 537\text{-}539 \text{ nm}$



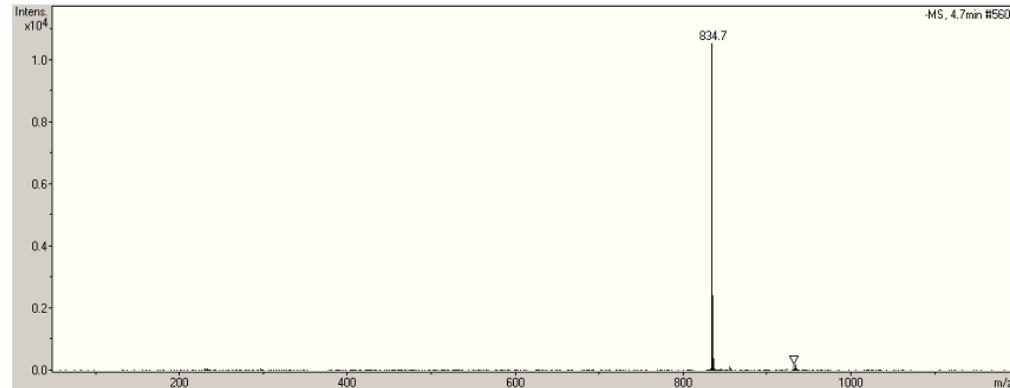
t=4.78 min  
 $\lambda_{\text{max}} = 533\text{-}535 \text{ nm}$



## MASS SPECTRA

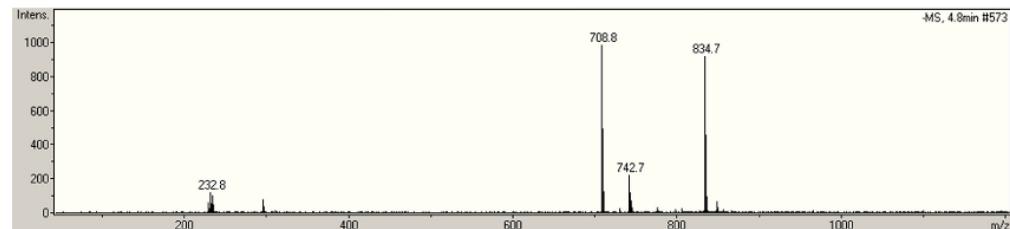
MS (negative mode)

t=4.7 min



m/z	I	Formula
834.7	10554	[M] <sup>-</sup>

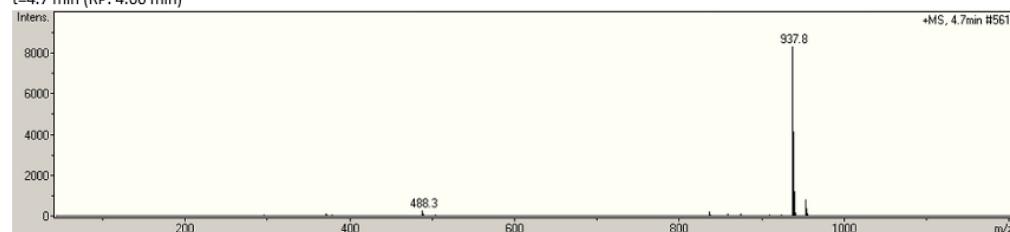
t=4.8 min



m/z	I	Formula
708.8	990	[M-I] <sup>-</sup>
742.7	221	unknown
834.7	925	[M] <sup>-</sup>

MS (positive mode)

t=4.7 min (RP: 4.66 min)



m/z	I	Formula
488.3	251	unknown
836.7	196	[M]•2H <sup>+</sup>
858.7	121	[M] <sup>-</sup> •H <sup>+</sup> •Na <sup>+</sup>
937.8	8366	[M] <sup>-</sup> •H <sup>+</sup> •[TEAH] <sup>+</sup>

## S-8.30. Fast Acid Magenta

### GENERAL INFORMATION

**Alternative names:** D&C Red 33

**Color Index Name:** Acid Red 33

**Color Index Number:** 17200

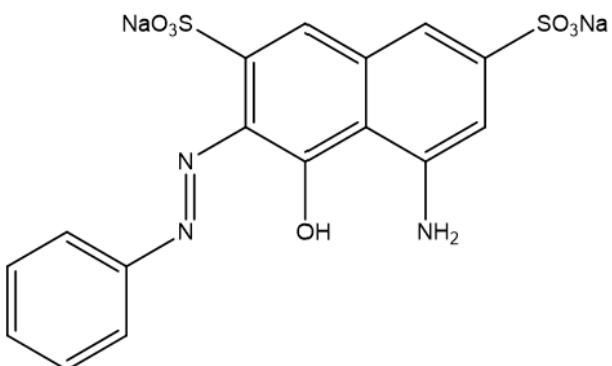
**Type of dye:** Monoazo

**Charge:** -2

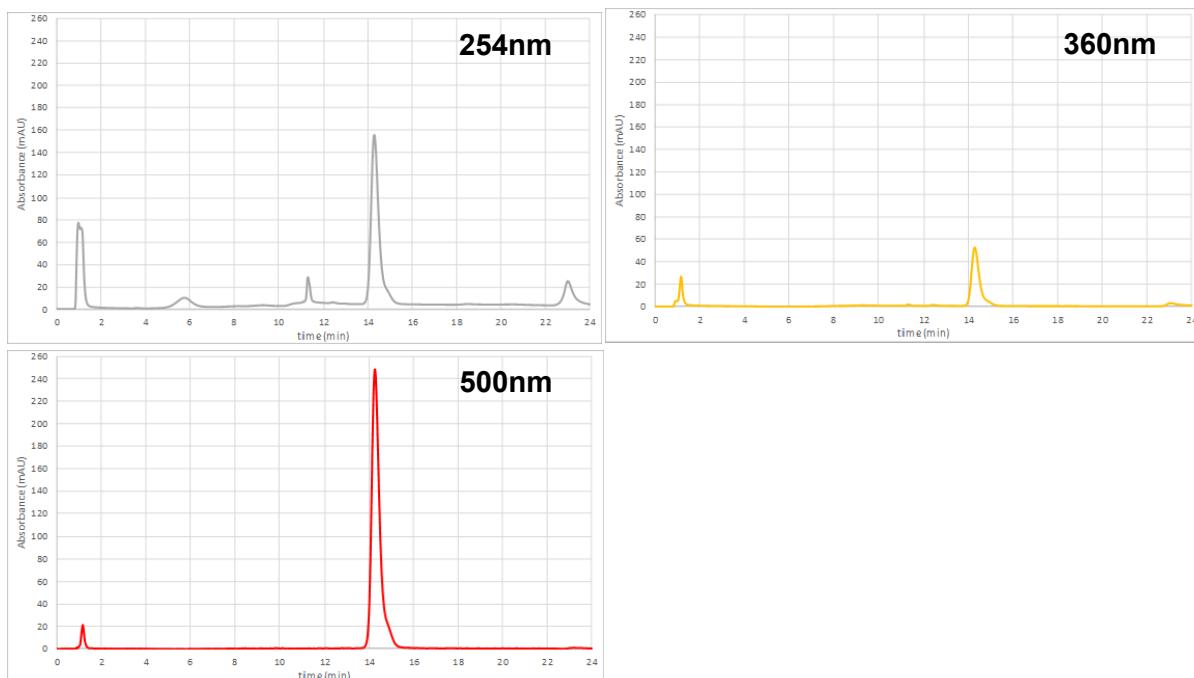
**Molecular Formula:** C<sub>16</sub>H<sub>11</sub>N<sub>3</sub>O<sub>7</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

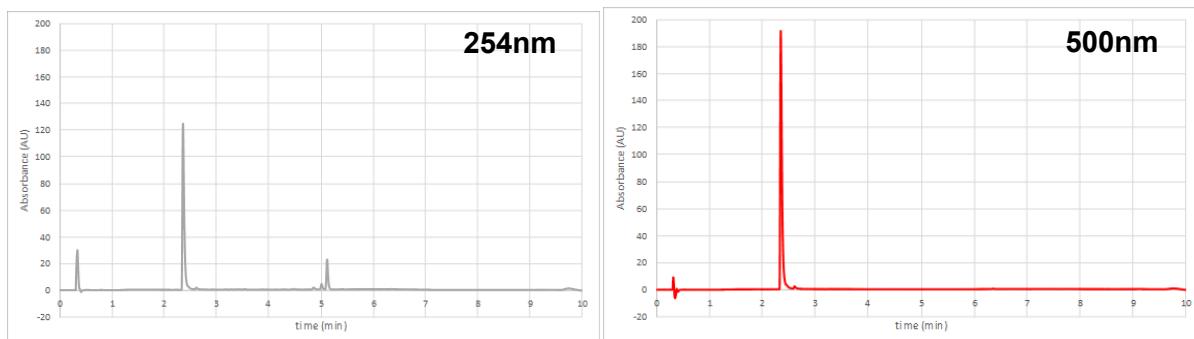
Full molecule:	467.38
Ion (-2)	421.41
Ion (-2), monoisotopic	421.00



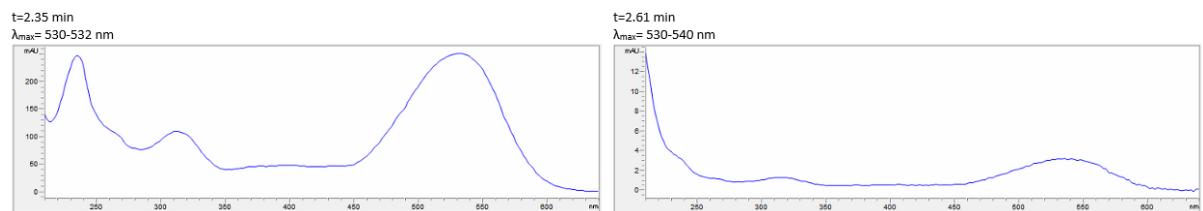
### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE



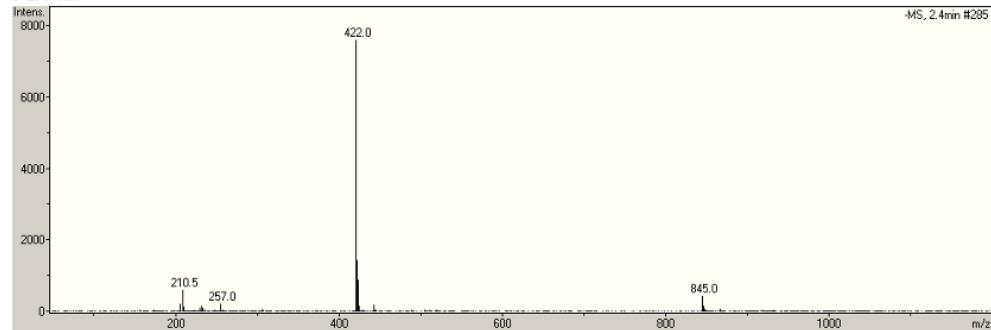
## UV-VIS SPECTRA



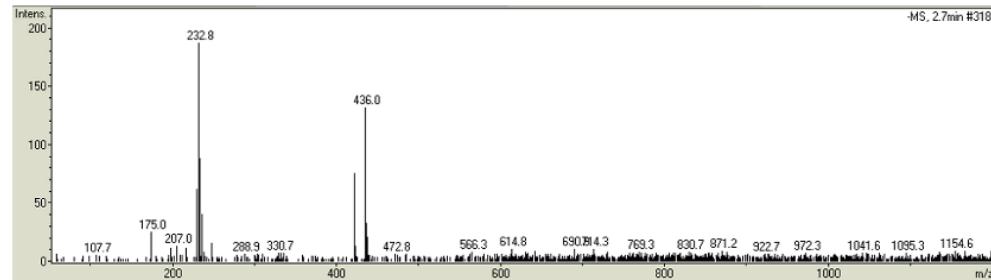
## MASS SPECTRA

MS (negative mode)

t=2.4 min

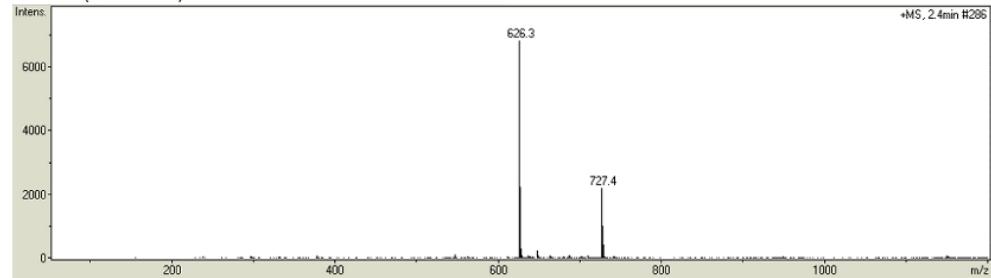


t=2.7 min



MS (positive mode)

t=2.4 min (RP: 2.35 min)



### S-8.31. Fast Red AV

#### GENERAL INFORMATION

**Color Index Name:** Acid Red 88

**Color Index Number:** 15620

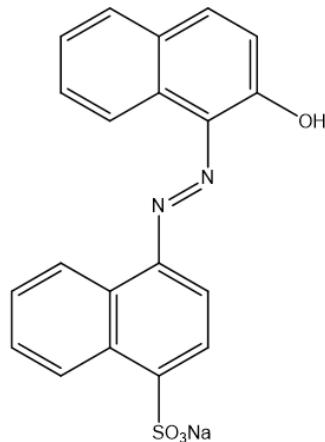
**Type of dye:** Monoazo

**Charge:** -1

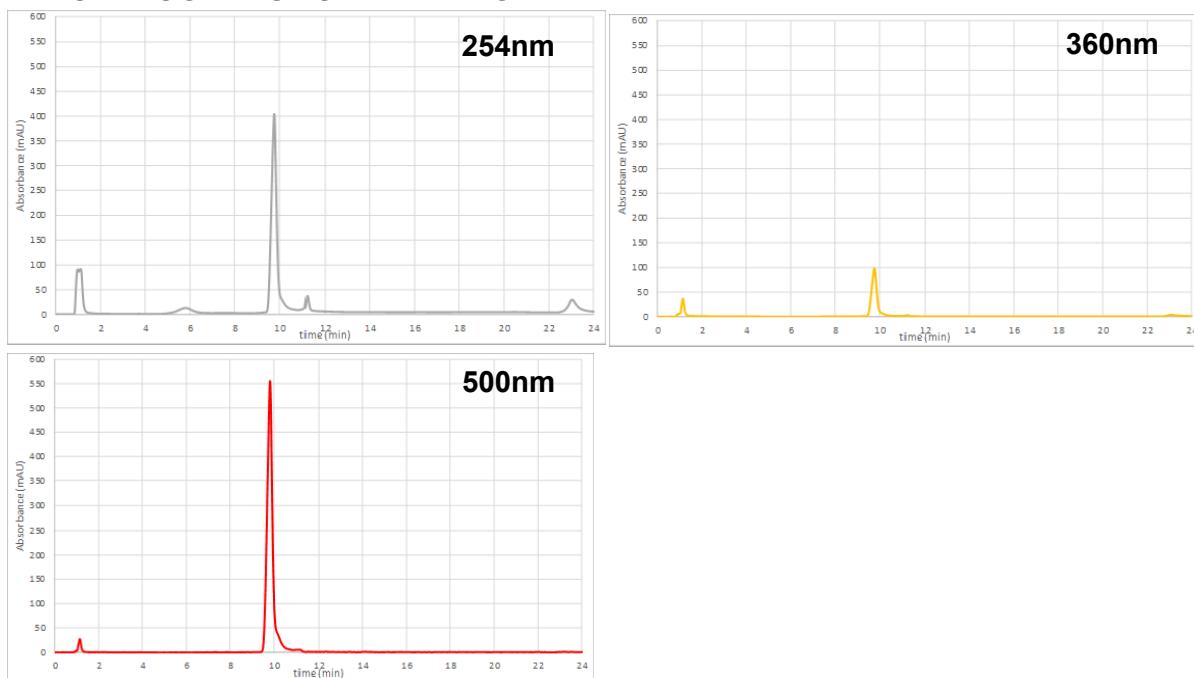
**Molecular Formula:** C<sub>20</sub>H<sub>13</sub>N<sub>2</sub>O<sub>4</sub>S (ion, -1)

**Molecular Weight**

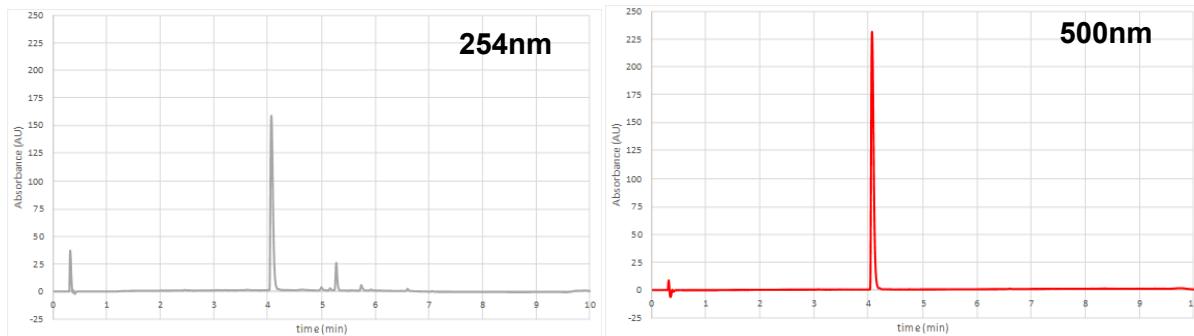
Full molecule:	400.38
Ion (-1)	377.39
Ion (-1), monoisotopic	377.06



#### CHROMATOGRAMS: ION-EXCHANGE

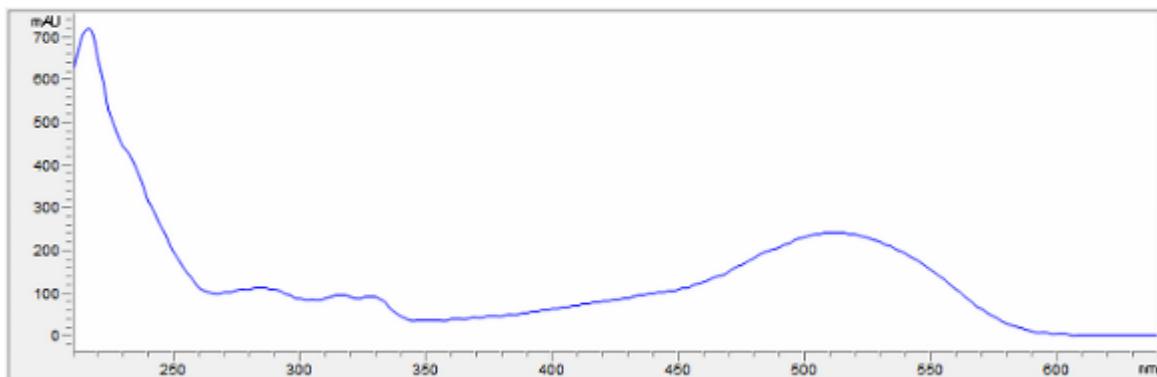


#### CHROMATOGRAMS: REVERSED-PHASE



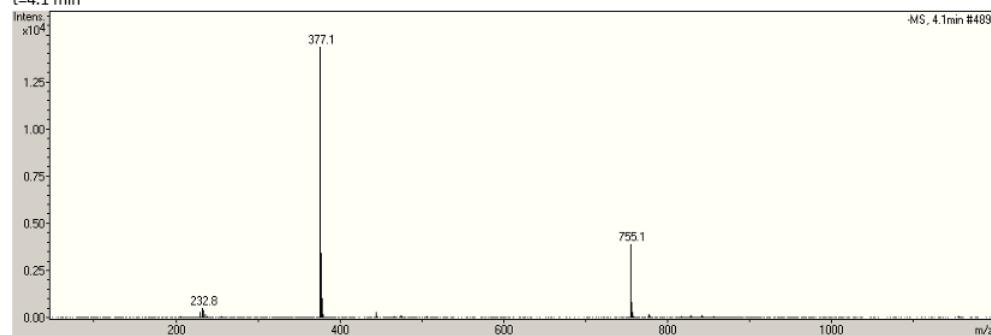
## UV-VIS SPECTRA

t=4.07 min  
 $\lambda_{\text{max}} = 510-514 \text{ nm}$



## MASS SPECTRA

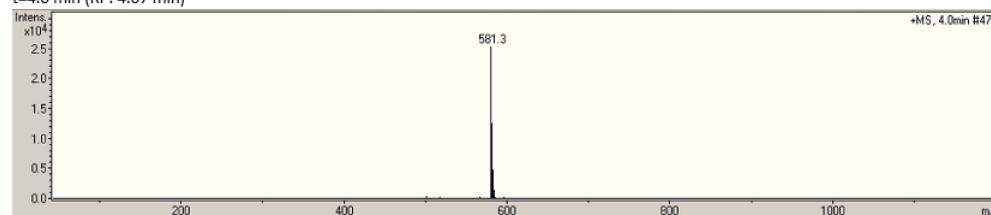
MS (negative mode)  
t=4.1 min



m/z	I	Formula
377.1	14398	[M] <sup>-</sup>
755.1	3915	2[M] <sup>-</sup> •H <sup>+</sup>

MS (positive mode)

t=4.0 min (RP: 4.07 min)



m/z	I	Formula
581.3	24614	[M] <sup>-</sup> •2[TEAH] <sup>+</sup>

## S-8.32 Fast Red B

### GENERAL INFORMATION

**Alternative names:** Bordeaux R

**Color Index Name:** Acid Red 17

**Color Index Number:** 16180

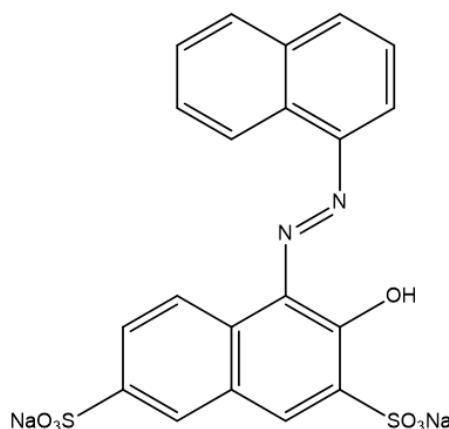
**Type of dye:** Monoazo

**Charge:** -2

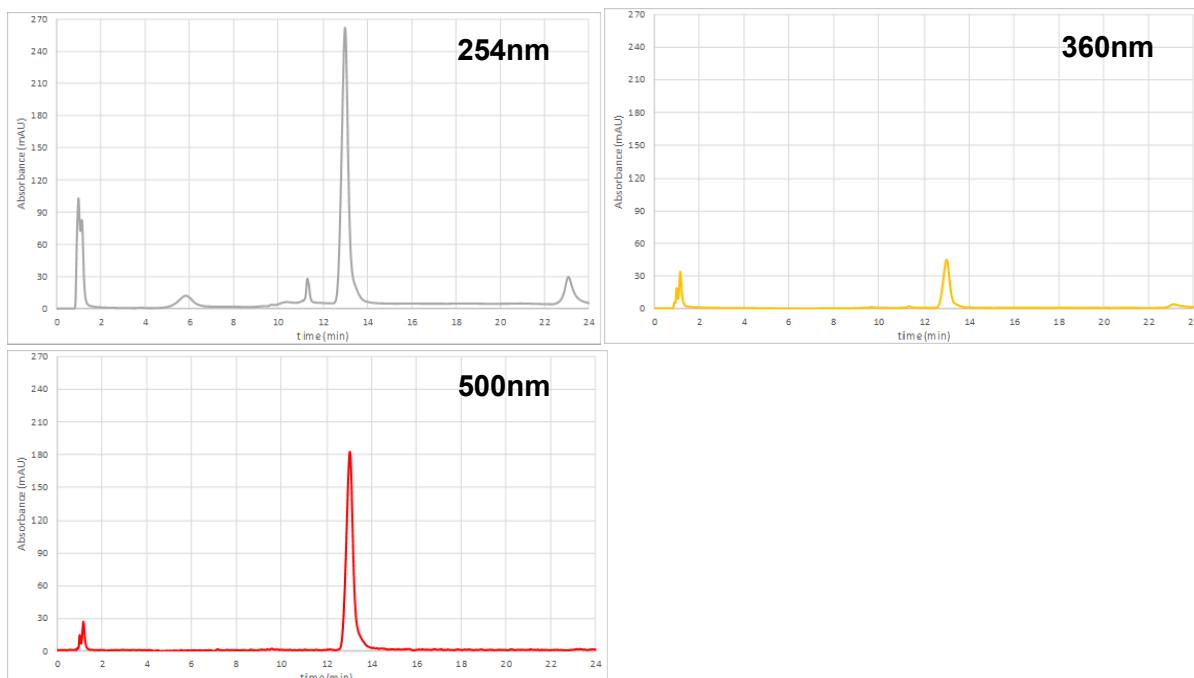
**Molecular Formula:** C<sub>20</sub>H<sub>12</sub>N<sub>2</sub>O<sub>7</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

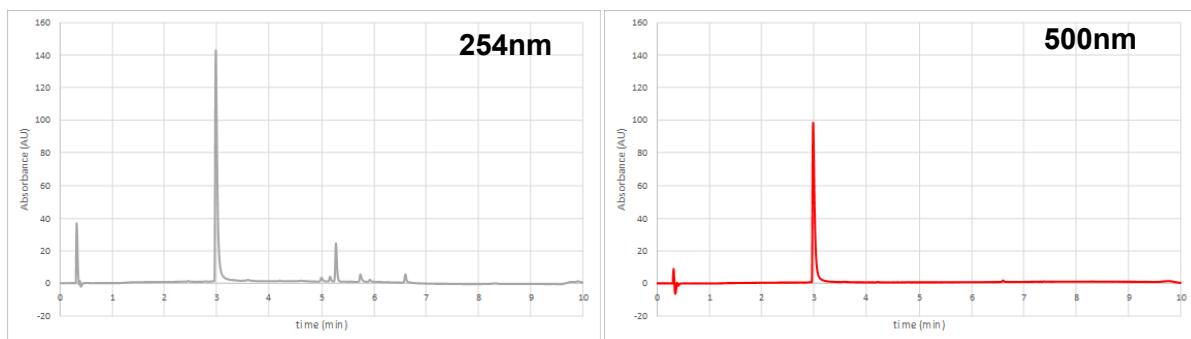
Full molecule:	502.43
Ion (-2)	456.45
Ion (-2), monoisotopic	456.01



### CHROMATOGRAMS: ION-EXCHANGE

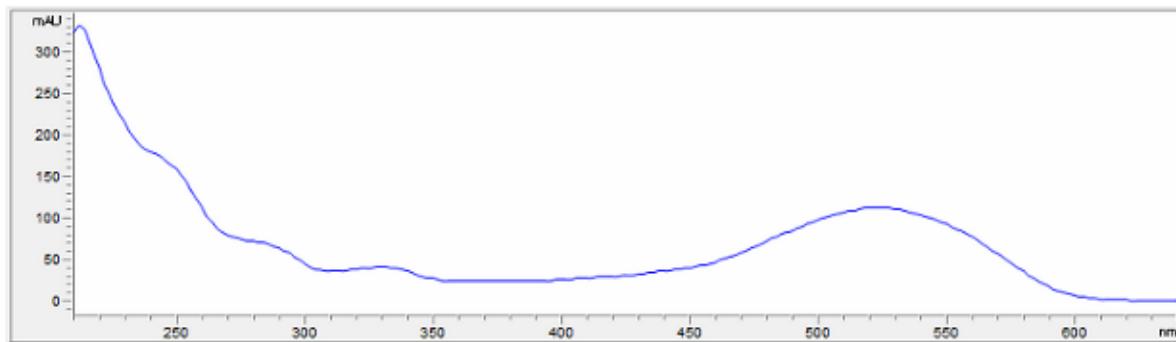


### CHROMATOGRAMS: REVERSED-PHASE



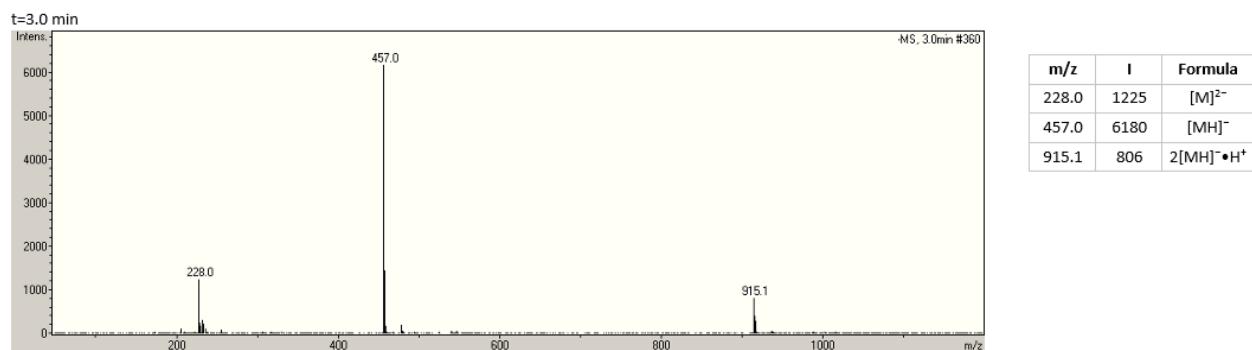
## UV-VIS SPECTRA

t=2.99 min  
 $\lambda_{\text{max}} = 521-525 \text{ nm}$

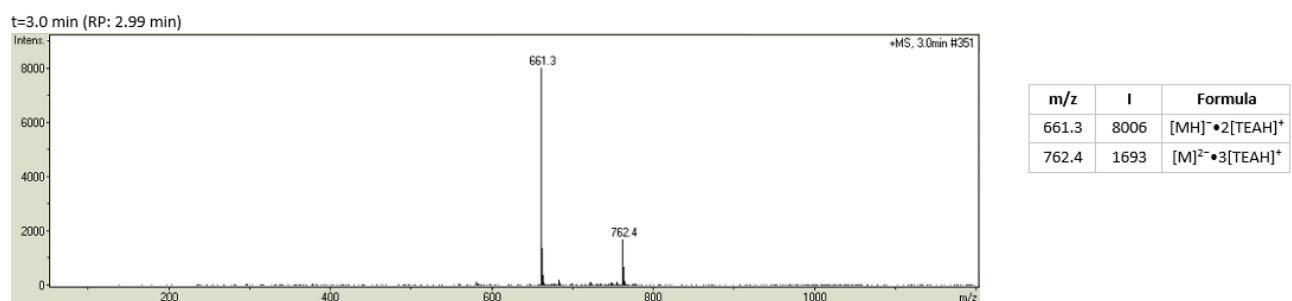


## MASS SPECTRA

MS (negative mode)



MS (positive mode)

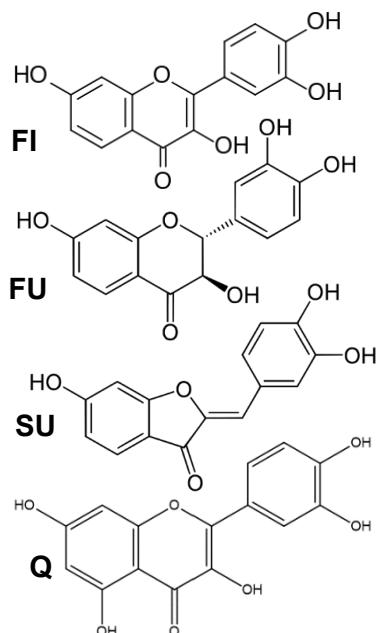


### S-8.33. Fisetin

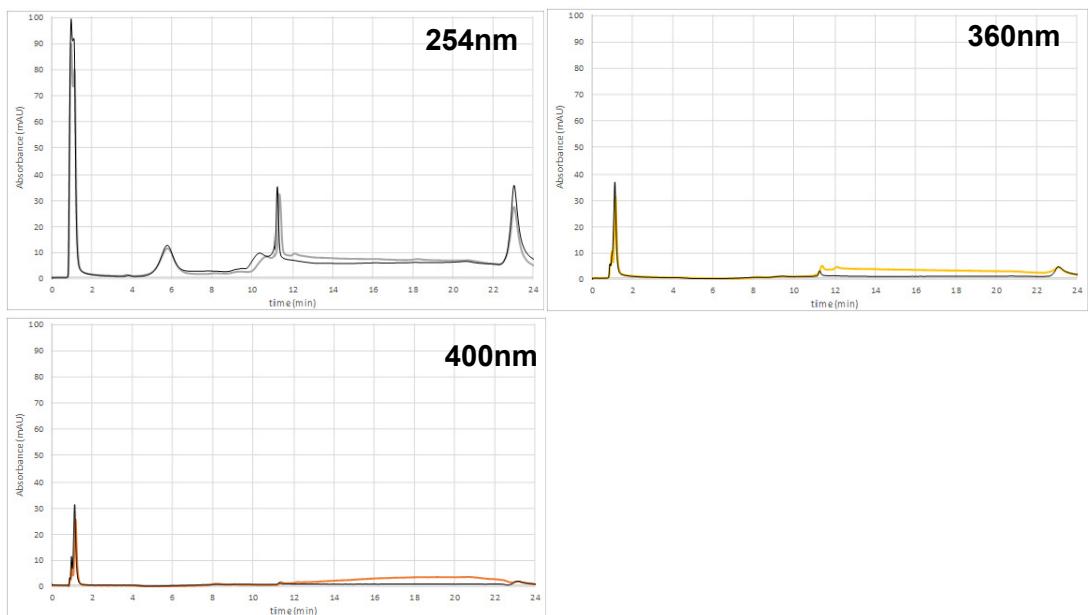
#### GENERAL INFORMATION

**Alternative names:** Young Fustic  
**Color Index Name:** Natural Brown 1  
**Color Index Number:** 75620  
**Type of dye:** Natural, Mordant dye  
**Scientific name of biological source:** *Cotinus coggygria* Scop.

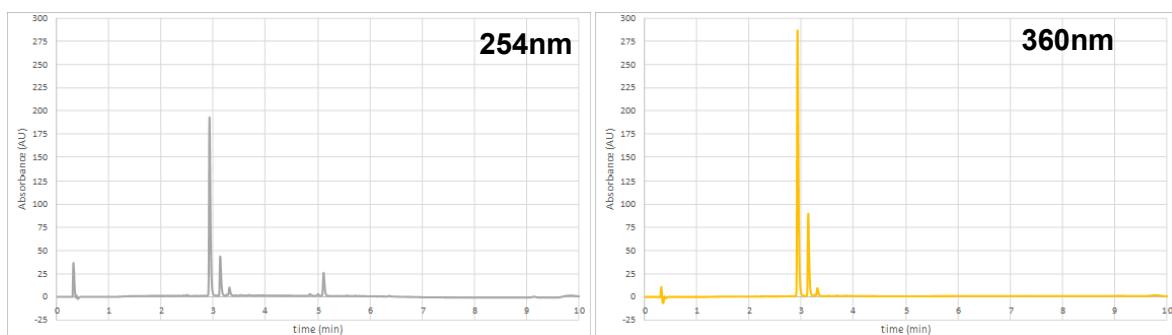
Name	Short	Mw	monoisotopic	Formula
Fisetin	[FI]	286.24	286.05	$C_{15}H_{10}O_6$
Fustin	[FU]	288.25	288.06	$C_{15}H_{12}O_6$
Sulfuretin	[SU]	270.24	270.05	$C_{15}H_{10}O_5$
Quercetin	[Q]	302.24	302.04	$C_{15}H_{10}O_7$

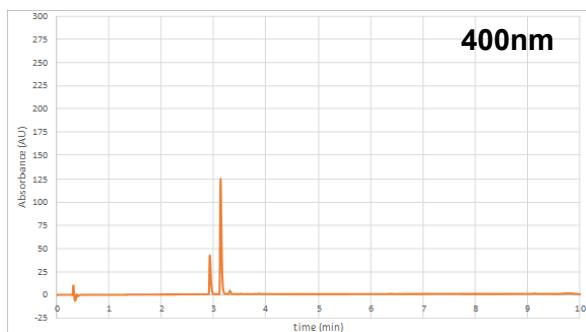


#### CHROMATOGRAMS: ION-EXCHANGE



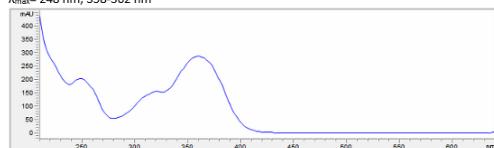
#### CHROMATOGRAMS: REVERSED-PHASE



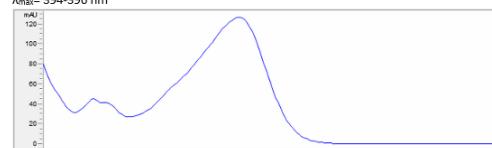


## UV-VIS SPECTRA

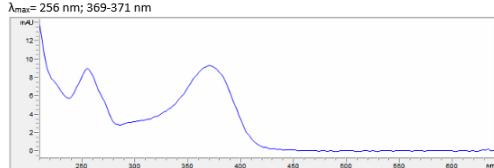
t=2.93 min  
 $\lambda_{max}= 248 \text{ nm}; 358-362 \text{ nm}$



t=3.14 min  
 $\lambda_{max}= 394-396 \text{ nm}$



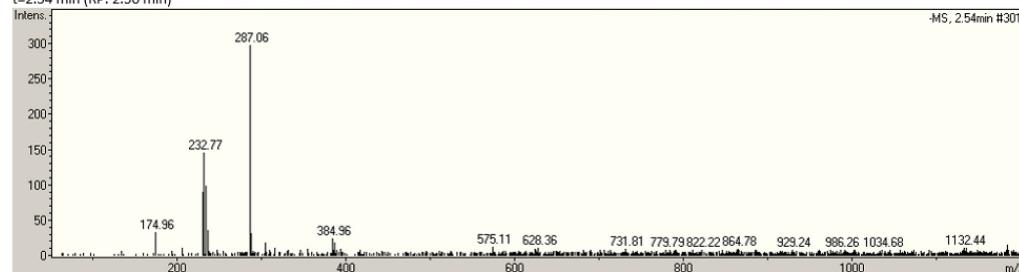
t=3.31 min  
 $\lambda_{max}= 256 \text{ nm}; 369-371 \text{ nm}$



## MASS SPECTRA

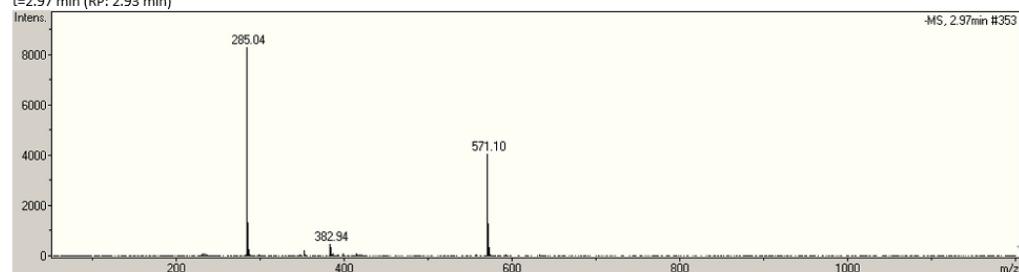
MS (negative mode)

t=2.54 min (RP: 2.50 min)



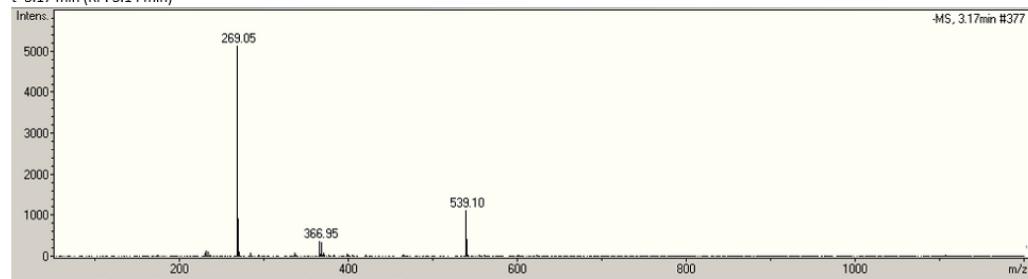
m/z	I	Formula
287.1	299	[FU] <sup>-</sup>
385.0	24	+97.9

t=2.97 min (RP: 2.93 min)

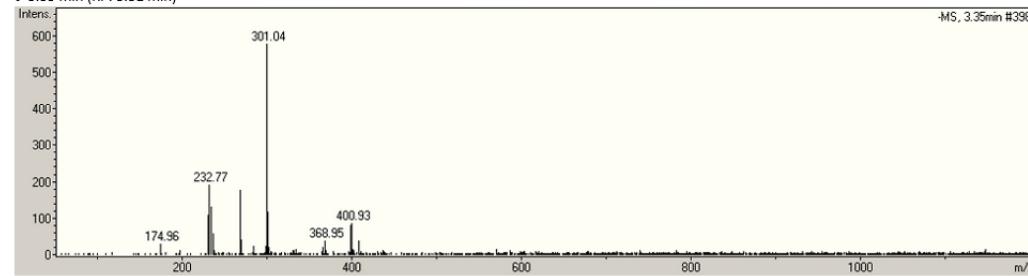


m/z	I	Formula
285.0	8317	[FJ] <sup>-</sup>
382.9	457	+97.9
571.1	4050	2[FJ] <sup>-</sup> •H <sup>+</sup>

t=3.17 min (RP: 3.14 min)



t=3.35 min (RP: 3.31 min)



### S-8.34. Flavazine L

#### GENERAL INFORMATION

**Color Index Name:** Acid Yellow 11

**Color Index Number:** 18820

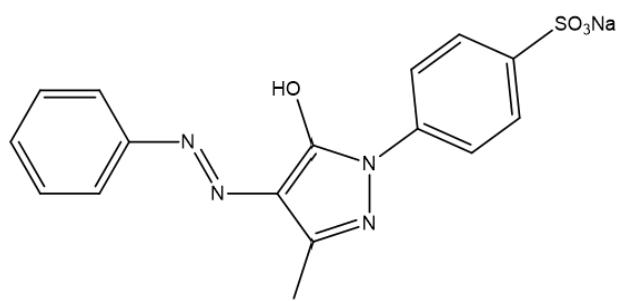
**Type of dye:** Monoazo

**Charge:** -1

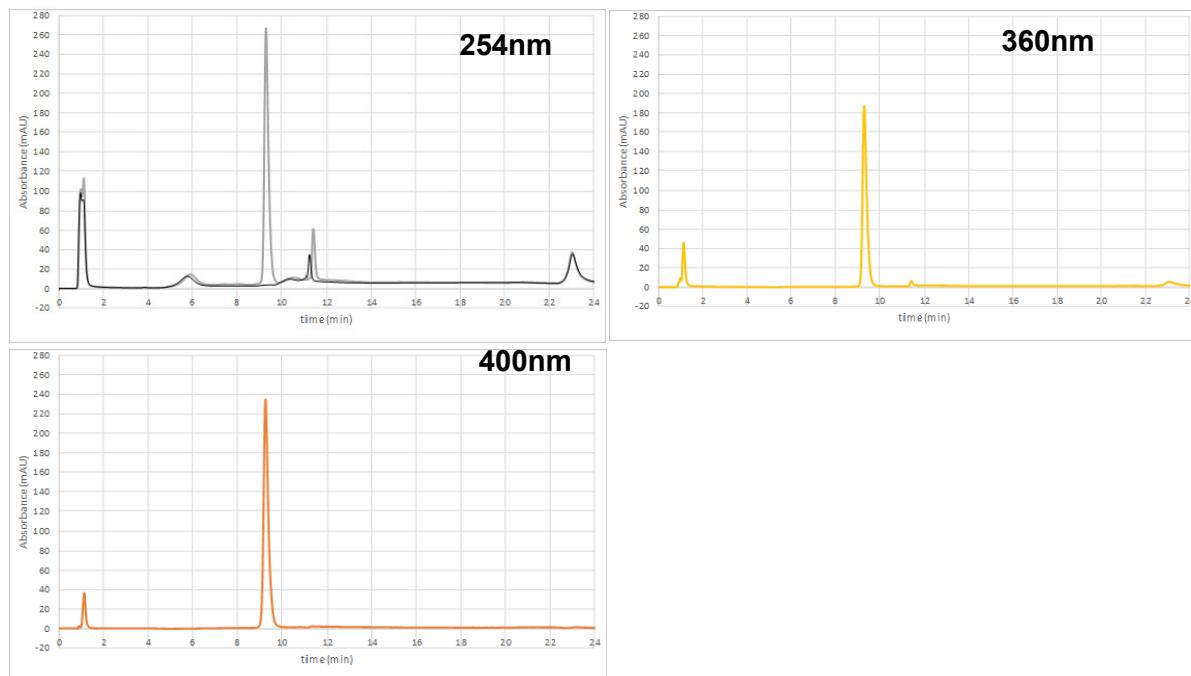
**Molecular Formula:** C<sub>16</sub>H<sub>13</sub>N<sub>4</sub>O<sub>4</sub>S (ion, -1)

**Molecular Weight**

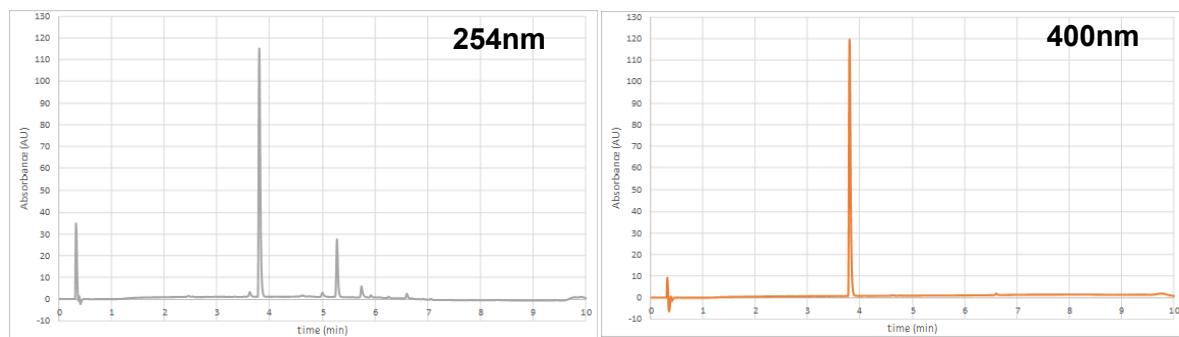
Full molecule:	380.35
Ion (-1)	357.36
Ion (-1), monoisotopic	357.07



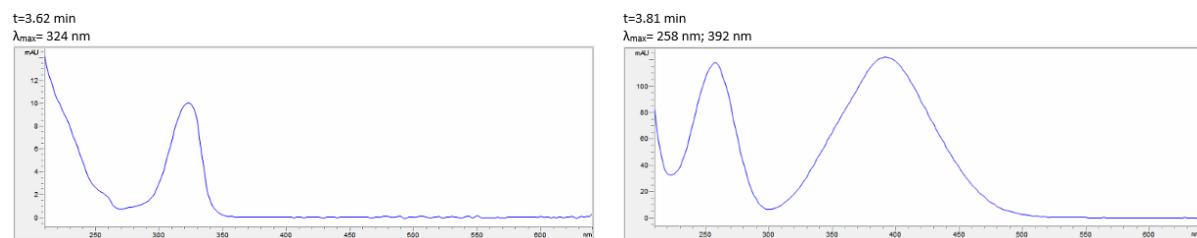
#### CHROMATOGRAMS: ION-EXCHANGE



#### CHROMATOGRAMS: REVERSED-PHASE



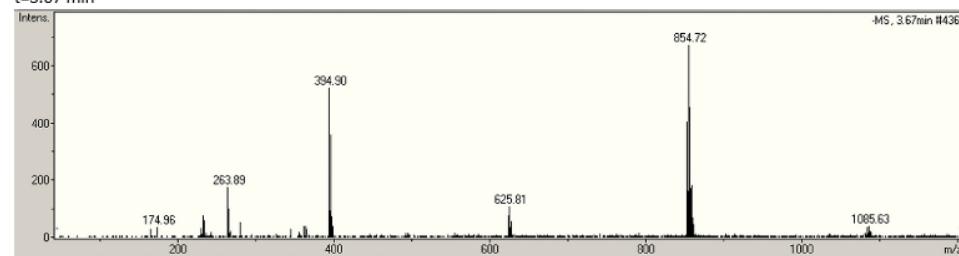
## UV-VIS SPECTRA



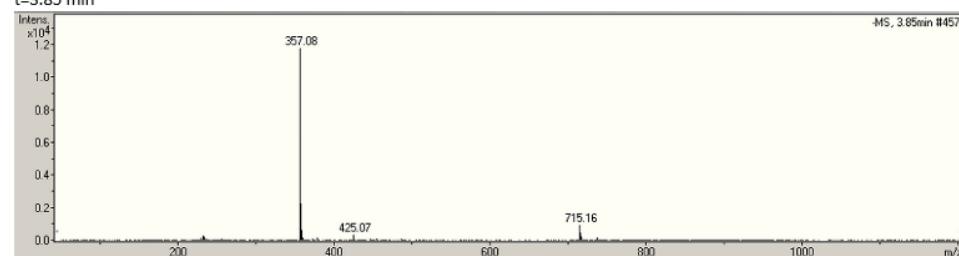
## MASS SPECTRA

### MS (negative mode)

t=3.67 min



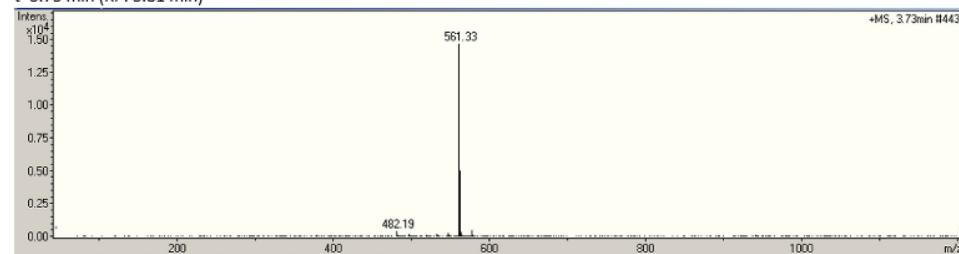
t=3.85 min



m/z	I	Formula
357.08	11816	[M] <sup>-</sup>
715.16	880	2[M] <sup>-</sup> •H <sup>+</sup>

### MS (positive mode)

t=3.73 min (RP: 3.81 min)



m/z	I	Formula
482.19	353	[M] <sup>+</sup> •Na <sup>+</sup> •[TEAH] <sup>+</sup>
561.33	14676	[M] <sup>+</sup> •2[TEAH] <sup>+</sup>

### S-8.35. Fuchsin

#### GENERAL INFORMATION

**Alternative names:** Basic Fuchsin; Magenta ABN

**Color Index Name:** Basic Violet 17

**Color Index Number:** 42510

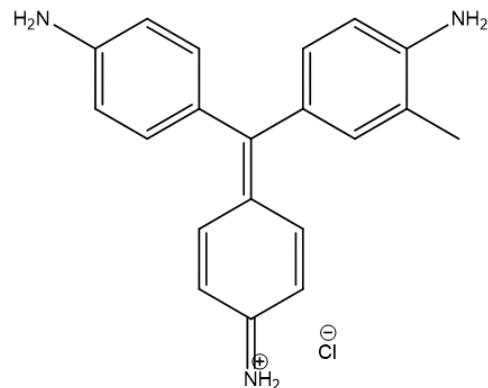
**Type of dye:** Triarylmethane

**Charge:** +1

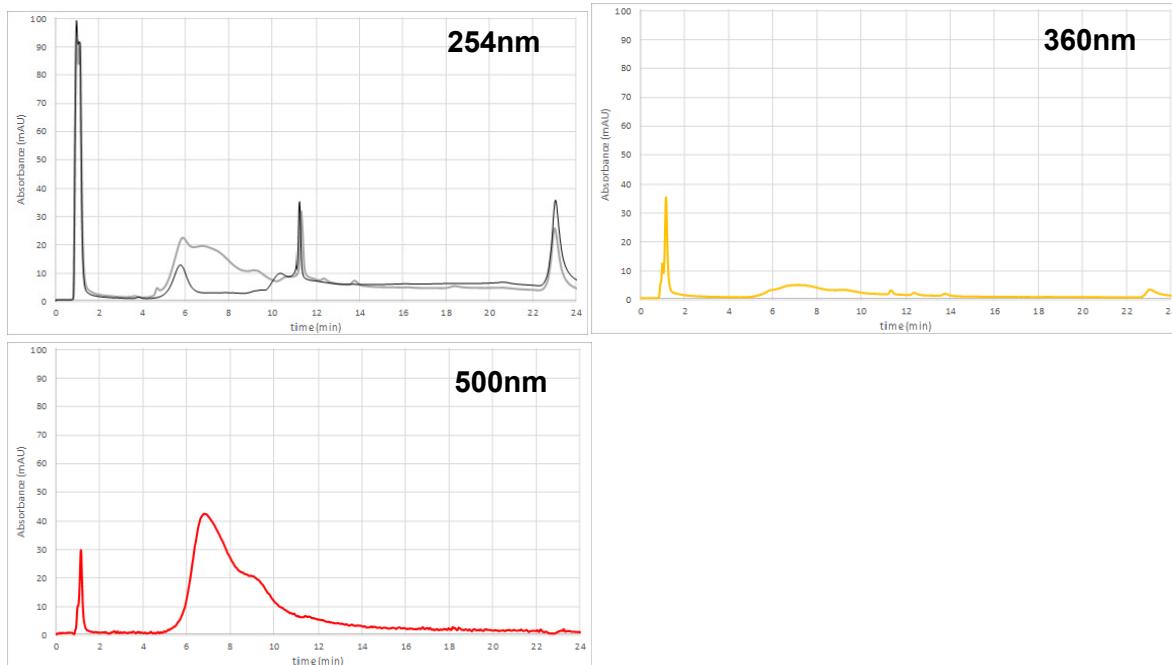
**Molecular Formula:** C<sub>20</sub>H<sub>20</sub>N<sub>3</sub> (ion, +1)

**Molecular Weight**

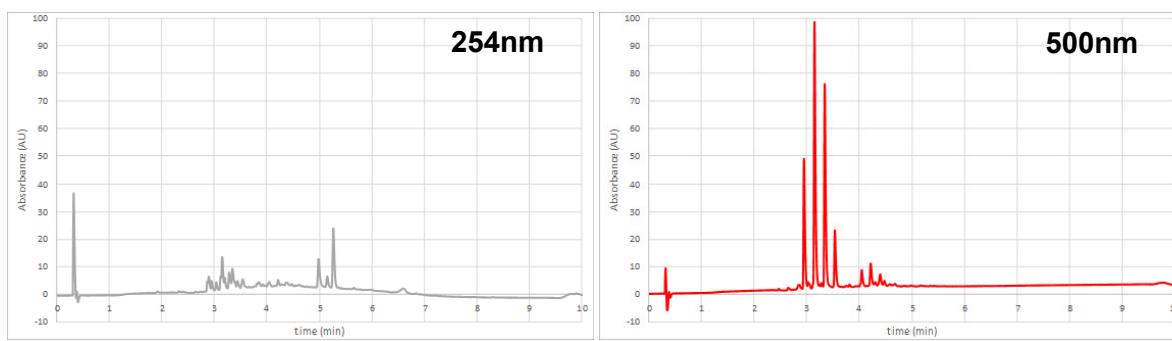
Full molecule:	337.85
Ion (+1)	302.39
Ion (+1), monoisotopic	302.17



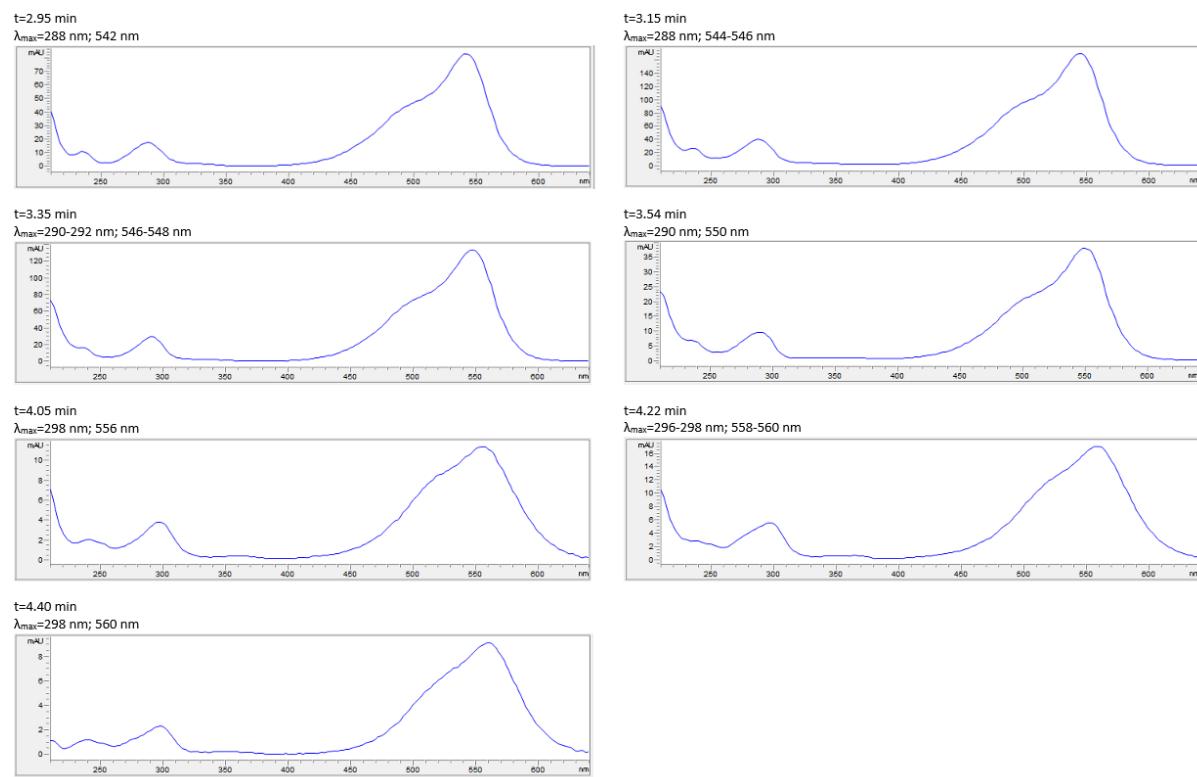
#### CHROMATOGRAMS: ION-EXCHANGE



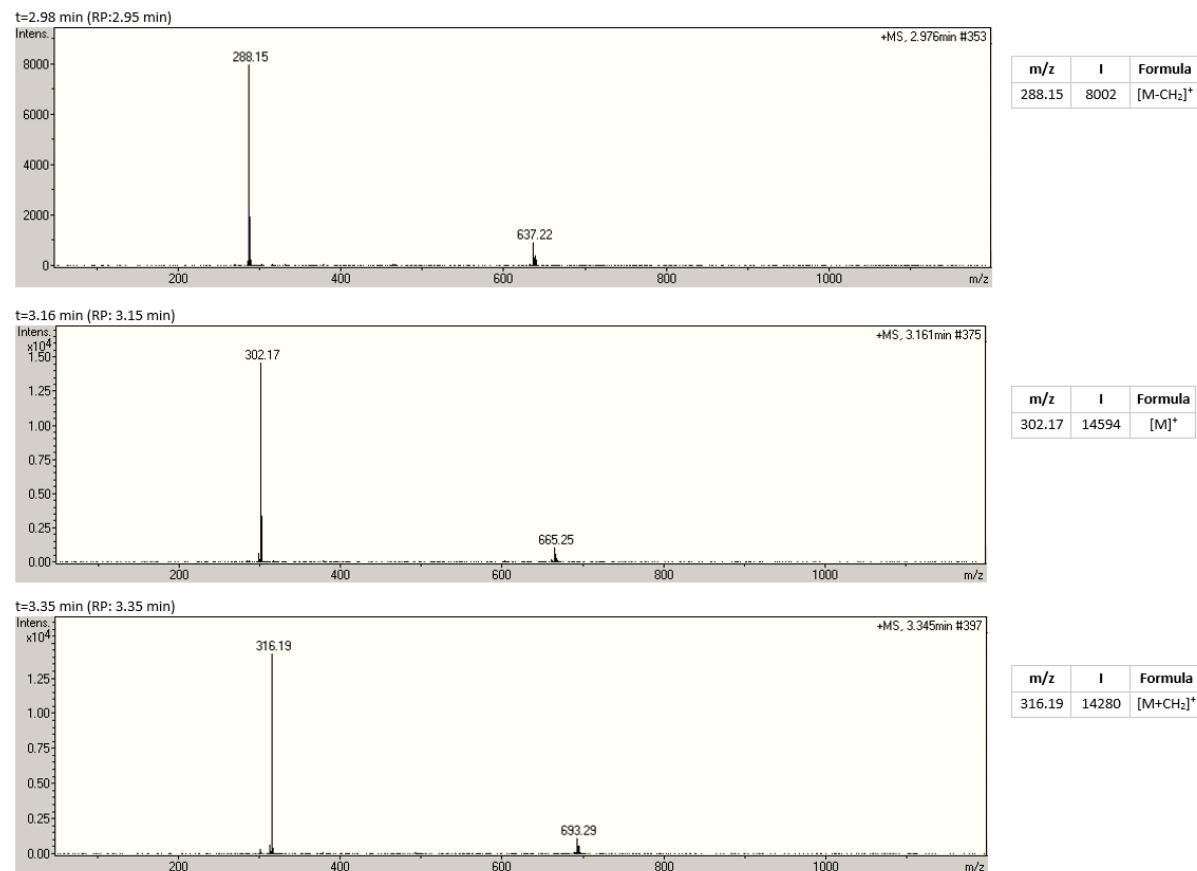
#### CHROMATOGRAMS: REVERSED-PHASE



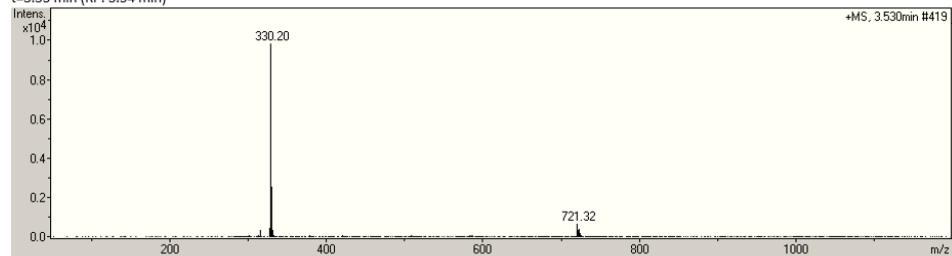
## UV-VIS SPECTRA



## MASS SPECTRA

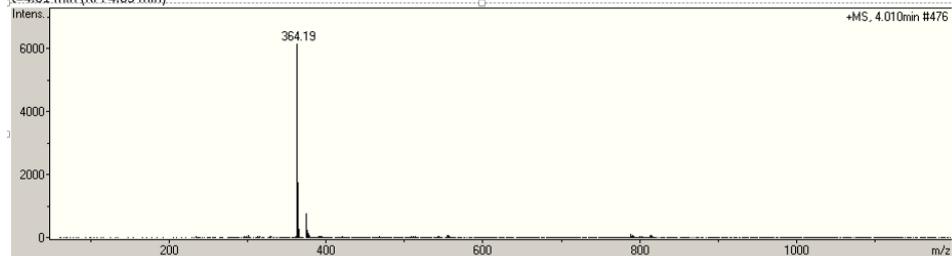


t=3.53 min (RP: 3.54 min)



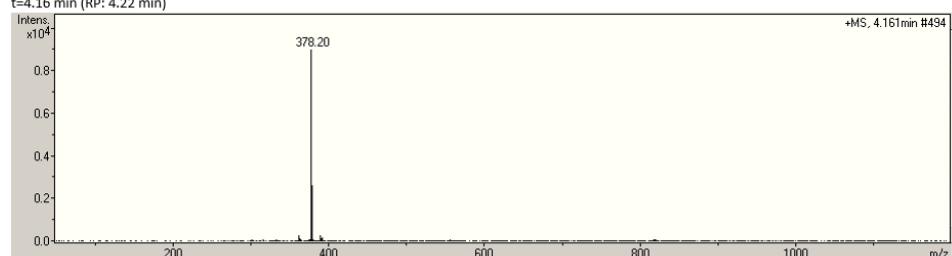
m/z	I	Formula
330.20	9843	[M+2CH <sub>3</sub> ] <sup>+</sup>

t=4.01 min (RP: 4.05 min)



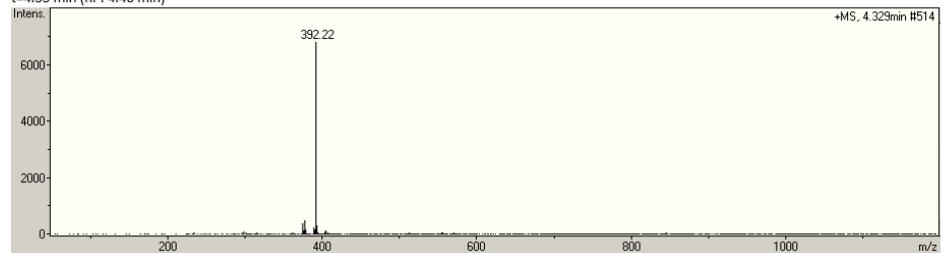
m/z	I	Formula
364.19	6176	[unknown] <sup>+</sup>

t=4.16 min (RP: 4.22 min)



m/z	I	Formula
378.20	9003	[unknown+CH <sub>2</sub> ] <sup>+</sup>

t=4.33 min (RP: 4.40 min)



m/z	I	Formula
392.22	6803	[unknown+2CH <sub>2</sub> ] <sup>+</sup>

### S-8.36. Haematin

#### GENERAL INFORMATION

**Alternative names:** Logwood (extract)

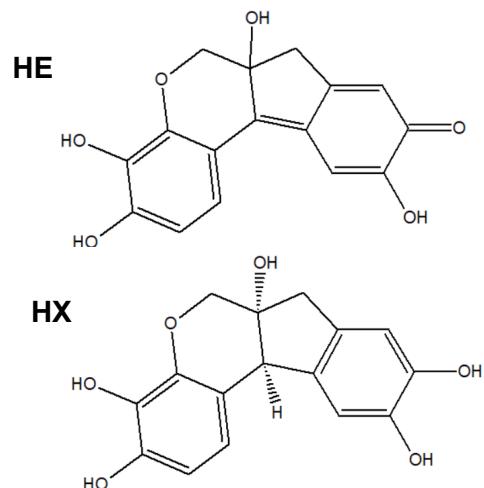
**Color Index Name:** Natural Black 1

**Color Index Number:** 75290

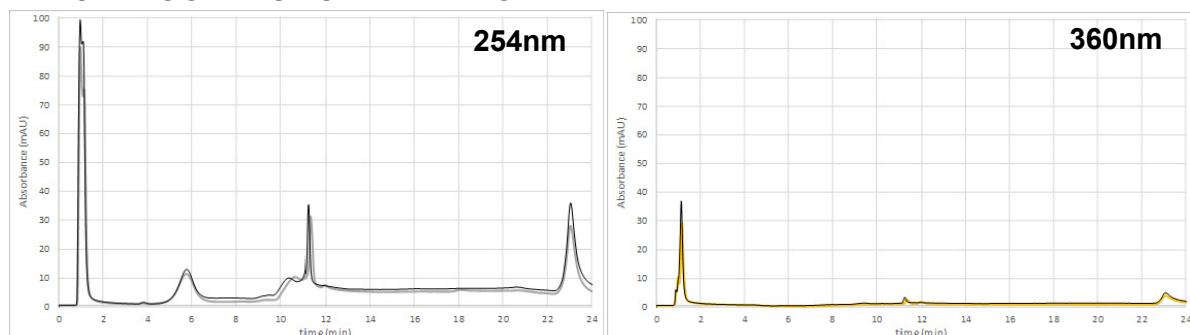
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Haematoxylum campechianum L.*

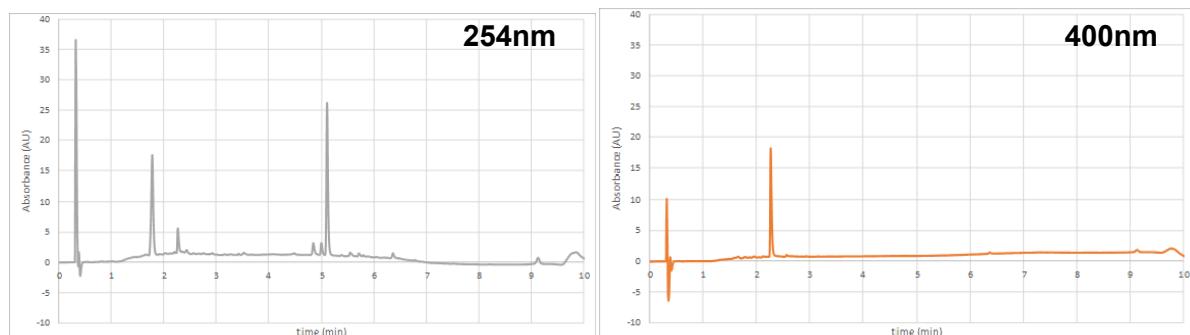
Name	Short	Mw	monoisotopic	Formula
Haematein	[HE]	300.26	300.06	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>
Haematoxylin	[HX]	302.28	302.08	C <sub>16</sub> H <sub>14</sub> O <sub>6</sub>



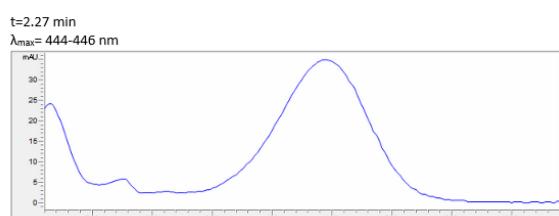
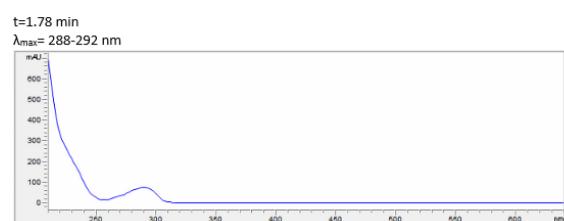
#### CHROMATOGRAMS: ION-EXCHANGE



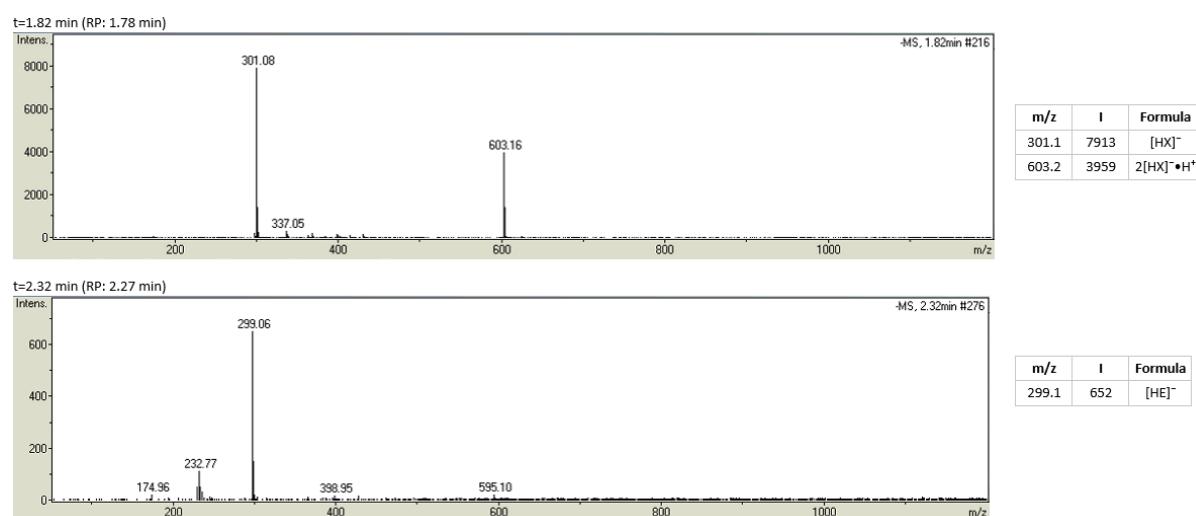
#### CHROMATOGRAMS: REVERSED-PHASE



#### UV-VIS SPECTRA



## MASS SPECTRA



### S-8.37. Indigo

#### GENERAL INFORMATION

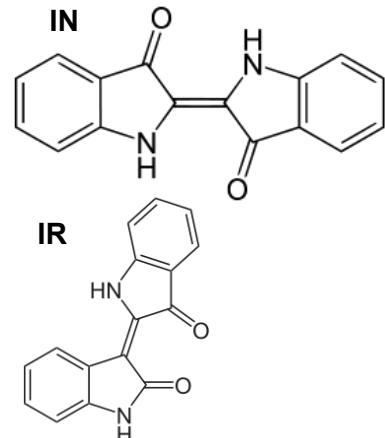
**Color Index Name:** Natural Blue 1; Vat Blue 1

**Color Index Number:** 75780; 73000

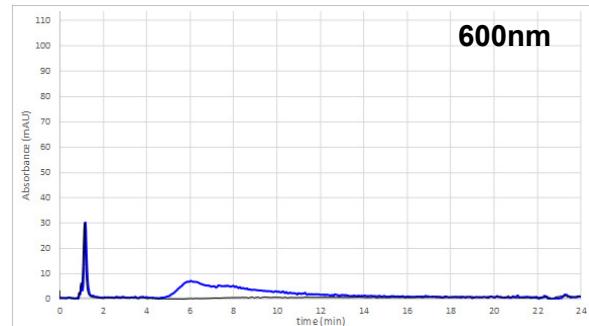
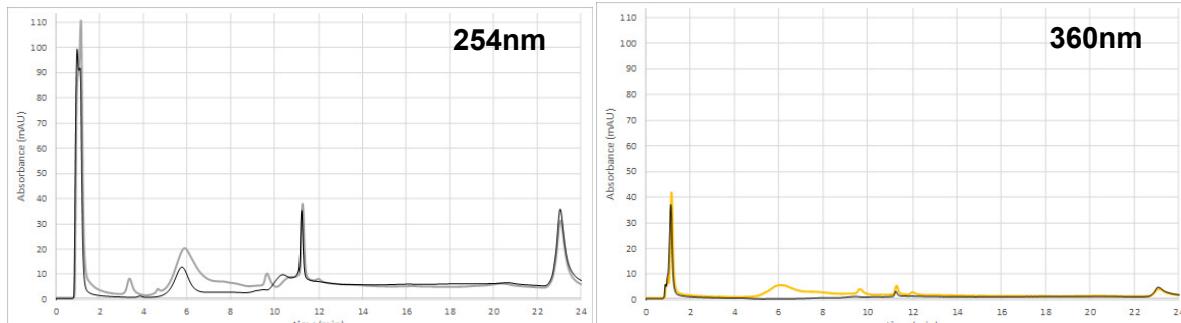
**Type of dye:** Natural, Vat dye

**Scientific name of biological source:** *Indigofera tinctoria L.*

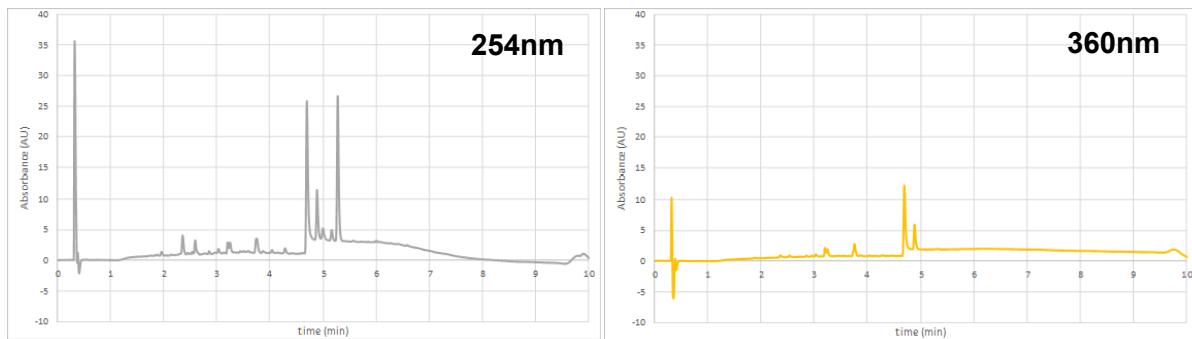
Name	Short	Mw	monoisotopic	Formula
Indigotin	[IN]	262.26	262.07	C <sub>16</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Indirubin	[IR]	262.26	262.07	C <sub>16</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>

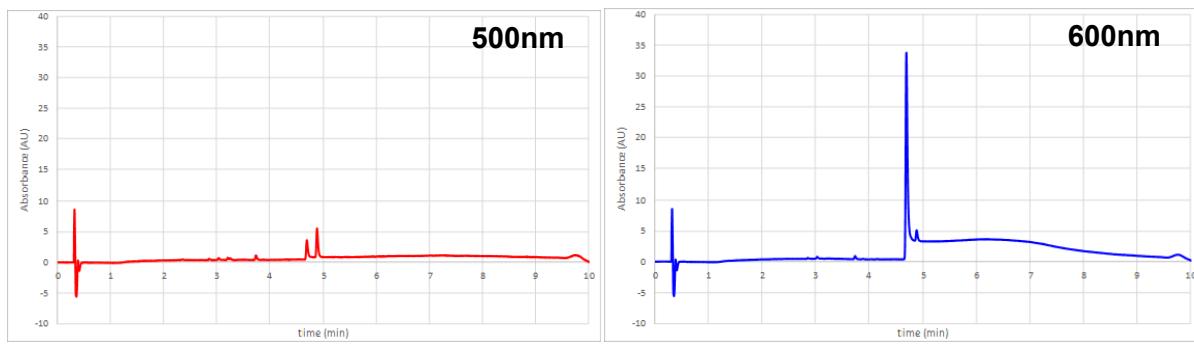


#### CHROMATOGRAMS: ION-EXCHANGE



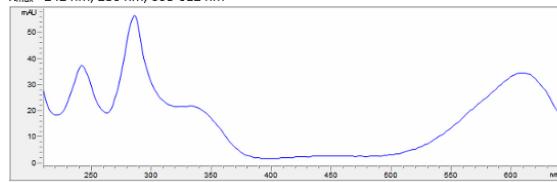
#### CHROMATOGRAMS: REVERSED-PHASE



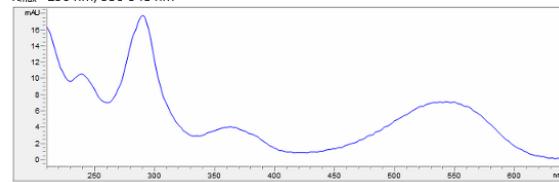


## UV-VIS SPECTRA

$t=4.68$  min  
 $\lambda_{\text{max}}=242$  nm; 286 nm; 608-612 nm

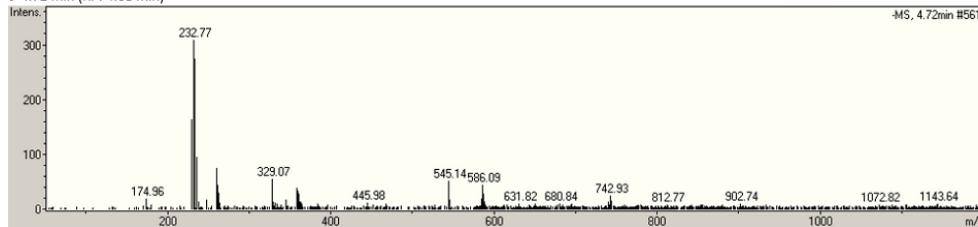


$t=4.88$  min  
 $\lambda_{\text{max}}=290$  nm; 536-548 nm



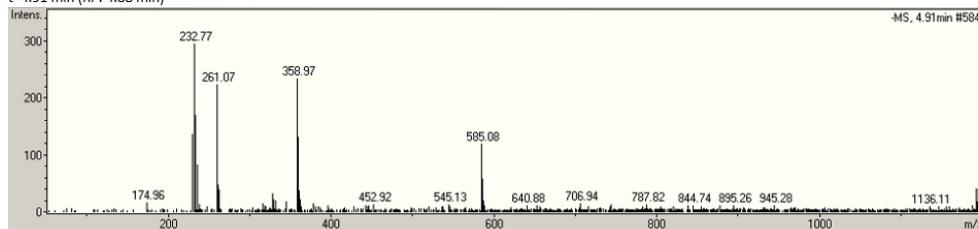
## MASS SPECTRA

$t=4.72$  min (RP: 4.68 min)



$m/z$	I	Formula
261.07	75	$[\text{IN}]^-$
358.98	39	$+97.9$

$t=4.91$  min (RP: 4.88 min)



$m/z$	I	Formula
261.07	225	$[\text{IR}]^-$
358.97	234	$+97.9$

## S-8.38. Indigo Carmine

### GENERAL INFORMATION

**Color Index Name:** Acid Blue 74; Food Blue 1  
**Color Index Number:** 73015

**Type of dye:** Indigoid

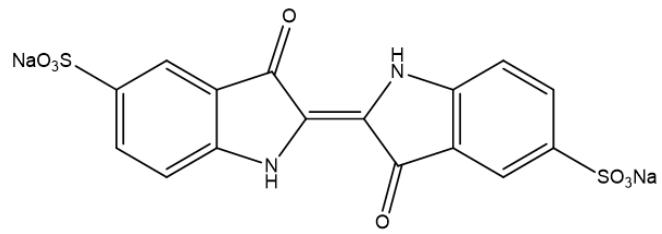
**Charge:** -2

**Related dye:** N2031 Indigo (natural); 2030 Indigoferin

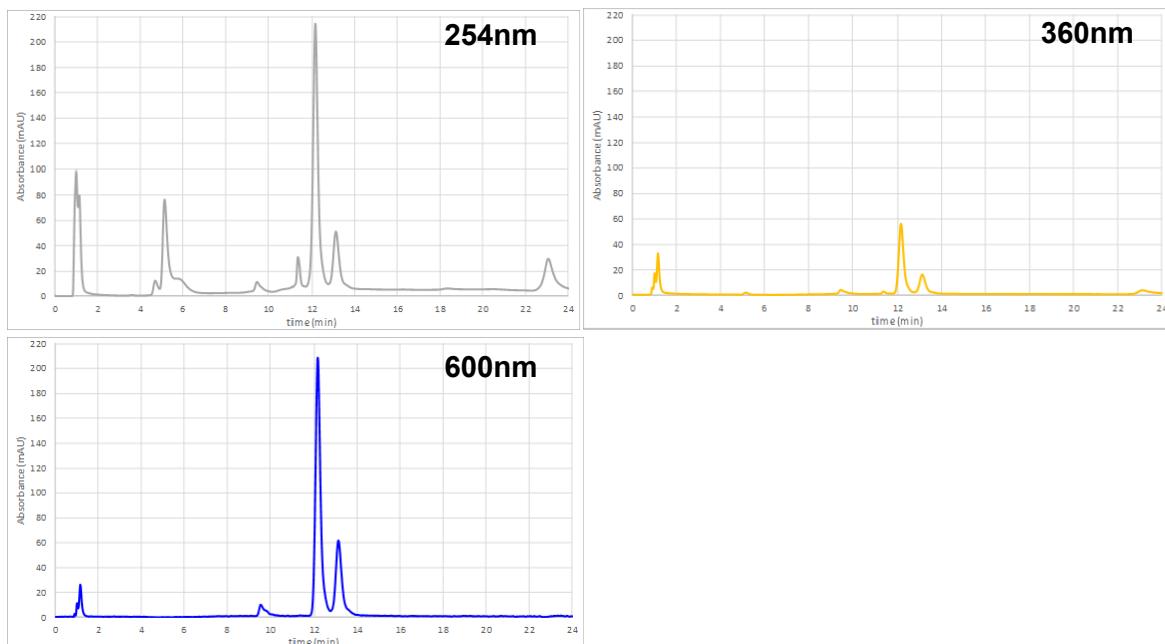
**Molecular Formula:** C<sub>16</sub>H<sub>8</sub>N<sub>2</sub>S<sub>2</sub>O<sub>2</sub> (ion, -2)

**Molecular Weight**

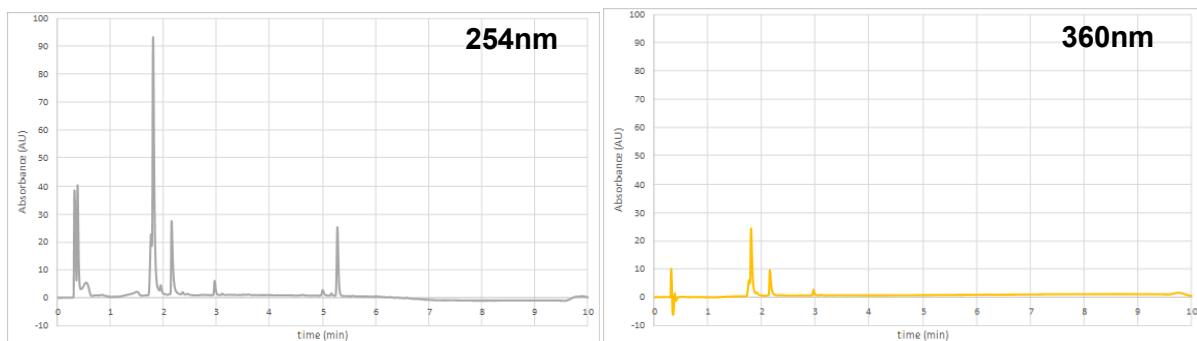
Full molecule:	466.35
Ion (-2)	420.37
Ion (-2), monoisotopic	419.97

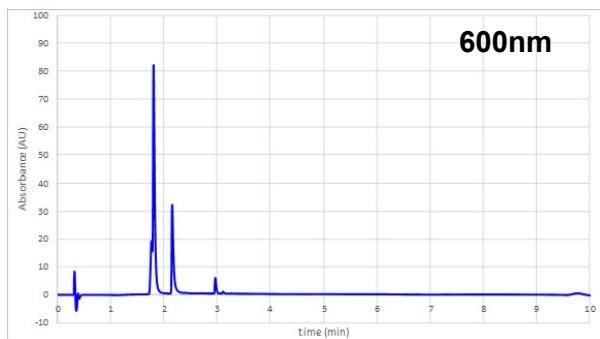


### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

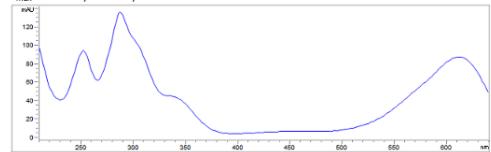




## UV-VIS SPECTRA

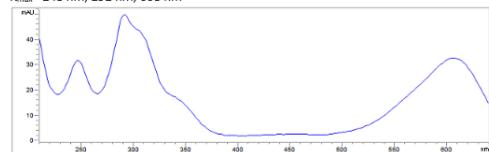
t=1.81 min

$\lambda_{\text{max}} = 252 \text{ nm}; 288 \text{ nm}; 612 \text{ nm}$



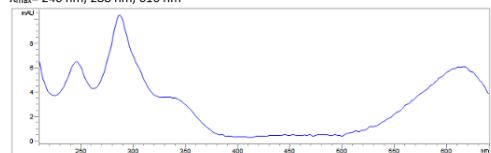
t=2.16 min

$\lambda_{\text{max}} = 248 \text{ nm}; 292 \text{ nm}; 608 \text{ nm}$



t=2.97 min

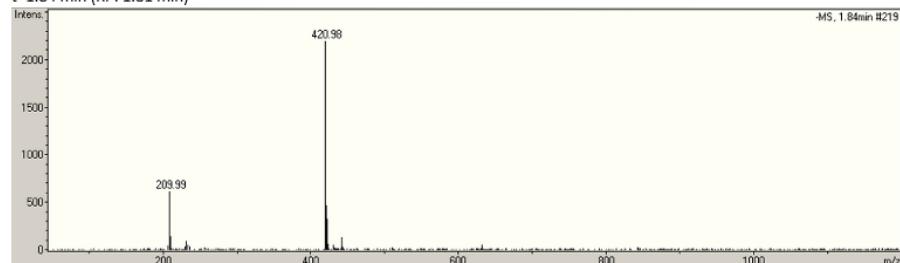
$\lambda_{\text{max}} = 246 \text{ nm}; 288 \text{ nm}; 616 \text{ nm}$



## MASS SPECTRA

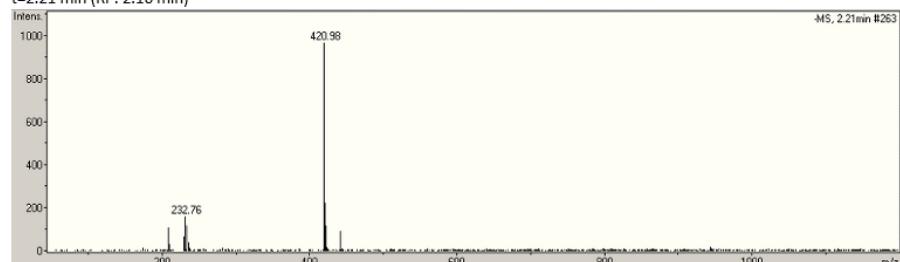
### MS (negative mode)

t=1.84 min (RP: 1.81 min)



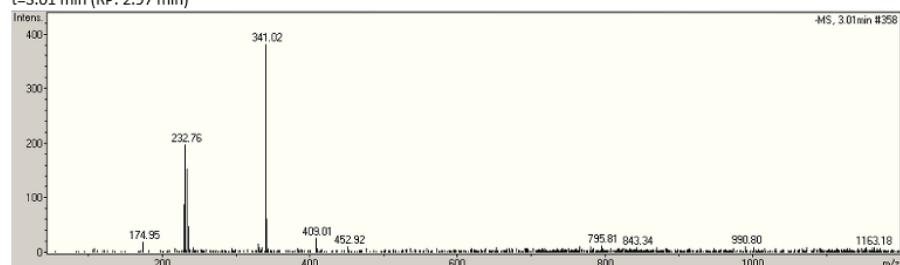
m/z	I	Formula
209.99	614	[M] <sup>2-</sup>
420.98	2199	[MH] <sup>-</sup>

t=2.21 min (RP: 2.16 min)



m/z	I	Formula
209.99	106	[M] <sup>2-</sup>
420.98	968	[MH] <sup>-</sup>

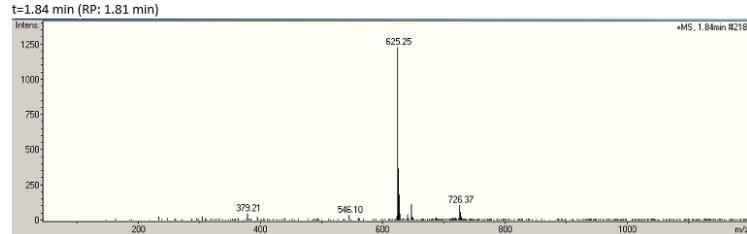
t=3.01 min (RP: 2.97 min)



m/z	I	Formula
341.02	383	unknown
409.01	25	unknown

**MS (positive mode)**

t=1.84 min (RP: 1.81 min)



+MS, 1.84min #218

m/z	I	Formula
546.10	32	[MH] <sup>+</sup> •Na <sup>+</sup> •[TEAH] <sup>+</sup>
625.25	1232	[MH] <sup>+</sup> •2[TEAH] <sup>+</sup>
726.37	102	[M] <sup>2-</sup> •3[TEAH] <sup>+</sup>

### S-8.39. Indigotin

#### GENERAL INFORMATION

**Color Index Name:** Vat Blue 1

**Color Index Number:** 73015

**Type of dye:** Indigoid

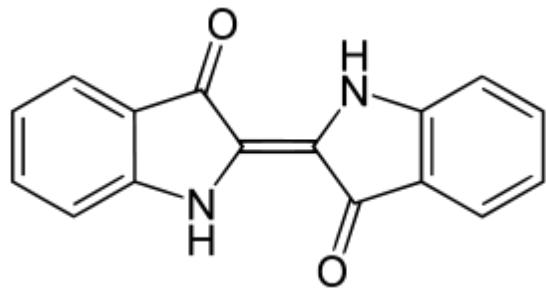
**Charge:** 0

**Related dye:** N2031 Indigo (natural)

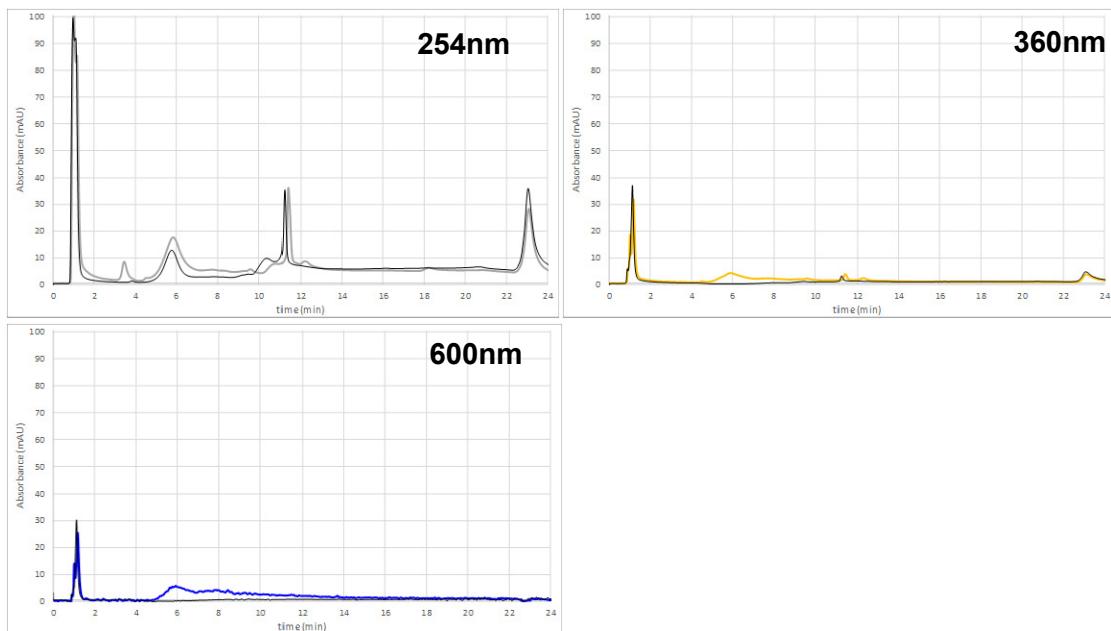
**Molecular Formula:** C<sub>16</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight**

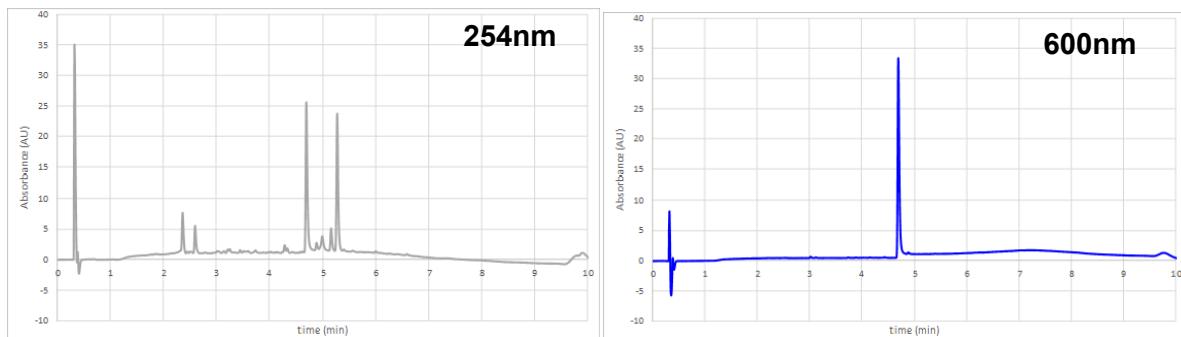
Full molecule:	262.26
Monoisotopic	262.07



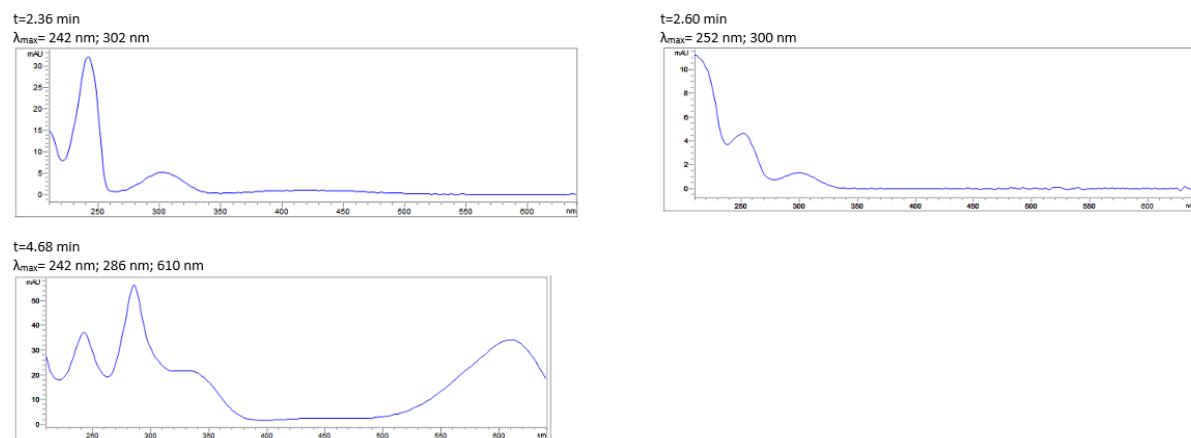
#### CHROMATOGRAMS: ION-EXCHANGE



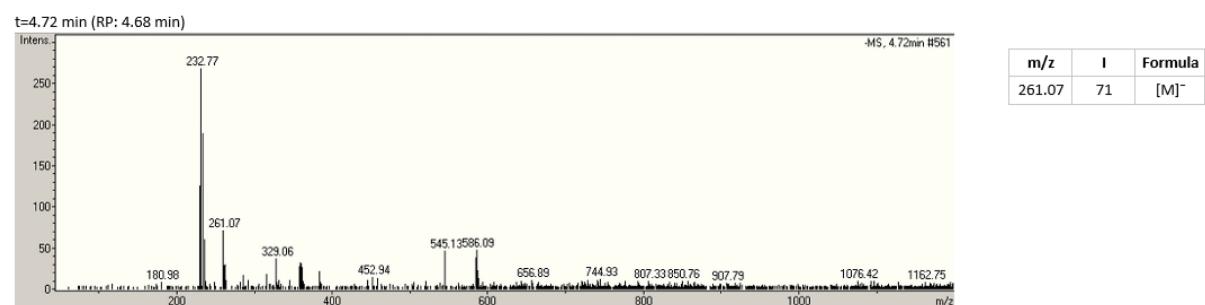
#### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA



## MASS SPECTRA



## S-8.40. Isatin

### GENERAL INFORMATION

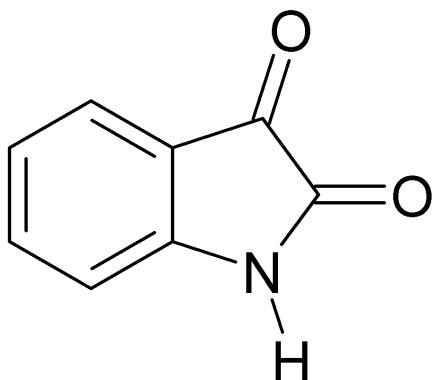
Alternative names: 1*H*-indole-2,3-dione

Color Index Name: n.a.

Color Index Number: n.a.

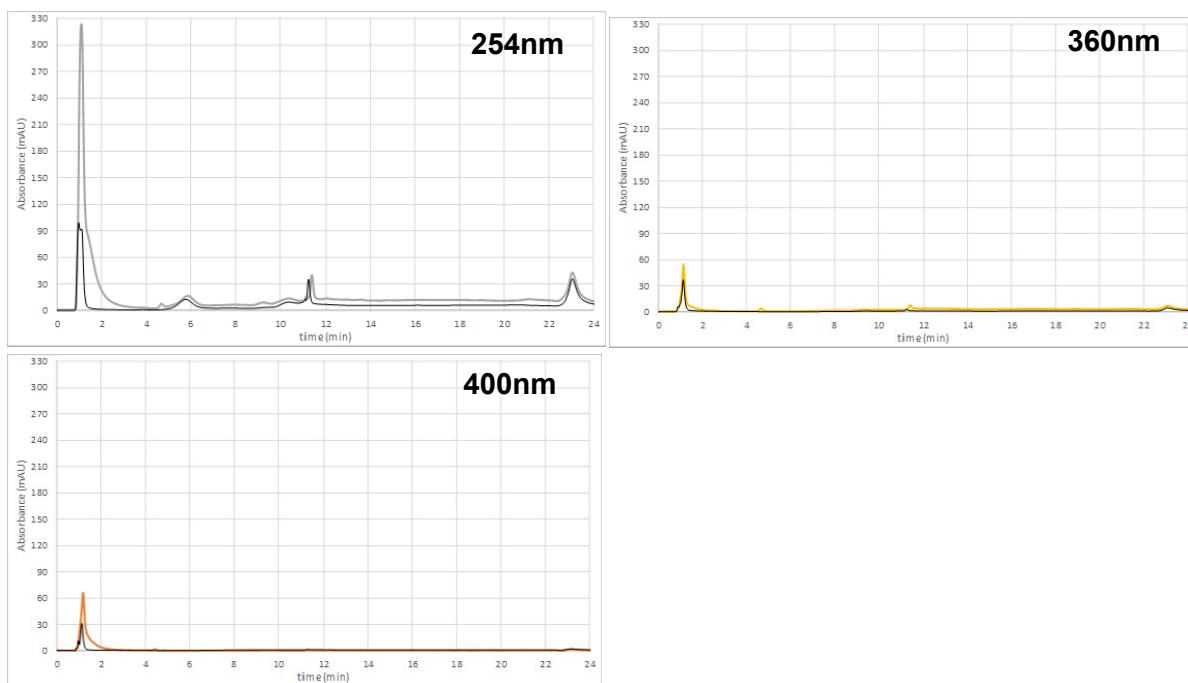
Type of dye: Natural

Scientific name of biological source: *Indigofera tinctoria L.*

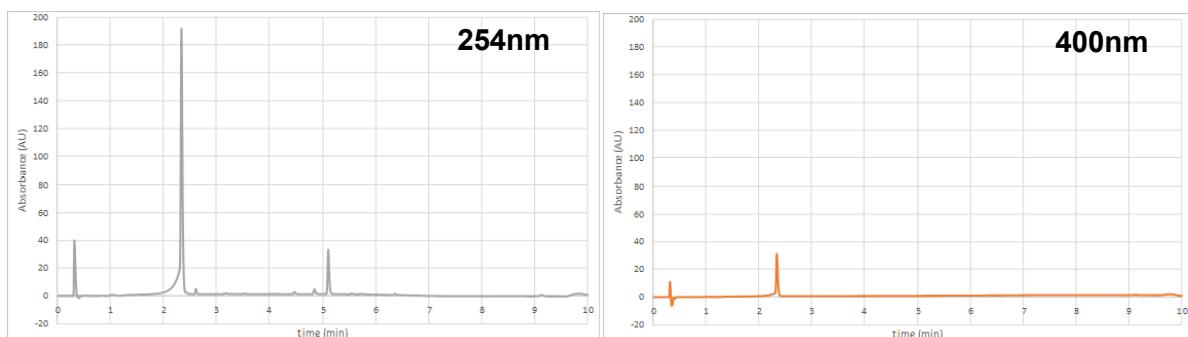


Name	Short	Mw	monoisotopic	Formula
Isatin	[IS]	147.13	147.03	C <sub>8</sub> H <sub>5</sub> NO <sub>2</sub>

### CHROMATOGRAMS: ION-EXCHANGE



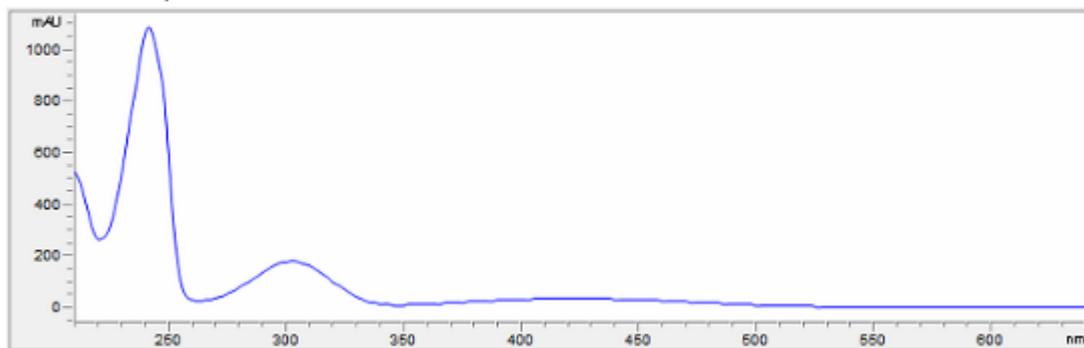
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

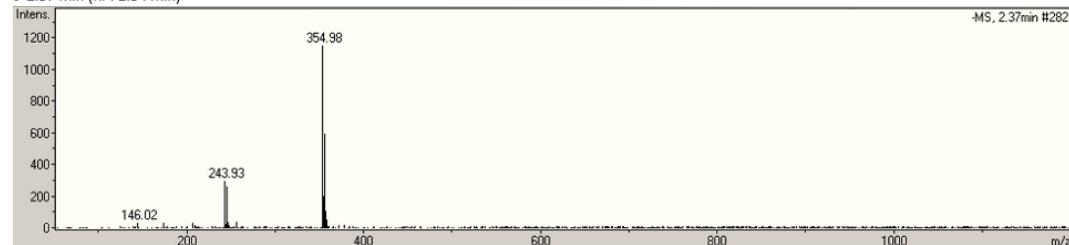
t=2.34 min

$\lambda_{\text{max}} = 242 \text{ nm}$ ; 300-304 nm



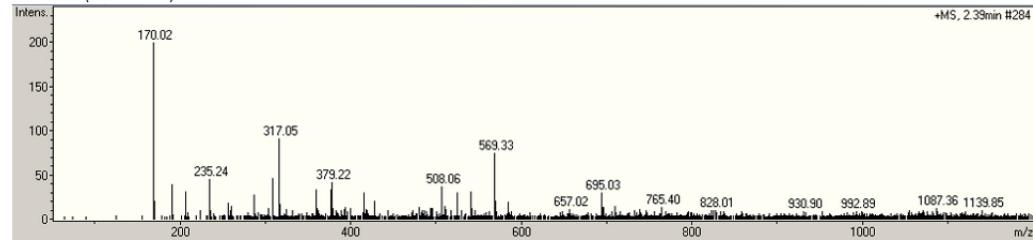
## MASS SPECTRA

t=2.37 min (RP: 2.34 min)



m/z	I	Formula
146.0	30	[IS] <sup>-</sup>
243.9	292	+97.9
355.0	1152	unknown

t=2.39 min (RP: 2.34 min)



m/z	I	Formula
170.0	200	[IS]•Na <sup>+</sup>
569.3	75	unknown

## S-8.41. Kaempferol

### GENERAL INFORMATION

**Alternative names:** Persian Berries

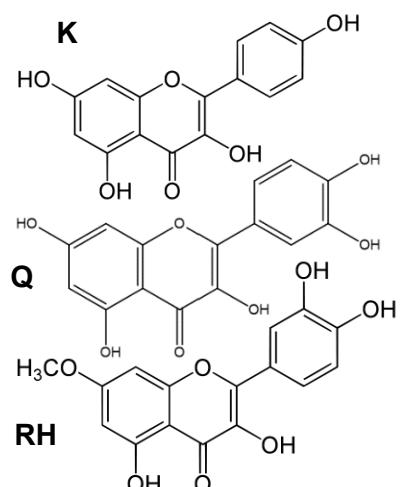
**Color Index Name:** n.a.

**Color Index Number:** n.a.

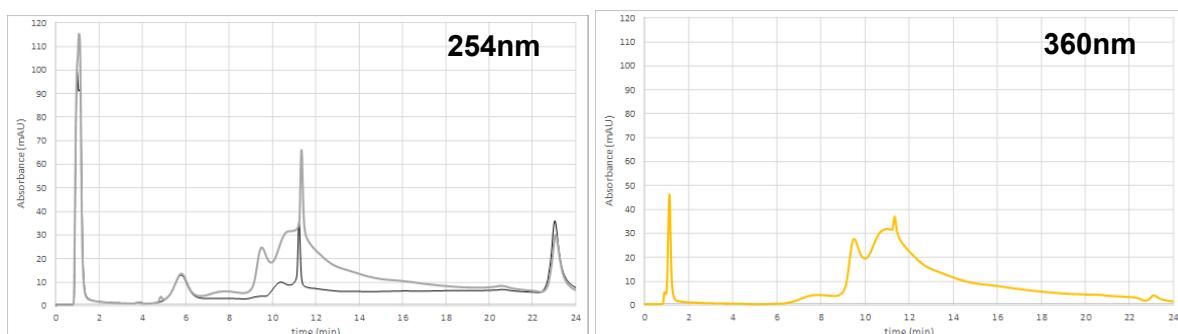
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Rhamnus Inectoria L./Saxatilis.*

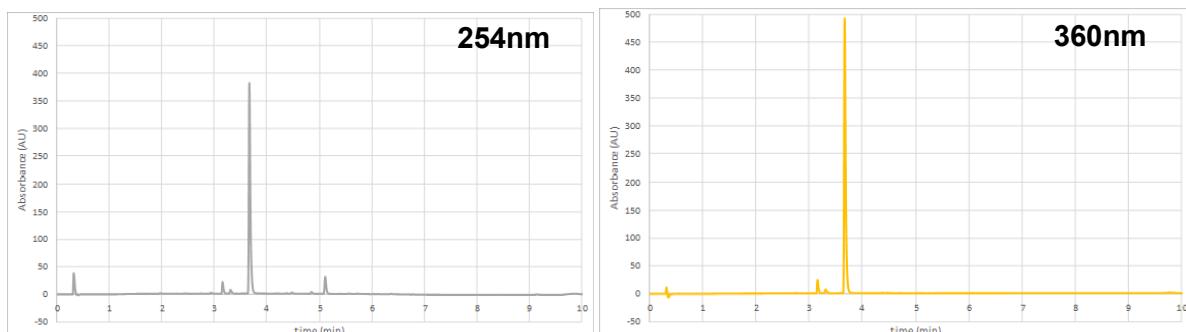
Name	Short	Mw	monoisotopic	Formula
Kaempferol	[K]	286.24	286.05	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>
Quercetin	[Q]	302.24	302.04	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>
Rhamnetin	[RH]	316.26	316.06	C <sub>16</sub> H <sub>12</sub> O <sub>7</sub>



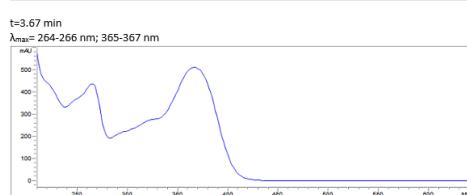
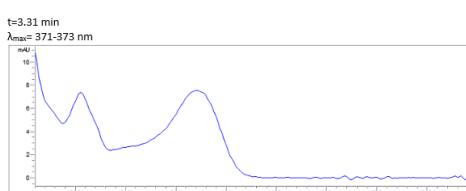
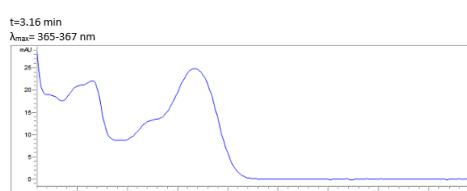
### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

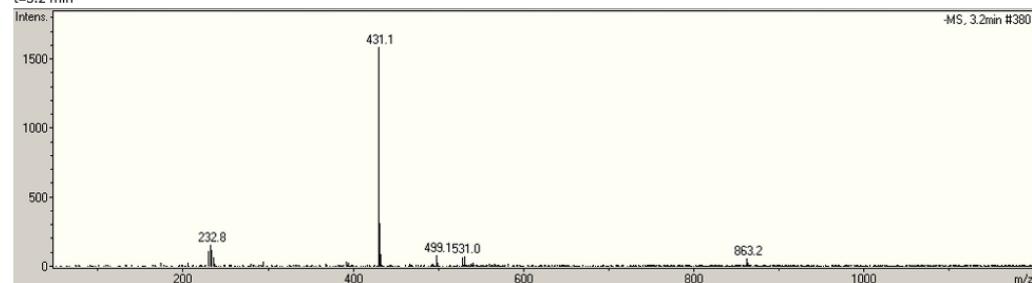


### UV-VIS SPECTRA

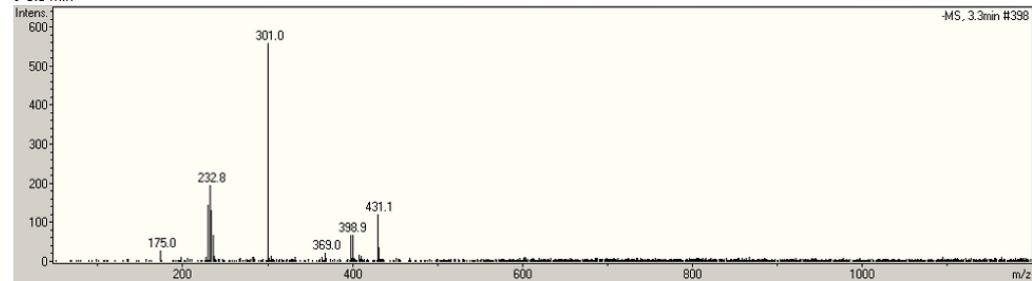


## MASS SPECTRA

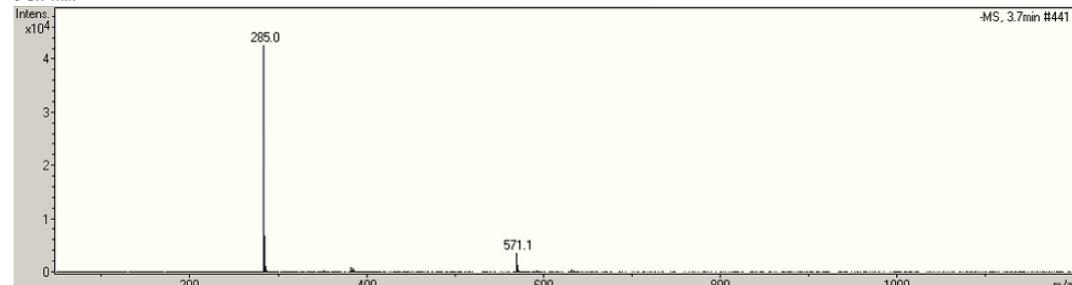
t=3.2 min



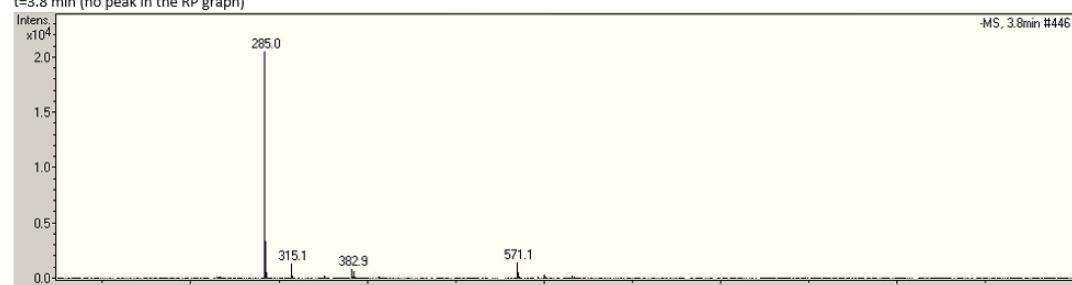
t=3.3 min



t=3.7 min



t=3.8 min (no peak in the RP graph)



## S-8.42. Lawsone

### GENERAL INFORMATION

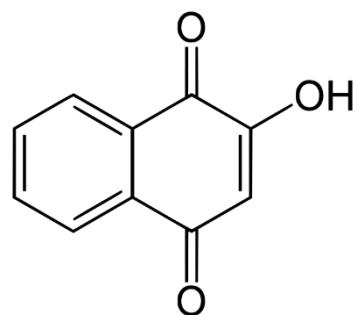
**Alternative names:** 2-hydroxy-1,4-naphthoquinone; Hennotannic acid

**Color Index Name:** Natural Orange 6

**Color Index Number:** 75480

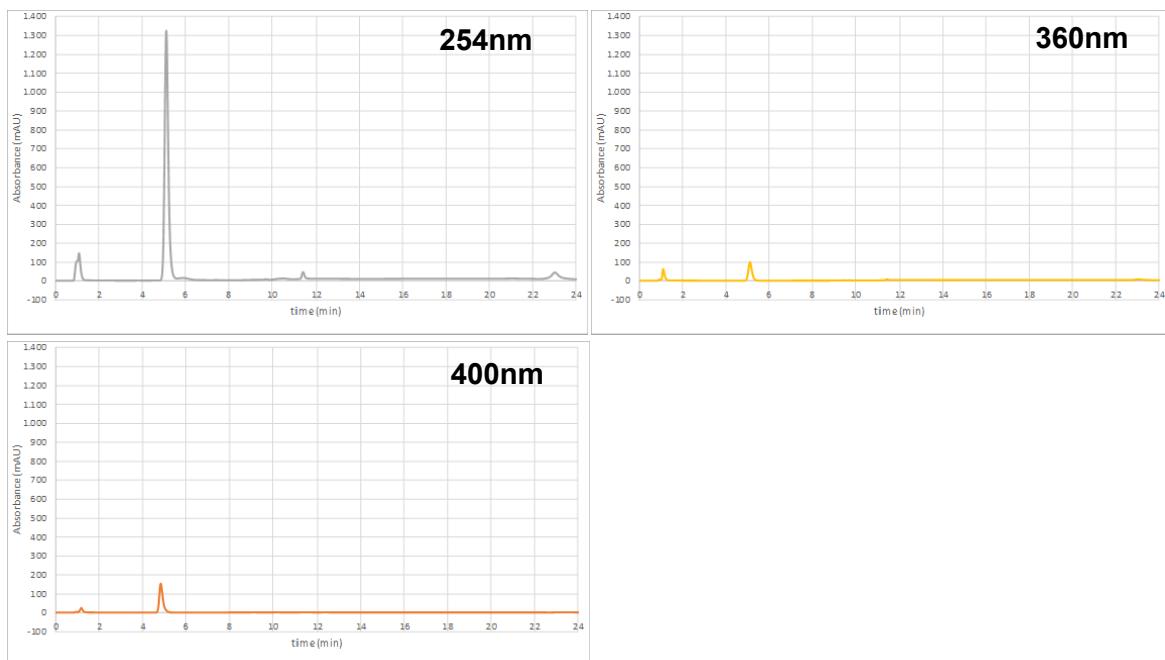
**Type of dye:** Natural

**Scientific name of biological source:** *Lawsonia inermis L.*

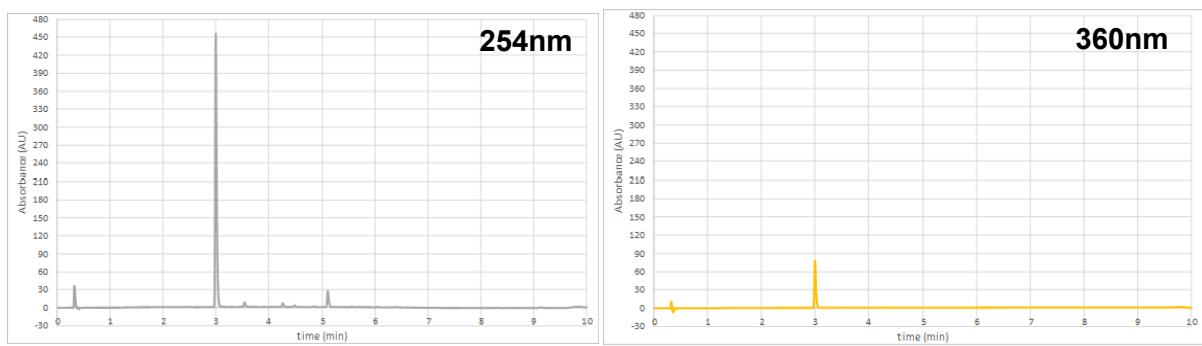


Name	Short	Mw	monoisotopic	Formula
Lawsone	[L]	174.15	174.03	C <sub>10</sub> H <sub>6</sub> O <sub>3</sub>

### CHROMATOGRAMS: ION-EXCHANGE



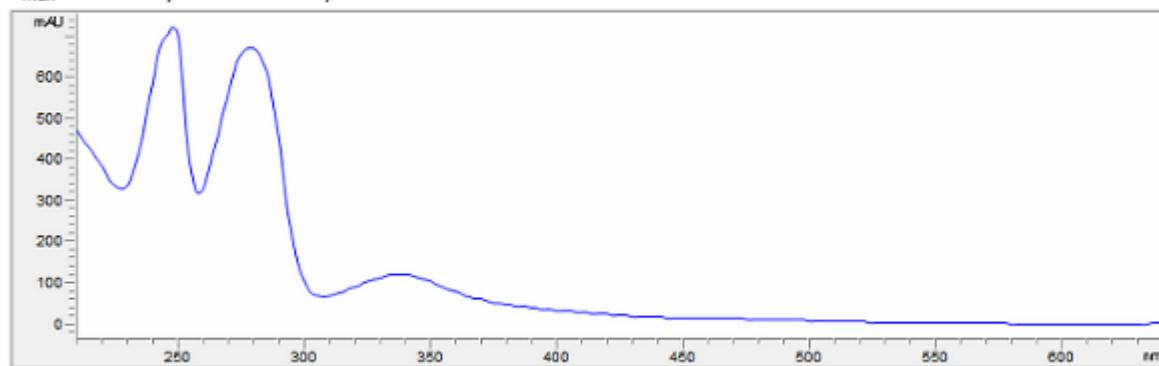
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

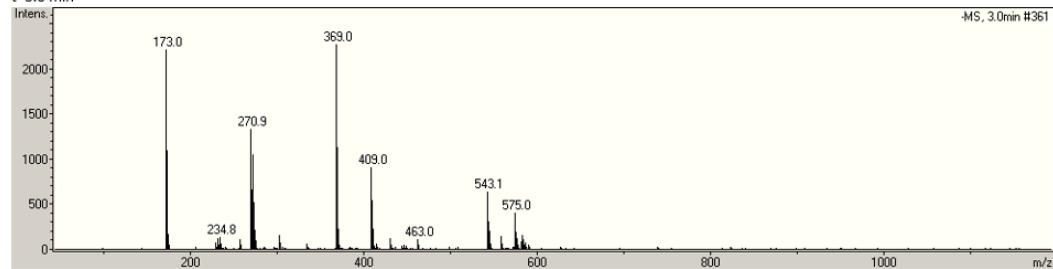
t=3.00 min

$\lambda_{\text{max}} = 248 \text{ nm}$ ; 278-280 nm; 336-338 nm



## MASS SPECTRA

t=3.0 min



$m/z$	I	Formula
173.0	2220	$[\text{L}]^-$
270.9	1334	$+97.9$
369.0	2281	$2[\text{L}]^- \bullet \text{Na}^+$
409.0	911	unknown
463.0	104	unknown
543.1	612	$3[\text{L}]^- \bullet \text{H}^+ \bullet \text{Na}^+$
575.0	402	$3[\text{L}]^- \bullet 2\text{Na}^+$

### S-8.43. Maclurin

#### GENERAL INFORMATION

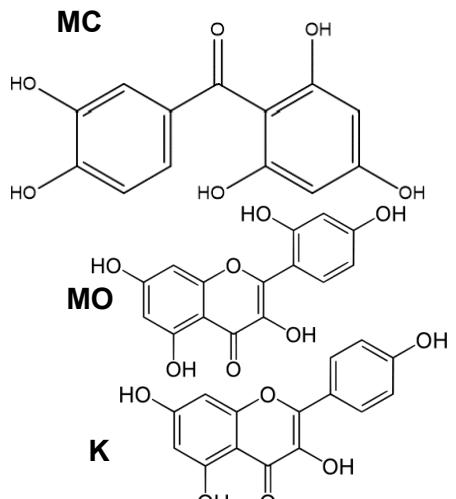
**Color Index Name:** Natural Yellow 11

**Color Index Number:** 75240

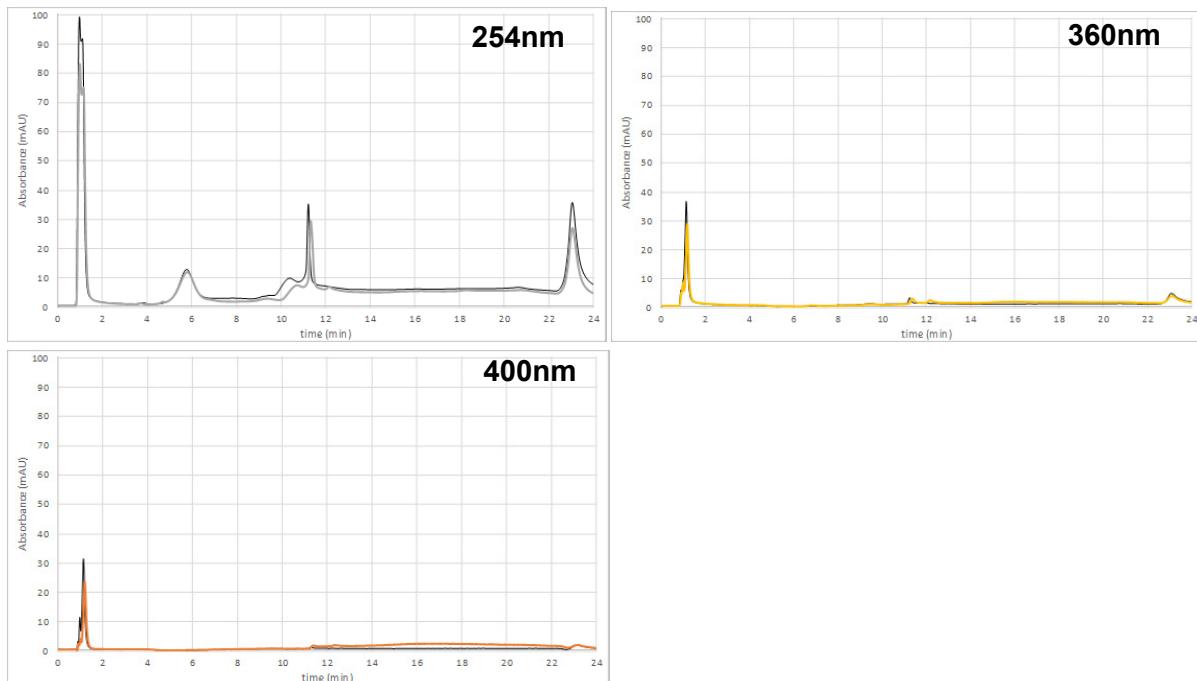
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Chlorophora/Maclura/Morus tinctoria L.*

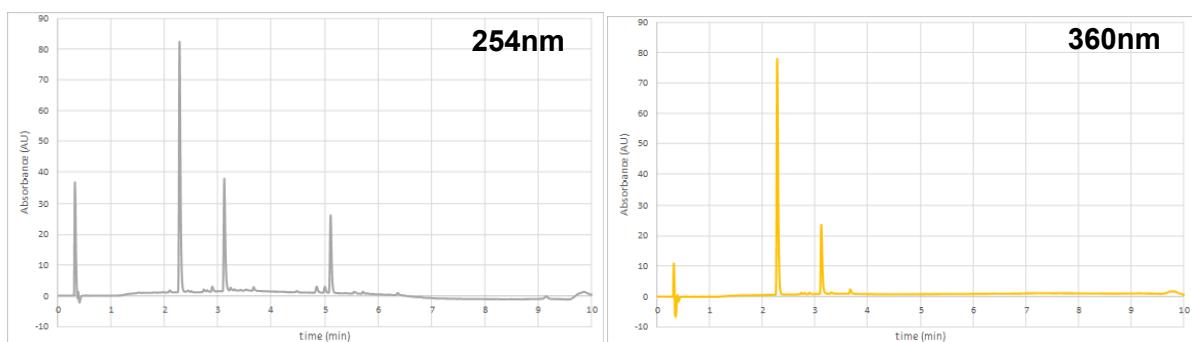
Name	Short	Mw	monoisotopic	Formula
Maclurin	[MC]	262.21	262.05	C <sub>13</sub> H <sub>10</sub> O <sub>6</sub>
Morin	[MO]	302.24	302.04	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>
Kaempferol	[K]	286.24	286.05	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>



#### CHROMATOGRAMS: ION-EXCHANGE

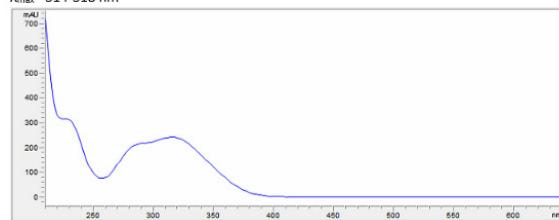


#### CHROMATOGRAMS: REVERSED-PHASE

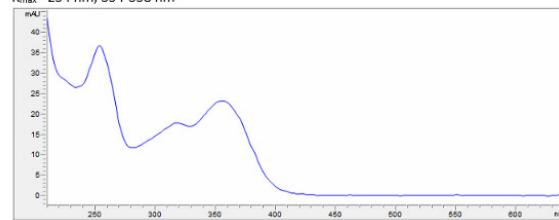


## UV-VIS SPECTRA

t=2.28 min  
 $\lambda_{\text{max}} = 314\text{-}318 \text{ nm}$

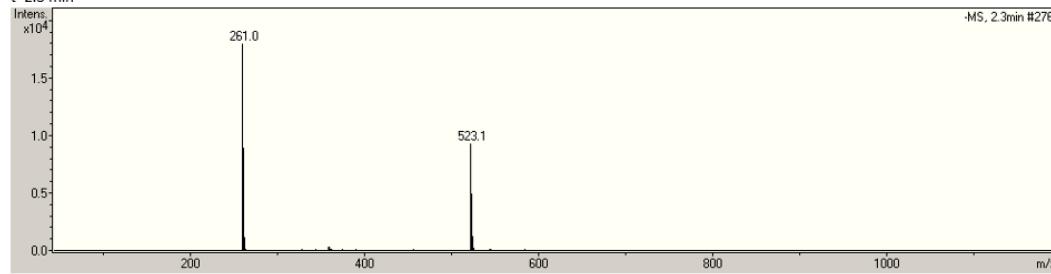


t=3.12 min  
 $\lambda_{\text{max}} = 254 \text{ nm}; 354\text{-}358 \text{ nm}$



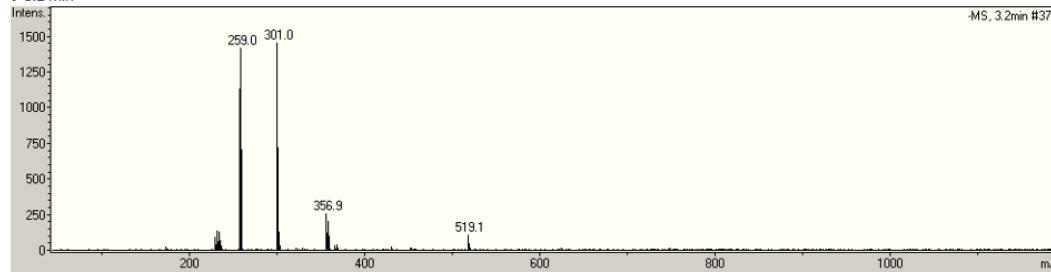
## MASS SPECTRA

t=2.3 min



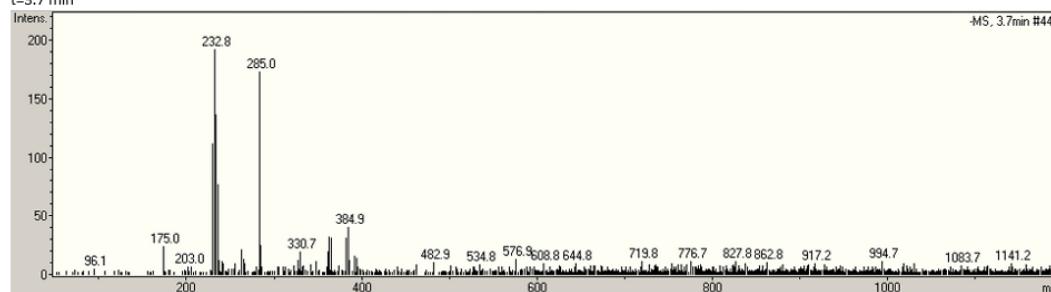
m/z	I	Formula
261.0	17983	[MO] <sup>-</sup>
523.1	9328	2[MC] <sup>-</sup> •H <sup>+</sup>

t=3.2 min



m/z	I	Formula
259.0	1425	unknown
301.0	1456	[MO] <sup>-</sup>
356.9	257	+97.9
519.1	166	2[unknown] <sup>-</sup> •H <sup>+</sup>

t=3.7 min



m/z	I	Formula
285.0	173	[K] <sup>-</sup>
384.9	40	+97.9

## S-8.44. Martius Yellow

### GENERAL INFORMATION

**Color Index Name:** Acid Yellow 24

**Color Index Number:** 10315

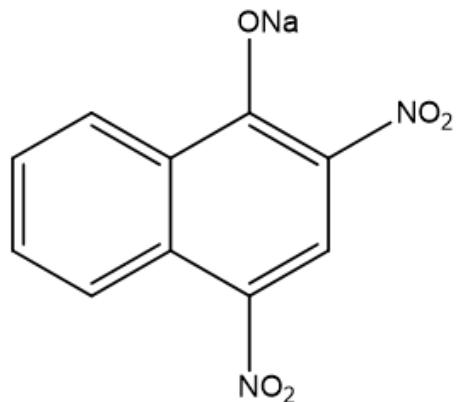
**Type of dye:** Nitro dye

**Charge:** 0

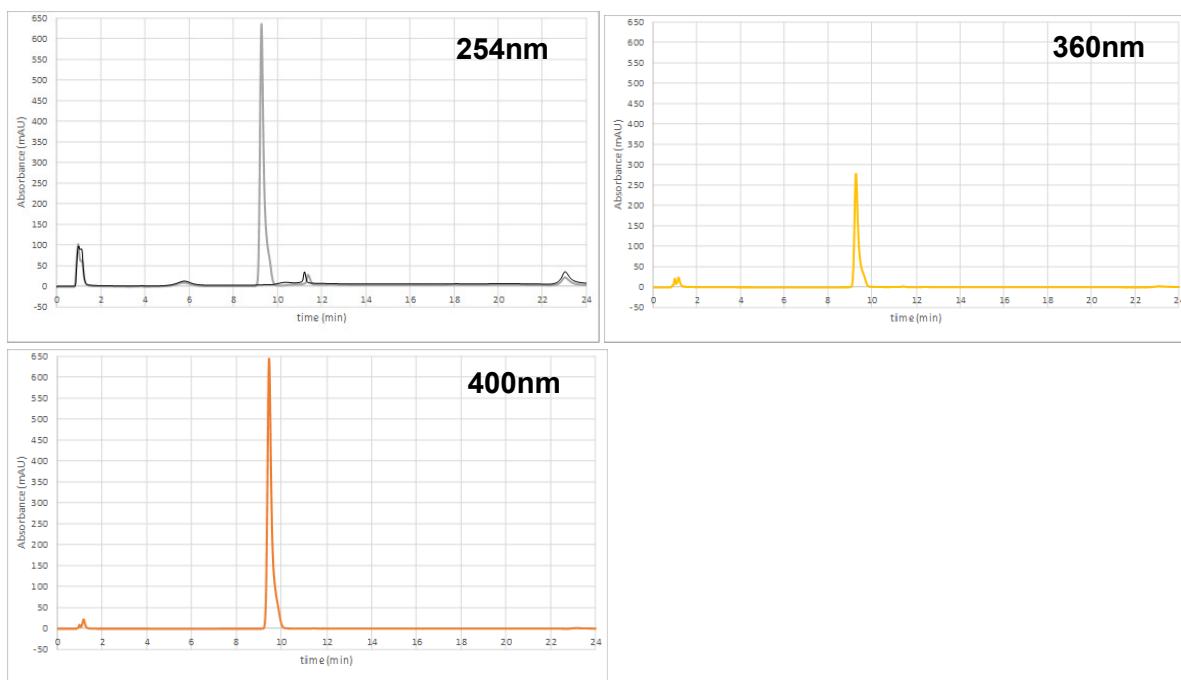
**Molecular Formula:** C<sub>10</sub>H<sub>6</sub>N<sub>2</sub>O<sub>5</sub> (ONa replaced with OH)

### Molecular Weight

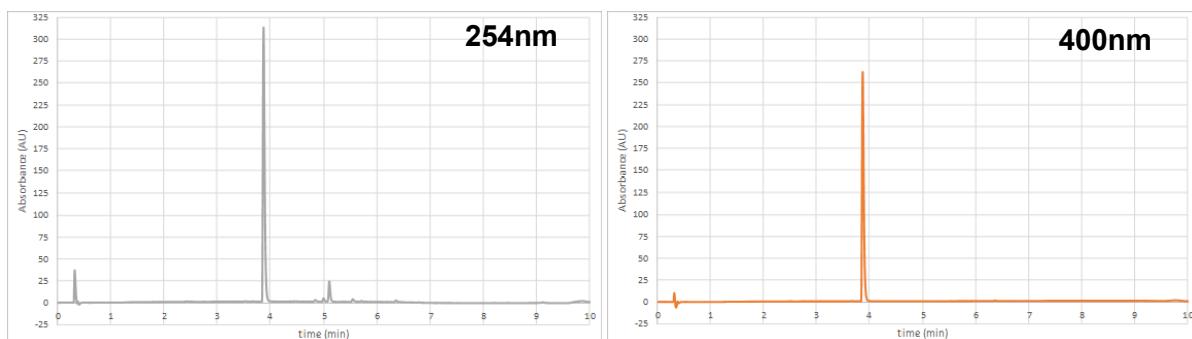
Full molecule:	256.15
ONa replaced with OH	234.17
Monoisotopic	234.03



### CHROMATOGRAMS: ION-EXCHANGE



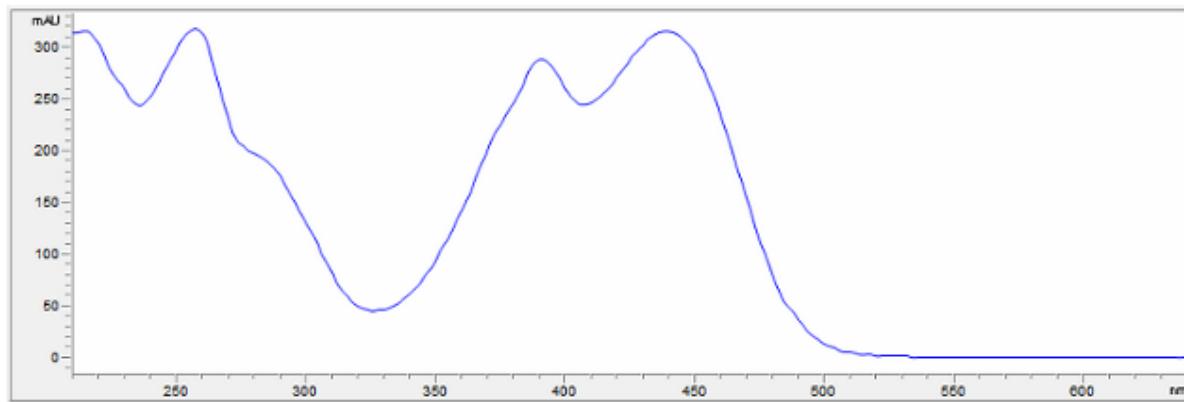
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

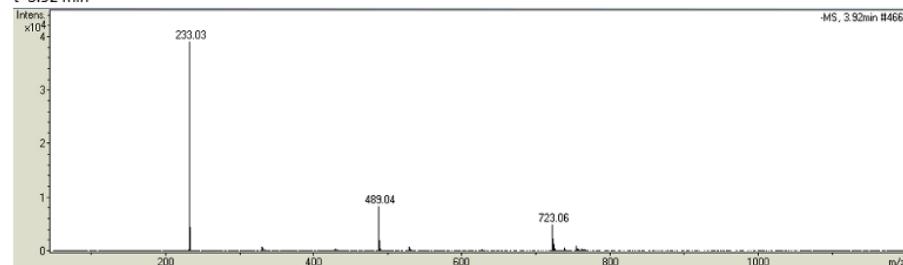
t=3.88 min

$\lambda_{\text{max}} = 258 \text{ nm}; 390-392 \text{ nm}; 440 \text{ nm}$



## MASS SPECTRA

t=3.92 min



m/z	I	Formula
233.03	39168	$[M]^-$
489.04	8347	$2[M]^- \bullet Na^+$
723.06	4817	$3[M]^- \bullet Na^+ \bullet H^+$

## S-8.45. Metanil Yellow

### GENERAL INFORMATION

**Color Index Name:** Acid Yellow 36

**Color Index Number:** 13065

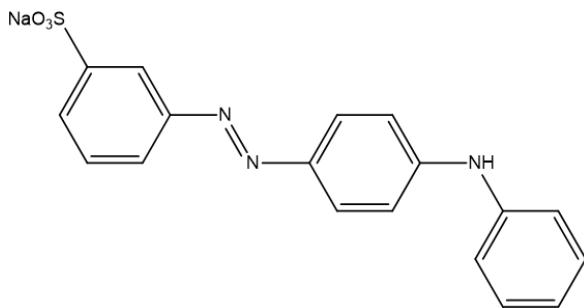
**Type of dye:** Monoazo

**Charge:** -1

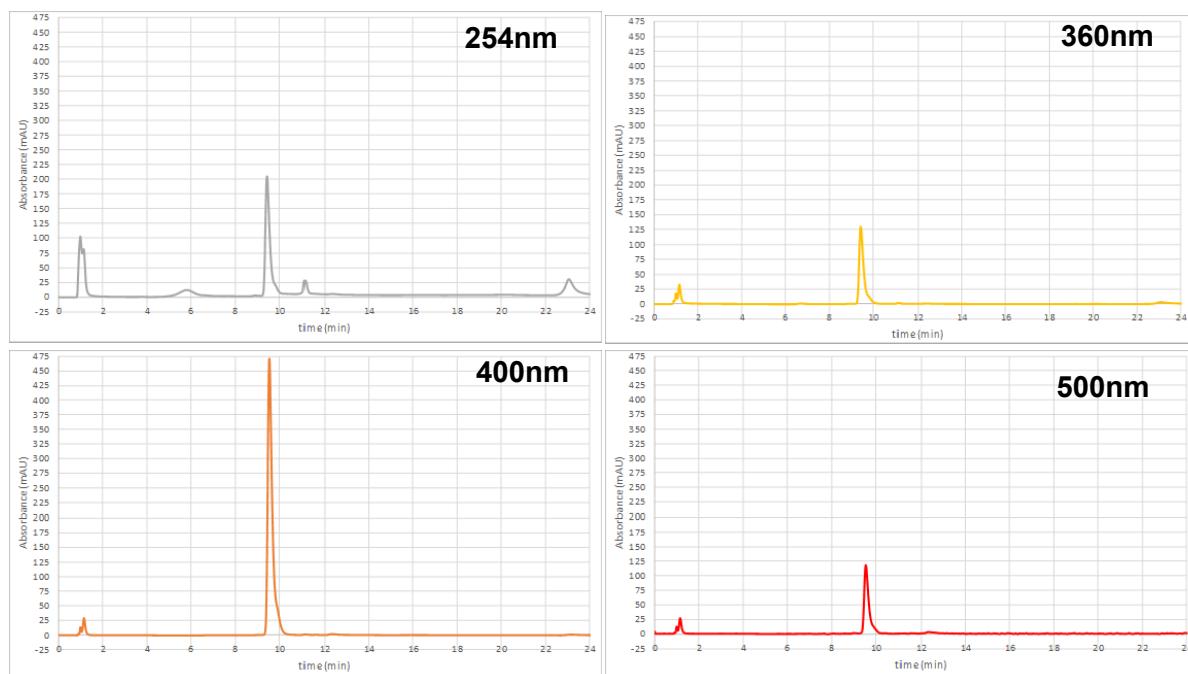
**Molecular Formula:** C<sub>18</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub>S (ion, -1)

**Molecular Weight**

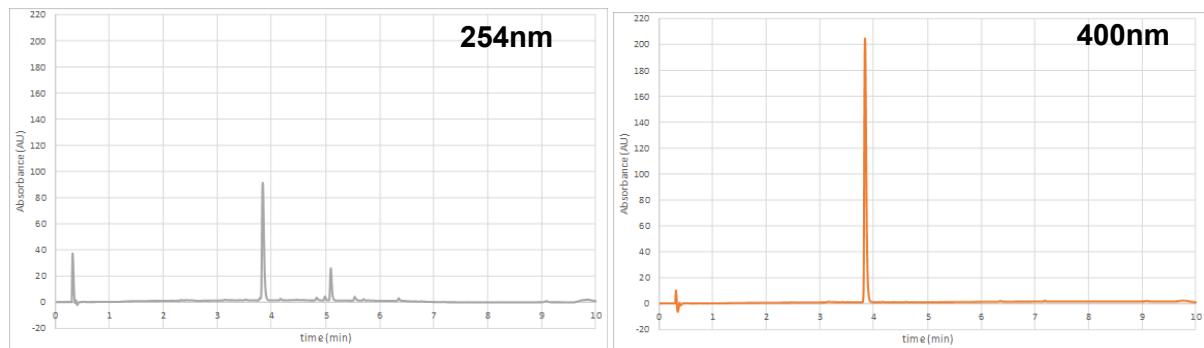
Full molecule:	375.38
Ion (-1)	352.39
Ion (-1), monoisotopic	352.08



### CHROMATOGRAMS: ION-EXCHANGE



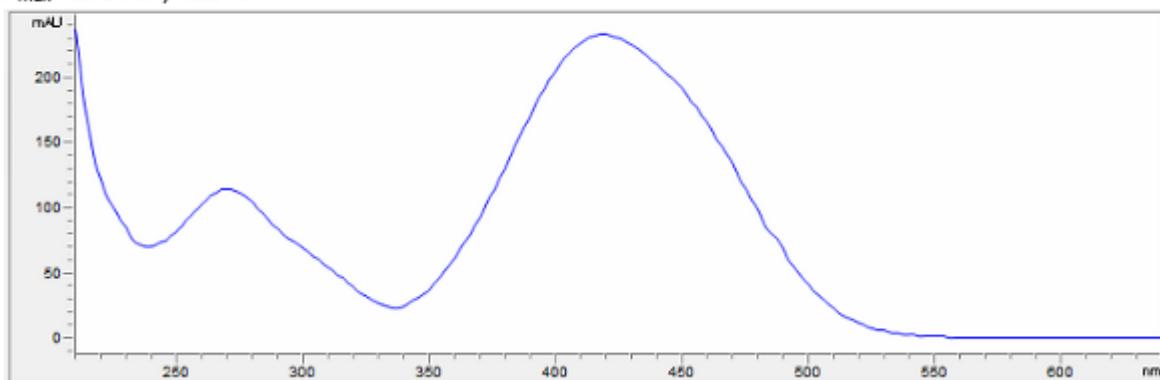
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

t=3.84 min

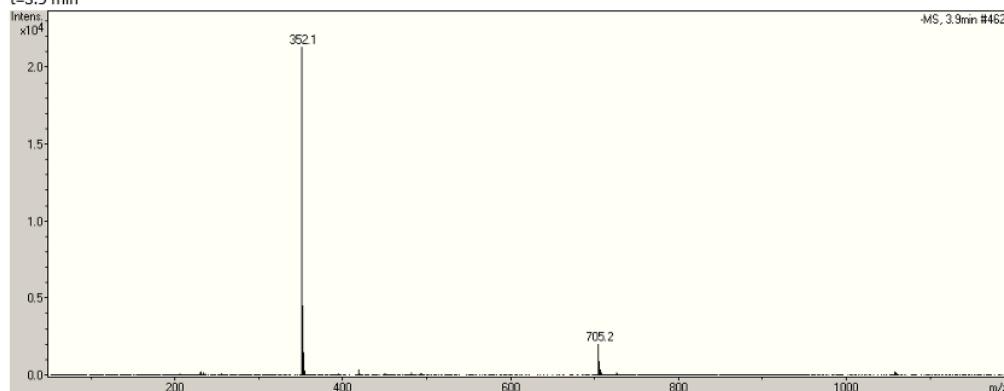
$\lambda_{\text{max}} = 270 \text{ nm}; 418 \text{ nm}$



## MASS SPECTRA

MS (negative mode)

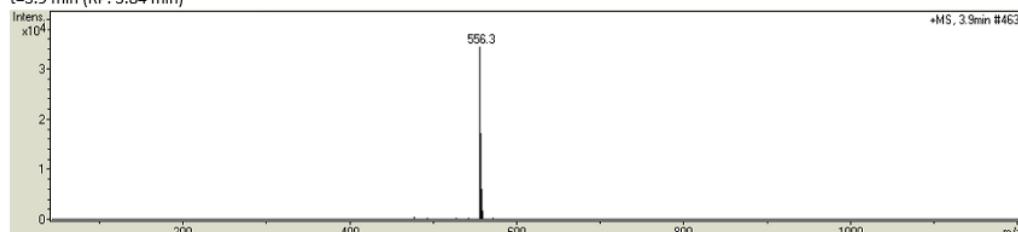
t=3.9 min



m/z	I	Formula
352.1	21361	$[\text{M}]^-$
705.2	1966	$2[\text{M}]^- \bullet \text{H}^+$

MS (positive mode)

t=3.9 min (RP: 3.84 min)



m/z	I	Formula
556.3	34658	$[\text{M}]^- \bullet 2[\text{TEAH}]^+$

## S-8.46. Methyl Violet

### GENERAL INFORMATION

**Color Index Name:** Basic Violet 1

**Color Index Number:** 42535

**Type of dye:** Triarylmethane

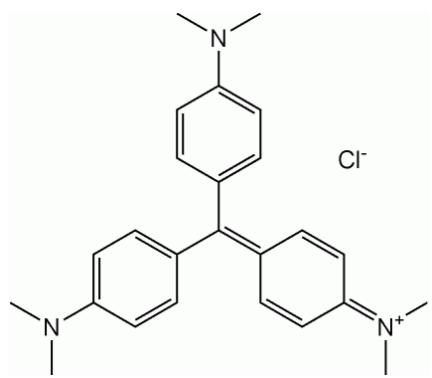
**Charge:** +1

**Related dyes:** Crystal Violet (only one of the compounds)

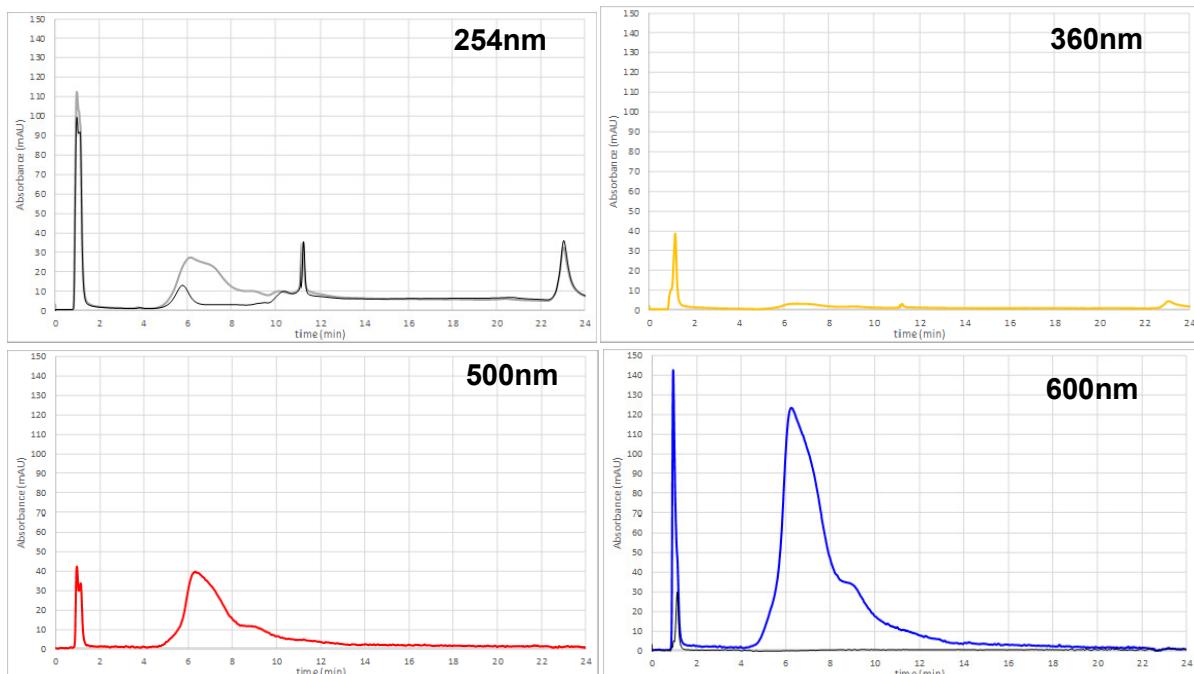
**Molecular Formula:** Mixture of tetra-, penta- and hexa-methylated pararosaniline, including Crystal Violet:  $C_{25}H_{30}N_3$  (ion, +1)

### Molecular Weight

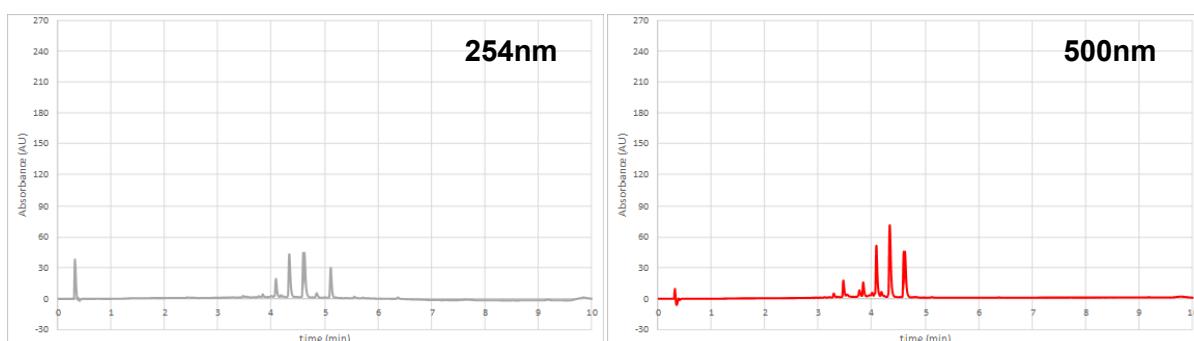
Crystal Violet:	407.98
Ion (+1)	372.53
Ion (+1), monoisotopic	372.24

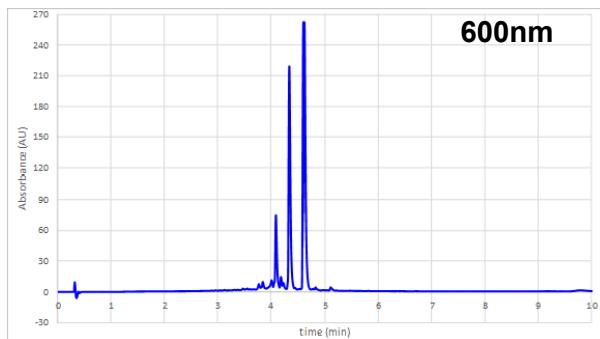


### CHROMATOGRAMS: ION-EXCHANGE

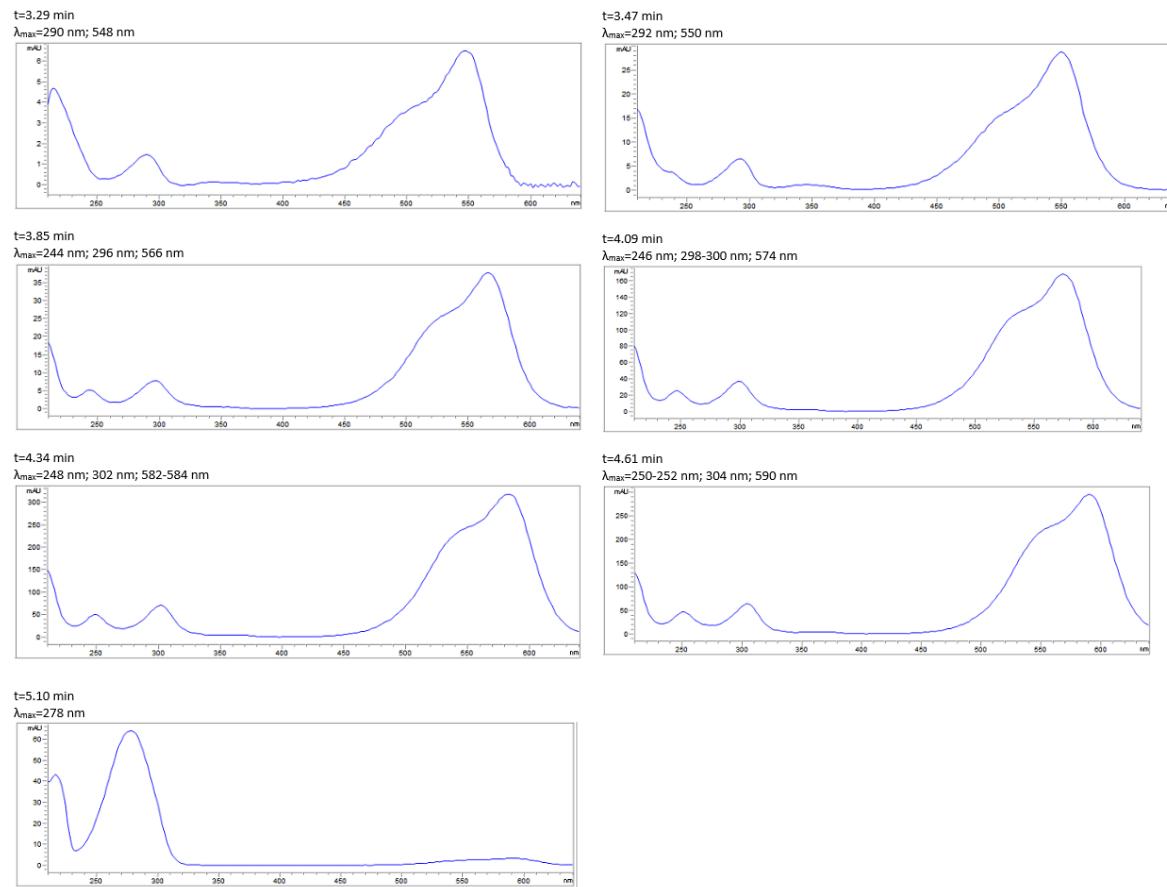


### CHROMATOGRAMS: REVERSED-PHASE

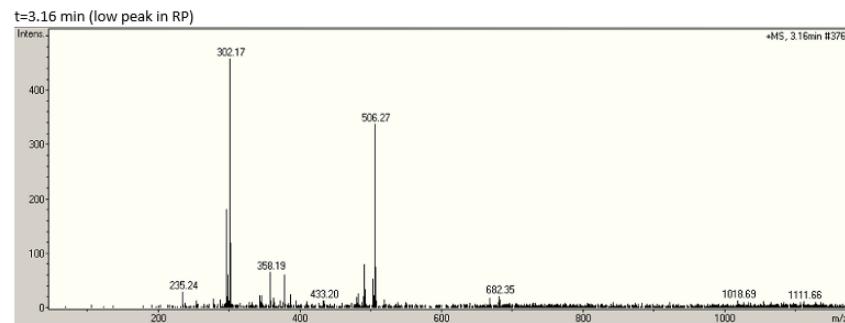




## UV-VIS SPECTRA

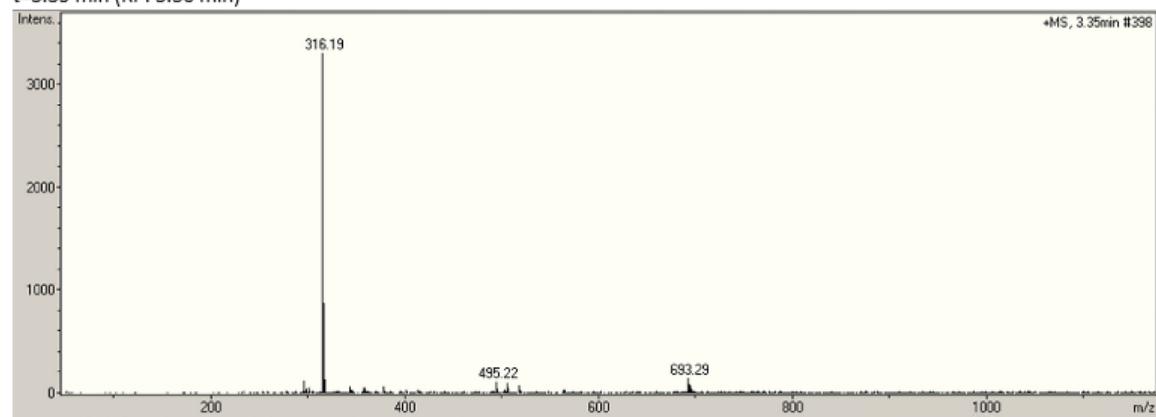


## MASS SPECTRA

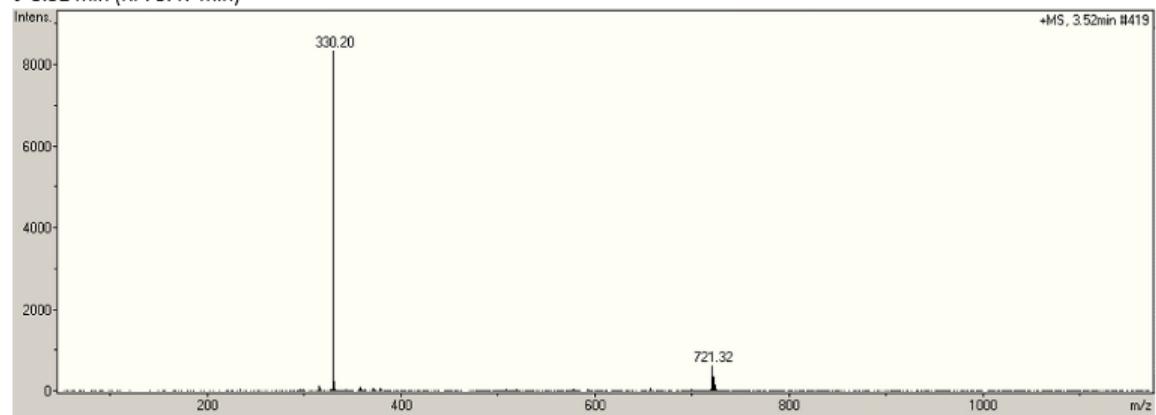


m/z	Time MS+	Time UV	I	Formula
302.17	3.16	no	459	[M-5CH <sub>2</sub> ] <sup>+</sup>
316.19	3.35	3.30	3313	[M-4CH <sub>2</sub> ] <sup>+</sup>
330.20	3.52	3.47	8361	[M-3CH <sub>2</sub> ] <sup>+</sup>
330.20	3.89	3.85	11606	[M-2CH <sub>2</sub> ] <sup>+</sup>
344.22	4.14	4.09	24767	[M-2CH <sub>2</sub> ] <sup>+</sup>
358.23	4.38	4.34	50123	[M-CH <sub>2</sub> ] <sup>+</sup>
372.25	4.65	4.61	57879	[M] <sup>+</sup>
386.27	4.85	no	4089	[M+CH <sub>2</sub> ] <sup>+</sup>
400.28	5.16	5.10	3856	[M+2CH <sub>2</sub> ] <sup>+</sup>

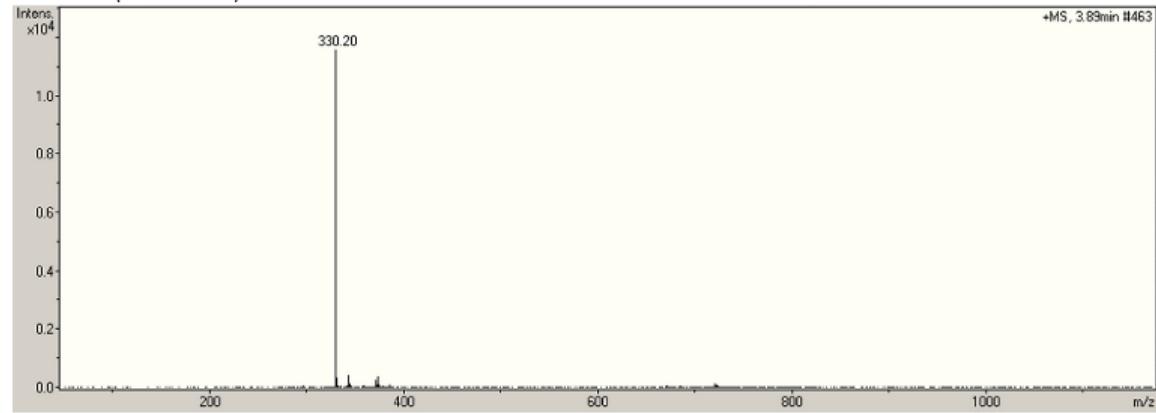
t=3.35 min (RP: 3.30 min)



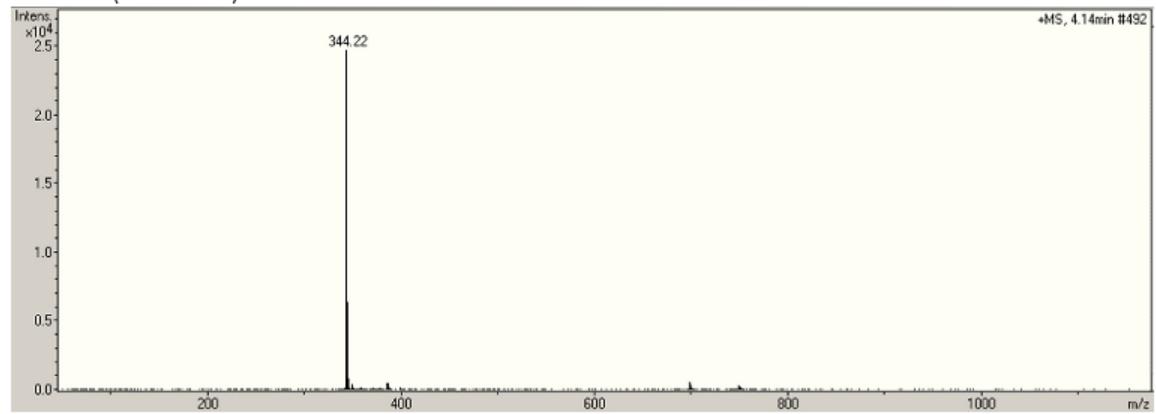
t=3.52 min (RP: 3.47 min)



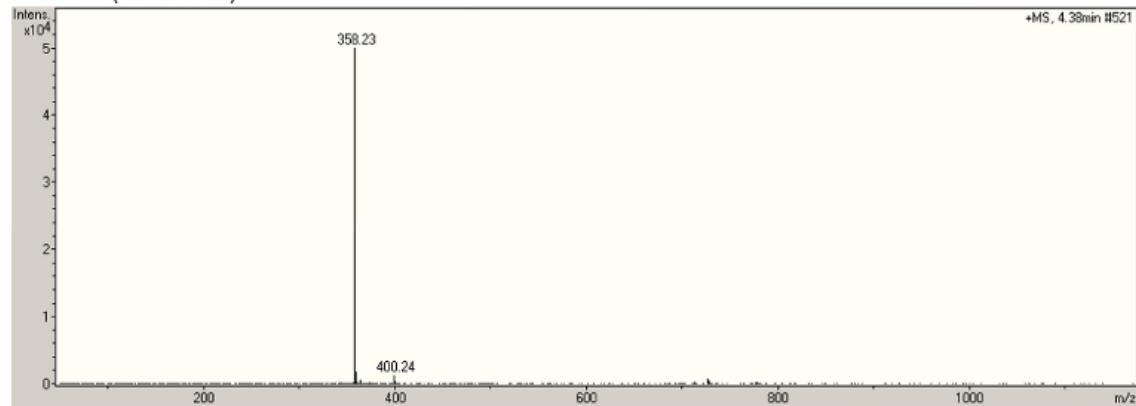
t=3.89 min (RP: 3.85 min)



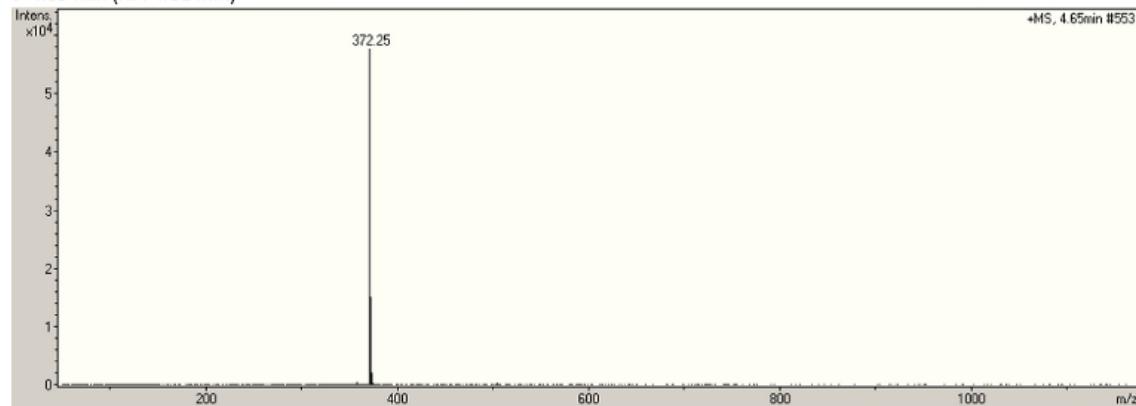
t=4.14 min (RP: 4.09 min)



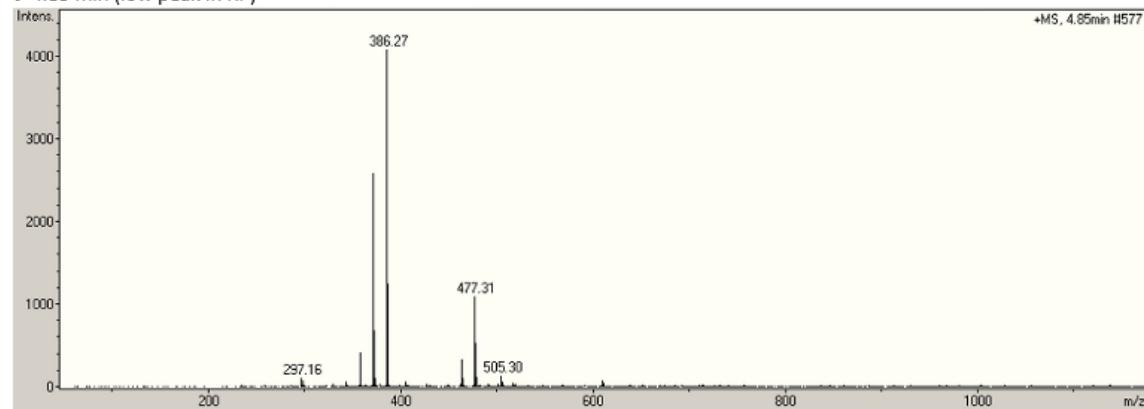
t=4.38 min (RP: 4.34 min)



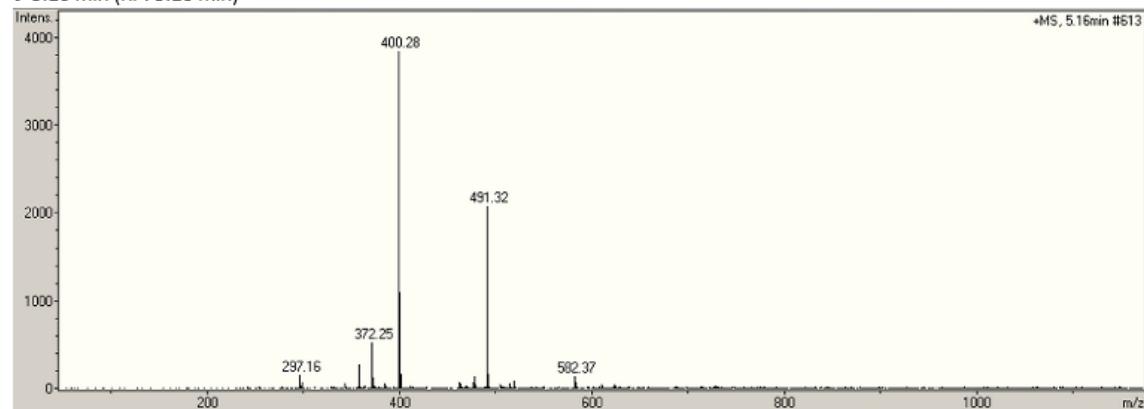
t=4.65 min (RP: 4.61 min)



t=4.85 min (low peak in RP)



t=5.16 min (RP: 5.10 min)



### S-8.47. Methylene Blue

#### GENERAL INFORMATION

**Color Index Name:** Basic Blue 9

**Color Index Number:** 52015

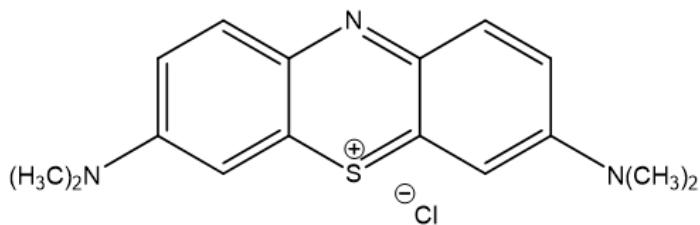
**Type of dye:** Diphenylmethane

**Charge:** +1

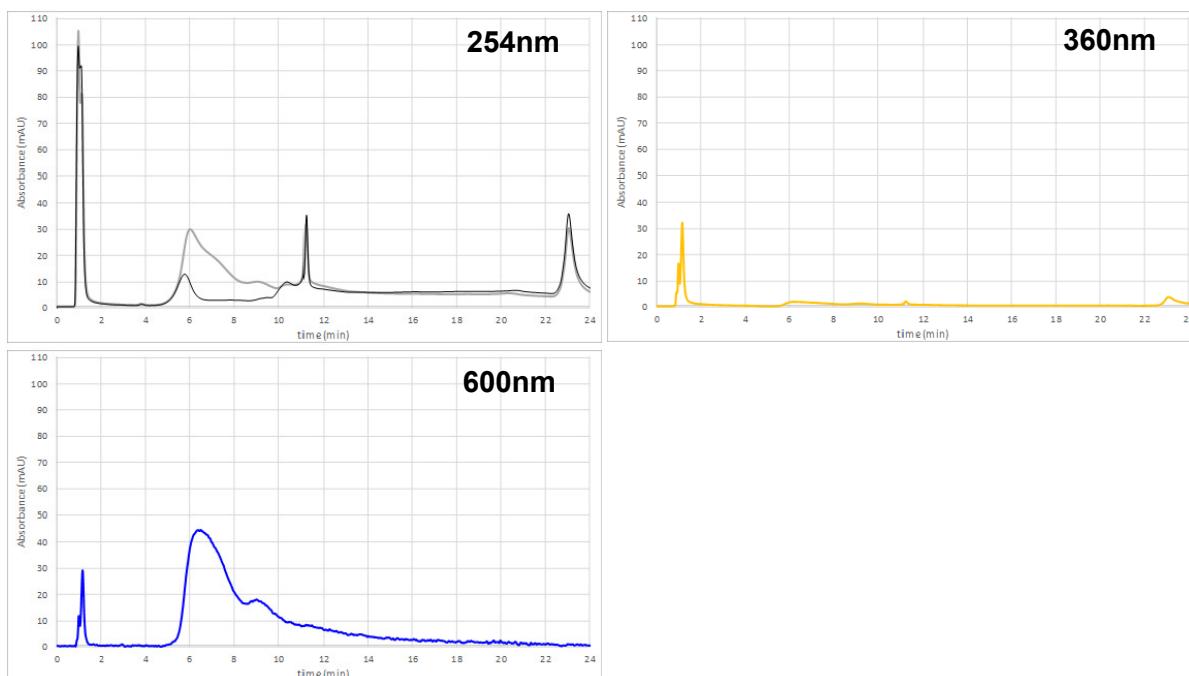
**Molecular Formula:** C<sub>16</sub>H<sub>18</sub>N<sub>3</sub>S (ion, +1)

**Molecular Weight**

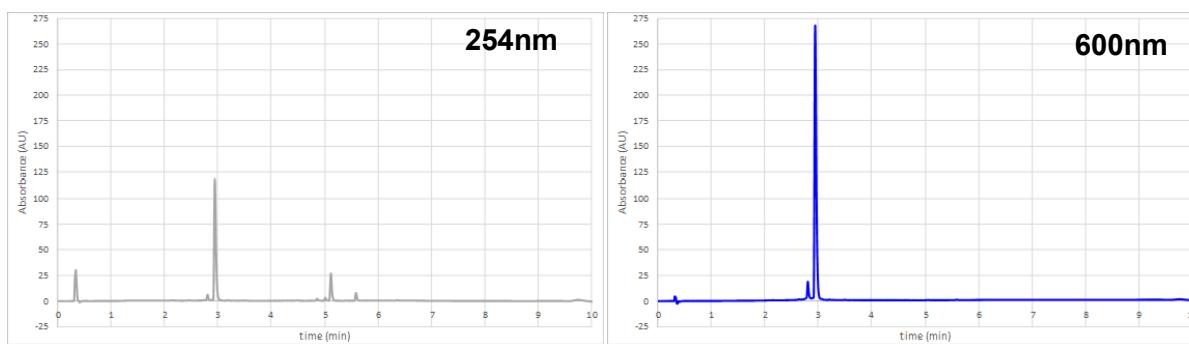
Full molecule:	319.85
Ion (+1)	284.40
Ion (+1), monoisotopic	284.12



#### CHROMATOGRAMS: ION-EXCHANGE



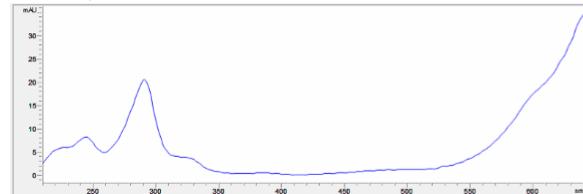
#### CHROMATOGRAMS: REVERSED-PHASE



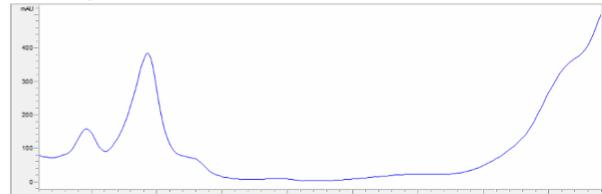
## UV-VIS SPECTRA

### DAD Spectra

$t=2.81$  min  
 $\lambda_{\text{max}} = 290 \text{ nm; } >640 \text{ nm}$



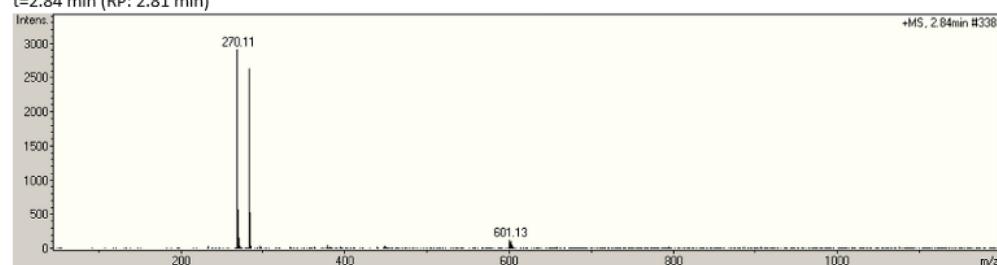
$t=2.95$  min  
 $\lambda_{\text{max}} = 284 \text{ nm; } >640 \text{ nm}$



## MASS SPECTRA

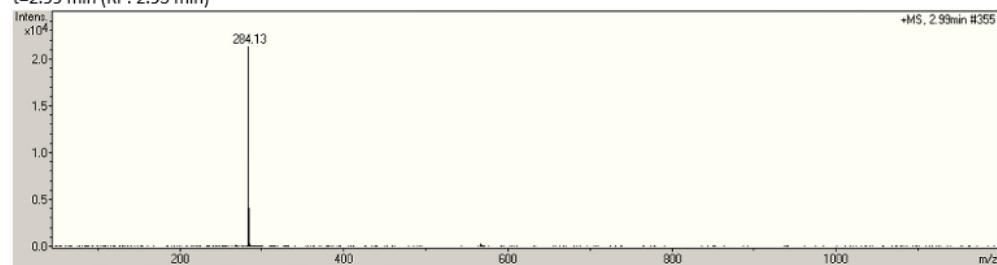
### MS (positive mode)

$t=2.84$  min (RP: 2.81 min)



m/z	I	Formula
270.11	2920	[M-CH <sub>2</sub> ] <sup>+</sup>

$t=2.99$  min (RP: 2.95 min)



m/z	I	Formula
284.13	21382	[M] <sup>+</sup>

## S-8.48. Morin

### GENERAL INFORMATION

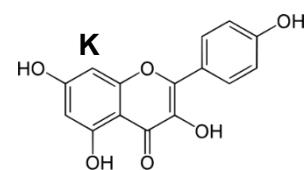
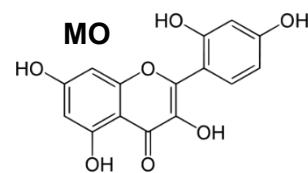
**Alternative names:** Old Fustic, Dyer's Mulberry

**Color Index Name:** Natural yellow 8

**Color Index Number:** 75660

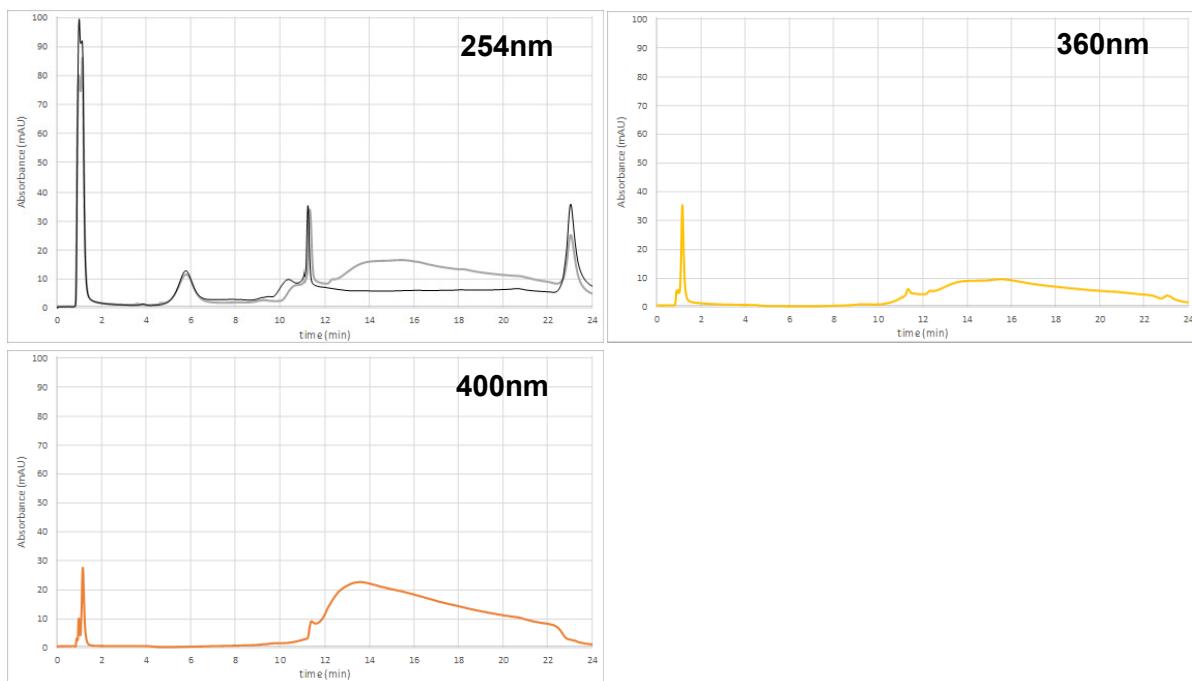
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Chlorophora/Maclura/Morus tinctoria L.*

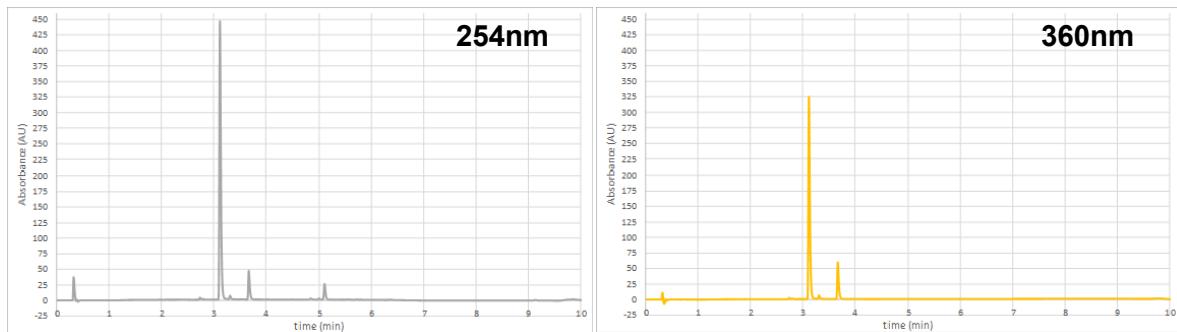


Name	Short	Mw	monoisotopic	Formula
Morin	[MO]	302.24	302.04	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>
Kaempferol	[K]	286.24	286.05	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>

### CHROMATOGRAMS: ION-EXCHANGE

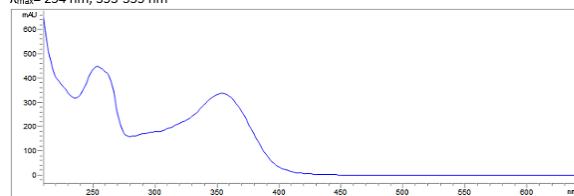


### CHROMATOGRAMS: REVERSED-PHASE

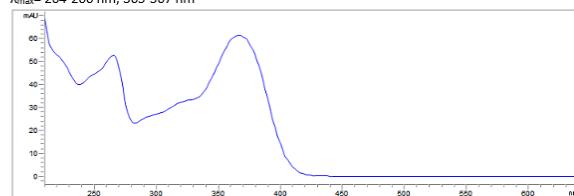


## UV-VIS SPECTRA

t=3.12 min  
 $\lambda_{\text{max}} = 254 \text{ nm; } 353-355 \text{ nm}$

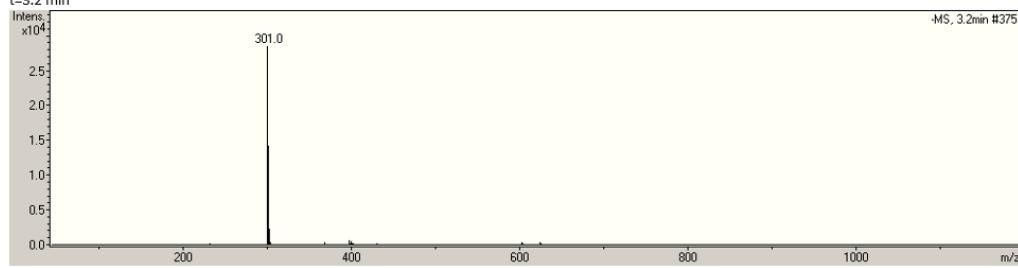


t=3.67 min  
 $\lambda_{\text{max}} = 264-266 \text{ nm; } 365-367 \text{ nm}$



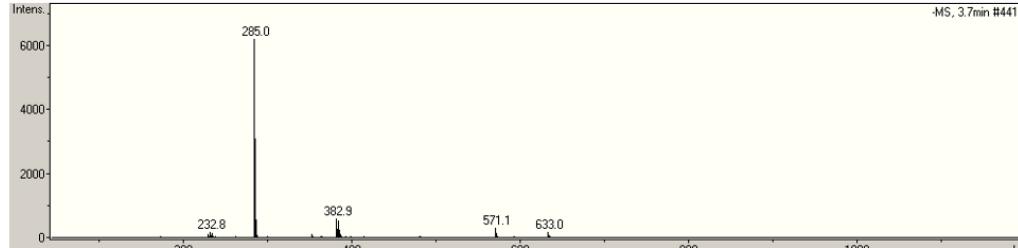
## MASS SPECTRA

t=3.2 min



m/z	I	Formula
301.0	28630	[MO] <sup>-</sup>
603.1	315	2[MO] <sup>-</sup> •H <sup>+</sup>

t=3.7 min



m/z	I	Formula
285.0	6233	[K] <sup>-</sup>
382.9	582	+97.9
571.1	279	2[K] <sup>-</sup> •H <sup>+</sup>
633.0	160	unknown

## S-8.49. Murexide

### GENERAL INFORMATION

Alternative name: Ammonium Purpurate

Color Index Name: Mordant Dye

Color Index Number: 56085

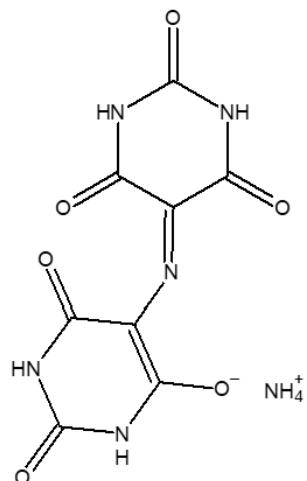
Type of dye: Aminoketone

Charge: 0

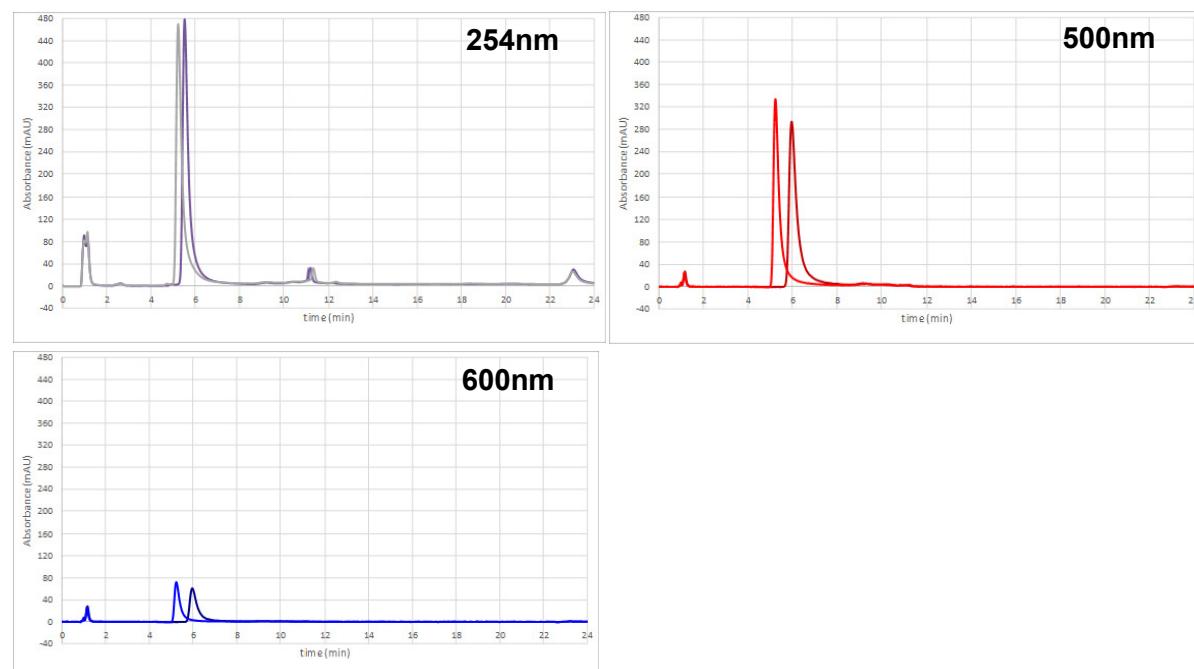
Molecular Formula: C<sub>8</sub>H<sub>4</sub>N<sub>5</sub>O<sub>6</sub> (ion, -1)

Molecular Weight

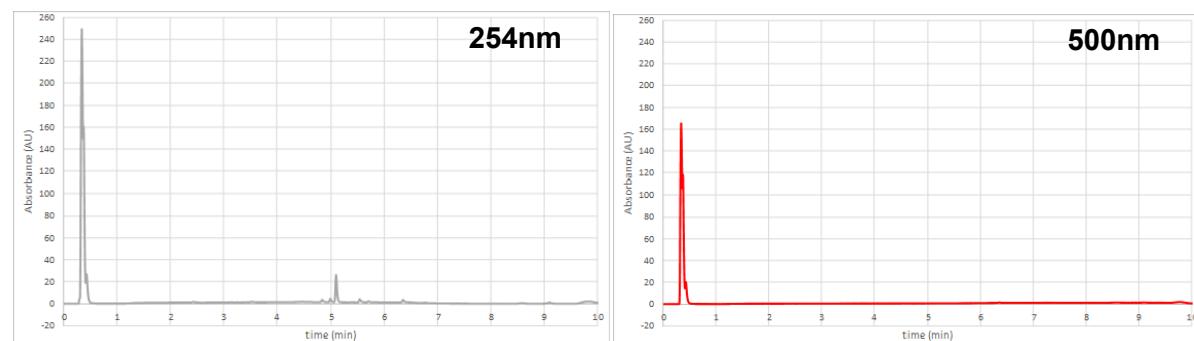
Full molecule:	284.19
Ion (-1)	266.15
Ion (-1), monoisotopic	266.02



### CHROMATOGRAMS: ION-EXCHANGE (double runs)



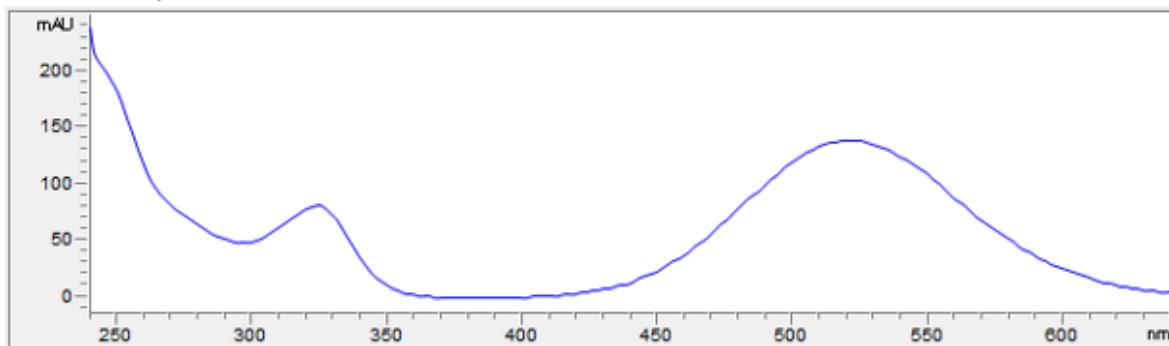
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

t=0.37 min

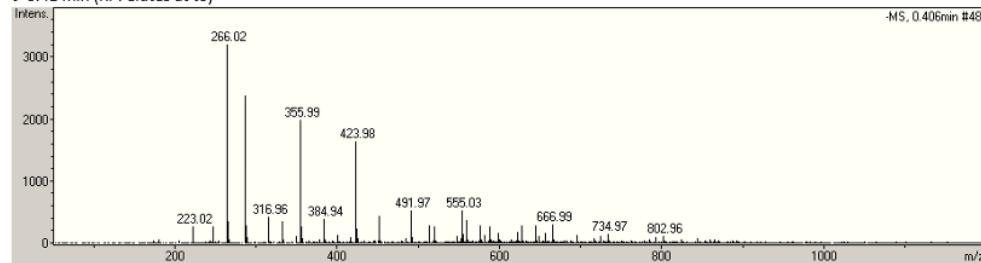
$\lambda_{\text{max}} = 324 \text{ nm; } 522 \text{ nm}$



## MASS SPECTRA

MS (negative mode)

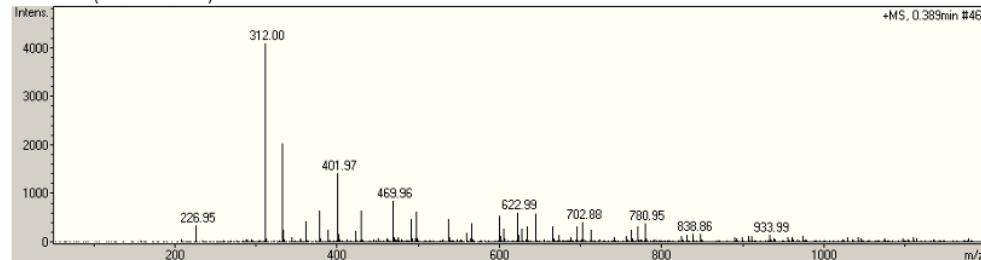
t=0.41 min (RP: elutes at t0)



m/z	I	Formula
266.02	3216	[M] <sup>-</sup>

MS (positive mode)

t=0.39 min (RP: elutes at t0)



m/z	I	Formula
312.00	3795	[M] <sup>+</sup> •2Na <sup>+</sup>

## S-8.50. Naphthol Yellow S

### GENERAL INFORMATION

**Color Index Name:** Acid Yellow 1

**Color Index Number:** 10316

**Type of dye:** Nitro

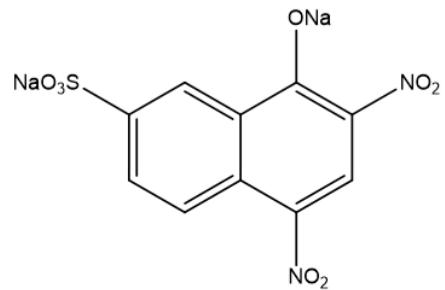
**Charge:** -1

**Molecular Formula:** C<sub>10</sub>H<sub>5</sub>N<sub>2</sub>O<sub>8</sub>S (ion, -1, replaced -ONa with -OH)

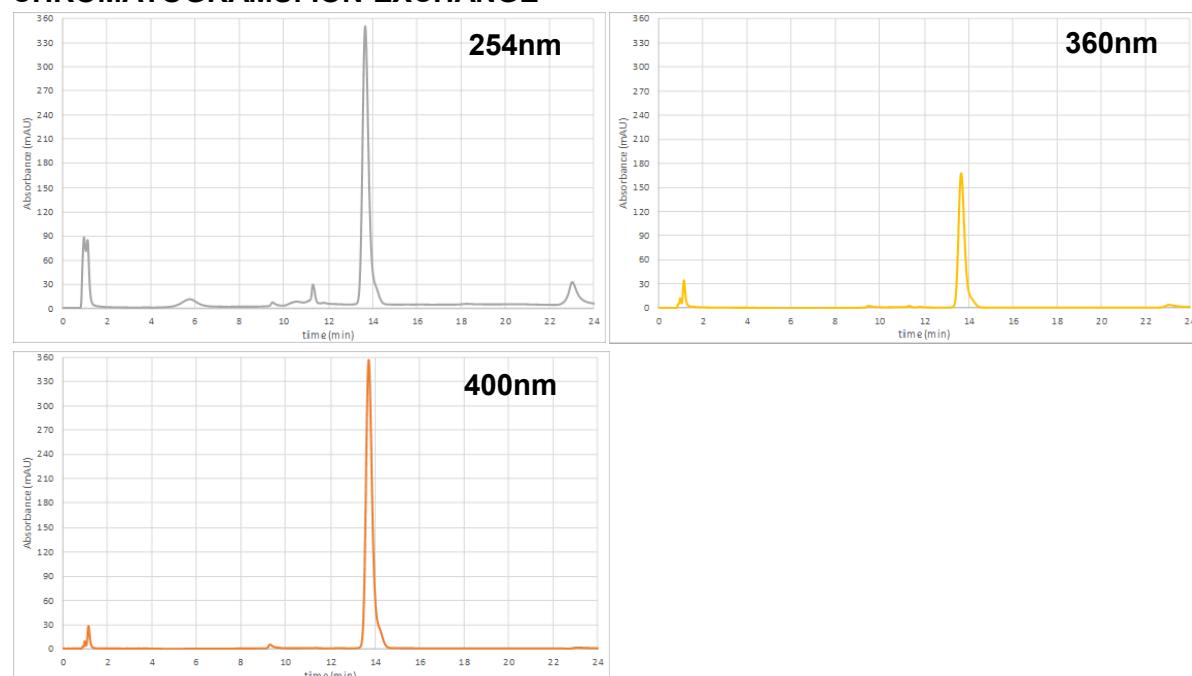
**Related dye:** Martius Yellow

**Molecular Weight**

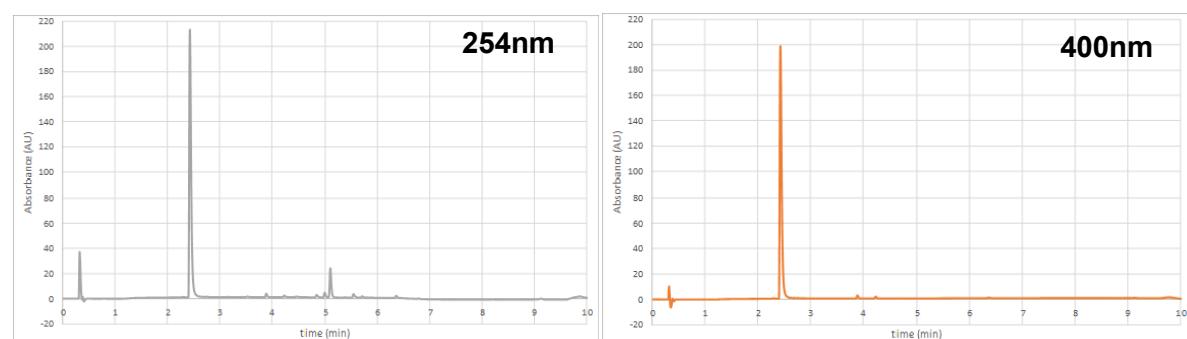
Full molecule:	358.19
Ion (-1)	313.22
Ion (-1), monoisotopic	312.98



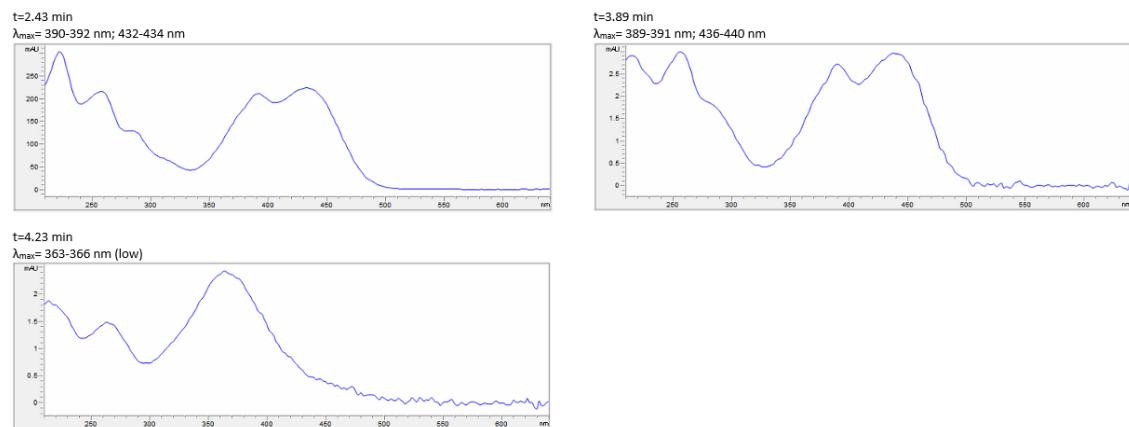
### CHROMATOGRAMS: ION-EXCHANGE



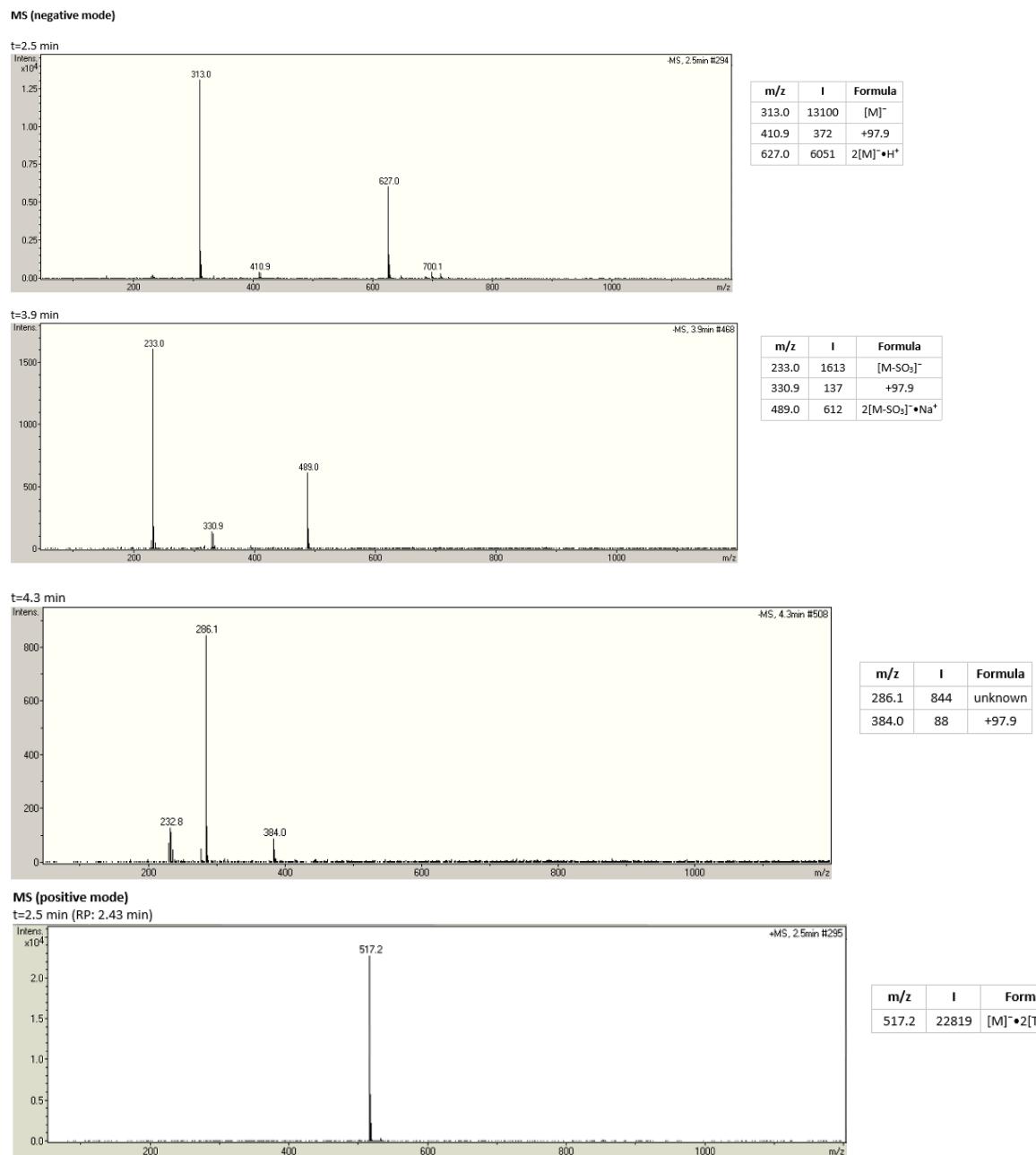
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA



## MASS SPECTRA



## S-8.51. Nigrosin

### GENERAL INFORMATION

**Color Index Name:** Acid Black 2

**Color Index Number:** 50420

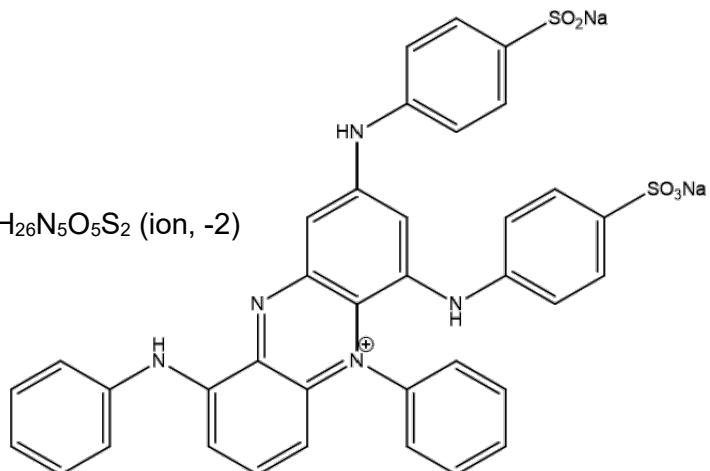
**Type of dye:** Azine

**Charge:** -2

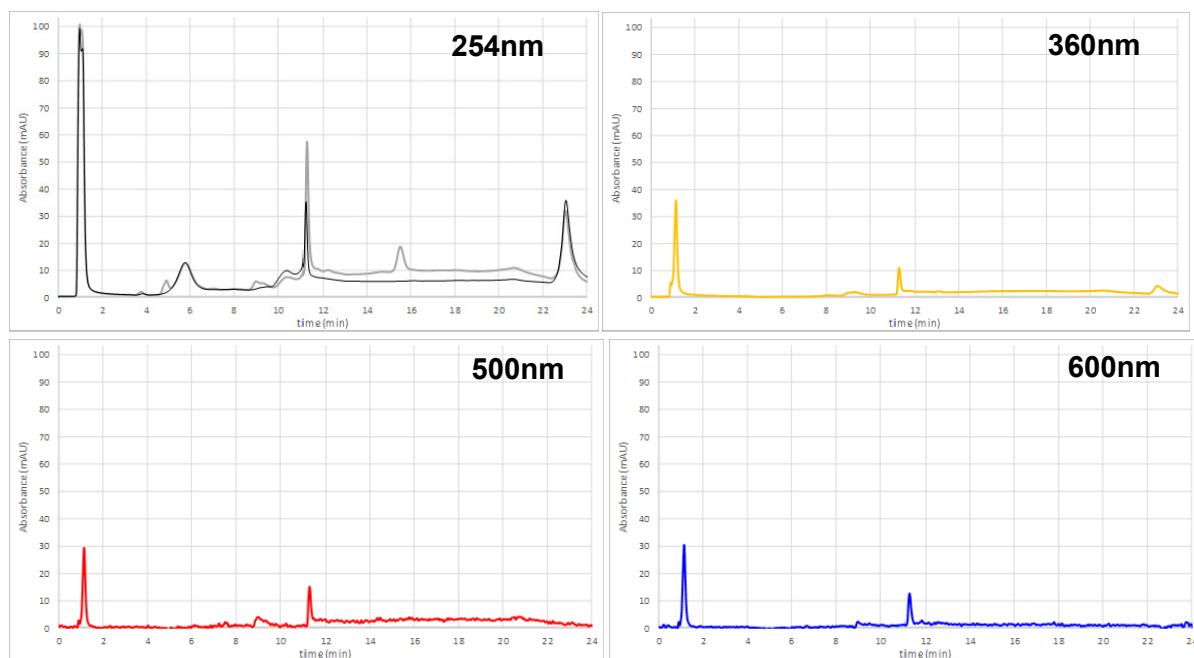
**Molecular Formula:** Complex mixture.  $C_{36}H_{26}N_5O_5S_2$  (ion, -2)

**Molecular Weight**

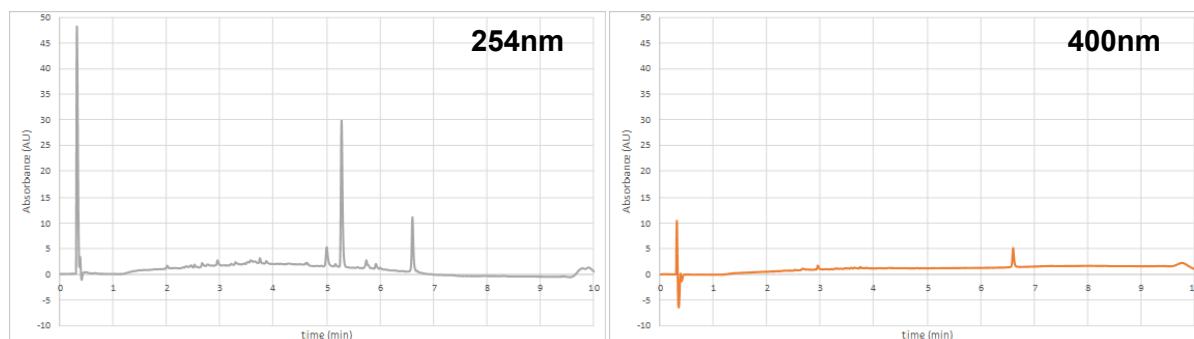
Sample molecule:	718.73
Ion (-2)	672.75
Ion (-2), monoisotopic	672.14

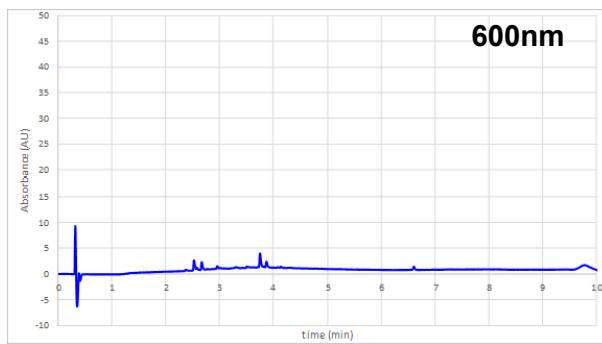


### CHROMATOGRAMS: ION-EXCHANGE



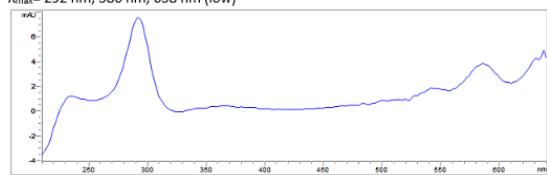
### CHROMATOGRAMS: REVERSED-PHASE



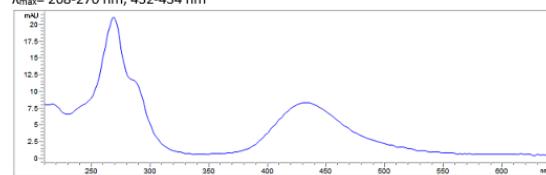


## UV-VIS SPECTRA

$t=3.76$  min  
 $\lambda_{\text{max}}=292$  nm; 586 nm; 638 nm (low)



$t=6.60$  min  
 $\lambda_{\text{max}}=268-270$  nm; 432-434 nm



Peak at 3.76 min is most likely nigrosine.

## MASS SPECTRA

No peaks detected in both positive and negative mode

## S-8.52. Orange I

### GENERAL INFORMATION

**Color Index Name:** Acid Orange 20

**Color Index Number:** 14600

**Type of dye:** Monoazo

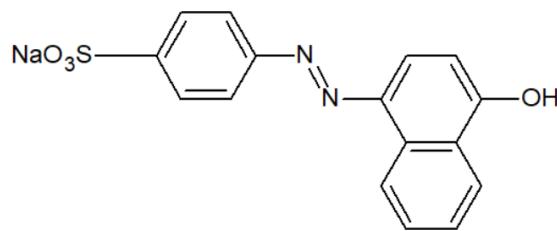
**Charge:** -1

**Molecular Formula:** C<sub>16</sub>H<sub>11</sub>N<sub>2</sub>O<sub>4</sub>S (ion, -1)

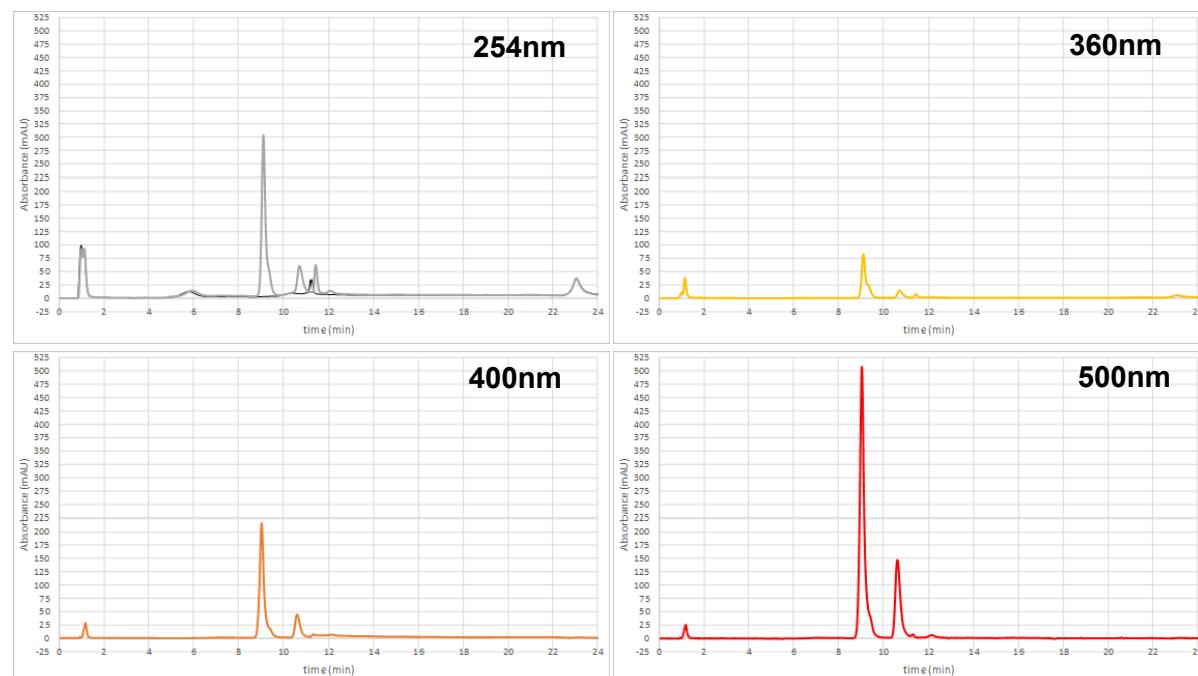
**Related dye:** Orange II

**Molecular Weight**

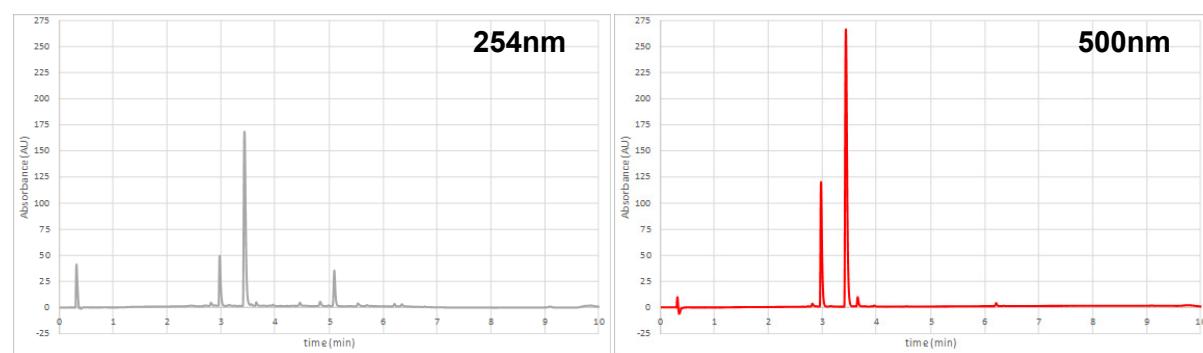
Full molecule:	350.32
Ion (-1)	327.34
Ion (-1), monoisotopic	327.04



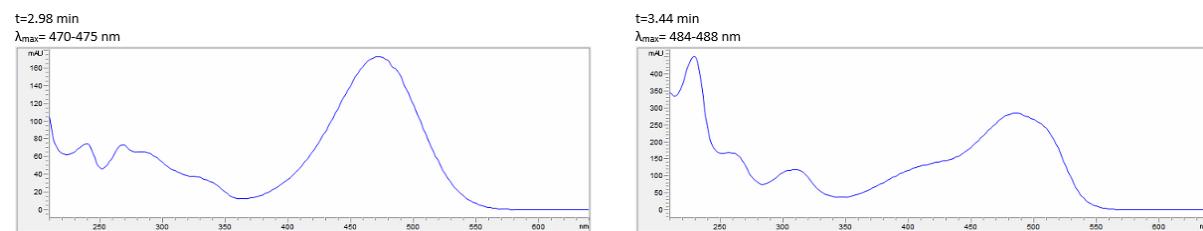
### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

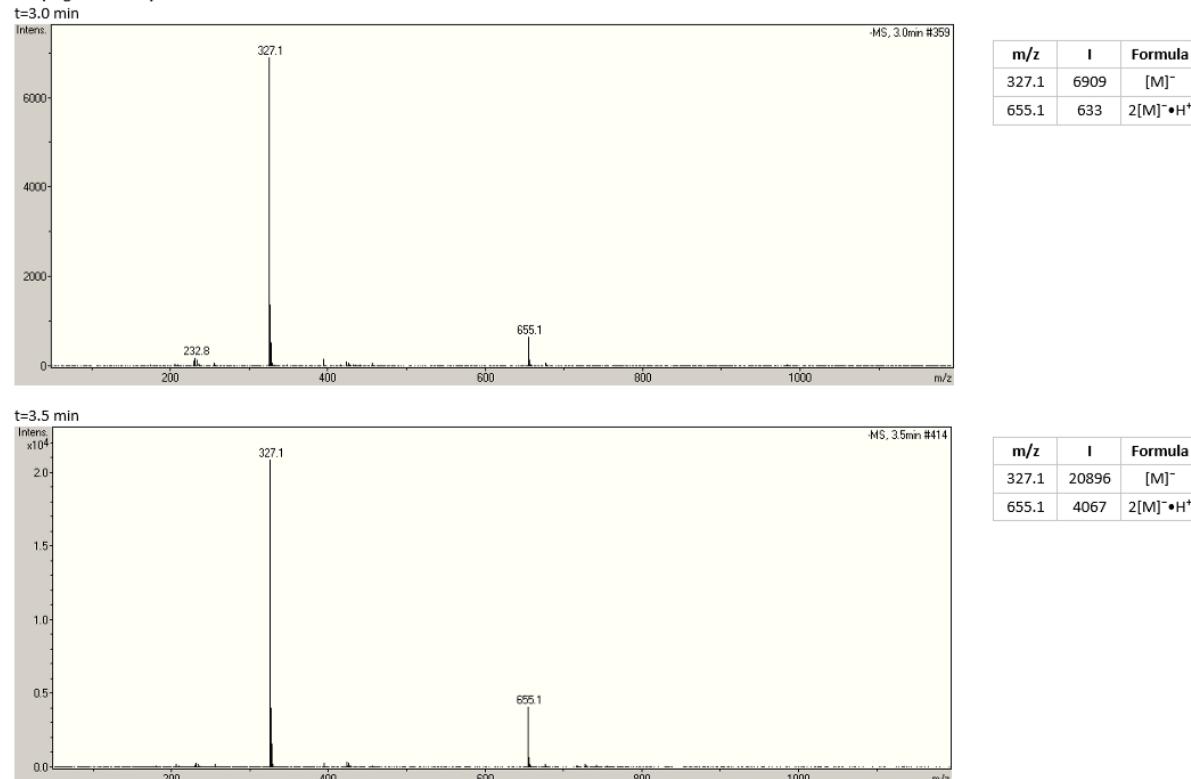


## UV-VIS SPECTRA

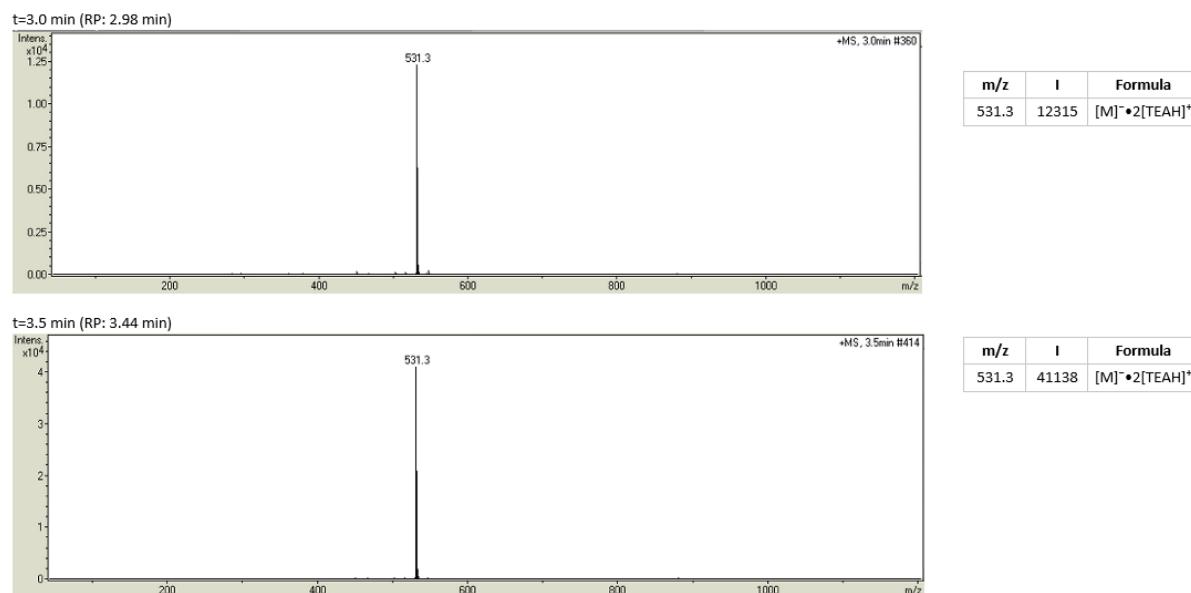


## MASS SPECTRA

### MS (negative mode)



### MS (positive mode)



### S-8.53. Orange II

#### GENERAL INFORMATION

Alternative names: Tropaeolin OOO

Color Index Name: Acid Orange 7

Color Index Number: 15510

Type of dye: Monoazo; Anthraquinone

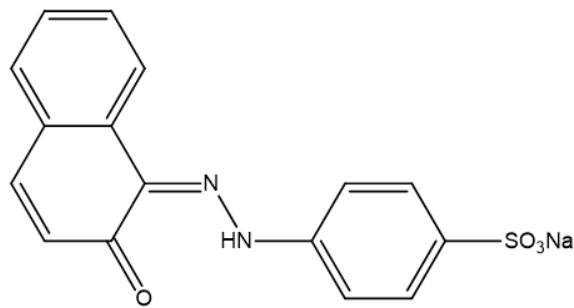
Charge: -1

Molecular Formula: C<sub>16</sub>H<sub>11</sub>N<sub>2</sub>O<sub>4</sub>S (ion, -1)

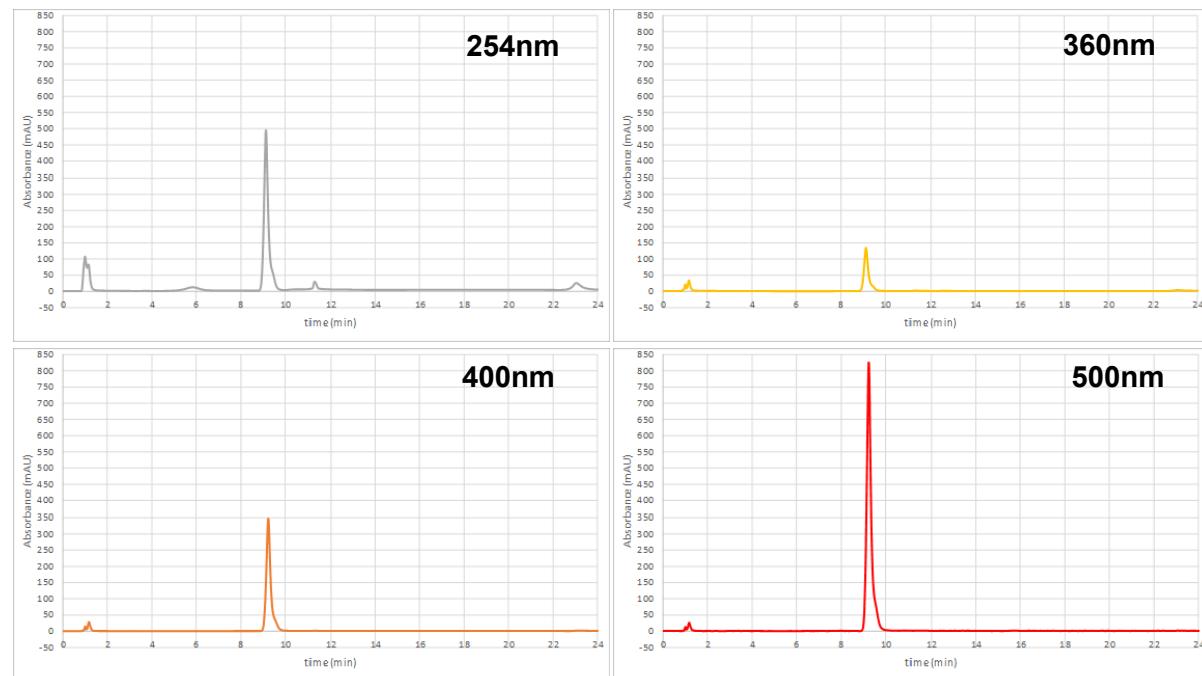
Related Dye: Orange I

#### Molecular Weight

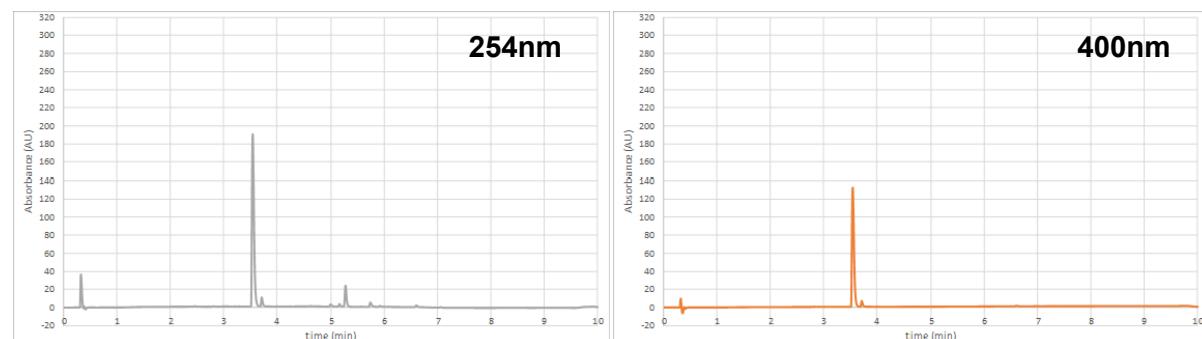
Full molecule:	350.32
Ion (-1)	327.34
Ion (-1), monoisotopic	327.04

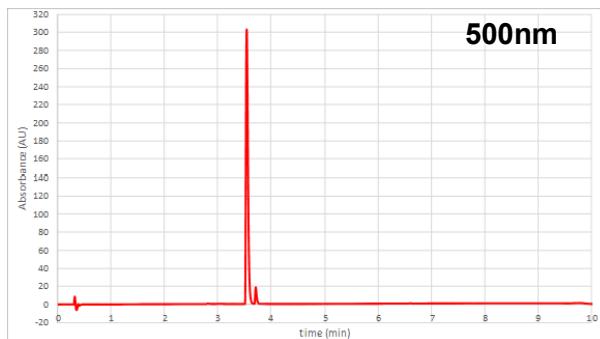


#### CHROMATOGRAMS: ION-EXCHANGE



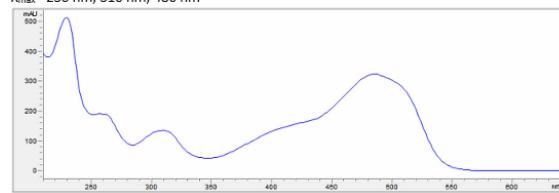
#### CHROMATOGRAMS: REVERSED-PHASE



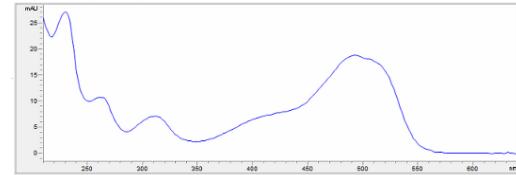


## UV-VIS SPECTRA

$t=3.54$  min  
 $\lambda_{\text{max}}= 230 \text{ nm}; 310 \text{ nm}; 486 \text{ nm}$



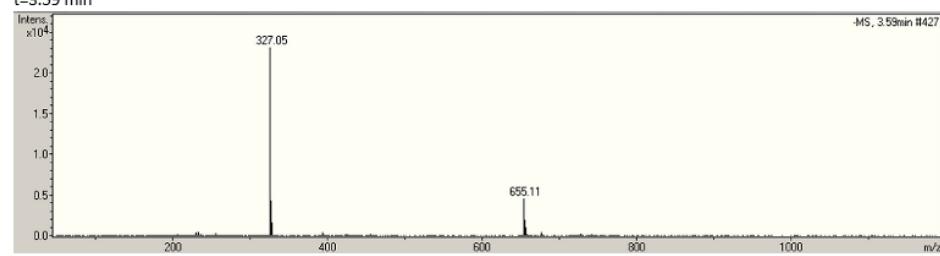
$T=3.71$  min  
 $\lambda_{\text{max}}= 230 \text{ nm}; 312 \text{ nm}; 494 \text{ nm}$



## MASS SPECTRA

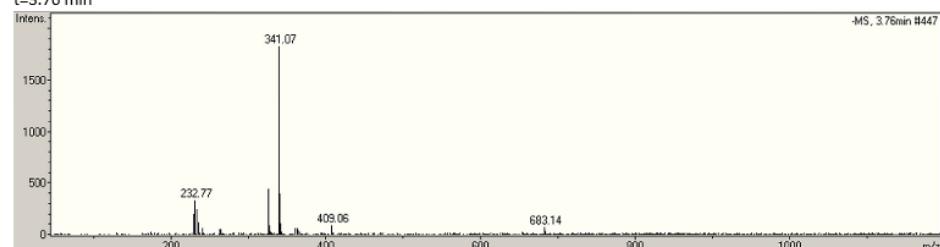
MS (negative mode)

$t=3.59$  min



$m/z$	I	Formula
327.05	23235	$[M]^-$
655.11	4518	$2[M]^- \bullet H^+$

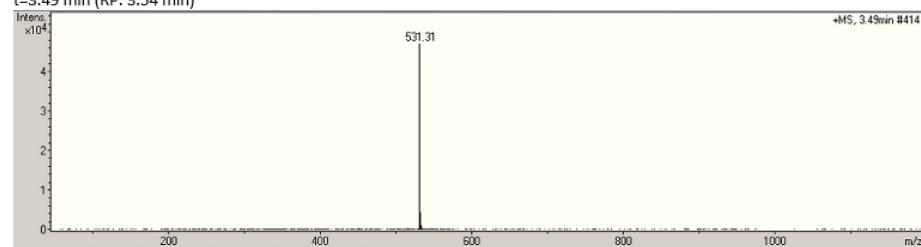
$t=3.76$  min



$m/z$	I	Formula
341.07	1829	$[M+CH_2]^-$
683.14	62	$2[M+CH_2]^- \bullet H^+$

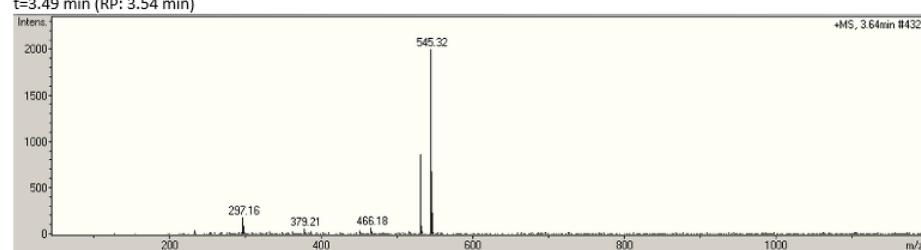
**MS (positive mode)**

t=3.49 min (RP: 3.54 min)



m/z	I	Formula
531.31	47025	$[M]^- \bullet 2[TEAH]^+$

t=3.49 min (RP: 3.54 min)



m/z	I	Formula
545.32	2005	$[M+CH_2]^- \bullet 2[TEAH]^+$

## S-8.54. Orange IV

### GENERAL INFORMATION

Alternative Name: Tropaeolin OO

Color Index Name: Acid Orange 5

Color Index Number: 13080

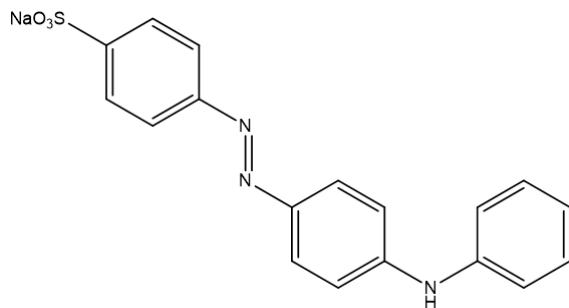
Type of dye: Monoazo

Charge: -1

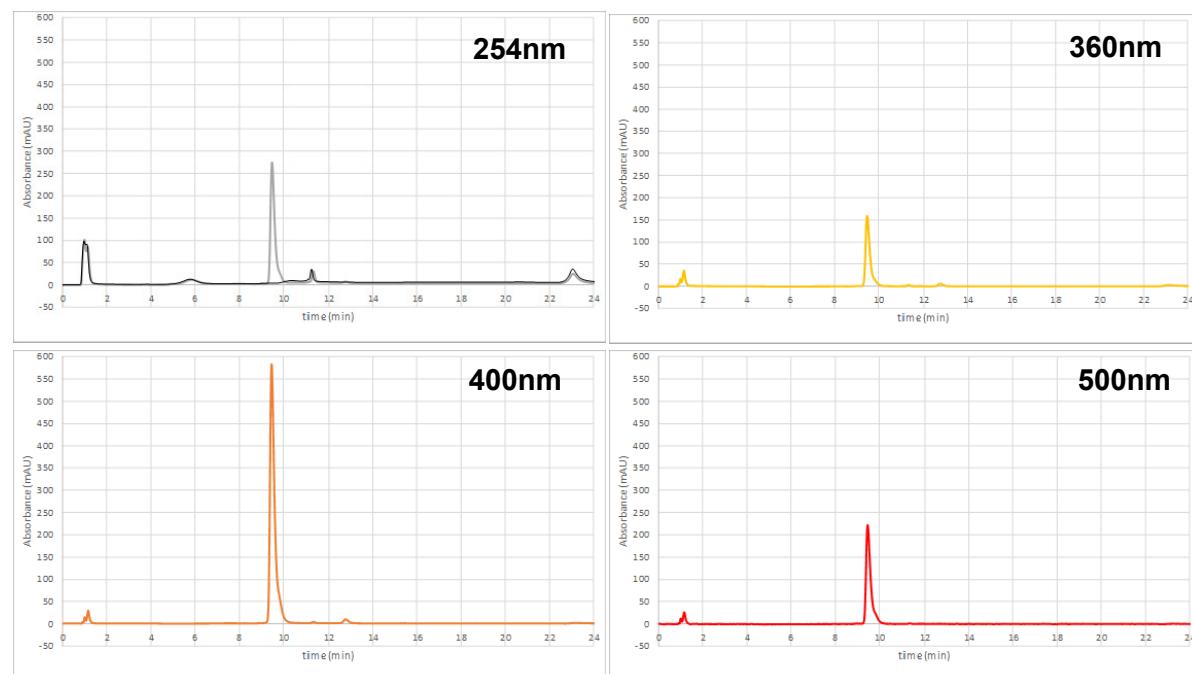
Molecular Formula: C<sub>18</sub>H<sub>14</sub>N<sub>3</sub>O<sub>3</sub>S (ion, -1)

Molecular Weight

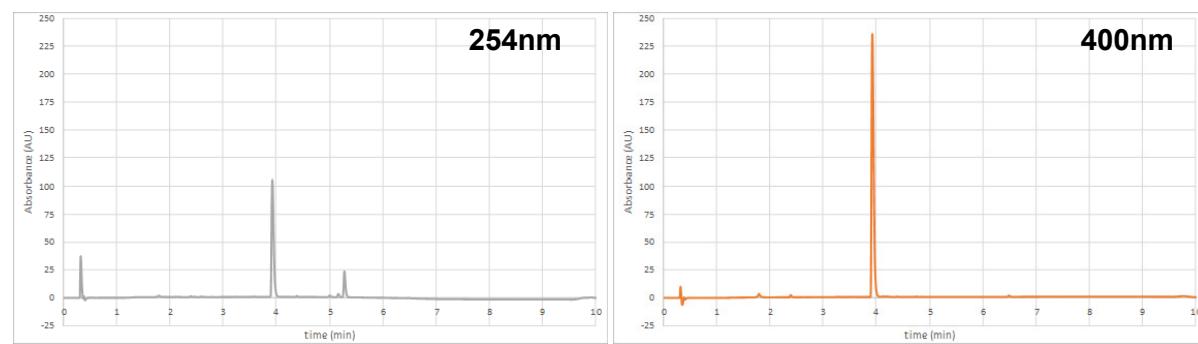
Full molecule:	375.38
Ion (-1)	352.39
Ion (-1), monoisotopic	352.08



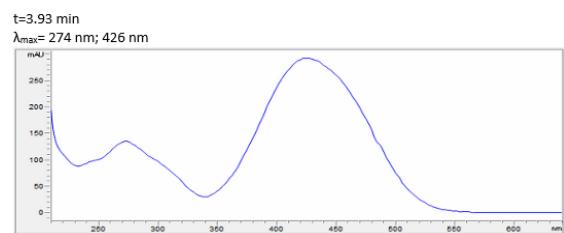
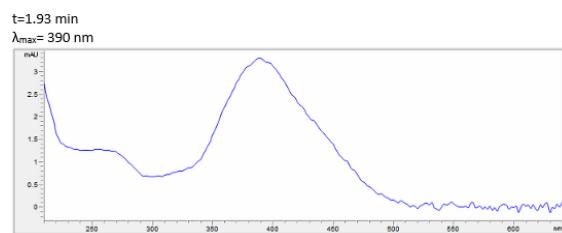
### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE



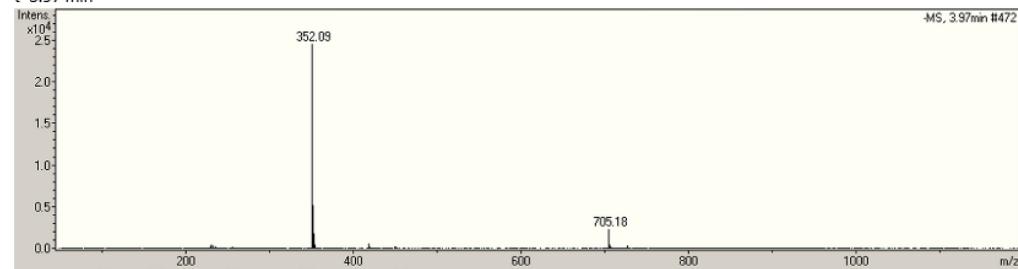
## UV-VIS SPECTRA



## MASS SPECTRA

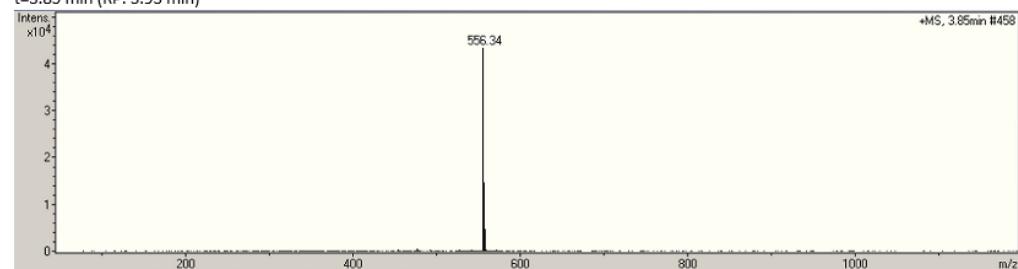
### MS (negative mode)

t=3.97 min



### MS (positive mode)

t=3.85 min (RP: 3.93 min)



## S-8.55. Orange GG

### GENERAL INFORMATION

Alternative names: Orange G

Color Index Name: Acid Orange 10

Color Index Number: 16230

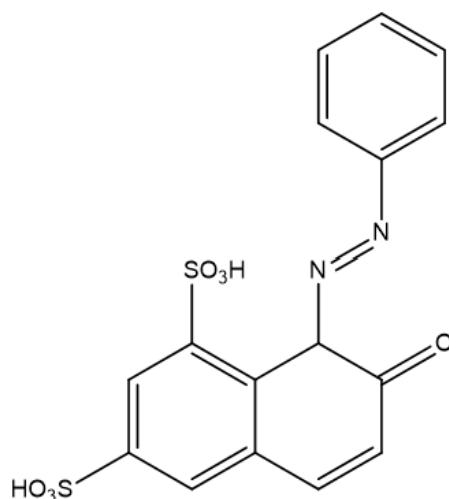
Type of dye: Monoazo

Charge: -2

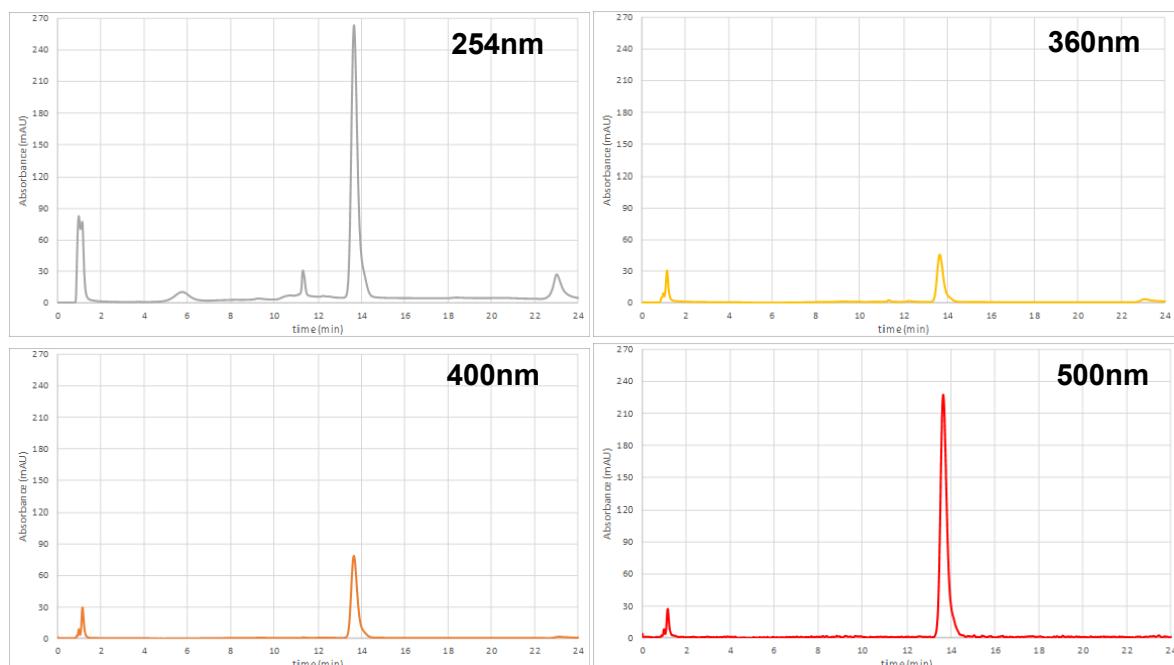
Molecular Formula: C<sub>16</sub>H<sub>10</sub>N<sub>2</sub>O<sub>7</sub>S<sub>2</sub> (ion, -2)

Molecular Weight

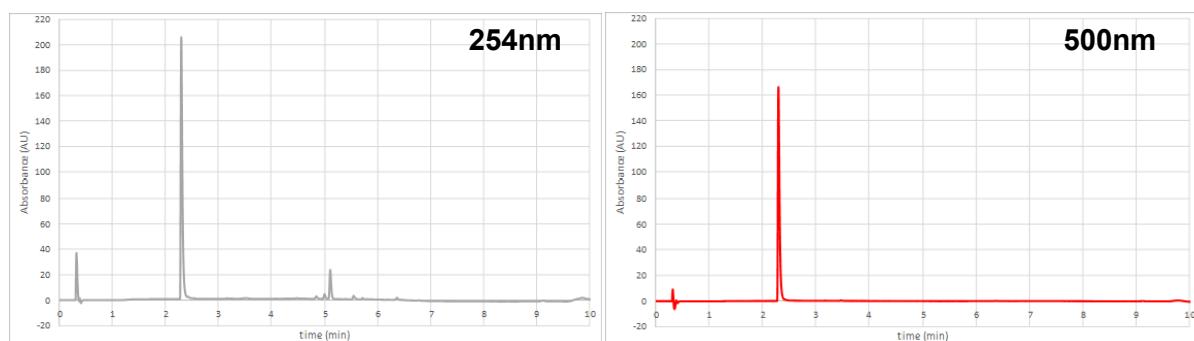
Full molecule:	452.37
Ion (-2)	406.39
Ion (-2), monoisotopic	405.99



### CHROMATOGRAMS: ION-EXCHANGE

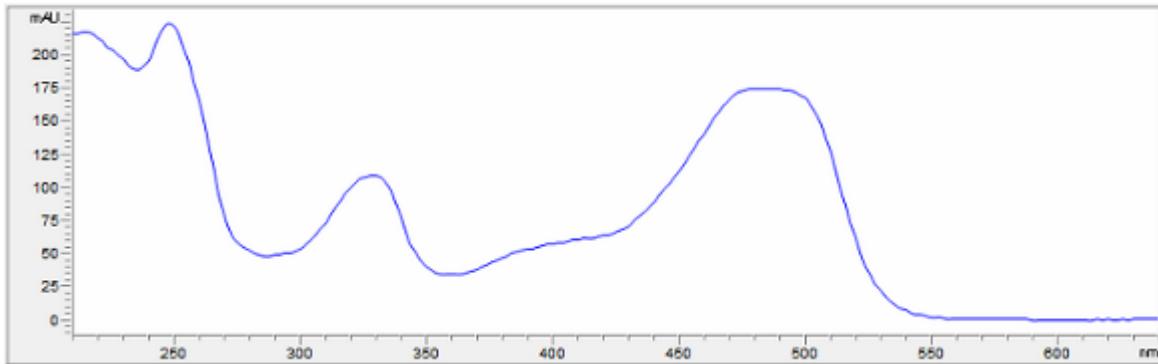


### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

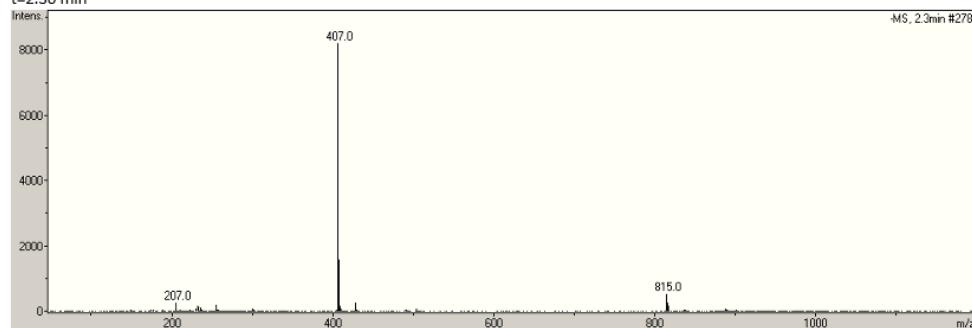
t=2.30 min  
 $\lambda_{\text{max}} = 478\text{-}490 \text{ nm}$



## MASS SPECTRA

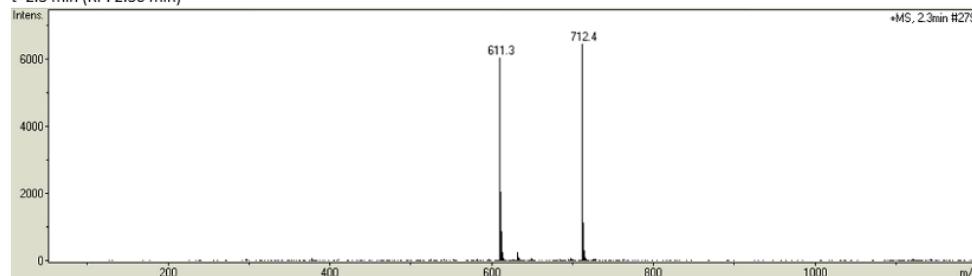
MS (negative mode)

t=2.30 min



MS (positive mode)

t=2.3 min (RP: 2.30 min)



## S-8.56. Orcein

### GENERAL INFORMATION

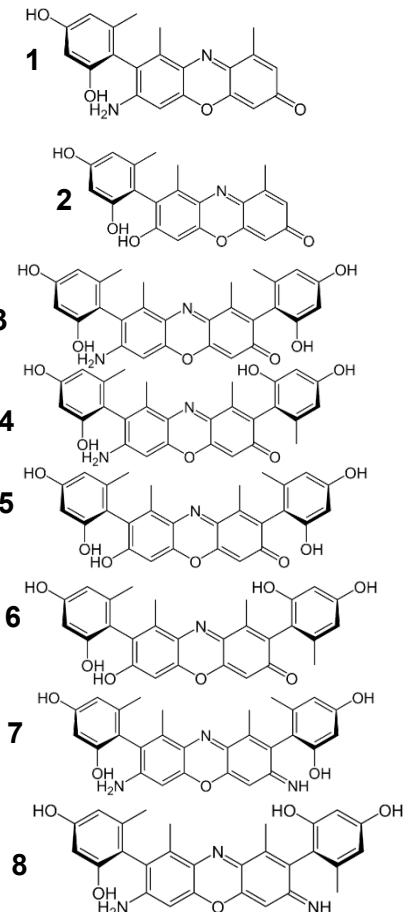
**Alternative names:** archil, orchil, lacmus

**Color Index Name:** Natural Red 28

**Color Index Number:** none

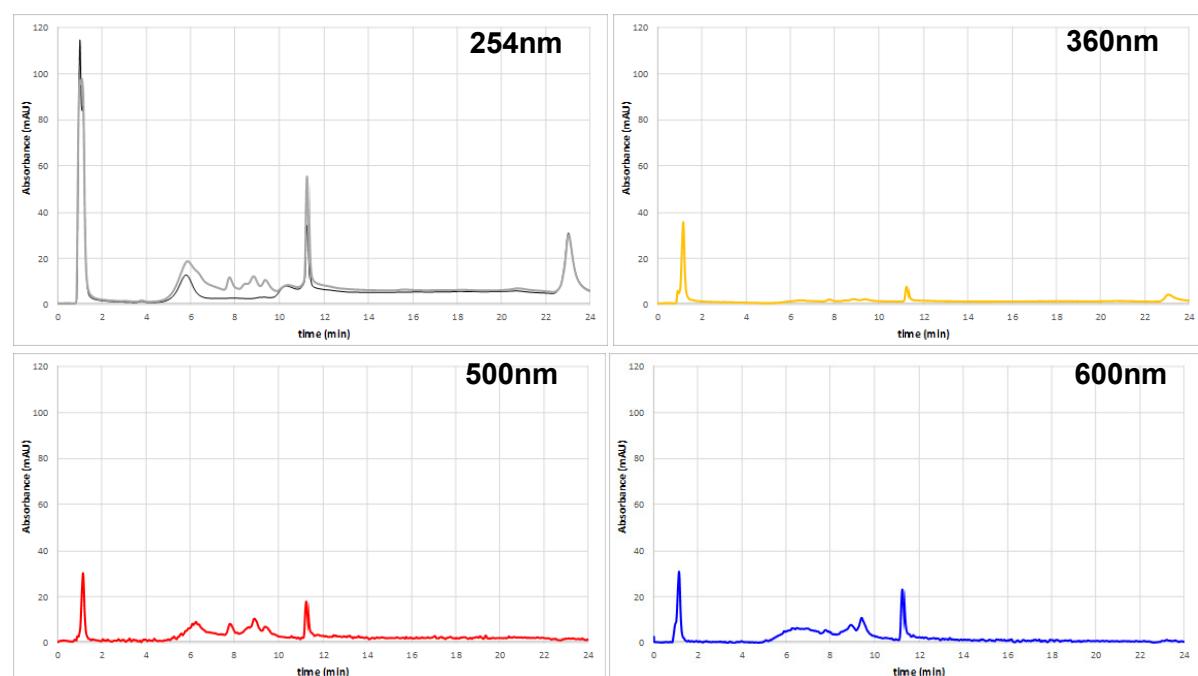
**Type of dye:** Natural

**Scientific name of biological source:** *Roccella tinctoria DC*

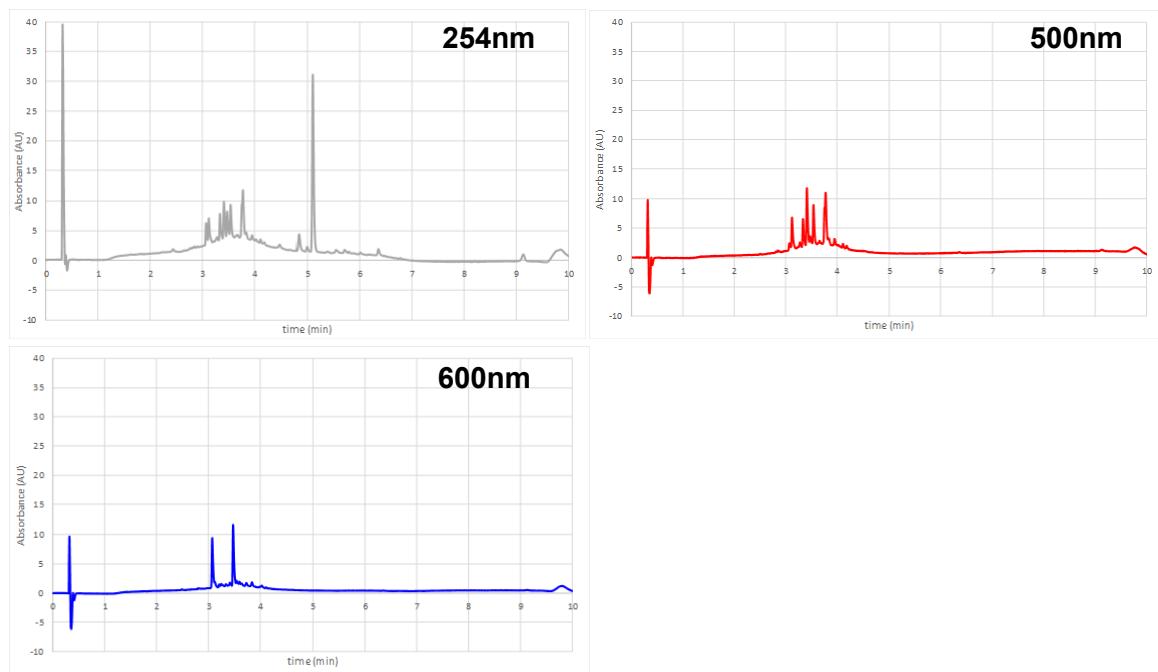


Name	#	Mw	Monoiso.	Formula	%
α-amino-orcein	1	362.38	362.13	C <sub>21</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>	10
α-hydroxy-orcein	2	363.36	363.11	C <sub>21</sub> H <sub>17</sub> NO <sub>5</sub>	10
β-amino-orcein	3	484.50	484.16	C <sub>28</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub>	6
γ-amino-orcein	4	484.50	484.16	C <sub>28</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub>	12
β-hydroxy-orcein	5	485.48	485.15	C <sub>28</sub> H <sub>23</sub> NO <sub>7</sub>	15
γ-hydroxy-orcein	6	485.48	485.15	C <sub>28</sub> H <sub>23</sub> NO <sub>7</sub>	10
β-amino-orcein-imine	7	483.51	483.18	C <sub>28</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub>	1-2
γ-amino-orcein-imine	8	483.51	483.18	C <sub>28</sub> H <sub>25</sub> N <sub>3</sub> O <sub>5</sub>	1-2

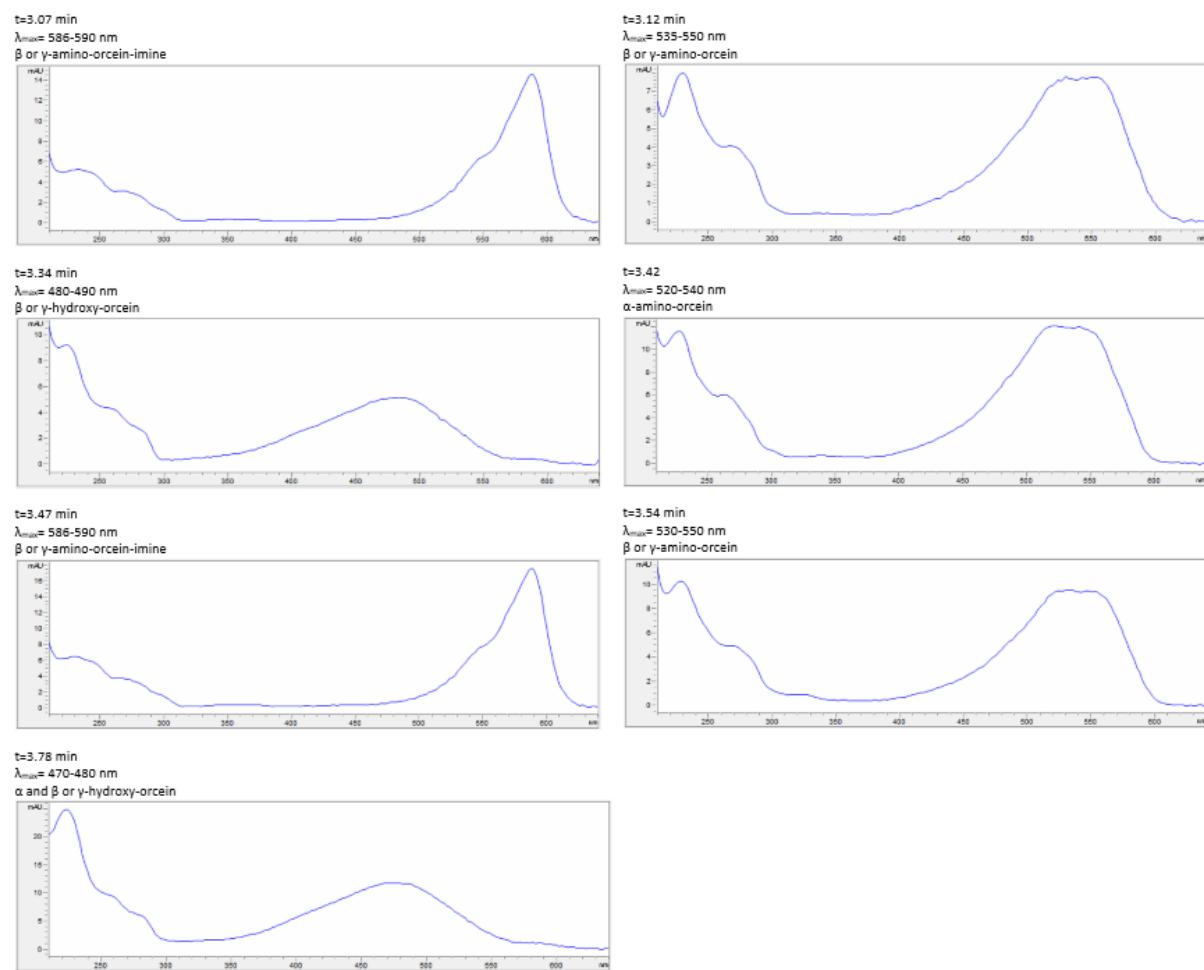
### CHROMATOGRAMS: ION-EXCHANGE



## CHROMATOGRAMS: REVERSED-PHASE



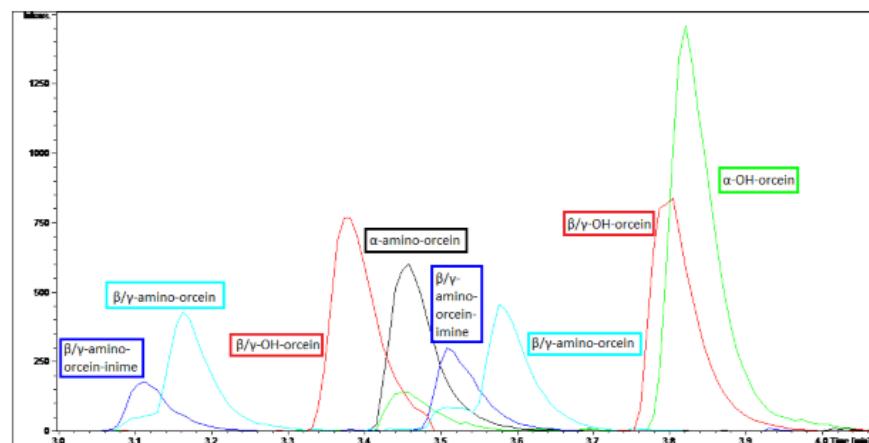
## UV-VIS SPECTRA



## MASS SPECTRA

### MS (negative mode)

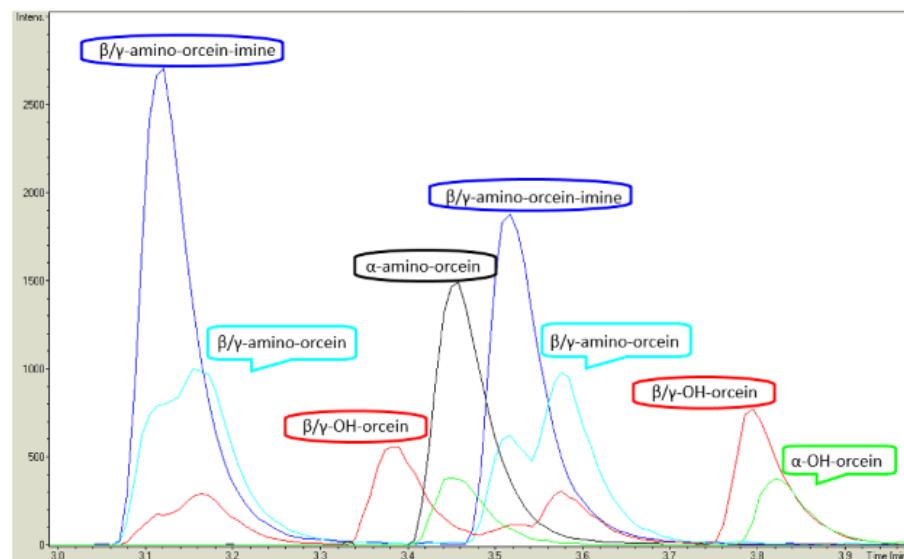
Each one of the 8 main components of the mixture has its own peak, well resolved and separated, eluting between minute 3 and 4. The pairs of  $\beta$  and  $\gamma$  isomers appear with separated peaks. However, in order to identify them, more information on their polarity is needed.



Rt	MS- peak	Intensity (-)	MS+ peak	Intensity (+)	Compound	Color	GM
3.11	482.2	177	484.2	2710	$\beta$ or $\gamma$ -amino-orcein-imine	Blue	
3.16	483.2	429	485.2	1003	$\beta$ or $\gamma$ -amino-orcein	Cyan	
3.38	484.1	719	486.2	559	$\beta$ or $\gamma$ -hydroxy-orcein	Red	
3.46	361.1	603	363.1	1494	$\alpha$ -amino-orcein	Black	
3.51	482.2	300	484.2	1880	$\beta$ or $\gamma$ -amino-orcein-imine	Blue	
3.57	483.2	458	485.2	979	$\beta$ or $\gamma$ -amino-orcein	Cyan	
3.80	484.1	841	486.2	774	$\beta$ or $\gamma$ -hydroxy-orcein	Red	
3.82	362.1	1461	364.1	375	$\alpha$ -hydroxy-orcein	Green	

### MS (positive mode)

The MS chromatogram in the positive mode looks just like the one in the negative mode, with the difference that every peak is shifted by +2 because the compounds are protonated instead of being deprotonated. The effect of proton-donor and acceptor properties of the compounds can be seen too: the imine compounds appear with the highest peaks in the positive mode, while they have the lowest peaks in the negative mode. Viceversa, the -OH compounds have the highest peaks in the negative mode and the lowest peaks in the positive mode. As for the negative mode, in the positive mode the isotopic peaks can be seen as well, and sometimes they are not well resolved from the actual compound.



### S-8.57. Patent Blue V

#### GENERAL INFORMATION

**Color Index Name:** Acid Blue 3

**Color Index Number:** 42051

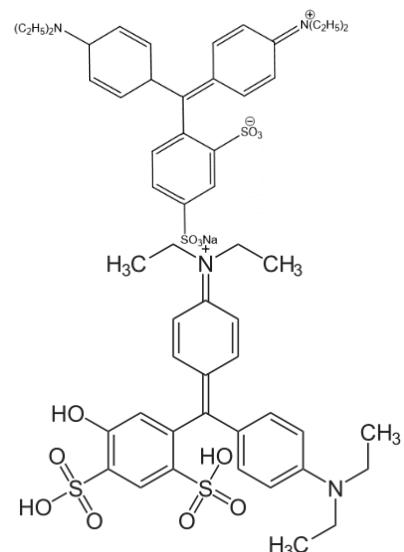
**Type of dye:** Triarylmethane

**Charge:** -2

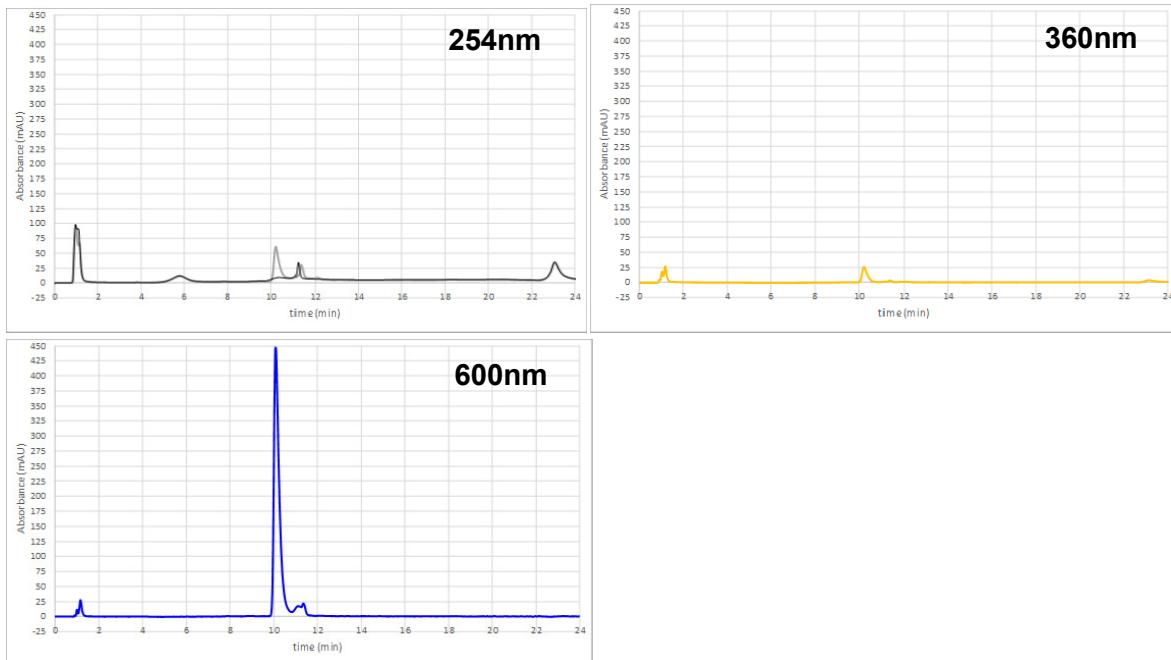
**Molecular Formula:** C<sub>27</sub>H<sub>31</sub>N<sub>2</sub>O<sub>6</sub>S<sub>2</sub> (ion, -1)

**Molecular Weight**

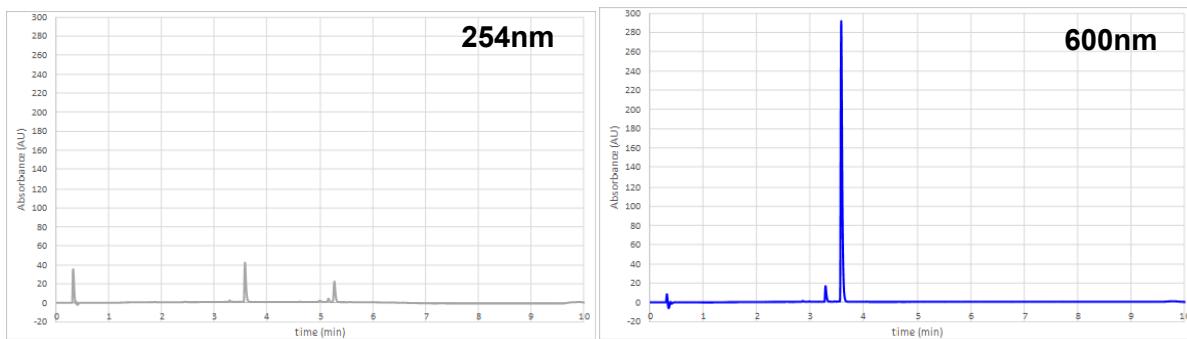
Full molecule:	566.66
Ion (-1)	543.68
Ion (-1), monoisotopic	543.16



#### CHROMATOGRAMS: ION-EXCHANGE

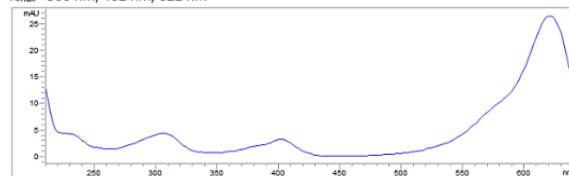


#### CHROMATOGRAMS: REVERSED-PHASE

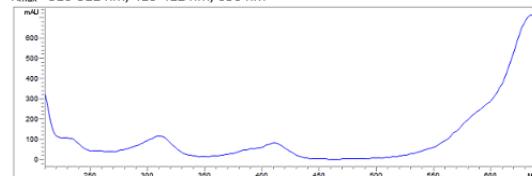


## UV-VIS SPECTRA

t=3.20 min  
 $\lambda_{\text{max}} = 306 \text{ nm}; 402 \text{ nm}; 622 \text{ nm}$



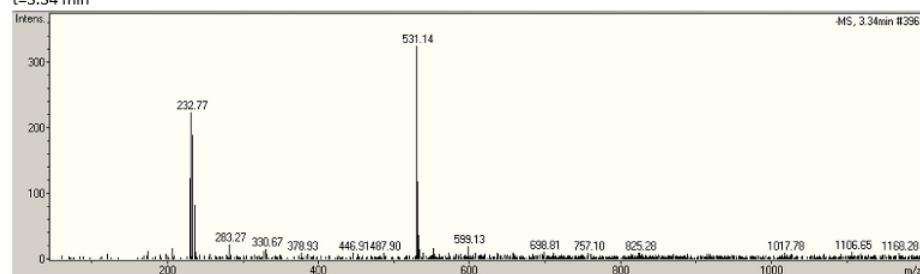
t=3.58 min  
 $\lambda_{\text{max}} = 310-312 \text{ nm}; 410-412 \text{ nm}; 636 \text{ nm}$



## MASS SPECTRA

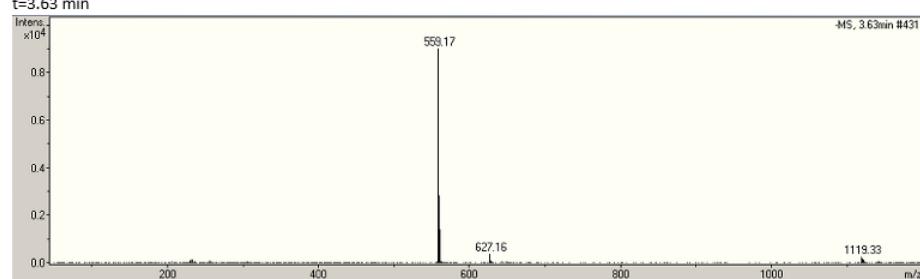
### MS (negative mode)

t=3.34 min



m/z	I	Formula
531.14	326	$[\text{M}-\text{C}_2\text{H}_4]^-$

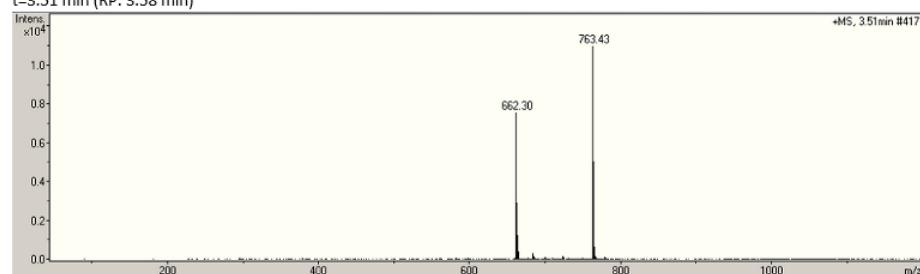
t=3.63 min



m/z	I	Formula
559.17	9013	$[\text{M}]^-$
1119.33	247	$2[\text{M}]^- \bullet \text{H}^+$

### MS (positive mode)

t=3.51 min (RP: 3.58 min)



m/z	I	Formula
662.30	7553	$[\text{MH}] \bullet [\text{TEAH}]^+$
763.43	11011	$[\text{M}]^- \bullet 2[\text{TEAH}]^+$

## S-8.58. Picric Acid

### GENERAL INFORMATION

**Alternative names:** 2,4,6-trinitrophenol (TNP)

**Color Index Name:** Acid Yellow

**Color Index Number:** 10305

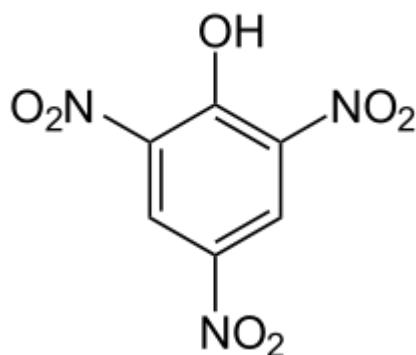
**Type of dye:** Nitro dye

**Charge:** 0

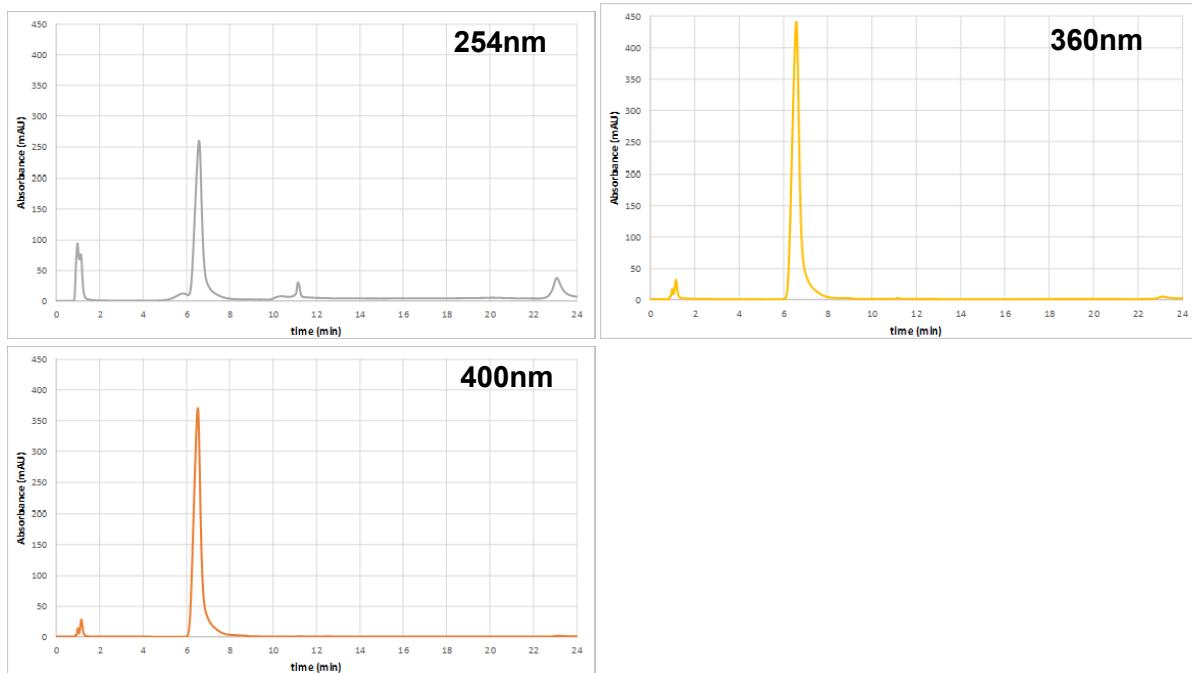
**Molecular Formula:** C<sub>6</sub>H<sub>3</sub>N<sub>3</sub>O<sub>7</sub>

**Molecular Weight**

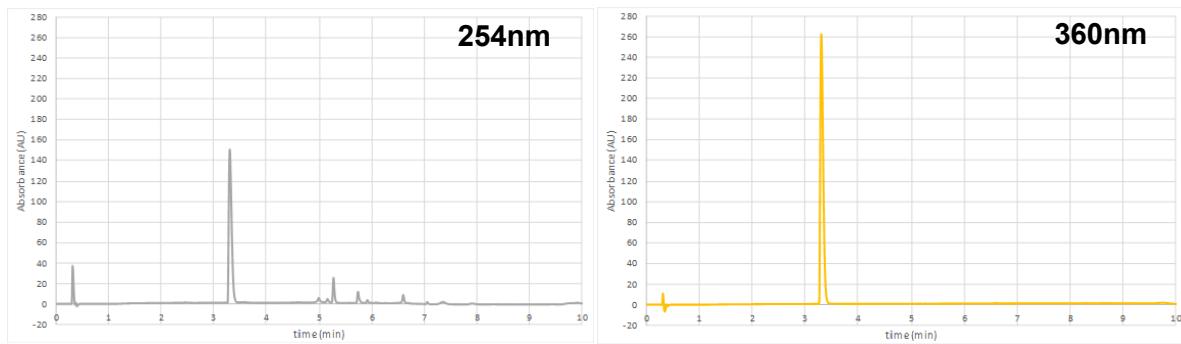
Full molecule:	229.10
Monoisotopic	229.00

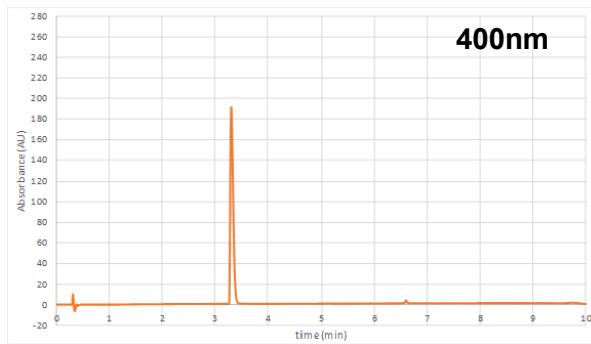


### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

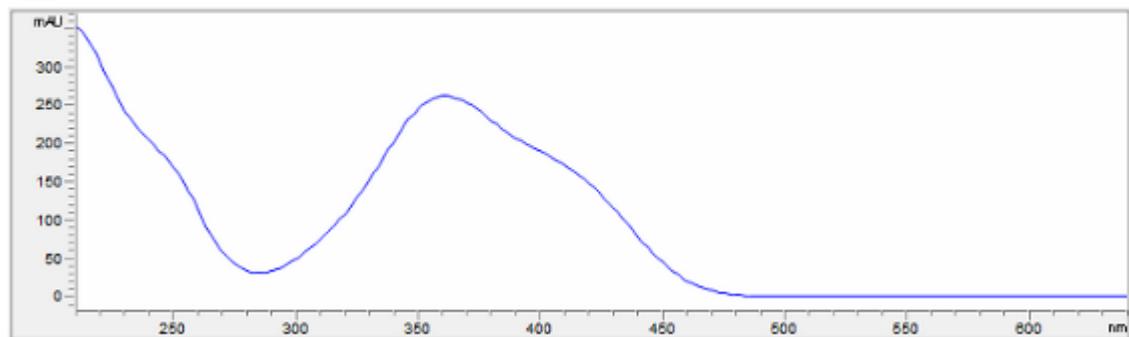




## UV-VIS SPECTRA

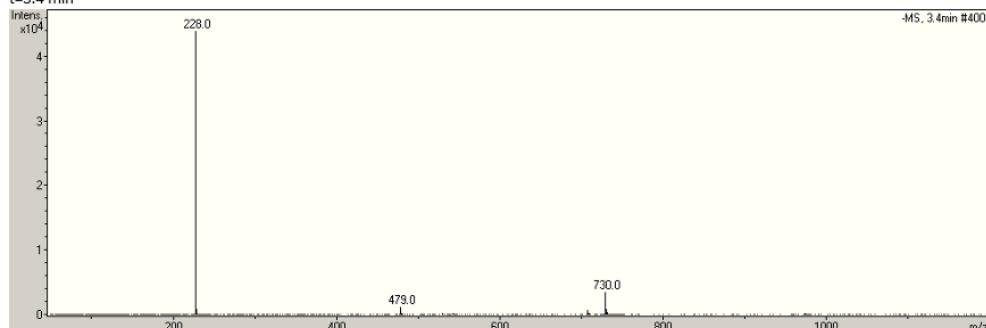
$t=3.34$  min

$\lambda_{\text{max}} = 360-362$  nm



## MASS SPECTRA

$t=3.4$  min



$m/z$	I	Formula
228.0	43989	$[M]^-$
479.0	1053	$2[M]^- \bullet Na^+$
730.0	3381	$3[M]^- \bullet 2Na^+$

## S-8.59. Ponceau 3RO

### GENERAL INFORMATION

**Color Index Name:** Acid Red 25

**Color Index Number:** 16050

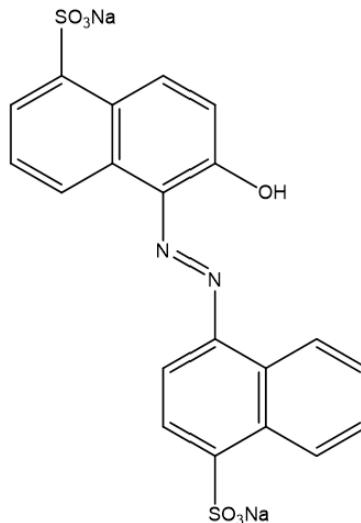
**Type of dye:** Monoazo

**Charge:** -2

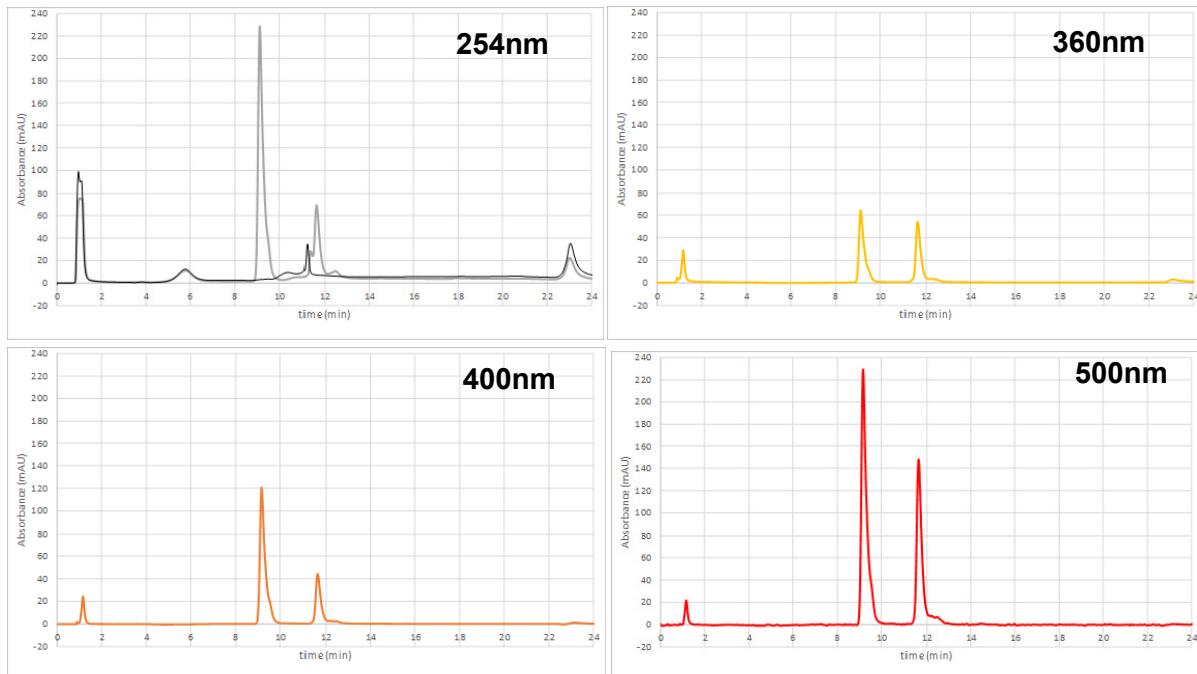
**Molecular Formula:** C<sub>20</sub>H<sub>12</sub>N<sub>2</sub>O<sub>7</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

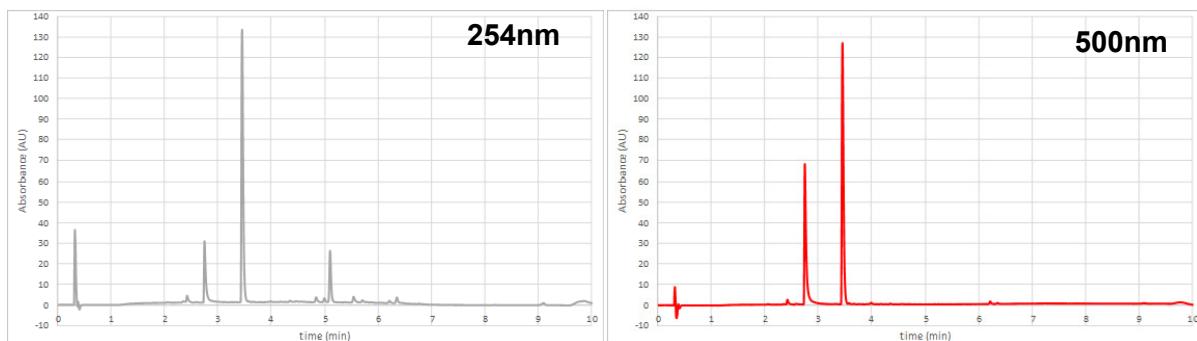
Full molecule:	502.43
Ion (-2)	456.45
Ion (-2), monoisotopic	456.01



### CHROMATOGRAMS: ION-EXCHANGE

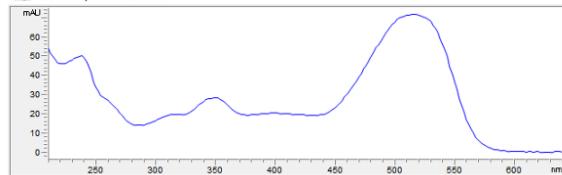


### CHROMATOGRAMS: REVERSED-PHASE

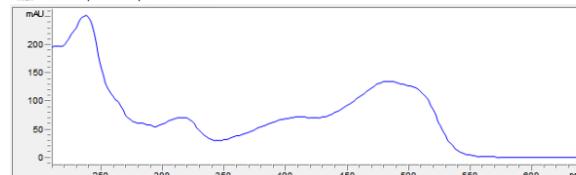


## UV-VIS SPECTRA

t=2.75 min  
 $\lambda_{\text{max}} = 350 \text{ nm}; 514-516 \text{ nm}$



t=3.46 min  
 $\lambda_{\text{max}} = 238 \text{ nm}; 316 \text{ nm}; 482-486 \text{ nm}$

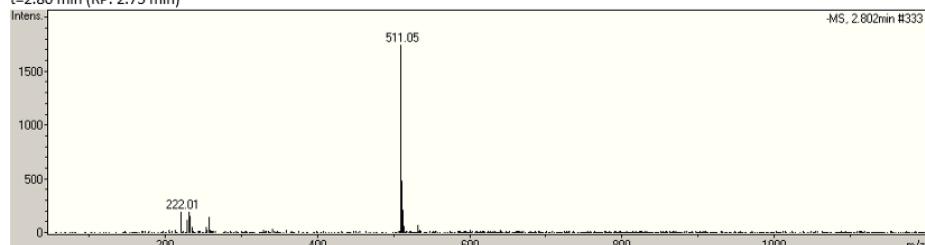


## MASS SPECTRA

The main component was not detected

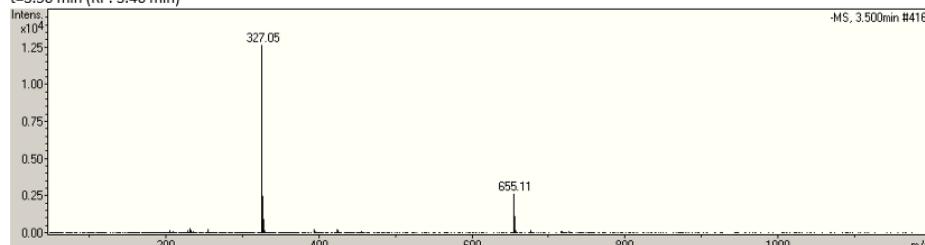
MS (negative mode)

t=2.80 min (RP: 2.75 min)



m/z	I	Formula
511.05	1751	[unknown] <sup>-</sup>

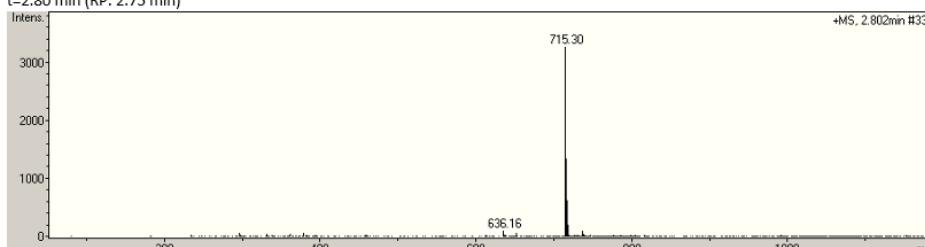
t=3.50 min (RP: 3.46 min)



m/z	I	Formula
327.05	12703	[COG] <sup>-</sup>
655.11	2635	2[COG] <sup>-</sup> •H <sup>+</sup>

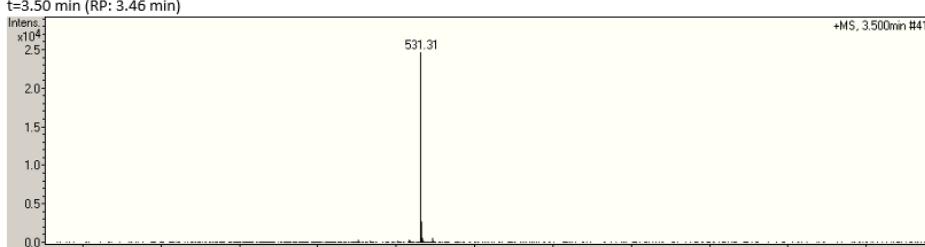
MS (positive mode)

t=2.80 min (RP: 2.75 min)



m/z	I	Formula
715.30	3274	[unknown] <sup>-</sup> •2[TEAH] <sup>+</sup>

t=3.50 min (RP: 3.46 min)



m/z	I	Formula
531.31	24274	[COG] <sup>-</sup> •2[TEAH] <sup>+</sup>

## S-8.60. Ponceau RR

### GENERAL INFORMATION

**Alternative names:** Scarlet RR

**Color Index Name:** Acid Red 26

**Color Index Number:** 16150

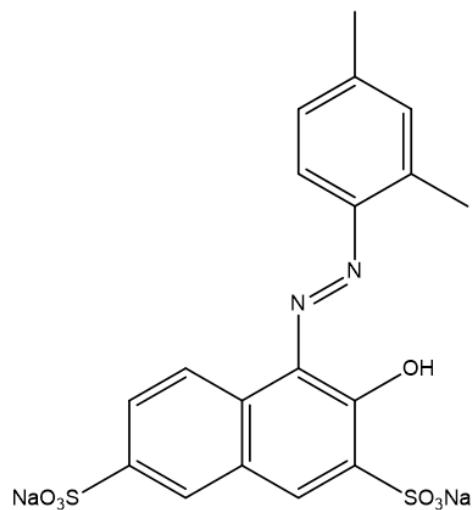
**Type of dye:** Monoazo

**Charge:** -2

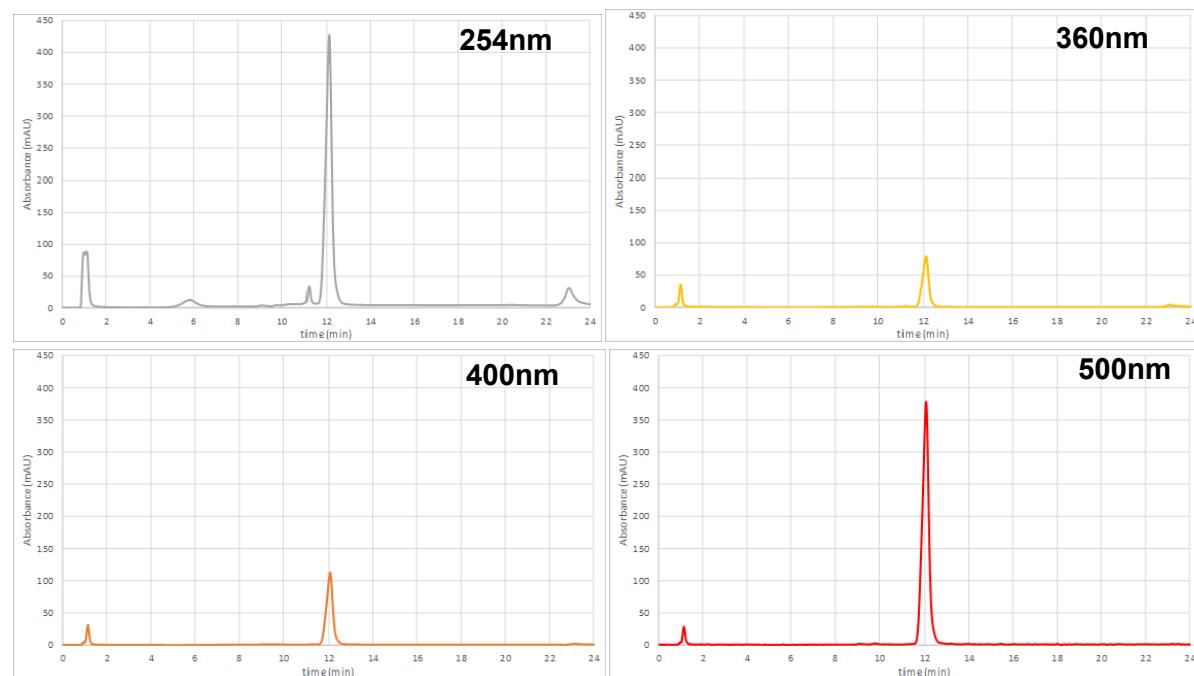
**Molecular Formula:** C<sub>18</sub>H<sub>14</sub>N<sub>2</sub>O<sub>7</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

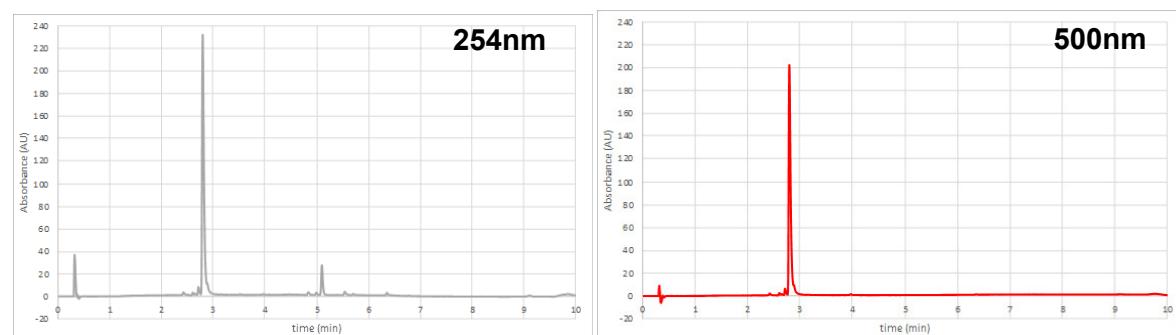
Full molecule:	480.42
Ion (-2)	434.44
Ion (-2), monoisotopic	434.03



### CHROMATOGRAMS: ION-EXCHANGE

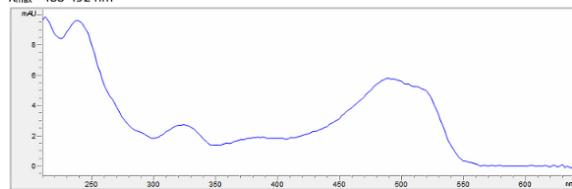


### CHROMATOGRAMS: REVERSED-PHASE

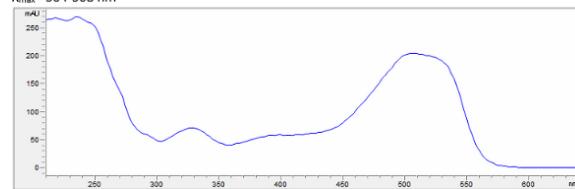


## UV-VIS SPECTRA

t=2.72 min  
 $\lambda_{\text{max}} = 488\text{-}492 \text{ nm}$



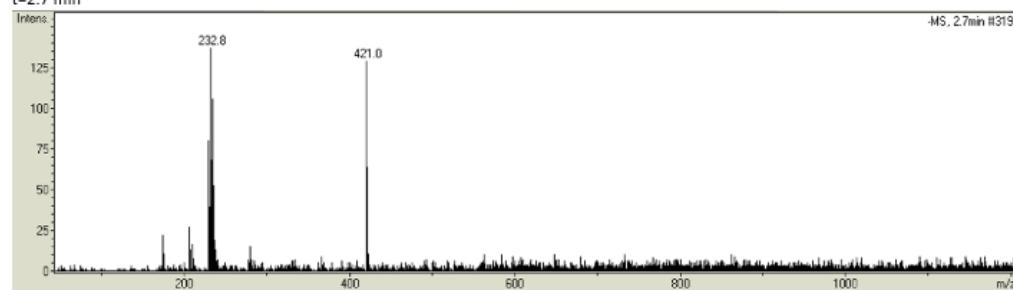
t=2.80 min  
 $\lambda_{\text{max}} = 504\text{-}508 \text{ nm}$



## MASS SPECTRA

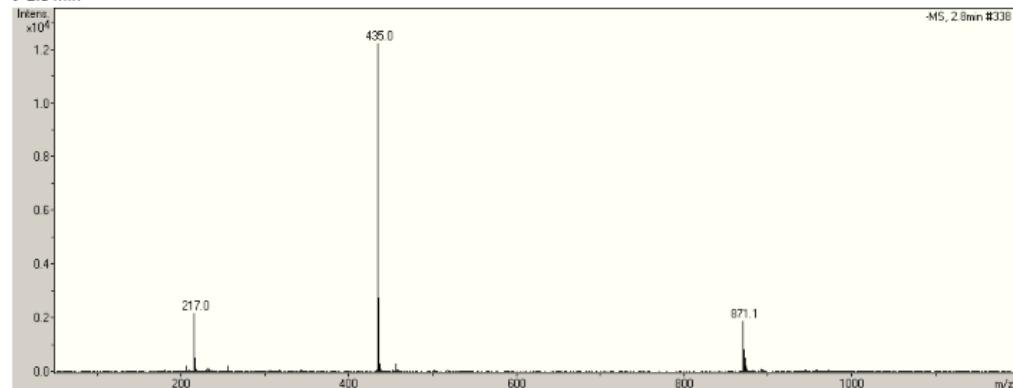
### MS (negative mode)

t=2.7 min



m/z	I	Formula
421.0	127	$[\text{MH}-\text{CH}_3]^-$

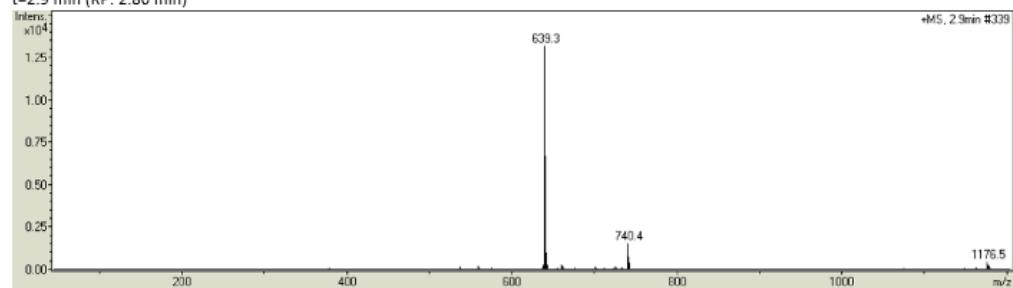
t=2.8 min



m/z	I	Formula
217.0	2146	$[\text{M}]^{2-}$
435.0	12240	$[\text{MH}]^-$
457.0	248	$[\text{M}]^{2-}\bullet\text{Na}^+$
871.1	1842	$2[\text{MH}]^- \bullet \text{H}^+$

### MS (positive mode)

t=2.9 min (RP: 2.80 min)



m/z	I	Formula
639.3	13235	$[\text{MH}]^- \bullet 2[\text{TEAH}]^*$
740.4	1511	$[\text{M}]^{2-} \bullet 3[\text{TEAH}]^*$
1176.5	403	$2[\text{MH}]^- \bullet 3[\text{TEAH}]^*$

## S-8.61. Purpurin

### GENERAL INFORMATION

**Alternative names:** Rose madder

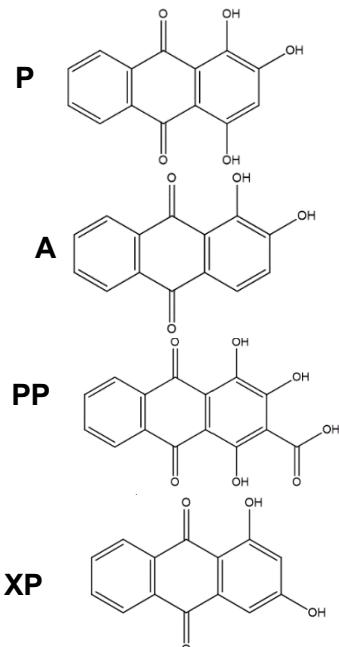
**Color Index Name:** Natural Red 8

**Color Index Number:** 58205; 75330; 75410; 75340

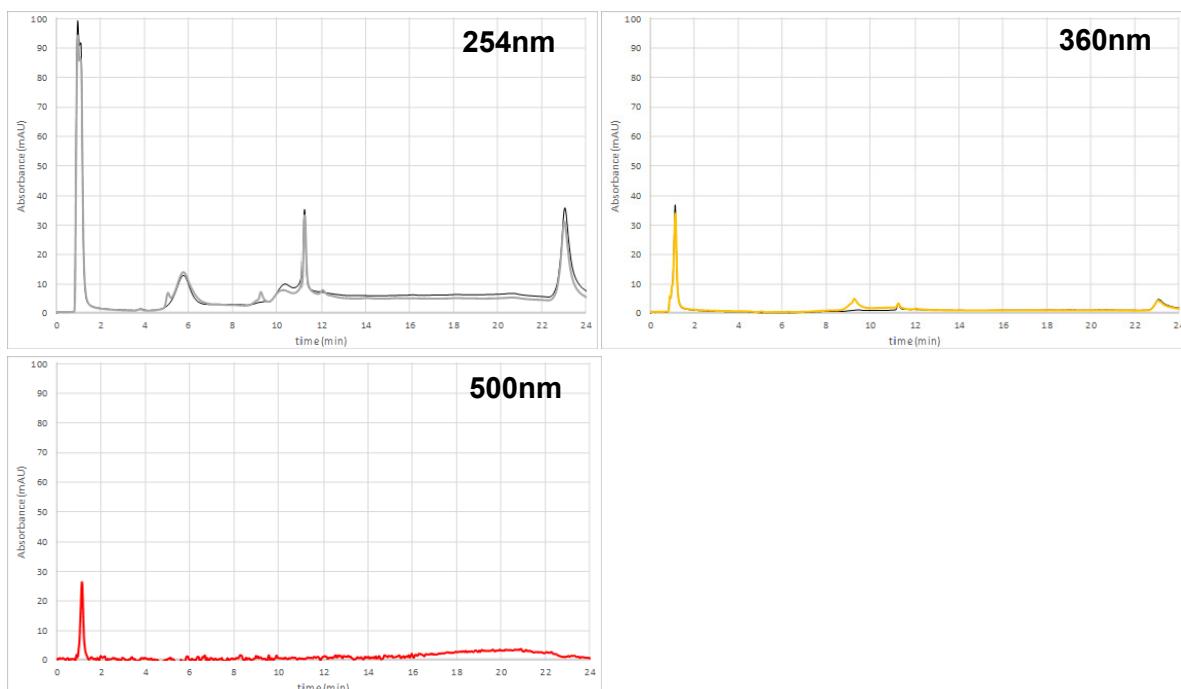
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Rubia tinctorum L.*

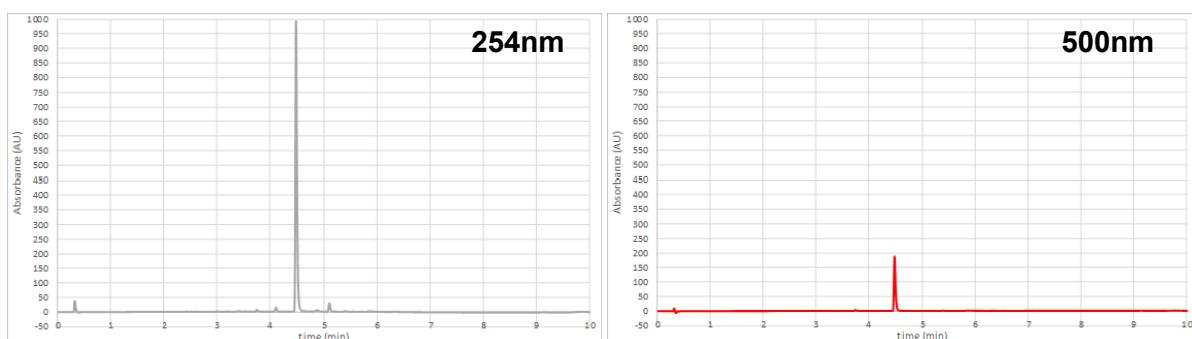
Name	Short	Mw	monoisotopic	Formula
Purpurin	[P]	256.21	256.04	C <sub>14</sub> H <sub>8</sub> O <sub>5</sub>
Alizarin	[A]	240.21	240.04	C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>
Pseudo-Purpurin	[PP]	300.22	300.03	C <sub>15</sub> H <sub>8</sub> O <sub>7</sub>
Xantho-Purpurin	[XP]	240.21	240.04	C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>



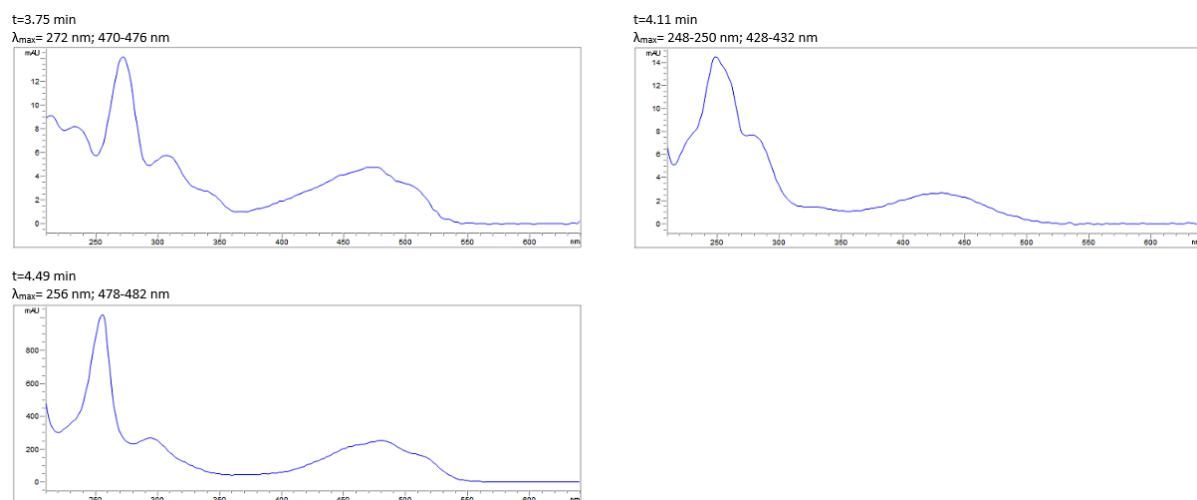
### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

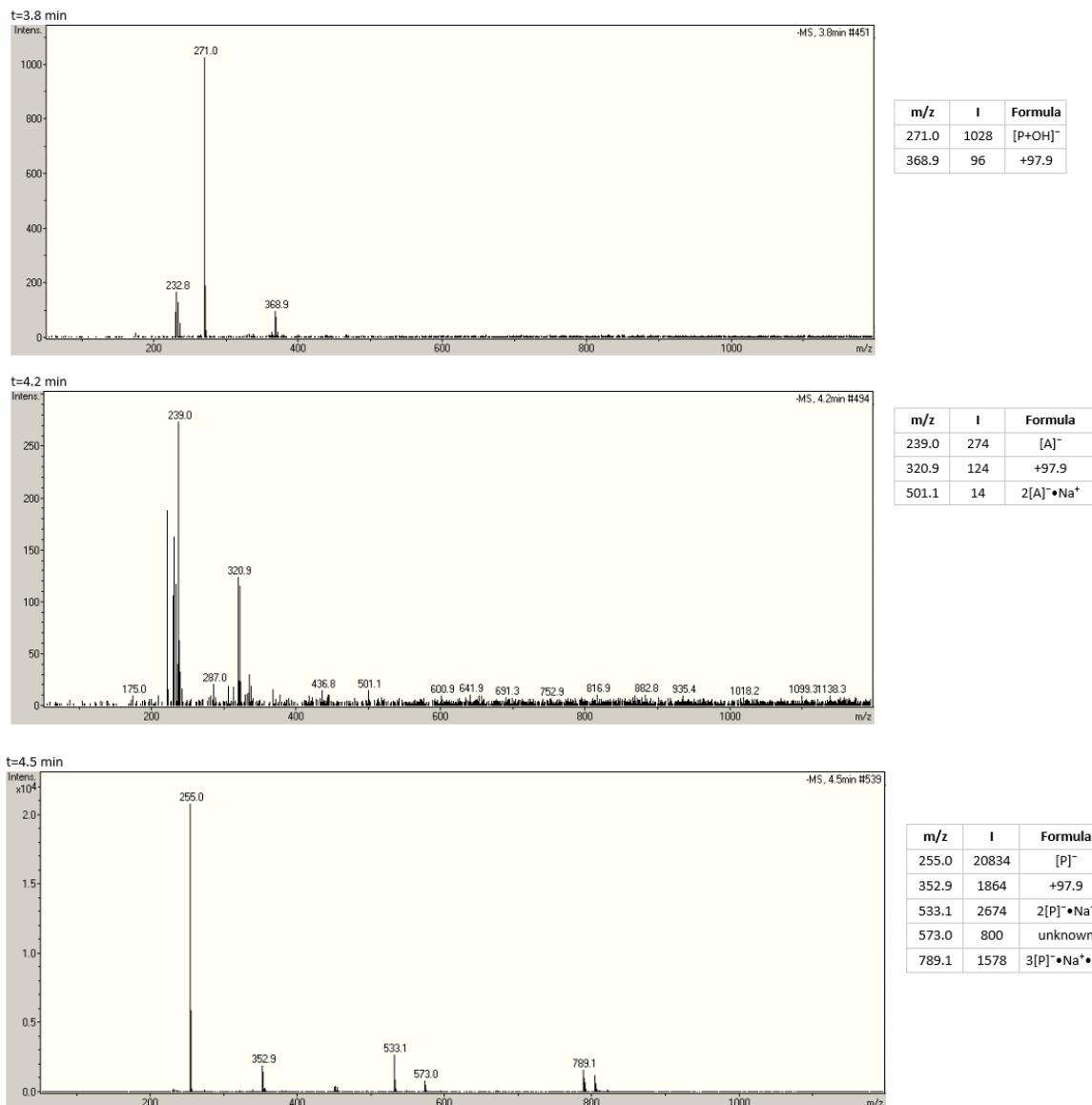


## UV-VIS SPECTRA



## MASS SPECTRA

MS (negative mode)



## S-8.62. Quercetin

### GENERAL INFORMATION

**Alternative names:** Quercitrin

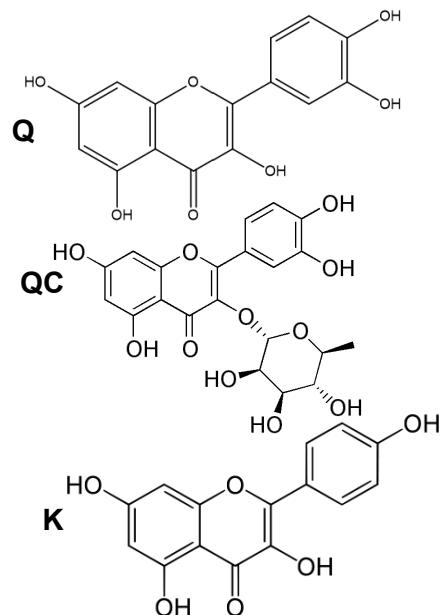
**Color Index Name:** n.a.

**Color Index Number:** n.a.

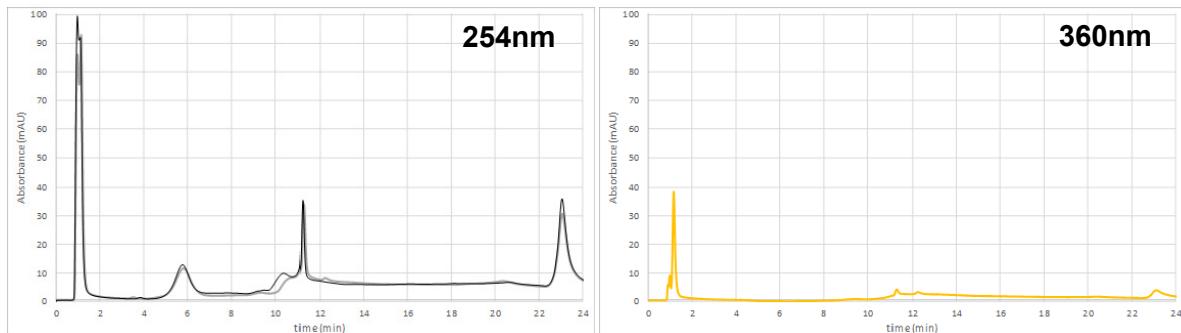
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Quercus velutina Lam.*

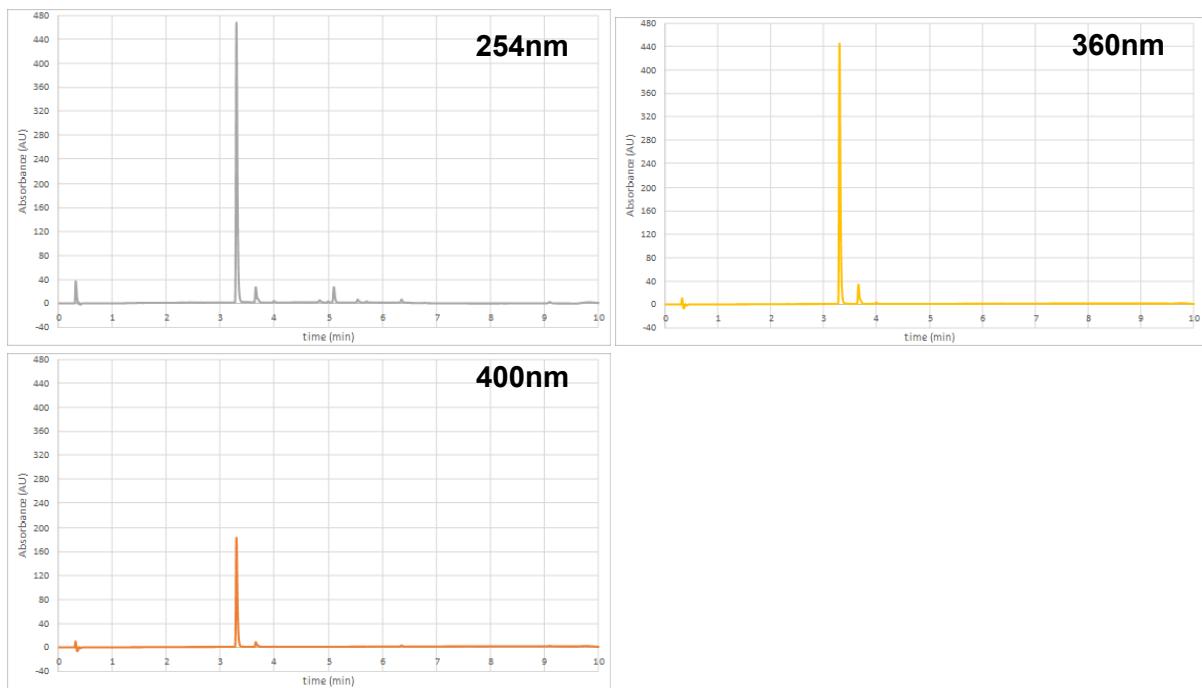
Name	Short	Mw	monoisotopic	Formula
Quercetin	[Q]	302.24	302.04	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>
Quercitrin	[QC]	448.38	448.10	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>
Kaempferol	[K]	286.24	286.05	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>



### CHROMATOGRAMS: ION-EXCHANGE

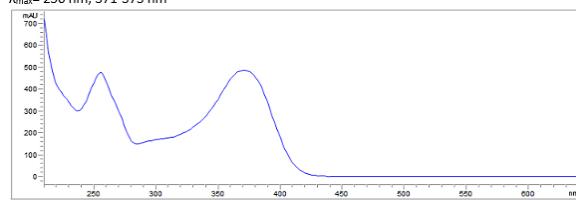


### CHROMATOGRAMS: REVERSED-PHASE

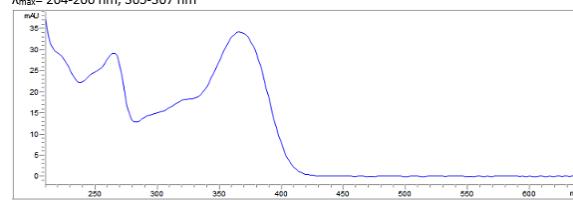


## UV-VIS SPECTRA

t=3.30 min  
 $\lambda_{\text{max}} = 256 \text{ nm; } 371-373 \text{ nm}$

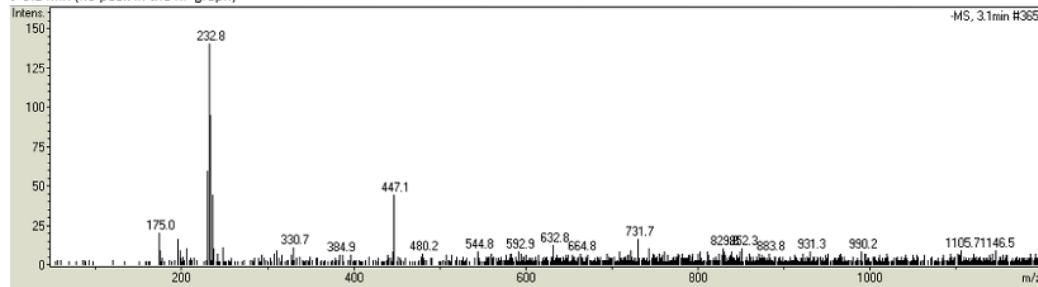


t=3.66 min  
 $\lambda_{\text{max}} = 264-266 \text{ nm; } 365-367 \text{ nm}$



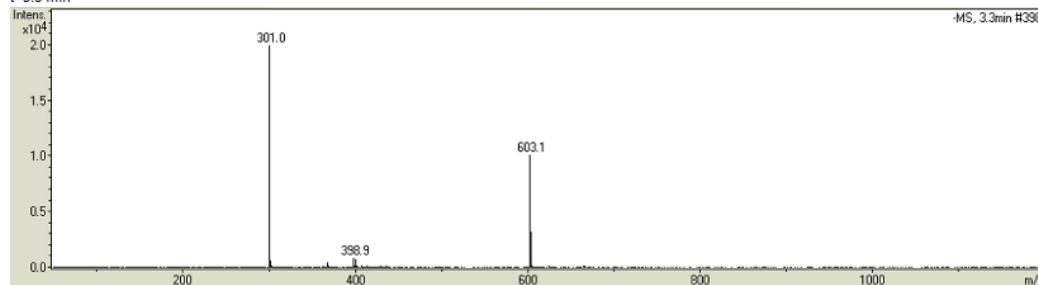
## MASS SPECTRA

t=3.1 min (no peak in the RP graph)



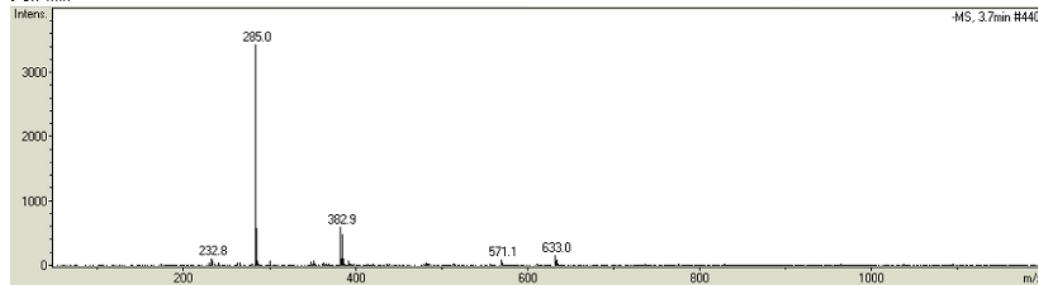
m/z	I	Formula
447.1	44	[QC] <sup>-</sup>

t=3.3 min



m/z	I	Formula
301.0	19997	[Q] <sup>-</sup>
398.9	762	+97.9
603.1	10099	2[Q] <sup>-</sup> •H <sup>+</sup>

t=3.7 min



m/z	I	Formula
285.0	3443	[K] <sup>-</sup>
382.9	595	+97.9
571.1	80	2[K] <sup>-</sup> •H <sup>+</sup>
633.0	143	unknown

### S-8.63. Quinoline Yellow

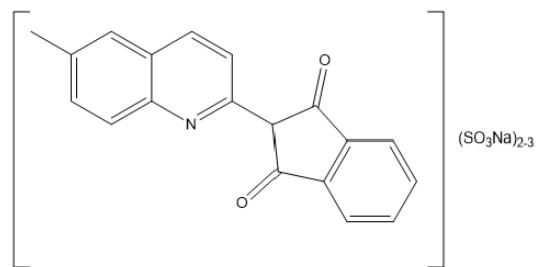
#### GENERAL INFORMATION

**Color Index Name:** Acid Yellow 3; Food Yellow 13

**Color Index Number:** 47005

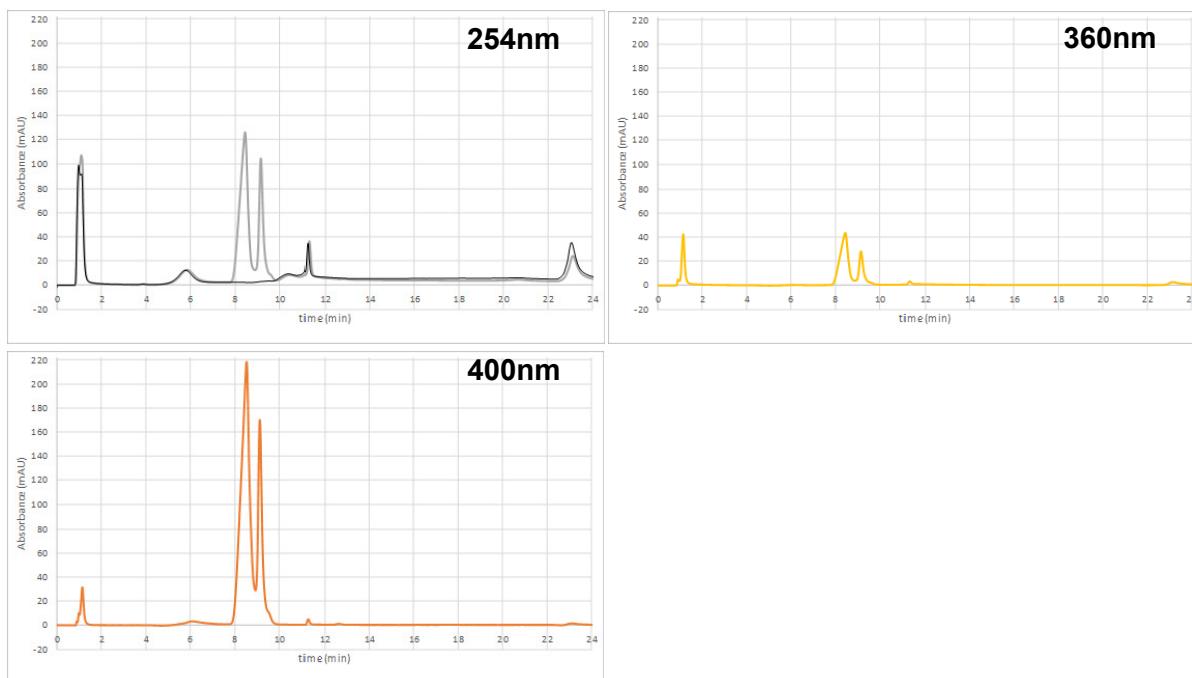
**Type of dye:** Quinoline

**Charge:** 0

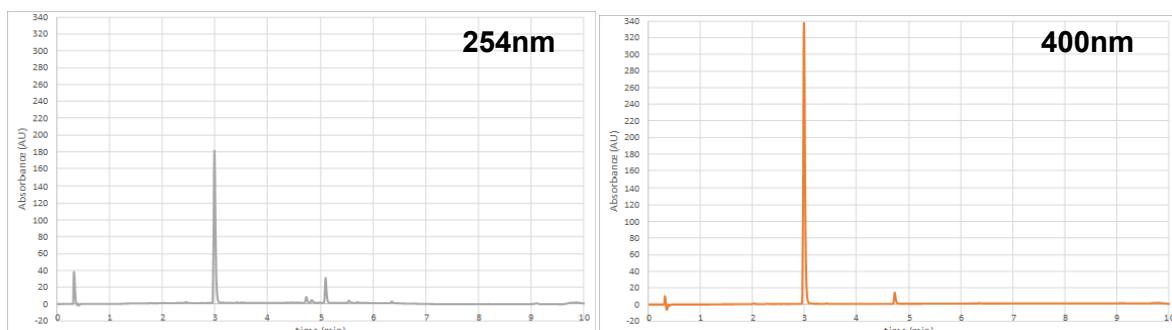


Molecule	Short	Formula (ion)	Full	Ion	Monoisotopic
Quinoline 3( $SO_3Na$ )	[Q3]	$C_{18}H_{10}NO_5S$	579.42	510.42	509.93
Quinoline 2( $SO_3Na$ )	[Q2]	$C_{18}H_9NO_8S_2$	477.38	431.40	430.98
Quinoline 1( $SO_3Na$ )	[Q1]	$C_{18}H_8NO_{11}S_3$	375.33	352.34	352.03

#### CHROMATOGRAMS: ION-EXCHANGE



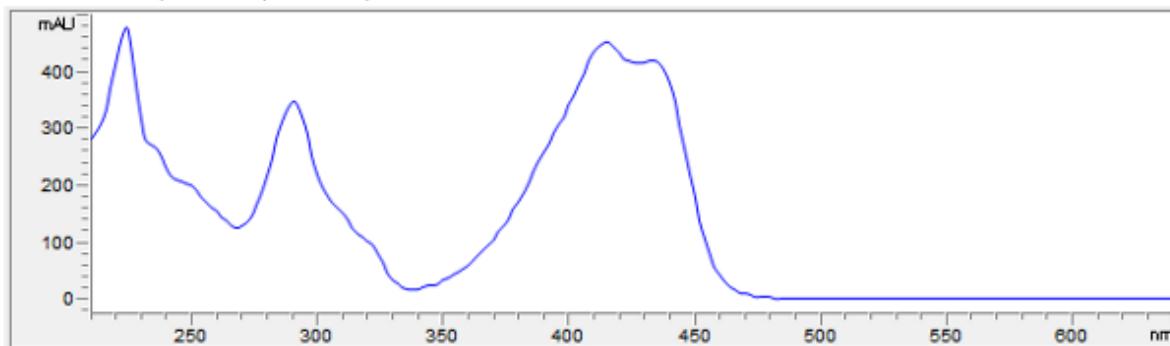
#### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

t=2.99 min

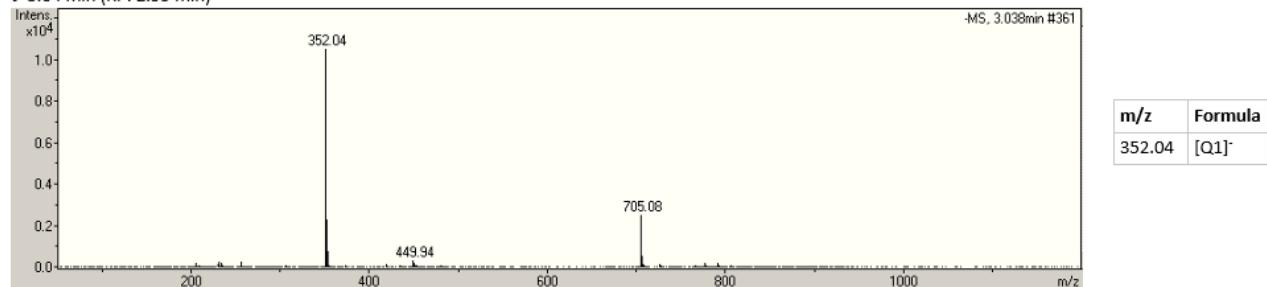
$\lambda_{\text{max}} = 224 \text{ nm}; 290 \text{ nm}; 414 \text{ nm}; 434 \text{ nm}$



## MASS SPECTRA

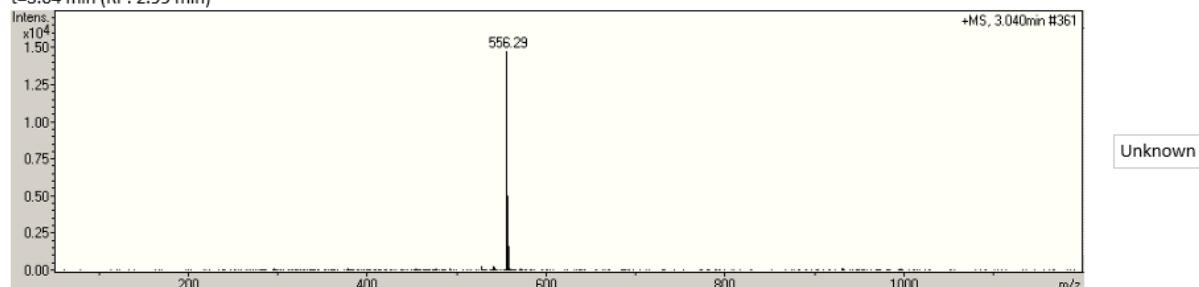
MS (negative mode)

t=3.04 min (RP: 2.99 min)



MS (positive mode)

t=3.04 min (RP: 2.99 min)

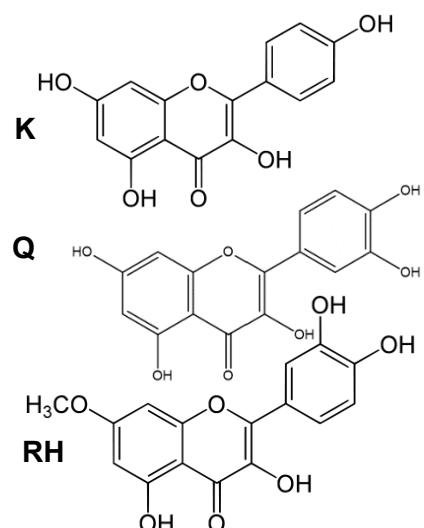


## S-8.64. Rhamnetin

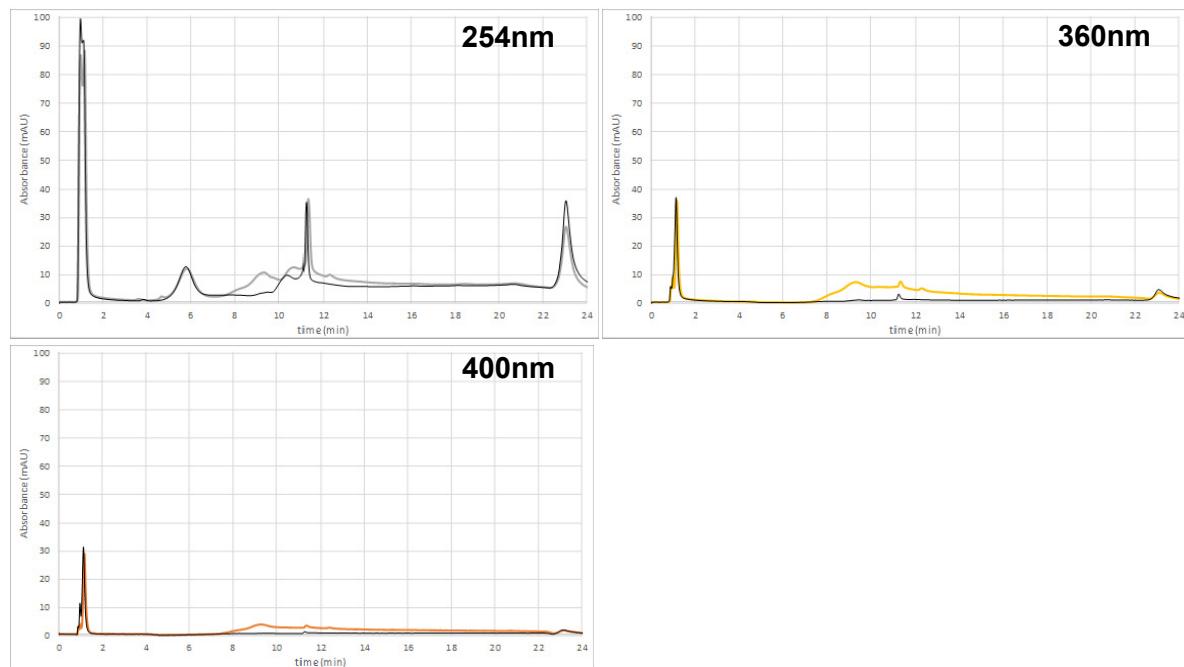
### GENERAL INFORMATION

**Alternative names:** Persian Berries  
**Color Index Name:** Natural Yellow 13  
**Color Index Number:** n.a.  
**Type of dye:** Natural, Mordant dye  
**Scientific name of biological source:** *Rhamnus Inectoria Lam.*

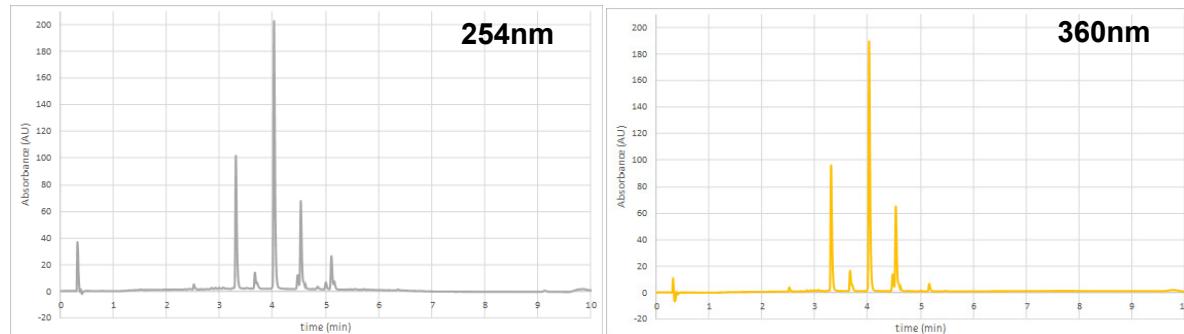
Name	Short	Mw	monoisotopic	Formula
Kaempferol	[K]	286.24	286.05	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>
Quercetin	[Q]	302.24	302.04	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>
Rhamnetin	[RH]	316.26	316.06	C <sub>16</sub> H <sub>12</sub> O <sub>7</sub>

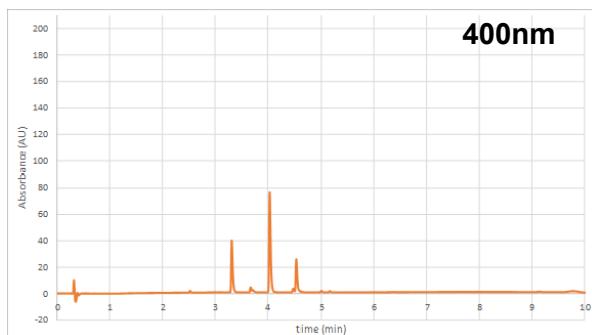


### CHROMATOGRAMS: ION-EXCHANGE



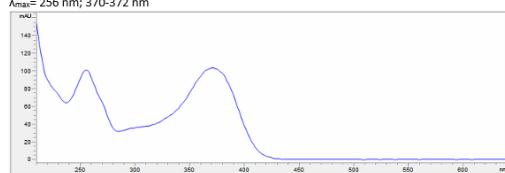
### CHROMATOGRAMS: REVERSED-PHASE



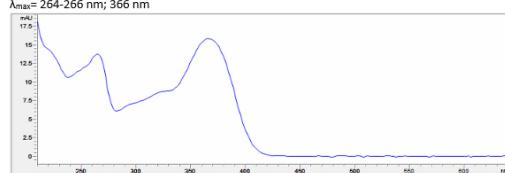


## UV-VIS SPECTRA

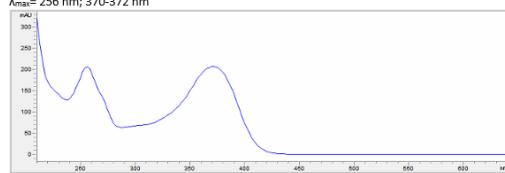
$t=3.31$  min  
 $\lambda_{\text{max}}= 256 \text{ nm}; 370-372 \text{ nm}$



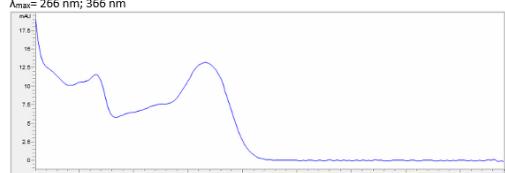
$t=3.67$  min  
 $\lambda_{\text{max}}= 264-266 \text{ nm}; 366 \text{ nm}$



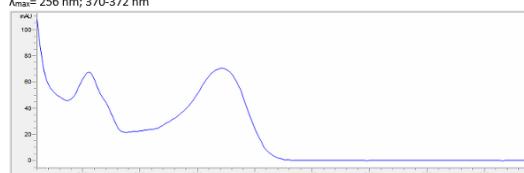
$t=4.04$  min  
 $\lambda_{\text{max}}= 256 \text{ nm}; 370-372 \text{ nm}$



$t=4.48$  min  
 $\lambda_{\text{max}}= 266 \text{ nm}; 366 \text{ nm}$

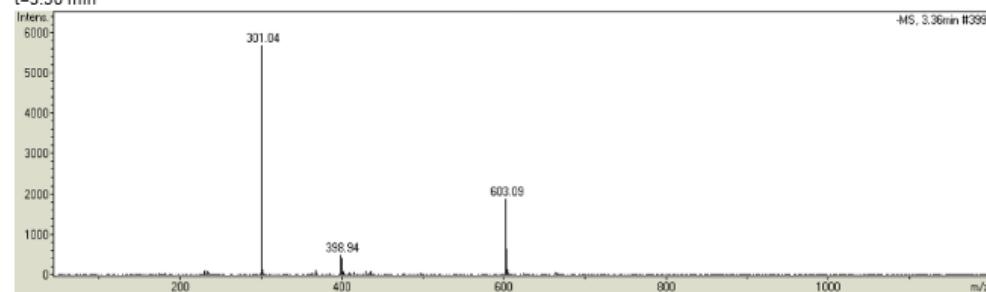


$t=4.54$  min  
 $\lambda_{\text{max}}= 256 \text{ nm}; 370-372 \text{ nm}$

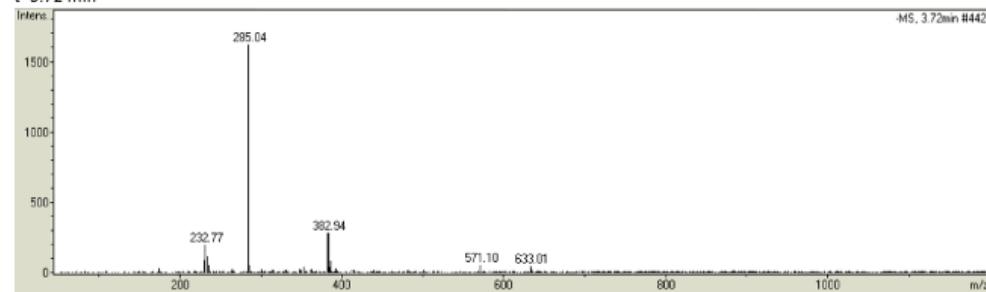


## MASS SPECTRA

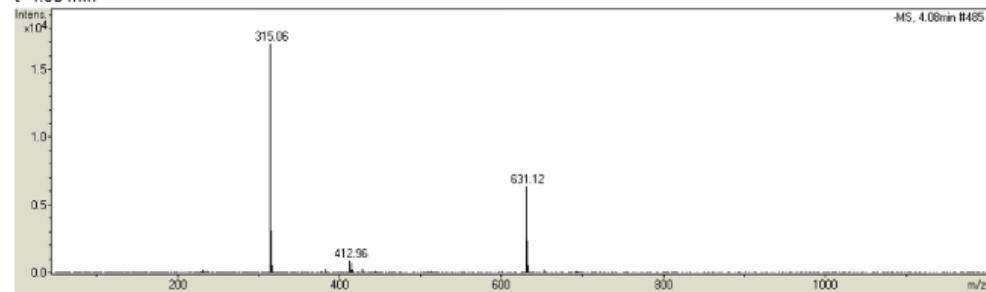
t=3.36 min



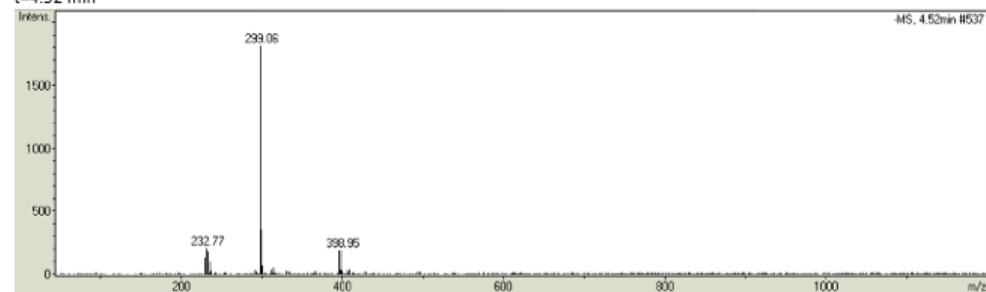
t=3.72 min



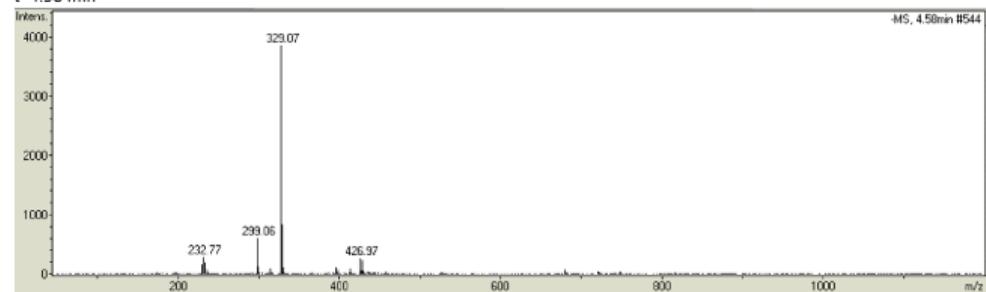
t=4.08 min



t=4.52 min



t=4.58 min



## S-8.65. Rhodamine 6G

### GENERAL INFORMATION

**Color Index Name:** Basic Red 1

**Color Index Number:** 45160

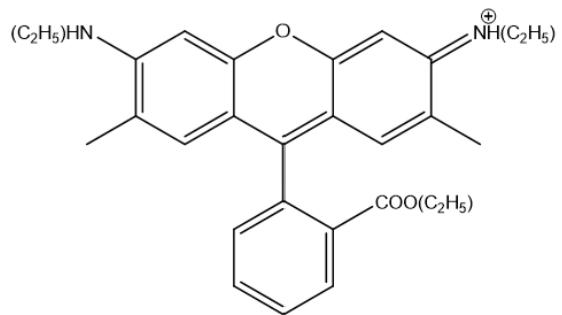
**Type of dye:** Xanthene

**Charge:** +1

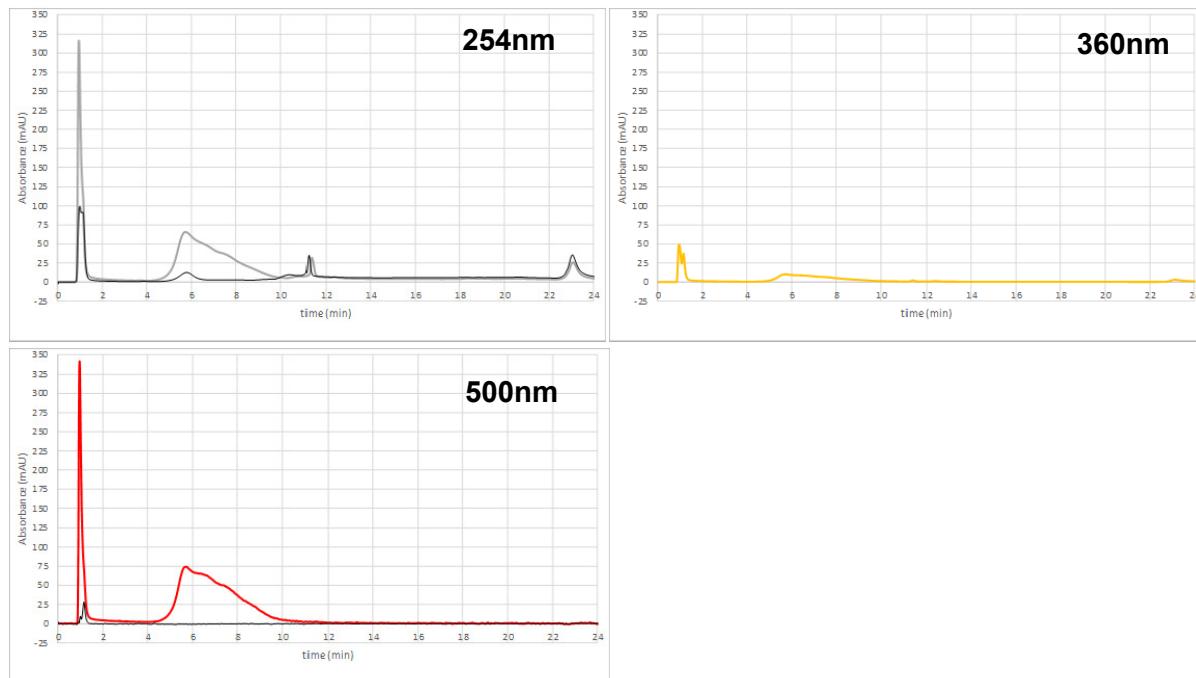
**Molecular Formula:** C<sub>28</sub>H<sub>31</sub>N<sub>2</sub>O<sub>3</sub> (ion, +1)

**Molecular Weight**

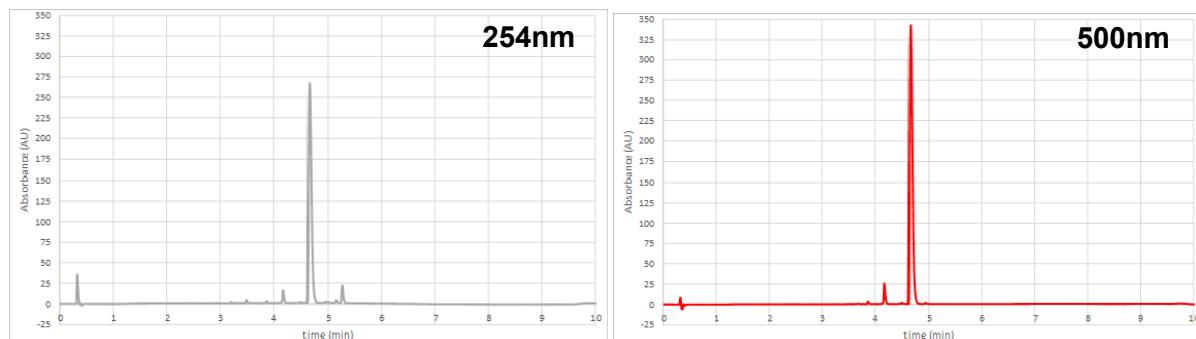
Full molecule:	479.01
Ion (+1)	443.56
Ion (+1), monoisotopic	443.23
Ion (-1), monoisotopic	441.22



### CHROMATOGRAMS: ION-EXCHANGE

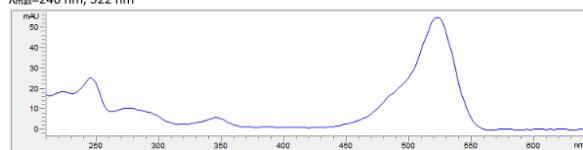


### CHROMATOGRAMS: REVERSED-PHASE

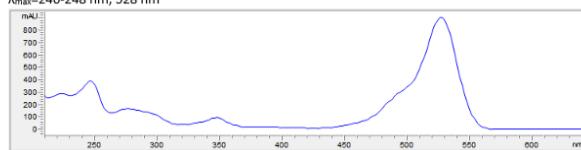


## UV-VIS SPECTRA

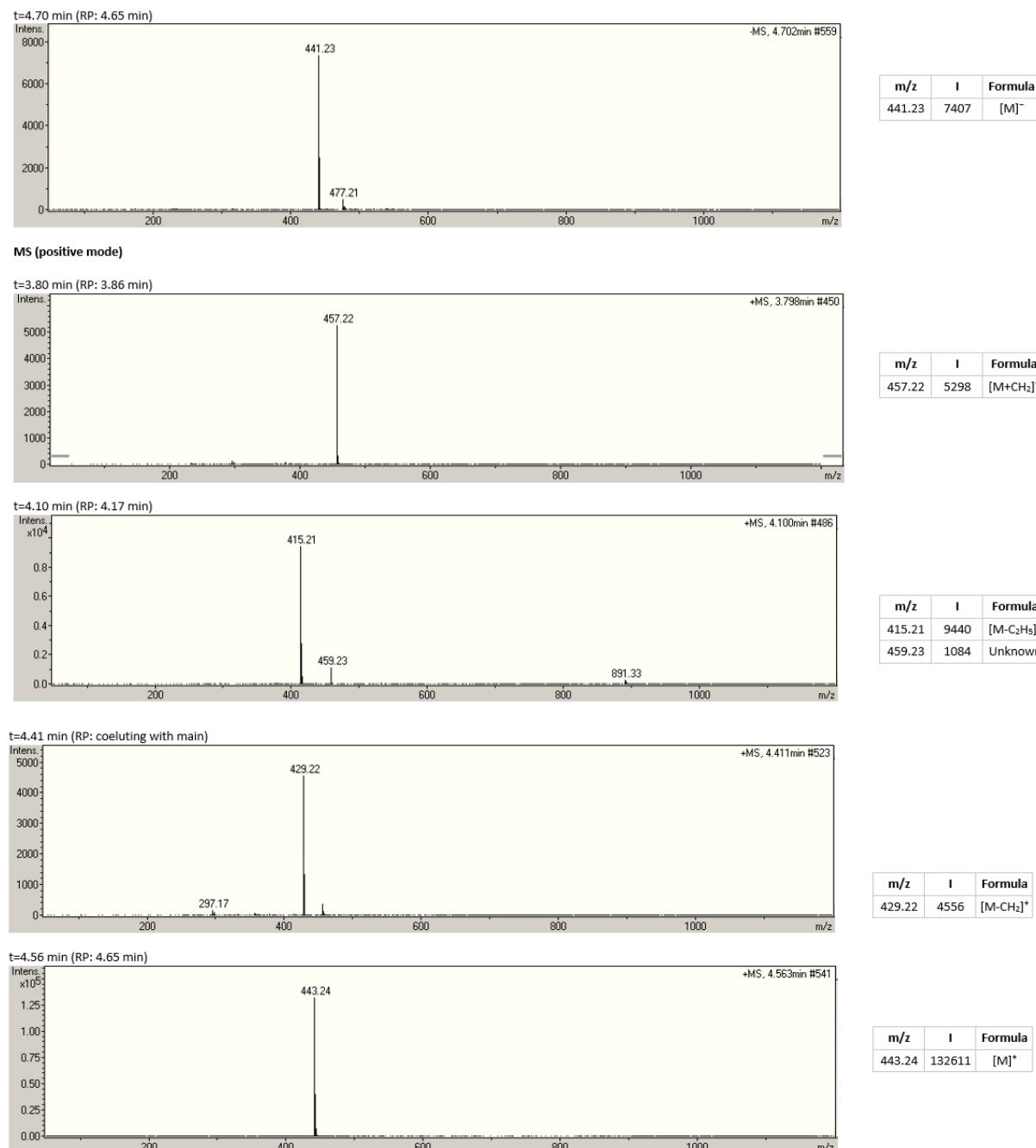
t=4.17 min  
 $\lambda_{\text{max}}=246 \text{ nm}; 522 \text{ nm}$



t=4.65 min  
 $\lambda_{\text{max}}=246-248 \text{ nm}; 528 \text{ nm}$



## MASS SPECTRA



## S-8.66. Rhodamine B

### GENERAL INFORMATION

**Color Index Name:** Basic Violet 10

**Color Index Number:** 45170

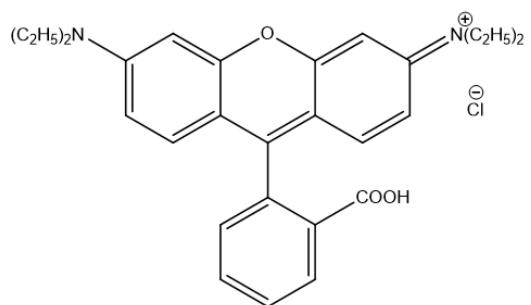
**Type of dye:** Xanthene

**Charge:** +1

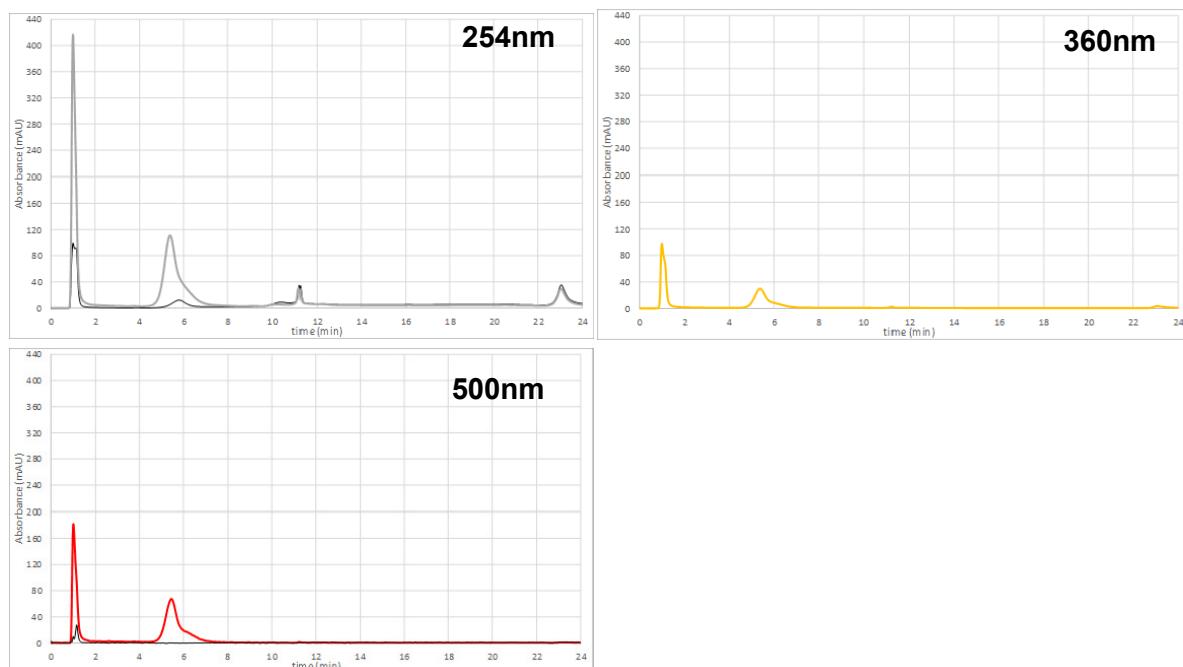
**Molecular Formula:** C<sub>28</sub>H<sub>31</sub>N<sub>2</sub>O<sub>3</sub> (ion, +1)

**Molecular Weight**

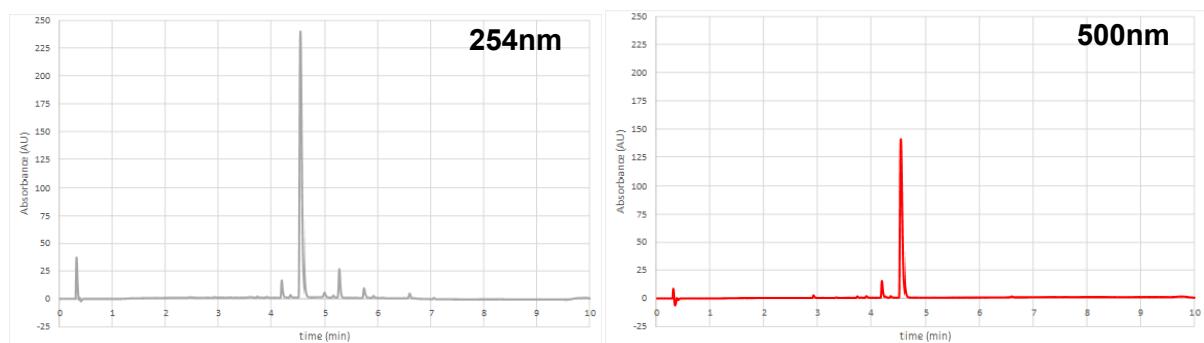
Full molecule:	479.01
Ion (+1)	443.56
Ion (+1), monoisotopic	443.23



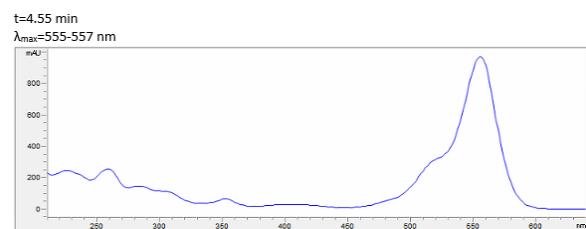
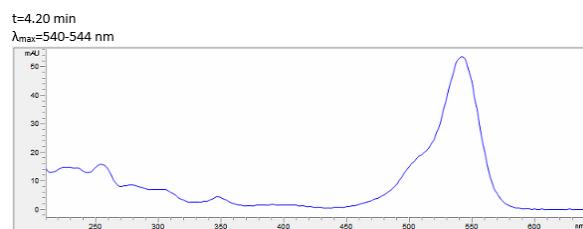
### CHROMATOGRAMS: ION-EXCHANGE



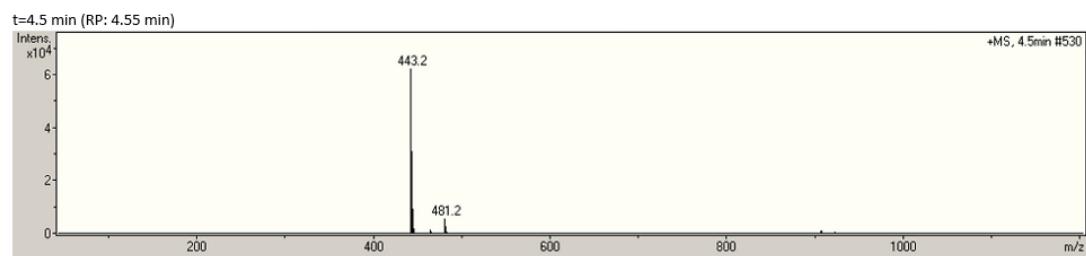
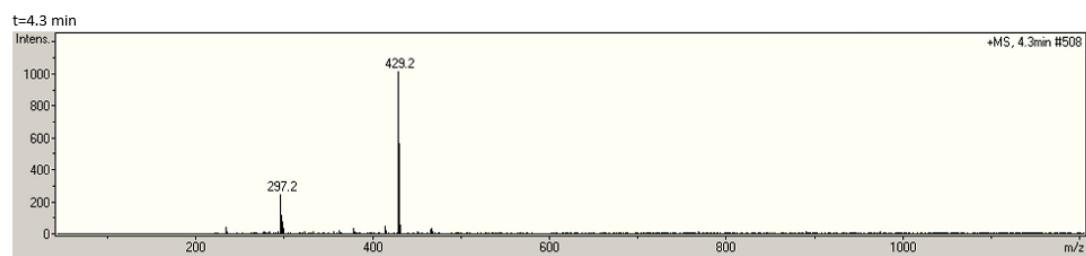
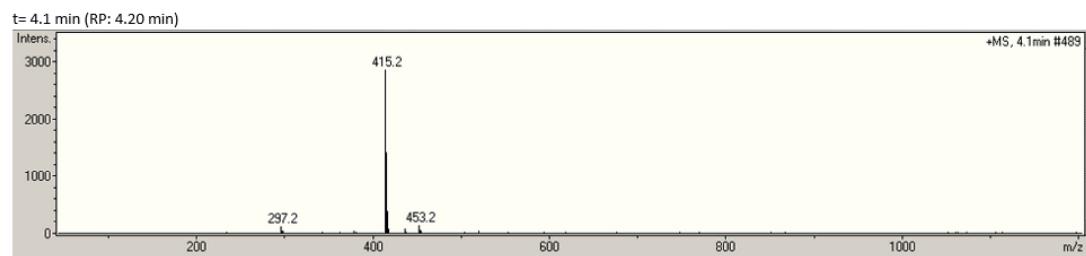
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA



## MASS SPECTRA



## S-8.67. Rutin

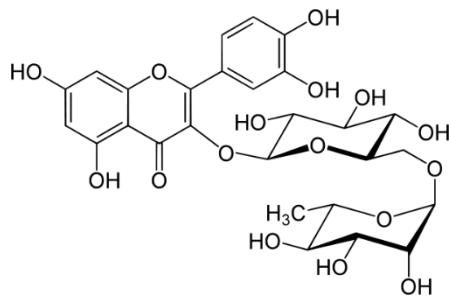
### GENERAL INFORMATION

**Color Index Name:** Natural yellow 10

**Color Index Number:** 75730

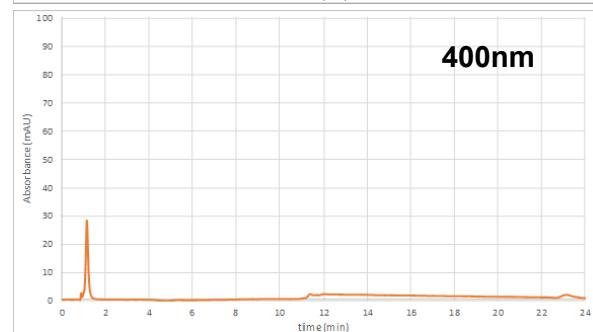
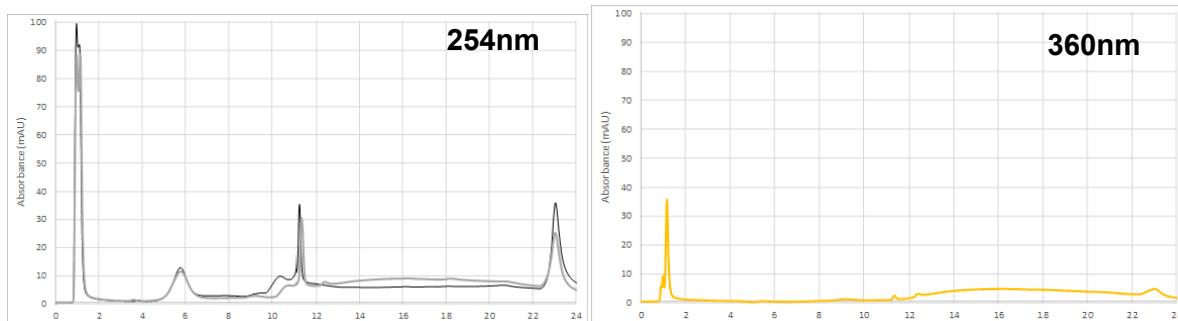
**Type of dye:** Natural

**Scientific name of biological source:** *Quercus Velutina Lam.*

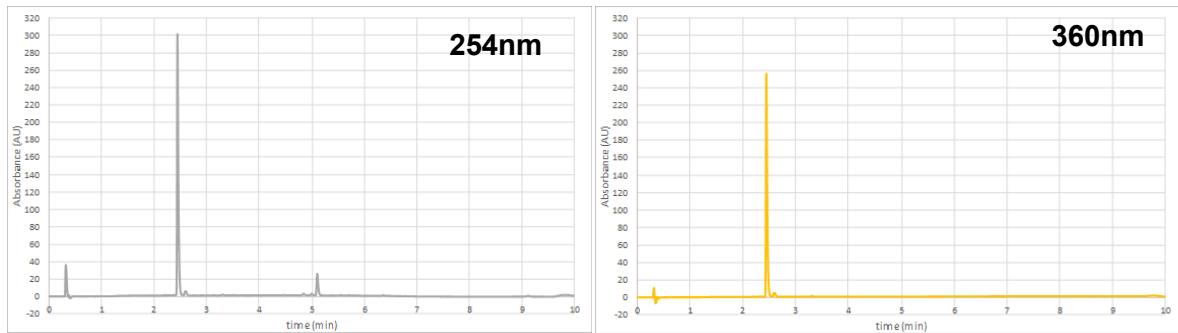


Name	Short	Mw	monoisotopic	Formula
Rutin	[RU]	610.52	610.15	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>

### CHROMATOGRAMS: ION-EXCHANGE



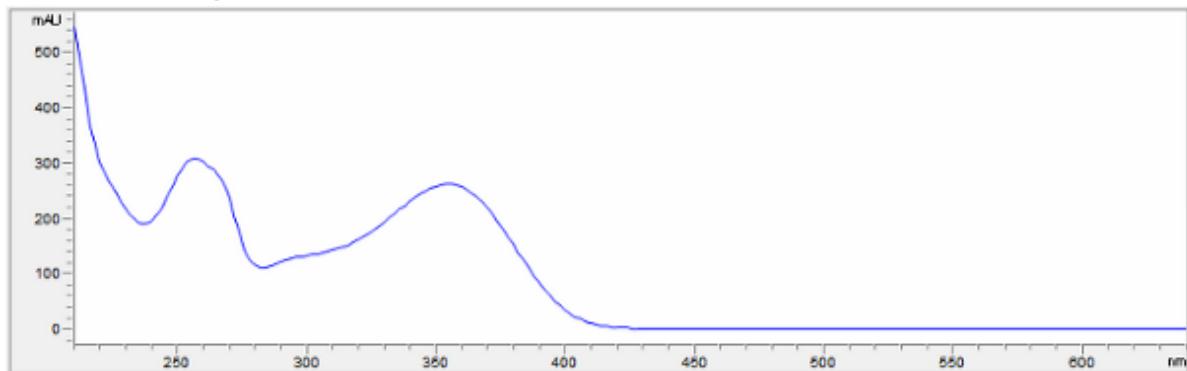
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

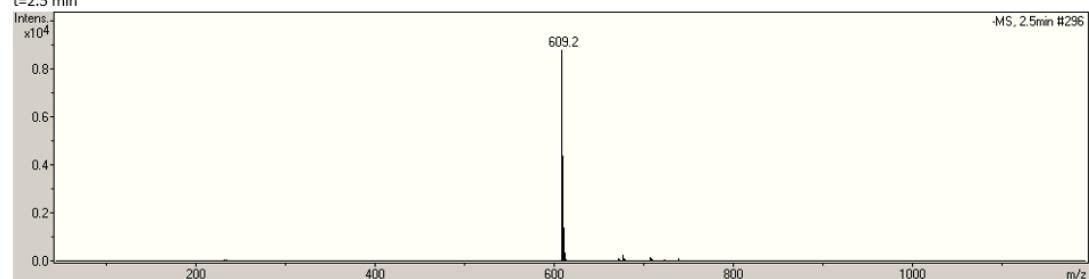
t=2.45 min

$\lambda_{\text{max}} = 256-258 \text{ nm}$ ; 353-357 nm

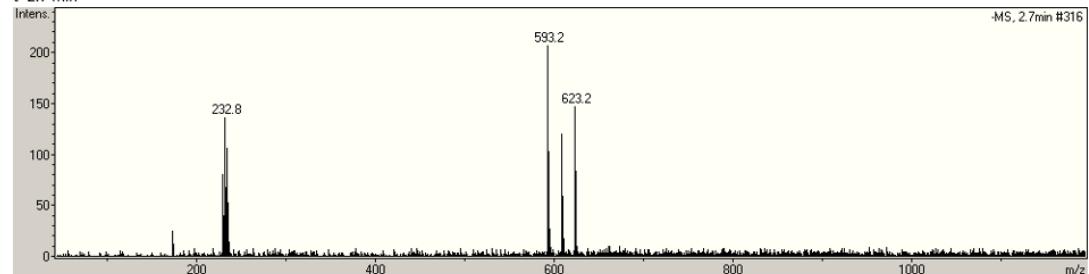


## MASS SPECTRA

t=2.5 min



t=2.7 min



## S-8.68. Safranine T

### GENERAL INFORMATION

**Alternative name:** Safranine O

**Color Index Name:** Basic Red 2

**Color Index Number:** 50240

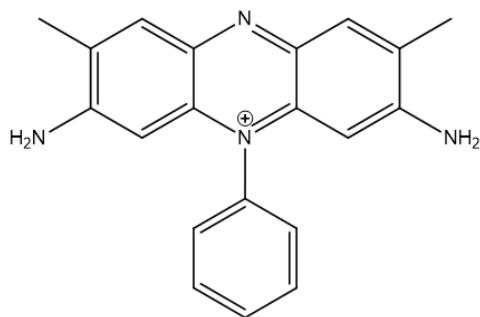
**Type of dye:** Azine, Phenazine

**Charge:** +1

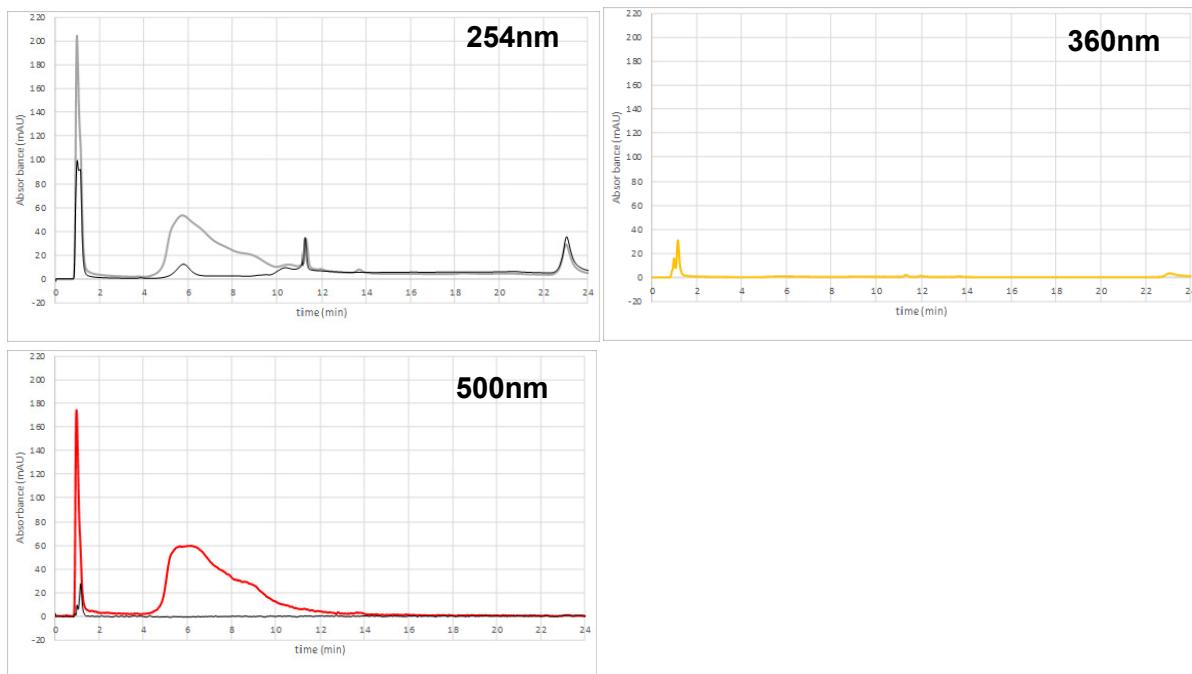
**Molecular Formula:** C<sub>28</sub>H<sub>31</sub>N<sub>2</sub>O<sub>3</sub> (ion, +1)

**Molecular Weight**

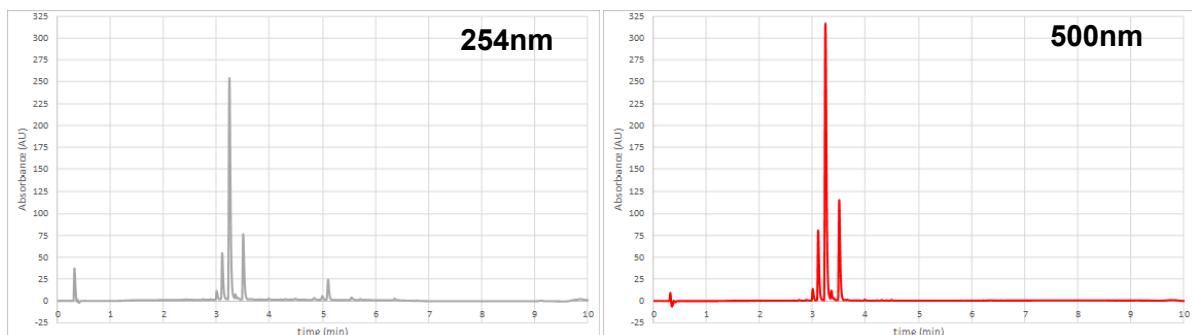
Full molecule (with Cl <sup>-</sup> )	350.84
Ion (+1)	315.39
Ion (+1), monoisotopic	315.16
Ion (-1), monoisotopic	313.15



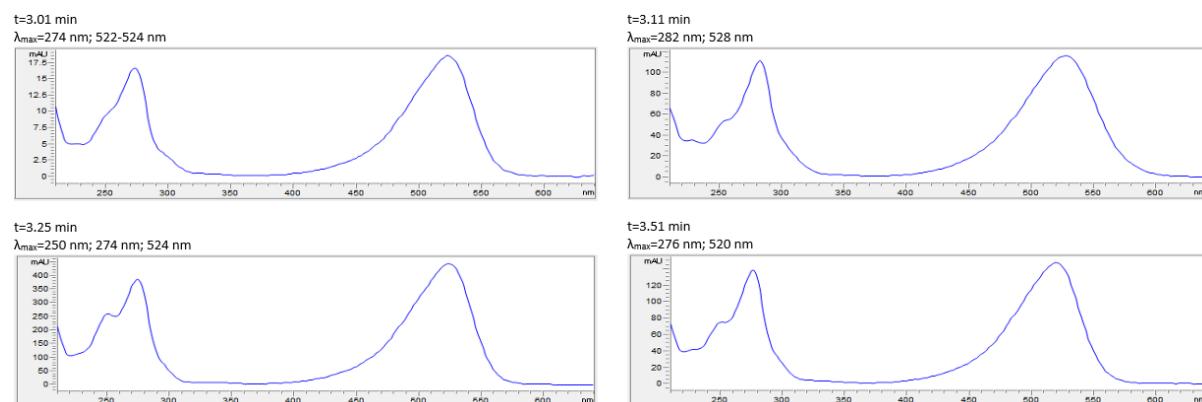
### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

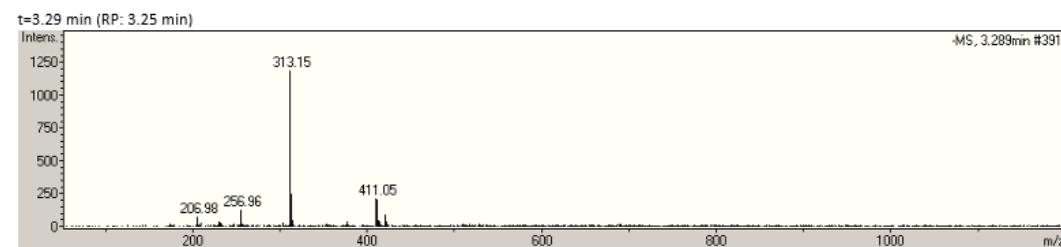


## UV-VIS SPECTRA



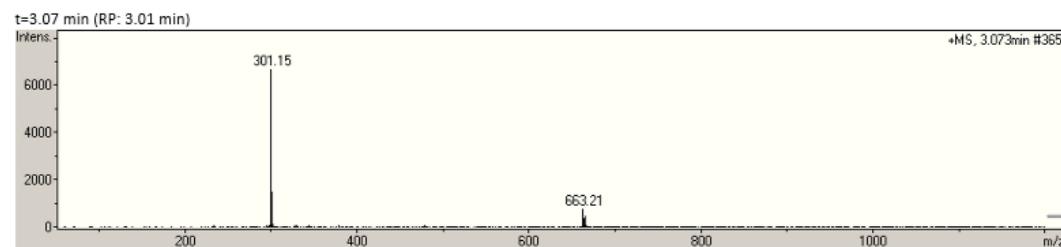
## MASS SPECTRA

### MS (negative mode)



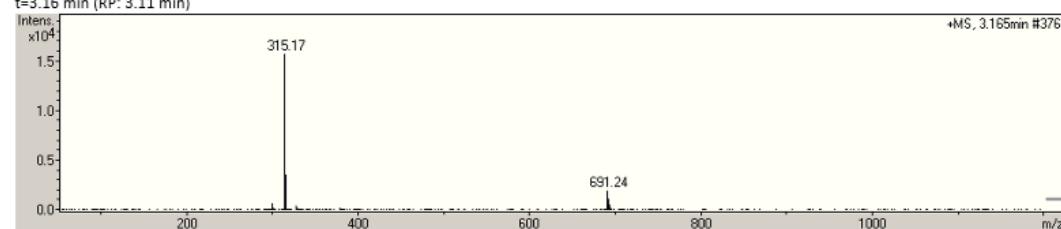
m/z	I	Formula
313.15	1191	[M] <sup>-</sup>
411.05	211	+97.9

### MS (positive mode)



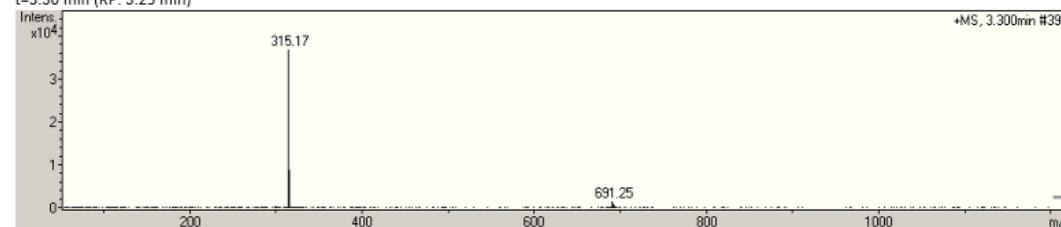
m/z	I	Formula
301.15	6672	[M-CH <sub>2</sub> ] <sup>+</sup>

### t=3.16 min (RP: 3.11 min)



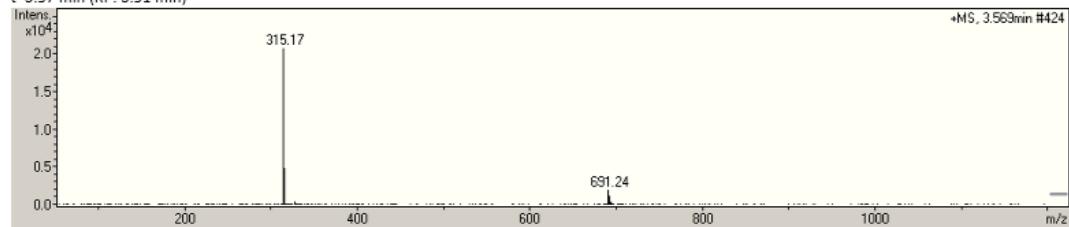
m/z	I	Formula
315.17	15805	[M (iso)] <sup>+</sup>

### t=3.30 min (RP: 3.25 min)



m/z	I	Formula
315.17	36895	[M] <sup>+</sup>

t=3.57 min (RP: 3.51 min)



+MS, 3.569min #424

m/z	I	Formula
315.17	20857	[M (iso)] <sup>*</sup>

## S-8.69. Sandelwood

### GENERAL INFORMATION

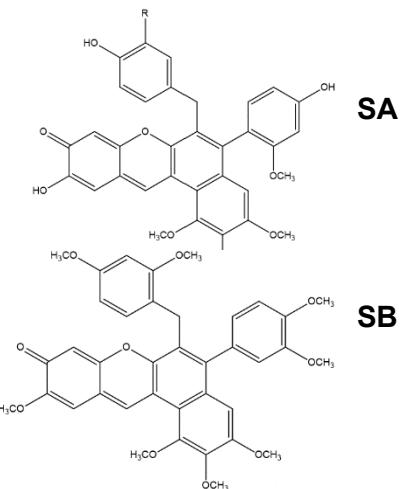
**Color Index Name:** Natural Red 22

**Color Index Number:** 75510; 75540; 75550

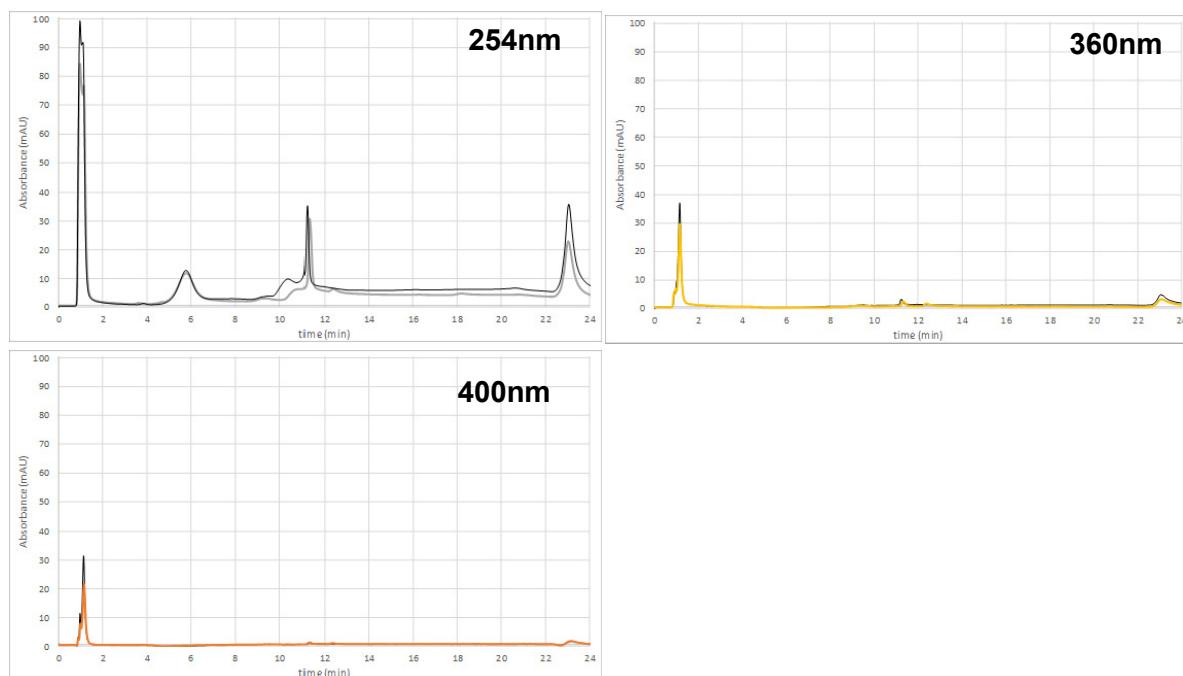
**Type of dye:** Natural, Mordant dye

**Scientific name of biological source:** *Pterocarpus santalinus L.*

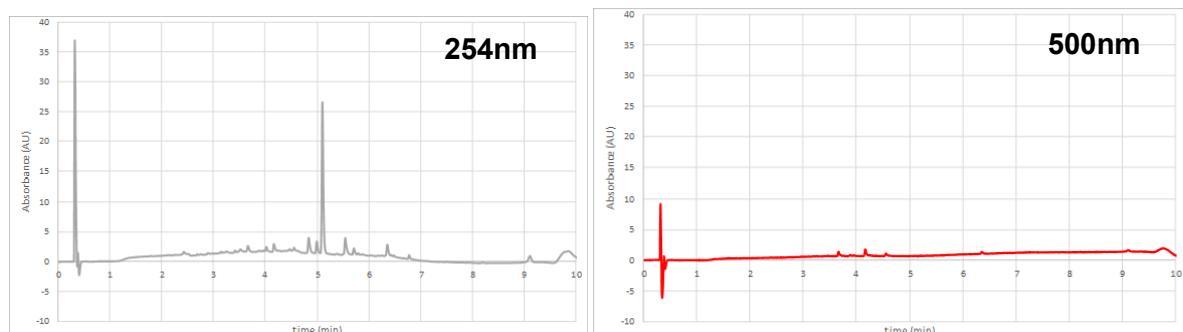
Name	Short	Mw	monoisotopic	Formula
Santalain A	[SA]	582.55	582.15	C <sub>33</sub> H <sub>26</sub> O <sub>10</sub>
Santalain B	[SB]	652.69	652.23	C <sub>38</sub> H <sub>36</sub> O <sub>10</sub>



### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE



**UV-VIS SPECTRA**

not available

**MASS SPECTRA**

not available

## S-8.70. Silk Scarlet N

### GENERAL INFORMATION

**Color Index Name:** Acid Red 9

**Color Index Number:** 15635

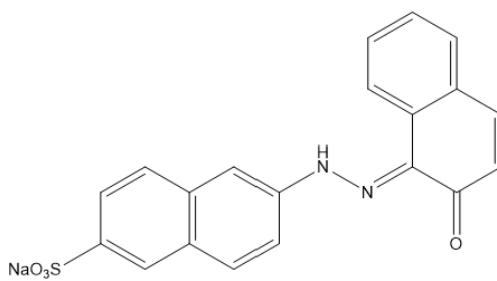
**Type of dye:** Monoazo

**Charge:** -1

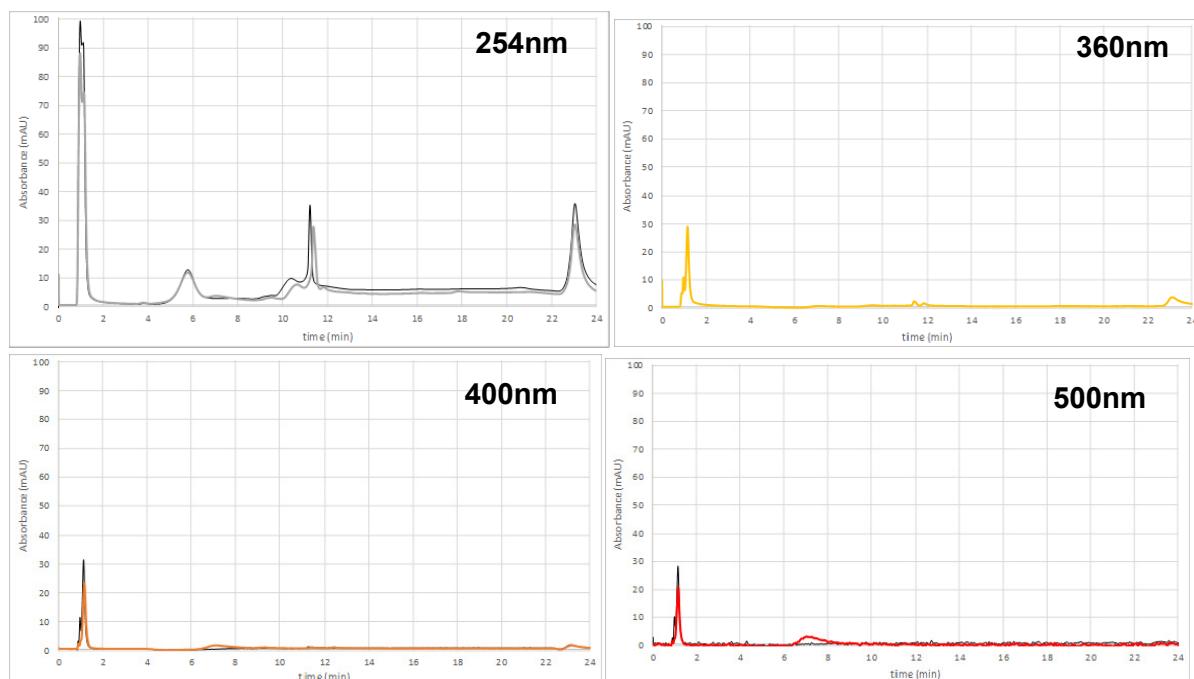
**Molecular Formula:** C<sub>20</sub>H<sub>13</sub>N<sub>2</sub>O<sub>4</sub>S (ion, -1)

**Molecular Weight**

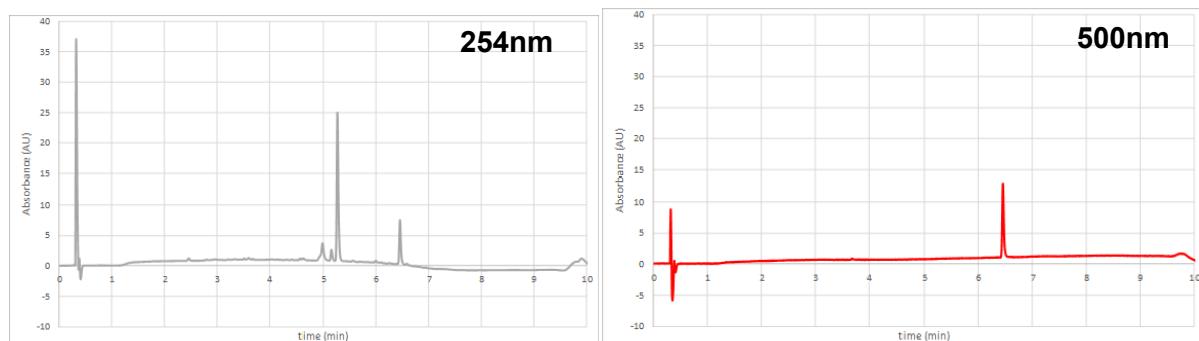
Full molecule:	400.38
Ion (-1)	377.39
Ion (-1), monoisotopic	377.06



### CHROMATOGRAMS: ION-EXCHANGE

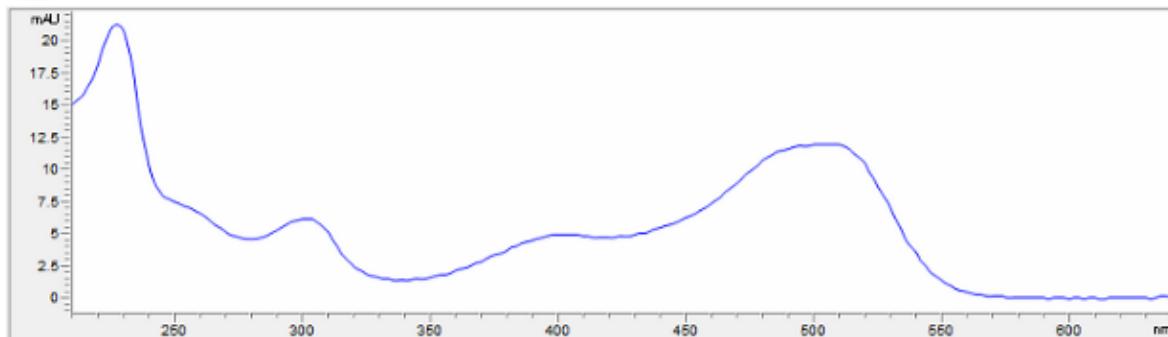


### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

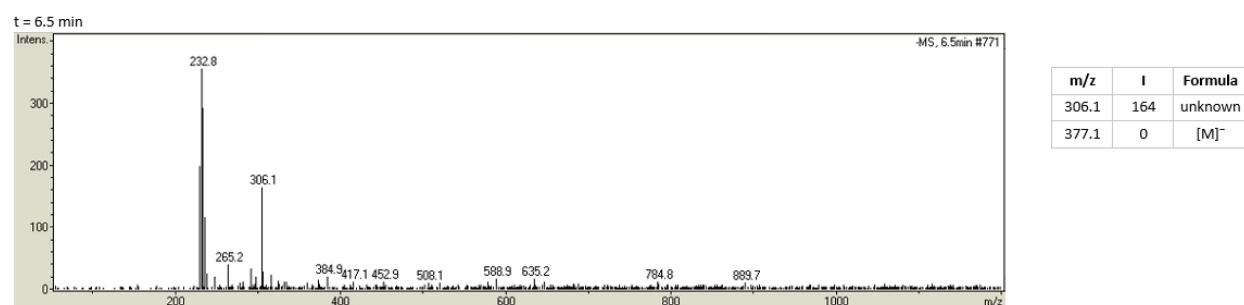
$t=6.45 \text{ min}$   
 $\lambda_{\max} = 500-504 \text{ nm}$



## MASS SPECTRA

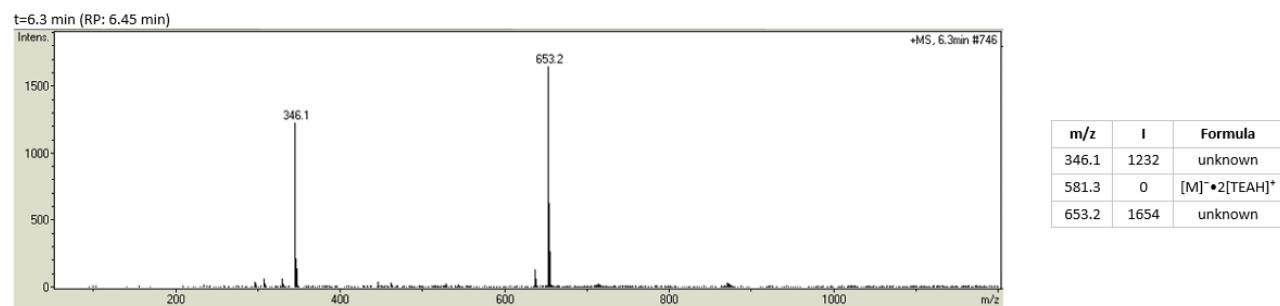
### MS (negative mode)

The expected peak  $[M]^-$  with  $m/z=377.1$  does not appear anywhere in the chromatogram. The MS- peaks generated by the peak at 6.45 in the RP separation do not seem to be linked to the compound Silk Scarlet N, and they have an intensity which is anyway too low to be significant.



### MS (positive mode)

The expected peak  $[M]^{+}\bullet 2[\text{TEAH}]^+$  with  $m/z=581.3$  does not appear anywhere in the chromatogram. The MS+ peaks generated by the peak at 6.45 in the RP separation do not seem to be linked to the compound Silk Scarlet N.



## S-8.71. Tartrazin

### GENERAL INFORMATION

**Color Index Name:** Acid Yellow 23

**Color Index Number:** 19140

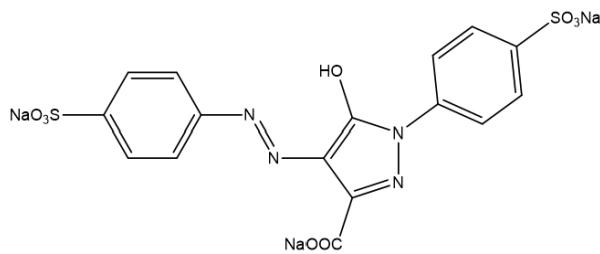
**Type of dye:** Monoazo; Pyrazolone

**Charge:** -3

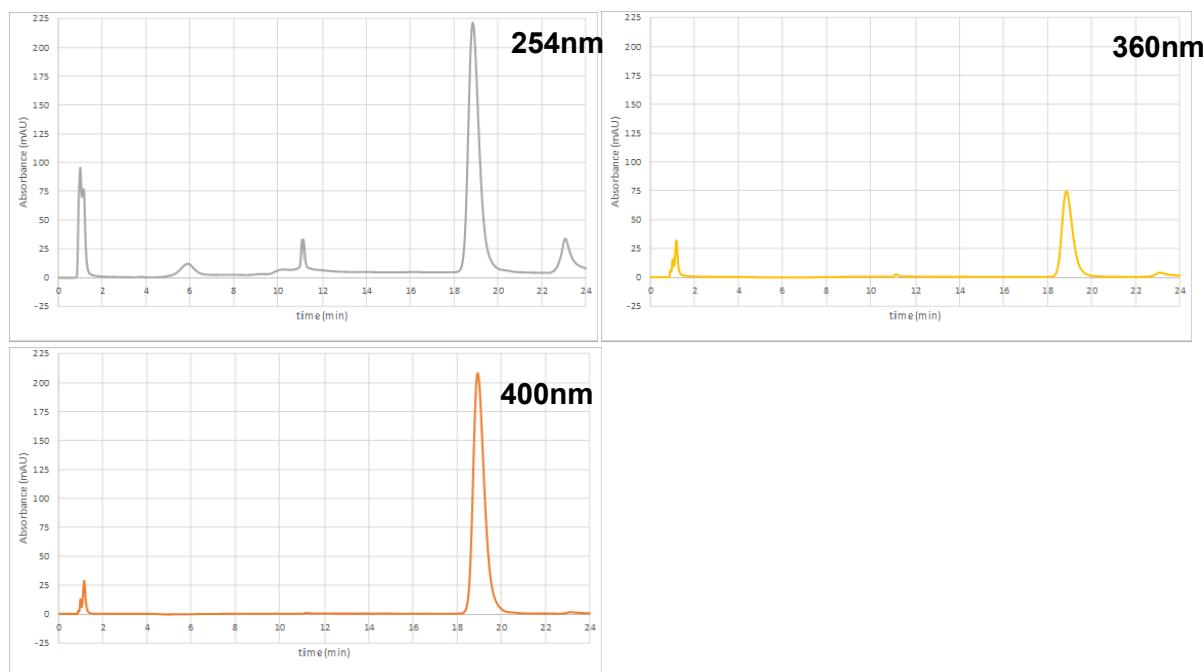
**Molecular Formula:** C<sub>16</sub>H<sub>9</sub>N<sub>4</sub>O<sub>9</sub>S<sub>2</sub> (ion, -3)

**Molecular Weight**

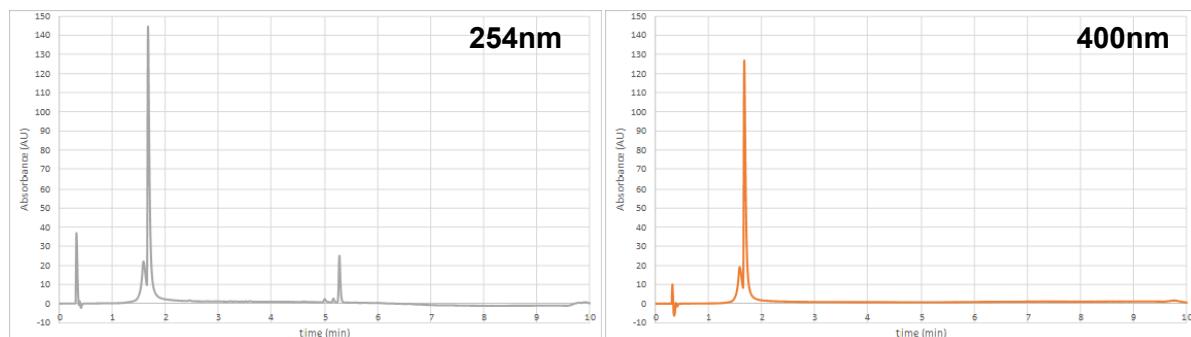
Full molecule:	534.36
Ion (-3)	465.39
Ion (-3), monoisotopic	464.98



### CHROMATOGRAMS: ION-EXCHANGE



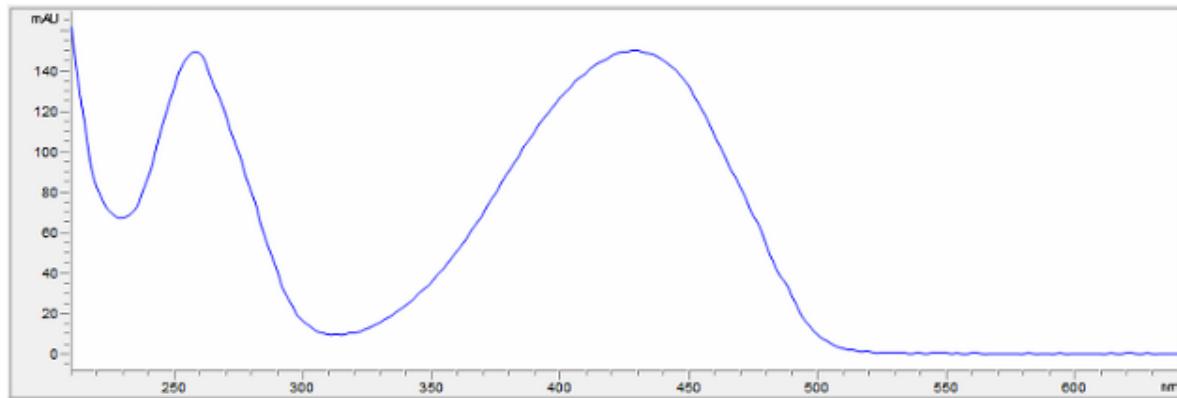
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

$t=1.67 \text{ min}$

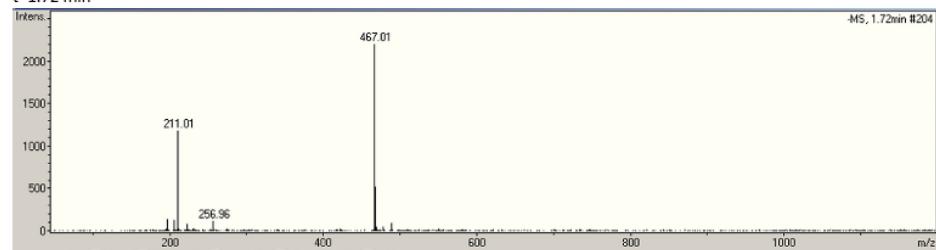
$\lambda_{\text{max}} = 258 \text{ nm}; 428 \text{ nm}$



## MASS SPECTRA

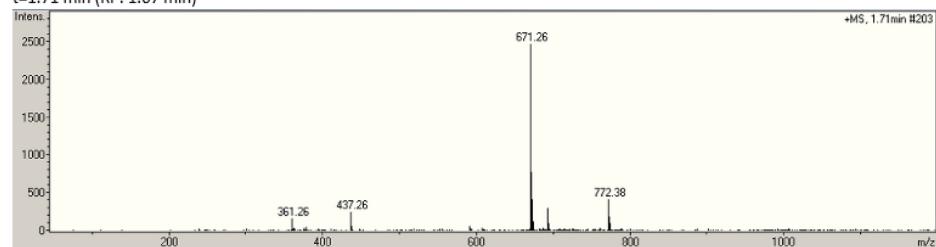
MS (negative mode)

$t=1.72 \text{ min}$



MS (positive mode)

$t=1.71 \text{ min} (\text{RP: } 1.67 \text{ min})$



## S-8.72. Turmeric

### GENERAL INFORMATION

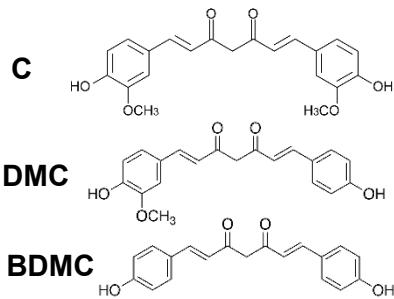
**Alternative names:** Curcumin

**Color Index Name:** Natural Yellow 3

**Color Index Number:** 75300

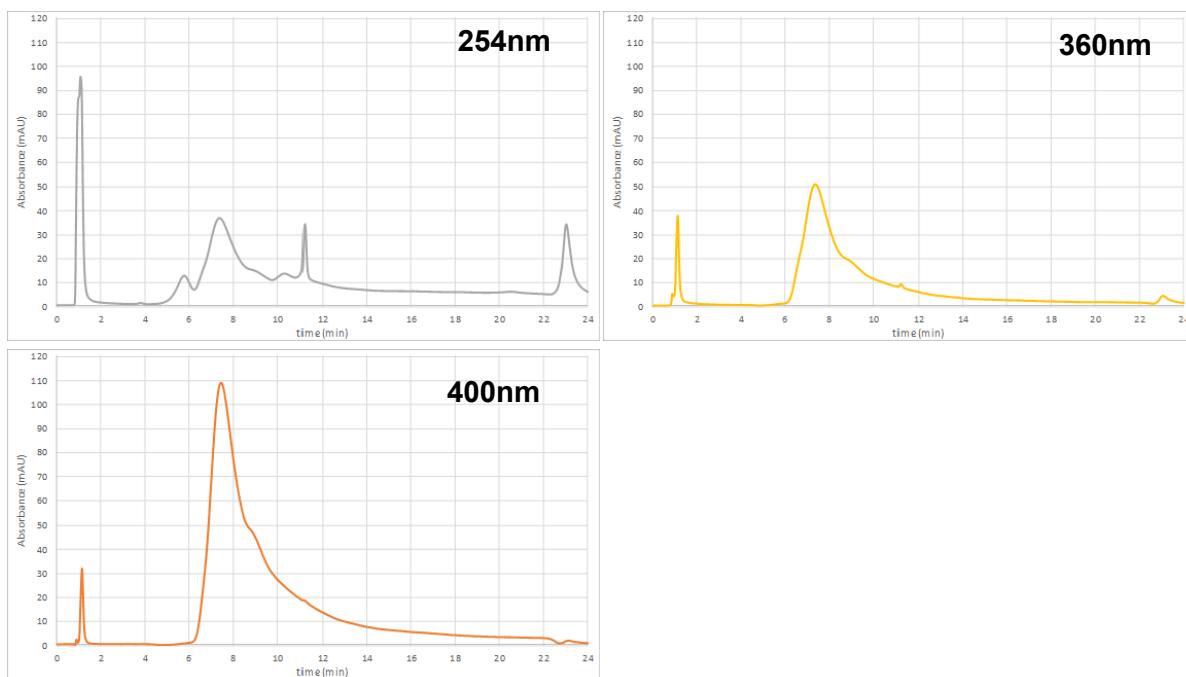
**Type of dye:** Natural

**Scientific name of biological source:** *Curcuma Longa*

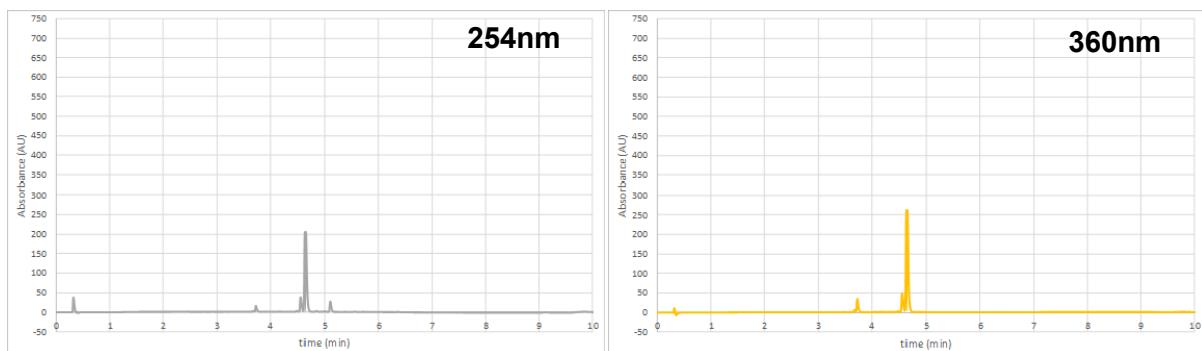


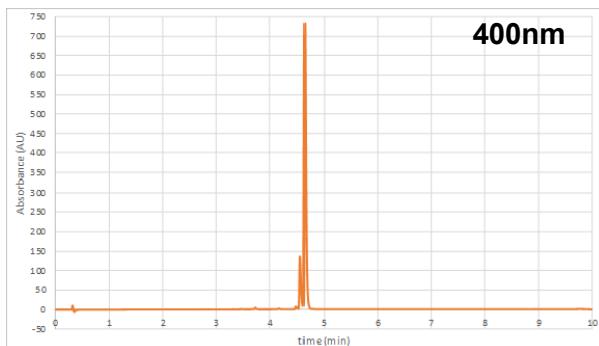
Name	Short	Mw	monoisotopic	Formula	%
Curcumin	[C]	368.38	368.13	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>	65-85
Demethoxy-curcumin	[DMC]	338.35	338.12	C <sub>20</sub> H <sub>18</sub> O <sub>5</sub>	12-25
Bis-demethoxy-curcumin	[BDMC]	308.33	308.10	C <sub>19</sub> H <sub>16</sub> O <sub>4</sub>	1-10

### CHROMATOGRAMS: ION-EXCHANGE

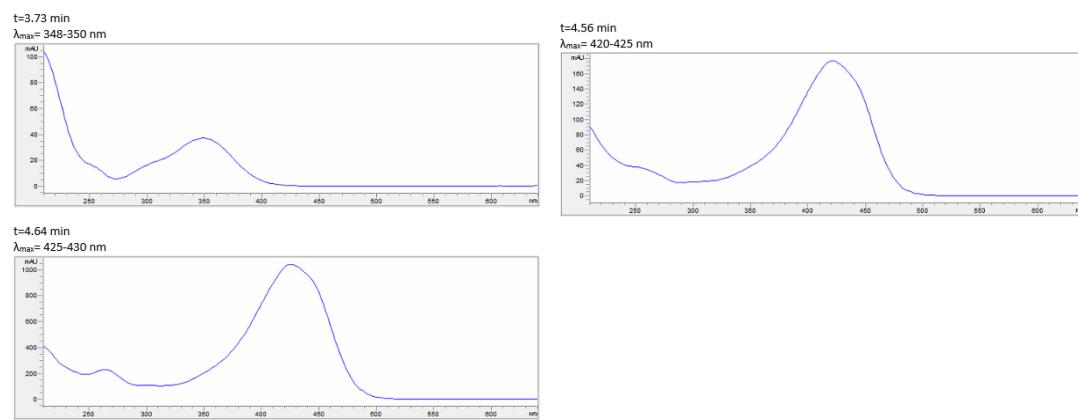


### CHROMATOGRAMS: REVERSED-PHASE



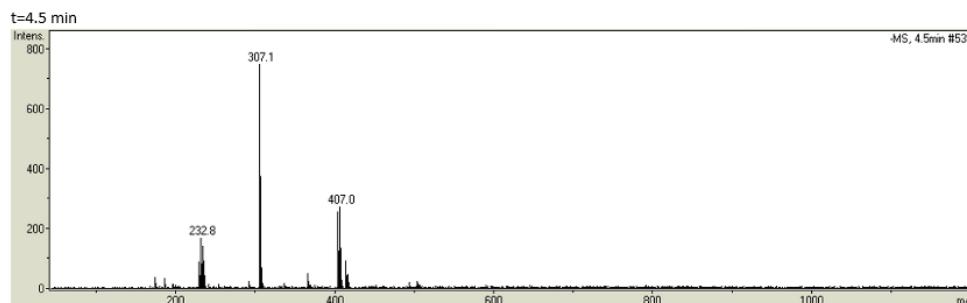
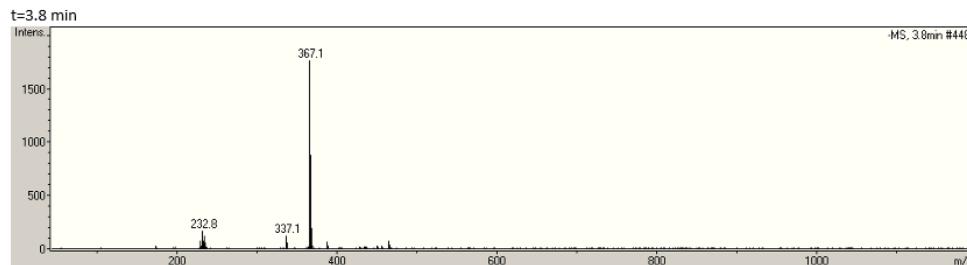


## UV-VIS SPECTRA

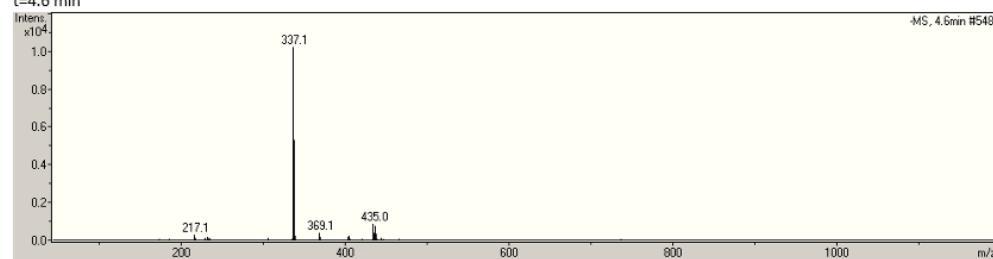


## MASS SPECTRA

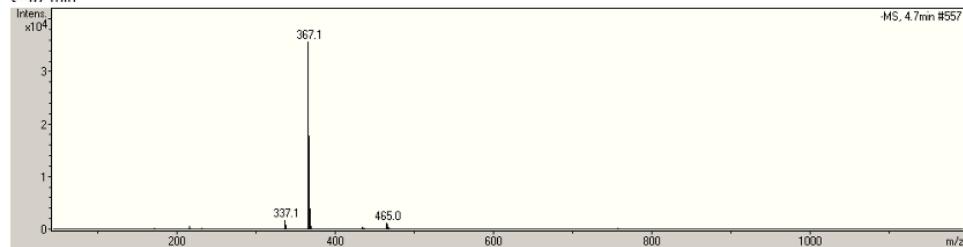
MS (negative mode)



t=4.6 min



t=4.7 min



### S-8.73. Uranine A

#### GENERAL INFORMATION

Alternative name: Fluorescein

Color Index Name: Acid Yellow 73

Color Index Number: 45350

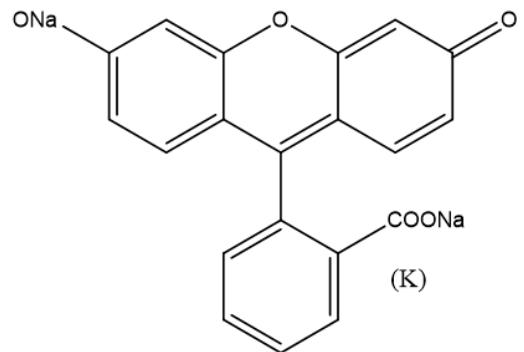
Type of dye: Xanthene

Charge: -1

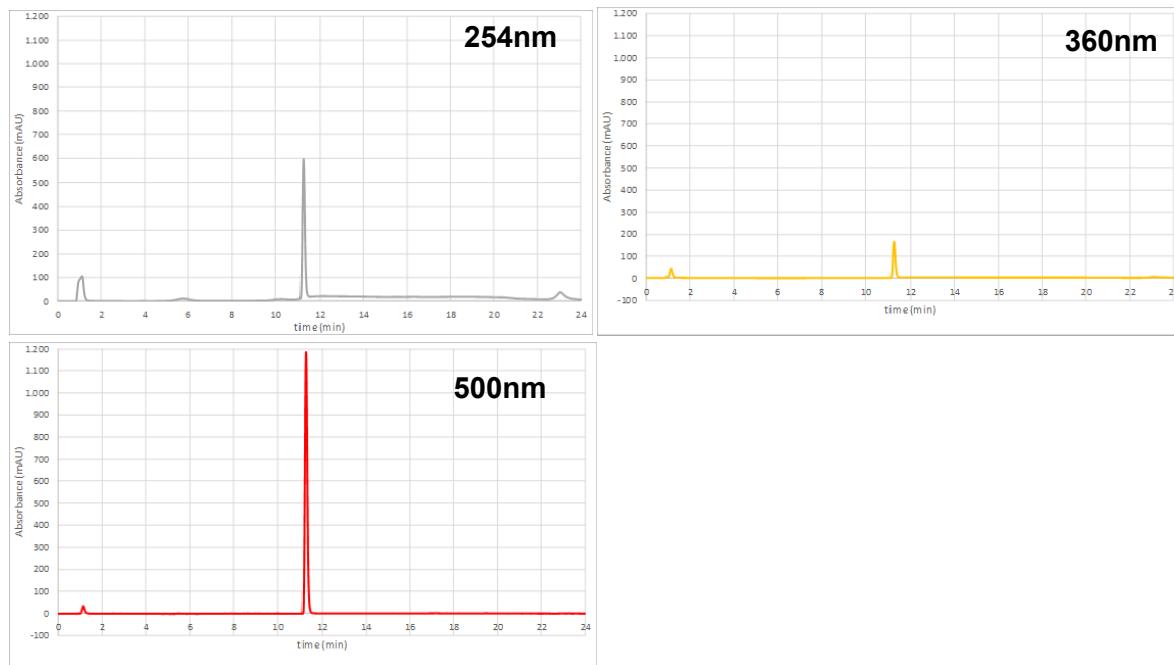
Molecular Formula: C<sub>20</sub>H<sub>11</sub>O<sub>5</sub> (ion, -1, ONa replaced with OH)

#### Molecular Weight

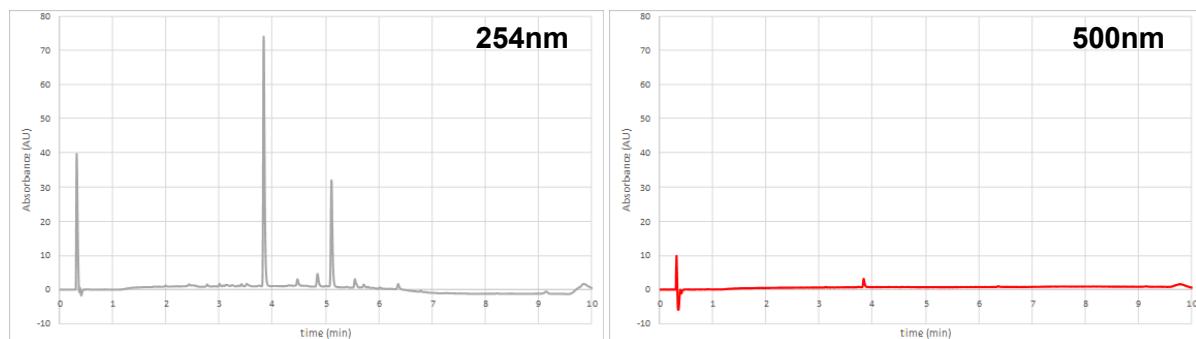
Full molecule:	376.27
Ion (-1)	331.30
Ion (-1), monoisotopic	331.06



#### CHROMATOGRAMS: ION-EXCHANGE



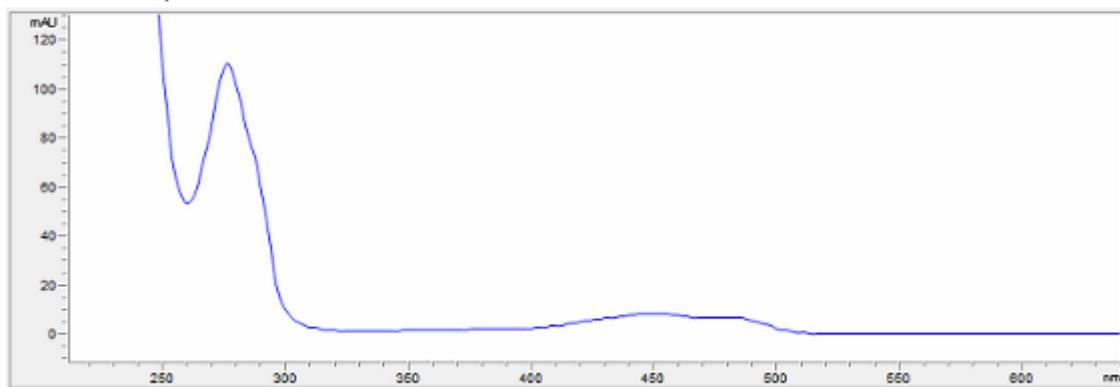
#### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

t=3.84 min

$\lambda_{\text{max}} = 276 \text{ nm}; 452 \text{ nm}$



## MASS SPECTRA

MS (negative mode)

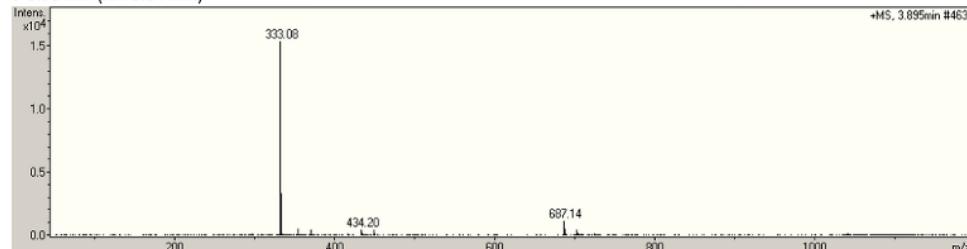
t=3.88 min



m/z	I	Formula
331.07	24527	[M] <sup>-</sup>
995.21	598	3[M] <sup>-</sup> •2H <sup>+</sup>

MS (positive mode)

t=3.90 min (RP: 3.84 min)



m/z	I	Formula
333.08	15421	[MH]•H <sup>+</sup>
434.20	424	[MH]•[TEAH] <sup>+</sup>
687.14	1068	2[MH]•Na <sup>+</sup>

## S-8.74. Vesuvine BA

### GENERAL INFORMATION

**Alternative name:** Bismark Brown Y

**Color Index Name:** Basic Brown 1

**Color Index Number:** 21000

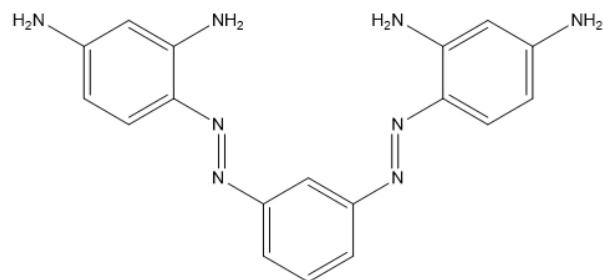
**Type of dye:** Diazo

**Charge:** 0

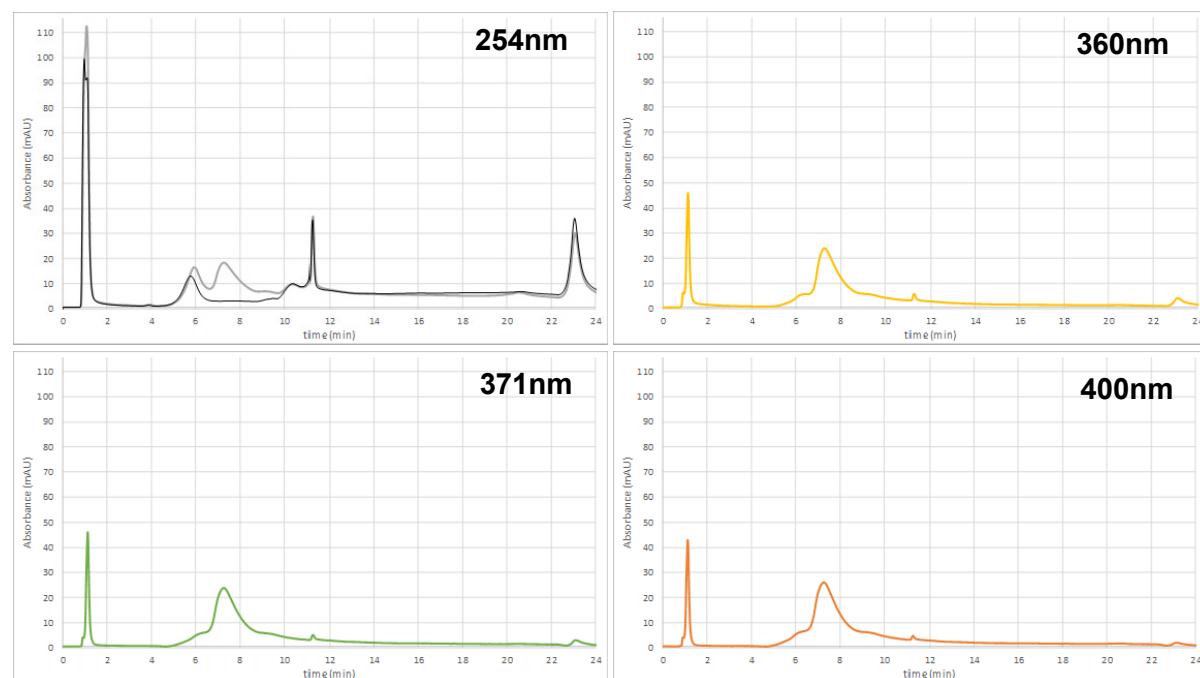
**Molecular Formula:** C<sub>18</sub>H<sub>18</sub>N<sub>8</sub>

**Molecular Weight**

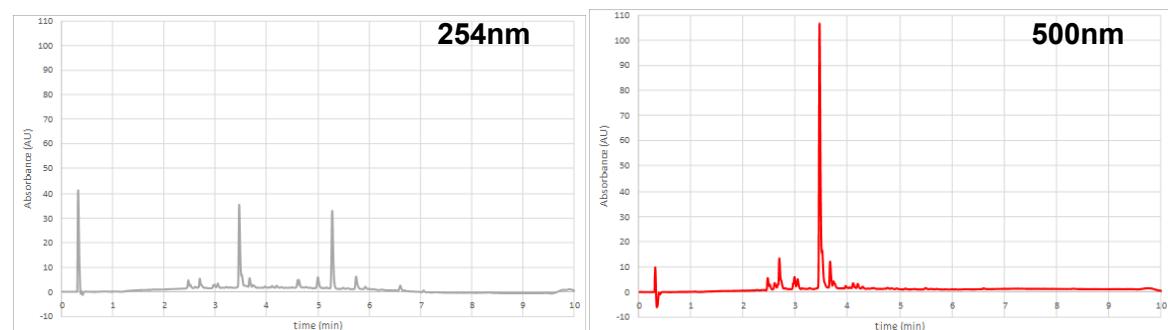
Full molecule:	346.39
Monoisotopic	346.17



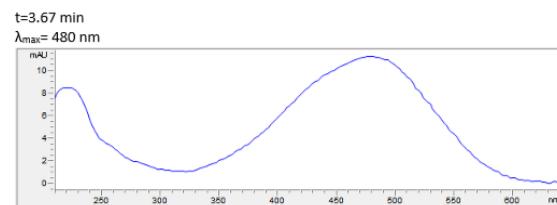
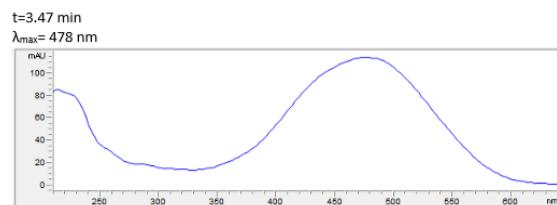
### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

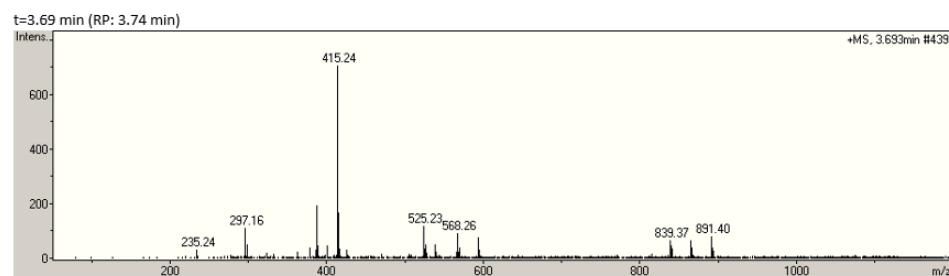
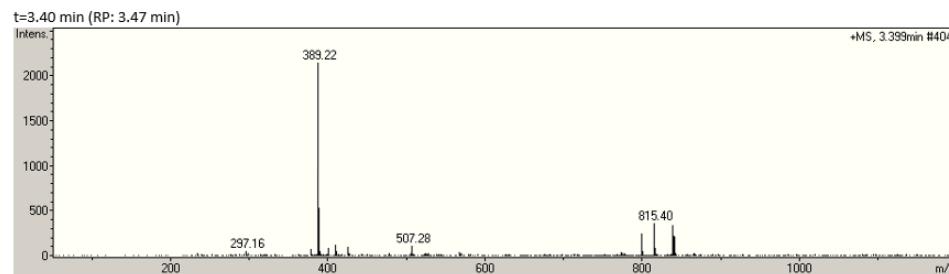
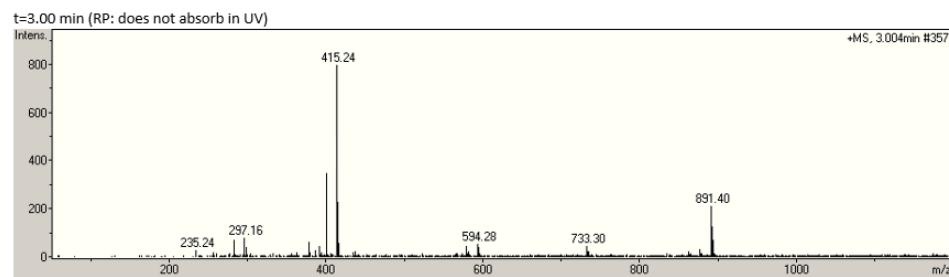


## UV-VIS SPECTRA



## MASS SPECTRA

MS (positive mode)

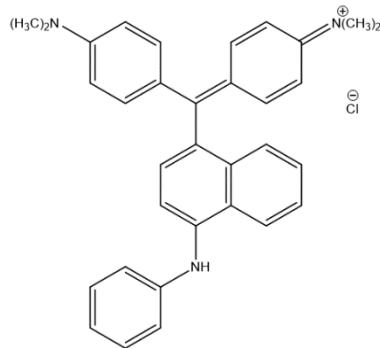


## S-8.75. Victoria Blue B

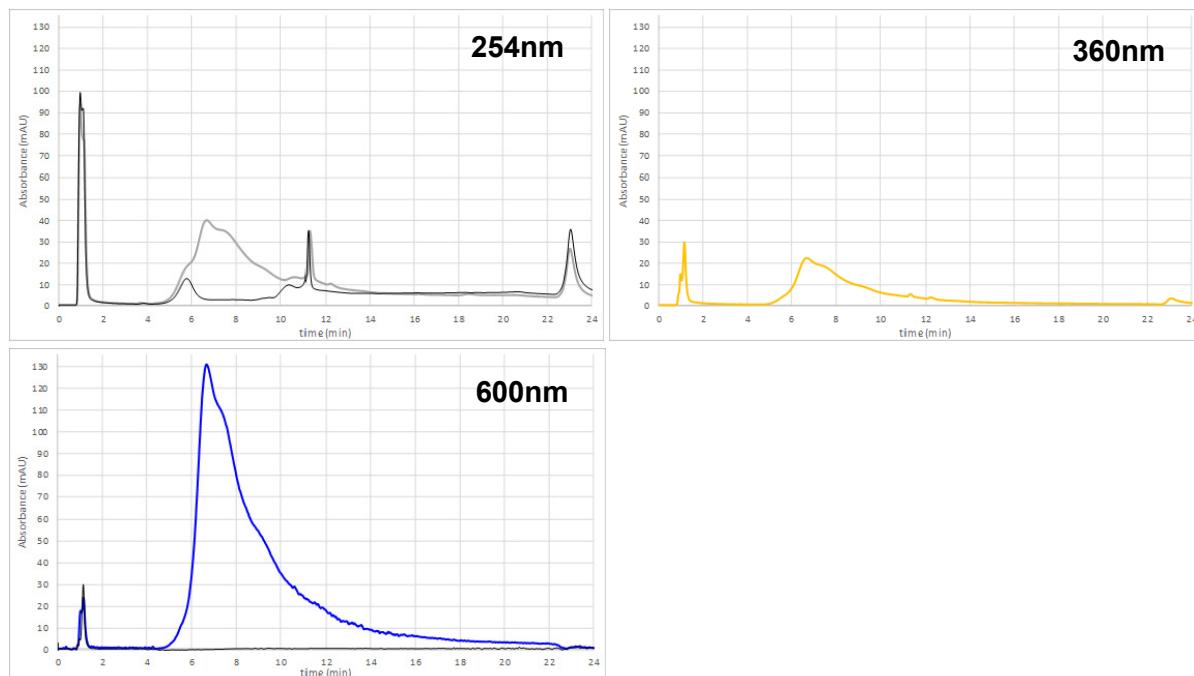
### GENERAL INFORMATION

**Color Index Name:** Basic Blue 26  
**Color Index Number:** 44045  
**Type of dye:** Triarylmethane  
**Charge:** +1  
**Molecular Formula:** C<sub>33</sub>H<sub>32</sub>N<sub>3</sub> (ion, +1)  
**Molecular Weight**

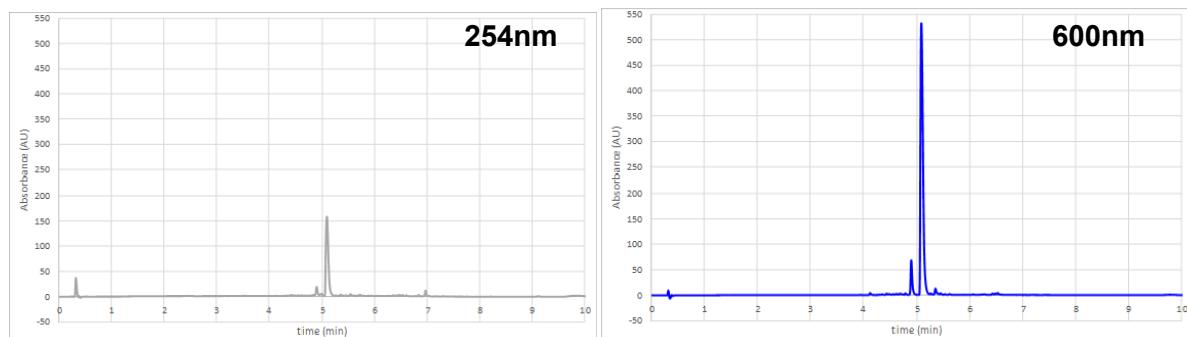
Full molecule:	506.08
Ion (+1)	470.63
Ion (+1), monoisotopic	470.26



### CHROMATOGRAMS: ION-EXCHANGE

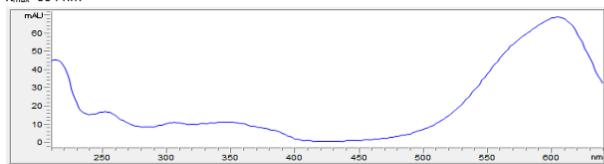


### CHROMATOGRAMS: REVERSED-PHASE

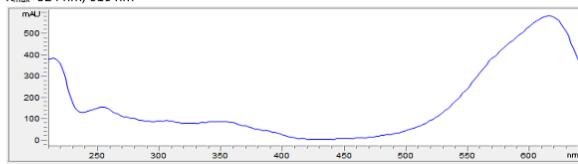


## UV-VIS SPECTRA

t=4.89 min  
 $\lambda_{\text{max}}=604 \text{ nm}$

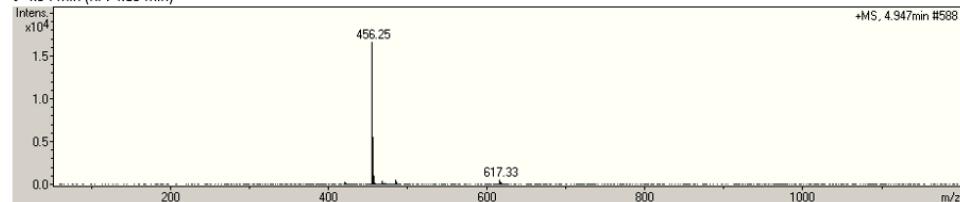


t=5.08 min  
 $\lambda_{\text{max}}=324 \text{ nm}; 616 \text{ nm}$



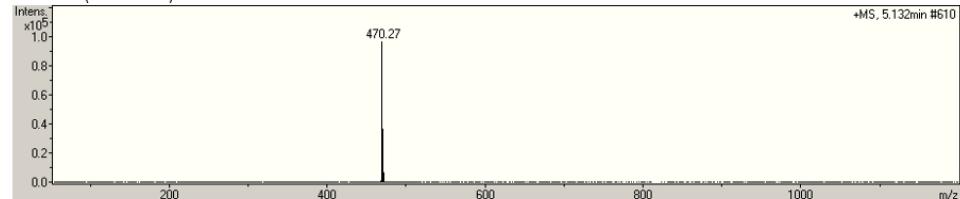
## MASS SPECTRA

t=4.94 min (RP: 4.89 min)



m/z	I	Formula
456.25	16618	[M-CH <sub>2</sub> ] <sup>+</sup>

t=5.13 min (RP: 5.08 min)



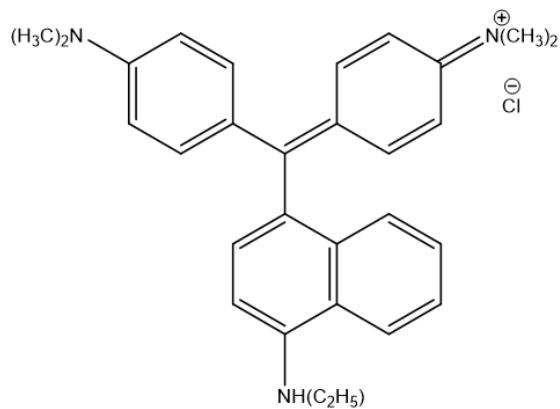
m/z	I	Formula
470.27	97256	[M] <sup>+</sup>

## S-8.76. Victoria Blue R

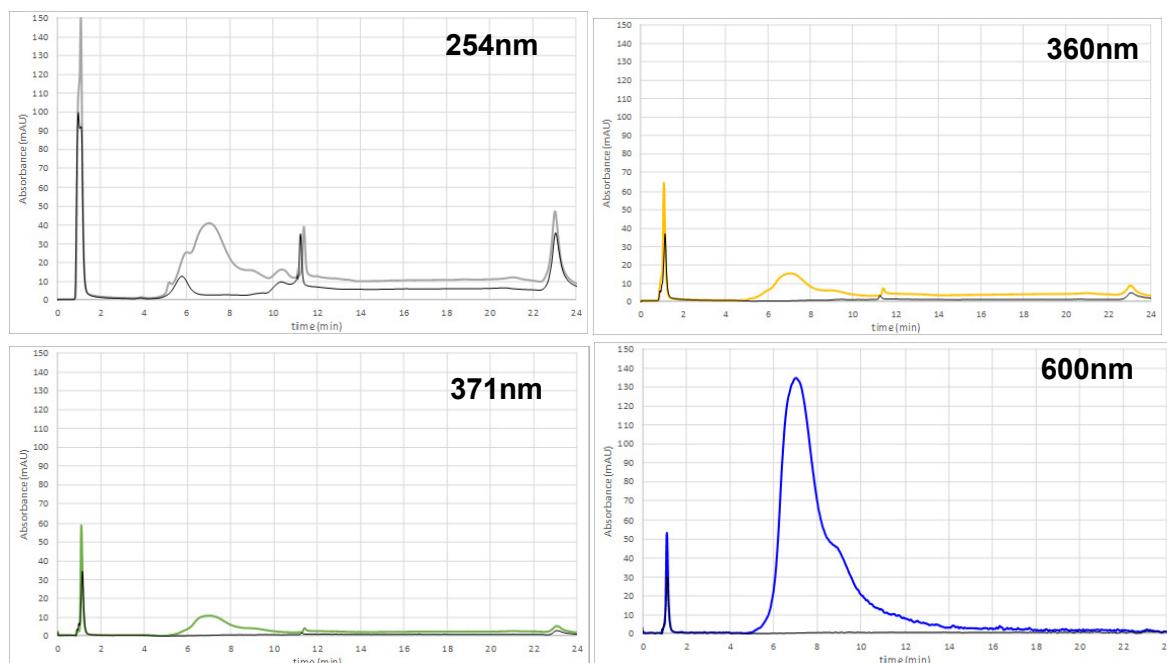
### GENERAL INFORMATION

**Color Index Name:** Basic Blue 11  
**Color Index Number:** 44040  
**Type of dye:** Triarylmethane  
**Charge:** +1  
**Molecular Formula:** C<sub>29</sub>H<sub>32</sub>N<sub>3</sub> (ion, +1)  
**Molecular Weight**

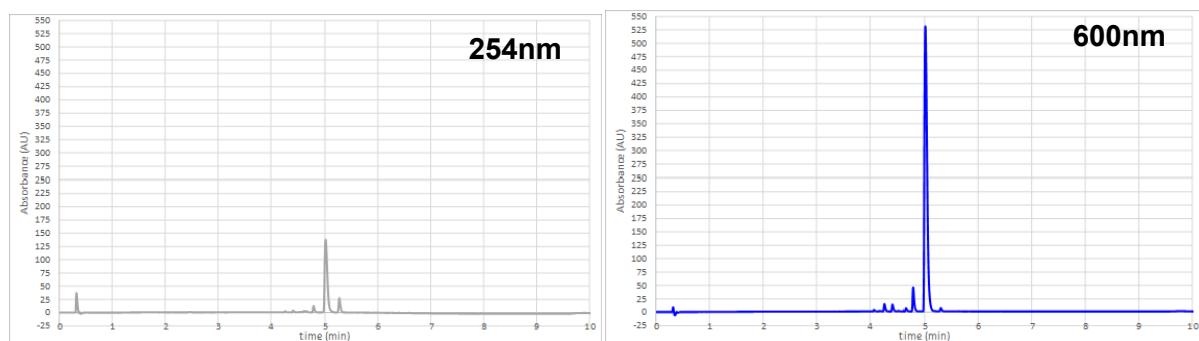
Full molecule:	458.04
Ion (+1)	422.58
Ion (+1), monoisotopic	422.26



### CHROMATOGRAMS: ION-EXCHANGE

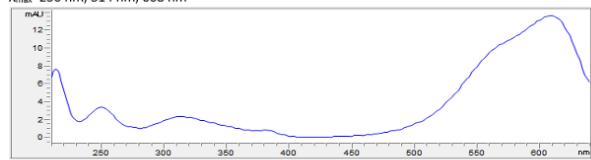


### CHROMATOGRAMS: REVERSED-PHASE

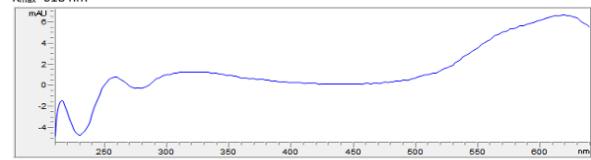


## UV-VIS SPECTRA

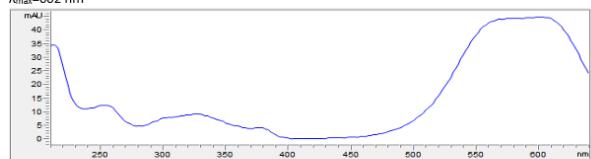
t=4.41 min  
 $\lambda_{\text{max}}=250 \text{ nm; } 314 \text{ nm; } 608 \text{ nm}$



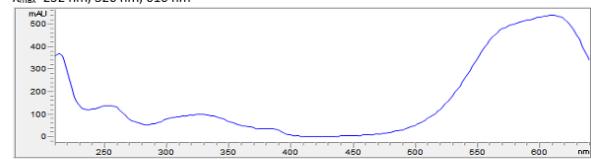
t=4.65 min  
 $\lambda_{\text{max}}=618 \text{ nm}$



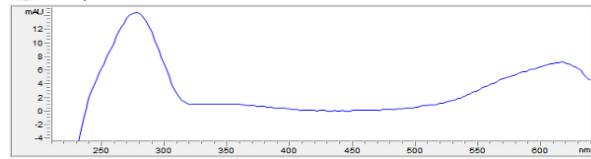
t=4.78 min  
 $\lambda_{\text{max}}=602 \text{ nm}$



t=5.10 min  
 $\lambda_{\text{max}}=252 \text{ nm; } 326 \text{ nm; } 610 \text{ nm}$

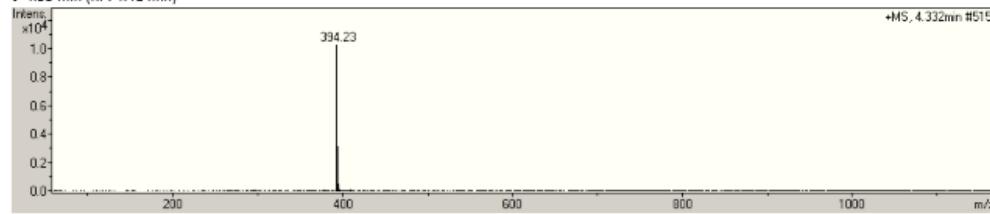


t=5.30 min  
 $\lambda_{\text{max}}=278 \text{ nm; } 616 \text{ nm}$

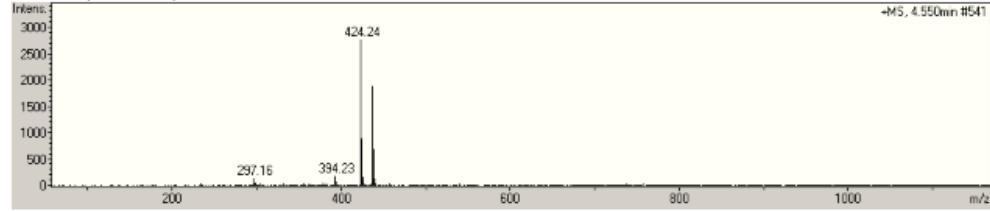


## MASS SPECTRA

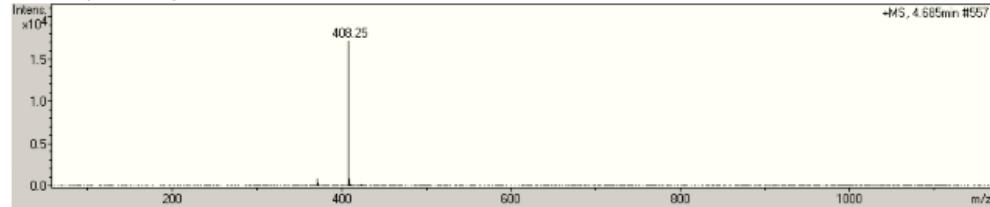
t=4.33 min (RP: 4.41 min)



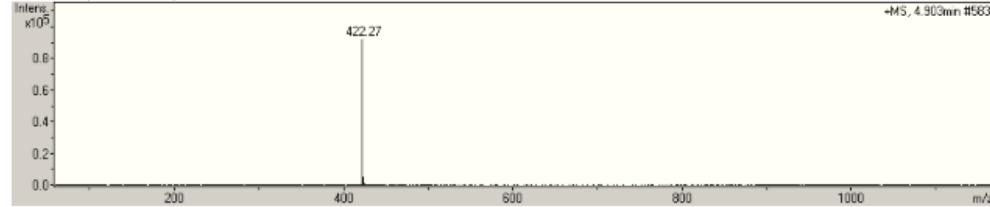
t=4.55 min (RP: 4.65 min)



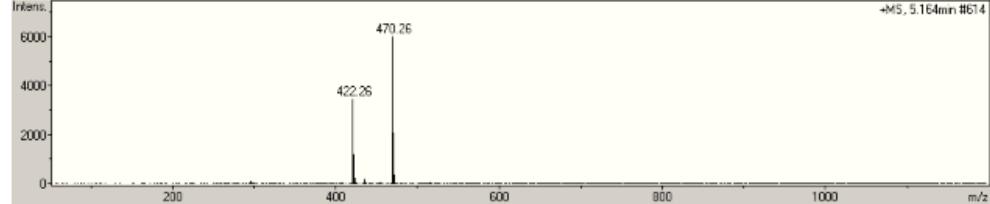
t=4.69 min (RP: 4.78 min)



t=4.90 min (RP: 5.10 min)



t=5.16 min (RP: 5.30 min)



## S-8.77. Water Blue IN

### GENERAL INFORMATION

**Alternative names:** Methyl Blue; Anilin Blue

**Color Index Name:** Acid Blue 93

**Color Index Number:** 42780

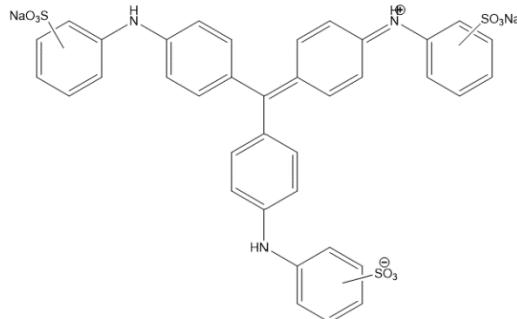
**Type of dye:** Triarylmethane

**Charge:** -3

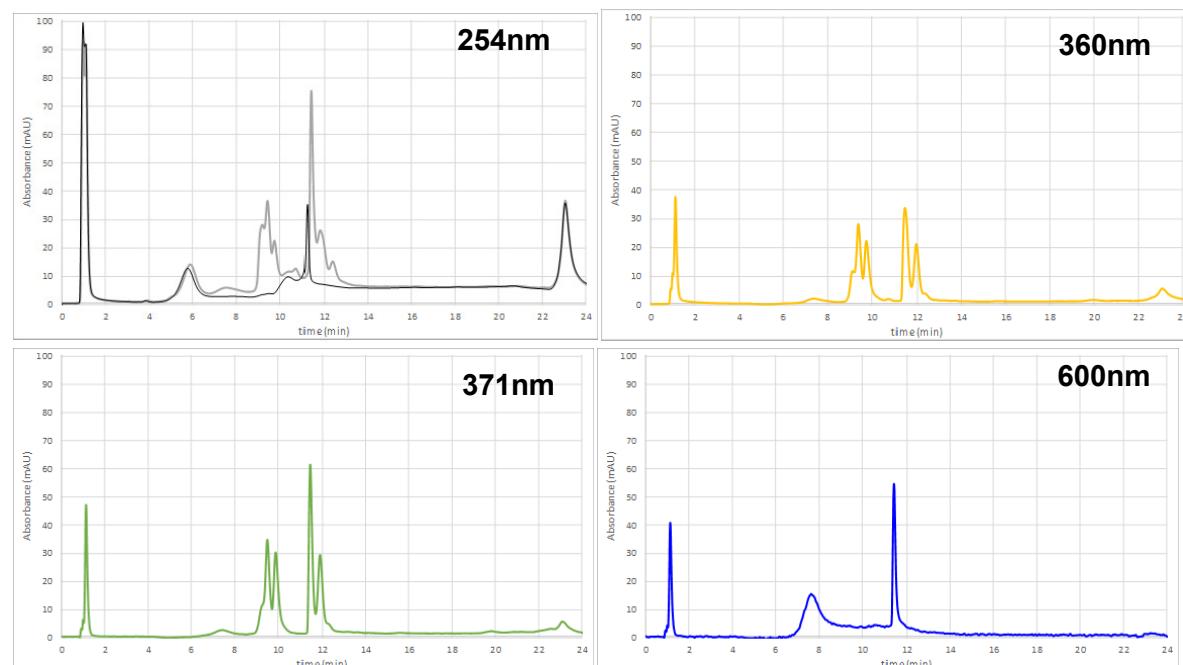
**Molecular Formula:** C<sub>37</sub>H<sub>27</sub>N<sub>3</sub>O<sub>9</sub>S<sub>3</sub> (ion, -3)

**Molecular Weight**

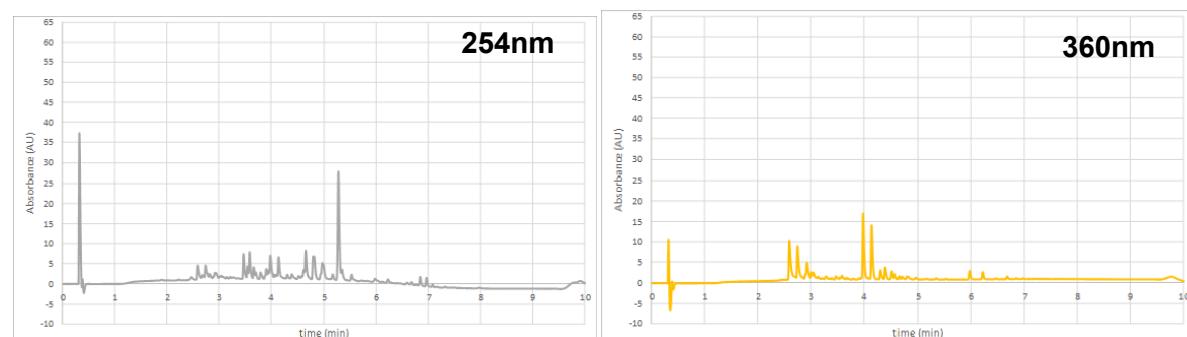
Full molecule:	799.80
Ion (-3)	753.82
Ion (-3), monoisotopic	753.09

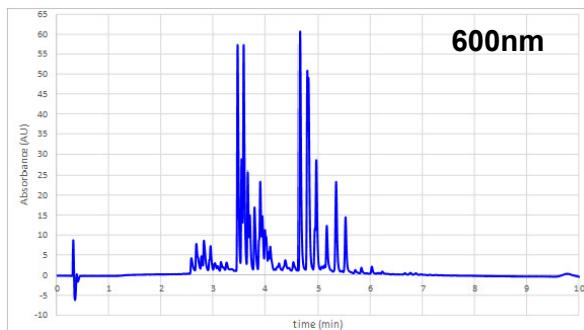


### CHROMATOGRAMS: ION-EXCHANGE

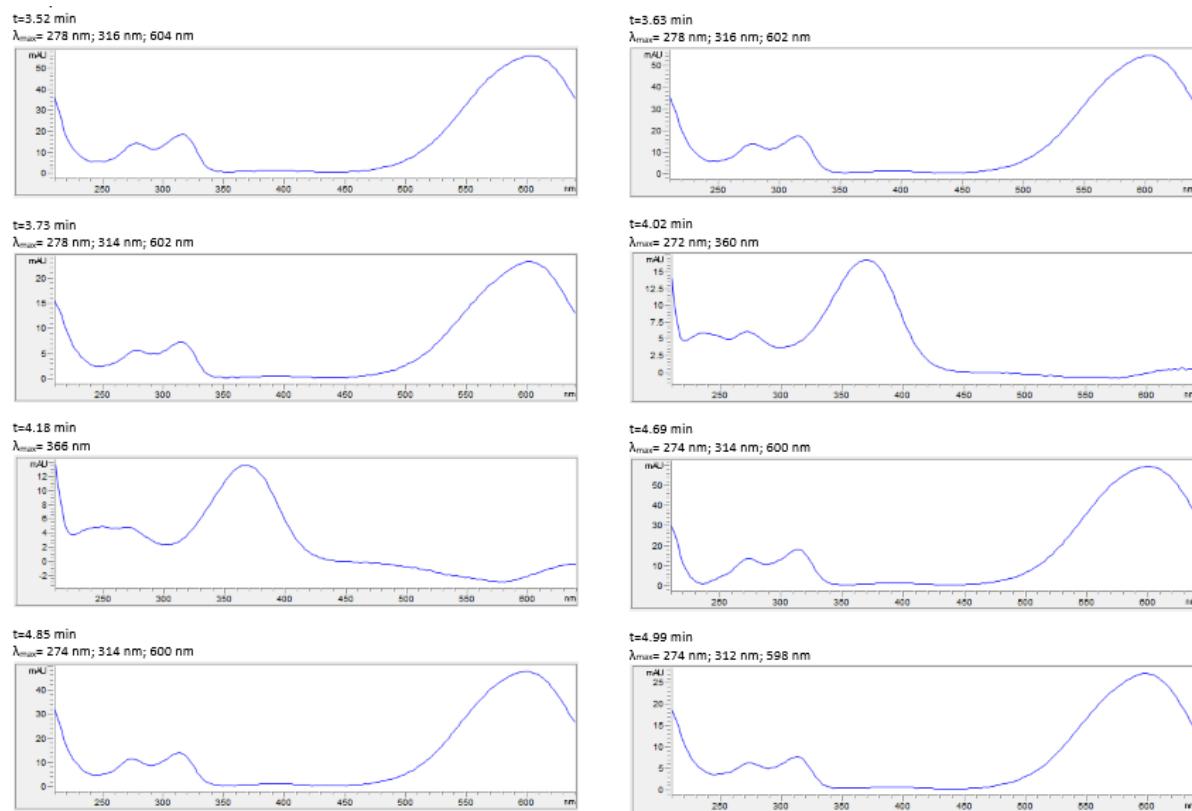


### CHROMATOGRAMS: REVERSED-PHASE

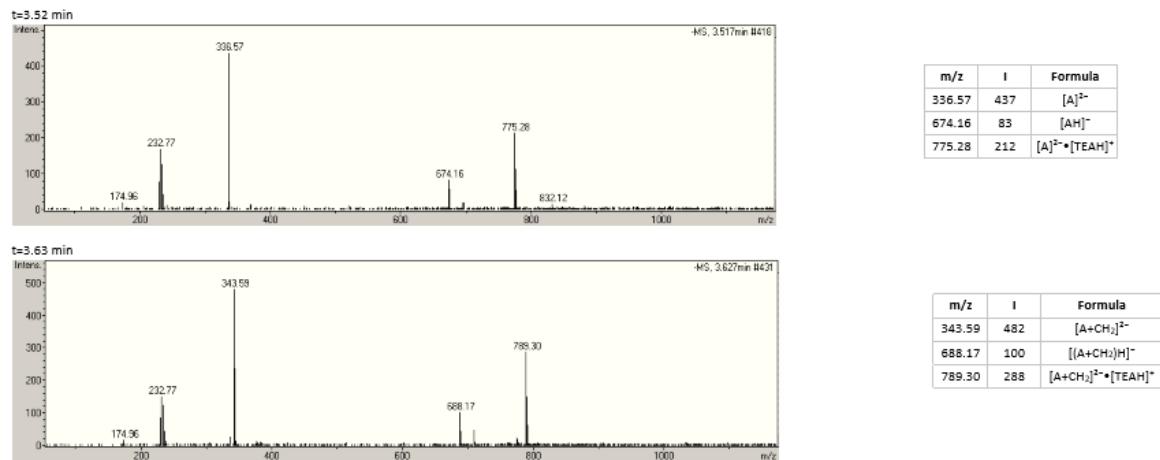


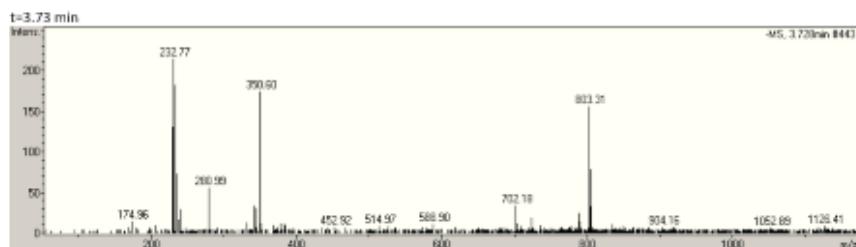


## UV-VIS SPECTRA

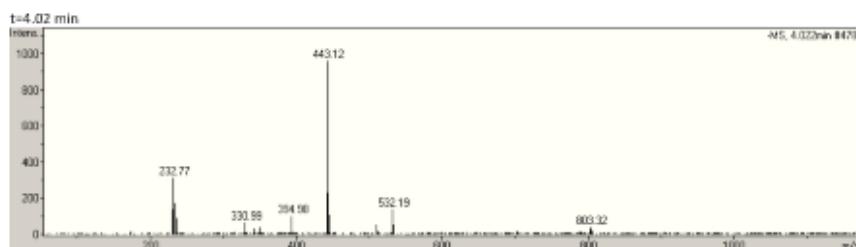


## MASS SPECTRA

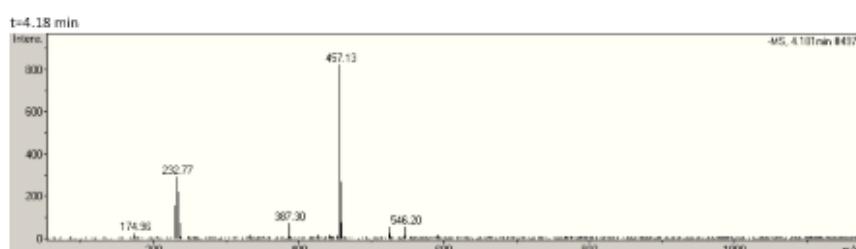




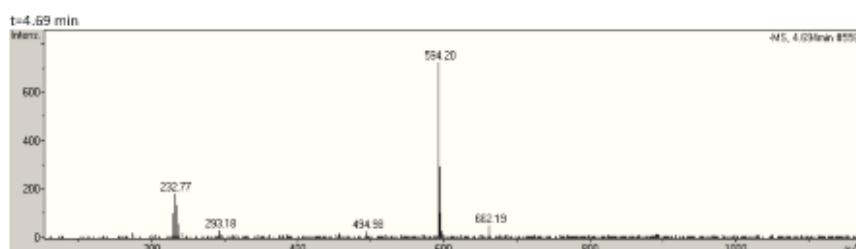
m/z	I	Formula
350.60	174	[A+2CH <sub>2</sub> ] <sup>2-</sup>
702.18	33	[(A+2CH <sub>2</sub> )H] <sup>-</sup>
803.31	156	[A+2CH <sub>2</sub> ] <sup>2-</sup> *[TEAH] <sup>+</sup>



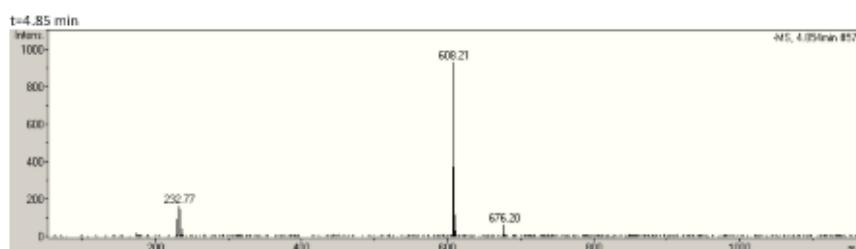
m/z	I	Formula
443.12	964	[B] <sup>-</sup>



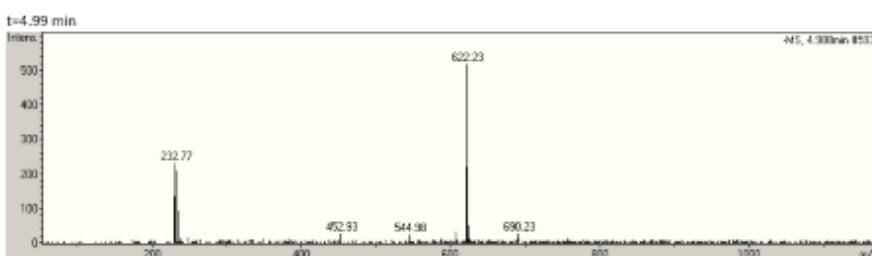
m/z	I	Formula
457.13	824	[B+CH <sub>2</sub> ] <sup>-</sup>



m/z	I	Formula
594.20	727	[A-SD <sub>1</sub> ] <sup>-</sup>



m/z	I	Formula
608.21	932	[(A+CH <sub>2</sub> )-SD <sub>1</sub> ] <sup>-</sup>



m/z	I	Formula
622.23	517	[(A+2CH <sub>2</sub> )-SO <sub>3</sub> ] <sup>-</sup>

Two unknown compounds were detected, indicated with A and B. These two components have mass 674.16 and 443.12 respectively.

## S-8.78. Wool Red B

### GENERAL INFORMATION

**Alternative Name:** Cloth Red B

**Color Index Name:** Acid Red 115

**Color Index Number:** 27200

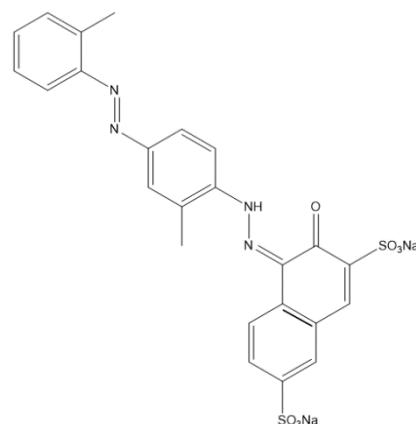
**Type of dye:** Diazo

**Charge:** -2

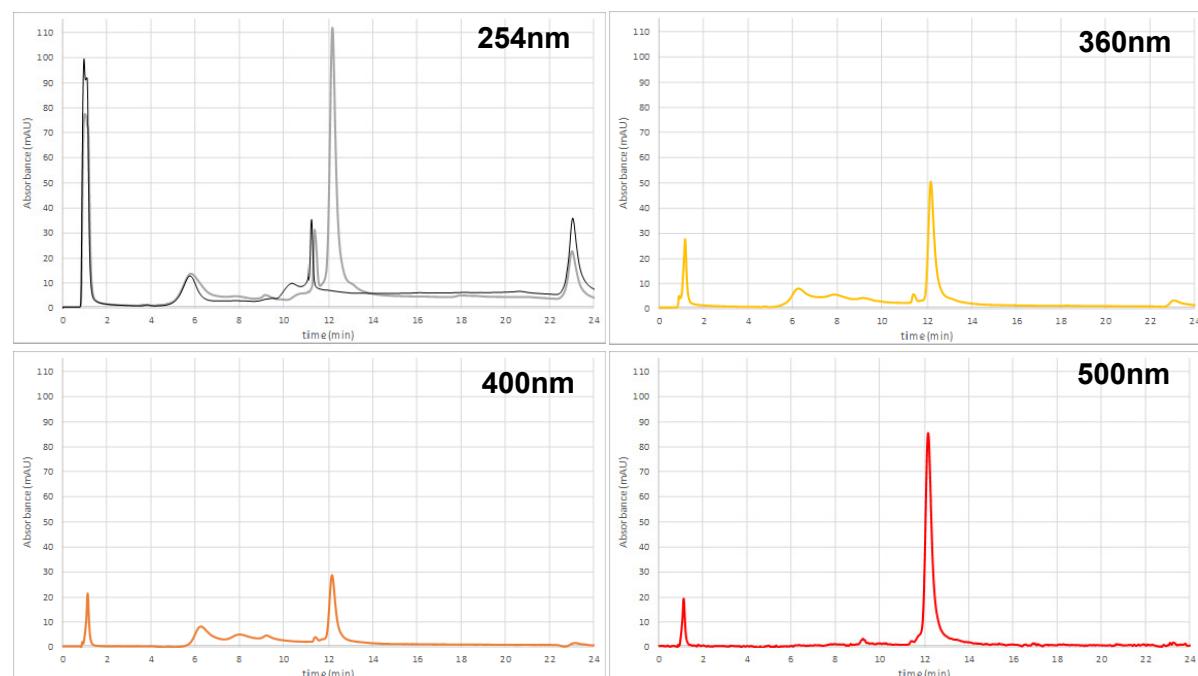
**Molecular Formula:** C<sub>24</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>S<sub>2</sub> (ion, -2)

**Molecular Weight**

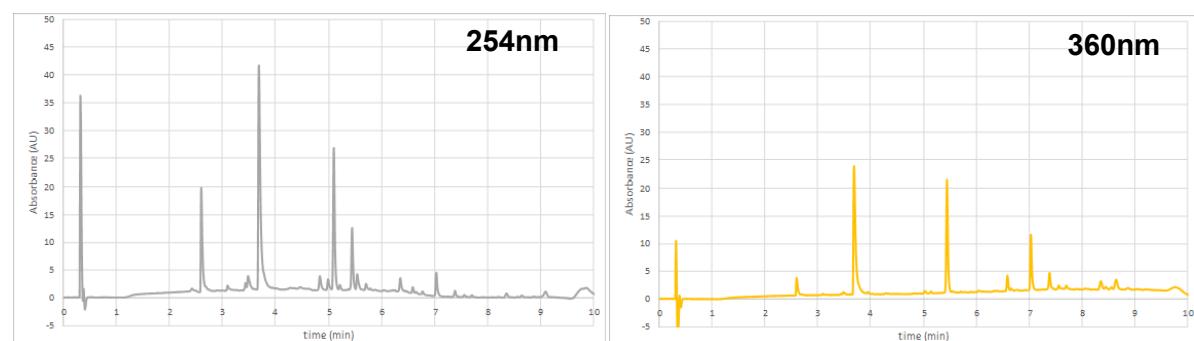
Full molecule:	584.53
Ion (-2)	538.55
Ion (-2), monoisotopic	538.06

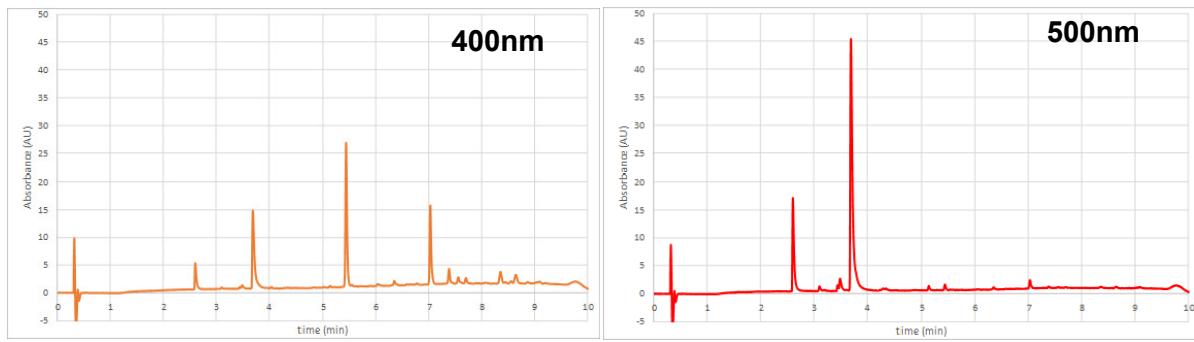


### CHROMATOGRAMS: ION-EXCHANGE

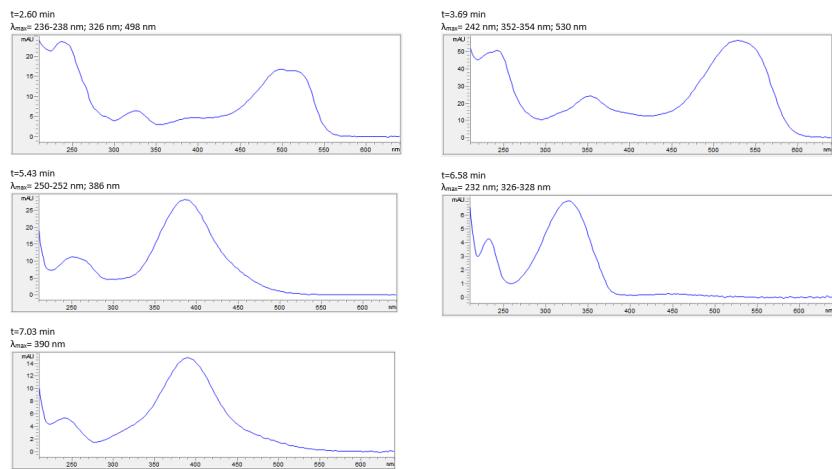


### CHROMATOGRAMS: REVERSED-PHASE





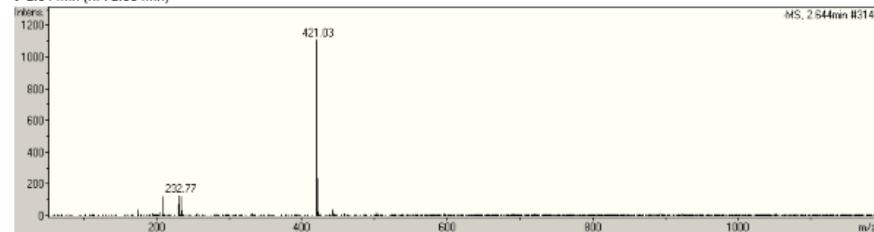
## UV-VIS SPECTRA



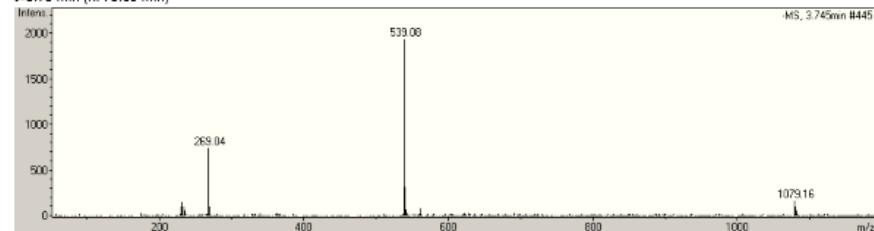
## MASS SPECTRA

MS (negative mode)

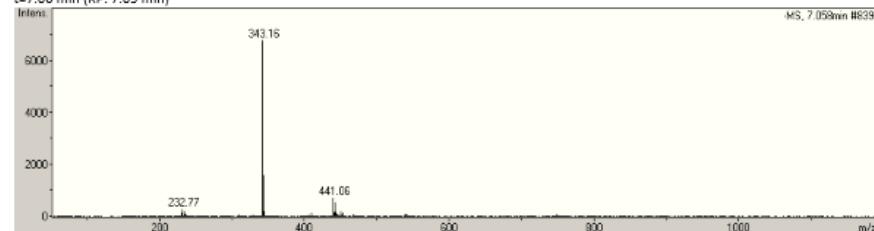
t=2.64 min (RP: 2.60 min)



t=3.75 min (RP: 3.69 min)

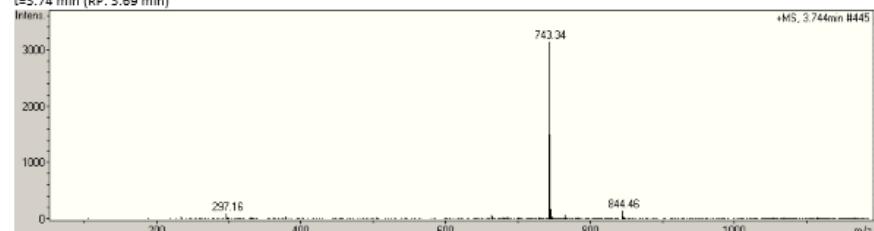


t=7.06 min (RP: 7.03 min)



MS (positive mode)

t=3.74 min (RP: 3.69 min)

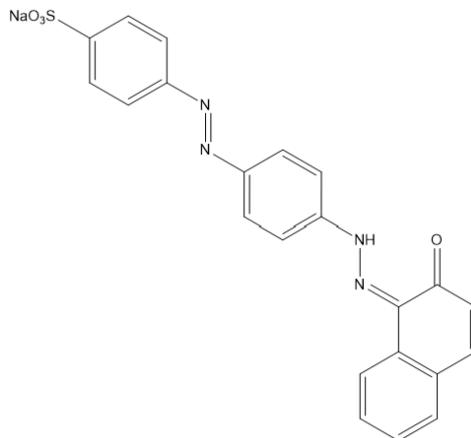


## S-8.79. Wool/Cloth Scarlet

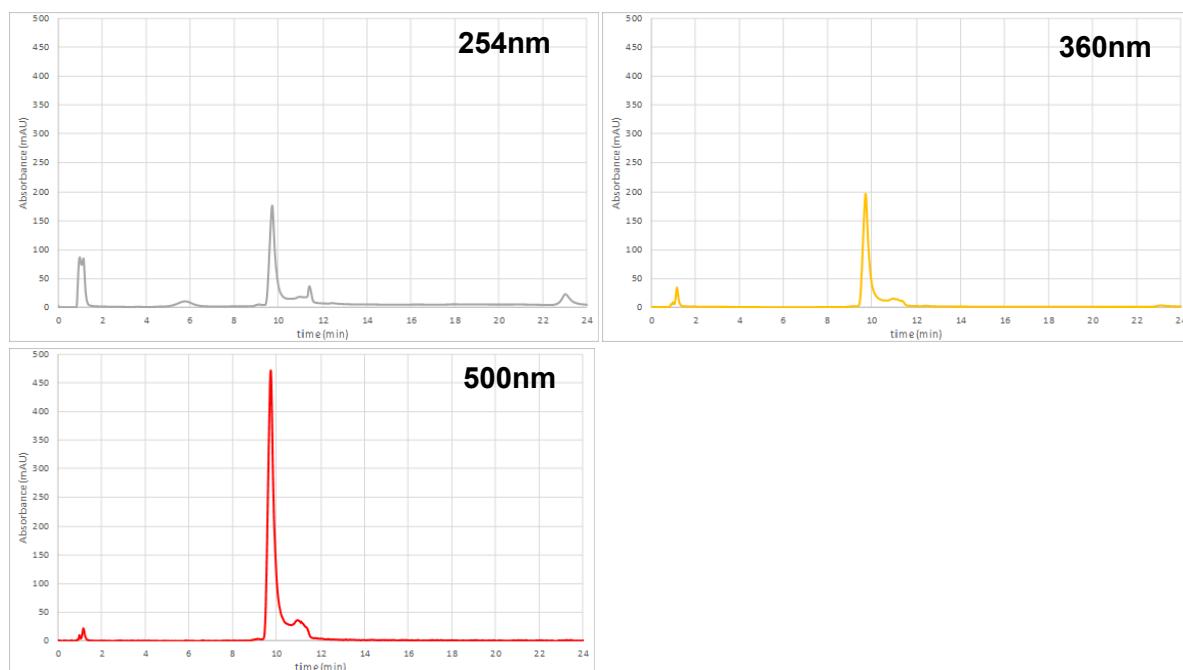
### GENERAL INFORMATION

**Color Index Name:** Acid Red 151  
**Color Index Number:** 26900  
**Type of dye:** Diazo  
**Charge:** -1  
**Molecular Formula:** C<sub>22</sub>H<sub>15</sub>N<sub>4</sub>O<sub>4</sub>S (ion, -1)  
**Molecular Weight**

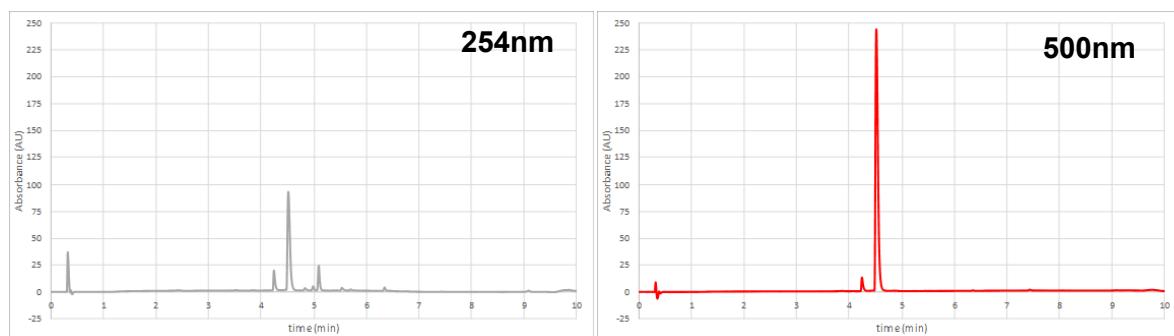
Full molecule:	454.43
Ion (-1)	431.44
Ion (-1), monoisotopic	431.08



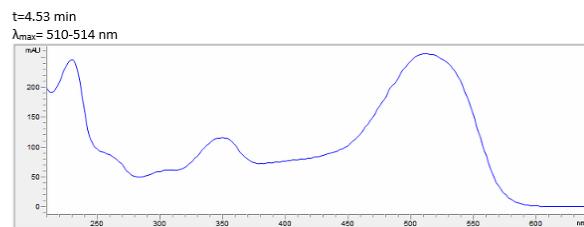
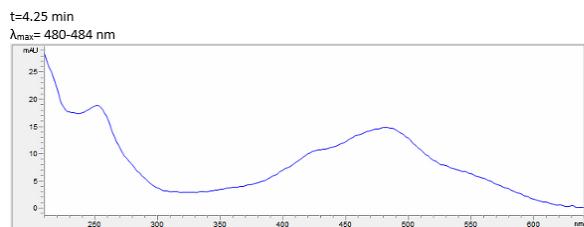
### CHROMATOGRAMS: ION-EXCHANGE



### CHROMATOGRAMS: REVERSED-PHASE

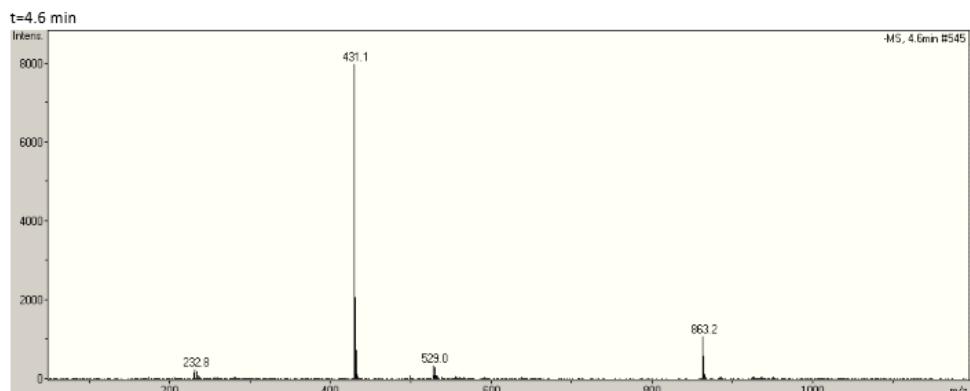
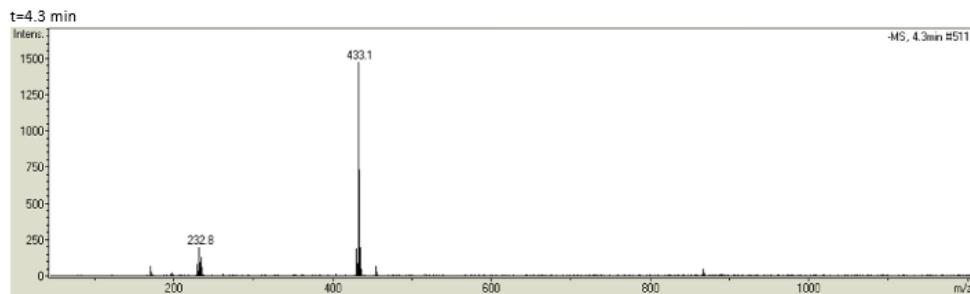


## UV-VIS SPECTRA

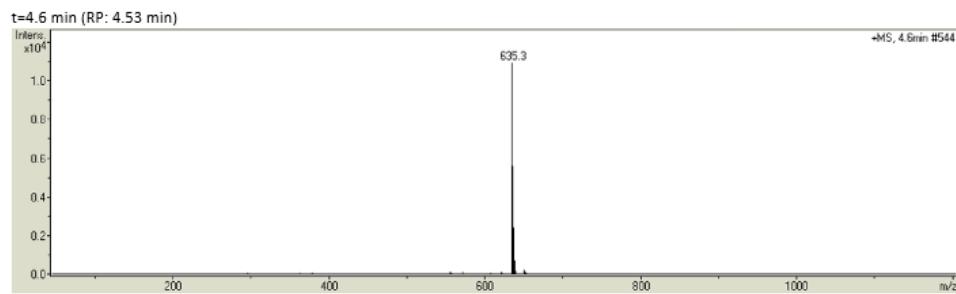
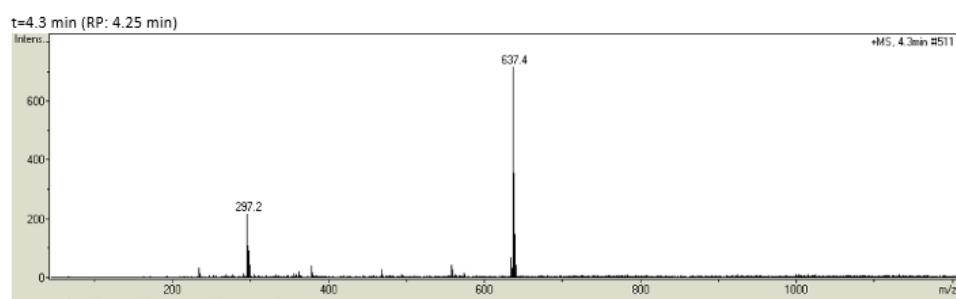


## MASS SPECTRA

MS (negative mode)



MS (positive mode)

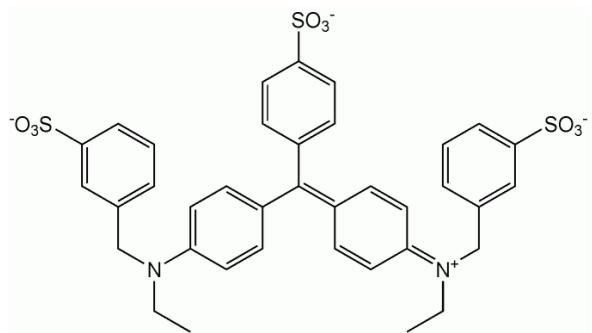


## S-8.80. Yellowish Light Green SF

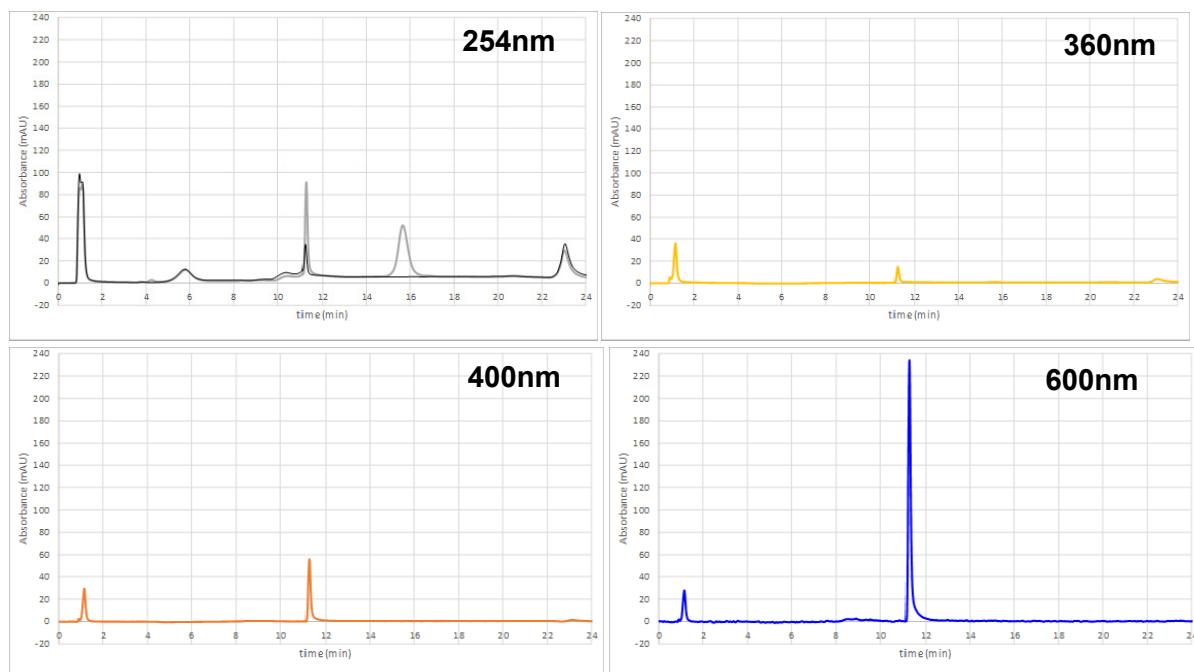
### GENERAL INFORMATION

**Color Index Name:** Acid Green 5  
**Color Index Number:** 42095  
**Type of dye:** Triarylmethane  
**Charge:** -3  
**Molecular Formula:** C<sub>37</sub>H<sub>34</sub>N<sub>2</sub>O<sub>9</sub>S<sub>3</sub> (ion, -3)  
**Molecular Weight**

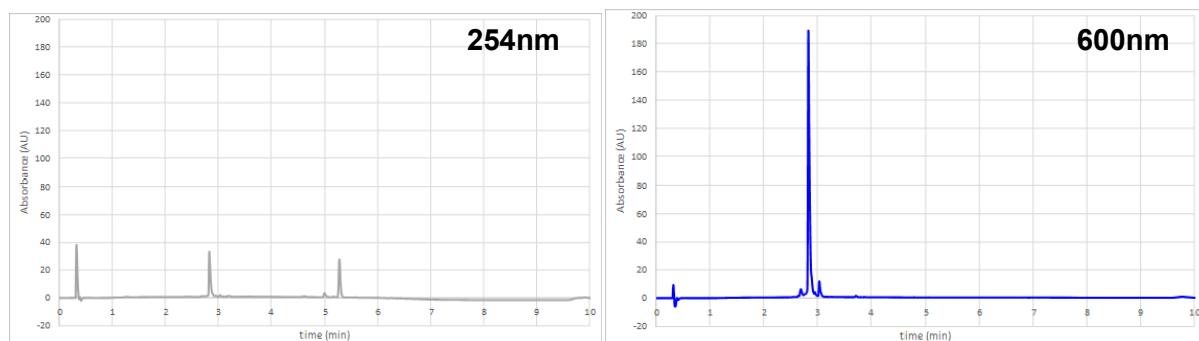
Full molecule:	792.85
Ion (-3)	746.87
Ion (-3), monoisotopic	746.13



### CHROMATOGRAMS: ION-EXCHANGE



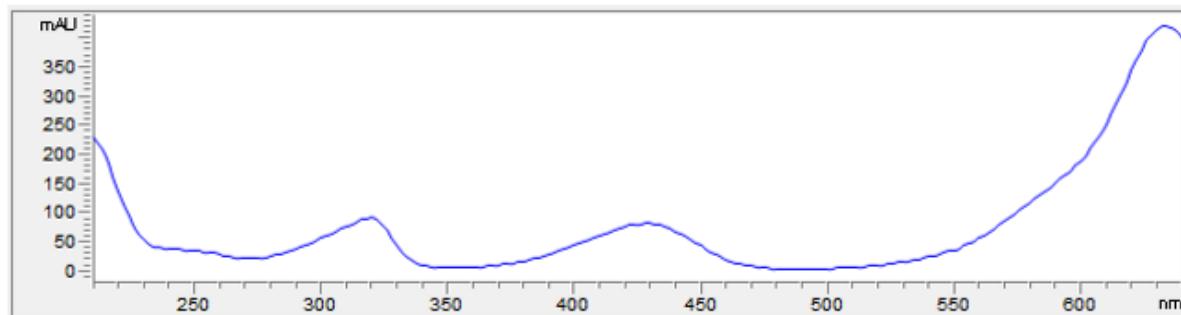
### CHROMATOGRAMS: REVERSED-PHASE



## UV-VIS SPECTRA

t=2.83 min

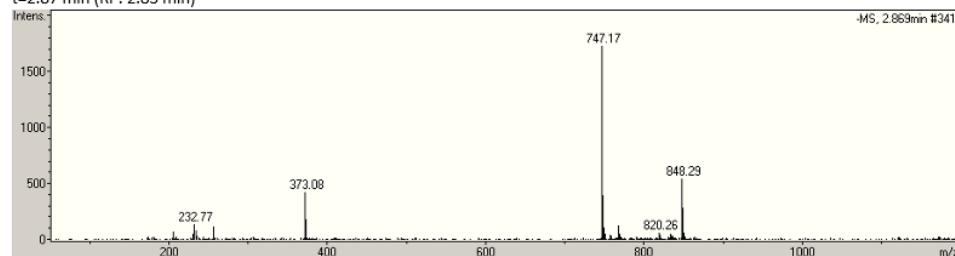
$\lambda_{\text{max}} = 320 \text{ nm}; 428 \text{ nm}; 632\text{-}634 \text{ nm}$



## MASS SPECTRA

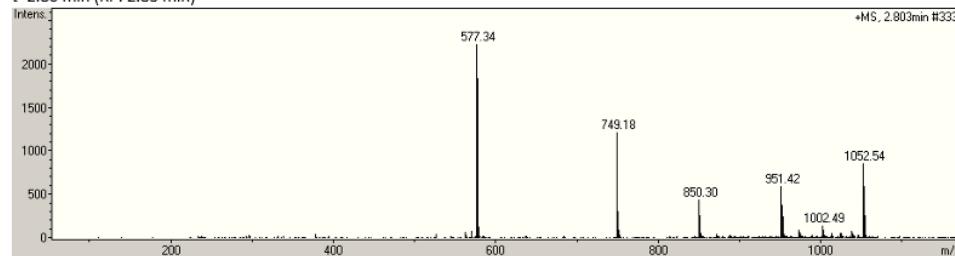
MS (negative mode)

t=2.87 min (RP: 2.83 min)



MS (positive mode)

t=2.80 min (RP: 2.83 min)



## References

- (1) Valianou, L.; Karapanagiotis, I.; Chryssoulakis, Y. Comparison of Extraction Methods for the Analysis of Natural Dyes in Historical Textiles by High-Performance Liquid Chromatography. *Anal. Bioanal. Chem.* **2009**, 395 (7), 2175–2189.  
<https://doi.org/10.1007/s00216-009-3137-6>.
- (2) Pirok, B. W. J.; Stoll, D. R.; Schoenmakers, P. J. Recent Developments in Two-Dimensional Liquid Chromatography: Fundamental Improvements for Practical Applications. *Anal. Chem.* **2018**, acs.analchem.8b04841.  
<https://doi.org/10.1021/acs.analchem.8b04841>.
- (3) Pirok, B. W. J.; Gargano, A. F. G.; Schoenmakers, P. J. Optimizing Separations in On-Line Comprehensive Two-Dimensional Liquid Chromatography. *J. Sep. Sci.* **2018**, 41 (1), 68–98. <https://doi.org/10.1002/jssc.201700863>.
- (4) Camenzuli, M.; Schoenmakers, P. J. A New Measure of Orthogonality for Multi-Dimensional Chromatography. *Anal. Chim. Acta* **2014**, 838, 93–101.  
<https://doi.org/10.1016/j.aca.2014.05.048>.