

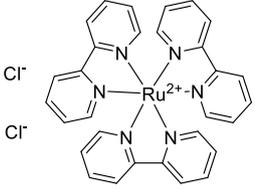
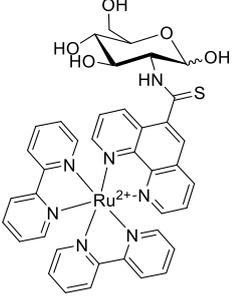
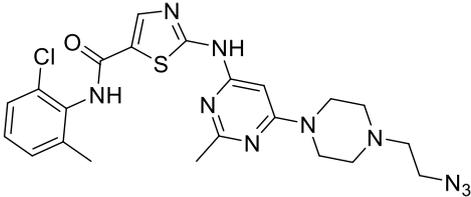
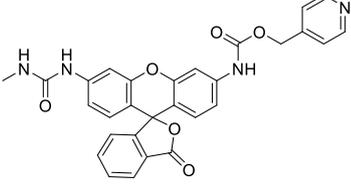
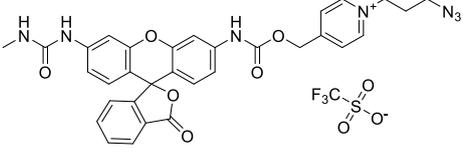
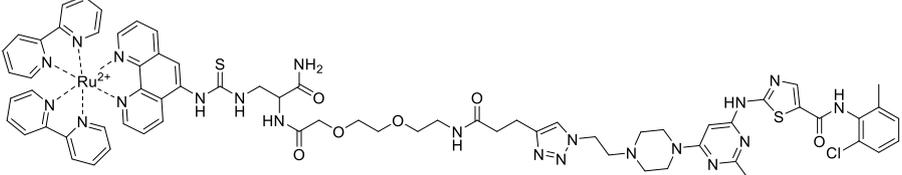
SUPPORTING INFORMATION

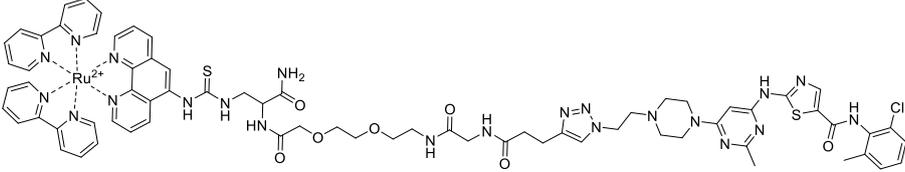
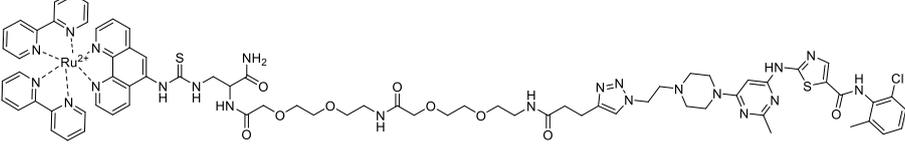
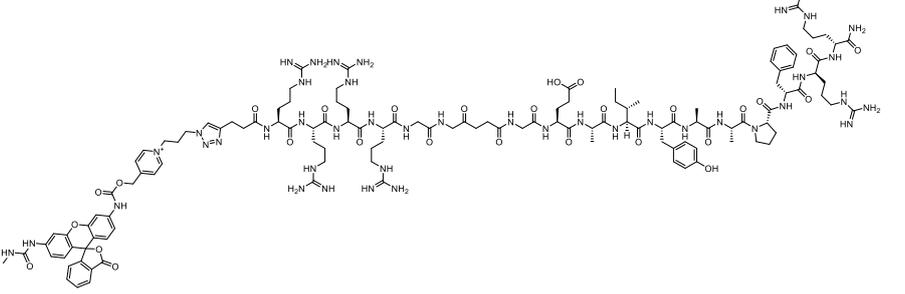
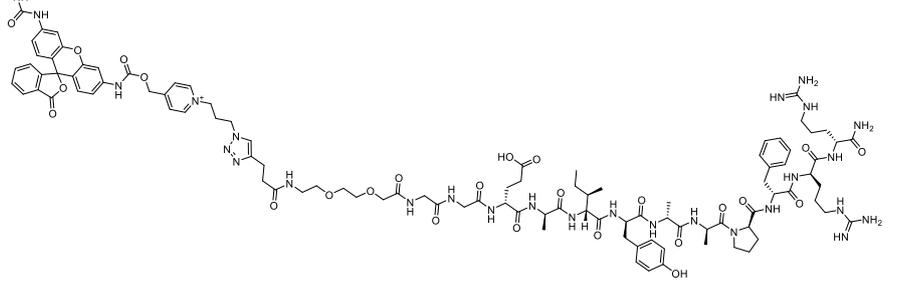
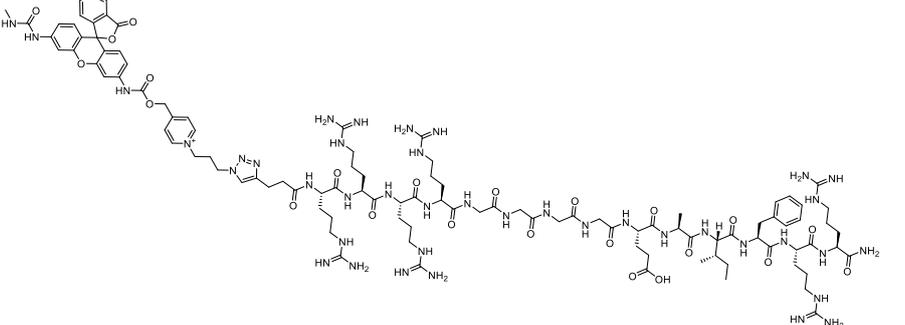
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Supplementary Figures

Figure S1: Peptide and Dasatinib probes used

	Peptide or Dasatinib Probe	Structure
1	Ruthenium trisbipyridine $\text{Ru}(\text{bpy})_3\text{Cl}_2$	
2	Glucosamine ruthenium GluAmRu^1	
3	Dasatinib Azide ²	
4	Rhodamine pyridine	
5	Rhodamine pyridinium	
6	Das-PEG-Ru	

7	Das-GPEG-Ru	
8	Das-PEG2-Ru	
9	PAbI-R4G2	
10	PAbI-PEG	
11	TR-PAbI-R4G2	

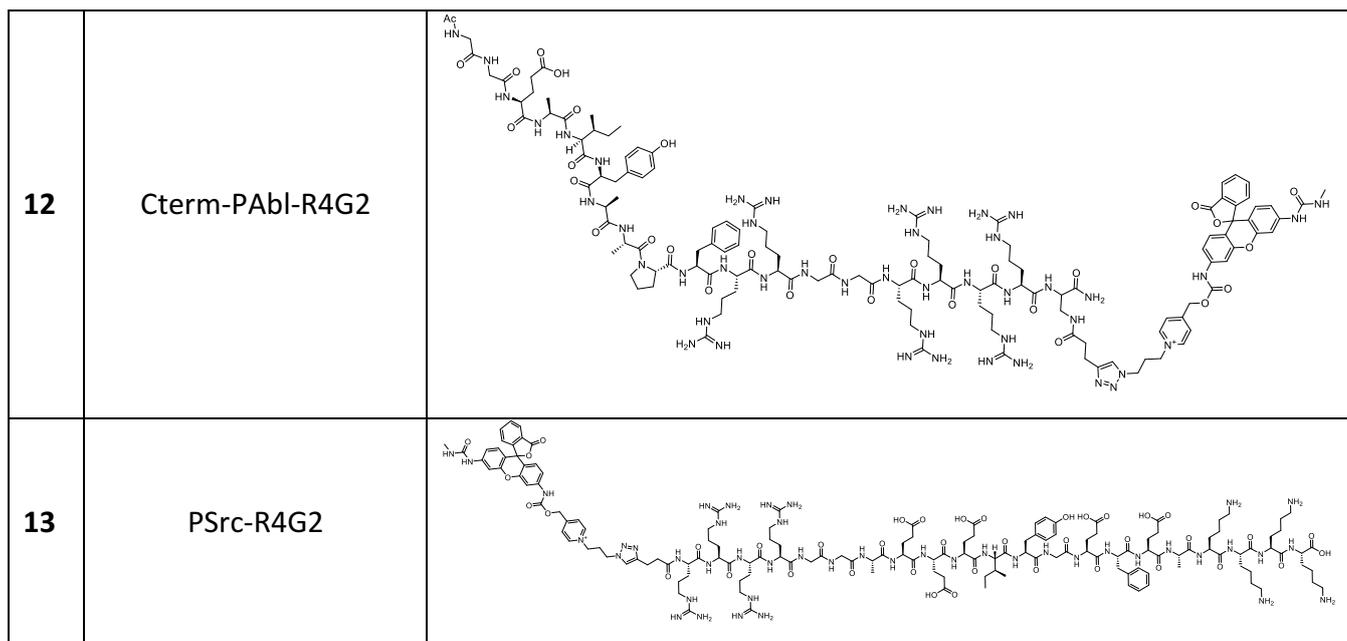


Figure S2 : Templated reaction between PAbI-R4G2 (9) and Das-GPEG-Ru (7)

Templated reaction between PAbI-R4G2 (9) and Das-GPEG-Ru (7) in presence of Abl or CA and dasatinib (3). Similar conditions as Fig 4B. with 90 minutes measurement of the kinase templated reaction. Grey curves shows the calculated signal to noise ratio (right axis)

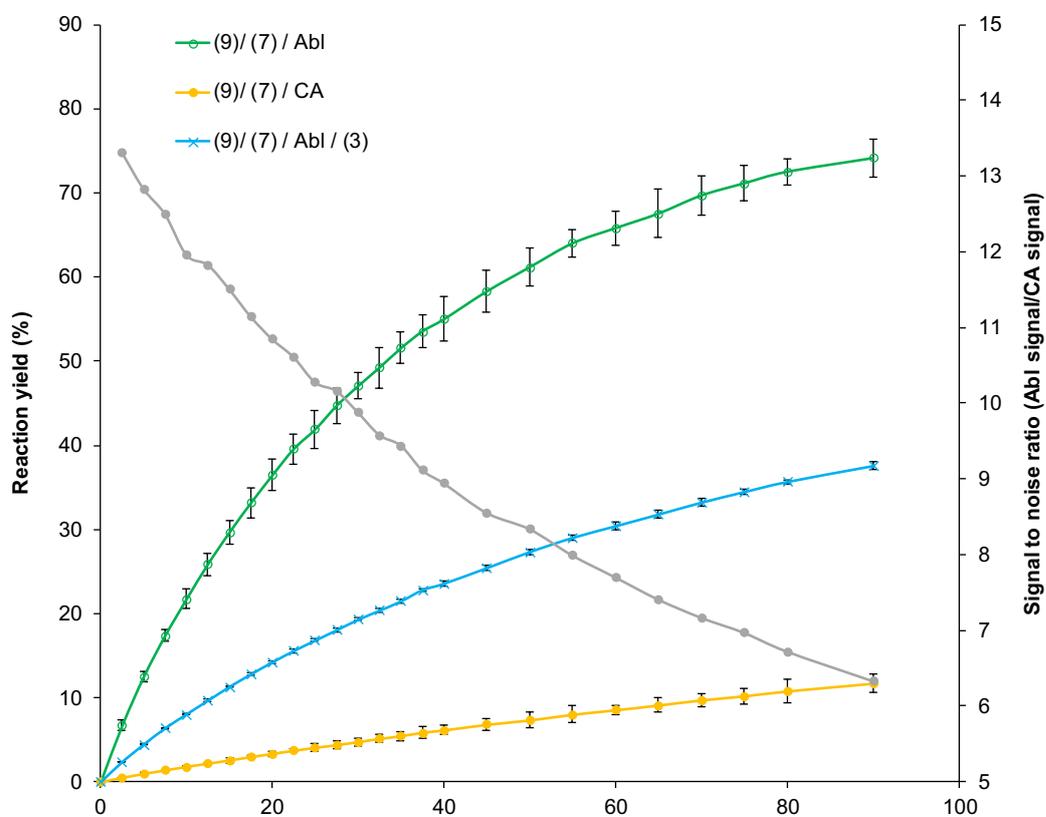
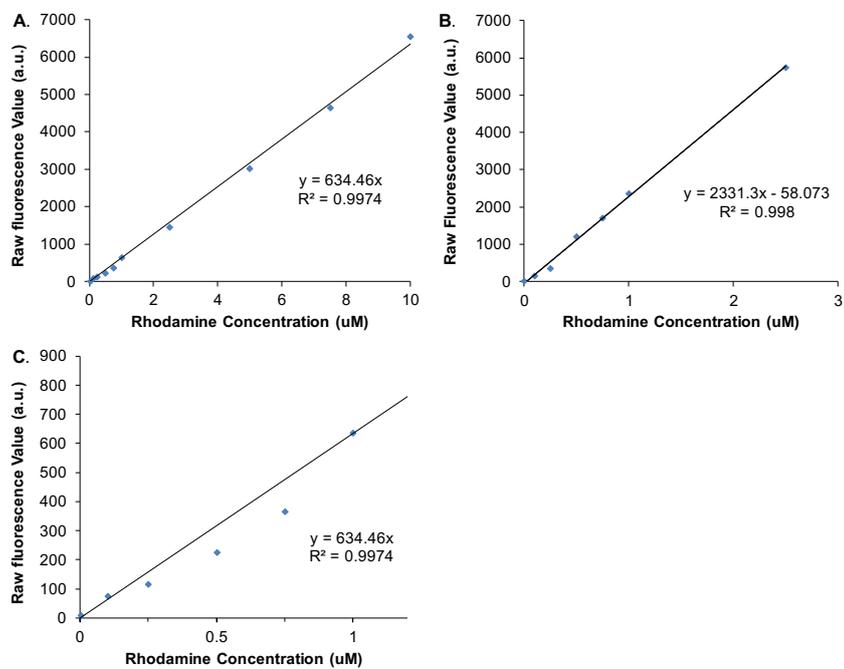


Figure S3: Rhodamine titration curve

- (A) Titration curve using 100 μL per well
- (B) Titration curve at 200 μL per well
- (C) Zoom between 0 and 1 μM of curve displayed in (A)



General techniques

Anhydrous solvents were obtained by passing them through a commercially available alumina column (Innovative technology, MA). Solid phase syntheses were performed with NovaPEG Rink amide resin obtained from EMD Millipore. Peptide synthesis was performed according to previously reported protocols³ using an automated peptide synthesizer (Intavis MultiPep instrument in 500 μ L fritted tubes.). LC-MS were recorded by using a Thermo Scientific Accela HPLC equipped with a Thermo C18 (5 cm x 2.1 mm, 1.9 μ m particles) Hypersil gold column coupled with A: Surveyor MSQ Plus spectrometer or B: LCQ Fleet mass spectrometer (both ESI, Thermo Scientific). Method: linear elution gradient for 95% H₂O 0.01% TFA to 90% MeCN 0.01% TFA in 4 minutes at a flow rate of 1.0 mL/min. The MALDI spectra were measured using Bruker Daltonics Autoflex TOF/TOF spectrometer. Final compounds were purified by reverse-phase chromatography using a Biotage Isolera ONE equipped with a Biotage SNAP Cartridge KP-C18-HS (linear gradient from 100% H₂O 0.01% TFA to 100% MeCN 0.01% TFA with a flow rate of 5 mL/min) or using an Agilent 1100 series HPLC equipped with DAD and with an Agilent ZORBAX Eclipse XDB-C18 (4.6 x 250 mm, 5 μ m) column (linear gradient from 100% H₂O 0.1% TFA to 100% MeCN 0.1% TFA with a flow rate of 1 mL/min). All kinases, were purchased from ProQinase, except the Abl kinase domain, which was expressed and purified according to the reported procedure.^{4, 5} Rhodamine **1**⁶, dasatinib azide² and glucosamine ruthenium⁷ were synthesized according to the reported procedures.

Resin Loading

The resin was washed with DMF and CH₂Cl₂ and treated with a preactivated (5 min) solution of the corresponding Fmoc-protected amino acid (5 equiv), HATU (4 equiv), DIPEA (5 equiv), and 2,6-lutidine (7.5 equiv) for 2 hrs in NMP. Following the reaction, the resin was washed with DMF (3x), CH₂Cl₂ (3x), DMF (3x) and CH₂Cl₂ (3x). The resin was capped for at least one hour using acetic anhydride (5.3 equiv) and 2,6-lutidine (6.4 equiv) in DMF (150 μ L / 5 mg resin)

Automated Peptide Synthesis

Peptides were synthesized in 500 mL fritted tubes by using an Intavis MultiPep instrument in a fully automated fashion. The resin (5 mg, 1 μ mol per column) was swollen in CH₂Cl₂ (300 μ L) for 20 min and deprotected using 20% piperidine in DMF (2x5 min). The resin was then washed with DMF and CH₂Cl₂ and treated with a preactivated (5 min) solution of the corresponding Fmoc-protected amino acid (5 equiv), HATU (4 equiv), DIPEA (5 equiv), and 2,6-lutidine (7.5 equiv) for 20 min in NMP. This process was repeated once (double couplings). Each coupling was followed by a capping step with Ac₂O (5.3 equiv) and 2,6-lutidine (6.4 equiv) in DMF (150 μ L per column).

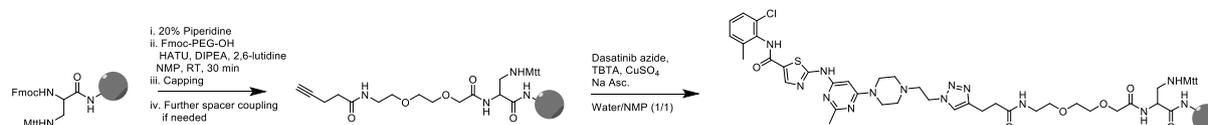
Fmoc deprotection (manual or on Intavis AG MultiPep RS Synthesizer)

To 5 mg of NovaPEG Rink amide resin were added 200 μ L of 20% piperidine solution in DMF. After 2 min, the resin was washed with 6 x 300 μ L DMF and the sequence was repeated a second time for 4 min. Finally, the resin was washed with 6 x 300 μ L of DMF and 6 x 300 μ L of CH₂Cl₂ and the washing cycle was repeated a second time.

Cleavage from the resin

5 mg of resin (0.44 mmol/g loading) were treated with 200 μ L TFA for 2 hours. After filtration of the resin, the resulting solution was precipitated in 12 mL of Et₂O, stored in a -20°C freezer for 5 min and centrifuged to recover the product as a pellet. The pellet was washed once more with ether following the previous process. The product was recovered as a pellet and dried under nitrogen flow and subsequently dissolved in water or 10% DMSO in water for purification.

Preparation of dasatinib derivatives

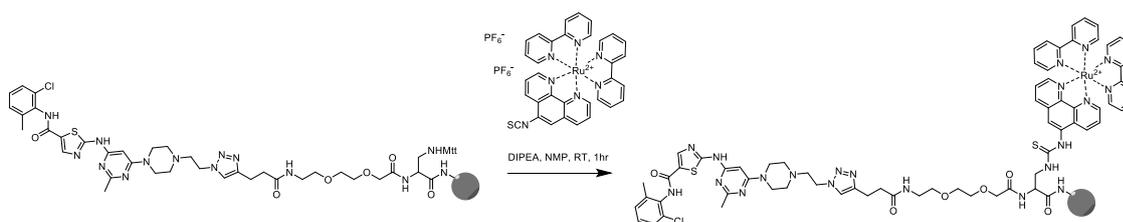


Rink amide NovaPEG resin was loaded with Fmoc-D-diaminopropionic(Mtt) acid at 0.44mmol/g.

Resins loaded with Fmoc-D-diaminopropionic(Mtt) acid (5 mg, 0.44 mmol/g, 2.2 μ mol) were deprotected at their alpha position and treated with a pre-activated (5 min) solution of 4-pentynoic acid (5 equiv), HATU (4 equiv), DIPEA (5 equiv) and 2,6-lutidine (7.5 equiv) for 60 min in NMP. After the reaction, the resins were washed with DMF and CH₂Cl₂ (5 times each). A capping step as described in the automated peptide synthesis was performed prior to click reaction.

TBTA (1.5 equiv, 3.75 μ mol, 2 mg) was suspended in 50 μ L of a solution of sodium ascorbate (2M in water, 198 mg/500 μ L) and 15 μ L of copper sulfate (64.2 mg/mL in water). The resulting black suspension was sonicated until color changed to beige. Dasatinib azide² (1.05 equiv, 2mg, 2.6 μ mol) was dissolved in 50 μ L NMP and the resulting solution was added to the previous suspension. The clear light orange mixture was transferred to the resin and was shaken overnight at room temperature. Subsequently, the resin was washed DMF (3 x 250 μ L), water (6 x 250 μ L), DMF (4 x 250 μ L) and CH₂Cl₂ (6 x 250 μ L).

Preparation of final Ruthenium derivatives



Dasatinib constructs on resin were deprotected at their C-terminus using a 150 μL per column of a solution of 244 mg HOBt in 20 mL of a 1:1 solution of 1,2-dichloroethane and hexafluoroisopropanol, this process was repeated 3 times, until no yellow color could be observed. The resin was subsequently washed with DMF, CH_2Cl_2 , DMF and CH_2Cl_2 (3 x each).

Ruthenium isothiocyanate (1.1 equiv, 2.75 μmol , 2.6 mg) was dissolved in 100 μL NMP and added to the resin. The resin was shaken for 1 hr, protected from light at room temperature. After reaction, the resin was washed with DMF, CH_2Cl_2 , DMF and CH_2Cl_2 (3 x each) and cleaved from resin using cleavage procedure. The final derivatives were purified by reverse phase HPLC.

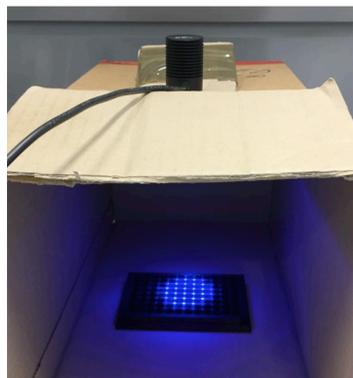
Rhodamine coupling to peptides

N-terminal deprotected peptides (5 mg 0.44 mmol/g, 2.2 μmol) were treated with a pre-activated (5 min) solution of 4-pentynoic acid (5 equiv), HATU (4 equiv), DIPEA (5 equiv) and 2,6-lutidine (7.5 equiv) for 60 min in NMP. After the reaction, the resins were washed with DMF and CH_2Cl_2 (5 times each).

TBTA (1.5 equiv, 3.75 μmol , 2 mg) was suspended in 50 μL of a solution of sodium ascorbate (2 M in water, 198 mg/500 μL) and 15 μL of copper sulfate (64.2 mg/mL in water). The resulting black suspension was sonicated until color changed to beige. Final Rhodamine derivative **3** (1.05 equiv, 2 mg, 2.6 μmol) was dissolved in 50 μL NMP and the resulting solution was added to the previous suspension. The clear light orange mixture was transferred to the resin and was shaken overnight at room temperature. Subsequently, the resin was washed DMF (3 x 250 μL), water (6 x 250 μL), DMF (4 x 250 μL) and CH_2Cl_2 (6 x 250 μL). The resin was suspended in TFA (200 μL) for 2 h. The solution was filtered and the product precipitated in diethyl ether (12 mL). After 5 min at -20°C (freezer) the precipitate was pelleted by centrifugation and the supernatant was removed. The pellet was washed with diethyl ether then dissolved in 300 μL of 10 % DMSO in water for HPLC purification as described in the general methods.

Template reaction procedure

Template reactions were carried out in opaque 96 well plates in 100 mM TBS (Tris Buffer Saline 150 mM NaCl) + 0,05% Tween 20 buffer and 20 mM of sodium ascorbate. Stock solutions of probes were made in 10% DMSO in mQ water at 1 mM and stored either at -20°C or in aliquots at -80°C. A stock solution of sodium ascorbate was made in water at 1 M. Stock solutions were diluted with reaction buffer to the desired concentration and used in the experiment. Each experiment was performed in triplicate. After measurement of initial fluorescence, the plate was irradiated using a 455 nm collimated LED lamp (www.thorlabs.com, 1W, 30cm distance) and the fluorescence of rhodamine (exc=490 nm; em=530 nm) was measured at different time points. The reactions were carried out in 200 μL volume at two different reagent concentrations: at higher concentration with 1 μM of peptide-rhodamine probe and 100nM of dasatinib-ruthenium probe and 100 nM of protein; at lower concentration using 500 nM of peptide-rhodamine probe and 100nM of dasatinib-ruthenium probe and 50 nM of template protein. The raw data was treated by subtracting the initial fluorescence value for each conditions and averaging the values of triplicate experiment while calculating a standard deviation. Picture of the LED setup below.



Cell Culture

A549 cells were grown in F12K medium (10% FCS, 1 x penstrep), K562 cells were grown in IMDM (10% FCS, 1 x penstrep), KCL-22 cells were grown in RPMI 1640 (10% FCS, 1 x penstrep), and SKBR-3 cells were grown in McCoy's 5A medium (10% FCS, 1 x penstrep) in accordance with ATCC and DSMZ recommendations.

Cell Experiments

Adherent cell lines, A549 and SKBR-3, were seeded in 35 mm glass bottom dishes and grown for 24h. Cells were then washed with DPBS and fixed for 20 min with 4% PFA. For K562, the cells were seeded in 35 mm glass bottom dishes, coated with poly-L-lysine and grown for 24h. Cells were then washed with DPBS and fixed with 4% PFA for 20 mins. For KCL-22, cells were seeded in 35 mm glass bottom dishes coated with poly-L-lysine and gently centrifuged (300 rpm, 3 min, rt). The cells were then fixed with 4% PFA for 20 mins.

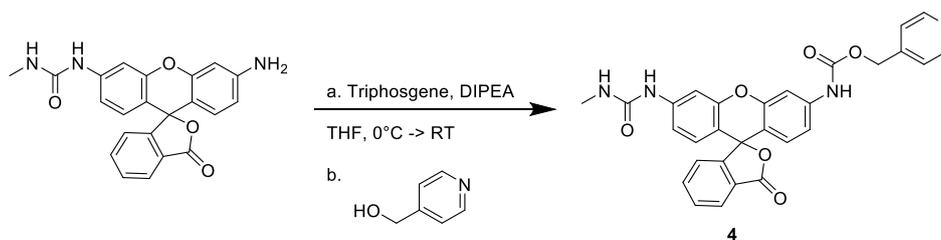
Peptide and Dasatinib conjugates were added to the cells in DPBS at the concentrations indicated and incubated at 37°C for 2 h. Sodium ascorbate (20 mM) was added and the cells were further incubated at 37°C for 1 h. The media was aspirated and replaced with 2 mL of DPBS containing 20 mM sodium ascorbate. The cells were then irradiated for 30 min with a 455 nm LED lamp. After irradiation the cells were imaged using confocal microscopy.

Confocal Microscopy

Images were acquired using a Zeiss LSM780 inverted confocal microscope, or a Leica SP8 inverted confocal microscope with 488 nm laserlines. Acquired images were analyzed and quantified using ImageJ software.

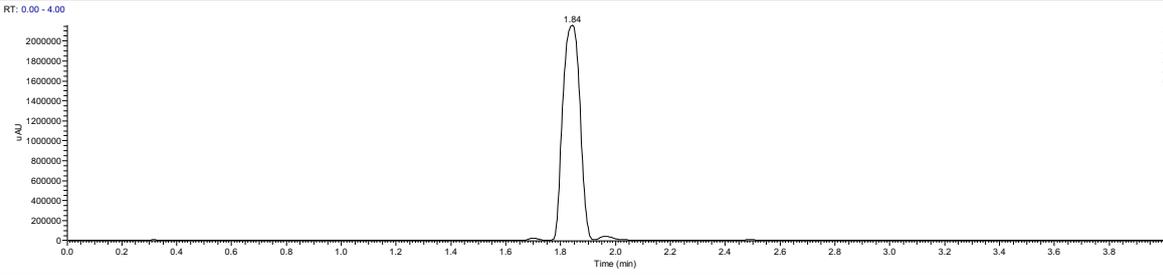
Structure and Characterization of probes

Rhodamine Pyridine Synthesis 4



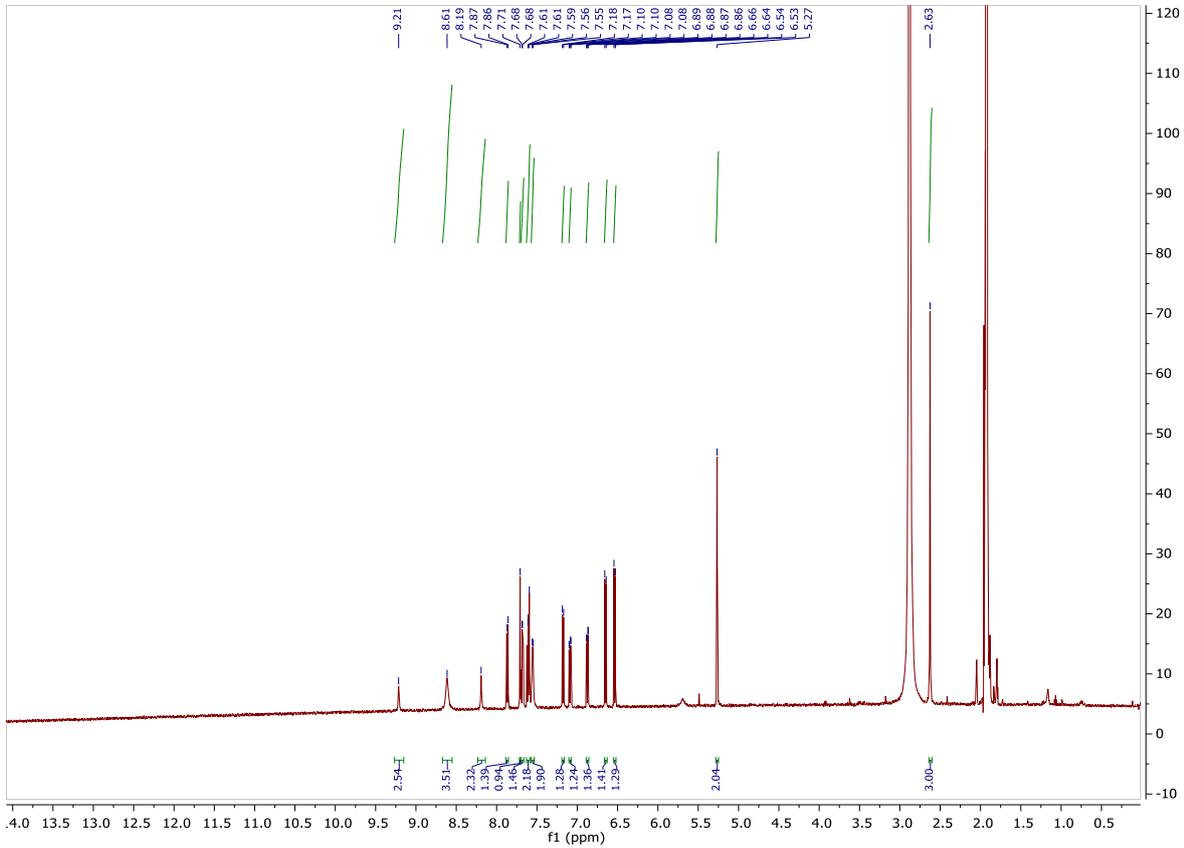
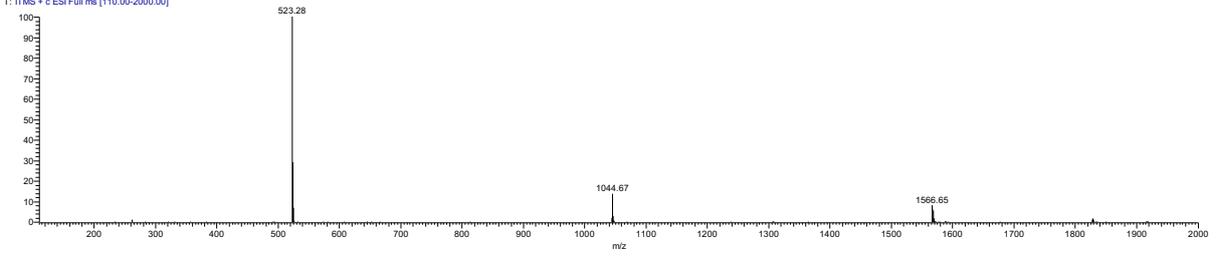
Rhodamine was synthesized as reported in Ref 6.

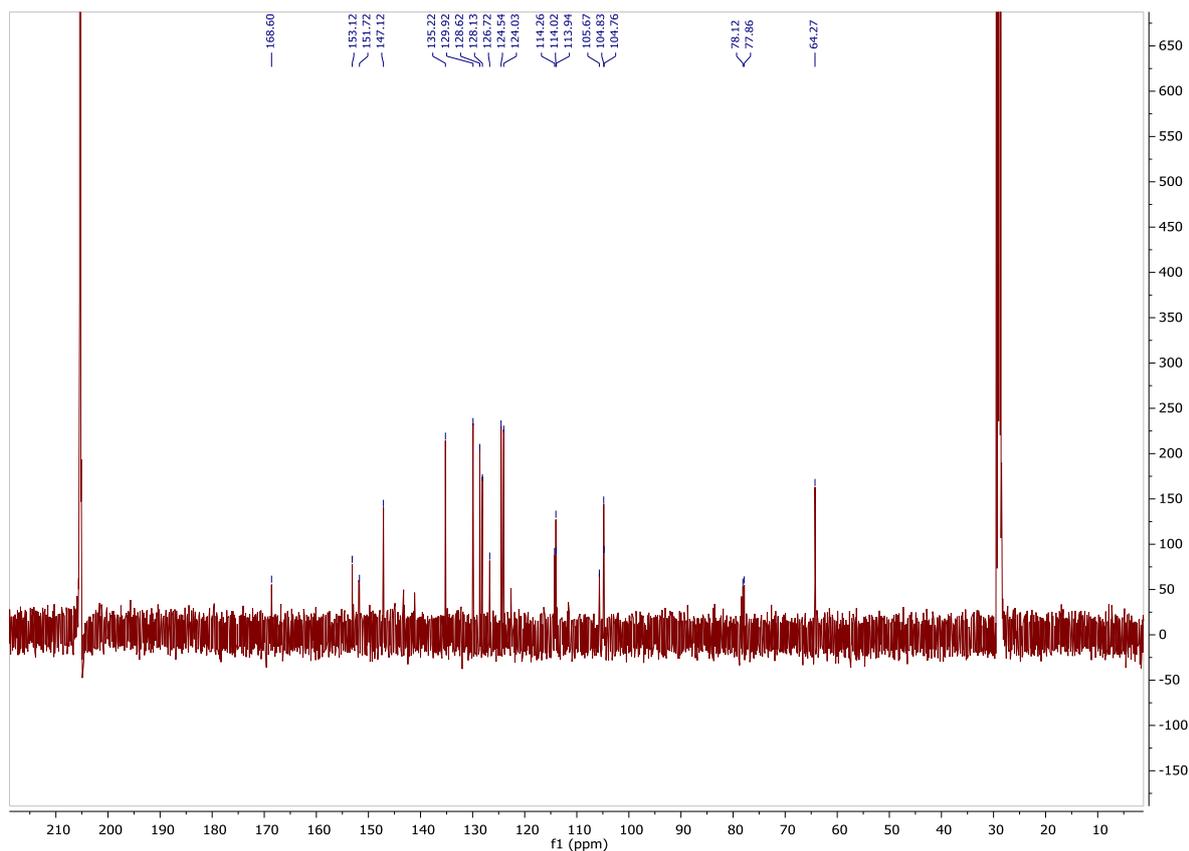
In a Schlenk flask, Rhodamine⁶ (100 mg, 0.26 mmol) and triphosgene (0.5 equiv, 38.5mg, 0.13 mmol) were suspended in dry tetrahydrofuran (5 mL). The suspension was cooled to 0°C with an ice bath and diisopropylethylamine (3.0 equiv, 0.77 mmol, 135 μ L) was added dropwise. The reaction turned from a red suspension to a clear purple solution within minutes. The ice bath was removed and the activation was continued for 1 hr at room temperature. The activation of Rhodamine to the Rhodamine isocyanate was monitored by TLC or LC/MS. 4-pyridine methanol (3.0 equiv, 84 mg, 0.77 mmol) was added to the previous solution. The reaction was monitored by TLC or LC/MS and stirred overnight under nitrogen at room temperature. The following day, the reaction mixture was concentrated *in vacuo* to remove THF and water and CH_2Cl_2 were added. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 . The combined organic layers were washed with brine, dried over sodium sulfate and concentrated under reduced pressure. Rhodamine-pyridine was purified by reverse phase using a biotage and a gradient from 5% to 50% acetonitrile to obtain 113 mg of Rhodamine-pyridine **2** as a red solid. Yield 84%. LC/MS ESI $t_r = 1.84$ min, m/z calculated = 522.15 m/z found 523.28 $[\text{M}+\text{H}^+]$. ^1H NMR (500 MHz, Acetone- d_6) δ 9.21 (s, 1H), 8.61 (s, 2H), 8.19 (s, 1H), 7.87 (dt, $J = 7.6, 1.0$ Hz, 1H), 7.71 (d, $J = 2.1$ Hz, 1H), 7.68 (td, $J = 7.5, 1.2$ Hz, 1H), 7.63 – 7.59 (m, 1H), 7.59 (s, 1H), 7.55 (d, $J = 5.2$ Hz, 2H), 7.18 (dt, $J = 7.7, 0.9$ Hz, 1H), 7.09 (dd, $J = 8.7, 2.2$ Hz, 1H), 6.87 (dd, $J = 8.7, 2.2$ Hz, 1H), 6.65 (d, $J = 8.6$ Hz, 1H), 6.54 (d, $J = 8.7$ Hz, 1H), 5.27 (s, 2H), 2.63 (s, 3H). ^{13}C NMR (126 MHz, Acetone) δ 168.60, 153.12, 151.72, 147.12, 135.22, 129.92, 128.62, 128.13, 126.72, 124.54, 124.03, 114.26, 114.02, 113.94, 105.67, 104.83, 104.76, 78.12, 77.86, 64.27.



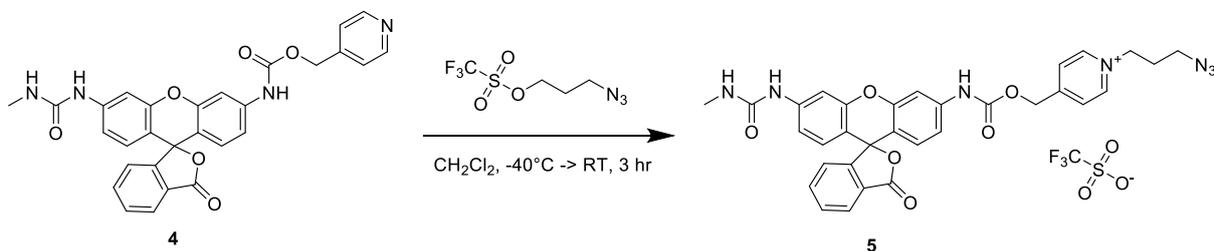
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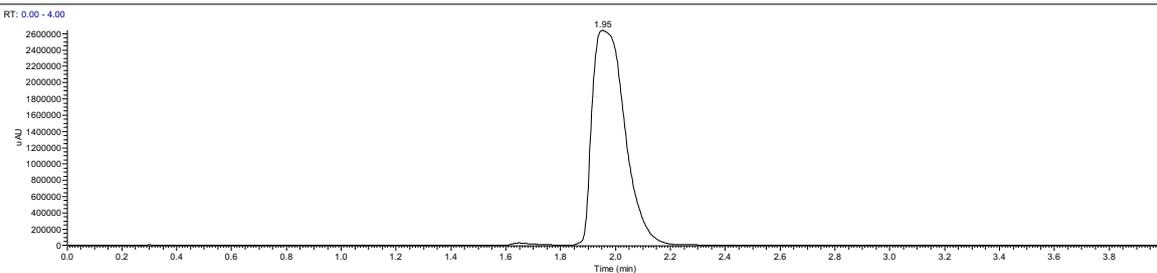




Rhodamine Azidopropyl-Pyridinium Synthesis 5



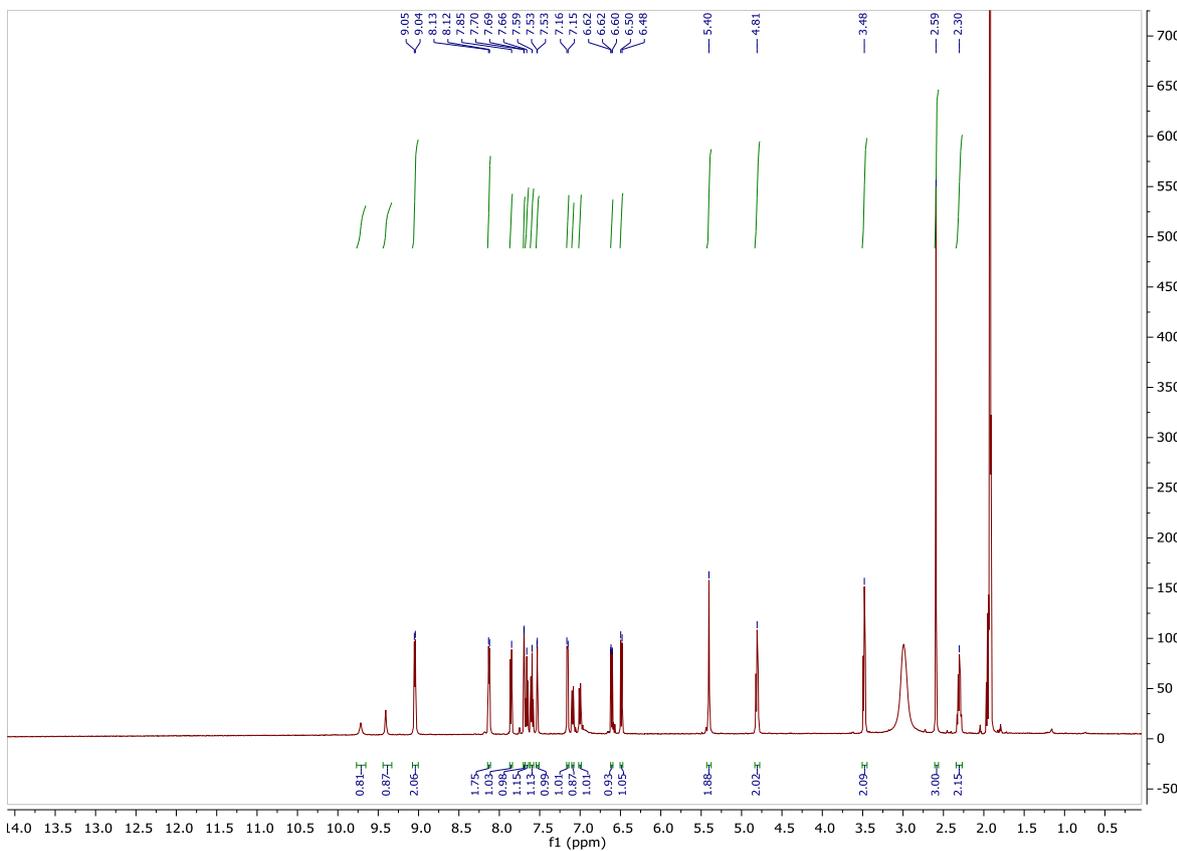
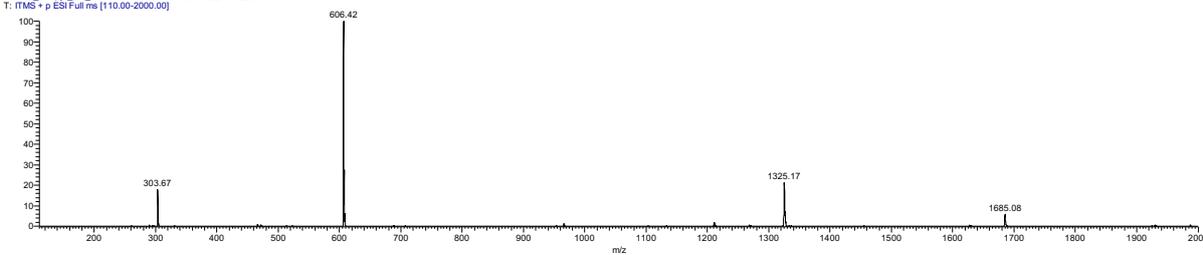
In a Schlenk flask, Rhodamine-pyridine **2** (1 equiv, 30 mg, 0.057 mmol) was suspended in dry CH_2Cl_2 (3 mL) and cooled to -40°C in an acetone/dry ice bath. Azidopropyl triflate (1.5 equiv, 0.0855 mmol) was added dropwise. The reaction was stirred for 30 min at -40°C , the ice bath was removed and the reaction mixture was allowed to warm to room temperature in 3 hrs. The reaction mixture was monitored by LC/MS and once alkylation was complete, the mixture was concentrated *in vacuo*. The alkylated rhodamine pyridinium was purified by reverse phase biotage or HPLC using gradient of respectively 5 to 50% and 10 to 80% acetonitrile in water. Lyophilization of the purified fractions gave 30 mg of rhodamine pyridinium **3** as a light orange solid. Yield (75%) LC-MS (ESI) RT = 1.95 min, m/z calculated = 606.21 m/z found = 303.67 $[\text{M}+\text{H}]^{2+}$, 606.42 $[\text{M}]^+$, ^1H NMR (500 MHz, Acetone- d_6) δ 9.18 (d, J = 6.3 Hz, 2H), 8.26 (d, J = 6.2 Hz, 2H), 7.98 (d, J = 7.5 Hz, 1H), 7.82 (d, J = 2.0 Hz, 1H), 7.79 (td, J = 1.2 Hz, 7.5 Hz, 1H), 7.72 (td, J = 1.0 Hz, 7.6 Hz, 1H), 7.66 (d, J = 2.2 Hz, 1H), 7.29 (d, J = 7.7 Hz, 1H), 7.22 (dd, J = 2.2 Hz, 8.8 Hz, 1H), 7.13 (dd, J = 2.1 Hz, 8.8 Hz, 1H), 6.74 (d, J = 8.7 Hz, 1H), 6.62 (d, J = 8.6 Hz) 5.53 (s, 2H), 4.94 (t, J = 7.3 Hz, 2H), 3.61 (t, J = 6.4 Hz, 2H), 2.72 (s, 3H), 2.43 (m, 2H). ^{13}C NMR (126 MHz, Acetone) δ 168.70, 157.87, 153.09, 152.58, 151.85, 151.63, 144.84, 144.06, 143.94, 140.99, 140.87, 135.23, 129.90, 128.53, 127.92, 126.71, 125.35, 124.52, 124.05, 114.32, 114.23, 114.14, 114.06, 113.91, 110.87, 105.85, 104.58, 104.51, 82.53, 63.60, 59.06, 47.83, 30.13.

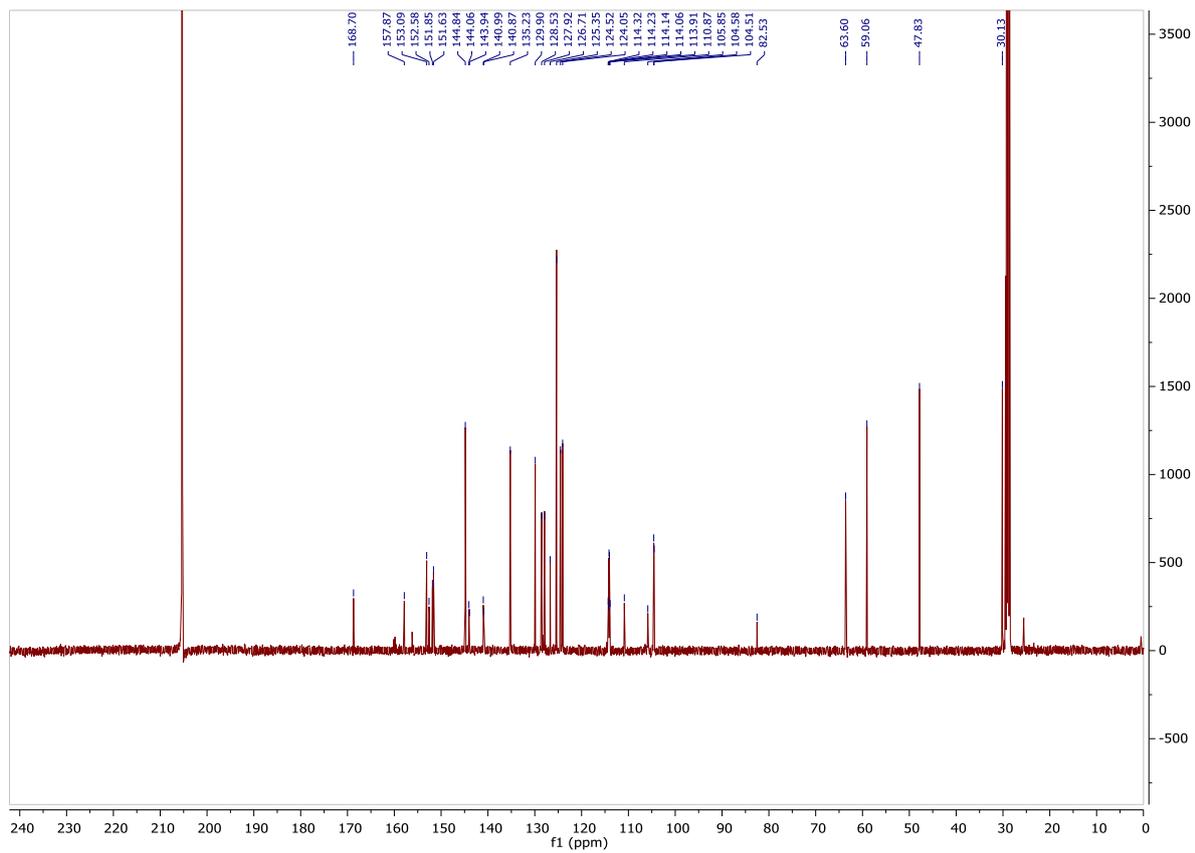


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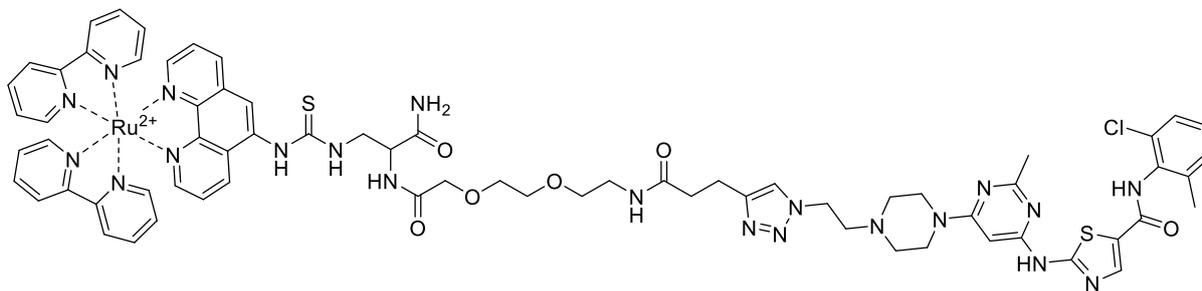
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MALDI-TOF and LC-MS (ESI) characterization of probes

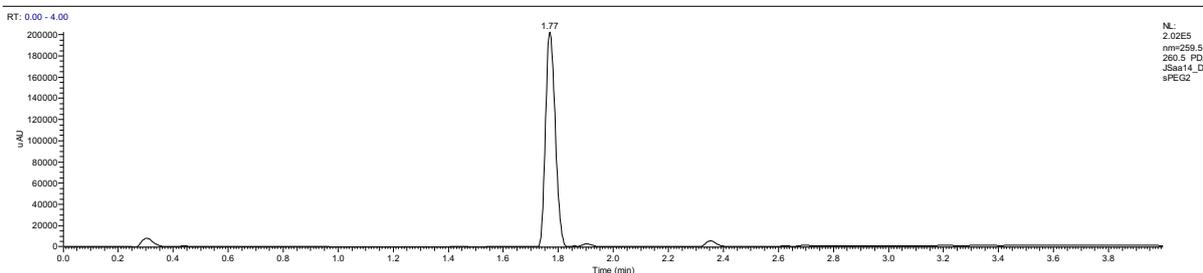
Das-PEG-Ru 6



Chemical Formula: $C_{69}H_{72}ClN_{21}O_6RuS_2^{2+}$ Exact Mass: 1491.41 LC-MS (ESI): RT= 1.77 min, m/z found = 325.67 [Ruthenium] $^{2+}$, 373.75 [M+2H] $^{4+}$, 497.50[M+H] $^{3+}$, 745.75 [M] $^{2+}$, 841.33 [M+H-Ruthenium] $^{+}$, 1490.08 [M-H] $^{+}$, MALDI-TOF found m/z = 839.40 [M+H-Ruthenium] $^{+}$, 1335.336 [M-H-bpy] $^{+}$, 1490.655 [M-H] $^{+}$

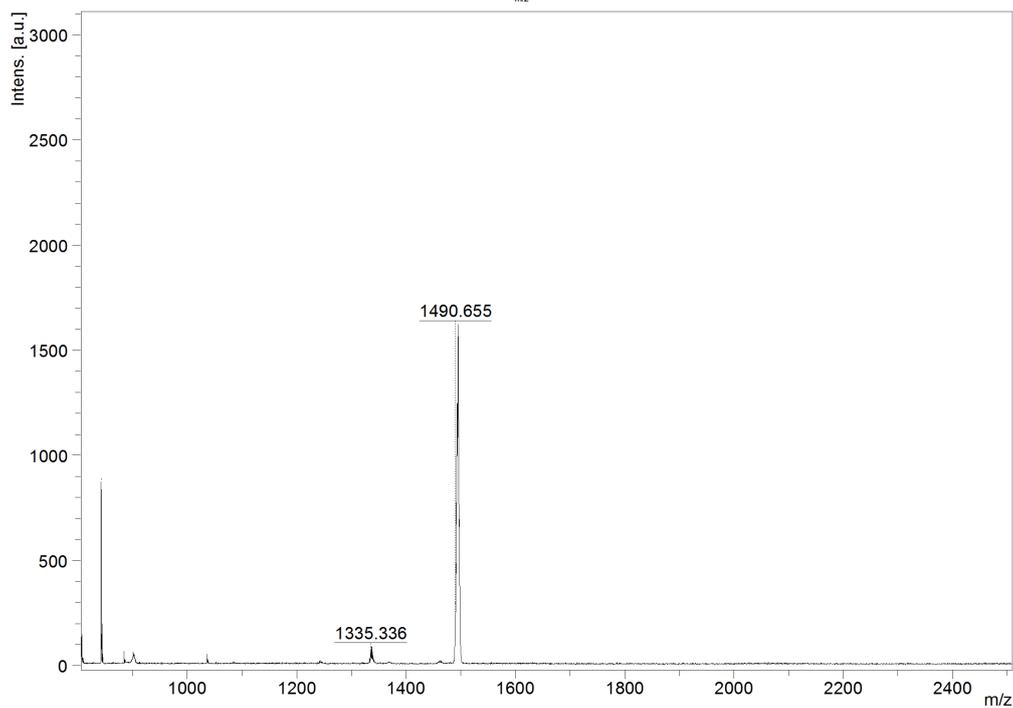
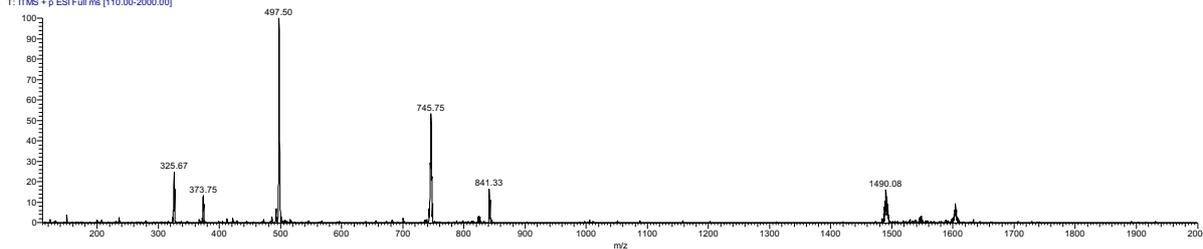
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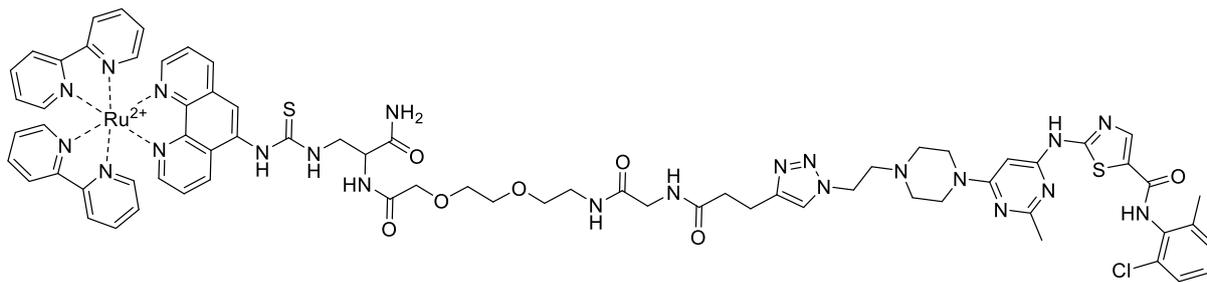


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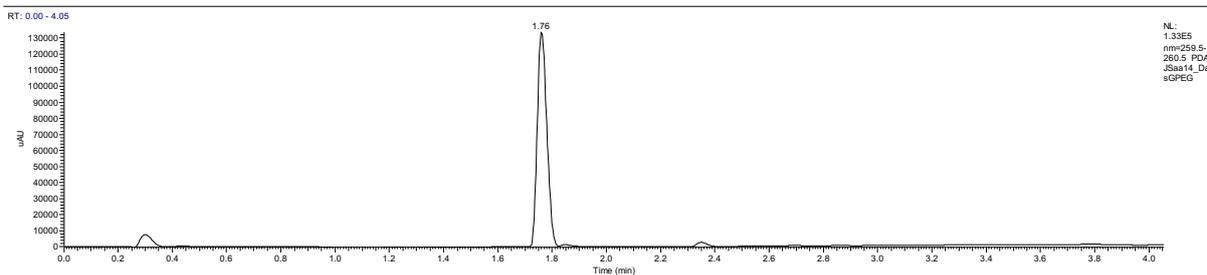
Das-GPEG-Ru 7



Chemical Formula: $C_{71}H_{75}ClN_{22}O_7RuS_2^{2+}$ Exact Mass: 1548.44 LC-MS (ESI): RT= 1.76 min m/z found = 325.67 [Ruthenium] $^{2+}$, 387.92 [M+2H] $^{4+}$, 516.67 [M+H] $^{3+}$, 774.25 [M] $^{2+}$, 898.33 [M+H-Ruthenium] $^{+}$, 1547.00 [M-H] $^{+}$ MALDI-TOF found m/z = 899.092 [M+H-Ruthenium] $^{+}$, 1392.368 [M-H-bpy] $^{+}$, 1548.640 [M-H] $^{+}$

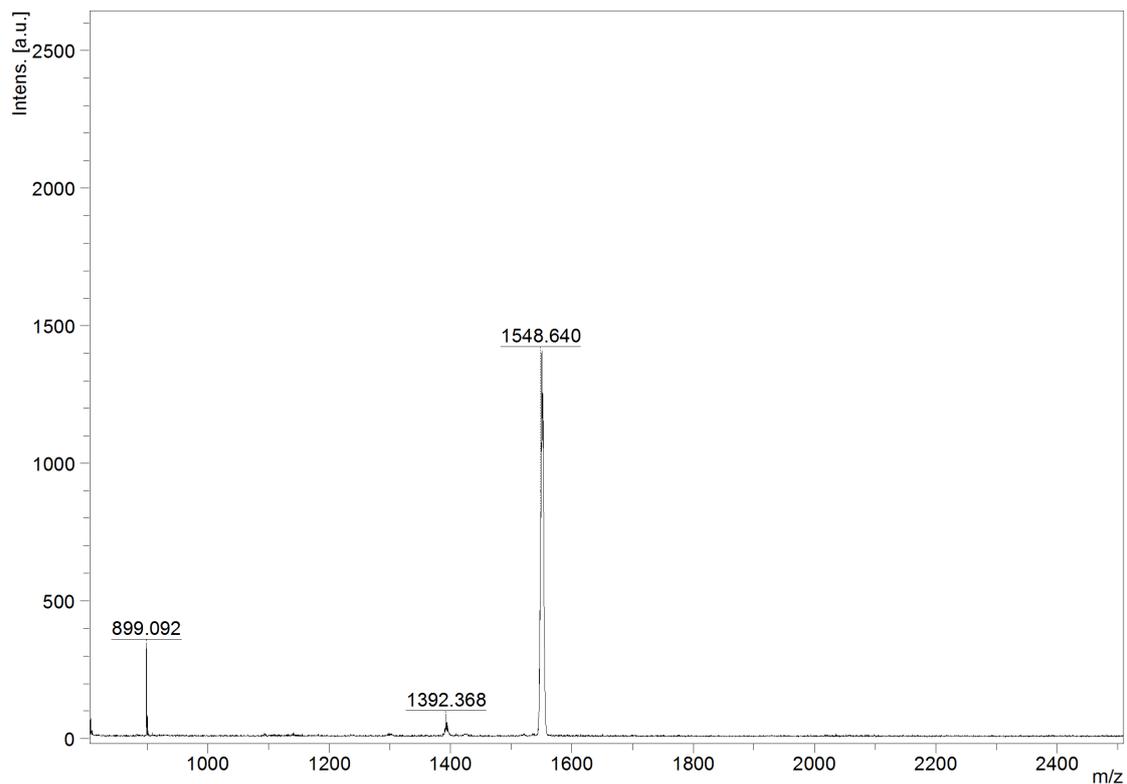
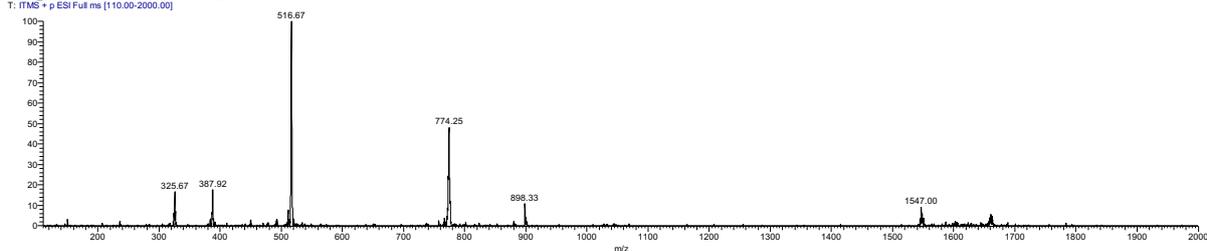
\\LCQFLEETPC\data\...JSaa14_DasGPEG

13/02/2017 12:50:34

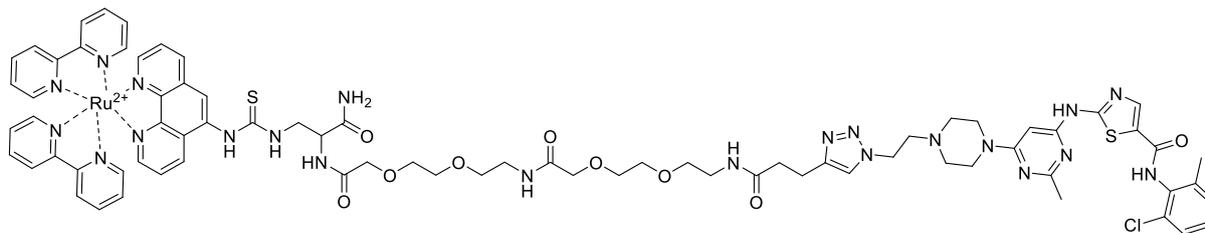


JSaa14_DasGPEG #121 RT: 1.76 AV: 1 NL: 1.45E4

T: (IMS+ p ESI Full ms [110.00-2000.00])



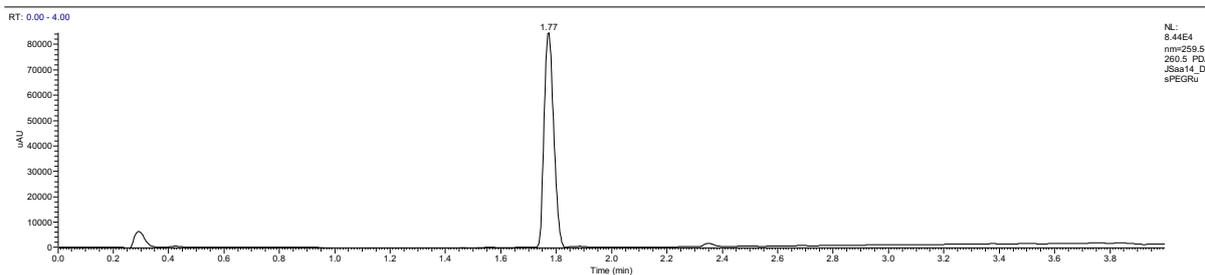
Das-PEG2-Ru 8



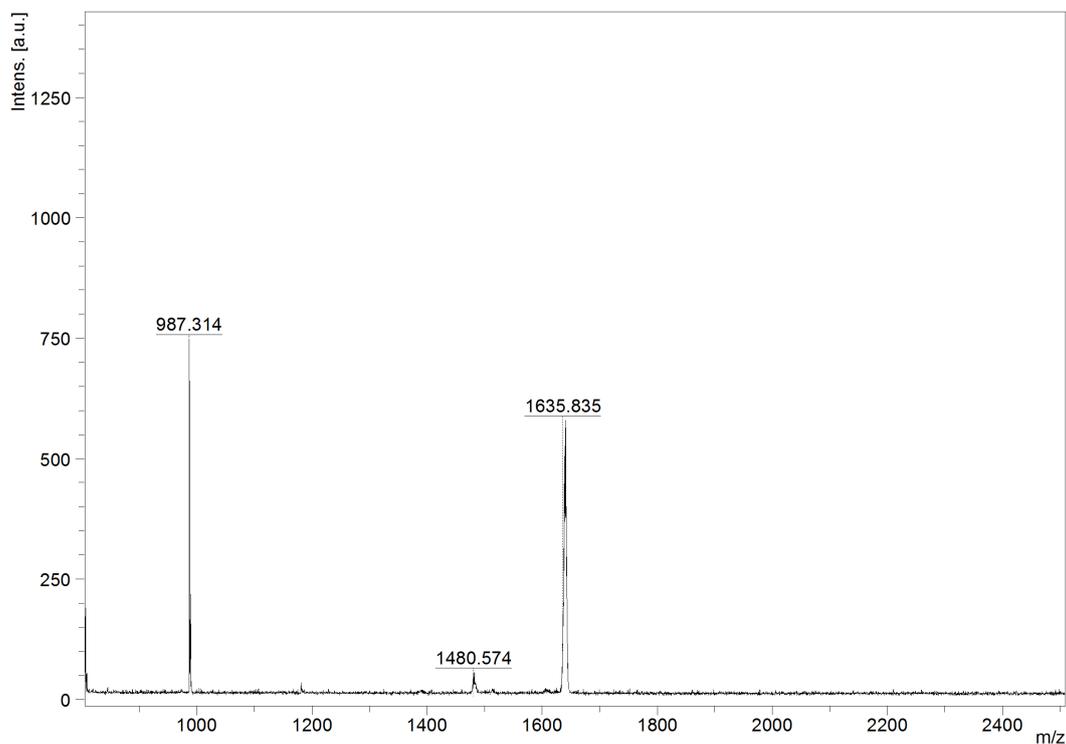
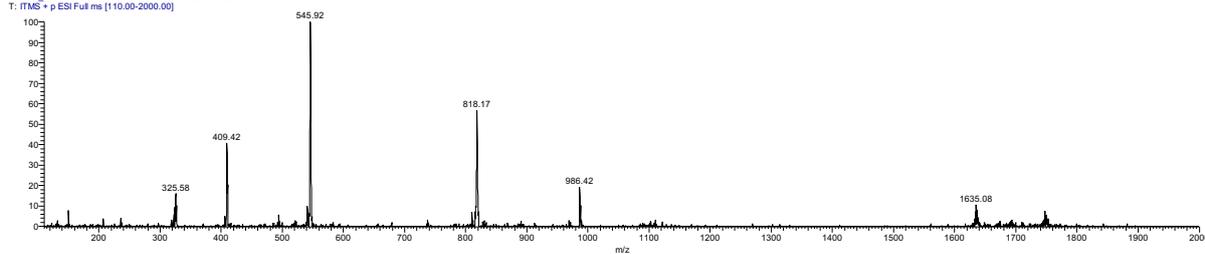
Chemical Formula: $C_{75}H_{83}ClN_{22}O_9RuS_2^{2+}$ Exact Mass: 1636.49 LC-MS (ESI) RT = 1.77 min m/z found = 325.58 [Ruthenium] $^{2+}$, 409.42 [M+2H] $^{4+}$, 545.92 [M+H] $^{3+}$, 818.17 [M] $^{2+}$, 986.42 [M+H-Ruthenium] $^{+}$, 1635.08 [M-H] $^{+}$ MALDI-TOF found m/z = 987.314 [M+H-Ruthenium] $^{+}$, 1480.574 [M-H-bpy] $^{+}$, 1635.835 [M-H] $^{+}$

\\LCOFLEETPC\data\...JSaa14_DasPEGRu

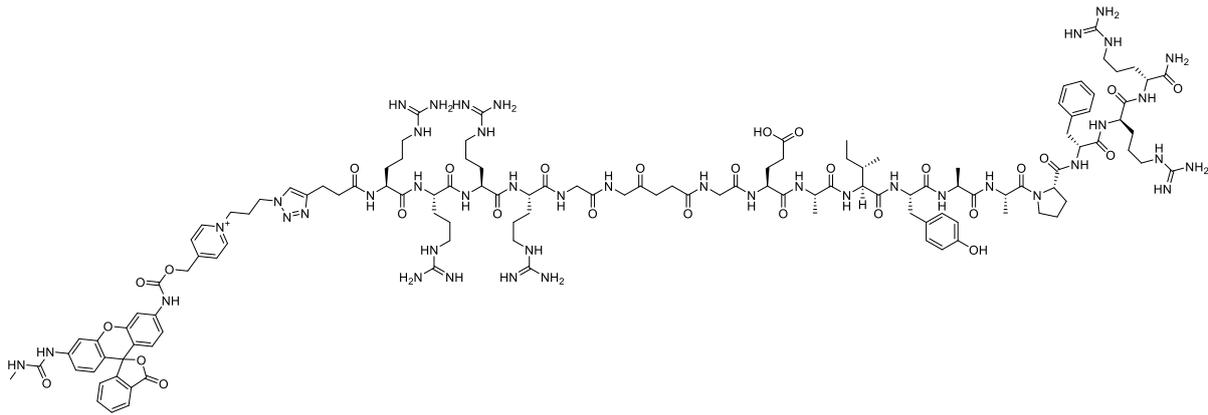
13/02/2017 12:12:12



JSaa14_DasPEGRu #122 RT: 1.77 AV: 1 NL: 8.16E3
T: (TMS + p ESI Full ms [110.00-2000.00])



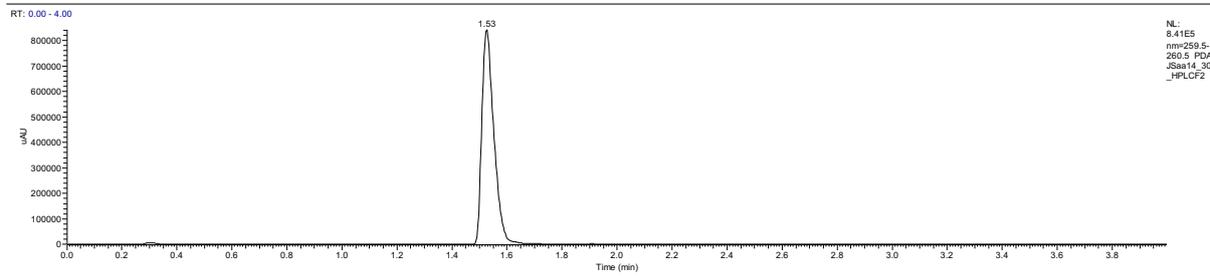
PAbI-R4G2 9



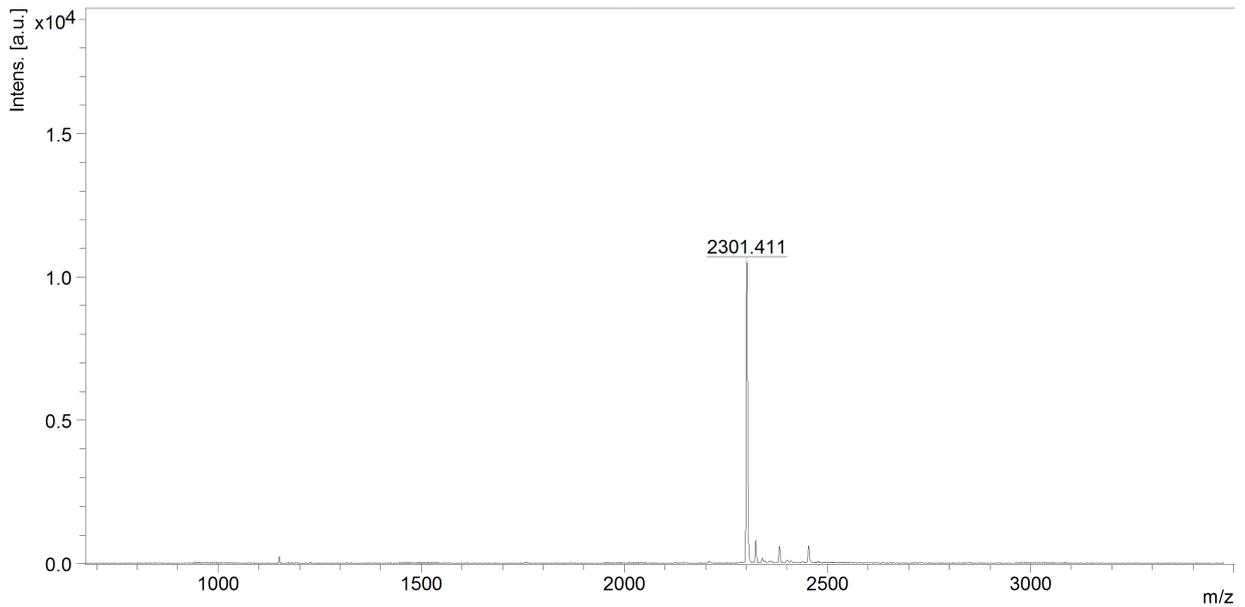
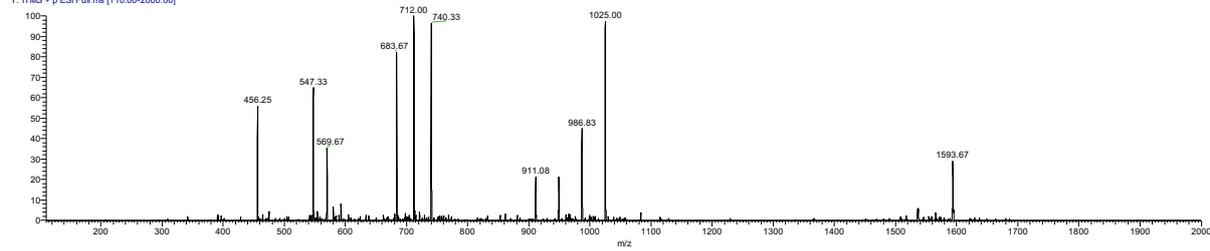
Chemical Formula: $C_{125}H_{178}N_{43}O_{28}^+$, Exact Mass: 2729,38 LC-MS (ESI): RT = 1.53 min m/z found: 456.25 [M+5H] $^{6+}$, 547.33 [M+4H] $^{5+}$, 569.67 [M+4H+TFA] $^{5+}$, 683.67 [M+3H] $^{4+}$, 712.00 [M+3H+TFA] $^{4+}$, 740.33 [M+3H+2TFA] $^{4+}$, 911.06 [M+2H] $^{3+}$, 986.23 [M+2H+2TFA] $^{3+}$, 1025.00 [M+2H+3TFA] $^{3+}$ 1593.67 [M+H+4TFA] $^{2+}$, MALDI-TOF m/z found = 2301.411 [M+H-Rhodamine] $^+$

ILCOFLEETPC\data1...JSaa14_30_HPLCF2

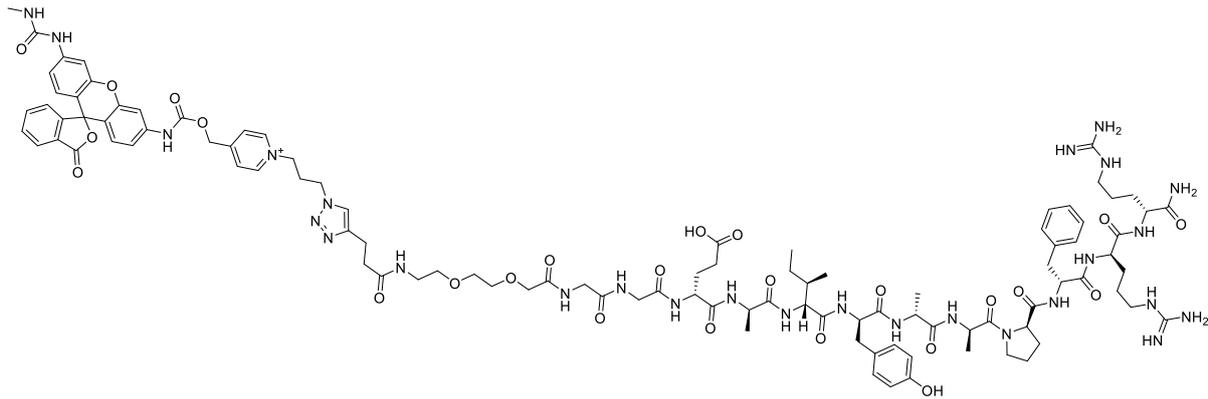
30/01/2017 16:52:14



JSaa14_30_HPLCF2 #102 RT: 1.52 AV: 1 NL: 8.29E4
T: FTMS + p ESI Full ms [110.00-2000.00]



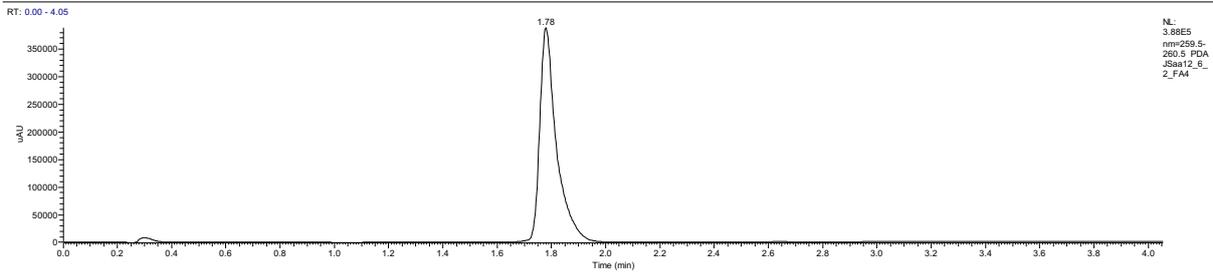
PAbI-PEG 10



Chemical Formula: $C_{102}H_{134}N_{27}O_{25}^+$ Exact Mass: 2137.00, LC-MS (ESI) RT = 1.78 min m/z found 535.50 $[M+4H]^{4+}$ 713.58 $[M+3H]^{3+}$, 1069.67 $[M+2H]^{2+}$, 1463.33 [MALDI-TOF found 1707.780 $[M+H\text{-rhodamine}]^+$

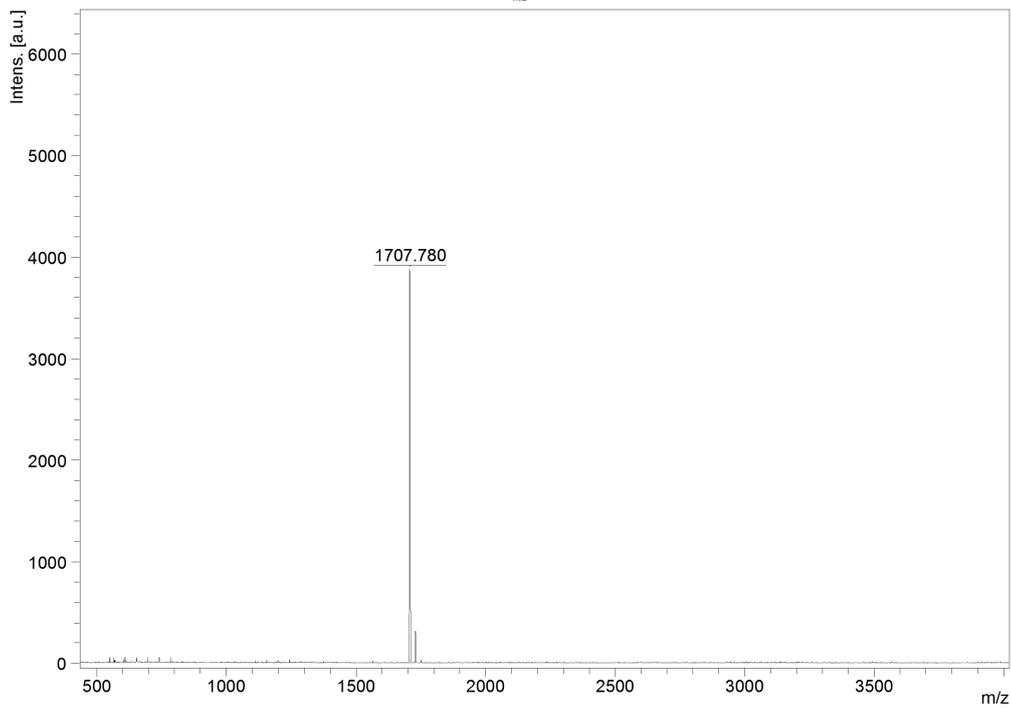
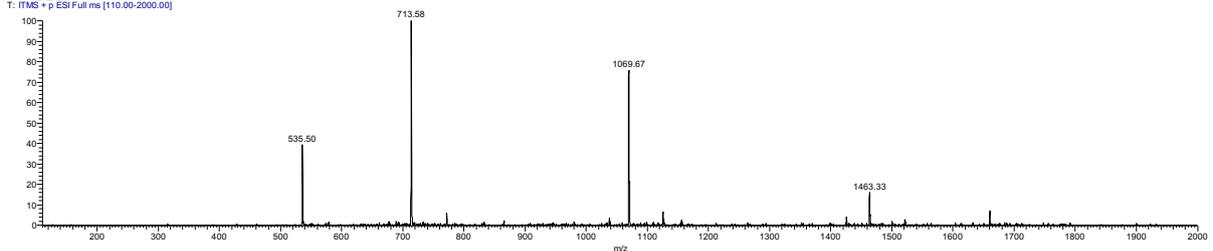
\\LCOFLEETPC\data_USaa12_6_2_FA4

16/09/2016 13:48:31

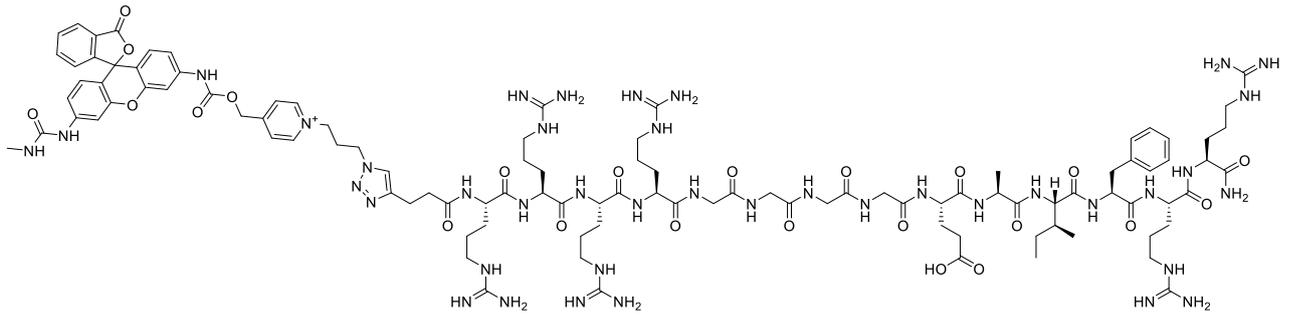


J.Saa12_6_2_FA4#113 RT: 1.78 Av: 1 NL: 6.56E4

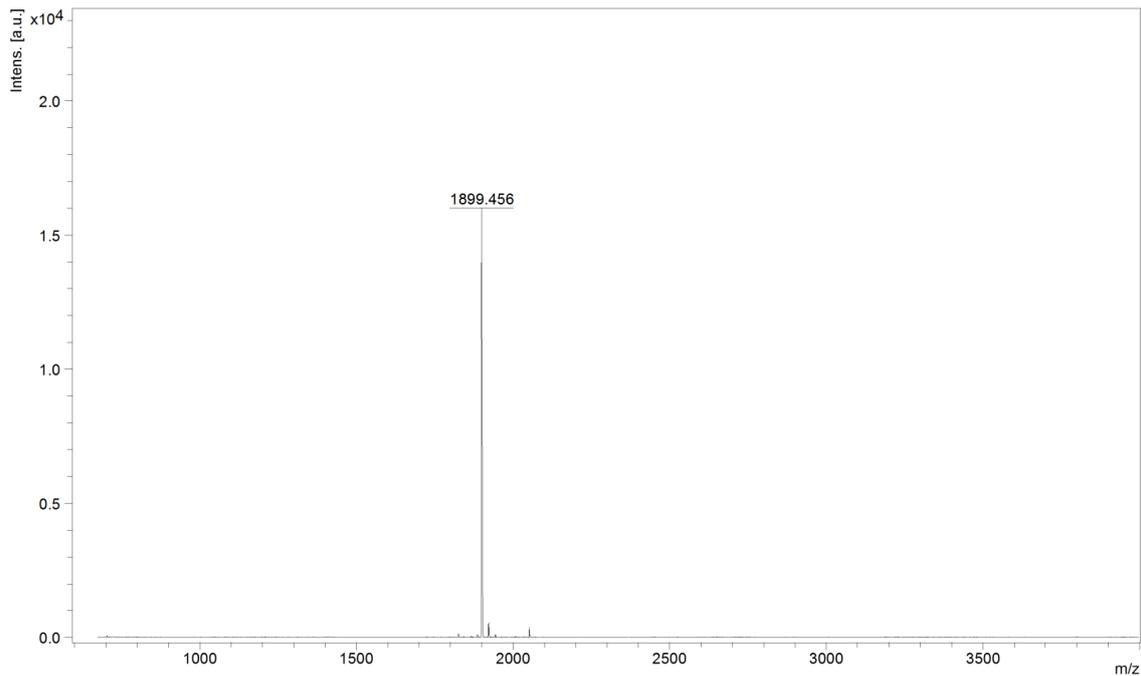
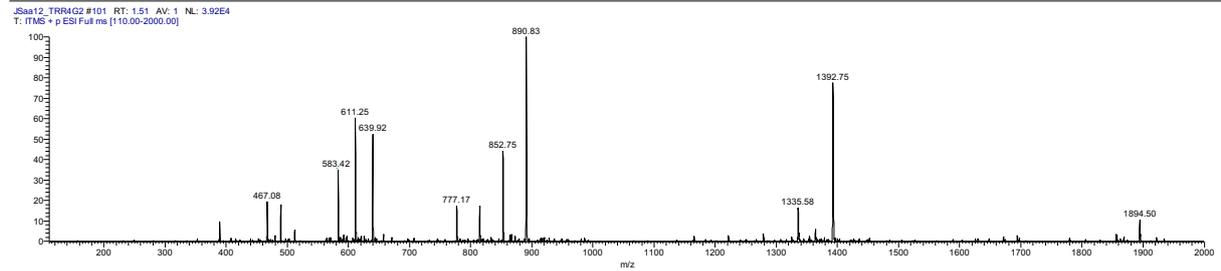
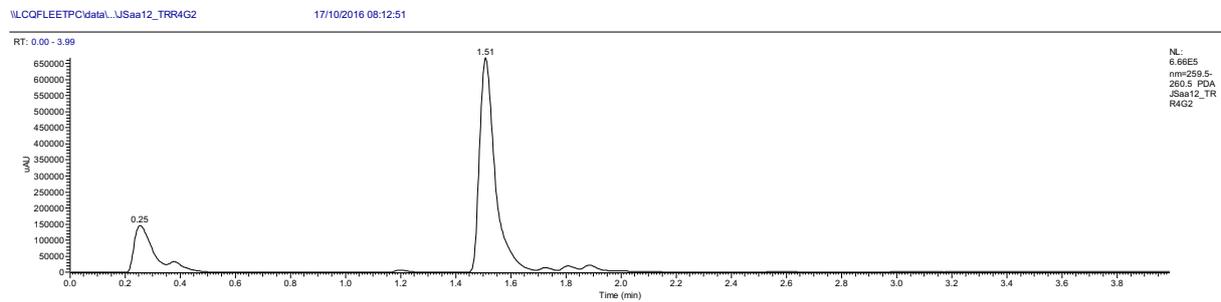
T: FTMS * p ESI Full ms [110.00-2000.00]



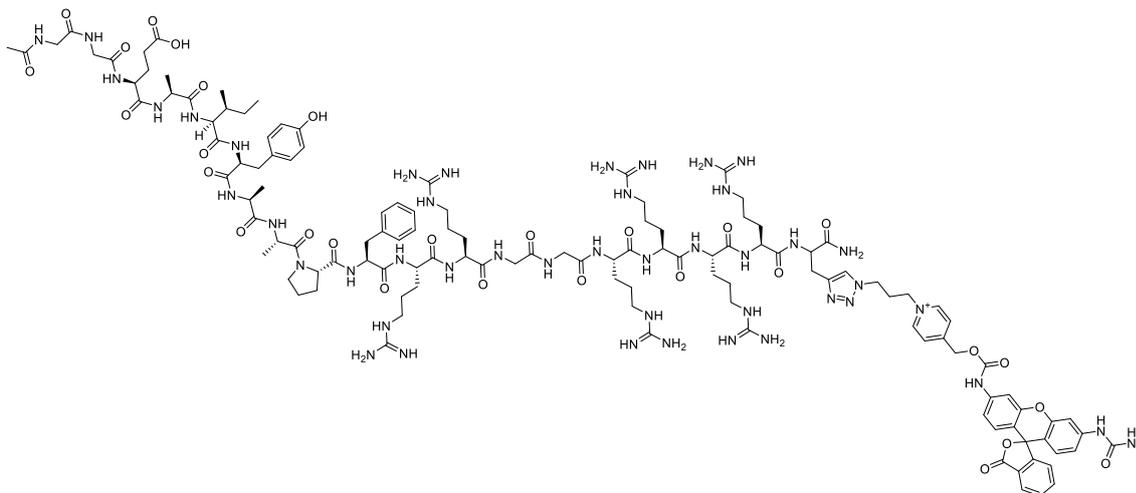
TR-PAbI-R4G2 11



Chemical Formula: $C_{104}H_{151}N_{40}O_{23}^+$ Exact Mass: 2328,19 LC-MS (ESI): RT= 1,51 min m/z found = 386,47 $[M+6H]^{6+}$, 467,08 $[M+5H]^{5+}$, 583,42 $[M+4H]^{4+}$, 611,25 $[M+4H+TFA]^{4+}$, 639,92 $[M+4H+2TFA]^{4+}$, 777,17 $[M+3H]^{3+}$, 852,75 $[M+3H+2TFA]^{3+}$, 890,83 $[M+3H+3TFA]^{3+}$, 1335,58 $[M+3H+3TFA]^{3+}$, 1392,75 $[M+2H+4TFA]^{2+}$, MALDI-TOF m/z found = 1899,456 $[M+H-Rhodamine]^+$



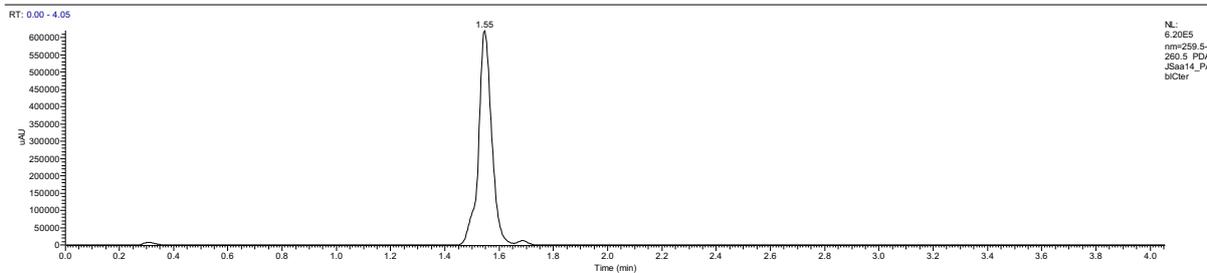
C-term-PAbI-R4G2 12



Chemical Formula: $C_{126}H_{180}N_{45}O_{29}^+$ Exact Mass: 2787.40, LC-MS (ESI) RT = 568.67 [M+4H]⁵⁺, 581.25 [M+4H+TFA]⁵⁺, 603.92 [M+4H+2TFA]⁺, 697.83 [M+3H]⁴⁺, 726.17 [M+3H+TFA]⁴⁺, 754.67 [M+3H+2TFA]⁴⁺, 783.17 [M+3H+TFA]⁴⁺, 930.00 [M+2H]³⁺, 968.08 [M+2H+TFA]³⁺, 1005.67 [M+2H+2TFA]³⁺, 1043.75 [M+2H+3TFA]³⁺, 1622.33 [M+4TFA]²⁺ MALDI-TOF m/z found 2358.507 [M+H-Rhodamine]⁺

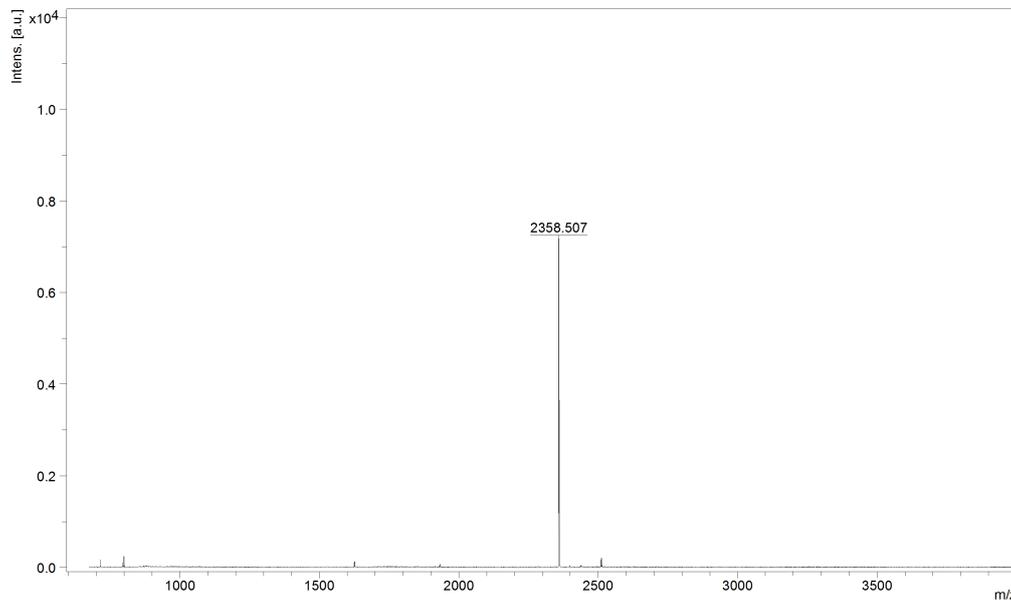
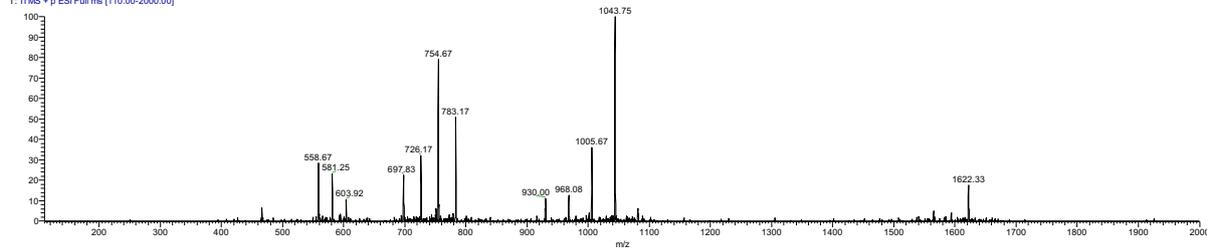
\\LCGFLEETPC\data\...USaa14_PAbICler

14/02/2017 09:37:34

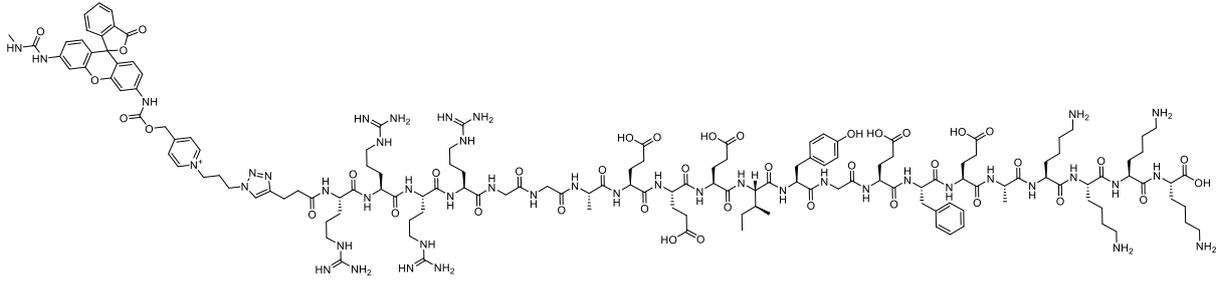


JSaa14_PAbICler #98 RT: 1.54 AV: 1 NL: 8.85E4

T: FIMS + p ESI Full ms [110.00-2000.00]



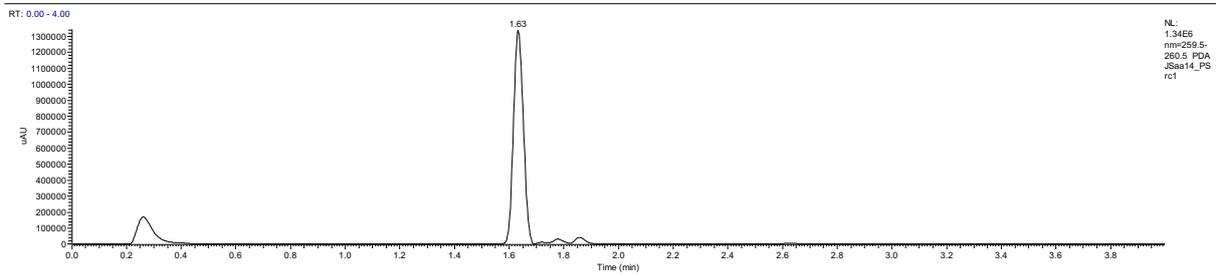
PSrc-R4G2 13



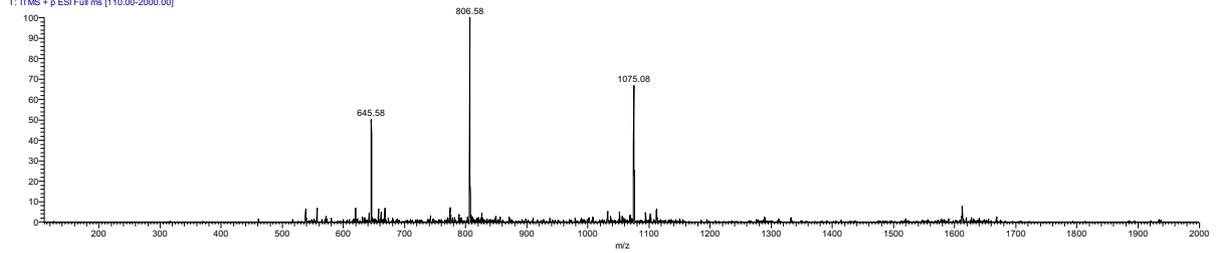
Chemical Formula: C₁₄₆H₂₁₃N₄₄O₄₀⁺ Exact Mass: 3222.60, LC-MS (ESI) RT = 1.63 min m/z found = 645.58 [M+5H]⁵⁺, 806.58 [M+4H]⁴⁺, 1075.08 [M+3H]³⁺, MALDI-TOF found: 2793.349 [M+H-Rhodamine]⁺

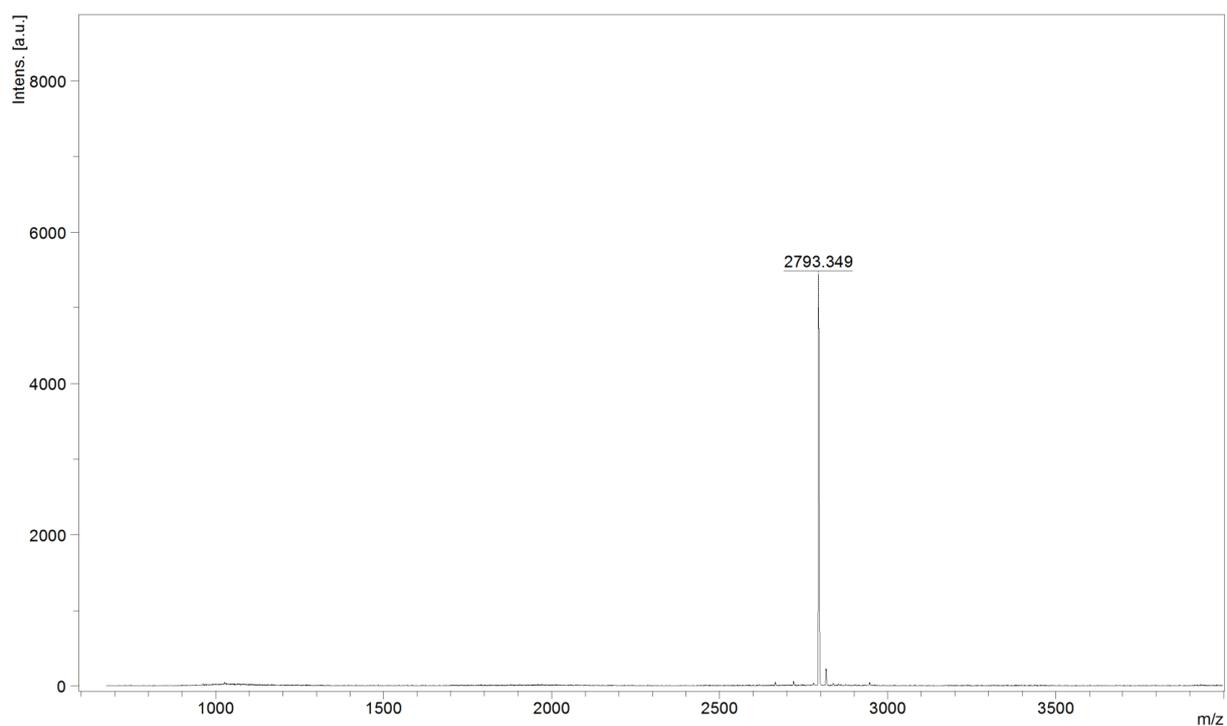
ILCQFLEETPC\data\...JSaa14_PSrc1

13/02/2017 09:11:54



JSaa14_PSrc1 #110 RT: 1.63 AV: 1 NL: 1.04E5
T: ITMS + p ESI Full ms [110.00-2000.00]





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