Supporting Information

Halogenated Corannulenes: Reaction Optimization & Purification by In Process Product Analysis

Table of contents:

1. General materials and methods:

Unless otherwise stated, all solvents were purchased from Heowns Biochem LLC or Concord Technology and used without further purification. Substrates and reagents were purchased from TCI or Heowns Biochem LLC and used as received.

Unless otherwise stated, all HPLC tests are performed on Shimazu LC-20AT. Column used is Agilent Zorbax CNl, 150 x 4.60 mm, 5 μm. Analytical method: mobile phase: *n*-hexane; flow rate: 0.5 mL/min; Sample injection volume: 2 μL detection: 254 nm.

^{1}H-NMR spectra were recorded on a Bruker Avance-400 or Bruker Avance-600 instrument and are reported relative to residual solvent: $CHCl_3$ (δ 7.26 ppm) or CH_2Cl_2 (δ 5.30 ppm). ^{13}C-NMR spectra were recorded on the same instrument and are reported relative to $CHCl_3$ (δ 77.16 ppm) or CH_2Cl_2 (δ 53.84 ppm). Data for ^{1}H-NMR are

reported as follows: chemical shift (δ/ ppm) (integration, multiplicity, coupling constant (Hz)). Multiplicities are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, br. s = broad singlet, app = apparent. Data for ^{13}C-NMR are reported in terms of chemical shift (δ/ ppm) and multiplicity (C, CH, CH_2 or CH_3). High resolution mass was obtained by SPST or China University of Petroleum. For accurate mass measurements the deviation from the calculated formula is reported in ppm.

2. Procedures for standard curve plotting

Corannulene **1**:

4.13 mg, 2.50 mg, 1.50 mg, 0.90 mg **1** (purity: 98 %) was added to four 25 mL beaker and dissolved in HPLC grade dichloromethane, respectively. The resulting solution was poured into four 25 mL volumetric flask and dilute with HPLC grade dichloromethane to volume, respectively, then named as solution I-IV (concentration: 0.659 mM, 0.395 mM, 0.237 mM, 0.142 mM, respectively). Solution I-IV was then directly tested in analytical HPLC.

Mono-bromocorannulene **2**-I:

14.25 mg, 8.55 mg, 5.13 mg, 3.08 mg **2**-I (purity: 98 %) was added to four 25 mL beaker and dissolved in HPLC grade dichloromethane, respectively. The resulting solution was poured into four 25 mL volumetric flask and dilute with HPLC grade dichloromethane to volume, respectively, then named as solution I-IV (concentration: 1.516 mM, 0.910 mM, 0.546 mM, 0.327 mM, respectively). Solution I-IV was then directly tested in analytical HPLC.

Mono-bromocorannulene **2**-Br:

14.25 mg, 6.5 mg, 3.6 mg, 2.6 mg **2**-Br (purity: 95 %) was added to four 10 mL beaker and dissolved in HPLC grade dichloromethane, respectively. The resulting solution was poured into four 10 mL volumetric flask and dilute with HPLC grade dichloromethane to volume, respectively, then named as solution I-IV (concentration: 4.370 mM, 1.973 mM, 1.093 mM, 0.789 mM, respectively). Solution I-IV was then directly tested in analytical HPLC.

Internal standard 1,3,5-trichlorobenzene:

235.0 mg, 141.0 mg, 84.6 mg, 50.8 mg, 30.5 mg 1,3,5-trichlorobenzene (purity: 99 %) was added to five 10 mL beaker and dissolved in HPLC grade dichloromethane, respectively. The resulting solution was poured into five 25 mL volumetric flask and

dilute with HPLC grade dichloromethane to volume, respectively, then named as solution I-V (concentration: 51.8 mM, 31.1 mM, 18.7 mM, 11.2 mM, 6.7 mM, respectively). Solution I-V was then directly tested in analytical HPLC.

3. Yield calculation methods:

With the addition of internal standard (IS):

The standard curves of **1** & **2**-I provided a correlation (c1, c2) between the concentration and the absorption integral (A1, A2) of HPLC:

$c1 = f(A1) \quad c2 = f'(A2)$

The standard curves of IS provided a correlation between the concentration (c0) and the absorption integral (A0) of HPLC:

$c0 = f''(A0)$

The dilution ratio (r) of the sample can be calculated: (c0' equals the concentration of IS in the reaction mixture, which is already known)

$r = c0/c0'$

The concentration of **1** & **2**-I (c1', c2') in the reaction mixture thus can be calculated:

$c1' = c1/r \quad c2' = c2/r$

Hence the yield & conversion of each compound can be calculated.

Without the addition of internal standard:

The crude product obtained from each entry is regarded as a mixture consisted of **1**, **2**-I & **2**-I_2. hence the mixture's total weight (m) equals the weight of **1** (m1), the weight of **2**-I (m2) and the weight of **2**-I_2 (m3):

$m = m1 + m2 + m3$

A small part of the mixture is sampled to test in HPLC: (m' represents sample's total mass; m1', m2' and m3' represents each compound's mass in the sample; r represents the sample/mixture ratio)

$m' = m1' + m2' + m3'$

$m'/m = m1'/m1 = m2'/m2 = m3'/m3 = r$

The amount (n') and concentration (c) of each compound in the sample can be calculated: (M represents molecular weight)

$n1' = m1'/M1 \quad n2' = m2'/M2 \quad n3' = m3'/M3$

$c1 = n1'/V \quad c2 = n2'/V \quad c3 = n3'/V$

So:

$m1^{'} = M1c1V = rm1 \quad m2^{'} = M2c2V = rm2 \quad m3^{'} = M3c3V = rm3$

$m^{'} = (M1c1 + M2c2 + M3c3)V = rm$

$r/V = (M1c1 + M2c2 + M3c3)/m = M1c1/m1 = M2c2/m2 = M3c3/m3$

The standard curves of **1** & **2**-I provided a correlation between the concentration and the absorption integral (A) of HPLC: (standard curve of **2**-I was applied to **2**-I_2)

$c1 = f(A1) \quad c2 = f'(A2) \quad c3 = f'(A3)$

According to two equations above, the weight of each compound in the mixture m1, m2 & m3 can be solved, hence the yield & conversion of each compound can be calculated.

4. Procedures for Au(III)-catalyzed iodination on 1

Entry 1:

An oven-dried 35 mL pressure flask was put into the glove-box and cooled down under reduced pressure. Gold(III) chloride (15.2 mg, 0.05 mmol), corannulene **1** (250.0 mg, 1.0 mmol) and *N*-iodosuccinimide (NIS) (225.0 mg, 1.0 mmol) was added into the flask in glove-box. The top of the flask was then covered by a rubber stopper and taken out of the glove-box. 16 mL dichloroethane was injected into the flask using a syringe and the flask was sealed with corresponding Teflon cap. The mixture in flask was stirred at 25 °C for 8 hours before heated to 80 °C and further stirred for 48 hours. Resulted reaction mixture in flask was cooled to room temperature, quenched by 5 mL 10 % NaOH solution and extract by dichloromethane (2×20 mL). The combined organic layer was washed with DI (deionized) water (2×20 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

Entry 2:

An oven-dried 35 mL pressure flask was put into the glove-box and cooled down under reduced pressure. Gold(III) chloride (15.2 mg, 0.05 mmol), corannulene **1** (250.0 mg, 1.0 mmol) and *N*-iodosuccinimide (NIS) (270.0 mg, 1.0 mmol) was added into the flask in glove-box. The top of the flask was then covered by a rubber stopper and taken out of the glove-box. 16 mL dichloroethane was injected into the flask using a syringe and the flask was sealed with corresponding Teflon cap. The mixture in flask was stirred at 25 °C for 8 hours before heated to 80 °C and further stirred for 48 hours. Resulted

reaction mixture in flask was cooled to room temperature, quenched by 5 mL 10 % NaOH solution and extract by dichloromethane (2×20 mL). The combined organic layer was washed with DI water (2×20 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

Entry 3:

An oven-dried 35 mL pressure flask was put into the glove-box and cooled down under reduced pressure. Gold(III) chloride (15.2 mg, 0.05 mmol), corannulene **1** (250.0 mg, 1.0 mmol) and *N*-iodosuccinimide (NIS) (337.5 mg, 1.0 mmol) was added into the flask in glove-box. The top of the flask was then covered by a rubber stopper and taken out of the glove-box. 16 mL dichloroethane was injected into the flask using a syringe and the flask was sealed with corresponding Teflon cap. The mixture in flask was stirred at 25 °C for 8 hours before heated to 80 °C and further stirred for 48 hours. Resulted reaction mixture in flask was cooled to room temperature, quenched by 5 mL 10 % NaOH solution and extract by dichloromethane (2×20 mL). The combined organic layer was washed with DI water (2×20 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

5. Procedures for catalyst selection tests

Entry 1:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (90.0 mg, 0.4 mmol) and 1,3,5-trichlorobenzene (90.0 mg, 0.4 mmol) was dissolved in 1 mL dichloroethane, then $FeCl_3$ (6.5 mg, 0.04 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C. The sampling was taken at 0.5 h, 1.0 h, 2.0 h and 4.0 h, each time 10 μL reaction mixture was sampled and diluted by HPLC grade DCM to 1.0 mL. The sample was then test in analytical HPLC to calculate the conversion rate and yield.

Entry 2:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (90.0 mg, 0.4 mmol) and 1,3,5-trichlorobenzene (90.0 mg, 0.4 mmol) was dissolved in 1 mL dichloroethane, then $AlCl_3$ (5.3 mg, 0.04 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C. The sampling was taken at 0.5 h, 1.0 h, 2.0 h and 4.0 h, each time 10 μL reaction mixture was sampled and diluted by HPLC

grade DCM to 1.0 mL. The sample was then test in analytical HPLC to calculate the conversion rate and yield.

Entry 3:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (90.0 mg, 0.4 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (5.0 μL, 0.04 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 4.0 h, the reaction mixture was then quenched by 5 mL 10 % NaOH solution, extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

Entry 4:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (90.0 mg, 0.4 mmol) was dissolved in 1 mL dichloroethane, the cap was sealed and the mixture was stirred at 80 °C. The sampling was taken at 0 h and 4.0 h, each time 10 μL reaction mixture was sampled and diluted by HPLC grade DCM to 1.0 mL. The sample was then test in analytical HPLC.

6. Procedures for condition selection tests

I-1:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (22.5 mg, 0.1 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (5.0 μL, 0.04 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 3 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-2:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (36.0 mg, 0.16 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (5.0 μL, 0.04 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 3 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered &

washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-3:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (45.0 mg, 0.2 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (5.0 μL, 0.04 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 3 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-4:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (54.0 mg, 0.24 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (5.0 μL, 0.04 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 3 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-5:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (67.5 mg, 0.3 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (5.0 μL, 0.04 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 3 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-6:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (90.0 mg, 0.4 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (5.0 μL, 0.04 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for

3 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-7:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (45.0 mg, 0.2 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (10.0 μL, 0.08 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 0.5 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-8:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (45.0 mg, 0.2 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (15.0 μL, 0.12 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 0.5 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-9:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (45.0 mg, 0.2 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (20.0 μL, 0.16 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 0.5 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-10:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide

(NIS) (45.0 mg, 0.2 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (25.0 μL, 0.2 mmol) was added and the cap was sealed. The mixture was stirred at 80 °C for 0.5 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-11:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (45.0 mg, 0.2 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (25.0 μL, 0.2 mmol) was added and the cap was sealed. The mixture was stirred at r.t. for 12 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-12:

To a 15 mL pressure tube, corannulene **1** (50.0 mg, 0.2 mmol), *N*-iodosuccinimide (NIS) (45.0 mg, 0.2 mmol) was dissolved in 1 mL dichloroethane, then $BF_3 \cdot Et_2O$ (10.0 μL, 0.08 mmol) was added and the cap was sealed. The mixture was stirred at r.t. for 12 h. Resulted reaction mixture was then allowed to cool to r.t., quenched by 5 mL 10 % NaOH solution and extract by DCM (2×5 mL). The organic layer was gathered & washed with water (2×5 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (mostly consisted of **1**, **2**-I & **2**-I_2) was obtained. The product was weighed & sampled to test in HPLC.

I-13 (gram-scale):

To a 50 mL round-bottom flask, corannulene **1** (1.0 g, 4.0 mmol), *N*-iodosuccinimide (NIS) (0.9 g, 4.0 mmol) was dissolved in 20 mL dichloroethane, then $BF_3 \cdot Et_2O$ (0.2 ml, 1.6 mmol) was added. The mixture was stirred at r.t. for 12 h and then quenched by 50 mL 10 % NaOH solution, extract by DCM (2×50 mL). The organic layer was gathered & washed with water (2×50 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product was obtained. The conversion rate (87.9 %) and yield of **2**-I (76.3 %, 86.9 % b.r.s.m.) was determined by analytical HPLC.

Br-1 (gram-scale):

To a 50 mL round-bottom flask, corannulene **1** (1.0 g, 4.0 mmol), *N*-bromosuccinimide (NBS) (712.0 mg, 4.0 mmol) was dissolved in 20 mL dichloroethane, then $BF_3 \cdot Et_2O$ (0.2 ml, 1.6 mmol) was added. The mixture was stirred at r.t. for 12 h and then quenched by 50 mL 10 % NaOH solution, extract by DCM (2×50 mL). The organic layer was gathered & washed with water (2×50 mL) and dried using anhydrous Na_2SO_4. The solvent was evaporated under vacuum and a crude product (total weight: 1.21 g) was obtained. The conversion rate (79.1%) and yield of **2**-Br (69.3 %, 87.5 % b.r.s.m.) was determined by analytical HPLC.

7. Procedures for purification of 2-I and 2-Br

Purification of **2-I**:

The gram-scale reaction (I-13) was repeated twice and the combined crude reaction mixture (total weight: 2.85 g) of **1**, **2**-I & **2**-I_2 was packed on a short silica plug and separated in to two portions (portion a: total weight 900 mg, 90 % **2**-I/ 10 % **2**-I_2, portion b: total weight 1900 mg, 13 % **1**/ 86 % **2**-I/ 1 % **2**-I_2). Portion a was then dissolved in HPLC grade DCM, mixed with kieselguhr and went on separation using Combiflash-Rf, gives 640 mg 93 % pure **2**-I. Multiple further separation attempt afforded about 200 mg 96 % pure **2**-I. ^{1}H-NMR data of **2**-I is consistent with reported values.

Purification of **2-Br**:

The crude reaction mixture of **1**, **2**-Br & **2**-Br_2 was packed on a short silica plug and separated in to two portions (portion a: total weight 515 mg, 90 % **2**-Br/ 10 % **2**-Br_2, portion b: total weight 685 mg, 30 % **1**/ 65 % **2**-Br/ 5 % **2**-Br_2). Portion a and b was then dissolved in HPLC grade DCM, mixed with kieselguhr and went on further separation using Combiflash-Rf, respectively. The separation process obtained 955 mg 98 % pure **2**-Br in total, as well as recovered 200 mg 98 % pure **1**. ^{1}H-NMR data of **2**-Br is consistent with reported values.

8. Preparation of *sym*-pentachlorocorannulene 3

Corannulene **1** (3 g, 12 mmol) dissolved in dichloromethane (156 mL) was cooled to -78 °C and iodine monochloride (25.3 g, 156 mmol) was added. The mixture was allowed to warm to room temperature over 10 hours and stirred an additional 3 days and 14 hours at ambient temperature. The solution was quenched by 156 mL 10% Vitamin C solution and washed with 300 mL water twice. The resulting yellow suspension was evaporated to dryness and a crude product (5.3 g, 35 % pure) was obtained. Triturated 3 times with cyclohexane (100 mL), the resulting yellowish solid (2.9 g, 58% pure) was recrystallized from 1,2-dichlorobenzene twice with a total amount of 500 mL to yield a pale-yellow solid (1.86 g, 85 % pure, 31 %). ^{1}H-NMR data is consistent with reported values.

9. Preparation of overchlorinated corannulene 6

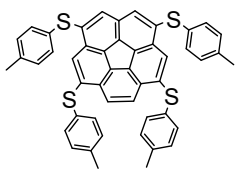
The filtrate of **2** after digesting in cyclohexane was separated by column chromatography with eluent of cyclohexane and used without further purification.

10. Preparation of 1,4,6,9-*tetrakis*(4-methoxyphenylthio)corannulene 7

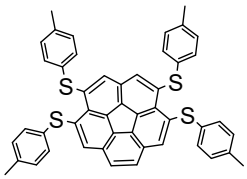
To a 10 mL round bottom flask equipped with a reflux condenser, DMI (5 mL, dried over MS) was added. 4-methylthiophenol (162 mg, 1.31 mmol) and sodium hydride (44 mg, 1.09 mmol, 60 % in mineral oil) were added and allowed to stir at room temperature for 10 minutes. **6** (50 mg, 0.110 mmol) was added and the solution was warmed to 60 °C for 18 hours. The solution was cooled, extracted three times with ethylacetate (15 mL) and washed with water. The organic layer was dried over magnesium sulfate, filtered, and evaporated. The product was purified by prep-TLC with hexane/dichloromethane (1:5) as eluent. The yield of a light-yellow solid was 10 mg (10 %).

Four tetrakis(phenylthio)corannulene are possible isomers. However, NOESY shows no cross peaks between the protons on corannulene ring. Compound **7a** is the possible structure through this point. Also, in compound **7b**, **7c** and **7d** there are two, one and one repulsion between the adjacent benzene rings. Compound **7a** is the most

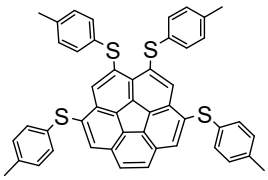
reasonable structure from the perspective of energy.



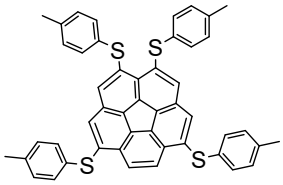
7a



7b



7c



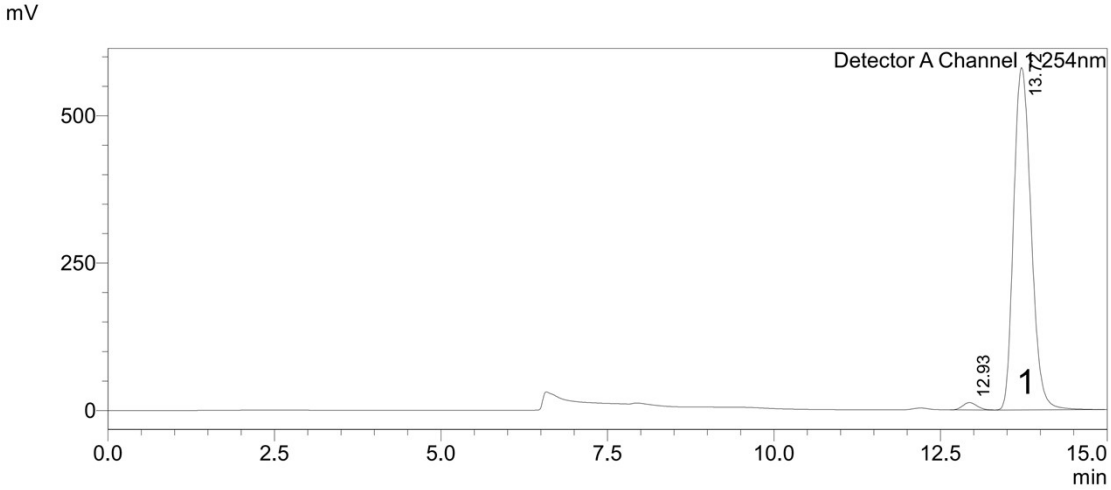
7d

9. HPLC traces & data plotting of standard curves

9.1 HPLC traces & data plotting of standard curves of compound 1

Trace 1: concentration 1.098 mM

Chromatogram:



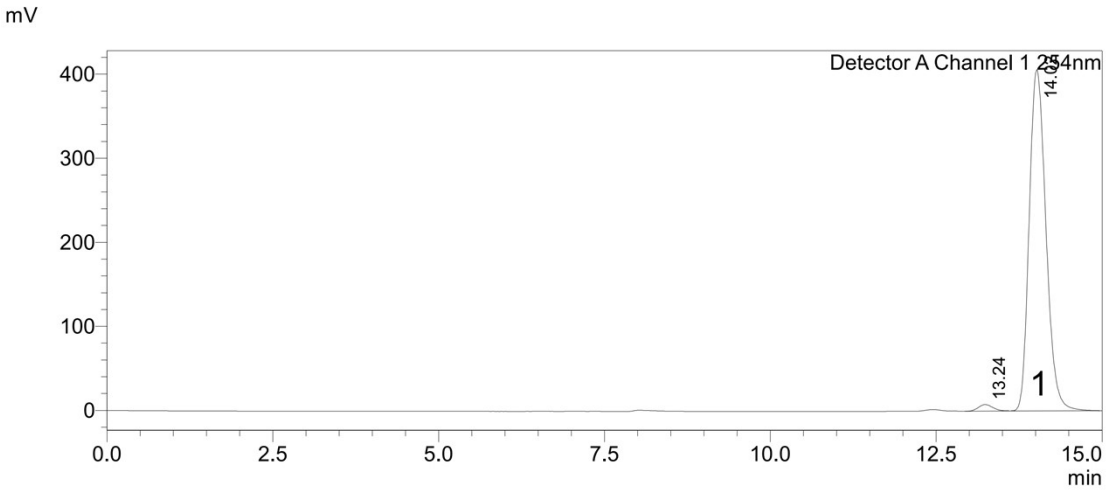
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.93	186000	12486	1.72	
2	13.72	10609733	580653	98.28	
Total		10795733	593139	100.00	

Trace 2: concentration 0.659 mM

Chromatogram:



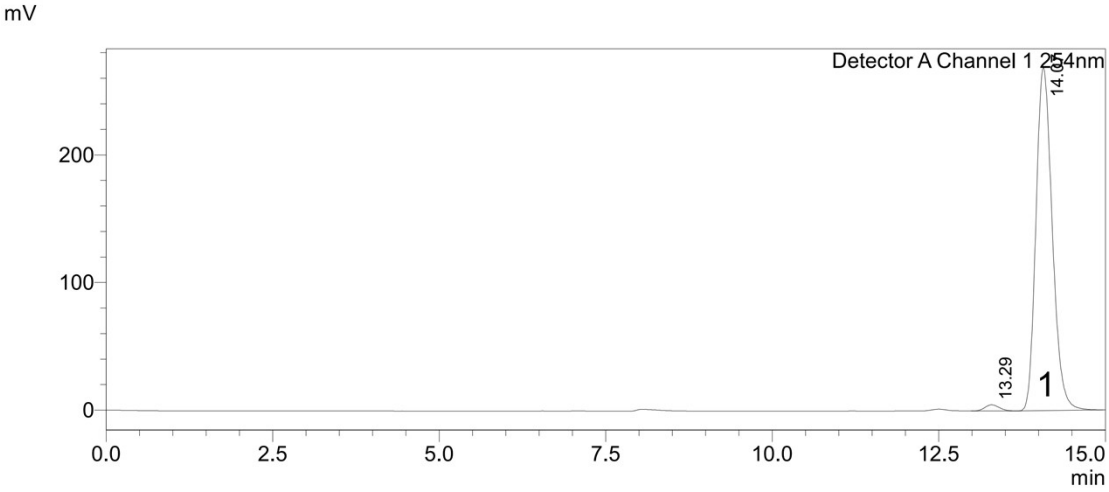
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	13.24	119833	7822	1.65	
2	14.02	7141018	405855	98.35	
Total		7260852	413677	100.00	

Trace 3: concentration 0.395 mM

Chromatogram:



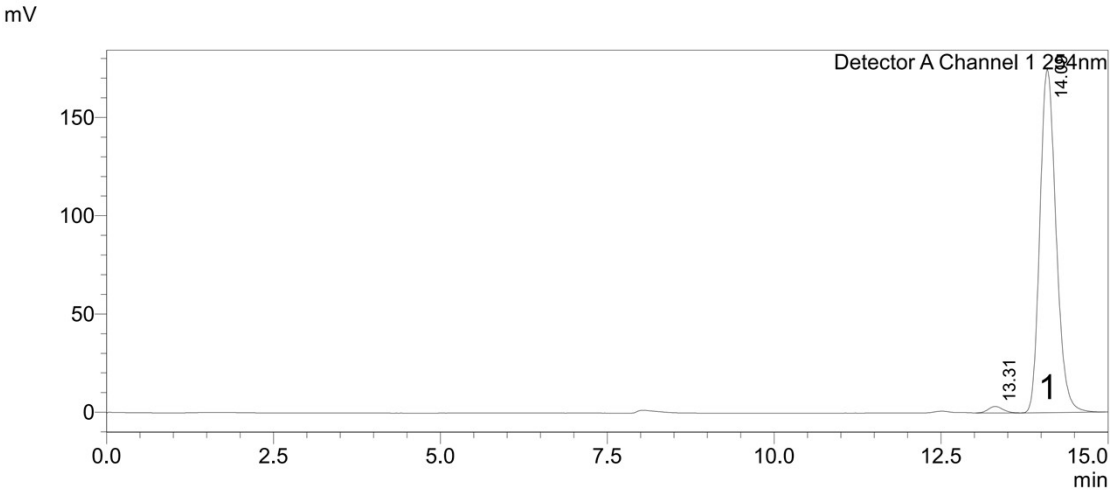
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	13.29	72936	4844	1.57	
2	14.07	4585688	268479	98.43	
Total		4658624	273322	100.00	

Trace 4: concentration 0.237 mM

Chromatogram:



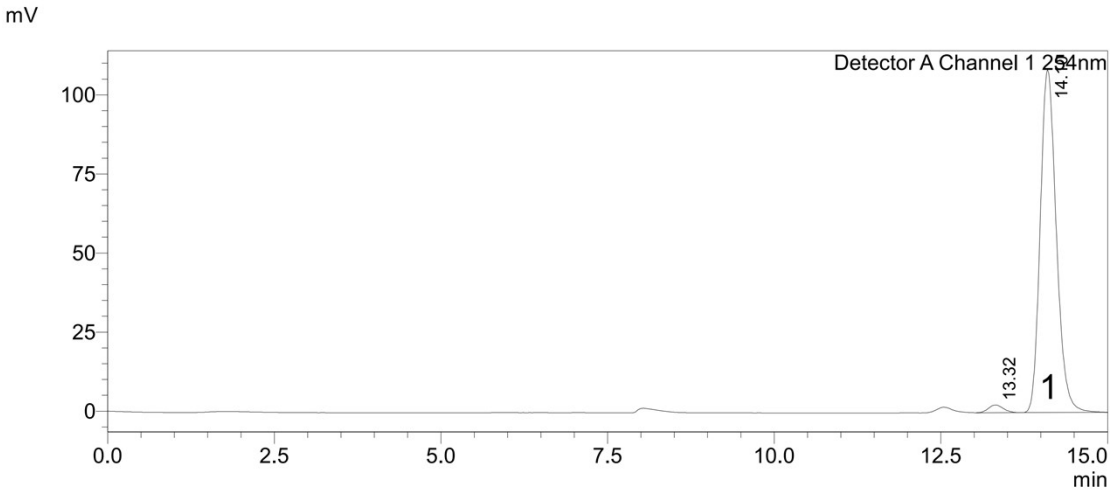
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	13.31	49746	3288	1.66	
2	14.09	2952387	174646	98.34	
Total		3002133	177934	100.00	

Trace 5: concentration 0.142 mM

Chromatogram:

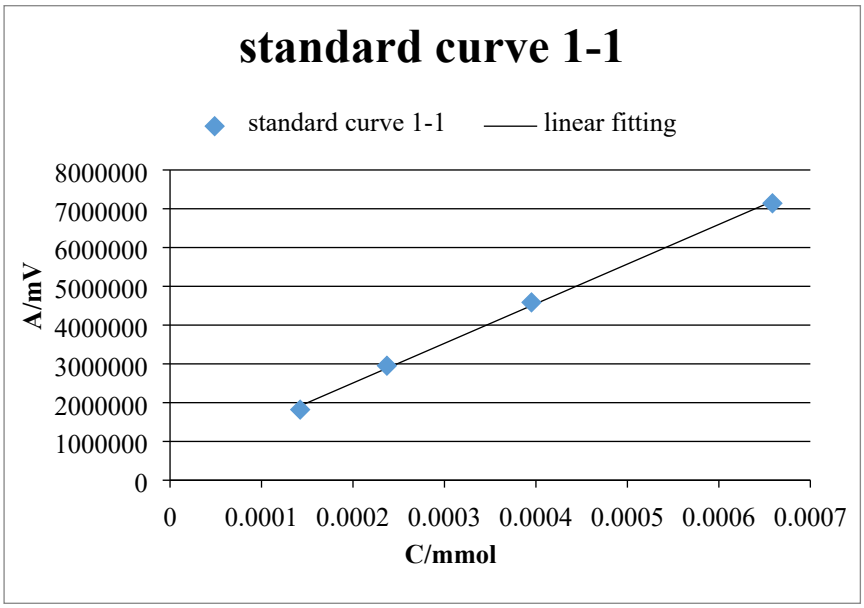


Peak Table:

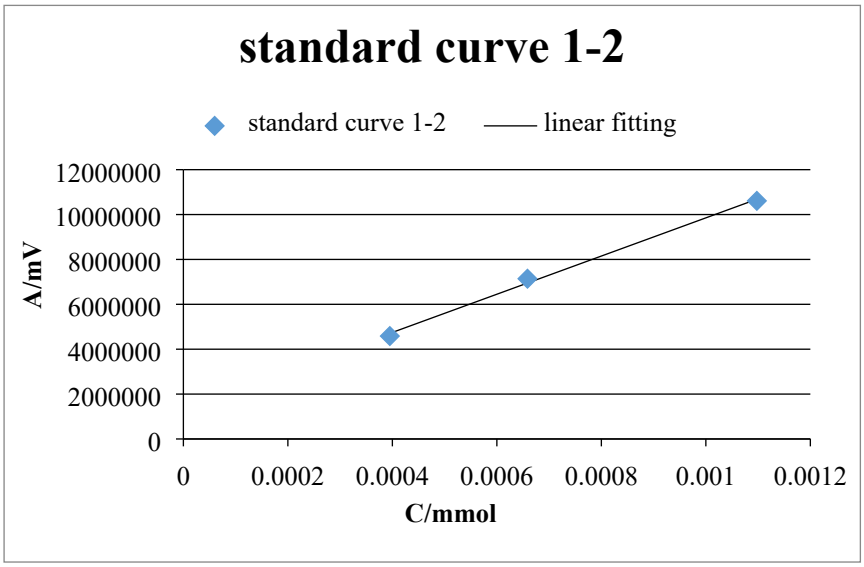
Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	13.32	37793	2446	2.03	
2	14.10	1820434	108323	97.97	
Total		1858227	110769	100.00	

Standard curve **1**-1: linear fitting of trace 2-5



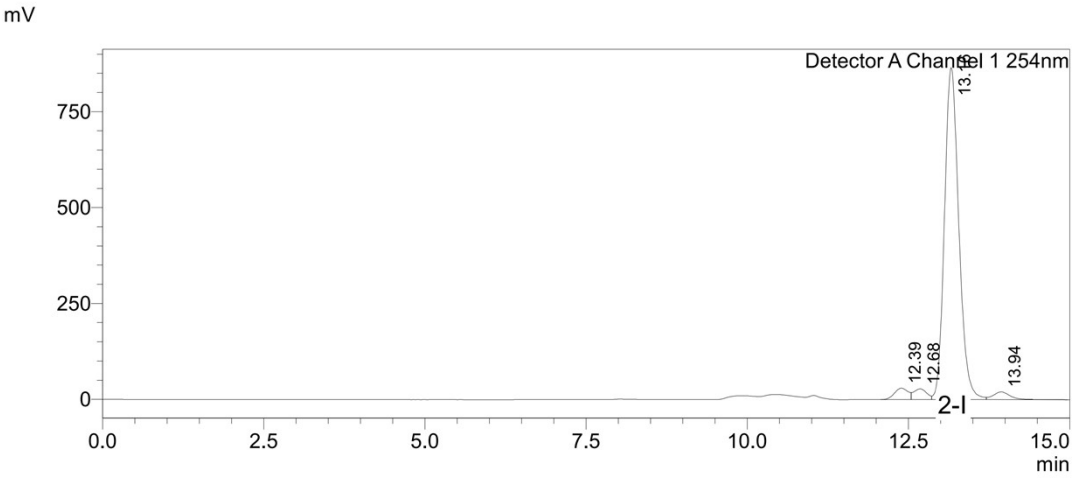
Standard curve **1**-2: linear fitting of trace 1-3



9.2 HPLC traces & data plotting of standard curves of compound 2-I

Trace 1: concentration 1.516 mM

Chromatogram:



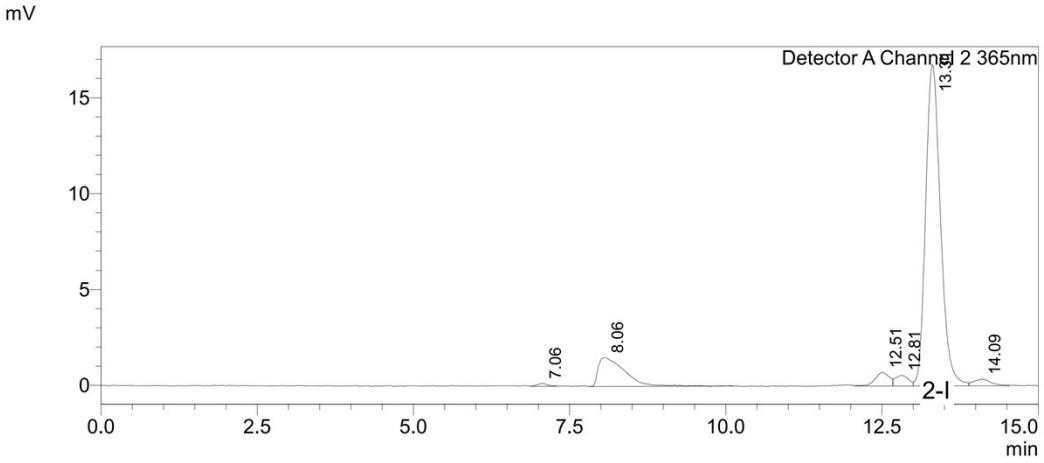
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.39	444940	29896	3.04	
2	12.68	394365	28069	2.70	
3	13.16	13402375	865156	91.68	
4	13.94	377710	20267	2.58	
Total		14619389	943388	100.00	

Trace 2: concentration 0.910 mM

Chromatogram:



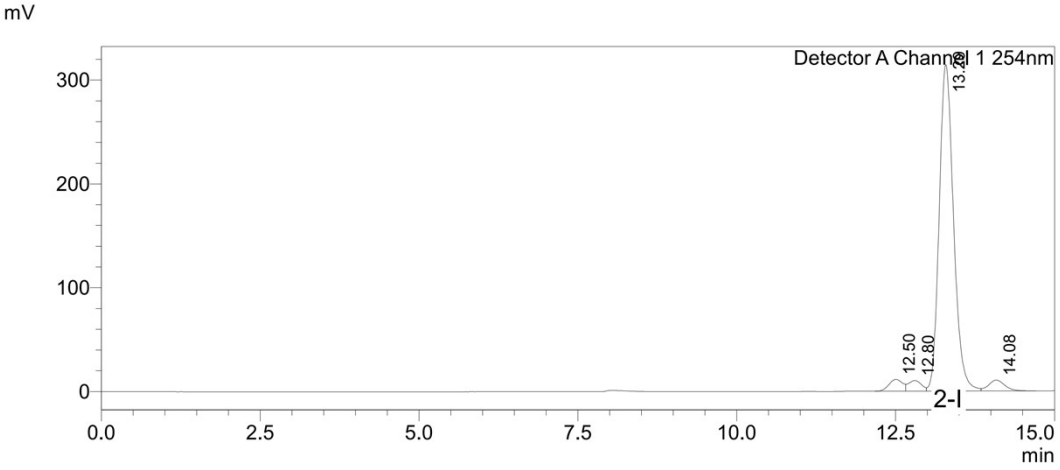
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.52	305976	19966	3.36	
2	12.82	244068	17349	2.68	
3	13.30	8286440	525592	90.91	
4	14.10	278729	14942	3.06	
Total		9115213	577848	100.00	

Trace 3: concentration 0.546 mM

Chromatogram:



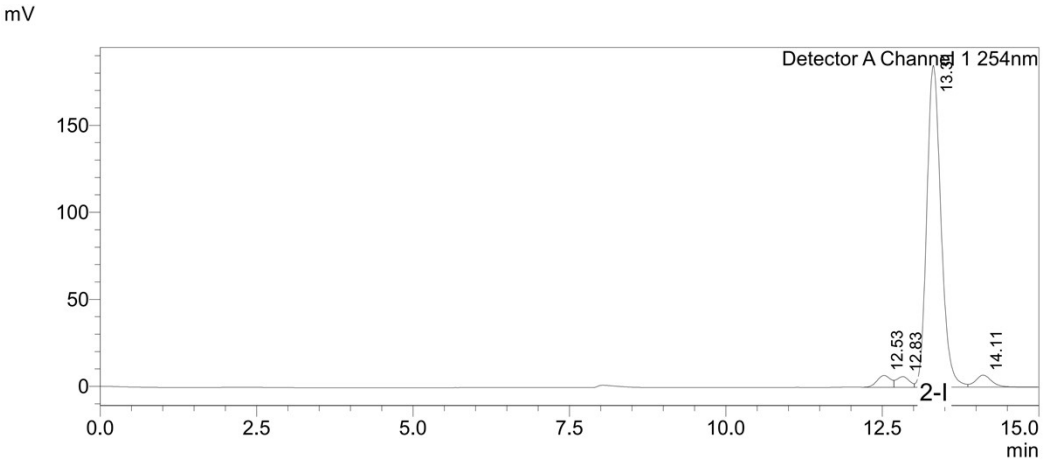
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.50	171394	11369	3.15	
2	12.80	147257	10252	2.70	
3	13.29	4940277	314251	90.71	
4	14.08	187108	10551	3.44	
Total		5446036	346423	100.00	

Trace 4: concentration 0.327 mM

Chromatogram:

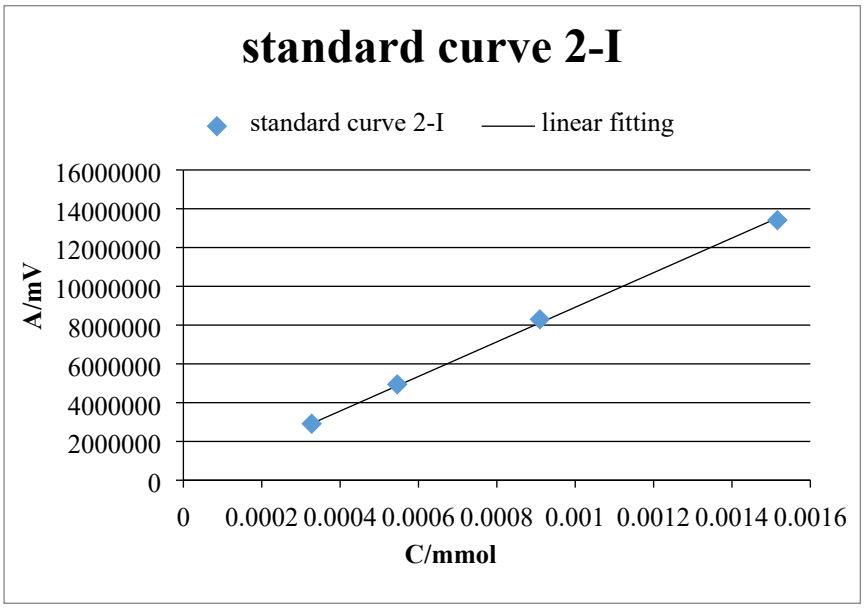


Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.53	102572	6748	3.17	
2	12.83	87298	6075	2.70	
3	13.31	2920016	184838	90.20	
4	14.11	127524	6962	3.94	
Total		3237410	204623	100.00	

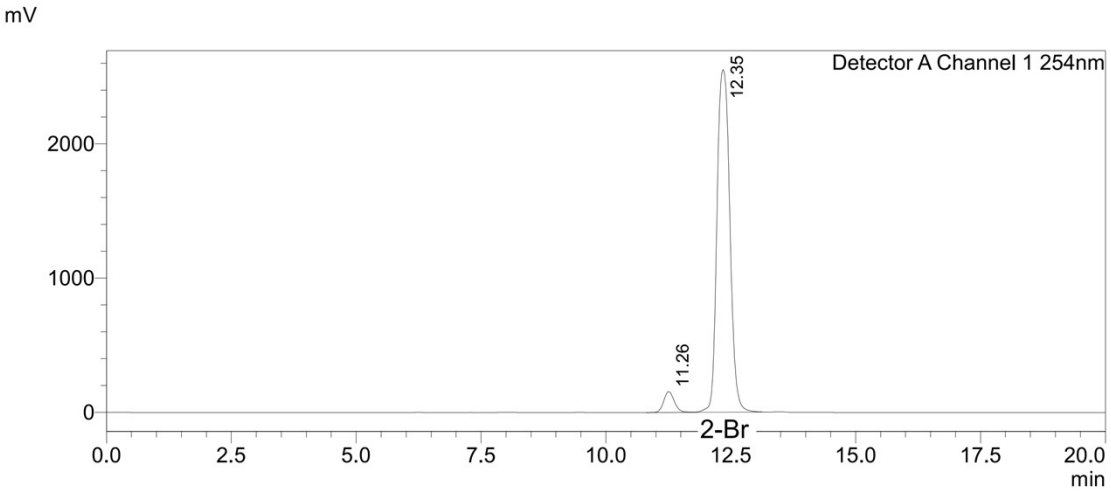
Standard curve **2**-I: linear fitting of trace 1-4



9.3 HPLC traces & data plotting of standard curves of compound 2-Br

Trace 1: concentration 4.370 mM

Chromatogram:



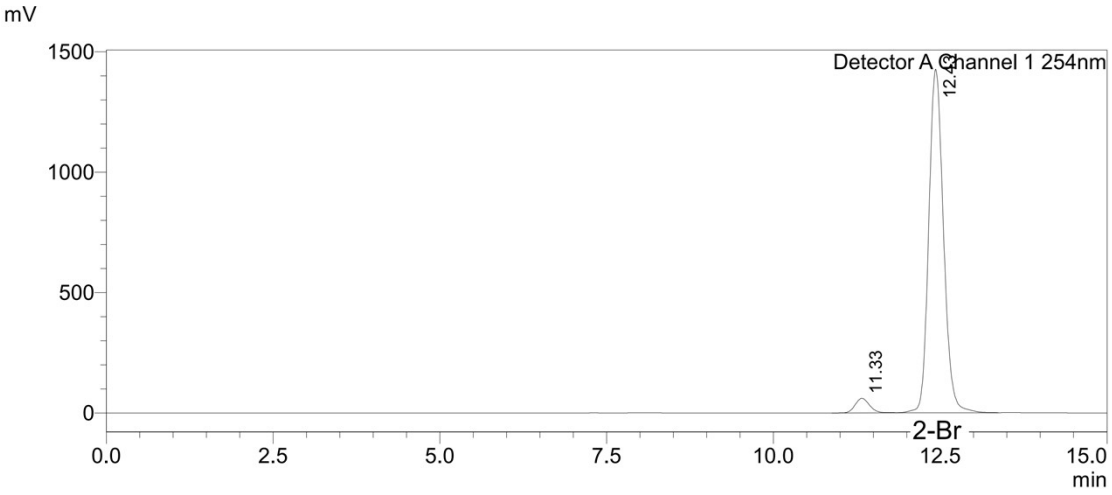
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	11.26	2308270	155391	4.81	
2	12.35	45724206	2549472	95.19	
Total		48032477	2704864	100.00	

Trace 2: concentration 1.973 mM

Chromatogram:



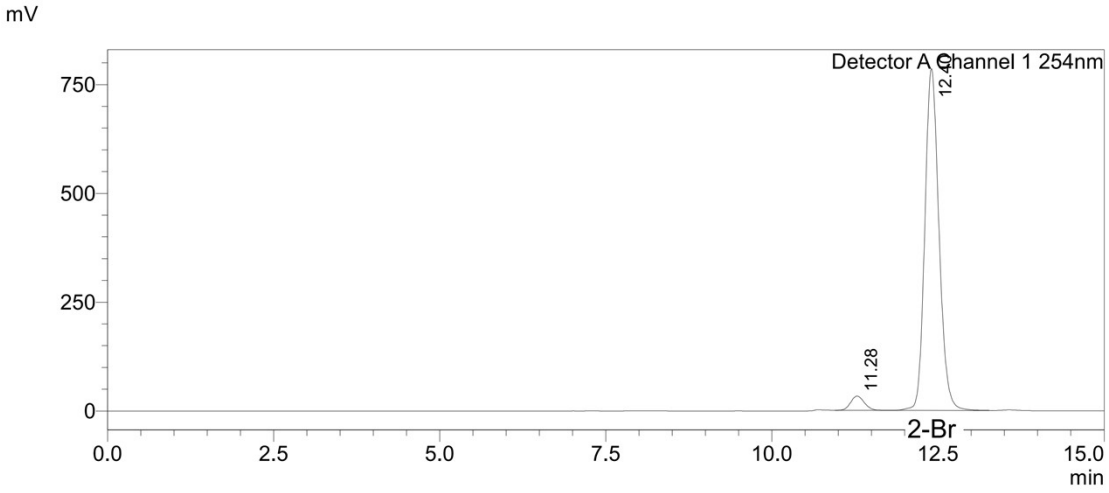
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	11.33	914801	60672	4.00	
2	12.43	21938526	1427358	96.00	
Total		22853327	1488030	100.00	

Trace 3: concentration 1.093 mM

Chromatogram:



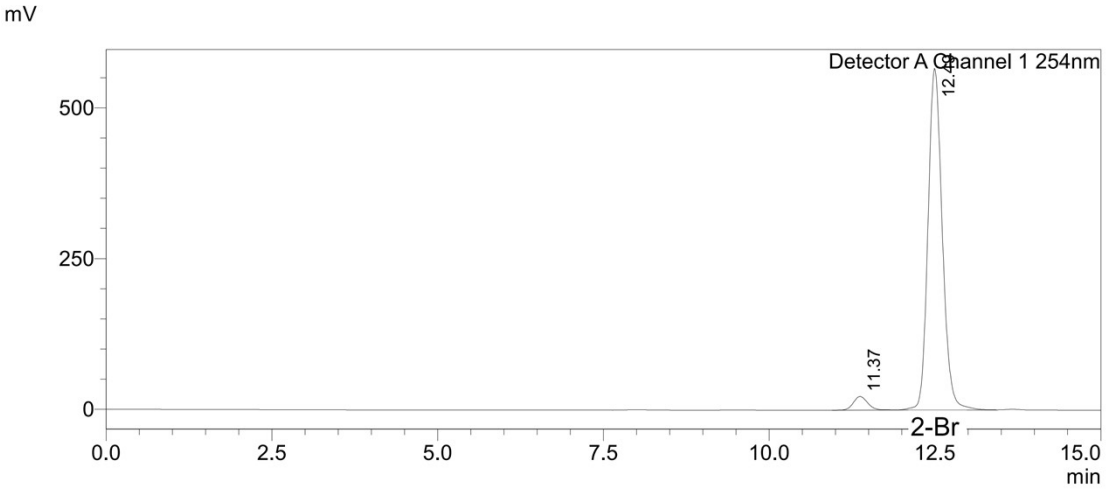
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	11.28	470154	32836	3.88	
2	12.40	11641601	784965	96.12	
Total		12111755	817801	100.00	

Trace 4: concentration 0.789 mM

Chromatogram:

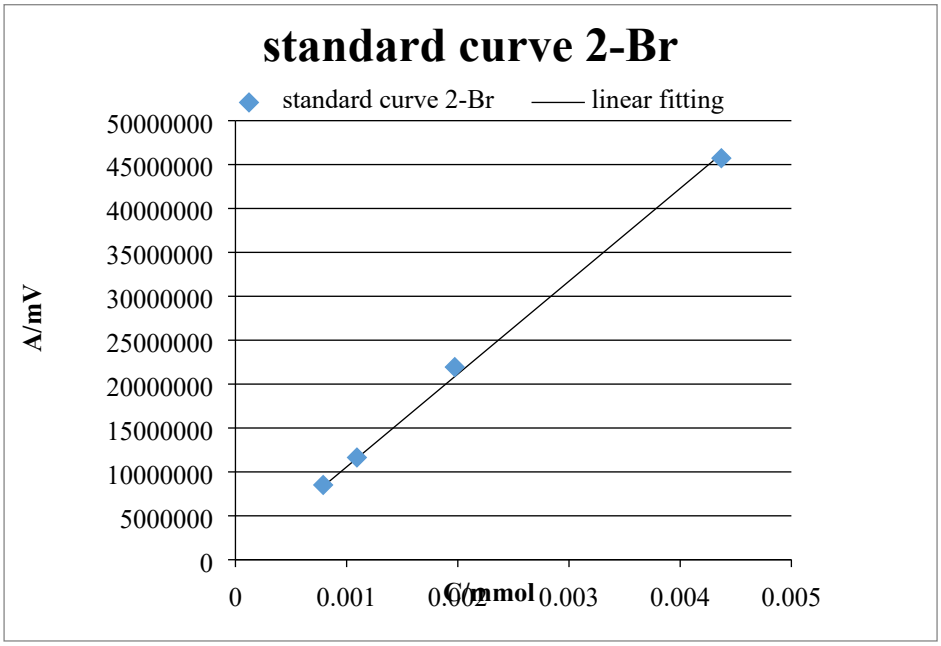


Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	11.37	341953	22679	3.86	
2	12.49	8512837	566426	96.14	
Total		8854790	589105	100.00	

Standard curve **2**-Br: linear fitting of trace 1-4

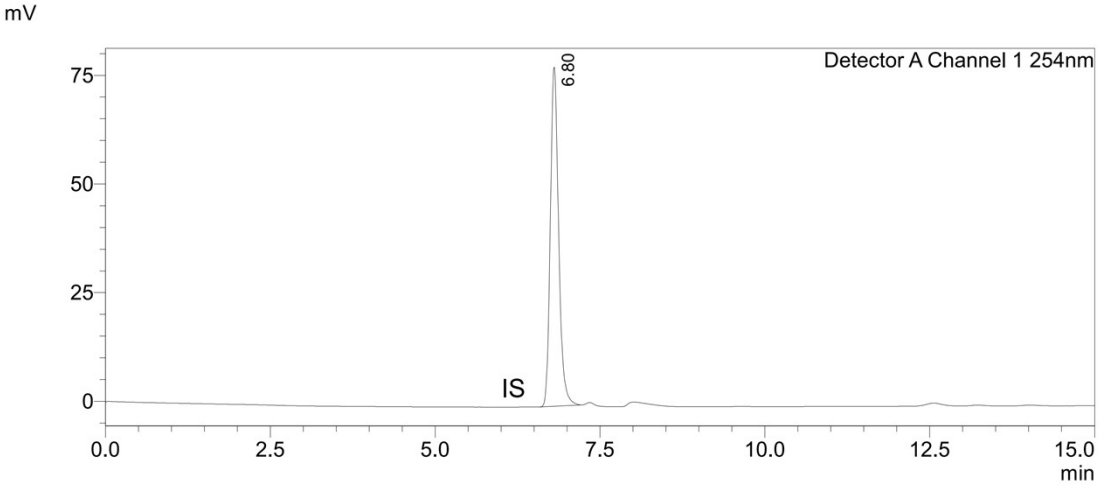


9.4 HPLC traces & data plotting of standard curves of internal standard 1,3,5-trichlorobenzene

IS: internal standard

Trace 1: concentration 51.8 mM

Chromatogram:



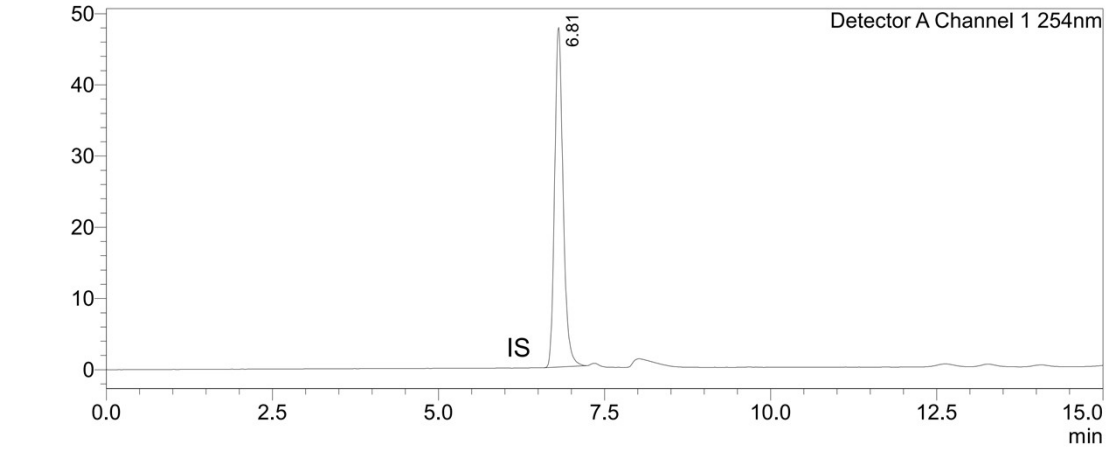
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.80	683770	77990	100.00	
Total		683770	77990	100.00	

Trace 2: concentration 31.1 mM

Chromatogram:



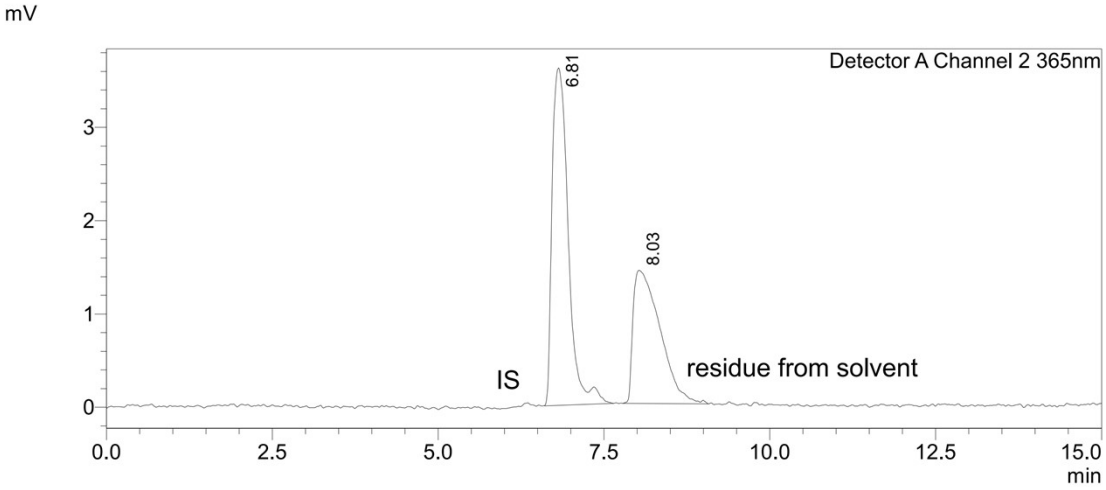
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.81	424109	47648	100.00	
Total		424109	47648	100.00	

Trace 3: concentration 18.7 mM

Chromatogram:



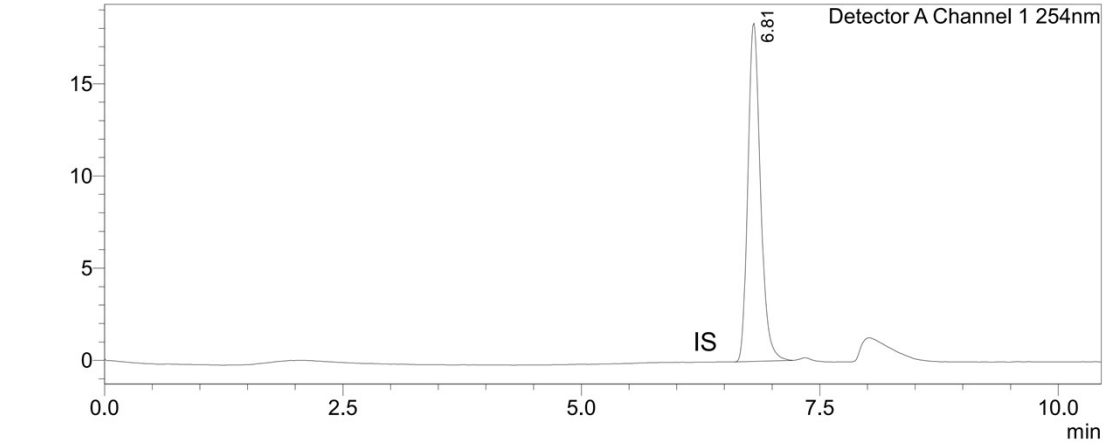
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.81	267947	29578	100.00	
Total		267947	29578	100.00	

Trace 4: concentration 11.2 mM

Chromatogram:



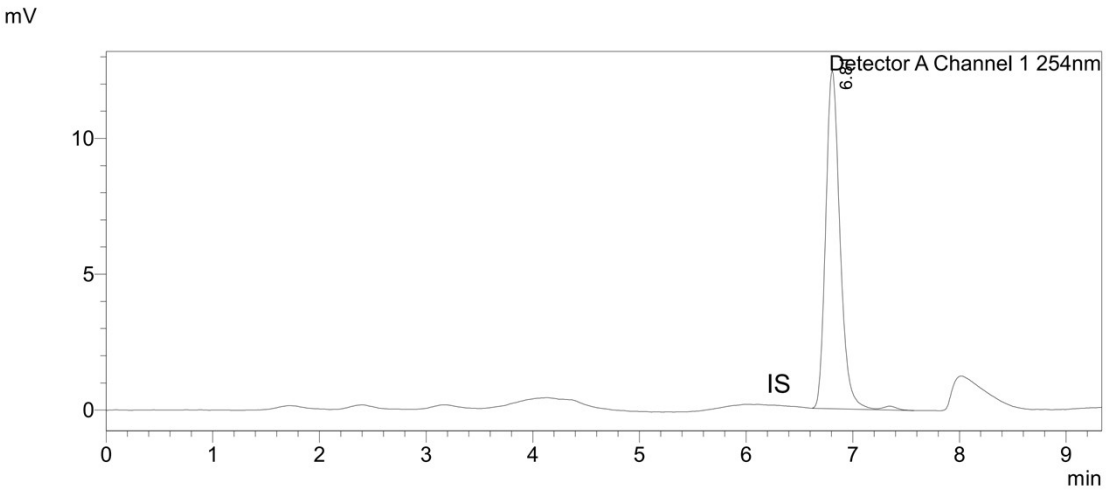
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.81	168452	18329	100.00	
Total		168452	18329	100.00	

Trace 5: concentration 6.7 mM

Chromatogram:

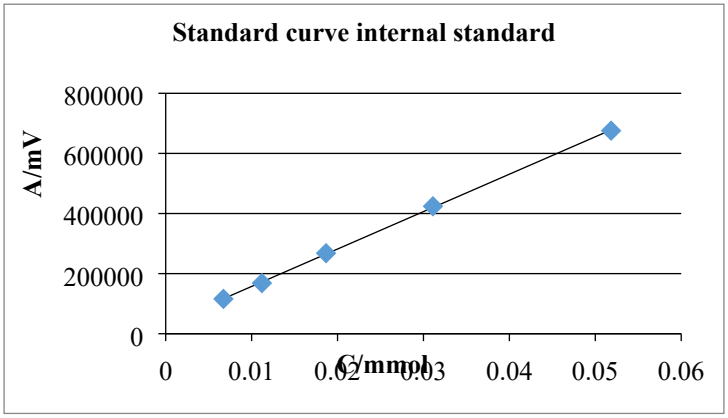


Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.81	115931	12446	100.00	
Total		115931	12446	100.00	

Standard curve internal standard: linear fitting of trace 1-5

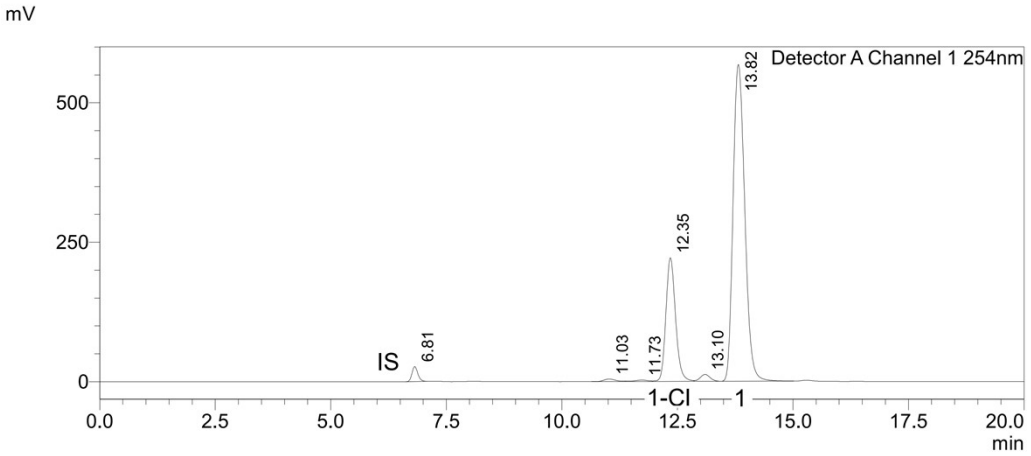


10. HPLC traces of catalyst selection tests

10.1 HPLC traces of Table 1, Entry 1

Trace 1: reaction time 0.5 h

Chromatogram:



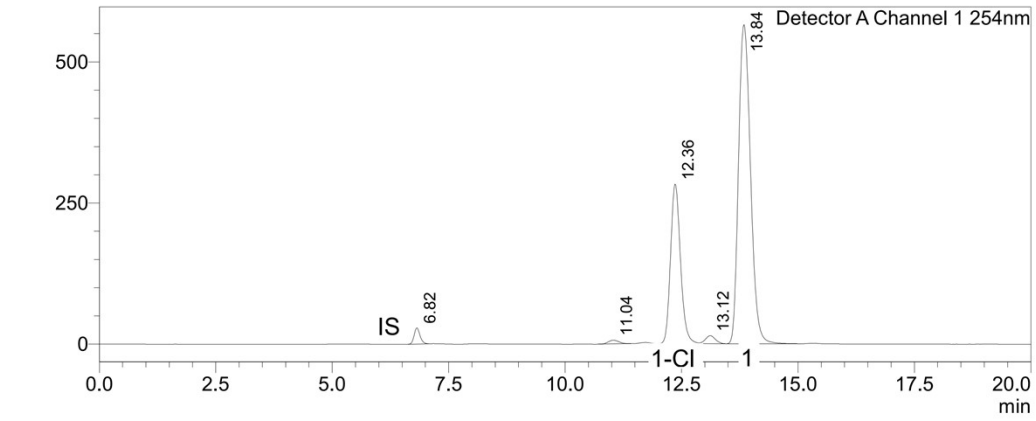
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.81	235983	26855	1.71	
2	11.03	81160	4555	0.59	
3	11.73	53211	2545	0.39	
4	12.35	3224060	221879	23.39	
5	13.10	184170	12378	1.34	
6	13.82	10002685	567856	72.58	
Total		13781269	836070	100.00	

Trace 2: reaction time 1.0 h

Chromatogram:



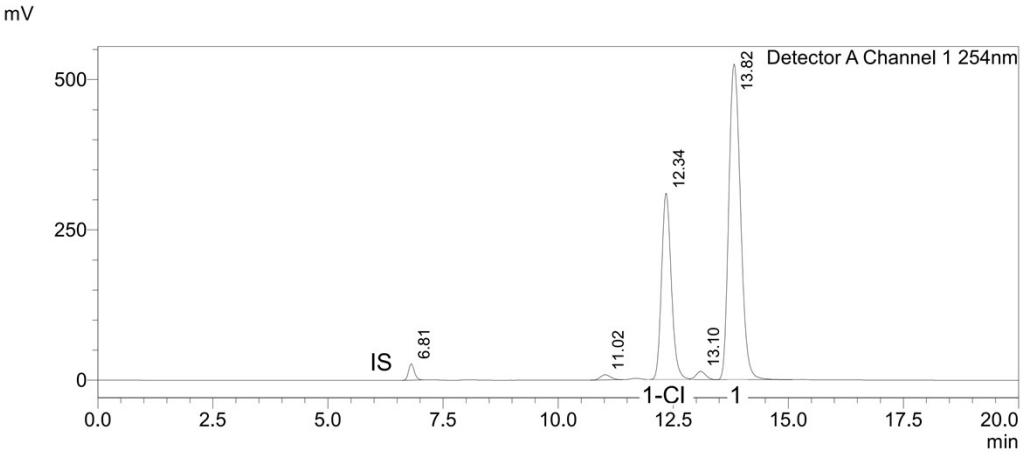
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.82	250785	28601	1.68	
2	11.04	104424	6606	0.70	
3	12.36	4192033	282304	28.12	
4	13.12	211698	14226	1.42	
5	13.84	10150816	565090	68.08	
Total		14909757	896826	100.00	

Trace 3: reaction time 2.0 h

Chromatogram:



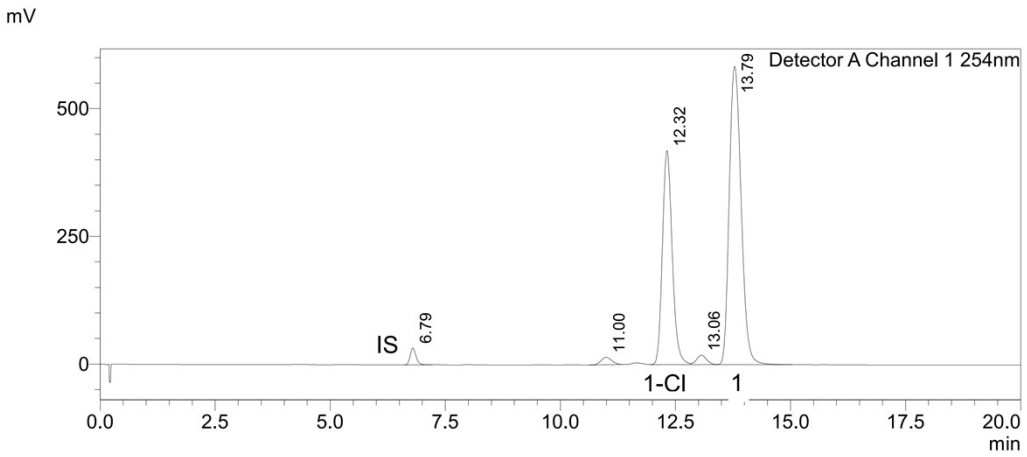
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.81	237804	27170	1.64	
2	11.02	135787	8706	0.94	
3	12.34	4585992	310027	31.68	
4	13.10	206442	13837	1.43	
5	13.82	9312102	524965	64.32	
Total		14478125	884705	100.00	

Trace 4: reaction time 4.0 h

Chromatogram:



Peak Table:

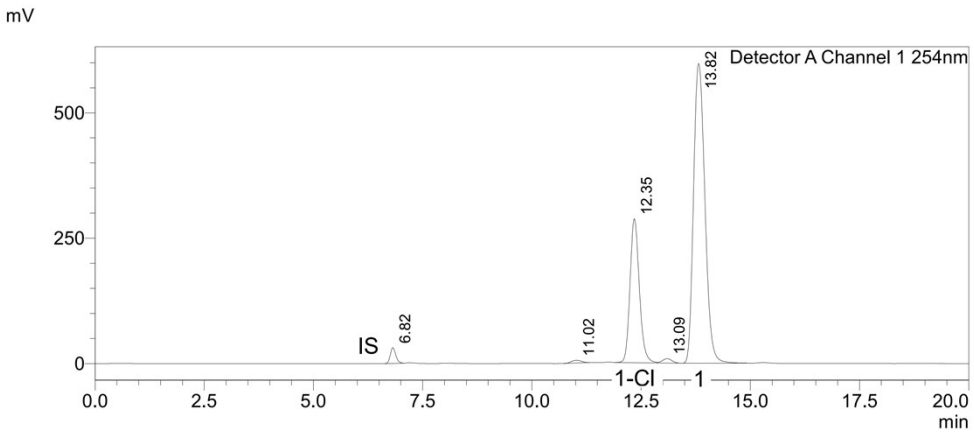
Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.79	293153	32988	1.67	
2	11.00	237766	14738	1.36	
3	12.32	6203596	418818	35.43	
4	13.06	274436	18363	1.57	
5	13.79	10500564	583543	59.97	
Total		17509514	1068451	100.00	

10.2 HPLC traces of Table 1, Entry 2

Trace 1: reaction time 0.5 h

Chromatogram:



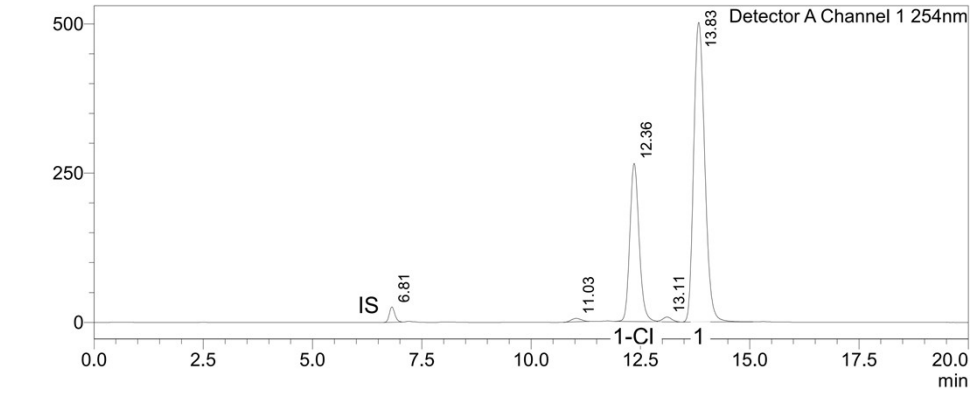
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.82	273780	31416	1.76	
2	11.02	86954	5363	0.56	
3	12.35	4276231	286904	27.45	
4	13.09	131353	8862	0.84	
5	13.82	10811647	597749	69.39	
Total		15579966	930294	100.00	

Trace 2: reaction time 1.0 h

Chromatogram:



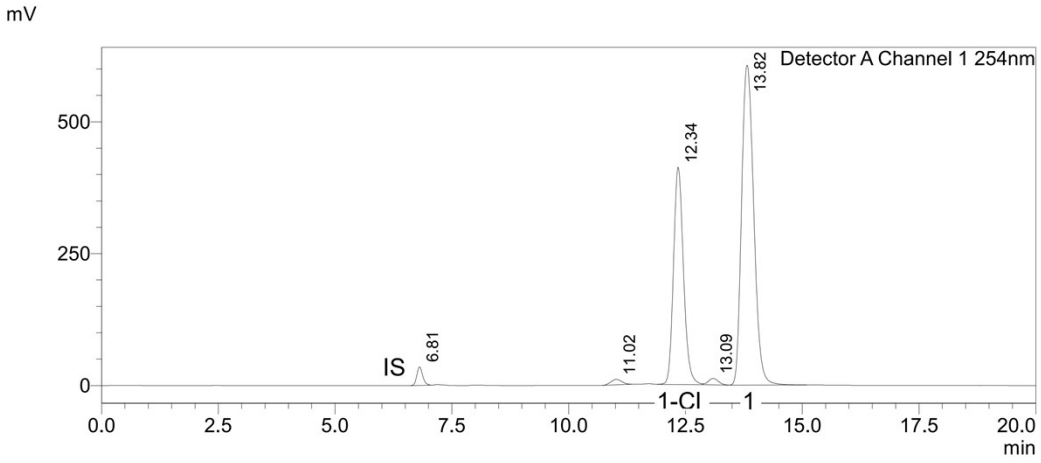
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.81	224934	25611	1.70	
2	11.03	89438	5641	0.68	
3	12.36	3927332	264920	29.77	
4	13.11	120184	8093	0.91	
5	13.83	8830763	501802	66.94	
Total		13192651	806068	100.00	

Trace 3: reaction time 2.0 h

Chromatogram:



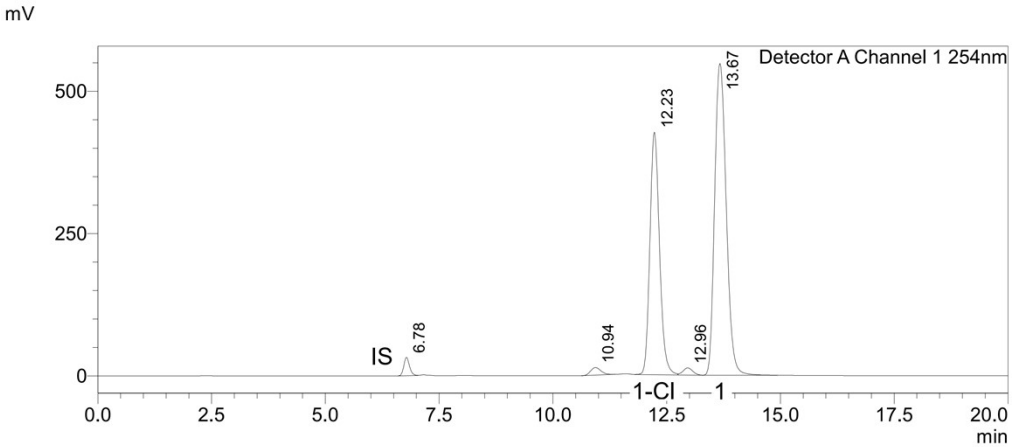
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.81	303920	35008	1.71	
2	11.02	167266	10284	0.94	
3	12.34	6134281	411820	34.49	
4	13.09	180810	12172	1.02	
5	13.82	10999885	606363	61.85	
Total		17786162	1075648	100.00	

Trace 4: reaction time 4.0 h

Chromatogram:



Peak Table:

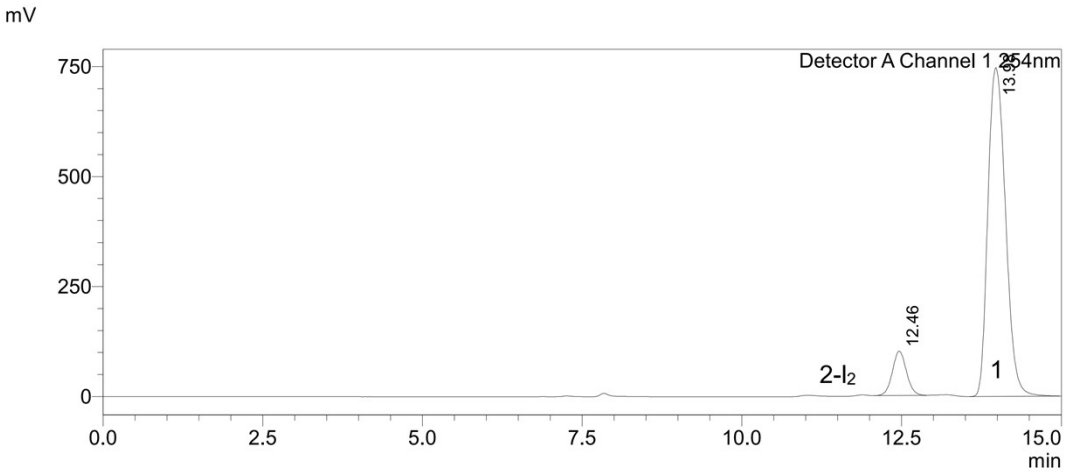
Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.78	277378	31980	1.67	
2	10.94	211048	13283	1.27	
3	12.23	6268538	425966	37.68	
4	12.96	183853	12592	1.11	
5	13.67	9695983	547490	58.28	
Total		16636800	1031311	100.00	

10.3 HPLC traces of Table 1, Entry 3

Trace 1: reaction time 1.0 h

Chromatogram:



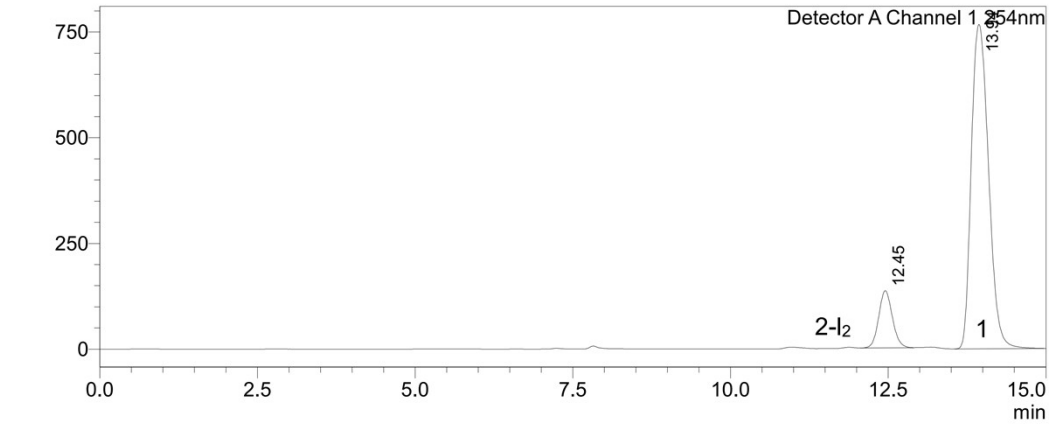
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.46	1549614	100864	9.75	
2	13.98	14343232	747150	90.25	
Total		15892845	848015	100.00	

Trace 2: reaction time 2.0 h

Chromatogram:



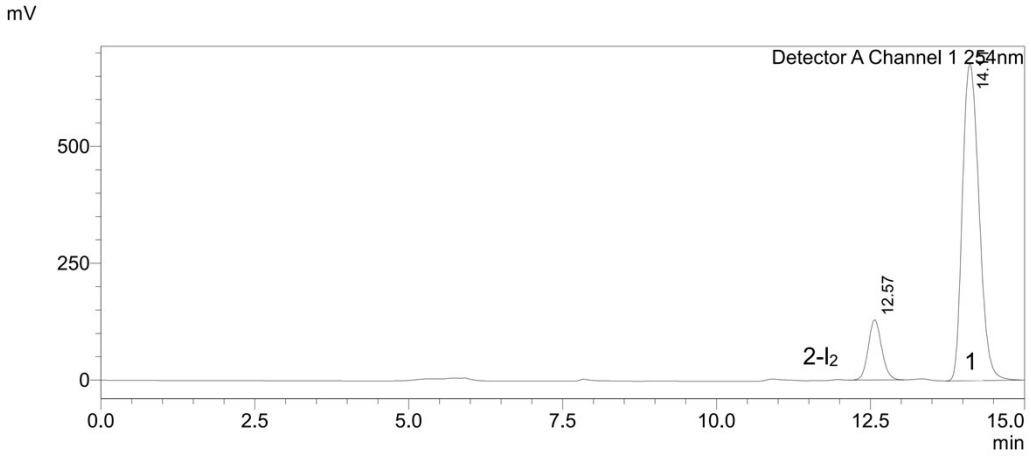
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.45	2032657	135311	12.24	
2	13.94	14575089	767208	87.76	
Total		16607746	902519	100.00	

Trace 3: reaction time 4.0 h

Chromatogram:



Peak Table:

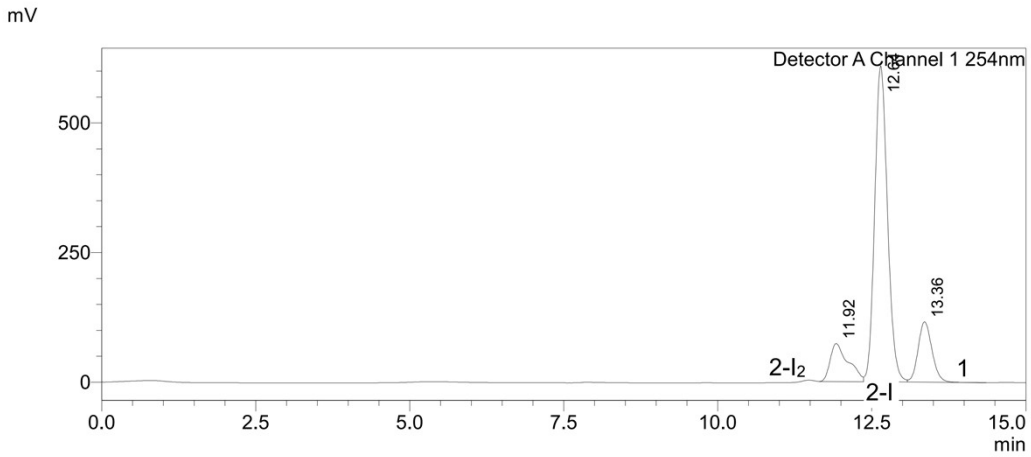
Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.57	1956354	128871	13.30	
2	14.11	12748656	677364	86.70	
Total		14705010	806235	100.00	

10.4 HPLC traces of Table 1, Entry 4

Trace 1: reaction time 4.0 h

Chromatogram:



Peak Table:

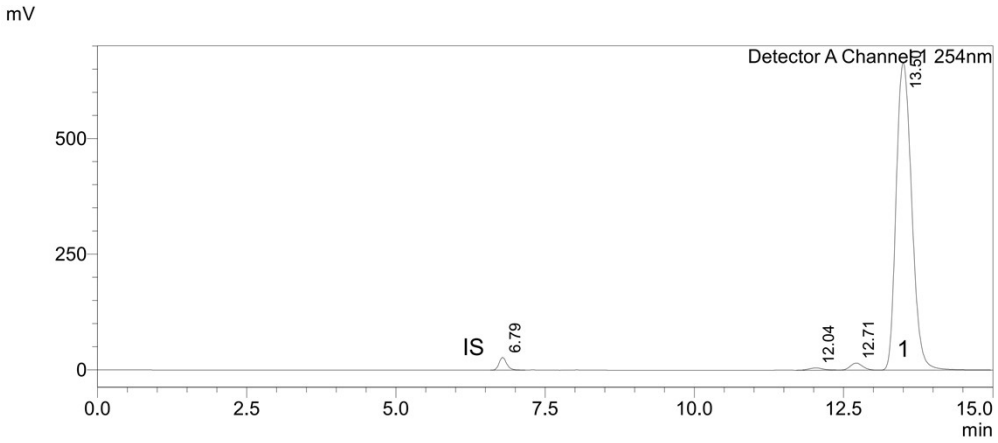
Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	11.92	1492229	73488	12.29	
2	12.64	8820659	609469	72.64	
3	13.36	1830369	116588	15.07	
Total		12143257	799546	100.00	

10.5 HPLC trace of Table 1, Entry 5

Trace 1: reaction time 0 h

Chromatogram:



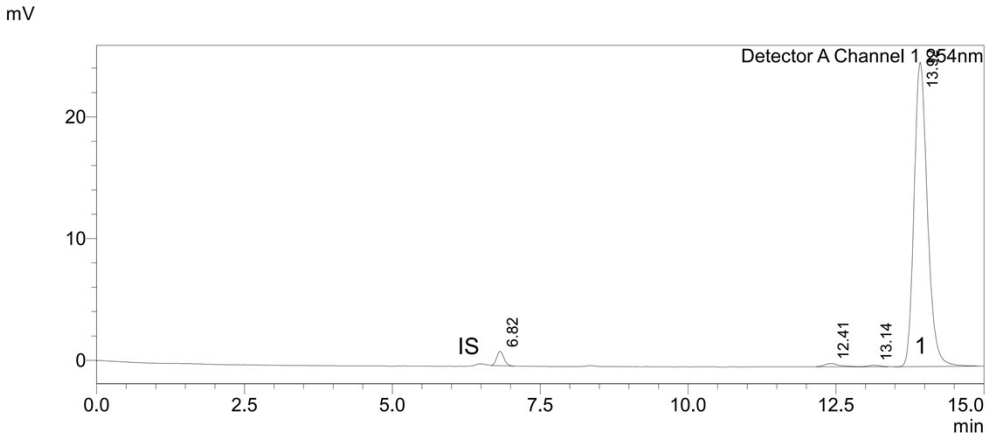
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.79	246166	27393	1.95	
2	12.04	83620	4848	0.66	
3	12.71	222919	15396	1.77	
4	13.50	12045786	663927	95.61	
Total		12598491	711564	100.00	

Trace 2: reaction time 4 h

Chromatogram:



Peak Table:

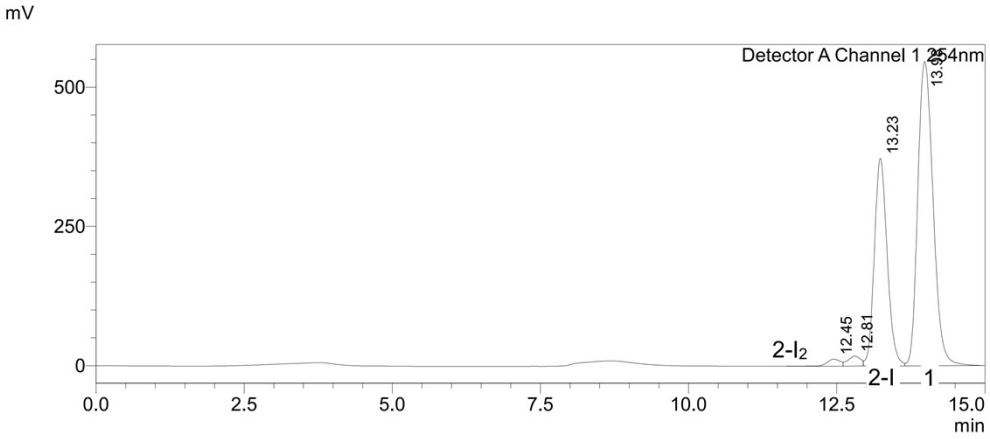
Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	6.82	9913	1168	2.41	
2	12.41	5005	273	1.22	
3	13.14	2063	132	0.50	
4	13.92	394071	24996	95.87	
Total		411052	26569	100.00	

11. HPLC traces of condition selection tests

Trace 1: I-1

Chromatogram:



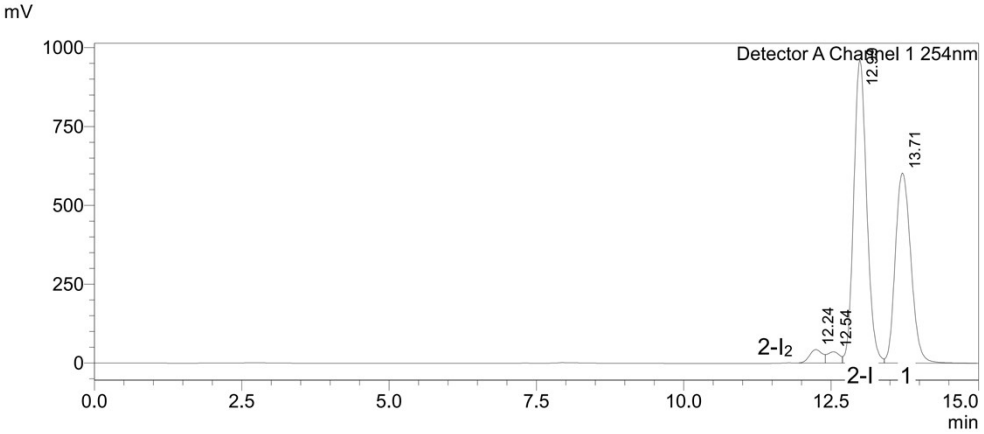
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.45	195036	12470	1.23	
2	12.81	266247	17904	1.67	
3	13.23	5637385	372883	35.42	
4	13.98	9817217	546284	61.68	
Total		15915885	949540	100.00	

Trace 2: I-2

Chromatogram:



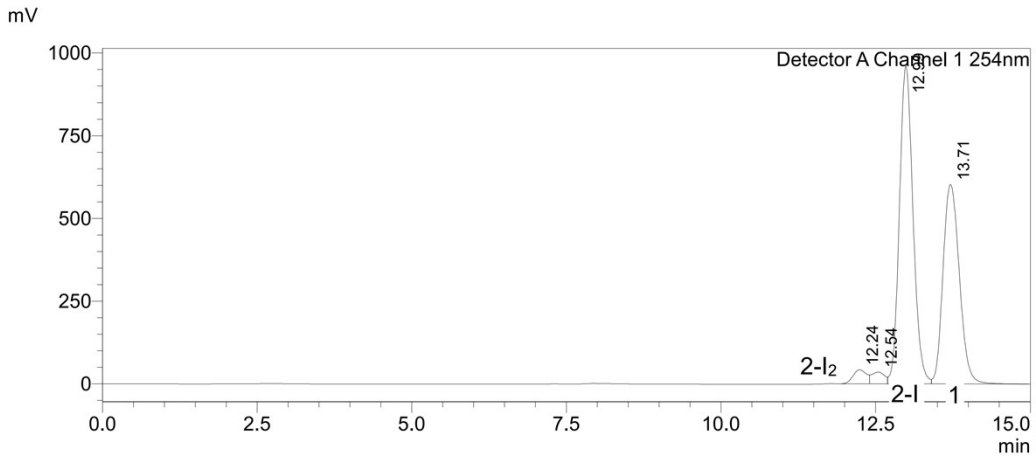
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.24	649241	42588	2.40	
2	12.54	519841	35546	1.92	
3	12.99	14752861	960372	54.58	
4	13.71	11107655	602993	41.09	
Total		27029598	1641499	100.00	

Trace 3: I-3

Chromatogram:



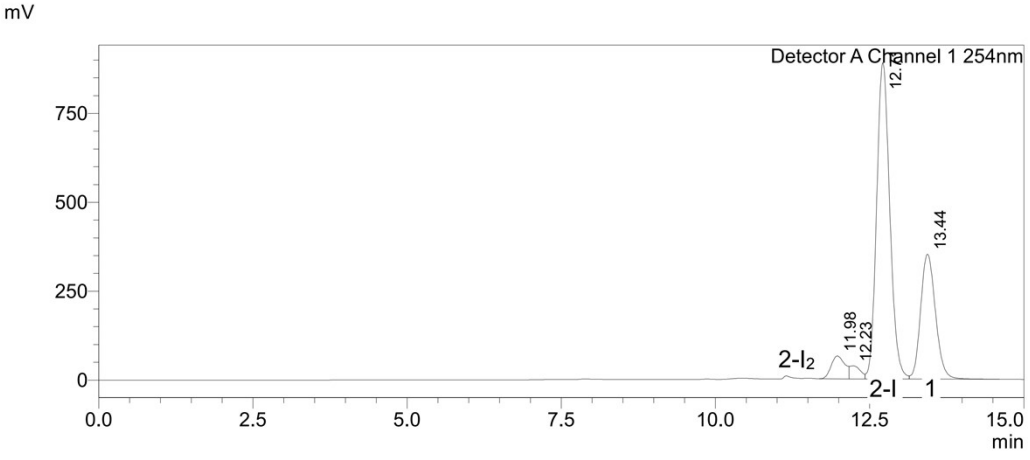
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.24	649241	42588	2.40	
2	12.54	519841	35546	1.92	
3	12.99	14752861	960372	54.58	
4	13.71	11107655	602993	41.09	
Total		27029598	1641499	100.00	

Trace 4: I-4

Chromatogram:



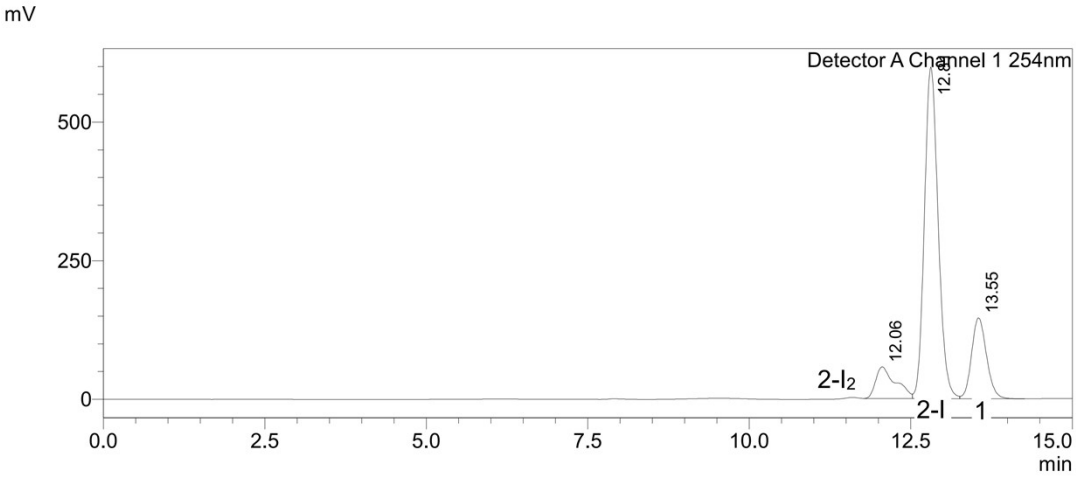
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	11.98	1008300	64528	4.91	
2	12.23	439113	36731	2.14	
3	12.71	13214599	889291	64.30	
4	13.44	5889896	351373	28.66	
Total		20551907	1341923	100.00	

Trace 5: I-5

Chromatogram:



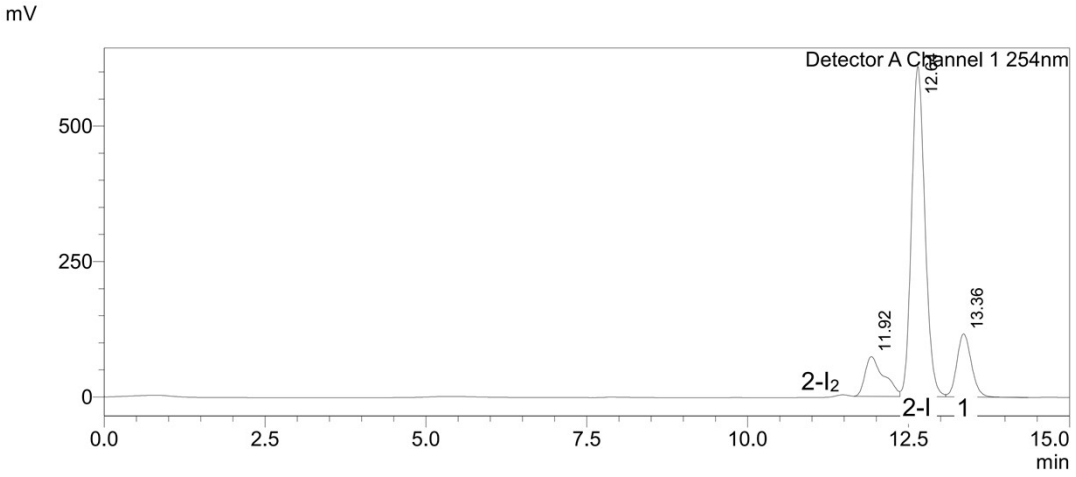
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.06	1219158	57181	9.82	
2	12.81	8856022	597846	71.30	
3	13.55	2345594	145910	18.88	
Total		12420775	800938	100.00	

Trace 6: I-6

Chromatogram:



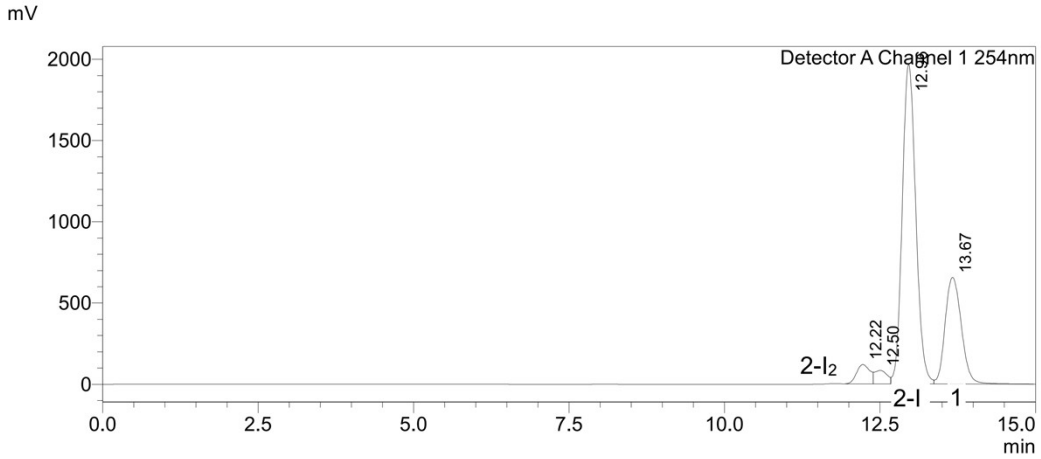
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	11.92	1492229	73488	12.29	
2	12.64	8820659	609469	72.64	
3	13.36	1830369	116588	15.07	
Total		12143257	799546	100.00	

Trace 7: I-7

Chromatogram:



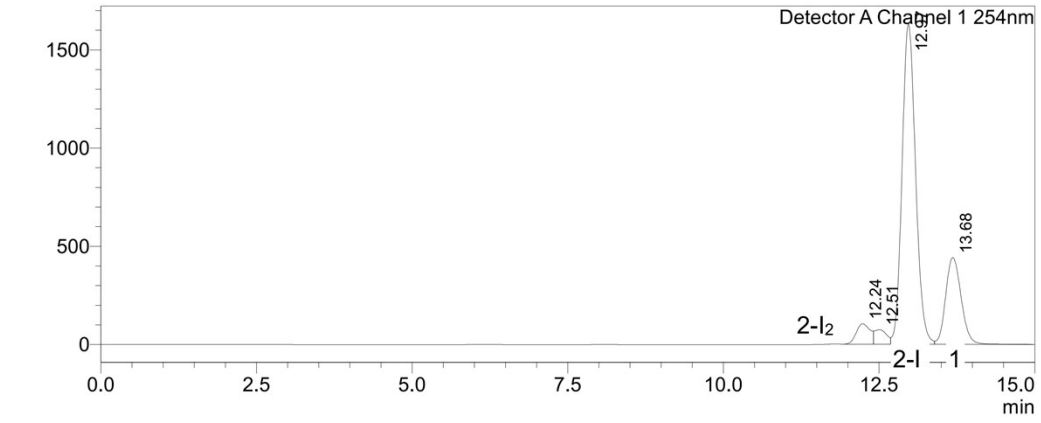
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.22	1798388	119195	4.02	
2	12.50	1160618	82683	2.59	
3	12.96	29863779	1966637	66.72	
4	13.67	11939328	655860	26.67	
Total		44762113	2824375	100.00	

Trace 8: I-8

Chromatogram:



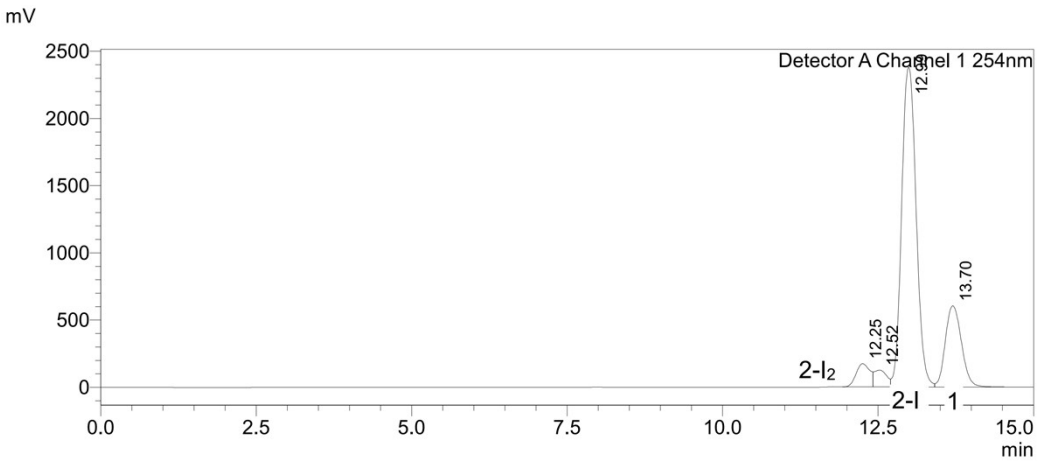
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.24	1621500	104151	4.64	
2	12.51	998691	73930	2.86	
3	12.97	24675931	1630637	70.61	
4	13.68	7650221	442074	21.89	
Total		34946343	2250792	100.00	

Trace 9: I-9

Chromatogram:



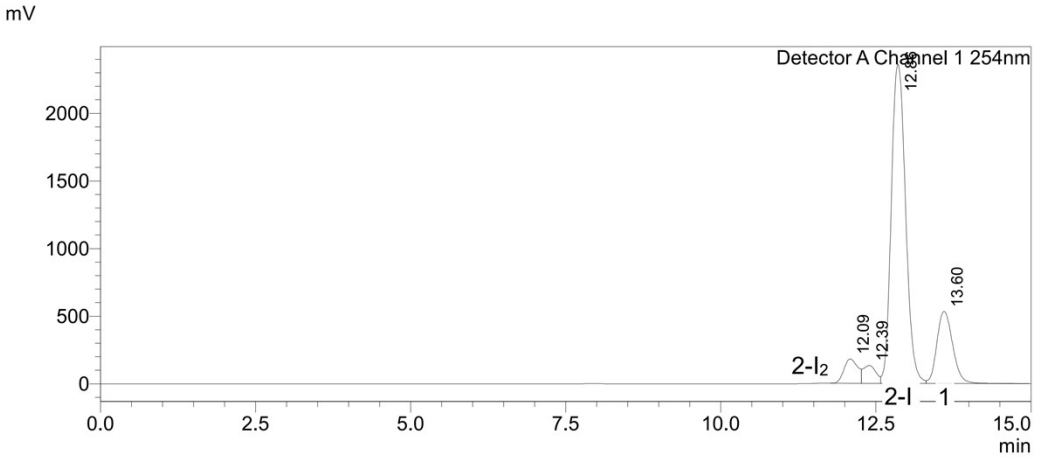
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.25	2678746	172917	4.98	
2	12.52	1749667	124820	3.25	
3	12.99	38435082	2378891	71.45	
4	13.70	10927092	604781	20.31	
Total		53790587	3281408	100.00	

Trace 10: I-10

Chromatogram:



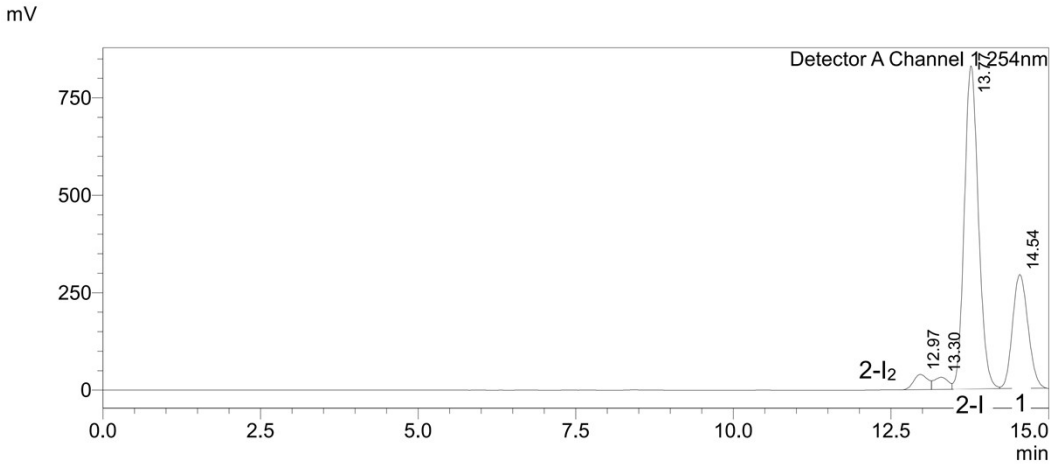
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.09	2813625	180626	5.41	
2	12.39	1889635	132037	3.63	
3	12.86	37861104	2358708	72.81	
4	13.60	9432239	533143	18.14	
Total		51996603	3204515	100.00	

Trace 11: I-11

Chromatogram:



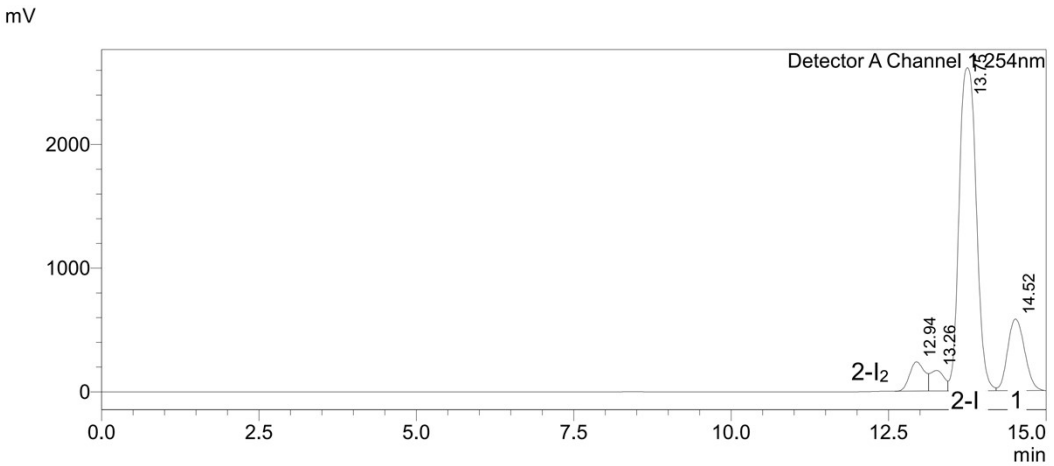
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.97	614039	39076	3.23	
2	13.30	487420	31200	2.56	
3	13.77	12939976	829149	67.99	
4	14.54	4991576	292181	26.23	
Total		19033010	1191607	100.00	

Trace 12: I-12

Chromatogram:



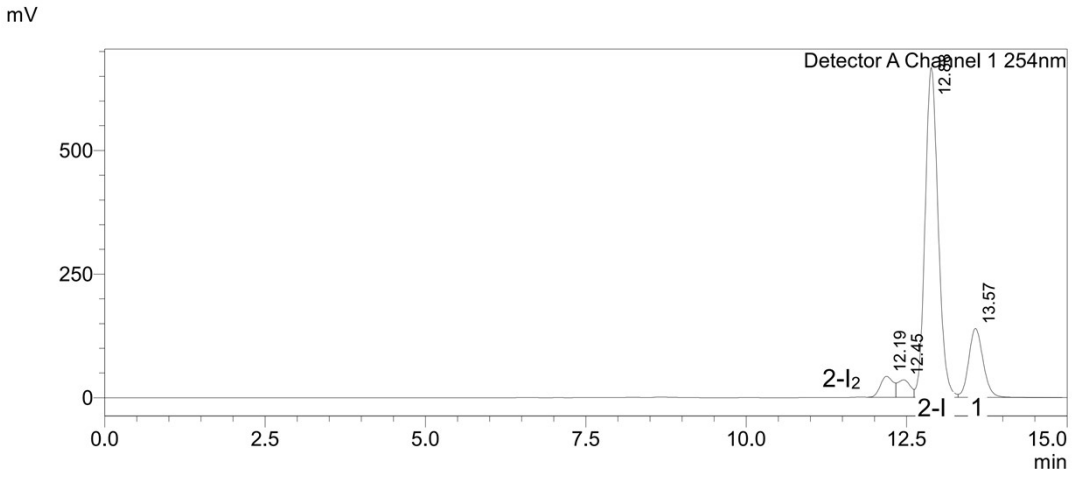
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.94	3932611	236805	5.88	
2	13.26	2543565	166223	3.81	
3	13.75	49515737	2613407	74.09	
4	14.52	10842132	578576	16.22	
Total		66834045	3595012	100.00	

Trace 13: I-13

Chromatogram:



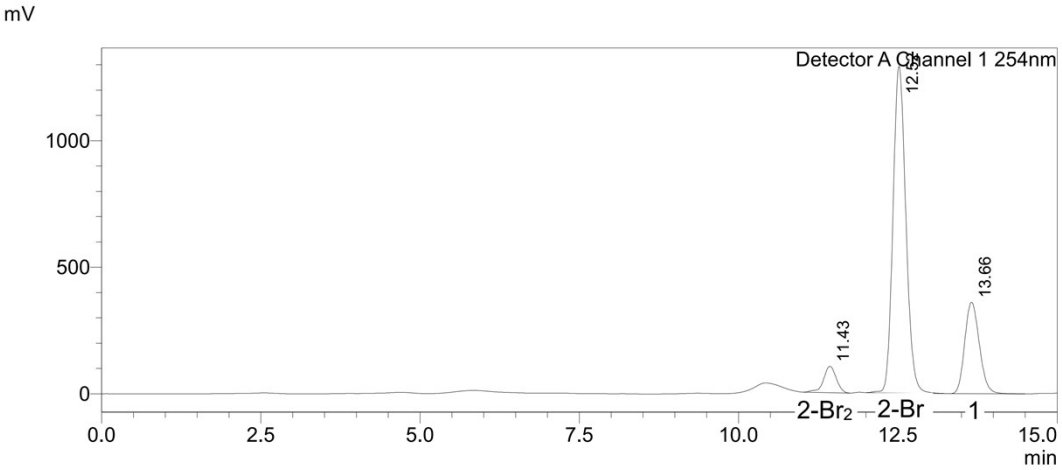
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	12.19	598241	42297	4.70	
2	12.45	485247	35219	3.82	
3	12.88	9452622	666984	74.33	
4	13.57	2180848	139462	17.15	
Total		12716958	883963	100.00	

Trace 14: Br-1

Chromatogram:



Peak Table:

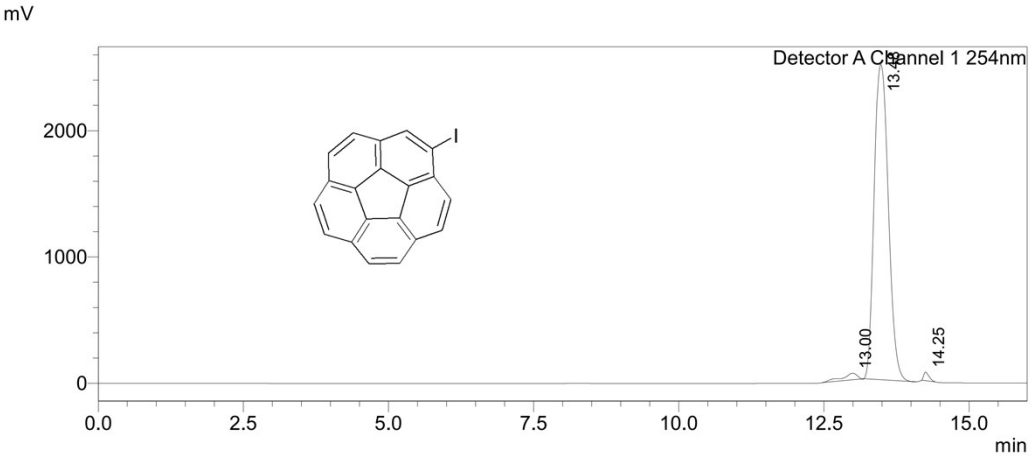
Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	11.43	1449005	104510	5.70	
2	12.52	18221566	1291616	71.62	
3	13.66	5772793	361528	22.69	
Total		25443364	1757654	100.00	

12. HPLC traces of purified 2-I, 2-Br & 2-Br_2

Trace 1: **2**-I (96.8 % purity)

Chromatogram:



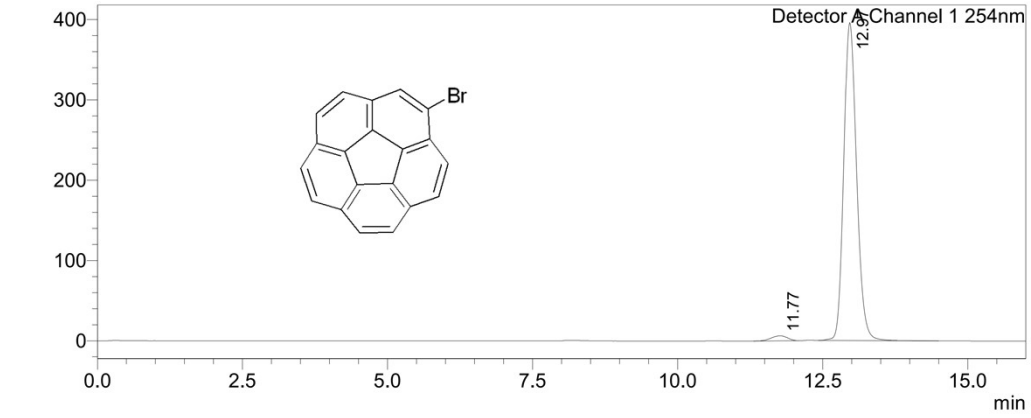
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	13.00	963828	52164	2.20	
2	13.48	42390834	2494868	96.80	
3	14.25	439051	68852	1.00	
Total		43793712	2615884	100.00	

Trace 2: **2**-Br (98.1 % purity)

Chromatogram:



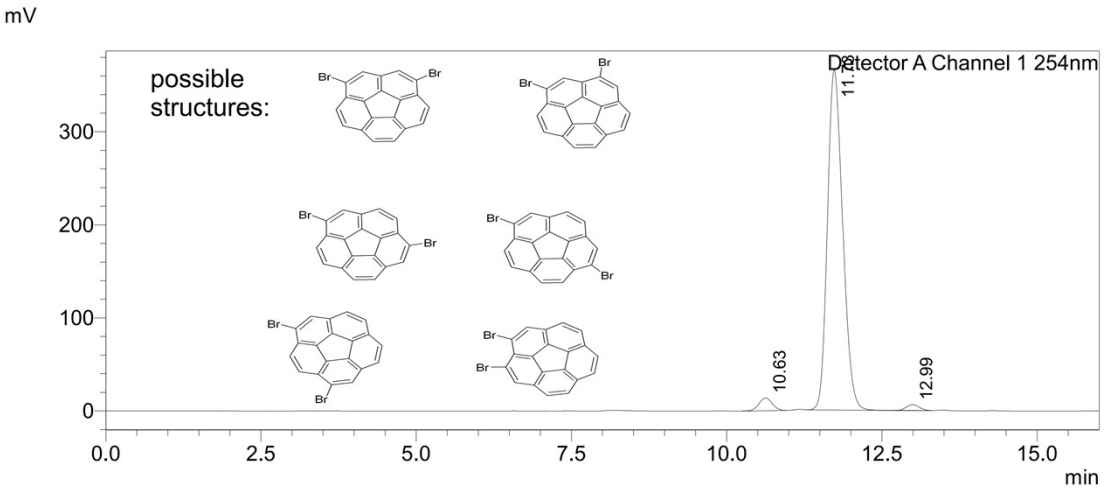
Peak Table:

Detector A Channel 1 254nm

Peak	Ret. Time	Area	Height	Area%	Compound Name
1	11.77	121654	6265	1.95	
2	12.97	6116968	395922	98.05	
Total		6238622	402188	100.00	

Trace 3: **2**-Br_2

Chromatogram:



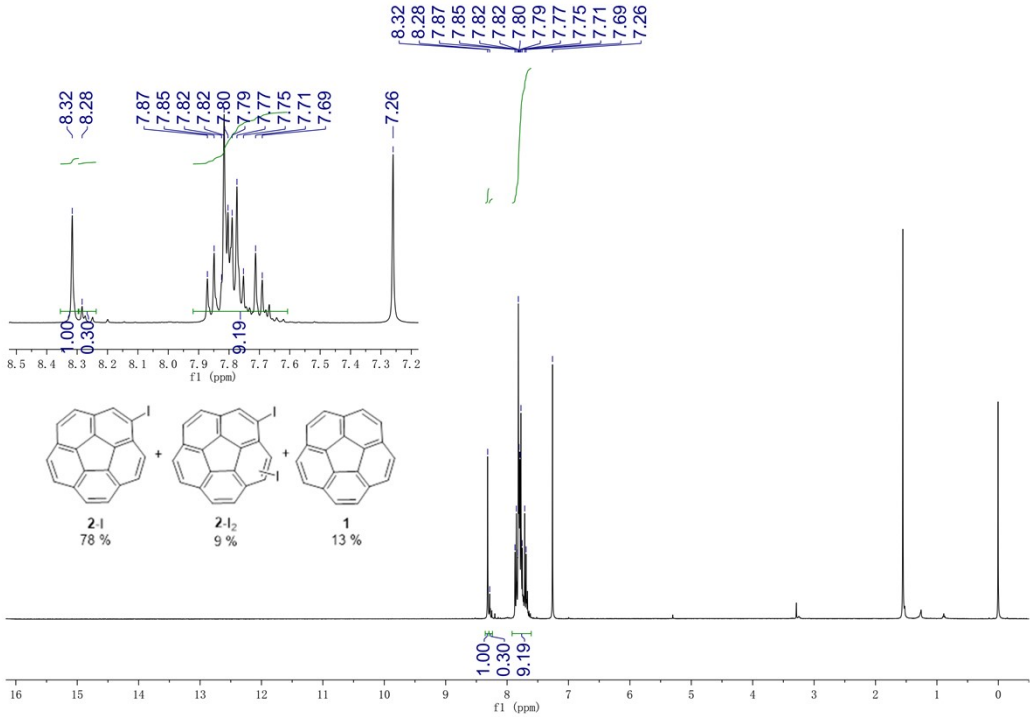
Peak Table:

Detector A Channel 1 254nm

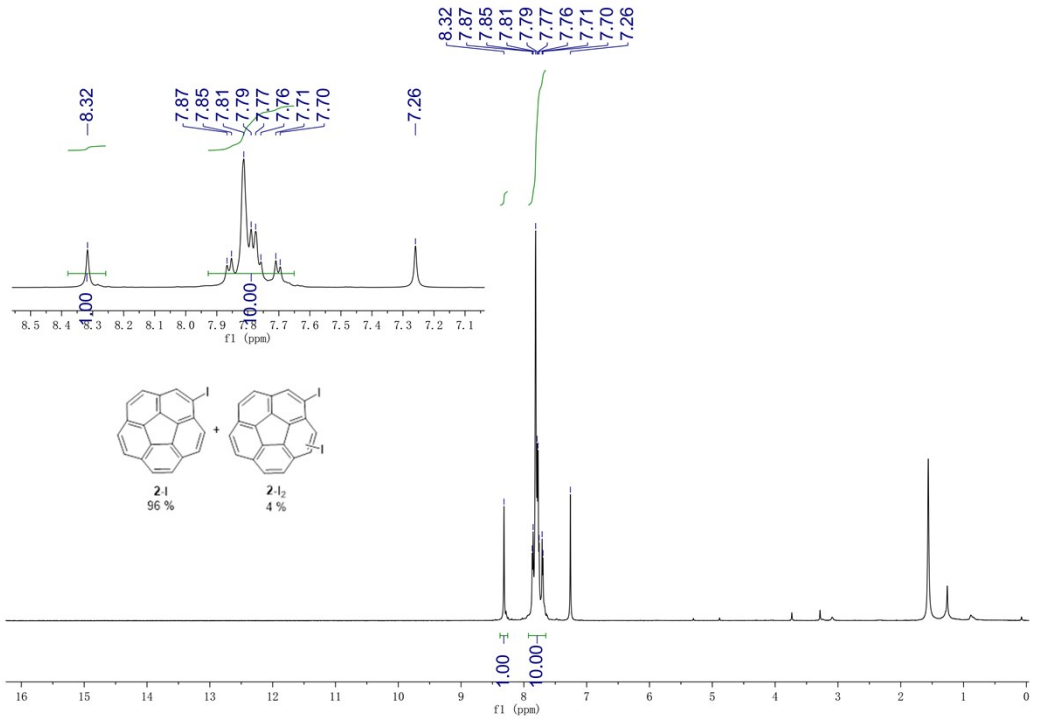
Peak	Ret. Time	Area	Height	Area%	Compound Name
1	10.63	205810	13626	3.14	
2	11.73	6248470	365290	95.47	
3	12.99	90743	6264	1.39	
Total		6545023	385180	100.00	

12. Copies of NMR spectra for crude and purified 2-I

Crude **2**-I:



Purified **2**-I:



13. Characterization of compounds 6-7

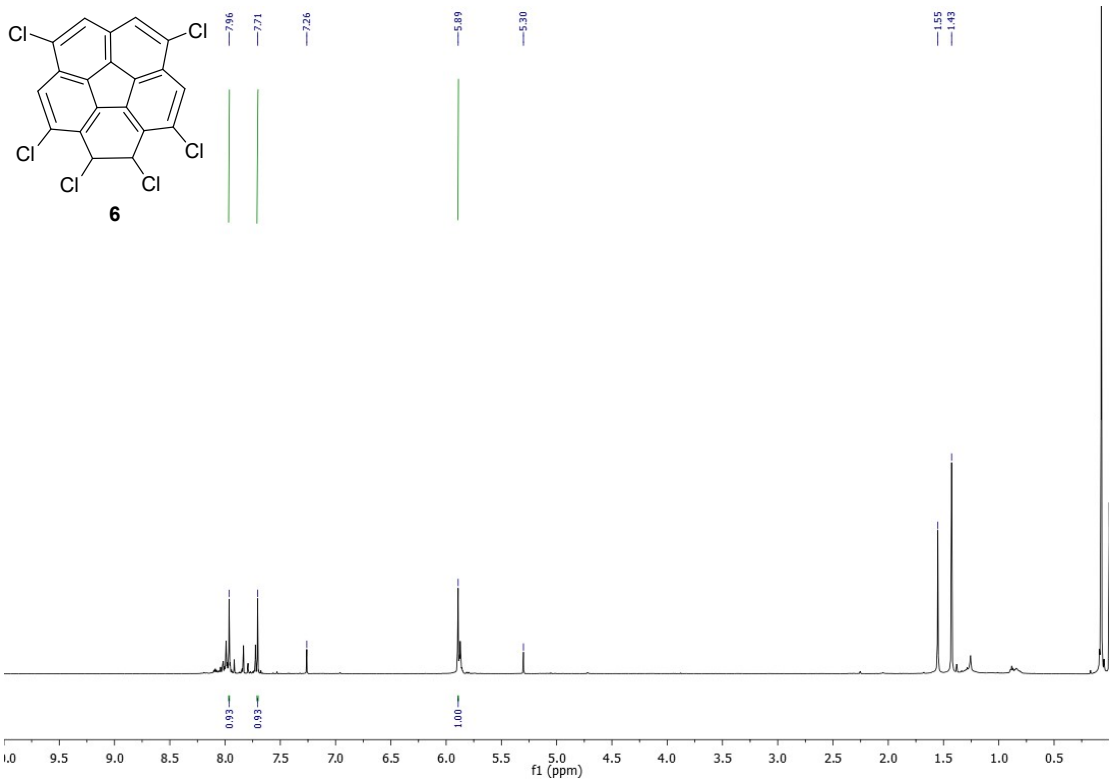
Compound **6**

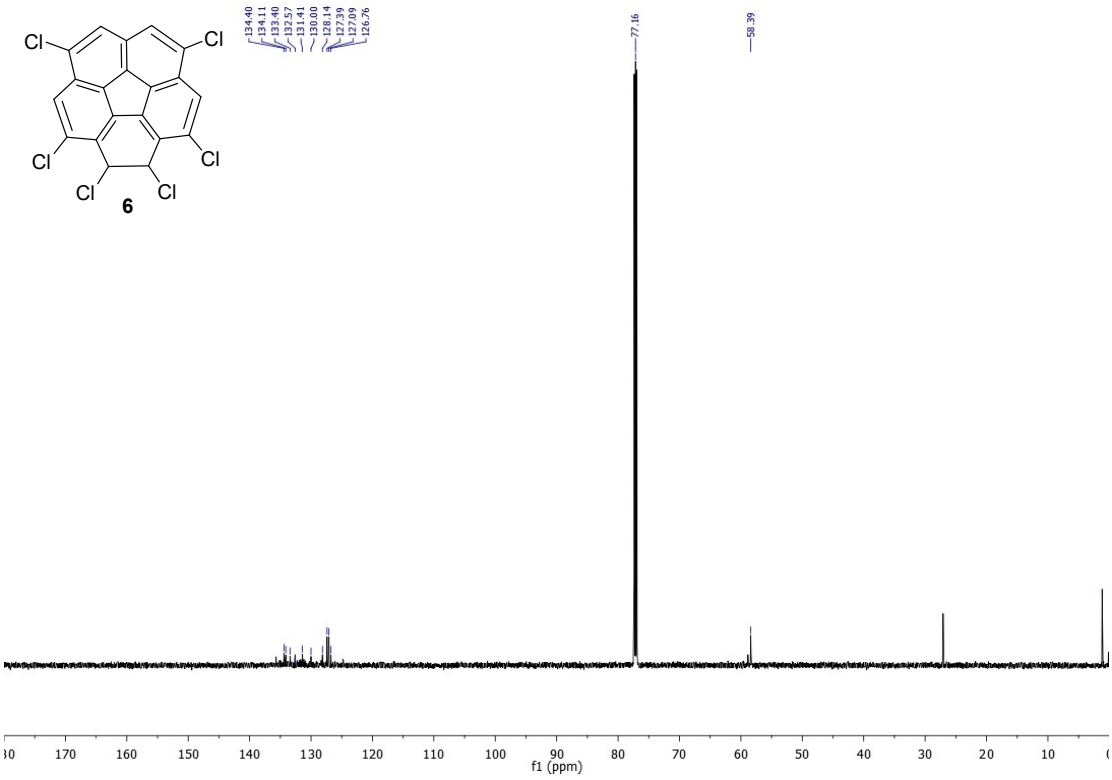
Spectroscopic data: ^{1}**H-NMR (400 MHz, $CDCl_3$):** δ/ppm 7.96 (2H, s), 7.71 (2H, s), 5.89 (2H, s). ^{13}**C-NMR (101 MHz, $CDCl_3$):** δ/ppm 58.39, 126.76, 127.09, 127.39, 128.14, 130.00, 131.41, 132.57, 133.40, 134.11, 134.40. **MALDI-TOF-MS ($C_{20}H_6Cl_6$):** Calculated 455.860, found 455.832.

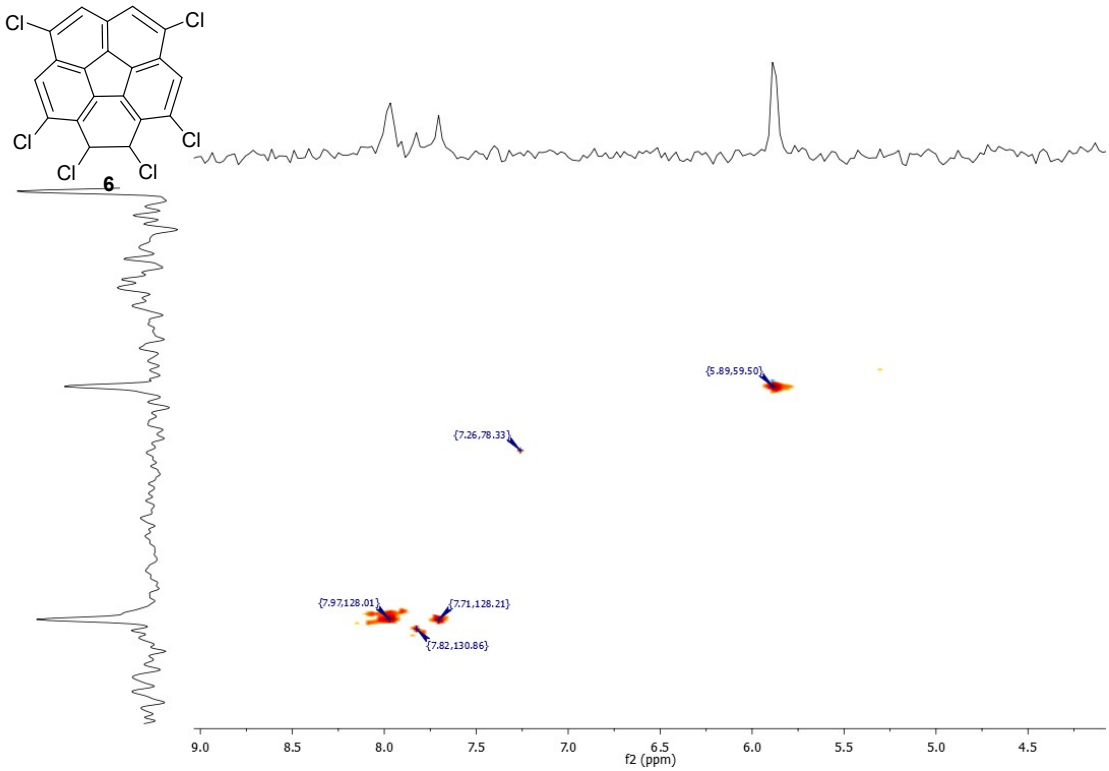
Compound **7**

Spectroscopic data: ^{1}**H-NMR (400 MHz, $CDCl_3$):** δ/ppm 7.84 (2H, s), 7.81 (2H, s), 7.60 (2H, s), 7.29 (4H, d, J = 8Hz), 7.24 (4H, d, J=8Hz), 7.10 (8H, t, J=8Hz). ^{13}**C-NMR (101 MHz, $CDCl_3$):** δ/ppm 21.30, 29.85, 126.90, 127.04, 128.37, 128.89, 129.22, 130.29, 130.30, 131.16, 131.28, 131.74, 131.98, 132.04, 132.13, 135.49, 136.32, 136.52, 137.28, 137.39, 137.47. **MALDI-TOF-MS($C_{48}H_{34}S_4$):** Calculated 738.154, found 738.075.

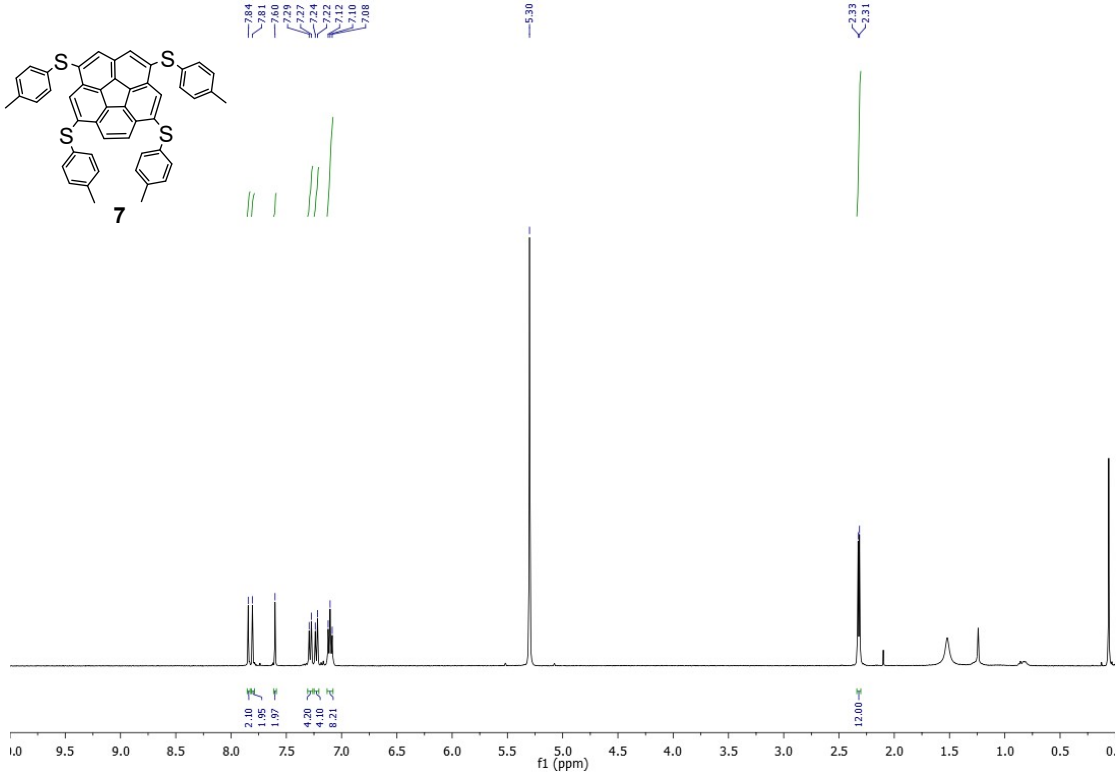
14. Copies of NMR spectra for 6-7


Cl
Cl
Cl
Cl
Cl
Cl
6
7.96
7.71
7.26
5.89
5.30
1.55
1.43
0.93
0.93
1.00
f1 (ppm)

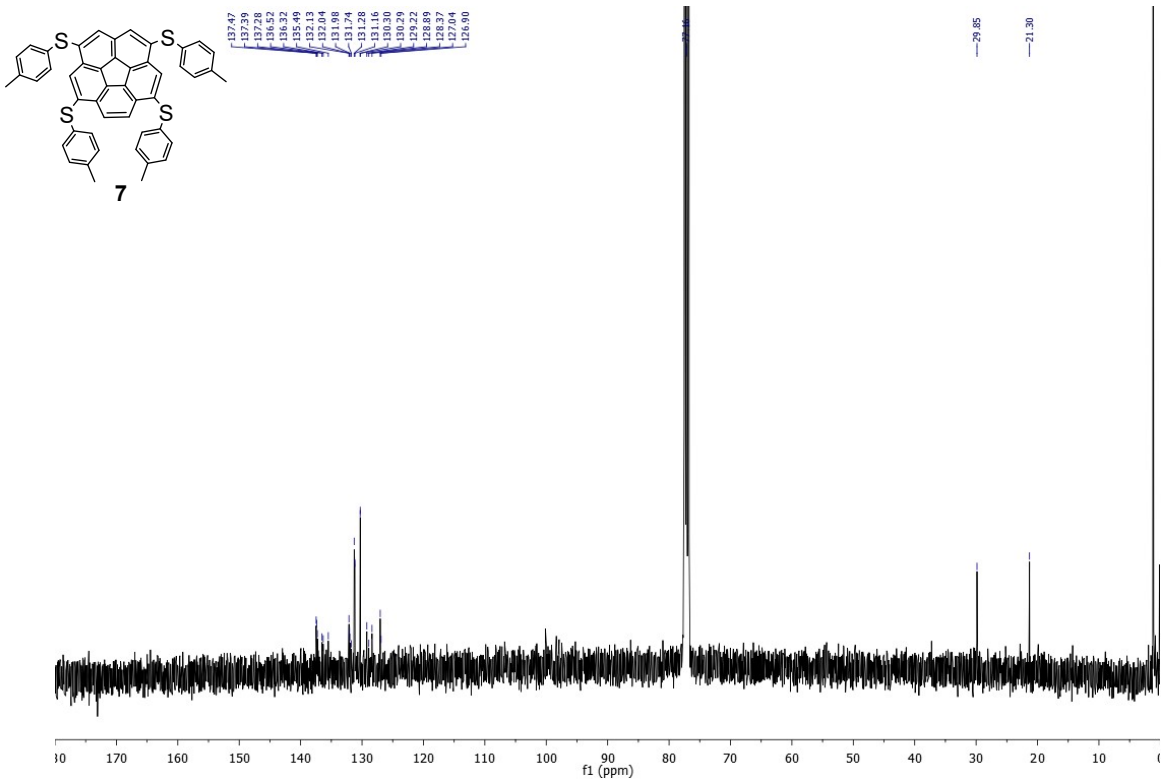

Cl
Cl
Cl
Cl
Cl
Cl
6
134.40
134.11
133.40
132.57
131.41
130.00
128.14
127.39
127.09
126.76
77.16
58.39
f1 (ppm)


Cl
Cl
Cl
Cl
Cl
Cl
{5.89,59.50}
{7.26,78.33}
{7.97,128.01}
{7.71,128.21}
{7.82,130.86}
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
f2 (ppm)

6


7.84
7.81
7.66
7.29
7.27
7.24
7.22
7.12
7.10
7.08
5.30
2.33
2.31
2.10
1.95
1.97
4.20
4.10
8.21
12.00
f1 (ppm)

7


7
137.47
137.39
137.28
136.52
136.32
135.49
132.13
132.04
131.98
131.74
131.28
131.16
130.30
130.29
129.22
128.89
128.37
127.04
126.90
29.85
21.30
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)