Supporting Information for:

Using a Build-and-Click Approach for Producing Structural and Functional Diversity in DNA-Targeted Hybrid Anticancer Agents

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1. Synthetic Procedures

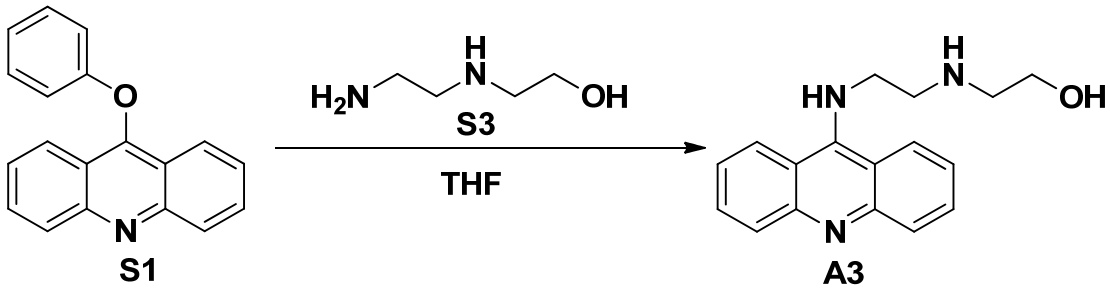
Acronyms used for reagents:

CDI: 1,1′-carbonyldiimidazole
DMF: Dimethylformamide
DCM: Dichloromethane
MeOH: Methanol
TEA: Triethanolamine
TFA: Trifluoroacetic acid

1.1. Synthetic procedures for building blocks

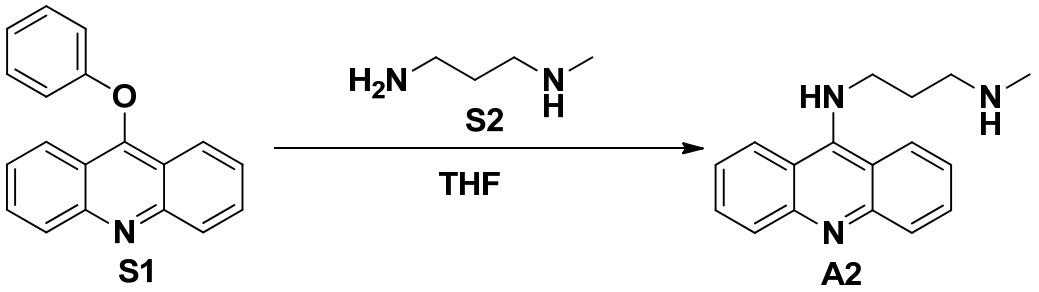
The synthetic precursors [$PtCl_2$(en)] **(S11),** cisplatin **(S12)**, and *rac*-1,3-diaminopropan-2-ol **(S13)**,[1] 9-phenoxyacridine (**S1**),[2] and building blocks N^1-(acridin-9-yl)-N^2-methylethane-1,2-diamine (**A1**),[2] and N^1-(acridin-9-yl)-N^3-methylpropane-1,3-diamine (**A2**)[3] were synthesized according to the cited methods.

Scheme 1. Synthesis of precursor A3.



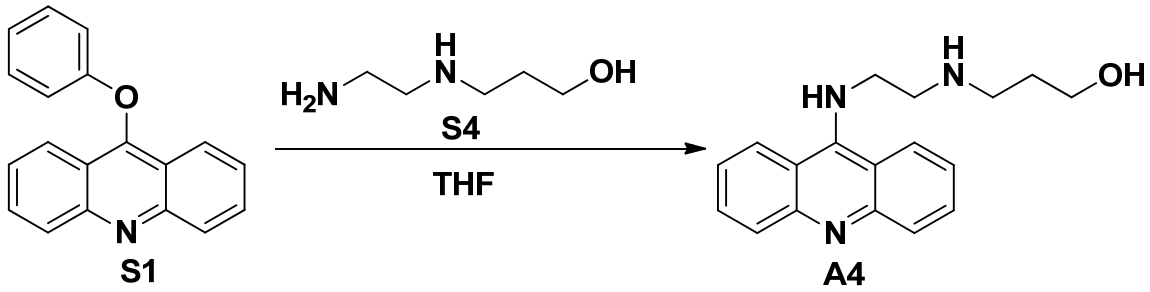
A mixture of phenoxyacridine (**S1**) (2.71 g, 0.01 mol) and 2-(2-aminoethylamino)ethanol (**S3**) (1.14 g, 0.011 mol) in 15 mL of anhydrous THF was refluxed for 16 h. The solvent was evaporated off and the residue was dissolved in 30 mL of acetone. To this solution were added 5 mL of concentrated HCl and the mixture was stirred at 4 °C for 3 hours. A yellow precipitate formed which was recovered by filtration, resuspended in 50 mL of 2 M ammonium hydroxide, and stirred at room temperature for 30 min. The aqueous phase was extracted with CH_2Cl_2 and the organic phase was collected, dried over Na_2SO_4, and concentrated using rotary evaporation, affording 2.57 g of the free base as an yellow solid (Yield: 92%). ^{1}H NMR ($(CD_3)_2SO$) δ 8.27 (d, J = 8.5 Hz, 2H), 7.69 (d, J = 7.6 Hz, 2H), 7.59 (t, J = 7.3 Hz, 1H), 7.26 (t, J = 7.5 Hz, 2H), 4.50 (s, 1H), 3.88 (t, J = 6.2 Hz, 2H), 3.47 (t, J = 5.7 Hz, 1H), 2.90 (t, J = 6.2 Hz, 2H), 2.63 (t, J = 5.7 Hz, 2H). ^{13}C NMR ($(CD_3)_2SO$) δ 151.70, 129.74, 124.84, 121.30, 60.39, 51.27, 50.18, 40.90. MS (ESI, positive-ion mode): calculated for $C_{17}H_{20}N_3O$ ($[M+H]^+$), 282.15; found: 282.3.

Scheme 2. Synthesis of precursor A2.



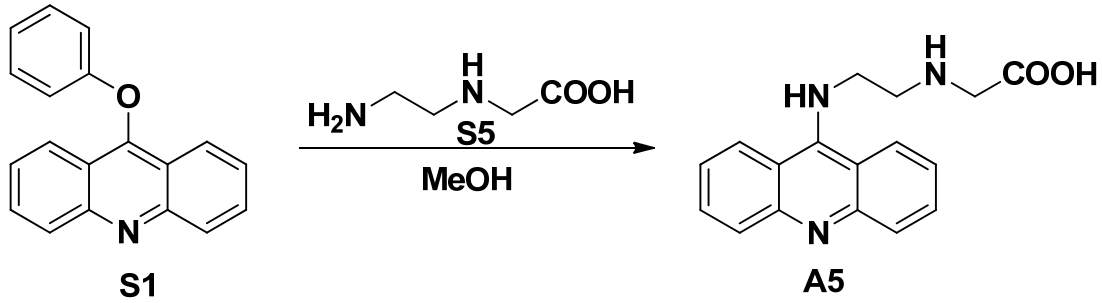
A2 was prepared using the procedure described for **A3**. Yield: 94%. ^{1}H NMR (300 MHz, $CDCl_3$) δ8.12 (d, J = 8.7， 2H), 8.02 (d, J = 8.7, 2H), 7.61 (t, J = 6.7 Hz, 2H), 7.25 (t, J = 7.5 Hz， 2H), 4.01 (t, J = 5.9 Hz, 2H), 2.96 - 2.75 (m, 2H), 2.53 (s, 3H), 1.94-1.68 (p, J = 5.9 Hz , 2H). MS (ESI, positive-ion mode): calculated for $C_{17}H_{20}N_3$ ($[M+H]^+$), 266.36; found: 266.2.

Scheme 3. Synthesis of precursor A4.



A4 was prepared using the procedure described for **A3**. Yield: 86%. ^{1}H NMR ($CDCl_3$) 8.11 (d, J = 8.5 Hz, 2H), 8.02 (d, J = 8.6 Hz, 2H), 7.72 - 7.54 (m, 2H), 7.35-7.29 (m, 2H), 3.87-3.82 (m, 4H), 3.16 - 2.64 (m, 4H), 1.79 (p, J = 6.5 Hz, 2H). ^{13}C-NMR ($CDCl_3$) 151.97, 147.93, 130.25, 127.65, 123.25, 122.70, 116.33, 62.15, 49.48, 48.91, 47.68, 31.98. MS (ESI, positive-ion mode): calculated for $C_{18}H_{22}N_3O$ ($[M+H]^+$), 296.38; found: 296.3.

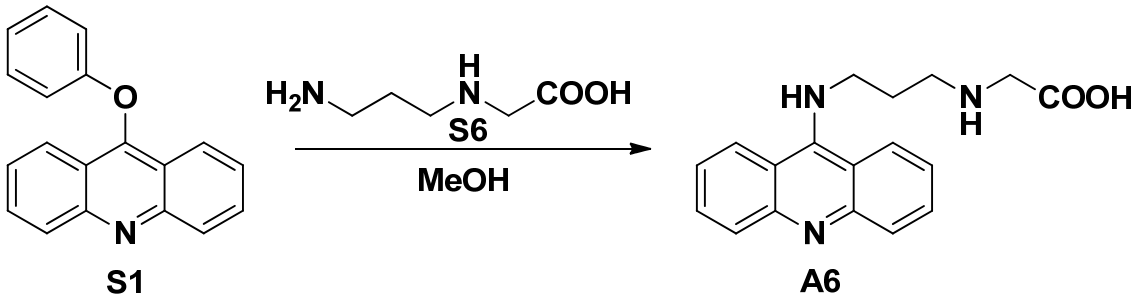
Scheme 4. Synthesis of precursor A5.



A mixture of phenoxyacridine (**S1**) (2.71 g, 0.01 mol) and 2-((2-aminoethyl)glycine (**S5**) (1.3 g, 0.011 mol) in 20 mL of dry MeOH was refluxed for 3 h. The yellow solid that precipitated

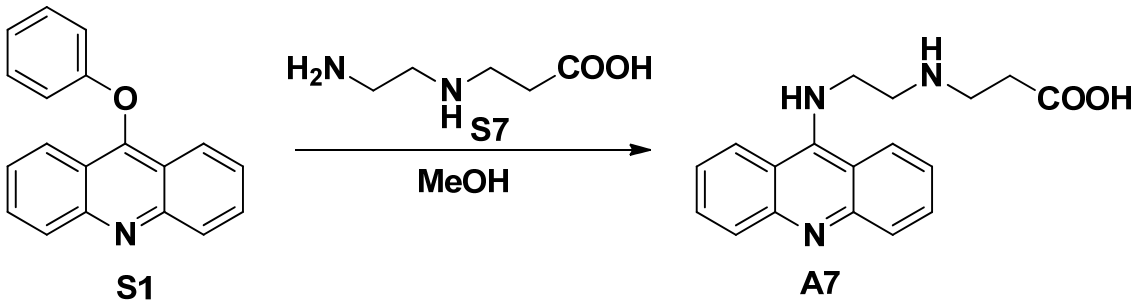
during the reaction was collected by filtration, washed with hot THF and ether, and dried in a vacuum, affording 2.55 g of the product as a yellow solid (Yield: 86 %). ^{1}H NMR ($(CD_3)_2SO$) 8.22 (m, 2H), 7.55 (t, J = 7.6 Hz, 2H), 7.43 (m, 2H), 7.15 (t, J = 7.6 Hz, 2H), 4.08 (d, J = 6.0 Hz, 2H), 3.22 (s, 2H), 3.16 (t, J = 5.9 Hz, 2H). A ^{13}C NMR spectrum of this compound was not obtained due to limited solubility of the compound. MS (ESI, positive-ion mode): calculated for $C_{17}H_{18}N_3O_2$ ($[M+H]^+$), 296.34; found: 296.3.

Scheme 5. Synthesis of precursor A6.



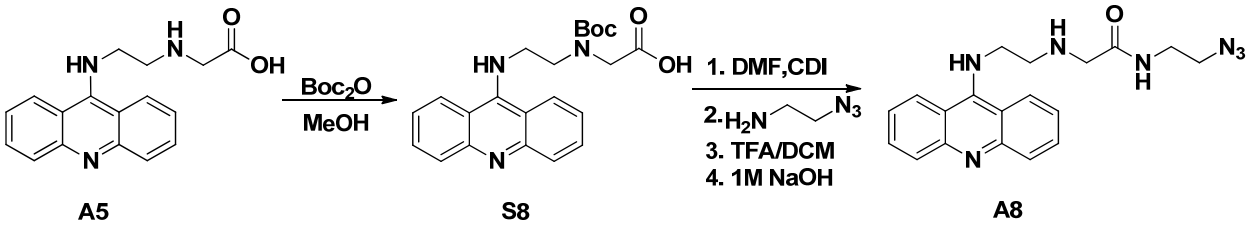
A6 was prepared using the procedure described for **A5**. Yield: 91%. ^{1}H NMR ($(CD_3)_2SO$) δ 8.21 (d, J = 8.4 Hz, 2H), 7.54 (m, 3H), 7.12-7.18 (m, 4H), 6.93-6.62 (m, 2H), 3.91 (t, J = 6.4 Hz, 2H), 3.21 (s, 2H), 3.01 (t, J = 7.2 Hz, 2H), 2.03 (p, J = 6.5 Hz, 2H). ^{13}C NMR ($(CD_3)_2SO$) δ 166.95, 157.31, 152.15, 130.13, 129.21, 125.84, 120.79, 118.56, 115.13, 49.87, 48.74, 45.42, 27.92. MS (ESI, positive-ion mode): calculated for $C_{18}H_{20}N_3O_2$ ($[M+H]^+$), 310.37; found: 310.2.

Scheme 6. Synthesis of precursor A7.



A7 was prepared using the procedure described for **A5**. Yield: 84%. ^{1}H NMR (D_2O) δ 8.04 (d, J = 8.7 Hz, 2H), 7.83 (dd, J = 8.4, 7.0 Hz, 2H), 7.58 - 7.34 (m, 4H), 4.33 (t, J = 6.1 Hz, 2H), 3.60 (t, J = 5.8 Hz, 1H), 3.33 (t, J = 6.3 Hz, 2H), 3.33 (t, J = 6.3 Hz, 2H). ^{13}C NMR (D_2O) δ 166.95, 157.31, 152.15, 130.13, 129.21, 125.84, 118.56, 115.13, 49.87, 48.80, 45.42, 27.92. MS (ESI, positive-ion mode): calculated for $C_{18}H_{20}N_3O_2$ ($[M+H]^+$), 310.37; found: 310.3.

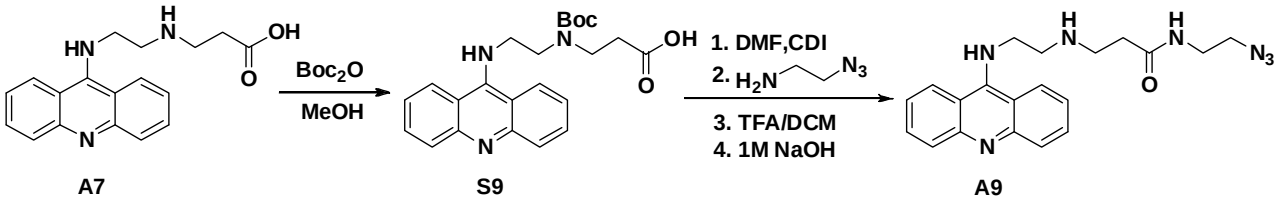
Scheme 7. Synthesis of precursor A8.



The Boc-protected acridine derivative (**S8**) (1.36 g, 4.6 mmol) was synthesized as follows. **A5** was suspended in 30 mL of anhydrous methanol, to which was added Boc_2O (1.3 g, 6 mmol) in 5 mL of anhydrous MeOH at 0-5 ºC maintained with an ice bath. The mixture was then stirred at room temperature for 4 h. The solvent was removed by rotary evaporation and residue was dissolved in 10 mL of dichloromethane and precipitated with 200 mL of anhydrous diethyl ether. The solid was recovered by filtration and dried in a vacuum affording 1.79 g (99%) of the product as a yellow solid, which was used in the next step without further purification.

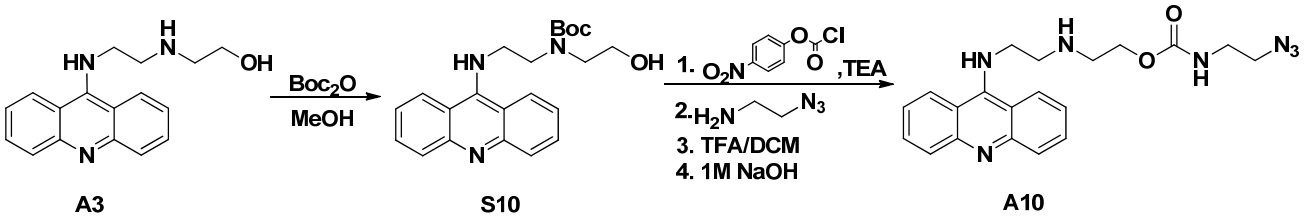
Compound **S8** (1 g, 2.52 mmol) and 1,1'-carbonyldiimidazole (CDI, 533 mg, 3.28 mmol) were combined in 20 mL of anhydrous DMF. The mixture was heated to 40-50 ºC and stirred for 6 h. Then the solution was cooled to 0-5 º C in an ice bath and 264 mg of 2-azidoethanamine dissolved in 3 mL of anhydrous DMF were added. The mixture was stirred at 0-5 º C for 4 h. DMF was removed by vacuum distillation at 35-40 ºC, and the residue was redissolved in 40 mL of dichloromethane and washed with 1 M HCl (3 × 20 mL). The organic phase was collected, dried with anhydrous Na_2SO_4, and concentrated to afford an orange oil. To remove the Boc group, the residue was dissolved in 6 mL of a 1:1 mixture of anhydrous dichloromethane and trifluoroacetic acid and stirred at room temperature for 3 h. The reaction was quenched by adding 10 mL of 1 M NaOH solution. The crude product was extracted from NaOH solution with DCM, dried over anhydrous Na_2SO_4, and concentrated. The product was purified by flash chromatography (Al_2O_3, DCM:MeOH, 30:1). Yield: 0.59 g (64 %). ^{1}H NMR ($CDCl_3$) δ 8.10 (d, J = 8.7 Hz, 2H), 7.97 (d, J = 8.6 Hz, 2H), 7.60 (t, J = 8.3, 6.8 Hz, 2H), 7.40 - 7.14 (m, 3H), 3.89 (t, J = 5.6 Hz, 2H), 3.50 - 3.23 (m, 6H), 2.99 (t, J = 5.6 Hz, 2H). ^{13}C NMR ($CDCl_3$) δ 172.56, 152.98, 146.04, 131.21, 125.75, 123.56, 122.97, 115.48, 50.72, 48.69, 48.47, 44.85, 38.82, 36.22. MS (ESI, positive-ion mode): calculated for $C_{19}H_{22}N_7O$ ($[M+H]^+$), 364.42; found: 364.3.

Scheme 8. Synthesis of precursor A9.



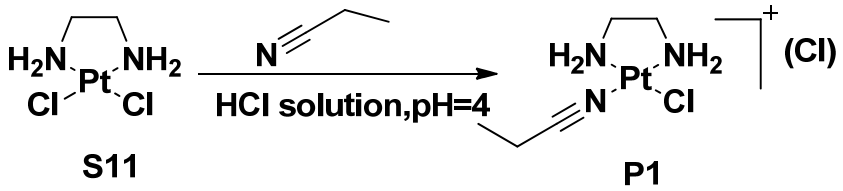
A9 was prepared using the procedure described for **A8**. Yield: 64%. ^{1}H NMR ($CDCl_3$) δ 8.09 (d, *J* = 8.7 Hz, 2H), 8.02 (d, *J* = 8.7 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 2H), 7.41 (s, 1H), 7.27 (t, *J* = 7.5 Hz, 2H), 4.95 (brs, 2H), 3.92 (t, *J* = 5.6 Hz, 2H), 3.44 (s, 4H), 2.91-3.14 (m, 4H), 2.53 (t, *J* = 6.0 Hz, 2H). ^{13}C NMR ($CDCl_3$) δ 152.09, 149.60, 129.65, 129.23, 123.60, 121.91, 115.75, 51.37, 51.32, 36.51, 29.15. MS (ESI, positive-ion mode): calculated for $C_{20}H_{24}N_7O$ ($[M+H]^+$), 378.45; found: 378.3.

Scheme 9. Synthesis of precursor A10.



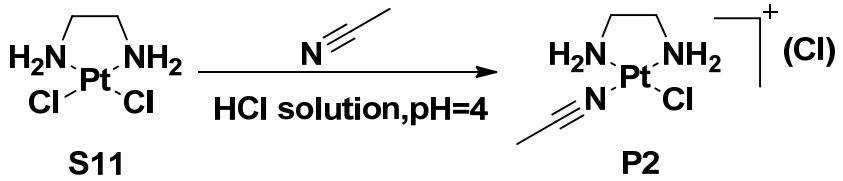
The Boc-protected acridine derivative (**S10**) was prepared as described for **S8** starting with compound **A3**. Compound **S10** (1 g, 2.62 mmol), TEA (793 mg, 7.85 mmol) and 4-nitrobenzyl chloroformate (732 mg, 3.4 mmol) were dissolved in 20 mL of anhydrous DCM. The mixture was stirred at room temperature for 16 h. Then 271 mg of 2-azidoethanamine dissolved in 5 mL of anhydrous DCM was added and the reaction was stirred for another 8 h. The solvent was removed using vacuum distillation and the residue was redissolved in 40 mL of DCM and washed with 1 M HCl (3 × 20 mL). The organic phase was collected, dried with anhydrous Na_2SO_4, and concentrated to afford an orange oil. To remove the Boc group, the orange oil was dissolved in 6 mL of a 1:1 mixture of anhydrous dichloromethane and trifluoroacetic acid and stirred at room temperature for 3 h. The reaction was quenched by adding 10 mL of 1 M NaOH solution. The crude product was extracted from NaOH solution with DCM, dried over anhydrous Na_2SO_4, and concentrated. The product was further purified by flash chromatography (Al_2O_3, DCM:MeOH, 30:1). Yield: 0.73 g (71 %). ^{1}H NMR ($CDCl_3$) δ 8.12 - 7.96 (m, 4H), 7.59 (t, *J* = 7.8 Hz, 2H), 7.23 (t, *J* = 7.6 Hz, 2H), 5.65 (brs, 1H), 4.27 (t, *J* = 4.8 Hz, 2H), 3.92 (t, *J* = 5.7 Hz, 1H), 3.61 - 3.20 (m, 4H), 3.01 (t, *J* = 5.7 Hz, 2H), 2.96 (t, *J* = 4.9 Hz, 2H). ^{13}C NMR ($CDCl_3$) δ 156.53, 152.69, 145.93, 131.22, 125.98, 123.3, 123.00, 115.07, 64.48, 50.97, 48.35, 48.17, 47.83, 40.45. MS (ESI, positive-ion mode): calculated for $C_{20}H_{24}N_7O_2$ ($[M+H]^+$), 394.45; found: 394.3.

Scheme 10. Synthesis of precursor P1[4].



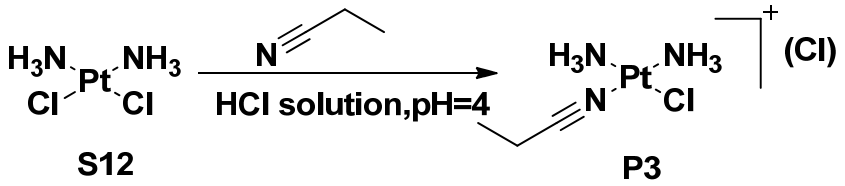
The complex [$PtCl_2$(en)] (**S11**) (0.50 g, 1.54 mmol) was heated under reflux in 25 mL of dilute HCl (pH 4) with propionitrile (6.85 mL, 98.5 mmol) until the yellow suspension turned into a colorless solution (~2 h). Solvent was removed by rotary evaporation, and the pale-yellow residue was redissolved in 10 mL of dry methanol. A small amount of an insoluble yellow solid was removed by membrane filtration and the colorless filtrate was added directly into 250 mL of vigorously stirred dry diethyl ether, affording **P1** as an off-white, extremely hygroscopic microcrystalline precipitate. Yield: 0.48 g (83%). ^{1}H NMR (D_2O) δ 5.72, 5.64 (2 br s，0.7 H, HD exchange), 2.87(q, J=7.5 Hz, 2H), 2.48 - 2.75 (m, Pt satellites, 4 H), 1.3 (t, J=7.5 Hz, 3H,).

Scheme 11. Synthesis of precursor P2[5].



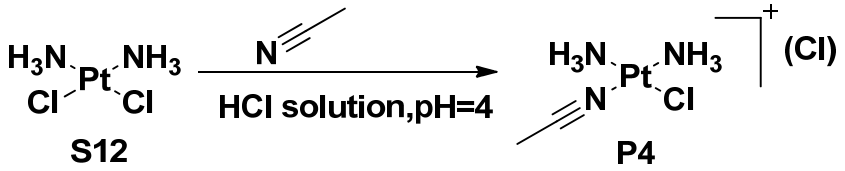
P2 was prepared using the similar procedure as described for **P1** as the white solid with the yield 89%. ^{1}H NMR (D_2O) δ 5.80, 5.65 (2 br s，1H, HD exchange), 2.87(q, J=7.5 Hz, 2H), 2.55 - 2.65 (m, Pt satellites, 4 H), 2.53 (s, 3H).

Scheme 12. Synthesis of precursor P3.



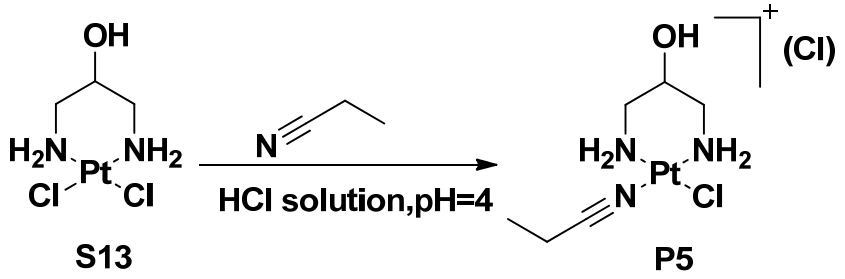
P3 was prepared using the procedure described for **P1**. Yield: 74%. ^{1}H NMR (D_2O) δ 2.89 (t, *J* = 7.6, 2H), 1.30 (t, *J* = 7.5, 3H).

Scheme 13. Synthesis of precursor P4.



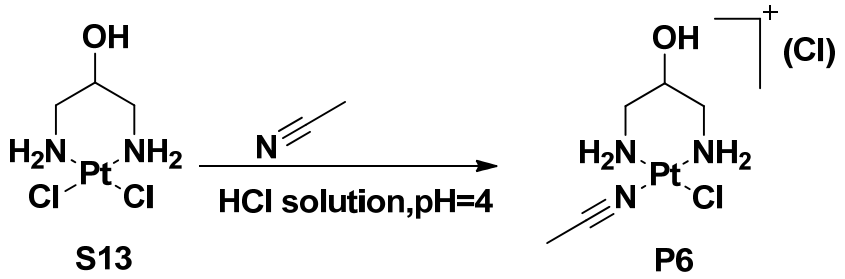
P4 was prepared using the procedure described for **P1**. Yield: 63%. ^{1}H NMR (D_2O) δ 2.53 (3 H, m, Pt satellites), 4.35, 4.48 (4 H, HD exchange, 2 br s).

Scheme 14. Synthesis of precursor P5.



P5 was prepared using the procedure described for **P1**. Yield: 91%. ^{1}H NMR (D_2O) δ 4.26 (m, 1H), 2.99 - 2.54 (m, 6H), 1.39 - 0.96 (t, *J* = 7.5 Hz, 3H).

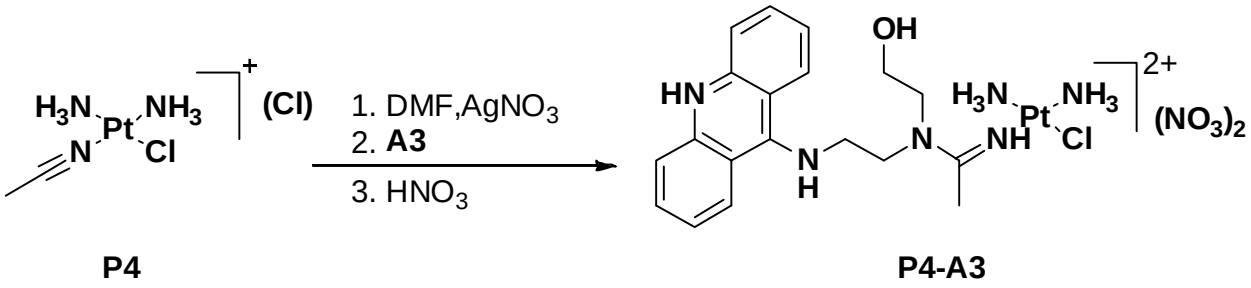
Scheme 15. Synthesis of precursor P6.



P6 was prepared using the procedure described for **P1.** Yield: 77%. ^{1}H NMR (D_2O) δ 4.28 (m, 1H), 2.85 - 2.53 (m, 4H), 2.53 (s, 3H).

1.2. Synthesis of Pt-Acridines

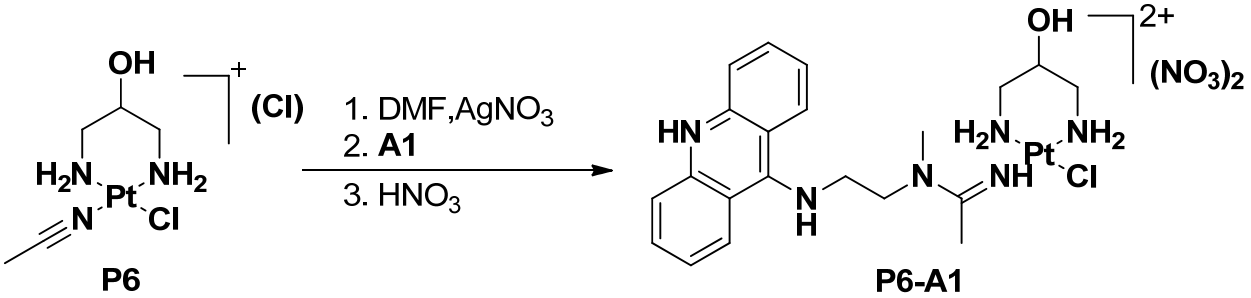
Scheme 16. Resynthesis of compound P4-A3.



P4 P4-A3

P4-A3 was prepared using the same procedure as described for **P1-A3** and was recovered with a yield of 87%. ^{1}H NMR (MeOD) δ 8.40 (d, *J* = 8.8 Hz, 2H), 7.87 (t, *J* = 6.8, 2H), 7.72 (dd, *J* = 8.7, 1.2 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 2H), 4.31 (t, *J* = 7.0 Hz, 2H), 4.10 (brs, 2H), 3.91 (t, *J* = 6.8 Hz, 1H), 3.75 (s, 2H), 3.65 (t, *J* = 4.9 Hz, 2H), 3.49 (t, *J* = 4.9 Hz, 2H), 2.58 (s, 3H). ^{13}C NMR (MeOD) δ 167.49, 160.02, 141.40, 136.55, 126.49, 125.30, 119.77, 114.14, 60.73, 49.86, 48.16, 47.39, 23.02. MS (ESI, positive-ion mode): for $C_{19}H_{28}ClN_6OPt$ ($[M]^+$), 587.00; found: 585.2.

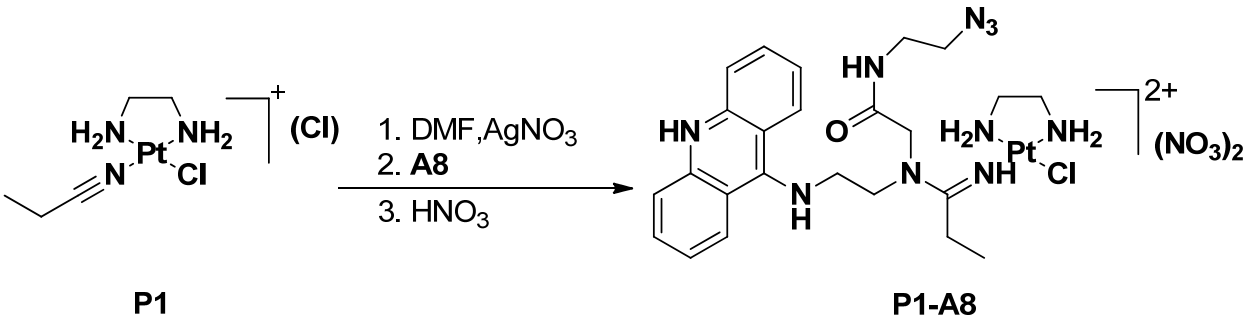
Scheme 17. Resynthesis of compound P6-A1.



P6 P6-A1

P6-A1 was prepared using the same procedure as described for **P1-A3** and was recovered with a yield of 92%. ^{1}H NMR (DMF-*d7*) δ 13.92 (s, 1H), 9.89 (s, 1H), 8.68 (d, *J* = 8.7 Hz, 2H), 7.9 - 8.11 (m, 4H), 7.62 (td, *J* = 6.4, 3.1 Hz, 2H), 6.21 (s, 1H), 5.65 (s, 1H), 5.60 (s, 1H), 5.13 (s, 2H), 4.87 (s, 1H), 4.50 (s, 2H),4.12 (t, *J* = 6.3 Hz 2H), 4.06 (s, 1H), 3.50 (s, 4H), 3.18 (s, 3H), 2.59-2.97 (m, 4H). ^{13}C NMR (DMF) δ 165.94, 158.64, 139.96, 135.33, 125.29, 123.91, 118.98, 112.80, 65.84, 48.38, 47.80, 33.79, 28.66. MS (ESI, positive-ion mode): for $C_{21}H_{30}ClN_6OPt$ ($[M]^+$), 613.04; found: 612.3.

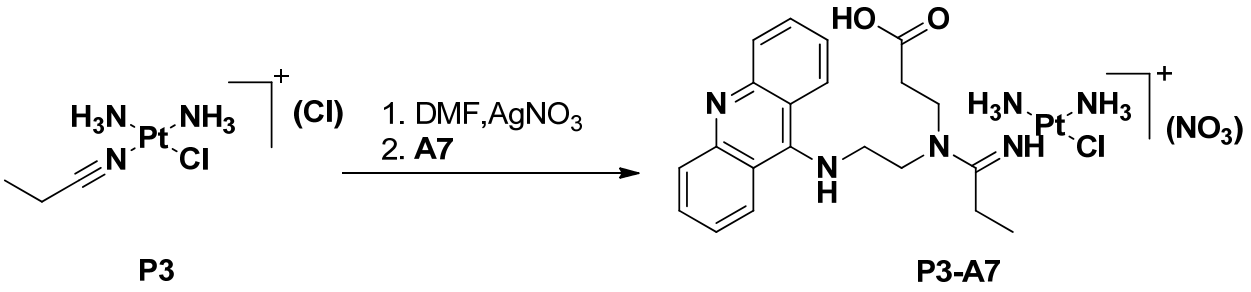
Scheme 18. Resynthesis of compound P1-A8.



P1 **P1-A8**

P1-A8 was prepared using the same procedure as described for **P1-A3** and was recovered with a yield of 81%. ^{1}H NMR (DMF-*d7*) δ 13.90 (s, 1H), 9.99 (s, 1H), 8.83 - 8.52 (m, 3H), 8.28 - 7.92 (m, 4H), 7.62 (td, *J* = 6.6, 1.5 Hz 2H), 6.73 (s, 1H), 5.84 (s, 2H), 5.51 (s, 2H), 4.54 (q, *J* = 5.7 Hz, 2H), 4.44 (s, 2H), 4.15 (t, *J* = 5.9 Hz, 2H), 3.44 - 3.52 (m , 4H), 3.06 (q, *J* = 7.9 Hz, 2H), 2.67 (s, 4H), 1.33 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (DMF-*d7*) δ 170.37, 169.56, 158.62, 140.17, 135.27, 125.92, 123.80, 118.90, 112.94, 50.32, 48.97, 48.79, 46.34, 38.78, 28.67, 11.00. MS (ESI, positive-ion mode): for $C_{24}H_{34}ClN_{10}OPt$ ($[M]^{+}$), 709.13; found: 708.5.

Scheme 19. Resynthesis of compound P3-A7.



P3 **P3-A7**

Platinum complex **P3** (354 mg, 1 mmol) was converted to its nitrate salt by reaction with $AgNO_3$ (162 mg, 0.95 mmol) in 7 mL of anhydrous DMF. AgCl was removed by syringe filtration, and the filtrate was cooled to -10 °C. Acridine precursor **A7** (310 mg, 0.1 mmol) was added to the solution, and the suspension was stirred at 4 °C for 5 days. The mixture was poured into 300 mL of vigorously stirred diethyl ether, and the precipitate was recovered by membrane filtration and dried in a vacuum overnight. The product was further purified by recrystallization from hot methanol to give 461.7 mg of the product as a yellow solid (Yield: 67%). ^{1}H NMR (MeOD) δ 8.29 (d, *J* = 8.6 Hz, 2H), 7.92 - 7.58 (m, 4H), 7.41 (t, *J* = 7.7 Hz, 2H), 4.06 (t, *J* = 6.5 Hz, 2H), 3.74 (t, *J* = 6.4 Hz, 2H), 3.63 (t, *J* = 6.5 Hz, 2H), 3.02 (t, *J* = 7.9 Hz, 2H), 2.35 (t, *J* = 6.4 Hz, 2H), 1.23 (t, *J* = 8.0 Hz, 2H). MS (ESI, positive-ion mode): for $C_{21}H_{30}ClN_6O2Pt$ ($[M]^{+}$), 629.04; found: 629.2.

2. LC-ESMS analysis of reaction mixtures

Abbreviations:

en = ethylenediamine; HPDA = 2-hydroxy-1,3-propanediamine ($pn^{2\text{-}OH}$)

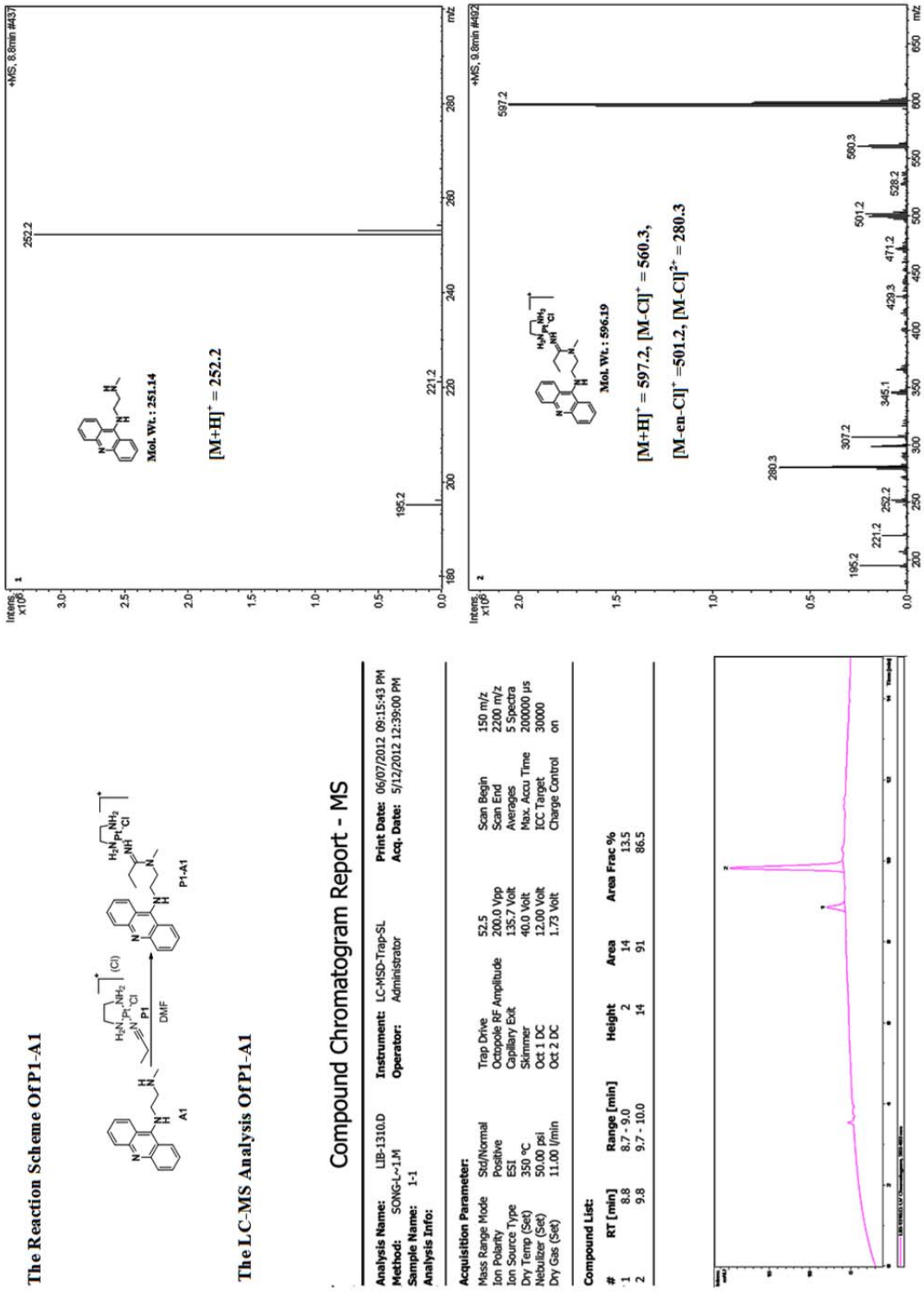
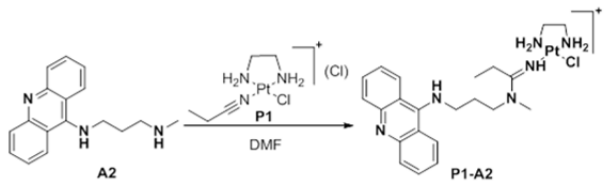


Figure S1.1. LC-ESMS analysis of reaction P1 + A1.

The Reaction Scheme Of P1-A2



The LC-MS Analysis Of P1-A2

Compound Chromatogram Report - MS

Analysis Name: 05121233.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/18/2012 03:32:27 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/10/2012 11:02:27 PM
Sample Name: 1-2
Analysis Info:

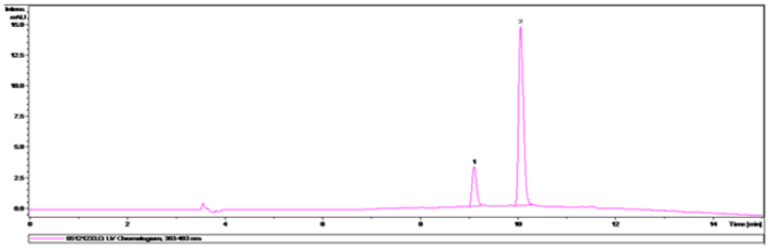
Acquisition Parameter:

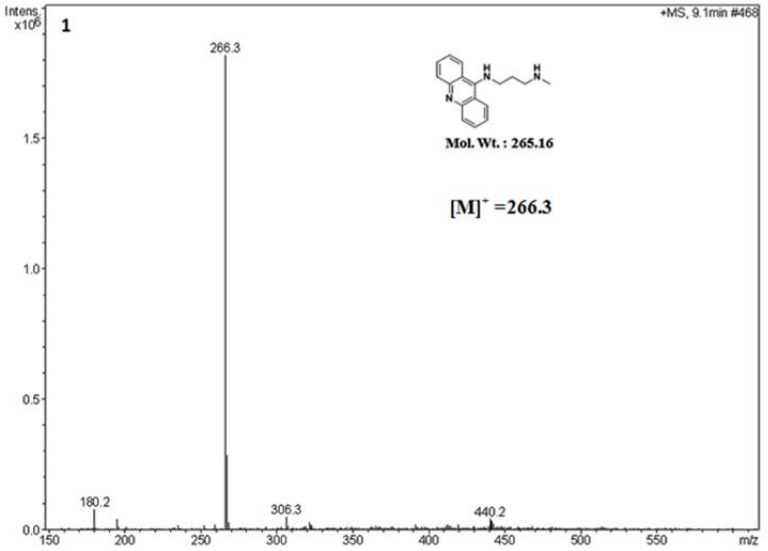
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.1	9.0 - 9.3	3	19	16.4
2	10.0	9.9 - 10.3	14	99	83.6

Chromatograms:





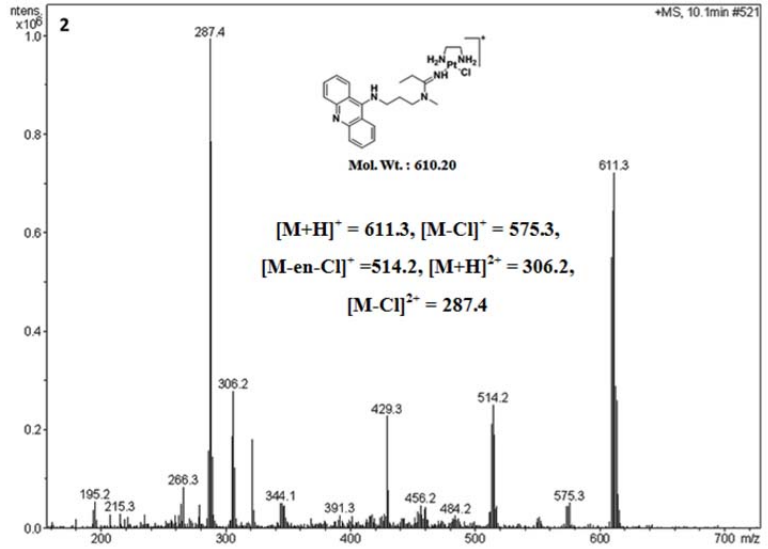
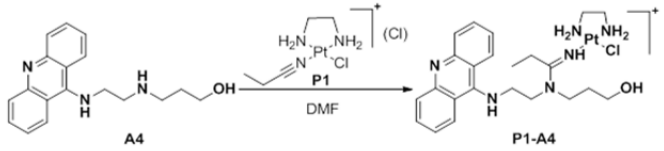


Figure S1.2 LC-ESMS analysis of reaction P1 + A2.

Figure S1.3 LC-ESMS analysis of reaction P1 + A3.

The Reaction Scheme Of P1-A4



The LC-MS Analysis Of P1-A4

Compound Chromatogram Report - MS

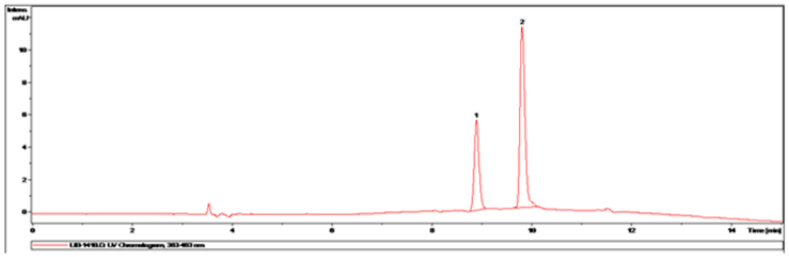
Analysis Name: LIB-1410.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 12:08:55 AM
Method: SONG-L~1.m **Operator:** Administrator **Acq. Date:** 5/12/2012 2:52:47 PM
Sample Name: 1-4
Analysis Info:

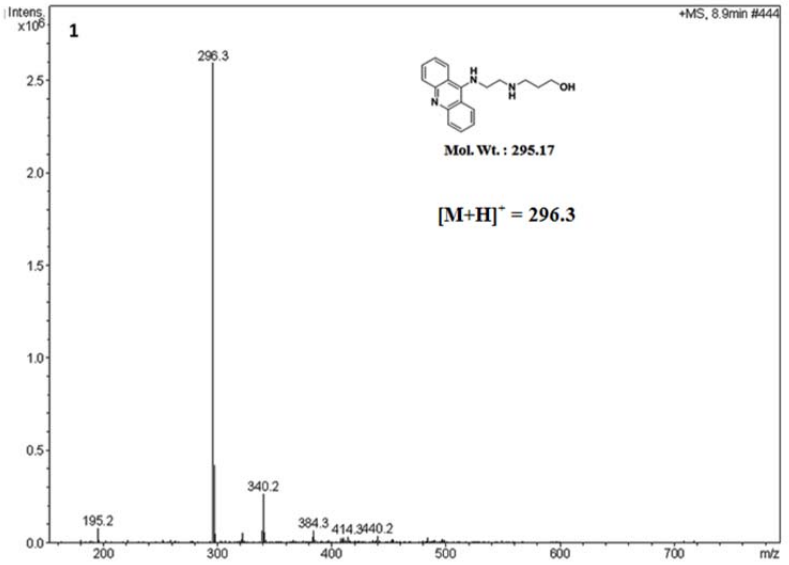
Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	8.9	8.7 - 9.1	5	37	32.8
2	9.8	9.6 - 10.1	11	75	67.2





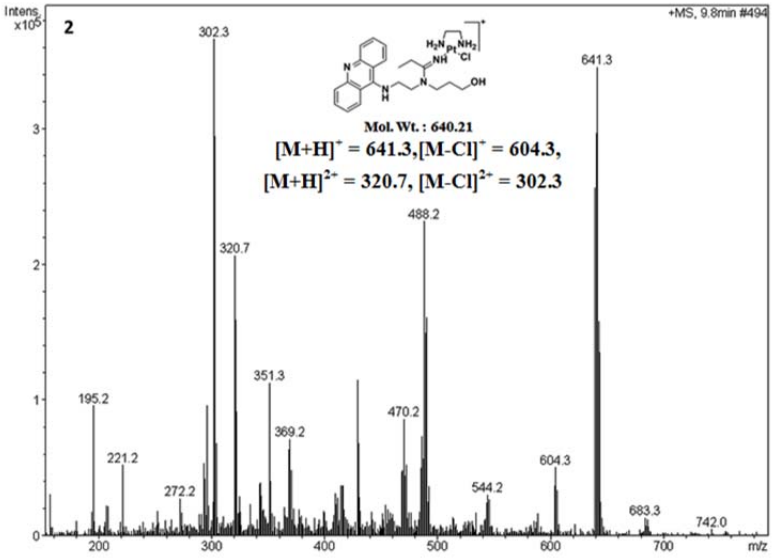
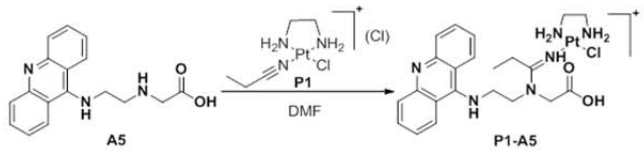


Figure S1.4 LC-ESMS analysis of reaction P1 + A4.

The Reaction Scheme Of P1-A5



The LC-MS Analysis Of P1-A5

Compound Chromatogram Report - MS

Analysis Name: LIB12010.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 12:11:42 AM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 9:00:58 PM
Sample Name: 1-5-1
Analysis Info:

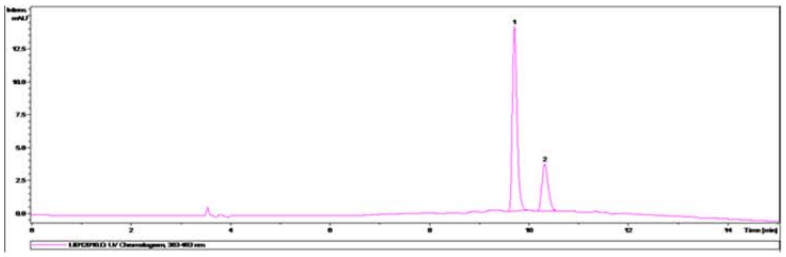
Acquisition Parameter:

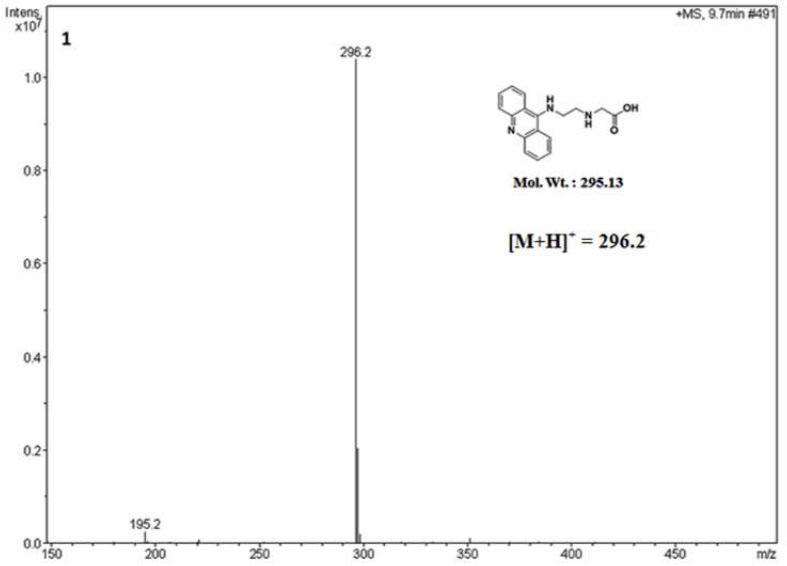
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.7	9.6 - 9.9	14	90	74.8
2	10.3	10.2 - 10.5	3	30	25.2

Chromatograms:





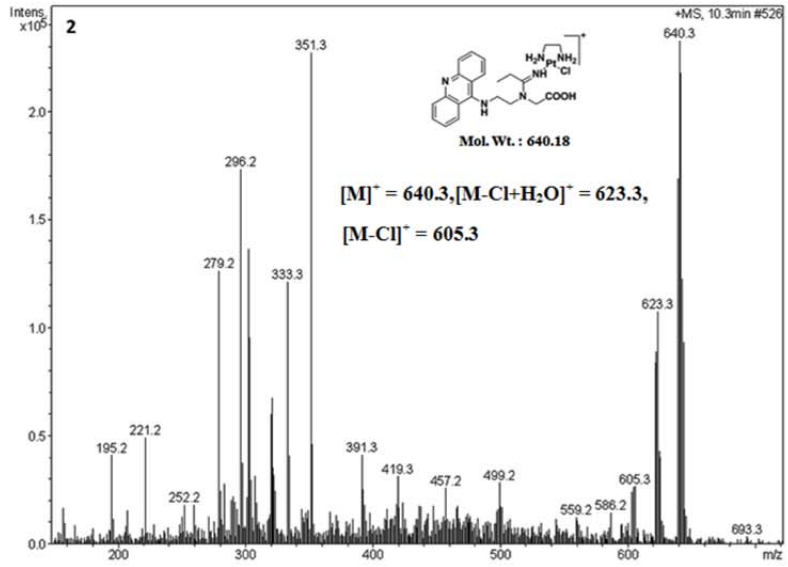
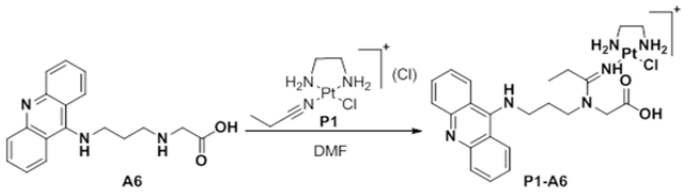


Figure S1.5 LC-ESMS analysis of reaction P1 + A5.

The Reaction Scheme Of P1-A6



The LC-MS Analysis Of P1-A6

Compound Chromatogram Report - MS

Analysis Name: 05221208.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 12:18:27 AM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/22/2012 1:24:03 PM
Sample Name: 1-6
Analysis Info:

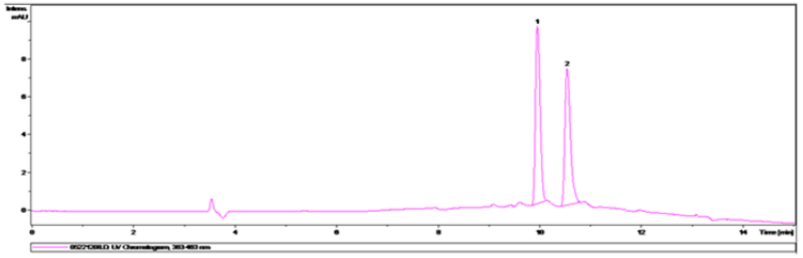
Acquisition Parameter:

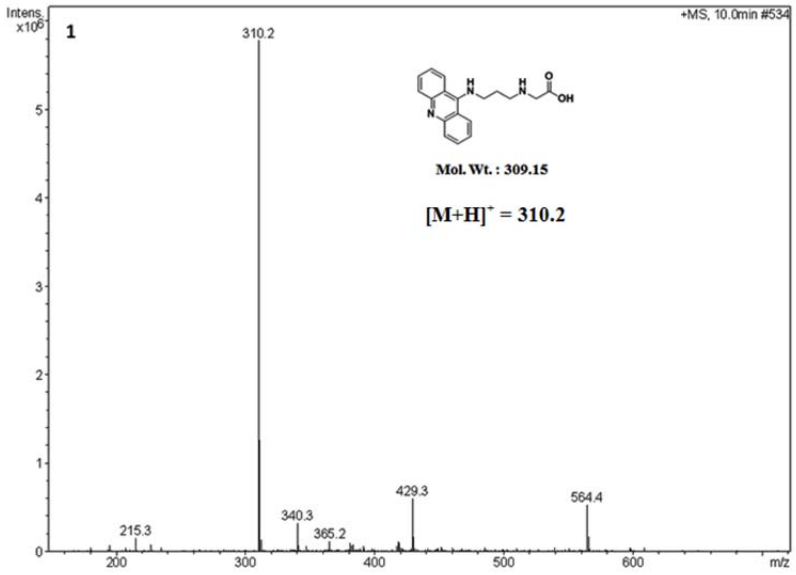
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.9	9.8 - 10.1	9	59	52.0
2	10.5	10.4 - 10.8	7	54	48.0

Chromatograms:





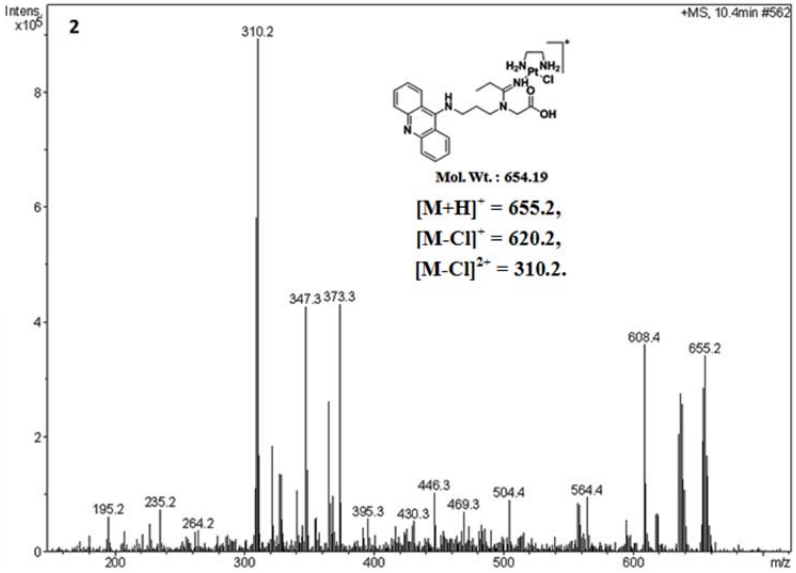
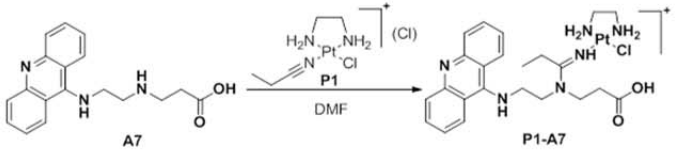


Figure S1.6 LC-ESMS analysis of reaction P1 + A6.

The Reaction Scheme Of P1-A7



The LC-MS Analysis Of P1-A7

Compound Chromatogram Report - MS

Analysis Name: LIB-6016.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 12:20:04 AM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/12/2012 1:24:20 AM
Sample Name: 1-7
Analysis Info:

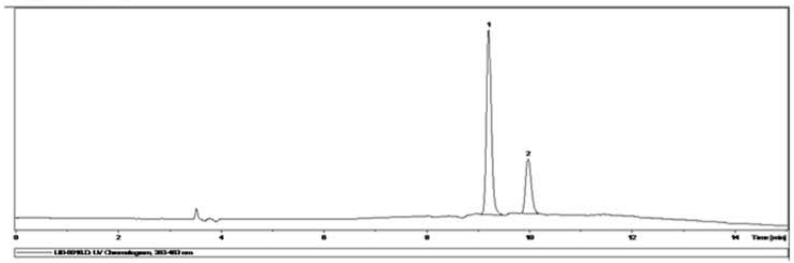
Acquisition Parameter:

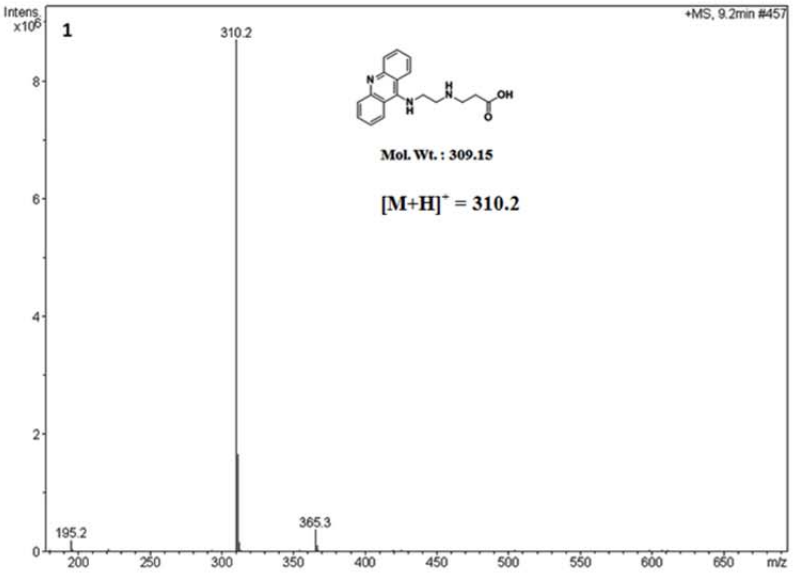
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.2	9.1 - 9.5	12	79	74.4
2	10.0	9.8 - 10.2	4	27	25.6

Chromatograms:





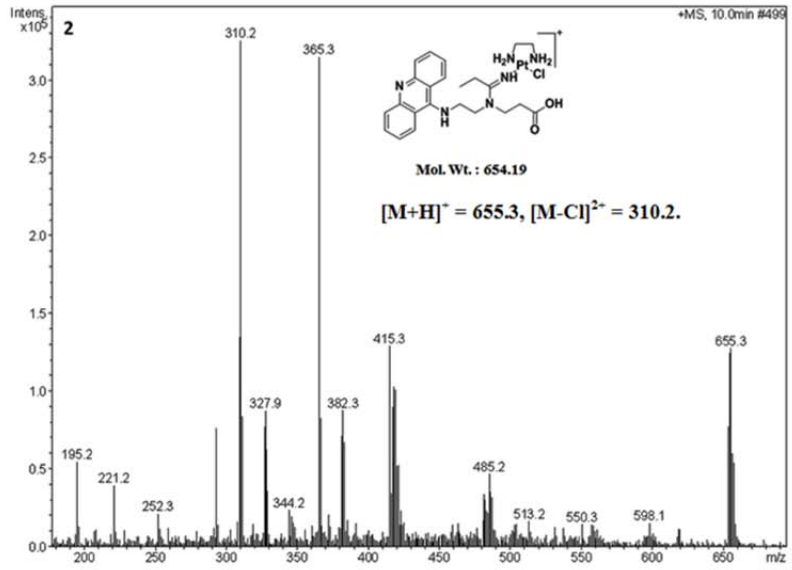
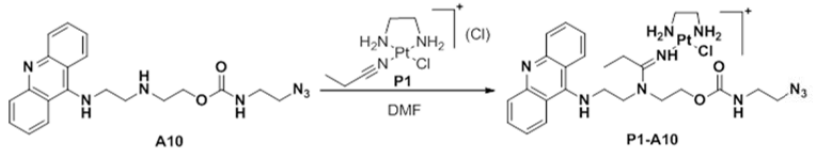


Figure S1.7 LC-ESMS analysis of reaction P1 and A7.

Figure S1.8 LC-ESMS analysis of reaction P1 + A8.

Figure S1.9 LC-ESMS analysis of reaction P1 + A9.

The Reaction Scheme Of P1-A10



The LC-MS Analysis Of P1-A10

Compound Chromatogram Report - MS

Analysis Name: LIB91025.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 12:24:39 AM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/13/2012 2:58:59 PM
Sample Name: 1-10
Analysis Info:

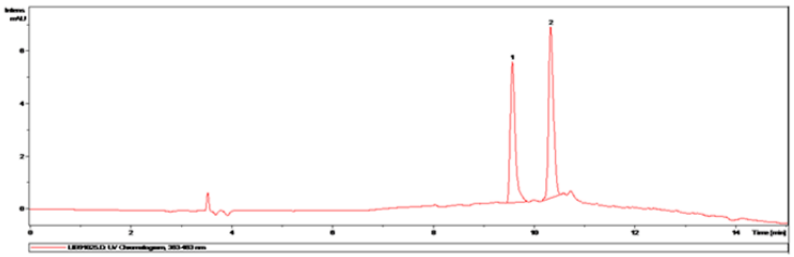
Acquisition Parameter:

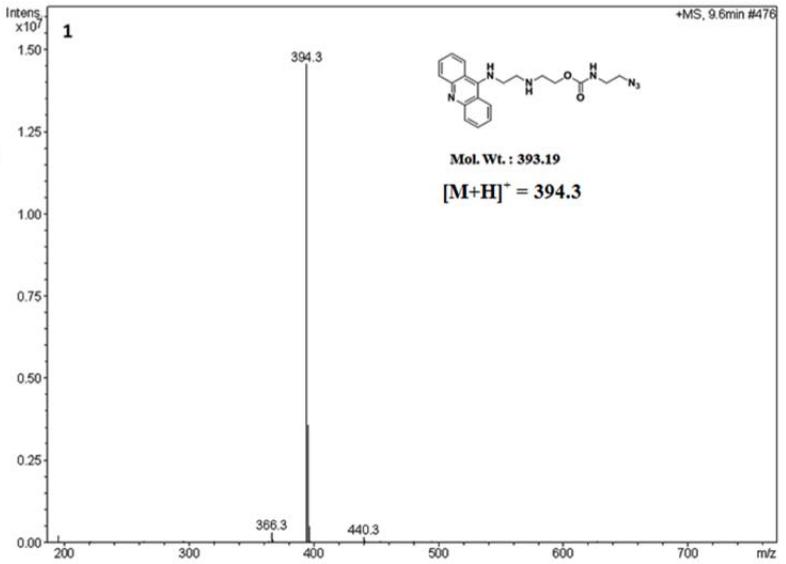
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.6	9.4 - 9.9	5	36	45.2
2	10.3	10.1 - 10.5	6	44	54.8

Chromatograms:





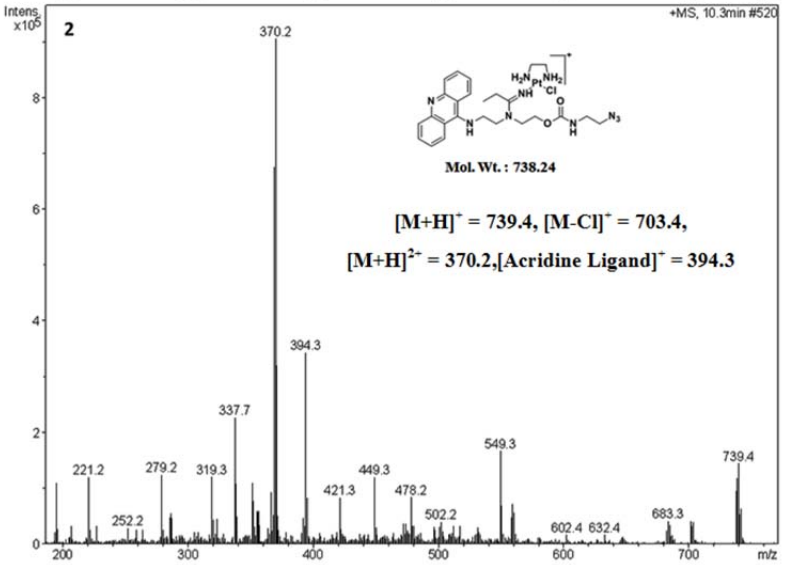
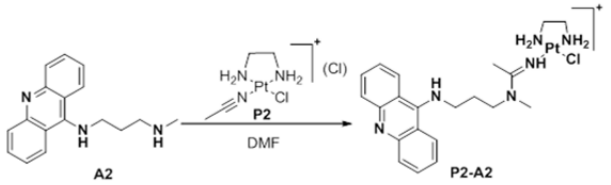


Figure S1.10 LC-ESMS analysis of reaction P1 + A10.

Figure S1.11. LC-ESMS analysis of reaction P2 + A1.

The Reaction Scheme Of P2-A2



The LC-MS Analysis Of P2-A2

Compound Chromatogram Report - MS

Analysis Name: 05121234.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 12:27:35 AM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/10/2012 11:27:01 PM
Sample Name: 2-2
Analysis Info:

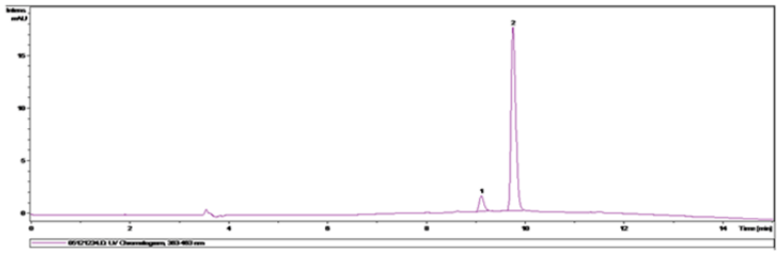
Acquisition Parameter:

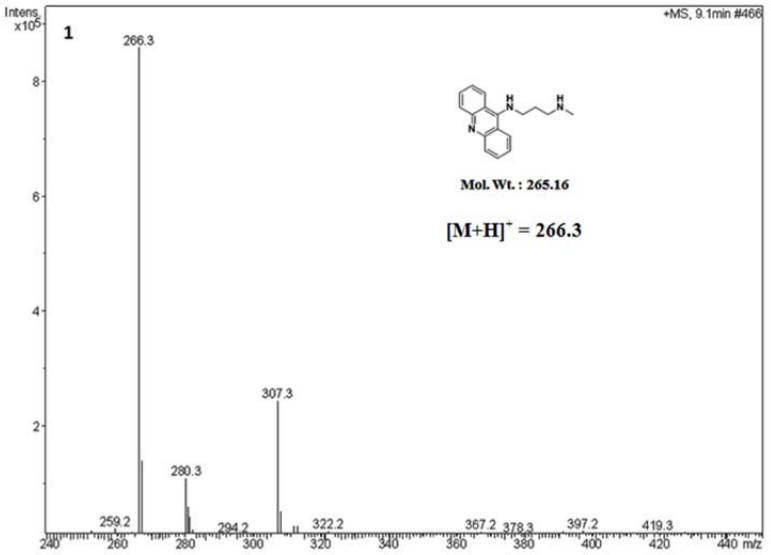
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.1	9.0 - 9.3	1	9	7.5
2	9.7	9.6 - 10.0	17	115	92.5

Chromatograms:





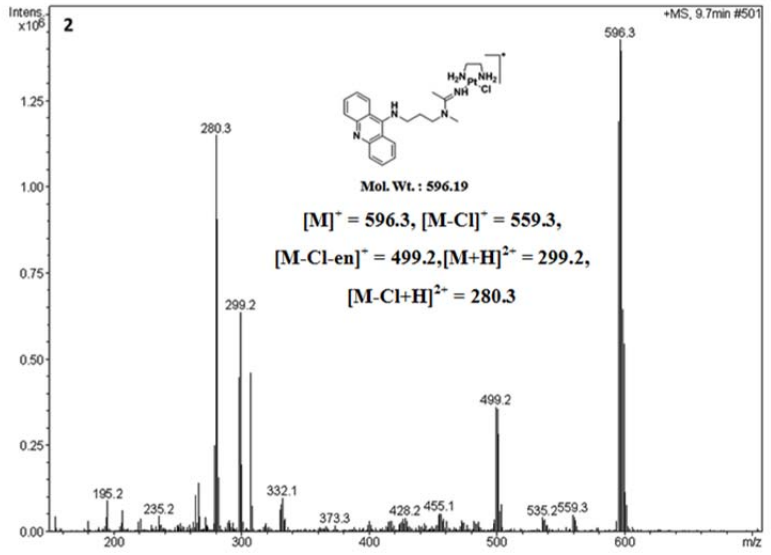
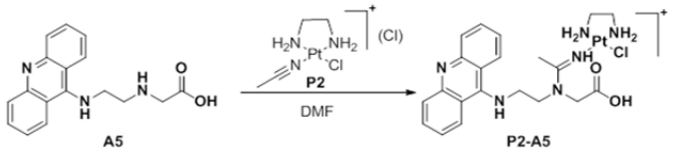


Figure S1.12. LC-ESMS analysis of reaction P2 + A2.

Figure S1.13. LC-ESMS analysis of reaction P2 + A3.

Figure S1.14. LC-ESMS analysis of reaction P2 + A4.

The Reaction Scheme Of P2-A5



The LC-MS Analysis Of P2-A5

Compound Chromatogram Report - MS

Analysis Name: LIB12011.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 04:49:11 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 9:23:01 PM
Sample Name: 2-5-1
Analysis Info:

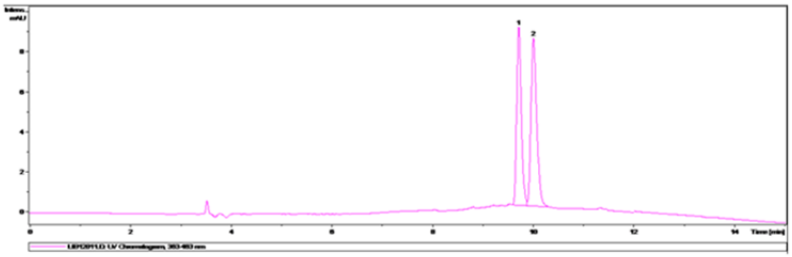
Acquisition Parameter:

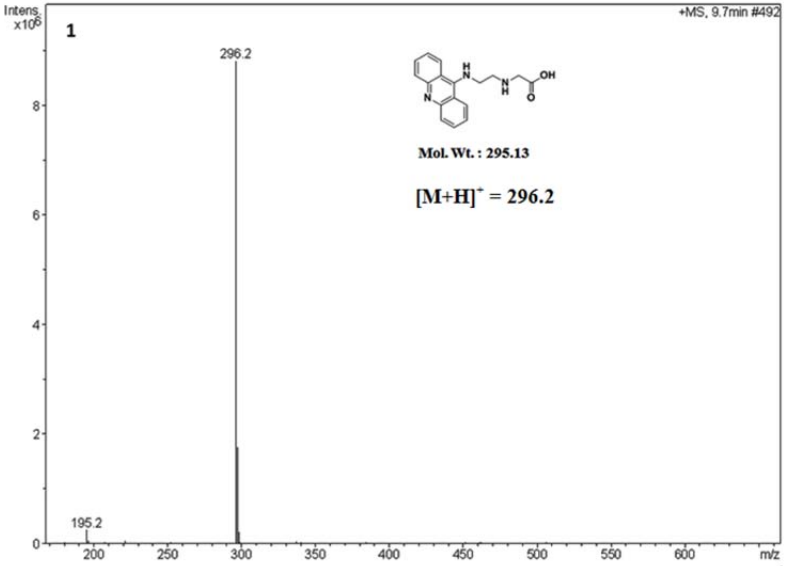
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.7	9.6 - 9.9	9	56	46.1
2	10.0	9.9 - 10.3	8	66	53.9

Chromatograms:





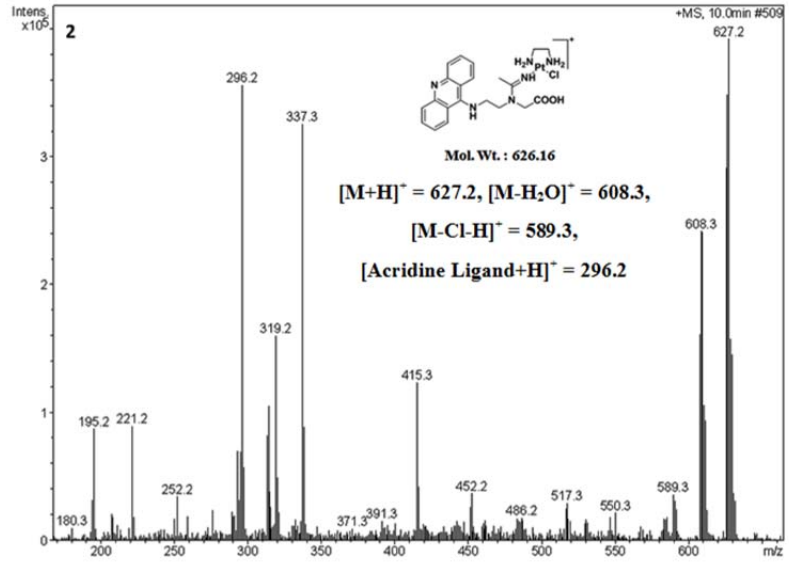


Figure S1.15. LC-ESMS analysis of reaction P2 + A5.

The Reaction Scheme Of P2-A6

The LC-MS Analysis Of P2-6

Compound Chromatogram Report - MS

Analysis Name: LIB-6011.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 04:50:33 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 11:34:04 PM
Sample Name: 2-6
Analysis Info:

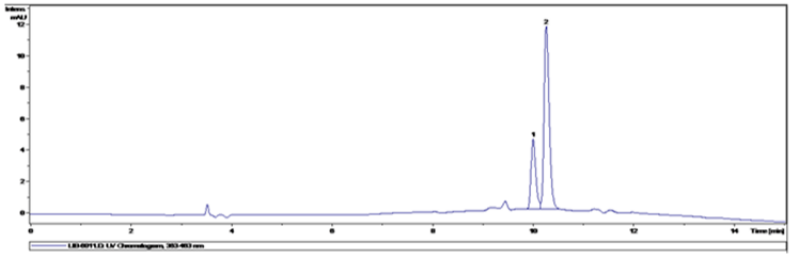
Acquisition Parameter:

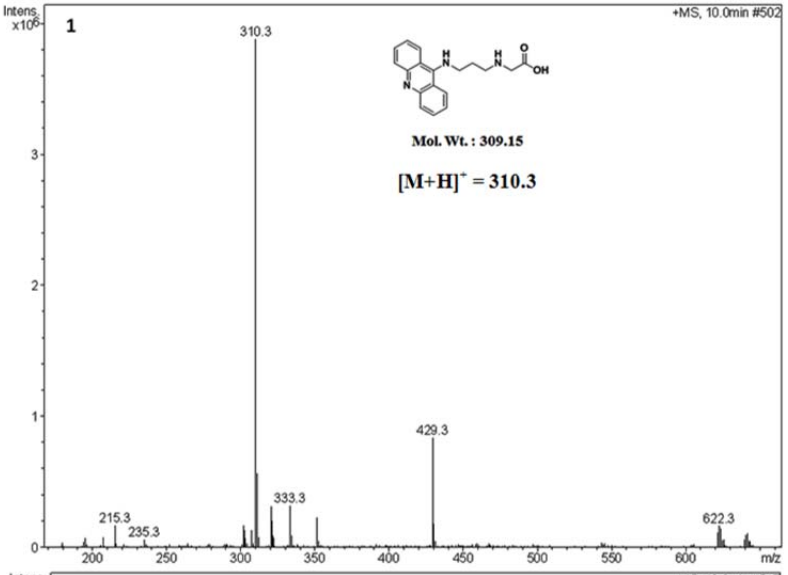
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	10.0	9.9 - 10.1	4	29	26.2
2	10.3	10.1 - 10.5	11	81	73.8

Chromatograms:





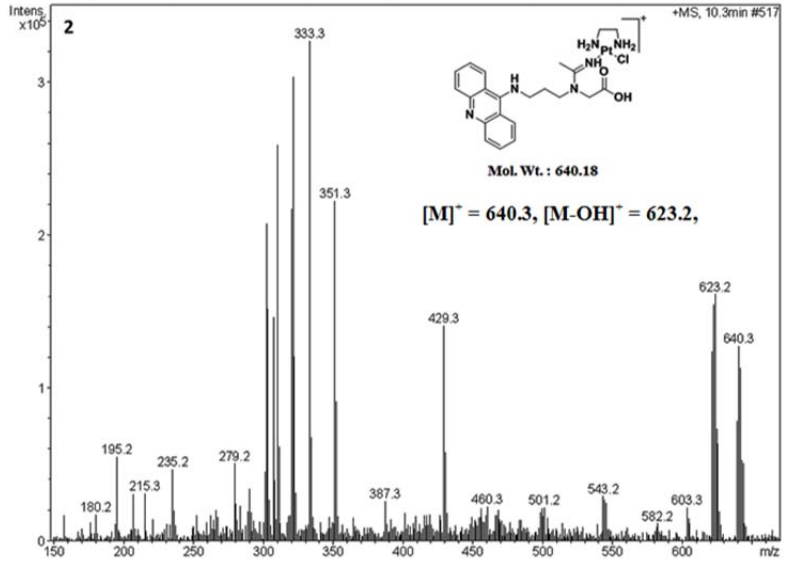
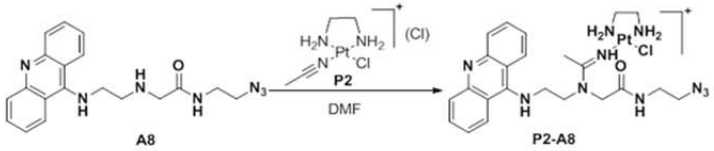


Figure S1.16. LC-ESMS analysis of reaction P2 + A6.

Figure S1.17 LC-ESMS analysis of reaction P2 + A7.

The Reaction Scheme Of P2-A8



The LC-MS Analysis Of P2-A8

Compound Chromatogram Report - MS

Analysis Name: LIB-1820.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 04:53:16 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/12/2012 10:34:40 PM
Sample Name: 2-8
Analysis Info:

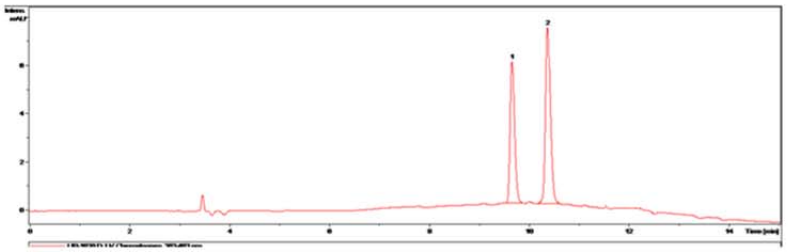
Acquisition Parameter:

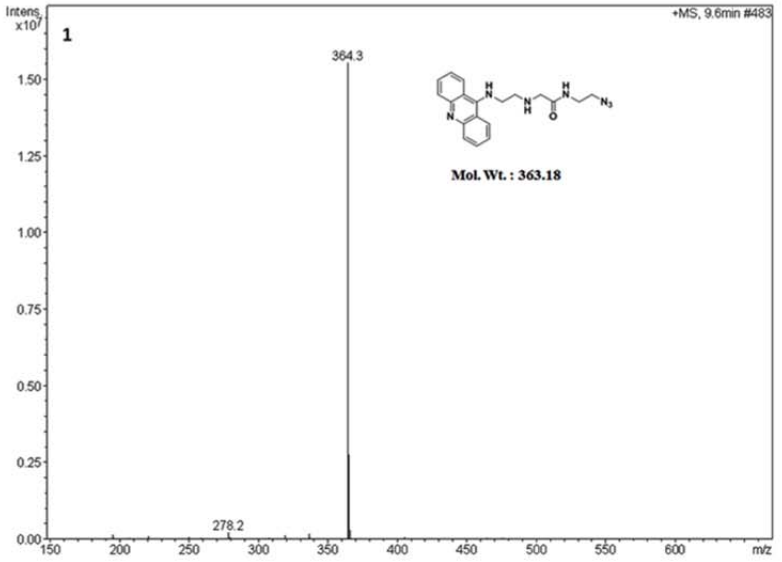
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.6	9.5 - 9.9	6	36	41.9
2	10.4	10.2 - 10.6	7	50	58.1

Chromatograms:





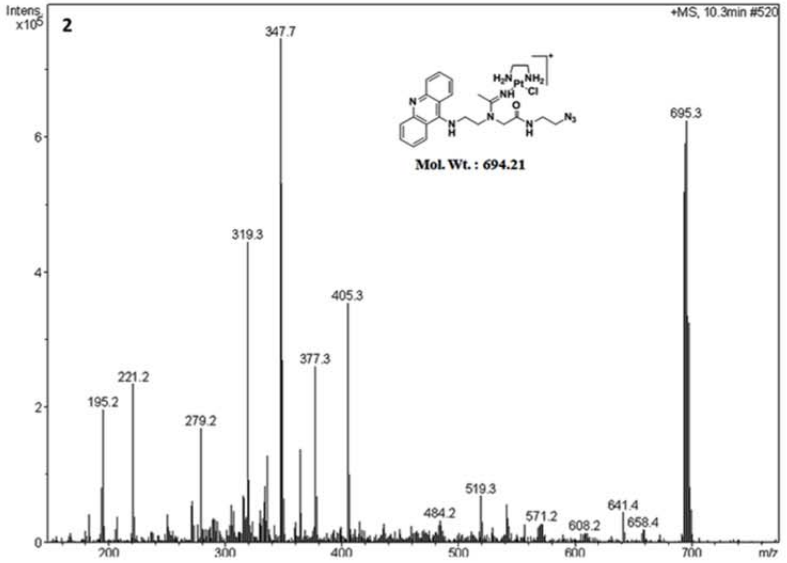


Figure S1.18 LC-ESMS analysis of reaction P2 + A8.

The Reaction Scheme Of P2-A9

The LC-MS Analysis Of P2-A9

Compound Chromatogram Report - MS

Analysis Name: LIB91020.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 04:54:48 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/13/2012 1:08:56 PM
Sample Name: 2-9
Analysis Info:

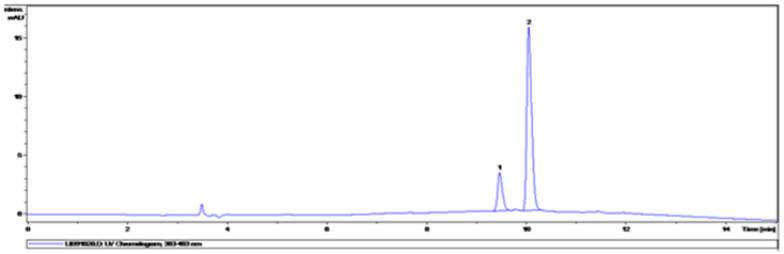
Acquisition Parameter:

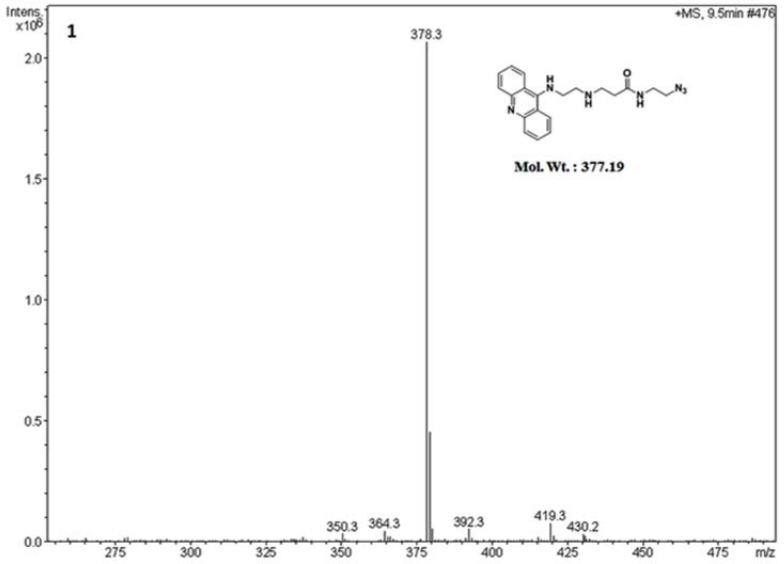
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.5	9.3 - 9.6	3	22	17.0
2	10.0	9.9 - 10.3	15	106	83.0

Chromatograms:





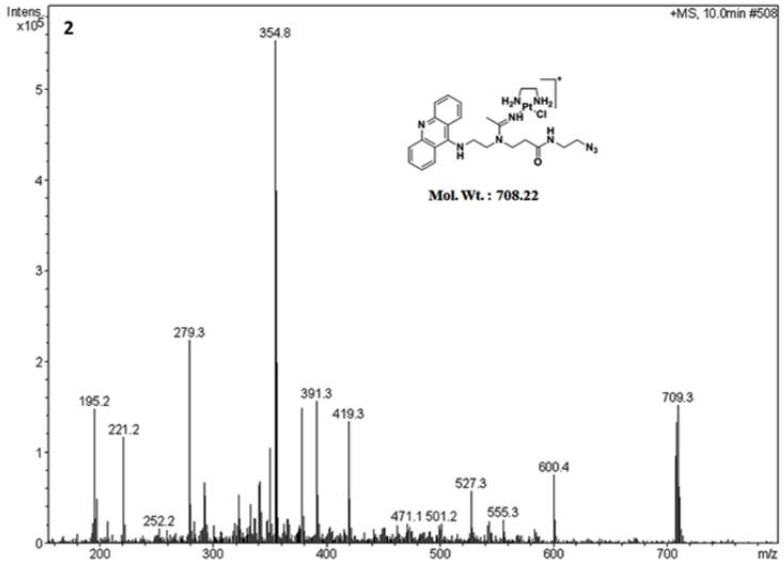


Figure S1.19 LC-ESMS analysis of reaction P2 + A9.

The Reaction Scheme Of P2-A10

The LC-MS Analysis Of P2-A10

Compound Chromatogram Report - MS

Analysis Name: LIB91026.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 04:56:33 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/13/2012 3:21:18 PM
Sample Name: 2-10
Analysis Info:

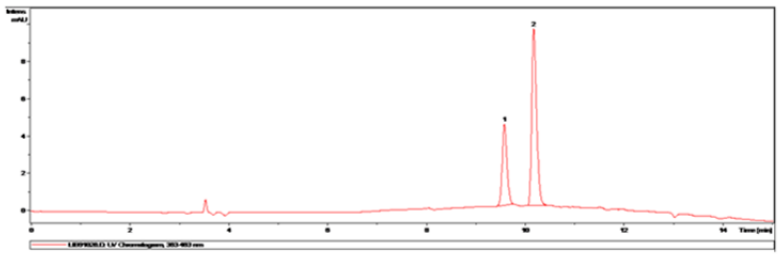
Acquisition Parameter:

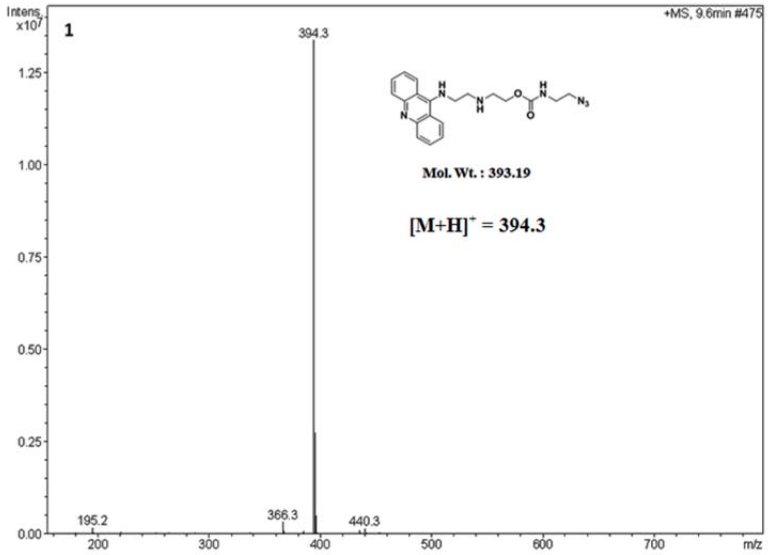
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.6	9.4 - 9.8	4	29	30.8
2	10.2	10.0 - 10.4	9	64	69.2

Chromatograms:





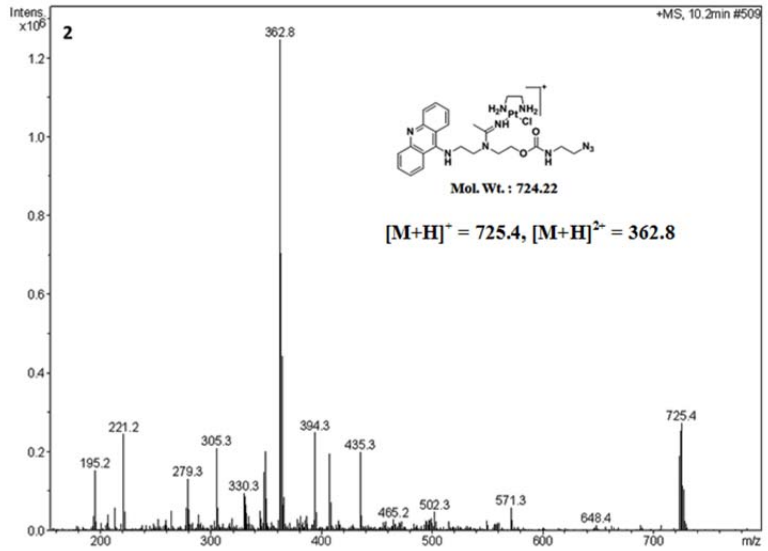
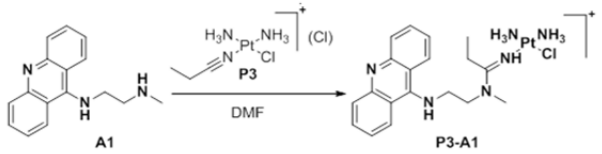


Figure S1.20 LC-ESMS analysis of reaction P2 + A10.

The Reaction Scheme Of P3-A1



The LC-MS Analysis Of P3-A1

Compound Chromatogram Report - MS

Analysis Name: 05121212.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 05:18:51 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/10/2012 7:14:02 PM
Sample Name: 3-1
Analysis Info:

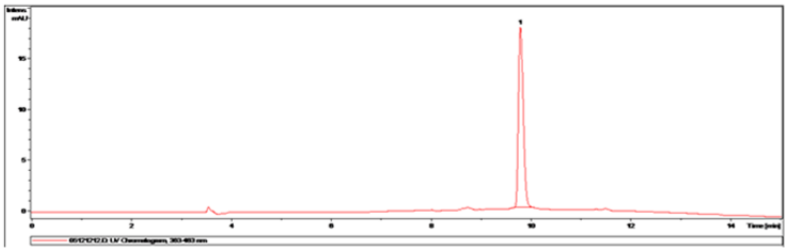
Acquisition Parameter:

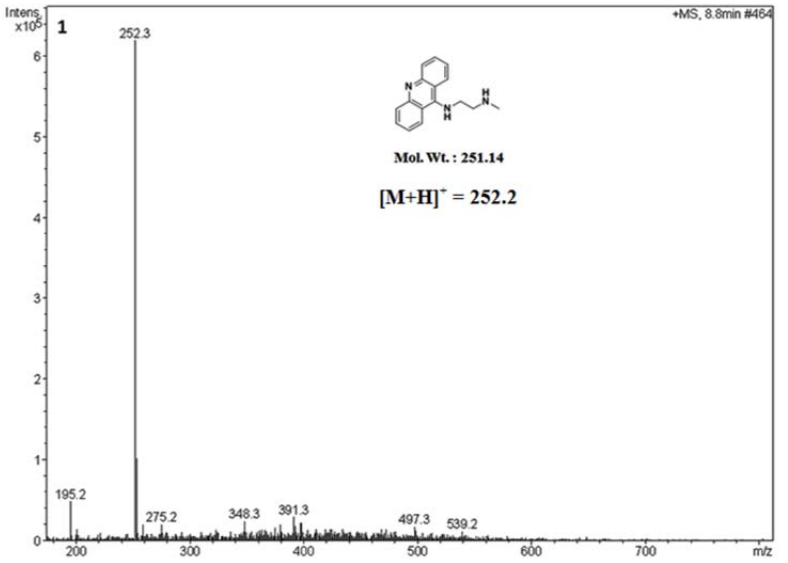
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.8	9.7 - 10.0	18	116	100.0

Chromatograms:





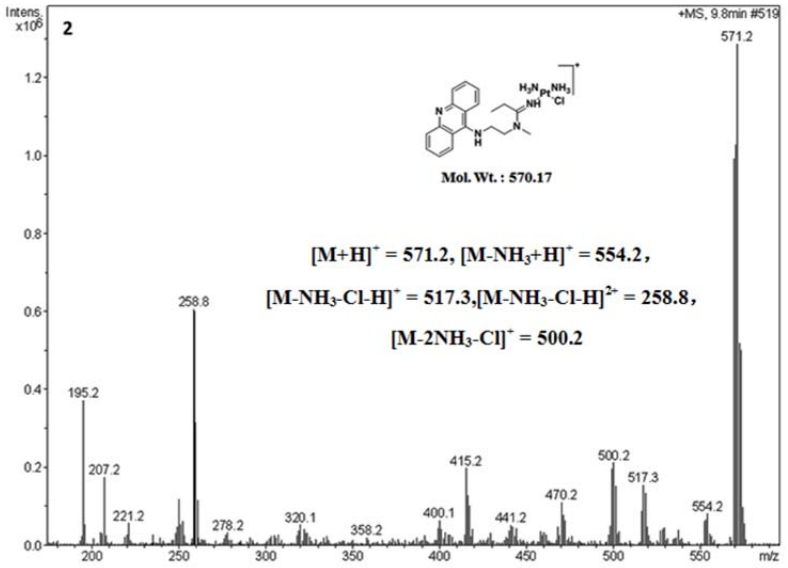


Figure S1.21. LC-ESMS analysis of reaction P3 + A1.

The Reaction Scheme Of P3-A2

The LC-MS Analysis Of P3-A2

Compound Chromatogram Report - MS

Analysis Name: 05121236.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 05:22:32 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 12:47:12 AM
Sample Name: 3-2
Analysis Info:

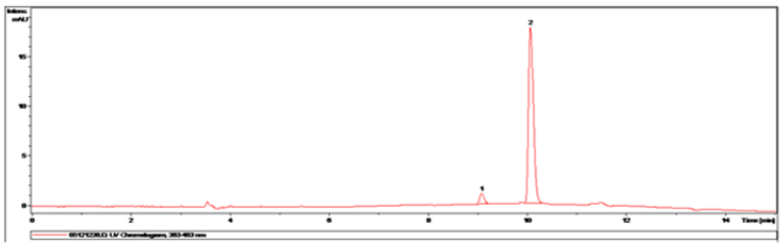
Acquisition Parameter:

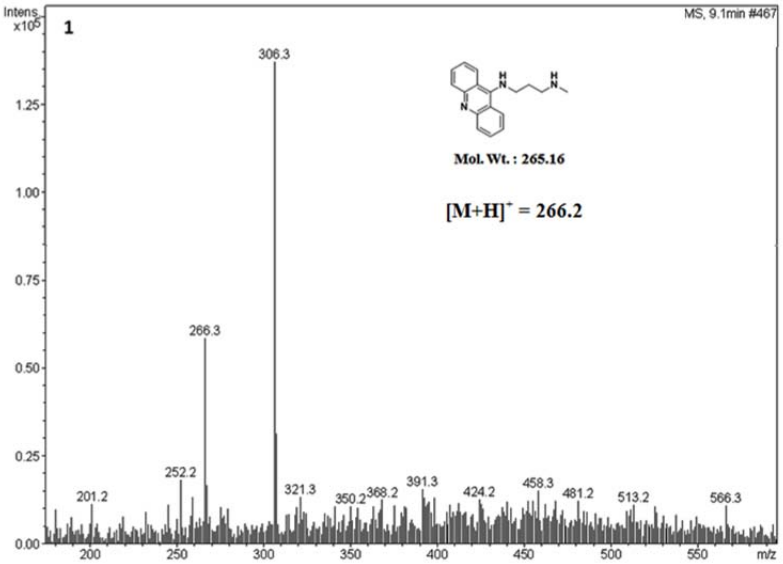
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	-1
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.1	9.0 - 9.2	1	6	4.9
2	10.1	9.9 - 10.3	18	121	95.1

Chromatograms:





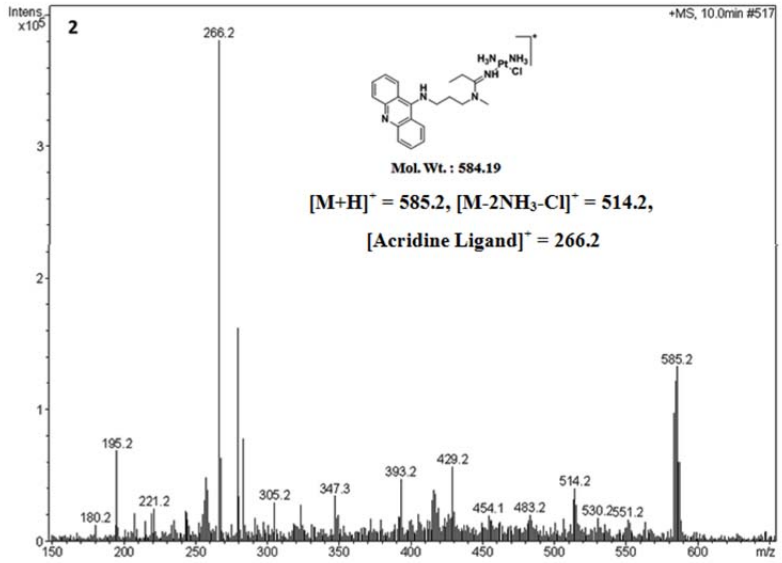
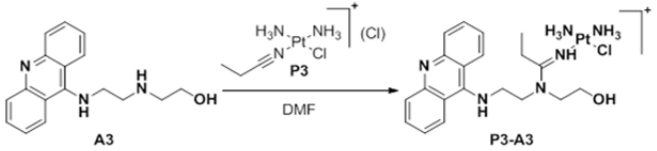


Figure S1.22. LC-ESMS analysis of reaction P3 + A2.

The Reaction Scheme Of P3-A3



The LC-MS Analysis Of P3-A3

Compound Chromatogram Report - MS

Analysis Name: LIB-1313.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 05:45:24 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/12/2012 1:44:57 PM
Sample Name: 3-3
Analysis Info:

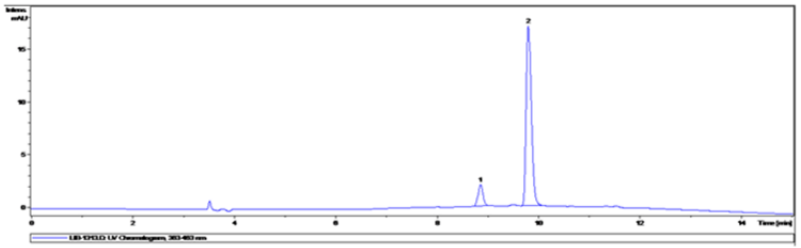
Acquisition Parameter:

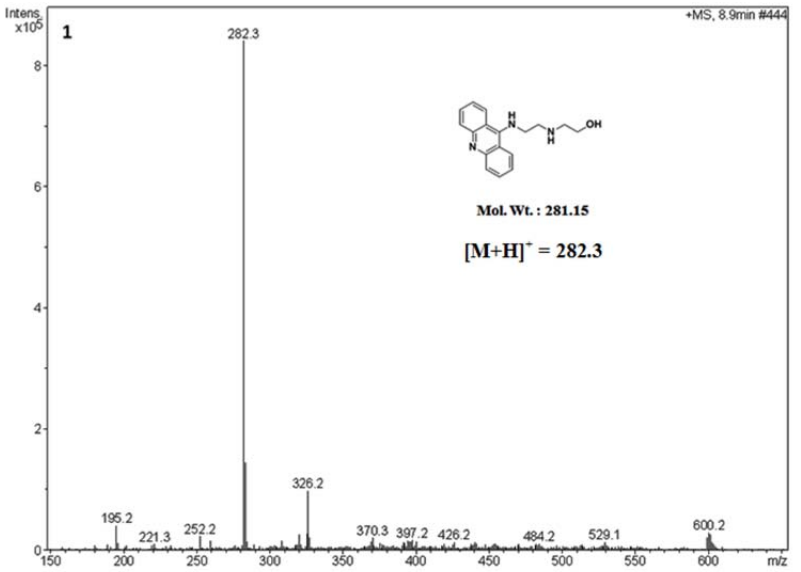
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	8.9	8.7 - 9.0	2	13	9.9
2	9.8	9.7 - 10.0	17	120	90.1

Chromatograms:





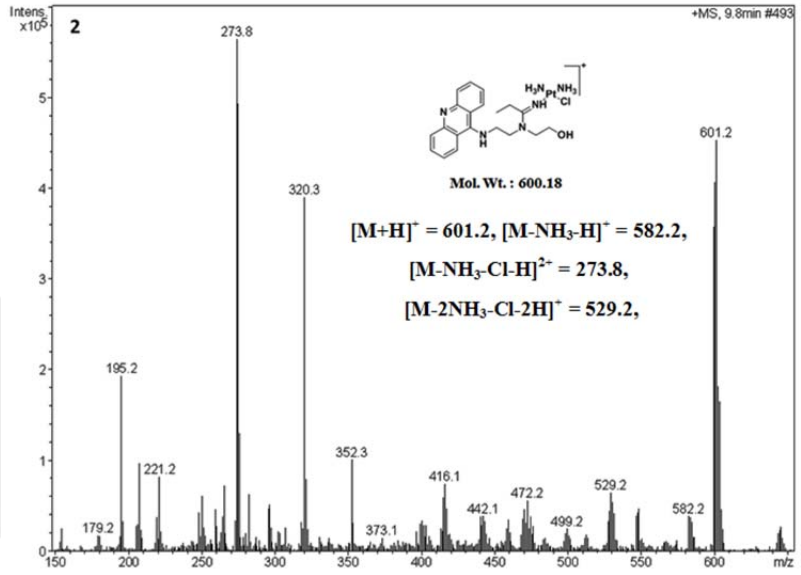


Figure S1.23. LC-ESMS analysis of reaction P3 + A3.

The Reaction Scheme Of P3-A4

The LC-MS Analysis Of P3-A4

Compound Chromatogram Report - MS

Analysis Name: LIB-1412.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 05:46:36 PM
Method: SONG-L~1.m **Operator:** Administrator **Acq. Date:** 5/12/2012 3:36:43 PM
Sample Name: 3-4
Analysis Info:

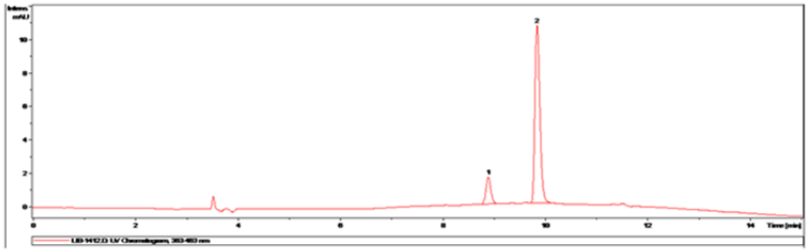
Acquisition Parameter:

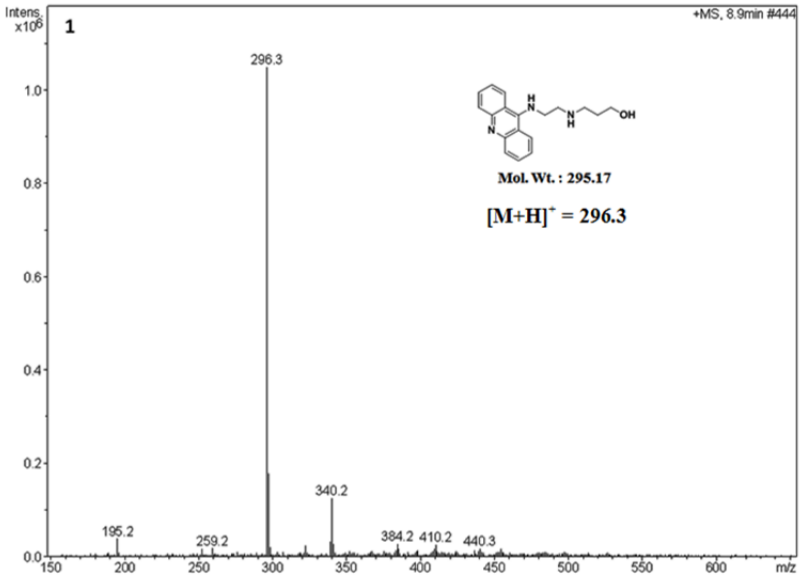
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	8.9	8.8 - 9.0	2	10	13.0
2	9.8	9.7 - 10.1	11	70	87.0

Chromatograms:





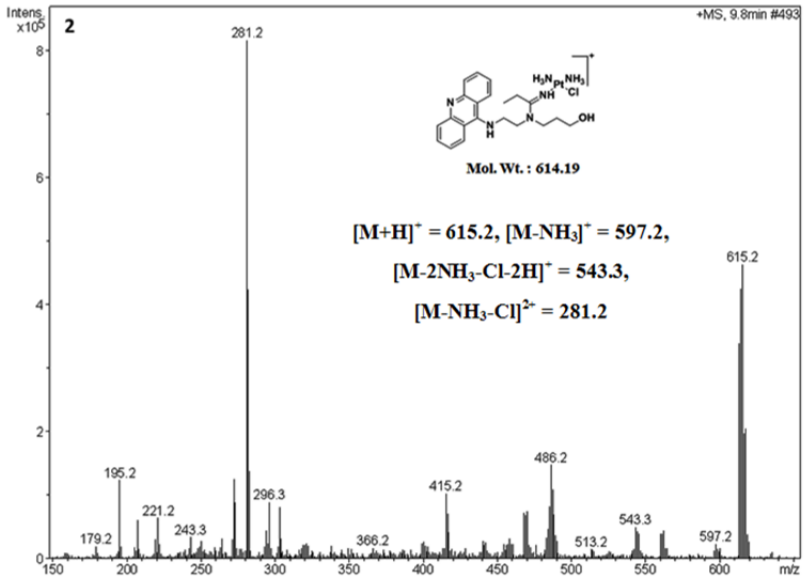
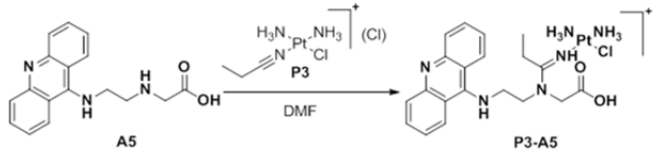


Figure S1.24. LC-ESMS analysis of reaction P3 + A4.

The Reaction Scheme Of P3-A5



The LC-MS Analysis Of P3-A5

Compound Chromatogram Report - MS

Analysis Name: LIB12012.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 05:52:19 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 9:45:05 PM
Sample Name: 3-5-1
Analysis Info:

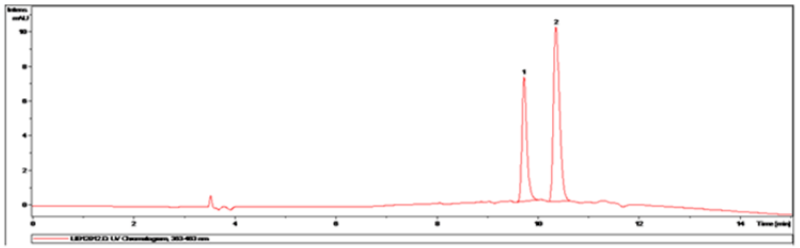
Acquisition Parameter:

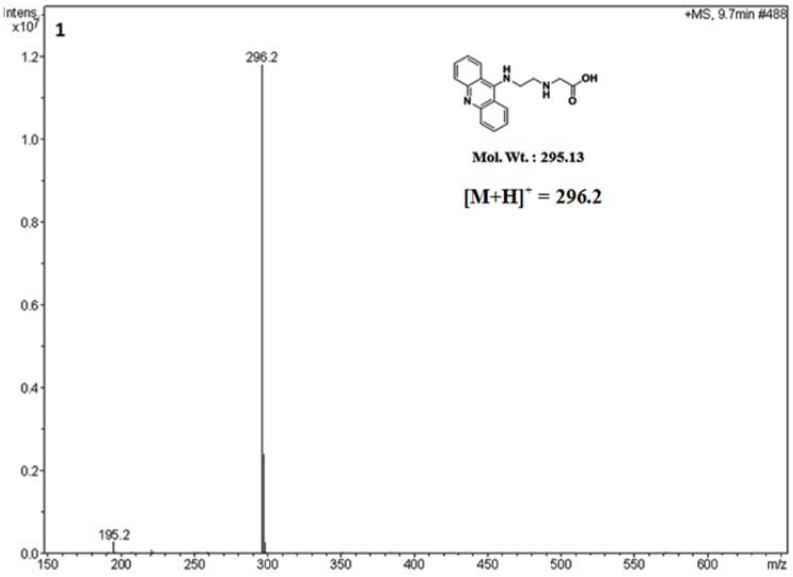
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.7	9.6 - 10.0	7	47	35.9
2	10.3	10.2 - 10.6	10	85	64.1

Chromatograms:





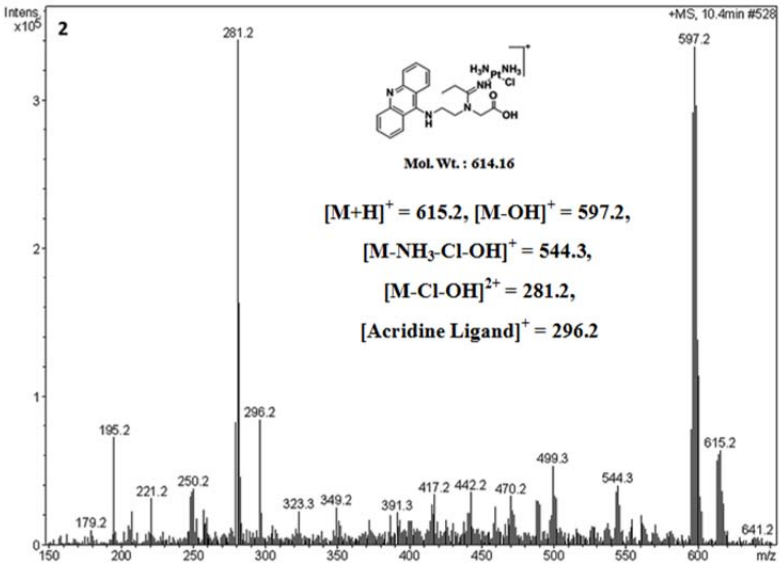
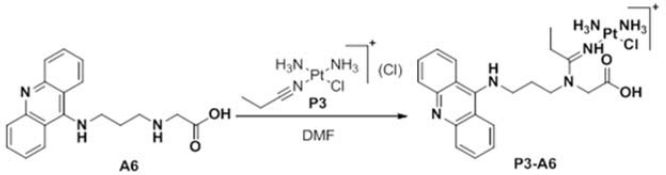


Figure S1.25. LC-ESMS analysis of reaction P3 + A5.

The Reaction Scheme Of P3-A6



The LC-MS Analysis Of P3-A6

Compound Chromatogram Report - MS

Analysis Name: LIB-6012.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 05:59:40 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 11:56:12 PM
Sample Name: 3-6
Analysis Info:

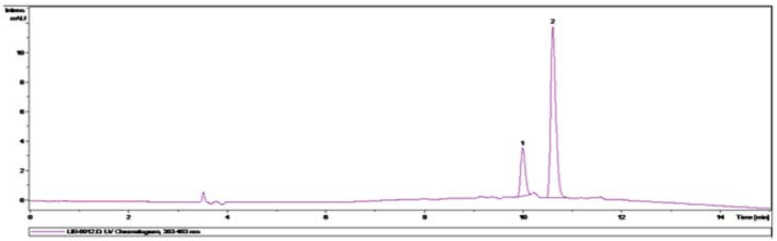
Acquisition Parameter:

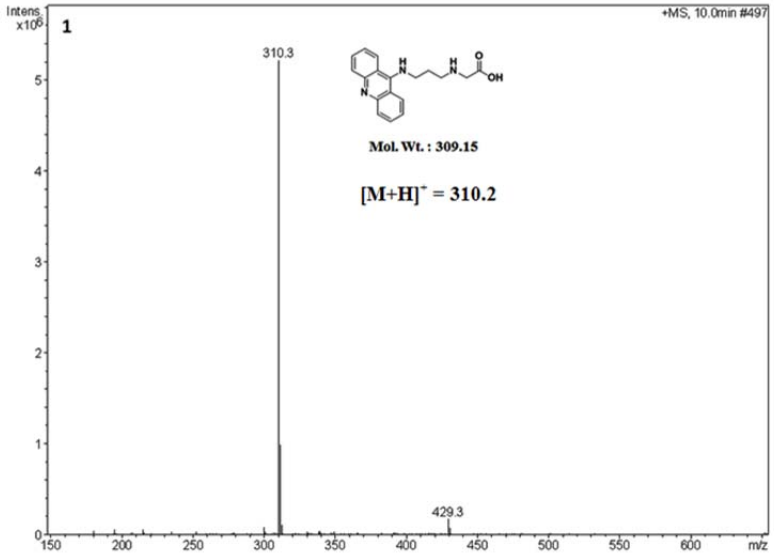
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	10.0	9.9 - 10.1	3	21	20.0
2	10.6	10.5 - 10.9	11	82	80.0

Chromatograms:





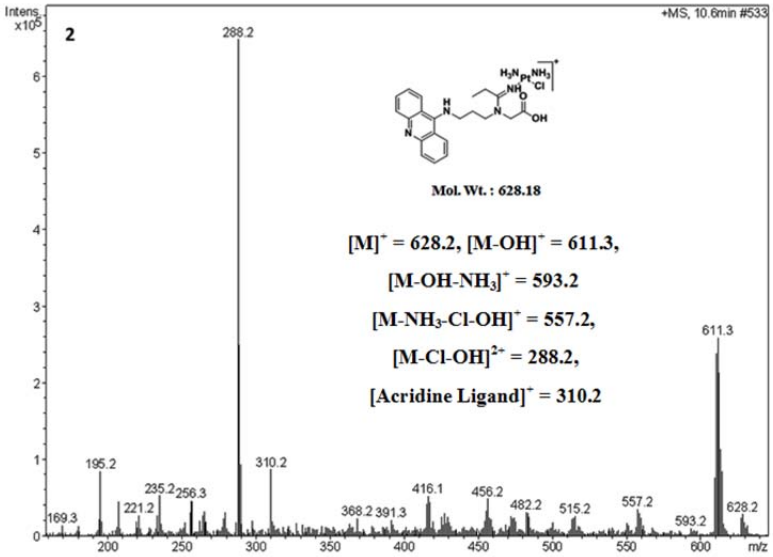
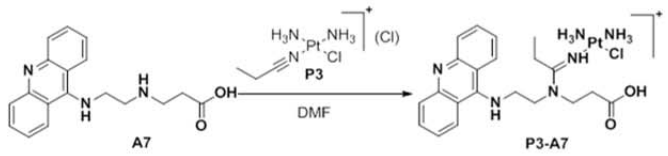


Figure S1.26. LC-ESMS analysis of reaction P3 + A6.

The Reaction Scheme Of P3-A7



The LC-MS Analysis Of P3-A7

Compound Chromatogram Report - MS

Analysis Name: LIB-7003.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:01:20 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/12/2012 9:59:28 AM
Sample Name: 3-7
Analysis Info:

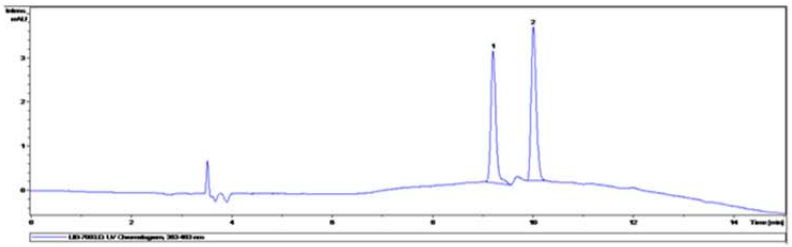
Acquisition Parameter:

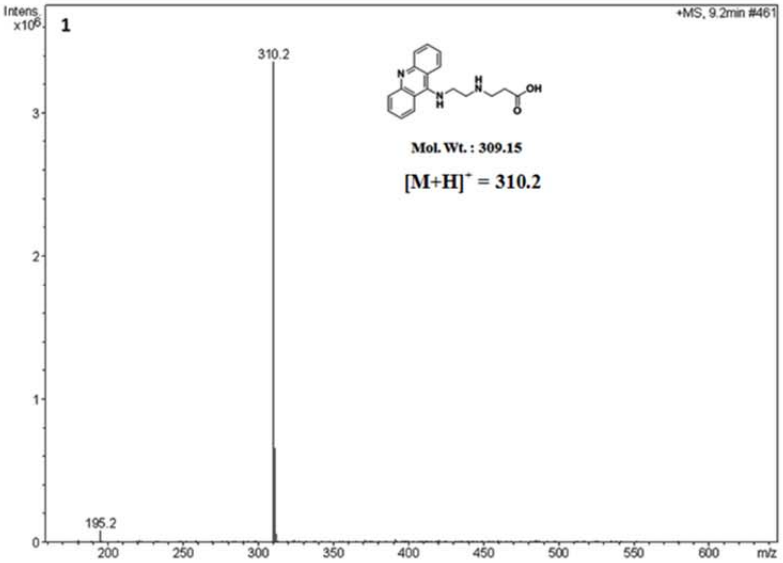
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.2	9.1 - 9.5	3	20	45.9
2	10.0	9.9 - 10.2	3	24	54.1

Chromatograms:





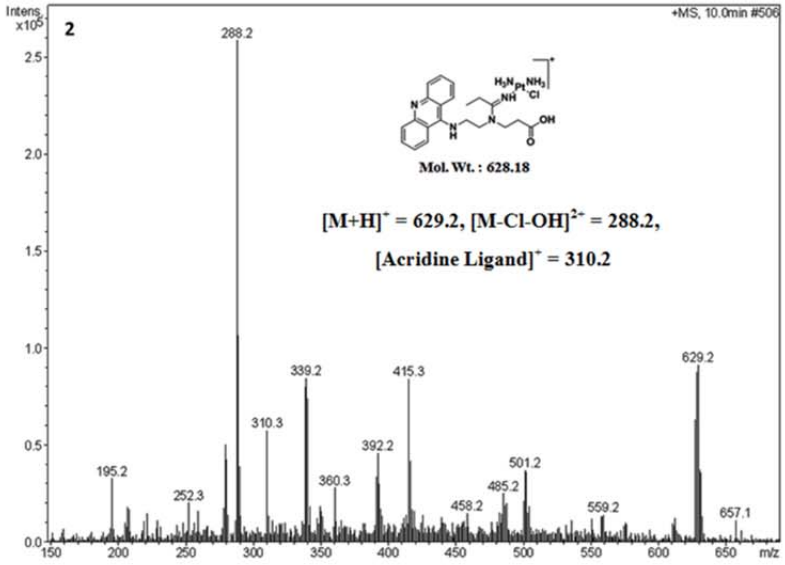
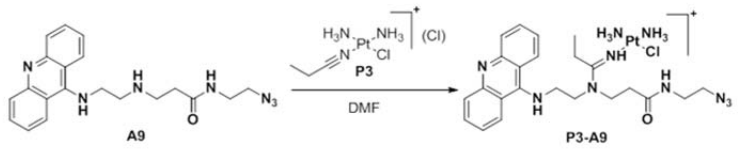


Figure S1.27. LC-ESMS analysis of reaction P3 + A7.

Figure S1.28. LC-ESMS analysis of reaction P3 + A8.

The Reaction Scheme Of P3-A9



The LC-MS Analysis Of P3-A9

Compound Chromatogram Report - MS

Analysis Name: LIB91021.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:05:40 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/13/2012 1:30:49 PM
Sample Name: 3-9
Analysis Info:

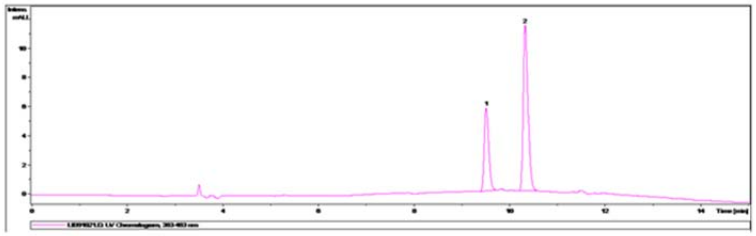
Acquisition Parameter:

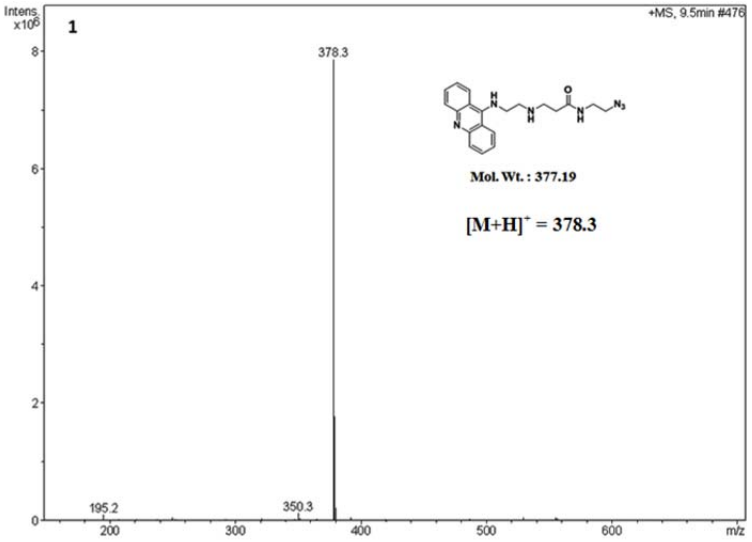
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.5	9.4 - 9.7	6	37	31.8
2	10.3	10.2 - 10.6	11	78	68.2

Chromatograms:





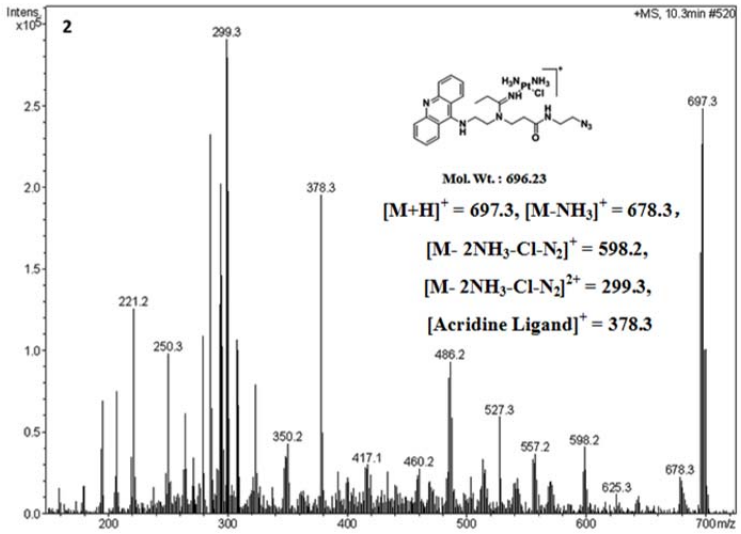


Figure S1.29. LC-ESMS analysis of reaction P3 + A9.

The Reaction Scheme Of P3-A10

The LC-MS Analysis Of P3-A10

Compound Chromatogram Report - MS

Analysis Name: LIB91027.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:06:46 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/13/2012 3:43:20 PM
Sample Name: 3-10
Analysis Info:

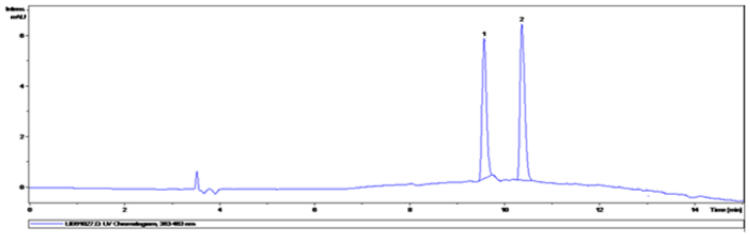
Acquisition Parameter:

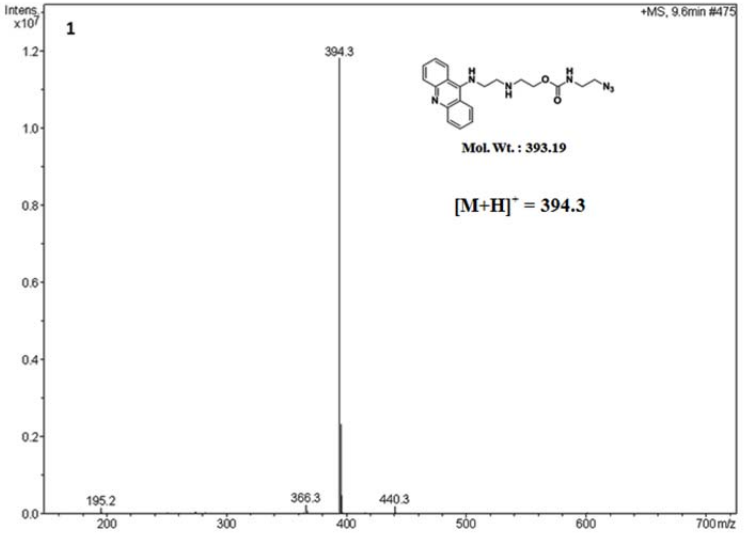
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.6	9.4 - 9.7	5	35	45.3
2	10.4	10.2 - 10.6	6	42	54.7

Chromatograms:





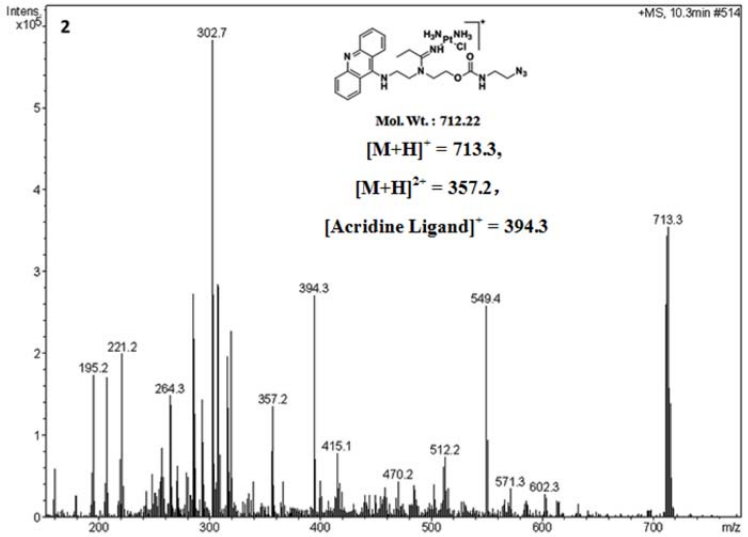
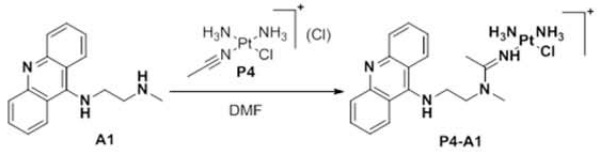


Figure S1.30. LC-ESMS analysis of reaction P3 + A10.

The Reaction Scheme Of P4-A1



The LC-MS Analysis Of P4-A1

Compound Chromatogram Report - MS

Analysis Name:	05121213.D	**Instrument:**	LC-MSD-Trap-SL	**Print Date:**	06/08/2012 06:08:25 PM
Method:	SONG-L~1.M	**Operator:**	Administrator	**Acq. Date:**	5/10/2012 7:38:31 PM
Sample Name:	4-1				
Analysis Info:					

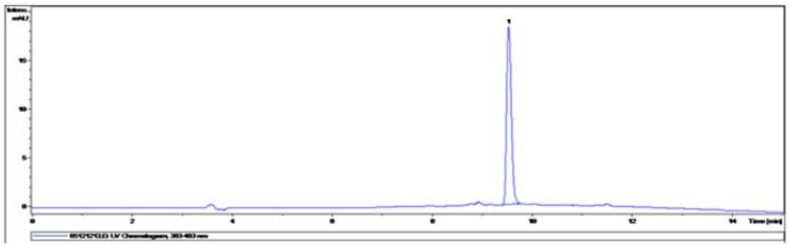
Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.5	9.4 - 9.7	18	116	100.0

Chromatograms:



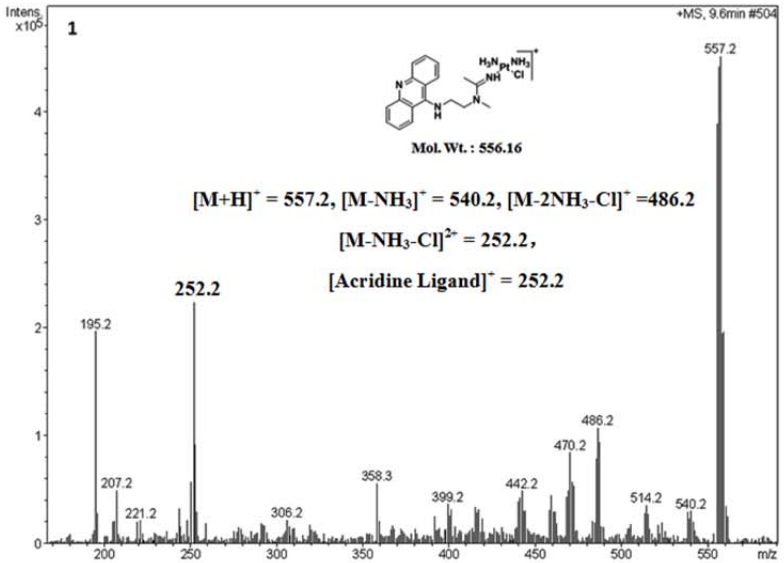


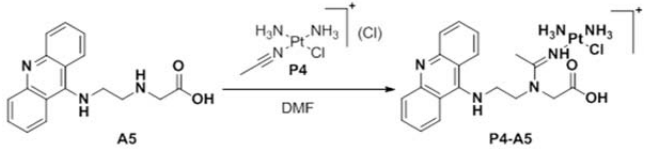
Figure S1.31. LC-ESMS analysis of reaction P4 + A1.

Figure S1.32. LC-ESMS analysis of reaction P4 + A2.

Figure S1.33. LC-ESMS analysis of reaction P4 + A3.

Figure S1.34. LC-ESMS analysis of reaction P4 + A4.

The Reaction Scheme Of P4-A5



The LC-MS Analysis Of P4-A5

Compound Chromatogram Report - MS

Analysis Name: LIB12013.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:16:06 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 10:07:11 PM
Sample Name: 4-5-1
Analysis Info:

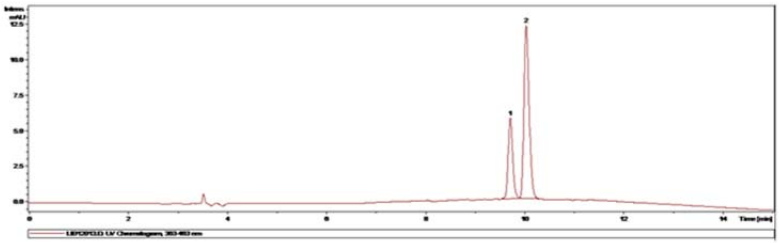
Acquisition Parameter:

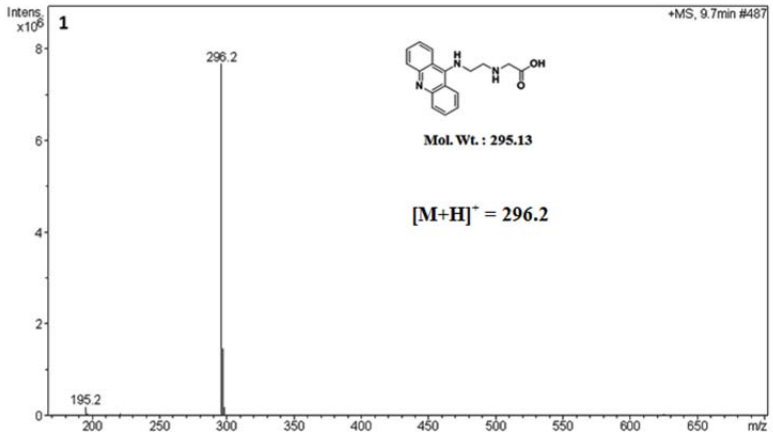
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.7	9.5 - 9.9	6	36	28.9
2	10.0	9.9 - 10.3	12	87	71.1

Chromatograms:





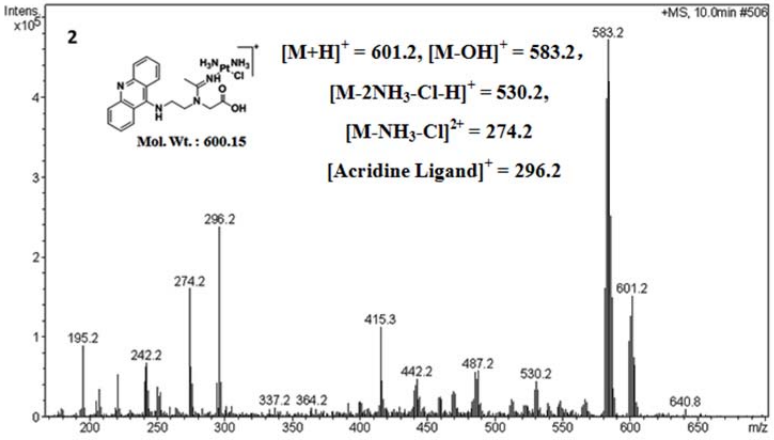
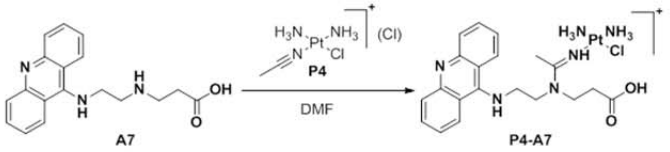


Figure S1.35. LC-ESMS analysis of reaction P4 + A5.

Figure S1.36. LC-ESMS analysis of reaction P4 + A6.

The Reaction Scheme Of P4-A7



The LC-MS Analysis Of P4-A7

Compound Chromatogram Report - MS

Analysis Name: LIB-7010.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:19:04 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/12/2012 11:27:15 AM
Sample Name: 4-7
Analysis Info:

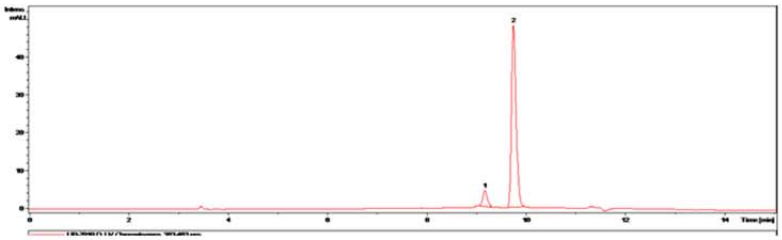
Acquisition Parameter:

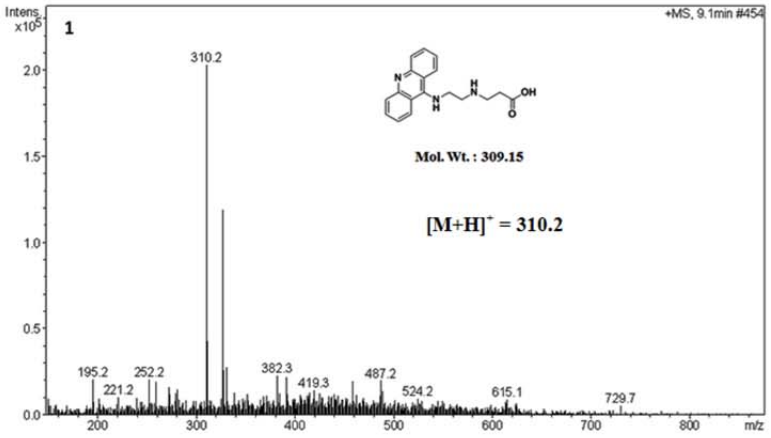
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	-1
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.2	9.0 - 9.3	4	27	8.0
2	9.7	9.6 - 10.0	48	309	92.0

Chromatograms:





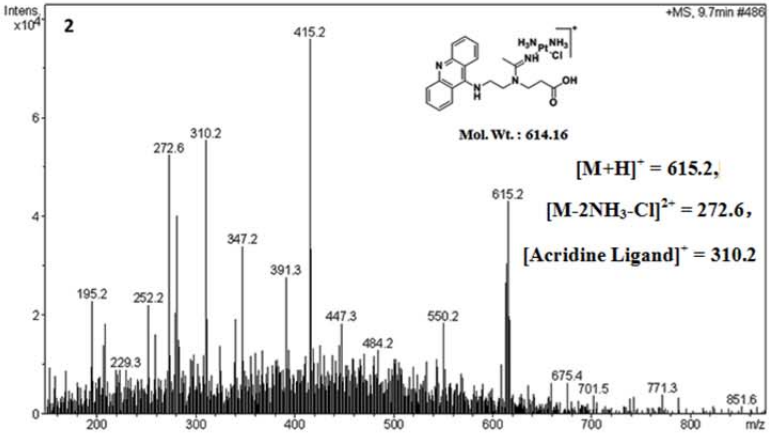
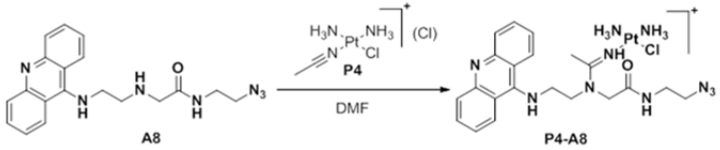


Figure S1.37. LC-ESMS analysis of reaction P4 + A7.

The Reaction Scheme Of P4-A8



The LC-MS Analysis Of P4-A8

Compound Chromatogram Report - MS

Analysis Name: LIB-1822.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:20:06 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/12/2012 11:18:32 PM
Sample Name: 4-8
Analysis Info:

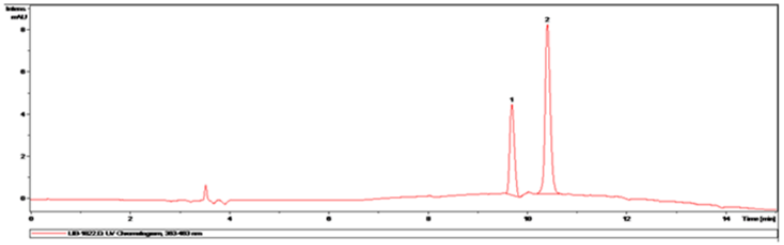
Acquisition Parameter:

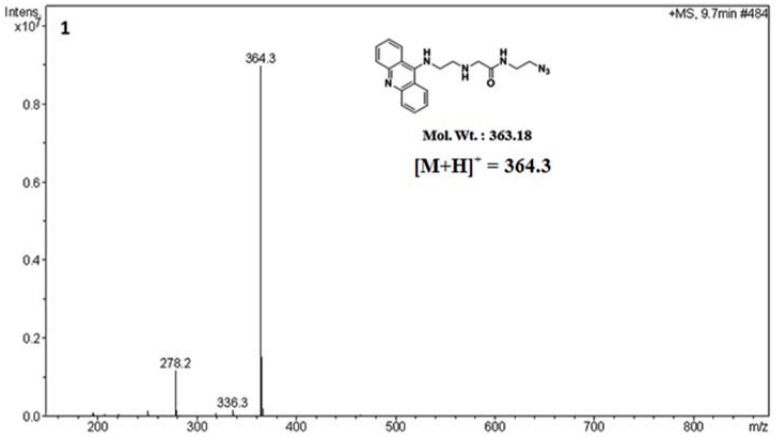
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.7	9.6 - 9.8	4	27	32.4
2	10.4	10.2 - 10.6	8	57	67.6

Chromatograms:





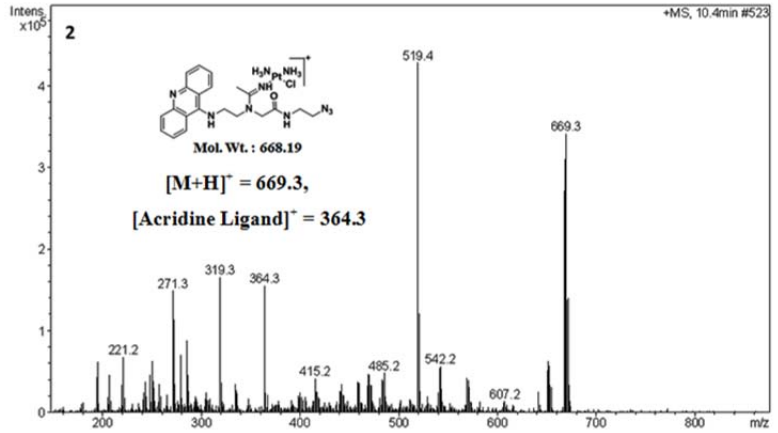
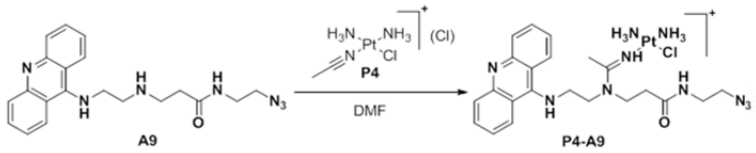


Figure S1.38. LC-ESMS analysis of reaction P4 + A8.

The Reaction Scheme Of P4-A9



The LC-MS Analysis Of P4-A9

Compound Chromatogram Report - MS

Analysis Name: LIB91022.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:21:52 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/13/2012 1:52:56 PM
Sample Name: 4-9
Analysis Info:

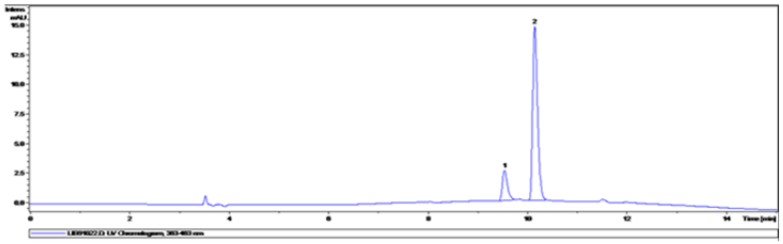
Acquisition Parameter:

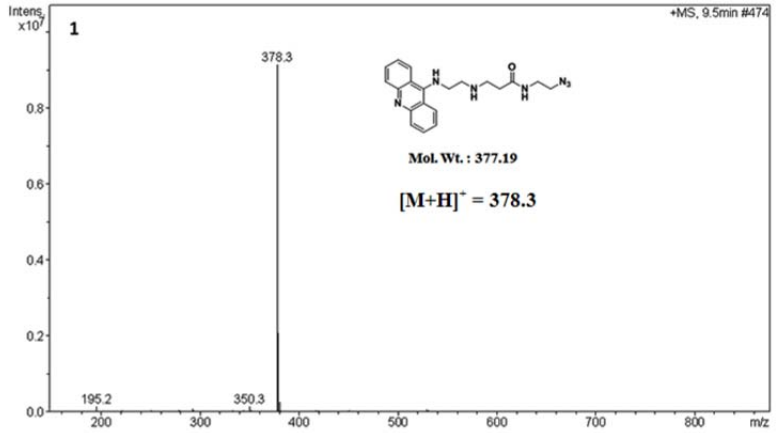
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.5	9.4 - 9.7	3	17	14.9
2	10.1	10.0 - 10.4	15	98	85.1

Chromatograms:





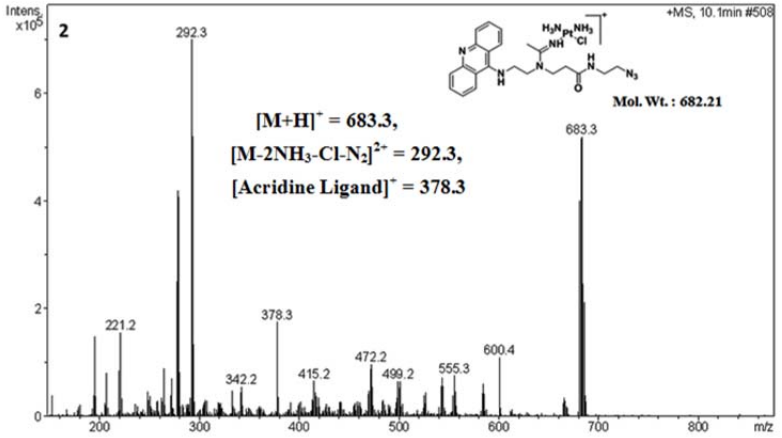
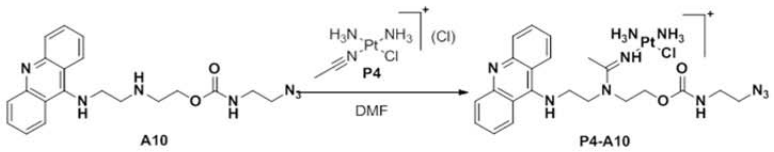


Figure S1.39. LC-ESMS analysis of reaction P4 + A9.

The Reaction Scheme Of P4-A10



The LC-MS Analysis Of P4-A10

Compound Chromatogram Report - MS

Analysis Name:	LIB91028.D	**Instrument:**	LC-MSD-Trap-SL	**Print Date:**	06/08/2012 06:22:52 PM
Method:	SONG-L~1.M	**Operator:**	Administrator	**Acq. Date:**	5/13/2012 4:05:30 PM
Sample Name:	4-10				
Analysis Info:					

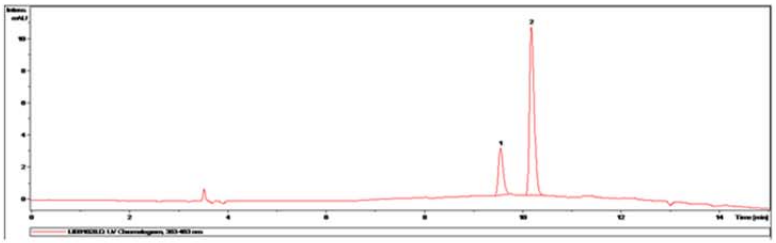
Acquisition Parameter:

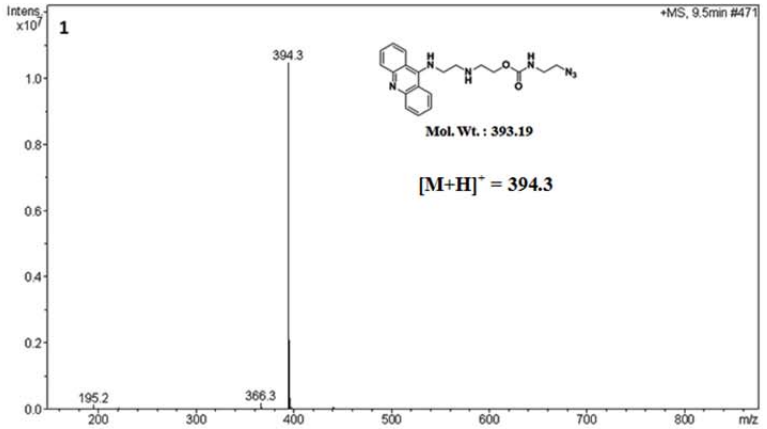
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.5	9.4 - 9.7	3	19	21.8
2	10.2	10.0 - 10.4	10	70	78.2

Chromatograms:





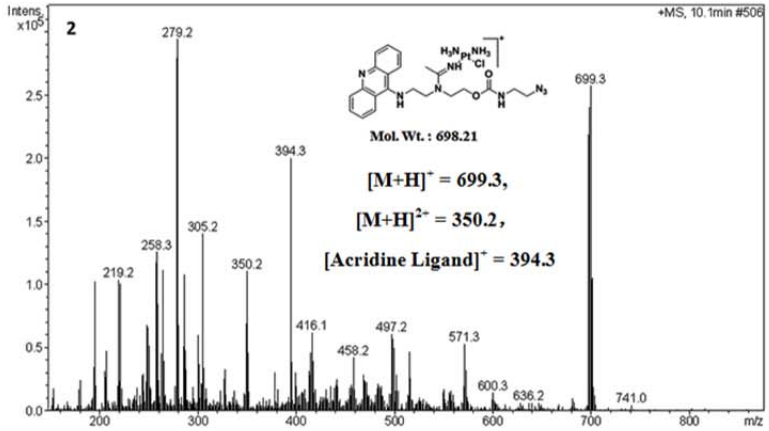
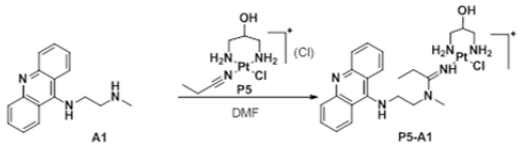


Figure S1.40. LC-ESMS analysis of reaction P4 + A10.

The Reaction Scheme Of P5-A1



The LC-MS Analysis Of P5-A1

Compound Chromatogram Report - MS

Analysis Name: LIB05121.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:25:34 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 4:50:20 PM
Sample Name: 5-1-2
Analysis Info:

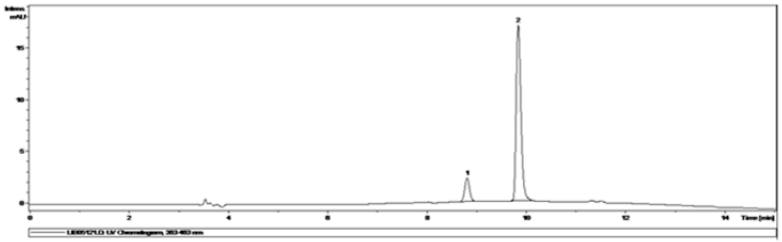
Acquisition Parameter:

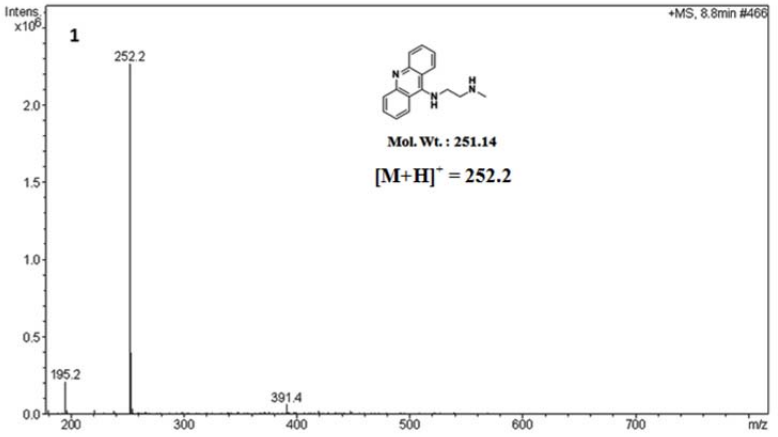
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	8.8	8.7 - 9.0	2	15	11.6
2	9.8	9.7 - 10.1	17	111	88.4

Chromatograms:





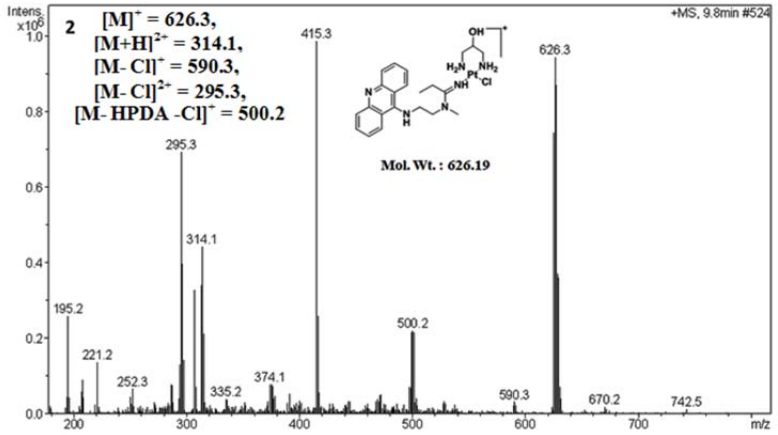
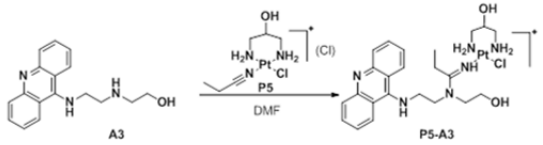


Figure S1.41. LC-ESMS analysis of reaction P5 + A1.

Figure S1.42. LC-ESMS analysis of reaction P5 + A2.

The Reaction Scheme Of P5-A3



The LC-MS Analysis Of P5-A3

Compound Chromatogram Report - MS

Analysis Name:	LIB-1314.D	**Instrument:**	LC-MSD-Trap-SL	**Print Date:**	06/08/2012 06:28:21 PM
Method:	SONG-L~1.M	**Operator:**	Administrator	**Acq. Date:**	5/12/2012 2:06:57 PM
Sample Name:	5-3				
Analysis Info:					

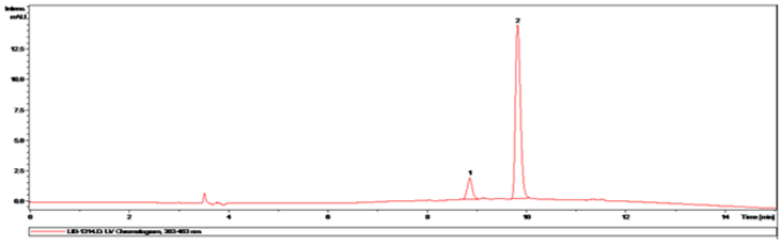
Acquisition Parameter:

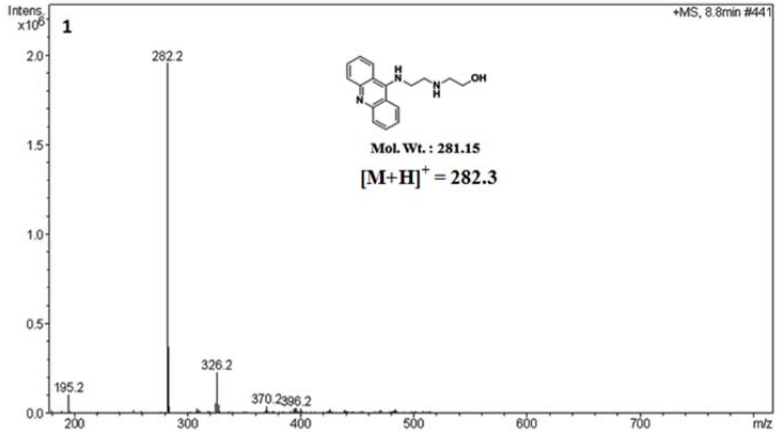
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	8.9	8.7 - 9.0	2	12	10.6
2	9.8	9.7 - 10.1	14	98	89.4

Chromatograms:





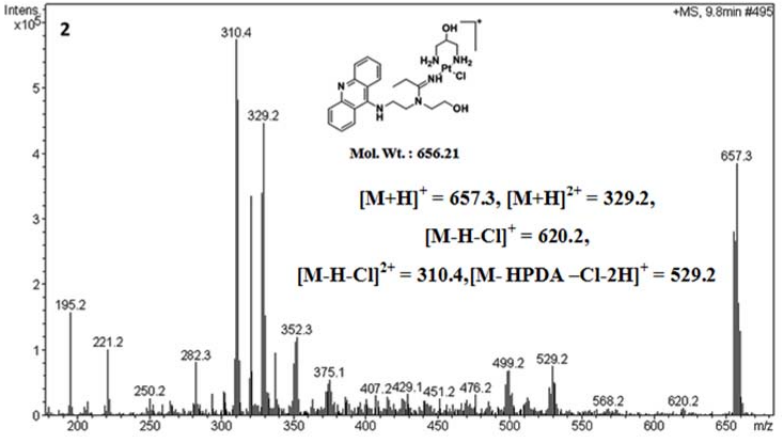
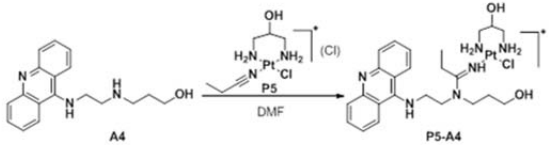


Figure S1.43. LC-ESMS analysis of reaction P5 + A3.

The Reaction Scheme Of P5-A4



The LC-MS Analysis Of P5-A4

Compound Chromatogram Report - MS

Analysis Name: LIB-1413.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:30:43 PM
Method: SONG-L~1.m **Operator:** Administrator **Acq. Date:** 5/12/2012 3:58:43 PM
Sample Name: 5-4
Analysis Info:

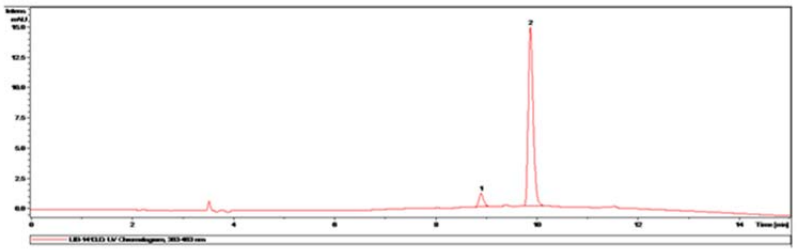
Acquisition Parameter:

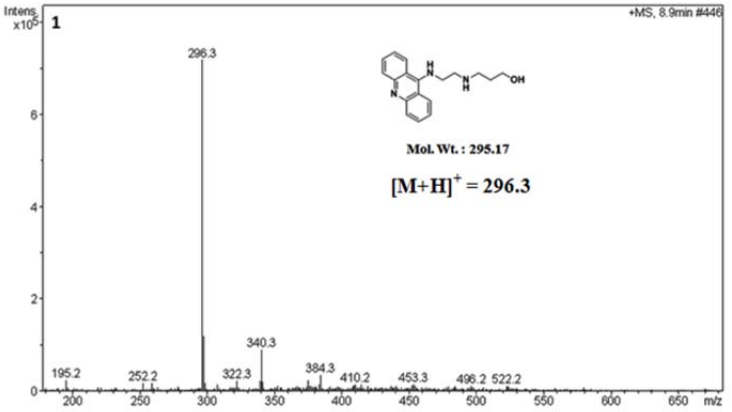
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	8.9	8.8 - 9.0	1	7	6.4
2	9.9	9.7 - 10.1	15	98	93.6

Chromatograms:





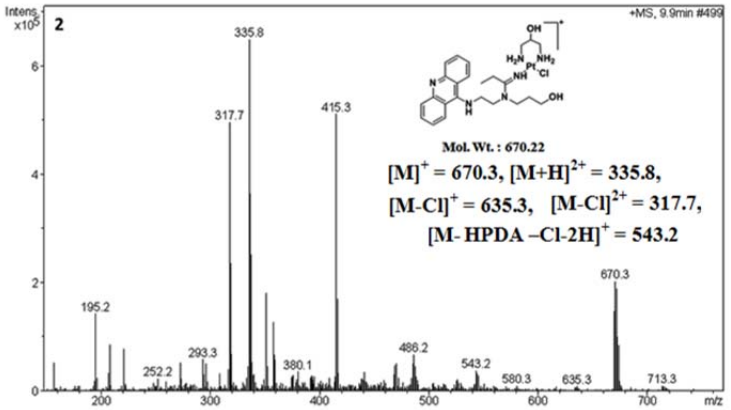
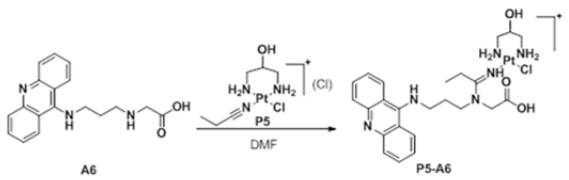


Figure S1.44. LC-ESMS analysis of reaction P5 + A4.

Figure S1.45. LC-ESMS analysis of reaction P5 + A5.

The Reaction Scheme Of P5-A6



The LC-MS Analysis Of P5-A6

Compound Chromatogram Report - MS

Analysis Name: LIB-6014.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:35:24 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/12/2012 12:40:14 AM
Sample Name: 5-6
Analysis Info:

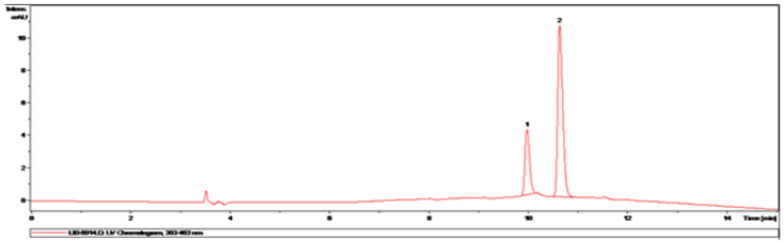
Acquisition Parameter:

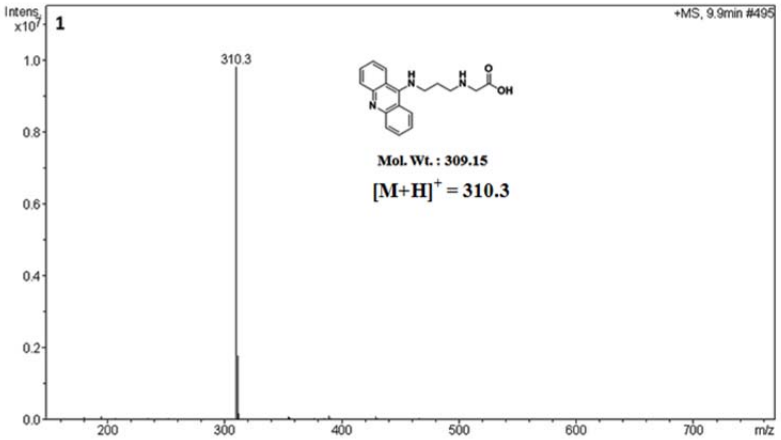
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	10.0	9.8 - 10.1	4	25	25.4
2	10.6	10.5 - 10.9	10	73	74.6

Chromatograms:





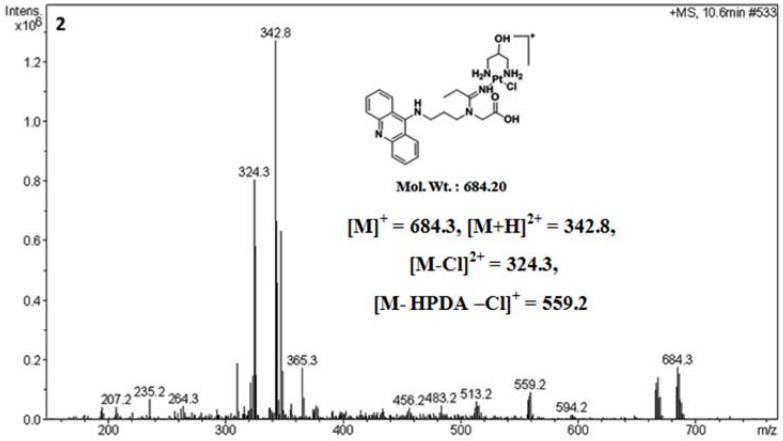
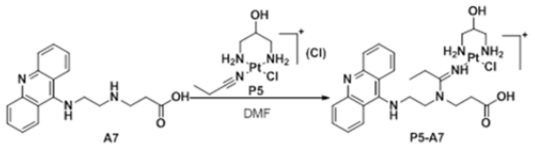


Figure S1.46. LC-ESMS analysis of reaction P5 + A6.

The Reaction Scheme Of P5-A7



The LC-MS Analysis Of P5-A7

Compound Chromatogram Report - MS

Analysis Name:	LIB-7011.D	**Instrument:**	LC-MSD-Trap-SL	**Print Date:**	06/08/2012 06:36:29 PM
Method:	SONG-L~1.M	**Operator:**	Administrator	**Acq. Date:**	5/12/2012 11:49:33 AM
Sample Name:	5-7				
Analysis Info:					

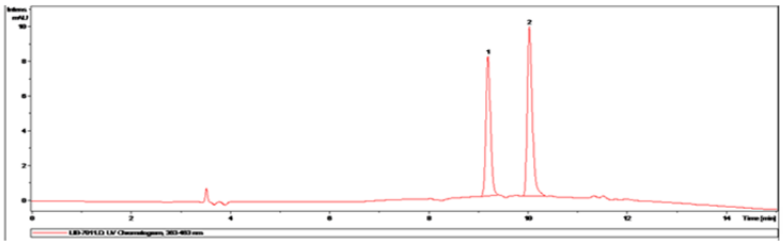
Acquisition Parameter:

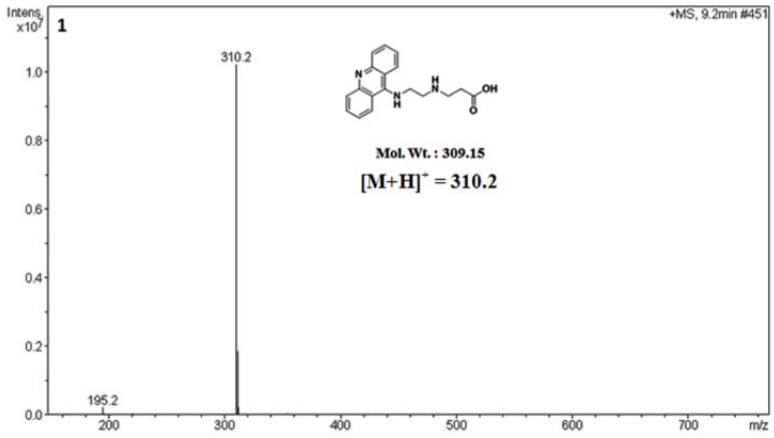
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.2	9.0 - 9.4	8	51	43.0
2	10.0	9.9 - 10.3	10	68	57.0

Chromatograms:





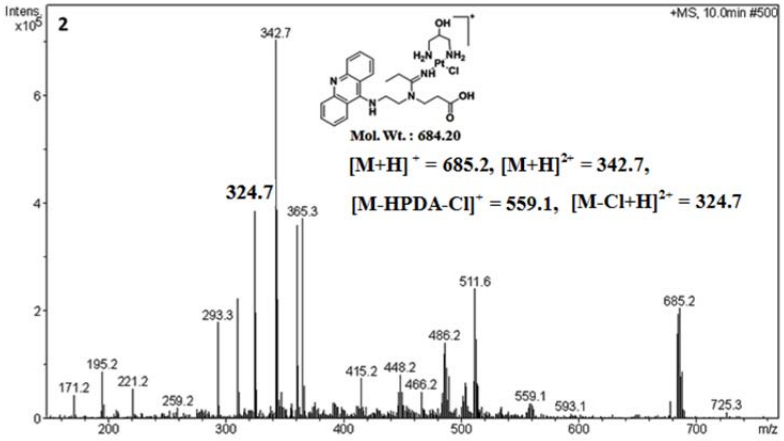
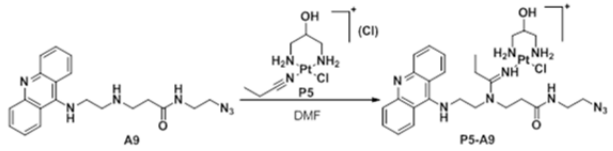


Figure S1.47. LC-ESMS analysis of reaction P5 + A7.

Figure S1.48. LC-ESMS analysis of reaction P5 + A8.

The Reaction Scheme Of P5-A9



The LC-MS Analysis Of P5-A9

Compound Chromatogram Report - MS

Analysis Name: LIB91023.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:40:31 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/13/2012 2:14:57 PM
Sample Name: 5-9
Analysis Info:

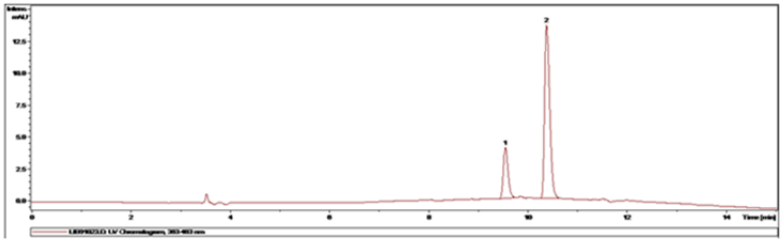
Acquisition Parameter:

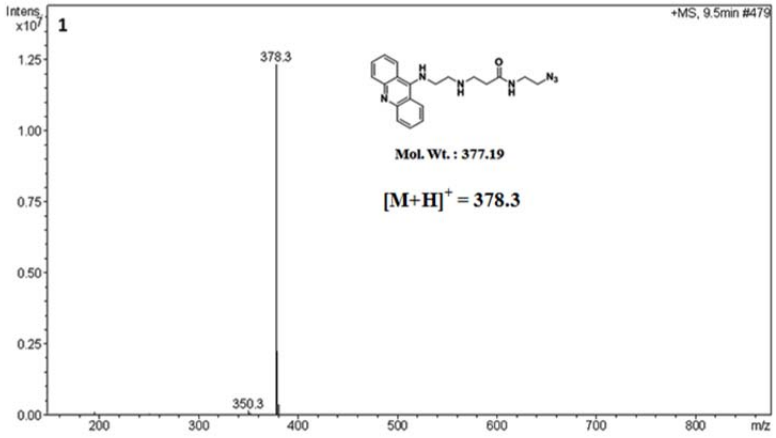
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.5	9.4 - 9.7	4	26	21.2
2	10.4	10.2 - 10.6	13	96	78.8

Chromatograms:





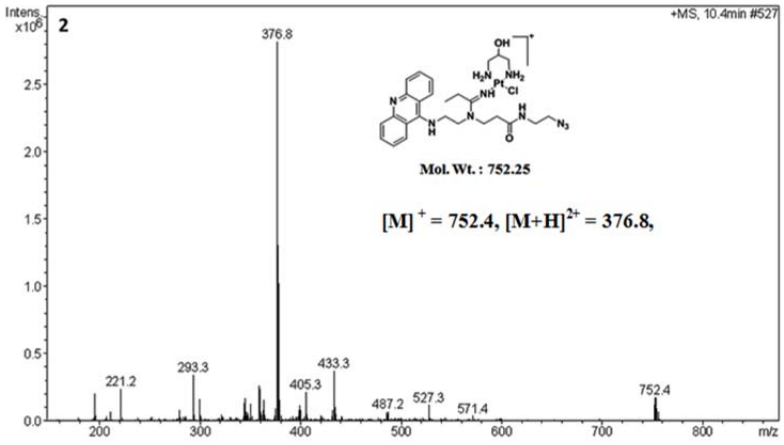
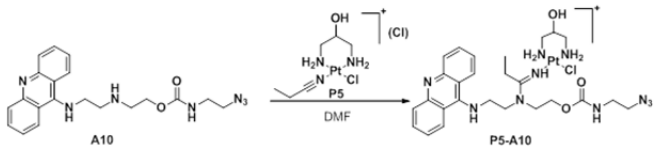


Figure S1.49. LC-ESMS analysis of reaction P5 + A9.

The Reaction Scheme Of P5-A10



The LC-MS Analysis Of P5-A10

Compound Chromatogram Report - MS

Analysis Name: LIB91029.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:42:21 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/13/2012 4:27:30 PM
Sample Name: 5-10
Analysis Info:

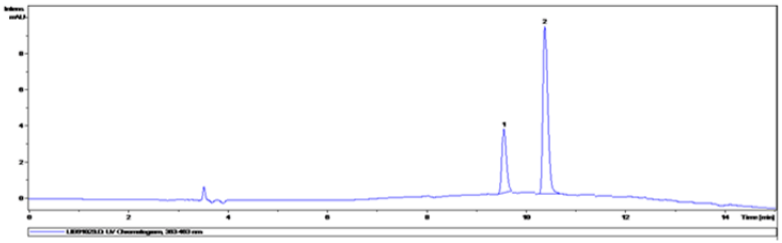
Acquisition Parameter:

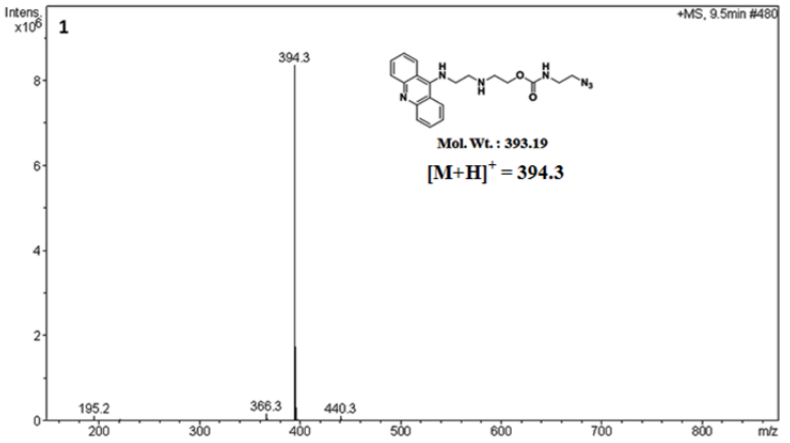
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.5	9.4 - 9.7	3	22	25.7
2	10.4	10.2 - 10.7	9	63	74.3

Chromatograms:





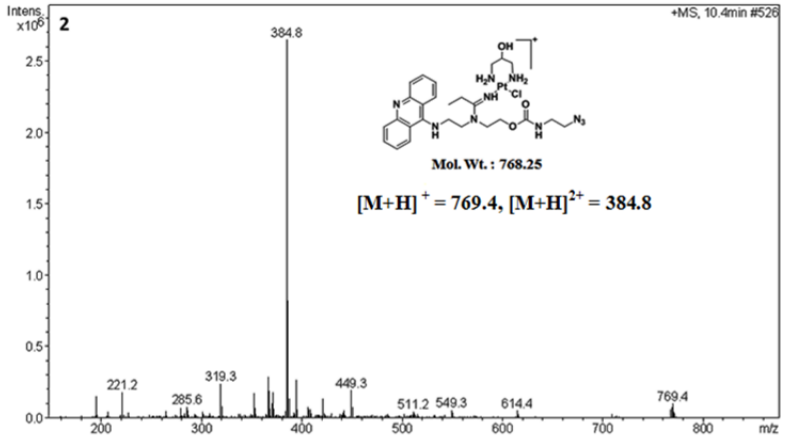
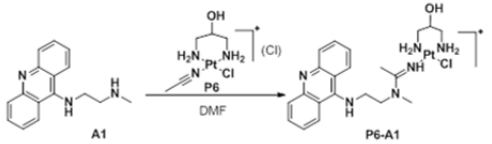


Figure S1.50. LC-ESMS analysis of reaction P5 + A10.

The Reaction Scheme Of P6-A1



The LC-MS Analysis Of P6-A1

Compound Chromatogram Report - MS

Analysis Name:	LIB05122.D	**Instrument:**	LC-MSD-Trap-SL	**Print Date:**	06/08/2012 06:43:50 PM
Method:	SONG-L~1.M	**Operator:**	Administrator	**Acq. Date:**	5/11/2012 5:13:49 PM
Sample Name:	6-1-2				
Analysis Info:					

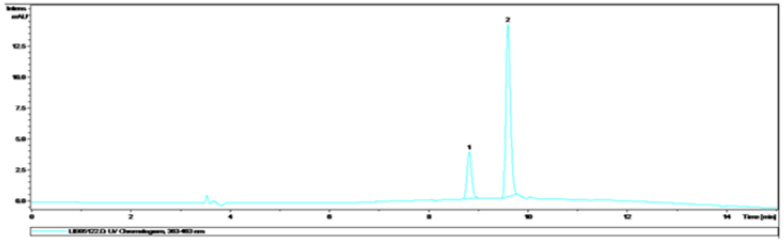
Acquisition Parameter:

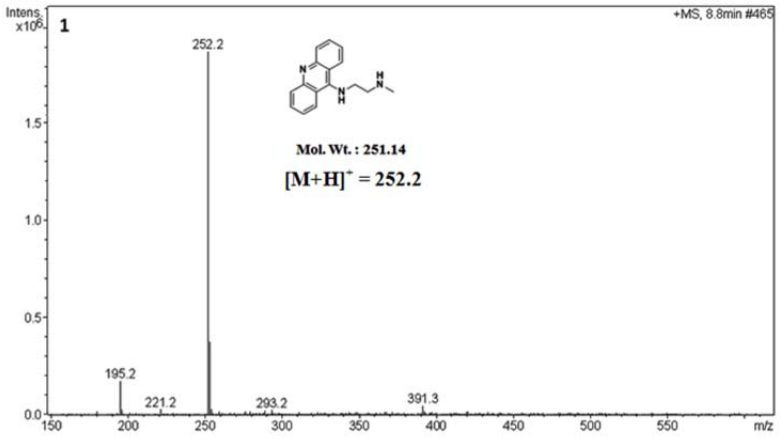
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	8.8	8.7 - 9.0	4	24	21.2
2	9.6	9.5 - 9.8	14	88	78.8

Chromatograms:





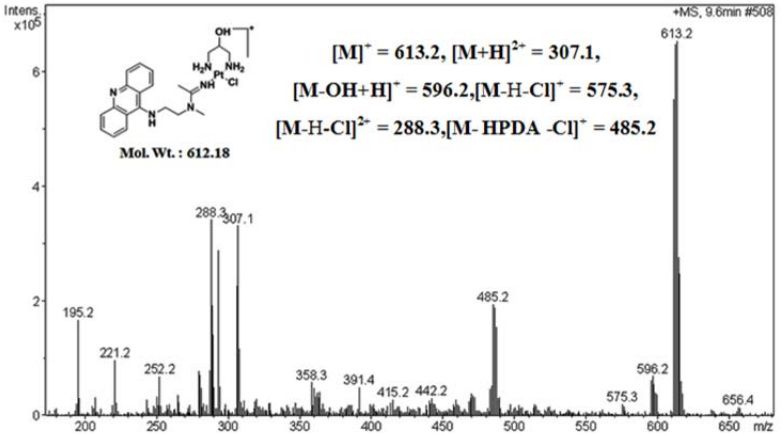
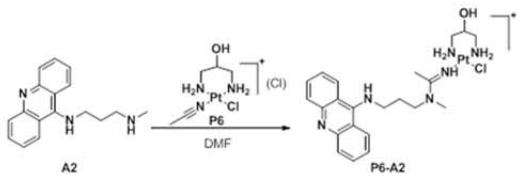


Figure S1.51. LC-ESMS analysis of reaction P6 + A1.

The Reaction Scheme Of P6-A2



The LC-MS Analysis Of P6-A2

Compound Chromatogram Report - MS

Analysis Name: LIB05125.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:45:34 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 6:24:23 PM
Sample Name: 6-2-2
Analysis Info:

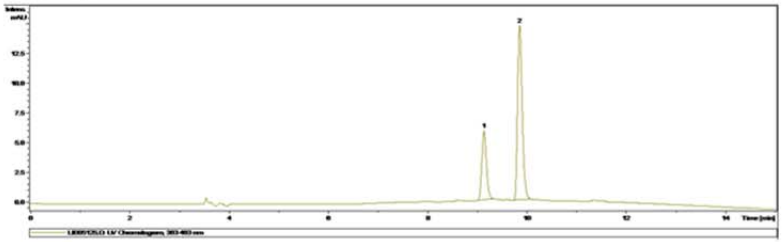
Acquisition Parameter:

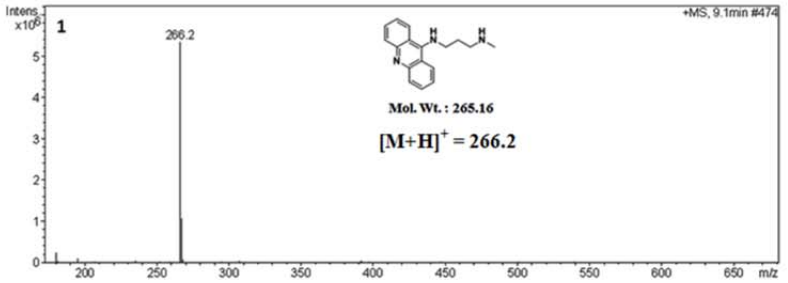
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.1	9.0 - 9.3	6	36	27.9
2	9.8	9.7 - 10.1	15	94	72.1

Chromatograms:





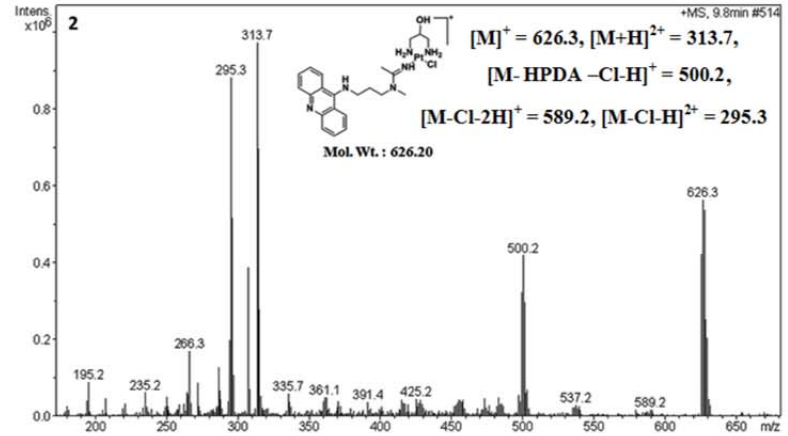
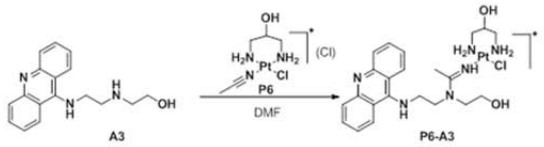


Figure S1.52. LC-ESMS analysis of reaction P6 + A2.

Figure S1.53. LC-ESMS analysis of reaction P6 + A3.

The Reaction Scheme Of P6-A4



The LC-MS Analysis Of P6-A4

Compound Chromatogram Report - MS

Analysis Name: 05121251.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:49:23 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 6:40:16 AM
Sample Name: 6-4
Analysis Info:

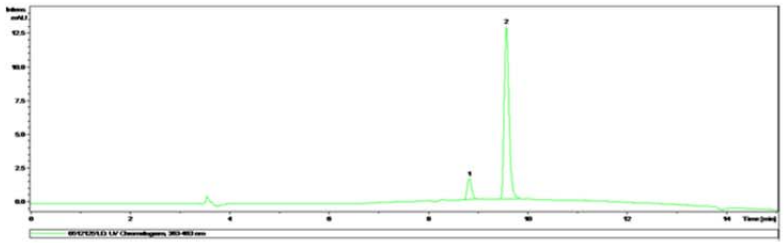
Acquisition Parameter:

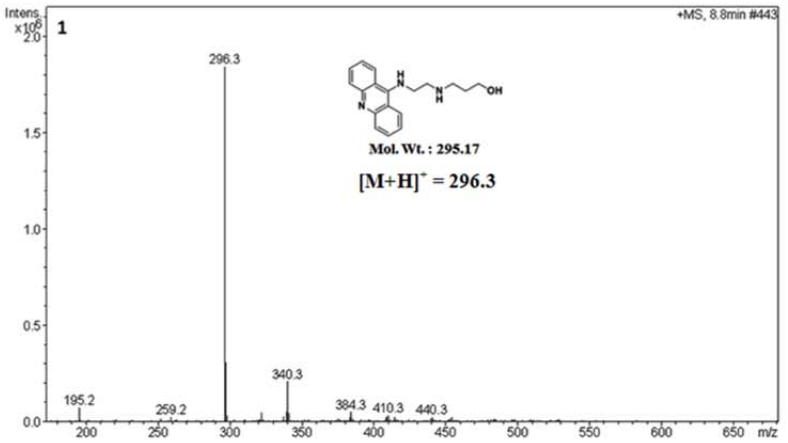
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	8.8	8.7 - 9.0	2	9	9.8
2	9.6	9.4 - 9.9	13	85	90.2

Chromatograms:





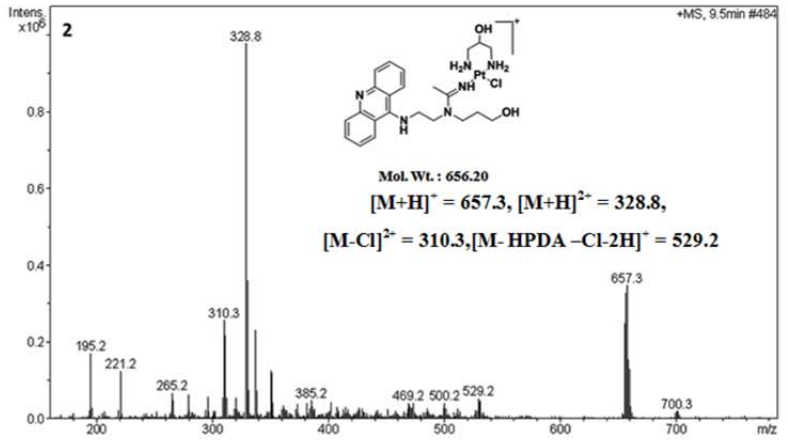
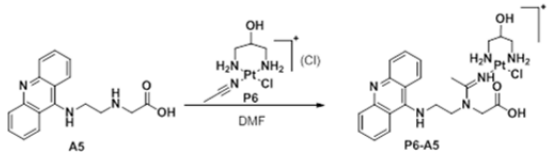


Figure S1.54. LC-ESMS analysis of reaction P6 + A4.

The Reaction Scheme Of P6-A5



The LC-MS Analysis Of P6-A5

Compound Chromatogram Report - MS

Analysis Name: LIB12015.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:52:12 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/11/2012 10:51:10 PM
Sample Name: 6-5-1
Analysis Info:

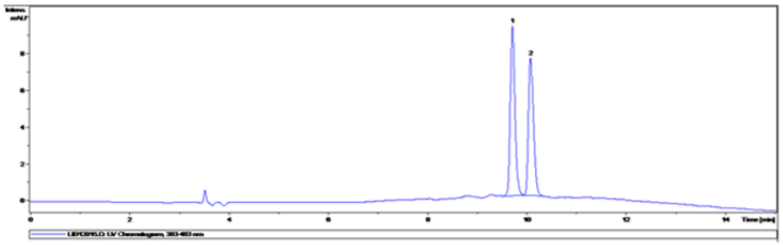
Acquisition Parameter:

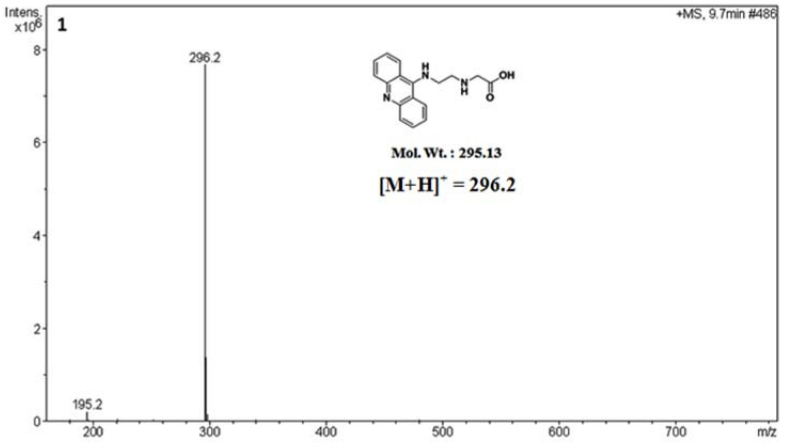
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.7	9.5 - 9.9	9	59	53.1
2	10.1	9.9 - 10.3	7	53	46.9

Chromatograms:





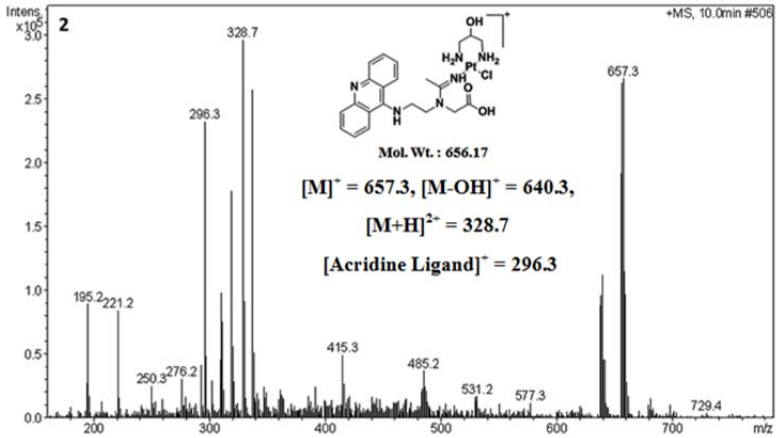
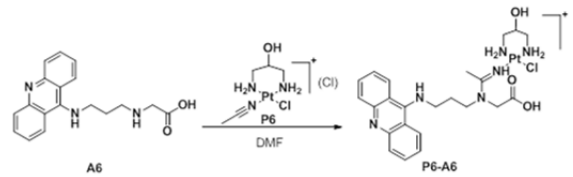


Figure S1.55. LC-ESMS analysis of reaction P6 + A5.

The Reaction Scheme Of P6-A6



The LC-MS Analysis Of P6-A6

Compound Chromatogram Report - MS

Analysis Name: LIB-6015.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:53:34 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/12/2012 1:02:13 AM
Sample Name: 6-6
Analysis Info:

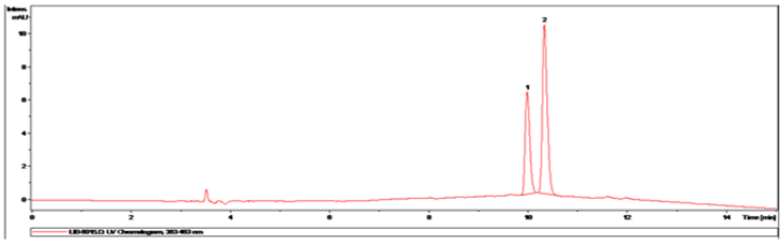
Acquisition Parameter:

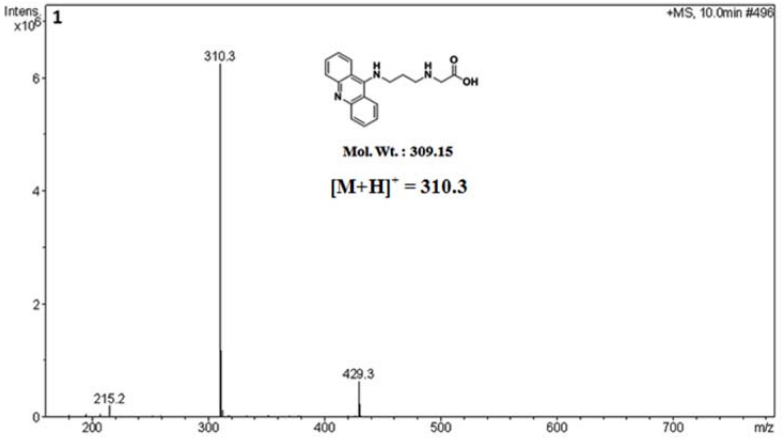
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	10.0	9.9 - 10.2	6	39	36.4
2	10.3	10.2 - 10.6	10	68	63.6

Chromatograms:





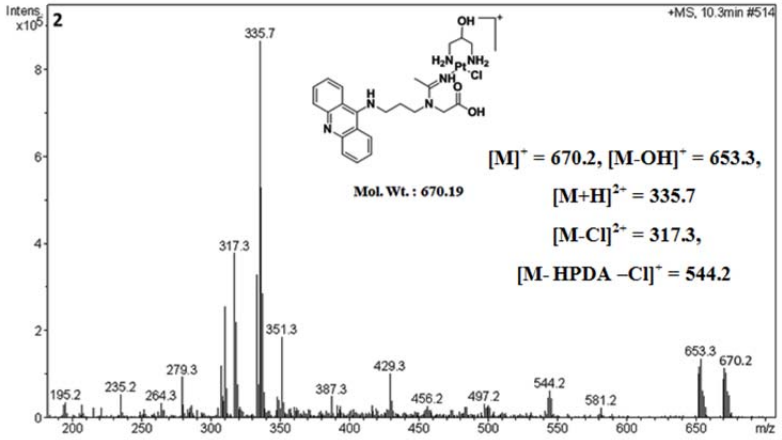
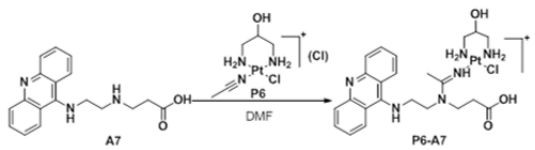


Figure S1.56. LC-ESMS analysis of reaction P6 + A6.

The Reaction Scheme Of P6-A7



The LC-MS Analysis Of P6-A7

Compound Chromatogram Report - MS

Analysis Name: LIB-7012.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/08/2012 06:57:22 PM
Method: SONG-L~1.M **Operator:** Administrator **Acq. Date:** 5/12/2012 12:11:37 PM
Sample Name: 6-7
Analysis Info:

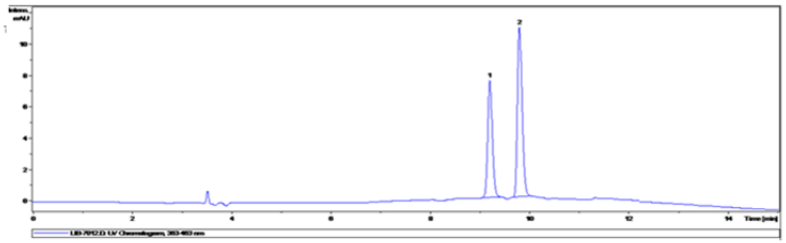
Acquisition Parameter:

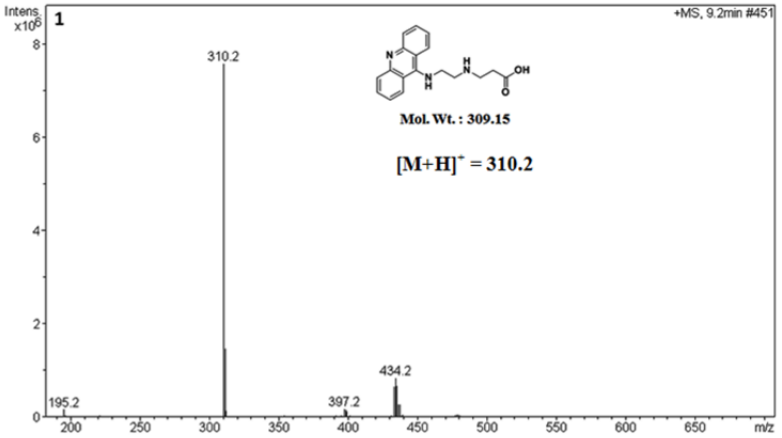
Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	9.2	9.0 - 9.4	7	48	40.2
2	9.8	9.7 - 10.0	11	71	59.8

Chromatograms:





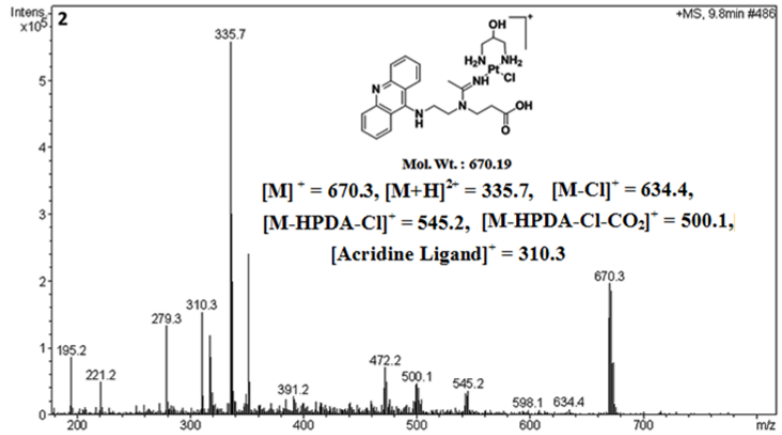


Figure S1.57. LC-ESMS analysis of reaction P6 + A7.

Figure S1.58. LC-ESMS analysis of reaction P6 + A8.

Figure S1.59. LC-ESMS analysis of reaction P6 + A9.

Figure S1.60. LC-ESMS analysis of reaction P6 + A10.

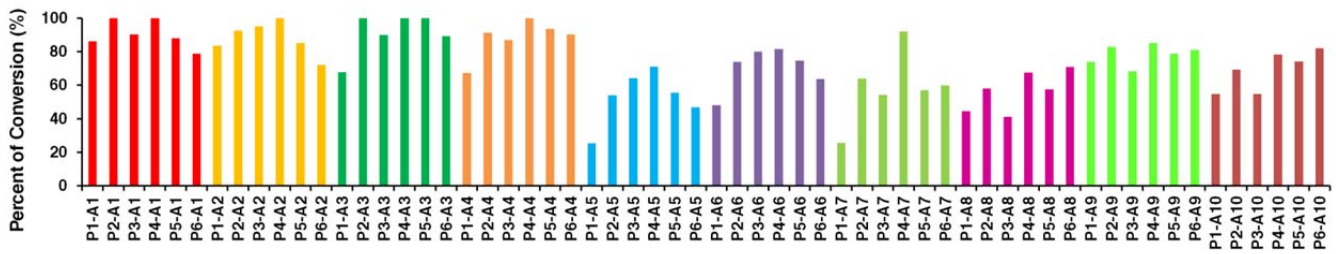


Figure S1.61. Percent conversion in 'click' reactions for platinum-acridines. Compounds are sorted and color-coded by common acridine moieties.

3. NMR spectra for purified compounds

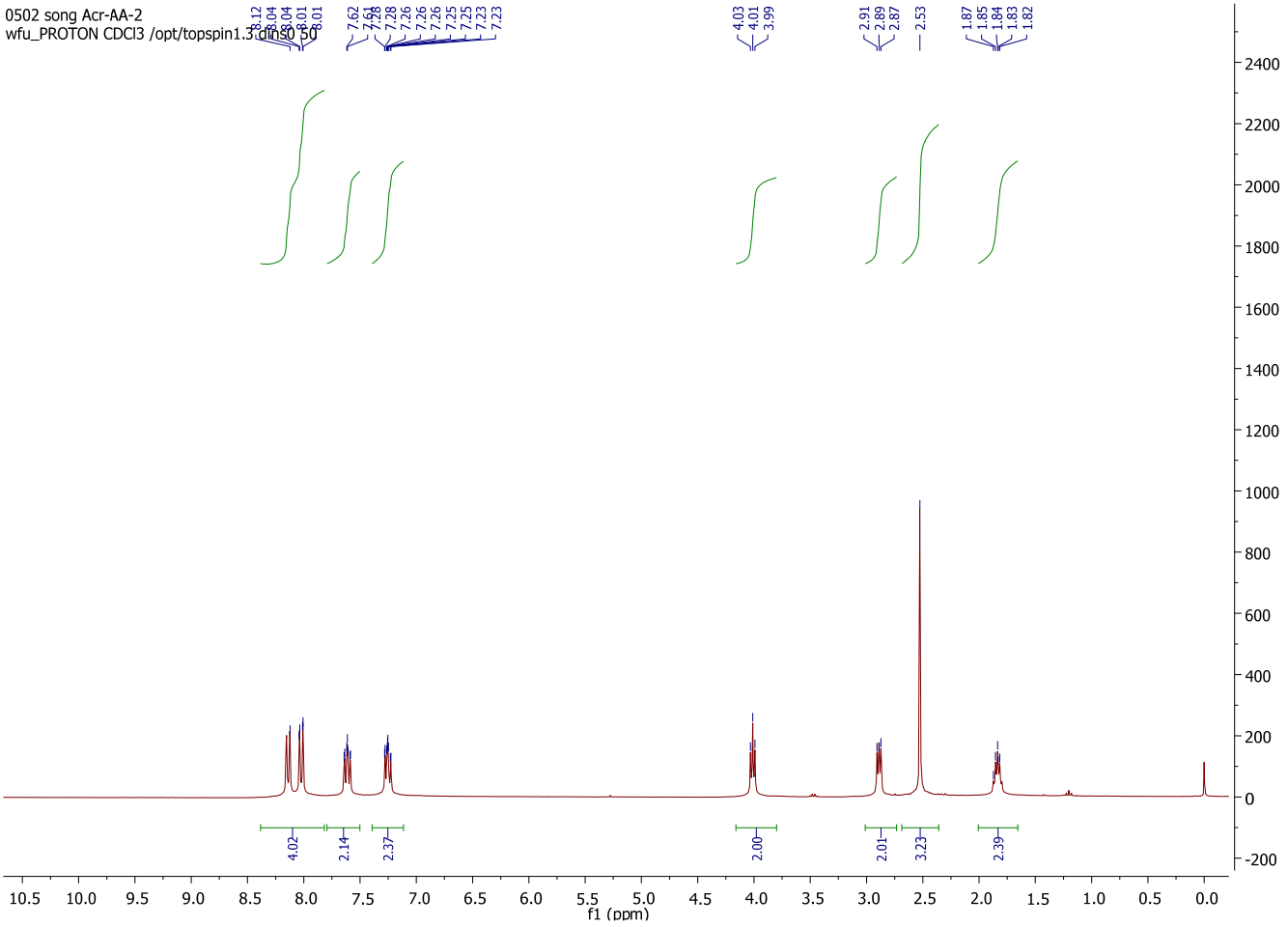


Figure S2.1. ^{1}H NMR spectrum of compound A2.

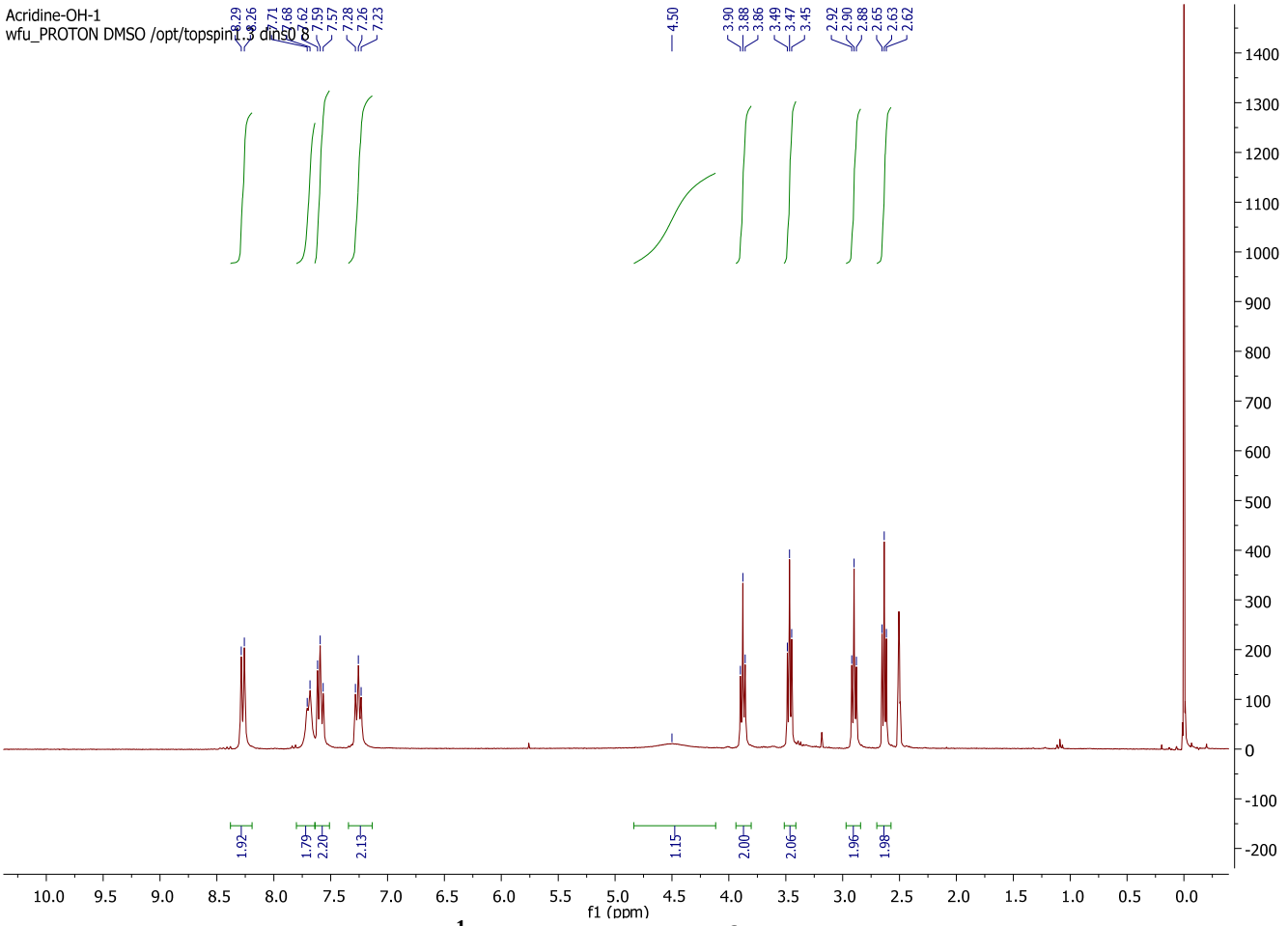


Figure S2.2. ^{1}H NMR spectrum of compound A3.

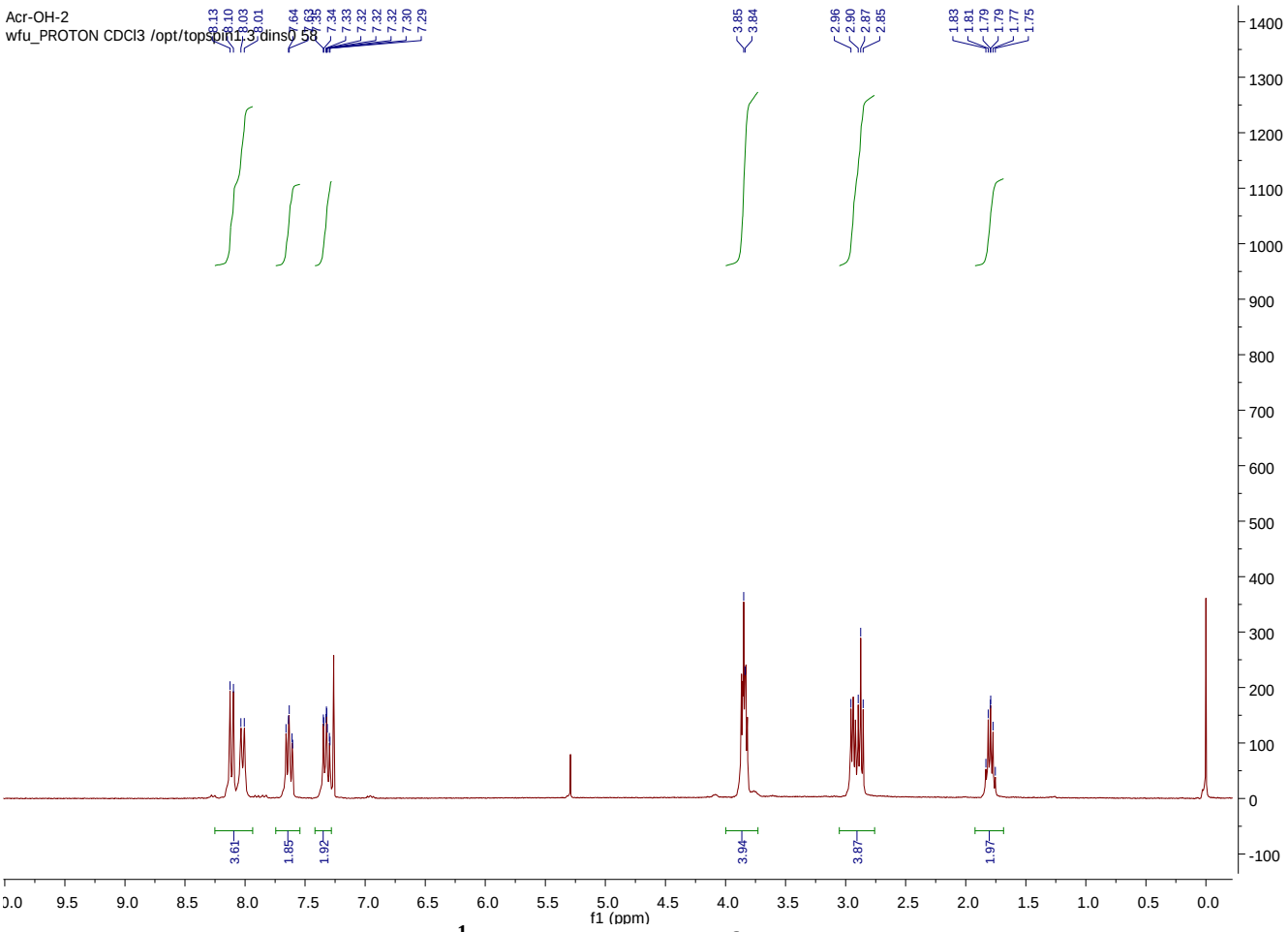


Figure S2.3. ^{1}H NMR spectrum of compound A4.

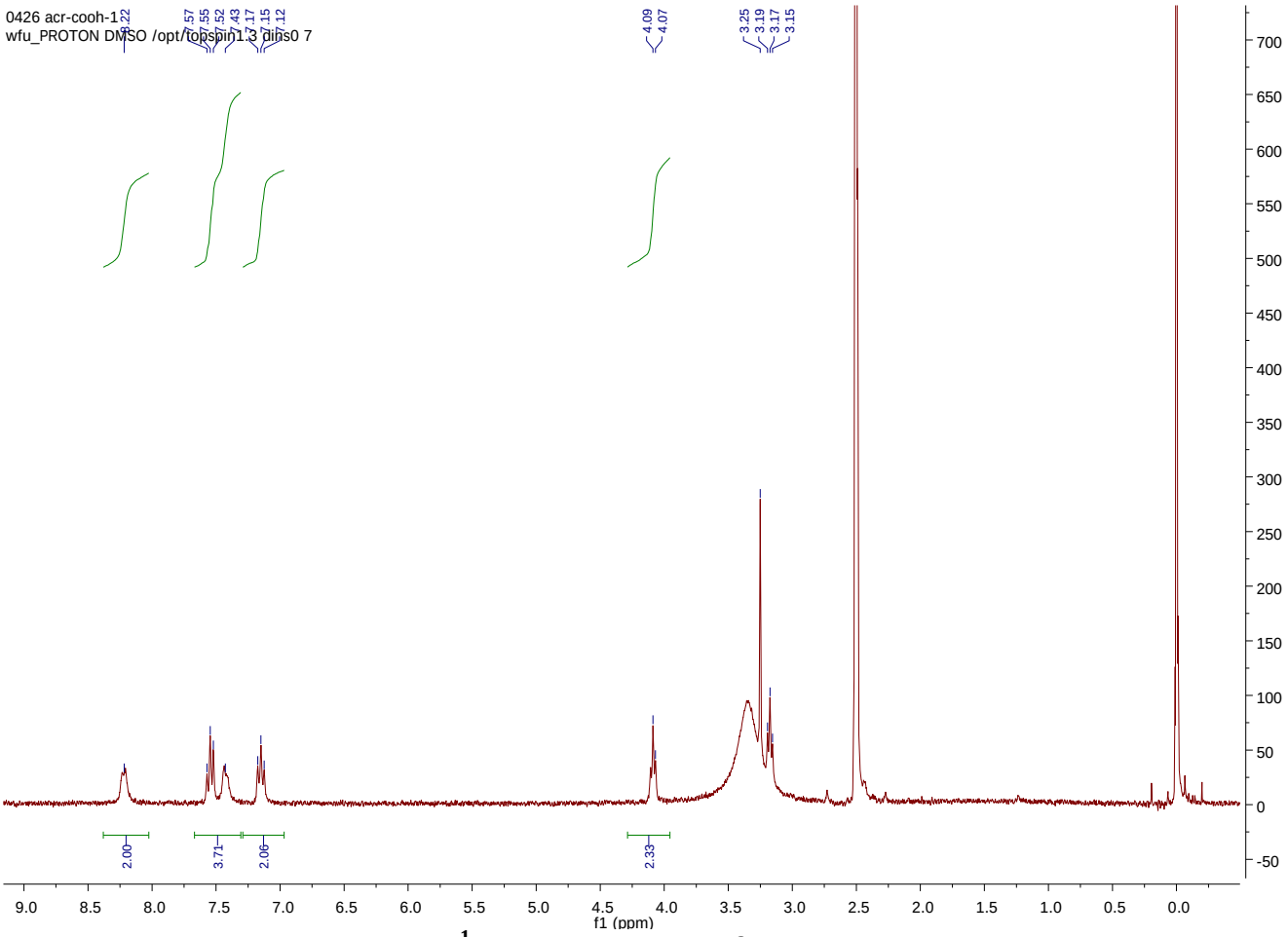


Figure S2.4. ^{1}H NMR spectrum of compound A5.

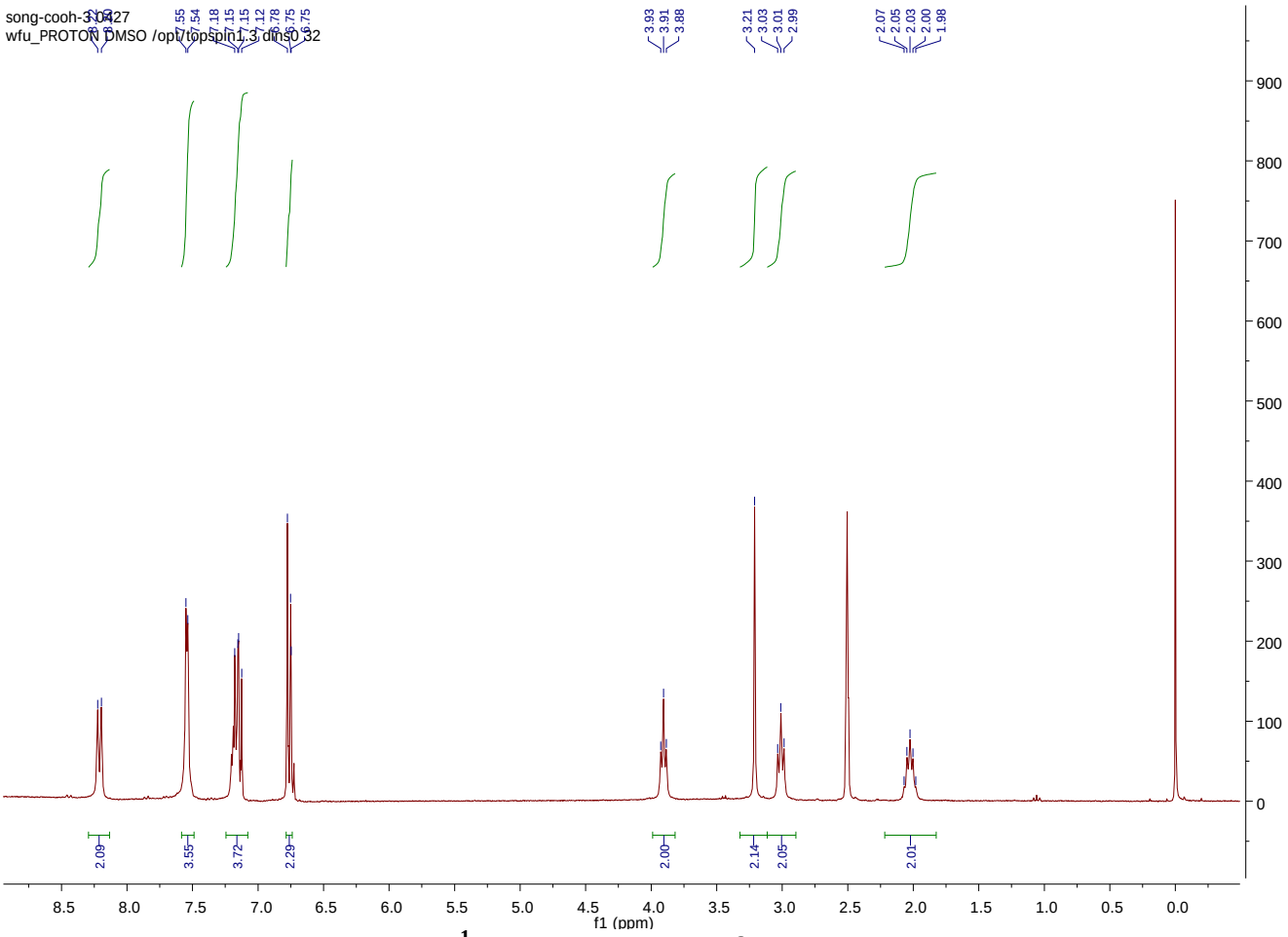


Figure S2.5. ^{1}H NMR spectrum of compound A6.

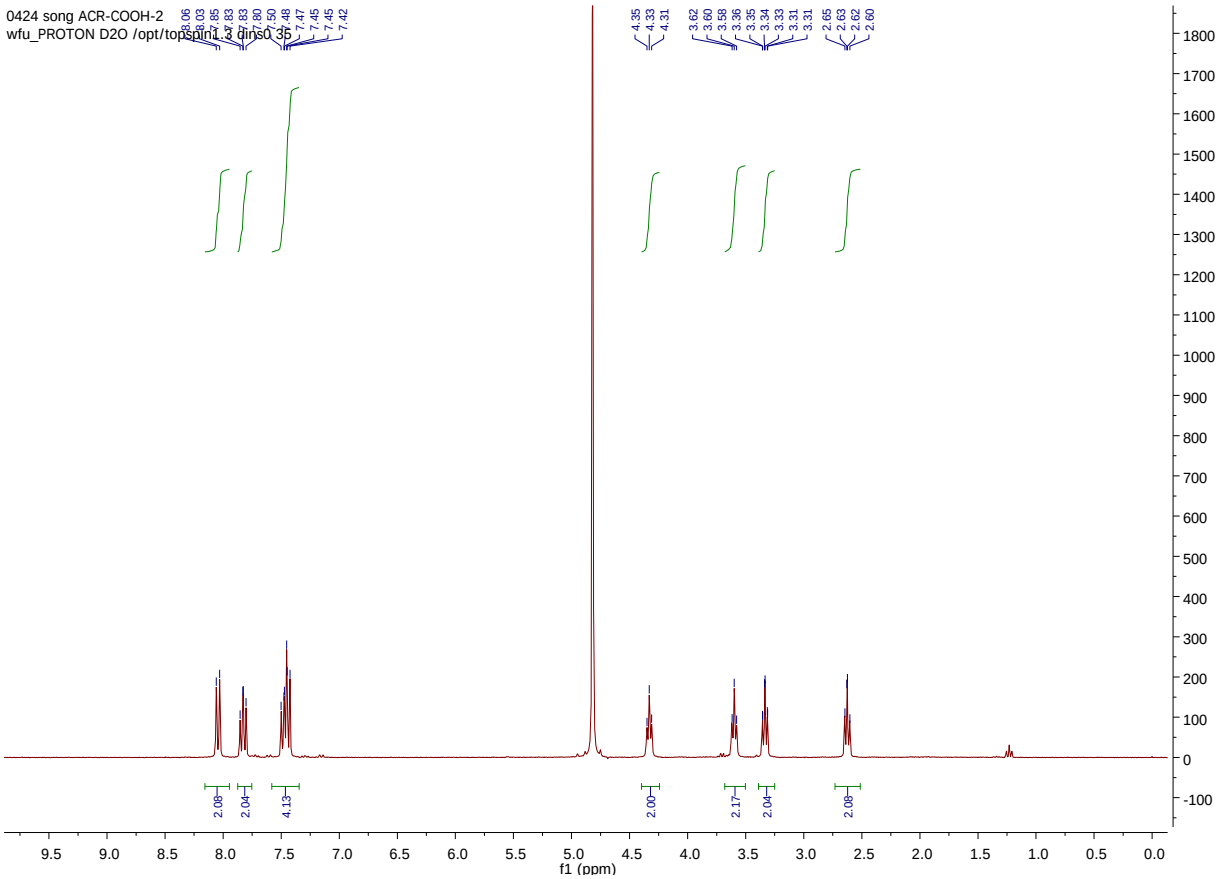


Figure S2.6. ^{1}H NMR spectrum of compound A7.

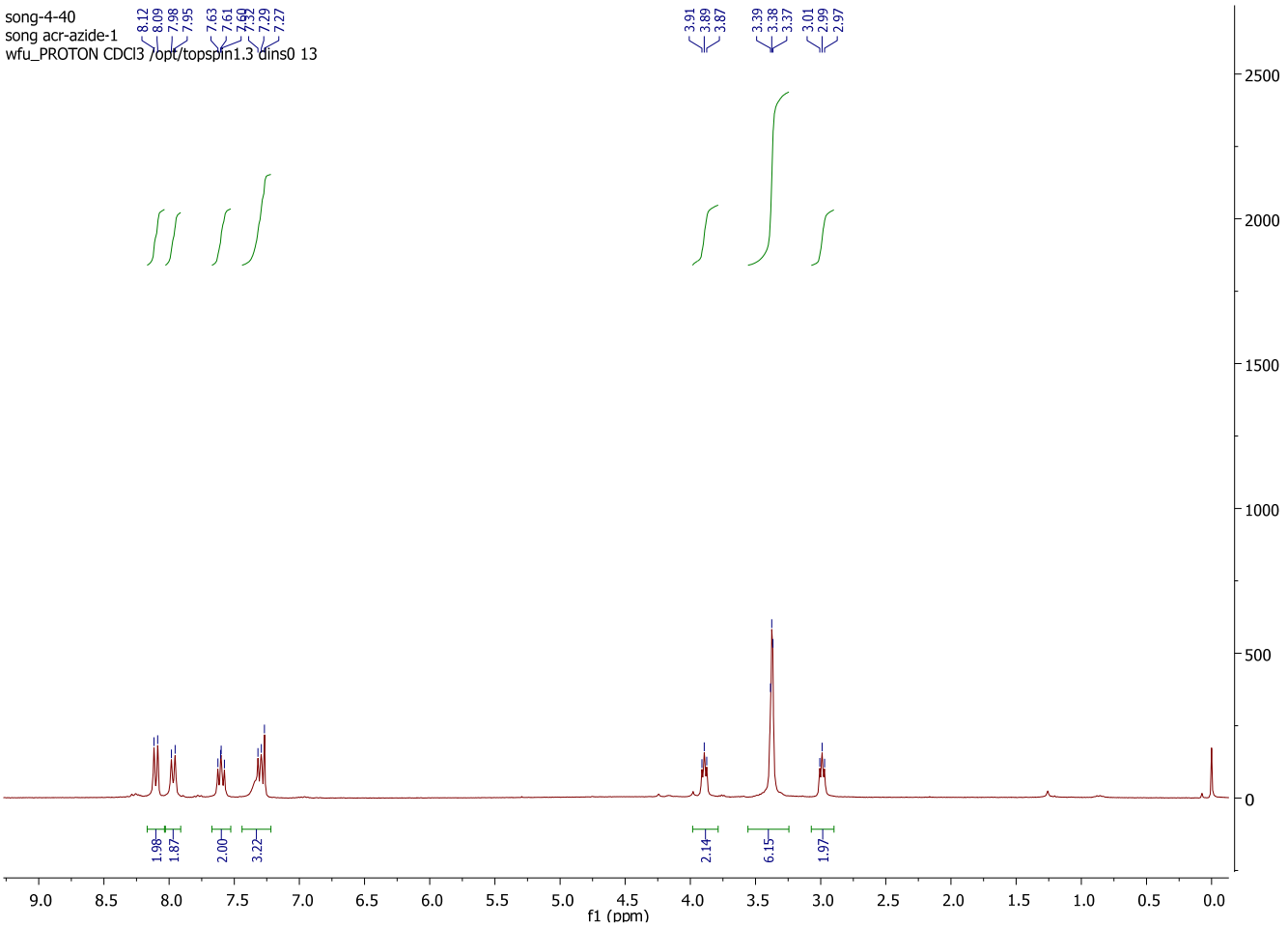


Figure S2.7. ^{1}H NMR spectrum of compound A8.

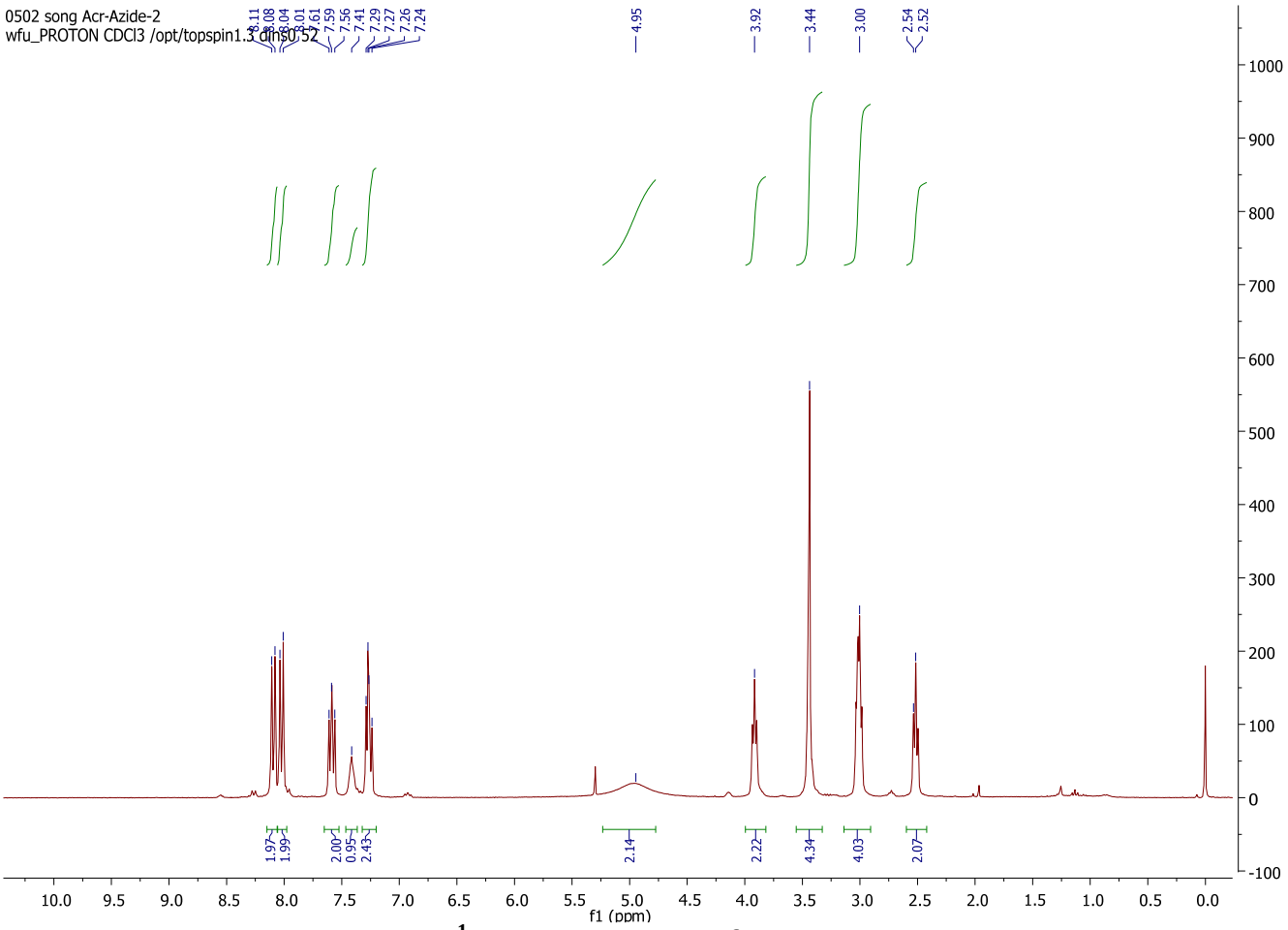


Figure S2.8. ^{1}H NMR spectrum of compound A9.

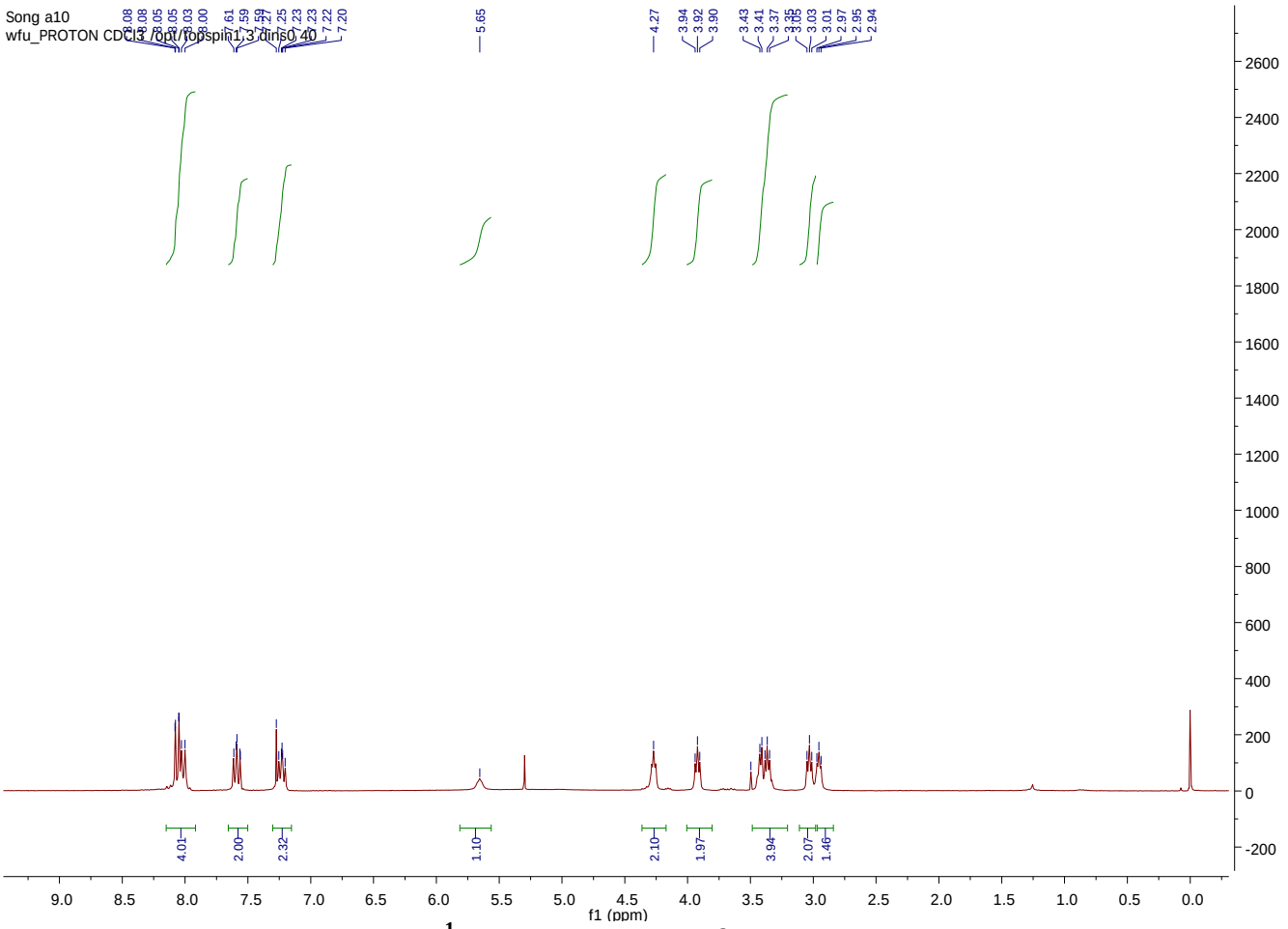


Figure S2.9. ^{1}H NMR spectrum of compound A10.

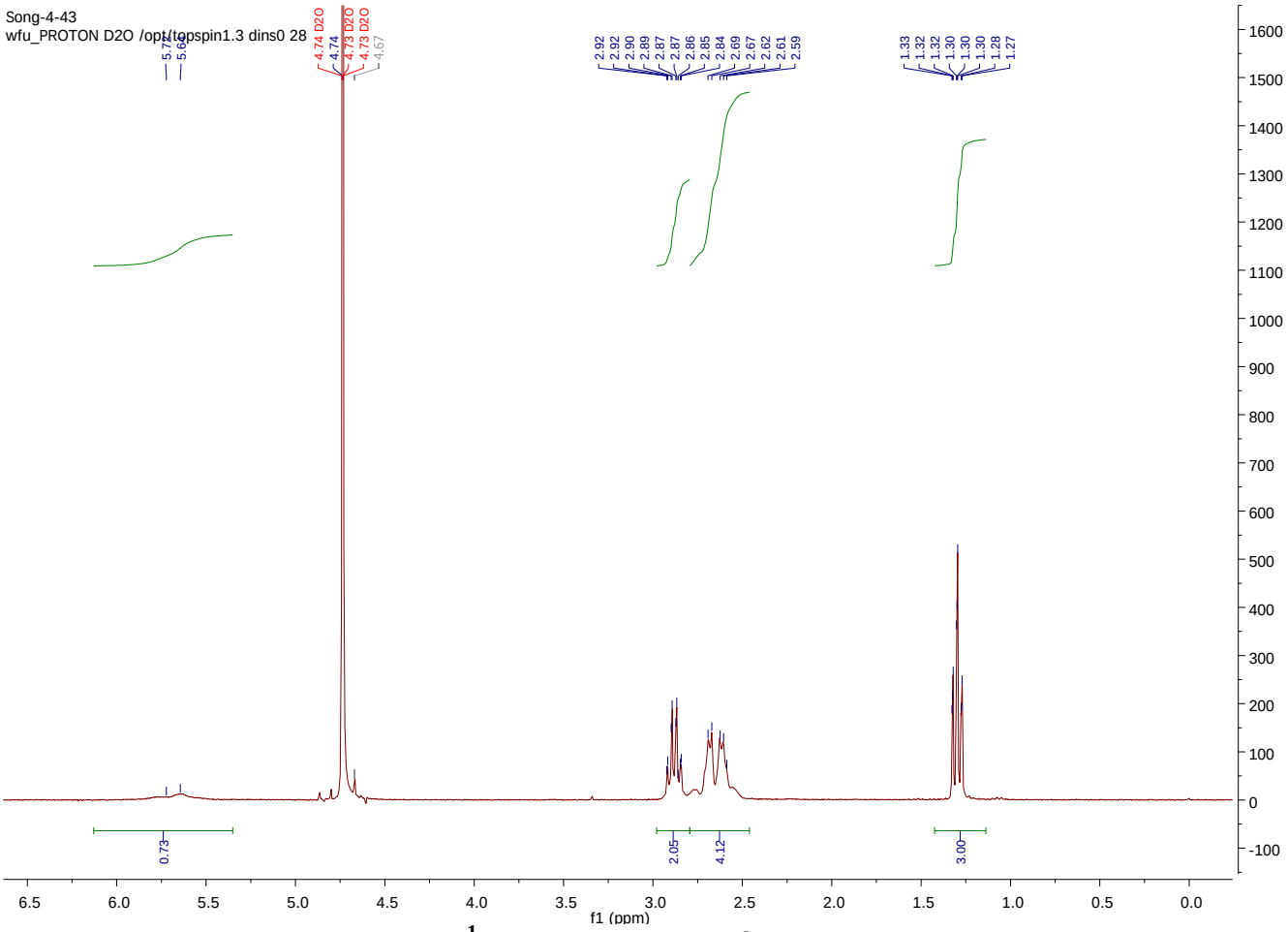


Figure S2.10. ^{1}H NMR spectrum of compound P1.

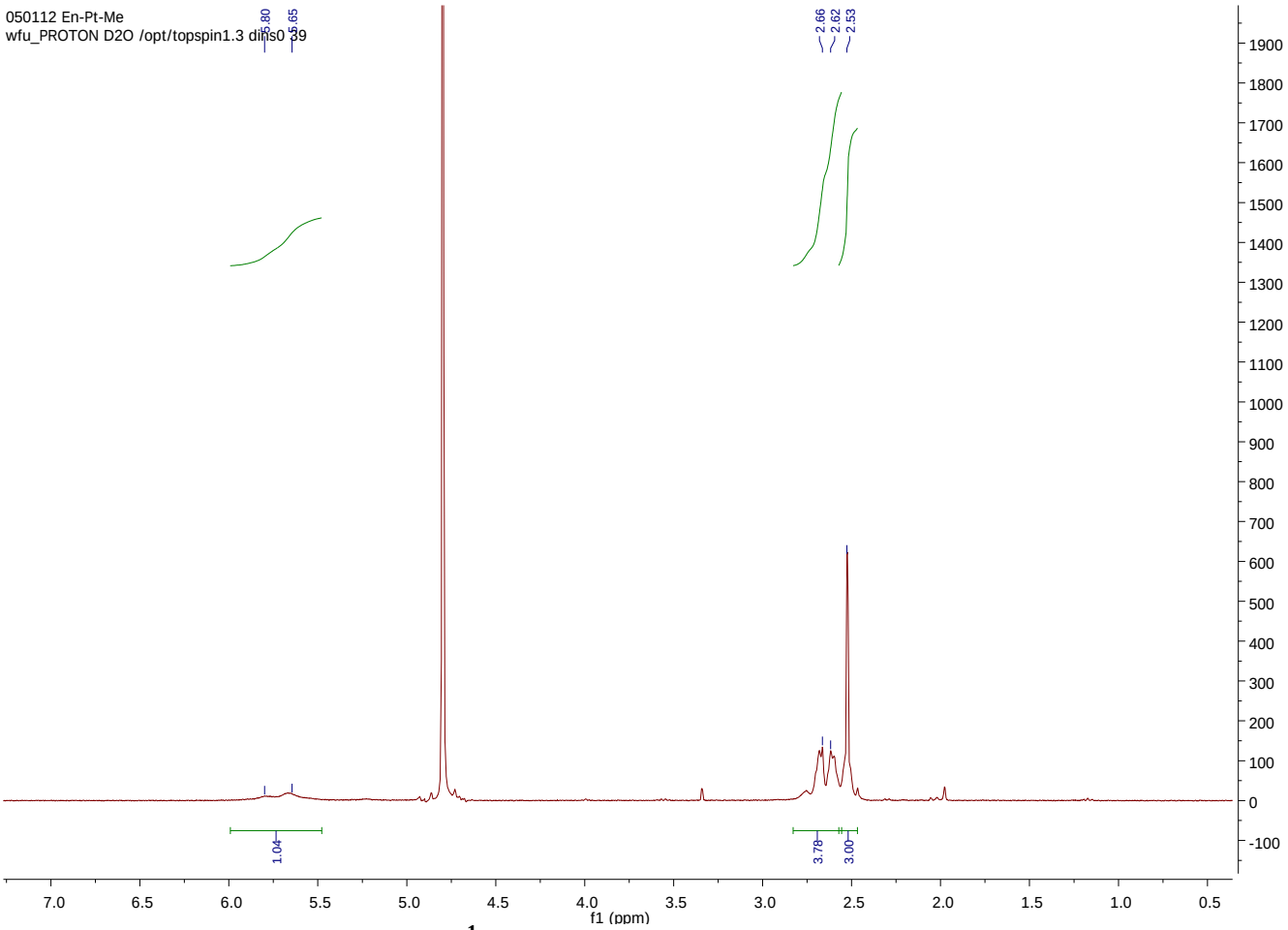


Figure S2.11. ^{1}H NMR spectrum of compound P2.

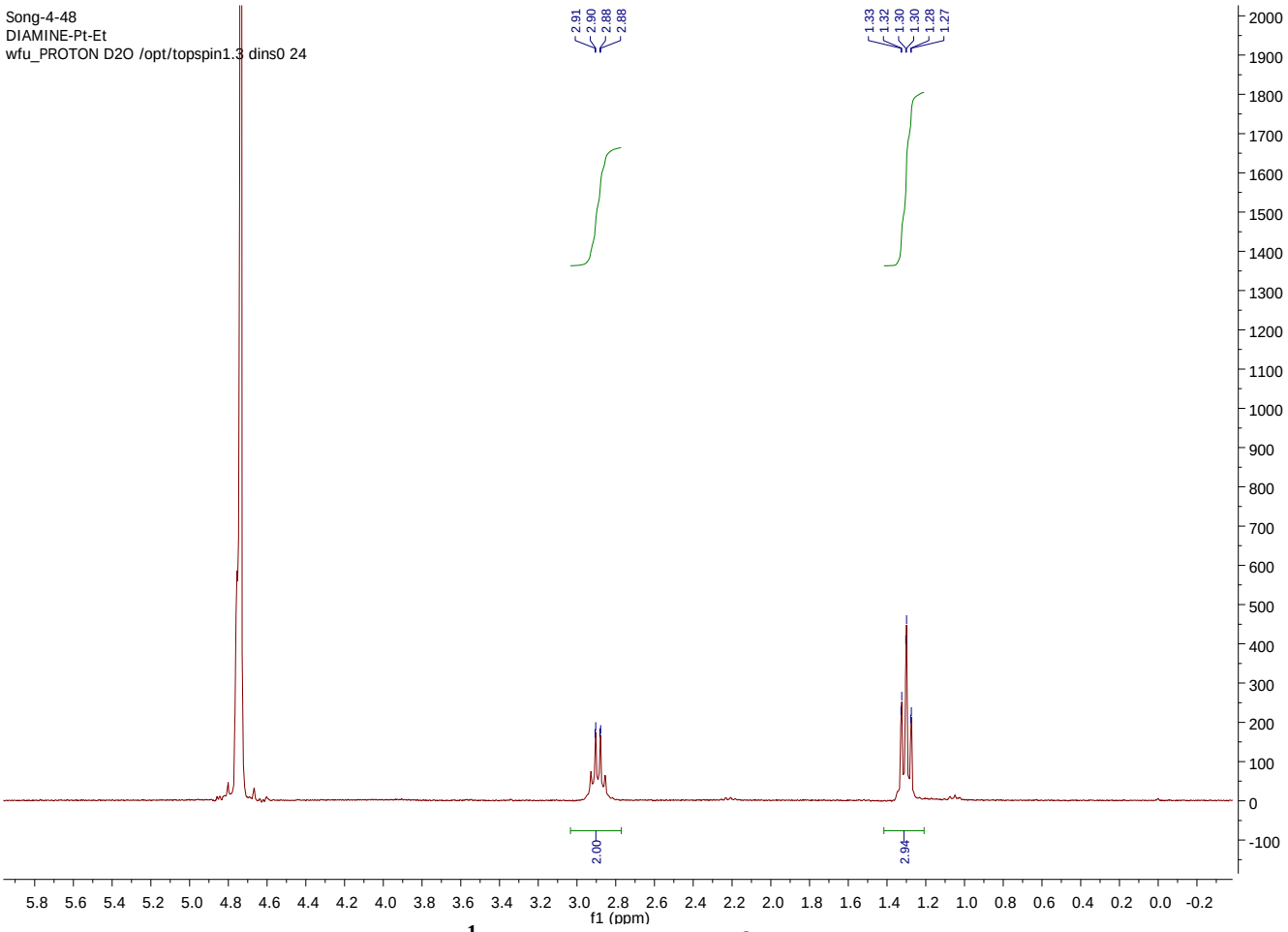


Figure S2.12. ^{1}H NMR spectrum of compound P3.

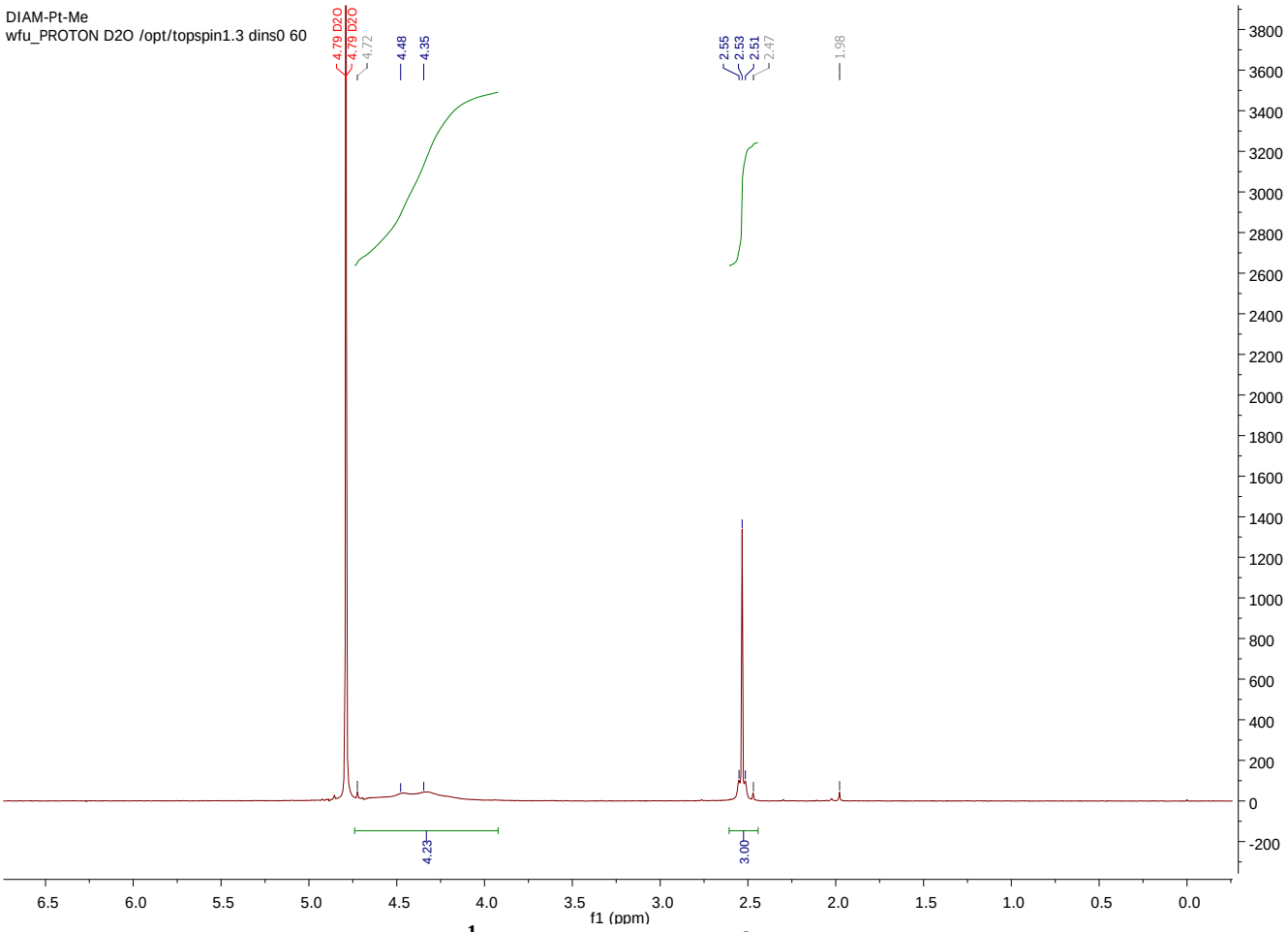


Figure S2.13. ^{1}H NMR spectrum of compound P4.

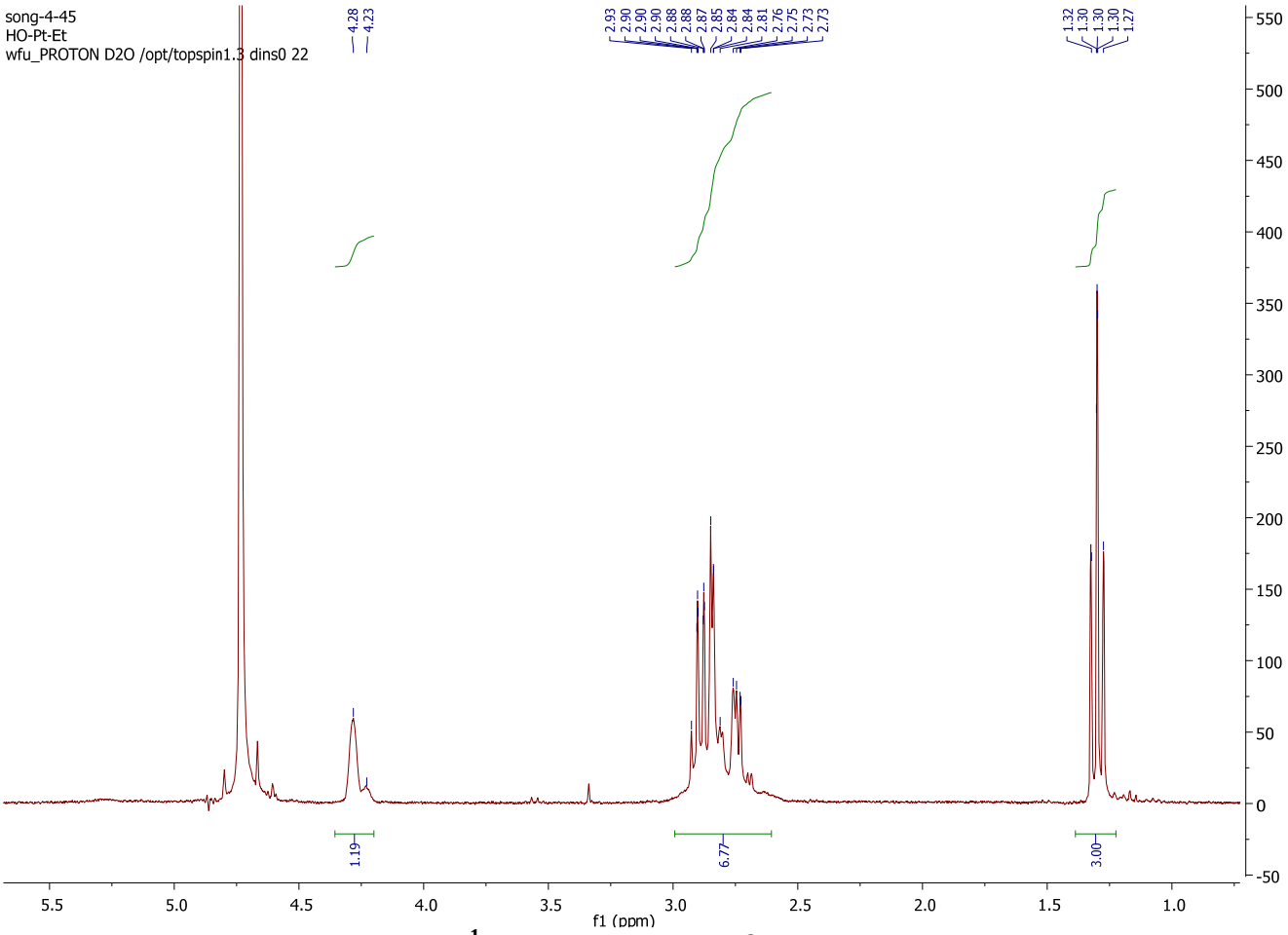


Figure S2.14. ^{1}H NMR spectrum of compound P5.

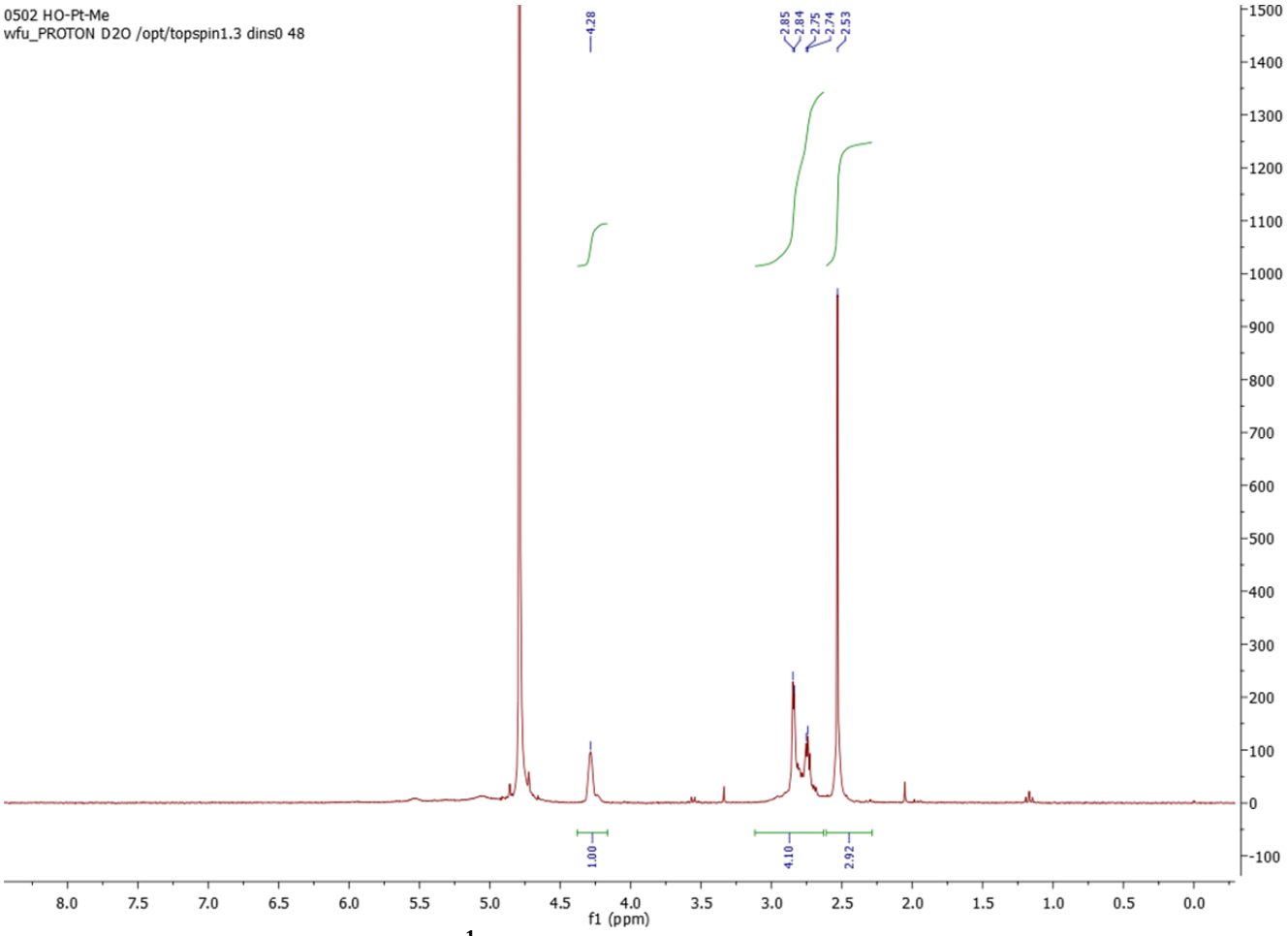


Figure S2.15. ^{1}H NMR spectrum of compound P6.

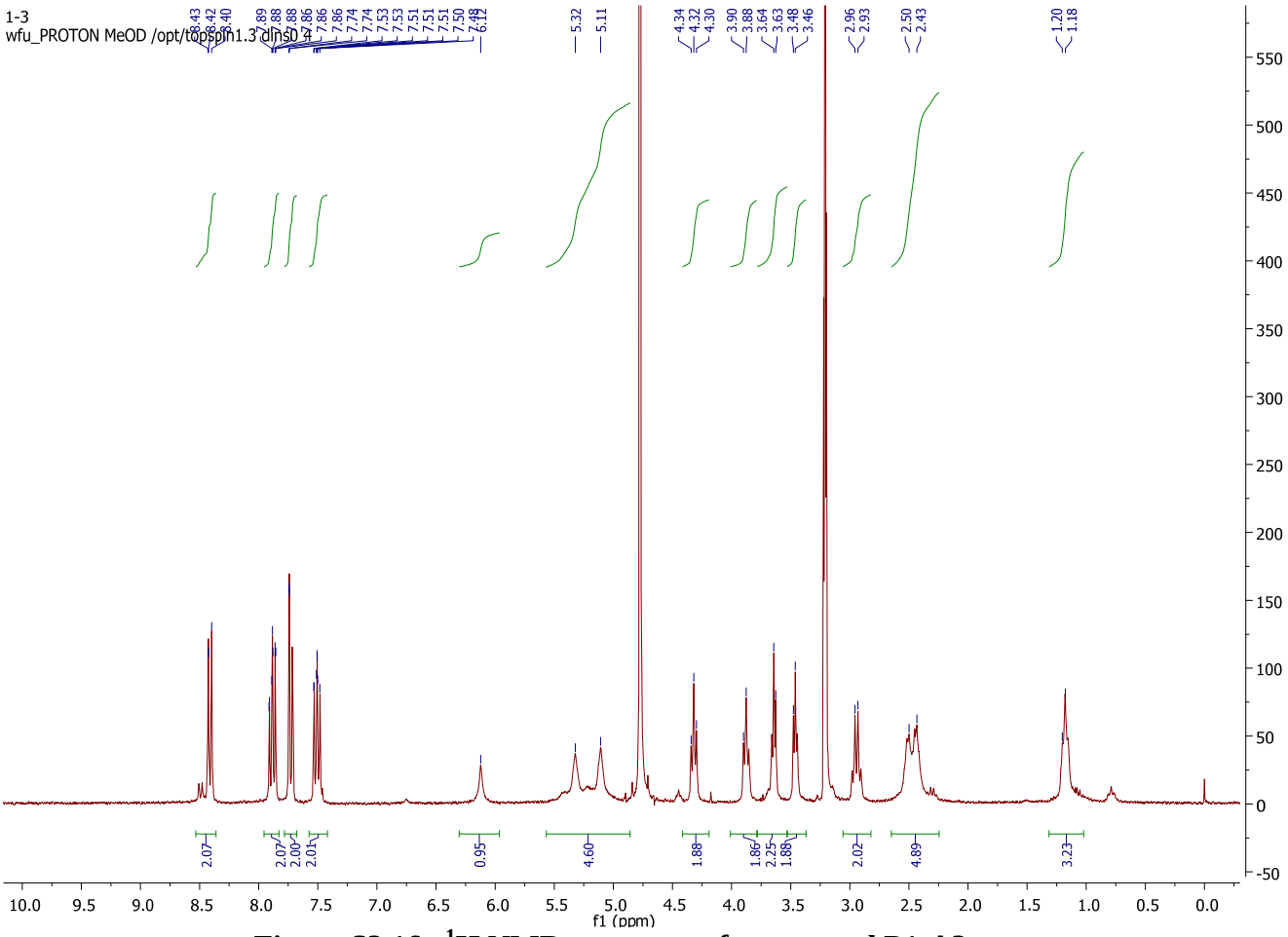


Figure S2.16. ^{1}H NMR spectrum of compound P1-A3.

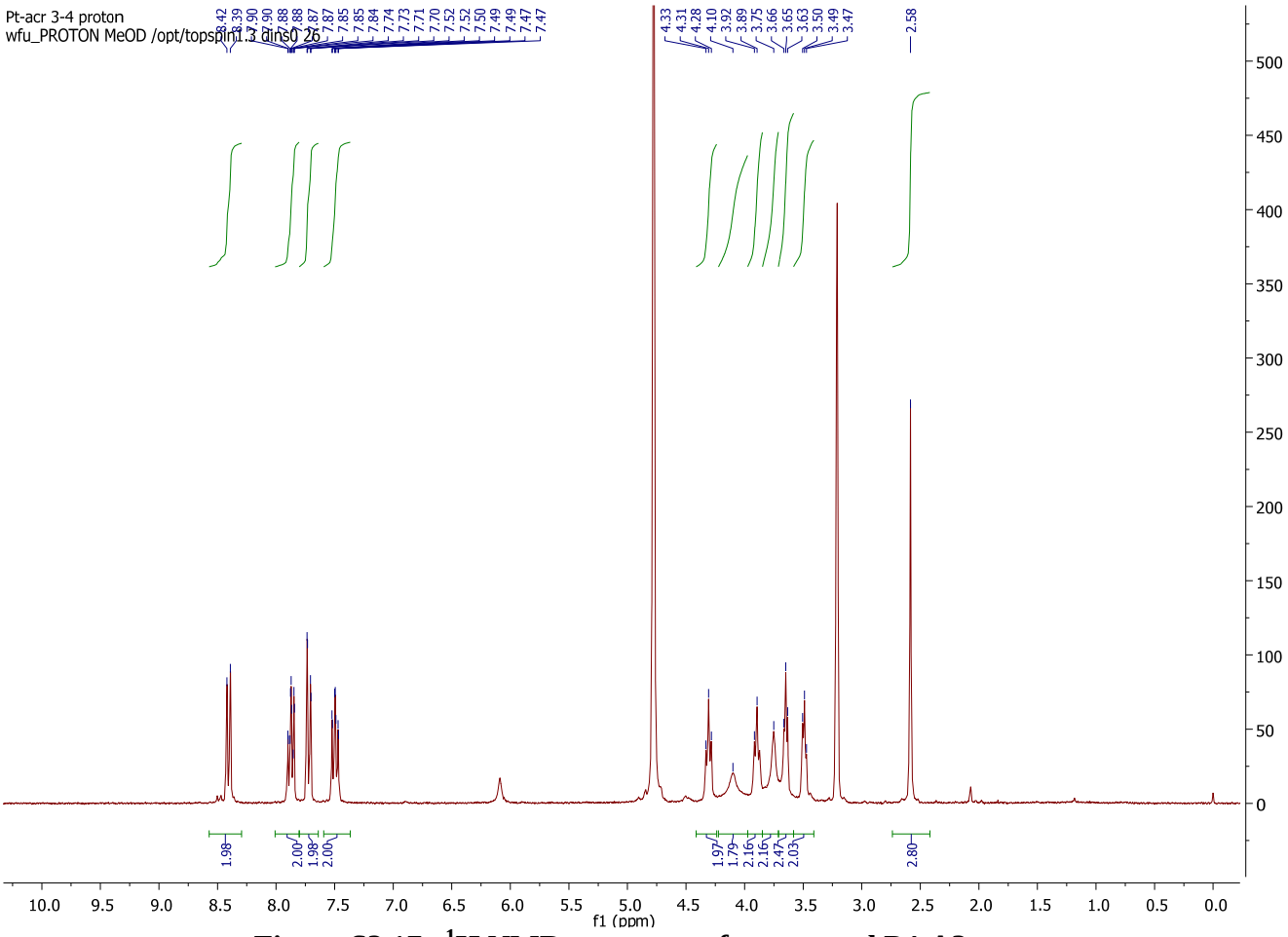


Figure S2.17. ^{1}H NMR spectrum of compound P4-A3.

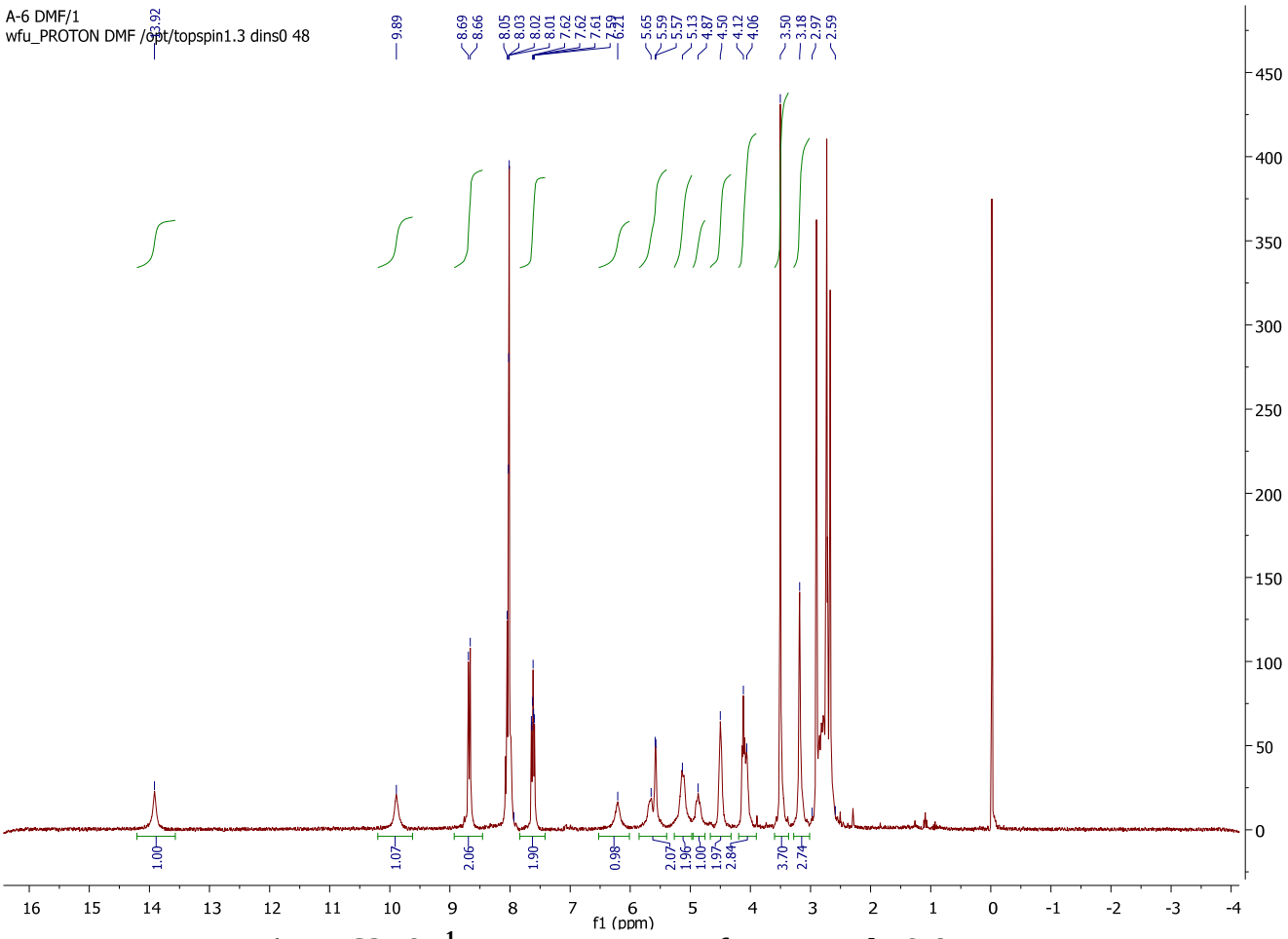


Figure S2.18. ^{1}H NMR spectrum of compound P6-A1.

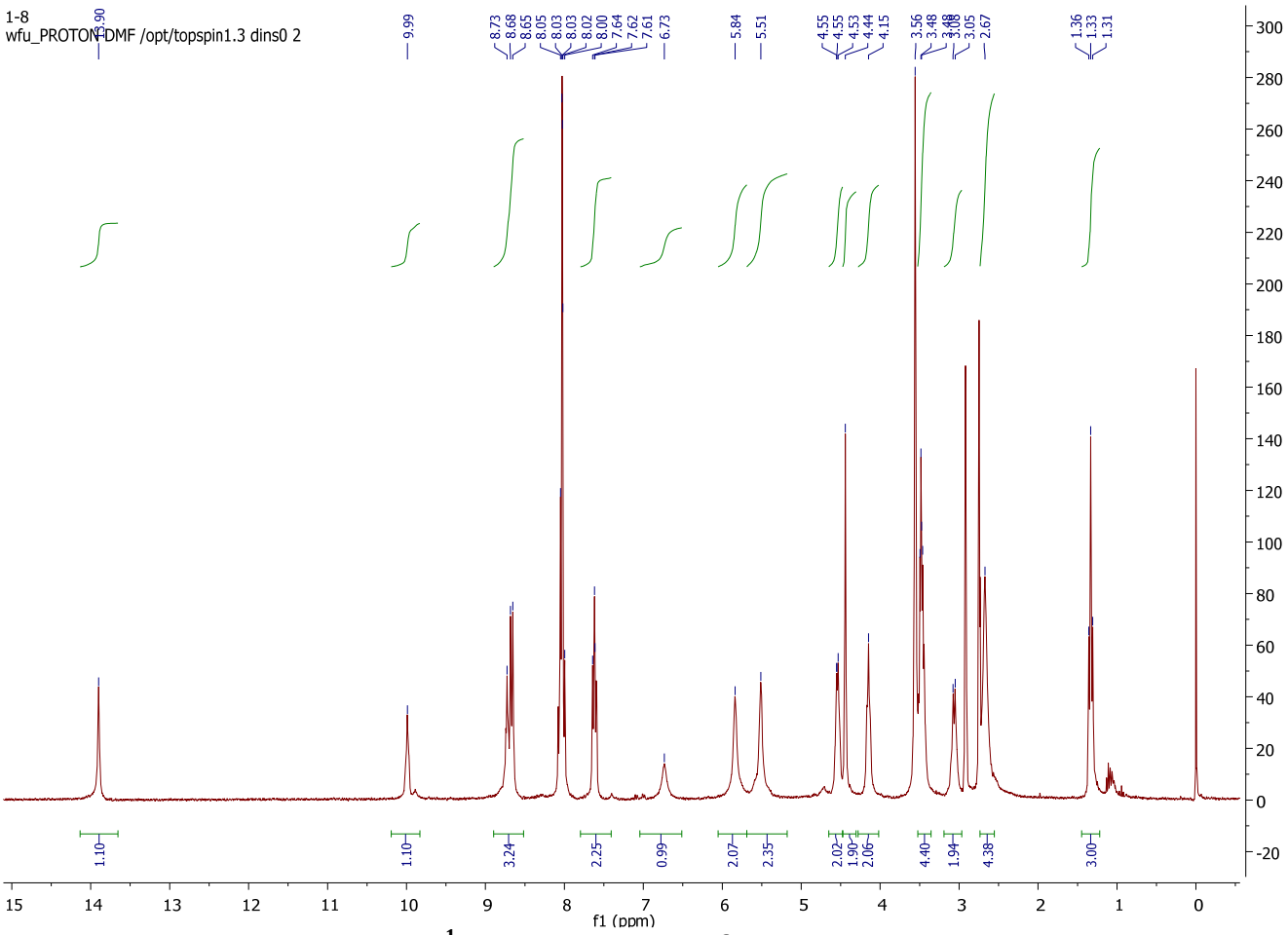


Figure S2.19. ^{1}H NMR spectrum of compound P1-A8.

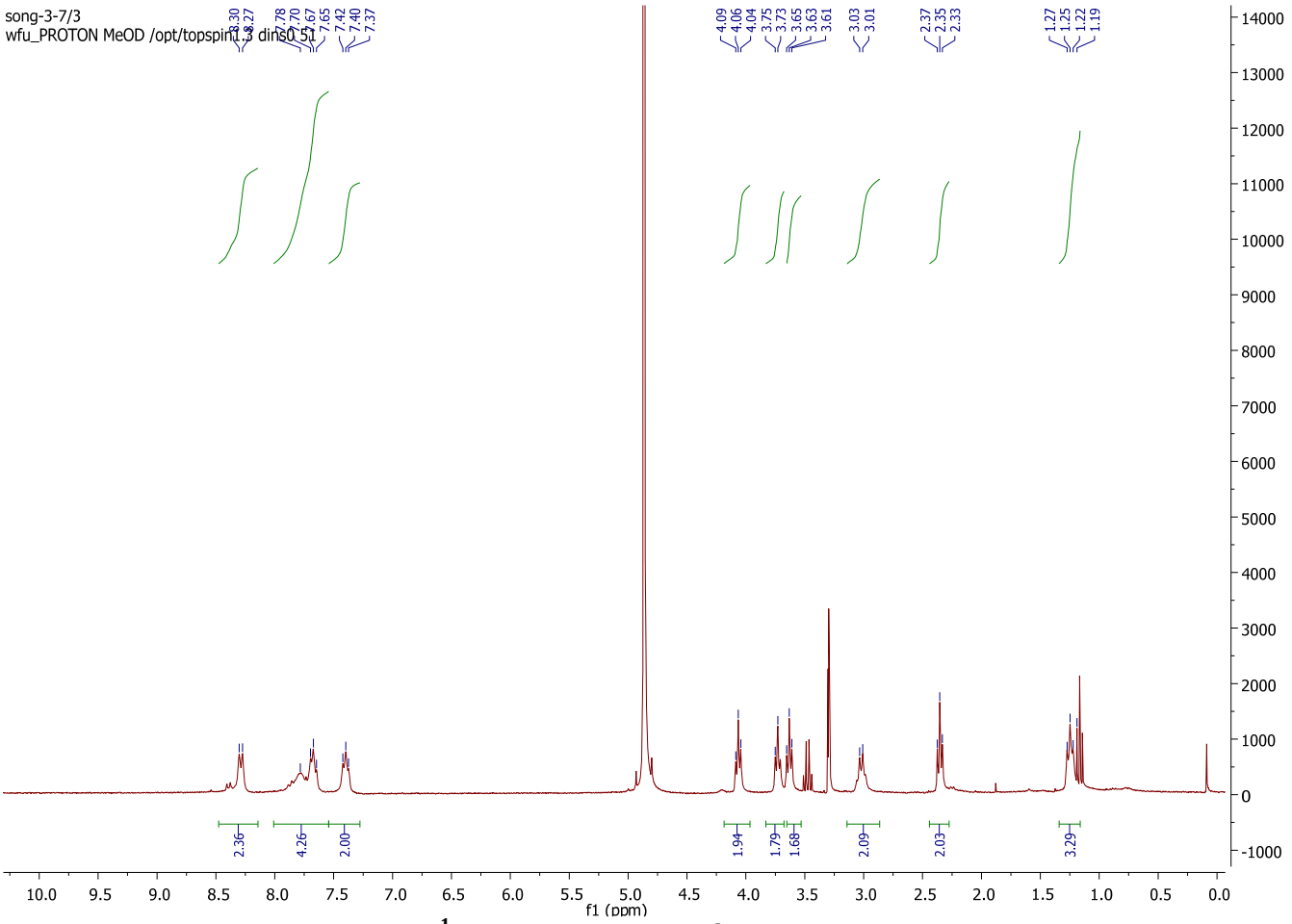


Figure S2.20. ^{1}H NMR spectrum of compound P3-A7.

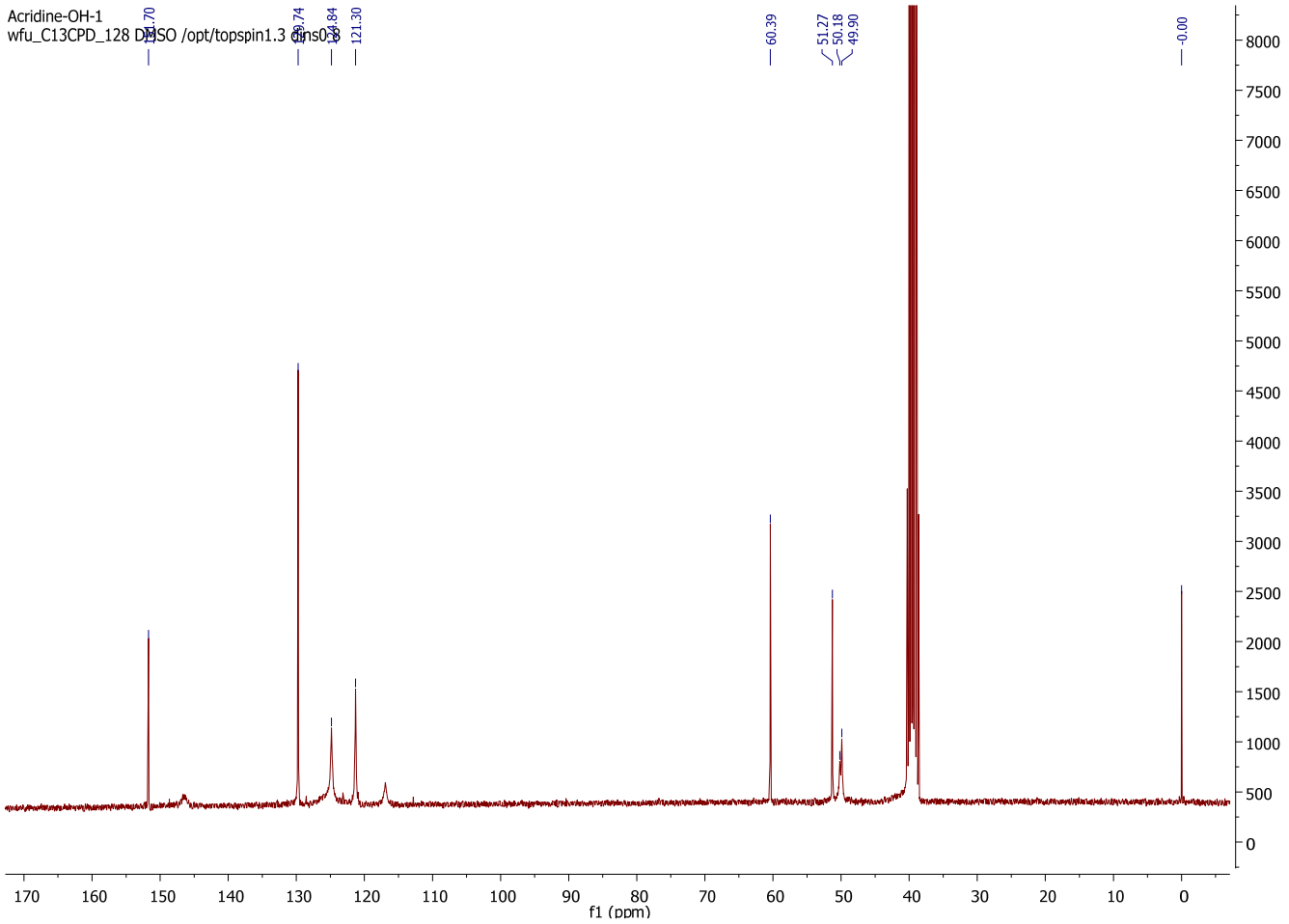


Figure S3.1. ^{13}C NMR spectrum of compound A3.

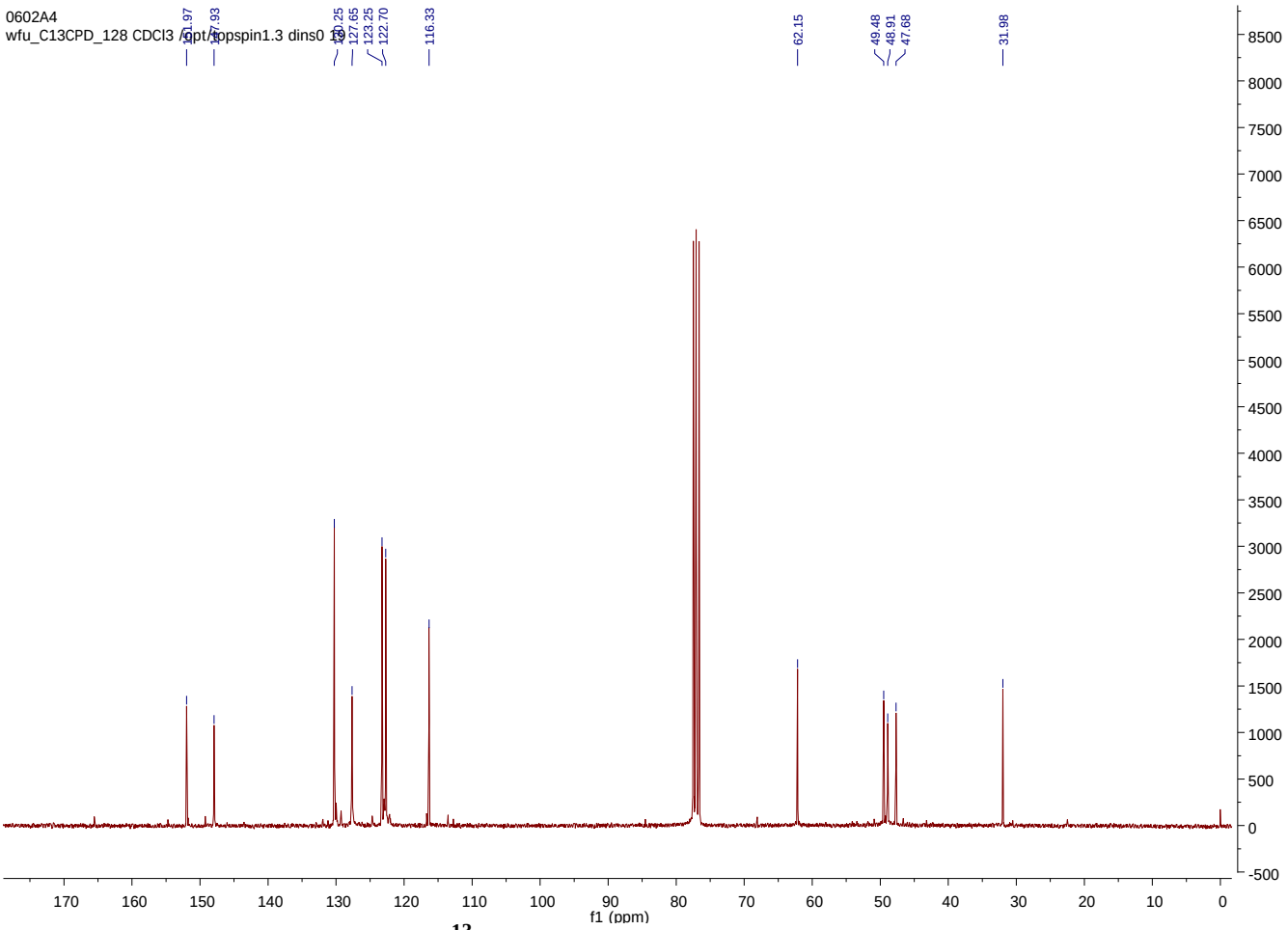


Figure S3.2. ^{13}C NMR spectrum of compound A4.

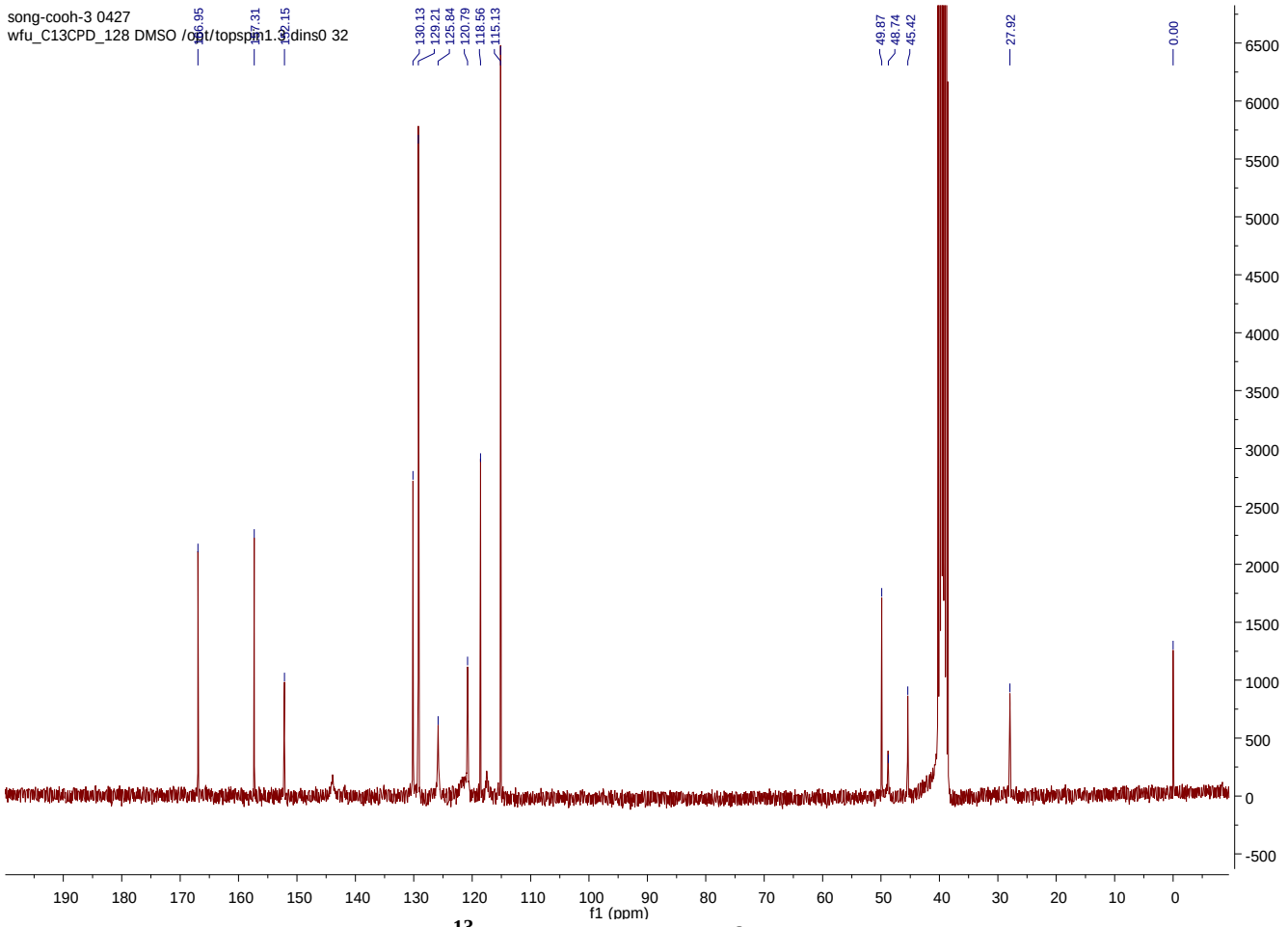


Figure S3.3. ^{13}C NMR spectrum of compound A6.

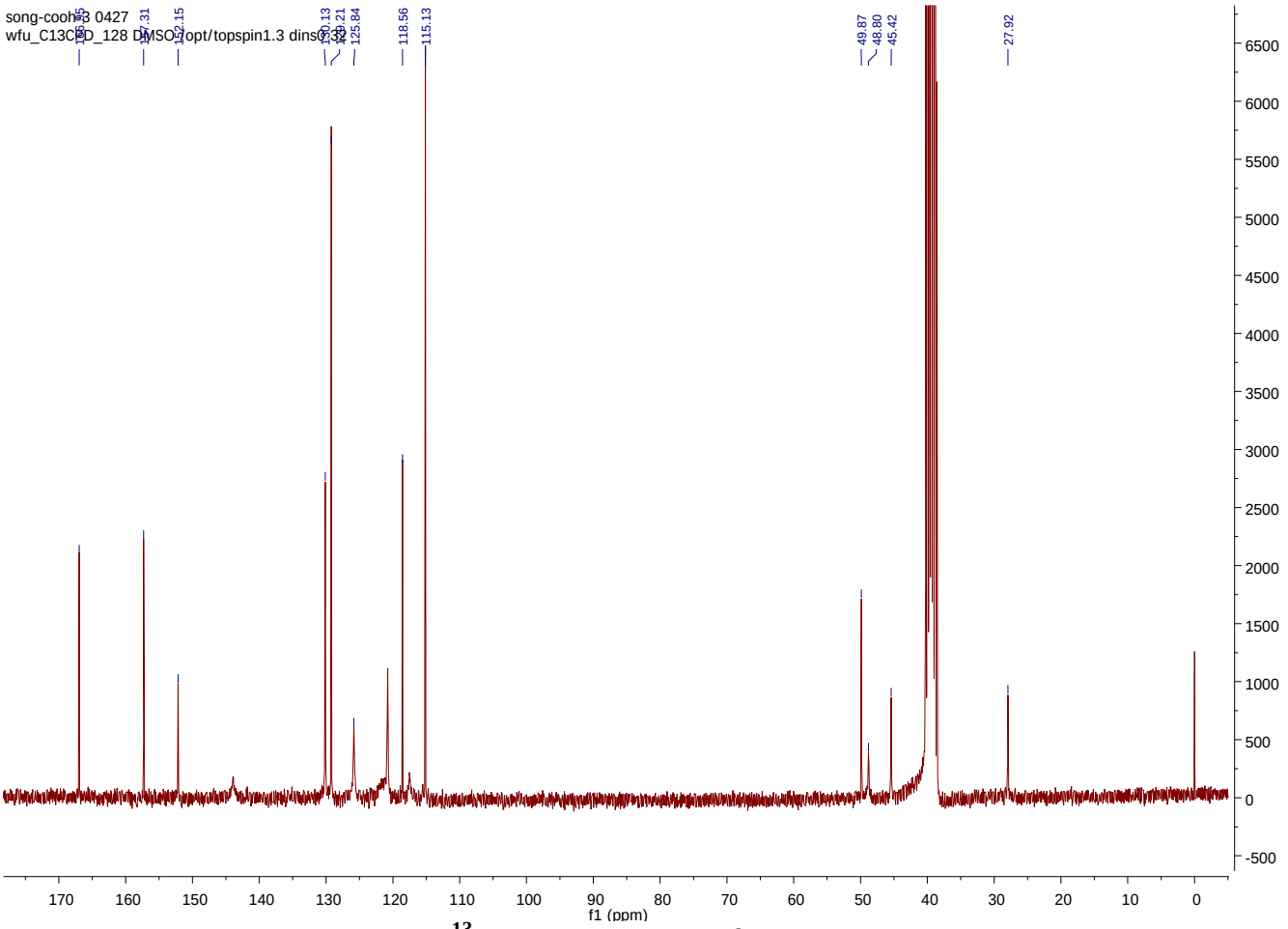


Figure S3.4. ^{13}C NMR spectrum of compound A7.

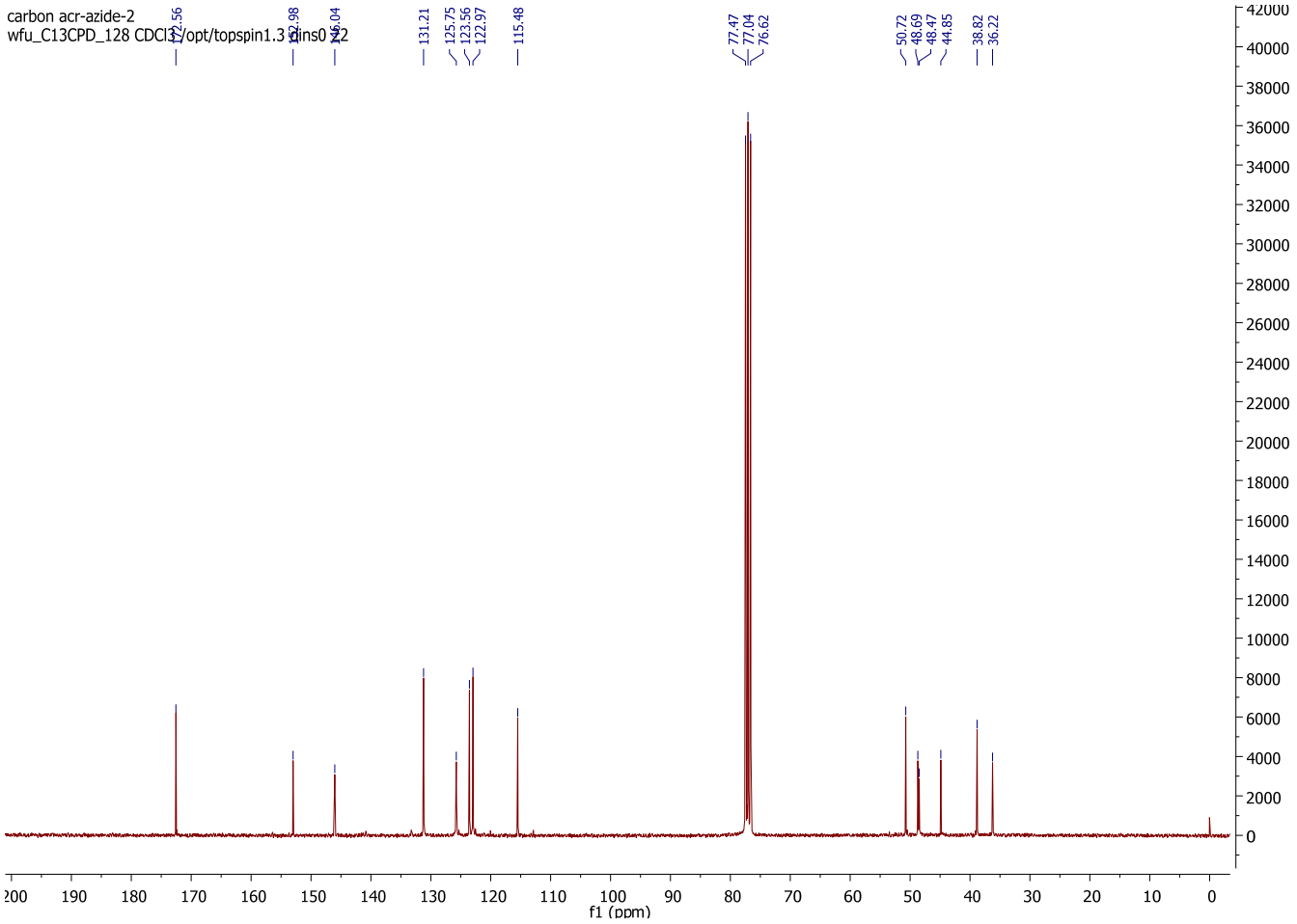


Figure S3.5. ^{13}C NMR spectrum of compound A8.

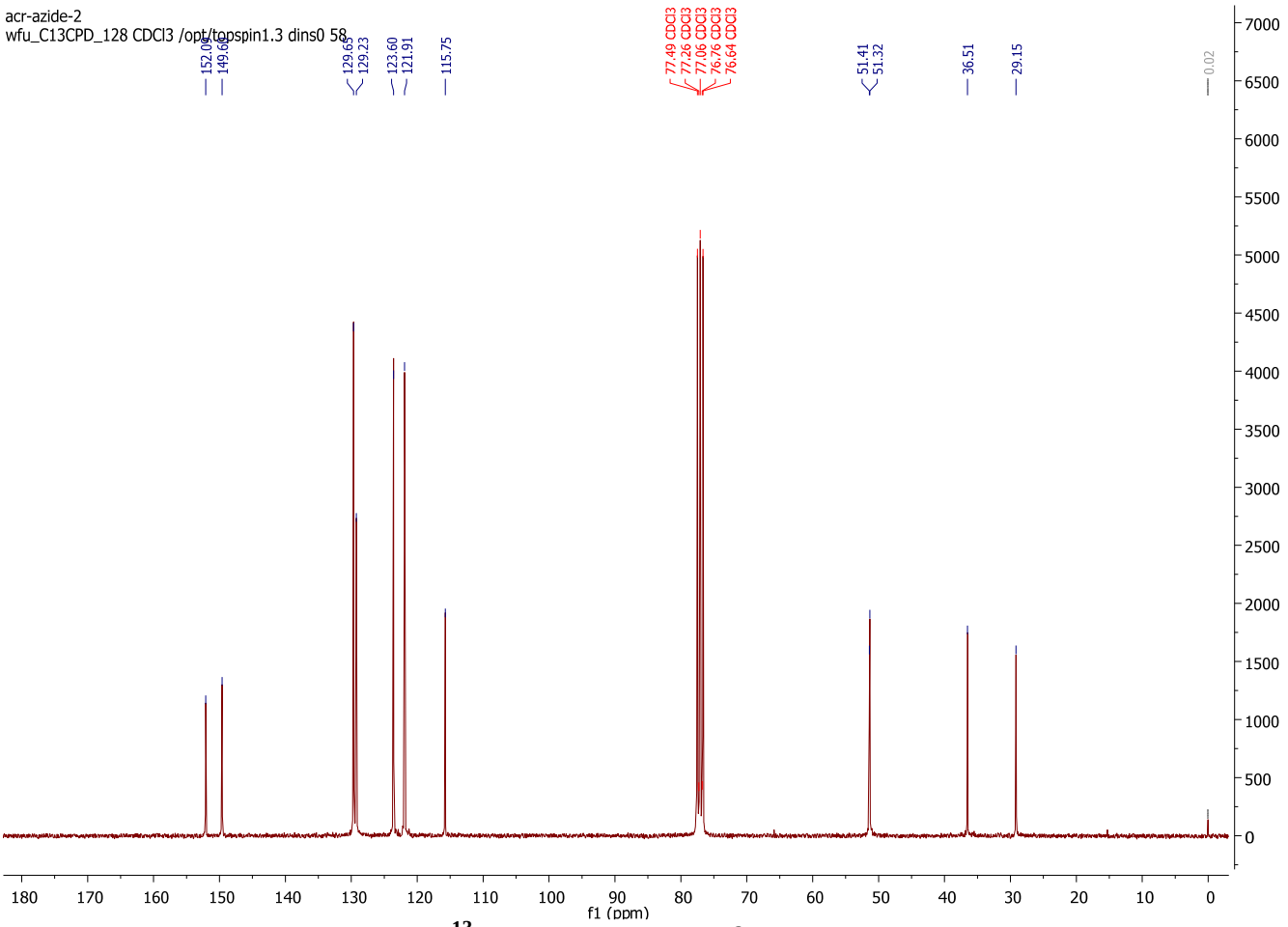


Figure S3.6. ^{13}C NMR spectrum of compound A9.

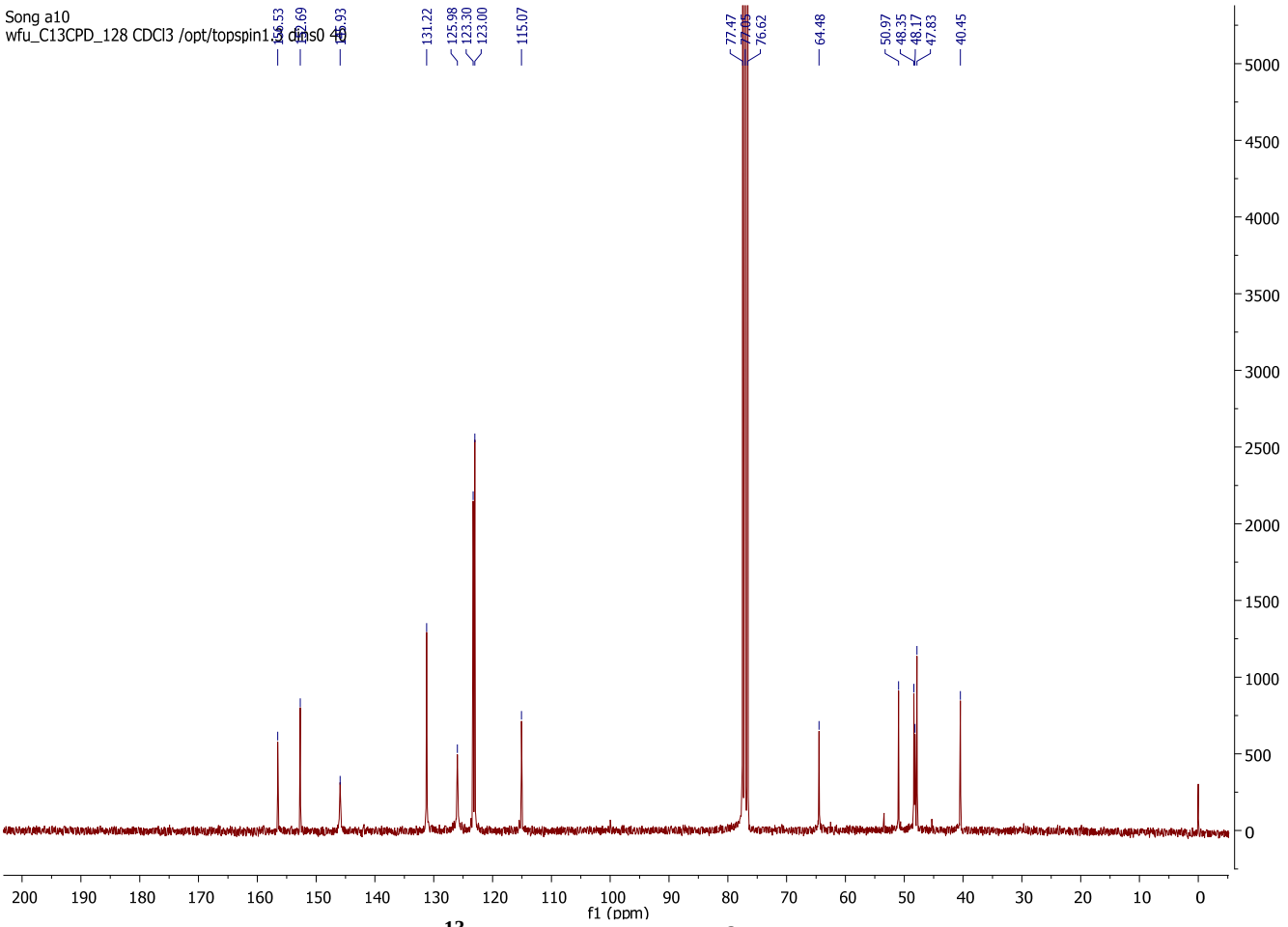


Figure S3.7. ^{13}C NMR spectrum of compound A10.

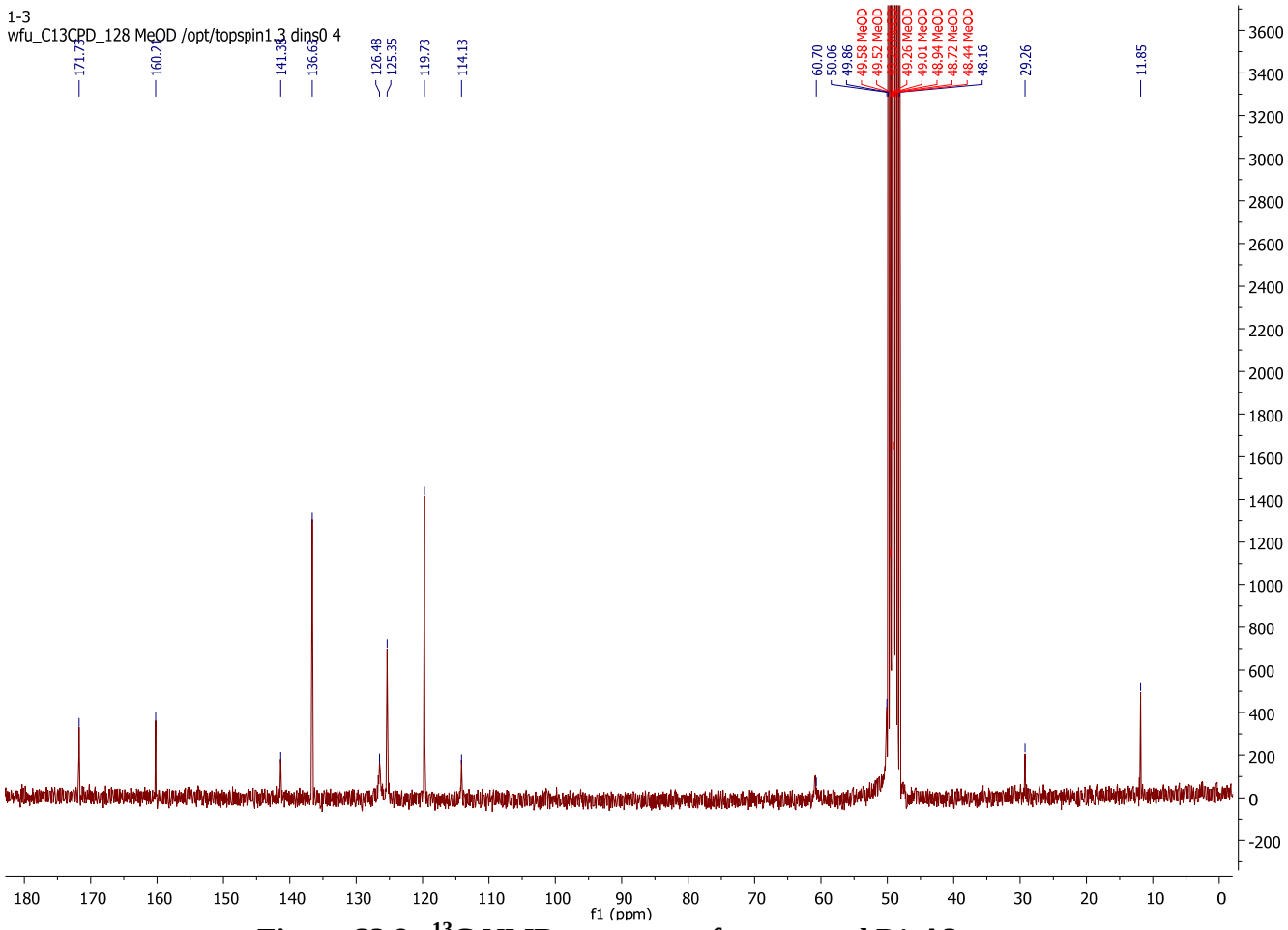


Figure S3.8. ^{13}C NMR spectrum of compound P1-A3.

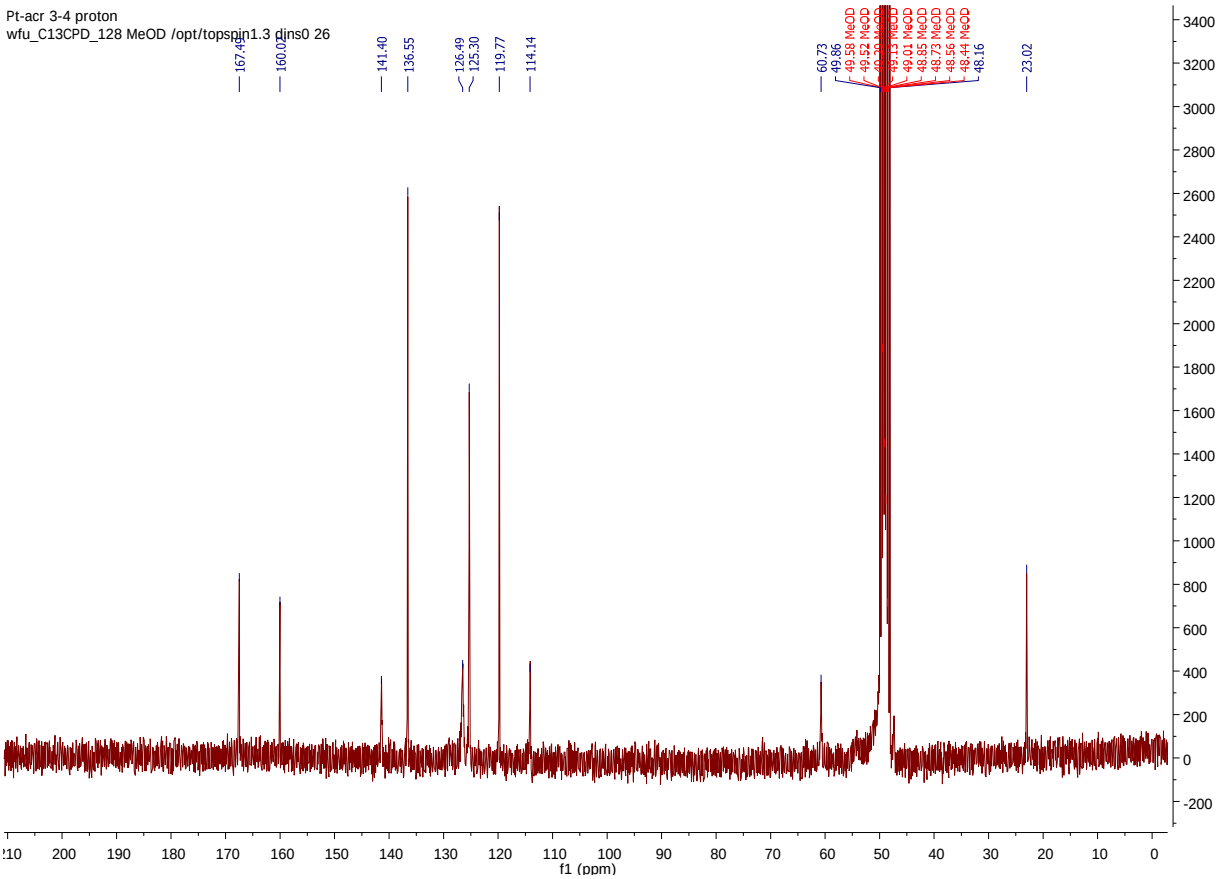


Figure S3.9. ^{13}C NMR spectrum of compound P4-A3.

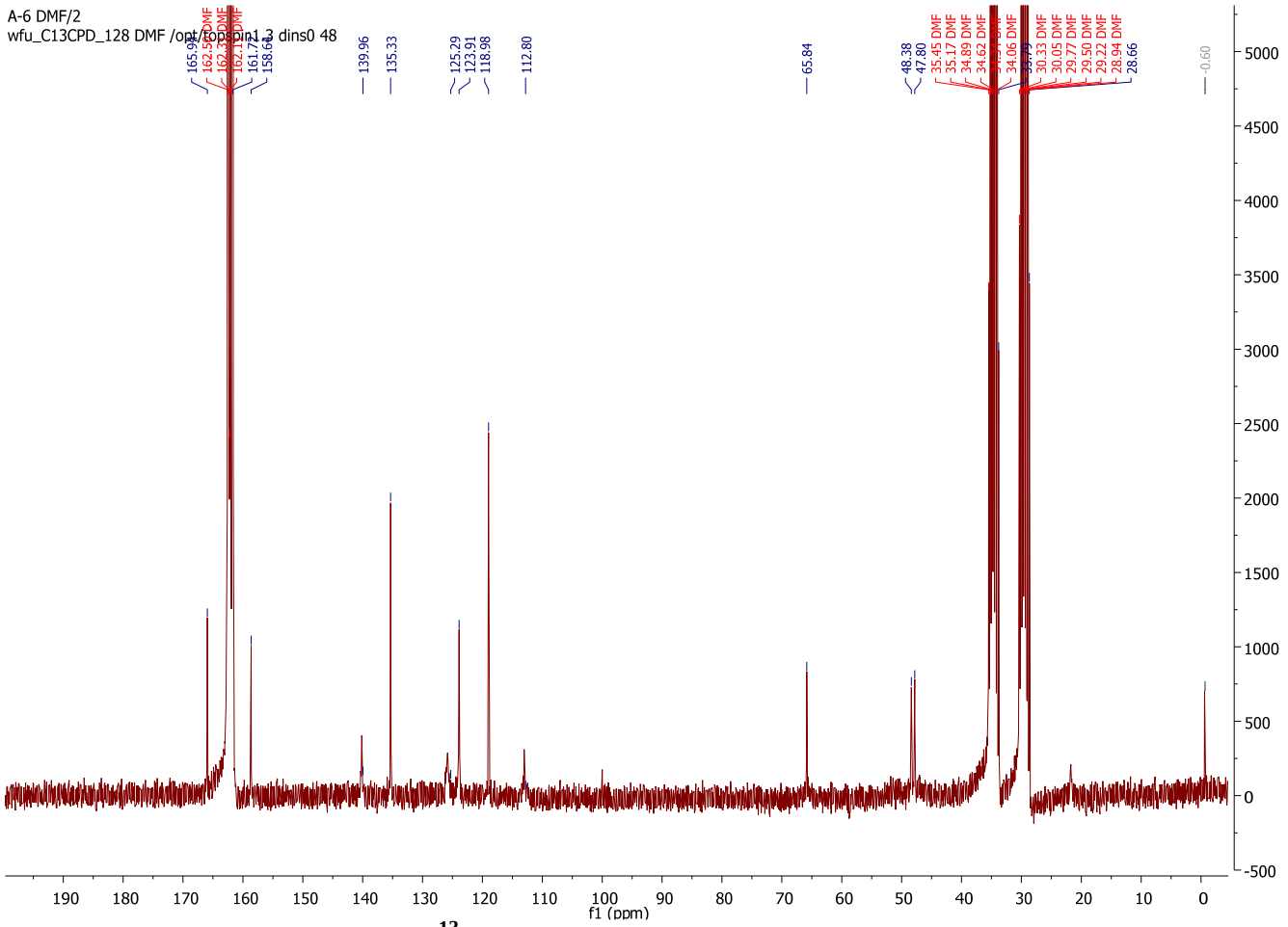


Figure S3.10. ^{13}C NMR spectrum of compound P6-A1.

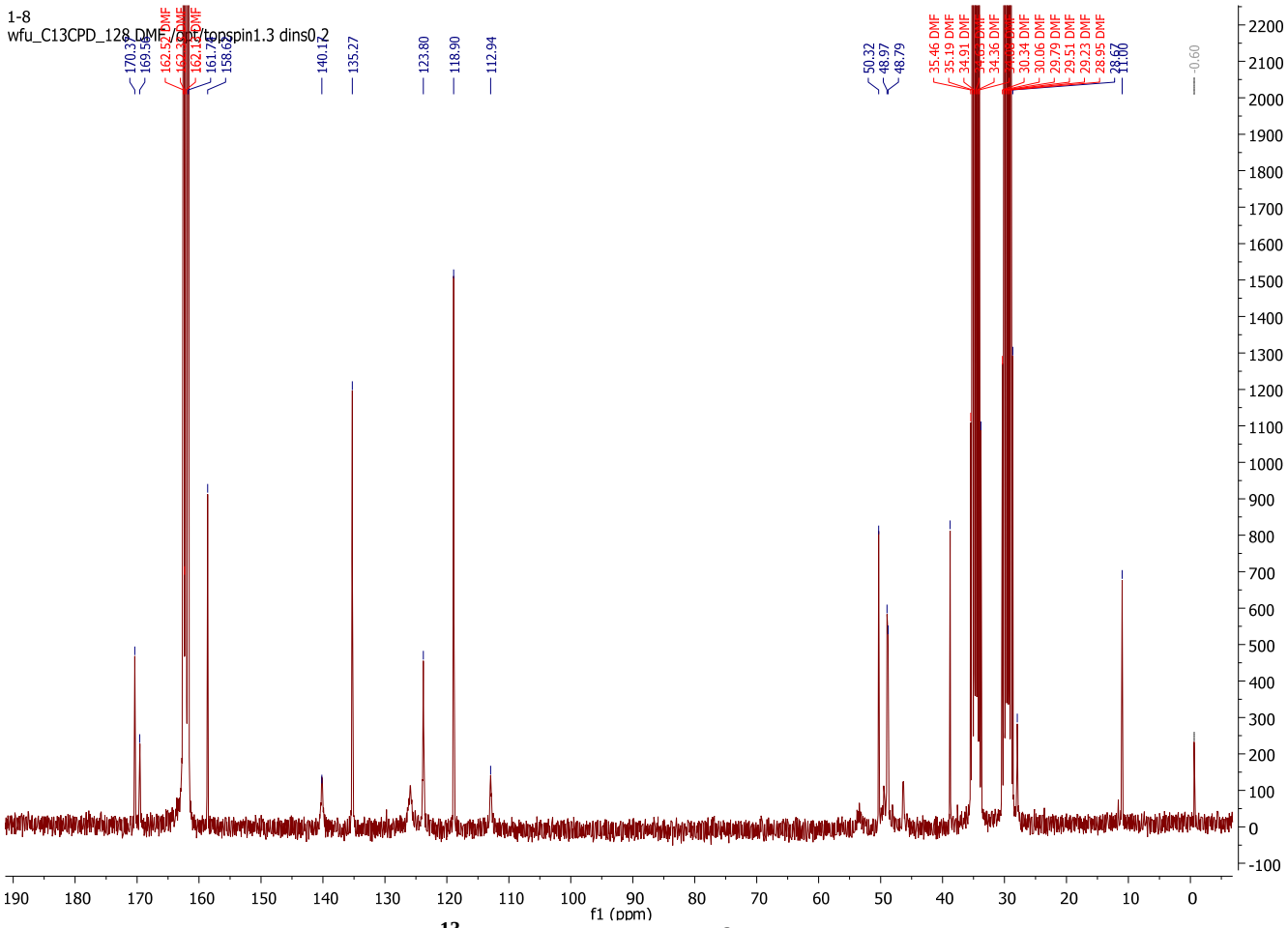


Figure S3.11. ^{13}C NMR spectrum of compound P1-A8.

4. LC-MS analysis of purified compounds

Compound Chromatogram Report - MS

Analysis Name: 04271219.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:13:15 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 4/28/2012 4:35:49 AM
Sample Name: Acridine-aa
Analysis Info: Free base

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	11.0	10.8 - 11.4	74	939	100.0

Chromatograms:

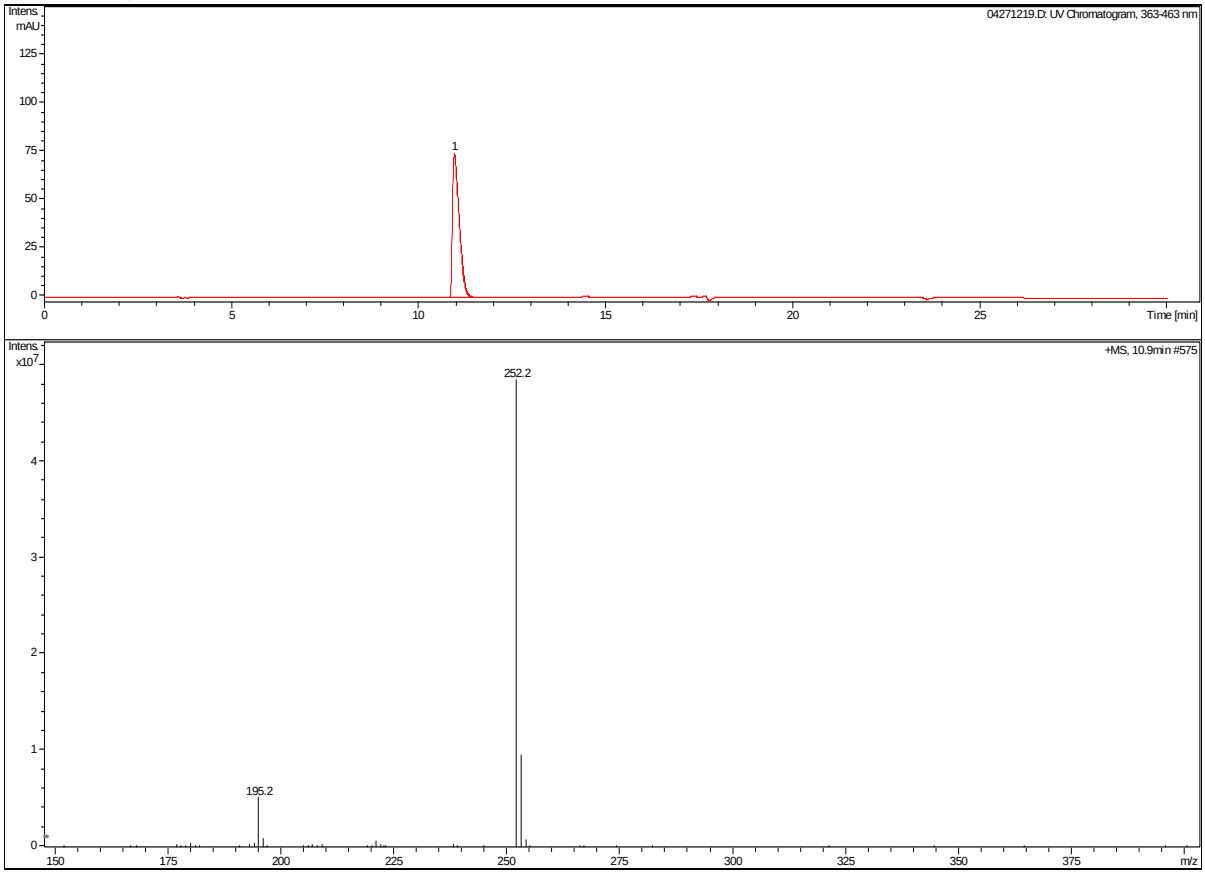


Figure S4.1. LC-MS analysis of compound A1.

Compound Chromatogram Report - MS

Analysis Name: 05021201.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:33:52 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 5/2/2012 2:34:16 PM
Sample Name: ACR-AA-2
Analysis Info: FREE BASE

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	11.8	11.7 - 12.3	81	1161	100.0

Chromatograms:

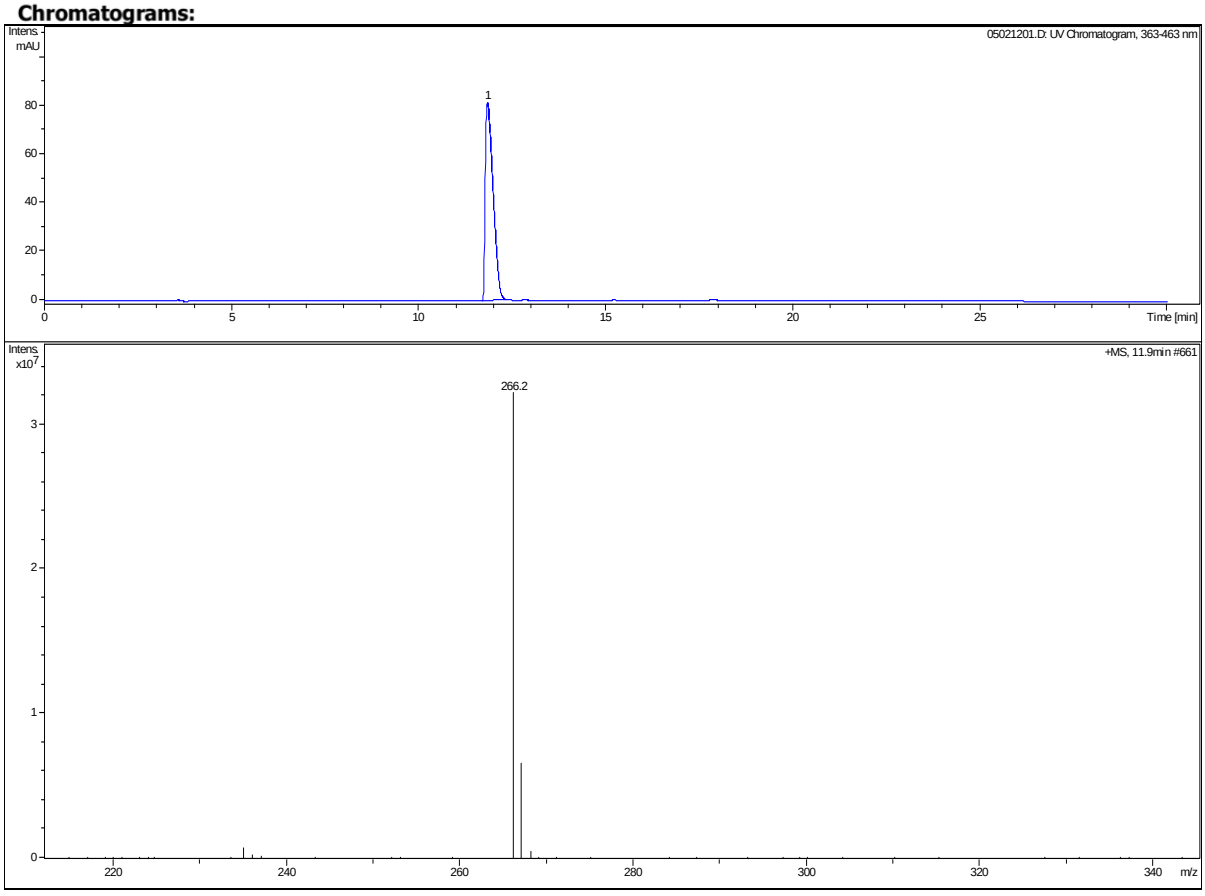


Figure S4.2. LC-MS analysis of compound A2.

Compound Chromatogram Report - MS

Analysis Name: 04271212.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:16:46 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 4/27/2012 8:46:30 PM
Sample Name: Acridine-OH-1
Analysis Info: Free base

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	11.0	10.9 - 11.6	135	2190	100.0

Chromatograms:

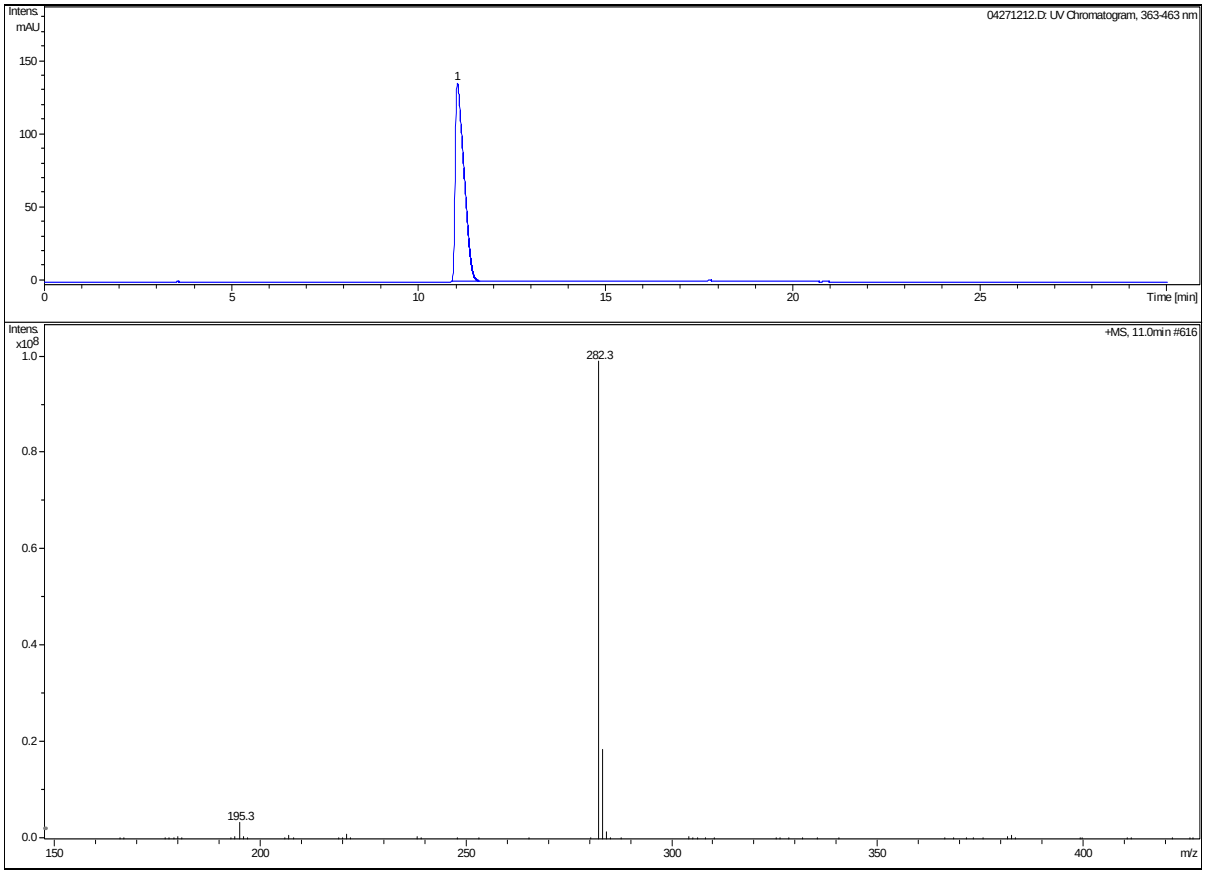


Figure S4.3. LC-MS analysis of compound A3.

Compound Chromatogram Report - MS

Analysis Name: 04271213.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:18:32 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 4/27/2012 9:28:49 PM
Sample Name: Acridine-OH-2
Analysis Info: Free base

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	11.3	11.1 - 11.7	73	885	100.0

Chromatograms:

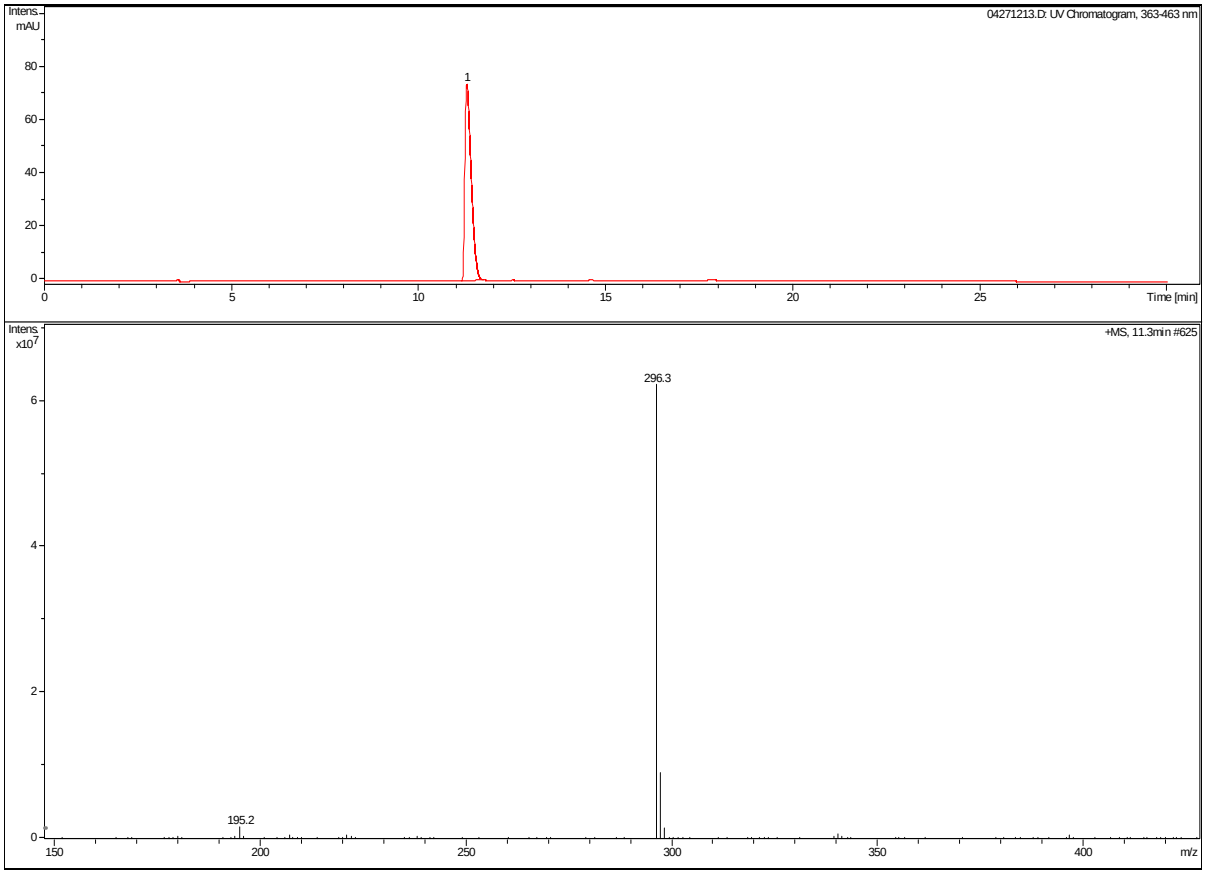


Figure S4.4. LC-MS analysis of compound A4.

Compound Chromatogram Report - MS

Analysis Name: 04271214.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:20:01 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 4/27/2012 10:08:42 PM
Sample Name: Acridine-COOH-1
Analysis Info: Free base

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	13.3	13.1 - 13.6	41	387	100.0

Chromatograms:

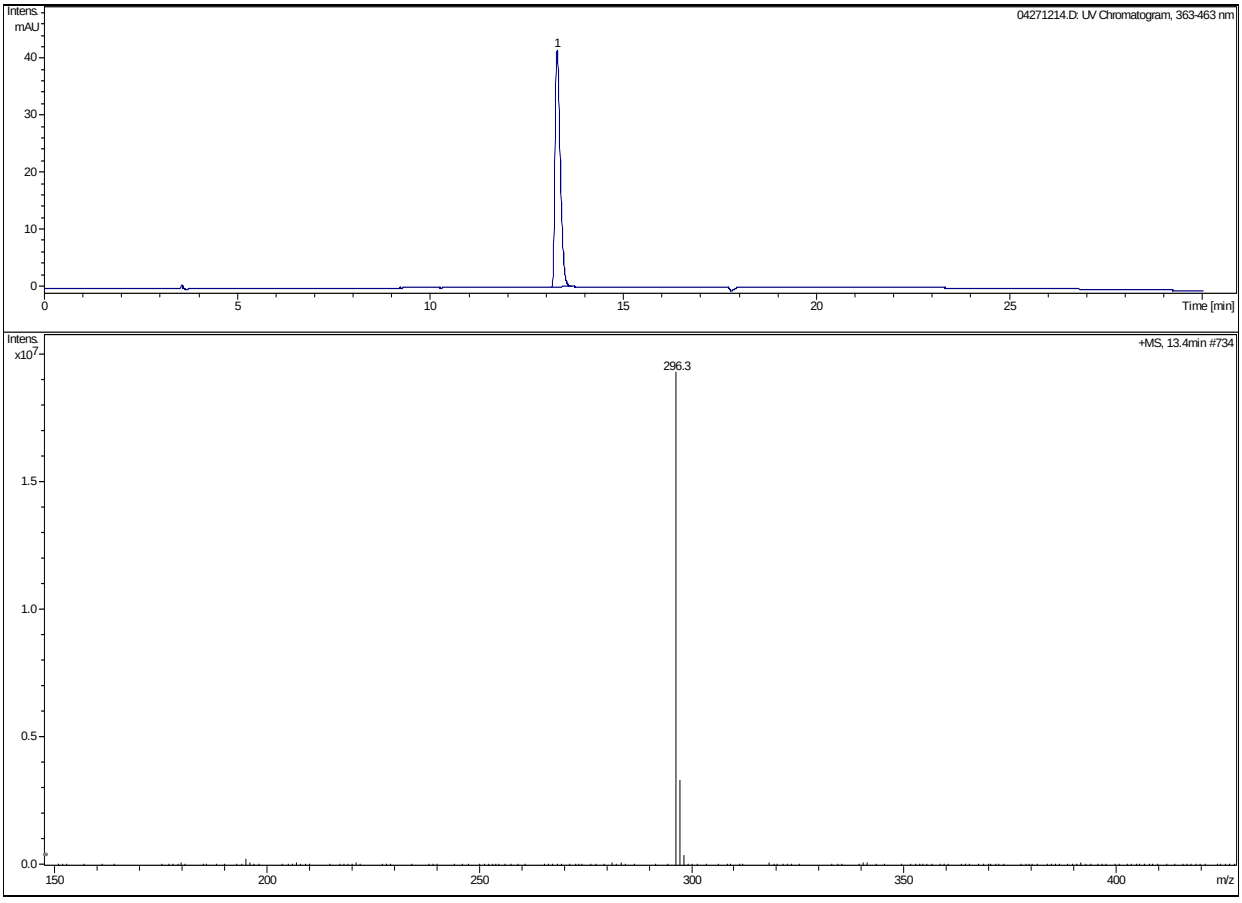


Figure S4.5. LC-MS analysis of compound A5.

Compound Chromatogram Report - MS

Analysis Name: 04271221.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:23:43 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 4/28/2012 10:58:15 AM
Sample Name: Acridine-COOH-2
Analysis Info: Free base

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	11.9	11.8 - 12.3	23	208	100.0

Chromatograms:

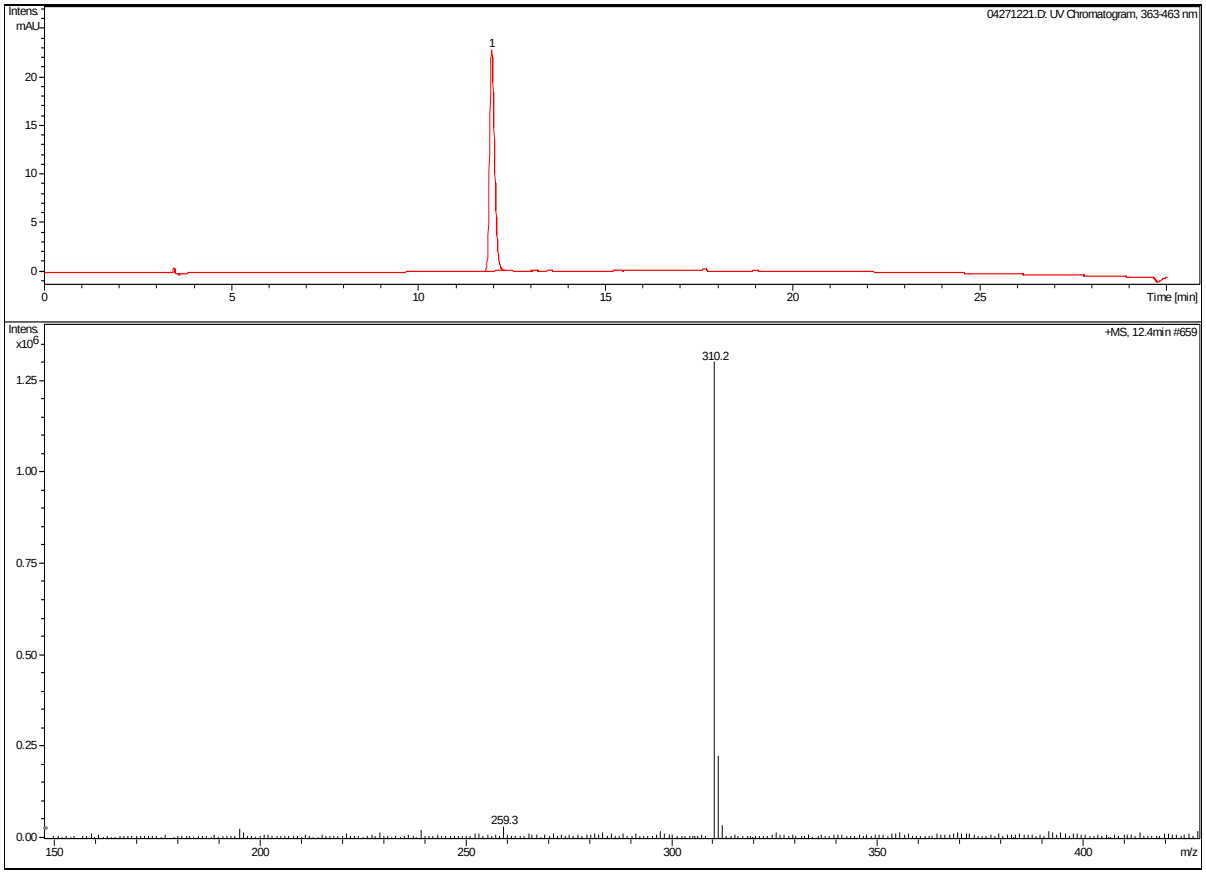


Figure S4.6. LC-MS analysis of compound A6.

Compound Chromatogram Report - MS

Analysis Name: 04271216.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:25:38 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 4/27/2012 11:50:30 PM
Sample Name: Acridine-COOH-3
Analysis Info: Free base

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	14.0	13.9 - 14.4	19	165	100.0

Chromatograms:

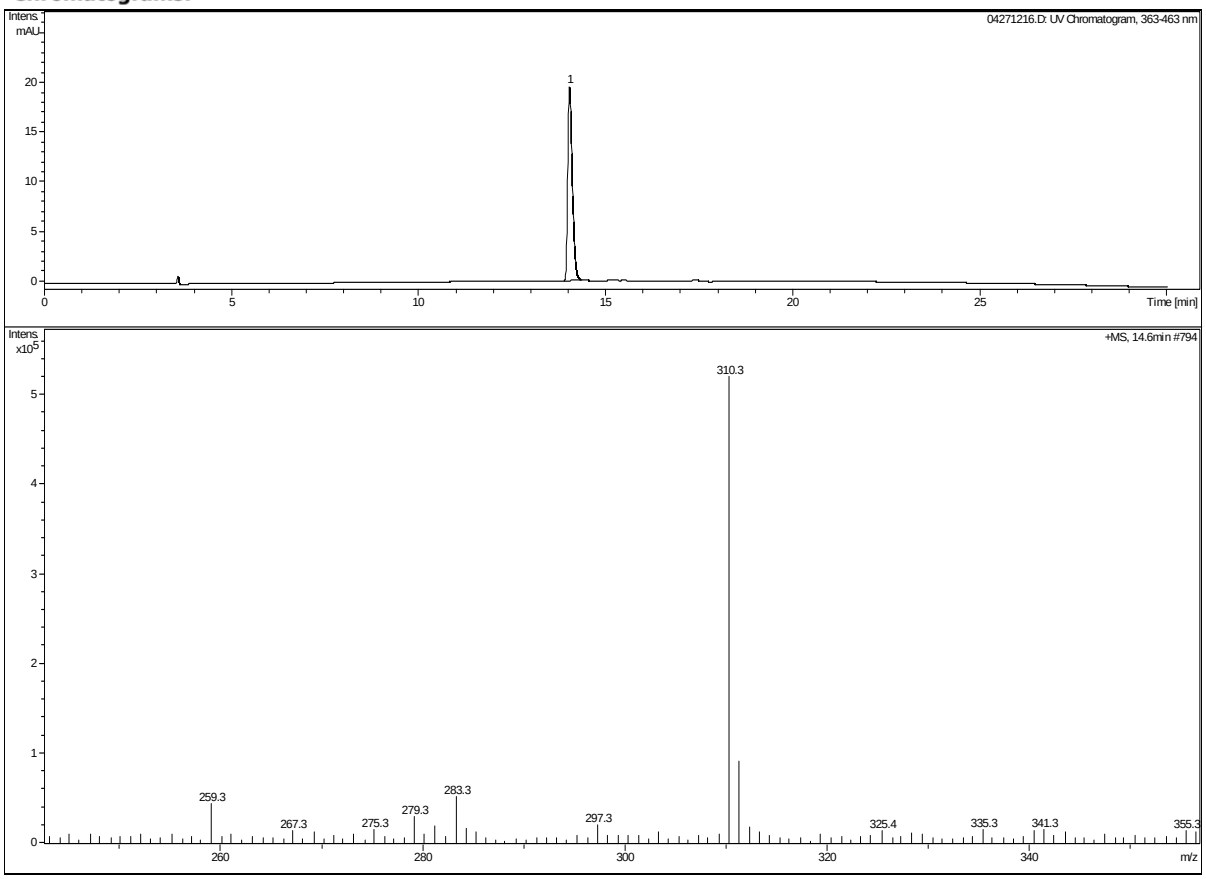


Figure S4.7. LC-MS analysis of compound A7.

Compound Chromatogram Report - MS

Analysis Name: 04271217.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:29:19 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 4/28/2012 1:32:02 AM
Sample Name: Acridine-azide-1
Analysis Info: Free base

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	13.3	12.7 - 13.7	21	223	100.0

Chromatograms:

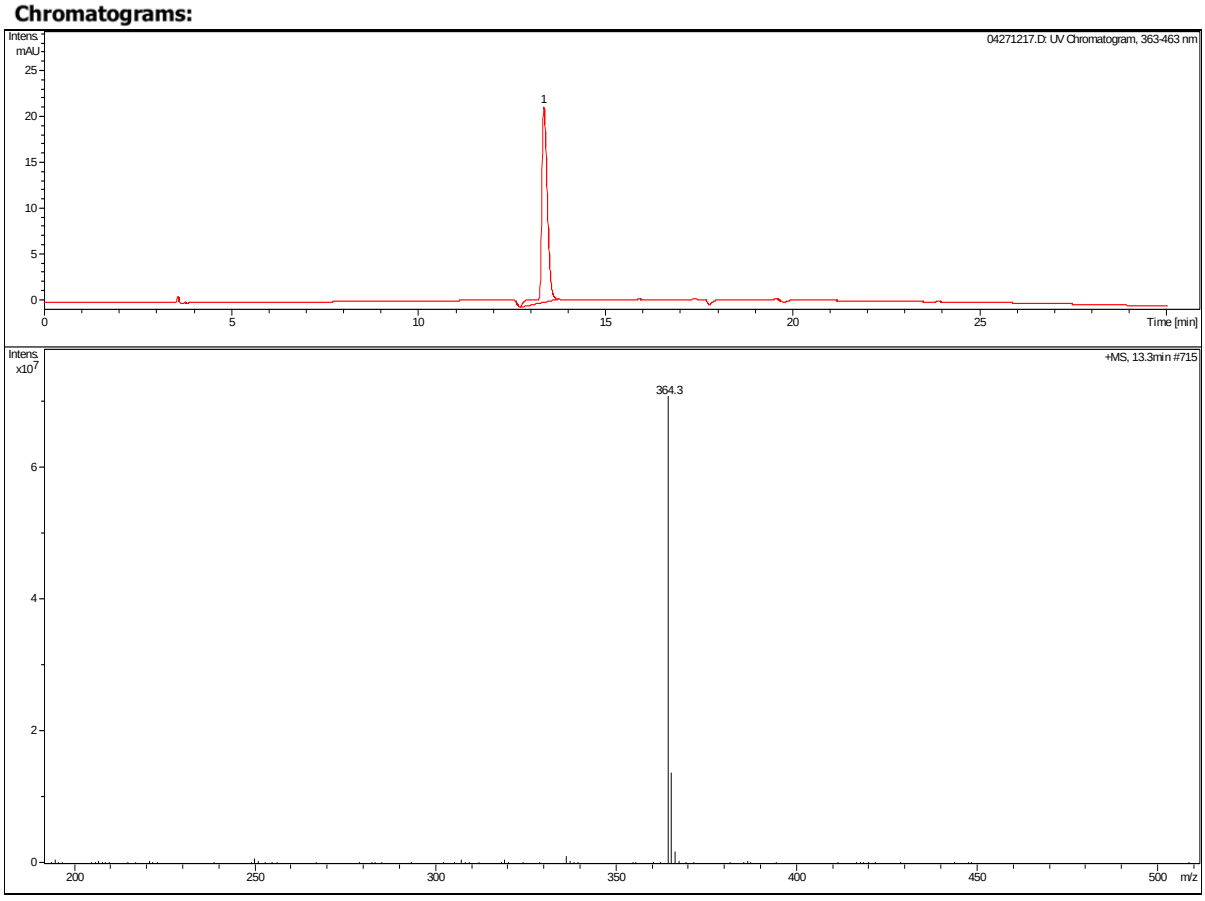


Figure S4.8. LC-MS analysis of compound A8.

Compound Chromatogram Report - MS

Analysis Name: 05021202.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:32:07 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 5/2/2012 3:17:52 PM
Sample Name: ACR-azide-2
Analysis Info: FREE BASE

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	13.1	12.9 - 13.5	39	464	100.0

Chromatograms:

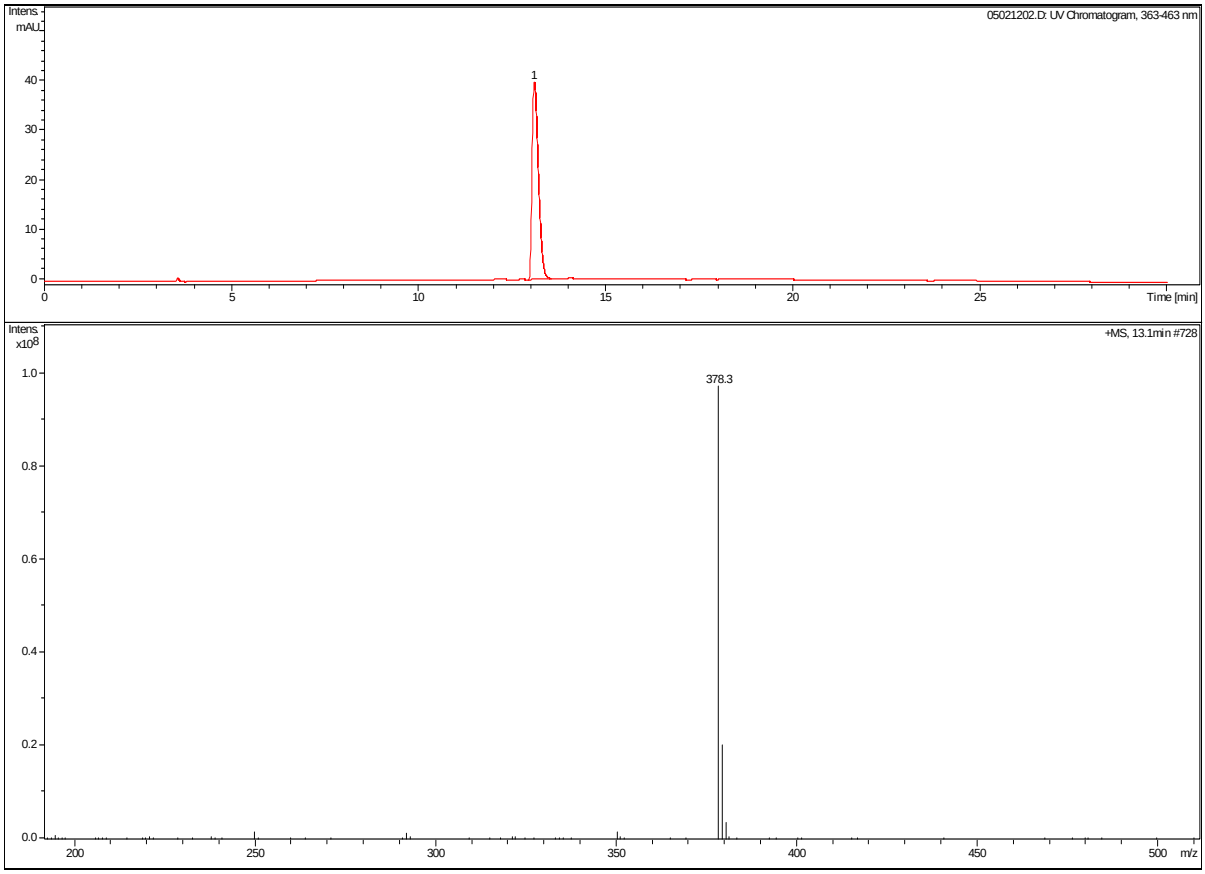


Figure S4.9. LC-MS analysis of compound A9.

Compound Chromatogram Report - MS

Analysis Name: 04271222.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:15:22 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 4/28/2012 11:36:27 AM
Sample Name: Acridine-Azide-3
Analysis Info: Free base

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	13.0	12.8 - 13.5	58	773	100.0

Chromatograms:

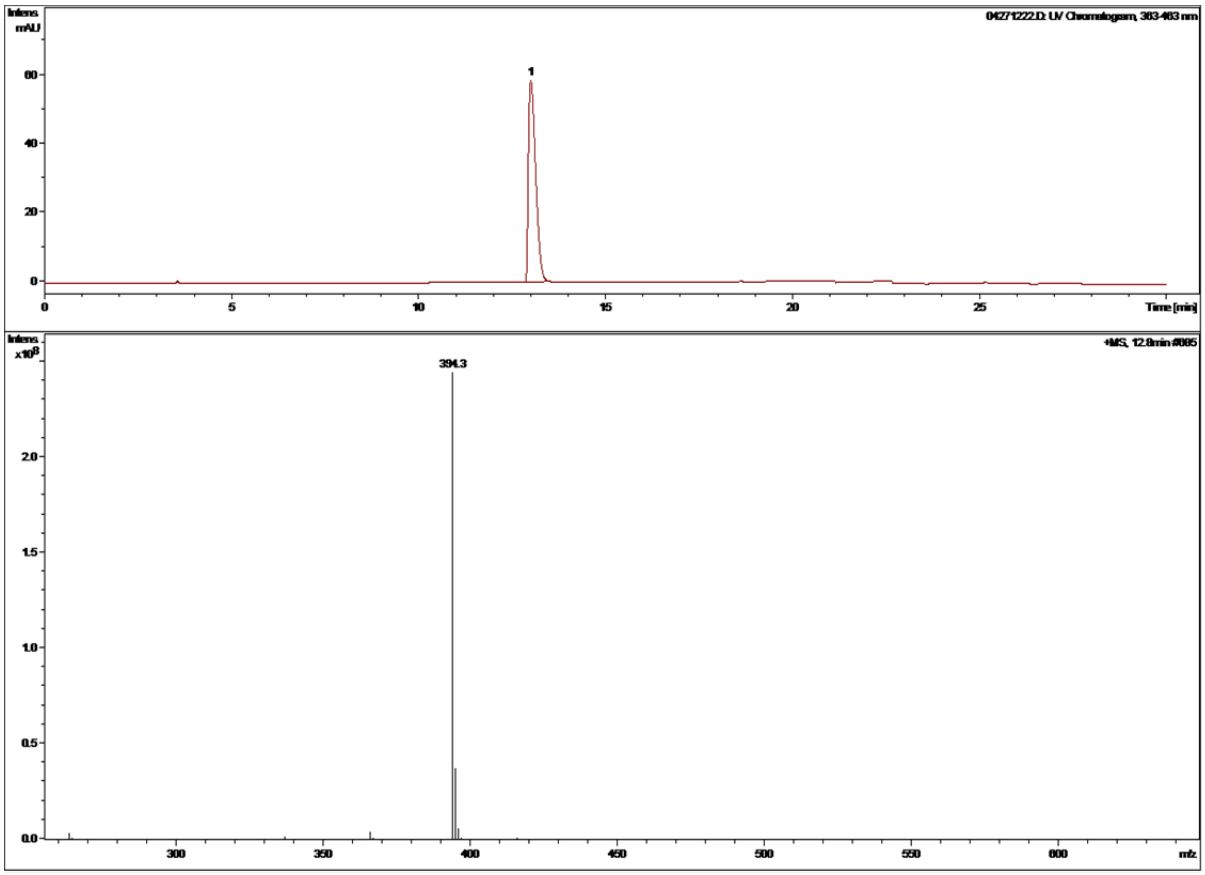


Figure S4.10. LC-MS analysis of compound A10.

Compound Chromatogram Report - MS

Analysis Name: 05261207.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:38:50 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 5/28/2012 4:20:45 PM
Sample Name: En-Pt-OH
Analysis Info: 1-3 N=2,2+

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	14.0	13.8 - 14.4	15	149	100.0

Chromatograms:

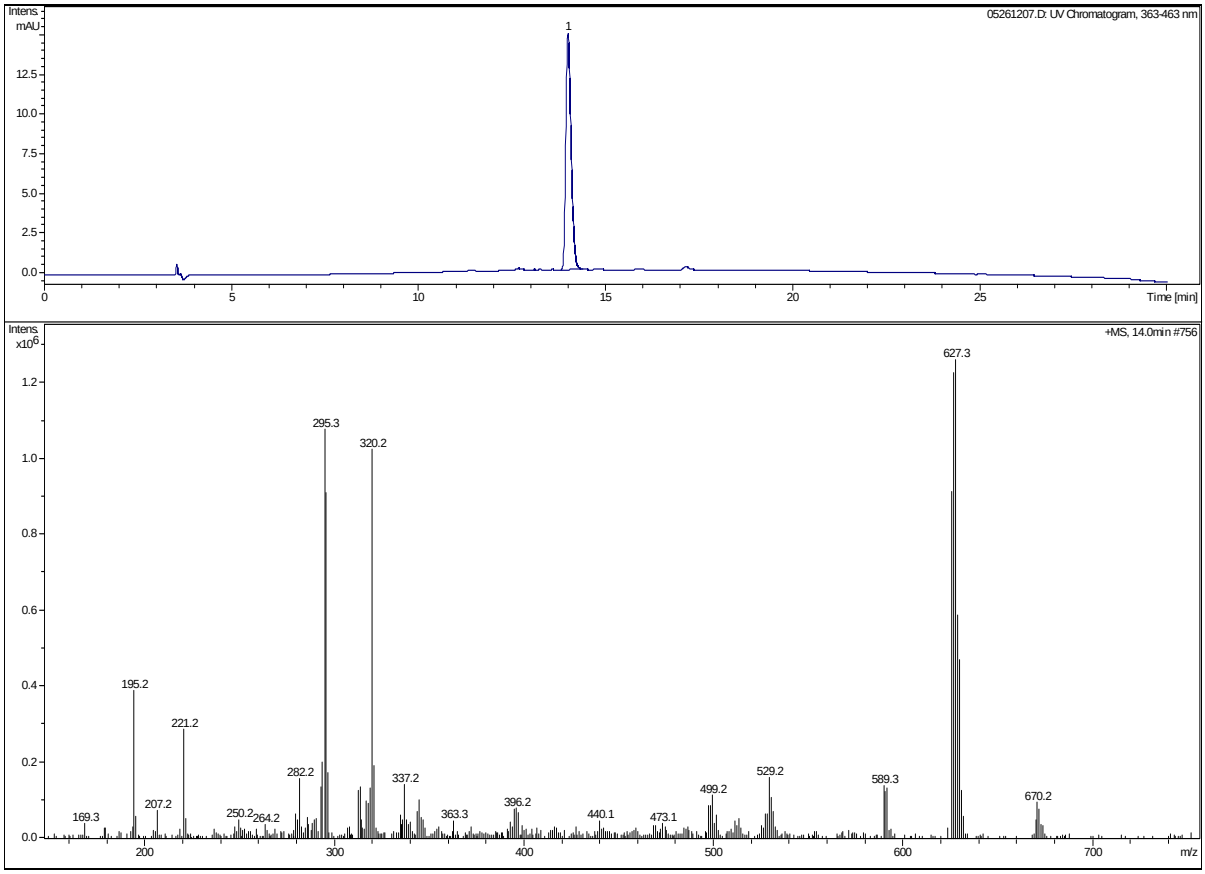


Figure S4.11. LC-MS analysis of compound P1-A3.

Compound Chromatogram Report - MS

Analysis Name: 05261205.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:46:43 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 5/28/2012 2:58:04 PM
Sample Name: diam-Pt-OH
Analysis Info: N=2,2+

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	10.0	9.8 - 10.2	19	141	100.0

Chromatograms:

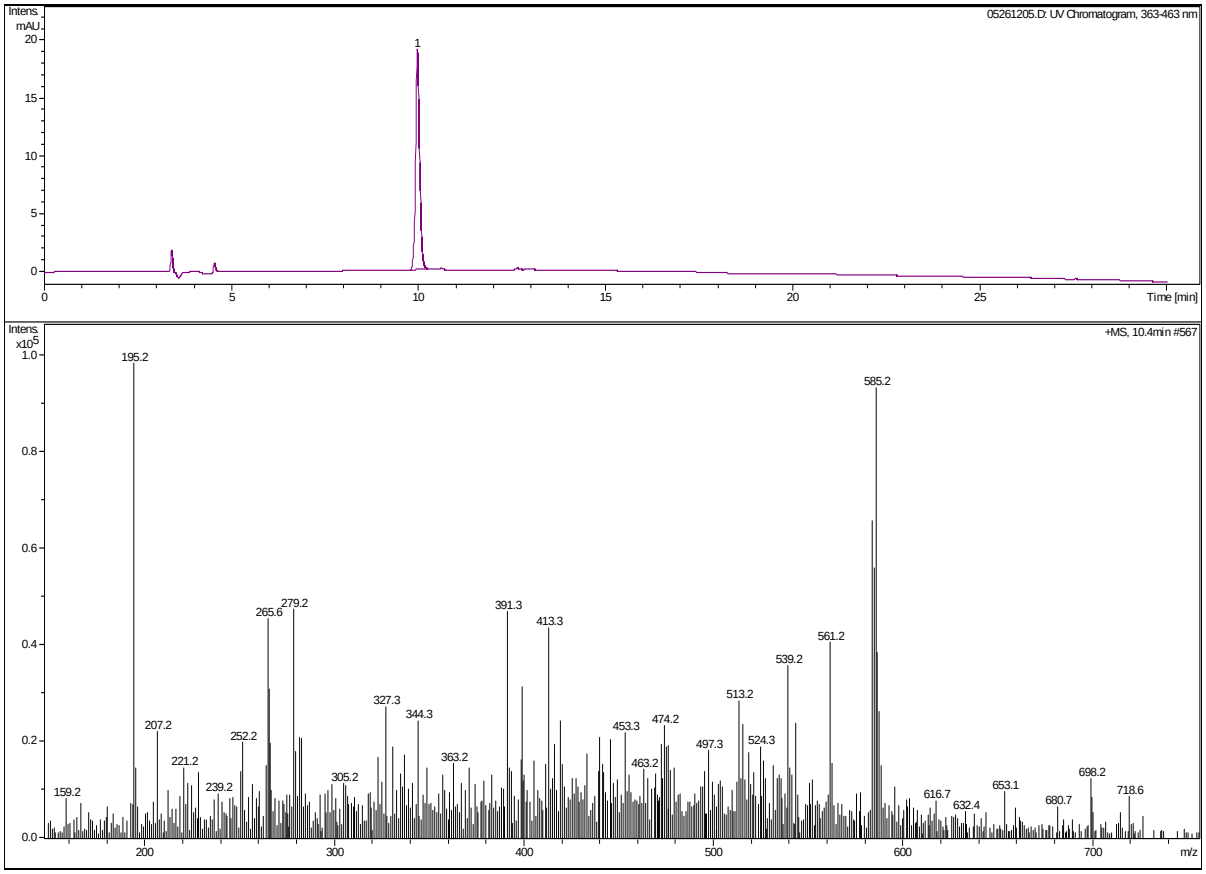


Figure S4.12. LC-MS analysis of compound P4-A3.

Compound Chromatogram Report - MS

Analysis Name: 06011211.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:47:38 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 6/1/2012 11:37:28 AM
Sample Name: 6-1
Analysis Info:

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	13.3	13.1 - 13.7	26	260	100.0

Chromatograms:

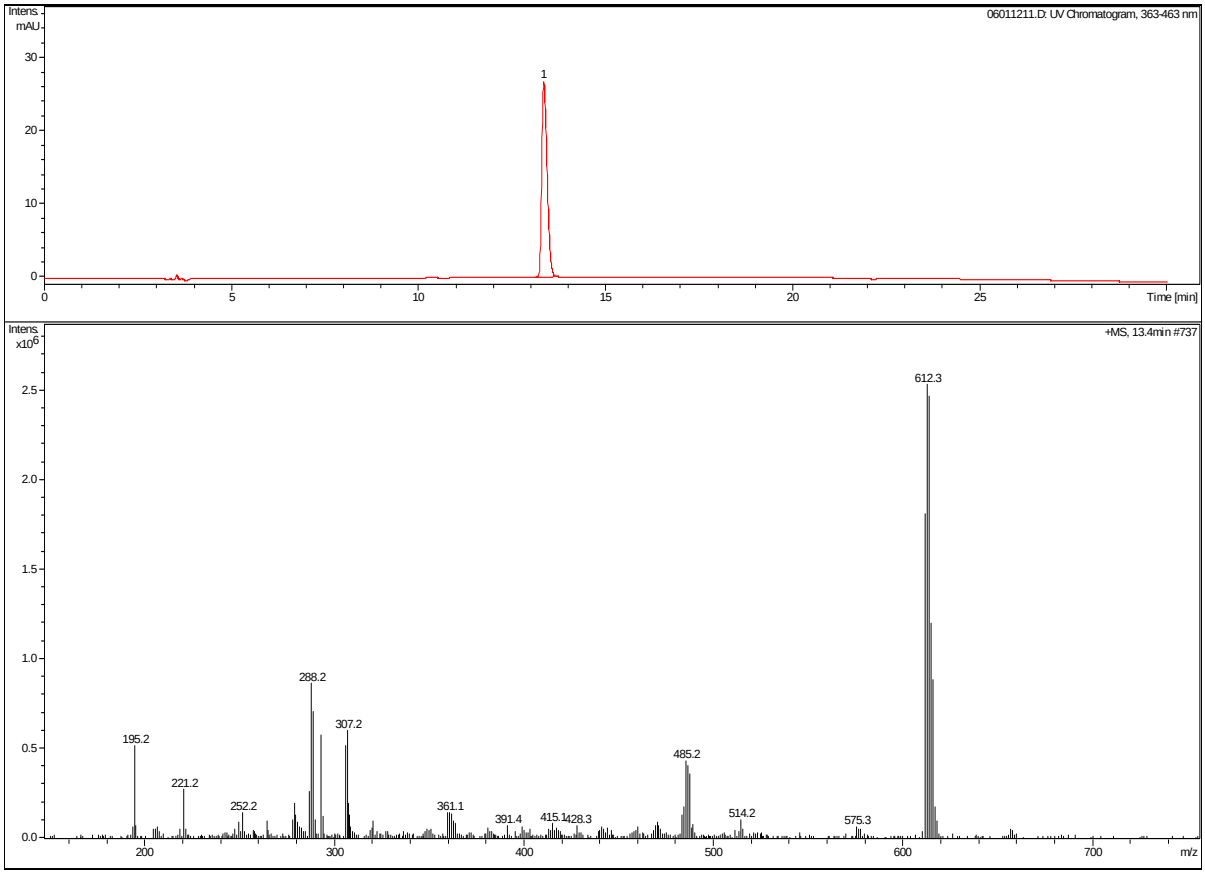


Figure S4.13. LC-MS analysis of compound P6-A1.

Compound Chromatogram Report - MS

Analysis Name: 02091211.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/30/2012 11:58:31 PM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 2/9/2012 4:31:15 PM
Sample Name: pt-azide
Analysis Info: n=1 2+

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	16.6	15.9 - 16.9	10	120	100.0

Chromatograms:

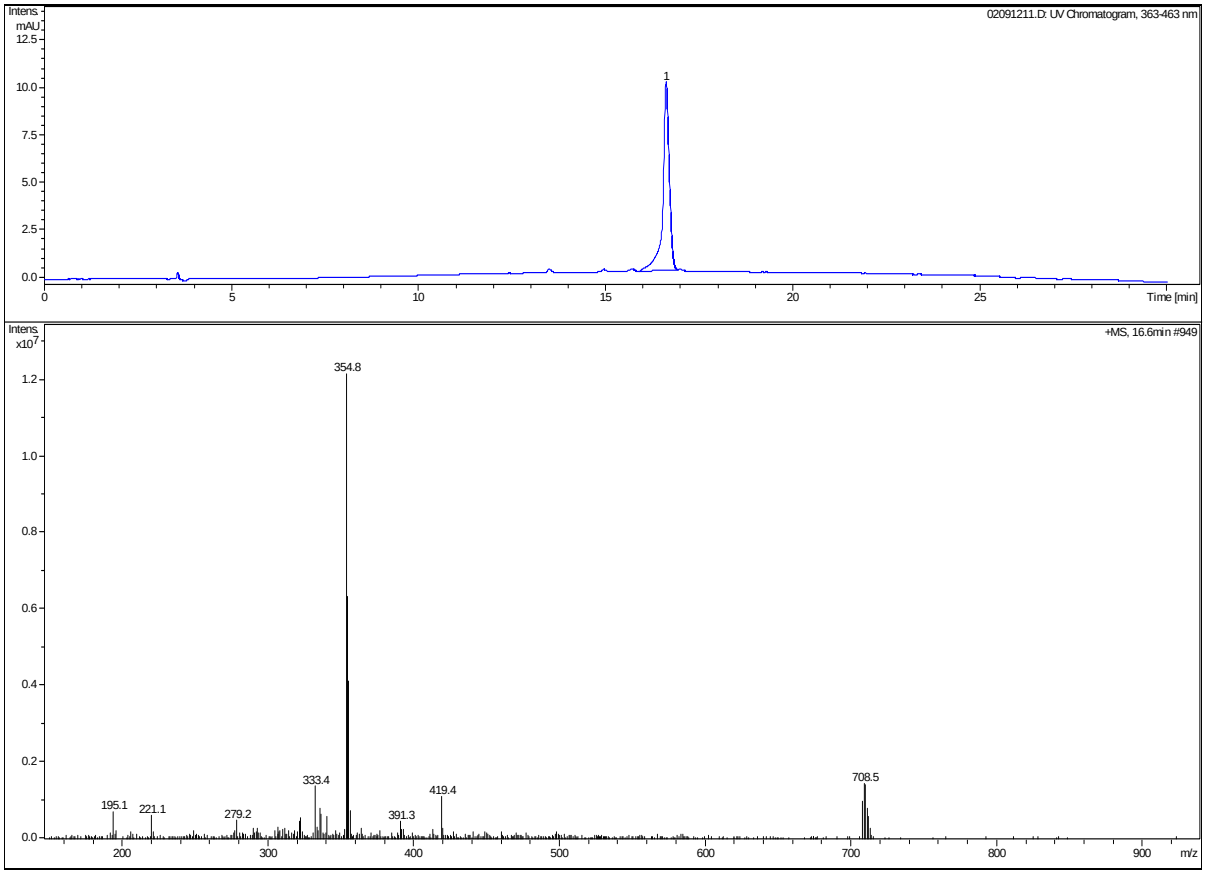


Figure S4.14. LC-MS analysis of compound P1-A8.

Compound Chromatogram Report - MS

Analysis Name: 06121202.D **Instrument:** LC-MSD-Trap-SL **Print Date:** 06/12/2012 11:43:54 AM
Method: PTAMID~1.M **Operator:** Administrator **Acq. Date:** 6/12/2012 10:35:00 AM
Sample Name: 3-7
Analysis Info:

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	52.5	Scan Begin	150 m/z
Ion Polarity	Positive	Octopole RF Amplitude	200.0 Vpp	Scan End	2200 m/z
Ion Source Type	ESI	Capillary Exit	135.7 Volt	Averages	5 Spectra
Dry Temp (Set)	350 °C	Skimmer	40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	50.00 psi	Oct 1 DC	12.00 Volt	ICC Target	30000
Dry Gas (Set)	11.00 l/min	Oct 2 DC	1.73 Volt	Charge Control	on

Compound List:

#	RT [min]	Range [min]	Height	Area	Area Frac %
1	14.4	14.2 - 14.8	30	341	100.0

Chromatograms:

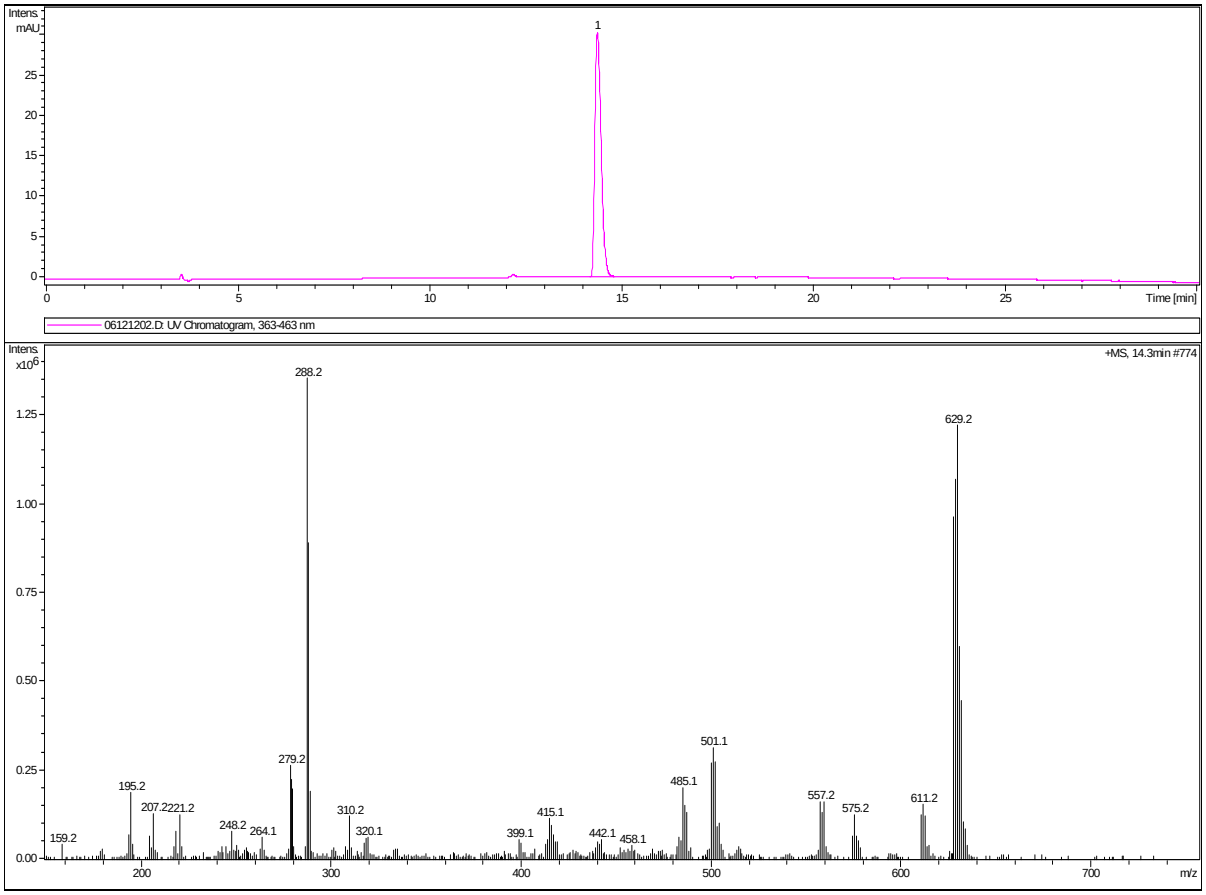


Figure S4.15. LC-MS analysis of compound P3-A7.

5. Cell proliferation assays

Cell culture. The human non-small cell lung cancer cell line, NCI-H460, was obtained from the American Type Culture Collection (Rockville, MD, USA) and was cultured in RPMI-1640 media (HyClone) containing 4.5 g/L glucose, 1.5 g/L sodium bicarbonate, 10 mM HEPES, and 110 mg/L sodium pyruvate supplemented with 10% fetal bovine serum (FBS), 10% penstrep (P&S), and 10% L-glutamine. Cells were incubated at a constant temperature at 37 °C in a humidified atmosphere containing 5% CO_2 and were subcultured every 2 to 3 days in order to maintain cells in logarithmic growth.

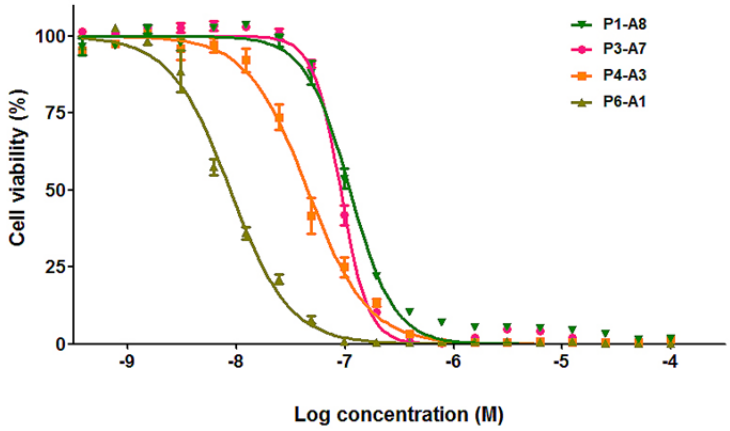


Figure S5.1. Drug-response curves for cell proliferation assays in NCI-H460 cells treated with selected compounds. Error bars indicate ± standard deviations from the mean for two independent experiments performed in triplicate.

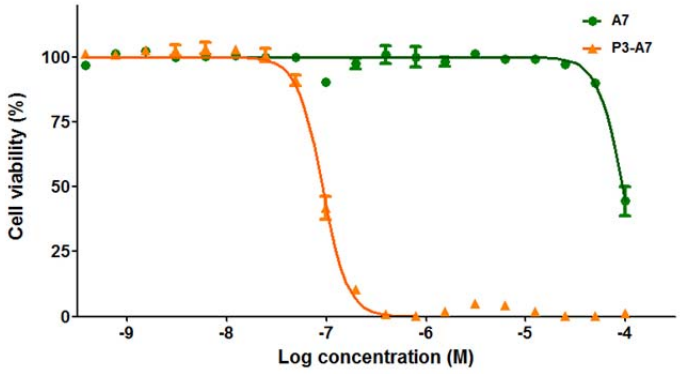


Figure S5.2. Drug-response curves for cell proliferation assays in NCI-H460 cells treated with **P3-A7** and the corresponding acridine ligand **A7**. Error bars indicate ± standard deviations from the mean for two independent experiments performed in triplicate.

6. References

[1] S. C. Dhara, *Indian Journal of Chemistry* **1970**, *8*, 193-194.

[2] E. T. Martins, H. Baruah, J. Kramarczyk, G. Saluta, C. S. Day, G. L. Kucera and U. Bierbach, *Journal of Medicinal Chemistry* **2001**, *44*, 4492-4496.

[3] T. M. Augustus, J. Anderson, S. M. Hess and U. Bierbach, *Bioorganic & Medicinal Chemistry Letters* **2003**, *13*, 855-858.

[4] Z. Ma, J. R. Choudhury, M. W. Wright, C. S. Day, G. Saluta, G. L. Kucera and U. Bierbach, *Journal of Medicinal Chemistry* **2008**, *51*, 7574-7580.

[5] L. A. Graham, G. M. Wilson, T. K. West, C. S. Day, G. L. Kucera and U. Bierbach, *ACS Medicinal Chemistry Letters* **2011***, 2*, 687-691.