

## SUPPORTING INFORMATION

### Oxidative Reactivities of 2-Furylquinolines: Ubiquitous Scaffolds in Common High-Throughput Screening Libraries

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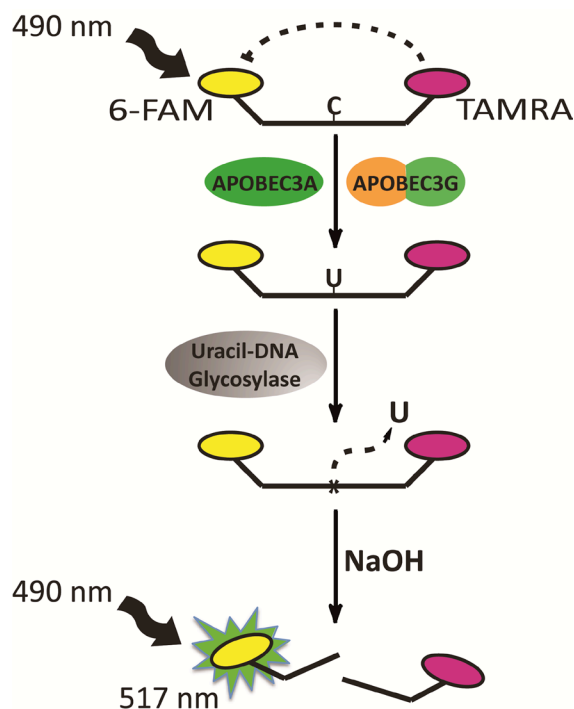
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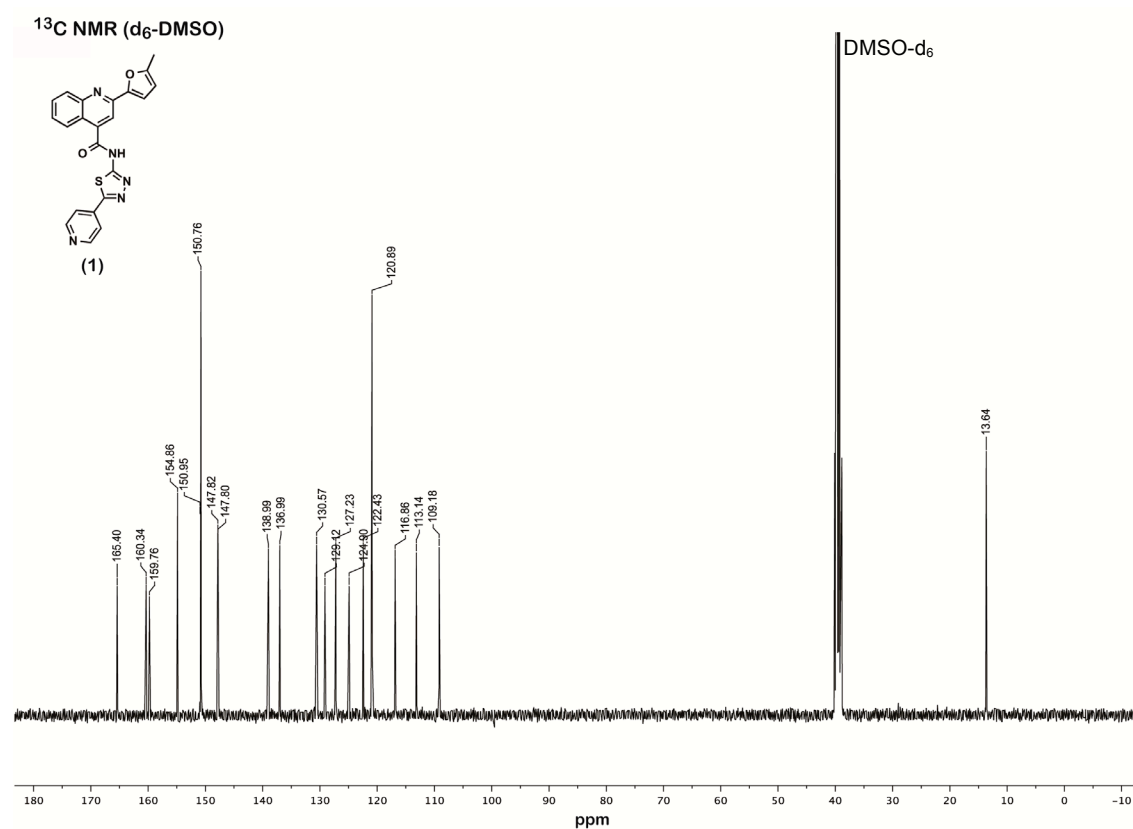
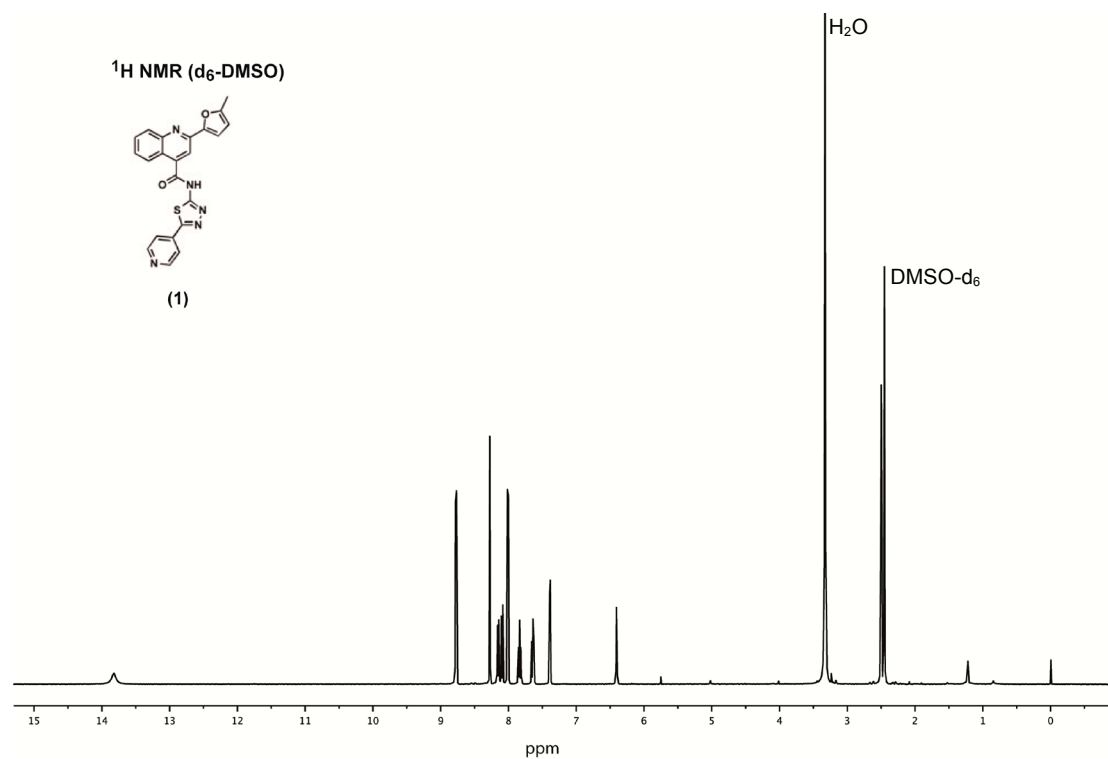
## I. Description & Graphical Representation of the HTS/In Vitro Assay

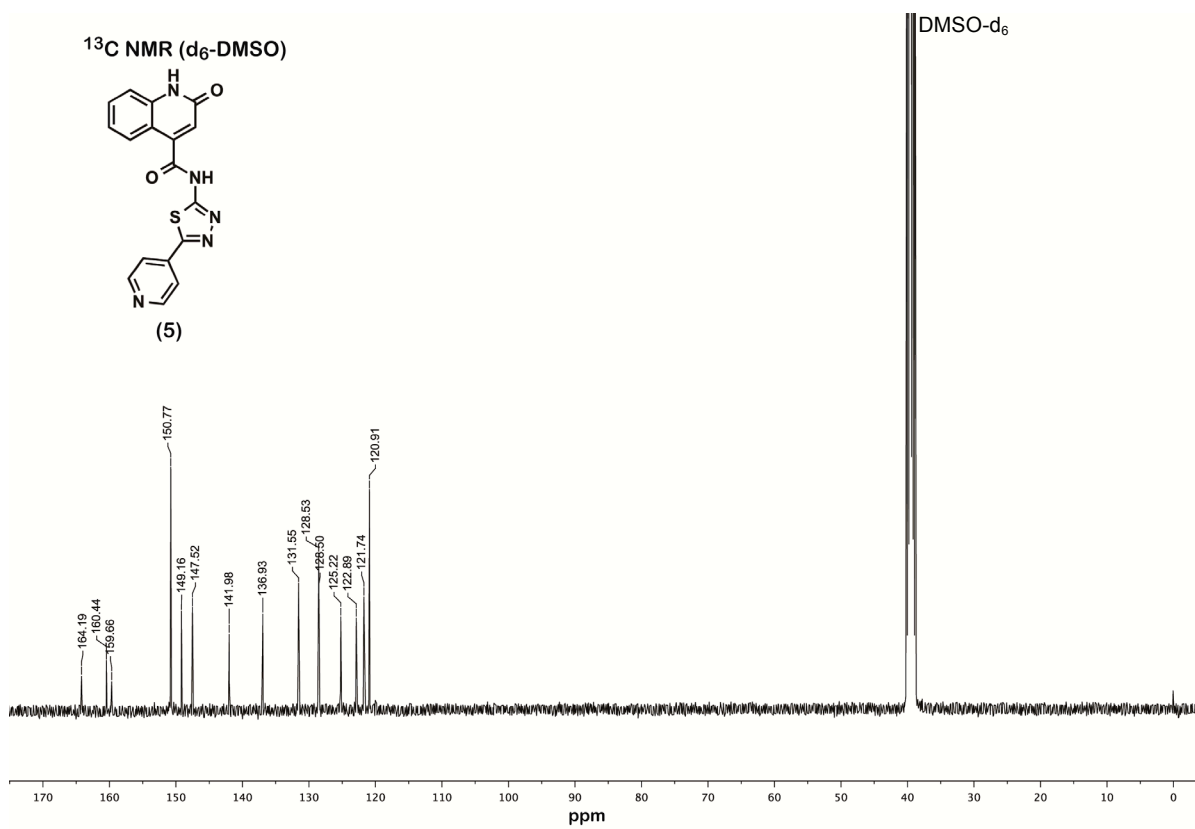
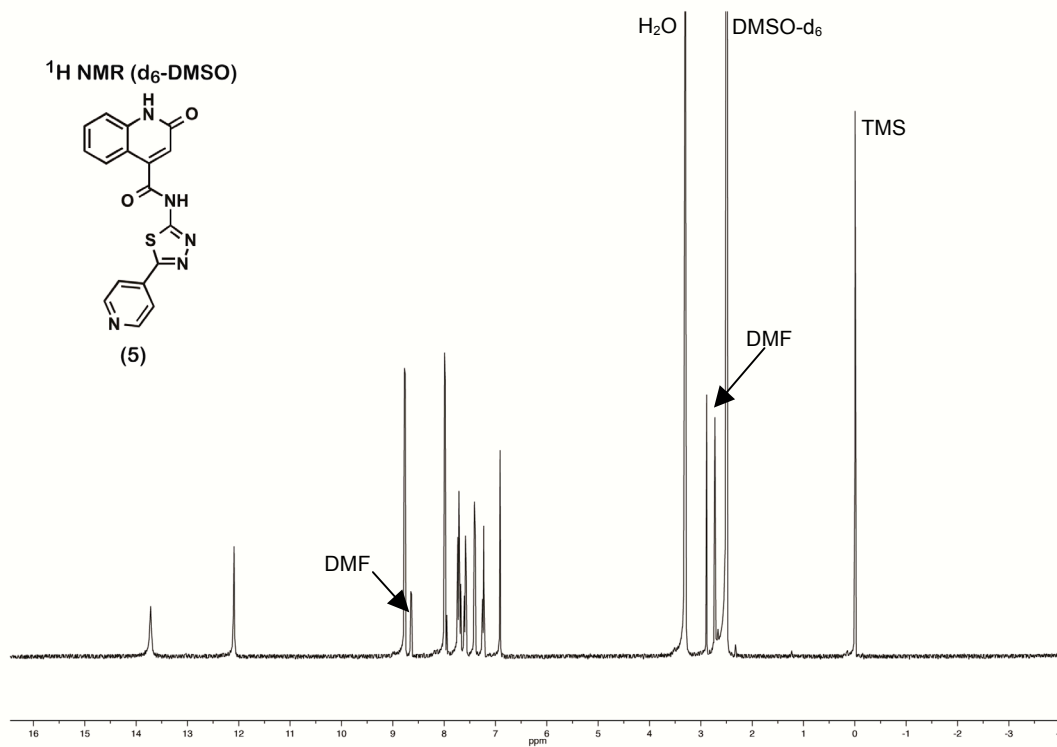


**Figure S1.** The HTS assay is published in Li, M.; et al. *ACS Chem. Biol.* **2012**, *7*, 506. To be classified as an APOBEC3 inhibitor, a 40% reduction in deaminase efficiency had to be observed in two independent experiments.

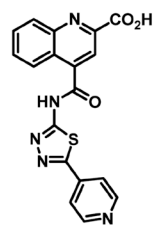
The *in vitro* assay was adapted from the HTS assay. In short, compounds were diluted with 50 mM Tris-Cl, pH 7.4, 150 mM NaCl, 10% glycerol, 0.5% Triton X-100, 1 mM PMSF (MP Biomedicals), 1 µg/mL Aprotinin (Sigma), 1 µg/mL Leupeptin (MP Biomedicals), and 1 µg/mL Pepstatin A (Fisher Scientific) to the following concentrations: 200 µM, 100 µM, 50 µM, 25 µM, 12.5 µM, 6.3 µM, 3.1 µM, and 1.6 µM. Proteins were diluted in the same buffer to working concentrations. 10 ng APOBEC3A, 40 ng APOBEC3B, and 100 ng APOBEC3G were used in each reaction. 10 pmol ssDNA substrate 5'-6-FAM-AAA-CCC-AAA-GAG-AGA-ATG-TGA-TAMRA-3' (Biosearch Technologies, Inc.) and 0.02 units of UDG (New England Biosciences) were diluted in 10 µL of 50 mM Tris-Cl, pH 7.4, 10 mM EDTA. Ten microliters of compound at various concentrations were incubated with 10 µL of protein and 10 µL of ssDNA substrate in Nunc 384-well black plates for 2 h at 37 °C. After which, 3 µL of 4 N NaOH was added, followed by mixing and incubating at 37 °C for another 30 min. Three microliters of 4 N HCl and 37 µL of 2 M Tris-Cl (pH 7.9) were then added for neutralization, and the relative deaminase activity was quantified by reading fluorescence with excitation at 490 nm and emission at 520 nm on a Synergy Mx Monochromator-based Multi-Mode (BioTek Instruments, Inc.). UDG assays omitted the deaminase and used a ssDNA substrate with a single uracil in place of the A3G-preferred cytosine (5'-6-FAM-AAA-CCU-AAA-GAG-AGA-ATG-TGA-TAMRA-3'). All compound stocks were suspended in 10 mM DMSO. IC<sub>50</sub>s were calculated in GraphPad Prism.

## II. Spectral Data of Synthesized Compounds

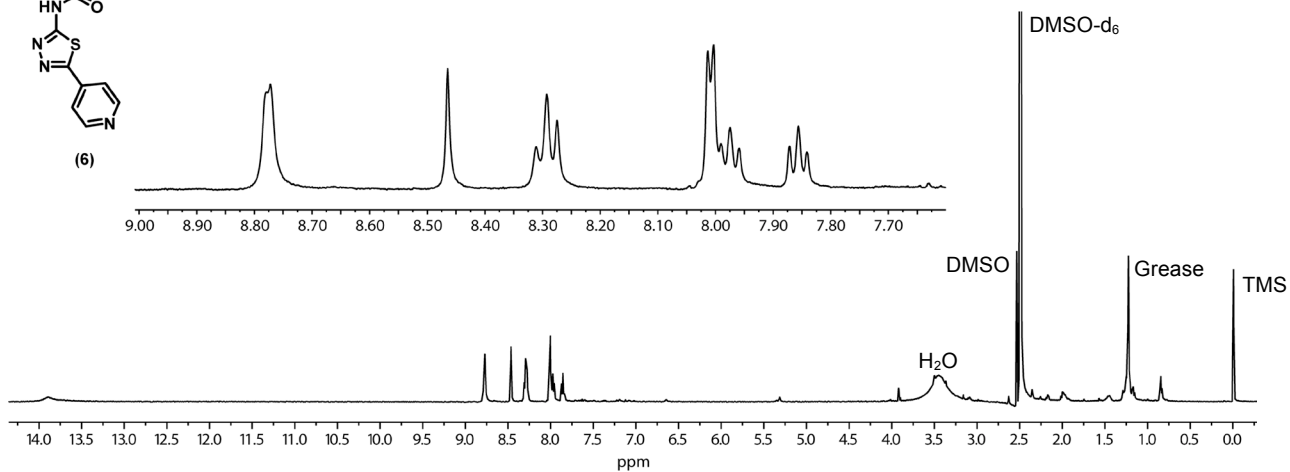




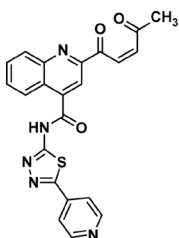
<sup>1</sup>H NMR (d<sub>6</sub>-DMSO)



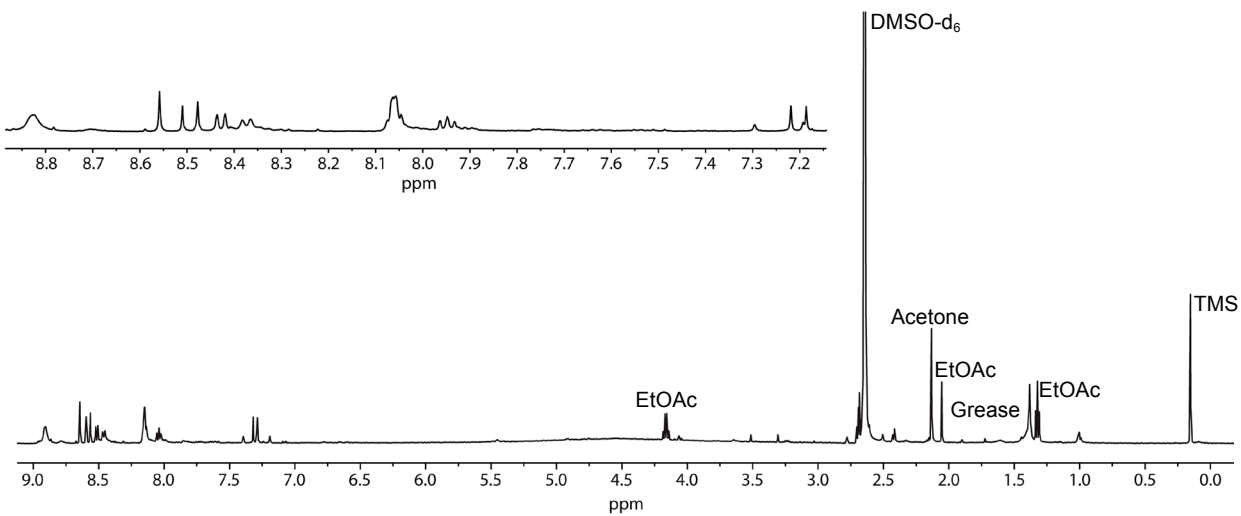
(6)



<sup>1</sup>H NMR (DMSO-d<sub>6</sub>)



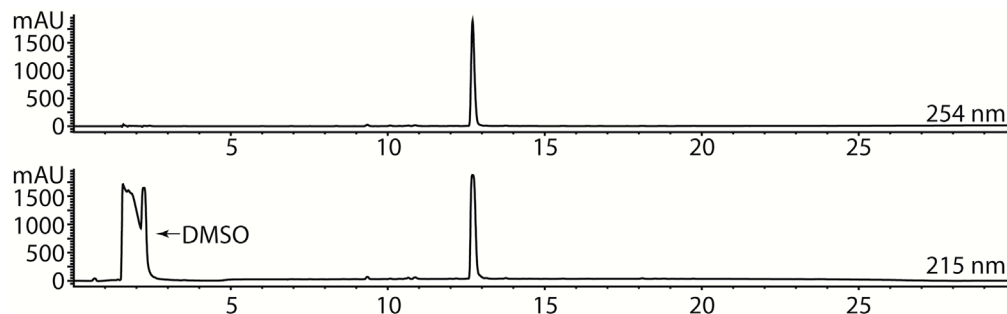
(8)



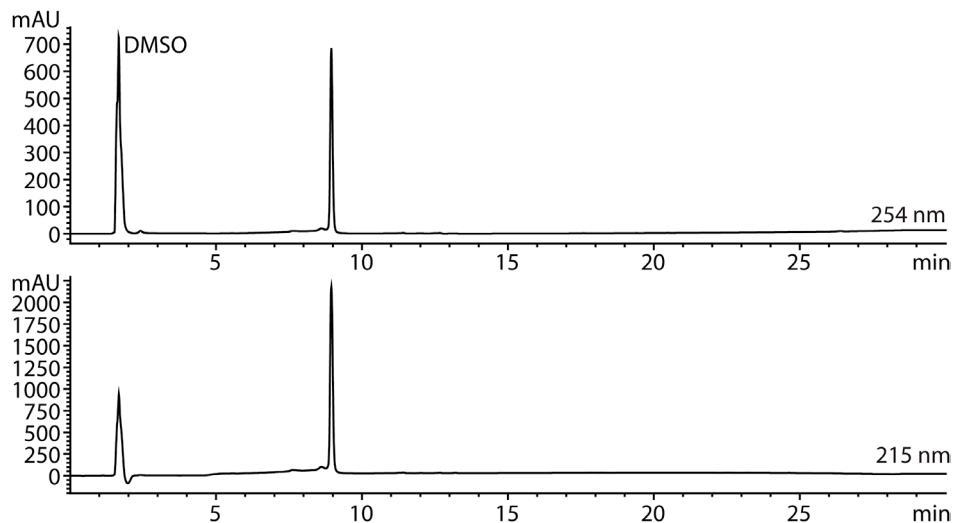
### III. HPLC Chromatograms of Synthesized & Isolated Compounds

**General Protocol for HPLC Analysis of Synthesized and Isolated Compounds.** DMSO stock solutions of newly synthesized molecules were dissolved in distilled and deionized water (ddH<sub>2</sub>O) containing trifluoroacetic acid (TFA, 0.1% v/v) and analyzed on an Agilent 1200 series instrument equipped with a diode array detector and Zorbax SB-C18 column (4.6 x 150 mm, 3.5 μm, Agilent Technologies). The analysis method (1 mL/min flow rate) involved isocratic 10% MeCN in ddH<sub>2</sub>O (both containing 0.1% TFA; 0 to 2 mins) followed by linear gradients of 10% to 85% MeCN in ddH<sub>2</sub>O (both containing 0.1% TFA; 2 to 24 mins) and 85% to 95% MeCN in ddH<sub>2</sub>O (both containing 0.1% TFA; 24 to 26 mins).

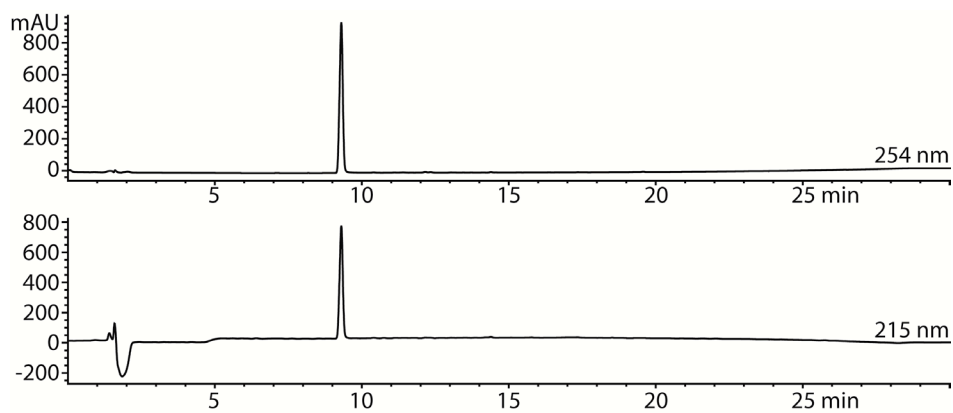
#### Synthesized 1:



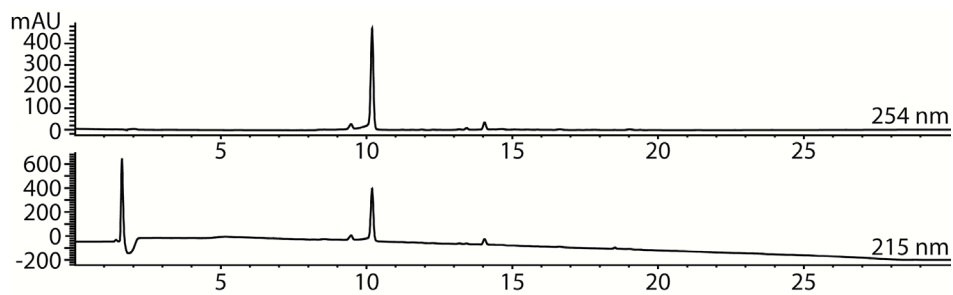
#### Synthesized 5:



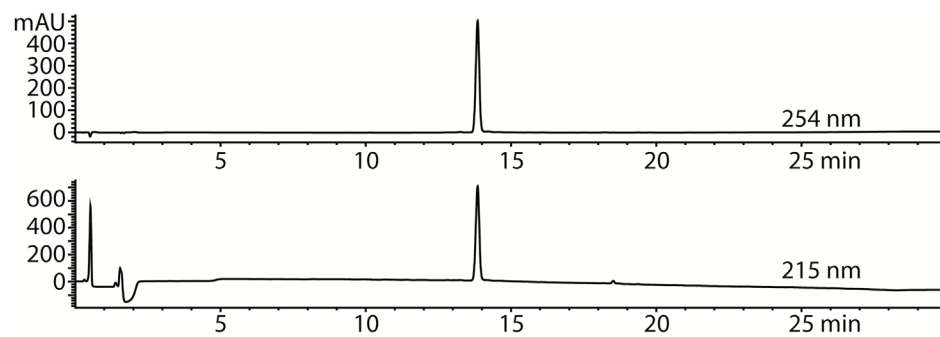
Synthesized **6**:



Isolated **7a-7b**:

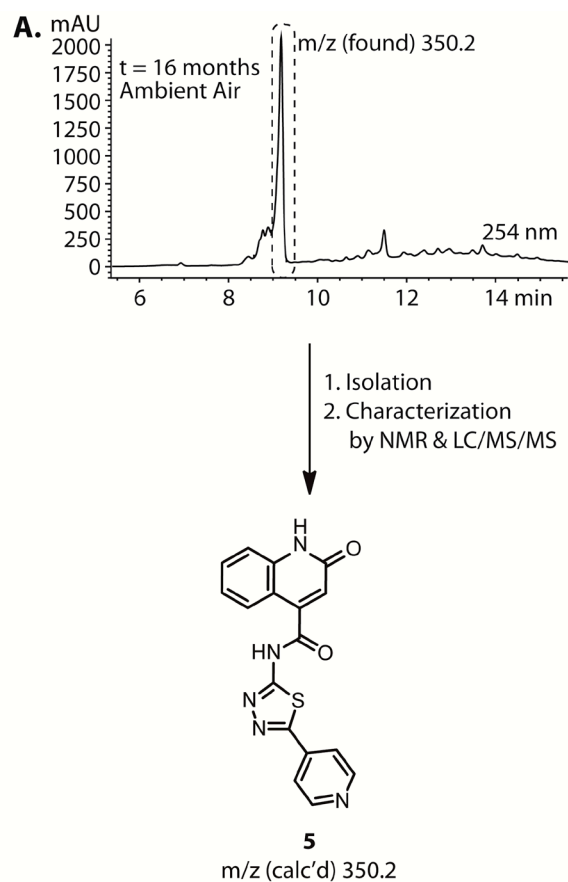


Synthesized **8**:

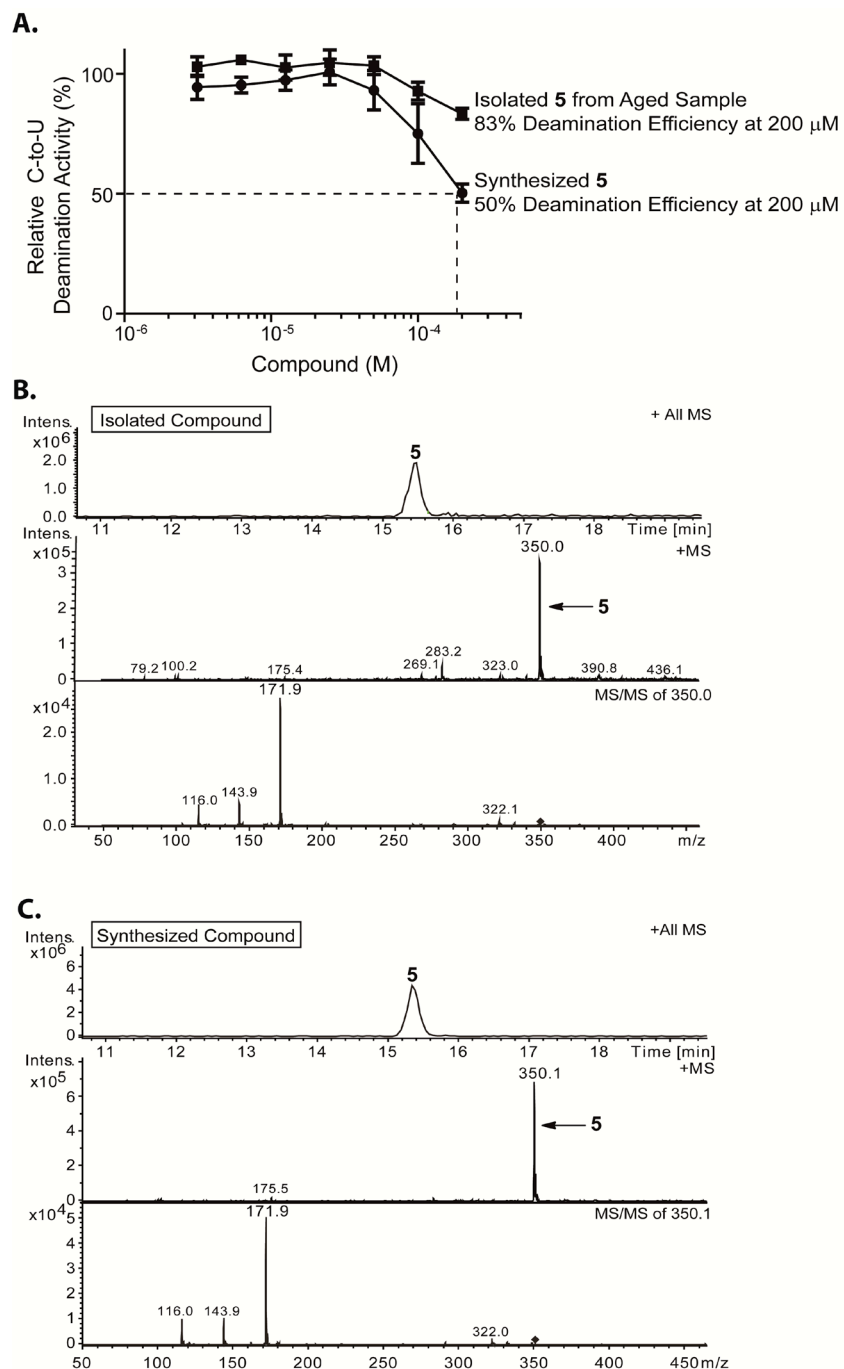




#### IV. Isolation, Synthesis & Biochemical Evaluation of **5**

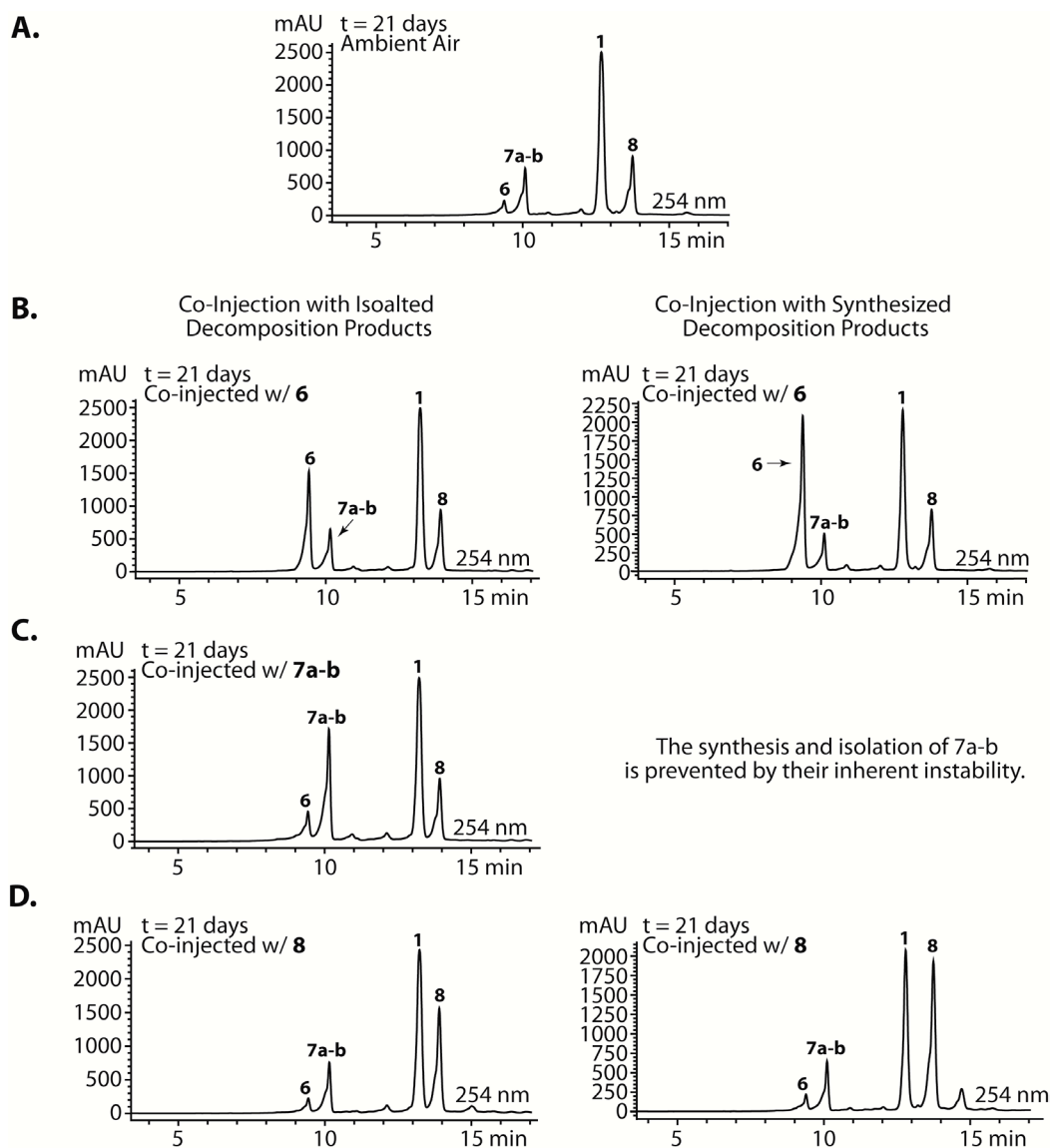


**Figure S2.** Analytical HPLC analysis of a 10 mM DMSO stock solution of **1**. After 16 months, **1** converted to **5** as determined by HPLC isolation and characterization by  $^1\text{H}$  and  $^{13}\text{C}$  NMR and LC-MS/MS.



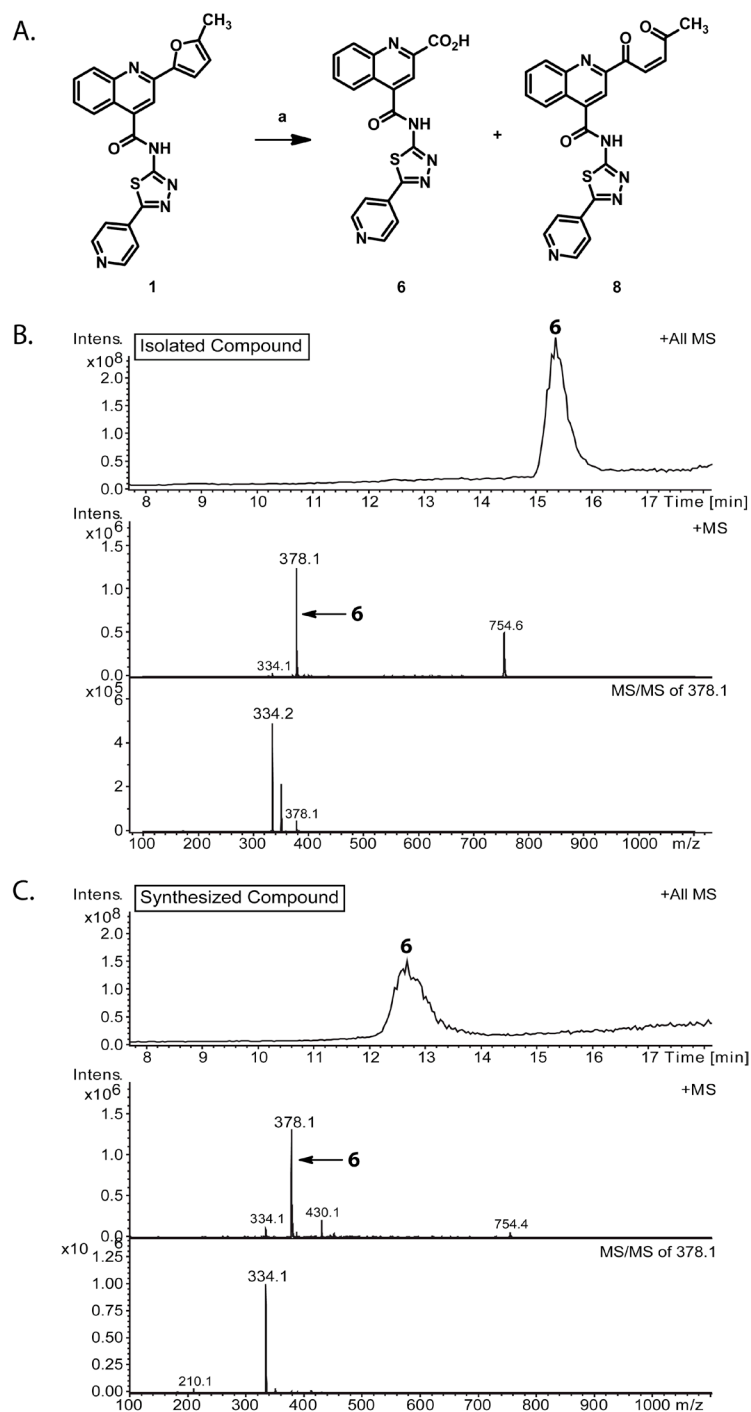
**Figure S3.** (A) Synthesis of **5**. *Reagents and conditions:* (a) PyBOP, NMM, DMF, 59%. (B) Dose response assays for A3G inhibition by **5** isolated from an aged DMSO stock solution (Figure S2) and synthesized **5**. Assays were performed in triplicate and deaminase activity was quantified as described previously.<sup>18</sup> Means  $\pm$  standard deviations are depicted on graph. (C) LC-MS/MS analysis of isolated **5** compared to the LC-MS/MS chromatogram of synthesized **5** (D).

## V. HPLC Chromatograms of Isolated & Synthesized Compounds Co-injected with 1

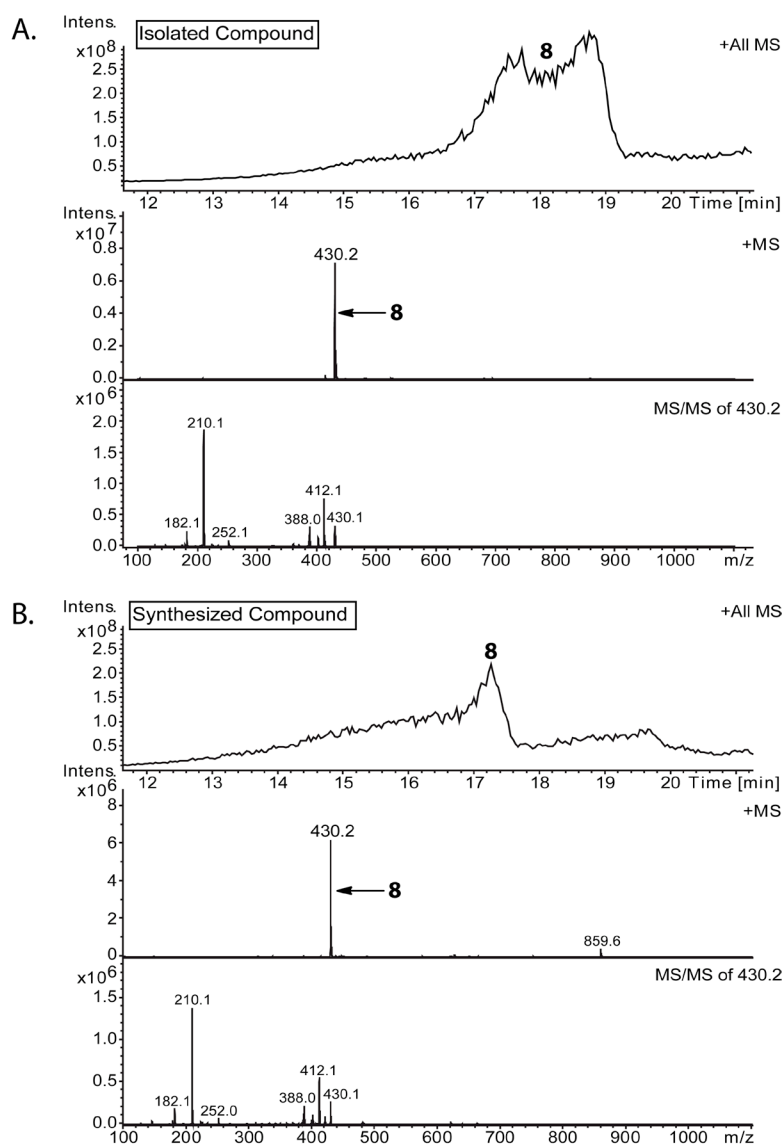


**Figure S4. General Protocol for HPLC Analysis.** Co-Injections of Isolated and Synthesized Decomposition Products **6**, **7a-b**, and **8** with Aged **1**. Ten mM DMSO stock solutions of **1** incubated for 21 days (A) were spiked with 10 mM DMSO stock solutions of standard (either isolated or synthesized **6** (B), **7a-b** (C), or **8** (D)) and diluted with biological grade MeOH so that the final concentration of each stock solution was 1 mM. The resulting solutions were analyzed by HPLC.

## VI. Synthesis & LC-MS/MS Analysis of Synthesized **6**

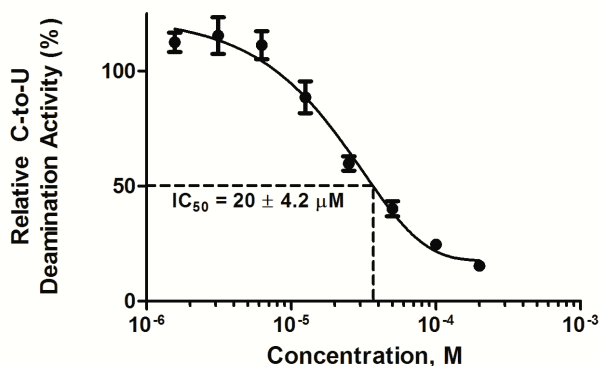


## VII. LC-MS/MS Analysis of Synthesized **8**

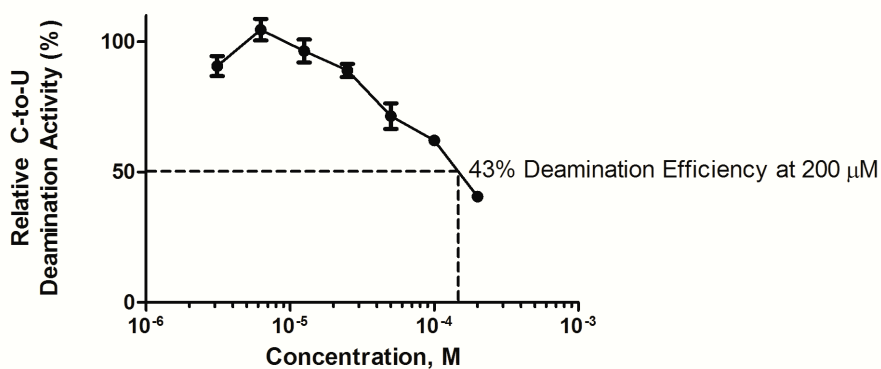


**Figure S6.** The synthesis of **8** is shown in Figure S4A. (A) LC-MS/MS analysis of isolated **6** compared to the LC-MS/MS chromatogram of synthesized **8** (B). The difference in retention time between the isolated and synthesized material is explained by differences in sample preparation. Isolated **8** was injected in a MeCN/H<sub>2</sub>O solution, while synthesized **8** was injected in a DMSO/MeOH solution.

### VIII. Biochemical Evaluation of 6 & 8



**Figure S7.** Dose response assays for A3G inhibition by synthesized **8**. Assays were performed in triplicate and deaminase activity was quantified as described previously.<sup>18</sup> Means  $\pm$  standard deviations are indicated.



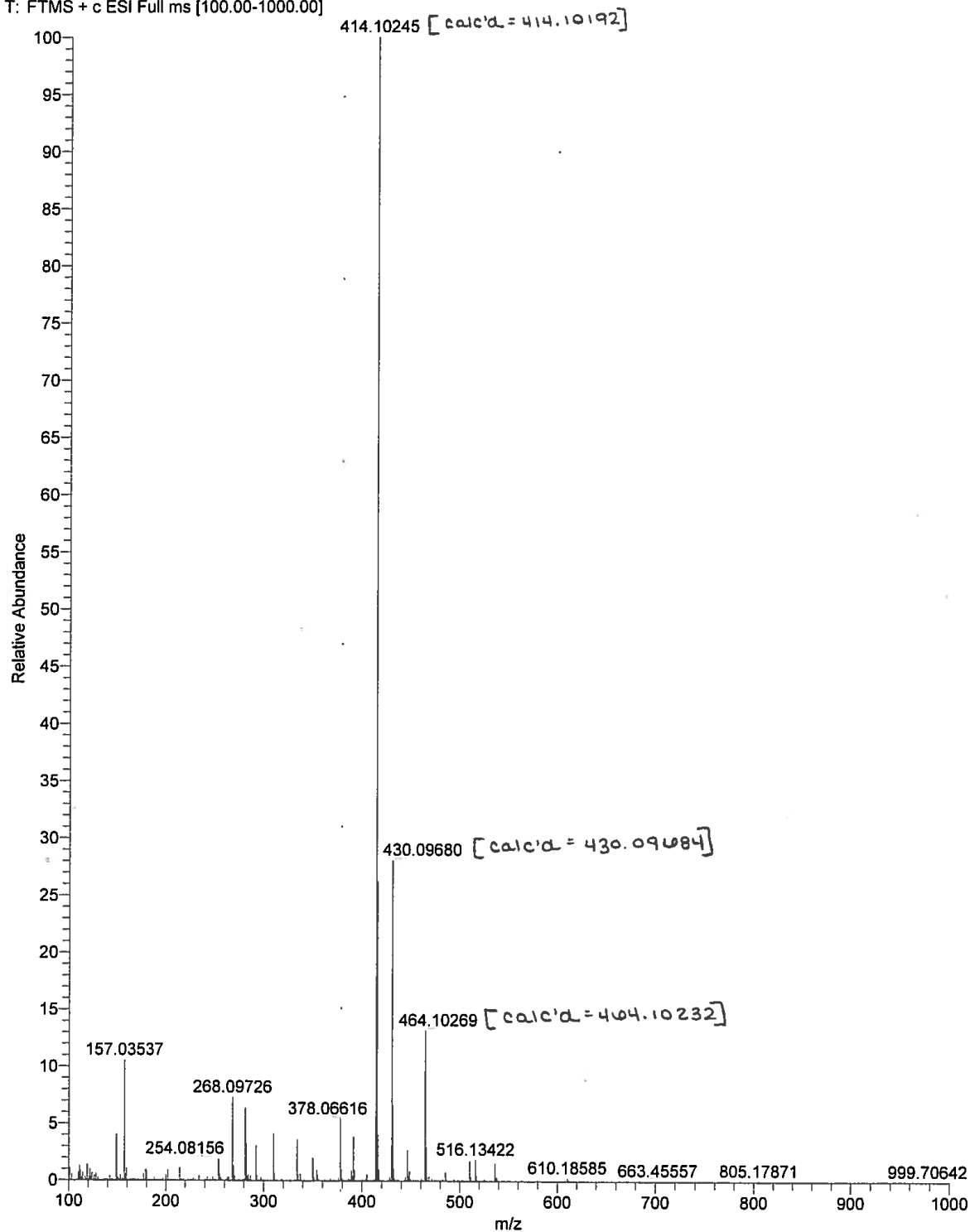
**Figure S8.** Dose response assays for A3G inhibition by synthesized **6**. Assays were performed in triplicate and deaminase activity was quantified as described previously.<sup>18</sup> Means  $\pm$  standard deviations are indicated.

# IX. High Resolution Mass Spectra of Aged 1 (t = 21 days) as 10 mM DMSO Stock

D:\Data\...MOHarkiO0514-1\ME03047

5/27/2014 1:44:38 PM

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T: FTMS + c ESI Full ms [100.00-1000.00]

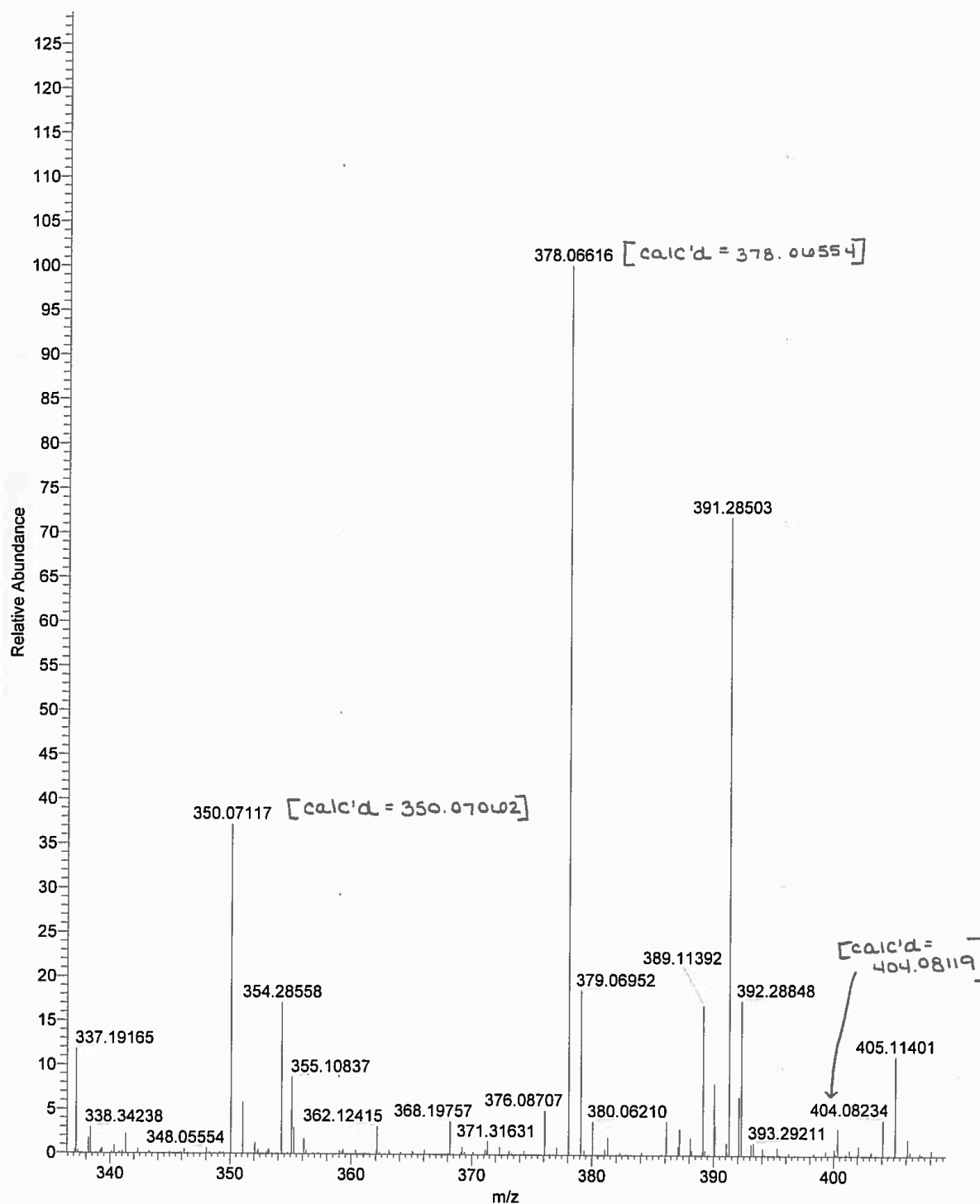


IX (Cont'd). Magnified HRMS of Aged 1 (t = 21 days) as 10 mM DMSO Stock. Spectrum from m/z = 335 – 410

D:\Data\...MOHarki00514-1\ME03047

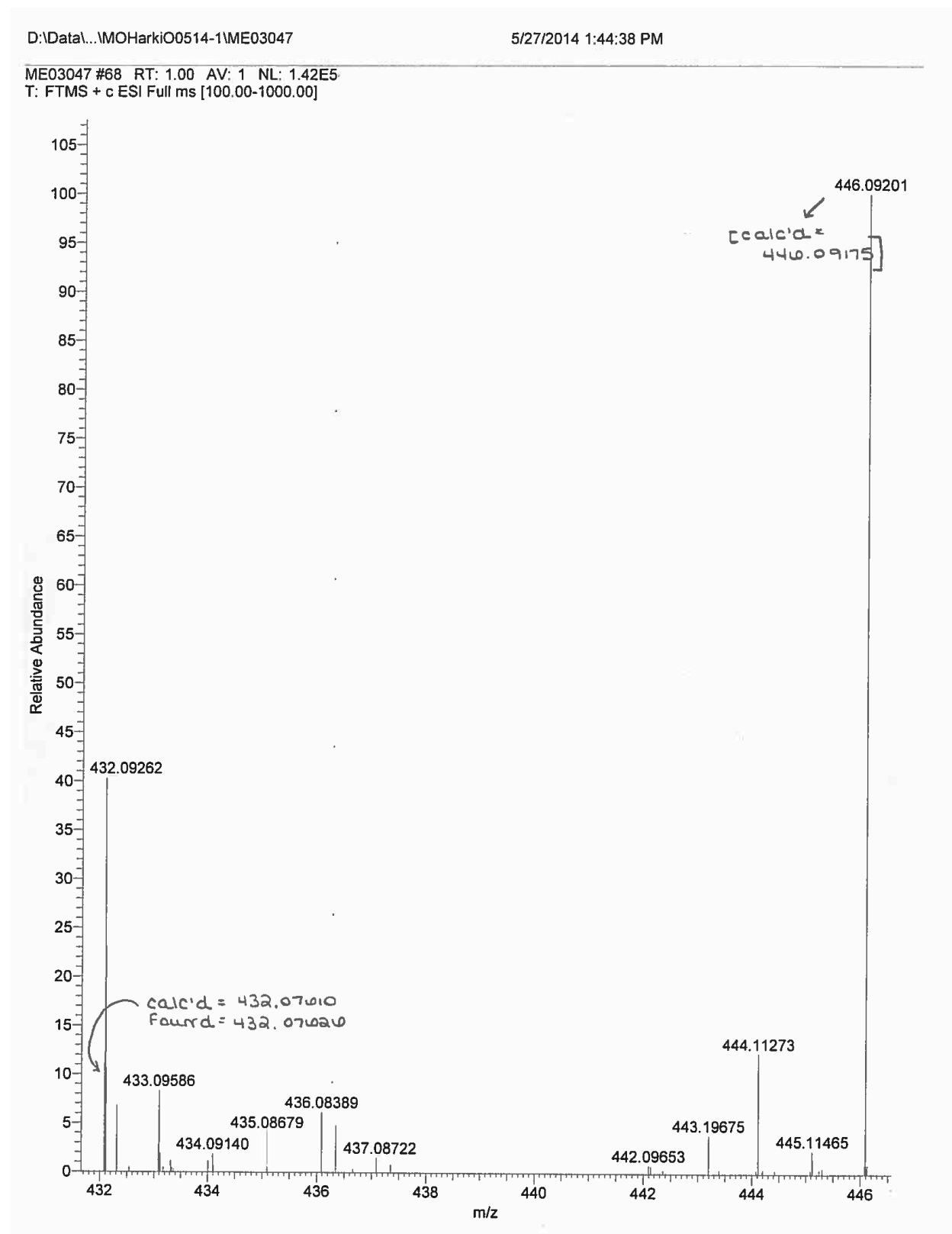
5/27/2014 1:44:38 PM

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T: FTMS + c ESI Full ms [100.00-1000.00]





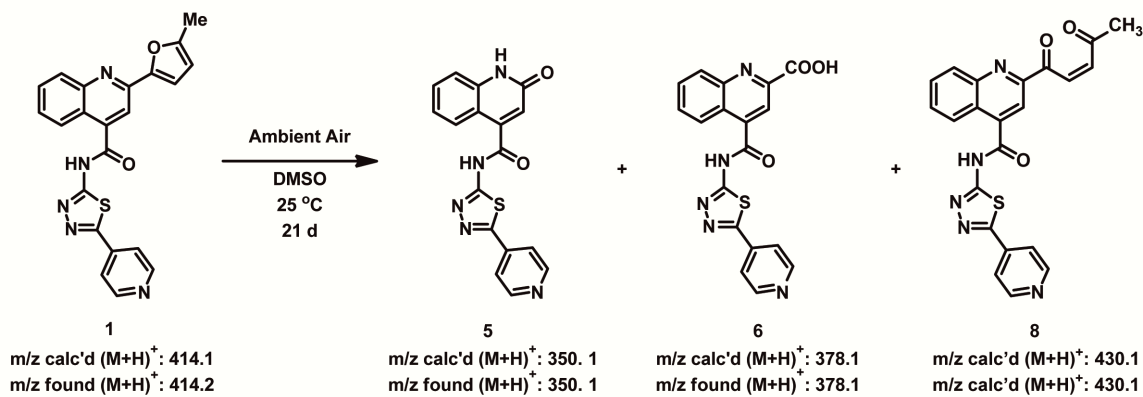
IX (Cont'd). Magnified HRMS of Aged 1 (t = 21 days) as 10 mM DMSO Stock. Spectrum from m/z = 430 – 450



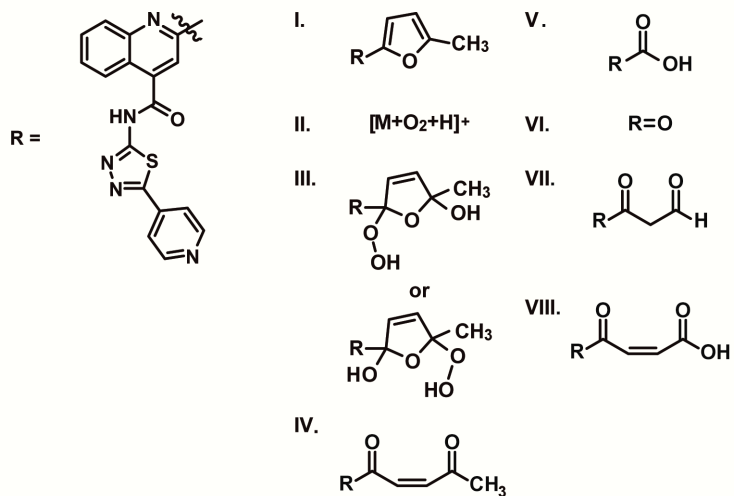
## X. LC/MS Analysis of Aged 1

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 21 d)

A.



B.

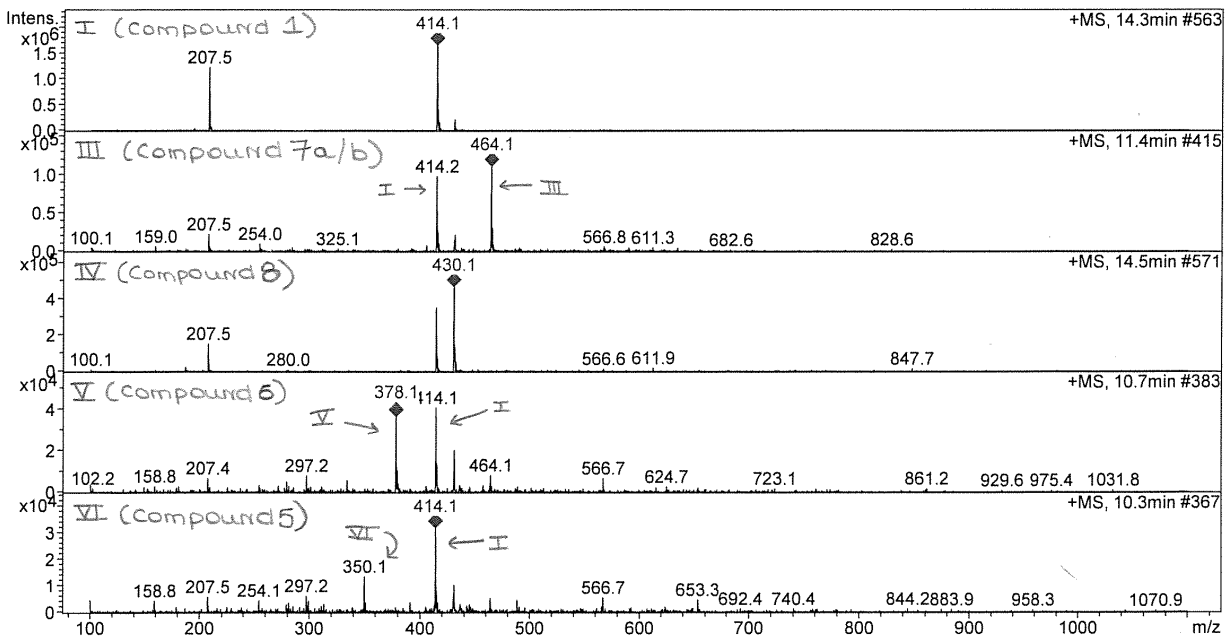
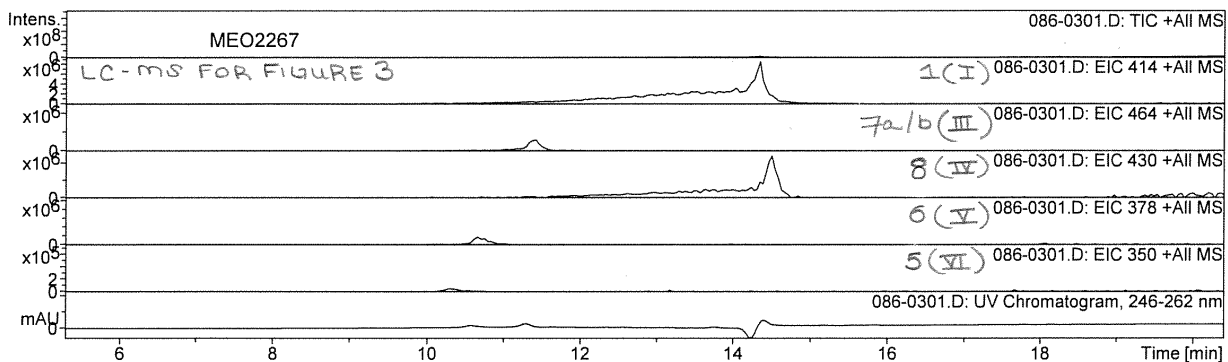


C.

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 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

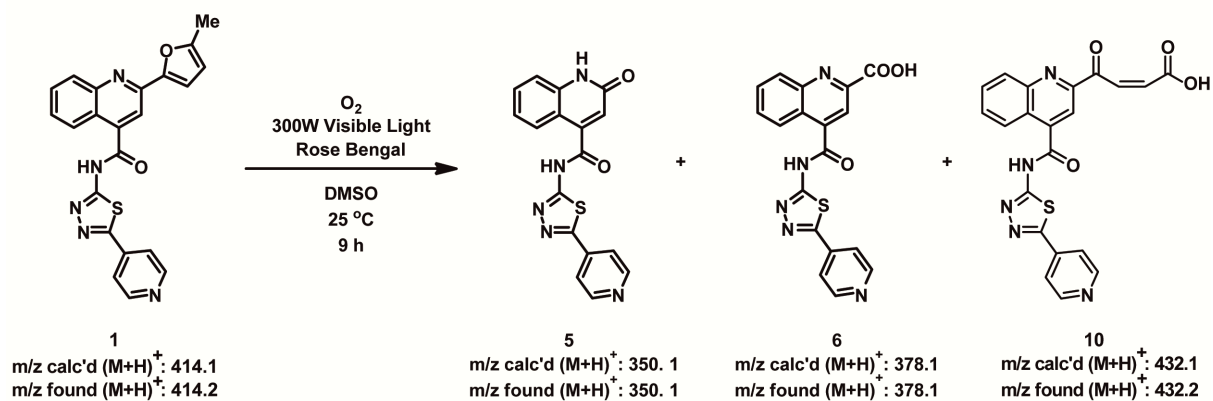
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Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	31098 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



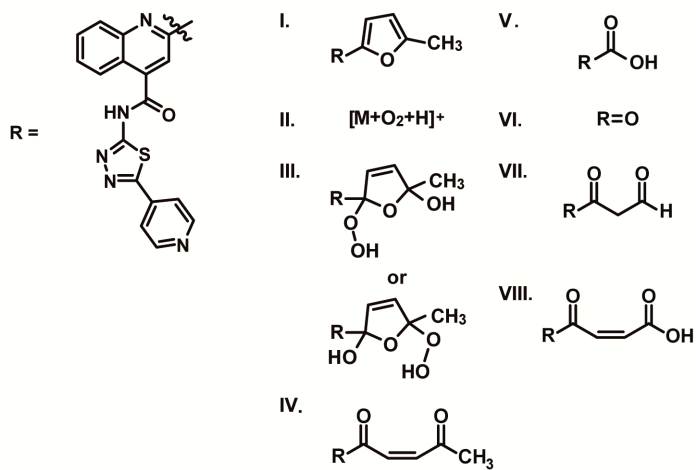
## XI. LC/MS Analysis of Aged 1

(Reaction Conditions: 10 mM DMSO Stock, O<sub>2</sub> Atmosphere, 300W Visible Light, RB, 25 °C, 9 h)

A.



B.

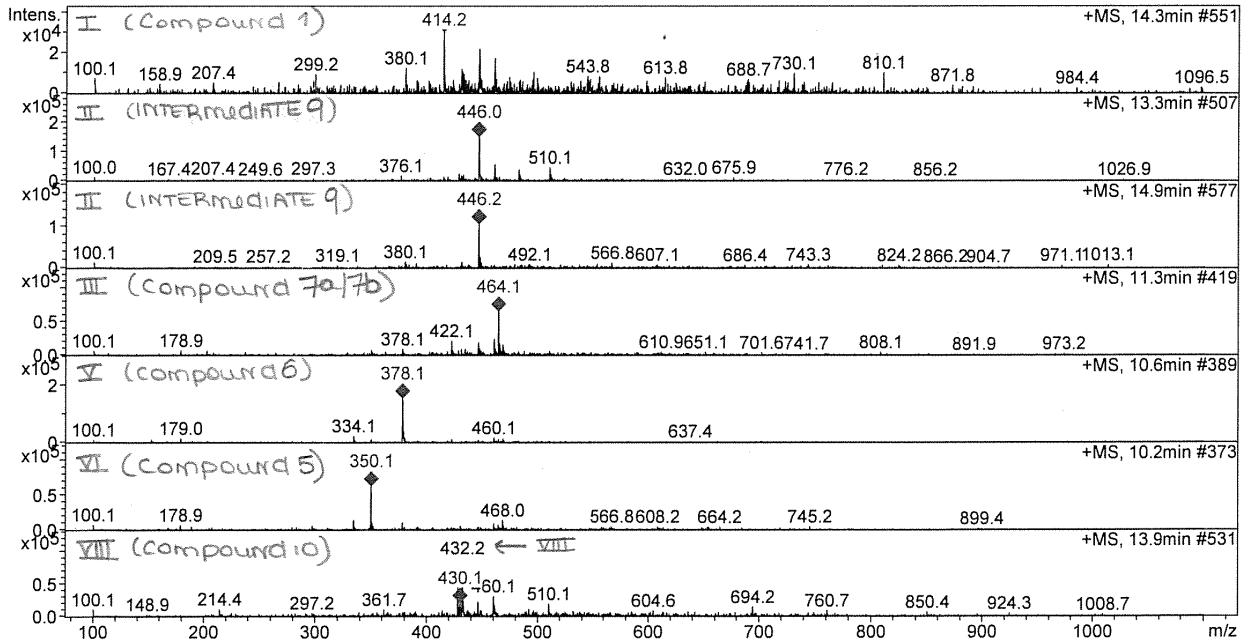
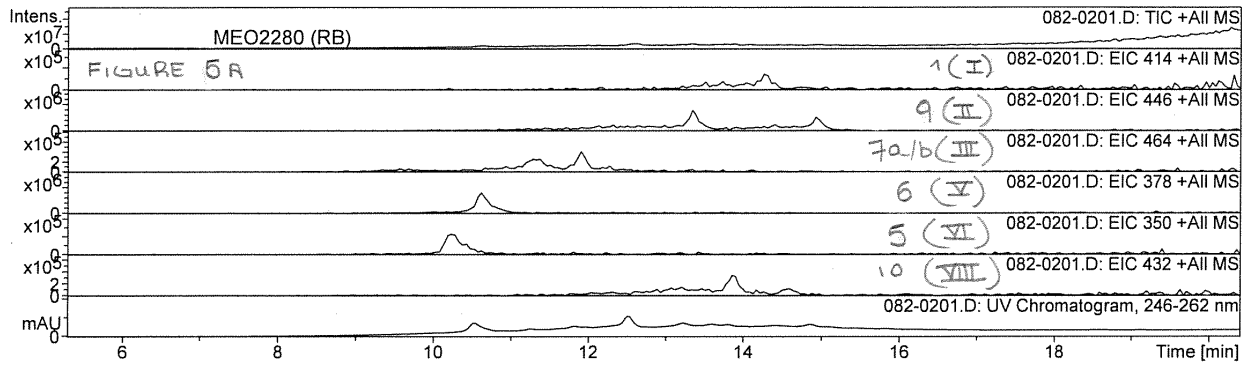


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 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

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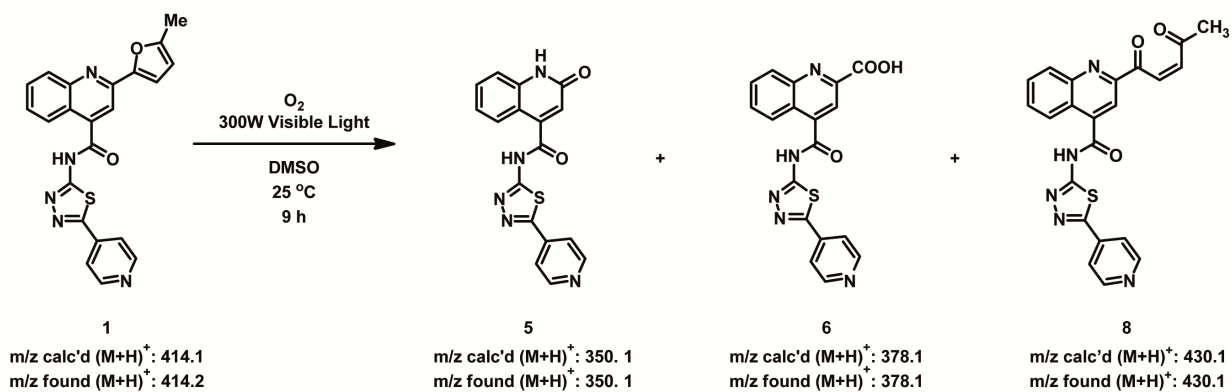
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	38837 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



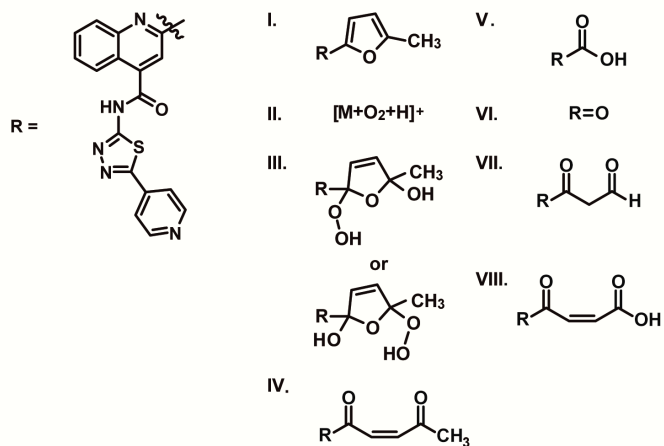
## XII. LC/MS Analysis of Aged 1

(Reaction Conditions: 10 mM DMSO Stock, O<sub>2</sub> Atmosphere, 300W Visible Light, 25 °C, 9 h)

A.



B.

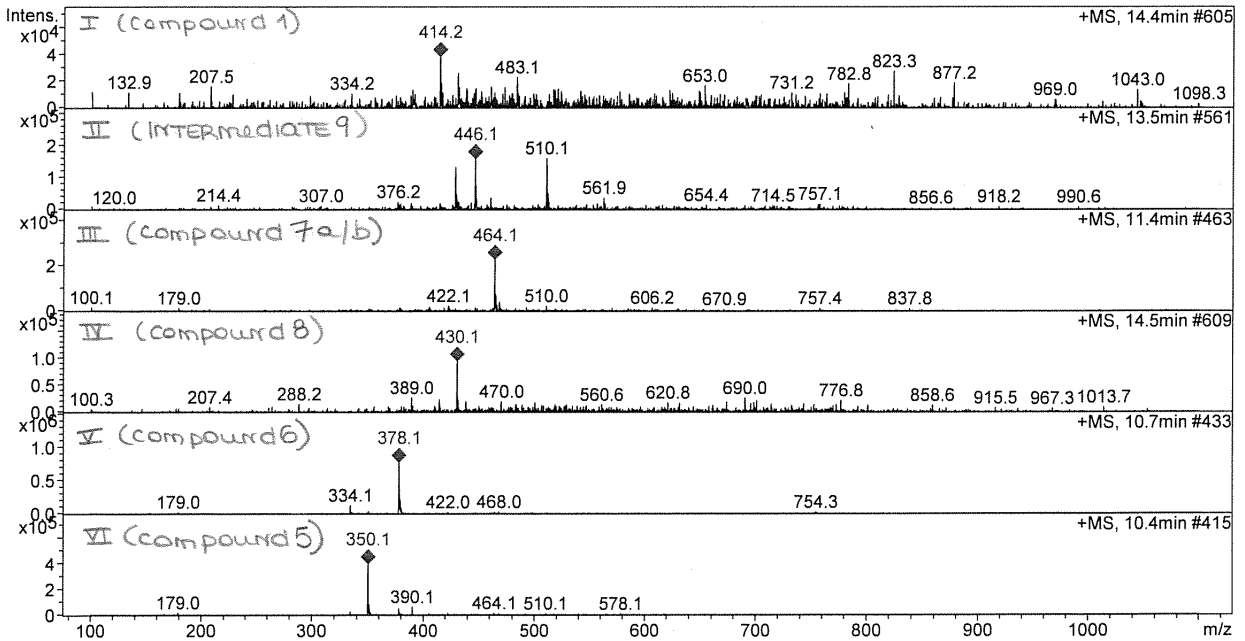
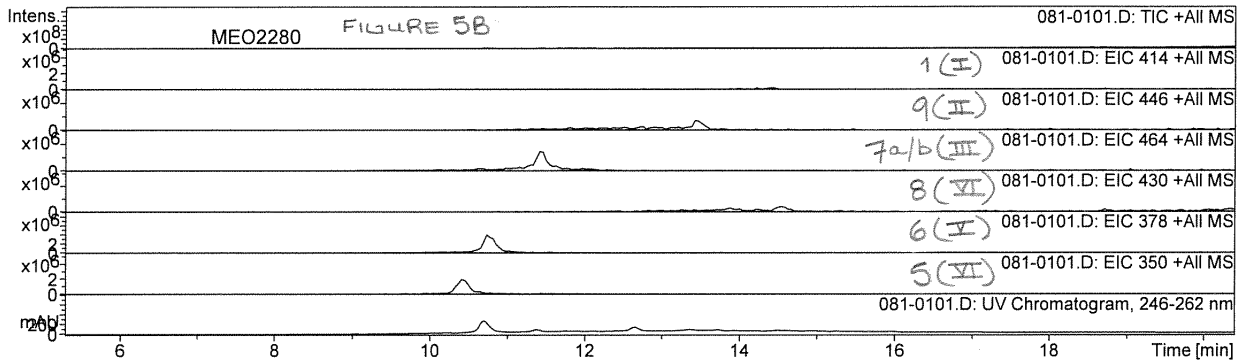


C.

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 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

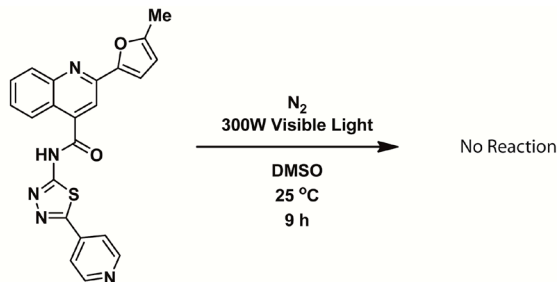
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	35189 µs	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



### XIII. LC/MS Analysis of Aged 1

(Reaction Conditions: 10 mM DMSO Stock, N<sub>2</sub> Atmosphere, 300W Visible Light, 25 °C, 9 h)

A.

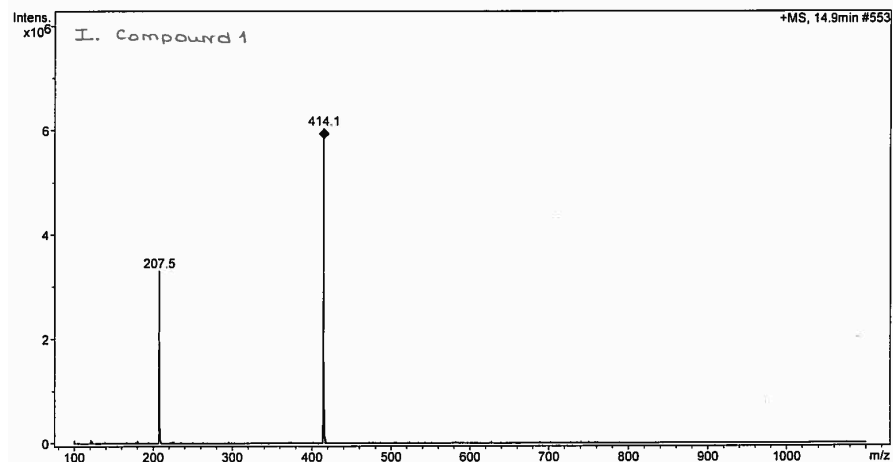
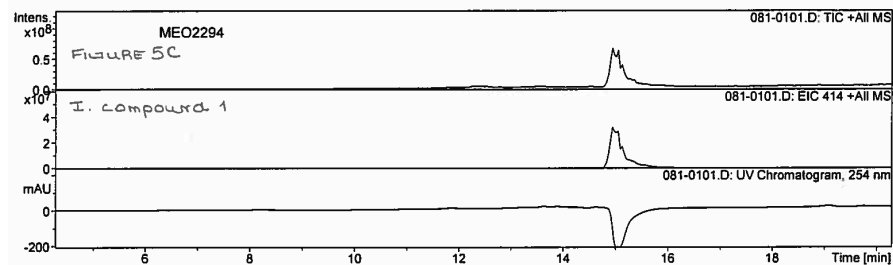


B.

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Method 130701A.M Instrument LC-MSD-Trap-SL  
Comment

#### Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	25880 µs	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

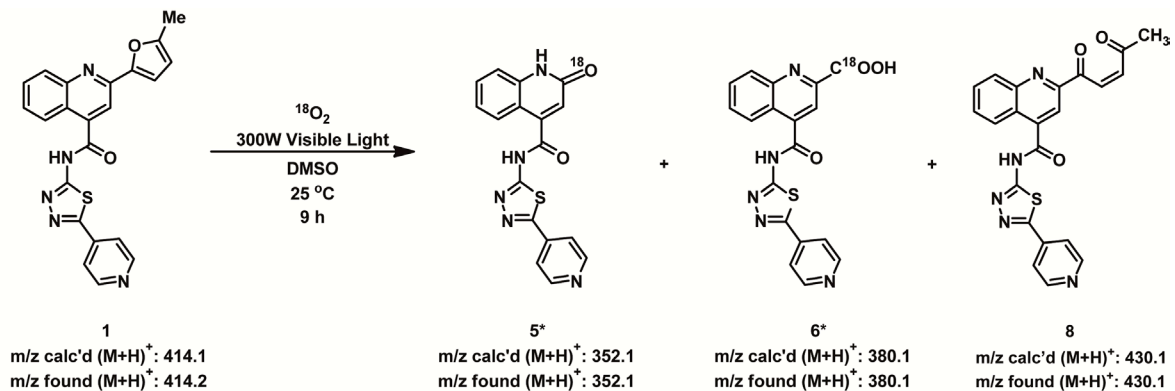




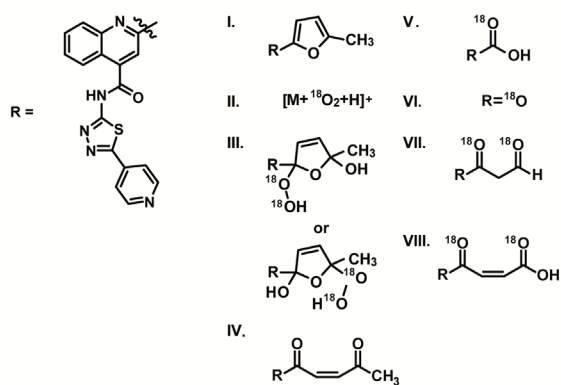
#### XIV. LC/MS Analysis of Aged 1

(Reaction Conditions: 10 mM DMSO Stock,  $^{18}\text{O}_2$  Atmosphere, 300W Visible Light, 25 °C, 9 h)

A.



B.

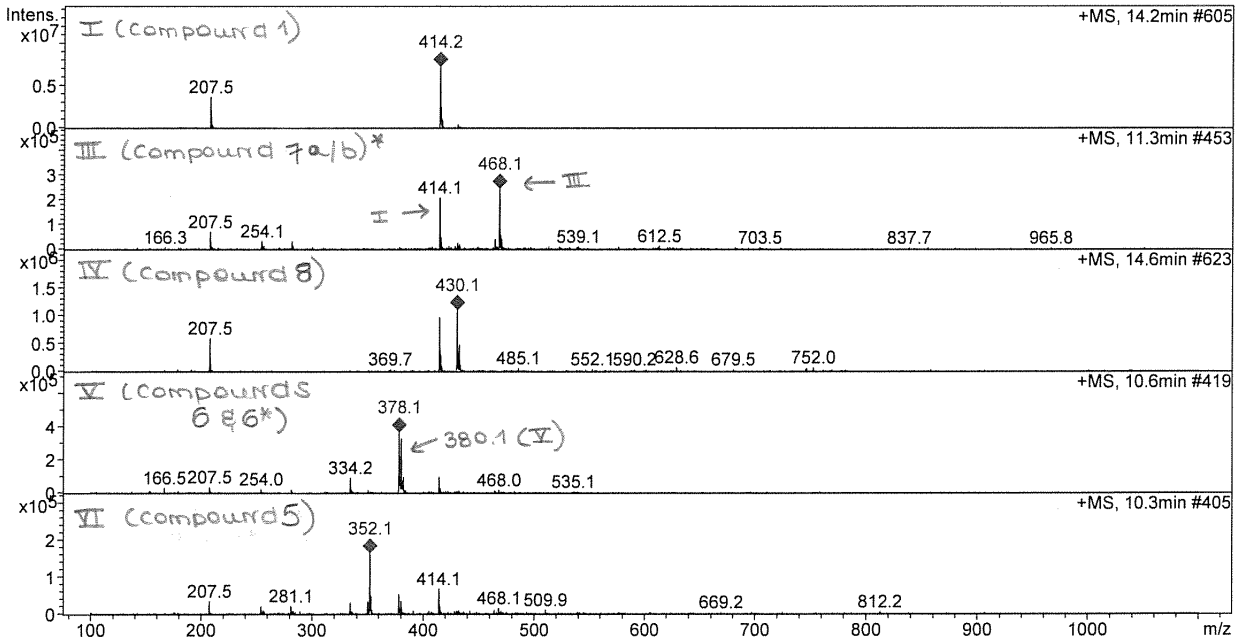
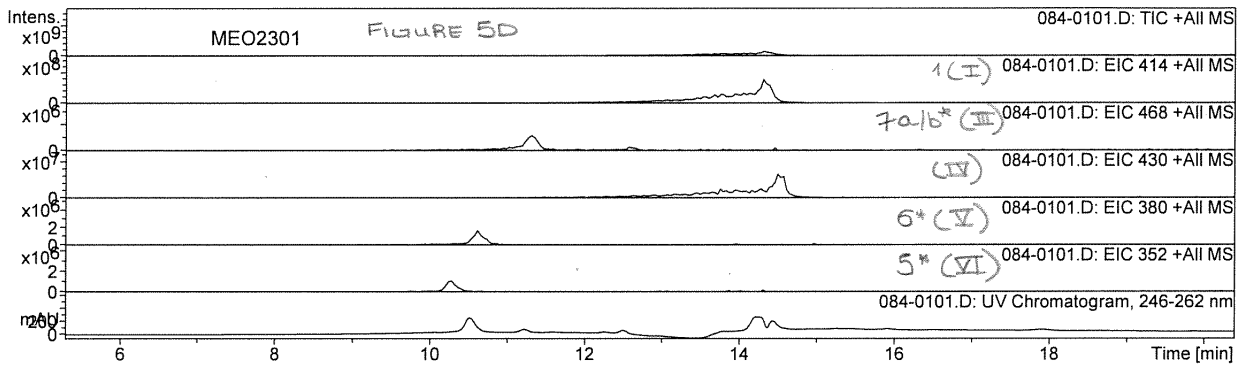


C.

Analysis Name 084-0101.D  
 Acquisition Date 08/16/2013 08:53:54 AM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

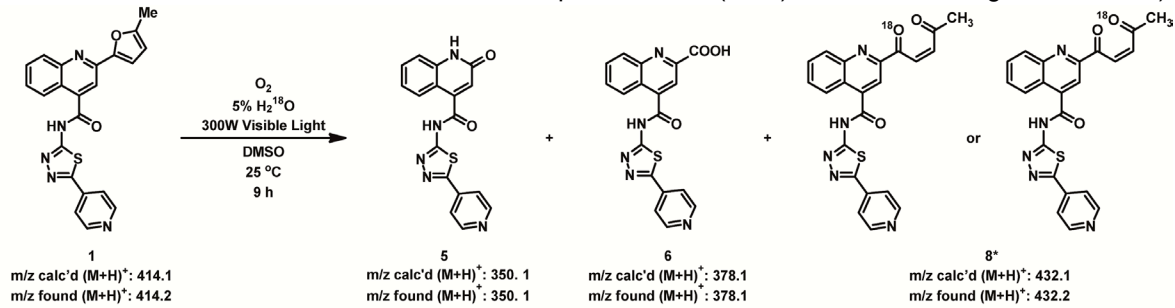
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	32489 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



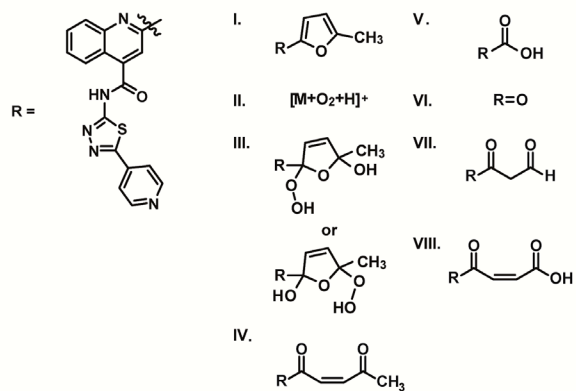
## XV. LC/MS Analysis of Aged 1

(Reaction Conditions: 10 mM DMSO Stock, O<sub>2</sub> Atmosphere, H<sub>2</sub><sup>18</sup>O (10%), 300W Visible Light, 25 °C, 9 h)

A.



B.

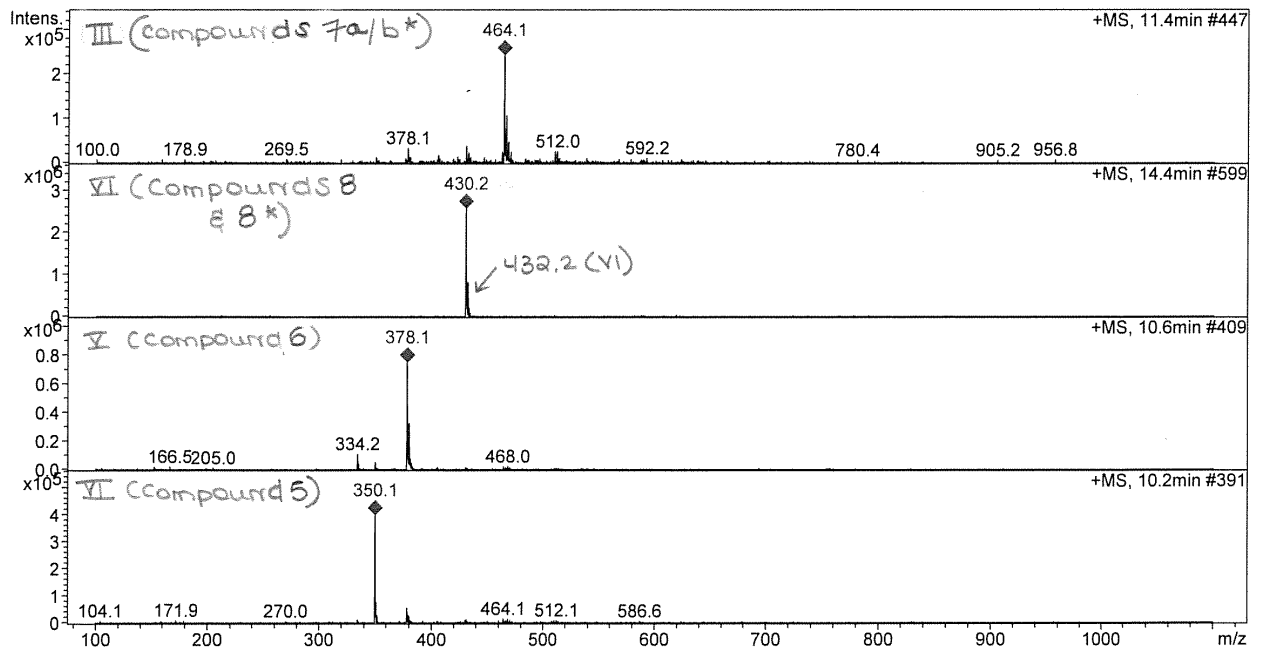
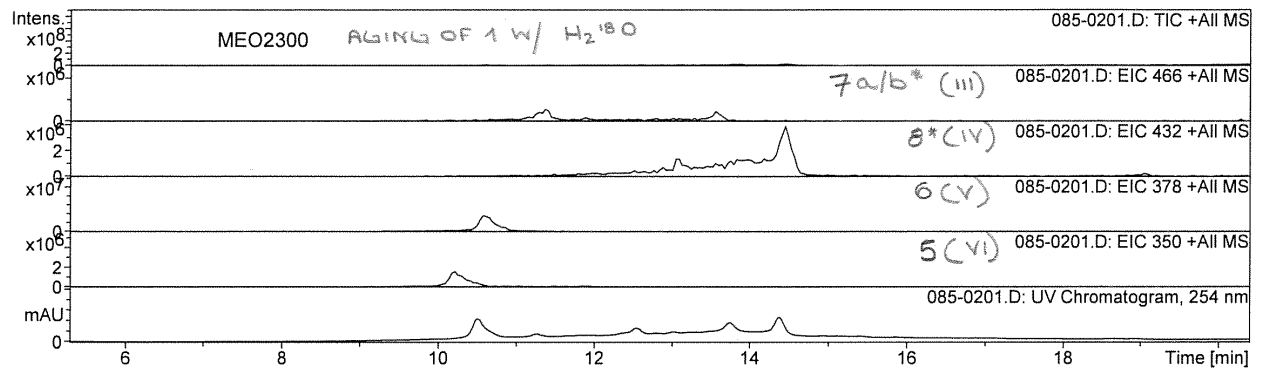


C.

Analysis Name 085-0201.D  
 Acquisition Date 08/16/2013 09:29:48 AM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	36545 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



## **XVI. Guide to SI Figures of the Aging Studies of Mechanistic Probes and Structurally Analogous 2-furylquinolines.**

The following pages include figures to support the aging studies of the mechanistic probes and structurally analogous 2-furylquinolines; the compounds included in Tables 1 and 2. For each compound, we have included:

(A) A scheme representing the reaction conditions and observed decomposition products for each studied probe. The masses depicted below each compound denote calculated and found masses. Masses were calculated for  $[M+H]^+$ .

(B) A calibration curve was performed for each studied probe to ensure consistency among injections. In short, we made DMSO stock solutions of each compound at 4-5 concentrations and spiked these stocks with 2.5  $\mu$ M rose bengal (RB). The calibration curves were generated by dividing the area under the curve (AUC) of each probe by the AUC of RB at each concentration. All calibration curves exhibited  $R^2 > 0.95$ .

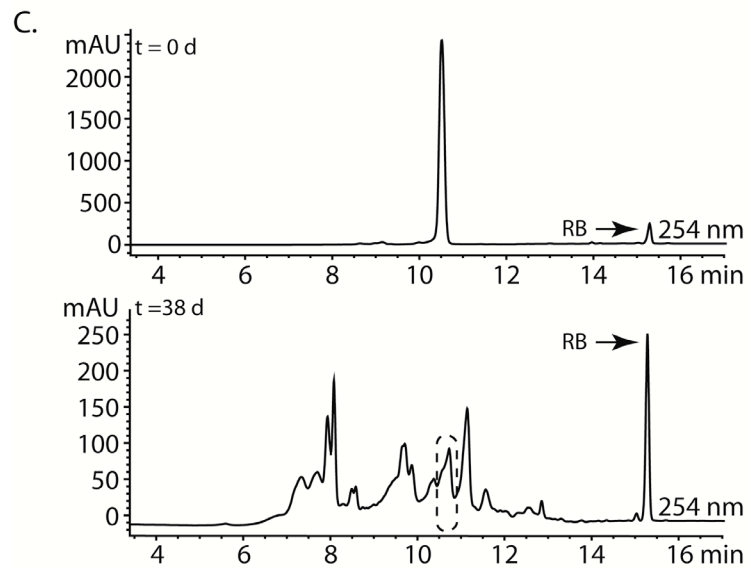
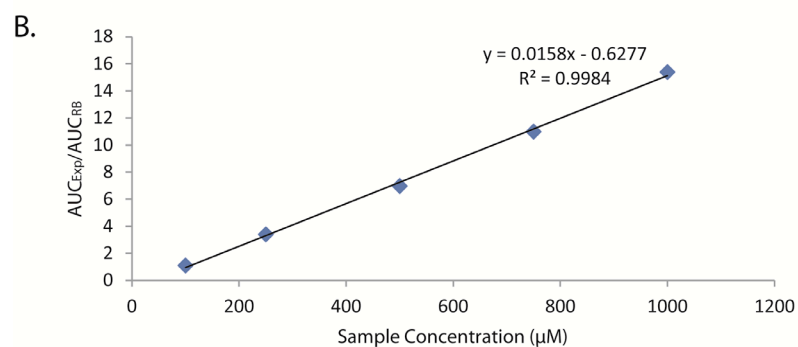
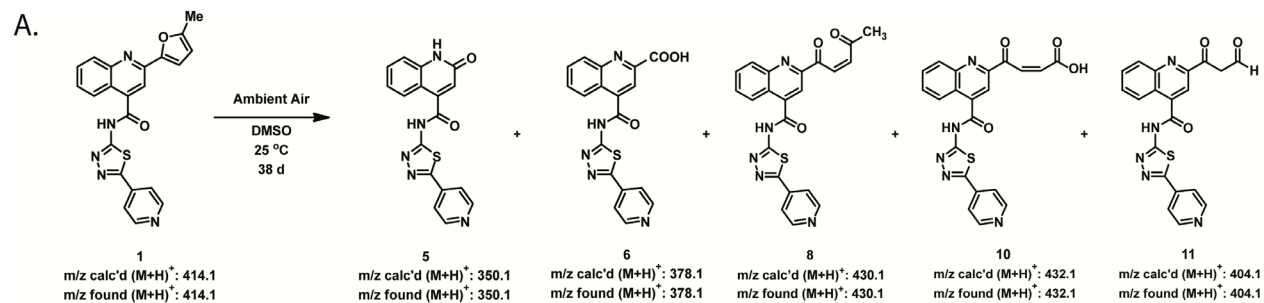
(C) HPLC chromatograms depicting the purity of the probe at time point 0 days, and the decomposition mixture at day 38. RB was spiked into the analyzed aliquot immediately prior to injection for quantification of the percent parent remaining (by fitting to the calibration curve in Panel B). In the  $t = 38$  d chromatogram, the peak corresponding to the starting material is denoted by a dashed oval.

(D). A structure-based key to describe how the LC-MS (E) is labeled. All possible decomposition intermediates and products are included.

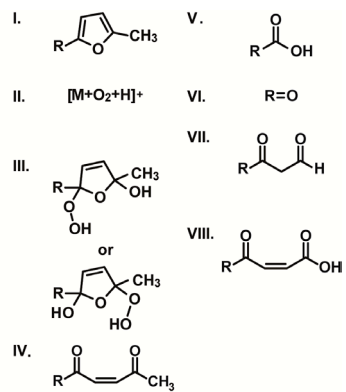
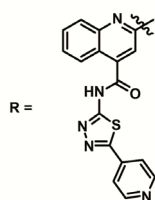
(E). LC-MS of the aged stock solution at 38 days. Included in the graphic are the total ion chromatogram (top), extracted ion current chromatograms for the starting material and all observed decomposition products and intermediates, and the UV chromatogram at 254 nm. Below, the mass spectrum corresponding to each chromatogram is depicted.

## XVII. HPLC & LC/MS Analysis of Aged 1

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)



D.



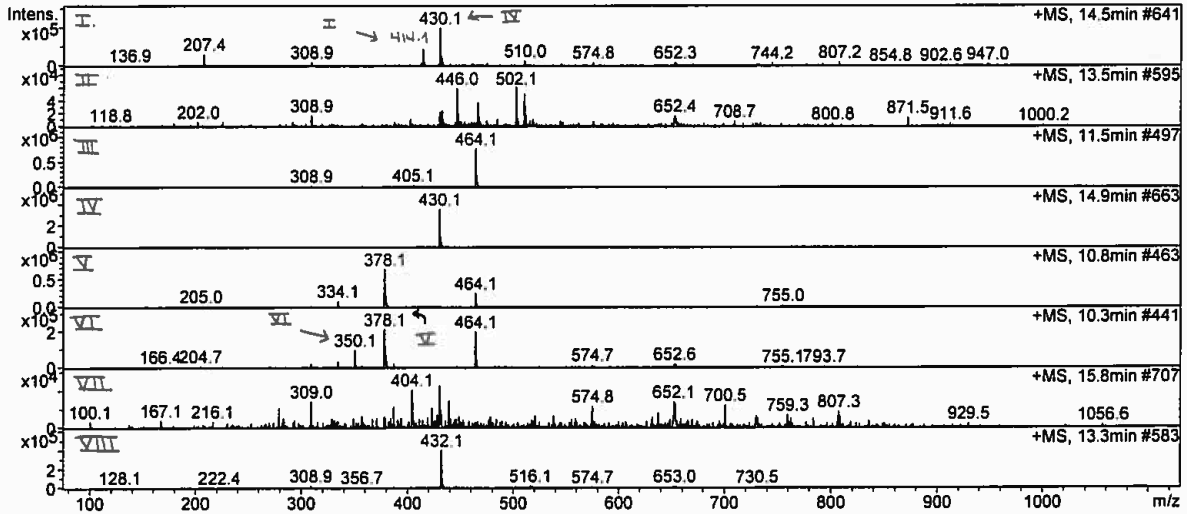
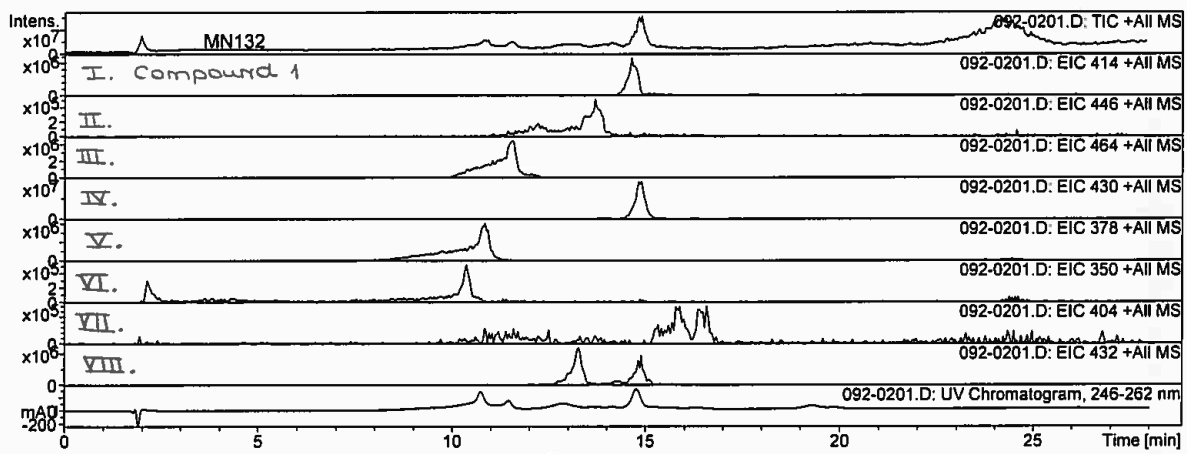
E.

Analysis Name 092-0201.D  
 Acquisition Date 08/05/2013 10:30:58 AM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

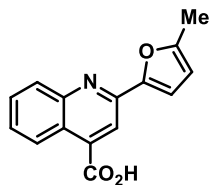
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	21353 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

Pubchem CID:1251050



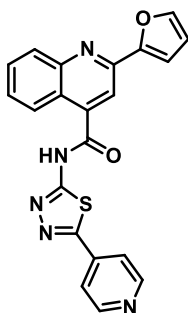


## XVIII. Experimental Procedures for the Synthesis of 12 – 24

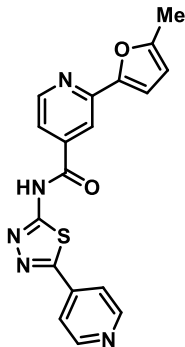


**2-(5-Methylfuran-2-yl)quinoline-4-carboxylic acid (12).** Synthesized as previously described.<sup>34</sup> Isolated as a brown powder (79%). <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) δ = 8.64 (d, *J* = 11.0 Hz, 1H), 7.87 (d, *J* = 10.5 Hz, 1H), 7.79 (s, 1H), 7.61 (ddd, *J* = 8.5 Hz, 6.0 Hz, 2.0 Hz, 1H), 7.41 (ddd, *J* = 8.5 Hz, 6.5 Hz, 2.0 Hz, 1H), 7.14 (d, *J* = 4.0 Hz, 1H), 6.31 (d, *J* = 4.5 Hz, 1H), 2.42 (s, 3H); LRMS-ESI<sup>+</sup> *m/z* [M + H]<sup>+</sup> calc'd for C<sub>15</sub>H<sub>11</sub>NO<sub>3</sub>: 254.1, found: 254.1.

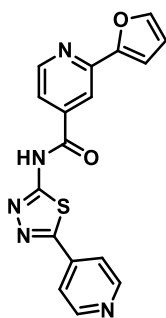
**General Procedure for the Coupling of 5-(Pyridin-4-yl)-1,3,4-thiadiazol-2-amine to Carboxylic Acids (Yielding Probes 13, 15, 17, 19, 21):** To a stirred solution of 5-(pyridin-4-yl)-1,3,4-thiadiazol-2-amine (**4**, 1 equiv.) in DMF (0.3 M) was added the appropriate carboxylic acid (1 equiv.), EDCI·HCl (1.2 equiv.), HOBT (1.2 equiv.), and NMM (6.0 equiv.), and the reaction was stirred at rt. After 24 h, the DMF was removed *in vacuo*, and the resulting residue was triturated with MeOH. The ppt was removed by filtration and purified over SiO<sub>2</sub> (0% to 30% MeOH in DCM) to yield the desired products.



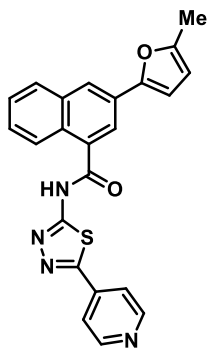
**2-(furan-2-yl)-N-(5-(pyridin-4-yl)-1,3,4-thiadiazol-2-yl)quinoline-4-carboxamide (13).** Yellow powder (24%). <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) δ = 13.85 (s, 1H), 8.78 (d, *J* = 4.5 Hz, 2H), 8.35 (s, 1H), 8.19 (d, *J* = 8.5 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 8.02 (m, 3H), 7.87 (t, *J* = 7.0 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.50 (d, *J* = 2.5 Hz, 1H), 6.79 (m, 1H); LRMS-ESI<sup>+</sup> *m/z* [M + H]<sup>+</sup> calc'd for C<sub>21</sub>H<sub>13</sub>N<sub>5</sub>O<sub>2</sub>S: 400.1, found: 400.2.



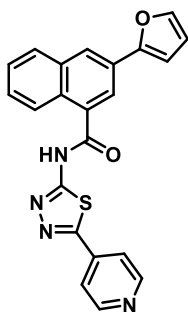
**2-(5-methylfuran-2-yl)-N-(5-(pyridin-4-yl)-1,3,4-thiadiazol-2-yl)isonicotinamide (15).** Yellow powder (6%).  $^1\text{H}$  (DMSO- $d_6$ ):  $\delta$  = 13.81 (bs, 1H), 8.77 (m, 3H), 8.31 (s, 1H), 7.97 (d,  $J$  = 4.2 Hz, 2H), 7.84 (d,  $J$  = 5.2 Hz, 1H), 7.12 (d,  $J$  = 3.3 Hz, 1H), 6.34 (d,  $J$  = 3.3 Hz, 1H), 2.42 (s, 3H); LRMS-ESI $^+$   $m/z$   $[\text{M} + \text{H}]^+$  calc'd for  $\text{C}_{18}\text{H}_{13}\text{N}_5\text{O}_2\text{S}$ : 364.1, found: 364.2.



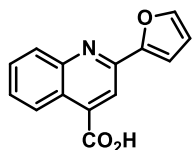
**2-(furan-2-yl)-N-(5-(pyridin-4-yl)-1,3,4-thiadiazol-2-yl)isonicotinamide (17).** White powder (9%).  $^1\text{H}$  (DMSO- $d_6$ ):  $\delta$  = 13.77 (bs, 1H), 8.82 (d,  $J$  = 5.0 Hz, 1H), 8.76 (d,  $J$  = 5.0 Hz, 2H), 8.40 (s, 1H), 7.97 (d,  $J$  = 4.5 Hz, 2H), 7.94 (m, 1H), 7.90 (d,  $J$  = 5.0 Hz, 1H), 7.23 (d,  $J$  = 3.0 Hz, 1H), 6.72 (m, 1H); LRMS-ESI $^+$   $m/z$   $[\text{M} + \text{H}]^+$  calc'd for  $\text{C}_{17}\text{H}_{11}\text{N}_5\text{O}_2\text{S}$ : 350.1, found: 350.2.



**3-(5-methylfuran-2-yl)-N-(5-(pyridin-4-yl)-1,3,4-thiadiazol-2-yl)-1-naphthamide (19)** Yellow powder (12%).  $^1\text{H}$  (DMSO- $d_6$ ):  $\delta$  = 13.57 (bs, 1H), 8.76 (d,  $J$  = 5.5 Hz, 2H), 8.45 (m, 1H), 8.34 (m, 1H), 8.28 (m, 1H), 8.21 (d,  $J$  = 8.0 Hz, 1H), 8.08 (d,  $J$  = 8.5 Hz, 1H), 7.99 (d,  $J$  = 5.5 Hz, 2H), 7.60 (m, 2H), 7.09 (d,  $J$  = 3.0 Hz, 1H), 6.30 (m, 1H); 2.41 (s, 3H); LRMS-ESI $^+$   $m/z$  [M + H] $^+$  calc'd for  $\text{C}_{23}\text{H}_{16}\text{N}_4\text{O}_2\text{S}$ : 413.1, found: 413.2.

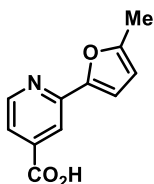


**3-(furan-2-yl)-N-(5-(pyridin-4-yl)-1,3,4-thiadiazol-2-yl)-1-naphthamide (21)**. Pale yellow powder (7%).  $^1\text{H}$  (DMSO- $d_6$ ):  $\delta$  = 13.61 (bs, 1H), 8.78 (dd,  $J$  = 4.5 Hz, 1.5 Hz, 2H), 8.45 (m, 1H), 8.35 (d,  $J$  = 1.5 Hz, 1H), 8.24 (dd,  $J$  = 6.5 Hz, 2.5 Hz, 1H), 8.12 (dd,  $J$  = 6.5 Hz, 2.0 Hz, 1H), 8.01 (dd,  $J$  = 4.5 Hz, 1.5 Hz, 2H), 7.89 (d,  $J$  = 1.0 Hz, 1H), 7.63 (m, 2H), 7.24 (d,  $J$  = 3.0 Hz, 1H), 6.71 (dd,  $J$  = 3.5 Hz, 2.0 Hz, 1H); LRMS-ESI $^+$   $m/z$  [M + H] $^+$  calc'd for  $\text{C}_{22}\text{H}_{14}\text{N}_4\text{O}_2\text{S}$ : 399.1, found: 399.1.

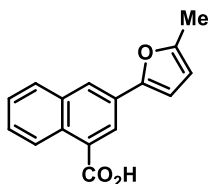


**2-(furan-2-yl)quinoline-4-carboxylic acid (14)** Synthesized as previously described.<sup>34</sup> Isolated as brown powder (34%). <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ = 8.63 (dd, *J* = 11.0 Hz, 2.0 Hz, 1H), 8.27 (s, 1H), 8.47 (dd, *J* = 11.0 Hz, 1.0 Hz, 1H), 7.97 (dd, *J* = 2.5 Hz, 1.0 Hz, 1H), 7.82 (ddd, *J* = 9.0 Hz, 7.0 Hz, 1.5 Hz, 1H), 7.66 (ddd, *J* = 9.0 Hz, 7.0 Hz, 1.5 Hz, 1H), 7.44 (dd, *J* = 4.5 Hz, 1.0 Hz, 1H), 6.75 (dd, *J* = 4.0 Hz, 2.0 Hz, 1H); LRMS-ESI<sup>+</sup> *m/z* [M + H]<sup>+</sup> calc'd for C<sub>22</sub>H<sub>15</sub>N<sub>5</sub>O<sub>2</sub>S: 414.1025, found: 414.1033. LRMS-ESI<sup>+</sup> *m/z* [M + H]<sup>+</sup> calc'd for C<sub>14</sub>H<sub>9</sub>NO<sub>3</sub>: 240.1, found: 240.1.

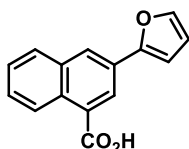
**General Procedure for Suzuki Coupling with 5-Methylfuran-2-Boronic Acid Pinacol Ester or Furan-2-Boronic Acid (Yielding Probes 16, 20, 22, 23):** To a mixture of the appropriate aromatic iodine or bromide (1 equiv.) in DMF/H<sub>2</sub>O (0.08 M, 5/1, v/v) was added boronic acid (1.5 equiv.), and Na<sub>2</sub>CO<sub>3</sub> (1.5 equiv.). The reaction mixture was degassed with bubbling N<sub>2</sub> for 10 min, and Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (5 mol %) was added. The reaction mixture was degassed with bubbling N<sub>2</sub> for 10 additional min, and then heated to 95 °C. After 2h, the reaction was cooled to rt, and the reaction was concentrated onto SiO<sub>2</sub>. SiO<sub>2</sub> purification (0% to 50% MeOH in DCM) provided the desired products.



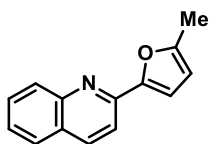
**2-(5-methylfuran-2-yl)isonicotinic acid (16).** Brown powder (>99%). <sup>1</sup>H (CD<sub>3</sub>OD): δ = 8.47 (d, *J* = 5.5 Hz, 1H), 8.15 (s, 1H), 7.63 (dd, *J* = 5.0 Hz, 1.0 Hz, 1H), 6.98 (d, *J* = 3.0 Hz, 1H), 6.19 (d, *J* = 3.0 Hz, 1H), 2.39 (s, 3H); LRMS-ESI<sup>+</sup> *m/z* [M + H]<sup>+</sup> calc'd for C<sub>11</sub>H<sub>9</sub>NO<sub>3</sub>: 204.1, found: 204.1.



**3-(5-methylfuran-2-yl)-1-naphthoic acid (20).** Brown Powder (21%).  $^1\text{H}$  ( $\text{CD}_3\text{OD}$ ):  $\delta$  = 8.80 (m, 1H), 8.42 (m, 1H), 8.25 (m, 1H), 7.92 (dd,  $J$  = 5.5 Hz, 3.5 Hz, 1H), 7.52 (m, 2H), 6.81 (d,  $J$  = 3.0 Hz, 1H), 6.17 (m, 1H), 2.41 (s, 3H); LRMS-ESI $^+$   $m/z$   $[\text{M} + \text{H}]^+$  calc'd for  $\text{C}_{16}\text{H}_{12}\text{O}_3$ : 253.1, found: 253.1.

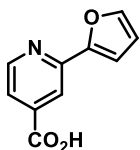


**3-(furan-2-yl)-N-(5-(pyridin-4-yl)-1,3,4-thiadiazol-2-yl)-1-naphthamide (22).** Pale yellow powder (48%).  $^1\text{H}$  ( $\text{CDCl}_3$ ):  $\delta$  = 9.01 (d,  $J$  = 8.5 Hz, 1H), 8.67 (m, 1H), 8.36 (m, 1H), 7.94 (d,  $J$  = 8.0 Hz, 1H), 7.62 (t,  $J$  = 8.0 Hz, 1H), 7.57 (m, 2H), 6.87 (d,  $J$  = 3.0 Hz, 1H), 6.56 (dd,  $J$  = 3.5 Hz, 2.0 Hz, 1H); LRMS-ESI $^+$   $m/z$   $[\text{M} + \text{H}]^+$  calc'd for  $\text{C}_{15}\text{H}_{10}\text{O}_3$ : 239.1, found: 239.1.

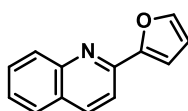


**2-(5-methylfuran-2-yl)quinoline (23).** White powder (48%).  $^1\text{H}$  ( $\text{CDCl}_3$ ):  $\delta$  = 8.14 (d,  $J$  = 9.0 Hz, 1H), 8.12 (d,  $J$  = 11 Hz, 1H), 7.79 (d,  $J$  = 8.5 Hz, 1H), 7.77 (d,  $J$  = 7.0 Hz, 1H), 7.70 (t,  $J$  = 7.0 Hz, 1H), 7.48 (t,  $J$  = 7.0 Hz, 1H), 7.13 (d,  $J$  = 2.5 Hz, 1 Hz, 1H), 6.20 (d,  $J$  = 2.0 Hz, 1H), 2.48 (s, 3H); LRMS-ESI $^+$   $m/z$   $[\text{M} + \text{H}]^+$  calc'd for  $\text{C}_{14}\text{H}_{11}\text{NO}$ : 210.1, found: 210.1.

**General Procedure for Stille Coupling with 2-(tributylstannyl)furan (Yielding Probes 18, 24):** To a suspension of 2-iodoisonicotinic acid (1 equiv.) and  $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$  (2 mol %) in anhydrous 1,4-dioxane (0.08 M) was added 2-(tributylstannyl)furan (4.5 equiv.), and the reaction was heated to 90  $^\circ\text{C}$ . After 14 h, the reaction was cooled to rt and the reaction mixture was filtered through a Celite pad. The filtrate was concentrated *in vacuo* and the resulting residue was triturated with hexanes. The ppt was removed by filtration to yield the desired product.



**2-(furan-2-yl)isonicotinic acid (18).** Tan powder (29%).  $^1\text{H}$  ( $\text{CD}_3\text{OD}$ ):  $\delta$  = 8.54 (d,  $J$  = 5.5 Hz, 1H), 8.24 (s, 1H), 7.71 (dd,  $J$  = 5.0 Hz, 1.0 Hz, 1H), 7.69 (d,  $J$  = 1 Hz, 1H), 7.12 (d,  $J$  = 3.5 Hz, 1H), 6.61 (dd,  $J$  = 3.5 Hz, 1.5 Hz, 1H); LRMS-ESI $^+$   $m/z$  [ $\text{M} + \text{H}$ ] $^+$  calc'd for  $\text{C}_{10}\text{H}_7\text{NO}_3$ : 190.0, found: 190.1.

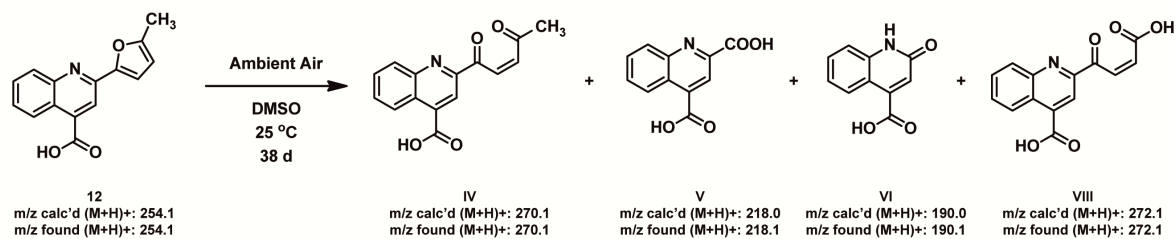


**2-(furan-2-yl)quinoline (24).** Tan powder (77%).  $^1\text{H}$  ( $\text{CDCl}_3$ ):  $\delta$  = 8.16 (d,  $J$  = 8.5 Hz, 1H), 8.13 (d,  $J$  = 8.5 Hz, 1H), 7.82 (d,  $J$  = 8.5 Hz, 1H), 7.78 (d,  $J$  = 8.5 Hz, 1H), 7.70 (t,  $J$  = 8.5 Hz, 1H), 7.63 (m, 1H), 7.50 (t,  $J$  = 8.0 Hz, 1H), 7.22 (d,  $J$  = 3.0 Hz, 1H), 6.59 (dd,  $J$  = 3.0 Hz, 1.5 Hz, 1H); LRMS-ESI $^+$   $m/z$  [ $\text{M} + \text{H}$ ] $^+$  calc'd for  $\text{C}_{13}\text{H}_9\text{NO}$ : 196.1, found: 196.1.

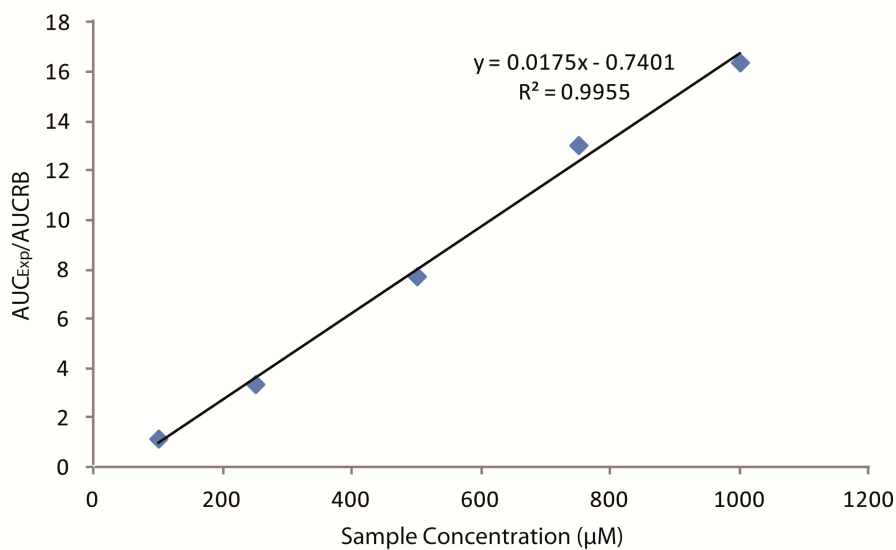
## XIX. HPLC & LC/MS Analysis of Aged 12

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

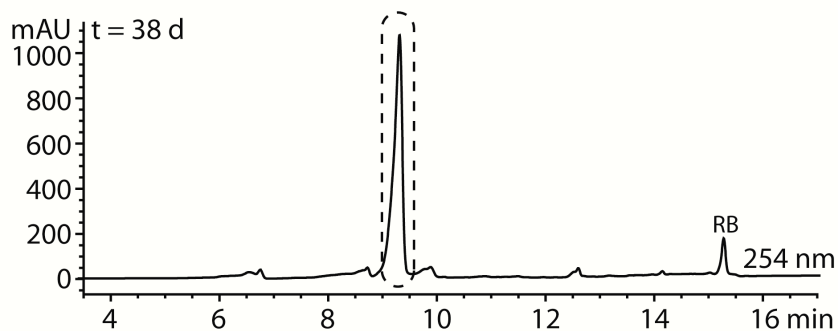
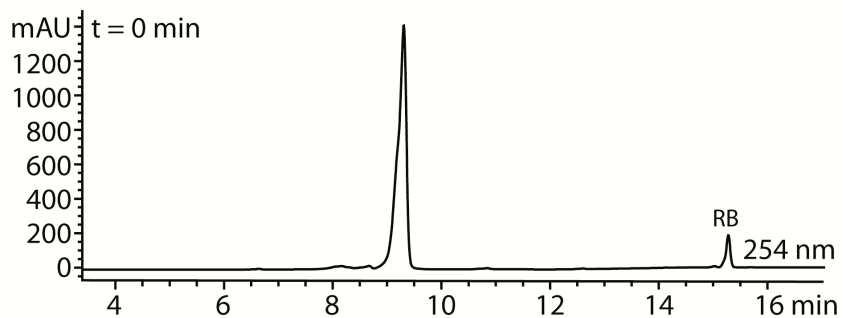
A.



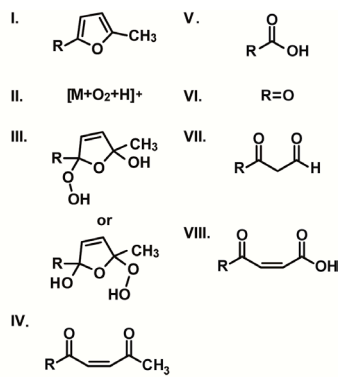
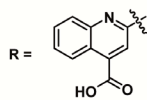
B.



C.



D.



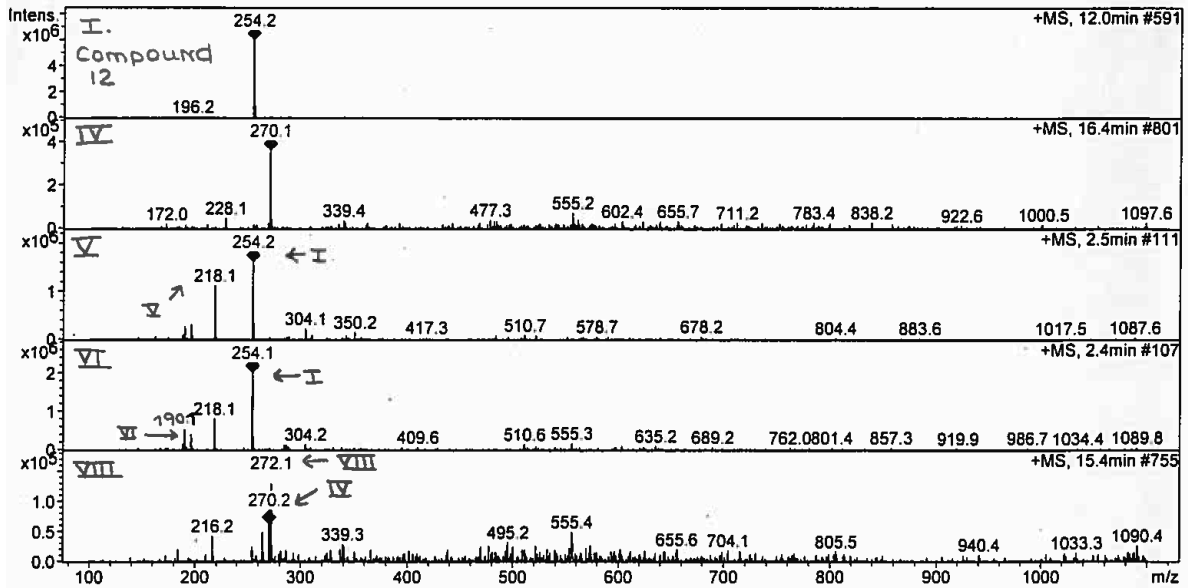
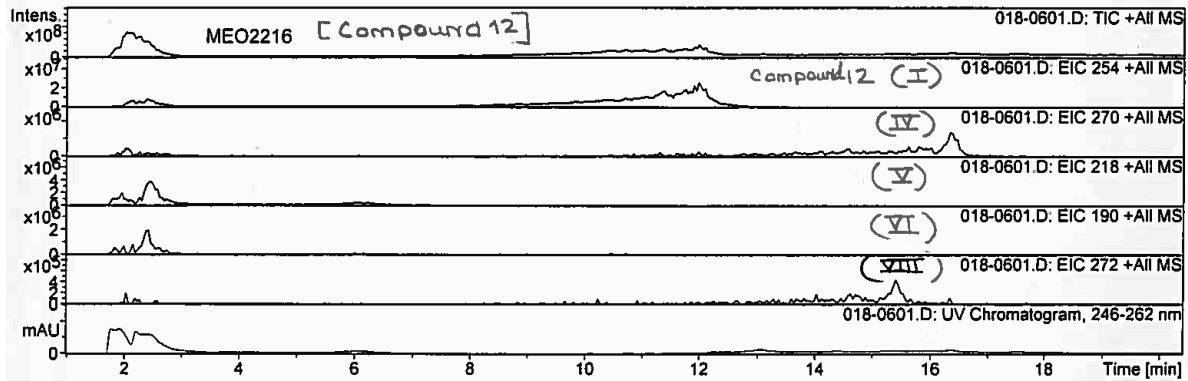


E.

Analysis Name 018-0601.D  
 Acquisition Date 09/01/2014 03:19:41 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

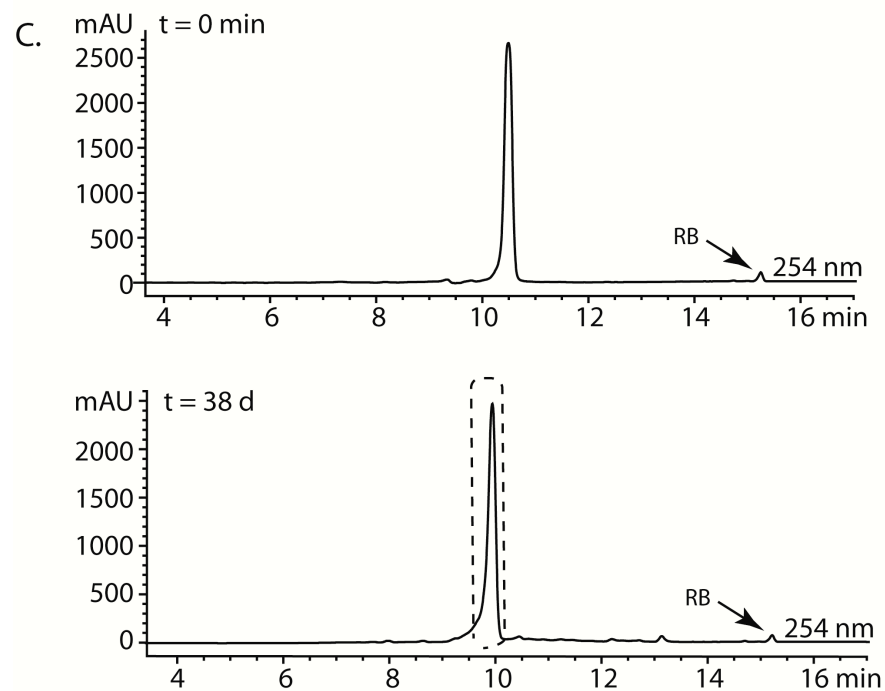
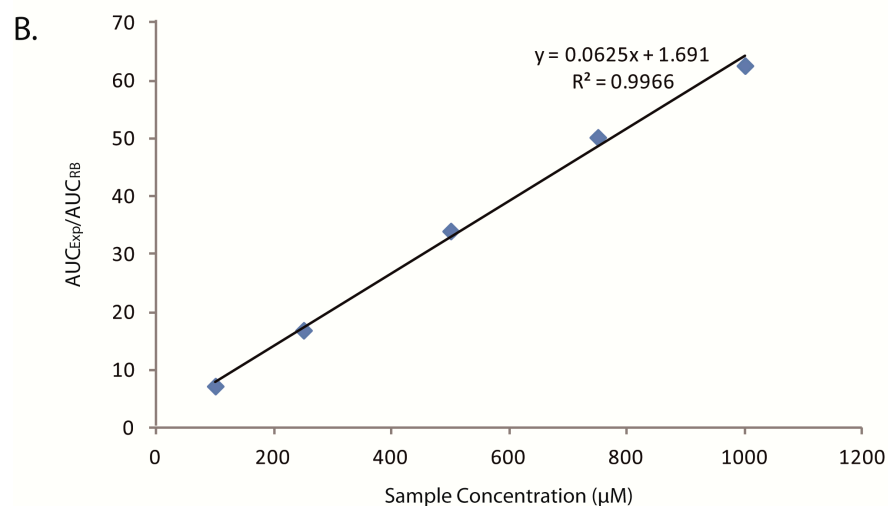
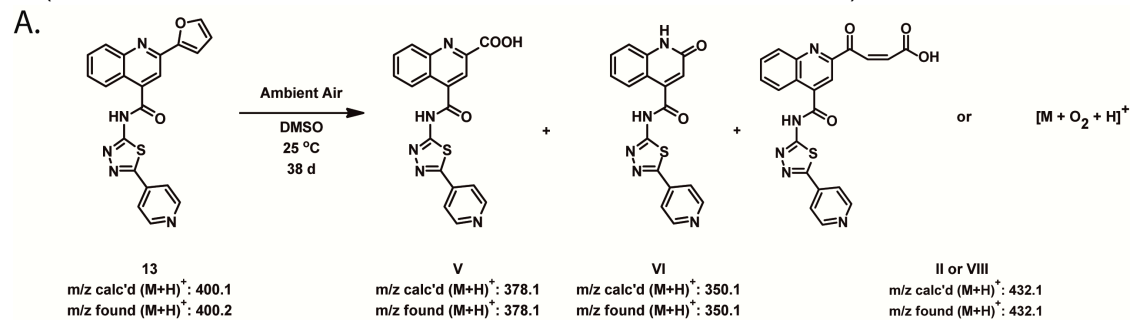
Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	11732 $\mu$ s	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

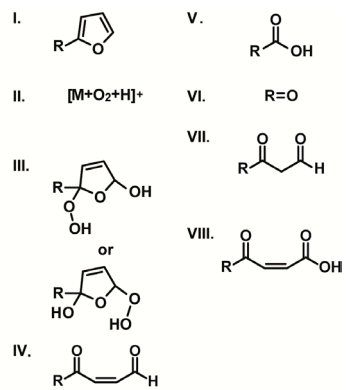
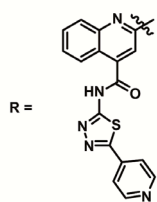


## XX. HPLC & LC/MS Analysis of Aged 13

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)



D.

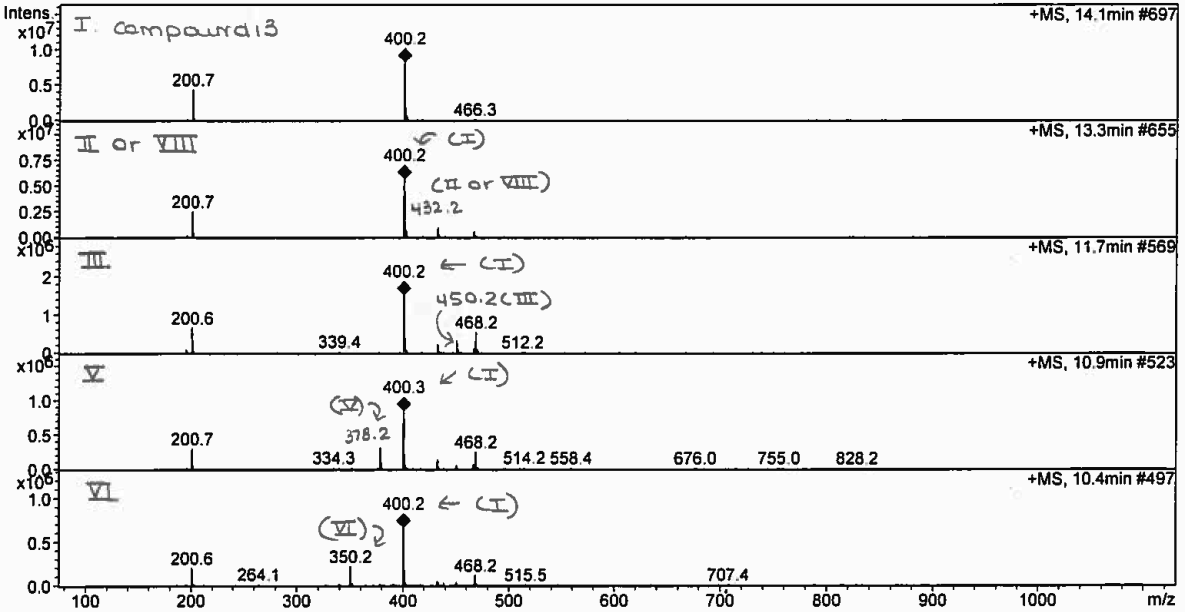
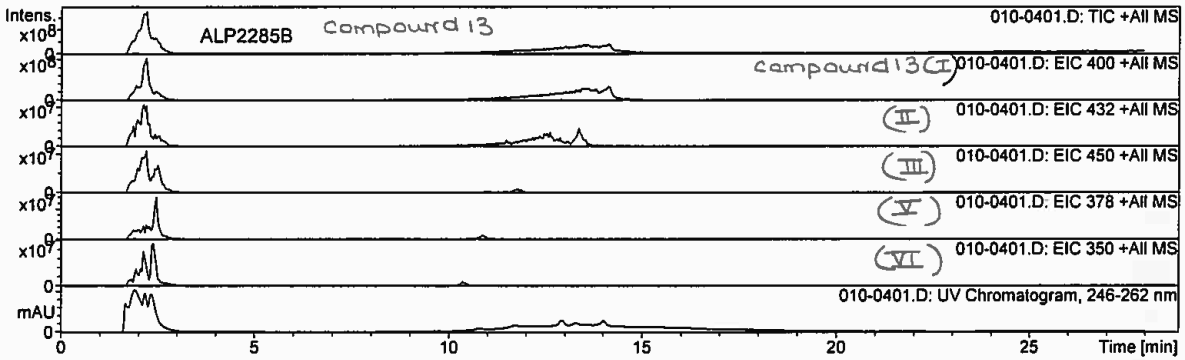


E.

Analysis Name	010-0401.D	Operator	Maggie Olson
Acquisition Date	09/01/2014 02:05:42 PM	Instrument	LC-MSD-Trap-SL
Method	130701A.M		
Comment			

Acquisition Parameters

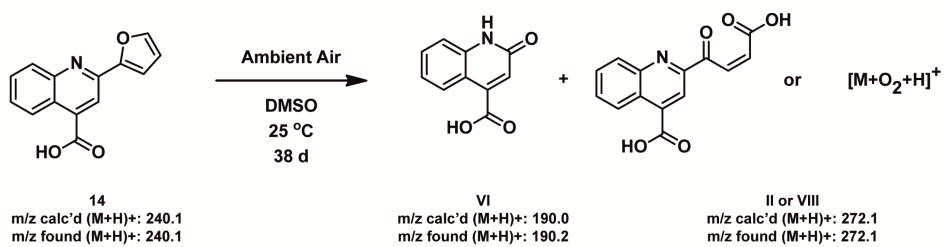
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	15293 $\mu$ s	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



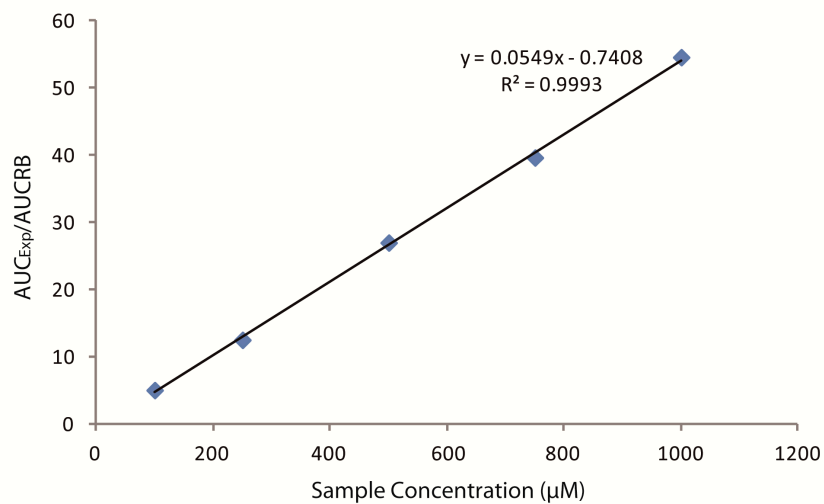
## XXI. HPLC & LC/MS Analysis of Aged 14

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

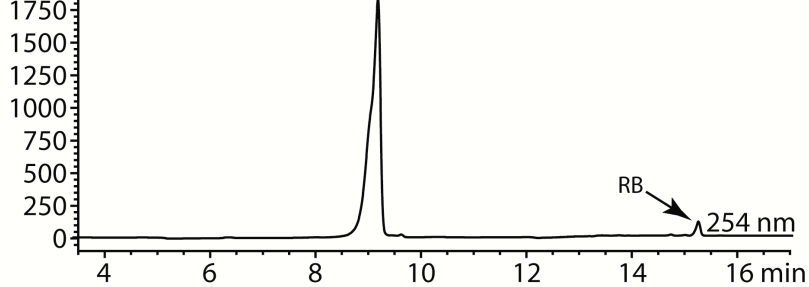
A.



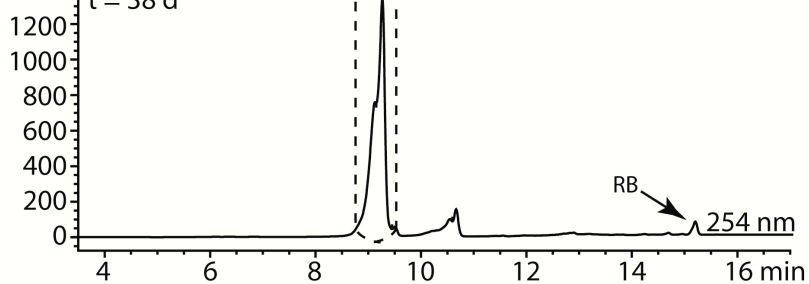
B.



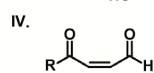
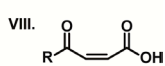
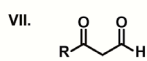
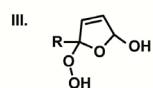
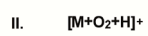
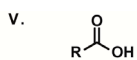
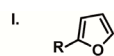
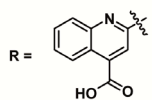
C. mAU t = 0 min



mAU t = 38 d



D.

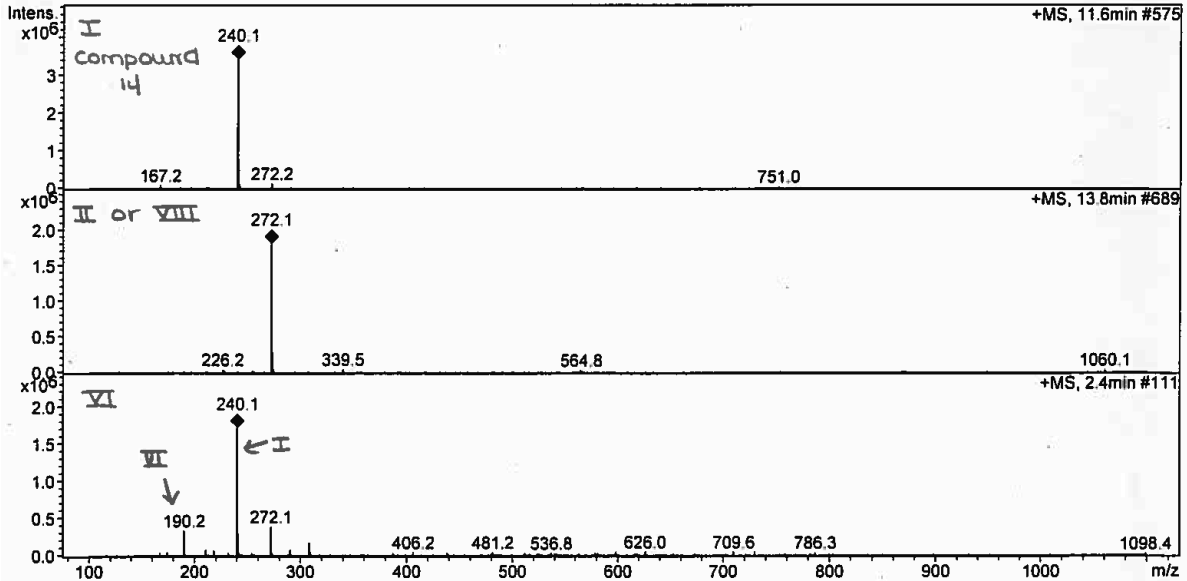
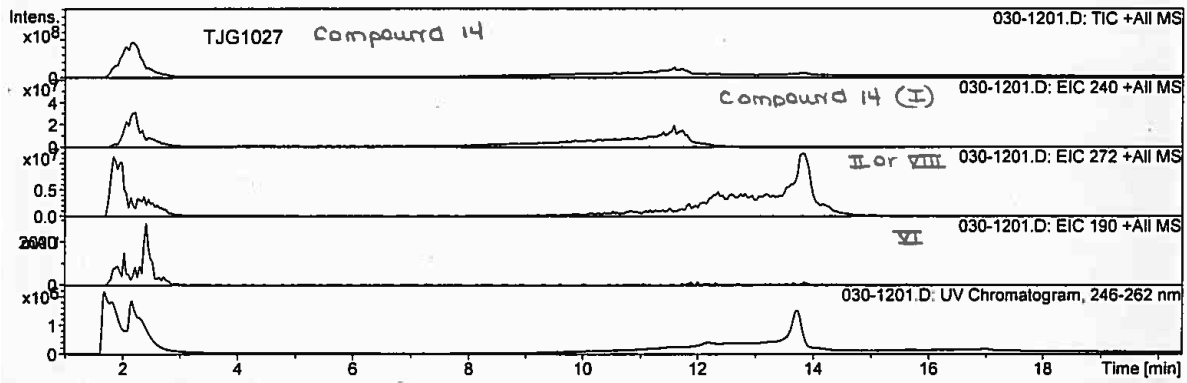


E.

Analysis Name	030-1201.D	Operator	Maggie Olson
Acquisition Date	09/01/2014 07:01:46 PM	Instrument	LC-MSD-Trap-SL
Method	130701A.M		
Comment			

Acquisition Parameters

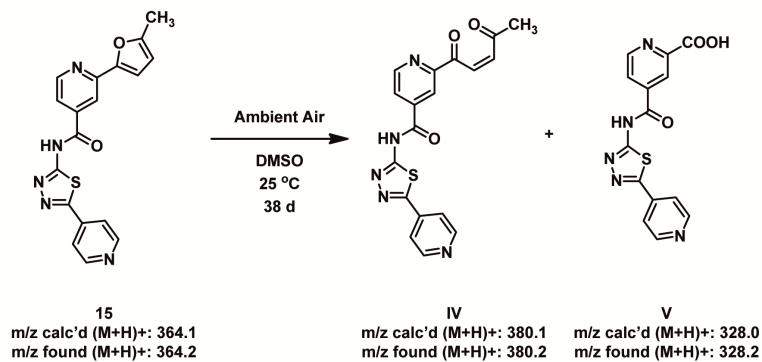
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	13815 $\mu$ s	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



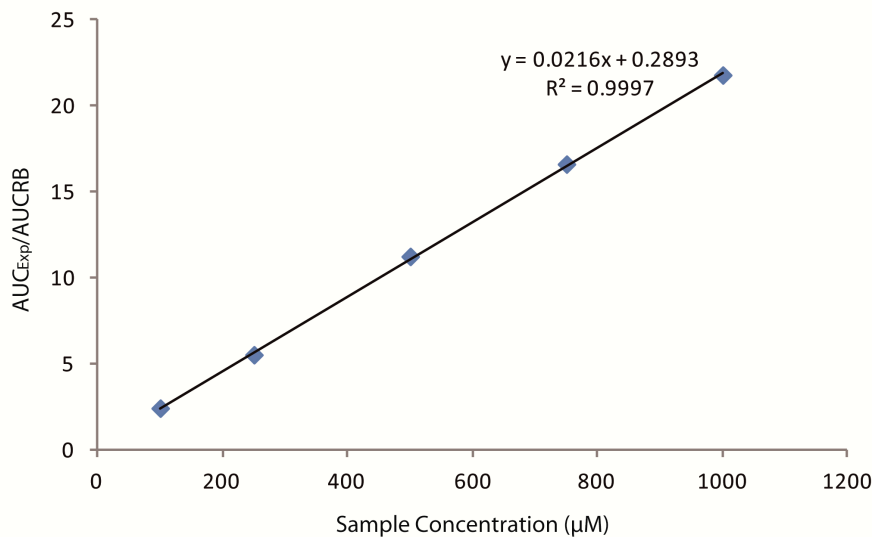
## XXII. HPLC & LC/MS Analysis of Aged 15

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

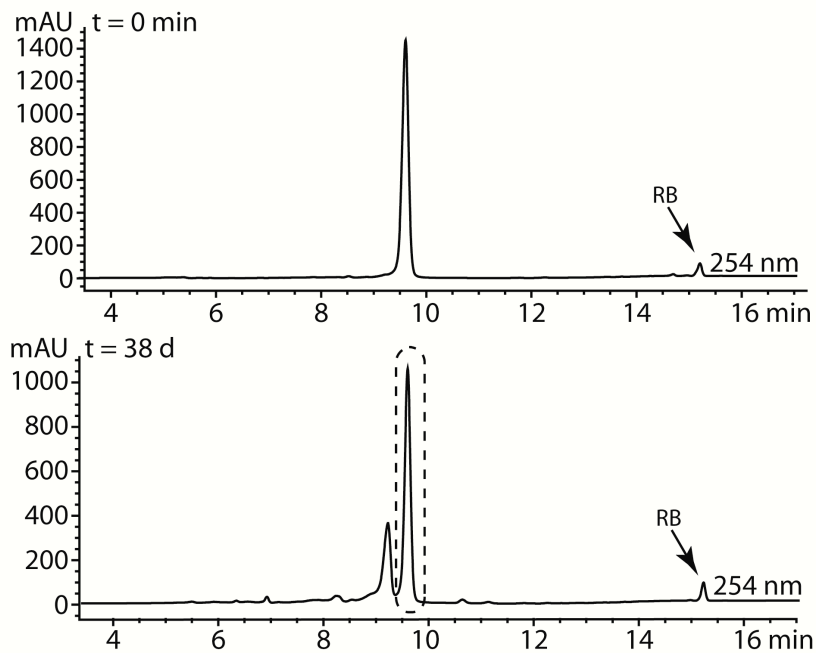
A.



B.

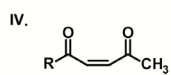
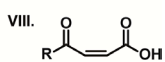
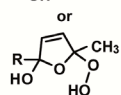
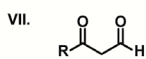
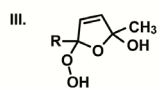
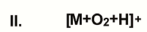
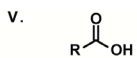
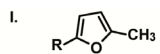
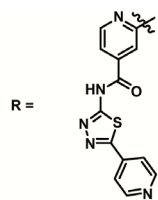


C.





D.

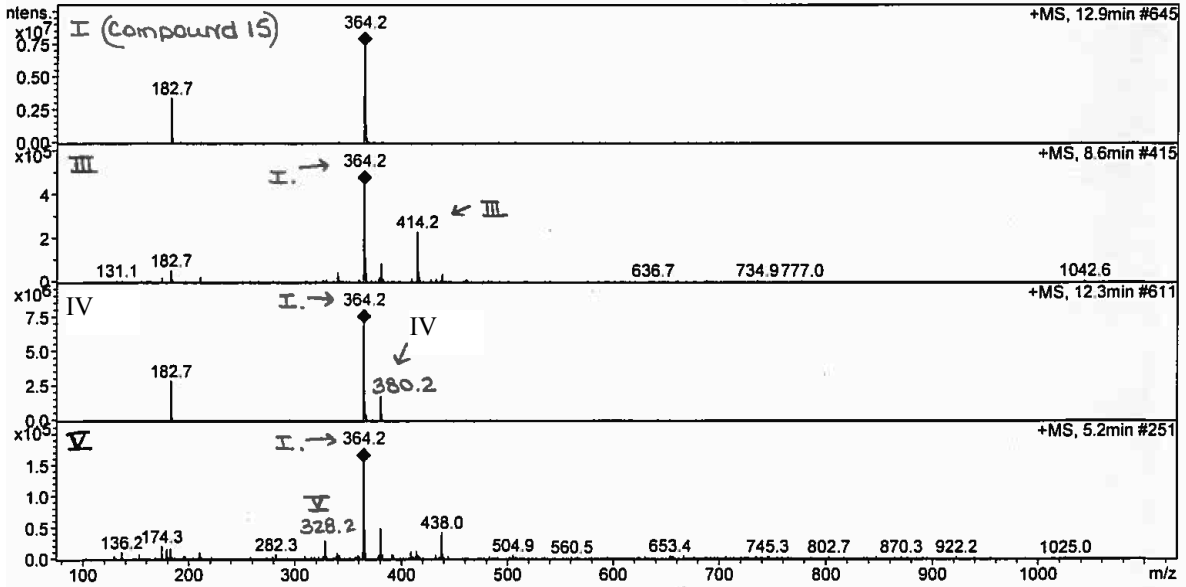
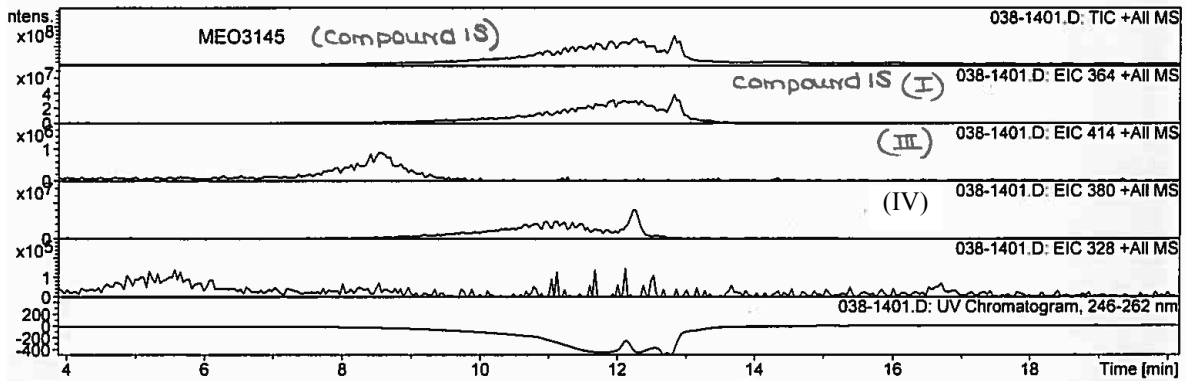


E.

Analysis Name 038-1401.D  
 Acquisition Date 09/01/2014 08:15:48 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

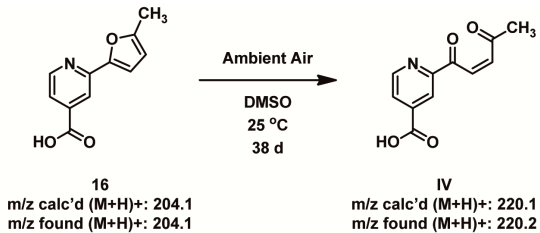
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	10997 µs	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Web. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



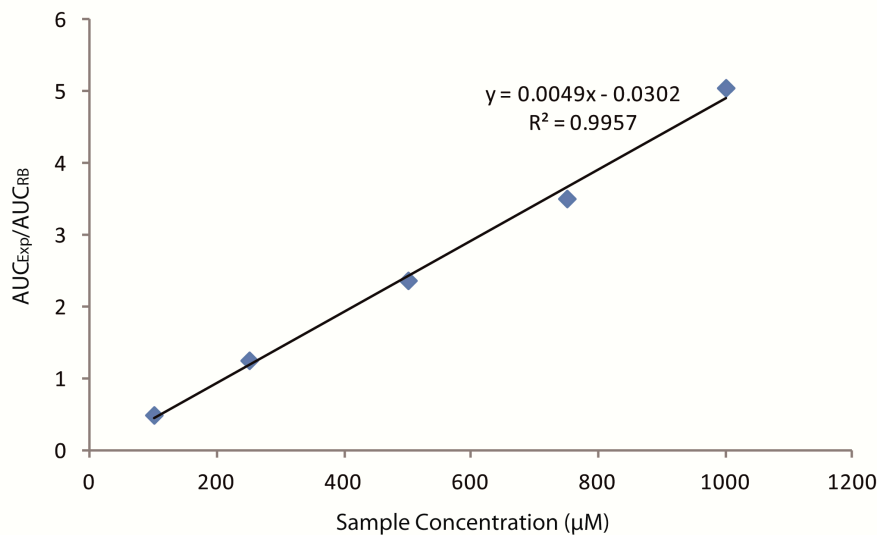
### XXIII. HPLC & LC/MS Analysis of Aged 16

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

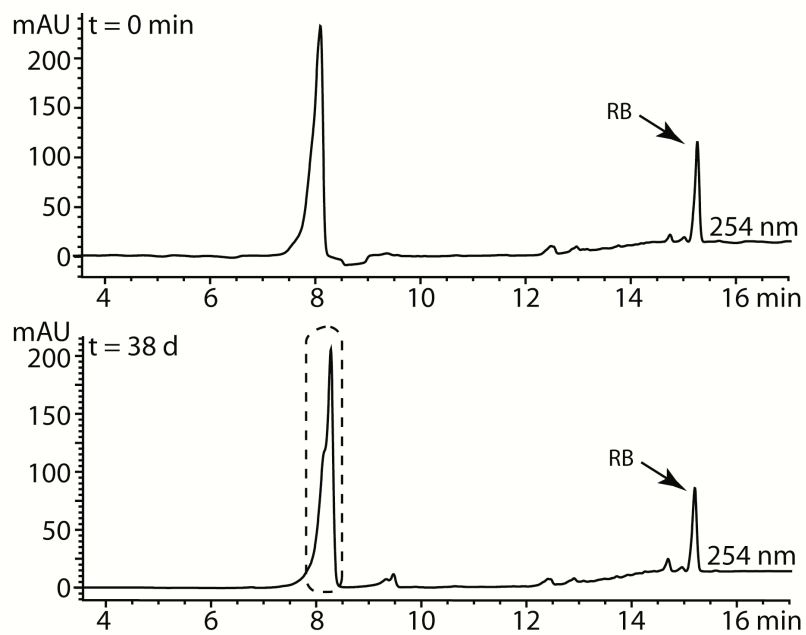
A.



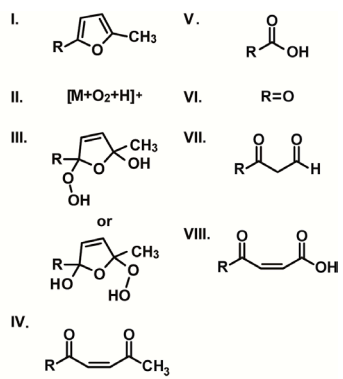
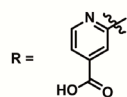
B.



C.



D.

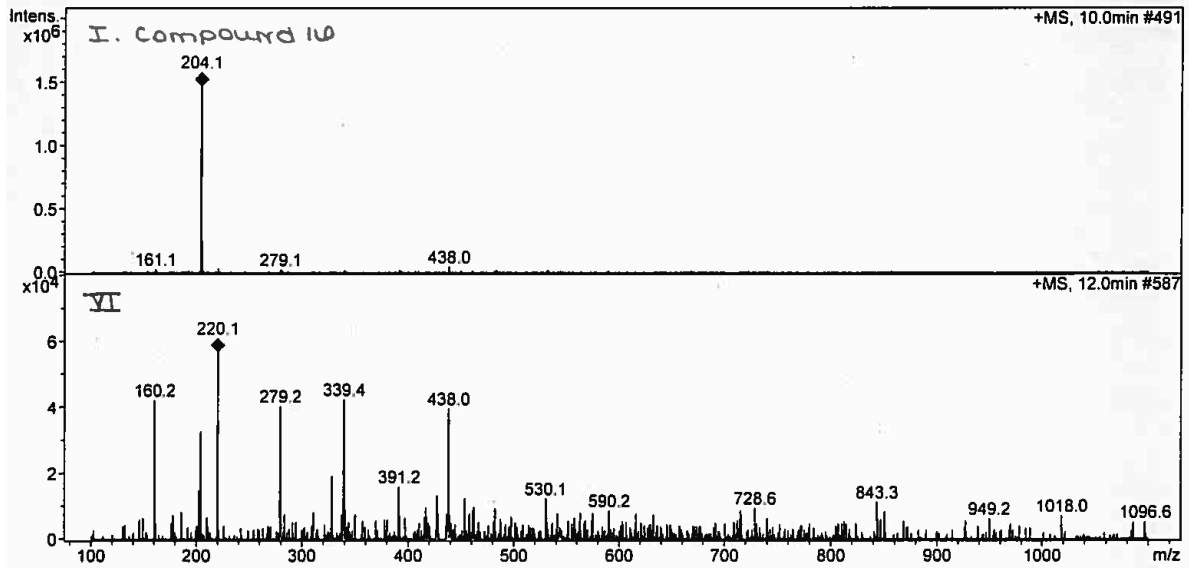
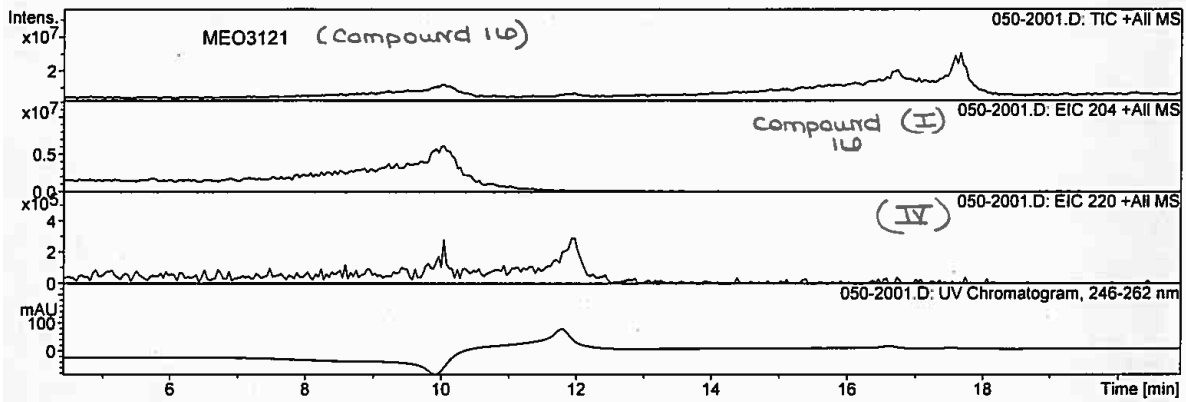


E.

Analysis Name	050-2001.D	Operator	Maggie Olson
Acquisition Date	09/01/2014 11:57:55 PM	Instrument	LC-MSD-Trap-SL
Method	130701A.M		
Comment			

Acquisition Parameters

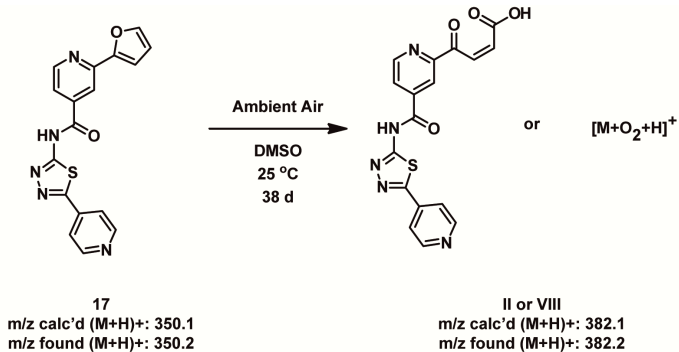
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	14793 µs	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



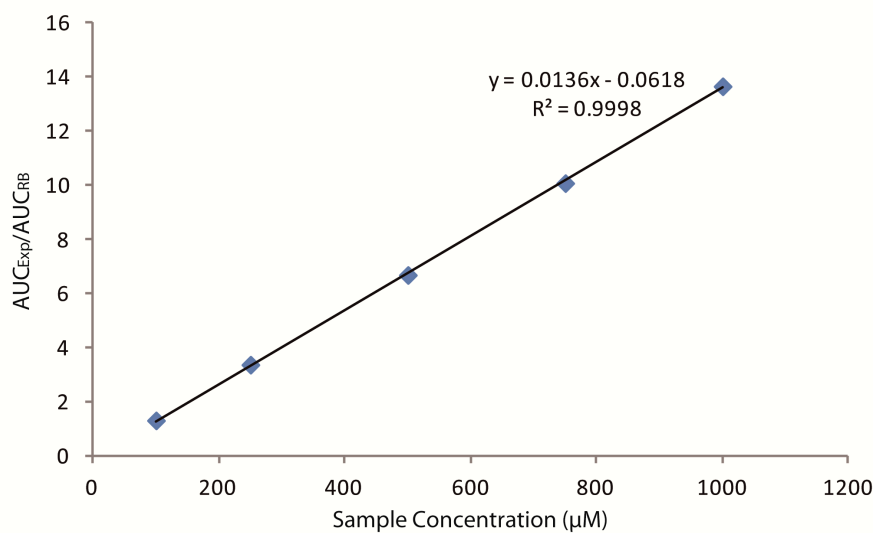
## XXIV. HPLC & LC/MS Analysis of Aged 17

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

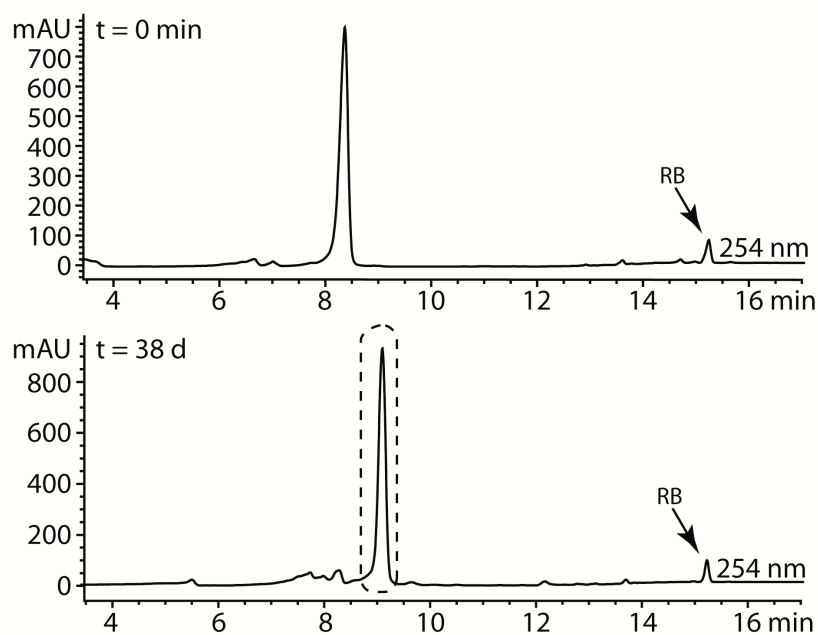
A.



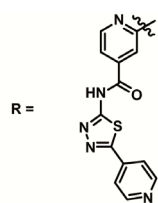
B.



C.



D.



I.



V.



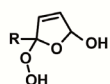
II.



VI.



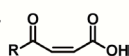
III.



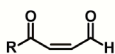
VII.



VIII.



IV.

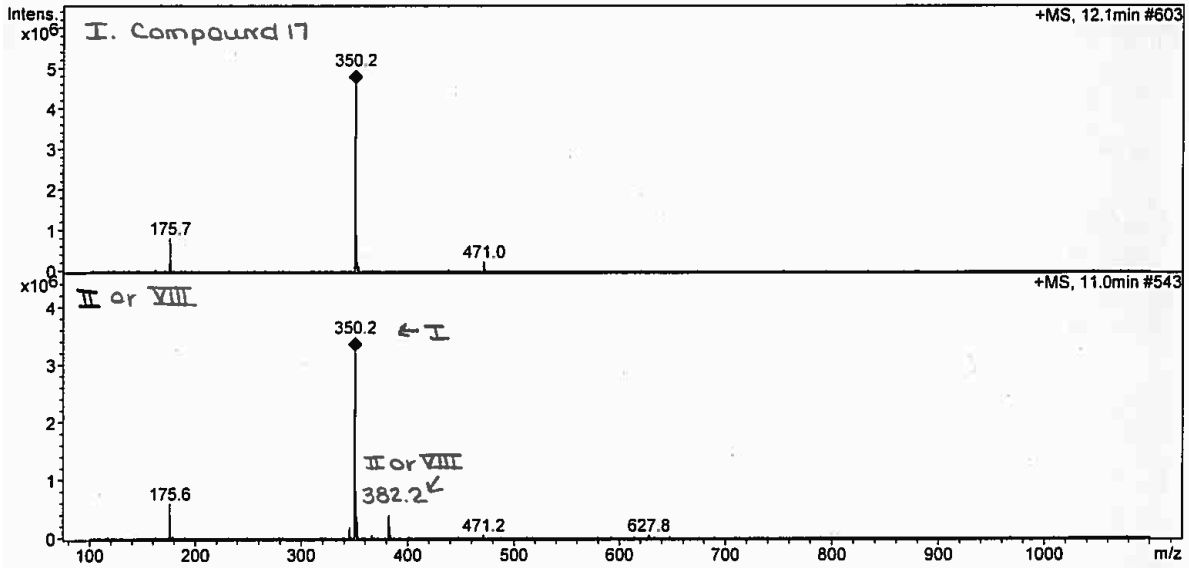
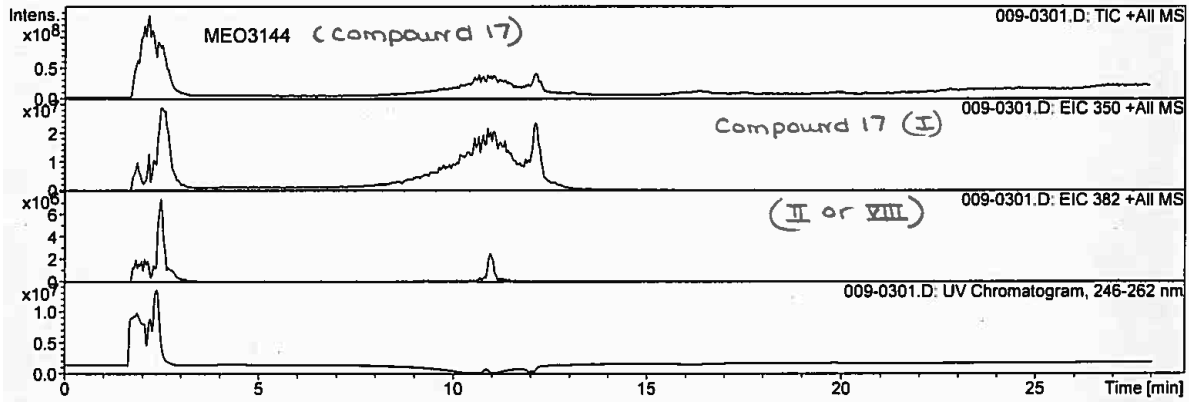


E.

Analysis Name 009-0301.D  
 Acquisition Date 09/01/2014 01:28:41 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	14740 $\mu$ s	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

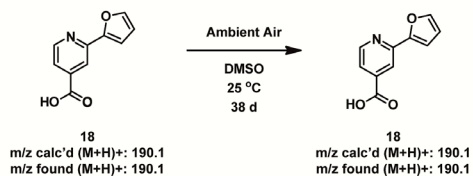




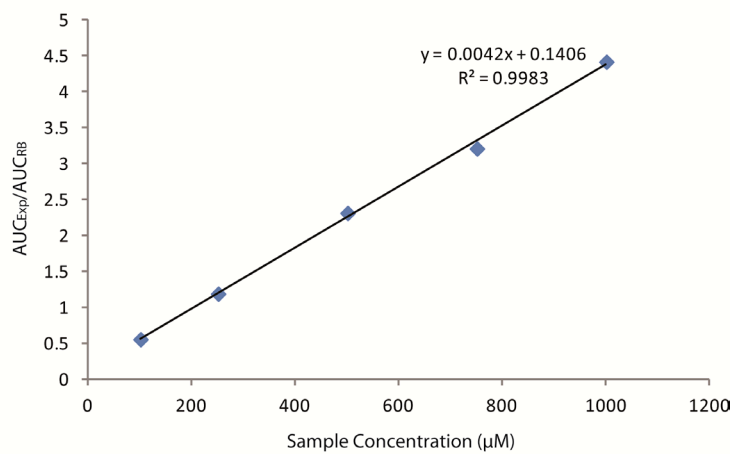
## XXV. HPLC & LC/MS Analysis of Aged 18

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

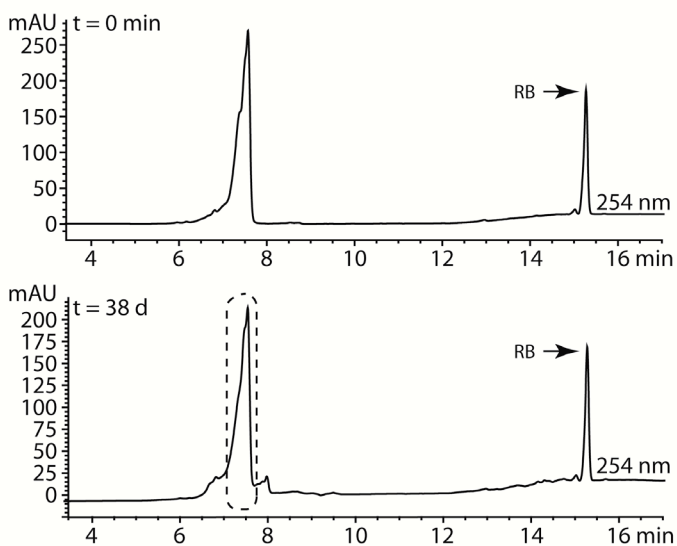
A.



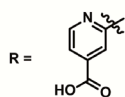
B.



C.



D.



I.



V.



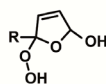
II.



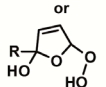
VI.



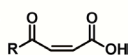
III.



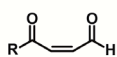
VII.



VIII.



IV.

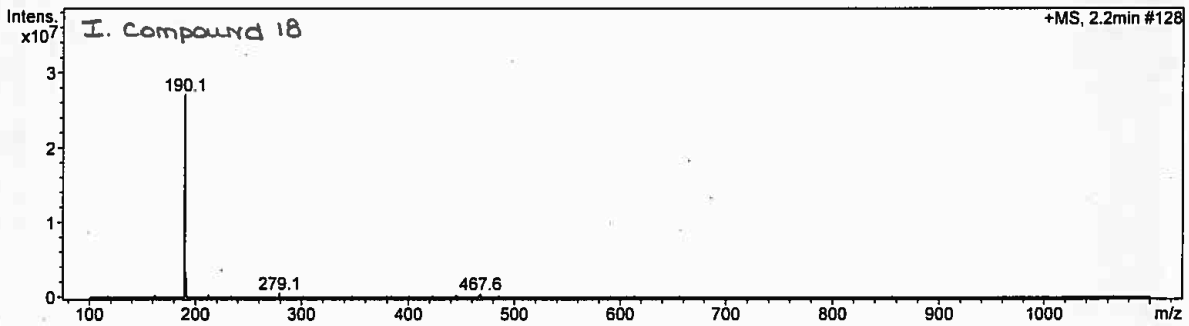
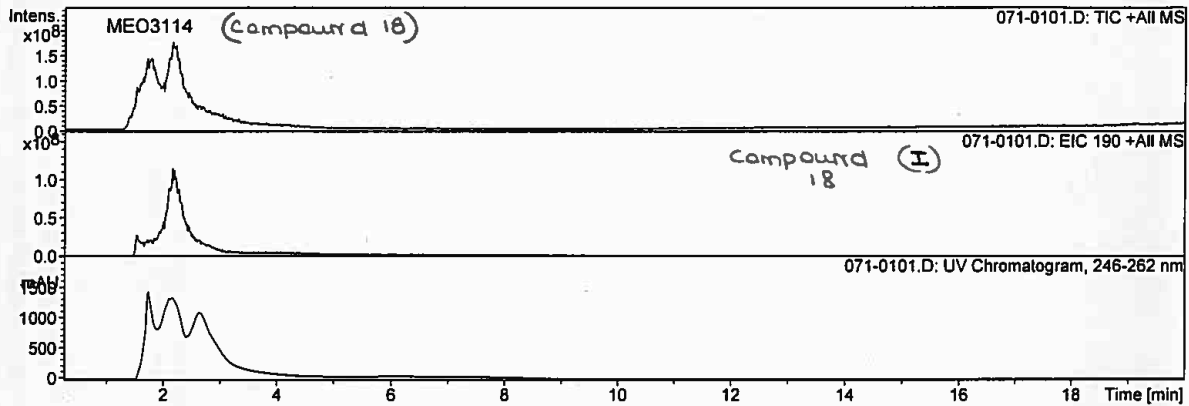


E.

Analysis Name 071-0101.D  
Acquisition Date 05/08/2015 08:51:26 PM Operator Rachit Shah  
Method 130701B.M Instrument LC-MSD-Trap-SL  
Comment

Acquisition Parameters

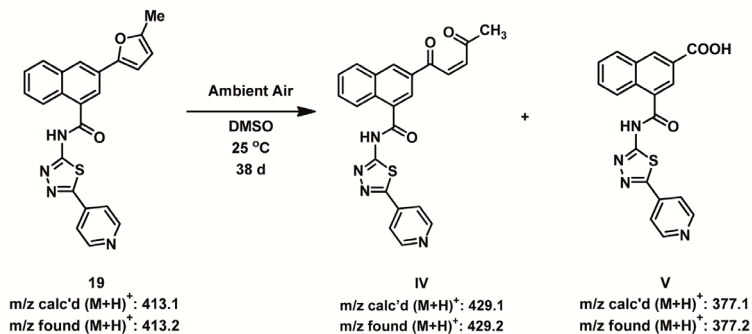
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	off
Accumulation Time	7130 $\mu$ s	Trap Drive	41.6	Multiplier Voltage	2256 Volt
Averages	8 Spectra	Octopole RF Amplitude	157.0 Vpp		
Dry Heat	on	Capillary Exit	103.1 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



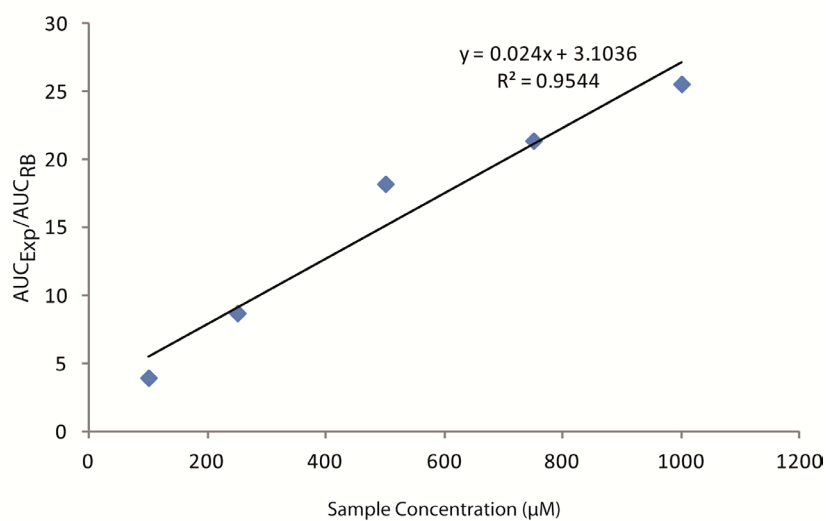
## XXVI. HPLC & LC/MS Analysis of Aged 19

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

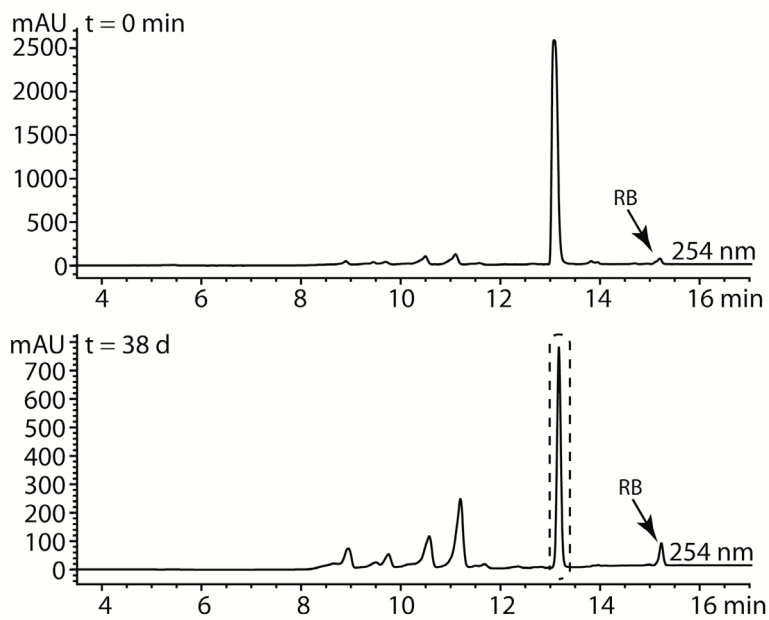
A.



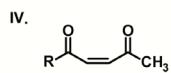
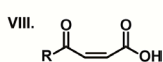
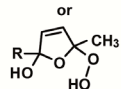
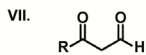
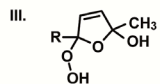
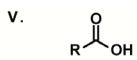
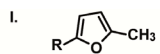
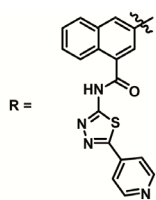
B.



C.



D.

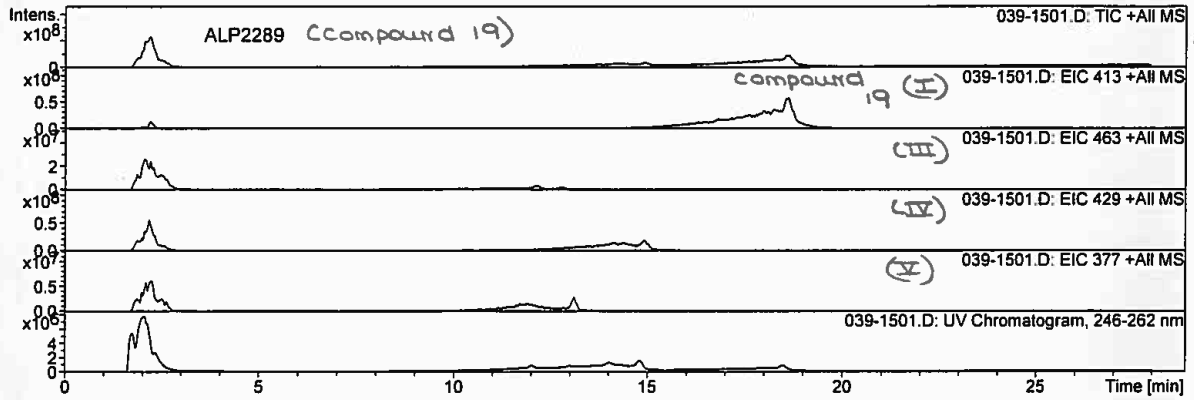


E.

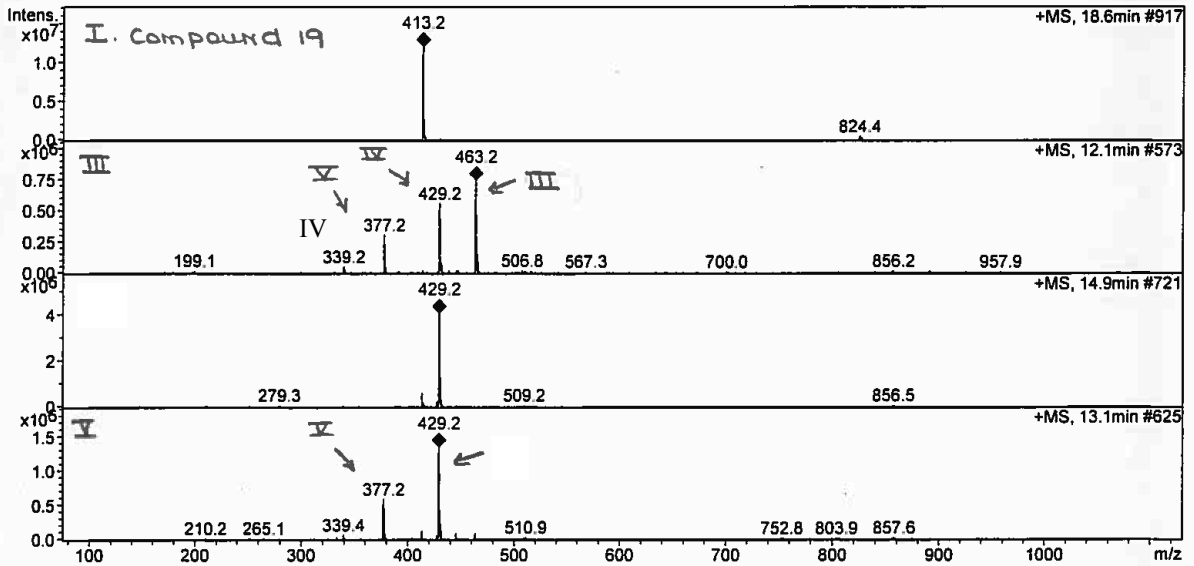
Analysis Name 039-1501.D  
 Acquisition Date 09/01/2014 08:52:52 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	11204 $\mu$ s	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



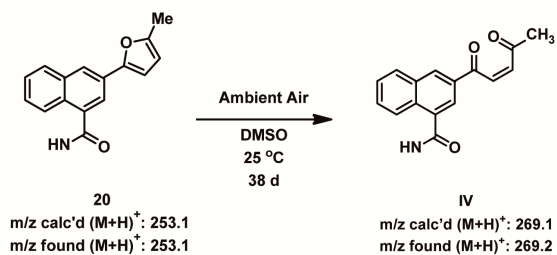
IV



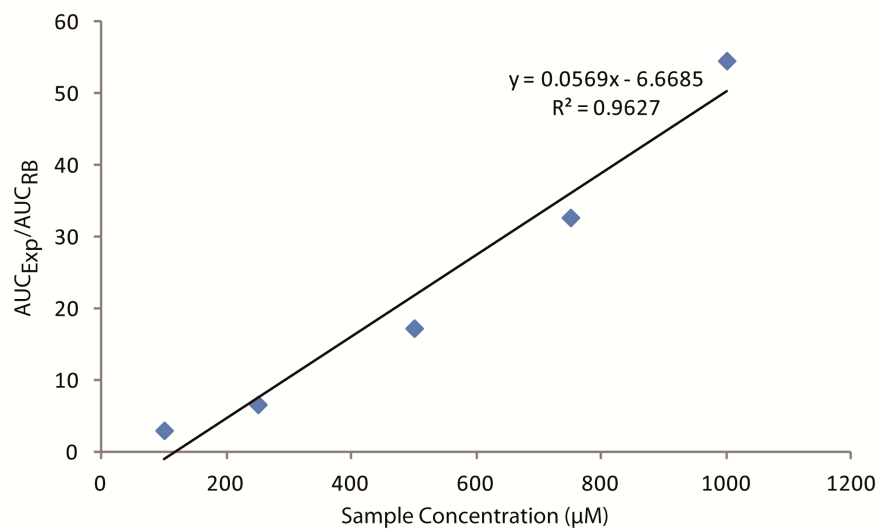
## XXVII. HPLC & LC/MS Analysis of Aged 20

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

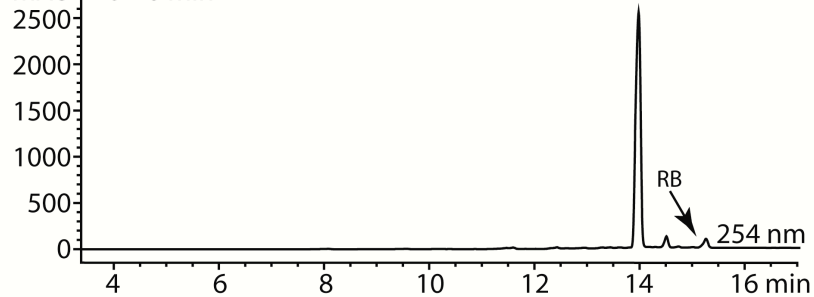
A.



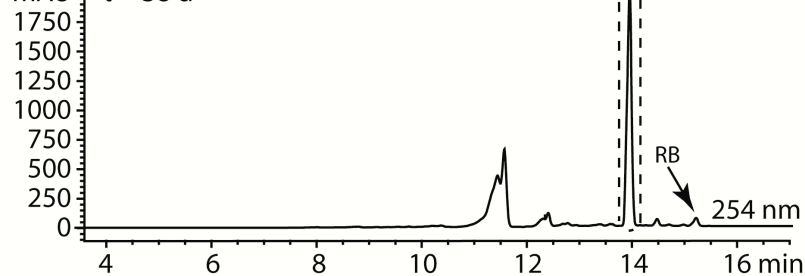
B.



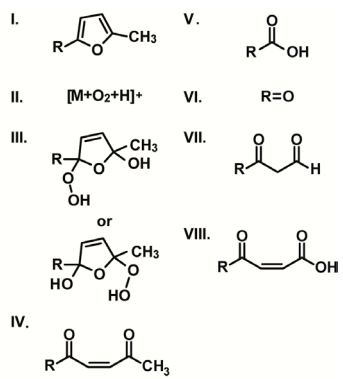
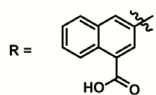
C. mAU t = 0 min



mAU t = 38 d



D.



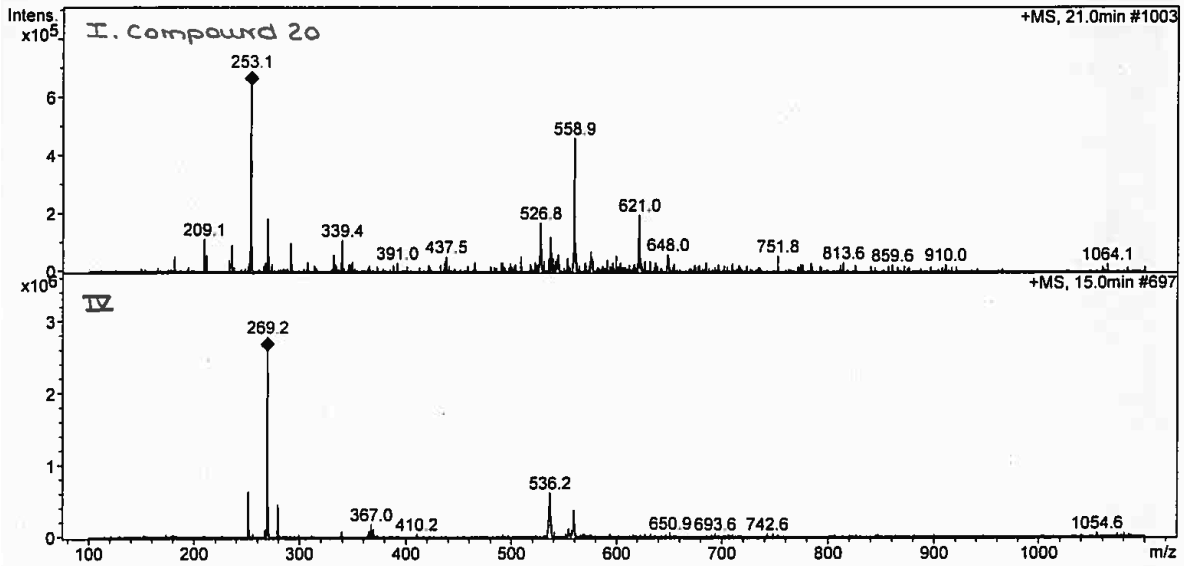
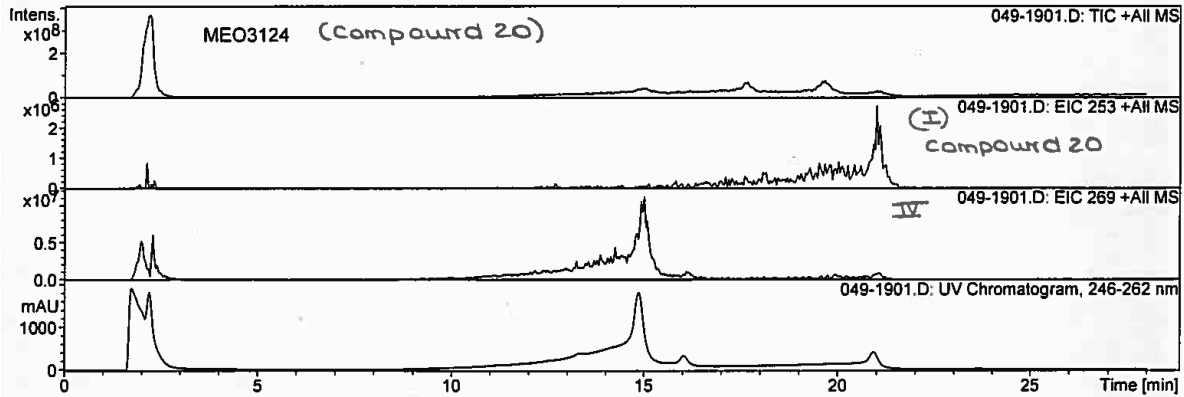


E.

Analysis Name 049-1901.D  
 Acquisition Date 09/01/2014 11:20:54 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

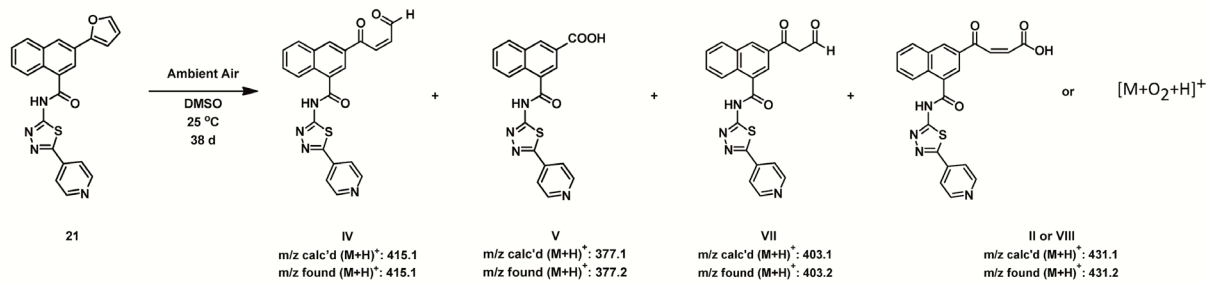
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	14805 $\mu$ s	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



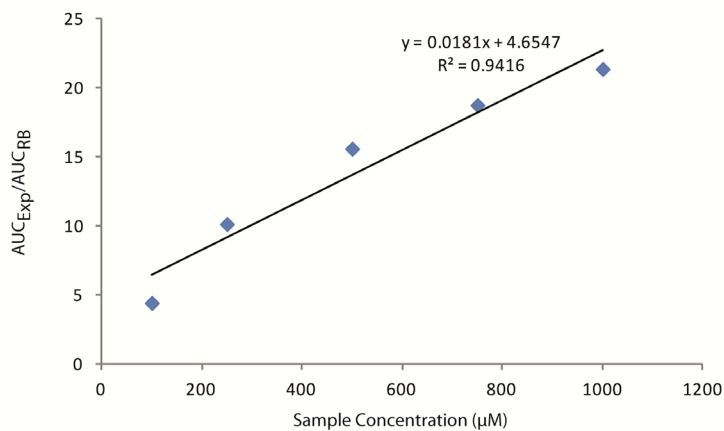
## XXVIII. HPLC & LC/MS Analysis of Aged 21

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

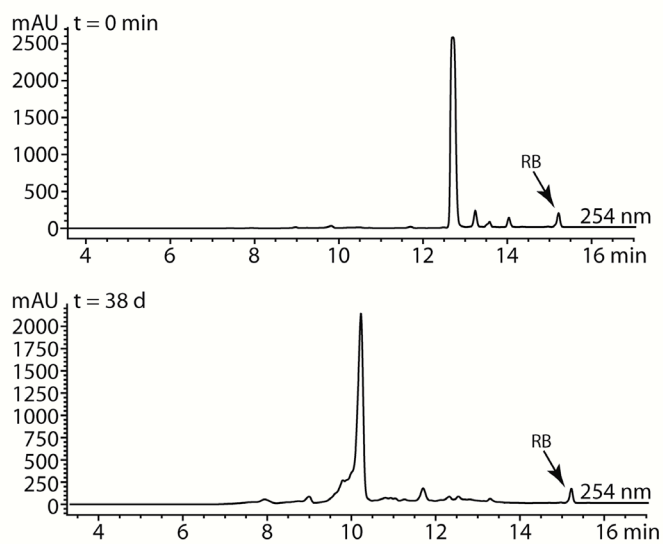
A.



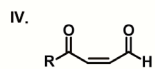
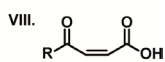
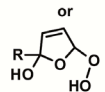
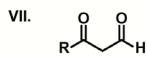
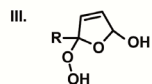
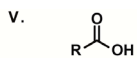
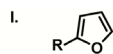
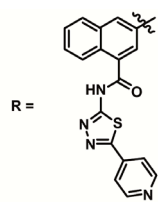
B.



C.



D.

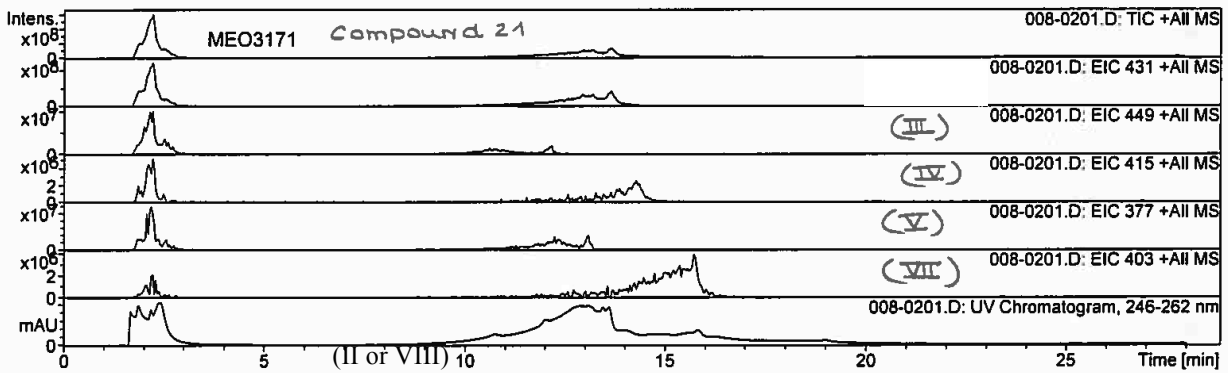


E.

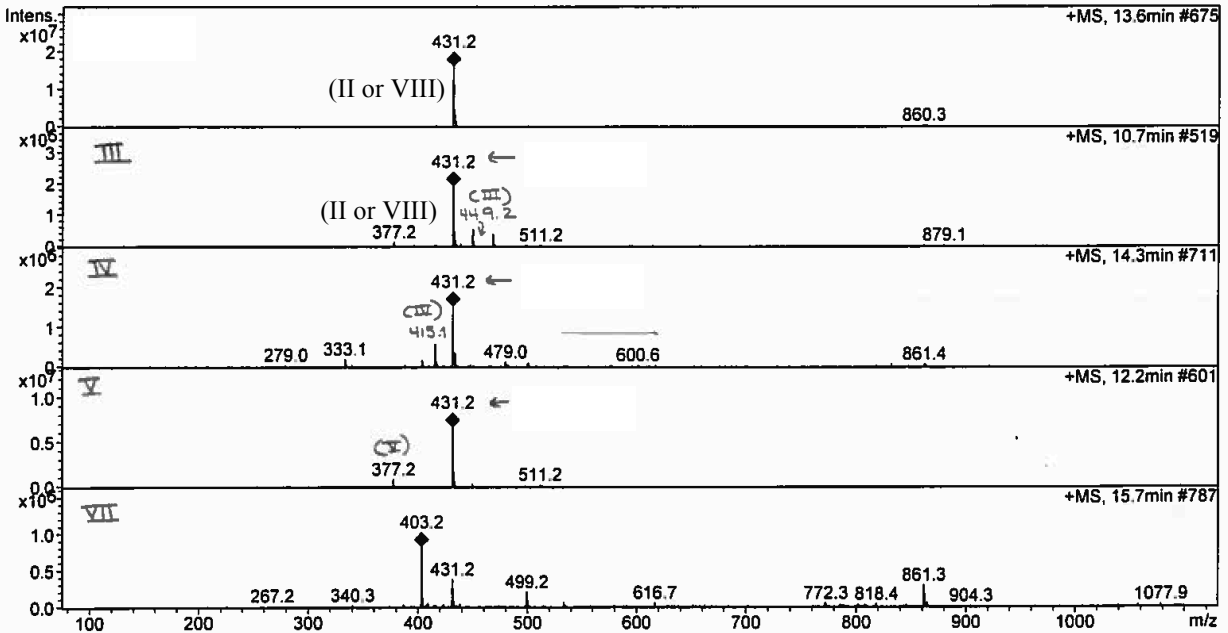
Analysis Name	008-0201.D	Operator	Maggie Olson
Acquisition Date	09/01/2014 12:51:40 PM	Instrument	LC-MSD-Trap-SL
Method	130701A.M		
Comment			

Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	13044 µs	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt (II or VIII)		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



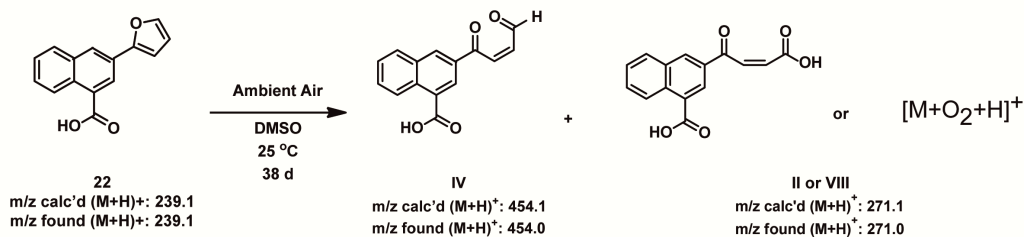
II or VIII



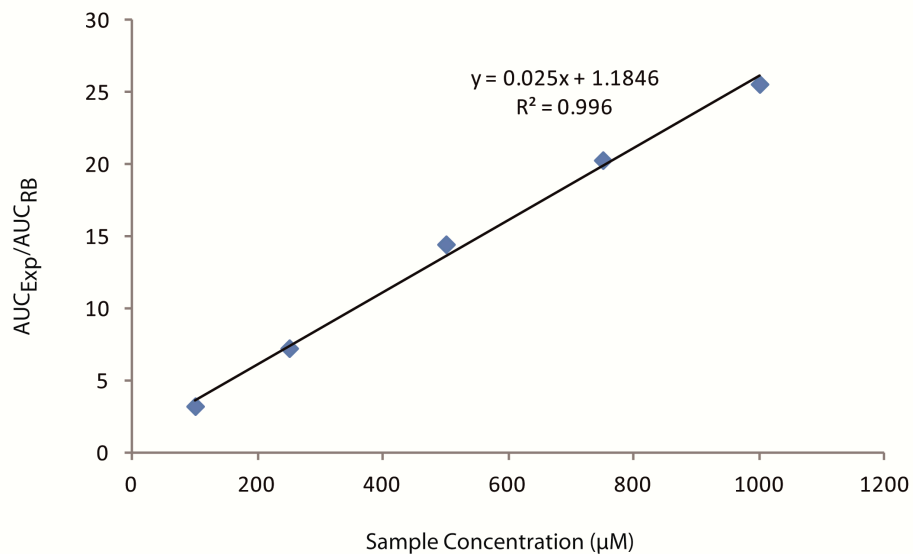
## XXIX. HPLC & LC/MS Analysis of Aged 22

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

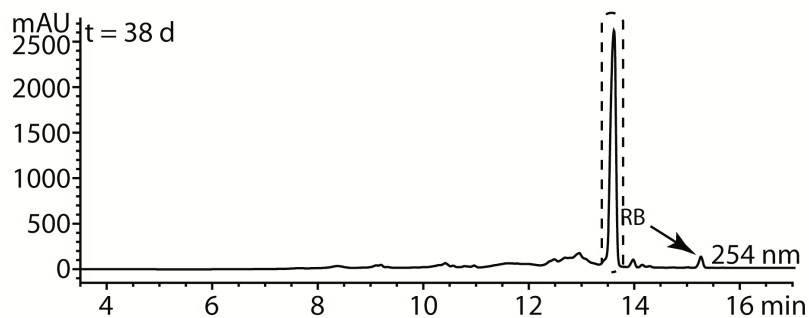
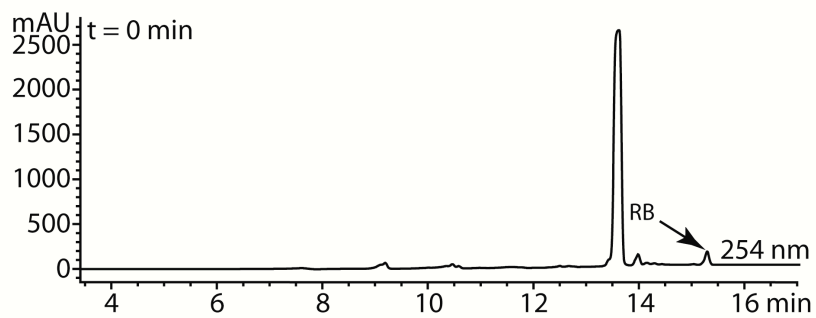
A.



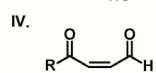
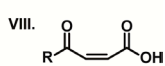
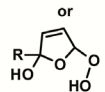
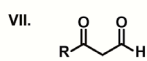
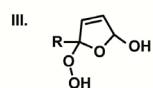
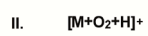
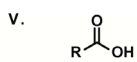
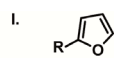
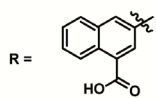
B.



C.



D.

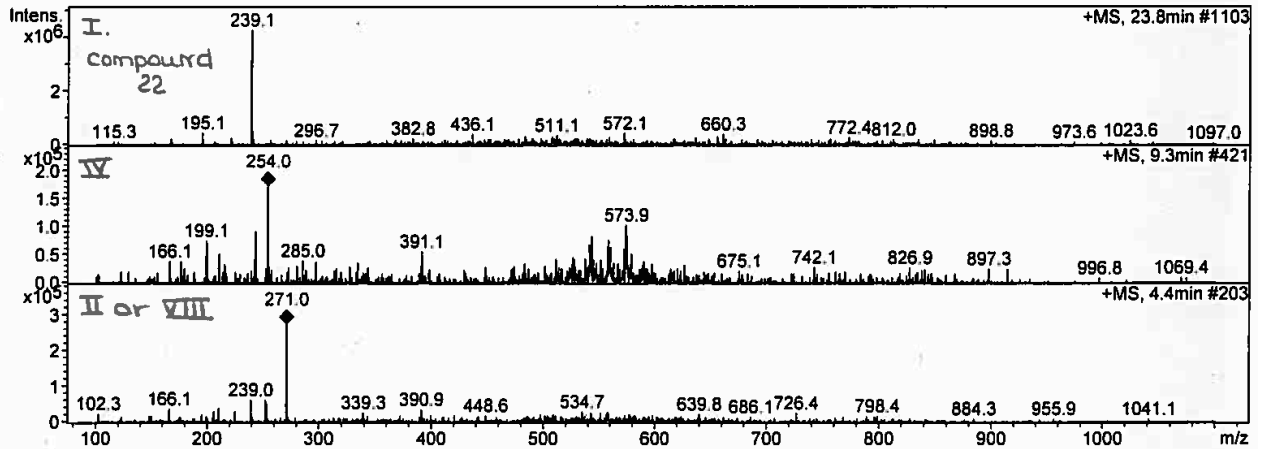
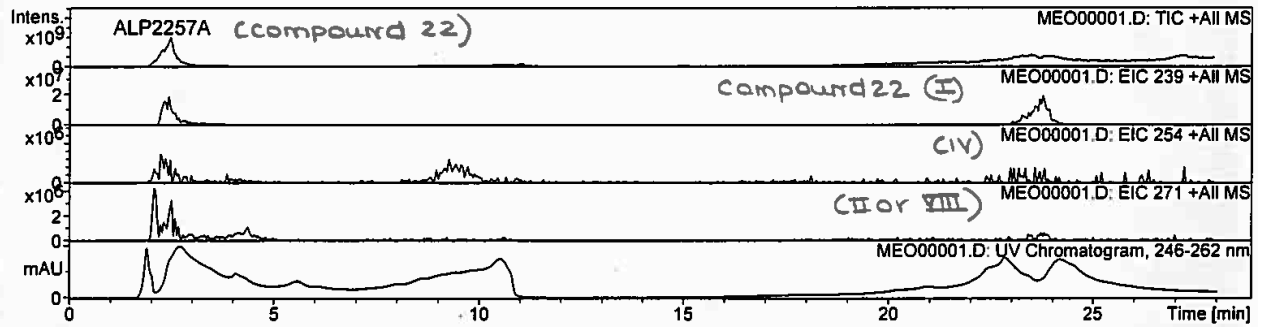


E.

Analysis Name MEO00001.D  
Acquisition Date 12/20/2014 04:00:08 PM Operator Rachit Shah  
Method 130701A.M Instrument LC-MSD-Trap-SL  
Comment

Acquisition Parameters

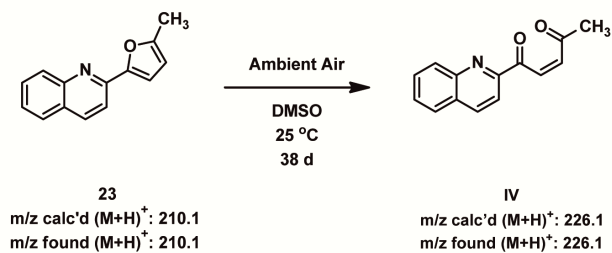
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	9644 $\mu$ s	Trap Drive	50.6	Multiplier Voltage	2256 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 $^{\circ}$ C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



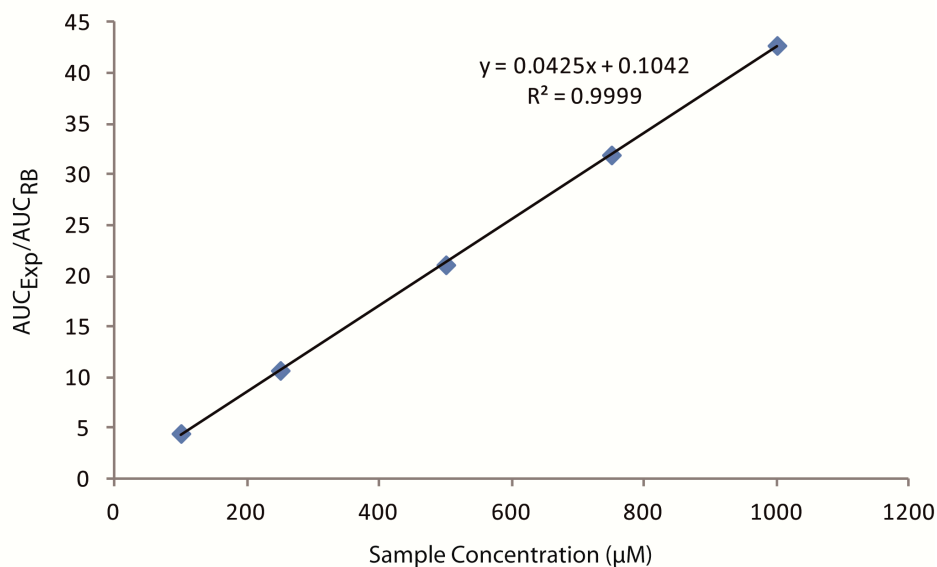
### XXX. HPLC & LC/MS Analysis of Aged 23

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

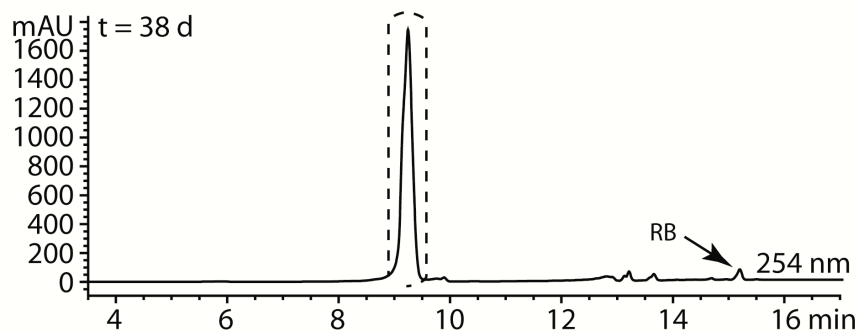
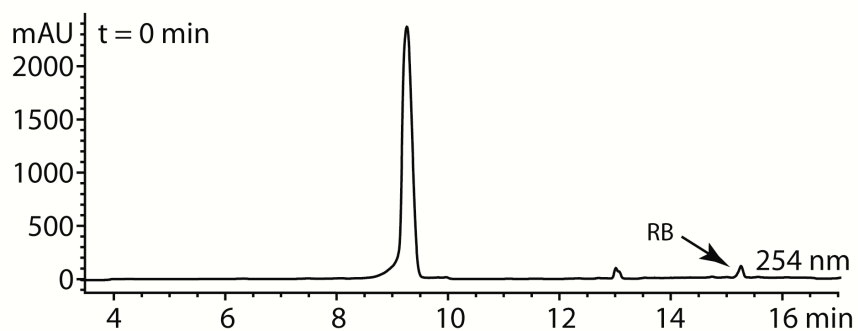
A.



B.

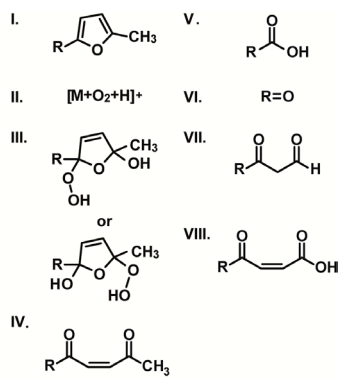
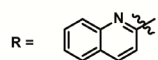


C.





D.

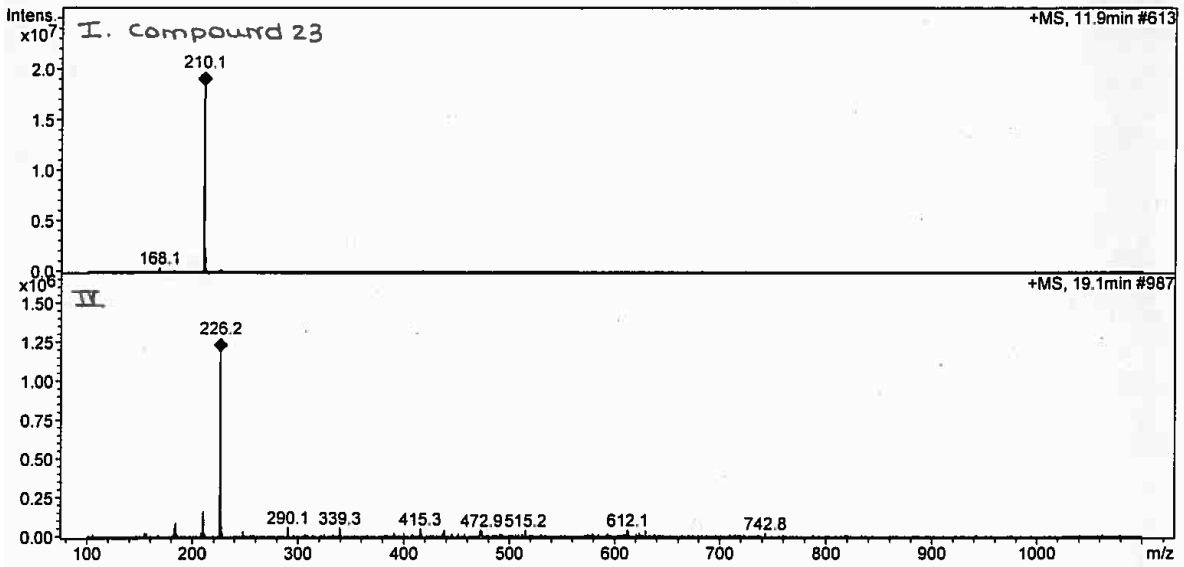
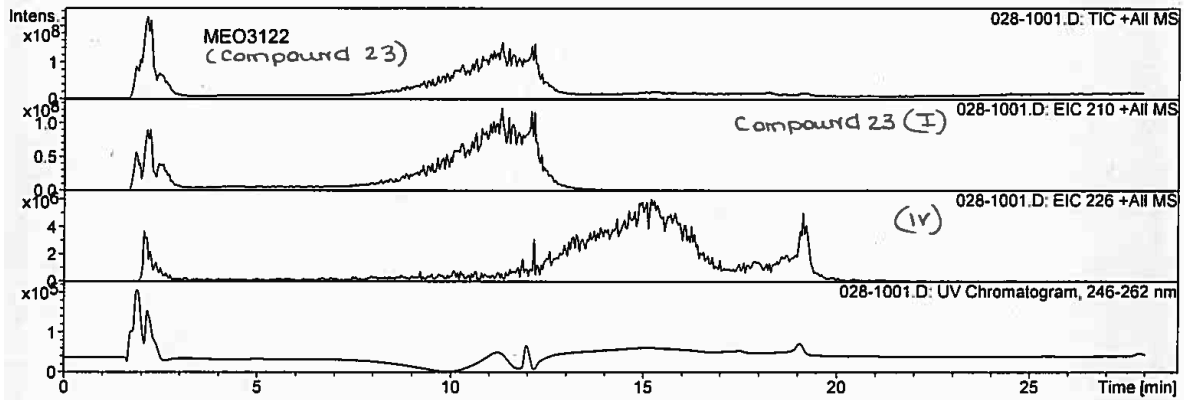


E.

Analysis Name	028-1001.D	Operator	Maggie Olson
Acquisition Date	09/01/2014 05:47:44 PM	Instrument	LC-MSD-Trap-SL
Method	130701A.M		
Comment			

Acquisition Parameters

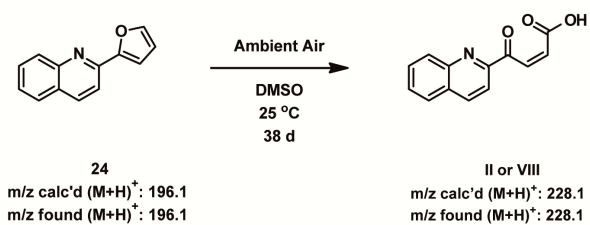
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	11782 $\mu$ s	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 $^{\circ}$ C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



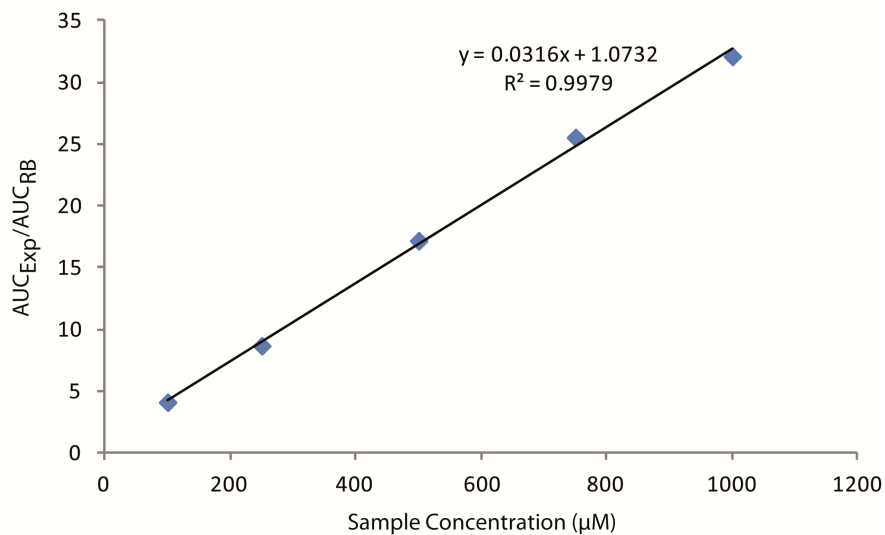
### XXXI. HPLC & LC/MS Analysis of Aged 24

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)

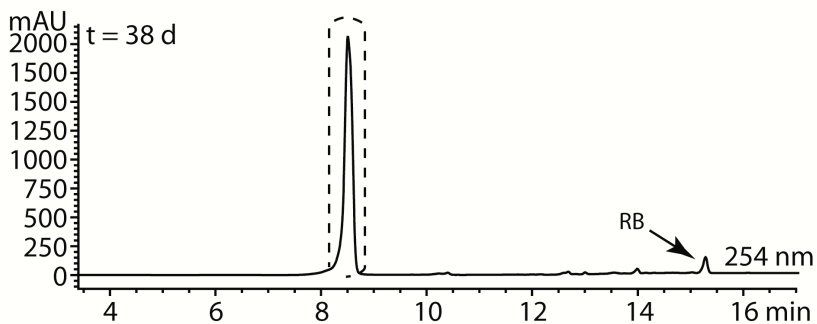
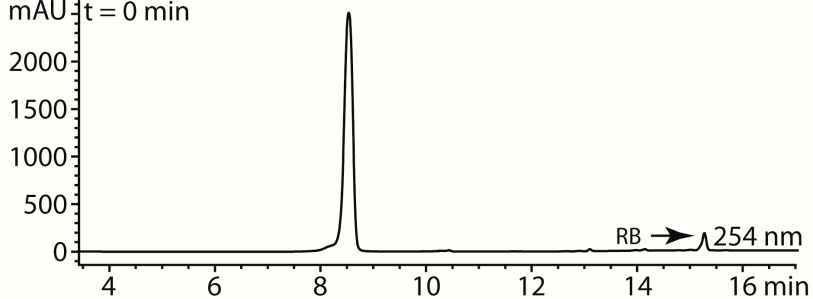
A.



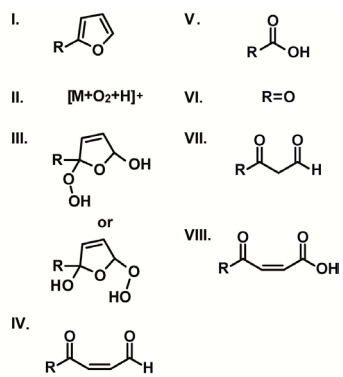
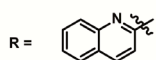
B.



C. mAU t = 0 min



D.

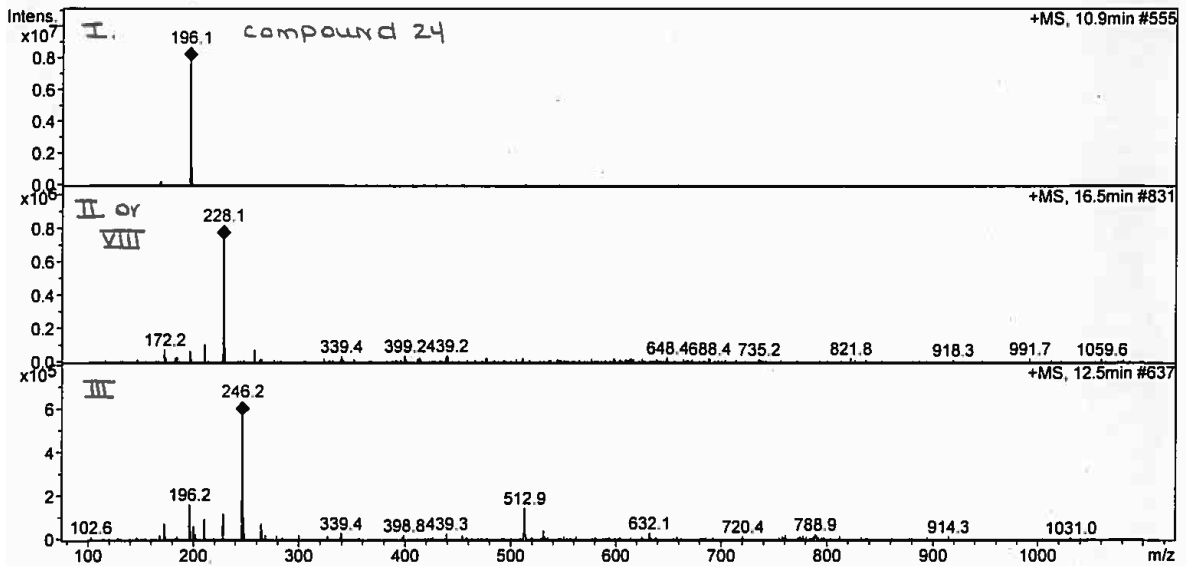
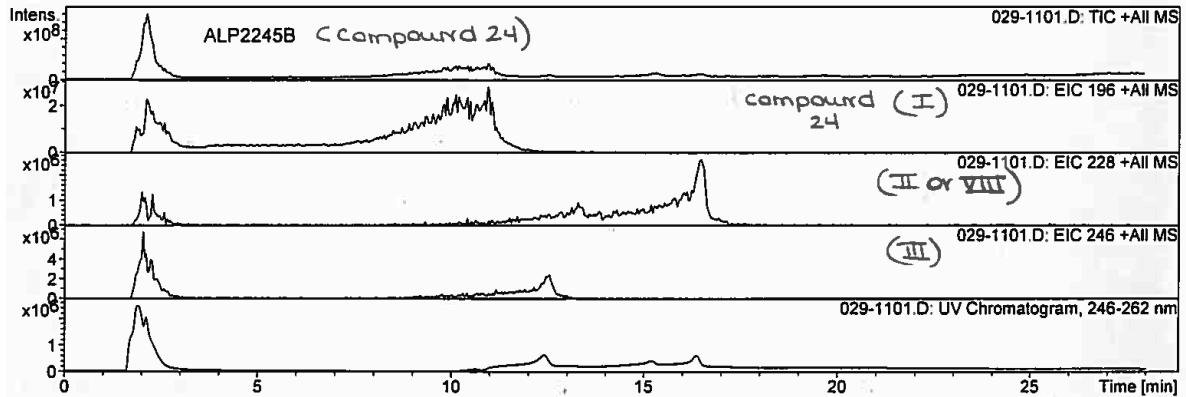


E.

Analysis Name 029-1101.D  
 Acquisition Date 09/01/2014 06:24:44 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

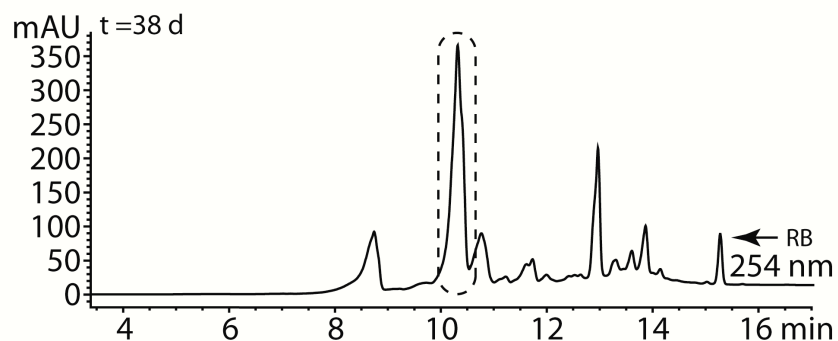
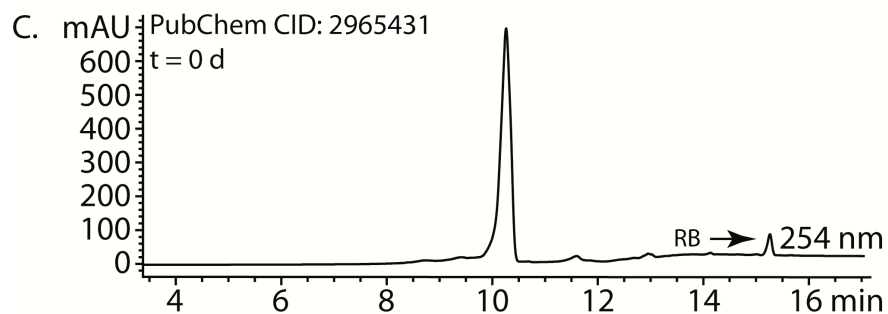
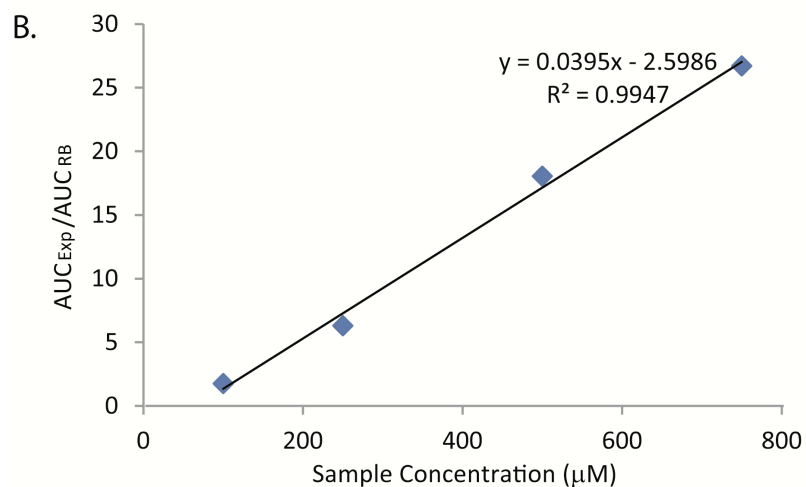
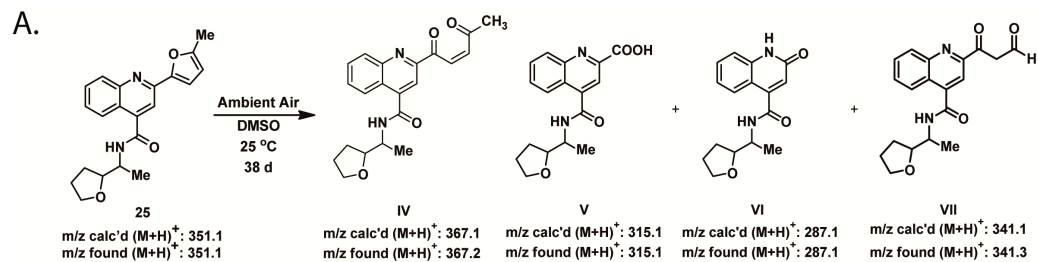
Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	12984 $\mu$ s	Trap Drive	50.6	Multiplier Voltage	2324 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		



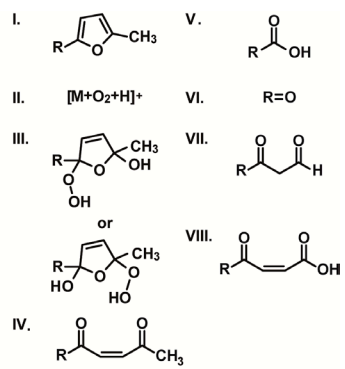
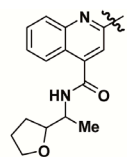
## XXXII. HPLC & LC/MS Analysis of Aged 25

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)



D.

R =



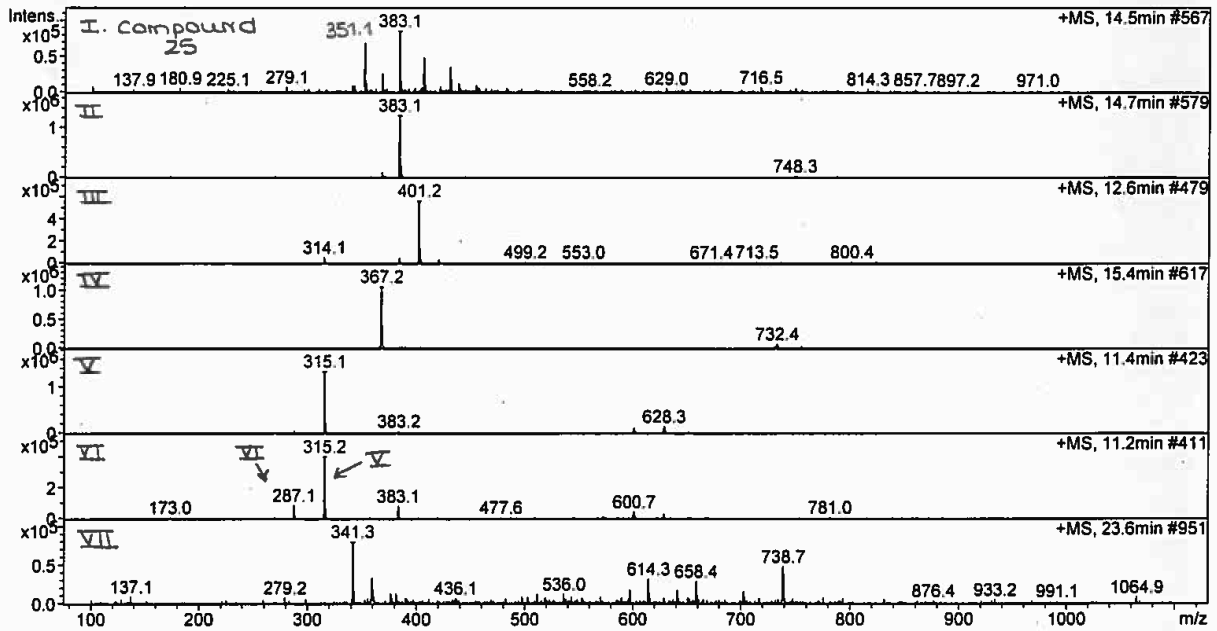
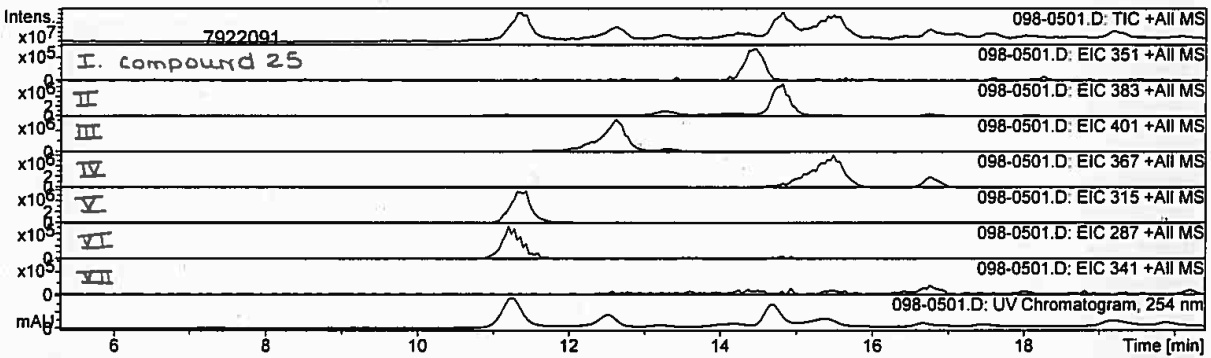
E.

Analysis Name 098-0501.D  
 Acquisition Date 08/06/2013 05:55:21 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	22117 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

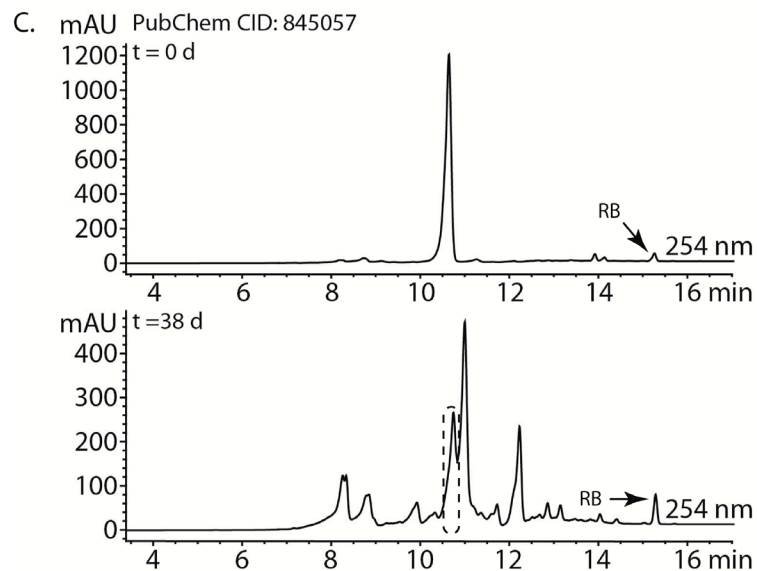
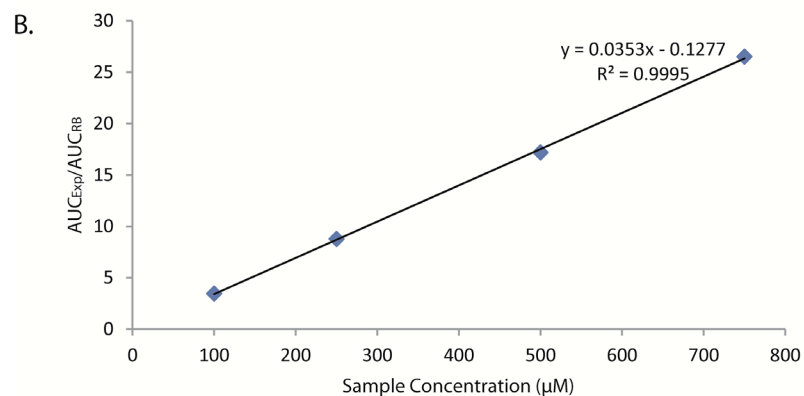
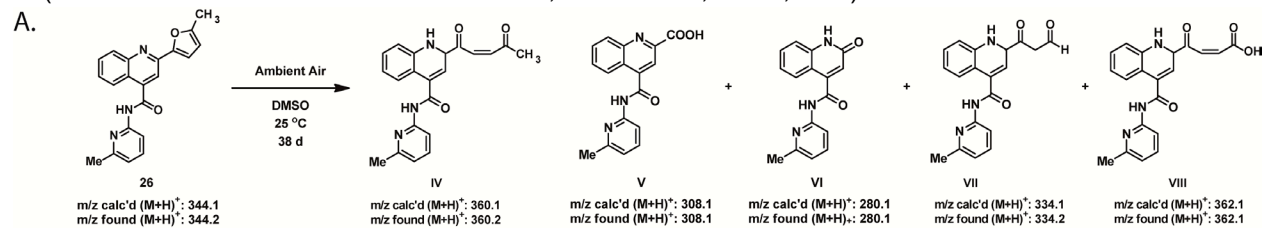
Pubchem CID: 2965431



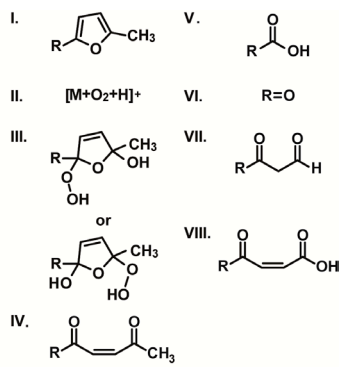
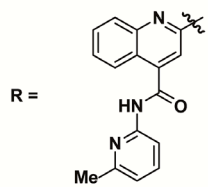


### XXXIII. HPLC & LC/MS Analysis of Aged 26

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)



D.



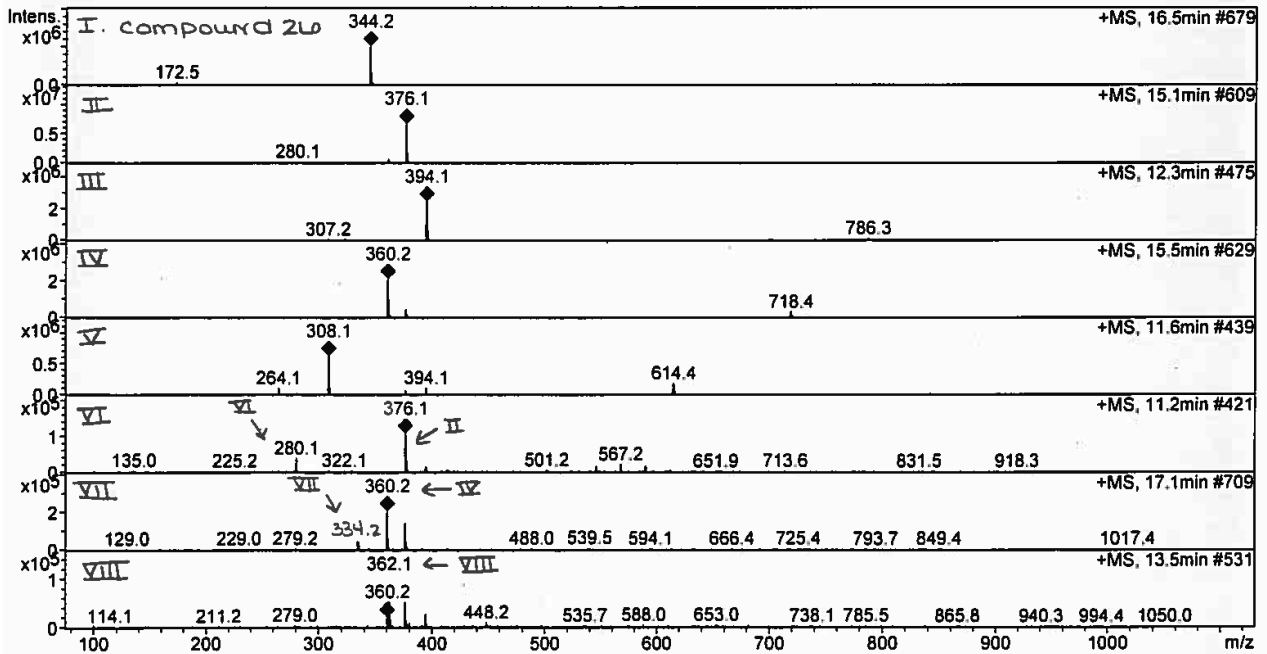
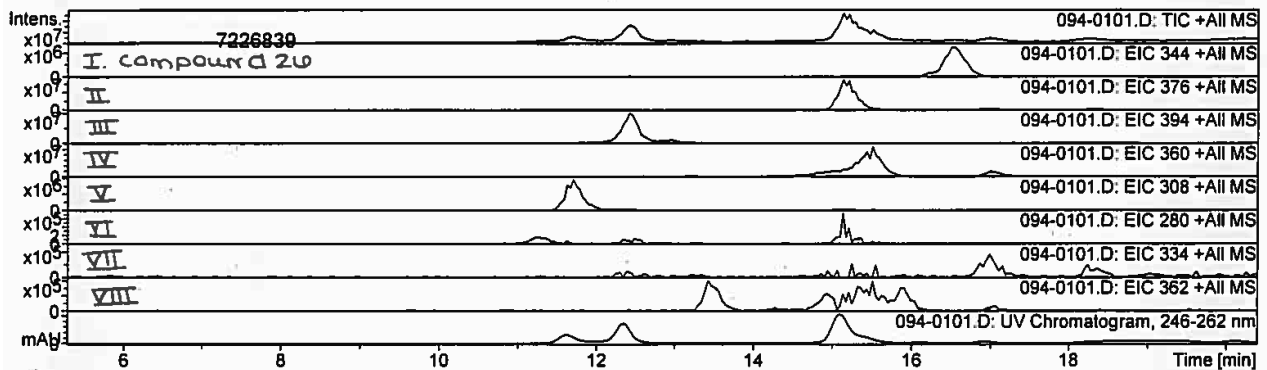
E.

Analysis Name 094-0101.D  
 Acquisition Date 08/06/2013 03:36:39 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

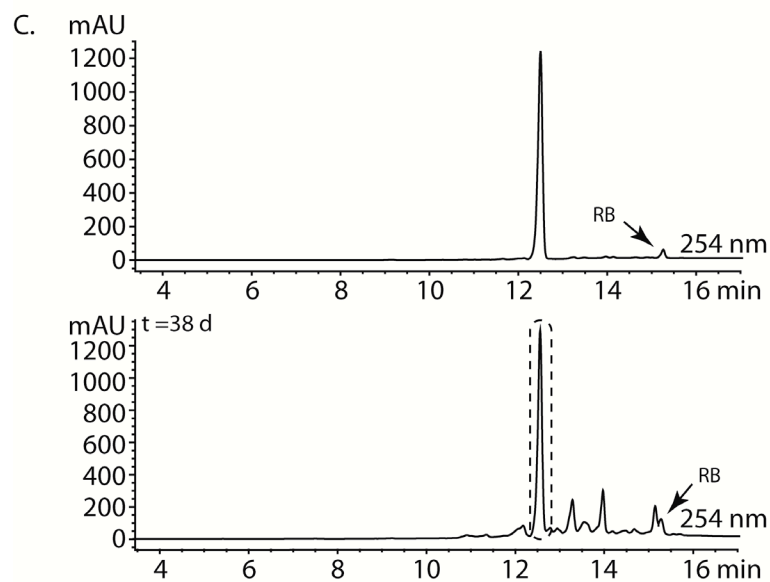
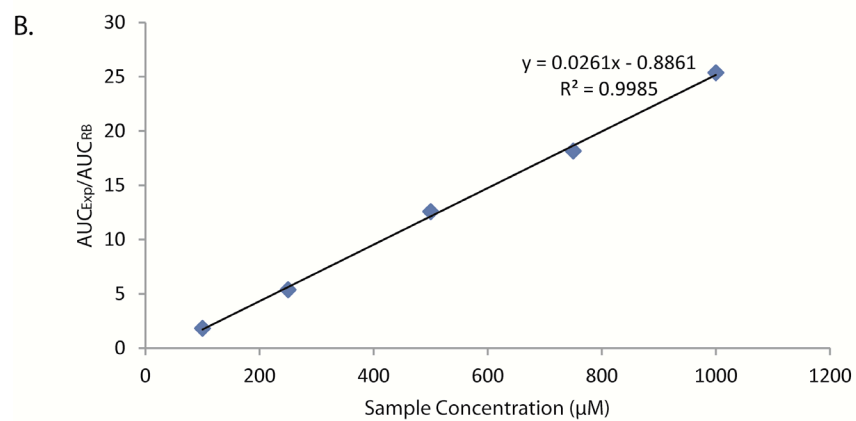
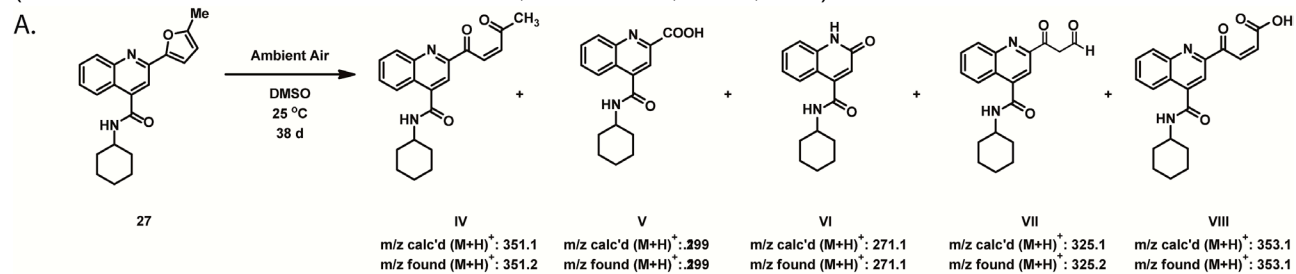
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	25020 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 $^{\circ}$ C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

PubChem CID: 845057

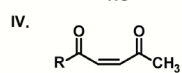
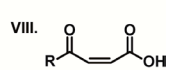
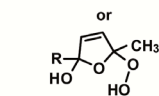
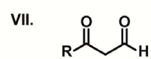
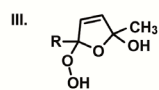
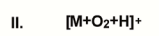
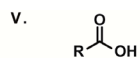
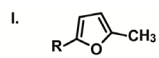
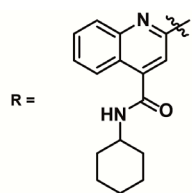


### XXXIV. HPLC & LC/MS Analysis of Aged 27

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)



D.



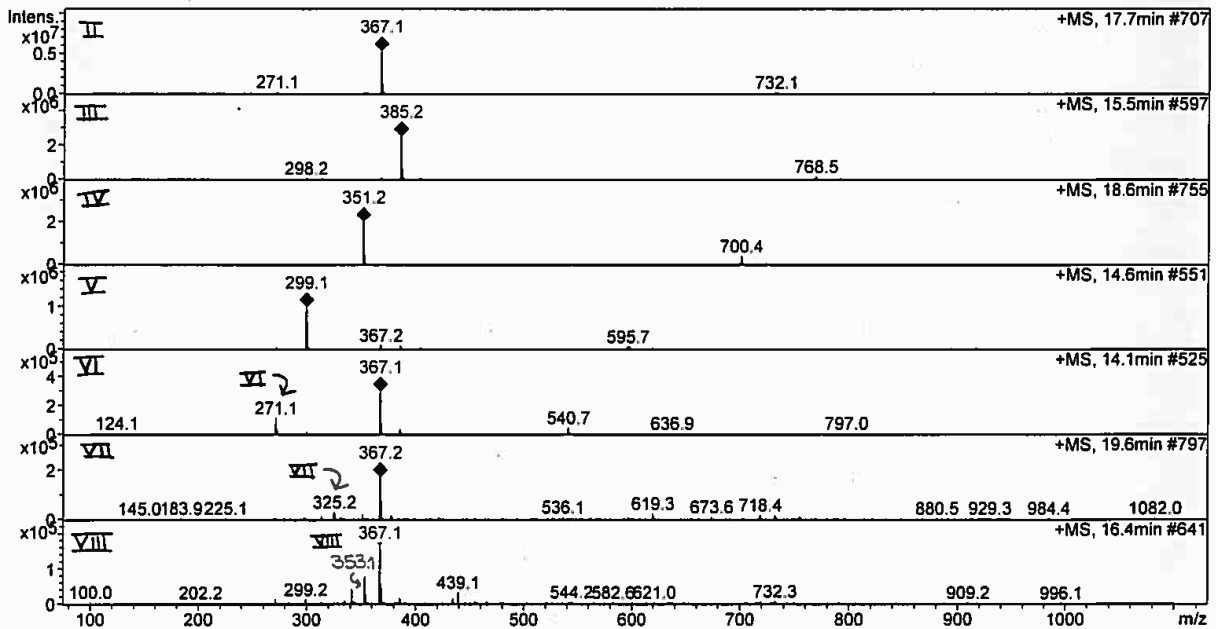
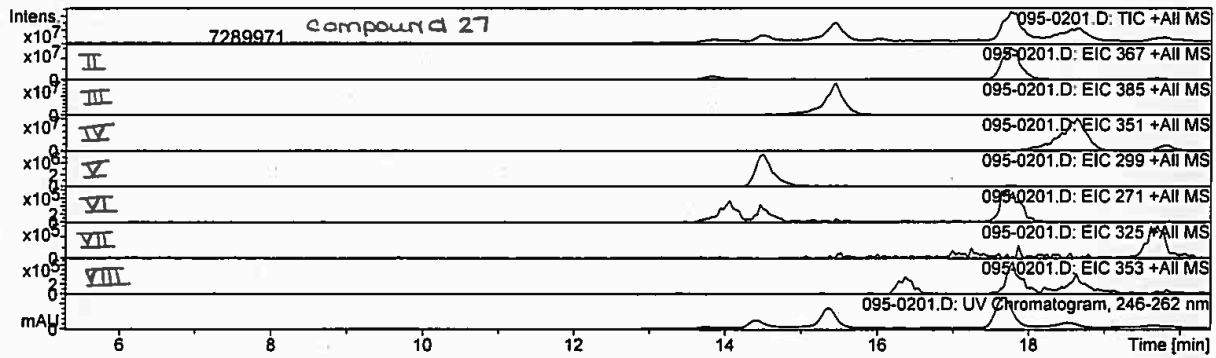
E.

Analysis Name 095-0201.D  
 Acquisition Date 08/06/2013 04:11:19 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

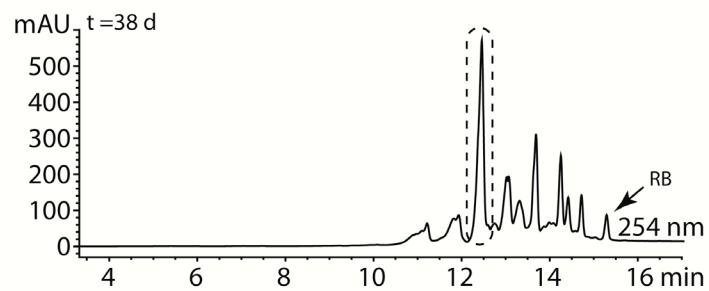
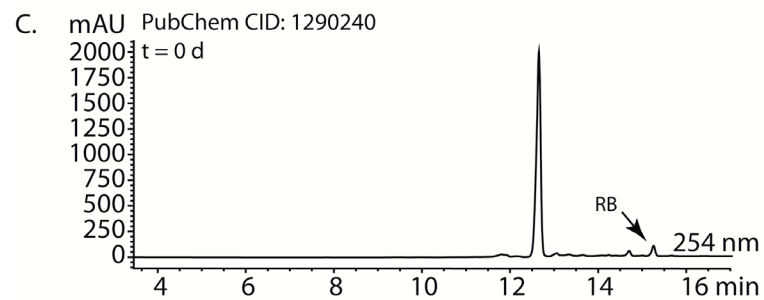
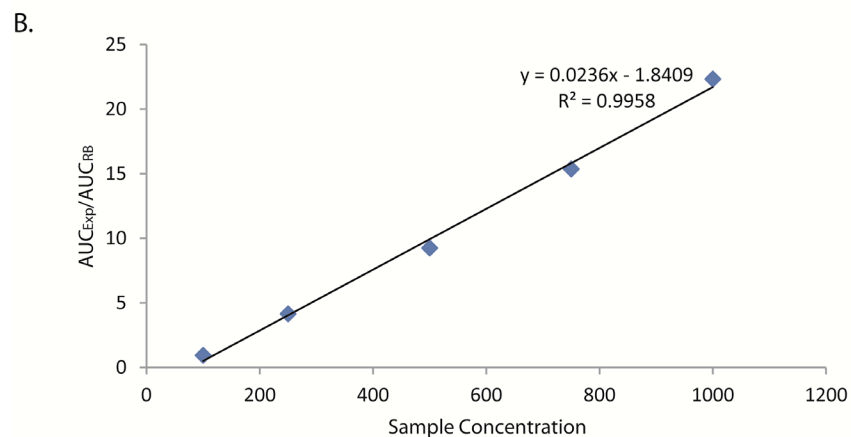
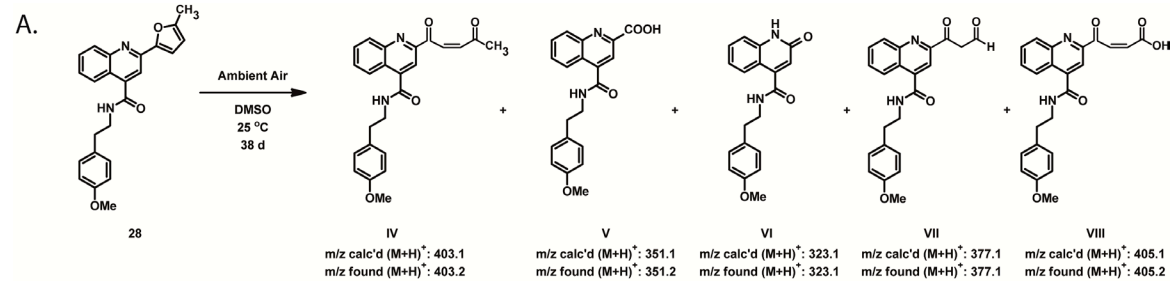
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	30071 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

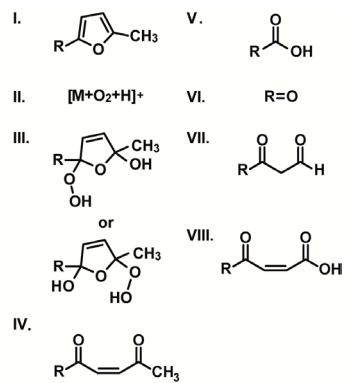
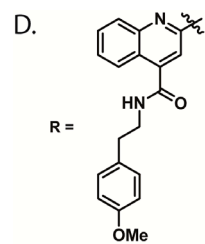
Pubchem CID: 898877



### XXXV. HPLC & LC/MS Analysis of Aged 28

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)







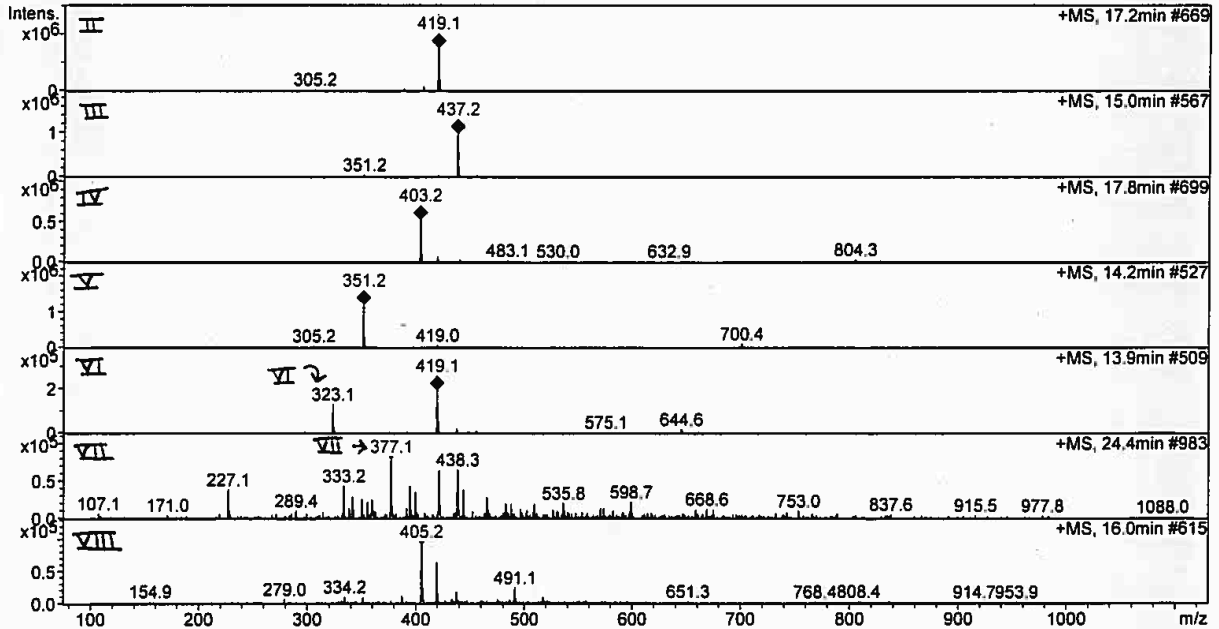
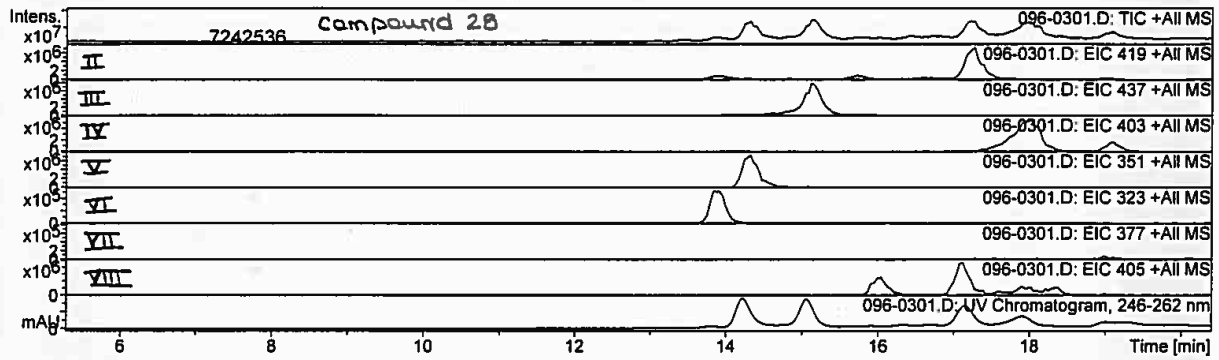
E.

Analysis Name 096-0301.D  
 Acquisition Date 08/06/2013 04:46:00 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

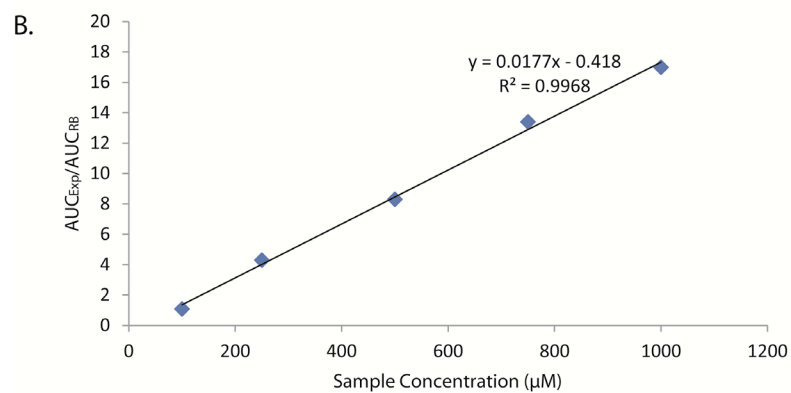
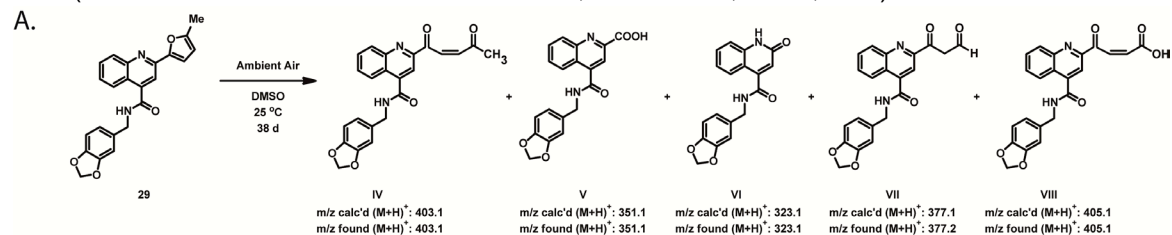
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	30000 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 $^{\circ}$ C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

Pubchem CID: 1290240

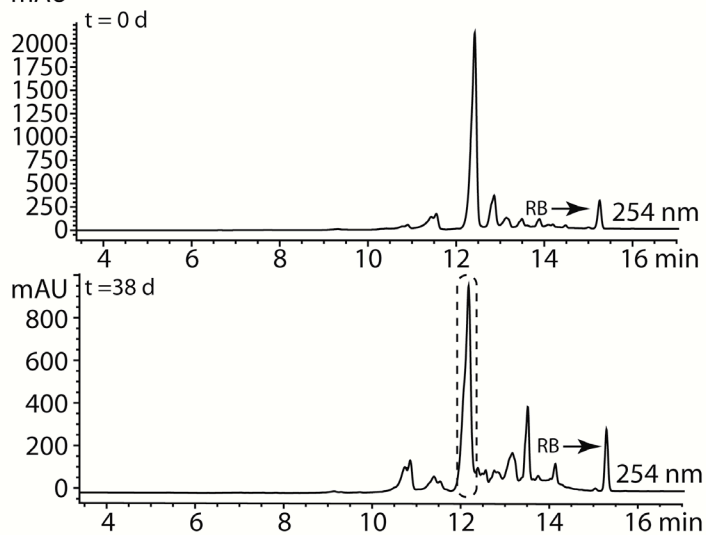


## XXXVI. HPLC & LC/MS Analysis of Aged 29

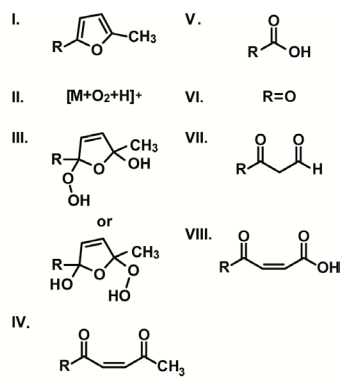
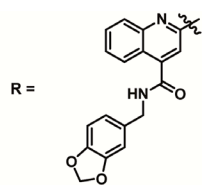
(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)



C. mAU PubChem CID: 1001397



D.



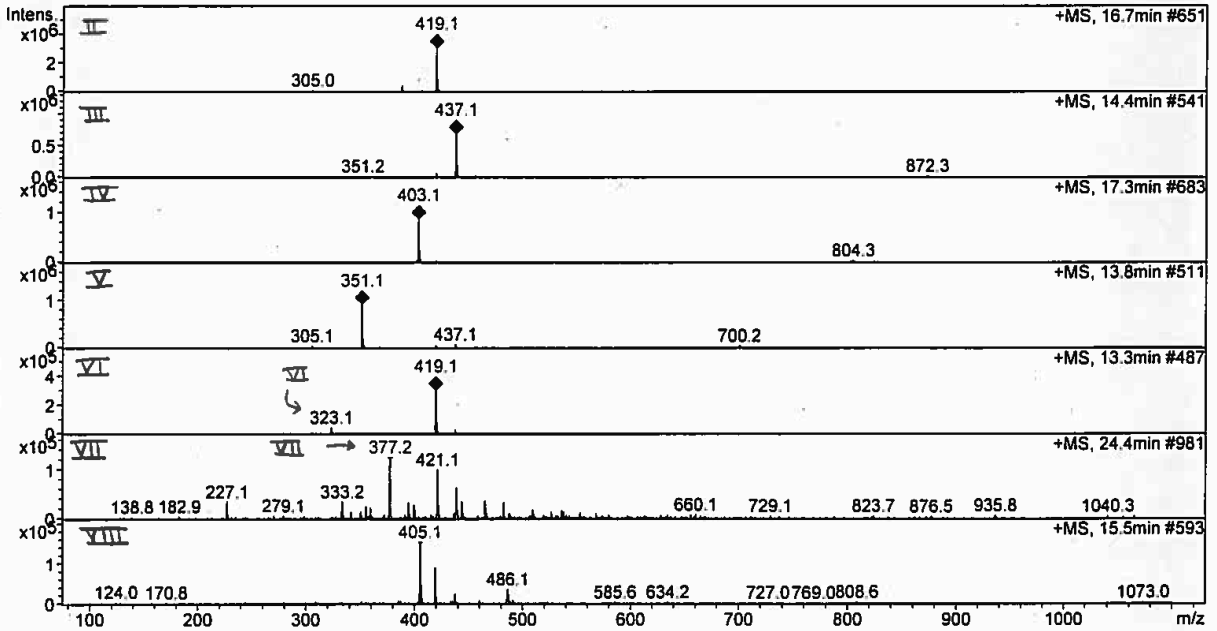
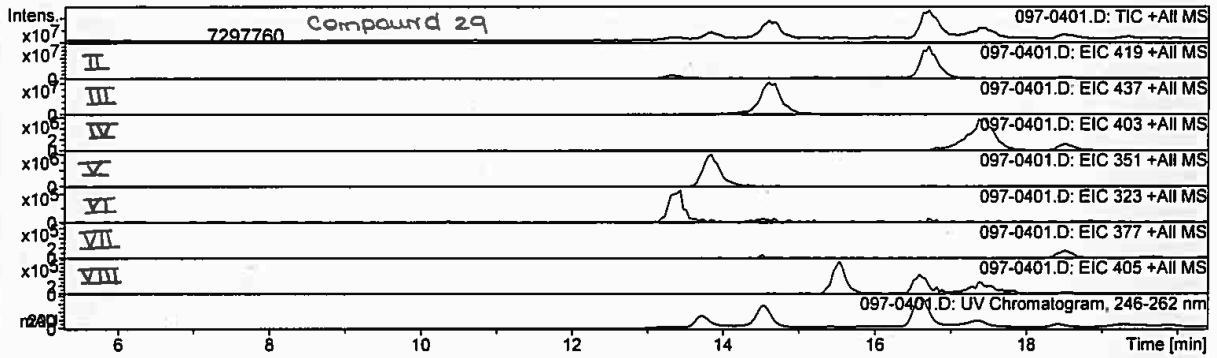
E.

Analysis Name 097-0401.D  
 Acquisition Date 08/06/2013 05:20:40 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

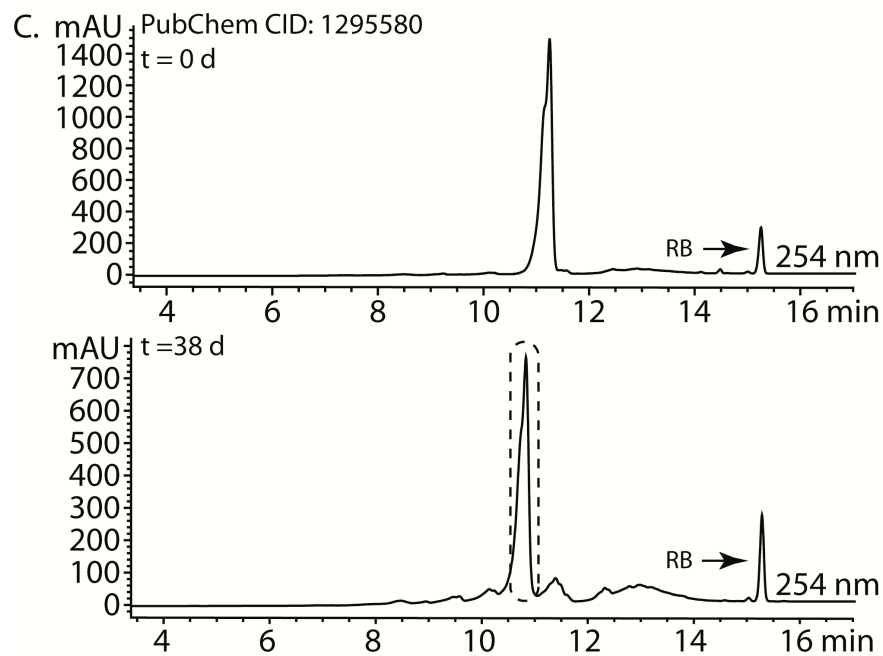
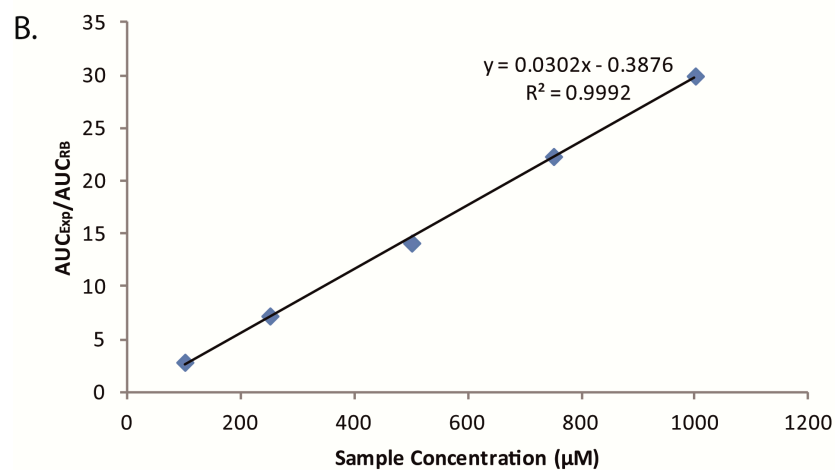
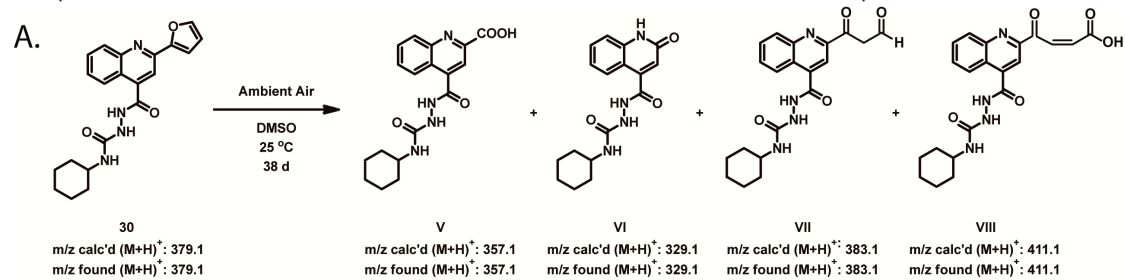
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	29931 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 $^{\circ}$ C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

Pubchem CID: 1001397

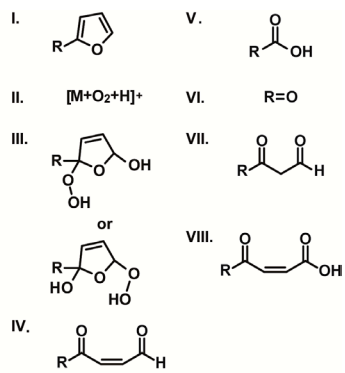
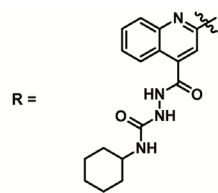


## XXXVII. HPLC & LC/MS Analysis of Aged 30

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)



D.



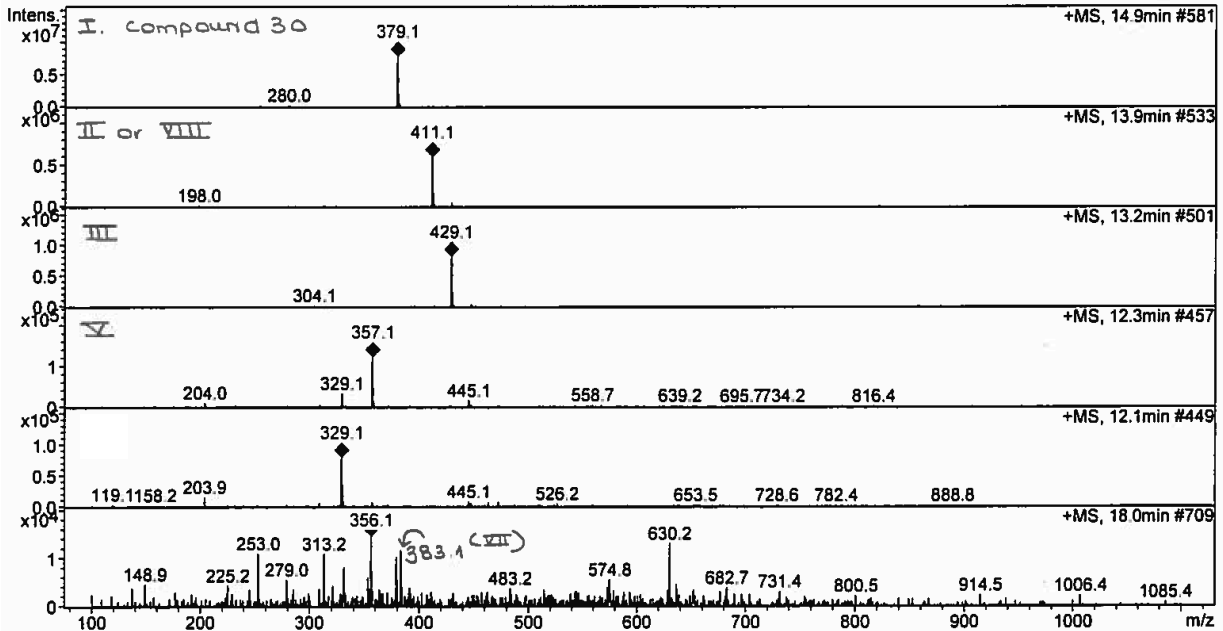
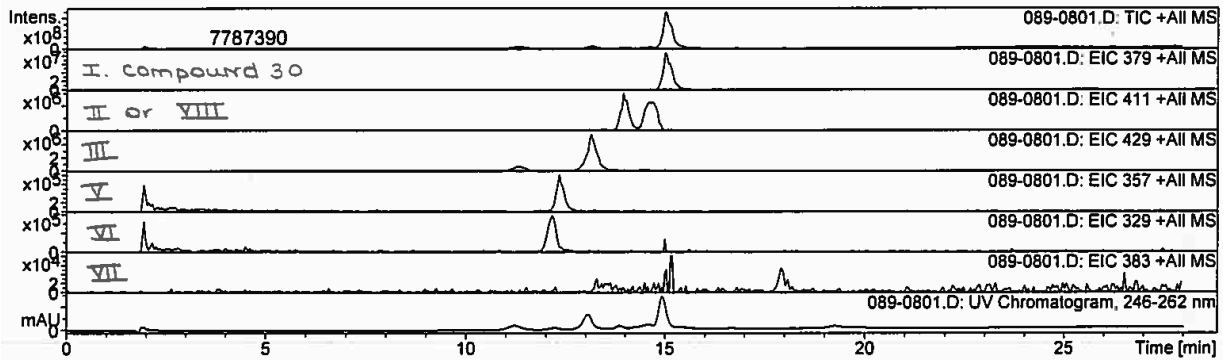
E.

Analysis Name 089-0801.D  
 Acquisition Date 08/06/2013 07:39:32 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	30412 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 $^{\circ}$ C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

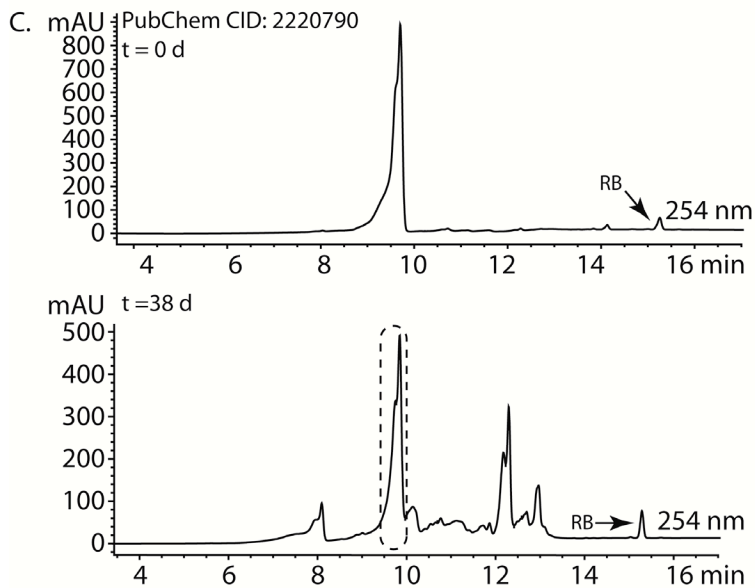
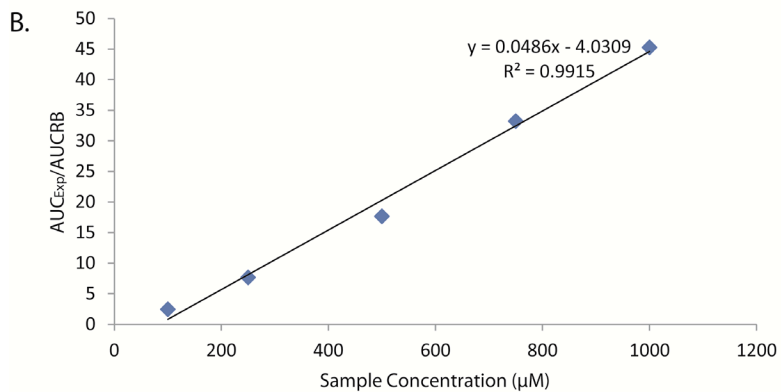
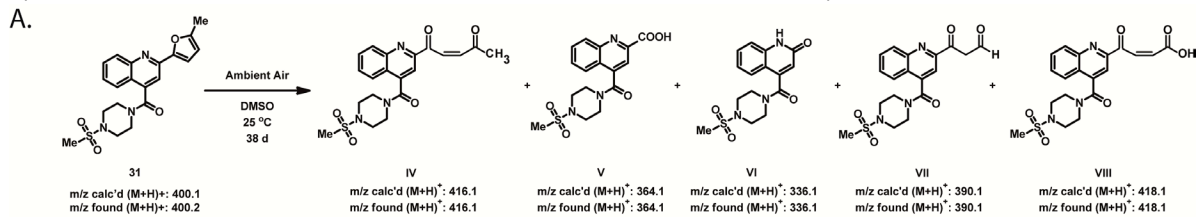
Pubchem CID: 1295580



VI

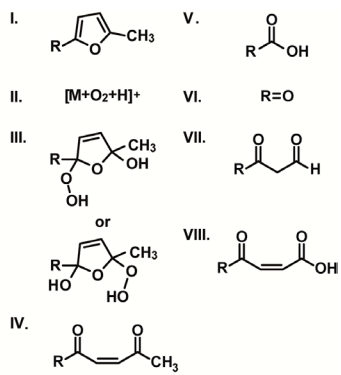
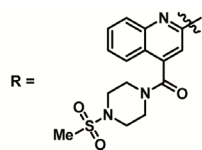
## XXXVIII. HPLC & LC/MS Analysis of Aged 31

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)





D.



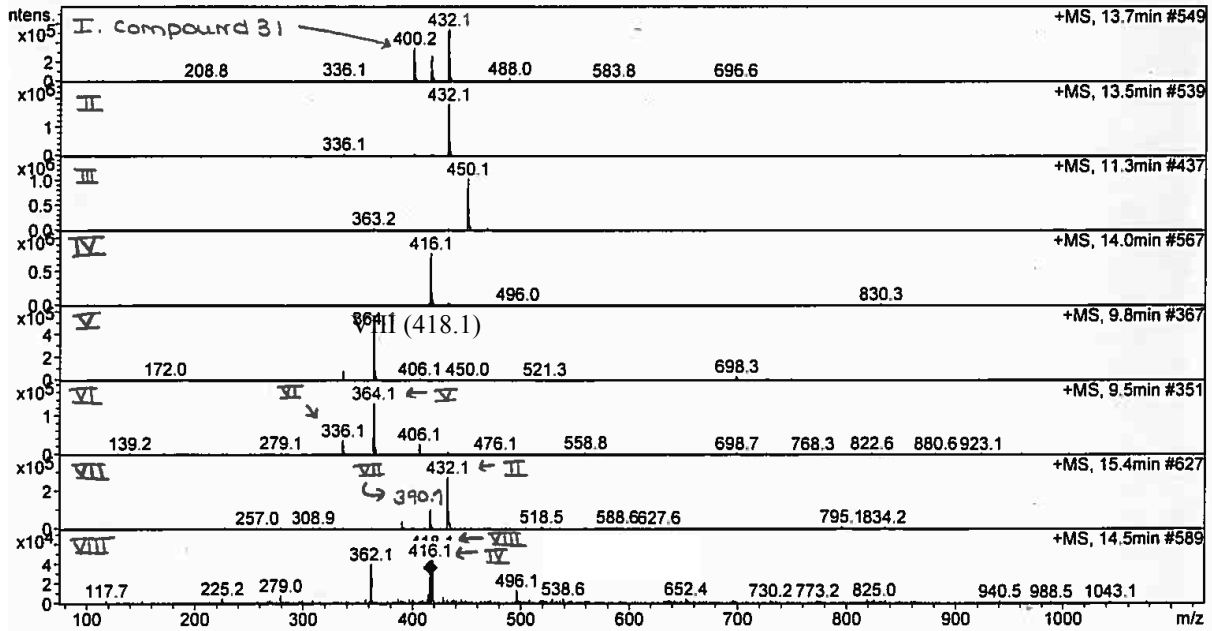
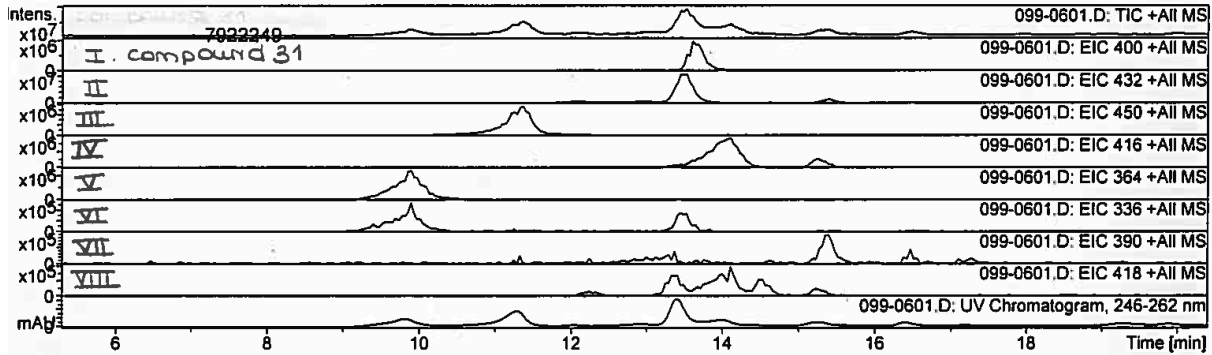
E.

Analysis Name 099-0601.D  
 Acquisition Date 08/06/2013 06:30:07 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

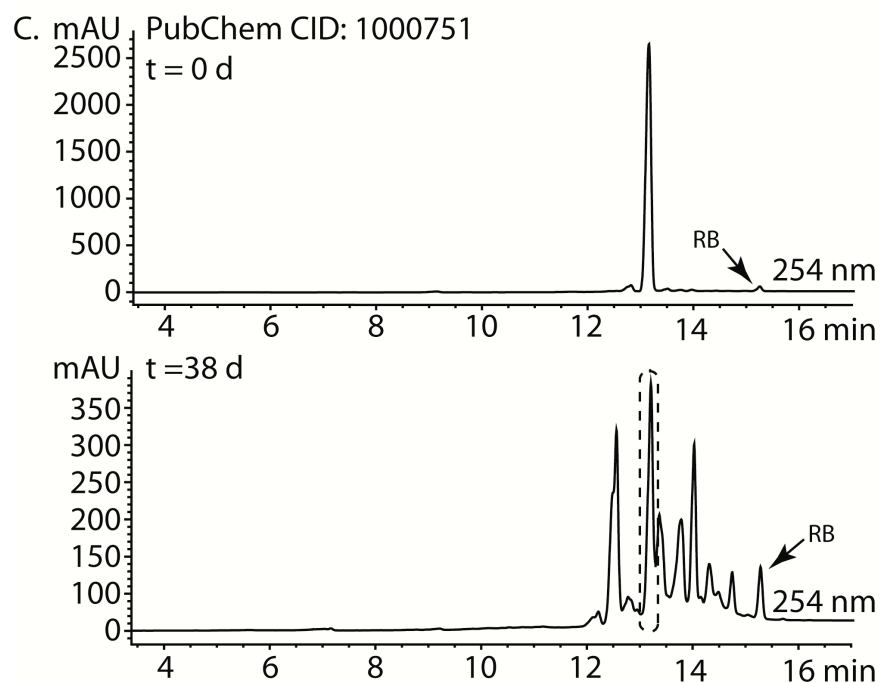
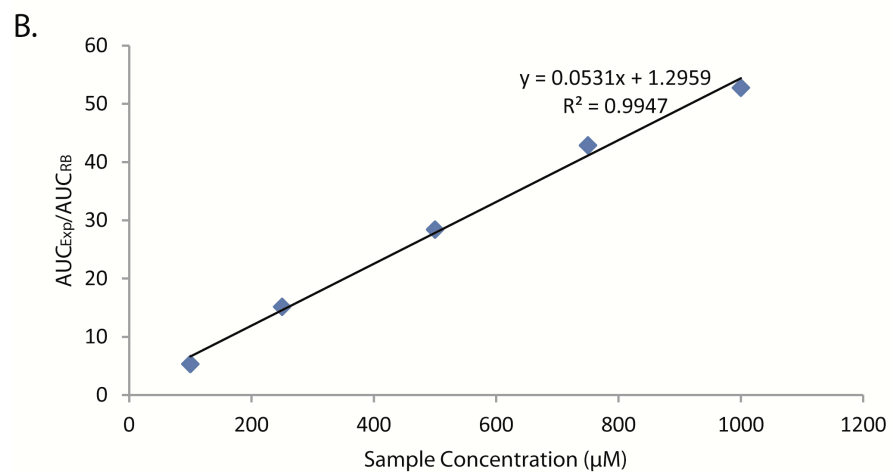
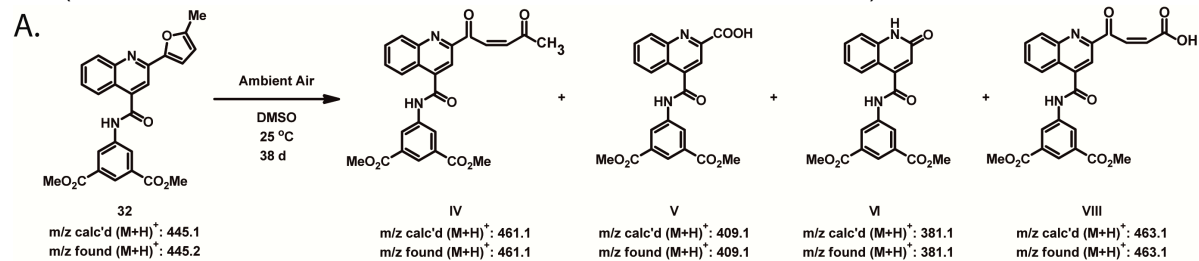
Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	29872 µs	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Web. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

Pubchem CID: 2220790

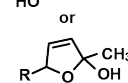
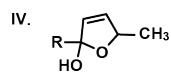
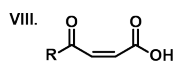
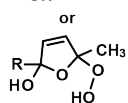
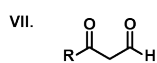
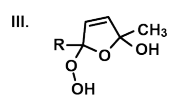
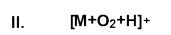
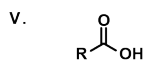
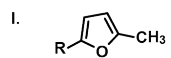
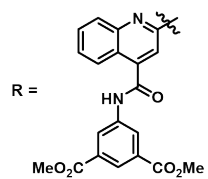


### XXXIX. HPLC & LC/MS Analysis of Aged 32

(Reaction Conditions: 10 mM DMSO Stock, Ambient Air, 25 °C, 38 d)



D.



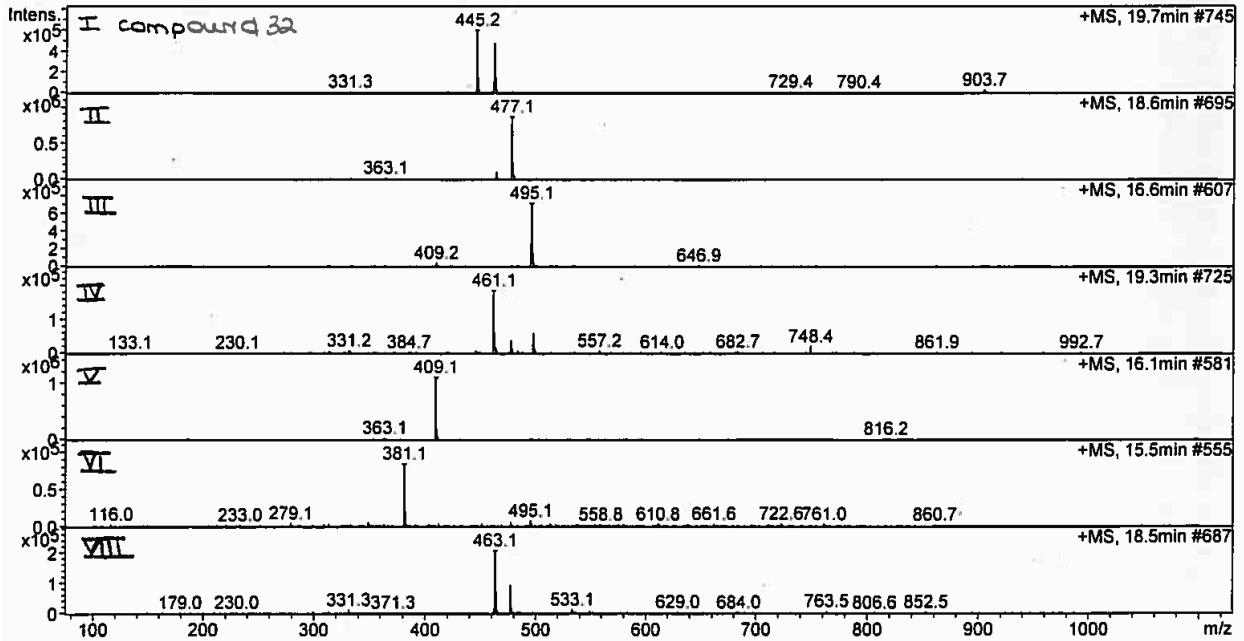
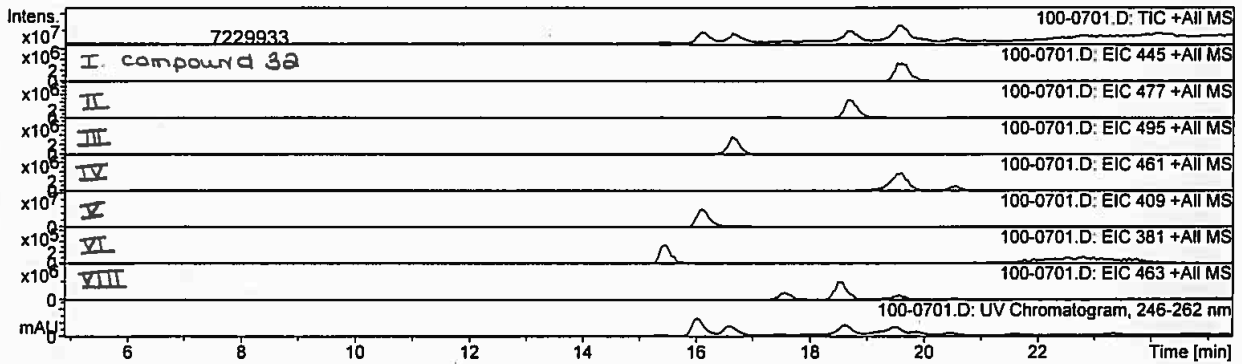
E.

Analysis Name 100-0701.D  
 Acquisition Date 08/06/2013 07:04:50 PM Operator Maggie Olson  
 Method 130701A.M Instrument LC-MSD-Trap-SL  
 Comment

Acquisition Parameters

Mass Range Mode	Std/Normal	Ion Polarity	Positive	Alternating Ion Polarity	off
Ion Source Type	ESI	Capillary Current Control	off	Auto MS/MS	on
Accumulation Time	29668 $\mu$ s	Trap Drive	51.9	Multiplier Voltage	2029 Volt
Averages	8 Spectra	Octopole RF Amplitude	179.2 Vpp		
Dry Heat	on	Capillary Exit	124.8 Volt		
Neb. Gas	on	Skimmer	40.0 Volt		
Dry Gas	on	Dry Temp (Set)	200 °C		
High Voltage	on	HV Capillary	3400 V		
		Scan Begin	100 m/z		
		Scan End	1100 m/z		

Pubchem CID: 1000751



## XXXX. SMILES Document

Compound	SMILE	% Parent Remaining
1	<chem>O=C(C1=CC(C2=CC=C(C)O2)=NC3=C1C=CC=C3)NC4=NN=C(C5=CC=NC=C5)S4</chem>	6 ± 1
2	<chem>O=C(C1=CC=CC=C1N2)C2=O</chem>	N/A
3	<chem>OC(C1=CC(C2=CC=C(C)O2)=NC3=CC=CC=C31)=O</chem>	N/A
4	<chem>NC1=NN=C(C2=CC=NC=C2)S1</chem>	N/A
5	<chem>O=C1C=C(C(NC2=NN=C(C3=CC=NC=C3)S2)=O)C4=CC=CC=C4N1</chem>	N/A
6	<chem>O=C(NC1=NN=C(C2=CC=NC=C2)S1)C3=CC(C(O)=O)=NC4=CC=CC=C43</chem>	N/A
7	<chem>O=C(NC1=NN=C(C2=CC=NC=C2)S1)C3=CC(C4(O)OC(C=C4)(O)C)=NC5=CC=CC=C53/ O=C(NC1=NN=C(C2=CC=NC=C2)S1)C3=CC(C4(O)OC(C)(OO)C=C4)=NC5=CC=CC=C53</chem>	N/A
8	<chem>O=C(C1=NC2=CC=CC=C2C(C(NC3=NN=C(C4=CC=NC=C4)S3)=O)=C1)/C=C\C(C)=O</chem>	N/A
9	<chem>O=C(NC1=NN=C(C2=CC=NC=C2)S1)C3=CC(C4(OO5)OC5(C=C4)C)=NC6=CC=CC=C63</chem>	N/A
10	<chem>O=C(C1=NC2=CC=CC=C2C(C(NC3=NN=C(C4=CC=NC=C4)S3)=O)=C1)/C=C\C(O)=O</chem>	N/A
11	<chem>O=C(C1=NC2=CC=CC=C2C(C(NC3=NN=C(C4=CC=NC=C4)S3)=O)=C1)CC([H])=O</chem>	N/A
12	<chem>O=C(O)C1=CC(C2=CC=C(C)O2)=NC3=C1C=CC=C3</chem>	83 ± 18
13	<chem>O=C(NC1=NN=C(C2=CC=NC=C2)S1)C3=CC(C4=CC=CO4)=NC5=C3C=CC=C5</chem>	101 ± 7
14	<chem>O=C(O)C1=CC(C2=CC=CO2)=NC3=C1C=CC=C3</chem>	69 ± 7
15	<chem>O=C(NC1=NN=C(C2=CC=NC=C2)S1)C3=CC(C4=CC=C(C)O4)=NC=C3</chem>	34 ± 4
16	<chem>O=C(O)C1=CC(C2=CC=C(C)O2)=NC=C1</chem>	85 ± 8
17	<chem>O=C(NC1=NN=C(C2=CC=NC=C2)S1)C3=CC(C4=CC=CO4)=NC=C3</chem>	90 ± 12
18	<chem>O=C(O)C1=CC(C2=CC=CO2)=NC=C1</chem>	92 ± 6
19	<chem>O=C(NC1=NN=C(C2=CC=NC=C2)S1)C3=CC(C4=CC=C(C)O4)=CC5=C3C=CC=C5</chem>	25 ± 1
20	<chem>CC(O1)=CC=C1C2=CC(C=CC=C3)=C3C(C(O)=O)=C2</chem>	82 ± 31
21	<chem>O=C(NC1=NN=C(C2=CC=NC=C2)S1)C3=CC(C4=CC=CO4)=CC5=C3C=CC=C5</chem>	0
22	<chem>O=C(O)C1=CC(C2=CC=CO2)=CC3=C1C=CC=C3</chem>	89 ± 8
23	<chem>CC(O1)=CC=C1C2=NC(C=CC=C3)=C3C=C2</chem>	102 ± 12
24	<chem>C12=C(C=CC=C2)N=C(C3=CC=CO3)C=C1</chem>	117 ± 16
25	<chem>O=C(C1=CC(C2=CC=C(C)O2)=NC3=C1C=CC=C3)NC(C)C4CCCO4</chem>	55 ± 4
26	<chem>O=C(C1=CC(C2=CC=C(C)O2)=NC3=C1C=CC=C3)NC4=NC(C)=CC=C4</chem>	73 ± 8
27	<chem>O=C(C1=CC(C2=CC=C(C)O2)=NC3=C1C=CC=C3)NC4CCCCC4</chem>	54 ± 19
28	<chem>O=C(C1=CC(C2=CC=C(C)O2)=NC3=C1C=CC=C3)NCCC4=CC=C(OC)C=C4</chem>	84 ± 32
29	<chem>O=C(C1=CC(C2=CC=C(C)O2)=NC3=C1C=CC=C3)NCC4=CC(OCO5)=C5C=C4</chem>	56 ± 28
30	<chem>O=C(NNC(NC1CCCC1)=O)C2=CC(C3=CC=CO3)=NC4=C2C=CC=C4</chem>	64 ± 19
31	<chem>O=C(C1=CC(C2=CC=C(C)O2)=NC3=C1C=CC=C3)N4CCN(S(=O)(C)=O)CC4</chem>	26 ± 4
32	<chem>O=C(C1=CC(C2=CC=C(C)O2)=NC3=C1C=CC=C3)NC4=CC(C(OC)=O)=CC(C(OC)=O)=C4</chem>	19 ± 10