## **Supporting Information**

Catalytic approach to *in vivo* metabolism of atractylenolide III using biomimetic ironporphyrin complexes

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Scheme S1. (a) Structure of iron(IV)-oxo porphyrin  $\pi$ -cation radical complex (1) and (b) expected organic products obtained from the reaction between 1 and AT-III (left and middle) or APAP (right).



Fig. S1. (a) Chromatogram of atractylenolide III, and (b) the mass spectra of molecular ion observed at m/z 248.93 and the fragmented ions (c) at m/z 248.93  $\rightarrow$  230.96 (MS<sup>2</sup>) and (d) at m/z 230.96  $\rightarrow$  213.16 (MS<sup>3</sup>) in the plasma sample obtained 1 h after the oral administration of atractylenolide III.



Fig. S2. (a) Chromatogram of the oxygenated atractylenolide III, (b) the mass spectra of the molecular ion at m/z 264.97, the fragmented ions at (c) m/z 264.97  $\rightarrow$  246.99 (MS<sup>2</sup>) and (d) at m/z 246.99  $\rightarrow$  229.13 (MS<sup>3</sup>) in the plasma sample obtained 1 h after the oral administration of atractylenolide III.



Fig. S3. UV-Vis spectral changes of 1 (0.025 mM) observed at -20 °C. The inset shows the time-courses that were monitored at 665 nm at -40 °C (black dot) and -20 °C (red dot) for the decay of 1.



Fig. S4. Plot of pseudo-first order rate constants ( $k_{obs}$ ) against the concentrations of AT-III to determine  $k_2$  in the oxidation of AT-III by 1.



**Fig. S5.** UV-Vis spectral changes of  $[(tmp^{+*})Fe^{IV}(O)]^+$  (0.025 mM) (1, red line) after the addition of 20 equiv of APAP at -20 °C, resulting in the formation of  $[Fe^{III}(tmp)](CF_3SO_3)$  (blue line). The inset shows the time-course of the formation of  $[Fe^{III}(tmp)](CF_3SO_3)$  (blue dot) and the decay of 1 (red dot), which were monitored at 505 and 665 nm, respectively.



**Fig. S6.** Cyclic voltammograms of (a) AT-III (2.0 mM) and (b) APAP (2.0 mM) in deaerated  $CH_3CN$  containing TBAPF<sub>6</sub> (0.10 M) with a glassy carbon working electrode at 298 K. The scan rate was 0.10 V s<sup>-1</sup>.



**Fig. S7.** GC data of the standard samples, namely, (a) AT-III, (b) APAP, (c) *m*-CPBA and (d) NAPQI as well as the products obtained from the oxygenation of AT-III by **1** in the (e) absence and (f) presence of APAP. The peak observed at 21.3 min corresponded to the oxygenated product of AT-III.



Fig. S8. (a) Chromatogram of oxygenated atractylenolide III, (b) the mass spectra of molecular ion at m/z 265.00, (c) the fragmented ions at m/z 265.00  $\rightarrow$  246.95 (MS<sup>2</sup>) and (d) at m/z 246.95  $\rightarrow$  229.12 (MS<sup>3</sup>) derived from the oxidation of atractylenolide III reacted with [(tmp<sup>+•</sup>)Fe<sup>IV</sup>(O)]<sup>+</sup> (1). The black arrow in (a) indicates the oxygenated atractylenolide III, which matches that observed in the plasma samples.

## Coordinates

The coordinates are provided in .xyz-format, with charge/multiplicity in parenthesis in the

comment row.

AT-III

(0/1)	
7 -3.36063 -0.89539 0.79099	
2 -3.26642 0.62031 1.03813	
2 -2.50649 1.31495 -0.06967	
2 -1.13626 0.73487 -0.38024	
2 -1.21307 -0.81227 -0.64247	
2 -1.98315 -1.50938 0.51104	
c -0.11520 1.11937 0.73750	
2 1.20762 0.50642 0.44077	
C 1.23030 -0.99794 0.25232	
C 0.21212 -1.41129 -0.80892	
2 2.42498 1.01199 0.17697	
3.3045/ -0.12/28 -0.22654	
7 2.50/51 -1.28290 -0.18528	
0 96984 -1 70240 1 43298	
7 2 94711 2 40994 0 19497	
2.34711 2.40334 0.13437	
4 - 4.04523 - 1.08260 - 0.05303	
4 -3.81332 -1.38827 1.66744	
4 -4.26804 1.06441 1.14852	
H -2.74425 0.78725 1.99928	
H -0.76607 1.20501 -1.30709	
H -2.09132 -2.57944 0.26415	
+ -1.37535 -1.47957 1.42729	
H -0.04992 2.21491 0.80977	
H -0.47208 0.74796 1.71262	
H 0.62572 -1.08271 -1.77505	
H 0.16246 -2.51191 -0.83392	
H -3.98674 2.77803 -0.50903	
H -2.43959 2.84290 -1.54968	
4 -2.01470 -2.13174 -2.19300	
4 -1.41085 -0.57704 -2.81337	
H -2.96853 -0.64460 -1.97133	
H 1.62330 -1.43443 2.09601	
1 3.3455/ 2.68686 -0./94/8	
1 2.1/2/4 3.13603 0.48012	
1 3./8895 2.49991 0.90111	
One also the second dimension of ATT III	
Jne electron oxidized A I-III	
38	
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38         (1/2)         -3.00112       -0.62191       1.50217         -3.42705       0.73487       0.99411         23.42705       0.73487       0.99411         23.42705       0.73487       0.99411         22.3064       0.84296       -0.70925         -1.23064       0.84296       -0.70925         2.1.23040       0.84296       -0.70925         2.1.23497       0.82053       1.31869         20.5149       1.22462       0.13728         1.23497       0.39119       0.12020         2.39800       -1.18117       0.27273         2.012255       -1.32510       -0.57773         2.35154       1.10094       0.07645         3.43637       0.15556       0.09554         2.86951       -1.42175       -0.03514         2.36355       1.42145       -0.99358         1.62359       -2.39797       -0.44367         2.46667       2.63582       0.02790         4.66108       0.42333       0.20546         -3.27730       -0.72534       2.53075         -4.49605       0.73609       0.94790         4.3.9447       1.54484       1.64719 <td></td>	
38         (1/2)         2 -3.00112 -0.62191 1.50217         2 -3.42705 0.73487 0.99411         2 -3.42705 0.73487 0.99411         2 -3.42705 0.973487 0.99411         2 -2.81976 0.99723 -0.40098         2 -1.29064 0.84296 -0.70925         2 -1.22485 -0.65115 -0.18445         2 -1.22485 -0.65115 -0.18445         2 -1.22485 -0.65115 -0.18445         2 -1.22487 0.39119 0.12020         2 1.39800 -1.18117 0.27273         0 .12255 -1.32510 -0.57773         2 .35154 1.10094 0.07645         2 .36155 1.4126 -0.3814         2 .86951 -1.12075 -0.03514         2 .86951 -1.12075 -0.03514         2 .86951 -1.42145 -0.99358         1 .62359 -2.39797 -0.44367         2 .246467 2.63582 0.02790         2 .46667 2.63582 0.02790         2 .46667 2.63582 0.02790         2 .46667 2.63582 0.02790         2 .46667 2.63582 0.02790         2 .46667 2.63582 0.02790         2 .46667 2.63582 0.02790         2 .46667 2.63582 0.02790         2 .46667 2.63582 0.02790         2 .46670 1.87348 1.64719         -3.2730 -0.72534 2.53075         4 .49605 0.73609 0.94790         -3.09453 1.51448 1.64719         -1.37665 -1.81716 1.62889         -0.0935	
38         (1/2)         2       -3.00112       -0.62191       1.50217         2       -3.42705       0.73487       0.99411         2       -3.42705       0.9723       -0.40098         2       -1.29064       0.84296       -0.70925         2       -1.29064       0.84296       -0.70925         2       -1.29064       0.84296       -0.70925         2       -1.2485       -0.65115       -0.18445         2       -1.51415       -0.82053       1.31869         2       -0.05149       1.20462       0.13728         2       1.23497       0.39119       0.12020         1.39800       -1.18117       0.2773         2       0.2555       -1.32510       -0.57773         2.35154       1.10094       0.07645         3.43637       0.15556       0.09554         2.86951       -1.42145       -0.99358         1.62359       -2.39797       -0.44367         2.24849       -1.32710       0.99358         1.62359       -2.379737       0.44367         2.46667       2.63582       0.02790         4.66108       0.42333       0.20546 <td></td>	
38         (1/2)         2       -3.00112       -0.62191       1.50217         2       -3.42705       0.73487       0.99411         2       -3.42705       0.73487       0.99411         2       -3.42705       0.73487       0.99411         2       -3.42705       0.9723       -0.40098         2       -1.29064       0.84296       -0.07925         2       -1.22485       -0.65115       -0.18445         2       -1.2104       1.20420       0.13728         2       -0.05149       1.20420       0.127273         2       .0.12255       -1.32510       -0.57773         2       .35154       1.10094       0.07645         2       .34637       0.15556       0.09554         2       .286951       -1.42175       -0.03314         2       .363455       1.44126       -1.38867         2       .286951       -1.42145       -0.99358         1.62359       -2.39797       -0.44367         2       .46667       2.63582       0.02790         0       4.66108       0.42333       0.20546         -3.4947       -1.37171 <t< td=""><td></td></t<>	
$\begin{array}{c} 38\\ (1/2)\\ (2)\\ (3)\\ (2)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3$	
38         (1/2)         2       -3.00112       -0.62191       1.50217         2       -3.42705       0.73487       0.99411         2       -3.42705       0.9723       -0.40098         2       -1.29064       0.84296       -0.70925         2       -1.29064       0.84296       -0.70925         2       -1.29064       0.84296       -0.10925         2       -1.29064       0.84296       -0.10925         2       -1.21064       0.84296       0.13728         2       -0.05149       1.20462       0.13728         2       -0.39119       0.12020       1.39800       -1.18117       0.27273         0.12255       -1.32510       -0.57773       2.35154       1.10094       0.07645         3.43637       0.15556       0.09554       2.86951       -1.12075       -0.03514         2.36355       1.42145       -0.99358       1.62359       -2.39797       -0.44367         2.28489       -1.42145       -0.99358       1.62359       -2.39797       -0.44367         2.46667       2.63582       0.02790       4.466108       0.42730       0.72534       2.53075         4.3.27	
$\begin{array}{c} 38\\ (1/2)\\ (2)\\ (3)\\ (2)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3$	
$\begin{array}{c} 38\\ (1/2)\\ (1/2)\\ (2-3,00112 -0.62191 1.50217\\ (2-3,42705 0.73487 0.99411\\ (2-2,81976 0.99723 -0.40098\\ (-1,29064 0.84296 -0.70925\\ (2-1,22485 -0.65115 -0.18445\\ (2-1,29064 0.84296 -0.70925\\ (2-1,22485 -0.65115 -0.18445\\ (2-1,21064 0.84296 0.13728\\ (2-1,21064 0.20462 0.13728\\ (2-1,22487 0.39119 0.12020\\ (2-3,2154 1.10094 0.07645\\ (2-3,43637 0.15556 0.09554\\ (2-3,63455 1.44126 -1.38867\\ (2-2,28489 -1.42145 -0.99358\\ (2-3,63455 1.44126 -1.38867\\ (2-2,28499 -1.42145 -0.99358\\ (2-3,63455 1.44126 -1.38867\\ (2-2,28499 -1.42145 -0.99358\\ (2-3,63455 1.44126 -1.38867\\ (2-2,28499 -2.39797 -0.44367\\ (2-2,63582 0.02790)\\ (2-66188 0.42333 0.20546\\ (2-3,49447 -1.37171 0.91952\\ (2-3,09453 1.51448 1.64719)\\ (-3,09453 1.51448 1.64719)\\ (-3,0360 1.87388 -0.42626\\ (-1.27885 -1.81716 1.62889\\ (0-20337 2.19103 -0.18494\\ (-0.36189 1.19988 1.16117\\ (0.33751 -0.97704 -1.56645\\ (-0.05983 -2.37944 -0.56862\\ (-3.23392 1.65392 -2.35771\\ (-2.25984 -2.04775 -0.126422\\ (-1.6693 -1.20399 -1.83964\\ (-2.44336 -2.37899 -1.44400\\ (-3,07822 -2.82779 -0.61709\\ (-3,0862) -2.8279 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82779 -0.61709\\ (-3,0862) -2.82$	
$\begin{array}{c} 38\\ (1/2)\\ (2-3,00112 -0.62191 1.50217\\ (2-3,42705 0.73487 0.99411\\ (2-2,81976 0.9723 -0.40098\\ (2-1,29064 0.84296 -0.70925\\ (2-1,22485 -0.65115 -0.184455\\ (2-1,51415 -0.82053 1.31869\\ (2-0,05149 1.20462 0.13728\\ (2-0,05149 1.20462 0.13728\\ (2-1,23497 0.39119 0.12020\\ (2-1,39800 -1.18117 0.2773\\ (2-2,35154 1.10094 0.07645\\ (2-3,35154 1.10094 0.07645\\ (2-3,35154 1.10094 0.07645\\ (2-3,35154 1.12075 -0.03514\\ (2-3,235154 1.12075 -0.03514\\ (2-3,235154 1.12075 -0.03514\\ (2-3,235154 1.12075 -0.03514\\ (2-3,2489 -1.42145 -0.99358\\ (2-2,28489 -1.42145 -0.99358\\ (2-2,28489 -1.42145 -0.99358\\ (2-2,28489 -1.42145 -0.99358\\ (2-2,28489 -1.42145 -0.99358\\ (2-2,28489 -1.42145 -0.99358\\ (2-2,28489 -1.37171 0.91952\\ (2-2,28489 -1.37171 0.91952\\ (2-2,28489 -1.37171 0.91952\\ (2-2,2730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3730 -0.72534 2.53075\\ (2-2,3739 -0.5682\\ (2-2,3739 -0.5682\\ (2-2,3789 -1.2039 -1.83964\\ (2-2,4336 -2.3789 -1.44400\\ (2-78282 -2.82779 -0.61709\\ (3-3,3507 2.91021 -0.48828\\ (3-2,91021 -0.48828\\ (3-$	
$\begin{array}{c} 38\\ (1/2)\\ (2)\\ (3)\\ (2)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3)\\ (3$	

4th carbon oxidized AT-III					
39 (0/1)					
-3.27200 -1.12755 0.83091					
C -3.20856 0.35461 1.22531 C -2.49111 1.19430 0.19142					
2 -1.10926 0.69428 -0.24455					
2 -1.16999 -0.84278 -0.64026					
2 -1.880/5 -1.65//5 0.4/301 2 -0.08819 0.95909 0.90555					
2 1.24028 0.39472 0.54820					
2 1.28556 -1.07365 0.19648					
2 0.26558 -1.37981 -0.90583					
2 3.34960 -0.14243 -0.16203					
0 2.61262 -1.29558 -0.28729					
C -1.95566 -1.00441 -1.96016					
0 1.09039 -1.82228 1.36559					
C 2.95245 2.33122 0.51662					
H -3.96651 -1.25416 -0.01610					
H -3.69152 -1.71754 1.66250					
H -4.21669 0.76104 1.40088 H -2 67092 0 43657 2 18868					
H -1.95155 -2.70860 0.14119					
H -1.25391 -1.67009 1.37622					
H -0.04202 2.04485 1.06692 H -0.44334 0.49009 1.83595					
H 0.65070 -0.91885 -1.82634					
H 0.22981 -2.46989 -1.08203					
H -2.46802 2.94793 -1.01315					
H -2.06397 -2.07251 -2.20741					
H -1.42833 -0.53610 -2.80589 H -2 96491 -0 57067 -1 90655					
H 1.12485 -2.76045 1.12825					
H 3.33960 2.71814 -0.44011					
H 2.16672 3.00962 0.87703 H 3.79497 2.35749 1.22702					
0 -0.59340 1.45093 -1.32908					
H -1.23002 1.41372 -2.05496					
10 <sup>th</sup> carbon oxidized AT-III					
10 <sup>th</sup> carbon oxidized AT-III					
10 <sup>th</sup> carbon oxidized AT-III 39 (0/1) 5 3.36993 0.66955 0.89940					
10 <sup>th</sup> carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 2 3.28904 -0.86383 0.99837 - 0.66955 0.99837					
10th carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 2 3.28904 -0.86383 0.99837 2 2.52043 -1.45405 -0.16265 2 1.14435 -0.85261 -0.40174					
10th carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 2 3.28904 -0.86383 0.99837 2 2.52043 -1.45405 -0.16265 2 1.14435 -0.85261 -0.40174 2 1.22258 0.70770 -0.52921					
10th carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 3 .28904 -0.86383 0.99837 2 .52043 -1.45405 -0.16265 1 .14435 -0.85261 -0.40174 1 .22258 0.70770 -0.52921 2 1.98736 1.29936 0.68426 2 0.14300 1.23642 0.69755					
10th carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 2 3.28904 -0.86383 0.99837 2 2.52043 -1.45405 -0.46265 1 1.14435 -0.85261 -0.40174 2 1.22258 0.70770 -0.52921 2 1.98736 1.29936 0.68426 2 0.14390 -1.32643 0.69795 2 -1.18509 -0.71166 0.44415					
10th carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 2 3.28904 -0.86383 0.99837 2 .52043 -1.45405 -0.16265 2 1.14435 -0.85261 -0.40174 1 .22258 0.70770 -0.52921 2 1.98736 1.29936 0.68426 2 0.14390 -1.32643 0.69795 2 -1.18509 -0.71166 0.44415 2 -1.24001 0.79751 0.35605					
10th carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 3 .28904 -0.86383 0.99837 2 .52043 -1.45405 -0.16265 2 1.14435 -0.85261 -0.40174 1 .22258 0.70770 -0.52921 2 1.98736 1.29936 0.68426 2 0.14390 -1.32643 0.69795 2 -1.18509 -0.71166 0.44415 2 -1.24001 0.79751 0.35605 2 -0.21263 1.33331 -0.66305 2 -2 39048 -1 22087 0 13224					
10th carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 2 .32804 -0.86383 0.99837 2 .52043 -1.45405 -0.16265 2 1.14435 -0.85261 -0.40174 1 .22258 0.70770 -0.52921 2 1.98736 1.29936 0.68426 2 0.14390 -1.32643 0.69795 2 -1.24001 0.79751 0.35605 2 -0.21263 1.33331 -0.66305 2 -3.29260 -0.07534 -0.18759					
10th carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 2 .32804 -0.86383 0.99837 2 .52043 -1.45405 -0.16265 2 1.14435 -0.85261 -0.40174 2 1.22258 0.70770 -0.52921 2 1.98736 1.29936 0.68426 2 0.14390 -1.32643 0.69795 2 -1.24001 0.79751 0.35605 2 -0.21263 1.33331 -0.66305 2 -3.29260 -0.07534 -0.18759 0 -2.57562 1.09076 -0.05232 0 -0.00254					
10th carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 2 3.28904 -0.86383 0.99837 2 .52043 -1.45405 -0.16265 2 1.14435 -0.85261 -0.40174 2 1.22258 0.70770 -0.52921 2 1.98736 1.29936 0.68426 2 0.14390 -1.32643 0.69795 2 -1.24001 0.79751 0.35605 2 -0.21263 1.33331 -0.66305 2 -3.29260 -0.07534 -0.18759 2 -3.29260 -0.07534 -0.18759 2 -2.57562 1.09076 -0.05232 2 3.01097 -2.43079 -0.35749 2 1.95505 1.07328 -1.83680					
$\begin{array}{l} 0^{th} \ carbon \ oxidized \ AT-III \\ \\ 39 \\ (0/1) \\ \hline 3.36993 \ 0.66955 \ 0.89940 \\ \hline 3.28904 \ -0.66333 \ 0.99837 \\ \hline 2.52043 \ -1.45405 \ -0.16265 \\ \hline 1.14435 \ -0.85261 \ -0.40174 \\ \hline 1.22258 \ 0.70770 \ -0.52921 \\ \hline 1.82736 \ 0.68426 \\ \hline 0.14390 \ -1.32643 \ 0.68426 \\ \hline 0.14390 \ -1.32643 \ 0.69795 \\ \hline -1.24001 \ 0.79751 \ 0.35605 \\ \hline -2.21263 \ 1.33331 \ -0.66305 \\ \hline -3.29260 \ -0.07534 \ -0.18759 \\ \hline -3.29260 \ -0.07534 \ -0.18759 \\ \hline 2.57562 \ 1.09076 \ -0.05232 \\ \hline 3.1097 \ -2.43079 \ -0.393749 \\ \hline 1.95505 \ 1.07328 \ -1.8580 \\ \hline 098723 \ 1.45111 \ 1.57494 \end{array}$					
10th carbon oxidized AT-III 39 (0/1) C 3.36993 0.66955 0.89940 C 3.28904 -0.86383 0.99837 C 2.52043 -1.45405 -0.16265 C 1.14435 -0.85261 -0.40174 C 1.22258 0.70770 -0.52921 C 1.98736 1.29936 0.68426 C 0.14390 -1.32643 0.69795 C -1.24001 0.79751 0.35605 C -0.21263 1.33331 -0.66305 C -2.39048 -1.22087 0.13224 C -3.29260 -0.07534 -0.18759 D -2.57562 1.09076 -0.05232 C 3.01097 -2.43079 -0.93749 C 1.95505 1.07328 -1.83680 D -0.98723 1.45111 1.57494 C -2.88164 -2.62702 0.04410					
10th carbon oxidized AT-III 39 (0/1) C 3.36993 0.66955 0.89940 C 3.28904 -0.86383 0.99837 C 2.52043 -1.45405 -0.16265 C 1.14435 -0.85261 -0.40174 C 1.22258 0.70770 -0.52921 C 1.98736 1.29936 0.68426 C 0.14390 -1.32643 0.69795 C -1.18509 -0.71166 0.44415 C -0.21263 1.33331 -0.66305 C -0.21263 1.33331 -0.66305 C -2.39048 -1.22087 0.13224 C -3.29260 -0.07534 -0.18759 D -2.57562 1.09076 -0.05232 C 3.01097 -2.43079 -0.93749 C -0.98723 1.45111 1.57494 C -2.88164 -2.62702 0.04410 D -4.44358 -0.0359 -0.52173 4.04914 0.94452 0.07588					
10th carbon oxidized AT-III 39 (0/1) 1 3.36993 0.66955 0.89940 2 3.28904 -0.86383 0.99837 2 .52043 -1.45405 -0.16265 1 .14435 -0.85261 -0.40174 1 .22258 0.70770 -0.52921 1 .98736 1.2936 0.68426 1 .14309 -1.32643 0.69795 1 -1.18509 -0.71166 0.44415 1 -1.24001 0.79751 0.35605 1 -0.21263 1.33331 -0.66305 2 -2.39048 -1.22087 0.13224 2 .329260 -0.07534 -0.18759 0 -2.57562 1.09076 -0.05232 2 .301097 -2.43079 -0.93749 1 .95505 1.07328 -1.83680 0 -0.98723 1.45111 1.57494 2 -2.88164 -2.62702 0.04410 0 -4.44358 -0.0359 -0.52173 4 .04914 0.94452 0.07588 4 .82190 1.0762 1.81834					
10th carbon oxidized AT-III 39 (0/1) 1 3.36993 0.66955 0.89940 2 3.28904 -0.86383 0.99837 2 .52043 -1.45405 -0.16265 1 .14435 -0.85261 -0.40174 1 .22258 0.70770 -0.52921 1 .98736 1.2936 0.68426 1 .14309 -1.32643 0.69795 1 -1.18509 -0.71166 0.44415 1 -1.24001 0.79751 0.35605 1 -0.21263 1.33331 -0.66305 2 -2.39048 -1.22087 0.13224 2 .329260 -0.07534 -0.18759 0 -2.57562 1.09076 -0.05232 2 .301097 -2.43079 -0.93749 1 .95505 1.07328 -1.83680 0 -0.98723 1.45111 1.57494 2 -2.88164 -2.62702 0.04410 0 -4.44358 -0.09359 -0.52173 4 .04914 0.94452 0.07588 4 .82190 1.07862 1.81834 4 .279747 -1.12825 1.94451					
$\begin{array}{l} 0^{th} \ carbon \ oxidized \ AT-III\\ \\ 39\\ (0/1)\\ \\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$					
$10^{th}$ carbon oxidized AT-III 39 (0/1) 2.3.2693 0.66955 0.89940 $3.28904 -0.86383 0.998372.52043 -1.45405 -0.162652.14435 -0.85261 -0.401741.22258 0.7077 0 -0.529211.18736 1.22936 0.684262.14390 -1.32643 0.69795-1.18509 -0.71166 0.44415-1.24001 0.79751 0.356052.2.30048 -1.22087 0.132242.3.29260 -0.07534 -0.187592.2.30048 -1.2207 0.0327492.301097 -2.43079 -0.937491.95505 1.07328 -1.836800 -0.98723 1.45111 1.574942.288164 -2.62702 0.04410-4.44358 -0.09359 -0.521734.04914 0.9452 0.075883.82190 1.07862 1.818344.29481 -1.30877 1.053832.77974 -1.12825 1.945110.75988 1.2254544 -1.358251.28818 2.38587 0.53681$					
$\begin{array}{l} 0^{th} \ carbon \ oxidized \ AT-III\\ \\ 39\\ (o/1)\\ \hline 3,36993 \ 0.66955 \ 0.89940\\ \hline 3,28904 \ -0.86383 \ 0.99837\\ \hline 2.52043 \ -1.45405 \ -0.16265\\ \hline 1.14435 \ -0.85261 \ -0.40174\\ \hline 1.22258 \ 0.70770 \ -0.52921\\ \hline 1.8736 \ 1.29936 \ 0.68426\\ \hline 0.14390 \ -1.32643 \ 0.69795\\ \hline -1.18509 \ -0.71166 \ 0.44415\\ \hline -1.24001 \ 0.79751 \ 0.35605\\ \hline -0.21263 \ 1.33331 \ -0.66305\\ \hline -2.39048 \ -1.22067 \ 0.13224\\ \hline -3.29260 \ -0.07534 \ -0.18759\\ \hline -2.57562 \ 1.09976 \ -0.52322\\ \hline 3.01097 \ -2.43079 \ -0.52173\\ \hline 4.04914 \ 0.94452 \ 0.07588\\ \hline 4.329481 \ -1.30877 \ 1.05383\\ \hline 4.29481 \ -1.30877 \ 1.05383\\ \hline 4.27974 \ -1.12825 \ 1.973681\\ \hline 4.7974 \ -1.12825 \ 1.95825\\ \hline 4.20818 \ 2.38587 \ 0.55681\\ \hline 1.38588 \ 1.07210 \ 1.59931\\ \hline 4.04904 \ -2.42474 \ 0.69801\\ \hline \end{array}$					
$\begin{array}{l} 0^{th} \ carbon \ oxidized \ AT-III\\ \\ 39\\ (o/1)\\ \hline 3,36993 \ 0.66955 \ 0.89940\\ \hline 3,28904 \ -0.86383 \ 0.99837\\ \hline 2,52043 \ -1.45405 \ -0.16265\\ \hline 1.14435 \ -0.85261 \ -0.40174\\ \hline 1.22258 \ 0.70770 \ -0.52921\\ \hline 1.98736 \ 1.29936 \ 0.68426\\ \hline 0.14390 \ -1.32643 \ 0.69795\\ \hline -1.24001 \ 0.79751 \ 0.35605\\ \hline -0.21263 \ 1.33331 \ -0.66305\\ \hline -2.39048 \ -1.22087 \ 0.13224\\ \hline -3.29260 \ -0.07534 \ -0.18759\\ \hline -2.57562 \ 1.09076 \ -0.5232\\ \hline 3.01097 \ -2.43079 \ -0.93749\\ \hline 1.9555 \ 1.07328 \ -1.83680\\ \hline 0.09732 \ 1.45111 \ 1.57494\\ \hline -2.88164 \ -2.62702 \ 0.04410\\ \hline 0.44358 \ -0.09359 \ -0.52173\\ \hline 4.04914 \ 0.94452 \ 0.07588\\ \hline 3.82190 \ 1.07862 \ 1.81834\\ \hline 4.29481 \ -1.30877 \ 1.05383\\ \hline 2.77974 \ -1.12825 \ 1.94451\\ \hline 0.75988 \ 1.24544 \ -1.35825\\ \hline 2.08618 \ 2.38587 \ 0.53681\\ \hline 1.38588 \ 1.17210 \ 1.59931\\ \hline 0.09043 \ -2.42410 \ 0.59031\\ \hline 0.05032 \ -1.01497 \ 1.69261\\ \hline \end{array}$					
$10^{th}$ carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 $3 .36993 0.66955 0.899402 .52043 -1.45405 -0.16265 2 1.14435 -0.85261 -0.401741.22258 0.70770 -0.529211.98736 1.29936 0.684262 0.14390 -1.32643 0.69795-1.18509 -0.71166 0.44415-1.24001 0.79751 0.356052 -0.21263 1.33331 -0.663052 -3.29260 -0.07534 -0.187592 -3.29260 -0.07534 -0.187592 -3.29260 -0.07534 -0.187592 -3.29260 -0.07534 -0.187592 -2.57562 1.09076 -0.052323 .01097 -2.43079 -0.937491 .95505 1.07328 -1.836802 -0.98723 1.45111 1.57494-2.88164 -2.62702 0.04410-4.44358 -0.09359 -0.521734 .04914 0.94452 0.075884 .32941 -1.30877 1.053834 .77974 -1.12825 1.944514 .29481 -1.30877 1.538354 .07598 -1.24544 -1.358254 .08818 2.38587 0.536811 .38858 1.17210 1.599314 .0.9043 -2.42481 0.698014 .005023 -1.01497 1.692614 .005023 -1.01497 1.65261$					
$\begin{array}{l} 0^{th} \ carbon \ oxidized \ AT-III\\ \\ 39\\ (o/1)\\ \hline 3,36993 \ 0.66955 \ 0.89940\\ \hline 3,28904 \ -0.86383 \ 0.99837\\ \hline 2.52043 \ -1.45405 \ -0.16265\\ \hline 1.14435 \ -0.85261 \ -0.40174\\ \hline 1.22258 \ 0.70770 \ -0.52921\\ \hline 1.98736 \ 1.29936 \ 0.68426\\ \hline 0.14390 \ -1.32643 \ 0.69795\\ \hline -1.18509 \ -0.71166 \ 0.44415\\ \hline -1.24001 \ 0.79751 \ 0.35605\\ \hline -0.21263 \ 1.33331 \ -0.66305\\ \hline -2.39260 \ -0.07534 \ -0.18759\\ \hline -3.29260 \ -0.07534 \ -0.18759\\ \hline -2.57562 \ 1.09076 \ -0.05232\\ \hline 3.01097 \ -2.43079 \ -0.93749\\ \hline 1.95505 \ 1.07328 \ -1.83680\\ \hline 098723 \ 1.45111 \ 1.57494\\ \hline 2.4355 \ -0.04410\\ \hline -4.44358 \ -0.09359 \ -0.52173\\ \hline 4.04914 \ 0.94452 \ 0.07588\\ \hline 3.82190 \ 1.07862 \ 1.81834\\ \hline 4.29491 \ -1.30877 \ 1.05383\\ \hline 2.77974 \ -1.12825 \ 1.94451\\ \hline 0.75998 \ -1.24544 \ -1.35825\\ \hline 2.08188 \ 2.38587 \ 0.53681\\ \hline 1.38858 \ 1.17210 \ 1.59931\\ \hline 0.09043 \ -2.42481 \ 0.69801\\ \hline 0.50323 \ -1.01497 \ 1.65261\\ \hline 4.00078 \ -2.86090 \ -0.75636\\ \hline 2.44126 \ -2.83498 \ -1.78002\\ \hline \end{array}$					
$10^{th}$ carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 $2 3.28904 - 0.66383 0.99837 2 .52043 - 1.45405 - 0.162651 .14435 - 0.85261 - 0.401741 .22258 0.70770 - 0.52921 1 .98736 1.29936 0.684260 .14390 - 1.32643 0.69795- 1.18509 - 0.71166 0.444152 - 1.24001 0.79751 0.35605- 0.21263 1.33331 - 0.66305- 3.29260 - 0.07534 - 0.187592 - 3.29260 - 0.07534 - 0.187592 - 2.57562 1.09076 - 0.052323 .01097 - 2.43079 - 0.937491 .95505 1.07328 - 1.836800 - 0.98723 1.45111 1.57494-2.88164 - 2.62702 0.044100 - 4.44358 - 0.09359 - 0.521734 .04914 0.94452 0.075884 .29491 - 1.30877 1.053834 .27974 - 1.12825 1.944514 .29481 - 1.30877 1.053834 .27974 - 1.12825 1.944514 .29481 - 1.30877 1.053834 .27974 - 1.12825 1.944511 .05998 - 1.24544 - 1.358254 .20818 2.38587 - 0.536814 .138858 1.17210 1.599314 0.09043 - 2.42481 0.6698010 .50323 - 1.01497 1.652614 .00078 - 2.86090 - 0.576364 .24412 - 0.34877 - 1.650164 .00078 - 2.84098 - 1.780021 .96144 2.16520 - 1.96866$					
$10^{h}$ carbon oxidized AT-III 39 (0/1) 2 3.36993 0.66955 0.89940 $2 3.28904 -0.66383 0.998372 .52043 -1.45405 -0.16265 2 1.14435 -0.85261 -0.401742 1.22258 0.70770 -0.529211.98736 1.29936 0.684260.14390 -1.32643 0.69795-1.18509 -0.71166 0.44415-1.24001 0.79751 0.35605-2.24263 1.33331 -0.66305-3.29260 -0.07334 -0.18759-3.29260 -0.07334 -0.187590.257562 1.09076 -0.052323.01097 -2.43079 -0.337491.95505 1.07328 -1.836800 -0.98723 1.45111 1.57494-2.88164 -2.62702 0.04410-4.44358 -0.09359 -0.521734 .04914 0.94452 0.075884 .29491 -1.30877 1.053834 .27974 -1.12825 1.944514 .29816 1.7210 1.599314 .09043 -2.42481 0.638014 .05938 -1.04544 -1.358254 .20818 2.38587 0.536811 .38858 1.17210 1.599310 .09043 -2.42481 0.638010 .50323 -1.01497 1.622614 .04078 -2.86090 -0.576364 .24412 -2.83498 -1.780021 .96144 2.16520 -1.968661 .44282 0.63141 -2.70717$					
$\begin{array}{l} 0^{th} \ carbon \ oxidized \ AT-III\\ \\ 39\\ (o/1)\\ \hline 3,36993 \ 0.66955 \ 0.89940\\ \hline 3,28904 \ -0.66333 \ 0.99837\\ \hline 2,52043 \ -1.45405 \ -0.16265\\ \hline 1.14435 \ -0.85261 \ -0.40174\\ \hline 1.22258 \ 0.70770 \ -0.52921\\ \hline 1.1425 \ -0.85261 \ -0.40174\\ \hline 1.22258 \ 0.70770 \ -0.52921\\ \hline 1.98736 \ 1.29936 \ 0.68426\\ \hline 0.14390 \ -1.32643 \ 0.69795\\ \hline -1.18509 \ -0.71166 \ 0.44415\\ \hline -1.24001 \ 0.79751 \ 0.35605\\ \hline -0.21263 \ 1.33331 \ -0.66305\\ \hline -2.329260 \ -0.07534 \ -0.18759\\ \hline -3.29260 \ -0.07534 \ -0.18759\\ \hline -3.29260 \ -0.07534 \ -0.18759\\ \hline -2.57562 \ 1.09076 \ -0.05232\\ \hline 3.01097 \ -2.43079 \ -0.393749\\ \hline 1.95505 \ 1.07328 \ -1.83680\\ \hline -0.98723 \ 1.45111 \ 1.57494\\ \hline -2.88164 \ -2.62702 \ 0.04410\\ \hline -4.44358 \ -0.09359 \ -0.52173\\ \hline 4.04914 \ 0.94452 \ 0.07588\\ \hline 3.82190 \ 1.07862 \ 1.81834\\ \hline 4.29481 \ -1.30877 \ 1.55383\\ \hline 2.77974 \ -1.12825 \ 1.94451\\ \hline 0.50323 \ -1.01497 \ 1.69801\\ \hline 4.060412 \ 1.03487 \ -1.65016\\ \hline 4.00078 \ -2.80398 \ -0.75636\\ \hline 2.44126 \ -2.80398 \ -0.75636\\ \hline 2.44126 \ -2.80398 \ -0.75636\\ \hline 2.44126 \ -2.83498 \ -1.78002\\ \hline 1.96144 \ 2.16520 \ -1.96866\\ \hline 1.44282 \ 0.63141 \ -2.70717\\ \hline 2.99176 \ 0.71047 \ -1.85099\\ \hline -1.73033 \ 1.28247 \ 2.17247\\ \hline .0.5032 \ -0.5035\\ \hline .0.5032 \ -0.5034 \ -0.50598\\ \hline .0.7263 \ -0.75636\\ \hline .0.99176 \ 0.71047 \ -1.85099\\ \hline -1.73033 \ 1.28247 \ 2.17247\\ \hline .0.5032 \ -0.75763\\ \hline .0.5032 \ -0.75763\\ \hline .0.5032 \ -0.75756\\ \hline .0.5032 \ -0.7556\\ \hline .0.5032 \ -0.7556\\ \hline .0.5032 \ -0.7556\\ \hline .0.5032 \ -0.5032 \ -0.7556\\ \hline$					
$\begin{array}{l} 0^{th} \ carbon \ oxidized \ AT-III\\ \\ 39\\ (0/1)\\ \hline \\ 2 \ 3.6993 \ 0.66955 \ 0.89940\\ \hline \\ 3.28904 \ -0.86383 \ 0.99837\\ \hline \\ 2.52043 \ -1.45405 \ -0.16265\\ \hline \\ 1.14435 \ -0.85261 \ -0.40174\\ \hline \\ 1.22258 \ 0.70770 \ -0.52921\\ \hline \\ 1.98736 \ 1.29936 \ 0.68426\\ \hline \\ 0.14390 \ -1.32643 \ 0.69795\\ \hline \\ -1.18509 \ -0.71166 \ 0.44415\\ \hline \\ -1.24001 \ 0.79751 \ 0.35605\\ \hline \\ -0.21263 \ 1.3331 \ -0.66305\\ \hline \\ -2.30048 \ -1.22087 \ 0.13224\\ \hline \\ 2.329260 \ -0.07534 \ -0.18759\\ \hline \\ -2.57562 \ 1.09076 \ -0.05232\\ \hline \\ 3.01097 \ -2.43079 \ -0.3749\\ \hline \\ 1.95505 \ 1.07328 \ -1.83680\\ \hline \\ -0.98723 \ 1.45111 \ 1.57494\\ \hline \\ -2.88164 \ -2.62702 \ 0.04410\\ \hline \\ -4.44358 \ -0.09359 \ -0.52173\\ \hline \\ 4.04914 \ 0.94452 \ 0.07588\\ \hline \\ 3.82190 \ 1.07862 \ 1.81834\\ \hline \\ 4.29481 \ -1.30877 \ 1.05383\\ \hline \\ 2.77974 \ -1.12825 \ 1.9451\\ \hline \\ 0.5982 \ 1.24544 \ -1.35825\\ \hline \\ 2.08818 \ 2.38587 \ 0.53681\\ \hline \\ 1.38858 \ 1.17210 \ 1.59931\\ \hline \\ 0.09043 \ -2.42481 \ 0.69801\\ \hline \\ 0.5032 \ -1.01497 \ 1.69261\\ \hline \\ 4.00078 \ -2.86090 \ -0.75636\\ \hline 2.44126 \ -2.83498 \ -1.78002\\ \hline \\ 1.96144 \ 2.16520 \ -1.96866\\ \hline 1.44282 \ 0.63141 \ -2.70717\\ \hline \\ 2.90176 \ 0.71047 \ -1.85099\\ \hline \\ -1.7303 \ 1.28274 \ 2.17247\\ \hline \\ -3.27243 \ -2.83755 \ -0.96485\\ \hline \end{array}$					
$\begin{array}{l} 10^{\rm th} \ carbon \ oxidized \ AT-III\\ 39\\ (0/1)\\ \hline 2 \ 3.36993 \ 0.66955 \ 0.89940\\ \hline 3.28904 \ -0.86383 \ 0.99837\\ \hline 2.52043 \ -1.45405 \ -0.16265\\ \hline 1.14435 \ -0.85261 \ -0.40174\\ \hline 1.22258 \ 0.70770 \ -0.52921\\ \hline 1.22258 \ 0.70770 \ -0.52921\\ \hline 1.225780 \ -1.32643 \ 0.68426\\ \hline 0.14390 \ -1.32643 \ 0.68426\\ \hline 0.14390 \ -1.32643 \ 0.68795\\ \hline -1.18509 \ -0.71166 \ 0.44415\\ \hline -1.24001 \ 0.79751 \ 0.35605\\ \hline -0.21263 \ 1.3331 \ -0.66305\\ \hline -0.21263 \ 1.3331 \ -0.66305\\ \hline -2.39048 \ -1.22070 \ -0.52322\\ \hline 2.301097 \ -2.43079 \ -0.93749\\ \hline 1.95505 \ 1.07328 \ -1.83680\\ \hline 0.98723 \ 1.45111 \ 1.57494\\ \hline 2.88164 \ -2.62702 \ 0.04410\\ \hline -4.44358 \ -0.09359 \ -0.52173\\ \hline 4 \ 0.4914 \ 0.94452 \ 0.07588\\ \hline 3.82190 \ 1.07862 \ 1.81834\\ \hline 4.29481 \ -1.30877 \ 1.05383\\ \hline 2.77974 \ -1.12825 \ 1.9451\\ \hline 0.5938 \ -1.24544 \ -1.35825\\ \hline 2.08188 \ 2.38587 \ 0.53681\\ \hline 1.38658 \ 1.17210 \ 1.59931\\ \hline 0.09043 \ -2.424280 \ 0.69801\\ \hline 4.00078 \ -2.86090 \ -0.75636\\ \hline 2.44126 \ -2.88169 \ -1.78002\\ \hline 1.96144 \ 2.16520 \ -1.96866\\ \hline 1.44262 \ 0.63141 \ -2.70177\\ \hline 2.99176 \ 0.71047 \ -1.85099\\ \ -1.7303 \ 1.22544 \ -2.77247\\ \ -3.27243 \ -2.83735 \ -0.96485\\ \hline -2.09159 \ -3.5519 \ 0.27651\\ \hline -3.7209 \ -2.78771 \ 0.73924 \ -0.57924 \ -0.57924 \ -0.57954 \ -0.57564 \ -0.67556 \ -0.75636 \ -0.756$					
$\begin{array}{l} 10^{\rm th} \ carbon \ oxidized \ AT-III\\ 39\\ (0/1)\\ \hline 3,36993 \ 0.66955 \ 0.89940\\ \hline 3,28904 \ -0.86383 \ 0.99837\\ \hline 2,52043 \ -1.45405 \ -0.16265\\ \hline 1.14435 \ -0.85261 \ -0.40174\\ \hline 1.22258 \ 0.70770 \ -0.52921\\ \hline 1.8736 \ 1.29936 \ 0.68426\\ \hline 0.14390 \ -1.32643 \ 0.69795\\ \hline -1.18509 \ -0.71166 \ 0.44415\\ \hline -1.24001 \ 0.79751 \ 0.35605\\ \hline -0.21263 \ 1.33331 \ -0.66305\\ \hline -2.39048 \ -1.22067 \ 0.13224\\ \hline -3.29260 \ -0.07534 \ -0.18759\\ \hline -2.39048 \ -1.22087 \ 0.13224\\ \hline -3.29260 \ -0.07534 \ -0.18759\\ \hline -2.39048 \ -1.22087 \ 0.13224\\ \hline -3.29260 \ -0.07534 \ -0.18759\\ \hline -2.39048 \ -1.22087 \ 0.13224\\ \hline -3.29260 \ -0.07534 \ -0.18759\\ \hline -2.39048 \ -1.2607 \ 0.05232\\ \hline 3.01097 \ -2.43079 \ -0.93749\\ \hline 1.95505 \ 1.07328 \ -1.83680\\ \hline -0.98723 \ 1.45111 \ 1.57494\\ \hline -2.88164 \ -2.62702 \ 0.04410\\ \hline -4.44358 \ -0.09359 \ -0.52173\\ \hline 4.04914 \ 0.94452 \ 0.07588\\ \hline 3.82190 \ 1.07862 \ 1.81834\\ \hline 4.29481 \ -1.30877 \ 1.05383\\ \hline 4.77974 \ -1.12825 \ 1.94451\\ \hline 0.60412 \ 1.03487 \ -1.65016\\ \hline 4.00078 \ -2.86080 \ -0.75636\\ \hline 2.44126 \ -2.84126 \ -1.38087 \ -1.78002\\ \hline H \ 0.60412 \ 1.03487 \ -1.65016\\ \hline 4.00078 \ -2.86089 \ -0.75636\\ \hline 2.44126 \ -2.81384 \ -1.78002\\ \hline H \ 0.6144 \ 2.16520 \ -1.780261\\ \hline -0.6142 \ 0.63141 \ -2.70717\\ \hline 2.99176 \ 0.71047 \ -1.85099\\ \hline -1.73033 \ 1.28247 \ 2.17247\\ -3.27243 \ -2.83735 \ -0.96485\\ \hline -2.09195 \ -3.3519 \ 0.27651\\ \hline -3.7209 \ -2.78771 \ 0.73924\\ \hline -0.18595 \ 2.73709 \ -0.63686\\ \hline \end{array}$					

Radio	cal on 4th	carbon of .	AT-III
$ \begin{array}{c} 3 \\ ( \ 0 \ ) \ ) \\ ( \ 0 \ ) \ ) \\ ( \ 0 \ ) \ ) \ ) \ ) \ ) \ ) \ ) \ ) \ )$	59030 -0 30720 0.2 30720 0.2 28660 0.2 28660 0.2 28460 0.1 28460 0.2 28520 -1 48160 -2 48360 -2 59340 -0 84720 -0	$\begin{array}{ccccc}$	0740 2620 2750 4240 1070 7320 12240 .14440 4970 00110 .67600 1420 .19170 0080 24210 5530 8220 4100 34580 77720 7150 62610 89250 3990 8460 8350 24220 5520 .64910 9040 1540 8130
Radio	cal on 10	<sup>th</sup> carbon of	AT-III
37 (0/1) C 3.3 C 2.4 C 1.1 C 1.1 C 2.6 C -1.1 C -1.1 C -1.1 C -1.1 C -1.1 C -1.1 C -1.1 C -2.6 C -2.2 C -2.2 C -2.2 C -2.2 C -2.2 C -2.4 C -1.1 C -1.	13250         -0           30620         0.3           19120         1.3           19810         -0           19810         -0           19810         -0           19810         -0           19810         -0           1030         -1           11030         1.1           18130         -2           41460         0.30340           30340         -1           59460         -1           05910         -2           88280         2           44720         -0           6490         -1           1950         0.6           72050         1.2           18660         1.9           1950         0.6           38100         -2           22060         2.3           35560         2.4           35510         -0           35110         -0           35110         -0           35110         -0           35110         -0           35110         -0           352         -0	.90790 -0. 59590 -1.0 31860 0.05 73150 0.34 81780 0.6 54760 -0. 0.6590 -0.8 46090 -0. 1.99720 -0. 0.99720 -0. 1.43560 0. 99720 -0. 1.30330 0.70 0.1190 2.0 0.3330 0.70 0.3330 0.70 0.3330 0.70 0.3330 0.70 0.3330 0.70 0.3330 0.70 0.3330 0.70 0.3330 0.70 0.3330 0.70 0.3330 0.2 42790 -1. 0.5540 -1. 0.5460 -1. 1.5200 -0.9 6390 -1.7 2.28270 1. 33040 0.48 90300 1.46 90300 1.46 0.7910 2.2 555310 2.0 0.74702 -2 74550 0.7	66900 0230 200 6530 44050 1120 49030 .27190 70680 27610 225380 23070 66740 1900 49180 9390 8530 9390 8530 9390 8530 9390 8550 14630 38060 1910 8250 35560 470 510 8280 3750 .18360 5980 .18360

Supporting Information, SI 12