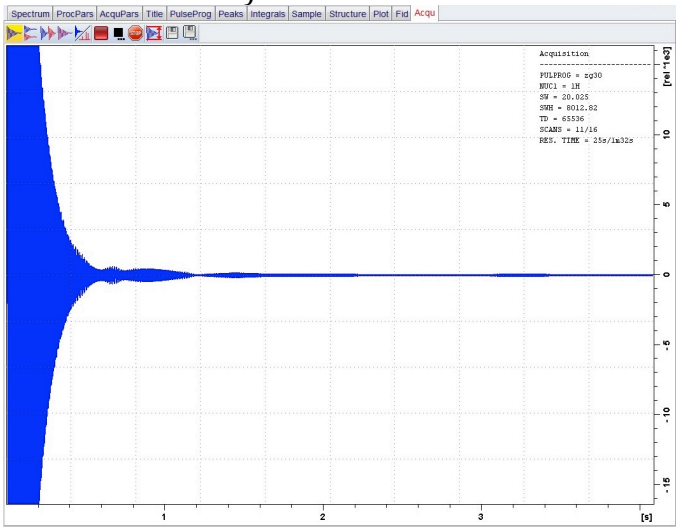
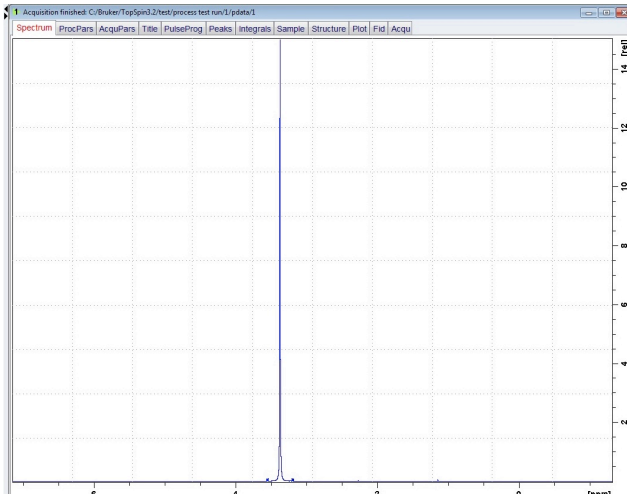
HOW TO PROCESS NMR SPECTRUM (SIMPLE)

1) AFTER THE ACQUISITION THE SPECTRUM TAB SHOULD HAVE YOUR FID (FREE INDUCTION DECAY) SPECTRUM.

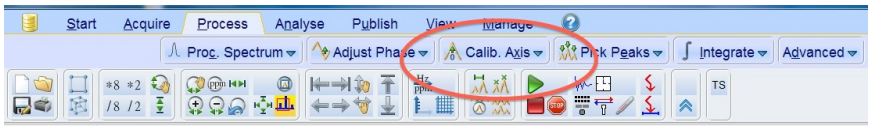


2) TO FOURIER TRANSFORM THIS SIGNAL ENTER "**FT**" FOR 1H OR "**EF**" FOR C13, INTO THE COMMAND BAR AT THE BOTTOM OF THE SCREEN.
3) THE SPECTRUM SHOULD LOOK SOMETHING LIKE THIS: IT IS OUT OF PHASE, TO CORRECT THE PHASE ENTER "**APK**" INTO THE COMMAND BAR.

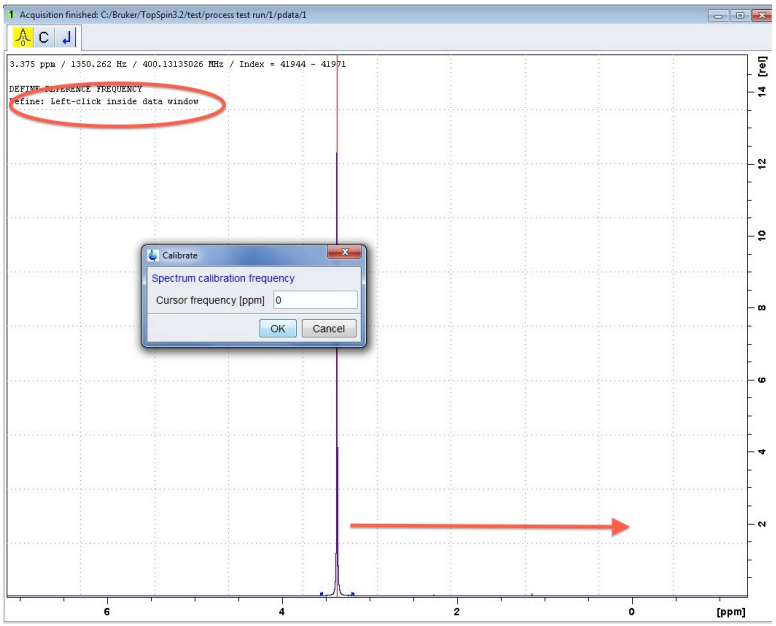
4) THE SPECTRUM SHOULD NOW LOOK LIKE A 'NORMAL' NMR SIGNAL WITH VERTICAL PEAKS



5) TO CALIBRATE THE AXIS, BY PUTTING TMS OR OTHER REFERENCE COMPOUND AT ZERO PPM, CLICK THE “CALIBRATE AXIS” BUTTON ON THE TOP TOOL BAR.



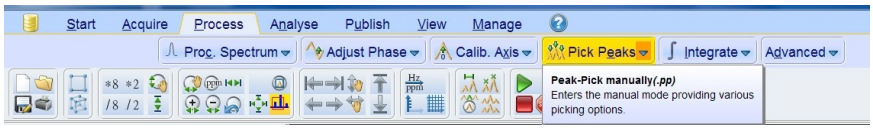
6) LEFT CLICK ON THE CENTER OF THE REFERENCE PEAK AND A WINDOW WILL POP UP. ENTER “0” AS THE VALUE FOR SPECTRUM CALIBRATION FREQUENCY. CLICK “OK”.



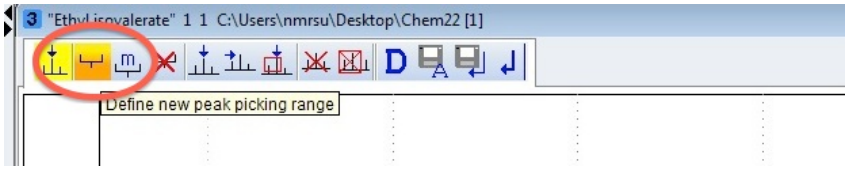
FOR PEAK PICKING GO TO NEXT PAGE

PICK PEAKS

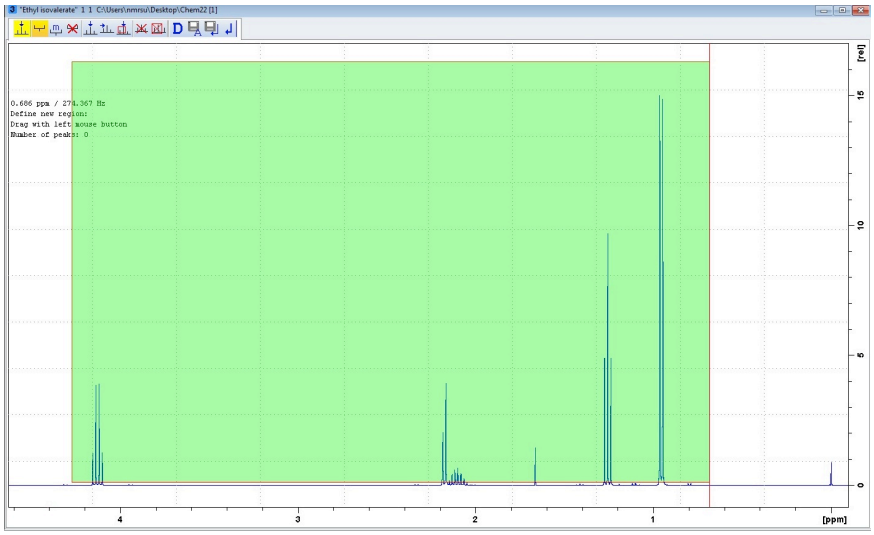
1) CLICK THE “PICK PEAKS” BUTTON AT THE TOP TOOL BAR.



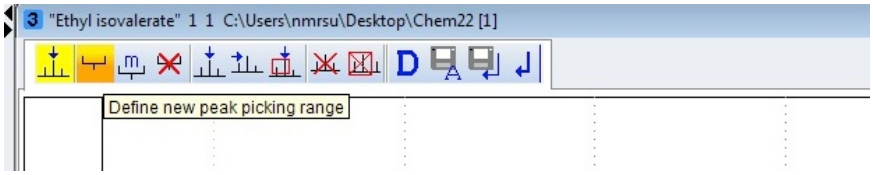
2) FROM THE TOP BUTTON BAR OF THE SPECTRUM WINDOW CLICK ON THE “DEFINE NEW PEAK PICKING RANGE” BUTTON IF NOT ALREADY ACTIVE.



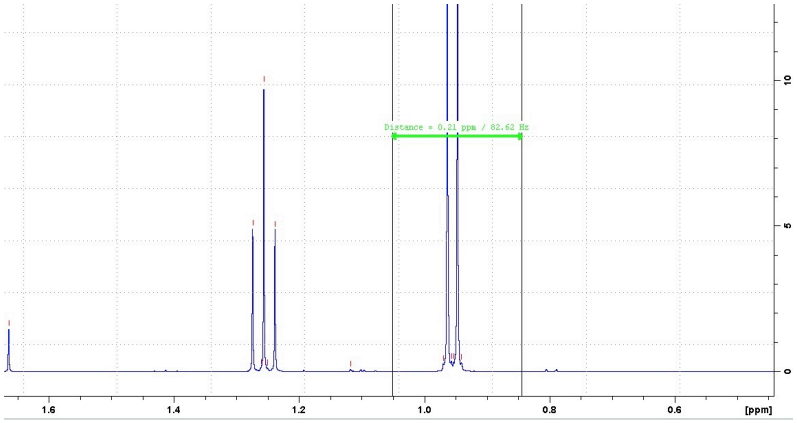
3) LEFT CLICK- HOLD ON THE MOUSE AND DRAG THE ‘GREEN BOX’ OVER THE PEAKS THAT YOU WOULD LIKE TO SELECT. **MAKE SURE THE BOX COVERS THE TOP OF THE PEAKS** OTHERWISE IT WILL NOT SELECT THEM. (hint- *SCROLLING UP/DOWN ON THE ROLLER OF THE MOUSE CAN INCREASE AND DECREASE THE INTENSITY OF THE PEAKS AND BRING THEM INTO FRAME*)



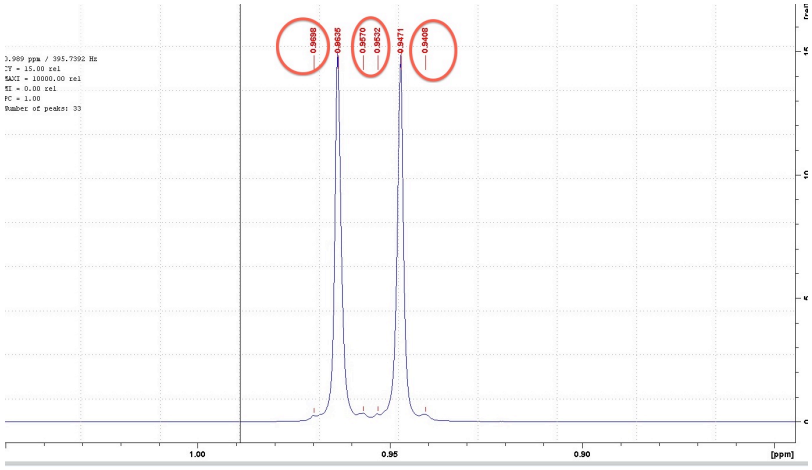
4) ONCE THE REGION IS DEFINED CLICK ON “DEFINE PEAK REGION” TO DEACTIVATE THE FUNCTION.



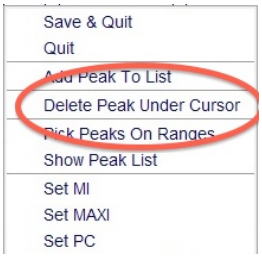
5) LEFT CLICK-HOLD AND DRAG TO ZOOM IN ON INDIVIDUAL PEAK(S).



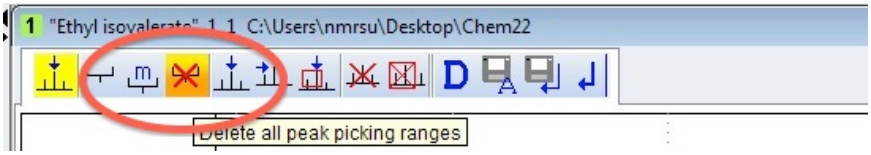
6) IF THERE ARE ERRANT PEAKS CHOSEN THEY CAN BE DELETED MANUALLY.



7) CLICK THE "MANUAL PICKING" BUTTON AND RIGHT CLICK ON PEAK. SELECT "DELETE PEAKS UNDER CURSOR".



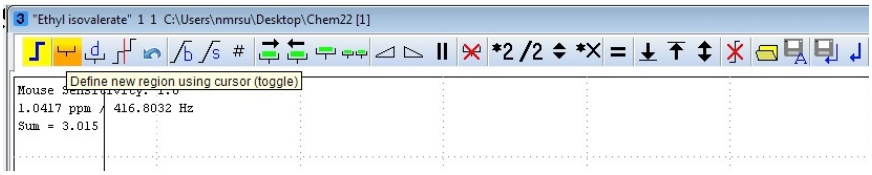
8) SELECT DELETE ALL PEAKS TO START OVER IF DESIRED.



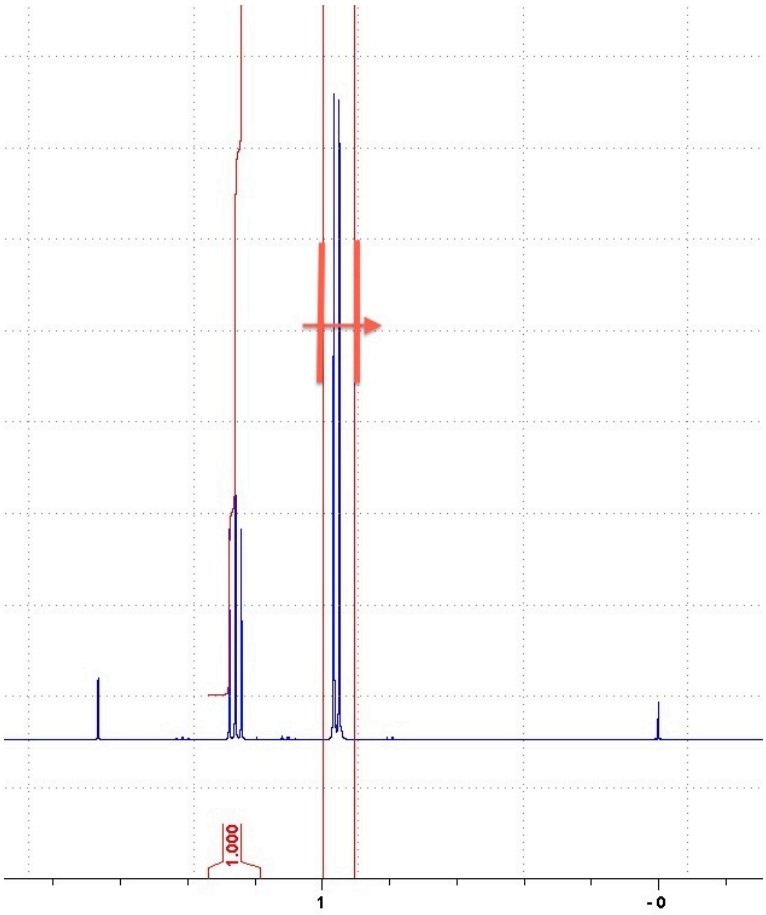
FOR INTERGRATION SEE NEXT PAGE

INTEGRATION

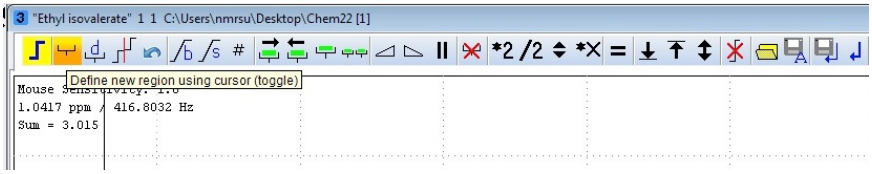
1) CLICK ON THE “INTEGRATION” BUTTON FROM THE TOP TOOLBAR.
2) CLICK ON THE “DEFINE NEW REGION…” BUTTON FROM THE TOP BUTTON BAR ON THE SPECTRUM WINDOW IF NOT ALREADY ACTIVE.



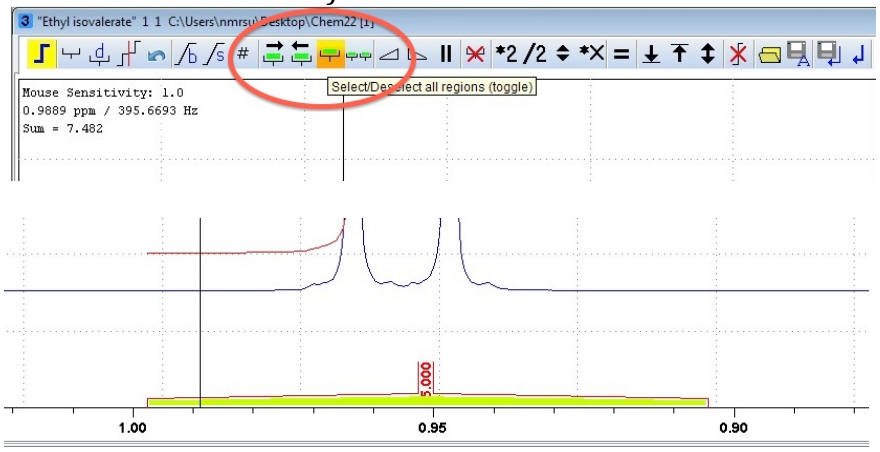
3) LEFT CLICK-HOLD AND DRAG OVER EACH INDIVIDUAL PEAK(S). A SINGLE RED VERTICAL LINE WILL SHOW UP ON THE INITIAL CLICK AND END ON THE OTHER END OF THE REGION.



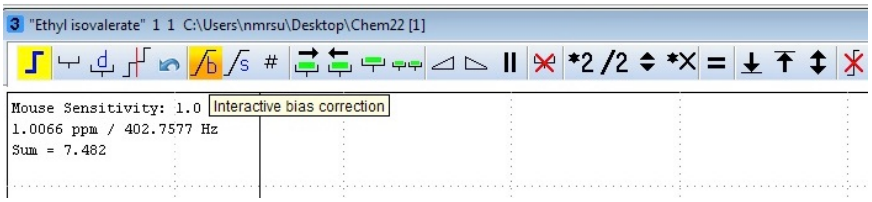
4) CLICK THE “DEFINE REGIONS” BUTTON AGAIN TO DEACTIVATE THE FUNCTION ONCE FINISHED. USE THE LEFT CLICK AND DRAG OVER EACH PEAK TO ZOOM IN.

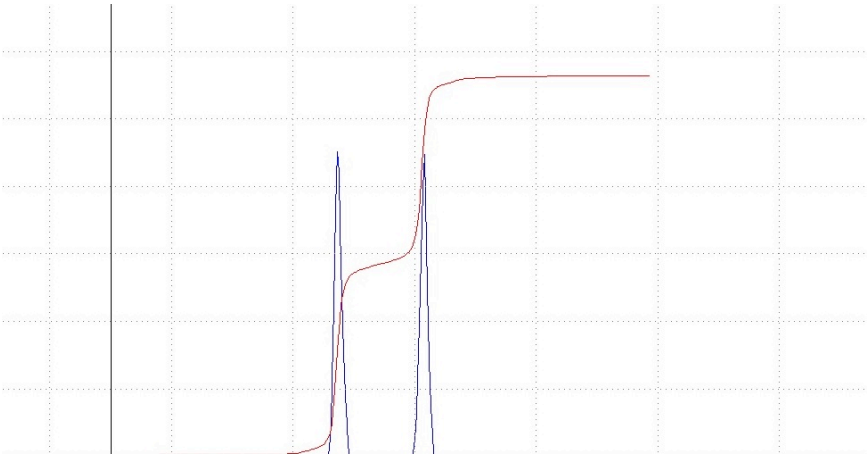


5) SELECT REGION BY USING THE “SELECT/DESELECT REGION” BUTTON TO PICK AN INDIVIDUAL PEAK OR PEAKS TO ADJUST BIAS AND SLOPE. ONCE SELECTED THE INTEGRATION NUMBER BELOW WILL HIGHLIGHT IN GREEN. *PEAKS CAN BE ADJUSTED INDIVIDUALLY OR AS A GROUP*.

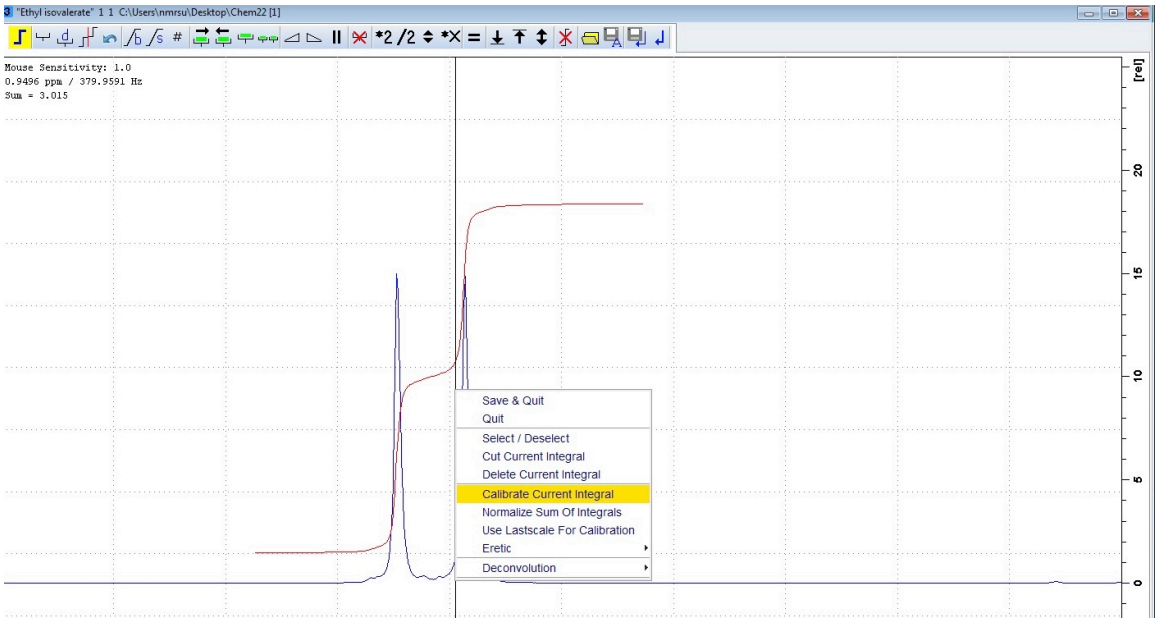


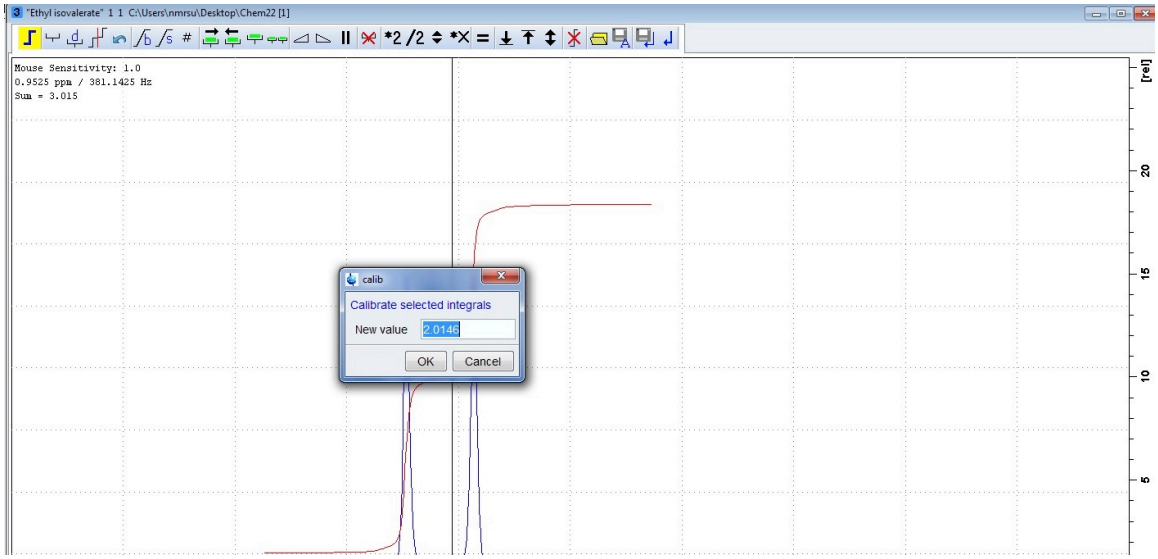
6) **LEFT CLICK AND HOLD** OVER THE BIAS OR SLOPE BUTTON AND SLIDE THE MOUSE UP OR DOWN TO ADJUST. THE GOAL IS TO HAVE THE ENDS OF THE INTEGRAL TO BE FLAT AND PARALLEL AT THE ENDS.





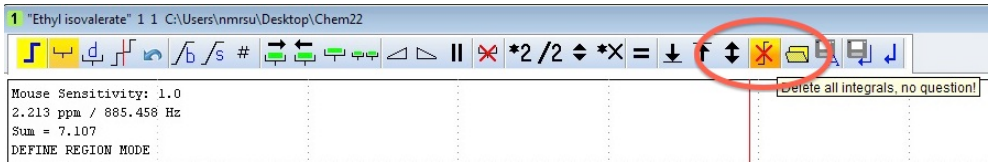
7) TO CALIBRATE THE INTEGRATION, SETTING A KNOWN VALUE OF A CERTAIN PEAK, RIGHT CLICK ON THE PEAK OF INTEREST. A POP UP WILL DISPLAY AND CLICK ON “CALIBRATE CURRENT INTEGRAL”. ENTER THE VALUE WANTED FOR THAT PEAK. ALL OTHER PEAKS WILL ADJUST TO THAT VALUE.



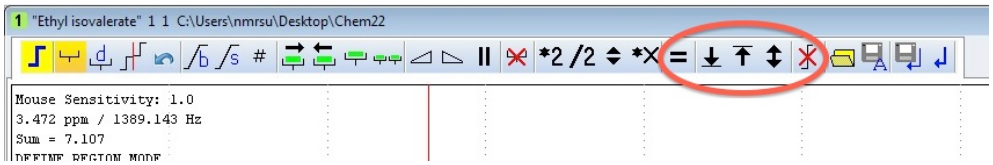


SEE NEXT PAGE FOR OTHER FUNCTIONS

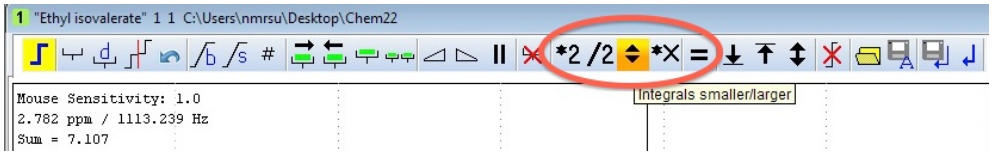
- TO DELETE ALL INTERGRALS AND START OVER SELECT “DELETE ALL INTEGRALS…” BUTTON.



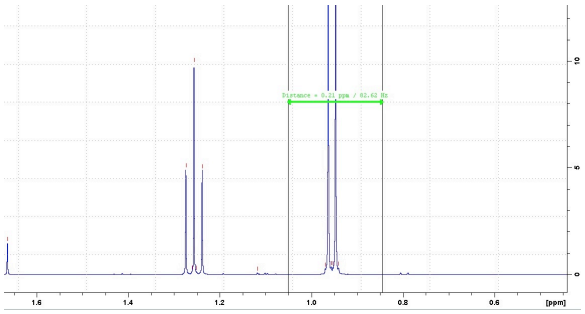
- TO MOVE THE INTEGRATION LINES ON THE SPECTRUM USE THE ARROW BUTTONS. UP AND DOWN ARROW MOVE THE INTEGRATION LINE A SET DISTANCE. A LEFT CLICK-HOLD ON “UP/DOWN ARROW” AND SLIDE MOUSE MOVE THEM A DESIRED DISTANCE.



- TO MAKE THE INTEGRATION LINES SMALLER/LARGER USE THE INDICATED BUTTONS. THE “*2 AND /2” EITHER DIVIDE OR MULTIPLY BY 2. THE “UP/DOWN” ARROW NEEDS A LEFT CLICK-HOLD AND TO DRAG MOUSE UP AND DOWN TO MAKE IT THE DESIRED SIZE.



- TO ZOOM IN, LEFT CLICK-HOLD AND DRAG ACROSS THE DESIRED AREA.



- TO RETURN TO THE PREVIOUS WINDOW SIZE, PRIOR TO ZOOMING, CLICK THE BUTTON FOR THE LAST WINDOW.