

Appendix 3 File formats for different proprietary instrument control software grouped by instrument or experiment type.

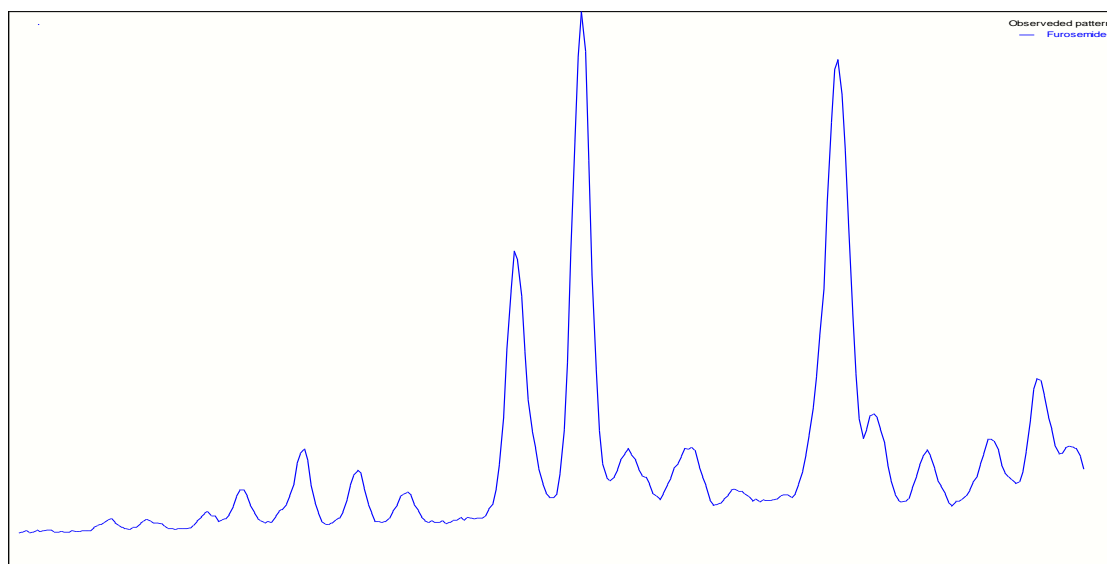
Instrument	Exporting File types
C2(PXRD)	1. DIFFRAC-AT → .raw 2. PLOTSO → .plt 3. DIFFRACPplus → .raw 4. OLD_DIFFRAC-AT → .raw
IR	1. Mattson Data File → .ras 2. ASCII Table → .tbl 3. Old Sadtler(pre 3.0) → .isp 4. New Sadtler → .irf 5. Spectra Calc & GRAMS → .spc 6. JCAMP – DX → .dx 7. Nicolet DX → .nic 8. Nicolet SX → .nic 9. Nicolet PCIR → .ird 10. Nicolet Omnic → .spa
IR Microscope	1. Spectra → .sp 2. Data Manager → .sp 3. Jcamp-DX → .dx 4. ASCII → .asc 5. Interferograms → .ig 6. Data Manager → .ig 7. Chromatograms → .chr 8. Data Manager → .chr 9. PE GRAMS → .spc 10. Spectacle → .irs 11. Omnic → .spa 12. Graphs → .gph 13. Graph Templates → .gfm
Digital Camera	1. .jpg (default) 2. .bmp 3. .tif
Robot	.mpt .s .csv
D8(PXRD)	.raw
DSC (Differential	1. Diamond DSC Data → .pdid 2. Diamond TG/DTA Data → .tdtd 3. DSC 7 Data → .dsd 4. DDSC Data → .ddd 5. Pyris 1 DSC Data → .dcd 6. Pyris 6 DSC Data → .d6d 7. TGA 7 Data → .tgd 8. High Temperature TGA 7 Data → .thd 9. Pyris 6 TGA Data → .t6d 10. DMA 7e Data → .dmd 11. DMA 7e (28-mm Furnace) Data → .d8d 12. TMA

Scanning Calorimetry)	7 Data → .tmd 13. TMA 7 (28-mm Furnace) Data → .t8d 14. DTA 7 Data → .dtd 15. Pyris 1 TGA Data → .tg1d 16. Pyris 1 TGA HT Data → .th1d, .tg1d 17. Diamond TG/DTA Data → .tdtd 18. Diamond TMA Data → .dtmd 19. Diamond TMAH Data → .dthd, .dtmd 20. Sapphire DSC Data → .drdd 21. ANF Data → .anf
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Samples for different files

(1) C2 (PXRD)

- DIFFRAC-AT(.raw), DIFFRACPplus (.raw), OLD_DIFFRAC-AT (.raw) opened with **poudrixmp**



- PLOTSO (.plt) opened with **notepad**

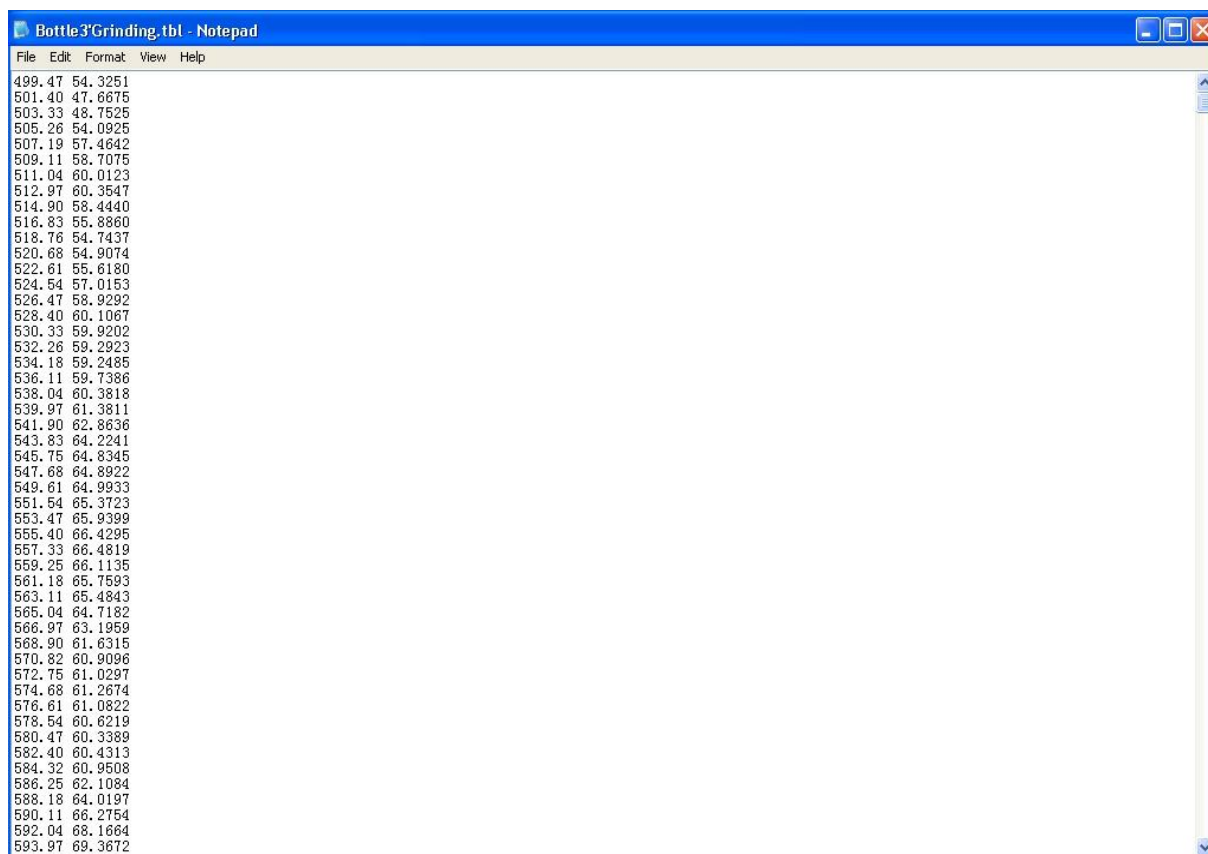
```
Furosemide+Pyridine After_01_2.plt - Notepad
File Edit Format View Help
!@!GADDS PLOTSO FILE: Chi integration type
!@!Title: Furosemide+Pyridine After Grading_22_11_2004
!@!Comment: Furosemide+Pyridine After Grading_22_11_2004
!@!Wavelengths 1.54184 1.54056 1.54439
!@!Integration range: 2Theta: 15.000 to 30.000 Gamma: -116.400 to -57.300
!@!Integration method: bin summation
!@!N
!@!SS
!@!M
!@!L 0.0 0.0 0.0 0.0 0.0
!@!XDegrees
!@!YCounts
15.00 177.29512
15.05 189.626846
15.10 206.717636
15.15 181.110382
15.20 188.221329
15.25 211.863144
15.30 198.345428
15.35 210.185379
15.40 212.889771
15.45 211.38858
15.50 182.031418
15.55 184.107773
15.60 195.611511
15.65 189.120407
15.70 184.861145
15.75 207.509888
15.80 195.57077
15.85 192.025208
15.90 203.497665
15.95 207.612732
16.00 207.23114
16.05 250.613449
16.10 283.751343
16.15 291.790619
16.20 317.335144
16.25 353.235565
16.30 365.751343
16.35 307.30072
16.40 272.128784
16.45 257.052063
16.50 234.741455
16.55 224.458618
16.60 248.767609
16.65 252.226746
16.70 308.227478
16.75 338.823853
16.80 360.257843
16.85 325.074402
```

(2) IR

- Mattson Data File (.ras) opened with **WinFIRST Lite**

See separate sheet.

- ASCII Table (.tbl) opened with **notepad**



Bottle3Grinding.tbl - Notepad

File Edit Format View Help

499.47	54.3251	
501.40	47.6675	
503.33	48.7525	
505.26	54.0925	
507.19	57.4642	
509.11	58.7075	
511.04	60.0123	
512.97	60.3547	
514.90	58.4440	
516.83	55.8860	
518.76	54.7437	
520.68	54.9074	
522.61	55.6180	
524.54	57.0153	
526.47	58.9292	
528.40	60.1067	
530.33	59.9202	
532.26	59.2923	
534.18	59.2485	
536.11	59.7386	
538.04	60.3818	
539.97	61.3811	
541.90	62.8636	
543.83	64.2241	
545.75	64.8345	
547.68	64.8922	
549.61	64.9933	
551.54	65.3723	
553.47	65.9399	
555.40	66.4295	
557.33	66.4819	
559.25	66.1135	
561.18	65.7593	
563.11	65.4843	
565.04	64.7182	
566.97	63.1959	
568.90	61.6315	
570.82	60.9096	
572.75	61.0297	
574.68	61.2674	
576.61	61.0822	
578.54	60.6219	
580.47	60.3389	
582.40	60.4313	
584.32	60.9508	
586.25	62.1084	
588.18	64.0197	
590.11	66.2754	
592.04	68.1664	
593.97	69.3672	

Opened with **WinFIRST Lite**

See separate sheet.

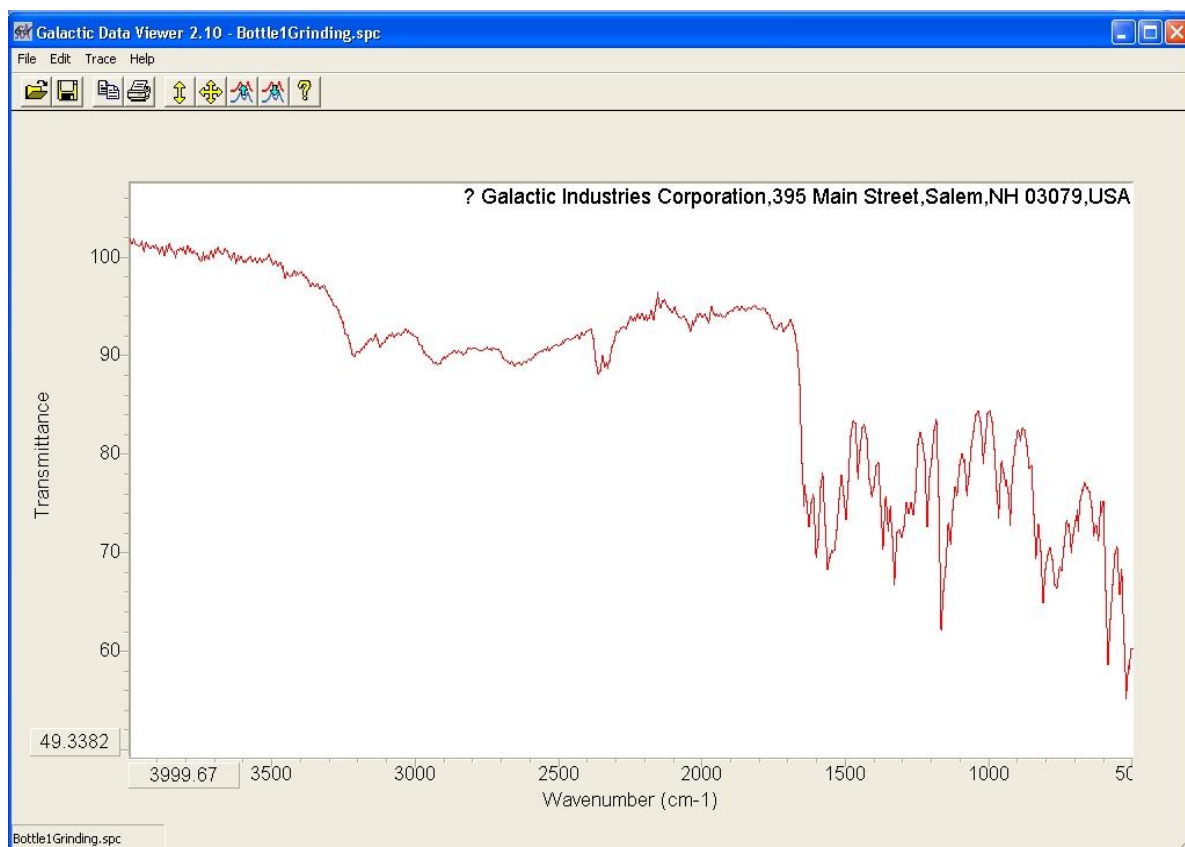
- Old Sadtler(pre 3.0) (.isp) opened with **WinFIRST Lite**

See separate sheet.

- New Sadtler (.irf) opened with **WinFIRST Lite**

See separate sheet.

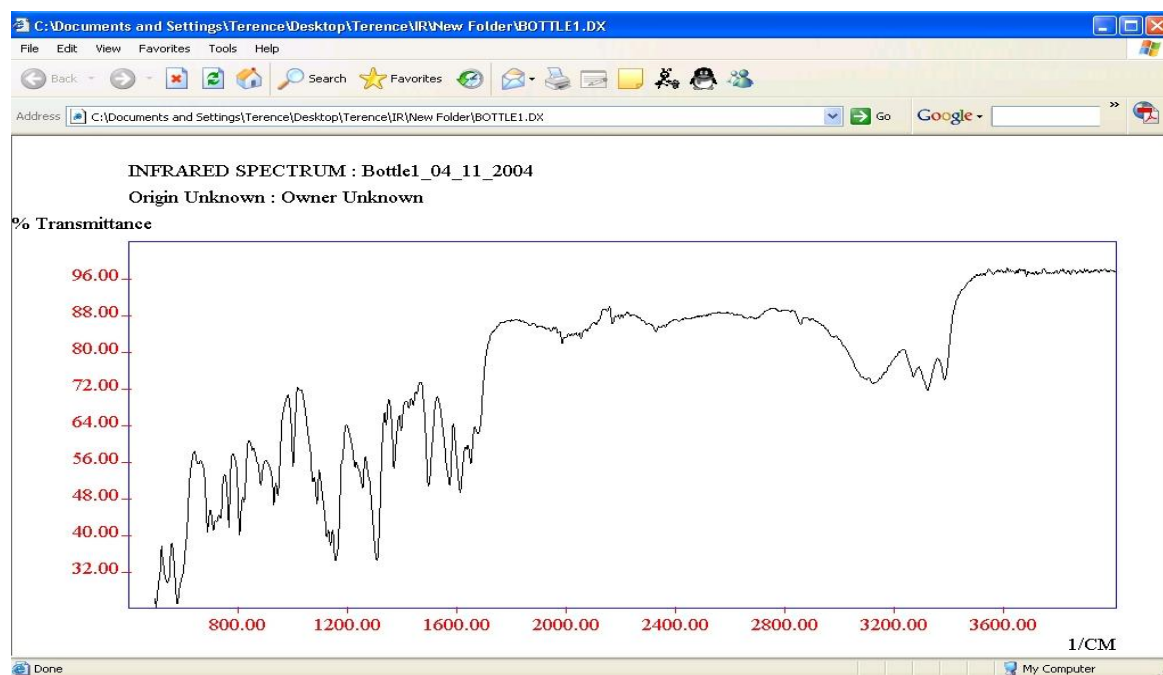
- Spectra Calc & GRAMS (.spc) opened with **Galactic Data Viewer**



Opened with **WinFIRST Lite**

See separate sheet.

- JCAMP – DX (.dx) opened with **IE explore**



Opened with **WinFIRST Lite**

See separate sheet.

Opened with **word**

```
##TITLE= Bottle1_04_11_2004
##JCAMP_DX= 4.24
##OWNER=
##ORIGIN=
##DATA TYPE= INFRARED SPECTRUM
##YUNITS= % Transmittance
##XUNITS= 1/CM
##FIRSTX= 499.47609046
##FIRSTY= 26.38117980
##LASTX= 3999.66568195
##XFACTOR= 1.00000000
##YFACTOR= 0.00112474
##MINY= 24.39409446
##MAXY= 98.10316467
##DELTAX= 1.92847911
##NPOINTS= 1816
##XYDATA= (X++(Y..Y))
499.47 23455 21688 22210 23635 24661 25568
511.04 26586 27265 27850 29489 32095 33655
522.61 33209 32007 31248 30555 29441 28397
534.18 27816 27386 26936 26669 26574 26569
545.75 26793 27223 27782 28846 30656 32549
557.33 33700 34041 33811 32999 31679 30159
568.90 28548 26773 25013 23635 22802 22439
580.47 22503 23061 24029 25057 25842 26369
592.04 26778 27164 27543 27968 28586 29463
603.61 30420 31283 32155 33169 34236 35400
615.18 37041 39310 41793 44061 46004 47500
626.75 48420 49045 49812 50685 51254 51421
638.32 51502 51695 51848 51683 51085 50287
649.89 49724 49575 49614 49596 49571 49700
661.46 49948 50147 50187 49992 49627 49319
673.03 49018 48501 47603 46232 44243 41651
684.61 38995 37040 36246 36605 37677 38907
696.18 39910 40476 40538 40152 39384 38334
707.75 37297 36717 36833 37443 38088 38430
...
...
...
3843.45 86866 86891 86835 86780 86713 86528
3855.02 86298 86262 86394 86561 86606 86543
3866.60 86599 86803 86910 86767 86581 86498
3924.45 86906 86878 86839 86862 86889 86822
3936.02 86661 86471 86363 86474 86774 87001
3947.59 86978 86827 86760 86799 86876 86978
3959.16 87059 87036 86935 86839 86732 86623
```

3993.88 86692 86629 86639 86782
##END=

- Nicolet DX (.nic) opened with **WinFIRST Lite**

See separate sheet.

- Nicolet SX (.nic) opened with **WinFIRST Lite**

See separate sheet.

- Nicolet PCIR (.ird) opened with **WinFIRST Lite**

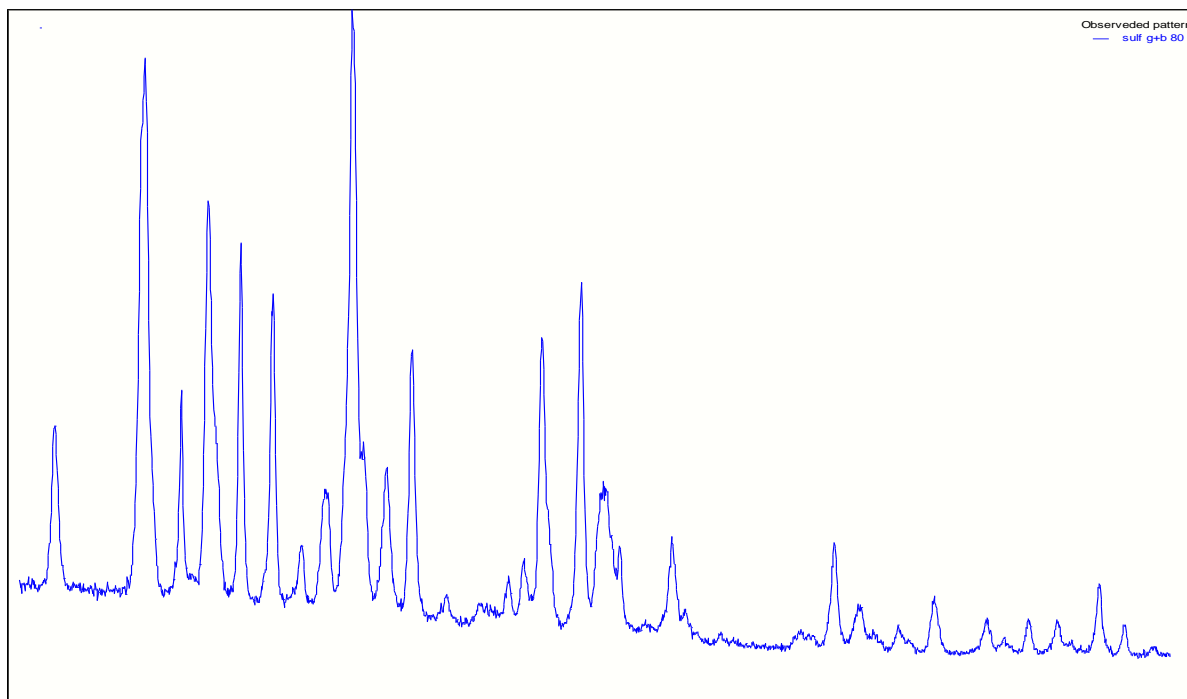
See separate sheet.

- Nicolet Omnic (.spa) opened with **WinFIRST Lite**

See separate sheet.

(3) D8 (PXRD)

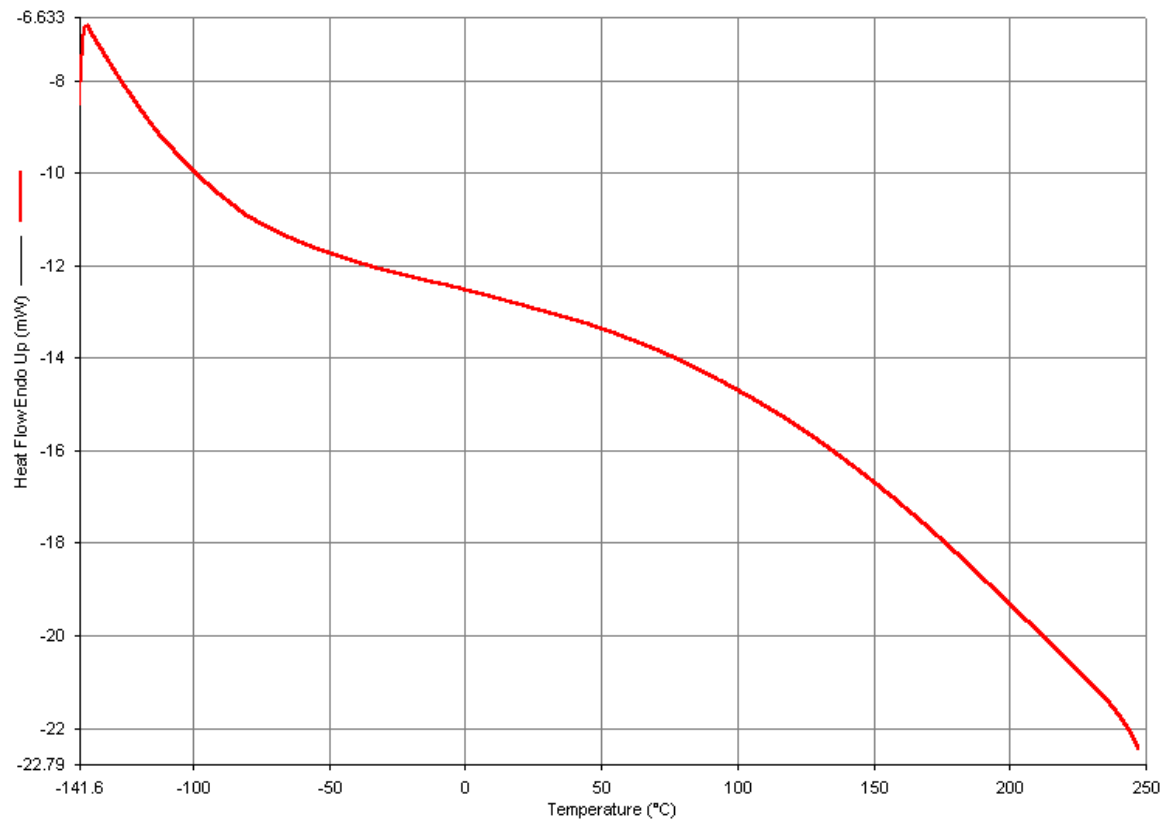
- .raw opened with **poudrixmp**



(4) DSC (Differential Scanning Calorimetry)

- Diamond DSC Data (.pdid), Diamond TG/DTA Data (.tdtd), DSC 7 Data (.dsd), DDSC Data (.ddd), Pyris 1 DSC Data (.dcd), Pyris 6 DSC Data (.d6d), TGA 7 Data (.tgd), High Temperature TGA 7 Data (.thd), Pyris 6 TGA Data (.t6d), DMA 7e Data (.dmd), DMA 7e (28-mm Furnace) Data (.d8d), TMA 7 Data (.tmd),

TMA 7 (28-mm Furnace) Data (.t8d), DTA 7 Data (.dtd), Pyris 1 TGA Data (.tg1d), Pyris 1 TGA HT Data (.th1d, .tg1d), Diamond TG/DTA Data (.tdtd), Diamond TMA Data (.dtmd), Diamond TMAH Data (.dthd, .dtmd), Sapphire DSC Data (.drdd) and ANF Data (.anf) opened with ***Pyris Series – Diamond DSC***



- ASCII (.txt) opened with ***notepad***

20rates38c2f45date22oct2004plot.txt - Notepad

File Edit Format View Help

Filename: C:\Program Files\Pyris\Data\Experimental\20rates38c2f45date22oct2004plot.pdid
 Operator ID:
 Sample ID:
 Comment:
 Serial Number:
 Data Collected: 22/10/2004 14:47:38
 Sample Weight: 0.000 mg
 Validation:
 Validated: No
 By:
 Date:
 Calibration Information
 Filename: C:\Program Files\Pyris\Calibrations\20rates38c2f46date22oct2004.pdic
 Date/Time:
 Initial Conditions
 Temperature: -140.00 磅
 Y Initial: 20.00 mW
 Sample Rate: Fast
 Baseline Filename:
 End Condition: Go To Load
 Total Points in Run: 23400
 Method Steps:
 Pre-Run Actions
 Start the Run
 Action occurs Immediately
 1) Heat from -140.00磅 to 250.00磅 at 20.00磅/min

1) Diamond DSC Temperature Scan

Time	Unsubtracted Heat Flow	Baseline Heat Flow	Program Temperature	Sample Temperature	Approx. Gas Flow	Heat Flow Calibration
0.000000	-8.520100	0.000000	-139.996000	-141.574000	0.000000	1.000000
0.000833	-8.521800	0.000000	-139.998000	-141.573000	0.000000	1.000000
0.001667	-8.519900	0.000000	-139.993000	-141.574000	0.000000	1.000000
0.002500	-8.519100	0.000000	-139.946000	-141.573000	0.000000	1.000000
0.003333	-8.513400	0.000000	-139.930000	-141.574000	0.000000	1.000000
0.004167	-8.502200	0.000000	-139.913000	-141.575000	0.000000	1.000000
0.005000	-8.486600	0.000000	-139.896000	-141.575000	0.000000	1.000000
0.005833	-8.468200	0.000000	-139.880000	-141.574000	0.000000	1.000000
0.006667	-8.448300	0.000000	-139.863000	-141.573000	0.000000	1.000000
0.007500	-8.427900	0.000000	-139.846000	-141.571000	0.000000	1.000000
0.008333	-8.408000	0.000000	-139.830000	-141.570000	0.000000	1.000000
0.009167	-8.389100	0.000000	-139.813000	-141.568000	0.000000	1.000000
0.010000	-8.371400	0.000000	-139.796000	-141.565000	0.000000	1.000000
0.010833	-8.354800	0.000000	-139.780000	-141.562000	0.000000	1.000000
0.011667	-8.340500	0.000000	-139.763000	-141.558000	0.000000	1.000000
0.012500	-8.326200	0.000000	-139.746000	-141.555000	0.000000	1.000000
0.013333	-8.313900	0.000000	-139.730000	-141.549000	0.000000	1.000000
0.014167	-8.301900	0.000000	-139.713000	-141.543000	0.000000	1.000000
0.015000	-8.290700	0.000000	-139.696000	-141.538000	0.000000	1.000000
0.015833	-8.279500	0.000000	-139.680000	-141.531000	0.000000	1.000000

20rates38c2f45date22oct2004plot.txt - Notepad

File Edit Format View Help

19.470000	-22.379800	0.000000	249.404000	246.739000	0.000000	1.000000
19.470833	-22.382000	0.000000	249.420000	246.755000	0.000000	1.000000
19.471667	-22.384200	0.000000	249.437000	246.771000	0.000000	1.000000
19.472500	-22.386400	0.000000	249.454000	246.788000	0.000000	1.000000
19.473333	-22.388600	0.000000	249.470000	246.805000	0.000000	1.000000
19.474167	-22.390900	0.000000	249.487000	246.822000	0.000000	1.000000
19.475000	-22.393100	0.000000	249.504000	246.838000	0.000000	1.000000
19.475833	-22.395400	0.000000	249.520000	246.855000	0.000000	1.000000
19.476667	-22.397700	0.000000	249.537000	246.872000	0.000000	1.000000
19.477500	-22.399900	0.000000	249.554000	246.890000	0.000000	1.000000
19.478333	-22.402200	0.000000	249.570000	246.907000	0.000000	1.000000
19.479167	-22.404500	0.000000	249.587000	246.922000	0.000000	1.000000
19.480000	-22.406700	0.000000	249.604000	246.939000	0.000000	1.000000
19.480833	-22.409000	0.000000	249.620000	246.955000	0.000000	1.000000
19.481667	-22.411300	0.000000	249.637000	246.972000	0.000000	1.000000
19.482500	-22.413600	0.000000	249.654000	246.989000	0.000000	1.000000
19.483333	-22.415900	0.000000	249.670000	247.005000	0.000000	1.000000
19.484167	-22.418200	0.000000	249.687000	247.021000	0.000000	1.000000
19.485000	-22.420500	0.000000	249.704000	247.038000	0.000000	1.000000
19.485833	-22.422800	0.000000	249.720000	247.054000	0.000000	1.000000
19.486667	-22.425100	0.000000	249.737000	247.071000	0.000000	1.000000
19.487500	-22.427400	0.000000	249.754000	247.088000	0.000000	1.000000
19.488333	-22.429700	0.000000	249.770000	247.105000	0.000000	1.000000
19.489167	-22.432000	0.000000	249.787000	247.122000	0.000000	1.000000
19.490000	-22.434300	0.000000	249.804000	247.140000	0.000000	1.000000
19.490833	-22.436600	0.000000	249.820000	247.157000	0.000000	1.000000
19.491667	-22.438800	0.000000	249.837000	247.174000	0.000000	1.000000
19.492500	-22.441100	0.000000	249.854000	247.191000	0.000000	1.000000
19.493333	-22.443300	0.000000	249.870000	247.207000	0.000000	1.000000
19.494167	-22.445600	0.000000	249.887000	247.223000	0.000000	1.000000
19.495000	-22.447800	0.000000	249.904000	247.241000	0.000000	1.000000
19.495833	-22.450200	0.000000	249.920000	247.258000	0.000000	1.000000
19.496667	-22.452400	0.000000	249.937000	247.274000	0.000000	1.000000
19.497500	-22.454800	0.000000	249.954000	247.291000	0.000000	1.000000
19.498333	-22.457100	0.000000	249.970000	247.307000	0.000000	1.000000
19.499167	-22.459400	0.000000	249.987000	247.326000	0.000000	1.000000

DIAMOND DSC AUTOTUNE CALIBRATION VALUES:
 Date: 22/10/2004 14:27:23
 Slope: 38
 Coarse Balance: 2
 Fine Balance: 45

DIAMOND DSC SAMPLE TEMPERATURE CALIBRATION VALUES:
 Reference Expected (磅) Measured (磅) Method
 Indium 156.600 156.600
 Zinc 419.470 419.470

NEWPAGE

```

20rates38c2f45date22oct2004plot.txt - Notepad
File Edit Format View Help

DIAMOND DSC FURNACE TEMPERATURE CALIBRATION VALUES:
Minimum 50.000 磅
Maximum 650.000 磅

FURNACE CALIBRATION COMPUTED RESULTS:
Date: 22/10/2004 14:27:19
Setpoints (磅) Boundaries (磅) y''
50.000 50.000 0
125.000 125.000 0
200.000 200.000 0
275.000 275.000 0
350.000 350.000 0
425.000 425.000 0
500.000 500.000 0
575.000 575.000 0
650.000 650.000 0

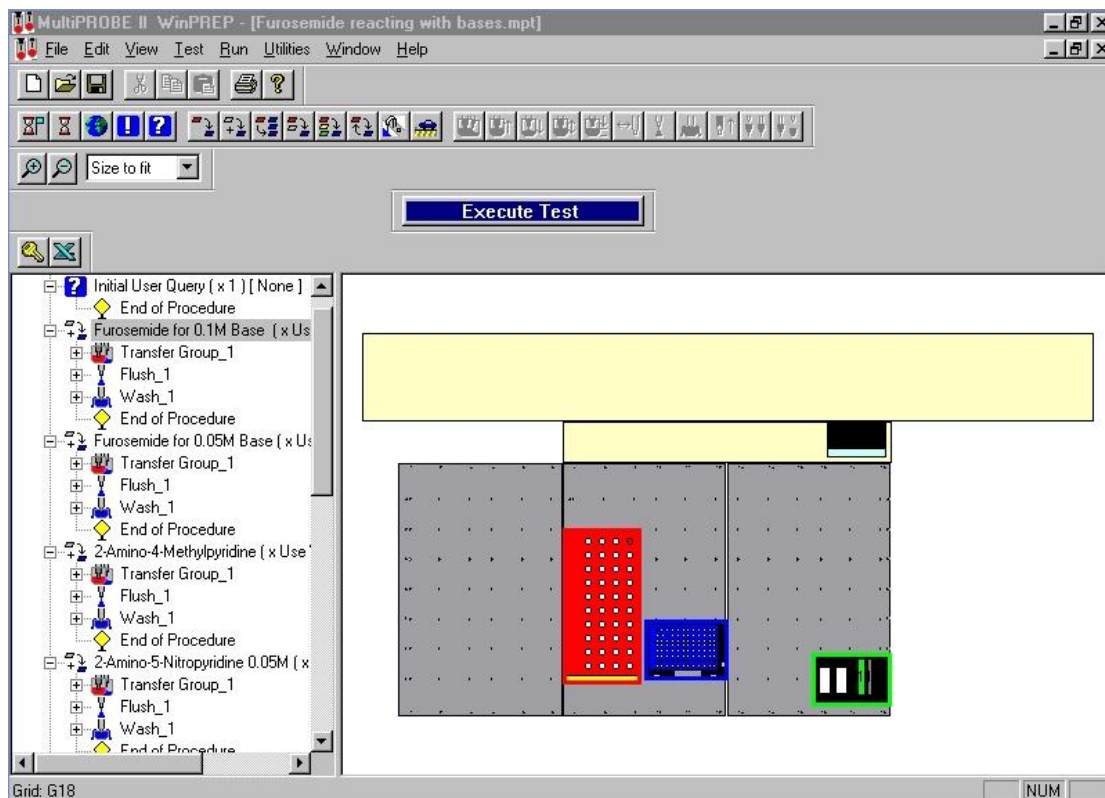
DIAMOND DSC HEAT FLOW CALIBRATION VALUES:
DIAMOND HEAT FLOW CALIBRATION COMPUTED RESULTS:
Date: 22/10/2004 14:27:19
K(Ts) = (0)Ts^3 + (0)Ts^2 + (0)Ts + (1)
Sapphire Cp Data:
Temperature (K) Measured Cp Ideal Cp
343.16 0.78566 0.86011
347.16 0.79251 0.86674
351.16 0.79975 0.87322
355.16 0.80787 0.87957
359.16 0.81695 0.88578
393.16 0.84811 0.93365
397.16 0.85325 0.93875
401.16 0.85933 0.94376
405.16 0.86560 0.94866
409.16 0.87303 0.95346

PROFILE VALUES FOR THIS DATA:
Software Version 6.0.0.0033
Firmware Version Part Number N5368010 Revision 0.01:.
Instrument Serial Number
Load Temperature 30.0 磅
Go To Temp Rate 500.0 磅/min
Maximum Allowed Temperature 300.0 磅
Helium Purge Was Used
Liquid Nitrogen Was Used
Data taken using the Normal Range
Filter Factor 3
Lag Compensation 0
Cooling Device CryoFill
Filter Algorithm: Adaptive Boxcar

```

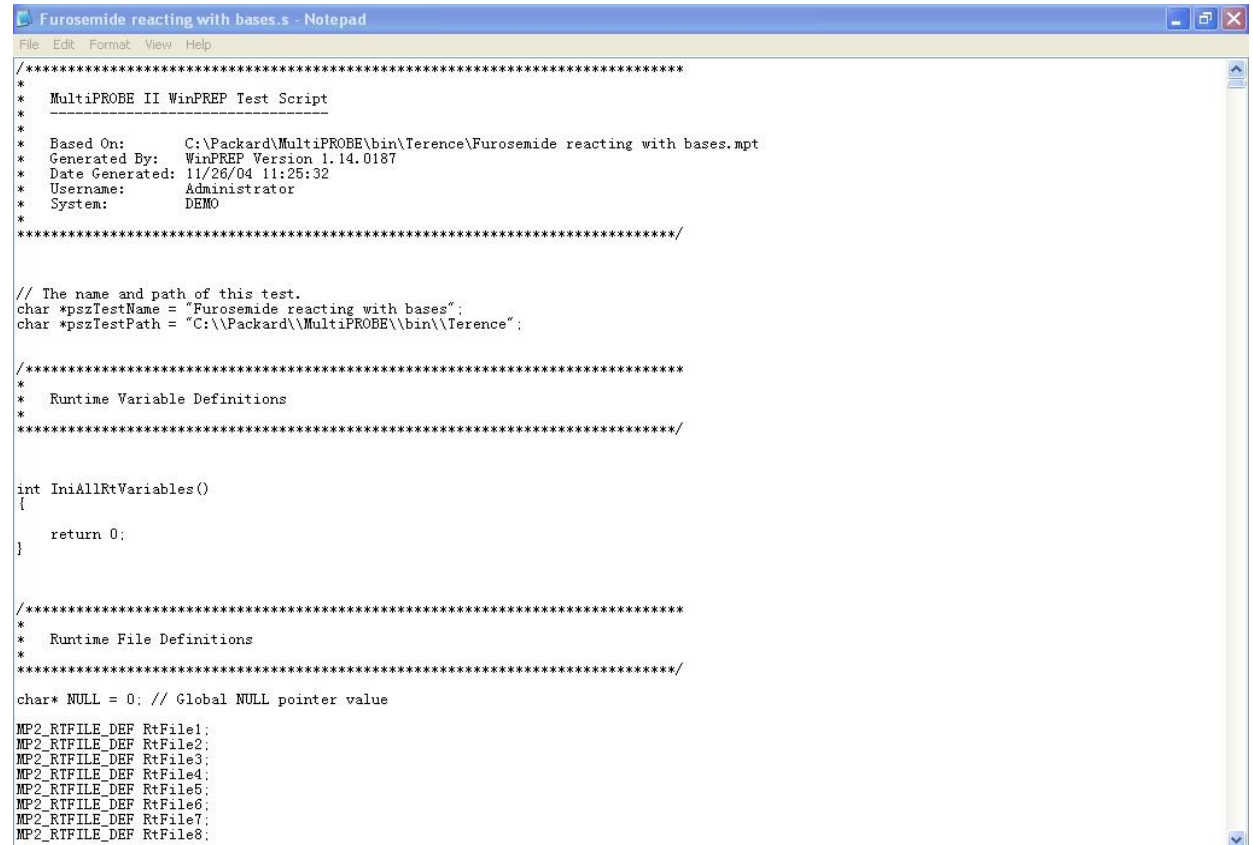
(5) Robot

- .mpt file opened with **MultiPROBE II WinPREP**



- .s file opened with **notepad**, .csv file open with **Microsoft Excel**

.s file is a test script. It contains all information about the project, which will run on the robot machine. In addition, .s file will also catch some information about sample's location from .csv file.



```

Furosemide reacting with bases.s - Notepad
File Edit Format View Help

/*****
 * MultiPROBE II WinPREP Test Script
 *
 * Based On:      C:\Packard\MultiPROBE\bin\Terence\Furosemide reacting with bases.mpt
 * Generated By:  WinPREP Version 1.14.0187
 * Date Generated: 11/26/04 11:25:32
 * Username:      Administrator
 * System:        DEMO
 */

// The name and path of this test.
char *pszTestName = "Furosemide reacting with bases";
char *pszTestPath = "C:\\Packard\\MultiPROBE\\bin\\Terence";

/*****
 * Runtime Variable Definitions
 */

int IniAllRtVariables()
{
    return 0;
}

/*****
 * Runtime File Definitions
 */

char* NULL = 0; // Global NULL pointer value
MP2_RTFILE_DEF RtFile1;
MP2_RTFILE_DEF RtFile2;
MP2_RTFILE_DEF RtFile3;
MP2_RTFILE_DEF RtFile4;
MP2_RTFILE_DEF RtFile5;
MP2_RTFILE_DEF RtFile6;
MP2_RTFILE_DEF RtFile7;
MP2_RTFILE_DEF RtFile8;

```

```
Furosemide reacting with bases.s - Notepad
File Edit Format View Help

//-----
// Aspirate
//-----
if( MSL_UseAspStep( 0, 1 ) )
{
    dAspVol = MSL_GetAspStepVol( 0 );

    if( nDspWells == nGrpWells )
        dWasteVol = PrfFileGetWastePercent( pPC->hPrfFile, dXfrVol ) * dXfrVol / 100.0;
    else
        dWasteVol = 0;

    dDspVol = 0.0;

    nRet = EGS_AspEx( pPC, 37, &M030000_Aspirate, 0,
                    // sample id
                    dAspVol, // aspirate volume
                    0.0, // pre-aspirate air volume (for blowout)
                    3.0, // post-aspirate air volume
                    dDspVol, // dispense back volume
                    dWasteVol ); // Waste volume

    if( nRet == -1 ) return nRet;
    if( nRet == -2 ) { bEOM = 1; break; }
    if( nRet == -3 ) break; // Skip Sample? // Specify additional aspirate details...
    EGS_SetAspDetails( 4, dLLSAspHeight, 1.0, PrfFileGetAspSpeed( pPC->hPrfFile, dAspVol ), PrfFileGetAspDelay( pPC->hPrfFile,
dAspVol ), dRetractFromLiqHeight, dRetractFromLiqSpeed, 0, 0, 0, dLLSclotDetHeight, 1 );
}

//-----
// Dispense
//-----
if( MSL_UseDspStep( 0, 1, &nDspWells ) )
{
    dDspVol = MSL_GetDspStepVol( 0 );

    dPostAir = 3.0;
    nDspMode = 0;

    nDspMax = 4; // Load maximum dispenses
    for( nDsp = 0; (nDsp < nDspMax) && (nDspWells > 0); nDsp++ )
    {
        nRet = EGS_DspEx( pPC, 40, &M030001_Dispense, 1,
                        dDspVol, // dispense volume
                        dPostAir, // post air volume
                        nDspMode, // dispense mode
                        0 ); // Reserved for blowout delay

        if( nRet == -1 ) return nRet;
        if( nRet == -2 ) { bEOM = 1; break; }
        nDspWells--;
        // Specify additional dispense details...
    }
}
```

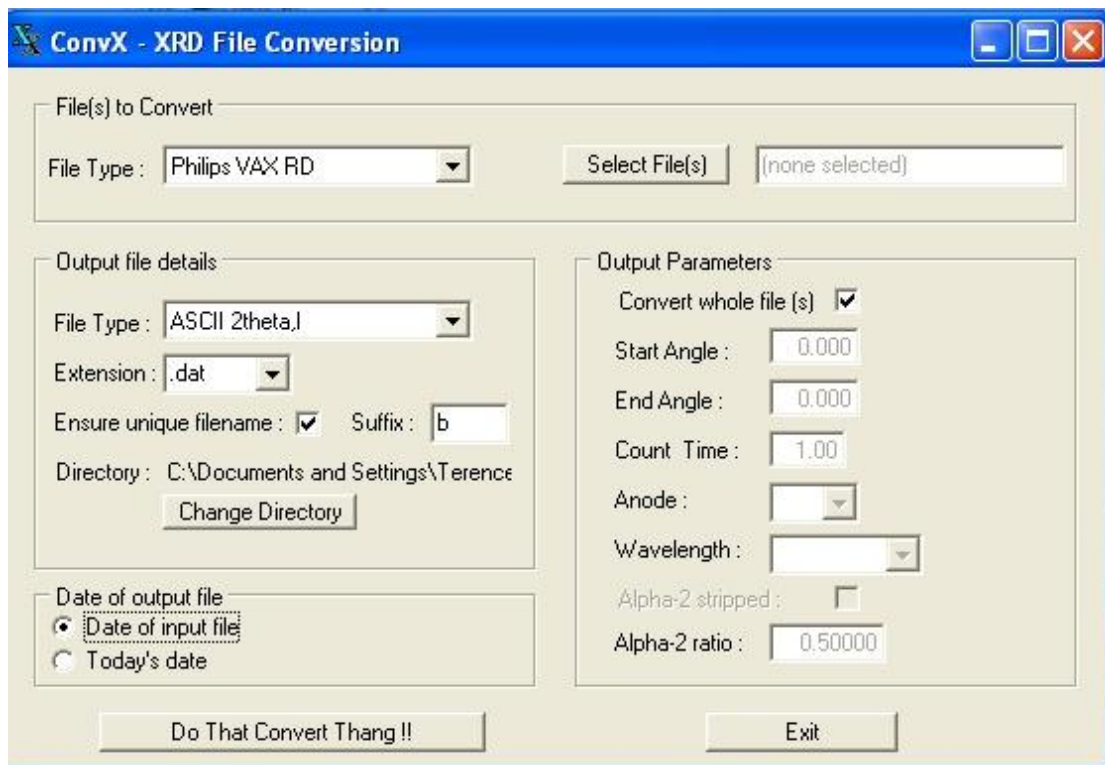
Microsoft Excel - Furosemide reacting with bases_M090001_Dispense.csv

Type a question for help

	A1		terence2														
	A	B	C	D	E	F	G	H	I	J	K	L	M				
1	terence2	49															
2																	
3																	
4																	
5																	
6																	
7																	
8																	
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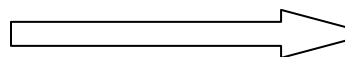
Furosemide reacting with bases_ /

Ready



Philips Vax RD (.rd)
 ASCII 2Theta (.dat)
 DiffracPLUS Raw (.raw)
 Philips PC RD (.rd)
 Philips PC SD (.sd)
 Sietronics CPI (.cpi)
 GSAS (.dat)
 DBW-based (.dat)
 ScanPI (.int)
 Diffrac-AT RAW (.raw)
 Diffrac-V1 RAW (.raw)

Converting



Philips Vax RD (.rd)
 ASCII 2Theta (.dat)
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