#### **TROUBLESHOOTING ON BRUKER INSTRUMENTS**

#### **General notes**

On the Bruker 500, three errors cause the queue to stop. On the Bruker 400, only one error is enough to cause it to stop. In either case, an email is sent to Robin. But, sometimes the errors are minor (eg missing sample or unshimmable sample), and also, sometimes it is quicker to try the below steps.

# To get the instrument back in working order, follow the below steps in order as far as possible

### Queue errors

1. Is IconNMR running? If so, click Change User, then log back in

IconNMR is the automation interface:

Control         Data Mathematics parked State State         Control         Contro         Control         Control	<ul> <li>Applicatio</li> </ul>	IN PACES	System	O O M		Q 0	2				_									12 1 1	-O.M. PROMS	8.32.36 PM
<pre>bit Bit Concept View Field Researcher Options Table greet  bit Concept Systematic Table  bit Concept Systematic Table Sy</pre>	٠						_			deards	INR A	demation)	en05-2	1016-045	5-stein							1000
	the Ban in	lojder Vi	es Figd	Barameter	n Options	Tools Help																
	15 P		Stop	# i															ZG in Progress	1 +		20 82
Defer         Defer         Description         Description <thdescription< th=""> <thdescription< th=""> <thdescript< td=""><td>Experiment</td><td>Table</td><td></td><td>-</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td>_</td><td>-</td><td></td></thdescript<></thdescription<></thdescription<>	Experiment	Table		-																_	-	
Image: Source of the second processing of the second procesing of the second processing of the second processing of	Holder	Tipe	Status	Name		No.	Solvert			Experimen					Pri	Par	TrielOrie		Time User	Start Time		1 1
****       #************************************	12.0	le 1	Finished	10-2112-7			SMM	denter		11111.111		bit lackin 715	expen		w24	Dia.	11		00.00 EF 14	07:34 This per	87,2854	
Image: Control of 12 (2 (3)       1       100000       1	¥ 30	Her 11	Queued																			
<ul> <li>3.1 (P 1 Finded (P 1 Finded (P 2 1 P 1 Finded (P 2 1 P 1 P 1 P 1 P 2 P 2 P 2 P 2 P 2 P</li></ul>		lie :	Queued	M1-81,61	1	1.	214542	10000	10000	N10,511		\$12 acah 63	3-6424	irrent.	() 第二	130.2	harmon	100			0 2010	
Image: State of the state	* 32	fer 11	Finished															100	periors-2016-0855-men Sc			
7.10       P - 1 Outstaf       P - 1 Outstaf       E       CDCI:       consistent of VL2, PEETIN:       Is as a proton outstaff.       IS A I       II       II       II       II       II       III       III       III       IIII       IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII		liter 1	Finished	mpitte		1	10450	1000	10000	NA PER	1014	15 mart (	company of	espective.	*2	180 A	PTINCE,	(1)(2)	34680		e 201m	
************************************	4 35	He-10	Queued													-		(mail)	aaaaa	000		
3.3 <ul> <li>1 - 0.00000 <ul> <li>2 - 0.00000 <li>2 - 0.00000 <li>2 - 0.00000 <li>2 - 0.00000 <li>2 - 0.00000 </li> <li>2 - 0.00000 <li>2 - 0.00000 </li> <li>2 - 0.00000 <li>2 - 0.00000 </li> <li>2 - 0.000000 </li> <li>2 - 0.000000 </li> <li>2 - 0.000000 </li> <li>2 - 0.000000 </li> <li>2 - 0.0000000 </li> <li>2 - 0.0000000000000000000000000000000000</li></li></li></li></li></li></li></li></li></li></li></li></li></li></li></li></li></li></li></ul></li></ul>		100	Queues	provide sets	011079		LDCI			N 10 Mills	10%	12 2011			<b>W.</b>	Mo .		000			0.2010	
Image: Property and product rates in the set of the set o	~ 33	iles 1	Queues	and the local			and in			ALL DOCT		11 months			-	-		21 22	224 💼 22 22	28 29 39		
• Source:	+ 34	10-10	Outunt															1 A A	ă ă ă ă ă ă	ăăă		
9       9		lie-	Queued	100m 714	entre.				arrest a	N.Le. Petr	tine	14 works			**	13		( ) (B)			9.2514	
	4.35	10-10	Queued													1.11		RO			1000	
b         B         Available         Diff         Construction         Diff         Construction         Diff         Construction         Diff         Construction         Diff         Diff <thdif< th=""> <thdif< th=""> <thdif< th=""></thdif<></thdif<></thdif<>		lie-	Queued.	249m 244	L.S.Adv	8 C	CDC/8	charge	arrest a	N34, PER	ttaka -	35 works	-		w X	13+±	H.				0.2215	
17     17 Probabel     1	b. 36	11 1	Available															(I) 🐨 🐨	<b>5) (H) (B) (B) (B)</b>			- 1
Image: Second 1/2 / Joint Color Management & Kill (MECC)       I state protein copyring & Kill (MECC) <thi &="" (mecc)<="" copyring="" kill="" protein="" state="" th=""> <thi< td=""><td>P 37</td><td>1 er 11</td><td>Finished</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td>22200</td><td></td><td>A second second</td><td></td><td>Contraction Contraction</td><td></td><td></td></thi<></thi>	P 37	1 er 11	Finished													22200		A second second		Contraction Contraction		
3.1          (* 1 Proubed		Her 1	Finished	804-09-17	41-24	F	CDCI	1 Property of		N 14, MIC	104	75 50017			<b>#</b> X	514	NGK-051	17.73.04	004537 Ainty	15:05 Wedge	1.06.3016	
***       3       ***       1       5       2       2       3       ***       1 </td <td>5 38</td> <td>Her 11</td> <td>Finished</td> <td></td> <td>-</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	5 38	Her 11	Finished													-						
Provided       provide		les .	Finished	808-09-17	Ad-day					w the provide state	104	28.0004.0			W.35	512	NUE-CD-1	tive3.be	and 11 woods	TRUCK WHERE	- 26 2016	
Summ         Summ         Summ         East         Description         Summ		iles 1	Frished					-		ALL MADE		The second of			-	121.4	Acres 1		STATUTE IN ADDRESS			
Submit         Submit<	-			the second		W																
Processing Experiments           Product         Marcine         No.         Experiment         Lock Shim         Acq         Proc         Hand         Theory (hang         Theory (hang         Theory (hang         Theory (hang         Theory (hang         Theory (hang         Accide           242 2016-01-011-02-10         2         215,213         - <td>Submit</td> <td></td> <td>Çancel</td> <td>Ed</td> <td>R.</td> <td>Qelete</td> <td>944</td> <td>1.</td> <td>CSBA</td> <td>1 I I</td> <td></td> <td>20</td> <td>Change Ster</td>	Submit		Çancel	Ed	R.	Qelete	944	1.	CSBA	1 I I											20	Change Ster
Chair         Header         Header         No.         Experiment         Load         ATM         Load         ATM <thload< th=""> <thload< th="">         Atm</thload<></thload<>	Preceding E	perment																				
243       254       255       254       2	e Date		0	Holder	Name	200003		. NO.	Exp	niment	Load	ATM	Loc	x Shim	Acq	Proc	User		Disk	Yitter/Onlg		
124 2016/00 41140.24     2016/00 41140.24     2016/00 41140.24     2016/00 41140.24     2016/00 41140.24     2016/00 41140.24     2016/00 41140.24     2016/00 41140.24     2016/00 4113737     41     2016/00 4113737     41     2016/00 4113737     41     2016/00 4113737     41     2016/00 4113737     41     2016/00 4113737     41     2016/00 4113737     41     2016/00 4	243 2016	01-08 11	49.49	25	PIC-1-64-9	eeco.		- 2	34.0	13		1					chang		/home/chang	Auclair		
Part 2016/02/00 1114/04       3       201002/00/00 1114/04       3       201002/00/00 1114/04       3       201002/00/00 1114/04       0       Part 2010/00/00 1114/04       0       Part 2010/00/00 1114/04       0       Part 2010/00/00/00/00/00/00/00/00/00/00/00/00/	242 2010	02-08 33	40.34	2	20140100	land of the second		1	mai	itenance.L5	Č.,					Ť.	Loany	10021	Interneticitation	Provident and		
2019 2019 01 11 2011 41       DD, Wolfen, hugs       2       2019 2010 01 11 2011 41       DD, Wolfen, hugs       2       2019 2010 01 11 2011 41       DD, Wolfen, hugs       2       2019 2010 01 11 2011 41       DD, Wolfen, hugs       2       2019 2010 01 11 2011 41       DD, Wolfen, hugs       2       2019 2010 01 11 2011 41       DD, Wolfen, hugs       2       2019 2010 01 11 2011 41       DD, Wolfen, hugs       2       2019 2010 01 11 2014 41       DD, Wolfen, hugs       2       2019 2010 01 11 2014 41       DD, Wolfen, hugs       2       2019 2010 01 11 2014 41       DD, Wolfen, hugs       2	245 2010	02-08-11	40.34		20160108			10	NP4	11000	1	1	-	1	-	1	macropro	ence.	mome/maintenance	Department.		
238 2016-01 00 113 021 42 DF, MC/145, Mp8 2 DF,	239 2016	01-08 11	33:41	41	DA NOFia	n smalle		1	10	NOTON	1	5	1	1	2	5	donaties		(hoine/docaties	Seiman		
212 212 212 212 212 212 212 212 212 212	238 2014	01-06-11	30.31	42	DR_NC/(a)	n bigð		2	- 202	31CPD		1	1		1	1	donatien		/home/donatien	Sleiman		
235     2056-036-01111.149     48     AD4+42-crude     1     15/m010n     2     2     1	236 2016	01-08 11	28:05	45	ACH-63-cr	n orgen nade		1	- 55	ROTON	5	5	5	5	5	5	domingu	42	(home/dominguez	Li		
235         235 <td>235 2016</td> <td>01-05 11</td> <td>11:49</td> <td>40</td> <td>ADH-62-cr</td> <td>ode</td> <td></td> <td>3</td> <td>- 32</td> <td>ROTON</td> <td>1</td> <td>1</td> <td>1</td> <td>1</td> <td>1</td> <td>1</td> <td>domingu</td> <td>43</td> <td>/home/dominguez</td> <td>11</td> <td></td> <td></td>	235 2016	01-05 11	11:49	40	ADH-62-cr	ode		3	- 32	ROTON	1	1	1	1	1	1	domingu	43	/home/dominguez	11		
232         233         234         3         5         7         4         matrixematics         3         4         2 <th2< th=""> <th2< th=""></th2<></th2<>	234 2016-233 2016-	01-08 11-01-01-01-01-01-01-01-01-01-01-01-01-0	05:30	16	ADH-61-C	ude		1	367	ROTON	5	5	5	5	5	5	yunliu	42	(home/dominguez (home/yunliu	U.		
211         22160108         2         materials/2-34         X         materials/2-34         X         materials/2-34         Opposite           230         20160108         2         materials/2-34         X         materials/2-34         X         materials/2-34         Opposite         Opposit         Opposite         Opposite	232 2016	01-06-10	55:49	15	ly-2-Me			1	16.	NOTON	2	1	2	2	1	~	yunku		/home/yunlia	11		
228 2016-03 10 413.5 5 20160108 2 maintenance maintenance 25 maint	231 2016	02-08-10	52:30		20160108				21	iterative SA	1	1	1	1	×		mainten	ence:	/homemaintenance	Department		
225 2316-31-08 10.513 45 wethodau honesteendoorus Lumb 226 2316-31-08 10.513 45 wethodau honesteendooru Lumb 227 2316-31-08 10.513 15 MA-123 228 2316-31-08 10.513 10 MA-123 228 2316-31-08 10.513 10 MA-123 228 2316-31-08 10.513 10 MA-123 228 2316-31-08 10.513 228 2316-31-08 10.513 228 2316	230 2016	01-08 10	47:35	5	20160108			2	mari 304	ntenance.13	1	1	1	1	1	1	maintena	ence .	/home/maintenance	Department		
1288 2016-01-00 10 12 128     45     xxx0-reflexuline     1     16,PMOTON     +     +     werdbaw     /home(werdbaw)     /home(werdbaw)       228 2016-01-00 100 131     1     10,PMOTON     +     +     +     werdbaw     /home(werdbaw)     /home(werdbaw)       228 2016-01-00 100 131     3     AM-123     10,PMOTON     +     +     +     werdbaw     /home(werdbaw)       228 2016-01-00 100 131     3     AM-123     15,PMOTON     +     +     werdbaw     /home(werdbaw)       228 2016-01-00 100 131     3     AM-123     15,PMOTON     +     +     werdbaw     /home(werdbaw)       228 2016-01-00 100 130     3     AM-123     15,PMOTON     +     +     werdbaw     /home(werdbaw)       228 2016-01-00 100 130     3     AM-123     15,PMOTON     +     +     werdbaw     /home(werdbaw)       228 2016-01-00 100 130     3     AM-123     15,PMOTON     +     +     werdbaw     /home(werdbaw)       228 2016-01-00 100 130     3     AM-123     10,PMOTON     +     +     werdbaw     /home(werdbaw)       228 2016-01-00 100 130     10,PMOTON     +     +     +     +     werdbaw     /home(werdbaw)       228 2016-01-00 100 130     10,PMOTON	229 2016	01-08-10	39-32	45	web-retiou	line .		2	24.4	:33		1			1	1	wenboxu		/home/wenboxu	Lumb		
228     228 <td>228 2016-</td> <td>01-08 10:</td> <td>12:28</td> <td>45</td> <td>KWD-reticu Toly/Ortad</td> <td>fine Indexed Frankline</td> <td>1.100</td> <td>1</td> <td>- 35</td> <td>ROTON</td> <td>3</td> <td>1</td> <td>1</td> <td>1</td> <td>3</td> <td>1</td> <td>wenboxu</td> <td></td> <td>/home/wenboxu /home/tuisun</td> <td>Lumb</td> <td></td> <td></td>	228 2016-	01-08 10:	12:28	45	KWD-reticu Toly/Ortad	fine Indexed Frankline	1.100	1	- 35	ROTON	3	1	1	1	3	1	wenboxu		/home/wenboxu /home/tuisun	Lumb		
San San A Barra La	226 2016	01-08-10	01:30	1	AM-123			â	- 560	ROTON	4	1	2	1	2	2	montagu	e.	/home/montagut	Ext-Castagner		
Search Peceding August Fe1317 fay 18 An System Fe1317	*) SOLA	03.08.00.		1	4183.884						_		_		1		1010-104		Part of the second second	Teasting		
🕼 Therminal 🔰 & Kontelletting Tales Schwarz (🖕 Kontelletting Tales Schwarz (🖕 Kontelletting Tales Schwarz (👘 Starting Tales Schwarzhold	Search Pres	eding				9.2												Barry	ate-25 Samuel Renau Burry and	PERMIT		Dare Main
	9 Il herr	inal			14 10	probability.			6 4.00	ution .			14	Bruker B	p/gen 3.5	Lpi 3 on av50	as most	& Kontell au	to Online Controls	E Starting Take	Screenshot	

Clicking Change User and logging back in will restart the queue if it has stopped. If the queue stopped because it couldn't find samples or because a sample or samples were unshimmable, then restarting the queue will work to get the spectrometer going again. If there is a more serious issue, however, this will not be enough.

## 2. Is TopSpin running? If so, close it by closing the Terminal window. Then go on to Step 3.

TopSpin is the program used for processing spectra. It is also in charge of automation, although IconNMR is usually used as a front end to TopSpin:



The Terminal window is open whenever TopSpin is running. To close it, just click on the upper right corner of the window:



TopSpin can sometimes take a few seconds to close all background processes, so wait some time before starting TopSpin again (Step 3).

3. Start TopSpin if it is not running or if you closed it in Step 2. Log in to IconNMR when prompted.

Use the icon at the top of the screen or the icon on the Desktop to restart TopSpin:



After some seconds, lconNMR will start, and there will be a prompt to log into lconNMR. Use your normal login and password, and the queue will start again. If there were samples queued previously, go to Step 4.

4. If there was a queue operating previously with samples waiting to be run, click Stop at the top of the IconNMR window. Then go to the IconNMR File menu and choose option 1. Then click Start.

Restarting lconNMR, as in Step 3, leads to a new run being started. If there were no samples queued previously, then it is fine to continue with this new run. But, if there were samples queued previously, you should:

Stop the current run by clicking on the red Stop icon:

	🛟 Applica	tions Places	System 🗞	2	🧅 🙆	2
	<b>\$</b>					
	<u>F</u> ile <u>R</u> un	Holder Vie	w Fi <u>n</u> d <u>P</u> ara	ameters Opt <u>i</u> o	ns T <u>o</u> ols <u>H</u> elp	
	2005		Stop 👥			
	262	00 🕶	3000 46	1		
	Experime	nt Table				
	Holder	Type S	Status Nan	ne	No.	Solvent
Then go to the F	ile mer	nu and cl	hoose the	e first run I	isted (or ty	pe 1):
			Applic	ations Places S	iystem 😰 🔗	
			4			
			File Run	Holder View	Find Parame	
			New			
			Open			
			Save			
			Save as e	xternal setup	st	
			Import Sp	readsheet (.xls	x)/.csv) file	
			Print (List	Setup)	p.	
			Print Histo	ory File	29	
			1 Jul03-20	)16-1800-barre	tt.set	
			2 Jun24-2	016-1442-lumb	-oce.set	
			<u>3</u> Jun16-2	016-1901-tjutri	ns.set	
			4 Jun15-2	016-1211-chido	hob.set	
			<u>5</u> May22-	2016-1839-mcg	illnmr.set	
			Close			
Now, start the run	n that i	s loaded	by clicki	ng on the	Start icon:	
	15	Applications	Places System	n 🗐 🔗 🖄	۵	5
	4					
	File	Run Hold	er <u>V</u> iew Fin	d Parameters	Options Tools	Help
	25	🖇 Start 📄	· II 😡	<b>#</b> i		
	Exp	periment Tab	le	1		
	H	older T	vpe St	atus Name		No.

Now IconNMR should be working again from where it left off.

### 5. If the above steps do not work, and/or you are at all confused, contact the Facility Manager

Robin's office phone (514-398-6219) usually forwards to her cell phone, or you can send an email: robin.stein@mcgill.ca.

If the instrument is in a state where it cannot be used by anyone, please leave a note at the spectrometer. Also, if the Bruker 400 is unusable, please go on FACES and block out the next few hours or overnight.