

Processing

Bucketing

Data Export

Data Type to Export:

- Data matrix
- Buckets table
- SNR matrix
- XLSX Workbook
- Spectral data

Export Format:

Tabular Separator Value (TXT)

noisy PPM range:

10.5 10.2

Export SNR Matrix



### Calculate Signal to Noise Ratio

(same as the Bruker TopSpin 'sino' command)

$$\text{SNR} (S_i, b_j) = \frac{\text{maxval}(S_i, b_j)}{2 \cdot \text{noise}(S_i)}$$

Where:

- **maxval** is the highest intensity in the spectral region defined by the bucket **j** on the spectrum **i**
- **noise** is the estimated noise in the given spectral region for each spectrum **i**

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Export SNR Matrix

noisy PPM range:

10.5 10.2

	A	B	C	D	E	F	G	H	I	J	K	L	M	B8_
1	SampleCo	Dose.Level	Caterogy	B9_3435	B9_1674	B9_1495	B8_9497	B8_9354	B8_8489	B8_8331	B8_7257	B8_7181	B8_7137	B8_
2	aq_179	BPA250ng	B	22.7	8.5	8.3	15.4	15.7	2.2	2.1	10.9	11.6	13.2	
3	aq_157	BPA250ng	B	19.4	8.1	7.8	26.2	27.6	1.9	1.9	25.3	25.2	26.5	
4	aq_154	BPA250ng	A	50.1	22.5	23.8	26.5	26.2	5.4	5.6	21.7	22.0	22.9	
5	aq_138-3	BPA250ng	A	38.1	17.9	18.7	28.3	27.7	10.5	11.2	30.0	30.2	30.8	
6	aq_138-1	BPA250ng	A	30.3	13.0	13.8	28.9	29.7	1.8	1.7	27.8	27.7	28.4	
7	aq_172	BPA250ng	B	53.9	25.5	25.0	36.7	36.0	5.8	6.1	30.4	30.4	30.3	
8	aq_135	BPA250ng	A	62.4	30.0	29.4	39.0	38.9	13.7	14.6	31.0	36.9	36.1	
9	aq_141	BPA250ng	A	32.5	14.9	14.8	40.0	40.2	2.1	1.9	37.6	38.5	38.5	
10	aq_133	BPA250ng	A	48.9	22.6	22.8	40.0	39.0	4.2	4.9	34.8	33.5	34.6	
11	aq_173	BPA250ng	B	18.7	8.5	8.7	40.5	39.7	0.9	1.3	32.0	34.3	34.7	
12	aq_165	BPA250ng	B	22.0	10.2	9.7	44.4	43.2	7.5	7.4	39.7	41.2	42.2	
13	aq_138-2	BPA250ng	A	33.8	14.8	16.6	44.7	42.8	1.9	2.1	37.0	38.0	39.1	
14	aq_155	BPA250ng	A	12.7	6.2	5.8	45.8	43.1	4.7	4.4	39.0	39.6	40.9	
15	aq_162	BPA25ng	B	64.7	32.8	33.1	26.8	26.0	20.6	22.5	23.3	24.8	25.4	
16	aq_181	BPA25ng	B	51.3	26.2	26.5	27.7	27.7	17.4	19.8	27.0	26.3	27.3	
17	aq_164	BPA25ng	B	47.2	22.2	22.3	28.3	28.5	13.1	14.1	23.3	27.7	28.4	
18	aq_152	BPA25ng	A	50.9	23.4	23.1	34.3	33.9	1.4	2.4	28.5	28.9	30.5	
19	aq_136	BPA25ng	A	29.9	13.2	13.5	39.0	38.5	3.4	4.5	32.7	33.3	34.2	
20	aq_166	BPA25ng	B	34.3	15.4	16.0	39.8	39.4	1.6	1.6	34.0	34.1	33.9	
21	aq_137	BPA25ng	A	22.8	9.8	10.5	40.6	39.9	0.6	0.9	32.6	34.3	34.4	
22	aq_177	BPA25ng	B	31.3	14.3	13.3	44.1	42.5	1.4	1.5	34.8	36.8	38.1	
23	aq_163	BPA25ng	B	32.2	14.9	14.7	44.7	43.1	5.7	6.6	40.4	41.7	42.4	
24	aq_149	BPA25ng	A	27.5	12.8	12.9	51.5	48.7	3.5	4.1	43.4	43.0	43.4	



# Excel

Conditional Formatting | Format as Table

Normal | Bad | Good

Neutral | Calculation | Check Cell

Highlight Cells Rules >

Greater Than...

Less Than...

Between...

Equal To...

Text that Contains...

A Date Occurring...

Duplicate Values...

More Rules...

	A	B		H	I	J	K	L	M				
1	Sampleco	Dose.Level		B8_9354	B8_8489	B8_8331	B8_7257	B8_7181	B8_7137	B8_...			
2	aq_179	BPA250ng		15.4	15.7	2.2	2.1	10.9	11.6	13.2			
3	aq_157	BPA250ng		26.2	27.6	1.9	1.9	25.3	25.2	26.5			
4	aq_154	BPA250ng		26.5	26.2	5.4	5.6	21.7	22.0	22.9			
5	aq_138-3	BPA250ng		28.3	27.7	10.5	11.2	30.0	30.2	30.8			
6	aq_138-1	BPA250ng		28.9	29.7	1.8	1.7	27.8	27.7	28.4			
7	aq_172	BPA250ng		36.7	36.0	5.8	6.1	30.4	30.4	30.3			
8	aq_135	BPA250ng		39.0	38.9	13.7	14.6	31.0	36.9	36.1			
9	aq_141	BPA250ng		40.0	40.2	2.1	1.9	37.6	38.5	38.5			
10	aq_133	BPA250ng		40.0	39.0	4.2	4.9	34.8	33.5	34.6			
11	aq_173	BPA250ng	B	40.5	39.7	0.9	1.3	32.0	34.3	34.7			
12	aq_165	BPA250ng	B	44.4	43.2	7.5	7.4	39.7	41.2	42.2			
13	aq_138-2	BPA250ng	A	33.8	14.8	16.6	44.7	42.8	1.9	2.1	37.0	38.0	39.1
14	aq_155	BPA250ng	A	12.7	6.2	5.8	45.8	43.1	4.7	4.4	39.0	39.6	40.9
15	aq_162	BPA25ng	B	64.7	32.8	33.1	26.8	26.0	20.6	22.5	23.3	24.8	25.4
16	aq_181	BPA25ng	B	51.3	26.2	26.5	27.7	27.7	17.4	19.8	27.0	26.3	27.3
17	aq_164	BPA25ng	B	47.2	22.2	22.3	28.3	28.5	13.1	14.1	23.3	27.7	28.4
18	aq_152	BPA25ng	A	50.9	23.4	23.1	34.3	33.9	1.4	2.4	28.5	28.9	30.5
19	aq_136	BPA25ng	A	29.9	13.2	13.5	39.0	38.5	3.4	4.5	32.7	33.3	34.2
20	aq_166	BPA25ng	B	34.3	15.4	16.0	39.8	39.4	1.6	1.6	34.0	34.1	33.9
21	aq_137	BPA25ng	A	22.8	9.8	10.5	40.6	39.9	0.6	0.9	32.6	34.3	34.4
22	aq_177	BPA25ng	B	31.3	14.3	13.3	44.1	42.5	1.4	1.5	34.8	36.8	38.1
23	aq_163	BPA25ng	B	32.2	14.9	14.7	44.7	43.1	5.7	6.6	40.4	41.7	42.4
24	aq_149	BPA25ng	A	27.5	12.8	12.9	51.5	48.7	3.5	4.1	43.4	43.0	43.4



# Excel

Conditional Formatting | Format as Table

Normal	Bad	Good
Neutral	Calculation	Check Cell

	A	B	I	J	K	L	M	N	O	P	Q	R	S	T	U
1	Sampleco	Dose.Level	B8_8489	B8_8331	B8_7257	B8_7181	B8_7137	B8_7049	B8_6172	B8_5873	B8_5412	B8_5226	B8_4879	B8_4609	B8_4415
2	aq_179	BPA250ng	2.2	2.1	10.9	11.6	13.2	12.2	110.0	8.6	3.0	1.2	1.1	0.5	31.4
3	aq_157	BPA250ng	1.9	1.9	25.3	25.2	26.5	24.5	83.9	12.2	1.1	3.4	0.5	7.8	28.6
4	aq_154	BPA250ng	5.4	5.6	21.7	22.0	22.9	21.8	146.9	21.3	1.4	5.0	2.9	7.1	74.1
5	aq_138-3	BPA250ng	10.5	11.2	30.0	30.2	30.8	29.7	144.6	35.3	2.9	4.1	2.3	6.8	59.9
6	aq_138-1	BPA250ng	1.8	1.7	27.8	27.7	28.4	27.3	112.8	12.2	2.1	4.1	0.5	8.0	42.9
7	aq_172	BPA250ng	5.8	6.1	30.4	30.4	30.3	30.7	172.2	11.8	2.1	6.7	4.8	9.6	82.9
8	aq_135	BPA250ng	13.7	14.6	31.0	36.9	36.1	33.0	358.8	69.9	5.0	6.7	9.7	12.6	99.7
9	aq_141	BPA250ng	2.1	1.9	37.6	38.5	38.5	37.1	186.6	18.7	2.6	5.6	1.1	8.3	49.6
10	aq_133	BPA250ng	4.2	4.9	34.8	33.5	34.6	32.0	171.1	12.6	2.5	4.1	3.9	7.8	72.3
11	aq_173	BPA250ng	0.9	1.3	32.0	34.3	34.7	33.3	181.7	53.9	2.1	4.6	6.0	5.1	28.8
12	aq_165	BPA250ng	7.5	7.4	39.7	41.2	42.2	39.7	62.7	20.7	2.2	4.8	1.1	9.6	34.7
13	aq_138-2	BPA250ng	1.9	2.1	37.0	38.0	39.1	36.2	180.4	34.8	3.7	5.2	7.0	7.6	48.5
14	aq_155	BPA250ng	4.7	4.4	39.0	39.6	40.9	39.7	75.8	7.6	1.2	5.5	1.0	9.3	22.6
15	aq_162	BPA25ng	20.6	22.5	23.3	24.8	25.4	24.4	340.9	108.1	4.0	2.8	1.1	10.3	99.3
16	aq_181	BPA25ng	17.4	19.8	27.0	26.3	27.3	24.7	341.8	45.8	4.3	4.9	2.3	11.0	86.7
17	aq_164	BPA25ng	13.1	14.1	23.3	27.7	28.4	26.4	190.1	6.9	1.5	5.9	1.1	6.3	76.8
18	aq_152	BPA25ng	1.4	2.4	28.5	28.9	30.5	29.8	168.7	15.1	2.8	3.6	6.1	7.9	74.0
19	aq_136	BPA25ng	3.4	4.5	32.7	33.3	34.2	33.4	116.9	28.6	2.2	5.1	1.3	9.4	43.5
20	aq_166	BPA25ng	1.6	1.6	34.0	34.1	33.9	32.8	235.7	47.3	3.2	4.0	7.4	6.5	51.1
21	aq_137	BPA25ng	0.6	0.9	32.6	34.3	34.4	32.4	183.3	43.5	2.4	2.9	3.6	7.6	31.4
22	aq_177	BPA25ng	1.4	1.5	34.8	36.8	38.1	34.9	214.8	36.5	2.6	4.8	4.0	5.9	44.0
23	aq_163	BPA25ng	5.7	6.6	40.4	41.7	42.4	39.7	114.6	6.4	1.7	6.6	1.8	11.1	52.4
24	aq_149	BPA25ng	3.5	4.1	43.4	43.0	43.4	42.2	174.3	11.1	3.0	5.0	3.0	9.3	42.4
25															
26									SNR<4						
27									SNR>10						



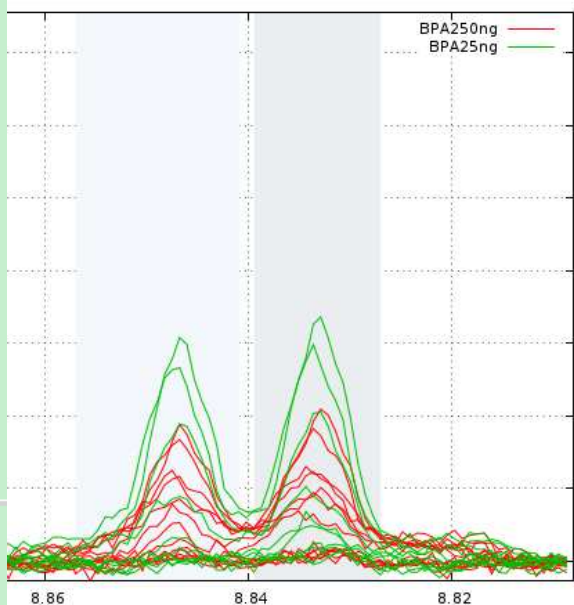
# Excel

Conditional Formatting | Format as Table

Normal | Bad | Good

Neutral | Calculation | Check Cell

	A	B	I	J	K	L	M	N	O	P	Q	R	S	T	U
1	Sampleco	Dose.Level	B8_8489	B8_8331	B8_7257	B8_7181	B8_7137	B8_7049	B8_6172	B8_5873	B8_5412	B8_5226	B8_4879	B8_4609	B8_4415
2	aq_179	BPA250ng	2.2	2.1	10.9	11.6	13.2	12.2	110.0	8.6	3.0	1.2	1.1	0.5	31.4
3	aq_157	BPA250ng	1.9	1.9						3.9	12.2	1.1	3.4	0.5	7.8
4	aq_154	BPA250ng	5.4	5.6						6.9	21.3	1.4	5.0	2.9	7.1
5	aq_138-3	BPA250ng	10.5	11.2						4.6	35.3	2.9	4.1	2.3	6.8
6	aq_138-1	BPA250ng	1.8	1.7						2.8	12.2	2.1	4.1	0.5	8.0
7	aq_172	BPA250ng	5.8	6.1						2.2	11.8	2.1	6.7	4.8	9.6
8	aq_135	BPA250ng	13.7	14.6						8.8	69.9	5.0	6.7	9.7	12.6
9	aq_141	BPA250ng	2.1	1.9						6.6	18.7	2.6	5.6	1.1	8.3
10	aq_133	BPA250ng	4.2	4.9						1.1	12.6	2.5	4.1	3.9	7.8
11	aq_173	BPA250ng	0.9	1.3						1.7	53.9	2.1	4.6	6.0	5.1
12	aq_165	BPA250ng	7.5	7.4						2.7	20.7	2.2	4.8	1.1	9.6
13	aq_138-2	BPA250ng	1.9	2.1						0.4	34.8	3.7	5.2	7.0	7.6
14	aq_155	BPA250ng	4.7	4.4						5.8	7.6	1.2	5.5	1.0	9.3
15	aq_162	BPA25ng	20.6	22.5						0.9	108.1	4.0	2.8	1.1	10.3
16	aq_181	BPA25ng	17.4	19.8						1.8	45.8	4.3	4.9	2.3	11.0
17	aq_164	BPA25ng	13.1	14.1						0.1	6.9	1.5	5.9	1.1	6.3
18	aq_152	BPA25ng	1.4	2.4						8.7	15.1	2.8	3.6	6.1	7.9
19	aq_136	BPA25ng	3.4	4.5						6.9	28.6	2.2	5.1	1.3	9.4
20	aq_166	BPA25ng	1.6	1.6						5.7	47.3	3.2	4.0	7.4	6.5
21	aq_137	BPA25ng	0.6	0.9						3.3	43.5	2.4	2.9	3.6	7.6
22	aq_177	BPA25ng	1.4	1.5						214.8	36.5	2.6	4.8	4.0	5.9
23	aq_163	BPA25ng	5.7	6.6						40.4	41.7	42.4	39.7	114.6	6.4
24	aq_149	BPA25ng	3.5	4.1						43.4	43.0	43.4	42.2	174.3	11.1
25															
26															
27															



SNR<4

SNR>10



# Excel

Conditional Formatting | Format as Table

Normal	Bad	Good
Neutral	Calculation	Check Cell

	A	B	I	J	K	L	M	N	O	P	Q	R	S	T	U
1	Sampleco	Dose.Level	B8_8489	B8_8331	B8_7257	B8_7181	B8_7137	B8_7049	B8_6172	B8_5873	B8_5412	B8_5226	B8_4879	B8_4609	B8_4415
2	aq_179	BPA250ng	2.2	2.1	10.9	11.6	12.2	12.2	110.0	8.6	3.0	1.2	1.1	0.5	31.4
3	aq_157	BPA250ng	1.9	1.9	25.3					2.2	1.1	3.4	0.5	7.8	28.6
4	aq_154	BPA250ng	5.4	5.6	21.7					1.3	1.4	5.0	2.9	7.1	74.1
5	aq_138-3	BPA250ng	10.5	11.2	30.0					5.3	2.9	4.1	2.3	6.8	59.9
6	aq_138-1	BPA250ng	1.8	1.7	27.8					2.2	2.1	4.1	0.5	8.0	42.9
7	aq_172	BPA250ng	5.8	6.1	30.4					1.8	2.1	6.7	4.8	9.6	82.9
8	aq_135	BPA250ng	13.7	14.6	31.0					9.9	5.0	6.7	9.7	12.6	99.7
9	aq_141	BPA250ng	2.1	1.9	37.6					8.7	2.6	5.6	1.1	8.3	49.6
10	aq_133	BPA250ng	4.2	4.9	34.8					2.6	2.5	4.1	3.9	7.8	72.3
11	aq_173	BPA250ng	0.9	1.3	32.0					3.9	2.1	4.6	6.0	5.1	28.8
12	aq_165	BPA250ng	7.5	7.4	39.7					0.7	2.2	4.8	1.1	9.6	34.7
13	aq_138-2	BPA250ng	1.9	2.1	37.0					4.8	3.7	5.2	7.0	7.6	48.5
14	aq_155	BPA250ng	4.7	4.4	39.0					7.6	1.2	5.5	1.0	9.3	22.6
15	aq_162	BPA25ng	20.6	22.5	23.3					8.1	4.0	2.8	1.1	10.3	99.3
16	aq_181	BPA25ng	17.4	19.8	27.0					5.8	4.3	4.9	2.3	11.0	86.7
17	aq_164	BPA25ng	13.1	14.1	23.3					6.9	1.5	5.9	1.1	6.3	76.8
18	aq_152	BPA25ng	1.4	2.4	28.5					5.1	2.8	3.6	6.1	7.9	74.0
19	aq_136	BPA25ng	3.4	4.5	32.7					8.6	2.2	5.1	1.3	9.4	43.5
20	aq_166	BPA25ng	1.6	1.6	34.0					7.3	3.2	4.0	7.4	6.5	51.1
21	aq_137	BPA25ng	0.6	0.9	32.6					3.5	2.4	2.9	3.6	7.6	31.4
22	aq_177	BPA25ng	1.4	1.5	34.8					6.5	2.6	4.8	4.0	5.9	44.0
23	aq_163	BPA25ng	5.7	6.6	40.4					6.4	1.7	6.6	1.8	11.1	52.4
24	aq_149	BPA25ng	3.5	4.1	43.4					1.1	3.0	5.0	3.0	9.3	42.4
25						8.54			8.52						
26										SNR<4					
27										SNR>10					