

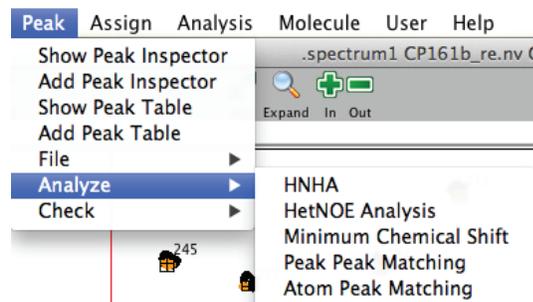
Transferring assignments from one peaklist to another in NMRViewJ

If you have a peaklist with assignments and need to populate another peaklist (of the same spectrum or a very related one), you can use peak-peak matching to transfer assignments.

In my case, Nicole assigned the RbmA FnIII-2 domain and wrote out a peaklist for the $^{15}\text{N}/^1\text{H}$ HSQC called "RbmAFnIII-2peaklist", but it wasn't loading properly onto my HSQC, no matter how I tried processing the data. I picked a new peaklist based off my spectrum CP161b.nv, then transferred the assignments from Nicole's peaklist to mine. I could open her peak list in the Peak Inspector window and see that she had all the proper assignments, they just wouldn't load onto my spectrum.

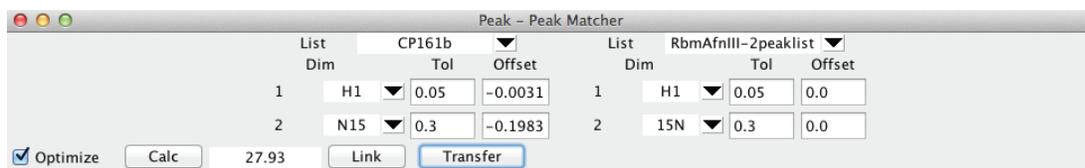
To use Peak Peak Matching, open both peak lists in the NMRViewJ session. Go to Peak --> Analyze --> Peak Peak Matching.

In the pop-up window, select the two peaklists from the dropdown menu (it doesn't matter which peaklist you put in which box). Select the dimension labels (H1, N15) and set the tolerances for each dimension; these values allow wiggle room when matching peaks up in the two dimensions. I typically use 0.05 ppm for ^1H and 0.3 ppm for ^{15}N .



Check the Optimize box, then click the Calc button. Click the Link button, then the Transfer button.

At this point, the assignments from one peak list should be transferred over to the other. The screenshot below shows the peak number from the first list (CP161b), the peak number for the corresponding peak in the second list (RbmAFnIII-2peaklist) and the assignments.



List	Dim	Tol	Offset
CP161b	H1	0.05	-0.0031
CP161b	N15	0.3	-0.1983
RbmAFnIII-2peaklist	H1	0.05	0.0
RbmAFnIII-2peaklist	15N	0.3	0.0

Optimize Calc 27.93 Link **Transfer**

match	peak1	label1	peak2	label2	score
<input checked="" type="checkbox"/>	1	63 225.H			0.056
<input checked="" type="checkbox"/>	2	72 234.H			0.043
<input checked="" type="checkbox"/>	3	86 249.H			0.017
<input checked="" type="checkbox"/>	4	13 171.H			0.061
<input checked="" type="checkbox"/>	6	107 270.H			0.083
<input checked="" type="checkbox"/>	8	25 184.H			0.029
<input checked="" type="checkbox"/>	9	10 168.H			0.042
<input checked="" type="checkbox"/>	10	53 214.H			0.097
<input checked="" type="checkbox"/>	11	52 213.H			0.035
<input checked="" type="checkbox"/>	12	38 198.H			0.201
<input checked="" type="checkbox"/>	13	62 224.H			0.044
<input checked="" type="checkbox"/>	14	68 230.H			0.03
<input checked="" type="checkbox"/>	15	9 167.H			0.056
<input checked="" type="checkbox"/>	16	60 222.H			0.034
<input checked="" type="checkbox"/>	17	92 255.H			0.125
<input checked="" type="checkbox"/>	18	29 189.H			0.017
<input checked="" type="checkbox"/>	19	87 250.H			0.07
<input checked="" type="checkbox"/>	20	91 254.H			0.052
<input checked="" type="checkbox"/>	21	106 269.H			0.079
<input checked="" type="checkbox"/>	22	84 247.H			0.113
<input checked="" type="checkbox"/>	23	75 237.H			0.054
<input checked="" type="checkbox"/>	24	43 203.H			0.153
<input checked="" type="checkbox"/>	25	77 239.H			0.056
<input checked="" type="checkbox"/>	26	30 190.H			0.119
<input checked="" type="checkbox"/>	27	80 242.H			0.049
<input checked="" type="checkbox"/>	28	105 268.H			0.075
<input checked="" type="checkbox"/>	29	93 256.H			0.049
<input checked="" type="checkbox"/>	30	46 206.H			0.479
<input checked="" type="checkbox"/>	31	42 202.H			0.009
<input checked="" type="checkbox"/>	32	81 244.H			0.049
<input checked="" type="checkbox"/>	33	76 238.H			0.078

If you want, you can verify that your new list has the assignments by looking at the Peak Table for the peaklist or by selecting the peaklist in the Peak Inspector and arrowing through the peak numbers to see the assignments written below.