

**DRCC results template for  
data submission:  
Data description & examples**

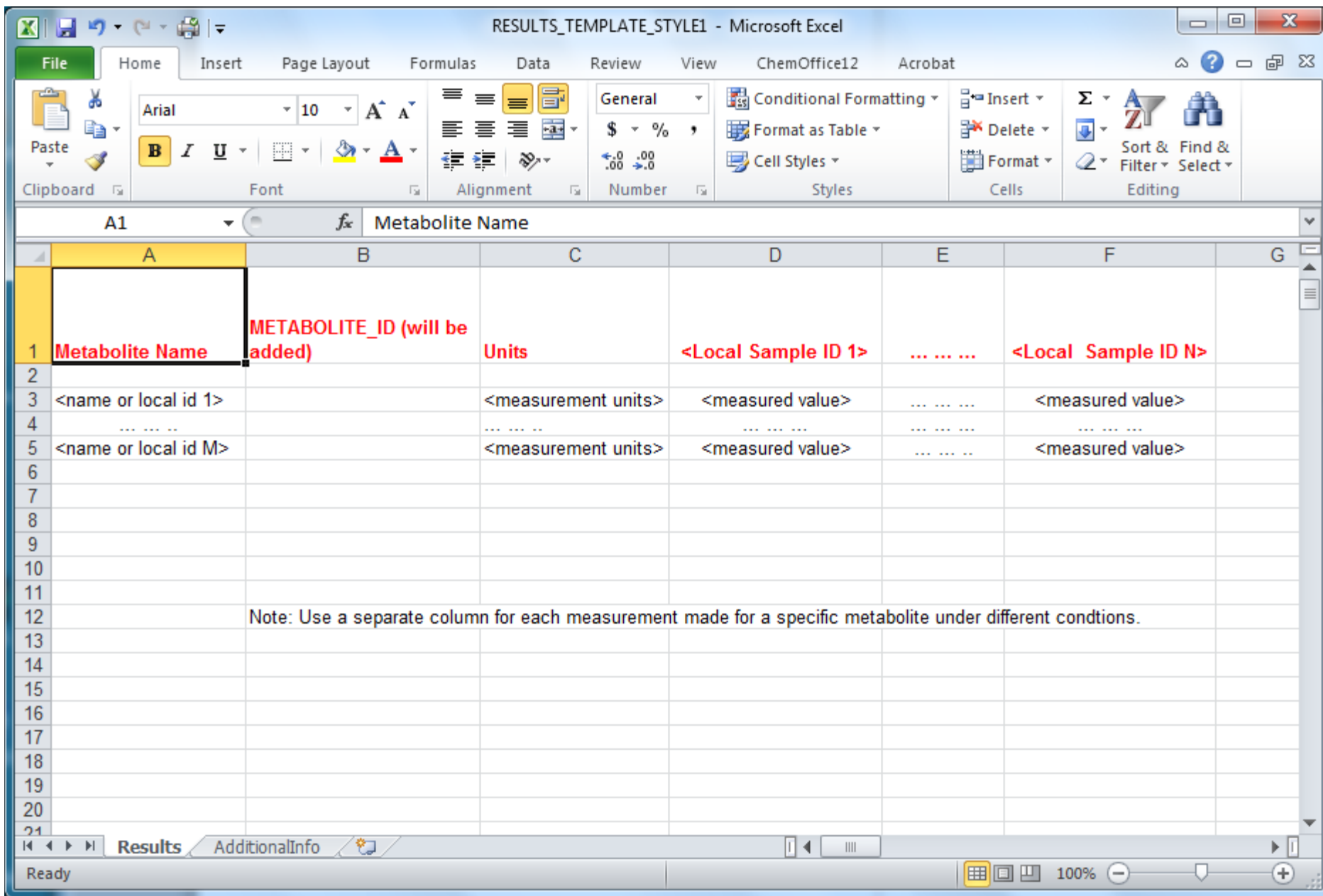
# DRCC results template

- **Results template data description**
- **Filling in results template for data submission**

# DRCC results template

- **Results template data description**
  - Results
  - AdditionalInfo
- Filling in results template for data submission

# DRCC results template: Results data



RESULTS\_TEMPLATE\_STYLE1 - Microsoft Excel

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Clipboard Font Alignment Number Styles Cells Editing

A1 *fx* Metabolite Name

	A	B	C	D	E	F	G	
1	Metabolite Name	METABOLITE_ID (will be added)	Units	<Local Sample ID 1>	... ..	<Local Sample ID N>		
2								
3	<name or local id 1>		<measurement units>	<measured value>	... ..	<measured value>		
4	... ..		... ..	... ..	... ..	... ..		
5	<name or local id M>		<measurement units>	<measured value>	... ..	<measured value>		
6								
7								
8								
9								
10								
11								
12	Note: Use a separate column for each measurement made for a specific metabolite under different conditions.							
13								
14								
15								
16								
17								
18								
19								
20								
21								

Ready Results AdditionalInfo 100%

# DRCC results template: Results data

The screenshot shows a Microsoft Excel window titled "RESULTS\_TEMPLATE - Microsoft Excel". The ribbon includes File, Home, Insert, Page Layout, Formulas, Data, Review, View, ChemOffice12, and Acrobat. The Home ribbon is active, showing options for Clipboard, Font, Alignment, Number, Styles, Cells, and Editing. The active cell is A1, containing the text "Metabolite Name".

	A	B	C	D	E	F	G	H	I
1	<b>Metabolite Name</b>	<b>Retention Index</b>	<b>Moverz Quant</b>	<b>Local ID</b>	<b>PubChem CID</b>	<b>KEGG ID</b>	<b>mass spectrum</b>		
2									
3	<name or local id>	<value>	<value>	<local id>	<pubchem cid>	<kedd id>	<peaks list>		
4									
5									
6									
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23									

The status bar at the bottom shows "Ready", "Results", "AdditionalInfo", and a zoom level of 100%.

# DRCC results template

- Results template data description
- **Filling in results template for data submission**
  - Results
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# Results example: Results data

stemcell\_Results - Microsoft Excel

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Clipboard Font Alignment Number Styles Cells Editing

A2 *fx* Betaine

	A	B	C	D	E	F	G	H	I	J
1	Name	METABOLITE_ID	units	iPSC-T1R1	iPSC-T1R2	iPSC-T1R3	iPSC-T2R1	iPSC-T2R2	iPSC-T2R3	m15-T1
2	Betaine		peak area	144301	146452	159604	54013	55288	50295	1
3	Taurine		peak area	459870	405380	459803	111315	103051	132147	5
4	Creatine		peak area	465781	456427	494302	39520	36568	48141	2
5	Carnitine		peak area	43557	49718	58249	16884	12434	17086	
6	Acetylcarnitine		peak area	23803	25064	28873	10445	13572	13467	
7	Pantothenic Acid		peak area	10585	9483	11310	8283	7752	8117	
8	Butyryl carnitine		peak area	2875	3040	3573	2267	1956	1746	
9	Adenosine		peak area		1607	322	10701	10157	9497	
10	Sphingosine		peak area	32290	24231	33665	30264	28371	25047	
11	lysoPC 14:0		peak area	1771	1438	1827	4500	2501	3434	
12	lysoPE 18:1		peak area	2066	1706	2133	5902	5823	6020	
13	lysoPC 16:1		peak area	2212	2663	3297	14685	8383	11877	
14	lysoPC 16:0		peak area	66055	62401	64752	106424	79105	89241	1
15	lysoPC 18:1		peak area	17191	17167	17290	73596	42590	60631	1
16	lysoPC 18:0		peak area	108693	103626	113683	108808	93930	93300	1
17	SM 32:1		peak area	29929	26473	29008	23607	20798	21648	
18	PE 32:1		peak area	18084	16551	17398	29767	30644	30625	
19	plasmeyl-PE 34:2		peak area	13998	15807	15077	25040	25195	26792	
20	SM 34:2		peak area	84947	79009	86398	71358	62355	62814	
21	plasmeyl PE 34:1		peak area	62490	69667	55648	71131	75987	70332	1

Ready | Results | 100%

# Results example: Results data

The screenshot shows a Microsoft Excel spreadsheet titled "seeds\_mutation\_results". The active cell is A2, containing the formula "2-ketoisocaproic acid". The spreadsheet displays a table with the following data:

	A	B	C	D	E	F	G	H	I	J
1	Name		units	343605	343609	343613	343617	343621	343625	343629
2	2-ketoisocaproic acid		peak area	153	1554	893	1059	1805	918	1418
3	2-hydroxyglutaric acid		peak area	5518	8163	5404	4970	6922	3307	6607
4	1-monostearin		peak area	545	1101	858	744	1118	525	718
5	1,2-anhydro-myo-inositol (put)		peak area	5941	9606	10012	23428	11462	8024	7204
6	xylose		peak area	13468	19504	28291	19315	91419	22487	24187
7	xylonic acid		peak area	6148	9981	9064	7749	10455	4695	8805
8	xylitol		peak area	20873	29632	25817	19862	27565	18829	21129
9	valine		peak area	216359	157090	178972	147961	246664	126174	158174
10	urea		peak area	11308	27529	3005	180	2889	16369	34169
11	tyrosine		peak area	14802	14999	18463	17424	25124	15513	12113
12	tryptophan		peak area	10184	13956	18968	16529	30378	13233	10133
13	trehalose		peak area	46057	37799	27129	27641	71559	28205	28105
14	trans-sinapinic acid		peak area	77860	101703	65309	131854	198955	78734	176734
15	tocopherol		peak area	6273	9185	8484	10132	18895	11558	17158
16	threonine		peak area	610091	785459	571898	433119	776503	519714	681714
17	threonic acid		peak area	345969	392747	289125	275419	439387	206812	148812
18	threitol		peak area	6730	7794	6373	6654	10444	5698	7948
19	sucrose		peak area	628350	525920	469748	256937	687102	330250	593250
20	succinic acid		peak area	166298	462425	278998	571399	660520	256130	496130
21	suband glucose		peak area	12758	8327	51775	6214	7658	22786	67786



# Results example: Additional Info data

seeds\_mutation\_results - Microsoft Excel

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Clipboard Font Alignment Number Styles Cells Editing

A2 fx 2-ketoisocaproic acid

	A	B	C	D	E	F	G	H	I	J	K
1	BinBase Name	ret index	quant mass	BinBase id	mass spectru	PubChem id	KEGG id				
2	2-ketoisocaproic aci	310629	200	213388	85:175.0 86:2	70	C00233				
3	2-hydroxyglutaric ac	506359	129	214409	85:1029.0 86:	43	n/a				
4	1-monostearin	959625	399	202835	85:6330.0 86:	24699	D01947				
5	1,2-anhydro-myo-ino	652000	318	214408	86:1.0 87:16.	119054	n/a				
6	xylose	542808	103	200500	85:565.0 86:8	6027	C00181				
7	xylonic acid	588743	292	208695	85:28.0 86:42	191545	n/a				
8	xylitol	563718	217	199436	85:46.0 86:52	6912	C00379				
9	valine	313224	144	199605	85:48.0 86:13	6287	C00183				
10	urea	328046	171	199594	85:882.0 86:7	1176	C00086				
11	tyrosine	671085	218	199781	86:146.0 89:8	6057	C00082				
12	tryptophan	779834	202	199775	86:27.0 87:27	6305	C00078				
13	trehalose	947837	191	199289	86:85.0 89:25	7427	C01083				
14	trans-sinapinic acid	788461	338	199228	88:1.0 89:471	637775	C00482				
15	tocopherol	1067178	237	199211	85:104.0 87:1	14985	C02477				
16	threonine	409403	117	199626	85:164.0 86:3	6288	C00188				
17	threonic acid	497167	292	199262	86:2.0 89:214	5282933	n/a				
18	threitol	467314	217	202661	85:64.0 87:55	169019	n/a				
19	sucrose	915457	271	202121	85:3981.0 86:	5988	C00089				
20	succinic acid	370518	147	199210	85:668.0 86:5	1110	C00042				
21	suberyl glycine	532293	188	200526	85:10.0 86:34	dioic acid glycine	n/a				
22	stearic acid	787358	117	199195	85:700.0 86:2	5281	C01530				
23	sophorose	953453	319	213152	87:120.0 89:9	441432	C08250				
24	shikimic acid	610984	204	199162	85:1162.0 86:	8742	C00493				

Ready

Results AdditionalInfo 100%

# Results example: Results data

4. PopGen Phenotypic and Normalized Binned Data - Microsoft Excel

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Clipboard Font Alignment Number Styles Cells Editing

A2 fx 5002\_0

	A	B	C	D	E	F	G	H	I	J
1	Sample ID	response to vaccination	gender	ethnicity	sample day	8.98	8.94	8.9	8.86	8.82
2	5002_0	low	male	hindu	0	-0.000063414	0.00010495	0.00018693	6.3373E-06	-0.000055306
3	5002_28	low	male	hindu	28	0.00001523	-0.000066187	-8.6966E-06	0.000014346	0.00025868
4	5065_0	low	male	hindu	0	-0.00001319	0.000072065	-0.000093369	0.000024221	0.00013183
5	5065_28	low	male	hindu	28	0.00011576	0.000029281	0.000016109	0.000029304	7.4869E-06
6	5070_0	high	female	hindu	0	-0.00028604	0.000075442	-0.000055027	-0.00016921	0.000034071
7	5070_28	high	female	hindu	28	0.00025546	0.000019766	0.000048745	0.000064593	-0.000014044
8	5089_0	high	female	hindu	0	-0.00013923	0.000010944	-0.000051583	-0.00012424	0.000022118
9	5089_28	high	female	hindu	28	-0.000076447	0.000018809	0.000033232	-8.0696E-06	0.000017087
10	5116_0	low	female	hindu	0	0.000045678	0.000073045	0.000056478	0.000086987	0.000089932
11	5116_28	low	female	hindu	28	-0.00011036	0.000093793	0.000039998	0.000011666	0.000050322
12	5124_0	low	female	hindu	0	-0.000011918	0.000047765	-4.1885E-06	0.000046208	0.000046096
13	5124_28	low	female	hindu	28	8.5185E-06	-0.000054427	0.00001034	-0.000012166	-0.000036294
14	5125_0	low	female	hindu	0	0.00016302	0.000099191	-5.4753E-06	0.00017272	7.4711E-06
15	5125_28	low	female	hindu	28	-0.000084807	0.00018861	0.000070657	5.4584E-06	0.000023563
16	5169_0	high	female	hindu	0	0.000090153	-0.000011298	0.00012638	-7.3946E-06	0.00013986
17	5169_28	high	female	hindu	28	-0.00021316	0.000058087	0.000054355	-0.00019528	-0.00020966
18	5184_0	low	female	hindu	0	0.000036514	-6.4931E-06	0.000010303	-0.000017828	9.5388E-06
19	5184_28	low	female	hindu	28	0.000045938	0.000028927	-0.000038203	-0.000037383	4.7235E-06
20	5195_0	high	female	hindu	0	0.00019587	-0.000059408	0.00008121	0.00014678	-0.00013963
21	5195_28	high	female	hindu	28	-0.000076111	-0.000097127	-0.000085462	-0.00026909	-0.000081732
22	5201_0	low	female	muslim	0	0.000053363	0.00012571	-0.000030238	0.000088402	-0.000011188
23	5201_28	low	female	muslim	28	0.000025464	-0.000086299	0.00012621	0.00023995	5.0463E-07

BinningResults

Ready 100%

**The End**