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Supporting information for article:

***Oscail*, a program package for small-molecule single-crystal crystallography with crystal morphology prediction and molecular modelling**

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Appendix A. Centroid distance matrix analysis for CSD code VUKRAW

Centroid Distance Matrix Calculation for VUKRAW

CELL 5.229 8.631 25.776 90.00 90.00 90.00

Cen - Cen Max. 5.30

Plane Slip Max. 1.50

down a

CMIN 5.23

	1	2	3	4	5	6	7	8
1	10.00	13.11	9.76	20.90	5.23	14.68	12.90	22.17
2	13.11	10.00	6.32	8.89	13.53	5.23	9.73	10.83
3	9.76	6.32	10.00	14.65	8.89	6.32	5.23	15.02
4	20.90	8.89	14.65	10.00	20.90	9.76	16.07	5.23
5	5.23	13.53	8.89	20.90	10.00	13.11	9.76	20.90
6	14.68	5.23	6.32	9.76	13.11	10.00	6.32	8.89
7	12.90	9.73	5.23	16.07	9.76	6.32	10.00	14.65
8	22.17	10.83	15.02	5.23	20.90	8.89	14.65	10.00

< 5.30 Angst

	1	2	3	4	5	6	7	8
1	0	0	0	0	1	0	0	0
2	0	0	0	0	0	1	0	0
3	0	0	0	0	0	0	1	0
4	0	0	0	0	0	0	0	1
5	1	0	0	0	0	0	0	0
6	0	1	0	0	0	0	0	0
7	0	0	1	0	0	0	0	0
8	0	0	0	1	0	0	0	0

1	5 Atoms < vdW sum + 1.0	17	60.71%
2	6 Atoms < vdW sum + 1.0	12	42.86%
3	7 Atoms < vdW sum + 1.0	12	42.86%
4	8 Atoms < vdW sum + 1.0	17	60.71%
5	1 Atoms < vdW sum + 1.0	12	42.86%
6	2 Atoms < vdW sum + 1.0	17	60.71%
7	3 Atoms < vdW sum + 1.0	17	60.71%
8	4 Atoms < vdW sum + 1.0	12	42.86%

Mean % 51.79%

1 1 1 1 1 1 1 1

Stacking Contacts 1s & 2s

8

0

down b


```

8  0  0  0  0  0  0  0  0
   0  0  0  0  0  0  0  0

```

Appendix B. Reduced cell cluster analysis of CSD codes starting with SUTHAZ

Total number of unique cell types 5

5 Clusters Match > 0.70

Cluster no. 1 7 files

1 suthaz01.ins	0.959
7 suthaz07.ins	0.959
8 suthaz08.ins	0.981
15 suthaz16.ins	0.962
23 suthaz28.ins	0.994
24 suthaz29.ins	0.958
34 suthaz43.ins	0.958

Cluster no. 2 8 files

2 suthaz02.ins	0.974
11 suthaz11.ins	0.974
12 suthaz12.ins	0.995
16 suthaz17.ins	0.977
20 suthaz25.ins	0.993
28 suthaz33.ins	0.972
29 suthaz34.ins	0.972
30 suthaz35.ins	0.972

Cluster no. 3 8 files

3 suthaz03.ins	0.967
9 suthaz09.ins	0.967
10 suthaz10.ins	0.999
17 suthaz18.ins	0.971
19 suthaz24.ins	0.997
25 suthaz30.ins	0.967
26 suthaz31.ins	0.967
27 suthaz32.ins	0.967

Cluster no. 4 8 files

4 suthaz04.ins	0.985
13 suthaz13.ins	0.985
14 suthaz14.ins	0.995
18 suthaz19.ins	0.969
21 suthaz26.ins	0.995
31 suthaz36.ins	0.975

32	suthaz37.ins		0.975
33	suthaz38.ins		0.975
	Cluster no.	5	3 files
5	suthaz05.ins		0.979
6	suthaz06.ins		0.979
22	suthaz27.ins		0.984

All in cluster(s)

- 1 suthaz01.ins
- 2 suthaz02.ins
- 3 suthaz03.ins
- 4 suthaz04.ins
- 5 suthaz05.ins
- 6 suthaz06.ins
- 7 suthaz07.ins
- 8 suthaz08.ins
- 9 suthaz09.ins
- 10 suthaz10.ins
- 11 suthaz11.ins
- 12 suthaz12.ins
- 13 suthaz13.ins
- 14 suthaz14.ins
- 15 suthaz16.ins
- 16 suthaz17.ins
- 17 suthaz18.ins
- 18 suthaz19.ins
- 19 suthaz24.ins
- 20 suthaz25.ins
- 21 suthaz26.ins
- 22 suthaz27.ins
- 23 suthaz28.ins
- 24 suthaz29.ins
- 25 suthaz30.ins
- 26 suthaz31.ins
- 27 suthaz32.ins
- 28 suthaz33.ins
- 29 suthaz34.ins
- 30 suthaz35.ins
- 31 suthaz36.ins
- 32 suthaz37.ins

33 suthaz38.ins

34 suthaz43.ins

Current CELLS

1	10.5540	13.2200	17.0500	90.000	108.060	90.000
2	17.5700	8.5740	15.5830	90.000	112.930	90.000
3	8.2390	15.5560	8.5920	90.000	90.000	86.340
4	10.8670	11.4560	8.5430	90.000	90.000	91.870
5	10.3990	15.1320	14.2800	90.000	91.210	90.000
6	14.3300	15.2730	10.4430	90.000	91.050	90.000
7	10.5010	12.9600	17.1760	90.000	107.650	90.000
8	10.5340	13.3880	17.0000	90.000	107.940	90.000
9	8.1900	8.5320	15.4470	90.000	94.140	90.000
10	8.2390	8.5950	15.5570	90.000	93.690	90.000
11	15.5040	8.4940	17.4270	90.000	112.760	90.000
12	15.6020	8.5620	17.6010	90.000	112.950	90.000
13	10.8200	8.4940	11.4030	90.000	91.860	90.000
14	10.8790	8.5500	11.4560	90.000	91.970	90.000
15	10.5340	12.9360	17.1910	90.000	107.770	90.000
16	17.4480	8.4980	15.5110	90.000	112.810	90.000
17	8.1930	8.5380	15.4370	90.000	94.010	90.000
18	10.7740	8.4670	11.3670	90.000	91.650	90.000
19	8.2310	8.5860	15.5490	90.000	93.690	90.000
20	17.5910	8.5440	15.5940	90.000	113.020	90.000
21	10.8600	8.5350	11.4390	90.000	91.940	90.000
22	10.4130	15.2430	14.3120	90.000	91.040	90.000
23	10.5300	13.1930	17.0400	90.000	107.960	90.000
24	10.5240	12.9020	17.2180	90.000	107.830	90.000
25	8.1900	8.5350	15.4500	90.000	94.150	90.000
26	8.1900	8.5350	15.4500	90.000	94.150	90.000
27	8.1900	8.5350	15.4500	90.000	94.150	90.000
28	17.4170	8.4910	15.4950	90.000	112.760	90.000
29	17.4170	8.4910	15.4950	90.000	112.760	90.000
30	17.4170	8.4910	15.4950	90.000	112.760	90.000
31	10.7890	8.4840	11.3980	90.000	91.640	90.000
32	10.7890	8.4840	11.3980	90.000	91.640	90.000
33	10.7890	8.4840	11.3980	90.000	91.640	90.000
34	10.5240	12.9020	17.2180	90.000	107.830	90.000

Niggli CELLS

1	10.5540	13.2200	17.0450	90.000	108.004	90.000
2	8.5740	15.5830	17.5700	112.930	90.000	90.000

3	8.2390	8.5920	15.5560	90.000	93.660	90.000
4	8.5430	10.8670	11.4560	91.870	90.000	90.000
5	10.3990	14.2800	15.1320	90.000	90.000	91.210
6	10.4430	14.3300	15.2730	90.000	90.000	91.050
7	10.5010	12.9600	17.1760	90.000	107.650	90.000
8	10.5340	13.3880	17.0000	90.000	107.940	90.000
9	8.1900	8.5320	15.4470	90.000	94.140	90.000
10	8.2390	8.5950	15.5570	90.000	93.690	90.000
11	8.4940	15.5040	17.4270	112.760	90.000	90.000
12	8.5620	15.6020	17.6010	112.950	90.000	90.000
13	8.4940	10.8200	11.4030	91.860	90.000	90.000
14	8.5500	10.8790	11.4560	91.970	90.000	90.000
15	10.5340	12.9360	17.1910	90.000	107.770	90.000
16	8.4980	15.5110	17.4480	112.810	90.000	90.000
17	8.1930	8.5380	15.4370	90.000	94.010	90.000
18	8.4670	10.7740	11.3670	91.650	90.000	90.000
19	8.2310	8.5860	15.5490	90.000	93.690	90.000
20	8.5440	15.5940	17.5910	113.020	90.000	90.000
21	8.5350	10.8600	11.4390	91.940	90.000	90.000
22	10.4130	14.3120	15.2430	90.000	90.000	91.040
23	10.5300	13.1930	17.0400	90.000	107.960	90.000
24	10.5240	12.9020	17.2110	90.000	107.765	90.000
25	8.1900	8.5350	15.4500	90.000	94.150	90.000
26	8.1900	8.5350	15.4500	90.000	94.150	90.000
27	8.1900	8.5350	15.4500	90.000	94.150	90.000
28	8.4910	15.4950	17.4170	112.760	90.000	90.000
29	8.4910	15.4950	17.4170	112.760	90.000	90.000
30	8.4910	15.4950	17.4170	112.760	90.000	90.000
31	8.4840	10.7890	11.3980	91.640	90.000	90.000
32	8.4840	10.7890	11.3980	91.640	90.000	90.000
33	8.4840	10.7890	11.3980	91.640	90.000	90.000
34	10.5240	12.9020	17.2110	90.000	107.765	90.000

Top Matches NIGGLI

	Match	File 1	File 2	Space Groups
24	34	1.00 SGm suthaz29.ins	suthaz43.ins	P21/c P21/c
25	26	1.00 SGm suthaz30.ins	suthaz31.ins	P21/c P21/c
25	27	1.00 SGm suthaz30.ins	suthaz32.ins	P21/c P21/c
26	27	1.00 SGm suthaz31.ins	suthaz32.ins	P21/c P21/c
28	29	1.00 SGm suthaz33.ins	suthaz34.ins	P21/c P21/c
28	30	1.00 SGm suthaz33.ins	suthaz35.ins	P21/c P21/c
29	30	1.00 SGm suthaz34.ins	suthaz35.ins	P21/c P21/c
31	32	1.00 SGm suthaz36.ins	suthaz37.ins	P21/n P21/n

31	33	1.00	SGm	suthaz36.ins	suthaz38.ins	P21/n	P21/n
32	33	1.00	SGm	suthaz37.ins	suthaz38.ins	P21/n	P21/n
9	25	1.00	SGm	suthaz09.ins	suthaz30.ins	P21/c	P21/c
9	26	1.00	SGm	suthaz09.ins	suthaz31.ins	P21/c	P21/c
9	27	1.00	SGm	suthaz09.ins	suthaz32.ins	P21/c	P21/c
3	10	1.00		suthaz03.ins	suthaz10.ins	P1121/b	P21/c
11	28	1.00		suthaz11.ins	suthaz33.ins	P21/a	P21/c
11	29	1.00		suthaz11.ins	suthaz34.ins	P21/a	P21/c
11	30	1.00		suthaz11.ins	suthaz35.ins	P21/a	P21/c
10	19	1.00	SGm	suthaz10.ins	suthaz24.ins	P21/c	P21/c
3	19	1.00		suthaz03.ins	suthaz24.ins	P1121/b	P21/c
11	16	1.00		suthaz11.ins	suthaz17.ins	P21/a	P21/c
4	14	1.00		suthaz04.ins	suthaz14.ins	P1121/n	P21/n
12	20	1.00		suthaz12.ins	suthaz25.ins	P21/a	P21/c
16	28	1.00	SGm	suthaz17.ins	suthaz33.ins	P21/c	P21/c
16	29	1.00	SGm	suthaz17.ins	suthaz34.ins	P21/c	P21/c
16	30	1.00	SGm	suthaz17.ins	suthaz35.ins	P21/c	P21/c
2	12	1.00		suthaz02.ins	suthaz12.ins	P21/c	P21/a
15	24	1.00	SGm	suthaz16.ins	suthaz29.ins	P21/c	P21/c
15	34	1.00	SGm	suthaz16.ins	suthaz43.ins	P21/c	P21/c
4	21	1.00		suthaz04.ins	suthaz26.ins	P1121/n	P21/n
9	17	0.99	SGm	suthaz09.ins	suthaz18.ins	P21/c	P21/c
17	25	0.99	SGm	suthaz18.ins	suthaz30.ins	P21/c	P21/c
17	26	0.99	SGm	suthaz18.ins	suthaz31.ins	P21/c	P21/c
17	27	0.99	SGm	suthaz18.ins	suthaz32.ins	P21/c	P21/c
1	23	0.99		suthaz01.ins	suthaz28.ins	P21/c	P21/n
14	21	0.99	SGm	suthaz14.ins	suthaz26.ins	P21/n	P21/n
6	22	0.99	SGm	suthaz06.ins	suthaz27.ins	P21/n	P21/n
18	31	0.99	SGm	suthaz19.ins	suthaz36.ins	P21/n	P21/n
18	32	0.99	SGm	suthaz19.ins	suthaz37.ins	P21/n	P21/n
18	33	0.99	SGm	suthaz19.ins	suthaz38.ins	P21/n	P21/n
2	20	0.99	SGm	suthaz02.ins	suthaz25.ins	P21/c	P21/c
7	15	0.99	SGm	suthaz07.ins	suthaz16.ins	P21/c	P21/c
13	31	0.99	SGm	suthaz13.ins	suthaz36.ins	P21/n	P21/n
13	32	0.99	SGm	suthaz13.ins	suthaz37.ins	P21/n	P21/n
13	33	0.99	SGm	suthaz13.ins	suthaz38.ins	P21/n	P21/n
7	24	0.99	SGm	suthaz07.ins	suthaz29.ins	P21/c	P21/c
7	34	0.99	SGm	suthaz07.ins	suthaz43.ins	P21/c	P21/c
13	21	0.99	SGm	suthaz13.ins	suthaz26.ins	P21/n	P21/n
4	13	0.99		suthaz04.ins	suthaz13.ins	P1121/n	P21/n
5	22	0.98	SGm	suthaz05.ins	suthaz27.ins	P21/n	P21/n
13	18	0.98	SGm	suthaz13.ins	suthaz19.ins	P21/n	P21/n

8	23	0.98		suthaz08.ins	suthaz28.ins	P21/c	P21/n
1	8	0.98	SGm	suthaz01.ins	suthaz08.ins	P21/c	P21/c
13	14	0.98	SGm	suthaz13.ins	suthaz14.ins	P21/n	P21/n
5	6	0.98	SGm	suthaz05.ins	suthaz06.ins	P21/n	P21/n
2	16	0.98	SGm	suthaz02.ins	suthaz17.ins	P21/c	P21/c
16	20	0.98	SGm	suthaz17.ins	suthaz25.ins	P21/c	P21/c
21	31	0.98	SGm	suthaz26.ins	suthaz36.ins	P21/n	P21/n
21	32	0.98	SGm	suthaz26.ins	suthaz37.ins	P21/n	P21/n
21	33	0.98	SGm	suthaz26.ins	suthaz38.ins	P21/n	P21/n
12	16	0.97		suthaz12.ins	suthaz17.ins	P21/a	P21/c
4	31	0.97		suthaz04.ins	suthaz36.ins	P1121/n	P21/n
4	32	0.97		suthaz04.ins	suthaz37.ins	P1121/n	P21/n
4	33	0.97		suthaz04.ins	suthaz38.ins	P1121/n	P21/n
17	19	0.97	SGm	suthaz18.ins	suthaz24.ins	P21/c	P21/c
2	11	0.97		suthaz02.ins	suthaz11.ins	P21/c	P21/a
11	20	0.97		suthaz11.ins	suthaz25.ins	P21/a	P21/c
2	28	0.97	SGm	suthaz02.ins	suthaz33.ins	P21/c	P21/c
2	29	0.97	SGm	suthaz02.ins	suthaz34.ins	P21/c	P21/c
2	30	0.97	SGm	suthaz02.ins	suthaz35.ins	P21/c	P21/c
20	28	0.97	SGm	suthaz25.ins	suthaz33.ins	P21/c	P21/c
20	29	0.97	SGm	suthaz25.ins	suthaz34.ins	P21/c	P21/c
20	30	0.97	SGm	suthaz25.ins	suthaz35.ins	P21/c	P21/c
11	12	0.97	SGm	suthaz11.ins	suthaz12.ins	P21/a	P21/a
10	17	0.97	SGm	suthaz10.ins	suthaz18.ins	P21/c	P21/c
3	17	0.97		suthaz03.ins	suthaz18.ins	P1121/b	P21/c
19	25	0.97	SGm	suthaz24.ins	suthaz30.ins	P21/c	P21/c
19	26	0.97	SGm	suthaz24.ins	suthaz31.ins	P21/c	P21/c
19	27	0.97	SGm	suthaz24.ins	suthaz32.ins	P21/c	P21/c
9	19	0.97	SGm	suthaz09.ins	suthaz24.ins	P21/c	P21/c
12	28	0.97		suthaz12.ins	suthaz33.ins	P21/a	P21/c
12	29	0.97		suthaz12.ins	suthaz34.ins	P21/a	P21/c
12	30	0.97		suthaz12.ins	suthaz35.ins	P21/a	P21/c
14	31	0.97	SGm	suthaz14.ins	suthaz36.ins	P21/n	P21/n
14	32	0.97	SGm	suthaz14.ins	suthaz37.ins	P21/n	P21/n
14	33	0.97	SGm	suthaz14.ins	suthaz38.ins	P21/n	P21/n
18	21	0.97	SGm	suthaz19.ins	suthaz26.ins	P21/n	P21/n
4	18	0.97		suthaz04.ins	suthaz19.ins	P1121/n	P21/n
10	25	0.97	SGm	suthaz10.ins	suthaz30.ins	P21/c	P21/c
10	26	0.97	SGm	suthaz10.ins	suthaz31.ins	P21/c	P21/c
10	27	0.97	SGm	suthaz10.ins	suthaz32.ins	P21/c	P21/c
9	10	0.97	SGm	suthaz09.ins	suthaz10.ins	P21/c	P21/c
3	25	0.97		suthaz03.ins	suthaz30.ins	P1121/b	P21/c

3	26	0.97	suthaz03.ins	suthaz31.ins	P1121/b	P21/c
3	27	0.97	suthaz03.ins	suthaz32.ins	P1121/b	P21/c
3	9	0.97	suthaz03.ins	suthaz09.ins	P1121/b	P21/c
15	23	0.97	suthaz16.ins	suthaz28.ins	P21/c	P21/n
7	23	0.96	suthaz07.ins	suthaz28.ins	P21/c	P21/n
14	18	0.96	SGm suthaz14.ins	suthaz19.ins	P21/n	P21/n
23	24	0.96	suthaz28.ins	suthaz29.ins	P21/n	P21/c
23	34	0.96	suthaz28.ins	suthaz43.ins	P21/n	P21/c

Minimum in Class Match 0.958 Maximum Out of Class Match 0.000

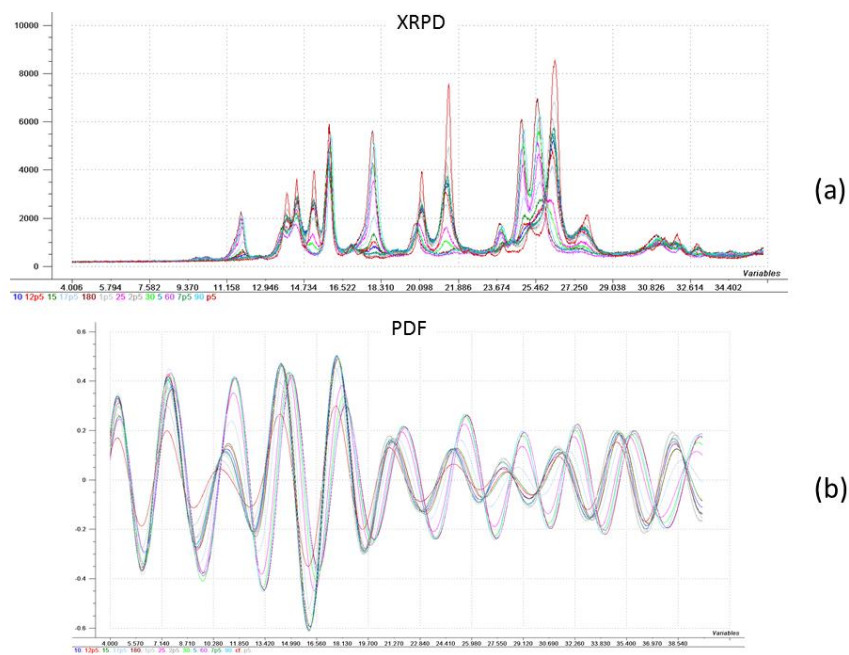


Figure S1 XRPD and PDF transform of room temperature ball milling of mefenamic acid.