Table S-4. Search A, 2-pyrrolidone and derivatives

Query	Refcode	C=O, Å	C-N, Å	C=O + C-N	Space Gp	Z	Z'	T
	ALODIP	1.223	1.342	2.565	P-1	2	1	29 5
1	AWUWOE	1.234	1.331	2.565	C2/c	8	1	29 3
1	BEYZAG	1.206	1.335	2.541	P21/c	4	1	29 5
1	BICDEW	1.244	1.336	2.58	C2/c	8	1	29 5
1	BICDIA	1.233	1.341	2.574	P21/c	4	1	29 5
1	BIXPUU	1.233	1.339	2.572	P21/c	8	2	29 3
1	BIXPUU	1.235	1.339	2.574	P21/c	8	2	29 3
	BOZZEW	1.223	1.331	2.554	C2/c	8	1	29 2
	BOZZIA	1.23	1.338	2.568	P-1	2	1	29 2
	BOZZOG	1.234	1.332	2.566	P-1	4	2	29 2
	BOZZOG	1.241	1.33	2.571	P-1	4	2	29 2
1	CAXKIV	1.241	1.322	2.563	P-1	4	2	29 5
1	CUQPIN	1.225	1.336	2.561	P21/c	4	1	29 5
1	DSZNDO10	1.238	1.329	2.567	C2/c	4	0.5	29 5
1	DXSEPO	1.235	1.33	2.565	Pbca	8	1	29 5
	DUBSOJ	1.242	1.339	2.581	P21/n	4	1	15 0
	DUBTOK	1.243	1.334	2.577	C2/c	8	1	15 0
	EHUBIT	1.231	1.333	2.564	P21/n	4	1	29 3
1	EZURUM	1.232	1.35	2.582	P21/c	4	1	17 3
1	EZUSAT	1.235	1.331	2.566	Pbca	8	1	12 3
1	GASSUP	1.256	1.355	2.611	P-1	2	1	15 0
1	GASTIE	1.234	1.343	2.577	P21/c	4	1	12 3
1	HIXMEH	1.235	1.336	2.571	P21/c	4	1	29 8
1	HIXQUA	1.231	1.343	2.574	P-1	2	1	18 3
1	HOMFIY	1.233	1.346	2.579	P-1	4	2	29 5
	HUKDIB	1.232	1.349	2.581	P21/c	4	1	15 5
	IRIPUV	1.232	1.346	2.578	P21/a	4	1	29 3
	IRIQAC	1.232	1.349	2.581	Pbca	8	1	29 3
	IROMIM	1.23	1.33	2.56	I2/a	16	2	17 3
	IROMIM	1.237	1.328	2.565	I2/a	16	2	17 3
1	JAFCOI	1.23	1.331	2.561	P21/n	4	1	29 5
1	JAFKAD	1.233	1.338	2.571	P-1	4	2	29 3

1	JAFKAD	1.233	1.337	2.57	P-1	4	2	29 3
1	LESJOJ	1.234	1.355	2.589	P21/n	4	1	10 0
1	MIXSIV	1.243	1.336	2.579	C2/c	8	1	19 0
1	MIXSOB	1.241	1.331	2.572	P21/c	4	1	19 0
1	MIZDAB	1.223	1.34	2.563	P-1	2	1	17 3
	NACMUB	1.232	1.34	2.572	P21/n	4	1	17 3
1	NAMWII	1.215	1.33	2.545	P-1	4	2	29 5
1	NAMWII	1.219	1.336	2.555	P-1	4	2	29 5
1	NEJTAY	1.232	1.346	2.578	P-1	2	1	16 3
1	NILYAI	1.237	1.335	2.572	P-1	2	1	17 3
	PUBJOM	1.245	1.324	2.569	P21/n	2	0.5	29 4
1	RAWZIZ	1.229	1.324	2.553	P21/n	4	1	19 3
1	RAZWOF	1.219	1.325	2.544	P-1	2	1	21 8
1	REDCAF	1.236	1.328	2.564	P21/a	4	1	29 8
1	RENTIN	1.223	1.343	2.566	P-1	2	1	29 5
1	RENTIN01	1.224	1.342	2.566	P-1	2	1	29 5
1	SANXOU	1.234	1.341	2.575	P21/n	4	1	29 5
1	SINXUI	1.232	1.329	2.561	C2/c	8	1	29 5
	UGIKOL	1.229	1.343	2.572	P21/n	4	1	29 6
	UNECAS	1.235	1.349	2.584	P21/n	4	1	17 3
1	VAXYOJ	1.223	1.344	2.567	P21/c	4	1	11 5
1	VUJVEB	1.227	1.331	2.558	P21/n	4	1	29 5
1	WEVLOY	1.227	1.344	2.571	P21/n	4	1	20 1
1	WOHRER	1.23	1.349	2.579	P21/n	4	1	15 0
1	ZIGQIO	1.242	1.336	2.578	P-1	2	1	29 5
1	ZIKXIA	1.237	1.338	2.575	P-1	2	1	29 5
1	YOPYAE	1.232	1.348	2.58	P21/n	4	1	20 0
1	AHCDLA	1.231	1.346	2.577	C2/c	8	1	29 5
	APAROZ	1.243	1.331	2.574	P21	2	1	29 4
	APAROZ	1.224	1.345	2.569	P21	2	1	29 4
1	AZPNOD	1.231	1.341	2.572	P21/21	4	1	29 5
1	AZPNOD	1.227	1.342	2.569	P21/21	4	1	29 5
1	BEWQAV01	1.222	1.35	2.572	P21/21	4	1	21 3
1	BIPVAX	1.219	1.327	2.546	P21	2	1	29 5

1	BIXQAB	1.228	1.333	2.561	Pbca	8	1	293
	BUHKIZ	1.218	1.34	2.558	P21	2	1	100
1	BURVUF	1.239	1.341	2.58	P2121 21	4	1	295
	BUWWAS	1.228	1.345	2.573	P21	2	1	150
1	CADBOY	1.221	1.338	2.559	P21/c	4	1	295
1	CAXKIV	1.231	1.324	2.555	P-1	4	2	295
1	CAZKUJ	1.22	1.351	2.571	P2121 21	4	1	295
1	CENBUT	1.229	1.346	2.575	P21/c	4	1	150
1	CIZMAA	1.228	1.347	2.575	P2121 21	4	1	130
1	COQSUX	1.226	1.339	2.565	P4121 2	8	1	100
	CUHMUO	1.228	1.339	2.567	P21	2	1	295
1	CYTOCH 10	1.232	1.328	2.56	P21	2	1	295
1	DICXET	1.228	1.334	2.562	P2121 21	4	1	293
1	DMAZNO	1.238	1.324	2.562	P21	2	1	295
1	DOGPAQ	1.244	1.324	2.568	Pn	2	1	295
1	DOGPAQ	1.234	1.342	2.576	Pn	2	1	295
1	DOGQAR	1.226	1.337	2.563	P21/c	4	1	295
1	DOGQAR	1.228	1.328	2.556	P21/c	4	1	295
	DUBTEA	1.239	1.338	2.577	P21/c	4	1	150
	DUBVAY	1.239	1.341	2.58	C2/c	8	1	150
	DUDMIZ	1.244	1.329	2.573	P21/c	4	1	150
1	DZSNON	1.228	1.327	2.555	P21/c	4	1	295
1	DZSNON	1.235	1.333	2.568	P21/c	4	1	295
1	ECOMAL	1.224	1.325	2.549	P2121 21	4	1	296
1	EYAZAF	1.23	1.341	2.571	P2121 21	4	1	293
1	FARYEC	1.237	1.332	2.569	P21	2	1	295
1	FEGSEP	1.25	1.314	2.564	Pbc21	4	1	295
1	FIHHEJ	1.217	1.346	2.563	P2121 21	4	1	295
1	FIJXOL	1.223	1.327	2.55	P21	4	2	295
1	FIJXOL	1.217	1.334	2.551	P21	4	2	295
1	FUVRUJ	1.22	1.359	2.579	P21/c	4	1	295
1	GASTEA	1.241	1.326	2.567	P21/c	4	1	150
1	GECKOO	1.228	1.317	2.545	P2121 21	4	1	295
1	GIBRAK	1.228	1.325	2.553	C2	4	1	295

					P2121			29
1	GIRFAP	1.232	1.336	2.568	21	4	1	3
	GIRSAB1							29
1	0	1.244	1.358	2.602	P21/c	4	1	5
					P2121			18
1	GUDSIH	1.244	1.336	2.58	21	4	1	0
					P2121			18
1	GUDSON	1.232	1.324	2.556	21	4	1	0
					P2121			20
	GUGHOG	1.216	1.329	2.545	21	4	1	8
								13
1	HACFUM	1.24	1.335	2.575	Pca21	8	2	3
								13
1	HACFUM	1.242	1.342	2.584	Pca21	8	2	3
								12
1	HACGAT	1.237	1.334	2.571	Pbc21	8	2	3
								12
1	HACGAT	1.242	1.329	2.571	Pbc21	8	2	3
								29
1	HAMCHC	1.247	1.336	2.583	P21/c	4	1	5
					P2121			29
1	HERKIZ	1.232	1.335	2.567	21	4	1	8
								29
1	HOMFIY	1.232	1.339	2.571	P-1	4	2	5
					P2121	1		21
1	HOVBUP	1.245	1.336	2.581	21	6	4	3
					P2121	1		21
1	HOVBUP	1.251	1.336	2.587	21	6	4	3
					P2121	1		21
1	HOVBUP	1.233	1.334	2.567	21	6	4	3
					P2121	1		21
1	HOVBUP	1.235	1.353	2.588	21	6	4	3
								16
	HUKDOH	1.246	1.334	2.58	Pbca	8	1	3
					P2121			29
1	IMPYRO	1.24	1.353	2.593	21	4	1	5
								29
1	JAFCIC	1.222	1.334	2.556	P21	2	1	5
					P2121			29
1	JAMJEM	1.226	1.334	2.56	21	4	1	5
								29
1	JOCVUT	1.222	1.332	2.554	C2/c	8	1	5
								16
1	KAFNEK	1.241	1.329	2.57	Pna21	4	1	3
					P2121			16
1	KAFNIO	1.239	1.334	2.573	21	8	2	3
					P2121			16
1	KAFNIO	1.243	1.329	2.572	21	8	2	3
					P2121			29
1	KAQNOF	1.238	1.338	2.576	21	8	2	5
					P2121			29
1	KAQNOF	1.231	1.324	2.555	21	8	2	5
								18
1	LANDUZ	1.238	1.331	2.569	P21	2	1	0
					P4121	1		10
1	LICTAT	1.236	1.338	2.574	2	6	2	0
					P4121	1		10
1	LICTAT	1.224	1.352	2.576	2	6	2	0
								10
1	LIWFIH	1.229	1.348	2.577	Pca21	4	1	0
					P2121			29
1	LIZDAA	1.212	1.34	2.552	21	4	1	5
					P2121			29
1	LPGHUR	1.218	1.332	2.55	21	4	1	5
					P2121	1		29
1	LPYGLU	1.24	1.341	2.581	21	2	3	5
					P2121	1		29
1	LPYGLU	1.238	1.335	2.573	21	2	3	5

					P2121	1		29
1	LPYGLU	1.233	1.338	2.571	21	2	3	5
								29
1	MALREX	1.213	1.351	2.564	Pbca	8	1	3
								29
1	MEJPIA	1.226	1.346	2.572	P43	8	2	5
								29
1	MEJPIA	1.228	1.329	2.557	P43	8	2	5
					P2121			29
	NAZLEG	1.235	1.332	2.567	21	8	2	5
					P2121			29
	NAZLEG	1.242	1.331	2.573	21	8	2	5
					P2121			21
1	NODMUP	1.23	1.356	2.586	21	4	1	3
								19
1	ODIBOT	1.231	1.344	2.575	P21	4	2	0
								19
1	ODIBOT	1.239	1.343	2.582	P21	4	2	0
					P2121			17
	OMANOG	1.231	1.347	2.578	21	4	1	3
								10
	OQAWOT	1.241	1.316	2.557	C2	4	1	0
								15
1	PELDIU	1.235	1.347	2.582	P21	4	2	0
								15
1	PELDIU	1.233	1.347	2.58	P21	4	2	0
					P2121			29
1	PEZHUX	1.24	1.34	2.58	21	4	1	5
	PGTAPA1							29
1	0	1.233	1.331	2.564	P21	4	2	5
	PGTAPA1							29
1	0	1.234	1.326	2.56	P21	4	2	5
	PYRGLU0							29
1	1	1.243	1.331	2.574	P21/a	4	1	5
								19
1	RAWZOF	1.225	1.315	2.54	P-1	4	2	3
								19
1	RAWZOF	1.226	1.317	2.543	P-1	4	2	3
								17
1	RENSUY	1.218	1.336	2.554	P21/c	4	1	3
					P2121			29
1	RUVZEN	1.231	1.334	2.565	21	4	1	5
					P2121			30
1	SAHDUB	1.22	1.325	2.545	21	4	1	1
					P2121			29
1	SHFRAP	1.234	1.321	2.555	21	4	1	5
					P2121			29
1	SHFSAP	1.21	1.35	2.56	21	4	1	5
								29
1	SINYAP	1.227	1.333	2.56	Pbcn	8	1	5
								29
1	SIZMAP	1.241	1.332	2.573	P21/a	4	1	5
								10
1	SOCBOC	1.225	1.354	2.579	P21	2	1	0
					P2121			10
1	SOCCAP	1.236	1.323	2.559	2	8	2	0
					P2121			10
1	SOCCAP	1.237	1.325	2.562	2	8	2	0
								29
1	TADPIY	1.227	1.331	2.558	Pbca	8	1	3
								12
	TADVAX	1.236	1.339	2.575	C2/c	8	1	3
								29
1	TANBIT	1.23	1.345	2.575	P-1	6	3	5
								29
1	TANBIT	1.233	1.344	2.577	P-1	6	3	5
								29
1	TANBIT	1.234	1.327	2.561	P-1	6	3	5

1	TIFHIA	1.234	1.335	2.569	P21	2	1	298
1	TIFHOG	1.226	1.336	2.562	P21	2	1	298
1	TIFHUM	1.219	1.337	2.556	P21 21	4	1	298
1	TUCLOS	1.223	1.334	2.557	P21	2	1	295
1	TUSJIA	1.229	1.344	2.573	P21	8	4	100
1	TUSJIA	1.228	1.342	2.57	P21	8	4	100
1	TUSJIA	1.228	1.343	2.571	P21	8	4	100
1	TUSJIA	1.229	1.344	2.573	P21	8	4	100
1	UBEDOU	1.246	1.319	2.565	P21/c	4	1	293
1	VEHQUU	1.246	1.334	2.58	C2	4	1	295
1	VEHWIO	1.246	1.321	2.567	P21	2	1	295
1	VEKGOI	1.222	1.322	2.544	P21	2	1	293
1	VERTOB	1.233	1.315	2.548	P21	2	1	295
1	VIHTEM	1.229	1.339	2.568	P-1	2	1	193
1	VUJTUP	1.233	1.337	2.57	P21/c	4	1	173
1	WAPDUN	1.213	1.318	2.531	P21	2	1	293
1	WAQNUX	1.232	1.344	2.576	P2121 21	4	1	120
1	WOHRIV	1.242	1.333	2.575	P21/n	4	1	150
1	WOHROB	1.251	1.325	2.576	P21/c	4	1	150
1	XATHAC	1.24	1.322	2.562	P21/c	8	2	295
1	XATHAC	1.239	1.325	2.564	P21/c	8	2	295
1	XELBEV	1.231	1.349	2.58	P21	4	2	295
1	XELBEV	1.24	1.364	2.604	P21	4	2	295
1	XEQVAR	1.237	1.344	2.581	P21	2	1	298
1	XEVCAC	1.234	1.339	2.573	P2121 21	4	1	122
	XUZTIW	1.23	1.328	2.558	P2121 21	4	1	293
1	YEQCAZ	1.227	1.349	2.576	Pbca	8	1	223
	YUGMAP	1.219	1.333	2.552	P2121 21	4	1	293
1	ZAQCUP	1.241	1.307	2.548	P21	2	1	295
1	ZELKUW	1.236	1.334	2.57	P21	4	2	173
1	ZELKUW	1.238	1.335	2.573	P21	4	2	173
1	ZENRUF	1.24	1.315	2.555	P2121 21	4	1	295
1	ZIKKEJ	1.228	1.341	2.569	P21	2	1	295
1	ZIKKEJ01	1.225	1.347	2.572	P21	2	1	107

1	ZTCDON10	1.225	1.331	2.556	P21/c	4	1	295
1	POQSEU	1.227	1.327	2.554	P21	2	1	292
1	YOPXIL	1.235	1.338	2.573	P21	2	1	200
ave,dimer		1.232305	1.337559	2.569864				
stdev		0.007957	0.007844	0.011261				
max,dimer		1.256	1.355	2.611				298
min,dimer		1.206	1.322	2.541				100
ave,nondi		1.231973	1.335356	2.567329				
stdev		0.008573	0.01019	0.011905				
max,nondi		1.251	1.364	2.604				301
min,nondi		1.21	1.307	2.531				100
rejected								
H missing	SUBYAP	1.219	1.367	2.586	P21/c	4	1	173
H missing	SUBYET	1.214	1.36	2.574	P21/c	4	1	173
H missing	GIRSEF10	1.226	1.34	2.566	P21/c	4	1	295
Co-crystals								
H2O	DUBTUQ	1.243	1.341	2.584	P21/c	4	1	150
Bipy	FUHRAC	1.235	1.335	2.57	P-1	2	1	98
Bipy	FUHRAC	1.239	1.337	2.576	P-1	2	1	98
cocryst	HUFZUE	1.262	1.318	2.58	P-1	2	1	110
H2O	TONQAO	1.246	1.318	2.564	C2/c	8	1	295
cocryst	UHACEM	1.247	1.322	2.569	P-1	1	0.5	120
cocryst	UHACUC	1.254	1.321	2.575	P21/n	2	0.5	120
CHCl3	UHUZED	1.238	1.333	2.571	P-1	2	1	153
BzCOOH	XOHXAU	1.249	1.319	2.568	P21/n	4	1	150
ions	ACXMPR	1.227	1.349	2.576	P212121	4	1	295
acetone	CHAETK	1.216	1.338	2.554	P1	1	1	295
cocryst	CIWHUM	1.228	1.325	2.553	P212121	4	1	113
H2O	CTOGBS20	1.232	1.326	2.558	P212121	4	1	295
H2O	DETQEZ	1.24	1.333	2.573	P21	2	1	293
H2O	DIPMUK	1.257	1.319	2.576	P21/c	4	1	193
CH3OH	DUVFEG	1.241	1.33	2.571	P1	1	1	93
H2O	ECAQII	1.211	1.32	2.531	Aba2	8	1	293
CH3CN	ECAQOO	1.214	1.343	2.557	P-1	2	1	293
H2O	EDEFOJ	1.237	1.326	2.563	P21	2	1	293

	EDIDUQ01				P2121			223
H2O		1.235	1.325	2.56	21	4	1	
								293
cocryst	HAZGUL	1.218	1.344	2.562	P21	2	1	
					P2121			150
H2O	HUGCOC	1.23	1.342	2.572	21	4	1	
								295
C3H7OH	KOVPOA	1.222	1.343	2.565	P21/c	4	1	
					P2121			293
ions	KUTCOS	1.218	1.332	2.55	21	4	1	
								297
H2O,ions	LGPYRG	1.222	1.315	2.537	P21	2	1	
					P2121			293
H2O	MILKOH	1.201	1.348	2.549	21	4	1	
					P2121			293
1	MILKOH	1.219	1.332	2.551	21	4	1	
					P2121			293
1	MILKOH	1.213	1.342	2.555	21	4	1	
H2O,cocryst	NOPZUO	1.249	1.322	2.571	P21	2	1	153
	PYDPYR10							293
H2O		1.246	1.308	2.554	P21/c	4	1	
	PYDPYR10							293
H2O		1.233	1.331	2.564	P21/c	4	1	
					P2121			293
H2O	PYLOCA	1.232	1.352	2.584	21	4	1	
								293
H2O	TONQES	1.233	1.325	2.558	P21/n	4	1	
								293
H2O	TUDPAJ	1.226	1.335	2.561	P21	2	1	
					P2121			293
CHCl3	VEKHAV	1.246	1.347	2.593	21	4	1	
								293
H2O	XOHBAX	1.227	1.333	2.56	P-1	4	2	
								293
H2O	XOHBAX	1.211	1.347	2.558	P-1	4	2	
								293
CH3OH	XUGZUV	1.225	1.333	2.558	C2	4	1	
					P2121			293
H2O	ZIHRAJ	1.231	1.341	2.572	21	4	1	
ave,cocrys		1.232128	1.332051	2.564179				
stdev		0.014045	0.010894	0.012494				
max,cocrys		1.262	1.352	2.593				298
min,cocrys		1.201	1.308	2.531				293

2-pyrrolidone and derivatives, 93-200K

Query	Refcode	C=O	C-N	C=O + C-N	Space Gp.	Z	Z	T
	DUBSOJ	1.242	1.339	2.581	P21/n	4	1	150
	DUBTOK	1.243	1.334	2.577	C2/c	8	1	150
1	EZURUM	1.232	1.35	2.582	P21/c	4	1	173
1	EZUSAT	1.235	1.331	2.566	Pbca	8	1	123
1	GASSUP	1.256	1.355	2.611	P-1	2	1	150
1	GASTIE	1.234	1.343	2.577	P21/c	4	1	123

1	HIXQUA	1.231	1.343	2.574	P-1	2	1	183
	HUKDIB	1.232	1.349	2.581	P21/c	4	1	155
	IROMIM	1.23	1.33	2.56	I2/a	16	2	173
	IROMIM	1.237	1.328	2.565	I2/a	16	2	173
1	LESJOJ	1.234	1.355	2.589	P21/n	4	1	100
1	MIXSIV	1.243	1.336	2.579	C2/c	8	1	190
1	MIXSOB	1.241	1.331	2.572	P21/c	4	1	190
1	MIZDAB	1.223	1.34	2.563	P-1	2	1	173
	NACMUB	1.232	1.34	2.572	P21/n	4	1	173
1	NEJTAY	1.232	1.346	2.578	P-1	2	1	163
1	NILYAI	1.237	1.335	2.572	P-1	2	1	173
1	RAWZIZ	1.229	1.324	2.553	P21/n	4	1	193
	UNECAS	1.235	1.349	2.584	P21/n	4	1	173
1	VAXYOJ	1.223	1.344	2.567	P21/c	4	1	115
1	WOHRER	1.23	1.349	2.579	P21/n	4	1	150
1	YOPYAE	1.232	1.348	2.58	P21/n	4	1	200
	BUHKIZ	1.218	1.34	2.558	P21	2	1	100
	BUWWAS	1.228	1.345	2.573	P21	2	1	150
1	CENBUT	1.229	1.346	2.575	P21/c	4	1	150
1	CIZMAA	1.228	1.347	2.575	P212121	4	1	130
1	COQSUX	1.226	1.339	2.565	P41212	8	1	100
1	DIPMUK	1.257	1.319	2.576	P21/c	4	1	193
	DUBTEA	1.239	1.338	2.577	P21/c	4	1	150
	DUBVAY	1.239	1.341	2.58	C2/c	8	1	150
	DUDMIZ	1.244	1.329	2.573	P21/c	4	1	150
1	GASTEA	1.241	1.326	2.567	P21/c	4	1	150
1	GUDSIH	1.244	1.336	2.58	P212121	4	1	180
1	GUDSON	1.232	1.324	2.556	P212121	4	1	180
1	HACFUM	1.24	1.335	2.575	Pca21	8	2	133
1	HACFUM	1.242	1.342	2.584	Pca21	8	2	133
1	HACGAT	1.237	1.334	2.571	Pbc21	8	2	123
1	HACGAT	1.242	1.329	2.571	Pbc21	8	2	123
	HUKDOH	1.246	1.334	2.58	Pbca	8	1	163
1	KAFNEK	1.241	1.329	2.57	Pna21	4	1	163

					P21212			16
1	KAFNIO	1.239	1.334	2.573	1	8	2	3
					P21212			16
1	KAFNIO	1.243	1.329	2.572	1	8	2	3
	LANDU							18
1	Z	1.238	1.331	2.569	P21	2	1	0
						1		10
1	LICTAT	1.236	1.338	2.574	P41212	6	2	0
						1		10
1	LICTAT	1.224	1.352	2.576	P41212	6	2	0
								10
1	LIWFIH	1.229	1.348	2.577	Pca21	4	1	0
								19
1	ODIBOT	1.231	1.344	2.575	P21	4	2	0
								19
1	ODIBOT	1.239	1.343	2.582	P21	4	2	0
	OMANO				P21212			17
	G	1.231	1.347	2.578	1	4	1	3
	OQAWO							10
	T	1.241	1.316	2.557	C2	4	1	0
								15
1	PELDIU	1.235	1.347	2.582	P21	4	2	0
								15
1	PELDIU	1.233	1.347	2.58	P21	4	2	0
	RAWZO							19
1	F	1.225	1.315	2.54	P-1	4	2	3
	RAWZO							19
1	F	1.226	1.317	2.543	P-1	4	2	3
	RENSU							17
1	Y	1.218	1.336	2.554	P21/c	4	1	3
	SOCBO							10
1	C	1.225	1.354	2.579	P21	2	1	0
	SOCCA							10
1	P	1.236	1.323	2.559	P21212	8	2	0
	SOCCA							10
1	P	1.237	1.325	2.562	P21212	8	2	0
								12
	TADVAX	1.236	1.339	2.575	C2/c	8	1	3
								10
1	TUSJIA	1.229	1.344	2.573	P21	8	4	0
								10
1	TUSJIA	1.228	1.342	2.57	P21	8	4	0
								10
1	TUSJIA	1.228	1.343	2.571	P21	8	4	0
								10
1	TUSJIA	1.229	1.344	2.573	P21	8	4	0
								19
1	VIHTEM	1.229	1.339	2.568	P-1	2	1	3
								17
1	VUJTUP	1.233	1.337	2.57	P21/c	4	1	3
	WAQNU				P21212			12
1	X	1.232	1.344	2.576	1	4	1	0
	WOHRI							15
1	V	1.242	1.333	2.575	P21/n	4	1	0
	WOHRO							15
1	B	1.251	1.325	2.576	P21/c	4	1	0
	XEVCA				P21212			12
1	C	1.234	1.339	2.573	1	4	1	2
	ZELKU							17
1	W	1.236	1.334	2.57	P21	4	2	3
	ZELKU							17
1	W	1.238	1.335	2.573	P21	4	2	3
	ZIKKEJ0							10
1	1	1.225	1.347	2.572	P21	2	1	7
								20
1	YOPXIL	1.235	1.338	2.573	P21	2	1	0
ave,dim er		1.234681818	1.340863636	2.575545455				

		0.007226	0.008865	0.011725				
stdev		844	64	947				
max,di								20
mer		1.256	1.355	2.611				0
min,dim								10
er		1.223	1.324	2.553				0
ave,non		1.234588	1.336509	2.571098				
di		235	804	039				
		0.007808	0.009388	0.009029				
stdev		141	019	407				
max,no								20
ndi		1.257	1.354	2.584				0
min,non								10
di		1.218	1.315	2.54				0
H								17
missing	SUBYAP	1.219	1.367	2.586	P21/c	4	1	3
H								17
missing	SUBYET	1.214	1.36	2.574	P21/c	4	1	3
	DUBTU							15
H2O	Q	1.243	1.341	2.584	P21/c	4	1	0
	FUHRA							
Bipy	C	1.235	1.335	2.57	P-1	2	1	98
	FUHRA							
Bipy	C	1.239	1.337	2.576	P-1	2	1	98
	HUFZU							11
cocryst	E	1.262	1.318	2.58	P-1	2	1	0
	UHACE						0.	12
cocryst	M	1.247	1.322	2.569	P-1	1	5	0
	UHACU						0.	12
cocryst	C	1.254	1.321	2.575	P21/n	2	5	0
	UHUZE							15
CHCl3	D	1.238	1.333	2.571	P-1	2	1	3
	XOHXA							15
BzCOOH	U	1.249	1.319	2.568	P21/n	4	1	0
	CIWHU				P21212			11
cocryst	M	1.228	1.325	2.553	1	4	1	3
	DUVFE							
CH2OH	G	1.241	1.33	2.571	P1	1	1	93
	HUGCO				P21212			15
H2O	C	1.23	1.342	2.572	1	4	1	0
H2O,coc	NOPZU							15
ry	O	1.249	1.322	2.571	P21	2	1	3
								19
H2O	DIPMUK	1.257	1.319	2.576	P21/c	4	1	3
ave,cocr								
y		1.244	1.328	2.572				
		0.010230	0.007820	0.006370				
stdev		673	912	002				
max,coc								19
ry		1.262	1.342	2.584				3
min,cocr								
y		1.228	1.318	2.553				93

Table S-5. Twelve representative primary amides (dimers/nondimers) (Gavezzotti, 2010)

REFCODE	C-N, Å	C=O, Å	*Cis* O=C-N-H, °	C-N + C=O
ACEMID03	1.335	1.247	-8.2	2.582
BZAMID01	1.333	1.24	6.4	2.573
CYANAC	1.327	1.2232	-0.8	2.5502
CYANAC	1.327	1.2292	2.0	2.5562
DIXTAF	1.332	1.243	4	2.575
IBURAM	1.320	1.2303	1.3	2.5503
JEXNAB	1.311	1.228	-1	2.539
MALOAM	1.318	1.241	1.5	2.559
MALOAM	1.310	1.239	-3.1	2.549
MALOAM	1.317	1.241	6.7	2.558
MALOAM	1.321	1.241	-8.1	2.562
ZZZKAY01	1.327	1.2536	5.9	2.5806
Average	1.323167	1.238025		2.561192
St.dev.	0.00831	0.00872		0.013688
Maximum	1.335	1.2536		2.582
Minimum	1.310	1.2232		2.539

Table S-6 Results: Search B (Derivatives of Naphtholactam)

Query	Refcode	C-N, Å	C=O, Å	C-N+C=O	C-N-C-C,⁰	R-factor	Space Gp. Symbol	Z	Z'	C=O H-bond	Study Temp.	Publication Year	Unique Chemical Units
1	QACQOA	1.376	1.226	2.602	-1.207	7.78	P21/c	4	1	NH…O,CH…O	228	1998	1
1	SOHCEY	1.389	1.23	2.619	-0.494	3.71	P21/c	4	1	CH…O	295	2008	1
1	XATHIK	1.389	1.221	2.61	-0.662	3.63	P-1	2	1	CH…O	295	2005	1
1	KAKMEP	1.393	1.221	2.614	-0.713	4.13	P21/c	4	1	CH…O	295	2005	1
1	KAKNAM	1.394	1.215	2.609	1.021	4.16	P21/n	4	1	CH…O	295	2005	1
1	SOHCAU	1.401	1.213	2.614	-0.141	4.64	Pbca	8	1	CH…O	295	2008	1
1	DUXXEA	1.415	1.219	2.634	0.835	4	P-1	4	2	2 CH…O	296	2010	1
1	RAKYUY	1.43	1.193	2.623	-0.17	3.24	P21/c	4	1	CH…O, Br	295	2005	1
1	DUXXIE	1.454	1.204	2.658	0.494	4.48	P-1	2	1	3 CH…O	296	2010	1
1	DUXXEA	1.46	1.209	2.669	1.681	4	P-1	4	2	3 CH…O	296	2010	1
average		1.4101	1.2151	2.6252									
stdev		0.0289 15	0.0109 49	0.0221 05									
max		1.46	1.23	2.669									
min		1.376	1.193	2.602									
Tetrahel.	AJEJUV	1.349	1.217	2.566	5.24	7	P21/n	4	1	NH…O	295	2008	1
trihel.	GUGMOL	1.397	1.233	2.63	0.159	6.56	P-1	4	2	CH…O	100	2009	1
trihel.	GUGMOL	1.401	1.227	2.628	-1.505	6.56	P-1	4	2	none	100	2009	1
co-cryst.	VIBSAA	1.366	1.211	2.577	1.252	14.7	P21/c	4	1	2 CH…O,H2O	295	1990	2
co-cryst.	XATLOU	1.398	1.222	2.62	0.185	5.35	P21/c	2	0.5	CHCl3	295	2005	2

Refcode	Compound Name
QACQOA	7-Amino-6,8-bis(4-methoxyphenyl)benz(c,d)indol-2(1H)-one
SOHCEY	5-Methyl-8-phenylbenzo(cd)furo(2,3-f)indol-4(5H)-one
XATHIK	6-(2-Anthracen-9-ylethenyl)-1-methyl-1,2-dihydro-1-azaacenaphthylen-2-one
KAKMEP	6-Formyl-1-methyl-benz(c,d)indol-2-one
KAKNAM	6-Formyl-1-t-butyl-benz(c,d)indol-2-one
SOHCAU	5-Methyl-7-phenylbenzo(cd)furo(2,3-f)indol-4(5H)-one
DUXXEA	S-Benzyl 2-oxobenzo[cd]indole-1(2H)-carbothioate
RAKYUY	6-(4-Bromophenyl)-1-methylbenz(c,d)indol-2-one
DUXXIE	1-(Benzyloxycarbonyl)benzo(c,d)indol-2-one
DUXXEA	S-Benzyl 2-oxobenzo[cd]indole-1(2H)-carbothioate
AJEJUV	6-(4-Iodobenzoyl)-7-(4-iodophenyl)indolo(3,4-jk)phenanthridin-5(4H)-one
GUGMOL	6-(4-Methoxyphenyl)-5-methyldibenzo[cd,f]indol-4(5H)-one
GUGMOL	6-(4-Methoxyphenyl)-5-methyldibenzo[cd,f]indol-4(5H)-one
VIBSAA	2,7,7-Trimethyl-1,9-dioxo-1,7,8,9-tetrahydro-2H-isoindolo(4,6-cd)indole monohydrate
XATLOU	3,7-Di-t-butyl-9,10-bis(1-butyl-2-oxo-1,2-dihydro-1-azaacenaphthylen-6-ylethynyl)anthracene chloroform solvate