Supplementary Material (ESI) for Chemical Communications

Correlation between molecular dipole moment and centrosymmetry in some crystalline diphenyl ethers.

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Appendix I

Table 1: List of CSD refcodes and dipole moments for compounds in space group *P*1 (60 compounds)

No	Refcodes	Dipole moment (D)	No	Refcodes	Dipole moment (D)
1	ABMHFO	2.913	31	RICRIE	5.610
2	BAQLIO	5.203	32	TEOXDE01	0.555
3	BXDABT	4.861	33	TILRUB	5.012
4	CILWOJ	0.226	34	VEGJOG	6.696
5	CTMTPS10	0.647	35	VOFFAX	4.503
6	FIYPEI	1.764	36	WATCID10	0.550
7	FOMANN	8.176	37	WEFDAM	2.331
8	HOBXEB	1.636	38	WICVUZ	5.662
9	HOVFON	4.013	39	WIMGOO10	0.387
10	JAQWED	6.512	40	WINWEV	7.005
11	JIPBIT	1.658	41	XIZTIJ	4.975
12	KASJET	1.523	42	XOVLUP	3.329
13	KOPROW	2.048	43	YAGXAF	1.160
14	LEMZAE	0.942	44	YEBGIV	7.387
15	LETBOB	3.793	45	YIJBUO	5.126
16	MAMNAC	1.037	46	YOGVOF	5.216
17	MASFOB	1.923	47	YOGWOG	2.063
18	MAZNIK	0.640	48	ZAQTOA	2.979
19	MEKLIX	3.913	49	ZAVZAX	2.659
20	MENBNB	6.354	50	ZUKMAT	2.988
21	MOYKOA	3.802	51	TAGBEJ	4.229
22	PABMOU	2.785	52	UJIPIM	3.087
23	PATCUI	3.029	53	ALULEY	3.429
24	PATPYS	0.413	54	BEFZOC	5.401
25	PEVLOR	1.195	55	EMIGEM	10.13
26	PICSEZ	2.856	56	ENIREY	2.143
27	PIKYIR	6.300	57	INANUG	1.383
28	PIVGAC	0.985	58	OKUFEF	4.511
29	QAMFAL	2.585	59	ASEZED	2.343
30	QERJEC	1.107	60	ISELAT	2.846

Table 2: List of CSD refcodes and dipole moments for compounds in space group $P\bar{1}$ (300 compounds)

No	Refcode	Dipole moment (D)	No	Refcode	Dipole moment (D)
1	ACAVAB	2.953	51	FABXAI	3.044
2	ADUQIZ	3.256	52	FAMCUR	1.125
3	BACBEN	5.330	53	FECHEA	2.985
4	BAGNUS	3.320	54	FENKAK	3.665
5	BANTIU	5.630	55	FEVPIF	2.820
6	BEBCUG	1.939	56	FIQDEO	3.814
7	BEJRIR	2.167	57	FOCFAE10	3.848
8	BELMUA	4.575	58	FOSRUA	2.129
9	BEQBOO	4.342	59	FUCFIS	3.957
10	BERSIA	2.562	60	FUMLAA	3.205
11	BFRNDX	4.429	61	FUWHOU	0.800
12	BIGBAU	3.271	62	GADNEE	2.486
13	BILKIQ01	2.667	63	GAKPOX	3.177
14	BIYNUS	1.303	64	GATRAU	1.917
15	BODFNB	3.461	65	GAZLAU	1.962
16	BONKEU	1.853	66	GEJHUY	4.327
17	BPAXEB	2.471	67	GESLOF	2.188
18	BUHXEH	3.831	68	GIGJOV	6.609
19	BUZXAV	1.382	69	GIKMIW	4.051
20	CAKREM	9.053	70	GISGAQ	4.658
21	CAVLAM	2.812	71	GOJKOF	0.069
22	CAZMOF10	2.639	72	GOVRIS	3.628
23	CESVOL	2.959	73	GUDWEH	9.567
24	CEYZIP	3.952	74	GUQYAS	3.953
25	CIMHUB	0.047	75	HABFUL	6.477
26	CIWMUQ	3.868	76	HABZAL	3.300
27	CMCDCN	3.637	77	HADHUQ	1.825
28	COCHEH	4.080	78	HADLUU	2.160
29	COPHIY	6.901	79	HALLEN	0.435
30	CPHTRI	0.072	80	HAXLEX	1.640
31	CUMKIE	2.439	81	HEGHIK	1.246
32	CYHXDN	3.585	82	HEKFIM	2.771
33	DAKTUE	2.123	83	HIFQOC	1.735
34	DARHUZ01	4.821	84	HIPSOO	2.954
35	DEKDIG	8.372	85	HNFMNO	3.534
36	DEMTEU	5.410	86	HOLSEG	5.962
37	DENCOO	0.214	87	HOVYAS01	1.925
38	DESJAM	2.168	88	HUFWOU	3.365
39	DFNAPQ	4.058	89	HUPQEO	3.336
40	DIHXEX	1.806	90	HUZLOD	2.317
41	DIWDOC	0.247	91	IDODEK	0.178
42	DOKZOS	1.019	92	IGIHUB	4.898
43	DONRUT	3.862	93	JACCOF	4.668
44	DOYNEK	1.439	94	JAHWAQ	2.637
45	DUDBOT	0.795	95	JAPPAR	7.276
46	DUWBEC	3.159	96	JAZFEV	4.815
47	EBEYEP	1.950	97	JEMXAA	6.085
48	EDAVAG	4.436	98	JIGXAY10	6.906
49	EDUWEF	1.111	99	JOBBEH	5.354
50	EMBPBL	4.675	100	JORGAY	0.670

Cont.

101	JOTVUJ	3.439	151	NOKXIU	0.917
102	JUHFAT	9.571	152	NOXZEF	2.298
103	JUNJEH	3.283	153	NUCHOI	4.759
104	JUVNUJ	7.607	154	NUNDEF	1.303
105	KAFBAU	2.054	155	NUZDIV	2.143
106	KAGXIZ	0.932	156	OBOHOC	3.096
107	KAMBUV	2.974	157	OCMETD10	0.032
108	KAPBOS	2.921	158	OFOKUP	2.316
109	KEDWAR	7.687	159	PABCOK10	4.412
110	KERQON	0.369	160	PAMGEP	3.949
111	KILGIV	3.190	161	PAZGAY	2.053
112	KIRFEW	4.590	162	PEFCAE	3.121
113	KOBFAI	2.476	163	PHXCBN	2.660
114	KOPZEU	5.231	164	PIGQUR	4.117
115	KUFJEA	4.863	165	PIKDAO	5.395
116	KUTGEL	6.783	166	PINWIS	0.584
117	LACTUE	3.029	167	PIQRAI	5.115
118	LALMEQ	2.349	168	PIRSAK01	2.978
119	LAQPOI	2.764	169	POBTOP10	0.088
120	LEBBOJ	4.101	170	POPZOJ	4.166
121	LEGSIZ	2.499	171	POWKUH	7.623
122	LELWEE	2.953	172	POZPOJ	5.497
123	LETMOM	2.979	173	PUNPOD	2.560
124	LIFCAE	3.140	174	PUVRIH	5.040
125	LIJQAW	2.892	175	PUZHIB	0.061
126	LIQROS	5.038	176	PYDMIM	5.241
127	LIYSAN	0.771	177	QAGNAN	1.056
128	LOSQEP	6.452	178	QAQJIB	2.471
129	LUCGAR	3.555	179	QEBXEA	2.440
130	LUMTAO	5.271	180	QETGUR	6.056
131	MALQIZ	1.889	181	QIJDAO	4.815
132	MBPHIN	1.242	182	QISTUH	4.406
133	MEBRUN	2.996	183	QOMSOA	4.818
134	MERJUO	1.639	184	QOQQIW	3.617
135	MEXGUR	5.642	185	RACBEC	5.564
136	MIWQIS	2.525	186	RAQSUX	5.517
137	MOCZIN	3.276	187	RECHIQ	2.320
138	MOKRIN	2.310	188	REMBIU	4.184
139	MOVBEE	4.796	189	REWDEC	1.779
140	MPYCHD	0.659	190	RIFWEI	1.120
141	MUGFOJ	1.568	191	RIKXEO	0.419
142	MUQMIU	3.574	192	RIYLEQ	5.218
143	MXBCUN	0.759	193	ROHHEB	3.834
144	NADVAP	0.249	194	RUHFIJ	5.522
145	NAQZOU	2.837	195	RUVCAM	2.320
146	NEDNAL	4.869	196	RUXSIM	2.590
147	NEQLUQ	4.681	197	SAMBIR	2.075
148	NIBPUJ	1.870	198	SAQZOY01	0.070
149	NIMFIY	2.612	199	SAXGED	0.882
150	NIXWIA	2.233	200	SAYDAX	4.178

Cont.

201	SEKKOI	3.586	251	XEZHEP	3.985
202	SERQEL	2.571	252	XIRYEC	2.311
203	SIYJAL	1.914	253	XIXJUJ	4.699
204	SOHRUC	6.965	254	XOKGEJ	2.946
205	SOXGAN	2.782	255	XOWWEL	6.495
206	SUMMES	0.931	256	XOZGAU	3.356
207	SURSUT	2.533	257	XUGYON	2.924
208	TABBEE	2.990	258	XURXUD	2.666
209	TAHKUI	2.477	259	YAHQUT	6.021
210	TAJWAC	6.493	260	YAWPER	1.699
211	TASPIM	1.060	261	YEGDET	5.987
212	TELNIH	7.470	262	YEMGAY	0.690
213	TEYDUW	4.262	263	YESCII	3.617
214	TIJXOZ	1.560	264	YIGFAV	0.826
215	TIQVUK	2.219	265	YIZPAY	2.596
216	TOBXOX	2.343	266	YORHOC	5.595
217	TOHZUL	4.853	267	YOWYAK	8.828
218	TOPSIA	3.586	268	YUFFAG	2.251
219	TUDRUF	2.403	269	YUPNUS	2.877
220	TURYUA	1.414	270	ZAGMUP	2.378
221	TUWDUK	3.538	271	ZAMVAK	0.615
222	UCOQAE	3.428	272	ZEBWUY	3.219
223	UDIMID	1.926	273	ZERPOB	3.282
224	UGEGIW	1.240	274	ZEYDOW	0.110
225	UHENEA	4.227	275	ZIFLOP	5.790
226	VALHAR	0.369	276	ZILTIX	3.508
227	VATCIC	9.997	277	ZIYLOI	1.328
228	VAYNEO	1.439	278	ZOKVAW	7.788
229	VEJGAS	3.505	279	ZUKQEB	2.797
230	VETNOX	3.268	280	ZUZFUV	4.194
231	VIDHOF	2.995	281	BAPVEU	4.376
232	VIWPIA	3.559	282	EJEVEU	3.882
233	VOCREK	3.72	283	EKUFIZ	3.542
234	VOMZAY	2.286	284	IJOKUN	3.685
235	VUBZOH	3.319	285	KABFEZ	6.600
236	WACDOT	2.161	286	OHOWOX	4.040
237	WANCAP	5.272	287	OJORUA	2.949
238	WEBBUA	3.426	288	TAHYOR	3.728
239	WEHPII	0.815	289	AKUPUR	1.022
240	WEPSEP	1.582	290	AMIZOL	3.155
241	WICLOJ	1.940	291	ELORIG	0.492
242	WIQLIR	2.589	292	IMIMAS	3.681
243	WOBPEI	1.271	293	OLEQEB	2.872
244	WOSKUK	0.934	294	OMOTOZ	1.223
245	WUHMOB	2.332	295	UNOHIO	5.816
246	WUQXUB	3.293	296	AROYEL	3.742
247	XARYIY	5.089	297	ASUYUI	5.774
248	XAXRIX	5.536	298	IPUROA	0.874
249	XAZXOL	0.326	299	IQULEL	5.947
250	XEQBAW	2.306	300	ITIHIC	3.255

Table 3: List of CSD refcodes and dipole moments for compounds in space group $P2_1$ (350 compounds)

No	Refcode	Dipole moment (D)	No	Refcode	Dipole moment (D)
1	ABAXES	5.840	51	DBXZCP01	3.665
2	ABULAK	3.119	52	DEANDB10	3.767
3	ACALPA	4.240	53	DEHPAH	3.993
4	ACDXYL10	3.706	54	DENXUP01	3.911
5	ACSESO10	3.996	55	DEVWOQ	3.810
6	ADUPIY	3.166	56	DIJVIB	5.138
7	AFUZOQ	3.119	57	DITBOX01	0.636
8	AHUBAG	2.788	58	DMBZAN11	0.574
9	AIPCUR10	7.221	59	DPCYPE01	0.449
10	AKUYUA	3.594	60	DUFJET10	3.109
11	AMAJUT	2.769	61	DUWGOR	3.883
12	AQEBIH	6.194	62	EADYAJ	3.151
13	ATEZOO	2.720	63	ECODUV	0.748
14	ATULOQ	4.230	64	ECUKAO	2.481
15	AWULUZ	2.223	65	EDIPEM	2.397
16	BADVEH01	3.635	66	EGEREN	6.137
17	BALSOW	4.742	67	EMINET	6.358
18	BAQMAH	5.957	68	EQUTOZ	6.673
19	BASZAW	3.484	69	FACWIQ	3.642
20	BAXFAI	4.545	70	FAFYEQ	6.275
21	BAXTUQ	2.186	71	FAMXUM	2.135
22	BAZTIF	2.898	72	FATCEI	3.056
23	BEDDOE	0.981	73	FEMTIA	1.843
24	BEKMIO	4.475	74	FEQPEW	5.317
25	BEPYIE	2.234	75	FEWWEJ01	0.407
26	BERFAF	4.737	76	FEZNED	4.668
27	BERLEP	2.134	77	FIJKOY	1.790
28	BEVVUT	3.003	78	FITGEU	2.069
29	BINPOD	1.944	79	FIXZER	3.786
30	BIXWOU10	3.394	80	FOJMAS	2.525
31	BLONGA10	1.570	81	FOVSEO	1.714
32	BOKPAS	6.252	82	FOZFEF	2.450
33	BOSLUQ10	2.022	83	FUCNAS	2.821
34	BOSYUD	5.919	84	FUDYEI	4.961
35	BRUCLA	7.288	85	FUNYAO	3.319
36	BUGPOI	5.852	86	GAHGAX	3.319
37	BUVRIT	2.833	87	GAPHIO	4.456
38	CANCOJ	4.31	88	GEMKIS	2.363
39	CAZJOC	3.865	89	GEPCOT01	2.349
40	CEVXEG	3.136	90	GEYSIM	1.778
41	CEYWOS	1.712	91	GIBYAR	2.203
42	CIFZOG	1.895	92	GIQMEY	2.518
43	CIMVEZ	2.426	93	GIVQUX	2.849
44	CIXXUC	1.747	94	GIWHUP	0.121
45	COLBOU	3.878	95	GOKPOL	6.171
46	CROVRN	7.175	96	GOPJOK	1.822
47	CUFJIW	4.495	97	GOYFAB	2.240
48	CUMDOD	2.336	98	GUJYAL	1.996
49	DABRON	3.903	99	GUNYUJ	1.913
50	DAJTEN	3.272	100	HABSAE	0.689

Cont.

101	HAGJIJ	2.079	151	LATWOS	4.647
102	HAWXUY	0.666	152	LEBKAE	2.985
103	HERSID	4.259	153	LETTAF	2.457
104	HEXXIR	2.523	154	LIMFAO	2.637
105	HISTIM	1.776	155	LIWFEC	2.495
106	HOMPEE	1.415	156	LODVEF	1.949
107	HOYGUX	3.038	157	LOHXAH	8.025
108	HUNZAR	4.460	158	LOLFAT	5.607
109	IDOKIV	1.902	159	LOTFEF	5.607
110	IHOYIN	4.170	160	LOYPEU	2.659
111	IKURUB	5.552	161	LURSAS	3.413
112	ILODAO	5.849	162	LUXVUV	2.393
113	INOJAW	3.966	163	MABCIC	2.853
114	IPEKET	2.786	164	MAJCIJ	3.382
115	IQADEJ	4.351	165	MAQMAS	1.730
116	IROQUB	2.908	166	MATALP	1.670
117	ISPCHX	6.116	167	MBZYAN01	1.499
118	IWECES	1.227	168	MEBYAS	2.337
119	JABFAT	4.586	169	MELXAC	1.143
120	JACZIW	2.165	170	MILZAI	1.345
121	JAYRAC	2.277	171	MIRSAH	3.486
122	JEGTUK	1.683	172	MIYSUI	2.039
123	JEJJIR10	1.322	173	MONTIS01	0.682
124	JEXLUT	6.204	174	MOYDUZ	3.569
125	JINNID	2.618	175	MULBOK	7.591
126	JIZFON	5.095	176	MXTDOB	4.726
127	JOBVOL	1.677	177	NAFQOA	3.343
128	JOHZAH	1.677	178	NAHVIB	5.983
129	JOTGAA	4.766	179	NATTAD	2.991
130	JOTJUX	3.222	180	NECNAK	1.125
131	JUPDIH	1.413	181	NEMROM	3.062
132	JUXHEP	4.417	182	NEQNIG	3.582
133	KADTAK	4.091	183	NFSIHN10	1.468
134	KAQNIZ	5.541	184	NIFDEL	6.926
135	KAVTAC	1.843	185	NIKZAI	4.179
136	KEDWUL	1.777	186	NOCPOK	5.093
137	KEFXEY	5.182	187	NOZXEF	0.980
138	KERZEM	3.439	188	NUGWOB	3.515
139	KIMCIS	0.265	189	NUKVEU	3.400
140	KIZZEY	1.744	190	NUSLUI	7.238
141	KOPREM	5.875	191	NUYPAY	3.068
142	KOSLEJ	2.617	192	OCICEI	3.324
143	KOSZEX	4.501	193	OCINOD	5.416
144	KOUMIN	2.707	194	OCOHAP	6.999
145	KUGSAG	4.923	195	ODEVEY	10.73
146	KUNFAA	2.960	196	ODOTAC	7.185
147	KURZAY	6.622	197	OHUVIW	3.688
148	KUVZEG	2.229	198	OKIQUU	1.414
149	LABNEI	5.566	199	OKUFIJ	6.532
150	LAKGAF	1.503	200	PABDAY	1.235

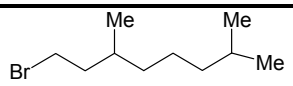
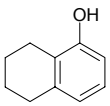
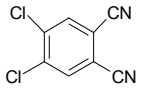
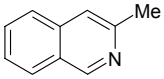
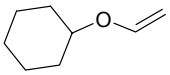
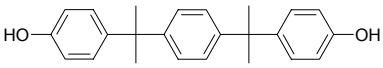
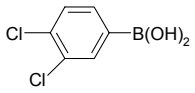
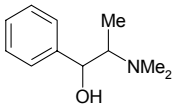
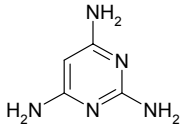
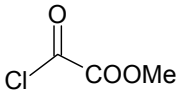
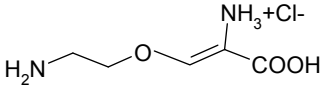
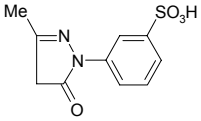
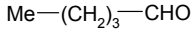
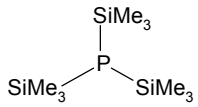
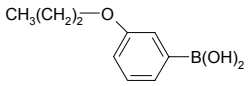
Cont.

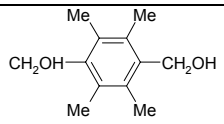
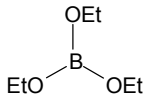
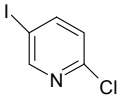
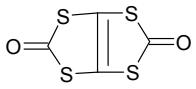
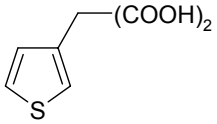
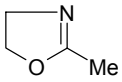
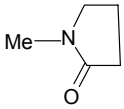
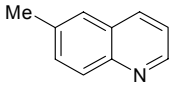
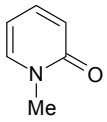
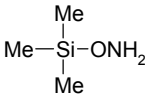
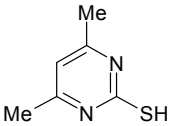
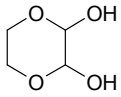
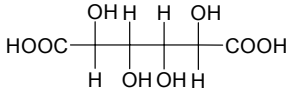
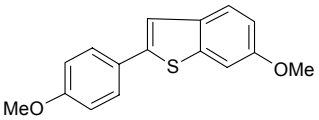
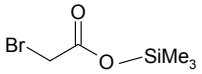
201	PAIDOP	0.971	251	TACHIO	1.701
202	PAZBAT	6.216	252	TACRIB02	3.054
203	PEPQOQ	5.756	253	TAFHOX01	5.65
204	PEXFED	5.272	254	TAHPEX	2.336
205	PFLUOR	0.144	255	TAHXAC	4.596
206	PIGTII	5.035	256	TATCUM	2.217
207	PILLEB	2.567	257	TAYWAR	3.332
208	PIQMEH	0.756	258	TEDQOI	4.091
209	PIZBAB	5.267	259	TEHHOD	2.277
210	PLBULD	4.177	260	TEKSOR	3.113
211	POKZEU	2.757	261	TERWES	3.580
212	PUDHAX	2.151	262	TEYMOZ	4.911
213	PUHWAQ	6.347	263	TIBGUG	3.713
214	QAGJUE	4.076	264	TIQFAA	2.713
215	QAPJIA	5.007	265	TOBBOB	1.855
216	QECFAF	3.306	266	TOHDUP	2.579
217	QEGYEG	4.641	267	TOLDUT	2.184
218	QETVUG	0.739	268	TOSNOE	0.984
219	QEYQIU	2.190	269	TRBZAM	5.044
220	QEZLOW	2.520	270	TRCHRN	3.968
221	QIMXIT	4.379	271	TTHBUD	0.220
222	QOTYAZ	8.549	272	TUPVEF	1.560
223	QOYBAH	4.808	273	TUWLIG	2.616
224	QUDVUG	4.206	274	UBUJEG	2.430
225	QUSZEJ	2.158	275	UFOBOG	1.538
226	RAHFAH	5.193	276	UGUGIM	0.691
227	RANWIM	2.302	277	UHUDIK	1.872
228	REBFOT	3.919	278	UHUHEK	3.603
229	REMTEI	2.454	279	UJEKAV	4.400
230	RICWIJ	2.005	280	UJELEA	2.080
231	RIGLUO	2.815	281	ULARAA	2.649
232	RIJGOG	5.253	282	UNOHAG	0.542
233	RIRRUF	3.919	283	VAKJOG	2.184
234	ROFHEZ	2.490	284	VAQJED	4.188
235	ROHFOJ	4.541	285	VAQQOU	3.468
236	RONKIO	0.680	286	VEJTEJ	4.032
237	RONKUA	0.414	287	VERJUX	1.402
238	RUWHAS01	1.951	288	VIDLUP	7.575
239	SAFFEK01	1.520	289	VIMGUT	8.112
240	SATHEA	0.839	290	VIXRID	3.191
241	SAVCOH	4.108	291	VOKWIB	4.712
242	SAWYIY	5.182	292	VOLRET	9.690
243	SEFSEB	3.224	293	VOMMEP	5.784
244	SEQFUP	4.523	294	VONBOP	3.726
245	SILFAU	4.523	295	VOTTED	1.952
246	SIZMET	4.523	296	VOWTIK	1.148
247	SOCGOG	5.947	297	VOXFOD	2.947
248	SONQER	2.473	298	VOYNEC	0.883
249	SOSFEL	3.791	299	VUKBUY	1.397
250	SUNDEK	3.791	300	VUMMIZ	4.159

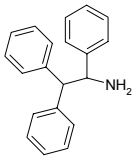
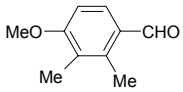
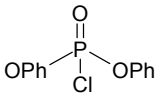
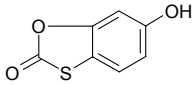
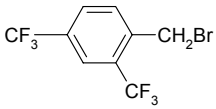
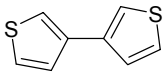
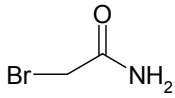
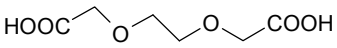
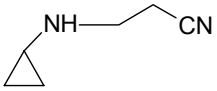
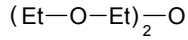
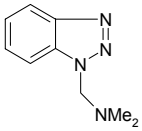
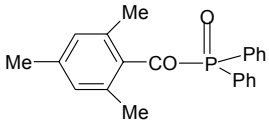
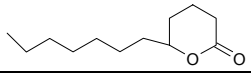
Cont.

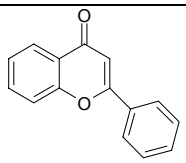
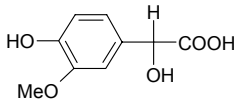
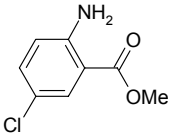
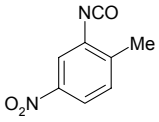
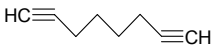
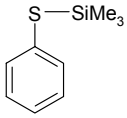
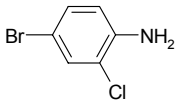
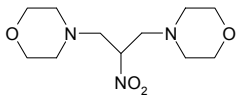
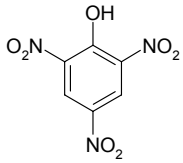
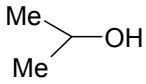
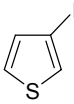
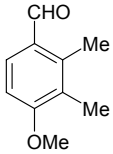
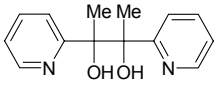
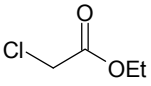
301	VUWJIG	2.692	326	YAZDEI	5.522
302	WAPWAL	3.543	327	YEMQAI	3.967
303	WEJZAM	5.294	328	YEVZEE	1.312
304	WEWYAY	1.512	329	YEZJUI	0.128
305	WIJYUJ	3.435	330	YIRQAR	2.649
306	WISDOR	2.812	331	YIZLOI	1.513
307	WODTOY	8.290	332	YOLPUK	3.377
308	WOMLOZ	3.066	333	YOXYEP	1.895
309	WOMMUG	2.668	334	YUFBEG	1.734
310	WOVVEI	2.670	335	YUSZUH	2.038
311	WUJWON	4.004	336	ZAHPOT	3.466
312	WUNWEH	3.512	337	ZAJZOZ	3.047
313	XARLOR	2.844	338	ZALREJ01	1.676
314	XATWAQ	6.865	339	ZATTAP	1.949
315	XEBBAH	3.894	340	ZAYRUM	3.771
316	XEHTUZ	2.887	341	ZECHOE	5.370
317	XEYHUE	2.689	342	ZELLOR	3.930
318	XIKCOJ01	1.930	343	ZELVER	5.213
319	XIQBAA	1.430	344	ZEXQAU	0.055
320	XOGCAX	3.331	345	ZIBXUD	5.989
321	XOQVAA	3.456	346	ZIVTAZ	3.592
322	XOYGAT	3.221	347	ZORBUD	1.763
323	XUHPAR	2.456	348	ZOWCOD	5.626
324	XUSYUF	2.477	349	ZUKTUU	1.718
325	YAGLUN	4.518	350	ZZZBZD10	2.660

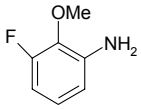
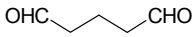
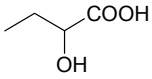
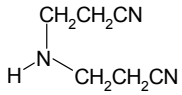
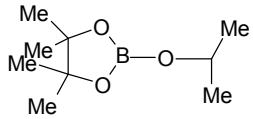
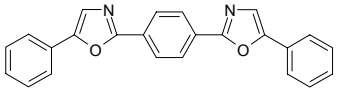
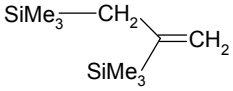
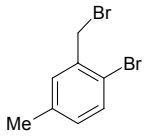
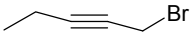
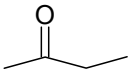
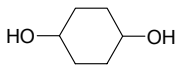
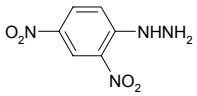
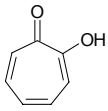
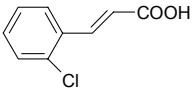
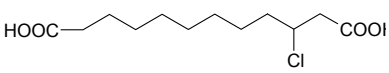
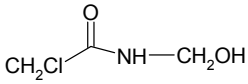
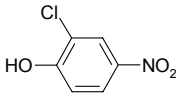
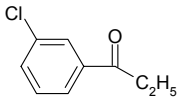
Table 4: 200 Compounds selected randomly from the Aldrich catalogue (2003-2004)

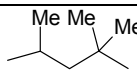
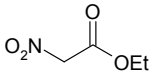
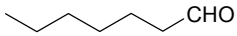
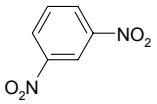
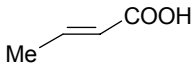
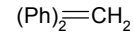
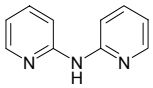
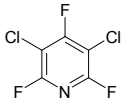
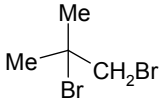
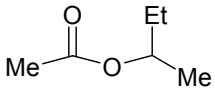
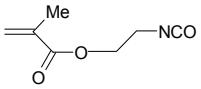
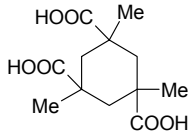
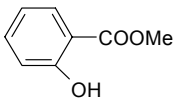
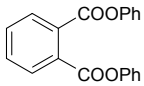
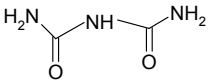
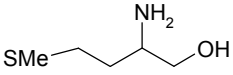
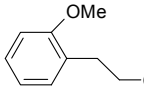
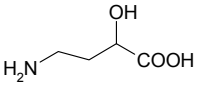
No	Page. No	Catalogue No	Compound name	Structure	Dipole moment (D)
1	283	55,489-8	1-Bromo-3,7,-dimethyloctane		1.799
2	1743	T1,340-4	5,6,7,8-Tetrahydro-1-naphthol		1.757
3	627	42,264-9	4,5-Dichlorophthalonitrile		3.486
4	1253	12,989-5	3-Methylisoquinoline		1.850
5	536	40,993-6	Cyclohexyl vinyl ether		1.839
6	1449	45,046-4	4,4'-(1,3-Phenylenediisopropylidine)bisphenol		2.188
7	625	47,191-7	3,4-Dichlorophenylboronic acid		1.714
8	1283	29,004-1	(1S,2S)-(+)-N-Methylpseudoephedrine		1.001
9	1803	T4,580-2	2,4,6-Triaminopyrimidine		1.733
10	1225	15,144-0	Methyl chlorooxoacetate		2.355
11	83	35,962-9	L-α-[2-(2-Aminoethoxy)vinyl]glycine hydrochloride		5.102
12	1702	56,689-0	1-(3-Sulfophenyl)-3-methyl-5-pyrazolone		6.189
13	1906	11,013-2	Valeraldehyde		2.563
14	1893	33,367-0	Tri(trimethylsilyl)phosphine		0.030
15	1593	55,771-4	3-Propoxyphenylboronic acid		4.521

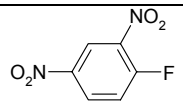
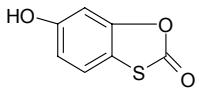
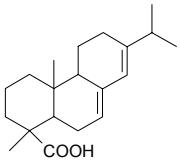
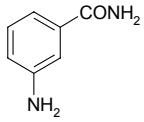
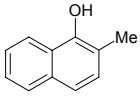
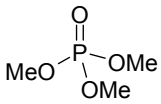
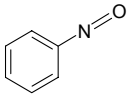
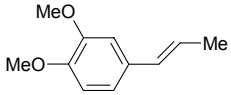
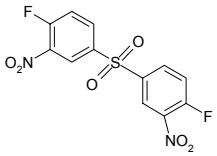
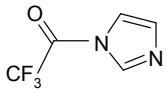
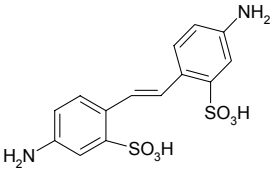
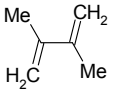
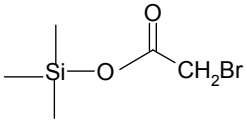
16	1761	16,220-5	2,3,5,6-Tetramethyl-p-xylene-α,α'-diol		0.020
17	1822	75,930-7	Triethyl borate		2.627
18	443	49,818-1	2-Chloro-5-iodopyridine		2.018
19	1765	27,845-9	1,3,4,6-Tetrathiapentalene-2,5-dione		0.009
20	1777	21-531-7	3-Thiophenemalonic acid		1.446
21	1267	13,744-8	2-Methyl-2-oxazoline		0.969
22	1286	24,279-9	1-Methyl-2-pyrrolidinone		3.589
23	1287	10,982-8	6-Methylquinoline		2.010
24	1984	M7,825-9	1-Methyl-2-pyridone		3.724
25	1869	92776	O-(Trimethylsilyl)hydroxylamine		0.559
26	740	13,801-0	4,6-Dimethyl-2-mercaptopyrimidine		2.706
27	770	25,624-2	1,4-Dioxane –2,3 diol		3.104
28	1313	M8,961-7	Mucic acid		3.523
29	1187	56,129-0	6-Methoxy-2-(4-methoxyphenyl)benzo[b]thiophene		0.625
30	1867	23,511-3	Trimethylsilylbromoacetate		1.477
31	915	49,324-6	2-Fluoro-2-methylphenylpyridine		3.147

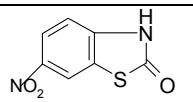
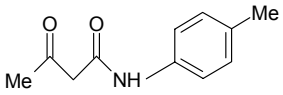
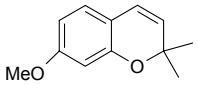
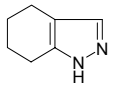
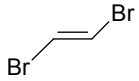
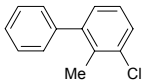
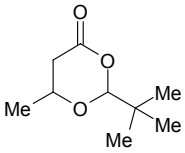
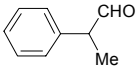
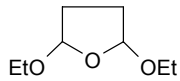
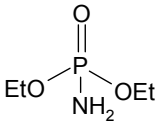
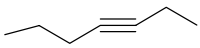
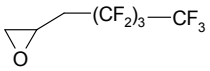
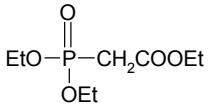
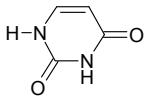
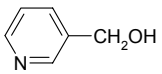
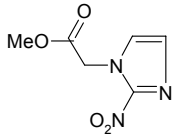
32	1877	55,324-7	R-(+)-1,2,2-Triphenylethylamine		1.663
33	741	15,201-3	2,3-Dimethyl-4-methoxybenzaldehyde		2.862
34	527	27,062-8	Cyclohexane		0.00
35	776	D20,655-5	Diphenyl chlorophosphate		3.023
36	1285	M7,880-1	1-Methylpyrrole		2.248
37	1022	21,707-7	6-Hydroxy-1,3-benzoxathiol-2-one		5.144
38	244	29,014-9	2,4-Bis(trifluoromethyl) benzly bromide		2.936
39	248	47,291-3	3,3'-Bithiophene		0.336
40	267	30,127-2	2-Bromoacetamide		2.936
41	771	40,698-8	3,6-Dioxaoctanedioic acid		5.610
42	543	56,020-0	3-(Cyclopropylamine) propinonitric		3.946
43	1597	P5-320,9	Propylene sulfide		2.326
44	649	30,827-7	Di (ethylone glycol) diethyl ether		1.241
45	723	46,560-7	N,N-Dimethylbenzotriazolemethanamine		4.190
46	1293	26,926-3	3-Methyltetrahydropyrane		1.522
47	785	41,595-2	Diphenyl (2,4,6)-trimethyl benzyle) phsphine oxide		4.599
48	801	29,807-7	δ-Dodecanolactone		4.689

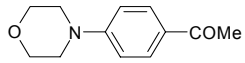
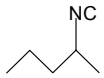
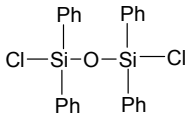
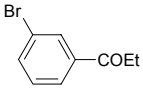
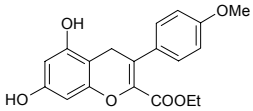
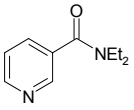
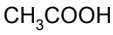
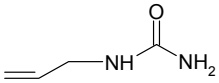
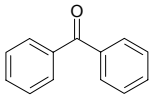
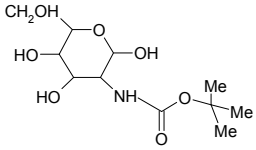
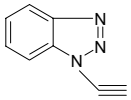
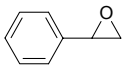
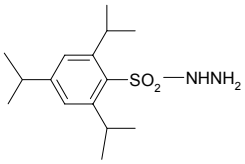
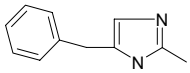
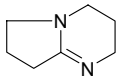
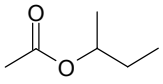
49	897	F60-2	Flavone		3.566
50	1035	23,542-3	3-Hydroxy-4-methoxymandelic acid		2.058
51	1209	30,510-3	Methyl-3-amino-5-chlorobenzoate		0.677
52	1265	47,834-2	2-Methyl-5-nitrophenylisocyanate		5.179
53	629	33,339-5	Dichlorosilane		1.758
54	1379	16,129-2	1,7-Octadiyne		0.281
55	1465	22,646-7	Phenyl thiotrimethyl silane		3.029
56	275	15,424-5	4-Bromo-2-chloroaniline		2.878
57	762	30,237-6	1,3-Dimorpholino-2-nitropropane		4.489
58	1477	19,737-8	Picric acid		1.531
59	1589	27,049-0	2-Propanol		1.691
60	1079	21,502-3	3-Iodothiophene		1.670
61	741	15,201-3	2,3-Dimethyl-4-methoxybenzenebenzaldehyde		3.636
62	789	26,944-1	2,3-Di-2-pyridyl-2,3-butane diol		4.714
63	845	E1,685-6	Ethylchloroacetate		2.090

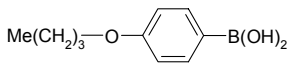
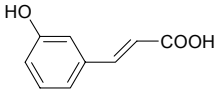
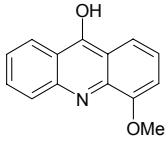
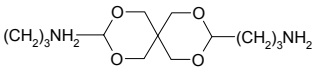
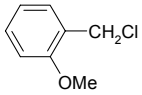
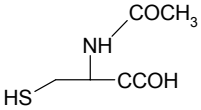
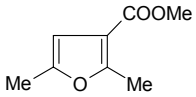
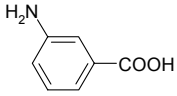
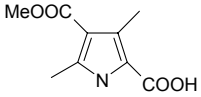
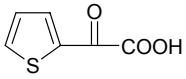
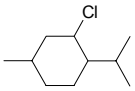
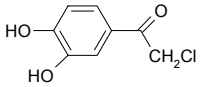
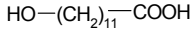
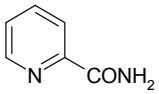
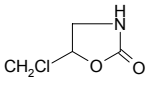
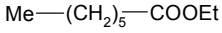
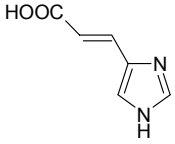
64	905	52,240-6	3-Fluoro-*o*-anisidine		1.972
65	953	34,085-5	Glutaric dialdehyde		3.259
66	1023	54917	(R)-2-Hydroxybutyric acid		3.746
67	1061	31,730-6	3,3'-Imonodipropionitrile		2.723
68	1099	41,714-9	2-Isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane		2.398
69	239	25,739-7	1,4-Bis(5-phenyloxazol-2-yl)benzene		3.318
70	247	43,417-5	2,3-Bis(trimethylsilyl)-1-propene		0.173
71	297	55,338-7	2-Bromo-5-methylbenzylbromide		2.574
72	305	42,953-8	1-Bromo-2-pentyne		1.783
73	329	23,029-4	2-Butanone		2.788
74	529	C10,120-6	1,4-Cyclohexanediol		0.000
75	767	D19-930-3	2,4-Dinitrophenylhydrazine		7.061
76	1897	T8,970-2	Tropolone		3.340
77	421	C3,139-2	2-Chlorocinnamic acid		3.122
78	429	39,621-4	3-Chlorododecanedioic acid		2.727
79	441	42,283-5	2-Chloro-N-(hydroxymethyl)acetamide		2.336
80	457	C6,120-8	2-Chloro-4-nitrophenol		4.617
81	469	24,819-3	3-Chloropropiophenone		4.398

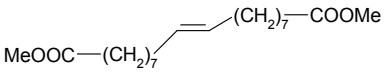
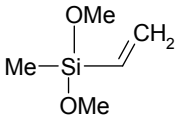
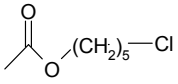
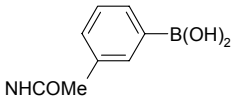
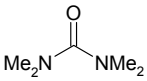
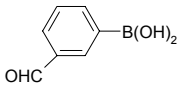
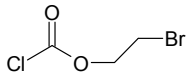
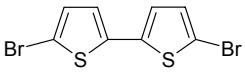
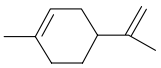
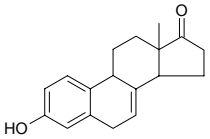
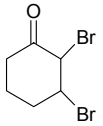
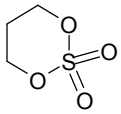
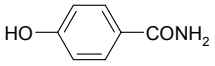
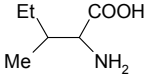
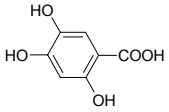
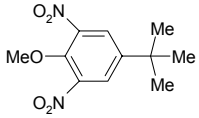
82	1863	15,501-2	2,2,4-Triethylpentane		0.014
83	877	19,233-3	Ethyl nitroacetate		5.346
84	975	H212-0	Heptaldehyde		2.554
85	763	D19,425-5	1,3-Dinitrobemzene		4.836
86	515	11,301-8	Crotonic acid		2.961
87	777	D20,680-6	1,1-Diphenylethylene		0.058
88	788	D21,640-2	2,2'-Dipyridylamine		1.001
89	631	24,801-0	3,5-Dichloro-2,4,6-trifluoropyridine		1.498
90	589	25,162-3	1,2-Dibromo-2-methylpropane		0.575
91	341	24,259-4	s-Butyl actetate		1.552
92	1095	47,706-0	2-Isocyanatoethyl methacrylate		3.941
93	1111	34,228-9	Kemp's triacid		1.811
94	1287	24,082-6	Methyl salicylate		2.217
95	782	10,588-0	Diphenyl phthalate		4.979
96	249	B5,420-7	Biuret		5.292
97	1177	47,001-5	(R)-(+)-Methioninol		2.163
98	1193	18,792-5	2-Methoxyphenethylalcohol		2.842
99	88	46,735-9	(S)-(-) 4-Amino-2-hydoxybutyric acid		2.569

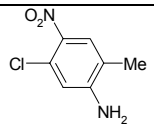
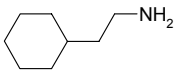
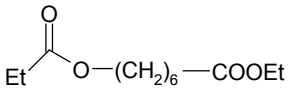
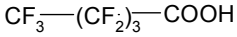
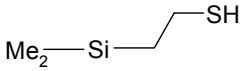
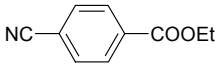
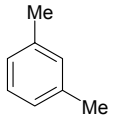
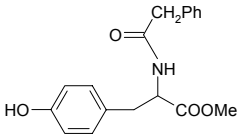
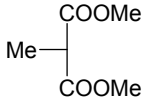
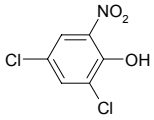
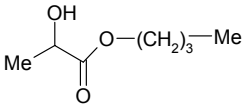
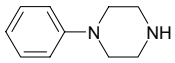
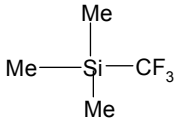
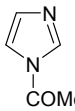
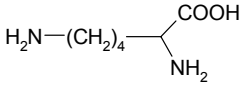
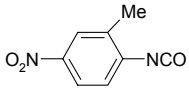
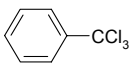
100	765	D19,680-0	2,4-Dinitrofluorobenzene		4.358
101	1022	21,707-7	6-Hydroxy-1,3-benzoxathiol-2-one		5.135
102	1	16,502-6	Abietic acid		2.098
103	69	25,301-4	3-Aminobenzamide		3.787
104	1261	16,284-1	2-Methyl-1-naphthol		1.227
105	1865	13,219-5	Trimethyl phosphate		2.815
106	1361	N2,460-9	Nitrosobenzene		2.747
107	707	D13,690-5	1,2-Dimethoxy-4-propenyl benzene		2.037
108	917	F1,170-0	4-Fluoro-3-nitrophenyl sulfone		8.223
109	1827	34,612-8	1-(Trifluoroacetyle)imidazole		0.909
110	573	46,226-8	4,4'-Diamino-2,2'stillbenedisulfonic acid		5.994
111	37	11,020-1	Acrolein		2.610
112	725	14-549-1	2,3-Dimethyl-1,3-butadiene		0.185
113	1867	23,511-3	Trimethylsilyl bromoacetate		1.546

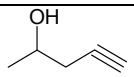
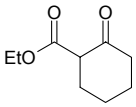
114	1345	44,192-9	6-Nitro-2-benzotriazolinone		3.607
115	9	53,706-3	*o*-Acetoacetoluidide		2.142
116	1583	19,585-5	Precocene 1		1.950
117	1741	44,552-5	4,5,6,7-Tetrahydroindazole		2.850
118	587	D4,080-9	1,2-Dibromoethylene		0.001
119	447	36,162-3	3-Chloro-2-methylbiphenyl		1.274
120	359	20264	(R)-2-tert-Butyl-6-methyl-1,3-dioxin-4-one		3.157
121	21	29,315-6	Acetyl-1-^{13}C chloride	CH_3COCl	2.738
122	1459	24,136-9	2-Phenylpropionaldehyde		2.656
123	639	26,264-1	2,5-Diethoxytetrahydroxyfuran		0.150
124	657	36,539-6	Diethyl phosphoramidate		2.307
125	979	38,361-0	3-Heptyne		0.108
126	1369	47,405-5	(2,2,3,3,4,4,5,5,5)-Nonefluoropentyl) oxirane		3.370
127	1825	29,318-0	Triethyl phosphonacetate		1.532
128	1904	48,626-4	Uracil		4.300
129	1612	P6,680-7	3-Pyridylcarbinol		0.992
130	1264	40,802-6	Methyl-2-nitro-1-imidaoleacetate		4.174

131	1312	11,986-5	4'-Morpholineacetophenone		3.309
132	1424	53,619-9	2-Pentyl isocyanide		3.043
133	630	45,483-4	1,3-Dichlorotetraphenyldisilaoxane		4.017
134	311	19,049-7	3-Bromopropiophenone		1.568
135	384	C330-8	2-Carbethoxy-5,7-dihydroxy-4'-methoxyisoflavone		2.877
136	655	D9,880-7	N,N'-Diethylnicotinamide		3.633
137	7	53,702-0	Acetic acid		1.890
138	56	A3,680-8	Allylurea		3.413
139	168	27,773-8	Benzophenone		2.971
140	334	38,131-4	N-(tert-Butoxycarbonyl)-D-glucosamine		3.734
141	1590	44,694-7	1-Propargyl-1H-benzotrizole		3.947
142	1695	54,009-9	(R)-(+)-Styrene oxide		1.811
143	1848	19,219-8	2,4,6-Triisopropylbenzenesulfonyl hydrazide		4.600
144	188	36,971-3	1-Benzyl-2-methylimidazole		3.932
145	160	31,995-3	Benzene		0.000
146	11	27,072-5	Acetone		2.921
147	575	13,658-1	1,5-Diazabicyclo[4.3.0]one-5-ene		2.587
148	341	24,259-4	s-Butyl acetate		1.706

149	340	54,250-4	4-Butoxyphenylboronic acid		3.896
150	1024	H2,3007	3-Hydroxycinnamic acid		1.462
151	1033	H3,590-0	9-Hydroxy-4-methoxyacridine		3.097
152	1761	45,447-8	2,4,8,10-Tetraoxaspiro[5.5]undeecane-3,9-dipropanamine		1.230
153	131	25,470-3	*o*-Anisoyl chloride		1.110
154	21	13,806-1	N-Acetyl-L-cysteine		1.687
155	1233	26,362-1	Methyl 2,5-dimethyl-3-furoate		2.193
156	69	12,767-1	3-Aminobenzoic acid		2.849
157	22	A1,500-2	4-Acetyl-3,5-dimethyl-2-pyrrolecarboxylic acid		2.576
158	1776	22,227-5	2-Thiopheneglyoxylic acid		3.270
159	1161	24,924-6	(-)-Menthyl chloride		1.639
160	424	C3,440-5	2-Chloro,3',4'-dihydroxyacetophenone		2.928
161	1025	19,878-1	12-Hydroxydodecanoic acid		2.055
162	1475	10,405-1	Picolinamide		2.972
163	449	13,565-8	5-Chloromethyl-2-oxazolidinone		5.439
164	1369	25,951-9	3-Nonanone		2.616
165	1905	28,746-6	*cis*-Vacecnic acid		2.726

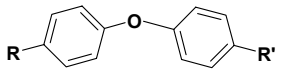
166	1266	26,803-8	Methyl oleate		4.551
167	703	44,620-3	Dimethoxymethylvinylsilane		0.894
168	458	38,787-8	5-Chloropentyl acetate		2.880
169	4	56,601-2	3-Acetamidophenylboronic acid		3.406
170	1760	T2,450-3	1,1,3,3-Tetramethyurea		3.166
171	935	44,165-1	3-Formylphenylboronic acid		4.501
172	285	36,897-0	2-Bromoethyl chloroformate		1.480
173	583	51,549-3	5,5'Dibromo-2,2'-bithiophene		0.256
174	1125	21,836-7	(S)-(-)-Limonene		0.378
175	817	49,252-3	Equiline		2.318
176	587	32,416-3	2,5-Dibromo-3-4-hexanedione		3.596
177	1585	46,416-3	1,3-Propanediol cyclic sulfate		4.372
178	1020	27,025-3	4-Hydroxybenzamide		2.791
179	1095	15,171-8	L-Isoleucine		3.051
180	1845	25,384-7	2,3,4-Trihydroxybenzoic acid		0.822
181	351	56-568,7	4-tert-Butyl-2,6-dinitroanisole		5.216

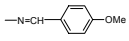
182	457	20,120-0	5-Chloro-4-nitro-o-toluidine		7.680
183	531	25,586-6	2-(1-Cyclohexyl)ethylamine		1.380
184	658	D10,060,9	Diethyl suberate		5.295
185	1368	39,657-5	Nonafluoropentanoic acid		1.433
186	1867	36,468-1	2-(Trimethylsilyl)ethanethiol		1.726
187	846	E1,860-3	Ethyl-4-cyanobenzoate		2.553
188	1921	29,632-5	m-Xylene		0.278
189	1940	54,703-4	Z-D-tyrosine methyl ester		6.973
190	741	34,028-6	Dimethyl methylmalonate		1.490
191	622	22,543-6	2,4-Dichloro-6-nitrophenol		3.040
192	356	28,332-0	Butyl lactate		2.117
193	1457	P3,000-4	1-Phenylpiperzine		1.535
194	1873	48,871-2	Trimethyl(trifluoromethyl) silane		3.778
195	24	37,710-4	1-Acetylindole		1.059
196	1144	28,170-0	D-Lysine		2.072
197	1264	47,818-0	2-Methyl-4-nitrophenylisocyanate		3.705
198	1816	14,789-3	α, α, α-Trichlorotoluene		2.279

199	1424	26,899-2	4-Pentyn-2-ol		1.415
200	847	E2,000-4	Ethyl-2-cyclohexanonecarboxylate		1.496

Appendix II

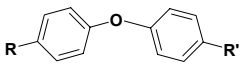
Table 5: Compounds synthesized in this study, their space groups and dipole moments.

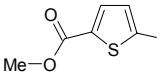
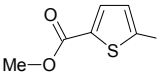
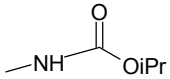
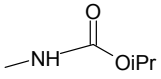
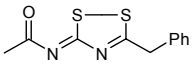
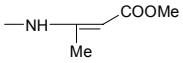
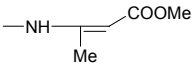
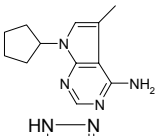
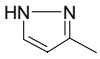
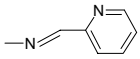
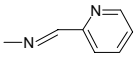
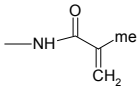
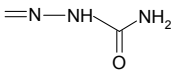
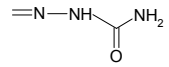
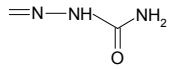
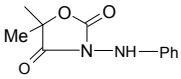
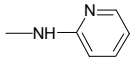
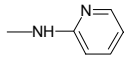
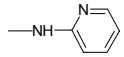
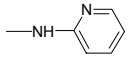


No	R	R'	Dipole moment (D)	SG (Z')	No	R	R'	Dipole moment (D)	SG
1	$-NH_2$	–OMe	2.272	$P2_1$ (1)	15	$-NH_2$	– Me	2.522	$P2_12_12_1$ (1)
2	–OH	$-NO_2$	5.269	$P2_1/n$ (1)	16	–CN	$-NO_2$	3.514	$P2_1/c$ (1)
3	–OMe	$-NO_2$	6.551	$P2_1/c$ (1)	17	–CN	–CN	1.376	$P2_1/c$ (1)
4	–I	$-NO_2$	2.880*	$P2_1/c$ (2)	18	–Me	–CN	4.198	$P2_1/c$ (1)
5	–Cl	$-NO_2$	5.044	$P2_1/m$ (1)	19	–OMe	–CN	4.418	$P2_1/c$ (1)
6	–Br	$-NO_2$	3.127*	$P2_1/n$ (2)	20	–H	$-NO_2$	5.791*	$P\bar{1}$ (2)
7	$-C_2H$	$-NO_2$	6.182*	$P2_1/c$ (2)	21	$-NMe_2$	$-NH_2$	2.146	$P2_1/c$ (1)
8	–I	–CN	1.470	$P2_12_12_1$ (1)	22	–OMe	–COOH	1.838	$Pbca$ (1)
9	–Cl	–CN	1.517	$P2_1/c$ (1)	23	$-NMe_2$	–OH	2.996	$C2/c$ (1)
10	$-C_2H$	–CN	3.143*	$P2_1/n$ (5)	24	$-NH_2$	–CN	4.756	$P2_1/n$ (1)
11	–Br	–CN	2.036	$P2_1/c$ (1)	25	$-NMe_2$	–OMe	3.648	Cc (1)
12	$-NMe_2$	$-NO_2$	8.007	$P2_1/n$ (1)	26	–OH		2.529	$Pna2_1$ (1)
13	$-NO_2$	$-NO_2$	3.472	$C2/m$ (0.5	27	–COOH	–COOH	2.302	$Pbca$ (1)
14	–Me	$-NO_2$	6.669	$P2_1/c$ (1)					

* For structures where Z' > 1, the average value of the dipole moment is given.

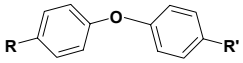
Table 6: Compounds from the CSD



NO	Refcode	R	R'	Dipole moment (D)	SG (Z')
1	BEQYOL			2.765	*Aba*2 (0.5)
2	EMOFER			0.324	*P*-1 (1)
3	ENANUC	$-NH_2$	–OH	3.419	Cc (1)
4	FUQBOI	$-NH_2$	$-NO_2$	6.475	$P2_1/c$ (1)
5	GOTPEK	–OMe		3.704	$P2_1/n$ (1)
6	HUHXIR			3.889	$P2_1/c$ (1)
7	ICAKOM	–H		4.021	*Pbca* (1)
8	NIBFIN	–H		2.953*	$P2_1/n$ (2)
9	QIKHOH			1.766	$P2_1/c$ (1)
10	SUCVER	$-NH_2$	$-NH_2$	3.089	$P2_12_12_1$ (1)
11	SUSCIS	–H		2.459	$P2_1$ (1)
12	SUSNID	–H		3.883	*Pbca* (1)
13	TUBQUC	–H		4.761	$P2_1/c$ (1)
14	TUBRAJ	–F		3.195	$P2_1/a$ (1)
15	TUBREN	–OMe		4.579	$P2_1/a$ (1)
16	XALTIN	–H		2.590	$P2_12_12_1$ (1)
17	XILQOY			2.040*	$P2_1/c$ (2)
18	XILQOY01			1.904*	*P*-1 (2)

* Where Z' > 1, the average value of the dipole moment is given.

Table7: List of compounds published but not yet in the CSD



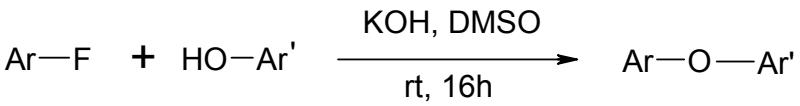
No	R	R'	Dipole moment (D)	SG (Z')	Reference no
1	$-NH_2$	–I	2.409	$Pna2_1$ (1)	9
2	$-NH_2$	–Cl	2.302	$Pna2_1$ (1)	9
3	$-NH_2$	$-C_2H$	2.367	$Pna2_1$ (1)	9
4	$-NH_2$	–Br	2.469	$Pna2_1$ (1)	9
5	–H	–H	1.297	$P2_12_12_1$ (1)	10
6	–H	–H	1.393	$P2_1/n$ (1)	10

* These references correspond to references in the main paper.

Appendix III

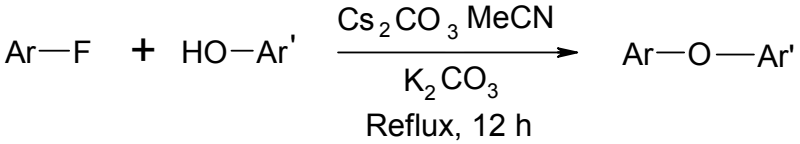
Synthesis

Method I



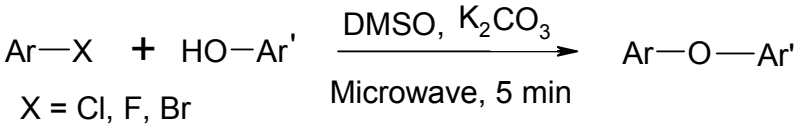
To a degassed solution of the phenol derivative (2 mmol) in DMSO, KOH (excess) and the appropriate fluoride derivative (2 mmol) were added and stirred at r.t. for 16 h. The reaction mixture was then poured in ice water and filtered. Purification by column chorography or recrystallization afforded the expected compounds.

Method II



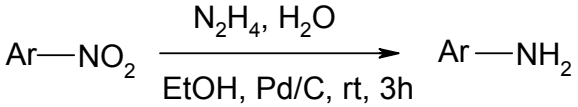
Equivalent amounts of the fluoride and the phenol were refluxed in MeCN with K_2CO_3 (2 equivalents) for 12 h. The usual work-up and purification by column chromatography afforded the required compounds.

Method III



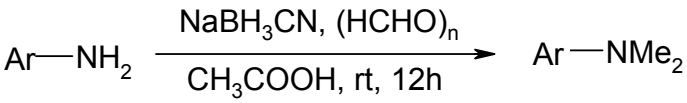
The appropriated aryl halide (10 mmol), phenol (10-12 mmol) and anhydrous K_2CO_3 were sequentially added to 50 ml of DMSO with the use of microwave power of 300 W for 5 min. After completion of the reaction, the mixture was cooled to r.t., poured into ice water and stirred for 30 min to precipitate the product, which was worked up as before.

Method IV



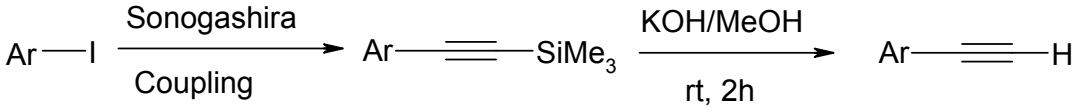
The nitro derivative (10 mmol) was dissolved in EtOH. A catalytic amount of Pd/C, $N_2H_4.H_2O$ (100 mmol) were added and stirred for 3 h at r.t. The reaction mixture was filtered and the product purified by recrystallisation.

Method V



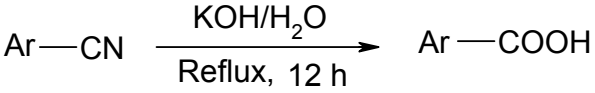
The aniline derivative (5 mmol), $NaBH_3CN$ (20 mmol) and $(HCHO)_n$ (50 mmol) were taken in 10 ml AcOH and stirred at r.t. for 12 h. The reaction mixture was made alkaline with excess NaOH and work up was as before.

Method VI



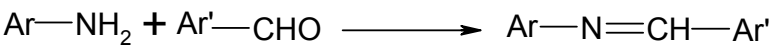
We followed the typical Sonogashira coupling procedure. [1]

Method VII



The appropriate cyanobezene derivative was refluxed in excess aqueous NaOH in H_2O for 12 h. The neutralization followed by the usual work-up and purification afforded the required acid.

Method VIII



The aniline (10 mmol) and benzaldehyde (10 mmol) were dissolved in MeOH and refluxed for 6 h. The product was purified by recrystallisation.

Table 8: Synthesis and characterization of compounds **1-27.**

Compound	Method used	Characterization	Reference
1	I and IV	^{1}H-NMR (DMSO-d^6) 6.84 (4H, m), 6.69 (2H, d, J8) 6.53 (2H, d, J8), 4.89 (2H, s) and 3.70 (3H, s); mp: 79˚C	-
2	I	^{1}H-NMR ($CDCl_3$); 8.21(2H, d, J8), 6.93 (6H, m); mp: 173˚C	-
3	I	^{1}H-NMR ($CDCl_3$); 8.20 (2H, d, J8), 6.82-7.22 (6H, m) and 3.76 (3H, s); mp: 110˚C	2
4	I	^{1}H-NMR ($CDCl_3$); 8.23 (2H, d, J8), 7.71 (2H, d, J8), 7.01 (2H, d, J8) and 6.91 (2H, d, J8); mp: 65˚C	3
5	I	^{1}H-NMR ($CDCl_3$); 8.23 (2H, d, J8), 7.55 (2H, d, J8) and 7.04 (4H, m); mp: 75˚C	4
6	I	^{1}H-NMR ($CDCl_3$); 8.21 (2H, d, J8), 7.44 (2H, d, J8) and 7.06 (4H, m); mp: 74˚C	-
7	I and VI	^{1}H-NMR ($CDCl_3$); 8.23 (2H, d, J8), 7.56 (2H, d, J8), 7.04 (4H, m) and 3.10 (1H, s); mp: 84˚C	5
8	II	^{1}H-NMR ($CDCl_3$); 7.70 (2H, d, J8), 7.60 (2H, d, J8), 7.99 (2H, d, J8) and 6.84 (2H, d, J8); mp: 81˚C	-
9	II	^{1}H-NMR ($CDCl_3$); 7.85 (2H, d, J8), 7.47 (2H, d, J8) and 7.06 (4H, m); mp: 83˚C,	-
10	II	^{1}H-NMR ($CDCl_3$); 7.64 (2H, d, J8), 7.53 (2H, d, J8), 7.02 (4H, m) and 3.09 (1H, s); mp: 76˚C	-
11	II	^{1}H-NMR ($CDCl_3$); 7.46 (2H, d, J8), 7.52 (2H, d, J8) and 6.55 (4H, m); mp: 85˚C	-
12	I and V	^{1}H-NMR ($CDCl_3$); 8.18 (2H, d, J8), 6.96 (4H, m), 6.77 (2H, d, J8) and 2.99 (6H, s); mp: 140˚C	-
13	I	^{1}H-NMR ($CDCl_3$); 8.33 (4H, d, J8) and 7.16 (4H, d, J8); mp: 145˚C	6
14	I	^{1}H-NMR ($CDCl_3$); 8.19 (2H, d, J8), 6.96-7.25 (6H, m) and 2.38 (3H, s); mp: 70˚C	2
15	I and VI	^{1}H-NMR (DMSO-d^6) 6.88 (4H, m), 6.69 (2H, d, J8) 6.53 (2H, d, J8), 4.85 (2H, s) and 2.26(3H, s); mp: 117˚C	-
16	III	^{1}H-NMR ($CDCl_3$); 8.28 (2H, d, J8), 7.71 (2H, d, J8) and 7.13 (4H, m); mp: 159	7
17	III	^{1}H-NMR ($CDCl_3$); 7.71 (4H, d, J8) and 7.13 (4H, d, J8); mp: 185˚C	7
18	III	^{1}H-NMR ($CDCl_3$); 7.57 (2H, d, J8), 7.19 (2H, d, J8), 6.96 (4H, m) and 2.37 (3H, s); mp: 70˚C	7
19	III	^{1}H-NMR ($CDCl_3$); 7.57 (2H, d, J8) and 6.95 (6H, m) and 3.83(3H, s), mp: 108˚C	7
20	I	^{1}H-NMR ($CDCl_3$); 8.22 (2H, d, J8), 7.43 (3H, m), 7.10 (2H, d, J8) and 7.01 (2H, d, J8); mp: 56˚C	2
21	I, IV and V	^{1}H-NMR ($CDCl_3$); 6.89 (2H, d, J8), 6.84 (2H, d, J8), 6.71 (2H, d, J8), 6.64 (2H, d, J8), 3.49 (2H, s) and 2.90 (6H, s), mp: 96˚C	-
22	III and VII	^{1}H-NMR ($CDCl_3$); 8.03 (2H, d, J8), 7.03 (2H, d, J8), 6.94 (4H, m) and 3.32 (3H, s), mp: 180˚C	-
23	I, IV and V	^{1}H-NMR ($CDCl_3$); 6.69-6.92 (8H, m) and 2.91 (6H, s), mp; 138˚C	-
24	III and IV	^{1}H-NMR ($CDCl_3$); 7.55 (2H, d, J8), 6.93 (4H, m) and 6.72 (2H, d, J8), mp: 106˚C	-
25	I, IV and V	^{1}H-NMR ($CDCl_3$); 6.75-6.92 (8H, m), 3.78 (3H, s) and 2.92 (6H, s); mp: 60˚C	-
26	I, IV and VIII	^{1}H-NMR ($CDCl_3$); 8.47 (1H, s), 7.8.7 (2H, d, J8), 6.99 (2H, d, J8), 6.93 (2H, d, J8), 6.96 (6H, m) and 3.87 (3H, s); mp: 157˚C	-
27	III and VII	^{1}H-NMR, 8.10 (4H, d, J8) and 7.02 (4H, d, J8); mp: ≈ 300˚C	8

Reference:

1. S. Takahashi, Y. Kuroyama, K. Sonogashira and N. Hagihara, *Synthesis,* 1980, 627.

2. S. M. S. Chauhan, N. Jin, A. Kumar, K. A. Srinivas; *Synthetic Communications*, 2003, **33**, 3607.

3. C. Bjorklund and R. Wahren, *Acta Chemica Scandinavica, Series B: Organic Chemistry and* Biochemistry, 1976, **B30**, 576.

4. W. Xu, R. Mohan, M. M. Morrissey; *Tetrahedron Letters*, 1997, **38***,* 7737.

5. R. D. Rutuja. V. M. Alexander and M. K. Bhushan, *Tetraredron Letters*. 2002, **43**, 9457.

6. A. D. Sagar, R. H. Tale and R. N. Adude, *Tetrahedron Letters*, 2003, **44**, 7061.

7. F. Li, Q. Wang, Z. Ding, and F. Tao, *Org. Lett*, 2003, **5**, 2169.

8. L. S. Shimizu, A. D. Hughes, M. D. Smith, M. J. Davis, B. P. Zhang, L. Zur and K. D. Shimizu, *J. Am. Chem. Soc*. 2003, **125**, 14972.

Table 9: Crystallographic data for compounds **1**-**27**

NO	Chemical formula	Solvent of crystallisation	Crystal system	Space Group	T(K)	Cell lengths (Å)	Cell angles (deg)	Z	V (Å^3)	R_{int}	Reflections with $I > 2\sigma(I)$	R_1 [$(I>2\sigma(I)$] wR_2	GOF	Structural description
1	$C_{13}H_{13}NO_2$	1:1 EtOAc–hexane	Monoclinic	$P2_1$	120(2)	7.5729(5) 5.4503(4) 13.4175(9)	90 94.077(2) 90	2	552.40(7)	0.0343	1989	0.0328	0.913	Structural pattern same as compounds in reference **9**.
2	$C_{12}H_9NO_4$	1:1 EtOAc–hexane	Monoclinic	$P2_1/n$	298(2)	11.2437(17) 5.3306(8) 17.601(3)	90 94.891(1) 90	4	1051.1(3)	0.0094	1674	0.0382	1.041	NO_2 forms dimer with O–H...O and C–H...O.
3	$C_{13}H_{11}NO_4$	1:1 EtOAc–hexane	Monoclinic	$P2_1/c$	120(2)	12.3992(3) 7.4839(2) 12.2812(3)	90 101.431(1) 90	4	1117.02(5)	0.0426	2039	0.0360	1.043	Close packing only with C–H...O.
4	$C_{12}H_8INO_3$	EtOAc	Monoclinic	$P2_1/n$	243(2)	9.547(14) 28.28(4) 10.080(14)	90 117.06(2) 90	8	2424(6)	0.0459	2198	0.0885	1.034	As in **3**.
5	$C_{12}H_8ClNO_3$	1:1 EtOAc–hexane	Monoclinic	$P2_1/m$	243(2)	10.0600(6) 7.2712(5) 15.6390(10)	90 97.4580(10) 90	4	1134.29(13)	0.0283	2467	0.0530	1.066	As in **3**.
6	$C_{12}H_8BrNO_3$	1:1 EtOAc–hexane	Monoclinic	$P2_1/n$	100(2)	9.1199(9) 27.782(3) 9.8887(9)	90 116.7450(10) 90	4	2237.4(4)	0.0282	3779	0.0411	1.035	As in **3**.
7	$C_{14}H_9NO_3$	$CDCl_3$	Monoclinic	$P2_1/c$	298(2)	14.866(2) 8.8944(14) 19.496(3)	90 111.771(2) 90	8	2393.9(6)	0.0398	2617	0.0736	1.023	As in **3**.
8	$C_{13}H_8INO$	EtOAc	Orthorhombic	$P2_12_12_1$	298(2)	5.325(4) 7.960(5) 28.285(19)	90 90 90	4	1198.8(14)	0.0286	1815	0.0503	1.129	Short C–I...N (d = 3.4 Å).
9	$C_{13}H_8ClNO$	Toluene	Monoclinic	$P2_1/c$	100(2)	12.3125(17) 7.3792(10) 11.8045(17)	90 98.385(2) 90	4	1061.0(3)	0.0649	2145	0.0443	1.076	Close packing only with C–H...N.
10	$C_{15}H_9NO$	EtOAc	Monoclinic	$P2_1/n$	100(2)	15.5731(11) 21.7581(16) 18.1368(13)	90 111.5700(10) 90	20	5715.1(7)	0.0712	6469	0.0493	0.920	Close packing only with C–H...N with

														additional C–H...π.
11	$C_{13}H_8BrNO$	Toluene	Monoclinic	$P2_1/c$	100(2)	12.3919(18) 7.3765(11) 11.9824(18)	90 98.842(2) 90	4	1082.3(3)	0.0404	1898	0.0324	1.264	Same as compound **9.**
12	$C_{14}H_{14}N_2O_3$	1:1 EtOAc–hexane	Monoclinic	$P2_1/n$	298(2)	5.8340(9) 28.698(4) 7.6833(12)	90 90.208(2) 90	4	1286.3(3)	0.0448	1852	0.0482	1.050	Closed pack structure with herringbone.
13	$C_{12}H_8N_2O_5$	1:0.5 $CHCl_3$–Benzene	Monoclinic	$C2/c$	100(2)	12.4081(17) 9.2706(17) 9.8031(13)	90 94.614(2) 90	4	1124.0(3)	0.0219	1010	0.0361	1.057	Close packed structure with C–H...O.
14	$C_{13\ 11}N\ O_3$	1:1 EtOAc–hexane	Monoclinic	$P2_1/c$	100(2)	7.6100(11) 8.8817(13) 16.410(2)	90 94.682(2) 90	4	1105.4(3)	0.0190	1907	0.0379	1.062	As above.
15	$C_{13}H_{13}NO$	1:1 EtOAc–hexane	Orthorhombic	$P2_12_12_1$	298(2)	5.8600(11) 7.8153(15) 23.130(4)	90 90 90	4	1059.3(3)	0.0379	1115	0.0407	1.091	As in **1**.
16	$C_{13}H_8N_2O_3$	1:1 EtOAc–hexane	Monoclinic	$P2_1/c$	298(2)	13.374(3) 7.2793(16) 11.782(3)	90 104.415(2) 90	4	1110.9(4)	0.0265	1361	0.0637	1.104	C–H...N dimer with additional C–H...O.
17	$C_{1\ 4}H_8\ N_2\ O$	1:1:0.5 EtOAc–MeCN–toluene	Monoclinic	$P2_1/c$	298(2)	12.5909(18) 7.4306(11) 11.8337(17)	90 96.601(2) 90	4	1099.8(3)	0.0296	1467	0.0442	1.041	C–H...N dimer.
18	$C_{14}H_{11}NO$	1:1 EtOAc–hexane	Monoclinic	$P2_1/c$	298(2)	12.5167(19) 6.7036(10) 13.680(2)	90 92.477(2) 90	4	1146.8(3)	0.0194	1585	0.0516	1.050	No specific interactions.
19	$C_{14}H_{11}NO_2$	1:1 EtOAc–hexane	Monoclinic	$P2_1/c$	298(2)	12.319(2) 7.9156(14) 12.276(2)	90 106.166(2) 90	4	1149.7(3)	0.0154	1815	0.0425	1.045	As in **18**.
20	$C_{12}H_9NO_3$	1:1 EtOAc–hexane	Triclinic	$P\bar{1}$	298(2)	6.7833(14) 8.9802(18) 17.306(4)	87.76(3) 88.25(3) 88.88(3)	4	1052.7(4)	0.0000	1371	0.0511	0.987	C–H...O dimer
21	$C_{14}H_{16}N_2O$	1:1 EtOAc–hexane	Monoclinic	$P2_1/c$	298(2)	9.0473(17) 17.419(3) 7.9560(15)	90 94.488(4) 90	4	1250.0(4)	0.1207	559	0.0425	0.617	N–H...N and C–H...O

22	$C_{14}H_{12}O_4$	1:2 MeOH–THF	Orthorhombic	*Pbca*	298(2)	7.4742(11) 5.9733(8) 53.194(7)	90 90 90	8	2374.9(6)	0.0550	1475	0.0730	1.143	Acid dimer and zigzag C–H...O.
23	$C_{14}H_{15}NO_2$	1:1 EtOAc–toluene	Monoclinic	*C*2/*c*	298(2)	18.654(4) 13.836(3) 9.885(2)	90 98.084(3) 90	8	2525.9(9)	0.0273	1446	0.0488	1.025	Forms square motif with O–H...N and C–H...O.
24	$C_{13}H_{10}N_2O$	Toluene	Monoclinic	$P2_1/n$	298(2)	11.6484(19) 5.6103(10) 16.746(3)	90 100.581(3) 90	4	1075.7(3)	0.0528	1121	0.0803	1.100	$–NH_2$ saturates its coordination
25	$C_{15}H_{17}NO_2$	EtOAc	Monoclinic	*Cc*	298(2)	28.046(5) 7.5638(14) 6.3222(12)	90 96.738(2) 90	4	1331.9(4)	0.0324	1641	0.0469	1.023	No specific interactions.
26	$C_{20}H_{17}NO_3$	MeOH	Orthorhombic	$Pna2_1$	298(2)	6.137(2) 7.451(2) 34.981(12)	90 90 90	4	1599.5(9)	0.0247	1278	0.0296	1.159	Molecules propagate with C–H...O.
27	$C_{14}H_{10}O_5$	1:1 MeOH–EtOAc	Orthorhombic	*Pbca*	298(2)	27.516(12) 14.904(7) 5.724(3)	90 90 90	8	2347.4(18)	0.2816	689	0.0638	0.930	Acid dimer