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**Supporting information for article:**

**2,2'-Dithiobispyrazine: about the disulfide bond**

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**Table S1** Selected geometrical parameters of disulphide compounds. For torsion angles absolute values are presented.

Refcode	C-S [Å]	C-S-S-C [°]	S-S [Å]
MAVKON	1.741	80.045	2.058
SASZAR	1.759	79.744	2.055
ABOJUX	1.76	89.712	2.057
ACEYEN	1.797	83.479	2.06
ACEYEN01	1.792	82.435	2.061
ADEPUJ	1.732	52.085	2.135
AFOPAO	1.791	96.757	2.061
AGOKOW	1.764	84.451	2.028
AGOKOW01	1.767	84.051	2.033
AHUFOZ	1.796	101.698	2.031
AHUFUF	1.784	83.687	2.019
ALENAI	1.807	92.015	2.011
ALITOF	1.78	89.4	2.038
APUZOD	1.79	103.372	2.044
AWUQUF	1.775	86.767	2.015
AXOZIZ	1.832	82.936	1.997
AYANUM	1.784	91.183	2.055
AYAXUV	1.784	89.439	2.051
AYIKOK	1.796	83.19	2.058
AYIKUQ	1.796	82.498	2.062
AYILAX	1.794	81.237	2.056
AYILEB	1.796	90.213	2.048
AYILIF	1.788	81.718	2.053
AYILOL	1.788	85.033	2.049
AYINED	1.797	93.777	2.055
AYIVAH	1.791	90.291	2.044
AZOTEP	1.75	83.62	2.071
AZOTEP01	1.726	80.21	2.079
AZOTEP01	1.739	100.771	2.079
AZOTEP01	1.739	77.812	2.082
AZOTEP01	1.745	95.489	2.089
BAFREF	1.786	87.55	2.018
BANHIK	1.787	76.561	2.04
BAZVEE	1.765	81.537	2.026
BEKDEA	1.814	90.457	2.043
BESCEJ	1.787	80.72	2.025
BESCEJ	1.791	82.574	2.029
BEWMAS	1.791	80.4	2.055
BIDHAX	1.786	97.933	2.022
BIDQEK	1.783	86.074	2.074
BIFBOK	1.772	94.422	2.041
BIFBOK	1.765	84.303	2.037
BIFBOK	1.771	93.904	2.034

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BIGLOU	1.785	87.878	2.028
BIPXAC	1.782	89.061	2.046
BIWTIN	1.799	91.279	2.032
BIYJUR	1.788	87.148	2.049
BIYJUR	1.79	91.055	2.052
BIZMAZ	1.783	87.1	2.052
BOMPAU	1.787	99.005	2.01
BOTSUZ	1.782	84.071	2.019
BOWGAV	1.825	85.35	2.013
BOWGID	1.751	87.595	2.072
BFPDPS	1.77	73.616	2.06
BUCKAM	1.756	106.244	2.052
BULWIQ	1.725	56.288	2.096
BURKIL	1.779	103.114	2.039
BUWVOH	1.739	62.292	2.1
BZTZLS	1.765	88.616	2.031
BZTZLS01	1.76	88.208	2.029
CABNIE	1.794	91.49	2.042
CAKMOS	1.776	93.715	2.049
CAPLEK	1.805	93.427	2.002
CAPLEK01	1.808	93.52	2.003
CAPLEK02	1.81	87.702	1.995
CAPLEK03	1.808	93.624	2.006
CAQLAJ	1.746	79.703	2.102
CAZTON	1.774	90.804	2.028
CAZTON01	1.778	91.281	2.031
CEHJUJ	1.784	68.154	2.045
CEYYAJ	1.768	92.873	2.058
CEYYAJ	1.769	86.153	2.058
CIKPOC	1.782	90.258	2.025
CINNUJ	1.78	79.265	2.049
CINXUS	1.797	94.493	2.038
COGHAI	1.781	88.527	2.019
COGHOY	1.78	85.505	2.032
COJMET	1.769	63.216	2.074
COQJIB	1.786	81.337	2.021
COQJIB01	1.792	75.509	2.037
COZYUL	1.754	101.654	2.045
CUHHET	1.786	96.23	2.05
CUSNUZ	1.762	86.581	2.021
CUTSAN	1.814	81.706	2.041
CUTSER	1.78	82.609	2.037
CUTSOB	1.821	82.575	2.037
CUVCUS	1.777	109.865	2.016
CUVDAZ	1.779	89.33	2.014
DADPDS	1.877	82.798	2.059
DADPDS01	1.766	89.48	2.061
DADPDS02	1.77	89.773	2.057

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DADPDS03	1.771	89.3	2.069
DADPDS04	1.766	89.296	2.06
DADPDS05	1.774	89.259	2.068
DARZOL	1.755	81.076	2.042
DARZUR	1.795	90.195	2.035
DBZOSS01	1.811	80.813	2.021
DBZOSS03	1.823	80.75	2.02
DBZOSS04	1.819	80.613	2.025
DBZOSS05	1.829	80.741	2.022
DCPHDS	1.778	103.604	2.041
DCPHDS02	1.777	103.503	2.042
DEHLIM	1.767	81.451	2.044
DEHLOS	1.764	107.161	2.067
DEMZEB	1.763	99.048	2.048
DEMZIF	1.755	82.426	2.044
DEWCAK	1.79	75.992	2.039
DEWCAK01	1.795	81.78	2.047
DEZJEY	1.762	80.336	2.025
DHDSPY	1.778	93.156	2.018
DHDSPY01	1.791	93.254	2.018
DIBYOF	1.79	104.667	2.044
DICZUL	1.759	88.218	2.029
DIFWUM	1.765	87.573	2.022
DILGEK	1.798	79.448	2.053
DILGEK01	1.795	84.452	2.055
DIRLEY	1.767	82.597	2.073
DONVOU	1.783	92.625	2.032
DOXJAE	1.78	87.203	2.03
DPTBUO	1.77	66.328	2.078
DPYSUL01	1.783	87.135	2.011
DPYSUL01	1.786	86.43	2.016
DPYSUL02	1.791	85.854	2.02
DPYSUL02	1.789	85.017	2.026
DQUNDS02	1.78	79.551	2.039
DRFURS	1.749	49.9	2.108
DTACAC10	1.745	68.577	2.082
DTCOPM	1.764	70.299	2.075
DUDCOU	1.77	91.473	2.043
DUWTUM	1.806	87.645	2.05
EBIHAB	1.762	80.071	2.063
EFAMII	1.767	88.226	2.029
EHIROD	1.774	92.924	2.025
ELAQOX	1.766	87.838	2.052
EMASIV	1.81	86.261	2.015
ENANEM	1.784	83.34	2.054
ENAXEX	1.809	88.808	2.02
ENAXEX	1.801	81.718	2.025
ETHUSS	1.812	90.217	1.997

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ETHUSS01	1.824	91.001	1.996
ETHUSS02	1.824	90.991	2.006
ETHUSS03	1.825	90.822	2.005
ETHUSS04	1.787	91.159	1.991
ETHUSS04	1.789	90.656	2.002
EWUCAA	1.741	61.227	2.096
EYUBUV	1.727	77.121	2.047
FADKOM	1.79	87.43	2.028
FAKNAK	1.738	70.886	2.11
FAMGEI	1.784	87.61	2.024
FARWIF	1.853	90.204	2.002
FARWIF	1.779	89.945	2.009
FARWIF	1.644	83.366	2.051
FARWIF	1.707	86.74	2.06
FAZBEN	1.834	83.758	1.998
FEBDUL	1.772	80.815	2.022
FEBZUJ	1.785	96.178	2.027
FEBZUJ	1.781	92.68	2.031
FEBZUJ	1.779	92.906	2.034
FECBAS	1.78	95.119	2.029
FECBEW	1.797	105.048	2.028
FEFDEA	1.783	82.74	2.029
FEFDEA	1.783	86.888	2.031
FEJRUH	1.762	73.507	2.045
FESVEE	1.698	62.8	2.141
FMCLTE	1.801	83.187	2.05
FMDCTE	1.805	88.943	2.026
FOASBH01	1.781	86.418	2.029
FOCCUW	1.729	84.043	2.095
FOCLAM	1.759	84.971	2.042
FOCXUQ	1.739	180	2.117
FOINSI01	1.783	94.087	2.024
FOVYOF	1.794	89.985	2.051
FOYSES	1.767	77.895	2.054
FUBSOM	1.776	89.696	2.078
FUCWAB	1.781	87.402	2.051
FUGQUT	1.784	97.626	2.026
FUGQUT01	1.789	87.298	2.006
FUGQUT01	1.8	87.999	2.018
FUGQUT01	1.734	91.286	2.022
FUGQUT01	1.774	87.019	2.025
FUGQUT02	1.766	92.876	2.014
FUGQUT02	1.778	91.014	2.014
FUGQUT02	1.738	89.22	2.017
FUGQUT02	1.757	83.893	2.026
FULXAN	1.807	85.993	2.034
FUQLIM	1.783	81.511	2.04
FUQLIM01	1.784	87.774	2.044

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FUQLIM02	1.771	82.116	2.038
FUQLIM03	1.802	81.988	2.032
FUQLIM04	1.758	81.312	2.037
FUQLIM05	1.785	80.55	2.042
FUQLIM06	1.783	80.134	2.039
FUQLIM07	1.797	79.423	2.093
FUQLIM08	1.809	78.371	2.044
FUQLIM09	1.827	78.434	2.029
FUQMEJ	1.777	89.923	2.048
FUXDUA	1.753	72.731	2.035
GADTOV	1.783	85.597	2.028
GADTOV	1.783	85.764	2.029
GADTOV	1.786	83.333	2.032
GADTOV	1.789	84.897	2.033
GADTOV01	1.785	83.357	2.027
GADTOV02	1.784	84.155	2.027
GANVEW	1.771	71.448	2.086
GAQVOL	1.783	91.822	2.016
GAYWIP	1.777	89.12	2.042
GEDNUA	1.79	101.047	2.068
GITPUW	1.78	94.529	2.038
GITQEH	1.777	102.683	2.029
GITQUX	1.756	97.997	2.011
GOJPEC	1.739	74.579	2.079
GOQLUW	1.829	88.412	2.005
GOQREM	1.776	79.892	2.014
GUDSUT	1.816	77.503	2.007
GUHBEQ	1.776	76.055	2.109
GUPDAZ	1.792	90.698	2.044
HACTOU	1.782	80.852	2.053
HACZET	1.774	98.486	2.034
HADLIH	1.716	61.596	2.117
HAMWEY	1.779	82.46	2.052
HESPED	1.784	87.142	2.029
HIFGIN	1.723	81.89	2.013
HIFGIN01	1.757	82.417	2.031
HIPGIZ	1.803	79.085	2.033
HIQJUM	1.815	85.169	1.997
HIRLEA	1.782	83.795	2.041
HISMEE	1.774	103.997	2.028
HISQUX	1.766	92.972	2.01
HISQUX	1.789	79.606	2.017
HIXPUB	1.783	88.353	2.025
HODREA	1.788	88.365	2.053
HOWPAK	1.753	82.479	2.028
HOWPOY	1.808	79.118	2.021
IDAHIE	1.769	80.207	2.074
IDEJEI	1.791	75.88	2.057

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IDEJIM	1.79	87.569	2.033
IDEJOS	1.793	76.657	2.061
IDEJUY	1.791	78.248	2.053
IDEKAF	1.793	79.735	2.045
IFUGAS	1.794	88.02	2.06
IFUPAB	1.773	87.288	2.013
IFUPAB	1.782	86.283	2.022
IGAPIR	1.797	92.246	2.052
IGAPIR01	1.779	90.278	2.038
IGOLAR	1.815	88.979	2.055
IGOLAR01	1.807	89.504	2.056
IKAZOK	1.78	92.873	2.051
IKIJER02	1.787	82.204	2.05
IKIJER02	1.788	83.163	2.044
INADOT	1.794	86.931	2.029
INADOT01	1.795	86.378	2.034
IPIXUB	1.787	86.726	2.026
IPIXUB01	1.791	86.523	2.025
IPIXUB02	1.737	87.437	2.033
IPIXUB03	1.779	85.757	2.022
IPIXUB04	1.784	85.067	2.019
IPIXUB05	1.778	84.825	2.029
IPIXUB06	1.786	86.416	2.024
IPIXUB07	1.765	75.331	2.001
IPIXUB07	1.763	89.515	2.022
IPIXUB08	1.775	99.364	2.058
IPIXUB09	1.78	99.331	2.086
IPIXUB10	1.755	101.191	2.064
IPIXUB11	1.777	84.607	2.027
IPIXUB12	1.764	99.155	2.042
IPIXUB13	1.776	76.467	2.022
IPIXUB13	1.779	89.129	2.033
IPIXUB14	1.791	78.107	1.983
IPIXUB14	1.793	92.232	2
IPIXUB15	1.754	91.205	2.014
IPIXUB15	1.753	73.588	2.035
IPIXUB16	1.766	99.358	2.108
IPQUNS10	1.797	86.556	2.038
IRITIO	1.782	90.808	2.011
IVIRAH	1.778	84.74	2.082
JAGFUV	1.793	85.066	2.048
JAGFUV	1.8	79.179	2.049
JAWCOZ	1.793	88.048	2.042
JAXPUW	1.728	77.549	2.105
JECYAZ	1.798	180	2.07
JEJYON	1.8	89.084	2.006
JEJYON	1.786	84.478	2.007
JEJYON	1.79	89.978	2.018

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JEJYON	1.805	88.442	2.016
JEPJIA	1.786	101.688	2.037
JESXEN	1.775	100.428	2.067
JIRXOA	1.774	95.515	2.029
JISZOB	1.8	93.441	2.038
JITWUH	1.789	83.191	2.045
JONREJ	1.795	103.191	2.057
JOPDAT	1.767	99.084	2.103
JUJYUL	1.801	90.547	2.018
JUJZAS	1.798	87.613	2.016
JUJZEW	1.803	85.89	2.025
JUWYIM	1.795	91.84	2.023
KADFAY	1.755	69.322	2.111
KADFAY01	1.756	69.67	2.087
KADFAY01	1.753	67.555	2.095
KAHRUK	1.744	79.981	2.058
KAPRAX	1.82	78.941	1.997
KAQZAF	1.787	104.062	2.083
KAYNON	1.759	82.366	2.051
KAYNUT	1.794	95.151	2.021
KAYNUT01	1.782	94.93	2.017
KAZHEA	1.821	89.272	1.993
KEJRAT	1.776	73.581	2.034
KIDPOC	1.779	85.893	2.07
KINLAX	1.781	85.767	2.027
KISCOG	1.773	90.279	2.055
KIWSEO	1.764	80.265	2.048
KIWWOC	1.77	180	2.117
KIWWOC01	1.76	180	2.103
KOZSOK	1.789	91.424	2.065
KUBLOJ	1.788	84.199	2.022
KUBNUT	1.776	69.167	2.044
KUJZIZ	1.77	91.021	2.071
KUSNOC	1.792	87.413	2.053
KUZSOO	1.79	88.852	2.051
KUZSUU	1.788	88.045	2.053
KUZVEH	1.795	88.73	2.059
LACTOB	1.769	96.104	2.024
LADQAI	1.787	77.433	2.06
LADQAI01	1.787	74.611	2.07
LAFNUD	1.786	91.319	2.066
LAGLUD	1.791	91.541	2.037
LAJYAZ	1.774	84.226	2.025
LAJYAZ01	1.775	85.26	2.021
LAJYAZ02	1.78	83.903	2.024
LAKFOT	1.761	92.151	2.077
LARTOQ	1.774	95.352	2.072
LEWPEI	1.76	85.426	2.086

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LEYZOG	1.771	75.478	2.025
LIDCUX	1.763	92.099	2.025
LIDCUX	1.762	93.17	2.027
LIRYER	1.791	88.508	2.038
LIRYIV	1.79	87.526	2.041
LIRYUH	1.776	80.339	2.049
LIRYUH01	1.778	80.889	2.051
LIRZES	1.783	78.947	2.055
LIRZIW	1.782	96.426	2.047
LIRZOC	1.788	96.293	2.056
LOSHOR	1.795	88.205	2.048
LUHGED	1.735	80.525	2.068
LUMMOW	1.719	67.352	2.126
LUMNAJ	1.712	58.755	2.145
MABRUE	1.775	115.469	2.107
MABVIY	1.775	82.025	2.022
MABVOE	1.769	96.89	2.031
MAGQOD	1.742	58.461	2.112
MAWTIN	1.801	84.706	2.039
MBTPDS	1.759	73.695	2.075
MEFCTE	1.782	98.616	2.012
METBZA10	1.789	84.272	2.047
METHUS	1.86	87.577	1.996
METHUS01	1.809	88.136	2.019
METHUS02	1.805	88.212	1.997
METHUS03	1.823	87.19	2.004
METHUS04	1.824	87.152	2.008
MEURDS	1.755	77.947	2.073
MIPSEK	1.784	76.005	2.045
MIPVAI	1.799	86.656	2.062
MIXPOY	1.802	86.052	2.044
MPPRDS	1.749	88.468	2.079
MUFNIK	1.794	81.522	2.057
MUFNIK01	1.798	79.779	2.057
MUSBK	1.731	169.998	2.157
MUYRIJ	1.791	88.725	2.039
MUYRIJ01	1.786	89.022	2.04
NAJNUJ	1.778	82.071	2.01
NASVOV	1.786	85.414	2.041
NELTUT	1.81	86.173	2.013
NIDDIN	1.796	84.601	2.04
NIDDIN	1.794	100.975	2.042
NIPHSS01	1.779	88.106	2.03
NOGBUJ	1.768	59.452	2.08
NUCNEG	1.806	82.445	2.058
NUJVEU	1.779	79.774	2.034
NUMXOJ	1.75	100.548	2.083
NUVFOZ	1.783	54.501	2.089

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OBAYOI	1.79	84.567	2.04
OBAYOI	1.796	94.99	2.048
OBAYUO	1.783	89.644	2.052
OBAYUO	1.787	89.948	2.046
OBAYUO	1.785	89.579	2.042
OBERUK	1.784	86.127	2.064
OBUPIM	1.785	95.7	2.052
OCAMUC	1.776	95.194	2.03
OCANIR	1.78	90.01	2.037
OCOYIO	1.77	180	2.113
ODNPDS02	1.784	84.41	2.057
ODNPDS10	1.785	85.109	2.043
ODNPDS11	1.793	85.491	2.059
ODOYOW	1.777	88.114	2.039
OKEGOC	1.802	86.235	2.045
OLINIJ	1.788	83.429	2.029
OPAQOM	1.775	82.646	2.016
OPAQOM01	1.783	82.721	2.011
OPIXES	1.781	78.933	2.04
OVIVAR	1.79	81.182	2.043
OWAZAP	1.758	88.679	2.059
OXAFEB	1.772	87.279	2.051
OXAFIF	1.764	78.344	2.039
OXEFII	1.785	78.912	2.028
OXEFII	1.792	90.091	2.03
OXEYEW	1.828	81.214	2.037
OXEYEW	1.833	77.46	2.038
OXEYIA	1.828	77.287	2.041
OXEYIA	1.832	81.244	2.042
PAMTED	1.744	78.493	2.062
PAWNUX	1.756	77.731	2.016
PAYXES	1.714	33.851	2.164
PAZDUP	1.78	88.774	2.032
PAZDUP01	1.78	88.774	2.032
PAZYIA	1.784	88.344	2.035
PAZYIA	1.795	90.978	2.041
PECWOL	1.81	90.585	1.996
PEDVUS	1.757	90.261	2.083
PEDWAZ	1.761	86.662	2.079
PEDYII	1.75	72.198	2.042
PEGPAV	1.826	85.843	1.993
PEGPAV01	1.821	89.099	1.993
PEGPAV01	1.821	87.773	2.002
PETNEI	1.766	97.761	2.073
PETNER	1.755	72.513	2.082
PETNER01	1.76	101.091	2.073
PHENSS01	1.789	84.987	2.023
PHENSS10	1.785	83.822	2.027

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PHENSS12	1.784	84.6	2.025
PHENSS13	1.794	84.445	2.034
PHENSS14	1.787	84.133	2.029
PIJSAD	1.755	77.771	2.056
PINPEH	1.78	86.245	2.034
PIPTHS	1.811	90.781	1.995
PIPTHS01	1.818	91.552	1.999
POHTEM	1.801	64.829	2.05
POYYEH	1.749	72.102	2.107
PTCARB10	1.747	86.847	2.035
PUCKEG	1.764	66.462	2.064
PUGHEF	1.79	83.028	2.058
PUGHEF01	1.784	83.028	2.05
PUJSIX	1.786	85.618	2.03
PUKRET	1.795	91.506	2.053
PUKRIX	1.788	81.239	2.054
PYMDSO	1.781	82.789	2.017
PYMDSO01	1.781	82.497	2.015
PYMSUL10	1.782	83.921	2.018
PYMSUL10	1.777	85.37	2.02
PYMSUL11	1.787	87.262	2.026
PYMSUL12	1.78	83.722	2.012
PYMSUL12	1.77	85.19	2.014
PYMSUL13	1.772	83.768	2.016
PYMSUL13	1.768	85.487	2.02
QADGUX	1.72	58.37	2.14
QAVMUY	1.801	83.78	2.026
QEDYAC	1.783	86.597	2.036
QENTEJ	1.791	85.521	2.051
QIZWOL	1.793	84.356	2.037
QIZWOL	1.784	83.85	2.039
QOBGAP	1.741	89.956	2.04
QOLQOY	1.777	84.712	2.077
QONJEK	1.777	89.067	2.065
QONJEK01	1.782	89.133	2.076
QOZZOV	1.774	78.596	2.021
QUCMIL	1.769	87.841	2.039
QUDESUL10	1.825	75.152	2.034
QUDESUL20	1.777	71.44	2.062
RATCAQ	1.783	84.151	2.037
REGPOI	1.787	90.701	2.047
REJNIG	1.798	80.863	2.057
RIPPUB	1.791	99.308	2.06
RIRPEN	1.767	89.888	2.054
RIRPOX	1.762	92.988	2.055
RISCUS	1.729	100.205	2.049
ROKPEN	1.739	76.438	2.091
ROKPIR	1.731	57.819	2.121

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ROVWUX	1.78	87.521	2.04
SACZEB	1.772	86.138	2.072
SAVTOB	1.779	89.043	2.026
SAVTOB01	1.799	89.107	2.031
SEBJUG	1.787	86.954	2.055
SEBJUG	1.788	87.719	2.066
SEDMEV	1.76	83.59	2.039
SEMZIU	1.781	84.639	2.026
SEMZIU	1.783	84.965	2.026
SEWSOE	1.784	87.759	2.019
SEYMEO	1.76	91.906	2.068
SEZZOP	1.785	99.467	2.062
SIBBEN	1.786	101.301	2.035
SIQBIE	1.796	80.059	2.057
SIQBUQ	1.798	88.378	2.056
SODKIG	1.793	85.899	2.05
SODKOM	1.793	94.948	2.051
SODKUS	1.785	84.539	2.042
SOHDUP	1.764	50.201	2.102
SOQMAO	1.79	127.145	2.073
SOSNAP	1.798	79.652	2.017
TABMUF	1.782	82.338	2.026
TABMUF	1.785	80.386	2.027
TADVIE	1.771	82.758	2.063
TAJMAS	1.757	74.136	2.039
TARFOK	1.732	63.315	2.097
TATNUY	1.786	84.265	2.04
TATPAG	1.774	99.884	2.038
TATPEK	1.783	82.902	2.028
TATPIO	1.786	101.705	2.035
TATPOU	1.757	81.576	2.044
TATPUA	1.775	180	2.104
TAWGEG	1.816	79.299	2.044
TAWGEG	1.807	73.203	2.048
TBMTZT	1.758	83.107	2.026
TEFSIH	1.784	74.358	2.032
TEGLOJ	1.765	86.24	2.077
TELMIJ	1.715	61.61	2.141
TELMOP	1.703	49.437	2.158
TESHUV	1.772	75.744	2.029
THPDCB	1.783	80.087	2.053
TIBFEQ	1.815	85.707	1.991
TIGQEG	1.786	84.661	2.044
TIPGIK	1.77	89.111	2.029
TIPGOQ	1.782	83.92	2.044
TIRVUM	1.747	93.095	2.081
TIRWOH	1.749	83.742	2.07
TOHHON	1.77	89.791	2.032

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TOKVUL	1.784	104.601	2.039
TOKVUL	1.766	104.929	2.044
TOLLEO	1.798	107.321	2.066
TOQFAI	1.779	86.313	2.027
TOQFEM	1.782	83.904	2.028
TOQFEM	1.782	81.607	2.03
TOZZIT	1.766	88.47	2.05
TOZZIT	1.769	88.163	2.055
TUPYOT	1.799	86.134	2.04
TURLUN	1.727	76.2	2.095
UBINUS	1.777	90.32	2.076
UCEVIH	1.736	90.914	2.099
UCIVAD	1.763	48.92	2.11
UDALER	1.849	89.738	2.014
UFAGIS	1.761	180	2.072
UFAGIS01	1.768	79.769	2.024
UFAGIS01	1.781	80.114	2.028
UFOMAF	1.783	89.091	2.055
UKESIM	1.741	81.953	2.022
UKESIM	1.757	82.203	2.022
ULOXIC	1.832	92.804	1.995
UPAXIT	1.754	98.275	2.064
UREKAE	1.762	84.189	2.067
URELIN	1.754	92.314	2.056
URELIN01	1.758	92.455	2.059
URELIN02	1.759	92.553	2.066
UVALIN	1.752	80.83	2.048
UVALIN01	1.754	80.518	2.047
VAHYAE	1.783	84.665	2.043
VAJKUO	1.781	99.117	2.02
VAVJOR	1.787	84.975	2.025
VAZCOP	1.755	85.428	2.026
VAZCOP	1.76	102.595	2.031
VAZCOP	1.75	92.213	2.028
VAZCOP01	1.755	89.081	2.039
VEGNAW	1.796	80.818	2.047
VEPDAV	1.785	84.018	2.037
VEPDAV	1.782	76.587	2.043
VIGSEJ	1.802	80.441	1.975
VINXOI	1.767	99.254	2.068
VOHFIH01	1.825	83.965	2.002
VOJFEI	1.783	80.673	2.054
VOKXIE	1.78	68.86	2.072
VOLHEL	1.78	76.883	2.067
VOLZAY	1.815	81.343	2.071
VORLOE	1.771	91.94	2.025
VORNUM	1.785	91.086	2.038
VOVKOG	1.751	55.835	2.08

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VUBPOA	1.813	86.637	2.033
VUHKEO	1.789	75.869	2.033
WAFFOA	1.781	86.137	2.03
WAFFOA01	1.779	86.794	2.028
WAFNEY	1.793	84.956	2.052
WAGLOH	1.779	104.784	2.023
WAKKAY	1.761	85.107	2.053
WAVDIJ	1.751	101.322	2.093
WEHQAB	1.796	77.168	2.039
WEWCOT	1.764	76.351	2.07
WEWGIP	1.759	84.221	2.029
WEYMEV	1.76	78.786	2.049
WICCUG	1.766	63.412	2.075
WIFXOB	1.749	70.701	2.072
WINMUC	1.788	86.255	2.048
WIWJUI	1.749	82.682	2.066
WIWKAP	1.751	88.151	2.065
WOBPOT	1.769	72.785	2.082
WONFOV	1.76	69.649	2.086
WONGEM	1.767	76.608	2.085
WONGOW	1.766	99.949	2.083
WOVHOH	1.789	85.469	2.037
WOVKUQ	1.787	86.79	2.047
WOVKUQ	1.785	90.732	2.051
WUBHOQ	1.799	87.276	2.067
WUBZUO	1.791	87.335	2.038
WUBZUO01	1.783	87.431	2.034
WURGAS	1.744	79.705	2.059
WURGUM	1.755	75.142	2.04
XACBOU	1.749	83.252	2.081
XACBUA	1.755	75.942	2.068
XACCAH	1.768	76.089	2.065
XACCEL	1.755	81.449	2.081
XAJRIJ	1.773	91.533	2.068
XAMJON	1.784	87.277	2.027
XANYIV	1.762	80.667	2.047
XANYIV01	1.763	80.186	2.049
XASBOK	1.787	82.731	2.067
XASNAG	1.785	87.656	2.028
XATVUM	1.782	93.363	2.044
XAVCAZ	1.749	74.11	2.048
XAZKUG	1.77	59.562	2.088
XAZTID	1.806	90.994	2.033
XEBDEO	1.782	90.413	2.042
XEBDEO02	1.787	91.09	2.05
XEBJOF	1.82	77.998	2.011
XEPZEZ	1.787	86.939	2.016
XEQBAW	1.788	89.603	2.012

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XEXFOV	1.799	92.512	2.053
XIMKOU	1.759	76.983	2.043
XIVBAF	1.748	78.84	2.085
XIVBAF01	1.744	77.914	2.089
XIVBEJ	1.74	92.55	2.095
XIVBEJ	1.744	94.556	2.086
XIWNAS	1.78	83.981	2.032
XIWNAS01	1.782	83.786	2.037
XIWNAS02	1.782	83.878	2.034
XOJRIA	1.78	91.613	2.047
XOSBUC	1.79	90.285	2.048
XUBVEW	1.787	94.876	2.025
XUGPEU	1.772	94.806	2.065
XULZAF	1.73	68.696	2.073
YAHMEB	1.811	82.035	2.025
YESHEJ	1.782	86.466	2.022
YIPQEU	1.738	68.549	2.098
YIPQIY	1.738	69.153	2.099
YIPQOE	1.734	96.688	2.092
YIPQUK	1.727	67.47	2.101
YIPVEY	1.734	65.276	2.088
YIRYEE	1.754	83.691	2.069
YIRYEE01	1.759	83.696	2.072
YIRYEE02	1.746	83.668	2.074
YISNOG	1.776	95.206	2.026
YIYGIY	1.814	61.887	2.034
YIYGOE	1.81	77.981	2.037
YOCHOQ	1.77	86.096	2.043
YOHYOK	1.768	138.283	2.237
YOQQIG	1.75	82.42	2.035
YOTJEX	1.784	81.329	2.015
YOVFAR	1.773	96.119	2.024
YOXGAT	1.778	83.123	2.021
YUCQIX	1.797	89.262	2.048
YUCQOD	1.799	85.592	2.05
YUCVAU	1.791	95.423	2.046
YUXPEN	1.785	84.494	2.022
YUXPEN01	1.79	84.191	2.027
YUXPEN02	1.787	84.711	2.021
YUXPEN03	1.797	84.442	2.025
ZAHFET	1.806	94.186	2.033
ZAJZIW	1.779	86.83	2.035
ZAQWUL	1.825	81.55	2.026
ZATKIO	1.788	90.005	2.032
ZAYNIW	1.814	84.998	2.04
ZAYNIW01	1.784	85.705	2.023
ZECQAC	1.745	64.075	2.109
ZELMEI	1.779	98.909	2.078

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ZELMIM	1.737	104.882	2.099
ZEMPUC	1.826	89.972	1.997
ZESLAN	1.782	85.526	2.047
ZESLAN	1.788	88.444	2.047
ZEXNEV	1.788	86.686	2.043
ZIJDON	1.774	80.787	2.046
ZIJLOV	1.788	131.933	2.021
ZIXCEQ	1.777	93.283	2.013
ZIXCEQ01	1.78	92.985	2.017
ZOFWOI	1.773	139.342	2.139
ZOMKUH	1.759	74.927	2.076
ZOMKUH01	1.759	74.927	2.076
BPHDSU01	1.779	102.991	2.037
DAVZAF	1.717	58.322	2.135
DAVZAF	1.727	61.611	2.138
FEGZIE	1.774	80.89	2.044
FEHBED	1.759	87.963	2.026
FEHBIH	1.776	87.697	2.037
FEHBON	1.784	86.075	2.03
FEHBUT	1.776	88.707	2.033
FUQLEI01	1.774	85.636	2.057
VAXQIY	1.76	180	2.11
BEPCAE	1.784	94.48	2.047
BEPCEI	1.784	94.644	2.048
BEPCIM	1.786	94.223	2.048
CELMEP	1.786	74.931	2.041
JECYAZ01	1.816	86.685	1.98
REKDUK	1.793	88.572	2.052
XEBDEO03	1.782	90.963	2.048
ZEPTUN	1.787	180	2.087
KEKGOA	1.767	87.393	2.052
KEKGOA	1.762	89.931	2.064
KENPIG	1.764	94.957	2.095
MEQZUH	1.791	91.252	2.043
TEVCAC	1.79	86.96	2.019
XEJGUS	1.738	89.158	2.079
mean value	1.778529	86.88039	2.045956
median	1.782	86.153	2.042
maximum	1.877	180	2.237
minimum	1.644	33.851	1.975
standard deviation	0.023419	14.94138	0.029354

**Table S2** Selected geometrical parameters of disulphide compounds with S-S...S intermolecular distances shorter than 4 Å. For torsion angles absolute values are presented.



Refcode	S-S [Å]	C-S [Å]	C-S-S-C [°]	S...S [Å]	S-S...S [°]
SASZAR	2.055	1.759	79.744	3.806	110.354
SASZAR	2.055	1.764	79.744	3.67	120.329
SASZAR	2.055	1.764	79.744	3.762	126.261
ADEPUU	2.135	1.732	52.085	3.645	163.831
AGOKOW	2.028	1.764	84.451	3.714	161.154
AGOKOW01	2.033	1.767	84.051	3.675	160.278
AHUFOZ	2.031	1.796	101.698	3.567	81.52
AHUFUF	2.019	1.78	83.687	3.675	89.992
AHUFUF	2.019	1.784	83.687	3.79	70.105
ALENAI	2.011	1.793	92.015	3.602	86.065
BIFBOK	2.037	1.784	84.303	3.733	107.606
BIFBOK	2.034	1.785	93.904	3.814	122.425
BIFBOK	2.034	1.785	93.904	3.829	91.702
BIFBOK	2.037	1.765	84.303	3.733	72.394
BIFBOK	2.037	1.765	84.303	3.829	74.152
BIFBOK	2.041	1.778	94.422	3.872	87.388
BIYJUR	2.049	1.789	87.148	3.738	104.95
BIYJUR	2.052	1.786	91.055	3.738	101.529
BOMPAU	2.01	1.787	99.005	3.596	115.038
BOWGAV	2.013	1.802	85.35	3.651	121.003
BOWGAV	2.013	1.802	85.35	3.651	90.343
BOWGID	2.072	1.755	87.595	3.739	164.405
BOWGID	2.072	1.751	87.595	3.603	138.965
BURKIL	2.039	1.779	103.114	3.66	121.682
BURKIL	2.039	1.779	103.114	3.813	115.502
BURKIL	2.039	1.779	103.114	3.66	120.66
BURKIL	2.039	1.779	103.114	3.813	114.575
BZTZLS	2.031	1.765	88.616	3.807	71.626
BZTZLS01	2.029	1.76	88.208	3.739	71.603
CAPLEK	2.002	1.805	93.427	3.736	122.106
CAPLEK01	2.003	1.808	93.52	3.739	122.167
CAPLEK02	1.995	1.81	87.702	3.693	116.506
CAPLEK03	2.006	1.808	93.624	3.736	122.143
CEHJUJ	2.045	1.762	68.154	3.555	88.987
CEHJUJ	2.045	1.784	68.154	3.862	65.01
CEYYAJ	2.058	1.768	92.873	3.652	62.983
CEYYAJ	2.058	1.769	86.153	3.587	64.183
CEYYAJ	2.058	1.755	92.873	3.201	164.307
CEYYAJ	2.058	1.76	86.153	3.445	160.691
COZYUL	2.045	1.774	101.654	3.598	106.582
COZYUL	2.045	1.754	101.654	3.598	161.196
DADPDS	2.059	1.877	82.798	3.836	145.967
DADPDS	2.059	1.888	82.798	3.836	96.105
DADPDS01	2.061	1.766	89.48	3.848	145.053
DADPDS01	2.061	1.746	89.48	3.848	95.793
DADPDS02	2.057	1.77	89.773	3.854	95.783
DADPDS02	2.057	1.759	89.773	3.854	145.389

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DADPDS03	2.069	1.771	89.3	3.826	95.706
DADPDS03	2.069	1.765	89.3	3.826	144.972
DADPDS04	2.06	1.766	89.296	3.863	145.255
DADPDS04	2.06	1.769	89.296	3.863	95.71
DADPDS05	2.068	1.774	89.259	3.821	95.751
DADPDS05	2.068	1.768	89.259	3.821	145.051
DARZUR	2.035	1.795	90.195	3.812	77.528
DCPHDS	2.041	1.778	103.604	3.759	117.402
DCPHDS	2.041	1.778	103.604	3.759	117.402
DCPHDS02	2.042	1.777	103.503	3.77	117.447
DCPHDS02	2.042	1.777	103.503	3.77	117.447
DEMZEB	2.048	1.763	99.048	3.846	87.434
DICZUL	2.029	1.759	88.218	3.626	79.68
DUDCOU	2.043	1.77	91.473	3.742	78.943
EFAMII	2.029	1.767	88.226	3.835	113.423
EFAMII	2.029	1.764	88.226	3.555	152.444
FARWIF	2.002	1.853	90.204	3.733	87.281
FARWIF	2.009	1.779	89.945	3.773	87.763
FARWIF	2.051	1.644	83.366	3.765	86.786
FARWIF	2.06	1.707	86.74	3.777	85.852
FARWIF	2.002	1.766	90.204	3.773	88.366
FARWIF	2.009	1.746	89.945	3.733	86.803
FARWIF	2.051	1.775	83.366	3.777	86.147
FARWIF	2.06	1.687	86.74	3.765	86.738
FOCLAM	2.042	1.767	84.971	3.719	81.624
FOINSI01	2.024	1.783	94.087	3.481	134.36
FOVYOF	2.051	1.782	89.985	3.413	151.466
FOVYOF	2.051	1.794	89.985	3.413	151.466
FUBSOM	2.078	1.776	89.696	3.674	73.339
FUBSOM	2.078	1.776	89.696	3.774	70.349
FUGQUT01	2.006	1.766	87.298	3.641	86.029
FUGQUT01	2.018	1.776	87.999	3.791	84.073
FUGQUT01	2.022	1.774	91.286	3.641	92.839
FUGQUT01	2.025	1.749	87.019	3.791	89.177
FUGQUT01	2.018	1.776	87.999	3.792	147.205
FUGQUT01	2.025	1.749	87.019	3.861	118.75
FUGQUT01	2.006	1.789	87.298	3.792	123.192
FUGQUT01	2.022	1.734	91.286	3.861	143.046
FUGQUT01	2.006	1.789	87.298	3.695	91.548
FUGQUT01	2.018	1.8	87.999	3.651	93.305
FUGQUT01	2.022	1.734	91.286	3.695	84.36
FUGQUT01	2.025	1.774	87.019	3.651	87.818
FUGQUT02	2.014	1.751	91.014	3.655	87.683
FUGQUT02	2.014	1.771	92.876	3.59	93.78
FUGQUT02	2.017	1.777	89.22	3.655	91.422
FUGQUT02	2.026	1.78	83.893	3.59	88.181
FUGQUT02	2.014	1.771	92.876	3.815	116.411
FUGQUT02	2.017	1.738	89.22	3.815	133.735

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FUGQUT02	2.014	1.766	92.876	3.691	85.584
FUGQUT02	2.014	1.778	91.014	3.658	91.393
FUGQUT02	2.017	1.738	89.22	3.658	87.557
FUGQUT02	2.026	1.757	83.893	3.691	90.679
GITQEH	2.029	1.777	102.683	3.572	89.47
GITQEH	2.029	1.759	102.683	3.572	90.53
GOQLUW	2.005	1.829	88.412	3.598	119.417
HISMEE	2.028	1.774	103.997	3.88	93.305
HOWPAK	2.028	1.753	82.479	3.639	82.863
HOWPOY	2.021	1.838	79.118	3.896	105.278
HOWPOY	2.021	1.808	79.118	3.896	74.722
HOWPOY	2.021	1.808	79.118	3.7	126.736
IFUPAB	2.022	1.767	86.283	3.586	128.1
IFUPAB	2.013	1.773	87.288	3.586	85.389
IKIJER02	2.05	1.787	82.204	3.731	108.083
IKIJER02	2.044	1.788	83.163	3.731	106.817
IPIXUB04	2.019	1.778	85.067	3.869	132.506
IPIXUB04	2.019	1.784	85.067	3.869	132.506
IPIXUB05	2.029	1.764	84.825	3.854	132.116
IPIXUB05	2.029	1.778	84.825	3.854	132.116
IPIXUB07	2.022	1.767	89.515	3.644	151.007
IPIXUB07	2.022	1.763	89.515	3.644	151.007
IPIXUB11	2.027	1.76	84.607	3.885	132.73
IPIXUB11	2.027	1.777	84.607	3.885	132.73
IPIXUB13	2.033	1.725	89.129	3.666	149.801
IPIXUB13	2.033	1.779	89.129	3.666	149.801
IPIXUB14	2	1.833	92.232	3.662	152.051
IPIXUB14	2	1.793	92.232	3.662	152.051
IPIXUB15	2.014	1.779	91.205	3.598	152.908
IPIXUB15	2.014	1.754	91.205	3.598	152.908
IRITIO	2.011	1.782	90.808	3.764	81.187
JEJYON	2.006	1.8	89.084	3.601	80.655
JEJYON	2.007	1.786	84.478	3.491	82.912
JEJYON	2.016	1.78	88.442	3.61	89.772
JEJYON	2.018	1.79	89.978	3.636	90.504
JEJYON	2.007	1.786	84.478	3.887	130.899
JEJYON	2.006	1.8	89.084	3.872	65.678
JEJYON	2.018	1.79	89.978	3.667	71.029
JEJYON	2.007	1.794	84.478	3.671	82.358
JEJYON	2.016	1.805	88.442	3.564	77.81
KADFAY	2.111	1.755	69.322	3.579	114.11
KADFAY	2.111	1.755	69.322	3.36	174.683
KADFAY	2.111	1.756	69.322	3.86	97.888
KADFAY	2.111	1.756	69.322	3.739	166.051
KADFAY	2.111	1.756	69.322	3.592	107.594
KADFAY01	2.095	1.753	67.555	3.648	149.805
KADFAY01	2.087	1.756	69.67	3.761	97.211
KADFAY01	2.095	1.753	67.555	3.786	98.946

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KADFAY01	2.095	1.753	67.555	3.808	161.113
KADFAY01	2.087	1.749	69.67	3.717	111.936
KADFAY01	2.095	1.752	67.555	3.752	122.105
KAHRUK	2.058	1.744	79.981	3.762	85.777
KAZHEA	1.993	1.813	89.272	3.809	78.079
KAZHEA	1.993	1.821	89.272	3.809	101.921
KIWVOC	2.117	1.77	180	3.763	75.619
KIWVOC	2.117	1.77	180	3.832	107.966
KIWVOC01	2.103	1.76	180	3.703	76.143
KIWVOC01	2.103	1.76	180	3.796	108.69
LAGLUD	2.037	1.791	91.541	3.886	71.172
LEWPEI	2.086	1.76	85.426	3.478	104.298
MABRUE	2.107	1.775	115.469	3.453	161.103
MABRUE	2.107	1.775	115.469	3.461	123.161
MBTPDS	2.075	1.751	73.695	3.688	162.569
MBTPDS	2.075	1.759	73.695	3.645	91.678
MBTPDS	2.075	1.759	73.695	3.828	153.742
METHUS03	2.004	1.823	87.19	3.873	87.703
METHUS04	2.008	1.824	87.152	3.872	87.696
NELTUT	2.013	1.805	86.173	3.857	77.347
NUMXOJ	2.083	1.75	100.548	3.416	168.029
NUMXOJ	2.083	1.767	100.548	3.866	150.649
NUMXOJ	2.083	1.767	100.548	3.602	159.132
OVIVAR	2.043	1.786	81.182	3.858	111.711
OXAFEB	2.051	1.772	87.279	3.591	79.192
OXAFEB	2.051	1.792	87.279	3.591	100.808
OXEFII	2.03	1.792	90.091	3.727	139.239
PEGPAV01	1.993	1.821	89.099	3.741	81.808
PEGPAV01	1.993	1.821	89.099	3.815	112.488
PEGPAV01	2.002	1.821	87.773	3.815	72.61
PETNEI	2.073	1.766	97.761	3.563	80.623
PETNEI	2.073	1.766	97.761	3.781	168.265
PETNER	2.082	1.755	72.513	3.877	171.985
PETNER	2.082	1.755	72.513	3.508	112.518
PETNER	2.082	1.755	72.513	3.767	156.191
PETNER	2.082	1.763	72.513	3.891	172.844
PETNER	2.082	1.763	72.513	3.476	92.291
PETNER01	2.073	1.76	101.091	3.574	149.544
PETNER01	2.073	1.764	101.091	3.727	107.728
PETNER01	2.073	1.764	101.091	3.579	156.461
PHENSS01	2.023	1.789	84.987	3.729	81.236
PHENSS01	2.023	1.788	84.987	3.729	130.314
PHENSS10	2.027	1.785	83.822	3.741	81.152
PHENSS10	2.027	1.804	83.822	3.741	130.303
PHENSS12	2.025	1.784	84.6	3.646	80.499
PHENSS12	2.025	1.783	84.6	3.867	150.84
PHENSS12	2.025	1.783	84.6	3.646	130.217
PHENSS13	2.034	1.794	84.445	3.894	150.816

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PHENSS13	2.034	1.794	84.445	3.894	68.468
PHENSS13	2.034	1.794	84.445	3.673	130.283
PHENSS14	2.029	1.787	84.133	3.647	80.45
PHENSS14	2.029	1.788	84.133	3.868	150.877
PHENSS14	2.029	1.788	84.133	3.647	130.198
PINPEH	2.034	1.78	86.245	3.763	79.649
PTCARB10	2.035	1.779	86.847	3.844	85.501
PYMDS	2.017	1.781	82.789	3.837	107.93
PYMDS	2.017	1.789	82.789	3.837	90.223
PYMDS01	2.015	1.781	82.497	3.813	90.09
PYMDS01	2.015	1.778	82.497	3.813	107.958
PYMSUL10	2.02	1.777	85.37	3.536	80.427
PYMSUL10	2.02	1.777	85.37	3.77	112.321
PYMSUL12	2.014	1.777	85.19	3.766	112.382
PYMSUL12	2.014	1.77	85.19	3.766	67.618
PYMSUL13	2.02	1.768	85.487	3.763	112.307
PYMSUL13	2.02	1.768	85.487	3.531	80.348
QAVMUY	2.026	1.802	83.78	3.887	83.048
QENTEJ	2.051	1.791	85.521	3.629	97.34
QENTEJ	2.051	1.791	85.521	3.686	83.254
QOBGAP	2.04	1.741	89.956	3.833	141.499
QOBGAP	2.04	1.741	89.956	3.853	92.418
QOBGAP	2.04	1.76	89.956	3.833	141.499
QOBGAP	2.04	1.76	89.956	3.853	87.582
QUCMIL	2.039	1.769	87.841	3.515	171.987
QUCMIL	2.039	1.769	87.841	3.787	78.095
RIRPEN	2.054	1.767	89.888	3.782	103.72
RIRPOX	2.055	1.766	92.988	3.791	109.052
SACZEB	2.072	1.776	86.138	3.388	92.959
SAVTOB01	2.031	1.784	89.107	3.542	95.625
SAVTOB01	2.031	1.799	89.107	3.542	84.375
SEBJUG	2.066	1.788	87.719	3.849	129.221
SEBJUG	2.055	1.783	86.954	3.849	143.255
SEMZIU	2.026	1.776	84.965	3.715	116.572
SEMZIU	2.026	1.786	84.639	3.671	105.652
SEMZIU	2.026	1.781	84.639	3.671	74.348
SEMZIU	2.026	1.783	84.965	3.715	63.428
SODKUS	2.042	1.785	84.539	3.669	119.827
TBMTZT	2.026	1.758	83.107	3.809	113.393
TBMTZT	2.026	1.758	83.107	3.823	77.309
TBMTZT	2.026	1.758	83.107	3.677	133.767
TELMIJ	2.141	1.715	61.61	3.457	103.054
TIBFEQ	1.991	1.833	85.707	3.876	91.979
TIBFEQ	1.991	1.833	85.707	3.621	103.302
TIBFEQ	1.991	1.815	85.707	3.621	76.698
TOZZIT	2.055	1.788	88.163	3.607	93.246
TOZZIT	2.055	1.769	88.163	3.607	86.754
UCEVIH	2.099	1.736	90.914	3.766	71.619

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UFAGIS01	2.028	1.781	80.114	3.894	108.418
UPAXIT	2.064	1.757	98.275	3.582	98
UVALIN	2.048	1.752	80.83	3.868	76.15
VAZCOP	2.026	1.755	85.428	3.86	120.001
VAZCOP	2.028	1.759	92.213	3.675	154.057
VAZCOP	2.028	1.759	92.213	3.892	83.844
VAZCOP	2.031	1.76	102.595	3.537	158.185
VAZCOP	2.031	1.76	102.595	3.732	74.553
VAZCOP	2.026	1.755	85.428	3.684	161.981
VAZCOP	2.028	1.75	92.213	3.86	126.77
VAZCOP	2.028	1.75	92.213	3.577	158.071
VAZCOP	2.028	1.75	92.213	3.782	76.094
VOVKOG	2.08	1.751	55.835	3.825	149.998
WAKKAY	2.053	1.769	85.107	3.626	100.339
WAVDIJ	2.093	1.751	101.322	3.782	152.071
WAVDIJ	2.093	1.751	101.322	3.635	159.043
WAVDIJ	2.093	1.751	101.322	3.733	65.9
WICCUG	2.075	1.766	63.412	3.852	108.912
WIFXOB	2.072	1.749	70.701	3.663	121.153
WIFXOB	2.072	1.749	70.701	3.731	85.178
WIFXOB	2.072	1.749	70.701	3.812	176.544
WIFXOB	2.072	1.749	70.701	3.772	78.201
WOVHOH	2.037	1.789	85.469	3.687	138.862
WOVKUQ	2.047	1.783	86.79	3.74	105.584
WOVKUQ	2.051	1.793	90.732	3.74	102.856
XAZKUG	2.088	1.77	59.562	3.896	168.079
XAZKUG	2.088	1.769	59.562	3.896	154.308
XAZTID	2.033	1.806	90.994	3.785	143.705
XAZTID	2.033	1.806	90.994	3.858	121.684
XAZTID	2.033	1.806	90.994	3.728	131.2
XAZTID	2.033	1.806	90.994	3.787	67.807
XAZTID	2.033	1.805	90.994	3.783	134.168
XUGPEU	2.065	1.772	94.806	3.718	75.611
YOHYOK	2.237	1.768	138.283	3.86	114.666
YOVFAR	2.024	1.773	96.119	3.775	74.975
YOVFAR	2.024	1.786	96.119	3.775	105.025
YUXPEN	2.022	1.785	84.494	3.644	80.666
YUXPEN	2.022	1.797	84.494	3.87	150.684
YUXPEN	2.022	1.797	84.494	3.644	130.246
YUXPEN01	2.027	1.79	84.191	3.637	80.352
YUXPEN01	2.027	1.79	84.191	3.898	135.161
YUXPEN01	2.027	1.789	84.191	3.856	151.044
YUXPEN01	2.027	1.789	84.191	3.637	130.256
YUXPEN01	2.027	1.789	84.191	3.898	135.161
YUXPEN02	2.021	1.787	84.711	3.727	81.267
YUXPEN02	2.021	1.786	84.711	3.727	130.449
YUXPEN03	2.025	1.797	84.442	3.646	80.361
YUXPEN03	2.025	1.796	84.442	3.863	150.968

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YUXPEN03	2.025	1.796	84.442	3.646	130.265
ZECQAC	2.109	1.745	64.075	3.761	101.224
ZESLAN	2.047	1.785	88.444	3.733	110.181
ZESLAN	2.047	1.786	85.526	3.864	105.678
ZESLAN	2.047	1.782	85.526	3.733	73.667
ZESLAN	2.047	1.788	88.444	3.864	70.456
ZIJLOV	2.021	1.788	131.933	3.865	78.437
ZIXCEQ	2.013	1.777	93.283	3.76	121.942
ZIXCEQ	2.013	1.781	93.283	3.655	106.467
ZIXCEQ	2.013	1.781	93.283	3.76	123.223
ZIXCEQ	2.013	1.781	93.283	3.365	94.971
ZIXCEQ	2.013	1.781	93.283	3.684	152.298
ZIXCEQ01	2.017	1.779	92.985	3.864	122.627
ZIXCEQ01	2.017	1.779	92.985	3.444	94.778
ZIXCEQ01	2.017	1.779	92.985	3.752	151.668
ZIXCEQ01	2.017	1.779	92.985	3.676	106.747
ZIXCEQ01	2.017	1.78	92.985	3.864	121.418
BPHDSU01	2.037	1.779	102.991	3.768	117.86
BPHDSU01	2.037	1.779	102.991	3.768	117.86
DAVZAF	2.135	1.719	58.322	3.799	101.414
DAVZAF	2.138	1.728	61.611	3.799	110.079
FEGZIE	2.044	1.774	80.89	3.874	92.996
VAXQIY	2.11	1.76	180	3.671	84.517
KEKGOA	2.064	1.762	89.931	3.606	75.8
KEKGOA	2.052	1.767	87.393	3.608	105.374
KEKGOA	2.064	1.762	89.931	3.526	78.133
XEJGUS	2.079	1.738	89.158	3.574	153.907
XEJGUS	2.079	1.738	89.158	3.805	161.838
mean value	2.042	1.775	88.751	3.723	110.790
median	2.033	1.776	87.719	3.739	106.747
minimum	1.991	1.644	52.085	3.201	62.983
maximum	2.237	1.888	180.000	3.998	176.544
standard deviation	0.032	0.024	15.208	0.122	29.336