

SUPPLEMENTARY INFORMATION

A. *IsoStar* Scatterplots

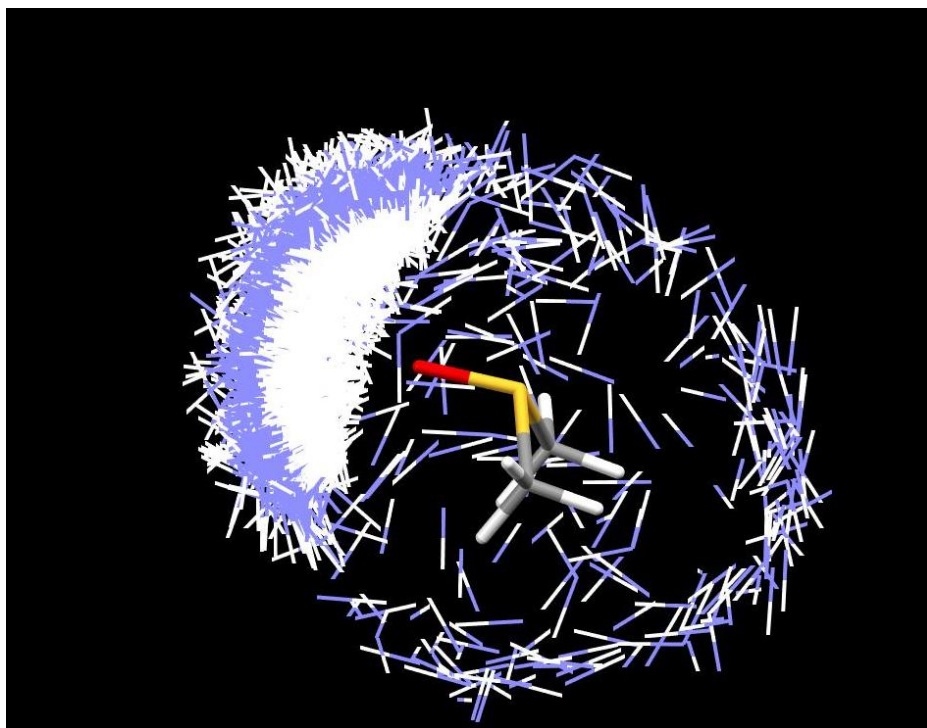


Figure A1: Scatterplot showing the distribution of -NH groups around DMSO as a central group.

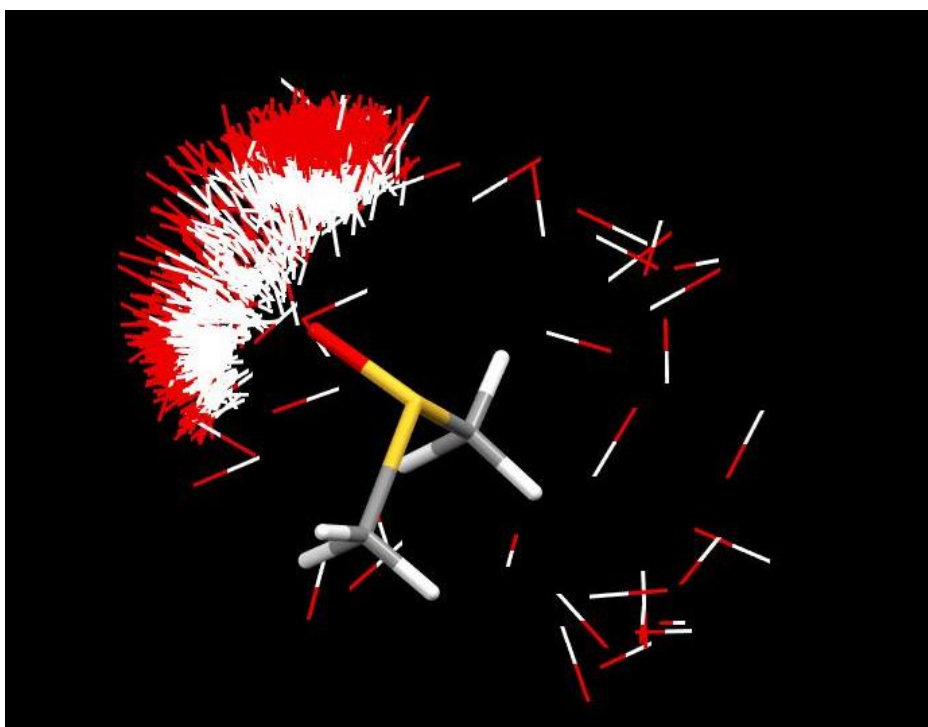


Figure A2: Scatterplot showing the distribution of -OH groups around DMSO as a central group.

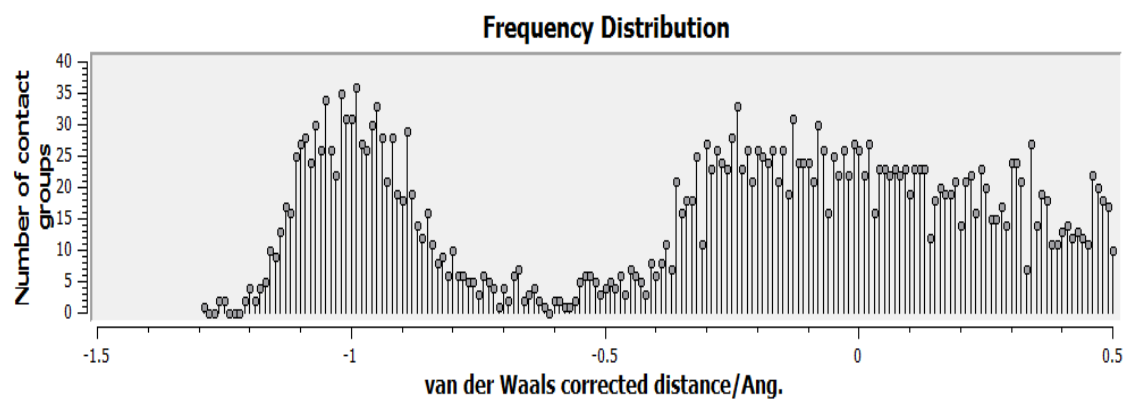


Figure A3: Frequency plot showing the distribution of the number of amino groups at different lengths.

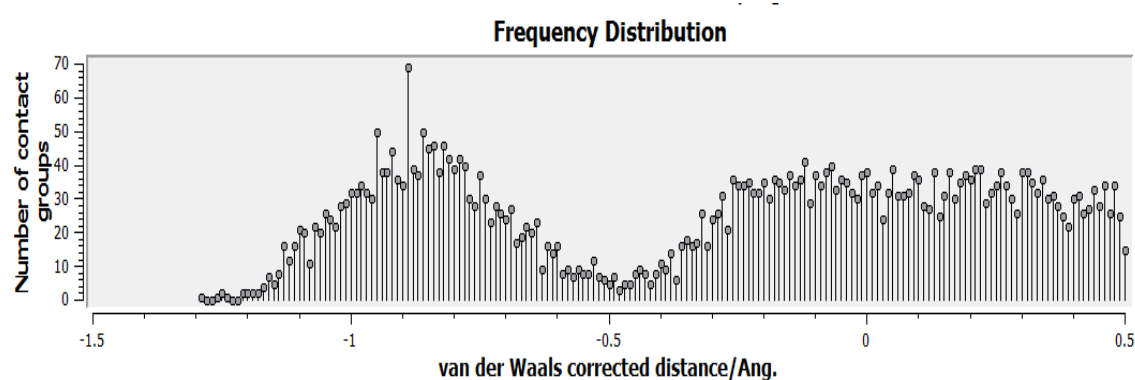


Figure A4: Frequency plot showing the distribution of the number of N/O/S-H groups at different lengths.

B. Descriptive Statistics

Table B1: Kruskal- Wallis H test.

	LogS
Chi-Square	2.290
df	2
Asymp. Sig.	0.318

Table B2: Multicollinearity Diagnostics

Table 2: Descriptive Statistics and Diagnostics									
		Diagnostics							
Model		Unstandardized Coefficients		Standardized Coefficients		t	Sig.	Collinearity Statistics	
		B	Std. Error	Beta				Tolerance	VIF
1	(Constant)	-4.202	1.579			-2.662	0.008		
	Angle1	0.014	0.007	0.073		1.959	0.051	0.651	1.535
	Dist1	0.480	0.315	0.059		1.524	0.128	0.608	1.645
	no_of_coordinates	-0.062	0.004	-0.539		-16.805	0.000	0.881	1.135
	no_of_interactions	-0.184	0.053	-0.114		-3.478	0.001	0.848	1.180

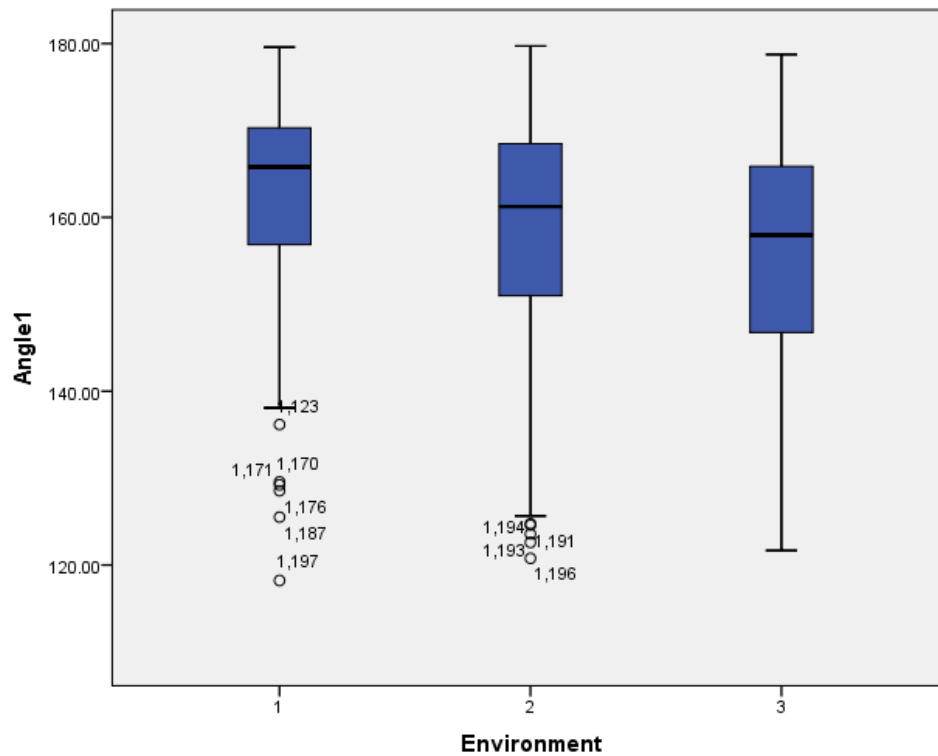


Figure B1: Boxplot of Angle1 according to each environment

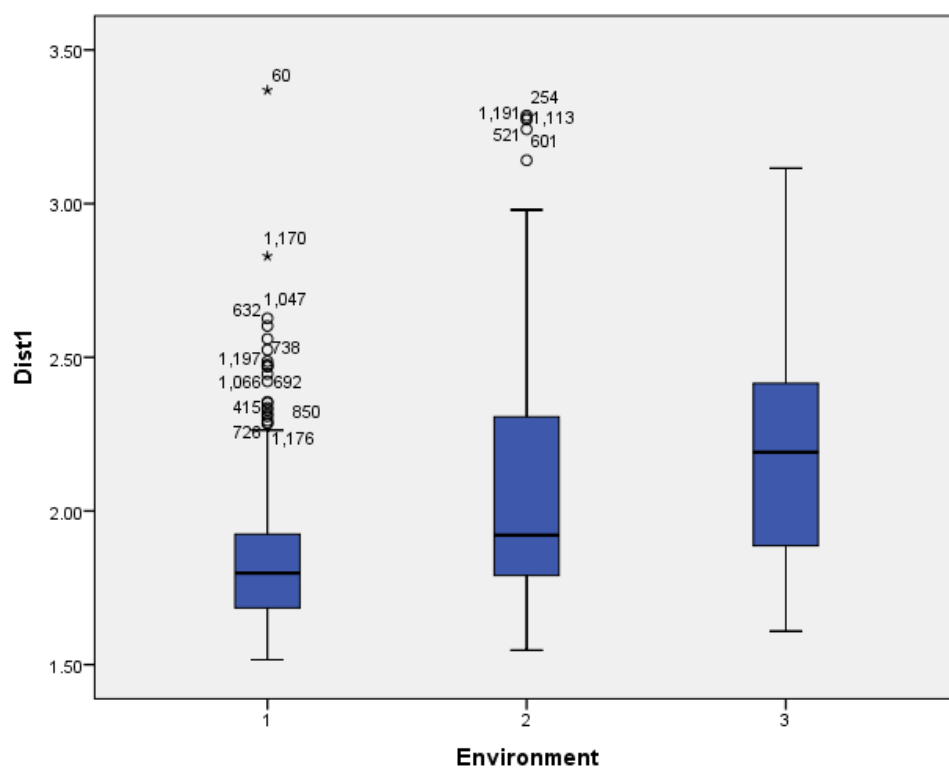


Figure B2: Boxplot of Dist1 according to each environment

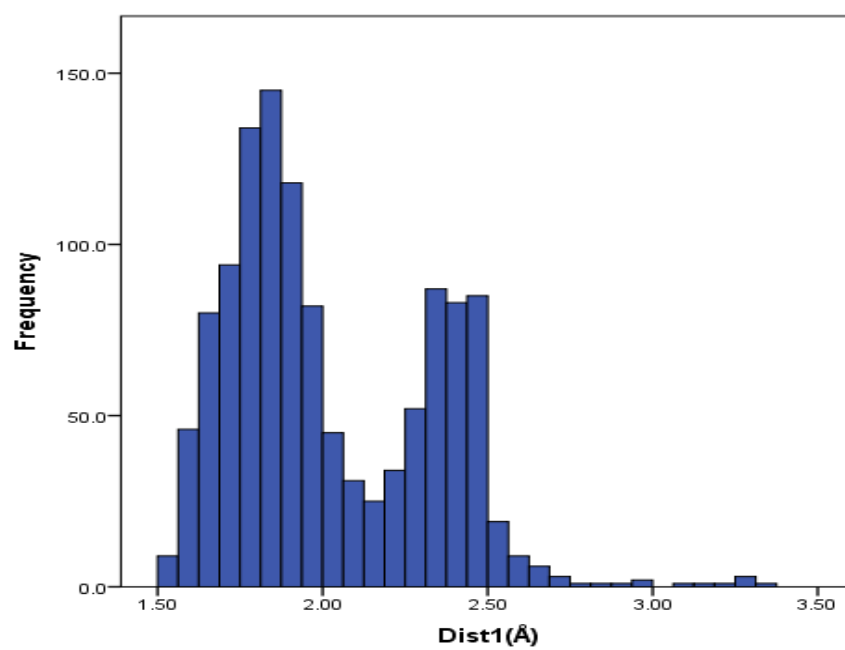


Figure B3: Histogram of Dist1.

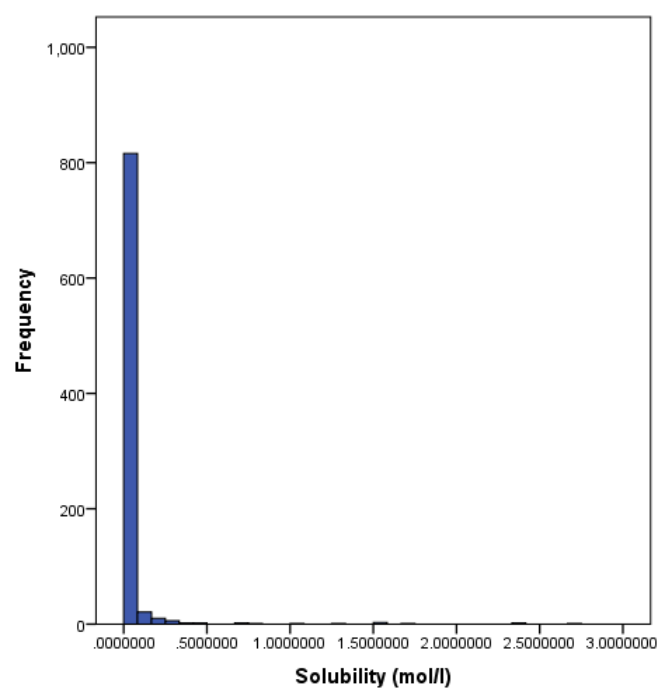


Figure B4: Histogram of solubility (mol/l).

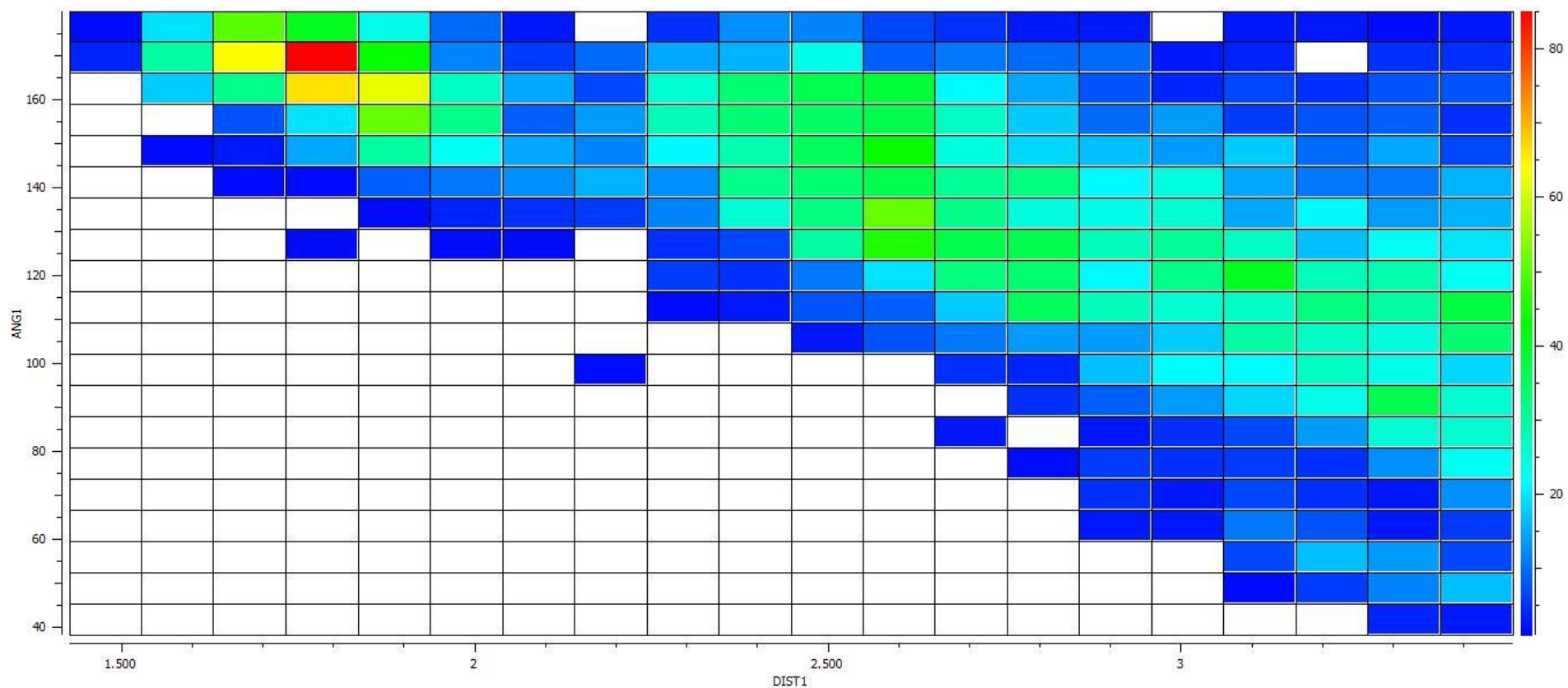


Figure B3: Heat plot of $\text{dist1}(\text{\AA})$ against $\text{ang1}(^{\circ})$, taking into account all the interactions detected by *ConQuest*. The coloured bar indicates the frequency scale, going from blue to red with an increase in numbers. One can easily notice the dominance of an inverse relationship between distance and angle of an interaction.

C. ANCOVA results

Dependent Variable: Log(Solubility)

Source	Type III Sum of Squares	df	Mean Square	F	Sig.
Corrected Model	1600.006 ^a	8	200.001	55.970	.000
Intercept	23.447	1	23.447	6.562	.011
Angle1	26.924	1	26.924	7.535	.006
Dist1	23.569	1	23.569	6.596	.010
no_of_coordinates	663.190	1	663.190	185.593	.000
Angle1 * Dist1	21.700	1	21.700	6.073	.014
no_of_interactions	194.205	1	194.205	54.348	.000
Environment	26.799	2	13.399	3.750	.024
no_of_coordinates * no_of_interactions	140.351	1	140.351	39.277	.000
Error	2590.684	725	3.573		
Total	23109.998	734			
Corrected Total	4190.690	733			

a. R Squared = .382 (Adjusted R Squared = .375)

Table C1: Tests between subjects

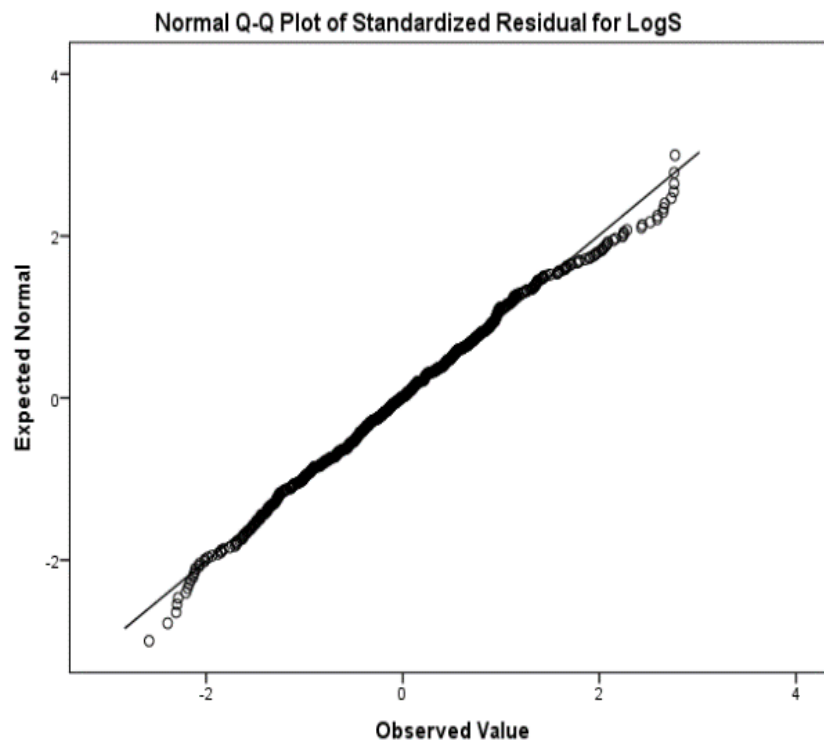


Figure C2:Q-Q plot of the standardised residuals for LogS.

D. Data: Chosen Interactions

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
AHUVUV	1	0.50	1.61	176.25	1
AJEFUS	2	1.00	1.76	165.36	1
AJIFAC	3	1.00	2.37	167.80	2
AJIFAC	3	1.00	1.87	160.39	2
AKAYEQ	4	0.50	1.90	161.79	2
AKAYEQ	4	0.50	1.97	161.70	2
AKEMAF	5	1.00	1.74	166.08	1
AKOCEK	6	1.00	1.89	165.23	2
AKOCEK	6	1.00	1.88	158.95	2
AKOJAN	7	1.00	1.85	140.27	1
AKUVEJ	8	1.00	1.85	166.36	2
AKUVEJ	8	1.00	1.89	145.11	2
ALEVUK	9	0.50	1.81	164.77	2
ALEVUK	9	0.50	1.87	143.20	2
ALOKOC	10	0.50	2.21	144.93	1
ALOKOC	10	0.50	2.42	174.22	2
ALOKOC	10	0.50	2.43	169.67	2
ALOSEB	11	1.00	1.89	150.92	2
ALOSEB	11	1.00	1.89	150.51	2
ALOSEB	11	1.00	1.91	145.29	2
ALOSEB	11	1.00	1.94	144.97	2
ALOSIF	12	1.00	1.79	176.15	2
ALOSIF	12	1.00	2.42	159.61	2
ALUBEQ	13	1.00	2.00	154.91	2
ALUBEQ	13	1.00	2.18	142.70	2
ALUCIV	14	1.00	1.87	140.94	1
ALUDUI	15	2.00	1.98	155.73	2
ALUDUI	15	2.00	2.15	149.20	2
ALUDUI	15	2.00	2.10	147.85	2
ALUDUI	15	2.00	2.22	143.85	2
ALUTOS	16	1.00	1.87	163.56	2
ALUTOS	16	1.00	2.36	137.15	2
AMEJIN	17	1.00	2.06	158.96	2
AMEJIN	17	1.00	2.07	157.23	2
AMEJIN	17	1.00	1.91	150.88	2
AMEJIN	17	1.00	1.93	145.29	2
ANUTOU	18	1.00	2.52	129.22	1
APAWOF	19	1.00	1.73	159.21	2
APAWOF	19	1.00	2.34	131.95	2
APUZAM	20	0.50	1.70	177.00	1
AQABUQ	21	1.00	2.18	155.70	2
AQABUQ	21	1.00	1.58	176.21	2
AQOTUX	22	1.00	1.69	169.20	1

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
ASALUB	23	1.00	2.47	165.20	3
ASALUB	23	1.00	1.86	157.97	3
ASALUB	23	1.00	2.01	154.88	3
ASEHUD	24	1.00	1.82	168.49	2
ASEHUD	24	1.00	1.96	139.88	2
AVECEL	25	0.50	2.41	141.04	2
AVECEL	25	0.50	2.54	137.83	2
AWETIH	26	1.00	1.96	157.23	1
AXIDEQ	27	1.00	2.30	167.77	2
AXIDEQ	27	1.00	2.18	146.48	2
AXIDEQ	27	1.00	2.37	145.87	2
AXIDEQ	27	1.00	1.65	163.70	2
AXIDIU	28	1.00	2.02	162.67	2
AXIDIU	28	1.00	1.87	153.66	2
AXIDIU	28	1.00	2.44	151.25	2
AXIDIU	28	1.00	2.31	153.18	2
AXOREK	29	0.50	1.90	155.83	2
AXOREK	29	0.50	1.98	149.23	2
AXUVAR	30	1.00	2.60	160.66	1
AXUVAR	30	1.00	1.69	170.51	2
AXUVAR	30	1.00	1.73	160.53	2
BACBIT	31	0.33	1.88	164.19	3
BACBIT	31	0.33	2.48	137.90	3
BACBIT	31	0.33	2.49	135.18	3
BAHBIW	32	1.00	1.95	164.33	2
BAHBIW	32	1.00	1.92	160.46	2
BAXNOD	33	1.00	2.39	175.69	2
BAXNOD	33	1.00	1.87	161.34	2
BAYLIY	34	1.00	1.85	155.72	1
BAZKUJ	35	1.00	3.37	175.53	1
BECWIR	36	2.00	1.87	171.70	2
BECWIR	36	2.00	1.92	160.91	2
BEHTAL	37	1.00	2.06	159.78	3
BEHTAL	37	1.00	2.14	156.55	3
BEHTAL	37	1.00	1.84	155.70	3
BEHTOZ	38	1.00	1.89	170.82	2
BEHTOZ	38	1.00	1.84	163.34	2
BEHTOZ	38	1.00	1.81	162.96	2
BEHTOZ	38	1.00	2.58	157.67	2
BICSAI	39	1.00	1.74	173.70	1
BICSAI	39	1.00	1.80	164.67	2
BICSAI	39	1.00	2.12	125.73	2
BIFJAD	40	1.00	2.39	173.96	2
BIFJAD	40	1.00	1.64	175.29	2
BIFVAP	41	1.00	1.65	164.95	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
BIFVAP	41	1.00	2.48	135.56	2
BIGTUH	42	1.00	1.71	174.99	2
BIGTUH	42	1.00	2.05	159.50	2
BILXEA	43	1.00	1.92	164.54	2
BILXEA	43	1.00	1.96	163.84	2
BILXEA	43	1.00	2.37	146.38	2
BILXEA	43	1.00	2.35	145.35	2
BIYSIN	44	1.00	2.26	169.26	1
BIYSIN	44	1.00	1.57	163.20	1
BOKHEQ	45	1.00	1.91	171.02	3
BOKHEQ	45	1.00	2.15	164.54	3
BOKHEQ	45	1.00	2.43	159.17	3
BUKDIW	46	0.50	2.32	173.94	2
BUKDIW	46	0.50	2.37	135.48	2
BULKIC	47	1.00	1.86	176.94	2
BULKIC	47	1.00	1.87	176.37	2
BUTTIU	48	1.00	1.96	166.09	2
BUTTIU	48	1.00	1.99	162.12	2
BUTTIU	48	1.00	2.40	152.26	2
BUTTIU	48	1.00	2.25	147.21	2
BUXPEP	49	1.00	1.80	175.36	3
BUXPEP	49	1.00	2.50	151.20	3
BUXPEP	49	1.00	2.70	148.79	3
BUYTIA	50	1.00	2.24	156.44	2
BUYTIA	50	1.00	2.30	131.92	2
CAMDOL	51	1.00	1.95	154.31	2
CAMDOL	51	1.00	1.88	165.60	2
CAZTAZ	52	0.50	1.85	166.25	2
CAZTAZ	52	0.50	2.27	165.12	2
CEGZIZ	53	1.00	2.49	127.26	2
CEGZIZ	53	1.00	1.70	175.20	2
CEKGAC	54	0.50	1.84	165.55	1
CEKGAC	54	0.50	1.92	151.44	1
CEKPUF	55	1.00	1.83	175.70	1
CELRAO02	56	1.00	2.49	160.50	2
CELRAO02	56	1.00	1.90	157.74	2
CELSOD	57	1.00	1.90	170.16	1
CEQBAC	58	1.00	1.86	171.59	2
CEQBAC	58	1.00	2.49	143.99	2
CETWIJ	59	1.00	1.91	173.34	2
CETWIJ	59	1.00	2.23	153.15	2
CIDNEJ	60	0.50	1.72	170.85	1
CIDNEJ	60	0.50	1.81	175.84	2
CIDNEJ	60	0.50	2.43	137.08	2
CIPYOR	61	1.00	1.87	164.38	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
CIPYOR	61	1.00	1.92	160.69	2
CIPYUX	62	1.00	1.80	165.96	2
CIPYUX	62	1.00	1.89	155.17	2
CIXHOH	63	0.50	2.23	166.67	3
CIXHOH	63	0.50	2.01	155.17	3
CIXHOH	63	0.50	2.36	152.28	3
COCKIQ	64	1.00	1.65	166.50	1
COGQAS	65	1.00	1.77	176.15	1
COKBEL	66	1.00	1.82	170.38	2
COKBEL	66	1.00	2.23	151.03	2
COKBEL	66	1.00	2.24	144.43	2
COKBEL	66	1.00	2.48	126.40	2
COKWAB	67	1.00	1.77	179.59	1
COQBEQ	68	1.00	1.96	168.68	2
COQBEQ	68	1.00	1.80	171.66	2
CORSOS	69	0.50	2.29	159.82	2
CORSOS	69	0.50	2.33	154.62	2
COVNAE	70	2.00	1.74	169.32	3
COVNAE	70	2.00	2.44	161.49	3
COVNAE	70	2.00	1.67	175.94	3
COXWES	71	1.00	1.82	167.52	2
COXWES	71	1.00	2.33	163.22	2
COZWUK	72	0.50	2.14	161.89	2
COZWUK	72	0.50	2.28	147.13	2
CUZVAW	73	1.00	2.06	162.38	2
CUZVAW	73	1.00	1.71	175.63	2
DACPAA	74	1.00	2.48	156.21	3
DACPAA	74	1.00	2.42	154.41	3
DACPAA	74	1.00	2.50	151.12	3
DAQRIX	75	1.00	2.46	161.80	2
DAQRIX	75	1.00	1.62	174.66	2
DEMTEV	76	1.00	1.66	175.90	1
DEMTEV	76	1.00	1.68	174.93	1
DEMTEV	76	1.00	1.66	174.80	1
DESTDM01	77	1.00	1.63	170.67	2
DESTDM01	77	1.00	2.44	162.64	2
DEWYEL	78	2.00	1.87	170.32	2
DEWYEL	78	2.00	1.80	167.68	2
DEWYEL	78	2.00	1.99	166.29	2
DEWYEL	78	2.00	1.95	153.25	2
DEWYIP	79	1.00	1.79	169.58	1
DEXZUC	80	1.00	1.96	164.58	2
DEXZUC	80	1.00	1.95	159.52	2
DIDTUH	81	0.50	1.70	170.20	2
DIDTUH	81	0.50	1.79	154.24	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
DIQCAJ	82	1.00	1.80	154.00	2
DIQCAJ	82	1.00	1.67	152.98	2
DISLUN	83	1.00	1.70	168.27	2
DISLUN	83	1.00	2.22	158.55	2
DISSAA	84	1.00	1.86	167.90	2
DISSAA	84	1.00	1.76	175.28	2
DISTIJ	85	1.00	1.88	160.91	2
DISTIJ	85	1.00	1.96	156.19	2
DISTUV	86	1.00	2.00	151.62	2
DISTUV	86	1.00	1.94	150.54	2
DISVAD	87	1.00	1.99	156.94	3
DISVAD	87	1.00	1.90	152.42	3
DISVAD	87	1.00	2.12	146.77	3
DIVLOK	88	1.00	1.86	149.33	2
DIVLOK	88	1.00	2.11	141.13	2
DUFXEI	89	1.00	2.11	150.13	1
DUFXEI	89	1.00	2.02	176.45	3
DUFXEI	89	1.00	1.97	176.30	3
DUFXEI	89	1.00	1.92	165.63	3
DUFXEI	89	1.00	1.94	164.20	3
DUFXEI	89	1.00	2.46	159.41	3
DUFXEI	89	1.00	2.26	157.98	3
DUKWAI	90	1.00	2.02	149.56	1
DUMNIK	91	1.00	1.86	159.38	2
DUMNIK	91	1.00	2.46	136.70	2
DUNFUP	92	0.50	2.06	172.89	2
DUNFUP	92	0.50	2.44	164.57	2
DUVRIW	93	2.00	2.56	143.88	1
ECELON01	94	1.00	1.76	173.37	2
ECELON01	94	1.00	1.77	166.68	2
ECEZUJ	95	1.00	1.66	143.12	1
ECEZUJ	95	1.00	1.84	177.46	2
ECEZUJ	95	1.00	2.39	147.26	2
ECIBAV	96	1.00	1.89	166.47	1
ECIBAV	96	1.00	2.48	156.34	1
ECIBAV	96	1.00	1.83	169.25	2
ECIBAV	96	1.00	2.69	158.91	2
ECIBAV	96	1.00	2.42	150.24	3
ECIBAV	96	1.00	2.49	149.51	3
ECIBAV	96	1.00	1.70	145.21	3
EFAJUR	97	0.17	1.62	166.06	1
EFIPEP	98	1.00	2.48	150.98	2
EFIPEP	98	1.00	2.47	142.17	2
EGIJAG	99	0.50	2.02	138.09	1
EJIVUO	100	0.50	2.39	167.32	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
EJIVUO	100	0.50	1.70	172.78	2
EJIWAV	101	1.00	2.33	142.98	2
EJIWAV	101	1.00	1.76	169.59	2
EMOREF	102	0.50	2.35	166.13	1
ENUDAU	103	2.00	1.95	162.25	2
ENUDAU	103	2.00	1.83	161.41	2
ENUDAU	103	2.00	1.84	159.10	2
ENUDAU	103	2.00	1.92	158.03	2
ENUDEY	104	1.00	1.87	160.39	2
ENUDEY	104	1.00	1.96	152.93	2
ENUDOI	105	1.00	1.89	149.82	2
ENUDOI	105	1.00	1.94	145.80	2
EPAVUN	106	2.00	1.69	169.51	2
EPAVUN	106	2.00	1.67	167.60	2
EPUJUW	107	1.00	1.62	168.33	1
EQAPUI	108	1.00	2.21	159.77	2
EQAPUI	108	1.00	1.88	156.69	2
EVAKUJ	109	1.00	1.86	171.10	2
EVAKUJ	109	1.00	1.80	168.75	2
EVALEU	110	1.00	1.84	151.66	1
EVUMOY	111	2.00	1.72	169.21	1
EVUWOJ	112	1.00	2.35	163.17	2
EVUWOJ	112	1.00	1.62	171.21	2
EYAMUN	113	1.00	1.72	167.68	1
EYOCEA	114	1.00	1.83	174.30	2
EYOCEA	114	1.00	3.24	124.60	2
FAFJEC	115	0.50	1.93	173.30	1
FAFJEC	115	0.50	1.87	167.04	2
FAFJEC	115	0.50	2.40	127.05	2
FAFSOW	116	2.00	1.91	156.34	2
FAFSOW	116	2.00	1.89	154.86	2
FAFSOW	116	2.00	1.97	153.84	2
FAFSOW	116	2.00	1.98	151.86	2
FAQRIY	117	1.00	1.83	168.96	2
FAQRIY	117	1.00	1.77	167.72	2
FAWZUA	118	1.00	1.83	166.74	2
FAWZUA	118	1.00	1.78	165.73	2
FAXBOX	119	1.00	1.80	155.04	2
FAXBOX	119	1.00	1.87	150.40	2
FAYGUI	120	1.00	2.07	164.52	1
FAYGUI	120	1.00	1.93	152.30	1
FAZSUV	121	1.00	2.12	167.78	1
FAZSUV	121	1.00	2.33	162.93	2
FAZSUV	121	1.00	2.10	161.16	2
FAZSUV	121	1.00	2.08	150.77	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
FAZSUV	121	1.00	2.24	147.93	2
FAZSUV	121	1.00	2.15	137.61	3
FAZSUV	121	1.00	2.19	137.03	3
FAZSUV	121	1.00	2.24	134.71	3
FEFJOR	122	0.50	2.35	156.64	3
FEFJOR	122	0.50	2.35	154.61	3
FEFJOR	122	0.50	1.63	174.05	3
FEPFEN	123	0.50	1.62	175.23	1
FERKAP	124	1.00	1.77	165.74	1
FERKAP	124	1.00	1.78	171.30	1
FEWBAK	125	1.00	2.34	167.77	2
FEWBAK	125	1.00	1.68	156.59	2
FEWHEW	126	0.50	2.37	162.39	2
FEWHEW	126	0.50	1.60	167.81	2
FICNAI	127	1.00	2.29	158.88	2
FICNAI	127	1.00	2.38	153.58	2
FIQNAV	128	1.00	2.29	167.73	2
FIQNAV	128	1.00	1.78	164.01	2
FOBWOJ	129	1.00	1.53	175.17	1
FOFLET	130	1.00	1.89	167.79	2
FOFLET	130	1.00	1.56	172.56	2
FOGWAZ	131	1.00	2.02	172.38	2
FOGWAZ	131	1.00	2.04	164.60	2
FOHDIQ	132	1.00	1.61	162.06	1
FOWRAM	133	0.50	1.92	166.44	3
FOWRAM	133	0.50	2.28	151.38	3
FOWRAM	133	0.50	2.34	139.48	3
FUDPIF	134	1.00	1.82	174.85	3
FUDPIF	134	1.00	2.41	146.75	3
FUDPIF	134	1.00	2.09	140.98	3
FUFQUS	135	1.00	1.84	165.02	2
FUFQUS	135	1.00	2.03	145.78	2
FUFQUS	135	1.00	2.42	145.46	2
FUFQUS	135	1.00	2.25	129.09	2
FULJIG	136	1.00	1.66	165.03	1
FULKIH	137	1.00	1.67	165.68	2
FULKIH	137	1.00	2.48	155.80	2
FUNLUX	138	1.00	2.26	145.87	1
FUWHIP	139	2.00	1.84	151.65	2
FUWHIP	139	2.00	1.86	151.04	2
FUWHIP	139	2.00	1.89	150.13	2
FUWHIP	139	2.00	1.88	149.75	2
FUWHUB	140	1.00	1.89	152.46	2
FUWHUB	140	1.00	1.98	148.15	2
FUZLES	141	1.00	1.72	171.66	3

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
FUZLES	141	1.00	1.90	170.28	3
FUZLES	141	1.00	2.24	147.43	3
GABPEG	142	1.00	1.74	157.68	1
GAGNEJ	143	1.00	1.74	177.91	2
GAGNEJ	143	1.00	1.78	152.67	2
GANJOW	144	1.00	1.67	176.21	2
GANJOW	144	1.00	1.63	173.03	2
GANJOW	144	1.00	1.65	162.34	2
GANJOW	144	1.00	1.69	162.05	2
GEKSOG	145	1.00	1.79	176.32	2
GEKSOG	145	1.00	1.68	169.97	2
GEMLUH	146	1.00	1.67	171.15	2
GEMLUH	146	1.00	1.73	164.48	2
GEWZUF	147	1.00	1.77	169.50	1
GEXZOA	148	1.00	2.34	158.07	3
GEXZOA	148	1.00	2.42	147.31	3
GEXZOA	148	1.00	1.96	146.33	3
GISXEN	149	1.00	1.68	162.39	1
GISXUB	150	0.50	2.00	154.91	2
GISXUB	150	0.50	2.16	142.59	2
GIVJOM	151	1.00	1.75	167.65	2
GIVJOM	151	1.00	2.43	138.19	2
GONQIL	152	1.00	1.93	165.05	2
GONQIL	152	1.00	1.97	161.58	2
GUBTEE	153	0.50	1.95	173.92	1
GUGCER	154	1.00	1.82	125.51	1
GULJAA	155	1.00	1.52	168.31	1
GUTBAZ	156	0.50	1.83	159.57	2
GUTBAZ	156	0.50	2.03	148.57	2
GUVDEG	157	1.00	1.79	171.93	2
GUVDEG	157	1.00	1.83	165.29	2
GUVDEG	157	1.00	2.43	160.21	2
GUVDEG	157	1.00	2.43	143.19	2
GUWDIL	158	0.50	1.64	176.45	1
GUWPUL	159	1.00	1.77	170.19	2
GUWPUL	159	1.00	2.50	145.92	2
HAKVAR01	160	1.00	2.44	164.97	3
HAKVAR01	160	1.00	2.45	160.50	3
HAKVAR01	160	1.00	2.04	124.76	3
HEBQAG	161	1.00	2.29	165.87	1
HEBQAG	161	1.00	2.12	139.37	1
HEBQAG	161	1.00	2.29	156.01	2
HEBQAG	161	1.00	2.98	142.13	2
HEGMOX	162	2.00	2.45	160.87	2
HEGMOX	162	2.00	1.81	158.34	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
HEGMOX	162	2.00	1.78	169.93	3
HEGMOX	162	2.00	2.26	155.47	3
HEGMOX	162	2.00	2.51	147.02	3
HEHMEO	163	1.00	1.80	166.30	3
HEHMEO	163	1.00	2.38	156.21	3
HEHMEO	163	1.00	2.31	146.51	3
HEHPAN	164	1.00	1.68	169.33	2
HEHPAN	164	1.00	1.81	162.65	2
HESBAJ	165	1.00	1.74	161.25	2
HESBAJ	165	1.00	1.89	159.07	2
HESBAJ	165	1.00	2.27	138.49	2
HESBAJ	165	1.00	2.35	133.63	2
HITFOG	166	1.00	1.83	171.77	2
HITFOG	166	1.00	1.78	156.00	2
HITFOG	166	1.00	2.29	153.12	2
HITFOG	166	1.00	2.12	143.77	2
HOMFEU	167	0.50	2.42	161.19	2
HOMFEU	167	0.50	1.68	166.66	2
HORQOU	168	1.00	1.52	168.62	1
HOYPAN	169	1.00	2.83	129.56	1
HOYVIB	170	1.00	1.79	164.65	3
HOYVIB	170	1.00	2.44	141.37	3
HOYVIB	170	1.00	2.48	133.78	3
HUCTUW	171	0.50	1.63	172.56	1
HUHLED	172	1.00	1.86	162.11	2
HUHLED	172	1.00	2.49	132.04	2
HUTSUM	173	1.00	1.68	173.47	1
HUTSUM	173	1.00	1.71	171.23	1
HUTSUM	173	1.00	1.80	162.01	1
HUTSUM	173	1.00	1.76	161.56	1
HUTSUM	173	1.00	2.47	164.87	2
HUTSUM	173	1.00	2.41	163.41	2
HUTSUM	173	1.00	1.73	162.26	2
HUTSUM	173	1.00	2.37	153.48	2
HUTSUM	173	1.00	1.71	174.71	2
HUTSUM	173	1.00	1.70	168.29	2
HUTSUM	173	1.00	1.72	174.08	3
HUTSUM	173	1.00	2.59	124.85	3
HUTSUM	173	1.00	2.39	144.71	3
HUVBUX	174	0.50	1.75	170.15	2
HUVBUX	174	0.50	1.91	139.82	2
HUVBUX	174	0.50	2.37	134.63	2
HUVBUX	174	0.50	1.73	166.59	2
HUVBUX	174	0.50	1.75	168.50	3
HUVBUX	174	0.50	1.93	160.86	3

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
HUVBUX	174	0.50	2.00	139.78	3
IBUXAF	175	1.00	2.13	163.74	2
IBUXAF	175	1.00	1.89	163.04	2
ICOLUI	176	0.50	1.80	178.87	2
ICOLUI	176	0.50	1.80	168.22	2
IFAHIG	177	1.00	1.73	169.15	1
IFOXUY	178	0.50	1.64	173.93	2
IFOXUY	178	0.50	2.31	149.56	2
IGARAL	179	0.50	1.57	170.67	1
IGARAL	179	0.50	2.48	158.86	3
IGARAL	179	0.50	2.44	139.64	3
IGARAL	179	0.50	1.63	159.60	3
IGARIT	180	2.00	1.77	167.33	2
IGARIT	180	2.00	1.72	164.06	2
IGARIT	180	2.00	1.71	160.56	2
IGARIT	180	2.00	1.80	153.68	2
IJASAP	181	1.00	1.97	152.46	2
IJASAP	181	1.00	2.32	120.77	2
IJINAS	182	1.00	2.29	145.19	2
IJINAS	182	1.00	2.52	129.01	2
IKEYAZ	183	1.00	2.41	130.56	2
IKEYAZ	183	1.00	1.61	162.84	2
IKIZAF	184	1.00	1.71	176.77	2
IKIZAF	184	1.00	1.74	176.34	2
IKIZOT	185	1.00	1.79	174.21	2
IKIZOT	185	1.00	1.70	173.83	2
ILEZEF	186	0.50	1.56	166.53	1
IMIGAO	187	1.00	1.72	165.54	2
IMIGAO	187	1.00	2.56	123.57	2
INUREQ	188	1.00	1.87	163.19	2
INUREQ	188	1.00	2.44	155.23	2
INUSOB	189	1.00	1.67	164.23	2
INUSOB	189	1.00	1.83	151.35	2
INUTAO	190	1.00	1.96	178.77	1
IPUGEH	191	1.00	1.85	154.55	3
IPUGEH	191	1.00	2.15	151.61	3
IPUGEH	191	1.00	2.50	135.07	3
IQIYOY	192	1.00	1.78	168.67	2
IQIYOY	192	1.00	2.45	142.83	2
IQOPUZ	193	1.00	1.96	163.25	2
IQOPUZ	193	1.00	1.79	174.86	2
IRUZOL	194	1.00	2.46	152.85	2
IRUZOL	194	1.00	2.03	145.26	2
IWOMUD	195	1.00	1.84	159.56	1
IXAJIC	196	0.50	1.89	164.89	3

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
IXAJIC	196	0.50	2.43	152.89	3
IXAJIC	196	0.50	2.31	152.72	3
IYILEH	197	0.50	1.97	167.30	1
JAFXIA	198	1.00	2.28	165.92	2
JAFXIA	198	1.00	2.23	142.18	2
JALDEG	199	1.00	1.91	157.78	1
JALDEG	199	1.00	1.82	155.23	1
JERQAZ	200	0.50	2.42	165.86	3
JERQAZ	200	0.50	2.45	155.07	3
JERQAZ	200	0.50	2.52	121.68	3
JEZRIP	201	1.00	1.81	161.20	2
JEZRIP	201	1.00	2.43	149.97	2
JOCYOR	202	1.00	1.71	171.03	2
JOCYOR	202	1.00	2.50	129.85	2
JOTSES	203	1.00	1.81	161.24	2
JOTSES	203	1.00	1.87	149.74	2
KAPVON	204	0.50	1.80	163.76	1
KAQXOQ	205	1.00	1.73	170.83	2
KAQXOQ	205	1.00	1.69	167.71	2
KEKFOW	206	0.50	1.66	170.55	1
KELPAU	207	1.00	2.42	152.29	2
KELPAU	207	1.00	1.77	167.52	2
KEZZOE	208	1.00	1.66	173.05	1
KIBBEC	209	1.00	1.83	177.87	2
KIBBEC	209	1.00	1.71	177.00	2
KICJUD	210	1.00	1.80	164.29	1
KIRPIM	211	1.00	2.42	163.44	2
KIRPIM	211	1.00	2.33	152.47	2
KIRPIM	211	1.00	1.68	175.26	2
KIRPIM	211	1.00	1.77	167.46	2
KOJKIF	212	1.00	1.80	168.46	2
KOJKIF	212	1.00	1.90	158.38	2
KOJKOL	213	1.00	1.78	168.85	2
KOJKOL	213	1.00	1.83	164.04	2
KOSHUV	214	0.50	2.40	159.66	2
KOSHUV	214	0.50	1.91	151.12	2
KOVHOS	215	1.00	1.73	176.82	2
KOVHOS	215	1.00	2.26	171.08	2
KOVLUE	216	0.50	1.69	172.53	2
KOVLUE	216	0.50	2.37	160.60	2
KOYPIX	217	0.50	1.87	157.72	2
KOYPIX	217	0.50	2.43	136.48	2
KUHXOC	218	1.00	2.44	150.79	2
KUHXOC	218	1.00	1.59	173.52	2
KUMHEF	219	2.00	1.83	173.56	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
KUMHEF	219	2.00	1.94	140.15	2
KUMHIJ10	220	1.00	1.81	170.25	2
KUMHIJ10	220	1.00	2.59	161.41	2
KUMHOP	221	0.50	2.47	152.86	2
KUMHOP	221	0.50	1.66	171.15	2
KUNYOJ	222	1.00	2.16	167.79	3
KUNYOJ	222	1.00	1.99	165.12	3
KUNYOJ	222	1.00	2.34	141.57	3
KUZNIE	223	1.00	1.64	175.84	2
KUZNIE	223	1.00	2.41	139.37	2
LAKZII	224	1.00	1.73	170.47	2
LAKZII	224	1.00	2.34	160.28	2
LAMHOX	225	1.00	1.69	165.21	1
LATNEB	226	1.00	1.78	171.33	1
LEDKUC	227	0.50	2.26	152.80	2
LEDKUC	227	0.50	2.37	134.95	2
LENPEA	228	0.50	2.12	171.33	2
LENPEA	228	0.50	2.41	164.41	2
LENPEA	228	0.50	2.61	159.01	2
LENPEA	228	0.50	2.64	158.41	2
LENRON	229	1.00	2.36	154.89	1
LIHYOS	230	1.00	1.86	160.99	2
LIHYOS	230	1.00	1.94	150.36	2
LINLOJ	231	1.00	2.24	141.15	2
LINLOJ	231	1.00	1.63	166.03	2
LISDAU	232	1.00	1.77	173.18	3
LISDAU	232	1.00	2.35	139.33	3
LISDAU	232	1.00	2.47	134.79	3
LOCDEN	233	0.50	2.00	172.23	2
LOCDEN	233	0.50	1.95	168.61	2
LOFZUD	234	0.50	1.84	171.11	2
LOFZUD	234	0.50	2.46	143.29	2
LONKEG	235	1.00	1.67	172.31	2
LONKEG	235	1.00	2.38	152.28	2
LOQRUG	236	2.00	2.29	152.80	1
LOQRUG	236	2.00	1.86	174.83	2
LOQRUG	236	2.00	1.92	163.76	2
LOQRUG	236	2.00	1.92	161.89	2
LOQRUG	236	2.00	2.31	160.39	2
LOQRUG	236	2.00	2.47	141.57	2
LOQRUG	236	2.00	1.89	175.79	2
LORXAS	237	1.00	1.99	162.28	1
LORXEW	238	1.00	1.94	174.58	2
LORXEW	238	1.00	2.05	145.77	2
LUDYEP	239	1.00	1.61	159.22	1

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
LUKMEL	240	1.00	2.32	145.44	2
LUKMEL	240	1.00	1.58	165.27	2
LUVMUK	241	0.50	2.51	176.78	2
LUVMUK	241	0.50	2.37	173.50	2
MACLIM	242	0.50	1.64	175.13	2
MACLIM	242	0.50	1.67	173.18	2
MADSOC	243	2.00	1.79	164.77	2
MADSOC	243	2.00	2.02	162.78	2
MANCEJ	244	1.00	2.11	175.42	3
MANCEJ	244	1.00	1.77	169.44	3
MANCEJ	244	1.00	2.44	151.46	3
MARJAR	245	0.50	2.35	175.32	2
MARJAR	245	0.50	1.75	165.55	2
MEKXAB	246	0.50	1.89	168.13	2
MEKXAB	246	0.50	1.89	154.97	2
MIFQID	247	1.00	1.73	173.11	1
MIFQID	247	1.00	1.71	163.93	2
MIFQID	247	1.00	2.38	127.04	2
MIFXUU	248	0.50	1.76	172.90	2
MIFXUU	248	0.50	2.49	130.27	2
MILHAR	249	1.00	1.82	164.77	2
MILHAR	249	1.00	1.86	155.69	2
MIPLUT	250	1.00	1.81	161.36	2
MIPLUT	250	1.00	1.97	153.02	2
MIPPEH	251	1.00	2.42	168.90	3
MIPPEH	251	1.00	1.74	165.47	3
MIPPEH	251	1.00	2.48	129.71	3
MIYTOF	252	1.00	2.22	170.95	2
MIYTOF	252	1.00	1.74	151.96	2
MOHNIH	253	1.00	1.67	154.55	2
MOHNIH	253	1.00	2.29	149.79	2
MONQOX	254	1.00	1.78	167.58	1
MUGCEX	255	1.00	1.83	163.78	2
MUGCEX	255	1.00	1.83	161.81	2
MUQZIJ	256	1.00	2.49	136.16	1
MURGUD	257	1.00	1.97	174.93	2
MURGUD	257	1.00	2.48	160.77	2
NADJIN	258	1.00	1.73	178.19	2
NADJIN	258	1.00	1.95	164.63	2
NADJIN	258	1.00	1.95	157.78	2
NADJIN	258	1.00	2.12	139.59	2
NAFSAQ	259	0.50	2.01	144.06	2
NAFSAQ	259	0.50	2.07	140.64	2
NAGJAJ	260	0.50	2.31	156.55	2
NAGJAJ	260	0.50	1.59	168.77	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
NAWQOS	261	1.00	1.91	157.66	2
NAWQOS	261	1.00	2.39	131.42	2
NEDJUD	262	1.00	1.81	166.08	1
NENSEF	263	2.00	2.03	155.88	3
NENSEF	263	2.00	2.00	155.25	3
NENSEF	263	2.00	2.01	152.09	3
NENSEF	263	2.00	1.91	151.42	3
NENSEF	263	2.00	2.01	150.80	3
NENSEF	263	2.00	2.01	150.32	3
NIFFIS	264	0.50	1.88	162.36	3
NIFFIS	264	0.50	2.32	138.78	3
NIFFIS	264	0.50	2.43	155.68	3
NIKWEK	265	1.00	1.84	170.17	1
NIMGAR	266	1.00	1.73	174.49	2
NIMGAR	266	1.00	1.86	170.44	2
NIMGAR01	267	1.00	1.73	174.41	2
NIMGAR01	267	1.00	1.86	174.36	2
NINFIB	268	1.00	1.75	169.26	2
NINFIB	268	1.00	2.43	136.23	2
NIPBUL	269	2.00	1.63	171.04	1
NIZJAI	270	1.00	1.90	162.92	2
NIZJAI	270	1.00	2.04	153.05	2
NIZJAI	270	1.00	1.95	170.18	3
NIZJAI	270	1.00	2.02	156.48	3
NIZJAI	270	1.00	2.20	151.28	3
NOJHOJ	271	1.00	1.83	168.04	3
NOJHOJ	271	1.00	1.93	148.55	3
NOJHOJ	271	1.00	2.32	144.00	3
NOLCEX	272	1.00	1.92	172.69	1
NOPZUO	273	1.00	1.91	153.00	1
NOSFAE	274	1.00	1.66	167.42	1
NUJHIK	275	1.00	1.74	174.20	2
NUJHIK	275	1.00	2.43	145.03	2
NUJHUW	276	1.00	1.87	171.06	3
NUJHUW	276	1.00	2.50	165.74	3
NUJHUW	276	1.00	2.29	164.91	3
NUJKIM	277	0.50	1.90	158.57	1
NUKQER	278	1.00	1.93	161.83	1
NUNFEI	279	1.00	1.77	171.34	2
NUNFEI	279	1.00	1.84	170.14	2
NUNFEI	279	1.00	1.82	165.12	2
NUNFEI	279	1.00	1.86	177.51	2
NUPYEE	280	1.00	1.83	162.86	2
NUPYEE	280	1.00	2.44	150.79	2
NUQXIH	281	2.00	1.67	163.08	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
NUQXIH	281	2.00	2.48	153.74	2
NUTSOK	282	1.00	1.66	155.01	3
NUTSOK	282	1.00	2.26	146.58	3
NUTSOK	282	1.00	2.44	137.74	3
NUVWAE	283	1.00	1.81	162.45	1
NUVWEI	284	2.00	1.83	166.43	1
NUXCIU	285	0.50	1.76	171.48	2
NUXCIU	285	0.50	2.52	137.36	2
NUXMUP	286	1.00	1.85	146.08	3
NUXMUP	286	1.00	2.39	142.37	3
NUXMUP	286	1.00	1.93	165.93	3
NUXPOM	287	1.00	2.41	153.76	2
NUXPOM	287	1.00	1.57	168.29	2
NUZKIC	288	1.00	2.48	153.56	2
NUZKIC	288	1.00	2.41	150.29	2
OBIZIJ	289	1.00	2.47	157.33	2
OBIZIJ	289	1.00	1.81	176.07	2
OCAFUU	290	1.00	1.90	156.28	2
OCAFUU	290	1.00	2.33	146.49	2
OCEHIN	291	1.00	2.44	122.61	2
OCEHIN	291	1.00	1.88	171.86	2
OCEHIN	291	1.00	2.12	167.13	3
OCEHIN	291	1.00	1.88	159.21	3
OCEHIN	291	1.00	2.03	158.13	3
ODEFEJ	292	1.00	1.77	171.60	3
ODEFEJ	292	1.00	1.83	161.76	3
ODEFEJ	292	1.00	2.47	131.69	3
ODIFIR	293	0.50	1.83	151.05	1
OFOMOM	294	0.50	2.34	154.02	2
OFOMOM	294	0.50	1.61	167.69	2
OFONAA	295	0.50	2.42	147.05	2
OFONAA	295	0.50	1.63	167.19	2
OHEXUW	296	0.50	1.58	170.32	1
OJANOE	297	0.50	2.33	155.11	2
OJANOE	297	0.50	1.69	149.56	2
OJICOB	298	1.00	1.85	175.42	1
OJIYOX	299	0.50	1.92	151.22	1
OKEJOE	300	6.00	1.87	170.20	1
OKEJOE	300	6.00	1.67	173.31	2
OKEJOE	300	6.00	1.68	171.46	2
OKEJOE	300	6.00	3.29	169.89	2
OKEJOE	300	6.00	1.65	168.23	2
OKEJOE	300	6.00	3.27	163.62	2
OKEJOE	300	6.00	3.14	161.52	2
OKITIN	301	0.50	1.83	158.69	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
OKITIN	301	0.50	1.88	157.51	2
OKITOT	302	0.50	1.90	157.24	1
OKUYOK	303	1.00	2.44	172.93	2
OKUYOK	303	1.00	1.78	166.55	2
OLIPK	304	1.00	1.82	163.34	2
OLIPK	304	1.00	2.10	147.81	2
OMELUP	305	1.00	1.91	165.91	2
OMELUP	305	1.00	1.77	165.17	2
OMEMAW	306	1.00	1.77	169.91	2
OMEMAW	306	1.00	1.87	168.46	2
OQAZAI	307	1.00	1.94	164.93	2
OQAZAI	307	1.00	2.41	138.89	2
OQAZAI	307	1.00	1.85	174.57	3
OQAZAI	307	1.00	2.08	162.62	3
OQAZAI	307	1.00	2.14	161.82	3
OQONUE	308	1.00	1.75	166.40	2
OQONUE	308	1.00	2.41	142.33	2
PADWID	309	1.00	2.43	173.48	2
PADWID	309	1.00	1.81	167.35	2
PAMSOM	310	1.00	1.55	172.70	1
PAZJUX	311	2.00	1.64	172.10	2
PAZJUX	311	2.00	2.30	135.42	2
PAZKIM	312	1.00	1.97	162.98	2
PAZKIM	312	1.00	2.28	133.95	2
PERWEQ	313	1.00	1.93	159.00	2
PERWEQ	313	1.00	1.99	151.56	2
PEYMUB	314	1.00	2.32	174.12	3
PEYMUB	314	1.00	2.33	161.20	3
PEYMUB	314	1.00	2.53	137.16	3
PIDLOF	315	1.00	1.97	159.94	2
PIDLOF	315	1.00	2.00	142.80	2
PIKQOR	316	0.50	2.47	178.75	3
PIKQOR	316	0.50	2.35	169.70	3
PIKQOR	316	0.50	2.32	163.01	3
PILGIC	317	1.00	2.47	141.39	1
PILWOX	318	1.00	1.70	164.39	1
PIWCAA	319	1.00	1.62	174.89	2
PIWCAA	319	1.00	2.46	125.64	2
PIWCAA	319	1.00	1.63	176.23	3
PIWCAA	319	1.00	2.46	149.80	3
PIWCAA	319	1.00	2.45	126.85	3
PUHHAC	320	1.00	1.83	153.91	2
PUHHAC	320	1.00	1.86	152.29	2
PUKRIY	321	1.00	1.77	169.18	2
PUKRIY	321	1.00	2.33	149.47	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
PUVVOR	322	0.50	1.64	177.09	1
QATYOA	323	1.00	2.45	148.26	2
QATYOA	323	1.00	1.61	173.00	2
QAWNIM	324	0.50	1.69	170.73	2
QAWNIM	324	0.50	2.45	168.38	2
QEKLEX	325	1.00	1.76	176.64	2
QEKLEX	325	1.00	1.83	165.18	2
QEWDED	326	1.00	1.84	174.63	1
QIMFOH	327	1.00	2.46	154.54	2
QIMFOH	327	1.00	1.55	168.15	2
QIVBUU	328	1.00	1.83	155.35	2
QIVBUU	328	1.00	2.29	152.43	2
QIWVAV	329	1.00	1.80	177.22	2
QIWVAV	329	1.00	1.93	147.82	2
QOFWEP	330	1.00	2.19	166.19	2
QOFWEP	330	1.00	2.34	165.82	2
QOJTAL	331	1.00	1.82	173.82	1
QOJTAL	331	1.00	1.77	173.97	2
QOJTAL	331	1.00	1.95	164.69	2
QOJTAL	331	1.00	2.32	155.58	2
QOJTAL	331	1.00	2.21	134.63	2
QOJTAL	331	1.00	1.76	170.44	3
QOJTAL	331	1.00	2.36	161.80	3
QOJTAL	331	1.00	2.21	143.39	3
QOPMUF	332	2.00	1.98	143.80	2
QOPMUF	332	2.00	1.99	142.29	2
QOPMUF	332	2.00	2.18	140.21	2
QOPMUF	332	2.00	2.19	139.50	2
QORZOM	333	1.00	2.31	157.24	1
QORZOM	333	1.00	1.91	171.17	2
QORZOM	333	1.00	1.97	160.14	2
QOTBIM	334	1.00	2.53	172.86	2
QOTBIM	334	1.00	1.70	172.43	2
QOVQAU	335	1.00	1.96	168.34	2
QOVQAU	335	1.00	1.96	134.77	2
QUCQUB	336	1.00	2.04	152.78	2
QUCQUB	336	1.00	2.04	146.54	2
QUCRAI	337	1.00	2.04	153.09	2
QUCRAI	337	1.00	2.52	146.66	2
QUFTUI	338	1.00	1.78	164.32	1
QUJDOO	339	1.00	1.90	162.48	2
QUJDOO	339	1.00	2.89	129.87	2
QULTIC	340	0.50	1.73	175.26	1
QUPRUP	341	1.00	1.87	177.65	2
QUPRUP	341	1.00	2.39	162.63	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
QUXDOE	342	1.00	1.97	159.01	1
RABJEL	343	1.00	1.77	152.28	2
RABJEL	343	1.00	1.77	144.50	2
RACTIA	344	0.50	1.64	162.91	1
RADHIP	345	0.50	1.69	172.33	2
RADHIP	345	0.50	1.74	171.04	2
RADJOX	346	0.50	1.72	156.27	1
RALZEJ	347	0.50	1.81	163.83	2
RALZEJ	347	0.50	2.40	130.66	2
RAPJOI	348	1.00	1.92	155.26	1
RAPVEK	349	1.00	1.79	162.57	1
RAWFAY	350	1.00	1.83	168.98	2
RAWFAY	350	1.00	2.50	138.87	2
RENMOM	351	1.00	1.86	169.93	2
RENMOM	351	1.00	1.97	136.56	2
REZRAR	352	1.00	1.85	154.08	2
REZRAR	352	1.00	2.03	148.71	2
REZRIZ	353	1.00	1.82	160.30	2
REZRIZ	353	1.00	2.11	140.07	2
REZRIZ01	354	1.00	1.81	161.68	3
REZRIZ01	354	1.00	2.16	143.51	3
REZRIZ01	354	1.00	2.35	142.58	3
RIGYEM	355	1.00	1.76	172.46	1
RIMSUD	356	1.00	1.91	176.04	2
RIMSUD	356	1.00	1.96	162.40	2
RIZQAU	357	0.50	1.83	166.31	2
RIZQAU	357	0.50	2.03	159.05	2
ROFBOF	358	1.00	1.95	152.81	2
ROFBOF	358	1.00	1.98	147.33	2
ROKPAK	359	1.00	1.82	164.39	3
ROKPAK	359	1.00	1.84	163.03	3
ROKPAK	359	1.00	2.41	135.48	3
ROMLIQ	360	1.00	2.22	164.11	3
ROMLIQ	360	1.00	1.83	161.63	3
ROMLIQ	360	1.00	2.36	137.52	3
ROVPOJ	361	1.00	1.86	154.75	1
RUKFUA	362	0.50	2.40	158.71	3
RUKFUA	362	0.50	2.41	132.93	3
RUKFUA	362	0.50	1.63	173.84	3
RUXPAC	363	0.50	2.45	166.61	2
RUXPAC	363	0.50	1.86	163.46	2
SAFLOD	364	1.00	1.72	160.91	2
SAFLOD	364	1.00	2.10	136.04	2
SAJREC	365	1.00	1.74	177.27	2
SAJREC	365	1.00	2.51	128.45	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
SAKMEY	366	0.50	1.90	138.75	1
SENTAH	367	1.00	2.40	158.66	2
SENTAH	367	1.00	2.36	150.79	2
SENTAH	367	1.00	1.89	173.41	3
SENTAH	367	1.00	2.68	164.76	3
SENTAH	367	1.00	1.86	158.80	3
SERNAG	368	1.00	1.69	165.08	2
SERNAG	368	1.00	2.42	152.09	2
SERZIA	369	1.00	1.70	176.71	3
SERZIA	369	1.00	1.88	146.32	3
SERZIA	369	1.00	2.50	127.20	3
SIGFIY	370	2.00	1.72	169.30	1
SIGFIY	370	2.00	1.79	147.07	2
SIGFIY	370	2.00	1.95	141.86	2
SIMCIB	371	1.00	1.78	172.76	3
SIMCIB	371	1.00	1.92	167.15	3
SIMCIB	371	1.00	2.26	163.41	3
SOCFEW	372	1.00	1.98	145.31	1
SOCFEW	372	1.00	1.93	168.40	2
SOCFEW	372	1.00	1.99	164.01	2
SOCFEW	372	1.00	2.33	158.36	2
SOCFEW	372	1.00	1.96	151.42	2
SOCFEW	372	1.00	1.95	146.30	2
SOCFEW	372	1.00	2.78	143.06	2
SOCFOG	373	1.00	1.88	172.12	1
SOCFOG	373	1.00	1.80	165.50	1
SOCFOG	373	1.00	1.93	161.31	1
SOFNUX	374	0.50	1.61	174.49	2
SOFNUX	374	0.50	2.49	130.16	2
SOPCOP	375	0.50	1.56	173.30	1
SOVYOT01	376	2.00	1.78	158.96	2
SOVYOT01	376	2.00	1.84	152.62	2
SOVYOT01	376	2.00	1.92	142.66	2
SOVYOT01	376	2.00	1.71	168.52	2
SOXROO	377	1.00	1.76	168.06	1
SUNZEG	378	0.50	1.93	162.47	2
SUNZEG	378	0.50	2.35	139.46	2
TACSEW	379	1.00	2.12	167.67	3
TACSEW	379	1.00	2.19	166.70	3
TACSEW	379	1.00	2.09	161.92	3
TACXAW	380	1.00	1.82	168.67	1
TAJGES	381	1.00	1.61	167.70	1
TAJGIW	382	1.00	1.60	171.74	1
TASZUK	383	0.50	2.00	143.61	2
TASZUK	383	0.50	2.44	132.25	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
TATJEF	384	0.50	1.75	164.92	2
TATJEF	384	0.50	2.38	136.43	2
TETQUG	385	1.00	1.65	162.59	2
TETQUG	385	1.00	1.65	160.72	2
TETQUG	385	1.00	2.45	146.54	2
TETQUG	385	1.00	2.53	134.30	2
TETYOI	386	0.50	1.91	159.88	1
TEWWEZ	387	1.00	2.20	166.41	1
TIHFUM	388	1.00	1.76	174.39	2
TIHFUM	388	1.00	2.37	135.88	2
TIHGAT	389	1.00	1.80	165.87	1
TIVNUI	390	1.00	1.88	168.43	3
TIVNUI	390	1.00	2.14	158.18	3
TIVNUI	390	1.00	2.05	156.23	3
TIVPEU	391	1.00	1.85	154.97	2
TIVPEU	391	1.00	1.97	148.85	2
TIVPIY	392	1.00	1.81	159.57	2
TIVPIY	392	1.00	1.92	153.67	2
TMADMS01	393	0.50	1.70	162.99	2
TMADMS01	393	0.50	1.60	168.06	2
TNIZMS	394	1.00	1.61	165.11	1
TOJCOL	395	0.50	1.79	165.58	1
TOKZUP	396	1.00	1.64	154.39	1
TOKZUP	396	1.00	1.84	153.40	2
TOKZUP	396	1.00	1.85	152.21	2
TOMPOC	397	1.00	1.66	170.80	1
TURCOA	398	1.00	1.58	172.82	1
TUVSOU	399	1.00	1.89	165.17	3
TUVSOU	399	1.00	2.49	162.78	3
TUVSOU	399	1.00	2.32	150.03	3
UCOVIS	400	1.00	1.60	161.35	2
UCOVIS	400	1.00	2.22	150.66	2
UCOVIS	400	1.00	1.78	141.82	2
UCOVIS	400	1.00	2.19	133.27	2
UCOVIS	400	1.00	1.66	175.37	3
UCOVIS	400	1.00	2.37	133.12	3
UCOVIS	400	1.00	2.45	126.83	3
UFUXUO	401	1.00	1.94	150.78	2
UFUXUO	401	1.00	1.66	173.77	2
UKUTUQ	402	1.00	1.79	168.17	1
ULEMUT	403	1.00	1.80	175.42	1
ULENUV	404	1.00	2.39	169.73	2
ULENUV	404	1.00	2.42	163.86	2
ULERIN	405	1.00	1.79	161.20	1
UMUMEV	406	1.00	1.89	156.88	1

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
UMUZOR	407	1.00	1.93	148.92	1
UMUZOR	407	1.00	1.85	164.45	2
UMUZOR	407	1.00	2.33	139.07	2
UNAYOY	408	2.00	1.74	177.53	2
UNAYOY	408	2.00	1.76	162.99	2
UNUNIC	409	0.50	2.33	172.43	2
UNUNIC	409	0.50	2.69	160.49	2
UPASIO	410	1.00	2.44	137.39	3
UPASIO	410	1.00	2.50	128.55	3
UPASIO	410	1.00	1.81	167.93	3
UPEQIR	411	1.00	1.86	174.86	2
UPEQIR	411	1.00	1.83	172.44	2
UQEHJ	412	1.00	1.83	166.30	2
UQEHJ	412	1.00	1.86	164.06	2
UQEHJ	412	1.00	1.93	162.60	2
UQEHJ	412	1.00	1.97	156.61	2
UROHOZ	413	1.00	2.26	134.98	2
UROHOZ	413	1.00	2.01	158.47	2
UTEPAM	414	1.00	1.85	167.48	1
UTOBIP	415	1.00	2.31	124.76	2
UTOBIP	415	1.00	1.61	167.97	2
UVAFOO	416	0.50	1.71	171.11	2
UVAFOO	416	0.50	2.24	142.54	2
UVETOF	417	0.33	2.19	161.67	2
UVETOF	417	0.33	1.88	159.52	2
UWALUB	418	2.00	1.83	149.04	1
UWALUB	418	2.00	2.66	150.96	2
UWALUB	418	2.00	2.33	147.15	2
UWEJIQ	419	1.00	1.75	166.11	1
UWEJIQ	419	1.00	1.67	170.90	1
UWEJIQ	419	1.00	1.76	152.20	1
UWEJIQ	419	1.00	1.62	175.67	2
UWEJIQ	419	1.00	2.42	173.42	2
UWEJUC	420	0.50	1.82	166.43	2
UWEJUC	420	0.50	1.86	151.67	2
UXAZOJ	421	1.00	2.34	172.67	2
UXAZOJ	421	1.00	1.77	165.97	2
UXOVIO	422	1.00	2.34	179.72	2
UXOVIO	422	1.00	1.81	159.73	2
UYAFIL	423	1.00	1.79	160.56	2
UYAFIL	423	1.00	2.41	143.25	2
UYORIK	424	1.00	1.99	174.89	2
UYORIK	424	1.00	1.97	174.32	2
UYORIK	424	1.00	2.22	140.35	2
UYORIK	424	1.00	2.32	135.30	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
VAMMED	425	1.00	1.81	159.71	1
VASQAH	426	1.00	1.64	164.75	2
VASQAH	426	1.00	2.98	132.61	2
VATLUZ	427	1.00	1.91	169.65	1
VATLUZ	427	1.00	1.81	166.30	1
VAWLIQ	428	1.00	1.84	162.26	2
VAWLIQ	428	1.00	1.84	171.92	2
VAWLOW	429	1.00	1.80	172.46	2
VAWLOW	429	1.00	1.83	169.01	2
VAWWAT	430	0.33	1.75	160.26	2
VAWWAT	430	0.33	2.51	138.13	2
VAXQOB	431	1.00	2.37	168.99	2
VAXQOB	431	1.00	2.36	133.58	2
VEGMOJ	432	1.00	1.72	167.14	2
VEGMOJ	432	1.00	2.33	128.59	2
VEKPOR	433	1.00	1.90	155.85	2
VEKPOR	433	1.00	2.26	153.34	2
VEKQOS	434	0.50	1.72	168.00	1
VEKQOS	434	0.50	1.73	173.18	2
VEKQOS	434	0.50	2.29	159.18	2
VELLUV	435	1.00	2.22	151.70	1
VEMKON	436	1.00	1.62	173.90	2
VEMKON	436	1.00	2.57	153.99	2
VEQFAA	437	1.00	1.79	170.29	1
VEVLUD	438	1.00	1.64	166.31	1
VEVMAK	439	1.00	1.59	171.98	1
VEVMAK	439	1.00	2.58	159.42	3
VEVMAK	439	1.00	2.59	157.42	3
VEVMAK	439	1.00	1.61	161.91	3
VEVMEO	440	1.00	1.60	173.00	1
VIDNEC	441	2.00	1.72	169.24	2
VIDNEC	441	2.00	1.71	166.87	2
VIDNEC	441	2.00	1.88	166.14	2
VIDNEC	441	2.00	1.84	162.13	2
VITCAD	442	2.00	1.74	172.09	2
VITCAD	442	2.00	1.98	147.78	2
VITCAD	442	2.00	1.95	145.74	2
VITCAD	442	2.00	1.73	167.39	2
VIWGEP	443	1.00	2.04	146.63	1
VIWGIT	444	1.00	1.94	178.58	2
VIWGIT	444	1.00	2.46	151.00	2
VOCYUI	445	0.50	1.90	157.35	2
VOCYUI	445	0.50	2.06	146.76	2
VODWIV	446	0.50	1.70	171.86	1
VODWIV	446	0.50	1.87	175.29	3

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
VODWIV	446	0.50	2.49	164.63	3
VODWIV	446	0.50	2.00	161.18	3
VOGDEC	447	1.00	1.59	176.78	1
VUYPOW	448	1.00	2.42	158.94	1
VUYPOW	448	1.00	1.81	157.21	3
VUYPOW	448	1.00	2.36	157.05	3
VUYPOW	448	1.00	2.26	137.13	3
VUYWAP	449	1.00	1.63	172.34	2
VUYWAP	449	1.00	1.81	169.60	2
VUZHEE	450	1.00	2.33	169.87	3
VUZHEE	450	1.00	1.85	168.19	3
VUZHEE	450	1.00	2.36	161.06	3
WABBAC	451	1.00	1.79	163.76	1
WABBAC	451	1.00	1.70	174.12	2
WABBAC	451	1.00	2.35	152.38	2
WAHTIK	452	1.00	2.14	165.12	1
WAHWAF	453	1.00	2.15	163.10	2
WAHWAF	453	1.00	2.44	132.18	2
WAMBOE	454	1.00	1.78	144.47	2
WAMBOE	454	1.00	1.90	135.38	2
WANGUO	455	1.00	2.38	169.18	2
WANGUO	455	1.00	2.31	163.43	2
WANGUO	455	1.00	2.40	147.35	2
WANGUO	455	1.00	2.30	144.95	2
WAYTUL	456	1.00	1.79	174.76	2
WAYTUL	456	1.00	1.74	176.31	2
WELYUI	457	1.00	1.70	169.77	1
WELZUK	458	1.00	1.68	167.70	2
WELZUK	458	1.00	2.36	149.73	2
WELZUK01	459	1.00	1.66	174.20	1
WERGIJ	460	1.00	1.81	160.87	2
WERGIJ	460	1.00	2.03	152.07	2
WIGJEC	461	1.00	1.87	159.90	3
WIGJEC	461	1.00	2.10	148.89	3
WIGJEC	461	1.00	2.39	140.16	3
WINZEZ	462	1.00	1.78	156.86	1
WOMFOU	463	0.50	1.73	170.92	2
WOMFOU	463	0.50	2.31	163.03	2
WOMFOU	463	0.50	1.81	170.39	3
WOMFOU	463	0.50	2.69	151.47	3
WOMFOU	463	0.50	2.51	145.35	3
WOMGIP	464	0.50	1.96	168.59	2
WOMGIP	464	0.50	2.07	131.23	2
WOPVOO	465	5.00	1.84	178.34	2
WOPVOO	465	5.00	1.83	165.42	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
WOPVOO	465	5.00	1.79	164.75	2
WOPVOO	465	5.00	1.77	164.37	2
WOPVOO	465	5.00	1.77	160.94	2
WOPVOO	465	5.00	1.84	150.36	2
WOPVOO	465	5.00	1.82	150.04	2
WOPVOO	465	5.00	1.73	169.49	2
WUVXEQ	466	0.50	1.85	168.32	1
WUYGIH	467	0.50	1.94	155.28	2
WUYGIH	467	0.50	2.33	136.68	2
XACWIK	468	1.00	1.78	173.46	2
XACWIK	468	1.00	2.42	168.18	2
XAHLAV	469	1.00	1.92	164.08	3
XAHLAV	469	1.00	2.45	162.67	3
XAHLAV	469	1.00	2.34	140.12	3
XAJHOI	470	3.00	2.63	142.73	1
XAJHOI	470	3.00	2.24	166.81	2
XAJHOI	470	3.00	2.05	161.30	2
XAJHOI	470	3.00	1.91	176.75	3
XAJHOI	470	3.00	2.42	174.98	3
XAJHOI	470	3.00	1.84	174.65	3
XAJHOI	470	3.00	1.90	169.95	3
XAJHOI	470	3.00	1.83	169.78	3
XAJHOI	470	3.00	1.88	163.68	3
XAJHOI	470	3.00	1.94	163.01	3
XAJHOI	470	3.00	2.38	137.85	3
XAJHOI	470	3.00	2.42	132.54	3
XAKMIG	471	1.00	2.24	151.30	2
XAKMIG	471	1.00	2.15	135.89	2
XALVUB	472	1.00	1.93	175.58	2
XALVUB	472	1.00	1.67	159.85	2
XAPCAU	473	0.50	1.91	160.82	2
XAPCAU	473	0.50	1.80	153.41	2
XAPVEP	474	1.00	1.90	156.11	2
XAPVEP	474	1.00	1.99	147.58	2
XAPVIT	475	1.00	1.92	156.49	2
XAPVIT	475	1.00	1.92	150.77	2
XAQVES	476	1.00	2.18	154.93	3
XAQVES	476	1.00	2.42	148.37	3
XAQVES	476	1.00	2.23	144.72	3
XAQVIW	477	1.00	2.31	164.96	3
XAQVIW	477	1.00	2.25	151.53	3
XAQVIW	477	1.00	2.37	141.61	3
XAQWET	478	1.00	2.30	165.47	2
XAQWET	478	1.00	1.69	172.48	2
XARBEZ	479	1.00	1.59	175.49	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
XARBEZ	479	1.00	1.93	163.46	2
XARCOK	480	1.00	2.32	165.35	2
XARCOK	480	1.00	2.39	155.91	2
XARCOK	480	1.00	1.92	154.35	2
XARCOK	480	1.00	1.86	153.42	2
XEBHAP	481	1.00	1.61	169.22	2
XEBHAP	481	1.00	2.33	159.10	2
XEJPAF	482	1.00	1.69	167.73	1
XENFAX	483	1.00	1.83	153.33	2
XENFAX	483	1.00	2.14	133.11	2
XEQWAR	484	1.00	2.47	156.59	1
XEQWAR	484	1.00	2.34	176.97	2
XEQWAR	484	1.00	2.18	157.07	2
XICMUT	485	2.00	2.41	159.27	2
XICMUT	485	2.00	2.42	159.14	2
XICMUT	485	2.00	1.60	169.43	2
XICMUT	485	2.00	1.59	164.38	2
XIFGAU	486	1.00	1.67	165.48	2
XIFGAU	486	1.00	1.88	161.45	2
XIJRAL	487	1.00	2.35	152.95	3
XIJRAL	487	1.00	2.44	137.02	3
XIJRAL	487	1.00	1.69	173.96	3
XIKLUA	488	1.00	1.77	173.79	2
XIKLUA	488	1.00	2.42	159.54	2
XIPKIS	489	1.00	1.79	165.20	1
XITMOD	490	0.50	2.32	169.05	2
XITMOD	490	0.50	2.67	166.86	2
XITMOD	490	0.50	1.73	164.50	2
XITMOD	490	0.50	1.97	132.75	2
XIZTAB	491	0.50	1.85	144.63	2
XIZTAB	491	0.50	1.80	144.85	2
XOBNAD	492	1.00	2.34	146.17	1
XOGWEX	493	1.00	1.63	172.22	2
XOGWEX	493	1.00	2.46	171.93	2
XOKDIK	494	1.00	1.77	164.16	2
XOKDIK	494	1.00	1.89	154.35	2
XOMBIL	495	1.00	1.80	165.04	2
XOMBIL	495	1.00	1.75	145.02	2
XOSFOB	496	1.00	1.78	172.26	2
XOSFOB	496	1.00	1.87	165.18	2
XOSFOB	496	1.00	1.85	164.53	2
XOSFOB	496	1.00	2.09	155.02	2
XOZHAX	497	0.50	1.71	157.75	1
XOZHAX	497	0.50	2.33	155.49	2
XOZHAX	497	0.50	1.76	154.44	2

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
XUCJEK	498	1.00	1.90	176.11	2
XUCJEK	498	1.00	2.29	164.12	2
XUDNUG	499	1.00	1.81	144.90	2
XUDNUG	499	1.00	2.12	143.73	2
XUKZIM	500	1.00	1.78	176.97	2
XUKZIM	500	1.00	1.71	169.66	2
XULMAS	501	0.50	1.70	175.19	3
XULMAS	501	0.50	2.31	144.33	3
XULMAS	501	0.50	2.44	143.32	3
XUXXUK	502	1.00	2.29	128.55	1
XUXYEV	503	1.00	1.68	173.65	2
XUXYEV	503	1.00	3.28	137.10	2
XUZYUN	504	1.00	2.38	158.74	2
XUZYUN	504	1.00	2.47	130.11	2
YARJEH	505	1.00	1.87	170.94	1
YARWOD	506	1.00	1.62	165.98	1
YARWOD	506	1.00	2.51	159.47	2
YARWOD	506	1.00	1.64	166.08	2
YERZOL	507	1.00	2.12	166.71	2
YERZOL	507	1.00	2.05	154.64	2
YICMUU	508	1.00	2.25	160.39	2
YICMUU	508	1.00	2.28	152.87	2
YIJBAW	509	1.00	1.93	166.52	2
YIJBAW	509	1.00	2.03	151.69	2
YILJIO	510	1.00	2.32	165.00	1
YILJIO	510	1.00	3.12	148.52	3
YILJIO	510	1.00	2.34	142.32	3
YILJIO	510	1.00	2.39	140.27	3
YINGOS	511	0.50	1.71	167.68	1
YINROE	512	0.50	1.73	173.98	2
YINROE	512	0.50	2.34	172.47	2
YIPFOU	513	0.50	1.56	151.17	1
YIPGAH	514	0.50	2.36	153.12	2
YIPGAH	514	0.50	1.57	168.01	2
YIPJEO	515	0.50	1.73	178.41	2
YIPJEO	515	0.50	2.45	177.47	2
YITKOB	516	1.00	2.62	137.26	2
YITKOB	516	1.00	1.83	173.99	2
YIZCUG	517	1.00	1.81	162.37	1
YIZCUG01	518	1.00	1.87	150.20	1
YIZGEU	519	2.00	1.80	165.93	1
YIZGEU	519	2.00	2.47	155.35	2
YIZGEU	519	2.00	1.94	143.33	2
YOJSUN	520	1.00	1.89	153.32	1
YOKHIP	521	1.00	2.02	172.12	3

Name	Solvate no.	Zprime	Dist1	Angle1	Environment
YOKHIP	521	1.00	2.46	159.39	3
YOKHIP	521	1.00	1.96	154.10	3
YOPFOZ	522	0.50	2.40	176.78	3
YOPFOZ	522	0.50	2.42	154.70	3
YOPFOZ	522	0.50	1.79	146.81	3
YOXZUG	523	1.00	1.64	169.35	1
YOXZUG	523	1.00	1.54	163.66	1
YOXZUG	523	1.00	1.58	159.33	2
YOXZUG	523	1.00	2.39	155.34	2
YOZWIV	524	1.00	1.77	166.35	1
YUNXAH	525	1.00	1.84	144.29	1
YUVQEM	526	0.50	2.33	170.90	3
YUVQEM	526	0.50	2.13	154.28	3
YUVQEM	526	0.50	2.47	124.09	3
ZAVCEE	527	0.50	2.33	143.85	1
ZIDLUV	528	1.00	2.26	164.81	1
ZIDLUV	528	1.00	2.11	151.48	1
ZIDLUV	528	1.00	2.45	118.22	1
ZITNUL	529	1.00	1.71	170.73	2
ZITNUL	529	1.00	1.68	166.49	2
ZITPAT	530	1.00	1.61	167.59	1
ZITPAT	530	1.00	1.67	174.02	2
ZITPAT	530	1.00	1.65	173.25	2
ZOFDIJ	531	0.50	1.60	162.70	1
ZUCREU	532	1.00	2.10	165.29	1
ZUGJEQ	533	1.00	2.30	154.72	2
ZUGJEQ	533	1.00	1.60	177.30	2
ZUKSON	534	0.50	1.68	172.07	2
ZUKSON	534	0.50	2.39	141.94	2
ZUQTEM	535	1.00	1.86	170.43	2
ZUQTEM	535	1.00	2.17	152.80	2