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Supplementary Materials: $RCH_3\cdots O$ Interactions in Biological Systems: Are They Trifurcated H-Bonds or Noncovalent Carbon Bonds?

Antonio Bauzá and Antonio Frontera

Table S1. Results from the PDB search. Distances in Å. Angles in degrees.

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
17	202-B	3ucb	2.93231	172.006
133	246	1gj8	2.90482	174.118
282	2001-X	2rbz	2.96481	171.068
372	303-A	4gr9	3.00791	177.233
592	1224-A	4awq	3.11099	170.206
592	1224-B	4awq	2.99529	175.910
861	201-D	4ggq	3.18859	171.357
0HK	2000-A	4daj	2.81268	170.204
0HK	2000-D	4daj	2.85544	176.297
0HK	2000-A	4u14	2.93495	177.414
0JZ	6002-B	3g60	3.16707	174.686
0MS	601-B	4dyp	2.92292	172.064
17E	502-F	4r85	3.19696	170.306
17E	501-E	4r85	3.13288	172.758
17E	501-B	4r85	3.15277	172.880
1EU	2-A	3fv5	3.11854	174.548
2KT	524-B	3tdf	2.86164	174.123
2L0	301-H	4no9	2.93815	177.652
2NR	1001-A	4nw5	3.17963	173.485
2OY	301-B	4nsy	3.01365	171.552
2OY	301-A	4nsy	3.03122	171.953
2OY	301-B	4nsv	3.16389	172.970
2OY	301-A	4nsv	3.15208	173.740
2VA	901	1wnz	3.15744	177.627
30B	500-D	3kee	3.08536	172.445
3BV	201-b	4qwl	3.00296	172.032
3BV	201-N	4qwl	3.01518	172.064
3G4	2007-D	3g49	2.71818	170.432
3PK	501-A	4k7r	3.15561	171.384
41Z	401-A	4xjt	2.78387	171.739
4MB	1603	2hds	3.09725	170.201
5MC	501-C	4jnp	3.16845	170.595
5MC	501-E	4jnp	3.16032	171.859
5MC	501-B	4jnp	3.19147	172.565
6HE	154-A	2ekt	3.19258	173.028
7DE	102	1y2j	3.17163	174.434
ACE-LEU-ALA-DCL-POL	1-c	4y74	3.089	177.740
ACE-XXXLXLXX-MLU-GLY	1-C	5ah4	3.08542	173.469
ACM	360-A	3ids	3.16417	175.031
ACT	1722-C	4aj9	3.11636	171.159
ACT	1342-A	2waa	2.89241	171.381

Table S1. *Cont.*

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
ACT	278-A	3spv	2.96125	171.713
ACT	1719-B	4aj9	2.91574	172.726
ACT	201-D	4oeq	2.97664	173.444
ACT	701	2eib	3.12191	174.011
ACT	1267-A	2vqp	2.60029	174.452
ACT	505-D	4e7c	2.97603	175.180
ACT	604-A	4fxz	3.15876	175.983
ACT	1429-A	3dx6	3.12013	176.001
ACT	503-A	4g2c	2.37662	178.039
ACY	1643-A	2wq8	3.03154	171.962
ACY	1-A	3avc	2.81985	172.496
ACY	1-A	3avk	2.81778	177.221
ADN	300	1mrj	2.86971	175.313
AITLIFI	1-D	2grm	3.19103	171.657
ARTMQTARKSTGAKAP	1-C	2v1d	2.51677	175.391
ARTX	1-B	3mea	3.15805	172.874
ARTXQTA	1-D	2gfa	3.19855	176.508
ASP-PLP	414-C	1gck	2.83737	178.223
AVI	401-A	4pin	3.04104	172.917
B12	1801-D	3kox	3.19133	170.448
B12	1801-C	3kox	3.19675	170.875
B35	449-A	3h0b	3.12119	170.166
BB2	194-D	3m6r	3.14671	175.819
BCL	852	1z9j	3.19297	170.849
BCL	1303-M	1ogv	3.19023	171.658
BCL	1304-M	2boz	3.14748	173.492
BCL	102-K	3wmo	3.15638	173.886
BCR	514-c	4tni	3.09282	170.005
BCR	488-C	3bz1	2.86004	170.622
BCR	488-C	3bz2	2.836	171.112
BCR	6050-d	3a0b	2.81223	172.971
BCR	528-B	3prq	2.79828	174.500
BCR	5528-B	3prr	2.80787	174.714
BCR	1050-D	3a0b	2.97563	177.140
BET	264-A	3t27	2.92384	176.262
BOG	705-C	4rry	3.09953	171.902
BTM	406-A	4ltz	3.09189	173.099
BU3	1030-G	3se9	2.78536	170.602
CAC	1301	1tye	2.99519	172.076
CL1	1226-B	3lw5	2.84455	170.329
CL1	510-P	4fby	3.07637	170.556
CL1	1139-X	2wsf	3.1243	171.203
CL1	510-C	4fby	3.05692	171.808
CL1	1215-B	2o01	3.09386	174.236
CL1	2013	1s5l	2.8707	175.318
CL1	13	1s5l	2.9428	176.241
CLA	606-C	2bhw	2.83179	170.080
CLA	510-C	4ixq	3.1079	170.113
CLA	604-H	1rwt	3.05008	170.131
CLA	510-c	4ixq	3.05504	170.327

Table S1. *Cont.*

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
CLA	21	2axt	3.09234	170.587
CLA	606-A	2bhw	2.82905	170.678
CLA	5021	2axt	3.1322	170.789
CLA	511-c	4il6	3.10622	171.476
CLA	604-A	1rwt	3.0716	172.017
CLA	501-C	4q54	3.19111	172.503
CLA	628-C	3arc	3.19138	172.522
CLA	501-C	4pbu	3.19043	172.526
CLA	510-c	4ixr	3.00388	172.637
CLA	1132-A	4kt0	3.18758	173.089
CLA	912-c	4q54	3.15385	174.288
CLA	912-c	4pbu	3.15477	174.293
CLA	638-c	3arc	3.1536	174.361
CLA	606-B	2bhw	2.81892	174.958
CLA	604-G	1rwt	3.03024	175.980
CLA	501-C	4il6	3.17522	178.033
CLR	253-A	3gki	3.17822	170.819
CNO	801	1k0y	2.95361	170.554
COH	154-X	2o5t	3.1698	174.726
COH	154-X	2o5s	3.14011	175.299
CRT	103-F	3wmo	3.1456	171.159
CWB	1207-A	2yme	3.09679	170.721
CXE	503-D	4mlb	3.10192	177.391
CYC	255-P	1ha7	3.12581	170.486
CYC	255-D	1ha7	3.17146	170.518
CYC	255-L	1ha7	3.143	170.538
CYC	184-H	2uul	3.11969	171.024
CYC	502	1jbo	3.0811	171.063
CYC	1081-B	2v8a	3.18787	172.361
CYC	255-J	1ha7	3.11275	172.792
CYC	255-R	1ha7	3.18645	173.810
CYC	202-D	4lm6	3.18577	176.149
CYC	202-B	4lm6	3.10814	177.212
CYC	184-L	2uun	2.93714	178.175
D2B	187-A	3nxo	3.17716	173.179
DDJ	801-A	3vlj	3.0404	171.076
DMA	998-B	3kef	2.93682	173.046
DMA	998-A	3kef	2.96085	175.875
DMS	103	2ohm	2.86718	170.400
DMS	8703-D	1jz7	2.95787	170.553
DMS	209-A	4mwm	2.91607	170.620
DMS	1702-A	4pzt	2.95009	170.728
DMS	8703-D	1jz3	2.95983	170.753
DMS	8419-C	1jyn	3.05791	170.820
DMS	1137-B	4ttg	3.13758	170.922
DMS	607-A	5ddb	3.19725	171.308
DMS	906-B	4ovz	3.18217	171.666
DMS	8703-D	1jz5	2.74312	171.669
DMS	7-B	3sl4	3.06951	172.059
DMS	215-B	4ow9	2.87469	172.530

Table S1. *Cont.*

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
DMS	8419-A	1jyv	3.0267	172.883
DMS	8425-B	1jyx	3.12719	174.182
DMS	1702-A	4pzs	2.81463	174.871
DMS	508-B	4ifv	3.08983	175.710
DMS	8419-C	1jz4	2.78859	176.074
DMS	366-A	3qyw	2.84432	177.096
DMS	1336-A	4btk	2.96152	177.570
DMS	8427-B	1jz4	3.04753	177.863
DMS	8703-D	1jz8	3.10617	179.070
DMS	202-A	4oxe	3.15477	179.742
DTM	187	1mvt	3.16439	174.324
EKRVASSVFITLAPP	6-K	4p3w	3.12073	172.213
EMC	451-A	1ems	3.04456	170.512
ENB	145	2d2d	2.76882	174.410
EOH	401-A	4mul	3.15687	174.757
EP	1001	1tvk	2.81752	176.073
FAD	7202	2pd7	2.95929	171.373
FAD	773-E	3red	3.15677	172.882
FAD	601-A	3t37	2.96313	173.827
FAD	1205	2b3d	3.07886	175.783
FMN	400-D	4laf	3.07578	171.160
FOK	2	1ab8	2.91949	171.336
FOK	1	1ab8	3.19797	177.564
G39	501-A	4gzt	2.64705	177.071
GEA	3990	1d8t	3.12067	172.425
GLY-TYR-GLU	756-F	3sv1	3.00056	171.360
GPP	903-H	1h48	3.00918	176.149
GPRV	1-J	2ffd	3.11013	172.963
HEA	559-A	3ehb	3.19788	171.673
HEA	559-A	3hb3	3.14137	171.702
HEA	2	1ar1	3.14634	173.002
HEB	201-A	4i0v	3.04968	171.968
HEB	201-C	4i0v	3.06206	172.323
HEB	201-A	4max	3.03947	172.960
HEB	201-C	4max	3.04076	173.985
HEB	201-B	4max	3.03155	175.494
HEB	201-B	4i0v	3.02716	176.465
HEEAVSVDRVL	1-C	3ln5	3.00961	172.731
HEM	1001-A	2yyw	3.16164	170.000
HEM	1-C	1thb	3.14033	170.039
HEM	142-A	1hbr	3.18989	170.047
HEM	147-D	3gdj	2.89786	170.051
HEM	125-A	1s6a	3.1304	170.111
HEM	142-R	1lfl	3.1289	170.115
HEM	1154-A	1gjn	3.1988	170.155
HEM	154-B	1yca	3.16279	170.156
HEM	1154-A	2v1j	3.14249	170.166
HEM	201-B	4n7p	3.18799	170.178
HEM	1154-A	2v1f	3.15493	170.239
HEM	139-B	3lb2	3.08545	170.320

Table S1. *Cont.*

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
HEM	1001-A	2ewk	3.19212	170.418
HEM	202-A	4ni1	3.16827	170.427
HEM	142-C	1y0d	3.17703	170.458
HEM	154-A	1mdn	3.18538	170.598
HEM	150-A	1c40	3.18165	170.654
HEM	142-A	3gou	3.17801	170.736
HEM	154-X	2frj	3.10204	170.739
HEM	143-A	1r1y	3.16071	170.815
HEM	201-D	4mqk	3.19865	170.831
HEM	154	1mti	3.13638	170.863
HEM	153-A	3arj	2.96567	170.874
HEM	143-C	1ouu	3.1808	170.923
HEM	201-G	4f4o	3.11316	170.945
HEM	200-C	3hrw	2.64638	170.948
HEM	154	1swm	3.17492	170.966
HEM	201-K	4f4o	3.16963	170.985
HEM	154-A	2g3h	3.17054	170.992
HEM	1154-A	2v1e	3.14556	171.021
HEM	147-B	1hbr	3.09325	171.055
HEM	1154-A	2v1g	3.12657	171.065
HEM	154-A	3ogb	3.06671	171.071
HEM	153-A	3a9m	2.95661	171.091
HEM	1-E	1hbs	2.86425	171.142
HEM	150-D	3a59	3.15746	171.188
HEM	201-A	3wtg	3.19199	171.200
HEM	1-A	1thb	3.16516	171.245
HEM	201-B	4fh6	3.07073	171.267
HEM	201-J	4f4o	3.11244	171.306
HEM	142-A	2d5z	3.19913	171.308
HEM	201-D	4f4o	3.1915	171.325
HEM	201-H	4mqk	3.05394	171.374
HEM	154-B	1mdn	3.18251	171.404
HEM	147-B	3at6	3.00466	171.411
HEM	142-A	1yhr	2.97058	171.419
HEM	201-A	4f4o	3.12827	171.422
HEM	154-A	3rgk	3.0866	171.424
HEM	201-B	4fh7	2.98051	171.456
HEM	154-A	1m6c	3.12207	171.478
HEM	147-D	3gou	3.03823	171.486
HEM	200-A	1hab	2.96536	171.546
HEM	500-B	3pt7	3.17667	171.621
HEM	154-A	3hc9	3.00322	171.628
HEM	154-A	3lr7	3.13929	171.749
HEM	148-B	3ic0	3.15425	171.753
HEM	148	2fal	3.08963	171.836
HEM	150-C	3mjp	3.12902	171.893
HEM	301-C	3bkn	3.08809	171.978
HEM	143-A	3onz	2.94366	172.044
HEM	201-D	4mqk	3.0809	172.097
HEM	142-A	3d1a	3.08844	172.127

Table S1. *Cont.*

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
HEM	147-A	1i3d	3.19019	172.132
HEM	200-D	1hac	3.03283	172.198
HEM	139-B	3oj1	3.03573	172.207
HEM	1154-A	2v1i	3.10932	172.213
HEM	202-A	4ns2	3.15814	172.216
HEM	201-B	4hsx	3.17349	172.358
HEM	147-B	3bcq	3.15024	172.363
HEM	142-C	1nej	3.05489	172.375
HEM	1154-A	2vly	3.12992	172.378
HEM	201-A	5cnc	3.05805	172.380
HEM	143-A	1r1x	3.04704	172.386
HEM	142-C	2rao	3.04793	172.386
HEM	147-B	1lfv	2.91578	172.389
HEM	142-I	2ri4	2.81567	172.464
HEM	139-B	3o7n	3.01775	172.475
HEM	144-A	2gkm	2.98354	172.638
HEM	144-B	3aq8	3.06103	172.667
HEM	154-A	1mnk	3.09057	172.696
HEM	1-A	2pgh	3.16417	172.770
HEM	125-A	2hz3	3.10073	172.772
HEM	139-B	3k3u	3.0852	172.776
HEM	142-E	3dhr	3.01093	172.790
HEM	147-B	3eu1	3.15449	172.827
HEM	125-A	1rtx	3.07579	172.861
HEM	142-A	2dn1	3.18716	172.980
HEM	154	2mgh	3.12935	173.003
HEM	148-B	3bj3	2.94846	173.030
HEM	144-B	3aq5	3.11474	173.070
HEM	191-B	2dc3	3.177	173.070
HEM	134-B	1gcw	2.95561	173.100
HEM	154	2mgb	3.19222	173.103
HEM	201-B	1v75	3.18585	173.183
HEM	154-B	1mnj	3.1237	173.208
HEM	154-B	1mwc	3.15619	173.348
HEM	143-C	3gqp	3.07397	173.383
HEM	500-B	3pt8	3.19322	173.471
HEM	1001-A	2yxc	3.19453	173.514
HEM	144-C	1v4u	2.99034	173.530
HEM	154-A	3lr9	3.11108	173.617
HEM	142-A	1yeq	3.00653	173.663
HEM	151	1hv4	3.08407	173.699
HEM	154-X	2fri	3.12526	173.723
HEM	500-A	3pi2	3.19334	173.776
HEM	142-A	1y8w	3.0957	173.780
HEM	1154-A	2vlz	3.15619	173.824
HEM	143-A	1ouu	3.18948	173.835
HEM	154-B	1m6c	3.1448	173.836
HEM	143-C	3bj3	3.17358	173.847
HEM	142-A	2ri4	2.86296	173.859
HEM	144-B	3aq9	3.09585	173.881

Table S1. *Cont.*

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
HEM	301-I	3bkn	3.18995	173.890
HEM	150-A	1a4f	3.01674	173.942
HEM	154-A	3hep	3.0798	174.048
HEM	500-A	3pt7	3.12	174.088
HEM	155	1hv4	3.12461	174.163
HEM	201-A	4yu3	3.12024	174.257
HEM	150-B	1faw	3.18358	174.282
HEM	1154-A	2v1h	3.13882	174.284
HEM	150-D	1faw	3.1836	174.284
HEM	154-A	3hen	3.09246	174.350
HEM	200-D	3hrw	3.13527	174.385
HEM	148-A	1dm1	3.17837	174.408
HEM	154-X	2frk	3.14399	174.444
HEM	804-A	1p2e	3.13865	174.511
HEM	144-A	2gkn	3.01761	174.524
HEM	201-A	5cne	3.07863	174.575
HEM	153	1hv4	3.11416	174.598
HEM	1-B	1hho	3.19704	174.616
HEM	144-A	3aq8	3.17804	174.638
HEM	201-A	5cn8	3.05486	174.787
HEM	202-C	4esa	3.19773	174.818
HEM	1154-A	2vm0	3.15271	174.835
HEM	157	1hv4	3.08549	174.868
HEM	200-A	2b7h	3.01147	174.888
HEM	202-A	4esa	3.19724	174.915
HEM	201-A	5cn4	3.08375	174.916
HEM	1154-A	2vlx	3.1409	175.002
HEM	201-A	5cnd	3.10538	175.012
HEM	139-B	3ok5	3.0806	175.037
HEM	201-A	5cnf	3.1422	175.058
HEM	1-A	1hgb	3.14982	175.178
HEM	144-A	2gln	3.08551	175.237
HEM	147-C	1cbm	3.16965	175.268
HEM	201-A	5cn5	3.13199	175.316
HEM	201-A	5cnb	3.07972	175.373
HEM	500-B	3pi3	3.11106	175.456
HEM	201-B	4mqk	3.14557	175.510
HEM	500-B	2olp	3.08653	175.747
HEM	154-A	5cn9	3.05943	175.799
HEM	500-A	3pi1	3.14278	175.967
HEM	500-A	2olp	3.13067	176.131
HEM	230	1f6h	3.133	176.213
HEM	201-A	5cng	3.08629	176.252
HEM	201-A	5cn7	3.11951	176.298
HEM	154-A	2frf	3.12774	176.453
HEM	154-B	1myj	3.12596	176.543
HEM	201-A	5cn6	3.12716	176.593
HEM	201-A	5cmv	3.05373	176.641
HEM	154-A	1pmb	3.17889	176.748
HEM	301-E	3bkn	2.954	176.804

Table S1. *Cont.*

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
HEM	142-C	2zlx	3.1588	176.808
HEM	144-A	1idr	3.05663	176.827
HEM	350-A	1gw2	3.14527	176.881
HEM	200-C	2b7h	2.9549	176.924
HEM	350-A	6atj	3.15681	176.985
HEM	153-A	3a5a	2.93907	177.096
HEM	201-J	4n7p	3.19664	177.317
HEM	301-K	3bkn	3.17855	177.772
HEM	134-D	1gcw	3.06024	177.993
HEM	147-B	1t1n	3.10262	178.210
HEM	148-B	1pbx	3.02127	178.311
HEM	350-A	1gwo	3.16438	178.503
HEM	144-B	3aq6	3.08089	178.546
HEM	500-A	3pt8	3.04338	178.582
HEM	1-C	1hgb	3.17766	178.793
HEM	301-B	3bkn	3.06199	179.239
HEM	144-A	3aq5	3.16426	179.300
HEM	147-B	1i3e	3.1459	179.422
IM1	400	1tcw	3.19661	170.412
IPA	1423-A	2wge	3.16162	170.699
IRC	410-A	3o3n	3.00816	173.197
IZN	400-D	4alx	3.09615	170.943
IZN	400-G	4alx	3.09507	170.990
IZN	400-I	4alx	3.00618	173.016
IZN	400-C	4alx	3.03594	178.921
JUS	1257-G	4bnn	2.97516	172.181
KLTPLCVTL	1-C	2x4o	3.18563	177.465
KMIDFATLSKLKKKYQIILD	461-C	3owt	3.09753	172.739
L1G	1506-A	2c0i	3.14259	176.707
LAC	398-C	2pi1	2.62355	174.117
LDA	504-B	2r4o	3.17536	170.119
LDA	272-B	3hb3	3.06733	175.960
LLFNILGGWV	1-P	3mrn	3.08161	173.561
LN5	500-B	3i4a	3.09279	170.965
LVEALYLVCGERGG	1-C	1jk8	3.18861	172.406
M8E	368-A	3dz6	3.13379	171.885
MBV	1207-A	1he3	2.44277	171.104
MD4	301-A	4wv9	3.14158	172.614
MER	401-A	2zd8	3.16572	176.866
MGR	200-A	3bqz	2.30038	171.640
MHZ	368-A	1i79	3.06086	173.191
MLK	301-A	3sh1	2.80704	172.716
MNH	154-X	2o5q	3.13356	171.301
MNR	154-X	2o5m	3.16627	170.940
MNR	154-X	2o5l	3.12392	171.977
MNR	154-X	2o58	3.15822	172.500
MNR	154-X	2o5o	3.08941	177.196
MPD	3-D	3dcx	3.0671	170.225
MPD	1214-C	2xz5	3.12841	173.397
MPD	7012	1loj	3.11008	173.892

Table S1. *Cont.*

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
MPD	607	2fuz	3.02932	174.591
MPD	401	2i1o	3.06772	176.879
MPD	303-A	4kea	3.16587	178.424
MRD	304-C	3no6	3.12467	173.368
MRD	942-A	4iib	3.18851	174.006
MUR	1670-A	3zfz	2.75521	171.616
NAG	1694-A	2iuf	3.17872	171.532
NAG	2-B	3bix	2.96511	172.352
NAG	701-A	4pbx	3.11122	172.370
NAG-NAG	606-C	4miv	2.88806	171.012
NAG-NAG	685A-H	2ajd	2.79123	171.963
NAG-NAG	401-C	04-jun	3.14107	172.485
NAG-NAG	700-B	3saj	3.02219	174.594
NAG-NAG	484-A	1ivd	2.73666	176.668
NAG-NAG	484-B	1ivd	2.73666	176.668
NAG-NAG	602-E	3al4	3.0144	176.776
NAG-NAG-BMA	5158-C	3i26	3.17925	176.723
NAG-NAG-BMA-MAN	2006-A	4g1e	3.05617	171.690
NAG-NAG-FUL	608	1maa	3.15409	171.064
NDG-NAG-BMA-MAN-MAN-MAN-MAN-MAN	1-C	1o7d	2.76558	170.160
NTE	201-A	3vau	3.18031	171.950
NVW	901-A	3w5e	3.12012	177.114
NZF	1501-A	4fnz	2.83425	172.815
OLO	800	4erk	3.14797	172.383
P68	501-H	4my1	2.94753	177.079
PDA	401-X	4zu8	3.15648	174.165
PDS	902	2i0e	3.08908	174.548
PE5	534-B	2yeq	3.04226	172.137
PFNVDDVLKFTFTGEK	195-K	2hzs	3.17648	170.650
PFNVDDVLKFTFTGEKH	195-L	2hzs	3.19186	171.587
PGO	1602	1iwp	3.11128	171.453
PHE-HIS-PRO-ACE-NH2	1-P	1mcj	3.12725	175.247
PLP	1430-B	2x5f	3.17444	171.597
PLP	342-A	3bm5	3.17903	171.605
PLP	600-E	2bwo	3.10407	171.974
PLP	500-B	3kgw	2.96157	172.201
PLP	342-B	1f2d	3.10003	172.835
PLP	600-D	2bwo	3.18388	173.607
PLP	500-C	3ele	3.06956	175.128
PSC	303-O	3x2q	3.10146	172.636
PTT	801	1b25	2.5019	171.084
PTT	802	1b25	2.59854	174.059
PTT	800	1b25	2.55502	174.468
PTT	803	1b25	2.59711	176.615
PVKKPKIRR	297-B	4wv6	2.87504	177.484
PWK	201-B	4pwk	2.7601	170.725
PYR-SMM	68-A	3ep7	3.10347	172.973
QO9	556-A	3qo9	3.13296	174.019

Table S1. *Cont.*

LIG ID	Ligand Position	PDB-ID	Distance D1	Angle A1
R19	800-B	1o6r	3.02895	170.151
R19	800-C	1o6r	2.99846	170.254
RVB	451-B	3rv7	3.09472	171.094
SAV	1167-A	3cjf	3.02923	175.114
SAZ	709	1yyr	3.05293	175.249
SIA	782	1yaj	3.11114	170.056
SLLMWITQV	1-F	3gjf	3.13352	177.269
SMM	368-A	3dz3	2.99456	170.533
SZ8	8-A	3rxk	3.10725	171.360
T9N	1296-C	4bcn	2.84052	172.499
TCU	1257-A	4bnm	2.96919	170.067
TCU	1258-E	4bnm	2.98999	173.779
TSHKLVQLLTT	629-B	3h0a	3.11589	171.345
TSSKIYDNKNQLIADL	51-A	2c5w	2.97245	174.300
TZZ	901	2d2h	3.14683	175.895
UQ1	614	1prc	2.80506	170.279
V55	1251-D	2vsu	3.13035	171.483
WYQ	701-A	3v94	2.95178	171.249
XRS	301-A	3zdh	3.01289	171.080
XRS	301-H	3zdh	3.1326	171.405
XRX	301-J	3zdg	3.16297	170.574
YLVTSV	2838-B	4g69	3.13192	171.079
ZGA	301-B	3vje	3.17192	173.626
ZZC	401-A	2wod	3.19099	171.349

Table S2. Cartesian coordinates of the complexes **4.**

Atom label	X	Y	Z
C	0.0000000	0.0000000	−0.8422047
H	0.5117758	0.8864217	−0.4924039
H	0.5117758	−0.8864217	−0.4924039
H	−1.0235516	0.0000000	−0.4924039
F	0.0000000	0.0000000	−2.2699532
O	−0.0000000	0.0000000	1.8118730
H	0.0000000	0.0000000	2.7774965

Table S3. Cartesian coordinates of the complexes **5.**

Atom label	X	Y	Z
C	1.8250870	−0.0105611	0.0000000
H	1.4743639	−0.5250440	−0.8898932
H	1.4756003	1.0174914	0.0000000
H	1.4743639	−0.5250440	0.8898932
F	3.2178835	−0.0121355	0.0000000
O	−1.1681595	0.0118500	0.0000000
C	−2.3819637	0.0138473	0.0000000
H	−2.9570417	0.9510356	0.0000000
H	−2.9601338	−0.9214397	0.0000000

Table S4. Cartesian coordinates of the complexes **6.**

Atom label	X	Y	Z
C	1.8248139	−0.0063718	0.0000000
H	1.4769565	−0.0063718	−0.8906732
H	1.4695958	−0.0063718	0.0000000
H	3.2176176	−0.5211124	0.8906732
F	3.2176176	0.0006390	0.0000000
O	−1.1678970	−0.0064234	0.0000000
C	−2.3816174	0.0071479	0.0000000
H	−2.9582129	0.0135826	0.9362674
H	−2.9582129	0.0135826	−0.9362674

Table S5. Cartesian coordinates of the complexes **8.**

Atom label	X	Y	Z
C	0.2266220	−0.6477647	0.0000000
H	0.6178936	0.6178936	0.6178936
H	0.6178936	0.6178936	0.6178936
H	0.6178936	0.6178936	0.6178936
O	2.9501204	0.0916592	0.0000000
C	4.1559667	0.2650364	0.0000000
H	4.5885122	1.2731810	0.0000000
H	4.8548831	−0.5805049	0.0000000
S	−1.5546561	−1.5546561	−1.5546561
C	−2.0427777	0.1558724	−1.3891897
H	−1.6796482	−0.3311471	−0.3311471
H	−3.1295302	0.1941599	−1.4007227
H	−1.6111157	1.1476873	−1.2760241
C	−2.0427777	0.1558724	1.3891897
H	−1.6111157	1.1476873	1.2760241
H	−3.1295302	0.1941599	1.4007227
H	−1.6796482	−0.3311471	2.2912353

Table S6. Cartesian coordinates of the complexes **9.**

Atom label	X	Y	Z
C	0.1742286	−0.4822514	0.0000988
H	0.6059202	−0.9356278	0.8883347
H	0.3252656	0.5939560	0.0000797
H	0.6059954	−0.9356699	−0.8880756
O	2.9301068	0.0298048	0.0001267
C	4.1390908	0.1797355	−0.0000597
H	4.7063033	0.2501127	−0.9364463
H	4.7066033	0.2500299	0.9361532
S	−1.5823512	−0.8518986	−0.0000098
C	−2.1558676	0.1298971	−1.3894915
H	−1.7507663	−0.3236219	−2.2911584
H	−3.2418221	0.0740611	−1.4023800
H	−1.8121587	1.1554767	−1.2758635
C	−2.1559933	0.1298719	1.3894392
H	−1.8122498	1.1554433	1.2758456
H	−3.2419529	0.0740779	1.4023157
H	−1.7509217	−0.3236967	2.2910911

Table S7. Cartesian coordinates of the complexes **11.**

Atom label	X	Y	Z
C	0.8054361	0.8054361	0.8054361
H	0.4674891	−0.5228008	−0.8890344
H	0.4549735	1.0191574	0.0000000
H	0.4674891	−0.5228008	0.8890344
O	−1.9409858	0.0081029	0.0000000
C	−3.1594971	0.0018961	0.0000000
H	−3.7349248	0.9354674	0.0000000
H	−3.7255021	−0.9374602	0.0000000
N	2.3131143	0.0043646	0.0000000
H	2.6815482	0.4819278	−0.8235831
H	2.6815482	0.4819278	0.8235831
H	2.6893112	0.9445553	0.0000000

Table S8. Cartesian coordinates of the complexes **12.**

Atom label	X	Y	Z
C	0.8054506	−0.0035601	0.0000000
H	0.4638428	−0.5162655	−0.8903560
H	0.4623113	1.0233596	0.0000000
H	0.4638428	−0.5162655	0.8903560
O	−1.9409510	−0.0059480	0.0000000
C	−3.1594425	0.0019382	0.0000000
H	−3.7302288	0.0056338	0.9364202
H	−3.7302288	0.0056338	−0.9364202
N	2.3131063	0.0002992	0.0000000
H	2.6875443	−0.9493516	0.0000000
H	2.6823766	0.4772630	−0.8234944
H	2.6823766	0.4772630	0.8234944