

## Supplementary Information

### An *in silico* Study of Benzophenone Derivatives as Potential Non-Competitive Inhibitors of *Trypanosoma cruzi* and *Leishmania amazonensis* Cysteine Proteinases

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**Table S1.** Configuration parameters of the centers of the search space for the molecular docking simulation for cruzain and Llacys1

Receptor	Binding site	Center of the search space / Å
Cruzain	P_1	$10.94 \times -0.35 \times 10.02$
	P_2	$5.99 \times -9.46 \times 0.69$
	P_3	$18.32 \times 5.01 \times 6.50$
Llacys1	P_1	$3.64 \times 3.73 \times 21.97$
	P_2	$7.76 \times -8.15 \times -0.72$
	P_3	$20.89 \times 2.90 \times 6.45$
	P_4	$13.00 \times 13.31 \times -2.84$

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ATOM 0.00	55	CZ2	TRP	4	46.570	35.910	55.230	1.00
ATOM 0.00	56	HZ2	TRP	4	45.510	36.020	55.430	1.00
ATOM 0.00	57	CH2	TRP	4	47.130	34.750	54.670	1.00
ATOM 0.00	58	HH2	TRP	4	46.560	33.890	54.350	1.00
ATOM 0.00	59	CZ3	TRP	4	48.540	34.680	54.480	1.00
ATOM 0.00	60	HZ3	TRP	4	49.040	33.900	53.930	1.00
ATOM 0.00	61	CE3	TRP	4	49.340	35.760	54.940	1.00
ATOM 0.00	62	HE3	TRP	4	50.400	35.760	54.740	1.00
ATOM 0.00	63	CD2	TRP	4	48.780	36.930	55.640	1.00
ATOM 0.00	64	C	TRP	4	52.790	38.580	57.620	1.00
ATOM 0.00	65	O	TRP	4	53.320	37.660	56.950	1.00
ATOM 0.00	66	N	ARG	5	53.520	39.380	58.390	1.00
ATOM 0.00	67	H	ARG	5	53.030	40.050	58.970	1.00
ATOM 0.00	68	CA	ARG	5	54.960	39.160	58.710	1.00
ATOM 0.00	69	HA	ARG	5	55.470	39.020	57.750	1.00
ATOM 0.00	70	CB	ARG	5	55.550	40.450	59.250	1.00
ATOM 0.00	71	HB1	ARG	5	56.630	40.380	59.260	1.00
ATOM 0.00	72	HB2	ARG	5	55.200	40.660	60.260	1.00
ATOM 0.00	73	CG	ARG	5	55.210	41.650	58.380	1.00
ATOM 0.00	74	HG1	ARG	5	54.150	41.890	58.330	1.00
ATOM 0.00	75	HG2	ARG	5	55.650	41.470	57.400	1.00
ATOM 0.00	76	CD	ARG	5	55.890	42.860	58.920	1.00
ATOM 0.00	77	HD1	ARG	5	55.950	43.560	58.090	1.00
ATOM 0.00	78	HD2	ARG	5	56.920	42.620	59.180	1.00
ATOM 0.00	79	NE	ARG	5	55.080	43.410	60.000	1.00
ATOM 0.00	80	HE	ARG	5	54.280	42.870	60.290	1.00
ATOM 0.00	81	CZ	ARG	5	55.430	44.280	60.890	1.00
ATOM 0.00	82	NH1	ARG	5	56.580	44.980	60.720	1.00













ATOM 0.00	223	N	ASN	15	63.560	50.880	48.860	1.00
ATOM 0.00	224	H	ASN	15	64.030	50.350	48.140	1.00
ATOM 0.00	225	CA	ASN	15	63.460	52.350	48.590	1.00
ATOM 0.00	226	HA	ASN	15	62.680	52.710	49.260	1.00
ATOM 0.00	227	CB	ASN	15	64.820	52.960	48.940	1.00
ATOM 0.00	228	HB1	ASN	15	65.560	52.890	48.140	1.00
ATOM 0.00	229	HB2	ASN	15	65.190	52.500	49.860	1.00
ATOM 0.00	230	CG	ASN	15	64.700	54.410	49.250	1.00
ATOM 0.00	231	OD1	ASN	15	63.780	55.080	48.880	1.00
ATOM 0.00	232	ND2	ASN	15	65.680	55.000	49.910	1.00
ATOM 0.00	233	1HD2	ASN	15	66.430	54.440	50.270	1.00
ATOM 0.00	234	2HD2	ASN	15	65.460	55.950	50.190	1.00
ATOM 0.00	235	C	ASN	15	63.110	52.680	47.100	1.00
ATOM 0.00	236	O	ASN	15	63.750	52.180	46.200	1.00
ATOM 0.00	237	N	GLN	16	62.220	53.710	46.820	1.00
ATOM 0.00	238	H	GLN	16	61.780	54.140	47.620	1.00
ATOM 0.00	239	CA	GLN	16	61.940	54.310	45.480	1.00
ATOM 0.00	240	HA	GLN	16	62.040	53.560	44.700	1.00
ATOM 0.00	241	CB	GLN	16	60.520	54.810	45.430	1.00
ATOM 0.00	242	HB1	GLN	16	59.830	54.030	45.760	1.00
ATOM 0.00	243	HB2	GLN	16	60.340	55.100	44.400	1.00
ATOM 0.00	244	CG	GLN	16	60.220	56.010	46.270	1.00
ATOM 0.00	245	HG1	GLN	16	60.600	56.830	45.670	1.00
ATOM 0.00	246	HG2	GLN	16	60.630	55.920	47.270	1.00
ATOM 0.00	247	CD	GLN	16	58.740	56.170	46.370	1.00
ATOM 0.00	248	OE1	GLN	16	58.130	55.540	47.160	1.00
ATOM 0.00	249	NE2	GLN	16	58.110	56.920	45.470	1.00
ATOM 0.00	250	1HE2	GLN	16	58.570	57.600	44.880	1.00







ATOM 0.00	335	HH2	TRP	23	55.220	51.660	36.270	1.00
ATOM 0.00	336	CZ3	TRP	23	53.840	51.130	37.790	1.00
ATOM 0.00	337	HZ3	TRP	23	53.850	50.120	37.420	1.00
ATOM 0.00	338	CE3	TRP	23	53.230	51.460	39.070	1.00
ATOM 0.00	339	HE3	TRP	23	52.680	50.680	39.570	1.00
ATOM 0.00	340	CD2	TRP	23	53.230	52.790	39.570	1.00
ATOM 0.00	341	C	TRP	23	53.420	51.060	42.630	1.00
ATOM 0.00	342	O	TRP	23	52.770	50.010	42.820	1.00
ATOM 0.00	343	N	ALA	24	54.540	51.050	41.890	1.00
ATOM 0.00	344	H	ALA	24	54.950	51.950	41.710	1.00
ATOM 0.00	345	CA	ALA	24	55.140	49.860	41.480	1.00
ATOM 0.00	346	HA	ALA	24	54.450	49.220	40.930	1.00
ATOM 0.00	347	CB	ALA	24	56.260	50.230	40.440	1.00
ATOM 0.00	348	HB1	ALA	24	56.660	49.340	39.960	1.00
ATOM 0.00	349	HB2	ALA	24	55.950	50.880	39.620	1.00
ATOM 0.00	350	HB3	ALA	24	57.110	50.610	41.010	1.00
ATOM 0.00	351	C	ALA	24	55.700	49.050	42.630	1.00
ATOM 0.00	352	O	ALA	24	55.480	47.820	42.670	1.00
ATOM 0.00	353	N	PHE	25	56.370	49.710	43.630	1.00
ATOM 0.00	354	H	PHE	25	56.480	50.710	43.530	1.00
ATOM 0.00	355	CA	PHE	25	56.720	49.050	44.840	1.00
ATOM 0.00	356	HA	PHE	25	57.340	48.210	44.530	1.00
ATOM 0.00	357	CB	PHE	25	57.610	49.960	45.750	1.00
ATOM 0.00	358	HB1	PHE	25	57.710	49.550	46.760	1.00
ATOM 0.00	359	HB2	PHE	25	57.160	50.910	46.030	1.00
ATOM 0.00	360	CG	PHE	25	58.970	50.150	45.250	1.00
ATOM 0.00	361	CD1	PHE	25	59.210	50.950	44.150	1.00
ATOM 0.00	362	HD1	PHE	25	58.380	51.380	43.600	1.00





































ATOM 0.00	811	HB1	ASH	57	55.360	53.170	33.030	1.00
ATOM 0.00	812	HB2	ASH	57	53.980	52.410	32.200	1.00
ATOM 0.00	813	CG	ASH	57	53.470	53.710	33.790	1.00
ATOM 0.00	814	OD1	ASH	57	53.430	54.800	34.390	1.00
ATOM 0.00	815	OD2	ASH	57	52.530	52.770	33.960	1.00
ATOM 0.00	816	HD2	ASH	57	51.960	52.910	34.720	1.00
ATOM 0.00	817	C	ASH	57	55.710	55.480	31.880	1.00
ATOM 0.00	818	O	ASH	57	56.670	55.720	31.140	1.00
ATOM 0.00	819	N	GLU	58	55.590	56.110	33.080	1.00
ATOM 0.00	820	H	GLU	58	54.780	55.960	33.660	1.00
ATOM 0.00	821	CA	GLU	58	56.550	57.100	33.480	1.00
ATOM 0.00	822	HA	GLU	58	57.500	56.820	33.010	1.00
ATOM 0.00	823	CB	GLU	58	56.070	58.420	32.870	1.00
ATOM 0.00	824	HB1	GLU	58	55.180	58.810	33.370	1.00
ATOM 0.00	825	HB2	GLU	58	55.740	58.210	31.850	1.00
ATOM 0.00	826	CG	GLU	58	57.020	59.620	32.720	1.00
ATOM 0.00	827	HG1	GLU	58	57.820	59.420	32.010	1.00
ATOM 0.00	828	HG2	GLU	58	57.480	59.820	33.690	1.00
ATOM 0.00	829	CD	GLU	58	56.350	60.950	32.180	1.00
ATOM 0.00	830	OE1	GLU	58	56.400	61.080	30.920	1.00
ATOM 0.00	831	OE2	GLU	58	55.820	61.870	32.910	1.00
ATOM 0.00	832	C	GLU	58	56.880	57.210	34.960	1.00
ATOM 0.00	833	O	GLU	58	56.800	58.240	35.610	1.00
ATOM 0.00	834	N	GLY	59	57.360	56.110	35.620	1.00
ATOM 0.00	835	H	GLY	59	57.390	55.290	35.030	1.00
ATOM 0.00	836	CA	GLY	59	57.630	55.860	37.040	1.00
ATOM 0.00	837	HA1	GLY	59	58.000	54.840	37.190	1.00
ATOM 0.00	838	HA2	GLY	59	56.680	55.930	37.570	1.00











ATOM 0.00	951	HB3	ALA	68	52.730	50.510	34.960	1.00
ATOM 0.00	952	C	ALA	68	51.470	47.680	33.510	1.00
ATOM 0.00	953	O	ALA	68	52.220	46.840	33.000	1.00
ATOM 0.00	954	N	MET	69	50.300	47.450	34.100	1.00
ATOM 0.00	955	H	MET	69	49.810	48.250	34.470	1.00
ATOM 0.00	956	CA	MET	69	49.640	46.120	34.300	1.00
ATOM 0.00	957	HA	MET	69	50.390	45.330	34.450	1.00
ATOM 0.00	958	CB	MET	69	48.810	46.010	35.590	1.00
ATOM 0.00	959	HB1	MET	69	48.440	45.010	35.840	1.00
ATOM 0.00	960	HB2	MET	69	47.960	46.700	35.560	1.00
ATOM 0.00	961	CG	MET	69	49.570	46.420	36.860	1.00
ATOM 0.00	962	HG1	MET	69	48.970	46.160	37.730	1.00
ATOM 0.00	963	HG2	MET	69	49.620	47.500	36.920	1.00
ATOM 0.00	964	SD	MET	69	51.210	45.740	37.210	1.00
ATOM 0.00	965	CE	MET	69	51.650	46.790	38.540	1.00
ATOM 0.00	966	HE1	MET	69	51.870	47.780	38.140	1.00
ATOM 0.00	967	HE2	MET	69	50.890	46.730	39.310	1.00
ATOM 0.00	968	HE3	MET	69	52.620	46.470	38.910	1.00
ATOM 0.00	969	C	MET	69	48.880	45.780	33.050	1.00
ATOM 0.00	970	O	MET	69	48.800	44.590	32.710	1.00
ATOM 0.00	971	N	ASN	70	48.390	46.730	32.220	1.00
ATOM 0.00	972	H	ASN	70	48.200	47.630	32.640	1.00
ATOM 0.00	973	CA	ASN	70	48.130	46.450	30.840	1.00
ATOM 0.00	974	HA	ASN	70	47.560	45.530	30.740	1.00
ATOM 0.00	975	CB	ASN	70	47.430	47.620	30.160	1.00
ATOM 0.00	976	HB1	ASN	70	48.260	48.300	29.950	1.00
ATOM 0.00	977	HB2	ASN	70	46.760	48.220	30.770	1.00
ATOM 0.00	978	CG	ASN	70	46.810	47.300	28.830	1.00







ATOM 0.00	1063	H	SER	75	52.850	42.970	27.230	1.00
ATOM 0.00	1064	CA	SER	75	54.390	42.350	25.960	1.00
ATOM 0.00	1065	HA	SER	75	54.260	42.110	24.900	1.00
ATOM 0.00	1066	CB	SER	75	54.970	43.760	26.150	1.00
ATOM 0.00	1067	HB1	SER	75	54.380	44.500	25.620	1.00
ATOM 0.00	1068	HB2	SER	75	55.930	43.800	25.640	1.00
ATOM 0.00	1069	OG	SER	75	55.200	43.900	27.590	1.00
ATOM 0.00	1070	HG	SER	75	54.540	44.580	27.760	1.00
ATOM 0.00	1071	C	SER	75	55.260	41.290	26.610	1.00
ATOM 0.00	1072	O	SER	75	56.140	40.810	25.920	1.00
ATOM 0.00	1073	N	HIP	76	54.970	40.930	27.850	1.00
ATOM 0.00	1074	H	HIP	76	54.190	41.420	28.250	1.00
ATOM 0.00	1075	CA	HIP	76	55.760	40.120	28.790	1.00
ATOM 0.00	1076	HA	HIP	76	56.500	39.450	28.350	1.00
ATOM 0.00	1077	CB	HIP	76	56.430	41.180	29.680	1.00
ATOM 0.00	1078	HB1	HIP	76	56.580	40.780	30.690	1.00
ATOM 0.00	1079	HB2	HIP	76	55.760	42.020	29.890	1.00
ATOM 0.00	1080	CG	HIP	76	57.720	41.720	29.180	1.00
ATOM 0.00	1081	ND1	HIP	76	57.950	42.860	28.400	1.00
ATOM 0.00	1082	HD1	HIP	76	57.220	43.350	27.910	1.00
ATOM 0.00	1083	CE1	HIP	76	59.290	43.040	28.160	1.00
ATOM 0.00	1084	HE1	HIP	76	59.750	43.780	27.520	1.00
ATOM 0.00	1085	NE2	HIP	76	59.890	41.970	28.730	1.00
ATOM 0.00	1086	HE2	HIP	76	60.880	41.810	28.590	1.00
ATOM 0.00	1087	CD2	HIP	76	58.970	41.120	29.340	1.00
ATOM 0.00	1088	HD2	HIP	76	59.260	40.230	29.880	1.00
ATOM 0.00	1089	C	HIP	76	54.840	39.120	29.580	1.00
ATOM 0.00	1090	O	HIP	76	55.020	38.880	30.810	1.00













































ATOM 0.00	1623	HG2	PRO	115	36.100	44.540	49.820	1.00
ATOM 0.00	1624	CB	PRO	115	35.220	46.400	48.890	1.00
ATOM 0.00	1625	HB1	PRO	115	34.600	46.700	49.730	1.00
ATOM 0.00	1626	HB2	PRO	115	34.520	45.820	48.290	1.00
ATOM 0.00	1627	CA	PRO	115	35.920	47.480	48.140	1.00
ATOM 0.00	1628	HA	PRO	115	35.380	47.830	47.270	1.00
ATOM 0.00	1629	C	PRO	115	36.340	48.740	49.020	1.00
ATOM 0.00	1630	O	PRO	115	37.170	48.640	49.910	1.00
ATOM 0.00	1631	N	HIP	116	35.820	49.920	48.700	1.00
ATOM 0.00	1632	H	HIP	116	35.060	49.940	48.030	1.00
ATOM 0.00	1633	CA	HIP	116	36.110	51.250	49.330	1.00
ATOM 0.00	1634	HA	HIP	116	37.150	51.390	49.610	1.00
ATOM 0.00	1635	CB	HIP	116	35.530	52.300	48.320	1.00
ATOM 0.00	1636	HB1	HIP	116	35.710	53.280	48.760	1.00
ATOM 0.00	1637	HB2	HIP	116	34.450	52.250	48.240	1.00
ATOM 0.00	1638	CG	HIP	116	36.210	52.240	46.990	1.00
ATOM 0.00	1639	ND1	HIP	116	35.830	53.010	45.900	1.00
ATOM 0.00	1640	HD1	HIP	116	35.020	53.630	45.910	1.00
ATOM 0.00	1641	CE1	HIP	116	36.670	52.790	44.860	1.00
ATOM 0.00	1642	HE1	HIP	116	36.550	53.170	43.860	1.00
ATOM 0.00	1643	NE2	HIP	116	37.610	51.990	45.280	1.00
ATOM 0.00	1644	HE2	HIP	116	38.270	51.570	44.640	1.00
ATOM 0.00	1645	CD2	HIP	116	37.300	51.560	46.550	1.00
ATOM 0.00	1646	HD2	HIP	116	37.770	50.830	47.200	1.00
ATOM 0.00	1647	C	HIP	116	35.370	51.400	50.630	1.00
ATOM 0.00	1648	O	HIP	116	34.440	52.170	50.790	1.00
ATOM 0.00	1649	N	ASP	117	35.640	50.550	51.640	1.00
ATOM 0.00	1650	H	ASP	117	36.030	49.670	51.360	1.00

























ATOM 0.00	1959	H	ALA	137	50.530	61.520	51.120	1.00
ATOM 0.00	1960	CA	ALA	137	51.510	61.320	53.020	1.00
ATOM 0.00	1961	HA	ALA	137	51.290	60.510	53.720	1.00
ATOM 0.00	1962	CB	ALA	137	52.690	60.850	52.220	1.00
ATOM 0.00	1963	HB1	ALA	137	53.070	61.730	51.690	1.00
ATOM 0.00	1964	HB2	ALA	137	53.400	60.430	52.930	1.00
ATOM 0.00	1965	HB3	ALA	137	52.360	60.170	51.430	1.00
ATOM 0.00	1966	C	ALA	137	51.840	62.630	53.800	1.00
ATOM 0.00	1967	O	ALA	137	52.780	62.650	54.540	1.00
ATOM 0.00	1968	N	THR	138	51.120	63.700	53.640	1.00
ATOM 0.00	1969	H	THR	138	50.250	63.560	53.150	1.00
ATOM 0.00	1970	CA	THR	138	51.570	65.040	53.900	1.00
ATOM 0.00	1971	HA	THR	138	52.560	65.080	53.440	1.00
ATOM 0.00	1972	CB	THR	138	50.650	66.120	53.290	1.00
ATOM 0.00	1973	HB	THR	138	50.840	67.120	53.680	1.00
ATOM 0.00	1974	CG2	THR	138	50.930	66.290	51.740	1.00
ATOM 0.00	1975	1HG2	THR	138	51.970	66.580	51.570	1.00
ATOM 0.00	1976	2HG2	THR	138	50.640	65.400	51.170	1.00
ATOM 0.00	1977	3HG2	THR	138	50.420	67.180	51.390	1.00
ATOM 0.00	1978	OG1	THR	138	49.270	65.800	53.460	1.00
ATOM 0.00	1979	HG1	THR	138	48.990	65.270	52.710	1.00
ATOM 0.00	1980	C	THR	138	51.690	65.230	55.430	1.00
ATOM 0.00	1981	O	THR	138	52.510	66.070	55.880	1.00
ATOM 0.00	1982	N	THR	139	51.000	64.460	56.270	1.00
ATOM 0.00	1983	H	THR	139	50.250	63.920	55.860	1.00
ATOM 0.00	1984	CA	THR	139	51.120	64.490	57.710	1.00
ATOM 0.00	1985	HA	THR	139	51.130	65.540	58.000	1.00
ATOM 0.00	1986	CB	THR	139	49.930	63.770	58.390	1.00





ATOM 0.00	2015	CE3	TRP	140	53.510	58.400	55.050	1.00
ATOM 0.00	2016	HE3	TRP	140	54.580	58.560	55.140	1.00
ATOM 0.00	2017	CD2	TRP	140	52.590	58.990	55.990	1.00
ATOM 0.00	2018	C	TRP	140	55.200	62.330	58.930	1.00
ATOM 0.00	2019	O	TRP	140	55.860	61.670	59.680	1.00
ATOM 0.00	2020	N	GLN	141	55.650	63.480	58.510	1.00
ATOM 0.00	2021	H	GLN	141	54.980	63.980	57.940	1.00
ATOM 0.00	2022	CA	GLN	141	56.740	64.310	59.090	1.00
ATOM 0.00	2023	HA	GLN	141	57.710	63.890	58.820	1.00
ATOM 0.00	2024	CB	GLN	141	56.720	65.730	58.450	1.00
ATOM 0.00	2025	HB1	GLN	141	57.540	66.180	59.020	1.00
ATOM 0.00	2026	HB2	GLN	141	55.860	66.310	58.780	1.00
ATOM 0.00	2027	CG	GLN	141	56.890	65.870	56.910	1.00
ATOM 0.00	2028	HG1	GLN	141	56.010	65.470	56.430	1.00
ATOM 0.00	2029	HG2	GLN	141	57.780	65.280	56.690	1.00
ATOM 0.00	2030	CD	GLN	141	57.000	67.310	56.420	1.00
ATOM 0.00	2031	OE1	GLN	141	57.180	68.270	57.170	1.00
ATOM 0.00	2032	NE2	GLN	141	56.580	67.670	55.220	1.00
ATOM 0.00	2033	1HE2	GLN	141	56.300	66.940	54.570	1.00
ATOM 0.00	2034	2HE2	GLN	141	56.570	68.640	54.930	1.00
ATOM 0.00	2035	C	GLN	141	56.660	64.370	60.580	1.00
ATOM 0.00	2036	O	GLN	141	57.720	64.490	61.190	1.00
ATOM 0.00	2037	N	LEU	142	55.470	64.180	61.290	1.00
ATOM 0.00	2038	H	LEU	142	54.610	64.180	60.760	1.00
ATOM 0.00	2039	CA	LEU	142	55.430	64.050	62.700	1.00
ATOM 0.00	2040	HA	LEU	142	56.130	64.840	62.980	1.00
ATOM 0.00	2041	CB	LEU	142	54.090	64.640	63.140	1.00
ATOM 0.00	2042	HB1	LEU	142	54.050	65.720	62.980	1.00



















































































