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Supplementary information

Effects of isosteric substitutions on the conformational preference and *cis-trans* isomerization of proline-containing peptides

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Table S1 Torsion angles (°) and thermodynamic properties (kcal/mol) of local minima and transition states of Ac-Pro-ψ[CS–NH]Me in water[a]

Conf.	Torsion angles					Thermodynamic properties			
	ω_0	ϕ_1	ψ_1	ω_1	$\chi_1{}^1$	$\Delta E_{e,0}{}^b$	$\Delta E_e{}^c$	ΔH^d	ΔG^e
cAd	1.7	-81.7	-14.9	-179.3	33.4	2.92	0.34	0.00	0.00
cFd	-5.6	-68.2	150.0	175.7	31.0	6.31	0.37	0.19	0.12
tFu	176.7	-58.4	142.1	176.2	-22.6	5.07	0.00	0.06	0.37
tAu	-177.2	-65.4	-26.5	-177.9	-24.0	6.06	0.23	0.27	0.81
cFu	-9.0	-55.3	143.2	176.9	-22.8	7.04	0.73	0.63	0.87
cAu	-2.6	-66.1	-26.9	-176.5	-22.0	3.94	1.46	1.44	1.90
tCd	-170.2	-87.1	62.0	179.4	34.2	0.00	1.99	1.95	2.74
ts1	119.0	-100.6	-14.6	-178.9	14.8	18.88	20.30	19.25	20.75
ts2	119.7	-106.0	-9.2	-178.6	-31.7	19.37	20.52	19.20	20.28
ts3	-59.9	-107.0	-1.1	179.4	22.6	19.70	20.19	18.87	20.10
ts4	-61.6	-92.2	-7.4	179.6	-37.8	19.99	19.94	18.66	19.60
cis%[f]									72.3

[a] Torsion angles are defined in Fig. 1. Calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in water. [b] Relative single-point electronic energies at the DSD-PBEP86-D3BJ/def2-TZVP level of theory. [c] Relative electronic energies in water. [d] Relative enthalpies at 25 °C in water. [e] Relative Gibbs free energies at 25 °C in water. [f] Population (%) of *cis* conformers calculated by Δ*G* values at 25 °C in water.

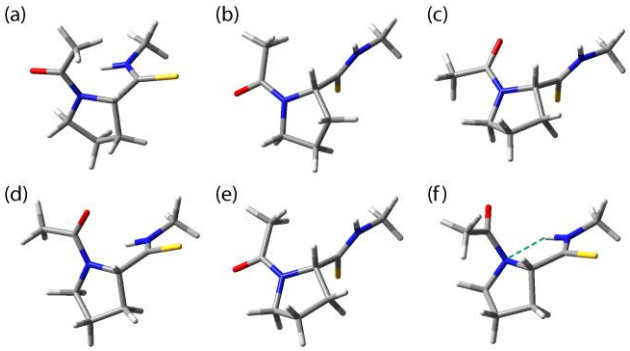

Fig. S1 The representative structures of Ac-Pro-ψ[CS–NH]Me optimized in water: local minima (a) cAd, (b) cFd, (c) tFu, (d) tAu, and (e) cFu (Δ*G* = 0.00, 0.12, 0.37, 0.81, and 0.87 kcal/mol, respectively) and transition state (f) ts4 (Δ*G* = 19.60 kcal/mol). Intramolecular H-bond is represented by dotted lines.

Table S2 Torsion angles (°) and thermodynamic properties (kcal/mol) of local minima and transition states of Ac-Pro-ψ[CSe–NH]Me in water[a]

Conf.	Torsion angles					Thermodynamic properties			
	ω_0	ϕ_1	ψ_1	ω_1	χ_1^1	$\Delta E_{e,0}$[b]	ΔE_e[c]	ΔH[d]	ΔG[e]
tFu	167.5	-50.7	145.2	174.5	-19.3	5.46	0.32	0.11	0.00
cAd	0.3	-81.1	-14.6	-178.6	34.0	2.84	0.49	0.28	0.16
tAd	-176.9	-74.7	-15.7	-178.1	31.8	5.19	0.00	0.00	0.24
tAu	-175.9	-69.1	-21.6	-175.1	-23.4	5.66	0.51	0.32	0.25
tFd	170.0	-60.5	151.9	175.5	30.9	4.85	0.39	0.40	0.62
cFd	-10.9	-67.0	159.6	177.1	34.1	6.72	0.72	0.80	1.41
cFu	-18.4	-49.7	145.4	175.8	-18.4	7.75	1.17	1.10	1.74
cAu	-1.0	-73.4	-20.9	-177.1	-19.4	3.73	1.63	1.64	1.92
tCd	-171.2	-86.7	65.9	178.1	33.9	0.00	2.63	2.45	2.74
ts1	119.0	-102.8	-14.4	-178.0	17.0	18.69	20.15	18.76	19.75
ts2	121.6	-107.1	-13.4	-176.4	-31.0	19.13	20.61	19.19	19.85
ts3	-59.1	-102.4	-10.7	-179.0	18.5	19.60	20.10	18.83	19.40
ts4	-61.2	-93.0	-13.8	-176.1	-37.4	19.77	19.96	18.79	19.59
cis%[f]									26.1

[a] Torsion angles are defined in Fig. 1. Calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in water. [b] Relative single-point electronic energies at the DSD-PBEP86-D3BJ/def2-TZVP level of theory. [c] Relative electronic energies in water. [d] Relative enthalpies at 25 °C in water. [e] Relative Gibbs free energies at 25 °C in water. [f] Population (%) of *cis* conformers calculated by ΔG values at 25 °C in water.

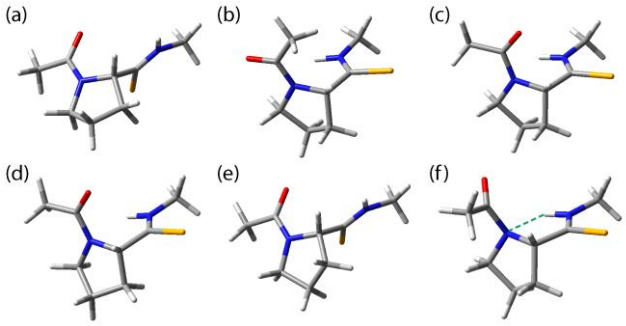

Fig. S2 The representative structures of Ac-Pro-ψ[CSe–NH]Me optimized in water: local minima (a) tFu, (b) cAd, (c) tAd, (d) tAu, and (e) tFd (ΔG = 0.00, 0.16, 0.24, 0.25, and 0.62 kcal/mol, respectively) and transition state (f) ts3 (ΔG = 19.40 kcal/mol). Intramolecular H-bond is represented by dotted lines.

Table S3 Absolute values of electronic energies, enthalpies, and Gibbs free energies in water at the SMD M06-2X/6-31+G(d) level of theory and single-point energies at the M06-2X/6-31+G(d) and DSD-PBEP86-D3BJ/def2-TZVP levels of theory for Ac-Pro-NHMe[a]

	SMD M06-2X/6-31+G(d)			M06-2X/6-31+G(d)	DSD-PBEP86-D3BJ/ def2-TZVP
Conf.	E_e[b]	H[b]	G[b]	E_e[c]	E_e[c]
tFu	-573.0641152	-572.837180	-572.890820	-573.030324	-573.233531
tFd	-573.0639107	-572.836788	-572.890516	-573.031881	-573.235250
cFd	-573.0625970	-572.835580	-572.891269	-573.029407	-573.232895
tAd	-573.0635739	-572.836656	-572.890320	-573.031830	-573.234649
cBd	-573.0629790	-572.836248	-572.890468	-573.034751	-573.237235
cFu	-573.0624482	-572.835264	-572.888665	-573.028649	-573.231991
tAu	-573.0626140	-572.835468	-572.888155	-573.030105	-573.232797
tCd	-573.0616941	-572.834923	-572.888283	-573.039985	-573.243387
cAu	-573.0607179	-572.833679	-572.886549	-573.032687	-573.235185
tCu	-573.0586672	-572.831598	-572.884875	-573.037098	-573.240184
ts1	-573.0304925	-572.805506	-572.857959	-573.008322	-573.211005
ts2	-573.0302529	-572.805356	-572.857497	-573.007155	-573.209840
ts3	-573.0311591	-572.805944	-572.858393	-573.006836	-573.209224
ts4	-573.0313552	-572.806067	-572.858204	-573.006009	-573.208475

[a] All energies are in hartees. The optimized structures were taken from ref. 71, except for cFd. [b] E_e is the electronic energy. H and G are the enthalpy and Gibbs free energy, respectively, calculated at 25℃ and 1 atm. [c] Single-point energy for the conformer optimized at the SMD M06-2X/6-31+G(d) level of theory in water.

Table S4 Absolute values of electronic energies, enthalpies, and Gibbs free energies in water at the SMD M06-2X/6-31+G(d) level of theory and single-point energies at the M06-2X/6-31+G(d) and DSD-PBEP86-D3BJ/def2-TZVP levels of theory for Ac-ψ(CS−NH)Pro-NHMe[a]

	SMD M06-2X/6-31+G(d)			M06-2X/6-31+G(d)	DSD-PBEP86-D3BJ/ def2-TZVP
Conf.	E_e[b]	H[b]	G[b]	E_e[c]	E_e[c]
tFu	-896.0056777	-895.780450	-895.834627	-895.975566	-895.177650
tAd	-896.0055842	-895.780315	-895.835314	-895.975452	-895.176958
tFd	-896.0062273	-895.780788	-895.834262	-895.977623	-895.179487
cFd	-896.0046816	-895.779350	-895.834057	-895.974005	-895.175821
cFu	-896.0041072	-895.778924	-895.833673	-895.972955	-895.174503
tAu	-896.0044369	-895.779228	-895.833305	-895.974226	-895.175807
cBd	-896.0047893	-895.779436	-895.834366	-895.980302	-895.181153
tCd	-896.0017306	-895.776481	-895.830570	-895.982019	-895.184301
cAu	-896.0022075	-895.776851	-895.830897	-895.977535	-895.178459
ts1	-895.9651167	-895.742119	-895.794503	-895.946233	-895.148551
ts2	-895.9636663	-895.740846	-895.794397	-895.944276	-895.146716
ts4	-895.9645298	-895.741261	-895.794411	-895.943089	-895.144981
ts3	-895.9648529	-895.741666	-895.794496	-895.944567	-895.146296

[a] All energies are in hartees. [b] E_e is the electronic energy. H and G are the enthalpy and Gibbs free energy, respectively, calculated at 25℃ and 1 atm. [c] Single-point energy for the conformer optimized at the SMD M06-2X/6-31+G(d) level of theory in water.

Table S5 Absolute values of electronic energies, enthalpies, and Gibbs free energies in water at the SMD M06-2X/6-31+G(d) level of theory and single-point energies at the M06-2X/6-31+G(d) and DSD-PBEP86-D3BJ/def2-TZVP levels of theory for Ac-ψ(CSe–NH)Pro-NHMe[a]

	SMD M06-2X/6-31+G(d)			M06-2X/6-31+G(d)	DSD-PBEP86-D3BJ/ def2-TZVP
Conf.	E_e[b]	H[b]	G[b]	E_e[c]	E_e[c]
tFu	-2897.3089609	-2897.083891	-2897.139721	-2897.276042	-2897.974490
tFd	-2897.3093787	-2897.083869	-2897.138804	-2897.277850	-2897.976324
tAd	-2897.3088289	-2897.083758	-2897.139536	-2897.276696	-2897.974592
cFd	-2897.3069233	-2897.081449	-2897.136506	-2897.274022	-2897.973479
tAu	-2897.3076621	-2897.082735	-2897.137281	-2897.275728	-2897.973324
cFu	-2897.3055503	-2897.080107	-2897.135412	-2897.272296	-2897.972015
cBd	-2897.3073908	-2897.082217	-2897.136930	-2897.281108	-2897.978896
cAu	-2897.3038786	-2897.078979	-2897.135249	-2897.276842	-2897.975490
tCd	-2897.3051210	-2897.079730	-2897.133791	-2897.284103	-2897.981607
tCu	-2897.3006033	-2897.075142	-2897.130176	-2897.279750	-2897.979274
ts1	-2897.2632582	-2897.040506	-2897.094419	-2897.244650	-2897.943825
ts2	-2897.2624677	-2897.039976	-2897.093979	-2897.243665	-2897.942303
ts3	-2897.2616147	-2897.038977	-2897.093402	-2897.241835	-2897.941758
ts4	-2897.2611585	-2897.038345	-2897.092500	-2897.240304	-2897.940021

[a] All energies are in hartees. [b] E_e is the electronic energy. H and G are the enthalpy and Gibbs free energy, respectively, calculated at 25℃ and 1 atm. [c] Single-point energy for the conformer optimized at the SMD M06-2X/6-31+G(d) level of theory in water.

Table S6 Absolute values of electronic energies, enthalpies, and Gibbs free energies in water at the SMD M06-2X/6-31+G(d) level of theory and single-point energies at the M06-2X/6-31+G(d) and DSD-PBEP86-D3BJ/def2-TZVP levels of theory for Ac-Pro-ψ(CS–NH)Me[a]

	SMD M06-2X/6-31+G(d)			M06-2X/6-31+G(d)	DSD-PBEP86-D3BJ/ def2-TZVP
Conf.	E_e[b]	H[b]	G[b]	E_e[c]	E_e[c]
cAd	-896.0061133	-895.781196	-895.836113	-895.981566	-895.182187
cFd	-896.0050529	-895.779877	-895.834930	-895.975143	-895.176785
tFu	-896.0056411	-895.780090	-895.834350	-895.977119	-895.178757
tAu	-896.0060342	-895.780508	-895.834072	-895.976303	-895.177181
cFu	-896.0044533	-895.779159	-895.833660	-895.973972	-895.175632
cAu	-896.0045781	-895.779146	-895.832852	-895.980180	-895.180557
tCd	-896.0025967	-895.777191	-895.830256	-895.985328	-895.186844
ts1	-895.9738109	-895.750026	-895.802026	-895.955636	-895.156756
ts2	-895.9737624	-895.750413	-895.803071	-895.955155	-895.155969
ts3	-895.9741296	-895.750771	-895.803214	-895.954476	-895.155444
ts4	-895.9747785	-895.751357	-895.804852	-895.954268	-895.154993

[a] All energies are in hartees. [b] E_e is the electronic energy. H and G are the enthalpy and Gibbs free energy, respectively, calculated at 25℃ and 1 atm. [c] Single-point energy for the conformer optimized at the SMD M06-2X/6-31+G(d) level of theory in water.

Table S7 Absolute values of electronic energies, enthalpies, and Gibbs free energies in water at the SMD M06-2X/6-31+G(d) level of theory and single-point energies at the M06-2X/6-31+G(d) and DSD-PBEP86-D3BJ/def2-TZVP levels of theory for Ac-Pro-ψ(CSe–NH)Me[a]

	SMD M06-2X/6-31+G(d)			M06-2X/6-31+G(d)	DSD-PBEP86-D3BJ/ def2-TZVP
Conf.	E_e[b]	H[b]	G[b]	E_e[c]	E_e[c]
tFu	-2897.3119251	-2897.086772	-2897.141471	-2897.281279	-2897.975449
cAd	-2897.3103396	-2897.085189	-2897.140017	-2897.284128	-2897.979620
tAd	-2897.3105778	-2897.085092	-2897.139290	-2897.279848	-2897.975877
tAu	-2897.3088878	-2897.083703	-2897.138558	-2897.278224	-2897.975133
tFd	-2897.3113299	-2897.085830	-2897.139991	-2897.281756	-2897.976416
cFd	-2897.3109641	-2897.085346	-2897.138815	-2897.278949	-2897.973447
cFu	-2897.3109455	-2897.085578	-2897.138741	-2897.278001	-2897.971794
cAu	-2897.3073360	-2897.081835	-2897.135941	-2897.281531	-2897.978211
tCd	-2897.3041449	-2897.078953	-2897.132576	-2897.285880	-2897.984149
ts1	-2897.2776070	-2897.054323	-2897.107173	-2897.257465	-2897.954360
ts2	-2897.2763869	-2897.053174	-2897.106840	-2897.256291	-2897.953664
ts3	-2897.2775986	-2897.054129	-2897.108315	-2897.255937	-2897.952915
ts4	-2897.2775740	-2897.053958	-2897.106999	-2897.255423	-2897.952648

[a] All energies are in hartees. [b] E_e is the electronic energy. H and G are the enthalpy and Gibbs free energy, respectively, calculated at 25℃ and 1 atm. [c] Single-point energy for the conformer optimized at the SMD M06-2X/6-31+G(d) level of theory in water.

Table S8 Absolute values of electronic energies, enthalpies, and Gibbs free energies in water at the SMD M06-2X/6-31+G(d) level of theory and single-point energies at the M06-2X/6-31+G(d) and DSD-PBEP86-D3BJ/def2-TZVP levels of theory for Ac-Ala-Pro-NHMe[a]

	SMD M06-2X/6-31+G(d)			M06-2X/6-31+G(d)	DSD-PBEP86-D3BJ/ def2-TZVP
Conf.	E_e[b]	H[b]	G[b]	E_e[c]	E_e[c]
FtFu	-820.3108405	-819.997454	-820.065209	-820.262546	-819.428058
EtFu	-820.3091907	-819.996041	-820.064636	-820.267147	-819.432420
AtFu	-820.3091130	-819.995777	-820.063537	-820.251397	-819.417326
EtAu	-820.3081270	-819.995392	-820.064632	-820.266114	-819.430869
FcBd	-820.3118790	-819.998867	-820.064741	-820.274672	-819.439253
EcBd	-820.3077537	-819.994882	-820.063342	-820.268861	-819.434028
FtAu	-820.3092387	-819.995759	-820.063165	-820.259389	-819.424717
EcFd	-820.3075667	-819.994386	-820.062432	-820.265837	-819.431792
FtCd	-820.3084432	-819.995354	-820.063048	-820.271136	-819.436253
AtAu	-820.3113315	-819.997958	-820.063222	-820.266862	-819.430832
EcFd	-820.3074395	-819.993941	-820.061153	-820.266445	-819.432382
AtBd	-820.3093095	-819.996376	-820.062715	-820.266863	-819.430959
EcFu	-820.3072839	-819.993746	-820.060811	-820.265611	-819.431539
EcAu	-820.3056915	-819.992680	-820.060642	-820.266211	-819.431848
FcBu	-820.3090049	-819.995684	-820.061328	-820.271285	-819.436001
EtCd	-820.3063176	-819.993137	-820.060336	-820.274227	-819.439073
DcAd	-820.3083979	-819.995426	-820.061451	-820.267714	-819.431178
DcFd	-820.3090598	-819.995907	-820.061195	-820.270501	-819.434142
DtCd	-820.3043791	-819.991398	-820.059735	-820.271313	-819.436100
F*tFu	-820.3041378	-819.991994	-820.058525	-820.250400	-819.415936
A*cAd	-820.3094083	-819.996188	-820.060774	-820.268227	-819.431167
AtCd	-820.3044854	-819.991207	-820.057868	-820.265327	-819.430281
ts	-820.2780454	-819.966996	-820.033767	-820.242002	-819.406450

[a] All energies are in hartees. [b] E_e is the electronic energy. H and G are the enthalpy and Gibbs free energy, respectively, calculated at 25℃ and 1 atm. [c] Single-point energy for the conformer optimized at the SMD M06-2X/6-31+G(d) level of theory in water.

Table S9 Absolute values of electronic energies, enthalpies, and Gibbs free energies in water at the SMD M06-2X/6-31+G(d) level of theory and single-point energies at the M06-2X/6-31+G(d) and DSD-PBEP86-D3BJ/def2-TZVP levels of theory for Ac-Ala-ψ(CS–NH)Pro-NHMe[a]

	SMD M06-2X/6-31+G(d)			M06-2X/6-31+G(d)	DSD-PBEP86-D3BJ/ def2-TZVP
Conf.	E_e[b]	H[b]	G[b]	E_e[c]	E_e[c]
FtAu	-1143.2505637	-1142.939329	-1143.012923	-1143.206321	-1142.162930
FtFu	-1143.2516287	-1142.941518	-1143.008789	-1143.210193	-1142.167098
FcBd	-1143.2526792	-1142.941427	-1143.009161	-1143.221601	-1142.177316
EcBd	-1143.2497381	-1142.938712	-1143.007600	-1143.213937	-1142.170933
AtFu	-1143.2499549	-1142.938318	-1143.007281	-1143.196329	-1142.153607
EtFu	-1143.2504679	-1142.939080	-1143.007007	-1143.211379	-1142.168653
EcFu	-1143.2495700	-1142.938308	-1143.006806	-1143.210181	-1142.167636
EcFd	-1143.2496735	-1142.938198	-1143.006554	-1143.210642	-1142.168262
FtAd	-1143.2529575	-1142.942328	-1143.007770	-1143.209320	-1142.165639
EtAu	-1143.2497954	-1142.938608	-1143.007138	-1143.209612	-1142.166350
AtAu	-1143.2526451	-1142.941217	-1143.007758	-1143.210505	-1142.165970
ts	-1143.2131760	-1142.904222	-1142.971718	-1143.180782	-1142.137526

[a] All energies are in hartees. [b] E_e is the electronic energy. H and G are the enthalpy and Gibbs free energy, respectively, calculated at 25℃ and 1 atm. [c] Single-point energy for the conformer optimized at the SMD M06-2X/6-31+G(d) level of theory in water.

Table S10 Absolute values of electronic energies, enthalpies, and Gibbs free energies in water at the SMD M06-2X/6-31+G(d) level of theory and single-point energies at the M06-2X/6-31+G(d) and DSD-PBEP86-D3BJ/def2-TZVP levels of theory for Ac-Ala-ψ(CSe–NH)Pro-NHMe[a]

	SMD M06-2X/6-31+G(d)			M06-2X/6-31+G(d)	DSD-PBEP86-D3BJ/ def2-TZVP
Conf.	E_e[b]	H[b]	G[b]	E_e[c]	E_e[c]
FtAu	-3144.5612650	-3144.250364	-3144.320216	-3144.515346	-3144.960689
FtFu	-3144.5622641	-3144.251067	-3144.319384	-3144.518697	-3144.964590
FcBd	-3144.5616475	-3144.250526	-3144.318533	-3144.529073	-3144.975231
EcBd	-3144.5572625	-3144.246217	-3144.316722	-3144.520991	-3144.968625
EcFu	-3144.5549033	-3144.245109	-3144.313135	-3144.513544	-3144.964333
EtAd	-3144.5592486	-3144.248009	-3144.316645	-3144.518286	-3144.965388
AtAu	-3144.5619757	-3144.250867	-3144.318800	-3144.516917	-3144.961685
EcFd	-3144.5555425	-3144.245007	-3144.312490	-3144.515585	-3144.966123
EtAu	-3144.5576176	-3144.246608	-3144.315598	-3144.516352	-3144.963547
FtCd	-3144.5585870	-3144.247346	-3144.315774	-3144.525430	-3144.970762
AtBd	-3144.5587995	-3144.248464	-3144.314779	-3144.516337	-3144.962076
FcAu	-3144.5572612	-3144.245703	-3144.313147	-3144.522534	-3144.968774
DcAd	-3144.5544125	-3144.243437	-3144.311036	-3144.516819	-3144.964236
DcFd	-3144.5557282	-3144.244157	-3144.310124	-3144.519221	-3144.967147
ts	-3144.5190244	-3144.210265	-3144.277375	-3144.487471	-3144.933618

[a] All energies are in hartees. [b] E_e is the electronic energy. H and G are the enthalpy and Gibbs free energy, respectively, calculated at 25℃ and 1 atm. [c] Single-point energy for the conformer optimized at the SMD M06-2X/6-31+G(d) level of theory in water.

Optimized Cartesian coordinates of representative structures of Ac-ψ(C**X**–NH)Pro-NHMe, Ac-Pro-ψ(C**X**–NH)Me, and Ac-Ala-ψ(C**X**–NH)Pro-NHMe (**X** = O, S, and Se) at the SMD M06-2X/6-31+G(d) level of theory in water (Shown in Fig. 2–7, and Fig. S1 and S2):

Ac-Pro-NHMe

(a) tFu

N	-1.111575	-0.043507	-0.123617
C	0.107939	0.665812	-0.506317
C	-2.17178	0.862507	0.345008
C	-0.177167	2.113335	-0.068877
C	1.333803	0.107369	0.205471
O	1.298569	-0.224939	1.400957
C	-1.7002	2.2184	-0.175158
C	-1.191941	-1.380266	-0.217162
O	-0.23803	-2.04739	-0.666167
C	-2.476009	-2.026271	0.229055
N	2.457781	0.070286	-0.51636
C	3.719016	-0.365296	0.060031
H	-2.346834	-3.108874	0.230593
H	-3.287704	-1.76288	-0.457699
H	-2.760915	-1.687287	1.229704
H	0.251871	0.601454	-1.591472
H	-2.223799	0.848813	1.44029
H	-3.139721	0.561168	-0.060436
H	0.132427	2.244046	0.974458
H	0.35999	2.833739	-0.688692
H	-2.110419	3.047921	0.404716
H	-1.999168	2.339247	-1.221843
H	2.42245	0.326458	-1.496131
H	3.999993	0.277121	0.898941
H	3.644724	-1.396469	0.416589
H	4.487392	-0.30681	-0.709798

(b) tFd

N	-1.149295	0.051238	-0.294793
C	0.153133	0.507856	-0.766792
C	-1.960605	1.13336	0.291704
C	0.032922	2.041336	-0.695994
C	1.26815	-0.004597	0.142344
O	1.105361	-0.140683	1.365716
C	-0.956328	2.27552	0.449486
C	-1.419841	-1.263016	-0.226138
O	-0.594709	-2.105377	-0.632929
C	-2.744817	-1.666194	0.361693
N	2.440998	-0.24068	-0.454522
C	3.614197	-0.648819	0.300044
H	-2.921537	-2.721506	0.151531
H	-3.563277	-1.065371	-0.044891
H	-2.724104	-1.517146	1.447198
H	0.331444	0.158704	-1.788135
H	-2.391968	0.815693	1.243322
H	-2.773706	1.402219	-0.392038
H	1.001747	2.522574	-0.540253
H	-0.384772	2.403082	-1.640604
H	-0.448297	2.194008	1.415083
H	-1.439026	3.253599	0.392978
H	2.510025	-0.147296	-1.461066
H	3.839775	0.08118	1.081653
H	3.45693	-1.626171	0.765085
H	4.458755	-0.711681	-0.385041

(c) cFd

N	-1.203306	0.045792	-0.213066
C	0.095502	0.419511	-0.765648
C	-1.927662	1.18664	0.369653
C	-0.001195	1.956008	-0.84711
C	1.240857	-0.006439	0.154096
O	1.088648	-0.122575	1.380174
C	-0.903472	2.320142	0.335333
C	-1.645683	-1.215256	-0.061489
O	-2.736991	-1.445827	0.494663
C	-0.78156	-2.3296	-0.593139
N	2.418095	-0.21096	-0.446078
C	3.615477	-0.524292	0.316633
H	-1.340318	-3.264366	-0.54025
H	0.127667	-2.426098	0.011084
H	-0.482106	-2.141819	-1.628422
H	0.239579	-0.022208	-1.755738
H	-2.25958	0.938414	1.380751
H	-2.81084	1.409794	-0.239314
H	0.979644	2.435651	-0.80958
H	-0.481745	2.222828	-1.793577
H	-0.324057	2.331674	1.263465
H	-1.376596	3.296771	0.212949
H	2.484264	-0.103147	-1.45191
H	3.501293	-1.48005	0.835378
H	4.455241	-0.591241	-0.373899
H	3.817191	0.256899	1.054407

(d) tAd

N	-1.009906	0.176963	-0.131673
C	0.17119	0.623425	-0.865986
C	-1.517998	1.194957	0.807979
C	0.195531	2.136581	-0.586993
C	1.470978	-0.04191	-0.418133
O	2.500657	0.123726	-1.096438
C	-0.406501	2.244433	0.817134
C	-1.577061	-1.023068	-0.365824
O	-1.084026	-1.817907	-1.187362
C	-2.813233	-1.356586	0.42438

N	1.463499	-0.755127	0.709434
C	2.665291	-1.397895	1.214543
H	-3.243725	-2.280513	0.037494
H	-3.550605	-0.55048	0.366321
H	-2.552632	-1.495284	1.479646
H	0.063672	0.401255	-1.931221
H	-1.697013	0.754804	1.792035
H	-2.458985	1.610571	0.43067
H	1.201722	2.553501	-0.66716
H	-0.448513	2.636763	-1.316937
H	0.34439	1.992444	1.573244
H	-0.793253	3.241798	1.036484
H	0.59251	-0.852332	1.218337
H	3.049253	-2.12018	0.489143
H	3.441415	-0.65466	1.416497
H	2.414379	-1.916722	2.138917

(e) ts1

N	0.871209	-0.062098	-0.331233
C	-0.033224	0.590384	0.651485
C	1.689384	1.003796	-0.968722
C	0.117488	2.110136	0.406384
C	-1.484077	0.149959	0.497882
O	-2.336269	0.55618	1.311586
C	0.739299	2.190369	-0.987911
C	1.687592	-1.093887	0.25934
O	2.5071	-0.838608	1.121705
C	1.456776	-2.472459	-0.268432
N	-1.78522	-0.652319	-0.52127
C	-3.129094	-1.160537	-0.732455
H	2.113642	-3.19421	0.218143
H	1.624813	-2.473437	-1.35105
H	0.407764	-2.744861	-0.106775
H	0.246043	0.342791	1.682173
H	2.016741	0.674858	-1.958533
H	2.572998	1.238761	-0.359759
H	-0.836584	2.634433	0.497769
H	0.80978	2.524689	1.144927
H	-0.021278	2.058847	-1.765285
H	1.261114	3.133908	-1.165458
H	-1.013143	-0.960856	-1.102024
H	-3.119537	-1.804321	-1.611364
H	-3.465563	-1.738104	0.133258
H	-3.830233	-0.338716	-0.900271

(f) ts3

N	0.79029	-0.118796	-0.437223
C	-0.033248	0.520936	0.616262
C	1.625695	0.932329	-1.077117
C	0.204885	2.03845	0.467061
C	-1.50793	0.152513	0.493939
O	-2.329031	0.624964	1.303009
C	0.759143	2.176963	-0.951474
C	1.56741	-1.22191	0.043218
O	1.426531	-2.320713	-0.459973
C	2.571366	-0.989881	1.144714
N	-1.855282	-0.690346	-0.476563
C	-3.224155	-1.14404	-0.644406
H	2.414698	-1.729119	1.934769
H	2.522114	0.01712	1.562956
H	3.571536	-1.152717	0.729064
H	0.257921	0.185014	1.620765
H	1.849764	0.64947	-2.108141
H	2.573375	1.074478	-0.53704
H	-0.706793	2.613108	0.645064
H	0.958803	2.356931	1.19347
H	-0.048556	2.151795	-1.69129
H	1.335556	3.093929	-1.0946
H	-1.113802	-1.026866	-1.081232
H	-3.25002	-1.866325	-1.45958
H	-3.584241	-1.622403	0.270656
H	-3.884413	-0.306583	-0.885835

Ac-ψ(CS–NH)Pro-NHMe

(a) tFu

N	-1.096045	0.195605	-0.025584
C	0.166361	0.763323	-0.511808
C	-2.063815	1.25587	0.334504
C	-0.002169	2.276851	-0.289348
C	1.373583	0.251979	0.265469
O	1.323535	0.049226	1.48817
C	-1.512614	2.482669	-0.381674
C	-1.355152	-1.107715	-0.003036
S	-0.27171	-2.262809	-0.583015
C	-2.698591	-1.505261	0.548483
N	2.508504	0.161966	-0.43565
C	3.748995	-0.278231	0.180062
H	-2.732875	-2.582389	0.703872
H	-3.488778	-1.22813	-0.159762
H	-2.903348	-0.993923	1.495121
H	0.281203	0.524678	-1.575432
H	-2.070522	1.393628	1.422045
H	-3.065844	0.980646	0.004366
H	0.348894	2.53845	0.715405
H	0.568174	2.850979	-1.021877
H	-1.844461	3.411628	0.086672
H	-1.834684	2.480165	-1.428082
H	2.466494	0.261312	-1.443208
H	4.022797	0.387047	1.002684
H	3.650945	-1.296861	0.568479
H	4.534285	-0.256007	-0.574685

(b) tAd

N	-0.840012	0.566923	-0.078032
C	0.344918	0.531629	-0.938065
C	-0.997142	1.87611	0.598271
C	0.768217	2.007392	-1.020625

C	1.470887	-0.339016	-0.384282
O	2.348415	-0.758623	-1.157868
C	0.33113	2.580462	0.329114
C	-1.680401	-0.459532	0.048332
S	-1.444474	-1.928564	-0.744205
C	-2.858498	-0.233035	0.955496
N	1.509507	-0.55762	0.93239
C	2.546379	-1.377723	1.537032
H	-3.541698	-1.079049	0.902084
H	-3.391514	0.683955	0.680888
H	-2.513926	-0.120302	1.990681
H	0.083967	0.115223	-1.913497
H	-1.198004	1.728957	1.661489
H	-1.839381	2.414209	0.149511
H	1.837708	2.114772	-1.21626
H	0.215709	2.485747	-1.835013
H	1.056756	2.325499	1.10811
H	0.214564	3.665833	0.310184
H	0.737465	-0.23558	1.505039
H	2.523231	-2.392926	1.129545
H	3.533198	-0.944776	1.354548
H	2.366788	-1.418395	2.610766

(c) tFd

N	-1.051909	0.357372	-0.15758
C	0.270559	0.54352	
C	-1.64673	1.638275	0.284739
C	0.354548	2.065569	-0.960359
C	1.361812	0.05155	0.196436
O	1.226348	0.103542	1.428879
C	-0.488976	2.628099	0.184714
C	-1.62042	-0.833211	-0.00652
S	-0.862677	-2.268986	-0.471846
C	-2.989882	-0.835269	0.615553
N	2.491636	-0.361952	-0.385086
C	3.632542	-0.803107	0.398833
H	-3.440397	-1.822452	0.525454
H	-3.639658	-0.092715	0.139966
H	-2.911206	-0.578402	1.679114
H	0.330095	-0.008519	-1.695467
H	-2.042572	1.540502	1.297422
H	-2.46652	1.904965	-0.391997
H	1.386252	2.424463	-0.960301
H	-0.098937	2.311633	-1.925699
H	0.084401	2.632934	1.116454
H	-0.841984	3.642974	-0.010012
H	2.527951	-0.432703	-1.395225
H	3.97	-0.006132	1.066498
H	3.375012	-1.680891	0.998842
H	4.440795	-1.060715	-0.284432

(d) cFd

N	0.846774	0.356499	0.250485
C	-0.514115	0.415364	0.791184
C	1.231116	1.624538	-0.394405
C	-0.769809	1.927019	0.898796
C	-1.498918	-0.251577	-0.174719
O	-1.215197	-0.451878	-1.365036
C	-0.030357	2.48421	-0.318539
C	1.610066	-0.730911	0.254366
S	3.153874	-0.747536	-0.426288
C	1.039438	-1.952481	0.927028
N	-2.683547	-0.578661	0.350223
C	-3.75274	-1.129112	-0.466981
H	1.718732	-2.794403	0.805377
H	0.063839	-2.220722	0.50433
H	0.899806	-1.761452	1.997568
H	-0.566559	-0.077173	1.764948
H	1.566536	1.427764	-1.415721
H	2.06848	2.06237	0.16016
H	-1.834931	2.167709	0.915141
H	-0.314228	2.289272	1.825664
H	-0.633313	2.351335	-1.222369
H	0.208754	3.54477	-0.217361
H	-2.862114	-0.369125	1.326201
H	-3.439902	-2.073557	-0.919767
H	-4.616015	-1.307872	0.172659
H	-4.030173	-0.430475	-1.261271

(e) ts1

N	-0.574089	0.087369	0.496918
C	0.272051	0.579724	-0.618337
C	-1.084851	1.261115	1.251577
C	0.322773	2.112094	-0.442274
C	1.676983	-0.013802	-0.602647
O	2.466741	0.265801	-1.525718
C	0.001399	2.303965	1.039533
C	-1.583353	-0.856822	0.115489
S	-2.841888	-0.472037	-0.854005
C	-1.369946	-2.219802	0.684103
N	2.012286	-0.805174	0.414697
C	3.323523	-1.421884	0.507287
H	-2.16899	-2.912119	0.419129
H	-1.280891	-2.143382	1.775226
H	-0.409365	-2.606255	0.317735
H	-0.155566	0.313163	-1.591507
H	-1.245391	0.986673	2.297749
H	-2.034095	1.61412	0.826142
H	1.284227	2.529267	-0.750535
H	-0.463803	2.566202	-1.053263
H	0.8752	2.081274	1.6621
H	-0.348326	3.31257	1.273056
H	1.287854	-1.015461	1.092967
H	3.374481	-1.988161	1.436609
H	3.497801	-2.09799	-0.334986
H	4.104289	-0.656608	0.50971

Ac-ψ(CSe–NH)Pro-NHMe

(a) tFu

N	-0.955882	0.745063	0.022981
C	0.374639	1.043853	-0.523367
C	-1.713119	1.987975	0.301921
C	0.481235	2.57445	-0.421837
C	1.482057	0.384314	0.2931
O	1.384796	0.238524	1.521216
C	-0.971422	3.036709	-0.516222
C	-1.438814	-0.470713	0.181355
Se	-0.535819	-1.96495	-0.356189
C	-2.816899	-0.568011	0.768762
N	2.599853	0.094541	-0.379109
C	3.743755	-0.502287	0.290593
H	-3.048312	-1.599326	1.029491
H	-3.552758	-0.219051	0.03369
H	-2.908035	0.063293	1.658968
H	0.416622	0.7049	-1.564791
H	-1.666937	2.204037	1.37549
H	-2.755449	1.867827	0.006576
H	0.899053	2.847607	0.553858
H	1.124511	2.978316	-1.205492
H	-1.124636	4.042597	-0.120544
H	-1.31382	3.009698	-1.555809
H	2.599065	0.169907	-1.389662
H	4.106387	0.152493	1.086749
H	3.47246	-1.470445	0.72325
H	4.534926	-0.646699	-0.444005

(b) tFd

N	-0.483229	1.075362	-0.126147
C	0.740921	0.577229	-0.758058
C	-0.367553	2.504981	0.24688
C	1.527146	1.860378	-1.071362
C	1.494845	-0.324397	0.221881
O	1.374688	-0.197628	1.4502
C	1.112618	2.813937	0.049694
C	-1.528534	0.322201	0.146026
Se	-1.587368	-1.453028	-0.282717
C	-2.692691	1.009848	0.796629
N	2.337567	-1.202076	-0.329049
C	3.183385	-2.053648	0.491892
H	-3.568298	0.362883	0.802526
H	-2.931911	1.943614	0.276409
H	-2.436408	1.263478	1.83314
H	0.490424	0.012755	-1.660025
H	-0.705386	2.648777	1.274801
H	-1.000371	3.099737	-0.420794
H	2.603398	1.68184	-1.117593
H	1.195855	2.242653	-2.041796
H	1.669074	2.590073	0.965023
H	1.275052	3.862968	-0.205572
H	2.377387	-1.281987	-1.338536
H	3.833768	-1.447756	1.128292
H	2.573531	-2.702891	1.126477
H	3.795699	-2.66837	-0.166691

(c) tAd

N	0.018955	1.089912	-0.012918
C	0.868329	0.312744	-0.922488
C	0.711346	2.301912	0.488562
C	2.049982	1.25333	-1.20495
C	1.333363	-1.016201	-0.330108
O	1.758887	-1.895192	-1.097463
C	2.163001	2.086292	0.073127
C	-1.227542	0.768325	0.284456
Se	-2.029405	-0.72338	-0.395735
C	-1.960261	1.721586	1.181087
N	1.3253	-1.162382	0.997091
C	1.752219	-2.402498	1.624152
H	-3.01008	1.445103	1.259757
H	-1.879182	2.745279	0.798894
H	-1.513993	1.706588	2.183389
H	0.309224	0.068654	-1.828436
H	0.5765	2.390779	1.568107
H	0.2768	3.182347	0.002698
H	2.958651	0.699315	-1.45067
H	1.791621	1.891405	-2.055253
H	2.69636	1.52855	0.84929
H	2.679759	3.034804	-0.085339
H	0.915828	-0.434461	1.571987
H	1.164433	-3.245097	1.248022
H	2.809631	-2.591367	1.421069
H	1.600706	-2.311092	2.69894

(d) cFd

N	0.272552	0.501364	0.301067
C	-1.111792	0.459633	0.791953
C	0.583437	1.797317	-0.33249
C	-1.501337	1.944436	0.852131
C	-1.996409	-0.312465	-0.191001
O	-1.662357	-0.491235	-1.371142
C	-0.748021	2.54473	-0.335499
C	1.109411	-0.512826	0.37344
Se	2.829399	-0.396211	-0.231196
C	0.606272	-1.763637	1.036556
N	-3.155075	-0.750539	0.309508
C	-4.137356	-1.424698	-0.524348
H	1.35181	-2.55427	0.972667
H	-0.321854	-2.114506	0.570271
H	0.39546	-1.562904	2.093905
H	-1.15408	-0.011416	1.776242
H	0.991092	1.623887	-1.33113
H	1.347154	2.302677	0.269043
H	-2.582807	2.088616	0.805859
H	-1.133959	2.361894	1.794491
H	-1.289161	2.348693	-1.266233
H	-0.604637	3.622884	-0.241231
H	-3.372802	-0.561414	1.281649

H	-3.728439	-2.358265	-0.919866
H	-5.010741	-1.648465	0.086602
H	-4.435321	-0.787062	-1.360967

(e) ts1

N	-0.054594	0.313523	0.628438
C	0.727798	0.608565	-0.595904
C	-0.511631	1.604353	1.193713
C	1.025996	2.129244	-0.518938
C	2.019744	-0.189177	-0.689871
O	2.636405	-0.226684	-1.77213
C	0.681268	2.503936	0.925349
C	-1.083773	-0.659445	0.4652
Se	-2.539216	-0.348756	-0.482828
C	-0.829352	-1.926683	1.202531
N	2.467765	-0.779795	0.41683
C	3.68887	-1.566408	0.430706
H	-1.643757	-2.644437	1.106151
H	-0.65456	-1.690743	2.260464
H	0.101372	-2.374787	0.828517
H	0.156619	0.3742	-1.501951
H	-0.753101	1.474683	2.252172
H	-1.400314	1.976784	0.666381
H	2.057865	2.356414	-0.798416
H	0.361642	2.657025	-1.209079
H	1.505287	2.260138	1.604195
H	0.435291	3.562827	1.037573
H	1.868579	-0.737011	1.234505
H	3.812632	-1.994879	1.424652
H	3.634867	-2.372952	-0.306124
H	4.553957	-0.9385	0.20057

Ac-Pro-ψ(CS–NH)Me

(a) cAd

N	-1.064728	0.230017	-0.50978
C	-0.099829	-0.607151	0.242479
C	-2.116098	-0.664461	-1.088887
C	-0.300635	-2.017002	-0.335862
C	1.335172	-0.120238	0.11365
S	2.5542	-0.839315	1.023197
C	-1.81066	-2.061758	-0.552026
C	-1.625106	1.278331	0.29353
O	-1.425191	2.439244	-0.009866
C	-2.434125	0.916322	1.513289
N	1.534343	0.855767	-0.749722
C	2.819406	1.47195	-1.021849
H	-3.326417	1.545665	1.553799
H	-1.828622	1.138056	2.399363
H	-2.715547	-0.138055	1.53725
H	-0.334736	-0.625289	1.315725
H	-2.035465	-0.628177	-2.178953
H	-3.116509	-0.310146	-0.817733
H	0.234209	-2.100621	-1.289701
H	0.072904	-2.783343	0.344985
H	-2.122775	-2.845969	-1.246091
H	-2.317266	-2.222163	0.406291
H	0.700693	1.218763	-1.210654
H	3.513955	0.738786	-1.440646
H	2.6641	2.279699	-1.735909
H	3.249753	1.871428	-0.099374

(b) cFd

N	-1.31081	0.022047	-0.287105
C	-0.044072	0.405216	-0.894666
C	-2.032593	1.153647	0.313369
C	-0.18793	1.934726	-1.035492
C	1.17639	0.033715	-0.049362
S	1.150577	-0.001847	1.626298
C	-1.078572	2.337165	0.144497
C	-1.733144	-1.242413	-0.113854
O	-2.79135	-1.482052	0.499995
C	-0.894909	-2.35073	-0.696876
N	2.257546	-0.218475	-0.772128
C	3.569268	-0.505511	-0.218788
H	-1.439257	-3.290721	-0.601669
H	0.054193	-2.435214	-0.15575
H	-0.668527	-2.166479	-1.75124
H	0.06212	-0.065189	-1.877371
H	-2.257264	0.935289	1.361063
H	-2.979115	1.302521	-0.218168
H	0.780034	2.441681	-1.040065
H	-0.691757	2.141416	-1.98485
H	-0.475844	2.462156	1.047502
H	-1.615527	3.269238	-0.044971
H	2.175311	-0.191798	-1.785099
H	3.52882	-1.399448	0.409563
H	4.256675	-0.670982	-1.047397
H	3.917924	0.3336	0.389386

(c) tFu

N	-1.233976	-0.015267	-0.212001
C	-0.027179	0.670922	-0.663525
C	-2.182833	0.895266	0.440866
C	-0.273535	2.142889	-0.268068
C	1.24615	0.128634	-0.018528
S	1.32731	-0.273765	1.608464
C	-1.797297	2.244596	-0.157466
C	-1.378001	-1.340433	-0.37114
O	-0.515792	-2.012429	-0.971854
C	-2.623516	-1.970174	0.19358
N	2.284383	0.079514	-0.837693
C	3.624543	-0.32109	-0.44758
H	-2.5492	-3.053371	0.09326
H	-3.507739	-1.619153	-0.349082
H	-2.750827	-1.705498	1.248149
H	0.055308	0.567986	-1.752815
H	-2.032142	0.881019	1.527816

H	-3.21098	0.604189	0.21966
H	0.181837	2.336936	0.708345
H	0.161379	2.827009	-0.999247
H	-2.118334	3.08184	0.466143
H	-2.247777	2.351851	-1.149759
H	2.13603	0.320074	-1.814182
H	4.0167	0.35519	0.316815
H	3.613039	-1.337409	-0.044721
H	4.259257	-0.284385	-1.33195

(d) tAu

N	-1.221859	0.042803	-0.065236
C	-0.014318	0.735054	-0.526064
C	-2.09199	0.912697	0.743541
C	-0.154021	2.149684	0.079618
C	1.282248	0.075197	-0.079309
S	2.695908	0.343786	-0.943701
C	-1.661051	2.306464	0.295273
C	-1.512012	-1.198923	-0.501706
O	-0.735979	-1.800927	-1.266895
C	-2.801647	-1.81753	-0.032357
N	1.219294	-0.633213	1.034056
C	2.352729	-1.301983	1.64872
H	-2.792577	-2.879414	-0.279798
H	-3.64623	-1.340005	-0.541341
H	-2.939879	-1.689636	1.044853
H	-0.008338	0.769256	-1.619059
H	-1.895106	0.752776	1.810887
H	-3.142819	0.702865	0.539323
H	0.368365	2.191527	1.042027
H	0.275947	2.904959	-0.58027
H	-1.903295	3.073213	1.034327
H	-2.157152	2.55653	-0.648554
H	0.305722	-0.751574	1.467064
H	2.786977	-2.026391	0.954
H	3.120976	-0.573252	1.920741
H	1.999028	-1.815104	2.542152

(e) cFu

N	1.291401	0.095417	-0.199649
C	0.117071	-0.636649	-0.676751
C	2.290636	-0.79016	0.407719
C	0.44615	-2.108666	-0.336531
C	-1.19077	-0.213816	-0.009945
S	-1.294972	0.140217	1.626521
C	1.972674	-2.13342	-0.238749
C	1.433812	1.432558	-0.196775
O	2.406777	1.971261	0.366866
C	0.397389	2.263776	-0.909046
N	-2.231328	-0.216265	-0.827293
C	-3.595611	0.082061	-0.427156
H	0.852629	3.216935	-1.183365
H	-0.441906	2.464173	-0.233738
H	0.011037	1.773653	-1.806438
H	0.022788	-0.512292	-1.762565
H	2.157835	-0.818647	1.496884
H	3.293439	-0.421125	0.185278
H	0.009441	-2.361076	0.635056
H	0.038272	-2.785487	-1.089733
H	2.339649	-2.976681	0.350484
H	2.421337	-2.180358	-1.236553
H	-2.067643	-0.413017	-1.81142
H	-3.655834	1.091908	-0.011849
H	-4.229368	0.00938	-1.309945
H	-3.934951	-0.629096	0.330641

(f) ts4

N	-1.064728	0.230017	-0.50978
C	-0.099829	-0.607151	0.242479
C	-2.116098	-0.664461	-1.088887
C	-0.300635	-2.017002	-0.335862
C	1.335172	-0.120238	0.11365
S	2.5542	-0.839315	1.023197
C	-1.81066	-2.061758	-0.552026
C	-1.625106	1.278331	0.29353
O	-1.425191	2.439244	-0.009866
C	-2.434125	0.916322	1.513289
N	1.534343	0.855767	-0.749722
C	2.819406	1.47195	-1.021849
H	-3.326417	1.545665	1.553799
H	-1.828622	1.138056	2.399363
H	-2.715547	-0.138055	1.53725
H	-0.334736	-0.625289	1.315725
H	-2.035465	-0.628177	-2.178953
H	-3.116509	-0.310146	-0.817733
H	0.234209	-2.100621	-1.289701
H	0.072904	-2.783343	0.344985
H	-2.122775	-2.845969	-1.246091
H	-2.317266	-2.222163	0.406291
H	0.700693	1.218763	-1.210654
H	3.513955	0.738786	-1.440646
H	2.6641	2.279699	-1.735909
H	3.249753	1.871428	-0.099374

Ac-Pro-ψ(CSe–NH)Me

(a) tFu

N	1.496943	0.089694	0.422673
C	0.368648	0.942782	0.77968
C	2.358996	0.71222	-0.59018
C	0.614364	2.248995	-0.010473
C	-0.965904	0.33866	0.378782
Se	-1.17903	-0.561245	-1.186077
C	2.105156	2.198504	-0.358083
C	1.500189	-1.211382	0.772356
O	0.674412	-1.654438	1.592729
C	2.540425	-2.086765	0.130996
N	-1.95107	0.593822	1.206712

C	-3.34413	0.231796	0.999254
H	2.370596	-3.120839	0.431854
H	3.547093	-1.779719	0.433182
H	2.476864	-2.005143	-0.959632
H	0.365241	1.123064	1.861048
H	2.045843	0.401997	-1.59575
H	3.400711	0.425119	-0.435901
H	0.015427	2.238373	-0.926242
H	0.332076	3.122325	0.580301
H	2.353696	2.802031	-1.233609
H	2.706845	2.545746	0.488221
H	-1.733994	1.103438	2.061275
H	-3.724359	0.6916	0.083571
H	-3.440113	-0.854129	0.919813
H	-3.911784	0.590529	1.856983

(b) cAd

N	-1.712004	0.150028	-0.174656
C	-0.390402	0.482478	-0.703442
C	-2.353396	1.281853	0.519831
C	-0.414422	2.024631	-0.690336
C	0.755408	-0.053292	0.148581
Se	2.440309	-0.064827	-0.53465
C	-1.257192	2.347566	0.546447
C	-2.34842	-1.02957	-0.339853
O	-3.488142	-1.201745	0.124952
C	-1.64235	-2.102721	-1.128027
N	0.459191	-0.46598	1.357228
C	1.409542	-0.982309	2.329292
H	-2.183471	-3.041551	-1.007696
H	-0.604108	-2.238556	-0.810632
H	-1.634139	-1.828426	-2.188955
H	-0.261598	0.092772	-1.715029
H	-2.685117	0.976296	1.515939
H	-3.230045	1.606257	-0.051452
H	0.588445	2.453943	-0.667777
H	-0.923223	2.364417	-1.59794
H	-0.653241	2.250833	1.455074
H	-1.671527	3.357418	0.51926
H	-0.52107	-0.438678	1.636368
H	0.856659	-1.249814	3.228833
H	1.914547	-1.864794	1.926938
H	2.15959	-0.222184	2.562576

(c) tAd

N	-1.675193	0.202561	-0.228766
C	-0.335715	0.613726	-0.642088
C	-2.375376	1.234112	0.562312
C	-0.338102	2.124487	-0.335297
C	0.777267	-0.101141	0.113165
Se	2.482662	0.004691	-0.516765
C	-1.261305	2.231342	0.880975
C	-2.182426	-0.991323	-0.603146
O	-1.494949	-1.799575	-1.252202
C	-3.596291	-1.290839	-0.186604
N	0.450054	-0.727612	1.216539
C	1.372565	-1.431187	2.093583
H	-3.925822	-2.205847	-0.679366
H	-4.267445	-0.466942	-0.44638
H	-3.641171	-1.430298	0.899319
H	-0.189319	0.411071	-1.70515
H	-2.825177	0.795136	1.456186
H	-3.164941	1.695677	-0.041177
H	0.667097	2.511568	-0.161263
H	-0.772801	2.650524	-1.191131
H	-0.731145	1.930182	1.790816
H	-1.650757	3.240575	1.029128
H	-0.534356	-0.731037	1.481865
H	1.886469	-2.222261	1.541336
H	2.116279	-0.736584	2.492829
H	0.794441	-1.864364	2.908795

(d) tAu

N	-1.665636	0.10769	-0.071605
C	-0.35835	0.677918	-0.398273
C	-2.492379	1.03255	0.721773
C	-0.395806	2.078627	0.257322
C	0.815247	-0.110415	0.144995
Se	2.473732	0.194564	-0.531601
C	-1.88913	2.389167	0.369883
C	-2.060481	-1.056667	-0.628391
O	-1.28655	-1.700103	-1.360143
C	-3.453782	-1.535482	-0.321795
N	0.576605	-0.904078	1.160553
C	1.579901	-1.664577	1.888403
H	-3.573247	-2.546628	-0.711487
H	-4.189447	-0.878074	-0.797425
H	-3.643896	-1.529216	0.755447
H	-0.247404	0.751029	-1.483644
H	-2.38415	0.809899	1.790383
H	-3.543517	0.943205	0.444825
H	0.055754	2.028746	1.254146
H	0.161739	2.803755	-0.337255
H	-2.105966	3.147934	1.124885
H	-2.281859	2.72822	-0.594295
H	-0.391808	-0.999821	1.465137
H	2.086823	-2.362759	1.217068
H	2.319973	-0.986644	2.321751
H	1.074413	-2.21599	2.679914

(e) tFd

N	1.494142	0.227945	0.489275
C	0.282719	0.857618	0.98674
C	2.159407	1.016578	-0.565495
C	0.430504	2.318118	0.522121
C	-0.976607	0.205455	0.426746
Se	-1.035713	-0.575817	-1.209592
C	1.228944	2.215277	-0.781863

C	1.71867	-1.077449	0.738529
O	0.997952	-1.711472	1.532567
C	2.86122	-1.726836	0.01
N	-2.021032	0.298856	1.218537
C	-3.366133	-0.150341	0.898925
H	3.07493	-2.693385	0.467336
H	3.759063	-1.102764	0.019659
H	2.569367	-1.881977	-1.036202
H	0.245126	0.789291	2.078932
H	2.271549	0.416695	-1.473233
H	3.152133	1.326516	-0.223518
H	-0.536821	2.811112	0.399183
H	1.000796	2.858822	1.283412
H	0.558559	2.024799	-1.623353
H	1.791694	3.127179	-0.993149
H	-1.89019	0.73919	2.127418
H	-3.73062	0.357612	0.002172
H	-3.370716	-1.229303	0.722118
H	-4.008366	0.087636	1.745909

(f) ts3

N	-1.604641	-0.111529	0.361589
C	-0.441113	0.520169	-0.297539
C	-2.449636	0.952088	0.961672
C	-0.506005	2.011219	0.113487
C	0.858718	-0.14335	0.140638
Se	2.418106	0.235219	-0.722263
C	-1.419485	2.005714	1.339576
C	-2.319763	-1.010316	-0.494509
O	-2.453237	-2.174004	-0.168184
C	-2.90859	-0.486133	-1.779213
N	0.769803	-0.972039	1.147764
C	1.87034	-1.702421	1.750073
H	-2.521195	-1.07879	-2.61312
H	-2.697071	0.57111	-1.948356
H	-3.99241	-0.635767	-1.741606
H	-0.483893	0.424102	-1.388528
H	-3.00556	0.548304	1.810905
H	-3.163499	1.358361	0.230133
H	0.484419	2.430994	0.298591
H	-0.975312	2.57829	-0.696474
H	-0.872414	1.694232	2.235846
H	-1.875957	2.980303	1.527794
H	-0.178697	-1.112984	1.505165
H	1.468211	-2.30268	2.565254
H	2.343013	-2.352244	1.008475
H	2.617736	-1.005507	2.137763

Ac-Ala-Pro-NHMe

(a) FtFu

H	-4.321209	-1.832466	-1.820286
H	-5.427825	-0.568165	-1.265234
H	-4.899803	-1.841807	-0.133614
C	-4.591595	-1.205776	-0.965487
O	-2.943451	0.481679	-1.428073
C	-3.416718	-0.334921	-0.618303
N	-2.896497	-0.468759	0.614065
H	-3.247785	-1.196101	1.227062
C	-1.720211	0.277245	1.012753
H	-1.946226	1.343407	0.936445
C	-1.342061	-0.069131	2.451256
C	-0.534711	-0.068558	0.110002
O	-0.395547	-1.212986	-0.353201
H	-0.463935	0.504953	2.759252
H	-2.168005	0.173154	3.125821
H	-1.111285	-1.136109	2.538556
N	0.385944	0.885631	-0.09072
C	0.346574	2.284799	0.37201
C	1.66956	0.540376	-0.704438
H	1.528522	0.303786	-1.765068
C	2.513101	1.815419	-0.519257
C	2.318752	-0.640657	0.009051
O	2.228167	-0.785519	1.238555
H	3.061337	1.754912	0.427924
H	3.231522	1.940687	-1.33138
C	1.466568	2.927093	-0.441455
H	1.846543	3.83694	0.027737
H	1.098971	3.174268	-1.443032
H	0.550602	2.334853	1.448477
H	-0.627678	2.732277	0.169068
N	3.045478	-1.4558	-0.76024
H	3.058564	-1.301651	-1.761475
C	3.793908	-2.568388	-0.198682
H	4.521977	-2.209612	0.533623
H	3.120519	-3.277809	0.290076
H	4.31837	-3.073416	-1.008644

(b) EtFu

H	-4.347299	-2.244079	-1.174801
H	-5.434222	-0.908942	-1.640407
H	-5.617636	-1.678867	-0.057879
C	-4.888333	-1.368315	-0.811222
O	-4.429231	0.723276	0.272521
C	-3.978893	-0.333771	-0.205533
N	-2.664587	-0.605027	-0.22129
H	-2.330639	-1.485299	-0.601201
C	-1.673087	0.294432	0.338999
H	-1.96423	1.317025	0.087188
C	-1.562419	0.142454	1.861811
C	-0.329392	-0.052185	-0.284386
O	-0.116553	-1.199313	-0.718135
H	-0.856585	0.86599	2.279956
H	-2.542336	0.308864	2.31739
H	-1.221036	-0.867083	2.113052
N	0.6226	0.887856	-0.291757
C	0.525051	2.284544	0.166798
C	1.988445	0.527015	-0.67818
H	2.018471	0.280771	-1.745238

C	2.800136	1.799021	-0.370352
C	2.485821	-0.655818	0.145062
O	2.185316	-0.778172	1.342974
H	3.194565	1.74247	0.6505
H	3.635333	1.915077	-1.063369
C	1.761264	2.918492	-0.46343
H	2.067226	3.825997	0.061197
H	1.558538	3.166236	-1.510574
H	0.575125	2.329557	1.260737
H	-0.408078	2.739061	-0.169186
N	3.307116	-1.500981	-0.483422
H	3.480554	-1.370349	-1.473231
C	3.888	-2.647517	0.195735
H	4.474937	-2.326209	1.059909
H	3.105832	-3.3323	0.535811
H	4.539767	-3.167299	-0.505274

(c) AtFu

H	2.505586	-0.848199	-2.941095
H	3.694004	-1.996732	-2.31167
H	3.941753	-0.246622	-2.068961
C	3.196007	-1.042922	-2.115113
O	1.514374	-2.030733	-0.712556
C	2.399741	-1.169659	-0.845621
N	2.687676	-0.310778	0.150587
H	3.332768	0.451569	-0.029493
C	1.915137	-0.292505	1.378505
H	1.976527	-1.283979	1.837274
C	2.474096	0.744187	2.349347
C	0.414818	-0.066406	1.173201
O	-0.376078	-0.672176	1.920645
H	1.89387	0.728277	3.275416
H	3.515003	0.508707	2.587664
H	2.428088	1.753118	1.927233
N	-0.034886	0.802705	0.255463
C	0.72648	1.676922	-0.659016
C	-1.483167	0.990459	0.107476
H	-1.887543	1.438257	1.02273
C	-1.605136	1.956624	-1.082182
C	-2.20113	-0.321903	-0.181763
O	-1.711079	-1.180904	-0.930951
H	-1.653521	1.383167	-2.01503
H	-2.500799	2.575531	-1.002843
C	-0.298489	2.746723	-1.02369
H	-0.055022	3.23983	-1.967241
H	-0.346421	3.503466	-0.2333
H	1.038049	1.113981	-1.546991
H	1.608418	2.088484	-0.167751
N	-3.419578	-0.446251	0.354166
H	-3.756759	0.272608	0.983322
C	-4.261375	-1.598508	0.078715
H	-4.436445	-1.696298	-0.996032
H	-3.794333	-2.517198	0.444324
H	-5.215326	-1.455274	0.584667

(d) EtAu

H	-5.471039	-0.167896	-1.652897
H	-5.74275	-1.285373	-0.30741
H	-4.530261	-1.678769	-1.556275
C	-4.98105	-0.872399	-0.974013
O	-4.325623	0.778635	0.640353
C	-3.973939	-0.115346	-0.150768
N	-2.683788	-0.441483	-0.327102
H	-2.42963	-1.173205	-0.983306
C	-1.605056	0.225373	0.376793
H	-1.84619	1.290533	0.427982
C	-1.411355	-0.333341	1.791643
C	-0.327656	0.009094	-0.423594
O	-0.2473	-0.915936	-1.249372
H	-0.633644	0.217979	2.328717
H	-2.347059	-0.245432	2.35001
H	-1.12592	-1.389462	1.741909
N	0.722484	0.801753	-0.156608
C	0.785016	1.980685	0.725088
C	2.003082	0.562111	-0.827699
H	1.852453	0.546411	-1.911246
C	2.885232	1.753181	-0.389134
C	2.664179	-0.755643	-0.451316
O	3.537367	-1.230922	-1.197479
H	3.514412	1.457106	0.457622
H	3.534342	2.082615	-1.201839
C	1.876699	2.813431	0.06059
H	2.310645	3.544648	0.74575
H	1.462043	3.341195	-0.804498
H	1.08163	1.675911	1.736155
H	-0.179691	2.486513	0.773227
N	2.331301	-1.315293	0.714348
H	1.601607	-0.891017	1.27669
C	2.964881	-2.538704	1.179972
H	2.835623	-3.339524	0.447018
H	4.033952	-2.380328	1.346934
H	2.493746	-2.831613	2.117601

(e) FcBd

H	-4.396115	1.953806	-0.672521
H	-4.949575	0.419229	0.05649
H	-4.432118	0.476466	-1.6475
C	-4.245138	0.87198	-0.644034
O	-1.872452	1.161878	-0.866259
C	-2.813829	0.58853	-0.287166
N	-2.586711	-0.320144	0.674967
H	-3.371131	-0.823903	1.074641
C	-1.24068	-0.734461	1.025175
H	-0.715175	0.125813	1.451174
C	-1.299258	-1.864703	2.049034
C	-0.515302	-1.222718	-0.234119
O	-1.128375	-1.854185	-1.108079
H	-0.28921	-2.17553	2.329861
H	-1.821557	-1.526575	2.948446

H	-1.828388	-2.727257	1.631423
N	0.800242	-0.978398	-0.34367
C	1.544998	-1.492847	-1.509851
C	1.693359	-0.373487	0.651001
H	1.387914	-0.631701	1.668903
C	3.047054	-1.001169	0.290998
C	1.770535	1.155375	0.583574
O	2.641102	1.743314	1.249384
H	3.883305	-0.417662	0.678992
H	3.090938	-2.009366	0.715023
C	2.986262	-1.063146	-1.236419
H	3.174784	-0.070157	-1.659852
H	3.707094	-1.762324	-1.664568
H	1.129931	-1.07756	-2.431727
H	1.441798	-2.582879	-1.54333
N	0.889776	1.802538	-0.17996
H	0.100675	1.298339	-0.58066
C	0.836392	3.255802	-0.19068
H	0.022354	3.562158	-0.847348
H	0.657738	3.64847	0.814961
H	1.775026	3.669667	-0.567213

(f) AtAu

H	1.855895	2.007473	2.571647
H	3.11425	2.848022	1.656676
H	3.404799	1.186837	2.235053
C	2.653976	1.871765	1.836584
O	1.115063	1.998176	-0.0036
C	2.047073	1.385113	0.551488
N	2.546328	0.260653	0.014615
H	3.244093	-0.267074	0.529869
C	1.99829	-0.312829	-1.202046
H	2.135283	0.407882	-2.014583
C	2.723112	-1.608793	-1.554383
C	0.484712	-0.537162	-1.163332
O	-0.154906	-0.376059	-2.217391
H	2.318873	-2.013035	-2.485643
H	3.788836	-1.408421	-1.697336
H	2.607341	-2.359855	-0.766755
N	-0.132014	-0.917314	-0.030533
C	0.456053	-1.312812	1.264379
C	-1.589705	-1.092366	-0.034436
H	-1.873159	-1.803719	-0.816569
C	-1.907228	-1.642362	1.371865
C	-2.378739	0.184115	-0.281592
O	-3.586996	0.093774	-0.569111
H	-2.170035	-0.815495	2.041631
H	-2.74372	-2.342321	1.343015
C	-0.58978	-2.275452	1.81792
H	-0.514767	-2.379917	2.902491
H	-0.46245	-3.261918	1.359705
H	0.56262	-0.433608	1.913308
H	1.43113	-1.779203	1.129399
N	-1.767544	1.354039	-0.094467
H	-0.760201	1.38253	0.054635
C	-2.479056	2.609974	-0.264487
H	-2.87139	2.703202	-1.281394
H	-3.31107	2.679109	0.441371
H	-1.78125	3.425604	-0.074769

(g) AtBd

H	3.055	3.172576	1.054767
H	3.245893	1.739804	2.099417
H	1.686542	2.60758	2.02394
C	2.557208	2.281084	1.447985
O	1.241549	1.881955	-0.52222
C	2.08149	1.450175	0.290343
N	2.586972	0.212565	0.165109
H	3.188207	-0.152495	0.896873
C	2.165139	-0.67874	-0.90071
H	2.490449	-0.254776	-1.856002
C	2.797077	-2.056529	-0.723784
C	0.647601	-0.813238	-1.054967
O	0.191256	-0.87552	-2.209504
H	2.498272	-2.704829	-1.551411
H	3.887226	-1.968233	-0.730511
H	2.485956	-2.520318	0.217048
N	-0.156217	-0.922717	0.020412
C	0.205364	-0.91736	1.458524
C	-1.593397	-1.133374	-0.166679
H	-1.7711	-1.732827	-1.062656
C	-2.001699	-1.863449	1.116392
C	-2.378473	0.16697	-0.344503
O	-3.61712	0.113247	-0.456279
H	-3.07063	-1.772439	1.318049
H	-1.754255	-2.924083	1.011467
C	-1.122814	-1.198904	2.176442
H	-1.576616	-0.25548	2.497374
H	-0.975949	-1.822596	3.06054
H	0.610291	0.049987	1.760553
H	0.953834	-1.689821	1.655304
N	-1.704818	1.317873	-0.374555
H	-0.68793	1.314937	-0.317078
C	-2.390145	2.588529	-0.546325
H	-2.946393	2.606206	-1.487639
H	-3.088311	2.763612	0.276997
H	-1.641636	3.380708	-0.556073

(h) ts

H	-5.601762	-0.117427	1.104679
H	-5.405889	-0.881125	-0.495614
H	-5.352056	0.893555	-0.326092
C	-5.08346	-0.057131	0.143694
O	-3.05992	0.760826	1.149422
C	-3.602188	-0.067012	0.396523
N	-2.873322	-1.01285	-0.224359
H	-3.319272	-1.656284	-0.869152
C	-1.440961	-1.073088	-0.032677
H	-1.22003	-1.212611	1.03015

C	-0.841347	-2.224073	-0.840796
C	-0.765413	0.213846	-0.479519
O	-1.206774	0.912586	-1.36725
H	0.245183	-2.247239	-0.720602
H	-1.249206	-3.175634	-0.489388
H	-1.073295	-2.10268	-1.903909
N	0.473325	0.495955	0.182403
C	0.428668	1.806752	0.907381
C	1.620734	0.523026	-0.759626
H	1.318673	0.183906	-1.756996
C	2.107018	1.979262	-0.772755
C	2.736104	-0.420262	-0.31129
O	3.784024	-0.497576	-0.981064
H	3.159601	2.063697	-1.052046
H	1.504991	2.549178	-1.488253
C	1.799607	2.430582	0.653526
H	2.542286	2.028217	1.351656
H	1.773155	3.517031	0.766645
H	0.213696	1.638959	1.965352
H	-0.357574	2.442898	0.483021
N	2.536025	-1.126218	0.800324
H	1.623491	-1.034175	1.236219
C	3.512321	-2.081079	1.29161
H	4.466374	-1.585708	1.490901
H	3.136244	-2.514846	2.217496
H	3.678054	-2.879546	0.562061

Ac-Ala-ψ(CS–NH)Pro-NHMe

(a) FtAu

H	-5.542907	0.069467	-0.959206
H	-4.999629	-1.466296	-0.220244
H	-4.423654	-0.987993	-1.834232
C	-4.702665	-0.618449	-0.841186
O	-3.20762	1.253125	-0.694822
C	-3.525078	0.127473	-0.279631
N	-2.822463	-0.485434	0.697576
H	-2.991211	-1.475605	0.84604
C	-1.53971	0.041017	1.111136
H	-1.698996	1.087966	1.371178
C	-1.031819	-0.714767	2.338327
C	-0.483204	-0.056741	0.002502
S	-0.550835	-1.275311	-1.15351
H	-0.071435	-0.308238	2.669255
H	-1.749179	-0.617744	3.157775
H	-0.897268	-1.776481	2.104648
N	0.521651	0.815344	0.071395
C	0.64516	1.981018	0.97761
C	1.690348	0.723239	-0.816178
H	1.35206	0.719604	-1.855818
C	2.53491	1.974422	-0.491077
C	2.51891	-0.538101	-0.606338
O	3.259019	-0.937735	-1.520561
H	3.341382	1.715291	0.202503
H	2.981813	2.387386	-1.396603
C	1.545162	2.921986	0.186932
H	2.034388	3.653563	0.833328
H	0.949344	3.455693	-0.560396
H	1.113829	1.66375	1.91716
H	-0.329727	2.417241	1.189013
N	2.501808	-1.102417	0.604622
H	1.824469	-0.782433	1.28778
C	3.288092	-2.289334	0.897056
H	3.005079	-3.11648	0.238646
H	4.353685	-2.083979	0.766707
H	3.102507	-2.57588	1.931616

(b) FtFu

H	-4.229555	-1.805124	-1.624588
H	-5.430303	-0.533203	-1.341714
H	-4.994142	-1.662156	-0.024969
C	-4.617532	-1.099542	-0.881672
O	-3.135082	0.75285	-1.260046
C	-3.505962	-0.160752	-0.505122
N	-2.92197	-0.359801	0.694428
H	-3.122694	-1.226477	1.182583
C	-1.703201	0.339292	1.039229
H	-1.910415	1.405931	0.945874
C	-1.311952	0.027573	2.48329
C	-0.532226	-0.042484	0.124414
S	-0.409144	-1.596095	-0.508561
H	-0.400392	0.566559	2.75579
H	-2.112852	0.335642	3.161171
H	-1.132583	-1.045826	2.606586
N	0.396007	0.890682	-0.055679
C	0.310328	2.310535	0.359765
C	1.688259	0.60406	-0.692122
H	1.522081	0.292503	-1.728852
C	2.458115	1.935735	-0.610305
C	2.452794	-0.47448	0.067734
O	2.387188	-0.565361	1.303027
H	3.064676	1.952837	0.301897
H	3.117685	2.062369	-1.470655
C	1.354763	2.986297	-0.519336
H	1.699907	3.929367	-0.090757
H	0.930237	3.183809	-1.509045
H	0.553241	2.397544	1.42543
H	-0.691279	2.701815	0.183118
N	3.281652	-1.217787	-0.671286
H	3.225175	-1.148314	-1.68072
C	4.105481	-2.257419	-0.077707
H	4.795345	-1.830392	0.654442
H	3.483681	-3.009218	0.417904
H	4.678618	-2.73462	-0.871625

(c) FcBd

H	-4.318762	2.243054	-0.611699
H	-4.836598	0.760009	0.242483
H	-4.332128	0.691787	-1.464221

C	-4.145708	1.17037	-0.496615
O	-1.7833	1.500938	-0.748722
C	-2.706393	0.938487	-0.13528
N	-2.46118	0.091358	0.881544
H	-3.234862	-0.463861	1.2318
C	-1.11846	-0.367797	1.176527
H	-0.521475	0.514508	1.424531
C	-1.166032	-1.308242	2.379872
C	-0.487738	-1.091289	-0.024495
S	-1.425019	-2.042491	-1.041268
H	-0.170925	-1.695416	2.613643
H	-1.545688	-0.77179	3.253904
H	-1.824505	-2.156432	2.165421
N	0.829082	-0.966915	-0.17106
C	1.570734	-1.674041	-1.237884
C	1.760638	-0.259687	0.729415
H	1.432933	-0.326724	1.769178
C	3.07248	-1.018073	0.501945
C	1.934291	1.230406	0.407201
O	2.85148	1.855377	0.964385
H	3.937819	-0.438323	0.825663
H	3.038936	-1.954061	1.068371
C	3.03038	-1.295493	-0.999918
H	3.288236	-0.388994	-1.558668
H	3.708097	-2.094214	-1.307212
H	1.184892	-1.371669	-2.214602
H	1.398744	-2.749252	-1.120581
N	1.091261	1.803377	-0.454233
H	0.238421	1.3179	-0.726055
C	1.124183	3.241632	-0.673907
H	0.935971	3.785569	0.257087
H	2.098022	3.541981	-1.067111
H	0.353325	3.492885	-1.401866

(d) EcBd

H	-4.660613	1.636564	-1.164889
H	-5.378872	0.51234	-0.002896
H	-4.533817	-0.123428	-1.437466
C	-4.534039	0.664224	-0.681432
O	-3.06295	1.57234	0.983001
C	-3.268468	0.688413	0.132302
N	-2.381683	-0.291938	-0.108746
H	-2.610597	-1.033653	-0.764867
C	-1.159022	-0.43684	0.660172
H	-0.797137	0.575788	0.852509
C	-1.419493	-1.146163	1.995696
C	-0.124749	-1.229362	-0.136766
S	-0.597641	-2.491468	-1.141625
H	-0.500003	-1.238735	2.581912
H	-2.14604	-0.569138	2.574613
H	-1.822302	-2.146679	1.811313
N	1.151831	-0.915844	0.064503
C	2.262767	-1.666556	-0.558423
C	1.652957	0.18004	0.911567
H	1.086015	0.253138	1.841731
C	3.106339	-0.236587	1.176468
C	1.585039	1.55315	0.237161
O	1.86179	2.558767	0.910034
H	3.726334	0.618006	1.454363
H	3.113957	-0.960226	1.997335
C	3.518745	-0.906808	-0.1344
H	3.779071	-0.152271	-0.883444
H	4.371388	-1.577873	-0.01491
H	2.115165	-1.705728	-1.640672
H	2.242722	-2.691895	-0.17338
N	1.2447	1.618765	-1.052239
H	1.035662	0.766082	-1.558687
C	1.155336	2.89287	-1.749247
H	2.112332	3.419281	-1.707409
H	0.897766	2.695008	-2.78882
H	0.3841	3.522873	-1.297827

(e) ts

H	-5.402475	0.498399	-1.372656
H	-5.185466	1.227691	0.244488
H	-5.199249	-0.541566	0.046653
C	-4.892682	0.405129	-0.410788
O	-2.90821	-0.372929	-1.517873
C	-3.408604	0.354136	-0.64393
N	-2.638898	1.124267	0.149212
H	-3.072423	1.630837	0.913961
C	-1.194893	1.049847	0.089712
H	-0.87328	1.258278	-0.936232
C	-0.596205	2.091138	1.039478
C	-0.644487	-0.327639	0.445376
S	-1.333681	-1.305656	1.549573
H	0.496352	2.052108	1.030603
H	-0.905699	3.093572	0.730277
H	-0.942711	1.905677	2.061692
N	0.560498	-0.642072	-0.250969
C	0.501707	-1.896671	-1.04796
C	1.792512	-0.661178	0.575477
H	1.55656	-0.631364	1.64525
C	2.511275	-1.972733	0.198481
C	2.685021	0.546013	0.303973
O	3.657293	0.772708	1.049022
H	3.598447	-1.870856	0.243074
H	2.206716	-2.758699	0.896951
C	1.966922	-2.278929	-1.19624
H	2.452894	-1.6528	-1.952481
H	2.088381	-3.326941	-1.480717
H	-0.007712	-1.70899	-1.997004
H	-0.041813	-2.678131	-0.500312
N	2.390305	1.304651	-0.752018
H	1.525025	1.086112	-1.237024
C	3.110801	2.533157	-1.032326
H	4.17106	2.325829	-1.198618
H	2.692488	2.983783	-1.931813
H	3.017595	3.237793	-0.199563

Ac-Ala-ψ(CSe–NH)Pro-NHMe

(a) FtAu

H	-5.368636	0.279064	-0.957665
H	-4.977427	-1.0389	0.187074
H	-4.288506	-1.036902	-1.452223
C	-4.588975	-0.402234	-0.61066
O	-2.989501	1.381291	-0.806519
C	-3.386836	0.387909	-0.1788
N	-2.744431	-0.046387	0.929068
H	-2.970978	-0.977513	1.266026
C	-1.432547	0.47079	1.252107
H	-1.532247	1.550688	1.364208
C	-0.942598	-0.129386	2.569932
C	-0.40309	0.156836	0.165786
Se	-0.519808	-1.398671	-0.7784
H	0.032958	0.288272	2.837092
H	-1.650757	0.104022	3.369539
H	-0.846814	-1.216961	2.479002
N	0.591588	1.011501	0.016744
C	0.717175	2.351041	0.644755
C	1.754142	0.733196	-0.846965
H	1.406023	0.567034	-1.870328
C	2.635319	1.991035	-0.735244
C	2.533587	-0.506404	-0.420395
O	3.215685	-1.113796	-1.260747
H	3.398369	1.849324	0.037382
H	3.135818	2.199526	-1.681964
C	1.65379	3.080972	-0.308776
H	2.14468	3.927581	0.174829
H	1.086656	3.446169	-1.170977
H	1.154476	2.237507	1.64359
H	-0.256361	2.831713	0.726356
N	2.540322	-0.824281	0.878751
H	1.89657	-0.351959	1.503725
C	3.225865	-2.013962	1.355712
H	2.843375	-2.908011	0.852436
H	4.300412	-1.938499	1.171852
H	3.049042	-2.101892	2.427131

(b) FtFu

H	-4.186878	-1.503211	-1.509002
H	-5.361655	-0.203133	-1.241421
H	-4.947643	-1.32361	0.089674
C	-4.560486	-0.780762	-0.774915
O	-3.014482	1.011777	-1.188738
C	-3.427541	0.136004	-0.412431
N	-2.865776	-0.041815	0.803961
H	-3.080397	-0.89944	1.303103
C	-1.616643	0.615739	1.120036
H	-1.782153	1.688836	1.020398
C	-1.205701	0.305081	2.55934
C	-0.481917	0.181368	0.192198
Se	-0.410034	-1.542834	-0.406152
H	-0.281611	0.832579	2.812046
H	-1.99177	0.633656	3.244957
H	-1.043235	-0.770691	2.686966
N	0.441188	1.077913	-0.081151
C	0.383599	2.521006	0.260741
C	1.729262	0.739436	-0.706424
H	1.555741	0.375156	-1.724413
C	2.520412	2.060322	-0.694053
C	2.466876	-0.307319	0.126074
O	2.339275	-0.356739	1.358937
H	3.131271	2.113687	0.213881
H	3.17846	2.128846	-1.56191
C	1.435147	3.132296	-0.655202
H	1.79745	4.088724	-0.273646
H	1.010944	3.288206	-1.65217
H	0.635875	2.650068	1.319628
H	-0.61513	2.913667	0.070874
N	3.341866	-1.064603	-0.540387
H	3.34752	-1.03138	-1.553399
C	4.162154	-2.04835	0.146925
H	4.733845	-1.57007	0.945601
H	3.539959	-2.837821	0.579899
H	4.850312	-2.487419	-0.574196

(c) FcBd

H	-3.631552	3.148642	-0.66532
H	-4.34363	1.910985	0.411302
H	-3.945305	1.515937	-1.278813
C	-3.633891	2.08921	-0.398655
O	-1.262218	1.969973	-0.74745
C	-2.238866	1.662945	-0.04473
N	-2.095827	0.918955	1.071757
H	-2.936345	0.52685	1.485213
C	-0.844968	0.249293	1.364821
H	-0.078902	1.023663	1.462103
C	-0.980312	-0.508985	2.685063
C	-0.443265	-0.719993	0.248193
Se	-1.725094	-1.639898	-0.662613
H	-0.060131	-1.049609	2.922433
H	-1.189817	0.196616	3.493363
H	-1.799153	-1.232947	2.61739
N	0.844988	-0.908689	0.039207
C	1.366948	-1.87571	-0.956063
C	1.958861	-0.290243	0.789683
H	1.695637	-0.149019	1.840538
C	3.082611	-1.316736	0.617361
C	2.38706	1.076268	0.240659
O	3.428433	1.589135	0.679566
H	4.060942	-0.876197	0.813658
H	2.917093	-2.141257	1.317508
C	2.884725	-1.780878	-0.825087
H	3.287041	-1.037014	-1.521014
H	3.362054	-2.740118	-1.033575
H	0.985833	-1.615579	-1.946702
H	0.99011	-2.868858	-0.690843

N	1.628152	1.660166	-0.688619
H	0.69206	1.306357	-0.871586
C	1.914844	3.014557	-1.134236
H	1.85503	3.722342	-0.301383
H	2.916413	3.06502	-1.567216
H	1.182441	3.286459	-1.893597

(d) EcBd

H	-4.399754	2.285604	-1.250417
H	-5.190574	1.477354	0.110881
H	-4.493474	0.50376	-1.210374
C	-4.366826	1.403368	-0.605291
O	-2.745106	2.380133	0.868126
C	-3.070738	1.411932	0.158945
N	-2.285814	0.328934	0.023253
H	-2.623475	-0.477735	-0.496088
C	-1.0669	0.163298	0.7953
H	-0.580119	1.140799	0.815465
C	-1.371867	-0.287066	2.232249
C	-0.155785	-0.867462	0.143899
Se	-0.863007	-2.349419	-0.645114
H	-0.452501	-0.412354	2.812927
H	-1.993835	0.468501	2.720067
H	-1.911255	-1.238749	2.212556
N	1.146148	-0.695574	0.273219
C	2.145949	-1.681197	-0.198422
C	1.80398	0.449113	0.931241
H	1.256839	0.75724	1.823835
C	3.186029	-0.110796	1.28833
C	1.920192	1.678368	0.026403
O	2.396015	2.721342	0.500826
H	3.91824	0.685824	1.431584
H	3.099863	-0.681236	2.218068
C	3.495001	-1.03732	0.112478
H	3.849631	-0.459209	-0.746878
H	4.248823	-1.788967	0.353526
H	1.985217	-1.880218	-1.260771
H	1.986564	-2.612691	0.355637
N	1.512622	1.584422	-1.241686
H	1.148419	0.705355	-1.591882
C	1.610906	2.720197	-2.145557
H	2.656317	3.002406	-2.297724
H	1.171901	2.437199	-3.101247
H	1.067792	3.576488	-1.73786

(e) ts

H	5.042959	0.967422	1.72041
H	4.898218	1.654937	0.075092
H	4.858603	-0.105984	0.320638
C	4.563383	0.860506	0.745239
O	2.522664	0.247536	1.856661
C	3.071571	0.847616	0.919653
N	2.343954	1.50338	-0.010761
H	2.814983	1.819152	-0.852791
C	0.904446	1.342069	-0.051457
H	0.487211	1.693852	0.897392
C	0.329173	2.171672	-1.201939
C	0.482341	-0.111095	-0.205786
Se	1.381297	-1.252642	-1.200876
H	-0.754585	2.041672	-1.272488
H	0.541146	3.231446	-1.033712
H	0.780792	1.855126	-2.148387
N	-0.694084	-0.455338	0.508986
C	-0.510096	-1.565274	1.479742
C	-1.88797	-0.753599	-0.32111
H	-1.609655	-0.957998	-1.361294
C	-2.530736	-1.9986	0.333448
C	-2.867469	0.412191	-0.365402
O	-3.791287	0.406595	-1.201513
H	-3.622563	-1.952461	0.312017
H	-2.21331	-2.891589	-0.213297
C	-1.936712	-2.013186	1.743193
H	-2.449622	-1.296856	2.39397
H	-1.976475	-3.000974	2.208911
H	0.014449	-1.196371	2.364968
H	0.071709	-2.38131	1.031014
N	-2.702392	1.389825	0.525437
H	-1.868191	1.33839	1.101859
C	-3.506899	2.598159	0.492868
H	-4.558323	2.366346	0.68201
H	-3.147064	3.27448	1.267649
H	-3.423935	3.089695	-0.481676