Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

An intraresidue H-bonding motif in selenocysteine and cysteine, revealed by gas phase laser spectroscopy and quantum chemistry calculations

G. Goldsztejn, V. Mundlapati, J. Donon, B. Tardivel, E. Gloaguen, V. Brenner and M. Mons*

Université Paris-Saclay, CEA, CNRS, LIDYL, 91191, Gif-sur-Yvette, France

Supplementary Information

Content

Fig. S1: H-bonding schemes in conformers A (5^{γ}-7-7) and B (5^{γ}-π-10) of the Ac-Cys-Phe-NH_2 and Ac-Sec-Phe-NH_2 molecules and of their truncated models.

Table S1: Structural parameters of the most stable theoretical conformations of Ac-Sec-Phe-NH_2

Table S2: Relevant NBO parameters for the 5^{γ} bonds of conformations A and B of the dipeptides, of the intrinsic models and for the H-bonds of the relevant intermolecular complexes of the Cys, Sec and Ser residues.

Table S3: Interatomic NH…Y distance (pm) and calculated raw harmonic NH stretch frequency frequency (cm^{-1}) for the 5^{γ} H-bond in conformations A and B of the dipeptides, in the intrinsic models and for the H-bonds of the relevant intermolecular complexes of the Cys, Sec and Ser residues.

Tables S4-S6 : RI-B97-D3(BJ)-abc/def2-TZVPPD structures of conformations A and B of the dipeptides, of the intrinsic models and of the relevant intermolecular complexes of the Cys, Sec and Ser residues.

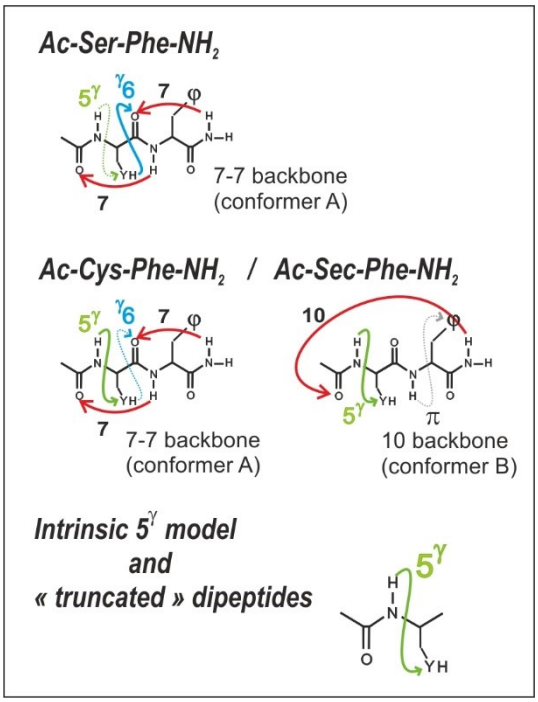

Figure S1 : Scheme of the H-bonding in conformers A (5^{γ}-7-7) and B (5^{γ}-π-10) of the Ac-Cys-Phe-NH_2 and Ac-Sec-Phe-NH_2 molecules, together with a truncated version of these molecules, in which the carbonyl of the first peptide bond is not a H-bond acceptor itself. For this purpose the C-terminal peptide link has been changed into a simple methyl group (bottom line); the Me group alone been optimized and the rest of the molecule being frozen. The intrinsic model is an optimized structure of the truncated dipeptide. Depending on the balance between proton donating and accepting properties of Ser and Cys, $^{\gamma}6$ and 5^{γ} side chain - main chain H-bonds are observed with various relative strengths, as determined from NH stretch spectral shifts (strong and weak H-bonds are figured by full and dotted arrow lines respectively).

Table S1: Structural parameters of the most stable theoretical conformations (a-j, see Table 1) of Ac-Sec-Phe-NH2 at the RI-B97-D3(BJ)-abc/def2-TZVPPD level : Ramachandran dihedral angles (ϕ and ψ) and side chain dihedrals of the Sec and Phe residues (in degrees)*; distances between i) the NH hydrogen of the Sec residue and the side chain Se atom (NH…Se) and ii) the H atom of the SeH group and the carbonyl acceptor oxygen atom of the Sec residue (SeH···OC), both given in pm. The a, g+ and g- notations correspond to the* anti, gauche+ *and* gauche- *orientations of the Sec (χ_{Sec}) and Phe (χ_{Phe}) side chains with respect to the backbone.*

		ϕ_{sec}	ψ_{sec}	χ_{sec}	ϕ_{phe}	ψ_{phe}	χ_{phe}	SeH-OC (pm)	NH-Se (pm)
a	5^{γ}-π-10-g+g+	-70	-9	56	-94	3	52	338	274
b	5^{γ}-f-7-g+g-	-95	-7	52	-87	70	-56	339	267
c	5-π-9^{γ}-ag+	-154	135	-175	-99	2	55	434	268
d	5^{γ}-f-10-g+g-	-70	-11	56	-97	1	-54	340	275
e	5-6^{γ}/π-9^{γ}-ag+	-157	148	-171	-88	-7	55	425	265
f	5-π-9^{γ}-ag+	-90	106	-179	-101	4	57	290	305
g	5^{γ}-5-π-g+a	-99	4	57	-162	160	-171	311	279
h	5^{γ}-7-7-g+g-	-140	41	58	-168	164	46	456	318
i	5^{γ}-7-7-g+g-	-83	55	52	-88	70	-60	251	266
j	5^{γ}-π-10-g-g+	-69	-20	-54	-82	-1	53	489	273

Table S2 : Detailed parameters of the NBO(i)→NBO(j) interactions at play in the 5^{γ} motif in the 5^{γ} H-bond in conformers A (γ-turns) and B (β-turns) of the Ac-Ser/Cys/Sec-Phe-NH_2 capped dipeptides, in the truncated version of these conformers centered on the Cys/Sec residue frozen in the geometry of the dipeptide (See Figure S1), in the optimized version of the truncated model, providing an intrinsic model for the 5^{γ} interaction, and in the corresponding intermolecular *trans-N*-methylacetamide---Me-YH (Y = Se, S and O) **complexes. Interaction energies E(2) and NBO energy difference Δε are given in kcal/mol ; NBO occupancy is close to 2 for the donor NBOs considered; the off-diagonal NBO Fock matrix elements F(i,j) are given in atomic units.**

	Sec					
	Intrinsic 5^{γ} model	5^{γ} model geom. A	Ac-Cys-Phe-NH_2 A 7-7	5^{γ} model geom. B	Ac-Cys-Phe-NH_2 B 10	MAA-Me-SeH complex
	5^{γ} H-bond					Intermolec.
$E_{(2)}(n_{S/Se}\rightarrow\sigma^*_{NHi})$	0.13	0.31	0.29	0.19	0.19	0.21
$n_{S/Se}$ occup.	1.961	1.960	1.960	1.961	1.960	1.962
F(i,j)	0.012	0.019	0.018	0.015	0.015	0.016
Δε	1.45	1.45	1.43	1.45	1.44	1.46
$E_{(2)}(n'_{S/Se}\rightarrow\sigma^*_{NHi})$	1.00	2.31	2.55	1.42	1.51	5.54
$n'_{S/Se}$ occup	1.919	1.915	1.912	1.918	1.914	1.916
F(i,j)	0.028	0.043	0.044	0.033	0.034	0.067
Δε	0.98	0.98	0.96	0.98	0.97	1.01
ΣE_{HB} *: Sum of E(2)*	*1.13*	*2.62*	*2.84*	*1.61*	*1.70*	*5.75*

	Cys						
	Intrinsic 5^{γ} model	5^{γ} model geom. A	Ac-Cys-Phe-NH_2 A 7-7	5^{γ} model geom. B	Ac-Cys-Phe-NH_2 B 10	MAA-Me-SH complex	
	5^{γ} H-bond					Intermolec.	
$E_{(2)}(n_{S/Se}\rightarrow\sigma^*_{NHi})$	0.13	0.28	0.29	0.18	0.19	0.36	
$n_{S/Se}$ occup.	1.956	1.956	1.956	1.956	1.956	1.957	
F(i,j)	0.012	0.018	0.018	0.015	0.015	0.021	
Δε	1.43	1.43	1.41	1.43	1.42	1.44	
$E_{(2)}(n'_{S/Se}\rightarrow\sigma^*_{NHi})$	0.88	1.86	2.09	1.17	1.15	5.93	
$n'_{S/Se}$ occup	1.911	1.908	1.905	1.910	1.908	1.909	
F(i,j)	0.027	0.039	0.041	0.031	0.030	.070	
Δε	1.01	1.01	0.99	1.01	0.99	1.04	
ΣE_{HB} *: Sum of E(2)*	*1.01*	*2.14*	*2.38*	*1.35*	*1.34*	*6.29*	

	Ser				
	Intrinsic 5^{γ} model	5^{γ} model geom. A	Ac-Ser-Phe-NH_2 A 7-7		MAA-Me-OH complex
	5^{γ} H-bond				Intermolec.
$E_{(2)}(n_{S/Se} \rightarrow \sigma^*_{NHi})$	< 0.05	< 0.05	< 0.05		3.19
$n_{S/Se}$ occup.	-	-	-		1.9
F(i,j)	-	-	-		0.063
$\Delta\varepsilon$	-	-	-		1.56
$E_{(2)}(n'_{S/Se} \rightarrow \sigma^*_{NHi})$	0.18	0.21	0.26		1.92
n'_O occup	1.923	1.922	1.918		1.
F(i,j)	0.013	0.014	0.015		0.043
$\Delta\varepsilon$	1.14	1.14	1.12		1.21
ΣE_{HB} *: Sum of E(2)*	*0.18*	*0.21*	*0.26*		*5.11*

Table S3 : Interatomic NH…Y distance (pm) and calculated raw harmonic NH stretch frequency (cm^{-1}) for the 5^{γ} H-bond in conformers A (γ-turns) and B (β-turns) of the Ac-Ser/Cys/Sec-Phe-NH_2 capped dipeptides, in the truncated version of these conformers centered on the Cys/Sec residue frozen in the geometry of the dipeptide (See Figure S1) and in the optimized version of the truncated model, providing an intrinsic model for the 5^{γ} interaction. Scaled frequencies for the intrinsic 5^{γ} motifs have been obtained using the procedure presented in Section 2, in order to provide a spectroscopic benchmark signature comparable to the experimental frequencies observed (Figure 8). For the sake of comparison the intermolecular H-bond in the fully optimized *trans*-methylacetamide – Me-YH complex is also provided.

Y	**O**				**S**				**Se**		
	NH…O	raw	scaled		NH…S	raw	scaled		NH…Se	raw	scaled
NH ··· Y											
In γ-turn env. (5^{γ}-7-7)	246	3550			259	3497			266	3481	
Truncated γ-turn	246	3549			259	3500			266	3483	
In β-turn env. (5^{γ}-π-10)	-	-			265	3513			274	3503	
Truncated β-turn	-	-			265	3515			274	3506	
Intrinsic 5^{γ} NH ··· Y	248	3564	3472		272	3533	3445		282	3528	3440
Intermolecular NH ··· Y											
trans-N-MAA ··· CH_3-YH	204	3501			254	3469			266	3472	

Table S4 : RI-B97-D3(BJ)-abc/def2-TZVPPD structures of conformations A and B of Ac-Cys-Phe-NH_2 , of the intrinsic Cys 5$^{\gamma}$ model and of the *trans*-*N*-methylacetamide···Me-SH intermolecular complex; xyz format, coordinates in Å.

Dipeptide Conformation A			Conformation B		
H	2.3799619	-2.0777625 -0.7104681	H	-0.0965168	1.7931385 -2.2115821
C	1.6623768	-2.6884212 -1.2676071	C	0.5200480	1.1496673 -2.8483544
H	2.0893827	-2.8959303 -2.2508058	H	0.1418824	1.2277996 -3.8699350
H	1.5019056	-3.6261667 -0.7289950	H	1.5519637	1.5081182 -2.8093075
C	0.3953114	-1.8823404 -1.4462568	C	0.3628143	-0.2812028 -2.3782302
O	0.2975786	-0.9846194 -2.2896029	O	-0.6666616	-0.9285629 -2.5708691
N	-0.6223447	-2.1941585 -0.6010314	N	1.4206967	-0.8001160 -1.6883957
H	-0.4790768	-2.8530131 0.1549186	H	2.2095545	-0.2117168 -1.4528159
C	-1.9206543	-1.5372840 -0.6228175	C	1.4101495	-2.1398214 -1.1286979
H	-2.1425683	-1.3079370 -1.6729362	H	0.9978862	-2.8213024 -1.8814894
C	-1.9065781	-0.1850218 0.1328041	C	0.4912162	-2.3301434 0.1031198
O	-2.6151911	0.0281869 1.1247995	O	0.3040056	-3.4519234 0.5571966
C	-3.0043519	-2.4798992 -0.0959555	C	2.8324617	-2.6011152 -0.7967342
H	-3.9529417	-1.9465982 -0.0262424	H	2.7847241	-3.5905408 -0.3410695
H	-3.1230054	-3.3155683 -0.7900772	H	3.4330698	-2.6625092 -1.7081368
S	-2.6363568	-3.2552225 1.5226504	S	3.7616175	-1.4606106 0.2984556
H	-2.6564652	-2.1014073 2.2149453	H	2.9417919	-1.5718296 1.3600753
N	-1.0727712	0.7260428 -0.4036158	N	-0.0504910	-1.1927747 0.5979771
H	-0.5409330	0.4453657 -1.2291680	H	0.1971948	-0.3204928 0.1538419
C	-0.8126208	2.0275948 0.2081824	C	-1.0624668	-1.1399512 1.6317207
H	-0.9114216	1.8907908 1.2902491	H	-0.9751021	-2.0534541 2.2261834
C	-1.8904157	3.0582554 -0.2311570	C	-2.5156227	-1.1335775 1.0937371
O	-1.6488098	3.9916614 -0.9825830	O	-3.4494759	-1.0554560 1.8850895
C	0.5942215	2.5121793 -0.1421804	C	-0.8217694	0.0925080 2.5380141
H	0.6511806	2.6841544 -1.2208461	H	-1.6617218	0.1516744 3.2337009
H	0.7280679	3.4945131 0.3239898	H	0.0914837	-0.0830348 3.1145005
C	1.6899573	1.5704443 0.3001470	C	-0.6901758	1.3643377 1.7355166
C	2.6118107	1.0674196 -0.6238112	C	0.5735970	1.8554276 1.3770850
H	2.5137797	1.3333919 -1.6726120	H	1.4643681	1.3492636 1.7424032
C	1.8244535	1.1966257 1.6445563	C	-1.8263045	2.0379389 1.2639536
H	1.1240615	1.5786140 2.3835376	H	-2.8116749	1.6698641 1.5344396
C	3.6503342	0.2270545 -0.2173848	C	0.7030272	2.9851898 0.5669481
H	4.3601624	-0.1441210 -0.9516719	H	1.6917818	3.3529651 0.3064736
C	2.8511600	0.3474361 2.0538856	C	-1.6998849	3.1653520 0.4533145
H	2.9385738	0.0721836 3.1013995	H	-2.5912337	3.6759196 0.0994889
C	3.7725191	-0.1387632 1.1230862	C	-0.4355567	3.6423166 0.0999447
H	4.5787292	-0.7935878 1.4416850	H	-0.3395279	4.5240050 -0.5274053
N	-3.1120416	2.8175414 0.3160144	N	-2.6714307	-1.2170948 -0.2467856
H	-3.2751309	1.9606213 0.8340292	H	-1.9059231	-1.2609153 -0.9086023
H	-3.8918496	3.3777457 0.0069461	H	-3.6137942	-1.2373405 -0.6047695

intrinsic Cys 5$^{\gamma}$ model			*trans*-methylacetamide···Me-SH complex		
H	-1.7158225	2.8451365 -1.3375819	C	1.6498138	1.2226425 0.5446049
C	-0.8043329	2.3355539 -1.6645629	H	0.7778380	1.8222348 0.2678526
H	-0.7587025	2.4136364 -2.7541199	C	1.2933242	-0.1558073 1.0836857
H	0.0626057	2.8415535 -1.2302110	O	2.1454544	-0.9284400 1.5132021
C	-0.9075943	0.8667590 -1.2855050	N	-0.0313433	-0.4712900 1.0516982
O	-1.7723187	0.1335066 -1.7547843	H	-0.6895879	0.1814416 0.6431595
N	0.0301497	0.4269747 -0.3943032	C	-0.5195500	-1.7611220 1.5070190
H	0.6747154	1.0829561 0.0246484	H	2.2966225	1.1009842 -0.3297053
C	0.0407901	-0.9284931 0.1368084	H	2.2253576	1.7567164 1.3052507
H	-0.4113454	-1.5577626 -0.6381607	H	-0.0250153	-2.5791503 0.9721745
C	-0.8073533	-1.0468638 1.4067286	H	-1.5960135	-1.8096747 1.3270556
C	1.4863054	-1.4070851 0.3217486	H	-0.3284101	-1.8996638 2.5764775
H	1.4988753	-2.4274432 0.7122937	C	-0.7713004	0.6112386 -2.3371586
H	2.0019845	-1.4068754 -0.6425367	H	-0.0359145	1.4133462 -2.4236175
S	2.5421362	-0.3479233 1.3874710	H	-1.1852602	0.3995181 -3.3239734
H	1.9143920	-0.5985924 2.5497440	S	-2.0687031	1.2315619 -1.2081134
H	-0.8038737	-2.0758179 1.7826869	H	-0.2840458	-0.2734679 -1.9239639
H	-1.8390417	-0.7634251 1.1849888	H	-2.8532665	0.1389317 -1.2456484
H	-0.4315695	-0.3857948 2.1946472			

Table S5 : RI-B97-D3(BJ)-abc/def2-TZVPPD structures of conformations A and B of Ac-Sec-Phe-NH_2 , of the intrinsic Sec 5^{γ} model and of the *trans*-methylacetamide···Me-SeH intermolecular complex ; xyz format, coordinates in Å.

Conformation A				Conformation B			
H	-3.1175	3.06714	-1.13987	H	1.36052	4.11089	0.56849
C	-2.31612	2.82873	-0.43164	C	1.43352	3.04598	0.33892
H	-1.39789	3.31526	-0.77191	H	2.24975	2.87466	-0.36762
H	-2.59645	3.21795	0.54677	H	1.66509	2.51588	1.26959
C	-2.17412	1.3237	-0.34244	C	0.09135	2.56057	-0.16746
O	-2.81811	0.64443	0.4638	O	-0.97211	2.89716	0.35274
N	-1.31751	0.7656	-1.23702	N	0.13511	1.68428	-1.21505
H	-0.69996	1.35037	-1.78837	H	1.02694	1.33064	-1.53864
C	-1.14225	-0.66918	-1.40891	C	-1.05549	1.05837	-1.76175
H	-2.12154	-1.12976	-1.2164	H	-1.82101	1.8335	-1.88438
C	-0.16685	-1.29123	-0.37524	C	-1.72296	0.00365	-0.84319
O	0.80922	-1.96996	-0.71462	O	-2.81668	-0.46059	-1.13825
C	-0.73854	-0.99526	-2.84351	C	-0.77647	0.4542	-3.13635
H	-0.4978	-2.05261	-2.93636	H	-1.66997	-0.05069	-3.49953
H	-1.55187	-0.7447	-3.52741	H	-0.47879	1.22613	-3.8494
Se	0.81744	0.03343	-3.53323	Se	0.73186	-0.84656	-3.17296
H	1.75892	-0.57221	-2.57501	H	0.08429	-1.79782	-2.25024
N	-0.50419	-1.04981	0.90525	N	-1.00155	-0.33557	0.24917
H	-1.37165	-0.54152	1.07736	H	-0.0968	0.0967	0.3656
C	0.33116	-1.44768	2.03441	C	-1.45473	-1.20252	1.31542
H	1.36282	-1.45271	1.66759	H	-2.25452	-1.83179	0.91342
C	-0.0143	-2.89342	2.48145	C	-2.08172	-0.44789	2.51453
O	-0.5703	-3.14867	3.53957	O	-2.44495	-1.0781	3.50174
C	0.19065	-0.4446	3.18188	C	-0.28544	-2.09703	1.79357
H	-0.8439	-0.44751	3.5365	H	-0.63914	-2.66048	2.65996
H	0.80069	-0.80817	4.01496	H	-0.05053	-2.80455	0.99321
C	0.61389	0.94638	2.77526	C	0.94027	-1.28622	2.13976
C	1.95596	1.22482	2.48244	C	1.95473	-1.08187	1.19273
H	2.69972	0.43655	2.57698	H	1.88332	-1.56402	0.22029
C	-0.32103	1.9803	2.65803	C	1.05665	-0.65903	3.38873
H	-1.36673	1.77976	2.87598	H	0.27783	-0.80841	4.13086
C	2.35281	2.4978	2.07756	C	3.05494	-0.27242	1.48171
H	3.39854	2.69365	1.8567	H	3.83294	-0.13163	0.73619
C	0.07287	3.25974	2.2612	C	2.15485	0.14962	3.67991
H	-0.66554	4.05319	2.1864	H	2.23061	0.62341	4.65468
C	1.40989	3.52223	1.96512	C	3.1572	0.34742	2.72746
H	1.71797	4.51746	1.65735	H	4.0146	0.97322	2.95833
N	0.37554	-3.83363	1.57811	N	-2.19502	0.89476	2.39622
H	0.74244	-3.55167	0.67588	H	-1.88714	1.42209	1.58868
H	0.10601	-4.79247	1.73665	H	-2.62781	1.39449	3.15743

intrinsic Sec 5^{γ} model				*trans*-methylacetamide···Me-SeH complex			
H	-1.7387612	2.8330091	-1.3776229	C	1.6554746	1.2235244	0.5540175
C	-0.8105491	2.3372194	-1.6775528	H	0.7833998	1.8279505	0.2883833
H	-0.7301793	2.4229646	-2.7645308	C	1.2993729	-0.1669173	1.0612594
H	0.0350865	2.8512194	-1.2117159	O	2.1550758	-0.9638721	1.4352467
C	-0.9070460	0.8648369	-1.3110828	N	-0.0301163	-0.4640625	1.0671692
O	-1.7475682	0.1241822	-1.8114401	H	-0.6927918	0.2122294	0.7074677
N	0.0093981	0.4318445	-0.3942976	C	-0.5228933	-1.7600777	1.4994250
H	0.6321904	1.0951129	0.0462209	H	2.3049506	1.1216892	-0.3205063
C	0.0224971	-0.9255950	0.1317476	H	2.2279087	1.7417158	1.3281801
H	-0.4500982	-1.5443289	-0.6404812	H	-0.0217128	-2.5675250	0.9556739
C	-0.8057632	-1.0440532	1.4143602	H	-1.5973792	-1.8058880	1.3073713
C	1.4607333	-1.4244862	0.2817862	H	-0.3429931	-1.9166818	2.5686240
H	1.4814287	-2.4384705	0.6837145	C	-0.7205365	0.6036126	-2.3584437
H	1.9696508	-1.4200799	-0.6848279	H	-0.0245229	1.4277996	-2.5176437
Se	2.6492984	-0.3043012	1.4248441	H	-1.1365815	0.2808525	-3.3117028
H	1.9821623	-0.6415321	2.6954371	Se	-2.1621478	1.3311400	-1.2129149
H	-0.8006898	-2.0741074	1.7870228	H	-0.2159974	-0.2143745	-1.8456049
H	-1.8396644	-0.7549490	1.2105123	H	-2.9585098	0.0888850	-1.2060016
H	-0.4121263	-0.3884855	2.1979062				

Table S6 : RI-B97-D3(BJ)-abc/def2-TZVPPD structures of conformation A of Ac-Ser-Phe-NH_2 , of the intrinsic Ser 5$^{\gamma}$ model and of the *trans*-methylacetamide···Me-OH intermolecular complex ; xyz format, coordinates in Å.

Conformation A H 2.3913247 -2.0761613 -0.7705884 C 1.6557892 -2.6939951 -1.2951940 H 2.0516744 -2.9174455 -2.2879923 H 1.5129477 -3.6240633 -0.7384722 C 0.3848337 -1.8879793 -1.4478071 O 0.2726631 -0.9876999 -2.2870275 N -0.6210526 -2.2015724 -0.5890219 H -0.4693120 -2.8691118 0.1540564 C -1.9235778 -1.5462896 -0.6048175 H -2.1724978 -1.3381543 -1.6523429 C -1.8888138 -0.1972616 0.1510023 O -2.5486890 -0.0061898 1.1853884 C -2.9706074 -2.4857598 -0.0049503 H -3.9534422 -1.9985372 -0.0444359 H -3.0115206 -3.4038061 -0.5982182 O -2.6353070 -2.8724749 1.3250341 H -2.6795999 -2.0527172 1.8431402 N -1.0915547 0.7289645 -0.4090920 H -0.5800258 0.4533097 -1.2492902 C -0.8129276 2.0240813 0.2092933 H -0.8998496 1.8777694 1.2908976 C -1.8934165 3.0594052 -0.2086752 O -1.6618803 4.0011298 -0.9521808 C 0.5934732 2.5002521 -0.1518871 H 0.6497941 2.6565633 -1.2329982 H 0.7305011 3.4882120 0.3010603 C 1.6857774 1.5600867 0.3035698 C 2.6045347 1.0387807 -0.6129957 H 2.5057077 1.2874206 -1.6659131 C 1.8201484 1.2075110 1.6536981 H 1.1222245 1.6038878 2.3873750 C 3.6409031 0.2022054 -0.1934984 H 4.3499381 -0.1821401 -0.9217753 C 2.8442987 0.3617818 2.0760273 H 2.9315064 0.1032511 3.1277922 C 3.7633663 -0.1418964 1.1526055 H 4.5681059 -0.7935169 1.4812867 N -3.1088331 2.8061912 0.3481988 H -3.2601628 1.9510942 0.8716261 H -3.8964420 3.3648745 0.0571222	
intrinsic Ser 5$^{\gamma}$ model H 3.5204175 -0.1587470 -0.4946302 C 2.7251090 -0.8593783 -0.7660795 H 3.0187716 -1.3411085 -1.7025983 H 2.6355708 -1.6187235 0.0161772 C 1.4454712 -0.0730187 -1.0039558 O 1.3523530 0.7611618 -1.8995207 N 0.4139266 -0.3627530 -0.1582205 H 0.5533611 -1.0084596 0.6046769 C -0.8681733 0.3303805 -0.2061396 H -1.0623998 0.5604776 -1.2597027 C -0.8299338 1.6470075 0.5795947 C -1.9607497 -0.6256111 0.2798557 H -2.9363517 -0.1217953 0.2325000 H -1.9957311 -1.5049128 -0.3694883 O -1.7129611 -1.1387256 1.5976309 H -1.8520602 -0.4250962 2.2309039 H -1.7911403 2.1683582 0.5102226 H -0.0542468 2.2988998 0.1713355 H -0.6012329 1.4720444 1.6374382	*trans*-*N*-methylacetamide···Me-OH complex C -1.6722734 1.3805314 0.7688354 H -0.8674656 1.8438350 0.1914275 C -1.3453146 -0.0260415 1.2511098 O -2.1497458 -0.6989891 1.8913941 N -0.1053170 -0.4839063 0.9243764 H 0.5205915 0.0991882 0.3840621 C 0.3389496 -1.8105519 1.3138411 H -2.5788202 1.3381880 0.1581621 H -1.8946467 2.0047973 1.6393848 H -0.3542138 -2.5765464 0.9504454 H 1.3287946 -1.9867431 0.8863761 H 0.3962535 -1.9064952 2.4038395 C 1.1729841 0.2936638 -2.3645942 H 0.1462430 -0.0441519 -2.2084919 H 1.1942117 0.9845796 -3.2170727 O 1.5758389 0.9431127 -1.1502551 H 1.8009926 -0.5790938 -2.5865876 H 2.4929374 1.2246232 -1.2362528