Supporting Information

On the interactions of fused pyrazole derivative with selected aminoacids – DFT calculations

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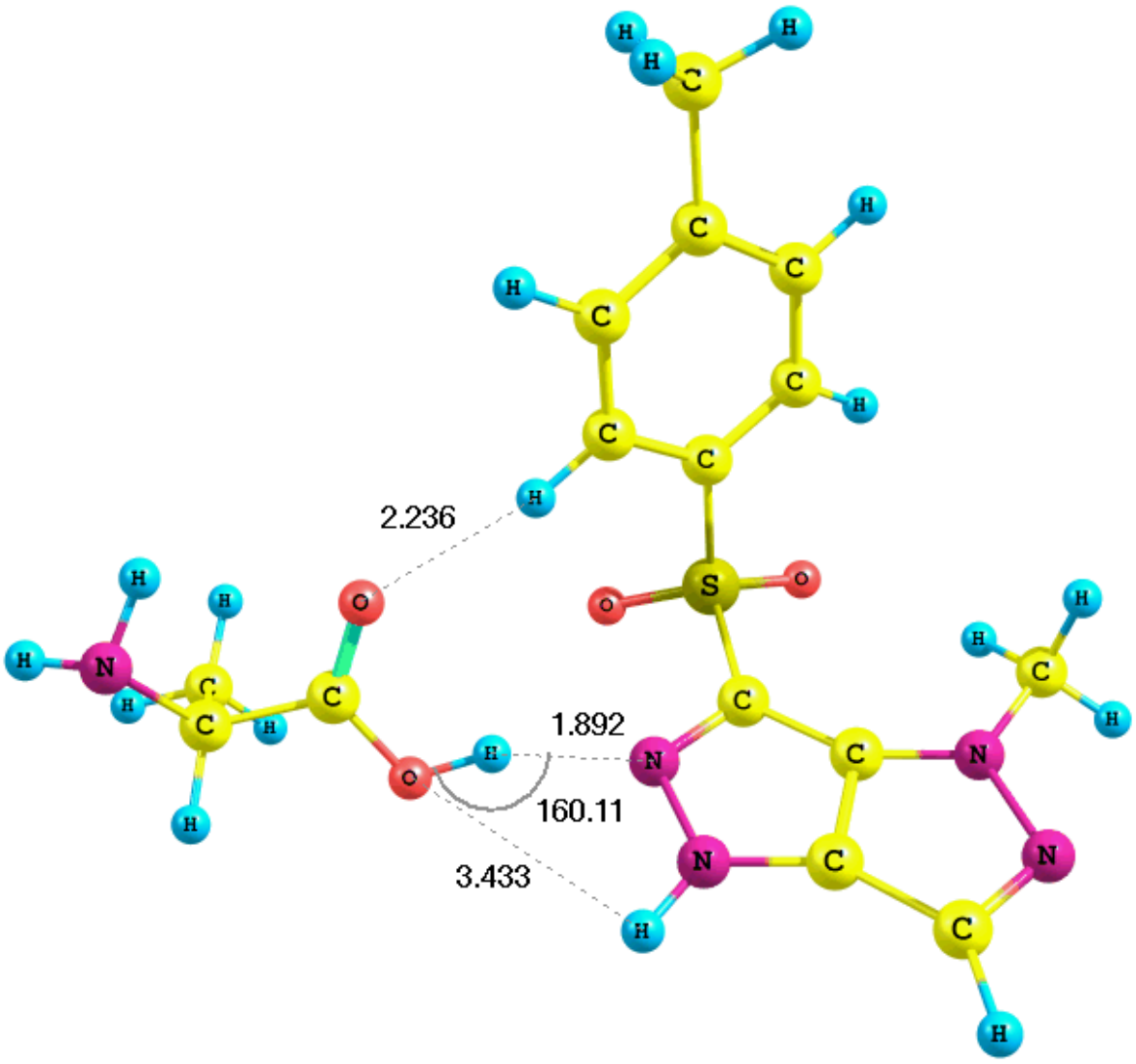

Figure S1. Structure of the 7–alanine adduct **7AlaB** optimized at the B3LYP/6-31G(d,p) level of theory.

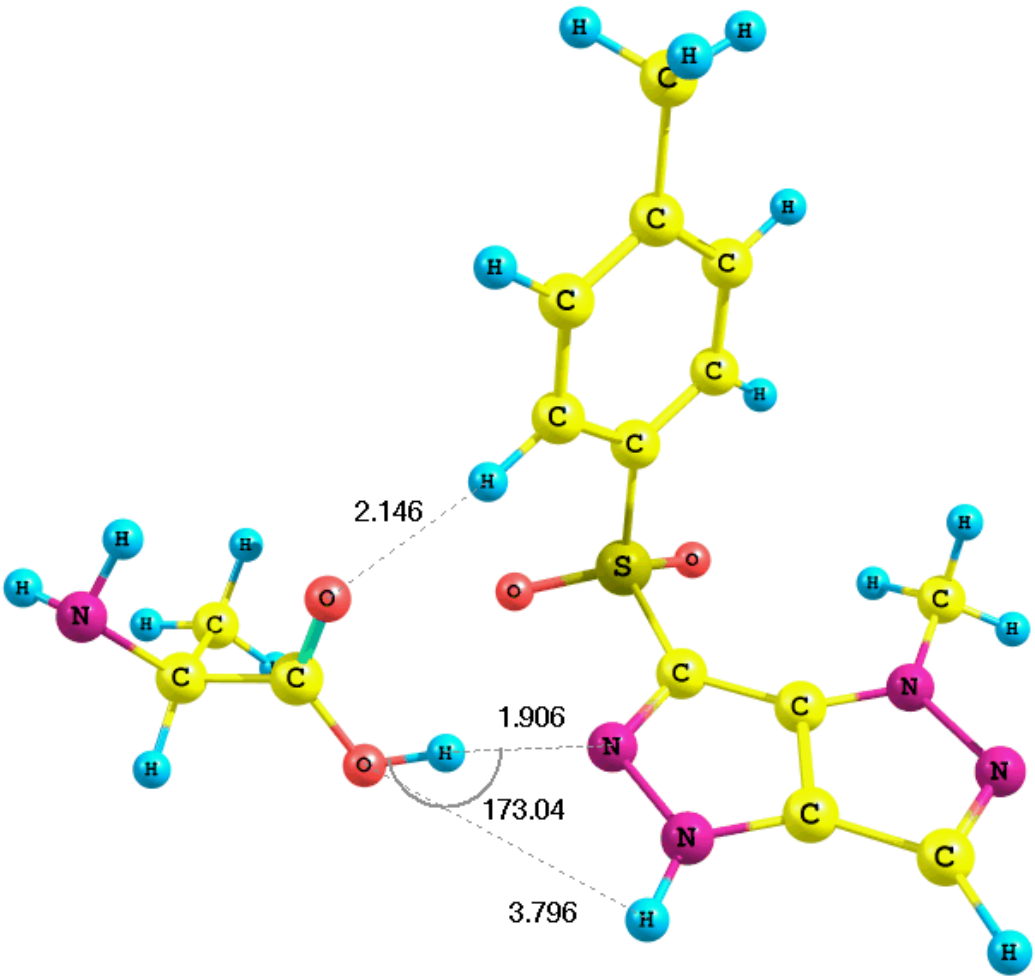

Figure S2. Structure of the **7**–alanine adduct **7AlaM** optimized at the M06L/6-31G(d,p) level of theory.

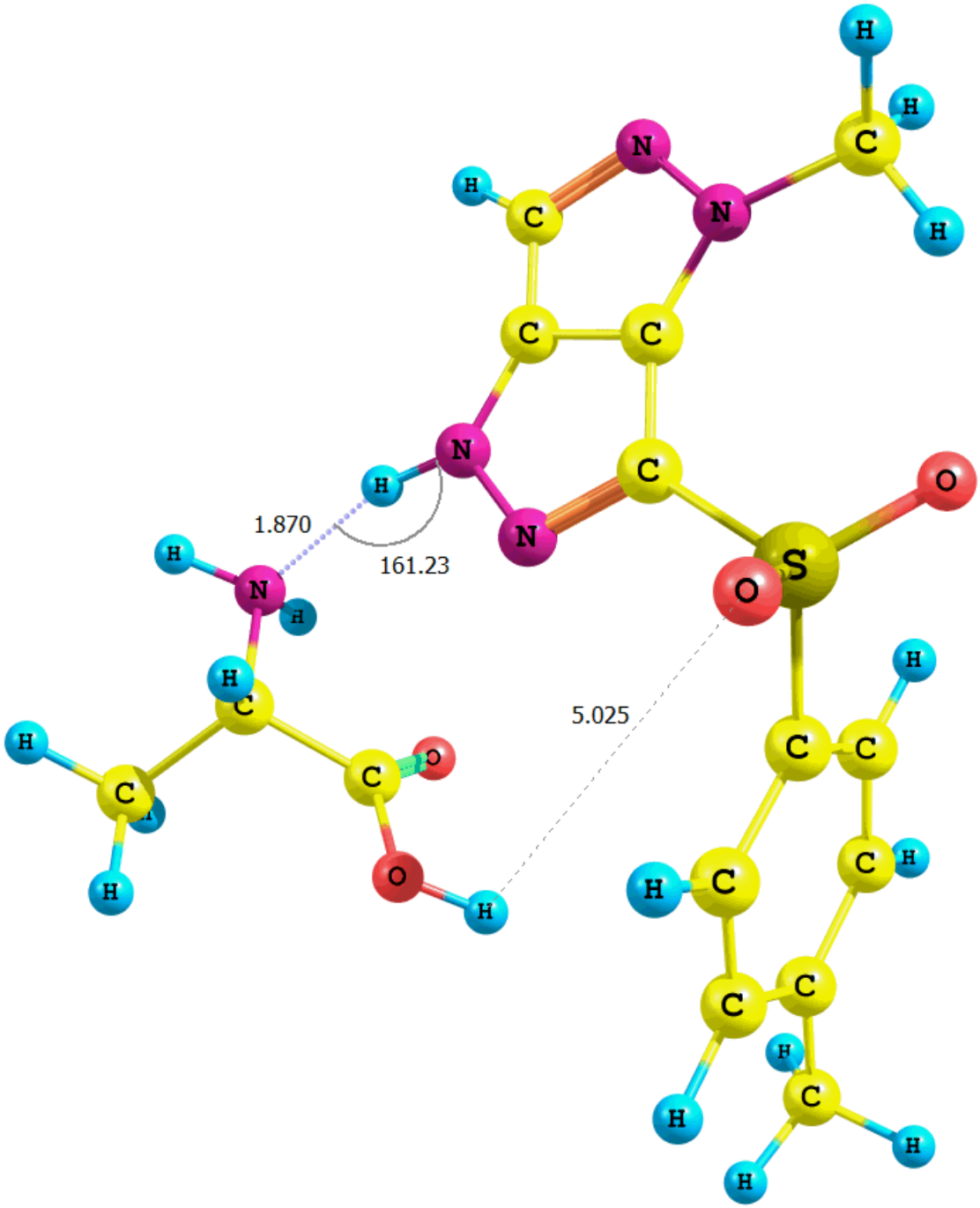

Figure S3. Structure of the **7**–alanine adduct **7AlaB-N** optimized at the B3LYP/6-31G(d,p) level of theory.

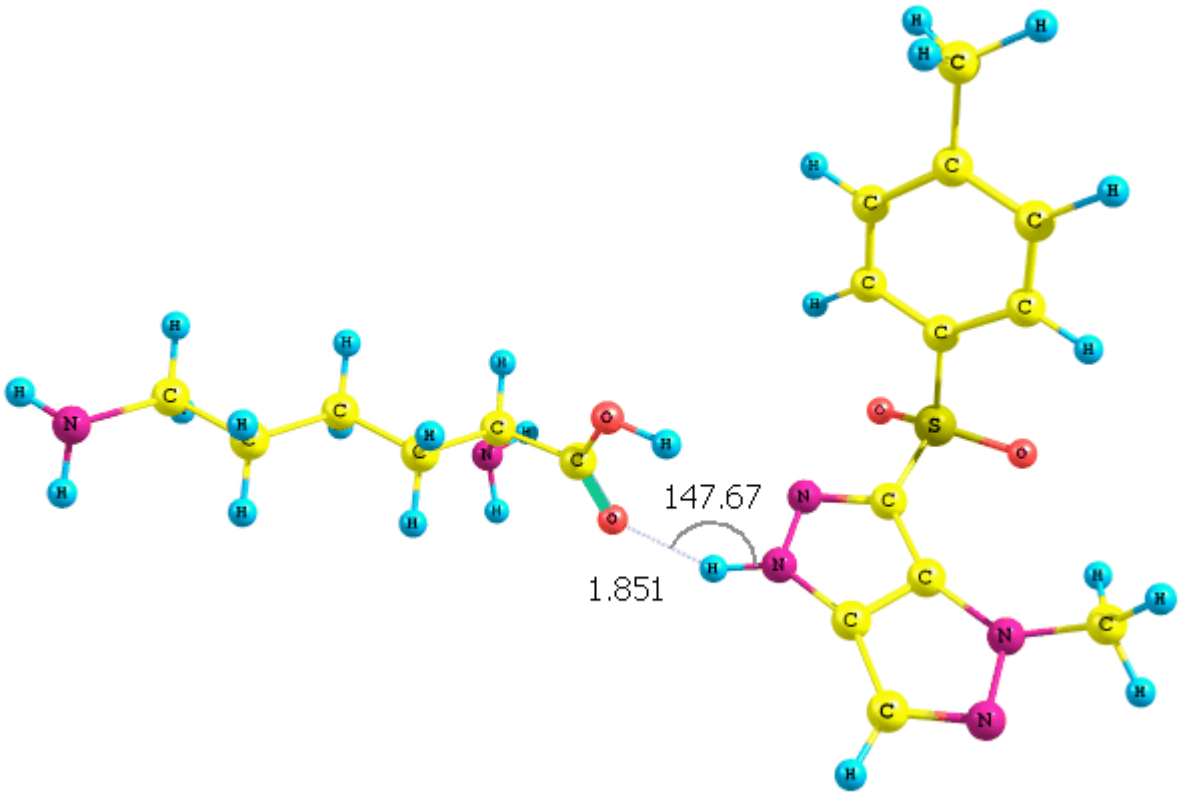

Figure S4. Structure of the **7**–lysine adduct **7LysB** optimized at the B3LYP/6-31G(d,p) level of theory.

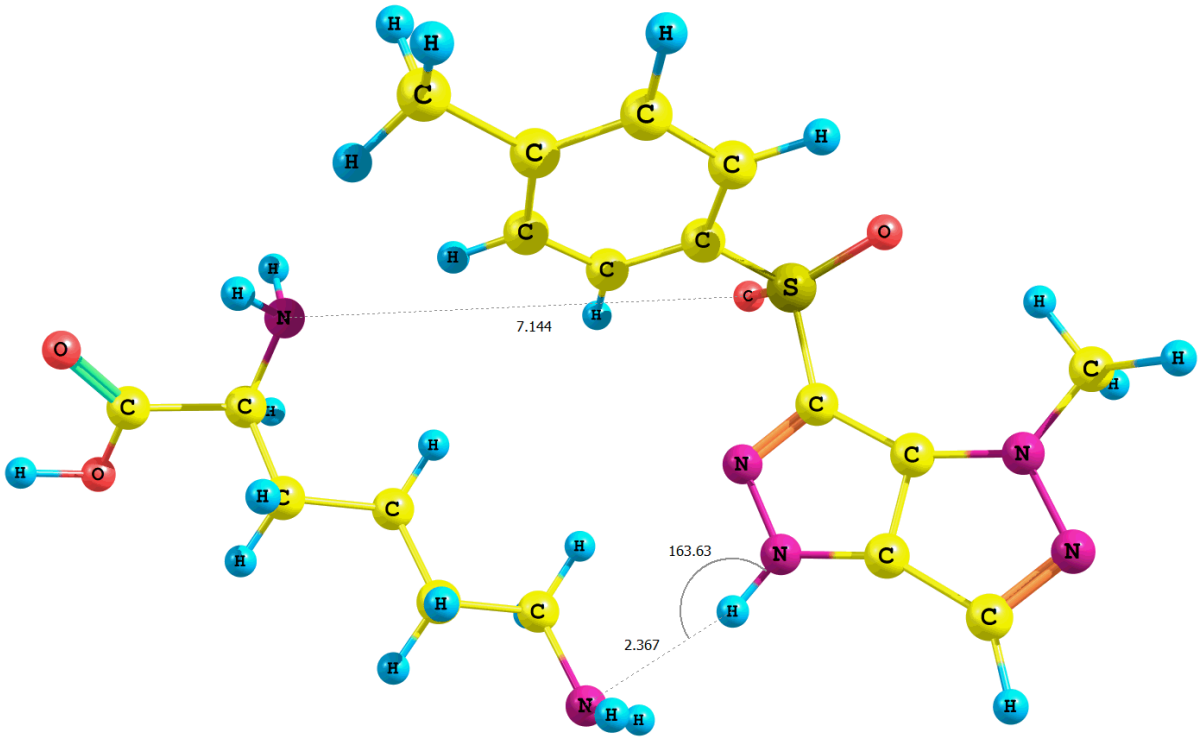

Figure S5. Structure of the **7**–lysine adduct **7LysP-N** optimized at the B3LYP/6-31G(d,p) level of theory.

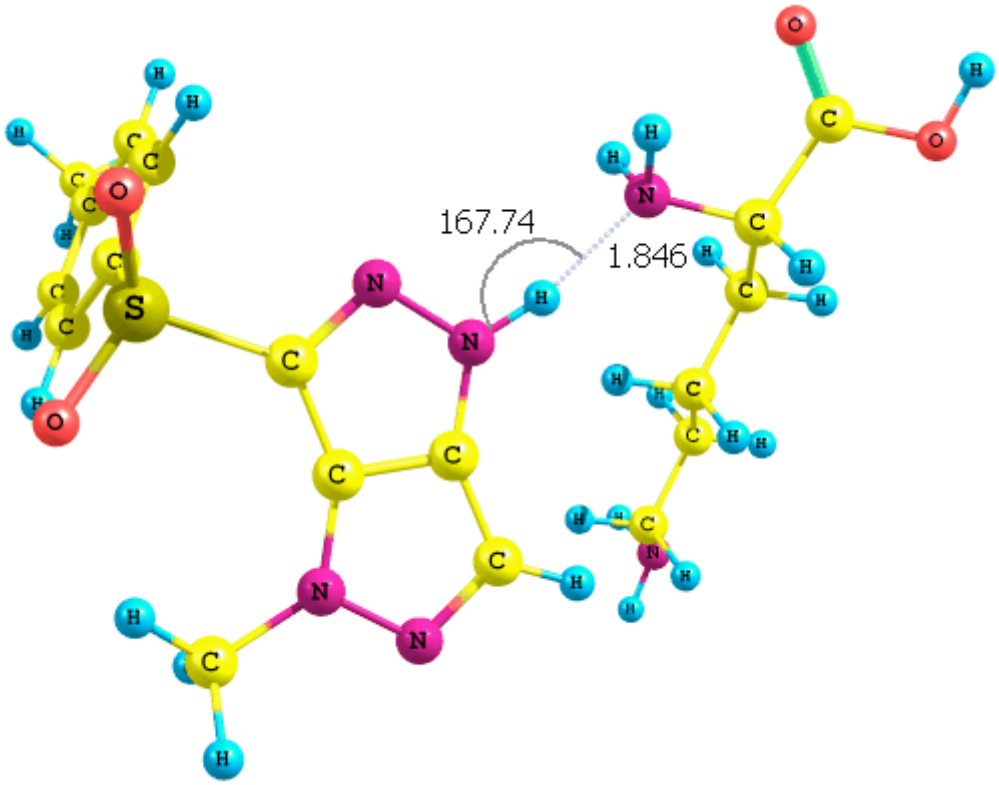

Figure S6. Structure of the **7**–lysine adduct **7LysP-αN** optimized at the PBE1PBE/6-31G(d,p) level of theory.

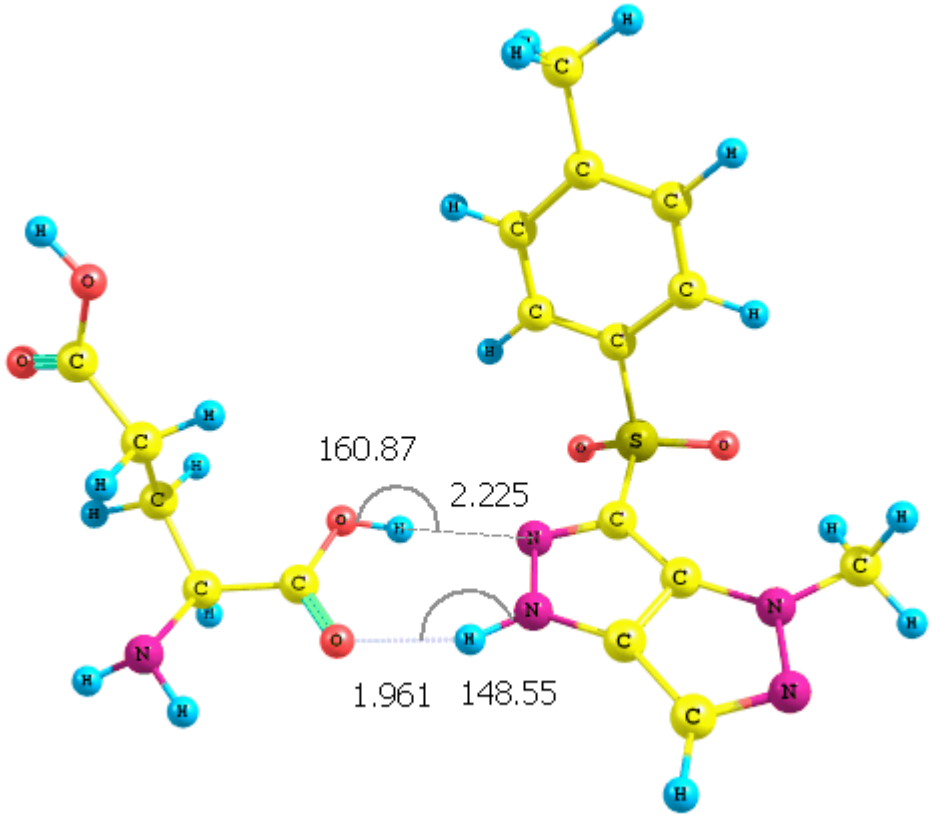

Figure S7. Structure of the **7**–glutamic acid adduct **7GluB6** optimized at the B3LYP/6-311+G(d,p) level of theory.

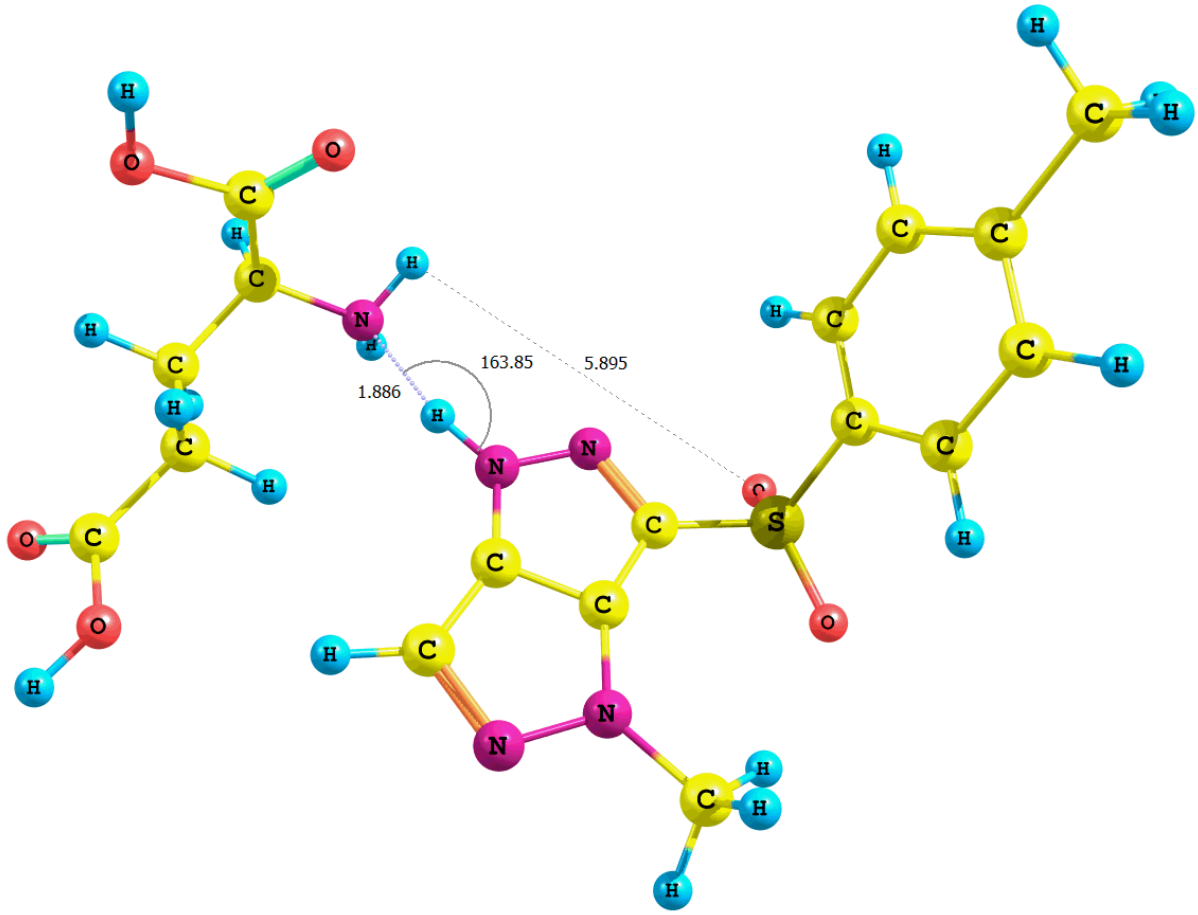

Figure S8. Structure of the 7–glutamic acid adduct **7GluB-αN** optimized at the B3LYP/6-31G(d,p) level of theory.

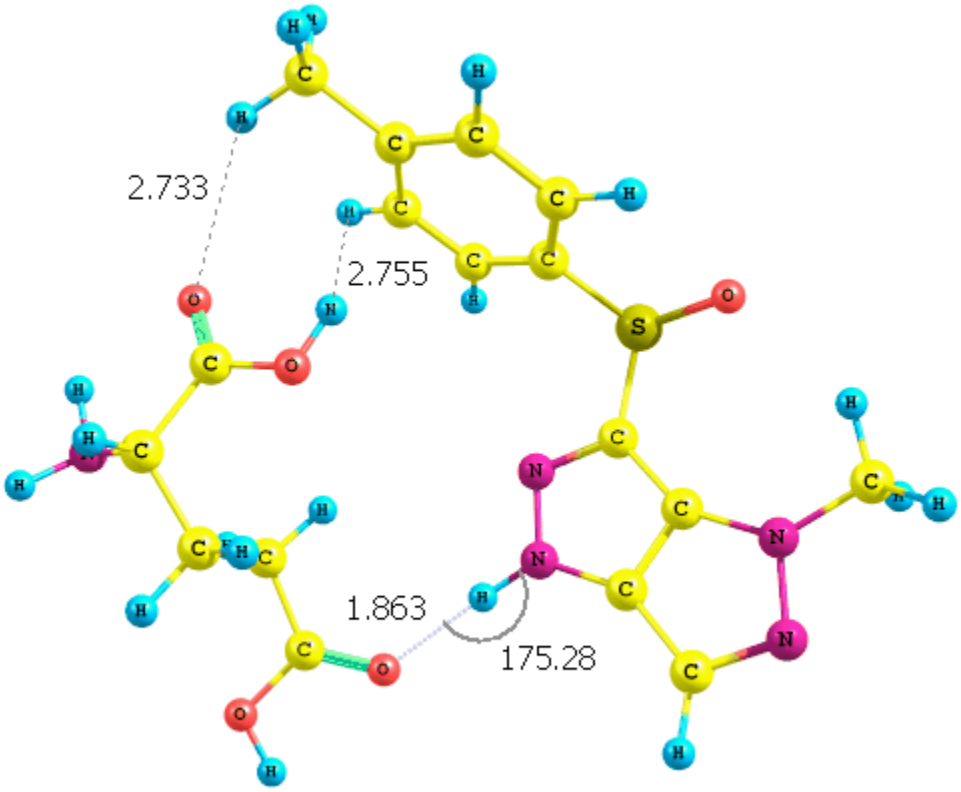

Figure S9. Structure of the **7**–glutamic acid adduct **7GluB-C** optimized at the B3LYP/6-31G(d,p) level of theory.

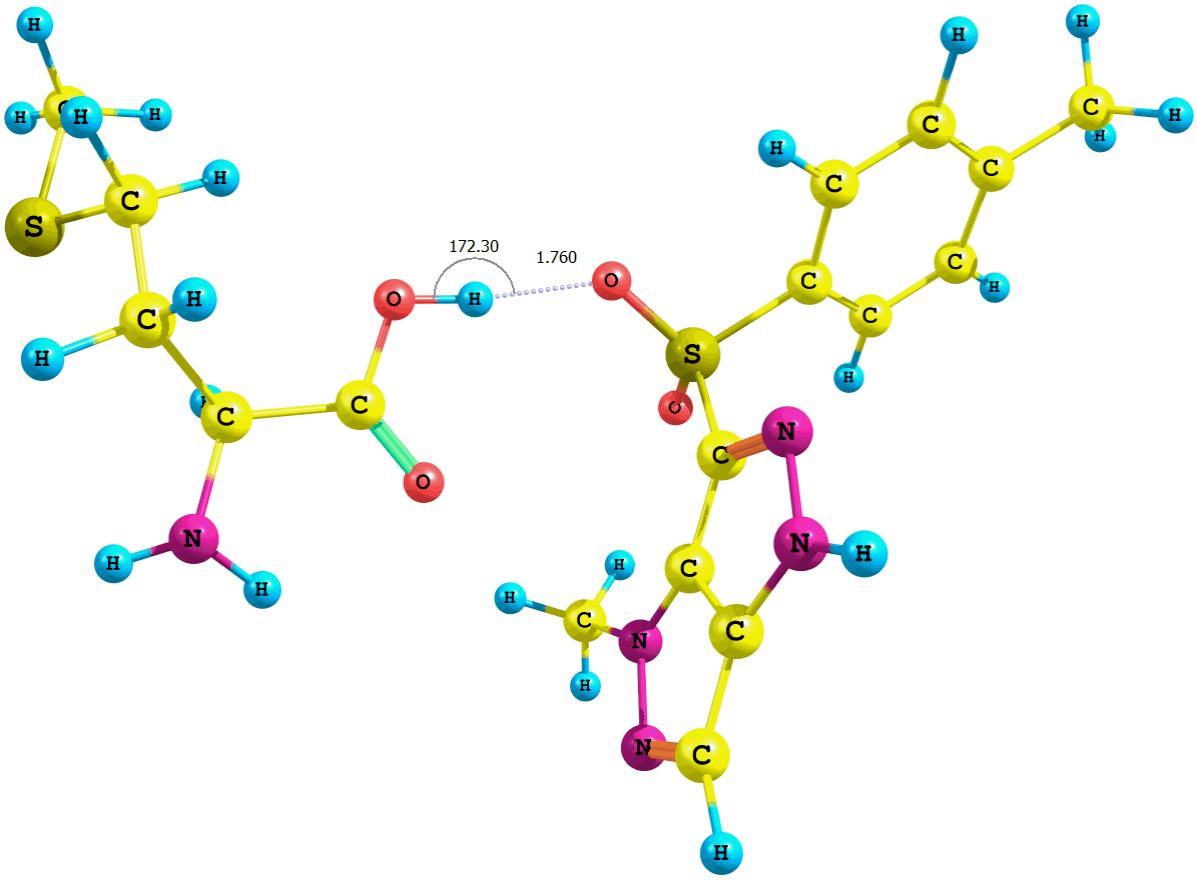

Figure S10. Structure of the **7**–methionine adduct **7MetB6** optimized at the B3LYP/6-311+G(d,p) level of theory.

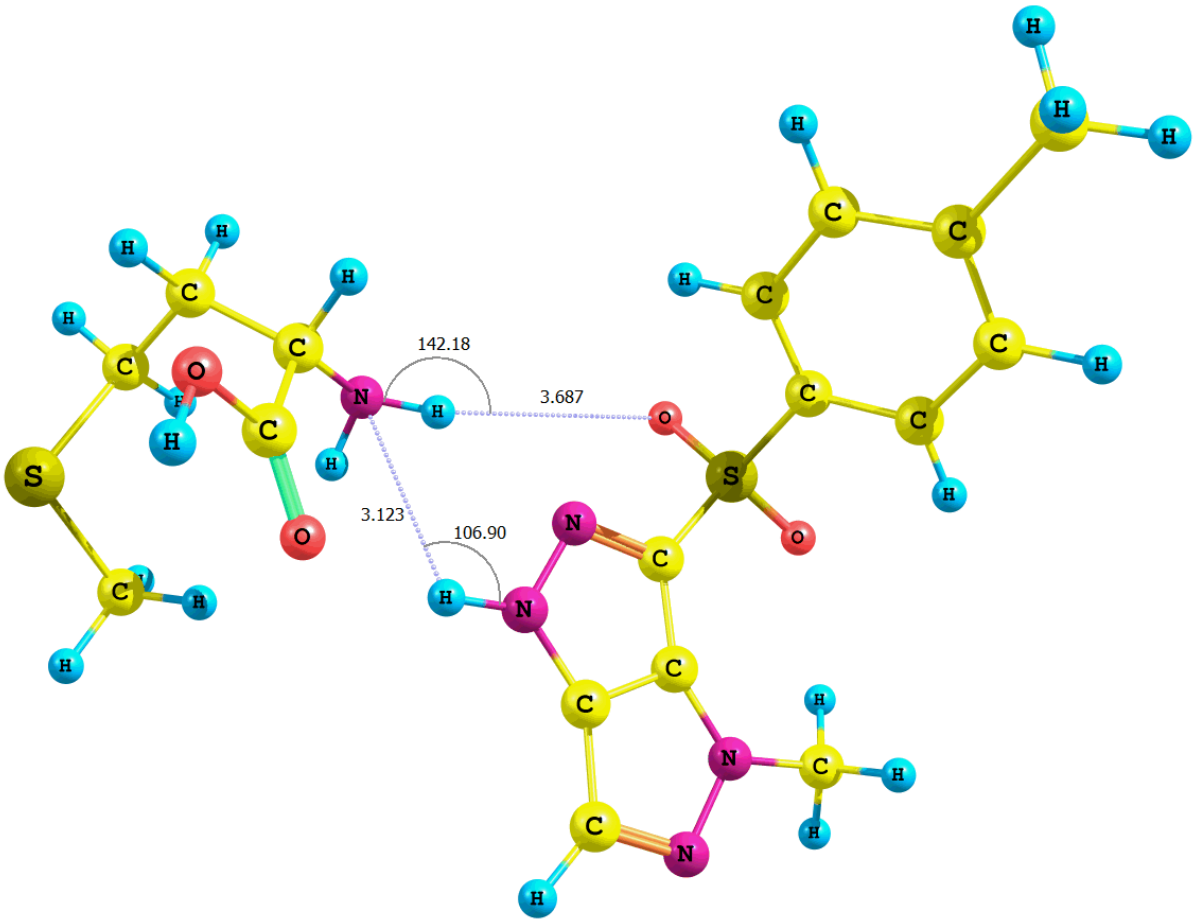

Figure S11. Structure of the 7–methionine adduct **7MetB-αN** optimized at the B3LYP/6-31G(d,p) level of theory.

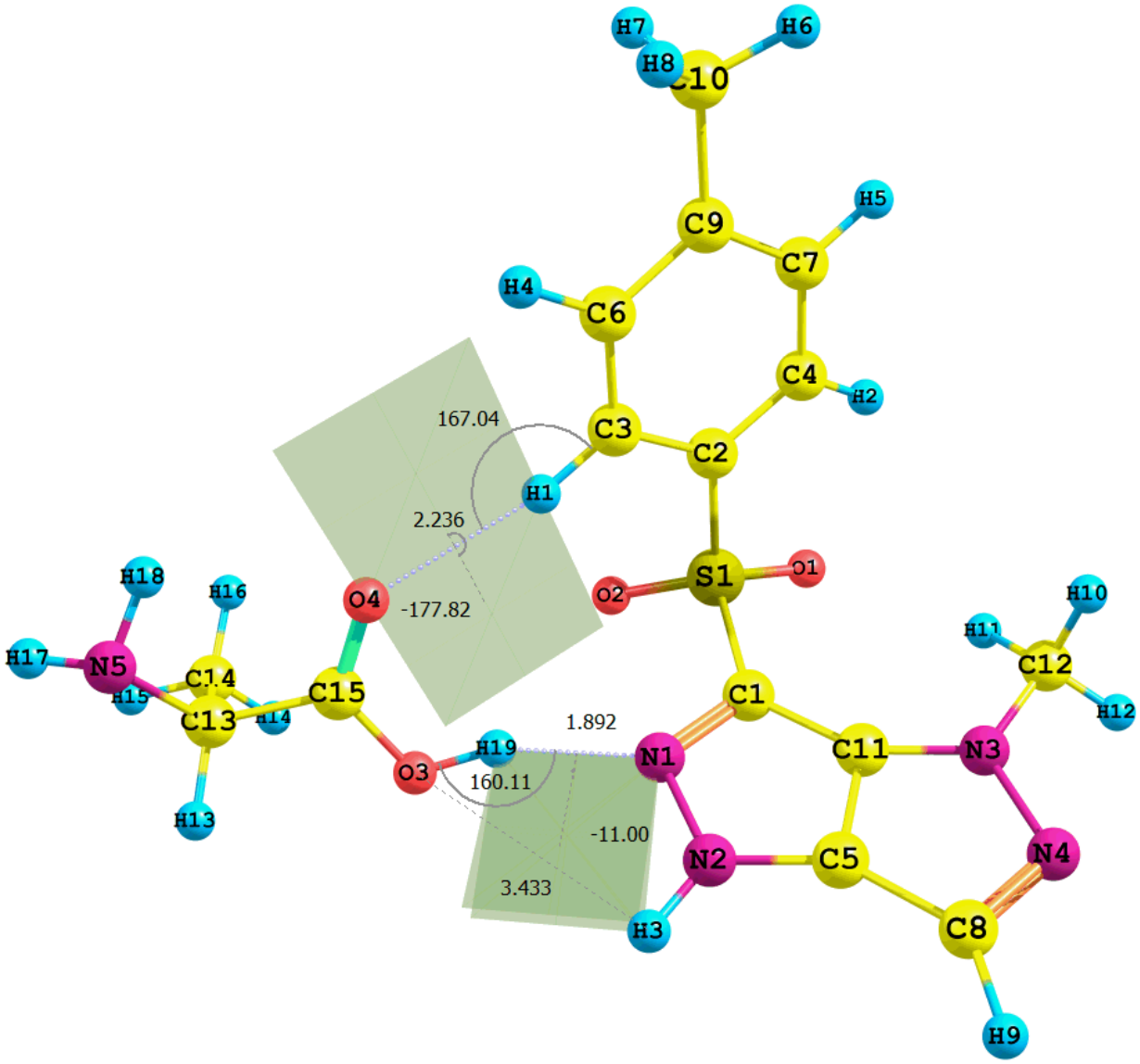

Figure S12. Hydrogen bond parameters within the **7**–alanine adduct **7AlaB**, interaction energy E = -9.36 (-8.77) kcal/mole, $J_{H\text{-}N}$ = -2.05 Hz, $J_{H\text{-}O}$ = 1.39 Hz.

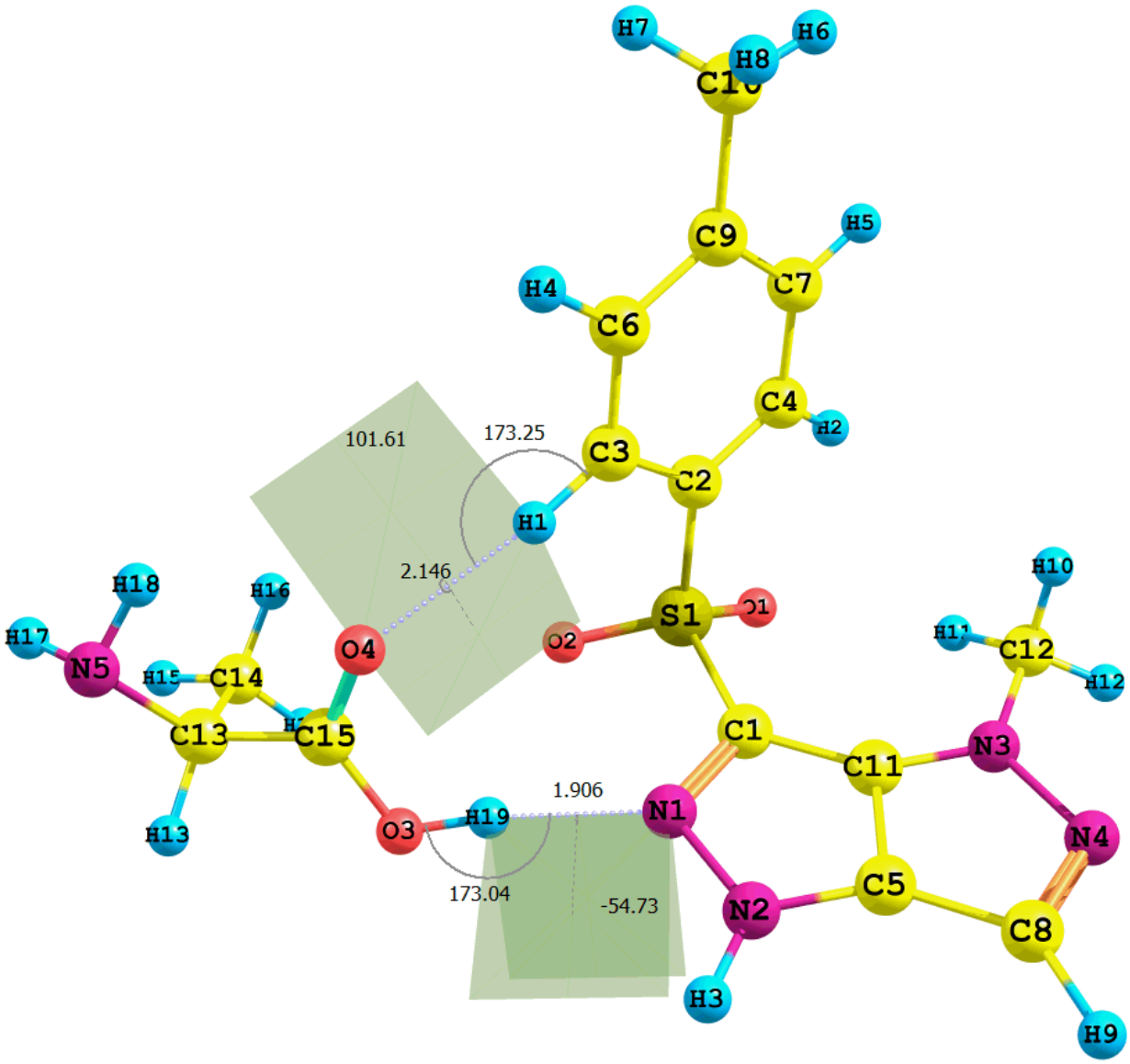

Figure S13. Hydrogen bond parameters within the **7**–alanine adduct **7AlaM**, interaction energy E = --8.56 (-8.07) kcal/mole, $J_{H\text{-}N}$ = -2.16 Hz, $J_{H\text{-}O}$ = 2.24 Hz.

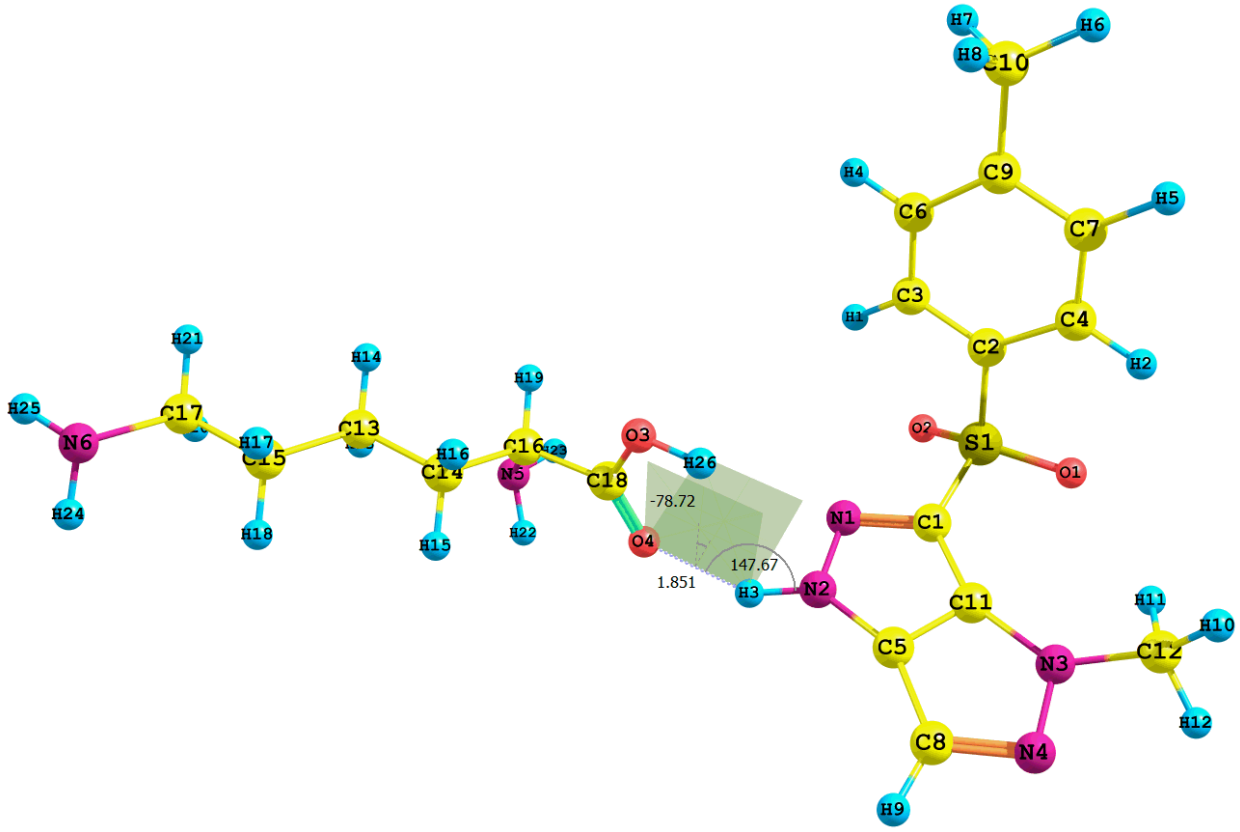

Figure S14. Hydrogen bond parameters within the **7**–lysine adduct **7LysB**, interaction energy E = -5.11 (-4.73) kcal/mole, $J_{H\text{-}O}$ = 5.16 Hz.

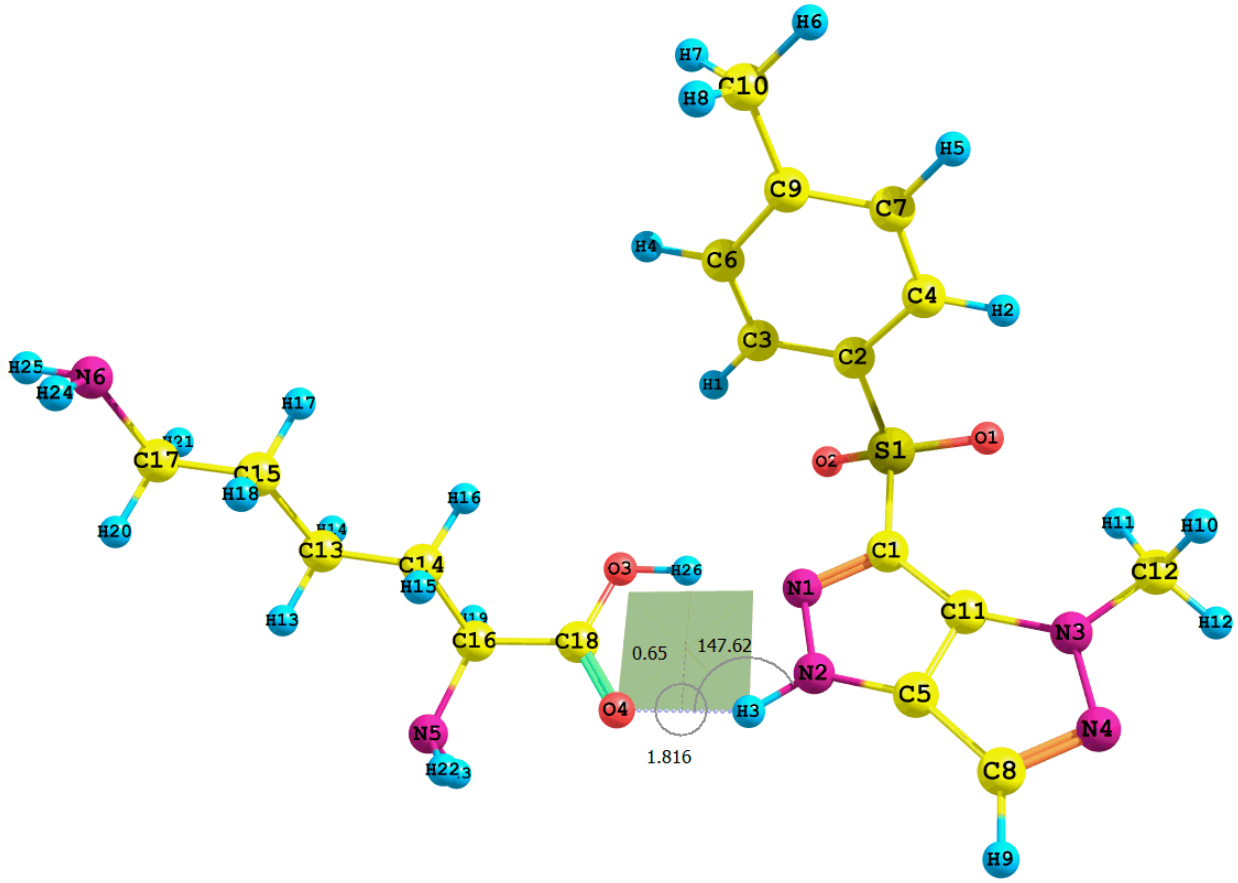

Figure S15. Hydrogen bond parameters within the **7**–lysine adduct **7LysP**, interaction energy E = -15.96 (-15.06) kcal/mole, $J_{H\text{-}O}$ = 5.78 Hz.

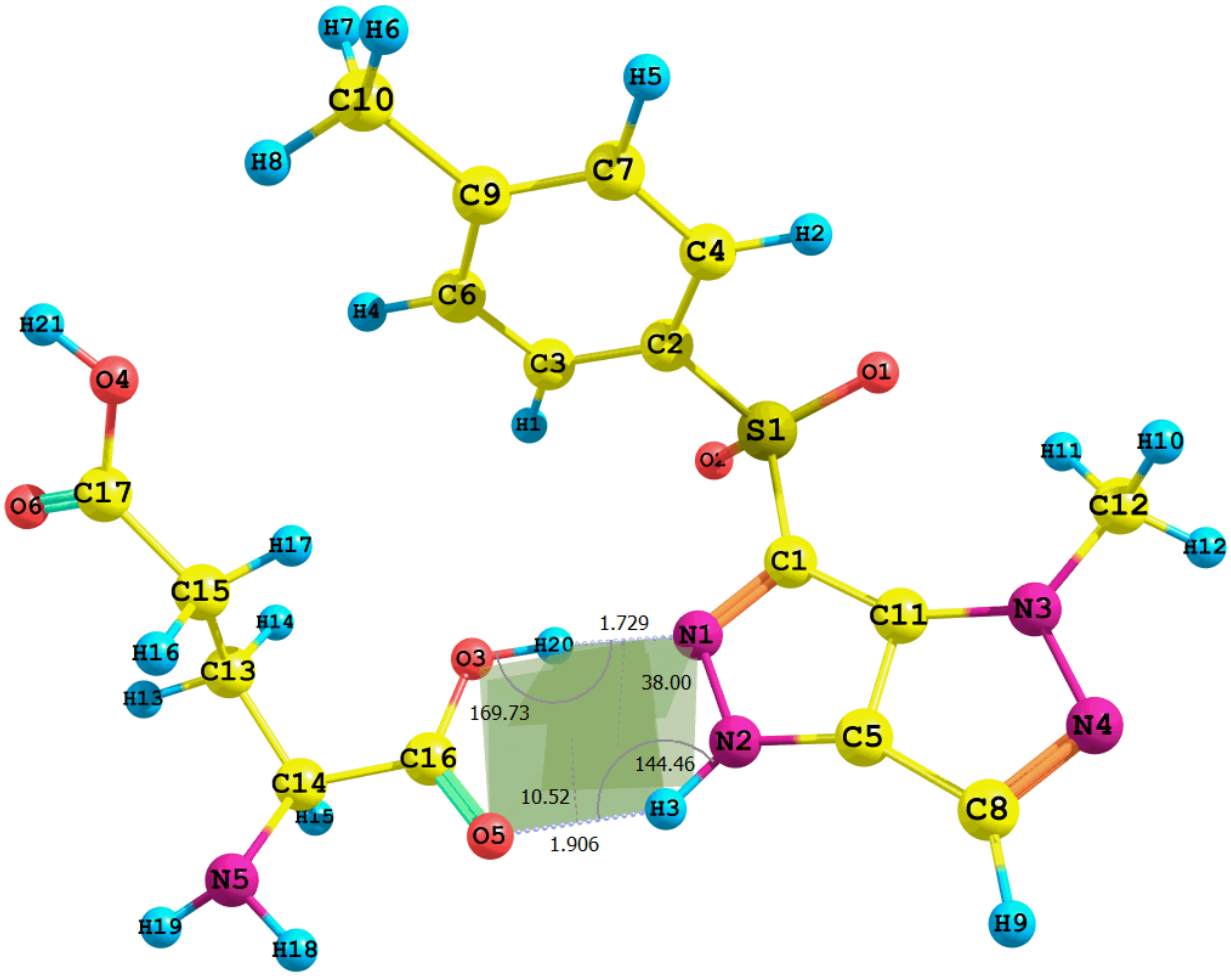

Figure S16. Hydrogen bond parameters within the **7**–glutamic acid adduct **7GluB**, interaction energy E = -15.88 (-14.85) kcal/mole, $J_{H\text{-}O}$ = 4.56 Hz, $J_{H\text{-}N}$ = -1.18 Hz.

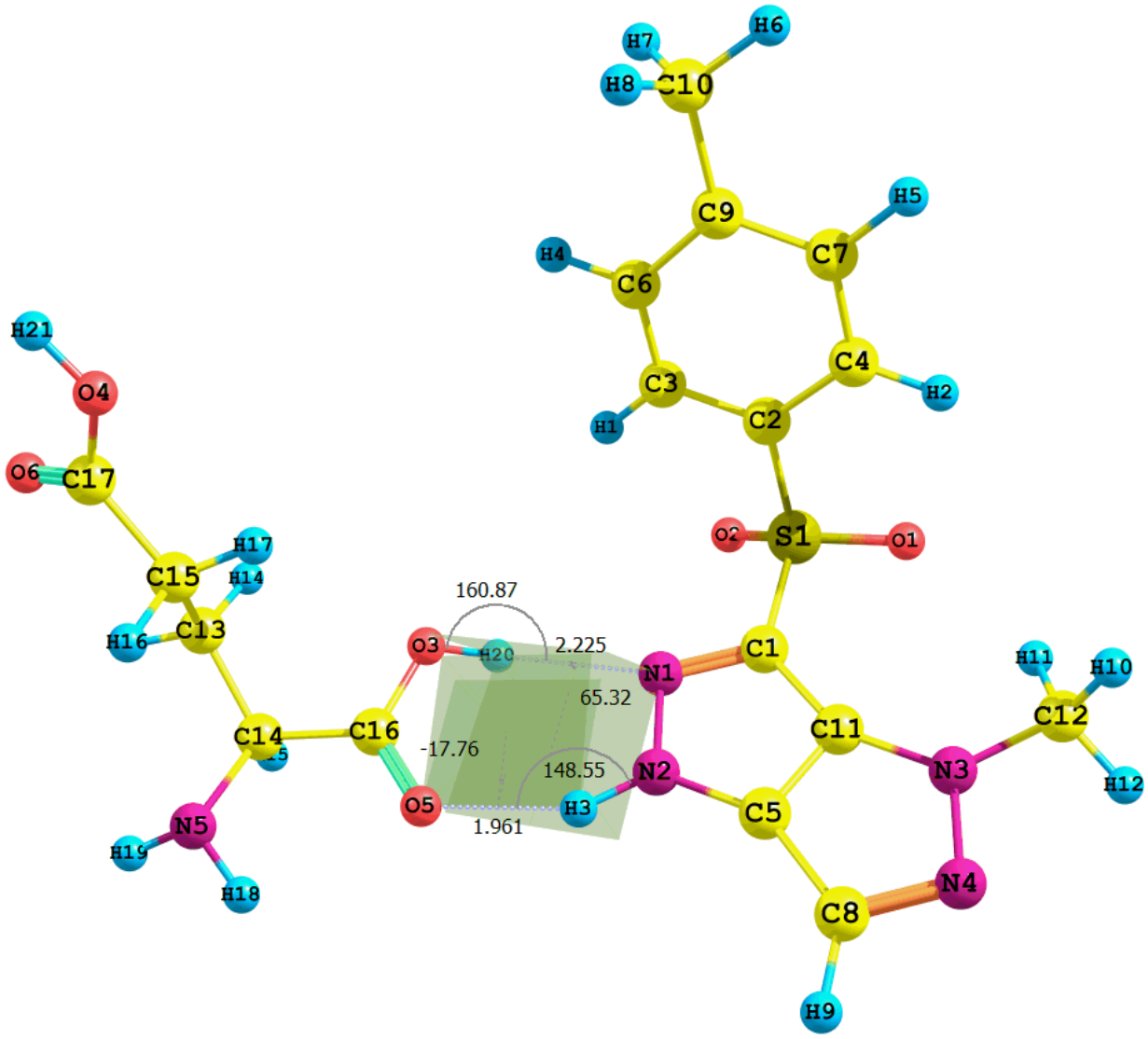

Figure S17. Hydrogen bond parameters within the **7**–glutamic acid adduct **7GluB6**, interaction energy E = -10.90 (-9.97) kcal/mole, $J_{H\text{-}O}$ = 4.17 Hz, $J_{H\text{-}N}$ = -9.38 Hz.

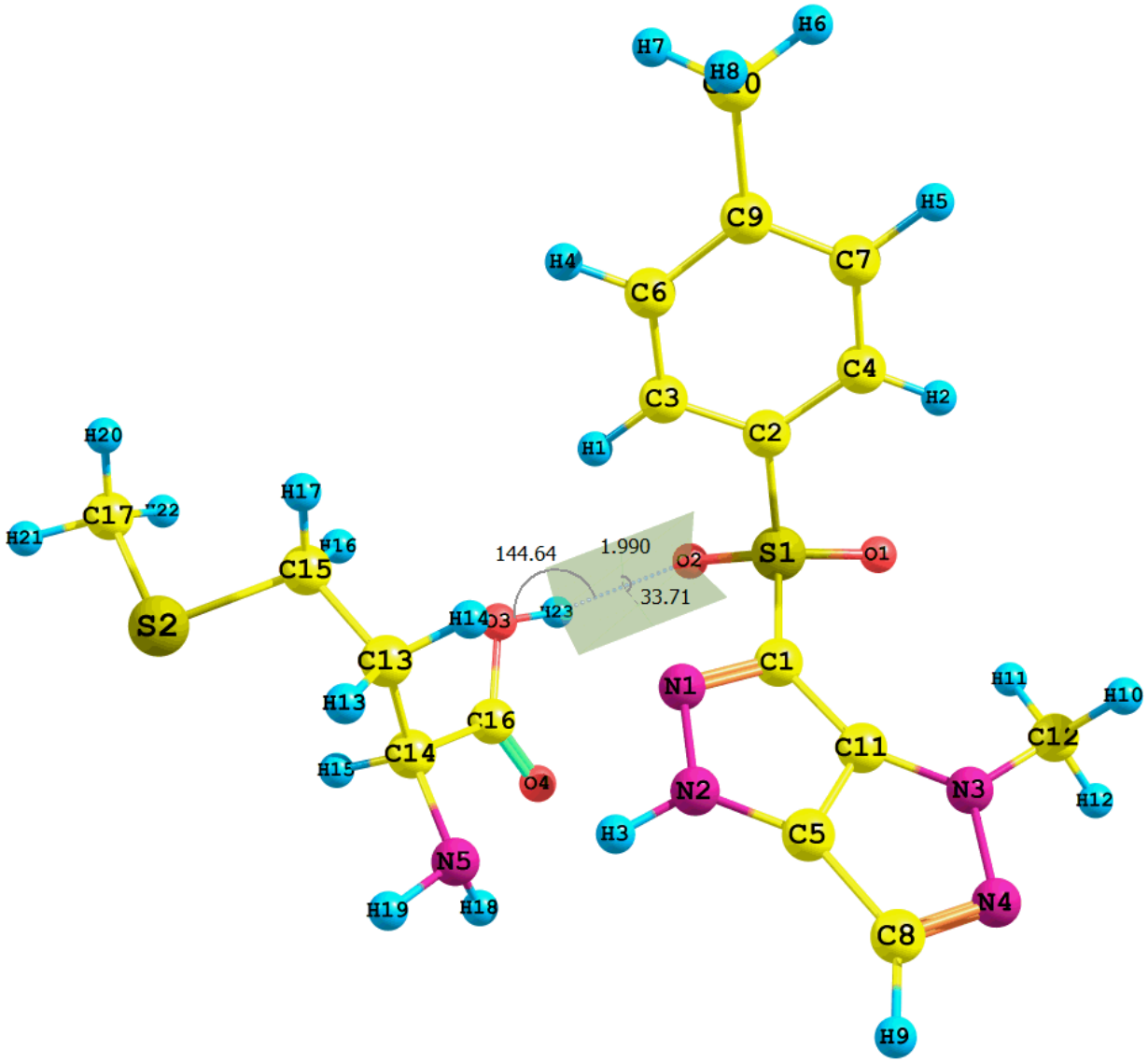

Figure S18. Hydrogen bond parameters within the **7**–methionine adduct **7MetB**, interaction energy E = -13.69 (-11.67) kcal/mole, $J_{H\text{-}O}$ = 4.03 Hz.

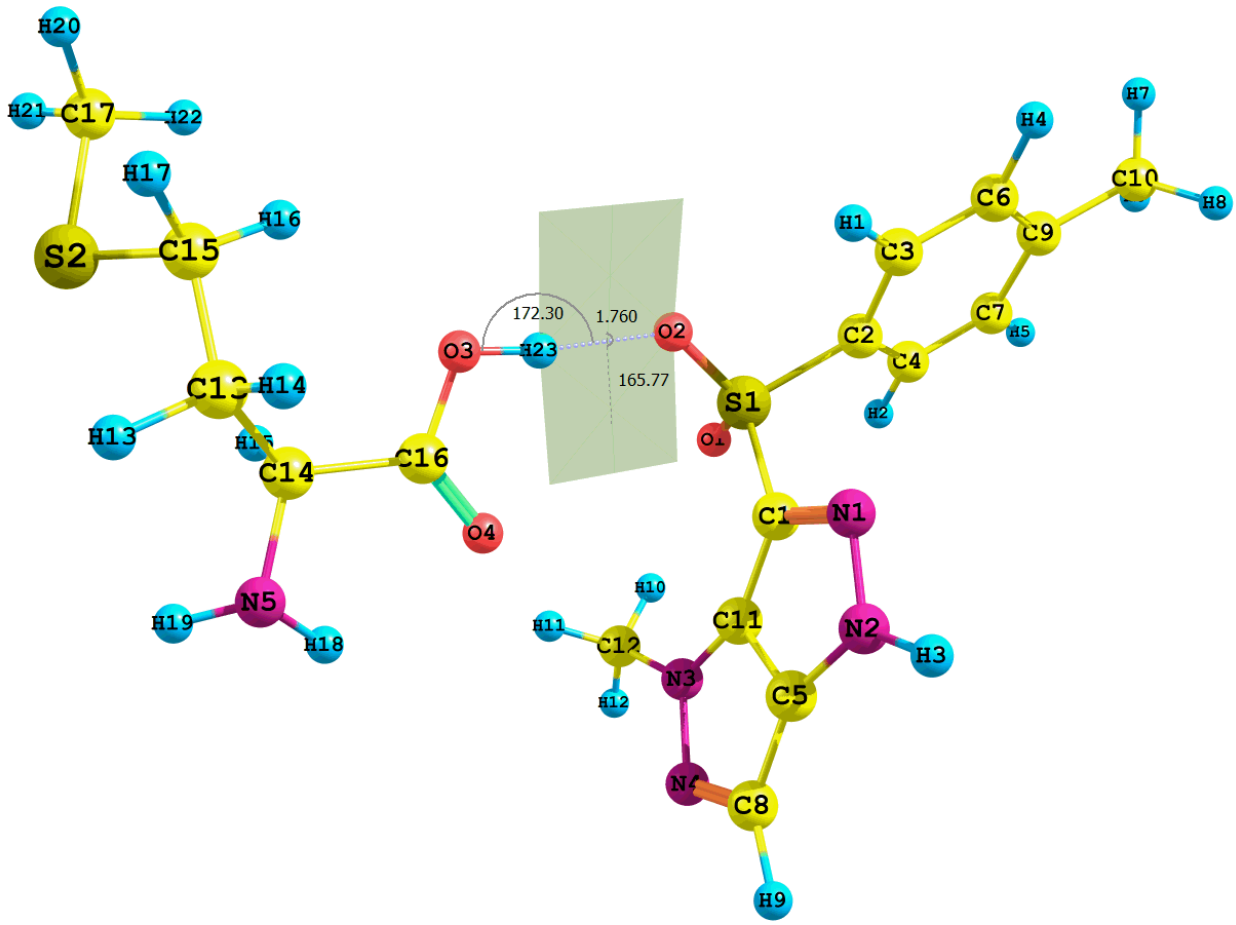

Figure S19. Hydrogen bond parameters within the **7**–methionine adduct **7MetB6**, interaction energy E = -8.63 (-8.39) kcal/mole, $J_{H\text{-}O}$ = 7.43 Hz.

Table S1. Values of electron densities (ρ) and Laplacian fields ($\nabla^2\rho$) (in eÅ) of the hydrogen-bonded **7–Ala** adducts.

Parameter	**Adduct**	**Hydrogen bond**	
		O-H···N	C-H···O=C
ρ	**7AlaB**	0.032687	0.014820
$\nabla^2\rho$	**7AlaB**	0.082415	0.042042
ρ	**7AlaM**	0.030902	0.017124
$\nabla^2\rho$	**7AlaM**	0.079888	0.052129

Table S2. Values of electron densities (ρ) and Laplacian fields ($\nabla^2\rho$) (in eÅ) of the hydrogen-bonded **7–Glu** adducts.

Parameter	**Adduct**	**Hydrogen bond**	
		N-H···O=C	O-H···N
ρ	**7GluB** (**7GluP**)	0.029184	0.048345
$\nabla^2\rho$	**7GluB** (**7GluP**)	0.083141	0.106983
ρ	**7GluB6**	0.024299	0.015119
$\nabla^2\rho$	**7GluB6**	0.090097	0.049104

Table S3. Values of electron densities (ρ) and Laplacian fields ($\nabla^2\rho$) (in eÅ) of the hydrogen-bonded **7–Met** adducts; nd – no data were calculated.

Parameter	**Adduct**	**Hydrogen bond**	
		N-H···NH_2	O-H···O_2S
ρ	**7MetB**	0.031705	0.021761
$\nabla^2\rho$	**7MetB**	0.067738	0.065721
ρ	**7MetB6**	nd	0.035009
$\nabla^2\rho$	**7MetB6**	nd	0.126416

Table S4. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7AlaB–7AlaB$_c$**) for compound 7 within the **7–Ala** adduct; absolute errors (δ_I–δ_{Ic}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.755 ppm for TMS (B3LYP/6-31G(d,p)/GIAO); MAD = 1.09.

Locant	δ_{exp}	7AlaB	7AlaB$_a$	7AlaB$_b$	7AlaB$_c$	Δ_{7AlaB}	Δ_{7AlaBa}	Δ_{7AlaBb}	Δ_{7AlaBc}	δ	$\Delta\delta$
A	2.37	2.22	2.26	2.24	2.24	0.15	0.11	0.14	0.14	0.13	6
B	7.65	7.06	7.19	7.15	7.16	0.59	0.46	0.50	0.49	0.51	7
NH	13.67	8.78	8.71	8.71	8.65	4.90	4.96	4.96	5.02	4.96	36
C	7.85	8.55	8.70	8.77	8.75	0.69	0.85	0.91	0.90	0.84	11
D	7.43	7.37	7.43	7.40	7.41	0.06	0.01	0.03	0.03	0.03	0
E	4.08	4.05	4.13	4.21	4.19	0.03	0.06	0.14	0.12	0.08	2

Table S5. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7AlaB6–7AlaB6$_c$**) for compound 7 within the **7–Ala** adduct; absolute errors (δ_{II}–δ_{IIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.9844 ppm for TMS (B3LYP/6-311+G(d,p)/GIAO); MAD = 1.82.

Locant	δ_{exp}	7AlaB6	7AlaB6$_a$	7AlaB6$_b$	7AlaB6$_c$	Δ_{7AlaB6}	$\Delta_{7AlaB6a}$	$\Delta_{7AlaB6b}$	$\Delta_{7AlaB6c}$	δ	$\Delta\delta$
A	2.37	2.35	2.61	2.36	7.68	0.02	0.24	0.02	5.31	1.40	59
B	7.65	6.98	7.53	7.40	7.24	0.67	0.12	0.25	0.41	0.36	5
NH	13.67	8.87	9.02	8.78	6.74	4.80	4.65	4.89	6.93	5.32	39
C	7.85	8.74	9.28	8.94	3.71	0.89	1.43	1.09	4.15	1.89	24
D	7.43	7.44	7.85	7.55	4.51	0.00	0.42	0.12	2.92	0.87	12
E	4.08	4.02	4.53	4.47	7.56	0.06	0.45	0.39	3.49	1.10	27

Table S6. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7AlaC–7AlaC$_c$**) for compound 7 within the **7–Ala** adduct; absolute errors (δ_{III}–δ_{IIIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.7749 ppm for TMS (CAM-B3LYP/6-31G(d,p)/GIAO); MAD = 1.12.

Locant	δ_{exp}	7AlaC	7AlaC$_a$	7AlaC$_b$	7AlaC$_c$	Δ_{7AlaC}	Δ_{7AlaCa}	Δ_{7AlaCb}	Δ_{7AlaCc}	δ	$\Delta\delta$
A	2.37	2.26	2.27	2.26	2.27	0.11	0.10	0.11	0.10	0.11	5
B	7.65	7.24	7.28	7.25	7.21	0.41	0.37	0.40	0.44	0.40	5
NH	13.67	8.78	8.78	8.79	8.79	4.89	4.89	4.89	4.88	4.89	36
C	7.85	9.00	8.98	9.02	9.00	1.15	1.13	1.17	1.15	1.15	15
D	7.43	7.49	7.49	7.48	7.49	0.06	0.06	0.04	0.05	0.05	1
E	4.08	4.20	4.20	4.23	4.20	0.13	0.12	0.15	0.13	0.13	3

Table S7. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7AlaP–7AlaP$_c$**) for compound 7 within the **7–Ala** adduct; absolute errors (δ_{IV}–δ_{IVc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.6651 ppm for TMS (PBE1PBE/6-31G(d,p)/GIAO); MAD = 1.13.

Locant	δ_{exp}	7AlaP	7AlaP$_a$	7AlaP$_b$	7AlaP$_c$	Δ_{7AlaP}	Δ_{7AlaPa}	Δ_{7AlaPb}	Δ_{7AlaPc}	δ	$\Delta\delta$
A	2.37	2.29	2.30	2.28	2.29	0.09	0.07	0.09	0.08	0.09	4
B	7.65	7.25	7.27	7.24	7.21	0.40	0.38	0.41	0.44	0.41	5
NH	13.67	8.72	8.72	8.72	8.70	4.95	4.95	4.95	4.97	4.96	36
C	7.85	8.96	8.93	8.99	8.97	1.11	1.08	1.14	1.11	1.11	14
D	7.43	7.55	7.55	7.53	7.53	0.11	0.12	0.09	0.10	0.10	1
E	4.08	4.18	4.19	4.23	4.21	0.10	0.11	0.16	0.13	0.13	3

Table S8. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7AlaM –7AlaM$_c$**) for compound 7 within the 7–**Ala** adduct; absolute errors (δ_V–δ_{Vc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.9579 ppm for TMS (M06L/6-31G(d,p)/GIAO); MAD = 0.97.

Locant	δ_{exp}	7AlaM	7AlaM$_a$	7AlaM$_b$	7AlaM$_c$	Δ_{7AlaM}	Δ_{7AlaMa}	Δ_{7AlaMb}	Δ_{7AlaMc}	Δ	$\Delta\delta$
A	2.37	2.29	2.30	2.28	2.29	0.09	0.07	0.09	0.08	0.09	4
B	7.65	7.25	7.27	7.24	7.21	0.40	0.38	0.41	0.44	0.41	5
NH	13.67	8.72	8.72	8.72	8.70	4.95	4.95	4.95	4.97	4.96	36
C	7.85	8.96	8.93	8.99	8.97	1.11	1.08	1.14	1.11	1.11	14
D	7.43	7.55	7.55	7.53	7.53	0.11	0.12	0.09	0.10	0.10	1
E	4.08	4.18	4.19	4.23	4.21	0.10	0.11	0.16	0.13	0.13	3

Table S9. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7LysB–7LysB$_c$**) for compound 7 within the **7–Lys** adduct; absolute errors (δ_{VI}–δ_{VIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.755 ppm for TMS (B3LYP/6-31G(d,p)/GIAO); MAD = 0.34.

Locant	δ_{exp}	7LysB	7LysB$_a$	7LysB$_b$	7LysB$_c$	Δ_{7LysB}	Δ_{7LysBa}	Δ_{7LysBb}	Δ_{7LysBc}	δ	$\Delta\delta$
A	2.37	2.26	2.24	2.22	2.27	0.12	0.13	0.15	0.10	0.13	5
B	7.65	7.23	7.24	7.12	7.24	0.42	0.41	0.53	0.41	0.44	6
NH	13.67	12.87	12.87	12.59	12.83	0.81	0.81	1.08	0.85	0.89	6
C	7.85	8.10	8.28	8.05	8.11	0.24	0.42	0.20	0.26	0.28	4
D	7.43	7.36	7.34	7.27	7.37	0.08	0.09	0.17	0.06	0.10	1
E	4.08	4.26	4.29	4.24	4.26	0.19	0.21	0.16	0.18	0.19	5

Table S10. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7LysB6–7LysB6$_c$**) for compound 7 within the **7–Lys** adduct; absolute errors (δ_{VII}–δ_{VIIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.9844 ppm for TMS (B3LYP/6-311+G(d,p)/GIAO); MAD = 0.37.

Locant	δ_{exp}	7LysB6	7LysB6$_a$	7LysB6$_b$	7LysB6$_c$	Δ_{7LysB6}	$\Delta_{7LysB6a}$	$\Delta_{7LysB6b}$	$\Delta_{7LysB6c}$	δ	$\Delta\delta$
A	2.37	2.31	2.47	2.49	2.55	0.06	0.09	0.12	0.18	0.11	5
B	7.65	7.23	7.36	7.40	7.46	0.42	0.29	0.25	0.19	0.29	4
NH	13.67	12.77	12.47	12.73	12.65	0.91	1.21	0.94	1.03	1.02	7
C	7.85	8.31	8.02	8.28	8.14	0.45	0.16	0.43	0.29	0.33	4
D	7.43	7.39	7.52	7.51	7.47	0.04	0.09	0.07	0.04	0.06	1
E	4.08	4.42	4.55	4.48	4.48	0.34	0.48	0.41	0.40	0.41	10

Table S11. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7LysC–7LysC$_c$**) for compound 7 within the **7–Lys** adduct; absolute errors (δ_{VIII}–δ_{VIIIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.7749 ppm for TMS (CAM-B3LYP/6-31G(d,p)/GIAO); MAD = 0.29.

Locant	δ_{exp}	7LysC	7LysC$_a$	7LysC$_b$	7LysC$_c$	Δ_{7LysC}	Δ_{7LysCa}	Δ_{7LysCb}	Δ_{7LysCc}	δ	$\Delta\delta$
A	2.37	2.28	2.27	2.28	2.29	0.09	0.10	0.09	0.08	0.09	4
B	7.65	7.31	7.31	7.31	7.31	0.34	0.34	0.34	0.34	0.34	4
NH	13.67	13.03	13.03	13.04	13.00	0.64	0.64	0.63	0.67	0.65	5
C	7.85	8.28	8.27	8.28	8.29	0.43	0.42	0.42	0.43	0.43	5
D	7.43	7.45	7.45	7.46	7.46	0.02	0.01	0.03	0.03	0.02	0
E	4.08	4.31	4.32	4.30	4.31	0.23	0.24	0.23	0.23	0.23	6

Table S12. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7LysM–7LysM$_c$**) for compound 7 within the **7–Lys** adduct; absolute errors (δ_X–δ_{Xc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.9579 ppm for TMS (M06L/6-31G(d,p)/GIAO); MAD = 0.41.

Locant	δ_{exp}	7LysM	7LysM$_a$	7LysM$_b$	7LysM$_c$	Δ_{7LysM}	Δ_{7LysMa}	Δ_{7LysMb}	Δ_{7LysMc}	δ	$\Delta\delta$
A	2.37	2.13	2.26	2.25	2.21	0.25	0.12	0.13	0.17	0.17	7
B	7.65	7.74	6.99	7.73	7.65	0.09	0.66	0.08	0.01	0.21	3
NH	13.67	12.14	12.49	12.59	12.37	1.53	1.18	1.08	1.31	1.27	9
C	7.85	7.97	8.16	8.27	8.30	0.11	0.31	0.42	0.45	0.32	4
D	7.43	7.14	7.16	7.07	7.05	0.29	0.27	0.36	0.39	0.33	4
E	4.08	4.52	4.22	4.15	4.16	0.44	0.14	0.07	0.09	0.19	5

Table S13. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7GluB–7GluB$_c$**) for compound 7 within the **7–Glu** adduct; absolute errors (δ_{XI}–δ_{XIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.755 ppm for TMS (B3LYP/6-31G(d,p)/GIAO); MAD = 0.39.

Locant	δ_{exp}	7GluB	7GluB$_a$	7GluB$_b$	7GluB$_c$	Δ_{7GluB}	Δ_{7GluBa}	Δ_{7GluBb}	Δ_{7GluBc}	δ	$\Delta\delta$
A	2.37	2.29	2.29	2.32	2.28	0.09	0.08	0.06	0.09	0.08	3
B	7.65	7.37	7.27	7.27	7.30	0.28	0.38	0.38	0.35	0.35	5
NH	13.67	12.25	12.28	12.29	12.29	1.42	1.39	1.39	1.38	1.40	10
C	7.85	8.05	8.07	8.09	8.08	0.20	0.22	0.24	0.22	0.22	3
D	7.43	7.51	7.49	7.53	7.50	0.07	0.05	0.10	0.07	0.07	1
E	4.08	4.32	4.32	4.32	4.30	0.24	0.25	0.24	0.23	0.24	6

Table S14. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7GluB6–7GluB6$_c$**) for compound 7 within the **7–Glu** adduct; absolute errors (δ_{XII}–δ_{XIIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.9844 ppm for TMS (B3LYP/6-311+G(d,p)/GIAO); MAD = 0.51.

Locant	δ_{exp}	7GluB6	7GluB6$_a$	7GluB6$_b$	7GluB6$_c$	Δ_{7GluB6}	$\Delta_{7GluB6a}$	$\Delta_{\&GluB6b}$	$\Delta_{7GluB6c}$	δ	$\Delta\delta$
A	2.37	2.31	2.50	2.42	2.44	0.06	0.13	0.04	0.07	0.08	3
B	7.65	7.38	7.34	7.49	7.39	0.27	0.31	0.16	0.27	0.25	3
NH	13.67	12.08	12.28	11.10	11.64	1.59	1.39	2.58	2.04	1.90	14
C	7.85	8.40	8.11	8.03	8.13	0.55	0.25	0.18	0.27	0.31	4
D	7.43	7.63	7.49	7.62	7.31	0.20	0.05	0.18	0.13	0.14	2
E	4.08	4.36	4.44	4.58	4.49	0.29	0.37	0.51	0.41	0.39	10

Table S15. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7GluC–7GluC$_c$**) for compound 7 within the **7–Glu** adduct; absolute errors (δ_{XIII}–δ_{XIIIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.7749 ppm for TMS (CAM-B3LYP/6-31G(d,p)/GIAO); MAD = 0.40.

Locant	δ_{exp}	7GluC	7GluC$_a$	7GluC$_b$	7GluC$_c$	Δ_{7GluC}	Δ_{7GluCa}	Δ_{7GluCb}	Δ_{7GluCc}	Δ	$\Delta\delta$
A	2.37	2.32	2.37	2.35	2.32	0.05	0.01	0.03	0.05	0.03	1
B	7.65	7.41	7.45	7.35	7.36	0.24	0.20	0.30	0.29	0.26	3
NH	13.67	12.46	12.45	12.48	12.49	1.21	1.22	1.19	1.18	1.20	9
C	7.85	8.24	8.29	8.26	8.25	0.39	0.44	0.41	0.40	0.41	5
D	7.43	7.62	7.66	7.64	7.62	0.19	0.22	0.20	0.19	0.20	3
E	4.08	4.38	4.40	4.38	4.37	0.30	0.32	0.31	0.29	0.31	7

Table S16. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7GluP–7GluP$_c$**) for compound 7 within the **7–Glu** adduct; absolute errors (δ_{XIV}–δ_{XIVc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.6651 ppm for TMS (PBE1PBE/6-31G(d,p)/GIAO); MAD = 0.39.

Locant	δ_{exp}	7GluP	7GluP$_a$	7GluP$_b$	7GluP$_c$	Δ_{7GluP}	Δ_{7GluPa}	Δ_{7GluPb}	Δ_{7GluPc}	δ	$\Delta\delta$
A	2.37	2.34	2.34	2.36	2.33	0.03	0.03	0.01	0.04	0.03	1
B	7.65	7.41	7.35	7.35	7.36	0.24	0.30	0.30	0.29	0.28	4
NH	13.67	12.57	12.56	12.57	12.56	1.10	1.12	1.10	1.11	1.11	8
C	7.85	8.23	8.25	8.26	8.26	0.38	0.39	0.40	0.40	0.39	5
D	7.43	7.62	7.62	7.65	7.64	0.19	0.18	0.22	0.21	0.20	3
E	4.08	4.38	4.40	4.38	4.36	0.30	0.32	0.30	0.29	0.30	7

Table S17. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7GluM–7GluM$_c$**) for compound 7 within the **7–Glu** adduct; absolute errors (δ_{XV}–δ_{XVc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.9579 ppm for TMS (M06L/6-31G(d,p)/GIAO); MAD = 0.46.

Locant	δ_{exp}	7GluM	7GluM$_a$	7GluM$_b$	7GluM$_c$	Δ_{7GluM}	Δ_{7GluMa}	Δ_{7GluMb}	Δ_{7GluMc}	δ	$\Delta\delta$
A	2.37	2.30	2.07	2.31	2.22	0.08	0.30	0.06	0.16	0.15	6
B	7.65	7.52	7.49	7.28	7.90	0.13	0.16	0.37	0.25	0.23	3
NH	13.67	12.08	12.22	11.46	11.62	1.59	1.45	2.21	2.06	1.83	13
C	7.85	7.93	8.04	8.02	7.93	0.07	0.19	0.16	0.07	0.12	2
D	7.43	7.42	7.18	7.19	7.26	0.01	0.26	0.25	0.17	0.17	2
E	4.08	4.33	4.13	4.42	4.35	0.26	0.06	0.34	0.27	0.23	6

Table S18. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7MetB –7MetB$_c$**) for compound 7 within the **7–Met** adduct; absolute errors (δ_{XVI}–δ_{XVIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.755 ppm for TMS (B3LYP/6-31G(d,p)/GIAO); MAD = 0.26.

Locant	δ_{exp}	7MetB	7MetB$_a$	7MetB$_b$	7MetB$_c$	Δ_{7MetB}	Δ_{7MetBa}	Δ_{7MetBb}	Δ_{7MetBc}	δ	$\Delta\delta$
A	2.37	2.28	2.28	2.27	2.24	0.10	0.10	0.11	0.13	0.11	5
B	7.65	7.17	7.14	7.18	7.30	0.48	0.51	0.47	0.35	0.45	6
NH	13.67	13.29	13.26	13.33	12.85	0.38	0.41	0.34	0.82	0.49	4
C	7.85	8.19	8.18	8.21	8.05	0.34	0.32	0.35	0.20	0.30	4
D	7.43	7.35	7.37	7.33	7.33	0.09	0.07	0.10	0.11	0.09	1
E	4.08	4.20	4.17	4.18	4.23	0.12	0.10	0.11	0.16	0.12	3

Table S19. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7MetB6–7MetB6$_c$**) for compound 7 within the **7–Met** adduct; absolute errors (δ_{XVII}–δ_{XVIIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.9844 ppm for TMS (B3LYP/6-311+G(d,p)/GIAO); MAD = 0.53.

Locant	δ_{exp}	7MetB6	7MetB6$_a$	7MetB6$_b$	7MetB6$_c$	Δ_{7MetB6}	$\Delta_{7MetB6a}$	$\Delta_{7MetB6b}$	$\Delta_{7MetB6c}$	δ	$\Delta\delta$
A	2.37	2.57	2.45	2.42	2.41	0.20	0.08	0.05	0.04	0.09	4
B	7.65	7.48	7.31	7.40	7.40	0.18	0.34	0.25	0.25	0.25	3
NH	13.67	8.23	12.58	12.88	12.53	5.44	1.10	0.79	1.14	2.12	15
C	7.85	8.14	8.19	8.38	8.21	0.29	0.34	0.53	0.36	0.38	5
D	7.43	7.48	7.57	7.51	7.45	0.04	0.13	0.08	0.02	0.07	1
E	4.08	4.61	4.32	4.19	4.26	0.54	0.24	0.11	0.18	0.27	7

Table S20. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7MetC–7MetC$_c$**) for compound 7 within the **7–Met** adduct; absolute errors (δ_{XVIII}–δ_{XVIIIc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.7749 ppm for TMS (CAM-B3LYP/6-31G(d,p)/GIAO); MAD = 0.23.

Locant	δ_{exp}	7MetC	7MetC$_a$	7MetC$_b$	7MetC$_c$	Δ_{7MetC}	Δ_{7MetCa}	Δ_{7MetCb}	Δ_{7MetCc}	δ	$\Delta\delta$
A	2.37	2.30	2.30	2.29	2.29	0.07	0.07	0.08	0.08	0.08	3
B	7.65	7.24	7.22	7.25	7.20	0.41	0.43	0.41	0.45	0.42	6
NH	13.67	13.53	13.51	13.55	13.48	0.14	0.16	0.12	0.19	0.15	1
C	7.85	8.43	8.43	8.44	8.43	0.58	0.57	0.59	0.58	0.58	7
D	7.43	7.45	7.46	7.43	7.44	0.01	0.02	0.00	0.00	0.01	0
E	4.08	4.24	4.23	4.24	4.23	0.16	0.15	0.16	0.16	0.16	4

Table S21. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7MetP–7MetP$_c$**) for compound 7 within the **7–Met** adduct; absolute errors (δ_{XIX}–δ_{XIXc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.6651 ppm for TMS (PBE1PBE/6-31G(d,p)/GIAO); MAD = 0.24.

Locant	δ_{exp}	7MetP	7MetP$_a$	7MetP$_b$	7MetP$_c$	Δ_{7MetP}	Δ_{7MetPa}	Δ_{7MetPb}	Δ_{7MetPc}	δ	$\Delta\delta$
A	2.37	2.29	2.32	2.31	2.31	0.08	0.05	0.06	0.07	0.07	3
B	7.65	7.23	7.20	7.23	7.19	0.42	0.45	0.42	0.46	0.44	6
NH	13.67	13.46	13.86	13.94	13.88	0.22	0.19	0.27	0.21	0.22	2
C	7.85	8.38	8.39	8.42	8.39	0.52	0.54	0.56	0.53	0.54	7
D	7.43	7.46	7.50	7.47	7.47	0.03	0.06	0.03	0.04	0.04	1
E	4.08	4.23	4.22	4.24	4.23	0.15	0.14	0.16	0.15	0.15	4

Table S22. Experimental (δ_{exp}) and calculated chemical shifts (rotamers **7MetM–7MetM$_c$**) for compound 7 within the 7–Met adduct; absolute errors (δ_{XX}– δ_{XXc}), average absolute error (δ), relative percentage errors ($\Delta\delta$); calculated NMR shielding for proton H_{ref} = 31.9579 ppm for TMS (M06L/6-31G(d,p)/GIAO); MAD = 0.49.

Locant	δ_{exp}	7MetM	7MetM$_a$	7MetM$_b$	7MetM$_c$	Δ_{7MetM}	Δ_{7MetMa}	Δ_{7MetMb}	Δ_{7MetMc}	δ	$\Delta\delta$
A	2.37	2.35	2.25	2.30	2.31	0.03	0.12	0.07	0.06	0.07	3
B	7.65	7.51	6.93	7.36	6.98	0.14	0.72	0.29	0.67	0.45	6
NH	13.67	9.03	13.05	13.09	13.12	4.65	0.63	0.58	0.55	1.60	12
C	7.85	8.43	8.30	8.23	8.30	0.58	0.45	0.38	0.45	0.46	6
D	7.43	7.37	7.44	7.36	7.26	0.07	0.00	0.08	0.17	0.08	1
E	4.08	3.81	4.43	4.38	4.25	0.27	0.35	0.31	0.17	0.27	7

Table S23. Hydrogen bonding within the 7–aminoacid adducts; hydrogen bond (HB) length (*d*), torsion angle (HB donor, α), dihedral angle (HB donor–acceptor, τ) and coupling constant (HB donor–acceptor, *J*) are given in Angstrőm [Å], degrees [°], and Herz, respectively.

Adduct	**Hydrogen bond**	***d***	**HB angle**		***J***
			θ	**τ**	
7–Ala					
7AlaB	O-H···N	1.892	160.1	-11.0	-2.05
7AlaM	O-H···N	1.906	173.0	-54.7	-2.16
7AlaB	C-H···O=C	2.236	167.0	-177.8	1.39
7AlaM	C-H···O=C	2.146	173.2	101.6	2.24
7–Lys					
7LysB	N-H···O=C	1.851	147.7	-78.7	5.16
7LysP	N-H···O=C	1.816	147.6	0.6	5.78
7–Glu					
7GluB	N-H···O=C	1.906	144.5	10.5	4.56
7GluB6	N-H···O=C	1.961	148.5	-17.8	4.17
7GluB	O-H···N	1.729	169.7	38.0	-1.18
7GluB6	O-H···N	2.225	160.9	65.3	-9.38
7–Met					
7MetB	O-H···O_2S	1.990	144.6	33.7	4.03
7MetB6	O-H···O_2S	1.760	172.3	165.8	7.43

Cartesian coordinates (charge=0, multiplicity=1)**:**

Adduct 7AlaB:

O	-4.639366000	-11.233900000	3.797372000
S	-3.367655000	-10.706917000	3.268262000
C	-2.169313000	-10.975154000	4.568997000
O	-3.230435000	-9.310651000	2.840880000
C	-2.839677000	-11.781354000	1.933462000
N	-1.061477000	-10.234058000	4.600122000
C	-1.708729000	-11.443503000	1.183921000
C	-3.584875000	-12.926761000	1.654644000
C	-0.963637000	-11.660687000	6.328197000
N	-0.335634000	-10.647629000	5.659281000
C	-1.328258000	-12.284953000	0.142652000
H	-1.131668000	-10.548961000	1.402033000
C	-3.187071000	-13.750019000	0.602359000
H	-4.464693000	-13.153437000	2.246291000
C	-0.949685000	-12.562504000	7.417513000
H	0.535703000	-10.181941000	5.858652000
C	-2.057289000	-13.443985000	-0.167568000
H	-0.447937000	-12.032023000	-0.442003000
H	-3.764768000	-14.642016000	0.375842000
C	-1.642727000	-14.323754000	-1.321630000
H	-2.101697000	-15.313914000	-1.257953000
H	-1.944893000	-13.880541000	-2.278268000
H	-0.556360000	-14.451675000	-1.355129000
N	-2.803958000	-12.893247000	6.324395000
C	-2.160091000	-11.901783000	5.643927000
N	-2.063073000	-13.294477000	7.388061000
C	-4.054501000	-13.568428000	6.016278000
H	-0.221594000	-12.711450000	8.200730000
H	-3.875912000	-14.457852000	5.402920000
H	-4.701984000	-12.877020000	5.476876000
H	-4.515467000	-13.868862000	6.957290000
O	-0.086615000	-7.830152000	3.436883000
O	0.358998000	-8.884253000	1.487841000
N	2.111502000	-6.895849000	0.791185000
C	1.071816000	-6.592701000	1.771637000
C	-0.047366000	-5.650746000	1.273201000
C	0.429689000	-7.903833000	2.209202000
H	1.532383000	-6.140113000	2.658114000
H	-0.784984000	-5.455103000	2.057343000
H	0.383997000	-4.693084000	0.962652000
H	-0.562401000	-6.092392000	0.413710000

H	2.325794000	-6.064424000	0.246796000
H	1.748085000	-7.598395000	0.150135000
H	-0.555210000	-8.673356000	3.657049000

Adduct 7AlaB$_a$:

O	-4.639366000	-11.233900000	3.797372000
S	-3.367655000	-10.706917000	3.268262000
C	-2.169313000	-10.975154000	4.568997000
O	-3.230435000	-9.310651000	2.840880000
C	-2.839677000	-11.781354000	1.933462000
N	-1.061477000	-10.234058000	4.600122000
C	-1.708729000	-11.443503000	1.183921000
C	-3.584875000	-12.926761000	1.654644000
C	-0.963637000	-11.660687000	6.328197000
N	-0.335634000	-10.647629000	5.659281000
C	-1.328258000	-12.284953000	0.142652000
H	-1.131668000	-10.548961000	1.402033000
C	-3.187071000	-13.750019000	0.602359000
H	-4.464693000	-13.153437000	2.246291000
C	-0.949685000	-12.562504000	7.417513000
H	0.535703000	-10.181941000	5.858652000
C	-2.057289000	-13.443985000	-0.167568000
H	-0.447937000	-12.032023000	-0.442003000
H	-3.764768000	-14.642016000	0.375842000
C	-1.642727000	-14.323754000	-1.321630000
H	-2.101697000	-15.313914000	-1.257953000
H	-1.944893000	-13.880541000	-2.278268000
H	-0.556360000	-14.451675000	-1.355129000
N	-2.803958000	-12.893247000	6.324395000
C	-2.160091000	-11.901783000	5.643927000
N	-2.063073000	-13.294477000	7.388061000
C	-4.054501000	-13.568428000	6.016278000
H	-0.221594000	-12.711450000	8.200730000
H	-3.875912000	-14.457852000	5.402920000
H	-4.701984000	-12.877020000	5.476876000
H	-4.515467000	-13.868862000	6.957290000
O	-0.086615000	-7.830152000	3.436883000
O	0.358998000	-8.884253000	1.487841000
N	2.111502000	-6.895849000	0.791185000
C	1.071816000	-6.592701000	1.771637000
C	-0.047366000	-5.650746000	1.273201000
C	0.429689000	-7.903833000	2.209202000
H	1.532383000	-6.140113000	2.658114000

H	-0.784984000	-5.455103000	2.057343000
H	0.383997000	-4.693084000	0.962652000
H	-0.562401000	-6.092392000	0.413710000
H	2.325794000	-6.064424000	0.246796000
H	1.748085000	-7.598395000	0.150135000
H	-0.555210000	-8.673356000	3.657049000

Adduct 7AlaB$_b$:

O	-4.144398000	-12.132113000	3.129992000
S	-2.925981000	-11.361371000	2.818828000
C	-2.056403000	-11.212264000	4.375637000
O	-2.992282000	-10.018422000	2.233638000
C	-1.869606000	-12.390820000	1.799803000
N	-1.158943000	-10.239271000	4.534005000
C	-0.696149000	-11.854173000	1.261622000
C	-2.253258000	-13.707712000	1.546414000
C	-1.217911000	-11.413998000	6.443650000
N	-0.653840000	-10.361539000	5.778958000
C	0.099323000	-12.669380000	0.461476000
H	-0.399799000	-10.827887000	1.459682000
C	-1.443192000	-14.501885000	0.736676000
H	-3.176031000	-14.089958000	1.968074000
C	-1.299390000	-12.168250000	7.637149000
H	0.030922000	-9.690079000	6.089208000
C	-0.258717000	-13.997804000	0.183141000
H	1.015614000	-12.261522000	0.043489000
H	-1.737100000	-15.527516000	0.530708000
C	0.602586000	-14.852571000	-0.714254000
H	0.402914000	-15.917486000	-0.567830000
H	0.412831000	-14.623942000	-1.770110000
H	1.666922000	-14.675504000	-0.532355000
N	-2.718741000	-13.028592000	6.227144000
C	-2.134061000	-11.993137000	5.558494000
N	-2.203043000	-13.134707000	7.477734000
C	-3.690539000	-14.004186000	5.759409000
H	-0.775482000	-12.062953000	8.575323000
H	-3.188879000	-14.893408000	5.363480000
H	-4.295179000	-13.546914000	4.976310000
H	-4.314284000	-14.291929000	6.605901000
O	-0.279203000	-7.819869000	3.369611000
O	0.725185000	-8.890970000	1.651315000
N	2.337641000	-6.720420000	1.211943000
C	1.074361000	-6.514383000	1.915993000
C	-0.006389000	-5.749943000	1.118768000
C	0.510654000	-7.878698000	2.295527000

H	1.265190000	-5.967179000	2.847187000
H	-0.918724000	-5.617146000	1.708049000
H	0.368340000	-4.759115000	0.840584000
H	-0.260150000	-6.292920000	0.202330000
H	2.568306000	-5.894100000	0.666638000
H	2.216884000	-7.494751000	0.562053000
H	-0.676034000	-8.709335000	3.547184000

Adduct 7AlaB$_c$:

O	-4.098274000	-9.457132000	6.646963000
S	-3.347403000	-9.222539000	5.399485000
C	-2.067799000	-10.472868000	5.379886000
O	-2.695808000	-7.938245000	5.122821000
C	-4.419222000	-9.642628000	4.025200000
N	-0.975457000	-10.279294000	4.640526000
C	-3.987099000	-9.404536000	2.716779000
C	-5.677981000	-10.181139000	4.291341000
C	-0.761979000	-12.274275000	5.642947000
N	-0.189916000	-11.364582000	4.798556000
C	-4.843012000	-9.725586000	1.667278000
H	-3.007395000	-8.981739000	2.511876000
C	-6.519396000	-10.488183000	3.223181000
H	-5.989867000	-10.340164000	5.317460000
C	-0.656381000	-13.516889000	6.309791000
H	0.701262000	-11.387462000	4.328200000
C	-6.117367000	-10.266885000	1.899466000
H	-4.513022000	-9.547953000	0.647349000
H	-7.503417000	-10.903921000	3.422040000
C	-7.039301000	-10.578625000	0.745945000
H	-7.844601000	-11.254326000	1.046032000
H	-7.503123000	-9.663393000	0.358482000
H	-6.496530000	-11.040768000	-0.084392000
N	-2.550227000	-12.620333000	6.903247000
C	-1.987912000	-11.727676000	6.038449000
N	-1.745762000	-13.702524000	7.054681000
C	-3.845687000	-12.583112000	7.562972000
H	0.127083000	-14.259696000	6.297606000
H	-4.604806000	-13.090883000	6.958773000
H	-4.132964000	-11.542141000	7.711070000
H	-3.750553000	-13.093719000	8.521393000
O	0.386944000	-8.209682000	3.267839000
O	-1.116681000	-8.221204000	1.580479000
N	0.701920000	-7.022303000	-0.079875000
C	0.880012000	-6.877172000	1.362780000
C	0.606457000	-5.462124000	1.920516000

C	-0.058249000	-7.854341000	2.061259000
H	1.905750000	-7.158850000	1.630128000
H	0.771863000	-5.419220000	3.001253000
H	1.276154000	-4.738880000	1.443024000
H	-0.426840000	-5.163816000	1.714663000
H	1.044378000	-6.191762000	-0.555684000
H	-0.295278000	-7.097739000	-0.270768000
H	-0.278511000	-8.788981000	3.716515000

Adduct 7AlaB6:

O	-4.604490000	-11.175054000	3.767244000
S	-3.318186000	-10.684302000	3.252618000
C	-2.137467000	-10.985962000	4.567665000
O	-3.140774000	-9.298649000	2.824377000
C	-2.807580000	-11.775925000	1.920190000
N	-1.011175000	-10.279494000	4.608017000
C	-1.703394000	-11.433448000	1.140003000
C	-3.537215000	-12.937562000	1.680022000
C	-0.968922000	-11.706342000	6.333738000
N	-0.305750000	-10.712483000	5.670624000
C	-1.331011000	-12.285966000	0.106409000
H	-1.139469000	-10.526503000	1.328093000
C	-3.149549000	-13.771683000	0.635248000
H	-4.399806000	-13.169310000	2.291779000
C	-0.990140000	-12.603168000	7.424906000
H	0.577740000	-10.275196000	5.878861000
C	-2.044396000	-13.461059000	-0.165330000
H	-0.470074000	-12.027355000	-0.500805000
H	-3.717290000	-14.675143000	0.439223000
C	-1.647610000	-14.352818000	-1.315015000
H	-1.987530000	-15.379063000	-1.161541000
H	-2.090703000	-13.995189000	-2.250814000
H	-0.564052000	-14.366890000	-1.452230000
N	-2.844978000	-12.880581000	6.319510000
C	-2.165679000	-11.912425000	5.641788000
N	-2.124027000	-13.297914000	7.386352000
C	-4.116500000	-13.516650000	6.006491000
H	-0.275350000	-12.774438000	8.213326000
H	-3.957938000	-14.422679000	5.415587000
H	-4.730070000	-12.814116000	5.445455000
H	-4.602133000	-13.779503000	6.944679000
O	0.011707000	-7.871193000	3.447466000
O	0.413784000	-8.875876000	1.473256000
N	2.077329000	-6.809295000	0.744778000
C	1.057799000	-6.566223000	1.762842000

C	-0.105276000	-5.651501000	1.318552000
C	0.478621000	-7.905051000	2.197297000
H	1.532419000	-6.116731000	2.640249000
H	-0.821195000	-5.494852000	2.129173000
H	0.289832000	-4.676759000	1.018906000
H	-0.631829000	-6.087777000	0.465407000
H	2.273935000	-5.963970000	0.220513000
H	1.753664000	-7.521475000	0.096682000
H	-0.438300000	-8.720282000	3.672562000

Adduct 7AlaB6$_a$:

O	-4.604490000	-11.175054000	3.767244000
S	-3.318186000	-10.684302000	3.252618000
C	-2.137467000	-10.985962000	4.567665000
O	-3.140774000	-9.298649000	2.824377000
C	-2.807580000	-11.775925000	1.920190000
N	-1.011175000	-10.279494000	4.608017000
C	-1.703394000	-11.433448000	1.140003000
C	-3.537215000	-12.937562000	1.680022000
C	-0.968922000	-11.706342000	6.333738000
N	-0.305750000	-10.712483000	5.670624000
C	-1.331011000	-12.285966000	0.106409000
H	-1.139469000	-10.526503000	1.328093000
C	-3.149549000	-13.771683000	0.635248000
H	-4.399806000	-13.169310000	2.291779000
C	-0.990140000	-12.603168000	7.424906000
H	0.577740000	-10.275196000	5.878861000
C	-2.044396000	-13.461059000	-0.165330000
H	-0.470074000	-12.027355000	-0.500805000
H	-3.717290000	-14.675143000	0.439223000
C	-1.647610000	-14.352818000	-1.315015000
H	-1.987530000	-15.379063000	-1.161541000
H	-2.090703000	-13.995189000	-2.250814000
H	-0.564052000	-14.366890000	-1.452230000
N	-2.844978000	-12.880581000	6.319510000
C	-2.165679000	-11.912425000	5.641788000
N	-2.124027000	-13.297914000	7.386352000
C	-4.116500000	-13.516650000	6.006491000
H	-0.275350000	-12.774438000	8.213326000
H	-3.957938000	-14.422679000	5.415587000
H	-4.730070000	-12.814116000	5.445455000
H	-4.602133000	-13.779503000	6.944679000
O	0.011707000	-7.871193000	3.447466000
O	0.413784000	-8.875876000	1.473256000
N	2.077329000	-6.809295000	0.744778000

C	1.057799000	-6.566223000	1.762842000
C	-0.105276000	-5.651501000	1.318552000
C	0.478621000	-7.905051000	2.197297000
H	1.532419000	-6.116731000	2.640249000
H	-0.821195000	-5.494852000	2.129173000
H	0.289832000	-4.676759000	1.018906000
H	-0.631829000	-6.087777000	0.465407000
H	2.273935000	-5.963970000	0.220513000
H	1.753664000	-7.521475000	0.096682000
H	-0.438300000	-8.720282000	3.672562000

Adduct 7AlaB6$_b$:

O	-4.097313000	-12.044778000	3.071545000
S	-2.848835000	-11.317311000	2.801309000
C	-2.013086000	-11.214273000	4.384599000
O	-2.852206000	-9.973474000	2.228036000
C	-1.802208000	-12.376524000	1.796283000
N	-1.097315000	-10.269425000	4.578739000
C	-0.633632000	-11.855425000	1.240275000
C	-2.188363000	-13.695976000	1.576035000
C	-1.234454000	-11.466267000	6.466581000
N	-0.626584000	-10.420103000	5.831794000
C	0.156470000	-12.688291000	0.456100000
H	-0.337997000	-10.826382000	1.411915000
C	-1.384389000	-14.508861000	0.781491000
H	-3.109580000	-14.068093000	2.005918000
C	-1.366988000	-12.229221000	7.647986000
H	0.067609000	-9.773695000	6.171586000
C	-0.203593000	-14.020574000	0.211293000
H	1.068695000	-12.290173000	0.024512000
H	-1.682857000	-15.535937000	0.600231000
C	0.650672000	-14.895676000	-0.671302000
H	0.443126000	-15.954782000	-0.506647000
H	0.459836000	-14.681072000	-1.728268000
H	1.714525000	-14.722677000	-0.491933000
N	-2.772198000	-13.034387000	6.193334000
C	-2.142185000	-12.009232000	5.552878000
N	-2.291288000	-13.165661000	7.451682000
C	-3.763071000	-13.975254000	5.690802000
H	-0.866488000	-12.151691000	8.599487000
H	-3.278537000	-14.885752000	5.328338000
H	-4.312330000	-13.501856000	4.879098000
H	-4.436766000	-14.227383000	6.508079000
O	-0.208857000	-7.827419000	3.402213000
O	0.791263000	-8.867801000	1.674077000

N	2.261795000	-6.609118000	1.135987000
C	1.015835000	-6.472068000	1.886374000
C	-0.131222000	-5.768373000	1.127753000
C	0.543542000	-7.858881000	2.299256000
H	1.214450000	-5.910554000	2.804429000
H	-1.024022000	-5.677916000	1.751306000
H	0.185285000	-4.762720000	0.836952000
H	-0.390827000	-6.323720000	0.222288000
H	2.449129000	-5.775806000	0.589633000
H	2.198036000	-7.401253000	0.503245000
H	-0.569111000	-8.724282000	3.603292000

Adduct 7AlaB6$_c$:

O	-4.230806000	-9.812342000	6.677874000
S	-3.468310000	-9.418780000	5.485081000
C	-2.147951000	-10.626849000	5.361202000
O	-2.852781000	-8.099534000	5.361922000
C	-4.502526000	-9.694116000	4.041338000
N	-1.136425000	-10.378079000	4.536856000
C	-4.158322000	-9.087364000	2.833720000
C	-5.645110000	-10.480681000	4.156252000
C	-0.737381000	-12.352219000	5.523928000
N	-0.291157000	-11.423781000	4.623827000
C	-4.972419000	-9.293689000	1.725450000
H	-3.287033000	-8.446648000	2.762181000
C	-6.448192000	-10.671236000	3.034672000
H	-5.908489000	-10.913864000	5.112586000
C	-0.515010000	-13.586029000	6.174160000
H	0.574721000	-11.389439000	4.107935000
C	-6.123250000	-10.089291000	1.804606000
H	-4.714360000	-8.815829000	0.786254000
H	-7.346166000	-11.273402000	3.121569000
C	-6.981835000	-10.320698000	0.586428000
H	-7.997273000	-10.611213000	0.862891000
H	-7.038473000	-9.423960000	-0.034754000
H	-6.565813000	-11.121874000	-0.033911000
N	-2.395384000	-12.788716000	6.922452000
C	-1.952966000	-11.871561000	6.016269000
N	-1.526985000	-13.822466000	7.005835000
C	-3.623511000	-12.806124000	7.704203000
H	0.298768000	-14.288625000	6.097836000
H	-4.341384000	-13.506195000	7.269684000
H	-4.038908000	-11.800202000	7.714858000
H	-3.385976000	-13.120328000	8.719932000
O	0.169218000	-8.449248000	3.039534000

O	-1.466301000	-7.750109000	1.664306000
N	0.400686000	-6.656539000	-0.029356000
C	0.762108000	-6.860506000	1.367631000
C	0.913414000	-5.570925000	2.208451000
C	-0.309257000	-7.729152000	2.011271000
H	1.705018000	-7.413643000	1.416422000
H	1.206404000	-5.797334000	3.236722000
H	1.685491000	-4.936239000	1.764861000
H	-0.025307000	-5.010676000	2.223858000
H	0.935846000	-5.900327000	-0.439095000
H	-0.587804000	-6.439970000	-0.109945000
H	-0.574806000	-8.909491000	3.479734000

Adduct 7AlaC:

O	-4.541589000	-11.075495000	3.766341000
S	-3.242606000	-10.625700000	3.259539000
C	-2.089932000	-10.957142000	4.566573000
O	-3.016429000	-9.248642000	2.839948000
C	-2.762395000	-11.721436000	1.945985000
N	-0.969489000	-10.256457000	4.640852000
C	-1.615980000	-11.440730000	1.207050000
C	-3.552479000	-12.830126000	1.672808000
C	-0.954831000	-11.714903000	6.327289000
N	-0.283141000	-10.708874000	5.698790000
C	-1.265994000	-12.304367000	0.181029000
H	-1.005068000	-10.568355000	1.423615000
C	-3.184185000	-13.677336000	0.636269000
H	-4.446357000	-13.009052000	2.258824000
C	-0.994748000	-12.641085000	7.393389000
H	0.598282000	-10.278016000	5.925592000
C	-2.040327000	-13.428163000	-0.121918000
H	-0.372319000	-12.097667000	-0.400015000
H	-3.797165000	-14.544660000	0.411297000
C	-1.655133000	-14.334088000	-1.259969000
H	-2.172998000	-15.293606000	-1.201616000
H	-1.909718000	-13.877711000	-2.222090000
H	-0.579189000	-14.525923000	-1.267419000
N	-2.821410000	-12.886872000	6.254689000
C	-2.133601000	-11.903503000	5.617523000
N	-2.122848000	-13.330193000	7.317365000
C	-4.084377000	-13.503652000	5.902536000
H	-0.290860000	-12.832226000	8.188600000
H	-3.925384000	-14.381507000	5.270052000
H	-4.692779000	-12.773868000	5.369227000
H	-4.577985000	-13.809801000	6.823652000

O	-0.064866000	-7.845938000	3.456537000
O	0.403746000	-8.927736000	1.542953000
N	2.000165000	-6.890363000	0.724448000
C	1.011283000	-6.609620000	1.751451000
C	-0.157444000	-5.718196000	1.302155000
C	0.437018000	-7.928214000	2.232875000
H	1.498279000	-6.134709000	2.610414000
H	-0.860801000	-5.542360000	2.119535000
H	0.221921000	-4.750670000	0.960980000
H	-0.696670000	-6.188574000	0.474819000
H	2.141515000	-6.075301000	0.137599000
H	1.652555000	-7.646255000	0.141179000
H	-0.496699000	-8.698766000	3.703405000

Adduct 7AlaC $_a$:

O	-4.541589000	-11.075495000	3.766341000
S	-3.242606000	-10.625700000	3.259539000
C	-2.089932000	-10.957142000	4.566573000
O	-3.016429000	-9.248642000	2.839948000
C	-2.762395000	-11.721436000	1.945985000
N	-0.969489000	-10.256457000	4.640852000
C	-1.615980000	-11.440730000	1.207050000
C	-3.552479000	-12.830126000	1.672808000
C	-0.954831000	-11.714903000	6.327289000
N	-0.283141000	-10.708874000	5.698790000
C	-1.265994000	-12.304367000	0.181029000
H	-1.005068000	-10.568355000	1.423615000
C	-3.184185000	-13.677336000	0.636269000
H	-4.446357000	-13.009052000	2.258824000
C	-0.994748000	-12.641085000	7.393389000
H	0.598282000	-10.278016000	5.925592000
C	-2.040327000	-13.428163000	-0.121918000
H	-0.372319000	-12.097667000	-0.400015000
H	-3.797165000	-14.544660000	0.411297000
C	-1.655133000	-14.334088000	-1.259969000
H	-2.172998000	-15.293606000	-1.201616000
H	-1.909718000	-13.877711000	-2.222090000
H	-0.579189000	-14.525923000	-1.267419000
N	-2.821410000	-12.886872000	6.254689000
C	-2.133601000	-11.903503000	5.617523000
N	-2.122848000	-13.330193000	7.317365000
C	-4.084377000	-13.503652000	5.902536000
H	-0.290860000	-12.832226000	8.188600000
H	-3.925384000	-14.381507000	5.270052000
H	-4.692779000	-12.773868000	5.369227000

H	-4.577985000	-13.809801000	6.823652000
O	-0.064866000	-7.845938000	3.456537000
O	0.403746000	-8.927736000	1.542953000
N	2.000165000	-6.890363000	0.724448000
C	1.011283000	-6.609620000	1.751451000
C	-0.157444000	-5.718196000	1.302155000
C	0.437018000	-7.928214000	2.232875000
H	1.498279000	-6.134709000	2.610414000
H	-0.860801000	-5.542360000	2.119535000
H	0.221921000	-4.750670000	0.960980000
H	-0.696670000	-6.188574000	0.474819000
H	2.141515000	-6.075301000	0.137599000
H	1.652555000	-7.646255000	0.141179000
H	-0.496699000	-8.698766000	3.703405000

Adduct 7AlaC$_b$:

O	-4.046647000	-11.850298000	3.094281000
S	-2.762680000	-11.191142000	2.842493000
C	-1.936362000	-11.160977000	4.412198000
O	-2.685738000	-9.840101000	2.302132000
C	-1.780695000	-12.277938000	1.837036000
N	-1.015115000	-10.239777000	4.645667000
C	-0.556332000	-11.832225000	1.345391000
C	-2.262900000	-13.547917000	1.549740000
C	-1.166809000	-11.506437000	6.474157000
N	-0.549175000	-10.443515000	5.885183000
C	0.190296000	-12.694300000	0.557839000
H	-0.188916000	-10.834270000	1.569434000
C	-1.499063000	-14.391217000	0.753791000
H	-3.227753000	-13.855776000	1.935430000
C	-1.308717000	-12.321497000	7.619342000
H	0.154049000	-9.820473000	6.247531000
C	-0.266086000	-13.979071000	0.248791000
H	1.148034000	-12.359131000	0.171309000
H	-1.868405000	-15.384765000	0.519169000
C	0.551927000	-14.886156000	-0.630063000
H	0.199683000	-15.918355000	-0.578973000
H	0.496177000	-14.567217000	-1.675899000
H	1.606487000	-14.870341000	-0.342953000
N	-2.713005000	-13.041645000	6.135138000
C	-2.074218000	-11.997957000	5.544682000
N	-2.238423000	-13.233649000	7.380796000
C	-3.713349000	-13.936331000	5.588914000
H	-0.806527000	-12.290515000	8.573908000
H	-3.244274000	-14.816640000	5.140640000

H	-4.284597000	-13.400362000	4.831538000
H	-4.363993000	-14.251966000	6.403104000
O	-0.253173000	-7.813202000	3.405537000
O	0.817178000	-8.927523000	1.773190000
N	2.207346000	-6.701067000	1.089162000
C	0.982017000	-6.528717000	1.850675000
C	-0.180506000	-5.887519000	1.076352000
C	0.527990000	-7.891478000	2.337739000
H	1.183767000	-5.918528000	2.738224000
H	-1.066161000	-5.779311000	1.706875000
H	0.111462000	-4.895206000	0.720597000
H	-0.443939000	-6.500774000	0.209657000
H	2.345723000	-5.918000000	0.459606000
H	2.124194000	-7.546902000	0.532412000
H	-0.588807000	-8.709928000	3.646806000

Adduct 7AlaC$_c$:

O	-3.927450000	-9.314805000	6.541111000
S	-3.196233000	-9.188906000	5.277802000
C	-1.978320000	-10.478365000	5.310900000
O	-2.498856000	-7.962493000	4.913256000
C	-4.299731000	-9.646915000	3.962748000
N	-0.870110000	-10.346951000	4.599415000
C	-3.883838000	-9.504235000	2.641171000
C	-5.565793000	-10.119454000	4.281266000
C	-0.762817000	-12.316129000	5.639783000
N	-0.135403000	-11.450338000	4.794115000
C	-4.765120000	-9.857639000	1.631673000
H	-2.895666000	-9.121648000	2.399571000
C	-6.432871000	-10.461531000	3.251913000
H	-5.864615000	-10.196361000	5.320171000
C	-0.726713000	-13.546713000	6.332856000
H	0.761133000	-11.522348000	4.341341000
C	-6.045478000	-10.340961000	1.917688000
H	-4.452831000	-9.748814000	0.597435000
H	-7.428504000	-10.823184000	3.489595000
C	-6.976993000	-10.733033000	0.802810000
H	-8.000512000	-10.858972000	1.161381000
H	-6.983357000	-9.980603000	0.010005000
H	-6.664332000	-11.678982000	0.348804000
N	-2.583596000	-12.562603000	6.859150000
C	-1.964395000	-11.716966000	5.994647000
N	-1.834069000	-13.665309000	7.049069000
C	-3.883647000	-12.445615000	7.488137000
H	0.022609000	-14.322882000	6.353710000

H	-4.654416000	-12.927649000	6.880298000
H	-4.119232000	-11.388482000	7.607370000
H	-3.834050000	-12.935718000	8.459346000
O	0.393230000	-8.178184000	3.288039000
O	-1.050390000	-8.340375000	1.573194000
N	0.593054000	-6.878610000	-0.016260000
C	0.768920000	-6.773826000	1.422289000
C	0.356004000	-5.424463000	2.031429000
C	-0.058047000	-7.859786000	2.083477000
H	1.817242000	-6.962690000	1.679099000
H	0.518214000	-5.409740000	3.111773000
H	0.944597000	-4.618200000	1.584214000
H	-0.702283000	-5.228084000	1.836412000
H	0.814549000	-5.996243000	-0.464679000
H	-0.381009000	-7.096693000	-0.206033000
H	-0.214868000	-8.827796000	3.716040000

Adduct 7AlaP:

O	-4.585991000	-11.117474000	3.771430000
S	-3.297109000	-10.640560000	3.261395000
C	-2.130906000	-10.951678000	4.560397000
O	-3.098425000	-9.259427000	2.837960000
C	-2.796114000	-11.728347000	1.949805000
N	-1.016724000	-10.232065000	4.623790000
C	-1.649553000	-11.429894000	1.214368000
C	-3.570810000	-12.849834000	1.672501000
C	-0.959385000	-11.691675000	6.308557000
N	-0.316071000	-10.675957000	5.671577000
C	-1.283925000	-12.287580000	0.186210000
H	-1.049143000	-10.549535000	1.435923000
C	-3.187229000	-13.689917000	0.633344000
H	-4.464150000	-13.041584000	2.257905000
C	-0.973516000	-12.618393000	7.372093000
H	0.560454000	-10.232083000	5.889396000
C	-2.042695000	-13.423235000	-0.122969000
H	-0.389910000	-12.066553000	-0.391085000
H	-3.788271000	-14.566065000	0.404505000
C	-1.644213000	-14.318884000	-1.260564000
H	-2.134059000	-15.293733000	-1.195848000
H	-1.922705000	-13.871594000	-2.221824000
H	-0.562298000	-14.479430000	-1.280564000
N	-2.807378000	-12.893627000	6.254936000
C	-2.147434000	-11.899841000	5.608985000
N	-2.093727000	-13.327862000	7.307304000
C	-4.057488000	-13.532067000	5.913433000

H	-0.259549000	-12.800217000	8.161489000
H	-3.886834000	-14.405857000	5.276471000
H	-4.685386000	-12.812486000	5.386443000
H	-4.537503000	-13.850345000	6.838814000
O	-0.083761000	-7.836840000	3.453315000
O	0.409472000	-8.929489000	1.548836000
N	2.039489000	-6.908414000	0.761801000
C	1.034614000	-6.617162000	1.766333000
C	-0.119410000	-5.718651000	1.295572000
C	0.438493000	-7.929099000	2.239647000
H	1.508414000	-6.142408000	2.635071000
H	-0.837156000	-5.533190000	2.099871000
H	0.274174000	-4.754011000	0.958586000
H	-0.648043000	-6.186916000	0.458820000
H	2.186240000	-6.096854000	0.171909000
H	1.688878000	-7.660907000	0.175392000
H	-0.526387000	-8.686116000	3.692824000

Adduct 7AlaP$_a$:

O	-4.585991000	-11.117474000	3.771430000
S	-3.297109000	-10.640560000	3.261395000
C	-2.130906000	-10.951678000	4.560397000
O	-3.098425000	-9.259427000	2.837960000
C	-2.796114000	-11.728347000	1.949805000
N	-1.016724000	-10.232065000	4.623790000
C	-1.649553000	-11.429894000	1.214368000
C	-3.570810000	-12.849834000	1.672501000
C	-0.959385000	-11.691675000	6.308557000
N	-0.316071000	-10.675957000	5.671577000
C	-1.283925000	-12.287580000	0.186210000
H	-1.049143000	-10.549535000	1.435923000
C	-3.187229000	-13.689917000	0.633344000
H	-4.464150000	-13.041584000	2.257905000
C	-0.973516000	-12.618393000	7.372093000
H	0.560454000	-10.232083000	5.889396000
C	-2.042695000	-13.423235000	-0.122969000
H	-0.389910000	-12.066553000	-0.391085000
H	-3.788271000	-14.566065000	0.404505000
C	-1.644213000	-14.318884000	-1.260564000
H	-2.134059000	-15.293733000	-1.195848000
H	-1.922705000	-13.871594000	-2.221824000
H	-0.562298000	-14.479430000	-1.280564000
N	-2.807378000	-12.893627000	6.254936000
C	-2.147434000	-11.899841000	5.608985000
N	-2.093727000	-13.327862000	7.307304000

C	-4.057488000	-13.532067000	5.913433000
H	-0.259549000	-12.800217000	8.161489000
H	-3.886834000	-14.405857000	5.276471000
H	-4.685386000	-12.812486000	5.386443000
H	-4.537503000	-13.850345000	6.838814000
O	-0.083761000	-7.836840000	3.453315000
O	0.409472000	-8.929489000	1.548836000
N	2.039489000	-6.908414000	0.761801000
C	1.034614000	-6.617162000	1.766333000
C	-0.119410000	-5.718651000	1.295572000
C	0.438493000	-7.929099000	2.239647000
H	1.508414000	-6.142408000	2.635071000
H	-0.837156000	-5.533190000	2.099871000
H	0.274174000	-4.754011000	0.958586000
H	-0.648043000	-6.186916000	0.458820000
H	2.186240000	-6.096854000	0.171909000
H	1.688878000	-7.660907000	0.175392000
H	-0.526387000	-8.686116000	3.692824000

Adduct 7AlaP$_b$:

O	-4.092559000	-11.921454000	3.095372000
S	-2.827261000	-11.231243000	2.827804000
C	-1.987214000	-11.163151000	4.388251000
O	-2.786604000	-9.885386000	2.268390000
C	-1.822309000	-12.305085000	1.832282000
N	-1.082197000	-10.215032000	4.600131000
C	-0.605003000	-11.837862000	1.337101000
C	-2.280622000	-13.588168000	1.553113000
C	-1.178491000	-11.462000000	6.445881000
N	-0.598892000	-10.394517000	5.832922000
C	0.158785000	-12.691121000	0.553078000
H	-0.255313000	-10.830802000	1.556458000
C	-1.500193000	-14.421560000	0.759619000
H	-3.240223000	-13.911467000	1.943149000
C	-1.285840000	-12.265849000	7.600234000
H	0.093487000	-9.751040000	6.178402000
C	-0.273190000	-13.988497000	0.250258000
H	1.110731000	-12.338635000	0.164521000
H	-1.851133000	-15.424263000	0.530215000
C	0.559859000	-14.883007000	-0.622184000
H	0.220627000	-15.920732000	-0.574683000
H	0.506818000	-14.563440000	-1.669266000
H	1.613727000	-14.853822000	-0.329283000
N	-2.689739000	-13.039324000	6.145237000
C	-2.088958000	-11.989562000	5.530994000

N	-2.197297000	-13.206518000	7.384082000
C	-3.666866000	-13.965421000	5.621215000
H	-0.774139000	-12.212339000	8.549575000
H	-3.176906000	-14.838287000	5.178071000
H	-4.260405000	-13.454243000	4.862114000
H	-4.301607000	-14.289685000	6.445865000
O	-0.281649000	-7.805113000	3.383162000
O	0.802394000	-8.925612000	1.760202000
N	2.248811000	-6.720144000	1.135175000
C	1.014110000	-6.531866000	1.872239000
C	-0.120852000	-5.856900000	1.087047000
C	0.520409000	-7.890448000	2.332226000
H	1.209589000	-5.936081000	2.773260000
H	-1.016534000	-5.735959000	1.703038000
H	0.199012000	-4.865582000	0.749368000
H	-0.382221000	-6.453216000	0.206638000
H	2.402674000	-5.937820000	0.508820000
H	2.152969000	-7.559111000	0.569620000
H	-0.635820000	-8.698755000	3.608864000

Adduct 7AlaP$_c$:

O	-3.984553000	-9.423013000	6.561997000
S	-3.240332000	-9.237767000	5.312754000
C	-2.006281000	-10.510989000	5.304761000
O	-2.558054000	-7.987625000	5.000371000
C	-4.320520000	-9.665131000	3.969212000
N	-0.892233000	-10.335128000	4.604254000
C	-3.892839000	-9.468203000	2.656296000
C	-5.584146000	-10.169661000	4.257920000
C	-0.763120000	-12.345461000	5.560298000
N	-0.148008000	-11.434378000	4.758382000
C	-4.759968000	-9.798973000	1.624164000
H	-2.906699000	-9.062013000	2.438715000
C	-6.436560000	-10.487202000	3.206542000
H	-5.891139000	-10.287542000	5.292041000
C	-0.715339000	-13.601935000	6.200018000
H	0.751791000	-11.475296000	4.309613000
C	-6.037618000	-10.312890000	1.878701000
H	-4.438215000	-9.647586000	0.597066000
H	-7.430182000	-10.871818000	3.421053000
C	-6.949497000	-10.681474000	0.743826000
H	-7.983666000	-10.793067000	1.078997000
H	-6.925605000	-9.925198000	-0.046254000
H	-6.642781000	-11.631601000	0.291217000
N	-2.588100000	-12.668718000	6.755281000

C	-1.980092000	-11.776733000	5.933819000
N	-1.828556000	-13.767015000	6.904272000
C	-3.892622000	-12.598452000	7.371933000
H	0.043971000	-14.369642000	6.195558000
H	-4.653391000	-13.047716000	6.725547000
H	-4.138536000	-11.551088000	7.552274000
H	-3.850777000	-13.147131000	8.312779000
O	0.384623000	-8.146538000	3.362438000
O	-1.037787000	-8.263365000	1.622589000
N	0.632809000	-6.765945000	0.098500000
C	0.787816000	-6.699088000	1.538963000
C	0.370150000	-5.367356000	2.181394000
C	-0.051354000	-7.798899000	2.161090000
H	1.833613000	-6.897030000	1.807080000
H	0.518143000	-5.381988000	3.265004000
H	0.967618000	-4.549734000	1.764734000
H	-0.685830000	-5.161619000	1.977682000
H	0.850357000	-5.866751000	-0.316482000
H	-0.341014000	-6.975590000	-0.103252000
H	-0.231474000	-8.804943000	3.764389000

Adduct 7AlaM:

O	-4.307178000	-10.607855000	3.731714000
S	-2.939284000	-10.357671000	3.268192000
C	-1.887438000	-10.871203000	4.600753000
O	-2.482829000	-9.038449000	2.843188000
C	-2.573547000	-11.541327000	1.991024000
N	-0.706603000	-10.275657000	4.786461000
C	-1.363657000	-11.441714000	1.301962000
C	-3.497224000	-12.541416000	1.702784000
C	-0.921682000	-11.873755000	6.350479000
N	-0.130624000	-10.883615000	5.844823000
C	-1.089485000	-12.372197000	0.309847000
H	-0.655110000	-10.648833000	1.537364000
C	-3.201846000	-13.459246000	0.700072000
H	-4.436229000	-12.579014000	2.247199000
C	-1.104541000	-12.879762000	7.318677000
H	0.767399000	-10.554394000	6.156372000
C	-1.998402000	-13.391134000	-0.007811000
H	-0.150890000	-12.305587000	-0.235771000
H	-3.918714000	-14.240598000	0.458171000
C	-1.682688000	-14.378822000	-1.088498000
H	-2.467986000	-15.131054000	-1.192841000
H	-1.565276000	-13.883521000	-2.058014000
H	-0.741500000	-14.901593000	-0.889987000

N	-2.877001000	-12.860885000	6.064258000
C	-2.070602000	-11.890555000	5.558553000
N	-2.286176000	-13.468722000	7.123373000
C	-4.142123000	-13.346945000	5.563732000
H	-0.474031000	-13.203846000	8.132767000
H	-3.992624000	-14.114407000	4.797061000
H	-4.699697000	-12.512747000	5.135244000
H	-4.691444000	-13.779650000	6.398809000
O	0.189827000	-7.793873000	3.615044000
O	0.694940000	-8.996738000	1.769600000
N	1.742187000	-6.774054000	0.581861000
C	0.801738000	-6.594135000	1.677483000
C	-0.580734000	-6.065949000	1.271268000
C	0.583892000	-7.931173000	2.350830000
H	1.230442000	-5.907599000	2.419624000
H	-1.241968000	-5.955360000	2.135641000
H	-0.485531000	-5.090400000	0.783918000
H	-1.058703000	-6.755972000	0.567437000
H	1.619439000	-6.024906000	-0.090284000
H	1.492474000	-7.638576000	0.108944000
H	-0.112000000	-8.672945000	3.942830000

Adduct 7AlaM$_a$:

O	-4.307178000	-10.607855000	3.731714000
S	-2.939284000	-10.357671000	3.268192000
C	-1.887438000	-10.871203000	4.600753000
O	-2.482829000	-9.038449000	2.843188000
C	-2.573547000	-11.541327000	1.991024000
N	-0.706603000	-10.275657000	4.786461000
C	-1.363657000	-11.441714000	1.301962000
C	-3.497224000	-12.541416000	1.702784000
C	-0.921682000	-11.873755000	6.350479000
N	-0.130624000	-10.883615000	5.844823000
C	-1.089485000	-12.372197000	0.309847000
H	-0.655110000	-10.648833000	1.537364000
C	-3.201846000	-13.459246000	0.700072000
H	-4.436229000	-12.579014000	2.247199000
C	-1.104541000	-12.879762000	7.318677000
H	0.767399000	-10.554394000	6.156372000
C	-1.998402000	-13.391134000	-0.007811000
H	-0.150890000	-12.305587000	-0.235771000
H	-3.918714000	-14.240598000	0.458171000
C	-1.682688000	-14.378822000	-1.088498000
H	-2.467986000	-15.131054000	-1.192841000
H	-1.565276000	-13.883521000	-2.058014000

H	-0.741500000	-14.901593000	-0.889987000
N	-2.877001000	-12.860885000	6.064258000
C	-2.070602000	-11.890555000	5.558553000
N	-2.286176000	-13.468722000	7.123373000
C	-4.142123000	-13.346945000	5.563732000
H	-0.474031000	-13.203846000	8.132767000
H	-3.992624000	-14.114407000	4.797061000
H	-4.699697000	-12.512747000	5.135244000
H	-4.691444000	-13.779650000	6.398809000
O	0.189827000	-7.793873000	3.615044000
O	0.694940000	-8.996738000	1.769600000
N	1.742187000	-6.774054000	0.581861000
C	0.801738000	-6.594135000	1.677483000
C	-0.580734000	-6.065949000	1.271268000
C	0.583892000	-7.931173000	2.350830000
H	1.230442000	-5.907599000	2.419624000
H	-1.241968000	-5.955360000	2.135641000
H	-0.485531000	-5.090400000	0.783918000
H	-1.058703000	-6.755972000	0.567437000
H	1.619439000	-6.024906000	-0.090284000
H	1.492474000	-7.638576000	0.108944000
H	-0.112000000	-8.672945000	3.942830000

Adduct 7AlaM$_b$:

O	-3.881487000	-11.298049000	3.017722000
S	-2.499245000	-10.831638000	2.874277000
C	-1.769397000	-11.010451000	4.480735000
O	-2.167788000	-9.493551000	2.395977000
C	-1.618939000	-12.035482000	1.904031000
N	-0.805716000	-10.174377000	4.875120000
C	-0.301985000	-11.769442000	1.525595000
C	-2.256329000	-13.219232000	1.545237000
C	-1.144584000	-11.658483000	6.527451000
N	-0.435648000	-10.569077000	6.111658000
C	0.374974000	-12.720369000	0.775224000
H	0.177533000	-10.834770000	1.812658000
C	-1.558535000	-14.154906000	0.788584000
H	-3.287125000	-13.386420000	1.843502000
C	-1.397523000	-12.605206000	7.538835000
H	0.273805000	-10.041071000	6.590967000
C	-0.237572000	-13.922530000	0.394586000
H	1.401540000	-12.525838000	0.472825000
H	-2.047174000	-15.080845000	0.493998000
C	0.510920000	-14.928074000	-0.424973000
H	-0.068219000	-15.842268000	-0.574233000

H	0.759904000	-14.528036000	-1.413600000
H	1.459210000	-15.203613000	0.047230000
N	-2.744372000	-13.043555000	5.892821000
C	-2.018233000	-11.969477000	5.484739000
N	-2.359596000	-13.436447000	7.132876000
C	-3.720309000	-13.815404000	5.158535000
H	-0.960114000	-12.731674000	8.517619000
H	-3.235662000	-14.593397000	4.559316000
H	-4.279373000	-13.148528000	4.500104000
H	-4.390212000	-14.284888000	5.877721000
O	-0.076954000	-7.674760000	3.623793000
O	1.093909000	-8.915131000	2.141537000
N	1.973877000	-6.653481000	0.899254000
C	0.780023000	-6.564688000	1.726109000
C	-0.533982000	-6.370439000	0.957316000
C	0.645433000	-7.846380000	2.518503000
H	0.888852000	-5.736465000	2.439140000
H	-1.390846000	-6.295938000	1.632963000
H	-0.489343000	-5.456357000	0.356683000
H	-0.709443000	-7.216428000	0.283879000
H	1.885795000	-6.016411000	0.115439000
H	2.005472000	-7.593662000	0.514118000

Adduct 7AlaM$_c$:

O	-4.501431000	-10.149590000	6.458473000
S	-4.790552000	-9.239511000	5.345181000
C	-3.319522000	-9.225247000	4.365749000
O	-5.228070000	-7.863508000	5.554530000
C	-5.984164000	-10.038274000	4.290134000
N	-3.169855000	-8.302832000	3.407815000
C	-6.673808000	-9.278198000	3.346535000
C	-6.201980000	-11.406690000	4.411491000
C	-1.355299000	-9.634856000	3.393521000
N	-1.984818000	-8.564869000	2.825250000
C	-7.592059000	-9.907038000	2.517964000
H	-6.487021000	-8.210458000	3.278994000
C	-7.128494000	-12.019275000	3.574316000
H	-5.660541000	-11.970428000	5.165748000
C	-0.214492000	-10.462477000	3.424951000
H	-1.618646000	-7.942105000	2.119699000
C	-7.834798000	-11.283681000	2.618182000
H	-8.136744000	-9.322990000	1.779377000
H	-7.311062000	-13.087726000	3.664350000
C	-8.843671000	-11.943113000	1.728718000

H	-8.787548000	-13.032455000	1.790588000
H	-9.863893000	-11.651328000	2.001488000
H	-8.705636000	-11.656540000	0.681740000
N	-1.573022000	-11.151955000	4.980152000
C	-2.208238000	-10.099993000	4.394975000
N	-0.370206000	-11.377772000	4.384426000
C	-2.043464000	-12.059376000	5.999557000
H	0.691983000	-10.436997000	2.829413000
H	-2.752342000	-12.784974000	5.586009000
H	-2.541389000	-11.500086000	6.791507000
H	-1.175862000	-12.590287000	6.388736000
O	0.708838000	-7.042965000	4.213603000
O	0.495969000	-7.448673000	2.002480000
N	2.610194000	-9.145672000	2.053961000
C	2.475020000	-8.209964000	3.158924000
C	3.549709000	-7.118541000	3.236143000
C	1.120928000	-7.550465000	3.042188000
H	2.479344000	-8.772978000	4.101670000
H	3.398904000	-6.460003000	4.096107000
H	4.539325000	-7.574371000	3.330439000
H	3.544661000	-6.507103000	2.327435000
H	3.575289000	-9.445960000	1.979563000
H	2.375100000	-8.663952000	1.191269000
H	-0.152634000	-6.624019000	4.064181000

Adduct 7LysB:

O	-4.399916000	-10.946267000	6.655317000
S	-3.440286000	-10.114579000	5.906725000
C	-2.342564000	-11.267903000	5.101795000
O	-2.613961000	-9.100642000	6.570707000
C	-4.329841000	-9.314594000	4.569496000
N	-1.248380000	-10.808577000	4.485338000
C	-3.750589000	-8.222391000	3.918301000
C	-5.594297000	-9.781041000	4.211767000
C	-1.261593000	-13.020063000	4.224866000
N	-0.599450000	-11.860302000	3.958088000
C	-4.451911000	-7.603734000	2.887964000
H	-2.776547000	-7.857598000	4.225672000
C	-6.282189000	-9.145342000	3.179443000
H	-6.034426000	-10.612450000	4.751033000
C	-1.291553000	-14.429229000	4.095161000
H	0.272695000	-11.633831000	3.467466000
C	-5.722947000	-8.055442000	2.499202000
H	-4.009945000	-6.750017000	2.381463000
H	-7.272077000	-9.497587000	2.902809000

C	-6.459691000	-7.388739000	1.363325000
H	-7.532124000	-7.596681000	1.403959000
H	-6.321074000	-6.303584000	1.380014000
H	-6.090901000	-7.747203000	0.394485000
N	-3.047158000	-13.848064000	5.247224000
C	-2.404159000	-12.677940000	4.962792000
N	-2.374063000	-14.899707000	4.710417000
C	-4.312618000	-14.077423000	5.925217000
H	-0.603624000	-15.105664000	3.610375000
H	-5.132109000	-14.157682000	5.203115000
H	-4.504467000	-13.243726000	6.599620000
H	-4.235615000	-15.011801000	6.482074000
O	0.186097000	-9.664278000	1.159823000
O	1.458671000	-10.327428000	2.908268000
N	3.286701000	-8.250190000	2.464445000
N	6.176794000	-8.168775000	-3.587809000
C	3.887362000	-8.077345000	-0.502897000
C	2.987523000	-9.119537000	0.169035000
C	4.630360000	-8.630811000	-1.723827000
C	2.297848000	-8.587994000	1.446857000
C	5.519987000	-7.591634000	-2.408719000
C	1.267939000	-9.614687000	1.924723000
H	4.599668000	-7.698271000	0.237838000
H	3.271826000	-7.219177000	-0.808586000
H	3.581416000	-10.004045000	0.440844000
H	2.216957000	-9.460715000	-0.531462000
H	3.920380000	-9.019886000	-2.464294000
H	5.251334000	-9.485109000	-1.414722000
H	1.743324000	-7.680120000	1.180483000
H	6.220584000	-7.171991000	-1.663606000
H	4.897134000	-6.755355000	-2.751009000
H	3.625650000	-9.117865000	2.877925000
H	2.832713000	-7.752567000	3.227144000
H	6.841545000	-8.880609000	-3.290008000
H	6.727179000	-7.455060000	-4.059989000
H	-0.448305000	-10.365910000	1.488868000

Adduct 7LysB$_a$:

O	-4.356548000	-10.339574000	6.233349000
S	-3.237608000	-9.782753000	5.451482000
C	-2.225092000	-11.186101000	5.014160000
O	-2.356656000	-8.744555000	5.997349000
C	-3.895082000	-9.186101000	3.892689000
N	-1.057239000	-10.983462000	4.394942000
C	-3.141257000	-8.290491000	3.129696000

C	-5.154964000	-9.610801000	3.472749000
C	-1.283527000	-13.183511000	4.651472000
N	-0.491684000	-12.182524000	4.176935000
C	-3.662269000	-7.828597000	1.925089000
H	-2.173451000	-7.952702000	3.483768000
C	-5.660542000	-9.133929000	2.264356000
H	-5.731867000	-10.284915000	4.096044000
C	-1.451325000	-14.575277000	4.846440000
H	0.417595000	-12.157350000	3.702797000
C	-4.924246000	-8.243897000	1.471340000
H	-3.083953000	-7.127252000	1.329757000
H	-6.645844000	-9.452989000	1.936052000
C	-5.464692000	-7.748740000	0.152122000
H	-6.543049000	-7.909623000	0.074444000
H	-5.268285000	-6.680735000	0.016789000
H	-4.990681000	-8.272982000	-0.686538000
N	-3.198789000	-13.587858000	5.694243000
C	-2.423728000	-12.578169000	5.200418000
N	-2.608914000	-14.790833000	5.467031000
C	-4.516134000	-13.541676000	6.308062000
H	-0.811380000	-15.404420000	4.584040000
H	-5.295680000	-13.757916000	5.570041000
H	-4.673939000	-12.546311000	6.721102000
H	-4.553249000	-14.294663000	7.096191000
O	0.704696000	-9.161552000	3.318578000
O	1.734953000	-11.130139000	2.896089000
N	3.974812000	-9.813069000	1.838898000
N	2.734983000	-5.856181000	-3.438210000
C	3.021363000	-7.629498000	-0.041263000
C	2.127248000	-8.627527000	0.701686000
C	2.461110000	-7.234651000	-1.412091000
C	2.726556000	-9.088818000	2.050555000
C	3.341031000	-6.226581000	-2.153598000
C	1.676493000	-9.905255000	2.807808000
H	4.020893000	-8.064582000	-0.148182000
H	3.139914000	-6.728329000	0.577320000
H	1.962828000	-9.516961000	0.076672000
H	1.141457000	-8.185759000	0.886315000
H	1.456050000	-6.806712000	-1.309700000
H	2.349666000	-8.136585000	-2.032612000
H	2.934843000	-8.196620000	2.653129000
H	4.363352000	-6.638234000	-2.240218000
H	3.426877000	-5.313325000	-1.550981000
H	3.745982000	-10.745745000	1.497599000
H	4.436610000	-9.963167000	2.733125000
H	2.734927000	-6.664483000	-4.057850000

H	3.307366000	-5.152736000	-3.899488000
H	0.020170000	-9.736833000	3.770418000

Adduct 7LysB$_b$:

O	-5.236389000	-12.771184000	2.657912000
S	-4.299212000	-11.653733000	2.442953000
C	-2.740296000	-12.211130000	3.109740000
O	-4.562474000	-10.312881000	2.976528000
C	-4.016527000	-11.501184000	0.677912000
N	-1.712383000	-11.357938000	3.169946000
C	-3.467430000	-10.320547000	0.171046000
C	-4.365652000	-12.555699000	-0.165176000
C	-0.995357000	-13.298232000	3.993638000
N	-0.664468000	-12.010262000	3.700636000
C	-3.259348000	-10.209924000	-1.200456000
H	-3.223676000	-9.501161000	0.838381000
C	-4.152037000	-12.423971000	-1.536225000
H	-4.816059000	-13.450722000	0.249362000
C	-0.577994000	-14.540693000	4.527687000
H	0.192437000	-11.454929000	3.798278000
C	-3.592395000	-11.257141000	-2.073825000
H	-2.838683000	-9.292065000	-1.602041000
H	-4.431187000	-13.237851000	-2.199662000
C	-3.336924000	-11.130620000	-3.555772000
H	-3.948607000	-11.831793000	-4.129545000
H	-3.550846000	-10.118776000	-3.912751000
H	-2.286355000	-11.341178000	-3.790492000
N	-2.665261000	-14.756905000	3.941208000
C	-2.336552000	-13.471112000	3.620769000
N	-1.594615000	-15.398406000	4.478802000
C	-3.899864000	-15.490862000	3.714746000
H	0.372930000	-14.846019000	4.938010000
H	-3.834206000	-16.087500000	2.798854000
H	-4.718361000	-14.777919000	3.624922000
H	-4.062416000	-16.157009000	4.562842000
O	-0.775350000	-8.824110000	2.638209000
O	1.050470000	-9.835852000	3.509004000
N	2.515051000	-7.444581000	3.395208000
N	3.197639000	-4.842523000	-2.754556000
C	2.077957000	-6.176788000	0.671107000
C	1.508758000	-7.520313000	1.137989000
C	2.395052000	-6.155127000	-0.828196000
C	1.260170000	-7.576411000	2.663215000
C	2.949347000	-4.812486000	-1.308069000
C	0.501653000	-8.864054000	2.993350000

H	2.977616000	-5.954036000	1.254924000
H	1.353571000	-5.382762000	0.902531000
H	2.202874000	-8.330843000	0.873347000
H	0.566507000	-7.731347000	0.619531000
H	1.498156000	-6.388142000	-1.415699000
H	3.125694000	-6.945744000	-1.056243000
H	0.605337000	-6.739246000	2.932738000
H	3.838763000	-4.554441000	-0.704297000
H	2.207265000	-4.027477000	-1.114253000
H	3.010992000	-8.332983000	3.335855000
H	2.319136000	-7.314800000	4.385277000
H	3.957232000	-5.491138000	-2.953589000
H	3.522232000	-3.930466000	-3.067679000
H	-1.223017000	-9.699522000	2.830436000

Adduct 7LysB$_c$:

O	1.321145000	-14.314750000	8.082976000
S	1.695659000	-13.233502000	7.153478000
C	0.650577000	-13.457712000	5.724046000
O	3.074325000	-13.065779000	6.681129000
C	1.164027000	-11.678299000	7.872410000
N	0.838903000	-12.686666000	4.647792000
C	1.707292000	-10.482084000	7.397365000
C	0.228113000	-11.686082000	8.906518000
C	-0.852991000	-14.055867000	4.178422000
N	-0.064225000	-13.045085000	3.719825000
C	1.291279000	-9.281575000	7.965512000
H	2.452277000	-10.495751000	6.609331000
C	-0.173042000	-10.473567000	9.464191000
H	-0.157861000	-12.629075000	9.277498000
C	-1.913008000	-14.953317000	3.906312000
H	-0.016040000	-12.522604000	2.838285000
C	0.344208000	-9.256124000	9.000986000
H	1.714644000	-8.348010000	7.605132000
H	-0.893941000	-10.473715000	10.277092000
C	-0.116588000	-7.944516000	9.588219000
H	-0.516475000	-8.075225000	10.597298000
H	0.700802000	-7.219058000	9.635286000
H	-0.910070000	-7.499713000	8.975196000
N	-1.203718000	-15.381610000	5.921451000
C	-0.423650000	-14.351431000	5.480693000
N	-2.106867000	-15.731845000	4.968332000
C	-1.238646000	-16.040739000	7.217010000
H	-2.520924000	-15.076475000	3.022502000
H	-2.023191000	-15.612277000	7.849496000

H	-0.271719000	-15.910665000	7.701156000
H	-1.448604000	-17.098841000	7.056596000
O	2.288668000	-10.656433000	3.475855000
O	0.790844000	-11.171648000	1.861530000
N	1.982066000	-9.368837000	0.075617000
N	2.133075000	-2.983259000	2.113325000
C	2.515522000	-6.761174000	1.523482000
C	1.828272000	-7.992038000	2.123541000
C	1.977990000	-5.443815000	2.093238000
C	2.309323000	-9.321011000	1.496117000
C	2.663960000	-4.209270000	1.505216000
C	1.718912000	-10.488739000	2.290211000
H	2.391675000	-6.785089000	0.435494000
H	3.596297000	-6.827147000	1.713900000
H	0.740770000	-7.917734000	1.979136000
H	2.000033000	-8.030672000	3.205137000
H	2.095590000	-5.418110000	3.183767000
H	0.896786000	-5.378644000	1.898997000
H	3.398844000	-9.375428000	1.608014000
H	2.575292000	-4.240056000	0.403698000
H	3.737455000	-4.253849000	1.729148000
H	0.984140000	-9.555411000	-0.014485000
H	2.441699000	-10.169529000	-0.352228000
H	1.160816000	-2.861802000	1.835390000
H	2.629565000	-2.173927000	1.747630000
H	1.848992000	-11.404751000	3.975914000

Adduct 7LysB6:

O	-3.995025000	-9.999890000	6.306266000
S	-2.996861000	-9.606112000	5.302612000
C	-2.109906000	-11.106142000	4.906681000
O	-2.009552000	-8.560827000	5.565240000
C	-3.874293000	-9.171636000	3.794326000
N	-0.947667000	-11.029369000	4.255848000
C	-3.241152000	-8.370201000	2.845572000
C	-5.176650000	-9.624024000	3.602063000
C	-1.359665000	-13.188998000	4.604782000
N	-0.496394000	-12.279976000	4.072972000
C	-3.925971000	-8.034306000	1.683401000
H	-2.239581000	-8.001344000	3.028277000
C	-5.846294000	-9.276378000	2.432120000
H	-5.663567000	-10.215609000	4.367121000
C	-1.638698000	-14.550359000	4.865134000

H	0.413898000	-12.362225000	3.612401000
C	-5.232988000	-8.485023000	1.454413000
H	-3.440435000	-7.403689000	0.946105000
H	-6.865145000	-9.617510000	2.282947000
C	-5.952968000	-8.133651000	0.176799000
H	-7.034250000	-8.236004000	0.286340000
H	-5.735636000	-7.108733000	-0.132892000
H	-5.638864000	-8.794084000	-0.638607000
N	-3.270740000	-13.381308000	5.709363000
C	-2.426597000	-12.466132000	5.152332000
N	-2.791222000	-14.635374000	5.521050000
C	-4.559091000	-13.190477000	6.358487000
H	-1.082501000	-15.442221000	4.626000000
H	-5.375105000	-13.367268000	5.652418000
H	-4.611724000	-12.170595000	6.733988000
H	-4.637403000	-13.900984000	7.180207000
O	1.087339000	-9.381090000	3.267175000
O	1.876250000	-11.450299000	2.856131000
N	4.377721000	-10.366375000	2.079798000
N	3.961880000	-6.490443000	-3.407202000
C	3.779958000	-8.164573000	0.048191000
C	2.759457000	-9.094798000	0.710857000
C	3.392411000	-7.785156000	-1.384747000
C	3.177455000	-9.540298000	2.130979000
C	4.395895000	-6.841920000	-2.048515000
C	1.987210000	-10.234002000	2.795030000
H	4.760579000	-8.648582000	0.060396000
H	3.874115000	-7.252848000	0.652303000
H	2.621429000	-9.994353000	0.097405000
H	1.786208000	-8.597290000	0.767187000
H	2.405912000	-7.308740000	-1.401899000
H	3.306153000	-8.697169000	-1.991095000
H	3.396273000	-8.644175000	2.719307000
H	5.397510000	-7.300423000	-2.014789000
H	4.455134000	-5.913521000	-1.470532000
H	4.141265000	-11.293479000	1.736730000
H	4.767559000	-10.492912000	3.008106000
H	3.972041000	-7.307125000	-4.010810000
H	4.584272000	-5.805699000	-3.823151000
H	0.311330000	-9.863443000	3.663931000

Adduct 7LysB6$_a$:

O	-4.046706000	-10.118529000	6.411755000
S	-3.107778000	-9.640144000	5.388008000
C	-2.179269000	-11.083454000	4.889632000

O	-2.152522000	-8.567223000	5.657931000
C	-4.062641000	-9.176091000	3.936792000
N	-1.047437000	-10.929592000	4.200155000
C	-3.500068000	-8.306941000	3.003327000
C	-5.353008000	-9.672197000	3.773966000
C	-1.359203000	-13.117777000	4.463143000
N	-0.554115000	-12.150645000	3.942546000
C	-4.244261000	-7.945981000	1.886130000
H	-2.506824000	-7.906833000	3.164607000
C	-6.082756000	-9.298747000	2.648762000
H	-5.785109000	-10.317221000	4.528700000
C	-1.573321000	-14.499836000	4.670670000
H	0.338273000	-12.173757000	3.442127000
C	-5.541050000	-8.438545000	1.687021000
H	-3.814351000	-7.262526000	1.161482000
H	-7.092883000	-9.673649000	2.523283000
C	-6.325777000	-8.057302000	0.456947000
H	-7.396715000	-8.210476000	0.602704000
H	-6.162786000	-7.010390000	0.190471000
H	-6.018346000	-8.663912000	-0.401665000
N	-3.215828000	-13.438461000	5.629155000
C	-2.431672000	-12.465107000	5.083379000
N	-2.694738000	-14.661878000	5.364932000
C	-4.483972000	-13.330559000	6.334629000
H	-0.992030000	-15.356287000	4.369740000
H	-5.320634000	-13.490328000	5.648880000
H	-4.554392000	-12.338304000	6.775596000
H	-4.508223000	-14.093237000	7.111607000
O	0.866972000	-9.149854000	3.207499000
O	1.727469000	-11.159828000	2.666192000
N	4.137808000	-9.927027000	1.823414000
N	3.290195000	-5.766207000	-3.401561000
C	3.343289000	-7.635494000	-0.043274000
C	2.403422000	-8.656907000	0.604518000
C	2.878298000	-7.203835000	-1.437794000
C	2.908005000	-9.159221000	1.976730000
C	3.795610000	-6.163331000	-2.080645000
C	1.781439000	-9.938145000	2.657432000
H	4.349164000	-8.061888000	-0.093907000
H	3.410070000	-6.753188000	0.606450000
H	2.285383000	-9.526086000	-0.055009000
H	1.409215000	-8.217080000	0.730605000
H	1.864336000	-6.791083000	-1.393257000
H	2.825334000	-8.084972000	-2.091718000
H	3.117805000	-8.286919000	2.603030000
H	4.824355000	-6.557801000	-2.107096000

H	3.818742000	-5.266229000	-1.452824000
H	3.923767000	-10.843119000	1.438619000
H	4.576409000	-10.088060000	2.724230000
H	3.329080000	-6.545986000	-4.051053000
H	3.852804000	-5.020870000	-3.798074000
H	0.131276000	-9.684990000	3.613492000

Adduct 7LysB6$_b$:

O	-5.257928000	-12.487053000	2.846643000
S	-4.260097000	-11.501757000	2.408591000
C	-2.694672000	-12.120440000	3.009114000
O	-4.354902000	-10.090903000	2.778728000
C	-4.141237000	-11.595886000	0.617033000
N	-1.629626000	-11.316762000	3.013559000
C	-3.638825000	-10.504552000	-0.089502000
C	-4.567951000	-12.746244000	-0.041168000
C	-0.965055000	-13.286171000	3.809815000
N	-0.589825000	-12.016040000	3.493859000
C	-3.552796000	-10.581641000	-1.475080000
H	-3.342773000	-9.606359000	0.437939000
C	-4.474541000	-12.804096000	-1.428671000
H	-4.988261000	-13.569426000	0.522875000
C	-0.581264000	-14.541058000	4.335823000
H	0.291333000	-11.502542000	3.578913000
C	-3.961343000	-11.730366000	-2.165445000
H	-3.170380000	-9.731559000	-2.030075000
H	-4.815956000	-13.693994000	-1.946568000
C	-3.836464000	-11.810402000	-3.666219000
H	-4.526150000	-12.545348000	-4.085792000
H	-4.038998000	-10.844481000	-4.134459000
H	-2.822209000	-12.106964000	-3.954608000
N	-2.701754000	-14.661612000	3.853282000
C	-2.327224000	-13.397299000	3.504039000
N	-1.638689000	-15.345670000	4.343497000
C	-3.983250000	-15.333948000	3.698964000
H	0.370169000	-14.890463000	4.702760000
H	-4.001514000	-15.920796000	2.776420000
H	-4.770863000	-14.583788000	3.671664000
H	-4.122637000	-16.000166000	4.549001000
O	-0.635805000	-8.731401000	2.619739000
O	1.175383000	-9.856792000	3.345150000
N	2.644435000	-7.437295000	3.503564000
N	3.471139000	-4.465483000	-2.479179000
C	2.249794000	-6.002829000	0.825499000
C	1.732419000	-7.392854000	1.207454000

C	2.642017000	-5.902483000	-0.652207000
C	1.421461000	-7.530374000	2.715573000
C	3.126924000	-4.508808000	-1.051702000
C	0.648292000	-8.831057000	2.938475000
H	3.104383000	-5.755200000	1.461586000
H	1.470512000	-5.261725000	1.045926000
H	2.476557000	-8.154388000	0.941490000
H	0.827523000	-7.620907000	0.635548000
H	1.794947000	-6.171412000	-1.293074000
H	3.435744000	-6.630974000	-0.866848000
H	0.757796000	-6.709566000	3.003548000
H	3.959755000	-4.214483000	-0.392568000
H	2.322108000	-3.785202000	-0.884001000
H	3.172516000	-8.301582000	3.418646000
H	2.430307000	-7.325751000	4.489210000
H	4.272359000	-5.058410000	-2.673824000
H	3.720931000	-3.524848000	-2.765680000
H	-1.102913000	-9.602931000	2.741110000

Adduct 7LysB6$_c$:

O	1.671047000	-14.310559000	7.883467000
S	1.806116000	-13.084993000	7.084702000
C	0.681591000	-13.291472000	5.711301000
O	3.094128000	-12.653621000	6.544859000
C	1.124927000	-11.724699000	8.043246000
N	0.787583000	-12.488241000	4.651247000
C	1.484948000	-10.417476000	7.719222000
C	0.266710000	-11.993684000	9.105702000
C	-0.912261000	-13.869960000	4.256339000
N	-0.170225000	-12.833672000	3.777047000
C	0.960243000	-9.369812000	8.467075000
H	2.179846000	-10.230690000	6.910012000
C	-0.246842000	-10.931154000	9.844213000
H	0.027673000	-13.017865000	9.363182000
C	-1.968266000	-14.780942000	4.024495000
H	-0.176447000	-12.314543000	2.895115000
C	0.083768000	-9.607121000	9.534570000
H	1.244060000	-8.351288000	8.224076000
H	-0.906916000	-11.136414000	10.680149000
C	-0.498049000	-8.458858000	10.320263000
H	-0.846348000	-8.782915000	11.302790000
H	0.235783000	-7.662170000	10.462961000
H	-1.353690000	-8.023439000	9.792953000
N	-1.120160000	-15.254359000	5.973875000
C	-0.393713000	-14.194663000	5.515977000

N	-2.073819000	-15.592511000	5.071365000
C	-1.049687000	-15.956086000	7.246749000
H	-2.630408000	-14.892885000	3.181297000
H	-1.773719000	-15.543567000	7.954879000
H	-0.043846000	-15.852349000	7.648641000
H	-1.281161000	-17.005200000	7.069251000
O	2.295583000	-10.531881000	3.333480000
O	0.661860000	-10.987654000	1.851570000
N	1.960975000	-9.402075000	-0.105927000
N	2.402137000	-2.909965000	1.598707000
C	2.619518000	-6.728959000	1.222007000
C	1.843146000	-7.891981000	1.846914000
C	2.120785000	-5.360059000	1.696252000
C	2.285029000	-9.272479000	1.309508000
C	2.909169000	-4.194683000	1.098292000
C	1.659033000	-10.361697000	2.181832000
H	2.549674000	-6.800829000	0.132943000
H	3.682445000	-6.835613000	1.474692000
H	0.770387000	-7.775048000	1.647008000
H	1.966399000	-7.877958000	2.934294000
H	2.173073000	-5.289640000	2.788400000
H	1.061107000	-5.247706000	1.429325000
H	3.369950000	-9.352683000	1.426802000
H	2.890110000	-4.273470000	-0.000863000
H	3.958450000	-4.275995000	1.401419000
H	0.961668000	-9.550787000	-0.217188000
H	2.419684000	-10.213204000	-0.507646000
H	1.455823000	-2.744040000	1.269557000
H	2.971747000	-2.138841000	1.266764000
H	1.847666000	-11.225878000	3.890015000

Adduct 7LysC:

O	-4.245686000	-10.163230000	6.101547000
S	-3.079676000	-9.721580000	5.333114000
C	-2.140844000	-11.190348000	5.022412000
O	-2.164946000	-8.707966000	5.842065000
C	-3.644345000	-9.196854000	3.730811000
N	-0.950162000	-11.090570000	4.443085000
C	-2.803312000	-8.430925000	2.929038000
C	-4.920145000	-9.546514000	3.309998000
C	-1.308540000	-13.243039000	4.808815000
N	-0.446615000	-12.319091000	4.312189000
C	-3.254009000	-8.024379000	1.683421000

H	-1.818837000	-8.147946000	3.284613000
C	-5.354812000	-9.126529000	2.060053000
H	-5.563335000	-10.120750000	3.966699000
C	-1.563718000	-14.608541000	5.072241000
H	0.479047000	-12.367565000	3.874816000
C	-4.530548000	-8.367729000	1.229029000
H	-2.607273000	-7.421639000	1.053138000
H	-6.354702000	-9.386851000	1.726988000
C	-4.995147000	-7.936875000	-0.135727000
H	-6.083722000	-7.965530000	-0.215060000
H	-4.662088000	-6.922160000	-0.366514000
H	-4.589435000	-8.596351000	-0.910030000
N	-3.271580000	-13.483426000	5.791129000
C	-2.423770000	-12.552081000	5.276613000
N	-2.745889000	-14.717982000	5.654102000
C	-4.596616000	-13.325048000	6.355702000
H	-0.965338000	-15.485664000	4.879750000
H	-5.363304000	-13.569697000	5.615531000
H	-4.716662000	-12.291434000	6.675227000
H	-4.692478000	-14.000691000	7.205161000
O	0.905430000	-9.411742000	3.351175000
O	1.851743000	-11.434201000	3.084255000
N	4.161354000	-10.315882000	2.016540000
N	3.347363000	-6.492951000	-3.384964000
C	3.417882000	-8.147787000	0.060790000
C	2.436182000	-9.042684000	0.810188000
C	2.920208000	-7.759883000	-1.328362000
C	2.970567000	-9.502210000	2.176812000
C	3.889241000	-6.855270000	-2.078257000
C	1.856750000	-10.219828000	2.926873000
H	4.380048000	-8.664246000	-0.007822000
H	3.595232000	-7.239215000	0.651548000
H	2.215914000	-9.935493000	0.209425000
H	1.485741000	-8.520466000	0.959347000
H	1.952346000	-7.250097000	-1.263785000
H	2.749726000	-8.669940000	-1.920500000
H	3.225907000	-8.610609000	2.759942000
H	4.876302000	-7.346928000	-2.123690000
H	4.031105000	-5.931056000	-1.506213000
H	3.878481000	-11.238972000	1.696161000
H	4.601914000	-10.465319000	2.919077000
H	3.289425000	-7.318621000	-3.974455000
H	3.970567000	-5.846516000	-3.858319000
H	0.182370000	-9.930259000	3.808835000

Adduct 7LysC$_a$:

O	-4.333532000	-10.315096000	6.191225000
S	-3.201675000	-9.778116000	5.432455000
C	-2.209325000	-11.184517000	5.016000000
O	-2.320861000	-8.759255000	5.988633000
C	-3.817119000	-9.180987000	3.875039000
N	-1.045436000	-11.000926000	4.403645000
C	-3.024407000	-8.329741000	3.110321000
C	-5.082740000	-9.561724000	3.451721000
C	-1.292390000	-13.182942000	4.673110000
N	-0.491246000	-12.196532000	4.195387000
C	-3.513716000	-7.868571000	1.899225000
H	-2.047393000	-8.025275000	3.468560000
C	-5.556994000	-9.085716000	2.236258000
H	-5.688086000	-10.204827000	4.079958000
C	-1.475925000	-14.570129000	4.875755000
H	0.416411000	-12.180617000	3.719854000
C	-4.781966000	-8.240532000	1.442823000
H	-2.904729000	-7.200291000	1.297972000
H	-6.549442000	-9.370947000	1.901551000
C	-5.288890000	-7.741189000	0.117020000
H	-6.359555000	-7.921965000	0.004222000
H	-5.110514000	-6.668757000	0.003625000
H	-4.777122000	-8.243959000	-0.709914000
N	-3.207089000	-13.563043000	5.705501000
C	-2.420883000	-12.568776000	5.211295000
N	-2.630945000	-14.763242000	5.489559000
C	-4.517286000	-13.495601000	6.320802000
H	-0.845503000	-15.407723000	4.619893000
H	-5.297063000	-13.744281000	5.595860000
H	-4.675390000	-12.484514000	6.691566000
H	-4.550684000	-14.212544000	7.140677000
O	0.675482000	-9.187118000	3.311940000
O	1.705192000	-11.145085000	2.908878000
N	3.897874000	-9.865937000	1.776236000
N	2.615532000	-5.841984000	-3.384781000
C	2.946250000	-7.647400000	-0.030982000
C	2.052189000	-8.628483000	0.720200000
C	2.360335000	-7.225102000	-1.375050000
C	2.679577000	-9.121320000	2.034726000
C	3.238341000	-6.229834000	-2.122178000
C	1.642613000	-9.926548000	2.805754000
H	3.930126000	-8.105612000	-0.169953000
H	3.103668000	-6.758085000	0.593761000
H	1.847641000	-9.502798000	0.087618000
H	1.084968000	-8.165934000	0.941201000

H	1.368911000	-6.777909000	-1.241123000
H	2.214256000	-8.114938000	-2.003295000
H	2.922203000	-8.244790000	2.645545000
H	4.249419000	-6.657787000	-2.234675000
H	3.352098000	-5.325762000	-1.512906000
H	3.643106000	-10.788462000	1.431619000
H	4.394669000	-10.029220000	2.646589000
H	2.579079000	-6.641911000	-4.010375000
H	3.176684000	-5.137696000	-3.853207000
H	0.001388000	-9.761995000	3.777274000

Adduct 7LysC_b:

O	-5.203155000	-12.748705000	2.624762000
S	-4.266728000	-11.637581000	2.441488000
C	-2.731026000	-12.204586000	3.116930000
O	-4.532563000	-10.313453000	2.988538000
C	-3.957774000	-11.460374000	0.699565000
N	-1.703241000	-11.366781000	3.187574000
C	-3.374597000	-10.288544000	0.226339000
C	-4.315668000	-12.487015000	-0.163424000
C	-1.012852000	-13.300980000	4.010281000
N	-0.669841000	-12.019341000	3.722555000
C	-3.140371000	-10.159684000	-1.133165000
H	-3.123451000	-9.487582000	0.912603000
C	-4.076256000	-12.337262000	-1.522955000
H	-4.792756000	-13.377215000	0.229835000
C	-0.610321000	-14.546835000	4.543973000
H	0.189606000	-11.470121000	3.822367000
C	-3.482505000	-11.179678000	-2.025816000
H	-2.690659000	-9.247099000	-1.512361000
H	-4.361801000	-13.131037000	-2.206183000
C	-3.200746000	-11.031066000	-3.496362000
H	-3.786538000	-11.736438000	-4.089050000
H	-3.428842000	-10.020542000	-3.844161000
H	-2.143016000	-11.216952000	-3.709821000
N	-2.683202000	-14.743703000	3.940587000
C	-2.342733000	-13.463870000	3.629186000
N	-1.629112000	-15.387314000	4.482596000
C	-3.921151000	-15.460421000	3.709260000
H	0.334258000	-14.861454000	4.960187000
H	-3.843757000	-16.085721000	2.815676000
H	-4.722698000	-14.735998000	3.576914000
H	-4.118534000	-16.094956000	4.572773000
O	-0.782327000	-8.863582000	2.616232000
O	1.024953000	-9.858856000	3.510625000

N	2.516025000	-7.518293000	3.329526000
N	3.080407000	-4.888701000	-2.776142000
C	2.027096000	-6.229016000	0.646216000
C	1.450356000	-7.561578000	1.112585000
C	2.304623000	-6.199580000	-0.853839000
C	1.246113000	-7.624206000	2.635317000
C	2.863380000	-4.865980000	-1.332226000
C	0.485081000	-8.897543000	2.977900000
H	2.943804000	-6.027779000	1.208783000
H	1.323225000	-5.426113000	0.902819000
H	2.124180000	-8.379040000	0.822516000
H	0.492115000	-7.752680000	0.618936000
H	1.390934000	-6.413268000	-1.419898000
H	3.016941000	-6.997249000	-1.107168000
H	0.609709000	-6.782141000	2.928623000
H	3.768078000	-4.625493000	-0.747554000
H	2.136343000	-4.075010000	-1.114797000
H	2.998885000	-8.410292000	3.252472000
H	2.356741000	-7.380810000	4.322870000
H	3.817825000	-5.550142000	-3.002628000
H	3.400884000	-3.981285000	-3.098991000
H	-1.230440000	-9.733599000	2.825498000

Adduct 7LysC_c:

O	1.237402000	-14.234483000	8.109373000
S	1.636800000	-13.191372000	7.161984000
C	0.624332000	-13.446398000	5.731683000
O	3.015905000	-13.051627000	6.712714000
C	1.110578000	-11.624078000	7.816131000
N	0.832155000	-12.708379000	4.647491000
C	1.644987000	-10.451648000	7.290202000
C	0.184906000	-11.593951000	8.850247000
C	-0.845882000	-14.073579000	4.183402000
N	-0.047407000	-13.080184000	3.715782000
C	1.228932000	-9.235617000	7.808115000
H	2.384657000	-10.495639000	6.498629000
C	-0.216336000	-10.365765000	9.358405000
H	-0.194368000	-12.523552000	9.258584000
C	-1.904544000	-14.971660000	3.915584000
H	0.016489000	-12.573071000	2.827480000
C	0.292238000	-9.173165000	8.843804000
H	1.644131000	-8.315751000	7.407780000
H	-0.932224000	-10.333414000	10.173822000
C	-0.165401000	-7.843306000	9.378661000
H	-0.606456000	-7.942407000	10.372518000

H	0.663409000	-7.134081000	9.441517000
H	-0.922856000	-7.401113000	8.723086000
N	-1.235981000	-15.349640000	5.942870000
C	-0.445288000	-14.339052000	5.490771000
N	-2.115765000	-15.715321000	4.988178000
C	-1.289762000	-15.977321000	7.247761000
H	-2.498613000	-15.113298000	3.025938000
H	-2.101925000	-15.555440000	7.846039000
H	-0.341049000	-15.809086000	7.754180000
H	-1.465232000	-17.043731000	7.109433000
O	2.286801000	-10.688259000	3.527420000
O	0.848146000	-11.229031000	1.886013000
N	2.002963000	-9.401268000	0.140717000
N	2.209687000	-3.067615000	2.203675000
C	2.565830000	-6.825661000	1.597514000
C	1.876691000	-8.049405000	2.192246000
C	2.041416000	-5.514498000	2.175382000
C	2.341756000	-9.367396000	1.551218000
C	2.733175000	-4.287707000	1.595555000
C	1.751304000	-10.533210000	2.332623000
H	2.435484000	-6.843826000	0.511304000
H	3.645961000	-6.899301000	1.781340000
H	0.790014000	-7.965305000	2.055557000
H	2.055863000	-8.098110000	3.270990000
H	2.162288000	-5.496194000	3.264362000
H	0.961679000	-5.439658000	1.984415000
H	3.430429000	-9.431404000	1.656079000
H	2.645062000	-4.312907000	0.495688000
H	3.804625000	-4.341539000	1.820507000
H	1.005788000	-9.582688000	0.054127000
H	2.461600000	-10.189334000	-0.306054000
H	1.237717000	-2.939804000	1.936248000
H	2.711267000	-2.256696000	1.855581000
H	1.844903000	-11.442389000	4.014506000

Adduct 7LysP:

O	-4.231130000	-10.149706000	6.120366000
S	-3.082020000	-9.706423000	5.326437000
C	-2.138174000	-11.169095000	5.008607000
O	-2.163337000	-8.679703000	5.804448000
C	-3.679420000	-9.204009000	3.729499000
N	-0.940990000	-11.060454000	4.435140000
C	-2.869712000	-8.409575000	2.919195000

C	-4.947297000	-9.599396000	3.318293000
C	-1.295258000	-13.218401000	4.770815000
N	-0.437126000	-12.284072000	4.293146000
C	-3.343927000	-8.020201000	1.675047000
H	-1.893056000	-8.092063000	3.270729000
C	-5.405480000	-9.196139000	2.068960000
H	-5.566056000	-10.194524000	3.982040000
C	-1.548150000	-14.585137000	5.017624000
H	0.493243000	-12.322428000	3.860377000
C	-4.613506000	-8.408955000	1.229040000
H	-2.722041000	-7.395781000	1.038795000
H	-6.398860000	-9.492340000	1.742852000
C	-5.102631000	-7.989531000	-0.127373000
H	-6.168006000	-8.197247000	-0.252139000
H	-4.942193000	-6.919813000	-0.293234000
H	-4.563674000	-8.523165000	-0.918446000
N	-3.262420000	-13.475674000	5.739969000
C	-2.419600000	-12.534173000	5.242346000
N	-2.736333000	-14.705506000	5.593185000
C	-4.587494000	-13.325852000	6.295382000
H	-0.947094000	-15.460282000	4.820375000
H	-5.349982000	-13.558886000	5.545438000
H	-4.709167000	-12.295989000	6.630759000
H	-4.690332000	-14.014951000	7.134458000
O	0.918428000	-9.390297000	3.369075000
O	1.866663000	-11.414756000	3.094740000
N	4.183959000	-10.280594000	2.057864000
N	3.421278000	-6.516524000	-3.368223000
C	3.451369000	-8.137627000	0.088641000
C	2.462877000	-9.024837000	0.834656000
C	2.971369000	-7.765176000	-1.308883000
C	2.987866000	-9.477235000	2.206874000
C	3.950907000	-6.873405000	-2.058338000
C	1.868935000	-10.197336000	2.946510000
H	4.416018000	-8.655283000	0.038961000
H	3.621584000	-7.222095000	0.673048000
H	2.245303000	-9.922098000	0.237076000
H	1.510382000	-8.500765000	0.974196000
H	2.003127000	-7.251089000	-1.262522000
H	2.803795000	-8.682990000	-1.892275000
H	3.231900000	-8.579436000	2.788651000
H	4.937181000	-7.372321000	-2.087684000
H	4.094077000	-5.945514000	-1.489742000
H	3.905043000	-11.203993000	1.734976000
H	4.606247000	-10.433035000	2.968278000
H	3.367711000	-7.347661000	-3.949867000

H	4.059497000	-5.884344000	-3.840134000
H	0.189017000	-9.911280000	3.816549000

Adduct 7LysP$_a$:

O	-4.305955000	-10.290877000	6.219844000
S	-3.185330000	-9.757090000	5.440983000
C	-2.197819000	-11.163128000	5.015800000
O	-2.295386000	-8.731448000	5.972686000
C	-3.823584000	-9.174713000	3.887894000
N	-1.027047000	-10.977759000	4.408526000
C	-3.056248000	-8.298012000	3.122975000
C	-5.081075000	-9.591931000	3.465742000
C	-1.284742000	-13.162147000	4.645215000
N	-0.481080000	-12.171150000	4.187503000
C	-3.562082000	-7.847228000	1.912152000
H	-2.088166000	-7.965501000	3.484088000
C	-5.571462000	-9.126093000	2.251157000
H	-5.667238000	-10.252906000	4.095936000
C	-1.475590000	-14.548677000	4.829429000
H	0.428643000	-12.150676000	3.712338000
C	-4.821422000	-8.255590000	1.455658000
H	-2.973521000	-7.158356000	1.311808000
H	-6.557574000	-9.438297000	1.917865000
C	-5.343947000	-7.773048000	0.133142000
H	-6.420132000	-7.938966000	0.041936000
H	-5.149712000	-6.705428000	-0.005459000
H	-4.855365000	-8.300864000	-0.694036000
N	-3.204763000	-13.547192000	5.665379000
C	-2.417273000	-12.548458000	5.189130000
N	-2.637108000	-14.745669000	5.437468000
C	-4.514183000	-13.480228000	6.271911000
H	-0.848675000	-15.387829000	4.567015000
H	-5.293428000	-13.700245000	5.535401000
H	-4.662835000	-12.476403000	6.669416000
H	-4.561406000	-14.219122000	7.072688000
O	0.699460000	-9.180683000	3.334059000
O	1.718114000	-11.144332000	2.912098000
N	3.910688000	-9.859430000	1.782137000
N	2.631941000	-5.866220000	-3.380132000
C	2.956116000	-7.652325000	-0.020964000
C	2.061387000	-8.626596000	0.734665000
C	2.374452000	-7.239830000	-1.367851000
C	2.693965000	-9.119443000	2.046295000
C	3.254276000	-6.251624000	-2.119990000
C	1.657129000	-9.923046000	2.818926000

H	3.941591000	-8.113227000	-0.153177000
H	3.113241000	-6.757898000	0.598764000
H	1.849697000	-9.502368000	0.104132000
H	1.095470000	-8.159931000	0.959696000
H	1.381597000	-6.790396000	-1.240621000
H	2.228440000	-8.135560000	-1.990016000
H	2.937071000	-8.239663000	2.655486000
H	4.266298000	-6.683992000	-2.226659000
H	3.371127000	-5.345187000	-1.512150000
H	3.650884000	-10.781053000	1.438991000
H	4.401750000	-10.028545000	2.654277000
H	2.597868000	-6.669836000	-4.000606000
H	3.202782000	-5.171959000	-3.851111000
H	0.020263000	-9.755877000	3.794577000

Adduct 7LysP_b:

O	-5.220581000	-12.674103000	2.681780000
S	-4.265299000	-11.587239000	2.450873000
C	-2.727301000	-12.164000000	3.109577000
O	-4.489846000	-10.240352000	2.962732000
C	-3.984151000	-11.467648000	0.699847000
N	-1.696639000	-11.323986000	3.186525000
C	-3.402215000	-10.312950000	0.179944000
C	-4.361863000	-12.521289000	-0.125562000
C	-0.992109000	-13.271712000	3.963821000
N	-0.660470000	-11.984681000	3.697320000
C	-3.189773000	-10.228173000	-1.188807000
H	-3.138255000	-9.491645000	0.838721000
C	-4.143880000	-12.415380000	-1.494324000
H	-4.838998000	-13.395808000	0.304761000
C	-0.583720000	-14.524738000	4.469841000
H	0.199052000	-11.432309000	3.797880000
C	-3.551268000	-11.275532000	-2.044950000
H	-2.742657000	-9.328797000	-1.604151000
H	-4.445705000	-13.229247000	-2.148204000
C	-3.291888000	-11.177059000	-3.520709000
H	-3.919133000	-11.871184000	-4.085536000
H	-3.480238000	-10.165613000	-3.891757000
H	-2.246467000	-11.416581000	-3.747746000
N	-2.660118000	-14.716251000	3.883804000
C	-2.330205000	-13.431885000	3.591229000
N	-1.603787000	-15.368884000	4.402352000
C	-3.895482000	-15.427023000	3.648425000
H	0.364669000	-14.847310000	4.873017000
H	-3.831274000	-16.022227000	2.732027000

H	-4.702544000	-14.700544000	3.554520000
H	-4.076903000	-16.091928000	4.493610000
O	-0.772079000	-8.827978000	2.654713000
O	1.042951000	-9.845110000	3.517220000
N	2.531632000	-7.498800000	3.354537000
N	3.122927000	-4.867673000	-2.728462000
C	2.047230000	-6.208038000	0.681489000
C	1.463485000	-7.537340000	1.142564000
C	2.336184000	-6.178489000	-0.814513000
C	1.261889000	-7.602949000	2.665161000
C	2.903666000	-4.848011000	-1.287840000
C	0.497238000	-8.875576000	3.001292000
H	2.961042000	-6.010412000	1.253346000
H	1.343545000	-5.402046000	0.934221000
H	2.132818000	-8.359055000	0.849099000
H	0.502453000	-7.722618000	0.648942000
H	1.425551000	-6.388528000	-1.389576000
H	3.047453000	-6.980453000	-1.062894000
H	0.626043000	-6.758431000	2.959144000
H	3.806560000	-4.612876000	-0.694444000
H	2.178301000	-4.053803000	-1.069179000
H	3.009265000	-8.393029000	3.271332000
H	2.369352000	-7.374536000	4.348841000
H	3.860635000	-5.530197000	-2.949365000
H	3.456476000	-3.961743000	-3.041083000
H	-1.222670000	-9.700772000	2.852963000

Adduct 7LysP$_c$:

O	1.337088000	-14.246627000	8.073480000
S	1.683611000	-13.165767000	7.146738000
C	0.654689000	-13.414676000	5.728711000
O	3.048413000	-12.960790000	6.675657000
C	1.111800000	-11.636750000	7.849837000
N	0.848100000	-12.667831000	4.643017000
C	1.621041000	-10.432563000	7.367962000
C	0.174536000	-11.665545000	8.877236000
C	-0.841878000	-14.023115000	4.193474000
N	-0.045483000	-13.030824000	3.725919000
C	1.168152000	-9.243808000	7.923101000
H	2.371362000	-10.433699000	6.583579000
C	-0.263621000	-10.464445000	9.422183000
H	-0.182371000	-12.619297000	9.252312000
C	-1.904252000	-14.916327000	3.935836000
H	0.011437000	-12.517821000	2.838406000
C	0.218323000	-9.239482000	8.951559000

H	1.564641000	-8.299917000	7.558242000
H	-0.987527000	-10.477900000	10.232642000
C	-0.281522000	-7.943939000	9.523016000
H	-0.685708000	-8.078845000	10.529452000
H	0.514335000	-7.195490000	9.570568000
H	-1.081739000	-7.528388000	8.899366000
N	-1.208609000	-15.311365000	5.948804000
C	-0.422067000	-14.300294000	5.497900000
N	-2.102472000	-15.669463000	5.008768000
C	-1.244586000	-15.943143000	7.247369000
H	-2.512228000	-15.053426000	3.054022000
H	-2.031157000	-15.505100000	7.870003000
H	-0.278059000	-15.802204000	7.731014000
H	-1.450543000	-17.004740000	7.106759000
O	2.292404000	-10.673044000	3.495001000
O	0.816331000	-11.201091000	1.878136000
N	1.971696000	-9.394018000	0.111149000
N	2.274864000	-3.064235000	2.100441000
C	2.587383000	-6.828169000	1.539962000
C	1.895652000	-8.036952000	2.157374000
C	2.081429000	-5.506355000	2.105003000
C	2.330505000	-9.363530000	1.513995000
C	2.775057000	-4.294247000	1.499912000
C	1.737286000	-10.516964000	2.311366000
H	2.444507000	-6.861219000	0.453913000
H	3.670193000	-6.909231000	1.712014000
H	0.806127000	-7.939621000	2.042595000
H	2.095854000	-8.082093000	3.233932000
H	2.215120000	-5.472645000	3.193529000
H	0.998630000	-5.426008000	1.926296000
H	3.421558000	-9.440762000	1.603824000
H	2.672868000	-4.336748000	0.399752000
H	3.850460000	-4.357810000	1.710181000
H	0.969422000	-9.554412000	0.044901000
H	2.399991000	-10.200980000	-0.331347000
H	1.302080000	-2.931620000	1.839607000
H	2.777190000	-2.265919000	1.726215000
H	1.847969000	-11.419083000	3.994491000

Adduct 7LysM:

O	-4.224039000	-10.153262000	6.152095000
S	-3.074870000	-9.701750000	5.363182000
C	-2.138173000	-11.163698000	5.029160000

O	-2.149412000	-8.674691000	5.830427000
C	-3.663307000	-9.212500000	3.756068000
N	-0.930220000	-11.053849000	4.464548000
C	-2.867749000	-8.384612000	2.964167000
C	-4.894627000	-9.676154000	3.303579000
C	-1.332444000	-13.227752000	4.749753000
N	-0.447766000	-12.297575000	4.299779000
C	-3.320939000	-8.022537000	1.704202000
H	-1.916691000	-8.023677000	3.345040000
C	-5.332865000	-9.300690000	2.038563000
H	-5.501374000	-10.306550000	3.947363000
C	-1.619796000	-14.591127000	4.959343000
H	0.483741000	-12.348046000	3.880865000
C	-4.556602000	-8.474035000	1.220848000
H	-2.709365000	-7.374434000	1.080637000
H	-6.296538000	-9.652127000	1.677176000
C	-5.033273000	-8.064730000	-0.138287000
H	-5.945849000	-8.593102000	-0.423872000
H	-5.246476000	-6.991072000	-0.177840000
H	-4.276330000	-8.261034000	-0.904126000
N	-3.321006000	-13.454705000	5.692677000
C	-2.445319000	-12.525289000	5.224484000
N	-2.823783000	-14.707619000	5.519955000
C	-4.652814000	-13.277345000	6.223093000
H	-1.039181000	-15.476789000	4.749507000
H	-5.376543000	-13.097325000	5.421243000
H	-4.667677000	-12.424080000	6.901145000
H	-4.919940000	-14.192553000	6.749158000
O	0.961369000	-9.312245000	3.430670000
O	1.889113000	-11.355174000	3.134042000
N	4.217244000	-10.216250000	2.090190000
N	3.357477000	-6.538936000	-3.376297000
C	3.459684000	-8.134713000	0.086730000
C	2.477422000	-8.991092000	0.868402000
C	2.943861000	-7.757222000	-1.292307000
C	3.012374000	-9.417590000	2.242344000
C	3.919016000	-6.899126000	-2.078443000
C	1.902588000	-10.135657000	2.993426000
H	4.412440000	-8.672136000	0.008194000
H	3.677695000	-7.221964000	0.660891000
H	2.237871000	-9.899129000	0.293516000
H	1.529397000	-8.456508000	1.005964000
H	1.988539000	-7.221151000	-1.216064000
H	2.726216000	-8.672758000	-1.864188000
H	3.260043000	-8.508372000	2.806175000
H	4.893952000	-7.422359000	-2.127901000

H	4.107576000	-5.970305000	-1.523414000
H	3.927615000	-11.142570000	1.784456000
H	4.626390000	-10.369532000	3.006264000
H	3.277075000	-7.378651000	-3.942118000
H	4.010750000	-5.942216000	-3.872305000
H	0.238826000	-9.838802000	3.872393000

Adduct 7LysM$_a$:

O	-4.263863000	-10.209166000	6.247961000
S	-3.131888000	-9.713793000	5.460978000
C	-2.176518000	-11.147815000	5.061194000
O	-2.215055000	-8.689495000	5.950887000
C	-3.745367000	-9.181777000	3.877113000
N	-0.988630000	-10.992323000	4.466547000
C	-2.965032000	-8.326900000	3.098873000
C	-4.980320000	-9.639418000	3.428402000
C	-1.340265000	-13.183069000	4.676669000
N	-0.486115000	-12.217885000	4.240252000
C	-3.437234000	-7.931689000	1.855823000
H	-2.011954000	-7.969111000	3.477477000
C	-5.438419000	-9.229075000	2.181437000
H	-5.575027000	-10.290086000	4.063308000
C	-1.595958000	-14.559033000	4.840974000
H	0.420592000	-12.231901000	3.769122000
C	-4.676516000	-8.376948000	1.376201000
H	-2.838566000	-7.260435000	1.244169000
H	-6.407211000	-9.571617000	1.825185000
C	-5.165209000	-7.948740000	0.027272000
H	-6.201862000	-8.248804000	-0.142414000
H	-5.103499000	-6.863246000	-0.096012000
H	-4.559412000	-8.389011000	-0.772339000
N	-3.295921000	-13.485708000	5.666375000
C	-2.451542000	-12.521833000	5.210660000
N	-2.781124000	-14.720725000	5.430305000
C	-4.613438000	-13.354299000	6.243470000
H	-1.006104000	-15.424500000	4.579829000
H	-5.363997000	-13.151616000	5.472493000
H	-4.621270000	-12.532094000	6.959137000
H	-4.849532000	-14.296148000	6.736435000
O	0.770400000	-9.141117000	3.415566000
O	1.723204000	-11.136531000	2.936114000
N	3.903542000	-9.885385000	1.721252000
N	2.470489000	-5.767758000	-3.300810000
C	2.922541000	-7.640018000	-0.008025000
C	2.040104000	-8.594741000	0.778551000

C	2.277753000	-7.170625000	-1.302374000
C	2.712886000	-9.121105000	2.054014000
C	3.142465000	-6.191924000	-2.076650000
C	1.691979000	-9.911995000	2.856828000
H	3.881902000	-8.130186000	-0.213998000
H	3.159577000	-6.769570000	0.621833000
H	1.769950000	-9.456362000	0.148390000
H	1.096372000	-8.105407000	1.049892000
H	1.305938000	-6.699449000	-1.103668000
H	2.060612000	-8.042589000	-1.938838000
H	3.007359000	-8.254066000	2.660647000
H	4.140721000	-6.645479000	-2.233602000
H	3.314284000	-5.299625000	-1.459823000
H	3.593457000	-10.794948000	1.386610000
H	4.408887000	-10.092567000	2.576762000
H	2.399769000	-6.564648000	-3.926631000
H	3.052084000	-5.094549000	-3.788157000
H	0.100084000	-9.715144000	3.880747000

Adduct 7LysM$_b$:

O	-5.254390000	-12.386506000	2.776321000
S	-4.216155000	-11.386517000	2.514870000
C	-2.728285000	-12.066328000	3.184870000
O	-4.315049000	-10.003181000	2.968237000
C	-3.901055000	-11.367200000	0.762948000
N	-1.659533000	-11.275470000	3.325332000
C	-3.243539000	-10.273789000	0.199779000
C	-4.296745000	-12.450590000	-0.015280000
C	-1.052722000	-13.324939000	3.957714000
N	-0.655279000	-12.032414000	3.797657000
C	-2.986598000	-10.275399000	-1.163708000
H	-2.952247000	-9.435270000	0.826499000
C	-4.032577000	-12.432626000	-1.380037000
H	-4.818888000	-13.281952000	0.449831000
C	-0.713452000	-14.632740000	4.358065000
H	0.232349000	-11.542347000	3.919389000
C	-3.376245000	-11.350292000	-1.974101000
H	-2.477151000	-9.426567000	-1.614458000
H	-4.342330000	-13.271666000	-1.998825000
C	-3.109871000	-11.325550000	-3.447254000
H	-3.262982000	-12.306407000	-3.903271000
H	-3.775087000	-10.619930000	-3.957238000
H	-2.086831000	-11.005572000	-3.666106000
N	-2.797235000	-14.668684000	3.744214000
C	-2.393384000	-13.382190000	3.563065000

N	-1.772948000	-15.428447000	4.212463000
C	-4.057043000	-15.291758000	3.411804000
H	0.211274000	-15.037620000	4.740674000
H	-4.082608000	-15.593568000	2.359241000
H	-4.868206000	-14.587909000	3.598120000
H	-4.166624000	-16.176918000	4.037116000
O	-0.719694000	-8.728858000	2.839603000
O	1.091252000	-9.870041000	3.573100000
N	2.722471000	-7.621458000	3.265789000
N	2.793189000	-4.860771000	-2.790952000
C	2.054013000	-6.239842000	0.688538000
C	1.429407000	-7.534199000	1.181872000
C	2.150340000	-6.174206000	-0.827190000
C	1.378654000	-7.633212000	2.712571000
C	2.751721000	-4.874898000	-1.332224000
C	0.572793000	-8.863112000	3.100048000
H	3.046269000	-6.127367000	1.142134000
H	1.458539000	-5.390886000	1.056075000
H	2.002246000	-8.392947000	0.798550000
H	0.412641000	-7.642392000	0.784584000
H	1.159979000	-6.302246000	-1.284002000
H	2.756764000	-7.018363000	-1.190973000
H	0.834894000	-6.755612000	3.087819000
H	3.733568000	-4.722154000	-0.842725000
H	2.122117000	-4.036696000	-1.004841000
H	3.122792000	-8.543048000	3.105493000
H	2.659199000	-7.548970000	4.276163000
H	3.454854000	-5.564202000	-3.105868000
H	3.171064000	-3.974865000	-3.109174000
H	-1.184739000	-9.583851000	3.056044000

Adduct 7LysM$_c$:

O	1.796040000	-14.222745000	7.878920000
S	1.887288000	-13.028835000	7.035103000
C	0.791452000	-13.317327000	5.680071000
O	3.147525000	-12.538445000	6.486814000
C	1.105533000	-11.684038000	7.902370000
N	0.923951000	-12.583978000	4.568917000
C	1.317796000	-10.377972000	7.460663000
C	0.286091000	-11.951510000	8.993801000
C	-0.841219000	-13.913404000	4.277233000
N	-0.055870000	-12.948398000	3.725898000
C	0.695640000	-9.333507000	8.128216000
H	1.972354000	-10.194092000	6.612546000
C	-0.326585000	-10.890604000	9.652653000

H	0.153778000	-12.976899000	9.327800000
C	-1.944442000	-14.778141000	4.129838000
H	-0.052685000	-12.461943000	2.826976000
C	-0.135014000	-9.571566000	9.232251000
H	0.858857000	-8.310978000	7.794950000
H	-0.961351000	-11.087635000	10.513521000
C	-0.796538000	-8.430777000	9.941730000
H	-1.398141000	-8.772766000	10.787057000
H	-0.059382000	-7.716703000	10.323035000
H	-1.454407000	-7.870548000	9.269138000
N	-1.093859000	-15.150589000	6.093934000
C	-0.322452000	-14.171605000	5.550086000
N	-2.086582000	-15.506688000	5.237613000
C	-1.051992000	-15.716478000	7.421947000
H	-2.626986000	-14.920961000	3.305518000
H	-1.613853000	-15.099448000	8.131622000
H	-0.014899000	-15.784733000	7.752563000
H	-1.503833000	-16.706721000	7.378628000
O	2.409039000	-10.585157000	3.350999000
O	0.816203000	-11.117630000	1.833453000
N	1.889341000	-9.346497000	-0.032440000
N	2.524943000	-3.018998000	1.864241000
C	2.661780000	-6.790128000	1.309425000
C	1.995001000	-7.970347000	1.996533000
C	2.259460000	-5.452969000	1.910205000
C	2.344209000	-9.316143000	1.347720000
C	2.931568000	-4.271030000	1.234540000
C	1.775603000	-10.443011000	2.196045000
H	2.419286000	-6.819181000	0.240297000
H	3.753698000	-6.908421000	1.372087000
H	0.901186000	-7.845474000	1.969705000
H	2.274174000	-8.003528000	3.056400000
H	2.492310000	-5.422795000	2.982745000
H	1.166813000	-5.335540000	1.839461000
H	3.437657000	-9.420872000	1.359941000
H	2.734480000	-4.323999000	0.145870000
H	4.020065000	-4.365921000	1.345208000
H	0.878871000	-9.463469000	-0.015150000
H	2.231569000	-10.196132000	-0.470002000
H	1.537301000	-2.867202000	1.682091000
H	3.003195000	-2.245163000	1.415767000
H	1.984314000	-11.320690000	3.872625000

Adduct 7GluB:

O	-4.511754000	-9.682767000	5.806173000
S	-3.269140000	-9.263661000	5.133055000
C	-2.047136000	-10.482496000	5.599817000
O	-2.692407000	-7.931582000	5.346345000
C	-3.470474000	-9.510902000	3.369030000
N	-0.811876000	-10.391674000	5.097697000
C	-2.632202000	-8.828728000	2.483682000
C	-4.437310000	-10.404128000	2.907162000
C	-0.857569000	-12.210928000	6.379820000
N	-0.095009000	-11.427126000	5.568056000
C	-2.758738000	-9.066760000	1.118136000
H	-1.898552000	-8.125108000	2.860688000
C	-4.552017000	-10.624790000	1.535732000
H	-5.088973000	-10.907658000	3.612798000
C	-0.919730000	-13.353432000	7.212358000
H	0.855253000	-11.506448000	5.197674000
C	-3.712815000	-9.970029000	0.623882000
H	-2.102153000	-8.554879000	0.420773000
H	-5.302168000	-11.319939000	1.168832000
C	-3.834748000	-10.208700000	-0.861040000
H	-4.324496000	-11.162267000	-1.075865000
H	-4.429639000	-9.418919000	-1.336295000
H	-2.849983000	-10.208696000	-1.337173000
N	-2.882913000	-12.409333000	7.262370000
C	-2.134009000	-11.630220000	6.428033000
N	-2.144716000	-13.451979000	7.723900000
C	-4.286824000	-12.307966000	7.629065000
H	-0.163903000	-14.082245000	7.464062000
H	-4.888113000	-13.017055000	7.051303000
H	-4.627657000	-11.294489000	7.423057000
H	-4.385029000	-12.538575000	8.690758000
O	0.817126000	-9.014163000	3.402219000
O	-0.197515000	-9.151548000	-1.559294000
O	2.085621000	-10.807326000	3.920911000
O	1.670307000	-7.905533000	-1.677062000
N	3.730858000	-10.365350000	1.810536000
C	2.283526000	-8.496873000	1.084788000
C	2.910810000	-9.248617000	2.272708000
C	1.358861000	-9.372139000	0.234865000
C	1.887003000	-9.782447000	3.273393000
C	1.000037000	-8.715587000	-1.075696000
H	3.093053000	-8.122224000	0.450339000
H	1.742949000	-7.622726000	1.458165000
H	3.479961000	-8.500113000	2.857726000
H	1.874542000	-10.313580000	0.003491000

H	0.441806000	-9.634193000	0.769555000
H	3.887319000	-11.007809000	2.582470000
H	4.633255000	-10.028015000	1.489710000
H	0.174676000	-9.421312000	4.060391000
H	-0.313200000	-8.701541000	-2.413901000

Adduct 7GluB$_a$:

O	0.646389000	-16.090089000	4.142404000
S	0.487441000	-14.756643000	3.534674000
C	0.247709000	-13.640421000	4.910742000
O	-0.554550000	-14.487841000	2.537272000
C	2.064021000	-14.253905000	2.845564000
N	0.136959000	-12.329507000	4.675177000
C	2.092543000	-13.266009000	1.858176000
C	3.240320000	-14.827395000	3.329094000
C	0.014191000	-12.603605000	6.880764000
N	-0.006749000	-11.705547000	5.857239000
C	3.323443000	-12.838072000	1.368690000
H	1.166788000	-12.845188000	1.482187000
C	4.462566000	-14.388282000	2.823444000
H	3.193193000	-15.607503000	4.081047000
C	-0.071829000	-12.816225000	8.277036000
H	-0.030533000	-10.683720000	5.812832000
C	4.524560000	-13.384888000	1.846570000
H	3.359042000	-12.059541000	0.612285000
H	5.382789000	-14.829201000	3.196759000
C	5.847523000	-12.908438000	1.299074000
H	6.667507000	-13.118492000	1.991122000
H	6.081065000	-13.409076000	0.351242000
H	5.823645000	-11.832430000	1.104224000
N	0.171991000	-14.768017000	7.339407000
C	0.176431000	-13.874033000	6.307566000
N	0.030847000	-14.120075000	8.524897000
C	0.359911000	-16.210386000	7.330000000
H	-0.204397000	-12.116119000	9.088250000
H	1.383403000	-16.467049000	7.620946000
H	0.167912000	-16.579660000	6.323735000
H	-0.336209000	-16.655205000	8.042484000
O	0.179252000	-10.388969000	2.763612000
O	4.453624000	-9.493057000	0.214545000
O	0.176132000	-9.177777000	4.667942000
O	3.219268000	-7.865024000	-0.724188000
N	0.990521000	-6.949612000	3.350861000
C	1.146604000	-8.251498000	1.254696000
C	0.373106000	-8.013999000	2.563637000

C	2.598712000	-8.683943000	1.477343000
C	0.250553000	-9.256362000	3.444155000
C	3.413542000	-8.611857000	0.209406000
H	1.142352000	-7.319759000	0.679992000
H	0.616149000	-8.996077000	0.654558000
H	-0.674365000	-7.795128000	2.277963000
H	3.062035000	-8.007933000	2.208143000
H	2.664027000	-9.693905000	1.890912000
H	0.653778000	-7.003814000	4.308395000
H	0.733327000	-6.042140000	2.974727000
H	0.109610000	-11.168902000	3.395263000
H	4.929355000	-9.340261000	-0.620064000

Adduct 7GluB$_b$:

O	-4.210403000	-13.684772000	3.478811000
S	-3.565149000	-12.390766000	3.192250000
C	-2.103748000	-12.358168000	4.222503000
O	-4.280848000	-11.121905000	3.367035000
C	-2.911929000	-12.439494000	1.523822000
N	-1.262793000	-11.323311000	4.131523000
C	-2.642037000	-11.239418000	0.861799000
C	-2.651051000	-13.671739000	0.923940000
C	-0.398337000	-12.730659000	5.624021000
N	-0.239588000	-11.543820000	4.975304000
C	-2.084317000	-11.284420000	-0.412800000
H	-2.867898000	-10.292246000	1.338515000
C	-2.096002000	-13.695699000	-0.354167000
H	-2.887414000	-14.590154000	1.450060000
C	0.115699000	-13.642778000	6.575896000
H	0.511115000	-10.849488000	4.944546000
C	-1.797118000	-12.508515000	-1.036758000
H	-1.856160000	-10.358402000	-0.932227000
H	-1.888322000	-14.651573000	-0.827161000
C	-1.196400000	-12.533590000	-2.420819000
H	-0.690496000	-13.481823000	-2.621666000
H	-1.972406000	-12.406636000	-3.185851000
H	-0.475339000	-11.720906000	-2.546996000
N	-1.760949000	-14.467955000	5.837279000
C	-1.599749000	-13.291099000	5.164075000
N	-0.716870000	-14.676112000	6.680800000
C	-2.798992000	-15.480351000	5.720604000
H	1.012982000	-13.602861000	7.175136000
H	-2.441124000	-16.331493000	5.132871000
H	-3.662253000	-15.037594000	5.226124000
H	-3.063721000	-15.823922000	6.721690000

O	-0.731408000	-8.979813000	2.850285000
O	0.362283000	-9.055740000	-2.093408000
O	1.165390000	-9.310735000	4.027519000
O	0.625786000	-6.845910000	-1.774163000
N	2.519155000	-7.511982000	2.512509000
C	0.517636000	-7.212453000	1.091810000
C	1.060662000	-7.432897000	2.514866000
C	0.878200000	-8.342206000	0.123477000
C	0.510648000	-8.684014000	3.198127000
C	0.612260000	-7.966044000	-1.313485000
H	0.932744000	-6.275383000	0.707072000
H	-0.567236000	-7.082617000	1.137941000
H	0.668395000	-6.604484000	3.136487000
H	1.950500000	-8.560025000	0.215837000
H	0.343697000	-9.266560000	0.358628000
H	2.831977000	-7.939719000	3.379915000
H	2.920568000	-6.581077000	2.454722000
H	-1.033611000	-9.815984000	3.321186000
H	0.244143000	-8.709929000	-2.994905000

Adduct 7GluB$_c$:

O	-4.553522000	-10.925317000	6.780446000
S	-3.430628000	-10.013364000	6.496856000
C	-2.068631000	-11.077765000	6.038443000
O	-2.950721000	-9.053895000	7.497900000
C	-3.797136000	-9.114067000	4.990253000
N	-0.916842000	-10.531471000	5.636771000
C	-3.141977000	-7.906175000	4.739669000
C	-4.704903000	-9.648776000	4.075857000
C	-0.664563000	-12.739958000	5.512776000
N	-0.071167000	-11.528852000	5.323734000
C	-3.392485000	-7.240340000	3.543105000
H	-2.453730000	-7.499228000	5.471899000
C	-4.945079000	-8.965168000	2.885403000
H	-5.215660000	-10.578475000	4.301672000
C	-0.536118000	-14.148092000	5.457391000
H	0.827520000	-11.235072000	4.933034000
C	-4.289513000	-7.760273000	2.596840000
H	-2.878510000	-6.307699000	3.329605000
H	-5.649444000	-9.376392000	2.167558000
C	-4.547647000	-7.019978000	1.307562000
H	-4.963216000	-7.680465000	0.541845000
H	-5.264143000	-6.203759000	1.462381000
H	-3.624923000	-6.576953000	0.921880000
N	-2.541570000	-13.709896000	6.188337000

C	-1.964109000	-12.490578000	5.979128000
N	-1.675848000	-14.704371000	5.861923000
C	-3.892007000	-14.046233000	6.611280000
H	0.297489000	-14.767243000	5.161545000
H	-4.512637000	-14.308067000	5.748486000
H	-4.324215000	-13.183500000	7.115837000
H	-3.838875000	-14.901245000	7.286493000
O	0.395674000	-8.201354000	5.111835000
O	-1.165986000	-5.252528000	1.300570000
O	1.835661000	-9.743383000	4.310745000
O	0.601519000	-4.012330000	1.927330000
N	3.179055000	-7.867239000	2.882679000
C	1.556106000	-6.152757000	3.617630000
C	2.359235000	-7.408286000	4.001203000
C	0.586955000	-6.384259000	2.455352000
C	1.494009000	-8.574800000	4.475235000
C	0.049746000	-5.090124000	1.895273000
H	2.263119000	-5.366895000	3.333349000
H	1.016204000	-5.789730000	4.496618000
H	2.952150000	-7.144388000	4.898713000
H	1.119883000	-6.899764000	1.645401000
H	-0.250316000	-7.025354000	2.744442000
H	3.466034000	-8.827711000	3.050939000
H	4.014377000	-7.295376000	2.803304000
H	-0.136229000	-9.008990000	5.388761000
H	-1.401139000	-4.378636000	0.943931000

Adduct 7GluB6:

O	-4.549408000	-9.671377000	6.097869000
S	-3.476876000	-9.270529000	5.177514000
C	-2.163586000	-10.453366000	5.444283000
O	-2.937836000	-7.915479000	5.198827000
C	-4.069888000	-9.592945000	3.506785000
N	-0.988512000	-10.250566000	4.859351000
C	-3.407110000	-9.013588000	2.429701000
C	-5.192263000	-10.387204000	3.315809000
C	-0.880873000	-12.169080000	6.036959000
N	-0.208134000	-11.276934000	5.241234000
C	-3.881529000	-9.245984000	1.146802000
H	-2.553175000	-8.374700000	2.607571000
C	-5.653801000	-10.607688000	2.020793000
H	-5.707452000	-10.803506000	4.170425000
C	-0.831067000	-13.355160000	6.800428000
H	0.746268000	-11.328921000	4.893223000
C	-5.007653000	-10.046715000	0.918658000

H	-3.380358000	-8.781273000	0.306213000
H	-6.538113000	-11.214469000	1.870009000
C	-5.504814000	-10.287965000	-0.484023000
H	-6.460029000	-10.812428000	-0.482229000
H	-5.635340000	-9.347203000	-1.023451000
H	-4.792571000	-10.892984000	-1.052244000
N	-2.825637000	-12.521516000	7.025771000
C	-2.167026000	-11.662471000	6.197113000
N	-2.014863000	-13.549681000	7.371586000
C	-4.208520000	-12.508353000	7.479804000
H	-0.028200000	-14.051679000	6.972977000
H	-4.821944000	-13.160846000	6.854406000
H	-4.586792000	-11.491470000	7.422685000
H	-4.235427000	-12.867673000	8.506234000
O	1.115501000	-8.715995000	3.125620000
O	1.632875000	-9.637122000	-2.093611000
O	2.233152000	-10.463451000	3.952768000
O	3.237114000	-8.098226000	-1.800265000
N	4.415438000	-10.024147000	2.377881000
C	3.081621000	-8.401956000	1.063262000
C	3.404068000	-8.972008000	2.459372000
C	2.555674000	-9.452286000	0.080169000
C	2.202936000	-9.502379000	3.228789000
C	2.535329000	-8.961012000	-1.342992000
H	4.007983000	-7.986134000	0.664429000
H	2.382135000	-7.569235000	1.153697000
H	3.734641000	-8.126786000	3.083613000
H	3.216847000	-10.324215000	0.098665000
H	1.556815000	-9.807184000	0.337509000
H	4.424958000	-10.604885000	3.209551000
H	5.340429000	-9.632453000	2.251066000
H	0.492782000	-8.995902000	3.772158000
H	1.696432000	-9.315448000	-3.003566000

Adduct 7GluB6$_a$:

O	0.541435000	-16.430392000	4.439065000
S	0.518978000	-15.201817000	3.631047000
C	0.315810000	-13.873944000	4.808799000
O	-0.451825000	-15.018587000	2.554624000
C	2.164945000	-14.961119000	2.943310000
N	0.123760000	-12.635386000	4.365556000
C	2.339145000	-14.065234000	1.889040000
C	3.232821000	-15.689977000	3.454040000
C	0.105686000	-12.562108000	6.601131000
N	0.004882000	-11.844792000	5.441540000

C	3.608691000	-13.898292000	1.351634000
H	1.490589000	-13.521446000	1.494118000
C	4.498435000	-15.511485000	2.899257000
H	3.068773000	-16.397967000	4.256581000
C	0.061220000	-12.550198000	8.013044000
H	-0.176248000	-10.859836000	5.288069000
C	4.707279000	-14.614843000	1.847418000
H	3.748647000	-13.207200000	0.526775000
H	5.332940000	-16.084968000	3.288166000
C	6.079794000	-14.413057000	1.255245000
H	6.795734000	-15.134876000	1.651807000
H	6.059085000	-14.517982000	0.167025000
H	6.457264000	-13.409899000	1.477616000
N	0.383887000	-14.610258000	7.390006000
C	0.316649000	-13.893413000	6.231417000
N	0.239578000	-13.790128000	8.459089000
C	0.659713000	-16.023611000	7.601568000
H	-0.084958000	-11.740654000	8.709724000
H	1.717638000	-16.177390000	7.830887000
H	0.400154000	-16.568589000	6.696915000
H	0.057461000	-16.366273000	8.441773000
O	-0.210366000	-9.736307000	2.096887000
O	4.463682000	-7.934168000	0.421746000
O	0.007298000	-9.166079000	4.256454000
O	3.100735000	-6.319457000	-0.333067000
N	0.544525000	-6.560436000	3.659275000
C	0.945007000	-7.270971000	1.325158000
C	0.065447000	-7.417686000	2.581213000
C	2.405242000	-7.653241000	1.566803000
C	-0.034657000	-8.845960000	3.091257000
C	3.316373000	-7.212869000	0.446454000
H	0.896194000	-6.227306000	1.004770000
H	0.521929000	-7.868405000	0.515245000
H	-0.969102000	-7.183418000	2.273364000
H	2.760935000	-7.158997000	2.478442000
H	2.530967000	-8.726960000	1.724667000
H	0.215251000	-6.881212000	4.562471000
H	0.259376000	-5.598900000	3.520408000
H	-0.265372000	-10.620889000	2.478531000
H	5.014081000	-7.573602000	-0.289562000

Adduct 7GluB6$_b$:

O	-4.304362000	-13.373084000	3.328884000
S	-3.448342000	-12.264738000	2.873906000
C	-2.055028000	-12.249287000	3.991501000

O	-3.960100000	-10.896123000	2.767487000
C	-2.749493000	-12.725292000	1.285371000
N	-1.189022000	-11.236867000	3.923167000
C	-2.119596000	-11.751394000	0.508324000
C	-2.849118000	-14.043384000	0.848735000
C	-0.453001000	-12.641518000	5.499172000
N	-0.230387000	-11.469943000	4.836058000
C	-1.572143000	-12.116721000	-0.715585000
H	-2.069749000	-10.726271000	0.855140000
C	-2.301278000	-14.388869000	-0.385541000
H	-3.362275000	-14.776090000	1.459914000
C	-0.027056000	-13.541155000	6.503546000
H	0.526584000	-10.785631000	4.871366000
C	-1.651371000	-13.438723000	-1.180247000
H	-1.074554000	-11.364948000	-1.320626000
H	-2.384245000	-15.412728000	-0.736181000
C	-1.042510000	-13.818642000	-2.507132000
H	-1.303009000	-14.840836000	-2.789600000
H	-1.381615000	-13.149570000	-3.303813000
H	0.050018000	-13.748897000	-2.470577000
N	-1.866853000	-14.339603000	5.656719000
C	-1.631259000	-13.182810000	4.973369000
N	-0.887100000	-14.553966000	6.571550000
C	-2.915750000	-15.331238000	5.478330000
H	0.826705000	-13.508301000	7.162163000
H	-2.563497000	-16.157393000	4.853461000
H	-3.770064000	-14.854739000	5.000566000
H	-3.192118000	-15.717814000	6.459032000
O	-0.554962000	-8.219981000	3.515161000
O	-0.838568000	-7.915725000	-1.572326000
O	1.358549000	-9.326980000	3.938383000
O	0.092060000	-5.906668000	-1.187788000
N	2.793041000	-7.714837000	2.297314000
C	0.686712000	-6.661136000	1.537087000
C	1.477832000	-7.242483000	2.724730000
C	0.425796000	-7.683971000	0.428018000
C	0.760739000	-8.381290000	3.445872000
C	-0.105780000	-7.044394000	-0.829479000
H	1.263947000	-5.830821000	1.120715000
H	-0.254695000	-6.240552000	1.898903000
H	1.533570000	-6.448709000	3.492397000
H	1.370320000	-8.177614000	0.168957000
H	-0.264275000	-8.468547000	0.747373000
H	3.171947000	-8.360036000	2.984429000
H	3.436470000	-6.936253000	2.201543000
H	-0.962639000	-9.007392000	3.946821000

H	-1.108305000	-7.435275000	-2.371994000

Adduct 7GluB6$_c$:

O	-4.313136000	-10.853794000	7.038728000
S	-3.367755000	-9.925411000	6.404623000
C	-2.030834000	-10.950838000	5.805477000
O	-2.775036000	-8.807594000	7.136600000
C	-4.144955000	-9.265764000	4.923857000
N	-0.885034000	-10.379373000	5.430557000
C	-3.651555000	-8.086023000	4.368869000
C	-5.233003000	-9.927485000	4.361390000
C	-0.655329000	-12.570602000	5.113743000
N	-0.057793000	-11.351075000	5.014406000
C	-4.253235000	-7.577554000	3.223720000
H	-2.825675000	-7.568073000	4.840269000
C	-5.823626000	-9.401152000	3.215818000
H	-5.623623000	-10.822951000	4.828219000
C	-0.533264000	-13.969428000	4.949379000
H	0.872664000	-11.049454000	4.718848000
C	-5.341488000	-8.227296000	2.625866000
H	-3.877231000	-6.655953000	2.792297000
H	-6.678759000	-9.906862000	2.780364000
C	-5.966315000	-7.679153000	1.367678000
H	-6.989274000	-8.038443000	1.240016000
H	-5.985328000	-6.586945000	1.376314000
H	-5.394574000	-7.988642000	0.486134000
N	-2.522955000	-13.581418000	5.745851000
C	-1.943109000	-12.353392000	5.619536000
N	-1.668000000	-14.547189000	5.329135000
C	-3.869224000	-13.940818000	6.166249000
H	0.289521000	-14.568384000	4.594183000
H	-4.514518000	-14.095207000	5.297210000
H	-4.267864000	-13.137162000	6.781885000
H	-3.813387000	-14.865400000	6.739003000
O	0.554898000	-8.013695000	5.253239000
O	0.342008000	-5.148386000	0.800064000
O	2.027082000	-9.540220000	4.503228000
O	1.465791000	-3.795833000	2.195873000
N	3.839086000	-7.656988000	3.791798000
C	2.048464000	-5.961275000	3.997529000
C	2.701330000	-7.222671000	4.597740000
C	1.497227000	-6.189574000	2.590870000
C	1.727592000	-8.384036000	4.762556000
C	1.123821000	-4.910368000	1.886616000
H	2.807366000	-5.175706000	3.961617000

H	1.260936000	-5.608220000	4.665998000
H	2.983614000	-6.971631000	5.634138000
H	2.255903000	-6.687908000	1.976348000
H	0.624141000	-6.847960000	2.595385000
H	4.022550000	-8.644669000	3.931491000
H	4.673377000	-7.130532000	4.021230000
H	-0.037110000	-8.806547000	5.388829000
H	0.176868000	-4.291515000	0.378445000

Adduct 7GluC:

O	-4.527098000	-9.794300000	5.742432000
S	-3.292743000	-9.337315000	5.100316000
C	-2.055776000	-10.515042000	5.579386000
O	-2.763635000	-7.999301000	5.332167000
C	-3.447728000	-9.577057000	3.346812000
N	-0.827175000	-10.399908000	5.090293000
C	-2.614082000	-8.867290000	2.488193000
C	-4.371097000	-10.494399000	2.862286000
C	-0.840118000	-12.202866000	6.371960000
N	-0.092129000	-11.408535000	5.564001000
C	-2.700876000	-9.102046000	1.124803000
H	-1.912824000	-8.143287000	2.886812000
C	-4.445756000	-10.713210000	1.493439000
H	-5.022159000	-11.019146000	3.552100000
C	-0.882873000	-13.343845000	7.205302000
H	0.861268000	-11.465314000	5.199419000
C	-3.609841000	-10.030399000	0.609187000
H	-2.047689000	-8.567837000	0.442364000
H	-5.162637000	-11.430094000	1.105223000
C	-3.686749000	-10.266737000	-0.874562000
H	-4.149804000	-11.228925000	-1.103101000
H	-4.285034000	-9.488686000	-1.360604000
H	-2.690025000	-10.243787000	-1.321202000
N	-2.857881000	-12.450256000	7.234659000
C	-2.121613000	-11.657247000	6.409876000
N	-2.102491000	-13.464507000	7.701610000
C	-4.257026000	-12.368104000	7.604813000
H	-0.113902000	-14.055591000	7.463212000
H	-4.830425000	-13.150206000	7.101245000
H	-4.636013000	-11.392041000	7.308103000
H	-4.344654000	-12.499194000	8.683502000
O	0.747010000	-8.982211000	3.407254000
O	-0.264085000	-9.098459000	-1.514233000
O	2.049080000	-10.733276000	3.932558000
O	1.548259000	-7.793233000	-1.595465000

N	3.658876000	-10.275280000	1.817472000
C	2.201999000	-8.417585000	1.121409000
C	2.842394000	-9.170020000	2.290994000
C	1.279562000	-9.293493000	0.282327000
C	1.830635000	-9.718746000	3.284139000
C	0.906631000	-8.633950000	-1.015010000
H	2.999619000	-8.032668000	0.480155000
H	1.658188000	-7.551293000	1.505093000
H	3.411613000	-8.427990000	2.880130000
H	1.796623000	-10.230371000	0.043105000
H	0.368724000	-9.560776000	0.823201000
H	3.821508000	-10.926511000	2.578355000
H	4.553414000	-9.939187000	1.479978000
H	0.114804000	-9.404747000	4.063629000
H	-0.390070000	-8.638307000	-2.359938000

Adduct 7GluC$_a$:

O	0.677759000	-16.052835000	4.144379000
S	0.500914000	-14.729608000	3.542228000
C	0.256246000	-13.626377000	4.909711000
O	-0.541753000	-14.475598000	2.556091000
C	2.054068000	-14.210283000	2.853762000
N	0.150926000	-12.323305000	4.679970000
C	2.066049000	-13.220968000	1.875666000
C	3.233104000	-14.771311000	3.327632000
C	0.015489000	-12.600430000	6.870265000
N	0.004488000	-11.702163000	5.852401000
C	3.284895000	-12.779078000	1.384558000
H	1.133244000	-12.809496000	1.507655000
C	4.443540000	-14.317688000	2.821895000
H	3.195076000	-15.555497000	4.075124000
C	-0.074651000	-12.815226000	8.264412000
H	-0.016816000	-10.681000000	5.807608000
C	4.488047000	-13.313523000	1.853846000
H	3.312213000	-11.997978000	0.631600000
H	5.370419000	-14.748138000	3.188211000
C	5.798736000	-12.819766000	1.304636000
H	6.623143000	-13.026926000	1.990202000
H	6.029766000	-13.310725000	0.353225000
H	5.759512000	-11.743793000	1.120042000
N	0.170826000	-14.755094000	7.328209000
C	0.175702000	-13.862298000	6.301433000
N	0.023894000	-14.111888000	8.503730000
C	0.318616000	-16.197208000	7.313384000
H	-0.205097000	-12.116824000	9.076598000

H	1.276168000	-16.482798000	7.754810000
H	0.276734000	-16.536693000	6.280260000
H	-0.489479000	-16.645053000	7.892740000
O	0.208702000	-10.413962000	2.764777000
O	4.456533000	-9.578179000	0.225763000
O	0.202392000	-9.206784000	4.656984000
O	3.209033000	-7.989855000	-0.731185000
N	1.058680000	-7.007813000	3.348252000
C	1.171991000	-8.302847000	1.258013000
C	0.415511000	-8.049369000	2.564337000
C	2.607079000	-8.766553000	1.478548000
C	0.281254000	-9.285851000	3.438298000
C	3.414024000	-8.712895000	0.212534000
H	1.188211000	-7.373372000	0.682222000
H	0.623797000	-9.035408000	0.661077000
H	-0.628160000	-7.808034000	2.291626000
H	3.087891000	-8.104395000	2.208380000
H	2.649861000	-9.778285000	1.888388000
H	0.736116000	-7.059684000	4.308887000
H	0.832214000	-6.091830000	2.978370000
H	0.133312000	-11.190124000	3.398160000
H	4.925286000	-9.437772000	-0.612915000

Adduct 7GluC$_b$:

O	-4.190459000	-13.648702000	3.459864000
S	-3.545036000	-12.362694000	3.187092000
C	-2.098590000	-12.342715000	4.214029000
O	-4.253096000	-11.101752000	3.368185000
C	-2.889832000	-12.399023000	1.536229000
N	-1.255924000	-11.320614000	4.129072000
C	-2.610776000	-11.198710000	0.890557000
C	-2.631959000	-13.622023000	0.930444000
C	-0.407028000	-12.729251000	5.608422000
N	-0.239745000	-11.545508000	4.965076000
C	-2.046258000	-11.234563000	-0.375065000
H	-2.836381000	-10.255965000	1.375490000
C	-2.069013000	-13.637556000	-0.338286000
H	-2.877883000	-14.542310000	1.447838000
C	0.101650000	-13.648564000	6.554075000
H	0.513368000	-10.854788000	4.935575000
C	-1.761334000	-12.450118000	-1.003479000
H	-1.809296000	-10.307441000	-0.886976000
H	-1.861209000	-14.588499000	-0.818994000
C	-1.150604000	-12.464097000	-2.378325000
H	-0.655889000	-13.415095000	-2.586632000

H	-1.918667000	-12.316819000	-3.145112000
H	-0.419659000	-11.659195000	-2.484206000
N	-1.768947000	-14.455637000	5.812619000
C	-1.602749000	-13.278736000	5.150404000
N	-0.733882000	-14.668912000	6.649576000
C	-2.819213000	-15.448846000	5.702963000
H	0.999498000	-13.618240000	7.151882000
H	-2.450544000	-16.335735000	5.181959000
H	-3.646347000	-15.016498000	5.143205000
H	-3.143619000	-15.731831000	6.704569000
O	-0.733486000	-9.001370000	2.839164000
O	0.310642000	-9.116859000	-2.075163000
O	1.150342000	-9.339809000	4.011492000
O	0.547588000	-6.917520000	-1.756928000
N	2.515100000	-7.593406000	2.473274000
C	0.509204000	-7.258518000	1.086404000
C	1.066201000	-7.479633000	2.495053000
C	0.828991000	-8.402262000	0.131418000
C	0.504006000	-8.713772000	3.182078000
C	0.551773000	-8.033341000	-1.298299000
H	0.938818000	-6.336371000	0.685424000
H	-0.570688000	-7.104519000	1.146539000
H	0.703598000	-6.643905000	3.121013000
H	1.894879000	-8.646923000	0.211314000
H	0.273651000	-9.309276000	0.381362000
H	2.833096000	-8.028859000	3.332810000
H	2.943967000	-6.678577000	2.394322000
H	-1.039771000	-9.831467000	3.315050000
H	0.181684000	-8.772418000	-2.973803000

Adduct 7GluC$_c$:

O	-4.579786000	-10.895704000	6.769452000
S	-3.454217000	-9.987240000	6.485301000
C	-2.087931000	-11.056768000	6.052163000
O	-2.983546000	-9.015749000	7.479088000
C	-3.806481000	-9.106036000	4.964644000
N	-0.931928000	-10.514523000	5.657139000
C	-3.147528000	-7.902100000	4.705149000
C	-4.706001000	-9.651260000	4.048289000
C	-0.678639000	-12.724143000	5.557624000
N	-0.083169000	-11.514945000	5.362863000
C	-3.385322000	-7.251345000	3.497727000
H	-2.466059000	-7.486588000	5.438902000
C	-4.933671000	-8.982584000	2.846945000
H	-5.220142000	-10.577456000	4.280755000

C	-0.549644000	-14.132738000	5.517675000
H	0.819727000	-11.225103000	4.979039000
C	-4.273681000	-7.782293000	2.549392000
H	-2.867942000	-6.322189000	3.277354000
H	-5.631440000	-9.402213000	2.127517000
C	-4.518421000	-7.058209000	1.248340000
H	-4.920983000	-7.729529000	0.485085000
H	-5.240913000	-6.243885000	1.384399000
H	-3.592929000	-6.615123000	0.869531000
N	-2.562727000	-13.687410000	6.222821000
C	-1.983012000	-12.470159000	6.007784000
N	-1.693559000	-14.685026000	5.915797000
C	-3.917358000	-14.019655000	6.635457000
H	0.287003000	-14.754741000	5.236760000
H	-4.527257000	-14.296634000	5.769755000
H	-4.356686000	-13.149608000	7.120895000
H	-3.870964000	-14.863516000	7.325088000
O	0.386490000	-8.189401000	5.123816000
O	-1.138621000	-5.279792000	1.269906000
O	1.834561000	-9.739290000	4.353069000
O	0.623777000	-4.033378000	1.898699000
N	3.192467000	-7.877671000	2.919885000
C	1.562094000	-6.155945000	3.620586000
C	2.361238000	-7.407388000	4.025187000
C	0.604126000	-6.399612000	2.451526000
C	1.491251000	-8.569135000	4.502237000
C	0.072073000	-5.111371000	1.873211000
H	2.271908000	-5.373117000	3.334908000
H	1.013712000	-5.783615000	4.490387000
H	2.944991000	-7.134282000	4.925947000
H	1.144806000	-6.923254000	1.651998000
H	-0.235740000	-7.037915000	2.739238000
H	3.477564000	-8.836390000	3.100873000
H	4.028666000	-7.306700000	2.843374000
H	-0.148267000	-8.994248000	5.403280000
H	-1.370640000	-4.409592000	0.902356000

Adduct 7GluP:

O	-4.500074000	-9.721846000	5.773024000
S	-3.268932000	-9.296420000	5.102242000
C	-2.042921000	-10.486942000	5.573808000
O	-2.708038000	-7.964516000	5.298270000
C	-3.458365000	-9.565178000	3.356791000
N	-0.806383000	-10.367705000	5.095420000
C	-2.630007000	-8.879304000	2.470831000

C	-4.401632000	-10.482057000	2.903655000
C	-0.837085000	-12.203243000	6.329171000
N	-0.083890000	-11.390277000	5.548452000
C	-2.742102000	-9.138330000	1.111631000
H	-1.914985000	-8.154491000	2.846336000
C	-4.501992000	-10.723790000	1.538591000
H	-5.047411000	-10.986892000	3.614995000
C	-0.892449000	-13.361298000	7.133997000
H	0.871464000	-11.442720000	5.185019000
C	-3.671222000	-10.066452000	0.626230000
H	-2.092858000	-8.622438000	0.409463000
H	-5.235074000	-11.439000000	1.174978000
C	-3.776845000	-10.327256000	-0.848547000
H	-4.239639000	-11.296011000	-1.053211000
H	-4.389622000	-9.559489000	-1.335638000
H	-2.789434000	-10.306860000	-1.318324000
N	-2.861570000	-12.459352000	7.173030000
C	-2.121108000	-11.650336000	6.371915000
N	-2.119399000	-13.488124000	7.620154000
C	-4.261350000	-12.382134000	7.523759000
H	-0.129841000	-14.084042000	7.383142000
H	-4.841245000	-13.112297000	6.951341000
H	-4.620214000	-11.378156000	7.298898000
H	-4.367365000	-12.596778000	8.588064000
O	0.773954000	-8.942861000	3.450501000
O	-0.181175000	-9.162450000	-1.522990000
O	2.066456000	-10.713510000	3.946465000
O	1.612875000	-7.827520000	-1.594288000
N	3.691861000	-10.221482000	1.857978000
C	2.212343000	-8.391292000	1.150012000
C	2.858647000	-9.130173000	2.324189000
C	1.321346000	-9.292045000	0.307543000
C	1.848753000	-9.686476000	3.314309000
C	0.968567000	-8.666248000	-1.010482000
H	3.007158000	-7.989770000	0.512860000
H	1.645683000	-7.535690000	1.528228000
H	3.410709000	-8.373781000	2.915830000
H	1.862563000	-10.225228000	0.098022000
H	0.403164000	-9.569535000	0.834110000
H	3.844781000	-10.873385000	2.620459000
H	4.590745000	-9.871836000	1.548787000
H	0.138077000	-9.373741000	4.100445000
H	-0.290722000	-8.723818000	-2.380270000

Adduct 7GluP$_a$:

O	0.637571000	-16.053686000	4.148041000
S	0.478824000	-14.724817000	3.551899000
C	0.275451000	-13.619427000	4.923064000
O	-0.568662000	-14.441430000	2.577337000
C	2.033803000	-14.230936000	2.850204000
N	0.146569000	-12.315052000	4.690351000
C	2.050334000	-13.244580000	1.866129000
C	3.211373000	-14.803800000	3.320438000
C	0.119804000	-12.575127000	6.886435000
N	0.050267000	-11.690124000	5.862064000
C	3.272705000	-12.816917000	1.365988000
H	1.117845000	-12.826539000	1.500962000
C	4.424916000	-14.364813000	2.804318000
H	3.168773000	-15.585485000	4.072169000
C	0.095141000	-12.781362000	8.282351000
H	0.020292000	-10.668339000	5.808664000
C	4.475398000	-13.362401000	1.830912000
H	3.302076000	-12.038316000	0.608584000
H	5.350157000	-14.805038000	3.166606000
C	5.785563000	-12.885729000	1.273774000
H	6.614544000	-13.108198000	1.950428000
H	6.000914000	-13.374761000	0.316326000
H	5.761788000	-11.807198000	1.094067000
N	0.314241000	-14.724971000	7.351273000
C	0.266779000	-13.844658000	6.318093000
N	0.218137000	-14.078636000	8.526881000
C	0.498220000	-16.158332000	7.337065000
H	-0.007141000	-12.080163000	9.097129000
H	1.516616000	-16.416256000	7.642213000
H	0.320206000	-16.520148000	6.324804000
H	-0.209042000	-16.610259000	8.034151000
O	0.131239000	-10.423011000	2.779335000
O	4.409171000	-9.493879000	0.237260000
O	0.187457000	-9.203199000	4.666437000
O	3.125835000	-7.934246000	-0.725168000
N	0.962612000	-7.003988000	3.321779000
C	1.084895000	-8.321205000	1.250448000
C	0.333691000	-8.064546000	2.558505000
C	2.529947000	-8.743008000	1.474148000
C	0.226658000	-9.294169000	3.444860000
C	3.344438000	-8.659137000	0.216207000
H	1.076397000	-7.399882000	0.658603000
H	0.550159000	-9.077347000	0.668525000
H	-0.718856000	-7.849894000	2.287929000
H	2.983665000	-8.064338000	2.209763000

H	2.603517000	-9.753637000	1.886942000
H	0.657049000	-7.062572000	4.287673000
H	0.695224000	-6.098774000	2.954399000
H	0.079386000	-11.196641000	3.420887000
H	4.879558000	-9.331613000	-0.594448000

Adduct 7GluP$_b$:

O	-4.184885000	-13.672619000	3.479701000
S	-3.546261000	-12.385309000	3.193682000
C	-2.092872000	-12.349550000	4.209083000
O	-4.255497000	-11.122426000	3.365135000
C	-2.895101000	-12.433185000	1.542035000
N	-1.269909000	-11.306128000	4.128652000
C	-2.631131000	-11.234438000	0.882721000
C	-2.622285000	-13.661552000	0.948307000
C	-0.367378000	-12.718098000	5.571931000
N	-0.240273000	-11.523415000	4.944473000
C	-2.065701000	-11.277133000	-0.384329000
H	-2.870537000	-10.289207000	1.358892000
C	-2.059665000	-13.683160000	-0.322422000
H	-2.857432000	-14.579858000	1.476805000
C	0.172410000	-13.638684000	6.495472000
H	0.498083000	-10.815082000	4.911492000
C	-1.765159000	-12.497284000	-1.001821000
H	-1.841843000	-10.350566000	-0.905865000
H	-1.841398000	-14.637533000	-0.794222000
C	-1.155889000	-12.518637000	-2.373880000
H	-0.664653000	-13.472869000	-2.580352000
H	-1.924052000	-12.369650000	-3.141932000
H	-0.420602000	-11.716544000	-2.484304000
N	-1.689683000	-14.475358000	5.770767000
C	-1.562054000	-13.289281000	5.121363000
N	-0.641597000	-14.681032000	6.588224000
C	-2.715229000	-15.487123000	5.655767000
H	1.077269000	-13.599378000	7.083432000
H	-2.343482000	-16.345351000	5.088356000
H	-3.571762000	-15.054463000	5.139590000
H	-2.998810000	-15.816143000	6.656664000
O	-0.794269000	-8.980944000	2.865289000
O	0.416733000	-9.098325000	-2.059423000
O	1.108204000	-9.294357000	4.020568000
O	0.577501000	-6.889569000	-1.742111000
N	2.420039000	-7.489019000	2.515685000
C	0.427582000	-7.233765000	1.099556000
C	0.971305000	-7.427754000	2.516734000

C	0.820525000	-8.363611000	0.159188000
C	0.439119000	-8.676331000	3.200513000
C	0.592700000	-8.005987000	-1.280706000
H	0.823107000	-6.293505000	0.701273000
H	-0.660308000	-7.128429000	1.140599000
H	0.564051000	-6.602672000	3.133454000
H	1.893078000	-8.567436000	0.285129000
H	0.291338000	-9.293191000	0.389627000
H	2.735615000	-7.925646000	3.375642000
H	2.813158000	-6.556980000	2.465282000
H	-1.081322000	-9.822731000	3.336491000
H	0.319397000	-8.757929000	-2.961629000

Adduct 7GluP$_c$:

O	-4.556812000	-10.937534000	6.714138000
S	-3.440769000	-10.026533000	6.446587000
C	-2.079591000	-11.073783000	6.004813000
O	-2.977521000	-9.068377000	7.443945000
C	-3.784153000	-9.139862000	4.946542000
N	-0.925077000	-10.519957000	5.640438000
C	-3.133692000	-7.930920000	4.709132000
C	-4.666210000	-9.682567000	4.017432000
C	-0.664681000	-12.709225000	5.463331000
N	-0.077868000	-11.495819000	5.319408000
C	-3.362123000	-7.271835000	3.508815000
H	-2.465858000	-7.518790000	5.458576000
C	-4.884572000	-9.005580000	2.823478000
H	-5.174840000	-10.615652000	4.237834000
C	-0.532299000	-14.111447000	5.373665000
H	0.825512000	-11.184336000	4.952257000
C	-4.231963000	-7.800266000	2.547304000
H	-2.851990000	-6.334673000	3.303123000
H	-5.570561000	-9.422109000	2.090666000
C	-4.464858000	-7.068864000	1.256978000
H	-4.865253000	-7.732248000	0.486206000
H	-5.184410000	-6.253563000	1.397404000
H	-3.534961000	-6.626652000	0.888328000
N	-2.542119000	-13.700929000	6.069618000
C	-1.970303000	-12.479429000	5.909107000
N	-1.675192000	-14.674858000	5.739990000
C	-3.884934000	-14.047460000	6.476358000
H	0.306743000	-14.723003000	5.076971000
H	-4.465479000	-14.396513000	5.617502000

H	-4.357546000	-13.160940000	6.898115000
H	-3.834036000	-14.843609000	7.220826000
O	0.349163000	-8.193057000	5.196004000
O	-1.130649000	-5.285028000	1.315795000
O	1.807756000	-9.700997000	4.389458000
O	0.569990000	-4.021650000	2.034866000
N	3.142475000	-7.802118000	3.025187000
C	1.488141000	-6.132115000	3.742883000
C	2.305561000	-7.367391000	4.126756000
C	0.563678000	-6.382144000	2.560455000
C	1.450800000	-8.542678000	4.571245000
C	0.038689000	-5.104831000	1.972263000
H	2.180434000	-5.325192000	3.480918000
H	0.917653000	-5.791344000	4.611618000
H	2.876619000	-7.104720000	5.038901000
H	1.130961000	-6.900847000	1.775018000
H	-0.277219000	-7.030230000	2.825405000
H	3.422087000	-8.765267000	3.179786000
H	3.976558000	-7.230298000	2.968677000
H	-0.178498000	-9.012252000	5.447232000
H	-1.355534000	-4.417082000	0.947863000

Adduct 7GluM:

O	-4.372635000	-9.498625000	5.867962000
S	-3.132536000	-9.150601000	5.170843000
C	-1.961515000	-10.395292000	5.635482000
O	-2.485822000	-7.850036000	5.309768000
C	-3.348568000	-9.474610000	3.434338000
N	-0.697645000	-10.266851000	5.219772000
C	-2.522618000	-8.830279000	2.513801000
C	-4.295029000	-10.408581000	3.023745000
C	-0.852243000	-12.232721000	6.256754000
N	-0.028424000	-11.366618000	5.605500000
C	-2.650062000	-9.137970000	1.166602000
H	-1.801332000	-8.093131000	2.854982000
C	-4.408492000	-10.702992000	1.669788000
H	-4.938088000	-10.882352000	3.760936000
C	-0.992287000	-13.464243000	6.925744000
H	0.931640000	-11.428637000	5.269163000
C	-3.584445000	-10.084022000	0.724269000
H	-2.012871000	-8.643025000	0.437448000
H	-5.148817000	-11.426961000	1.337009000
C	-3.677674000	-10.433077000	-0.728235000
H	-4.573373000	-11.018309000	-0.949243000
H	-3.692643000	-9.536750000	-1.355932000

H	-2.807066000	-11.018451000	-1.042570000
N	-2.933108000	-12.487486000	6.965134000
C	-2.116811000	-11.632641000	6.291791000
N	-2.253403000	-13.604172000	7.334539000
C	-4.354846000	-12.401625000	7.204600000
H	-0.271890000	-14.240363000	7.136193000
H	-4.922947000	-12.792593000	6.353956000
H	-4.630638000	-11.359145000	7.360647000
H	-4.582571000	-12.995610000	8.088720000
O	0.839393000	-8.742619000	3.540555000
O	-0.335436000	-9.588548000	-1.385285000
O	2.116334000	-10.550296000	3.991851000
O	1.291904000	-8.051869000	-1.619029000
N	3.691406000	-10.090463000	1.854058000
C	2.103642000	-8.377749000	1.106137000
C	2.837924000	-8.999731000	2.295053000
C	1.195417000	-9.373549000	0.406546000
C	1.891241000	-9.525798000	3.357013000
C	0.759359000	-8.908246000	-0.948458000
H	2.844785000	-8.009335000	0.388531000
H	1.533709000	-7.506296000	1.441888000
H	3.385048000	-8.181651000	2.804189000
H	1.741783000	-10.318413000	0.275225000
H	0.310877000	-9.618622000	1.007254000
H	3.917692000	-10.672389000	2.653265000
H	4.558479000	-9.720840000	1.484397000
H	0.248257000	-9.162021000	4.228532000
H	-0.508862000	-9.248368000	-2.276031000

Adduct 7GluM$_a$:

O	0.456390000	-16.148518000	3.615183000
S	0.873323000	-14.843554000	3.092920000
C	0.527399000	-13.689453000	4.381405000
O	0.362440000	-14.315783000	1.835049000
C	2.650472000	-14.844498000	3.005988000
N	0.614925000	-12.380130000	4.121941000
C	3.299345000	-13.829347000	2.306690000
C	3.365051000	-15.856299000	3.635340000
C	0.064595000	-12.630241000	6.285968000
N	0.331158000	-11.749358000	5.276717000
C	4.684155000	-13.839042000	2.243280000
H	2.712623000	-13.056035000	1.818587000
C	4.753238000	-15.851823000	3.556595000
H	2.828233000	-16.640849000	4.161660000
C	-0.300742000	-12.819226000	7.630761000

H	0.353354000	-10.734371000	5.284188000
C	5.432436000	-14.846938000	2.865020000
H	5.202106000	-13.055569000	1.693508000
H	5.323161000	-16.645610000	4.035263000
C	6.925793000	-14.836458000	2.789497000
H	7.358779000	-15.749147000	3.205258000
H	7.275995000	-14.738042000	1.757449000
H	7.347090000	-13.990610000	3.343351000
N	-0.097879000	-14.787854000	6.737037000
C	0.188207000	-13.909420000	5.736897000
N	-0.384620000	-14.126056000	7.887547000
C	-0.036148000	-16.229311000	6.748184000
H	-0.503361000	-12.108053000	8.418835000
H	0.927431000	-16.576716000	7.135337000
H	-0.166132000	-16.596210000	5.731552000
H	-0.830216000	-16.605136000	7.393654000
O	-0.858899000	-8.469031000	3.288027000
O	0.977524000	-8.474162000	-1.500243000
O	0.970681000	-9.083140000	4.455020000
O	1.033414000	-6.263567000	-1.072360000
N	2.482107000	-7.151200000	3.301174000
C	0.663268000	-6.747181000	1.713724000
C	1.041553000	-7.046016000	3.163307000
C	1.134040000	-7.830023000	0.762206000
C	0.411530000	-8.312041000	3.698717000
C	1.036745000	-7.407643000	-0.671970000
H	1.129307000	-5.799956000	1.422284000
H	-0.417557000	-6.595608000	1.630316000
H	0.590024000	-6.250546000	3.791466000
H	2.188751000	-8.046492000	0.979291000
H	0.597174000	-8.774410000	0.901688000
H	2.707687000	-7.634342000	4.162969000
H	2.891013000	-6.227444000	3.349128000
H	-1.194131000	-9.276181000	3.680279000
H	0.962673000	-8.113939000	-2.398881000

Adduct 7GluM$_b$:

O	-4.291066000	-13.489515000	3.553507000
S	-3.613483000	-12.223704000	3.263217000
C	-2.157117000	-12.243733000	4.270944000
O	-4.267723000	-10.928723000	3.420187000
C	-2.939428000	-12.301392000	1.618778000
N	-1.306089000	-11.213812000	4.207519000
C	-2.679629000	-11.114636000	0.934756000
C	-2.631286000	-13.538122000	1.059741000

C	-0.411471000	-12.724633000	5.579247000
N	-0.262420000	-11.501177000	5.004512000
C	-2.097358000	-11.176739000	-0.323656000
H	-2.944261000	-10.162451000	1.385589000
C	-2.050829000	-13.580604000	-0.202571000
H	-2.857416000	-14.448838000	1.607621000
C	0.116336000	-13.701872000	6.445926000
H	0.505342000	-10.830348000	4.972101000
C	-1.768007000	-12.407008000	-0.908772000
H	-1.887047000	-10.258651000	-0.867540000
H	-1.812476000	-14.541941000	-0.652080000
C	-1.114595000	-12.455882000	-2.254499000
H	-1.069349000	-13.474728000	-2.646342000
H	-1.649832000	-11.836006000	-2.980976000
H	-0.093440000	-12.063811000	-2.205798000
N	-1.791584000	-14.448738000	5.720569000
C	-1.632832000	-13.236328000	5.124093000
N	-0.723624000	-14.734903000	6.509342000
C	-2.829002000	-15.437703000	5.534971000
H	1.029390000	-13.718666000	7.021716000
H	-2.641321000	-16.043662000	4.642623000
H	-3.790387000	-14.938404000	5.417192000
H	-2.832691000	-16.082294000	6.412838000
O	-0.762909000	-8.878752000	2.860776000
O	0.379531000	-9.395644000	-2.022256000
O	1.143991000	-9.306981000	3.992685000
O	0.574586000	-7.160815000	-1.845026000
N	2.550025000	-7.644815000	2.395571000
C	0.552300000	-7.314151000	1.011457000
C	1.105247000	-7.481369000	2.426003000
C	0.811847000	-8.528628000	0.137485000
C	0.506004000	-8.662017000	3.167414000
C	0.578611000	-8.249922000	-1.315400000
H	1.025433000	-6.440341000	0.549932000
H	-0.519188000	-7.097441000	1.058280000
H	0.769448000	-6.602685000	3.012676000
H	1.861020000	-8.834620000	0.257017000
H	0.208367000	-9.391129000	0.443486000
H	2.853702000	-8.027561000	3.284745000
H	2.994312000	-6.741989000	2.281767000
H	-1.085833000	-9.678090000	3.367150000
H	0.278375000	-9.113269000	-2.943939000

Adduct 7GluM$_c$:

O	-4.427567000	-10.850673000	6.895238000

S	-3.308063000	-9.955909000	6.593161000
C	-1.981925000	-11.024223000	6.106946000
O	-2.786159000	-8.991412000	7.556161000
C	-3.673968000	-9.079830000	5.088516000
N	-0.792507000	-10.490561000	5.809390000
C	-2.992838000	-7.895805000	4.809617000
C	-4.607610000	-9.601748000	4.197953000
C	-0.646865000	-12.681363000	5.427135000
N	0.012422000	-11.491085000	5.411240000
C	-3.254035000	-7.234857000	3.617117000
H	-2.284303000	-7.497005000	5.529590000
C	-4.859438000	-8.923024000	3.011506000
H	-5.137462000	-10.516509000	4.449277000
C	-0.595685000	-14.071516000	5.204087000
H	0.927859000	-11.200568000	5.068191000
C	-4.184307000	-7.738637000	2.698470000
H	-2.732929000	-6.306981000	3.391395000
H	-5.595223000	-9.315806000	2.313649000
C	-4.434938000	-7.033618000	1.402088000
H	-5.388423000	-7.329853000	0.958036000
H	-4.439553000	-5.947074000	1.529823000
H	-3.644690000	-7.261725000	0.678798000
N	-2.597915000	-13.606627000	5.910363000
C	-1.945808000	-12.413590000	5.873731000
N	-1.781985000	-14.608344000	5.491316000
C	-3.980625000	-13.888587000	6.219896000
H	0.210535000	-14.704870000	4.865908000
H	-4.633380000	-13.625429000	5.381390000
H	-4.288322000	-13.310374000	7.090905000
H	-4.059368000	-14.956263000	6.418546000
O	0.452538000	-8.090517000	5.361191000
O	-1.229029000	-5.939636000	1.002895000
O	1.898700000	-9.614193000	4.531492000
O	0.135202000	-4.341698000	1.809627000
N	3.164323000	-7.747011000	3.055527000
C	1.378048000	-6.161286000	3.614214000
C	2.297585000	-7.273140000	4.122014000
C	0.460193000	-6.637473000	2.503228000
C	1.527454000	-8.455040000	4.679713000
C	-0.192510000	-5.507085000	1.769226000
H	1.994579000	-5.338339000	3.236161000
H	0.795722000	-5.756096000	4.447412000
H	2.844608000	-6.870608000	4.997354000
H	1.046802000	-7.218250000	1.777930000
H	-0.316123000	-7.318438000	2.873994000
H	3.526774000	-8.660032000	3.308605000

H	3.952132000	-7.120099000	2.948860000
H	-0.026365000	-8.912569000	5.667823000
H	-1.554313000	-5.151190000	0.542516000

Adduct 7MetB:

O	-4.437470000	-9.411394000	6.336226000
S	-3.993761000	-8.699709000	5.124879000
C	-2.355318000	-9.288692000	4.773220000
O	-3.968168000	-7.222340000	5.098930000
C	-5.011601000	-9.240603000	3.752012000
N	-1.691114000	-8.725284000	3.763807000
C	-4.999766000	-8.515411000	2.557681000
C	-5.811984000	-10.371705000	3.904665000
C	-0.295555000	-10.145951000	4.768353000
N	-0.456953000	-9.251013000	3.745692000
C	-5.799161000	-8.946510000	1.503613000
H	-4.383082000	-7.628194000	2.465271000
C	-6.608495000	-10.784045000	2.837395000
H	-5.819763000	-10.902214000	4.850315000
C	0.569280000	-11.043339000	5.438464000
H	0.226267000	-8.727613000	3.173764000
C	-6.610883000	-10.085793000	1.622947000
H	-5.800401000	-8.385685000	0.572768000
H	-7.242002000	-11.659140000	2.952692000
C	-7.451990000	-10.553891000	0.460501000
H	-8.267556000	-11.202435000	0.791059000
H	-7.885992000	-9.709793000	-0.083952000
H	-6.847168000	-11.124226000	-0.255137000
N	-1.346523000	-11.105170000	6.469846000
C	-1.517165000	-10.214103000	5.451789000
N	-0.083397000	-11.610034000	6.451913000
C	-2.307545000	-11.608603000	7.436225000
H	1.602965000	-11.294759000	5.252144000
H	-2.743894000	-12.554195000	7.096665000
H	-3.098553000	-10.869810000	7.561367000
H	-1.787834000	-11.775061000	8.380494000
S	-0.865529000	-4.539536000	-0.790293000
O	-2.392300000	-5.778321000	3.217337000
O	-0.547399000	-5.906654000	4.510550000
N	0.877097000	-6.990224000	2.493095000
C	-1.034080000	-6.714968000	0.944895000
C	-0.259972000	-6.113623000	2.130684000
C	-1.905414000	-5.719824000	0.170230000
C	-1.075044000	-5.930979000	3.418335000
C	-2.152459000	-3.364695000	-1.334336000

H	-0.306258000	-7.161818000	0.255635000
H	-1.660753000	-7.532730000	1.312593000
H	0.083262000	-5.104777000	1.847158000
H	-2.541586000	-5.154794000	0.855639000
H	-2.549538000	-6.262603000	-0.528896000
H	1.264835000	-6.635526000	3.367010000
H	1.600446000	-6.914108000	1.781752000
H	-2.898138000	-3.857753000	-1.963725000
H	-1.651840000	-2.592607000	-1.922234000
H	-2.644069000	-2.894666000	-0.478608000
H	-2.852537000	-5.935223000	4.069772000

Adduct 7MetB_a:

O	-5.207201000	-6.709193000	6.688704000
S	-3.890025000	-6.987052000	6.089674000
C	-3.403454000	-5.501479000	5.246595000
O	-3.721371000	-8.121682000	5.158261000
C	-2.705589000	-7.207066000	7.417350000
N	-2.280621000	-5.529063000	4.528324000
C	-1.452208000	-7.758228000	7.137174000
C	-3.061847000	-6.839690000	8.713742000
C	-3.232537000	-3.538990000	4.198841000
N	-2.164401000	-4.344267000	3.910040000
C	-0.547338000	-7.930154000	8.179717000
H	-1.200988000	-8.052361000	6.124045000
C	-2.141355000	-7.024321000	9.744721000
H	-4.049312000	-6.435472000	8.906683000
C	-3.871145000	-2.292166000	3.998612000
H	-1.471546000	-4.324901000	3.143587000
C	-0.873343000	-7.564620000	9.495743000
H	0.427694000	-8.362959000	7.972145000
H	-2.415665000	-6.749097000	10.759320000
C	0.129873000	-7.738362000	10.609923000
H	-0.350455000	-7.703751000	11.591202000
H	0.660876000	-8.691380000	10.523564000
H	0.885436000	-6.943743000	10.583770000
N	-5.117813000	-3.441557000	5.363266000
C	-4.055453000	-4.249437000	5.083216000
N	-4.996638000	-2.254536000	4.709894000
C	-6.225994000	-3.646660000	6.280226000
H	-3.588588000	-1.447806000	3.387331000
H	-6.027508000	-3.167075000	7.244762000
H	-6.362486000	-4.717323000	6.428944000
H	-7.121812000	-3.205566000	5.841287000
S	2.750176000	-8.246964000	2.037455000

O	-1.520287000	-8.267192000	3.354623000
O	-2.590818000	-7.037568000	1.794504000
N	-0.548733000	-5.278600000	1.680510000
C	0.786992000	-6.668994000	3.232929000
C	-0.230536000	-6.669045000	2.079248000
C	1.556194000	-7.982136000	3.416374000
C	-1.578264000	-7.332836000	2.393988000
C	3.248865000	-9.968178000	2.385599000
H	1.505034000	-5.858871000	3.052217000
H	0.265425000	-6.423999000	4.162738000
H	0.196023000	-7.241092000	1.238550000
H	0.865750000	-8.828244000	3.453935000
H	2.114778000	-7.952367000	4.357306000
H	-1.331110000	-5.324163000	1.028012000
H	0.244566000	-4.881772000	1.182244000
H	3.724790000	-10.051525000	3.366313000
H	3.972377000	-10.252437000	1.618732000
H	2.392173000	-10.645045000	2.332104000
H	-2.433567000	-8.437389000	3.670755000

Adduct 7MetB_b:

O	-4.206491000	-9.805308000	6.532658000
S	-3.676496000	-8.843785000	5.550052000
C	-2.115020000	-9.494384000	5.008029000
O	-3.478987000	-7.428835000	5.927387000
C	-4.744637000	-8.867061000	4.110462000
N	-1.380631000	-8.749388000	4.181439000
C	-4.628735000	-7.857834000	3.151322000
C	-5.690820000	-9.882917000	3.982511000
C	-0.167735000	-10.543524000	4.715476000
N	-0.215238000	-9.385100000	3.988372000
C	-5.473195000	-7.883661000	2.045648000
H	-3.898334000	-7.066385000	3.278647000
C	-6.529824000	-9.887536000	2.869281000
H	-5.775119000	-10.639829000	4.754306000
C	0.581665000	-11.684550000	5.088080000
H	0.527649000	-8.803871000	3.566280000
C	-6.431717000	-8.896450000	1.883879000
H	-5.394233000	-7.099508000	1.297422000
H	-7.276263000	-10.670586000	2.768502000
C	-7.321705000	-8.924585000	0.665268000
H	-8.246506000	-9.475486000	0.856552000
H	-7.586785000	-7.914122000	0.340516000

H	-6.816318000	-9.414039000	-0.176399000
N	-1.338493000	-11.816145000	6.104559000
C	-1.395600000	-10.661861000	5.380692000
N	-0.141612000	-12.435039000	5.917426000
C	-2.360164000	-12.456961000	6.914753000
H	1.581309000	-11.988828000	4.815007000
H	-2.881466000	-13.232167000	6.342913000
H	-3.075620000	-11.700721000	7.236245000
H	-1.876943000	-12.916006000	7.778195000
S	-0.063528000	-3.617571000	0.883922000
O	-1.755919000	-5.706944000	4.445007000
O	0.054563000	-6.359050000	5.623128000
N	1.368947000	-7.028825000	3.364884000
C	-0.481543000	-6.147743000	1.977714000
C	0.339097000	-5.968883000	3.266579000
C	-1.233568000	-4.896933000	1.509021000
C	-0.463813000	-6.043595000	4.572612000
C	-1.217576000	-2.218120000	0.678126000
H	0.203288000	-6.468729000	1.182489000
H	-1.195387000	-6.963446000	2.124608000
H	0.795202000	-4.965087000	3.253139000
H	-1.818531000	-4.471938000	2.328298000
H	-1.919600000	-5.163985000	0.698842000
H	1.780391000	-6.963120000	4.295648000
H	2.106526000	-6.845301000	2.688572000
H	-1.996673000	-2.451961000	-0.052366000
H	-0.632486000	-1.373092000	0.309458000
H	-1.676032000	-1.942074000	1.631289000
H	-2.235409000	-6.032411000	5.237016000

Adduct 7MetB_c:

O	-6.112854000	-7.810396000	5.724123000
S	-4.763684000	-7.398121000	5.297035000
C	-4.967378000	-6.710736000	3.664516000
O	-3.645455000	-8.346244000	5.240489000
C	-4.263654000	-6.010387000	6.319337000
N	-3.885941000	-6.498468000	2.906911000
C	-2.925501000	-5.608938000	6.323380000
C	-5.213587000	-5.363570000	7.109305000
C	-5.648067000	-5.814400000	1.730058000
N	-4.293965000	-5.960423000	1.745762000
C	-2.546643000	-4.536060000	7.124691000
H	-2.195211000	-6.137198000	5.719989000
C	-4.813323000	-4.294363000	7.908575000
H	-6.240565000	-5.711446000	7.109190000

C	-6.793154000	-5.408036000	1.003571000
H	-3.548222000	-5.770719000	1.068143000
C	-3.480997000	-3.859915000	7.924514000
H	-1.506588000	-4.221839000	7.136315000
H	-5.546736000	-3.793326000	8.534395000
C	-3.062302000	-2.680175000	8.767325000
H	-3.719384000	-2.552400000	9.631846000
H	-2.036697000	-2.791768000	9.130534000
H	-3.102094000	-1.751154000	8.185339000
N	-7.481774000	-6.160681000	2.928643000
C	-6.123374000	-6.285980000	2.962204000
N	-7.877386000	-5.620087000	1.746083000
C	-8.468357000	-6.437501000	3.959593000
H	-6.885618000	-4.993542000	0.010876000
H	-8.709016000	-5.529390000	4.522541000
H	-8.063848000	-7.189208000	4.636831000
H	-9.373106000	-6.806675000	3.475598000
S	2.684715000	-8.862703000	2.112342000
O	-1.172138000	-6.826404000	2.664952000
O	-1.726140000	-5.858315000	0.704875000
N	0.865507000	-5.369532000	0.109322000
C	1.565665000	-6.315617000	2.270995000
C	0.584408000	-6.425711000	1.083021000
C	1.769704000	-7.595318000	3.089195000
C	-0.886919000	-6.324502000	1.472602000
C	2.479018000	-10.305206000	3.212651000
H	2.529674000	-5.989691000	1.863476000
H	1.234387000	-5.512951000	2.938288000
H	0.679025000	-7.445913000	0.664408000
H	0.809035000	-8.014223000	3.396193000
H	2.349594000	-7.367264000	3.989193000
H	0.074628000	-5.288959000	-0.524684000
H	1.678552000	-5.626762000	-0.443435000
H	2.938607000	-10.126736000	4.188405000
H	2.984671000	-11.146701000	2.734473000
H	1.422547000	-10.553660000	3.342896000
H	-2.159252000	-6.780785000	2.838658000

Adduct 7MetB6:

O	-4.367537000	-8.652666000	5.019697000
S	-4.130498000	-9.135345000	3.655127000
C	-2.758191000	-10.269863000	3.764144000
O	-3.869211000	-8.164614000	2.572090000
C	-5.526761000	-10.126737000	3.131549000
N	-2.586402000	-11.185581000	2.816772000

C	-5.783640000	-10.296775000	1.773076000
C	-6.341811000	-10.701177000	4.103014000
C	-0.910096000	-11.394702000	4.297366000
N	-1.471751000	-11.864720000	3.140915000
C	-6.877545000	-11.063859000	1.390050000
H	-5.145727000	-9.825361000	1.037136000
C	-7.433029000	-11.463869000	3.698151000
H	-6.135691000	-10.535161000	5.153046000
C	0.131964000	-11.495255000	5.245056000
H	-1.178221000	-12.622677000	2.547065000
C	-7.714728000	-11.661627000	2.341390000
H	-7.088625000	-11.195030000	0.334045000
H	-8.079551000	-11.904487000	4.449356000
C	-8.883013000	-12.511461000	1.908781000
H	-9.629842000	-12.596731000	2.700340000
H	-9.369357000	-12.097313000	1.022498000
H	-8.551461000	-13.524345000	1.655994000
N	-1.175105000	-9.875564000	5.885590000
C	-1.724675000	-10.346728000	4.733596000
N	-0.048701000	-10.565958000	6.180514000
C	-1.528557000	-8.693851000	6.661427000
H	0.973585000	-12.166310000	5.302182000
H	-2.612307000	-8.601213000	6.695543000
H	-1.104730000	-7.803428000	6.194030000
H	-1.123516000	-8.826425000	7.662834000
S	-0.081342000	-2.520440000	0.878266000
O	-1.867958000	-6.374511000	2.021069000
O	-0.739878000	-7.250486000	3.751840000
N	1.544083000	-5.948426000	3.091347000
C	0.501886000	-5.239767000	0.972279000
C	0.298339000	-5.473677000	2.486979000
C	-0.451655000	-4.236738000	0.317926000
C	-0.805776000	-6.472339000	2.822760000
C	-1.564444000	-1.662970000	0.249777000
H	1.533328000	-4.900112000	0.837286000
H	0.430217000	-6.196454000	0.446735000
H	-0.051236000	-4.524655000	2.926949000
H	-1.488039000	-4.466854000	0.564599000
H	-0.336340000	-4.274408000	-0.767941000
H	1.346346000	-6.439753000	3.957084000
H	2.164540000	-5.172655000	3.292227000
H	-1.635703000	-1.746467000	-0.836340000
H	-1.460266000	-0.610507000	0.515641000
H	-2.470137000	-2.058330000	0.713041000
H	-2.557093000	-7.023761000	2.298301000

Adduct 7MetB6$_a$:

O	-5.136435000	-6.891185000	6.629855000
S	-3.758722000	-7.095761000	6.164498000
C	-3.310951000	-5.609420000	5.292088000
O	-3.420972000	-8.246972000	5.312282000
C	-2.688310000	-7.165489000	7.606163000
N	-2.188857000	-5.611865000	4.579313000
C	-1.414506000	-7.718804000	7.489228000
C	-3.152543000	-6.671732000	8.821710000
C	-3.198248000	-3.655941000	4.226728000
N	-2.105348000	-4.431571000	3.950387000
C	-0.596938000	-7.765515000	8.612351000
H	-1.080667000	-8.116806000	6.539429000
C	-2.318978000	-6.728943000	9.935444000
H	-4.156353000	-6.272612000	8.895380000
C	-3.875493000	-2.436208000	4.001551000
H	-1.434623000	-4.389130000	3.172432000
C	-1.031030000	-7.268569000	9.848853000
H	0.392935000	-8.201980000	8.529673000
H	-2.680441000	-6.355771000	10.887679000
C	-0.121756000	-7.301623000	11.051635000
H	-0.688503000	-7.240575000	11.982634000
H	0.475410000	-8.216240000	11.074089000
H	0.575370000	-6.456938000	11.032979000
N	-5.091264000	-3.605171000	5.376745000
C	-4.000159000	-4.379187000	5.116521000
N	-5.003187000	-2.429037000	4.706124000
C	-6.201319000	-3.835094000	6.288149000
H	-3.620707000	-1.592596000	3.380445000
H	-6.019219000	-3.344982000	7.248776000
H	-6.313039000	-4.906847000	6.439088000
H	-7.103173000	-3.420035000	5.840329000
S	2.772311000	-8.235757000	1.646915000
O	-1.423496000	-8.349577000	3.264480000
O	-2.610480000	-7.087406000	1.828475000
N	-0.560300000	-5.333043000	1.572771000
C	0.857882000	-6.754406000	3.020391000
C	-0.234968000	-6.731182000	1.937144000
C	1.657126000	-8.058065000	3.102299000
C	-1.558011000	-7.396511000	2.334571000
C	3.275015000	-9.978134000	1.849410000
H	1.547695000	-5.926808000	2.820899000
H	0.400369000	-6.551902000	3.991447000
H	0.128632000	-7.296487000	1.065939000
H	0.989244000	-8.919499000	3.139388000
H	2.269211000	-8.057273000	4.007226000

H	-1.367760000	-5.343847000	0.952821000
H	0.215174000	-4.928046000	1.056669000
H	3.799894000	-10.127976000	2.794646000
H	3.954862000	-10.209681000	1.028931000
H	2.411457000	-10.643094000	1.793242000
H	-2.298817000	-8.537081000	3.658578000

Adduct 7MetB6$_b$:

O	-4.217850000	-9.579389000	6.544712000
S	-3.764545000	-8.726656000	5.438517000
C	-2.190216000	-9.383033000	4.927763000
O	-3.616737000	-7.274749000	5.624934000
C	-4.880107000	-8.975576000	4.051863000
N	-1.435090000	-8.648757000	4.116713000
C	-4.922636000	-8.031572000	3.027200000
C	-5.693244000	-10.104644000	4.027334000
C	-0.257131000	-10.460001000	4.665388000
N	-0.277374000	-9.299392000	3.940533000
C	-5.790656000	-8.235924000	1.961119000
H	-4.297882000	-7.148790000	3.076541000
C	-6.556851000	-10.290875000	2.951158000
H	-5.664827000	-10.810105000	4.848258000
C	0.474330000	-11.605489000	5.052817000
H	0.490211000	-8.740306000	3.546414000
C	-6.615780000	-9.367348000	1.901837000
H	-5.833841000	-7.500515000	1.164557000
H	-7.200444000	-11.163883000	2.932993000
C	-7.532530000	-9.587591000	0.724695000
H	-8.338960000	-10.280923000	0.970592000
H	-7.979283000	-8.649299000	0.387361000
H	-6.980434000	-10.009067000	-0.122242000
N	-1.463427000	-11.713752000	6.037140000
C	-1.495607000	-10.562784000	5.308341000
N	-0.272711000	-12.342362000	5.869717000
C	-2.506527000	-12.340234000	6.833763000
H	1.472980000	-11.923161000	4.799559000
H	-3.046782000	-13.086455000	6.244141000
H	-3.197175000	-11.570495000	7.172526000
H	-2.037569000	-12.829392000	7.686288000
S	0.300896000	-3.433429000	0.970573000
O	-1.691730000	-5.540645000	4.398778000
O	0.014110000	-6.310665000	5.648214000
N	1.444398000	-6.930182000	3.430200000
C	-0.317148000	-5.945388000	1.997391000
C	0.445078000	-5.841671000	3.330012000

C	-0.971831000	-4.643871000	1.526496000
C	-0.426481000	-5.934085000	4.588365000
C	-0.728448000	-1.931499000	0.848868000
H	0.389020000	-6.285141000	1.231428000
H	-1.081006000	-6.721566000	2.083609000
H	0.925931000	-4.853110000	3.378027000
H	-1.556851000	-4.193541000	2.329110000
H	-1.639732000	-4.851053000	0.687209000
H	1.841092000	-6.913938000	4.367676000
H	2.201307000	-6.756739000	2.775373000
H	-1.526219000	-2.060892000	0.115273000
H	-0.074025000	-1.124191000	0.518769000
H	-1.153688000	-1.669576000	1.819225000
H	-2.242089000	-5.871577000	5.136338000

Adduct 7MetB6$_c$:

O	-6.188342000	-7.348900000	5.223949000
S	-4.753818000	-7.129797000	4.999778000
C	-4.628093000	-6.271170000	3.445143000
O	-3.819849000	-8.266584000	4.971457000
C	-4.163606000	-5.983237000	6.251690000
N	-3.428474000	-6.156643000	2.884086000
C	-2.796606000	-5.887240000	6.505997000
C	-5.084716000	-5.213901000	6.956492000
C	-4.915708000	-5.306864000	1.457479000
N	-3.592032000	-5.559777000	1.695529000
C	-2.354744000	-4.996167000	7.477051000
H	-2.097755000	-6.511030000	5.963375000
C	-4.622335000	-4.328709000	7.926649000
H	-6.144050000	-5.325932000	6.762839000
C	-5.885147000	-4.800939000	0.562293000
H	-2.799039000	-5.639146000	1.046149000
C	-3.255678000	-4.200298000	8.197455000
H	-1.292412000	-4.922906000	7.684971000
H	-5.337208000	-3.735442000	8.486717000
C	-2.758275000	-3.218272000	9.228446000
H	-3.536688000	-2.970790000	9.952759000
H	-1.897879000	-3.614522000	9.772607000
H	-2.441485000	-2.284182000	8.751991000
N	-6.941842000	-5.493353000	2.334305000
C	-5.624462000	-5.736365000	2.584792000
N	-7.089326000	-4.918814000	1.113961000
C	-8.101784000	-5.670370000	3.193761000
H	-5.781652000	-4.379048000	-0.424447000
H	-8.330094000	-4.744583000	3.729662000

H	-7.891341000	-6.463948000	3.907879000
H	-8.950929000	-5.939784000	2.567498000
S	2.714259000	-7.497404000	2.052097000
O	-1.455371000	-8.544008000	3.385465000
O	-2.600812000	-8.840819000	1.470921000
N	-1.278532000	-6.792355000	0.286050000
C	0.124597000	-6.510132000	2.305559000
C	-0.598757000	-7.511399000	1.387880000
C	1.272097000	-7.102491000	3.128281000
C	-1.669546000	-8.366069000	2.076458000
C	3.717614000	-8.473600000	3.222498000
H	0.516873000	-5.701183000	1.679197000
H	-0.604562000	-6.056405000	2.980791000
H	0.143170000	-8.225573000	1.000108000
H	0.953653000	-8.013660000	3.635975000
H	1.593396000	-6.381469000	3.883526000
H	-1.849293000	-7.460735000	-0.227672000
H	-0.584082000	-6.424985000	-0.357766000
H	3.995767000	-7.876564000	4.092867000
H	4.624349000	-8.769157000	2.693862000
H	3.184094000	-9.370780000	3.541036000
H	-2.282738000	-8.852604000	3.806094000

Adduct 7MetC:

O	-4.407810000	-9.467115000	6.302450000
S	-3.944972000	-8.715927000	5.134562000
C	-2.318110000	-9.296233000	4.784760000
O	-3.908920000	-7.248343000	5.170350000
C	-4.935394000	-9.188269000	3.737164000
N	-1.650938000	-8.720947000	3.795905000
C	-4.881718000	-8.429453000	2.571529000
C	-5.757340000	-10.301680000	3.838074000
C	-0.272505000	-10.156699000	4.770554000
N	-0.426346000	-9.242216000	3.770283000
C	-5.662226000	-8.810619000	1.492161000
H	-4.244243000	-7.553644000	2.520341000
C	-6.534959000	-10.663943000	2.745920000
H	-5.794255000	-10.858814000	4.767011000
C	0.585550000	-11.069493000	5.425042000
H	0.251365000	-8.723735000	3.190289000
C	-6.495318000	-9.931424000	1.560068000
H	-5.632196000	-8.223799000	0.578959000
H	-7.187876000	-11.528118000	2.818818000
C	-7.317776000	-10.343654000	0.369288000
H	-8.145292000	-10.993509000	0.660761000

H	-7.731823000	-9.474647000	-0.147942000
H	-6.705776000	-10.892149000	-0.354408000
N	-1.324590000	-11.142696000	6.442841000
C	-1.486762000	-10.233619000	5.446064000
N	-0.072160000	-11.646263000	6.417629000
C	-2.285284000	-11.647998000	7.401128000
H	1.617436000	-11.323438000	5.236119000
H	-2.682269000	-12.614695000	7.078975000
H	-3.100677000	-10.931572000	7.487519000
H	-1.784766000	-11.770288000	8.361354000
S	-1.040460000	-4.660436000	-0.767617000
O	-2.426492000	-5.829531000	3.275408000
O	-0.562258000	-5.944681000	4.520793000
N	0.836496000	-6.986614000	2.490579000
C	-1.117099000	-6.787866000	0.999960000
C	-0.326220000	-6.151722000	2.146865000
C	-2.024723000	-5.822669000	0.240541000
C	-1.111006000	-5.973721000	3.444603000
C	-2.349782000	-3.514544000	-1.272052000
H	-0.400364000	-7.230169000	0.298307000
H	-1.713965000	-7.610895000	1.400241000
H	-0.019472000	-5.139481000	1.840433000
H	-2.641896000	-5.254477000	0.939265000
H	-2.688182000	-6.385740000	-0.421741000
H	1.226269000	-6.622713000	3.358021000
H	1.544416000	-6.900694000	1.767579000
H	-3.115805000	-4.023338000	-1.860978000
H	-1.887394000	-2.745192000	-1.891718000
H	-2.810919000	-3.037224000	-0.405009000
H	-2.869048000	-5.995436000	4.135151000

Adduct 7MetC_a:

O	-5.182017000	-6.665045000	6.685324000
S	-3.896539000	-6.954053000	6.047596000
C	-3.411515000	-5.476917000	5.217850000
O	-3.779042000	-8.069691000	5.100111000
C	-2.685416000	-7.211809000	7.321897000
N	-2.298120000	-5.502737000	4.501250000
C	-1.449703000	-7.760640000	6.990660000
C	-2.999792000	-6.874769000	8.630563000
C	-3.234077000	-3.518283000	4.189325000
N	-2.175590000	-4.325593000	3.892012000
C	-0.518440000	-7.959803000	7.996704000
H	-1.231605000	-8.031434000	5.963444000
C	-2.053337000	-7.086784000	9.624833000

H	-3.978753000	-6.470250000	8.860074000
C	-3.865788000	-2.268154000	3.999700000
H	-1.468443000	-4.300216000	3.141098000
C	-0.802556000	-7.624420000	9.324158000
H	0.447316000	-8.391624000	7.751529000
H	-2.293544000	-6.834809000	10.653036000
C	0.230534000	-7.828425000	10.399096000
H	-0.220062000	-7.819571000	11.393507000
H	0.755067000	-8.778539000	10.270646000
H	0.983953000	-7.034408000	10.369731000
N	-5.108792000	-3.415929000	5.351396000
C	-4.055580000	-4.224518000	5.062863000
N	-4.981881000	-2.235102000	4.709407000
C	-6.222802000	-3.630898000	6.251088000
H	-3.579024000	-1.419920000	3.396994000
H	-6.062973000	-3.105356000	7.196548000
H	-6.315110000	-4.699294000	6.439589000
H	-7.129216000	-3.250153000	5.780659000
S	2.705152000	-8.251814000	2.252426000
O	-1.574696000	-8.235774000	3.392144000
O	-2.586255000	-6.984675000	1.826643000
N	-0.524450000	-5.280986000	1.728447000
C	0.730261000	-6.653268000	3.346959000
C	-0.237719000	-6.658991000	2.160293000
C	1.472509000	-7.969124000	3.570157000
C	-1.595182000	-7.298969000	2.442347000
C	3.179457000	-9.956193000	2.642106000
H	1.463258000	-5.854903000	3.182541000
H	0.175502000	-6.389766000	4.250706000
H	0.209529000	-7.251507000	1.346971000
H	0.768440000	-8.803476000	3.585998000
H	1.990188000	-7.940244000	4.533001000
H	-1.294476000	-5.325019000	1.063674000
H	0.284095000	-4.898594000	1.247524000
H	3.614926000	-10.026906000	3.641050000
H	3.930739000	-10.259466000	1.911849000
H	2.323881000	-10.630373000	2.566648000
H	-2.495303000	-8.389184000	3.694623000

Adduct 7MetC_b:

O	-4.175510000	-9.800152000	6.518211000
S	-3.621215000	-8.830460000	5.572160000
C	-2.080774000	-9.492258000	5.028986000
O	-3.399184000	-7.439984000	5.988685000
C	-4.664836000	-8.792619000	4.134578000

N	-1.344130000	-8.760329000	4.207048000
C	-4.511010000	-7.769403000	3.203642000
C	-5.628594000	-9.777922000	3.973918000
C	-0.160359000	-10.561643000	4.722351000
N	-0.195299000	-9.401684000	4.005521000
C	-5.336966000	-7.751445000	2.091409000
H	-3.761897000	-7.000586000	3.357991000
C	-6.449134000	-9.738899000	2.854166000
H	-5.738928000	-10.548352000	4.728203000
C	0.574082000	-11.713719000	5.084523000
H	0.542509000	-8.835077000	3.559327000
C	-6.312921000	-8.733624000	1.897391000
H	-5.229829000	-6.955314000	1.360708000
H	-7.212252000	-10.500083000	2.724969000
C	-7.184499000	-8.711355000	0.670941000
H	-8.098668000	-9.289488000	0.819768000
H	-7.466033000	-7.690484000	0.401570000
H	-6.657777000	-9.141282000	-0.187474000
N	-1.332149000	-11.821331000	6.106437000
C	-1.375971000	-10.666554000	5.391697000
N	-0.153254000	-12.449109000	5.909546000
C	-2.350039000	-12.440295000	6.929493000
H	1.565889000	-12.032522000	4.802285000
H	-2.851213000	-13.245267000	6.384900000
H	-3.079151000	-11.681389000	7.208794000
H	-1.874466000	-12.853793000	7.818642000
S	-0.242651000	-3.763889000	0.821489000
O	-1.760890000	-5.763344000	4.468222000
O	0.076341000	-6.410681000	5.583850000
N	1.336108000	-7.057646000	3.312596000
C	-0.576642000	-6.252657000	1.982410000
C	0.284722000	-6.030227000	3.229099000
C	-1.361403000	-5.026249000	1.521681000
C	-0.472477000	-6.099356000	4.553338000
C	-1.412933000	-2.394073000	0.632798000
H	0.082530000	-6.579102000	1.169718000
H	-1.268074000	-7.076045000	2.176693000
H	0.714000000	-5.017272000	3.181820000
H	-1.911905000	-4.591820000	2.358551000
H	-2.082282000	-5.319255000	0.753294000
H	1.765967000	-6.978237000	4.232235000
H	2.050573000	-6.872947000	2.614942000
H	-2.221765000	-2.656525000	-0.052371000
H	-0.861611000	-1.550920000	0.214690000
H	-1.830992000	-2.097098000	1.596762000
H	-2.219154000	-6.091515000	5.271264000

Adduct 7MetC_c:

O	-6.318193000	-7.214822000	5.154529000
S	-4.893464000	-7.179501000	4.820777000
C	-4.760354000	-6.281129000	3.310354000
O	-4.140465000	-8.431721000	4.675189000
C	-4.056840000	-6.196820000	6.041963000
N	-3.561262000	-6.160700000	2.761285000
C	-2.666885000	-6.224927000	6.108478000
C	-4.807870000	-5.428027000	6.919860000
C	-5.020797000	-5.263105000	1.355645000
N	-3.706018000	-5.536961000	1.594204000
C	-2.030627000	-5.456230000	7.069823000
H	-2.100840000	-6.845210000	5.422232000
C	-4.150584000	-4.668282000	7.878578000
H	-5.889740000	-5.445152000	6.857151000
C	-5.979640000	-4.713239000	0.474702000
H	-2.879927000	-5.577445000	0.977736000
C	-2.758648000	-4.665975000	7.964228000
H	-0.946835000	-5.473805000	7.135134000
H	-4.729905000	-4.071309000	8.576070000
C	-2.049665000	-3.818514000	8.985719000
H	-2.704902000	-3.570263000	9.823134000
H	-1.167359000	-4.327225000	9.381431000
H	-1.711030000	-2.876727000	8.541214000
N	-7.048761000	-5.445362000	2.209831000
C	-5.740575000	-5.717795000	2.456471000
N	-7.181869000	-4.833326000	1.013857000
C	-8.211980000	-5.651034000	3.047246000
H	-5.862069000	-4.257258000	-0.496503000
H	-8.501237000	-4.720370000	3.543185000
H	-7.971747000	-6.402896000	3.797242000
H	-9.035561000	-5.991475000	2.419974000
S	2.499593000	-7.116742000	2.568275000
O	-1.649844000	-8.434538000	3.412238000
O	-2.583575000	-8.727873000	1.391814000
N	-1.305520000	-6.598146000	0.393423000
C	-0.129925000	-6.260503000	2.534467000
C	-0.679174000	-7.283596000	1.535881000
C	0.944692000	-6.803885000	3.473857000
C	-1.746725000	-8.218458000	2.099114000
C	3.424880000	-8.004216000	3.848136000
H	0.285162000	-5.420493000	1.965631000
H	-0.961070000	-5.862953000	3.121813000
H	0.148241000	-7.933823000	1.211604000

H	0.607542000	-7.733240000	3.937307000
H	1.141377000	-6.077754000	4.267486000
H	-1.803277000	-7.302437000	-0.147840000
H	-0.585880000	-6.196537000	-0.199974000
H	3.578851000	-7.379493000	4.730483000
H	4.398379000	-8.258819000	3.427196000
H	2.914755000	-8.925738000	4.135882000
H	-2.502024000	-8.804252000	3.728008000

Adduct 7MetP:

O	-4.407810000	-9.467115000	6.302450000
S	-3.944972000	-8.715927000	5.134562000
C	-2.318110000	-9.296233000	4.784760000
O	-3.908920000	-7.248343000	5.170350000
C	-4.935394000	-9.188269000	3.737164000
N	-1.650938000	-8.720947000	3.795905000
C	-4.881718000	-8.429453000	2.571529000
C	-5.757340000	-10.301680000	3.838074000
C	-0.272505000	-10.156699000	4.770554000
N	-0.426346000	-9.242216000	3.770283000
C	-5.662226000	-8.810619000	1.492161000
H	-4.244243000	-7.553644000	2.520341000
C	-6.534959000	-10.663943000	2.745920000
H	-5.794255000	-10.858814000	4.767011000
C	0.585550000	-11.069493000	5.425042000
H	0.251365000	-8.723735000	3.190289000
C	-6.495318000	-9.931424000	1.560068000
H	-5.632196000	-8.223799000	0.578959000
H	-7.187876000	-11.528118000	2.818818000
C	-7.317776000	-10.343654000	0.369288000
H	-8.145292000	-10.993509000	0.660761000
H	-7.731823000	-9.474647000	-0.147942000
H	-6.705776000	-10.892149000	-0.354408000
N	-1.324590000	-11.142696000	6.442841000
C	-1.486762000	-10.233619000	5.446064000
N	-0.072160000	-11.646263000	6.417629000
C	-2.285284000	-11.647998000	7.401128000
H	1.617436000	-11.323438000	5.236119000
H	-2.682269000	-12.614695000	7.078975000
H	-3.100677000	-10.931572000	7.487519000
H	-1.784766000	-11.770288000	8.361354000
S	-1.040460000	-4.660436000	-0.767617000
O	-2.426492000	-5.829531000	3.275408000
O	-0.562258000	-5.944681000	4.520793000
N	0.836496000	-6.986614000	2.490579000

C	-1.117099000	-6.787866000	0.999960000
C	-0.326220000	-6.151722000	2.146865000
C	-2.024723000	-5.822669000	0.240541000
C	-1.111006000	-5.973721000	3.444603000
C	-2.349782000	-3.514544000	-1.272052000
H	-0.400364000	-7.230169000	0.298307000
H	-1.713965000	-7.610895000	1.400241000
H	-0.019472000	-5.139481000	1.840433000
H	-2.641896000	-5.254477000	0.939265000
H	-2.688182000	-6.385740000	-0.421741000
H	1.226269000	-6.622713000	3.358021000
H	1.544416000	-6.900694000	1.767579000
H	-3.115805000	-4.023338000	-1.860978000
H	-1.887394000	-2.745192000	-1.891718000
H	-2.810919000	-3.037224000	-0.405009000
H	-2.869048000	-5.995436000	4.135151000

Adduct 7MetP_a:

O	-5.194398000	-6.697190000	6.680247000
S	-3.904352000	-6.986493000	6.049833000
C	-3.416737000	-5.514524000	5.215102000
O	-3.771930000	-8.109022000	5.112091000
C	-2.699090000	-7.225500000	7.333098000
N	-2.318230000	-5.557691000	4.469329000
C	-1.454044000	-7.763498000	7.010915000
C	-3.024526000	-6.884275000	8.640544000
C	-3.214009000	-3.548844000	4.198911000
N	-2.185957000	-4.379293000	3.870934000
C	-0.524472000	-7.947808000	8.024137000
H	-1.229113000	-8.037928000	5.984785000
C	-2.079917000	-7.082280000	9.641895000
H	-4.010579000	-6.488870000	8.861804000
C	-3.822204000	-2.285385000	4.036574000
H	-1.490406000	-4.364111000	3.103449000
C	-0.819015000	-7.608581000	9.350839000
H	0.447958000	-8.371130000	7.785471000
H	-2.328812000	-6.828144000	10.668778000
C	0.208519000	-7.794556000	10.430213000
H	-0.247382000	-7.789379000	11.423330000
H	0.749229000	-8.737543000	10.307388000
H	0.951263000	-6.988737000	10.402899000
N	-5.057856000	-3.415382000	5.406827000
C	-4.033557000	-4.246425000	5.089951000
N	-4.922596000	-2.233218000	4.775701000
C	-6.146071000	-3.613299000	6.334490000

H	-3.534166000	-1.436835000	3.433547000
H	-5.933139000	-3.127688000	7.292239000
H	-6.278812000	-4.683944000	6.491207000
H	-7.050219000	-3.177725000	5.907179000
S	2.695656000	-8.190365000	2.211401000
O	-1.570956000	-8.272250000	3.352023000
O	-2.601840000	-7.033176000	1.785720000
N	-0.571530000	-5.296552000	1.704919000
C	0.700379000	-6.646810000	3.325826000
C	-0.261639000	-6.666374000	2.136204000
C	1.470542000	-7.945384000	3.538529000
C	-1.608500000	-7.331990000	2.408095000
C	3.189253000	-9.892989000	2.561862000
H	1.416436000	-5.829041000	3.172242000
H	0.135640000	-6.404573000	4.231680000
H	0.203263000	-7.253331000	1.324875000
H	0.783520000	-8.796674000	3.553094000
H	1.994158000	-7.910903000	4.499894000
H	-1.338688000	-5.358842000	1.037837000
H	0.230063000	-4.903626000	1.221890000
H	3.634973000	-9.981057000	3.556491000
H	3.939155000	-10.171689000	1.818562000
H	2.340341000	-10.576894000	2.477285000
H	-2.488593000	-8.440556000	3.646664000

Adduct 7MetP_b:

O	-4.170979000	-9.799078000	6.538348000
S	-3.629329000	-8.824621000	5.588525000
C	-2.086208000	-9.470425000	5.037134000
O	-3.420656000	-7.429088000	5.996338000
C	-4.676692000	-8.804303000	4.153615000
N	-1.349202000	-8.714536000	4.230655000
C	-4.530649000	-7.785583000	3.213833000
C	-5.637309000	-9.797701000	4.002137000
C	-0.159768000	-10.524705000	4.699100000
N	-0.202165000	-9.348408000	4.014509000
C	-5.360691000	-7.779751000	2.101816000
H	-3.784973000	-7.010565000	3.362739000
C	-6.462293000	-9.769979000	2.883306000
H	-5.740961000	-10.563315000	4.764189000
C	0.576810000	-11.681385000	5.033812000
H	0.535359000	-8.764974000	3.580272000
C	-6.333858000	-8.769456000	1.916299000
H	-5.259297000	-6.987001000	1.364927000
H	-7.223220000	-10.536390000	2.762116000

C	-7.205952000	-8.763053000	0.693703000
H	-8.137324000	-9.309375000	0.862640000
H	-7.457758000	-7.743650000	0.388050000
H	-6.693672000	-9.238974000	-0.150770000
N	-1.326855000	-11.822102000	6.052377000
C	-1.379691000	-10.651713000	5.368359000
N	-0.149599000	-12.441772000	5.842528000
C	-2.342228000	-12.462188000	6.854406000
H	1.570791000	-11.991488000	4.746652000
H	-2.854334000	-13.242470000	6.282312000
H	-3.064281000	-11.707895000	7.167559000
H	-1.864186000	-12.913725000	7.724722000
S	-0.215763000	-3.789984000	0.819530000
O	-1.755448000	-5.722140000	4.482697000
O	0.083928000	-6.362500000	5.604042000
N	1.330729000	-7.039555000	3.338886000
C	-0.583124000	-6.253382000	2.002647000
C	0.281329000	-6.015754000	3.242936000
C	-1.353386000	-5.028616000	1.521657000
C	-0.470288000	-6.064234000	4.570986000
C	-1.357417000	-2.402683000	0.626035000
H	0.071459000	-6.602504000	1.193589000
H	-1.284456000	-7.066957000	2.212857000
H	0.708599000	-4.999844000	3.177983000
H	-1.907050000	-4.577335000	2.350363000
H	-2.072013000	-5.324960000	0.750046000
H	1.760342000	-6.943369000	4.257336000
H	2.045046000	-6.860027000	2.640434000
H	-2.169029000	-2.648911000	-0.064164000
H	-0.786851000	-1.570061000	0.209252000
H	-1.774021000	-2.095227000	1.589068000
H	-2.207530000	-6.037565000	5.291077000

Adduct 7MetP_c:

O	-6.318837000	-7.265131000	5.149865000
S	-4.890494000	-7.218805000	4.829120000
C	-4.748410000	-6.321088000	3.320601000
O	-4.119379000	-8.461591000	4.695783000
C	-4.077335000	-6.220619000	6.053295000
N	-3.545384000	-6.224480000	2.765485000
C	-2.685917000	-6.232675000	6.133233000
C	-4.846512000	-5.453276000	6.920627000
C	-4.986698000	-5.278097000	1.373300000
N	-3.681682000	-5.588357000	1.607322000

C	-2.066273000	-5.450070000	7.097210000
H	-2.107102000	-6.852687000	5.455445000
C	-4.205705000	-4.680233000	7.882269000
H	-5.928732000	-5.484080000	6.846900000
C	-5.935111000	-4.699827000	0.502316000
H	-2.853278000	-5.643251000	0.987875000
C	-2.812000000	-4.660981000	7.981671000
H	-0.981850000	-5.455714000	7.172759000
H	-4.798950000	-4.085512000	8.571813000
C	-2.124437000	-3.799821000	9.001935000
H	-2.785652000	-3.566121000	9.840190000
H	-1.229127000	-4.287299000	9.397973000
H	-1.807638000	-2.848994000	8.557373000
N	-7.015671000	-5.418188000	2.233761000
C	-5.716816000	-5.724705000	2.477667000
N	-7.141249000	-4.794585000	1.046553000
C	-8.174237000	-5.596125000	3.076378000
H	-5.813193000	-4.240140000	-0.467460000
H	-8.418333000	-4.667706000	3.602678000
H	-7.959483000	-6.379739000	3.803183000
H	-9.018588000	-5.882314000	2.448021000
S	2.491773000	-7.041237000	2.519738000
O	-1.608369000	-8.475909000	3.401046000
O	-2.542723000	-8.779232000	1.379232000
N	-1.314338000	-6.617879000	0.394581000
C	-0.151196000	-6.258535000	2.537826000
C	-0.674812000	-7.288530000	1.534449000
C	0.950045000	-6.777886000	3.455705000
C	-1.718225000	-8.253380000	2.091240000
C	3.444733000	-7.962360000	3.748215000
H	0.229263000	-5.396284000	1.975092000
H	-0.989628000	-5.895661000	3.140634000
H	0.173399000	-7.917679000	1.212445000
H	0.646028000	-7.722364000	3.916706000
H	1.139880000	-6.052509000	4.253927000
H	-1.792965000	-7.336267000	-0.145947000
H	-0.601783000	-6.204540000	-0.198480000
H	3.610481000	-7.368112000	4.650991000
H	4.413773000	-8.191631000	3.299940000
H	2.948923000	-8.900727000	4.011171000
H	-2.449381000	-8.867172000	3.711889000

Adduct 7MetM:

O	-3.571079000	-9.346092000	6.611910000
S	-3.080645000	-8.549726000	5.485548000

C	-1.868127000	-9.545361000	4.671791000
O	-2.513909000	-7.214634000	5.687914000
C	-4.386480000	-8.454034000	4.279552000
N	-0.864813000	-8.971320000	4.002880000
C	-4.180795000	-7.740963000	3.097995000
C	-5.581681000	-9.123965000	4.521800000
C	-0.685737000	-11.205261000	3.758418000
N	-0.155719000	-9.981215000	3.459990000
C	-5.194146000	-7.709375000	2.151198000
H	-3.240719000	-7.224025000	2.910203000
C	-6.588938000	-9.069785000	3.563959000
H	-5.711658000	-9.668979000	5.452296000
C	-0.607902000	-12.606031000	3.635779000
H	0.667747000	-9.750480000	2.929631000
C	-6.412310000	-8.367766000	2.367675000
H	-5.027917000	-7.163877000	1.223623000
H	-7.529772000	-9.584862000	3.744787000
C	-7.501718000	-8.305841000	1.342493000
H	-8.283828000	-9.043907000	1.535572000
H	-7.977925000	-7.319112000	1.331840000
H	-7.114614000	-8.476541000	0.333534000
N	-2.340528000	-12.161681000	4.866013000
C	-1.808760000	-10.952031000	4.546494000
N	-1.620610000	-13.164722000	4.301622000
C	-3.564478000	-12.460976000	5.572159000
H	0.106115000	-13.234865000	3.124960000
H	-4.423973000	-12.444098000	4.893530000
H	-3.713591000	-11.720075000	6.358633000
H	-3.469987000	-13.456654000	6.003351000
S	-2.066942000	-7.196098000	0.148845000
O	-1.397103000	-5.917186000	3.469888000
O	-1.184992000	-3.719953000	3.940584000
N	-0.522904000	-3.122259000	1.390231000
C	-0.048220000	-5.470953000	0.989755000
C	-1.012337000	-4.467282000	1.645050000
C	-0.445099000	-6.938455000	0.949849000
C	-1.185864000	-4.634410000	3.144697000
C	-2.236532000	-8.962635000	0.482337000
H	0.110067000	-5.114245000	-0.035786000
H	0.926658000	-5.380397000	1.483172000
H	-2.024423000	-4.662528000	1.235523000
H	-0.501331000	-7.362375000	1.956325000
H	0.305344000	-7.496299000	0.374992000
H	-0.881431000	-2.507911000	2.114201000
H	-0.874120000	-2.789034000	0.501234000
H	-1.402302000	-9.528874000	0.055732000

H	-3.162673000	-9.304834000	0.016569000
H	-2.297820000	-9.156566000	1.558615000
H	-1.585339000	-6.011595000	4.423236000

Adduct 7MetM$_a$:

O	-5.147734000	-6.602881000	6.806725000
S	-3.918365000	-6.902937000	6.070084000
C	-3.377594000	-5.383697000	5.357969000
O	-3.918332000	-7.927753000	5.014865000
C	-2.638397000	-7.328566000	7.226880000
N	-2.166150000	-5.345275000	4.798158000
C	-1.435060000	-7.853938000	6.753338000
C	-2.856106000	-7.128675000	8.585435000
C	-3.186472000	-3.413486000	4.341820000
N	-2.037341000	-4.140478000	4.213305000
C	-0.438980000	-8.168156000	7.665313000
H	-1.291586000	-8.008068000	5.686603000
C	-1.847452000	-7.460776000	9.483968000
H	-3.808339000	-6.731816000	8.923856000
C	-3.863852000	-2.209075000	4.068479000
H	-1.287862000	-4.084173000	3.506073000
C	-0.626515000	-7.976799000	9.041646000
H	0.503318000	-8.578969000	7.308124000
H	-2.009826000	-7.318938000	10.549966000
C	0.464728000	-8.314387000	10.009729000
H	0.121482000	-8.252651000	11.044975000
H	0.852176000	-9.324273000	9.842736000
H	1.314766000	-7.631496000	9.903025000
N	-5.208270000	-3.445932000	5.241557000
C	-4.072965000	-4.181445000	5.103070000
N	-5.077627000	-2.243979000	4.620004000
C	-6.396907000	-3.726701000	6.012013000
H	-3.561470000	-1.340199000	3.503021000
H	-6.277990000	-3.408932000	7.052949000
H	-6.594814000	-4.798162000	5.995834000
H	-7.224907000	-3.179115000	5.563080000
S	2.567565000	-8.169059000	2.439438000
O	-1.682761000	-8.010662000	3.320529000
O	-2.601674000	-6.415637000	2.011425000
N	-0.355100000	-4.959101000	2.018614000
C	0.679204000	-6.530748000	3.600920000
C	-0.221978000	-6.379652000	2.370851000
C	1.332458000	-7.894592000	3.755224000
C	-1.635536000	-6.915835000	2.547502000
C	2.910168000	-9.917541000	2.729318000

H	1.463840000	-5.765354000	3.537415000
H	0.094986000	-6.298067000	4.498730000
H	0.221760000	-6.973081000	1.548752000
H	0.583437000	-8.691777000	3.707222000
H	1.833138000	-7.959497000	4.728156000
H	-1.087998000	-4.887406000	1.316623000
H	0.507374000	-4.639250000	1.591012000
H	3.326689000	-10.081993000	3.727177000
H	3.646948000	-10.236097000	1.990384000
H	2.008238000	-10.523581000	2.606567000
H	-2.619302000	-8.167716000	3.558341000

Adduct 7MetM_b:

O	-4.215488000	-9.923155000	6.371604000
S	-3.661192000	-8.909420000	5.472298000
C	-2.111537000	-9.541755000	4.923835000
O	-3.463750000	-7.531195000	5.945521000
C	-4.659224000	-8.831884000	4.005342000
N	-1.452676000	-8.906812000	3.951551000
C	-4.478069000	-7.787211000	3.098478000
C	-5.610668000	-9.822707000	3.788817000
C	-0.112155000	-10.503687000	4.755816000
N	-0.256892000	-9.512897000	3.826136000
C	-5.265806000	-7.751862000	1.956717000
H	-3.730905000	-7.021613000	3.294044000
C	-6.396182000	-9.763066000	2.643269000
H	-5.731851000	-10.617009000	4.519072000
C	0.703854000	-11.520152000	5.291306000
H	0.457380000	-8.951875000	3.338167000
C	-6.237388000	-8.732544000	1.712559000
H	-5.131858000	-6.944963000	1.238879000
H	-7.147891000	-10.528847000	2.466868000
C	-7.099139000	-8.659518000	0.490095000
H	-7.602507000	-9.608872000	0.292279000
H	-7.876944000	-7.895508000	0.600014000
H	-6.518750000	-8.391219000	-0.397396000
N	-1.177023000	-11.572604000	6.375140000
C	-1.311454000	-10.567945000	5.470016000
N	0.047803000	-12.152851000	6.264923000
C	-2.133397000	-12.088373000	7.326383000
H	1.711782000	-11.820508000	5.046113000
H	-2.943746000	-12.621430000	6.820910000
H	-2.570512000	-11.272013000	7.902939000
H	-1.597090000	-12.772700000	7.981834000
S	-0.383571000	-3.792571000	0.939394000

O	-1.770294000	-5.876137000	4.477551000
O	0.032347000	-6.794439000	5.481836000
N	1.277305000	-7.167426000	3.136448000
C	-0.710091000	-6.339377000	1.939972000
C	0.196875000	-6.171301000	3.162460000
C	-1.500097000	-5.096984000	1.559042000
C	-0.510159000	-6.332560000	4.499674000
C	-1.543357000	-2.410466000	0.906297000
H	-0.081250000	-6.637592000	1.090799000
H	-1.398765000	-7.172325000	2.121522000
H	0.587279000	-5.135748000	3.155569000
H	-2.048971000	-4.708563000	2.423110000
H	-2.228292000	-5.341515000	0.777051000
H	1.741724000	-7.129309000	4.041306000
H	1.959493000	-6.899169000	2.435224000
H	-2.367028000	-2.595368000	0.210981000
H	-0.995926000	-1.529603000	0.567479000
H	-1.946375000	-2.208336000	1.902641000
H	-2.213687000	-6.190297000	5.291582000

Adduct 7MetM$_c$:

O	-6.346974000	-7.147741000	5.193918000
S	-4.928980000	-7.191348000	4.829724000
C	-4.784506000	-6.312843000	3.308967000
O	-4.229105000	-8.475695000	4.690060000
C	-4.013951000	-6.205548000	5.992068000
N	-3.563437000	-6.145561000	2.795157000
C	-2.621932000	-6.293781000	6.026521000
C	-4.705791000	-5.350842000	6.843222000
C	-5.033775000	-5.332594000	1.325980000
N	-3.713108000	-5.532156000	1.609489000
C	-1.925198000	-5.504178000	6.929947000
H	-2.102799000	-6.972528000	5.353839000
C	-3.988428000	-4.571594000	7.744343000
H	-5.790150000	-5.316448000	6.801123000
C	-5.990776000	-4.837630000	0.418657000
H	-2.878264000	-5.565188000	1.004139000
C	-2.593440000	-4.631446000	7.799644000
H	-0.839800000	-5.568335000	6.972084000
H	-4.519846000	-3.907021000	8.421709000
C	-1.822496000	-3.776201000	8.756991000
H	-2.473428000	-3.319124000	9.505958000
H	-1.053906000	-4.351077000	9.282328000
H	-1.304476000	-2.964377000	8.234260000
N	-7.074464000	-5.602137000	2.137613000

C	-5.760950000	-5.808906000	2.421893000
N	-7.213537000	-5.003251000	0.924870000
C	-8.241038000	-5.828326000	2.957930000
H	-5.874460000	-4.391934000	-0.558024000
H	-8.456110000	-4.959540000	3.588506000
H	-8.067971000	-6.692104000	3.599004000
H	-9.088675000	-6.006668000	2.296812000
S	2.386112000	-6.982371000	2.757935000
O	-1.679282000	-8.470853000	3.465235000
O	-2.640988000	-8.670133000	1.430847000
N	-1.278946000	-6.570632000	0.469540000
C	-0.254728000	-6.200998000	2.680260000
C	-0.722963000	-7.237893000	1.655734000
C	0.813279000	-6.700310000	3.640092000
C	-1.796968000	-8.191282000	2.157772000
C	3.276514000	-7.898024000	4.033783000
H	0.133880000	-5.333031000	2.131253000
H	-1.121826000	-5.843649000	3.246638000
H	0.145223000	-7.875625000	1.401354000
H	0.500654000	-7.638977000	4.109556000
H	0.979266000	-5.963541000	4.434039000
H	-1.729160000	-7.288712000	-0.093850000
H	-0.518514000	-6.187100000	-0.081766000
H	3.412752000	-7.295748000	4.936516000
H	4.260323000	-8.147402000	3.633235000
H	2.758114000	-8.826291000	4.289721000
H	-2.510163000	-8.901407000	3.748915000

Adduct 7AlaB-N:

O	1.803532000	-2.784255000	0.478665000
S	0.893819000	-1.764401000	1.038002000
C	1.449790000	-0.216983000	0.361546000
O	0.716190000	-1.644602000	2.492101000
C	-0.732082000	-2.019735000	0.314791000
N	0.629690000	0.837912000	0.342554000
C	-1.867658000	-1.715641000	1.061486000
C	-0.835895000	-2.551888000	-0.972344000
C	2.595886000	1.493618000	-0.495611000
N	1.320926000	1.866980000	-0.178595000
C	-3.127091000	-1.941181000	0.499930000
H	-1.759809000	-1.320154000	2.064974000
C	-2.097521000	-2.763411000	-1.519366000
H	0.061459000	-2.803022000	-1.527454000
C	3.850917000	1.875699000	-1.027734000
H	0.805330000	2.756623000	-0.312363000

C	-3.262067000	-2.463119000	-0.794870000
H	-4.017866000	-1.728679000	1.086458000
H	-2.182674000	-3.175000000	-2.521438000
C	-4.623303000	-2.726027000	-1.391836000
H	-4.699242000	-2.316904000	-2.404549000
H	-4.817606000	-3.802580000	-1.463778000
H	-5.420077000	-2.286051000	-0.786484000
N	3.994728000	-0.227944000	-0.488750000
C	2.723208000	0.141260000	-0.156039000
N	4.675398000	0.829691000	-1.006153000
C	4.691410000	-1.481340000	-0.251716000
H	4.189971000	2.823907000	-1.418417000
H	5.307577000	-1.708980000	-1.123227000
H	3.951215000	-2.265015000	-0.094440000
H	5.335494000	-1.404045000	0.630425000
O	-2.827485000	1.415871000	0.678934000
O	-2.177922000	2.090595000	-1.376004000
N	-0.576408000	4.016302000	-0.332150000
C	-1.620958000	3.458604000	0.542506000
C	-2.742440000	4.449333000	0.907057000
C	-2.213024000	2.251048000	-0.174845000
H	-1.150871000	3.093010000	1.460959000
H	-3.480354000	3.979376000	1.563024000
H	-2.324938000	5.314681000	1.431992000
H	-3.253435000	4.805217000	0.006235000
H	-0.354034000	4.968012000	-0.051462000
H	-0.937820000	4.041859000	-1.285130000
H	-3.113322000	0.635285000	0.171008000

Adduct 7LysP-N:

O	-3.821433000	-10.035908000	4.609686000
S	-2.546410000	-9.447708000	4.182205000
C	-1.295654000	-10.531326000	4.818614000
O	-2.202194000	-8.073586000	4.533549000
C	-2.411479000	-9.627639000	2.421839000
N	-0.050777000	-10.410844000	4.375917000
C	-1.419775000	-8.927493000	1.737897000
C	-3.289530000	-10.476527000	1.756886000
C	-0.065548000	-12.034728000	5.908367000
N	0.684094000	-11.314522000	5.028231000
C	-1.298566000	-9.097351000	0.365214000
H	-0.755459000	-8.263474000	2.280838000
C	-3.163315000	-10.625399000	0.380515000
H	-4.058873000	-10.998241000	2.316822000
C	-0.113984000	-13.054268000	6.881351000

H	1.665029000	-11.385248000	4.793847000
C	-2.169145000	-9.946694000	-0.329920000
H	-0.508599000	-8.575736000	-0.174306000
H	-3.846836000	-11.282893000	-0.150663000
C	-2.048852000	-10.101770000	-1.819274000
H	-2.459666000	-11.056019000	-2.159672000
H	-2.594654000	-9.305399000	-2.339046000
H	-1.004857000	-10.042485000	-2.139217000
N	-2.119651000	-12.268968000	6.676414000
C	-1.369788000	-11.550773000	5.801026000
N	-1.360023000	-13.167869000	7.325446000
C	-3.520189000	-12.142703000	7.010659000
H	0.662034000	-13.695082000	7.273481000
H	-3.997913000	-13.121902000	6.938707000
H	-3.979466000	-11.448156000	6.307537000
H	-3.630004000	-11.765121000	8.030830000
O	4.792064000	-7.212157000	-2.775253000
O	3.006613000	-7.966145000	-3.904824000
N	1.403080000	-7.865443000	-1.630681000
N	3.773206000	-11.138320000	3.746591000
C	3.027221000	-8.867247000	0.771466000
C	3.444791000	-8.887046000	-0.693624000
C	3.569189000	-10.056911000	1.556602000
C	2.843289000	-7.725750000	-1.501184000
C	3.244261000	-9.974219000	3.042098000
C	3.525029000	-7.649111000	-2.859216000
H	1.933224000	-8.843500000	0.831470000
H	3.385682000	-7.934296000	1.229827000
H	3.130997000	-9.830461000	-1.161794000
H	4.537518000	-8.844225000	-0.770262000
H	4.657459000	-10.135923000	1.441010000
H	3.147031000	-10.985508000	1.145453000
H	3.065822000	-6.792577000	-0.968701000
H	2.159912000	-9.819353000	3.165731000
H	3.733702000	-9.088655000	3.464968000
H	1.228234000	-8.520751000	-2.390171000
H	1.007283000	-6.986147000	-1.949406000
H	3.314332000	-12.003792000	3.487743000
H	3.790546000	-11.033202000	4.753050000
H	5.148331000	-7.230506000	-3.676241000

Adduct 7GluB-αN:

O	-3.535225000	-2.284938000	0.894247000
S	-2.962716000	-1.002116000	1.319356000
C	-1.297180000	-1.007849000	0.736599000

O	-2.967942000	-0.596166000	2.720635000
C	-3.765852000	0.278919000	0.380311000
N	-0.484585000	-0.011466000	1.081901000
C	-3.629741000	1.605797000	0.781764000
C	-4.524339000	-0.063112000	-0.733190000
C	0.671699000	-1.402262000	-0.217093000
N	0.692585000	-0.248898000	0.506981000
C	-4.261153000	2.597982000	0.045195000
H	-3.041307000	1.844478000	1.661576000
C	-5.152848000	0.944529000	-1.456485000
H	-4.625274000	-1.107332000	-1.010758000
C	1.385888000	-2.316090000	-1.024266000
H	1.460987000	0.411906000	0.702316000
C	-5.031378000	2.284990000	-1.081440000
H	-4.159481000	3.636430000	0.350198000
H	-5.750827000	0.685005000	-2.326242000
C	-5.734331000	3.367622000	-1.849544000
H	-5.984124000	3.042730000	-2.862821000
H	-6.670388000	3.651426000	-1.354297000
H	-5.119299000	4.269333000	-1.921424000
N	-0.624371000	-3.088479000	-0.803817000
C	-0.615875000	-1.926818000	-0.099720000
N	0.579268000	-3.313459000	-1.364581000
C	-1.714676000	-3.996166000	-1.070399000
H	2.414846000	-2.313807000	-1.356259000
H	-2.141800000	-3.809617000	-2.061182000
H	-2.482931000	-3.849028000	-0.311502000
H	-1.331706000	-5.017020000	-1.034980000
O	4.688543000	3.192851000	-1.033495000
O	5.030308000	-2.011026000	-1.184151000
O	2.494321000	3.433289000	-0.634623000
O	6.513295000	-1.114539000	0.241313000
N	2.546617000	1.755442000	1.460336000
C	4.850195000	1.096464000	0.814096000
C	3.834859000	2.229356000	0.968724000
C	4.407475000	0.010034000	-0.150692000
C	3.574604000	2.997852000	-0.314942000
C	5.444209000	-1.067713000	-0.316751000
H	5.035642000	0.654765000	1.799134000
H	5.803637000	1.517510000	0.485602000
H	4.289550000	2.978003000	1.642273000
H	3.486936000	-0.474289000	0.190784000
H	4.187233000	0.415899000	-1.145904000
H	1.858739000	2.496571000	1.346926000
H	2.605600000	1.534788000	2.449107000
H	4.430895000	3.732379000	-1.796284000

H	5.734193000	-2.675220000	-1.226135000

Adduct 7MetB-αN:

O	3.595948000	1.238269000	1.803289000
S	2.509417000	0.270973000	1.558272000
C	1.375570000	1.104826000	0.466259000
O	1.743400000	-0.317691000	2.662351000
C	3.189968000	-1.076118000	0.584793000
N	0.198155000	0.537777000	0.186742000
C	2.533022000	-2.307973000	0.569437000
C	4.374976000	-0.882315000	-0.124527000
C	0.290637000	2.481092000	-0.919048000
N	-0.453138000	1.369413000	-0.645715000
C	3.072011000	-3.350971000	-0.178495000
H	1.629111000	-2.443494000	1.152767000
C	4.899740000	-1.938508000	-0.867020000
H	4.884790000	0.073349000	-0.072360000
C	0.370978000	3.723027000	-1.592280000
H	-1.388444000	1.097910000	-0.951490000
C	4.256806000	-3.183037000	-0.911513000
H	2.570731000	-4.315195000	-0.187144000
H	5.828009000	-1.796475000	-1.413683000
C	4.815425000	-4.314061000	-1.740354000
H	5.886511000	-4.188239000	-1.920048000
H	4.662594000	-5.281156000	-1.252121000
H	4.322046000	-4.363285000	-2.718932000
N	2.222035000	3.472396000	-0.473285000
C	1.494067000	2.345843000	-0.216093000
N	1.541015000	4.295232000	-1.314646000
C	3.570308000	3.827841000	-0.063420000
H	-0.337779000	4.220699000	-2.237417000
H	4.300004000	3.534961000	-0.826206000
H	3.799576000	3.316263000	0.870422000
H	3.610120000	4.909415000	0.069924000
S	-6.308410000	-0.071427000	0.034786000
O	-3.832354000	-1.721676000	-2.125775000
O	-2.950512000	0.214375000	-1.428641000
N	-2.517576000	-0.857121000	1.206726000
C	-4.515095000	-2.218457000	0.674889000
C	-3.169915000	-1.637029000	0.174849000
C	-5.513032000	-1.209901000	1.254197000
C	-3.311309000	-0.926363000	-1.177155000
C	-5.516969000	1.532711000	0.419590000
H	-4.985990000	-2.790987000	-0.129616000
H	-4.264396000	-2.921718000	1.477207000

H	-2.533963000	-2.505333000	-0.043741000
H	-5.047360000	-0.607279000	2.038974000
H	-6.331954000	-1.760750000	1.725011000
H	-2.935432000	0.065062000	1.285121000
H	-1.528932000	-0.709790000	1.009680000
H	-5.604858000	1.767354000	1.483224000
H	-6.066985000	2.287348000	-0.147331000
H	-4.472117000	1.554612000	0.102802000
H	-3.899813000	-1.189735000	-2.937155000

Adduct 7LysP-αN:

O	-4.817873000	-11.106972000	4.246975000
S	-3.956370000	-9.925516000	4.374976000
C	-2.308052000	-10.548231000	4.466176000
O	-4.152909000	-8.955663000	5.446628000
C	-4.024390000	-9.045252000	2.829251000
N	-1.304931000	-9.704426000	4.699476000
C	-3.523580000	-7.746745000	2.761423000
C	-4.589956000	-9.658717000	1.717818000
C	-0.434370000	-11.741723000	4.499299000
N	-0.183434000	-10.421766000	4.717767000
C	-3.588903000	-7.064445000	1.555043000
H	-3.098457000	-7.286926000	3.647629000
C	-4.650248000	-8.957487000	0.518268000
H	-4.987896000	-10.664339000	1.807166000
C	0.085478000	-13.049344000	4.385029000
H	0.705760000	-9.926404000	4.911546000
C	-4.152741000	-7.655929000	0.417648000
H	-3.201177000	-6.050708000	1.492662000
H	-5.095591000	-9.427899000	-0.354558000
C	-4.243728000	-6.891912000	-0.872441000
H	-4.424520000	-7.557106000	-1.720543000
H	-5.065944000	-6.167633000	-0.839179000
H	-3.325819000	-6.329779000	-1.068803000
N	-2.057139000	-13.189905000	4.124793000
C	-1.812597000	-11.867954000	4.322114000
N	-0.910572000	-13.895304000	4.153923000
C	-3.299924000	-13.863084000	3.830536000
H	1.098959000	-13.414863000	4.462871000
H	-3.397900000	-14.045261000	2.755311000
H	-4.123986000	-13.234316000	4.167092000
H	-3.307543000	-14.819174000	4.355578000
O	5.417027000	-8.328089000	6.663866000
O	3.827604000	-6.809417000	6.208741000
N	2.053979000	-8.736158000	5.328636000

N	4.390983000	-13.498597000	1.174455000
C	3.483576000	-11.030310000	3.938727000
C	4.131579000	-9.747429000	4.447304000
C	4.243038000	-11.648772000	2.770427000
C	3.417188000	-9.130091000	5.655527000
C	3.620351000	-12.949374000	2.280932000
C	4.216894000	-7.952996000	6.196107000
H	2.449672000	-10.829087000	3.633650000
H	3.429975000	-11.754518000	4.764587000
H	4.166358000	-9.001279000	3.640251000
H	5.170802000	-9.945534000	4.730241000
H	5.285453000	-11.846463000	3.048232000
H	4.277122000	-10.929948000	1.938711000
H	3.378727000	-9.883495000	6.453764000
H	2.553091000	-12.774654000	2.051163000
H	3.641551000	-13.681434000	3.098918000
H	2.089036000	-8.022794000	4.602914000
H	1.644828000	-8.259175000	6.129070000
H	4.287469000	-12.903050000	0.358260000
H	4.020588000	-14.405371000	0.910109000
H	5.854317000	-7.522767000	6.978886000

Adduct 7GluB-C:

O	-5.502826000	-10.163757000	5.326092000
S	-4.253903000	-9.377576000	5.280061000
C	-2.989650000	-10.452716000	5.921663000
O	-4.171922000	-8.069656000	5.943945000
C	-3.819963000	-9.138611000	3.553858000
N	-1.701207000	-10.192470000	5.678501000
C	-2.893911000	-8.152005000	3.211278000
C	-4.429676000	-9.927034000	2.578824000
C	-1.797334000	-11.978720000	7.026157000
N	-0.986301000	-11.118911000	6.341157000
C	-2.568459000	-7.967362000	1.868646000
H	-2.443463000	-7.540767000	3.984881000
C	-4.099783000	-9.724730000	1.238695000
H	-5.156726000	-10.676329000	2.872074000
C	-1.888958000	-13.108908000	7.872886000
H	0.033161000	-11.106398000	6.272031000
C	-3.168251000	-8.746286000	0.861018000
H	-1.837144000	-7.213932000	1.592496000
H	-4.576120000	-10.331958000	0.473929000
C	-2.820527000	-8.507030000	-0.588159000
H	-3.140803000	-9.339033000	-1.220939000
H	-3.312213000	-7.600141000	-0.959731000

H	-1.742214000	-8.367058000	-0.710392000
N	-3.921042000	-12.451196000	7.452546000
C	-3.115091000	-11.578586000	6.779056000
N	-3.171674000	-13.368210000	8.121153000
C	-5.362955000	-12.435763000	7.636088000
H	-1.116485000	-13.731052000	8.300132000
H	-5.728687000	-13.463297000	7.602404000
H	-5.809009000	-11.845733000	6.836513000
H	-5.624185000	-11.994949000	8.603743000
O	-0.259676000	-10.376519000	1.836667000
O	3.928039000	-11.220142000	5.228661000
O	0.571743000	-8.597926000	0.725466000
O	1.886539000	-11.236914000	6.140422000
N	3.135184000	-9.364210000	1.216124000
C	2.279044000	-11.134698000	2.716144000
C	2.089003000	-10.364125000	1.393783000
C	2.196317000	-10.215667000	3.951152000
C	0.734696000	-9.664106000	1.286090000
C	2.613699000	-10.924227000	5.210671000
H	3.265552000	-11.609233000	2.683786000
H	1.531628000	-11.930115000	2.784724000
H	2.064150000	-11.122454000	0.588216000
H	2.863973000	-9.364023000	3.783173000
H	1.176226000	-9.852794000	4.094748000
H	2.799679000	-8.635378000	0.591834000
H	3.964881000	-9.781473000	0.807037000
H	-1.084795000	-9.859823000	1.750179000
H	4.097829000	-11.685773000	6.065595000