Electronic Supplementary Information (ESI†)

Probing chirality recognition of protonated glutamic acid dimers by gas-phase vibrational spectroscopy and first-principles simulations

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Experimental and Computational Methods

IRPD spectroscopy

IRPD spectra of LL-/LD-Glu_2H^+-H_2 are recorded in the XH stretch (ν_{XH}, X=O, N) and fingerprint ranges (2600-3600 and 1100-1900 cm^{-1}, respectively) employing a cryogenic quadrupole ion trap (QIT) tandem mass spectrometer.[54] LL-/LD-Glu_2H^+ ions are generated in a continuous electrospray ionization (ESI) source using 10^{-4} M of L-/D-Glu dissolved in methanol, water, and formic acid (100:10:1). Naturally, L- and D-Glu have equal physical properties such as molecular weight. To distinguish LL- and LD-Glu_2H^+ by means of mass spectrometry, L-Glu-2,3,3,4,4-d_5 (L-d_5-L-Glu_2H^+) with five deuterium atoms substituted at its alkyl chain is used. The effect of deuteration on the IR frequencies of L-$GluH^+$ and LL-Glu_2H^+ is monitored by IRPD spectroscopy of all possible isotopologues (L-$GluH^+$ m/z 148, L-d_5-$GluH^+$ m/z 153, LL-Glu_2H^+ m/z 295, L-d_5-L-Glu_2H^+ m/z 200, L-d_5-L-d_5-Glu_2H^+ m/z 205, L-d_5-D-Glu_2H^+ m/z 200). Furthermore, ^{15}N-isotope labeling is employed to disentangle the XH stretches by the same approach of isotopologue-selective IRPD spectroscopy. Natural L- and D-Glu (Sigma Aldrich, 99% purity), deuterated L-Glu-2,3,3,4,4-d_5 (Sigma Aldrich, 97% purity), and ^{15}N-labeled L-Glu-^{15}N (Sigma Aldrich, 98% purity) are used without further purification. The ESI-generated ions pass through a glass capillary heated to 60°C before entering vacuum. Behind a skimmer, LL-/LD-Glu_2H^+ are size-selected by a first quadrupole mass spectrometer, deflected by a quadrupole bender, and guided through an octopole to a gold-coated copper QIT mounted onto the cold head of a closed-cycle cryostat. The QIT held at 10 K is filled with He/H_2 (80:20) buffer gas through a pulsed nozzle (pulse duration ca. 120 μs) to form cold LL-/LD-Glu_2H^+-H_2 in the QIT. Recent analysis of the internal temperature of protonated tyrosine results in T_{int}≈13 K.[54] In the XH stretch range, IRPD spectra are recorded using the idler of a pulsed tuneable IR optical parametric oscillator (IR-OPO, Laservision, bandwidth 1.7 cm^{-1}) pumped by a nanosecond injection seeded Nd:YAG laser operated at 10 Hz (Continuum Surelite II). To produce IR-radiation in the fingerprint range, signal and idler outputs of the OPO are difference-frequency-mixed in an $AgGaSe_2$ crystal. Resonant vibrational excitation followed by fast internal vibrational energy redistribution induces dissociation of LL-/LD-Glu_2H^+-H_2. Predominantly, loss of the weakly bound H_2 tag is observed. The maximum internal energy stored in the clusters is limited by the dissociation energy of the weakest bound cluster unit (H_2). Therefore, tagging ensures single-photon dissociation of internally cold clusters. The fragment ions are ejected into a time-of-flight mass spectrometer and detected by a dynode converter detector. The fragment ion current is recorded as a function of the IR laser frequency to generate IRPD spectra. The ion source is triggered at twice the laser frequency (20 Hz) to measure the background signal induced by metastable decay. Fragmentation signal of alternating triggers is subtracted. The measured spectra are plotted as fragmentation yield $R=I_f/(I_p + I_f)$, where I_p and I_f refer to the abundances of parent and fragment ions, respectively. All spectra are normalized by IR laser intensity fluctuations. In the XH stretch range the IR-OPO provides 0.7-10 mJ/pulse, in the fingerprint range 0.5-1.3 mJ/pulse.

IR-IR hole burning spectroscopy

To record conformer-selective IR-IR hole burning spectra of LL-/LD-Glu_2H^+-H_2 in the XH stretch range, a typical pump-probe spectroscopy scheme is applied. After a delay of 3 ms, the radiation of the probe laser (IR-OPO, Laservision, bandwidth >5 cm^{-1}) pumped by a nanosecond Nd:YAG laser (Continuum Surelite II) is introduced into the QIT. The probe laser is set at a conformer-specific transition in the IRPD spectrum, thus generating a constant fragmentation signal of this cluster conformer. The pump laser is the same IR-OPO as used for IRPD spectroscopy. Resonant excitation of any of the conformers present in the trap by the pump laser leads to fragmentation of the corresponding cluster (loss of H_2 ligands). All fragments induced by the pump laser are removed from the trap by a so-called "tickle" RF pulse applied to the QIT before the probe laser is introduced. When the pump laser hits a transition of the conformer currently probed, the constant fragmentation signal produced by the probe laser is depleted (burnt). Thus, by scanning the pump laser, a conformer-specific IR-dip spectrum is recorded. The measured IR-dip spectra are corrected for laser-off background signal, but are not normalized for laser intensity due to saturation effects. Four to five IR-dip spectra are averaged to achieve satisfactory signal-to-noise ratio.

IRMPD spectroscopy

In the fingerprint range (1000-2000 cm^{-1}), also Infrared Multiple Photon Dissociation (IRMPD) spectra of LL-/LD-Glu_2H^+ are recorded at room temperature in a FT-ICR mass spectrometer coupled to the Infrared Free Electron Laser (IR-FEL) at the Centre de Laser Infrarouge d´Orsay (CLIO), France.[72,73] LL-/LD-Glu_2H^+ are generated by ESI, mass selected and confined in the FT-ICR cell. Here they are irradiated by 8 μs fixed-wavelength macropulses of the IR-FEL beam focused into the center of the trap. Resonant absorption of multiple IR photons leads to fragmentation into $GluH^+$. IRMPD spectra are obtained by scanning the IR-FEL (step size 3 cm^{-1}) and recording the fragmentation efficiency R as a function of the IR frequency, $R=\ln(I_p/(I_p + I_f))$, with I_p (LL-/LD-Glu_2H^+) and I_f (L-/D-$GluH^+$) being parent and fragment ion currents, respectively. Measured spectra are normalized for IR-FEL flux, $\Phi_{IR} \sim P_{IR}/\nu_{IR}$, because the power of the FEL operating at 44.5 MeV electron energy and 25 Hz increases from 400 mW (2000 cm^{-1}) to 1600 mW (1000 cm^{-1}) as the frequency changes.

Computational methods

Presampling of the potential-energy surface (PES) of LL-/LD-Glu_2H^+ is accomplished by basin hopping employing the MM3Pro force field as implemented in the TINKER molecular modeling software.[57–60] To this end, six different input structures are generated, which differ in (i) relative chirality (LL/LD), and (ii) protonation state ($GluH^+$ protonated at the amino group (α-COOH, γ-COOH, NH_3^+) and either canonical Glu (α-COOH, γ-COOH, NH_2) or zwitterionic Glu ((a) α-COO^-, γ-COOH, NH_3^+ or (b) α-COOH, γ-COO^-, NH_3^+)). Initial low energy conformers are found by chemical intuition and relaxation at the PBE0+vdW^{TS}/light level. More than 500000 structures are found by the force-field approach. The 1200 lowest-energy conformers are subjected to geometry relaxation using density-functional theory (DFT) at the dispersion-corrected PBE+vdW^{TS}/light level.[61,62] Thus, after clustering (a computational method to sort objects on the basis of a similarity criterion), 625 (309 LL and 316 LD) conformers are found within $\Delta E \approx 160$ kJ/mol. All DFT calculations are performed with FHI-aims, which employs numeric atom-centered basis functions

for the Kohn-Sham orbitals.[61] For the elements contained in Glu (H, C, N, O), light settings include the so-called tier1 basis sets[61] and are used for initial relaxation. Corresponding tight settings include the larger tier2 basis sets and ensure that energy differences are converged to a few meV.

In a second step, the PES of LL-/LD-Glu_2H^+ is scanned in more detail by replica-exchange molecular dynamics (REMD) simulations.[63–65] Multiple independent molecular dynamics (MD) trajectories of non-interacting copies (replicas) of the system are simultaneously generated at different temperatures. At fixed time intervals (0.04 ps), neighboring pairs of replicas are eventually swapped based on a Metropolis criterion. Thus, individual replicas traverse a wide temperature range to overcome barriers, which ensures efficient sampling of the PES. After each swap, the MD velocities are scaled to fit the canonical ensemble.[63] A script-based REMD scheme implemented in FHI-aims is used. All DFT calculations within the REMD run are performed at the PBE/light level. REMD simulations are run separately for LL- and LD-Glu_2H^+. Therefore, the respective 12 most stable conformers found by presampling are sorted into individual replicas at 12 temperatures (T=300.00, 328.53, 360.41, 395.73, 435.02, 478.72, 527.30, 581.31, 641.34, 707.97, 782.16, 864.59 K). These temperatures are chosen such that swap acceptance rates are reliable and LL- and LD-Glu_2H^+ are not destroyed during REMD. Every REMD interval of 0.04 ps contains 40 MD steps of 0.001 ps. For both LL- and LD-Glu_2H^+, two REMD simulations are performed consecutively with a total duration of 158 ps (LL) and 139 ps (LD). Structures are extracted from the MD trajectories every 0.04 ps just before the next attempt to swap replicas. To reduce the number of structures for further treatment, the resulting conformers are clustered (sorted into structural families, called clusters) using the *gromos* algorithm (cutoff 0.05 nm) as implemented in the GROMACS program.[66,67] A sequential clustering scheme is employed. First, all cluster centres of an initial clustering step are relaxed at the PBE+vdW^{TS}/light level. Second, the relaxed geometries are again clustered. The cluster centres are subjected to geometry optimization at the PBE+vdW^{TS}/tight level. Thus, more than 500 relaxed structures are generated within ΔE=42 (LL) to 250 kJ/mol (LD.)

Harmonic vibrational analysis of the most stable conformers of LL- and LD-Glu_2H^+ is accomplished at the many-body dispersion (MBD) corrected hybrid DFT level PBE0+MBD/tight.[68] Harmonic frequencies are used to calculate zero-point corrected energies (E_0) and Helmholtz free energies at 15 K (F_{15}) and 300 K (F_{300}).[69] Calculated linear IR absorption spectra are linearly scaled by factors of 0.93 (2600-3600 cm^{-1}) to roughly adjust the experimental free OH stretching vibration (band A), and 0.955 (1100-1900 cm^{-1}) adjust the CO stretching vibrations (bands K1-K4).

Some noncovalent interaction types and their strengths are determined using the noncovalent interaction (NCI) approach. To this end, the reduced gradient of the electron density ($s(\rho)\sim|grad(\rho)|/\rho^{4/3}$) is evaluated as a function of the electron density ρ oriented by the sign of the second eigenvalue λ_2 of the Hessian, $\rho^*=\rho\cdot sign(\lambda_2)$. The ρ^* values provide a measure of the strengths of the noncovalent interactions (H-bonds, electrostatic, inductive, and dispersive interactions). By use of a BGR color code covering the range $-1.25<\rho^*<1.25$ a.u., a representation of the isosurfaces with an isosurface value of 0.5 a.u. is derived. Blue and red surfaces correspond

to attractive (negative λ_2) and repulsive (positive λ_2) interactions, respectively. Green surfaces correlate with ρ^* values close to zero, indicating weak interactions (mostly dispersion).

Figure S1

Additional stable structures of LD-Glu_2H^+ with intra- (red) and intermolecular (black) H-bonds (R, Å). Relative energies (ΔE_0, kJ/mol) and binding energies (D_0, kJ/mol) calculated at the PBE0+MBD/tight level are also given.

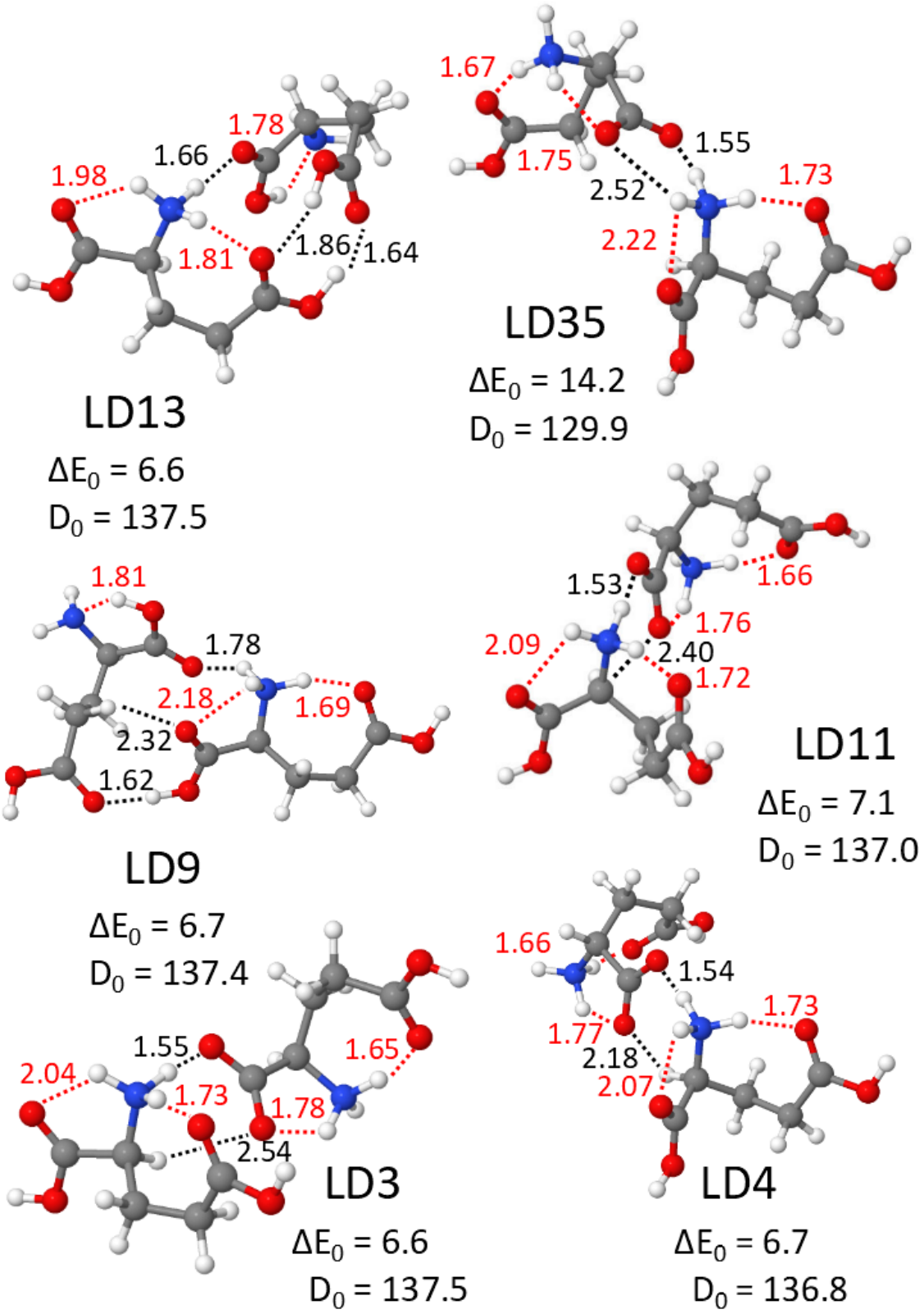

Figure S2

Additional stable structures of LL-Glu_2H^+ with intra- (red) and intermolecular (black) H-bonds (R, Å). Relative energies (ΔE_0, kJ/mol) and binding energies (D_0, kJ/mol) calculated at the PBE0+MBD/tight level are also given.

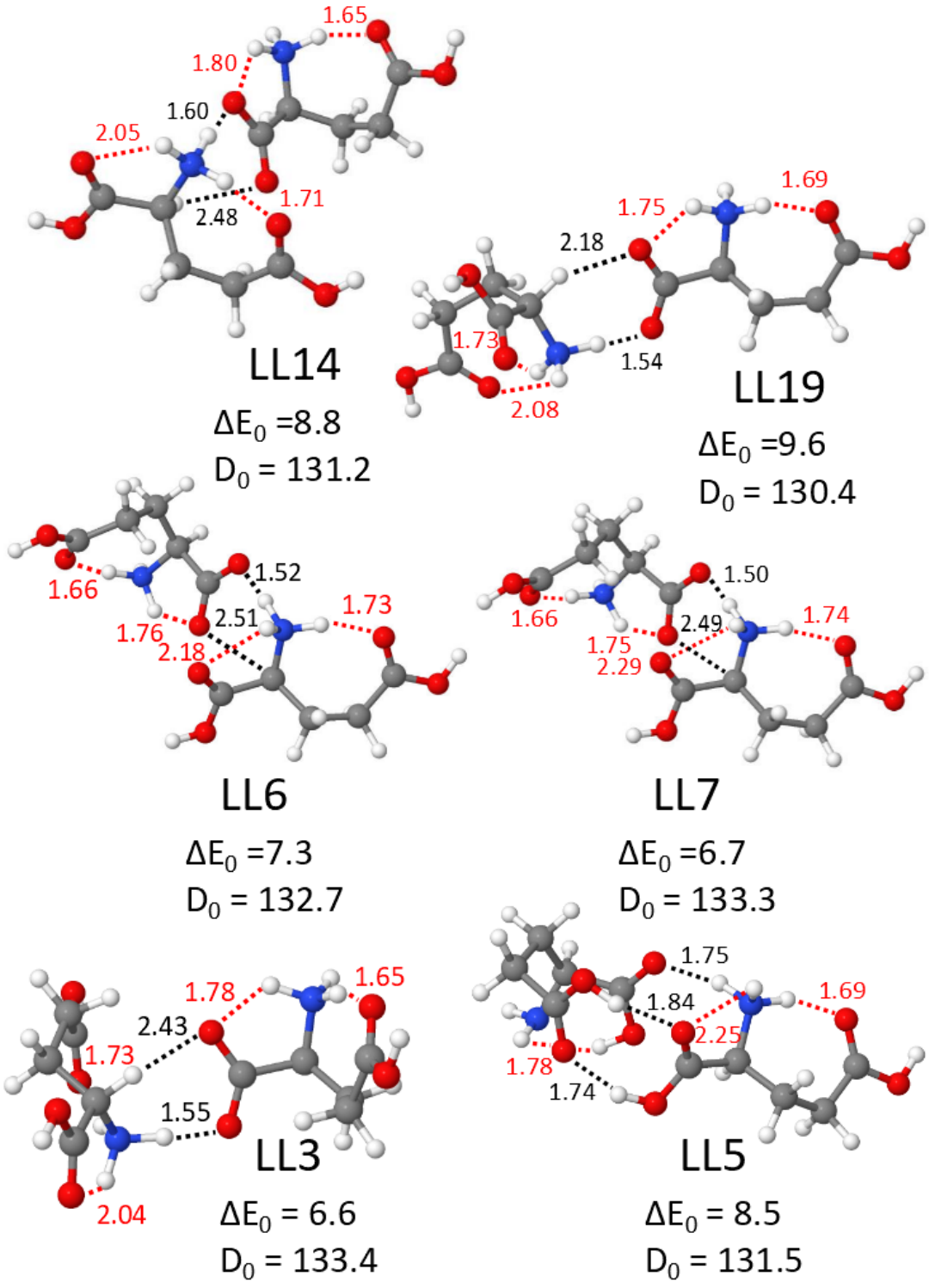

Figure S3

Low-frequency normal modes of selected conformers (cm^{-1}) calculated at the PBE0+MBD/tight level. Spectra highlighted in green belong to LD6 and LD11 that benefit most by entropy, those highlighted in red spectra belong to LD1 and LL1 that are disfavoured by temperature effects.

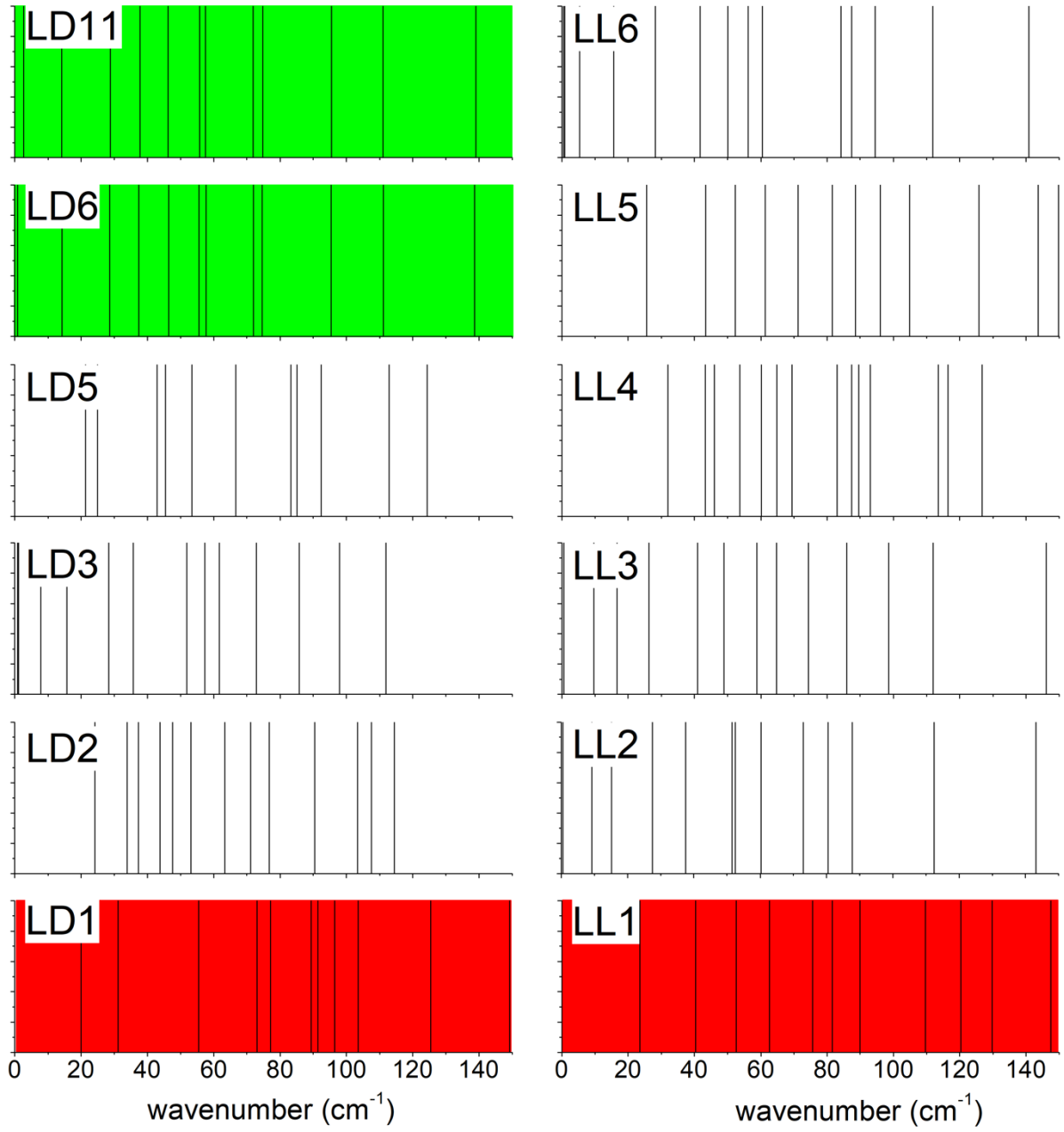

Figure S4

Noncovalent interaction in LD1 and LL1 visualized via the reduced gradient $s(\rho)\sim|\mathrm{grad}(\rho)|/\rho^{4/3}$ as a function of the oriented electron density $\rho^{*}=\rho\cdot\mathrm{sign}(\lambda_2)$ using the NCI Plot Software. BGR color coding ($-1.25<\lambda^{*}<1.25$ a.u.) is used for the isosurfaces (isosurface value of 0.5 a.u.), blue: attractive interactions (negative λ_2), red: repulsive interactions (positive λ_2), green: weak interactions ($\lambda_2\sim0$).

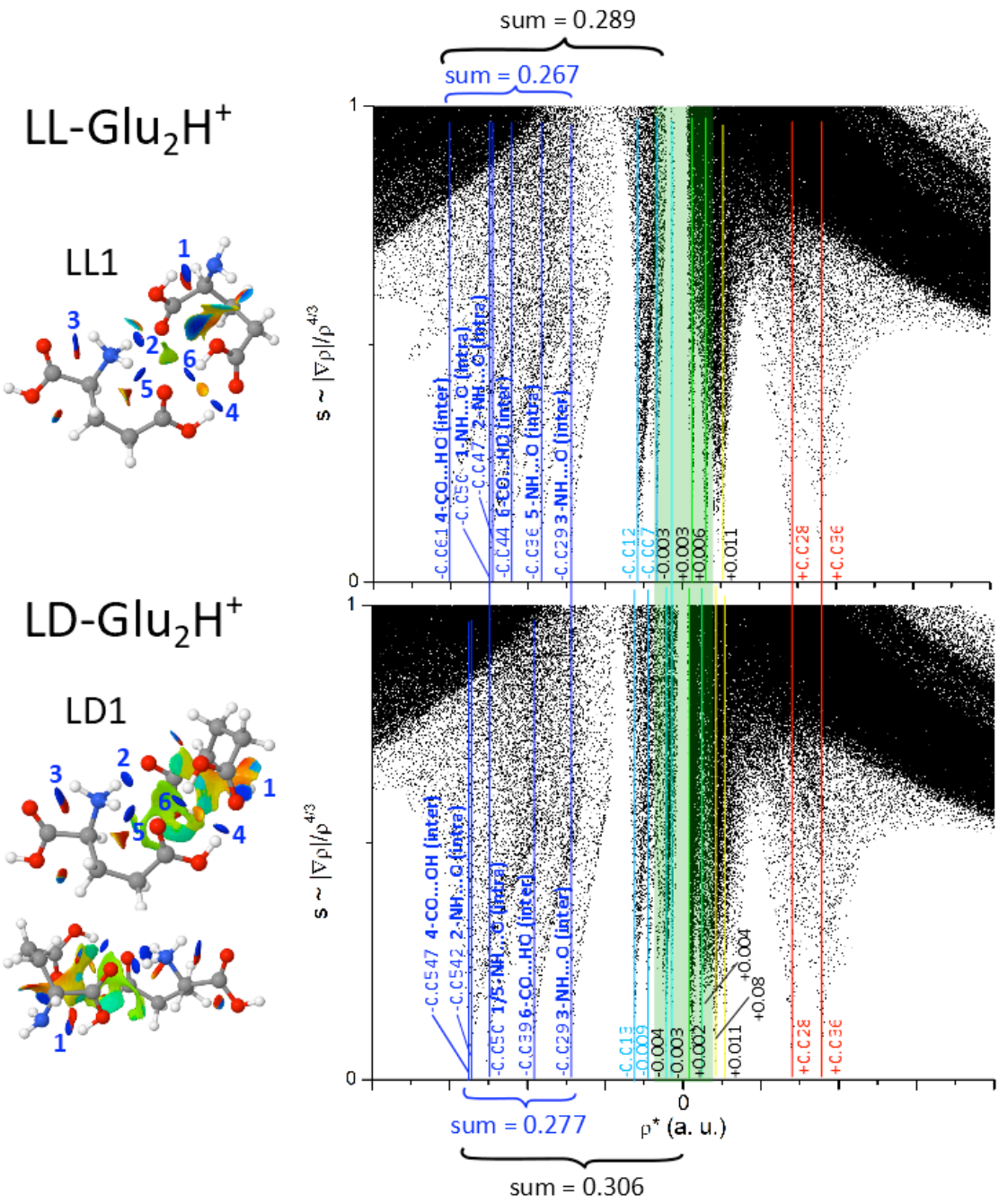

Figure S5

IRPD spectra of cryogenic LL-/LD-Glu_2H^+-H_2 in the XH stretch range. From top to bottom: LL-Glu_2H^+ (m/z 297, both ^{15}N-labelled), LL-Glu_2H^+ (m/z 296, one ^{15}N-labeled), LL-Glu_2H^+ (m/z 295, unlabelled), LD-Glu_2H^+ (m/z 295, unlabelled), LD-Glu_2H^+ (m/z 296, one ^{15}N-labeled). For comparison, the IRPD spectrum of L-$GluH^+$ is also shown.[50] By analogy, the transitions of LL-/LD-Glu_2H^+ can be assigned to bound stretches of the NH_3^+ group (ν^b_{NH3}), free stretches of NH_3^+ (ν^f_{NH3}) and free OH stretches (ν^f_{OH}) as illustrated by their colour. ^{15}N-labeling induces a typical red shift of 8 cm^{-1} of its NH stretching modes (ν_{NH}), which helps to distinguish them from OH stretches (ν_{OH}). Bands J-D of LL-Glu_2H^+ are red-shifted by 8 cm^{-1} upon ^{15}N-labelling supporting this assignment. Only transition Y may be attributed to an OH mode. Band B is assigned to ν^b_{OH} because it is insensitive to ^{15}N-labelling. In case of LD-Glu_2H^+, bands J-C are assigned to ν^b_{NH3} and ν^f_{NH3}, and transitions A and B are assigned to ν^f_{OH} and ν^b_{OH}, respectively. Bands E-C are characteristic signatures of heterochiral LD-Glu_2H^+ compared to homochiral LL-Glu_2H^+. ^{15}N-labelling only changes their intensities and may indicate a shift of "half of the peaks" related to "half of the molecule" as only L-Glu is labelled.

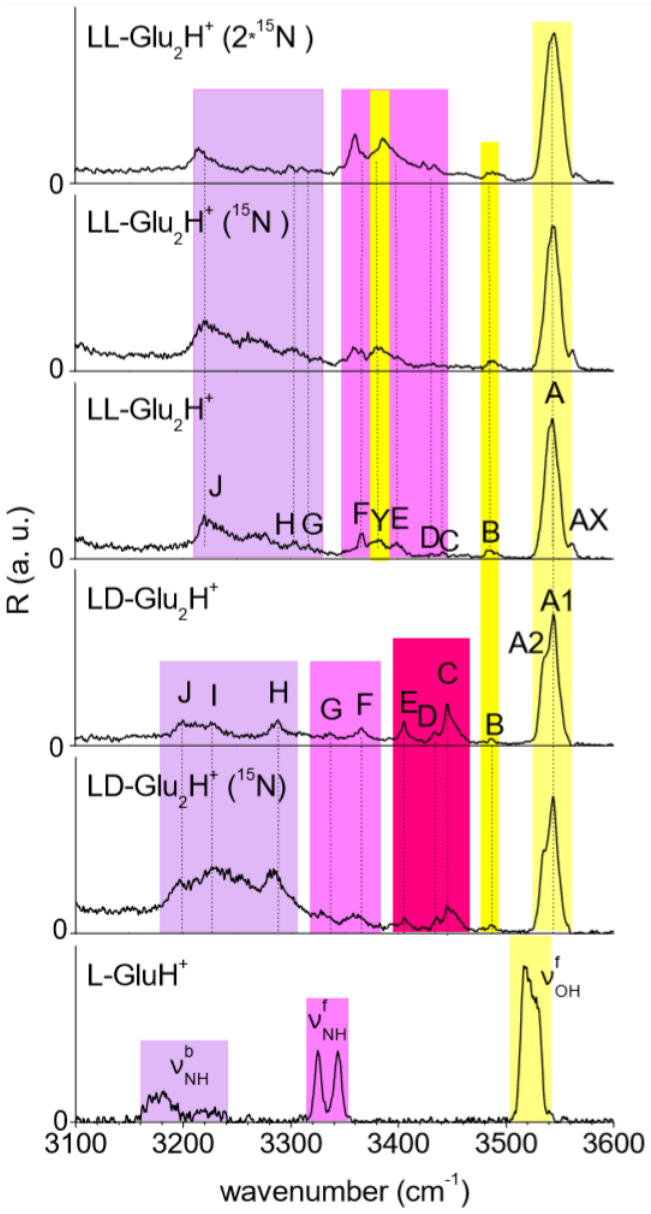

Figure S6

IR-dip spectra of LL-/LD-Glu_2H^+-H_2; arrows indicate the bands probed, dashed lines indicate that all bands in the IRPD spectra are covered by IR-IR hole burning. Overlapping bands in the IR-dip spectra of LD-Glu_2H^+ appear at ≈3445, 3405, and 3290 cm^{-1}.

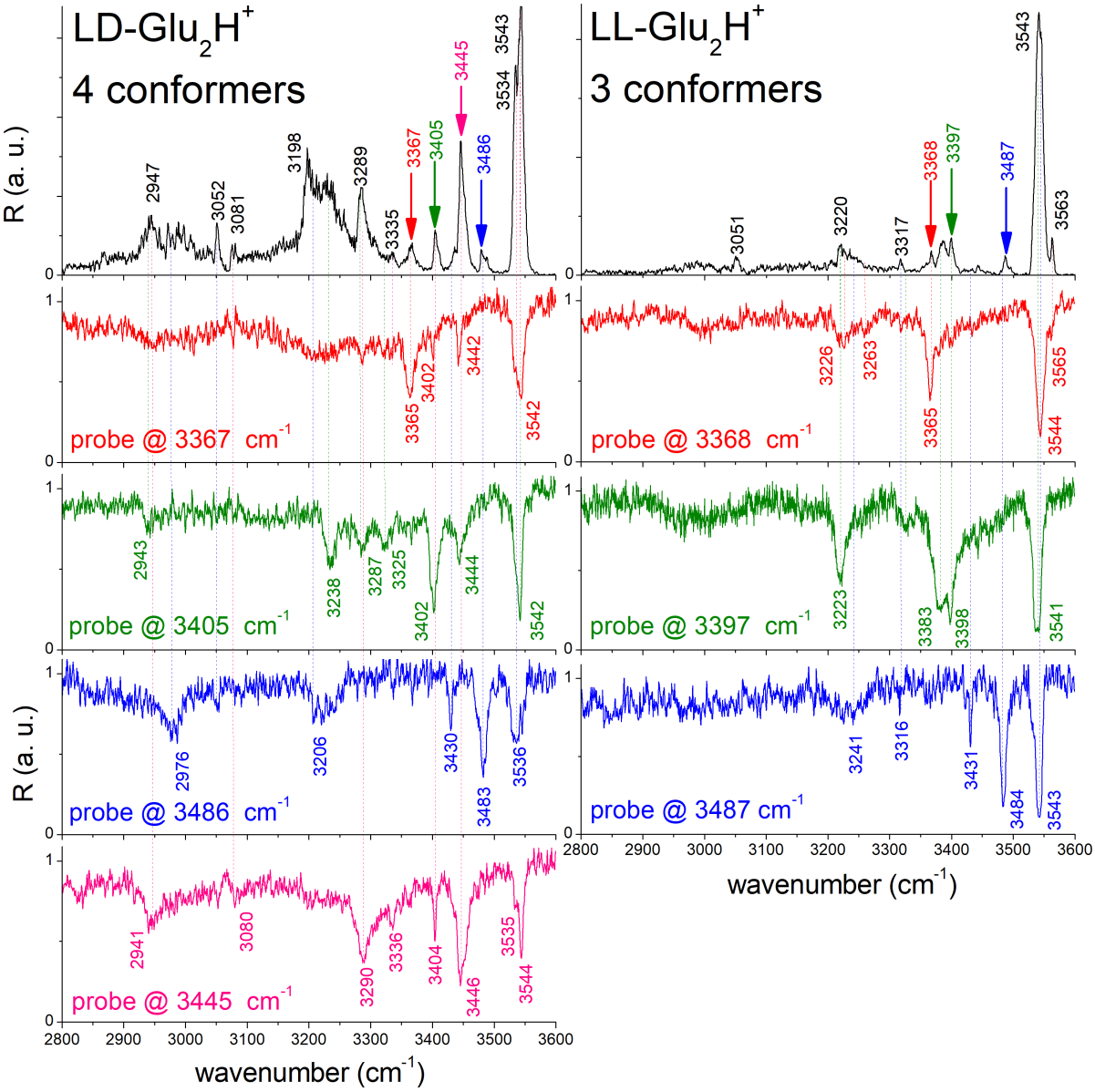

Figure S7

IRPD spectra and IR-IR hole burning spectra of LL-/LD-Glu_2H^+-H_2 recorded in the full measured XH stretch range and calculated IR absorption spectra of the assigned conformers (stick spectra and convolution with Lorentzian profile, FWHM 8 cm^{-1}). Left: Four dominant conformers of LD-Glu_2H^+ probed at 3445, 3486, 3367, and 3405 cm^{-1}. Right: Three dominant conformers of LL-Glu_2H^+ probed at 3368, 3397, and 3487 cm^{-1} as indicated by arrows in the IRPD spectrum.

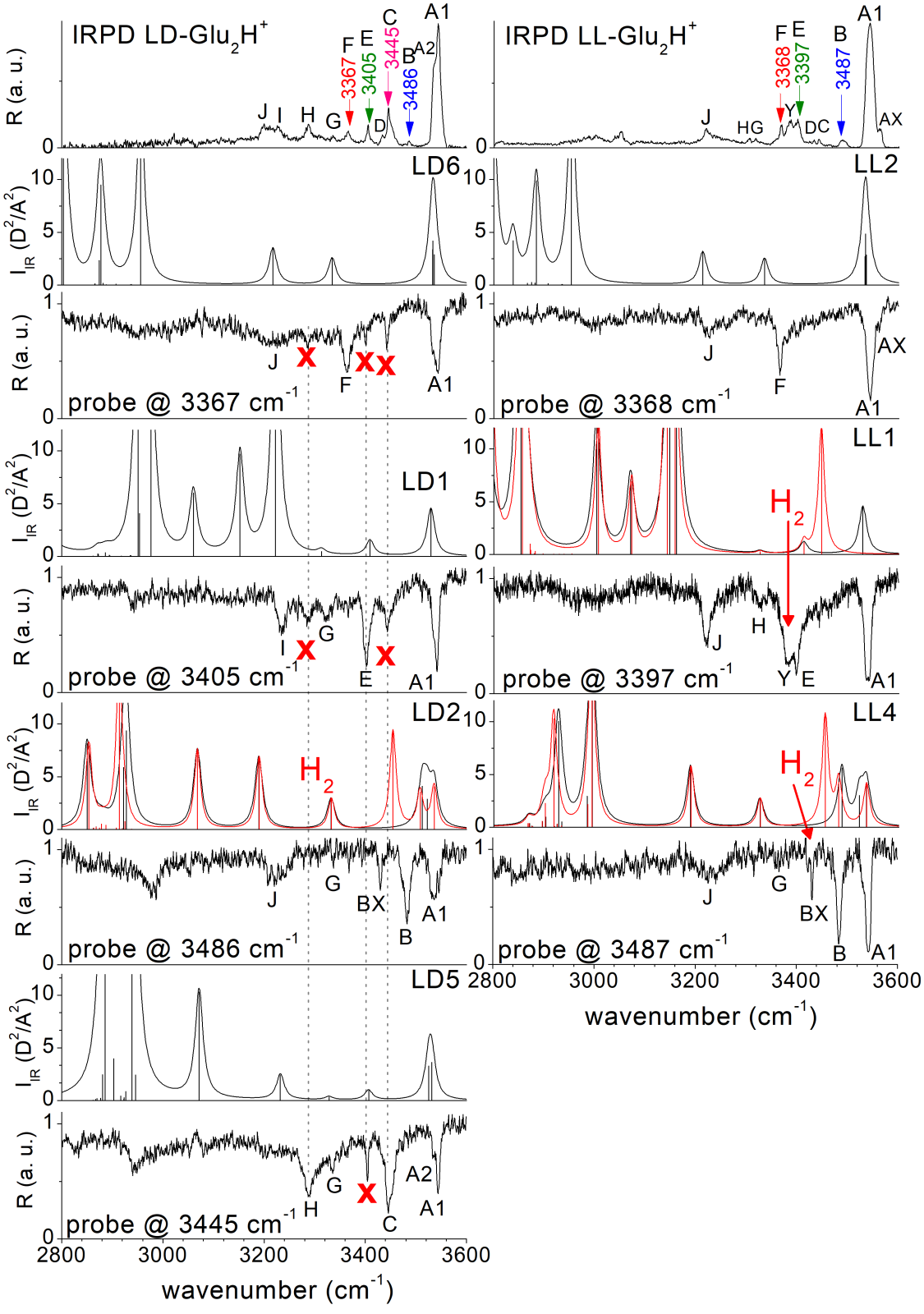

Figure S8

IR-dip spectra of cryogenic LL-/LD-Glu_2H^+-H_2 compared to the scaled (0.93) linear IR absorption spectra of additional most stable conformers calculated at the PBE0+MBD/tight level (stick spectra and convolution with Lorentzian profile, FWHM 10 cm^{-1}). Left: LD-Glu_2H^+ probed at 3367, 3405, 3486, and 3445 cm^{-1}. Right: LD-Glu_2H^+ probed at 3368, 3397, and 3487 cm^{-1} (see also Figure S7).

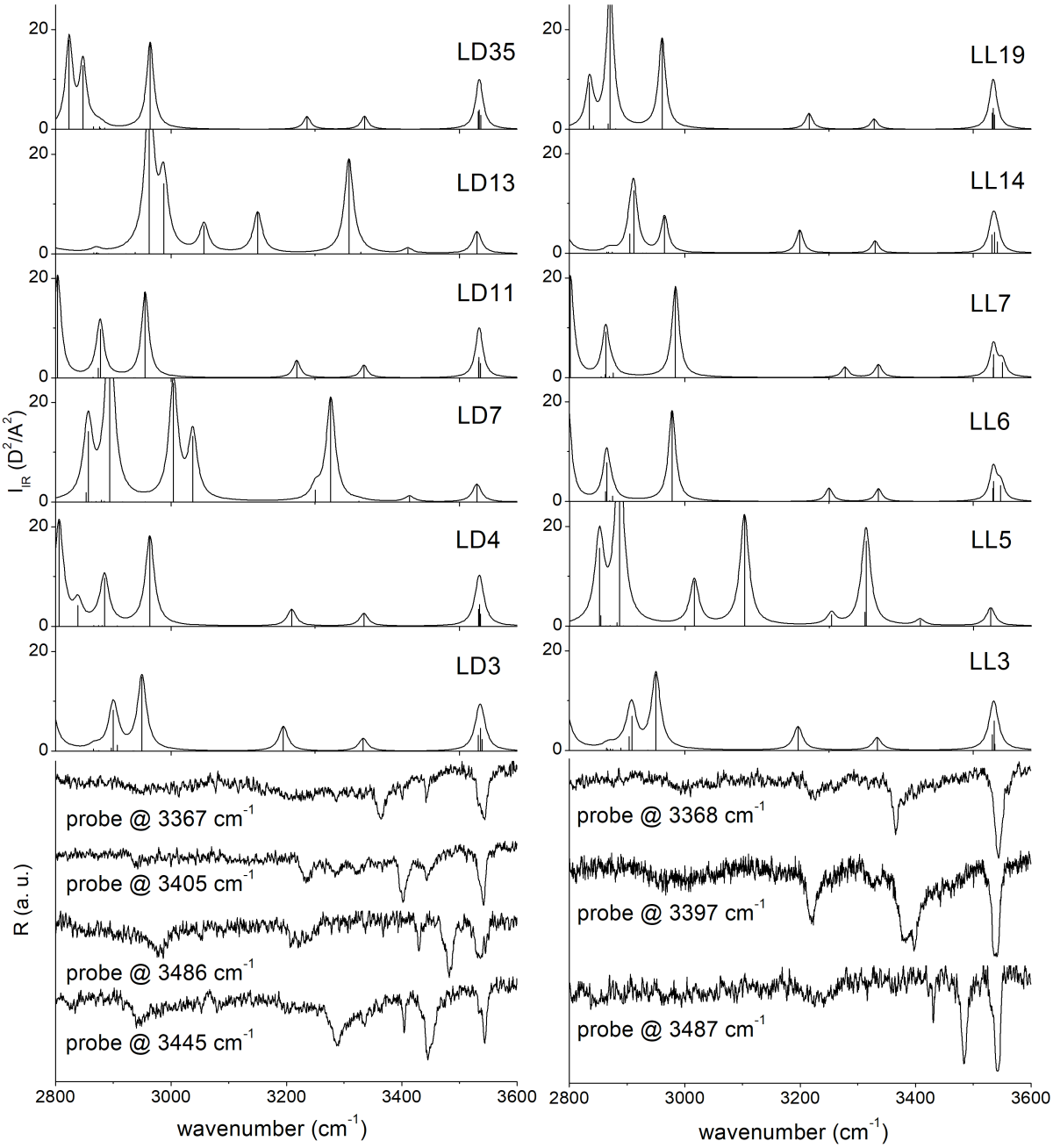

Figure S9

IRPD and IR-IR hole burning spectra of LL-/LD-Glu_2H^+-H_2 in the XH stretch range compared to IR absorption spectra of the assigned conformers (stick spectra and convolution with Lorentzian profile, FWHM 8 cm^{-1}) as calculated by Gaussian09 and FHI-aims. Black traces: PBE0+MBD/tight (FHI-aims); blue traces: PBE0/cc-pVTZ (G09); green traces: B3LYP/cc-pVTZ (G09), red traces: corresponding H_2-tagged conformers. Left: LL-Glu_2H^+ probed at 3368, 3397, and 3487 cm^{-1}. Right: LD-Glu_2H^+ probed at 3445, 3486, 3367, and 3405 cm^{-1} (see also Figure S7).

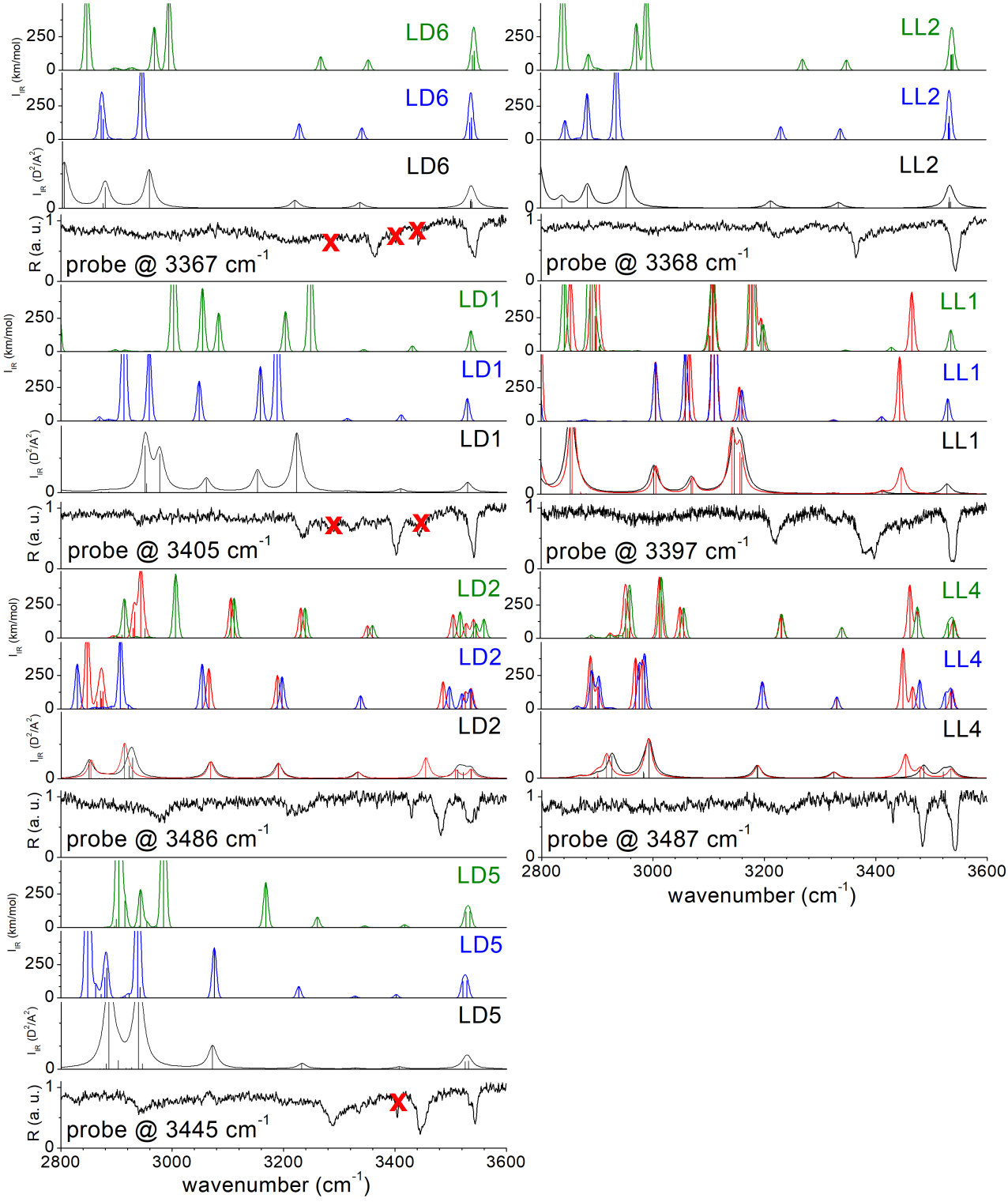

Figure S10

Structures of relevant H_2-tagged LL-/LD-Glu_2H^+-H_2 isomers with H_2 binding energies (D_0, kJ/mol) and lengths of intermolecular H-bonds (R, Å) calculated at the PBE0+MBD/tight level.

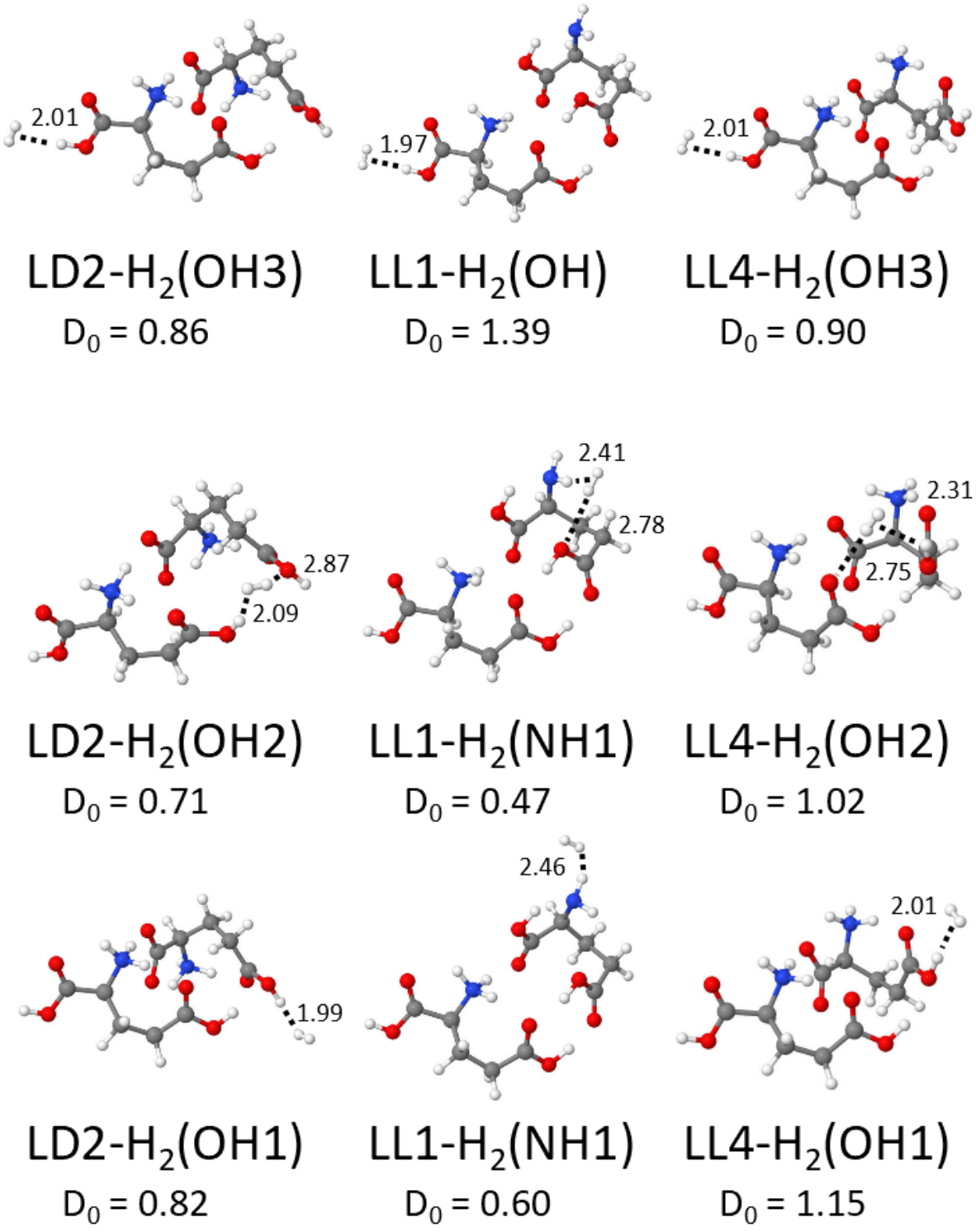

Figure S11

IR-dip spectrum of cryogenic LD-Glu_2H^+-H_2 probed at 3486 cm^{-1} compared to the scaled (0.93) linear IR absorption spectra of relevant H_2-tagged LD2 isomers calculated at the PBE0+MBD/tight level with FHI-aims (black) and at the B3LYP/cc-pVTZ level with Gaussian09 (red, scaled by 0.95).

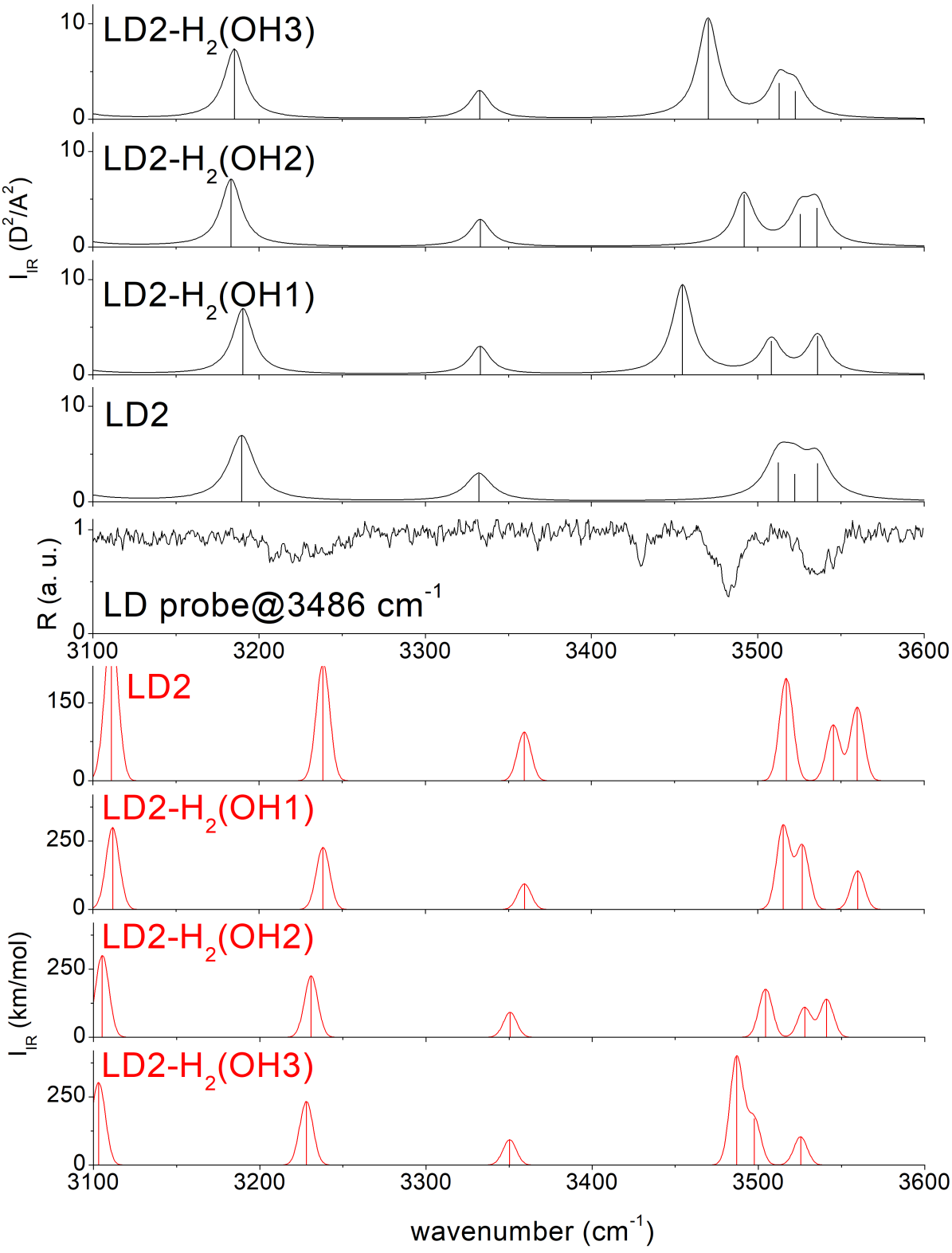

Figure S12

IR-dip spectrum of cryogenic LL-Glu_2H^+-H_2 probed at 3397 cm^{-1} compared to the scaled (0.93) linear IR absorption spectra of relevant H_2-tagged LL1 isomers calculated at the PBE0+MBD/tight level with FHI-aims (black) and at the B3LYP/cc-pVTZ level with Gaussian09 (red, scaled by 0.95).

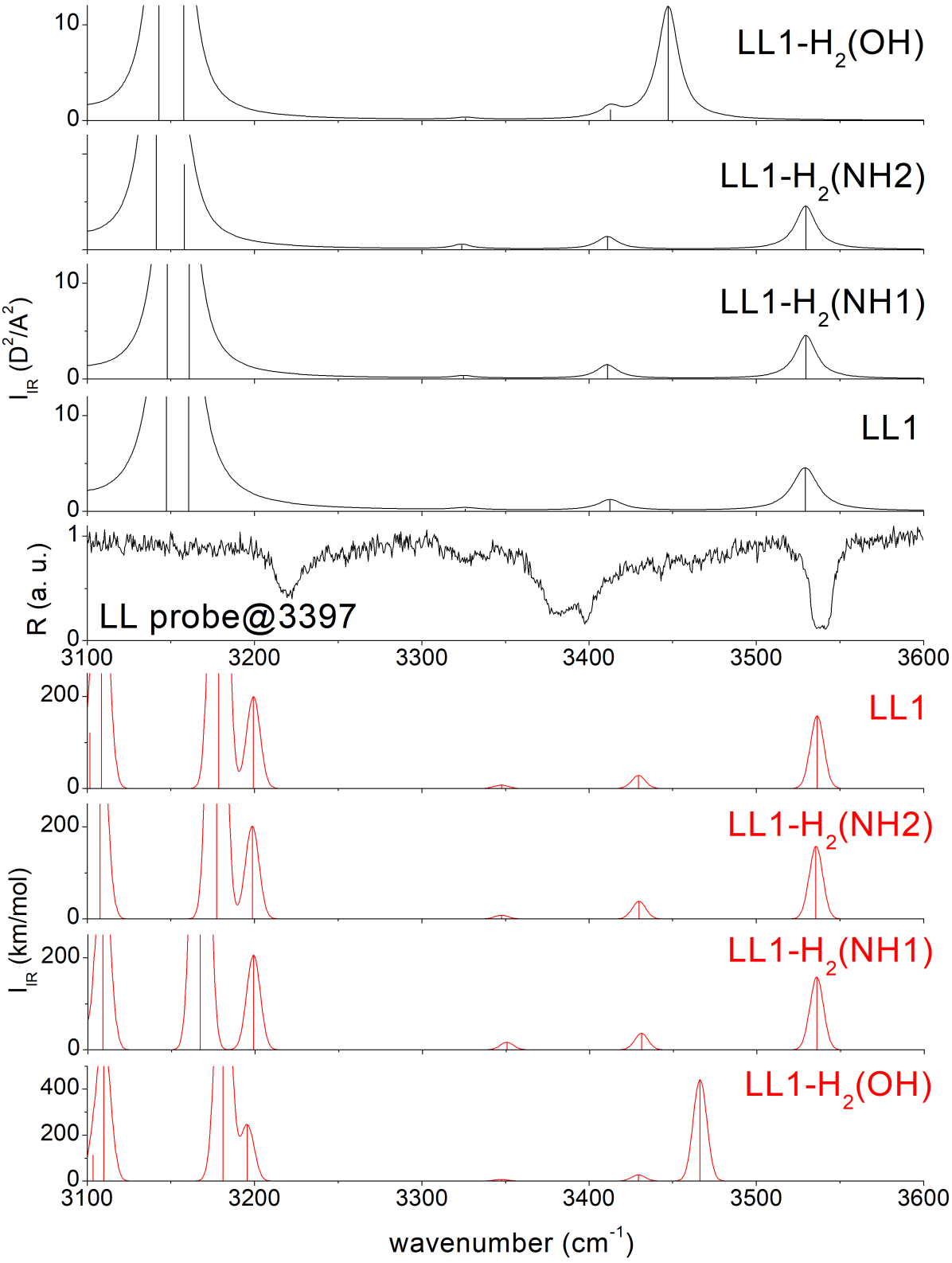

Figure S13

IR-dip spectrum of cryogenic LL-Glu_2H^+-H_2 probed at 3487 cm^{-1} compared to the linear IR absorption spectra of relevant H_2-tagged LL4 isomers calculated at the PBE0+MBD/tight level with FHI-aims (black, scaled by 0.93) and at the B3LYP/cc-pVTZ level with Gaussian09 (red, scaled by 0.95).

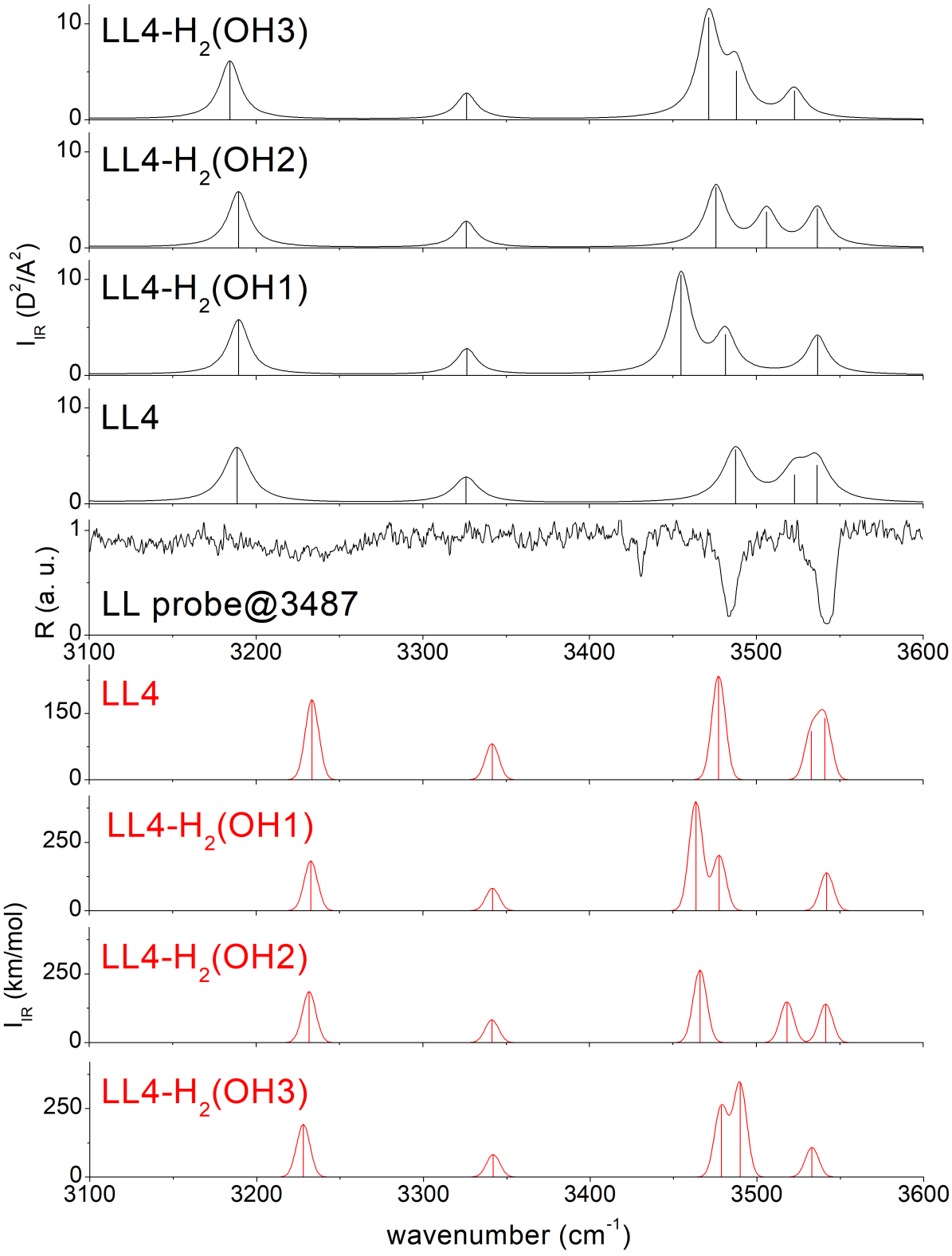

Figure S14

IRPD spectra of cryogenic LL-/LD-Glu_2H^+ in the fingerprint range. From top to bottom: LL-Glu_2H^+ (m/z 305, both deuterated), LL-Glu_2H^+ (m/z 300, one deuterated), LL-Glu_2H^+ (m/z 295, unlabeled), LD-Glu_2H^+ (m/z 295, unlabelled). The two lowest spectra correspond to L-$GluH^+$ (m/z 153, deuterated) and L-$GluH^+$ (m/z 148) to illustrate the effect of deuteration. Dotted lines are IRMPD spectra measured with the CLIO-FEL. There is an apparent effect of deuteration of the alkyl chain on the skeletal modes of the fingerprint range. Any deuteration effect is however negligible in the XH stretch range, because the CH-stretches (ν_{CH}) are too weak to be observed. Comparison of the IRPD spectra of natural (m/z 295), partially deuterated (m/z 300), and fully deuterated (m/z 305) LL-Glu_2H^+ reveals the effects of deuteration, which are confirmed by comparison to natural (m/z 148) and deuterated (m/z 152) L-$GluH^+$ (lowest two spectra). Deuteration influences δ_{CH} (1450 cm^{-1}): band M of fully deuterated LL-Glu_2H^+ (m/z 305) is red-shifted and overlaps with band N ($\Delta\nu\approx32$ cm^{-1}). All modes affected by deuteration are mainly skeletal CH bending modes (δ_{CH}), overlapping partly with NH bending modes (δ_{NH}, bands N, M) and OH bending modes (δ_{OH}, band O). Deuteration-induced effects must carefully be distinguished from chirality effects, which are most prominent for ν_{CO} (K1-K5) and δ_{NH} (N).

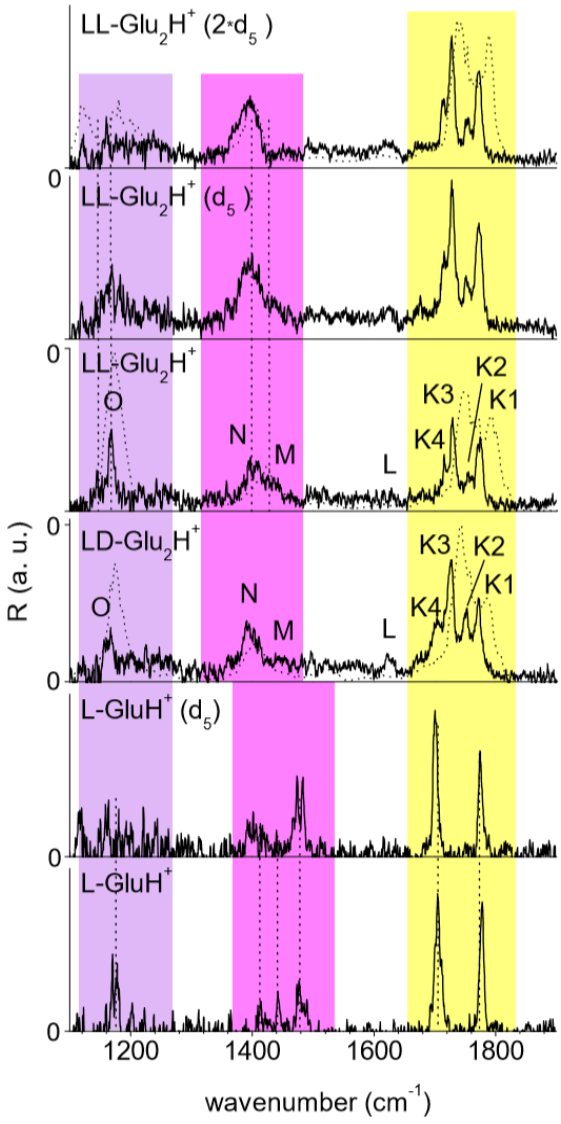

Figure S15

IRPD spectra of cryogenic LL- and LD-Glu_2H^+-H_2 in the fingerprint range (1100-1900 cm^{-1}) compared to the scaled (0.955) linear IR absorption spectra of additional most stable conformers calculated at the PBE0+MBD/tight level (stick spectra and convolution with Lorentzian profile, FWHM 10 cm^{-1}).

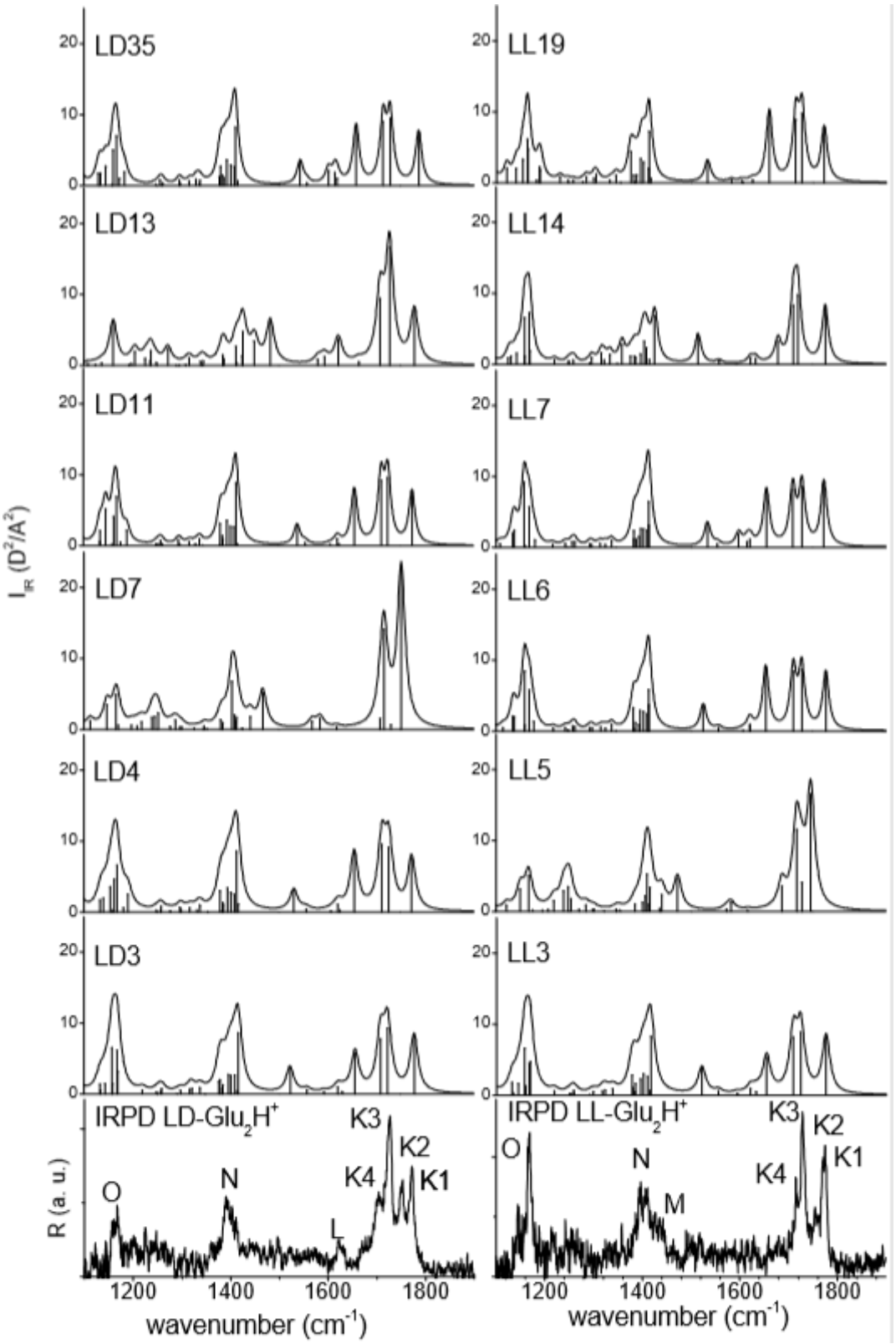

Figure S16

Mass spectra of the sprayed solution containing L-d_5-Glu and D-Glu taken at different ESI and ion optics conditions. The tables included in the individual plots indicate the observed ratio of L- and D-Glu (top left two entries). Expected ratios of DD-/LD- and LL-Glu_2H^+ (top right three entries) are calculated from these values assuming no preference for a certain diastereomer. We compare the expected ratios to the observed ratios of DD-/LD- and LLGlu_2H^+ (bottom three entries) and do not find any clear indication for any preferred formation of homo- or heterochiral dimers.

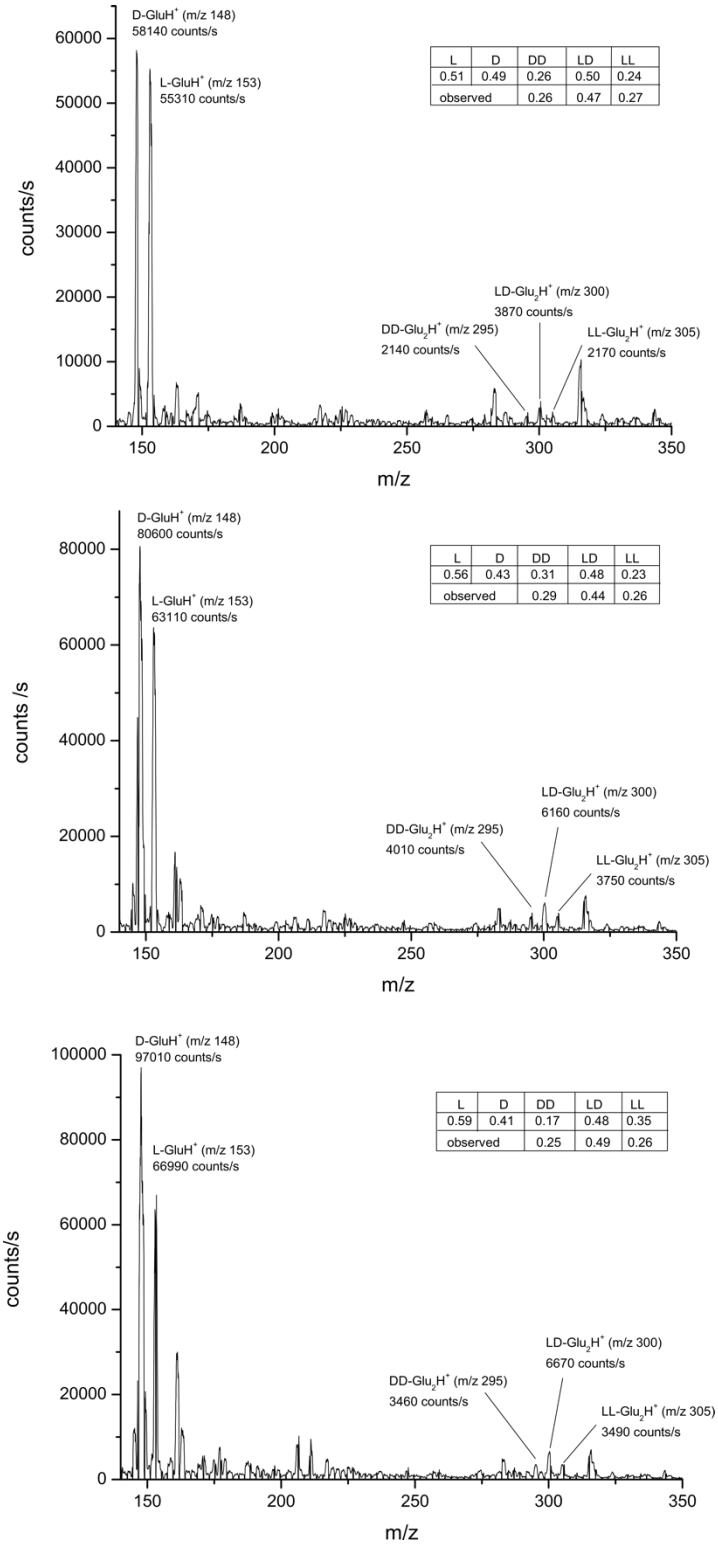

Figure S17
Collision-induced dissociation (CID) efficiency of LL-/LD-Glu_2H^+ as a function of the RF amplitude of the QIT (see also Figure 6).

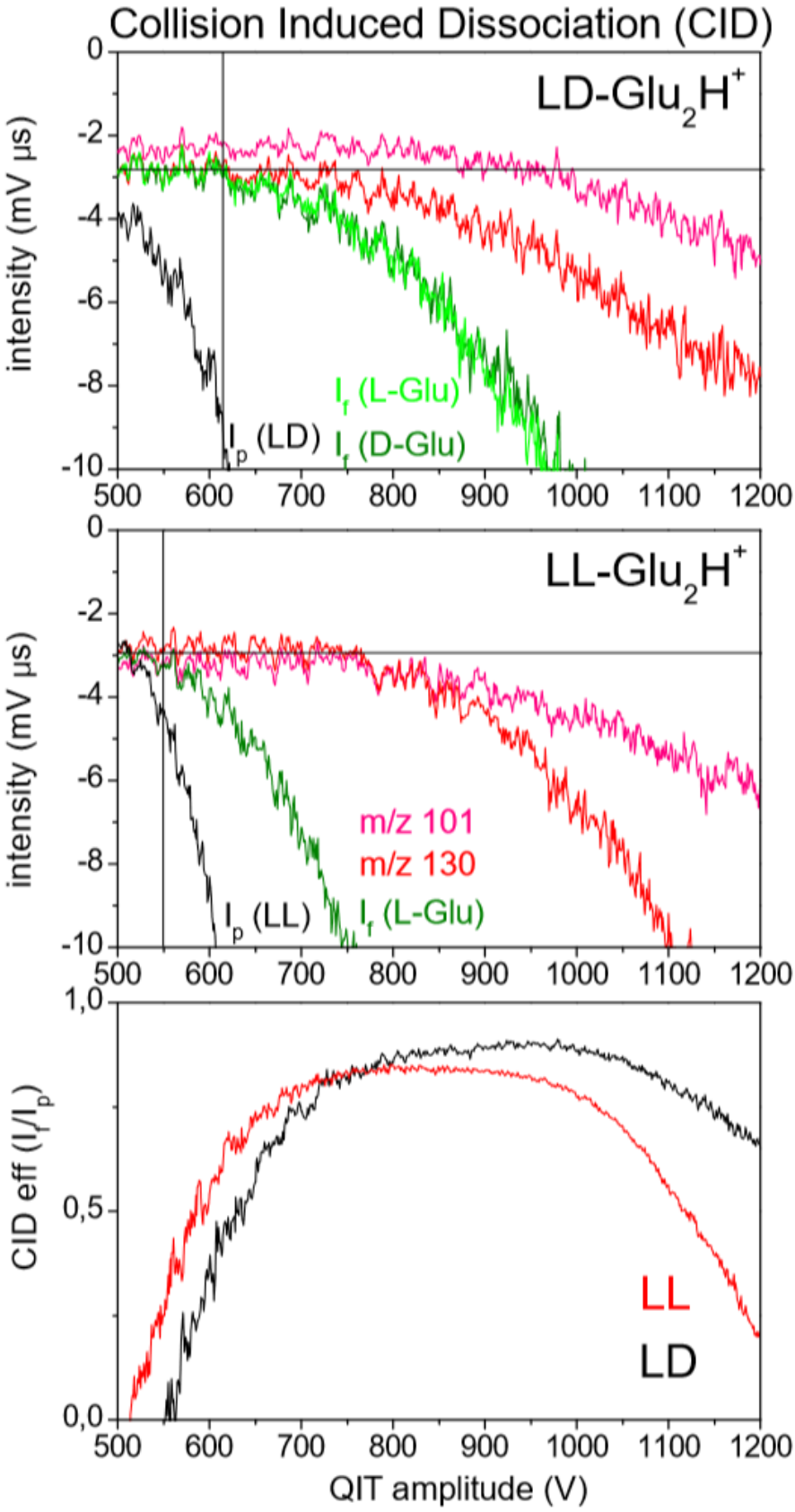

Figure S18

Extended energy hierarchy diagram of the most stable LL- and LD-Glu_2H^+ (ΔE<20 kJ/mol) at the PBE0+MBD/tight level (Table S3).

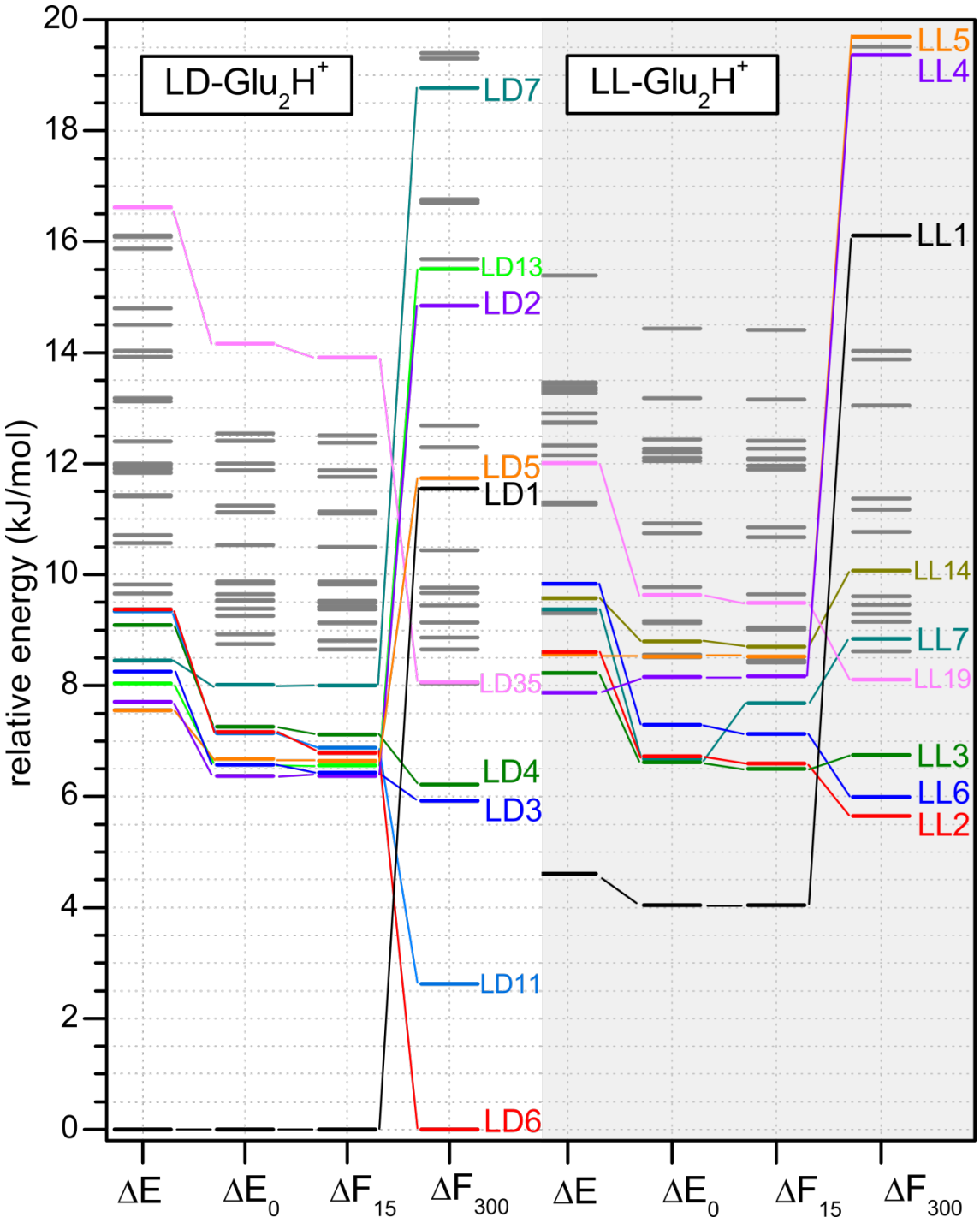

Figure S19

IRPD spectra of cryogenic LL-/LD-Glu_2H^+-H_2 recorded in the XH stretch range. From top to bottom: LD-Glu_2H^+ (m/z 300, L-enantiomer is deuterated), LL-Glu_2H^+ (m/z 305, both L-enantiomers are deuterated), LL-Glu_2H^+ (m/z 295, unlabelled), DD-Glu_2H^+ (m/z 295, unlabelled). The bottom two IRPD spectra of unlabelled LL- and DD-Glu_2H^+ are identical, which is not surprising because these LL and DD dimers are enantiomers, which have the same physical properties (apart from tiny effects of parity violation). Furthermore, the IRPD spectrum of labelled LL-Glu_2H^+ (m/z 305) resembles the one of unlabelled LL- and DD-Glu_2H^+. This emphasizes that (i) deuteration has no impact on the modes in the XH stretch range and (ii) the same ensemble of conformers is probed. Hence, we conclude that deuteration does not significantly alter the chemistry of the probed dimers or at least not at a scale detectable by IR spectroscopy. The spectrum of LD-Glu_2H^+ is clearly different. Yet, deuteration has no impact on the XH stretching modes (X=O, N) and hence does not distort the IRPD spectrum in this range.

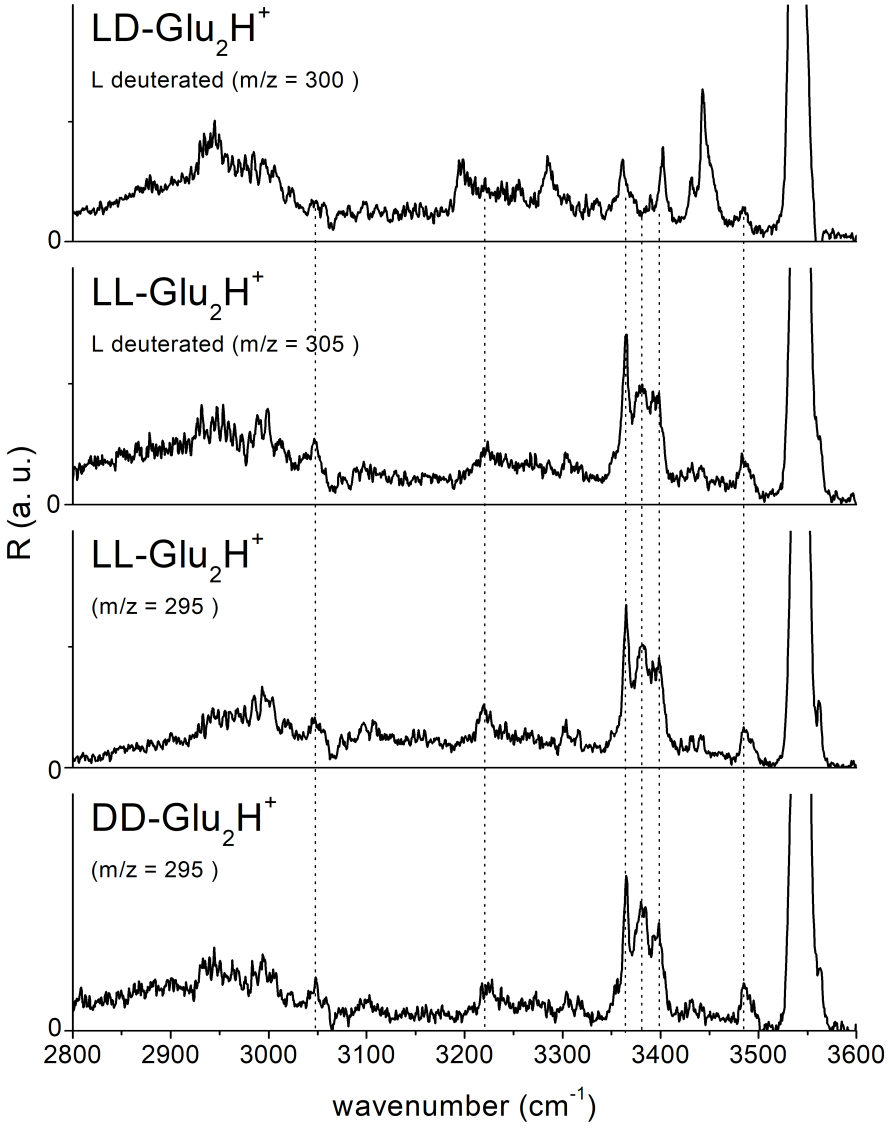

Table S1

Positions and assignments of major bands in the IRPD spectra[a] of LL-/LD-Glu_2H^+ in the XH stretch range (X=O, N, 3200-3600 cm^{-1}) and scaled frequencies calculated at the PBE0+MBD/tight level.[b]

species	IRPD	IR-dip	calculated	isomer	assignment
LD	A1 3543 (20)	3542	3536 (2.9) / 3534 (4.2) / 3533 (3.3)	LD6	ν^{f}_{OH}
		3542	3530 (4.5)	LD1	ν^{f}_{OH}
		3544	3531 (3.6)	LD5	ν^{f}_{OH}
LD	A2 3534 (15)	3536	3536 (4.0) / 3522 (2.9)	LD2	ν^{f}_{OH}
		3535	3536 (4.0)	LD2-H_2(OH1)	ν^{f}_{OH}
			3526 (3.3)	LD5	ν^{f}_{OH}
LD	B 3486 (10)	3483	3512 (4.1)	LD2	ν^{b}_{OH}
		3430	3508 (3.5)	LD2-H_2(OH1)	ν^{b}_{OH}
LD	C 3445 (15)	3442			
		3444			
		3446	3407 (0.9)	LD5	$\nu^{f(as)}_{NH2}$
LD	D 3434 (5)	3430	3455 (9.3)	LD2-H_2(OH1)	ν^{b}_{OH}
LD	E 3405 (8)	3402			
		3402	3409 (1.5)	LD1	$\nu^{f(as)}_{NH2}$
		3404			
LD	F 3367 (15)	3365	3334 (2.5)	LD6	ν^{f}_{NH3}
LD	G 3335 (20)	3325	3313 (0.5)	LD1	$\nu^{f(s)}_{NH2}$
		3336	3328 (0.3)	LD5	$\nu^{f(s)}_{NH2}$
LD	H 3289 (25)	3288			
		3287			
		3290	3232 (2.4)	LD5	ν^{b}_{NH3}
LD	I 3228 (>25)	3238	3152 (9.7)	LD1	ν^{b}_{NH3}
LD	J 3198 (>25)	3206	3190 (6.9)	LD2	ν^{b}_{NH3}
			3217 (3.5)	LD6	ν^{b}_{NH3}
LL	AX 3563 (5)	3565	3536 (2.8)	LL2	ν^{f}_{OH}
LL	A1 3543 (20)	3544	3534 (4.8) / 3533 (2.7)	LL2	ν^{f}_{OH}
		3541	3529 (4.5)	LL1	ν^{f}_{OH}
		3543	3536 (4.0) /3523 (3.0)	LL4	ν^{f}_{OH}
			3537 (4.0)	LL4-H_2(OH1)	ν^{f}_{OH}
LL	B 3487 (10)	3484	3488 (5.6)	LL4	ν^{b}_{OH}
			3481 (4.3)	LL4-H_2(OH1)	ν^{b}_{OH}
LL	C 3441 (5)				
LL	D 3432 (3)	3431	3455 (10.5)	LL4-H_2(OH1)	ν^{b}_{OH}
LL	E 3397 (10)	3398	3413 (1.1)	LL1	$\nu^{f(as)}_{NH2}$
LL	Y 3381 (10)	3383	3447 (11.9)	LL1-H_2(OH)	ν^{b}_{OH}
LL	F 3368 (10)	3365	3335 (2.5)	LL2	ν^{f}_{NH3}
LL	G 3317 (10)	3316	3326 (2.7)	LL4	ν^{f}_{NH3}
LL	H 3305 (10)	3325	3326 (0.2)	LL1	$\nu^{f(s)}_{NH2}$
LL	J 3220 (>25)	3263 / 3226	3231 (3.1)	LL2	ν^{b}_{NH3}
		3223	3161 (16.6)	LL1	$\nu^{b}_{NH3} + \nu^{b}_{OH}$
		3241	3189 (5.8)	LL4	ν^{b}_{NH3}

[a] Band widths (FWHM, cm^{-1}) are listed in parentheses.

[b] IR intensities ($D^2/Å^2$) are listed in parentheses. The scaling factor is 0.93.

Table S2

Positions and assignments of major bands in the IRPD spectra[a] of LL-/LD-Glu_2H^+ in the fingerprint range (1100-1900 cm^{-1}) and scaled frequencies calculated at the PBE0+MBD/tight level.[b]

species	IRPD	calculated	isomer	assignment
LD	K1 1774 (10)	1779 (7.8) 1776 (8.2) 1774 (7.5)	LD1 LD2 LD6	$\nu_{\alpha CO}$ $\nu_{\alpha CO}$ $\nu_{\alpha CO}$
LD	K2 1751 (10)	1735 (13.5) 1754 (18.1) 1743 (5.8)	LD1 LD5 LD5	$\nu_{\gamma CO}$ $\nu_{\alpha CO}$ $\nu_{\gamma CO}$
LD	K3 1728 (10)	1728 (6.0) 1724 (9.6) 1717 (11.1)	LD2 LD6 LD5	$\nu_{\gamma CO}$ $\nu_{\gamma CO}$ $\nu_{\gamma CO}$
LD	K4 1715 (8)	1710 (9.2) 1697 (10.3)	LD6 LD1	$\nu_{\gamma CO}$ $\nu_{\gamma CO}$
LD	L 1619 (20)	1656 (7.8) 1619 (5.9)	LD6 LD1	ν_{COO-} δ_{NH3}
LD	N 1390 (30)	1413 (8.8) 1411 (5.1) / 1402 (5.5) 1418 (4.2) 1409 (4.0)	LD6 LD2 LD1 LD5	δ^u_{NH3} δ^u_{NH3} δ^b_{OH} δ^b_{OH}
LD	O 1165 (15)	1160 (6.5) 1168 (6.9) / 1162 (4.1) / 1146 (5.1) 1177 (6.8) / 1160 (6.6) 1166 (5.5)	LD1 LD6 LD2 LD5	δ^f_{OH} δ^f_{OH} δ^f_{OH} δ^f_{OH}
LL	K1 1774 (10)	1779 (7.9) 1771 (7.6) 1774 (8.4)	LL1 LL2 LL4	$\nu_{\alpha CO}$ $\nu_{\alpha CO}$ $\nu_{\alpha CO}$
LL	K2 1751 (10)	1726 (9.5)	LL2	$\nu_{\gamma CO}$
LL	K3 1728 (10)	1737 (21.2) 1732 (11.9)	LL1 LL4	$\nu_{\gamma CO}$ $\nu_{\gamma CO}$
LL	K4 1715 (8)	1711 (8.8)	LL2	$\nu_{\gamma CO}$
LL	M 1432 (25)	1485 (6.5) / 1461 (3.9)	LL1	δ^u_{NH3}
LL	N 1400 (30)	1417 (8.0) 1414 (4.7) 1406 (7.4)	LL2 LL4 LL1	δ^u_{NH3} δ^u_{NH3} δ^b_{OH}
LL	O 1167 (15)	1159 (6.2) 1167 (5.8) / 1163 (5.7) 1172 (2.3) / 1162 (6.1) / 1156 (7.7)	LL1 LL-2 LL4	δ^f_{OH} δ^f_{OH} δ^f_{OH}

[a] Band widths (FWHM, cm^{-1}) are listed in parentheses.

[b] IR intensities ($D^2/Å^2$) are listed in parentheses. The scaling factor is 0.955.

Table S3

Relative electronic energies (ΔE), zero-point corrected energies (ΔE_0), relative free energies at 15 and 300 K (ΔF_{15} and ΔF_{300}, kJ/mol), and binding energies (D_0) of the most stable LL- and LD-Glu_2H^+ (ΔE<15 kJ/mol). All values are given in kJ/mol.

conformer	ΔE	ΔE_0	ΔF_{15}	ΔF_{300}	D_0
LD1	0.0	0.0	0.0	11.6	144.1
LD2	7.7	6.4	6.4	14.9	137.7
LD3	8.3	6.6	6.4	5.9	137.5
LD4	9.1	7.3	7.1	6.2	136.8
LD5	7.6	6.7	6.6	11.7	137.4
LD6	9.4	5.8	5.4	0.0	138.3
LD7	8.5	8.0	8.0	18.8	136.0
LD8	9.0	7.3	7.1	6.3	136.8
LD9	7.6	6.7	6.4	11.8	137.4
LD10	7.6	6.7	6.7	11.9	137.4
LD11	9.3	7.1	6.9	2.6	137.0
LD12	8.5	8.0	8.0	18.8	136.0
LD13	8.0	6.6	6.6	15.5	137.5
LD35	16.6	14.2	13.9	8.1	129.9
LL1	4.6	4.0	4.0	16.1	140.0
LL2	8.6	6.7	6.6	5.6	133.3
LL3	8.2	6.6	6.5	6.8	133.4
LL4	7.9	8.2	8.2	19.3	131.8
LL5	8.6	8.5	8.5	19.7	131.5
LL6	9.8	7.3	7.1	6.0	132.7
LL7	9.4	6.7	7.7	8.8	133.3
LL8	8.6	8.5	8.5	19.7	131.5
LL9	9.8	7.3	7.1	5.9	132.7
LL10	9.4	6.7	6.6	8.9	133.3
LL11	10.2	7.7	7.5	6.8	132.3
LL12	11.3	9.2	9.0	9.3	130.8
LL13	11.3	9.1	9.0	9.2	130.9
LL14	8.6	8.8	8.7	10.1	131.2
LL19	12.0	9.6	9.5	8.1	130.4

Table S4

Unscaled low-frequency normal modes of selected conformers (cm^{-1}) calculated at the PBE0+MBD/tight level.

mode no.	1	2	3	4	5	6	7	8	9	10
LD1 [a]	19.9	31.2	55.4	73.8	77.1	89.4	91.4	96.5	103.5	125.5
LD2 [a]	24.2	33.9	37.4	43.8	47.9	53.1	63.3	71.2	76.70	90.4
LD3	7.8	15.6	28.3	35.7	51.9	57.3	61.6	72.8	85.7	97.9
LD5 [a]	21.3	24.9	43.0	45.4	53.5	66.6	83.3	85.1	92.5	113.0
LD6 [a]	14.2	28.6	37.5	46.4	55.6	57.6	72.0	74.5	95.4	111.2
LD11	2.6	14.2	28.8	37.8	46.2	55.7	57.5	71.9	74.8	95.5
LL1 [a]	23.5	40.3	52.6	62.6	75.6	81.6	90.0	109.7	120.4	129.8
LL2 [a]	9.2	15.1	27.5	37.5	51.5	52.4	60.2	72.9	80.4	87.7
LL3	9.6	16.6	26.3	40.9	49.0	58.8	64.8	74.4	86.0	98.6
LL4 [a]	34.0	45.5	47.4	56.8	69.7	77.7	85.4	89.2	92.8	112.8
LL5	25.6	43.4	52.3	61.3	71.3	81.5	88.6	96.1	104.8	125.8
LL6	5.4	15.6	28.2	41.7	50.1	56.2	60.4	84.1	87.4	94.5

[a] Assigned conformers.

XYZ-files

Cartesian coordinates of all LL and LD structures of Glu2H+

LD1

N	-1.21654	-1.43205	1.08003
C	-1.80512	-0.47274	2.05206
C	-2.34694	-1.32309	3.19444
O	-2.35825	-2.52363	3.15417
H	-1.47241	-2.38038	1.38444
H	-0.17191	-1.34544	0.99575
H	-1.57362	-1.22035	0.13610
H	-1.00427	0.15620	2.44863
C	-2.89960	0.39669	1.42588
C	-2.39380	1.57528	0.60878
C	-1.63143	1.23182	-0.63775
O	-1.58656	0.09431	-1.10624
O	-1.01844	2.24812	-1.16219
H	-3.50061	0.79763	2.24137
H	-3.56361	-0.23490	0.83022
H	-1.76102	2.23168	1.20945
H	-3.24065	2.19304	0.29700
H	-0.36078	1.92832	-1.84353
O	-2.78526	-0.57842	4.19354
H	-3.12126	-1.15809	4.89464
N	3.46368	1.50771	-0.71529
C	3.23919	0.08390	-0.52107
C	1.92617	-0.06875	0.25037
O	1.46561	1.04993	0.75560
H	2.12012	1.73338	0.42716
H	4.43833	1.76562	-0.64982
H	3.08617	1.83956	-1.59572
H	3.98471	-0.27383	0.19728
C	3.32157	-0.84699	-1.73772
C	2.64653	-0.34836	-3.02430
C	1.24844	0.11387	-2.76584
O	1.00486	1.27990	-2.48183
O	0.33929	-0.82994	-2.79169
H	4.37252	-1.01894	-1.97114
H	2.89732	-1.80816	-1.44587
H	3.19710	0.48887	-3.45176
H	2.64029	-1.16156	-3.74891
H	-0.49648	-0.47455	-2.41008
O	1.37269	-1.13866	0.41886

LD2

N	-1.35436	-1.57579	1.27144
C	-1.64180	-0.41604	2.14769
C	-2.18867	-0.98621	3.44584
O	-2.41401	-2.15625	3.60185
H	-0.29374	-1.66910	1.08447
H	-1.78239	-1.42977	0.34584
H	-1.72101	-2.41847	1.72606
H	-0.69361	0.08484	2.36139
C	-2.61202	0.58614	1.52033
C	-2.02074	1.47474	0.43471
C	-1.77723	0.81196	-0.88681
O	-1.87431	-0.37556	-1.11715
O	-1.41996	1.68228	-1.82420
H	-2.95391	1.23897	2.32289
H	-3.49484	0.05852	1.14928
H	-1.06448	1.89781	0.75304
H	-2.68254	2.32342	0.25036
H	-1.27834	1.19587	-2.65137
O	-2.37355	-0.04475	4.35970
H	-2.71817	-0.46098	5.16419
N	3.31816	1.04139	-0.30657
C	2.95942	-0.41093	-0.29558
C	1.61910	-0.49753	0.46593
O	1.16285	-1.64756	0.60805
H	3.25176	1.42152	-1.27151
H	2.54661	1.45495	0.27195
H	4.22925	1.23802	0.09589
H	3.71600	-0.94576	0.27736
C	2.86262	-1.02395	-1.68804
C	1.66110	-0.61388	-2.53166
C	1.71290	0.77562	-3.08813
O	2.54621	1.61620	-2.82351
O	0.72094	1.02154	-3.94199
H	3.78964	-0.84493	-2.23711
H	2.79435	-2.09965	-1.52942
H	1.56398	-1.28941	-3.38474
H	0.72238	-0.72692	-1.97948
H	0.84629	1.91728	-4.29335
O	1.12612	0.59039	0.82736

LD3

N	-1.39610	-1.39621	1.17387
C	-1.67449	-0.33662	2.16885
C	-1.87811	-1.03519	3.50239
O	-1.95021	-2.22945	3.61121
H	-1.96687	-1.24111	0.32231
H	-1.62161	-2.29983	1.60142
H	-0.35377	-1.36867	0.89903
H	-0.78736	0.29715	2.23885
C	-2.88032	0.53257	1.81267
C	-2.68699	1.44820	0.60798
C	-2.88462	0.78778	-0.72355
O	-2.80666	-0.40521	-0.93609
O	-3.15138	1.66001	-1.68445
H	-3.07588	1.16189	2.68040
H	-3.76233	-0.09891	1.67750
H	-1.67619	1.86770	0.59465
H	-3.37436	2.29245	0.66405
H	-3.25543	1.17199	-2.51507
O	-1.96890	-0.17056	4.50352
H	-2.10853	-0.66622	5.32450
N	2.90813	1.72235	-0.56768
C	2.88329	0.31546	-0.06858
C	1.40296	0.02854	0.27752
O	1.13805	-1.15780	0.55631
H	3.63692	2.29106	-0.14843
H	3.00718	1.71905	-1.61091
H	1.95600	2.06573	-0.30548
H	3.43417	0.28877	0.87269
C	3.50740	-0.69349	-1.02130
C	2.74308	-1.01212	-2.30210
C	2.79967	0.03834	-3.36957
O	3.03051	1.22000	-3.18567
O	2.55339	-0.44599	-4.57301
H	4.53129	-0.39343	-1.25683
H	3.57782	-1.62080	-0.45375
H	3.11788	-1.94040	-2.73410
H	1.68615	-1.20116	-2.08814
H	2.58250	0.28279	-5.21184
O	0.63871	1.01335	0.25984

LD4

N	-1.47422	-1.13822	0.85322
C	-1.35361	0.10830	1.64482
C	-1.78040	-0.21000	3.06267
O	-2.05893	-1.31888	3.43406
H	-0.57923	-1.30331	0.27288
H	-2.30786	-1.08362	0.23997
H	-1.60688	-1.91629	1.50582
H	-0.28462	0.35117	1.67846
C	-2.08340	1.29856	1.02551
C	-3.60569	1.32329	1.11123
C	-4.32579	0.39089	0.18020
O	-3.82623	-0.55203	-0.39792
O	-5.60509	0.70456	0.05396
H	-1.76344	1.38866	-0.01482
H	-1.71135	2.18582	1.53710
H	-3.96810	2.33117	0.90278
H	-3.96003	1.10322	2.12316
H	-6.02370	0.05632	-0.53264
O	-1.78157	0.87121	3.83391
H	-2.01364	0.60127	4.73522
N	4.03846	-0.19258	-0.05081
C	3.10796	-1.23758	-0.57231
C	1.71453	-0.85785	-0.01837
O	1.69995	0.05939	0.82406
H	4.28210	0.47206	-0.82169
H	3.44274	0.29603	0.65786
H	4.88212	-0.57024	0.36846
H	3.38101	-2.18560	-0.10685
C	3.15209	-1.41029	-2.08353
C	2.54399	-0.29787	-2.93028
C	3.35536	0.95801	-3.03411
O	4.22656	1.30306	-2.25690
O	3.01914	1.69367	-4.07864
H	4.17801	-1.61042	-2.40183
H	2.58061	-2.31495	-2.28841
H	2.36913	-0.65901	-3.94435
H	1.55592	-0.01721	-2.55178
H	3.56025	2.49815	-4.07625
O	0.75887	-1.52489	-0.46485

LD5

N	-1.43090	-0.66949	1.39274
C	-1.67572	0.43928	0.43936
C	-0.31920	1.09660	0.22220
O	0.55935	0.99167	1.04677
H	-2.33720	-0.98251	1.79878
H	-0.80048	-0.32529	2.12204
H	-0.91255	-1.41302	0.88181
H	-2.00281	0.00188	-0.50456
C	-2.69915	1.44772	0.95883
C	-4.16664	1.07175	0.79203
C	-4.67063	-0.05905	1.64278
O	-3.98286	-0.90960	2.17322
O	-5.98686	-0.05243	1.74434
H	-2.54378	2.36966	0.39698
H	-2.47752	1.68540	2.00262
H	-4.38258	0.80045	-0.24647
H	-4.79290	1.94076	0.99747
H	-6.26221	-0.81847	2.27132
O	-0.25665	1.74002	-0.91069
H	0.67379	2.07705	-1.07223
N	3.60480	-2.66270	-0.93882
C	2.36617	-2.07060	-1.43074
C	1.34139	-2.10986	-0.29717
O	1.83103	-2.45092	0.86774
H	2.78980	-2.64077	0.67797
H	3.71620	-3.61820	-1.25318
H	4.42554	-2.15098	-1.23396
H	1.93003	-2.64226	-2.25426
C	2.53685	-0.63045	-1.91690
C	3.14346	0.30937	-0.86883
C	3.16881	1.71659	-1.38939
O	2.19073	2.42670	-1.51393
O	4.37805	2.12591	-1.73398
H	3.16346	-0.64722	-2.81168
H	1.55467	-0.26373	-2.21876
H	2.53372	0.32409	0.03715
H	4.15833	0.01786	-0.60228
H	4.31195	3.03458	-2.06701
O	0.17150	-1.82582	-0.46231

LD6

N	-1.37605	-1.24408	0.94478
C	-1.32383	-0.15642	1.94748
C	-2.06464	-0.63369	3.18061
O	-2.51186	-1.74347	3.29253
H	-1.67176	-2.10276	1.41689
H	-0.40460	-1.38784	0.49135
H	-2.08013	-1.01220	0.21997
H	-0.27364	-0.02583	2.22291
C	-1.80299	1.18991	1.40955
C	-3.30094	1.38048	1.19938
C	-3.88893	0.68796	0.00421
O	-3.37207	-0.22384	-0.60825
O	-5.07340	1.17957	-0.32248
H	-1.25214	1.39292	0.48927
H	-1.47468	1.93978	2.12866
H	-3.52282	2.44393	1.09771
H	-3.87933	1.05772	2.07099
H	-5.41776	0.67568	-1.07547
O	-2.13225	0.31014	4.11268
H	-2.57260	-0.06254	4.89141
N	3.87221	0.54844	-0.12521
C	3.23047	-0.78405	-0.32969
C	1.77191	-0.61134	0.15607
O	1.01165	-1.57473	-0.07249
H	3.15573	1.04721	0.45343
H	4.76823	0.50154	0.34919
H	3.97501	1.03045	-1.04867
H	3.70626	-1.48918	0.35324
C	3.35571	-1.32423	-1.74674
C	2.53037	-0.63910	-2.83041
C	3.03369	0.69829	-3.28247
O	3.77262	1.42728	-2.64609
O	2.57581	1.03590	-4.47463
H	4.40859	-1.35668	-2.03704
H	3.01574	-2.35794	-1.69327
H	2.47037	-1.28084	-3.71007
H	1.49437	-0.50348	-2.50362
H	2.91613	1.91578	-4.69817
O	1.51659	0.46029	0.73647

LD7

N	-1.51875	-0.81197	0.49739
C	-1.59474	0.63606	0.80886
C	-0.16137	1.06332	1.08072
O	0.62271	0.28182	1.58232
H	-0.98306	-0.92864	-0.39245
H	-2.48479	-1.20183	0.47888
H	-0.96602	-1.27536	1.22210
H	-1.94131	1.15020	-0.08816
C	-2.50668	0.93586	1.99809
C	-3.99855	1.02453	1.69849
C	-4.68264	-0.24948	1.29008
O	-4.13554	-1.23604	0.83665
O	-5.98990	-0.18021	1.45364
H	-2.20831	1.90851	2.39242
H	-2.31165	0.21354	2.79494
H	-4.19008	1.74805	0.89940
H	-4.52312	1.41556	2.57095
H	-6.38858	-1.00720	1.14107
O	0.08996	2.27980	0.70141
H	1.07796	2.40425	0.63500
N	3.46809	-2.23092	-1.75729
C	2.49656	-1.31443	-2.33285
C	1.24751	-1.36365	-1.45097
O	1.21135	-2.39280	-0.63797
H	4.02815	-2.69853	-2.45645
H	4.08345	-1.77006	-1.09840
H	2.09815	-2.82948	-0.77156
H	2.13998	-1.76777	-3.26501
C	2.96089	0.09974	-2.69868
C	3.82695	0.84291	-1.67282
C	3.08181	1.09556	-0.40112
O	2.54750	2.14928	-0.12507
O	3.01461	0.01326	0.36478
H	3.54604	0.03002	-3.61649
H	2.07674	0.69486	-2.93354
H	4.73801	0.28310	-1.45419
H	4.11471	1.80491	-2.09121
H	2.35662	0.16226	1.07816
O	0.32534	-0.57303	-1.52712

LD8

N	-1.47415	-1.13884	0.85368
C	-1.35339	0.10790	1.64486
C	-1.78058	-0.20972	3.06274
O	-2.05941	-1.31837	3.43454
H	-0.57933	-1.30394	0.27310
H	-2.30798	-1.08450	0.24065
H	-1.60650	-1.91677	1.50650
H	-0.28432	0.35043	1.67869
C	-2.08260	1.29813	1.02484
C	-3.60490	1.32361	1.11046
C	-4.32541	0.39089	0.18010
O	-3.82629	-0.55267	-0.39738
O	-5.60457	0.70504	0.05366
H	-1.76255	1.38746	-0.01554
H	-1.71020	2.18554	1.53589
H	-3.96682	2.33151	0.90126
H	-3.95936	1.10448	2.12255
H	-6.02346	0.05666	-0.53260
O	-1.78161	0.87181	3.83356
H	-2.01382	0.60226	4.73495
N	4.03827	-0.19278	-0.05066
C	3.10785	-1.23777	-0.57241
C	1.71440	-0.85840	-0.01832
O	1.69975	0.05858	0.82441
H	4.28159	0.47222	-0.82133
H	3.44265	0.29543	0.65835
H	4.88209	-0.57050	0.36824
H	3.38105	-2.18586	-0.10717
C	3.15206	-1.41003	-2.08367
C	2.54358	-0.29761	-2.93013
C	3.35446	0.95860	-3.03358
O	4.22548	1.30374	-2.25621
O	3.01801	1.69441	-4.07792
H	4.17807	-1.60967	-2.40199
H	2.58096	-2.31486	-2.28886
H	2.36890	-0.65854	-3.94432
H	1.55536	-0.01747	-2.55162
H	3.55891	2.49903	-4.07540
O	0.75880	-1.52541	-0.46493

LD9

N	-1.43087	-0.66942	1.39283
C	-1.67569	0.43930	0.43939
C	-0.31918	1.09664	0.22222
O	0.55937	0.99173	1.04679
H	-2.33717	-0.98243	1.79886
H	-0.80047	-0.32518	2.12213
H	-0.91250	-1.41297	0.88194
H	-2.00276	0.00185	-0.50451
C	-2.69916	1.44774	0.95880
C	-4.16663	1.07172	0.79197
C	-4.67061	-0.05907	1.64275
O	-3.98282	-0.90956	2.17326
O	-5.98684	-0.05252	1.74424
H	-2.54380	2.36966	0.39692
H	-2.47756	1.68546	2.00259
H	-4.38252	0.80036	-0.24653
H	-4.79293	1.94071	0.99735
H	-6.26217	-0.81856	2.27124
O	-0.25664	1.74004	-0.91067
H	0.67380	2.07708	-1.07221
N	3.60476	-2.66272	-0.93890
C	2.36612	-2.07060	-1.43075
C	1.34139	-2.10987	-0.29714
O	1.83107	-2.45097	0.86774
H	2.78983	-2.64084	0.67792
H	3.71615	-3.61821	-1.25330
H	4.42550	-2.15099	-1.23403
H	1.92994	-2.64223	-2.25427
C	2.53681	-0.63044	-1.91689
C	3.14345	0.30936	-0.86882
C	3.16881	1.71658	-1.38937
O	2.19074	2.42671	-1.51389
O	4.37806	2.12589	-1.73396
H	3.16340	-0.64720	-2.81168
H	1.55462	-0.26370	-2.21872
H	2.53372	0.32408	0.03717
H	4.15831	0.01783	-0.60229
H	4.31196	3.03456	-2.06699
O	0.17150	-1.82580	-0.46222

LD10

N	-1.22749	0.76480	1.54313
C	-1.76530	0.07167	0.34789
C	-0.79446	0.39368	-0.78055
O	-0.09062	1.37596	-0.73125
H	-1.96930	0.82380	2.27149
H	-0.91943	1.69757	1.25535
H	-0.37370	0.25214	1.84451
H	-1.72861	-1.00126	0.53953
C	-3.18427	0.51651	-0.00273
C	-4.31329	-0.12554	0.79492
C	-4.42053	0.26672	2.24104
O	-3.52887	0.74534	2.91461
O	-5.61745	0.01044	2.73540
H	-3.34621	0.25136	-1.04830
H	-3.24647	1.60672	0.04889
H	-4.23193	-1.21717	0.77362
H	-5.26988	0.10011	0.32216
H	-5.62319	0.24766	3.67565
O	-0.83481	-0.49297	-1.73645
H	-0.11837	-0.31124	-2.41388
N	4.47053	-0.53576	0.74639
C	3.18643	-1.18396	0.50603
C	2.11557	-0.40997	1.27467
O	2.52343	0.72533	1.78224
H	3.49031	0.75888	1.54693
H	5.01798	-1.02983	1.43951
H	5.03490	-0.46681	-0.08988
H	3.15793	-2.20650	0.89173
C	2.80918	-1.24548	-0.97499
C	2.80197	0.12108	-1.66934
C	2.31621	-0.01924	-3.08230
O	1.16257	-0.22941	-3.40048
O	3.28110	0.08531	-3.98047
H	3.51162	-1.91587	-1.47571
H	1.82118	-1.70258	-1.04695
H	2.11244	0.80534	-1.17017
H	3.79264	0.57306	-1.68460
H	2.89328	-0.02449	-4.86279
O	0.97290	-0.80839	1.38516

LD11

N	-1.37271	-1.24920	0.94572
C	-1.32398	-0.17084	1.95844
C	-2.08163	-0.65375	3.17924
O	-2.53866	-1.76094	3.27597
H	-1.67703	-2.11063	1.40715
H	-0.39809	-1.39316	0.49881
H	-2.06900	-1.00692	0.21672
H	-0.27626	-0.04977	2.24692
C	-1.78827	1.18335	1.42724
C	-3.28251	1.38556	1.20205
C	-3.86145	0.70836	-0.00626
O	-3.34498	-0.20285	-0.61997
O	-5.03740	1.21305	-0.34357
H	-1.22514	1.39067	0.51545
H	-1.46333	1.92455	2.15680
H	-3.49640	2.45135	1.10825
H	-3.87292	1.05810	2.06384
H	-5.37670	0.71827	-1.10485
O	-2.15197	0.28198	4.11923
H	-2.60365	-0.09437	4.88967
N	3.86018	0.57238	-0.13483
C	3.23110	-0.76809	-0.32577
C	1.77168	-0.60479	0.16063
O	1.02030	-1.57743	-0.05813
H	3.14014	1.06936	0.44089
H	4.75778	0.53860	0.33771
H	3.95599	1.04695	-1.06290
H	3.71480	-1.46219	0.36287
C	3.35910	-1.32019	-1.73799
C	2.52458	-0.65374	-2.82626
C	3.01273	0.68479	-3.29136
O	3.74564	1.42701	-2.66337
O	2.54829	1.00711	-4.48520
H	4.41168	-1.34453	-2.03018
H	3.02987	-2.35679	-1.67421
H	2.46986	-1.30402	-3.69997
H	1.48779	-0.52627	-2.49878
H	2.87885	1.88847	-4.71740
O	1.50673	0.46958	0.73141

LD12

N	-1.51899	-0.81163	0.49666
C	-1.59493	0.63632	0.80856
C	-0.16152	1.06346	1.08039
O	0.62249	0.28188	1.58198
H	-0.98329	-0.92810	-0.39320
H	-2.48505	-1.20147	0.47809
H	-0.96627	-1.27524	1.22124
H	-1.94163	1.15073	-0.08825
C	-2.50667	0.93578	1.99804
C	-3.99862	1.02436	1.69880
C	-4.68271	-0.24967	1.29045
O	-4.13570	-1.23593	0.83627
O	-5.98987	-0.18077	1.45498
H	-2.20830	1.90839	2.39249
H	-2.31137	0.21333	2.79470
H	-4.19038	1.74791	0.89979
H	-4.52300	1.41530	2.57142
H	-6.38858	-1.00773	1.14235
O	0.08993	2.27992	0.70108
H	1.07794	2.40428	0.63469
N	3.46802	-2.23103	-1.75698
C	2.49672	-1.31446	-2.33280
C	1.24750	-1.36343	-1.45116
O	1.21107	-2.39248	-0.63803
H	4.02811	-2.69882	-2.45601
H	4.08336	-1.77019	-1.09805
H	2.09785	-2.82928	-0.77142
H	2.14027	-1.76780	-3.26500
C	2.96132	0.09964	-2.69864
C	3.82724	0.84277	-1.67264
C	3.08187	1.09552	-0.40110
O	2.54747	2.14927	-0.12526
O	3.01456	0.01331	0.36489
H	3.54665	0.02977	-3.61632
H	2.07728	0.69485	-2.93373
H	4.73822	0.28290	-1.45382
H	4.11516	1.80474	-2.09102
H	2.35642	0.16234	1.07813
O	0.32542	-0.57273	-1.52759

LD13

N	-1.05728	-1.33576	1.04922

C	-1.79750	-0.37171	1.90871
C	-2.07583	-1.11076	3.21145
O	-1.81619	-2.27436	3.36013
H	-1.50020	-1.37522	0.11856
H	-1.08135	-2.24999	1.51975
H	-0.06076	-1.05304	0.86957
H	-1.13834	0.47065	2.13422
C	-3.08929	0.12483	1.25081
C	-2.89142	1.22677	0.21947
C	-2.04568	0.83732	-0.96021
O	-1.89332	-0.33220	-1.30728
O	-1.47733	1.84366	-1.55189
H	-3.72788	0.51989	2.03997
H	-3.61808	-0.72603	0.81440
H	-2.45672	2.11942	0.67075
H	-3.86527	1.53117	-0.17438
H	-0.74570	1.50485	-2.14281
O	-2.62216	-0.31873	4.11635
H	-2.78514	-0.82929	4.92450
N	4.15581	1.55576	0.07114
C	3.49818	0.35114	-0.42471
C	2.12533	0.28100	0.24213
O	1.42673	-0.71727	0.20511
H	4.87270	1.35370	0.75568
H	4.57816	2.09594	-0.67266
H	2.57221	1.95848	0.77874
H	4.01855	-0.56060	-0.11754
C	3.42550	0.38072	-1.95824
C	2.54417	-0.67153	-2.61186
C	1.09296	-0.29019	-2.59226
O	0.72636	0.87057	-2.51124
O	0.26874	-1.30971	-2.68359
H	3.07742	1.36757	-2.27241
H	4.44902	0.26173	-2.31619
H	2.82014	-0.76542	-3.66611
H	2.65893	-1.66091	-2.17048
H	-0.64195	-0.98321	-2.52337
O	1.77047	1.36677	0.87560

LD14

N	-1.67875	-1.43519	1.44493
C	-1.77734	-0.29409	2.38258
C	-1.80858	-0.88194	3.78244
O	-1.89177	-2.06134	3.99612
H	-0.69214	-1.46190	1.01016
H	-2.37294	-1.32964	0.68235
H	-1.85142	-2.29619	1.97315
H	-0.86912	0.30401	2.27502
C	-2.99162	0.59921	2.13026
C	-2.94253	1.40592	0.83638
C	-3.36484	0.65237	-0.38944
O	-3.37166	-0.55630	-0.50349
O	-3.73157	1.45747	-1.37572
H	-3.03619	1.30324	2.96060
H	-3.90560	0.00126	2.17532
H	-1.92829	1.76882	0.64153
H	-3.57827	2.28773	0.91821
H	-3.97576	0.91040	-2.13742
O	-1.73696	0.05862	4.71468
H	-1.77073	-0.36921	5.58351
N	2.55391	1.44824	-0.84764
C	2.36761	-0.02366	-0.67607
C	1.01139	-0.17636	0.05646
O	0.34718	0.87130	0.18977
H	2.87152	1.67173	-1.81590
H	1.59996	1.81114	-0.60694
H	3.21721	1.83495	-0.18219
H	3.16021	-0.41649	-0.03884
C	2.32759	-0.76779	-2.00332
C	3.63741	-0.89225	-2.77188
C	4.06497	0.34215	-3.51197
O	3.66649	1.46958	-3.28637
O	4.95033	0.08335	-4.45618
H	1.98305	-1.77193	-1.75593
H	1.55795	-0.32735	-2.64368
H	4.46471	-1.17517	-2.11276
H	3.56609	-1.69943	-3.50224
H	5.20445	0.91667	-4.88186
O	0.72605	-1.33394	0.41536

LD15

N	-1.82707	-1.40418	1.32170
C	-1.73230	-0.40847	2.41296
C	-1.79744	-1.18364	3.71718

O	-2.03309	-2.36067	3.76881
H	-2.09349	-2.30347	1.73463
H	-0.87149	-1.49389	0.82960
H	-2.53079	-1.10091	0.62361
H	-0.75324	0.07165	2.34069
C	-2.81667	0.66685	2.35274
C	-2.70156	1.63481	1.17914
C	-3.27601	1.12777	-0.10994
O	-3.45821	-0.04035	-0.38612
O	-3.56508	2.10715	-0.95409
H	-2.73078	1.24519	3.27209
H	-3.80369	0.19728	2.36744
H	-1.65367	1.87815	0.97599
H	-3.19923	2.57528	1.41630
H	-3.91502	1.71215	-1.76689
O	-1.56782	-0.40539	4.76618
H	-1.63048	-0.94651	5.56763
N	2.70046	1.19238	-0.75583
C	2.30309	-0.24668	-0.79860
C	0.96571	-0.32007	-0.02074
O	0.46802	0.77652	0.30505
H	1.81931	1.64489	-0.41217
H	3.43403	1.37147	-0.07597
H	3.01800	1.51759	-1.69480
H	3.05013	-0.84381	-0.27522
C	2.10634	-0.75738	-2.21895
C	3.35577	-0.94784	-3.06990
C	3.94409	0.31253	-3.63503
O	3.72910	1.43584	-3.21948
O	4.75106	0.08021	-4.65348
H	1.62129	-1.72724	-2.10783
H	1.39208	-0.11392	-2.74067
H	4.15055	-1.45095	-2.50945
H	3.13758	-1.60851	-3.91014
H	5.11637	0.92432	-4.96044
O	0.52614	-1.46814	0.17700

LD16

N	-1.29934	-1.27586	1.50095
C	-1.21979	0.11238	2.01193
C	-0.65664	0.02366	3.41843
O	-0.48946	-1.01869	3.99319
H	-1.18979	-1.91392	2.29517
H	-0.52619	-1.44985	0.78775
H	-2.21400	-1.42434	1.02931
H	-0.51680	0.65656	1.37742
C	-2.56477	0.83931	1.99915
C	-3.09795	1.19631	0.61520
C	-3.77920	0.07365	-0.10734
O	-3.62771	-1.10920	0.12713
O	-4.58321	0.50457	-1.06615
H	-2.41869	1.76947	2.54755
H	-3.30354	0.25853	2.55793
H	-2.29033	1.53660	-0.04015
H	-3.80778	2.02048	0.68911
H	-4.97405	-0.26629	-1.50436
O	-0.38475	1.22127	3.91865
H	-0.04585	1.10680	4.81927
N	2.10243	-1.79861	-2.35409
C	1.15736	-0.64951	-2.50102
C	0.39023	-0.53906	-1.16222
O	0.55714	-1.52875	-0.38621
H	1.75105	-2.28530	-1.50388
H	2.11473	-2.41973	-3.15721
H	3.06632	-1.42810	-2.17164
H	0.42005	-0.92965	-3.25490
C	1.82787	0.64466	-2.93787
C	2.68312	1.37081	-1.90554
C	4.01199	0.74838	-1.60234
O	4.31201	-0.41416	-1.80682
O	4.85925	1.60251	-1.05814
H	2.40101	0.47272	-3.85220
H	1.01362	1.31781	-3.20387
H	2.86854	2.39415	-2.23375
H	2.14431	1.46651	-0.95760
H	5.68630	1.13580	-0.86244
O	-0.30449	0.45712	-0.98540

LD17

N	-2.12432	-0.81934	0.25737
C	-1.72517	-0.44559	1.63379
C	-2.28709	-1.49230	2.57280
O	-2.84909	-2.48493	2.19364
H	-2.90627	-0.21480	-0.05459

H	-2.45478	-1.78810	0.27325
H	-1.28193	-0.73247	-0.41267
H	-0.63265	-0.53276	1.67311
C	-2.08766	0.99129	2.00364
C	-3.55030	1.30463	2.29984
C	-4.46049	1.36755	1.10740
O	-4.21647	0.91304	0.00900
O	-5.60011	1.98104	1.38434
H	-1.71289	1.64778	1.21537
H	-1.51408	1.23159	2.89840
H	-3.62190	2.26533	2.81214
H	-3.98653	0.58303	2.99767
H	-6.15657	1.96667	0.59085
O	-2.05696	-1.19063	3.84598
H	-2.39161	-1.91583	4.39471
N	3.46599	-0.66789	-0.57961
C	2.33243	-0.57371	-1.54768
C	1.05507	-0.58477	-0.67143
O	-0.02199	-0.64178	-1.29541
H	2.97783	-0.48642	0.33215
H	3.86755	-1.60046	-0.54306
H	4.21467	0.01761	-0.81573
H	2.32962	-1.45614	-2.18795
C	2.37959	0.69674	-2.38428
C	3.46371	0.78838	-3.45096
C	4.83836	1.11100	-2.94047
O	5.21039	0.97549	-1.79023
O	5.63622	1.56252	-3.89095
H	1.41038	0.74613	-2.88075
H	2.43123	1.56580	-1.72214
H	3.54311	-0.14128	-4.02395
H	3.20279	1.55342	-4.18358
H	6.51086	1.73132	-3.50803
O	1.24703	-0.51619	0.55805

LD18

N	-1.81982	-1.29055	0.82855
C	-1.34562	-0.41092	1.92221
C	-1.01943	-1.31724	3.09499
O	-1.28050	-2.49045	3.10936
H	-2.66553	-0.87664	0.38748
H	-2.02847	-2.21073	1.22801
H	-1.06788	-1.38350	0.07874
H	-0.43000	0.07583	1.57930
C	-2.36035	0.66234	2.31730
C	-2.56806	1.77051	1.29005
C	-3.48276	1.41783	0.15631
O	-3.76556	0.28960	-0.19605
O	-3.96500	2.48829	-0.45448
H	-1.98340	1.12358	3.22970
H	-3.31342	0.19227	2.57423
H	-1.61784	2.06689	0.83553
H	-2.97194	2.65927	1.77557
H	-4.52931	2.19291	-1.18474
O	-0.42651	-0.65687	4.08024
H	-0.25693	-1.27694	4.80538
N	1.63208	-1.16192	-3.01462
C	1.14547	0.17589	-2.55779
C	0.31552	-0.07383	-1.27638
O	0.05727	-1.29620	-1.05611
H	1.52487	-1.31403	-4.01276
H	2.63832	-1.27250	-2.74082
H	1.04762	-1.82517	-2.46530
H	0.44505	0.54112	-3.31044
C	2.25186	1.20635	-2.38664
C	3.18243	1.03971	-1.19036
C	4.18862	-0.06589	-1.29359
O	4.10411	-1.03282	-2.02926
O	5.20953	0.09954	-0.47275
H	2.83107	1.28254	-3.31010
H	1.74205	2.16082	-2.26025
H	3.73086	1.96627	-1.01723
H	2.60661	0.87139	-0.27482
H	5.80831	-0.65721	-0.56718
O	-0.02432	0.90547	-0.61927

LD19

N	-1.66381	-1.15809	0.99961
C	-1.59546	0.09758	1.78194
C	-1.88269	-0.24867	3.22790
O	-2.02214	-1.37598	3.62113
H	-0.82108	-1.22612	0.32765
H	-2.55699	-1.19342	0.47503

H	-1.64647	-1.94361	1.65585
H	-0.55229	0.43318	1.73605
C	-2.47083	1.21485	1.21756
C	-3.97758	1.11675	1.43059
C	-4.69407	0.10544	0.58309
O	-4.17050	-0.81080	-0.01605
O	-6.00099	0.31329	0.56028
H	-2.24606	1.31600	0.15355
H	-2.13340	2.13724	1.68946
H	-4.43830	2.08632	1.23500
H	-4.22643	0.89489	2.47308
H	-6.41245	-0.38188	0.02462
O	-1.93105	0.83400	3.99627
H	-2.06623	0.54970	4.91274
N	3.65936	0.21154	-0.29743
C	2.67220	-0.64505	-1.02028
C	1.36401	-0.52971	-0.19899
O	0.43785	-1.28196	-0.55847
H	3.03529	0.74088	0.36018
H	4.31212	-0.33447	0.25767
H	4.19322	0.80798	-0.96491
H	3.01104	-1.68112	-1.00292
C	2.43148	-0.18220	-2.45009
C	3.55246	-0.41445	-3.45555
C	4.70054	0.54919	-3.36854
O	4.96322	1.24399	-2.40516
O	5.42921	0.56620	-4.46971
H	1.55550	-0.73779	-2.78517
H	2.14422	0.87319	-2.44637
H	3.97070	-1.42229	-3.36480
H	3.15971	-0.35912	-4.47182
H	6.16403	1.18665	-4.34633
O	1.37764	0.31587	0.71634

LD20

N	-1.64354	-1.15698	1.02877
C	-1.60119	0.12324	1.77226
C	-1.87702	-0.18506	3.22899
O	-1.99076	-1.30266	3.65673
H	-2.53636	-1.22749	0.50714
H	-1.60872	-1.92142	1.70881
H	-0.80017	-1.22788	0.35798
H	-0.56575	0.48007	1.71311
C	-2.50265	1.20316	1.17703
C	-4.00633	1.07806	1.39751
C	-4.70196	0.02592	0.58293
O	-4.15930	-0.89576	0.00970
O	-6.01331	0.20341	0.55818
H	-2.28278	1.27701	0.10974
H	-2.18476	2.14670	1.61979
H	-4.48906	2.03078	1.17414
H	-4.24775	0.88229	2.44695
H	-6.41026	-0.51657	0.04479
O	-1.94702	0.91916	3.96430
H	-2.07360	0.65997	4.88941
N	3.65382	0.27217	-0.30189
C	2.68405	-0.62241	-1.00195
C	1.37175	-0.50655	-0.18734
O	1.36805	0.36517	0.70327
H	3.01853	0.80908	0.33866
H	4.31457	-0.24586	0.27031
H	4.17900	0.85837	-0.98512
H	3.04107	-1.65137	-0.95361
C	2.43947	-0.20565	-2.44523
C	3.56723	-0.44775	-3.44069
C	4.69885	0.53708	-3.37860
O	4.94628	1.26464	-2.43558
O	5.43141	0.53329	-4.47732
H	1.57419	-0.78591	-2.76607
H	2.13402	0.84426	-2.47303
H	4.00196	-1.44542	-3.31998
H	3.17672	-0.42823	-4.45916
H	6.15538	1.16931	-4.37011
O	0.45994	-1.28516	-0.52680

LL1

N	-1.53442	-0.46522	0.96513
C	-1.56479	-0.18872	2.42586
C	-2.83058	-0.85979	2.94715
O	-3.62133	-1.39650	2.21947

H	-1.43950	0.42184	0.44906
H	-2.40768	-0.94740	0.71461
H	-0.71767	-1.03818	0.64130
H	-0.71057	-0.68205	2.89528
C	-1.54712	1.31045	2.73509
C	-0.18467	1.97569	2.61790
C	0.40547	2.02939	1.23684
O	-0.25120	1.78949	0.22177
O	1.66151	2.34093	1.22949
H	-1.88573	1.43166	3.76343
H	-2.28140	1.81552	2.10229
H	0.54830	1.50351	3.27496
H	-0.25675	3.01102	2.96293
H	2.05966	2.19696	0.31811
O	-2.92455	-0.77130	4.26147
H	-3.73867	-1.21222	4.54996
N	0.42239	-1.60208	-3.87879
C	1.15353	-1.93324	-2.66489
C	0.24529	-1.59179	-1.48476
O	-1.01198	-1.40413	-1.82161
H	0.60068	-2.25129	-4.63258
H	0.62523	-0.66486	-4.20383
H	-0.99493	-1.45777	-2.81933
H	1.21402	-3.02619	-2.61076
C	2.58819	-1.41691	-2.52592
C	2.83746	0.05825	-2.86162
C	2.14737	0.98094	-1.90805
O	2.71587	1.55275	-0.99933
O	0.84476	1.07112	-2.12856
H	3.21772	-2.00704	-3.19307
H	2.92581	-1.62467	-1.50914
H	2.51599	0.28877	-3.87928
H	3.90555	0.25437	-2.79815
H	0.41974	1.53682	-1.36753
O	0.61001	-1.55212	-0.32490

LL2

N	-0.38393	1.37694	1.05999
C	-1.06533	0.24386	1.72797
C	-2.55230	0.52942	1.70588
O	-3.03471	1.46723	1.12847
H	0.34793	1.01218	0.35519
H	0.06218	1.98379	1.77284
H	-1.09335	1.92835	0.56922
H	-0.89839	-0.63473	1.09296
C	-0.50516	-0.07314	3.11304
C	-0.85327	0.87272	4.25744
C	-0.13732	2.19258	4.25581
O	0.43734	2.68186	3.30537
O	-0.20513	2.79614	5.43141
H	0.57861	-0.17488	3.02403
H	-0.88297	-1.06027	3.37795
H	-0.63602	0.38845	5.21073
H	-1.92541	1.09017	4.29271
H	0.24747	3.65066	5.36408
O	-3.24396	-0.38958	2.36982
H	-4.18670	-0.18413	2.27987
N	1.78948	-2.82965	-2.06006
C	2.25982	-1.43181	-1.82627
C	1.22091	-0.80618	-0.86575
O	0.37912	-1.59359	-0.39355
H	2.51581	-3.52915	-1.94519
H	1.36605	-2.89936	-3.01534
H	1.03950	-2.93145	-1.33679
H	3.20175	-1.48568	-1.27879
C	2.48662	-0.63286	-3.10163
C	1.25095	-0.20661	-3.88677
C	0.57323	-1.28920	-4.67136
O	0.67834	-2.48416	-4.46271
O	-0.18842	-0.81239	-5.63900
H	3.18201	-1.16812	-3.75263
H	2.99398	0.27819	-2.78613
H	1.51341	0.58842	-4.58555
H	0.49911	0.23201	-3.22297
H	-0.61818	-1.55579	-6.08922
O	1.34890	0.41779	-0.65910

LL3

N	-2.03762	-0.52806	1.09453
C	-0.99287	-0.24692	2.10509
C	-0.89815	-1.47861	2.98771
O	0.11344	-1.39819	3.84182
H	-1.58023	-0.68137	0.13093
H	-2.53877	-1.37465	1.38111

H	0.11828	-2.20013	4.38584
H	-0.04525	-0.12077	1.57498
C	-1.26698	1.00912	2.93189
C	-1.15341	2.32348	2.16605
C	-2.36933	2.69282	1.36961
O	-3.23035	1.91933	1.00331
O	-2.41173	3.98552	1.08294
H	-0.52489	1.02328	3.72947
H	-2.24503	0.92877	3.41346
H	-0.31712	2.29228	1.46041
H	-0.94783	3.14345	2.85455
H	-3.20971	4.15321	0.55913
O	-1.66017	-2.40412	2.90589
H	-2.68902	0.27565	1.02420
N	1.71858	1.24003	-2.68112
C	0.60663	0.25034	-2.79644
C	0.01194	0.13276	-1.37329
O	-0.81654	-0.78512	-1.21168
H	2.63468	0.73101	-2.68103
H	1.54892	1.65467	-1.73691
H	1.71085	1.94930	-3.40717
H	-0.16875	0.69660	-3.42092
C	1.02012	-1.07714	-3.41522
C	1.88458	-2.00467	-2.56859
C	3.31930	-1.59978	-2.41581
O	3.75745	-0.47485	-2.57693
O	4.09590	-2.60777	-2.06332
H	1.49262	-0.89942	-4.38432
H	0.08926	-1.60635	-3.61607
H	1.87130	-3.00959	-2.99205
H	1.46709	-2.11304	-1.56251
H	5.00172	-2.27846	-1.95776
O	0.41209	0.97539	-0.54577

LL4

N	-2.04108	-0.29325	0.84770
C	-1.45784	-0.28828	2.21095
C	-2.49410	-0.92712	3.11897
O	-3.59964	-1.21699	2.74593
H	-1.54683	-0.99734	0.21561
H	-1.89777	0.63198	0.40727
H	-3.03666	-0.52393	0.92921
H	-0.56359	-0.91584	2.19325
C	-1.08429	1.11546	2.69093
C	0.18219	1.69686	2.07830
C	0.07129	2.14857	0.65381
O	-0.88504	1.97727	-0.07640
O	1.16648	2.77219	0.24335
H	-0.92369	1.04914	3.76666
H	-1.93128	1.79081	2.54226
H	1.00192	0.97483	2.11313
H	0.51220	2.55896	2.66180
H	1.05838	2.99670	-0.69542
O	-2.02846	-1.11417	4.34473
H	-2.72699	-1.51847	4.88120
N	0.73119	-2.29263	-2.85301
C	1.57200	-2.01802	-1.64572
C	0.59028	-1.52643	-0.55358
O	-0.62226	-1.80493	-0.79789
H	1.03896	-3.09373	-3.39638
H	0.71550	-1.43321	-3.43829
H	-0.21898	-2.43194	-2.45332
H	1.95342	-2.98100	-1.30241
C	2.74920	-1.09438	-1.94122
C	2.48203	0.40340	-1.89922
C	1.47095	0.91981	-2.87006
O	0.86367	0.26566	-3.69122
O	1.27931	2.23503	-2.75197
H	3.19696	-1.37859	-2.89692
H	3.50449	-1.29627	-1.18260
H	3.40999	0.95018	-2.08646
H	2.16711	0.69448	-0.89589
H	0.62428	2.50379	-3.41497
O	1.05568	-0.94060	0.41892

LL5

N	-1.88482	0.04767	0.58332
C	-0.78406	0.55127	1.44183
C	0.30880	-0.50093	1.34785
O	0.02436	-1.66644	1.16370
H	-2.73413	0.62665	0.75632
H	-2.06914	-0.92724	0.82905
H	-1.55932	0.04503	-0.41047

H	-0.40661	1.46933	0.98984
C	-1.22214	0.78514	2.88701
C	-1.92648	2.10640	3.17311
C	-3.29140	2.28723	2.57131
O	-3.73226	1.67868	1.61551
O	-3.98204	3.22589	3.18961
H	-0.31921	0.77261	3.49953
H	-1.82816	-0.05974	3.22444
H	-1.32134	2.95020	2.82607
H	-2.02033	2.24388	4.25084
H	-4.83636	3.33132	2.74277
O	1.51008	-0.00642	1.44396
H	2.13862	-0.64085	1.00971
N	2.71380	0.66499	-2.93313
C	1.46543	-0.04176	-3.17462
C	0.51747	0.32140	-2.02929
O	0.87999	1.39481	-1.36556
H	3.34691	0.12222	-2.35633
H	3.18603	0.93200	-3.78570
H	1.77059	1.62030	-1.75721
H	0.98532	0.43530	-4.03686
C	1.52391	-1.54145	-3.48470
C	2.49355	-2.37497	-2.63671
C	2.18072	-2.24049	-1.18097
O	2.64247	-1.33417	-0.50122
O	1.32051	-3.12574	-0.73651
H	1.82347	-1.66221	-4.52627
H	0.51370	-1.94349	-3.39513
H	3.52353	-2.05672	-2.79595
H	2.40601	-3.41794	-2.93706
H	0.99484	-2.84458	0.14425
O	-0.50733	-0.28120	-1.77533

LL6

N	-0.77785	0.76638	3.54771
C	-1.33148	-0.37600	2.76184
C	-0.52215	-0.39132	1.44459
O	-0.91157	-1.20936	0.58509
H	-1.45874	1.56182	3.53747
H	-0.53156	0.52406	4.50192
H	1.77512	3.03815	-0.97299
H	-1.09441	-1.29689	3.29577
C	-2.83704	-0.30978	2.54877
C	-3.35819	0.77046	1.60598
C	-3.38708	2.15953	2.16833
O	-2.70497	2.55980	3.09435
O	-4.24110	2.94497	1.53806
H	-3.34457	-0.24598	3.51418
H	-3.10929	-1.27181	2.11589
H	-4.37097	0.52469	1.28554
H	-2.76619	0.80900	0.68549
H	-4.19178	3.83123	1.92792
O	0.43015	0.40749	1.38166
H	0.06780	1.02419	2.98451
N	0.38531	-0.93135	-1.65658
C	1.59916	-0.12207	-1.42563
C	1.14542	1.32657	-1.38975
O	0.05573	1.68309	-1.74991
H	-0.23683	-0.40956	-2.27653
H	-0.15292	-1.08672	-0.72350
H	0.65078	-1.83214	-2.09247
H	1.98207	-0.35948	-0.43145
C	2.67488	-0.33312	-2.49357
C	3.52802	-1.58780	-2.35005
C	2.85808	-2.88748	-2.69418
O	1.66035	-3.06903	-2.76382
O	3.73553	-3.85471	-2.90816
H	3.35270	0.51827	-2.43256
H	2.21740	-0.29475	-3.48578
H	3.90920	-1.68782	-1.32877
H	4.41449	-1.50353	-2.98025
H	3.25044	-4.67200	-3.09896
O	2.10806	2.12904	-0.95715

LL7

N	-1.89900	0.24895	0.42367
C	-1.05499	0.49773	1.60875
C	-0.07627	-0.65902	1.69672
O	0.83778	-0.44951	2.63477
H	-1.33685	0.44077	-0.49430
H	-2.16317	-0.73576	0.40077
H	1.42837	-1.21603	2.66090
H	-0.45618	1.38914	1.40895

C	-1.86446	0.65778	2.89804
C	-2.46697	2.03568	3.14443
C	-3.61847	2.42827	2.26331
O	-3.90674	1.91405	1.20269
O	-4.30404	3.44038	2.76984
H	-1.18772	0.45828	3.72845
H	-2.64085	-0.11092	2.93991
H	-1.70772	2.81704	3.03758
H	-2.80924	2.10744	4.17777
H	-5.01316	3.67126	2.15055
O	-0.14807	-1.64402	1.01075
H	-2.74918	0.83594	0.48982
N	3.05852	0.72469	-2.07855
C	1.68995	0.56153	-2.65332
C	0.72517	0.72984	-1.45930
O	-0.48317	0.55567	-1.72162
H	2.84451	1.03471	-1.10026
H	3.62898	1.40515	-2.56992
H	3.54069	-0.20384	-2.04492
H	1.51083	1.38534	-3.34446
C	1.48394	-0.75466	-3.39072
C	1.45222	-2.02421	-2.54343
C	2.78988	-2.52374	-2.08929
O	3.79275	-1.84301	-1.96880
O	2.78403	-3.81410	-1.80751
H	2.22251	-0.85148	-4.18989
H	0.51123	-0.66407	-3.87296
H	0.97263	-2.82914	-3.10081
H	0.84007	-1.89138	-1.64398
H	3.66820	-4.06633	-1.50037
O	1.25195	1.00357	-0.36528

LL8

N	-1.88484	0.04748	0.58339
C	-0.78413	0.55104	1.44199
C	0.30878	-0.50111	1.34797
O	0.02443	-1.66663	1.16384
H	-2.73414	0.62648	0.75635
H	-2.06919	-0.92744	0.82904
H	-1.55931	0.04488	-0.41040
H	-0.40667	1.46913	0.99007
C	-1.22236	0.78485	2.88713
C	-1.92643	2.10626	3.17323
C	-3.29115	2.28753	2.57108
O	-3.73211	1.67885	1.61542
O	-3.98145	3.22673	3.18893
H	-0.31954	0.77205	3.49981
H	-1.82864	-0.05991	3.22438
H	-1.32096	2.94996	2.82652
H	-2.02057	2.24359	4.25096
H	-4.83570	3.33239	2.74203
O	1.51002	-0.00646	1.44400
H	2.13864	-0.64079	1.00973
N	2.71352	0.66520	-2.93323
C	1.46526	-0.04177	-3.17460
C	0.51730	0.32123	-2.02922
O	0.87964	1.39470	-1.36550
H	3.34684	0.12252	-2.35659
H	3.18555	0.93244	-3.78585
H	1.77018	1.62037	-1.75714
H	0.98498	0.43519	-4.03679
C	1.52398	-1.54145	-3.48469
C	2.49374	-2.37486	-2.63672
C	2.18090	-2.24041	-1.18098
O	2.64253	-1.33402	-0.50126
O	1.32079	-3.12575	-0.73649
H	1.82355	-1.66214	-4.52626
H	0.51383	-1.94365	-3.39512
H	3.52368	-2.05648	-2.79596
H	2.40633	-3.41783	-2.93709
H	0.99511	-2.84459	0.14427
O	-0.50738	-0.28157	-1.77523

LL9

N	-0.77785	0.76638	3.54771
C	-1.33148	-0.37600	2.76184
C	-0.52215	-0.39132	1.44459
O	-0.91157	-1.20936	0.58509
H	-1.45874	1.56181	3.53747
H	-0.53156	0.52406	4.50192
H	1.77511	3.03815	-0.97299
H	-1.09441	-1.29689	3.29577
C	-2.83704	-0.30978	2.54877

C	-3.35819	0.77046	1.60597
C	-3.38708	2.15953	2.16833
O	-2.70497	2.55980	3.09435
O	-4.24109	2.94497	1.53806
H	-3.34458	-0.24598	3.51418
H	-3.10929	-1.27181	2.11588
H	-4.37096	0.52469	1.28553
H	-2.76619	0.80900	0.68549
H	-4.19178	3.83123	1.92792
O	0.43015	0.40749	1.38166
H	0.06780	1.02419	2.98451
N	0.38531	-0.93135	-1.65658
C	1.59916	-0.12207	-1.42563
C	1.14541	1.32657	-1.38975
O	0.05573	1.68309	-1.74990
H	-0.23683	-0.40957	-2.27653
H	-0.15292	-1.08672	-0.72350
H	0.65078	-1.83214	-2.09247
H	1.98207	-0.35948	-0.43145
C	2.67488	-0.33311	-2.49357
C	3.52802	-1.58780	-2.35005
C	2.85808	-2.88748	-2.69418
O	1.66035	-3.06903	-2.76382
O	3.73554	-3.85471	-2.90816
H	3.35269	0.51827	-2.43256
H	2.21740	-0.29475	-3.48578
H	3.90920	-1.68782	-1.32877
H	4.41449	-1.50353	-2.98025
H	3.25044	-4.67200	-3.09895
O	2.10806	2.12904	-0.95715

LL10

N	-1.89950	0.24933	0.42282
C	-1.05558	0.49727	1.60812
C	-0.07675	-0.65944	1.69540
O	0.83698	-0.45056	2.63392
H	-1.33703	0.44094	-0.49508
H	-2.16455	-0.73512	0.39961
H	1.42757	-1.21710	2.65978
H	-0.45682	1.38887	1.40893
C	-1.86519	0.65641	2.89744
C	-2.46699	2.03436	3.14522
C	-3.61745	2.42906	2.26368
O	-3.90569	1.91612	1.20242
O	-4.30213	3.44155	2.77068
H	-1.18876	0.45565	3.72782
H	-2.64201	-0.11193	2.93832
H	-1.70710	2.81534	3.04023
H	-2.81015	2.10484	4.17836
H	-5.01065	3.67375	2.15118
O	-0.14816	-1.64388	1.00859
H	-2.74917	0.83704	0.48897
N	3.05826	0.72539	-2.07888
C	1.68979	0.56150	-2.65369
C	0.72484	0.73023	-1.45987
O	-0.48341	0.55542	-1.72223
H	2.84410	1.03611	-1.10086
H	3.62864	1.40555	-2.57073
H	3.54058	-0.20305	-2.04449
H	1.51051	1.38487	-3.34532
C	1.48421	-0.75516	-3.39040
C	1.45265	-2.02428	-2.54244
C	2.79037	-2.52320	-2.08780
O	3.79297	-1.84205	-1.96733
O	2.78492	-3.81345	-1.80546
H	2.22295	-0.85223	-4.18940
H	0.51157	-0.66506	-3.87286
H	0.97334	-2.82962	-3.09949
H	0.84032	-1.89115	-1.64314
H	3.66913	-4.06520	-1.49804
O	1.25137	1.00486	-0.36596

LL11

N	-1.79217	-0.00154	0.73955
C	-0.99282	0.54064	1.85745
C	-0.01202	-0.55133	2.24735
O	-0.11242	-1.68821	1.87113
H	-1.90475	-1.00687	0.88526
H	-1.26543	0.12853	-0.20297
H	-2.71690	0.46355	0.71852
H	-0.40420	1.37905	1.48099
C	-1.84356	0.96229	3.05769
C	-2.55054	2.30756	2.94206

C	-3.74091	2.35263	2.02687
O	-3.99702	1.54321	1.15996
O	-4.50379	3.40872	2.25905
H	-1.17092	1.03088	3.91263
H	-2.56281	0.17280	3.29127
H	-1.85970	3.08644	2.60386
H	-2.88778	2.63147	3.92769
H	-5.23857	3.40111	1.62681
O	0.91997	-0.09888	3.07432
H	1.50306	-0.83620	3.30682
N	3.04972	0.61821	-1.99963
C	1.65374	0.53477	-2.52252
C	0.75387	0.47314	-1.26640
O	1.33110	0.63330	-0.17548
H	3.53233	-0.30063	-2.13905
H	2.88599	0.77641	-0.97636
H	3.59508	1.36893	-2.41058
H	1.42962	1.47305	-3.03126
C	1.42305	-0.61308	-3.49477
C	1.44195	-2.02565	-2.91893
C	2.80038	-2.57828	-2.60880
O	3.79912	-1.91524	-2.39459
O	2.81619	-3.89808	-2.57423
H	2.12278	-0.53617	-4.33030
H	0.42744	-0.44724	-3.90500
H	0.95727	-2.71421	-3.61154
H	0.85370	-2.08263	-1.99708
H	3.71073	-4.19064	-2.34151
O	-0.45979	0.27520	-1.48428

LL12

N	-1.41471	1.77071	1.43631
C	-1.85470	0.46632	1.98082
C	-3.37054	0.44702	1.89495
O	-4.02105	1.40401	1.57120
H	-0.94414	1.62191	0.47741
H	-0.72965	2.21151	2.07734
H	-2.24195	2.36608	1.32979
H	-1.45780	-0.31617	1.32910
C	-1.37661	0.20897	3.40948
C	0.12719	-0.00092	3.55818
C	0.93164	1.26295	3.62550
O	0.57122	2.34690	3.21474
O	2.11906	1.07765	4.18369
H	-1.87532	-0.70016	3.74384
H	-1.71810	1.01465	4.06456
H	0.52488	-0.57782	2.71697
H	0.34005	-0.57731	4.45869
H	2.58872	1.92540	4.18244
O	-3.86872	-0.73853	2.21938
H	-4.83461	-0.69112	2.15771
N	2.29586	-1.12720	-1.61298
C	1.34332	-0.05312	-2.02467
C	0.53796	0.28539	-0.74559
O	0.73709	-0.46204	0.23330
H	2.31478	-1.89653	-2.31760
H	1.91273	-1.40237	-0.67665
H	3.23982	-0.77654	-1.47787
H	1.90463	0.82921	-2.33296
C	0.39822	-0.50150	-3.13040
C	0.99167	-0.68739	-4.52149
C	1.77352	-1.95368	-4.71972
O	2.24494	-2.63470	-3.82823
O	1.91500	-2.26541	-5.99453
H	-0.36214	0.27747	-3.18767
H	-0.11845	-1.41389	-2.81892
H	1.65148	0.14381	-4.79107
H	0.19813	-0.67585	-5.26993
H	2.44416	-3.07529	-6.06020
O	-0.23858	1.25362	-0.84491

LL13

N	-2.31606	-0.42329	1.26215
C	-1.36851	-0.16106	2.36884
C	-1.48325	-1.33260	3.32798
O	-2.31374	-2.19358	3.21482
H	-2.88569	0.42193	1.07325
H	-2.91599	-1.20757	1.53616
H	-1.76706	-0.67608	0.36908
H	-0.36021	-0.15211	1.94717
C	-1.61725	1.16707	3.08290
C	-1.31354	2.41138	2.25409
C	-2.41154	2.82469	1.32002
O	-3.29276	2.09865	0.90782
O	-2.32031	4.09785	0.96417
H	-0.96242	1.17801	3.95361

H	-2.64285	1.19795	3.45983
H	-0.42183	2.26002	1.63720
H	-1.09926	3.25679	2.90816
H	-3.04701	4.29333	0.35349
O	-0.56742	-1.27854	4.28576
H	-0.69296	-2.04010	4.87164
N	1.89909	0.84858	-2.21062
C	0.96558	-0.31717	-2.21984
C	0.08424	-0.13930	-0.95861
O	0.42344	0.78006	-0.18638
H	1.75750	1.22524	-1.24243
H	2.87481	0.54428	-2.42017
H	1.62568	1.56862	-2.87326
H	0.33110	-0.26542	-3.10493
C	1.69542	-1.65165	-2.15957
C	2.45385	-2.08804	-3.40696
C	3.77416	-1.40729	-3.62496
O	4.11499	-0.35604	-3.11557
O	4.55397	-2.07290	-4.45633
H	0.91998	-2.39099	-1.95874
H	2.36270	-1.66192	-1.29292
H	1.85887	-1.93417	-4.31318
H	2.64509	-3.16146	-3.37049
H	5.37856	-1.57664	-4.57467
O	-0.85240	-0.95155	-0.84352

LL14

N	-1.58622	-0.95119	1.21326
C	-1.22319	-0.21830	2.44798
C	-1.51327	-1.15601	3.60662
O	-1.05012	-0.68052	4.75398
H	-0.70382	-1.29659	0.72604
H	-2.17415	-1.74751	1.47759
H	-1.27486	-1.30661	5.45873
H	-0.15081	-0.01729	2.41276
C	-1.97533	1.10312	2.60933
C	-1.55760	2.21413	1.65221
C	-2.13215	2.11382	0.27186
O	-2.59561	1.10921	-0.23071
O	-2.08243	3.26663	-0.37815
H	-1.77752	1.45062	3.62307
H	-3.05180	0.92339	2.54418
H	-0.47112	2.23938	1.52883
H	-1.84743	3.18344	2.05907
H	-2.46050	3.13337	-1.26012
O	-2.10110	-2.19608	3.47553
H	-2.09010	-0.31435	0.56466
N	2.80832	-1.95299	-1.29988
C	2.69253	-0.55973	-0.76972
C	1.31063	-0.46665	-0.08095
O	0.72418	-1.58318	0.05929
H	2.03102	-2.45249	-0.82024
H	3.70443	-2.38872	-1.10481
H	2.63041	-1.94330	-2.33296
H	3.43956	-0.44723	0.01735
C	2.92743	0.51773	-1.81825
C	1.83221	0.72690	-2.85842
C	1.73505	-0.32253	-3.92380
O	2.16928	-1.45710	-3.84017
O	1.09882	0.10436	-4.99945
H	3.89015	0.35317	-2.30821
H	3.01757	1.44949	-1.26094
H	1.97447	1.68659	-3.35646
H	0.85115	0.79335	-2.37699
H	1.04582	-0.62423	-5.63706
O	0.92412	0.64289	0.27293

LL15

N	-1.97952	0.24195	1.02372
C	-1.46004	-0.26812	2.31361
C	-2.60382	-1.01847	2.97269
O	-3.72976	-0.99568	2.55289
H	-3.00251	0.19236	1.05142
H	-1.60921	-0.35620	0.22330
H	-1.65830	1.21982	0.87909
H	-0.65375	-0.97022	2.09299
C	-0.92598	0.83392	3.22896
C	0.37982	1.48084	2.77891
C	0.23594	2.52342	1.71213
O	-0.70978	2.63654	0.95738
O	1.27827	3.33857	1.66024
H	-0.74697	0.37070	4.19893
H	-1.69870	1.59215	3.38165

H	1.07204	0.73245	2.38192
H	0.87765	1.94621	3.62998
H	1.12707	3.97846	0.94860
O	-2.20463	-1.67854	4.05070
H	-2.97229	-2.12443	4.43928
N	0.40620	-2.42000	-2.70336
C	1.29755	-1.96711	-1.59158
C	0.40555	-1.16728	-0.61301
O	-0.83793	-1.26642	-0.84541
H	-0.54813	-2.25306	-2.32252
H	0.53748	-3.39410	-2.95800
H	0.56073	-1.80618	-3.53910
H	1.62541	-2.85782	-1.05359
C	2.52775	-1.20542	-2.06213
C	2.31156	0.21021	-2.58563
C	1.69653	0.31501	-3.94811
O	1.04114	-0.55247	-4.49660
O	1.92509	1.48369	-4.51907
H	3.07393	-1.80260	-2.79633
H	3.17100	-1.12494	-1.18655
H	3.26277	0.74281	-2.61404
H	1.67995	0.78274	-1.89868
H	1.48159	1.49877	-5.38120
O	0.96231	-0.54257	0.28453

LL16

N	-1.60297	-0.93172	1.20467
C	-1.22151	-0.23011	2.45199
C	-1.54940	-1.17447	3.59504
O	-2.17025	-2.19261	3.44538
H	-2.21768	-1.71244	1.45419
H	-0.73096	-1.29759	0.71382
H	-2.08241	-0.26845	0.56426
H	-0.14273	-0.06526	2.42485
C	-1.92958	1.11344	2.62934
C	-1.46616	2.22510	1.69463
C	-2.02634	2.16445	0.30617
O	-2.52470	1.18614	-0.21456
O	-1.92094	3.32194	-0.32892
H	-1.72899	1.43744	3.65028
H	-3.01093	0.97154	2.55245
H	-0.37803	2.21912	1.58481
H	-1.73129	3.19662	2.11312
H	-2.29461	3.21498	-1.21632
O	-1.07793	-0.73108	4.75182
H	-1.32719	-1.35957	5.44610
N	2.73998	-2.01506	-1.36020
C	2.67365	-0.63244	-0.79497
C	1.30336	-0.51413	-0.08735
O	0.68461	-1.61530	0.03380
H	2.54895	-1.97437	-2.39004
H	1.95375	-2.50227	-0.88235
H	3.62470	-2.48254	-1.18792
H	3.43300	-0.56231	-0.01481
C	2.92907	0.46285	-1.81999
C	1.82661	0.73312	-2.83805
C	1.67830	-0.28676	-3.92591
O	2.07934	-1.43547	-3.87764
O	1.03565	0.18518	-4.97879
H	3.87886	0.27952	-2.32818
H	3.05751	1.37705	-1.24153
H	1.99398	1.69905	-3.31593
H	0.85557	0.82100	-2.34002
H	0.94906	-0.52564	-5.63258
O	0.95467	0.59805	0.29637

LL17

N	-1.90558	0.06516	0.87196
C	-1.06760	0.46372	2.02654
C	-1.36377	-0.49749	3.15855
O	-2.08053	-1.45534	3.04000
H	-2.28638	-0.86587	1.06274
H	-1.31212	0.03690	-0.03011
H	-2.69853	0.72513	0.77234
H	-0.02639	0.29537	1.72608
C	-1.20763	1.93765	2.40202
C	-2.48189	2.37349	3.11722
C	-3.71347	2.46129	2.26278
O	-3.85114	1.95242	1.16980
O	-4.67177	3.16564	2.84350
H	-1.06000	2.53222	1.49788
H	-0.36884	2.16758	3.05846
H	-2.33069	3.35585	3.56742

H	-2.72146	1.71503	3.95803
H	-5.44727	3.16552	2.26203
O	-0.71862	-0.16649	4.27149
H	-0.90540	-0.84045	4.94224
N	3.13694	0.06994	-1.71729
C	1.76048	-0.17883	-2.24073
C	0.82781	-0.00376	-1.01637
O	1.40267	0.13143	0.08103
H	3.48347	0.99302	-1.96228
H	3.80413	-0.65046	-2.06827
H	2.97403	0.04651	-0.68053
H	1.51439	0.57682	-2.98703
C	1.59922	-1.57798	-2.81833
C	2.29188	-1.86950	-4.14392
C	3.77087	-2.11210	-4.05440
O	4.48431	-1.77007	-3.13024
O	4.24353	-2.74424	-5.11294
H	0.52616	-1.70433	-2.96241
H	1.89815	-2.31645	-2.06891
H	2.14249	-1.05671	-4.86225
H	1.84710	-2.74905	-4.61141
H	5.20144	-2.85204	-5.00833
O	-0.39299	-0.04153	-1.26336

LL18

N	-1.92168	0.13581	0.82623
C	-1.09191	0.42001	2.01992
C	-1.47158	-0.58330	3.08871
O	-2.23864	-1.48956	2.89994
H	-2.67189	0.84639	0.74585
H	-2.36095	-0.77987	0.95604
H	-1.30745	0.12114	-0.06209
H	-0.05479	0.20739	1.73369
C	-1.15650	1.87664	2.47494
C	-2.42136	2.34614	3.18541
C	-3.62366	2.55326	2.31017
O	-3.76191	2.11559	1.18686
O	-4.55499	3.27837	2.90899
H	-0.95231	2.51048	1.60931
H	-0.32270	2.02045	3.16157
H	-2.22567	3.29145	3.69402
H	-2.71958	1.65723	3.98191
H	-5.31408	3.35616	2.31129
O	-0.83739	-0.35275	4.23283
H	-1.07968	-1.05063	4.85995
N	3.18052	-0.02626	-1.63713
C	1.80652	-0.16299	-2.20631
C	0.85291	0.00411	-0.99712
O	-0.36075	0.05433	-1.27508
H	2.98814	-0.09416	-0.60739
H	3.58794	0.88558	-1.82349
H	3.81295	-0.76663	-2.01016
H	1.62635	0.64418	-2.91661
C	1.57795	-1.51776	-2.86182
C	2.28798	-1.78175	-4.18395
C	3.74701	-2.11778	-4.07199
O	4.45385	-1.86890	-3.11362
O	4.21026	-2.72060	-5.15159
H	0.50361	-1.57067	-3.03840
H	1.81162	-2.31106	-2.14600
H	2.20648	-0.92543	-4.86146
H	1.80478	-2.60744	-4.70812
H	5.15687	-2.89163	-5.02983
O	1.40472	0.04545	0.11952

LL19

N	-0.82657	1.41897	1.31935
C	-1.13606	0.17584	2.06251
C	-2.62916	0.15375	2.31403
O	-3.38591	0.97229	1.86412
H	-0.16750	1.20519	0.49097
H	-0.39913	2.11125	1.96165
H	-1.70670	1.80763	0.96964
H	-0.91498	-0.65445	1.38085
C	-0.28367	-0.01220	3.31592
C	-0.60825	0.84464	4.53483
C	-0.19580	2.28591	4.45070
O	0.08729	2.88037	3.43139
O	-0.18010	2.86806	5.63925
H	0.76399	0.11390	3.03417
H	-0.39684	-1.05523	3.61030
H	-0.12611	0.42177	5.41759
H	-1.67769	0.83077	4.76730

H	0.06460	3.79850	5.52138
O	-2.99103	-0.88508	3.05869
H	-3.95633	-0.87618	3.14314
N	1.54055	-2.28782	-2.24907
C	1.54317	-0.79429	-2.23744
C	0.74009	-0.40186	-0.97218
O	0.17943	-1.34372	-0.37907
H	1.32155	-2.65187	-3.20120
H	0.81393	-2.50114	-1.52174
H	2.42483	-2.67940	-1.93789
H	2.56723	-0.43463	-2.13484
C	0.88516	-0.19834	-3.47394
C	1.64063	-0.31694	-4.79193
C	1.57572	-1.66590	-5.44807
O	1.28881	-2.70674	-4.88741
O	1.87883	-1.61755	-6.73232
H	0.76253	0.86094	-3.24802
H	-0.12297	-0.60866	-3.58178
H	2.70023	-0.06861	-4.67144
H	1.25664	0.41047	-5.50847
H	1.84111	-2.51623	-7.09439
O	0.72547	0.81460	-0.70255

LL20

N	-1.52081	-0.67370	1.44363
C	-1.40418	-0.01069	2.76719
C	-2.59615	-0.48789	3.58620
O	-3.42853	-1.23139	3.14141
H	-1.57145	0.05624	0.69843
H	-2.35521	-1.27194	1.45509
H	-0.66305	-1.21771	1.20459
H	-0.49896	-0.37638	3.25832
C	-1.35360	1.51124	2.65511
C	-0.10085	2.07138	1.99712
C	-0.03324	1.94804	0.49703
O	-0.83129	1.30941	-0.17625
O	0.98200	2.59306	-0.00380
H	-1.40890	1.90233	3.67039
H	-2.24632	1.86548	2.13279
H	0.80626	1.61311	2.40200
H	-0.01024	3.13434	2.22839
H	1.03886	2.47598	-0.99276
O	-2.57940	0.00573	4.81203
H	-3.34895	-0.33175	5.29574
N	1.74682	-2.99339	-2.58358
C	2.04923	-2.04558	-1.51638
C	0.87646	-2.05542	-0.54000
O	-0.18179	-2.69780	-0.97223
H	2.22911	-3.87373	-2.45302
H	2.00313	-2.64243	-3.49719
H	0.11039	-3.07114	-1.85018
H	2.93770	-2.32607	-0.94509
C	2.25884	-0.62012	-2.03083
C	1.03888	-0.04894	-2.76199
C	1.34990	1.32577	-3.27547
O	1.37462	2.32758	-2.59249
O	1.63467	1.34604	-4.56807
H	3.12833	-0.62821	-2.69241
H	2.50672	0.01496	-1.17927
H	0.19591	0.05477	-2.07563
H	0.73943	-0.67800	-3.59960
H	1.84346	2.25854	-4.82239
O	0.89920	-1.48372	0.53218