Distinguishing Isomeric Peptides: The Unimolecular Reactivity and Structures of (LeuPro)M^+ and (ProLeu)M^+ (M = alkali metal)

Yasaman Jami-Alahmadi, Bryan D. Linford, and Travis D. Fridgen*

Department of Chemistry, Memorial University, St. John's, NL, A1N 4T8

*tfridgen@mun.ca

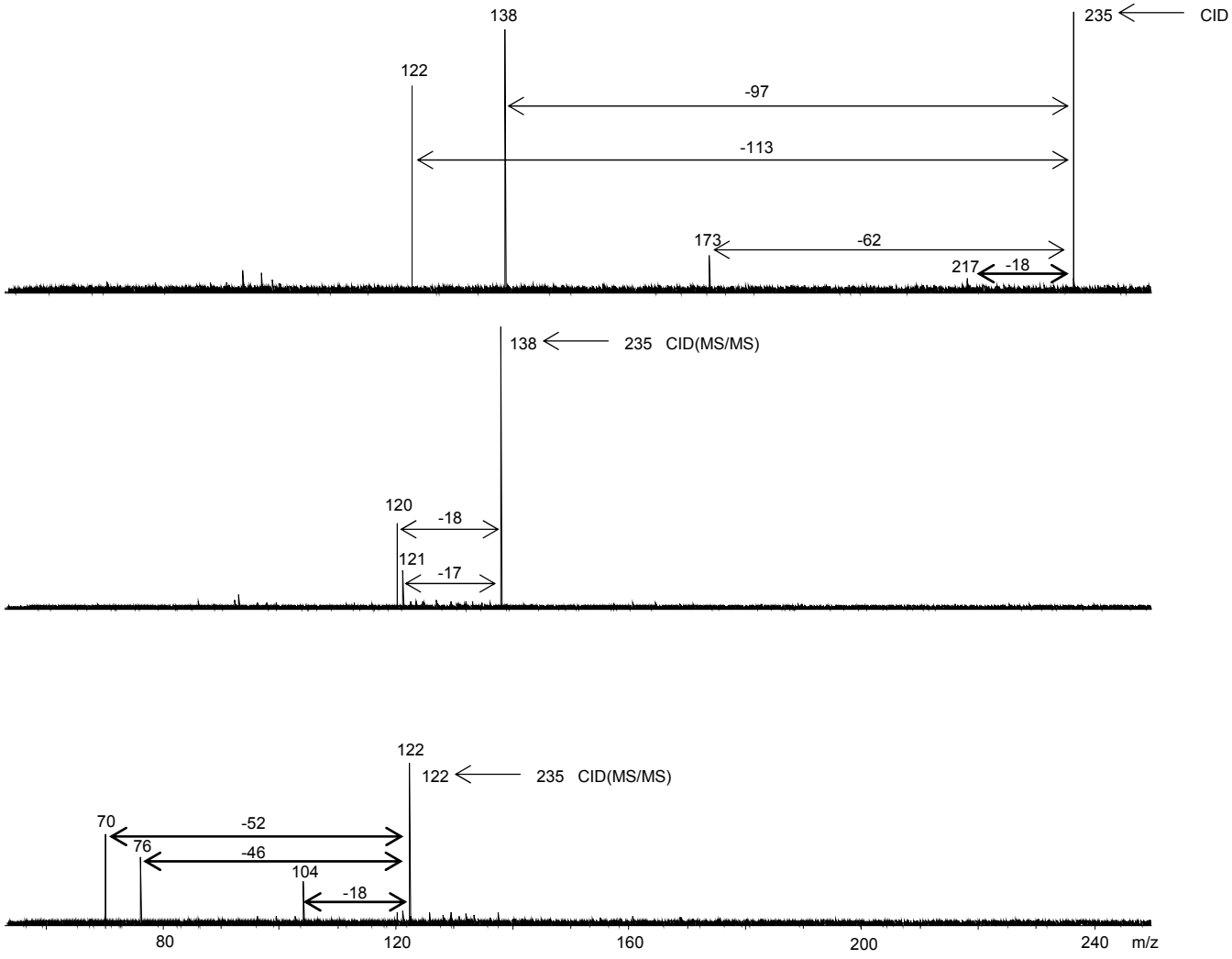

Figure S1. SORI/CID MS/MS spectra of **[Li(ProLeu)]**$^+$

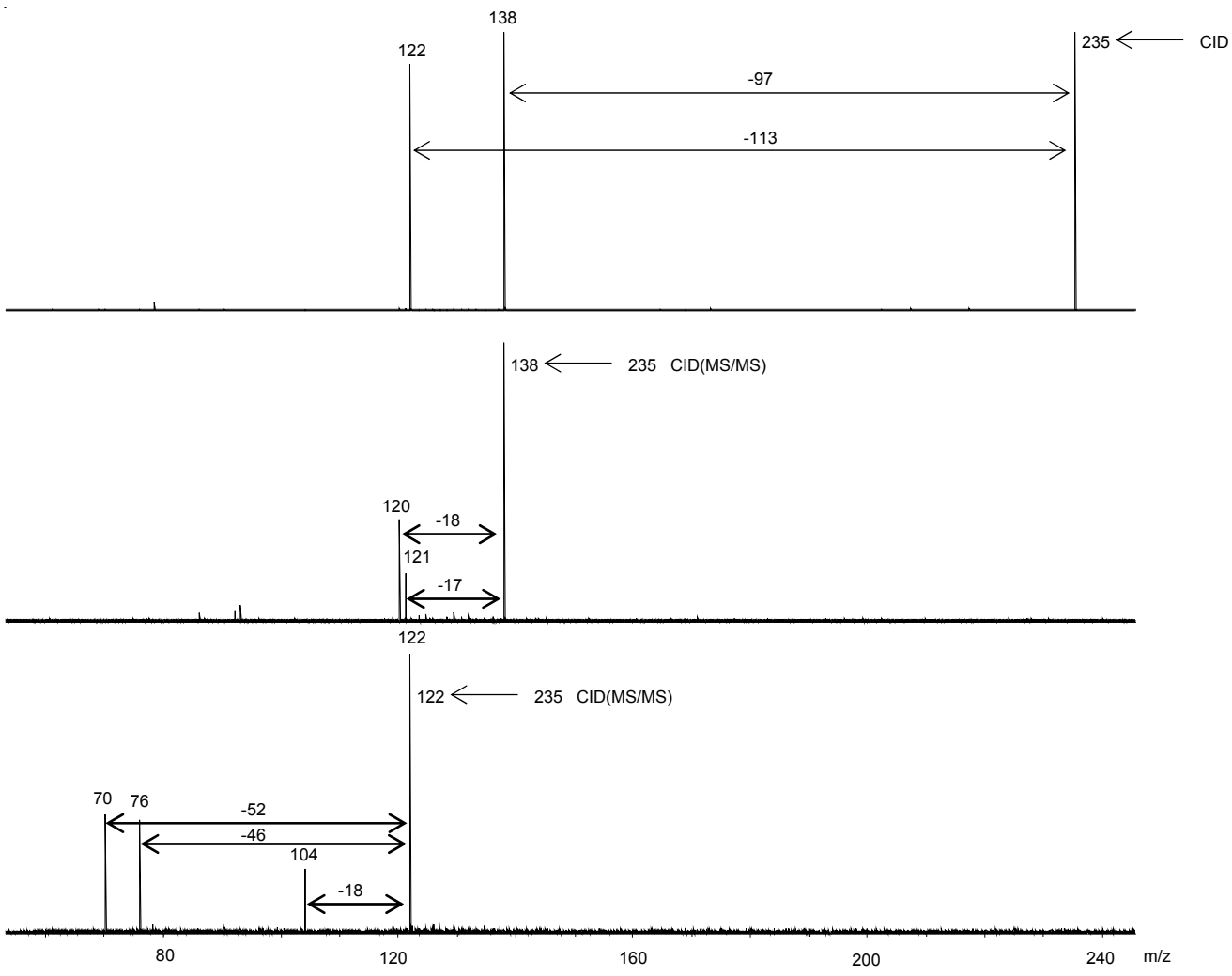

Figure S2. SORI/CID MS/MS spectra of [Li(LeuPro)]$^+$

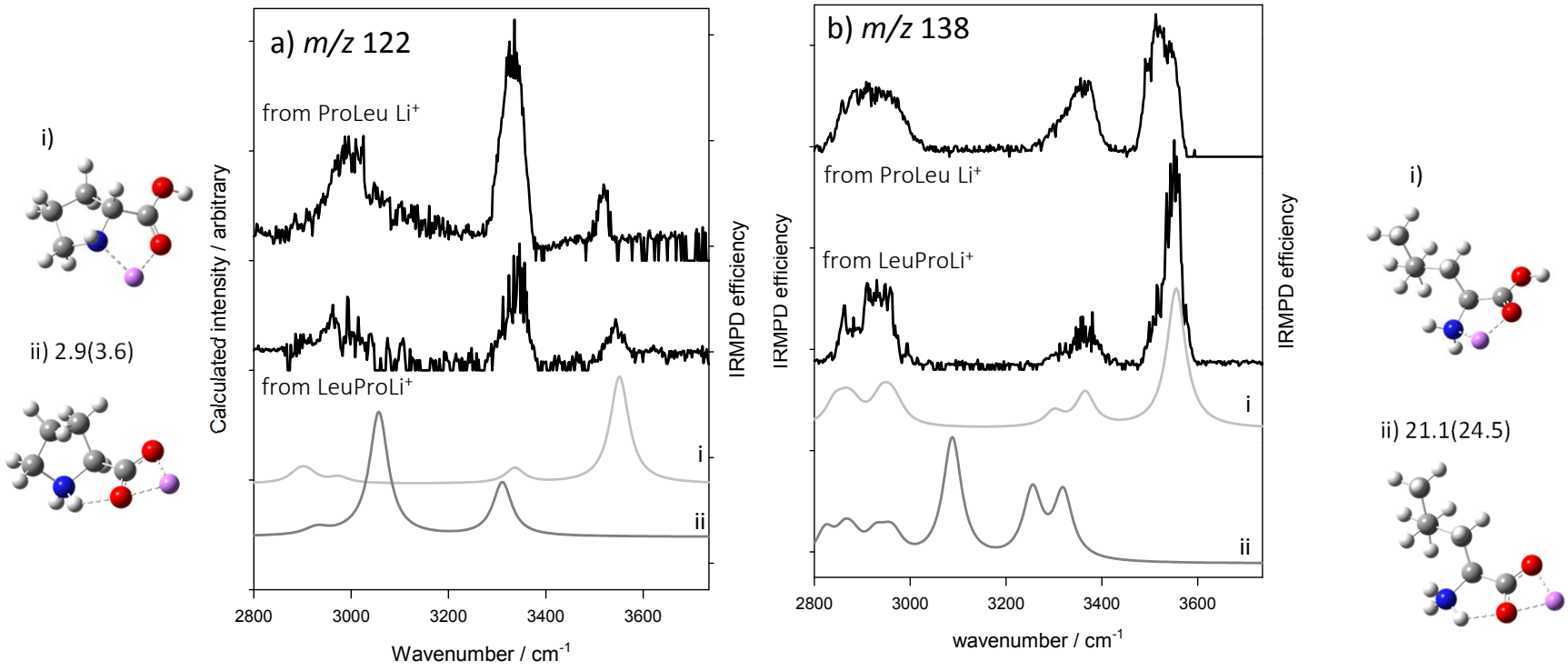

Figure S3. Comparison of the experimental IRMPD spectra of the a) m/z 122 and b) m/z 138 fragment ions from CID of (ProLeu)-Li^+ and (LeuPro)-Li^+ with the calculated spectra of proline-Li^+ and leucine-Li^+**.** Energies are M06-2XD3/6-31+G(d,p) 298 K Gibbs energies (and enthalpies) and in kJ mol^{-1}.

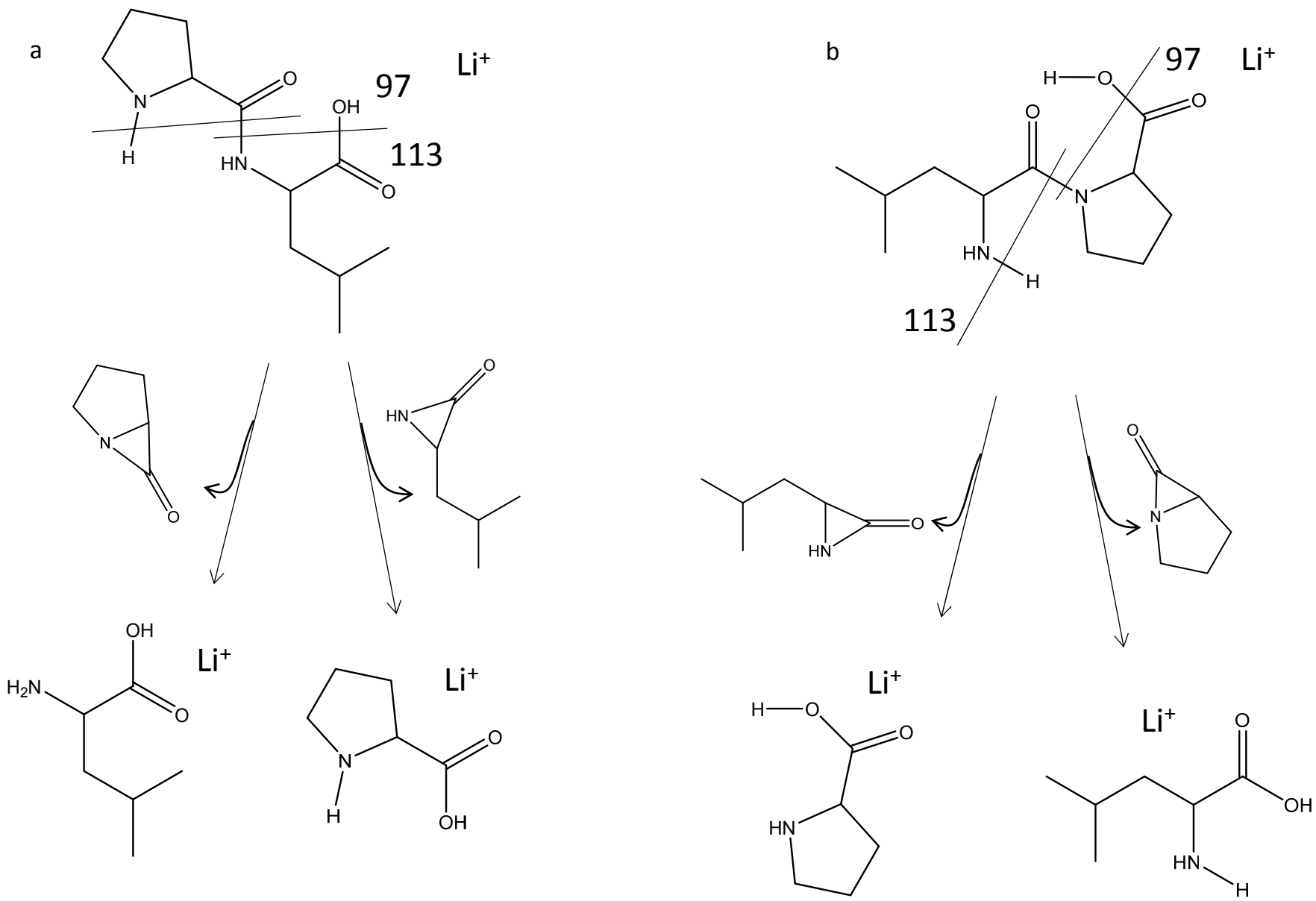

Figure S4. Proposed mechanism for the dissociation of (ProLeu)Li^+ and (LeuPro)Li^+ forming (Pro)Li^+ (m/z 122) and (Leu)Li^+ (m/z 138).

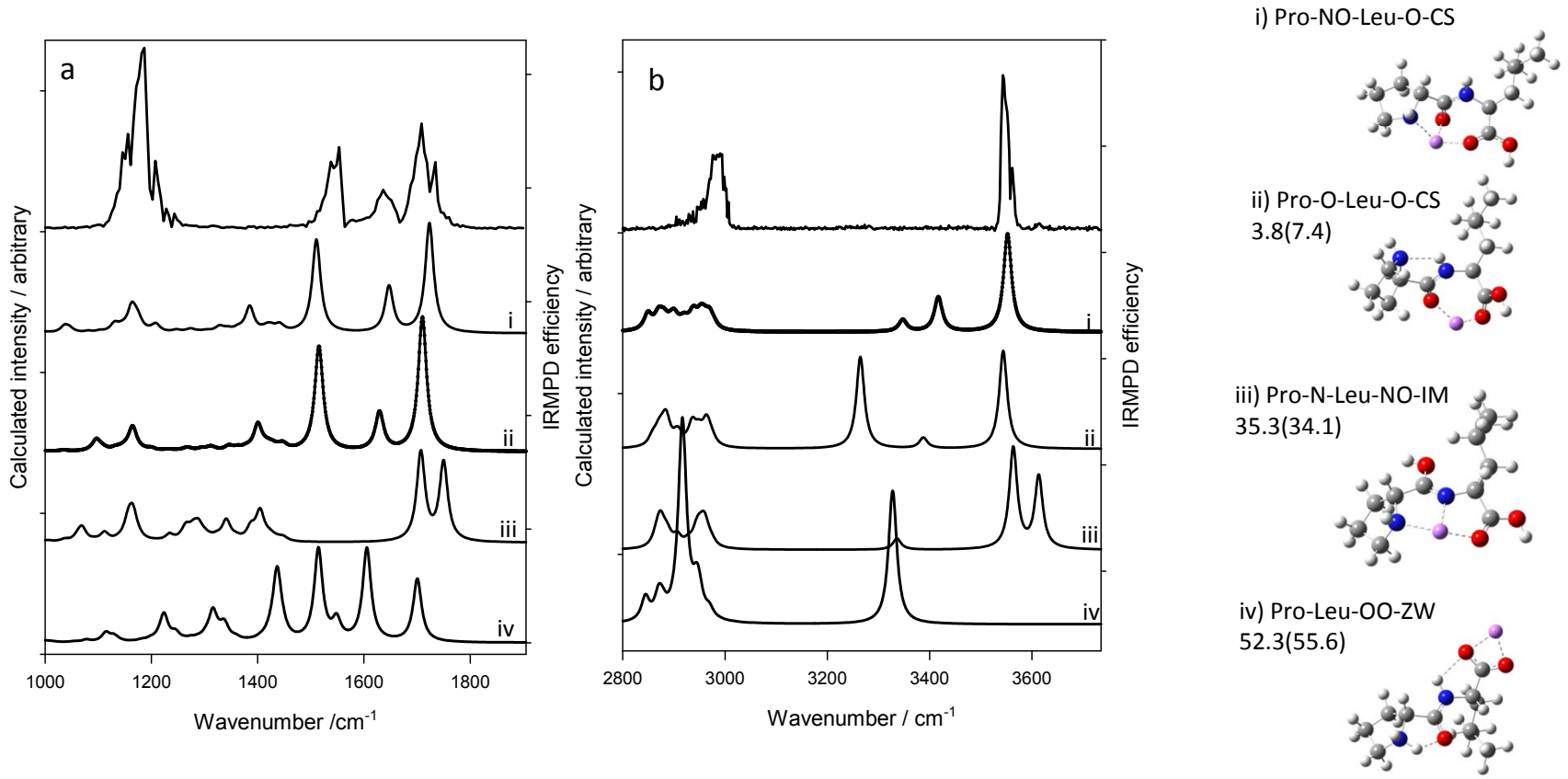

Figure S5. Comparison of the experimental IRMPD spectrum and calculated IR spectra of the lowest energy structures of each form of the (ProLeu)-Li^+ complex a) from 1000 to 1900 cm^{-1}, b) from 2700 to 3800 cm^{-1}.
Energies are M06-2XD3/6-311++G(3df,3pd)//6- 31+G(d,p), 298 K Gibbs energies (and enthalpies) and in kJ mol^{-1}.

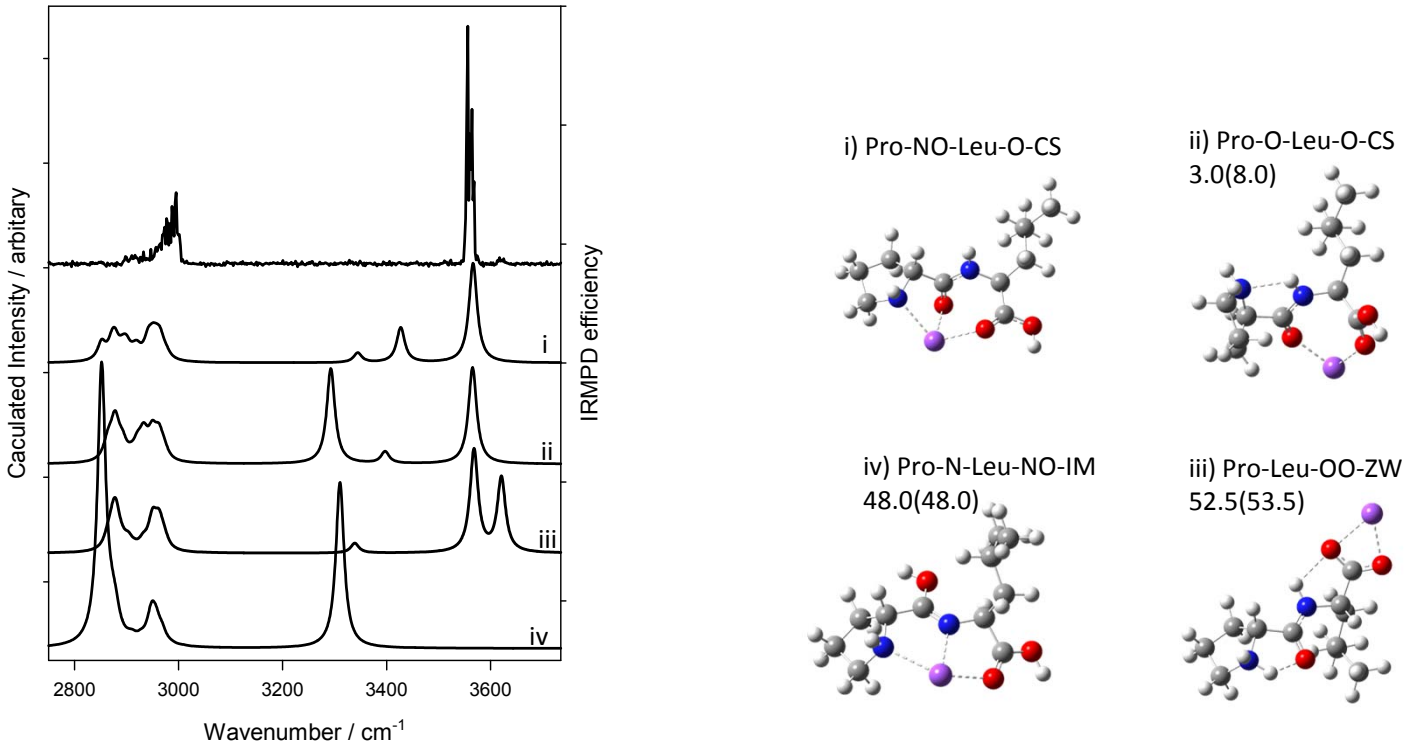

Figure S6. Comparison of the experimental IRMPD spectrum and calculated IR spectra of the lowest energy structures of each form of the (ProLeu)-Na^+ complex from 2700 to 3800 cm^{-1}.
Energies are M06-2XD3/6-311++G(3df,3pd)//6- 31+G(d,p), 298 K Gibbs energies (and enthalpies) and in kJ mol^{-1}.

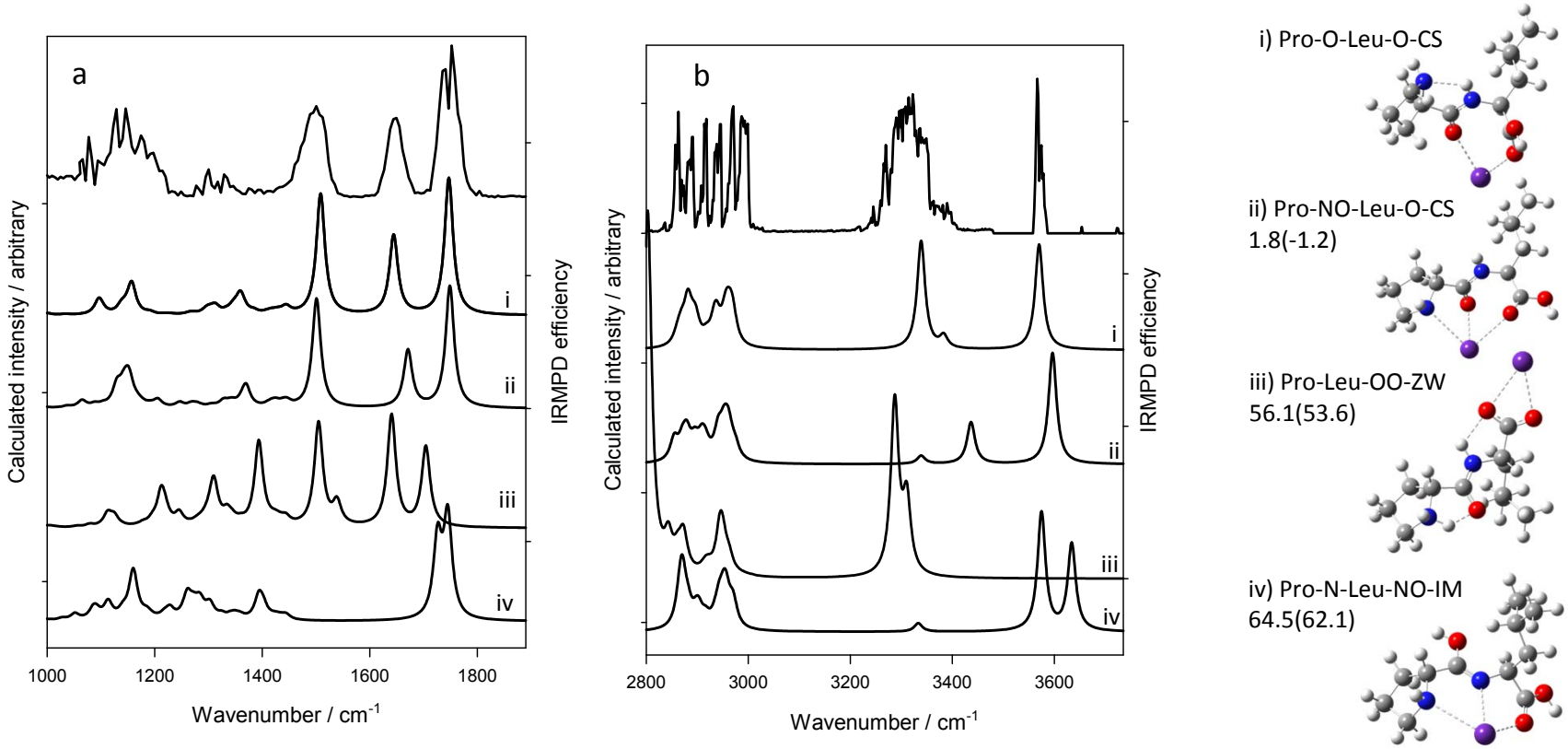

Figure S7. Comparison of the experimental IRMPD spectrum and calculated IR spectra of the lowest energy structures of each form of the (ProLeu)-Rb^+ complex a) from 1000 to 1900 cm^{-1}, b) from 2700 to 3800 cm^{-1}.
Energies are M06-2XD3/6-311++G(3df,3pd)//6- 31+G(d,p), 298 K Gibbs energies (and enthalpies) and in kJ mol^{-1}.

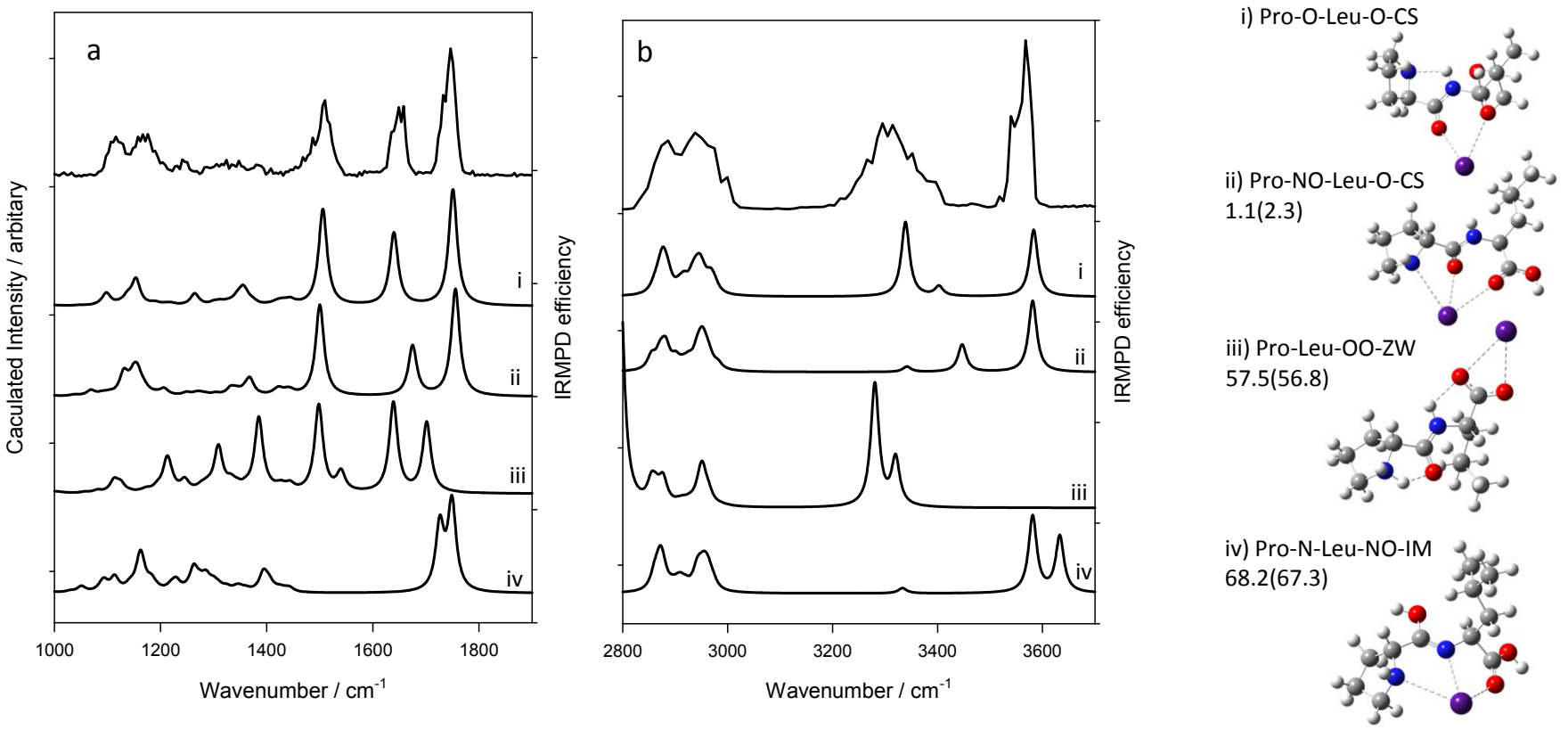

Figure S8. Comparison of the experimental IRMPD spectrum and calculated IR spectra of the lowest energy structures of each form of the (ProLeu)-Cs^+ complex a) from 1000 to 1900 cm^{-1}, b) from 2700 to 3800 cm^{-1}.
Energies are M06-2XD3/6-311++G(3df,3pd)//6- 31+G(d,p), 298 K Gibbs energies (and enthalpies) and in kJ mol^{-1}.

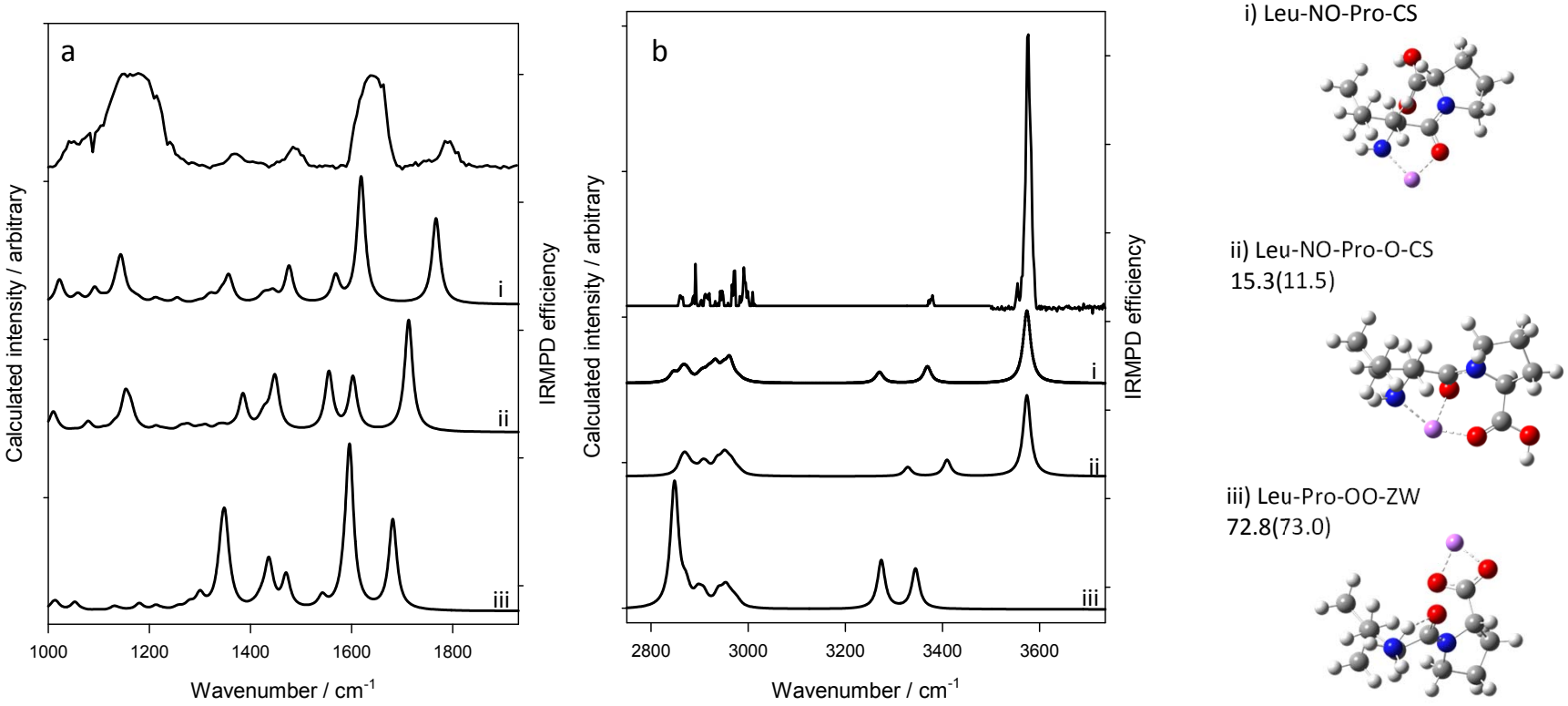

Figure S9. Comparison of the experimental IRMPD spectrum and calculated IR spectra of the lowest energy structures of each form of the (LeuPro)-Li^+ complex a) from 1000 to 1900 cm^{-1}, b) from 2700 to 3800 cm^{-1}.
Energies are M06-2XD3/6-311++G(3df,3pd)//6- 31+G(d,p), 298 K Gibbs energies (and enthalpies) and in kJ mol^{-1}.

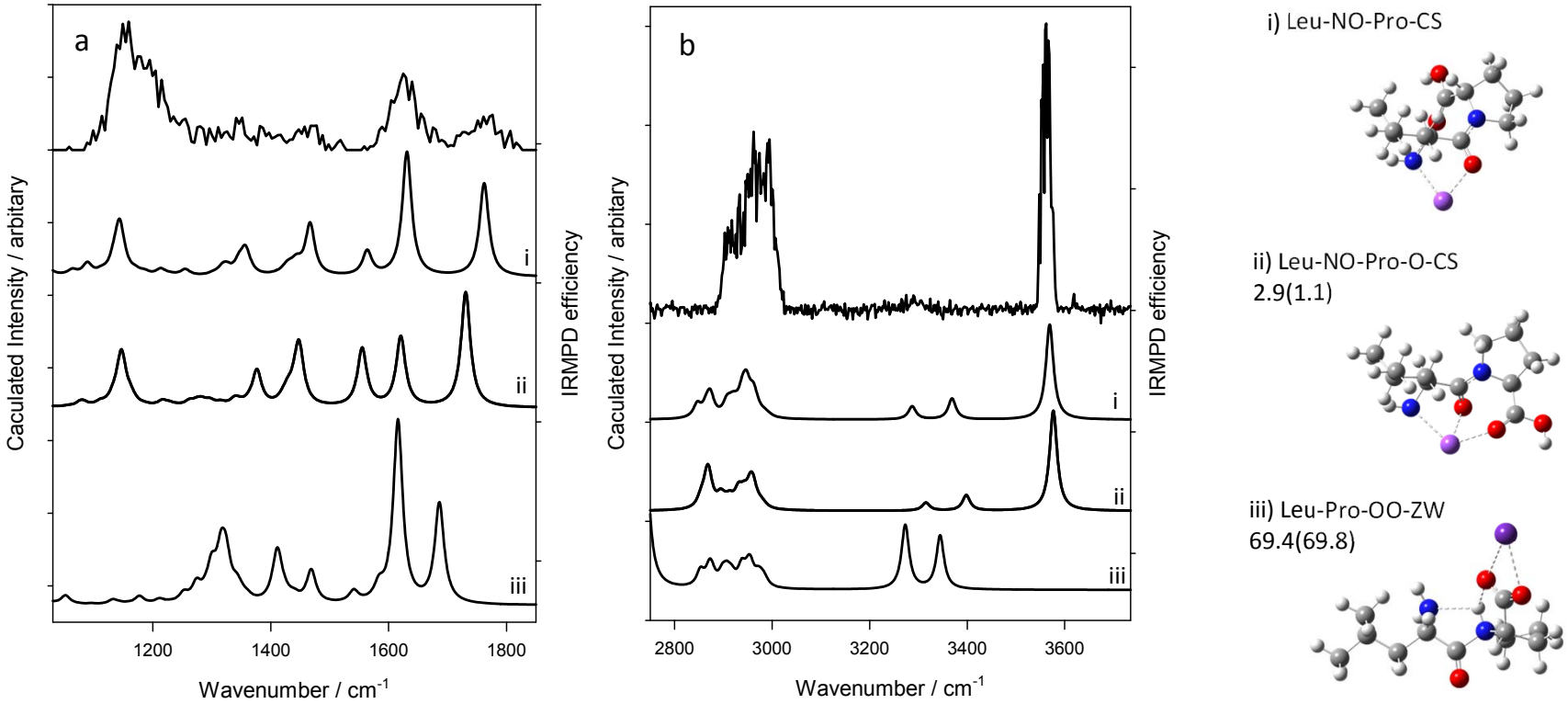

Figure S10. Comparison of the experimental IRMPD spectrum and calculated IR spectra of the lowest energy structures of each form of the (LeuPro)-Na^+ complex from 2700 to 3800 cm^{-1}.
Energies are M06-2XD3/6-311++G(3df,3pd)//6- 31+G(d,p), 298 K Gibbs energies (and enthalpies) and in kJ mol^{-1}.

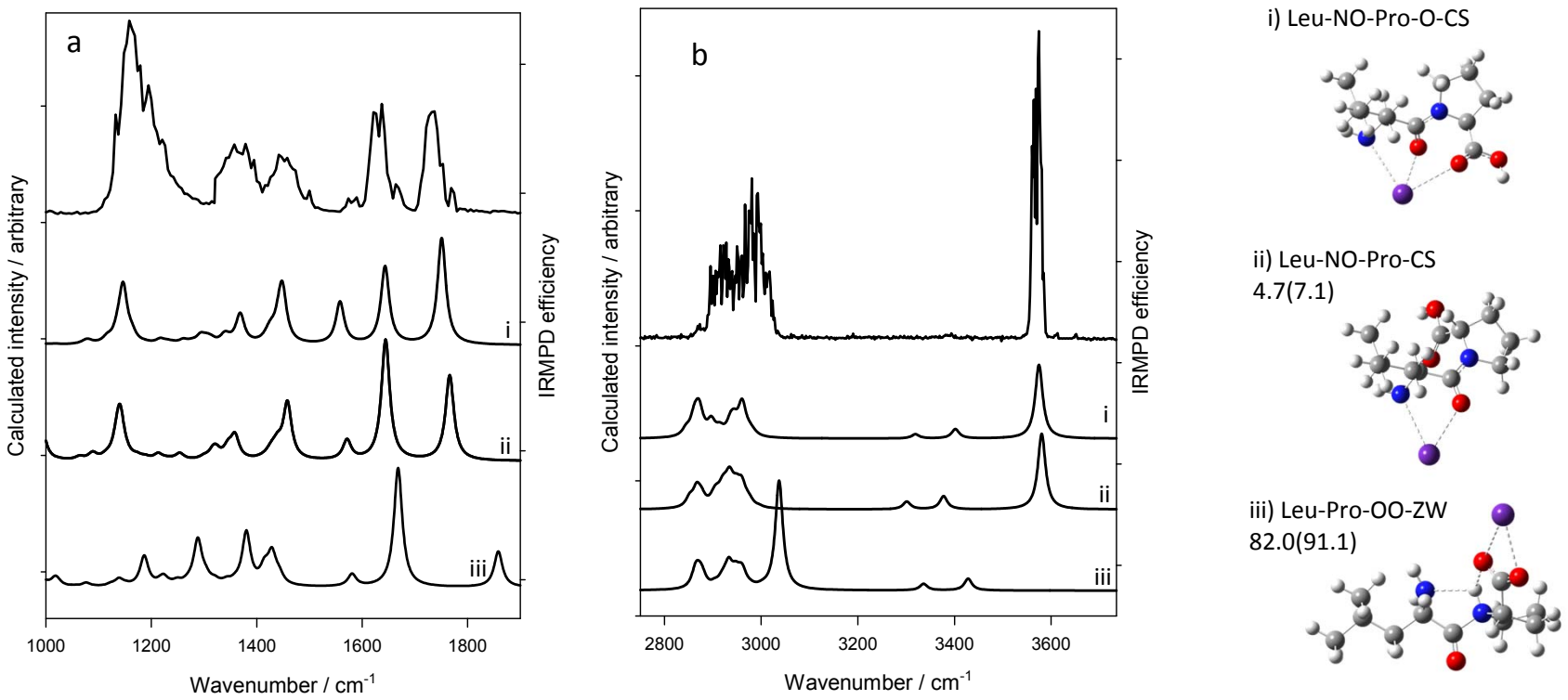

Figure S11. Comparison of the experimental IRMPD spectrum and calculated IR spectra of the lowest energy structures of each form of the (LeuPro)-Rb^+ complex a) from 1000 to 1900 cm^{-1}, b) from 2700 to 3800 cm^{-1}.
Energies are M06-2XD3/6-311++G(3df,3pd)//6- 31+G(d,p), 298 K Gibbs energies (and enthalpies) and in kJ mol^{-1}.

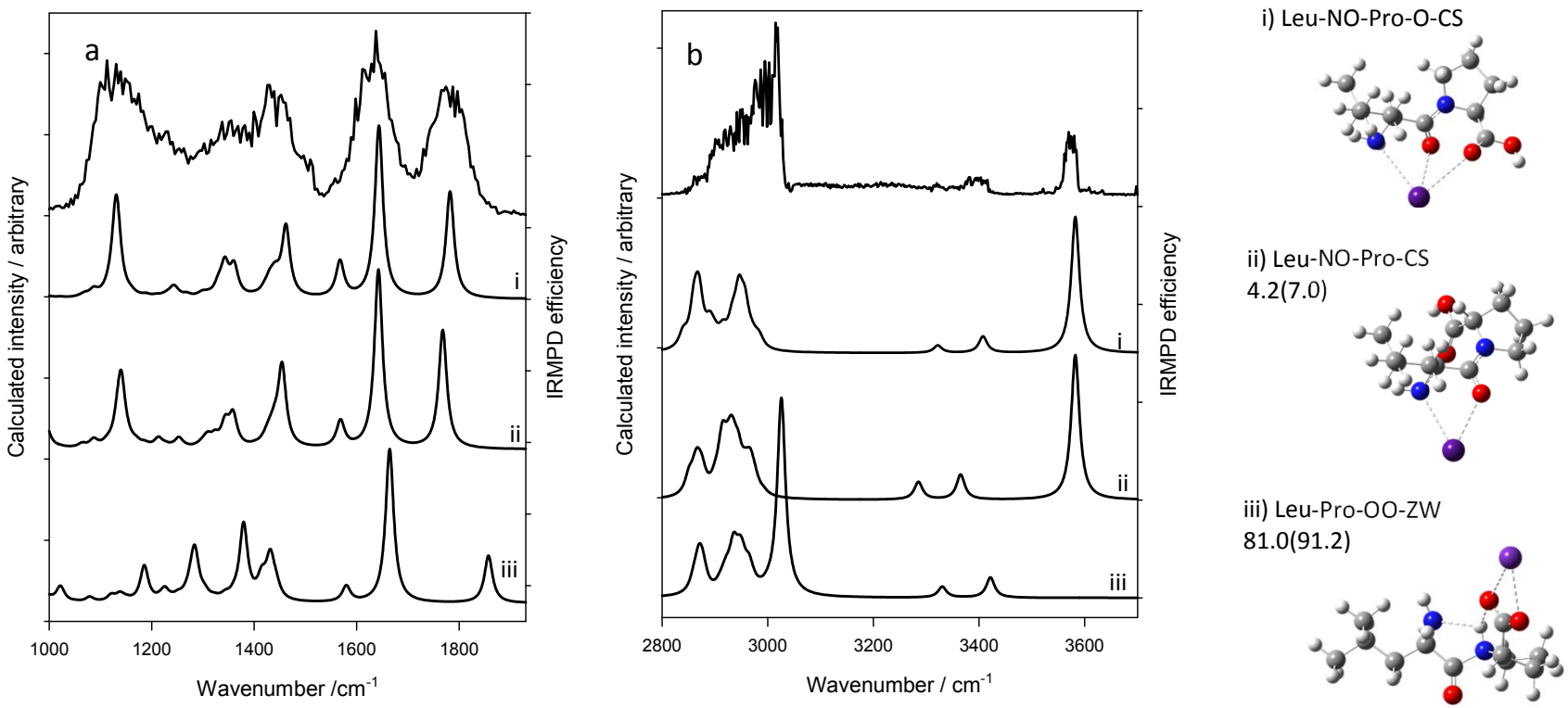

Figure S12. Comparison of the experimental IRMPD spectrum and calculated IR spectra of the lowest energy structures of each form of the (LeuPro)-Cs^+ complex a) from 1000 to 1900 cm^{-1}, b) from 2700 to 3800 cm^{-1}.
Energies are M06-2XD3/6-311++G(3df,3pd)//6- 31+G(d,p), 298 K Gibbs energies (and enthalpies) and in kJ mol^{-1}.

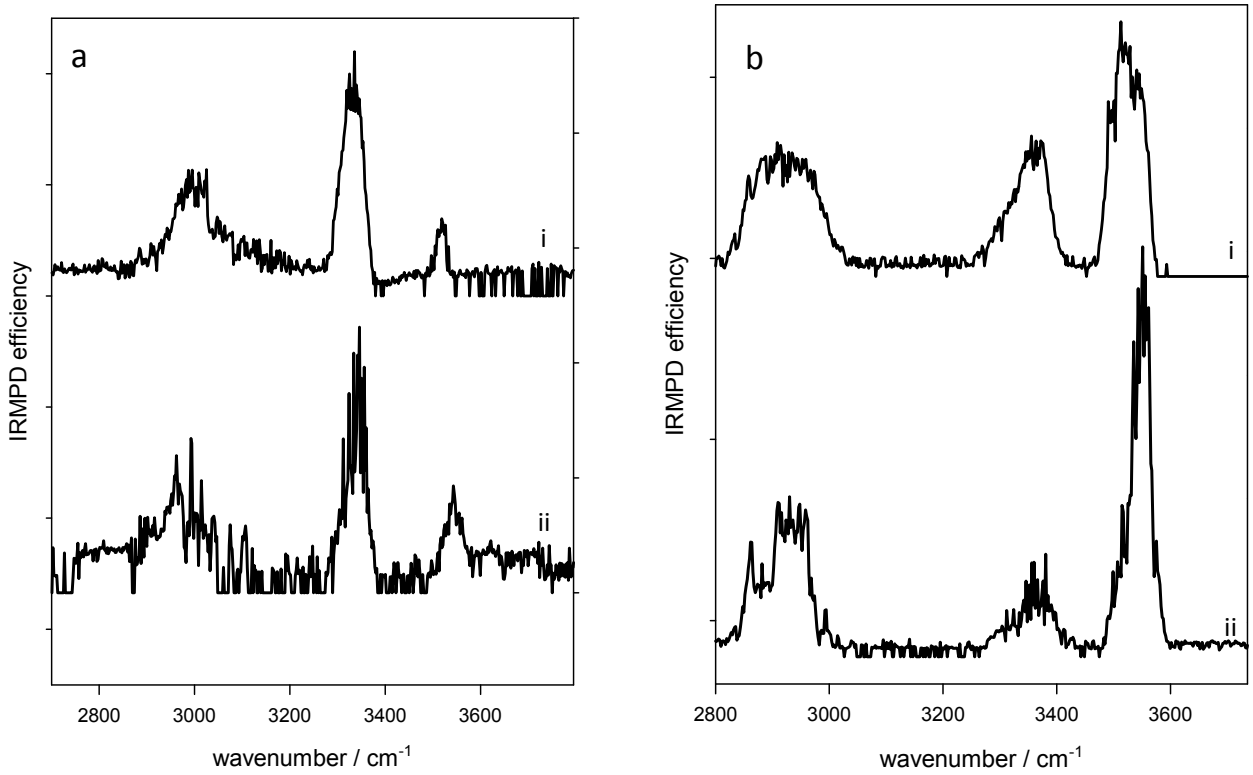

Figure S13. Comparison of the experimental IRMPD from 2700 to 3800 cm^{-1} of the a)(pro)Li^+ and b)(Leu)Li^+ complex resulted from i) cleavage of ProLeu and ii) cleavage of LeuPro dipeptides using CID experiment.

Figure S14.
Comparison of computed (unscaled) B3LYP and B3LYPD3 spectra for some ProLeu-M^+ and LeuProM^+.

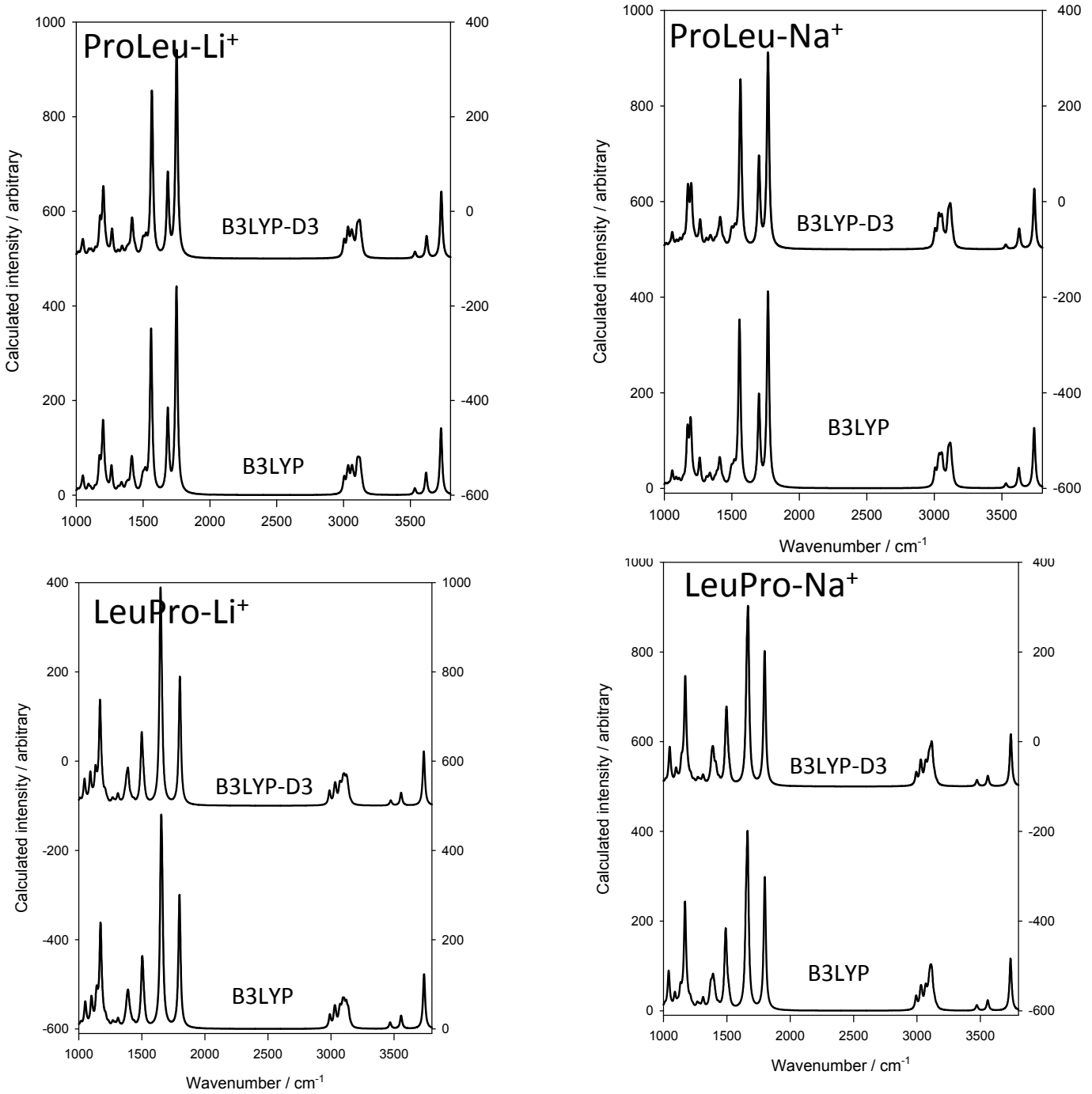

Table 1. Comparison of M06-2X/6-31+G(d,p) and M06-2X/6-311++G(3df,3pd)//6- 31+G(d,p), relative Gibbs energies (and enthalpies) of the lowest energy structures of each forms of the $[M(ProLeu)]^+$ complex at 298 K.

Structure	$\Delta_{rel}G(\Delta_{rel}H)$/kJ mol^{-1} M06-2X/6-31+G(d,p)	$\Delta_{rel}G(\Delta_{rel}H)$/kJ mol^{-1} M06-2X/6-311++G(3df,3pd)// 6-31+G(d,p)	$\Delta_{rel}G(\Delta_{rel}H)$/kJ mol^{-1} B3LYP/6-31+G(d,p)	$\Delta_{rel}G(\Delta_{rel}H)$/kJ mol^{-1} B3LYP/6-311++G(3df,3pd)// 6-31+G(d,p)
Li-Pro-NO-Leu-O-CS	0(0)	0(0)	2.6(-1.3)	4.1(0.1)
Li-Pro-O-Leu-O-CS	4.7(8.2)	3.8(7.4)	0(0)	0(0)
Li-Pro-Leu-OO-ZW	53.3(56.6)	52.3(55.6)	39.9(39.6)	41.0(40.8)
Li-Pro-N-Leu-NO-IM	35.0(33.8)	35.3(34.1)	41.0(36.6)	42.2(37.7)
Na-Pro-NO-Leu-O-CS	0(0)	0(0)	0(0)	0(0)
Na-Pro-O-Leu-O-CS	3.7(8.7)	3.0(8.0)	2.1(4.1)	1.1(3.1)
Na-Pro-Leu-OO-ZW	51.4(52.5)	52.5(53.5)	40.2(40.1)	42.4(42.4)
Na-Pro-N-Leu-NO-IM	48.2(48.3)	48.0(48.0)	57.4(54.1)	56.6(53.4)
Rb-Pro-O-Leu-O-CS	0(0)	0(0)	0(0)	0(0)
Rb-Pro-NO-Leu-O-CS	2.9(-0.1)	1.8(-1.2)	6.2(2.4)	4.9(1.2)
Rb-Pro-Leu-OO-ZW	54.7(52.2)	56.1(53.6)	50.9(46.9)	53.5(49.4)
Rb-Pro-N-Leu-NO-IM	66.3(63.9)	64.5(62.1)	78.0(72.3)	75.9(70.3)
Cs-Pro-O-Leu-O-CS	0(0)	0(0)	0(0)	0(0)
Cs-Pro-NO-Leu-O-CS	3.0(4.1)	1.1(2.3)	9.9(5.7)	8.2(3.9)
Cs-Pro-Leu-OO-ZW	58.0(57.4)	57.5(56.8)	56.1(51.6)	56.5(52.0)
Cs-Pro-N-Leu-NO-IM	71.7(70.9)	68.2(67.3)	86.5(78.5)	82.9(74.8)

Table 2. Comparison of M06-2X/6-31+G(d,p) and M06-2X/6-311++G(3df,3pd)//6- 31+G(d,p), relative Gibbs energies (and enthalpies) of the lowest energy structures of each forms of the $[M(LeuPro)]^+$ complex at 298 K.

Structure	$\Delta_{rel}G(\Delta_{rel}H)$/kJ mol^{-1} M06-2X/6-31+G(d,p)	$\Delta_{rel}G(\Delta_{rel}H)$/kJ mol^{-1} M06-2X/6-311++G(3df,3pd)// 6-31+G(d,p)	$\Delta_{rel}G(\Delta_{rel}H)$/kJ mol^{-1} B3LYP/6-31+G(d,p)	$\Delta_{rel}G(\Delta_{rel}H)$/kJ mol^{-1} B3LYP/6-311++G(3df,3pd)// 6-31+G(d,p)
Li-Leu-NO-Pro-CS	0(0)	0(0)	0(0)	0(0)
Li-Leu-O-Pro-O-CS	14.1(15.8)	12.1(13.8)	10.7(11.2)	9.3(9.8)
Li-Leu-Pro-OO-ZW	74.8(74.9)	72.8(73.0)	66.0(63.8)	65.6(63.4)
Na-Leu-NO-Pro-CS	0(0)	0(0)	0(0)	0(0)
Na-Leu-O-Pro-O-CS	12.0(14.9)	9.8(12.7)	7.8(10.1)	6.2(8.6)
Na-Leu-Pro-OO-ZW	70.4(70.8)	69.4(69.8)	64.1(61.2)	64.8(61.9)
Rb-Leu-NO-Pro-O-CS	0(0)	0(0)	0(0)	0(0)
Rb-Leu-NO-Pro-CS	3.2(5.7)	4.7(7.1)	1.1(3.2)	1.8(4.0)
Rb-Leu-Pro-OO-ZW	79.3(88.5)	82.0(91.1)	73.0(81.4)	75.6(84.0)
Cs-Leu-NO-Pro-O-CS	0(0)	0(0)	0(0)	0(0)
Cs-Leu-NO-Pro-CS	3.3(8.9)	2.8(8.4)	2.1(7.7)	1.1(6.6)
Cs-Leu-Pro-OO-ZW	79.1(89.3)	81.0(91.2)	75.9(83.1)	77.4(84.6)

Table 3a
Pro-NO-Leu-O-CS
0(0) kJ mol^{-1}

N	-2.90333900	0.39162000	-0.81045400
C	-4.23990100	0.19308800	-0.17240600
C	-2.07545400	-0.81643800	-0.47216700
H	-5.01215400	0.66838400	-0.78033800
H	-4.23554200	0.66894700	0.81483300
C	-4.38855000	-1.31722700	-0.02291800
C	-2.97142700	-1.73287400	0.38290400
C	-0.89601200	-0.23860200	0.29486700
H	-5.13825100	-1.59810300	0.71933800
H	-4.66765500	-1.76885700	-0.98131600
H	-2.80533600	-1.51420300	1.44232700
H	-2.75649900	-2.78797300	0.20580300
O	-0.01369300	2.38872200	-0.38795800
O	-1.12087600	0.47393200	1.28340400
C	1.05600000	1.96782700	0.02854500
C	1.41661300	0.49741700	0.24636000
O	2.05049300	2.76713900	0.35882200
N	0.33566000	-0.34840700	-0.22363600
H	1.51530700	0.37882000	1.33278900
C	2.73976100	0.13390600	-0.44171900
H	3.51802000	0.77588000	-0.01632000
H	2.67171200	0.38432500	-1.50944200
C	3.15072100	-1.33650800	-0.27387200
H	2.42847900	-1.97362800	-0.80565400
C	3.17052400	-1.76023300	1.19533100
C	4.51927800	-1.54724500	-0.92458200
H	3.82299800	-1.10021600	1.77926600
H	3.55712300	-2.77784900	1.29379500
H	2.17373800	-1.74721200	1.64937600
H	5.28738200	-0.97154100	-0.39674300
H	4.52030500	-1.23298100	-1.97277300
H	4.80698000	-2.60091700	-0.88775800
H	0.47719500	-0.88397000	-1.07016400
Li	-1.80673100	1.89152100	0.10699600
H	1.78661300	3.69454400	0.23404900
H	-3.02623700	0.42585900	-1.81905000
H	-1.74694700	-1.31338500	-1.39057600

Table 3b
Pro-O-Leu-O-CS
3.8(7.4) kJ mol^{-1}

N	-2.01120200	-1.62784800	-0.18810900
C	-3.03462300	-1.54172000	-1.25470700
C	-2.21937100	-0.50651700	0.73774700
H	-3.32057400	-2.54206000	-1.58408900
H	-2.61222000	-1.01299400	-2.11781000
C	-4.17863600	-0.73159300	-0.64360100
C	-3.41874900	0.30776500	0.18401000
H	-2.43187900	-0.85047800	1.75670500
C	-0.98418300	0.36610200	0.84401700
H	-4.83535500	-0.27949000	-1.38985900
H	-4.78592500	-1.36788300	0.00920500
H	-3.05757900	1.11180200	-0.46904800
H	-4.00415000	0.76193900	0.98434600
O	0.80784300	3.03500900	0.02412600
O	-0.94531300	1.32343500	1.64423400
H	1.58591900	3.02399800	-2.14272200
C	1.25931700	2.05590200	-0.56100800
C	1.34264300	0.67094800	0.08227700
O	1.68797000	2.11878000	-1.79970700
N	0.02286700	0.05761500	0.02373600
H	1.57802800	0.85404600	1.13814000
C	2.39325800	-0.23985900	-0.54962400
H	3.36689400	0.25708200	-0.45254100
H	2.19361100	-0.32851000	-1.62377200
C	2.47417100	-1.63491300	0.08927000
H	1.54390500	-2.17757400	-0.13277600
C	2.63642200	-1.56630100	1.60854800
C	3.62760200	-2.40952300	-0.55073900
H	3.51070800	-0.96200200	1.87954500
H	2.78709200	-2.56670100	2.02212400
H	1.75658700	-1.14080800	2.10478100
H	4.58620200	-1.92984400	-0.32369800
H	3.52291000	-2.45907000	-1.63879900
H	3.66667000	-3.43257800	-0.16829900
H	-2.08143100	-2.51235600	0.30192900
H	-0.14405200	-0.78067900	-0.53758500
Li	-0.23270800	2.96208100	1.55615800

Table 3c
Pro-N-Leu-NO-IM
35.3(34.1) kJ mol^{-1}

N	2.57999200	0.28653400	1.08531100
C	3.81048100	0.72519000	0.36760700
C	2.09175700	-0.93776900	0.38644600
H	4.47024300	1.25900500	1.05416100
H	3.52588300	1.41320500	-0.43766000
C	4.40449500	-0.55214700	-0.21841600
C	3.14749200	-1.28174300	-0.69899200
C	0.70875000	-0.70765400	-0.19963200
H	5.11817100	-0.36712500	-1.02330700
H	4.91030700	-1.12696300	0.56476200
H	2.83946700	-0.87764400	-1.67097400
H	3.29742000	-2.35901900	-0.80717000
O	-0.36078700	2.84351900	0.28280900
O	0.24949300	-1.58229700	-1.10294100
C	-1.22005300	2.20917400	-0.31737700
C	-1.24159500	0.68944200	-0.38596300
O	-2.22996700	2.78253300	-0.93840600
N	0.03481000	0.29765900	0.17563800
H	-1.36033100	0.38447200	-1.43377800
C	-2.43067700	0.17418900	0.45368800
H	-3.34061600	0.66640500	0.08926200
H	-2.27316100	0.49939600	1.49065500
C	-2.62735200	-1.34565400	0.41003600
H	-1.68063200	-1.82779400	0.69223500
C	-3.02920900	-1.82576100	-0.98529900
C	-3.68760700	-1.74238100	1.43976800
H	-3.96548500	-1.34884400	-1.29724400
H	-3.19350200	-2.90693800	-0.98404000
H	-2.26591400	-1.61316100	-1.73892500
H	-4.64822900	-1.27037000	1.20446400
H	-3.40089400	-1.43976300	2.45153500
H	-3.84126700	-2.82481500	1.44070900
H	0.90423700	-2.25560900	-1.33476400
Li	1.03062500	1.70708500	1.05583100
H	-2.17683100	3.74770200	-0.83275300
H	2.84981200	0.01851500	2.02893300
H	2.00703300	-1.76061800	1.10687000

Table 3d
Pro-Leu-OO-ZW
52.3(55.6) kJ mol^{-1}

N	-3.19166500	-0.50454600	-1.02315700
C	-4.20341100	0.32156500	-0.25871000
C	-2.14665500	-0.99927100	-0.05091900
H	-5.18352300	0.21028100	-0.72161000
H	-3.87999500	1.36220400	-0.33188900
C	-4.08168200	-0.20751200	1.16465400
C	-2.57218200	-0.42173400	1.31177600
H	-2.14836100	-2.09189700	-0.05763500
C	-0.81906000	-0.42688300	-0.58000800
H	-4.48231600	0.49957500	1.89259100
H	-4.62451000	-1.15245100	1.27217600
H	-2.06495200	0.53424000	1.48162100
H	-2.30795800	-1.09527000	2.12824400
O	3.74406400	-1.49662400	-0.45820600
O	-0.87686200	0.37298800	-1.51749700
C	2.55954500	-1.56172600	-0.04948000
C	1.62544800	-0.38541600	-0.31910900
O	2.12244500	-2.54948900	0.62182000
N	0.27712000	-0.80941700	0.05817800
H	1.63437500	-0.16091700	-1.39002200
C	2.10110200	0.82939700	0.49223400
H	3.15544500	0.99314000	0.23809400
H	2.06257500	0.55848700	1.55649100
C	1.31262700	2.12229000	0.25669100
H	0.24430100	1.91569100	0.42554300
C	1.48717900	2.64271400	-1.17074900
C	1.75731700	3.17674400	1.27250100
H	2.54646900	2.83421900	-1.37709800
H	0.94775800	3.58521000	-1.30397800
H	1.10754600	1.93965700	-1.91639500
H	2.82263400	3.40115500	1.14744600
H	1.60436700	2.83609300	2.30157600
H	1.20376200	4.11016100	1.13624500
H	-3.63621800	-1.27451400	-1.52439600
H	0.25954300	-1.58920000	0.71280100
H	-2.63389500	0.06993100	-1.70102000
Li	3.91207300	-3.14802100	0.40128100

Table 4a
Pro-NO-Leu-O-CS
0(0) kJ mol^{-1}

N	-2.95087000	0.08846400	-0.83227500
C	-4.16460600	-0.27459800	-0.04979700
C	-1.92605700	-0.96208900	-0.53912500
H	-5.05716300	0.10534100	-0.55164200
H	-4.09870000	0.18848800	0.94178200
C	-4.11130300	-1.79323800	0.08531500
C	-2.61955600	-2.02970800	0.34089400
C	-0.79483000	-0.26306500	0.19932400
H	-4.74117500	-2.17301300	0.89226500
H	-4.42798200	-2.26719800	-0.85040500
H	-2.38823900	-1.83896100	1.39348300
H	-2.28719200	-3.03852800	0.09028900
O	0.21165100	2.42101600	-0.46219000
O	-1.04081600	0.41680900	1.20124000
C	1.23772000	1.95374600	-0.00015400
C	1.52957300	0.46814500	0.20131800
O	2.24549500	2.70561300	0.41263200
N	0.44160700	-0.33040900	-0.32429000
H	1.57445900	0.32722500	1.28888000
C	2.86729900	0.06052200	-0.43063700
H	3.64905200	0.67633500	0.02607900
H	2.85206700	0.31126400	-1.50041200
C	3.22140300	-1.42258200	-0.24556700
H	2.49735900	-2.03560700	-0.80223400
C	3.17154500	-1.84232500	1.22386500
C	4.60529600	-1.68217600	-0.84417700
H	3.82266900	-1.20222500	1.83099700
H	3.51975100	-2.87212300	1.33887500
H	2.15900300	-1.79311300	1.63866600
H	5.37246700	-1.12915000	-0.29113900
H	4.65484100	-1.37274400	-1.89277800
H	4.85707600	-2.74450900	-0.79344100
H	0.59390100	-0.84492000	-1.18130800
Na	-1.97236300	2.13562200	0.06069600
H	2.02696000	3.64397300	0.28821500
H	-3.18430700	0.02951500	-1.82012100
H	-1.56356500	-1.39157700	-1.47875600

Table 4b
Pro-O-Leu-O-CS
3.0(8.0) kJ mol^{-1}

N	1.94359300	-2.01557600	-0.28406900
C	2.98464600	-2.28468700	0.73150100
C	2.20800700	-0.71969400	-0.91989500
H	3.82963300	-2.84371200	0.30840800
H	2.56740700	-2.86314700	1.55891900
C	3.43520000	-0.88515000	1.14171000
C	3.45084200	-0.14729900	-0.20015700
H	2.37850900	-0.79708200	-1.99969700
C	1.01841200	0.22145200	-0.76540700
H	2.70039600	-0.43800800	1.82177900
H	4.40568700	-0.88398200	1.64094100
H	3.42020600	0.94120200	-0.11806900
H	4.34698000	-0.41683200	-0.76614400
O	-0.80908700	2.83240800	0.67469700
O	1.00762700	1.34027200	-1.30795700
H	-0.82233100	2.16943800	2.88680000
C	-1.00141500	1.69341200	1.07084800
C	-1.23974600	0.50194700	0.14485000
O	-0.99493300	1.37554200	2.35287000
N	0.00753100	-0.22492000	-0.01109000
H	-1.50426800	0.93293000	-0.82706400
C	-2.35453900	-0.41662300	0.64418900
H	-3.26886400	0.18512800	0.73164900
H	-2.10721300	-0.76215600	1.65455300
C	-2.63208300	-1.61828700	-0.27251600
H	-1.76039900	-2.28771300	-0.24541700
C	-2.86499400	-1.19697000	-1.72418300
C	-3.83269300	-2.39411000	0.27159600
H	-3.67096300	-0.45564400	-1.78881500
H	-3.16025200	-2.05813900	-2.32916300
H	-1.96634300	-0.77084300	-2.18416200
H	-4.74028800	-1.78203200	0.22307200
H	-3.67982100	-2.69040700	1.31380400
H	-4.00856100	-3.29998300	-0.31433000
H	1.86068600	-2.76580800	-0.96017800
H	0.13417000	-1.16779000	0.35763100
Na	0.24809900	3.34802900	-1.21731800

Table 4c
Pro-N-Leu-NO-IM
48.0(48.0) kJ mol^{-1}

N	2.59669000	0.07191800	1.03197900
C	3.83581600	0.49243400	0.32603600
C	2.02270100	-1.05686900	0.25628200
H	4.54017700	0.93107000	1.03592700
H	3.58216500	1.25599900	-0.42048100
C	4.34625500	-0.76470500	-0.37229400
C	3.04001500	-1.38333900	-0.87510100
C	0.64253200	-0.74948500	-0.29818600
H	5.05217200	-0.55673900	-1.17862400
H	4.83443400	-1.42613400	0.35154700
H	2.73681000	-0.89538200	-1.80907700
H	3.12711500	-2.45689200	-1.06254300
O	-0.68337100	2.85733400	0.01044700
O	0.14862200	-1.63239100	-1.18513900
C	-1.41971100	2.08100900	-0.57660800
C	-1.32187500	0.56726900	-0.49314200
O	-2.43074000	2.48348500	-1.32937900
N	-0.01467700	0.27139900	0.06456900
H	-1.46362700	0.15468000	-1.49948600
C	-2.45259400	0.07479100	0.43993800
H	-3.40020300	0.49524700	0.08124900
H	-2.26413700	0.49290200	1.43793500
C	-2.58498900	-1.44984800	0.53192600
H	-1.59971000	-1.87093800	0.77807000
C	-3.06529000	-2.05523000	-0.78795000
C	-3.54879800	-1.80316600	1.66698200
H	-4.05220700	-1.65782800	-1.05140300
H	-3.15901900	-3.14142500	-0.69938900
H	-2.38005100	-1.85153800	-1.61538900
H	-4.54193900	-1.38229400	1.47358800
H	-3.19878700	-1.41478400	2.62848500
H	-3.66011600	-2.88694600	1.75970100
H	0.78654400	-2.32131800	-1.41519100
Na	1.04140400	1.95498000	1.19174100
H	-2.48058300	3.45384100	-1.31434200
H	2.86521100	-0.28704600	1.94440100
H	1.90575200	-1.92706200	0.91531100

Table 4d
Pro-Leu-OO-ZW
52.5(53.5) kJ mol^{-1}

N	-3.33780700	-0.90668400	-1.02149600
C	-4.40609000	-0.31459800	-0.13279000
C	-2.17029100	-1.30581700	-0.15151500
H	-5.38577300	-0.49280700	-0.57545500
H	-4.21566200	0.76021700	-0.08581800
C	-4.15153700	-0.98999700	1.20832300
C	-2.62114000	-1.00033700	1.29028700
H	-1.95844600	-2.36600500	-0.30897400
C	-1.00842600	-0.42110300	-0.64523900
H	-4.61622300	-0.44402600	2.03084400
H	-4.55297800	-2.00895100	1.20668200
H	-2.24695800	-0.01634100	1.59212000
H	-2.23244100	-1.73851200	1.99313100
O	3.67668000	-0.45993100	-0.57916300
O	-1.26257500	0.40856800	-1.52534700
C	2.55437500	-0.82380300	-0.16367600
C	1.37669700	0.13231500	-0.39026600
O	2.32685500	-1.90171400	0.46679200
N	0.15569900	-0.59682700	-0.04369400
H	1.33360500	0.40333200	-1.44928400
C	1.56589600	1.38126700	0.48307900
H	2.55298000	1.79427500	0.24189200
H	1.59918900	1.05450900	1.53194500
C	0.50001300	2.46959900	0.31442400
H	-0.49159100	2.01232000	0.45583000
C	0.54790800	3.10065000	-1.07765800
C	0.68756100	3.53709000	1.39502100
H	1.52901000	3.55757900	-1.25149700
H	-0.20641900	3.88796600	-1.16953000
H	0.35829500	2.37018300	-1.86811100
H	1.67227600	4.00813600	1.29847500
H	0.61621600	3.11048700	2.40078600
H	-0.06699100	4.32380900	1.30393200
H	-3.69394200	-1.69344500	-1.56509500
H	0.32922400	-1.40309500	0.55605100
H	-2.90854300	-0.19555400	-1.66845700
Na	4.51658700	-2.30604300	0.28260600

Table 5a
Pro-O-Leu-O-CS
0(0) kJ mol^{-1}

N	2.21171800	2.34139600	-0.67119200
C	2.55850900	3.28998900	0.40664500
C	0.75036200	2.36297700	-0.83288500
H	3.55333700	3.70630600	0.23802400
H	2.57669500	2.75384300	1.36379200
C	1.43289900	4.32480100	0.40347700
C	0.20613700	3.44926000	0.13719800
H	0.46866700	2.59610200	-1.86590400
C	0.12819500	1.01485900	-0.51628700
H	1.35729600	4.88515400	1.33814500
H	1.58085300	5.03881700	-0.41426800
H	-0.13013700	2.98137700	1.06995900
H	-0.64116800	3.98708300	-0.29050300
O	-1.65803700	-1.60614800	1.31697700
O	-1.09758900	0.82474300	-0.59321400
H	-0.71063500	-0.55771400	3.14585700
C	-0.52685100	-1.16262700	1.36959600
C	0.48865800	-1.26367900	0.23770500
O	-0.03959900	-0.55069400	2.44435600
N	0.96947200	0.05407700	-0.11843400
H	-0.06139500	-1.68962200	-0.60862500
C	1.64845900	-2.18307600	0.63734600
H	1.22474800	-3.16310700	0.89315600
H	2.11359500	-1.78560700	1.54741100
C	2.71018100	-2.37162100	-0.45688600
H	3.21238800	-1.40959400	-0.63205300
C	2.09870400	-2.83871300	-1.77820600
C	3.76587100	-3.36245100	0.03758900
H	1.51876300	-3.75821200	-1.63166600
H	2.88375000	-3.05534200	-2.50754600
H	1.44173000	-2.08314400	-2.22189400
H	3.32143700	-4.35209100	0.19233900
H	4.20809600	-3.03790400	0.98438300
H	4.57165900	-3.46828500	-0.69341100
H	2.66753000	2.60886600	-1.53594400
H	1.95365000	0.31164200	-0.08285000
Rb	-3.47524700	-0.38320000	-0.43183000

Table 5b
Pro-NO-Leu-O-CS
1.8(-1.2) kJ mol^{-1}

N	2.47800100	1.17757700	-0.82449500
C	3.34247200	1.89579900	0.14109400
C	1.11124100	1.72823900	-0.64048500
H	4.38294300	1.86733000	-0.19122500
H	3.26909800	1.39661600	1.11468000
C	2.75048200	3.30130100	0.23360000
C	1.24410600	3.01328800	0.22916000
C	0.26685500	0.68933600	0.08163600
H	3.06956400	3.84624700	1.12444700
H	3.03819300	3.88590700	-0.64701300
H	0.90164700	2.80655000	1.24765400
H	0.64802700	3.83532900	-0.17104700
O	-0.24474600	-2.23761900	-0.53613800
O	0.69179700	0.11161200	1.08382400
C	-1.28992300	-1.94485700	0.00876600
C	-1.84333300	-0.53444900	0.18349700
O	-2.10070100	-2.84735500	0.55290200
N	-0.95959200	0.43766700	-0.41973500
H	-1.86018000	-0.36305300	1.26767700
C	-3.26466900	-0.41394200	-0.38474300
H	-3.89246700	-1.14019900	0.14215700
H	-3.25681400	-0.71141500	-1.44259500
C	-3.88220900	0.98488300	-0.24237400
H	-3.32182500	1.68912300	-0.87460900
C	-3.82596500	1.49129800	1.19913700
C	-5.32346300	0.94985100	-0.75453700
H	-4.30373200	0.77592400	1.87910300
H	-4.35828200	2.44173100	1.29081600
H	-2.79958800	1.65841100	1.54312500
H	-5.93725400	0.29422500	-0.12710200
H	-5.37704400	0.58063300	-1.78337100
H	-5.76832100	1.94813800	-0.73012200
H	-1.24753600	0.88046600	-1.28124600
H	-1.72852000	-3.73449700	0.42431800
H	2.78582700	1.42416100	-1.76180700
H	0.67492700	1.95022400	-1.61981400
Rb	2.48562500	-1.72476100	0.00465900

Table 5c
Pro-Leu-OO-ZW
56.1(53.6) kJ mol^{-1}

N	-3.93360900	-1.54097900	-0.99867800
C	-5.08551700	-1.33507000	-0.04471400
C	-2.66302500	-1.64424700	-0.19208400
H	-5.98881800	-1.77579800	-0.46599300
H	-5.22051900	-0.25587800	0.05890200
C	-4.58360800	-1.96532200	1.24807800
C	-3.11277900	-1.53733900	1.27782300
H	-2.17671500	-2.59731900	-0.41282800
C	-1.81569100	-0.44940900	-0.67305900
H	-5.14563800	-1.61340000	2.11468500
H	-4.67492000	-3.05578200	1.20331500
H	-3.02102000	-0.49972100	1.61611700
H	-2.49551300	-2.15897900	1.92778300
O	2.71315000	0.78854100	-0.71740900
O	-2.34507500	0.32338000	-1.48267300
C	1.75296800	0.09995500	-0.31475600
C	0.34801500	0.71745900	-0.47513900
O	1.82208200	-1.03189400	0.25041800
N	-0.61654400	-0.33042300	-0.13624800
H	0.19787300	1.00945900	-1.51888700
C	0.22357700	1.93145000	0.45447300
H	1.05320200	2.60552300	0.20908100
H	0.38617400	1.58117600	1.48377600
C	-1.10161600	2.69767900	0.37501300
H	-1.92692300	1.98286300	0.51855100
C	-1.28431900	3.37801300	-0.98234400
C	-1.16560800	3.72789800	1.50422900
H	-0.47123200	4.09147500	-1.16013200
H	-2.22674300	3.93356700	-1.01125000
H	-1.30184700	2.65833400	-1.80440200
H	-0.35258500	4.45598900	1.40333100
H	-1.07191700	3.25564600	2.48756500
H	-2.10961500	4.28038400	1.47987000
H	-4.07616500	-2.35685400	-1.59428200
H	-0.18448900	-1.09213100	0.39040000
H	-3.74092700	-0.69106100	-1.59674600
Rb	4.58929100	-0.94660200	0.13913000

Table 5d
Pro-N-Leu-NO-IM
64.5(62.1) kJ mol^{-1}

N	-2.41056900	-0.64339000	-0.83131600
C	-3.50116300	-0.48024900	0.15287700
C	-1.60252600	-1.78244600	-0.36170400
H	-4.34211100	0.05441600	-0.29612200
H	-3.12751300	0.10946400	1.00158600
C	-3.83832400	-1.89732900	0.61498400
C	-2.44634800	-2.53006800	0.72610100
C	-0.25856600	-1.37042900	0.20864000
H	-4.39007800	-1.93032700	1.55655300
H	-4.43579900	-2.40355800	-0.15049000
H	-2.03155300	-2.34029100	1.72229400
H	-2.46457100	-3.61139500	0.56929500
O	0.61882400	2.33787300	1.25037500
O	0.47547800	-2.38805800	0.71151300
C	1.38391500	1.43643600	1.53641000
C	1.46348400	0.09849600	0.82574700
O	2.30365700	1.54863200	2.48874900
N	0.16340300	-0.17462600	0.22997300
H	1.76947200	-0.65763000	1.55716700
C	2.55125900	0.23611900	-0.26534500
H	3.45713400	0.64896500	0.19723500
H	2.19415700	0.97484300	-0.99664700
C	2.91130800	-1.06972000	-0.98322700
H	1.98202900	-1.53910000	-1.33626900
C	3.63598800	-2.04436800	-0.05399200
C	3.77801500	-0.75149500	-2.20373000
H	4.57162600	-1.60149900	0.30642200
H	3.89027300	-2.96440000	-0.58825700
H	3.03104400	-2.32323300	0.81265900
H	4.70797100	-0.25958300	-1.89643000
H	3.26105700	-0.08823500	-2.90465800
H	4.04793200	-1.66554300	-2.73964100
H	0.00527400	-3.23166100	0.67891600
Rb	-1.24548500	2.11925000	-0.81113300
H	2.25960400	2.44075400	2.87041900
H	-2.82853300	-0.90857200	-1.71943000
H	-1.39023500	-2.44681600	-1.20893700

Table 6a
Pro-O-Leu-O-CS
0(0) kJ mol^{-1}

N	2.70220500	2.25255600	-0.87494700
C	3.19162800	3.23290400	0.11959200
C	1.24143600	2.35606800	-0.98239300
H	3.50856300	4.16915400	-0.35823500
H	4.04184400	2.82429600	0.67121000
C	1.97008100	3.48234800	1.00117000
C	0.83247600	3.49347100	-0.02320900
H	0.90625000	2.55587000	-2.00633300
C	0.56485200	1.05200400	-0.56849600
H	1.84002100	2.65604100	1.71045100
H	2.04546900	4.41124900	1.56935400
H	-0.16105400	3.33881500	0.40218300
H	0.82811500	4.44137000	-0.56967500
O	-1.24145600	-1.41906300	1.49663600
O	-0.67084700	0.92078200	-0.58268500
H	-0.16575700	-0.25706700	3.18090300
C	-0.10342500	-0.99585000	1.44645300
C	0.84093900	-1.20544900	0.26947800
O	0.45991900	-0.31381900	2.44103200
N	1.37451800	0.06391100	-0.17138800
H	0.22248500	-1.63482300	-0.52674800
C	1.96481900	-2.17503700	0.65301100
H	1.49932700	-3.12008000	0.96213000
H	2.49227100	-1.77430800	1.52722900
C	2.96499800	-2.45826700	-0.47767300
H	3.51316900	-1.53232700	-0.70257200
C	2.27158500	-2.92589800	-1.75754000
C	3.98228500	-3.49499600	0.00288600
H	1.64780000	-3.80606300	-1.55906100
H	3.01143500	-3.20809800	-2.51147100
H	1.63981500	-2.14643600	-2.19652100
H	3.49070100	-4.45502000	0.19690300
H	4.47566900	-3.17501400	0.92569700
H	4.75409300	-3.66109700	-0.75314200
H	3.16243300	2.35045300	-1.77175600
H	2.36816100	0.28384600	-0.16438800
Cs	-3.27943400	-0.18449100	-0.28438800

Table 6b
Pro-NO-Leu-O-CS
1.1(2.3) kJ mol^{-1}

N	1.93839500	1.72380300	-0.87391200
C	2.67481800	2.54490200	0.11249500
C	0.50279100	2.04294800	-0.68482900
H	3.70767800	2.69030600	-0.21377300
H	2.67957400	2.01536700	1.07340600
C	1.86927900	3.83786700	0.23676900
C	0.42536800	3.32018100	0.20440400
C	-0.16307900	0.87471000	0.02575600
H	2.09239100	4.39932200	1.14640700
H	2.07121300	4.48571800	-0.62321600
H	0.10586700	3.04727900	1.21466300
H	-0.28436100	4.04754000	-0.19338300
O	-0.24663200	-2.11348400	-0.61699600
O	0.34343000	0.37183700	1.03022400
C	-1.32668800	-1.97827700	-0.07955700
C	-2.05981000	-0.65771400	0.13072300
O	-2.01340800	-2.99636100	0.43357400
N	-1.33213600	0.43127200	-0.48059000
H	-2.05840300	-0.50125600	1.21751000
C	-3.50559300	-0.71496500	-0.38058200
H	-4.01332600	-1.52352800	0.15538400
H	-3.50432800	-0.99386700	-1.44345100
C	-4.29012800	0.59118700	-0.18516000
H	-3.85789800	1.36625600	-0.83466500
C	-4.22159500	1.08909600	1.25889400
C	-5.73999800	0.37453800	-0.62223500
H	-4.56666000	0.31346400	1.95308100
H	-4.86544600	1.96258200	1.39246500
H	-3.20722700	1.38301500	1.54948400
H	-6.23155700	-0.35608500	0.02969400
H	-5.79945300	0.00397400	-1.65026800
H	-6.30622500	1.30782800	-0.56575200
H	-1.68434100	0.82310500	-1.34298900
H	-1.52167800	-3.82027600	0.28846200
H	2.20567200	2.03330000	-1.80471800
H	0.03477000	2.20383900	-1.66127300
Cs	2.56546600	-1.27302100	0.05309000

Table 6c
Pro-Leu-OO-ZW
57.5(56.8) kJ mol^{-1}

N	-4.31540800	-1.72680900	-1.00239700
C	-5.47778800	-1.60494900	-0.04737500
C	-3.04050100	-1.73587300	-0.19657000
H	-6.34897800	-2.10473200	-0.47038100
H	-5.68571700	-0.53786200	0.06109100
C	-4.93244400	-2.20437600	1.24270100
C	-3.49500300	-1.67444100	1.27436100
H	-2.47997200	-2.64513800	-0.42553300
C	-2.29045900	-0.47404000	-0.67007600
H	-5.51738300	-1.89653000	2.11085600
H	-4.94753600	-3.29835500	1.19317100
H	-3.47580600	-0.63615600	1.62212800
H	-2.83512400	-2.25724300	1.91850200
O	2.13672700	1.10118000	-0.65872000
O	-2.87795000	0.25505000	-1.48072200
C	1.22493200	0.33599200	-0.28440600
C	-0.22070300	0.85452300	-0.45459000
O	1.36408900	-0.80378900	0.25090600
N	-1.10875300	-0.26168400	-0.12482000
H	-0.38098400	1.13448400	-1.50023900
C	-0.44435800	2.05616800	0.47126600
H	0.33899200	2.78710800	0.23677800
H	-0.27130700	1.71956400	1.50345400
C	-1.81885700	2.72748800	0.37188900
H	-2.59514100	1.96005700	0.51622500
C	-2.03498200	3.38056400	-0.99404700
C	-1.96312600	3.76302400	1.48929000
H	-1.26750800	4.14234700	-1.17397100
H	-3.01076200	3.87445700	-1.03556000
H	-2.00052800	2.65239900	-1.80810400
H	-1.19974600	4.54265400	1.38659900
H	-1.84685500	3.30826900	2.47840900
H	-2.94209400	4.25012000	1.45046300
H	-4.39824800	-2.55099200	-1.59767500
H	-0.61838000	-0.99314900	0.39444300
H	-4.18444200	-0.86387100	-1.59948100
Cs	4.28388100	-0.64785400	0.08223600

Table 6d
Pro-N-Leu-NO-IM
68.2(67.3) kJ mol^{-1}

N	2.08159200	1.27695300	-0.78613700
C	3.12286400	1.41008800	0.25205800
C	1.05008100	2.27331300	-0.45902000
H	4.07305500	1.00512800	-0.10608200
H	2.81321900	0.83863000	1.13829400
C	3.16892800	2.90159900	0.58453200
C	1.68152600	3.27542400	0.56819900
C	-0.21062400	1.66199900	0.12108500
H	3.64567000	3.12104900	1.54204100
H	3.71293000	3.43767600	-0.20006200
H	1.24822200	3.12048900	1.56233700
H	1.51551300	4.31873100	0.28859100
O	-0.42770300	-1.99796300	1.64091300
O	-1.16170300	2.56158200	0.46360800
C	-1.34672300	-1.21486000	1.78451200
C	-1.63677500	-0.03073400	0.88253400
O	-2.26554200	-1.35060200	2.73602200
N	-0.38194000	0.41703800	0.29344100
H	-2.12900500	0.74055800	1.48440700
C	-2.60705200	-0.53215700	-0.21287300
H	-3.44265400	-1.05265100	0.27299600
H	-2.06797400	-1.27628600	-0.81618800
C	-3.16740200	0.56572000	-1.12412900
H	-2.32724200	1.17143200	-1.49256500
C	-4.14055100	1.47704900	-0.37500200
C	-3.85716000	-0.07847700	-2.32870000
H	-4.99680100	0.89904600	-0.00869300
H	-4.52678300	2.25435000	-1.04071300
H	-3.67152200	1.97577800	0.47722000
H	-4.68388800	-0.71927700	-2.00150400
H	-3.16326500	-0.69419900	-2.90998400
H	-4.27177400	0.68318000	-2.99470200
H	-0.87036100	3.47239700	0.32508100
Cs	1.53782600	-1.84157800	-0.52985900
H	-2.08069600	-2.15854400	3.24243000
H	2.49191300	1.53714600	-1.67924200
H	0.75034300	2.79626300	-1.37606300

Table 7a
Leu-NO-Pro-CS
0(0) kJ mol^{-1}

N	-1.19756300	-0.77452400	-0.41153500
C	-2.31540800	-1.71632600	-0.65121800
C	-1.57747200	0.60982900	-0.69596300
H	-2.42861400	-2.37140700	0.21348600
H	-2.07593300	-2.33129200	-1.52411700
C	-3.50797700	-0.79311600	-0.90004000
C	-2.86770100	0.45482200	-1.51563300
H	-0.80472600	1.14175200	-1.26231400
C	-1.78214700	1.36531100	0.62313400
H	-3.99504100	-0.54158300	0.04834800
H	-4.25379200	-1.25001200	-1.55152600
H	-3.49027100	1.34810400	-1.46855400
H	-2.59881500	0.27248700	-2.56008700
O	-2.40998800	2.52147600	0.43155900
O	-1.38730000	0.97790600	1.69909500
H	-2.49306100	2.98617500	1.28088700
C	-0.12155200	-1.15235200	0.27244300
C	1.03394600	-0.18115400	0.50616800
O	0.00263000	-2.32326800	0.69828300
N	1.45920900	-0.38649100	1.90896100
H	0.72129900	0.85189300	0.34614500
C	2.16183600	-0.52042000	-0.47673800
H	2.41936800	-1.58408800	-0.38209100
H	1.76604300	-0.38949300	-1.49380400
C	3.42875100	0.33610600	-0.33096700
H	3.90949100	0.09951200	0.63055300
C	4.41862900	-0.03886700	-1.43579800
C	3.11976500	1.83434900	-0.36563400
H	4.00752700	0.21516200	-2.41923900
H	5.35977900	0.50354700	-1.31562700
H	4.64229800	-1.10989200	-1.42923000
H	2.51996500	2.16492900	0.48978700
H	4.04445100	2.41675200	-0.35576400
H	2.57604700	2.09371200	-1.28247300
H	2.35471100	0.07295600	2.06322900
H	0.78585200	0.09217300	2.51151600
Li	1.20504600	-2.38409800	2.05628800

Table 7b
Leu-NO-Pro-O-CS
15.3(11.5) kJ mol^{-1}

N	0.91894100	0.51055800	-0.55486100
C	0.57543000	1.93799400	-0.39518100
C	2.34840200	0.27287000	-0.34560000
H	0.17814200	2.12772600	0.60727000
H	-0.16176000	2.23750300	-1.14178900
C	1.93137500	2.61991000	-0.58220600
C	2.89620700	1.64414800	0.09430400
H	2.82318900	-0.07298300	-1.27223600
C	2.58165100	-0.81781500	0.69219700
H	1.95438200	3.61627200	-0.13845500
H	2.16250000	2.70891600	-1.64817600
H	2.83424600	1.74390000	1.18332900
H	3.93781100	1.77300500	-0.19947300
O	3.86305400	-0.90980500	0.99193100
O	1.73151900	-1.52860600	1.20837700
H	4.00524000	-1.61614600	1.64477800
C	0.17360600	-0.53142400	-0.95285400
C	-1.35890800	-0.59019800	-0.78864000
O	0.74197200	-1.58039900	-1.31077700
N	-1.59253200	-2.01519700	-0.43444500
H	-1.81451100	-0.34015600	-1.75679400
C	-1.93722800	0.31564700	0.30310500
H	-1.34462100	0.20347800	1.22227700
H	-1.83998100	1.35639400	-0.01895000
C	-3.42600200	0.09099600	0.62056400
H	-3.55198100	-0.88789100	1.10523800
C	-3.88461300	1.14555000	1.63015700
C	-4.29198700	0.13657700	-0.64013200
H	-3.82833400	2.14781200	1.19042700
H	-4.92084800	0.97076000	1.93033100
H	-3.26532200	1.13396300	2.53232700
H	-4.06250600	-0.67084100	-1.34434800
H	-5.35057400	0.05092000	-0.38181200
H	-4.15524900	1.09004000	-1.16422300
H	-2.52034300	-2.11823100	-0.03307100
H	-1.58059900	-2.57813100	-1.28336000
Li	0.29210200	-2.51296600	0.32043900

Table 7c
Leu-Pro-OO-ZW
72.8(73.0) kJ mol^{-1}

N	-0.70245800	-0.89389400	0.09708500
C	-0.48696000	-1.29424700	1.49517900
C	-2.06994800	-0.40884300	-0.13011000
H	-0.10691500	-0.44774500	2.07907000
H	0.21876600	-2.12569500	1.56392400
C	-1.90366400	-1.66331700	1.93599100
C	-2.75774900	-0.59983900	1.23797500
H	-2.54729600	-0.99391800	-0.92126300
C	-2.07594900	1.05879600	-0.55036000
H	-2.01146700	-1.65273300	3.02180700
H	-2.15720000	-2.66348200	1.57089800
H	-2.72224400	0.33709300	1.80392900
H	-3.80370300	-0.88293200	1.12182500
O	-1.03473300	1.76662400	-0.40009700
O	-3.15945400	1.52565700	-0.98548700
H	1.40519600	-1.28302700	-2.66159900
C	0.14911400	-0.89039200	-0.91851800
C	1.65483900	-1.11581600	-0.67464800
O	-0.17242900	-0.67096500	-2.09458200
N	2.10227800	-1.70201500	-1.99115500
H	1.88532000	-1.82329600	0.12374800
C	2.36800300	0.23232800	-0.49880600
H	3.45375500	0.06289700	-0.55876100
H	2.07439600	0.86911400	-1.34396800
C	2.05955900	0.96064200	0.81567800
H	0.96962200	1.04778900	0.90357500
C	2.64599000	0.21905700	2.01889900
C	2.62184400	2.38147600	0.73807600
H	2.29286100	-0.81444200	2.10636900
H	3.74009100	0.19245900	1.95551300
H	2.38363800	0.72953000	2.94977900
H	2.42911100	2.92018200	1.66945200
H	3.70634400	2.36760700	0.57911500
H	2.15906300	2.94231200	-0.07898700
H	3.06040000	-1.44128000	-2.23306100
H	2.01202200	-2.71994600	-2.03141000
Li	-2.17934500	3.10042100	-1.11209100

Table 7d
Leu-NO-Pro-CS
0(0) kJ mol^{-1}

N	1.28519400	0.50265700	-0.69064400
C	2.33999200	1.41313700	-1.18700100
C	1.78386100	-0.85625900	-0.49181200
H	2.34403800	2.32448100	-0.58778700
H	2.11755400	1.68311900	-2.22433900
C	3.61487800	0.57935000	-1.06493500
C	3.11737200	-0.85514600	-1.25912700
H	1.09875400	-1.61143900	-0.89254600
C	1.95276000	-1.14163300	1.00391100
H	4.04897400	0.69844600	-0.06631200
H	4.36971200	0.86849000	-1.79738400
H	3.79974800	-1.62127800	-0.89104600
H	2.91201500	-1.05059000	-2.31544800
O	2.63784200	-2.26380800	1.21175100
O	1.49294600	-0.45790100	1.88956600
H	2.69852300	-2.42905100	2.16714200
C	0.12615700	0.99467600	-0.23934700
C	-0.95398700	0.04392400	0.28035300
O	-0.11170900	2.21532100	-0.27700600
N	-1.41304700	0.57491700	1.57907500
H	-0.55186500	-0.96513500	0.39665200
C	-2.09752700	-0.00239100	-0.73962000
H	-2.43220000	1.02180900	-0.95415700
H	-1.69011100	-0.39455900	-1.68226700
C	-3.29914100	-0.86597200	-0.32744400
H	-3.79663900	-0.39124000	0.53193500
C	-4.31196900	-0.90605700	-1.47361400
C	-2.88116600	-2.28263600	0.07272400
H	-3.88142200	-1.40891600	-2.34675500
H	-5.21069900	-1.45492500	-1.18076600
H	-4.61423100	0.10035100	-1.77924300
H	-2.25335000	-2.30303100	0.97061600
H	-3.76047300	-2.89867000	0.27800000
H	-2.32351300	-2.76222200	-0.74093400
H	-2.20912200	0.02578500	1.89732900
H	-0.66852800	0.40831100	2.25866200
Na	-1.60020000	2.90385400	1.15460300

Table 8a
Leu-NO-Pro-O-CS
2.9(1.1) kJ mol^{-1}

N	0.92819900	0.69857800	-0.51994400
C	0.59467600	2.11285700	-0.27565500
C	2.35242600	0.43894200	-0.32669700
H	0.23600600	2.25195300	0.75002500
H	-0.17072500	2.45348500	-0.97646100
C	1.94795500	2.79942600	-0.46347900
C	2.91954700	1.78943300	0.15383800
H	2.81635100	0.11995800	-1.26830900
C	2.57583300	-0.69006700	0.66918800
H	1.98604100	3.77614400	0.02124600
H	2.15793100	2.93105800	-1.52942500
H	2.88014200	1.84803400	1.24695500
H	3.95595300	1.92308100	-0.15579900
O	3.86890000	-0.84586100	0.91191400
O	1.71454100	-1.37388200	1.19317600
H	4.00193000	-1.56777200	1.54815900
C	0.16968700	-0.30317400	-0.99634400
C	-1.36574200	-0.24656800	-0.93285700
O	0.71290100	-1.34523700	-1.39591200
N	-1.79815700	-1.65008300	-1.06150100
H	-1.71900200	0.37780100	-1.76901800
C	-1.89448800	0.32520300	0.39108300
H	-1.35776000	-0.14672200	1.22786400
H	-1.66791600	1.39368500	0.43813900
C	-3.40911900	0.17761500	0.60453900
H	-3.65528200	-0.88946400	0.69706500
C	-3.79869300	0.84739700	1.92386100
C	-4.20656100	0.77448200	-0.55728000
H	-3.60422600	1.92510200	1.88026000
H	-4.86288300	0.70897700	2.13114600
H	-3.23461600	0.43465800	2.76617300
H	-4.02330500	0.26430200	-1.50966700
H	-5.27967700	0.71440100	-0.35826300
H	-3.95393500	1.83313100	-0.69205700
H	-2.81257900	-1.69897200	-1.02550000
H	-1.51583700	-2.00551600	-1.97315800
Na	0.02083900	-2.69274700	0.25510300

Table 8b
Leu-Pro-OO-ZW
69.4(69.8) kJ mol^{-1}

N	0.26264000	-1.22890700	0.12165800
C	-0.14737500	-1.88661900	-1.12664200
C	1.72108500	-1.06034200	0.20137300
H	-0.34767800	-1.13925100	-1.90319900
H	-1.04057600	-2.49821100	-0.97604300
C	1.09814600	-2.70474600	-1.46913300
C	2.23637000	-1.75823400	-1.07382800
H	2.09664100	-1.53051400	1.11444500
C	2.11747800	0.42193000	0.22136900
H	1.12393300	-2.99208600	-2.52165600
H	1.12183300	-3.61334500	-0.85941500
H	2.39370900	-1.01447900	-1.86222400
H	3.18528300	-2.26375900	-0.89593100
O	1.25529600	1.29255600	-0.09186000
O	3.31705400	0.65774600	0.49969200
H	-1.62282600	-0.39197500	2.88095200
C	-0.48715200	-0.76414600	1.10684100
C	-2.01605600	-0.63867500	0.93912300
O	-0.04370000	-0.36303500	2.19459700
N	-2.48788600	-0.73357900	2.36776200
H	-2.47867900	-1.43562800	0.35469300
C	-2.37505000	0.76320000	0.42557200
H	-3.46160100	0.90411500	0.53063600
H	-1.87171000	1.48672000	1.08109400
C	-1.98246000	1.04627100	-1.03004000
H	-0.91388400	0.82241400	-1.13633900
C	-2.81676000	0.21748200	-2.00900800
C	-2.16313800	2.53972600	-1.30644200
H	-2.74790100	-0.86108800	-1.83066300
H	-3.87454800	0.49845200	-1.94537200
H	-2.49122800	0.39545900	-3.03787400
H	-1.91217100	2.77084700	-2.34499000
H	-3.20183500	2.84786800	-1.13793600
H	-1.51562600	3.13883300	-0.65980500
H	-3.30125000	-0.14481600	2.55567700
H	-2.68862600	-1.69035500	2.66660400
Na	2.88961300	2.79045300	0.21880500

Table 8c
Leu-NO-Pro-O-CS
0(0) kJ mol^{-1}

N	-1.00860100	-1.23294600	-0.42314800
C	-0.72048800	-2.62717500	-0.05028700
C	-2.42879200	-0.92520800	-0.30670400
H	-0.40291100	-2.68852200	0.99678400
H	0.06423900	-3.04409900	-0.68591700
C	-2.08184000	-3.29959400	-0.23134500
C	-3.05007600	-2.21873600	0.25790000
H	-2.84659400	-0.67605900	-1.29040900
C	-2.66736700	0.28104000	0.58609700
H	-2.16263300	-4.23035500	0.33230900
H	-2.25539100	-3.51703800	-1.28983800
H	-3.05674100	-2.18634200	1.35288600
H	-4.07634200	-2.35375600	-0.08354000
O	-3.97216300	0.50946300	0.71424800
O	-1.81676300	0.95743700	1.12752200
H	-4.11154400	1.26988200	1.30100400
C	-0.20309800	-0.32101400	-1.00167200
C	1.31376600	-0.53429500	-0.98841800
O	-0.68083300	0.71053300	-1.48989400
N	1.91152500	0.69090700	-1.52677300
H	1.53119400	-1.42090300	-1.60689900
C	1.84557600	-0.77647600	0.43311200
H	1.46479700	0.01437000	1.09641400
H	1.44617900	-1.71789100	0.82241400
C	3.37580400	-0.84126200	0.54182000
H	3.79127300	0.13726400	0.26304700
C	3.77106400	-1.11380900	1.99429100
C	3.96247900	-1.90911300	-0.38428800
H	3.40802100	-2.09708700	2.31462800
H	4.85788300	-1.10584800	2.11171600
H	3.35324800	-0.36355100	2.67327100
H	3.78806600	-1.69506100	-1.44451000
H	5.04335500	-1.99105800	-0.24276600
H	3.52467100	-2.89060500	-0.16465900
H	2.90846600	0.55347200	-1.66688500
H	1.50385700	0.89688600	-2.43609200
Rb	0.24222600	2.73499900	0.09130900

Table 8d
Leu-NO-Pro-CS
4.7(7.1) kJ mol^{-1}

N	-1.59797500	-0.46221500	-0.81728400
C	-2.21022700	-1.63560200	-1.47245900
C	-2.60188700	0.45936000	-0.29533400
H	-1.74333600	-2.54724200	-1.09637100
H	-2.03237700	-1.57899800	-2.55156500
C	-3.69242600	-1.50758000	-1.12110000
C	-3.89418500	0.00442100	-0.99566700
H	-2.37333300	1.50335300	-0.53538700
C	-2.68423800	0.35003500	1.22865100
H	-3.89500000	-1.99693900	-0.16211900
H	-4.33878500	-1.96027900	-1.87422700
H	-4.78468800	0.29516900	-0.43787600
H	-3.93695000	0.46916000	-1.98497600
O	-3.72307300	1.03207000	1.71038900
O	-1.89442100	-0.24970600	1.92096200
H	-3.72858700	0.95833300	2.67874000
C	-0.28312300	-0.45530900	-0.53862200
C	0.32798000	0.75498400	0.16968400
O	0.44828100	-1.39384400	-0.88417400
N	1.09687500	0.25606500	1.32172700
H	-0.46133100	1.44049800	0.49369600
C	1.22861100	1.49685400	-0.82386600
H	1.95428200	0.78690600	-1.24238700
H	0.60371200	1.83008500	-1.66502600
C	1.96401000	2.71497200	-0.24773600
H	2.68330000	2.36605600	0.50869000
C	2.76439200	3.39887400	-1.35797200
C	1.00478100	3.70669300	0.41419300
H	2.09104500	3.79989900	-2.12377200
H	3.35271800	4.23060700	-0.96131200
H	3.45131500	2.70065300	-1.84668100
H	0.50188800	3.28645400	1.29217300
H	1.54115500	4.60090500	0.74268900
H	0.23249700	4.02606800	-0.29637200
H	1.55109900	1.04552000	1.77669800
H	0.42887200	-0.10958800	2.00196300
Rb	2.76275100	-2.01453900	0.32476400

Table 9a
Leu-Pro-OO-ZW
82.0(91.1) kJ mol^{-1}

N	-0.31561000	1.60411200	0.28392300
C	-0.21327100	2.92778000	1.00306100
C	0.74811700	1.58196600	-0.80348100
H	-0.47082400	2.76865000	2.05118400
H	-0.93402800	3.60142300	0.53365900
C	1.21853500	3.36987600	0.72737500
C	1.41004200	2.96035600	-0.73546700
H	0.27386000	1.38995800	-1.76930500
C	1.70417800	0.40799900	-0.47924500
H	1.91771500	2.83425000	1.37866800
H	1.34553800	4.44064000	0.89503800
H	2.45264400	2.88834300	-1.04821400
H	0.89214300	3.66158900	-1.39633400
O	2.73144900	0.33509000	-1.17537000
O	1.34762700	-0.36785900	0.45409100
H	-0.06267100	0.82212600	0.92526300
C	-1.69128100	1.30943300	-0.24334700
C	-2.20543600	-0.04874500	0.20105100
O	-2.22270200	2.12192400	-0.93218800
N	-1.92451100	-0.15057600	1.63068700
H	-1.55163900	-0.77142500	-0.31190600
C	-3.65673400	-0.24706400	-0.23215300
H	-4.26446100	0.55611500	0.20592600
H	-3.71854700	-0.11833900	-1.32028800
C	-4.23943300	-1.61121300	0.15576300
H	-4.24558100	-1.68663300	1.25253200
C	-5.68684800	-1.70343200	-0.32980900
C	-3.40793900	-2.76790000	-0.40270400
H	-5.72896500	-1.66455100	-1.42412500
H	-6.14654400	-2.64218300	-0.00953500
H	-6.29264500	-0.87979400	0.05984500
H	-2.40028700	-2.81092600	0.02710800
H	-3.88899200	-3.72627800	-0.18945900
H	-3.30853900	-2.68117500	-1.49158900
H	-2.71398700	0.17418100	2.18264200
H	-1.72350900	-1.10520600	1.90698500
Rb	3.71674600	-1.86521900	0.11354300

Table 9b
Leu-NO-Pro-O-CS
0(0) kJ mol^{-1}

N	1.42642600	1.23432300	-0.41664600
C	1.51862600	2.64957300	-0.02469300
C	2.71230000	0.55802500	-0.29982000
H	1.23221700	2.77861300	1.02563700
H	0.86971000	3.26838200	-0.64855800
C	3.00808700	2.94062000	-0.20811400
C	3.65898000	1.63753000	0.26402500
H	3.04680800	0.20410100	-1.28307800
C	2.61977400	-0.66574300	0.59608900
H	3.33410600	3.81066500	0.36405700
H	3.22763500	3.11679900	-1.26575000
H	3.66807500	1.59622400	1.35864100
H	4.68110600	1.49819900	-0.08790800
O	3.81749500	-1.23350700	0.72808200
O	1.61895900	-1.08937100	1.13588800
H	3.74777400	-1.99794100	1.32180500
C	0.41043100	0.58136900	-1.01647500
C	-0.98820000	1.20405800	-1.00389900
O	0.59452600	-0.53321600	-1.51940400
N	-1.89468000	0.22819300	-1.61247900
H	-0.93944500	2.14963600	-1.56888500
C	-1.45102600	1.50479600	0.43044700
H	-1.31735600	0.60006500	1.04203100
H	-0.80568500	2.26905900	0.87459800
C	-2.90300600	1.98958100	0.54698400
H	-3.56983900	1.18476900	0.20738400
C	-3.22803000	2.27326700	2.01468100
C	-3.15436200	3.23311700	-0.30873400
H	-2.61120500	3.09655100	2.39295400
H	-4.27621200	2.55920900	2.13575200
H	-3.04189200	1.39715300	2.64440800
H	-3.03215400	3.04352000	-1.38081600
H	-4.17098000	3.60613800	-0.15877400
H	-2.46233100	4.03730800	-0.02997900
H	-2.80287400	0.65513100	-1.77190600
H	-1.53001900	-0.05914400	-2.51787000
Cs	-0.93525300	-2.42982700	0.05183000

Table 9c
Leu-NO-Pro-CS
4.2(7.0) kJ mol^{-1}

N	-1.84465400	-0.62217200	-0.82792300
C	-2.18789600	-1.89129000	-1.50031000
C	-3.02100900	0.04049800	-0.27518300
H	-1.51610600	-2.67859600	-1.15491400
H	-2.05209800	-1.77514900	-2.58089900
C	-3.65148200	-2.11168300	-1.12026900
C	-4.18993300	-0.68756200	-0.96296600
H	-3.04090700	1.11195100	-0.50181300
C	-3.05298900	-0.10373500	1.24709600
H	-3.71580100	-2.64826400	-0.16743000
H	-4.19336500	-2.68873700	-1.87085500
H	-5.11229300	-0.61584100	-0.38605100
H	-4.35697700	-0.23087600	-1.94273300
O	-4.20361700	0.34118600	1.75308100
O	-2.14662300	-0.53656000	1.92052000
H	-4.17828900	0.25303700	2.71984000
C	-0.55829200	-0.32198000	-0.57424100
C	-0.21848600	0.97724200	0.15911800
O	0.35766400	-1.06065100	-0.96013600
N	0.63465900	0.63068200	1.30579600
H	-1.13663400	1.47805500	0.48410300
C	0.51619700	1.90346700	-0.81602100
H	1.38109600	1.36321400	-1.22277500
H	-0.15104500	2.10421800	-1.66656700
C	0.97140200	3.24431100	-0.22422300
H	1.72648800	3.04941900	0.55219300
C	1.64213900	4.08074600	-1.31586000
C	-0.18777700	4.01770400	0.40774700
H	0.92182600	4.32922900	-2.10343100
H	2.02999500	5.01857100	-0.90937800
H	2.47468600	3.54333900	-1.78107000
H	-0.62070100	3.50124400	1.27156300
H	0.14561600	5.00090300	0.75033500
H	-0.98689800	4.17561500	-0.32680300
H	0.90267100	1.48820900	1.78433000
H	0.06494200	0.10539500	1.97006500
Cs	2.93551100	-1.28695700	0.21600200

Table 9d
Leu-Pro-OO-ZW
81.0(91.2) kJ mol^{-1}

N	-0.97295000	1.72326400	0.23736300
C	-1.17220100	3.02241100	0.97781400
C	0.13997400	1.93177000	-0.77642200
H	-1.51214100	2.79231700	1.98872300
H	-1.93795300	3.58426000	0.43686200
C	0.19130400	3.69147100	0.86711400
C	0.58961000	3.38421800	-0.57916400
H	-0.25174600	1.74920500	-1.77980000
C	1.23252700	0.87797800	-0.46810200
H	0.89595000	3.24000200	1.57383300
H	0.13157200	4.76031400	1.07901400
H	1.65848700	3.47391100	-0.77802600
H	0.04987600	4.04197900	-1.26643700
O	2.28866600	0.98527900	-1.11403000
O	0.94112300	0.00596000	0.40152600
H	-0.61117400	0.99334200	0.88658900
C	-2.23879900	1.18040200	-0.36002000
C	-2.59745800	-0.19253200	0.17972700
O	-2.81368400	1.83934300	-1.16804700
N	-2.37847900	-0.15246000	1.62342300
H	-1.82793600	-0.85544000	-0.24622500
C	-3.98623100	-0.61878500	-0.29353400
H	-4.71704200	0.12507600	0.05161300
H	-4.00995800	-0.58562100	-1.39007100
C	-4.40127800	-2.01483200	0.18607600
H	-4.45227600	-2.00434200	1.28422600
C	-5.79814200	-2.34211900	-0.34435200
C	-3.39717000	-3.08795300	-0.23966800
H	-5.79127800	-2.39789000	-1.43867200
H	-6.14594300	-3.30543700	0.03809500
H	-6.52588700	-1.57962400	-0.05050300
H	-2.41478900	-2.95794700	0.22914600
H	-3.75634000	-4.08267600	0.03753000
H	-3.25759000	-3.07569400	-1.32739400
H	-3.22915600	0.11184400	2.11363600
H	-2.08547100	-1.05493400	1.98135700
Cs	3.60998500	-1.30191100	0.06724700

leupro-li AIM Results

BCP #	Name	Atoms	Rho	DelSqRho	Ellipticity	K	BPL - GBL_I
1	BCP1	N1 - C17	0.339976	-0.85832	0.142133	0.56308	0.000345
2	BCP2	N1 - C2	0.243432	-0.60584	0.025154	0.304041	0.000543
3	BCP3	N1 - C3	0.258583	-0.70729	0.009754	0.318054	0.000513
4	BCP4	C2 - C6	0.247094	-0.56918	0.0168	0.199951	0.000323
5	BCP5	C2 - H4	0.285438	-1.04058	0.025012	0.297754	0.000235
6	BCP6	C2 - H5	0.282385	-1.00613	0.031231	0.290807	0.000285
7	BCP7	C6 - H11	0.279871	-0.98325	0.003253	0.2878	0.000102
8	BCP8	C6 - C7	0.2426	-0.53935	0.000306	0.193362	0.000271
9	BCP9	C3 - C7	0.241274	-0.54137	0.019217	0.195108	0.000473
10	BCP10	C3 - H8	0.280754	-0.99819	0.030733	0.288742	0.000169
11	BCP11	C3 - C9	0.252651	-0.61452	0.096315	0.208782	0.000488
12	BCP12	C6 - H10	0.27696	-0.94848	0.008923	0.281239	0.000229
13	BCP13	C7 - H12	0.281757	-1.00353	0.006688	0.291534	0.00015
14	BCP14	C7 - H13	0.27872	-0.96583	0.011065	0.284668	0.000268
15	BCP15	C9 - O14	0.310987	-0.24573	0.039234	0.490301	0.001109
16	BCP16	C9 - O15	0.410252	0.278732	0.086507	0.695395	0.000242
17	BCP17	O14 - H16	0.351983	-2.1257	0.014961	0.596296	0.000765
18	BCP18	O15 - H21	0.012529	0.048983	1.435105	-0.0016	0.437886
19	BCP19	C17 - C18	0.255554	-0.62582	0.068622	0.212334	0.00053
20	BCP20	C17 - O19	0.373427	-0.03477	0.023139	0.62218	0.000039
21	BCP21	C18 - H21	0.286331	-1.02502	0.023793	0.297725	0.00013
22	BCP22	O15 - H36	0.008887	0.035388	0.930117	-0.00104	0.20577
23	BCP23	C18 - N20	0.254739	-0.68342	0.025226	0.28408	0.000118
24	BCP24	N20 - H35	0.336747	-1.76736	0.033533	0.495105	0.00039
25	BCP25	N20 - Li37	0.030343	0.183932	0.064086	-0.00733	0.002619
26	BCP26	C18 - C22	0.242574	-0.54765	0.017544	0.19481	0.000661
27	BCP27	C22 - H23	0.274089	-0.92603	0.008569	0.276439	0.000259
28	BCP28	C22 - H24	0.273774	-0.92799	0.008179	0.276251	0.000189
29	BCP29	C25 - H26	0.273109	-0.90726	0.007913	0.274094	0.000066
30	BCP30	C25 - C28	0.243515	-0.54934	0.000565	0.193861	0.000156
31	BCP31	C22 - C25	0.241254	-0.53736	0.009213	0.191188	0.000525
32	BCP32	C27 - H30	0.276415	-0.95146	0.007085	0.282186	0.000203
33	BCP33	C25 - C27	0.243316	-0.54918	0.004764	0.194122	0.000103
34	BCP34	C28 - H32	0.27247	-0.91193	0.008072	0.275354	0.000229
35	BCP35	C27 - H29	0.27373	-0.92744	0.007158	0.277113	0.000276
36	BCP36	C27 - H31	0.274906	-0.93644	0.008185	0.279416	0.000228
37	BCP37	C28 - H33	0.276582	-0.95478	0.004661	0.282687	0.000159
38	BCP38	C28 - H34	0.272169	-0.91527	0.006907	0.274428	0.000228
39	BCP39	N20 - H36	0.333456	-1.7553	0.031902	0.490301	0.000315
40	BCP40	O19 - Li37	0.041444	0.319161	0.016213	-0.01322	0.002458
41	BCP41	O19 - Li37	0.000004	0.000001	6.153649	0.000003	10.69091

leupro-na AIM Results

BCP #	Name	Atoms	Rho	DelSqRho	Ellipticity	K	BPL - GBL_I
1	BCP1	N1 - C17	0.334085	-0.85694	0.133493	0.548383	0.000299
2	BCP2	N1 - C2	0.245488	-0.62172	0.027613	0.305553	0.000496
3	BCP3	N1 - C3	0.260332	-0.71799	0.011403	0.319344	0.000525
4	BCP4	C6 - C7	0.243106	-0.54164	0.000565	0.194091	0.000262
5	BCP5	C2 - H4	0.28525	-1.03702	0.024451	0.297234	0.000225
6	BCP6	C2 - H5	0.281923	-1.00114	0.030602	0.289803	0.00027
7	BCP7	C2 - C6	0.247335	-0.57018	0.016761	0.200153	0.000303
8	BCP8	C6 - H11	0.279568	-0.97968	0.002974	0.28717	0.000098
9	BCP9	C3 - C7	0.240342	-0.53689	0.019672	0.193481	0.000475
10	BCP10	C3 - H8	0.28099	-0.99852	0.030904	0.289079	0.000159
11	BCP11	C3 - C9	0.253464	-0.61876	0.097838	0.210294	0.000463
12	BCP12	C6 - H10	0.276857	-0.94707	0.008377	0.281095	0.000217
13	BCP13	C7 - H12	0.281572	-1.00076	0.006675	0.29108	0.000152
14	BCP14	C7 - H13	0.278726	-0.96539	0.01075	0.284698	0.000258
15	BCP15	C9 - O14	0.309824	-0.24885	0.042889	0.487895	0.001109
16	BCP16	C9 - O15	0.410221	0.282284	0.085819	0.695025	0.000253
17	BCP17	O14 - H16	0.352387	-2.12375	0.015161	0.596204	0.000768
18	BCP18	O15 - H21	0.011386	0.044696	2.035357	-0.00149	0.628369
19	BCP19	O15 - H36	0.011203	0.041804	0.243901	-0.00085	0.087903
20	BCP20	C17 - C18	0.254102	-0.61917	0.061999	0.209833	0.000455
21	BCP21	C17 - O19	0.379898	0.014948	0.03447	0.635264	0.000059
22	BCP22	C18 - N20	0.257478	-0.69703	0.029404	0.286738	0.000116
23	BCP23	N20 - H35	0.337099	-1.75794	0.035933	0.494653	0.000379
24	BCP24	N20 - Na37	0.023598	0.129983	0.014846	-0.00512	0.00196
25	BCP25	C18 - H21	0.285024	-1.00964	0.023352	0.29503	0.00014
26	BCP26	C18 - C22	0.243587	-0.55225	0.018514	0.195598	0.000593
27	BCP27	C22 - C25	0.241563	-0.53872	0.008891	0.191381	0.000457
28	BCP28	C22 - H23	0.273399	-0.91909	0.007772	0.275303	0.000246
29	BCP29	C22 - H24	0.273701	-0.92694	0.007131	0.276071	0.000167
30	BCP30	C25 - H26	0.273112	-0.90695	0.007043	0.274135	0.00005
31	BCP31	C25 - C28	0.243435	-0.54898	0.000209	0.193767	0.000141
32	BCP32	C27 - H29	0.273765	-0.9278	0.006716	0.277188	0.000264
33	BCP33	C25 - C27	0.243379	-0.54937	0.004765	0.194099	0.000095
34	BCP34	C27 - H30	0.276233	-0.94947	0.006787	0.281845	0.000195
35	BCP35	C28 - H32	0.272457	-0.91188	0.007644	0.275367	0.000222
36	BCP36	C27 - H31	0.274545	-0.9329	0.007879	0.278796	0.000223
37	BCP37	C28 - H33	0.276324	-0.95188	0.004623	0.282148	0.00016
38	BCP38	C28 - H34	0.272385	-0.91704	0.006425	0.274817	0.000216
39	BCP39	N20 - H36	0.334557	-1.75997	0.033283	0.492409	0.00033
40	BCP40	O19 - Na37	0.02988	0.205526	0.039005	-0.00885	0.003999