Supplementary Materials

The Proton Dissociation of Bio-Protic Ionic Liquids: [AAE]X Amino Acid Ionic Liquids

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The Hammett functions for [AA]X PILs in water.

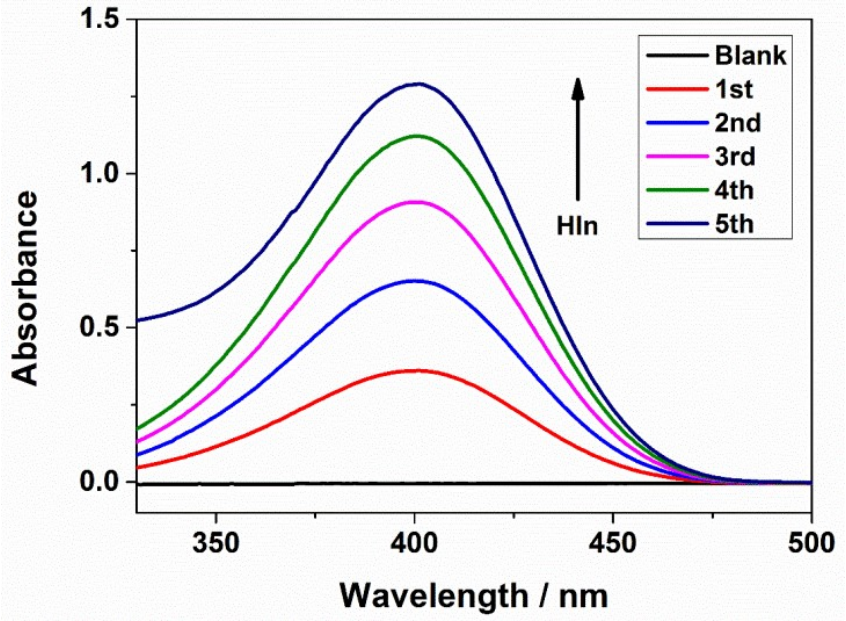
Table 1. The Hammett functions for [ValC$_1$]NO$_3$ in water.

Concentration/mol·L^{-1}	A_{max} (solvent)	A_{max} (compound)	H_0
0.0010	0.7612	0.7519	6.03
0.0025	0.7612	0.7375	5.61
0.0050	0.7612	0.7124	5.28
0.0075	0.7612	0.6875	5.09
0.0100	0.7612	0.6550	4.91
0.0250	0.7612	0.5731	4.60
0.0500	0.7612	0.4862	4.37

Table 2. The Hammett functions for [PheC$_1$]NO$_3$ in water.

Concentration/mol·L^{-1}	A_{max} (solvent)	A_{max} (compound)	H_0
0.0010	0.7612	0.7342	5.55
0.0025	0.7612	0.7092	5.25
0.0050	0.7612	0.6740	5.01
0.0075	0.7612	0.6413	4.85
0.0100	0.7612	0.6088	4.72
0.0250	0.7612	0.5371	4.50
0.0500	0.7612	0.4700	4.33

UV-Vis spectra of the titration of [AAE]X.



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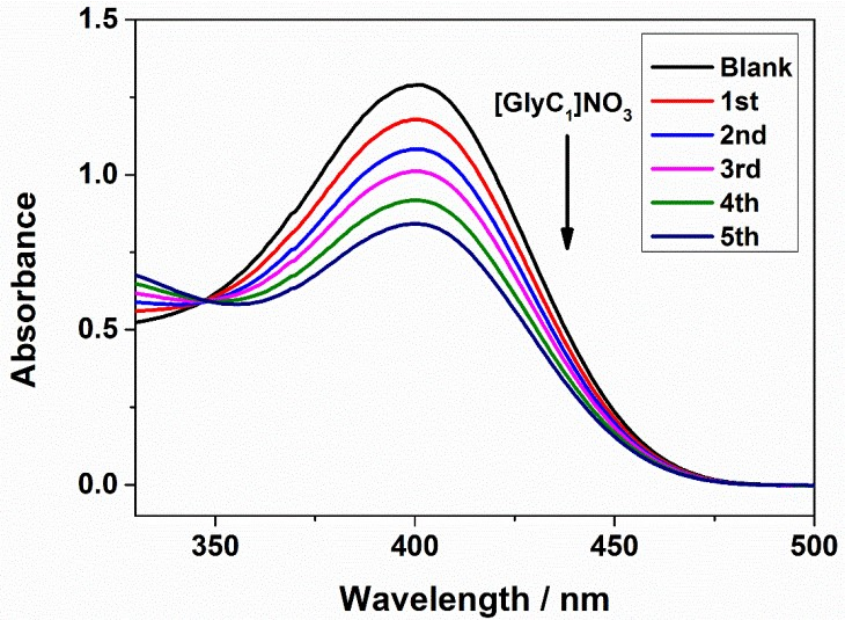
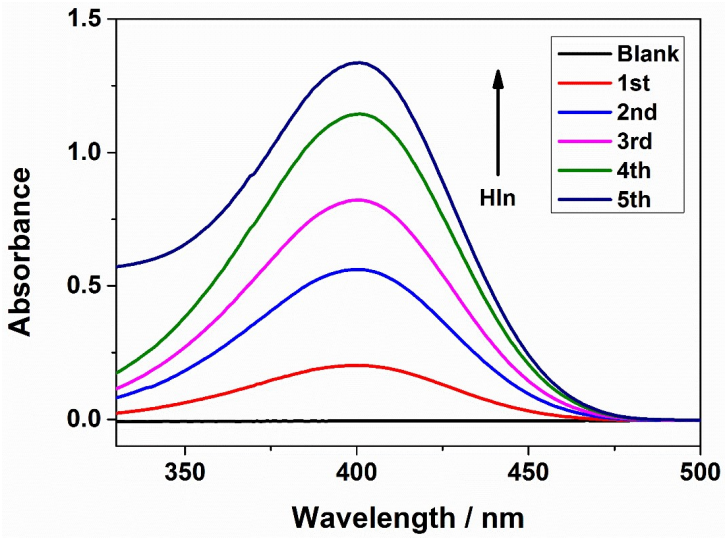


(b)

Figure S1. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of $[GlyC_1]NO_3$ in water.



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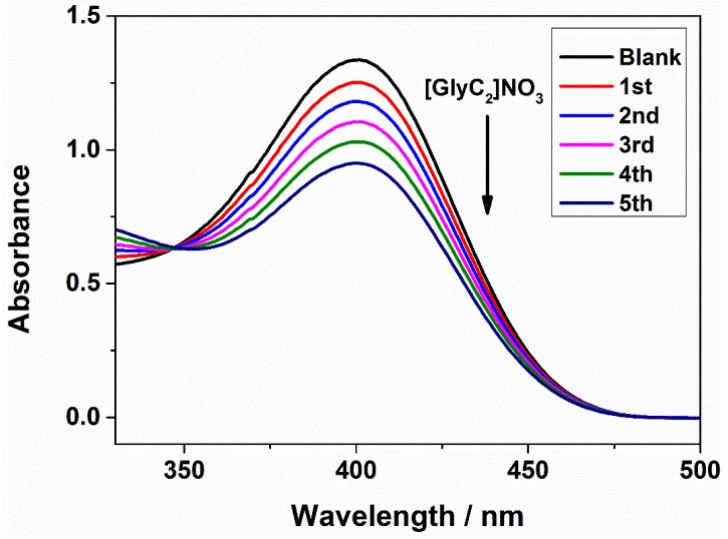
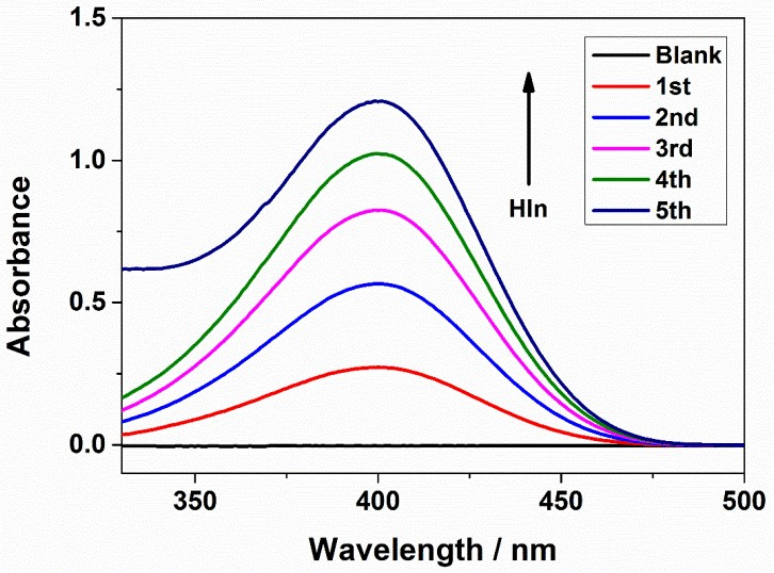


(b)

Figure S2. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of $[GlyC_2]NO_3$ in water.



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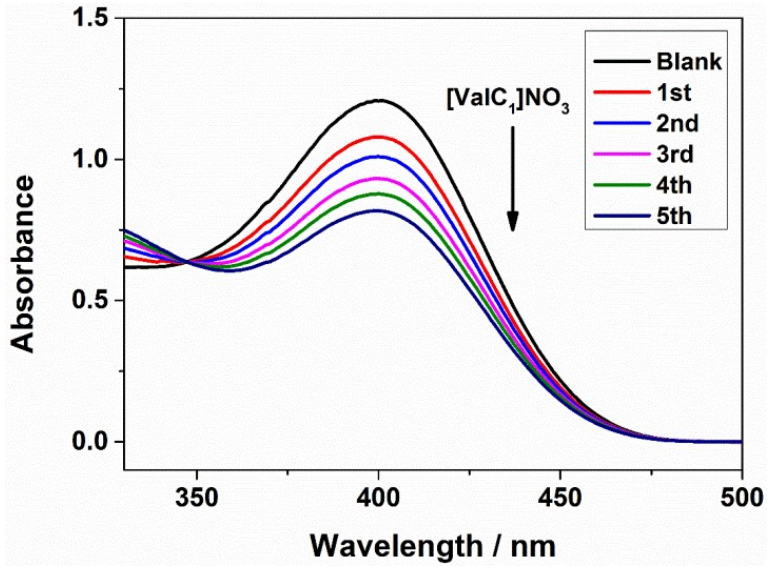
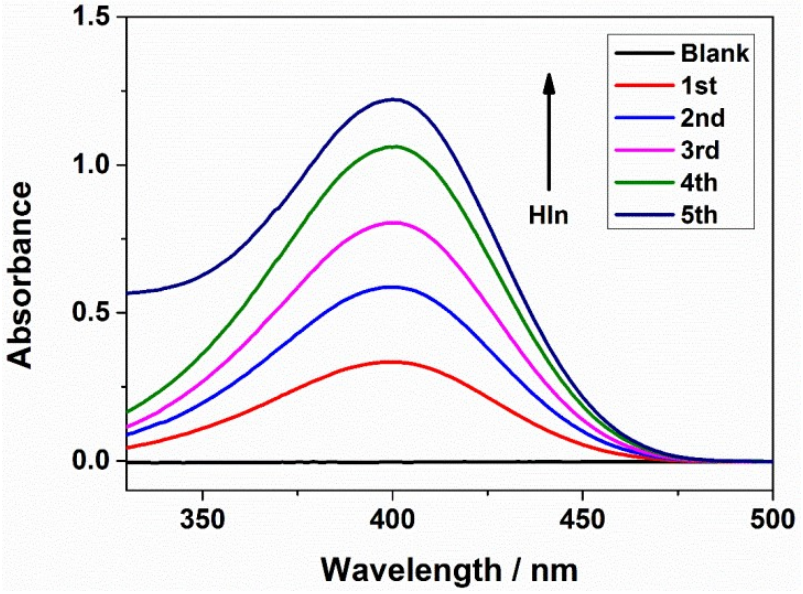


(b)

Figure S3. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of [ValC$_1$]NO$_3$ in water.



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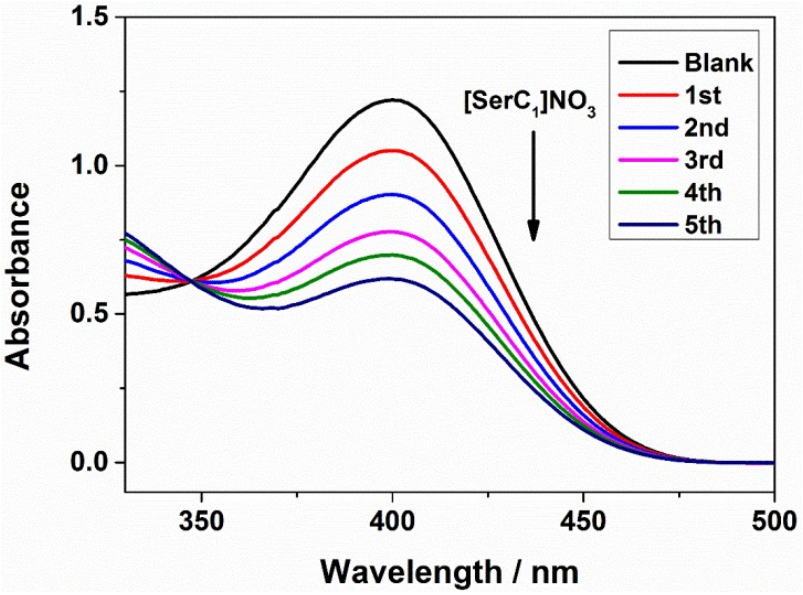
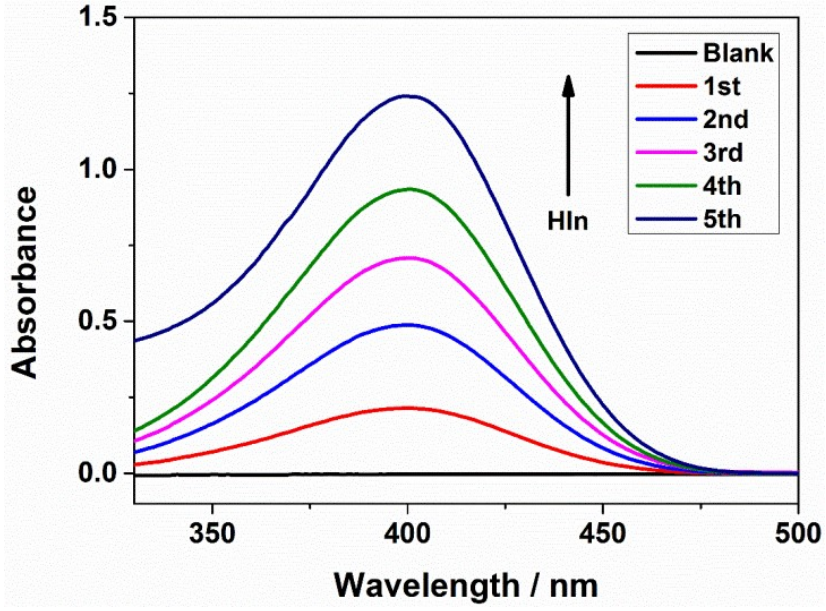


(b)

Figure S4. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of [SerC1]NO3 in water.



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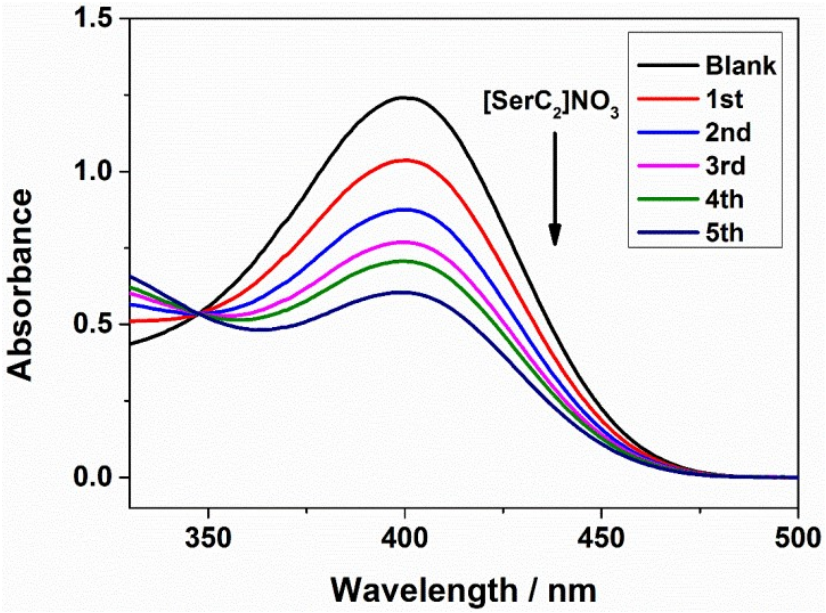
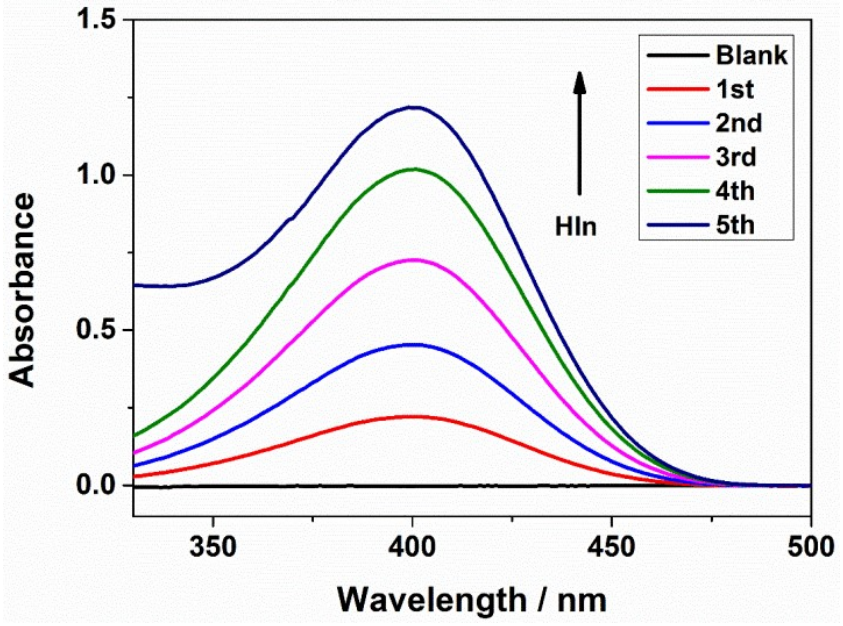


(b)

Figure S5. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of $[SerC_2]NO_3$ in water.



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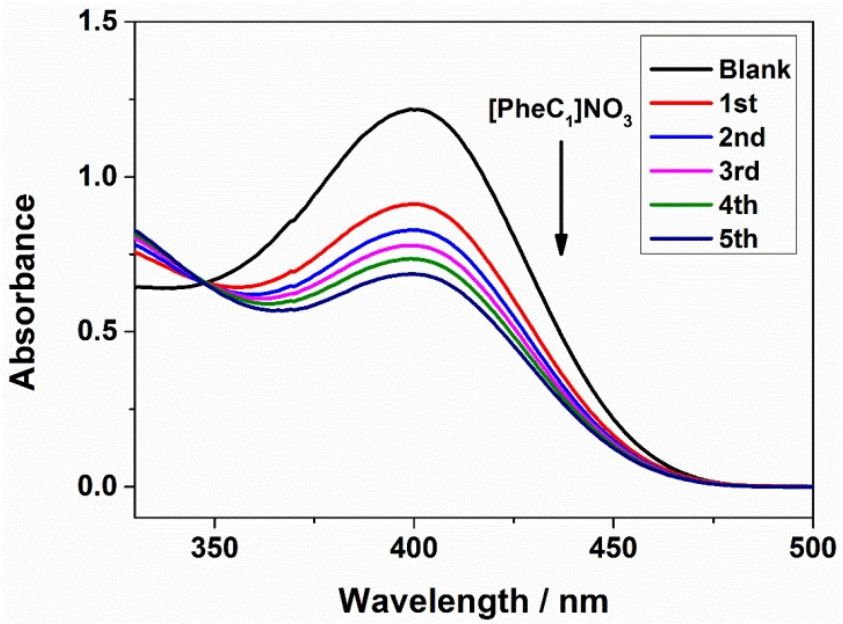
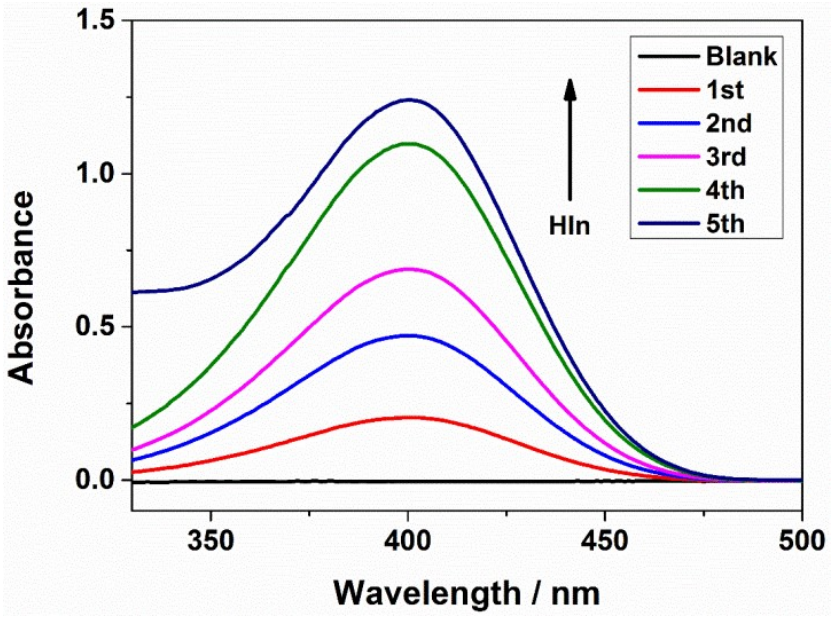


(b)

Figure S6. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of $[PheC_1]NO_3$ in water.



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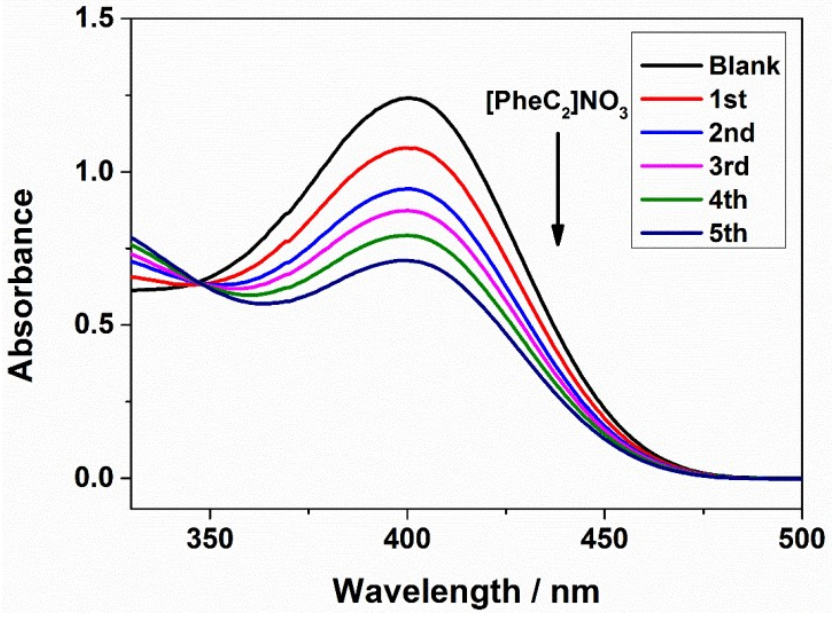
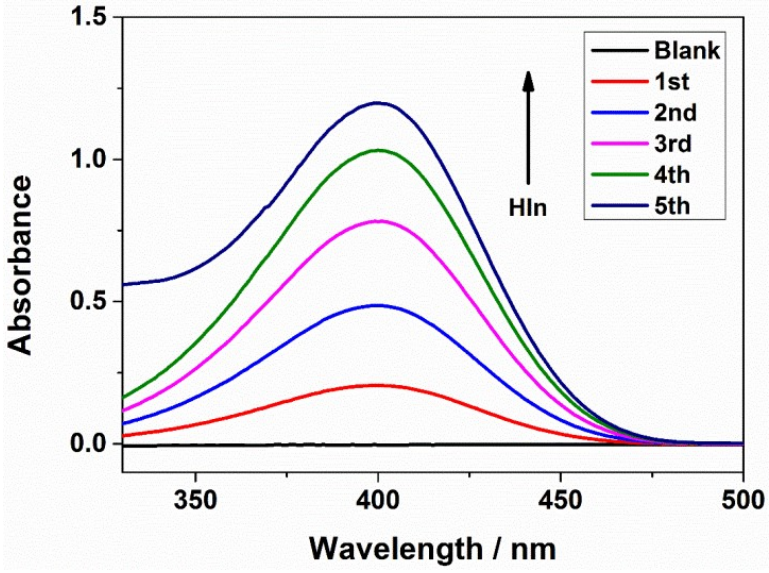


(b)

Figure S7. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of $[PheC_2]NO_3$ in water.



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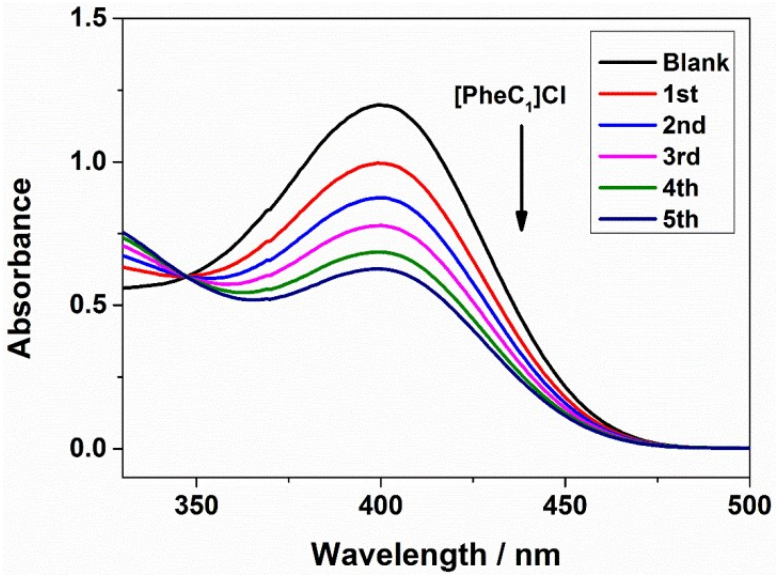
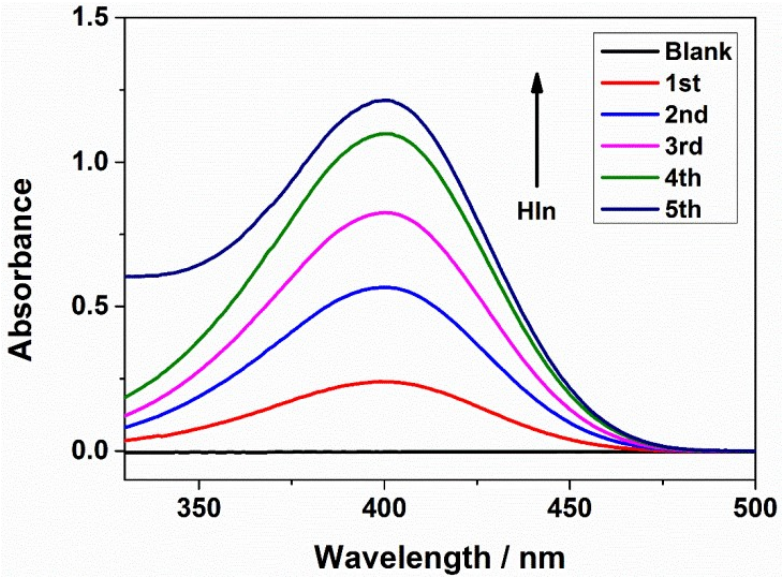


(b)

Figure S8. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of [PheC$_1$]Cl in water.



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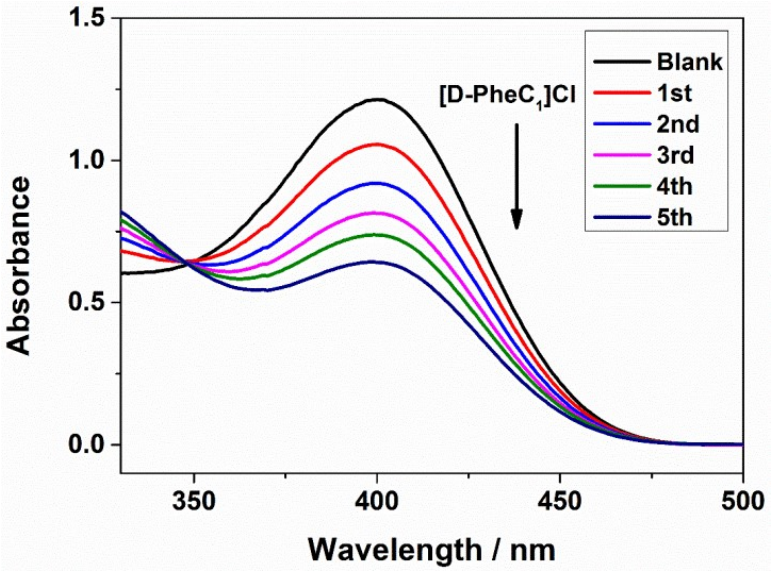
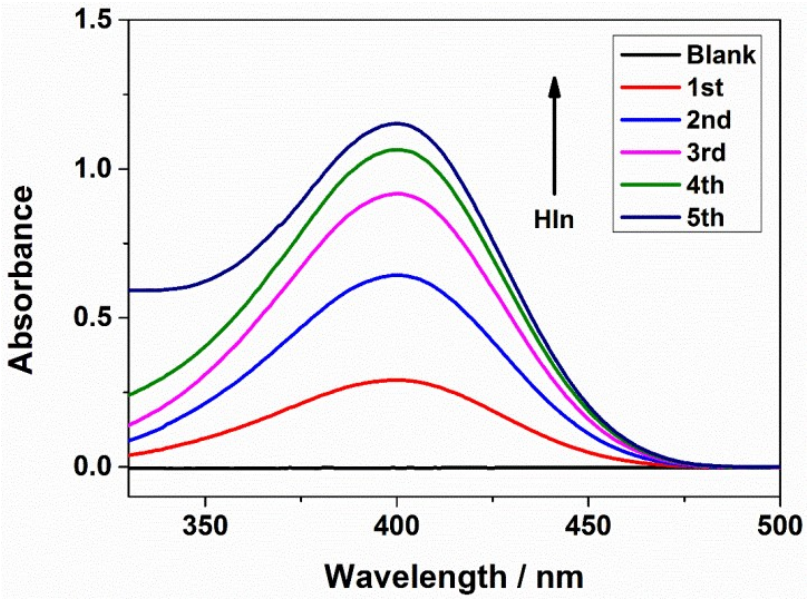


(b)

Figure S9. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of [D-PheC1]Cl in water.



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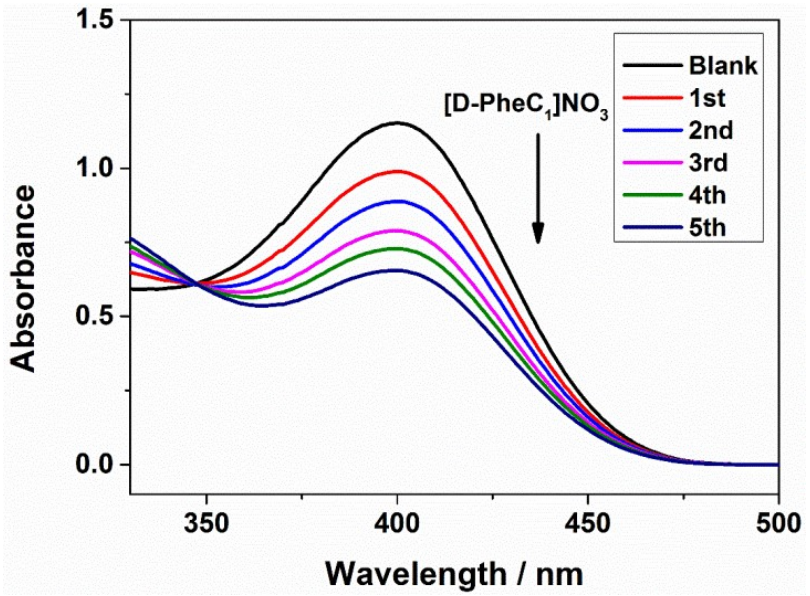
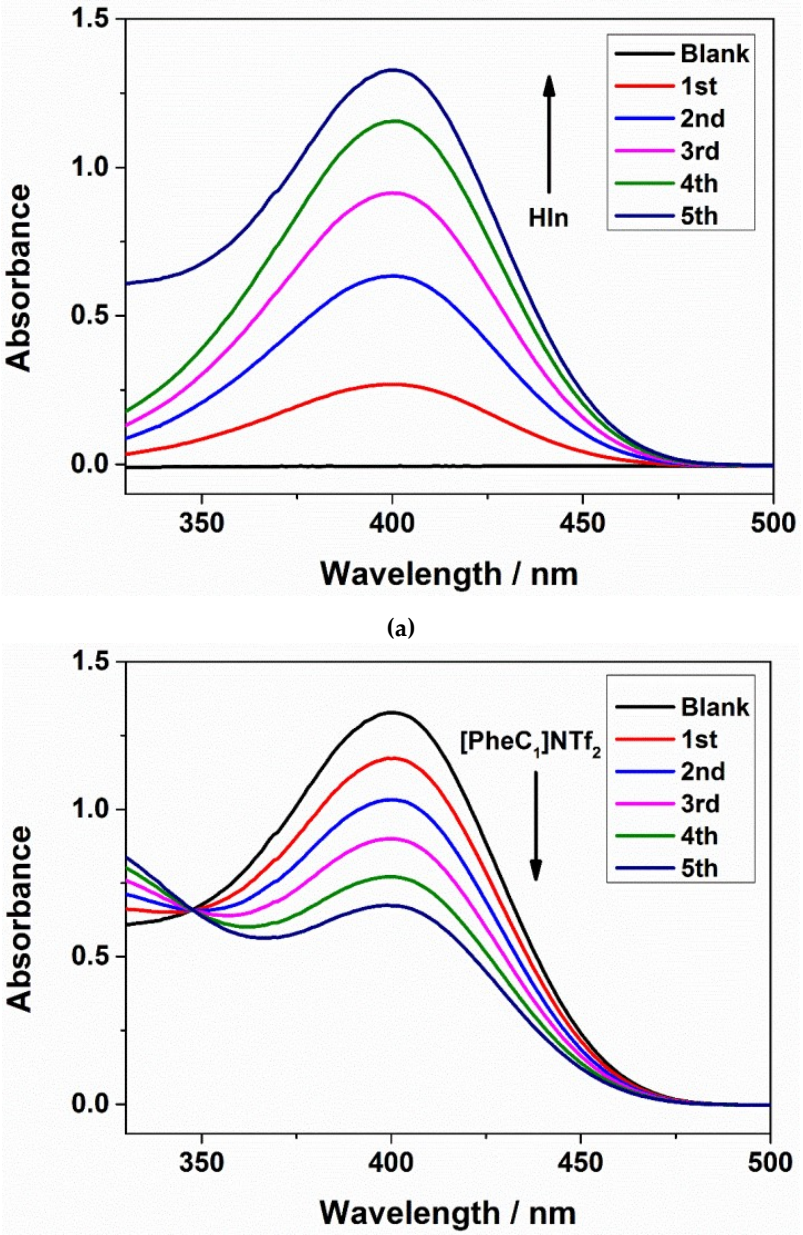


(b)

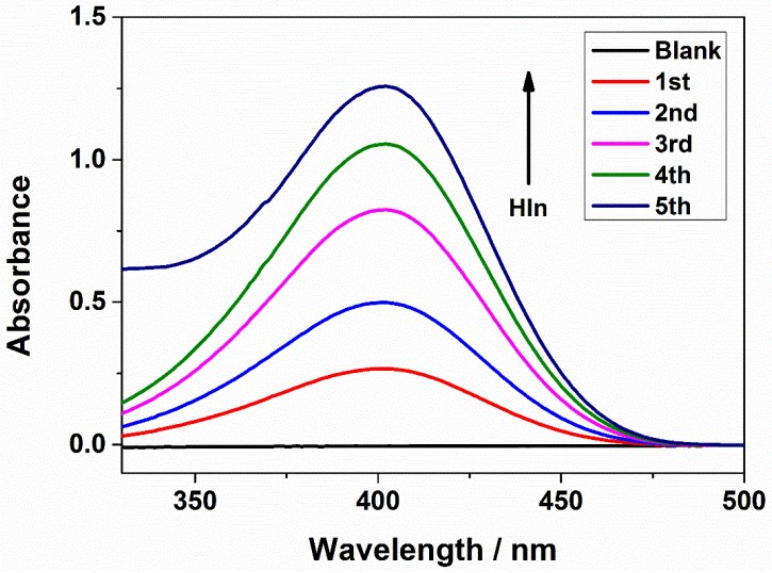
Figure S10. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of [D-PheC1]NO3 in water.



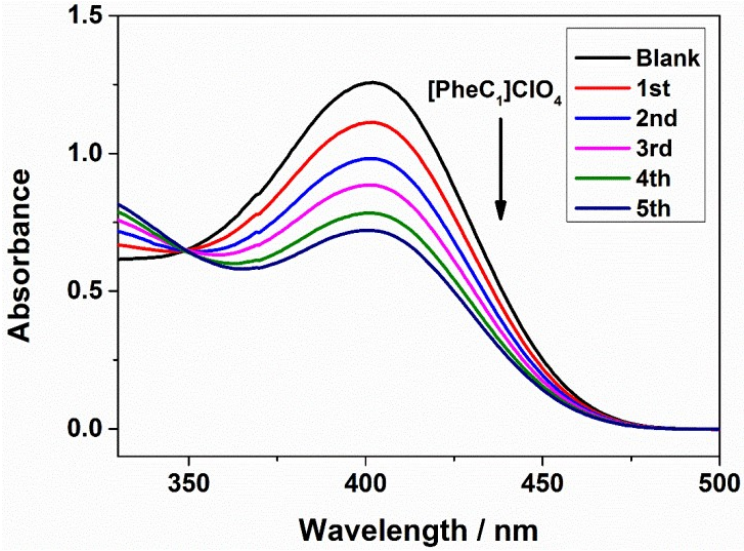
(a)

(b)

Figure S11. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of [PheC$_1$]NTf$_2$ in water.

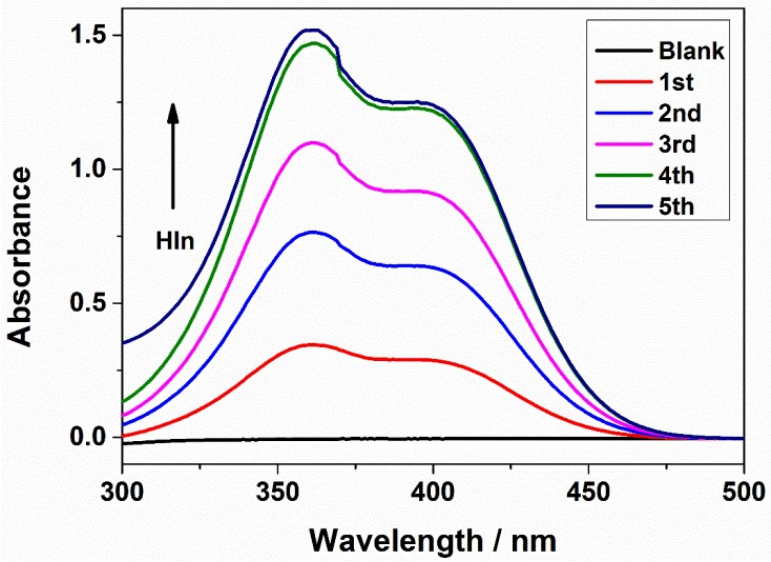


(a)

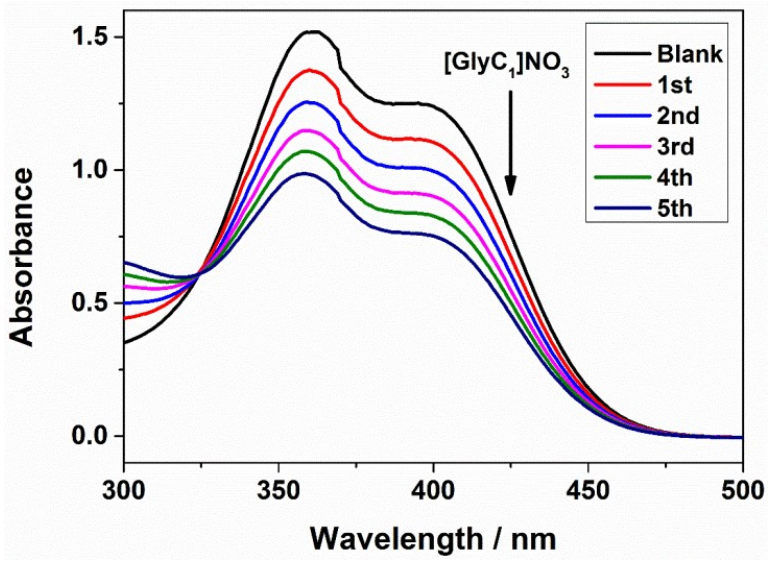


(b)

Figure S12. (**a**) The increasing absorbance during the deprotonation of the acid indicator (4-nitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (4-nitrophenolate) during the titration of $[PheC_1]ClO_4$ in water.

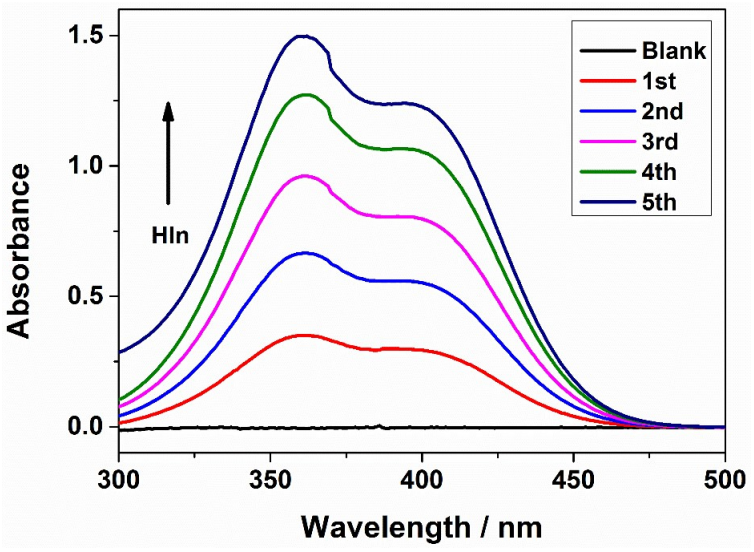


(a)



(b)

Figure S13. (**a**) The increasing absorbance during the deprotonation of the acid indicator (2,4-dinitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (2,4-dinitrophenolate) during the titration of $[GlyC_1]NO_3$ in ethanol.



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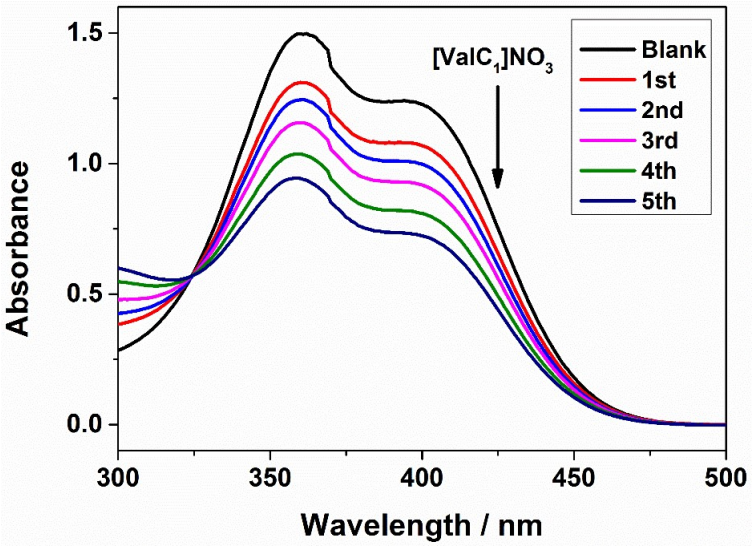
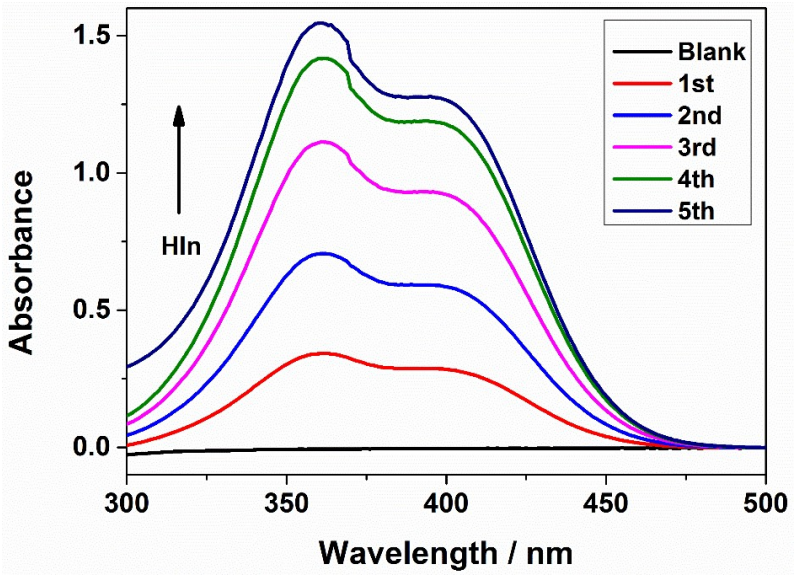


(b)

Figure S14. (**a**) The increasing absorbance during the deprotonation of the acid indicator (2,4-dinitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (2,4-dinitrophenolate) during the titration of [ValC1]NO3 in ethanol.



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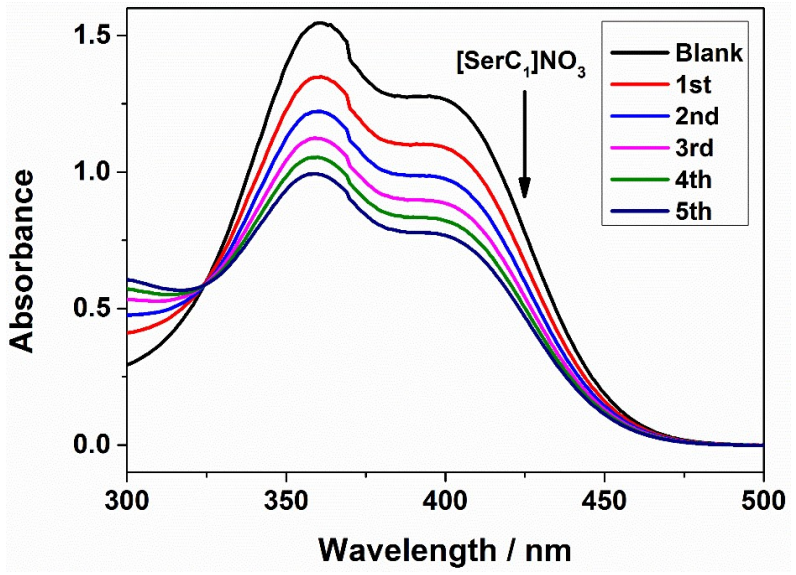
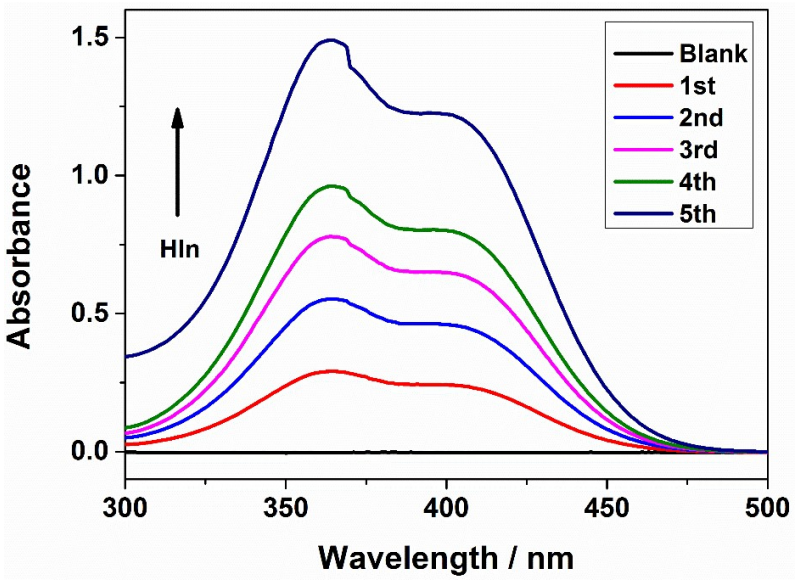


(b)

Figure S15. (**a**) The increasing absorbance during the deprotonation of the acid indicator (2,4-dinitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (2,4-dinitrophenolate) during the titration of [SerC1]NO3 in ethanol.



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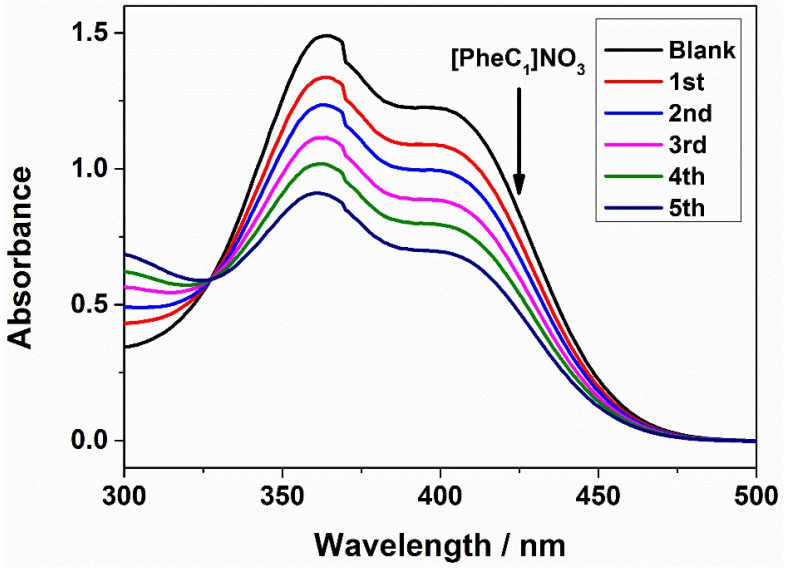
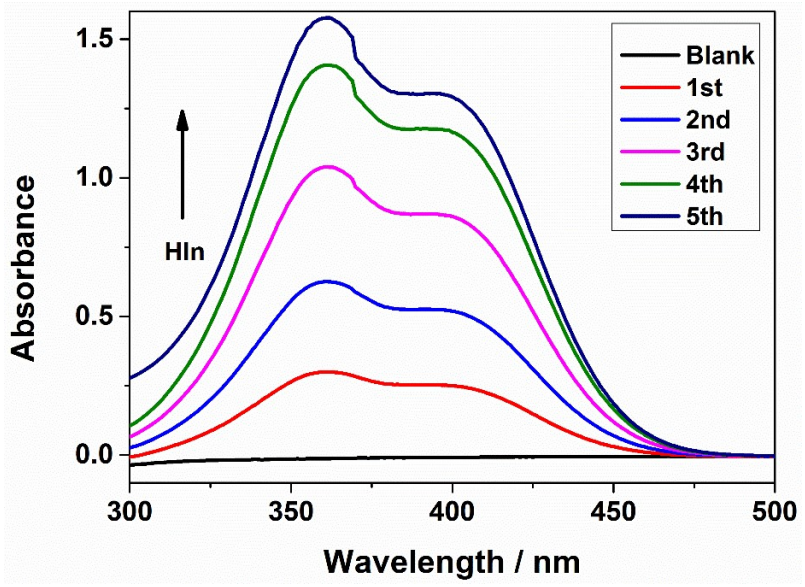


(b)

Figure S16. (**a**) The increasing absorbance during the deprotonation of the acid indicator (2,4-dinitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (2,4-dinitrophenolate) during the titration of [PheC1]NO3 in ethanol.



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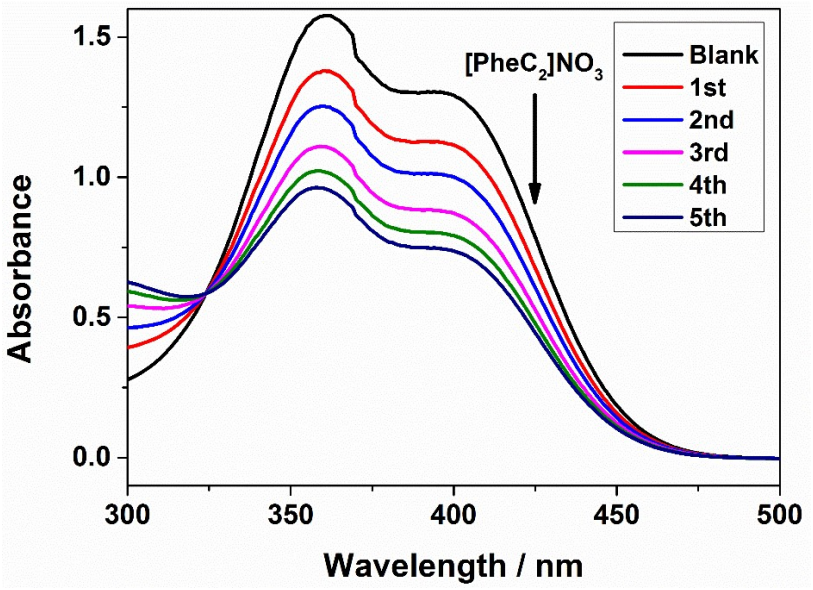

(b)

Figure S17. (**a**) The increasing absorbance during the deprotonation of the acid indicator (2,4-dinitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (2,4-dinitrophenolate) during the titration of [PheC2]NO3 in ethanol.

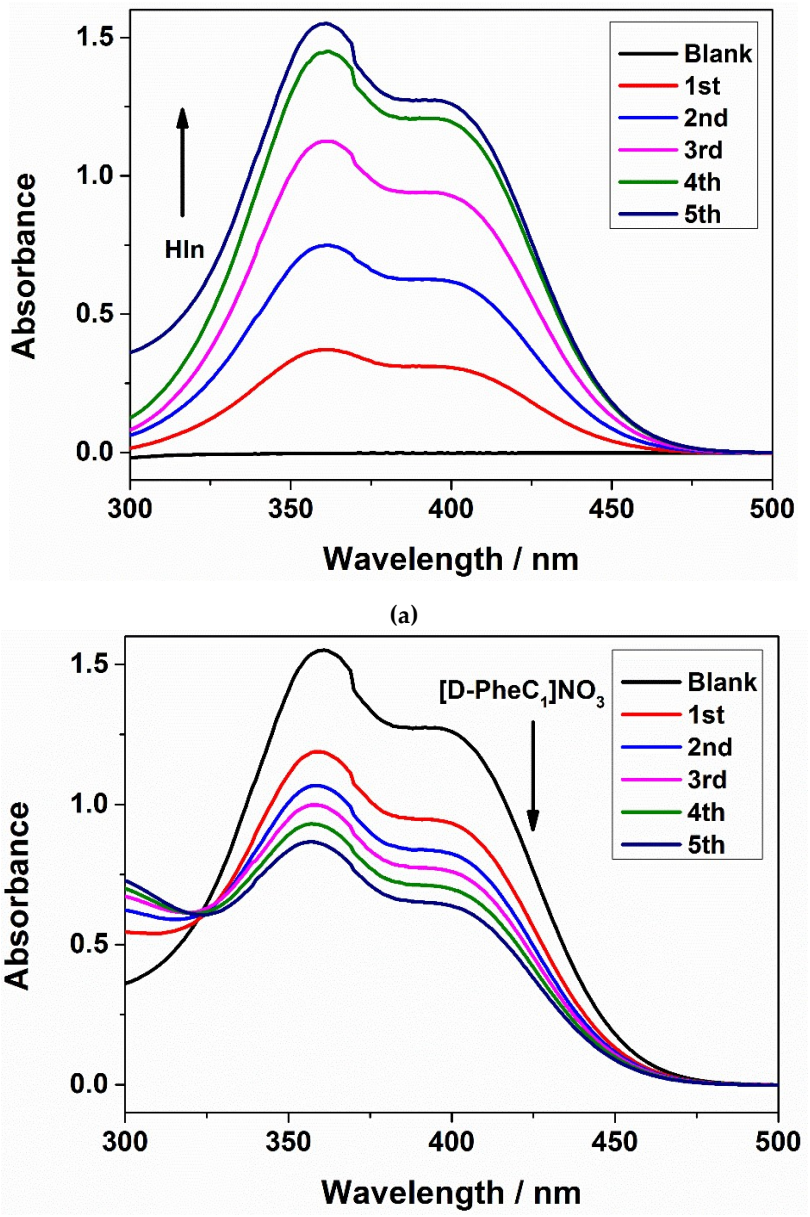

Figure S18. (**a**) The increasing absorbance during the deprotonation of the acid indicator (2,4-dinitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (2,4-dinitrophenolate) during the titration of [D-PheC1]NO3 in ethanol.

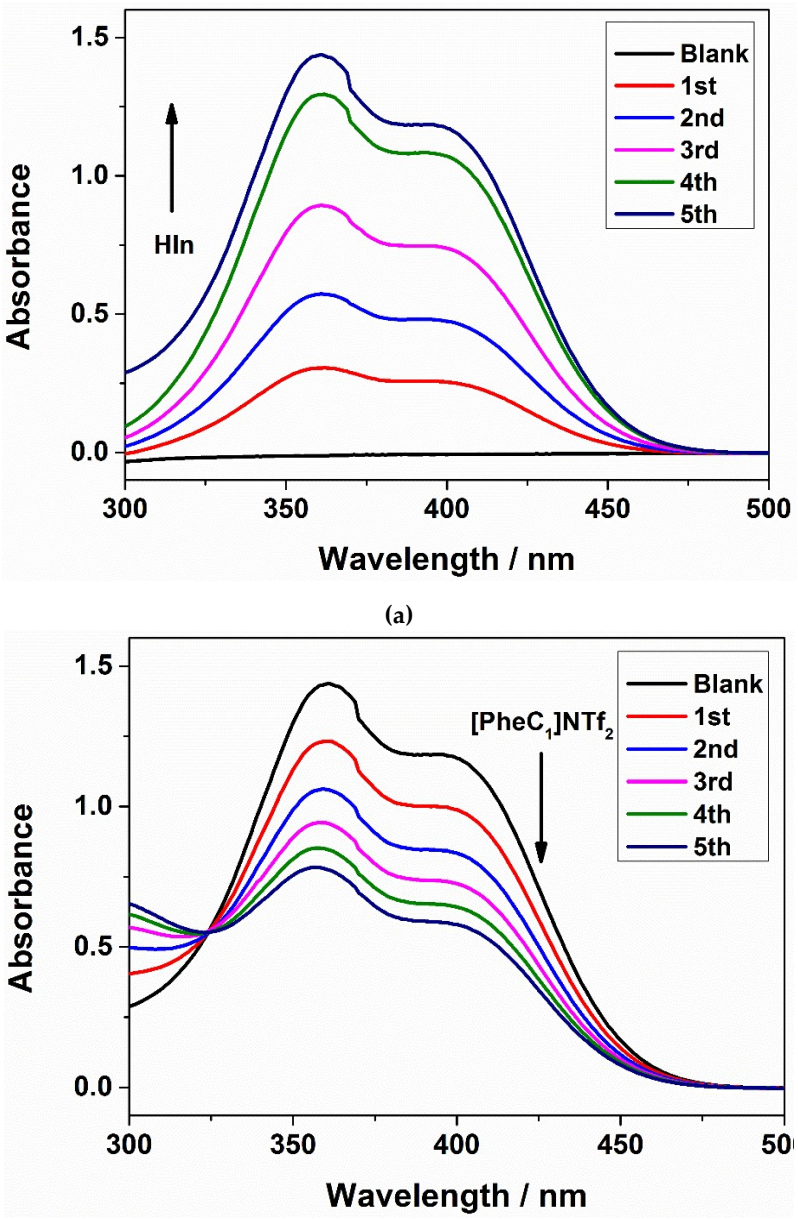

Figure S18. (**a**) The increasing absorbance during the deprotonation of the acid indicator (2,4-dinitrophenol) by the base. (**b**) The decreasing absorbance of the acid indicator anion (2,4-dinitrophenolate) during the titration of [PheC1]NTf_2 in ethanol.

The optimized geometry coordinates of [AAE]X.

The optimized geometry coordinates (Å) (B3LYP/6-311++G(d,p) level)

[GlyC1]+

C	1.15736700	−0.83142200	0.00022400
C	−0.10147200	0.04680400	−0.00003500
H	1.19788600	−1.46272100	−0.88621800
H	1.19763300	−1.46182100	0.88735300
O	0.00377400	1.25482500	0.00009800

O	−1.19023800	−0.66888800	−0.00022700
C	−2.47414900	0.04265500	0.00001700
H	−2.54187600	0.65975000	−0.89390700
H	−3.22221400	−0.74331900	−0.00314400
H	−2.54414600	0.65451200	0.89738300
H	2.91084300	0.04703500	−0.82808400
H	1.86825200	1.08090800	0.00039800
H	2.91179600	0.04656400	0.82706400
N	2.31758000	0.13476700	−0.00015000

GlyC$_1$

C	1.24658600	−0.72955800	0.00038000
C	−0.03365700	0.10293100	0.00009800
H	1.21224100	−1.39103500	−0.87073400
H	1.21259400	−1.38962700	0.87259100
O	−0.08246500	1.30842400	0.00021300
O	−1.12257400	−0.69246100	−0.00021000
C	−2.40014400	−0.02589400	−0.00009600
H	−2.50442400	0.59686300	−0.88955000
H	−3.14254700	−0.82074100	0.00042800
H	−2.50392300	0.59762500	0.88887500
N	2.48750400	0.02015800	−0.00038600
H	2.53824600	0.62634800	−0.81256700
H	2.53888900	0.62688700	0.81134800

[GlyC$_2$*]*$^+$

C	−1.57639400	−0.89895400	−0.00013100
C	−0.44553900	0.14167700	−0.00015700
H	−1.53222300	−1.52931300	0.88669100
H	−1.53258700	−1.52906100	−0.88714400
O	−0.72066900	1.32438500	0.00029800
O	0.72837100	−0.41663100	−0.00070400
C	1.92543200	0.47082900	−0.00061100
H	1.85288300	1.09740500	−0.88968100
H	1.85182100	1.09886700	0.88732600
C	3.14412800	−0.41756600	0.00078300
H	3.17699200	−1.05033600	−0.88771200
H	4.03574400	0.21421500	0.00046900
H	3.17632300	−1.04851800	0.89059500
H	−3.43129400	−0.26064000	0.82810400
H	−2.52933300	0.90115000	0.00034500
H	−3.43178600	−0.26048600	−0.82718200
N	−2.85484600	−0.09589000	0.00030500

GlyC$_2$

C	1.65807200	−0.81825600	0.00006500
C	0.52134000	0.20271700	0.00004500
H	1.52228200	−1.46593300	−0.87157100
H	1.52243200	−1.46567400	0.87191900
O	0.66442700	1.40133800	0.00013200
O	−0.67644600	−0.41361000	−0.00009200
C	−1.85188000	0.43786800	−0.00016700

H	−1.81493400	1.08032300	0.88247600
H	−1.81508200	1.07997700	−0.88307100
C	−3.07030300	−0.46171400	0.00010200
H	−3.08662100	−1.09980200	0.88645600
H	−3.97742900	0.14859000	0.00005800
H	−3.08676000	−1.10013700	−0.88600700
N	3.00029600	−0.26966700	−0.00010300
H	3.14327600	0.32249900	−0.81171200
H	3.14354600	0.32231500	0.81159000

[ValC$_1$]$^+$

C	0.56236600	0.50174100	−0.70076200
H	0.49897500	0.33956000	−1.77738100
C	1.60779700	−0.46365000	−0.08290500
C	−0.84980900	0.44417600	−0.08763200
H	2.57436600	−0.12383500	−0.48102400
C	1.65258400	−0.38560300	1.45020300
C	1.40209100	−1.90083700	−0.58145400
O	−1.27782600	1.37372000	0.56585700
H	0.72877400	−0.76200500	1.89750100
H	2.47226300	−1.00085900	1.82447900
H	1.81806900	0.62739500	1.83323600
H	1.39189500	−1.95335600	−1.67299700
H	2.22489000	−2.52420000	−0.22694500
H	0.47029800	−2.32850800	−0.21002600
O	−1.47438800	−0.67196500	−0.36495600
C	−2.83304200	−0.82869500	0.16065800
H	−3.15306600	−1.80501200	−0.18915700
H	−2.80956800	−0.78501200	1.24804700
H	−3.46665900	−0.03839100	−0.23794600
H	1.91699600	2.02501400	−0.07273500
H	0.95712500	2.50406000	−1.33672400
H	0.27484000	2.34208000	0.18491200
N	0.98094100	1.95231900	−0.47701300

ValC$_1$

C	−0.53379900	−0.51826400	−0.74803900
H	−0.30911400	−0.24054500	−1.78065600
C	−1.58545700	0.50117100	−0.21998200
C	0.77786200	−0.44429300	0.04000800
H	−2.45020500	0.33540500	−0.87174100
C	−2.02778300	0.22050300	1.22245700
C	−1.13140000	1.95712400	−0.38928500
O	1.01545600	−1.07629300	1.04262200
H	−1.20254900	0.33659600	1.93067100
H	−2.81778500	0.91915000	1.51200800
H	−2.43031600	−0.78896000	1.33349700
H	−0.81754600	2.16579200	−1.41592500
H	−1.95291300	2.63619100	−0.14501900
H	−0.29374700	2.20379100	0.26938000
O	1.65739200	0.41346300	−0.51861100
C	2.91577700	0.56938500	0.16686600

H	3.48520700	1.27923500	−0.42892000
H	2.75574200	0.95441600	1.17488900
H	3.43596600	−0.38729800	0.22803400
N	−1.09519600	−1.86904300	−0.75517000
H	−0.52781300	−2.48531800	−1.32820200
H	−1.08253700	−2.25627100	0.18393700

[SerC₁]⁺

C	0.73480600	0.24302800	−0.71796600
H	0.64626000	0.43149000	−1.78951200
C	1.41694600	−1.10223600	−0.45731900
C	−0.66097300	0.40678500	−0.08103100
H	2.28294000	−1.22359100	−1.11787400
O	−0.93266900	1.39548000	0.56139500
O	−1.44791800	−0.59944000	−0.36862800
C	−2.82363800	−0.53845500	0.13215000
H	−3.28784600	−1.45318100	−0.22235100
H	−2.80887200	−0.49633900	1.21969200
H	−3.31702000	0.34095800	−0.27787800
O	1.81019700	−1.04972200	0.90889600
H	2.20864600	−1.87930000	1.19484400
H	0.70014900	−1.90116400	−0.65821300
H	2.09141000	0.92488700	0.68806700
H	2.20739100	1.79665600	−0.74401500
H	0.89230700	2.03000400	0.29961800
N	1.56355700	1.34347200	−0.09438500

SerC₁

C	0.80434900	0.31321800	−0.67601300
H	0.66722500	0.43239200	−1.76092800
C	1.41418700	−1.07953100	−0.42086700
C	−0.58609900	0.45178000	−0.06046100
H	2.33922000	−1.15942900	−1.01022500
O	−0.92534600	1.35568400	0.66505900
O	−1.40010400	−0.53799900	−0.45556200
C	−2.74300200	−0.50394700	0.06881900
H	−3.24243500	−1.36919900	−0.36051000
H	−2.72353700	−0.57104700	1.15687800
H	−3.24305600	0.41839600	−0.22894600
N	1.68570400	1.32618100	−0.09283900
H	2.31995400	1.71725200	−0.77792600
H	1.14180600	2.07491100	0.32430700
O	1.67146400	−1.26734000	0.95644800
H	2.10439900	−0.45187200	1.25198000
H	0.73177600	−1.86655300	−0.74117300

[SerC₂]⁺

C	1.18237500	−0.12482900	0.73197000
H	1.09296800	−0.27719400	1.80908000
C	1.52834900	1.33181900	0.41671500
C	−0.10312500	−0.65641500	0.05954100
H	2.30645800	1.69446700	1.09803500

O	−0.08681600	−1.71063700	−0.53764100
O	−1.12419500	0.13127000	0.26695800
C	−2.44044200	−0.29040900	−0.27885500
H	−2.32508800	−0.36529300	−1.36037200
H	−2.65042700	−1.28078400	0.12550400
O	1.98695600	1.31305100	−0.93001300
H	2.18952800	2.20044300	−1.24634900
H	0.62972800	1.93857200	0.54639700
H	2.73952100	−0.51992400	−0.57586500
H	2.97115500	−1.29014900	0.90017300
H	1.80111200	−1.85567500	−0.19117300
N	2.27888100	−1.01993700	0.20075600
C	−3.45634500	0.74487100	0.13640100
H	−4.43364800	0.45313700	−0.25571600
H	−3.53470500	0.81321000	1.22289500
H	−3.21119700	1.72904700	−0.26696400

$SerC_2$

C	−1.25839800	−0.16480700	−0.70158400
H	−1.09617900	−0.25251400	−1.78614300
C	−1.51327500	1.31923700	−0.37391600
C	0.01781800	−0.68818700	−0.04331700
H	−2.35586400	1.66521300	−0.99027900
O	0.07523900	−1.69638700	0.62035700
O	1.07186500	0.08907100	−0.32375400
C	2.34611000	−0.30789200	0.25107900
H	2.23307200	−0.35238900	1.33604100
H	2.58765400	−1.31180600	−0.10499900
O	−1.78972200	1.48605800	1.00272200
H	−2.42602600	0.78891600	1.22398500
H	−0.63944000	1.92505300	−0.61279700
C	3.37833900	0.71480500	−0.17434600
H	4.35260000	0.44535900	0.24205500
H	3.46984100	0.75273100	−1.26217600
H	3.11502000	1.71094800	0.18759300
N	−2.39618600	−0.95316800	−0.22475100
H	−3.07030300	−1.12915200	−0.95908500
H	−2.07969500	−1.83905500	0.15696000

$[PheC_1]^+$

C	−1.10651900	1.31199800	−0.35063800
H	−1.78934500	2.02170300	−0.82305500
C	−0.03682600	0.84524700	−1.36678800
C	−1.96897800	0.20634400	0.28481600
H	0.30500200	1.71860700	−1.92830800
O	−2.11792900	0.14388200	1.48582000
O	−2.51703200	−0.57034000	−0.61896000
C	−3.43051200	−1.60894400	−0.14130000
H	−3.75316400	−2.12859000	−1.03800400
H	−2.90038200	−2.27650900	0.53573700
H	−4.27179300	−1.14268500	0.36879100
C	1.14105800	0.15570900	−0.71064800

C	2.30781600	0.88163600	−0.42631300
C	1.08305900	−1.19628200	−0.34751100
C	3.38789200	0.27230900	0.21587200
H	2.39818900	1.91372100	−0.75571300
C	2.16204600	−1.80365900	0.28949100
H	0.20384300	−1.78447300	−0.58803000
C	3.31324200	−1.06987500	0.57771300
H	4.28878900	0.84128900	0.41277200
H	2.10969000	−2.85369700	0.55184700
H	4.15301500	−1.54794000	1.06751900
H	−0.54283000	0.19034600	−2.07794400
H	−0.49758700	3.02886200	0.76863400
H	−0.98066500	1.68362200	1.67507600
H	0.51654100	1.70527900	0.91655900
N	−0.46761400	2.01074600	0.83301000

PheC₁

C	−1.20304400	1.36616800	−0.35621500
H	−1.97766600	1.83829600	−0.97112400
C	−0.09160700	0.90416800	−1.33669500
C	−1.89115500	0.18048500	0.33784700
H	0.24390100	1.79997000	−1.86420000
O	−1.96932100	0.02511200	1.53120500
O	−2.44177800	−0.66670200	−0.55932300
C	−3.14960300	−1.79649600	−0.01231000
H	−3.52117100	−2.35112300	−0.87119900
H	−2.47732500	−2.41440300	0.58442500
H	−3.97630700	−1.45975400	0.61457900
C	1.09224600	0.22766100	−0.67901700
C	2.17999700	0.97711500	−0.21292600
C	1.12848400	−1.16322600	−0.52034900
C	3.26554600	0.35631800	0.40300200
H	2.17577300	2.05430700	−0.34092600
C	2.21251100	−1.78712000	0.09396000
H	0.30474600	−1.76322400	−0.89332200
C	3.28435600	−1.02833700	0.56073500
H	4.09925300	0.95440800	0.75430200
H	2.22275200	−2.86614500	0.20250800
H	4.12995600	−1.51243700	1.03619800
H	−0.54031900	0.23347200	−2.07188300
N	−0.69832700	2.36370400	0.57334900
H	−1.45055000	2.71062900	1.15965100
H	−0.02235000	1.94237800	1.20429000

[PheC₂]⁺

C	0.54226500	1.55587300	0.44517800
H	1.12675800	2.29967800	0.99111600
C	−0.33222400	0.74054900	1.42753600
C	1.53037800	0.74726900	−0.41844800
H	−0.76338700	1.43069800	2.15724900
O	1.57520600	0.90921900	−1.62026500
O	2.28634600	−0.04050000	0.30280300

C	3.34450000	−0.80690200	−0.39920900
H	2.85035800	−1.42451100	−1.14971400
H	3.98203000	−0.08128900	−0.90511500
C	4.08305900	−1.61640400	0.63869600
H	3.41997300	−2.32430300	1.13940600
H	4.87364500	−2.18522800	0.14335700
H	4.54743300	−0.97319700	1.38823900
C	−1.43246900	−0.03511100	0.73354000
C	−2.72797200	0.49912700	0.66125100
C	−1.17727300	−1.26857900	0.11971600
C	−3.74253900	−0.17943000	−0.01731800
H	−2.96254800	1.42444500	1.18137600
C	−2.19049900	−1.94586400	−0.55388200
H	−0.19072100	−1.71434800	0.18919500
C	−3.47257000	−1.40051500	−0.62905100
H	−4.74200300	0.23791100	−0.04956400
H	−1.98271000	−2.90521900	−1.01287700
H	−4.25940200	−1.93328700	−1.14938500
H	0.34204400	0.08072000	1.97587000
H	−0.44361800	3.28283400	−0.34219600
H	0.17474500	2.18865000	−1.47836900
H	−1.23418800	1.83571700	−0.63312000
N	−0.31125300	2.29584300	−0.56483200

PheC$_2$

C	−0.57695700	1.68672300	−0.41564500
H	−1.28352200	2.23918600	−1.04532600
C	0.32963800	0.88011700	−1.38363200
C	−1.43801600	0.77039200	0.46891400
H	0.79991600	1.61114800	−2.04528500
O	−1.43446700	0.77317300	1.67544600
O	−2.23750500	−0.02460600	−0.27335100
C	−3.13204100	−0.90697000	0.45294800
H	−2.53206100	−1.56947600	1.08097900
H	−3.75794200	−0.30074800	1.11162300
C	−3.95146600	−1.67261600	−0.56533600
H	−3.31087300	−2.27036500	−1.21774300
H	−4.63964400	−2.34776600	−0.04968000
H	−4.53942600	−0.99330600	−1.18655900
C	1.39714600	0.04811100	−0.70511000
C	2.65280500	0.59363400	−0.40911100
C	1.15398800	−1.28576400	−0.35446700
C	3.63166200	−0.16736400	0.22814700
H	2.86328100	1.62104600	−0.68635300
C	2.13053400	−2.04970300	0.28140900
H	0.19364400	−1.73174000	−0.59184100
C	3.37278300	−1.49146100	0.57761600
H	4.59843400	0.27298100	0.44636500
H	1.92338200	−3.08211100	0.54109000
H	4.13454400	−2.08527300	1.07016800
H	−0.30773300	0.23898400	−1.99566100
N	0.20054500	2.65433700	0.34196300

H	−0.41187800	3.22447100	0.91634700
H	0.82138400	2.17347800	0.98698200

[D−PheC$_1$]$^+$

C	1.10637500	1.31205900	−0.35016500
H	1.78897100	2.02209800	−0.82237200
C	0.03677300	0.84545300	−1.36660900
C	1.96907600	0.20635700	0.28494200
H	−0.30477800	1.71898500	−1.92803300
H	0.54277100	0.19057600	−2.07776400
C	−1.14125200	0.15588200	−0.71077600
O	2.11769600	0.14329000	1.48595400
C	−2.30814400	0.88148200	−0.42681000
C	−1.08287100	−1.19613000	−0.34729200
H	−2.39884700	1.91350000	−0.75632600
C	−3.38824300	0.27192600	0.21539700
C	−2.16169800	−1.80362400	0.28965300
H	−0.20347300	−1.78408500	−0.58772400
H	−4.28932700	0.84073500	0.41195300
C	−3.31324200	−1.07005200	0.57755100
H	−2.10925700	−2.85358200	0.55234600
H	−4.15287200	−1.54835400	1.06737600
O	2.51750200	−0.56972700	−0.61918100
C	3.43122200	−1.60826300	−0.14191300
H	3.74854200	−2.13207000	−1.03808900
H	4.27595100	−1.14144400	0.36194800
H	2.90330700	−2.27201700	0.54053000
H	0.49617600	3.02831000	0.76940700
H	−0.51688900	1.70392500	0.91721700
H	0.98028800	1.68350100	1.67581700
N	0.46712500	2.01012500	0.83366600

D−PheC$_1$

C	1.20273000	1.36638400	−0.35574200
H	1.97738600	1.83896600	−0.97028200
C	0.09155300	0.90452300	−1.33655000
C	1.89098800	0.18057700	0.33791000
H	−0.24400200	1.80038900	−1.86391400
H	0.54046900	0.23404200	−2.07180500
C	−1.09226500	0.22776900	−0.67908000
O	1.96914300	0.02476700	1.53119500
C	−2.18046400	0.97686300	−0.21351300
C	−1.12783600	−1.16308600	−0.51988500
H	−2.17672100	2.05401600	−0.34184200
C	−3.26587900	0.35574700	0.40237400
C	−2.21170600	−1.78728900	0.09433600
H	−0.30358100	−1.76266900	−0.89236700
H	−4.09993800	0.95358600	0.75326300
C	−3.28407000	−1.02884500	0.56053700
H	−2.22147600	−2.86627300	0.20329800
H	−4.12955400	−1.51323000	1.03591500
O	2.44181500	−0.66618800	−0.55958600

C	3.15011200	−1.79588400	−0.01298000
H	3.52285300	−2.34943700	−0.87205700
H	3.97598300	−1.45907400	0.61496900
H	2.47781300	−2.41489700	0.58260200
N	0.69758300	2.36336800	0.57419000
H	0.02145900	1.94166600	1.20472400
H	1.44958700	2.71015600	1.16085500

H_3O^+

O	0.00000300	0.00002800	−0.06915700
H	−0.78749300	−0.52584700	0.18439200
H	−0.06184000	0.94443300	0.18445800
H	0.84930600	−0.41881000	0.18440500

H_2O

O	0.00000000	0.00000000	0.11704100
H	0.00000000	0.76348700	−0.46816500
H	0.00000000	−0.76348700	−0.46816500

$EtOH_2^+$

C	−1.27517800	−0.27947300	−0.02593700
H	−1.32931100	−0.97383600	0.81631200
H	−1.31778700	−0.82180700	−0.97122900
H	−2.16100700	0.36205300	0.03247700
C	−0.08290700	0.62254800	0.05131800
H	0.03625300	1.28909300	−0.79959100
H	0.04437100	1.14226000	0.99918000
O	1.20049700	−0.27713400	−0.08665500
H	1.22188000	−1.03935100	0.52091300
H	2.05014000	0.20020600	−0.05711000

EtOH

C	1.22356400	−0.22355400	0.00000600
H	1.29174600	−0.85987300	−0.88568400
H	1.29173600	−0.85980600	0.88574000
H	2.07458400	0.46354700	−0.00001700
C	−0.08147300	0.54986700	−0.00000500
H	−0.13968500	1.19452500	0.88775100
H	−0.13965600	1.19446700	−0.88780300
O	−1.15506700	−0.39631100	−0.00000800
H	−1.99073300	0.07974300	0.00006500