

Supporting Information

For

Using differential mobility spectrometry to measure ion solvation: An examination of the roles of solvents and ionic structures for separating quinoline-based drugs

Chang Liu,^a J. C. Yves Le Blanc,^a Jefry Shields,^b John S. Janiszewski,^b Christian Ieritano,^c Gene F. Ye,^c Gillian F. Hawes,^c W. Scott Hopkins^{*c}, and J. Larry Campbell^{*a,c}

^aSCIEX, 71 Four Valley Drive, Concord, ON, Canada. Email: larry.campbell@sciex.com.

^bGroton lab, Pfizer Global Research and Development, Groton, CT, USA

^cDepartment of Chemistry, University of Waterloo, Waterloo, ON, Canada. Email: scott.hopkins@uwaterloo.ca.

Contents

Figure S1. Cross sectional schematic of the DMS-MS.....	4
Figure S2. 2,6- and 2,8-Dimethylquinolinium Water Binding Energies	5
Table S1. Mass spectrometer parameters used to detect the ions of this study	6
2,6-dimethylquinolinium XYZ Coordinates	7
1 water.....	7
2 water.....	8
3 water.....	9
4 water.....	10
5 water.....	11
6 water.....	12
7 water.....	13
8 water.....	14
2,8-dimethylquinolinium XYZ Coordinates	15
1 water.....	15
2 water.....	16
3 water.....	17
4 water.....	18
5 water.....	19
6 water.....	20
7 water.....	21
8 water.....	22
6-amino-2-methylquinolinium•H ₂ O XYZ Coordinates	23
8-amino-2-methylquinolinium•H ₂ O XYZ Coordinates	24
6-methoxy-2-methylquinolinium•H ₂ O XYZ Coordinates	25
8-methoxy-2-methylquinolinium•H ₂ O XYZ Coordinates	26
7-chloro-2-methylquinolinium•H ₂ O XYZ Coordinates	27
8-chloro-2-methylquinolinium•H ₂ O XYZ Coordinates	28
2-methyl-6-nitroquinolinium•H ₂ O XYZ Coordinates	29
2-methyl-8-nitroquinolinium•H ₂ O XYZ Coordinates	30

Figure S1. Cross sectional schematic of the DMS-MS.

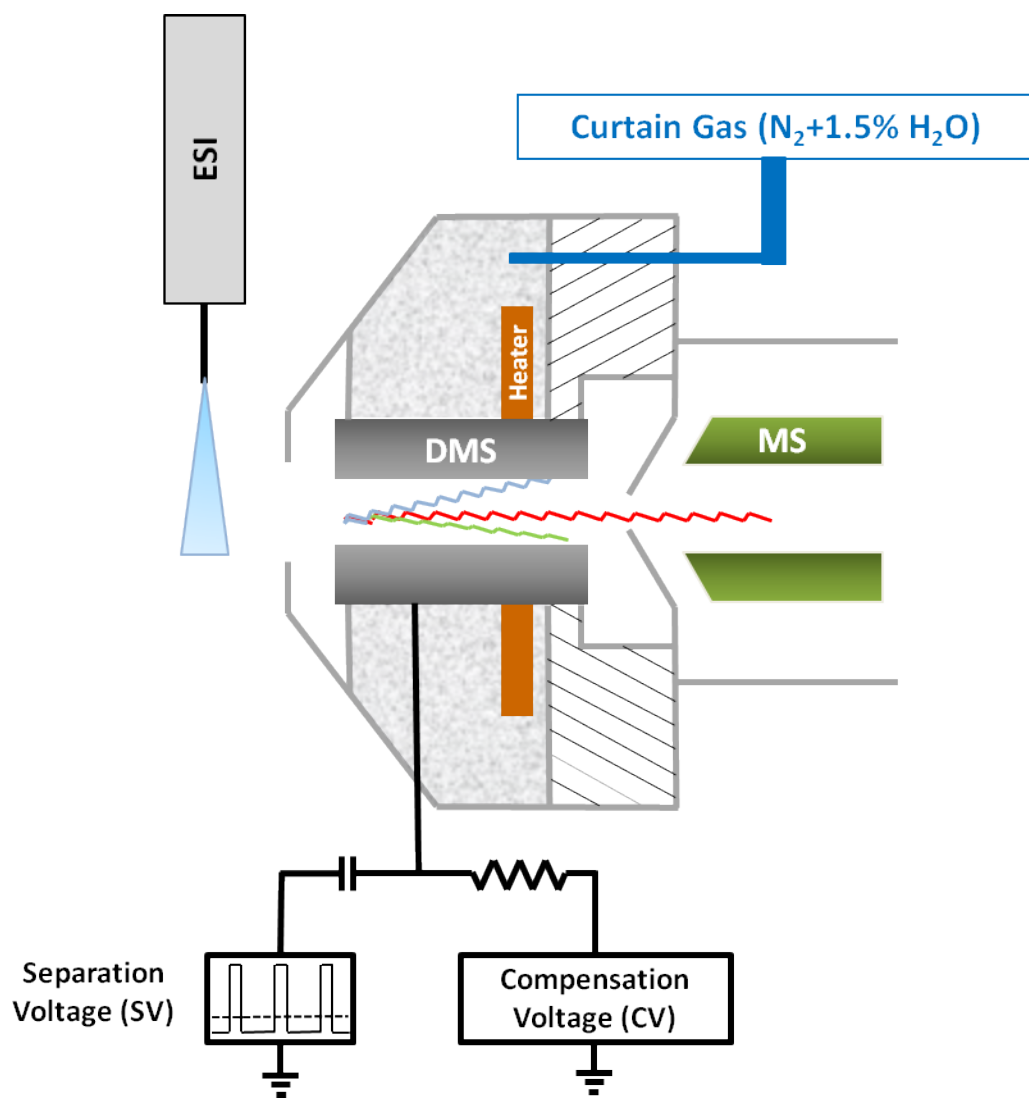


Figure S2. 2,6- and 2,8-Dimethylquinolinium Water Binding Energies

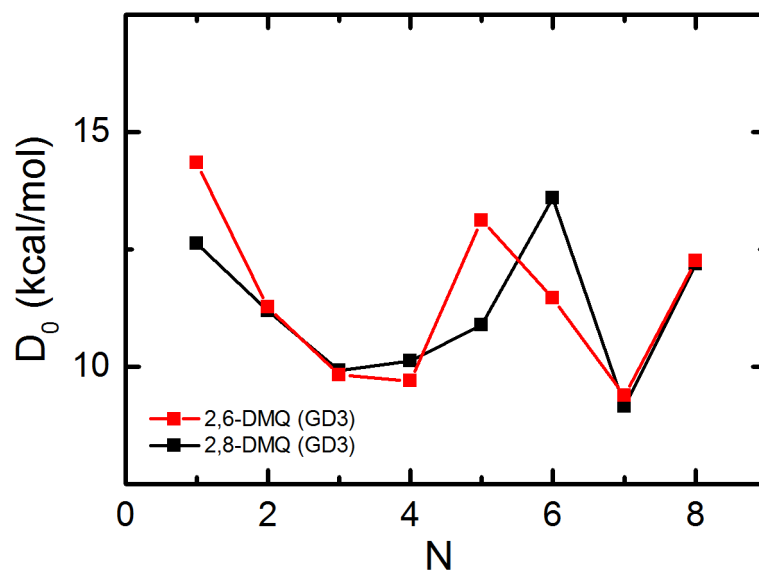


Figure S2. Calculated binding energies for loss of a single water from an N water cluster. Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory and include GD3 dispersion correction. Red points are for clusters containing 2,6-dimethylquinolinium, and black points are for clusters containing 2,8-dimethylquinolinium. Lines serve only as a guide to the eye.

Table S1. Mass spectrometer parameters used to detect the ions of this study

Analyte	Q1	Q3	Collision energy (eV _{Lab})
8-amino-2-methylquinoline	159.1	117.0	47
6-amino-2-methylquinoline	159.1	117.0	47
8-methoxy-2-methylquinoline	174.1	131.0	43
6-methoxy-2-methylquinoline	174.1	131.0	39
2,8-dimethylquinoline	158.1	91.0	47
2,6-dimethylquinoline	158.1	91.0	47
8-chloro-2-methylquinoline	178.1	178.1	10
7-chloro-2-methylquinoline	178.1	115.1	53
2-methyl-8-nitroquinoline	189.2	143.0	30
2-methyl-6-nitroquinoline	189.2	143.0	30

2,6-dimethylquinolinium XYZ Coordinates

1 water

C	2.08869100	1.40883200	0.00001600
C	0.71368700	1.45166000	0.00010100
C	-0.00150600	0.24079700	0.00005400
C	0.68370600	-1.00230900	-0.00008500
C	2.09954400	-0.99820700	-0.00017100
C	2.81098700	0.18335900	-0.00012100
H	2.64492700	2.33994200	0.00005600
H	0.17924100	2.39435400	0.00020700
C	-0.09684700	-2.18296300	-0.00013800
H	2.62008600	-1.94941200	-0.00027900
C	-1.47190600	-2.12378200	-0.00005000
C	-2.12482500	-0.87848000	0.00010000
H	0.40370000	-3.14514900	-0.00025400
H	-2.07161300	-3.02437300	-0.00009300
N	-1.37874000	0.23114000	0.00013800
H	-1.85581100	1.14421400	0.00021500
C	-3.61541200	-0.74757000	0.00030000
H	-4.03319200	-1.24400700	-0.87962300
H	-4.03281700	-1.24285100	0.88106400
H	-3.93423800	0.29490600	-0.00029100
C	4.31532600	0.20953700	-0.00020500
H	4.69205000	0.73788400	0.88035400
H	4.73721800	-0.79581800	-0.00034500
H	4.69195000	0.73808900	-0.88068500
O	-2.62621300	2.77422600	0.00000600
H	-2.89479200	3.28762900	0.77078300
H	-2.89450000	3.28755900	-0.77091900

2 water

C	1.89011600	-1.81844800	0.27650400
C	0.60842200	-1.33040100	0.37948300
C	0.38615100	0.04193400	0.16195600
C	1.46581500	0.90514100	-0.16017600
C	2.76853800	0.35861900	-0.25626100
C	2.99734900	-0.98459900	-0.04349300
H	2.06697300	-2.87532800	0.44443000
H	-0.22615900	-1.97718100	0.62279000
C	1.17206400	2.27444400	-0.36750400
H	3.59116700	1.02089300	-0.50234400
C	-0.11594700	2.74571700	-0.25911100
C	-1.16487700	1.86493200	0.06361700
H	1.97970200	2.95484600	-0.61490700
H	-0.34542900	3.79134400	-0.41664900
N	-0.87863200	0.57504800	0.25736400
H	-1.65248200	-0.07548300	0.49867500
C	-2.58560300	2.31575000	0.19945500
H	-2.92198900	2.77356000	-0.73462800
H	-3.25015400	1.48824400	0.44719600
H	-2.66179200	3.07730800	0.98028300
C	4.37371600	-1.58513800	-0.14008400
H	5.12470900	-0.83663700	-0.39454000
H	4.66077900	-2.04749000	0.80879900
H	4.40048200	-2.36847200	-0.90309100
O	-2.89716800	-1.18661300	0.88649200
H	-3.47187800	-1.64928600	0.24051900
H	-3.20324900	-1.43936500	1.76326800
O	-4.47725300	-2.44564400	-0.96783600
H	-4.34497900	-3.33824800	-1.30497600
H	-5.37438400	-2.19368400	-1.21193200

3 water

C	2.30776100	-1.96479200	0.28586100
C	1.10881700	-1.31831600	0.47490900
C	1.03442100	0.06216500	0.21088300
C	2.17574300	0.77186100	-0.24518200
C	3.38928100	0.06499700	-0.42604900
C	3.47336200	-1.28695900	-0.16773200
H	2.37108900	-3.02849700	0.48841200
H	0.22692600	-1.84554600	0.81874300
C	2.02990100	2.15779300	-0.49453800
H	4.25961200	0.61026300	-0.77414300
C	0.82237800	2.78736800	-0.30001900
C	-0.29032500	2.05494000	0.15521700
H	2.88676900	2.72336600	-0.84434300
H	0.70517300	3.84610600	-0.49028700
N	-0.14357000	0.74932300	0.38873900
H	-0.96672200	0.20546800	0.72999500
C	-1.62883000	2.68214600	0.39109400
H	-1.97280400	3.17967200	-0.51926900
H	-2.37231800	1.94534000	0.69461500
H	-1.54963000	3.44628300	1.16949400
C	4.75379300	-2.05613800	-0.35116000
H	4.61861200	-2.86510800	-1.07496400
H	5.56305000	-1.41589600	-0.70367500
H	5.06737200	-2.51428400	0.59137200
O	-4.05744300	-1.68597400	-0.48258500
H	-4.98007400	-1.37474600	-0.56984000
H	-4.03165800	-2.57612900	-0.84578100
O	-2.25900100	-0.72868700	1.24638100
H	-2.54485200	-0.91858100	2.14490200
H	-2.94390900	-1.09943100	0.63642100
O	-6.67333100	-0.81086400	-0.72617700
H	-7.40657900	-1.04982500	-0.14947500
H	-7.06468600	-0.43989400	-1.52401100

4 water

C	1.13328600	2.34635500	0.41432800
C	0.63112300	1.06907700	0.50000000
C	1.48171600	-0.01432400	0.20987500
C	2.83110100	0.20927300	-0.16844700
C	3.30484500	1.54149600	-0.24389200
C	2.48064900	2.60942800	0.04164100
H	0.48228000	3.18495200	0.63668900
H	-0.39846500	0.88181000	0.78082100
C	3.62951400	-0.92496700	-0.45223000
H	4.33646100	1.70918300	-0.53318000
C	3.10898400	-2.19483200	-0.36364200
C	1.76628500	-2.38231400	0.01724000
H	4.66414200	-0.78126500	-0.74434600
H	3.71380200	-3.06521200	-0.58164900
N	1.02203000	-1.30796100	0.28513600
H	0.02590400	-1.44811400	0.57302600
C	1.14289100	-3.73781400	0.13843800
H	0.08183200	-3.67288700	0.37858400
H	1.26398900	-4.28847700	-0.79783800
H	1.64933200	-4.31103200	0.92031700
C	2.96558000	4.03245600	-0.02988200
H	2.36232200	4.61214400	-0.73450200
H	2.88010500	4.51901800	0.94624400
H	4.00731300	4.08898100	-0.34726600
O	-3.39742800	-1.20712500	-0.87944400
H	-3.99610900	-0.42539400	-0.85575400
H	-3.85739100	-1.89446100	-1.36961900
O	-7.51714000	1.06065400	0.41387800
H	-7.76207600	1.59660800	1.17517400
H	-8.32405100	0.63233800	0.11019300
O	-5.00955700	0.96396000	-0.78801600
H	-5.03842700	1.61741300	-1.49297400
H	-5.88409700	0.98736100	-0.35478700
O	-1.56852800	-1.66844400	0.97438100
H	-1.98162400	-1.78749900	1.83446700
H	-2.29405700	-1.51511200	0.31348400

5 water

C	1.59744200	-2.16501400	-0.01164900
C	0.78857800	-1.05246200	-0.00650800
C	1.39167000	0.21995800	-0.00194000
C	2.80551800	0.34812300	-0.00291100
C	3.59671600	-0.82606500	-0.00760900
C	3.01674100	-2.07708800	-0.01172400
H	1.13639400	-3.14689200	-0.01639900
H	-0.29039700	-1.15607300	-0.00848600
C	3.34679700	1.65660400	0.00080200
H	4.67631000	-0.72346400	-0.00811600
C	2.52625200	2.76000000	0.00549700
C	1.12700600	2.59918400	0.00698300
H	4.42433200	1.78096900	0.00001800
H	2.93389400	3.76238000	0.00847200
N	0.62556800	1.36259700	0.00329200
H	-0.41794600	1.24921000	0.00721700
C	0.18272600	3.76114400	0.01094500
H	0.37735000	4.39432800	0.88069900
H	0.34718300	4.37465600	-0.87923600
H	-0.85755200	3.43749800	0.03173700
C	3.83936900	-3.33750200	-0.01657400
H	4.90848800	-3.12255900	-0.01645800
H	3.61491200	-3.94921200	0.86211900
H	3.61387900	-3.94319600	-0.89915800
O	-2.42933900	-2.23164200	-0.11743900
H	-2.65140300	-3.15854000	-0.25395900
H	-2.82792700	-1.73937900	-0.86422200
O	-3.42723700	-0.56589200	1.79680900
H	-3.05682400	-1.33847900	1.31443900
H	-3.36565500	-0.75194900	2.73921700
O	-3.63876800	-0.34207300	-1.75094700
H	-3.81616800	-0.29842800	-2.69599700
H	-4.50263700	-0.26053200	-1.27922900
O	-5.60052400	-0.26688400	0.05203600
H	-5.08369200	-0.28784400	0.87712500
H	-6.41364800	0.21709600	0.22248000
O	-2.07544300	1.18175800	0.03167400
H	-2.51399300	0.77745600	0.80295700
H	-2.55628800	0.82135100	-0.73719500

6 water

C	1.58594200	-2.09665000	-0.01693800
C	0.84781600	-0.93745400	-0.03132200
C	1.52420600	0.29615900	-0.02698500
C	2.94283500	0.34182800	0.00133400
C	3.66226900	-0.87771900	0.02110300
C	3.00804700	-2.09177500	0.00972300
H	1.06284800	-3.04658500	-0.02820700
H	-0.23293100	-0.96732600	-0.03713600
C	3.55734700	1.61709700	0.00232300
H	4.74589100	-0.84002100	0.04248800
C	2.80061700	2.76547800	-0.02824500
C	1.39504500	2.68461100	-0.06281600
H	4.63996400	1.68071500	0.02414500
H	3.26533200	3.74270500	-0.03128600
N	0.82405800	1.47896700	-0.05831400
H	-0.22410200	1.41916400	-0.10320400
C	0.51555500	3.89602700	-0.09356300
H	0.85473900	4.58610600	-0.86941700
H	-0.52581900	3.63281400	-0.27853500
H	0.58124400	4.42432900	0.86255800
C	3.75458800	-3.39871100	0.02448700
H	3.47609800	-3.99397300	0.89905100
H	3.51201600	-3.99250100	-0.86171800
H	4.83442000	-3.24768400	0.04667800
O	-1.86364800	1.39378300	-0.27912300
H	-2.47113100	1.30230000	0.47908100
H	-2.25896600	0.85294600	-0.98941700
O	-2.09351400	-2.61460600	-0.64428600
H	-2.44243400	-3.50777100	-0.72332700
H	-2.15967700	-2.36243800	0.30477000
O	-3.07868600	-0.49852900	-1.98518600
H	-2.71916600	-1.34535100	-1.62084500
H	-2.99235200	-0.53506500	-2.94343000
O	-3.77749000	0.66749900	1.66290600
H	-4.16205800	1.22661500	2.34570000
H	-4.49209400	0.46906300	1.00850200
O	-2.12139600	-1.53882900	1.84237400
H	-2.74377400	-0.78892400	1.93668500
H	-2.09307400	-1.98751900	2.69276100
O	-5.30784600	0.11326600	-0.44305200
H	-6.15759200	-0.30028300	-0.61839900
H	-4.69075600	-0.14809100	-1.15298100

7 water

C	-3.29850600	1.18967200	0.35110200
C	-1.96799200	0.85589700	0.44891300
C	-1.58042600	-0.47009000	0.17947000
C	-2.55215100	-1.44069000	-0.18439100
C	-3.91079500	-1.04961900	-0.27336000
C	-4.29869100	0.24661400	-0.01289600
H	-3.59801200	2.21092500	0.56123600
H	-1.23477100	1.59918900	0.73423600
C	-2.10416000	-2.75757800	-0.43615500
H	-4.64649200	-1.79641700	-0.55104700
C	-0.77101500	-3.08217300	-0.33152300
C	0.17149800	-2.10153200	0.02683900
H	-2.82777700	-3.51671400	-0.71318300
H	-0.42429500	-4.08889600	-0.52114800
N	-0.26251800	-0.85722200	0.26353000
H	0.44477900	-0.13855100	0.52597900
C	1.63548300	-2.37457100	0.14068100
H	2.02261400	-2.05840300	1.11208300
H	1.83879000	-3.43638200	0.01131400
H	2.18167000	-1.81963200	-0.62758900
C	-5.73648100	0.68347200	-0.09934700
H	-5.85418100	1.48426300	-0.83528900
H	-6.39247500	-0.13952700	-0.38511500
H	-6.08014900	1.07492300	0.86260000
O	2.78541600	2.16396100	-1.31426300
H	1.96847300	2.69526400	-1.48992700
H	3.51572500	2.79039400	-1.26768300
O	0.20133700	3.25708700	1.38406800
H	0.82449500	2.51542100	1.52639700
H	0.30371300	3.87165900	2.11683100
O	0.45015300	3.44020800	-1.33462400
H	0.25364400	3.59360300	-0.38709700
H	0.06140000	4.15951800	-1.84033100
O	1.71118100	1.00005800	0.99977400
H	2.37607300	0.52770300	1.55813400
H	2.20936500	1.36069100	0.23805700
O	3.52804000	-0.52832800	2.24696000
H	4.16510400	-0.83716000	1.56398000
H	4.01343800	-0.41784300	3.06964700
O	4.92306600	-1.32399300	0.06679500
H	4.52083600	-1.01958600	-0.77160200
H	5.84933100	-1.51288800	-0.10697700
O	3.41325100	-0.41485200	-2.06263900
H	3.54969700	-0.58055500	-3.00064700
H	3.17649000	0.53001700	-1.97214900

8 water

C	4.11391300	-1.98713400	0.02633700
C	2.85137900	-1.44476200	0.00472800
C	2.71553200	-0.04502900	-0.08525000
C	3.86421900	0.78678200	-0.15878200
C	5.14603000	0.18295700	-0.13183700
C	5.28794500	-1.18455700	-0.03937300
H	4.22434700	-3.06424700	0.09202200
H	1.96402900	-2.06545900	0.04458200
C	3.65364400	2.18143300	-0.25978700
H	6.02099900	0.82130900	-0.18785500
C	2.37957200	2.70413000	-0.28729400
C	1.26446200	1.84955100	-0.20867900
H	4.51239800	2.84150600	-0.31917400
H	2.21580700	3.77017100	-0.36957800
N	1.47356600	0.53512000	-0.10752500
H	0.63003700	-0.10816500	-0.04075900
C	-0.15392600	2.32945500	-0.23839600
H	-0.68582500	2.02755300	0.66910200
H	-0.18765900	3.41486400	-0.32434000
H	-0.68489900	1.88922100	-1.08762200
C	6.63924100	-1.84707400	-0.01111900
H	7.44832600	-1.11766800	-0.06319600
H	6.76499100	-2.43076500	0.90547200
H	6.74870300	-2.53796800	-0.85220700
O	-6.03782300	-0.00105700	-0.31066900
H	-5.46271200	0.77468400	-0.13960800
H	-6.94472700	0.26436900	-0.12776600
O	-2.46789700	0.11487900	-1.59392900
H	-3.12234800	-0.47678100	-2.00752500
H	-2.99915300	0.77232200	-1.11316400
O	-0.61988600	-1.08908500	-0.02318800
H	-1.31423000	-0.73168100	-0.62737700
H	-1.08724200	-1.31056900	0.80285100
O	-4.67693800	-1.52993500	-2.20689600
H	-5.39719200	-0.99918000	-1.82058200
H	-5.00466200	-1.90657500	-3.02973800
O	-2.48185800	1.29636800	2.22149700
H	-2.62783400	1.64611900	3.10645400
H	-2.42996300	0.31793800	2.31443800
O	-4.43124700	-2.14256100	0.63776500
H	-5.13073000	-1.47272200	0.54674000
H	-4.24241200	-2.39319700	-0.27832600
O	-4.03282200	1.84861900	0.08113300
H	-3.52528300	1.73619200	0.92239900
H	-4.10258700	2.79450000	-0.08481700
O	-2.37925000	-1.44148400	2.14943000
H	-2.27855600	-2.04525700	2.89273500
H	-3.16688200	-1.75680400	1.62508700

2,8-dimethylquinolinium XYZ Coordinates

1 water

C	-2.47501900	1.34851800	-0.00415700
C	-1.09090800	1.34744600	0.02148100
C	-0.45097700	0.08369200	0.00964700
C	-1.20297400	-1.12573800	-0.01421900
C	-2.61634100	-1.06044100	-0.03836300
C	-3.23853700	0.16288600	-0.03604200
H	-2.99253600	2.30111400	0.00322900
C	-0.50009200	-2.35234000	-0.00856600
H	-3.18698500	-1.98113000	-0.05756000
C	0.87376500	-2.38239600	0.01927300
C	1.60136400	-1.18169000	0.03225000
H	-1.06354400	-3.27900700	-0.02346100
H	1.41623600	-3.31833600	0.02849600
N	0.92919200	-0.02124000	0.02600400
H	1.49130100	0.83824500	0.01978300
C	3.09737900	-1.16417000	0.02954200
H	3.46322500	-1.43321800	-0.96698300
H	3.49825800	-0.18697000	0.29183900
H	3.47868900	-1.91264600	0.72667500
C	-0.31009000	2.63392300	0.07272700
H	0.37786700	2.72962800	-0.77102600
H	-0.98419900	3.48956300	0.05232500
H	0.28386900	2.70306400	0.98938400
H	-4.31941000	0.22742300	-0.05522100
O	2.92087200	2.11881500	-0.08018600
H	3.14988000	2.76679200	0.59607100
H	3.39060700	2.39549900	-0.87552700

2 water

C	-1.39355500	-2.50190500	0.16300500
C	-0.37110700	-1.57204200	0.23739000
C	-0.73200700	-0.20913200	0.08536500
C	-2.08502300	0.17465500	-0.14427500
C	-3.08636600	-0.82345200	-0.21169000
C	-2.73984800	-2.14199000	-0.05725600
H	-1.14776300	-3.55160300	0.27751600
C	-2.37383800	1.54904700	-0.30192100
H	-4.11434600	-0.52883400	-0.38541400
C	-1.37808500	2.49454600	-0.23742000
C	-0.05166200	2.09864400	-0.00142900
H	-3.40007700	1.85159600	-0.47997700
H	-1.59336200	3.54711500	-0.36287800
N	0.21659300	0.79415300	0.14921700
H	1.20508700	0.54932200	0.33248600
C	1.06611400	3.08711300	0.11701300
H	0.85196100	3.97092900	-0.48404000
H	1.15937300	3.41140500	1.15935800
H	2.01877800	2.65709700	-0.18948300
C	1.05566400	-1.99852500	0.45986500
H	1.69419200	-1.73861200	-0.38949700
H	1.48724300	-1.52649800	1.34607000
H	1.10958600	-3.07853000	0.59569400
H	-3.49578200	-2.91606600	-0.10523000
O	2.99087500	0.55583100	0.57305000
H	3.54752700	-0.10762100	0.11714800
H	3.51767700	0.91221500	1.29514800
O	4.33420400	-1.38419000	-0.85565000
H	4.79389600	-1.17591700	-1.67695700
H	4.78750100	-2.14995000	-0.48553700

3 water

C	0.49054900	-2.72791100	-0.11651600
C	0.04522800	-1.41854000	-0.17002200
C	1.02976300	-0.40237200	-0.06551200
C	2.40714900	-0.72545000	0.10484100
C	2.80012600	-2.08424600	0.15371900
C	1.85068900	-3.06814400	0.03996000
H	-0.23954800	-3.52547200	-0.19557700
C	3.33403300	0.33485900	0.22613300
H	3.84838500	-2.32610500	0.28180900
C	2.92129300	1.64464000	0.18092700
C	1.56094700	1.94372500	-0.00336900
H	4.38423600	0.09964600	0.36101000
H	3.62517100	2.45996700	0.28036400
N	0.68677400	0.93545000	-0.11979600
H	-0.30297800	1.20679700	-0.27844700
C	1.06364900	3.35198700	-0.10437600
H	1.12298600	3.68662200	-1.14593000
H	0.02727900	3.43906700	0.21877300
H	1.69279500	4.01515500	0.48979400
C	-1.41845300	-1.09933700	-0.31556000
H	-1.79921700	-0.54568800	0.54702000
H	-1.61615300	-0.49006500	-1.20077000
H	-2.00291800	-2.01459000	-0.40394600
H	2.13720700	-4.11208200	0.07399200
O	-1.82766300	2.06645600	-0.51213900
H	-2.62408000	1.72457800	-0.04272200
H	-2.14342300	2.56317400	-1.27291300
O	-5.21554700	-1.25078700	-0.11515900
H	-5.54219400	-1.95301100	0.45815500
H	-5.82729200	-1.21027900	-0.85860300
O	-3.86357500	0.96941800	0.86582200
H	-4.41261500	1.44467000	1.49683500
H	-4.39062200	0.21351100	0.54017400

4 water

C	-1.42753400	-2.72366800	-0.00003500
C	-0.70831400	-1.54019800	-0.00004100
C	-1.45830400	-0.33467900	-0.00001200
C	-2.88323700	-0.35750900	0.00001100
C	-3.56038300	-1.59945700	0.00002100
C	-2.83662500	-2.76523100	-0.00000300
H	-0.88008900	-3.65950800	-0.00005700
C	-3.57522600	0.87662400	0.00001500
H	-4.64379800	-1.60980200	0.00004200
C	-2.89397400	2.06716300	0.00000000
C	-1.48673200	2.06934300	-0.00001300
H	-4.65983600	0.86827500	0.00003900
H	-3.41466800	3.01565600	0.00000400
N	-0.83544300	0.90079600	-0.00001400
H	0.21274700	0.96042800	0.00001200
C	-0.71134300	3.35045700	0.00000700
H	-0.98479600	3.94063500	-0.87935500
H	-0.98468700	3.94054700	0.87946400
H	0.36339300	3.18309400	-0.00005400
C	0.79769700	-1.55753200	-0.00008100
H	1.21534300	-1.06135600	-0.87964400
H	1.21539200	-1.06147100	0.87952200
H	1.15582400	-2.58729900	-0.00015700
H	-3.34111200	-3.72368300	0.00000400
O	3.39899900	0.08262100	-1.84848700
H	4.17907100	-0.24747000	-1.37335200
H	3.68493200	0.28520100	-2.74478000
O	3.39899800	0.08242500	1.84854300
H	4.17908800	-0.24762600	1.37341500
H	3.68487500	0.28488100	2.74488100
O	1.84293700	1.45507000	0.00009100
H	2.35599400	1.13359000	-0.76647800
H	2.35594400	1.13348000	0.76664500
O	5.44342000	-0.82325800	-0.00004000
H	6.29722600	-0.37285300	-0.00001800
H	5.64628200	-1.76704000	-0.00010600

5 water

C	3.94056000	-1.97387500	-0.00000500
C	2.61171700	-1.58813500	0.00001000
C	2.34811500	-0.19252000	0.00000000
C	3.41250000	0.75585500	-0.00002600
C	4.75219300	0.29821800	-0.00004100
C	5.00696600	-1.04951200	-0.00003100
H	4.17050500	-3.03340800	0.00000200
C	3.08282400	2.12953800	-0.00004000
H	5.55734600	1.02325900	-0.00006000
C	1.77203500	2.54298500	-0.00002700
C	0.73739700	1.59206900	0.00000300
H	3.88413400	2.86063300	-0.00005900
H	1.51569600	3.59358700	-0.00003700
N	1.05567000	0.29060600	0.00001600
H	0.23956600	-0.37425400	0.00004700
C	-0.70921300	1.97803900	0.00001200
H	-1.22248500	1.57531100	0.87742900
H	-0.80625300	3.06292900	0.00004500
H	-1.22247100	1.57536600	-0.87744200
C	1.50599700	-2.60945000	0.00002900
H	0.85821900	-2.50871500	0.87396200
H	0.85826300	-2.50877700	-0.87394700
H	1.92191800	-3.61673900	0.00007300
H	6.02675500	-1.41442700	-0.00004100
O	-1.25055700	-1.15424200	0.00010800
H	-1.80171400	-0.89983500	-0.76508000
H	-1.80174400	-0.89981800	0.76526800
O	-5.04532100	0.62338900	-0.00002400
H	-5.82564300	0.02746900	-0.00005900
H	-5.40050800	1.51949300	-0.00000700
O	-2.95253700	0.08250600	-1.82364200
H	-3.22754400	-0.14386600	-2.71737300
H	-3.76524300	0.27607300	-1.31904300
O	-7.26074300	-0.99423200	-0.00010000
H	-7.71383400	-1.35054600	0.77141300
H	-7.71417400	-1.34999600	-0.77166700
O	-2.95260500	0.08261200	1.82373100
H	-3.22764200	-0.14363900	2.71748300
H	-3.76529100	0.27613000	1.31908400

6 water

C	-3.28445800	-1.49737400	0.29619100
C	-2.04859500	-1.37977200	-0.31457600
C	-1.54723900	-0.06728200	-0.50402900
C	-2.29093700	1.07199000	-0.09065900
C	-3.55074800	0.88980900	0.52727500
C	-4.03532300	-0.38014900	0.71897100
H	-3.69258800	-2.48962200	0.45270100
C	-1.72945400	2.35132200	-0.30654700
H	-4.11684800	1.76001800	0.83800300
C	-0.49951900	2.49245300	-0.89759200
C	0.22023400	1.35504900	-1.30189100
H	-2.28806700	3.22769700	0.00432300
H	-0.05963800	3.46669100	-1.05963100
N	-0.31909300	0.14694200	-1.09603100
H	0.25162900	-0.66596400	-1.38222100
C	1.56994800	1.45580400	-1.93422400
H	1.78115000	0.60536600	-2.58031600
H	1.64470200	2.38208900	-2.50463600
H	2.33749400	1.48304900	-1.15439600
C	-1.27093200	-2.59371400	-0.74607700
H	-1.06235500	-2.57330600	-1.81983400
H	-0.31707100	-2.65644100	-0.21641100
H	-1.83787000	-3.50091100	-0.53713300
H	-4.99924600	-0.53379400	1.18866200
O	1.64036900	-1.71006100	-1.90749000
H	1.63312100	-2.50233700	-2.45263900
H	2.37389300	-1.80912700	-1.26679200
O	3.47936500	-1.73200500	0.17172600
H	3.77133000	-0.79403200	0.31562900
H	4.27179500	-2.27868300	0.20364300
O	1.92361300	2.20574800	1.55060900
H	1.22645500	1.57678000	1.84425900
H	1.98968200	2.88270700	2.23103000
O	1.20065600	-2.17943100	1.69252400
H	1.30441600	-2.83266000	2.39185700
H	2.06946200	-2.10954900	1.24635100
O	0.07759900	0.28638900	2.09044200
H	-0.59103600	0.27829600	2.78157000
H	0.44691000	-0.62280700	2.04225700
O	4.01403200	0.85571400	0.50498400
H	4.86935700	1.28038000	0.61883900
H	3.34403800	1.39792000	0.98371100

7 water

C	3.79199100	2.22414800	-0.37428700
C	2.57534100	1.56526800	-0.37599200
C	2.59037000	0.18399300	-0.05163500
C	3.80954400	-0.48310700	0.26189300
C	5.02353200	0.24512300	0.24702000
C	5.00952000	1.58020600	-0.06759300
H	3.80915900	3.28021500	-0.61919000
C	3.75543400	-1.85927200	0.57789300
H	5.94820300	-0.26655800	0.48578300
C	2.56034500	-2.53801400	0.58447000
C	1.36749000	-1.86411200	0.27291800
H	4.67710000	-2.37841600	0.81778500
H	2.51502100	-3.59084900	0.82704400
N	1.42616200	-0.55814900	-0.02801800
H	0.51847900	-0.09877400	-0.25517600
C	0.03599000	-2.54505800	0.27382200
H	-0.47535300	-2.41968800	-0.68435100
H	0.15961000	-3.60918000	0.46916600
H	-0.61217300	-2.12094700	1.04660600
C	1.29813000	2.29119800	-0.70725800
H	0.80002400	1.85571600	-1.57737100
H	0.58483500	2.25004900	0.12003600
H	1.50541300	3.33873100	-0.92503300
H	5.93074100	2.14946900	-0.08280000
O	-2.90596700	2.46458400	-0.36382100
H	-2.17324900	1.84046100	-0.56432800
H	-2.73082700	3.28519100	-0.83493500
O	-4.38723700	-1.73884500	-0.48030800
H	-4.82903100	-0.84935500	-0.48873600
H	-5.08290600	-2.40450800	-0.46670200
O	-1.17586200	0.33434700	-0.55963700
H	-1.65508600	-0.04875700	0.22540700
H	-1.49512100	-0.22574200	-1.30279800
O	-5.26261600	0.77805800	-0.29781200
H	-5.33305800	0.99700800	0.64267400
H	-4.58913900	1.40166700	-0.61628100
O	-3.88624500	1.64282000	2.11758300
H	-3.99084600	2.16331600	2.92035900
H	-3.47703300	2.21704700	1.44400000
O	-2.22455700	-1.59066200	-2.16843800
H	-3.06811800	-1.76826100	-1.69866500
H	-2.40009700	-1.68889600	-3.10927500
O	-2.55247400	-0.75168200	1.45926400
H	-3.03127000	-0.03489300	1.91554300
H	-3.23486500	-1.27819400	1.00521400

8 water

C	4.61416200	-2.02361500	-0.05353000
C	3.30562900	-1.57573200	-0.01687300
C	3.10387000	-0.17154000	-0.08745600
C	4.20928500	0.72448500	-0.17507000
C	5.52581900	0.20466200	-0.20707700
C	5.71972700	-1.15191800	-0.15059500
H	4.79632300	-3.09119700	-0.00280300
C	3.94230400	2.11097900	-0.22480400
H	6.36205800	0.89020800	-0.27576900
C	2.65276100	2.58482700	-0.19084800
C	1.57731600	1.68319100	-0.11618800
H	4.77517100	2.80290000	-0.28965000
H	2.44404400	3.64534300	-0.22685900
N	1.83520500	0.37010100	-0.06865400
H	0.98790000	-0.25607200	-0.04491100
C	0.14981400	2.13385800	-0.10155600
H	-0.36287100	1.81035200	-1.01184900
H	-0.39305500	1.70538100	0.74456300
H	0.10258800	3.22067100	-0.04222000
C	2.15744000	-2.54137000	0.10656400
H	1.59087000	-2.36656000	1.02610500
H	1.44922400	-2.44739800	-0.71875000
H	2.52603700	-3.56663600	0.13009000
H	6.72108800	-1.56391400	-0.17612000
O	-5.89475500	0.32698700	-0.25089300
H	-5.28523700	1.05404200	-0.00227400
H	-6.78753900	0.60790700	-0.02639700
O	-2.34233000	0.44738400	-1.56924200
H	-3.01980300	-0.08460500	-2.02431500
H	-2.84480500	1.07227100	-1.01923900
O	-0.50747100	-0.96508000	-0.14463900
H	-1.18263800	-0.49796900	-0.68978800
H	-0.99045000	-1.30787100	0.62775800
O	-4.62379000	-1.04145300	-2.32475600
H	-5.31310900	-0.52269500	-1.87128600
H	-4.97263200	-1.29446000	-3.18535900
O	-2.24723900	1.13420900	2.33193200
H	-2.34451400	1.39458700	3.25352900
H	-2.24964700	0.15039200	2.31853300
O	-4.39623800	-1.99286500	0.42067600
H	-5.05444700	-1.27654400	0.42007600
H	-4.23559600	-2.14777500	-0.52168300
O	-3.80883200	2.03347100	0.31992700
H	-3.29035500	1.78738200	1.12524300
H	-3.83520700	2.99513100	0.28095200
O	-2.28782100	-1.58192800	1.95966300
H	-2.22515600	-2.26666100	2.63360600
H	-3.09563500	-1.78967200	1.41265900

6-amino-2-methylquinolinium•H₂O XYZ Coordinates

C	2.11821700	-0.89430900	0.00004500
C	-0.00315600	0.22872700	0.00007400
C	-0.70242400	-1.01145100	-0.00004600
C	0.08244600	-2.19268000	-0.00012700
C	1.45793800	-2.13457400	-0.00008200
C	-0.71951500	1.44246300	0.00015600
C	-2.10884500	-1.01133400	-0.00008400
H	-0.41606000	-3.15574300	-0.00022700
H	2.05149300	-3.03885300	-0.00014100
C	-2.82082800	0.18529800	-0.00000300
C	-2.08918100	1.41502800	0.00012000
H	-2.63410800	-1.95953500	-0.00017700
C	3.60828800	-0.74243100	0.00018000
H	3.94342200	-0.19155500	0.88342400
H	4.09327600	-1.71718600	-0.00047900
H	3.94349700	-0.19029500	-0.88224200
N	1.36928500	0.21596600	0.00010600
H	1.84593400	1.12829600	0.00017600
H	-2.63866800	2.35006700	0.00019100
H	-0.18413100	2.38451600	0.00025900
N	-4.18236800	0.21880500	-0.00002700
H	-4.68582800	1.08929300	0.00000000
H	-4.72667500	-0.62720200	-0.00014100
O	2.55596400	2.81839000	-0.00018500
H	2.85738700	3.31499200	0.76884100
H	2.85669900	3.31426600	-0.76995000

8-amino-2-methylquinolinium•H₂O XYZ Coordinates

C	1.63857400	-1.18308200	-0.05094400
C	-0.42048300	0.06733000	-0.01432400
C	-1.17236300	-1.14147700	0.04553300
C	-0.45448600	-2.36165100	0.07478200
C	0.91895600	-2.38659700	0.03025100
C	-1.06722000	1.33424100	-0.03741400
C	-2.58233600	-1.08758700	0.05922900
H	-1.01136000	-3.29080200	0.12749100
H	1.46594400	-3.31992600	0.04700700
C	-3.20446900	0.13970300	0.00997300
C	-2.45919400	1.32848600	-0.03241800
H	-3.15114500	-2.00747000	0.10487800
H	-4.28581700	0.20113500	0.01488200
C	3.13250800	-1.14534100	-0.12561200
H	3.56090700	-1.59194100	0.77611200
H	3.47640300	-1.73952800	-0.97612100
H	3.51263100	-0.12960600	-0.22967700
N	0.95694000	-0.03134800	-0.06514500
H	1.51135400	0.82663400	-0.12322500
H	-2.98225300	2.27819100	-0.05840600
N	-0.34276100	2.50944000	-0.14609200
H	-0.88456900	3.35965900	-0.09471800
H	0.54598800	2.59028900	0.32962900
O	2.71138200	2.33045900	0.17756600
H	2.97356900	2.93031000	-0.53091500
H	3.30112000	2.51859200	0.91685000

6-methoxy-2-methylquinolinium•H₂O XYZ Coordinates

C	1.84610500	1.12889600	0.00010100
C	0.47825600	1.29607700	0.00017700
C	-0.35667400	0.16821900	0.00006800
C	0.20314900	-1.14028600	-0.00012400
C	1.59974700	-1.28674200	-0.00022700
C	2.42344000	-0.16980500	-0.00012200
H	2.47928300	2.00520300	0.00023300
H	0.04514600	2.28931600	0.00035900
C	-0.69922900	-2.23727000	-0.00022400
H	2.04916400	-2.27185800	-0.00038800
C	-2.05752400	-2.03541800	-0.00012700
C	-2.58295300	-0.72753600	0.00010500
H	-0.30024400	-3.24562900	-0.00040400
H	-2.74688100	-2.86948200	-0.00022300
N	-1.72887200	0.29823800	0.00015700
H	-2.11068100	1.25407900	0.00029100
C	-4.05294100	-0.44938000	0.00045000
H	-4.51872700	-0.90190000	-0.87916600
H	-4.51787300	-0.89988400	0.88156800
H	-4.26671700	0.61955100	-0.00062300
O	3.74549700	-0.40394800	-0.00013800
C	4.67169800	0.69171400	0.00029400
H	5.65783100	0.23425500	0.00048900
H	4.55439900	1.30474900	-0.89795600
H	4.55388200	1.30460300	0.89855800
O	-2.71355700	2.98180400	-0.00027100
H	-2.93590200	3.51915400	0.76841500
H	-2.93452200	3.51651600	-0.77119700

8-methoxy-2-methylquinolinium•H₂O XYZ Coordinates

C	-2.62627900	-0.07534700	-0.00695200
C	-1.36707800	0.49512300	0.00248600
C	-0.23453600	-0.36169600	0.00439000
C	-0.39341800	-1.77107300	-0.01135600
C	-1.69807700	-2.32023000	-0.02323900
C	-2.78357900	-1.47890900	-0.01920600
H	-3.50795000	0.55048800	-0.00703600
C	0.78422600	-2.55621000	-0.01647600
H	-1.82168000	-3.39577800	-0.03489500
C	2.02767000	-1.96944700	-0.00622700
C	2.15124400	-0.56836400	0.01510900
H	0.69362900	-3.63680100	-0.03129400
H	2.92824700	-2.56865800	-0.01381300
N	1.03396000	0.16943100	0.01954400
H	1.12775300	1.19643200	0.03363200
C	3.47846500	0.11992100	0.06358100
H	4.23957000	-0.49465000	-0.41719300
H	3.44335600	1.09770500	-0.41576000
H	3.77936500	0.26228500	1.10741500
H	-3.78649500	-1.88755900	-0.02715500
O	-1.08394800	1.81611100	0.01018700
C	-2.16852100	2.75566700	0.07654300
H	-1.70369100	3.73797600	0.11203000
H	-2.80241600	2.67901100	-0.81084100
H	-2.76104100	2.59795000	0.98150700
O	1.86034800	2.93705800	-0.12202200
H	2.28765500	3.49502800	0.53694700
H	1.41407200	3.53859500	-0.72760200

7-chloro-2-methylquinolinium•H₂O XYZ Coordinates

C	-2.19114500	-0.01129900	0.00000900
C	-0.97690000	0.64506500	0.00000700
C	0.19445500	-0.12715900	0.00000100
C	0.14612100	-1.54716900	-0.00000300
C	-1.12485900	-2.17459600	0.00000000
C	-2.27373800	-1.42446600	0.00000500
H	-0.92479200	1.72616300	0.00001000
C	1.36997600	-2.25310900	-0.00001000
H	-1.17956100	-3.25673700	-0.00000400
H	-3.24733300	-1.89674400	0.00000700
C	2.57337000	-1.58305700	-0.00001200
C	2.59602700	-0.17822200	-0.00000800
H	1.35273200	-3.33752700	-0.00001400
H	3.51356300	-2.11826200	-0.00001800
N	1.43147500	0.48164000	-0.00000200
H	1.44935700	1.51192300	0.00000000
C	3.86848000	0.60786500	-0.00000400
H	4.46391700	0.35105000	-0.88028500
H	3.68665000	1.68258600	-0.00004700
H	4.46386900	0.35111500	0.88032900
Cl	-3.65990100	0.91105000	0.00001700
O	1.35407900	3.32435900	-0.00001500
H	1.34810600	3.90455400	-0.76993000
H	1.34812900	3.90456700	0.76989000

8-chloro-2-methylquinolinium•H₂O XYZ Coordinates

C	2.53912300	1.00293000	0.00003400
C	1.16034800	1.04194400	0.00002400
C	0.42235600	-0.16307400	0.00000000
C	1.12038700	-1.40383900	-0.00001800
C	2.53440400	-1.41143600	-0.00000900
C	3.22815800	-0.22518800	0.00001700
H	3.09004100	1.93488100	0.00005400
C	0.35282600	-2.59394500	-0.00004800
H	3.05481400	-2.36143900	-0.00002400
H	4.31085700	-0.22138100	0.00002500
C	-1.01825300	-2.55043000	-0.00005800
C	-1.68684900	-1.31206700	-0.00003400
H	0.86803100	-3.54821000	-0.00006600
H	-1.60985100	-3.45628000	-0.00008400
N	-0.95850500	-0.18712000	-0.00000900
H	-1.46820900	0.70917000	0.00000000
C	-3.17956500	-1.23389600	0.00001200
H	-3.56968600	-1.75509900	-0.87893600
H	-3.56956700	-1.75429200	0.87949900
H	-3.54548800	-0.20992300	-0.00041100
Cl	0.34468100	2.58301500	0.00004700
O	-2.91516700	2.00602400	-0.00004800
H	-3.11350200	2.55364800	-0.76808500
H	-3.11376000	2.55331900	0.76815600

2-methyl-6-nitroquinolinium•H₂O XYZ Coordinates

C	-1.50012100	1.37849100	0.00003500
C	-0.12487200	1.43199400	-0.00001200
C	0.60580800	0.22905800	-0.00008900
C	-0.05001000	-1.03070200	-0.00019300
C	-1.46350000	-1.06036100	-0.00011500
C	-2.14721600	0.12785800	0.00003200
H	-2.09934400	2.27929100	0.00006300
H	0.39629200	2.38150600	-0.00003800
C	0.74973100	-2.20043900	-0.00019900
H	-2.00214000	-1.99929700	-0.00014900
C	2.12126900	-2.11291100	-0.00011000
C	2.74893200	-0.85233200	-0.00001700
H	0.26505800	-3.17056600	-0.00032300
H	2.73991500	-3.00057100	-0.00007800
N	1.98354300	0.24444300	-0.00006900
H	2.44486200	1.16776700	0.00000500
C	4.23521700	-0.69661100	0.00026100
H	4.65845900	-1.18727900	0.88111700
H	4.65915600	-1.18973300	-0.87885900
H	4.53962800	0.34987000	-0.00101300
N	-3.64008300	0.09702400	0.00011500
O	-4.17107400	-1.00037200	0.00045000
O	-4.21179700	1.17394700	-0.00028500
O	3.14916400	2.82651100	0.00004800
H	3.40611600	3.34656900	-0.77022900
H	3.40600800	3.34721700	0.76992000

2-methyl-8-nitroquinolinium•H₂O XYZ Coordinates

C	-2.66069700	-0.07496200	0.06146800
C	-1.38292100	0.43342200	-0.04706500
C	-0.25518600	-0.42842800	-0.04171000
C	-0.48746100	-1.82957300	0.04726900
C	-1.81215200	-2.32292000	0.13839700
C	-2.88098800	-1.45968500	0.15250700
H	-3.49184900	0.61860700	0.06400000
C	0.63461300	-2.69549300	0.04220700
H	-1.96519700	-3.39402400	0.19885600
C	1.90952300	-2.19824500	-0.04348800
C	2.11563300	-0.80772600	-0.10398800
H	0.46878100	-3.76542300	0.10284100
H	2.77034400	-2.85329600	-0.05854600
N	1.05087700	0.00389300	-0.09603300
H	1.22565300	1.01705900	-0.10618500
C	3.48254100	-0.20918300	-0.16148300
H	4.11547500	-0.79594800	-0.82971700
H	3.46248400	0.82914000	-0.48690600
H	3.93567000	-0.24878200	0.83516100
H	-3.89388800	-1.83397700	0.22531300
N	-1.25303000	1.89851400	-0.19619800
O	-2.17955000	2.59382700	0.16121100
O	-0.20840400	2.31585800	-0.69937800
O	2.18048000	2.62814300	0.58251900
H	2.81319300	2.98866000	1.21256900
H	1.65676600	3.37526600	0.26873700