Supporting Information


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Fig. S1  Schematic of experimental setup: (1) sparger; (2) cold trap; (3) emission cell; (4) optical chopper; (5) InGaAs photodetector; (6) reaction vessel; (7) mechanical pump; (8) pressure relay; (9) piston pump; (10) UV-Vis spectrometer; (11) fluorometer; (12) peristaltic pump; (13) two-position switching valve; (14) θ-ESI emitter; (15a – b) syringe pumps; and (16) tandem MS.
Calibration of $[^1\text{O}_2]$ in solution  In the experiment, chemically generated $[^1\text{O}_2]$ was continuously bubbled into the reaction vessel. $[^1\text{O}_2]$ had a longer lifetime in the interior of bubbles (because of reduced encounters with water) than in bulk solution. After diffusing into the bulk water, $[^1\text{O}_2]$ could travel $\sim 150$ nm within a lifetime of $\sim 2 \mu$s. Therefore, $[^1\text{O}_2]$ reactions occurred both at the gas/solution interface and in the bulk solution. On the basis of the steady concentration of airborne $[^1\text{O}_2]$ (determined on the basis of its emission intensity) and the continuously bubbling of $[^1\text{O}_2]$ into the solution, quasi-steady-state $[^1\text{O}_2]_{\text{sol}}$ was assumed for the solution reaction and its amount was determined as

$$[^1\text{O}_2]_{\text{sol}} = m(I_{\text{EM}} - I_B) \quad (S1)$$

where $I_{\text{EM}}$ is the $[^1\text{O}_2]$ emission intensity (mV) measured by the lock-in amplifier in the gas phase, $I_B (= 43$ mV) represents a threshold $[^1\text{O}_2]$ emission intensity below which all of the airborne $[^1\text{O}_2]$ quenched in the bubbles and/or during diffusion before reaching aqueous substrates as we determined in the previous experiment, and $m$ is a scaling factor (M·mV$^{-1}$).

To validate this assumption and calibrate the value of the scaling factor $m$, 3-(10-(2-carboxy-ethyl)-anthracen-9-yl)-propionic acid (ADPA, Aldrich) was used as a calibration compound. ADPA is known to react with $[^1\text{O}_2]$ chemically (i.e. without physical quenching) and produces an endoperoxide via a $[4 + 2]$ cycloaddition accompanied by bleaching of the absorption band of ADPA. To take into account the physical quenching of $[^1\text{O}_2]$ by LysNH$_2$ ($N^{\alpha}$-acetyl-L-lysine-methyl ester, 15 mM) in the actual reaction solution, the calibration experiment was carried out in the presence of the same LysNH$_2$ concentration in the ADPA solution. pH of the ADPA solution (0.1 mM) was maintained at 10.0 using borax/NaOH buffer. The rate law for the decay of ADPA could be described as

$$\ln \frac{A_t}{A_0} = -k_r \int[^1\text{O}_2]_{\text{sol},t} dt \quad (S2)$$

where $A_t$ and $A_0$ are the ADPA peak absorption (at 378.7 nm) at different reaction times and time zero, respectively; and $[^1\text{O}_2]_{\text{sol},t}$ represents the $[^1\text{O}_2]_{\text{sol}}$ at the time instant $t$. The combination of Eqs (S1) and (S2) gives

$$\ln \frac{A_t}{A_0} = -k_r m \int (I_{\text{EM},t} - I_B) dt \quad (S3)$$
Figure S2a shows the absorption changes of ADPA throughout the reaction, and the plot of 

$$\ln \frac{A_t}{A_0} \text{ vs. } \int (I_{EM, t} - I_B) dt$$

is depicted in Figure S2b. The observation of a linear relationship between 

$$\ln \frac{A_t}{A_0} \text{ and } \int (I_{EM, t} - I_B) dt$$

has verified the pseudo first-order consumption of ADPA and the linear dependence of $[^{1}O_2]_{sol}$ on $I_{EM}$. Accordingly, the value of $m (8.39 \times 10^{-15} \text{ M} \cdot \text{mV}^{-1})$ was extracted from the slope of the calibration plot using the reaction rate $k_r$ of $8.2 \times 10^7 \text{ M}^{-1} \cdot \text{s}^{-1}$ for ADPA + $^{1}O_2$.

During the experiment, emission of airborne $^{1}O_2$ was continuously monitored, and the Eq. S1 was used to determine $[^{1}O_2]_{sol}$ in the reactions.

Fig. S2 (a) UV-Vis absorption spectra of ADPA over the course of the reaction with $^{1}\text{O}_2$; and (b) the linear relationship of $\int_{t}^{t'} (I_{EM,t} - 43) dt$ against $\ln\left(\frac{A_t}{A_0}\right)$. 

In($\frac{A_t}{A_0}$) = $-6.88 \times 10^{-7} \cdot \int_{t}^{t'} (I_{EM,t} - 43) dt$.
Fig. S3  Stable conformers of neutral LysNH₂ (Nα-acetyl-L-lysine-methyl ester). Relative energies (kJ/mol, including ZPE and thermal corrections at 298 K) were calculated at the SMD-ωB97XD/6-31+G(d,p) level of theory. Populations for major conformers are indicated in parenthesis.
Fig. S3 (Continued.)
Fig. S4  Stable conformers of protonated LysNH₃⁺ (protonated Nα-acetyl-L-lysine-methyl ester). Relative energies (kJ/mol, including ZPE and thermal corrections at 298 K) were calculated at the SMD-ωB97XD/6-31+G(d,p) level of theory. Populations for major conformers are indicated in parenthesis.
Fig. S4  (Continued.)
Cartesian coordinates for the structures in Fig. S3, optimized at SMD-ωB97XD/6-31+ G(d,p).

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Cartesian coordinates for the structures in Fig. 3, optimized at SMD-ωB97X/6-31+G(d,p). For each TS, the vibrational mode corresponding to TS imaginary frequency is indicated by displacement vectors.

\[9\text{MG} – \text{H}^–\]

| C1  | -1.190857  | 1.319433  | 0.000905 |
| C2  | 0.199251   | 0.983609  | -0.002827|
| C3  | -1.587902  | -0.999143 | -0.007401|
| C4  | 2.327108   | 0.897920  | 0.000700 |
| N5  | -2.055509  | 0.262396  | -0.002194|
| C6  | 1.345055   | 1.768339  | 0.001351 |
| N7  | 1.904677   | -0.406387 | 0.001114 |
| N8  | -0.311909  | -1.409633 | -0.001908|
| C9  | 0.533861   | -0.362272 | -0.001549|
| N10 | -2.545918  | -1.990753 | -0.073125|
| H11 | -2.246048  | -2.900256 | 0.249531 |
| C17 | 2.217125   | -1.989677 | -0.457838|
| H18 | 2.293194   | -2.04466  | 0.611562 |
| H19 | 1.710625   | -2.813242 | -0.961719|
| H20 | 3.214980   | -1.874000 | -0.880803|

\[8-\text{OO9MG} – \text{H}^–\]

| C1  | -1.516584  | 1.443926  | -0.094996|
| C2  | -0.152981  | 0.865988  | -0.276995|
| C3  | -2.232087  | -0.768373 | 0.164264 |
| C4  | 1.971672   | 0.393111  | -0.614610|
| C5  | -2.504363  | 0.554947  | 0.123795 |
| C6  | 0.966138   | 1.451783  | -0.458170|
| N7  | 1.230053   | -0.872411 | -0.468930|
| N8  | -1.036179  | -1.422512 | -0.013874|
| C9  | -0.039678  | -0.602361 | -0.236855|
| N10 | -3.266174  | -1.567613 | 0.406866 |
| H11 | -3.136589  | -2.568215 | 0.439480 |
| H12 | -4.184819  | -1.173890 | 0.547160 |
| C17 | 1.866151   | -2.172672 | -0.415100|
| H18 | 1.933406   | -2.521172 | 0.618958 |
| H19 | 1.292360   | -2.888174 | -1.006799|
| H20 | 2.868611   | -2.085916 | -0.833643|
C17 2.377352  -1.715952  -0.593757  
H18 1.911113  -2.570186  -1.084900  
H19 3.349173  -1.541804  -1.057548  
H20 2.515844  -1.941481  0.467932  

[4,8-OO-9MG – H]–  
C1  -1.510809  1.323977  -0.137634  
C2  -0.063284  0.991911  -0.237190  
C3  -1.836162  -1.000309  0.008767  
C4  2.047513  0.767659  -0.261252  
N5  -2.335666  0.285966  0.007631  
N6  0.960321  1.745959  -0.405071  
N7  1.551336  -0.455698  -0.843824  
N8  -0.582543  -1.437266  -0.067004  
C9  0.352991  -0.426790  -0.038866  
N10  -2.801922  -1.935133  0.101082  
H11  -2.562049  -2.913850  0.097331  
H12  -3.769424  -1.655580  0.091769  
O13  -1.892721  2.514608  -0.194902  
H14  3.027593  1.107014  -0.579582  
O15  2.120535  0.490816  1.165322  
O16  0.941110  -0.304781  1.383397  
C17  2.420805  -1.622780  -0.673090  
H18  1.962108  -2.482893  -0.161363  
H19  3.371933  -1.420724  -0.168509  
H20  2.611442  -1.867914  0.375702  

[8-OOH9MG – H]–  
C1  -1.554614  1.472626  -0.013309  
C2  -0.264787  0.857423  -0.097331  
C3  -2.408056  -0.716111  0.098624  
C4  1.777183  0.344767  -0.256996  
N5  -2.611095  0.614369  0.083307  
N6  1.005590  1.395341  -0.213493  
N7  -1.117859  -0.857178  -0.183186  
N8  0.685282  -1.476760  0.033370  
C9  -0.210808  -0.567568  -0.036029  
N10  2.924721  -1.892452  0.036043  
O11  1.706142  2.560876  -0.004900  
O12  -3.297832  0.846931  0.044754  
C13  -2.321911  -1.938730  0.014549  
H14  -1.975969  -2.621729  -0.762123  
H15  -2.194282  -2.400782  0.995726  
H16  -3.374830  -1.713366  -0.149870  
H17  3.836721  -1.435332  0.061188  

TS3a– (water-assisted addition)
[5-OH9MOG – \( \text{H}_2\text{O} \)]

C1  1.336312  -1.208552  -0.419561  
C2  0.069001  -0.799612  0.338860  
C3  2.056623  1.012180  -0.108182  
C4  -2.148885  -0.388403  -0.116498  
C5  2.294656  -0.296769  0.510609  
N6  -1.177067  -1.354580  -0.095505  
N7  -1.525523  0.855230  0.016936  
N8  0.739582  1.550650  -0.051173  
C9  -0.175442  0.671937  0.093108  
N10  3.009834  1.842676  0.138207  
O11  1.429270  -2.388654  -0.834654  
H12  1.098193  -0.810171  2.025155  
O13  0.217189  -1.074361  1.725184  
O14  -3.350961  -0.559786  -0.267157  
C15  -2.181710  2.123149  -0.246039  
H16  -1.927998  2.835667  0.539665  
H17  -1.871773  2.521239  -1.215343  
H18  -3.257968  1.956458  -0.246391  
H19  -1.425738  -2.310400  0.126910  
H20  3.895532  1.344966  0.047896  

**TS3b** (water-assisted proton transfer)

C1  -0.846542  1.670544  -0.420385  
C2  0.091054  0.768930  0.419469  
C3  -1.863824  -2.388654  -0.834654  
C4  2.326464  0.217189  -0.460393  
C5  -1.218710  2.123149  -0.246391  
H16  -1.927998  2.835667  0.539665  
H17  -1.871773  2.521239  -1.215343  
H18  -3.257968  1.956458  -0.246391  
H19  -1.425738  -2.310400  0.126910  
H20  3.895532  1.344966  0.047896  

[5-OH9MOG – \( \text{H}_2\text{O} \)]

C1  1.244930  -1.313892  -0.352922  
C2  0.001286  -0.854382  0.407806  
C3  2.030232  0.845029  -0.097864  
C4  -2.192511  -0.336743  -0.128016  
N5  2.276832  -0.431008  -0.407069  
N7  -1.946999  0.884703  0.096968  
N8  0.790179  1.470443  -0.004539  
C9  -0.178711  0.624380  0.118211  
O11  3.064312  1.666609  0.048893  
H11  2.910720  2.646081  0.236244  
H12  4.006205  1.310718  -0.026828  
O13  1.345455  -2.475850  -0.773502  
H14  -1.606022  -2.264617  0.165405  
O15  0.189728  -1.089213  1.735898  
O16  -3.407004  -0.415274  -0.267313  
C17  -2.087039  2.187948  -0.238639  
H18  -1.847613  2.533321  -1.247131  
H19  -3.166662  2.099668  -0.127516  
H20  -1.708633  2.902176  0.493141  

**TS3c**

C1  0.227571  -0.958919  -0.778596  
C2  0.002686  0.445368  -0.589371  
C3  -2.134550  0.486613  -0.003366  
C4  -0.675098  -0.981575  0.912019  
C5  2.174527  0.068033  -0.115110  
N6  -1.901650  -0.493429  0.925753  
N7  -1.177718  1.072219  -0.714002  
O8  -0.113240  1.748546  1.682865  
N9  1.183847  1.043837  -0.222134  
N10  -3.402542  0.902050  -0.131543  
H11  -4.108632  0.543149  0.491989  
H12  -3.612727  1.698628  -0.713572  
O13  3.314660  0.258387  0.312395  
N14  1.626792  -1.098026  -0.546660
S36

O15  -0.431561  -1.815400  -1.473881
H16  2.085712  -1.989007  -0.413359
C17  1.281139  2.320070  0.470686
H18  2.279819  2.728563  0.320937
H20  0.548297  3.004761  0.045623

[9MSp – H]–
C1  -0.620417  1.470337  -0.173450
C2  0.107909  0.126255  -0.205701
C3  2.246850  -0.149230  -0.349070
C4  0.759041  -0.128345  1.193836
C5  -2.188794  -0.185335  -0.303609
N6  2.068466  -0.281006  1.019016
N7  1.202185  0.064195  -1.125545
O8  0.097693  -0.173888  2.248843
N9  -0.992173  -0.797392  -0.458204
N10  3.504205  -0.216351  -0.831246
H11  4.234029  -0.561742  -0.227475
H12  3.641342  -0.290940  -1.827895
O13  -3.304428  -0.699325  -0.280922
N14  -1.950549  1.189279  -0.192005
H16  1.202185  0.064195  -1.125545
C17  -0.830036  -2.230062  -0.282222
H18  -0.834198  -2.504452  0.777806
H19  -1.638797  -2.750627  -0.795099
H20  0.117714  -2.528093  -0.732730

[5-OH9MOG – HN7]–
C1  1.194492  -1.302841  -0.416379
C2  -0.058036  -0.857750  0.349624
C3  1.993427  0.858163  -0.118923
C4  -2.168844  -0.418530  -0.121370
N5  2.220157  -0.419999  -0.466448
N6  -1.312760  -1.420198  -0.016197
N7  -1.509509  0.876562  0.051412
N8  0.773659  1.485018  0.043665
C9  -0.210262  0.637915  0.148619
N10  3.050145  1.655557  -0.004963
H11  2.926560  2.632869  0.216000
H12  3.978808  1.284418  -0.142500
O13  1.281702  -2.449595  -0.873539
H16  1.202185  0.064195  -1.125545
C17  -0.830036  -2.230062  -0.282222
H18  -0.834198  -2.504452  0.777806
H19  -1.638797  -2.750627  -0.795099
H20  0.117714  -2.528093  -0.732730

[5-OH9MOG – HN7]–·2H2O
C1  0.183671  0.130824  0.144620
C2  -1.158164  -0.572236  0.164614
C3  -2.183640  1.383917  -0.128050
C4  0.041526  1.358726  -0.766632
C5  0.510807  -2.048925  -0.128771
N6  -1.146701  2.000003  -0.718909
N7  -2.306991  0.035581  0.158338
O8  1.000093  1.759610  -1.436260
N9  -0.908645  -1.875037  0.160628
N10  -3.268687  2.105465  0.125134
H11  -3.285613  3.090446  -0.095827
H12  -4.089614  1.664041  0.513342
O13  0.966460  -3.191417  -0.291239
N14  1.131037  -0.877388  -0.198350
O15  0.424898  0.711878  1.435319
H16  0.558611  -0.012740  2.063755
O18  1.202185  0.064195  -1.125545
H17  3.429559  1.233890  0.681089
O18  3.095946  1.822459  1.386358
H19  2.160397  1.568208  1.457322
H20  3.703728  0.444233  -1.458955
O21  3.720256  -0.052957  -0.633072
H22  2.790673  -3.903531  -0.518372
C23  -1.895871  -2.934817  0.140652
H24  -2.603305  -2.791853  0.959005
H25  -2.434713  -2.942378  -0.810542
H26  -1.381013  -3.885368  0.273479

TS3d– (water-assisted addition)
C1  -0.107482  -0.348918  0.477779
C2  -0.083965  1.125414  0.140048
C3  1.251031  1.001025  -0.066238
C4  0.946172  -0.952784  -0.497597
C5  -2.197437  0.343785  0.066383
N6  -2.217819  -0.276537  -0.279847
N7  0.993156  1.810551  -0.054038
O8  0.561796  -1.049674  -1.736654
N9  -1.360995  1.519686  0.034917
N10  3.288598  1.721779  0.157537
H11  4.163751  1.280410  -0.085656
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[5-LysNH-9MSp – HN3]−

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Cartesian coordinates for the structures in Fig. 4, optimized at SMD-ωB97XD/6-31+G(d,p). For each TS, the vibrational mode corresponding to TS imaginary frequency is indicated by displacement vectors.

**9MG**

C1 -1.130432  1.366537  0.000875  
C2  0.241414  0.997063  -0.001077  
H3 -2.959548  0.438671  -0.004438  
C4 -1.546751  -1.064071  -0.001877  
C5  2.359148  0.896134  0.000086  
N6 -1.963105  0.243970  0.000419  
N7  1.385500  1.737349  -0.00548  
N8  1.925935  -0.405795  0.000059  
N9 -0.276917  -1.415763  0.000943  
C10  0.562575  -0.354584  -0.000815  
N11 -2.515236  -2.005900  -0.054389  
H12 -2.233634  -2.954567  0.148069  
H13 -3.461809  -1.753510  0.194714  
O14 -1.629272  2.503642  0.003123  
H15  3.414849  1.128636  0.000417  
C16  2.757222  -1.598271  0.002873  
H17  2.562901  -2.191816  0.897670  
H18  2.558060  -2.199230  -0.885866  
H19  3.801056  -1.286002  -0.001323  

**TS1 (open-shell)**

C1  0.032083  0.872266  -0.436413  
C2  0.210123  -0.544415  -0.356655  
C3 -2.515236  -2.005900  -0.054389  
C4 -2.233634  -2.954567  0.148069  
C5  2.359148  0.896134  0.000086  
N6 -2.217524  0.392359  0.001323  
N7  1.185302  -1.598271  0.002873  
N8  1.925935  -0.405795  0.000059  
N9 -0.276917  -1.415763  0.000943  
C10  0.562575  -0.354584  -0.000815  
N11 -2.515236  -2.005900  -0.054389  
H12 -2.233634  -2.954567  0.148069  
H13 -3.461809  -1.753510  0.194714  
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H15  3.414849  1.128636  0.000417  
C16  2.757222  -1.598271  0.002873  
H17  2.562901  -2.191816  0.897670  
H18  2.558060  -2.199230  -0.885866  
H19  3.801056  -1.286002  -0.001323  

**8-OO9MG**

C1 -1.450682  1.480298  -0.105006  
C2 -0.109610  0.871849  -0.278785  
H3  2.359148  0.896134  0.000086  
N6 -1.963105  0.243970  0.000419  
N7  1.385500  1.773749  -0.00548  
N8  1.925935  -0.405795  0.000059  
N9 -0.276917  -1.415763  0.000943  
C10  0.562575  -0.354584  -0.000815  
N11 -2.515236  -2.005900  -0.054389  
H12 -2.233634  -2.954567  0.148069  
H13 -3.461809  -1.753510  0.194714  
O14 -1.629272  2.503642  0.003123  
H15  3.414849  1.128636  0.000417  
C16  2.757222  -1.598271  0.002873  
H17  2.562901  -2.191816  0.897670  
H18  2.558060  -2.199230  -0.885866  
H19  3.801056  -1.286002  -0.001323  

**TS2**
O15  1.004905  0.031056  1.568665
O16  2.214075  0.590227  1.153001
H17  -3.220526  0.534122  0.153001
C18  2.348239  -1.810764  -0.532083
H19  1.857579  -2.655067  -1.015676
H20  3.325673  -1.664153  -0.991704
H21  2.469558  -2.020205  0.534684

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C1  -1.450621  1.372863  -0.146483
C2  -0.021560  1.003510  -0.242667
C3  -1.794619  -1.063377  0.006591
C4  2.080411  0.762232  -0.254745
N5  -2.241967  0.266714  0.006010
N6  1.000738  1.754002  -0.406261
N7  1.577940  -0.454183  -0.841210
N8  -0.547238  -1.442997  -0.065643
C9  0.388234  -0.418340  -0.027893
N10  -2.778996  -1.962504  0.088417
H11  -2.542131  -2.943254  0.108014
H12  -3.752147  -1.694265  0.074487
O13  -1.892986  2.509844  -0.197009
H14  3.064659  1.096082  -0.564116
O15  2.444529  -1.625963  -0.671972
H19  1.984814  -2.481810  -1.165635
H20  3.395726  -1.420743  -1.165009
H21  2.631643  -1.873215  0.376496

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C1  -1.532661  1.438400  -0.128479
C2  -0.169773  0.858001  -0.105411
C3  -2.239144  -0.796777  0.178684
C4  1.941119  0.377890  -0.650750
N5  -2.514236  0.568645  0.086033
N6  1.040767  1.440836  -0.222098
N7  1.145399  -0.849558  -0.183209
N8  -1.199269  -1.394798  0.030153
C9  -0.174440  -0.523245  -0.074345
N10  -3.503012  -1.529537  0.152351
H11  -3.408986  -2.520030  0.322988
H12  -4.383230  -1.092798  0.388602
O13  -1.748037  2.715827  -0.019603
H14  3.928697  1.109129  1.140014
O15  3.151264  0.396674  -0.439496
O16  3.783475  0.193007  0.848774
H17  -3.461719  0.957335  0.151233
C18  1.713405  -2.188069  -0.215897
H19  1.216325  -2.774915  -0.989096
H20  2.773851  -2.107866  -0.448737
H21  1.588098  -2.672712  0.753635

9MOGx
C1  1.366246  1.418465  -0.005306
C2  -0.042711  0.918912  -0.008393
C3  1.989472  -0.824544  0.004111
C4  -2.170404  0.527968  0.004456
N5  2.325627  0.466716  0.004816
N6  -1.149277  1.557580  0.005670
N7  -1.571514  -0.732983  -0.038393
N8  0.712490  -1.415132  -0.017134
C9  -0.232510  -0.548002  -0.023577
N10  2.962706  -1.718533  0.026361
H11  2.747519  -2.063977  0.026404
H12  3.927114  -1.414151  0.044691
O13  1.595988  2.629737  -0.009841
O14  -3.353627  0.751804  0.038051
C15  -2.276930  -2.004508  -0.008842
H16  -1.908407  -2.647631  -0.800422
H17  -2.127567  -2.846354  0.966745
H18  -3.336760  -1.807623  -0.155024

8-OOH9MG
C1  -1.491802  1.502970  -0.015551
C2  -0.224219  0.865433  -0.015411
C3  -2.374318  -0.796945  0.099522
C4  1.808994  0.351890  -0.268097
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N6  1.040667  1.403190  -0.222096
N7  1.145399  -0.849558  -0.183209
N8  -1.199269  -1.394798  0.030153
C9  -0.174440  -0.523245  -0.074345
N10  -3.503012  -1.529537  0.152351
H11  -3.408886  -2.520030  0.322988
H12  -4.383230  -1.092798  0.388602
O13  -1.748037  2.715827  -0.019603
H14  3.928697  1.109129  1.140014
O15  3.151264  0.396674  -0.439496
O16  3.783475  0.193007  0.848774
H17  -3.461719  0.957335  0.151233
C18  1.713405  -2.188069  -0.215897
H19  1.216325  -2.774915  -0.989096
H20  2.773851  -2.107866  -0.448737
H21  1.588098  -2.672712  0.753635
TS3a (water-assisted addition)

C1  -0.201119  0.485214  0.013710  
C2  0.191336  -0.961985  -0.188853  
C3  2.356128  -0.431138  -0.029932  
C4  0.914898  1.201710  0.783319  
C5  -1.969919  -0.770360  0.381273  
N6  2.171940  0.741651  0.602550  
N7  1.409703  -1.396049  -0.321933  
O8  0.657871  2.209186  1.453147  
N9  -1.513975  0.467269  0.544583  
N10  -0.935322  -1.658461  -0.141464  
N11  3.601448  -0.764119  -0.342974  
H12  4.364391  -0.141926  -0.118200  
H13  3.791821  -1.654354  -0.779491  
O14  -1.727268  3.105064  -0.966629  
H15  -2.281118  2.802511  -0.223256  
H16  -1.228793  3.881457  -0.659519  
O17  -0.271948  1.123797  -1.305396  
H18  -1.054880  2.316892  -1.164142  
H19  0.603703  1.287804  -1.690049  
C21  -1.056618  -3.100907  -0.217557  
H22  -2.098409  -3.347139  -0.418947  
H23  -0.435140  -3.472882  -1.032819  
H24  -0.745216  -3.566351  0.721458  

5-OHMOG

C1  1.255012  -1.302843  -0.396633  
C2  -0.010686  -0.839311  0.335534  
C3  2.031697  0.859953  -0.112548  
C4  -2.195484  -0.323543  -0.141278  
N5  2.234934  -0.476338  -0.434032  
N6  -1.269046  -1.332236  -0.129154  
N7  -1.500670  0.898640  -0.015062  
N8  0.788095  1.48382  -0.017885  
C9  -0.184084  0.647506  0.096857  
N10  3.061868  1.672130  0.050184  
H11  2.910993  2.651119  0.249362  
H12  4.003889  1.313695  -0.021317  
O13  1.328918  -2.455591  -0.827954  

TS3b

C1  0.270653  -0.949591  -0.814160  
C2  0.046624  0.460192  -0.523034  
C3  -2.132186  0.551633  -0.075561  
C4  -0.635986  -0.994072  0.883370  
C5  2.221799  0.038483  -0.110748  
N6  -1.908219  -0.510103  0.788030  
N7  -1.114921  1.119622  -0.676143  
O8  -0.223864  -1.769438  1.712820  
N9  1.225541  1.026968  -0.155206  
N10  -3.379586  0.985552  -0.206863  
H11  -4.143177  0.547273  0.288072  
H12  -3.564205  1.790807  -0.787799  
O13  3.366910  0.214420  0.282599  
O14  1.650732  -1.135388  -0.557800  
O15  -0.407923  -1.740119  -1.528429  
H16  2.133436  -2.002575  -0.573088  
H17  -2.627583  -0.805875  1.443300  
C18  1.363556  2.297887  0.544172  
H19  1.188085  2.165644  1.614335  
H20  2.370226  2.678103  0.377266  
H21  0.640651  3.001371  0.133631  

9MSp

C1  -0.653471  1.478850  -0.141064  
C2  0.068841  0.118736  -0.188150  
C3  2.228522  -0.130786  -0.458636  
C4  0.720052  -0.140238  1.197818  
C5  -2.274845  -0.171388  -0.302805  
N6  2.040653  -0.258330  0.921341  
N7  1.14055  0.073942  -1.144713  
O8  0.158171  -0.221441  2.275054  
N9  -1.028853  -0.794614  -0.433889  
N10  3.465519  -0.219216  -0.945047
5-OH9MOG·2H2O

C1  0.160723  0.085297  0.207981
C2  -1.278398  -0.382150  0.117614
C3  -1.932749  1.745226  -0.062772
C4  0.281525  1.381788  -0.605973
C5  0.040970  -2.176282  -0.208739
N6  -0.773965  2.211795  -0.549627
N7  -2.292650  2.117951  -0.549627
O8  1.331729  -3.341743  -0.377215
N9  -1.276693  -1.723266  0.041407
N10  -2.894271  2.609538  0.205308
H11  -2.734460  3.599867  -0.377215
H12  -3.797919  2.281840  0.157669
O13  0.347394  -3.341743  -0.377215
N14  -0.804066  -1.394956  0.571176
N15  0.481130  0.010896  1.978597
H16  -0.284410  0.010388  2.568853
H17  -0.479298  -2.351970  0.550152
N18  2.229226  -2.174605  0.041526
O19  2.369856  -1.051056  0.477095
H20  2.249987  -0.981538  1.438985
H21  1.430588  -2.307090  -1.289656
O22  1.935886  -3.020572  -0.759634
H23  1.290994  -3.641334  -0.392715
C24  -3.211354  1.050376  -0.603357
H25  -3.054557  1.200135  -1.674339
H26  -4.113383  0.462097  -0.442229
H27  -3.320240  2.016062  -0.109266

gem-9Mdiol

C1  -0.033625  -0.705369  0.466121
C2  -0.364872  0.742974  0.143876
C3  1.836811  1.178640  0.006687
C4  1.207075  -1.042137  -0.385625
C5  -2.281246  -0.436163  -0.001595
N6  2.227341  -0.508034  -0.185752
N7  0.510342  1.665094  -0.018297
N8  -1.708449  0.850359  0.028336
N9  2.739191  2.153360  0.213185
H10  3.725045  1.943954  0.182487

TS3c (water-assisted addition)
H11  2.437732  3.113543  0.266453
O12  -3.472952  -0.660140  -0.147808
N13  -1.275328  -1.345052  1.807986
H15  -1.474996  -2.304041  0.384791
O16  0.765796  -1.095039  -1.715000
H17  1.540255  -0.975715  -2.278565
H18  2.197644  -2.261283  0.757832
O19  1.704702  -2.317828  -0.071047
H20  -0.379079  -0.603832  2.388281
C21  -2.426196  2.060441  -0.333796
H22  -2.22836  2.326842  -1.373570
H23  -3.491560  1.877441  -0.202212
H24  -2.116541  2.871823  0.324948

LysNH₃⁺
N1  -5.541400  -0.702935  0.108660
C2  -4.272147  -0.003797  -0.255529
H3  -4.264558  0.940959  0.289215
H4  -4.323904  0.203849  -1.325077
C5  -3.070358  -0.863022  0.093342
H6  -3.130755  -1.812362  -0.452142
H7  -3.089524  -1.096160  1.164942
C8  -1.765931  -0.147443  -0.235732
C9  -1.765931  -0.147443  -0.235732
H9  -1.765931  -0.147443  -0.235732
H10  -1.730488  0.809763  0.280285
C11  -0.551585  -0.999242  0.109454
H12  -0.639793  -1.982122  -0.365948
H13  -0.517709  -1.160076  1.193796
C14  0.784878  -0.395462  -0.343073
H15  -0.089524  -0.961600  1.164942
C16  0.784878  -0.395462  -0.343073
H16  -0.089524  -0.961600  1.164942
H17  1.540255  -0.975715  -2.278565
H18  2.197644  -2.261283  0.757832
O19  1.704702  -2.317828  -0.071047
H20  -0.379079  -0.603832  2.388281
C21  -2.426196  2.060441  -0.333796
H22  -2.22836  2.326842  -1.373570
H23  -3.491560  1.877441  -0.202212
H24  -2.116541  2.871823  0.324948

Weak Complex of 9MOGOX with LysNH₃⁺

LysNH₃⁺
C1  -3.989202  1.160689  -0.146511
C2  -3.049945  0.107871  -0.640893

5-LysNH₂⁺-9MOG'
Cartesian coordinates for the structures in Fig. 5, optimized at SMD-oB97XD/6-31+G(d,p). For each TS, the vibrational mode corresponding to TS imaginary frequency is indicated by displacement vectors.

**Fig. 5a**

[5-MeNH-9MSp – H]−

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**Fig. 5b**

5-MeNH2+–9MOG

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5-MeNH₂⁺-9MOG_HT1

C1  -1.189248  -0.885776  -0.826523
C2  0.043171  -0.700416  0.054728
C3  -1.877181  1.294184  -0.000821
C4  2.255394  -0.202867  -0.319384
N5  -2.138664  0.104378  -0.629554
N6  1.280708  -1.132271  -0.538402
N7  1.608967  0.985504  0.132726
N8  -0.623106  1.693402  0.321209
C9  0.297171  0.781636  0.198052
N10 -2.872404  2.112698  0.223259
H11 -2.683980  3.017302  0.637667
O12 -1.392168  -1.847056  -1.535351
O13  3.448797  -0.300437  -0.503421
C14  2.278051  2.276040  0.213765
H15  2.138088  2.827605  -0.717802
H16  1.861679  2.834979  1.050552
H17  3.337888  2.095507  0.384236
H18  -3.825548  1.873212  -0.024145
N19 -0.164825  -1.279352  1.381415
H20 -0.860875  -0.735231  1.886985
C21 -0.566247  -2.691544  1.385723
H22 -0.596376  -3.019354  2.425440
H23 -1.549397  -2.873145  0.936255
H24  0.179503  -3.296909  0.866646
H25 -3.059751  -0.49216  -1.034709
H26  1.535128  -2.112792  -0.568754

[TSHT2 + H]⁺

C1  1.189268  0.785138  -0.901472
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C3  1.760641  -1.399634  0.011395
C4  -2.261689  0.381727  -0.295627
N5  2.070453  -0.257081  -0.687125
N6  -1.283535  1.322546  -0.436907
N7  -1.684716  -0.883999  0.095721
N8  0.496543  -1.717915  0.361034
C9  -0.372267  -0.754044  0.192432
N10 2.725891  -2.248083  0.259058
H11 2.508587  -3.122880  0.720627
O12 1.430663  1.693549  -1.663260
O13  -3.463786  0.518123  -0.435823
C14  -2.428456  -2.128416  0.197016
5-MeNH₂⁺-9MOG_HT2

[TScO + H]^+

[IMG + H]^+

\[
\begin{align*}
C1 & = -1.091568 \quad 0.588426 \quad 1.450877 \\
C2 & = 0.483555 \quad 0.831160 \quad -0.462943
\end{align*}
\]