Supporting Information

Effects of Substituents on the Properties of Metal-Free MRI Contrast Agents

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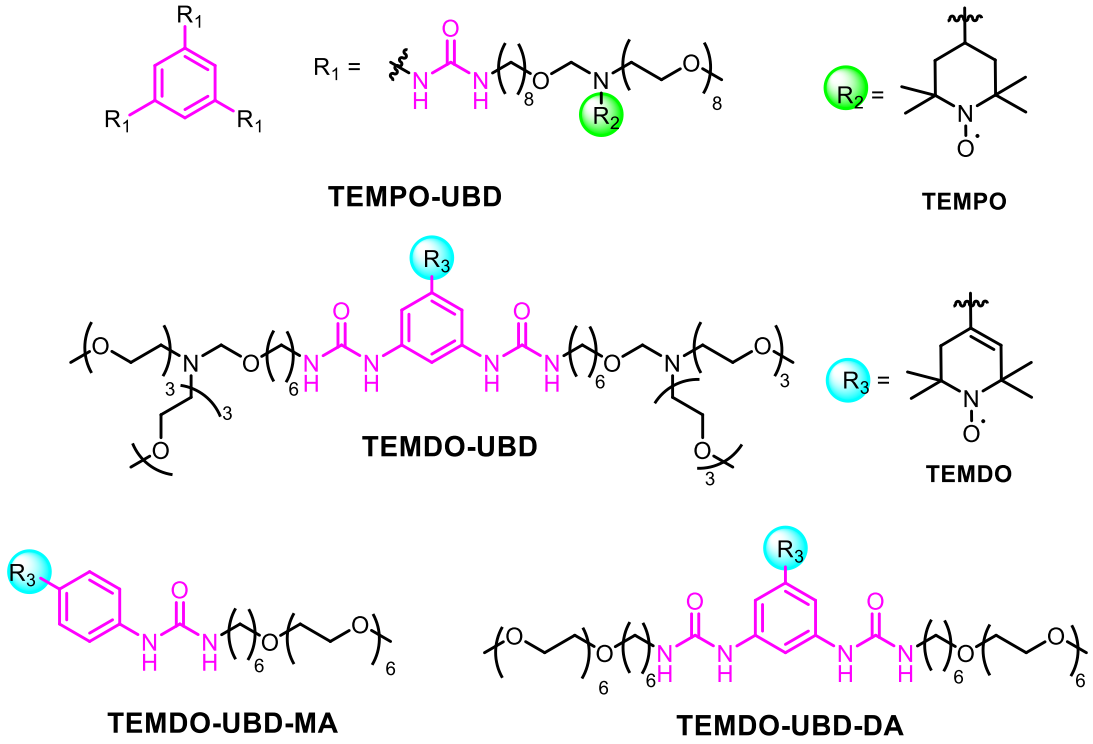
Scheme S1. Molecular structures consisted of UBD frameworks carrying stable radicals.



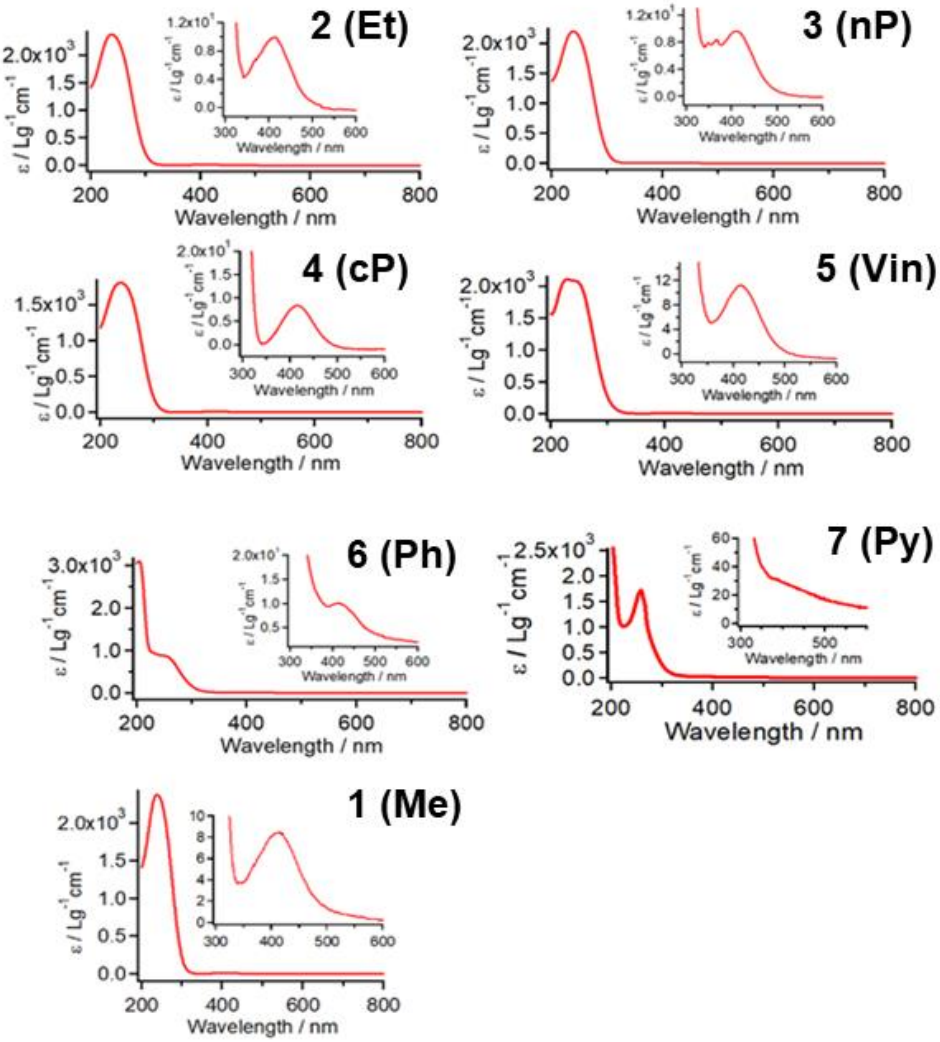


Figure S1. UV-vis spectra of the given **DAD–X** in water.

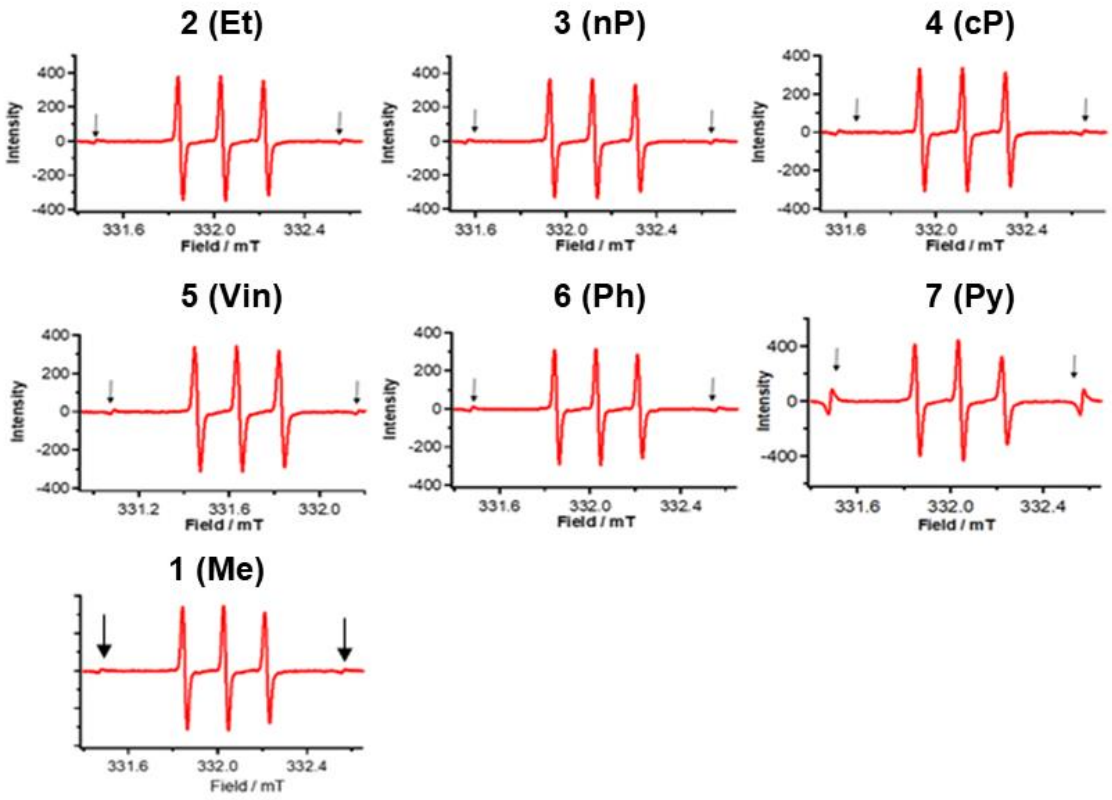


Figure S2. ESR spectra of the given **DAD**–**X** in PBS. The arrows indicate the signals of Mn(II) ions that were used as the standard signals.

Table S1. Estimated τ_R Values of **DAD-X** in Water Solutions

DAD-X	**1 (Me)**	**8 (Py)**	**5 (Vin)**	**2 (Et)**	**4 (cP)**	**3 (nP)**	**6 (Ph)**
τ_R (10^{-11} s)	7.6	7.9	5.5	3.5	4.6	6.4	6.3

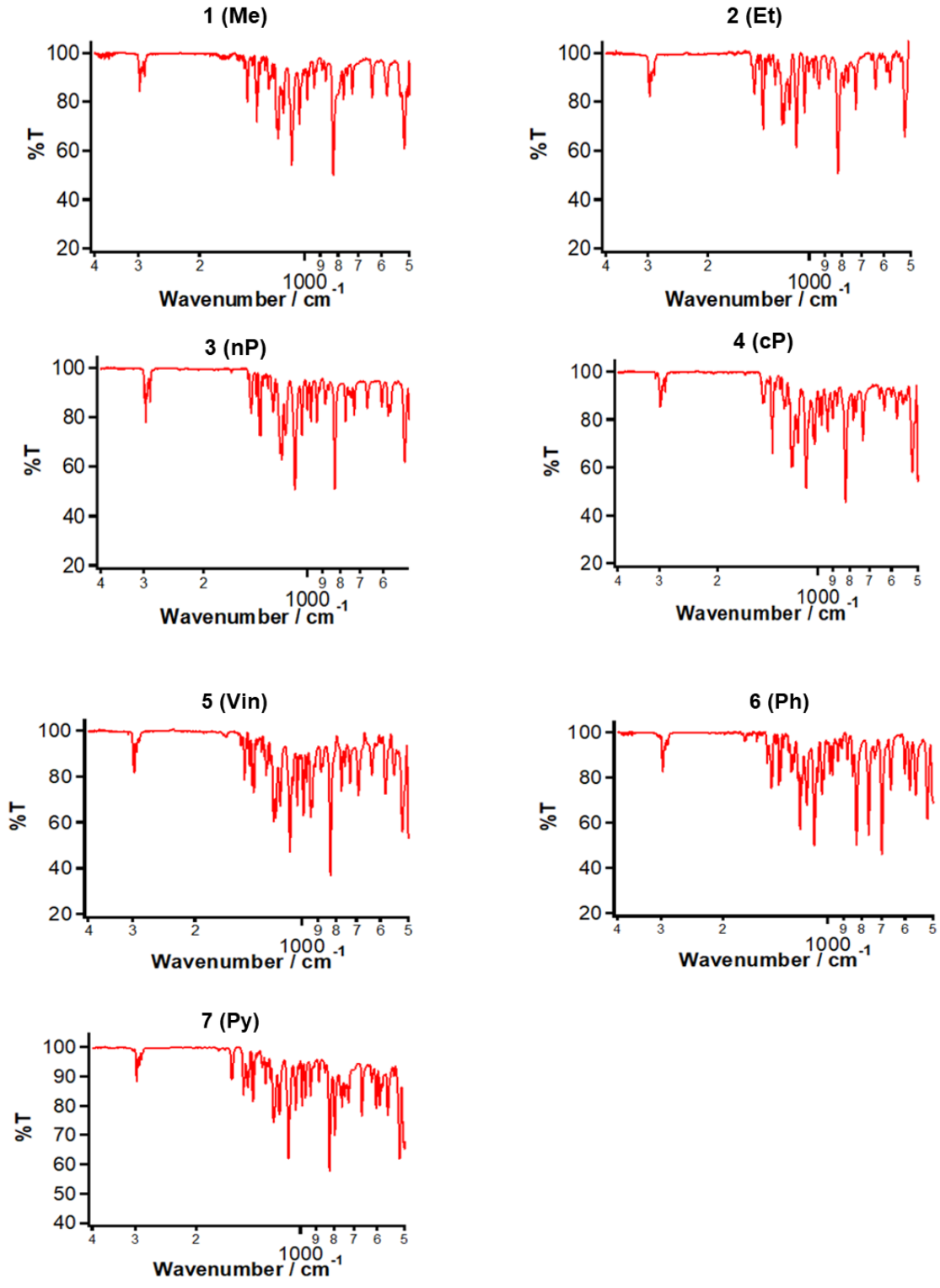


Figure S3. IR spectra of the given **DAD–X** with the use of a NaCl block.

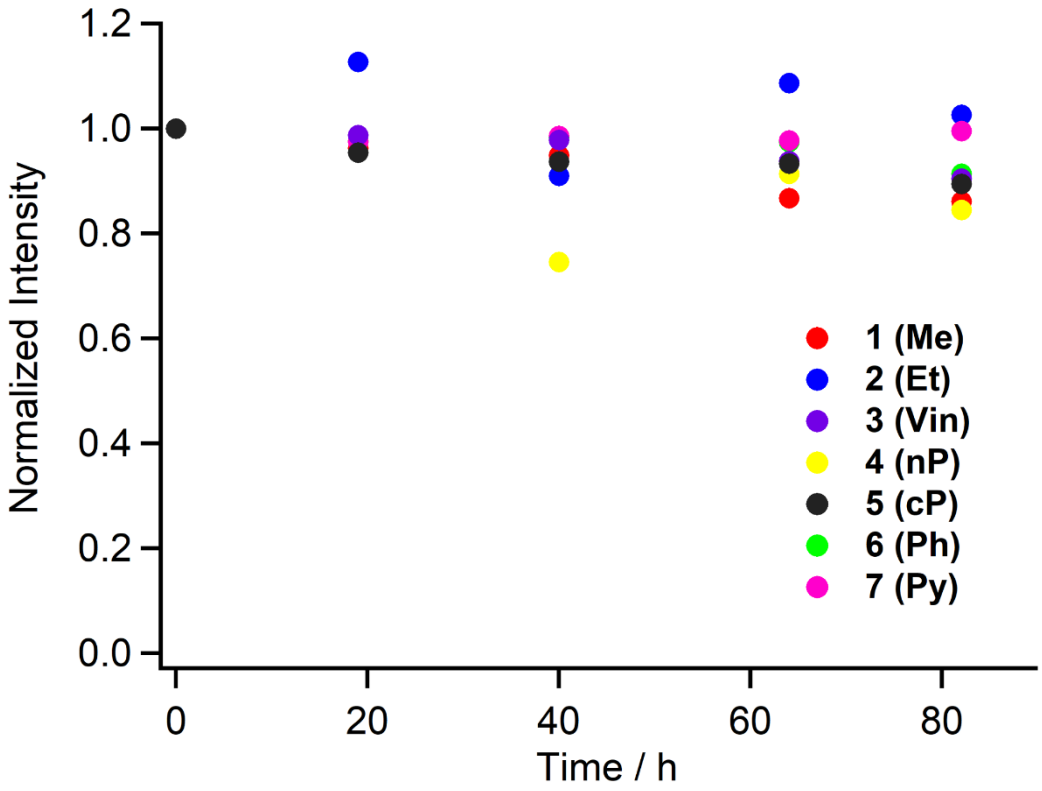


Figure S4. Stability check of **DAD-X** by change of ESR signal. The double integration of ESR signals for the corresponding 1 mM water solutions of **DAD-X** were monitored at 23 ˚C until 82 h.

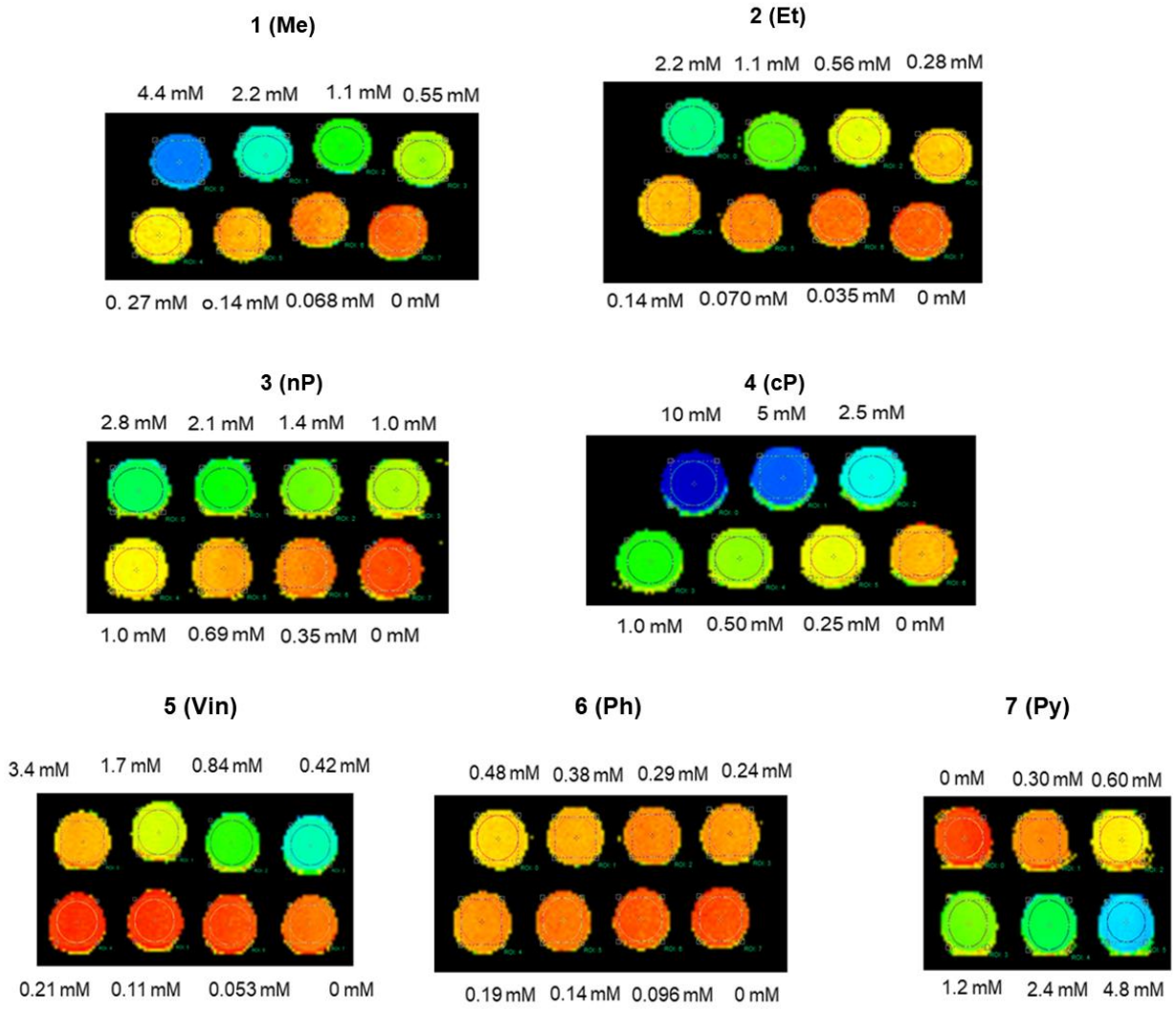


Figure S5-1. Estimated T_1-weighted images (phantom images) of the **DAD**–**X** solutions in PBS. The solution concentrations are listed in these images.

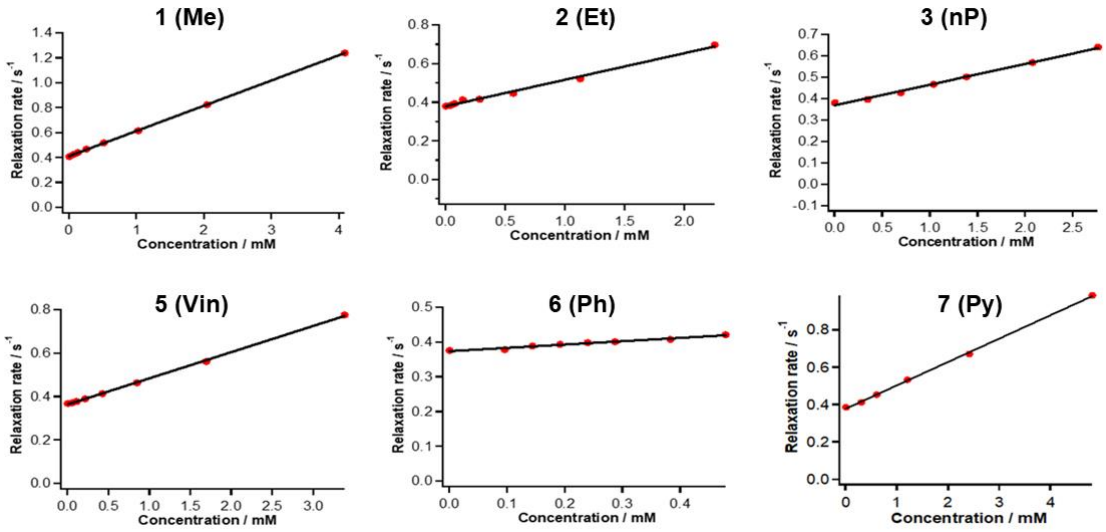


Figure S5-2. Plots of relaxation time *vs.* concentration for the given **DAD**–**X** in PBS.

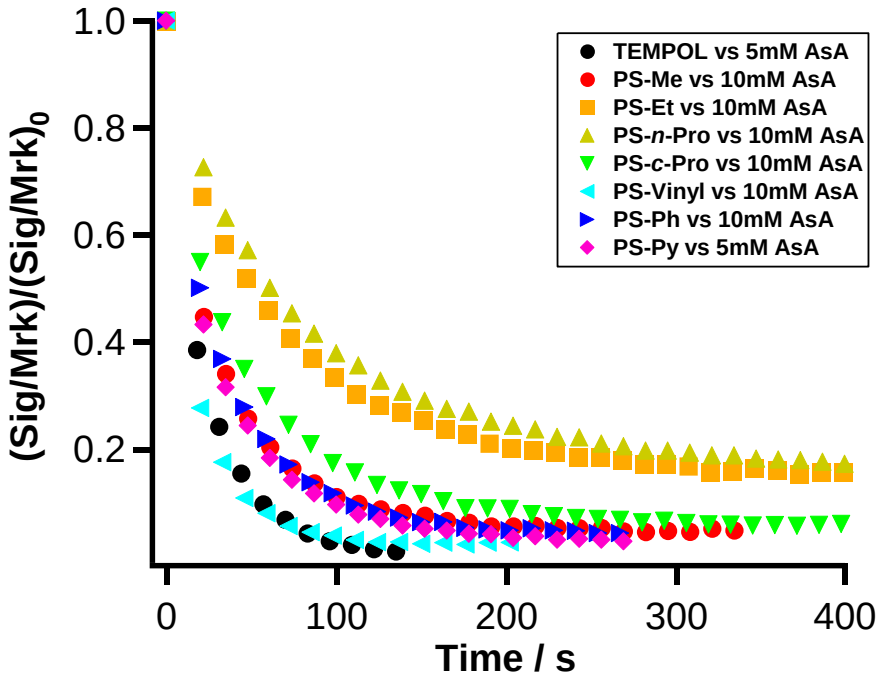
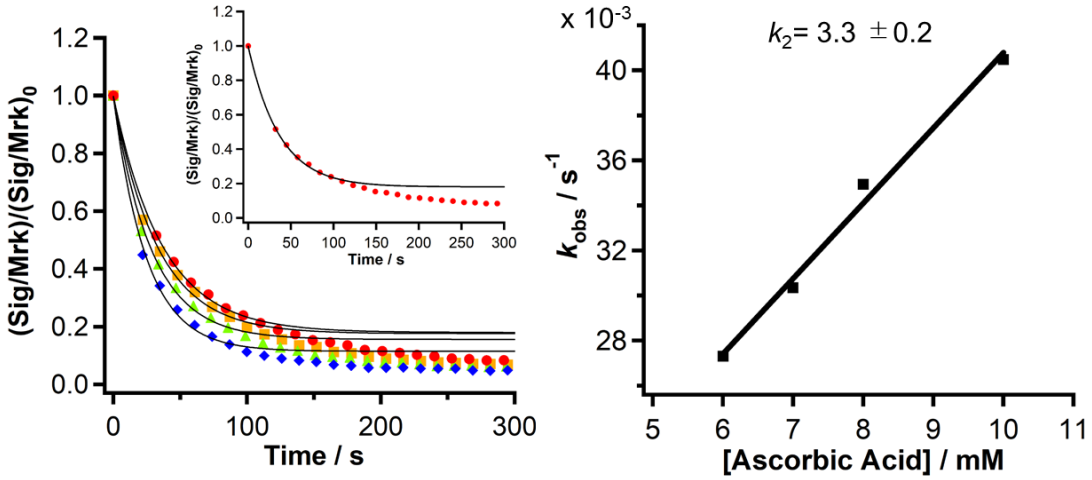
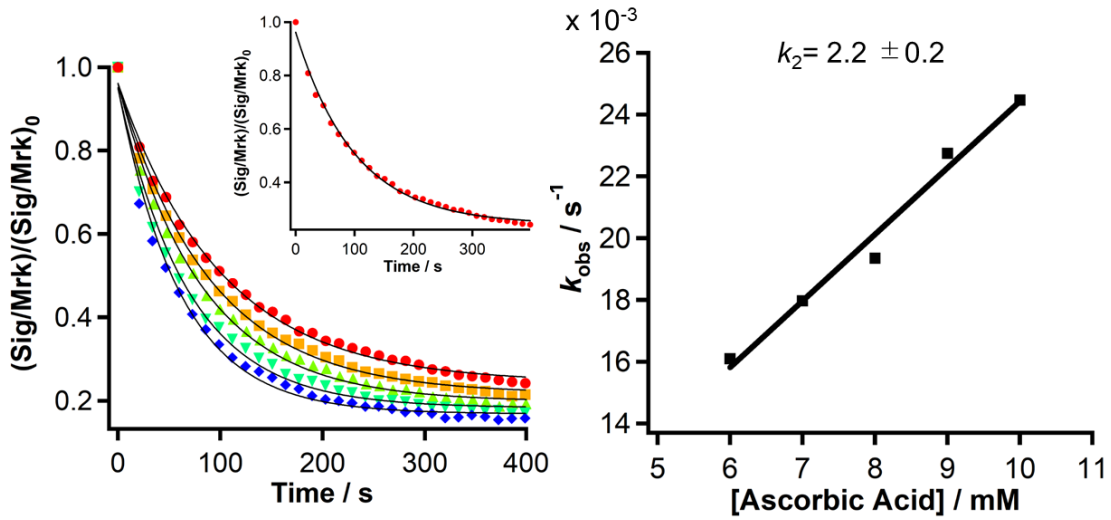


Figure S6. Time-dependent decay curves obtained from the ESR intensities of **DAD**–**X** (50 μM) for various concentrations of ascorbic acid.

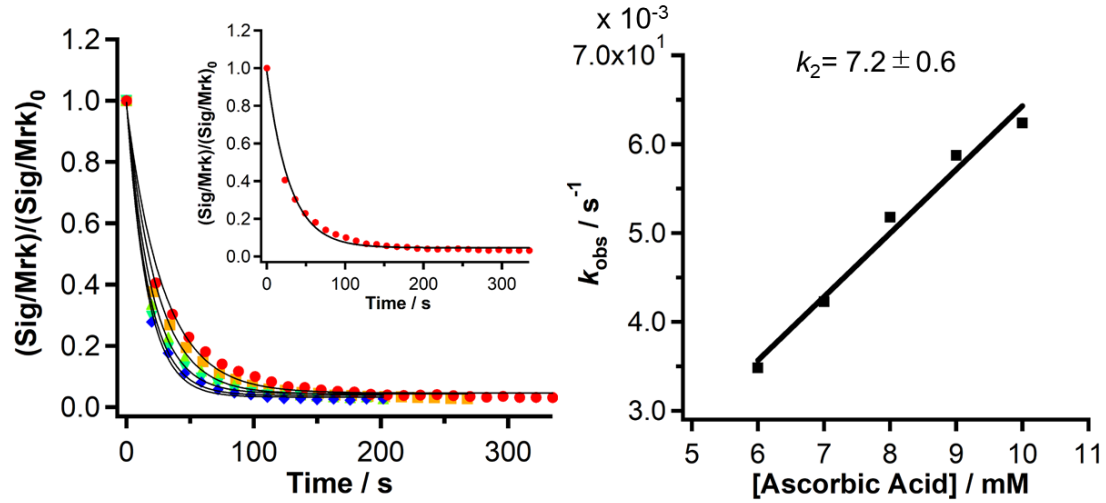
(a)


(Sig/Mrk)/(Sig/Mrk)0
Time / s
x 10-3
kobs / s-1
k2= 3.3 ±0.2
[Ascorbic Acid] / mM

(b)


(Sig/Mrk)/(Sig/Mrk)0
Time / s
x 10-3
kobs / s-1
k2= 2.2 ±0.2
[Ascorbic Acid] / mM

(c)



(d)

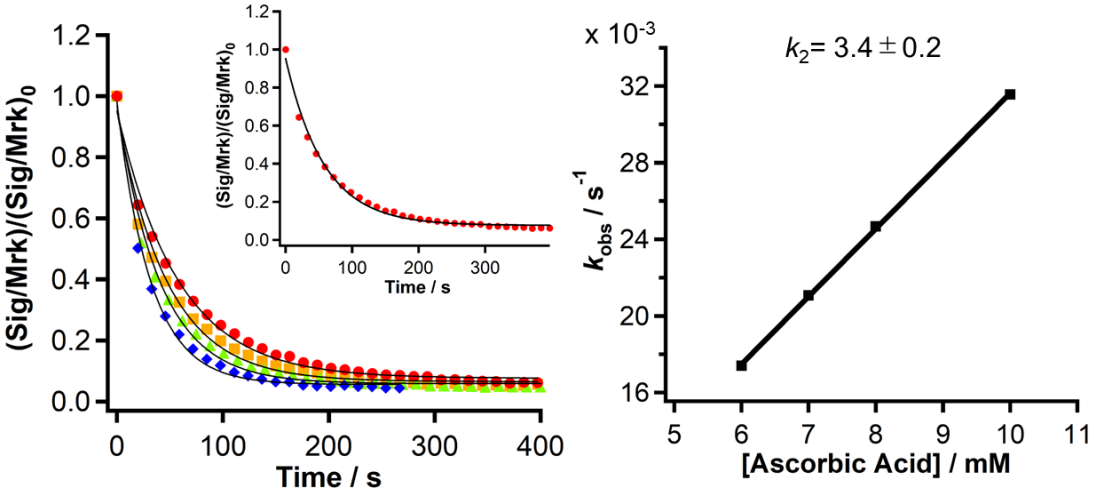


Figure S7. (Left) Time-dependent decay curves obtained from the ESR intensities of (a) **1 (Me)**, (b) **2 (Et)**, (c) **5 (Vin)**, and (d) **6 (Ph)** at various concentrations of the ascorbic acid (AsA). Solid lines indicate the curve fitting according to equation 2. Red, orange, green, sky blue, and blue colored circles represent 6, 7, 8, 9, and 10 mM of AsA. Inset show the result of 6 mM. (Right) Plots of the resulting k_{obs} values *vs.* concentration of AsA.

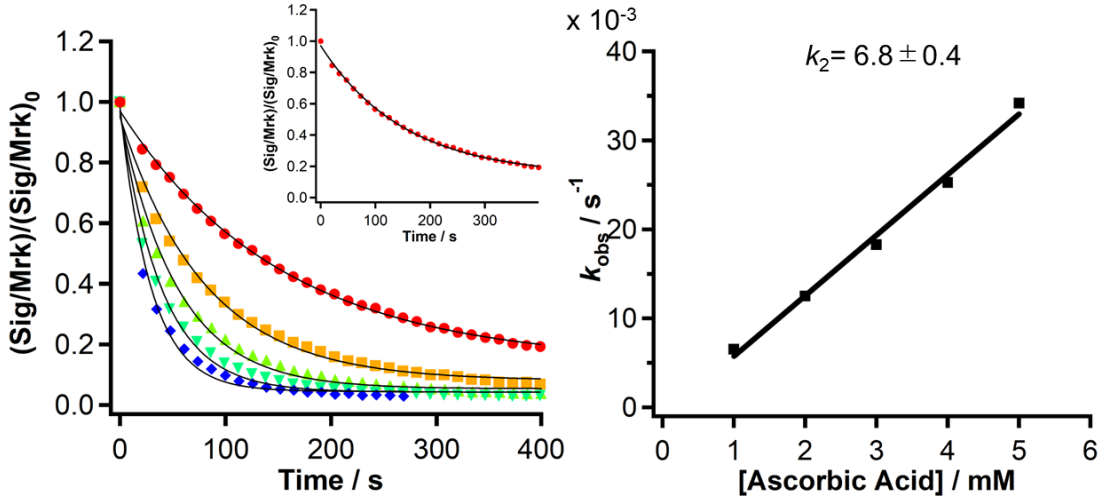


Figure S8. (Left) Time-dependent decay curves obtained from the ESR intensities of **8 (Py)** at various concentrations of ascorbic acid (AsA). Solid lines indicate the curve fitting according to equation 2. Red, orange, green, sky blue, and blue colored circles represent 1, 2, 3, 4, and 5 mM of AsA. Inset show the result of 6 mM. (Right) Plots of the resulting k_{obs} values *vs.* concentration of AsA.

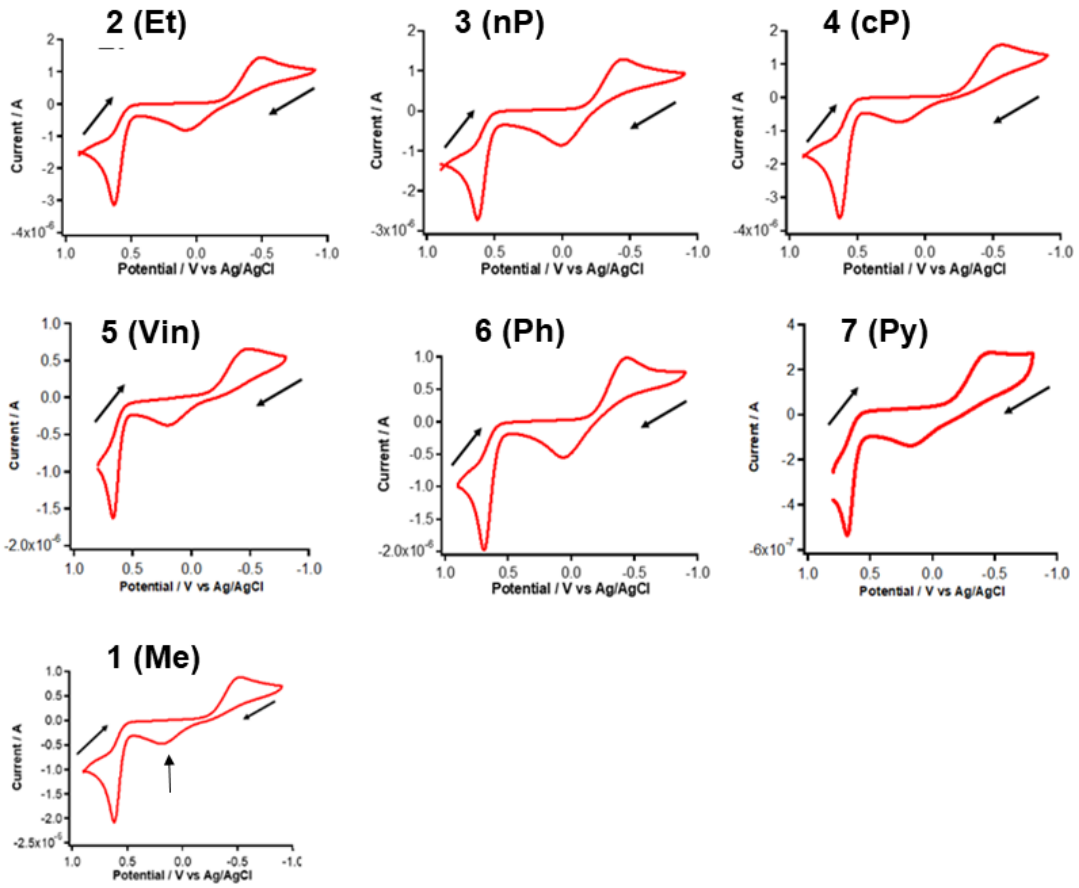


Figure S9. Cyclic voltammograms of the **DAD**–**X** solutions in PBS.

Table S2. Estimated Redox Potentials of **DAD-X**.[†]

DAD-X	**1 (Me)**	**7 (Py)**	**5 (Vin)**	**2 (Et)**	**4 (cP)**	**5 (nP)**	**6 (Ph)**
	Oxidation (OP) and reduction (RP) potentials[*]						
OP[††]	0.83[**], 0.77[#]	0.90[**], 0.83[#]	0.86[**], 0.80[#]	0.83[**], 0.78[#]	0.82[**], 0.78[#]	0.83[**], 0.76[#]	0.92[**], 0.84[#]
RP[††]	-0.16[**], -0.23[#]	-0.11[**], -0.14[#]	-0.13[**], -0.14[#]	-0.10[**], -0.15[#]	-0.11[**], -0.15[#]	-0.075[#]	0.0030[**], -0.0030[#]
logP[##]	1.87	2.19	2.46	2.50	2.53	3.09	3.17

[†]**DAD-X** is alligned in the order of log*P*. [††]OP: oxidation potential, RP: reduction potential. [*]Glassy carbon electrode, Ag/AgCl, Pt, sweep rate 4 $mV \cdot s^{-1}$, all potentials shown are versus SHE. [**]Obtained by SHACV. [#]Obtained by DPV. [##]UB3LYP-D3(BJ)/6-311G**//UB3LYP-D3(BJ)/6-31G*.

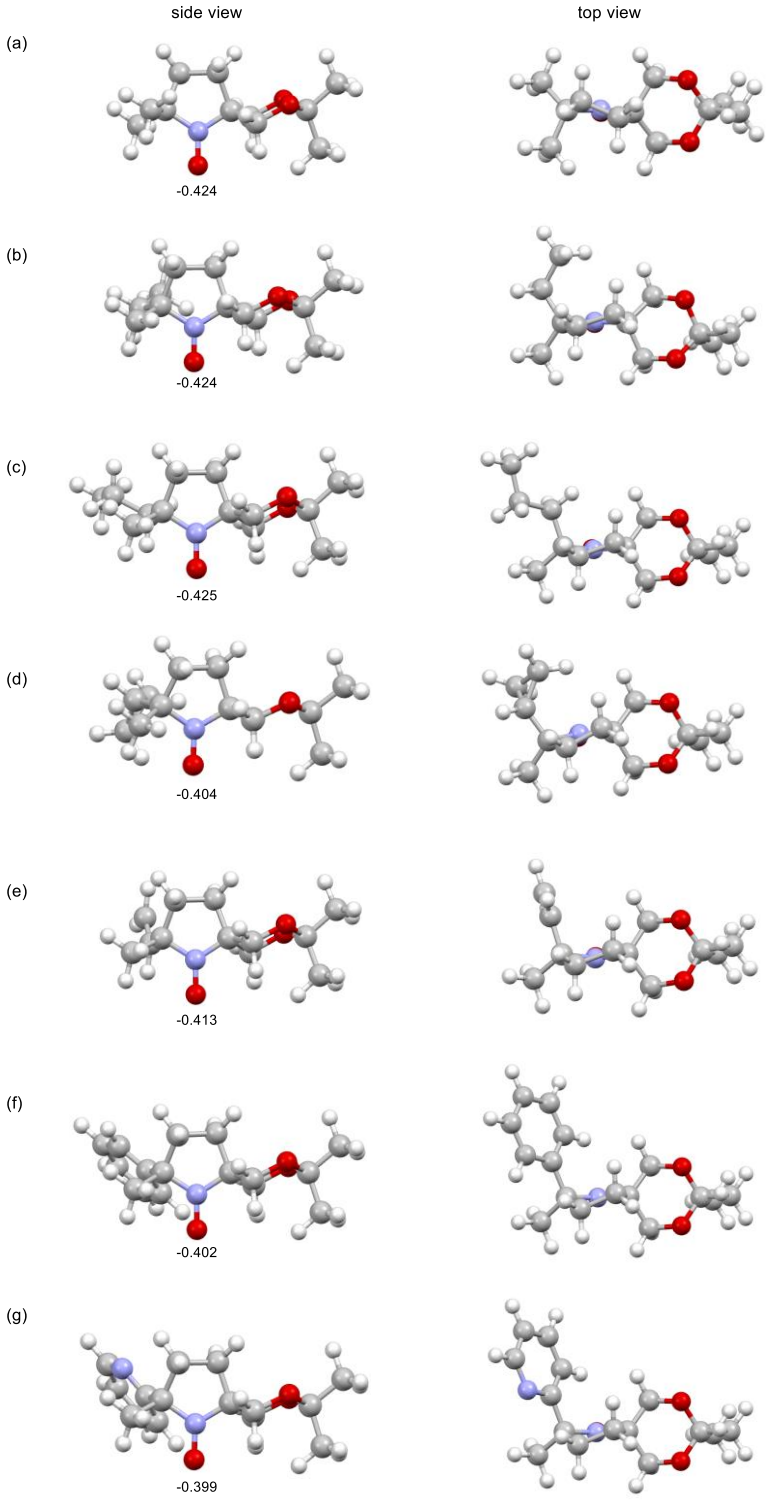


Figure S10. Optimized structures and Mulliken charges of the oxygen atom in NO for (a) **1 (Me)**, (b) **2 (Et)**, (c) **3 (nP)**, (d) **4 (cP)**, (e) **5 (Vin)**, (f) **6 (Ph)**, and (g) **7 (Py)**. The gray, blue, red, and white atoms denote C, N, O, H atoms, respectively.

Table S3. Solvation Gibbs Free Energies ($-\Delta G_{sol}$, J) and log*P* Values in *n*-Octanol and Water Solvents Based on DFT Calculations.

Radical	$-\Delta G_{sol\ (n\text{-octanol})}$ (J)	$-\Delta G_{sol\ (water)}$ (J)	log*P*
1 (Me)	-43843.22	-33170.57	1.87
2 (Et)	-46980.70	-32734.73	2.50
3 (nP)	-48983.95	-31319.59	3.09
4 (cP)	-47434.91	-32981.53	2.53
5 (Vin)	-44113.65	-30043.60	2.46
6 (Ph)	-53922.52	-35801.32	3.17
7 (Py)	-51522.81	-39041.18	2.19

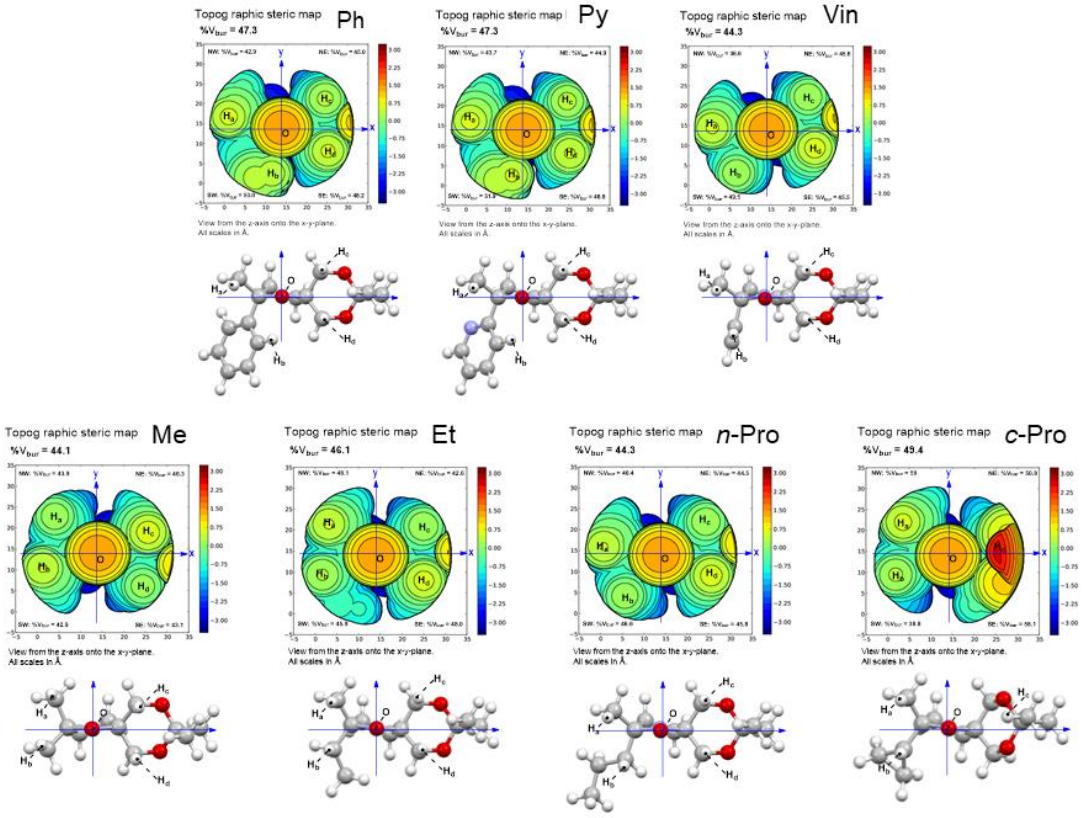


Figure S11. Space filling models of **DAD-X**. Phrase of $\%V_{bur}$ indicates the percentage of the buried volume.

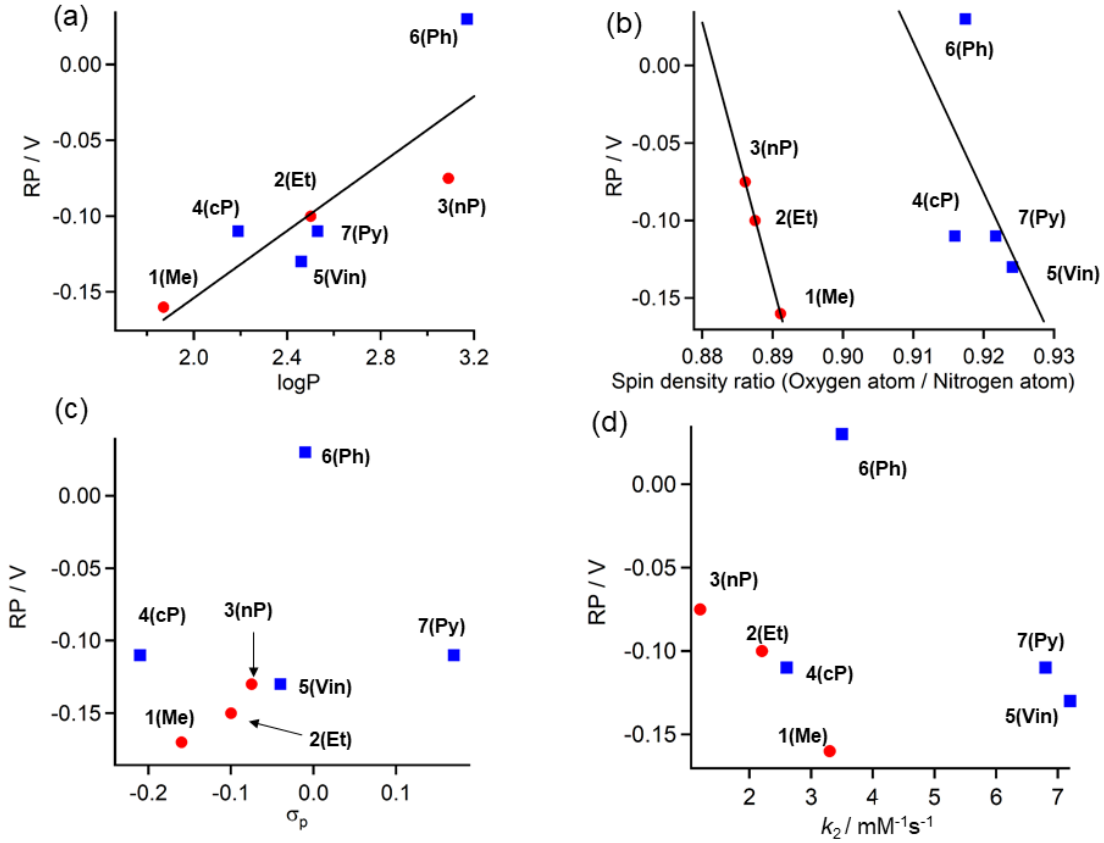


Figure S12. Correlations between RP and various parameters. (a) *reduction potential* vs log*P*. (b) *reduction potential* vs SDR. (c) *reduction potential* vs σ_P. (d) *reduction potential* vs k_2. The solid lines indicate least-squares fitting lines.

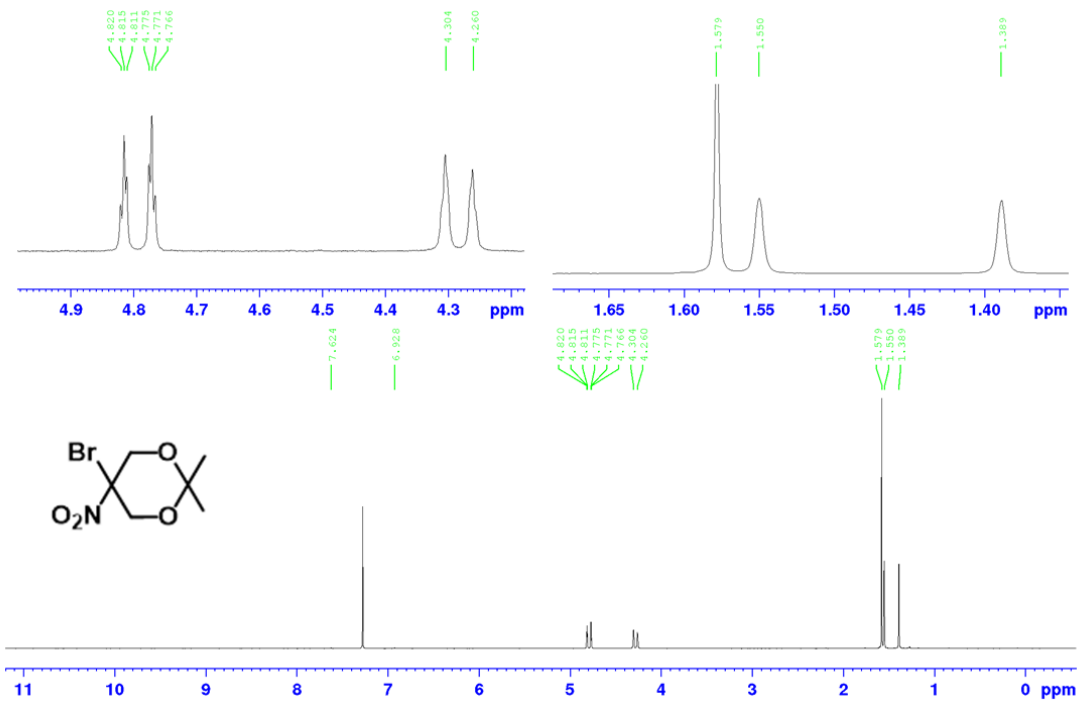


Figure S13. ^{1}H NMR spectrum of (**1**) in $CDCl_3$.

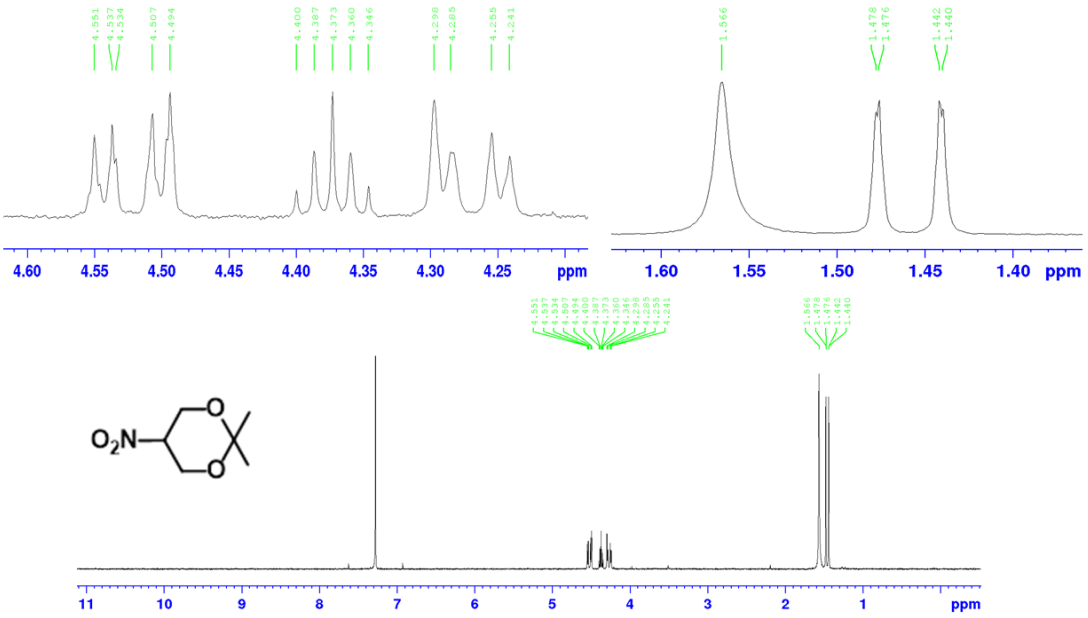


Figure S14. ^{1}H NMR spectrum of (**2**) in $CDCl_3$.

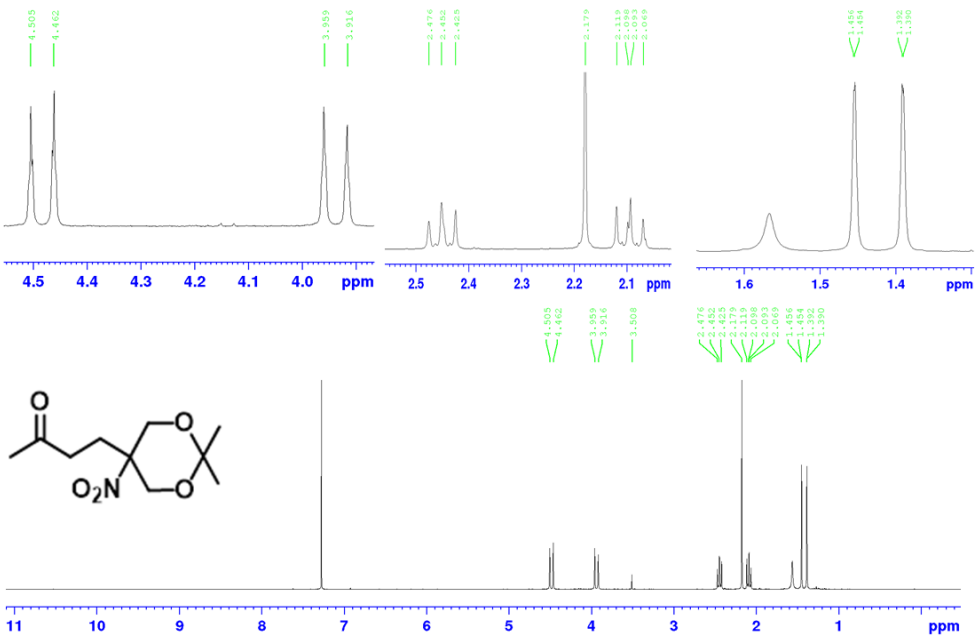


Figure S15. ^{1}H NMR spectrum of (**3**) in $CDCl_3$.

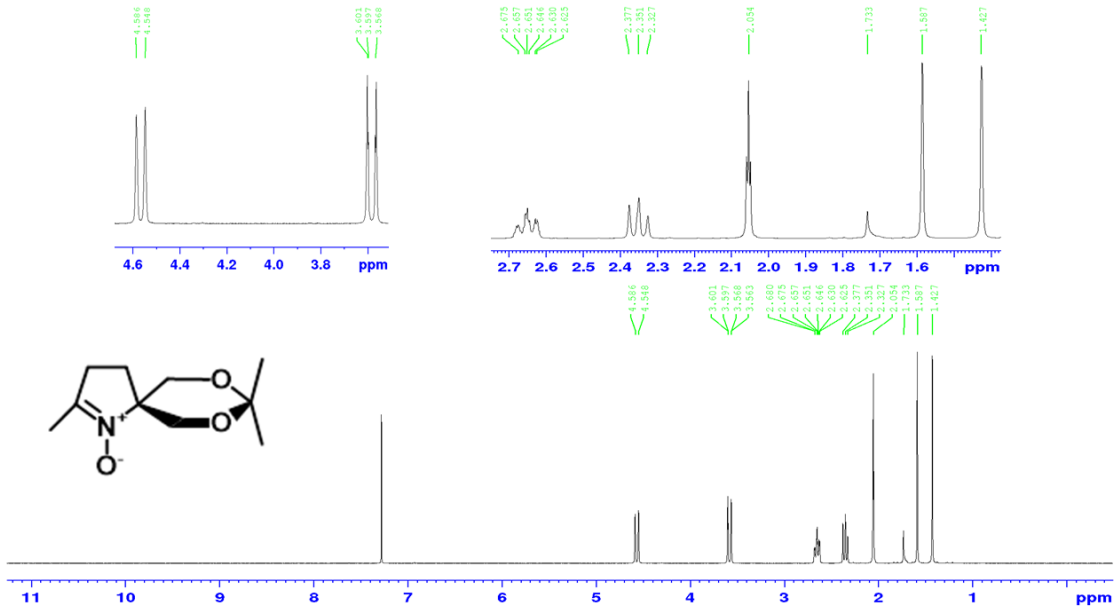


Figure S16. ^{1}H NMR spectrum of (**4**) in $CDCl_3$.

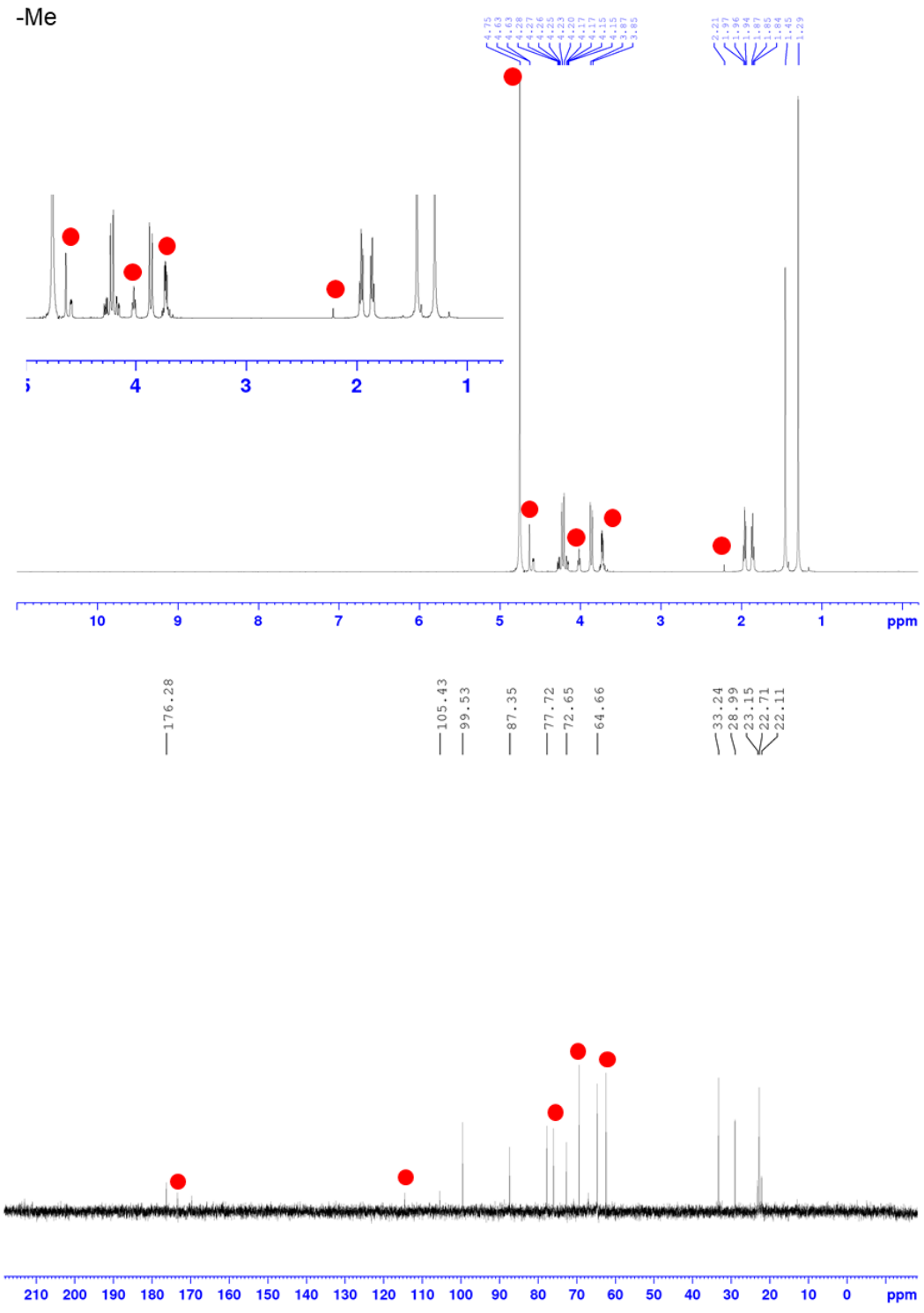


Figure S17. ^{1}H (upper) and ^{13}C (lower) NMR spectra of the hydroxylamine derivative derived from a reduction reaction of **1(Me)** by ascorbic acid (AsA) in D_2O. Reddish filled circles indicate the peaks of AsA and/or that oxidation product, and H_2O.

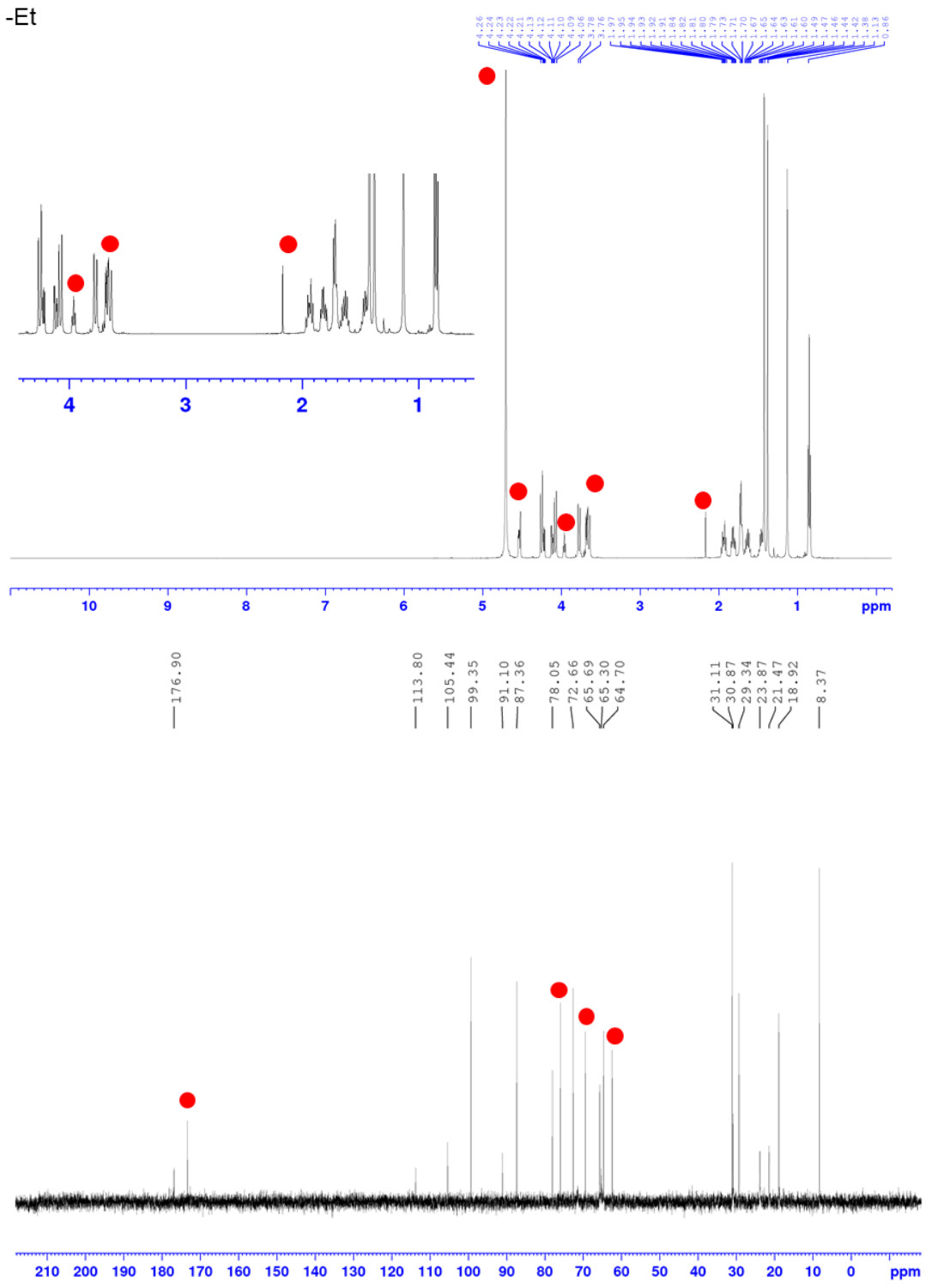


Figure S18. ^{1}H (upper) and ^{13}C (lower) NMR of the hydroxylamine derivative derived from a reduction reaction of **2(Et)** by ascorbic acid (AsA) in D_2O. Reddish filled circles indicate the peaks of AsA and/or that oxidation product, and H_2O.

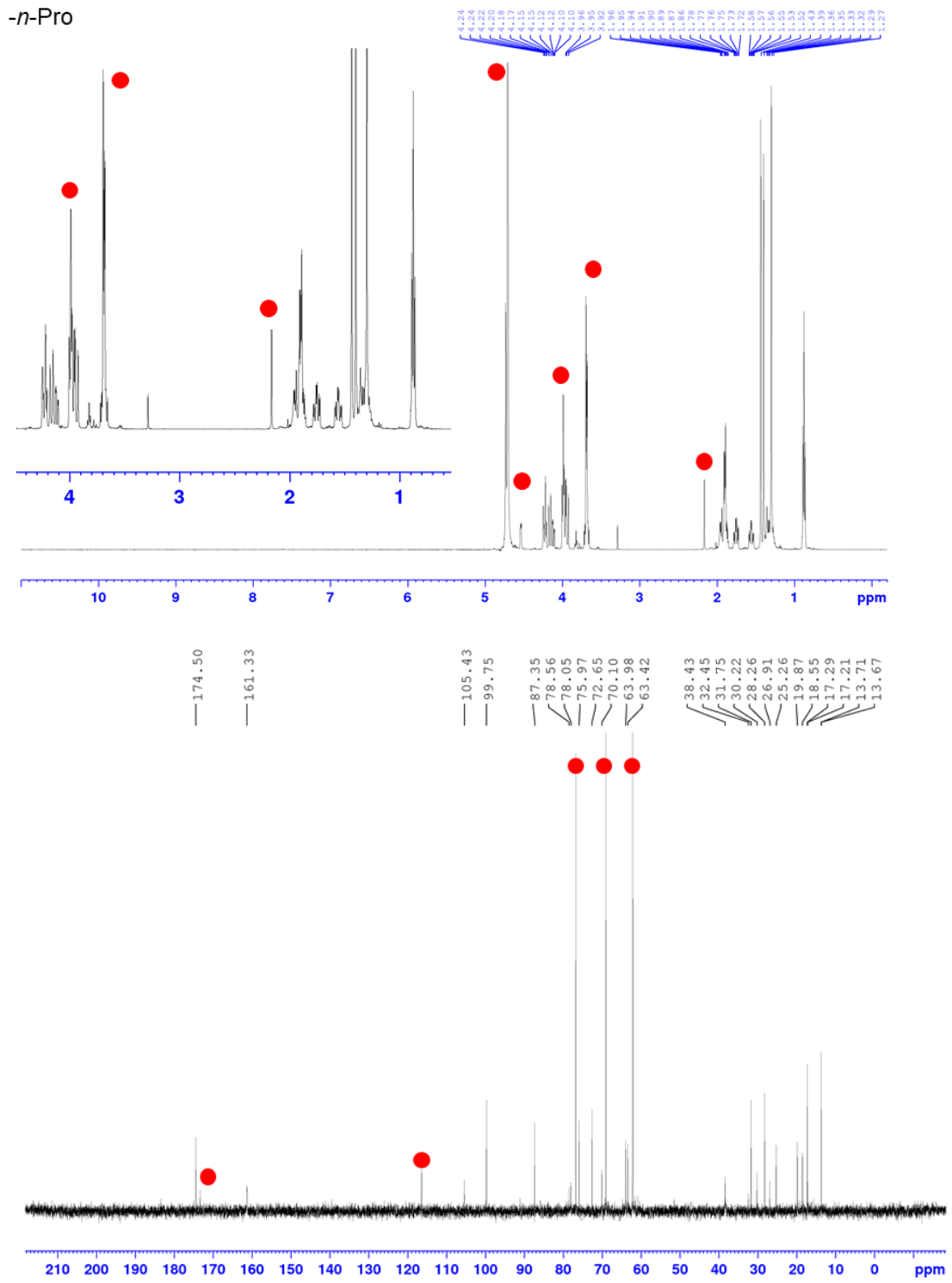


Figure S19. ^{1}H (upper) and ^{13}C (lower) NMR of the hydroxylamine derivative derived from a reduction reaction of **3(nP)** by ascorbic acid (AsA) in D_2O. Reddish filled circles indicate the peaks of AsA and/or that oxidation product, and H_2O.

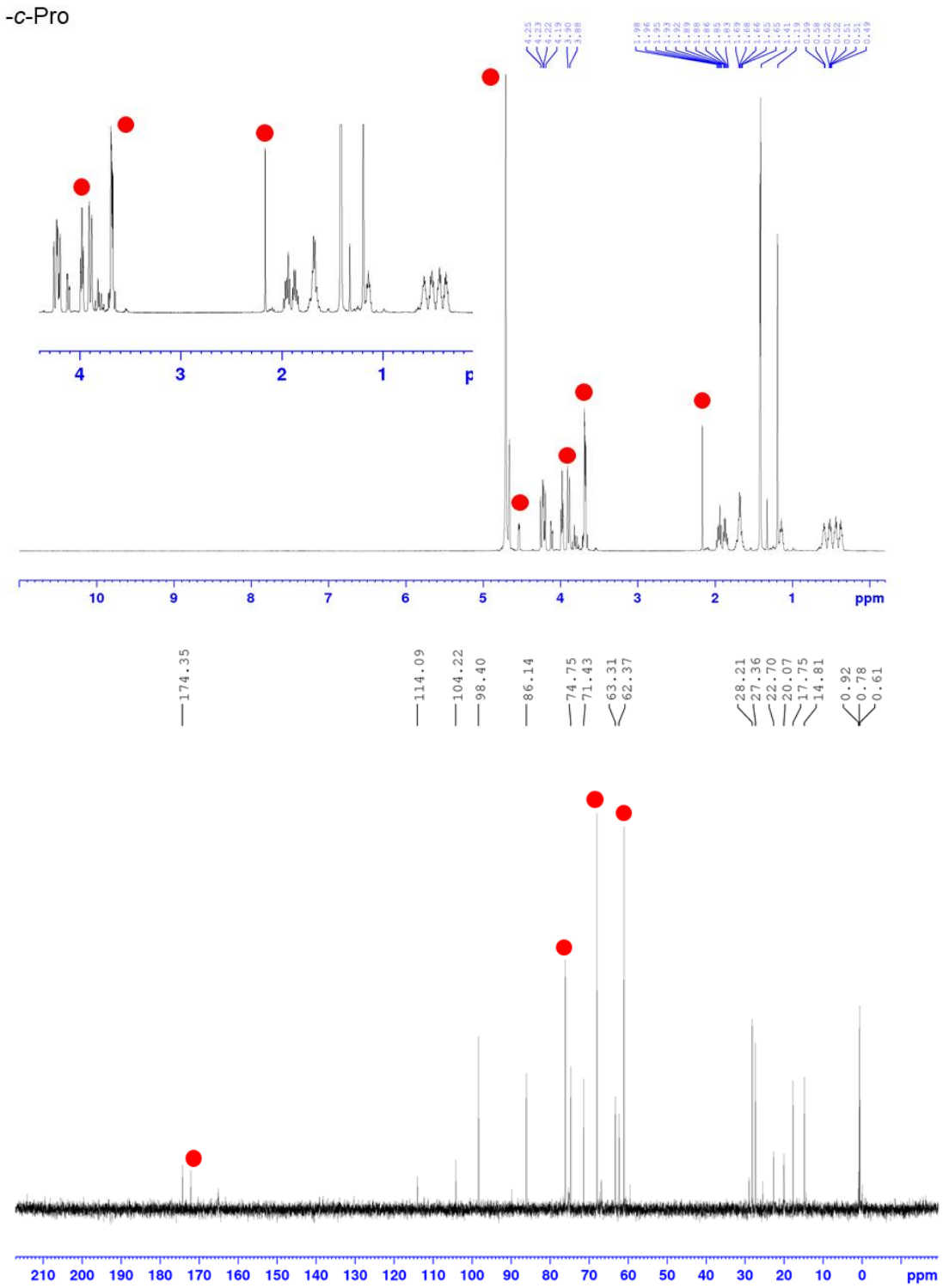


Figure S20. ^{1}H (upper) and ^{13}C (lower) NMR of the hydroxylamine derivative derived from a reduction reaction of **4(cP)** by ascorbic acid (AsA) in D_2O. Reddish filled circles indicate the peaks of AsA and/or that oxidation product, and H_2O.

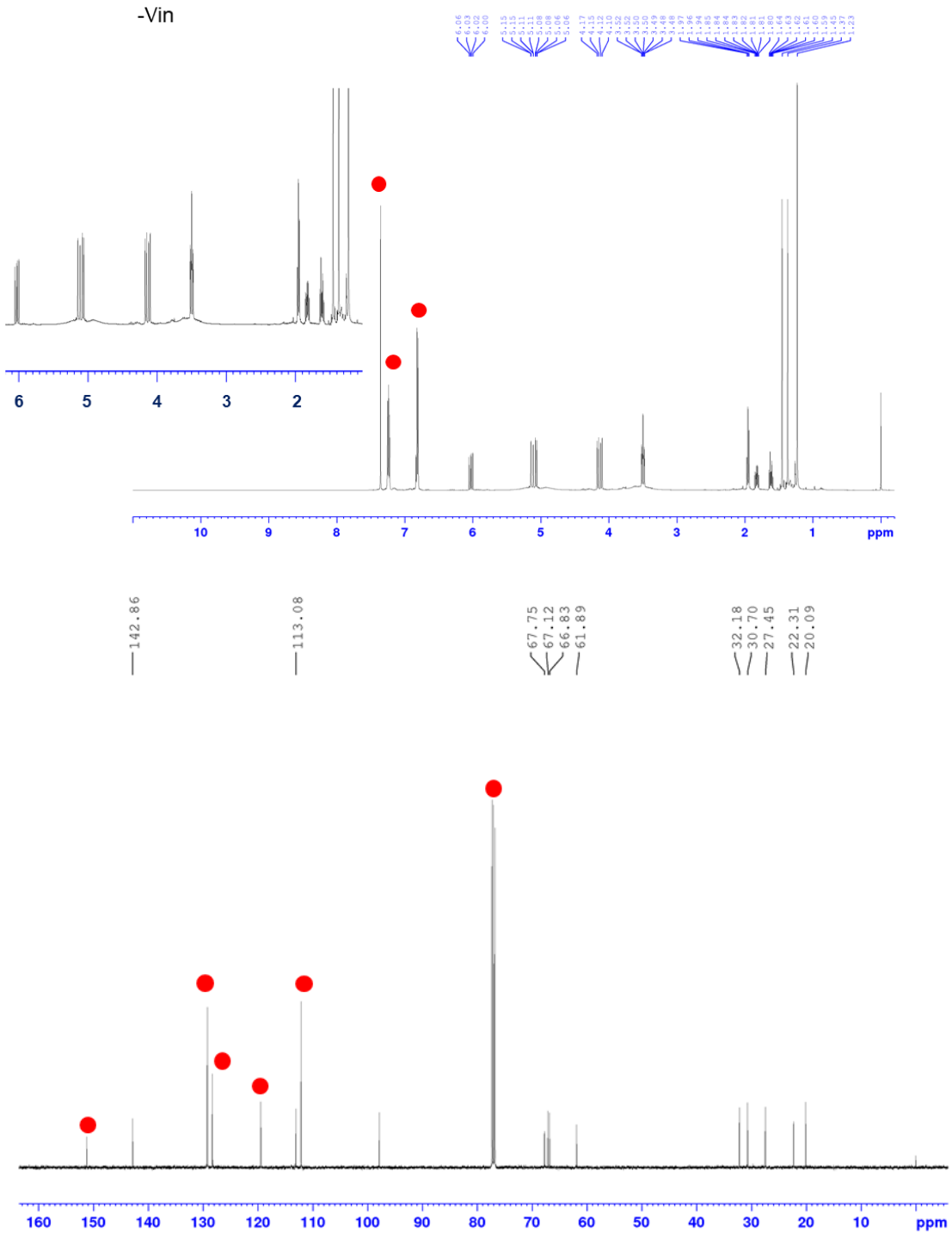


Figure S21. ^{1}H (upper) and ^{13}C (lower) NMR of the hydroxylamine derivative derived from a reduction reaction of **5(Vin)** by phenylhydrazine (PH) in $CDCl_3$. Reddish filled circles indicate the peaks of PH and/or that oxidation product, and $CHCl_3$.

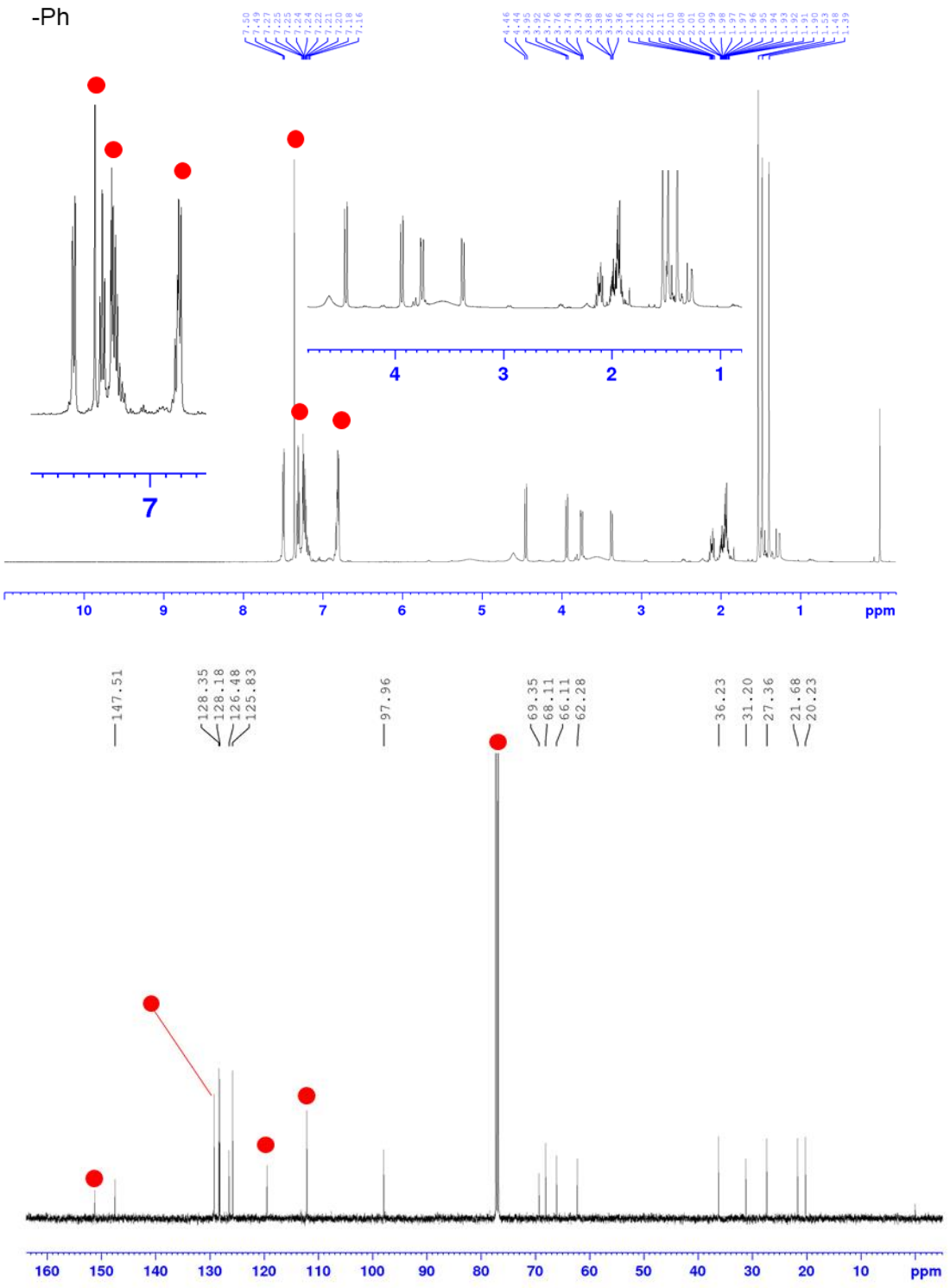


Figure S22. ^{1}H (upper) and ^{13}C (lower) NMR of the hydroxylamine derivative derived from a reduction reaction of **6(Ph)**by phenylhydrazine (PH) in $CDCl_3$. Reddish filled circles indicate the peaks of PH and/or that oxidation product, and $CHCl_3$

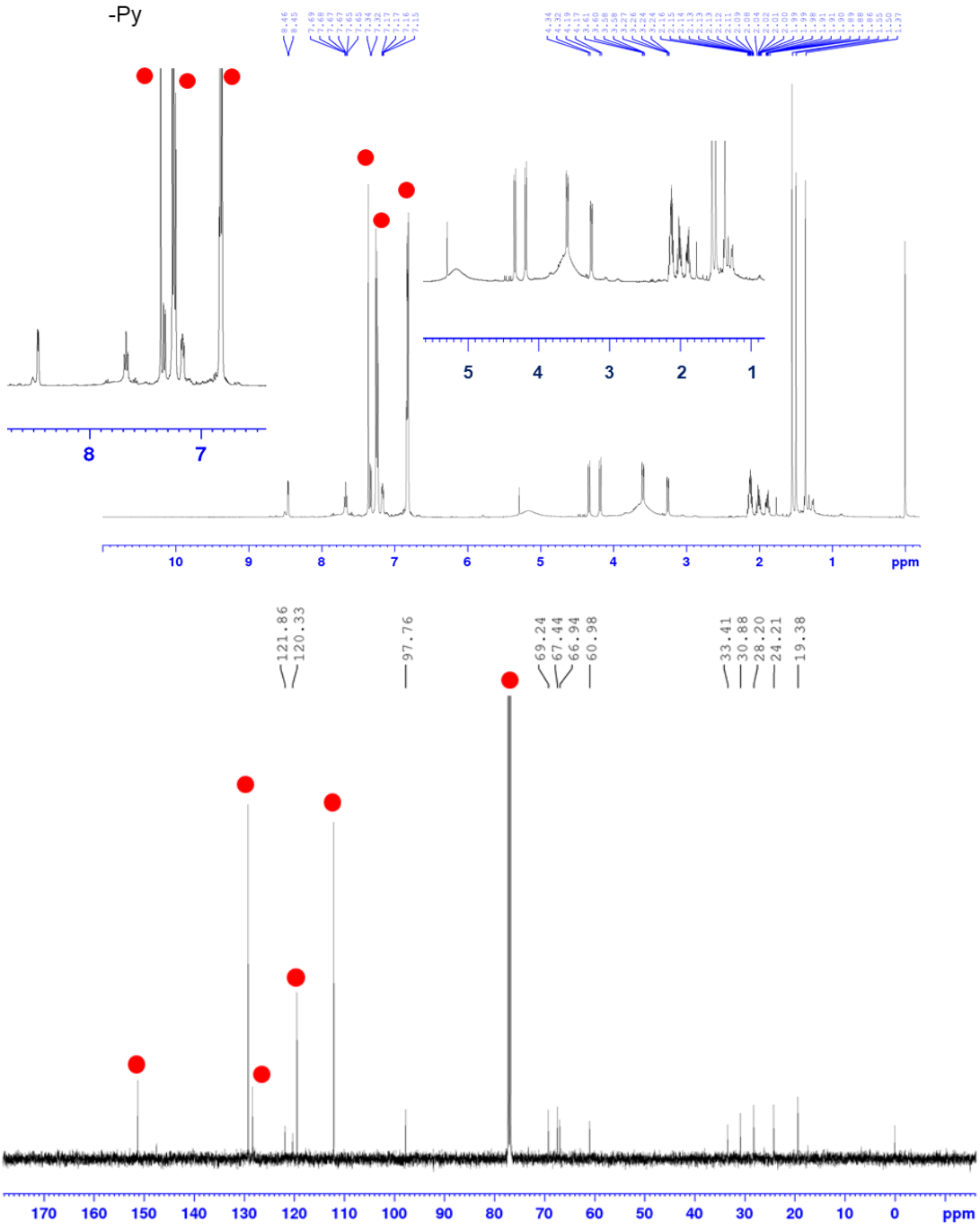
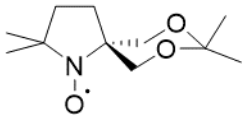


Figure S23. ^{1}H (upper) and ^{13}C (lower) NMR of the hydroxylamine derivative derived from a reduction reaction of **7(Py)**by phenylhydrazine (PH) in $CDCl_3$. Reddish filled circles indicate the peaks of PH and/or that oxidation product, and $CHCl_3$.

Cartesian coordinates

Me in water (the most stable conformer)

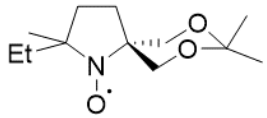


B3LYP-D3(BJ)/6-311G**/smd=water//B3LYP-D3(BJ)/6-31G*/smd=water
Electronic Energy (EE) = -711.840084 a.u.
EE + Thermal Free Energy Correction = -711.576293 a.u.

Cartesian coordinates

Symbol	X	Y	Z
H	-0.059854	-2.216195	-0.296878
C	0.622224	-1.522439	0.198841
C	2.032362	-1.534573	-0.417835
C	2.639262	-0.16935	-0.052253
N	1.415451	0.680554	-0.020346
C	0.149062	-0.068933	0.051926
H	0.663894	-1.790665	1.259128
H	1.968551	-1.625737	-1.507563
H	2.643859	-2.359652	-0.044462
O	1.465736	1.958813	0.086694
C	3.273879	-0.161951	1.345868
H	4.203915	-0.739359	1.337741
H	2.600615	-0.598427	2.090847
H	3.503803	0.865246	1.647058
C	3.614106	0.370721	-1.094653
H	4.495834	-0.276138	-1.142325
H	3.942771	1.381008	-0.831777
H	3.151946	0.399358	-2.086598
C	-0.707598	0.429379	1.221212
H	-0.252823	0.160858	2.17767
H	-0.80823	1.519119	1.174004
C	-0.653895	0.16105	-1.241879
H	-0.160556	-0.30975	-2.095407
H	-0.735612	1.237759	-1.433642
O	-1.93871	-0.452457	-1.139883
O	-1.982697	-0.214598	1.192363
C	-2.72112	-0.022119	-0.019424
C	-3.893998	-0.983685	0.055738
H	-3.524718	-2.006377	0.175106
H	-4.487784	-0.923214	-0.860344
H	-4.53243	-0.732335	0.906971
C	-3.179531	1.427595	-0.178481
H	-2.348021	2.133786	-0.228848
H	-3.810589	1.704984	0.670815
H	-3.765873	1.523612	-1.096828

Et in water (the most stable conformer)

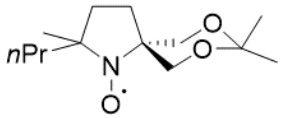


B3LYP-D3(BJ)/6-311G**/smd=water//B3LYP-D3(BJ)/6-31G*/smd=water
Electronic Energy (EE) = -751.168437 a.u.
EE + Thermal Free Energy Correction = -750.877721 a.u.

Cartesian coordinates

Symbol	X	Y	Z
H	-0.58079	1.775166	1.119465
C	-0.463521	0.706311	1.317205
C	-1.824493	0.050584	1.625693
C	-2.416875	-0.396874	0.272122
N	-1.20533	-0.436333	-0.592247
C	0.040119	0.00117	0.052178
H	0.245968	0.595062	2.139959
H	-2.497494	0.733124	2.150447
H	-1.681144	-0.827827	2.26223
O	-1.22932	-0.922397	-1.780419
C	-3.027526	-1.799302	0.337379
H	-3.894273	-1.794615	1.006081
H	-2.298951	-2.521127	0.720998
H	-3.356065	-2.127471	-0.653531
C	-3.435251	0.587732	-0.338588
H	-4.341494	0.544976	0.277286
H	-3.706221	0.202184	-1.329026
C	0.910283	-1.230961	0.368114
H	0.453391	-1.837331	1.153766
H	1.011979	-1.844266	-0.535256
C	0.842523	0.904666	-0.888441
H	0.334915	1.860918	-1.034181
H	0.962764	0.419207	-1.863053
O	2.106974	1.210101	-0.296335
O	2.18136	-0.822098	0.872089
C	2.91048	0.066644	0.015876
C	4.063983	0.589347	0.853519
H	3.675045	1.091146	1.744205
H	4.658322	1.300153	0.273137
H	4.708251	-0.23841	1.162093
C	3.397654	-0.64372	-1.247443
H	2.580491	-1.035521	-1.856688
H	4.0459	-1.4795	-0.968888
H	3.973218	0.056944	-1.859328
C	-2.961911	2.034893	-0.468385
H	-3.737386	2.643799	-0.945986
H	-2.057939	2.10703	-1.083457
H	-2.746075	2.482906	0.507396

_n_Pr in water (the most stable conformer)

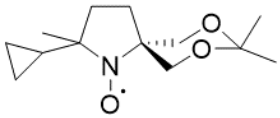


B3LYP-D3(BJ)/6-311G**/smd=water//B3LYP-D3(BJ)/6-31G*/smd=water
Electronic Energy (EE) = -790.496884 a.u.
EE + Thermal Free Energy Correction = -790.180000 a.u.

Cartesian coordinates

Symbol	X	Y	Z
H	0.354099	-1.531181	1.113009
C	0.122687	-0.485108	1.335534
C	1.411016	0.301756	1.636853
C	1.964012	0.701809	0.259041
N	0.691876	0.887768	-0.494014
C	-0.469752	0.19563	0.091414
H	-0.581861	-0.470503	2.169757
H	2.129756	-0.283945	2.21398
H	1.178846	1.207317	2.207898
O	0.649701	1.427364	-1.658526
C	2.744687	2.012647	0.267335
H	3.624389	1.920987	0.910052
H	2.124116	2.826946	0.65439
H	3.080061	2.275846	-0.740747
C	2.746899	-0.438824	-0.432276
H	2.847513	-0.174518	-1.492628
H	2.140418	-1.352826	-0.393397
C	-1.55593	1.225445	0.446888
H	-1.233385	1.861908	1.274405
H	-1.760075	1.859324	-0.424417
C	-1.075202	-0.781184	-0.923285
H	-0.396627	-1.617436	-1.106648
H	-1.261983	-0.266023	-1.872009
O	-2.273745	-1.348457	-0.391919
O	-2.734582	0.556832	0.897278
C	-3.276875	-0.393122	-0.02802
C	-4.32286	-1.172498	0.749357
H	-3.855271	-1.660625	1.609457
H	-4.775619	-1.934421	0.109182
H	-5.107182	-0.498515	1.104262
C	-3.873511	0.297108	-1.255453
H	-3.136563	0.869109	-1.823353
H	-4.663784	0.983131	-0.937018
H	-4.308275	-0.454572	-1.920598
C	4.130472	-0.7316	0.15541
H	4.047961	-0.905085	1.23601
H	4.78249	0.140454	0.027912
C	4.780266	-1.949313	-0.504259
H	5.770985	-2.148738	-0.079932
H	4.902793	-1.795228	-1.583328
H	4.167628	-2.848175	-0.364034

_c_-Pr in water (the most stable conformer)

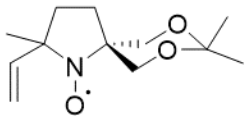


B3LYP-D3(BJ)/6-311G**/smd=water//B3LYP-D3(BJ)/6-31G*/smd=water
Electronic Energy (EE) = -789.249085 a.u.
EE + Thermal Free Energy Correction = -788.952280 a.u.

Cartesian coordinates

Symbol	X	Y	Z
C	-3.634132	-1.425413	0.521534
C	-2.880023	-1.795911	-0.73492
C	-3.233526	-0.357638	-0.461286
C	3.492237	-0.383416	1.453261
C	4.28556	-0.126038	-0.929713
C	3.083897	-0.150675	-0.001822
C	0.938268	-1.240269	0.103742
C	1.145738	1.209672	0.431052
C	-2.838788	1.825987	0.69728
C	0.223582	0.097786	-0.108571
N	-1.049286	0.128436	0.632548
C	-2.193551	0.711872	-0.126475
C	-1.484402	1.230744	-1.395842
C	-0.224589	0.361467	-1.549386
H	-3.090252	-1.47357	1.459873
H	-4.686886	-1.684246	0.592
H	-1.844863	-2.102434	-0.621439
H	-3.414019	-2.306877	-1.531087
H	-4.037573	0.055999	-1.066378
H	2.642762	-0.391369	2.139449
H	4.176499	0.409709	1.768255
H	4.007319	-1.344822	1.536222
H	3.953119	0.037531	-1.958948
H	4.96539	0.679991	-0.640784
H	4.821673	-1.077282	-0.873758
O	2.435922	1.116102	-0.170981
O	2.237445	-1.197175	-0.489839
H	0.405713	-2.051363	-0.39749
H	1.20358	1.134298	1.522896
H	0.76083	2.197979	0.169243
H	-2.104313	2.597594	0.949964
H	-3.641824	2.288913	0.114853
H	0.994079	-1.4658	1.17475
O	-1.090436	-0.082176	1.89935
H	-1.20327	2.279182	-1.252107
H	-2.138303	1.1746	-2.269216
H	-0.463404	-0.585406	-2.042382
H	0.560339	0.856453	-2.124956
H	-3.266663	1.428847	1.621838

Vin in water (the most stable conformer)

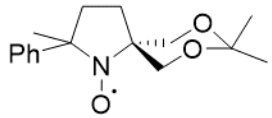


B3LYP-D3(BJ)/6-311G**/smd=water//B3LYP-D3(BJ)/6-31G*/smd=water
Electronic Energy (EE) = -749.927662 a.u.
EE + Thermal Free Energy Correction = -749.659561 a.u.

Cartesian coordinates

Symbol	X	Y	Z
H	-0.572975	1.962954	0.450487
C	-0.51994	1.035934	1.027675
C	-1.929309	0.581675	1.448342
C	-2.463736	-0.205344	0.246478
N	-1.20019	-0.851995	-0.225354
C	0.01673	-0.102378	0.141082
H	0.13381	1.211658	1.884567
H	-2.577375	1.414915	1.72541
H	-1.870883	-0.095222	2.306875
O	-1.190822	-1.773735	-1.117099
C	-3.488761	-1.279489	0.604585
H	-4.39829	-0.802397	0.981673
H	-3.092788	-1.945141	1.378508
H	-3.749701	-1.876675	-0.274068
C	-2.973644	0.641743	-0.905534
H	-3.11468	0.074594	-1.82531
C	0.980034	-1.036823	0.890412
H	0.580123	-1.297769	1.873293
H	1.12351	-1.95746	0.312393
C	0.734724	0.39042	-1.121935
H	0.147613	1.16524	-1.620252
H	0.880999	-0.443619	-1.816787
O	1.977314	0.99497	-0.761512
O	2.21916	-0.369869	1.131114
C	2.868811	0.134455	-0.042633
C	3.988786	1.028449	0.459329
H	3.572804	1.824001	1.084346
H	4.517369	1.476939	-0.386142
H	4.699071	0.443702	1.050021
C	3.39493	-0.998352	-0.924738
H	2.603188	-1.654166	-1.293049
H	4.101776	-1.605319	-0.351693
H	3.915761	-0.573804	-1.787882
C	-3.243816	1.946181	-0.884109
H	-3.117486	2.560027	0.003513
H	-3.614566	2.451749	-1.772162

Ph in water (the most stable conformer)

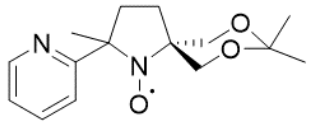


B3LYP-D3(BJ)/6-311G**/smd=water//B3LYP-D3(BJ)/6-31G*/smd=water
Electronic Energy (EE) = -903.640394 a.u.
EE + Thermal Free Energy Correction = -903.327008 a.u.

Cartesian coordinates

Symbol	X	Y	Z
H	-0.137321	-0.507053	-1.764622
C	0.286862	0.45708	-1.466859
C	-0.823254	1.512671	-1.344231
C	-1.451165	1.24516	0.03909
N	-0.24286	0.824848	0.793214
C	0.87073	0.356023	-0.050641
H	1.052032	0.731493	-2.195814
H	-1.555762	1.448395	-2.150246
H	-0.395885	2.521074	-1.348831
O	-0.191531	0.792192	2.07456
C	-2.057635	2.487486	0.693354
H	-2.917844	2.82772	0.110369
H	-1.321548	3.296352	0.736253
H	-2.395856	2.260982	1.708196
C	2.082074	1.283506	0.156861
H	1.891144	2.270254	-0.271814
H	2.273184	1.398838	1.230039
C	1.289581	-1.062468	0.356317
H	0.518435	-1.786127	0.084514
H	1.446948	-1.106518	1.439782
O	2.465826	-1.442499	-0.359107
O	3.223853	0.768581	-0.527103
C	3.585401	-0.570672	-0.167444
C	4.624729	-1.004077	-1.186013
H	4.205073	-0.936671	-2.193922
H	4.930553	-2.035999	-0.993656
H	5.504964	-0.358821	-1.121461
C	4.123434	-0.644712	1.261965
H	3.395636	-0.322171	2.009566
H	5.007087	-0.006087	1.349538
H	4.411131	-1.675417	1.488403
C	-2.477502	0.106097	-0.008169
C	-4.424118	-1.923488	-0.131699
C	-2.354173	-1.048014	0.77317
C	-3.593538	0.233403	-0.847937
C	-4.559146	-0.770411	-0.909321
C	-3.319491	-2.056719	0.708954
H	-1.511138	-1.163041	1.444075
H	-3.710192	1.124968	-1.457105
H	-5.415513	-0.652888	-1.567271
H	-3.203574	-2.946442	1.321349
H	-5.173468	-2.708166	-0.181007

Py in water (the most stable conformer)



B3LYP-D3(BJ)/6-311G**/smd=water//B3LYP-D3(BJ)/6-31G*/smd=water
Electronic Energy (EE) = -919.445469 a.u.
EE + Thermal Free Energy Correction = -919.141919 a.u.

Cartesian coordinates

Symbol	X	Y	Z
H	-0.142271	-0.553793	-1.741734
C	0.270767	0.424493	-1.475074
C	-0.850937	1.472403	-1.39446
C	-1.471774	1.251188	-0.004021
N	-0.259837	0.887162	0.769932
C	0.850892	0.376469	-0.053209
H	1.037041	0.679985	-2.209619
H	-1.592978	1.363522	-2.185326
H	-0.43712	2.485115	-1.439543
O	-0.20269	0.92564	2.050692
C	-2.128876	2.491835	0.598845
H	-3.002678	2.764378	0.001539
H	-1.426797	3.331261	0.602626
H	-2.454809	2.295336	1.62408
C	2.071722	1.297306	0.118579
H	1.889974	2.27112	-0.342479
H	2.270618	1.444672	1.186483
C	1.256435	-1.027558	0.412538
H	0.475769	-1.75399	0.177211
H	1.421087	-1.024948	1.495907
O	2.423543	-1.451423	-0.292906
O	3.201885	0.745011	-0.555334
C	3.55386	-0.583719	-0.149396
C	4.575034	-1.066678	-1.164012
H	4.140283	-1.036008	-2.167321
H	4.874465	-2.092925	-0.934833
H	5.460768	-0.426197	-1.138118
C	4.109187	-0.608519	1.275105
H	3.389873	-0.260233	2.019355
H	4.99391	0.032359	1.329693
H	4.399652	-1.630993	1.533348
C	-2.465091	0.080578	-0.013159
C	-4.334481	-1.925755	-0.132389
N	-3.433653	0.157904	-0.941483
C	-2.384652	-0.975526	0.898953
C	-3.333306	-1.995206	0.833484
C	-4.340789	-0.827904	-0.98996
H	-1.603489	-0.999629	1.648092
H	-3.287723	-2.828603	1.52814
H	-5.108613	-0.733369	-1.754611
H	-5.09239	-2.696794	-0.222591