Systematic Characterisation of the Structure and Radical Scavenging Potency of Pu'Er Tea (普洱茶) Polyphenol Theaflavin

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Figure Captions

Table Captions

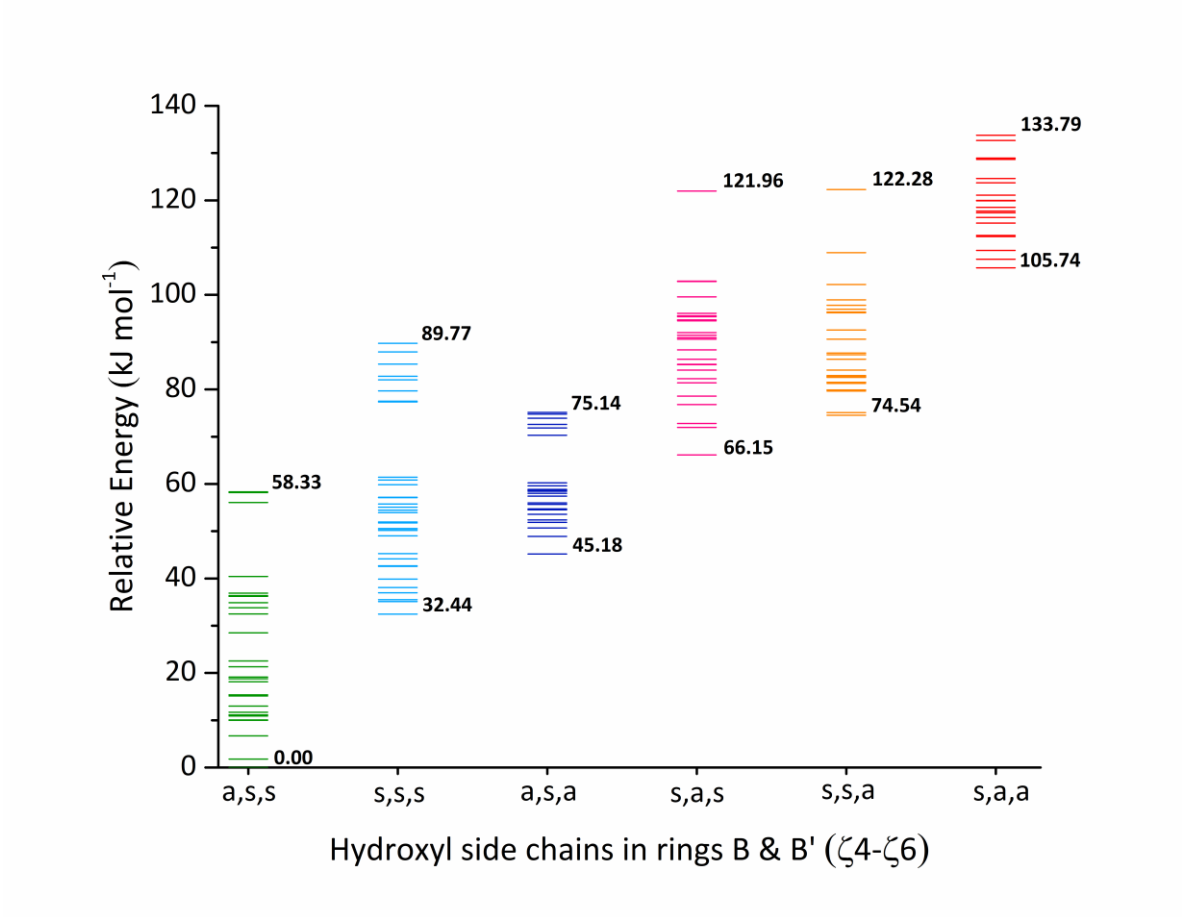

Fig.S1 Relative free-energies (kJ) of neutral theaflavin in relation to the configuration adopted at the hydroxyl side chains of rings B and B' (ζ4 – ζ6), derived from determinations at the B3LYP/6-31G(d,p)) level of theory, in the gas phase.

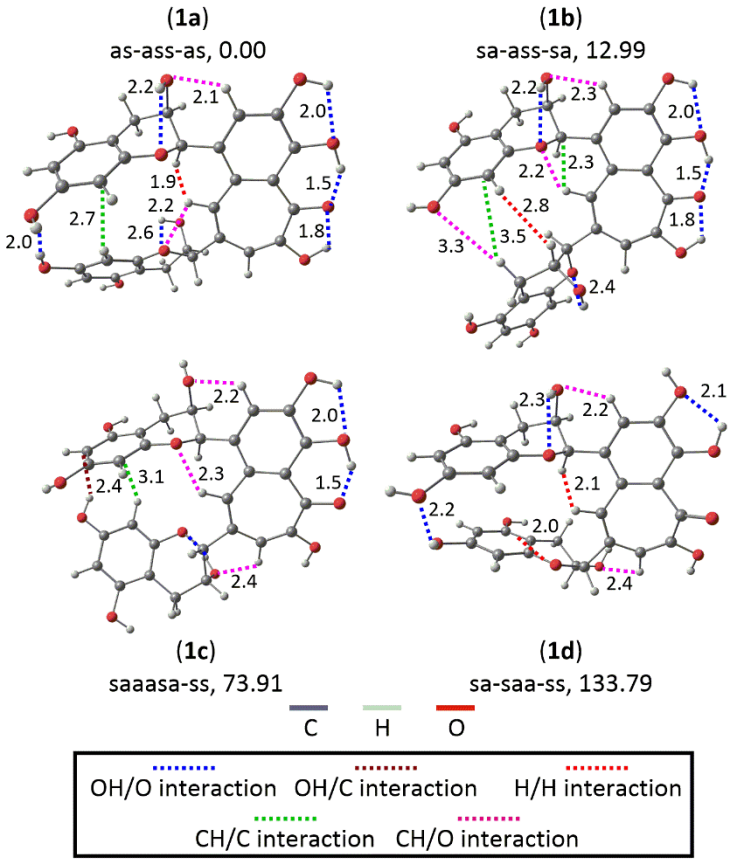

*Fig.S2 Intramolecular interactions of selected conformations of theaflavin: as-ass-as (**1a**), sa-ass-sa (**1b**), saaasa-ss (**1c**) and sa-saa-ss (**1d**), derived from determinations at the B3LYP/6-31G(d,p)) level of theory, in the gas phase. Dashed lines show selected intracmolecular NCIs (Å). Carbon, oxygen and hydrogen are represented by dark grey, red and light grey spheres, respectively.*

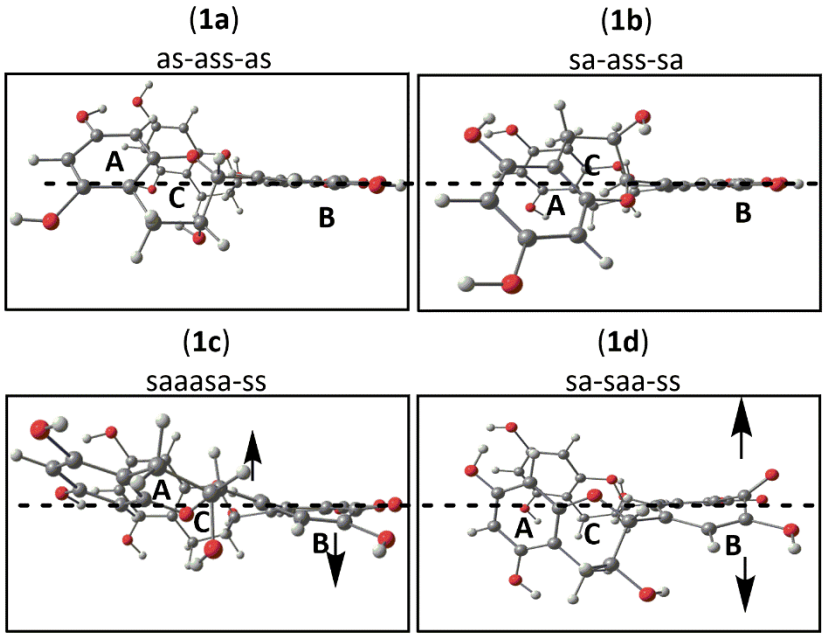

*Fig.S3 Perpendicular view of the planar B' ring of optimised theaflavin conformers **1a** – **1d**, derived from determinations at the B3LYP/6-31G(d,p)) level of theory, in the gas phase. The dashed lines are on the planar B'-ring. The carbon atom is represented by dark grey, oxygen by red and hydrogen light grey. ζ1 – ζ9 = dihedral angle of the hydroxyl side chains where s = syn, a = anti, - = gauche-, + = gauche+ and the A, C, B', B represent the rings in theaflavin*

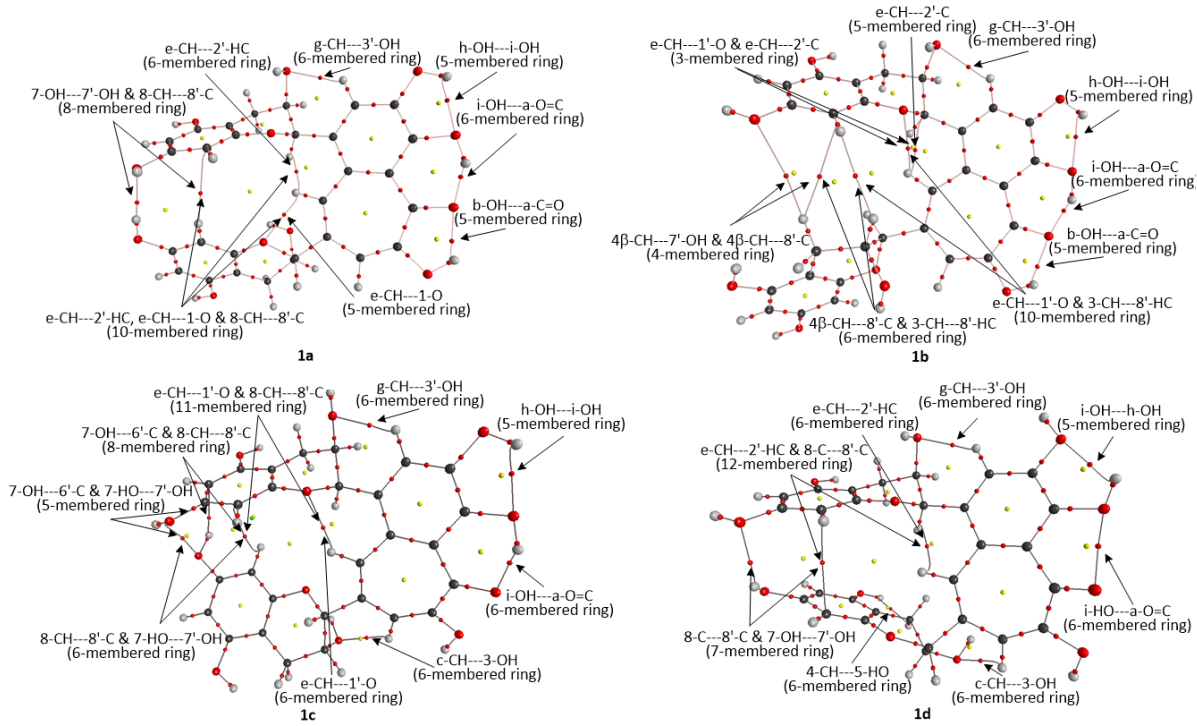

*Fig.S4 AIM analysis for the theaflavin conformers **1a** – **1d**. The wave function were generated from geometry optimisation at the B3LYP/6-31G(d,p) level of theory, in the gas phase. Bond and ring critical points (BCPs and RCPs, respectively) are represented by dimminuitive red and yellow dots, respectively. Pink-grey like lines trace bond paths between atomic-centres and passing through BCPs. Carbon, oxygen and hydrogen atoms are represented by dark grey, red and light grey spheres, respectively.*

*Table S1 Rho-b values ($\bar{e}$•bohr^{-3}) emerging from Bader Atoms-In-Molecules analyses of bond critical points (BCP) and ring critical points (RCP) for selected non-covalent intra-molecular interactions (NCIs) in conformers **1a**, **1b**, **1c**, **1d**, as derived from wavefunctions generated from structures residing at stable minima on the B3LYP/6-31G(d,p) gas-phase hypersurface.*

	bcp		rcp	
	Rho charge density p(r)	Laplacian of Rho $\nabla^2\rho(r)$	Rho charge density p(r)	Laplacian of Rho $\nabla^2\rho(r)$
1a (as-ass-as, 0.00 kJ mol^{-1})				
g-CH/3'-OH	0.0188	-0.0147	0.012	-0.0166
h-OH/i-O	0.0229	-0.0226	0.0219	-0.0319
i-OH/C=O /i-OH/h-O[a]	0.0743	-0.0464	0.0209	-0.0349
b-OH/a-C=O	0.0414	-0.0336	0.0325	-0.0548
7-OH/7'-O	0.0229	-0.015	NA	NA
8-CH/8'-C	0.0085	-0.0068	NA	NA
e-CH/1-O	0.0171	-0.0177	0.0165	-0.023
e-CH/2'-HC	0.0177	-0.0195	0.0158	-0.023
7-OH/7'-O & 8-CH/8'-C	NA	NA	0.0057	-0.006
8-CH/8'-C & e-CH/1-O & e-CH/2'-HC	NA	NA	0.0011	-0.0014
1b (sa-ass-sa, 12.99 kJ mol^{-1})				
g-CH/3'-OH	0.0176	-0.0143	0.0121	-0.0168
h-OH/i-O	0.0220	-0.0220	0.0213	-0.0304
i-OH/C=O /i-OH/h-O[a]	0.0749	-0.0462	0.0209	-0.0350
b-OH/a-C=O	0.0408	-0.0333	0.0322	-0.0542
7-OH/7'-O	NA	NA	NA	NA
4β-CH/7'-O	0.0014	-0.0015	NA	NA
4β-CH/8'-C	0.0018	-0.0014	NA	NA
3-CH/8'-CH	0.0022	-0.0018	NA	NA
e-CH/1-O	NA	NA	NA	NA
e-CH/2'-HC / e-CH/2'-HC[a]	0.0169[a]	-0.0200[a]	0.0159[a]	-0.0230[a]
e-CH/1'-O	0.0172	-0.0158	NA	NA
8-CH/7'-O & 8-CH/8'-C	NA	NA	0.0014	-0.0015
8-CH/8'-C & 3-CH/8'-CH	NA	NA	0.0017	-0.0014
3-CH/8'-CH & e-CH/1'-O	NA	NA	0.0011	-0.0010
e-CH/1'-O & e-CH/2'-HC	NA	NA	0.0165	-0.0185
7-OH/7'-O & 8-CH/8'-C	NA	NA	NA	NA
8-CH/8'-C & e-CH/1-O & e-CH/2'-HC	NA	NA	NA	NA
1c (saaasa-ss, 73.91 kJ mol^{-1})				
g-CH/3'-OH	0.0176	-0.0141	0.0109	-0.0155
h-OH/i-O	0.0225	-0.0223	0.0216	-0.0313
i-OH/C=O /i-OH/h-O[a]	0.0759	-0.0447	0.0212	-0.0358
b-OH/a-C=O	NA	NA	NA	NA
c-CH/3-OH	0.0139	-0.0120	0.0116	-0.0153
7-OH/6'-C	0.0133	-0.0091	NA	NA
7-OH/7'-O	0.0048	-0.0058	NA	NA
8-CH/7'-O	NA	NA	NA	NA
8-CH/8'-C	0.0047	-0.0037	NA	NA
e-CH/1-O	NA	NA	NA	NA
e-CH/2'-HC	NA	NA	NA	NA
e-CH/1'-O	0.0152	-0.0132	0.0141	-0.0167
7-OH/6'-C & 7-OH/7'-O	NA	NA	0.0048	-0.0057
7-OH/7'-O & 8-CH/8'-C	NA	NA	0.0043	-0.0035
8-CH/8'-C & e-CH/1'-O	NA	NA	0.0009	-0.0011
8-CH/8'-C & e-CH/1-O & e-CH/2'-HC	NA	NA	NA	NA
1d (sa-saa-ss, 133.79 kJ mol^{-1})				
g-CH/3'-OH	0.0209	-0.0161	0.0125	-0.0178
h-OH/i-O	NA	NA	NA	NA
i-OH/C=O /i-OH/h-O[a]	0.0206[a]	-0.0218[a]	0.0200	-0.0287
b-OH/a-C=O / a-C=O/h-O[a]	0.0146[a]	-0.0143[a]	0.0140	-0.0183
c-CH/3-OH	0.0134	-0.0125	0.0108	-0.0129
c-CH/1-O	NA	NA	NA	NA
7-OH/7'-O	0.0154	-0.0120	NA	NA
8-CH/8'-C	NA	NA	NA	NA
8-C/8'-C	0.0048	-0.0030	NA	NA
e-CH/1-O	NA	NA	NA	NA
4β-CH/5-HO	0.0135	-0.0141	0.0132	-0.0164
e-CH/2'-HC / e-CH/2'-HC[a]	0.0132[a]	-0.0157[a]	0.0130	-0.0172
7-OH/7'-O & 8-CH/8'-C	NA	NA	0.0041	-0.0035
8-CH/8'-C & e-CH/2'-HC	NA	NA	0.0011	-0.0012
8-CH/8'-C & e-CH/1-O & e-CH/2'-HC	NA	NA	NA	NA

*Table S2 Rho-b values ($\bar{e}$•bohr^{-3}) emerging from Bader Atoms-In-Molecules analyses of bond critical points (BCP) and ring critical points (RCP) for selected non-covalent intra-molecular interactions (NCIs) in conformers **1a**, **1b**, **1c**, **1d**, as derived from wavefunctions generated from structures residing at stable minima on the B3LYP/6-31G(d,p) (SCRF, PCM, Solvent=H_2O) hypersurface.*

	BCP		RCP	
	Rho charge density p(r)	Laplacian of Rho ∇^2p(r)	Rho charge density p(r)	Laplacian of Rho ∇^2p(r)
1a-H_2O (as-ass-as, 0.00 kJ mol^{-1})				
g-CH/3'-OH	0.0190	-0.0148	0.0120	-0.0167
h-OH/i-O	0.0221	-0.0221	0.0209	-0.0351
i-OH/C=O /i-OH/h-O[a]	0.0753	-0.0464	0.0209	-0.0351
b-OH/a-C=O	0.0409	-0.0333	0.0323	-0.0542
7-OH/7'-O	0.0247	-0.0163	NA	NA
8-CH/8'-C	0.0087	-0.0069	NA	NA
e-CH/1-O	0.0177	-0.0182	0.0169	-0.0240
e-CH/2'-HC	0.0176	-0.0194	0.0158	-0.0229
7-OH/7'-O & 8-CH/8'-C	NA	NA	0.0057	-0.0060
8-CH/8'-C & e-CH/1-O & e-CH/2'-HC	NA	NA	0.0011	-0.0014
1b-H_2O (sa-ass-sa, 8.61 kJ mol^{-1})				
g-CH/3'-OH	0.0176	-0.0143	0.0121	-0.0168
h-OH/i-O	0.0220	-0.0220	0.0213	-0.0304
i-OH/C=O /i-OH/h-O[a]	0.0749	-0.0462	0.0209	-0.0350
b-OH/a-C=O	0.0408	-0.0333	0.0322	-0.0542
7-OH/7'-O	NA	NA	NA	NA
4β-CH/7'-O	NA	NA	NA	NA
4β-CH/8'-C	NA	NA	NA	NA
3-CH/8'-CH	0.0013	-0.0010	NA	NA
e-CH/1-O	NA	NA	NA	NA
e-CH/2'-HC / e-CH/2'-HC[a]	0.0169	-0.0196	0.0158	-0.0228
e-CH/1'-O	0.0158	-0.0151	NA	NA
8-CH/7'-O & 8-CH/8'-C	NA	NA	NA	NA
8-CH/8'-C & 3-CH/8'-CH	NA	NA	NA	NA
3-CH/8'-CH & e-CH/1'-O	NA	NA	0.0007	-0.0007
e-CH/1'-O & e-CH/2'-HC	NA	NA	0.0157	-0.0168
7-OH/7'-O & 8-CH/8'-C	NA	NA	NA	NA
8-CH/8'-C & e-CH/1-O & e-CH/2'-HC	NA	NA	NA	NA
1c-H_2O (saaasa-ss, 50.19 kJ mol^{-1})				
g-CH/3'-OH	0.0183	-0.0145	0.0112	-0.0159
h-OH/i-O	0.0219	-0.0218	0.0214	-0.0362
i-OH/C=O /i-OH/h-O[a]	0.0759	-0.0447	0.0212	-0.0358
b-OH/a-C=O	NA	NA	NA	NA
c-CH/3-OH	NA	NA	NA	NA
c-CH/3-CH	0.0125	-0.0140	0.0120	-0.0159
7-OH/6'-C	0.0111	-0.0073	NA	NA
7-OH/7'-O	NA	NA	NA	NA
8-CH/7'-O	NA	NA	NA	NA
8-CH/8'-C	NA	NA	NA	NA
8-CH/8'a-C	0.0050	-0.0040	NA	NA
e-CH/1-O	0.0175	-0.0200	NA	NA
e-CH/2'-HC	0.0157	-0.0196	0.0154	-0.0216
e-CH/1'-O	0.0147	-0.0134	NA	NA
7-OH/6'-C & 7-OH/7'-O	NA	NA	NA	NA
7-OH/6'-C & 8-CH/8α'-C	NA	NA	0.0037	-0.0032
7-OH/7'-O & 8-CH/8'-C	NA	NA	0.0043	-0.0035
8-CH/8'-C & e-CH/1'-O	NA	NA	NA	NA
e-CH/1'-O & e-CH/2'-HC	NA	NA	0.0144	-0.0159
8-CH/8α'-C & e-CH/1'-O & e-CH/1-O	NA	NA	0.0011	-0.0013
1d-H_2O (sa-saa-ss, 103.54 kJ mol^{-1})				
g-CH/3'-OH	0.0202	-0.0158	0.0125	-0.0177
h-OH/i-O	NA	NA	NA	NA
i-OH/C=O /i-OH/h-O[a]	0.0217[a]	-0.0225[a]	0.0209	-0.0306
b-OH/a-C=O / a-C=O/h-O[a]	0.0153[a]	-0.0148[a]	0.0143	-0.0193
c-CH/3-OH	0.0132	-0.0120	0.0106	-0.0126
c-CH/1-O	NA	NA	NA	NA
4β-CH/5-HO	0.0129	-0.0139	0.0128	-0.0157
7-OH/7'-O	0.0161	-0.0119	NA	NA
8-CH/8'-C	NA	NA	NA	NA
8-C/8'-C	0.0049	-0.0031	NA	NA
e-CH/1-O	NA	NA	NA	NA
e-CH/2'-HC / e-CH/2'-HC[a]	0.0133	-0.0160	0.0132	-0.0175
7-OH/7'-O & 8-C/8'-C	NA	NA	0.0040	-0.0035
8-C/8'-C & e-CH/2'-HC	NA	NA	0.0011	-0.0011
8-CH/8'-C & e-CH/1-O & e-CH/2'-HC	NA	NA	NA	NA

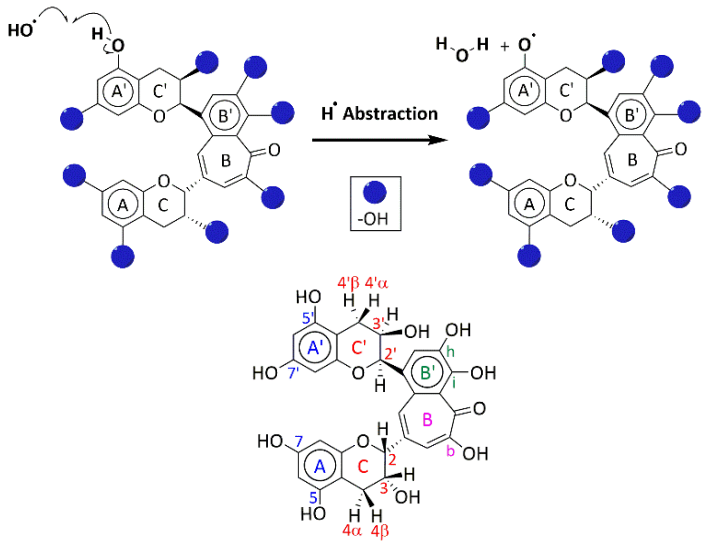

Fig.S5 Schematic of hydrogen radical abstraction at –OH and selected C-H theaflavin sites and with corresponding labels (colouring and numbering system).

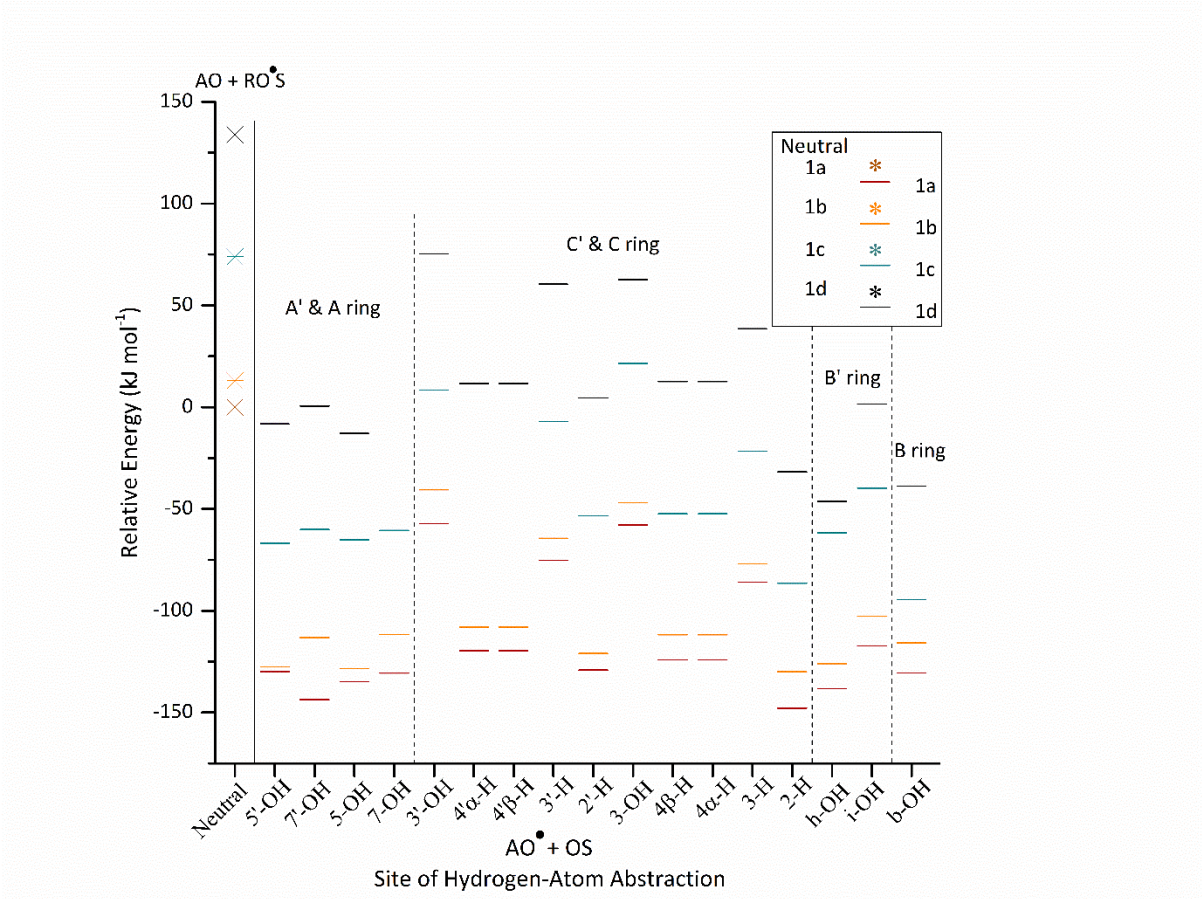

*Fig.S6 Relative energies of conformers **1a** - **1d** at their corresponding H-atom abstraction sites, derived from determinations at the UB3LYP/6-31G(d,p)) level of theory, in the gas phase. AO = antioxidant, RO•S = reactive oxygen species, AO• = antioxidant radical and OS = oxygen species. Key: left - neutral conformer and right - the corresponding antioxidant radical conformer.*

*Table S3 Energetics and Cartesian coordinates of the neutral conformer **1a** (as-ass-as) pre-radical capture by DFT calculations B3LYP/6-31G(d,p), in the gas phase*

Zero-point correction= 0.497689 (Hartree/Particle)
Thermal correction to Energy= 0.531779
Thermal correction to Enthalpy= 0.532723
Thermal correction to Gibbs Free Energy= 0.433798
Sum of electronic and zero-point Energies= -2021.741331
Sum of electronic and thermal Energies= -2021.707241
Sum of electronic and thermal Enthalpies= -2021.706296
Sum of electronic and thermal Free Energies= -2021.805222

Coordinates:

6	-2.608488	-0.052009	-0.035353
6	-3.95942	-0.553309	-0.229878
6	-5.044025	0.377937	-0.186146
6	-4.82338	1.736762	0.05675
6	-3.535096	2.204304	0.278497
6	-2.441401	1.346484	0.248814
1	-3.395796	3.262474	0.464503
6	-1.405809	-0.831376	-0.111182
6	-4.354798	-1.935162	-0.461742
6	-1.169835	-2.175557	-0.249966
6	-3.487273	-3.118847	-0.501829
6	-2.127127	-3.207011	-0.406903
8	-5.58157	-2.241476	-0.634984
8	-4.174744	-4.263922	-0.682372
1	-5.111163	-3.970619	-0.748848
8	-5.875311	2.589716	0.086213
8	-6.340259	0.05725	-0.362526
1	-6.669238	2.054557	-0.083112
1	-6.349516	-0.937206	-0.52026
6	-1.071761	1.918478	0.566756
8	-0.354699	2.094499	-0.691391
6	-0.992237	3.265196	1.308972
6	0.959857	2.477057	-0.558613
6	0.473147	3.486969	1.718645
6	1.418086	3.124534	0.593302
6	2.787082	3.439819	0.646593
6	1.798099	2.18462	-1.640021
6	3.65848	3.132114	-0.399724
6	3.146318	2.5036	-1.53477
8	3.214847	4.065377	1.781932
8	4.05412	2.145882	-2.516315
1	4.160841	4.248057	1.70962
1	3.569946	1.908808	-3.319482
8	-1.46924	4.341669	0.507418
1	-1.184405	4.163361	-0.401594
1	-0.511765	1.196668	1.17312
6	0.263924	-2.680246	-0.151986
8	1.158236	-1.670828	-0.632568
6	0.656281	-3.075032	1.295317
1	-0.076848	-3.791797	1.677426
6	2.504143	-1.846303	-0.40286
6	2.054331	-3.702009	1.266643
1	2.002668	-4.706062	0.823896
6	2.99418	-2.808351	0.488872
6	3.344536	-0.966495	-1.088199
6	4.390798	-2.865529	0.653354
1	2.905437	-0.238593	-1.755551
6	4.720116	-1.023415	-0.867436
6	5.253169	-1.992869	-0.00665
8	4.852982	-3.820253	1.518271
1	5.814409	-3.747979	1.579385
1	0.37167	-3.570763	-0.788421
1	0.599733	4.53736	1.998764
1	0.704598	2.896911	2.61554
1	-1.625626	3.240267	2.200877
1	4.71763	3.36329	-0.344364
1	1.389415	1.664458	-2.500295
1	6.327446	-2.034465	0.146179
1	2.411552	-3.834652	2.292262
1	-1.749629	-4.223857	-0.492475
1	-0.495034	-0.256067	-0.064857
8	0.590931	-1.951013	2.160361
1	1.3552	-1.391987	1.959332
8	5.590575	-0.168416	-1.46633
1	5.100148	0.553843	-1.898854

*Table S4 Energetics and Cartesian coordinates of the neutral conformer **1b** (sa-ass-sa) pre-radical capture by DFT calculations B3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.496322 (Hartree/Particle)
Thermal correction to Energy= 0.531147
Thermal correction to Enthalpy= 0.532091
Thermal correction to Gibbs Free Energy= 0.429194
Sum of electronic and zero-point Energies= -2021.733146
Sum of electronic and thermal Energies= -2021.698321
Sum of electronic and thermal Enthalpies= -2021.697377
Sum of electronic and thermal Free Energies= -2021.800274

Coordinates:

6	-2.341123	-1.063428	0.157816
6	-3.0333	-2.330124	0.016608
6	-4.462235	-2.319832	-0.030273
6	-5.181106	-1.122566	0.045585
6	-4.512504	0.084888	0.206377
6	-3.12612	0.132828	0.285715
1	-5.099703	0.993996	0.250239
6	-0.91925	-0.887133	0.150037
6	-2.424731	-3.651162	-0.069353
6	0.142214	-1.752466	0.05161
6	-0.992615	-3.984027	-0.053174
6	0.101571	-3.164079	-0.021216
8	-3.154696	-4.692706	-0.161974
8	-0.768916	-5.310657	-0.111445
1	-1.667708	-5.705566	-0.161385
8	-6.533489	-1.149776	-0.023687
8	-5.233454	-3.41614	-0.156134
1	-6.786516	-2.082925	-0.127202
1	-4.590683	-4.190798	-0.190157
6	-2.456557	1.466501	0.567422
8	-1.75671	1.899868	-0.632642
6	-3.341019	2.648773	0.995518
6	-0.922398	2.984416	-0.442137
6	-2.411509	3.79138	1.453271
6	-1.195821	3.929775	0.55756
6	-0.293358	5.000125	0.681245
6	0.174951	3.081517	-1.294491
6	0.822718	5.12145	-0.14942
6	1.049037	4.1582	-1.134506
8	-0.458957	5.97404	1.62309
8	2.132864	4.206832	-1.965946
1	-1.270572	5.810239	2.120233
1	2.647695	4.999672	-1.765441
8	-4.193507	3.06957	-0.059033
1	-3.693757	2.961214	-0.883178
1	-1.707651	1.326102	1.358926
6	1.506696	-1.087133	-0.054509
8	2.486042	-1.908703	0.599037
6	1.965089	-0.847915	-1.510642
1	1.183441	-0.305078	-2.049142
6	3.783996	-1.441955	0.564285
6	3.255364	-0.012257	-1.475077
1	2.995072	1.043356	-1.304964
6	4.206598	-0.524355	-0.412094
6	4.644849	-1.963938	1.527124
6	5.552879	-0.122118	-0.365179
1	4.281642	-2.669706	2.263432
6	5.977361	-1.549714	1.527355
6	6.439062	-0.623937	0.588265
8	6.063029	0.777492	-1.258032
1	5.364129	1.068904	-1.857526
1	1.470212	-0.114537	0.454377
1	-3.017379	4.707715	1.452557
1	-2.104901	3.60689	2.494264
1	-3.99117	2.357439	1.826134
1	1.493211	5.963652	-0.008578
1	0.341083	2.338392	-2.064521
1	7.469914	-0.283358	0.580425
1	3.704231	-0.075469	-2.47595
1	1.053823	-3.680675	-0.044961
1	-0.613428	0.148414	0.178003
8	2.131129	-2.072435	-2.203215
1	2.755518	-2.611489	-1.696323
8	6.793012	-2.078174	2.485814
1	7.680277	-1.710339	2.38173

*Table S5 Energetics and Cartesian coordinates of the neutral conformer **1c** (saaasa-ss) pre-radical capture by DFT calculations B3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.495981 (Hartree/Particle)
Thermal correction to Energy= 0.530777
Thermal correction to Enthalpy= 0.531721
Thermal correction to Gibbs Free Energy= 0.430510
Sum of electronic and zero-point Energies= -2021.711599
Sum of electronic and thermal Energies= -2021.676803
Sum of electronic and thermal Enthalpies= -2021.675859
Sum of electronic and thermal Free Energies= -2021.777070

Coordinates

6	-2.619787	-0.039846	0.098801
6	-3.946201	0.508243	0.248718
6	-5.029415	-0.396208	0.447178
6	-4.826806	-1.784127	0.422325
6	-3.560509	-2.30131	0.186855
6	-2.465398	-1.457828	0.019723
1	-3.433316	-3.375909	0.153145
6	-1.404282	0.73246	0.150196
6	-4.337978	1.924484	0.169125
6	-1.15328	2.061307	-0.04323
6	-3.470931	2.997973	-0.365212
6	-2.108317	3.055119	-0.411872
8	-5.509283	2.275261	0.448502
8	-4.221853	4.059633	-0.76248
1	-3.632656	4.748163	-1.10083
8	-5.884547	-2.611146	0.605745
8	-6.306078	-0.023131	0.645985
1	-6.659974	-2.040028	0.741171
1	-6.279513	0.988953	0.657353
6	-1.113151	-2.044073	-0.353411
8	-0.263773	-2.084982	0.813619
6	-1.101865	-3.425011	-1.024545
6	1.020084	-2.506193	0.593176
6	0.320267	-3.665563	-1.561814
6	1.370506	-3.234149	-0.559774
6	2.72469	-3.571153	-0.717216
6	1.959833	-2.14845	1.560304
6	3.692667	-3.201902	0.222075
6	3.296296	-2.491117	1.364442
8	3.170553	-4.283873	-1.795301
8	4.191916	-2.086896	2.307728
1	2.436191	-4.461069	-2.396237
1	5.080763	-2.09615	1.92659
8	-1.461983	-4.398675	-0.05298
1	-1.463562	-5.264713	-0.481122
1	-0.644836	-1.364144	-1.078919
6	0.302595	2.477103	0.176515
8	1.126884	1.614461	-0.641621
6	0.713483	3.918539	-0.148706
1	0.073501	4.630348	0.38227
6	2.479489	1.700856	-0.360455
6	2.173955	4.130071	0.305469
1	2.173236	4.406831	1.370961
6	3.037334	2.90394	0.085628
6	3.228986	0.543889	-0.550315
6	4.420653	2.899936	0.350858
1	2.733852	-0.365565	-0.87064
6	4.593567	0.57692	-0.254223
6	5.199479	1.755512	0.185666
8	5.065642	4.020389	0.795449
1	4.442833	4.75653	0.842158
1	0.555221	2.280872	1.229038
1	0.417431	-4.737077	-1.798213
1	0.431619	-3.128093	-2.515609
1	-1.814311	-3.416088	-1.862196
1	4.716966	-3.536165	0.085497
1	1.660334	-1.569342	2.424444
1	6.258015	1.781424	0.413249
1	2.550632	5.000163	-0.249933
1	-1.691454	3.986211	-0.788905
1	-0.526175	0.148514	0.394773
8	0.540153	4.183265	-1.534838
1	0.83092	3.384941	-2.003277
8	5.376624	-0.538259	-0.362498
1	4.814446	-1.283499	-0.630936

*Table S6 Energetics and Cartesian coordinates of the neutral conformer **1d** (sa-saa-ss) pre-radical capture by DFT calculations B3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.495715 (Hartree/Particle)
Thermal correction to Energy= 0.531118
Thermal correction to Enthalpy= 0.532062
Thermal correction to Gibbs Free Energy= 0.430881
Sum of electronic and zero-point Energies= -2021.689431
Sum of electronic and thermal Energies= -2021.654028
Sum of electronic and thermal Enthalpies= -2021.653084
Sum of electronic and thermal Free Energies= -2021.754265

Coordinates

6	-2.325757	-0.510085	0.123542
6	-3.735043	-0.560684	0.356501
6	-4.459409	-1.740114	0.078813
6	-3.78986	-2.871036	-0.392775
6	-2.415425	-2.853783	-0.567659
6	-1.670541	-1.69988	-0.324857
1	-1.908481	-3.758273	-0.887597
6	-1.512509	0.682646	0.334158
6	-4.53217	0.531442	0.993908
6	-1.870812	1.997825	0.332748
6	-4.385847	1.92594	0.478933
6	-3.206021	2.545602	0.226764
8	-5.356479	0.308372	1.863738
8	-5.579702	2.563496	0.42585
1	-5.437735	3.483811	0.16092
8	-4.588484	-3.962055	-0.642339
8	-5.803405	-1.787581	0.230603
1	-4.042593	-4.72016	-0.886201
1	-6.090131	-2.679951	-0.018416
6	-0.174106	-1.72931	-0.582973
8	0.496623	-1.819423	0.702011
6	0.367246	-2.875091	-1.459509
6	1.878089	-1.824342	0.666422
6	1.849903	-2.601297	-1.750607
6	2.582059	-2.205552	-0.486242
6	3.985349	-2.217244	-0.406119
6	2.519881	-1.468883	1.851533
6	4.656298	-1.861277	0.763393
6	3.912076	-1.475406	1.876897
8	4.764909	-2.574672	-1.468616
8	4.519227	-1.025425	3.028686
1	4.208214	-2.73943	-2.239886
1	5.471712	-1.175156	2.952263
8	0.212559	-4.144549	-0.83114
1	0.397646	-4.013397	0.111636
1	0.133882	-0.788445	-1.05666
6	-0.796866	3.085947	0.486499
8	0.366549	2.594321	1.160254
6	-0.419845	3.815868	-0.833822
1	0.135607	4.716171	-0.55182
6	1.553865	2.392521	0.499387
6	0.486929	2.94634	-1.70226
1	0.772656	3.54669	-2.576443
6	1.68351	2.516684	-0.890979
6	2.631868	2.046246	1.31443
6	2.957713	2.285687	-1.444098
1	2.483543	1.968503	2.385807
6	3.876758	1.814131	0.72629
6	4.051134	1.940312	-0.653524
8	3.182758	2.376327	-2.791577
1	2.360465	2.61191	-3.239109
1	-1.207565	3.844646	1.162873
1	2.264673	-3.523005	-2.180496
1	1.932593	-1.817259	-2.518444
1	-0.193134	-2.923568	-2.398301
1	5.741259	-1.844274	0.765056
1	1.943864	-1.16514	2.716361
1	5.015603	1.749845	-1.107056
1	-0.092551	2.087797	-2.077866
1	-3.256988	3.615453	0.027265
1	-0.459194	0.494642	0.498103
8	-1.557368	4.287712	-1.540003
1	-2.029245	3.516682	-1.886527
8	4.967392	1.462887	1.468676
1	4.668461	1.077359	2.306633

*Table S7 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 5'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483980 (Hartree/Particle)
Thermal correction to Energy= 0.517910
Thermal correction to Enthalpy= 0.518854
Thermal correction to Gibbs Free Energy= 0.419487
Sum of electronic and zero-point Energies= -2021.111160
Sum of electronic and thermal Energies= -2021.077230
Sum of electronic and thermal Enthalpies= -2021.076285
Sum of electronic and thermal Free Energies= -2021.175653

Coordinates:

6	-2.600625	-0.058588	-0.026467
6	-3.9478	-0.562273	-0.23638
6	-5.036698	0.363455	-0.183029
6	-4.823276	1.719424	0.083246
6	-3.537653	2.189951	0.314612
6	-2.440293	1.337284	0.274956
1	-3.40538	3.246487	0.513884
6	-1.395781	-0.833434	-0.096848
6	-4.335285	-1.941889	-0.495169
6	-1.152442	-2.175053	-0.248655
6	-3.46245	-3.1215	-0.547281
6	-2.102941	-3.207424	-0.435241
8	-5.558961	-2.249376	-0.684597
8	-4.142892	-4.265323	-0.756029
1	-5.080188	-3.975975	-0.826527
8	-5.878279	2.567214	0.122397
8	-6.329883	0.040266	-0.371442
1	-6.670274	2.032728	-0.057897
1	-6.334354	-0.951079	-0.548457
6	-1.072672	1.907852	0.599723
8	-0.341915	2.057784	-0.659424
6	-0.991547	3.265795	1.322417
6	0.961752	2.462749	-0.515333
6	0.474568	3.502388	1.724567
6	1.41339	3.132735	0.608026
6	2.828151	3.495149	0.681673
6	1.817331	2.159101	-1.592584
6	3.698216	3.143252	-0.427525
6	3.18406	2.496813	-1.526291
8	3.276638	4.101283	1.683531
8	4.046329	2.117277	-2.537062
1	3.539929	1.913569	-3.335675
8	-1.474868	4.330806	0.509762
1	-1.214965	4.135272	-0.40284
1	-0.518946	1.191385	1.218388
6	0.282573	-2.667091	-0.120522
8	1.174704	-1.683319	-0.660954
6	0.672601	-2.973579	1.348874
1	-0.061123	-3.66785	1.769595
6	2.519405	-1.833273	-0.408406
6	2.071436	-3.596419	1.359754
1	2.025825	-4.620957	0.966484
6	3.009839	-2.736714	0.542724
6	3.361837	-0.99012	-1.137895
6	4.405336	-2.772172	0.725224
1	2.929365	-0.32236	-1.870219
6	4.735991	-1.021261	-0.898396
6	5.267134	-1.931577	0.024861
8	4.864453	-3.669295	1.649402
1	5.823788	-3.581484	1.723283
1	0.396087	-3.593146	-0.701948
1	0.609434	4.554909	1.991587
1	0.722881	2.92745	2.62676
1	-1.621245	3.248384	2.21705
1	4.748387	3.399935	-0.35828
1	1.403544	1.626072	-2.443622
1	6.339579	-1.950703	0.193122
1	2.425141	-3.677198	2.391959
1	-1.721116	-4.221601	-0.530672
1	-0.487126	-0.258553	-0.024109
8	0.606615	-1.799067	2.145745
1	1.407535	-1.286583	1.963765
8	5.607688	-0.199219	-1.53892
1	5.121251	0.517568	-1.982706

*Table S8 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 7'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.484205 (Hartree/Particle)
Thermal correction to Energy= 0.518017
Thermal correction to Enthalpy= 0.518961
Thermal correction to Gibbs Free Energy= 0.419709
Sum of electronic and zero-point Energies= -2021.116419
Sum of electronic and thermal Energies= -2021.082607
Sum of electronic and thermal Enthalpies= -2021.081663
Sum of electronic and thermal Free Energies= -2021.180915

Coordinates:

6	-2.604844	-0.062209	-0.038815
6	-3.952434	-0.572368	-0.225307
6	-5.042153	0.35373	-0.191929
6	-4.829142	1.716185	0.038074
6	-3.542973	2.19321	0.252335
6	-2.444967	1.340766	0.227526
1	-3.413152	3.254566	0.425744
6	-1.399008	-0.836011	-0.102076
6	-4.340526	-1.959542	-0.438817
6	-1.155784	-2.182301	-0.206632
6	-3.468095	-3.14009	-0.447509
6	-2.107676	-3.221341	-0.340881
8	-5.5648	-2.272659	-0.615434
8	-4.14921	-4.291479	-0.606298
1	-5.086486	-4.005644	-0.688139
8	-5.884957	2.563987	0.061356
8	-6.335544	0.023783	-0.364623
1	-6.676739	2.024554	-0.104574
1	-6.33878	-0.972419	-0.515684
6	-1.076678	1.917526	0.53676
8	-0.346387	2.044988	-0.72358
6	-0.998041	3.295811	1.214705
6	0.972247	2.40558	-0.603374
6	0.467615	3.542009	1.613778
6	1.423884	3.126833	0.52859
6	2.814282	3.456227	0.608071
6	1.823553	2.067536	-1.633532
6	3.698581	3.100145	-0.37995
6	3.237586	2.36869	-1.541803
8	3.171042	4.134476	1.733903
8	4.036417	1.96189	-2.427173
1	4.11745	4.330347	1.703569
8	-1.467434	4.335916	0.365199
1	-1.244497	4.083739	-0.543974
1	-0.525876	1.215379	1.174578
6	0.282264	-2.665973	-0.079075
8	1.16242	-1.711236	-0.682276
6	0.696856	-2.89544	1.397819
1	-0.032505	-3.559037	1.87206
6	2.51397	-1.852585	-0.450223
6	2.092771	-3.523329	1.414798
1	2.03571	-4.565314	1.071752
6	3.017878	-2.706204	0.540551
6	3.342669	-1.052305	-1.24014
6	4.416118	-2.736571	0.700144
1	2.908006	-0.429816	-2.009652
6	4.722264	-1.072002	-1.019513
6	5.26602	-1.933555	-0.055079
8	4.890892	-3.587318	1.662027
1	5.853303	-3.51111	1.69778
1	0.386145	-3.621343	-0.612965
1	0.601163	4.60408	1.844769
1	0.708911	2.999668	2.539248
1	-1.626246	3.312177	2.110418
1	4.758625	3.325701	-0.314599
1	1.456821	1.526536	-2.497249
1	6.341346	-1.947025	0.09601
1	2.464332	-3.556694	2.443421
1	-1.726183	-4.238382	-0.399203
1	-0.489989	-0.257987	-0.067221
8	0.656817	-1.676319	2.129391
1	1.457891	-1.185186	1.895302
8	5.582898	-0.287987	-1.71205
1	5.09611	0.434338	-2.155899

*Table S9 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 3'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483089 (Hartree/Particle)
Thermal correction to Energy= 0.517181
Thermal correction to Enthalpy= 0.518125
Thermal correction to Gibbs Free Energy= 0.418343
Sum of electronic and zero-point Energies= -2021.083267
Sum of electronic and thermal Energies= -2021.049175
Sum of electronic and thermal Enthalpies= -2021.048230
Sum of electronic and thermal Free Energies= -2021.148013

Coordinates:

6	-2.606353	-0.020882	-0.026317
6	-3.965976	-0.487559	-0.234058
6	-5.02481	0.473841	-0.220248
6	-4.770865	1.8309	0.003462
6	-3.473768	2.263889	0.2464
6	-2.406398	1.375138	0.24543
1	-3.315005	3.320002	0.44157
6	-1.42095	-0.826086	-0.094142
6	-4.392995	-1.862615	-0.448248
6	-1.212665	-2.174488	-0.236134
6	-3.551458	-3.066207	-0.475845
6	-2.192489	-3.184951	-0.387094
8	-5.626057	-2.141967	-0.619039
8	-4.264799	-4.196659	-0.644196
1	-5.194577	-3.883642	-0.714214
8	-5.798395	2.71226	0.007296
8	-6.326448	0.184326	-0.406614
1	-6.605252	2.198322	-0.166419
1	-6.361761	-0.812913	-0.540035
6	-1.021992	1.902096	0.566504
8	-0.295202	2.035621	-0.656267
6	-0.966555	3.249393	1.378982
6	0.995438	2.466765	-0.544503
6	0.530912	3.476049	1.735881
6	1.453897	3.131648	0.597164
6	2.812533	3.492659	0.627018
6	1.829848	2.188852	-1.633011
6	3.681282	3.189777	-0.421769
6	3.171519	2.53417	-1.543413
8	3.234438	4.145123	1.75014
8	4.07794	2.173937	-2.524804
1	4.170427	4.366508	1.658795
1	3.592211	1.935995	-3.326917
8	-1.408963	4.288447	0.625469
1	-0.495847	1.188968	1.215778
6	0.214581	-2.701846	-0.155394
8	1.115512	-1.700454	-0.641179
6	0.617779	-3.112519	1.284203
1	-0.117601	-3.826897	1.666687
6	2.461253	-1.876788	-0.412403
6	2.010551	-3.74989	1.236391
1	1.948531	-4.745853	0.777104
6	2.951463	-2.848666	0.46851
6	3.301403	-0.987761	-1.086958
6	4.348155	-2.907735	0.632336
1	2.86235	-0.249492	-1.743337
6	4.677279	-1.048719	-0.868359
6	5.210241	-2.028395	-0.018833
8	4.810363	-3.871818	1.486682
1	5.771827	-3.800459	1.548422
1	0.301749	-3.589395	-0.799139
1	0.670963	4.517672	2.041048
1	0.746567	2.866024	2.623272
1	-1.550547	3.093845	2.303652
1	4.735657	3.443739	-0.378858
1	1.422118	1.65693	-2.486359
1	6.28465	-2.072468	0.132234
1	2.373323	-3.902448	2.257247
1	-1.838339	-4.210303	-0.471204
1	-0.498	-0.270901	-0.051318
8	0.570981	-1.995178	2.159401
1	1.351988	-1.454835	1.971832
8	5.549852	-0.189493	-1.457527
1	5.065645	0.538023	-1.888053

*Table S10 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site h-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.484724 (Hartree/Particle)
Thermal correction to Energy= 0.518623
Thermal correction to Enthalpy= 0.519567
Thermal correction to Gibbs Free Energy= 0.420104
Sum of electronic and zero-point Energies= -2021.114256
Sum of electronic and thermal Energies= -2021.080357
Sum of electronic and thermal Enthalpies= -2021.079413
Sum of electronic and thermal Free Energies= -2021.178876

Coordinates:

6	2.64649	-0.001403	0.035268
6	4.015376	-0.461022	0.226978
6	5.08043	0.496609	0.178356
6	4.840259	1.925784	-0.080144
6	3.466398	2.302555	-0.315474
6	2.430042	1.418034	-0.273483
1	3.291143	3.351935	-0.520047
6	1.478996	-0.793309	0.115474
6	4.434847	-1.83272	0.472546
6	1.261895	-2.158186	0.263088
6	3.591396	-3.035739	0.535203
6	2.226971	-3.162297	0.439441
8	5.665889	-2.119924	0.643266
8	4.299306	-4.1579	0.733005
1	5.232287	-3.845599	0.790797
8	5.775686	2.739658	-0.102307
8	6.345807	0.19183	0.354481
1	6.374025	-0.804864	0.516503
6	1.029942	1.923231	-0.591265
8	0.323649	2.05979	0.672361
6	0.881109	3.262115	-1.337239
6	-1.005607	2.39935	0.56464
6	-0.599452	3.410284	-1.727583
6	-1.509058	3.021626	-0.581855
6	-2.888298	3.294075	-0.605554
6	-1.807609	2.092768	1.668821
6	-3.724655	2.970854	0.464539
6	-3.166662	2.371425	1.593641
8	-3.361004	3.89503	-1.735786
8	-4.038336	2.000645	2.602648
1	-4.308693	4.057434	-1.640539
1	-3.528744	1.801411	3.400319
8	1.318149	4.365314	-0.552566
1	1.048041	4.192352	0.361569
1	0.507286	1.173119	-1.197745
6	-0.162879	-2.673911	0.124232
8	-1.071815	-1.715801	0.674432
6	-0.540689	-2.965226	-1.352994
1	0.208294	-3.637072	-1.782886
6	-2.414755	-1.889223	0.416999
6	-1.926432	-3.61662	-1.376062
1	-1.859308	-4.646922	-1.001274
6	-2.883894	-2.790495	-0.546776
6	-3.272744	-1.071046	1.154217
6	-4.278011	-2.852344	-0.731547
1	-2.851002	-0.390981	1.880648
6	-4.644949	-1.124268	0.909706
6	-5.157002	-2.036755	-0.023076
8	-4.717817	-3.748732	-1.666761
1	-5.679405	-3.684878	-1.735009
1	-0.258581	-3.612045	0.689134
1	-0.778057	4.450114	-2.017785
1	-0.816797	2.799134	-2.613813
1	1.502141	3.259533	-2.238021
1	-4.79118	3.170194	0.432827
1	-1.362902	1.594797	2.524245
1	-6.228749	-2.076604	-0.19287
1	-2.275721	-3.686656	-2.410621
1	1.874441	-4.18659	0.535945
1	0.552687	-0.246692	0.050725
8	-0.49568	-1.776394	-2.129269
1	-1.300992	-1.276311	-1.93183
8	-5.531671	-0.32012	1.551992
1	-5.05624	0.393163	2.015194

*Table S11 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site i-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.485012 (Hartree/Particle)
Thermal correction to Energy= 0.519097
Thermal correction to Enthalpy= 0.520041
Thermal correction to Gibbs Free Energy= 0.419677
Sum of electronic and zero-point Energies= -2021.105555
Sum of electronic and thermal Energies= -2021.071470
Sum of electronic and thermal Enthalpies= -2021.070526
Sum of electronic and thermal Free Energies= -2021.170890

Coordinates:

6	2.667297	-0.050899	0.09213
6	4.000527	-0.527589	0.296702
6	5.118353	0.412279	0.157956
6	4.806579	1.807848	-0.15979
6	3.509341	2.256241	-0.354232
6	2.455394	1.362574	-0.252886
1	3.32946	3.299893	-0.581468
6	1.465309	-0.822972	0.186203
6	4.399779	-1.886789	0.651586
6	1.236432	-2.180419	0.224186
6	3.537043	-3.105241	0.506298
6	2.189432	-3.220961	0.2997
8	5.551774	-2.178429	1.023334
8	4.256627	-4.211956	0.668107
1	5.155247	-3.839088	0.898117
8	5.862633	2.601942	-0.262639
8	6.341325	0.170606	0.261781
1	6.615115	1.976822	-0.087048
6	1.058525	1.873076	-0.568145
8	0.37065	2.063186	0.700205
6	0.913565	3.188583	-1.355164
6	-0.961351	2.395667	0.592429
6	-0.570239	3.341362	-1.730531
6	-1.471446	2.987738	-0.566811
6	-2.851206	3.257895	-0.590182
6	-1.757003	2.11212	1.707013
6	-3.681167	2.959933	0.491921
6	-3.117073	2.386363	1.631574
8	-3.330336	3.82962	-1.732733
8	-3.983921	2.036517	2.651126
1	-4.279109	3.986903	-1.639527
1	-3.470398	1.838015	3.446455
8	1.376053	4.31019	-0.610148
1	1.093083	4.17852	0.307225
1	0.521035	1.107009	-1.139388
6	-0.198754	-2.669363	0.083449
8	-1.091004	-1.717	0.669262
6	-0.590944	-2.910456	-1.398871
1	0.14652	-3.576481	-1.85652
6	-2.436209	-1.857503	0.411028
6	-1.984541	-3.544881	-1.428513
1	-1.927639	-4.583725	-1.076519
6	-2.925392	-2.724129	-0.574787
6	-3.276817	-1.041712	1.171384
6	-4.320707	-2.753656	-0.75744
1	-2.839909	-0.389266	1.914394
6	-4.650142	-1.061941	0.929
6	-5.182059	-1.939611	-0.025671
8	-4.780741	-3.61594	-1.714868
1	-5.741238	-3.532524	-1.776761
1	-0.303797	-3.622044	0.621673
1	-0.742583	4.375214	-2.045294
1	-0.802899	2.710491	-2.598729
1	1.521826	3.152417	-2.263902
1	-4.748413	3.155319	0.460359
1	-1.307871	1.632875	2.570781
1	-6.254732	-1.953861	-0.19382
1	-2.341898	-3.587324	-2.461749
1	1.821256	-4.244026	0.279563
1	0.551675	-0.25251	0.196247
8	-0.542285	-1.698519	-2.138922
1	-1.344297	-1.201037	-1.922398
8	-5.520231	-0.256463	1.593108
1	-5.029964	0.437022	2.070193

*Table S12 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site b-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483893 (Hartree/Particle)
Thermal correction to Energy= 0.518017
Thermal correction to Enthalpy= 0.518962
Thermal correction to Gibbs Free Energy= 0.418742
Sum of electronic and zero-point Energies= -2021.110799
Sum of electronic and thermal Energies= -2021.076674
Sum of electronic and thermal Enthalpies= -2021.075730
Sum of electronic and thermal Free Energies= -2021.175950

Coordinates:

6	2.627783	-0.079613	0.030618
6	3.980074	-0.544068	0.282483
6	5.033223	0.409544	0.261613
6	4.797368	1.761876	-0.076064
6	3.510495	2.193953	-0.35867
6	2.436605	1.311014	-0.306362
1	3.350384	3.239236	-0.593292
6	1.450145	-0.868951	0.124267
6	4.418625	-1.917237	0.569547
6	1.228133	-2.248832	0.257938
6	3.603008	-3.207743	0.401767
6	2.164775	-3.256417	0.365576
8	5.598213	-2.134807	0.920645
8	4.250641	-4.25564	0.343909
8	5.83601	2.619115	-0.104572
8	6.310029	0.133502	0.536775
1	6.629721	2.107278	0.132572
1	6.304777	-0.8597	0.790702
6	1.050448	1.843095	-0.62812
8	0.3719	2.051916	0.642788
6	0.922869	3.15599	-1.422057
6	-0.95379	2.40542	0.540997
6	-0.561087	3.331853	-1.789391
6	-1.461945	2.998022	-0.618888
6	-2.838044	3.286901	-0.635399
6	-1.746206	2.140878	1.662399
6	-3.665554	3.007326	0.45389
6	-3.102289	2.434005	1.594174
8	-3.316622	3.858429	-1.778433
8	-3.96531	2.105863	2.624575
1	-4.262805	4.027972	-1.680559
1	-3.447401	1.917567	3.419557
8	1.408555	4.273879	-0.685755
1	1.122229	4.154448	0.232294
1	0.495028	1.085126	-1.192226
6	-0.215124	-2.730374	0.131399
8	-1.093929	-1.770766	0.73315
6	-0.625463	-2.966681	-1.343381
1	0.101021	-3.64211	-1.804473
6	-2.441325	-1.878221	0.470226
6	-2.026428	-3.582677	-1.361942
1	-1.981495	-4.618995	-1.001101
6	-2.949627	-2.739506	-0.511141
6	-3.265267	-1.035683	1.220891
6	-4.344798	-2.739507	-0.696186
1	-2.815641	-0.386234	1.959402
6	-4.638628	-1.027591	0.975795
6	-5.188736	-1.901536	0.0282
8	-4.822335	-3.597459	-1.648975
1	-5.780715	-3.493487	-1.712411
1	-0.317379	-3.682364	0.669731
1	-0.718293	4.367026	-2.107853
1	-0.809098	2.701149	-2.653435
1	1.525689	3.104918	-2.33377
1	-4.729936	3.218482	0.42782
1	-1.297946	1.661091	2.526293
1	-6.261199	-1.892479	-0.141566
1	-2.390639	-3.629228	-2.392592
1	1.805885	-4.28268	0.406524
1	0.526099	-0.316366	0.081662
8	-0.567698	-1.754718	-2.087002
1	-1.374392	-1.25906	-1.883609
8	-5.493893	-0.198457	1.629909
1	-4.993831	0.50014	2.089151

*Table S13 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 3-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483531 (Hartree/Particle)
Thermal correction to Energy= 0.517417
Thermal correction to Enthalpy= 0.518361
Thermal correction to Gibbs Free Energy= 0.419167
Sum of electronic and zero-point Energies= -2021.083849
Sum of electronic and thermal Energies= -2021.049963
Sum of electronic and thermal Enthalpies= -2021.049019
Sum of electronic and thermal Free Energies= -2021.148213

Coordinates:

6	2.593407	-0.022276	0.015623
6	3.95796	-0.483767	0.219017
6	5.01795	0.472626	0.141118
6	4.76061	1.817854	-0.139494
6	3.458465	2.248252	-0.357416
6	2.386838	1.365102	-0.295959
1	3.290199	3.298631	-0.562405
6	1.414747	-0.835101	0.098473
6	4.388509	-1.846425	0.497596
6	1.216744	-2.181852	0.274007
6	3.552112	-3.051248	0.585148
6	2.195267	-3.182159	0.481191
8	5.622553	-2.115433	0.678479
8	4.269199	-4.167805	0.814802
1	5.197672	-3.846725	0.868699
8	5.789695	2.695698	-0.202316
8	6.323347	0.191434	0.318747
1	6.598864	2.187038	-0.023648
1	6.360209	-0.795387	0.511191
6	0.996873	1.900148	-0.59297
8	0.308306	2.068992	0.681147
6	0.868433	3.238271	-1.343941
6	-1.018108	2.41984	0.579171
6	-0.611977	3.423277	-1.716354
6	-1.518914	3.05158	-0.563239
6	-2.895695	3.333933	-0.584738
6	-1.822275	2.111806	1.681657
6	-3.733916	3.010163	0.483701
6	-3.179732	2.397407	1.607236
8	-3.365531	3.945225	-1.711033
8	-4.055238	2.019945	2.611433
1	-4.316169	4.092688	-1.621867
1	-3.545962	1.796667	3.402854
8	1.343459	4.332538	-0.565006
1	1.073932	4.163467	0.350395
1	0.439532	1.161985	-1.181318
6	-0.209003	-2.712295	0.147356
8	-1.111665	-1.741178	0.650813
6	-0.529938	-3.081525	-1.338073
1	0.147308	-3.894814	-1.655013
6	-2.451636	-1.894584	0.39378
6	-1.996271	-3.631394	-1.387614
1	-1.936463	-4.667061	-1.027375
6	-2.929029	-2.79512	-0.562141
6	-3.299955	-1.058104	1.120563
6	-4.32001	-2.825256	-0.769472
1	-2.870432	-0.3751	1.83983
6	-4.670742	-1.089173	0.866194
6	-5.191021	-1.99562	-0.068358
8	-4.766354	-3.713953	-1.710825
1	-5.721979	-3.612206	-1.808846
1	-0.310283	-3.638538	0.732771
1	-0.769107	4.467466	-2.004091
1	-0.854353	2.817092	-2.599286
1	1.478284	3.219775	-2.252319
1	-4.799486	3.214743	0.452654
1	-1.381291	1.602861	2.532643
1	-6.262112	-2.020176	-0.245051
1	-2.332092	-3.682153	-2.427008
1	1.843885	-4.204796	0.599197
1	0.485825	-0.292824	0.015687
8	-0.473338	-2.000436	-2.15606
8	-5.550215	-0.271093	1.501483
1	-5.067878	0.42975	1.976618

*Table S14 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 5-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.484116 (Hartree/Particle)
Thermal correction to Energy= 0.518010
Thermal correction to Enthalpy= 0.518955
Thermal correction to Gibbs Free Energy= 0.419640
Sum of electronic and zero-point Energies= -2021.113082
Sum of electronic and thermal Energies= -2021.079188
Sum of electronic and thermal Enthalpies= -2021.078244
Sum of electronic and thermal Free Energies= -2021.177558

Coordinates:

6	-2.59484	-0.024911	-0.033582
6	-3.95322	-0.501783	-0.234315
6	-5.021244	0.448023	-0.189896
6	-4.777447	1.802249	0.059692
6	-3.481466	2.246775	0.284764
6	-2.403485	1.369507	0.253761
1	-3.323699	3.301894	0.473428
6	-1.406421	-0.82588	-0.102237
6	-4.371087	-1.875877	-0.474304
6	-1.192738	-2.173568	-0.240792
6	-3.523553	-3.075043	-0.515114
6	-2.16584	-3.188361	-0.409745
8	-5.601325	-2.159746	-0.655232
8	-4.22934	-4.206436	-0.705777
1	-5.1606	-3.898022	-0.775747
8	-5.813635	2.673178	0.090542
8	-6.322059	0.15131	-0.371282
1	-6.617513	2.154172	-0.0822
1	-6.349824	-0.841389	-0.534776
6	-1.023094	1.914422	0.569542
8	-0.305215	2.067403	-0.691947
6	-0.910446	3.261827	1.305147
6	1.017129	2.418882	-0.565633
6	0.56219	3.451146	1.707745
6	1.495448	3.058021	0.58262
6	2.872479	3.338986	0.631333
6	1.844195	2.103054	-1.649968
6	3.73227	3.008829	-0.418611
6	3.199036	2.395018	-1.55167
8	3.318171	3.954704	1.763483
8	4.093486	2.017375	-2.540521
1	4.268481	4.114243	1.691515
1	3.605359	1.839147	-3.356461
8	-1.368371	4.34555	0.503069
1	-1.0908	4.161569	-0.406958
1	-0.477815	1.183668	1.178611
6	0.230629	-2.700063	-0.121455
8	1.148447	-1.719659	-0.634337
6	0.611196	-3.061299	1.339394
1	-0.13139	-3.764495	1.728134
6	2.480762	-1.912266	-0.365271
6	2.006122	-3.696599	1.341231
1	1.959893	-4.711865	0.924677
6	2.951546	-2.837656	0.545373
6	3.355556	-1.058937	-1.073704
6	4.397477	-2.932965	0.754465
1	2.922873	-0.352663	-1.770039
6	4.749796	-1.104358	-0.855414
6	5.270665	-2.041509	0.018819
8	4.859942	-3.759666	1.578485
1	0.329303	-3.608313	-0.732596
1	0.715337	4.500232	1.979186
1	0.782856	2.862917	2.608409
1	-1.539059	3.254077	2.200688
1	4.796258	3.217862	-0.369813
1	1.41873	1.596192	-2.510173
1	6.337448	-2.10991	0.195106
1	2.372835	-3.806606	2.36586
1	-1.806293	-4.211621	-0.495294
1	-0.486587	-0.267018	-0.044305
8	0.542153	-1.916812	2.177294
1	1.335157	-1.387554	2.012177
8	5.594191	-0.261601	-1.500539
1	5.097796	0.454692	-1.938385

*Table S15 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 7-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483839 (Hartree/Particle)
Thermal correction to Energy= 0.517771
Thermal correction to Enthalpy= 0.518715
Thermal correction to Gibbs Free Energy= 0.419227
Sum of electronic and zero-point Energies= -2021.111348
Sum of electronic and thermal Energies= -2021.077417
Sum of electronic and thermal Enthalpies= -2021.076472
Sum of electronic and thermal Free Energies= -2021.175960

Coordinates:

6	-2.608565	-0.020122	-0.046912
6	-3.978452	-0.456166	-0.248747
6	-4.975193	0.53783	-0.488399
6	-4.648573	1.898035	-0.503008
6	-3.350389	2.309562	-0.224712
6	-2.339177	1.386968	0.019746
1	-3.137763	3.371614	-0.201148
6	-1.463721	-0.876964	0.031894
6	-4.473172	-1.823912	-0.193498
6	-1.32251	-2.236862	0.142884
6	-3.702078	-3.039831	0.101447
6	-2.350571	-3.206584	0.226381
8	-5.710175	-2.075532	-0.371599
8	-4.47619	-4.139608	0.188948
1	-5.38285	-3.808324	0.000313
8	-5.615604	2.813229	-0.747904
8	-6.279134	0.280648	-0.709403
1	-6.440423	2.316955	-0.884394
1	-6.370408	-0.71762	-0.638595
6	-0.977267	1.895337	0.476166
8	-0.042711	1.858554	-0.639479
6	-0.931469	3.316875	1.069905
6	1.25361	2.249645	-0.345179
6	0.448186	3.516867	1.707391
6	1.538543	3.037177	0.77647
6	2.879529	3.421182	0.960168
6	2.240001	1.861326	-1.261608
6	3.883871	3.041765	0.076012
6	3.563758	2.26148	-1.044479
8	3.137688	4.188085	2.063348
8	4.588652	1.956782	-1.879082
1	4.070517	4.439596	2.057708
1	4.432149	1.134603	-2.380602
8	-1.19189	4.31195	0.084085
1	-0.705799	4.055499	-0.713843
1	-0.596637	1.217707	1.25127
6	0.095129	-2.785136	0.220005
8	0.885625	-2.061198	-0.740939
6	0.748061	-2.685625	1.617803
1	0.123549	-3.233832	2.329143
6	2.246327	-2.126437	-0.675756
6	2.146773	-3.318895	1.55366
1	2.063339	-4.410572	1.453858
6	2.924161	-2.746225	0.398704
6	2.935161	-1.492591	-1.691655
6	4.354402	-2.756912	0.379533
1	2.397995	-1.01953	-2.503574
6	4.376334	-1.417423	-1.664078
6	5.069743	-2.130073	-0.611976
8	4.930719	-3.408208	1.428758
1	5.892426	-3.336666	1.35921
1	0.087648	-3.844787	-0.07076
1	0.581004	4.579571	1.931001
1	0.494472	2.988504	2.66958
1	-1.713043	3.426997	1.827465
1	4.918451	3.331691	0.233142
1	1.954501	1.294249	-2.139108
1	6.154807	-2.096018	-0.609405
1	2.677872	-3.13783	2.492462
1	-2.048975	-4.241902	0.370184
1	-0.524443	-0.352752	-0.051408
8	0.79452	-1.352331	2.100023
1	1.414197	-0.846634	1.55463
8	4.998843	-0.721906	-2.51252

*Table S16 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 4'α-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483993 (Hartree/Particle)
Thermal correction to Energy= 0.518243
Thermal correction to Enthalpy= 0.519187
Thermal correction to Gibbs Free Energy= 0.419121
Sum of electronic and zero-point Energies= -2021.106889
Sum of electronic and thermal Energies= -2021.072639
Sum of electronic and thermal Enthalpies= -2021.071695
Sum of electronic and thermal Free Energies= -2021.171761

Coordinates:

6	2.601832	-0.050679	0.0381
6	3.948165	-0.563335	0.240258
6	5.042329	0.356178	0.187423
6	4.835365	1.712372	-0.077681
6	3.552361	2.191244	-0.305029
6	2.44777	1.348215	-0.260347
1	3.42343	3.245039	-0.517709
6	1.39453	-0.822512	0.115305
6	4.330831	-1.945856	0.48985
6	1.14849	-2.165376	0.252654
6	3.455799	-3.123664	0.529132
6	2.096359	-3.203449	0.420009
8	5.553817	-2.259836	0.677612
8	4.134021	-4.272244	0.7226
1	5.071513	-3.983894	0.796242
8	5.896403	2.553689	-0.121135
8	6.33524	0.025632	0.371606
1	6.684491	2.012438	0.055858
1	6.334084	-0.966037	0.546078
6	1.079509	1.929214	-0.570125
8	0.385527	2.133333	0.701036
6	0.971995	3.231467	-1.388173
6	-0.931179	2.480081	0.59585
6	-0.487628	3.532758	-1.575922
6	-1.397497	3.160542	-0.569212
6	-2.795306	3.460188	-0.609347
6	-1.765266	2.171829	1.663706
6	-3.644905	3.127769	0.436835
6	-3.120734	2.489249	1.567095
8	-3.231417	4.097971	-1.730356
8	-4.021726	2.119297	2.547254
1	-4.18046	4.264189	-1.656213
1	-3.534344	1.865475	3.343485
8	1.643605	4.357029	-0.795853
1	1.246493	4.489519	0.077542
1	0.504067	1.194094	-1.145039
6	-0.286931	-2.660336	0.135493
8	-1.180216	-1.654394	0.62653
6	-0.669627	-3.027888	-1.321677
1	0.062512	-3.742975	-1.708797
6	-2.524767	-1.821813	0.385567
6	-2.071539	-3.646952	-1.316132
1	-2.0292	-4.659643	-0.89252
6	-3.012863	-2.763949	-0.528134
6	-3.366754	-0.954225	1.084292
6	-4.408602	-2.812519	-0.702531
1	-2.929506	-0.244561	1.771994
6	-4.740891	-1.001231	0.853633
6	-5.272206	-1.949836	-0.030696
8	-4.868718	-3.747833	-1.589194
1	-5.829403	-3.670533	-1.655515
1	-0.405294	-3.560933	0.75543
1	-0.811794	4.133194	-2.415958
1	1.469203	3.08306	-2.351799
1	-4.706857	3.349659	0.395417
1	-1.355352	1.646052	2.520215
1	-6.345588	-1.984083	-0.191401
1	-2.421153	-3.75756	-2.346969
1	1.71098	-4.217412	0.504112
1	0.487048	-0.243094	0.061306
8	-0.589231	-1.89104	-2.168155
1	-1.349363	-1.327409	-1.964468
8	-5.611101	-0.154449	1.46567
1	-5.116995	0.553262	1.91661

*Table S17 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 4′β-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483992 (Hartree/Particle)
Thermal correction to Energy= 0.518243
Thermal correction to Enthalpy= 0.519187
Thermal correction to Gibbs Free Energy= 0.419118
Sum of electronic and zero-point Energies= -2021.106890
Sum of electronic and thermal Energies= -2021.072639
Sum of electronic and thermal Enthalpies= -2021.071695
Sum of electronic and thermal Free Energies= -2021.171764

Coordinates:

6	2.601815	-0.050585	0.038062
6	3.948171	-0.563186	0.240035
6	5.042321	0.356347	0.186868
6	4.835267	1.712511	-0.078295
6	3.55221	2.191332	-0.305455
6	2.447641	1.348294	-0.260462
1	3.423224	3.245109	-0.518191
6	1.394576	-0.822472	0.11538
6	4.330935	-1.945681	0.489802
6	1.148577	-2.165323	0.253009
6	3.455898	-3.123448	0.529959
6	2.096463	-3.203308	0.420912
8	5.553945	-2.259575	0.677447
8	4.134157	-4.271938	0.723923
1	5.071695	-3.983591	0.796979
8	5.896263	2.553864	-0.122007
8	6.335274	0.025889	0.370949
1	6.684415	2.012655	0.054833
1	6.334116	-0.96571	0.545746
6	1.079317	1.929225	-0.57013
8	0.385333	2.132983	0.701018
6	0.971752	3.231577	-1.387999
6	-0.931296	2.48001	0.596023
6	-0.487883	3.532822	-1.575698
6	-1.397695	3.160579	-0.568937
6	-2.79551	3.460263	-0.608901
6	-1.765291	2.171773	1.663978
6	-3.645008	3.127824	0.437319
6	-3.12076	2.489176	1.567509
8	-3.231685	4.098121	-1.729855
8	-4.021689	2.119174	2.54764
1	-4.180762	4.264173	-1.655728
1	-3.534277	1.864411	3.343551
8	1.643361	4.35706	-0.795563
1	1.246027	4.489749	0.077695
1	0.504011	1.194112	-1.145215
6	-0.286814	-2.660384	0.135694
8	-1.180234	-1.654419	0.626511
6	-0.669311	-3.028153	-1.321456
1	0.062906	-3.743278	-1.70836
6	-2.524742	-1.821907	0.385355
6	-2.071211	-3.647263	-1.316014
1	-2.028907	-4.659874	-0.892206
6	-3.012684	-2.764151	-0.528305
6	-3.36684	-0.95425	1.083866
6	-4.408391	-2.812706	-0.702971
1	-2.929668	-0.244542	1.771572
6	-4.740921	-1.001276	0.852963
6	-5.272104	-1.949917	-0.031395
8	-4.86836	-3.748106	-1.58961
1	-5.829033	-3.670811	-1.65611
1	-0.40523	-3.56089	0.755742
1	-0.812143	4.133228	-2.415733
1	1.468935	3.083301	-2.35166
1	-4.706965	3.349711	0.396002
1	-1.355305	1.645879	2.520386
1	-6.345457	-1.984153	-0.192283
1	-2.420667	-3.758049	-2.34688
1	1.711083	-4.21723	0.505465
1	0.487082	-0.243098	0.061219
8	-0.588856	-1.891477	-2.168158
1	-1.34865	-1.327487	-1.964199
8	-5.611269	-0.154463	1.46484
1	-5.117236	0.553135	1.91601

*Table S18 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 3′-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.484225 (Hartree/Particle)
Thermal correction to Energy= 0.518470
Thermal correction to Enthalpy= 0.519415
Thermal correction to Gibbs Free Energy= 0.418983
Sum of electronic and zero-point Energies= -2021.089638
Sum of electronic and thermal Energies= -2021.055392
Sum of electronic and thermal Enthalpies= -2021.054448
Sum of electronic and thermal Free Energies= -2021.154880

Coordinates:

6	2.593372	-0.056258	0.024415
6	3.933333	-0.587049	0.224501
6	5.051937	0.281461	0.023899
6	4.874536	1.596981	-0.410187
6	3.593452	2.101272	-0.590915
6	2.463325	1.328674	-0.343273
1	3.510185	3.118373	-0.953278
6	1.373935	-0.810003	0.091478
6	4.28935	-1.942742	0.622848
6	1.110557	-2.140043	0.312396
6	3.390967	-3.088067	0.792056
6	2.035612	-3.161777	0.633344
8	5.506631	-2.257823	0.842726
8	4.039485	-4.217068	1.13924
1	4.983253	-3.945362	1.186718
8	5.954811	2.379939	-0.640932
8	6.340796	-0.068178	0.193483
1	6.736961	1.834625	-0.449501
1	6.316615	-1.026355	0.506033
6	1.103589	1.970457	-0.57893
8	0.338408	1.91031	0.683029
6	1.04724	3.40115	-1.028398
6	-0.927473	2.43307	0.600781
6	-0.331179	3.79483	-1.473501
6	-1.329542	3.286506	-0.438228
6	-2.671489	3.701132	-0.450142
6	-1.807969	2.04822	1.619973
6	-3.581164	3.299093	0.52933
6	-3.12914	2.474251	1.558778
8	-3.033444	4.52835	-1.475401
8	-4.074225	2.040185	2.474067
1	-3.964554	4.766993	-1.378709
1	-3.617033	1.677663	3.245575
8	1.612432	4.354666	-0.209215
1	2.211906	3.932439	0.422912
1	0.546672	1.381828	-1.319938
6	-0.3172	-2.641537	0.14229
8	-1.231707	-1.617999	0.546991
6	-0.635226	-3.069433	-1.314315
1	0.115716	-3.794035	-1.643335
6	-2.567364	-1.825186	0.281892
6	-2.033741	-3.697727	-1.343553
1	-2.000317	-4.699594	-0.893973
6	-3.012277	-2.805738	-0.612497
6	-3.443211	-0.957801	0.93456
6	-4.402485	-2.88755	-0.818426
1	-3.038477	-0.21609	1.605785
6	-4.809716	-1.038813	0.674744
6	-5.30035	-2.023204	-0.194077
8	-4.82191	-3.85941	-1.686176
1	-5.781946	-3.803681	-1.778487
1	-0.465078	-3.51605	0.792516
1	-0.399634	4.883377	-1.557993
1	-0.559243	3.383389	-2.465204
1	-4.619645	3.614563	0.507024
1	-1.451464	1.375031	2.3926
1	-6.368373	-2.085653	-0.380079
1	-2.342573	-3.837013	-2.383991
1	1.631947	-4.157582	0.803122
1	0.479505	-0.230903	-0.070572
8	-0.524626	-1.965539	-2.199686
1	-1.279077	-1.384219	-2.026593
8	-5.705167	-0.190269	1.24592
1	-5.227299	0.525928	1.701945

*Table S19 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 2'-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483151 (Hartree/Particle)
Thermal correction to Energy= 0.517892
Thermal correction to Enthalpy= 0.518836
Thermal correction to Gibbs Free Energy= 0.416810
Sum of electronic and zero-point Energies= -2021.109028
Sum of electronic and thermal Energies= -2021.074286
Sum of electronic and thermal Enthalpies= -2021.073342
Sum of electronic and thermal Free Energies= -2021.175368

Coordinates:

6	2.60668	-0.047349	0.061897
6	3.941626	-0.608301	0.216623
6	5.067393	0.209354	-0.083153
6	4.91258	1.538782	-0.524705
6	3.661689	2.110255	-0.576824
6	2.496279	1.375755	-0.251434
1	3.600055	3.172265	-0.780285
6	1.393067	-0.790692	0.042713
6	4.271043	-1.950779	0.679095
6	1.096698	-2.110116	0.327406
6	3.342364	-3.03677	0.98046
6	1.985914	-3.100848	0.794029
8	5.488205	-2.289838	0.872916
8	3.95663	-4.143105	1.450465
1	4.910029	-3.903948	1.447046
8	6.018014	2.266641	-0.812002
8	6.350831	-0.180753	0.021533
1	6.780844	1.688815	-0.639228
1	6.310023	-1.118129	0.39778
6	1.281786	2.126298	-0.250822
8	0.307831	1.769891	0.659776
6	1.075243	3.41035	-1.008585
6	-0.944131	2.33084	0.622293
6	-0.370419	3.511432	-1.516847
6	-1.340634	3.177213	-0.414425
6	-2.665037	3.646339	-0.385973
6	-1.793772	1.969901	1.672976
6	-3.553421	3.277096	0.625914
6	-3.105652	2.429146	1.640472
8	-3.037239	4.467212	-1.409766
8	-4.043238	2.019505	2.568291
1	-3.959427	4.729878	-1.291303
1	-3.587709	1.609595	3.31676
8	1.44878	4.572228	-0.247195
1	0.891531	4.599966	0.543486
6	-0.322592	-2.605213	0.092087
8	-1.248254	-1.584876	0.498623
6	-0.61451	-3.001007	-1.376998
1	0.140417	-3.722061	-1.704486
6	-2.578604	-1.802937	0.223878
6	-2.014578	-3.625128	-1.448108
1	-1.989878	-4.642115	-1.033301
6	-3.007376	-2.761937	-0.7011
6	-3.470598	-0.969626	0.900279
6	-4.395403	-2.854874	-0.916417
1	-3.080469	-0.248487	1.601966
6	-4.833744	-1.0602	0.631421
6	-5.308179	-2.020741	-0.271443
8	-4.798628	-3.80548	-1.814489
1	-5.759153	-3.761407	-1.907897
1	-0.493506	-3.49273	0.717983
1	-0.540284	4.524814	-1.890441
1	-0.506678	2.831125	-2.369136
1	1.749223	3.419763	-1.866366
1	-4.582486	3.622364	0.631832
1	-1.430463	1.292438	2.438226
1	-6.37432	-2.091432	-0.465028
1	-2.306196	-3.728077	-2.497751
1	1.56077	-4.071125	1.041572
1	0.531622	-0.219585	-0.263793
8	-0.48271	-1.883791	-2.242943
1	-1.212277	-1.279833	-2.043498
8	-5.742804	-0.240862	1.228512
1	-5.273289	0.456263	1.717843

*Table S20 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 4β-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483992 (Hartree/Particle)
Thermal correction to Energy= 0.518244
Thermal correction to Enthalpy= 0.519189
Thermal correction to Gibbs Free Energy= 0.419256
Sum of electronic and zero-point Energies= -2021.108758
Sum of electronic and thermal Energies= -2021.074505
Sum of electronic and thermal Enthalpies= -2021.073561
Sum of electronic and thermal Free Energies= -2021.173494

Coordinates:

6	-2.59015	-0.091705	-0.018639
6	-3.918429	-0.645607	-0.227913
6	-5.039078	0.243427	-0.209382
6	-4.873152	1.614449	0.005399
6	-3.605909	2.135286	0.226386
6	-2.479664	1.319406	0.233003
1	-3.509481	3.202885	0.382723
6	-1.359208	-0.830013	-0.048247
6	-4.257304	-2.042176	-0.461944
6	-1.068265	-2.160525	-0.209669
6	-3.340504	-3.186829	-0.534719
6	-1.979607	-3.22215	-0.427589
8	-5.471146	-2.397867	-0.631757
8	-3.977971	-4.35289	-0.757612
1	-4.926571	-4.099242	-0.810963
8	-5.956958	2.427327	0.004843
8	-6.319866	-0.129706	-0.393282
1	-6.72784	1.858311	-0.16053
1	-6.288699	-1.126928	-0.532968
6	-1.140252	1.95873	0.555211
8	-0.395611	2.116586	-0.690155
6	-1.13576	3.33604	1.244627
6	0.898729	2.556983	-0.535966
6	0.306449	3.635418	1.684046
6	1.296718	3.26776	0.600816
6	2.650309	3.638691	0.681937
6	1.781865	2.255516	-1.57942
6	3.56606	3.321574	-0.322809
6	3.114468	2.628184	-1.445638
8	3.017317	4.326468	1.802162
8	4.068323	2.258585	-2.378562
1	3.9574	4.543625	1.751333
1	3.621255	1.980546	-3.190165
8	-1.632178	4.359084	0.387102
1	-1.329984	4.146966	-0.509015
1	-0.564682	1.286989	1.202909
6	0.383398	-2.620158	-0.133996
8	1.243032	-1.487778	-0.321285
6	0.73432	-3.338527	1.192929
1	0.139675	-4.256663	1.250524
6	2.590558	-1.726829	-0.258941
6	2.199122	-3.650107	1.212945
6	3.087786	-2.823947	0.502494
6	3.417159	-0.828188	-0.910664
6	4.512227	-2.967543	0.52276
1	2.9713	-0.008312	-1.454717
6	4.805864	-0.979177	-0.819288
6	5.352289	-2.067879	-0.116071
8	4.985917	-4.031213	1.23406
1	5.951683	-4.026008	1.203786
1	0.571383	-3.331595	-0.952703
1	0.381938	4.700505	1.924155
1	0.536696	3.0918	2.61018
1	-1.792491	3.319291	2.119715
1	4.61348	3.595831	-0.244983
1	1.420071	1.687401	-2.430368
1	6.431959	-2.176541	-0.070648
1	2.572296	-4.437394	1.855418
1	-1.559712	-4.219037	-0.542965
1	-0.473044	-0.222609	0.04232
8	0.32221	-2.568175	2.330605
1	0.969908	-1.856561	2.430853
8	5.666797	-0.106971	-1.40266
1	5.174295	0.658513	-1.751517

*Table S21 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 4α-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483991 (Hartree/Particle)
Thermal correction to Energy= 0.518245
Thermal correction to Enthalpy= 0.519189
Thermal correction to Gibbs Free Energy= 0.419253
Sum of electronic and zero-point Energies= -2021.108758
Sum of electronic and thermal Energies= -2021.074505
Sum of electronic and thermal Enthalpies= -2021.073560
Sum of electronic and thermal Free Energies= -2021.173497

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Coordinates:

6	-2.590165	-0.091801	-0.018582
6	-3.918407	-0.645825	-0.227932
6	-5.039129	0.243082	-0.209184
6	-4.873329	1.614099	0.005728
6	-3.606119	2.135063	0.226612
6	-2.479803	1.319294	0.233141
1	-3.509762	3.202662	0.382981
6	-1.35917	-0.830006	-0.048124
6	-4.257084	-2.042353	-0.462403
6	-1.068073	-2.160472	-0.209655
6	-3.340142	-3.186934	-0.53522
6	-1.979262	-3.222172	-0.427864
8	-5.470832	-2.398127	-0.6326
8	-3.977509	-4.352973	-0.758375
1	-4.926109	-4.099335	-0.81187
8	-5.957223	2.426869	0.005375
8	-6.319932	-0.130118	-0.392996
1	-6.728036	1.857817	-0.160185
1	-6.288844	-1.127211	-0.533157
6	-1.140381	1.958695	0.555273
8	-0.395728	2.116421	-0.690089
6	-1.135955	3.336094	1.244521
6	0.89858	2.55695	-0.535961
6	0.306234	3.635533	1.683957
6	1.296514	3.267908	0.600738
6	2.650045	3.639065	0.681754
6	1.78173	2.255453	-1.579387
6	3.565788	3.322012	-0.323018
6	3.114279	2.628386	-1.445734
8	3.016995	4.327062	1.801867
8	4.06815	2.258857	-2.37866
1	3.957031	4.544402	1.750937
1	3.621134	1.981379	-3.19048
8	-1.63238	4.35902	0.386863
1	-1.329772	4.14708	-0.509157
1	-0.564823	1.287042	1.203056
6	0.383609	-2.619937	-0.133694
8	1.243199	-1.487452	-0.32069
6	0.734389	-3.338306	1.193288
1	0.139846	-4.256526	1.250756
6	2.590713	-1.726659	-0.258656
6	2.199237	-3.649757	1.213486
1	2.572419	-4.436801	1.85625
6	3.087927	-2.823657	0.502934
6	3.417318	-0.828403	-0.910878
6	4.512335	-2.967396	0.523145
1	2.971552	-0.008629	-1.455157
6	4.806025	-0.979533	-0.819603
6	5.352436	-2.068009	-0.11608
8	4.986024	-4.03084	1.234765
1	5.951779	-4.02586	1.20417
1	0.571888	-3.331313	-0.952389
1	0.38169	4.700617	1.924087
1	0.536474	3.091909	2.610094
1	-1.792709	3.319441	2.119591
1	4.613144	3.596565	-0.245334
1	1.419985	1.687172	-2.430244
1	6.4321	-2.176723	-0.07066
1	-1.559276	-4.219014	-0.543292
1	-0.473098	-0.222505	0.04268
8	0.322084	-2.568086	2.330911
1	0.969715	-1.856439	2.431339
8	5.666944	-0.107674	-1.403593
1	5.174496	0.658112	-1.751829

*Table S22 Energetics and Cartesian coordinates of the conformer **1a** (as-ass-as) post-radical capture via HAB at site 3-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.484206 (Hartree/Particle)
Thermal correction to Energy= 0.518473
Thermal correction to Enthalpy= 0.519417
Thermal correction to Gibbs Free Energy= 0.418923
Sum of electronic and zero-point Energies= -2021.093651
Sum of electronic and thermal Energies= -2021.059385
Sum of electronic and thermal Enthalpies= -2021.058441
Sum of electronic and thermal Free Energies= -2021.158935

Coordinates:

6	-2.596129	-0.085388	-0.051786
6	-3.924168	-0.642713	-0.250755
6	-5.041532	0.250268	-0.275631
6	-4.874426	1.625518	-0.090736
6	-3.610554	2.145725	0.148617
6	-2.486122	1.327078	0.183816
1	-3.513495	3.21394	0.30078
6	-1.361147	-0.820223	-0.103836
6	-4.268607	-2.048318	-0.41346
6	-1.082299	-2.158657	-0.187787
6	-3.362072	-3.202019	-0.364079
6	-2.001189	-3.234355	-0.267929
8	-5.481035	-2.40554	-0.589687
8	-4.009591	-4.380444	-0.465081
1	-4.953921	-4.125465	-0.56284
8	-5.956071	2.441184	-0.126401
8	-6.321192	-0.124648	-0.465763
1	-6.725797	1.870092	-0.28964
1	-6.291931	-1.126342	-0.56878
6	-1.152388	1.962156	0.537775
8	-0.390312	2.159237	-0.691293
6	-1.168203	3.32083	1.264564
6	0.898071	2.606301	-0.50325
6	0.26324	3.616541	1.737486
6	1.271277	3.291207	0.657618
6	2.619087	3.674619	0.769017
6	1.800717	2.339028	-1.538918
6	3.553346	3.392997	-0.228555
6	3.127212	2.720782	-1.374131
8	2.961676	4.337305	1.9123
8	4.100265	2.381492	-2.296537
1	3.901403	4.5598	1.883101
1	3.670957	2.083133	-3.110471
8	-1.653456	4.364894	0.425213
1	-1.323265	4.183659	-0.46781
1	-0.582941	1.274044	1.173132
6	0.370418	-2.630084	-0.190682
8	1.246445	-1.49955	-0.426425
6	0.783742	-3.359703	1.051065
6	2.592757	-1.738642	-0.302683
6	2.192484	-3.886398	1.00996
1	2.230466	-4.837743	0.459417
6	3.10777	-2.863551	0.354297
6	3.424349	-0.768879	-0.867491
6	4.506922	-2.983608	0.410505
1	2.969595	0.081227	-1.355176
6	4.807771	-0.903807	-0.767306
6	5.359878	-2.026074	-0.134592
8	4.984491	-4.095926	1.054029
1	5.950095	-4.068447	1.048886
1	0.509042	-3.319917	-1.037324
1	0.326867	4.673702	2.01336
1	0.483576	3.043598	2.648231
1	-1.842384	3.27728	2.125234
1	4.596973	3.673741	-0.126605
1	1.459252	1.78736	-2.408873
1	6.439374	-2.125202	-0.069708
1	2.551155	-4.122101	2.020446
1	-1.57927	-4.236673	-0.276443
1	-0.472962	-0.207474	-0.094784
8	0.318787	-2.781404	2.207429
1	0.778375	-3.178481	2.959526
8	5.66834	0.018294	-1.27694
1	5.170844	0.783329	-1.617089

Table S23 Energetics and Cartesian coordinates of the conformer 1a (as-ass-as) post-radical capture via HAB at site 2-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.

Zero-point correction= 0.484138 (Hartree/Particle)
Thermal correction to Energy= 0.518465
Thermal correction to Enthalpy= 0.519409
Thermal correction to Gibbs Free Energy= 0.418919
Sum of electronic and zero-point Energies= -2021.117304
Sum of electronic and thermal Energies= -2021.082978
Sum of electronic and thermal Enthalpies= -2021.082033
Sum of electronic and thermal Free Energies= -2021.182524

Coordinates:

6	-2.55486	-0.216771	-0.039234
6	-3.806323	-0.934795	-0.254162
6	-4.944562	-0.206379	-0.709941
6	-4.896538	1.182298	-0.889849
6	-3.742517	1.882243	-0.559575
6	-2.597438	1.224612	-0.126394
1	-3.753296	2.96295	-0.637347
6	-1.275824	-0.80415	0.153592
6	-4.047356	-2.338509	0.01914
6	-0.859666	-2.125137	0.450539
6	-3.104774	-3.284649	0.641219
6	-1.761862	-3.188608	0.811128
8	-5.191165	-2.858872	-0.186953
8	-3.701805	-4.438898	1.023865
1	-4.629201	-4.346349	0.72046
8	-5.99774	1.839315	-1.328497
8	-6.142412	-0.75585	-0.98025
1	-6.691221	1.168254	-1.446818
1	-6.046591	-1.731164	-0.743794
6	-1.425989	2.056233	0.356267
8	-0.441725	2.186518	-0.716275
6	-1.721796	3.486866	0.850156
6	0.727092	2.810801	-0.345816
6	-0.460367	4.01237	1.550434
6	0.77908	3.679983	0.749826
6	2.027189	4.2479	1.059352
6	1.850427	2.529435	-1.132057
6	3.17241	3.96857	0.312172
6	3.064518	3.10749	-0.7802
8	2.053029	5.089351	2.13342
8	4.23488	2.798701	-1.44852
1	2.94694	5.438014	2.246687
1	4.015847	2.374474	-2.290281
8	-2.105119	4.346585	-0.219437
1	-1.560591	4.104188	-0.983564
1	-0.93747	1.525825	1.182157
6	0.520504	-2.435289	0.435416
8	1.37717	-1.395075	0.175613
6	1.155238	-3.769686	0.748455
1	0.410027	-4.559637	0.675849
6	2.715319	-1.607276	-0.103443
6	2.287212	-4.07291	-0.239103
1	1.861831	-4.299478	-1.227007
6	3.217509	-2.892672	-0.311107
6	3.505321	-0.458557	-0.177575
6	4.588633	-2.999538	-0.601539
1	3.056565	0.508206	0.011865
6	4.859001	-0.601324	-0.495676
6	5.406941	-1.875938	-0.695823
8	5.067006	-4.263385	-0.804156
1	6.017586	-4.217972	-0.970657
1	-0.554729	5.095511	1.675179
1	-0.386562	3.587894	2.560635
1	-2.560539	3.474855	1.552126
1	4.135222	4.40384	0.56101
1	1.760629	1.827669	-1.954408
1	6.461267	-1.962956	-0.940511
1	2.817212	-4.969123	0.093864
1	-1.334368	-4.07336	1.266866
1	-0.450366	-0.12132	0.014724
8	1.614823	-3.815218	2.105277
1	2.398649	-3.24925	2.164474
8	5.702982	0.455221	-0.621578
1	5.204607	1.292121	-0.648795

*Table S24 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 5'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482661 (Hartree/Particle)
Thermal correction to Energy= 0.517318
Thermal correction to Enthalpy= 0.518262
Thermal correction to Gibbs Free Energy= 0.413853
Sum of electronic and zero-point Energies= -2021.106005
Sum of electronic and thermal Energies= -2021.071348
Sum of electronic and thermal Enthalpies= -2021.070404
Sum of electronic and thermal Free Energies= -2021.174813

Coordinates:

6	-2.214715	-1.223596	0.147138
6	-2.808529	-2.536224	-0.029061
6	-4.234056	-2.635074	-0.078423
6	-5.043394	-1.499948	0.035517
6	-4.469565	-0.251269	0.235631
6	-3.089925	-0.096841	0.312841
1	-5.12486	0.607471	0.315024
6	-0.809495	-0.939107	0.139575
6	-2.1029	-3.805725	-0.145229
6	0.312874	-1.723144	0.034672
6	-0.650716	-4.032227	-0.116177
6	0.377352	-3.133276	-0.056476
8	-2.751663	-4.895758	-0.273266
8	-0.327565	-5.336738	-0.195487
1	-1.193146	-5.797043	-0.26634
8	-6.389243	-1.629134	-0.033551
8	-4.918646	-3.782431	-0.237881
1	-6.571253	-2.575461	-0.163225
1	-4.21848	-4.504782	-0.292904
6	-2.533874	1.278565	0.637283
8	-1.905616	1.820937	-0.566999
6	-3.508513	2.352618	1.154267
6	-1.253976	3.01982	-0.380425
6	-2.684093	3.562196	1.624156
6	-1.577277	3.880568	0.657355
6	-0.83265	5.134579	0.782975
6	-0.256716	3.33156	-1.320162
6	0.202481	5.42646	-0.191317
6	0.467049	4.545171	-1.213794
8	-1.093984	5.933462	1.712212
8	1.420508	4.742288	-2.16807
1	1.84602	5.59765	-2.018859
8	-4.453003	2.729782	0.158705
1	-3.992988	2.718247	-0.693955
1	-1.747778	1.17599	1.397115
6	1.631153	-0.967308	-0.052655
8	2.64847	-1.723276	0.620129
6	2.093545	-0.700397	-1.503086
1	1.287978	-0.200479	-2.04859
6	3.924991	-1.202068	0.583101
6	3.335292	0.204401	-1.453302
1	3.017846	1.241356	-1.265602
6	4.311044	-0.270911	-0.396007
6	4.806011	-1.686609	1.54693
6	5.641596	0.181692	-0.352905
1	4.471153	-2.404272	2.285129
6	6.12143	-1.220571	1.545418
6	6.546743	-0.282113	0.60171
8	6.118	1.096629	-1.24877
1	5.41579	1.344322	-1.863534
1	1.522021	0.001475	0.453955
1	-3.344162	4.427843	1.733924
1	-2.264249	3.375663	2.621977
1	-4.086228	1.954174	1.993784
1	0.741613	6.361661	-0.074521
1	-0.04338	2.644648	-2.131271
1	7.564061	0.09671	0.590534
1	3.786106	0.18248	-2.455053
1	1.365598	-3.576728	-0.076409
1	-0.583587	0.117091	0.183434
8	2.335626	-1.90922	-2.199465
1	3.000709	-2.40656	-1.7019
8	6.956537	-1.713702	2.504783
1	7.828866	-1.311489	2.401263

*Table S25 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 7'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482852 (Hartree/Particle)
Thermal correction to Energy= 0.517424
Thermal correction to Enthalpy= 0.518368
Thermal correction to Gibbs Free Energy= 0.415762
Sum of electronic and zero-point Energies= -2021.102237
Sum of electronic and thermal Energies= -2021.067665
Sum of electronic and thermal Enthalpies= -2021.066721
Sum of electronic and thermal Free Energies= -2021.169326

Coordinates:

6	-2.395879	-0.951269	0.168429
6	-3.133836	-2.19384	0.05795
6	-4.562771	-2.134426	0.034536
6	-5.239619	-0.911801	0.099052
6	-4.526942	0.274636	0.221218
6	-3.138645	0.274365	0.278234
1	-5.083209	1.203535	0.252043
6	-0.968527	-0.828247	0.151584
6	-2.572621	-3.536462	-0.021215
6	0.061875	-1.72952	0.041485
6	-1.152351	-3.919231	-0.037646
6	-0.028851	-3.138538	-0.031366
8	-3.340478	-4.552272	-0.08329
8	-0.976663	-5.252167	-0.095021
1	-1.888581	-5.617951	-0.118911
8	-6.592789	-0.892929	0.052628
8	-5.372096	-3.204818	-0.059155
1	-6.880631	-1.818085	-0.029719
1	-4.756567	-4.002275	-0.091068
6	-2.417243	1.586782	0.513379
8	-1.692564	1.94873	-0.702043
6	-3.241171	2.830775	0.87711
6	-0.755224	2.940364	-0.513435
6	-2.253441	3.952398	1.275856
6	-0.991356	3.96054	0.444553
6	0.004903	4.963591	0.618122
6	0.390695	2.900388	-1.272108
6	1.176462	4.943197	-0.109435
6	1.427835	3.892659	-1.072633
8	-0.161407	5.966061	1.526623
8	2.520901	3.812787	-1.691712
1	-1.034332	5.909901	1.935454
8	-4.07108	3.240859	-0.196415
1	-3.590123	3.043683	-1.01561
1	-1.676442	1.444716	1.31227
6	1.446864	-1.110063	-0.077716
8	2.404303	-1.95645	0.572706
6	1.906119	-0.894067	-1.538358
1	1.13453	-0.342578	-2.082777
6	3.710709	-1.507367	0.542762
6	3.214931	-0.087197	-1.514183
1	2.982222	0.980294	-1.382596
6	4.145337	-0.591151	-0.428924
6	4.562374	-2.044526	1.505276
6	5.492784	-0.193236	-0.369261
1	4.189719	-2.750083	2.237074
6	5.899306	-1.644521	1.510489
6	6.370731	-0.712103	0.582983
8	6.013491	0.707703	-1.252605
1	5.302749	1.115164	-1.764929
1	1.443864	-0.133485	0.425493
1	-2.796192	4.902909	1.179567
1	-1.987641	3.841379	2.33865
1	-3.901025	2.622034	1.724548
1	1.936925	5.698869	0.046893
1	0.545238	2.118536	-2.005652
1	7.402278	-0.373531	0.587013
1	3.67704	-0.189695	-2.505012
1	0.904472	-3.687226	-0.074377
1	-0.622134	0.193577	0.182494
8	2.039107	-2.131464	-2.215791
1	2.676447	-2.666507	-1.720893
8	6.707792	-2.188302	2.466893
1	7.598596	-1.827881	2.367079

*Table S26 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 3'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481849 (Hartree/Particle)
Thermal correction to Energy= 0.516638
Thermal correction to Enthalpy= 0.517582
Thermal correction to Gibbs Free Energy= 0.413479
Sum of electronic and zero-point Energies= -2021.073304
Sum of electronic and thermal Energies= -2021.038515
Sum of electronic and thermal Enthalpies= -2021.037571
Sum of electronic and thermal Free Energies= -2021.141674

Coordinates:

6	-2.070764	-1.401906	0.120351
6	-2.573868	-2.749791	-0.063975
6	-3.988814	-2.942403	-0.132063
6	-4.873741	-1.864873	-0.017001
6	-4.385904	-0.584499	0.210868
6	-3.020907	-0.340669	0.296847
1	-5.098719	0.225624	0.322494
6	-0.689559	-1.01597	0.093837
6	-1.782846	-3.968912	-0.163822
6	0.484426	-1.723305	0.010923
6	-0.319824	-4.095997	-0.092186
6	0.644478	-3.128403	-0.03526
8	-2.353853	-5.100194	-0.301084
8	0.091762	-5.377109	-0.134318
1	-0.738032	-5.89616	-0.223863
8	-6.207142	-2.083227	-0.096652
8	-4.592875	-4.132485	-0.303839
1	-6.32449	-3.037551	-0.241157
1	-3.845932	-4.806547	-0.349376
6	-2.5448	1.060524	0.633421
8	-2.027547	1.676357	-0.538214
6	-3.611431	2.003954	1.332437
6	-1.557357	2.96053	-0.415905
6	-2.838643	3.281422	1.753939
6	-1.902987	3.77058	0.678494
6	-1.377811	5.07609	0.692986
6	-0.739839	3.406624	-1.45266
6	-0.549839	5.54742	-0.325009
6	-0.241515	4.707724	-1.398919
8	-1.644983	5.950453	1.707672
8	0.563946	5.109426	-2.4246
1	-2.214105	5.529194	2.363787
1	0.817743	6.031079	-2.284156
8	-4.608972	2.308502	0.472357
1	-1.747134	1.004094	1.388772
6	1.748933	-0.884042	-0.0967
8	2.794696	-1.524721	0.649648
6	2.233554	-0.676362	-1.549651
1	1.412074	-0.270642	-2.1466
6	4.036599	-0.926888	0.603945
6	3.406141	0.316509	-1.524709
1	3.011164	1.335891	-1.400814
6	4.385584	-0.031698	-0.421925
6	4.924694	-1.298115	1.610997
6	5.684269	0.505894	-0.381016
1	4.618642	-1.991933	2.383695
6	6.208408	-0.751223	1.605607
6	6.595188	0.155791	0.615856
8	6.124105	1.395111	-1.319995
1	5.416604	1.578945	-1.95097
1	1.55939	0.104844	0.342606
1	-3.591595	4.042866	2.000794
1	-2.30738	3.04437	2.688323
1	-3.954389	1.451861	2.226729
1	-0.16407	6.560178	-0.262063
1	-0.510085	2.756413	-2.287355
1	7.586819	0.597483	0.601345
1	3.88343	0.27335	-2.513283
1	1.660486	-3.504044	-0.030086
1	-0.540016	0.054957	0.095401
8	2.583371	-1.90569	-2.15997
1	3.285194	-2.307452	-1.627726
8	7.051663	-1.133799	2.607884
1	7.900085	-0.685846	2.494141

*Table S27 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site h-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483361 (Hartree/Particle)
Thermal correction to Energy= 0.518007
Thermal correction to Enthalpy= 0.518951
Thermal correction to Gibbs Free Energy= 0.415754
Sum of electronic and zero-point Energies= -2021.106576
Sum of electronic and thermal Energies= -2021.071930
Sum of electronic and thermal Enthalpies= -2021.070986
Sum of electronic and thermal Free Energies= -2021.174183

#

Coordinates:

6	-2.070764	-1.401906	0.120351
6	-2.573868	-2.749791	-0.063975
6	-3.988814	-2.942403	-0.132063
6	-4.873741	-1.864873	-0.017001
6	-4.385904	-0.584499	0.210868
6	-3.020907	-0.340669	0.296847
1	-5.098719	0.225624	0.322494
6	-0.689559	-1.01597	0.093837
6	-1.782846	-3.968912	-0.163822
6	0.484426	-1.723305	0.010923
6	-0.319824	-4.095997	-0.092186
6	0.644478	-3.128403	-0.03526
8	-2.353853	-5.100194	-0.301084
8	0.091762	-5.377109	-0.134318
1	-0.738032	-5.89616	-0.223863
8	-6.207142	-2.083227	-0.096652
8	-4.592875	-4.132485	-0.303839
1	-6.32449	-3.037551	-0.241157
1	-3.845932	-4.806547	-0.349376
6	-2.5448	1.060524	0.633421
8	-2.027547	1.676357	-0.538214
6	-3.611431	2.003954	1.332437
6	-1.557357	2.96053	-0.415905
6	-2.838643	3.281422	1.753939
6	-1.902987	3.77058	0.678494
6	-1.377811	5.07609	0.692986
6	-0.739839	3.406624	-1.45266
6	-0.549839	5.54742	-0.325009
6	-0.241515	4.707724	-1.398919
8	-1.644983	5.950453	1.707672
8	0.563946	5.109426	-2.4246
1	-2.214105	5.529194	2.363787
1	0.817743	6.031079	-2.284156
8	-4.608972	2.308502	0.472357
1	-1.747134	1.004094	1.388772
6	1.748933	-0.884042	-0.0967
8	2.794696	-1.524721	0.649648
6	2.233554	-0.676362	-1.549651
1	1.412074	-0.270642	-2.1466
6	4.036599	-0.926888	0.603945
6	3.406141	0.316509	-1.524709
1	3.011164	1.335891	-1.400814
6	4.385584	-0.031698	-0.421925
6	4.924694	-1.298115	1.610997
6	5.684269	0.505894	-0.381016
1	4.618642	-1.991933	2.383695
6	6.208408	-0.751223	1.605607
6	6.595188	0.155791	0.615856
8	6.124105	1.395111	-1.319995
1	5.416604	1.578945	-1.95097
1	1.55939	0.104844	0.342606
1	-3.591595	4.042866	2.000794
1	-2.30738	3.04437	2.688323
1	-3.954389	1.451861	2.226729
1	-0.16407	6.560178	-0.262063
1	-0.510085	2.756413	-2.287355
1	7.586819	0.597483	0.601345
1	3.88343	0.27335	-2.513283
1	1.660486	-3.504044	-0.030086
1	-0.540016	0.054957	0.095401
8	2.583371	-1.90569	-2.15997
1	3.285194	-2.307452	-1.627726
8	7.051663	-1.133799	2.607884
1	7.900085	-0.685846	2.494141

*Table S28 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site i-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483624 (Hartree/Particle)
Thermal correction to Energy= 0.518432
Thermal correction to Enthalpy= 0.519376
Thermal correction to Gibbs Free Energy= 0.415479
Sum of electronic and zero-point Energies= -2021.097194
Sum of electronic and thermal Energies= -2021.062386
Sum of electronic and thermal Enthalpies= -2021.061442
Sum of electronic and thermal Free Energies= -2021.165339

Coordinates:

6	2.408192	-1.074236	-0.151834
6	3.122333	-2.310833	-0.063116
6	4.569625	-2.270866	0.168712
6	5.219971	-0.957969	0.225163
6	4.528729	0.227522	0.021133
6	3.160433	0.188934	-0.189847
1	5.060891	1.170646	0.047972
6	0.990478	-0.916379	-0.178426
6	2.563971	-3.650312	-0.207947
6	-0.064351	-1.806324	-0.106374
6	1.102424	-4.001233	-0.186674
6	-0.016805	-3.212121	-0.10628
8	3.27741	-4.663664	-0.336281
8	0.943817	-5.316944	-0.244729
1	1.891934	-5.633791	-0.314353
8	6.522775	-0.996048	0.462888
8	5.341703	-3.234866	0.363374
1	6.694021	-1.971899	0.546329
6	2.446289	1.487814	-0.527357
8	1.679012	1.910605	0.631145
6	3.296506	2.700196	-0.945331
6	0.806405	2.954867	0.381077
6	2.332981	3.781084	-1.476587
6	1.077777	3.886268	-0.631884
6	0.135193	4.913084	-0.815767
6	-0.323417	3.024679	1.191495
6	-1.015644	5.004763	-0.029639
6	-1.236829	4.057588	0.971726
8	0.293071	5.870623	-1.774377
8	-2.351401	4.076898	1.761938
1	1.125863	5.730316	-2.242822
1	-2.899043	4.834925	1.517961
8	4.076321	3.190576	0.13472
1	3.531485	3.114526	0.933472
1	1.743545	1.293504	-1.348722
6	-1.429747	-1.148511	0.035945
8	-2.430898	-1.990436	-0.548644
6	-1.820674	-0.878786	1.508244
1	-1.019489	-0.319531	1.999036
6	-3.727069	-1.518331	-0.476838
6	-3.117816	-0.052455	1.513804
1	-2.873483	1.003328	1.322936
6	-4.108434	-0.579612	0.495535
6	-4.623832	-2.056505	-1.396271
6	-5.453175	-0.169638	0.488784
1	-4.29115	-2.779014	-2.130744
6	-5.954045	-1.635973	-1.355429
6	-6.375966	-0.687269	-0.42042
8	-5.925002	0.752721	1.379181
1	-5.201541	1.060954	1.939947
1	-1.421756	-0.188608	-0.498007
1	2.893335	4.725688	-1.481847
1	2.077974	3.549794	-2.521994
1	3.999923	2.420092	-1.735025
1	-1.716164	5.81257	-0.217361
1	-0.484295	2.295842	1.975911
1	-7.404105	-0.340603	-0.382463
1	-3.525958	-0.108836	2.532272
1	-0.961106	-3.742752	-0.090942
1	0.662497	0.111982	-0.171885
8	-1.943572	-2.090457	2.22913
1	-2.568528	-2.653532	1.74967
8	-6.806626	-2.180697	-2.271083
1	-7.688759	-1.80878	-2.141001

*Table S29 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site b-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482431 (Hartree/Particle)
Thermal correction to Energy= 0.517300
Thermal correction to Enthalpy= 0.518245
Thermal correction to Gibbs Free Energy= 0.414456
Sum of electronic and zero-point Energies= -2021.102340
Sum of electronic and thermal Energies= -2021.067471
Sum of electronic and thermal Enthalpies= -2021.066526
Sum of electronic and thermal Free Energies= -2021.170315

Coordinates:

6	2.32271	-1.130998	-0.148816
6	2.994458	-2.400695	0.040139
6	4.392027	-2.39403	0.281759
6	5.134762	-1.190838	0.265383
6	4.499214	0.017385	0.010421
6	3.125925	0.066941	-0.203936
1	5.090704	0.924669	0.01166
6	0.917011	-0.95119	-0.189757
6	2.390794	-3.737447	-0.019646
6	-0.174761	-1.841753	-0.212316
6	0.987519	-4.084266	-0.53883
6	-0.15035	-3.205958	-0.386317
8	3.062259	-4.743307	0.292784
8	0.843881	-5.211539	-1.00957
8	6.461534	-1.236533	0.493644
8	5.118802	-3.486042	0.52941
1	6.69067	-2.17047	0.645972
1	4.440285	-4.251294	0.525808
6	2.483569	1.399451	-0.554189
8	1.734128	1.869098	0.598952
6	3.402808	2.55814	-0.975781
6	0.932546	2.968306	0.347205
6	2.508352	3.69387	-1.511726
6	1.264017	3.879949	-0.665896
6	0.390895	4.966644	-0.849173
6	-0.189645	3.113536	1.15859
6	-0.74991	5.135368	-0.061521
6	-1.03231	4.205273	0.940676
8	0.610231	5.911354	-1.808784
8	-2.140028	4.300481	1.734339
1	1.43144	5.716683	-2.278198
1	-2.632941	5.096768	1.495735
8	4.210217	3.00291	0.10419
1	3.66265	2.95719	0.903353
1	1.772411	1.238577	-1.375321
6	-1.51868	-1.142195	-0.045539
8	-2.567759	-1.985895	-0.529123
6	-1.826243	-0.791898	1.428662
1	-0.992924	-0.225324	1.853874
6	-3.846437	-1.470625	-0.42695
6	-3.105335	0.062144	1.464071
1	-2.846607	1.104039	1.22107
6	-4.155576	-0.477139	0.515386
6	-4.797152	-2.022707	-1.281002
6	-5.487027	-0.027705	0.548718
1	-4.518515	-2.788393	-1.993934
6	-6.111693	-1.559885	-1.202305
6	-6.463761	-0.557444	-0.29501
8	-5.892717	0.946931	1.415787
1	-5.138033	1.253065	1.935024
1	-1.51509	-0.212582	-0.632901
1	3.126057	4.602107	-1.522563
1	2.238325	3.47344	-2.555682
1	4.088791	2.233203	-1.763834
1	-1.394883	5.988302	-0.248467
1	-0.39855	2.397532	1.943623
1	-7.479085	-0.178815	-0.228003
1	-3.464443	0.053601	2.502245
1	-1.097657	-3.719411	-0.506644
1	0.608084	0.084271	-0.14671
8	-1.93349	-1.968668	2.206357
1	-2.511281	-2.581703	1.728395
8	-7.01975	-2.119003	-2.053745
1	-7.884233	-1.715154	-1.902234

*Table S30 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 3-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481942 (Hartree/Particle)
Thermal correction to Energy= 0.516559
Thermal correction to Enthalpy= 0.517503
Thermal correction to Gibbs Free Energy= 0.414182
Sum of electronic and zero-point Energies= -2021.076334
Sum of electronic and thermal Energies= -2021.041717
Sum of electronic and thermal Enthalpies= -2021.040773
Sum of electronic and thermal Free Energies= -2021.144094

Coordinates:

6	-2.232879	-1.202143	0.144838
6	-2.81677	-2.521501	-0.004384
6	-4.241285	-2.63371	-0.012048
6	-5.058487	-1.502638	0.10492
6	-4.491822	-0.245127	0.266125
6	-3.112209	-0.079957	0.31071
1	-5.153378	0.609563	0.335311
6	-0.830593	-0.906206	0.115993
6	-2.101046	-3.784686	-0.143504
6	0.292785	-1.682299	-0.020439
6	-0.644223	-3.997892	-0.193579
6	0.375967	-3.089361	-0.152775
8	-2.744206	-4.879564	-0.242093
8	-0.315091	-5.295548	-0.31847
1	-1.176996	-5.765958	-0.351096
8	-6.403573	-1.645488	0.070429
8	-4.920542	-3.787826	-0.139304
1	-6.58013	-2.59482	-0.044758
1	-4.21644	-4.504395	-0.210951
6	-2.552929	1.305055	0.590681
8	-1.915461	1.798019	-0.619148
6	-3.529892	2.402855	1.043044
6	-1.187683	2.960859	-0.449513
6	-2.697342	3.62256	1.485784
6	-1.527184	3.87755	0.556596
6	-0.735954	5.035444	0.651072
6	-0.131825	3.16519	-1.334497
6	0.334029	5.268204	-0.215394
6	0.62816	4.32953	-1.206509
8	-0.97104	5.991836	1.596126
8	1.668448	4.490389	-2.076683
1	-1.744089	5.748187	2.121168
1	2.104999	5.33298	-1.894386
8	-4.440893	2.747903	0.010217
1	-3.951759	2.696659	-0.82563
1	-1.781363	1.225128	1.369044
6	1.60454	-0.932989	-0.093838
8	2.560623	-1.587826	0.705358
6	2.128175	-0.765613	-1.605893
1	1.318062	-0.210154	-2.115918
6	3.86472	-1.160107	0.637027
6	3.403394	0.110445	-1.513412
1	3.078177	1.155544	-1.39654
6	4.318919	-0.329648	-0.400486
6	4.700483	-1.627487	1.648836
6	5.679246	0.029244	-0.374031
1	4.311222	-2.270201	2.428086
6	6.042495	-1.250884	1.633811
6	6.539377	-0.416464	0.62848
8	6.229167	0.83755	-1.328694
1	5.551511	1.093987	-1.966834
1	1.473352	0.102486	0.248438
1	-3.384565	4.479175	1.510175
1	-2.345868	3.46013	2.516159
1	-4.132355	2.051977	1.886488
1	0.916218	6.17701	-0.098209
1	0.088373	2.437914	-2.10618
1	7.57952	-0.106328	0.605349
1	3.903889	0.039209	-2.489129
1	1.371738	-3.512798	-0.231296
1	-0.60918	0.149394	0.168172
8	2.359176	-1.981613	-2.118106
8	6.833777	-1.72102	2.641211
1	7.734972	-1.398533	2.510095

*Table S31 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 5-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482740 (Hartree/Particle)
Thermal correction to Energy= 0.517372
Thermal correction to Enthalpy= 0.518316
Thermal correction to Gibbs Free Energy= 0.414529
Sum of electronic and zero-point Energies= -2021.106940
Sum of electronic and thermal Energies= -2021.072308
Sum of electronic and thermal Enthalpies= -2021.071364
Sum of electronic and thermal Free Energies= -2021.175151

Coordinates:

6	-2.211613	-1.226224	0.151747
6	-2.784385	-2.55056	-0.001242
6	-4.208336	-2.674318	-0.029613
6	-5.035315	-1.551061	0.074359
6	-4.480568	-0.288903	0.244716
6	-3.103672	-0.111579	0.307435
1	-5.149829	0.560357	0.307584
6	-0.811642	-0.916889	0.135446
6	-2.057221	-3.808005	-0.116877
6	0.323435	-1.679608	0.013426
6	-0.600828	-4.005813	-0.127703
6	0.411512	-3.088021	-0.090263
8	-2.688355	-4.911482	-0.217227
8	-0.254766	-5.30461	-0.2171
1	-1.113501	-5.780584	-0.263548
8	-6.379692	-1.704255	0.022076
8	-4.87534	-3.836018	-0.162721
1	-6.545832	-2.655193	-0.094708
1	-4.163176	-4.546294	-0.217834
6	-2.561008	1.278167	0.593733
8	-1.931998	1.785756	-0.61439
6	-3.549854	2.361548	1.055719
6	-1.223524	2.96028	-0.442569
6	-2.729412	3.585743	1.508056
6	-1.568504	3.863716	0.573989
6	-0.794684	5.03321	0.670372
6	-0.181237	3.190275	-1.33676
6	0.26249	5.290979	-0.204483
6	0.560679	4.36645	-1.208097
8	-1.036294	5.977854	1.626339
8	1.583743	4.551455	-2.09115
1	-1.802621	5.71834	2.153581
1	2.027921	5.38684	-1.895044
8	-4.464913	2.707248	0.026501
1	-3.976196	2.666211	-0.810163
1	-1.787115	1.203969	1.370282
6	1.626665	-0.901182	-0.075718
8	2.635791	-1.610807	0.67412
6	2.124095	-0.670705	-1.52301
1	1.3259	-0.177421	-2.084874
6	3.91492	-1.126421	0.582275
6	3.369476	0.223883	-1.476532
1	3.078049	1.266295	-1.288065
6	4.321911	-0.250541	-0.412994
6	4.811069	-1.603561	1.557844
6	5.715465	0.197274	-0.426503
1	4.462239	-2.291735	2.319054
6	6.163058	-1.183008	1.552244
6	6.614068	-0.299886	0.597993
8	6.116528	0.986885	-1.313249
1	1.487115	0.08335	0.389803
1	-3.426088	4.434287	1.545229
1	-2.37092	3.416102	2.534927
1	-4.14815	1.996543	1.89615
1	0.830042	6.208867	-0.086663
1	0.043025	2.474552	-2.117995
1	7.642143	0.047862	0.565873
1	3.866451	0.22493	-2.451102
1	1.406493	-3.512664	-0.143208
1	-0.6035	0.14211	0.182382
8	2.359522	-1.898447	-2.194574
1	3.128121	-2.320858	-1.786278
8	6.941703	-1.703696	2.54117
1	7.839769	-1.35637	2.454316

*Table S32 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 7-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482935 (Hartree/Particle)
Thermal correction to Energy= 0.517467
Thermal correction to Enthalpy= 0.518411
Thermal correction to Gibbs Free Energy= 0.415870
Sum of electronic and zero-point Energies= -2021.101702
Sum of electronic and thermal Energies= -2021.067170
Sum of electronic and thermal Enthalpies= -2021.066226
Sum of electronic and thermal Free Energies= -2021.168767

Coordinates:

6	-2.411367	-0.901663	0.162634
6	-3.203443	-2.10982	0.038163
6	-4.625608	-1.983031	-0.028706
6	-5.24381	-0.728346	0.010861
6	-4.479684	0.423271	0.158147
6	-3.095479	0.357696	0.257377
1	-4.990564	1.378343	0.175584
6	-0.980071	-0.842233	0.161952
6	-2.703777	-3.47778	-0.008407
6	0.007879	-1.792344	0.085297
6	-1.302347	-3.926006	0.031757
6	-0.14468	-3.197482	0.048876
8	-3.514458	-4.458007	-0.082966
8	-1.187494	-5.266625	0.012051
1	-2.114752	-5.589643	-0.035949
8	-6.591819	-0.644614	-0.078704
8	-5.483033	-3.014219	-0.141677
1	-6.922118	-1.554862	-0.167437
1	-4.908133	-3.840283	-0.14593
6	-2.318791	1.633561	0.529233
8	-1.556355	1.980788	-0.662153
6	-3.100439	2.90005	0.913673
6	-0.613893	2.968747	-0.452742
6	-2.07875	3.96452	1.36975
6	-0.820303	3.953404	0.523707
6	0.193814	4.91453	0.677703
6	0.524321	2.925118	-1.254726
6	1.354842	4.890845	-0.099111
6	1.51193	3.892502	-1.061679
8	0.101503	5.91528	1.599946
8	2.636169	3.793973	-1.835388
1	-0.744922	5.8575	2.061531
1	3.232135	4.523651	-1.619524
8	-3.890244	3.370128	-0.167739
1	-3.380017	3.210395	-0.977018
1	-1.601766	1.443044	1.339578
6	1.416242	-1.229865	-0.0406
8	2.354635	-2.12794	0.578096
6	1.870195	-1.016544	-1.499822
1	1.127629	-0.412975	-2.028286
6	3.667984	-1.705938	0.582595
6	3.218992	-0.274015	-1.477521
1	3.038461	0.803655	-1.339782
6	4.138073	-0.792922	-0.397636
6	4.501999	-2.236087	1.541326
6	5.502282	-0.386224	-0.343801
1	4.130147	-2.937482	2.278496
6	5.899176	-1.851954	1.582424
6	6.364801	-0.894506	0.601865
8	5.996799	0.51356	-1.242945
1	5.291206	0.833716	-1.819283
1	1.461284	-0.263957	0.479437
1	-2.59154	4.934249	1.314904
1	-1.830178	3.789232	2.427649
1	-3.790988	2.688635	1.735688
1	2.113449	5.649425	0.067234
1	0.63334	2.159109	-2.012379
1	7.402804	-0.585479	0.629346
1	3.677049	-0.396456	-2.468542
1	0.761377	-3.792427	0.049171
1	-0.592244	0.165484	0.168314
8	1.942795	-2.244507	-2.198754
1	2.440633	-2.866921	-1.648608
8	6.67365	-2.325427	2.452766

*Table S33 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 4'α-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482741 (Hartree/Particle)
Thermal correction to Energy= 0.517668
Thermal correction to Enthalpy= 0.518612
Thermal correction to Gibbs Free Energy= 0.415282
Sum of electronic and zero-point Energies= -2021.099894
Sum of electronic and thermal Energies= -2021.064967
Sum of electronic and thermal Enthalpies= -2021.064023
Sum of electronic and thermal Free Energies= -2021.167354

Coordinates:

6	-2.391475	-0.971732	0.142422
6	-3.111998	-2.225245	0.020244
6	-4.540996	-2.186302	-0.003651
6	-5.233167	-0.974672	0.081806
6	-4.538439	0.220496	0.221264
6	-3.149899	0.243544	0.269573
1	-5.104214	1.14191	0.276844
6	-0.965549	-0.829583	0.122749
6	-2.533306	-3.559767	-0.065532
6	0.075846	-1.71979	0.027851
6	-1.109345	-3.925422	-0.056952
6	0.003116	-3.130722	-0.03421
8	-3.286635	-4.5857	-0.14751
8	-0.916203	-5.257308	-0.108628
1	-1.824322	-5.631391	-0.150116
8	-6.587157	-0.975251	0.040936
8	-5.337035	-3.266993	-0.111844
1	-6.860245	-1.903849	-0.051767
1	-4.71101	-4.054732	-0.154497
6	-2.445245	1.562675	0.533861
8	-1.726329	1.963849	-0.673168
6	-3.268376	2.777955	0.996744
6	-0.81673	2.969727	-0.470322
6	-2.313052	3.916854	1.224894
6	-1.095921	3.967648	0.515679
6	-0.105691	4.986224	0.676347
6	0.313061	2.999252	-1.26809
6	1.037558	5.021599	-0.112032
6	1.240775	4.034769	-1.085029
8	-0.249754	5.965667	1.609902
8	2.355514	4.007857	-1.871093
1	-0.963779	5.725018	2.21545
1	2.914001	4.767198	-1.656723
8	-4.30105	3.154677	0.074557
1	-3.870222	3.28245	-0.784141
1	-1.696321	1.402261	1.321409
6	1.456822	-1.090054	-0.082667
8	2.407435	-1.915486	0.608689
6	1.940905	-0.905164	-1.53837
1	1.18005	-0.359806	-2.103585
6	3.717035	-1.483771	0.577138
6	3.251906	-0.101659	-1.509928
1	3.019915	0.965419	-1.374783
6	4.175808	-0.606633	-0.419924
6	4.552366	-1.998767	1.566014
6	5.531314	-0.237756	-0.367051
1	4.161894	-2.67308	2.317674
6	5.895031	-1.619014	1.571681
6	6.392402	-0.733438	0.612137
8	6.075031	0.622621	-1.278988
1	5.392191	0.907624	-1.899701
1	1.43782	-0.102049	0.396497
1	-2.672663	4.759909	1.807852
1	-3.795787	2.523228	1.922271
1	1.764983	5.810014	0.055959
1	0.470713	2.243843	-2.028031
1	7.431836	-0.41998	0.60781
1	3.711439	-0.206969	-2.502525
1	0.942882	-3.669424	-0.057952
1	-0.634982	0.197937	0.144881
8	2.086482	-2.152234	-2.194646
1	2.694563	-2.689962	-1.66695
8	6.684706	-2.13975	2.555772
1	7.582665	-1.798658	2.452422

*Table S34 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 4'β-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482742 (Hartree/Particle)
Thermal correction to Energy= 0.517669
Thermal correction to Enthalpy= 0.518613
Thermal correction to Gibbs Free Energy= 0.415284
Sum of electronic and zero-point Energies= -2021.099893
Sum of electronic and thermal Energies= -2021.064967
Sum of electronic and thermal Enthalpies= -2021.064022
Sum of electronic and thermal Free Energies= -2021.167351

Coordinates:

6	-2.391562	-0.971542	0.142495
6	-3.112243	-2.224924	0.020273
6	-4.541252	-2.185828	-0.003079
6	-5.233266	-0.974131	0.082822
6	-4.538341	0.220932	0.222103
6	-3.149767	0.243818	0.269966
1	-5.104022	1.142396	0.277821
6	-0.965654	-0.829565	0.122709
6	-2.53376	-3.55947	-0.066296
6	0.075603	-1.719876	0.027474
6	-1.109875	-3.925321	-0.058225
6	0.002691	-3.130764	-0.035181
8	-3.287275	-4.585257	-0.148606
8	-0.916917	-5.257202	-0.110685
1	-1.825103	-5.631131	-0.152174
8	-6.587263	-0.974549	0.042439
8	-5.337438	-3.26642	-0.111207
1	-6.860492	-1.903097	-0.050381
1	-4.711494	-4.054225	-0.154628
6	-2.444886	1.562844	0.53411
8	-1.726162	1.963881	-0.673126
6	-3.267719	2.77827	0.997164
6	-0.816364	2.969612	-0.47051
6	-2.312202	3.917066	1.224951
6	-1.095258	3.967714	0.515424
6	-0.104891	4.986216	0.675708
6	0.31331	2.998897	-1.268447
6	1.038205	5.021372	-0.112893
6	1.241146	4.034362	-1.085761
8	-0.248601	5.965767	1.609208
8	2.355719	4.007227	-1.872068
1	-0.962756	5.725445	2.214722
1	2.914421	4.766433	-1.657775
8	-4.300697	3.155003	0.075347
1	-3.870137	3.283036	-0.783444
1	-1.695779	1.402334	1.321458
6	1.45666	-1.090277	-0.082728
8	2.407144	-1.916079	0.608408
6	1.940935	-0.904926	-1.538317
1	1.180195	-0.359335	-2.103462
6	3.716741	-1.484332	0.577262
6	3.251988	-0.101519	-1.509433
1	3.020044	0.965536	-1.374018
6	4.17568	-0.606841	-0.419412
6	4.551902	-1.999644	1.566118
6	5.531163	-0.237929	-0.366151
1	4.161311	-2.674219	2.317482
6	5.894554	-1.619853	1.572164
6	6.392079	-0.73392	0.613028
8	6.075024	0.622767	-1.277704
1	5.392241	0.908124	-1.898317
1	1.437756	-0.10245	0.396799
1	-2.671645	4.760204	1.807909
1	-3.794844	2.523665	1.922894
1	1.765707	5.809779	0.054806
1	0.470739	2.243395	-2.028347
1	7.431502	-0.42042	0.60902
1	3.711681	-0.206587	-2.501981
1	0.94237	-3.669598	-0.059252
1	-0.634979	0.197906	0.145171
8	2.086529	-2.151788	-2.194993
1	2.694555	-2.689697	-1.667417
8	6.684061	-2.140903	2.556226
1	7.582028	-1.799741	2.453168

*Table S35 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 3'-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482776 (Hartree/Particle)
Thermal correction to Energy= 0.517774
Thermal correction to Enthalpy= 0.518719
Thermal correction to Gibbs Free Energy= 0.414779
Sum of electronic and zero-point Energies= -2021.082742
Sum of electronic and thermal Energies= -2021.047744
Sum of electronic and thermal Enthalpies= -2021.046799
Sum of electronic and thermal Free Energies= -2021.150739

Coordinates:

6	-2.316428	-1.102635	0.159947
6	-2.978632	-2.384941	0.005288
6	-4.404126	-2.433758	0.110076
6	-5.147501	-1.28179	0.381102
6	-4.507733	-0.055521	0.512859
6	-3.128209	0.064374	0.376481
1	-5.124874	0.80328	0.748533
6	-0.898344	-0.896909	0.161638
6	-2.341903	-3.673161	-0.245161
6	0.179513	-1.725349	-0.033822
6	-0.90677	-3.95894	-0.366957
6	0.167958	-3.117879	-0.278019
8	-3.050325	-4.725438	-0.380316
8	-0.653821	-5.261625	-0.595782
1	-1.541978	-5.681158	-0.621122
8	-6.492992	-1.365274	0.507865
8	-5.147449	-3.547768	-0.017085
1	-6.725547	-2.300757	0.378689
1	-4.485444	-4.287749	-0.197167
6	-2.517308	1.445193	0.582667
8	-1.650744	1.76802	-0.561774
6	-3.443348	2.616751	0.733114
6	-0.945844	2.940326	-0.409045
6	-2.720889	3.856933	1.182549
6	-1.389031	3.968587	0.44275
6	-0.57489	5.108555	0.547312
6	0.235819	3.043065	-1.14275
6	0.620955	5.229754	-0.163619
6	1.014801	4.192536	-1.010536
8	-0.912664	6.160676	1.350333
8	2.180203	4.237283	-1.725872
1	-1.758965	5.984191	1.780202
1	2.619583	5.081274	-1.557361
8	-4.324026	2.877053	-0.290555
1	-4.455631	2.077246	-0.820816
1	-1.875097	1.426856	1.475428
6	1.533214	-1.032059	-0.056167
8	2.508369	-1.882748	0.566242
6	2.027329	-0.682328	-1.478876
1	1.247998	-0.121959	-2.002128
6	3.801029	-1.401865	0.590982
6	3.296577	0.17384	-1.345216
1	3.010762	1.207279	-1.09896
6	4.231702	-0.40686	-0.303242
6	4.650847	-1.988998	1.525965
6	5.572193	0.004103	-0.199436
1	4.282404	-2.753608	2.198094
6	5.978483	-1.563464	1.582991
6	6.446658	-0.56229	0.728139
8	6.088367	0.975071	-1.010179
1	5.39282	1.320553	-1.584388
1	1.464455	-0.098501	0.518042
1	-3.364306	4.720906	0.970766
1	-2.559541	3.824755	2.271086
1	1.215547	6.1302	-0.044206
1	0.537942	2.243423	-1.807139
1	7.473379	-0.211563	0.766975
1	3.771328	0.199808	-2.335713
1	1.129836	-3.601391	-0.397253
1	-0.615	0.132169	0.318273
8	2.243306	-1.850947	-2.250949
1	2.907646	-2.384774	-1.791578
8	6.782833	-2.157826	2.512007
1	7.667489	-1.773902	2.45419

*Table S36 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 2'-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481877 (Hartree/Particle)
Thermal correction to Energy= 0.517247
Thermal correction to Enthalpy= 0.518191
Thermal correction to Gibbs Free Energy= 0.412723
Sum of electronic and zero-point Energies= -2021.103151
Sum of electronic and thermal Energies= -2021.067781
Sum of electronic and thermal Enthalpies= -2021.066837
Sum of electronic and thermal Free Energies= -2021.172305

Coordinates:

6	2.074695	-1.41536	-0.110047
6	2.549933	-2.773722	0.087356
6	3.922115	-3.058633	-0.162443
6	4.814699	-2.052602	-0.586067
6	4.39604	-0.744669	-0.677008
6	3.054778	-0.375069	-0.410413
1	5.147922	0.012128	-0.863842
6	0.708202	-1.026365	-0.165988
6	1.757989	-3.913362	0.535854
6	-0.474068	-1.669198	0.140893
6	0.322071	-3.946644	0.818232
6	-0.633527	-2.982557	0.627872
8	2.315924	-5.044316	0.738188
8	-0.093536	-5.143592	1.279723
1	0.720149	-5.69404	1.289763
8	6.107406	-2.381496	-0.821706
8	4.493121	-4.267879	-0.02208
1	6.190063	-3.33125	-0.630094
1	3.755811	-4.867195	0.324393
6	2.780907	1.025712	-0.436179
8	1.778803	1.504687	0.383513
6	3.63972	2.038595	-1.141856
6	1.414526	2.832572	0.386873
6	2.775079	3.188645	-1.685875
6	1.869798	3.715779	-0.601118
6	1.423325	5.045587	-0.518965
6	0.569087	3.220132	1.424076
6	0.57224	5.468467	0.504905
6	0.149571	4.551428	1.47009
8	1.786662	5.991699	-1.43105
8	-0.68253	4.904058	2.491797
1	2.360533	5.596868	-2.100227
1	-0.871988	5.849819	2.434088
8	4.713569	2.540693	-0.331024
1	4.327719	2.917259	0.47288
6	-1.730302	-0.824885	0.00254
8	-2.801541	-1.656898	-0.471851
6	-2.179735	-0.149219	1.317944
1	-1.340522	0.414236	1.734345
6	-4.033808	-1.05377	-0.602587
6	-3.3431	0.801901	0.995643
1	-2.940015	1.720322	0.543426
6	-4.349756	0.132826	0.081716
6	-4.949168	-1.714673	-1.419131
6	-5.642323	0.651772	-0.109557
1	-4.668736	-2.627462	-1.929335
6	-6.22545	-1.171619	-1.570392
6	-6.579554	0.014854	-0.923059
8	-6.048952	1.806444	0.497719
1	-5.326621	2.163422	1.030008
1	-1.546939	-0.034738	-0.738588
1	3.470558	3.955432	-2.050904
1	2.199138	2.832971	-2.552411
1	4.137199	1.549015	-1.980617
1	0.252547	6.505683	0.525279
1	0.263663	2.512689	2.184694
1	-7.565188	0.45576	-1.036157
1	-3.798588	1.088522	1.953632
1	-1.643013	-3.302127	0.856375
1	0.567167	-0.014631	-0.51861
8	-2.527953	-1.108047	2.301098
1	-3.243163	-1.650796	1.938785
8	-7.095489	-1.842994	-2.379773
1	-7.935483	-1.366314	-2.403188

*Table S37 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 4β-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482854 (Hartree/Particle)
Thermal correction to Energy= 0.517693
Thermal correction to Enthalpy= 0.518637
Thermal correction to Gibbs Free Energy= 0.414933
Sum of electronic and zero-point Energies= -2021.100862
Sum of electronic and thermal Energies= -2021.066023
Sum of electronic and thermal Enthalpies= -2021.065079
Sum of electronic and thermal Free Energies= -2021.168783

Coordinates:

6	-2.23886	-1.146989	0.140783
6	-2.905709	-2.428233	0.000563
6	-4.335155	-2.451075	-0.012876
6	-5.079571	-1.273257	0.105679
6	-4.435204	-0.054844	0.276223
6	-3.047965	0.026285	0.316172
1	-5.042045	0.838277	0.361724
6	-0.821442	-0.935452	0.087983
6	-2.271315	-3.735283	-0.111077
6	0.254444	-1.780933	-0.020914
6	-0.833803	-4.038468	-0.100576
6	0.240876	-3.194631	-0.078142
8	-2.980155	-4.790866	-0.210925
8	-0.581669	-5.360893	-0.15755
1	-1.472	-5.774099	-0.207701
8	-6.432447	-1.331655	0.071879
8	-5.084075	-3.562705	-0.139153
1	-6.665791	-2.26857	-0.04315
1	-4.424269	-4.321342	-0.20356
6	-2.408126	1.373155	0.609375
8	-1.802936	1.877944	-0.612344
6	-3.313614	2.494985	1.146055
6	-1.054574	3.030341	-0.46151
6	-2.40726	3.654352	1.598694
6	-1.30163	3.919077	0.596428
6	-0.498028	5.070427	0.659141
6	-0.078472	3.261955	-1.428114
6	0.492329	5.329	-0.289765
6	0.690895	4.42295	-1.333945
8	-0.647607	5.997708	1.650486
8	1.64351	4.618391	-2.292804
1	-1.367911	5.73236	2.236403
1	2.090361	5.458383	-2.124575
8	-4.247616	2.930385	0.168273
1	-3.799778	2.883352	-0.690503
1	-1.607545	1.233199	1.348235
6	1.611657	-1.106563	-0.142442
8	2.580306	-1.890933	0.58382
6	2.079983	-0.909572	-1.601554
1	1.383473	-0.210576	-2.078745
6	3.850475	-1.381428	0.60875
6	3.4713	-0.357136	-1.592504
6	4.308406	-0.574656	-0.482032
6	4.663384	-1.72921	1.672282
6	5.645515	-0.076823	-0.378211
1	4.287549	-2.356973	2.470553
6	5.983134	-1.256422	1.697429
6	6.47034	-0.420064	0.682977
8	6.1624	0.743916	-1.334878
1	5.440762	1.087442	-1.878921
1	1.563717	-0.111403	0.31917
1	-3.055674	4.532983	1.717835
1	-1.992102	3.419922	2.590816
1	-3.897345	2.134037	1.998359
1	1.085752	6.233464	-0.197381
1	0.072877	2.558453	-2.237412
1	7.478816	-0.018886	0.715055
1	3.845959	0.072769	-2.517069
1	1.204122	-3.690345	-0.105925
1	-0.540448	0.108358	0.093948
8	1.976441	-2.108464	-2.378088
1	2.703295	-2.685757	-2.103995
8	6.749715	-1.624069	2.761041
1	7.629232	-1.234065	2.669554

*Table S38 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 4α-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482852 (Hartree/Particle)
Thermal correction to Energy= 0.517690
Thermal correction to Enthalpy= 0.518634
Thermal correction to Gibbs Free Energy= 0.414937
Sum of electronic and zero-point Energies= -2021.100865
Sum of electronic and thermal Energies= -2021.066027
Sum of electronic and thermal Enthalpies= -2021.065083
Sum of electronic and thermal Free Energies= -2021.168779

Coordinates:

6	-2.239203	-1.146496	0.141144
6	-2.906326	-2.42763	0.000896
6	-4.335782	-2.450243	-0.012343
6	-5.079931	-1.272236	0.106013
6	-4.435339	-0.053921	0.276359
6	-3.048084	0.026945	0.316402
1	-5.042019	0.839335	0.361595
6	-0.821688	-0.935316	0.088606
6	-2.272284	-3.734793	-0.111031
6	0.253941	-1.781045	-0.020827
6	-0.834851	-4.038301	-0.101662
6	0.240003	-3.194701	-0.079108
8	-2.981523	-4.790193	-0.210389
8	-0.582939	-5.36074	-0.159548
1	-1.473316	-5.773851	-0.209063
8	-6.432835	-1.330399	0.072247
8	-5.084748	-3.561788	-0.13842
1	-6.666331	-2.267287	-0.042682
1	-4.424772	-4.32053	-0.20271
6	-2.408013	1.373689	0.609487
8	-1.802054	1.877925	-0.612152
6	-3.31347	2.495967	1.145317
6	-1.053345	3.030087	-0.461275
6	-2.407148	3.655419	1.597802
6	-1.300813	3.919368	0.596108
6	-0.496874	5.070478	0.658844
6	-0.076541	3.260959	-1.427345
6	0.49423	5.328284	-0.289503
6	0.693172	4.421728	-1.333163
8	-0.646827	5.99827	1.649643
8	1.646541	4.616385	-2.291438
1	-1.367363	5.73324	2.23542
1	2.09335	5.456452	-2.12347
8	-4.247074	2.930978	0.167002
1	-3.799007	2.883176	-0.691612
1	-1.607777	1.233765	1.348727
6	1.611337	-1.106891	-0.141952
8	2.580039	-1.892116	0.583228
6	2.079216	-0.908442	-1.600992
1	1.382766	-0.208692	-2.077157
6	3.850216	-1.382563	0.608561
6	3.470752	-0.356471	-1.591844
1	3.845254	0.074255	-2.516095
6	4.308037	-0.574955	-0.481658
6	4.663175	-1.731173	1.671766
6	5.645171	-0.077321	-0.377646
1	4.287338	-2.359569	2.469533
6	5.982963	-1.258438	1.697138
6	6.47007	-0.421351	0.683255
8	6.162034	0.743962	-1.333853
1	5.440293	1.088348	-1.877236
1	1.563675	-0.112191	0.320683
1	-3.055423	4.53427	1.716086
1	-1.99264	3.421437	2.590304
1	-3.897587	2.13554	1.997577
1	1.087938	6.232558	-0.197079
1	0.075055	2.557111	-2.236297
1	7.478577	-0.02026	0.715472
1	1.20315	-3.690573	-0.107516
1	-0.540339	0.1084	0.095263
8	1.975092	-2.106392	-2.378899
1	2.701772	-2.684263	-2.105565
8	6.749627	-1.626838	2.760414
1	7.629194	-1.236917	2.669047

*Table S39 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 3-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482875 (Hartree/Particle)
Thermal correction to Energy= 0.517811
Thermal correction to Enthalpy= 0.518755
Thermal correction to Gibbs Free Energy= 0.414778
Sum of electronic and zero-point Energies= -2021.087435
Sum of electronic and thermal Energies= -2021.052498
Sum of electronic and thermal Enthalpies= -2021.051554
Sum of electronic and thermal Free Energies= -2021.155531

Coordinates:

6	2.348452	-1.039779	-0.190814
6	3.041704	-2.307239	-0.045593
6	4.469975	-2.295295	0.006796
6	5.186688	-1.095535	-0.054569
6	4.516756	0.113276	-0.20359
6	3.131824	0.160103	-0.296124
1	5.103373	1.023279	-0.223347
6	0.927355	-0.866896	-0.209483
6	2.434434	-3.628381	0.049489
6	-0.134362	-1.733298	-0.10802
6	1.000662	-3.962218	0.061849
6	-0.096015	-3.142722	0.013846
8	3.164126	-4.669269	0.14246
8	0.779092	-5.284826	0.161272
1	1.678968	-5.679842	0.198673
8	6.537446	-1.119754	0.023515
8	5.244102	-3.389895	0.130687
1	6.794244	-2.052625	0.120571
1	4.606113	-4.166852	0.161805
6	2.461087	1.497669	-0.563819
8	1.694913	1.873387	0.612068
6	3.352443	2.706935	-0.891164
6	0.834234	2.935779	0.403412
6	2.436582	3.86747	-1.335476
6	1.157038	3.936376	-0.524559
6	0.229565	4.981176	-0.675196
6	-0.336979	2.944925	1.155212
6	-0.95722	5.021528	0.060228
6	-1.234267	3.997967	0.968621
8	0.436902	6.006153	-1.553029
8	-2.39263	3.963018	1.695021
1	1.296907	5.899638	-1.97928
1	-2.930224	4.733391	1.468107
8	4.150693	3.074191	0.223614
1	3.605167	2.936639	1.013843
1	1.757921	1.378403	-1.400357
6	-1.504569	-1.06372	-0.036769
8	-2.496635	-1.972943	-0.584535
6	-1.893104	-0.635373	1.348955
6	-3.797471	-1.531319	-0.511078
6	-3.239695	0.019494	1.446545
1	-3.136403	1.109711	1.311931
6	-4.203492	-0.557273	0.418292
6	-4.688884	-2.115486	-1.410544
6	-5.552626	-0.167301	0.389617
1	-4.343993	-2.860458	-2.116441
6	-6.024831	-1.715311	-1.390828
6	-6.465758	-0.73393	-0.499566
8	-6.040914	0.781365	1.245767
1	-5.325716	1.11132	1.804275
1	-1.502316	-0.168813	-0.673655
1	3.028811	4.787295	-1.236049
1	2.204122	3.747703	-2.404809
1	4.04438	2.465087	-1.703738
1	-1.644397	5.847152	-0.097626
1	-0.552469	2.138181	1.844911
1	-7.500052	-0.40438	-0.476305
1	-3.612139	-0.139946	2.46731
1	-1.053118	-3.652996	0.047655
1	0.614378	0.165004	-0.258387
8	-1.587271	-1.439716	2.41612
1	-0.754763	-1.901938	2.234481
8	-6.867536	-2.311598	-2.286126
1	-7.75424	-1.945543	-2.172264

*Table S40 Energetics and Cartesian coordinates of the conformer **1b** (sa-ass-sa) post-radical capture via HAB at site 2-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483197 (Hartree/Particle)
Thermal correction to Energy= 0.518108
Thermal correction to Enthalpy= 0.519052
Thermal correction to Gibbs Free Energy= 0.416357
Sum of electronic and zero-point Energies= -2021.108841
Sum of electronic and thermal Energies= -2021.073931
Sum of electronic and thermal Enthalpies= -2021.072987
Sum of electronic and thermal Free Energies= -2021.175682

Coordinates:

6	2.112013	-1.420032	-0.059456
6	2.626113	-2.781409	0.020192
6	4.010775	-2.972049	0.308115
6	4.871609	-1.883596	0.494272
6	4.399342	-0.586221	0.324011
6	3.067188	-0.336218	0.024983
1	5.100927	0.231433	0.436442
6	0.750249	-1.037705	-0.133172
6	1.870397	-3.998624	-0.202113
6	-0.454895	-1.754926	-0.298789
6	0.439872	-4.109633	-0.552546
6	-0.535499	-3.164726	-0.570718
8	2.438862	-5.137328	-0.143046
8	0.076515	-5.381809	-0.831801
1	0.893003	-5.905788	-0.685128
8	6.175384	-2.103267	0.791617
8	4.607315	-4.172112	0.425369
1	6.291165	-3.067763	0.831735
1	3.884558	-4.847449	0.232646
6	2.65849	1.082654	-0.338443
8	1.865044	1.669244	0.732387
6	3.791929	2.083227	-0.628381
6	1.298676	2.895673	0.425574
6	3.169027	3.351314	-1.236639
6	1.896933	3.747862	-0.516576
6	1.264086	4.979708	-0.75284
6	0.132597	3.229166	1.112521
6	0.09529	5.345454	-0.083833
6	-0.463261	4.463629	0.843879
8	1.757752	5.880588	-1.653599
8	-1.621697	4.754948	1.509424
1	2.58294	5.545587	-2.02706
1	-1.899401	5.650269	1.274987
8	4.52338	2.393177	0.549875
1	3.887276	2.393483	1.282115
1	2.021332	1.037503	-1.232782
6	-1.679767	-1.047971	-0.206123
8	-2.814803	-1.815089	-0.298829
6	-1.855235	0.406291	0.142232
1	-0.986961	0.97698	-0.182637
6	-4.07975	-1.277943	-0.189343
6	-3.099029	0.99296	-0.539822
1	-2.905774	1.104583	-1.616402
6	-4.289487	0.104097	-0.286235
6	-5.107972	-2.193838	0.007683
6	-5.615255	0.555431	-0.176648
1	-4.902521	-3.254101	0.081012
6	-6.412402	-1.704908	0.110275
6	-6.672686	-0.334824	0.024184
8	-5.942937	1.876363	-0.266764
1	-5.142543	2.400384	-0.400507
1	3.931672	4.139303	-1.168679
1	2.974306	3.179913	-2.30646
1	4.505728	1.652386	-1.336826
1	-0.357741	6.307508	-0.303614
1	-0.316391	2.535649	1.813305
1	-7.681282	0.058994	0.102571
1	-3.2298	2.001448	-0.127111
1	-1.520221	-3.55574	-0.795833
1	0.608999	0.014532	0.048119
8	-1.901199	0.604498	1.561814
1	-2.708415	0.185695	1.89515
8	-7.402948	-2.6214	0.302072
1	-8.252297	-2.164374	0.359343

*Table S41 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 5'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482889 (Hartree/Particle)
Thermal correction to Energy= 0.517257
Thermal correction to Enthalpy= 0.518201
Thermal correction to Gibbs Free Energy= 0.418331
Sum of electronic and zero-point Energies= -2021.087146
Sum of electronic and thermal Energies= -2021.052777
Sum of electronic and thermal Enthalpies= -2021.051833
Sum of electronic and thermal Free Energies= -2021.151704

Coordinates:

6	2.619151	-0.006228	-0.084992
6	3.92532	0.593268	-0.220262
6	5.037292	-0.265226	-0.459796
6	4.881466	-1.659459	-0.495041
6	3.635826	-2.229178	-0.270949
6	2.514548	-1.431046	-0.059815
1	3.545282	-3.308166	-0.280437
6	1.377827	0.724936	-0.112993
6	4.269483	2.017699	-0.08495
6	1.082096	2.042061	0.09836
6	3.362653	3.045692	0.473021
6	1.99841	3.059374	0.499767
8	5.43031	2.416824	-0.342134
8	4.073773	4.119094	0.9082
1	3.459004	4.778659	1.258669
8	5.964133	-2.440915	-0.722087
8	6.299111	0.158356	-0.648078
1	6.719977	-1.839425	-0.835163
1	6.239819	1.168809	-0.609939
6	1.194047	-2.079337	0.320626
8	0.294642	-2.070955	-0.81844
6	1.240901	-3.499388	0.907528
6	-0.959542	-2.542711	-0.54923
6	-0.150012	-3.822886	1.470184
6	-1.235964	-3.35532	0.54219
6	-2.617898	-3.765291	0.790852
6	-1.978716	-2.124873	-1.424079
6	-3.654954	-3.280111	-0.102126
6	-3.32984	-2.482287	-1.177904
8	-2.88831	-4.510019	1.762318
8	-4.24131	-1.959404	-2.039334
1	-5.101431	-1.90902	-1.595314
8	1.600953	-4.397148	-0.137718
1	1.573927	-5.294429	0.219747
1	0.730789	-1.45523	1.097579
6	-0.379266	2.417138	-0.148632
8	-1.20559	1.591228	0.709066
6	-0.817552	3.868406	0.082317
1	-0.170597	4.557568	-0.469455
6	-2.552349	1.642919	0.397937
6	-2.26609	4.026585	-0.425992
1	-2.239054	4.234901	-1.506469
6	-3.114058	2.800736	-0.151471
6	-3.296754	0.49321	0.655127
6	-4.487902	2.756532	-0.459978
1	-2.80192	-0.379777	1.064767
6	-4.650818	0.486535	0.314762
6	-5.257133	1.615337	-0.236289
8	-5.132542	3.830351	-1.003858
1	-4.521607	4.574072	-1.080103
1	-0.618954	2.154244	-1.1892
1	-0.255365	-4.89991	1.649465
1	-0.274163	-3.357799	2.457305
1	1.983741	-3.516967	1.718424
1	-4.671734	-3.612726	0.084709
1	-1.740953	-1.482823	-2.263998
1	-6.308818	1.609447	-0.49476
1	-2.675103	4.921653	0.062585
1	1.543696	3.969282	0.88582
1	0.521133	0.115768	-0.371808
8	-0.6926	4.215899	1.455335
1	-0.975576	3.43888	1.962869
8	-5.427898	-0.632644	0.475197
1	-4.900493	-1.314841	0.917937

*Table S42 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 7'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481771 (Hartree/Particle)
Thermal correction to Energy= 0.516820
Thermal correction to Enthalpy= 0.517765
Thermal correction to Gibbs Free Energy= 0.412958
Sum of electronic and zero-point Energies= -2021.080286
Sum of electronic and thermal Energies= -2021.045237
Sum of electronic and thermal Enthalpies= -2021.044293
Sum of electronic and thermal Free Energies= -2021.149099

Coordinates:

6	-2.080612	-1.3839	0.107462
6	-2.564246	-2.739761	-0.050065
6	-3.976261	-2.949177	-0.080713
6	-4.874303	-1.879817	0.05294
6	-4.401223	-0.592109	0.244091
6	-3.03482	-0.331364	0.29033
1	-5.11854	0.212882	0.332358
6	-0.700755	-0.979087	0.044418
6	-1.770356	-3.976841	-0.166784
6	0.472012	-1.676581	-0.033791
6	-0.30042	-4.078121	-0.060577
6	0.63759	-3.089273	-0.02994
8	-2.349586	-5.079603	-0.333641
8	0.08247	-5.381883	-0.048123
1	1.048249	-5.419446	-0.015809
8	-6.2053	-2.125064	0.007775
8	-4.570531	-4.143156	-0.233248
1	-6.301124	-3.083119	-0.132938
1	-3.795478	-4.799257	-0.325295
6	-2.571769	1.083237	0.602256
8	-2.037703	1.674211	-0.602778
6	-3.592011	2.051135	1.218053
6	-1.537439	2.943793	-0.500124
6	-2.830055	3.313462	1.658535
6	-1.865901	3.784068	0.596899
6	-1.287449	5.08378	0.656215
6	-0.712214	3.379767	-1.515449
6	-0.45495	5.545816	-0.338353
6	-0.136865	4.707245	-1.474829
8	-1.558291	5.925493	1.699378
8	0.633568	5.107377	-2.385749
1	-2.033114	5.456947	2.396506
8	-4.56802	2.365571	0.235157
1	-5.228007	2.946754	0.635684
1	-1.756301	1.020204	1.338274
6	1.737474	-0.846297	-0.173241
8	2.739533	-1.389935	0.704182
6	2.306402	-0.788445	-1.609391
1	1.514799	-0.466553	-2.291654
6	3.995538	-0.829427	0.631767
6	3.464777	0.218459	-1.621566
1	3.058131	1.239798	-1.591231
6	4.400708	-0.043667	-0.458016
6	4.850097	-1.125507	1.695805
6	5.715309	0.46625	-0.424273
1	4.482517	-1.737386	2.513582
6	6.148496	-0.612779	1.67979
6	6.588403	0.18843	0.624326
8	6.202083	1.251777	-1.428395
1	5.502112	1.446721	-2.064212
1	1.520026	0.183303	0.141571
1	-3.562069	4.102526	1.887001
1	-2.300856	3.103011	2.601204
1	-4.045516	1.57265	2.0979
1	-0.021574	6.537115	-0.283761
1	-0.483491	2.736744	-2.356935
1	7.591868	0.595138	0.62144
1	3.983286	0.107664	-2.583515
1	1.672321	-3.420143	-0.013248
1	-0.564782	0.09276	0.009285
8	2.71433	-2.070214	-2.062827
1	3.510606	-2.311336	-1.567771
8	7.037716	-0.855747	2.685856
1	6.613853	-1.407332	3.356221

*Table S43 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 3'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482006 (Hartree/Particle)
Thermal correction to Energy= 0.516549
Thermal correction to Enthalpy= 0.517494
Thermal correction to Gibbs Free Energy= 0.416380
Sum of electronic and zero-point Energies= -2021.057372
Sum of electronic and thermal Energies= -2021.022829
Sum of electronic and thermal Enthalpies= -2021.021885
Sum of electronic and thermal Free Energies= -2021.122999

Coordinates:

6	-2.617203	-0.071809	0.103249
6	-3.950517	0.453982	0.260121
6	-5.018927	-0.46866	0.456372
6	-4.797245	-1.854551	0.417621
6	-3.524421	-2.350353	0.170772
6	-2.443316	-1.486782	0.014916
1	-3.385812	-3.424067	0.100706
6	-1.412959	0.716879	0.158923
6	-4.362284	1.865057	0.191784
6	-1.179882	2.049528	-0.03171
6	-3.511446	2.954824	-0.338621
6	-2.149511	3.031807	-0.391219
8	-5.537144	2.196787	0.476675
8	-4.279188	4.006481	-0.726095
1	-3.703412	4.706414	-1.064364
8	-5.841599	-2.697552	0.592217
8	-6.298992	-0.115626	0.661053
1	-6.627369	-2.141613	0.730706
1	-6.288958	0.896621	0.677912
6	-1.080041	-2.039986	-0.347117
8	-0.252405	-2.115455	0.808107
6	-1.078079	-3.4382	-1.103829
6	1.040449	-2.52316	0.596626
6	0.378409	-3.65321	-1.58833
6	1.402335	-3.237954	-0.559693
6	2.759126	-3.584029	-0.693035
6	1.961436	-2.172039	1.582304
6	3.711343	-3.218837	0.262939
6	3.300646	-2.513931	1.40398
8	3.222323	-4.287845	-1.766712
8	4.179825	-2.119585	2.364303
1	2.488669	-4.520106	-2.349986
1	5.080775	-2.178583	2.018204
8	-1.469874	-4.415757	-0.257344
1	-0.602735	-1.369135	-1.074762
6	0.27298	2.480204	0.18095
8	1.099616	1.611597	-0.627653
6	0.672196	3.9201	-0.163663
1	0.031745	4.633553	0.364535
6	2.453358	1.710453	-0.355171
6	2.134487	4.146465	0.278447
1	2.138337	4.438607	1.339776
6	3.005126	2.92321	0.070941
6	3.209371	0.556154	-0.535285
6	4.390387	2.932154	0.326868
1	2.719487	-0.36041	-0.843437
6	4.576246	0.602673	-0.251126
6	5.176112	1.791222	0.170314
8	5.030582	4.062171	0.752771
1	4.403932	4.79537	0.793992
1	0.528459	2.299826	1.235785
1	0.476959	-4.71895	-1.839033
1	0.497043	-3.091872	-2.527299
1	-1.757499	-3.307933	-1.965517
1	4.737897	-3.550687	0.137446
1	1.646321	-1.605716	2.449236
1	6.236158	1.827724	0.389146
1	2.501962	5.010992	-0.291511
1	-1.747659	3.970647	-0.764979
1	-0.525596	0.146869	0.401062
8	0.485081	4.168754	-1.550622
1	0.786101	3.371891	-2.014854
8	5.36739	-0.506105	-0.354514
1	4.811232	-1.259612	-0.610213

*Table S44 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site h-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482871 (Hartree/Particle)
Thermal correction to Energy= 0.517401
Thermal correction to Enthalpy= 0.518345
Thermal correction to Gibbs Free Energy= 0.417799
Sum of electronic and zero-point Energies= -2021.084610
Sum of electronic and thermal Energies= -2021.050081
Sum of electronic and thermal Enthalpies= -2021.049136
Sum of electronic and thermal Free Energies= -2021.149683

Coordinates:

6	2.6617	-0.060427	-0.107275
6	3.996769	0.491404	-0.196182
6	5.082943	-0.394306	-0.473962
6	4.893205	-1.855168	-0.59089
6	3.554747	-2.34244	-0.342602
6	2.499784	-1.514689	-0.099418
1	3.423628	-3.417001	-0.363748
6	1.458296	0.689171	-0.13842
6	4.381178	1.897452	-0.003352
6	1.190156	2.033356	0.052945
6	3.483438	2.956394	0.509119
6	2.114473	3.022443	0.461883
8	5.567545	2.264782	-0.185166
8	4.201197	4.008032	0.969392
1	3.593578	4.691991	1.284992
8	5.845293	-2.605171	-0.849389
8	6.320728	0.007311	-0.632552
1	6.291054	1.020546	-0.514588
6	1.150868	-2.10262	0.299719
8	0.253911	-2.058113	-0.825683
6	1.149482	-3.523023	0.884133
6	-1.028076	-2.47573	-0.571761
6	-0.249728	-3.774173	1.474148
6	-1.337097	-3.263535	0.552268
6	-2.689674	-3.583442	0.756199
6	-2.003137	-2.044566	-1.470434
6	-3.692517	-3.138852	-0.110436
6	-3.336694	-2.368976	-1.22728
8	-3.09891	-4.34952	1.811517
8	-4.270211	-1.885915	-2.094074
1	-2.338017	-4.597852	2.351199
1	-5.119	-1.813781	-1.63395
8	1.442605	-4.435519	-0.164378
1	1.48024	-5.325185	0.210375
1	0.733212	-1.45986	1.088649
6	-0.263675	2.433624	-0.196202
8	-1.09593	1.630852	0.671067
6	-0.669644	3.896696	0.02559
1	-0.014542	4.567765	-0.538808
6	-2.448331	1.710382	0.376582
6	-2.119747	4.082685	-0.465396
1	-2.10284	4.274345	-1.549167
6	-2.992793	2.882354	-0.160136
6	-3.210212	0.577351	0.645432
6	-4.374381	2.871814	-0.434982
1	-2.725828	-0.311685	1.032334
6	-4.571082	0.600956	0.332704
6	-5.164206	1.748664	-0.19471
8	-5.006314	3.961641	-0.963518
1	-4.378681	4.688719	-1.060226
1	-0.506192	2.165954	-1.235516
1	-0.354334	-4.857121	1.644789
1	-0.30684	-3.298301	2.464756
1	1.901752	-3.577485	1.683986
1	-4.716414	-3.459896	0.055719
1	-1.733468	-1.41937	-2.311965
1	-6.220417	1.76636	-0.433553
1	-2.498005	4.995645	0.014841
1	1.678761	3.95754	0.805929
1	0.576333	0.101384	-0.359914
8	-0.520693	4.252925	1.394592
1	-0.836693	3.495133	1.911624
8	-5.365243	-0.500975	0.504224
1	-4.815375	-1.227263	0.840295

*Table S45 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site i-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483234 (Hartree/Particle)
Thermal correction to Energy= 0.518228
Thermal correction to Enthalpy= 0.519172
Thermal correction to Gibbs Free Energy= 0.417238
Sum of electronic and zero-point Energies= -2021.075373
Sum of electronic and thermal Energies= -2021.040380
Sum of electronic and thermal Enthalpies= -2021.039436
Sum of electronic and thermal Free Energies= -2021.141369

Coordinates:

6	-2.645455	-0.048387	0.189514
6	-3.936914	0.479948	0.35188
6	-5.094453	-0.404758	0.291161
6	-4.839621	-1.832917	0.100974
6	-3.557022	-2.343782	-0.064577
6	-2.471564	-1.480852	-0.049732
1	-3.415458	-3.407153	-0.20985
6	-1.435324	0.734634	0.286795
6	-4.245982	1.901886	0.658621
6	-1.220404	2.058482	0.02042
6	-3.545957	2.953254	-0.15237
6	-2.203989	3.02167	-0.380397
8	-5.11798	2.235967	1.441258
8	-4.401572	3.920125	-0.547926
1	-3.918784	4.588084	-1.05667
8	-5.924408	-2.599455	0.066637
8	-6.298616	-0.069114	0.362505
1	-6.661256	-1.950246	0.188972
6	-1.086874	-2.001194	-0.405791
8	-0.304812	-2.10001	0.800026
6	-1.003483	-3.325778	-1.175881
6	0.993896	-2.506643	0.640057
6	0.453531	-3.498991	-1.639084
6	1.428016	-3.150735	-0.53377
6	2.78712	-3.497502	-0.607347
6	1.853784	-2.239589	1.704752
6	3.678142	-3.222138	0.435286
6	3.195307	-2.603831	1.597577
8	3.313493	-4.131805	-1.69744
8	4.003638	-2.317192	2.653624
1	2.640703	-4.218201	-2.384196
1	4.921934	-2.504419	2.417594
8	-1.40412	-4.374489	-0.304402
1	-1.329829	-5.210676	-0.782666
1	-0.612938	-1.249764	-1.053736
6	0.234186	2.511126	0.17458
8	1.050269	1.575256	-0.563815
6	0.619017	3.916083	-0.305027
1	-0.016714	4.669787	0.169644
6	2.410213	1.708519	-0.344362
6	2.088151	4.187568	0.084622
1	2.112876	4.562343	1.119394
6	2.964425	2.958249	-0.048783
6	3.170306	0.548415	-0.453357
6	4.359136	2.999599	0.146273
1	2.67858	-0.39457	-0.663197
6	4.548148	0.629431	-0.23693
6	5.150895	1.855978	0.053507
8	5.003177	4.167733	0.445853
1	4.367939	4.894554	0.458539
1	0.50106	2.427747	1.238947
1	0.584782	-4.543034	-1.963909
1	0.614918	-2.876158	-2.531683
1	-1.662265	-3.264373	-2.054581
1	4.707585	-3.559004	0.352235
1	1.486881	-1.737991	2.591088
1	6.218796	1.919601	0.222243
1	2.43441	5.007518	-0.559678
1	-1.831392	3.907378	-0.889843
1	-0.550214	0.171844	0.553425
8	0.404357	4.039436	-1.705129
1	0.70319	3.20702	-2.103181
8	5.346119	-0.47506	-0.285974
1	4.785485	-1.257882	-0.412304

*Table S46 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site b-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482863 (Hartree/Particle)
Thermal correction to Energy= 0.517410
Thermal correction to Enthalpy= 0.518355
Thermal correction to Gibbs Free Energy= 0.417894
Sum of electronic and zero-point Energies= -2021.097229
Sum of electronic and thermal Energies= -2021.062682
Sum of electronic and thermal Enthalpies= -2021.061738
Sum of electronic and thermal Free Energies= -2021.162198

Coordinates:

6	2.633001	0.041327	-0.05872
6	3.952665	0.614542	-0.214348
6	5.03495	-0.250038	-0.511214
6	4.859647	-1.651758	-0.553548
6	3.612111	-2.205708	-0.293902
6	2.511774	-1.394171	-0.040147
1	3.503794	-3.282734	-0.3117
6	1.42171	0.783789	-0.055162
6	4.31787	2.025426	-0.057594
6	1.13679	2.157602	0.091274
6	3.451687	3.093353	0.619363
6	2.015459	3.155389	0.458404
8	5.455895	2.425406	-0.378751
8	4.050183	3.979809	1.228572
8	5.919461	-2.438554	-0.826566
8	6.283372	0.162635	-0.752635
1	6.682175	-1.849903	-0.965013
1	6.235222	1.178241	-0.702581
6	1.185727	-2.031973	0.347556
8	0.311654	-2.037538	-0.796254
6	1.230501	-3.442582	0.953867
6	-0.95826	-2.500301	-0.561143
6	-0.170313	-3.744155	1.514928
6	-1.258377	-3.286435	0.566338
6	-2.602459	-3.650901	0.752264
6	-1.93194	-2.114562	-1.481447
6	-3.604851	-3.251662	-0.136342
6	-3.257495	-2.481389	-1.255836
8	-3.0025	-4.419066	1.809726
8	-4.193344	-2.038416	-2.141286
1	-2.246639	-4.618399	2.375966
1	-5.043727	-1.957391	-1.685019
8	1.590822	-4.358463	-0.072028
1	1.60119	-5.247264	0.306561
1	0.72725	-1.398774	1.120061
6	-0.330277	2.507948	-0.170661
8	-1.14256	1.636937	0.647285
6	-0.800519	3.943972	0.096839
1	-0.165116	4.660363	-0.432493
6	-2.493742	1.676594	0.344192
6	-2.247077	4.083422	-0.422286
1	-2.216787	4.305555	-1.499997
6	-3.076453	2.841708	-0.166098
6	-3.217687	0.511224	0.580973
6	-4.454515	2.788103	-0.453126
1	-2.706036	-0.36882	0.953066
6	-4.57678	0.495258	0.261274
6	-5.206089	1.63219	-0.246483
8	-5.120646	3.868095	-0.958913
1	-4.51798	4.619177	-1.02888
1	-0.538086	2.269677	-1.22532
1	-0.236276	-4.828426	1.697395
1	-0.266566	-3.260642	2.498769
1	1.964661	-3.453442	1.772743
1	-4.620666	-3.60216	0.018856
1	-1.67064	-1.485161	-2.322437
1	-6.261197	1.619254	-0.490469
1	-2.672174	4.965971	0.074998
1	1.616661	4.124638	0.736074
1	0.534525	0.185422	-0.213123
8	-0.696039	4.258866	1.475715
1	-0.969201	3.467953	1.965515
8	-5.334841	-0.636926	0.407913
1	-4.768394	-1.342682	0.759505

*Table S47 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 3-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481623 (Hartree/Particle)
Thermal correction to Energy= 0.516363
Thermal correction to Enthalpy= 0.517307
Thermal correction to Gibbs Free Energy= 0.415906
Sum of electronic and zero-point Energies= -2021.052296
Sum of electronic and thermal Energies= -2021.017556
Sum of electronic and thermal Enthalpies= -2021.016612
Sum of electronic and thermal Free Energies= -2021.118013

Coordinates:

6	-2.618401	-0.048759	0.085744
6	-3.955274	0.468153	0.243141
6	-5.023724	-0.463133	0.387668
6	-4.795181	-1.844918	0.301303
6	-3.515876	-2.328746	0.064364
6	-2.43445	-1.458818	-0.04854
1	-3.367833	-3.398412	-0.014002
6	-1.417119	0.741737	0.168427
6	-4.369733	1.879827	0.22398
6	-1.186894	2.079091	0.015161
6	-3.518699	2.990049	-0.263097
6	-2.157353	3.073076	-0.307433
8	-5.54734	2.198637	0.51233
8	-4.287708	4.051612	-0.621322
1	-3.711989	4.759614	-0.942414
8	-5.839742	-2.69819	0.430859
8	-6.309048	-0.121928	0.587429
1	-6.628094	-2.148634	0.579826
1	-6.301378	0.887827	0.649114
6	-1.061336	-2.002994	-0.410067
8	-0.252213	-2.084003	0.784028
6	-0.999735	-3.346935	-1.148742
6	1.038522	-2.500215	0.604607
6	0.445988	-3.533169	-1.643907
6	1.446895	-3.161553	-0.569523
6	2.804409	-3.506625	-0.670392
6	1.923413	-2.223122	1.647284
6	3.719899	-3.216932	0.347398
6	3.261813	-2.588738	1.514461
8	3.305305	-4.154932	-1.764417
8	4.094321	-2.291225	2.549945
1	2.61577	-4.247885	-2.433607
1	5.005915	-2.488122	2.296661
8	-1.375948	-4.376919	-0.243652
1	-1.343964	-5.219178	-0.715786
1	-0.583209	-1.281056	-1.086231
6	0.264737	2.504108	0.232983
8	1.091847	1.574015	-0.426738
6	0.66365	3.99733	-0.155948
1	0.026553	4.623618	0.500561
6	2.448029	1.721512	-0.263868
6	2.153193	4.192878	0.232604
1	2.17321	4.518313	1.284542
6	3.010621	2.967962	0.034401
6	3.207829	0.568489	-0.439217
6	4.415938	3.011427	0.152884
1	2.709251	-0.369638	-0.65313
6	4.591805	0.649305	-0.284812
6	5.204666	1.873802	0.001023
8	5.072328	4.175183	0.44248
1	4.440317	4.902763	0.494836
1	0.485206	2.47862	1.312571
1	0.569941	-4.584513	-1.94743
1	0.586275	-2.930059	-2.553455
1	-1.681272	-3.305678	-2.010773
1	4.74748	-3.554163	0.244519
1	1.576429	-1.7109	2.53559
1	6.279257	1.938682	0.11882
1	2.517838	5.040112	-0.365912
1	-1.755976	4.022529	-0.655638
1	-0.531594	0.164654	0.394541
8	0.416508	4.198771	-1.463374
8	5.389208	-0.449871	-0.391686
1	4.825933	-1.232232	-0.511551

*Table S48 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 5-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482444 (Hartree/Particle)
Thermal correction to Energy= 0.517026
Thermal correction to Enthalpy= 0.517970
Thermal correction to Gibbs Free Energy= 0.416954
Sum of electronic and zero-point Energies= -2021.085532
Sum of electronic and thermal Energies= -2021.050950
Sum of electronic and thermal Enthalpies= -2021.050006
Sum of electronic and thermal Free Energies= -2021.151023

Coordinates:

6	-2.605623	-0.092673	0.103553
6	-3.95302	0.396807	0.259176
6	-5.000865	-0.556012	0.416444
6	-4.742675	-1.933377	0.345422
6	-3.45445	-2.39167	0.106631
6	-2.39282	-1.499515	-0.020524
1	-3.284299	-3.458619	0.037793
6	-1.42224	0.725056	0.183382
6	-4.398226	1.79902	0.22705
6	-1.219331	2.065261	0.01641
6	-3.572017	2.923005	-0.269097
6	-2.212629	3.032346	-0.321381
8	-5.582927	2.093594	0.513012
8	-4.364011	3.967256	-0.628915
1	-3.803779	4.690799	-0.942614
8	-5.767732	-2.807842	0.489022
8	-6.292304	-0.240369	0.616052
1	-6.567157	-2.274069	0.636582
1	-6.305535	0.770793	0.666214
6	-1.013224	-2.015434	-0.395461
8	-0.180129	-2.064766	0.785217
6	-0.93259	-3.366605	-1.119138
6	1.115416	-2.450642	0.586585
6	0.508003	-3.527044	-1.637954
6	1.518694	-3.117923	-0.586548
6	2.88101	-3.437484	-0.705121
6	2.013568	-2.134524	1.607599
6	3.808304	-3.111834	0.291824
6	3.35721	-2.474426	1.457624
8	3.377369	-4.09086	-1.796945
8	4.200509	-2.138442	2.471022
1	2.672411	-4.237741	-2.440029
1	5.113432	-2.309148	2.203363
8	-1.267635	-4.393067	-0.194613
1	-1.244214	-5.238871	-0.660942
1	-0.56204	-1.289062	-1.085526
6	0.222302	2.530337	0.232889
8	1.071355	1.63111	-0.528292
6	0.602353	3.964319	-0.161648
1	-0.043175	4.679144	0.358524
6	2.419318	1.800439	-0.294534
6	2.064577	4.231298	0.246544
1	2.109242	4.556399	1.294476
6	2.944023	3.024038	0.066303
6	3.220773	0.654108	-0.453307
6	4.387724	3.118105	0.290341
1	2.743377	-0.282444	-0.722443
6	4.61356	0.722843	-0.222434
6	5.19448	1.923978	0.131294
8	4.903969	4.21424	0.617641
1	0.471913	2.394802	1.295923
1	0.649332	-4.579805	-1.928625
1	0.619666	-2.934371	-2.558161
1	-1.629873	-3.35185	-1.96918
1	4.838374	-3.43869	0.180452
1	1.670133	-1.619463	2.495725
1	6.259779	1.999732	0.313398
1	2.444807	5.073936	-0.339762
1	-1.834574	3.987983	-0.675777
1	-0.524567	0.169443	0.419013
8	0.377975	4.173298	-1.552076
1	0.700046	3.382143	-2.009888
8	5.394477	-0.386357	-0.337854
1	4.829738	-1.164189	-0.486223

*Table S49 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 7-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481544 (Hartree/Particle)
Thermal correction to Energy= 0.516668
Thermal correction to Enthalpy= 0.517613
Thermal correction to Gibbs Free Energy= 0.412163
Sum of electronic and zero-point Energies= -2021.079893
Sum of electronic and thermal Energies= -2021.044768
Sum of electronic and thermal Enthalpies= -2021.043824
Sum of electronic and thermal Free Energies= -2021.149273

Coordinates:

6	-2.241242	-1.164804	0.109014
6	-2.898378	-2.444008	-0.053643
6	-4.321326	-2.457828	-0.154204
6	-5.067738	-1.272676	-0.070077
6	-4.431098	-0.059106	0.13838
6	-3.045217	0.011723	0.243866
1	-5.032288	0.839091	0.193806
6	-0.818652	-0.952269	0.072165
6	-2.275464	-3.778963	-0.100447
6	0.248814	-1.804925	0.064348
6	-0.846382	-4.07381	0.142739
6	0.219502	-3.22358	0.165658
8	-2.98341	-4.795783	-0.30416
8	-0.658153	-5.412348	0.27854
1	0.283502	-5.581415	0.419424
8	-6.416136	-1.332727	-0.177659
8	-5.066447	-3.562266	-0.326873
1	-6.638235	-2.270189	-0.313546
1	-4.389266	-4.318526	-0.381672
6	-2.398754	1.34787	0.581127
8	-1.725614	1.851527	-0.590763
6	-3.299414	2.450456	1.155971
6	-1.044442	3.031149	-0.435847
6	-2.3874	3.588513	1.646646
6	-1.300082	3.898264	0.639658
6	-0.533141	5.073403	0.710056
6	-0.089193	3.316815	-1.411391
6	0.432652	5.38265	-0.248475
6	0.641419	4.50066	-1.311276
8	-0.697104	5.982177	1.719022
8	1.575239	4.740186	-2.279911
1	-1.333072	5.644868	2.361843
1	1.990332	5.596042	-2.110312
8	-4.176433	2.89336	0.129012
1	-4.718385	3.609997	0.484066
1	-1.637924	1.168123	1.355581
6	1.60662	-1.146204	-0.114052
8	2.586904	-1.844508	0.681395
6	2.116002	-1.131072	-1.569869
1	1.351573	-0.696238	-2.218911
6	3.867026	-1.334008	0.647543
6	3.390879	-0.270578	-1.618997
1	3.106924	0.793379	-1.625621
6	4.311084	-0.556064	-0.455284
6	4.701035	-1.64831	1.697254
6	5.646536	-0.060893	-0.43832
1	4.349216	-2.246591	2.529075
6	6.069483	-1.171643	1.707793
6	6.507333	-0.355223	0.59624
8	6.120112	0.711169	-1.458588
1	5.41973	0.893839	-2.097482
1	1.54626	-0.109063	0.24008
1	-3.017416	4.47313	1.829645
1	-1.965861	3.305256	2.623178
1	-3.859433	2.037311	2.007886
1	1.001233	6.301727	-0.146094
1	0.068084	2.634945	-2.237947
1	7.523422	0.020515	0.595498
1	3.893259	-0.475366	-2.574139
1	1.193441	-3.692777	0.283095
1	-0.541996	0.089638	-0.014722
8	2.339349	-2.442694	-2.054936
1	2.911648	-2.894576	-1.418125
8	6.843252	-1.450138	2.659413

*Table S50 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 3'-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483042 (Hartree/Particle)
Thermal correction to Energy= 0.517719
Thermal correction to Enthalpy= 0.518663
Thermal correction to Gibbs Free Energy= 0.418138
Sum of electronic and zero-point Energies= -2021.064010
Sum of electronic and thermal Energies= -2021.029333
Sum of electronic and thermal Enthalpies= -2021.028388
Sum of electronic and thermal Free Energies= -2021.128913

Coordinates:

6	-2.634024	-0.027469	0.099117
6	-3.939128	0.577475	0.228992
6	-5.058732	-0.275347	0.452379
6	-4.912983	-1.669715	0.459133
6	-3.669992	-2.244035	0.235741
6	-2.536477	-1.453824	0.059843
1	-3.601458	-3.322395	0.20626
6	-1.391774	0.703779	0.137663
6	-4.27828	2.00373	0.100576
6	-1.096322	2.018947	-0.088538
6	-3.374499	3.022676	-0.475
6	-2.011053	3.031273	-0.506995
8	-5.434228	2.409207	0.370523
8	-4.085272	4.091967	-0.922121
1	-3.469509	4.745268	-1.282436
8	-6.003759	-2.449099	0.657186
8	-6.318838	0.154058	0.640944
1	-6.756537	-1.844365	0.772673
1	-6.251906	1.164548	0.621419
6	-1.209856	-2.102825	-0.299326
8	-0.312827	-2.086762	0.874282
6	-1.181945	-3.490402	-0.861153
6	0.963418	-2.511763	0.6136
6	0.173759	-3.829653	-1.430052
6	1.273634	-3.305621	-0.511422
6	2.623548	-3.630219	-0.722071
6	1.95021	-2.086158	1.504968
6	3.630402	-3.196172	0.144191
6	3.280995	-2.42006	1.25904
8	3.023412	-4.402284	-1.777929
8	4.222168	-1.940767	2.120306
1	2.266957	-4.606117	-2.341606
1	5.060045	-1.841823	1.643963
8	-1.790656	-4.448721	-0.084822
1	-1.554164	-5.326241	-0.413817
1	-0.725065	-1.472564	-1.055629
6	0.364095	2.402721	0.152085
8	1.190435	1.572882	-0.699498
6	0.793156	3.854222	-0.099876
1	0.143851	4.547708	0.443701
6	2.539214	1.637378	-0.395747
6	2.242738	4.02998	0.397589
1	2.220992	4.2474	1.476471
6	3.098386	2.808625	0.128102
6	3.286044	0.487396	-0.635486
6	4.475161	2.778403	0.423316
1	2.790649	-0.399883	-1.012145
6	4.64139	0.492635	-0.302368
6	5.248469	1.637132	0.215221
8	5.118647	3.867	0.941264
1	4.501354	4.605723	1.01395
1	0.607831	2.15318	1.1949
1	0.256897	-4.921275	-1.553938
1	0.267601	-3.397756	-2.439139
1	4.651405	-3.527046	-0.02056
1	1.689946	-1.452885	2.34351
1	6.301369	1.640233	0.468919
1	2.639972	4.924752	-0.10135
1	-1.554717	3.933392	-0.908848
1	-0.537165	0.096612	0.409644
8	0.662232	4.180078	-1.478382
1	0.947296	3.395061	-1.972441
8	5.416633	-0.630187	-0.440346
1	4.86343	-1.339155	-0.805877

*Table S51 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 2'-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482033 (Hartree/Particle)
Thermal correction to Energy= 0.516915
Thermal correction to Enthalpy= 0.517859
Thermal correction to Gibbs Free Energy= 0.416795
Sum of electronic and zero-point Energies= -2021.081283
Sum of electronic and thermal Energies= -2021.046401
Sum of electronic and thermal Enthalpies= -2021.045457
Sum of electronic and thermal Free Energies= -2021.146521

Coordinates:

6	-2.637655	-0.020389	-0.251289
6	-3.94363	-0.649011	-0.123311
6	-5.107472	0.165413	-0.171177
6	-5.015723	1.572225	-0.265649
6	-3.789499	2.181421	-0.331225
6	-2.575794	1.440827	-0.325277
1	-3.768801	3.254759	-0.472734
6	-1.403071	-0.729728	-0.324806
6	-4.237346	-2.082932	0.077143
6	-1.048785	-2.037536	-0.068277
6	-3.260661	-3.105059	0.478235
6	-1.896552	-3.077842	0.385756
8	-5.42446	-2.495805	0.009552
8	-3.891751	-4.222627	0.932559
1	-3.221935	-4.874195	1.182051
8	-6.158756	2.296049	-0.318418
8	-6.368089	-0.289216	-0.126992
1	-6.889119	1.653905	-0.286187
1	-6.263825	-1.307592	-0.100536
6	-1.402176	2.257564	-0.31459
8	-0.239016	1.818632	-0.892888
6	-1.366117	3.65456	0.236126
6	0.98224	2.374393	-0.574038
6	-0.133868	3.809982	1.152904
6	1.107539	3.304825	0.465425
6	2.406951	3.722586	0.789932
6	2.066969	1.900912	-1.303838
6	3.52551	3.241945	0.100988
6	3.345965	2.335092	-0.950962
8	2.651799	4.619999	1.791407
8	4.397603	1.829502	-1.653996
1	1.824641	4.846906	2.234732
1	5.174623	1.798152	-1.075393
8	-1.32839	4.563031	-0.868582
1	-1.240083	5.461599	-0.520046
6	0.429439	-2.344843	-0.294226
8	1.199416	-1.625203	0.704721
6	0.8999	-3.80643	-0.232427
1	0.280456	-4.438204	-0.87682
6	2.561418	-1.624566	0.46327
6	2.363046	-3.86681	-0.710776
1	2.377451	-3.898862	-1.810874
6	3.174234	-2.689735	-0.207983
6	3.27174	-0.514606	0.915768
6	4.563487	-2.595343	-0.420174
1	2.737323	0.296838	1.396681
6	4.638852	-0.445843	0.648945
6	5.299198	-1.488129	-0.000647
8	5.256287	-3.581061	-1.064007
1	4.659623	-4.307322	-1.28448
1	0.710112	-1.940783	-1.27679
1	-0.041281	4.876132	1.414276
1	-0.33099	3.277184	2.094542
1	-2.260933	3.817903	0.846226
1	4.508404	3.625903	0.355117
1	1.931327	1.172404	-2.09265
1	6.362043	-1.433297	-0.201358
1	2.770776	-4.823415	-0.35571
1	-1.388658	-3.984617	0.707185
1	-0.566464	-0.111001	-0.607629
8	0.766507	-4.325164	1.087217
1	1.013516	-3.604877	1.688846
8	5.378794	0.66609	0.972143
1	4.793413	1.311005	1.396912

*Table S52 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 4β-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482367 (Hartree/Particle)
Thermal correction to Energy= 0.517240
Thermal correction to Enthalpy= 0.518184
Thermal correction to Gibbs Free Energy= 0.416988
Sum of electronic and zero-point Energies= -2021.080795
Sum of electronic and thermal Energies= -2021.045923
Sum of electronic and thermal Enthalpies= -2021.044978
Sum of electronic and thermal Free Energies= -2021.146174

Coordinates:

6	-2.596822	-0.104063	0.082453
6	-3.952358	0.356996	0.264653
6	-4.983812	-0.619018	0.391071
6	-4.703787	-1.988195	0.271838
6	-3.408363	-2.417499	0.020771
6	-2.361869	-1.504893	-0.081307
1	-3.220373	-3.479029	-0.078547
6	-1.42573	0.730658	0.155139
6	-4.422037	1.750994	0.302406
6	-1.243617	2.079774	0.033392
6	-3.61794	2.916947	-0.121624
6	-2.261674	3.049274	-0.203589
8	-5.61332	2.008793	0.602231
8	-4.42755	3.97838	-0.38311
1	-3.878827	4.725378	-0.659729
8	-5.715187	-2.883214	0.386818
8	-6.279814	-0.333412	0.60669
1	-6.521467	-2.36568	0.554127
1	-6.307063	0.676544	0.695579
6	-0.971387	-1.996813	-0.448291
8	-0.170462	-2.082059	0.752135
6	-0.860966	-3.31949	-1.219414
6	1.127137	-2.475067	0.585765
6	0.594796	-3.448844	-1.703352
6	1.570009	-3.093343	-0.599999
6	2.933335	-3.419093	-0.681219
6	1.985584	-2.22206	1.656854
6	3.823213	-3.150549	0.365658
6	3.330024	-2.570499	1.544114
8	3.466637	-4.026525	-1.782979
8	4.134075	-2.302618	2.609567
1	2.792091	-4.110726	-2.468459
1	5.050652	-2.506795	2.381436
8	-1.210912	-4.385514	-0.346118
1	-1.155306	-5.212353	-0.842675
1	-0.509244	-1.245013	-1.102177
6	0.202031	2.553666	0.208555
8	1.039954	1.647818	-0.550777
6	0.567424	3.995427	-0.178665
1	0.027682	4.686328	0.480321
6	2.382814	1.771886	-0.298149
6	2.048762	4.178678	-0.01469
6	2.913562	3.066978	-0.02116
6	3.168623	0.639538	-0.388749
6	4.327947	3.128218	0.201249
1	2.707852	-0.318016	-0.603123
6	4.551138	0.756736	-0.175736
6	5.129588	2.000855	0.117105
8	4.933986	4.311583	0.503086
1	4.25982	4.953047	0.764165
1	0.469556	2.436271	1.270049
1	0.750288	-4.484595	-2.043609
1	0.730759	-2.808827	-2.58791
1	-1.535382	-3.276608	-2.086877
1	4.85583	-3.476318	0.276358
1	1.611233	-1.745777	2.553988
1	6.193334	2.07678	0.306319
1	2.424531	5.197708	-0.027112
1	-1.909143	4.032889	-0.501628
1	-0.511235	0.183813	0.335559
8	0.123203	4.340674	-1.501425
1	0.560059	3.722093	-2.105584
8	5.37057	-0.326023	-0.217097
1	4.831164	-1.127364	-0.333103

*Table S53 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 4α-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482372 (Hartree/Particle)
Thermal correction to Energy= 0.517244
Thermal correction to Enthalpy= 0.518188
Thermal correction to Gibbs Free Energy= 0.416997
Sum of electronic and zero-point Energies= -2021.080790
Sum of electronic and thermal Energies= -2021.045918
Sum of electronic and thermal Enthalpies= -2021.044974
Sum of electronic and thermal Free Energies= -2021.146166

Coordinates:

6	-2.596789	-0.10418	0.082563
6	-3.952381	0.356796	0.264812
6	-4.983663	-0.619307	0.391677
6	-4.703482	-1.988492	0.273003
6	-3.408083	-2.417736	0.0217
6	-2.361741	-1.505046	-0.080899
1	-3.219982	-3.479261	-0.077406
6	-1.425772	0.730635	0.155037
6	-4.422205	1.750803	0.301952
6	-1.243801	2.079741	0.033004
6	-3.618152	2.91662	-0.122619
6	-2.261895	3.049083	-0.204415
8	-5.613507	2.008707	0.601464
8	-4.427841	3.977856	-0.384662
1	-3.879179	4.724641	-0.661978
8	-5.714735	-2.883617	0.388573
8	-6.279737	-0.333893	0.607262
1	-6.521082	-2.366128	0.555684
1	-6.307317	0.675942	0.695589
6	-0.9713	-1.996914	-0.448148
8	-0.169964	-2.081764	0.752052
6	-0.860993	-3.319806	-1.218953
6	1.127595	-2.474745	0.585391
6	0.594622	-3.449213	-1.70331
6	1.570137	-3.093348	-0.600346
6	2.933413	-3.419195	-0.681835
6	1.986345	-2.221474	1.65617
6	3.823608	-3.15028	0.364702
6	3.330777	-2.569901	1.543156
8	3.466384	-4.027067	-1.783476
8	4.13515	-2.301567	2.608192
1	2.791628	-4.11166	-2.468701
1	5.051534	-2.506802	2.380242
8	-1.210543	-4.385639	-0.345269
1	-1.155117	-5.212593	-0.841654
1	-0.509398	-1.245254	-1.102362
6	0.201797	2.553709	0.208164
8	1.039759	1.648368	-0.551823
6	0.567152	3.995647	-0.178309
1	0.027343	4.686269	0.480907
6	2.382583	1.772143	-0.298484
6	2.048501	4.17886	-0.014221
1	2.424154	5.197938	-0.026648
6	2.913283	3.067156	-0.020924
6	3.168277	0.639765	-0.388882
6	4.327554	3.128264	0.201996
1	2.707543	-0.317688	-0.603795
6	4.550769	0.756791	-0.175251
6	5.12915	2.000819	0.117955
8	4.933608	4.311452	0.504373
1	4.259355	4.953147	0.764666
1	0.469526	2.435716	1.269532
1	0.750043	-4.485072	-2.043285
1	0.730297	-2.809475	-2.588109
1	-1.535702	-3.277215	-2.086202
1	4.856116	-3.476388	0.275299
1	1.612212	-1.744957	2.553273
1	6.192826	2.076701	0.307604
1	-1.909367	4.032608	-0.502754
1	-0.511191	0.183955	0.335603
8	0.123059	4.341508	-1.500999
1	0.559925	3.723104	-2.105336
8	5.370042	-0.32602	-0.216382
1	4.830591	-1.127298	-0.332725

*Table S54 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 3-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482314 (Hartree/Particle)
Thermal correction to Energy= 0.517415
Thermal correction to Enthalpy= 0.518359
Thermal correction to Gibbs Free Energy= 0.415185
Sum of electronic and zero-point Energies= -2021.067286
Sum of electronic and thermal Energies= -2021.032185
Sum of electronic and thermal Enthalpies= -2021.031241
Sum of electronic and thermal Free Energies= -2021.134415

Coordinates:

6	-2.549265	-0.146812	0.005112
6	-3.94877	0.195101	0.160917
6	-4.91513	-0.835908	-0.035415
6	-4.529109	-2.137589	-0.39212
6	-3.189496	-2.4479	-0.561835
6	-2.203776	-1.481598	-0.381155
1	-2.918782	-3.464175	-0.81765
6	-1.441763	0.743013	0.233491
6	-4.527789	1.506788	0.506787
6	-1.360483	2.081366	0.490175
6	-3.783636	2.779679	0.652287
6	-2.438512	3.001494	0.64534
8	-5.76742	1.623121	0.666629
8	-4.648789	3.811255	0.834481
1	-4.143228	4.62903	0.938749
8	-5.482002	-3.082273	-0.56926
8	-6.243591	-0.678168	0.089605
1	-6.334398	-2.649112	-0.389307
1	-6.358765	0.290733	0.370905
6	-0.750557	-1.866986	-0.619863
8	-0.131408	-2.070588	0.666219
6	-0.456049	-3.071711	-1.5258
6	1.185315	-2.435801	0.665603
6	1.0613	-3.081318	-1.78788
6	1.834436	-2.877939	-0.501511
6	3.200598	-3.182914	-0.397497
6	1.841388	-2.351028	1.895285
6	3.892519	-3.079157	0.814709
6	3.191609	-2.692292	1.965036
8	3.927068	-3.619546	-1.469283
8	3.793235	-2.608065	3.18531
1	3.407132	-3.526697	-2.277224
1	4.71889	-2.873263	3.104732
8	-0.874006	-4.25777	-0.863489
1	-0.645002	-5.012078	-1.421996
1	-0.243497	-1.027167	-1.113077
6	0.025178	2.727086	0.596673
8	1.014827	1.675788	0.636631
6	0.304524	3.691814	-0.523036
6	2.30347	1.949841	0.242983
6	1.677387	4.297804	-0.488907
1	1.730038	5.060479	0.303
6	2.703763	3.192176	-0.268794
6	3.187498	0.879698	0.375106
6	4.060088	3.327409	-0.62431
1	2.82601	-0.056419	0.785002
6	4.516056	1.045847	-0.016838
6	4.965994	2.274765	-0.506771
8	4.552823	4.502395	-1.125006
1	3.854903	5.168723	-1.133109
1	0.095982	3.276657	1.547849
1	1.324231	-4.045043	-2.250625
1	1.295352	-2.307169	-2.534062
1	-0.993315	-2.934859	-2.476062
1	4.938422	-3.370589	0.850361
1	1.306085	-2.020548	2.776242
1	5.998492	2.408702	-0.804726
1	1.84429	4.809207	-1.445791
1	-2.133404	4.03924	0.790093
1	-0.474061	0.269441	0.227772
8	-0.099513	3.346031	-1.786968
1	-0.856765	2.743259	-1.714233
8	5.4177	0.026119	0.066785
1	4.949267	-0.784332	0.32328

*Table S55 Energetics and Cartesian coordinates of the conformer **1c** (saaasa-ss) post-radical capture via HAB at site 2-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482091 (Hartree/Particle)
Thermal correction to Energy= 0.517423
Thermal correction to Enthalpy= 0.518368
Thermal correction to Gibbs Free Energy= 0.413920
Sum of electronic and zero-point Energies= -2021.090975
Sum of electronic and thermal Energies= -2021.055642
Sum of electronic and thermal Enthalpies= -2021.054698
Sum of electronic and thermal Free Energies= -2021.159146

Coordinates:

6	-2.624149	-0.016913	0.006148
6	-3.957398	0.519739	0.205802
6	-5.022787	-0.393899	0.443476
6	-4.813022	-1.783466	0.421463
6	-3.549181	-2.294813	0.157793
6	-2.468272	-1.448574	-0.057271
1	-3.414653	-3.368989	0.137815
6	-1.423154	0.738112	-0.046704
6	-4.356417	1.931431	0.178597
6	-1.148747	2.108895	-0.209189
6	-3.50196	3.054978	-0.288522
6	-2.152518	3.122386	-0.419755
8	-5.528593	2.263782	0.479773
8	-4.277461	4.143541	-0.556848
1	-3.706738	4.864519	-0.855612
8	-5.860568	-2.614142	0.644331
8	-6.293492	-0.033248	0.688277
1	-6.632864	-2.044102	0.801684
1	-6.27305	0.981925	0.692699
6	-1.120422	-2.041395	-0.430386
8	-0.273892	-2.0517	0.741329
6	-1.092521	-3.433322	-1.076499
6	1.00428	-2.496556	0.556659
6	0.337496	-3.662884	-1.603153
6	1.375152	-3.229348	-0.587581
6	2.727495	-3.587681	-0.706674
6	1.918443	-2.173121	1.560217
6	3.673377	-3.2473	0.267367
6	3.250331	-2.555614	1.411661
8	3.19364	-4.300716	-1.775996
8	4.113225	-2.205025	2.405555
1	2.479308	-4.441294	-2.409968
1	5.018528	-2.402096	2.130835
8	-1.445701	-4.398512	-0.094575
1	-1.439831	-5.269466	-0.512559
1	-0.655636	-1.377163	-1.171705
6	0.20925	2.50544	-0.237946
8	1.11092	1.476426	-0.305814
6	0.755165	3.90597	-0.306769
1	0.018943	4.600056	0.101323
6	2.466598	1.66366	-0.159865
6	2.050631	4.03542	0.515849
1	1.7964	4.062309	1.585488
6	2.998536	2.899621	0.214126
6	3.242166	0.5338	-0.395198
6	4.398609	2.960892	0.362545
1	2.761704	-0.397163	-0.670999
6	4.622316	0.628323	-0.209457
6	5.209141	1.84468	0.150655
8	5.033313	4.110879	0.735868
1	4.383173	4.810207	0.879015
1	0.445787	-4.733058	-1.840051
1	0.451568	-3.123049	-2.555306
1	-1.799373	-3.444607	-1.918905
1	4.695333	-3.598587	0.155427
1	1.599649	-1.604176	2.424147
1	6.280346	1.92026	0.290591
1	2.479063	5.013808	0.261576
1	-1.77687	4.083982	-0.763349
1	-0.529798	0.151197	0.084734
8	0.95105	4.343483	-1.660425
1	1.614947	3.763263	-2.061135
8	5.43633	-0.453118	-0.369447
1	4.883271	-1.231742	-0.546327

*Table S56 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 5'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482334 (Hartree/Particle)
Thermal correction to Energy= 0.517506
Thermal correction to Enthalpy= 0.518450
Thermal correction to Gibbs Free Energy= 0.416901
Sum of electronic and zero-point Energies= -2021.063892
Sum of electronic and thermal Energies= -2021.028720
Sum of electronic and thermal Enthalpies= -2021.027776
Sum of electronic and thermal Free Energies= -2021.129325

Coordinates:

6	-2.32441	-0.493266	0.126078
6	-3.731704	-0.527839	0.371439
6	-4.469371	-1.702199	0.107481
6	-3.814395	-2.842364	-0.36368
6	-2.441581	-2.839455	-0.552034
6	-1.684195	-1.69101	-0.322252
1	-1.94515	-3.749726	-0.871767
6	-1.496807	0.690872	0.324407
6	-4.511793	0.578253	1.005763
6	-1.838777	2.010061	0.321172
6	-4.35257	1.968088	0.479839
6	-3.167188	2.573971	0.219322
8	-5.333209	0.371707	1.882241
8	-5.539898	2.616802	0.426405
1	-5.391009	3.533102	0.151506
8	-4.625647	-3.926704	-0.598213
8	-5.811878	-1.736182	0.271862
1	-4.091634	-4.687485	-0.859616
1	-6.110308	-2.625657	0.026054
6	-0.19312	-1.729628	-0.6043
8	0.499458	-1.771969	0.679727
6	0.340688	-2.895443	-1.46133
6	1.874271	-1.815822	0.613149
6	1.822977	-2.645223	-1.763675
6	2.55509	-2.231096	-0.518313
6	4.015442	-2.295535	-0.478235
6	2.551753	-1.442186	1.789428
6	4.690344	-1.896526	0.742666
6	3.963463	-1.477919	1.830815
8	4.660655	-2.691099	-1.476658
8	4.533189	-1.03474	2.999134
1	5.491798	-1.151361	2.93669
8	0.166377	-4.155628	-0.813949
1	0.371723	-4.02488	0.123795
1	0.107961	-0.800718	-1.105011
6	-0.747928	3.082354	0.458351
8	0.407041	2.581139	1.143406
6	-0.357842	3.779105	-0.875528
1	0.211477	4.676573	-0.612695
6	1.592328	2.35639	0.489724
6	0.536011	2.876925	-1.724707
1	0.8338	3.453564	-2.61026
6	1.725233	2.447309	-0.902296
6	2.669136	2.02347	1.315243
6	2.999617	2.197026	-1.448392
1	2.52163	1.986161	2.389257
6	3.916177	1.783131	0.73381
6	4.091885	1.867849	-0.647957
8	3.229201	2.259928	-2.793572
1	2.403222	2.450093	-3.255673
1	-1.144693	3.860209	1.120752
1	2.27198	-3.552843	-2.176679
1	1.931693	-1.872467	-2.537172
1	-0.227368	-2.951551	-2.395062
1	5.775473	-1.920259	0.740281
1	1.987696	-1.115228	2.654915
1	5.056527	1.667137	-1.096538
1	-0.055936	2.019609	-2.082727
1	-3.206417	3.642719	0.011484
1	-0.444662	0.490643	0.479061
8	-1.488486	4.252818	-1.590058
1	-1.974805	3.48251	-1.91785
8	5.008318	1.456872	1.486648
1	4.70965	1.150534	2.355528

*Table S57 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 7'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482394 (Hartree/Particle)
Thermal correction to Energy= 0.517401
Thermal correction to Enthalpy= 0.518345
Thermal correction to Gibbs Free Energy= 0.417392
Sum of electronic and zero-point Energies= -2021.061025
Sum of electronic and thermal Energies= -2021.026018
Sum of electronic and thermal Enthalpies= -2021.025074
Sum of electronic and thermal Free Energies= -2021.126027

Coordinates:

6	2.362456	-0.411761	-0.097908
6	3.775615	-0.311907	-0.285764
6	4.615999	-1.390413	0.069187
6	4.061096	-2.576715	0.55488
6	2.686119	-2.717646	0.661308
6	1.829234	-1.663015	0.350645
1	2.274077	-3.671263	0.974299
6	1.429	0.681404	-0.332513
6	4.466076	0.821778	-0.974948
6	1.639981	2.027593	-0.390306
6	4.149377	2.224937	-0.577896
6	2.905537	2.723948	-0.361532
8	5.337576	0.628976	-1.805528
8	5.257146	3.003006	-0.592412
1	5.007017	3.918199	-0.399643
8	4.96885	-3.556101	0.879861
8	5.960847	-1.286239	-0.025022
1	4.508142	-4.374162	1.10486
1	6.338434	-2.132133	0.26236
6	0.33635	-1.8583	0.519387
8	-0.24969	-1.951093	-0.811853
6	-0.145122	-3.105461	1.279048
6	-1.627671	-1.953688	-0.84414
6	-1.668133	-2.992942	1.475868
6	-2.371573	-2.46943	0.247724
6	-3.796482	-2.450445	0.168947
6	-2.240881	-1.454348	-1.969837
6	-4.443692	-1.928043	-0.926236
6	-3.685993	-1.370391	-2.02371
8	-4.559759	-2.936981	1.187114
8	-4.25311	-0.754791	-2.968083
1	-4.002556	-3.242277	1.91364
8	0.178697	-4.302214	0.582711
1	0.124438	-4.0968	-0.364163
1	-0.097273	-0.980389	1.015386
6	0.440273	2.980397	-0.523954
8	-0.694752	2.314729	-1.091974
6	0.070706	3.731962	0.789906
1	-0.561624	4.579235	0.506495
6	-1.873912	2.161828	-0.396999
6	-0.735083	2.83222	1.725721
1	-0.991045	3.431747	2.609193
6	-1.957307	2.347244	0.989428
6	-2.976363	1.782005	-1.163267
6	-3.213963	2.148457	1.594184
1	-2.868619	1.653907	-2.233659
6	-4.207941	1.581747	-0.525891
6	-4.330405	1.76776	0.855208
8	-3.396148	2.302787	2.942448
1	-2.560645	2.559836	3.35205
1	0.721622	3.744001	-1.259562
1	-2.033839	-3.994078	1.74217
1	-1.880117	-2.333218	2.331735
1	0.34102	-3.1677	2.25768
1	-5.524606	-1.87097	-0.954642
1	-1.659188	-1.043497	-2.785734
1	-5.28205	1.607976	1.346485
1	-0.094146	2.00639	2.073883
1	2.838143	3.804525	-0.243275
1	0.395283	0.388736	-0.454462
8	1.198216	4.311279	1.427677
1	1.748441	3.591002	1.767736
8	-5.325231	1.213534	-1.205074
1	-5.08184	0.773153	-2.040985

*Table S58 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 3'-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481181 (Hartree/Particle)
Thermal correction to Energy= 0.516560
Thermal correction to Enthalpy= 0.517504
Thermal correction to Gibbs Free Energy= 0.415020
Sum of electronic and zero-point Energies= -2021.031382
Sum of electronic and thermal Energies= -2020.996003
Sum of electronic and thermal Enthalpies= -2020.995059
Sum of electronic and thermal Free Energies= -2021.097543

Coordinates:

6	-2.286137	-0.568813	0.12932
6	-3.686268	-0.710954	0.37318
6	-4.325576	-1.946354	0.128413
6	-3.580759	-3.037667	-0.327263
6	-2.215295	-2.922698	-0.530996
6	-1.555968	-1.71407	-0.316056
1	-1.649793	-3.782738	-0.881125
6	-1.545129	0.668625	0.345104
6	-4.551685	0.342633	0.984995
6	-1.976374	1.961161	0.335641
6	-4.481647	1.736862	0.447372
6	-3.339155	2.427526	0.204016
8	-5.372228	0.088861	1.849618
8	-5.711771	2.296401	0.366412
1	-5.625057	3.219781	0.088583
8	-4.302975	-4.185483	-0.54868
8	-5.660575	-2.086962	0.291854
1	-3.705945	-4.916359	-0.753174
1	-5.883258	-3.004814	0.070625
6	-0.067008	-1.627717	-0.580431
8	0.615507	-1.717808	0.659351
6	0.505024	-2.688288	-1.625428
6	1.98616	-1.743702	0.635589
6	1.997226	-2.319362	-1.833866
6	2.702898	-2.03681	-0.535868
6	4.106398	-2.07397	-0.433998
6	2.614085	-1.48244	1.852536
6	4.761414	-1.805753	0.765699
6	4.004343	-1.491362	1.8954
8	4.902347	-2.357967	-1.506778
8	4.594712	-1.120224	3.078915
1	4.362732	-2.445793	-2.302063
1	5.552801	-1.216099	2.990441
8	0.389425	-3.94579	-1.15383
1	0.180619	-0.667701	-1.053983
6	-0.963271	3.104685	0.494751
8	0.210736	2.691261	1.201689
6	-0.591072	3.823744	-0.8311
1	-0.059966	4.740791	-0.556083
6	1.393342	2.447944	0.546617
6	0.341451	2.960621	-1.678653
1	0.641948	3.562193	-2.547291
6	1.526008	2.534159	-0.846743
6	2.466061	2.106498	1.371923
6	2.796318	2.263679	-1.391558
1	2.314854	2.059601	2.444807
6	3.708814	1.844309	0.792131
6	3.88479	1.92666	-0.591037
8	3.020126	2.303869	-2.742001
1	2.209995	2.571254	-3.194036
1	-1.424401	3.854781	1.146958
1	2.461778	-3.160647	-2.366436
1	2.027708	-1.453271	-2.512367
1	-0.06864	-2.509045	-2.554733
1	5.846357	-1.795825	0.78274
1	2.026272	-1.244887	2.729915
1	4.847033	1.710967	-1.037892
1	-0.225298	2.098845	-2.066197
1	-3.452858	3.490144	-0.009195
1	-0.486237	0.539082	0.527142
8	-1.734074	4.256487	-1.553036
1	-2.177289	3.469327	-1.901053
8	4.799411	1.508225	1.5415
1	4.507587	1.158576	2.396161

*Table S59 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site h-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483736 (Hartree/Particle)
Thermal correction to Energy= 0.518451
Thermal correction to Enthalpy= 0.519395
Thermal correction to Gibbs Free Energy= 0.418231
Sum of electronic and zero-point Energies= -2021.078350
Sum of electronic and thermal Energies= -2021.043635
Sum of electronic and thermal Enthalpies= -2021.042691
Sum of electronic and thermal Free Energies= -2021.143855

Coordinates:

6	-2.362232	-0.529491	0.104913
6	-3.777963	-0.553907	0.33661
6	-4.502044	-1.71302	0.021913
6	-3.860838	-2.908329	-0.519081
6	-2.435432	-2.876952	-0.657291
6	-1.705997	-1.755214	-0.363101
1	-1.956552	-3.789494	-0.987314
6	-1.537465	0.627848	0.303374
6	-4.573306	0.522321	0.998505
6	-1.874338	1.962944	0.371744
6	-4.384044	1.941772	0.575343
6	-3.184775	2.545334	0.346063
8	-5.44378	0.270029	1.813779
8	-5.549262	2.619873	0.581048
1	-5.38645	3.54868	0.359834
8	-4.600042	-3.882255	-0.803388
8	-5.818334	-1.82209	0.148097
1	-5.999165	-2.734484	-0.188112
6	-0.199219	-1.78682	-0.595031
8	0.443761	-1.78399	0.701398
6	0.356967	-2.983164	-1.39089
6	1.827894	-1.803089	0.695633
6	1.844098	-2.72239	-1.669992
6	2.552243	-2.256933	-0.416647
6	3.953634	-2.274314	-0.306577
6	2.446976	-1.383391	1.8718
6	4.602844	-1.850711	0.852649
6	3.838392	-1.395939	1.924893
8	4.752055	-2.698346	-1.32847
8	4.428702	-0.873597	3.057137
1	4.209606	-2.932685	-2.091976
1	5.368881	-1.101113	3.046176
8	0.189636	-4.211906	-0.697918
1	0.327281	-4.033743	0.244605
1	0.104458	-0.876619	-1.130263
6	-0.762127	3.016415	0.490229
8	0.401169	2.473055	1.115211
6	-0.422153	3.753257	-0.839131
1	0.134613	4.655406	-0.566831
6	1.59179	2.336936	0.438558
6	0.472369	2.895544	-1.732483
1	0.724846	3.500021	-2.613629
6	1.696541	2.488663	-0.950542
6	2.688121	2.015235	1.235728
6	2.971332	2.31147	-1.523056
1	2.555281	1.913218	2.306852
6	3.932113	1.828706	0.62864
6	4.084237	1.985826	-0.75074
8	3.179794	2.435784	-2.869652
1	2.34433	2.635963	-3.309727
1	-1.128667	3.778985	1.187767
1	2.263926	-3.667957	-2.038166
1	1.943753	-1.983916	-2.479772
1	-0.183304	-3.082397	-2.337381
1	5.68753	-1.837457	0.875506
1	1.856274	-1.028154	2.706481
1	5.048251	1.834309	-1.219732
1	-0.102452	2.028214	-2.095352
1	-3.209462	3.626468	0.214964
1	-0.476276	0.433742	0.383268
8	-1.582138	4.221793	-1.507486
1	-2.05487	3.45275	-1.857099
8	5.037105	1.491669	1.352719
1	4.753161	1.108466	2.197913

*Table S60 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site i-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.483069 (Hartree/Particle)
Thermal correction to Energy= 0.518083
Thermal correction to Enthalpy= 0.519027
Thermal correction to Gibbs Free Energy= 0.417553
Sum of electronic and zero-point Energies= -2021.060116
Sum of electronic and thermal Energies= -2021.025102
Sum of electronic and thermal Enthalpies= -2021.024158
Sum of electronic and thermal Free Energies= -2021.125632

Coordinates:

6	-2.349492	-0.527648	0.136171
6	-3.731231	-0.588685	0.370277
6	-4.532404	-1.783535	0.043092
6	-3.782216	-2.952429	-0.4068
6	-2.403574	-2.903281	-0.563994
6	-1.679591	-1.738072	-0.325778
1	-1.871721	-3.799763	-0.867621
6	-1.534029	0.659454	0.341909
6	-4.521965	0.472635	1.050841
6	-1.911818	1.973395	0.341639
6	-4.419885	1.865199	0.518496
6	-3.250257	2.502316	0.242445
8	-5.299239	0.230984	1.955755
8	-5.621621	2.475686	0.468158
1	-5.510296	3.387364	0.160709
8	-4.511644	-4.050122	-0.660805
8	-5.771991	-1.816633	0.099741
1	-3.926785	-4.765487	-0.95125
6	-0.180813	-1.747038	-0.582159
8	0.47965	-1.80812	0.704577
6	0.38037	-2.890861	-1.449217
6	1.863765	-1.798615	0.677627
6	1.859322	-2.593103	-1.734342
6	2.578376	-2.182952	-0.46705
6	3.981459	-2.181425	-0.376586
6	2.4919	-1.42703	1.864345
6	4.639706	-1.810197	0.795225
6	3.88435	-1.42097	1.899916
8	4.772628	-2.539604	-1.429273
8	4.478402	-0.954733	3.050899
1	4.226183	-2.713988	-2.205686
1	5.43136	-1.108877	2.99033
8	0.240272	-4.159292	-0.818073
1	0.456979	-4.035975	0.118778
1	0.103818	-0.804314	-1.068017
6	-0.847595	3.073631	0.478032
8	0.323431	2.597206	1.146695
6	-0.488793	3.798189	-0.850715
1	0.059626	4.705269	-0.577162
6	1.508251	2.401878	0.478133
6	0.42113	2.932982	-1.720299
1	0.697082	3.532759	-2.597957
6	1.626188	2.516728	-0.913988
6	2.594084	2.070978	1.288507
6	2.898689	2.291598	-1.474259
1	2.453541	2.000828	2.361455
6	3.836937	1.845152	0.693605
6	4.000181	1.960866	-0.688534
8	3.114197	2.372761	-2.823475
1	2.290288	2.608287	-3.268039
1	-1.262119	3.832233	1.151708
1	2.289942	-3.509343	-2.159783
1	1.933397	-1.810162	-2.503952
1	-0.174732	-2.952543	-2.39026
1	5.724346	-1.782803	0.804507
1	1.907004	-1.122281	2.722792
1	4.963354	1.776667	-1.147387
1	-0.152618	2.068445	-2.091359
1	-3.318267	3.569806	0.036224
1	-0.477007	0.482238	0.493184
8	-1.636535	4.254596	-1.549143
1	-2.096758	3.479178	-1.901331
8	4.935141	1.509664	1.430961
1	4.645576	1.148355	2.282742

*Table S61 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site b-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482406 (Hartree/Particle)
Thermal correction to Energy= 0.517734
Thermal correction to Enthalpy= 0.518678
Thermal correction to Gibbs Free Energy= 0.416340
Sum of electronic and zero-point Energies= -2021.074948
Sum of electronic and thermal Energies= -2021.039620
Sum of electronic and thermal Enthalpies= -2021.038676
Sum of electronic and thermal Free Energies= -2021.141014

Coordinates:

6	-2.345064	-0.49303	0.138405
6	-3.754308	-0.586361	0.371522
6	-4.446439	-1.776978	0.111984
6	-3.745565	-2.894147	-0.368807
6	-2.373406	-2.838299	-0.558867
6	-1.656026	-1.666886	-0.318271
1	-1.845241	-3.727871	-0.885749
6	-1.573428	0.708585	0.366016
6	-4.555779	0.509611	1.003172
6	-1.952026	2.060907	0.420714
6	-4.508294	1.911355	0.399549
6	-3.236537	2.596248	0.32833
8	-5.291377	0.305787	1.949031
8	-5.56638	2.46368	0.098318
8	-4.512302	-4.002518	-0.602347
8	-5.781139	-1.860689	0.296834
1	-3.956132	-4.740604	-0.884029
1	-6.059704	-2.757725	0.056089
6	-0.158667	-1.662238	-0.585717
8	0.513256	-1.766185	0.692937
6	0.393854	-2.777153	-1.496762
6	1.896462	-1.774754	0.657454
6	1.871157	-2.475203	-1.783155
6	2.60109	-2.124612	-0.504477
6	4.004569	-2.145753	-0.420917
6	2.535895	-1.457013	1.85395
6	4.673259	-1.829417	0.760733
6	3.928402	-1.469292	1.882537
8	4.785789	-2.474301	-1.49083
8	4.532549	-1.049819	3.04514
1	4.234438	-2.596688	-2.273671
1	5.485782	-1.193344	2.966989
8	0.256627	-4.067801	-0.909095
1	0.50345	-3.981042	0.024354
1	0.12846	-0.707049	-1.043823
6	-0.845201	3.125972	0.545213
8	0.316451	2.605663	1.199527
6	-0.478723	3.837465	-0.787739
1	0.122694	4.711272	-0.516256
6	1.487517	2.383981	0.513003
6	0.378007	2.932469	-1.673065
1	0.662158	3.519998	-2.556305
6	1.581865	2.478145	-0.883121
6	2.581438	2.045393	1.309124
6	2.840625	2.222284	-1.461496
1	2.458576	1.993917	2.385341
6	3.810503	1.793592	0.696385
6	3.950216	1.88408	-0.690171
8	3.033014	2.279779	-2.81524
1	2.208831	2.538486	-3.246625
1	-1.225754	3.896868	1.222384
1	2.293987	-3.374287	-2.250825
1	1.943334	-1.659707	-2.518294
1	-0.170375	-2.805652	-2.43382
1	5.758211	-1.816287	0.765187
1	1.959375	-1.175418	2.7259
1	4.902498	1.679037	-1.162734
1	-0.23406	2.091431	-2.035761
1	-3.338305	3.676574	0.260091
1	-0.509632	0.547196	0.482941
8	-1.608605	4.361013	-1.456878
1	-2.173319	3.622801	-1.72808
8	4.918912	1.458727	1.418887
1	4.643996	1.117694	2.283259

*Table S62 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 3-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481306 (Hartree/Particle)
Thermal correction to Energy= 0.516483
Thermal correction to Enthalpy= 0.517427
Thermal correction to Gibbs Free Energy= 0.415796
Sum of electronic and zero-point Energies= -2021.036813
Sum of electronic and thermal Energies= -2021.001636
Sum of electronic and thermal Enthalpies= -2021.000692
Sum of electronic and thermal Free Energies= -2021.102322

Coordinates:

6	-2.326575	-0.534292	0.152534
6	-3.742398	-0.549331	0.344333
6	-4.479198	-1.727607	0.101972
6	-3.816532	-2.887807	-0.308824
6	-2.441217	-2.893945	-0.472785
6	-1.683581	-1.742111	-0.257097
1	-1.943331	-3.812063	-0.767108
6	-1.493956	0.638488	0.404025
6	-4.543983	0.60251	0.862782
6	-1.826928	1.959641	0.355638
6	-4.332849	1.944772	0.237887
6	-3.12297	2.526499	0.066239
8	-5.416222	0.466724	1.702006
8	-5.505841	2.577076	-0.001624
1	-5.322701	3.457922	-0.359924
8	-4.626648	-3.976387	-0.524355
8	-5.825928	-1.750002	0.22714
1	-4.091018	-4.744366	-0.760108
1	-6.123084	-2.643009	-0.006983
6	-0.191393	-1.784427	-0.536464
8	0.512924	-1.882562	0.731276
6	0.316548	-2.936907	-1.424771
6	1.892962	-1.887048	0.652013
6	1.791438	-2.677281	-1.759503
6	2.560783	-2.276352	-0.519508
6	3.966052	-2.286609	-0.485624
6	2.573478	-1.51911	1.811885
6	4.674545	-1.915471	0.656674
6	3.96544	-1.519488	1.788835
8	4.710515	-2.651919	-1.569692
8	4.610191	-1.041208	2.910635
1	4.128572	-2.842016	-2.316195
1	5.554826	-1.232911	2.828863
8	0.17086	-4.202068	-0.784916
1	0.379793	-4.066389	0.152255
1	0.112018	-0.844098	-1.014115
6	-0.794257	3.028568	0.693337
8	0.398681	2.523869	1.263058
6	-0.416084	4.000729	-0.534904
1	0.246115	4.739333	-0.039512
6	1.551184	2.365789	0.528367
6	0.39894	3.176667	-1.550525
1	0.671803	3.853527	-2.371182
6	1.61448	2.63386	-0.848171
6	2.661784	1.952445	1.262765
6	2.869337	2.472016	-1.471591
1	2.559207	1.77346	2.327051
6	3.88312	1.797026	0.604781
6	3.994816	2.058338	-0.764417
8	3.038932	2.704076	-2.808082
1	2.18921	2.934619	-3.204715
1	-1.226459	3.68207	1.458139
1	2.186967	-3.60586	-2.192778
1	1.859278	-1.899806	-2.535243
1	-0.271829	-2.985346	-2.345995
1	5.758772	-1.89264	0.621778
1	2.026689	-1.210838	2.693946
1	4.941045	1.925414	-1.273706
1	-0.255148	2.401611	-1.970439
1	-3.116823	3.57771	-0.228034
1	-0.466791	0.422124	0.671027
8	-1.521734	4.576742	-1.031247
8	5.007599	1.395954	1.260392
1	4.758322	0.97181	2.096967

*Table S63 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 5-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482469 (Hartree/Particle)
Thermal correction to Energy= 0.517545
Thermal correction to Enthalpy= 0.518489
Thermal correction to Gibbs Free Energy= 0.417156
Sum of electronic and zero-point Energies= -2021.065804
Sum of electronic and thermal Energies= -2021.030729
Sum of electronic and thermal Enthalpies= -2021.029785
Sum of electronic and thermal Free Energies= -2021.131118

Coordinates:

6	-2.329047	-0.494028	0.12856
6	-3.735767	-0.532007	0.3733
6	-4.46888	-1.710936	0.117208
6	-3.8101	-2.851292	-0.348491
6	-2.437505	-2.843721	-0.539379
6	-1.685271	-1.690924	-0.315374
1	-1.938563	-3.75351	-0.856986
6	-1.504466	0.69318	0.324228
6	-4.519446	0.578563	0.9956
6	-1.849445	2.011138	0.30447
6	-4.362867	1.961437	0.450647
6	-3.179366	2.568298	0.185656
8	-5.341289	0.379642	1.873355
8	-5.553162	2.603755	0.380096
1	-5.406284	3.515254	0.088606
8	-4.617785	-3.94016	-0.576117
8	-5.811058	-1.749122	0.283818
1	-4.080785	-4.70175	-0.828602
1	-6.106588	-2.640913	0.04308
6	-0.192923	-1.723045	-0.589043
8	0.489447	-1.788452	0.69398
6	0.346927	-2.879268	-1.450632
6	1.867922	-1.791312	0.649966
6	1.827461	-2.603354	-1.754794
6	2.566622	-2.183436	-0.501783
6	3.970919	-2.193364	-0.428443
6	2.516081	-1.422272	1.829307
6	4.64794	-1.827196	0.735839
6	3.908069	-1.435411	1.849326
8	4.745469	-2.559662	-1.489042
8	4.520952	-0.972902	2.996445
1	4.190432	-2.709022	-2.264923
1	5.466755	-1.169047	2.941495
8	0.197541	-4.14041	-0.805103
1	0.381458	-3.997975	0.136068
1	0.107826	-0.789074	-1.080231
6	-0.76571	3.090004	0.434348
8	0.396183	2.594199	1.126764
6	-0.376676	3.784489	-0.907167
1	0.179541	4.690619	-0.644131
6	1.568499	2.376541	0.455266
6	0.52791	2.888302	-1.748388
1	0.870438	3.409621	-2.645664
6	1.701577	2.474584	-0.914621
6	2.667406	2.04009	1.278484
6	3.011817	2.242098	-1.518146
1	2.515818	1.988763	2.351823
6	3.939036	1.79662	0.712869
6	4.121419	1.899986	-0.65072
8	3.160884	2.326095	-2.762337
1	-1.162096	3.867419	1.096687
1	2.245437	-3.529878	-2.170232
1	1.901553	-1.831868	-2.535687
1	-0.217221	-2.940941	-2.386185
1	5.732828	-1.810372	0.732322
1	1.943514	-1.122142	2.69792
1	5.088348	1.712589	-1.101449
1	-0.045688	2.011175	-2.088772
1	-3.220109	3.63126	-0.047884
1	-0.453719	0.494829	0.489592
8	-1.515634	4.244486	-1.618144
1	-1.944223	3.474119	-2.017736
8	5.005939	1.481832	1.501454
1	4.698641	1.023836	2.300986

*Table S64 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 4'α-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482150 (Hartree/Particle)
Thermal correction to Energy= 0.517689
Thermal correction to Enthalpy= 0.518634
Thermal correction to Gibbs Free Energy= 0.416207
Sum of electronic and zero-point Energies= -2021.055828
Sum of electronic and thermal Energies= -2021.020289
Sum of electronic and thermal Enthalpies= -2021.019345
Sum of electronic and thermal Free Energies= -2021.121771

Coordinates:

6	-2.336874	-0.466356	0.134491
6	-3.745255	-0.451265	0.376746
6	-4.527425	-1.593603	0.10279
6	-3.915575	-2.751359	-0.379276
6	-2.542471	-2.801457	-0.557887
6	-1.738825	-1.688284	-0.312958
1	-2.07958	-3.722844	-0.893846
6	-1.475148	0.694957	0.327411
6	-4.487427	0.676543	1.018512
6	-1.781393	2.023432	0.309425
6	-4.294732	2.057738	0.484569
6	-3.094021	2.624394	0.208612
8	-5.305174	0.493785	1.903674
8	-5.462934	2.741574	0.436235
1	-5.28784	3.650976	0.154023
8	-4.766395	-3.801491	-0.632788
8	-5.871486	-1.576105	0.264504
1	-4.257659	-4.576958	-0.901307
1	-6.20283	-2.451338	0.010261
6	-0.243868	-1.787232	-0.563263
8	0.413305	-1.912097	0.731916
6	0.276964	-2.909177	-1.485405
6	1.783457	-1.888037	0.711858
6	1.768225	-2.79833	-1.569683
6	2.486008	-2.309811	-0.461549
6	3.913977	-2.261362	-0.399262
6	2.437925	-1.512078	1.873212
6	4.578203	-1.889067	0.758395
6	3.836667	-1.516185	1.885603
8	4.672991	-2.600317	-1.478776
8	4.451988	-1.068395	3.029117
1	4.129014	-2.547993	-2.276151
1	5.404396	-1.215022	2.943362
8	-0.087077	-4.238432	-1.0593
1	0.285802	-4.35278	-0.172331
1	0.107686	-0.852591	-1.018616
6	-0.664538	3.071413	0.430277
8	0.479923	2.548424	1.114313
6	-0.267398	3.748787	-0.912626
1	0.308577	4.645066	-0.660471
6	1.670992	2.327438	0.4686
6	0.621517	2.831137	-1.750363
1	0.915747	3.393865	-2.646215
6	1.811221	2.413291	-0.923374
6	2.740965	1.9958	1.300102
6	3.087042	2.158208	-1.461488
1	2.584079	1.946518	2.372083
6	3.986875	1.737732	0.726467
6	4.172781	1.825323	-0.654325
8	3.323072	2.212554	-2.808413
1	2.501531	2.421736	-3.270238
1	-1.041774	3.864365	1.086613
1	2.264539	-3.322843	-2.380557
1	-0.188007	-2.797555	-2.47057
1	5.661889	-1.834568	0.749298
1	1.87496	-1.20522	2.745796
1	5.138701	1.61613	-1.09642
1	0.027502	1.969013	-2.093144
1	-3.102823	3.69168	-0.009417
1	-0.428034	0.469798	0.483341
8	-1.392763	4.223372	-1.635469
1	-1.891546	3.452813	-1.943524
8	5.067043	1.391119	1.48858
1	4.748488	1.070293	2.345617

*Table S65 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 4'-β-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482150 (Hartree/Particle)
Thermal correction to Energy= 0.517690
Thermal correction to Enthalpy= 0.518634
Thermal correction to Gibbs Free Energy= 0.416200
Sum of electronic and zero-point Energies= -2021.055828
Sum of electronic and thermal Energies= -2021.020288
Sum of electronic and thermal Enthalpies= -2021.019344
Sum of electronic and thermal Free Energies= -2021.121778

Coordinates:

6	-2.33689	-0.466399	0.134431
6	-3.745314	-0.451431	0.37657
6	-4.52733	-1.593883	0.102545
6	-3.915281	-2.751556	-0.379487
6	-2.542162	-2.801504	-0.558001
6	-1.738658	-1.688253	-0.312972
1	-2.079187	-3.722776	-0.894145
6	-1.475274	0.694941	0.327464
6	-4.487688	0.676223	1.018335
6	-1.781534	2.023423	0.309769
6	-4.294894	2.057601	0.484957
6	-3.094156	2.624394	0.209325
8	-5.30574	0.493221	1.903194
8	-5.463046	2.741544	0.436921
1	-5.287903	3.651005	0.154934
8	-4.765984	-3.801723	-0.633316
8	-5.871394	-1.576626	0.264077
1	-4.256936	-4.577981	-0.898947
1	-6.202476	-2.452094	0.010287
6	-0.243664	-1.787121	-0.563163
8	0.413413	-1.912159	0.731997
6	0.277312	-2.908783	-1.485594
6	1.783572	-1.887992	0.712007
6	1.768592	-2.797993	-1.569626
6	2.486266	-2.309523	-0.46141
6	3.91421	-2.261062	-0.399043
6	2.437954	-1.512228	1.873478
6	4.578324	-1.889049	0.758796
6	3.8367	-1.516437	1.886008
8	4.673319	-2.599688	-1.478504
8	4.45196	-1.069111	3.029742
1	4.129213	-2.548105	-2.275831
1	5.404355	-1.215835	2.944019
8	-0.086793	-4.238264	-1.06025
1	0.286966	-4.353457	-0.173762
1	0.107919	-0.852414	-1.018378
6	-0.664618	3.071344	0.430554
8	0.479896	2.548151	1.114291
6	-0.267703	3.748867	-0.912349
1	0.30828	4.645137	-0.660188
6	1.670937	2.327428	0.468439
6	0.621115	2.831293	-1.750303
1	0.915231	3.394085	-2.646143
6	1.810965	2.413402	-0.923534
6	2.741027	1.995885	1.299812
6	3.086746	2.158447	-1.461819
1	2.584262	1.946525	2.371808
6	3.986891	1.737984	0.726016
6	4.172605	1.825584	-0.654805
8	3.322623	2.213034	-2.80876
1	2.500761	2.421036	-3.270546
1	-1.041686	3.864225	1.087081
1	2.264755	-3.322223	-2.380783
1	-0.187498	-2.796675	-2.470792
1	5.662013	-1.834531	0.749769
1	1.874863	-1.205645	2.746079
1	5.138477	1.616454	-1.097036
1	0.027041	1.969196	-2.093041
1	-3.102993	3.691807	-0.008104
1	-0.428113	0.469841	0.483151
8	-1.393185	4.223459	-1.634993
1	-1.892399	3.452907	-1.942374
8	5.067179	1.391501	1.488011
1	4.748772	1.071208	2.345298

*Table S66 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 3'-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482490 (Hartree/Particle)
Thermal correction to Energy= 0.517875
Thermal correction to Enthalpy= 0.518819
Thermal correction to Gibbs Free Energy= 0.416794
Sum of electronic and zero-point Energies= -2021.037511
Sum of electronic and thermal Energies= -2021.002126
Sum of electronic and thermal Enthalpies= -2021.001181
Sum of electronic and thermal Free Energies= -2021.103206

Coordinates:

6	-2.27149	0.533239	-0.128044
6	-3.686492	0.562826	-0.331809
6	-4.457885	1.642221	0.147658
6	-3.832194	2.69908	0.809027
6	-2.448289	2.738822	0.906819
6	-1.648256	1.705427	0.413135
1	-1.988845	3.584702	1.408076
6	-1.443969	-0.640557	-0.364041
6	-4.450246	-0.431637	-1.14934
6	-1.803939	-1.953096	-0.477884
6	-4.305178	-1.880282	-0.839789
6	-3.13445	-2.509248	-0.562688
8	-5.247659	-0.075082	-1.999749
8	-5.47927	-2.540629	-0.980503
1	-5.333935	-3.485541	-0.827958
8	-4.674037	3.667998	1.299228
8	-5.805992	1.642201	0.026718
1	-4.162969	4.397526	1.671531
1	-6.134978	2.45677	0.437124
6	-0.139268	1.849141	0.576795
8	0.502579	1.578871	-0.714684
6	0.351036	3.200722	1.016102
6	1.870323	1.747514	-0.740146
6	1.81252	3.210365	1.349586
6	2.563278	2.492579	0.232243
6	3.958275	2.592062	0.102406
6	2.531803	1.140945	-1.808717
6	4.644309	1.974305	-0.942854
6	3.916705	1.24843	-1.883143
8	4.716125	3.296966	0.994621
8	4.548532	0.545915	-2.892585
1	4.154381	3.639589	1.700732
1	5.463862	0.853034	-2.952914
8	0.002019	4.281451	0.236286
1	-0.733966	4.035462	-0.344675
1	0.240866	1.102306	1.288399
6	-0.717726	-3.039036	-0.547062
8	0.507652	-2.530058	-1.078776
6	-0.49247	-3.80147	0.791177
1	0.067399	-4.710881	0.550283
6	1.639644	-2.414393	-0.30692
6	0.344371	-2.971179	1.763574
1	0.516976	-3.590918	2.653458
6	1.631676	-2.575454	1.08496
6	2.802051	-2.10427	-1.009812
6	2.857183	-2.412918	1.759554
1	2.759464	-1.999212	-2.087714
6	3.992866	-1.922718	-0.303035
6	4.031581	-2.088953	1.083393
8	2.953322	-2.549704	3.118443
1	2.080312	-2.738306	3.484717
1	-1.05542	-3.780422	-1.281036
1	2.139622	4.254968	1.435009
1	1.986244	2.725289	2.32146
1	5.726742	2.042897	-0.980307
1	1.974719	0.568177	-2.538471
1	4.954506	-1.944362	1.630851
1	-0.242774	-2.098038	2.089785
1	-3.184544	-3.595188	-0.490703
1	-0.379661	-0.452683	-0.391402
8	-1.708008	-4.255858	1.365574
1	-2.203565	-3.477458	1.658419
8	5.1509	-1.579131	-0.934237
1	4.931656	-1.206035	-1.804237

*Table S67 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 2'-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481683 (Hartree/Particle)
Thermal correction to Energy= 0.517553
Thermal correction to Enthalpy= 0.518498
Thermal correction to Gibbs Free Energy= 0.414971
Sum of electronic and zero-point Energies= -2021.057763
Sum of electronic and thermal Energies= -2021.021893
Sum of electronic and thermal Enthalpies= -2021.020949
Sum of electronic and thermal Free Energies= -2021.124476

Coordinates:

6	-2.276812	0.56292	-0.212311
6	-3.698299	0.619361	-0.371136
6	-4.429297	1.7333	0.081704
6	-3.755531	2.829562	0.645544
6	-2.381276	2.865282	0.682235
6	-1.592626	1.771344	0.236001
1	-1.890612	3.78782	0.97373
6	-1.502562	-0.647543	-0.365843
6	-4.511194	-0.385922	-1.129631
6	-1.8995	-1.958188	-0.433718
6	-4.397558	-1.827227	-0.786575
6	-3.238746	-2.480774	-0.507153
8	-5.324904	-0.032023	-1.967167
8	-5.58827	-2.46556	-0.901892
1	-5.46105	-3.408548	-0.724515
8	-4.572075	3.853735	1.061055
8	-5.781247	1.760307	0.01359
1	-4.038625	4.609309	1.338349
1	-6.071267	2.616646	0.364366
6	-0.180107	1.985103	0.290131
8	0.612261	1.308402	-0.609055
6	0.459227	3.050586	1.140239
6	1.967357	1.538522	-0.702001
6	1.895438	2.667953	1.522209
6	2.659336	2.227471	0.301074
6	4.042761	2.395831	0.124803
6	2.58685	1.029297	-1.839404
6	4.69968	1.884035	-0.996364
6	3.966711	1.18403	-1.953537
8	4.821181	3.04522	1.037211
8	4.573404	0.576734	-3.028798
1	4.284714	3.305937	1.796619
1	5.505475	0.834198	-3.046476
8	0.421597	4.36177	0.541418
1	0.851849	4.301473	-0.323867
6	-0.836582	-3.068353	-0.432118
8	0.386639	-2.638071	-1.040375
6	-0.592928	-3.709011	0.962757
1	-0.058461	-4.650374	0.798314
6	1.533599	-2.459258	-0.308089
6	0.282258	-2.809495	1.835669
1	0.469147	-3.349256	2.773709
6	1.557347	-2.495617	1.09278
6	2.68269	-2.215852	-1.061096
6	2.796855	-2.273987	1.722632
1	2.615315	-2.208622	-2.143367
6	3.888147	-1.976749	-0.398943
6	3.957255	-2.01561	0.995154
8	2.921033	-2.28173	3.085912
1	2.059026	-2.455711	3.484512
1	-1.204611	-3.866199	-1.087345
1	2.33779	3.553408	1.995838
1	1.873262	1.87056	2.278803
1	-0.128017	3.161784	2.054513
1	5.776215	1.998957	-1.071711
1	2.015141	0.495416	-2.586758
1	4.892237	-1.825873	1.507218
1	-0.281267	-1.899669	2.095082
1	-3.317744	-3.563379	-0.406829
1	-0.432719	-0.506116	-0.353867
8	-1.807214	-4.076792	1.597026
1	-2.300298	-3.263399	1.778667
8	5.03768	-1.694882	-1.080138
1	4.808859	-1.401302	-1.975346

*Table S68 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 4β-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481670 (Hartree/Particle)
Thermal correction to Energy= 0.517280
Thermal correction to Enthalpy= 0.518224
Thermal correction to Gibbs Free Energy= 0.415658
Sum of electronic and zero-point Energies= -2021.055399
Sum of electronic and thermal Energies= -2021.019789
Sum of electronic and thermal Enthalpies= -2021.018845
Sum of electronic and thermal Free Energies= -2021.121411

Coordinates:

6	-2.303824	-0.50689	0.114717
6	-3.703117	-0.594677	0.388359
6	-4.406666	-1.788917	0.124038
6	-3.726319	-2.896647	-0.385611
6	-2.358708	-2.84395	-0.602373
6	-1.634623	-1.675745	-0.364649
1	-1.840093	-3.730447	-0.952654
6	-1.518448	0.708658	0.309192
6	-4.509182	0.48112	1.042993
6	-1.918981	2.010264	0.293057
6	-4.425782	1.863466	0.484098
6	-3.27345	2.510404	0.184899
8	-5.291939	0.248868	1.947562
8	-5.644444	2.45388	0.42752
1	-5.541017	3.364402	0.115232
8	-4.506409	-4.003608	-0.62479
8	-5.743337	-1.870447	0.322755
1	-3.950941	-4.742604	-0.903098
1	-6.017845	-2.765839	0.071095
6	-0.142035	-1.669567	-0.638206
8	0.528531	-1.794333	0.644779
6	0.419322	-2.770197	-1.558561
6	1.907486	-1.8032	0.619565
6	1.899017	-2.45994	-1.832027
6	2.621968	-2.127033	-0.543986
6	4.024379	-2.149759	-0.448388
6	2.537534	-1.514551	1.829161
6	4.683927	-1.86134	0.746391
6	3.928866	-1.531369	1.870909
8	4.814432	-2.453542	-1.519677
8	4.520776	-1.147536	3.05317
1	4.265806	-2.56893	-2.305654
1	5.478091	-1.254668	2.967497
8	0.285229	-4.069351	-0.988204
1	0.486321	-3.982793	-0.043811
1	0.146087	-0.706739	-1.078205
6	-0.888383	3.143132	0.406238
8	0.276215	2.743045	1.143542
6	-0.531029	3.817868	-0.964426
1	-0.248456	4.856989	-0.736152
6	1.482378	2.500208	0.551124
6	0.608782	3.129507	-1.63615
6	1.674575	2.653003	-0.853551
6	2.504236	2.083988	1.393399
6	2.981818	2.352854	-1.355895
1	2.309125	1.98406	2.455609
6	3.765767	1.803751	0.850929
6	4.00673	1.939078	-0.523889
8	3.259329	2.472609	-2.68735
1	2.569965	3.004837	-3.106506
1	-1.342121	3.916769	1.034873
1	2.32756	-3.351118	-2.30991
1	1.972377	-1.63363	-2.554812
1	-0.138114	-2.787391	-2.500037
1	5.768937	-1.853786	0.761881
1	1.951876	-1.257239	2.702673
1	4.987999	1.726004	-0.929008
1	0.65965	3.222411	-2.717913
1	-3.361319	3.563128	-0.079817
1	-0.457751	0.551828	0.458554
8	-1.66623	3.951317	-1.810705
1	-1.921648	3.057582	-2.083691
8	4.81423	1.412012	1.625707
1	4.487029	1.022738	2.451252

*Table S69 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 4α-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481671 (Hartree/Particle)
Thermal correction to Energy= 0.517280
Thermal correction to Enthalpy= 0.518224
Thermal correction to Gibbs Free Energy= 0.415661
Sum of electronic and zero-point Energies= -2021.055398
Sum of electronic and thermal Energies= -2021.019789
Sum of electronic and thermal Enthalpies= -2021.018845
Sum of electronic and thermal Free Energies= -2021.121408

Coordinates:

6	-2.304021	-0.506572	0.114445
6	-3.703373	-0.593942	0.38799
6	-4.407308	-1.787887	0.123317
6	-3.727292	-2.895747	-0.386473
6	-2.359619	-2.843515	-0.603005
6	-1.635152	-1.675625	-0.36496
1	-1.841282	-3.730195	-0.953226
6	-1.518271	0.708694	0.308955
6	-4.509126	0.481806	1.043076
6	-1.918384	2.010457	0.293332
6	-4.425223	1.864452	0.485074
6	-3.272703	2.511119	0.185968
8	-5.292058	0.249278	1.947439
8	-5.643625	2.455468	0.429234
1	-5.539892	3.366058	0.117251
8	-4.507739	-4.00239	-0.625953
8	-5.744023	-1.869023	0.321872
1	-3.952507	-4.741512	-0.904397
1	-6.018799	-2.764268	0.069986
6	-0.142479	-1.670023	-0.638226
8	0.527803	-1.794424	0.644924
6	0.418656	-2.771336	-1.557887
6	1.906787	-1.803573	0.619926
6	1.898515	-2.461803	-1.831252
6	2.621357	-2.128327	-0.543301
6	4.023754	-2.151301	-0.447487
6	2.536711	-1.514219	1.829422
6	4.683184	-1.862141	0.747173
6	3.928027	-1.531245	1.871348
8	4.8139	-2.455862	-1.518478
8	4.51989	-1.146562	3.053394
1	4.265228	-2.573051	-2.304157
1	5.477094	-1.255173	2.968352
8	0.284004	-4.070095	-0.98676
1	0.483966	-3.982803	-0.04219
1	0.146057	-0.707512	-1.078654
6	-0.887325	3.142888	0.4063
8	0.27729	2.742128	1.143194
6	-0.530233	3.817722	-0.964438
1	-0.247538	4.856804	-0.736069
6	1.483442	2.499758	0.550554
6	0.60944	3.129439	-1.636461
1	0.660195	3.222339	-2.718215
6	1.675432	2.653045	-0.854078
6	2.505441	2.083338	1.392572
6	2.982709	2.35337	-1.356653
1	2.310407	1.98287	2.454746
6	3.766954	1.803488	0.84988
6	4.007773	1.939472	-0.524921
8	3.260059	2.473758	-2.688088
1	2.570486	3.005944	-3.106949
1	-1.340536	3.916669	1.035148
1	2.326759	-3.353476	-2.308499
1	1.97236	-1.635999	-2.554559
1	-0.138597	-2.788829	-2.49947
1	5.768192	-1.854672	0.762788
1	1.95098	-1.256224	2.702683
1	4.98906	1.726788	-0.930202
1	-3.36028	3.564055	-0.078007
1	-0.457564	0.551573	0.457906
8	-1.665595	3.951342	-1.810378
1	-1.921519	3.057631	-2.082968
8	4.815496	1.411369	1.624293
1	4.488445	1.02234	2.450018

*Table S70 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 3-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.481630 (Hartree/Particle)
Thermal correction to Energy= 0.517390
Thermal correction to Enthalpy= 0.518335
Thermal correction to Gibbs Free Energy= 0.415384
Sum of electronic and zero-point Energies= -2021.045280
Sum of electronic and thermal Energies= -2021.009520
Sum of electronic and thermal Enthalpies= -2021.008576
Sum of electronic and thermal Free Energies= -2021.111526

Coordinates:

6	-2.372189	-0.496508	0.138353
6	-3.785856	-0.470304	0.339213
6	-4.561576	-1.621559	0.083871
6	-3.939784	-2.795672	-0.347394
6	-2.56617	-2.843575	-0.517543
6	-1.771296	-1.718974	-0.289802
1	-2.099124	-3.772637	-0.828032
6	-1.501352	0.648842	0.397264
6	-4.543623	0.698052	0.883376
6	-1.788641	1.977024	0.347125
6	-4.295452	2.042345	0.277532
6	-3.072265	2.586614	0.075433
8	-5.414127	0.577632	1.727834
8	-5.453587	2.719391	0.074872
1	-5.245267	3.607123	-0.249908
8	-4.786765	-3.855845	-0.576367
8	-5.908803	-1.602057	0.215753
1	-4.274171	-4.639935	-0.809625
1	-6.233289	-2.483494	-0.025642
6	-0.282192	-1.804867	-0.56846
8	0.41692	-1.953785	0.698653
6	0.193134	-2.955136	-1.477009
6	1.79552	-1.989087	0.620555
6	1.675833	-2.730851	-1.805868
6	2.454435	-2.367293	-0.559825
6	3.858925	-2.408436	-0.526995
6	2.484038	-1.666281	1.789061
6	4.575787	-2.081216	0.623497
6	3.875513	-1.700443	1.766506
8	4.594669	-2.765488	-1.620462
8	4.530676	-1.275628	2.903608
1	4.006503	-2.930013	-2.368145
1	5.473016	-1.471844	2.807305
8	0.01224	-4.226254	-0.858067
1	0.207564	-4.105337	0.084204
1	0.053401	-0.86462	-1.023925
6	-0.686134	3.028707	0.628084
8	0.464845	2.420417	1.222877
6	-0.301891	3.864765	-0.555157
6	1.656915	2.329519	0.549318
6	0.677671	3.34189	-1.548663
1	1.050667	4.186063	-2.154322
6	1.822031	2.70207	-0.792186
6	2.717529	1.828178	1.306034
6	3.101375	2.542277	-1.355967
1	2.545592	1.564637	2.343539
6	3.973754	1.689905	0.713209
6	4.175416	2.046235	-0.622627
8	3.354478	2.879943	-2.661036
1	2.524479	3.075847	-3.112069
1	-1.090519	3.704514	1.394488
1	2.047796	-3.663796	-2.250728
1	1.765344	-1.945513	-2.571653
1	-0.395174	-2.971301	-2.399503
1	5.660278	-2.083419	0.589307
1	1.94376	-1.367527	2.678407
1	5.145738	1.92416	-1.087143
1	0.202414	2.639011	-2.264354
1	-3.045896	3.632914	-0.224824
1	-0.480537	0.401039	0.66039
8	-1.234502	4.804549	-0.922723
1	-0.900289	5.297786	-1.684343
8	5.04701	1.209777	1.404051
1	4.736562	0.747797	2.199029

*Table S71 Energetics and Cartesian coordinates of the conformer **1d** (sa-saa-ss) post-radical capture via HAB at site 2-H by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.482639 (Hartree/Particle)
Thermal correction to Energy= 0.518015
Thermal correction to Enthalpy= 0.518960
Thermal correction to Gibbs Free Energy= 0.417120
Sum of electronic and zero-point Energies= -2021.072789
Sum of electronic and thermal Energies= -2021.037413
Sum of electronic and thermal Enthalpies= -2021.036469
Sum of electronic and thermal Free Energies= -2021.138309

Coordinates:

6	-2.474157	-0.190081	-0.061665
6	-3.656357	-0.893744	-0.461902
6	-4.875904	-0.205974	-0.610034
6	-4.929876	1.176142	-0.390744
6	-3.786671	1.882011	-0.048912
6	-2.566622	1.231737	0.124999
1	-3.841861	2.958379	0.082074
6	-1.185958	-0.807437	0.123558
6	-3.675303	-2.337658	-0.850515
6	-0.831755	-2.131086	0.445018
6	-3.011859	-3.333949	0.047431
6	-1.777531	-3.231655	0.586703
8	-4.28802	-2.734782	-1.826642
8	-3.778808	-4.449612	0.179211
1	-3.291043	-5.102264	0.701641
8	-6.172098	1.744218	-0.551354
8	-6.015236	-0.86025	-0.934581
1	-6.112225	2.701438	-0.441209
1	-6.726201	-0.201709	-0.969024
6	-1.360173	2.033031	0.565393
8	-0.517427	2.264053	-0.603615
6	-1.5991	3.411669	1.205218
6	0.692854	2.86509	-0.341812
6	-0.256915	3.913669	1.768192
6	0.8783	3.666403	0.79531
6	2.150362	4.236082	0.976814
6	1.703334	2.65205	-1.280004
6	3.192494	4.014458	0.073473
6	2.953684	3.219295	-1.045723
8	2.437006	5.027882	2.050184
8	3.95285	2.919837	-1.94779
1	1.654242	5.11404	2.609191
1	4.750628	3.415015	-1.715318
8	-2.133119	4.344008	0.270557
1	-1.719514	4.14764	-0.584542
1	-0.777091	1.440025	1.280144
6	0.537592	-2.427802	0.673181
8	1.412821	-1.371099	0.557527
6	1.116176	-3.804338	0.949977
1	0.919413	-4.451228	0.085939
6	2.690435	-1.578646	0.059317
6	2.634251	-3.760721	1.212502
1	3.006154	-4.787611	1.119545
6	3.342544	-2.783325	0.316413
6	3.259453	-0.533168	-0.653971
6	4.643372	-2.923473	-0.200025
1	2.698118	0.378876	-0.811888
6	4.557718	-0.704022	-1.151965
6	5.245836	-1.901537	-0.934711
8	5.389684	-4.051398	-0.001758
1	4.882549	-4.688059	0.517332
1	-0.378694	4.986057	1.973133
1	-0.06226	3.417607	2.731089
1	-2.329439	3.329909	2.015908
1	4.16511	4.454048	0.270562
1	1.516456	2.03971	-2.153507
1	6.248193	-2.034445	-1.32286
1	2.778572	-3.48052	2.267089
1	-1.409239	-4.098089	1.128845
1	-0.34431	-0.135961	0.051802
8	0.474745	-4.484856	2.042254
1	0.461525	-3.871009	2.791217
8	5.191348	0.26469	-1.862457
1	4.619583	1.048506	-1.948533

*Table S72 Energetics and Cartesian coordinates of the neutral conformer **1a-H_2O** (as-ass-as) pre-radical capture by DFT calculations B3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.496174 (Hartree/Particle)
Thermal correction to Energy= 0.530472
Thermal correction to Enthalpy= 0.531416
Thermal correction to Gibbs Free Energy= 0.432093
Sum of electronic and zero-point Energies= -2021.770045
Sum of electronic and thermal Energies= -2021.735747
Sum of electronic and thermal Enthalpies= -2021.734803
Sum of electronic and thermal Free Energies= -2021.834126

Coordinates:

6	-2.609231	-0.054867	-0.031219
6	-3.95898	-0.556865	-0.231098
6	-5.04414	0.37574	-0.204376
6	-4.822244	1.736301	0.022809
6	-3.534823	2.204137	0.248443
6	-2.44103	1.346784	0.239286
1	-3.392449	3.263484	0.42355
6	-1.406276	-0.836201	-0.091978
6	-4.352737	-1.941333	-0.452768
6	-1.168275	-2.180382	-0.230687
6	-3.484347	-3.123539	-0.485014
6	-2.124553	-3.212968	-0.38928
8	-5.579948	-2.248487	-0.626427
8	-4.171478	-4.272378	-0.66146
1	-5.109486	-3.985442	-0.730721
8	-5.871608	2.597021	0.034802
8	-6.339191	0.051225	-0.38548
1	-6.672177	2.071029	-0.134006
1	-6.343209	-0.946244	-0.530682
6	-1.074285	1.925556	0.563605
8	-0.350275	2.098286	-0.689737
6	-1.00591	3.272872	1.305819
6	0.965406	2.489458	-0.548621
6	0.454932	3.494976	1.72682
6	1.409876	3.13911	0.607675
6	2.778026	3.46072	0.674005
6	1.811673	2.201512	-1.624424
6	3.65937	3.154178	-0.364792
6	3.160189	2.524258	-1.506187
8	3.192772	4.087847	1.812003
8	4.078742	2.171032	-2.474987
1	4.140471	4.274575	1.753989
1	3.614785	1.932126	-3.291251
8	-1.479644	4.351567	0.498372
1	-1.165712	4.190268	-0.404771
1	-0.517368	1.210804	1.179826
6	0.267166	-2.684997	-0.143513
8	1.154427	-1.652713	-0.593601
6	0.661524	-3.120206	1.289587
1	-0.053138	-3.869855	1.640232
6	2.50511	-1.837959	-0.394031
6	2.072989	-3.717721	1.250942
1	2.031548	-4.71949	0.803167
6	3.004444	-2.813247	0.476106
6	3.334927	-0.953427	-1.086558
6	4.404125	-2.878404	0.616767
1	2.890044	-0.21959	-1.743702
6	4.713912	-1.019089	-0.889008
6	5.259275	-1.998977	-0.047824
8	4.878051	-3.845354	1.458747
1	5.842147	-3.78146	1.509864
1	0.380486	-3.554684	-0.804984
1	0.57782	4.543736	2.015594
1	0.674202	2.899118	2.622336
1	-1.64641	3.246805	2.191639
1	4.715768	3.392731	-0.296544
1	1.415732	1.693454	-2.497365
1	6.334604	-2.051181	0.091683
1	2.430642	-3.850498	2.276453
1	-1.742993	-4.228151	-0.471927
1	-0.496898	-0.259116	-0.035689
8	0.55788	-2.031545	2.199619
1	1.232989	-1.380525	1.958524
8	5.575832	-0.158208	-1.498084
1	5.077448	0.569237	-1.918266

*Table S73 Energetics and Cartesian coordinates of the neutral conformer **1b-H_2O** (sa-ass-sa) pre-radical capture by DFT calculations B3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.494835 (Hartree/Particle)
Thermal correction to Energy= 0.529912
Thermal correction to Enthalpy= 0.530856
Thermal correction to Gibbs Free Energy= 0.427089
Sum of electronic and zero-point Energies= -2021.763102
Sum of electronic and thermal Energies= -2021.728025
Sum of electronic and thermal Enthalpies= -2021.727081
Sum of electronic and thermal Free Energies= -2021.830848

Coordinates:

6	-2.15793	-1.31614	0.154064
6	-2.69052	-2.65477	-0.02702
6	-4.11073	-2.82235	-0.05907
6	-4.96967	-1.72782	0.071191
6	-4.45301	-0.45361	0.268574
6	-3.08328	-0.23157	0.331902
1	-5.1458	0.373791	0.355293
6	-0.76811	-0.96246	0.147562
6	-1.92549	-3.88661	-0.16903
6	0.390204	-1.68837	0.018483
6	-0.46583	-4.03796	-0.17776
6	0.518182	-3.09181	-0.11307
8	-2.5225	-5.00778	-0.29746
8	-0.07694	-5.32629	-0.29663
1	-0.91908	-5.83041	-0.35371
8	-6.3124	-1.91552	0.016418
8	-4.74014	-4.00276	-0.21883
1	-6.46148	-2.86729	-0.11803
1	-4.00287	-4.68649	-0.28814
6	-2.58998	1.173894	0.639672
8	-2.00301	1.723472	-0.57322
6	-3.61467	2.204435	1.14283
6	-1.37881	2.948185	-0.41942
6	-2.83994	3.452341	1.599304
6	-1.74564	3.819586	0.617224
6	-1.06337	5.047743	0.680925
6	-0.4053	3.264456	-1.36575
6	-0.08017	5.395218	-0.24882
6	0.240154	4.499731	-1.27234
8	-1.33027	5.971522	1.650859
8	1.192665	4.776586	-2.21037
1	-2.00874	5.63778	2.253344
1	1.576437	5.646924	-2.03271
8	-4.5724	2.529416	0.137752
1	-4.09965	2.552689	-0.70877
1	-1.80349	1.116983	1.402676
6	1.674725	-0.87419	-0.04386
8	2.705111	-1.59502	0.655143
6	2.148578	-0.57906	-1.48379
1	1.337936	-0.08525	-2.02575
6	3.976862	-1.06807	0.608269
6	3.368136	0.34966	-1.41288
1	3.025657	1.371342	-1.19879
6	4.353821	-0.12906	-0.36605
6	4.86745	-1.55718	1.564244
6	5.683859	0.328015	-0.32556
1	4.537937	-2.28316	2.297658
6	6.182217	-1.08824	1.559063
6	6.598197	-0.14046	0.620147
8	6.155394	1.250778	-1.21535
1	5.44692	1.535828	-1.80817
1	1.514406	0.086284	0.461809
1	-3.56991	4.265157	1.702975
1	-2.42374	3.265595	2.599212
1	-4.17588	1.797544	1.98819
1	0.418518	6.355166	-0.16035
1	-0.15622	2.563434	-2.15328
1	7.614492	0.240052	0.611067
1	3.822599	0.367434	-2.41168
1	1.527322	-3.48368	-0.16357
1	-0.59221	0.100838	0.222719
8	2.418469	-1.77668	-2.20094
1	3.164938	-2.22003	-1.772
8	7.02514	-1.58733	2.509868
1	7.899253	-1.18505	2.407805

*Table S74 Energetics and Cartesian coordinates of the neutral conformer **1c-H_2O** (saaasa-ss) pre-radical capture by DFT calculations B3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.494628 (Hartree/Particle)
Thermal correction to Energy= 0.529737
Thermal correction to Enthalpy= 0.530681
Thermal correction to Gibbs Free Energy= 0.427682
Sum of electronic and zero-point Energies= -2021.748062
Sum of electronic and thermal Energies= -2021.712954
Sum of electronic and thermal Enthalpies= -2021.712010
Sum of electronic and thermal Free Energies= -2021.815009

Coordinates:

6	-2.34791	-0.48334	0.11753
6	-3.76042	-0.50117	0.360521
6	-4.50933	-1.66856	0.084686
6	-3.87034	-2.81339	-0.39667
6	-2.49427	-2.82615	-0.57409
6	-1.72339	-1.69096	-0.33085
1	-2.01298	-3.74177	-0.89818
6	-1.50325	0.68572	0.316825
6	-4.53529	0.611286	0.976768
6	-1.82475	2.011166	0.328105
6	-4.33917	2.002967	0.489565
6	-3.14256	2.593041	0.24296
8	-5.40911	0.403184	1.813579
8	-5.51318	2.683496	0.46122
1	-5.35176	3.596473	0.178575
8	-4.69548	-3.8772	-0.64155
8	-5.85838	-1.69782	0.237574
1	-4.2004	-4.61393	-1.02545
1	-6.16188	-2.56054	-0.09055
6	-0.22802	-1.75458	-0.59801
8	0.4447	-1.80788	0.692625
6	0.293076	-2.93521	-1.43714
6	1.825279	-1.85221	0.660062
6	1.779447	-2.69523	-1.73429
6	2.52086	-2.28327	-0.48013
6	3.923886	-2.32734	-0.39297
6	2.473699	-1.47892	1.837429
6	4.602471	-1.95433	0.769211
6	3.866053	-1.51926	1.87098
8	4.699567	-2.73142	-1.44199
8	4.476875	-1.05423	3.012791
1	4.146031	-2.9319	-2.20892
1	5.422067	-1.26275	2.976715
8	0.111636	-4.18616	-0.77354
1	0.289067	-4.04052	0.168348
1	0.090671	-0.83701	-1.10663
6	-0.72278	3.070142	0.479429
8	0.432667	2.530829	1.14173
6	-0.33041	3.809653	-0.8315
1	0.238635	4.695596	-0.53163
6	1.628878	2.359108	0.488349
6	0.566827	2.939437	-1.70825
1	0.853405	3.536201	-2.58247
6	1.765655	2.511651	-0.8985
6	2.704013	2.009615	1.308845
6	3.046519	2.308635	-1.44515
1	2.550671	1.905028	2.377091
6	3.955216	1.79913	0.726357
6	4.138054	1.958532	-0.64934
8	3.290441	2.435051	-2.7846
1	2.463855	2.597781	-3.25856
1	-1.10652	3.830216	1.1692
1	2.179588	-3.63055	-2.1456
1	1.874305	-1.93168	-2.51876
1	-0.2639	-2.99742	-2.37595
1	5.687135	-1.97534	0.783661
1	1.903879	-1.13589	2.692152
1	5.107965	1.785291	-1.10018
1	-0.00726	2.078318	-2.08119
1	-3.16807	3.664394	0.054708
1	-0.45119	0.469872	0.447575
8	-1.46013	4.312606	-1.52842
1	-1.91121	3.568543	-1.9538
8	5.046172	1.440759	1.468091
1	4.753166	1.004862	2.28527

*Table S75 Energetics and Cartesian coordinates of the neutral conformer **1d-H_2O** (sa-saa-ss) pre-radical capture by DFT calculations B3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.494924 (Hartree/Particle)
Thermal correction to Energy= 0.530399
Thermal correction to Enthalpy= 0.531343
Thermal correction to Gibbs Free Energy= 0.429717
Sum of electronic and zero-point Energies= -2021.729481
Sum of electronic and thermal Energies= -2021.694006
Sum of electronic and thermal Enthalpies= -2021.693062
Sum of electronic and thermal Free Energies= -2021.794688

Coordinates:

6	-2.60923	-0.05487	-0.03122
6	-3.95898	-0.55687	-0.2311
6	-5.04414	0.37574	-0.20438
6	-4.82224	1.736301	0.022809
6	-3.53482	2.204137	0.248443
6	-2.44103	1.346784	0.239286
1	-3.39245	3.263484	0.42355
6	-1.40628	-0.8362	-0.09198
6	-4.35274	-1.94133	-0.45277
6	-1.16828	-2.18038	-0.23069
6	-3.48435	-3.12354	-0.48501
6	-2.12455	-3.21297	-0.38928
8	-5.57995	-2.24849	-0.62643
8	-4.17148	-4.27238	-0.66146
1	-5.10949	-3.98544	-0.73072
8	-5.87161	2.597021	0.034802
8	-6.33919	0.051225	-0.38548
1	-6.67218	2.071029	-0.13401
1	-6.34321	-0.94624	-0.53068
6	-1.07429	1.925556	0.563605
8	-0.35028	2.098286	-0.68974
6	-1.00591	3.272872	1.305819
6	0.965406	2.489458	-0.54862
6	0.454932	3.494976	1.72682
6	1.409876	3.13911	0.607675
6	2.778026	3.46072	0.674005
6	1.811673	2.201512	-1.62442
6	3.65937	3.154178	-0.36479
6	3.160189	2.524258	-1.50619
8	3.192772	4.087847	1.812003
8	4.078742	2.171032	-2.47499
1	4.140471	4.274575	1.753989
1	3.614785	1.932126	-3.29125
8	-1.47964	4.351567	0.498372
1	-1.16571	4.190268	-0.40477
1	-0.51737	1.210804	1.179826
6	0.267166	-2.685	-0.14351
8	1.154427	-1.65271	-0.5936
6	0.661524	-3.12021	1.289587
1	-0.05314	-3.86986	1.640232
6	2.50511	-1.83796	-0.39403
6	2.072989	-3.71772	1.250942
1	2.031548	-4.71949	0.803167
6	3.004444	-2.81325	0.476106
6	3.334927	-0.95343	-1.08656
6	4.404125	-2.8784	0.616767
1	2.890044	-0.21959	-1.7437
6	4.713912	-1.01909	-0.88901
6	5.259275	-1.99898	-0.04782
8	4.878051	-3.84535	1.458747
1	5.842147	-3.78146	1.509864
1	0.380486	-3.55468	-0.80498
1	0.57782	4.543736	2.015594
1	0.674202	2.899118	2.622336
1	-1.64641	3.246805	2.191639
1	4.715768	3.392731	-0.29654
1	1.415732	1.693454	-2.49737
1	6.334604	-2.05118	0.091683
1	2.430642	-3.8505	2.276453
1	-1.74299	-4.22815	-0.47193
1	-0.4969	-0.25912	-0.03569
8	0.55788	-2.03155	2.199619
1	1.232989	-1.38053	1.958524
8	5.575832	-0.15821	-1.49808
1	5.077448	0.569237	-1.91827

*Table S76 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) post-radical capture via HAB at site 5'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482518 (Hartree/Particle)
Thermal correction to Energy= 0.516689
Thermal correction to Enthalpy= 0.517633
Thermal correction to Gibbs Free Energy= 0.417710
Sum of electronic and zero-point Energies= -2021.141037
Sum of electronic and thermal Energies= -2021.106866
Sum of electronic and thermal Enthalpies= -2021.105922
Sum of electronic and thermal Free Energies= -2021.205845

Coordinates:

6	-2.599559	-0.055244	-0.024236
6	-3.948325	-0.552225	-0.239504
6	-5.032448	0.381349	-0.204349
6	-4.81032	1.737978	0.04605
6	-3.523315	2.201503	0.283066
6	-2.430811	1.342827	0.264711
1	-3.38208	3.25833	0.472763
6	-1.39855	-0.838256	-0.082868
6	-4.341971	-1.93261	-0.486163
6	-1.16103	-2.181376	-0.23374
6	-3.475371	-3.115825	-0.526595
6	-2.116599	-3.21009	-0.416082
8	-5.567967	-2.234578	-0.676367
8	-4.162635	-4.260403	-0.726876
1	-5.09948	-3.970923	-0.801508
8	-5.858519	2.599525	0.067051
8	-6.326288	0.061331	-0.398099
1	-6.659282	2.077827	-0.113893
1	-6.330503	-0.933457	-0.56147
6	-1.063884	1.911994	0.600642
8	-0.322454	2.061309	-0.65089
6	-0.988732	3.265179	1.332639
6	0.978337	2.476044	-0.498935
6	0.474009	3.49174	1.748807
6	1.419697	3.137289	0.633288
6	2.832198	3.506077	0.715875
6	1.837997	2.192749	-1.579067
6	3.709333	3.167248	-0.389631
6	3.207103	2.532795	-1.500861
8	3.273278	4.108779	1.726672
8	4.077641	2.168464	-2.500946
1	3.593665	1.983841	-3.320124
8	-1.46391	4.342087	0.525609
1	-1.16144	4.183253	-0.381602
1	-0.517891	1.19666	1.2258
6	0.273766	-2.681734	-0.124422
8	1.160138	-1.671267	-0.627738
6	0.666659	-3.047568	1.328681
1	-0.047807	-3.782463	1.70984
6	2.50912	-1.83205	-0.403792
6	2.079542	-3.640427	1.320737
1	2.04553	-4.657687	0.909059
6	3.009327	-2.758811	0.517824
6	3.340254	-0.975467	-1.13108
6	4.407716	-2.802531	0.678604
1	2.899663	-0.294607	-1.846315
6	4.717599	-1.01721	-0.913124
6	5.261979	-1.94651	-0.01647
8	4.879938	-3.722582	1.571341
1	5.842855	-3.648341	1.629809
1	0.38777	-3.582215	-0.742408
1	0.607247	4.539715	2.034415
1	0.707526	2.898761	2.642619
1	-1.624863	3.241456	2.221412
1	4.758751	3.426534	-0.314584
1	1.431762	1.686843	-2.449172
1	6.335849	-1.978165	0.139393
1	2.432851	-3.733896	2.35198
1	-1.736322	-4.224964	-0.506563
1	-0.488066	-0.265623	-0.008244
8	0.559788	-1.918889	2.188708
1	1.273625	-1.30561	1.960627
8	5.581304	-0.182176	-1.555043
1	5.08579	0.530898	-1.999251

*Table S77 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) post-radical capture via HAB at site 7'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482595 (Hartree/Particle)
Thermal correction to Energy= 0.516702
Thermal correction to Enthalpy= 0.517646
Thermal correction to Gibbs Free Energy= 0.417668
Sum of electronic and zero-point Energies= -2021.144001
Sum of electronic and thermal Energies= -2021.109894
Sum of electronic and thermal Enthalpies= -2021.108950
Sum of electronic and thermal Free Energies= -2021.208928

Coordinates:

6	-2.600635	-0.06326	-0.030994
6	-3.94806	-0.573989	-0.222341
6	-5.038745	0.352554	-0.19809
6	-4.824597	1.715725	0.021023
6	-3.539091	2.193	0.236779
6	-2.440284	1.342093	0.226262
1	-3.405261	3.254653	0.402933
6	-1.394387	-0.839247	-0.085049
6	-4.33533	-1.962271	-0.432594
6	-1.150231	-2.184268	-0.207444
6	-3.461703	-3.140635	-0.451826
6	-2.101358	-3.222909	-0.353913
8	-5.560886	-2.276445	-0.604214
8	-4.143132	-4.294283	-0.615803
1	-5.082583	-4.013147	-0.689019
8	-5.878644	2.570136	0.033115
8	-6.331765	0.019526	-0.37314
1	-6.677174	2.039162	-0.129818
1	-6.330673	-0.978834	-0.513684
6	-1.075707	1.928984	0.540001
8	-0.342914	2.059859	-0.71922
6	-1.007581	3.303528	1.226874
6	0.971717	2.436062	-0.598245
6	0.456336	3.554824	1.62518
6	1.416301	3.15471	0.540268
6	2.806672	3.493704	0.629021
6	1.826347	2.119951	-1.630267
6	3.696143	3.146006	-0.358867
6	3.239231	2.424609	-1.525069
8	3.149793	4.163977	1.756512
8	4.043231	2.018736	-2.41289
1	4.097255	4.36481	1.747773
8	-1.493242	4.350723	0.38989
1	-1.213462	4.152617	-0.517259
1	-0.522957	1.233138	1.180907
6	0.287853	-2.676241	-0.102512
8	1.166063	-1.677604	-0.640859
6	0.697386	-3.004116	1.354984
1	-0.012625	-3.728385	1.763858
6	2.519268	-1.836746	-0.433743
6	2.109777	-3.597711	1.345471
1	2.069465	-4.626182	0.96301
6	3.029617	-2.739948	0.506101
6	3.34163	-1.003094	-1.196168
6	4.429972	-2.782795	0.649349
1	2.900375	-0.339214	-1.926206
6	4.722334	-1.03765	-0.990628
6	5.27633	-1.944882	-0.07653
8	4.912317	-3.680985	1.559699
1	5.875866	-3.605745	1.604111
1	0.397266	-3.592307	-0.698038
1	0.586398	4.614534	1.868324
1	0.698214	3.002928	2.544103
1	-1.632159	3.306348	2.123873
1	4.752858	3.38106	-0.284165
1	1.467001	1.589051	-2.503701
1	6.351821	-1.971956	0.069751
1	2.47618	-3.663078	2.374359
1	-1.715273	-4.237205	-0.423481
1	-0.486569	-0.25955	-0.033192
8	0.600475	-1.853165	2.186446
1	1.308431	-1.244192	1.93028
8	5.574592	-0.218421	-1.66472
1	5.075267	0.529131	-2.055447

*Table S78 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) post-radical capture via HAB at site 3'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481672 (Hartree/Particle)
Thermal correction to Energy= 0.515929
Thermal correction to Enthalpy= 0.516873
Thermal correction to Gibbs Free Energy= 0.416866
Sum of electronic and zero-point Energies= -2021.112446
Sum of electronic and thermal Energies= -2021.078190
Sum of electronic and thermal Enthalpies= -2021.077246
Sum of electronic and thermal Free Energies= -2021.177252

Coordinates:

6	-2.604728	-0.02086	-0.020866
6	-3.964776	-0.480792	-0.237212
6	-5.019656	0.486498	-0.23705
6	-4.759075	1.842304	-0.01701
6	-3.461414	2.267629	0.23519
6	-2.396981	1.375751	0.246051
1	-3.300304	3.322635	0.43398
6	-1.423156	-0.833101	-0.077362
6	-4.396936	-1.855564	-0.447507
6	-1.219481	-2.182421	-0.221056
6	-3.560794	-3.062054	-0.467371
6	-2.20289	-3.189102	-0.375547
8	-5.631194	-2.128427	-0.623319
8	-4.279273	-4.191996	-0.634322
1	-5.2092	-3.880933	-0.70852
8	-5.779415	2.7357	-0.024688
8	-6.320439	0.200417	-0.433185
1	-6.595418	2.235793	-0.198965
1	-6.355831	-0.799073	-0.5585
6	-1.012209	1.903395	0.570697
8	-0.287698	2.045975	-0.655016
6	-0.969473	3.249642	1.38084
6	1.009811	2.472625	-0.538403
6	0.532039	3.479538	1.740906
6	1.458803	3.141236	0.60516
6	2.817547	3.508787	0.642313
6	1.847204	2.194773	-1.623849
6	3.690771	3.204371	-0.402668
6	3.190129	2.543846	-1.527098
8	3.230001	4.164261	1.764197
8	4.103732	2.187935	-2.497941
1	4.169627	4.382859	1.688418
1	3.636679	1.946695	-3.311912
8	-1.39795	4.298678	0.63234
1	-0.483618	1.192177	1.217487
6	0.206891	-2.715218	-0.146958
8	1.104772	-1.700367	-0.616831
6	0.609798	-3.151435	1.283377
1	-0.110105	-3.893317	1.639967
6	2.4538	-1.882368	-0.407607
6	2.014672	-3.762956	1.233496
1	1.962172	-4.759455	0.775392
6	2.950195	-2.857157	0.464889
6	3.286261	-0.995067	-1.09457
6	4.34918	-2.919726	0.614024
1	2.843505	-0.260449	-1.752753
6	4.664282	-1.059691	-0.890092
6	5.206369	-2.039046	-0.046048
8	4.820064	-3.885843	1.458399
1	5.783662	-3.819689	1.515907
1	0.294904	-3.590194	-0.805073
1	0.668961	4.517855	2.05787
1	0.732335	2.85884	2.623614
1	-1.548528	3.102864	2.307497
1	4.742693	3.465407	-0.352144
1	1.448823	1.670328	-2.485725
1	6.281027	-2.089727	0.098951
1	2.375258	-3.909318	2.256024
1	-1.849565	-4.214545	-0.456853
1	-0.498565	-0.281395	-0.021985
8	0.526508	-2.060866	2.19328
1	1.234056	-1.43769	1.97234
8	5.53089	-0.199445	-1.493792
1	5.040366	0.529147	-1.92

*Table S79 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site h-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.483683 (Hartree/Particle)
Thermal correction to Energy= 0.517636
Thermal correction to Enthalpy= 0.518580
Thermal correction to Gibbs Free Energy= 0.419021
Sum of electronic and zero-point Energies= -2021.148653
Sum of electronic and thermal Energies= -2021.114700
Sum of electronic and thermal Enthalpies= -2021.113756
Sum of electronic and thermal Free Energies= -2021.213315

Coordinates:

6	-2.642743	0.001333	-0.035897
6	-4.009495	-0.453912	-0.229286
6	-5.068933	0.509884	-0.196549
6	-4.824725	1.936171	0.041418
6	-3.455656	2.312135	0.279081
6	-2.421823	1.424043	0.258897
1	-3.271764	3.361959	0.471894
6	-1.47811	-0.795346	-0.106086
6	-4.43803	-1.825069	-0.460675
6	-1.268168	-2.161868	-0.25339
6	-3.601322	-3.031794	-0.512716
6	-2.23676	-3.163449	-0.421612
8	-5.672367	-2.103726	-0.627617
8	-4.311586	-4.153827	-0.697884
1	-5.246877	-3.852082	-0.757967
8	-5.764585	2.757056	0.04695
8	-6.338343	0.203312	-0.37445
1	-6.357395	-0.803233	-0.520873
6	-1.023607	1.932252	0.586003
8	-0.310327	2.070644	-0.671427
6	-0.88613	3.268597	1.338921
6	1.021005	2.417636	-0.552689
6	0.589369	3.415747	1.741994
6	1.509585	3.03942	0.600616
6	2.888151	3.318525	0.639511
6	1.832224	2.117354	-1.651161
6	3.735664	2.998753	-0.423089
6	3.191945	2.399178	-1.560456
8	3.347201	3.91902	1.774423
8	4.076968	2.033648	-2.555297
1	4.297822	4.081634	1.695061
1	3.588818	1.825978	-3.365966
8	-1.319743	4.377471	0.551799
1	-1.008364	4.227999	-0.354004
1	-0.506257	1.185248	1.199137
6	0.156151	-2.685848	-0.134972
8	1.061239	-1.702699	-0.649443
6	0.531435	-3.03505	1.329142
1	-0.202168	-3.745709	1.719314
6	2.407253	-1.888041	-0.414375
6	1.92966	-3.660726	1.33544
1	1.872314	-4.683347	0.94033
6	2.882017	-2.812635	0.522753
6	3.258322	-1.058244	-1.147406
6	4.278423	-2.883629	0.691504
1	2.833311	-0.364852	-1.859347
6	4.633102	-1.123865	-0.919925
6	5.153635	-2.055023	-0.010491
8	4.726442	-3.801515	1.599193
1	5.690086	-3.744455	1.664162
1	0.251406	-3.599564	-0.735904
1	0.763633	4.452472	2.046648
1	0.794361	2.794326	2.623297
1	-1.515409	3.261507	2.232893
1	4.799963	3.205286	-0.376143
1	1.401287	1.631702	-2.520193
1	6.225765	-2.106953	0.152173
1	2.276537	-3.746066	2.369656
1	-1.884765	-4.187844	-0.513028
1	-0.550108	-0.251074	-0.038212
8	0.446907	-1.88622	2.163815
1	1.20432	-1.317577	1.961762
8	5.515	-0.310132	-1.563521
1	5.034412	0.411216	-2.01404

*Table S80 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site i-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.483972 (Hartree/Particle)
Thermal correction to Energy= 0.518127
Thermal correction to Enthalpy= 0.519071
Thermal correction to Gibbs Free Energy= 0.418583
Sum of electronic and zero-point Energies= -2021.138839
Sum of electronic and thermal Energies= -2021.104684
Sum of electronic and thermal Enthalpies= -2021.103739
Sum of electronic and thermal Free Energies= -2021.204228

Coordinates:

6	-2.671033	-0.056971	-0.077259
6	-4.012729	-0.53169	-0.277966
6	-5.11582	0.433785	-0.221961
6	-4.791035	1.833879	0.050001
6	-3.495562	2.269922	0.274604
6	-2.450609	1.363508	0.233816
1	-3.307276	3.316836	0.476899
6	-1.47279	-0.830248	-0.154454
6	-4.423145	-1.904476	-0.541074
6	-1.235672	-2.188129	-0.22896
6	-3.541092	-3.112334	-0.461082
6	-2.184426	-3.226519	-0.318466
8	-5.60497	-2.222091	-0.805724
8	-4.255296	-4.227645	-0.602471
1	-5.173961	-3.863479	-0.75494
8	-5.831833	2.656075	0.081457
8	-6.341726	0.213671	-0.375629
1	-6.597169	2.051569	-0.0989
6	-1.058333	1.877681	0.572945
8	-0.349582	2.062138	-0.681526
6	-0.934496	3.193257	1.364848
6	0.979539	2.416692	-0.552789
6	0.539925	3.34294	1.770593
6	1.462636	3.009442	0.61784
6	2.83864	3.300106	0.664543
6	1.792901	2.153369	-1.658962
6	3.688386	3.018328	-0.406892
6	3.150035	2.445056	-1.56036
8	3.292367	3.872086	1.816015
8	4.038465	2.114409	-2.563831
1	4.241464	4.045603	1.741533
1	3.552608	1.919648	-3.379071
8	-1.381411	4.320064	0.611437
1	-1.048781	4.214299	-0.293057
1	-0.532243	1.118504	1.162209
6	0.201631	-2.678979	-0.119685
8	1.084477	-1.682781	-0.645596
6	0.593442	-3.011573	1.343925
1	-0.124954	-3.731347	1.745442
6	2.435276	-1.845226	-0.422318
6	2.001807	-3.614162	1.342908
1	1.957853	-4.64047	0.955626
6	2.933107	-2.756649	0.515861
6	3.266382	-1.00617	-1.167836
6	4.331884	-2.80472	0.672082
1	2.823806	-0.32422	-1.880315
6	4.643966	-1.048406	-0.951954
6	5.187376	-1.966206	-0.042364
8	4.802623	-3.710155	1.58084
1	5.765846	-3.637929	1.636131
1	0.310926	-3.594399	-0.716051
1	0.703968	4.371772	2.106036
1	0.75163	2.697573	2.632808
1	-1.562541	3.154267	2.258858
1	4.750848	3.232706	-0.354186
1	1.366297	1.687182	-2.540693
1	6.261603	-1.99958	0.111226
1	2.359022	-3.686095	2.374617
1	-1.81076	-4.247197	-0.333111
1	-0.559895	-0.258046	-0.142103
8	0.496841	-1.858595	2.171406
1	1.23819	-1.27505	1.95315
8	5.507508	-0.224242	-1.607399
1	5.012682	0.491343	-2.051445

*Table S81 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) post-radical capture via HAB at site b-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482756 (Hartree/Particle)
Thermal correction to Energy= 0.517003
Thermal correction to Enthalpy= 0.517947
Thermal correction to Gibbs Free Energy= 0.416192
Sum of electronic and zero-point Energies= -2021.144148
Sum of electronic and thermal Energies= -2021.109901
Sum of electronic and thermal Enthalpies= -2021.108956
Sum of electronic and thermal Free Energies= -2021.210712

Coordinates:

6	2.627268	-0.076835	0.019023
6	3.987071	-0.542166	0.24854
6	5.038315	0.417517	0.210037
6	4.786236	1.779309	-0.080916
6	3.492136	2.21067	-0.329026
6	2.424793	1.322167	-0.290752
1	3.321845	3.260041	-0.534292
6	1.455721	-0.869472	0.089917
6	4.433549	-1.909641	0.527883
6	1.233695	-2.247026	0.255456
6	3.598659	-3.195861	0.520317
6	2.168001	-3.245318	0.434868
8	5.64457	-2.133649	0.775084
8	4.236925	-4.254185	0.624001
8	5.813741	2.646903	-0.110087
8	6.321916	0.141339	0.433334
1	6.62591	2.14826	0.092345
1	6.328118	-0.865084	0.641297
6	1.037183	1.86063	-0.607137
8	0.34591	2.031441	0.659654
6	0.921076	3.192135	-1.372148
6	-0.979645	2.402359	0.554186
6	-0.556587	3.373903	-1.753512
6	-1.470032	3.025186	-0.597744
6	-2.843708	3.328979	-0.622474
6	-1.783417	2.122473	1.663329
6	-3.684191	3.032206	0.452472
6	-3.138334	2.429599	1.587382
8	-3.305288	3.930045	-1.756123
8	-4.017348	2.08839	2.596105
1	-4.252109	4.109072	-1.667268
1	-3.523246	1.882561	3.403692
8	1.397376	4.296019	-0.602587
1	1.083096	4.171316	0.306107
1	0.491253	1.120848	-1.202801
6	-0.206283	-2.737135	0.123066
8	-1.086837	-1.75371	0.685674
6	-0.598456	-3.023025	-1.346513
1	0.116823	-3.737529	-1.762927
6	-2.435802	-1.879595	0.434195
6	-2.011733	-3.611732	-1.368949
1	-1.981643	-4.645047	-0.999326
6	-2.938611	-2.756513	-0.534372
6	-3.261887	-1.039848	1.185584
6	-4.335215	-2.770339	-0.714406
1	-2.817014	-0.383134	1.920334
6	-4.636416	-1.047616	0.946868
6	-5.184401	-1.931772	0.007162
8	-4.810095	-3.642504	-1.653191
1	-5.770033	-3.54519	-1.724777
1	-0.316755	-3.669808	0.690186
1	-0.709205	4.41311	-2.061468
1	-0.789538	2.753564	-2.628556
1	1.535336	3.161355	-2.276119
1	-4.74483	3.258838	0.416722
1	-1.351219	1.632414	2.529132
1	-6.256502	-1.938135	-0.163868
1	-2.362332	-3.661765	-2.404188
1	1.800995	-4.264983	0.525251
1	0.530761	-0.322543	0.009345
8	-0.490427	-1.848114	-2.14505
1	-1.251824	-1.284465	-1.94372
8	-5.493979	-0.221007	1.607145
1	-4.993523	0.479125	2.069233

*Table S82 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) post-radical capture via HAB at site 3-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481805 (Hartree/Particle)
Thermal correction to Energy= 0.515827
Thermal correction to Enthalpy= 0.516771
Thermal correction to Gibbs Free Energy= 0.417440
Sum of electronic and zero-point Energies= -2021.112469
Sum of electronic and thermal Energies= -2021.078448
Sum of electronic and thermal Enthalpies= -2021.077504
Sum of electronic and thermal Free Energies= -2021.176835

Coordinates:

6	-2.601159	-0.058989	-0.009773
6	-3.949312	-0.564521	-0.219219
6	-5.03614	0.364522	-0.19714
6	-4.818167	1.726789	0.030242
6	-3.532831	2.198717	0.258885
6	-2.437073	1.344373	0.257156
1	-3.394071	3.259182	0.429454
6	-1.39878	-0.839733	-0.056333
6	-4.339712	-1.949741	-0.447046
6	-1.159635	-2.183131	-0.206375
6	-3.468711	-3.130636	-0.488272
6	-2.109506	-3.218122	-0.387065
8	-5.564877	-2.258113	-0.624604
8	-4.151911	-4.278244	-0.68019
1	-5.090806	-3.994287	-0.749216
8	-5.868513	2.583747	0.037038
8	-6.329519	0.039476	-0.383817
1	-6.668117	2.056779	-0.134362
1	-6.333814	-0.957463	-0.529489
6	-1.072755	1.932253	0.577555
8	-0.351112	2.095276	-0.677432
6	-1.01167	3.286984	1.307337
6	0.96203	2.497465	-0.541871
6	0.448197	3.52065	1.724872
6	1.403557	3.161293	0.607294
6	2.769744	3.492201	0.66905
6	1.808489	2.204594	-1.616148
6	3.651761	3.180901	-0.36778
6	3.154995	2.53687	-1.502131
8	3.181609	4.132725	1.800338
8	4.075363	2.177382	-2.467538
1	4.128636	4.322527	1.741068
1	3.613104	1.932821	-3.283173
8	-1.49195	4.355783	0.490816
1	-1.174073	4.191689	-0.410436
1	-0.512461	1.227734	1.202034
6	0.275621	-2.676652	-0.127186
8	1.156955	-1.679679	-0.580067
6	0.676511	-3.184029	1.354547
1	-0.05685	-3.982245	1.571127
6	2.506899	-1.854853	-0.381872
6	2.103818	-3.766581	1.230827
1	2.022116	-4.750988	0.749236
6	3.012971	-2.845242	0.467144
6	3.32454	-0.946876	-1.056866
6	4.414463	-2.891736	0.613865
1	2.870001	-0.202432	-1.694953
6	4.703908	-1.004503	-0.86378
6	5.25832	-1.993942	-0.037519
8	4.897872	-3.865687	1.440834
1	5.860322	-3.787057	1.502731
1	0.395397	-3.583365	-0.734188
1	0.565271	4.572384	2.004942
1	0.67226	2.93321	2.624713
1	-1.651273	3.2652	2.193882
1	4.706799	3.426265	-0.303234
1	1.414495	1.686357	-2.483969
1	6.334351	-2.038442	0.098506
1	2.498198	-3.945894	2.235409
1	-1.724715	-4.230893	-0.480224
1	-0.489062	-0.264799	0.027327
8	0.600788	-2.142161	2.196946
8	5.559425	-0.130312	-1.458087
1	5.059002	0.592252	-1.885456

*Table S83 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site 5-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482896 (Hartree/Particle)
Thermal correction to Energy= 0.516935
Thermal correction to Enthalpy= 0.517879
Thermal correction to Gibbs Free Energy= 0.418253
Sum of electronic and zero-point Energies= -2021.142770
Sum of electronic and thermal Energies= -2021.108731
Sum of electronic and thermal Enthalpies= -2021.107787
Sum of electronic and thermal Free Energies= -2021.207413

Coordinates:

6	-2.595224	-0.032508	-0.029979
6	-3.949925	-0.518593	-0.234539
6	-5.023897	0.426682	-0.210921
6	-4.786545	1.784765	0.017107
6	-3.49414	2.237761	0.244708
6	-2.410909	1.367211	0.23863
1	-3.339583	3.29575	0.417552
6	-1.401465	-0.828417	-0.08203
6	-4.358924	-1.898402	-0.458881
6	-1.179012	-2.175013	-0.22027
6	-3.503729	-3.090861	-0.490623
6	-2.145639	-3.196592	-0.38835
8	-5.588446	-2.191134	-0.636977
8	-4.203126	-4.230865	-0.673227
1	-5.137671	-3.933494	-0.745463
8	-5.825423	2.657693	0.026421
8	-6.322096	0.117981	-0.39585
1	-6.632229	2.141767	-0.143916
1	-6.338553	-0.878833	-0.541409
6	-1.037207	1.928855	0.562414
8	-0.307058	2.074604	-0.690802
6	-0.949146	3.283101	1.289061
6	1.013991	2.444548	-0.551161
6	0.514808	3.487676	1.709258
6	1.466667	3.101309	0.597602
6	2.839898	3.401246	0.663921
6	1.857971	2.127958	-1.621325
6	3.718253	3.068893	-0.369815
6	3.210195	2.435118	-1.504587
8	3.261761	4.034486	1.794995
8	4.125476	2.056033	-2.469643
1	4.212514	4.205714	1.738214
1	3.663569	1.850086	-3.296223
8	-1.407	4.35935	0.469656
1	-1.094257	4.185321	-0.431506
1	-0.493889	1.212708	1.189177
6	0.248159	-2.697949	-0.120299
8	1.156682	-1.677562	-0.572404
6	0.628372	-3.134893	1.317034
1	-0.091406	-3.885095	1.654851
6	2.493234	-1.890467	-0.347782
6	2.03951	-3.737116	1.295087
1	2.005838	-4.742188	0.854214
6	2.975262	-2.853672	0.517536
6	3.356185	-1.021072	-1.04579
6	4.425694	-2.968926	0.685296
1	2.91798	-0.292098	-1.714219
6	4.75887	-1.085842	-0.859822
6	5.290159	-2.055559	-0.03342
8	4.902618	-3.837892	1.460092
1	0.359175	-3.568041	-0.780362
1	0.654139	4.538202	1.983636
1	0.723554	2.900874	2.613141
1	-1.589958	3.27642	2.175002
1	4.777772	3.293465	-0.303804
1	1.454685	1.61964	-2.490802
1	6.360605	-2.138109	0.115268
1	2.403223	-3.863352	2.318893
1	-1.775727	-4.215958	-0.471682
1	-0.486547	-0.261319	-0.017885
8	0.513512	-2.051966	2.230943
1	1.182495	-1.390346	2.002533
8	5.589446	-0.224409	-1.495691
1	5.084695	0.502876	-1.913677

*Table S84 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site 7-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482090 (Hartree/Particle)
Thermal correction to Energy= 0.516623
Thermal correction to Enthalpy= 0.517567
Thermal correction to Gibbs Free Energy= 0.415743
Sum of electronic and zero-point Energies= -2021.137732
Sum of electronic and thermal Energies= -2021.103199
Sum of electronic and thermal Enthalpies= -2021.102255
Sum of electronic and thermal Free Energies= -2021.204078

Coordinates:

6	-2.569511	-0.154702	-0.01737
6	-3.885151	-0.729238	-0.250631
6	-5.023543	0.136597	-0.213288
6	-4.883923	1.501881	0.048893
6	-3.62795	2.039678	0.292675
6	-2.485036	1.248805	0.277214
1	-3.550498	3.102888	0.482174
6	-1.323085	-0.866778	-0.055666
6	-4.194375	-2.125929	-0.524999
6	-1.00876	-2.190579	-0.225151
6	-3.257168	-3.253469	-0.589972
6	-1.898195	-3.26872	-0.457491
8	-5.398026	-2.497744	-0.728906
8	-3.870726	-4.430788	-0.833126
1	-4.823098	-4.197657	-0.907916
8	-5.981621	2.299192	0.069994
8	-6.295526	-0.256936	-0.41875
1	-6.748541	1.732317	-0.121432
1	-6.240421	-1.246918	-0.597047
6	-1.154963	1.905369	0.614663
8	-0.419796	2.075253	-0.629804
6	-1.181082	3.271157	1.325123
6	0.846907	2.61225	-0.510529
6	0.255652	3.602654	1.75127
6	1.22665	3.341555	0.620859
6	2.535244	3.859482	0.63407
6	1.697419	2.417564	-1.60423
6	3.413075	3.677707	-0.43436
6	2.981098	2.961018	-1.556309
8	2.892201	4.559113	1.751232
8	3.877287	2.811368	-2.576051
1	3.796173	4.88952	1.651402
1	3.45768	2.336595	-3.307281
8	-1.718629	4.300141	0.49236
1	-1.38918	4.143861	-0.405811
1	-0.576736	1.238385	1.264673
6	0.442931	-2.629486	-0.094599
8	1.31253	-1.526184	-0.41072
6	0.795142	-3.130583	1.324183
1	0.107395	-3.93163	1.606559
6	2.663072	-1.765655	-0.315924
6	2.230744	-3.674004	1.308799
1	2.237479	-4.688424	0.886455
6	3.16049	-2.800819	0.513702
6	3.507	-0.932786	-1.018799
6	4.575624	-2.994913	0.581101
1	3.112462	-0.133992	-1.634219
6	4.943685	-1.109471	-0.937906
6	5.446008	-2.186575	-0.109507
8	4.969398	-4.022706	1.378949
1	5.936007	-4.080249	1.384927
1	0.638441	-3.439878	-0.808861
1	0.295293	4.653891	2.052845
1	0.520494	3.014242	2.63979
1	-1.826801	3.218398	2.206078
1	4.41865	4.085559	-0.412287
1	1.346201	1.854602	-2.462895
1	6.52063	-2.328884	-0.054448
1	2.592704	-3.774754	2.337045
1	-1.456528	-4.256404	-0.568144
1	-0.451485	-0.240601	0.050011
8	0.608928	-2.104617	2.28852
1	1.121681	-1.331675	2.009633
8	5.723231	-0.355001	-1.576969

*Table S85 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site 4'α-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482670 (Hartree/Particle)
Thermal correction to Energy= 0.517040
Thermal correction to Enthalpy= 0.517984
Thermal correction to Gibbs Free Energy= 0.417880
Sum of electronic and zero-point Energies= -2021.135918
Sum of electronic and thermal Energies= -2021.101548
Sum of electronic and thermal Enthalpies= -2021.100604
Sum of electronic and thermal Free Energies= -2021.200708

Coordinates:

6	-2.602214	-0.055188	-0.037699
6	-3.947097	-0.569493	-0.243538
6	-5.042158	0.351542	-0.212471
6	-4.834414	1.710734	0.031558
6	-3.552702	2.190598	0.263444
6	-2.44782	1.347667	0.244437
1	-3.420202	3.246337	0.463425
6	-1.393904	-0.828125	-0.101122
6	-4.327931	-1.956059	-0.475873
6	-1.145592	-2.171446	-0.232427
6	-3.451869	-3.132434	-0.49961
6	-2.092524	-3.212099	-0.392018
8	-5.551147	-2.272137	-0.662809
8	-4.129665	-4.286207	-0.680084
1	-5.068817	-4.005279	-0.758447
8	-5.893171	2.560331	0.053358
8	-6.333576	0.016111	-0.400894
1	-6.687966	2.027675	-0.121721
1	-6.326917	-0.979579	-0.557596
6	-1.083265	1.936659	0.562447
8	-0.38438	2.146955	-0.702917
6	-0.989496	3.233093	1.39191
6	0.934573	2.500834	-0.586282
6	0.466112	3.540446	1.588388
6	1.385949	3.175902	0.58795
6	2.783964	3.478179	0.646267
6	1.777612	2.201552	-1.648448
6	3.644939	3.1509	-0.39226
6	3.134326	2.519134	-1.533761
8	3.205288	4.108554	1.775176
8	4.046696	2.157627	-2.500532
1	4.155908	4.28138	1.717693
1	3.582036	1.908573	-3.313571
8	-1.669389	4.363794	0.80804
1	-1.257142	4.525847	-0.053923
1	-0.508318	1.205206	1.141424
6	0.29222	-2.665579	-0.129476
8	1.176398	-1.636056	-0.591652
6	0.679687	-3.074024	1.313667
1	-0.033656	-3.821115	1.672369
6	2.52655	-1.812152	-0.381645
6	2.094315	-3.664571	1.294369
1	2.061133	-4.67408	0.863734
6	3.025585	-2.768742	0.509289
6	3.356494	-0.938201	-1.087144
6	4.424718	-2.824924	0.658884
1	2.912227	-0.222305	-1.764103
6	4.734608	-0.993994	-0.880816
6	5.279719	-1.954093	-0.01722
8	4.898063	-3.773701	1.521388
1	5.861709	-3.705725	1.575444
1	0.415073	-3.545682	-0.775134
1	0.78007	4.130177	2.439967
1	-1.489077	3.070272	2.351588
1	4.704803	3.377044	-0.334673
1	1.381953	1.693392	-2.521677
1	6.35444	-1.998124	0.129732
1	2.446211	-3.777591	2.324229
1	-1.702821	-4.224679	-0.467758
1	-0.488057	-0.245743	-0.044793
8	0.565082	-1.970587	2.204519
1	1.243595	-1.323722	1.961789
8	5.595705	-0.141406	-1.503029
1	5.094282	0.574806	-1.937327

*Table S86 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site 4'β-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482670 (Hartree/Particle)
Thermal correction to Energy= 0.517040
Thermal correction to Enthalpy= 0.517984
Thermal correction to Gibbs Free Energy= 0.417881
Sum of electronic and zero-point Energies= -2021.135918
Sum of electronic and thermal Energies= -2021.101548
Sum of electronic and thermal Enthalpies= -2021.100604
Sum of electronic and thermal Free Energies= -2021.200707

Coordinates:

6	-2.602177	-0.05491	-0.037804
6	-3.947221	-0.56907	-0.243407
6	-5.042162	0.352085	-0.211997
6	-4.834182	1.711249	0.03199
6	-3.552363	2.190964	0.263515
6	-2.447562	1.34792	0.244336
1	-3.419713	3.24671	0.463349
6	-1.394025	-0.828029	-0.101356
6	-4.32829	-1.95554	-0.475839
6	-1.145963	-2.171392	-0.232732
6	-3.452416	-3.132019	-0.499835
6	-2.093084	-3.211885	-0.39229
8	-5.551581	-2.271413	-0.662677
8	-4.130403	-4.285668	-0.680438
1	-5.069528	-4.004572	-0.758619
8	-5.89283	2.56098	0.054074
8	-6.333676	0.016808	-0.400015
1	-6.687728	2.028438	-0.120885
1	-6.327203	-0.97886	-0.556903
6	-1.082873	1.936708	0.562288
8	-0.383888	2.14675	-0.703087
6	-0.988969	3.233258	1.391546
6	0.935093	2.500497	-0.586394
6	0.466656	3.540398	1.588134
6	1.386505	3.175517	0.587817
6	2.784573	3.477525	0.646225
6	1.778123	2.201219	-1.648584
6	3.645542	3.150251	-0.392311
6	3.134882	2.518553	-1.533842
8	3.205946	4.107755	1.77521
8	4.047214	2.156867	-2.500561
1	4.156582	4.280491	1.717745
1	3.582589	1.907933	-3.313657
8	-1.668623	4.363912	0.807406
1	-1.256235	4.525801	-0.054519
1	-0.508129	1.205167	1.14133
6	0.291745	-2.665832	-0.129795
8	1.176147	-1.636763	-0.592582
6	0.679189	-3.073865	1.313475
1	-0.034316	-3.820715	1.672359
6	2.526221	-1.812611	-0.381983
6	2.093682	-3.664668	1.294333
1	2.060352	-4.67415	0.863649
6	3.025107	-2.768907	0.509367
6	3.356325	-0.938767	-1.087437
6	4.424185	-2.824863	0.659539
1	2.912299	-0.223081	-1.764779
6	4.734368	-0.994344	-0.88055
6	5.279315	-1.954085	-0.01647
8	4.897324	-3.773325	1.522489
1	5.860937	-3.70518	1.576918
1	0.414259	-3.546219	-0.775127
1	0.780723	4.130308	2.439538
1	-1.488659	3.070633	2.351205
1	4.705424	3.37628	-0.33463
1	1.382423	1.693021	-2.521776
1	6.353986	-1.997878	0.130908
1	2.445494	-3.777779	2.324208
1	-1.703552	-4.224525	-0.468106
1	-0.48807	-0.245799	-0.045137
8	0.564822	-1.970156	2.204005
1	1.244062	-1.3239	1.96168
8	5.595593	-0.141844	-1.502754
1	5.09427	0.574515	-1.936932

*Table S87 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) post-radical capture via HAB at site 3'-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482628 (Hartree/Particle)
Thermal correction to Energy= 0.517103
Thermal correction to Enthalpy= 0.518047
Thermal correction to Gibbs Free Energy= 0.417138
Sum of electronic and zero-point Energies= -2021.117909
Sum of electronic and thermal Energies= -2021.083434
Sum of electronic and thermal Enthalpies= -2021.082490
Sum of electronic and thermal Free Energies= -2021.183398

Coordinates:

6	2.59982	-0.046343	0.033613
6	3.942417	-0.569443	0.233185
6	5.055579	0.310946	0.0503
6	4.868589	1.630565	-0.366003
6	3.584252	2.126225	-0.547177
6	2.459079	1.341877	-0.318193
1	3.495032	3.148492	-0.892312
6	1.385219	-0.809524	0.091244
6	4.305276	-1.929101	0.612643
6	1.128879	-2.144201	0.291828
6	3.414677	-3.084178	0.752724
6	2.060455	-3.167104	0.591588
8	5.523819	-2.237701	0.836743
8	4.072025	-4.217322	1.078403
1	5.014347	-3.943004	1.138462
8	5.941881	2.429842	-0.583494
8	6.345705	-0.033796	0.222377
1	6.735287	1.898024	-0.399106
1	6.323237	-0.996654	0.521434
6	1.095295	1.97195	-0.562927
8	0.324015	1.926565	0.696968
6	1.024542	3.393334	-1.03914
6	-0.950266	2.436061	0.596812
6	-0.35533	3.749504	-1.510745
6	-1.354495	3.258093	-0.467151
6	-2.702306	3.657142	-0.499701
6	-1.830308	2.071455	1.623634
6	-3.613304	3.26802	0.484347
6	-3.15866	2.478598	1.541523
8	-3.066523	4.452127	-1.547522
8	-4.104495	2.060646	2.45817
1	-4.001188	4.688919	-1.466346
1	-3.661583	1.728676	3.25327
8	1.559755	4.377104	-0.232601
1	2.160142	3.990332	0.421884
1	0.545497	1.370092	-1.297272
6	-0.299306	-2.649365	0.129407
8	-1.209089	-1.615721	0.527847
6	-0.623681	-3.089969	-1.319938
1	0.110419	-3.83642	-1.635368
6	-2.549256	-1.826804	0.28737
6	-2.033045	-3.69497	-1.346434
1	-2.00502	-4.700559	-0.906278
6	-3.004096	-2.805172	-0.603125
6	-3.415449	-0.965055	0.961239
6	-4.397692	-2.891083	-0.788376
1	-3.00396	-0.230515	1.636974
6	-4.785726	-1.050656	0.72183
6	-5.288814	-2.030544	-0.145068
8	-4.828848	-3.859494	-1.651457
1	-5.791586	-3.810152	-1.734075
1	-0.447689	-3.515898	0.787668
1	-0.442305	4.83337	-1.634197
1	-0.563312	3.298929	-2.48949
1	-4.654739	3.57011	0.441489
1	-1.47376	1.436638	2.427686
1	-6.358135	-2.100282	-0.319127
1	-2.344631	-3.821117	-2.38779
1	1.660556	-4.167501	0.739928
1	0.487997	-0.231393	-0.060788
8	-0.484137	-2.002633	-2.226885
1	-1.1659	-1.349642	-2.010864
8	-5.674485	-0.205928	1.315994
1	-5.189746	0.508497	1.772014

*Table S88 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) post-radical capture via HAB at site 2'-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481467 (Hartree/Particle)
Thermal correction to Energy= 0.516393
Thermal correction to Enthalpy= 0.517337
Thermal correction to Gibbs Free Energy= 0.414986
Sum of electronic and zero-point Energies= -2021.138662
Sum of electronic and thermal Energies= -2021.103736
Sum of electronic and thermal Enthalpies= -2021.102792
Sum of electronic and thermal Free Energies= -2021.205143

Coordinates:

6	2.608754	-0.024435	0.075158
6	3.953595	-0.563969	0.228671
6	5.065777	0.269509	-0.074832
6	4.887307	1.591291	-0.530551
6	3.628526	2.143423	-0.584271
6	2.473256	1.399304	-0.239429
1	3.550856	3.199811	-0.809331
6	1.409107	-0.78744	0.050555
6	4.302357	-1.901501	0.694346
6	1.135299	-2.119748	0.307047
6	3.393384	-3.008507	0.964999
6	2.040474	-3.101338	0.758736
8	5.525064	-2.214046	0.907032
8	4.024637	-4.112517	1.427735
1	4.973435	-3.856679	1.446281
8	5.979928	2.337104	-0.833578
8	6.356247	-0.100901	0.032636
1	6.759176	1.780768	-0.661457
1	6.325908	-1.033943	0.421296
6	1.253059	2.136985	-0.22313
8	0.284356	1.761608	0.678269
6	1.016636	3.406636	-0.999307
6	-0.983685	2.302827	0.633999
6	-0.423591	3.44654	-1.527369
6	-1.394184	3.112357	-0.425541
6	-2.729895	3.552141	-0.414265
6	-1.82245	1.9513	1.694673
6	-3.611705	3.184988	0.604639
6	-3.147144	2.378453	1.645938
8	-3.117102	4.336697	-1.458707
8	-4.077532	1.975277	2.57963
1	-4.043125	4.594996	-1.347926
1	-3.626602	1.61425	3.357386
8	1.336979	4.586208	-0.237919
1	0.711149	4.64452	0.499205
6	-0.278765	-2.629676	0.065194
8	-1.207486	-1.631701	0.521955
6	-0.580403	-2.978852	-1.412189
1	0.164084	-3.701038	-1.758895
6	-2.539744	-1.832658	0.243616
6	-1.985762	-3.588612	-1.498728
1	-1.960466	-4.618434	-1.118554
6	-2.974848	-2.749039	-0.720387
6	-3.424088	-1.025252	0.960978
6	-4.364263	-2.824831	-0.938585
1	-3.030402	-0.342653	1.698911
6	-4.78814	-1.095118	0.687506
6	-5.271267	-2.011502	-0.256429
8	-4.775727	-3.733046	-1.873762
1	-5.737033	-3.681013	-1.970165
1	-0.432106	-3.540611	0.658697
1	-0.620803	4.443345	-1.931165
1	-0.522845	2.739564	-2.362285
1	1.700688	3.430943	-1.848002
1	-4.647843	3.506891	0.594685
1	-1.44666	1.318878	2.491204
1	-6.336423	-2.069752	-0.457939
1	-2.27851	-3.654415	-2.551101
1	1.631233	-4.084451	0.979576
1	0.536652	-0.224179	-0.240278
8	-0.437367	-1.840031	-2.254405
1	-1.151693	-1.22319	-2.03749
8	-5.690598	-0.293603	1.322243
1	-5.215445	0.388333	1.832071

*Table S89 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site 4β-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482612 (Hartree/Particle)
Thermal correction to Energy= 0.516954
Thermal correction to Enthalpy= 0.517898
Thermal correction to Gibbs Free Energy= 0.417742
Sum of electronic and zero-point Energies= -2021.137554
Sum of electronic and thermal Energies= -2021.103212
Sum of electronic and thermal Enthalpies= -2021.102268
Sum of electronic and thermal Free Energies= -2021.202424

Coordinates:

6	-2.593325	-0.074933	-0.016941
6	-3.929837	-0.606112	-0.230588
6	-5.035795	0.302124	-0.213279
6	-4.844953	1.66875	0.004829
6	-3.568997	2.166718	0.230558
6	-2.456626	1.333504	0.238882
1	-3.450995	3.23129	0.390994
6	-1.375114	-0.833718	-0.045993
6	-4.289834	-1.997558	-0.46607
6	-1.103381	-2.168196	-0.211492
6	-3.391326	-3.156034	-0.534476
6	-2.030927	-3.216058	-0.42805
8	-5.509739	-2.332945	-0.638679
8	-4.048663	-4.314599	-0.754543
1	-4.993805	-4.049315	-0.8135
8	-5.91273	2.506669	0.003789
8	-6.322301	-0.051291	-0.401296
1	-6.700665	1.962288	-0.166206
1	-6.303732	-1.048996	-0.542466
6	-1.105468	1.950163	0.561817
8	-0.368859	2.106631	-0.68688
6	-1.075105	3.317807	1.268545
6	0.937761	2.525737	-0.5379
6	0.375006	3.582339	1.701701
6	1.352839	3.213918	0.606802
6	2.714631	3.559119	0.686773
6	1.806458	2.224227	-1.592507
6	3.618208	3.238487	-0.328496
6	3.148391	2.570515	-1.460586
8	3.099954	4.222723	1.814254
8	4.089777	2.201909	-2.402187
1	4.046413	4.419296	1.76988
1	3.644837	1.947441	-3.224434
8	-1.560823	4.363786	0.425818
1	-1.242119	4.177696	-0.470953
1	-0.539981	1.265517	1.2036
6	0.343228	-2.643769	-0.130452
8	1.208405	-1.526094	-0.379935
6	0.696681	-3.3044	1.224763
1	0.109464	-4.224143	1.315218
6	2.556594	-1.755979	-0.296628
6	2.163042	-3.605479	1.264744
6	3.054189	-2.811105	0.522043
6	3.382144	-0.884878	-0.985814
6	4.480474	-2.945556	0.561715
1	2.939218	-0.099608	-1.581112
6	4.77145	-1.018942	-0.869008
6	5.320697	-2.06886	-0.110681
8	4.95317	-3.970587	1.325138
1	5.920952	-3.96378	1.313438
1	0.515099	-3.393534	-0.915977
1	0.472413	4.641315	1.961485
1	0.594222	3.017351	2.617032
1	-1.725888	3.301382	2.147087
1	4.669581	3.495158	-0.2495
1	1.433067	1.68714	-2.457975
1	6.399492	-2.170216	-0.043962
1	2.531971	-4.362912	1.944776
1	-1.62384	-4.218039	-0.543155
1	-0.480539	-0.240339	0.054009
8	0.274	-2.495001	2.336427
1	0.871728	-1.733997	2.37475
8	5.629419	-0.161807	-1.481048
1	5.133589	0.592863	-1.85517

*Table S90 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site 4α-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482618 (Hartree/Particle)
Thermal correction to Energy= 0.516956
Thermal correction to Enthalpy= 0.517900
Thermal correction to Gibbs Free Energy= 0.417764
Sum of electronic and zero-point Energies= -2021.137549
Sum of electronic and thermal Energies= -2021.103211
Sum of electronic and thermal Enthalpies= -2021.102267
Sum of electronic and thermal Free Energies= -2021.202403

Coordinates:

6	-2.593353	-0.075293	-0.017092
6	-3.929626	-0.606917	-0.230968
6	-5.035883	0.300971	-0.214315
6	-4.845559	1.667663	0.003763
6	-3.569821	2.166094	0.22976
6	-2.457195	1.333255	0.238478
1	-3.45224	3.230725	0.390114
6	-1.374828	-0.833638	-0.046019
6	-4.289112	-1.998607	-0.465992
6	-1.102626	-2.168104	-0.210792
6	-3.390266	-3.156945	-0.532936
6	-2.029868	-3.21646	-0.426483
8	-5.508797	-2.334504	-0.638967
8	-4.047236	-4.315913	-0.752074
1	-4.992427	-4.051072	-0.811951
8	-5.913618	2.505247	0.002323
8	-6.322164	-0.052942	-0.402725
1	-6.701352	1.960535	-0.167537
1	-6.303005	-1.050732	-0.543307
6	-1.10631	1.950402	0.561637
8	-0.369457	2.107196	-0.686881
6	-1.076726	3.318088	1.268304
6	0.936977	2.526818	-0.537479
6	0.373125	3.583191	1.70194
6	1.351432	3.215158	0.607356
6	2.713092	3.560776	0.687778
6	1.806113	2.225672	-1.59182
6	3.617111	3.240434	-0.327179
6	3.147909	2.572365	-1.459461
8	3.097824	4.224508	1.815397
8	4.089677	2.20405	-2.400735
1	4.044188	4.421589	1.771244
1	3.645179	1.949406	-3.22317
8	-1.562521	4.363795	0.425292
1	-1.243577	4.177625	-0.471379
1	-0.540713	1.265963	1.203547
6	0.344179	-2.643308	-0.130323
8	1.209125	-1.524891	-0.377537
6	0.697921	-3.306135	1.223667
1	0.110962	-4.226155	1.312835
6	2.55738	-1.755192	-0.295886
6	2.164416	-3.606839	1.263076
1	2.533635	-4.365102	1.94207
6	3.055333	-2.811507	0.520961
6	3.382516	-0.883196	-0.984386
6	4.481632	-2.946222	0.55949
1	2.939269	-0.096947	-1.578113
6	4.771887	-1.017702	-0.86884
6	5.321513	-2.068734	-0.112335
8	4.954679	-3.972335	1.321208
1	5.922457	-3.965878	1.308692
1	0.516419	-3.391514	-0.917246
1	0.470023	4.642195	1.961796
1	0.592261	3.018246	2.617321
1	-1.727804	3.301472	2.146628
1	4.668382	3.497426	-0.247819
1	1.433156	1.688531	-2.457448
1	6.400338	-2.170385	-0.046655
1	-1.622464	-4.218395	-0.540862
1	-0.480484	-0.239811	0.053459
8	0.274992	-2.498674	2.336762
1	0.86984	-1.735314	2.373601
8	5.629539	-0.159788	-1.480242
1	5.133423	0.595061	-1.853828

*Table S91 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site 3-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.483099 (Hartree/Particle)
Thermal correction to Energy= 0.517380
Thermal correction to Enthalpy= 0.518324
Thermal correction to Gibbs Free Energy= 0.418187
Sum of electronic and zero-point Energies= -2021.122679
Sum of electronic and thermal Energies= -2021.088399
Sum of electronic and thermal Enthalpies= -2021.087454
Sum of electronic and thermal Free Energies= -2021.187592

Coordinates:

6	-2.600065	-0.073059	-0.050024
6	-3.934854	-0.611755	-0.252411
6	-5.040123	0.297156	-0.28212
6	-4.852281	1.669369	-0.098509
6	-3.581587	2.170739	0.14587
6	-2.468996	1.337644	0.187005
1	-3.46599	3.236691	0.299357
6	-1.375062	-0.824797	-0.100756
6	-4.296969	-2.013609	-0.412616
6	-1.110919	-2.166163	-0.189265
6	-3.404772	-3.177931	-0.360382
6	-2.044169	-3.230108	-0.268099
8	-5.514037	-2.354898	-0.589986
8	-4.06815	-4.350446	-0.457498
1	-5.01077	-4.088922	-0.554736
8	-5.919894	2.507089	-0.139301
8	-6.323939	-0.062339	-0.476523
1	-6.705448	1.957877	-0.304395
1	-6.305119	-1.065014	-0.575568
6	-1.126878	1.954782	0.544114
8	-0.368843	2.150677	-0.686014
6	-1.122127	3.303905	1.287674
6	0.92982	2.580733	-0.50027
6	0.315806	3.568608	1.757573
6	1.315904	3.243496	0.669451
6	2.670962	3.605727	0.781969
6	1.821212	2.317188	-1.545656
6	3.59652	3.323596	-0.224607
6	3.155681	2.677114	-1.380671
8	3.027004	4.245105	1.932893
8	4.117978	2.342673	-2.312376
1	3.970633	4.45803	1.909242
1	3.690013	2.076822	-3.140071
8	-1.597502	4.369164	0.462911
1	-1.249866	4.215297	-0.429158
1	-0.567533	1.255927	1.175622
6	0.3362	-2.654074	-0.185891
8	1.217945	-1.537657	-0.487422
6	0.75786	-3.322984	1.085868
6	2.564967	-1.766898	-0.344497
6	2.163249	-3.858122	1.057056
1	2.190066	-4.823795	0.532157
6	3.0807	-2.858977	0.365838
6	3.394141	-0.815872	-0.945779
6	4.481683	-2.966894	0.439877
1	2.941816	0.005288	-1.483211
6	4.777579	-0.934555	-0.822564
6	5.333195	-2.023586	-0.137052
8	4.961852	-4.046456	1.129442
1	5.928631	-4.012537	1.147344
1	0.459669	-3.382217	-1.000207
1	0.398029	4.619754	2.051934
1	0.523439	2.976922	2.658661
1	-1.792303	3.259031	2.150373
1	4.642997	3.590953	-0.119816
1	1.471209	1.796962	-2.430888
1	6.411558	-2.115189	-0.052098
1	2.521597	-4.062096	2.072939
1	-1.633108	-4.236806	-0.281938
1	-0.480064	-0.222057	-0.086052
8	0.302103	-2.693418	2.218454
1	0.758158	-3.060202	2.989715
8	5.634297	-0.021647	-1.360982
1	5.131803	0.73247	-1.72475

*Table S92 Energetics and Cartesian coordinates of the conformer **1α-H_2O** (as-ass-as) post-radical capture via HAB at site 2-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482770 (Hartree/Particle)
Thermal correction to Energy= 0.517195
Thermal correction to Enthalpy= 0.518139
Thermal correction to Gibbs Free Energy= 0.417743
Sum of electronic and zero-point Energies= -2021.144655
Sum of electronic and thermal Energies= -2021.110230
Sum of electronic and thermal Enthalpies= -2021.109286
Sum of electronic and thermal Free Energies= -2021.209682

Coordinates:

6	-2.560511	-0.210566	-0.044602
6	-3.820788	-0.911193	-0.267298
6	-4.954967	-0.16219	-0.702813
6	-4.89203	1.228041	-0.854684
6	-3.727824	1.908481	-0.517724
6	-2.587189	1.233426	-0.103109
1	-3.723817	2.990439	-0.573119
6	-1.287065	-0.813372	0.135479
6	-4.071893	-2.318077	-0.022595
6	-0.877995	-2.141258	0.412836
6	-3.133051	-3.285667	0.568487
6	-1.788664	-3.207812	0.736767
8	-5.221268	-2.825657	-0.236478
8	-3.737267	-4.451039	0.918154
1	-4.666779	-4.343975	0.624736
8	-5.987228	1.912419	-1.275149
8	-6.159355	-0.697058	-0.978022
1	-6.696908	1.260822	-1.407903
1	-6.068531	-1.677415	-0.761997
6	-1.401515	2.046779	0.37994
8	-0.446298	2.202371	-0.711971
6	-1.678525	3.460936	0.92834
6	0.739301	2.810692	-0.352635
6	-0.39546	3.952702	1.612526
6	0.822255	3.642447	0.769706
6	2.08282	4.191451	1.068903
6	1.837874	2.549987	-1.178165
6	3.206863	3.929074	0.283504
6	3.065793	3.108745	-0.83663
8	2.141892	4.994804	2.169342
8	4.215338	2.816261	-1.544542
1	3.042118	5.332872	2.278402
1	3.977617	2.462605	-2.415115
8	-2.086615	4.361674	-0.103133
1	-1.541173	4.168544	-0.881242
1	-0.900842	1.492541	1.181505
6	0.503948	-2.450814	0.413312
8	1.353227	-1.41656	0.126078
6	1.144751	-3.76588	0.792193
1	0.413617	-4.569442	0.737052
6	2.700315	-1.624025	-0.127992
6	2.304143	-4.098186	-0.151068
1	1.901712	-4.381849	-1.133226
6	3.220949	-2.910587	-0.265651
6	3.470597	-0.46822	-0.255637
6	4.597029	-3.012629	-0.538598
1	3.005126	0.501175	-0.131868
6	4.829303	-0.606777	-0.554402
6	5.399923	-1.881062	-0.681305
8	5.093488	-4.276094	-0.676232
1	6.044765	-4.232734	-0.847527
1	-0.479563	5.030944	1.78167
1	-0.304854	3.48877	2.603343
1	-2.498031	3.429319	1.651049
1	4.177211	4.348107	0.528391
1	1.725976	1.88693	-2.028822
1	6.457073	-1.971223	-0.911149
1	2.836066	-4.969669	0.239483
1	-1.366988	-4.116382	1.148528
1	-0.456947	-0.132189	0.020441
8	1.570053	-3.739096	2.164929
1	2.362779	-3.183501	2.214983
8	5.655309	0.459842	-0.724685
1	5.139835	1.283703	-0.826461

*Table S93 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 5'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481455 (Hartree/Particle)
Thermal correction to Energy= 0.516346
Thermal correction to Enthalpy= 0.517291
Thermal correction to Gibbs Free Energy= 0.412911
Sum of electronic and zero-point Energies= -2021.137263
Sum of electronic and thermal Energies= -2021.102371
Sum of electronic and thermal Enthalpies= -2021.101427
Sum of electronic and thermal Free Energies= -2021.205807

Coordinates:

6	-2.101629	-1.359444	0.137183
6	-2.602527	-2.708285	-0.057638
6	-4.018379	-2.911205	-0.079003
6	-4.903593	-1.841989	0.083675
6	-4.417109	-0.559813	0.302232
6	-3.052344	-0.303384	0.349093
1	-5.128406	0.247449	0.422792
6	-0.721234	-0.970092	0.112612
6	-1.808669	-3.919214	-0.220631
6	0.453935	-1.667816	-0.017969
6	-0.345755	-4.037063	-0.21944
6	0.615249	-3.068486	-0.145442
8	-2.378682	-5.051596	-0.36884
8	0.073738	-5.315243	-0.341284
1	-0.755464	-5.838941	-0.409081
8	-6.241496	-2.063344	0.042245
8	-4.619314	-4.103734	-0.253914
1	-6.368202	-3.015704	-0.109852
1	-3.866183	-4.767607	-0.343712
6	-2.593177	1.106928	0.681168
8	-2.073131	1.713177	-0.541967
6	-3.622515	2.086742	1.273923
6	-1.537112	2.971415	-0.382699
6	-2.870094	3.349383	1.722192
6	-1.873919	3.788436	0.684712
6	-1.257583	5.114179	0.769174
6	-0.650312	3.392246	-1.388399
6	-0.33698	5.522789	-0.272925
6	-0.057991	4.680905	-1.32481
8	-1.535965	5.878393	1.727108
8	0.781046	4.984761	-2.349027
1	1.137757	5.876753	-2.226427
8	-4.65578	2.408282	0.343577
1	-4.245017	2.50052	-0.529573
1	-1.768761	1.054875	1.402293
6	1.72113	-0.826444	-0.077211
8	2.755443	-1.517447	0.646089
6	2.210105	-0.540225	-1.513784
1	1.398462	-0.06865	-2.073951
6	4.0168	-0.965326	0.612016
6	3.41108	0.412219	-1.437551
1	3.047177	1.430223	-1.242691
6	4.390083	-0.032306	-0.369402
6	4.901234	-1.422466	1.589281
6	5.709439	0.453348	-0.313494
1	4.57448	-2.144743	2.327569
6	6.20576	-0.925849	1.599187
6	6.617304	0.017448	0.653821
8	6.176907	1.37366	-1.207984
1	5.472827	1.637429	-1.815658
1	1.534282	0.136874	0.413713
1	-3.592138	4.149326	1.911754
1	-2.361918	3.164236	2.677767
1	-4.115198	1.62833	2.135506
1	0.10786	6.509373	-0.192037
1	-0.416294	2.730469	-2.214511
1	7.625214	0.419673	0.65633
1	3.879804	0.424928	-2.429758
1	1.63344	-3.436605	-0.19031
1	-0.571399	0.097787	0.181359
8	2.513858	-1.741008	-2.211884
1	3.265604	-2.161637	-1.769426
8	7.042767	-1.393435	2.570961
1	7.90977	-0.973889	2.478046

*Table S94 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 7'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481479 (Hartree/Particle)
Thermal correction to Energy= 0.516367
Thermal correction to Enthalpy= 0.517311
Thermal correction to Gibbs Free Energy= 0.413117
Sum of electronic and zero-point Energies= -2021.133699
Sum of electronic and thermal Energies= -2021.098811
Sum of electronic and thermal Enthalpies= -2021.097867
Sum of electronic and thermal Free Energies= -2021.202061

Coordinates:

6	-2.133409	-1.324638	0.15327
6	-2.649932	-2.670481	-0.018851
6	-4.068207	-2.857047	-0.040376
6	-4.941193	-1.77386	0.093104
6	-4.440193	-0.492288	0.28059
6	-3.07278	-0.251934	0.330935
1	-5.144469	0.324909	0.370386
6	-0.747937	-0.954433	0.140241
6	-1.870188	-3.89322	-0.161865
6	0.418885	-1.666661	0.011542
6	-0.408597	-4.027024	-0.175481
6	0.563882	-3.068811	-0.115819
8	-2.453699	-5.021672	-0.284956
8	-0.004541	-5.310376	-0.292129
1	-0.840124	-5.825716	-0.344877
8	-6.281354	-1.979541	0.050094
8	-4.682744	-4.045594	-0.191615
1	-6.419382	-2.933517	-0.080587
1	-3.937346	-4.720209	-0.264992
6	-2.597044	1.160736	0.626696
8	-2.028428	1.7141	-0.599218
6	-3.629236	2.183241	1.125819
6	-1.409249	2.93705	-0.470117
6	-2.865908	3.45048	1.551571
6	-1.783863	3.827762	0.571657
6	-1.115693	5.087141	0.654683
6	-0.459639	3.270672	-1.408988
6	-0.158319	5.449871	-0.266067
6	0.206135	4.556596	-1.343722
8	-1.411901	5.976418	1.640787
8	1.082415	4.875011	-2.191637
1	-2.068913	5.616064	2.251498
8	-4.607812	2.484304	0.137002
1	-4.160727	2.489223	-0.723649
1	-1.802256	1.120246	1.381279
6	1.694259	-0.838131	-0.053551
8	2.730861	-1.544253	0.65071
6	2.166879	-0.545475	-1.494509
1	1.352076	-0.062502	-2.039982
6	3.997351	-1.004663	0.602657
6	3.377109	0.395583	-1.427176
1	3.024597	1.415167	-1.219656
6	4.366108	-0.067155	-0.376235
6	4.89123	-1.479548	1.562685
6	5.691291	0.403972	-0.335877
1	4.567888	-2.204883	2.299473
6	6.201098	-0.997087	1.557168
6	6.608749	-0.050048	0.613871
8	6.15511	1.326817	-1.229552
1	5.44455	1.603874	-1.823638
1	1.522563	0.123031	0.447109
1	-3.598933	4.260809	1.6517
1	-2.428343	3.290678	2.547769
1	-4.167492	1.785682	1.98984
1	0.337581	6.410954	-0.194851
1	-0.197834	2.581704	-2.203459
1	7.620989	0.341084	0.604456
1	3.832674	0.412049	-2.425466
1	1.577661	-3.448195	-0.167373
1	-0.582697	0.110642	0.212821
8	2.449422	-1.743971	-2.20513
1	3.202894	-2.175366	-1.776253
8	7.047424	-1.48224	2.512114
1	7.917484	-1.071372	2.409578

*Table S95 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 3'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480293 (Hartree/Particle)
Thermal correction to Energy= 0.515343
Thermal correction to Enthalpy= 0.516287
Thermal correction to Gibbs Free Energy= 0.411626
Sum of electronic and zero-point Energies= -2021.105146
Sum of electronic and thermal Energies= -2021.070097
Sum of electronic and thermal Enthalpies= -2021.069153
Sum of electronic and thermal Free Energies= -2021.173813

Coordinates:

6	-2.286557	-1.130803	0.140706
6	-2.907702	-2.434186	-0.016975
6	-4.33602	-2.512941	-0.001805
6	-5.119047	-1.367278	0.157863
6	-4.518642	-0.125615	0.32348
6	-3.136686	0.013928	0.330829
1	-5.152661	0.744632	0.432372
6	-0.87624	-0.8721	0.111435
6	-2.227038	-3.712272	-0.181122
6	0.230596	-1.672898	-0.029183
6	-0.781091	-3.959538	-0.220857
6	0.264264	-3.081297	-0.165385
8	-2.898169	-4.792079	-0.299625
8	-0.480664	-5.270133	-0.352828
1	-1.355671	-5.716649	-0.393987
8	-6.472255	-1.471723	0.157273
8	-5.043503	-3.651705	-0.137543
1	-6.684862	-2.413042	0.035282
1	-4.353203	-4.37929	-0.236759
6	-2.539962	1.386681	0.600032
8	-1.919866	1.862587	-0.631717
6	-3.445928	2.510175	1.134975
6	-1.12313	2.97088	-0.477229
6	-2.594133	3.730765	1.333471
6	-1.444507	3.922227	0.541935
6	-0.568929	5.049692	0.643329
6	-0.071582	3.140672	-1.359853
6	0.491902	5.231464	-0.235029
6	0.733117	4.284317	-1.240278
8	-0.754132	6.003659	1.597744
8	1.761511	4.407109	-2.123623
1	-1.372532	5.682176	2.268753
1	2.253167	5.220646	-1.941061
8	-4.568313	2.806442	0.281073
1	-4.204766	3.034374	-0.588235
1	-1.747292	1.279442	1.351826
6	1.567556	-0.948659	-0.091625
8	2.533443	-1.717162	0.648983
6	2.092933	-0.724418	-1.526679
1	1.327713	-0.198684	-2.10335
6	3.833755	-1.263956	0.627755
6	3.365232	0.130939	-1.446917
1	3.081155	1.178016	-1.273467
6	4.290914	-0.374343	-0.358472
6	4.667471	-1.774402	1.623015
6	5.64299	0.008702	-0.289954
1	4.276703	-2.460141	2.365039
6	6.005892	-1.378718	1.646044
6	6.501867	-0.482301	0.695533
8	6.190464	0.878077	-1.189958
1	5.516825	1.179628	-1.81449
1	1.464265	0.034469	0.384113
1	-2.974644	4.505522	1.99124
1	-3.889909	2.189085	2.082414
1	1.129305	6.102715	-0.120849
1	0.124972	2.40622	-2.131712
1	7.537775	-0.158796	0.707975
1	3.847208	0.090022	-2.432148
1	1.244125	-3.539101	-0.232132
1	-0.626984	0.175701	0.18729
8	2.30847	-1.955331	-2.20498
1	3.020025	-2.427405	-1.74813
8	6.79085	-1.89621	2.635854
1	7.688828	-1.546072	2.550554

*Table S96 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site h-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482198 (Hartree/Particle)
Thermal correction to Energy= 0.517003
Thermal correction to Enthalpy= 0.517947
Thermal correction to Gibbs Free Energy= 0.414128
Sum of electronic and zero-point Energies= -2021.142039
Sum of electronic and thermal Energies= -2021.107234
Sum of electronic and thermal Enthalpies= -2021.106290
Sum of electronic and thermal Free Energies= -2021.210109

Coordinates:

6	-2.228749	-1.300752	0.142321
6	-2.792473	-2.629705	-0.010089
6	-4.214161	-2.765819	-0.106392
6	-5.115388	-1.608524	-0.079239
6	-4.494811	-0.326581	0.139316
6	-3.148637	-0.162577	0.271066
1	-5.161745	0.52516	0.186757
6	-0.85609	-0.976223	0.156337
6	-2.048394	-3.879178	-0.066869
6	0.308378	-1.733358	0.077592
6	-0.589958	-4.060714	-0.032147
6	0.420327	-3.128472	0.00739
8	-2.659906	-4.995583	-0.15745
8	-0.224503	-5.349808	-0.082715
1	-1.070785	-5.850218	-0.13597
8	-6.347007	-1.750605	-0.216299
8	-4.827256	-3.92536	-0.236039
1	-4.088708	-4.624587	-0.229254
6	-2.606331	1.221888	0.607776
8	-1.943121	1.742418	-0.573025
6	-3.606523	2.294214	1.07182
6	-1.269678	2.938143	-0.386644
6	-2.794085	3.502783	1.568166
6	-1.642481	3.822249	0.636196
6	-0.906402	5.016766	0.736186
6	-0.241586	3.209318	-1.287271
6	0.13451	5.31835	-0.145618
6	0.458527	4.411296	-1.157542
8	-1.173115	5.950076	1.696308
8	1.466146	4.642343	-2.048748
1	-1.895043	5.649814	2.264981
1	1.88285	5.493198	-1.851745
8	-4.50468	2.665944	0.029956
1	-3.996917	2.679475	-0.796109
1	-1.862163	1.119242	1.408159
6	1.595945	-0.926848	0.009043
8	2.643643	-1.677244	0.638484
6	2.01286	-0.590097	-1.442623
1	1.186613	-0.075731	-1.939533
6	3.916403	-1.151254	0.564509
6	3.241601	0.327545	-1.391
1	2.914446	1.345712	-1.13952
6	4.261197	-0.184815	-0.394024
6	4.836167	-1.671456	1.474327
6	5.593999	0.266477	-0.387222
1	4.529193	-2.4175	2.19724
6	6.151988	-1.20633	1.436953
6	6.538587	-0.233052	0.511663
8	6.038188	1.212919	-1.265557
1	5.310894	1.519637	-1.823738
1	1.459049	0.015937	0.553824
1	-3.489953	4.347682	1.644513
1	-2.430232	3.293516	2.583787
1	-4.220467	1.909332	1.890126
1	0.674816	6.252299	-0.028719
1	0.006939	2.501495	-2.068683
1	7.555862	0.14344	0.477022
1	3.659192	0.367135	-2.405112
1	1.422225	-3.540971	-0.008124
1	-0.655408	0.083932	0.203987
8	2.242464	-1.771569	-2.196138
1	3.00075	-2.231982	-1.807721
8	7.024715	-1.73546	2.342963
1	7.895603	-1.330243	2.22603

*Table S97 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site i-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482455 (Hartree/Particle)
Thermal correction to Energy= 0.517473
Thermal correction to Enthalpy= 0.518417
Thermal correction to Gibbs Free Energy= 0.413956
Sum of electronic and zero-point Energies= -2021.132154
Sum of electronic and thermal Energies= -2021.097136
Sum of electronic and thermal Enthalpies= -2021.096192
Sum of electronic and thermal Free Energies= -2021.200653

Coordinates:

6	-2.270224	-1.279177	0.139693
6	-2.862478	-2.581348	0.018574
6	-4.31001	-2.673677	-0.193878
6	-5.082089	-1.431026	-0.206276
6	-4.506556	-0.190388	0.022117
6	-3.140369	-0.096799	0.21863
1	-5.127526	0.696279	0.029198
6	-0.877382	-0.979595	0.16372
6	-2.173225	-3.860386	0.11039
6	0.26159	-1.759938	0.088405
6	-0.688605	-4.060647	0.111687
6	0.347101	-3.163668	0.066236
8	-2.782318	-4.95259	0.177497
8	-0.392117	-5.358365	0.139399
1	-1.300837	-5.775036	0.174451
8	-6.381563	-1.579238	-0.428562
8	-4.99248	-3.706132	-0.400906
1	-6.478232	-2.559989	-0.538108
6	-2.55892	1.264016	0.580355
8	-1.867665	1.78399	-0.584808
6	-3.53036	2.360162	1.052288
6	-1.154465	2.951405	-0.365873
6	-2.683422	3.530501	1.58169
6	-1.510349	3.828249	0.669129
6	-0.734537	4.994197	0.801637
6	-0.104756	3.202035	-1.246994
6	0.328275	5.275237	-0.060675
6	0.634834	4.376197	-1.085132
8	-0.981837	5.918381	1.775505
8	1.662388	4.587666	-1.958015
1	-1.720273	5.632618	2.330324
1	2.105166	5.420176	-1.740474
8	-4.401736	2.781814	0.006503
1	-3.87658	2.821719	-0.807897
1	-1.827535	1.125408	1.386335
6	1.565719	-0.984114	-0.024818
8	2.603659	-1.72657	0.631176
6	1.980564	-0.718347	-1.491102
1	1.160483	-0.210971	-2.005274
6	3.882948	-1.221117	0.534322
6	3.224993	0.179948	-1.483557
1	2.915544	1.213835	-1.277346
6	4.239171	-0.302268	-0.466031
6	4.796928	-1.712765	1.465722
6	5.577357	0.132371	-0.478796
1	4.480954	-2.422572	2.220555
6	6.11848	-1.266455	1.407727
6	6.516297	-0.339095	0.440984
8	6.032746	1.034435	-1.397295
1	5.309209	1.324316	-1.969183
1	1.452614	-0.015539	0.478047
1	-3.351242	4.396811	1.667487
1	-2.338537	3.288998	2.596694
1	-4.169047	1.981012	1.854185
1	0.898935	6.187427	0.08104
1	0.130339	2.499866	-2.037639
1	7.537858	0.023632	0.390376
1	3.640292	0.166992	-2.499385
1	1.339643	-3.597692	0.049091
1	-0.654976	0.076489	0.181266
8	2.186065	-1.933848	-2.196288
1	2.927463	-2.399087	-1.781858
8	6.985503	-1.766479	2.335628
1	7.862063	-1.380264	2.198412

*Table S98 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site b-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481359 (Hartree/Particle)
Thermal correction to Energy= 0.516469
Thermal correction to Enthalpy= 0.517413
Thermal correction to Gibbs Free Energy= 0.412840
Sum of electronic and zero-point Energies= -2021.137389
Sum of electronic and thermal Energies= -2021.102279
Sum of electronic and thermal Enthalpies= -2021.101335
Sum of electronic and thermal Free Energies= -2021.205908

Coordinates:

6	2.204855	-1.293887	-0.150741
6	2.78101	-2.609588	0.062967
6	4.183617	-2.70241	0.272108
6	5.013978	-1.558633	0.206233
6	4.465098	-0.312652	-0.067103
6	3.09711	-0.161133	-0.253686
1	5.1223	0.546719	-0.105716
6	0.820961	-1.002544	-0.186123
6	2.080901	-3.894393	0.061477
6	-0.335514	-1.806155	-0.170753
6	0.633206	-4.155381	-0.365147
6	-0.415941	-3.176917	-0.271089
8	2.692511	-4.946528	0.368434
8	0.368766	-5.315375	-0.708957
8	6.337948	-1.691905	0.404277
8	4.832484	-3.837641	0.531066
1	6.518839	-2.633595	0.57535
1	4.098937	-4.549814	0.555957
6	2.558323	1.216079	-0.616888
8	1.891701	1.758008	0.553964
6	3.562571	2.277935	-1.09635
6	1.22501	2.953826	0.346266
6	2.755791	3.480825	-1.614702
6	1.603889	3.819803	-0.689931
6	0.873461	5.015966	-0.81069
6	0.196098	3.244405	1.240077
6	-0.167291	5.336887	0.064314
6	-0.497578	4.447654	1.090032
8	1.145835	5.932406	-1.785461
8	-1.505419	4.698113	1.975734
1	1.865615	5.619037	-2.349701
1	-1.918478	5.547096	1.763593
8	4.459552	2.663283	-0.057832
1	3.945855	2.71039	0.763416
1	1.814768	1.102325	-1.415167
6	-1.629714	-1.012037	-0.041477
8	-2.709919	-1.772446	-0.598742
6	-1.97185	-0.672036	1.427382
1	-1.125123	-0.156902	1.887957
6	-3.970054	-1.220098	-0.491179
6	-3.202085	0.247206	1.437712
1	-2.881971	1.268756	1.189137
6	-4.262513	-0.243431	0.473622
6	-4.928334	-1.724901	-1.368995
6	-5.584429	0.236731	0.506709
1	-4.660112	-2.479897	-2.098028
6	-6.232276	-1.231692	-1.291576
6	-6.567759	-0.246151	-0.359415
8	-5.97978	1.195851	1.394838
1	-5.227734	1.489256	1.926829
1	-1.533767	-0.073435	-0.602834
1	3.454736	4.321863	-1.704511
1	2.393001	3.255329	-2.627157
1	4.178696	1.877269	-1.905555
1	-0.702695	6.271502	-0.068561
1	-0.058424	2.549532	2.031224
1	-7.575273	0.152014	-0.294267
1	-3.579844	0.27212	2.467861
1	-1.404455	-3.614277	-0.355303
1	0.593793	0.054436	-0.191336
8	-2.164916	-1.856296	2.186234
1	-2.848428	-2.382387	1.745382
8	-7.145131	-1.745766	-2.166448
1	-8.002557	-1.320627	-2.023742

*Table S99 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 3-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480582 (Hartree/Particle)
Thermal correction to Energy= 0.515447
Thermal correction to Enthalpy= 0.516392
Thermal correction to Gibbs Free Energy= 0.412123
Sum of electronic and zero-point Energies= -2021.107155
Sum of electronic and thermal Energies= -2021.072290
Sum of electronic and thermal Enthalpies= -2021.071346
Sum of electronic and thermal Free Energies= -2021.175615

Coordinates:

6	2.204855	-1.293887	-0.150741
6	2.78101	-2.609588	0.062967
6	4.183617	-2.70241	0.272108
6	5.013978	-1.558633	0.206233
6	4.465098	-0.312652	-0.067103
6	3.09711	-0.161133	-0.253686
1	5.1223	0.546719	-0.105716
6	0.820961	-1.002544	-0.186123
6	2.080901	-3.894393	0.061477
6	-0.335514	-1.806155	-0.170753
6	0.633206	-4.155381	-0.365147
6	-0.415941	-3.176917	-0.271089
8	2.692511	-4.946528	0.368434
8	0.368766	-5.315375	-0.708957
8	6.337948	-1.691905	0.404277
8	4.832484	-3.837641	0.531066
1	6.518839	-2.633595	0.57535
1	4.098937	-4.549814	0.555957
6	2.558323	1.216079	-0.616888
8	1.891701	1.758008	0.553964
6	3.562571	2.277935	-1.09635
6	1.22501	2.953826	0.346266
6	2.755791	3.480825	-1.614702
6	1.603889	3.819803	-0.689931
6	0.873461	5.015966	-0.81069
6	0.196098	3.244405	1.240077
6	-0.167291	5.336887	0.064314
6	-0.497578	4.447654	1.090032
8	1.145835	5.932406	-1.785461
8	-1.505419	4.698113	1.975734
1	1.865615	5.619037	-2.349701
1	-1.918478	5.547096	1.763593
8	4.459552	2.663283	-0.057832
1	3.945855	2.71039	0.763416
1	1.814768	1.102325	-1.415167
6	-1.629714	-1.012037	-0.041477
8	-2.709919	-1.772446	-0.598742
6	-1.97185	-0.672036	1.427382
1	-1.125123	-0.156902	1.887957
6	-3.970054	-1.220098	-0.491179
6	-3.202085	0.247206	1.437712
1	-2.881971	1.268756	1.189137
6	-4.262513	-0.243431	0.473622
6	-4.928334	-1.724901	-1.368995
6	-5.584429	0.236731	0.506709
1	-4.660112	-2.479897	-2.098028
6	-6.232276	-1.231692	-1.291576
6	-6.567759	-0.246151	-0.359415
8	-5.97978	1.195851	1.394838
1	-5.227734	1.489256	1.926829
1	-1.533767	-0.073435	-0.602834
1	3.454736	4.321863	-1.704511
1	2.393001	3.255329	-2.627157
1	4.178696	1.877269	-1.905555
1	-0.702695	6.271502	-0.068561
1	-0.058424	2.549532	2.031224
1	-7.575273	0.152014	-0.294267
1	-3.579844	0.27212	2.467861
1	-1.404455	-3.614277	-0.355303
1	0.593793	0.054436	-0.191336
8	-2.164916	-1.856296	2.186234
1	-2.848428	-2.382387	1.745382
8	-7.145131	-1.745766	-2.166448
1	-8.002557	-1.320627	-2.023742

*Table S100 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 5-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481656 (Hartree/Particle)
Thermal correction to Energy= 0.516435
Thermal correction to Enthalpy= 0.517380
Thermal correction to Gibbs Free Energy= 0.413595
Sum of electronic and zero-point Energies= -2021.137326
Sum of electronic and thermal Energies= -2021.102547
Sum of electronic and thermal Enthalpies= -2021.101602
Sum of electronic and thermal Free Energies= -2021.205387

Coordinates:

6	-2.088422	-1.376103	0.149934
6	-2.56695	-2.735322	-0.029234
6	-3.979103	-2.960384	-0.055422
6	-4.881303	-1.901573	0.079288
6	-4.415955	-0.60775	0.276029
6	-3.056048	-0.330287	0.333264
1	-5.141286	0.190692	0.367331
6	-0.714034	-0.96631	0.137777
6	-1.753066	-3.935253	-0.174479
6	0.47202	-1.645169	0.006417
6	-0.288274	-4.027563	-0.187534
6	0.656677	-3.042426	-0.125473
8	-2.304352	-5.079397	-0.301487
8	0.152115	-5.298971	-0.30727
1	-0.668828	-5.837237	-0.361194
8	-6.215337	-2.14357	0.029668
8	-4.561195	-4.165004	-0.213572
1	-6.32639	-3.100238	-0.10695
1	-3.797942	-4.818779	-0.286562
6	-2.61892	1.093688	0.641255
8	-2.06447	1.669867	-0.574208
6	-3.68153	2.079999	1.155044
6	-1.491777	2.919866	-0.422756
6	-2.954408	3.356784	1.610391
6	-1.88488	3.77203	0.620265
6	-1.254112	5.027471	0.681753
6	-0.54247	3.28008	-1.377889
6	-0.297209	5.419734	-0.257447
6	0.049819	4.541942	-1.28765
8	-1.548987	5.935588	1.658472
8	0.978662	4.862563	-2.235337
1	-2.199433	5.56809	2.272148
1	1.32753	5.747593	-2.058297
8	-4.658494	2.369155	0.157786
1	-4.192448	2.418874	-0.691307
1	-1.825401	1.067673	1.398576
6	1.722659	-0.780886	-0.053894
8	2.771281	-1.454852	0.6766
6	2.19953	-0.474355	-1.492613
1	1.378125	0.010606	-2.026697
6	4.027542	-0.914831	0.588293
6	3.40631	0.469237	-1.422479
1	3.066046	1.487591	-1.192048
6	4.389122	0.003767	-0.383935
6	4.951877	-1.380735	1.542905
6	5.763368	0.508093	-0.393515
1	4.63876	-2.104478	2.286675
6	6.287666	-0.903907	1.540237
6	6.692683	0.023151	0.607092
8	6.122522	1.341601	-1.262744
1	1.522238	0.175837	0.44336
1	-3.715891	4.138868	1.723762
1	-2.522478	3.183064	2.605978
1	-4.220023	1.64812	2.002755
1	0.16069	6.399973	-0.170915
1	-0.271049	2.591797	-2.169257
1	7.705804	0.410933	0.582718
1	3.890324	0.524564	-2.401917
1	1.680426	-3.393916	-0.179087
1	-0.581231	0.103252	0.211359
8	2.479837	-1.664575	-2.219643
1	3.267852	-2.077032	-1.837449
8	7.09107	-1.419287	2.506885
1	7.978513	-1.038723	2.432106

*Table S101 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 7-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481460 (Hartree/Particle)
Thermal correction to Energy= 0.516332
Thermal correction to Enthalpy= 0.517276
Thermal correction to Gibbs Free Energy= 0.413109
Sum of electronic and zero-point Energies= -2021.133403
Sum of electronic and thermal Energies= -2021.098532
Sum of electronic and thermal Enthalpies= -2021.097588
Sum of electronic and thermal Free Energies= -2021.201755

Coordinates:

6	-2.200856	-1.32727	0.150281
6	-2.68153	-2.623711	-0.028634
6	-4.107518	-2.791659	-0.070123
6	-4.957822	-1.689689	0.053948
6	-4.431441	-0.419667	0.252612
6	-3.060247	-0.209208	0.323319
1	-5.117635	0.41371	0.334413
6	-0.697324	-0.946985	0.152881
6	-1.930836	-3.87461	-0.166526
6	0.402403	-1.69591	0.031165
6	-0.472494	-4.038386	-0.166897
6	0.519159	-3.100562	-0.097899
8	-2.536652	-4.990828	-0.296883
8	-0.093936	-5.330132	-0.281969
1	-0.940002	-5.827148	-0.343128
8	-6.301781	-1.866032	-0.008096
8	-4.746059	-3.966876	-0.231915
1	-6.458203	-2.816682	-0.142175
1	-4.014255	-4.656943	-0.296245
6	-2.556725	1.192412	0.632072
8	-1.958333	1.735391	-0.57821
6	-3.575395	2.23229	1.128193
6	-1.3246	2.95495	-0.422466
6	-2.792623	3.474156	1.58742
6	-1.689773	3.830794	0.611013
6	-0.997438	5.053185	0.676981
6	-0.343162	3.26169	-1.363729
6	-0.006142	5.391067	-0.247689
6	0.312252	4.49155	-1.268276
8	-1.261874	5.980468	1.644243
8	1.272306	4.759066	-2.201308
1	-1.946516	5.653298	2.243344
1	1.662477	5.626339	-2.022602
8	-4.524701	2.564093	0.117366
1	-4.047053	2.582236	-0.726527
1	-1.77502	1.12981	1.399533
6	1.694137	-0.892773	-0.025016
8	2.714431	-1.621427	0.680643
6	2.178515	-0.603562	-1.462648
1	1.375144	-0.103582	-2.009753
6	3.990864	-1.105374	0.640218
6	3.405521	0.31484	-1.386091
1	3.070564	1.339677	-1.175201
6	4.381237	-0.170874	-0.333162
6	4.871906	-1.600795	1.601774
6	5.714871	0.274917	-0.285807
1	4.532136	-2.322985	2.334248
6	6.190626	-1.143063	1.603354
6	6.619895	-0.200079	0.665586
8	6.199205	1.192471	-1.174112
1	5.496503	1.482763	-1.771241
1	1.539182	0.069694	0.478535
1	-3.516221	4.293287	1.685983
1	-2.383619	3.285184	2.589874
1	-4.144756	1.831294	1.970913
1	0.500197	6.346853	-0.157642
1	-0.095666	2.557545	-2.148978
1	7.639428	0.171758	0.66171
1	3.865687	0.327441	-2.382351
1	1.525192	-3.501067	-0.142259
1	-0.512802	0.11488	0.227681
8	2.442198	-1.804375	-2.176765
1	3.182459	-2.253497	-1.743102
8	7.02395	-1.648055	2.559486

*Table S102 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 4'-α-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481034 (Hartree/Particle)
Thermal correction to Energy= 0.516271
Thermal correction to Enthalpy= 0.517215
Thermal correction to Gibbs Free Energy= 0.412732
Sum of electronic and zero-point Energies= -2021.129658
Sum of electronic and thermal Energies= -2021.094420
Sum of electronic and thermal Enthalpies= -2021.093476
Sum of electronic and thermal Free Energies= -2021.197959

Coordinates:

6	-2.088422	-1.376103	0.149934
6	-2.56695	-2.735322	-0.029234
6	-3.979103	-2.960384	-0.055422
6	-4.881303	-1.901573	0.079288
6	-4.415955	-0.60775	0.276029
6	-3.056048	-0.330287	0.333264
1	-5.141286	0.190692	0.367331
6	-0.714034	-0.96631	0.137777
6	-1.753066	-3.935253	-0.174479
6	0.47202	-1.645169	0.006417
6	-0.288274	-4.027563	-0.187534
6	0.656677	-3.042426	-0.125473
8	-2.304352	-5.079397	-0.301487
8	0.152115	-5.298971	-0.30727
1	-0.668828	-5.837237	-0.361194
8	-6.215337	-2.14357	0.029668
8	-4.561195	-4.165004	-0.213572
1	-6.32639	-3.100238	-0.10695
1	-3.797942	-4.818779	-0.286562
6	-2.61892	1.093688	0.641255
8	-2.06447	1.669867	-0.574208
6	-3.68153	2.079999	1.155044
6	-1.491777	2.919866	-0.422756
6	-2.954408	3.356784	1.610391
6	-1.88488	3.77203	0.620265
6	-1.254112	5.027471	0.681753
6	-0.54247	3.28008	-1.377889
6	-0.297209	5.419734	-0.257447
6	0.049819	4.541942	-1.28765
8	-1.548987	5.935588	1.658472
8	0.978662	4.862563	-2.235337
1	-2.199433	5.56809	2.272148
1	1.32753	5.747593	-2.058297
8	-4.658494	2.369155	0.157786
1	-4.192448	2.418874	-0.691307
1	-1.825401	1.067673	1.398576
6	1.722659	-0.780886	-0.053894
8	2.771281	-1.454852	0.6766
6	2.19953	-0.474355	-1.492613
1	1.378125	0.010606	-2.026697
6	4.027542	-0.914831	0.588293
6	3.40631	0.469237	-1.422479
1	3.066046	1.487591	-1.192048
6	4.389122	0.003767	-0.383935
6	4.951877	-1.380735	1.542905
6	5.763368	0.508093	-0.393515
1	4.63876	-2.104478	2.286675
6	6.287666	-0.903907	1.540237
6	6.692683	0.023151	0.607092
8	6.122522	1.341601	-1.262744
1	1.522238	0.175837	0.44336
1	-3.715891	4.138868	1.723762
1	-2.522478	3.183064	2.605978
1	-4.220023	1.64812	2.002755
1	0.16069	6.399973	-0.170915
1	-0.271049	2.591797	-2.169257
1	7.705804	0.410933	0.582718
1	3.890324	0.524564	-2.401917
1	1.680426	-3.393916	-0.179087
1	-0.581231	0.103252	0.211359
8	2.479837	-1.664575	-2.219643
1	3.267852	-2.077032	-1.837449
8	7.09107	-1.419287	2.506885
1	7.978513	-1.038723	2.432106

*Table S103 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 4'β-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481031 (Hartree/Particle)
Thermal correction to Energy= 0.516269
Thermal correction to Enthalpy= 0.517214
Thermal correction to Gibbs Free Energy= 0.412728
Sum of electronic and zero-point Energies= -2021.129660
Sum of electronic and thermal Energies= -2021.094422
Sum of electronic and thermal Enthalpies= -2021.093478
Sum of electronic and thermal Free Energies= -2021.197963

Coordinates:

6	-2.286557	-1.130803	0.140706
6	-2.907702	-2.434186	-0.016975
6	-4.33602	-2.512941	-0.001805
6	-5.119047	-1.367278	0.157863
6	-4.518642	-0.125615	0.32348
6	-3.136686	0.013928	0.330829
1	-5.152661	0.744632	0.432372
6	-0.87624	-0.8721	0.111435
6	-2.227038	-3.712272	-0.181122
6	0.230596	-1.672898	-0.029183
6	-0.781091	-3.959538	-0.220857
6	0.264264	-3.081297	-0.165385
8	-2.898169	-4.792079	-0.299625
8	-0.480664	-5.270133	-0.352828
1	-1.355671	-5.716649	-0.393987
8	-6.472255	-1.471723	0.157273
8	-5.043503	-3.651705	-0.137543
1	-6.684862	-2.413042	0.035282
1	-4.353203	-4.37929	-0.236759
6	-2.539962	1.386681	0.600032
8	-1.919866	1.862587	-0.631717
6	-3.445928	2.510175	1.134975
6	-1.12313	2.97088	-0.477229
6	-2.594133	3.730765	1.333471
6	-1.444507	3.922227	0.541935
6	-0.568929	5.049692	0.643329
6	-0.071582	3.140672	-1.359853
6	0.491902	5.231464	-0.235029
6	0.733117	4.284317	-1.240278
8	-0.754132	6.003659	1.597744
8	1.761511	4.407109	-2.123623
1	-1.372532	5.682176	2.268753
1	2.253167	5.220646	-1.941061
8	-4.568313	2.806442	0.281073
1	-4.204766	3.034374	-0.588235
1	-1.747292	1.279442	1.351826
6	1.567556	-0.948659	-0.091625
8	2.533443	-1.717162	0.648983
6	2.092933	-0.724418	-1.526679
1	1.327713	-0.198684	-2.10335
6	3.833755	-1.263956	0.627755
6	3.365232	0.130939	-1.446917
1	3.081155	1.178016	-1.273467
6	4.290914	-0.374343	-0.358472
6	4.667471	-1.774402	1.623015
6	5.64299	0.008702	-0.289954
1	4.276703	-2.460141	2.365039
6	6.005892	-1.378718	1.646044
6	6.501867	-0.482301	0.695533
8	6.190464	0.878077	-1.189958
1	5.516825	1.179628	-1.81449
1	1.464265	0.034469	0.384113
1	-2.974644	4.505522	1.99124
1	-3.889909	2.189085	2.082414
1	1.129305	6.102715	-0.120849
1	0.124972	2.40622	-2.131712
1	7.537775	-0.158796	0.707975
1	3.847208	0.090022	-2.432148
1	1.244125	-3.539101	-0.232132
1	-0.626984	0.175701	0.18729
8	2.30847	-1.955331	-2.20498
1	3.020025	-2.427405	-1.74813
8	6.79085	-1.89621	2.635854
1	7.688828	-1.546072	2.550554

*Table S104 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 3'-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481549 (Hartree/Particle)
Thermal correction to Energy= 0.516643
Thermal correction to Enthalpy= 0.517587
Thermal correction to Gibbs Free Energy= 0.413833
Sum of electronic and zero-point Energies= -2021.111925
Sum of electronic and thermal Energies= -2021.076832
Sum of electronic and thermal Enthalpies= -2021.075887
Sum of electronic and thermal Free Energies= -2021.179642

Coordinates:

6	-2.105727	-1.368011	0.156528
6	-2.587293	-2.721947	-0.055601
6	-3.981729	-2.986205	0.120951
6	-4.861927	-1.975279	0.514778
6	-4.399483	-0.675944	0.680416
6	-3.064271	-0.345387	0.473779
1	-5.118461	0.070929	0.994677
6	-0.7295	-0.963249	0.149102
6	-1.792572	-3.881261	-0.444399
6	0.445285	-1.620694	-0.121879
6	-0.342902	-3.942251	-0.655519
6	0.608932	-2.973391	-0.50573
8	-2.352084	-5.011668	-0.640525
8	0.078838	-5.169808	-1.030137
1	-0.740322	-5.712471	-1.055388
8	-6.17127	-2.260654	0.717783
8	-4.563933	-4.188521	-0.047085
1	-6.287081	-3.21009	0.540114
1	-3.817705	-4.80539	-0.328805
6	-2.656607	1.106475	0.695392
8	-1.915677	1.576027	-0.487616
6	-3.743391	2.114979	0.931216
6	-1.451696	2.869842	-0.397445
6	-3.194715	3.437935	1.382413
6	-1.996877	3.801612	0.506104
6	-1.428802	5.087245	0.519312
6	-0.414196	3.202663	-1.270415
6	-0.3858	5.444389	-0.338645
6	0.109721	4.496424	-1.237086
8	-1.877819	6.064705	1.36239
8	1.126554	4.777698	-2.104622
1	-2.561771	5.714653	1.948849
1	1.409559	5.694801	-1.98175
8	-4.708848	2.266112	-0.039983
1	-4.776914	1.460662	-0.574489
1	-1.971618	1.168379	1.551932
6	1.710662	-0.778976	-0.047273
8	2.740451	-1.574087	0.56858
6	2.215175	-0.269578	-1.415482
1	1.405579	0.274535	-1.908377
6	3.9991	-1.020075	0.634545
6	3.404103	0.670108	-1.170572
1	3.025455	1.639603	-0.818948
6	4.374918	0.063616	-0.176778
6	4.879262	-1.628943	1.529398
6	5.691789	0.537678	-0.031275
1	4.551022	-2.464574	2.135613
6	6.181339	-1.136581	1.630823
6	6.595269	-0.048447	0.857689
8	6.161807	1.593608	-0.759138
1	5.457494	1.960183	-1.310629
1	1.519456	0.096599	0.5853
1	-3.986039	4.192637	1.29583
1	-2.906476	3.384854	2.441578
1	0.018092	6.450824	-0.295372
1	-0.022756	2.464899	-1.960384
1	7.601246	0.351793	0.934784
1	3.885636	0.848395	-2.140635
1	1.622945	-3.303224	-0.697262
1	-0.584182	0.076298	0.401641
8	2.545965	-1.34337	-2.287184
1	3.313211	-1.802495	-1.915089
8	7.013059	-1.756011	2.518515
1	7.878867	-1.324533	2.502908

*Table S105 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 2'-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480570 (Hartree/Particle)
Thermal correction to Energy= 0.516077
Thermal correction to Enthalpy= 0.517021
Thermal correction to Gibbs Free Energy= 0.411885
Sum of electronic and zero-point Energies= -2021.133894
Sum of electronic and thermal Energies= -2021.098387
Sum of electronic and thermal Enthalpies= -2021.097442
Sum of electronic and thermal Free Energies= -2021.202579

Coordinates:

6	1.975116	-1.512151	-0.11152
6	2.348876	-2.897649	0.118857
6	3.678913	-3.30271	-0.179695
6	4.624758	-2.388902	-0.690451
6	4.314383	-1.053275	-0.802342
6	3.0276	-0.560308	-0.46717
1	5.113476	-0.371395	-1.064822
6	0.643371	-1.021026	-0.172138
6	1.488246	-3.945964	0.655176
6	-0.581037	-1.563056	0.169732
6	0.067726	-3.84709	0.97817
6	-0.821156	-2.83035	0.738785
8	1.966198	-5.105776	0.904962
8	-0.426953	-4.98033	1.529772
1	0.340237	-5.593935	1.550387
8	5.87289	-2.832143	-0.988174
8	4.155367	-4.551387	-0.014818
1	5.896174	-3.780541	-0.773372
1	3.391298	-5.066473	0.400738
6	2.874477	0.854227	-0.466104
8	1.93086	1.394068	0.375422
6	3.784296	1.809438	-1.192378
6	1.66498	2.748336	0.398137
6	2.984103	3.012703	-1.714407
6	2.146986	3.598401	-0.604499
6	1.794342	4.955632	-0.505317
6	0.891342	3.187862	1.469671
6	1.017743	5.434068	0.554006
6	0.571629	4.546708	1.536958
8	2.184316	5.878567	-1.430322
8	-0.186264	4.953162	2.594842
1	2.649518	5.446503	-2.159631
1	-0.336802	5.907443	2.538197
8	4.902889	2.227799	-0.391014
1	4.558721	2.740329	0.355805
6	-1.785431	-0.65712	-0.030544
8	-2.883282	-1.464446	-0.496709
6	-2.2202	0.104089	1.241115
1	-1.364204	0.667233	1.621347
6	-4.105652	-0.84528	-0.626929
6	-3.353949	1.0689	0.868433
1	-2.927876	1.940368	0.353005
6	-4.390814	0.375166	0.008138
6	-5.048008	-1.528905	-1.396055
6	-5.680252	0.904304	-0.184213
1	-4.789739	-2.469668	-1.867016
6	-6.320282	-0.97554	-1.548535
6	-6.643964	0.245308	-0.950316
8	-6.062502	2.09053	0.375005
1	-5.323713	2.48631	0.856878
1	-1.547088	0.086949	-0.80117
1	3.71171	3.734057	-2.104631
1	2.361225	2.692502	-2.560473
1	4.229425	1.292942	-2.043258
1	0.768688	6.489632	0.591725
1	0.55938	2.496953	2.234786
1	-7.625647	0.692586	-1.069779
1	-3.792293	1.435088	1.805638
1	-1.847115	-3.05839	1.003489
1	0.574327	-0.019797	-0.574267
8	-2.59328	-0.787974	2.284096
1	-3.396854	-1.250793	2.004671
8	-7.214909	-1.672182	-2.30891
1	-8.05431	-1.191908	-2.338854

*Table S106 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 4β-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481190 (Hartree/Particle)
Thermal correction to Energy= 0.516328
Thermal correction to Enthalpy= 0.517272
Thermal correction to Gibbs Free Energy= 0.412854
Sum of electronic and zero-point Energies= -2021.130918
Sum of electronic and thermal Energies= -2021.095780
Sum of electronic and thermal Enthalpies= -2021.094836
Sum of electronic and thermal Free Energies= -2021.199254

Coordinates:

6	-2.143505	-1.272191	0.155214
6	-2.732871	-2.588381	-0.016324
6	-4.15867	-2.702459	0.002036
6	-4.970589	-1.578831	0.178628
6	-4.399231	-0.327549	0.369132
6	-3.020405	-0.156622	0.378673
1	-5.055971	0.524016	0.495192
6	-0.741737	-0.97068	0.099496
6	-2.021477	-3.847553	-0.19462
6	0.382326	-1.741985	-0.061423
6	-0.570046	-4.056614	-0.239837
6	0.450623	-3.149789	-0.196555
8	-2.665624	-4.942864	-0.318652
8	-0.23505	-5.358979	-0.373331
1	-1.097586	-5.828825	-0.413702
8	-6.320505	-1.716524	0.175271
8	-4.837731	-3.856385	-0.146645
1	-6.509882	-2.660599	0.037252
1	-4.129598	-4.56599	-0.25287
6	-2.465403	1.228733	0.671655
8	-1.94219	1.775017	-0.570905
6	-3.422834	2.280771	1.256669
6	-1.295434	2.991902	-0.458128
6	-2.580517	3.496702	1.676472
6	-1.563744	3.85904	0.612123
6	-0.867547	5.081106	0.625275
6	-0.40521	3.308486	-1.483141
6	0.033355	5.428627	-0.384379
6	0.253547	4.539186	-1.439357
8	-1.042282	5.999317	1.621267
8	1.118471	4.818637	-2.45793
1	-1.664351	5.662769	2.280408
1	1.51453	5.689498	-2.31351
8	-4.436247	2.653756	0.325208
1	-4.021383	2.684702	-0.550717
1	-1.634191	1.138716	1.381661
6	1.701756	-0.990161	-0.143852
8	2.695861	-1.751211	0.576426
6	2.177191	-0.718541	-1.588047
1	1.464798	-0.018285	-2.038681
6	3.948551	-1.199543	0.623323
6	3.550329	-0.12589	-1.550233
6	4.389263	-0.352678	-0.443474
6	4.759844	-1.544242	1.689998
6	5.714456	0.175231	-0.317247
1	4.391902	-2.198651	2.471121
6	6.065136	-1.032306	1.742429
6	6.538154	-0.165102	0.74722
8	6.229664	1.01973	-1.253724
1	5.523397	1.345742	-1.828871
1	1.595092	-0.015819	0.348976
1	-3.277587	4.324522	1.85757
1	-2.088765	3.275998	2.634171
1	-3.938249	1.875465	2.131463
1	0.545937	6.384122	-0.333345
1	-0.230214	2.610819	-2.29333
1	7.537001	0.256135	0.798897
1	3.902434	0.375971	-2.445869
1	1.442177	-3.581136	-0.272093
1	-0.522449	0.085217	0.167643
8	2.113328	-1.888274	-2.420904
1	2.876414	-2.440225	-2.195444
8	6.82839	-1.397697	2.808242
1	7.695974	-0.972357	2.749154

*Table S107 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 4α-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481182 (Hartree/Particle)
Thermal correction to Energy= 0.516322
Thermal correction to Enthalpy= 0.517266
Thermal correction to Gibbs Free Energy= 0.412838
Sum of electronic and zero-point Energies= -2021.130926
Sum of electronic and thermal Energies= -2021.095786
Sum of electronic and thermal Enthalpies= -2021.094842
Sum of electronic and thermal Free Energies= -2021.199270

Coordinates:

6	-2.143292	-1.272618	0.15501
6	-2.732431	-2.588971	-0.016316
6	-4.158224	-2.703282	0.001837
6	-4.970314	-1.579713	0.177896
6	-4.399206	-0.328301	0.368266
6	-3.020404	-0.157129	0.378095
1	-5.056123	0.52318	0.493905
6	-0.741475	-0.970976	0.099684
6	-2.020825	-3.848105	-0.194015
6	0.382706	-1.742191	-0.060968
6	-0.56937	-4.056915	-0.239672
6	0.451179	-3.149963	-0.196207
8	-2.664774	-4.943584	-0.317603
8	-0.234172	-5.359216	-0.373313
1	-1.096586	-5.82933	-0.413115
8	-6.320227	-1.7176	0.174263
8	-4.837008	-3.857361	-0.146669
1	-6.509443	-2.661725	0.036381
1	-4.128568	-4.566787	-0.252478
6	-2.465657	1.228278	0.671349
8	-1.942322	1.774958	-0.570985
6	-3.423342	2.28007	1.256413
6	-1.295934	2.992019	-0.457876
6	-2.581214	3.495913	1.676807
6	-1.564441	3.858736	0.612655
6	-0.868661	5.081036	0.626127
6	-0.405891	3.309209	-1.482859
6	0.032096	5.429143	-0.38345
6	0.25249	4.540102	-1.438728
8	-1.043914	5.999045	1.622227
8	1.117302	4.820107	-2.45724
1	-1.664102	5.661176	2.28246
1	1.513062	5.691069	-2.312611
8	-4.436487	2.653314	0.324775
1	-4.021396	2.684559	-0.551028
1	-1.634532	1.138234	1.381495
6	1.702064	-0.990077	-0.143271
8	2.696565	-1.75122	0.576155
6	2.176763	-0.717515	-1.587493
1	1.464068	-0.01713	-2.037416
6	3.949197	-1.199319	0.622908
6	3.549895	-0.12477	-1.55002
1	3.901495	0.377494	-2.445668
6	4.389348	-0.351829	-0.443628
6	4.760879	-1.544519	1.68913
6	5.714424	0.176309	-0.317545
1	4.393243	-2.199417	2.469976
6	6.066079	-1.032323	1.741383
6	6.538549	-0.164507	0.746475
8	6.229152	1.021548	-1.253531
1	5.522733	1.347687	-1.828412
1	1.595244	-0.016076	0.3502
1	-3.278298	4.323661	1.858129
1	-2.089582	3.274818	2.634487
1	-3.938917	1.874416	2.130947
1	0.544437	6.384751	-0.332103
1	-0.230774	2.611881	-2.293315
1	7.537309	0.256951	0.79807
1	1.442811	-3.581173	-0.271536
1	-0.522265	0.084945	0.167859
8	2.112779	-1.886718	-2.421107
1	2.875324	-2.439286	-2.19531
8	6.829808	-1.398039	2.806738
1	7.697301	-0.972537	2.747483

*Table S108 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 3-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481478 (Hartree/Particle)
Thermal correction to Energy= 0.516628
Thermal correction to Enthalpy= 0.517572
Thermal correction to Gibbs Free Energy= 0.413569
Sum of electronic and zero-point Energies= -2021.115451
Sum of electronic and thermal Energies= -2021.080300
Sum of electronic and thermal Enthalpies= -2021.079356
Sum of electronic and thermal Free Energies= -2021.183360

Coordinates:

6	2.210146	-1.242426	-0.1861
6	2.782639	-2.563891	-0.000733
6	4.207429	-2.691635	0.006919
6	5.032947	-1.573136	-0.134536
6	4.477857	-0.312477	-0.315459
6	3.102003	-0.130056	-0.364916
1	5.147328	0.53426	-0.396406
6	0.810352	-0.933699	-0.193569
6	2.054958	-3.813642	0.178447
6	-0.322363	-1.68714	-0.012957
6	0.601691	-4.000445	0.263165
6	-0.409091	-3.08282	0.197508
8	2.685585	-4.917636	0.297256
8	0.253223	-5.29207	0.451141
1	1.110288	-5.773081	0.479269
8	6.3812	-1.722612	-0.098764
8	4.872319	-3.853526	0.1594
1	6.559042	-2.669821	0.032936
1	4.155308	-4.556651	0.246423
6	2.563051	1.263801	-0.64799
8	1.905815	1.744212	0.557674
6	3.561674	2.355282	-1.066531
6	1.210751	2.929778	0.406269
6	2.756387	3.593701	-1.499024
6	1.589262	3.862866	-0.570038
6	0.833457	5.046813	-0.637323
6	0.150833	3.13923	1.286406
6	-0.234519	5.290963	0.230316
6	-0.569648	4.332031	1.189715
8	1.105245	6.024676	-1.551315
8	-1.609626	4.501735	2.058239
1	1.851996	5.763876	-2.107378
1	-2.039356	5.351157	1.884865
8	4.466399	2.667143	-0.010085
1	3.960043	2.629079	0.816358
1	1.810502	1.201243	-1.444762
6	-1.630953	-0.906643	0.009919
8	-2.657402	-1.724686	-0.638117
6	-2.091386	-0.490428	1.370109
6	-3.939316	-1.237551	-0.585609
6	-3.35956	0.32008	1.356629
1	-3.12127	1.371294	1.132548
6	-4.335107	-0.241932	0.327025
6	-4.836219	-1.808871	-1.491356
6	-5.674004	0.183233	0.270836
1	-4.499369	-2.572474	-2.182152
6	-6.162307	-1.374523	-1.498452
6	-6.590647	-0.371717	-0.624794
8	-6.157768	1.152698	1.10491
1	-5.443975	1.523141	1.640861
1	-1.521103	0.000397	-0.596312
1	3.455322	4.439567	-1.518923
1	2.4047	3.444745	-2.529597
1	4.170424	2.011713	-1.907257
1	-0.789154	6.219673	0.140503
1	-0.115577	2.382336	2.014347
1	-7.616274	-0.016232	-0.626846
1	-3.8088	0.313197	2.359327
1	-1.406818	-3.493273	0.306629
1	0.596522	0.11671	-0.322165
8	-1.908551	-1.44347	2.339508
1	-2.370098	-1.176882	3.147634
8	-7.004615	-1.961526	-2.399579
1	-7.886186	-1.571953	-2.315302

*Table S109 Energetics and Cartesian coordinates of the conformer **1b-H_2O** (sa-ass-sa) post-radical capture via HAB at site 2-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481571 (Hartree/Particle)
Thermal correction to Energy= 0.516796
Thermal correction to Enthalpy= 0.517740
Thermal correction to Gibbs Free Energy= 0.414246
Sum of electronic and zero-point Energies= -2021.138875
Sum of electronic and thermal Energies= -2021.103650
Sum of electronic and thermal Enthalpies= -2021.102705
Sum of electronic and thermal Free Energies= -2021.206199

Coordinates:

6	2.068089	-1.47503	-0.07802
6	2.564515	-2.842711	0.036814
6	3.967546	-3.049577	0.211436
6	4.860594	-1.973956	0.249884
6	4.395259	-0.676382	0.064417
6	3.04681	-0.408545	-0.118753
1	5.114762	0.132822	0.074303
6	0.711035	-1.06832	-0.093219
6	1.770957	-4.053392	-0.034112
6	-0.5171	-1.764028	-0.154917
6	0.316089	-4.154303	-0.259026
6	-0.638795	-3.190739	-0.295465
8	2.31999	-5.200587	0.063071
8	-0.09487	-5.438936	-0.401033
1	0.721708	-5.97119	-0.284576
8	6.186679	-2.201776	0.434011
8	4.548585	-4.256133	0.348512
1	6.30138	-3.164007	0.516661
1	3.79515	-4.921631	0.272828
6	2.631389	1.015232	-0.454297
8	1.983163	1.60575	0.709432
6	3.735835	1.995335	-0.888564
6	1.440938	2.863882	0.507855
6	3.059236	3.273507	-1.408808
6	1.928922	3.710204	-0.499702
6	1.326941	4.976396	-0.608963
6	0.419034	3.237109	1.379451
6	0.305042	5.384821	0.251449
6	-0.142827	4.508887	1.243304
8	1.714045	5.879986	-1.557761
8	-1.144406	4.842181	2.109475
1	2.408895	5.503664	-2.114626
1	-1.46144	5.733621	1.906855
8	4.629467	2.290819	0.183544
1	4.096723	2.339965	0.99246
1	1.895801	0.982752	-1.268023
6	-1.725264	-1.025988	-0.095651
8	-2.872629	-1.77542	-0.083831
6	-1.887386	0.46062	0.091033
1	-0.986886	0.983107	-0.224846
6	-4.128886	-1.203251	-0.138668
6	-3.067738	0.982004	-0.740072
1	-2.797962	0.960728	-1.804422
6	-4.293807	0.148573	-0.463103
6	-5.189101	-2.062628	0.133498
6	-5.614372	0.627331	-0.521747
1	-5.011382	-3.100612	0.386027
6	-6.486133	-1.545613	0.072623
6	-6.705187	-0.204472	-0.253346
8	-5.907025	1.919597	-0.842919
1	-5.099849	2.400968	-1.070305
1	3.837529	4.044276	-1.476248
1	2.695553	3.09414	-2.430317
1	4.339839	1.553008	-1.685141
1	-0.127028	6.373224	0.131358
1	0.0476	2.541633	2.121517
1	-7.708269	0.205791	-0.30993
1	-3.213129	2.032957	-0.464398
1	-1.643707	-3.573275	-0.426803
1	0.596062	-0.002511	0.008203
8	-2.0357	0.78931	1.481266
1	-2.910206	0.483902	1.767254
8	-7.508362	-2.405558	0.342958
1	-8.352429	-1.937003	0.276403

*Table S110 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 5'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481475 (Hartree/Particle)
Thermal correction to Energy= 0.516338
Thermal correction to Enthalpy= 0.517282
Thermal correction to Gibbs Free Energy= 0.414410
Sum of electronic and zero-point Energies= -2021.121855
Sum of electronic and thermal Energies= -2021.086992
Sum of electronic and thermal Enthalpies= -2021.086048
Sum of electronic and thermal Free Energies= -2021.188920

Coordinates:

6	-2.607854	-0.033768	0.064422
6	-3.941806	0.497358	0.229932
6	-5.022397	-0.426158	0.366057
6	-4.809543	-1.807011	0.269317
6	-3.535678	-2.303158	0.028521
6	-2.442672	-1.44864	-0.077319
1	-3.399662	-3.373463	-0.063438
6	-1.397592	0.74109	0.137907
6	-4.341102	1.911187	0.234447
6	-1.151536	2.08215	0.027629
6	-3.478734	3.030562	-0.185527
6	-2.11498	3.095489	-0.238587
8	-5.529779	2.23239	0.508281
8	-4.228896	4.129774	-0.465333
1	-3.644792	4.856317	-0.728171
8	-5.862128	-2.655934	0.393293
8	-6.30432	-0.07021	0.569226
1	-6.652014	-2.107512	0.540255
1	-6.275776	0.943034	0.627592
6	-1.082999	-2.023205	-0.443125
8	-0.255517	-2.06537	0.753444
6	-1.047367	-3.398346	-1.12623
6	1.011964	-2.545286	0.570376
6	0.3871	-3.648742	-1.609921
6	1.382754	-3.287061	-0.543936
6	2.768825	-3.745182	-0.655914
6	1.932737	-2.24739	1.590117
6	3.706732	-3.397888	0.39492
6	3.281769	-2.684759	1.493174
8	3.127229	-4.429151	-1.647012
8	4.077751	-2.336764	2.535013
1	4.97725	-2.663222	2.384193
8	-1.441851	-4.385235	-0.173134
1	-1.471683	-5.237024	-0.63064
1	-0.600576	-1.333465	-1.146688
6	0.307505	2.497863	0.242175
8	1.125563	1.60141	-0.549076
6	0.716949	3.928954	-0.12409
1	0.089836	4.652825	0.402785
6	2.485764	1.717885	-0.343922
6	2.179458	4.150106	0.308207
1	2.191047	4.419011	1.373784
6	3.047777	2.933854	0.060757
6	3.247612	0.575607	-0.592673
6	4.44584	2.959742	0.22988
1	2.753985	-0.338833	-0.902119
6	4.6308	0.643768	-0.411781
6	5.237397	1.834439	-0.002259
8	5.099565	4.090601	0.630291
1	4.467353	4.805723	0.784106
1	0.554643	2.334152	1.300797
1	0.512817	-4.699099	-1.894433
1	0.579658	-3.070328	-2.523109
1	-1.731611	-3.380776	-1.984217
1	4.725632	-3.760972	0.303636
1	1.6157	-1.673917	2.453605
1	6.30988	1.883699	0.145047
1	2.546198	5.024801	-0.243964
1	-1.71551	4.0649	-0.520221
1	-0.510607	0.150222	0.31836
8	0.519268	4.164287	-1.514782
1	0.82168	3.369753	-1.981605
8	5.444506	-0.435098	-0.609297
1	4.90508	-1.212181	-0.818186

*Table S111 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 7'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481349 (Hartree/Particle)
Thermal correction to Energy= 0.516273
Thermal correction to Enthalpy= 0.517217
Thermal correction to Gibbs Free Energy= 0.414628
Sum of electronic and zero-point Energies= -2021.117915
Sum of electronic and thermal Energies= -2021.082991
Sum of electronic and thermal Enthalpies= -2021.082047
Sum of electronic and thermal Free Energies= -2021.184636

Coordinates:

6	-2.607854	-0.033768	0.064422
6	-3.941806	0.497358	0.229932
6	-5.022397	-0.426158	0.366057
6	-4.809543	-1.807011	0.269317
6	-3.535678	-2.303158	0.028521
6	-2.442672	-1.44864	-0.077319
1	-3.399662	-3.373463	-0.063438
6	-1.397592	0.74109	0.137907
6	-4.341102	1.911187	0.234447
6	-1.151536	2.08215	0.027629
6	-3.478734	3.030562	-0.185527
6	-2.11498	3.095489	-0.238587
8	-5.529779	2.23239	0.508281
8	-4.228896	4.129774	-0.465333
1	-3.644792	4.856317	-0.728171
8	-5.862128	-2.655934	0.393293
8	-6.30432	-0.07021	0.569226
1	-6.652014	-2.107512	0.540255
1	-6.275776	0.943034	0.627592
6	-1.082999	-2.023205	-0.443125
8	-0.255517	-2.06537	0.753444
6	-1.047367	-3.398346	-1.12623
6	1.011964	-2.545286	0.570376
6	0.3871	-3.648742	-1.609921
6	1.382754	-3.287061	-0.543936
6	2.768825	-3.745182	-0.655914
6	1.932737	-2.24739	1.590117
6	3.706732	-3.397888	0.39492
6	3.281769	-2.684759	1.493174
8	3.127229	-4.429151	-1.647012
8	4.077751	-2.336764	2.535013
1	4.97725	-2.663222	2.384193
8	-1.441851	-4.385235	-0.173134
1	-1.471683	-5.237024	-0.63064
1	-0.600576	-1.333465	-1.146688
6	0.307505	2.497863	0.242175
8	1.125563	1.60141	-0.549076
6	0.716949	3.928954	-0.12409
1	0.089836	4.652825	0.402785
6	2.485764	1.717885	-0.343922
6	2.179458	4.150106	0.308207
1	2.191047	4.419011	1.373784
6	3.047777	2.933854	0.060757
6	3.247612	0.575607	-0.592673
6	4.44584	2.959742	0.22988
1	2.753985	-0.338833	-0.902119
6	4.6308	0.643768	-0.411781
6	5.237397	1.834439	-0.002259
8	5.099565	4.090601	0.630291
1	4.467353	4.805723	0.784106
1	0.554643	2.334152	1.300797
1	0.512817	-4.699099	-1.894433
1	0.579658	-3.070328	-2.523109
1	-1.731611	-3.380776	-1.984217
1	4.725632	-3.760972	0.303636
1	1.6157	-1.673917	2.453605
1	6.30988	1.883699	0.145047
1	2.546198	5.024801	-0.243964
1	-1.71551	4.0649	-0.520221
1	-0.510607	0.150222	0.31836
8	0.519268	4.164287	-1.514782
1	0.82168	3.369753	-1.981605
8	5.444506	-0.435098	-0.609297
1	4.90508	-1.212181	-0.818186

*Table S112 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 3'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480783 (Hartree/Particle)
Thermal correction to Energy= 0.515465
Thermal correction to Enthalpy= 0.516409
Thermal correction to Gibbs Free Energy= 0.415120
Sum of electronic and zero-point Energies= -2021.098092
Sum of electronic and thermal Energies= -2021.063411
Sum of electronic and thermal Enthalpies= -2021.062467
Sum of electronic and thermal Free Energies= -2021.163756

Coordinates:

6	-1.827826	-1.63033	0.106122
6	-2.134284	-3.028323	-0.117491
6	-3.509869	-3.414101	-0.174486
6	-4.535953	-2.48047	0.022202
6	-4.229251	-1.156629	0.29544
6	-2.909336	-0.720463	0.345277
1	-5.044651	-0.463597	0.474804
6	-0.515278	-1.045173	0.044873
6	-1.186503	-4.142927	-0.275018
6	0.738343	-1.58744	-0.028377
6	0.274043	-4.066057	-0.099784
6	1.080111	-2.966761	-0.028565
8	-1.616858	-5.303031	-0.526797
8	0.818211	-5.311622	-0.08474
1	1.778461	-5.237459	0.018428
8	-5.82883	-2.886933	-0.034823
8	-3.940897	-4.666889	-0.399026
1	-5.816211	-3.841707	-0.222209
1	-3.082926	-5.204291	-0.522273
6	-2.632359	0.732007	0.690663
8	-2.324877	1.434543	-0.511417
6	-3.781544	1.475091	1.487565
6	-2.08857	2.783968	-0.413392
6	-3.19212	2.863231	1.870008
6	-2.474196	3.518511	0.72033
6	-2.209872	4.901937	0.699056
6	-1.483644	3.372491	-1.523428
6	-1.600072	5.518492	-0.394158
6	-1.246552	4.747353	-1.505975
8	-2.53752	5.718028	1.743543
8	-0.649983	5.290935	-2.60502
1	-2.872456	5.199884	2.487527
1	-0.539175	6.243277	-2.47396
8	-4.882763	1.638653	0.716999
1	-1.777835	0.797646	1.375683
6	1.892859	-0.60248	-0.14207
8	2.965362	-1.075325	0.694194
6	2.411802	-0.411308	-1.583917
1	1.575995	-0.10323	-2.217446
6	4.163139	-0.400518	0.624211
6	3.489059	0.681526	-1.572371
1	3.003503	1.663143	-1.488313
6	4.472617	0.456769	-0.442031
6	5.058419	-0.656777	1.666119
6	5.735878	1.08092	-0.410278
1	4.76847	-1.33038	2.465846
6	6.304478	-0.028225	1.649826
6	6.649631	0.846921	0.616338
8	6.13574	1.944875	-1.389992
1	5.424715	2.080083	-2.03086
1	1.565434	0.37629	0.229964
1	-4.022574	3.48476	2.227872
1	-2.530823	2.690899	2.730286
1	-3.962199	0.880291	2.39884
1	-1.407445	6.58604	-0.36228
1	-1.205953	2.769361	-2.37922
1	7.61339	1.342159	0.611726
1	3.989471	0.655286	-2.548579
1	2.145475	-3.169653	0.026813
1	-0.517701	0.03591	0.02972
8	2.8881	-1.631853	-2.137245
1	3.694208	-1.880847	-1.661872
8	7.232015	-0.223768	2.632022
1	6.880324	-0.842193	3.287784

*Table S113 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site h-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482238 (Hartree/Particle)
Thermal correction to Energy= 0.516864
Thermal correction to Enthalpy= 0.517808
Thermal correction to Gibbs Free Energy= 0.416667
Sum of electronic and zero-point Energies= -2021.126799
Sum of electronic and thermal Energies= -2021.092173
Sum of electronic and thermal Enthalpies= -2021.091229
Sum of electronic and thermal Free Energies= -2021.192371

Coordinates:

6	-2.650385	-0.118128	0.082774
6	-4.013717	0.346806	0.208593
6	-5.048238	-0.624639	0.385616
6	-4.779222	-2.069962	0.367622
6	-3.417206	-2.45981	0.103556
6	-2.405621	-1.557592	-0.041506
1	-3.220404	-3.521807	0.024323
6	-1.49091	0.690511	0.150396
6	-4.476524	1.738056	0.161295
6	-1.293388	2.059104	0.060059
6	-3.648402	2.90242	-0.20279
6	-2.280158	3.031922	-0.198027
8	-5.693924	2.008664	0.359762
8	-4.427139	3.969044	-0.485871
1	-3.872048	4.731551	-0.709436
8	-5.699517	-2.893659	0.544629
8	-6.311885	-0.305551	0.567671
1	-6.322478	0.723592	0.54349
6	-1.01312	-2.045706	-0.429222
8	-0.187356	-2.050249	0.756623
6	-0.906329	-3.408116	-1.126502
6	1.114829	-2.451644	0.583613
6	0.536186	-3.54772	-1.637766
6	1.53027	-3.139352	-0.570004
6	2.892262	-3.478093	-0.651998
6	1.987833	-2.142191	1.628126
6	3.79819	-3.159111	0.367236
6	3.329311	-2.507472	1.515501
8	3.406402	-4.150585	-1.721706
8	4.152199	-2.185865	2.553623
1	2.727013	-4.278442	-2.397685
1	5.053726	-2.476191	2.355085
8	-1.218658	-4.42848	-0.180813
1	-1.23682	-5.271539	-0.65458
1	-0.588979	-1.322443	-1.137481
6	0.152921	2.519642	0.266868
8	0.99064	1.625728	-0.499055
6	0.520974	3.952809	-0.137453
1	-0.11812	4.673116	0.379613
6	2.349779	1.781514	-0.300211
6	1.981159	4.224163	0.274191
1	1.994177	4.524275	1.331346
6	2.881271	3.025874	0.055575
6	3.135846	0.649276	-0.506808
6	4.279157	3.092986	0.214111
1	2.66535	-0.290672	-0.772193
6	4.517124	0.755952	-0.329513
6	5.096574	1.97817	0.023451
8	4.906907	4.254279	0.567506
1	4.258001	4.95918	0.696698
1	0.394717	2.389239	1.332087
1	0.689326	-4.594	-1.93543
1	0.651413	-2.944071	-2.54814
1	-1.601245	-3.427785	-1.975331
1	4.832011	-3.479568	0.279219
1	1.628384	-1.613577	2.50261
1	6.167628	2.058743	0.167807
1	2.317203	5.092853	-0.306218
1	-1.919816	4.028229	-0.43106
1	-0.572293	0.139688	0.292128
8	0.299225	4.149348	-1.529795
1	0.644295	3.366467	-1.986453
8	5.349222	-0.315488	-0.478937
1	4.817226	-1.122321	-0.580192

*Table S114 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site i-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482461 (Hartree/Particle)
Thermal correction to Energy= 0.517605
Thermal correction to Enthalpy= 0.518549
Thermal correction to Gibbs Free Energy= 0.415957
Sum of electronic and zero-point Energies= -2021.117406
Sum of electronic and thermal Energies= -2021.082262
Sum of electronic and thermal Enthalpies= -2021.081318
Sum of electronic and thermal Free Energies= -2021.183911

Coordinates:

6	-2.629018	-0.001008	0.054649
6	-3.977033	0.498711	0.235133
6	-5.023683	-0.439751	0.430127
6	-4.783493	-1.83079	0.343247
6	-3.50502	-2.302354	0.070512
6	-2.437784	-1.424857	-0.075824
1	-3.345984	-3.3701	-0.012251
6	-1.452538	0.788154	0.101666
6	-4.403576	1.896522	0.208002
6	-1.219177	2.175798	0.035659
6	-3.58271	3.072593	-0.323344
6	-2.150337	3.161946	-0.216552
8	-5.571921	2.211563	0.535206
8	-4.229658	4.0269	-0.777391
8	-5.805424	-2.690733	0.512646
8	-6.292078	-0.108952	0.683458
1	-6.609481	-2.168179	0.681651
1	-6.290495	0.907314	0.726587
6	-1.06942	-1.97684	-0.455285
8	-0.255292	-2.022083	0.738196
6	-1.020532	-3.341078	-1.155376
6	1.029967	-2.47675	0.572003
6	0.418606	-3.547793	-1.653347
6	1.422893	-3.17945	-0.580416
6	2.771283	-3.569907	-0.657716
6	1.910105	-2.202105	1.620315
6	3.684656	-3.287046	0.365379
6	3.236846	-2.618883	1.512574
8	3.263134	-4.26057	-1.726408
8	4.067665	-2.329911	2.554032
1	2.584854	-4.352776	-2.409213
1	4.959197	-2.650311	2.356594
8	-1.391498	-4.346326	-0.214524
1	-1.44434	-5.187585	-0.689017
1	-0.604738	-1.27459	-1.158082
6	0.245742	2.574318	0.249539
8	1.05261	1.649335	-0.513762
6	0.677967	3.990523	-0.152466
1	0.060629	4.7383	0.351193
6	2.414204	1.744316	-0.295762
6	2.142375	4.199143	0.282305
1	2.153504	4.495912	1.340532
6	2.993562	2.963581	0.072653
6	3.153339	0.579427	-0.494645
6	4.390536	2.969169	0.251941
1	2.646601	-0.338503	-0.770352
6	4.53514	0.625454	-0.2966
6	5.161563	1.820329	0.069599
8	5.062885	4.101093	0.618473
1	4.443799	4.834426	0.735314
1	0.475648	2.430795	1.315575
1	0.527069	-4.601071	-1.945809
1	0.567299	-2.954119	-2.565452
1	-1.707252	-3.326625	-2.011129
1	4.706072	-3.645666	0.280387
1	1.568131	-1.659346	2.493133
1	6.232896	1.853851	0.22967
1	2.524064	5.053703	-0.290812
1	-1.79934	4.168174	-0.411259
1	-0.540691	0.219098	0.206683
8	0.49203	4.191631	-1.548716
1	0.804855	3.389248	-1.994456
8	5.322745	-0.48031	-0.437697
1	4.759361	-1.263258	-0.555411

*Table S115 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site b-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482033 (Hartree/Particle)
Thermal correction to Energy= 0.516795
Thermal correction to Enthalpy= 0.517739
Thermal correction to Gibbs Free Energy= 0.416241
Sum of electronic and zero-point Energies= -2021.133672
Sum of electronic and thermal Energies= -2021.098910
Sum of electronic and thermal Enthalpies= -2021.097966
Sum of electronic and thermal Free Energies= -2021.199464

Coordinates:

6	-2.629018	-0.001008	0.054649
6	-3.977033	0.498711	0.235133
6	-5.023683	-0.439751	0.430127
6	-4.783493	-1.83079	0.343247
6	-3.50502	-2.302354	0.070512
6	-2.437784	-1.424857	-0.075824
1	-3.345984	-3.3701	-0.012251
6	-1.452538	0.788154	0.101666
6	-4.403576	1.896522	0.208002
6	-1.219177	2.175798	0.035659
6	-3.58271	3.072593	-0.323344
6	-2.150337	3.161946	-0.216552
8	-5.571921	2.211563	0.535206
8	-4.229658	4.0269	-0.777391
8	-5.805424	-2.690733	0.512646
8	-6.292078	-0.108952	0.683458
1	-6.609481	-2.168179	0.681651
1	-6.290495	0.907314	0.726587
6	-1.06942	-1.97684	-0.455285
8	-0.255292	-2.022083	0.738196
6	-1.020532	-3.341078	-1.155376
6	1.029967	-2.47675	0.572003
6	0.418606	-3.547793	-1.653347
6	1.422893	-3.17945	-0.580416
6	2.771283	-3.569907	-0.657716
6	1.910105	-2.202105	1.620315
6	3.684656	-3.287046	0.365379
6	3.236846	-2.618883	1.512574
8	3.263134	-4.26057	-1.726408
8	4.067665	-2.329911	2.554032
1	2.584854	-4.352776	-2.409213
1	4.959197	-2.650311	2.356594
8	-1.391498	-4.346326	-0.214524
1	-1.44434	-5.187585	-0.689017
1	-0.604738	-1.27459	-1.158082
6	0.245742	2.574318	0.249539
8	1.05261	1.649335	-0.513762
6	0.677967	3.990523	-0.152466
1	0.060629	4.7383	0.351193
6	2.414204	1.744316	-0.295762
6	2.142375	4.199143	0.282305
1	2.153504	4.495912	1.340532
6	2.993562	2.963581	0.072653
6	3.153339	0.579427	-0.494645
6	4.390536	2.969169	0.251941
1	2.646601	-0.338503	-0.770352
6	4.53514	0.625454	-0.2966
6	5.161563	1.820329	0.069599
8	5.062885	4.101093	0.618473
1	4.443799	4.834426	0.735314
1	0.475648	2.430795	1.315575
1	0.527069	-4.601071	-1.945809
1	0.567299	-2.954119	-2.565452
1	-1.707252	-3.326625	-2.011129
1	4.706072	-3.645666	0.280387
1	1.568131	-1.659346	2.493133
1	6.232896	1.853851	0.22967
1	2.524064	5.053703	-0.290812
1	-1.79934	4.168174	-0.411259
1	-0.540691	0.219098	0.206683
8	0.49203	4.191631	-1.548716
1	0.804855	3.389248	-1.994456
8	5.322745	-0.48031	-0.437697
1	4.759361	-1.263258	-0.555411

*Table S116 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 3-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480273 (Hartree/Particle)
Thermal correction to Energy= 0.515144
Thermal correction to Enthalpy= 0.516088
Thermal correction to Gibbs Free Energy= 0.413816
Sum of electronic and zero-point Energies= -2021.092992
Sum of electronic and thermal Energies= -2021.058122
Sum of electronic and thermal Enthalpies= -2021.057178
Sum of electronic and thermal Free Energies= -2021.159449

Coordinates:

6	-2.614116	-0.049703	0.05054
6	-3.96949	0.420702	0.221982
6	-5.018796	-0.546474	0.261433
6	-4.753338	-1.909214	0.075763
6	-3.456029	-2.34429	-0.155585
6	-2.393	-1.446595	-0.173852
1	-3.276545	-3.401261	-0.309232
6	-1.429612	0.759014	0.173884
6	-4.416866	1.815053	0.333516
6	-1.222258	2.11077	0.144773
6	-3.584521	2.997749	0.038995
6	-2.223801	3.111718	-0.00799
8	-5.620858	2.072986	0.602653
8	-4.368044	4.09546	-0.129687
1	-3.809238	4.864986	-0.312912
8	-5.777075	-2.799524	0.110486
8	-6.318018	-0.251831	0.453567
1	-6.589725	-2.290885	0.274854
1	-6.329618	0.752029	0.59461
6	-0.99802	-1.954821	-0.50527
8	-0.255546	-2.082098	0.733559
6	-0.874233	-3.263494	-1.295616
6	1.043619	-2.50277	0.618356
6	0.597577	-3.405785	-1.717346
6	1.525798	-3.104799	-0.557622
6	2.883768	-3.46626	-0.575582
6	1.848477	-2.304655	1.742573
6	3.724392	-3.252501	0.524766
6	3.187324	-2.693186	1.692092
8	3.458087	-4.059859	-1.661126
8	3.937994	-2.486358	2.811351
1	2.827261	-4.104715	-2.392605
1	4.844769	-2.786489	2.656157
8	-1.277429	-4.342044	-0.454036
1	-1.286395	-5.146698	-0.990391
1	-0.495709	-1.198834	-1.121212
6	0.224681	2.577192	0.333352
8	1.073009	1.551752	-0.133682
6	0.622093	3.973982	-0.33442
1	-0.015825	4.720534	0.171152
6	2.430071	1.750804	-0.110186
6	2.101532	4.256133	0.022432
1	2.114284	4.697417	1.029467
6	2.981894	3.03551	-0.050502
6	3.202403	0.593281	-0.203236
6	4.390485	3.115882	-0.071835
1	2.714364	-0.372734	-0.253399
6	4.590992	0.716389	-0.211793
6	5.193115	1.978049	-0.147785
8	5.043237	4.313835	-0.011968
1	4.409935	5.038682	0.071297
1	0.41634	2.756031	1.402506
1	0.750787	-4.429887	-2.083893
1	0.787714	-2.738651	-2.569063
1	-1.508521	-3.20116	-2.188875
1	4.754811	-3.592406	0.478995
1	1.438078	-1.842581	2.632259
1	6.27251	2.074479	-0.147307
1	2.44416	5.038716	-0.667017
1	-1.867563	4.123148	-0.17698
1	-0.526283	0.186463	0.30951
8	0.380834	3.887275	-1.657509
8	5.410419	-0.371076	-0.271939
1	4.872691	-1.180426	-0.236294

*Table S117 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 5-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481036 (Hartree/Particle)
Thermal correction to Energy= 0.515906
Thermal correction to Enthalpy= 0.516850
Thermal correction to Gibbs Free Energy= 0.414592
Sum of electronic and zero-point Energies= -2021.124946
Sum of electronic and thermal Energies= -2021.090076
Sum of electronic and thermal Enthalpies= -2021.089132
Sum of electronic and thermal Free Energies= -2021.191390

Coordinates:

6	-2.527413	-0.163529	-0.04529
6	-3.936803	0.145304	0.104671
6	-4.882239	-0.896965	-0.150162
6	-4.465928	-2.18195	-0.51994
6	-3.116301	-2.468465	-0.656327
6	-2.150691	-1.491539	-0.440658
1	-2.821863	-3.47647	-0.919299
6	-1.445668	0.75912	0.15113
6	-4.541588	1.426285	0.504372
6	-1.391402	2.072254	0.522686
6	-3.82155	2.659296	0.871286
6	-2.480127	2.91624	0.867316
8	-5.799135	1.531734	0.571681
8	-4.69895	3.627566	1.246882
1	-4.209631	4.430165	1.479621
8	-5.396482	-3.145514	-0.741141
8	-6.217205	-0.75801	-0.056364
1	-6.265568	-2.735724	-0.587206
1	-6.342463	0.216286	0.217408
6	-0.6882	-1.860231	-0.641562
8	-0.08941	-1.979114	0.67369
6	-0.351326	-3.109456	-1.464337
6	1.234903	-2.316581	0.719067
6	1.170238	-3.109627	-1.694022
6	1.91265	-2.818015	-0.40574
6	3.282648	-3.090412	-0.253617
6	1.863259	-2.141932	1.9566
6	3.949659	-2.894104	0.964387
6	3.218718	-2.452537	2.076151
8	4.04033	-3.576291	-1.277275
8	3.791171	-2.284467	3.301106
1	3.520127	-3.617088	-2.09134
1	4.7278	-2.524238	3.257872
8	-0.762879	-4.265458	-0.738434
1	-0.609399	-5.035809	-1.302958
1	-0.187003	-1.040898	-1.170797
6	-0.031279	2.766149	0.550929
8	0.987194	1.754186	0.655208
6	0.201931	3.67149	-0.684942
1	-0.556553	4.458802	-0.67084
6	2.250039	2.019196	0.206877
6	1.602223	4.294171	-0.603224
1	1.633667	5.030606	0.210586
6	2.619993	3.209985	-0.38561
6	3.159168	0.950478	0.365984
6	4.005003	3.360766	-0.832238
1	2.806052	0.036523	0.832302
6	4.49534	1.073279	-0.078148
6	4.924383	2.254965	-0.648233
8	4.3822	4.429481	-1.378268
1	0.032172	3.398547	1.446739
1	1.451457	-4.093833	-2.092491
1	1.412553	-2.376585	-2.475422
1	-0.866511	-3.044571	-2.431346
1	4.99629	-3.171617	1.047256
1	1.302063	-1.769026	2.804814
1	5.945864	2.37407	-0.990236
1	1.823089	4.837522	-1.525611
1	-2.206693	3.923699	1.18159
1	-0.466415	0.337085	0.004953
8	0.000425	2.964147	-1.901384
1	0.742568	2.354806	-2.025877
8	5.371235	0.043325	0.052528
1	4.91261	-0.746769	0.390025

*Table S118 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 7-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480905 (Hartree/Particle)
Thermal correction to Energy= 0.516108
Thermal correction to Enthalpy= 0.517052
Thermal correction to Gibbs Free Energy= 0.412161
Sum of electronic and zero-point Energies= -2021.120816
Sum of electronic and thermal Energies= -2021.085613
Sum of electronic and thermal Enthalpies= -2021.084669
Sum of electronic and thermal Free Energies= -2021.189561

Coordinates:

6	-2.046568	-1.401579	0.101386
6	-2.545503	-2.748477	-0.090687
6	-3.96071	-2.938003	-0.145977
6	-4.843589	-1.863855	0.02218
6	-4.355426	-0.587855	0.259676
6	-2.987507	-0.340913	0.309409
1	-5.05974	0.224082	0.387866
6	-0.663337	-1.010593	0.041249
6	-1.763036	-3.98851	-0.211914
6	0.500802	-1.726849	-0.005369
6	-0.309092	-4.115075	-0.007981
6	0.645044	-3.140406	0.040941
8	-2.348885	-5.081313	-0.449998
8	0.049955	-5.424994	0.058961
1	1.00821	-5.485562	0.185209
8	-6.18152	-2.08497	-0.03713
8	-4.565286	-4.123467	-0.345233
1	-6.302257	-3.036084	-0.203278
1	-3.793569	-4.77789	-0.456896
6	-2.509334	1.064727	0.64959
8	-2.004633	1.674638	-0.561879
6	-3.509947	2.018355	1.315815
6	-1.522696	2.956374	-0.445239
6	-2.735612	3.266626	1.765637
6	-1.819874	3.762221	0.666057
6	-1.262976	5.053128	0.682126
6	-0.736946	3.406664	-1.50759
6	-0.4694	5.530747	-0.36371
6	-0.219054	4.701845	-1.460246
8	-1.477383	5.919212	1.718372
8	0.546169	5.106187	-2.517498
1	-1.97455	5.482147	2.422712
1	0.845688	6.013886	-2.367618
8	-4.519776	2.355591	0.365758
1	-5.174395	2.905817	0.817877
1	-1.676655	0.981623	1.36041
6	1.777404	-0.912582	-0.144441
8	2.789405	-1.504888	0.699849
6	2.326668	-0.836299	-1.582466
1	1.549289	-0.435819	-2.237475
6	4.032946	-0.924842	0.681978
6	3.535837	0.112985	-1.588216
1	3.175249	1.151653	-1.578002
6	4.452456	-0.122415	-0.41439
6	4.866574	-1.193951	1.744851
6	5.762213	0.446216	-0.373884
1	4.531966	-1.815708	2.566878
6	6.205543	-0.642599	1.779071
6	6.617252	0.19757	0.676019
8	6.215141	1.241914	-1.380458
1	5.528206	1.396516	-2.042941
1	1.588506	0.109831	0.203387
1	-3.468184	4.036751	2.043897
1	-2.17573	3.026474	2.680208
1	-3.9433	1.520031	2.192625
1	-0.061271	6.534897	-0.306933
1	-0.53227	2.756649	-2.34991
1	7.611147	0.629428	0.691332
1	4.069612	-0.029767	-2.53603
1	1.669102	-3.493699	0.122221
1	-0.516493	0.059849	-0.003536
8	2.643513	-2.120148	-2.098919
1	3.324031	-2.517089	-1.535716
8	6.978875	-0.879507	2.745732

*Table S119 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 4'α-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481055 (Hartree/Particle)
Thermal correction to Energy= 0.516228
Thermal correction to Enthalpy= 0.517172
Thermal correction to Gibbs Free Energy= 0.414614
Sum of electronic and zero-point Energies= -2021.113412
Sum of electronic and thermal Energies= -2021.078239
Sum of electronic and thermal Enthalpies= -2021.077295
Sum of electronic and thermal Free Energies= -2021.179853

Coordinates:

6	-2.619408	-0.033343	0.074023
6	-3.947999	0.518282	0.220547
6	-5.045749	-0.387502	0.337668
6	-4.853964	-1.769862	0.231518
6	-3.584677	-2.285936	0.010321
6	-2.47323	-1.451715	-0.066824
1	-3.466291	-3.356944	-0.094288
6	-1.400322	0.727257	0.159594
6	-4.327327	1.937821	0.223517
6	-1.136884	2.064201	0.034904
6	-3.449315	3.042304	-0.201091
6	-2.084987	3.087012	-0.250062
8	-5.511716	2.276895	0.494506
8	-4.18324	4.149475	-0.493104
1	-3.587856	4.866373	-0.757039
8	-5.922598	-2.602657	0.328999
8	-6.324864	-0.012183	0.525677
1	-6.705614	-2.042374	0.467529
1	-6.280557	0.999433	0.595556
6	-1.113141	-2.047634	-0.40245
8	-0.312735	-2.108578	0.811865
6	-1.066136	-3.413968	-1.100498
6	0.984077	-2.511997	0.64861
6	0.36903	-3.727753	-1.396874
6	1.359724	-3.285365	-0.498042
6	2.747829	-3.613883	-0.608061
6	1.885982	-2.17166	1.644828
6	3.663074	-3.266872	0.380776
6	3.22476	-2.564964	1.516049
8	3.22689	-4.315331	-1.671699
8	4.072452	-2.209184	2.518038
1	2.57623	-4.318672	-2.387598
1	4.969177	-2.509661	2.311273
8	-1.631838	-4.413176	-0.224075
1	-1.49611	-5.271471	-0.650089
1	-0.606517	-1.363656	-1.094282
6	0.326297	2.466074	0.247967
8	1.133339	1.560722	-0.543458
6	0.748214	3.892972	-0.122717
1	0.128475	4.623739	0.403445
6	2.495873	1.667871	-0.347011
6	2.213727	4.103189	0.303533
1	2.232487	4.369482	1.369703
6	3.071173	2.880963	0.048575
6	3.245552	0.518644	-0.595335
6	4.470701	2.896029	0.205246
1	2.742507	-0.395897	-0.888472
6	4.629876	0.574514	-0.422009
6	5.250952	1.762642	-0.026959
8	5.137215	4.02366	0.595221
1	4.511785	4.74453	0.749768
1	0.573813	2.30221	1.306462
1	0.58738	-4.41922	-2.20429
1	-1.650313	-3.349922	-2.028222
1	4.697814	-3.579876	0.278053
1	1.562077	-1.598121	2.505008
1	6.324697	1.802898	0.114079
1	2.583504	4.976807	-0.248406
1	-1.670595	4.046957	-0.542045
1	-0.522858	0.1268	0.355517
8	0.550381	4.126187	-1.514078
1	0.841425	3.32601	-1.978513
8	5.427274	-0.517228	-0.615277
1	4.868649	-1.29216	-0.782543

*Table S120 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 4'β-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481054 (Hartree/Particle)
Thermal correction to Energy= 0.516226
Thermal correction to Enthalpy= 0.517170
Thermal correction to Gibbs Free Energy= 0.414619
Sum of electronic and zero-point Energies= -2021.113412
Sum of electronic and thermal Energies= -2021.078241
Sum of electronic and thermal Enthalpies= -2021.077296
Sum of electronic and thermal Free Energies= -2021.179848

Coordinates:

6	-2.619367	-0.03351	0.074039
6	-3.947955	0.517979	0.220851
6	-5.045653	-0.387891	0.337944
6	-4.853796	-1.770209	0.231411
6	-3.584485	-2.286142	0.009988
6	-2.473091	-1.451818	-0.067075
1	-3.466031	-3.35712	-0.094838
6	-1.400377	0.727179	0.159636
6	-4.327341	1.937494	0.224165
6	-1.137083	2.064141	0.034874
6	-3.449649	3.041904	-0.201263
6	-2.085319	3.086838	-0.250095
8	-5.511628	2.276532	0.495655
8	-4.183814	4.148792	-0.493686
1	-3.588637	4.865614	-0.758298
8	-5.922364	-2.603103	0.328819
8	-6.324727	-0.012612	0.526154
1	-6.705402	-2.042917	0.467604
1	-6.280236	0.999009	0.596412
6	-1.112952	-2.047523	-0.402801
8	-0.312468	-2.108267	0.811514
6	-1.065698	-3.413851	-1.100813
6	0.984315	-2.511742	0.648404
6	0.369527	-3.727424	-1.397191
6	1.360114	-3.284993	-0.498321
6	2.748227	-3.613563	-0.608135
6	1.88607	-2.171706	1.644865
6	3.66333	-3.266811	0.380915
6	3.224828	-2.565135	1.516294
8	3.227346	-4.314935	-1.671854
8	4.07234	-2.209715	2.518549
1	2.576775	-4.317884	-2.387849
1	4.968967	-2.510756	2.312174
8	-1.631156	-4.413142	-0.224322
1	-1.496171	-5.271329	-0.650785
1	-0.606433	-1.363452	-1.094624
6	0.326074	2.466193	0.247863
8	1.13318	1.560986	-0.54373
6	0.747859	3.89313	-0.122847
1	0.12814	4.623877	0.403366
6	2.49571	1.668119	-0.347089
6	2.213413	4.103471	0.303268
1	2.232229	4.369931	1.369395
6	3.070929	2.881259	0.048478
6	3.24541	0.518899	-0.595269
6	4.470429	2.896343	0.205344
1	2.742438	-0.395646	-0.888512
6	4.629721	0.574775	-0.421735
6	5.250716	1.762921	-0.026642
8	5.13689	4.023975	0.595397
1	4.511481	4.744977	0.749413
1	0.573748	2.30228	1.306304
1	0.588132	-4.418486	-2.204874
1	-1.649885	-3.34997	-2.028531
1	4.698023	-3.580091	0.278451
1	1.562028	-1.59835	2.505116
1	6.324434	1.803182	0.114605
1	2.583108	4.977027	-0.24883
1	-1.671073	4.046839	-0.542106
1	-0.522861	0.126777	0.355507
8	0.549884	4.126293	-1.514191
1	0.84052	3.325919	-1.978551
8	5.427122	-0.516951	-0.615087
1	4.868421	-1.292218	-0.780672

*Table S121 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 3'-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481413 (Hartree/Particle)
Thermal correction to Energy= 0.516571
Thermal correction to Enthalpy= 0.517515
Thermal correction to Gibbs Free Energy= 0.414924
Sum of electronic and zero-point Energies= -2021.099440
Sum of electronic and thermal Energies= -2021.064282
Sum of electronic and thermal Enthalpies= -2021.063338
Sum of electronic and thermal Free Energies= -2021.165929

Coordinates:

6	-2.623675	-0.081192	0.076581
6	-3.966846	0.422553	0.25238
6	-5.032866	-0.520907	0.361577
6	-4.797832	-1.893088	0.215748
6	-3.515879	-2.361385	-0.036849
6	-2.432795	-1.489735	-0.103669
1	-3.374546	-3.423648	-0.18177
6	-1.429016	0.717242	0.164503
6	-4.3902	1.82865	0.294731
6	-1.20801	2.062848	0.054859
6	-3.554924	2.969493	-0.121794
6	-2.193774	3.059495	-0.193698
8	-5.579455	2.123467	0.59365
8	-4.32963	4.057174	-0.379423
1	-3.763346	4.797437	-0.642972
8	-5.837256	-2.763118	0.303327
8	-6.320351	-0.191935	0.575653
1	-6.636785	-2.233381	0.465291
1	-6.307439	0.818119	0.672087
6	-1.054373	-2.025906	-0.455629
8	-0.248776	-2.085535	0.788159
6	-0.904427	-3.338024	-1.157408
6	1.049052	-2.496205	0.622948
6	0.506319	-3.542353	-1.647104
6	1.489498	-3.157548	-0.542448
6	2.849826	-3.504792	-0.608908
6	1.911312	-2.224839	1.689031
6	3.737842	-3.226204	0.437642
6	3.250629	-2.601763	1.5935
8	3.378833	-4.153169	-1.686522
8	4.054615	-2.31894	2.657412
1	2.718447	-4.242564	-2.386727
1	4.958045	-2.609199	2.467676
8	-1.512699	-4.408161	-0.544862
1	-1.220762	-5.229103	-0.967163
1	-0.558111	-1.295347	-1.10375
6	0.245889	2.510998	0.245782
8	1.072727	1.568161	-0.476149
6	0.637498	3.915027	-0.232248
1	0.012579	4.672235	0.248068
6	2.432661	1.712922	-0.288938
6	2.103584	4.185802	0.160873
1	2.124541	4.54137	1.200747
6	2.985451	2.964631	0.003235
6	3.200991	0.559965	-0.442612
6	4.384658	3.017022	0.154342
1	2.71459	-0.38389	-0.66138
6	4.584447	0.65333	-0.277188
6	5.184408	1.881678	0.015505
8	5.031563	4.184748	0.448404
1	4.393297	4.904947	0.540755
1	0.493045	2.431408	1.314334
1	0.645626	-4.592194	-1.939859
1	0.676508	-2.940267	-2.550824
1	4.768563	-3.560711	0.364326
1	1.542116	-1.715736	2.571058
1	6.25734	1.952782	0.150782
1	2.451104	5.017782	-0.465014
1	-1.818963	4.039979	-0.46992
1	-0.531523	0.14241	0.341996
8	0.415263	4.042273	-1.633027
1	0.723875	3.219744	-2.043809
8	5.398216	-0.437657	-0.380815
1	4.850718	-1.236924	-0.458841

*Table S122 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 2'-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.479897 (Hartree/Particle)
Thermal correction to Energy= 0.515574
Thermal correction to Enthalpy= 0.516518
Thermal correction to Gibbs Free Energy= 0.411637
Sum of electronic and zero-point Energies= -2021.123043
Sum of electronic and thermal Energies= -2021.087367
Sum of electronic and thermal Enthalpies= -2021.086423
Sum of electronic and thermal Free Energies= -2021.191304

Coordinates:

6	2.557666	0.034291	-0.00371
6	3.890799	-0.522061	0.116021
6	4.983996	0.240169	-0.38084
6	4.790775	1.517304	-0.955506
6	3.545947	2.101322	-0.953994
6	2.416862	1.418114	-0.43631
1	3.463348	3.132228	-1.276869
6	1.34568	-0.711322	0.078696
6	4.26336	-1.802435	0.735339
6	1.067271	-1.961228	0.57391
6	3.33332	-2.744545	1.371513
6	1.972975	-2.827539	1.236778
8	5.480489	-2.142495	0.792545
8	4.010321	-3.688869	2.081641
1	3.376979	-4.304551	2.478548
8	5.871068	2.189321	-1.430499
8	6.267115	-0.15817	-0.344841
1	6.646527	1.624219	-1.269093
1	6.226181	-1.065876	0.123937
6	1.205302	2.159207	-0.340326
8	0.345361	1.838489	0.681431
6	0.884209	3.383236	-1.144856
6	-0.911327	2.394431	0.769391
6	-0.611826	3.387816	-1.51182
6	-1.45333	3.138431	-0.285545
6	-2.761885	3.61778	-0.112549
6	-1.589767	2.14955	1.961671
6	-3.481038	3.382427	1.065719
6	-2.883399	2.658674	2.102434
8	-3.405402	4.343174	-1.072132
8	-3.522983	2.411957	3.281368
1	-2.862938	4.39841	-1.870427
1	-4.402763	2.814388	3.262031
8	1.240979	4.531391	-0.357958
1	1.03853	5.320327	-0.882697
6	-0.340563	-2.520869	0.42556
8	-1.25243	-1.429963	0.231491
6	-0.481728	-3.508482	-0.754448
1	0.245603	-4.315792	-0.634778
6	-2.557667	-1.732391	-0.083983
6	-1.903569	-4.090472	-0.744219
1	-1.973987	-4.846316	0.050087
6	-2.934094	-2.997052	-0.55568
6	-3.464036	-0.679211	0.055408
6	-4.297119	-3.178371	-0.863803
1	-3.115185	0.279809	0.422423
6	-4.800995	-0.8979	-0.277347
6	-5.228887	-2.148645	-0.731706
8	-4.775235	-4.374218	-1.320715
1	-4.06558	-5.030435	-1.340939
1	-0.616829	-3.050006	1.348862
1	-0.84057	4.3585	-1.971232
1	-0.787749	2.629394	-2.286723
1	1.467369	3.357713	-2.071581
1	-4.484625	3.784698	1.16251
1	-1.12456	1.576985	2.754457
1	-6.2695	-2.320054	-0.980686
1	-2.047887	-4.614112	-1.697656
1	1.522178	-3.704938	1.701374
1	0.483534	-0.197023	-0.317896
8	-0.162073	-2.878567	-1.98737
1	-0.733541	-2.102263	-2.079713
8	-5.743133	0.084784	-0.167476
1	-5.318727	0.898638	0.141374

*Table S123 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 4β-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481184 (Hartree/Particle)
Thermal correction to Energy= 0.516284
Thermal correction to Enthalpy= 0.517229
Thermal correction to Gibbs Free Energy= 0.414619
Sum of electronic and zero-point Energies= -2021.116237
Sum of electronic and thermal Energies= -2021.081136
Sum of electronic and thermal Enthalpies= -2021.080192
Sum of electronic and thermal Free Energies= -2021.182802

Coordinates:

6	-2.594427	-0.093139	0.034979
6	-3.959159	0.352103	0.216965
6	-4.991822	-0.635545	0.235608
6	-4.701614	-1.99129	0.039579
6	-3.395401	-2.402536	-0.184776
6	-2.34884	-1.486964	-0.196843
1	-3.197557	-3.455995	-0.338472
6	-1.425638	0.738055	0.125078
6	-4.433159	1.73393	0.376386
6	-1.2389	2.093718	0.143635
6	-3.616023	2.947405	0.203721
6	-2.258536	3.083942	0.118698
8	-5.653145	1.956793	0.616638
8	-4.410127	4.052357	0.178539
1	-3.857889	4.84024	0.068858
8	-5.710969	-2.899607	0.060602
8	-6.297421	-0.368337	0.42372
1	-6.531831	-2.404001	0.225348
1	-6.323665	0.638964	0.568634
6	-0.945228	-1.977908	-0.51946
8	-0.200181	-2.05854	0.722253
6	-0.796649	-3.303706	-1.276274
6	1.104686	-2.462921	0.621255
6	0.678605	-3.432158	-1.691321
6	1.599311	-3.087884	-0.53766
6	2.962862	-3.428808	-0.543345
6	1.903624	-2.224373	1.742404
6	3.79705	-3.175239	0.554119
6	3.247485	-2.595869	1.706277
8	3.549268	-4.041706	-1.611519
8	3.99106	-2.350456	2.822225
1	2.921247	-4.11587	-2.342892
1	4.900648	-2.6488	2.680687
8	-1.183298	-4.368921	-0.410196
1	-1.166006	-5.187487	-0.925092
1	-0.456683	-1.230277	-1.156095
6	0.212697	2.575409	0.264214
8	1.040809	1.591284	-0.397359
6	0.551902	3.965675	-0.301275
1	0.050251	4.728385	0.303608
6	2.391522	1.759286	-0.245939
6	2.036503	4.177912	-0.231191
6	2.916777	3.082541	-0.151421
6	3.187781	0.628738	-0.269444
6	4.341007	3.179735	-0.026166
1	2.730982	-0.350069	-0.359516
6	4.57868	0.780705	-0.168955
6	5.153351	2.054894	-0.042107
8	4.953756	4.391113	0.100146
1	4.299159	5.067021	0.325526
1	0.488126	2.583309	1.329854
1	0.848093	-4.462959	-2.031474
1	0.860775	-2.784242	-2.559449
1	-1.428408	-3.273984	-2.173106
1	4.831895	-3.503118	0.520422
1	1.483696	-1.746562	2.619224
1	6.226739	2.16113	0.063633
1	2.394913	5.196305	-0.342341
1	-1.919174	4.111109	0.031449
1	-0.502389	0.18562	0.186065
8	0.032106	4.152348	-1.628773
1	0.474664	3.501778	-2.194459
8	5.416665	-0.290534	-0.164647
1	4.893535	-1.111113	-0.173898

*Table S124 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 4α-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481185 (Hartree/Particle)
Thermal correction to Energy= 0.516287
Thermal correction to Enthalpy= 0.517231
Thermal correction to Gibbs Free Energy= 0.414561
Sum of electronic and zero-point Energies= -2021.116236
Sum of electronic and thermal Energies= -2021.081134
Sum of electronic and thermal Enthalpies= -2021.080190
Sum of electronic and thermal Free Energies= -2021.182859

Coordinates:

6	-2.59453	-0.093168	0.035539
6	-3.959176	0.352271	0.217584
6	-4.9918	-0.635351	0.237708
6	-4.701774	-1.991247	0.042459
6	-3.395676	-2.402692	-0.182352
6	-2.349086	-1.487151	-0.195516
1	-3.198	-3.456257	-0.335535
6	-1.425702	0.737912	0.125557
6	-4.433041	1.734342	0.375461
6	-1.238896	2.09365	0.142245
6	-3.616052	2.947408	0.19944
6	-2.25854	3.083796	0.114229
8	-5.652745	1.957582	0.61667
8	-4.410231	4.052244	0.171196
1	-3.857989	4.839881	0.05983
8	-5.711116	-2.899512	0.064675
8	-6.297335	-0.367998	0.426403
1	-6.531917	-2.403786	0.229365
1	-6.323576	0.639265	0.570568
6	-0.945622	-1.978139	-0.518809
8	-0.199916	-2.058904	0.722493
6	-0.797564	-3.303927	-1.275781
6	1.104907	-2.463222	0.62069
6	0.677435	-3.432565	-1.691603
6	1.598824	-3.088279	-0.538483
6	2.962373	-3.4292	-0.544977
6	1.904541	-2.224528	1.741314
6	3.797262	-3.175447	0.551921
6	3.248389	-2.595935	1.704364
8	3.548127	-4.042199	-1.613441
8	3.992671	-2.350326	2.819797
1	2.919585	-4.116654	-2.34434
1	4.902226	-2.648487	2.677663
8	-1.183863	-4.369119	-0.409522
1	-1.167021	-5.187683	-0.924435
1	-0.457395	-1.230394	-1.155533
6	0.212662	2.575148	0.263715
8	1.040884	1.591963	-0.399264
6	0.552272	3.966284	-0.299377
1	0.05036	4.728062	0.306499
6	2.391523	1.759485	-0.246648
6	2.036882	4.178152	-0.228217
1	2.395514	5.196677	-0.337475
6	2.91695	3.082495	-0.149675
6	3.187631	0.628836	-0.271179
6	4.341147	3.179314	-0.023324
1	2.730769	-0.349785	-0.362953
6	4.578466	0.780437	-0.169215
6	5.153293	2.054342	-0.040272
8	4.95408	4.390332	0.105152
1	4.299392	5.066345	0.329928
1	0.487883	2.581291	1.329412
1	0.846652	-4.463396	-2.031802
1	0.859159	-2.784706	-2.559866
1	-1.429786	-3.274152	-2.172282
1	4.83207	-3.50339	0.517664
1	1.485171	-1.746614	2.618343
1	6.226625	2.160196	0.066405
1	-1.919222	4.110703	0.02399
1	-0.502616	0.185283	0.18792
8	0.033277	4.155127	-1.626852
1	0.475831	3.505157	-2.193235
8	5.416258	-0.290968	-0.165385
1	4.892971	-1.111456	-0.176274

*Table S125 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 3-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481308 (Hartree/Particle)
Thermal correction to Energy= 0.516473
Thermal correction to Enthalpy= 0.517417
Thermal correction to Gibbs Free Energy= 0.413897
Sum of electronic and zero-point Energies= -2021.105183
Sum of electronic and thermal Energies= -2021.070017
Sum of electronic and thermal Enthalpies= -2021.069073
Sum of electronic and thermal Free Energies= -2021.172593

Coordinates:

6	-2.550542	-0.119232	-0.016944
6	-3.945305	0.241735	0.148758
6	-4.928353	-0.775185	-0.056566
6	-4.562179	-2.078169	-0.420167
6	-3.226838	-2.408511	-0.589445
6	-2.225269	-1.461007	-0.40414
1	-2.969511	-3.426539	-0.852815
6	-1.430631	0.75899	0.185328
6	-4.500974	1.556187	0.514086
6	-1.331785	2.089094	0.480332
6	-3.740524	2.804352	0.723167
6	-2.391901	3.011054	0.704744
8	-5.747743	1.691089	0.656024
8	-4.585461	3.837716	0.976665
1	-4.070214	4.645809	1.116266
8	-5.527666	-3.013928	-0.602736
8	-6.255223	-0.594742	0.071332
1	-6.379529	-2.576373	-0.430027
1	-6.345318	0.380698	0.348323
6	-0.779602	-1.876911	-0.637957
8	-0.162659	-2.046228	0.662038
6	-0.504881	-3.119545	-1.494137
6	1.152404	-2.428929	0.672224
6	1.010528	-3.169115	-1.754621
6	1.78848	-2.929744	-0.476442
6	3.151917	-3.248853	-0.36
6	1.811459	-2.301794	1.89836
6	3.848592	-3.105232	0.847059
6	3.158419	-2.65823	1.980848
8	3.87181	-3.735309	-1.412169
8	3.763004	-2.531823	3.196994
1	3.335474	-3.731452	-2.216668
1	4.689245	-2.803478	3.128162
8	-0.942772	-4.276382	-0.78435
1	-0.829242	-5.038447	-1.369159
1	-0.259553	-1.06436	-1.158945
6	0.057331	2.727681	0.553847
8	1.049104	1.667234	0.619564
6	0.343454	3.655987	-0.591489
6	2.335585	1.933096	0.222757
6	1.711874	4.269708	-0.552469
1	1.755713	5.035989	0.234015
6	2.738229	3.167559	-0.310222
6	3.221372	0.863627	0.375552
6	4.095855	3.297519	-0.660263
1	2.857861	-0.070121	0.789443
6	4.551385	1.024234	-0.011518
6	5.002931	2.245625	-0.519813
8	4.594713	4.461342	-1.178277
1	3.913912	5.147299	-1.17242
1	0.140345	3.301966	1.486885
1	1.248793	-4.154797	-2.176933
1	1.263055	-2.429918	-2.52704
1	-1.037271	-3.015894	-2.448377
1	4.89068	-3.406058	0.898352
1	1.282491	-1.924834	2.765329
1	6.038212	2.376608	-0.8122
1	1.893531	4.774807	-1.508726
1	-2.075231	4.035329	0.899016
1	-0.466809	0.283392	0.11518
8	-0.043009	3.277263	-1.852166
1	-0.824819	2.704802	-1.788732
8	5.458414	0.008281	0.095221
1	5.001883	-0.796473	0.390756

*Table S126 Energetics and Cartesian coordinates of the conformer **1c-H_2O** (saaasa-ss) post-radical capture via HAB at site 2-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481417 (Hartree/Particle)
Thermal correction to Energy= 0.516733
Thermal correction to Enthalpy= 0.517677
Thermal correction to Gibbs Free Energy= 0.414361
Sum of electronic and zero-point Energies= -2021.127517
Sum of electronic and thermal Energies= -2021.092202
Sum of electronic and thermal Enthalpies= -2021.091257
Sum of electronic and thermal Free Energies= -2021.194574

Coordinates:

6	-2.622975	0.004211	0.001875
6	-3.959062	0.541647	0.19623
6	-5.034836	-0.376151	0.382423
6	-4.831527	-1.762522	0.314626
6	-3.564662	-2.271298	0.05631
6	-2.473539	-1.42794	-0.10546
1	-3.434494	-3.344588	-0.008683
6	-1.418184	0.752003	-0.023463
6	-4.347601	1.953942	0.209627
6	-1.131781	2.126604	-0.143496
6	-3.479776	3.090874	-0.176713
6	-2.128551	3.15282	-0.304496
8	-5.53366	2.280445	0.490947
8	-4.237286	4.209674	-0.370327
1	-3.656331	4.947454	-0.60576
8	-5.885837	-2.602141	0.487809
8	-6.308888	-0.013021	0.615514
1	-6.667415	-2.04406	0.64297
1	-6.274778	1.003174	0.644813
6	-1.123368	-2.025114	-0.466666
8	-0.303376	-2.053305	0.729842
6	-1.091246	-3.409825	-1.124614
6	0.976041	-2.519277	0.572498
6	0.346239	-3.649632	-1.617673
6	1.360613	-3.25386	-0.563332
6	2.707643	-3.64846	-0.63913
6	1.863305	-2.227803	1.611262
6	3.627769	-3.346741	0.372714
6	3.187463	-2.654045	1.507476
8	3.191269	-4.365229	-1.695218
8	4.024043	-2.348077	2.540986
1	2.506538	-4.472896	-2.369268
1	4.912081	-2.680547	2.347901
8	-1.47635	-4.386562	-0.158992
1	-1.536531	-5.238435	-0.613178
1	-0.638475	-1.356535	-1.188712
6	0.229864	2.51603	-0.169088
8	1.125345	1.481738	-0.181912
6	0.78242	3.912129	-0.301366
1	0.062776	4.629055	0.093362
6	2.48889	1.673121	-0.11793
6	2.093513	4.06544	0.485637
1	1.864968	4.114259	1.558852
6	3.033063	2.922911	0.185542
6	3.253468	0.534114	-0.356353
6	4.438267	2.995916	0.249825
1	2.765446	-0.406068	-0.584661
6	4.642189	0.643866	-0.263248
6	5.240254	1.874277	0.025315
8	5.091976	4.155763	0.547585
1	4.457033	4.863629	0.722313
1	0.443955	-4.713812	-1.873051
1	0.497793	-3.090581	-2.551238
1	-1.776519	-3.411164	-1.981828
1	4.648194	-3.708372	0.288587
1	1.528246	-1.662883	2.472717
1	6.318271	1.958085	0.096775
1	2.515902	5.036754	0.203577
1	-1.752282	4.13509	-0.575291
1	-0.528981	0.152591	0.071215
8	0.94847	4.279015	-1.681179
1	1.656008	3.729395	-2.051036
8	5.462136	-0.42982	-0.448032
1	4.922491	-1.230798	-0.546549

*Table S127 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 5'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481326 (Hartree/Particle)
Thermal correction to Energy= 0.516811
Thermal correction to Enthalpy= 0.517755
Thermal correction to Gibbs Free Energy= 0.414727
Sum of electronic and zero-point Energies= -2021.104587
Sum of electronic and thermal Energies= -2021.069102
Sum of electronic and thermal Enthalpies= -2021.068157
Sum of electronic and thermal Free Energies= -2021.171185

Coordinates:

6	-2.328841	-0.491105	0.124706
6	-3.738483	-0.528928	0.378885
6	-4.47001	-1.710929	0.118189
6	-3.816518	-2.847942	-0.363683
6	-2.443162	-2.837593	-0.560773
6	-1.689763	-1.688157	-0.330017
1	-1.949599	-3.743862	-0.892443
6	-1.498553	0.688195	0.321624
6	-4.525545	0.579289	0.987352
6	-1.83501	2.009401	0.328524
6	-4.347752	1.969644	0.48625
6	-3.159189	2.574751	0.236403
8	-5.39542	0.369007	1.827473
8	-5.53128	2.632522	0.44915
1	-5.382899	3.544885	0.157338
8	-4.626396	-3.926914	-0.591903
8	-5.8161	-1.762808	0.286345
1	-4.122406	-4.661282	-0.968879
1	-6.108147	-2.633183	-0.031965
6	-0.199463	-1.719773	-0.622572
8	0.496429	-1.748992	0.662867
6	0.34003	-2.880833	-1.479778
6	1.868933	-1.809315	0.602769
6	1.820523	-2.614865	-1.780526
6	2.553006	-2.219348	-0.529034
6	4.013043	-2.300091	-0.474608
6	2.543422	-1.45792	1.787505
6	4.685669	-1.931309	0.755584
6	3.957372	-1.515634	1.844429
8	4.664001	-2.683917	-1.478751
8	4.512461	-1.101262	3.021498
1	5.47096	-1.241128	2.994076
8	0.178548	-4.149048	-0.842121
1	0.384743	-4.03504	0.097766
1	0.090693	-0.793307	-1.131064
6	-0.742227	3.07815	0.469751
8	0.414141	2.561728	1.150014
6	-0.344371	3.789807	-0.853607
1	0.234887	4.674793	-0.570723
6	1.600399	2.346738	0.493831
6	0.540131	2.891892	-1.715538
1	0.841128	3.471186	-2.596605
6	1.730357	2.454209	-0.897464
6	2.677714	2.008354	1.319334
6	3.004302	2.210644	-1.445584
1	2.531818	1.952567	2.392582
6	3.925528	1.778771	0.736122
6	4.098478	1.878111	-0.646062
8	3.239105	2.28739	-2.788923
1	2.411958	2.447627	-3.262925
1	-1.133305	3.849692	1.141865
1	2.270505	-3.513836	-2.211034
1	1.914634	-1.828173	-2.541059
1	-0.224547	-2.933229	-2.41465
1	5.769506	-1.978073	0.771505
1	1.97879	-1.137218	2.655113
1	5.064841	1.686111	-1.096649
1	-0.049012	2.037051	-2.079145
1	-3.198499	3.643988	0.038331
1	-0.444531	0.484371	0.454355
8	-1.471214	4.290812	-1.556058
1	-1.926151	3.544593	-1.973411
8	5.024423	1.453922	1.479955
1	4.744939	1.156653	2.359181

*Table S128 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 7'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481700 (Hartree/Particle)
Thermal correction to Energy= 0.516773
Thermal correction to Enthalpy= 0.517717
Thermal correction to Gibbs Free Energy= 0.416542
Sum of electronic and zero-point Energies= -2021.101952
Sum of electronic and thermal Energies= -2021.066879
Sum of electronic and thermal Enthalpies= -2021.065935
Sum of electronic and thermal Free Energies= -2021.167110

Coordinates:

6	-2.328841	-0.491105	0.124706
6	-3.738483	-0.528928	0.378885
6	-4.47001	-1.710929	0.118189
6	-3.816518	-2.847942	-0.363683
6	-2.443162	-2.837593	-0.560773
6	-1.689763	-1.688157	-0.330017
1	-1.949599	-3.743862	-0.892443
6	-1.498553	0.688195	0.321624
6	-4.525545	0.579289	0.987352
6	-1.83501	2.009401	0.328524
6	-4.347752	1.969644	0.48625
6	-3.159189	2.574751	0.236403
8	-5.39542	0.369007	1.827473
8	-5.53128	2.632522	0.44915
1	-5.382899	3.544885	0.157338
8	-4.626396	-3.926914	-0.591903
8	-5.8161	-1.762808	0.286345
1	-4.122406	-4.661282	-0.968879
1	-6.108147	-2.633183	-0.031965
6	-0.199463	-1.719773	-0.622572
8	0.496429	-1.748992	0.662867
6	0.34003	-2.880833	-1.479778
6	1.868933	-1.809315	0.602769
6	1.820523	-2.614865	-1.780526
6	2.553006	-2.219348	-0.529034
6	4.013043	-2.300091	-0.474608
6	2.543422	-1.45792	1.787505
6	4.685669	-1.931309	0.755584
6	3.957372	-1.515634	1.844429
8	4.664001	-2.683917	-1.478751
8	4.512461	-1.101262	3.021498
1	5.47096	-1.241128	2.994076
8	0.178548	-4.149048	-0.842121
1	0.384743	-4.03504	0.097766
1	0.090693	-0.793307	-1.131064
6	-0.742227	3.07815	0.469751
8	0.414141	2.561728	1.150014
6	-0.344371	3.789807	-0.853607
1	0.234887	4.674793	-0.570723
6	1.600399	2.346738	0.493831
6	0.540131	2.891892	-1.715538
1	0.841128	3.471186	-2.596605
6	1.730357	2.454209	-0.897464
6	2.677714	2.008354	1.319334
6	3.004302	2.210644	-1.445584
1	2.531818	1.952567	2.392582
6	3.925528	1.778771	0.736122
6	4.098478	1.878111	-0.646062
8	3.239105	2.28739	-2.788923
1	2.411958	2.447627	-3.262925
1	-1.133305	3.849692	1.141865
1	2.270505	-3.513836	-2.211034
1	1.914634	-1.828173	-2.541059
1	-0.224547	-2.933229	-2.41465
1	5.769506	-1.978073	0.771505
1	1.97879	-1.137218	2.655113
1	5.064841	1.686111	-1.096649
1	-0.049012	2.037051	-2.079145
1	-3.198499	3.643988	0.038331
1	-0.444531	0.484371	0.454355
8	-1.471214	4.290812	-1.556058
1	-1.926151	3.544593	-1.973411
8	5.024423	1.453922	1.479955
1	4.744939	1.156653	2.359181

*Table S129 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 3'-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480463 (Hartree/Particle)
Thermal correction to Energy= 0.515920
Thermal correction to Enthalpy= 0.516864
Thermal correction to Gibbs Free Energy= 0.414564
Sum of electronic and zero-point Energies= -2021.072104
Sum of electronic and thermal Energies= -2021.036647
Sum of electronic and thermal Enthalpies= -2021.035703
Sum of electronic and thermal Free Energies= -2021.138004

Coordinates:

6	-2.317958	-0.534101	0.112879
6	-3.724924	-0.624213	0.366808
6	-4.408914	-1.838047	0.120408
6	-3.71161	-2.95667	-0.344723
6	-2.341091	-2.890813	-0.549733
6	-1.634999	-1.710194	-0.331566
1	-1.817723	-3.77553	-0.901158
6	-1.52681	0.670853	0.316572
6	-4.554735	0.459667	0.962432
6	-1.906153	1.980633	0.327893
6	-4.417586	1.854072	0.458682
6	-3.247459	2.500343	0.223247
8	-5.425554	0.224522	1.794669
8	-5.621692	2.47652	0.407799
1	-5.501221	3.392418	0.113946
8	-4.47962	-4.067104	-0.560893
8	-5.751659	-1.939283	0.283502
1	-3.947004	-4.792888	-0.914536
1	-6.008782	-2.827126	-0.016422
6	-0.143094	-1.683474	-0.605587
8	0.537871	-1.721519	0.64764
6	0.38698	-2.827336	-1.562969
6	1.908454	-1.793752	0.628031
6	1.894242	-2.529106	-1.797432
6	2.613494	-2.183272	-0.522536
6	4.015587	-2.265229	-0.413363
6	2.54488	-1.485817	1.830114
6	4.680457	-1.950448	0.77211
6	3.9353	-1.546659	1.882066
8	4.803698	-2.642456	-1.462403
8	4.531889	-1.142627	3.048595
1	4.271925	-2.76243	-2.260529
1	5.485982	-1.298847	2.993111
8	0.252881	-4.046971	-0.988445
1	0.130198	-0.760557	-1.132489
6	-0.850975	3.083302	0.498653
8	0.315349	2.595193	1.180502
6	-0.46371	3.838675	-0.803401
1	0.084206	4.733811	-0.491526
6	1.509096	2.407558	0.52632
6	0.45695	2.992237	-1.678713
1	0.752812	3.606113	-2.537998
6	1.648516	2.558084	-0.860535
6	2.581012	2.050629	1.348947
6	2.928574	2.342419	-1.405118
1	2.424878	1.948788	2.417181
6	3.831919	1.833509	0.768492
6	4.016754	1.986585	-0.607738
8	3.174661	2.464392	-2.744302
1	2.351074	2.639531	-3.21907
1	-1.27622	3.826267	1.182262
1	2.330065	-3.413769	-2.27854
1	1.939224	-1.713212	-2.531869
1	-0.168373	-2.720429	-2.510042
1	5.764331	-1.989567	0.80053
1	1.966766	-1.172273	2.690422
1	4.986404	1.807826	-1.056904
1	-0.103283	2.13284	-2.075933
1	-3.32206	3.568515	0.029566
1	-0.468343	0.500829	0.46064
8	-1.599103	4.32195	-1.505083
1	-2.022145	3.574052	-1.951951
8	4.923499	1.474071	1.508469
1	4.636343	1.085515	2.349477

*Table S130 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site h-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.483061 (Hartree/Particle)
Thermal correction to Energy= 0.517865
Thermal correction to Enthalpy= 0.518809
Thermal correction to Gibbs Free Energy= 0.417512
Sum of electronic and zero-point Energies= -2021.117369
Sum of electronic and thermal Energies= -2021.082565
Sum of electronic and thermal Enthalpies= -2021.081621
Sum of electronic and thermal Free Energies= -2021.182919

Coordinates:

6	-2.378239	-0.501239	0.091882
6	-3.797264	-0.500915	0.331489
6	-4.541604	-1.644649	0.005139
6	-3.924732	-2.844275	-0.54899
6	-2.501125	-2.842395	-0.682295
6	-1.74709	-1.74118	-0.378029
1	-2.038955	-3.760589	-1.018206
6	-1.530877	0.632978	0.280168
6	-4.57401	0.585114	0.989503
6	-1.836223	1.977587	0.377765
6	-4.340221	2.006852	0.618934
6	-3.126287	2.587989	0.395011
8	-5.488348	0.335156	1.768262
8	-5.4827	2.718801	0.671371
1	-5.307522	3.647532	0.453145
8	-4.684039	-3.804231	-0.844522
8	-5.863717	-1.736904	0.129884
1	-6.059143	-2.636383	-0.231929
6	-0.240385	-1.80967	-0.60766
8	0.396676	-1.782587	0.695068
6	0.295446	-3.037498	-1.366685
6	1.780044	-1.830929	0.69907
6	1.789025	-2.817563	-1.639564
6	2.500522	-2.332167	-0.395133
6	3.901186	-2.372695	-0.272743
6	2.400155	-1.387663	1.866983
6	4.552798	-1.927011	0.87892
6	3.791567	-1.424097	1.933454
8	4.70016	-2.841574	-1.275451
8	4.379998	-0.879738	3.053137
1	4.164988	-3.093858	-2.040072
1	5.312425	-1.140627	3.08227
8	0.088394	-4.247477	-0.641353
1	0.237283	-4.054053	0.296691
1	0.079587	-0.923242	-1.169414
6	-0.697278	3.001527	0.47992
8	0.460489	2.412651	1.085643
6	-0.35442	3.741456	-0.848634
1	0.209455	4.636162	-0.566821
6	1.6573	2.309566	0.415765
6	0.535316	2.88554	-1.748819
1	0.784841	3.487997	-2.63028
6	1.764674	2.486633	-0.969897
6	2.75363	1.988353	1.216501
6	3.04335	2.334373	-1.538509
1	2.618953	1.864216	2.284917
6	4.001205	1.821558	0.612382
6	4.157138	2.005831	-0.76362
8	3.264093	2.488128	-2.878733
1	2.42555	2.619332	-3.341285
1	-1.030462	3.767295	1.189166
1	2.194654	-3.777735	-1.982201
1	1.907243	-2.104224	-2.466819
1	-0.235295	-3.147314	-2.316059
1	5.636851	-1.944364	0.919247
1	1.811522	-0.993463	2.685975
1	5.124373	1.868353	-1.23225
1	-0.028277	2.012277	-2.108939
1	-3.13014	3.671438	0.299338
1	-0.471566	0.420086	0.311587
8	-1.513559	4.225368	-1.505482
1	-1.967806	3.477106	-1.920068
8	5.108802	1.478636	1.334559
1	4.829858	1.065784	2.169103

*Table S131 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site i-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482758 (Hartree/Particle)
Thermal correction to Energy= 0.517776
Thermal correction to Enthalpy= 0.518720
Thermal correction to Gibbs Free Energy= 0.417110
Sum of electronic and zero-point Energies= -2021.106005
Sum of electronic and thermal Energies= -2021.070986
Sum of electronic and thermal Enthalpies= -2021.070042
Sum of electronic and thermal Free Energies= -2021.171652

Coordinates:

6	-2.376491	-0.495402	0.126191
6	-3.762039	-0.521452	0.374681
6	-4.585364	-1.699906	0.048246
6	-3.868816	-2.872496	-0.44218
6	-2.48763	-2.862237	-0.598003
6	-1.735492	-1.724287	-0.341446
1	-1.986614	-3.770284	-0.914109
6	-1.526518	0.660673	0.321713
6	-4.528319	0.558367	1.039896
6	-1.861443	1.988862	0.343219
6	-4.36655	1.953226	0.545714
6	-3.177522	2.55867	0.275404
8	-5.369701	0.330677	1.902811
8	-5.544389	2.612874	0.526559
1	-5.410774	3.520174	0.21079
8	-4.632397	-3.936856	-0.721423
8	-5.829095	-1.728124	0.132042
1	-4.082207	-4.663515	-1.054362
6	-0.235945	-1.772304	-0.599131
8	0.41924	-1.788555	0.695023
6	0.302771	-2.959451	-1.418247
6	1.802808	-1.824768	0.678439
6	1.789201	-2.706977	-1.702378
6	2.512853	-2.272806	-0.445516
6	3.915173	-2.308598	-0.340882
6	2.433484	-1.426345	1.856509
6	4.577177	-1.910575	0.822247
6	3.825924	-1.458356	1.906814
8	4.705573	-2.727357	-1.372197
8	4.421524	-0.96691	3.044945
1	4.163756	-2.946216	-2.142412
1	5.365486	-1.183683	3.030729
8	0.121323	-4.204139	-0.745805
1	0.333194	-4.06536	0.189849
1	0.062944	-0.858353	-1.127107
6	-0.760805	3.052382	0.469414
8	0.401262	2.518418	1.119323
6	-0.392223	3.785062	-0.853518
1	0.171111	4.678113	-0.564669
6	1.595079	2.361015	0.455843
6	0.505631	2.918657	-1.733762
1	0.778881	3.514845	-2.612606
6	1.716443	2.507151	-0.932731
6	2.680362	2.029925	1.269418
6	2.994821	2.314564	-1.489597
1	2.536969	1.930346	2.339453
6	3.928533	1.829127	0.6772
6	4.09698	1.980919	-0.70123
8	3.225992	2.4355	-2.831475
1	2.394035	2.585096	-3.300303
1	-1.13996	3.814912	1.158552
1	2.201589	-3.643467	-2.098117
1	1.885035	-1.952232	-2.494919
1	-0.2432	-3.03604	-2.362223
1	5.66166	-1.924818	0.849736
1	1.851617	-1.071129	2.69793
1	5.064608	1.81573	-1.159924
1	-0.062173	2.050478	-2.099933
1	-3.216173	3.629528	0.08821
1	-0.470642	0.452044	0.427683
8	-1.535759	4.27162	-1.537594
1	-1.972849	3.525383	-1.973555
8	5.028497	1.486042	1.411736
1	4.744648	1.077065	2.24579

*Table S132 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site b-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481880 (Hartree/Particle)
Thermal correction to Energy= 0.517212
Thermal correction to Enthalpy= 0.518156
Thermal correction to Gibbs Free Energy= 0.415998
Sum of electronic and zero-point Energies= -2021.115703
Sum of electronic and thermal Energies= -2021.080371
Sum of electronic and thermal Enthalpies= -2021.079427
Sum of electronic and thermal Free Energies= -2021.181585

Coordinates:

6	-2.378739	-0.437737	0.113881
6	-3.793756	-0.462584	0.360076
6	-4.543844	-1.614542	0.082423
6	-3.905451	-2.759297	-0.429157
6	-2.529047	-2.77395	-0.609471
6	-1.75268	-1.647802	-0.347119
1	-2.05265	-3.68857	-0.941875
6	-1.546828	0.718369	0.318949
6	-4.538779	0.653032	1.00714
6	-1.854653	2.086396	0.40739
6	-4.407377	2.080223	0.486683
6	-3.111194	2.687348	0.374223
8	-5.334159	0.456147	1.914491
8	-5.453333	2.717543	0.298029
8	-4.732387	-3.805352	-0.683962
8	-5.882504	-1.646356	0.269138
1	-4.245365	-4.559098	-1.047135
1	-6.204108	-2.508746	-0.042439
6	-0.253951	-1.722757	-0.608104
8	0.405116	-1.759092	0.685325
6	0.257575	-2.919187	-1.431637
6	1.786519	-1.830668	0.66666
6	1.748997	-2.70148	-1.717868
6	2.484619	-2.289026	-0.460774
6	3.885877	-2.3582	-0.358662
6	2.428837	-1.455003	1.846187
6	4.559021	-1.982782	0.805532
6	3.820086	-1.519336	1.893907
8	4.664578	-2.789373	-1.394088
8	4.428756	-1.046968	3.033337
1	4.117043	-2.982325	-2.167172
1	5.368373	-1.281447	3.01432
8	0.049665	-4.161189	-0.761075
1	0.251502	-4.023625	0.177003
1	0.070375	-0.816736	-1.13343
6	-0.695352	3.094755	0.508176
8	0.447995	2.498985	1.138194
6	-0.32186	3.805306	-0.825948
1	0.273146	4.681861	-0.550456
6	1.637593	2.330443	0.468236
6	0.541337	2.909257	-1.712699
1	0.819426	3.494011	-2.597635
6	1.750986	2.474458	-0.921407
6	2.72278	1.984325	1.274987
6	3.023302	2.264913	-1.486202
1	2.584787	1.887197	2.345919
6	3.964036	1.765016	0.674681
6	4.125381	1.914695	-0.704749
8	3.248246	2.383921	-2.82914
1	2.416129	2.549622	-3.292299
1	-1.022908	3.876652	1.200131
1	2.138587	-3.646322	-2.116966
1	1.861136	-1.946755	-2.508356
1	-0.291692	-2.981045	-2.37484
1	5.642938	-2.021905	0.830913
1	1.856769	-1.090476	2.690364
1	5.087658	1.736201	-1.169694
1	-0.051444	2.05496	-2.071238
1	-3.15058	3.771676	0.319676
1	-0.487087	0.509014	0.374274
8	-1.4578	4.324972	-1.493631
1	-1.964963	3.584611	-1.858051
8	5.063673	1.406354	1.402126
1	4.779555	0.999382	2.237053

*Table S133 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 3-OH by DFT calculations UB3LYP/6-31G(d,p), in the gas phase.*

Zero-point correction= 0.480391 (Hartree/Particle)
Thermal correction to Energy= 0.515661
Thermal correction to Enthalpy= 0.516605
Thermal correction to Gibbs Free Energy= 0.414811
Sum of electronic and zero-point Energies= -2021.074095
Sum of electronic and thermal Energies= -2021.038826
Sum of electronic and thermal Enthalpies= -2021.037882
Sum of electronic and thermal Free Energies= -2021.139676

Coordinates:

6	2.344134	-0.500012	-0.140784
6	3.762811	-0.501653	-0.346801
6	4.509958	-1.674562	-0.09662
6	3.86405	-2.837332	0.335698
6	2.48734	-2.855837	0.500936
6	1.717167	-1.715555	0.276411
1	2.003764	-3.778111	0.801766
6	1.493952	0.659564	-0.372483
6	4.552634	0.646867	-0.87282
6	1.806997	1.9874	-0.358905
6	4.318377	2.009882	-0.317992
6	3.102011	2.581231	-0.144706
8	5.465685	0.493948	-1.676981
8	5.484022	2.683175	-0.15706
1	5.300714	3.574512	0.17703
8	4.687653	-3.905489	0.555913
8	5.860244	-1.698038	-0.225472
1	4.192368	-4.653842	0.91685
1	6.160066	-2.56926	0.083484
6	0.223151	-1.778906	0.555154
8	-0.470824	-1.829126	-0.723493
6	-0.282453	-2.963584	1.399032
6	-1.85178	-1.866054	-0.661867
6	-1.762025	-2.726582	1.725493
6	-2.525521	-2.303702	0.48888
6	-3.930429	-2.339989	0.432172
6	-2.523536	-1.476223	-1.820644
6	-4.631721	-1.94939	-0.710316
6	-3.916503	-1.505477	-1.822165
8	-4.685571	-2.750185	1.493399
8	-4.550577	-1.013347	-2.940574
1	-4.117718	-2.965889	2.245616
1	-5.49234	-1.236181	-2.89813
8	-0.113396	-4.210545	0.724455
1	-0.312452	-4.060734	-0.212491
1	-0.086396	-0.861519	1.070109
6	0.739128	3.037354	-0.632424
8	-0.445989	2.5157	-1.209995
6	0.354297	3.938274	0.64938
1	-0.305745	4.706546	0.200976
6	-1.609325	2.348422	-0.494864
6	-0.457947	3.053576	1.617413
1	-0.720687	3.673752	2.482669
6	-1.680376	2.567135	0.88953
6	-2.716	1.972565	-1.256559
6	-2.942643	2.402219	1.496137
1	-2.607645	1.825341	-2.324916
6	-3.943145	1.801396	-0.613798
6	-4.065223	2.022372	0.76207
8	-3.130552	2.59483	2.834803
1	-2.282634	2.755507	3.27067
1	1.136343	3.740169	-1.371231
1	-2.154394	-3.665644	2.135514
1	-1.843005	-1.969633	2.517828
1	0.293057	-3.031171	2.326068
1	-5.716508	-1.961396	-0.700861
1	-1.970982	-1.127725	-2.684419
1	-5.016949	1.877185	1.259118
1	0.187672	2.243921	1.979493
1	3.095477	3.647459	0.083091
1	0.455576	0.42994	-0.574661
8	1.465067	4.471182	1.182915
8	-5.066217	1.424542	-1.288795
1	-4.818226	0.993229	-2.123841

*Table S134 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 5-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482061 (Hartree/Particle)
Thermal correction to Energy= 0.517083
Thermal correction to Enthalpy= 0.518027
Thermal correction to Gibbs Free Energy= 0.416835
Sum of electronic and zero-point Energies= -2021.104568
Sum of electronic and thermal Energies= -2021.069546
Sum of electronic and thermal Enthalpies= -2021.068602
Sum of electronic and thermal Free Energies= -2021.169794

Coordinates:

6	-2.527413	-0.163529	-0.04529
6	-3.936803	0.145304	0.104671
6	-4.882239	-0.896965	-0.150162
6	-4.465928	-2.18195	-0.51994
6	-3.116301	-2.468465	-0.656327
6	-2.150691	-1.491539	-0.440658
1	-2.821863	-3.47647	-0.919299
6	-1.445668	0.75912	0.15113
6	-4.541588	1.426285	0.504372
6	-1.391402	2.072254	0.522686
6	-3.82155	2.659296	0.871286
6	-2.480127	2.91624	0.867316
8	-5.799135	1.531734	0.571681
8	-4.69895	3.627566	1.246882
1	-4.209631	4.430165	1.479621
8	-5.396482	-3.145514	-0.741141
8	-6.217205	-0.75801	-0.056364
1	-6.265568	-2.735724	-0.587206
1	-6.342463	0.216286	0.217408
6	-0.6882	-1.860231	-0.641562
8	-0.08941	-1.979114	0.67369
6	-0.351326	-3.109456	-1.464337
6	1.234903	-2.316581	0.719067
6	1.170238	-3.109627	-1.694022
6	1.91265	-2.818015	-0.40574
6	3.282648	-3.090412	-0.253617
6	1.863259	-2.141932	1.9566
6	3.949659	-2.894104	0.964387
6	3.218718	-2.452537	2.076151
8	4.04033	-3.576291	-1.277275
8	3.791171	-2.284467	3.301106
1	3.520127	-3.617088	-2.09134
1	4.7278	-2.524238	3.257872
8	-0.762879	-4.265458	-0.738434
1	-0.609399	-5.035809	-1.302958
1	-0.187003	-1.040898	-1.170797
6	-0.031279	2.766149	0.550929
8	0.987194	1.754186	0.655208
6	0.201931	3.67149	-0.684942
1	-0.556553	4.458802	-0.67084
6	2.250039	2.019196	0.206877
6	1.602223	4.294171	-0.603224
1	1.633667	5.030606	0.210586
6	2.619993	3.209985	-0.38561
6	3.159168	0.950478	0.365984
6	4.005003	3.360766	-0.832238
1	2.806052	0.036523	0.832302
6	4.49534	1.073279	-0.078148
6	4.924383	2.254965	-0.648233
8	4.3822	4.429481	-1.378268
1	0.032172	3.398547	1.446739
1	1.451457	-4.093833	-2.092491
1	1.412553	-2.376585	-2.475422
1	-0.866511	-3.044571	-2.431346
1	4.99629	-3.171617	1.047256
1	1.302063	-1.769026	2.804814
1	5.945864	2.37407	-0.990236
1	1.823089	4.837522	-1.525611
1	-2.206693	3.923699	1.18159
1	-0.466415	0.337085	0.004953
8	0.000425	2.964147	-1.901384
1	0.742568	2.354806	-2.025877
8	5.371235	0.043325	0.052528
1	4.91261	-0.746769	0.390025

*Table S135 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 7-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481138 (Hartree/Particle)
Thermal correction to Energy= 0.516831
Thermal correction to Enthalpy= 0.517775
Thermal correction to Gibbs Free Energy= 0.413163
Sum of electronic and zero-point Energies= -2021.099189
Sum of electronic and thermal Energies= -2021.063496
Sum of electronic and thermal Enthalpies= -2021.062552
Sum of electronic and thermal Free Energies= -2021.167165

Coordinates:

6	-2.238134	-0.590885	0.117867
6	-3.646242	-0.758191	0.3265
6	-4.27864	-1.959082	-0.070389
6	-3.529243	-2.990912	-0.641076
6	-2.154762	-2.864068	-0.784541
6	-1.496834	-1.69173	-0.419994
1	-1.583895	-3.695446	-1.18262
6	-1.510779	0.63296	0.415617
6	-4.525587	0.21319	1.03459
6	-1.953646	1.918875	0.522869
6	-4.454607	1.660848	0.697366
6	-3.318961	2.380625	0.506921
8	-5.38522	-0.157527	1.828724
8	-5.682884	2.234467	0.741722
1	-5.605876	3.181104	0.548073
8	-4.249022	-4.095769	-1.004067
8	-5.620459	-2.126239	0.050879
1	-3.674248	-4.764251	-1.40179
1	-5.837161	-2.984605	-0.349482
6	0.006358	-1.604453	-0.623846
8	0.618548	-1.789573	0.682562
6	0.663788	-2.596307	-1.599827
6	1.998354	-1.767132	0.732143
6	2.133852	-2.184177	-1.769754
6	2.780215	-1.943802	-0.420737
6	4.17606	-1.933221	-0.247012
6	2.554618	-1.609778	2.001617
6	4.763706	-1.781308	1.010281
6	3.944356	-1.62015	2.130419
8	5.034089	-2.084543	-1.299982
8	4.453603	-1.461635	3.387314
1	4.539014	-2.131568	-2.128972
1	5.420109	-1.46438	3.345027
8	0.567099	-3.948925	-1.154488
1	0.745064	-3.954924	-0.201799
1	0.268772	-0.604308	-0.984969
6	-0.946356	3.065461	0.680459
8	0.294889	2.620979	1.256715
6	-0.679153	3.876903	-0.616591
1	-0.121187	4.769629	-0.315925
6	1.43133	2.470493	0.508738
6	0.181899	3.073781	-1.593287
1	0.409174	3.713112	-2.453804
6	1.43682	2.620147	-0.903357
6	2.583195	2.161767	1.201792
6	2.654025	2.389103	-1.611906
1	2.570542	2.066672	2.280877
6	3.833006	1.974914	0.496834
6	3.81912	2.082154	-0.945869
8	2.707241	2.488466	-2.969096
1	1.821	2.579141	-3.344953
1	-1.351935	3.763196	1.420013
1	2.636279	-2.996135	-2.310132
1	2.188023	-1.290794	-2.407072
1	0.15415	-2.554324	-2.566188
1	5.84571	-1.777514	1.094488
1	1.91597	-1.477839	2.866648
1	4.741844	1.923006	-1.491451
1	-0.39424	2.215798	-1.971417
1	-3.448745	3.458289	0.430007
1	-0.442002	0.510141	0.524435
8	-1.865659	4.36341	-1.215823
1	-2.331102	3.621052	-1.628839
8	4.8988	1.72424	1.122398

*Table S136 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 4'-α-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481607 (Hartree/Particle)
Thermal correction to Energy= 0.517136
Thermal correction to Enthalpy= 0.518080
Thermal correction to Gibbs Free Energy= 0.415946
Sum of electronic and zero-point Energies= -2021.094853
Sum of electronic and thermal Energies= -2021.059324
Sum of electronic and thermal Enthalpies= -2021.058379
Sum of electronic and thermal Free Energies= -2021.160513

Coordinates:

6	-2.353432	-0.447307	0.124441
6	-3.764079	-0.407236	0.375301
6	-4.565074	-1.538793	0.097778
6	-3.978628	-2.704115	-0.398053
6	-2.604815	-2.77725	-0.578067
6	-1.780931	-1.681422	-0.327481
1	-2.162908	-3.706117	-0.918894
6	-1.466615	0.692047	0.313751
6	-4.489075	0.732865	1.001928
6	-1.74192	2.028298	0.315683
6	-4.252621	2.113431	0.503364
6	-3.038575	2.657219	0.237832
8	-5.355546	0.557513	1.853682
8	-5.402618	2.834052	0.48238
1	-5.213044	3.738519	0.190029
8	-4.849508	-3.72895	-0.652939
8	-5.913438	-1.509767	0.260442
1	-4.384107	-4.483833	-1.038794
1	-6.256723	-2.355873	-0.07153
6	-0.286622	-1.808938	-0.580529
8	0.366005	-1.908394	0.721715
6	0.218049	-2.957015	-1.477547
6	1.737896	-1.920118	0.708562
6	1.712207	-2.882377	-1.550662
6	2.436506	-2.391545	-0.448353
6	3.865864	-2.383291	-0.370233
6	2.392671	-1.52204	1.862767
6	4.530789	-1.98917	0.782185
6	3.791814	-1.559129	1.890991
8	4.632801	-2.782214	-1.423432
8	4.404215	-1.087692	3.024259
1	4.098575	-2.809582	-2.229459
1	5.347465	-1.306785	2.994122
8	-0.178076	-4.274661	-1.040637
1	0.187507	-4.399663	-0.151779
1	0.07563	-0.891751	-1.060688
6	-0.603683	3.051127	0.445218
8	0.537401	2.477604	1.103875
6	-0.199867	3.762838	-0.878408
1	0.387993	4.641592	-0.594169
6	1.734696	2.297137	0.455752
6	0.677794	2.861942	-1.744366
1	0.966982	3.437698	-2.631594
6	1.874472	2.43358	-0.932261
6	2.806175	1.951061	1.281864
6	3.155167	2.218391	-1.47465
1	2.649969	1.859123	2.350928
6	4.05642	1.726089	0.703347
6	4.24324	1.869277	-0.673445
8	3.402641	2.330555	-2.814553
1	2.578373	2.496141	-3.291589
1	-0.956018	3.831521	1.129193
1	2.197308	-3.398094	-2.372903
1	-0.230998	-2.845073	-2.469105
1	5.615636	-1.979863	0.79246
1	1.830998	-1.173433	2.720873
1	5.213032	1.68629	-1.12066
1	0.08839	2.002727	-2.097205
1	-3.026732	3.726762	0.039017
1	-0.42105	0.44302	0.43715
8	-1.320662	4.278167	-1.580296
1	-1.790301	3.536456	-1.989416
8	5.141861	1.365358	1.452094
1	4.836472	0.984322	2.291042

*Table S137 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 4'-β-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481614 (Hartree/Particle)
Thermal correction to Energy= 0.517139
Thermal correction to Enthalpy= 0.518083
Thermal correction to Gibbs Free Energy= 0.415963
Sum of electronic and zero-point Energies= -2021.094845
Sum of electronic and thermal Energies= -2021.059320
Sum of electronic and thermal Enthalpies= -2021.058376
Sum of electronic and thermal Free Energies= -2021.160496

Coordinates:

6	-2.353321	-0.447548	0.124417
6	-3.764005	-0.407741	0.375182
6	-4.564755	-1.539492	0.097623
6	-3.978009	-2.704764	-0.397945
6	-2.604171	-2.777622	-0.577887
6	-1.780553	-1.681578	-0.32743
1	-2.162046	-3.706464	-0.918492
6	-1.466704	0.69195	0.313807
6	-4.489331	0.732217	1.001656
6	-1.742238	2.02816	0.315843
6	-4.25298	2.112853	0.503342
6	-3.038991	2.65684	0.23795
8	-5.356052	0.556642	1.853138
8	-5.403043	2.833384	0.482396
1	-5.213524	3.737895	0.190152
8	-4.848598	-3.729941	-0.65253
8	-5.913157	-1.510746	0.260035
1	-4.383373	-4.483838	-1.040519
1	-6.256222	-2.356688	-0.072594
6	-0.286184	-1.808803	-0.580495
8	0.366516	-1.908081	0.721653
6	0.21857	-2.956815	-1.477493
6	1.738418	-1.919798	0.708443
6	1.712713	-2.881898	-1.550851
6	2.436973	-2.391023	-0.448545
6	3.866326	-2.382724	-0.370496
6	2.39323	-1.522018	1.862758
6	4.531322	-1.988789	0.781927
6	3.79237	-1.559028	1.890896
8	4.633107	-2.781802	-1.423822
8	4.404822	-1.08771	3.024172
1	4.099321	-2.806439	-2.230253
1	5.348084	-1.30674	2.993956
8	-0.177028	-4.274535	-1.040159
1	0.188006	-4.398863	-0.15098
1	0.075823	-0.891531	-1.060693
6	-0.604239	3.051233	0.445543
8	0.536991	2.478048	1.104251
6	-0.200488	3.763184	-0.877961
1	0.387455	4.641844	-0.593593
6	1.734149	2.297391	0.455919
6	0.677073	2.862412	-1.744115
1	0.966264	3.43827	-2.631276
6	1.873774	2.433909	-0.932107
6	2.805712	1.951174	1.281873
6	3.154396	2.218697	-1.474655
1	2.649619	1.859148	2.350947
6	4.055903	1.726279	0.703215
6	4.242561	1.86955	-0.6736
8	3.401712	2.330965	-2.814581
1	2.577364	2.496411	-3.291526
1	-0.956824	3.831481	1.129548
1	2.198015	-3.397548	-2.372991
1	-0.230706	-2.845268	-2.468969
1	5.616163	-1.97939	0.792129
1	1.831542	-1.173567	2.720912
1	5.212297	1.686585	-1.120942
1	0.087626	2.003255	-2.097029
1	-3.027302	3.726395	0.039191
1	-0.421103	0.443084	0.437258
8	-1.321357	4.278689	-1.579608
1	-1.790485	3.537185	-1.989681
8	5.141422	1.365457	1.451769
1	4.836206	0.984565	2.290843

*Table S138 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 3'-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.482179 (Hartree/Particle)
Thermal correction to Energy= 0.517446
Thermal correction to Enthalpy= 0.518390
Thermal correction to Gibbs Free Energy= 0.416748
Sum of electronic and zero-point Energies= -2021.078213
Sum of electronic and thermal Energies= -2021.042947
Sum of electronic and thermal Enthalpies= -2021.042002
Sum of electronic and thermal Free Energies= -2021.143644

Coordinates:

6	-2.28996	0.504619	-0.117906
6	-3.708521	0.508212	-0.328287
6	-4.49719	1.573637	0.159342
6	-3.894915	2.633168	0.83967
6	-2.51021	2.699826	0.933971
6	-1.692215	1.690539	0.424747
1	-2.071697	3.548056	1.448831
6	-1.437562	-0.649802	-0.339698
6	-4.453378	-0.496043	-1.140892
6	-1.763312	-1.969737	-0.482206
6	-4.258661	-1.943257	-0.885079
6	-3.074515	-2.551142	-0.613178
8	-5.303652	-0.145722	-1.954683
8	-5.410314	-2.636569	-1.074812
1	-5.250947	-3.580026	-0.920571
8	-4.755174	3.567108	1.342346
8	-5.849358	1.562848	0.039037
1	-4.272593	4.297804	1.752936
1	-6.184548	2.34911	0.500693
6	-0.187059	1.874898	0.582155
8	0.463302	1.57811	-0.706194
6	0.277266	3.247902	0.980473
6	1.825736	1.77572	-0.738905
6	1.738213	3.291153	1.311136
6	2.50486	2.560197	0.212612
6	3.898858	2.678924	0.076799
6	2.497761	1.154752	-1.794199
6	4.596238	2.046783	-0.955236
6	3.881556	1.283745	-1.877579
8	4.648755	3.417807	0.947864
8	4.518176	0.567055	-2.870042
1	4.094751	3.761935	1.661227
1	5.425678	0.892394	-2.965482
8	-0.089691	4.305251	0.177225
1	-0.913027	4.096691	-0.290484
1	0.2103	1.159151	1.314213
6	-0.653149	-3.030775	-0.533163
8	0.567612	-2.48532	-1.056488
6	-0.419812	-3.786459	0.807324
1	0.146799	-4.691457	0.565337
6	1.70532	-2.389454	-0.292827
6	0.412551	-2.949701	1.778119
1	0.584717	-3.559183	2.673161
6	1.702576	-2.564258	1.097652
6	2.866471	-2.07961	-1.002254
6	2.931976	-2.415275	1.766445
1	2.82101	-1.960452	-2.078481
6	4.060767	-1.906658	-0.300345
6	4.105471	-2.088051	1.084393
8	3.042765	-2.568366	3.120923
1	2.170416	-2.716379	3.510402
1	-0.961911	-3.780739	-1.269888
1	2.051419	4.340445	1.376615
1	1.919028	2.831151	2.292371
1	5.676243	2.139172	-1.006845
1	1.951029	0.55051	-2.506778
1	5.031292	-1.949165	1.630104
1	-0.164976	-2.069243	2.095596
1	-3.102042	-3.638329	-0.574803
1	-0.377487	-0.441349	-0.317023
8	-1.633601	-4.250377	1.376749
1	-2.122007	-3.484897	1.714053
8	5.219441	-1.55768	-0.933501
1	5.001489	-1.151481	-1.79108

*Table S139 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 2'-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481143 (Hartree/Particle)
Thermal correction to Energy= 0.516987
Thermal correction to Enthalpy= 0.517931
Thermal correction to Gibbs Free Energy= 0.414369
Sum of electronic and zero-point Energies= -2021.098167
Sum of electronic and thermal Energies= -2021.062323
Sum of electronic and thermal Enthalpies= -2021.061379
Sum of electronic and thermal Free Energies= -2021.164941

Coordinates:

6	-2.296904	0.528148	-0.185518
6	-3.725122	0.54048	-0.350361
6	-4.489116	1.615342	0.14142
6	-3.853292	2.713436	0.751597
6	-2.481946	2.805247	0.769985
6	-1.652343	1.761734	0.272357
1	-2.036779	3.73512	1.101711
6	-1.485186	-0.651097	-0.324996
6	-4.502877	-0.464728	-1.135493
6	-1.832192	-1.975846	-0.451101
6	-4.317564	-1.911453	-0.900207
6	-3.140465	-2.535459	-0.617272
8	-5.376122	-0.099541	-1.921386
8	-5.468169	-2.601961	-1.121789
1	-5.310018	-3.547205	-0.979355
8	-4.707527	3.674274	1.216942
8	-5.845941	1.612097	0.081768
1	-4.218488	4.406443	1.61739
1	-6.152463	2.418554	0.528662
6	-0.256582	2.043208	0.271996
8	0.541346	1.360376	-0.615197
6	0.366526	3.174338	1.051263
6	1.896153	1.605276	-0.719814
6	1.811666	2.846771	1.445297
6	2.579924	2.347263	0.24964
6	3.962072	2.521282	0.061494
6	2.519748	1.045576	-1.831493
6	4.625513	1.957274	-1.032449
6	3.899271	1.204923	-1.955775
8	4.735985	3.22079	0.939546
8	4.508599	0.545451	-2.996249
1	4.198716	3.544909	1.675354
1	5.427578	0.84209	-3.072132
8	0.288053	4.43363	0.356491
1	0.792853	4.350591	-0.466372
6	-0.733892	-3.049365	-0.426023
8	0.486475	-2.559445	-1.006181
6	-0.497771	-3.697133	0.966983
1	0.044009	-4.633408	0.798099
6	1.634194	-2.418564	-0.267426
6	0.363972	-2.803254	1.858866
1	0.539638	-3.344138	2.796562
6	1.64991	-2.491985	1.132362
6	2.787778	-2.168938	-1.013557
6	2.890293	-2.304907	1.770735
1	2.726104	-2.126322	-2.095002
6	3.992434	-1.954634	-0.342459
6	4.056216	-2.03687	1.050677
8	3.019678	-2.359284	3.13099
1	2.151598	-2.471362	3.541319
1	-1.056106	-3.85323	-1.096691
1	2.239222	3.765153	1.863455
1	1.808604	2.098753	2.249564
1	-0.209329	3.329869	1.964244
1	5.699437	2.083104	-1.123884
1	1.953243	0.470616	-2.552267
1	4.990562	-1.865737	1.572099
1	-0.193671	-1.890711	2.115535
1	-3.182993	-3.623134	-0.590266
1	-0.423227	-0.478442	-0.24109
8	-1.71955	-4.080236	1.578294
1	-2.208995	-3.274085	1.79977
8	5.146295	-1.657969	-1.012585
1	4.925006	-1.319283	-1.896222

*Table S140 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 4β-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480559 (Hartree/Particle)
Thermal correction to Energy= 0.516413
Thermal correction to Enthalpy= 0.517357
Thermal correction to Gibbs Free Energy= 0.413935
Sum of electronic and zero-point Energies= -2021.093873
Sum of electronic and thermal Energies= -2021.058019
Sum of electronic and thermal Enthalpies= -2021.057075
Sum of electronic and thermal Free Energies= -2021.160498

Coordinates:

6	-2.312853	-0.487915	0.101815
6	-3.716825	-0.560343	0.380728
6	-4.433137	-1.746166	0.099799
6	-3.770015	-2.85776	-0.424166
6	-2.398461	-2.821312	-0.631172
6	-1.659442	-1.666989	-0.380027
1	-1.894634	-3.713784	-0.983709
6	-1.510355	0.714064	0.283341
6	-4.512732	0.510979	1.042739
6	-1.891758	2.022985	0.30113
6	-4.396472	1.910264	0.555389
6	-3.236278	2.545165	0.255456
8	-5.341252	0.255925	1.91183
8	-5.598656	2.541699	0.57448
1	-5.485238	3.46147	0.290448
8	-4.565875	-3.942254	-0.675036
8	-5.776079	-1.822736	0.288276
1	-4.050214	-4.665212	-1.058225
1	-6.05946	-2.691967	-0.04034
6	-0.16399	-1.684109	-0.650648
8	0.496465	-1.746642	0.645056
6	0.393083	-2.829291	-1.515782
6	1.875706	-1.792946	0.637222
6	1.878402	-2.550533	-1.784712
6	2.595371	-2.184915	-0.501997
6	3.995786	-2.241346	-0.382293
6	2.497576	-1.466095	1.842172
6	4.648321	-1.917293	0.809171
6	3.888394	-1.51693	1.908638
8	4.794423	-2.612089	-1.426492
8	4.469349	-1.102521	3.082575
1	4.258297	-2.776542	-2.214055
1	5.423875	-1.260254	3.040626
8	0.231113	-4.105455	-0.896648
1	0.420068	-3.995223	0.047571
1	0.131506	-0.747386	-1.138024
6	-0.841092	3.139341	0.382878
8	0.328259	2.718105	1.106233
6	-0.498377	3.795925	-0.999886
1	-0.21583	4.837307	-0.784355
6	1.536033	2.495525	0.506577
6	0.638471	3.109063	-1.677372
6	1.714521	2.644303	-0.900331
6	2.567089	2.097768	1.348387
6	3.020349	2.350275	-1.409702
1	2.381169	1.998026	2.412129
6	3.827187	1.824266	0.799789
6	4.055264	1.952835	-0.577753
8	3.300907	2.459403	-2.739021
1	2.567495	2.890221	-3.19914
1	-1.268306	3.926775	1.011658
1	2.298944	-3.460312	-2.231318
1	1.970106	-1.751909	-2.533554
1	-0.15094	-2.873553	-2.463149
1	5.732191	-1.948042	0.849064
1	1.908547	-1.152372	2.695224
1	5.034775	1.742122	-0.990347
1	0.680381	3.197711	-2.759094
1	-3.314671	3.609957	0.046772
1	-0.44559	0.544301	0.375649
8	-1.645394	3.914915	-1.83259
1	-1.873027	3.024707	-2.140819
8	4.886336	1.442815	1.567162
1	4.575207	1.061747	2.404022

*Table S141 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 4α-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480542 (Hartree/Particle)
Thermal correction to Energy= 0.516485
Thermal correction to Enthalpy= 0.517430
Thermal correction to Gibbs Free Energy= 0.413544
Sum of electronic and zero-point Energies= -2021.093882
Sum of electronic and thermal Energies= -2021.057938
Sum of electronic and thermal Enthalpies= -2021.056994
Sum of electronic and thermal Free Energies= -2021.160880

Coordinates:

6	-2.297426	-0.509533	0.104689
6	-3.700708	-0.602477	0.381188
6	-4.399346	-1.799073	0.102073
6	-3.719337	-2.902225	-0.417745
6	-2.348428	-2.845599	-0.623404
6	-1.626528	-1.67984	-0.374234
1	-1.83107	-3.73122	-0.973636
6	-1.51311	0.704622	0.289456
6	-4.514118	0.458939	1.037681
6	-1.914716	2.007485	0.302699
6	-4.419381	1.856351	0.540828
6	-3.26777	2.507791	0.244147
8	-5.338352	0.195943	1.908358
8	-5.632066	2.467668	0.548049
1	-5.532104	3.387032	0.257627
8	-4.498744	-3.998969	-0.667038
8	-5.741358	-1.894294	0.28865
1	-3.970367	-4.717784	-1.040592
1	-6.011526	-2.769224	-0.035887
6	-0.130854	-1.676862	-0.644423
8	0.530743	-1.733822	0.650857
6	0.439868	-2.813114	-1.512901
6	1.910466	-1.767309	0.642977
6	1.921534	-2.516674	-1.78139
6	2.634339	-2.150435	-0.496654
6	4.035089	-2.195734	-0.376122
6	2.52914	-1.435918	1.848369
6	4.684186	-1.8673	0.815892
6	3.920459	-1.473375	1.915112
8	4.837392	-2.558305	-1.420446
8	4.497147	-1.053464	3.088697
1	4.302744	-2.729037	-2.207673
1	5.453572	-1.198538	3.045489
8	0.294156	-4.09316	-0.897458
1	0.485311	-3.984214	0.046455
1	0.152472	-0.735217	-1.129565
6	-0.886511	3.143655	0.404421
8	0.293395	2.743251	1.122112
6	-0.549938	3.835687	-0.960101
1	-0.265019	4.87054	-0.717088
6	1.490409	2.50711	0.505468
6	0.582875	3.166954	-1.662168
1	0.655855	3.352985	-2.729749
6	1.649044	2.651851	-0.904697
6	2.536734	2.126011	1.335573
6	2.938374	2.322571	-1.435385
1	2.369462	2.0428	2.403847
6	3.790398	1.855905	0.770693
6	3.990546	1.949087	-0.614242
8	3.19214	2.393259	-2.7728
1	2.37206	2.542698	-3.262125
1	-1.332313	3.909441	1.046781
1	2.351522	-3.419444	-2.233166
1	2.00458	-1.71296	-2.525789
1	-0.104311	-2.861374	-2.459969
1	5.768285	-1.888438	0.856223
1	1.937143	-1.127985	2.701483
1	4.957147	1.711977	-1.042594
1	-3.361589	3.570017	0.029124
1	-0.446752	0.549682	0.390373
8	-1.69949	3.980307	-1.786672
1	-1.918176	3.102339	-2.134035
8	4.86511	1.495427	1.526445
1	4.570752	1.133884	2.377636

*Table S142 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 3-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.480909 (Hartree/Particle)
Thermal correction to Energy= 0.516665
Thermal correction to Enthalpy= 0.517609
Thermal correction to Gibbs Free Energy= 0.414613
Sum of electronic and zero-point Energies= -2021.086854
Sum of electronic and thermal Energies= -2021.051099
Sum of electronic and thermal Enthalpies= -2021.050155
Sum of electronic and thermal Free Energies= -2021.153151

Coordinates:

6	-2.382844	-0.471102	0.130062
6	-3.799196	-0.434054	0.343587
6	-4.583199	-1.580983	0.078417
6	-3.97606	-2.755413	-0.372787
6	-2.600766	-2.813577	-0.54266
6	-1.795885	-1.699594	-0.306274
1	-2.146189	-3.745652	-0.8589
6	-1.497794	0.661428	0.375774
6	-4.548116	0.730079	0.892804
6	-1.769179	1.995579	0.357615
6	-4.278598	2.089776	0.349134
6	-3.050136	2.625256	0.146336
8	-5.458965	0.592908	1.704112
8	-5.427929	2.801928	0.213239
1	-5.218392	3.693668	-0.10331
8	-4.833302	-3.797758	-0.605939
8	-5.934954	-1.563162	0.210524
1	-4.362108	-4.546323	-0.996844
1	-6.261314	-2.418354	-0.115656
6	-0.305604	-1.801678	-0.58519
8	0.385584	-1.903726	0.693882
6	0.169997	-2.981098	-1.452822
6	1.764604	-1.965951	0.631438
6	1.656209	-2.775356	-1.773369
6	2.428997	-2.390003	-0.529935
6	3.832967	-2.453392	-0.476057
6	2.444585	-1.618274	1.798907
6	4.542599	-2.104548	0.67496
6	3.836401	-1.676921	1.798851
8	4.579299	-2.852537	-1.547862
8	4.480731	-1.2297	2.930974
1	4.006886	-3.034656	-2.305503
1	5.416899	-1.474125	2.883199
8	-0.031042	-4.236194	-0.801884
1	0.15773	-4.103258	0.139826
1	0.032835	-0.881125	-1.075656
6	-0.640408	3.031149	0.584009
8	0.504968	2.407884	1.182881
6	-0.260795	3.809136	-0.639143
6	1.702879	2.315845	0.517454
6	0.704525	3.230665	-1.615931
1	1.056176	4.035403	-2.278914
6	1.864107	2.647869	-0.835254
6	2.765494	1.850183	1.296793
6	3.14689	2.486045	-1.38983
1	2.59564	1.614477	2.341237
6	4.023165	1.699988	0.710262
6	4.223964	2.020983	-0.634616
8	3.40951	2.781317	-2.700187
1	2.589155	2.975634	-3.172619
1	-1.015663	3.742351	1.332897
1	2.027184	-3.717157	-2.19691
1	1.756431	-2.008628	-2.554084
1	-0.405805	-3.015992	-2.381547
1	5.62695	-2.137926	0.664429
1	1.899332	-1.28182	2.672088
1	5.196808	1.89229	-1.094038
1	0.229978	2.476367	-2.273473
1	-3.019323	3.682484	-0.109124
1	-0.467312	0.402006	0.581203
8	-1.185203	4.743682	-1.023399
1	-0.927176	5.12803	-1.873928
8	5.101346	1.246324	1.415889
1	4.7981	0.762352	2.20257

*Table S143 Energetics and Cartesian coordinates of the conformer **1d-H_2O** (sa-saa-ss) post-radical capture via HAB at site 2-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.481984 (Hartree/Particle)
Thermal correction to Energy= 0.517360
Thermal correction to Enthalpy= 0.518304
Thermal correction to Gibbs Free Energy= 0.416525
Sum of electronic and zero-point Energies= -2021.112370
Sum of electronic and thermal Energies= -2021.076994
Sum of electronic and thermal Enthalpies= -2021.076050
Sum of electronic and thermal Free Energies= -2021.177829

Coordinates:

6	-2.486845	-0.181087	-0.054662
6	-3.682204	-0.872359	-0.457138
6	-4.893443	-0.162787	-0.597683
6	-4.933362	1.218149	-0.367349
6	-3.777918	1.907214	-0.025175
6	-2.566138	1.242391	0.139714
1	-3.821716	2.982107	0.113128
6	-1.203586	-0.803986	0.122895
6	-3.730893	-2.313054	-0.827991
6	-0.846212	-2.13441	0.417284
6	-3.03836	-3.320367	0.025623
6	-1.792216	-3.233404	0.541593
8	-4.415173	-2.715559	-1.764857
8	-3.796168	-4.449887	0.137562
1	-3.309605	-5.10691	0.657326
8	-6.165636	1.793802	-0.52125
8	-6.053364	-0.791527	-0.919133
1	-6.131303	2.737432	-0.312232
1	-6.757816	-0.123532	-0.879052
6	-1.349943	2.032714	0.582109
8	-0.502557	2.235797	-0.589115
6	-1.569995	3.417194	1.214528
6	0.712347	2.837276	-0.338524
6	-0.220768	3.902691	1.770733
6	0.907228	3.644226	0.792125
6	2.184336	4.210002	0.959201
6	1.713752	2.616905	-1.286011
6	3.218724	3.981373	0.047058
6	2.968613	3.182716	-1.067692
8	2.485425	5.006531	2.024767
8	3.957704	2.877142	-1.977824
1	1.721736	5.082148	2.613079
1	4.747789	3.403779	-1.785086
8	-2.101194	4.353364	0.277183
1	-1.67867	4.173762	-0.577034
1	-0.781127	1.439002	1.306702
6	0.52399	-2.43955	0.630013
8	1.394918	-1.383396	0.493416
6	1.10813	-3.816564	0.906878
1	0.943517	-4.449577	0.026136
6	2.687934	-1.588449	0.039802
6	2.617788	-3.764691	1.209635
1	2.998617	-4.787251	1.123346
6	3.342034	-2.784771	0.328483
6	3.265711	-0.542294	-0.669176
6	4.656913	-2.91736	-0.15295
1	2.700671	0.362586	-0.852915
6	4.577935	-0.704221	-1.12975
6	5.269642	-1.89473	-0.882261
8	5.410921	-4.033536	0.072638
1	4.910558	-4.672459	0.597914
1	-0.3249	4.974735	1.980194
1	-0.028272	3.40418	2.730903
1	-2.296339	3.34727	2.028638
1	4.196166	4.416391	0.228081
1	1.517914	2.003156	-2.156971
1	6.285315	-2.021594	-1.238714
1	2.737698	-3.477929	2.264185
1	-1.416945	-4.116463	1.049825
1	-0.363875	-0.128327	0.078962
8	0.442532	-4.515299	1.967839
1	0.456188	-3.943133	2.750151
8	5.223344	0.262999	-1.834738
1	4.669212	1.064573	-1.906341

*Table S144 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) transition state via HAB at site 2-H by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.503614 (Hartree/Particle)
Thermal correction to Energy= 0.540185
Thermal correction to Enthalpy= 0.541129
Thermal correction to Gibbs Free Energy= 0.436032
Sum of electronic and zero-point Energies= -2097.486892
Sum of electronic and thermal Energies= -2097.450321
Sum of electronic and thermal Enthalpies= -2097.449377
Sum of electronic and thermal Free Energies= -2097.554474

Coordinates:

6	-2.605763	-0.151578	-0.024709
6	-3.858891	-0.858116	-0.185974
6	-5.013482	-0.112873	-0.573711
6	-4.961258	1.278577	-0.719504
6	-3.790203	1.960122	-0.442343
6	-2.62184	1.283444	-0.095043
1	-3.794419	3.042459	-0.497133
6	-1.30502	-0.766094	0.067415
6	-4.095792	-2.260736	0.093462
6	-0.921745	-2.057565	0.378029
6	-3.146373	-3.191812	0.72376
6	-1.789082	-3.097711	0.849573
8	-5.244685	-2.780852	-0.081614
8	-3.726045	-4.32624	1.168231
1	-4.670856	-4.251251	0.892644
8	-6.079775	1.96095	-1.085492
8	-6.232639	-0.658286	-0.784465
1	-6.790257	1.30596	-1.181933
1	-6.130664	-1.630893	-0.577401
6	-1.426737	2.102106	0.355562
8	-0.474995	2.243492	-0.743205
6	-1.703513	3.515949	0.897579
6	0.704568	2.858856	-0.39069
6	-0.425644	4.026865	1.562126
6	0.788663	3.713382	0.718937
6	2.047776	4.276648	1.006203
6	1.812905	2.5941	-1.20155
6	3.170859	4.014037	0.223297
6	3.030214	3.166586	-0.870303
8	2.095422	5.103663	2.093228
8	4.183745	2.874748	-1.571307
1	2.99304	5.443108	2.196054
1	3.9631	2.428458	-2.408018
8	-2.128163	4.400248	-0.152291
1	-1.601574	4.177411	-0.935017
1	-0.907953	1.549971	1.15747
6	0.525686	-2.412712	0.192444
8	1.387855	-1.287765	0.318264
6	1.140207	-3.720033	0.776203
1	0.433973	-4.546627	0.6402
6	2.740145	-1.489498	0.075217
6	2.424071	-4.023056	0.001904
1	2.151193	-4.353006	-1.017563
6	3.287212	-2.779098	-0.064794
6	3.498173	-0.32526	-0.014084
6	4.681459	-2.850326	-0.264248
1	3.021604	0.634752	0.102192
6	4.87279	-0.438072	-0.28255
6	5.473137	-1.70943	-0.377939
8	5.20285	-4.113211	-0.370451
1	6.162708	-4.047952	-0.503112
1	-0.524646	5.114993	1.719454
1	-0.325286	3.586228	2.562584
1	-2.524016	3.490934	1.620297
1	4.130559	4.44462	0.459844
1	1.705822	1.90221	-2.034688
1	6.533617	-1.783156	-0.573267
1	2.956442	-4.849983	0.475496
1	-1.341474	-3.959677	1.325413
1	-0.487624	-0.104543	-0.189603
8	1.352546	-3.623325	2.197269
1	2.055186	-2.9619	2.343026
8	5.675885	0.640489	-0.442682
1	5.149332	1.437241	-0.622186
1	0.654698	-2.620134	-0.929782
8	0.530755	-2.420757	-2.5342
1	-0.349683	-2.834693	-2.600873

*Table S145 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) transition state via HAB at site b-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.504020 (Hartree/Particle)
Thermal correction to Energy= 0.539475
Thermal correction to Enthalpy= 0.540419
Thermal correction to Gibbs Free Energy= 0.438434
Sum of electronic and zero-point Energies= -2097.505584
Sum of electronic and thermal Energies= -2097.470129
Sum of electronic and thermal Enthalpies= -2097.469185
Sum of electronic and thermal Free Energies= -2097.571169

Coordinates:

6	2.384879	0.34235	-0.120915
6	3.792863	-0.015946	-0.012449
6	4.759883	1.032612	-0.084399
6	4.374421	2.370022	-0.221627
6	3.030371	2.705299	-0.35154
6	2.045762	1.731012	-0.328092
1	2.768024	3.749922	-0.466406
6	1.292213	-0.568464	-0.064317
6	4.357208	-1.359462	0.129662
6	1.217487	-1.933485	0.14317
6	3.639438	-2.596821	0.468004
6	2.271586	-2.813682	0.426987
8	5.615163	-1.523847	0.007386
8	4.381416	-3.637164	0.790894
1	5.35808	-3.391737	1.073657
8	5.319683	3.335038	-0.249402
8	6.093267	0.860986	-0.001789
1	6.177927	2.884798	-0.163112
1	6.226694	-0.136303	0.015181
6	0.608856	2.160585	-0.566573
8	-0.078692	2.165866	0.717675
6	0.355158	3.536878	-1.209972
6	-1.432155	2.405173	0.646924
6	-1.138861	3.619018	-1.563389
6	-1.997849	3.075298	-0.442496
6	-3.394175	3.239138	-0.436814
6	-2.195661	1.946307	1.725675
6	-4.190201	2.763489	0.606402
6	-3.573949	2.118352	1.678703
8	-3.925627	3.890961	-1.511751
8	-4.404212	1.593672	2.653383
1	-4.883027	3.961448	-1.402503
1	-3.871224	1.353323	3.424045
8	0.739525	4.603845	-0.348648
1	0.499799	4.340063	0.552558
1	0.114021	1.424253	-1.211359
6	-0.146652	-2.601248	0.028835
8	-1.149494	-1.715549	0.540338
6	-0.497383	-2.995481	-1.428818
1	0.312923	-3.609853	-1.832649
6	-2.466324	-2.051235	0.319112
6	-1.812894	-3.781108	-1.417494
1	-1.640792	-4.787867	-1.01324
6	-2.845524	-3.034139	-0.602976
6	-3.399057	-1.311479	1.048022
6	-4.226696	-3.259263	-0.755132
1	-3.044031	-0.560542	1.73875
6	-4.759925	-1.531622	0.840294
6	-5.181229	-2.526014	-0.053425
8	-4.578607	-4.232673	-1.6502
1	-5.542286	-4.283782	-1.695379
1	-0.146554	-3.516122	0.63808
1	-1.390479	4.665019	-1.764019
1	-1.33379	3.069457	-2.494119
1	0.955984	3.64274	-2.118229
1	-5.269547	2.878416	0.596033
1	-1.702941	1.415722	2.533861
1	-6.244025	-2.69649	-0.19662
1	-2.159398	-3.917561	-2.446372
1	2.008157	-3.844727	0.651345
1	0.317681	-0.118409	-0.162106
8	-0.567961	-1.844925	-2.259453
1	-1.403142	-1.398355	-2.058494
8	-5.719194	-0.815233	1.483364
1	-5.311342	-0.064294	1.951211
8	6.620396	-2.953858	1.648601
1	7.208432	-2.872579	0.878534

*Table S146 Energetics and Cartesian coordinates of the conformer **1a-H_2O** (as-ass-as) transition state via HAB at site h-OH by DFT calculations UB3LYP/6-31G(d,p), in the solvent H_2O.*

Zero-point correction= 0.505627 (Hartree/Particle)
Thermal correction to Energy= 0.541700
Thermal correction to Enthalpy= 0.542644
Thermal correction to Gibbs Free Energy= 0.438799
Sum of electronic and zero-point Energies= -2097.507260
Sum of electronic and thermal Energies= -2097.471188
Sum of electronic and thermal Enthalpies= -2097.470244
Sum of electronic and thermal Free Energies= -2097.574089

Coordinates:

6	-2.363162	-0.184644	-0.088149
6	-3.692506	-0.711077	-0.327575
6	-4.799549	0.203483	-0.351414
6	-4.632818	1.565876	-0.032903
6	-3.344885	2.050322	0.226821
6	-2.235493	1.228763	0.201967
1	-3.238671	3.105337	0.446422
6	-1.145676	-0.930335	-0.121659
6	-4.050473	-2.102557	-0.550636
6	-0.869384	-2.27324	-0.269407
6	-3.156708	-3.262515	-0.575827
6	-1.792807	-3.321995	-0.460509
8	-5.273578	-2.441366	-0.711369
8	-3.808707	-4.425293	-0.762466
1	-4.755152	-4.169734	-0.842586
8	-5.679307	2.387618	0.039048
8	-6.052415	-0.158547	-0.650483
1	-6.028431	-1.178083	-0.702871
6	-0.884135	1.836027	0.541945
8	-0.158333	2.007248	-0.707268
6	-0.852768	3.191287	1.271385
6	1.142171	2.449691	-0.571623
6	0.600577	3.446516	1.699049
6	1.564322	3.127036	0.576761
6	2.917835	3.507272	0.632112
6	1.992672	2.188543	-1.650015
6	3.8045	3.231968	-0.410967
6	3.325579	2.573168	-1.544664
8	3.312761	4.157843	1.763848
8	4.250645	2.258516	-2.520764
1	4.252115	4.381171	1.700475
1	3.791191	2.005516	-3.33536
8	-1.347981	4.24981	0.452162
1	-1.028442	4.088873	-0.448926
1	-0.324241	1.136446	1.173133
6	0.575049	-2.736684	-0.127368
8	1.44198	-1.726521	-0.660462
6	0.958378	-3.038797	1.344381
1	0.256029	-3.774726	1.745566
6	2.790698	-1.828608	-0.396959
6	2.383861	-3.598584	1.370602
1	2.378082	-4.623589	0.977246
6	3.302053	-2.708384	0.564124
6	3.605507	-0.95616	-1.122628
6	4.696082	-2.690229	0.763048
1	3.153779	-0.297995	-1.851396
6	4.976118	-0.931827	-0.864212
6	5.533513	-1.817692	0.068349
8	5.180327	-3.56568	1.694132
1	6.136906	-3.447611	1.778132
1	0.712948	-3.658253	-0.708239
1	0.696991	4.4932	2.004134
1	0.831989	2.841859	2.585619
1	-1.496448	3.158717	2.154703
1	4.84971	3.517721	-0.352559
1	1.612493	1.656766	-2.515626
1	6.602659	-1.79856	0.256051
1	2.724012	-3.664936	2.408288
1	-1.387948	-4.327579	-0.544686
1	-0.251306	-0.335517	-0.0285
8	0.818407	-1.880478	2.158809
1	1.54594	-1.278679	1.94319
8	5.819198	-0.068092	-1.494869
1	5.30538	0.616577	-1.965158
1	-6.536795	1.870519	0.189636
8	-7.713003	0.946894	0.796216
1	-8.214045	0.707188	-0.003154