

Electronic Supporting Information

Theoretical Studies on the Antioxidant Activity of Viniferifuran

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1. Thermal energies of all stationary points.

Table S1.

Structures	E_{ele}	E_0	E	H	G	$E_{\text{ele}}(\text{gas})$	$E_{\text{ele}}(\text{benzene})$	$E_{\text{ele}}(\text{methanol})$	$E_{\text{ele}}(\text{water})$
H•	-0.49813	-0.49813	-0.49672	-0.49577	-0.50879	-0.49820	-0.49790	-0.49800	-0.49608
resveratrol	-766.26057	-766.03170	-766.01680	-766.01586	-766.07489	-766.27536	-766.29781	-766.31180	-766.30555
viniferifuran	-1530.15526	-1529.73770	-1529.70945	-1529.70851	-1529.79688	-1530.18238	-1530.21836	-1530.23694	-1530.22730
RES•+	-765.99435	-765.76480	-765.75011	-765.74917	-765.80799	-766.00588	-766.06591	-766.10627	-766.10062
RES-12-O•	-765.61761	-765.40197	-765.38729	-765.38634	-765.44603	-765.63245	-765.65644	-765.66959	-765.66416
RES-12O•	-765.70854	-765.49360	-765.47897	-765.47803	-765.53652	-765.73038	-765.78683	-765.83367	-765.83002
VIN•+	-1529.90988	-1529.49235	-1529.46379	-1529.46285	-1529.55517	-1529.93368	-1530.00111	-1530.04028	-1530.03045
VIN-5O•	-1529.51414	-1529.10980	-1529.08176	-1529.08081	-1529.16955	-1529.54136	-1529.57872	-1529.59678	-1529.58783
VIN-12O•	-1529.51150	-1529.10754	-1529.07920	-1529.07826	-1529.16939	-1529.53883	-1529.57722	-1529.59593	-1529.58671
VIN-3'O•	-1529.50039	-1529.09677	-1529.06843	-1529.06749	-1529.15795	-1529.52759	-1529.56560	-1529.58395	-1529.57468
VIN-5'O•	-1529.50358	-1529.09970	-1529.07169	-1529.07074	-1529.15941	-1529.53074	-1529.56797	-1529.58520	-1529.57634
VIN-12'O•	-1529.51121	-1529.10685	-1529.07889	-1529.07795	-1529.16639	-1529.53836	-1529.57552	-1529.59330	-1529.58432
VIN-5O•	-1529.60094	-1529.19742	-1529.16933	-1529.16839	-1529.25667	-1529.63521	-1529.70432	-1529.75797	-1529.75114
VIN-12O•	-1529.60985	-1529.20603	-1529.17813	-1529.17719	-1529.26504	-1529.64312	-1529.70947	-1529.75662	-1529.74960
VIN-3'O•	-1529.60522	-1529.20163	-1529.17345	-1529.17251	-1529.26125	-1529.63951	-1529.70592	-1529.75726	-1529.75016
VIN-5'O•	-1529.60235	-1529.19924	-1529.17074	-1529.16979	-1529.26022	-1529.63800	-1529.70666	-1529.75947	-1529.75244
VIN-12'O•	-1529.60797	-1529.20417	-1529.17606	-1529.17511	-1529.26392	-1529.64131	-1529.70888	-1529.75869	-1529.75147

Notes) E_{ele} : Electronic energy, $E_0 = E_{\text{ele}} + \text{Zero-point correction}$, $E = E_{\text{ele}} + \text{thermal correction to Energy}$, $H = E_{\text{ele}} + \text{thermal correction to Enthalpy}$, $G = E_{\text{ele}} + \text{thermal correction to Gibbs Free Energy}$, which are at M06-2X/6-311G(d,p) theoretical level. $E_{\text{ele}}(\text{gas})$, $E_{\text{ele}}(\text{benzene})$, $E_{\text{ele}}(\text{methanol})$, $E_{\text{ele}}(\text{water})$ are electronic energies from single point calculations in the corresponding medium at M06-2X/6-311++G(d,p) theoretical level.

Table S2.

Structures	E _{ele}	E ₀	E	H	G	E _{ele} (gas)	E _{ele} (benzene)	E _{ele} (methanol)	E _{ele} (water)
•OH	-75.72061	-75.71198	-75.70962	-75.70868	-75.72890	-75.72660	-75.73018	-75.73416	-75.73600
H ₂ O	-76.41234	-76.39069	-76.38785	-76.38691	-76.40832	-76.42088	-76.42534	-76.43479	-76.43477
TS(RES-12OH•OH)	-841.98454	-841.74850	-841.73127	-841.73033	-841.79606	-842.00428	-842.02780	-842.05823	-842.05408
TS(VIN-5OH•OH)	-1605.88070	-1605.45603	-1605.42566	-1605.42472	-1605.52003	-1605.91212	-1605.95226	-1605.98919	-1605.98130
TS(VIN-12OH•OH)	-1605.87909	-1605.45475	-1605.42388	-1605.42293	-1605.51953	-1605.91100	-1605.94884	-1605.98154	-1605.97463
TS(VIN-3'OH•OH)	-1605.87517	-1605.45135	-1605.42047	-1605.41953	-1605.51672	-1605.90718	-1605.94543	-1605.98096	-1605.97355
TS(VIN-5'OH•OH)	-1605.87652	-1605.45246	-1605.42192	-1605.42097	-1605.51618	-1605.90731	-1605.93211	-1605.98021	-1605.97369
TS(VIN-12'OH•OH)	-1605.87890	-1605.45463	-1605.42385	-1605.42291	-1605.51870	-1605.91117	-1605.94813	-1605.98655	-1605.97922
VIN-C1•OH	-1605.91468	-1605.48368	-1605.45359	-1605.45264	-1605.54647	-1605.94542	-1605.98208	-1606.00519	-1605.99691
VIN-C2•OH	-1605.90066	-1605.46947	-1605.43939	-1605.43844	-1605.53232	-1605.93163	-1605.96816	-1605.99195	-1605.98301
VIN-C3•OH	-1605.90833	-1605.47734	-1605.44737	-1605.44642	-1605.53892	-1605.94040	-1605.97803	-1606.00422	-1605.99587
VIN-C4•OH	-1605.92429	-1605.49228	-1605.46186	-1605.46091	-1605.55745	-1605.95644	-1605.99561	-1606.02015	-1606.01095
VIN-C5•OH	-1605.92045	-1605.48900	-1605.45899	-1605.45805	-1605.55192	-1605.95194	-1605.98962	-1606.01350	-1606.00461
VIN-C6•OH	-1605.92895	-1605.49630	-1605.46644	-1605.46549	-1605.55952	-1605.95867	-1605.99556	-1606.01510	-1606.00532
VIN-C7•OH	-1605.94559	-1605.51360	-1605.48359	-1605.48265	-1605.57541	-1605.97646	-1606.01282	-1606.03570	-1606.02707
VIN-C8•OH	-1605.94263	-1605.50995	-1605.48040	-1605.47946	-1605.57107	-1605.97253	-1606.00871	-1606.03228	-1606.02344
VIN-C9•OH	-1605.91234	-1605.48085	-1605.45105	-1605.45010	-1605.54197	-1605.94285	-1605.97922	-1606.00239	-1605.99340
VIN-C10•OH	-1605.90964	-1605.47928	-1605.44867	-1605.44773	-1605.54299	-1605.94176	-1605.98006	-1606.00549	-1605.99662
VIN-C11•OH	-1605.91158	-1605.47973	-1605.44976	-1605.44882	-1605.54197	-1605.94318	-1605.98035	-1606.00449	-1605.99576
VIN-C12•OH	-1605.92811	-1605.49622	-1605.46666	-1605.46572	-1605.55695	-1605.95791	-1605.99415	-1606.01573	-1606.00662
VIN-C13•OH	-1605.90743	-1605.47605	-1605.44605	-1605.44510	-1605.53749	-1605.93880	-1605.97552	-1605.99965	-1605.99113
VIN-C14•OH	-1605.93064	-1605.49762	-1605.46823	-1605.46728	-1605.55815	-1605.96003	-1605.99636	-1606.01581	-1606.00620
VIN-C1'•OH	-1605.89958	-1605.46868	-1605.43866	-1605.43772	-1605.53149	-1605.92997	-1605.96623	-1605.98864	-1605.97972
VIN-C2'•OH	-1605.92020	-1605.48824	-1605.45798	-1605.45703	-1605.55165	-1605.95057	-1605.98757	-1606.00851	-1605.99930

VIN-C3'-•OH	-1605.90897	-1605.47879	-1605.44834	-1605.44739	-1605.54298	-1605.94049	-1605.97852	-1606.00426	-1605.99462
VIN-C4'-•OH	-1605.91983	-1605.48720	-1605.45732	-1605.45637	-1605.54904	-1605.94981	-1605.98663	-1606.01071	-1606.00184
VIN-C5'-•OH	-1605.91341	-1605.48280	-1605.45272	-1605.45178	-1605.54506	-1605.94426	-1605.98108	-1606.00485	-1605.99645
VIN-C6'-•OH	-1605.91243	-1605.48093	-1605.45044	-1605.44950	-1605.54442	-1605.94314	-1605.98012	-1606.00527	-1605.99631
VIN-C7'-•OH	-1605.93178	-1605.50054	-1605.47036	-1605.46941	-1605.56334	-1605.96155	-1605.99844	-1606.02371	-1606.01436
VIN-C8'-•OH	-1605.94153	-1605.50947	-1605.47970	-1605.47876	-1605.57163	-1605.97157	-1606.00873	-1606.03250	-1606.02379
VIN-C9'-•OH	-1605.90122	-1605.47039	-1605.44026	-1605.43931	-1605.53244	-1605.93223	-1605.96864	-1605.99270	-1605.98378
VIN-C10'-•OH	-1605.90878	-1605.47821	-1605.44773	-1605.44679	-1605.54139	-1605.94108	-1605.97856	-1606.00392	-1605.99517
VIN-C11'-•OH	-1605.91054	-1605.47875	-1605.44873	-1605.44779	-1605.54096	-1605.94216	-1605.97976	-1606.00447	-1605.99570
VIN-C12'-•OH	-1605.92176	-1605.49055	-1605.46058	-1605.45963	-1605.55254	-1605.95352	-1605.99025	-1606.01329	-1606.00452
VIN-C13'-•OH	-1605.91608	-1605.48369	-1605.45408	-1605.45314	-1605.54461	-1605.94559	-1605.98107	-1605.99964	-1605.99058
VIN-C14'-•OH	-1605.91510	-1605.48339	-1605.45347	-1605.45253	-1605.54501	-1605.94661	-1605.98305	-1606.00807	-1605.99906
TS(VIN-C2-•OH)	-1605.87805	-1605.44921	-1605.41871	-1605.41777	-1605.51322	-1605.91143	-1605.94912	-1605.97525	-1605.96645
TS(VIN-C4-•OH)	-1605.88530	-1605.45589	-1605.42564	-1605.42469	-1605.51924	-1605.91860	-1605.95646	-1605.97837	-1605.96941
TS(VIN-C5-•OH)	-1605.88020	-1605.45216	-1605.42159	-1605.42065	-1605.51558	-1605.91332	-1605.95097	-1605.97338	-1605.96458
TS(VIN-C6-•OH)	-1605.89176	-1605.46229	-1605.43216	-1605.43121	-1605.52513	-1605.92228	-1605.95862	-1605.97710	-1605.96801
TS(VIN-C7-•OH)	-1605.88787	-1605.45897	-1605.42878	-1605.42783	-1605.52120	-1605.91903	-1605.95645	-1605.98116	-1605.97299
TS(VIN-C8-•OH)	-1605.88662	-1605.45813	-1605.42768	-1605.42674	-1605.52092	-1605.91809	-1605.95562	-1605.98061	-1605.97239
TS(VIN-C12-•OH)	-1605.88752	-1605.45808	-1605.42838	-1605.42744	-1605.51900	-1605.91804	-1605.95540	-1605.97853	-1605.96964
TS(VIN-C14-•OH)	-1605.89536	-1605.46541	-1605.43574	-1605.43480	-1605.52618	-1605.92560	-1605.96247	-1605.98311	-1605.97424
TS(VIN-C5'-•OH)	-1605.87860	-1605.45046	-1605.42010	-1605.41915	-1605.51221	-1605.90911	-1605.94503	-1605.96910	-1605.96067
TS(VIN-C7'-•OH)	-1605.88523	-1605.45684	-1605.42616	-1605.42522	-1605.52150	-1605.91810	-1605.95592	-1605.98164	-1605.97283
TS(VIN-C8'-•OH)	-1605.88610	-1605.45753	-1605.42710	-1605.42615	-1605.52028	-1605.91791	-1605.95598	-1605.98351	-1605.97513
TS(VIN-C12'-•OH)	-1605.87886	-1605.45081	-1605.42042	-1605.41948	-1605.51351	-1605.91221	-1605.94914	-1605.97203	-1605.96347

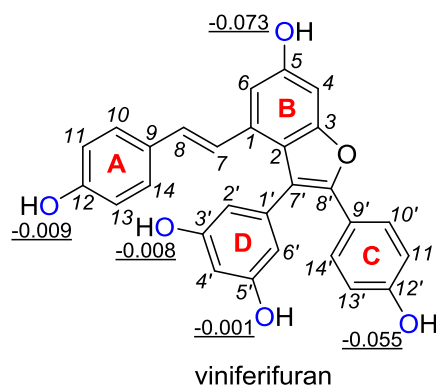
Notes: VIN-C1-•OH means the addition product of viniferifuran and •OH, where new O-H bond formed with C1 at viniferifuran.

Table S3.

Structures	E _{ele}	E ₀	E	H	G	E _{ele} (gas)	E _{ele} (benzene)	E _{ele} (methanol)	E _{ele} (water)
H₂O₂	-151.52765	-151.50038	-151.49716	-151.49621	-151.52198	-151.53531	-151.54128	-151.55215	-151.55103
•OOH	-150.88467	-150.87001	-150.86716	-150.86622	-150.89215	-150.89058	-150.89641	-150.90335	-150.90325
TS(RES-12OH-•OOH)	-917.13399	-916.89368	-916.87568	-916.87473	-916.94357	-917.15420	-917.18032	-917.20102	-917.19530
TS(VIN-5OH-•OOH)	-1681.03043	-1680.60141	-1680.57003	-1680.56909	-1680.66712	-1681.06296	-1681.10257	-1681.12927	-1681.12013
TS(VIN-12OH-•OOH)	-1681.02820	-1680.59925	-1680.56773	-1680.56679	-1680.66580	-1681.06059	-1681.10100	-1681.12721	-1681.11784
TS(VIN-3'OH-•OOH)	-1681.02322	-1680.59501	-1680.56340	-1680.56246	-1680.66281	-1681.05499	-1681.09561	-1681.11500	-1681.10690
TS(VIN-5'OH-•OOH)	-1681.02998	-1680.60178	-1680.57049	-1680.56955	-1680.66596	-1681.06116	-1681.09970	-1681.11300	-1681.10575
TS(VIN-12'OH-•OOH)	-1681.02877	-1680.60001	-1680.56848	-1680.56754	-1680.66684	-1681.06094	-1681.10096	-1681.12671	-1681.11735
VIN-C7-•OOH	-1681.06943	-1680.63348	-1680.60253	-1680.60158	-1680.69629	-1681.10088	-1681.13825	-1681.16251	-1681.15336
VIN-C8-•OOH	-1681.06487	-1680.62931	-1680.59815	-1680.59721	-1680.69343	-1681.09702	-1681.13453	-1681.16006	-1681.15057
VIN-C7'-•OOH	-1681.05297	-1680.61801	-1680.58684	-1680.58590	-1680.68123	-1681.08519	-1681.12299	-1681.15005	-1681.14135
VIN-C8'-•OOH	-1681.06699	-1680.63137	-1680.60048	-1680.59954	-1680.69483	-1681.09899	-1681.13727	-1681.16315	-1681.15380
TS(VIN-C7-•OOH)	-1681.03520	-1680.60131	-1680.57015	-1680.56921	-1680.66482	-1681.06746	-1681.10589	-1681.13260	-1681.12336
TS(VIN-C8-•OOH)	-1681.03217	-1680.59801	-1680.56701	-1680.56606	-1680.66145	-1681.06422	-1681.10268	-1681.12840	-1681.11932
TS(VIN-C7'-•OOH)	-1681.02608	-1680.59283	-1680.56147	-1680.56052	-1680.65678	-1681.05880	-1681.09694	-1681.12517	-1681.11630
TS(VIN-C8'-•OOH)	-1681.03686	-1680.60289	-1680.57186	-1680.57092	-1680.66607	-1681.06864	-1681.10720	-1681.13381	-1681.12435

Notes: VIN-C1-•OOH means the addition product of viniferifuran and •OOH, where new O-H bond formed with C1 at viniferifuran.

2. The 2Pz coefficients of HOMO orbital in viniferifuran.



3. Cartesian coordinates of all computed structures.

Viniferifuran_conf1				H	-1.726555	-3.846358	0.802651
C	1.825931	2.770790	0.047928	C	-1.734376	1.701632	0.570888
C	0.705958	1.953327	0.215359	H	-1.612377	0.864270	1.250627
C	-0.550697	2.557118	0.403721	C	-2.839381	1.778340	-0.175564
C	-0.613928	3.945637	0.384526	H	-2.915520	2.557854	-0.930742
C	0.536531	4.731615	0.206196	C	-3.889875	0.750633	-0.183420
C	1.788651	4.155247	0.038923	C	-4.650831	0.556352	-1.343938
C	2.541276	0.697693	-0.083711	C	-4.100680	-0.125036	0.888389
C	1.198456	0.590343	0.124932	C	-5.559814	-0.486350	-1.450752
H	-1.572494	4.429906	0.545419	H	-4.513906	1.228797	-2.184475
H	2.671598	4.764996	-0.091389	C	-5.011093	-1.164719	0.796138
C	3.339955	-1.553567	-0.798976	H	-3.548784	0.009904	1.811086
C	3.607100	-0.281820	-0.283982	C	-5.737140	-1.358402	-0.378875
C	4.932370	0.054235	0.019954	H	-6.139982	-0.643471	-2.351261
C	5.958119	-0.856456	-0.162346	H	-5.152943	-1.837646	1.635665
C	5.675672	-2.127627	-0.658709	O	6.717051	-2.985191	-0.814760
C	4.363551	-2.471084	-0.980121	H	6.395035	-3.817191	-1.171434
H	2.327885	-1.824851	-1.072327	O	0.475849	6.091550	0.200749
H	5.151406	1.043470	0.401833	H	-0.434491	6.369000	0.329471
H	6.984848	-0.606097	0.072382	O	-6.633073	-2.365062	-0.531226
H	4.144110	-3.453797	-1.385425	H	-6.618938	-2.927477	0.247651
O	2.936482	2.014094	-0.122418	O	0.278731	-3.645239	2.399914
C	0.412687	-0.654727	0.278514	H	1.066752	-3.369949	2.875697
C	0.749690	-1.564220	1.280903	O	-2.562091	-2.317338	-1.087994
C	-0.681677	-0.906555	-0.549921	H	-2.894166	-1.504004	-1.486166
C	-0.010498	-2.721028	1.445542	Viniferifuran_conf2			
H	1.600869	-1.365570	1.924199	C	1.826684	2.765156	0.051637
C	-1.461597	-2.044449	-0.340491	C	0.706443	1.953823	0.218340
H	-0.943244	-0.204375	-1.333225	C	-0.551492	2.564332	0.405807
C	-1.123144	-2.961908	0.648170				

C	-0.614273	3.949153	0.385088	H	1.203636	6.518628	0.093233
C	0.538646	4.732273	0.205026	O	-6.635707	-2.355142	-0.528519
C	1.789855	4.153327	0.041176	H	-6.623674	-2.915638	0.251751
C	2.538986	0.692566	-0.080291	O	0.278306	-3.653789	2.388807
C	1.195539	0.589573	0.127652	H	1.065784	-3.379077	2.865783
H	-1.557770	4.457832	0.540050	O	-2.569103	-2.311649	-1.088329
H	2.690323	4.740686	-0.092285	H	-2.903930	-1.496296	-1.480238
C	3.332977	-1.557324	-0.804152				
C	3.602621	-0.289075	-0.281772	Viniferifuran_conf3			
C	4.928003	0.040382	0.028528	C	1.831573	2.762463	0.055872
C	5.951388	-0.872770	-0.155351	C	0.712385	1.943619	0.223082
C	5.666275	-2.140339	-0.659226	C	-0.544422	2.547561	0.408830
C	4.354000	-2.477495	-0.986490	C	-0.608529	3.936274	0.389995
H	2.320752	-1.823672	-1.081804	C	0.541458	4.722977	0.213996
H	5.149286	1.026464	0.417267	C	1.793674	4.146819	0.047354
H	6.978157	-0.627382	0.084456	C	2.549472	0.689965	-0.075452
H	4.132341	-3.457448	-1.397236	C	1.206685	0.581020	0.133312
O	2.936686	2.009092	-0.118428	H	-1.567820	4.419745	0.548994
C	0.408089	-0.654803	0.279088	H	2.676789	4.756586	-0.081844
C	0.747080	-1.568280	1.277266	C	3.355420	-1.560921	-0.784815
C	-0.687797	-0.903081	-0.548160	C	3.618678	-0.284923	-0.279157
C	-0.012756	-2.725684	1.438652	C	4.944341	0.061452	0.011051
H	1.599419	-1.372257	1.919832	C	5.974434	-0.843049	-0.176238
C	-1.467350	-2.041893	-0.341841	C	5.695886	-2.118450	-0.663441
H	-0.951446	-0.197564	-1.327697	C	4.383428	-2.472088	-0.971291
C	-1.126707	-2.963490	0.642203	H	2.342609	-1.841122	-1.045550
H	-1.730046	-3.848360	0.794513	H	5.160154	1.053333	0.387618
C	-1.735189	1.708651	0.573887	H	7.001278	-0.585287	0.049712
H	-1.612629	0.870346	1.252394	H	4.166879	-3.459167	-1.367328
C	-2.840318	1.787257	-0.171745	O	2.942340	2.007237	-0.115035
H	-2.917764	2.570249	-0.922975	C	0.419527	-0.663394	0.289153
C	-3.890632	0.759249	-0.180460	C	0.751477	-1.570246	1.291193
C	-4.650623	0.564649	-1.341554	C	-0.676528	-0.909215	-0.545715
C	-4.103008	-0.115557	0.891711	C	-0.015924	-2.722751	1.455009
C	-5.560077	-0.477734	-1.448542	H	1.595952	-1.397079	1.945985
H	-4.513071	1.237163	-2.181897	C	-1.462440	-2.038369	-0.338285
C	-5.014079	-1.154756	0.799361	H	-0.931185	-0.205901	-1.330188
H	-3.552430	0.020495	1.815029	C	-1.128458	-2.956924	0.655474
C	-5.739068	-1.348810	-0.376191	H	-1.755895	-3.830831	0.792655
H	-6.139825	-0.634830	-2.349333	C	-1.730740	1.694446	0.570422
H	-5.157676	-1.826638	1.639452	H	-1.616055	0.857605	1.252285
O	6.705316	-3.000677	-0.816358	C	-2.830803	1.776320	-0.182706
H	6.381400	-3.830130	-1.177230	H	-2.897711	2.555201	-0.939349
O	0.356982	6.081118	0.212709	C	-3.887926	0.755441	-0.195157

C	-4.636924	0.557428	-1.362919
C	-4.119737	-0.107958	0.882010
C	-5.555456	-0.476763	-1.470743
H	-4.483666	1.220869	-2.207774
C	-5.040538	-1.138819	0.788741
H	-3.577731	0.031751	1.809882
C	-5.755711	-1.335510	-0.392246
H	-6.127399	-0.635745	-2.376182
H	-5.202273	-1.800032	1.634091
O	6.741527	-2.970072	-0.825170
H	6.419132	-3.810609	-1.160669
O	0.480203	6.083132	0.209222
H	-0.429991	6.359830	0.340353
O	-6.662898	-2.332641	-0.544807
H	-6.677564	-2.876498	0.247019
O	0.356907	-3.580971	2.441330
H	-0.242237	-4.331692	2.451601
O	-2.565789	-2.311772	-1.082257
H	-2.897404	-1.498662	-1.481534

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C	1.832630	2.756640	0.059705
C	0.713078	1.943982	0.225734
C	-0.545022	2.554674	0.410344
C	-0.608584	3.939697	0.390233
C	0.543978	4.723497	0.212978
C	1.795269	4.144709	0.049933
C	2.547349	0.684622	-0.072398
C	1.203945	0.580101	0.135581
H	-1.552771	4.447605	0.543514
H	2.695943	4.732073	-0.082207
C	3.348443	-1.565051	-0.790131
C	3.614330	-0.292471	-0.277205
C	4.940211	0.047300	0.019440
C	5.967906	-0.859749	-0.169273
C	5.686564	-2.131639	-0.663875
C	4.373856	-2.478961	-0.977643
H	2.335397	-1.840318	-1.055245
H	5.158373	1.036085	0.402793
H	6.994860	-0.606978	0.061822
H	4.154987	-3.463342	-1.379085
O	2.942840	2.001997	-0.110900
C	0.414951	-0.663519	0.289315
C	0.748589	-1.574032	1.287518

C	-0.682650	-0.905714	-0.544361
C	-0.018933	-2.726750	1.448672
H	1.594222	-1.403426	1.941482
C	-1.468617	-2.035381	-0.339515
H	-0.939128	-0.199181	-1.325276
C	-1.132837	-2.957707	0.650162
H	-1.760557	-3.831694	0.785550
C	-1.731373	1.701392	0.572705
H	-1.616157	0.863541	1.253270
C	-2.831668	1.785291	-0.179420
H	-2.900109	2.567795	-0.931976
C	-3.888649	0.764153	-0.192495
C	-4.636666	0.565561	-1.360787
C	-4.122095	-0.098098	0.885217
C	-5.555668	-0.468334	-1.468594
H	-4.482773	1.228893	-2.205578
C	-5.043522	-1.128494	0.792028
H	-3.581435	0.042952	1.813667
C	-5.757592	-1.325847	-0.389470
H	-6.127189	-0.627466	-2.374280
H	-5.206977	-1.788477	1.638032
O	6.729851	-2.986106	-0.826562
H	6.405363	-3.824363	-1.165741
O	0.361983	6.072532	0.221474
H	1.209333	6.509973	0.106902
O	-6.665375	-2.322755	-0.541861
H	-6.682931	-2.863802	0.251807
O	0.355345	-3.588699	2.431306
H	-0.245505	-4.338058	2.441258
O	-2.573206	-2.305765	-1.082423
H	-2.907792	-1.490664	-1.475358

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C	1.658945	2.865794	0.064624
C	0.604886	1.932315	0.216408
C	-0.732941	2.416199	0.413392
C	-0.916635	3.768745	0.434669
C	0.168680	4.739426	0.268422
C	1.513147	4.218422	0.081491
C	2.553805	0.868230	-0.094765
C	1.204537	0.645156	0.118620
H	-1.900226	4.190812	0.604718
H	2.338048	4.907395	-0.037975
C	3.519839	-1.322328	-0.792884

C	3.685958	-0.020278	-0.304810	C	1.527970	2.716298	-0.180254
C	4.985727	0.441851	-0.047150	C	0.543761	1.726857	0.054158
C	6.082204	-0.375208	-0.243492	C	-0.800974	2.121465	0.182805
C	5.901422	-1.676167	-0.714209	C	-1.084893	3.478532	0.065779
C	4.616755	-2.143328	-0.993498	C	-0.056603	4.459325	-0.104814
H	2.531350	-1.691308	-1.034721	C	1.283920	4.062335	-0.267895
H	5.124779	1.453396	0.312548	C	2.567517	0.782227	-0.188249
H	7.088195	-0.030236	-0.042144	C	1.254137	0.470691	0.042126
H	4.477217	-3.147803	-1.379639	H	-2.113323	3.818281	0.072420
O	2.835066	2.197761	-0.116192	H	2.063911	4.797123	-0.408007
C	0.572424	-0.683603	0.284956	C	3.719537	-1.355873	-0.752897
C	1.019298	-1.517733	1.309202	C	3.774351	-0.020214	-0.338270
C	-0.447951	-1.103549	-0.567260	C	5.028596	0.557696	-0.094728
C	0.450029	-2.780233	1.467183	C	6.189968	-0.178925	-0.233782
H	1.813474	-1.184245	1.969094	C	6.120179	-1.514234	-0.630269
C	-1.029327	-2.358013	-0.373155	C	4.880827	-2.097409	-0.894641
H	-0.799136	-0.451930	-1.360000	H	2.766120	-1.814720	-0.982173
C	-0.577575	-3.204356	0.632502	H	5.082198	1.596097	0.206714
H	-1.031492	-4.176053	0.774201	H	7.162455	0.256670	-0.043523
C	-1.842451	1.458507	0.544108	H	4.826616	-3.130085	-1.223771
H	-1.658011	0.594458	1.173670	O	2.746575	2.136957	-0.309856
C	-2.991464	1.570972	-0.129441	C	0.720362	-0.887163	0.291937
H	-3.129997	2.439786	-0.769663	C	1.225483	-1.629754	1.358438
C	-4.075589	0.581429	-0.159264	C	-0.269250	-1.426933	-0.529874
C	-5.275090	0.891492	-0.813546	C	0.747234	-2.918710	1.589280
C	-3.946057	-0.700143	0.388510	H	1.994906	-1.204511	1.994459
C	-6.308645	-0.024553	-0.910400	C	-0.760944	-2.705547	-0.262613
H	-5.396490	1.875770	-1.253038	H	-0.666940	-0.847141	-1.356117
C	-4.968320	-1.631441	0.286863	C	-0.249723	-3.460562	0.786487
H	-3.031825	-0.988984	0.894600	H	-0.633966	-4.452070	0.985223
C	-6.157098	-1.295803	-0.360549	C	-1.862225	1.117142	0.348261
H	-7.236875	0.218322	-1.411825	H	-1.624799	0.283006	0.998876
H	-4.835637	-2.625867	0.701181	C	-3.027593	1.144752	-0.306569
O	7.008998	-2.435088	-0.886920	H	-3.234432	1.984832	-0.966261
H	6.760287	-3.300378	-1.223405	C	-4.048469	0.089996	-0.288227
O	-0.054285	5.954548	0.293051	C	-5.276115	0.305329	-0.927697
O	-7.191280	-2.164808	-0.492662	C	-3.829169	-1.165370	0.291285
H	-6.966367	-2.997474	-0.069139	C	-6.250739	-0.676757	-0.981198
O	0.850635	-3.639179	2.437783	H	-5.467542	1.267647	-1.390241
H	1.550939	-3.232466	2.955112	C	-4.791456	-2.162008	0.233394
O	-2.055972	-2.807705	-1.139197	H	-2.891882	-1.381031	0.791589
H	-2.454601	-2.068244	-1.609615	C	-6.009591	-1.920284	-0.401204
				H	-7.200942	-0.506808	-1.471383
				H	-4.588363	-3.133868	0.672188

TS(VIN-5OH-•OH)

O	7.287640	-2.191304	-0.748691	C	-1.896612	1.321878	0.414486
H	7.112148	-3.090381	-1.039391	H	-1.625470	0.375077	0.863357
O	-0.349972	5.741030	-0.098230	C	-3.154039	1.497247	-0.053058
H	-1.191008	5.811651	0.511877	H	-3.410463	2.445388	-0.519669
O	-6.988499	-2.856594	-0.491342	C	-4.185025	0.494292	-0.063030
H	-6.704506	-3.660404	-0.048039	C	-5.475911	0.839075	-0.556397
O	1.210123	-3.691299	2.604447	C	-3.953760	-0.856140	0.342639
H	1.883761	-3.208209	3.090443	C	-6.478450	-0.077796	-0.636636
O	-1.756361	-3.267878	-0.995964	H	-5.647666	1.863850	-0.869598
H	-2.191618	-2.589143	-1.522185	C	-4.932787	-1.794391	0.255910
O	-2.181567	5.450113	1.497778	H	-2.976571	-1.145415	0.712459
H	-1.722922	5.157433	2.297558	C	-6.267739	-1.463934	-0.235628
VIN-12O•				H	-7.464695	0.177795	-1.004771
C	1.525609	2.824840	0.040749	H	-4.758913	-2.824960	0.541302
C	0.516575	1.860794	0.151481	O	7.179163	-2.203271	-0.660487
C	-0.815882	2.295315	0.300841	H	6.990609	-3.069404	-1.031458
C	-1.050112	3.672600	0.317601	O	-0.234598	5.941241	0.237157
C	-0.009523	4.600784	0.202840	H	-1.174939	6.106600	0.341498
C	1.312300	4.189998	0.061103	O	-7.162222	-2.308285	-0.312605
C	2.519188	0.872493	-0.087798	O	0.790834	-3.734429	2.325696
C	1.195323	0.582036	0.065662	H	1.459774	-3.323943	2.880194
H	-2.061941	4.034333	0.471236	O	-1.900135	-2.924871	-1.418009
H	2.115047	4.909352	-0.020569	H	-2.199218	-2.215234	-1.993777
C	3.641717	-1.245331	-0.776526	TS(VIN-12OH•-OH)			
C	3.713658	0.047105	-0.248513	C	2.141006	2.755695	0.126639
C	4.967990	0.557752	0.109549	C	1.026717	1.913524	0.209219
C	6.113740	-0.203942	-0.033451	C	-0.246159	2.496009	0.360947
C	6.026294	-1.497861	-0.544638	C	-0.318998	3.886604	0.411271
C	4.786621	-2.013672	-0.919625	C	0.824355	4.692775	0.322324
H	2.688289	-1.650459	-1.091707	C	2.089041	4.137196	0.178345
H	5.036107	1.564213	0.502886	C	2.902662	0.704847	-0.048467
H	7.086853	0.181024	0.243438	C	1.554014	0.565078	0.096328
H	4.718818	-3.013791	-1.335609	H	-1.286282	4.355663	0.563808
O	2.733045	2.228315	-0.096623	H	2.970993	4.759016	0.116551
C	0.601968	-0.768410	0.179981	C	3.784624	-1.492784	-0.832728
C	0.997238	-1.603581	1.222415	C	3.995909	-0.247344	-0.234373
C	-0.357052	-1.200415	-0.737943	C	5.293479	0.092132	0.168737
C	0.436131	-2.875867	1.337762	C	6.345215	-0.791461	0.002426
H	1.743034	-1.261705	1.932431	C	6.117391	-2.037887	-0.577983
C	-0.930477	-2.463828	-0.588770	C	4.834094	-2.383340	-0.998774
H	-0.664934	-0.547635	-1.548690	H	2.796424	-1.764430	-1.182683
C	-0.533775	-3.308873	0.441802	H	5.470353	1.062435	0.615653
H	-0.981664	-4.287716	0.549168	H	7.350776	-0.538632	0.313585

H	4.658139	-3.345734	-1.468755	C	1.156187	4.212790	0.043137
O	3.272510	2.026752	-0.022512	C	2.495085	0.954607	-0.125017
C	0.816696	-0.714211	0.183570	C	1.183183	0.602612	-0.001939
C	1.175180	-1.642816	1.159784	H	-2.207834	3.926529	0.417566
C	-0.228322	-0.997627	-0.697264	H	1.937808	4.956926	-0.013976
C	0.495423	-2.857115	1.241865	C	3.741315	-1.071564	-0.879796
H	1.987704	-1.417820	1.842827	C	3.727378	0.178728	-0.254975
C	-0.920096	-2.203677	-0.578309	C	4.932264	0.695838	0.238389
H	-0.509627	-0.275713	-1.457028	C	6.109829	-0.022542	0.135662
C	-0.558639	-3.141603	0.381826	C	6.105796	-1.278684	-0.470091
H	-1.099175	-4.074787	0.466332	C	4.917973	-1.798819	-0.981395
C	-1.447657	1.656072	0.435881	H	2.831423	-1.472010	-1.309892
H	-1.338020	0.724167	0.978735	H	4.935040	1.673445	0.704298
C	-2.602864	1.937999	-0.180460	H	7.045451	0.367791	0.515335
H	-2.680535	2.867161	-0.741239	H	4.916659	-2.765272	-1.475133
C	-3.773464	1.060885	-0.246644	O	2.648462	2.313532	-0.119053
C	-4.961508	1.539964	-0.816048	C	0.703168	-0.790337	0.114156
C	-3.745923	-0.274720	0.192090	C	1.277263	-1.614856	1.107578
C	-6.082452	0.737821	-0.929392	C	-0.264235	-1.314010	-0.710271
H	-5.002142	2.565734	-1.166363	C	0.900908	-2.964676	1.257710
C	-4.845435	-1.097968	0.053356	H	2.032219	-1.191369	1.763270
H	-2.845869	-0.683406	0.637072	C	-0.714832	-2.687717	-0.553198
C	-6.027448	-0.596344	-0.512830	H	-0.730931	-0.721560	-1.489271
H	-7.006324	1.107564	-1.356044	C	-0.072712	-3.500298	0.454168
H	-4.813384	-2.126009	0.394210	H	-0.390368	-4.528308	0.569669
O	7.181966	-2.869200	-0.714015	C	-1.997397	1.243128	0.282789
H	6.899865	-3.684425	-1.137156	H	-1.744580	0.279117	0.710250
O	0.748899	6.050010	0.385673	C	-3.246675	1.447963	-0.153294
H	-0.168749	6.312966	0.490959	H	-3.510843	2.417028	-0.571370
O	-7.105335	-1.362790	-0.718807	C	-4.316634	0.442248	-0.145050
H	-7.091560	-2.203912	-0.138246	C	-5.658423	0.834486	-0.067185
O	0.811740	-3.800880	2.164888	C	-4.038212	-0.923144	-0.251246
H	1.546492	-3.487472	2.698968	C	-6.682276	-0.097764	-0.053298
O	-1.974477	-2.517097	-1.375677	H	-5.900969	1.890146	-0.005363
H	-2.262310	-1.732157	-1.851986	C	-5.053545	-1.866082	-0.249296
O	-7.328647	-2.775956	1.127633	H	-3.019299	-1.261495	-0.388205
H	-8.251067	-2.613147	1.375315	C	-6.380930	-1.456049	-0.140593
VIN-3'O•				H	-7.720728	0.200449	0.016308
C	1.410899	2.854841	0.000489	H	-4.807942	-2.918009	-0.358673
C	0.437374	1.849514	0.074152	O	7.286891	-1.941814	-0.539263
C	-0.913631	2.233633	0.209044	H	7.161178	-2.778447	-0.994984
C	-1.183962	3.600608	0.265480	O	-0.458690	5.899933	0.242344
C	-0.177813	4.570855	0.179489	H	-1.407480	6.021171	0.329410
				O	-7.420763	-2.330892	-0.133576

H	-7.081329	-3.226185	-0.213979	H	5.586213	2.042668	0.673724
O	1.473082	-3.754061	2.200596	C	4.983068	-1.565158	-0.538623
H	2.144521	-3.259333	2.677989	H	2.932912	-1.020586	-0.727742
O	-1.637239	-3.139505	-1.255654	C	6.267804	-1.155457	-0.184060
TS(VIN-3'OH--OH)				H	7.484011	0.448371	0.530361
C	-1.656275	2.898556	0.009340	H	4.805671	-2.589160	-0.852472
C	-0.633458	1.956980	-0.147135	O	-7.235801	-2.252152	0.411649
C	0.691705	2.413428	-0.282562	H	-7.039719	-3.117260	0.780812
C	0.902872	3.789603	-0.230992	O	0.066200	6.042041	-0.017902
C	-0.150210	4.698887	-0.057187	H	1.006521	6.214344	-0.109650
C	-1.464620	4.267676	0.062321	O	7.341867	-1.987023	-0.231591
C	-2.624263	0.929216	0.031304	H	7.060240	-2.851563	-0.541769
C	-1.296836	0.665913	-0.131442	O	-0.977484	-3.595537	-2.513019
H	1.909534	4.170671	-0.373068	H	-1.661735	-3.166524	-3.033854
H	-2.277604	4.969652	0.182310	O	1.861152	-2.848627	1.130196
C	-3.724567	-1.220193	0.656565	H	1.921408	-2.350462	2.049614
C	-3.806782	0.077872	0.144957	O	1.444496	-2.232576	3.293260
C	-5.059960	0.567828	-0.243957	H	1.558996	-3.091640	3.725544
C	-6.193481	-0.219804	-0.148957	VIN-5'O•			
C	-6.094444	-1.519855	0.343764	C	1.850711	2.739545	0.033513
C	-4.856827	-2.015371	0.750297	C	0.731985	1.921615	0.204580
H	-2.773345	-1.606917	1.000784	C	-0.525208	2.523360	0.390400
H	-5.136251	1.579523	-0.622449	C	-0.591573	3.911673	0.362755
H	-7.165642	0.149611	-0.449567	C	0.557438	4.698763	0.179601
H	-4.781283	-3.019749	1.154784	C	1.810864	4.123327	0.016064
O	-2.857434	2.278793	0.109745	C	2.572277	0.666348	-0.079656
C	-0.692798	-0.672366	-0.299857	C	1.228299	0.559985	0.125377
C	-1.123688	-1.489045	-1.351080	H	-1.550597	4.395146	0.522736
C	0.297116	-1.120772	0.567224	H	2.692962	4.734032	-0.115460
C	-0.583136	-2.762902	-1.515957	C	3.392794	-1.586951	-0.767983
H	-1.890492	-1.125627	-2.027850	C	3.644353	-0.310253	-0.258836
C	0.846131	-2.397963	0.379905	C	4.962225	0.034702	0.066782
H	0.636409	-0.504400	1.391514	C	5.994317	-0.872969	-0.088324
C	0.393071	-3.230429	-0.645529	C	5.726379	-2.150587	-0.577019
H	0.813925	-4.219218	-0.769703	C	4.422338	-2.502190	-0.921748
C	1.801589	1.470001	-0.475957	H	2.388529	-1.866555	-1.060006
H	1.579394	0.595358	-1.077676	H	5.169858	1.026988	0.446850
C	3.015709	1.607937	0.068436	H	7.014940	-0.617271	0.166093
H	3.216212	2.483666	0.682520	H	4.213933	-3.490268	-1.319109
C	4.119054	0.646330	-0.042782	O	2.962343	1.982285	-0.128780
C	5.414362	1.029785	0.325128	C	0.436825	-0.679152	0.287857
C	3.925794	-0.672561	-0.468108	C	0.741864	-1.596127	1.265835
C	6.481514	0.150180	0.250797	C	-0.674254	-0.913961	-0.554517

C	-0.058977	-2.795234	1.444763	C	5.758258	-0.623889	-0.183020
H	1.583827	-1.456157	1.933306	C	5.505557	-1.784459	-0.913376
C	-1.515349	-2.033685	-0.370141	C	4.226503	-2.025928	-1.415625
H	-0.894946	-0.209927	-1.349585	H	2.216993	-1.299480	-1.578967
C	-1.215450	-2.963496	0.591951	H	4.930171	1.177392	0.623251
H	-1.840972	-3.835002	0.735953	H	6.759004	-0.456339	0.193702
C	-1.708591	1.668595	0.569028	H	4.034879	-2.914354	-2.009447
H	-1.591836	0.847200	1.269902	O	2.693209	2.314054	-0.169624
C	-2.817217	1.742129	-0.173488	C	0.359511	-0.504452	0.229846
H	-2.889698	2.513936	-0.936991	C	0.782501	-1.376804	1.258557
C	-3.885271	0.733062	-0.158792	C	-0.725776	-0.854059	-0.548235
C	-4.671226	0.550531	-1.305278	C	0.180531	-2.678016	1.378595
C	-4.095930	-0.132827	0.921365	H	1.378657	-0.987236	2.070785
C	-5.602149	-0.474062	-1.391793	C	-1.425432	-2.065062	-0.298250
H	-4.537431	1.218432	-2.149973	H	-1.087515	-0.181012	-1.317943
C	-5.027268	-1.155447	0.848513	C	-0.970624	-2.976967	0.632930
H	-3.529667	-0.002639	1.836107	H	-1.465796	-3.930055	0.758361
C	-5.777393	-1.339198	-0.313422	C	-1.942248	1.732776	0.562325
H	-6.201750	-0.622464	-2.280880	H	-1.783111	0.917486	1.262020
H	-5.170412	-1.819672	1.694676	C	-3.029541	1.719953	-0.212777
O	6.773260	-3.003942	-0.703673	H	-3.139278	2.478332	-0.985076
H	6.459564	-3.850848	-1.031752	C	-4.009423	0.623530	-0.218700
O	0.495409	6.057672	0.165894	C	-4.696765	0.321671	-1.402280
H	-0.413469	6.337037	0.300992	C	-4.221553	-0.206100	0.888633
O	-6.694485	-2.327120	-0.447136	C	-5.534377	-0.781013	-1.494038
H	-6.688908	-2.881913	0.337482	H	-4.560960	0.958585	-2.270307
O	0.227026	-3.628259	2.321180	C	-5.062200	-1.304601	0.811283
O	-2.601522	-2.235116	-1.159849	H	-3.730752	0.016452	1.828828
H	-2.951045	-1.389191	-1.465747	C	-5.714620	-1.604864	-0.384454
TS(VIN-5'OH--OH)				H	-6.059065	-1.020384	-2.410378
C	1.546519	3.009259	0.035746	H	-5.209506	-1.937332	1.680519
C	0.471463	2.132406	0.199555	O	6.543314	-2.633869	-1.113670
C	-0.813192	2.663087	0.407060	H	6.244898	-3.394888	-1.618671
C	-0.952279	4.045404	0.414561	O	0.021938	6.248771	0.265160
C	0.154602	4.894688	0.244966	H	-0.898785	6.476377	0.416052
C	1.434384	4.389556	0.056344	O	-6.540361	-2.670222	-0.524099
C	2.363026	0.982562	-0.156917	H	-6.540132	-3.187076	0.286019
C	1.033586	0.800771	0.075213	O	0.736080	-3.554984	2.160556
H	-1.934748	4.474631	0.586586	H	1.777856	-3.219811	2.113884
H	2.281618	5.048784	-0.070158	O	-2.525573	-2.384058	-1.006676
C	3.205944	-1.114988	-1.175716	H	-2.894046	-1.598570	-1.431045
C	3.444649	0.038820	-0.427418	O	2.814770	-2.465629	1.709502
C	4.736546	0.277999	0.051788	H	3.099285	-2.641703	0.803217

VIN-12'O•

C	1.954313	2.681376	0.064496
C	0.808253	1.892845	0.221628
C	-0.436496	2.529078	0.418062
C	-0.457983	3.915528	0.413579
C	0.717909	4.671571	0.243950
C	1.955605	4.064944	0.070805
C	2.614627	0.588894	-0.098076
C	1.252158	0.526680	0.112637
H	-1.401247	4.427191	0.578610
H	2.854370	4.652638	-0.050892
C	3.300482	-1.743642	-0.663633
C	3.628862	-0.401276	-0.310634
C	5.000070	-0.030930	-0.199568
C	5.989184	-0.947446	-0.382030
C	5.690016	-2.335059	-0.713451
C	4.277819	-2.669178	-0.857461
H	2.262632	-2.016470	-0.802568
H	5.238431	0.996007	0.046007
H	7.035829	-0.684953	-0.285915
H	4.046599	-3.688561	-1.141946
O	3.041524	1.899401	-0.111210
C	0.415699	-0.681685	0.280705
C	0.683178	-1.556197	1.334035
C	-0.664921	-0.915526	-0.569123
C	-0.136316	-2.667794	1.527417
H	1.523974	-1.367363	1.993498
C	-1.501072	-2.008541	-0.334895
H	-0.872198	-0.235024	-1.387020
C	-1.233974	-2.892578	0.704660
H	-1.880273	-3.742825	0.876887
C	-1.644828	1.707223	0.574126
H	-1.557070	0.867838	1.256602
C	-2.735203	1.818466	-0.189526
H	-2.773393	2.599318	-0.946290
C	-3.819622	0.827872	-0.212761
C	-4.564896	0.655962	-1.386901
C	-4.080021	-0.034270	0.858862
C	-5.506499	-0.355401	-1.506804
H	-4.390443	1.320680	-2.226679
C	-5.024362	-1.041684	0.754068
H	-3.541402	0.086440	1.791441
C	-5.733962	-1.215795	-0.434392
H	-6.075812	-0.496150	-2.416861

H	-5.206778	-1.704164	1.593998
O	6.579358	-3.174880	-0.871430
O	0.693776	6.027419	0.254165
H	-0.207244	6.333244	0.387025
O	-6.660564	-2.190254	-0.600463
H	-6.686161	-2.747956	0.181634
O	0.076756	-3.558575	2.528964
H	0.876125	-3.318928	3.005363
O	-2.589157	-2.267713	-1.101804
H	-2.867605	-1.464752	-1.557312

TS(VIN-12'OH•OH)

C	1.117240	3.170828	0.049773
C	0.140521	2.184726	0.211485
C	-1.198483	2.580089	0.394450
C	-1.481268	3.940058	0.373293
C	-0.469285	4.899892	0.199284
C	0.859845	4.531381	0.038783
C	2.155007	1.238100	-0.078218
C	0.841797	0.919077	0.122696
H	-2.505102	4.266136	0.529998
H	1.634661	5.274430	-0.086911
C	3.303661	-0.879504	-0.730180
C	3.362289	0.445290	-0.268533
C	4.616498	1.013604	-0.003167
C	5.774265	0.276353	-0.162433
C	5.705923	-1.041924	-0.627063
C	4.457850	-1.615408	-0.910353
H	2.346211	-1.325967	-0.966243
H	4.669748	2.039172	0.339060
H	6.748212	0.697773	0.052066
H	4.412906	-2.641304	-1.256023
O	2.334466	2.601396	-0.112663
C	0.257047	-0.431697	0.277724
C	0.717164	-1.269448	1.293654
C	-0.776884	-0.853064	-0.558801
C	0.140245	-2.527370	1.462441
H	1.520351	-0.937915	1.943759
C	-1.377460	-2.094424	-0.344684
H	-1.133063	-0.205430	-1.351722
C	-0.914230	-2.940647	0.656746
H	-1.376262	-3.906219	0.812987
C	-2.232047	1.548406	0.560452
H	-1.981230	0.741836	1.241977

C	-3.333812	1.449078	-0.188216	O	4.226184	2.426633	-0.351717
H	-3.530047	2.205128	-0.945614	H	3.548438	3.091238	-0.499052
C	-4.209962	0.269372	-0.193668	O	4.700024	-2.231914	0.424146
C	-4.931313	-0.045189	-1.353099	H	5.625183	-1.974582	0.449051
C	-4.280224	-0.624908	0.881055	C	0.258330	-0.471722	-0.109178
C	-5.665055	-1.218121	-1.455999	H	-0.035784	-1.508285	-0.250280
H	-4.902587	0.638174	-2.195531	C	-0.687047	0.459613	0.062138
C	-5.016184	-1.794757	0.792912	H	-0.384892	1.479371	0.288446
H	-3.756260	-0.401768	1.802953	C	-2.136784	0.237356	0.022076
C	-5.702688	-2.103853	-0.381253	C	-2.995205	1.193879	0.578772
H	-6.213559	-1.467450	-2.355528	C	-2.716452	-0.896414	-0.556894
H	-5.050416	-2.478956	1.634602	C	-4.369299	1.023854	0.585448
O	6.856031	-1.695567	-0.829358	H	-2.570409	2.087031	1.024490
H	6.712015	-2.702008	-0.882047	C	-4.090443	-1.079312	-0.557474
O	-0.746455	6.231377	0.192725	H	-2.088928	-1.639851	-1.033908
H	-1.689825	6.360868	0.318159	C	-4.923571	-0.120783	0.018339
O	-6.429172	-3.238988	-0.530081	H	-5.030880	1.761609	1.021387
H	-6.328465	-3.789177	0.251183	H	-4.521341	-1.963246	-1.017459
O	0.554640	-3.388627	2.428224	O	-6.276384	-0.244569	0.044784
H	1.305781	-3.007441	2.890463	H	-6.529697	-1.070978	-0.374427
O	-2.415569	-2.538048	-1.098657				
H	-2.856667	-1.789717	-1.517456	RES-12-O•			
O	6.532492	-3.925981	-0.173004	C	-3.877780	-1.139431	-0.000003
H	7.319403	-4.090304	0.367896	C	-2.495780	-1.321287	-0.000062
				C	-1.643505	-0.217152	-0.000074
•OH				C	-2.188957	1.077005	-0.000041
O	-0.000000	-0.000000	0.107936	C	-3.565144	1.241020	0.000003
H	0.000000	0.000000	-0.863486	C	-4.420407	0.137424	0.000022
				H	-2.104558	-2.330835	-0.000082
H ₂ O				H	-1.550636	1.952621	-0.000063
O	-0.000000	0.000000	0.117887	H	-5.491377	0.305184	0.000042
H	-0.000000	0.756241	-0.471547	O	-4.158734	2.461893	0.000034
H	-0.000000	-0.756241	-0.471547	H	-3.484597	3.146418	-0.000168
				O	-4.646878	-2.256616	0.000003
resveratrol				H	-5.575259	-2.008972	0.000188
C	3.933065	-1.132070	0.203674	C	-0.205018	-0.468351	-0.000107
C	2.553806	-1.322160	0.141491	H	0.067700	-1.518710	-0.000315
C	1.708548	-0.236104	-0.073193	C	0.774021	0.466587	0.000098
C	2.258405	1.041293	-0.248824	H	0.495375	1.516218	0.000280
C	3.633469	1.214245	-0.184599	C	2.188362	0.216886	0.000074
C	4.482755	0.132553	0.045335	C	3.076535	1.331240	0.000029
H	2.159371	-2.321579	0.275608	C	2.753374	-1.095232	0.000112
H	1.620169	1.890355	-0.467315	C	4.427431	1.171155	-0.000039
H	5.552732	0.302345	0.083085	H	2.646729	2.327672	0.000030

C	4.097921	-1.282687	0.000055	C	-0.122272	3.525932	0.889138
H	2.097755	-1.957291	0.000217	C	1.166028	4.134314	0.833340
C	5.029071	-0.156949	-0.000052	C	2.318048	3.344419	0.615752
H	5.107372	2.014407	-0.000087	C	2.455180	-0.145241	0.109269
H	4.537850	-2.272742	0.000095	C	1.099274	-0.028710	0.294502
O	6.249726	-0.322193	-0.000066	H	-0.966706	4.175711	1.084620
TS(RES-12OH-•OH)				H	3.298862	3.796703	0.573909
C	4.325352	1.302573	0.158083	C	2.840551	-2.433153	-0.801684
C	2.936534	1.383870	0.072836	C	3.327375	-1.276235	-0.183998
C	2.177882	0.226023	-0.083218	C	4.691773	-1.203456	0.129554
C	2.823350	-1.015172	-0.176183	C	5.540927	-2.259844	-0.142636
C	4.206420	-1.079417	-0.091679	C	5.040046	-3.414218	-0.743814
C	4.969136	0.075499	0.079915	C	3.688075	-3.494280	-1.076559
H	2.466587	2.356880	0.141788	H	1.797422	-2.500306	-1.083601
H	2.254032	-1.922219	-0.346072	H	5.080637	-0.304839	0.591498
H	6.048251	-0.010984	0.136120	H	6.595005	-2.215001	0.099445
O	4.891108	-2.250315	-0.180402	H	3.300892	-4.384318	-1.562047
H	4.268963	-2.972241	-0.301159	O	3.075953	1.065690	0.217678
O	5.004377	2.467885	0.318162	C	0.106932	-1.127912	0.316882
H	5.946202	2.284428	0.365084	C	0.245803	-2.154722	1.250546
C	0.716543	0.352838	-0.146928	C	-0.977048	-1.123401	-0.560613
H	0.352764	1.359864	-0.330229	C	-0.703992	-3.174117	1.297888
C	-0.163717	-0.639402	0.043378	H	1.090123	-2.153916	1.932325
H	0.207901	-1.627130	0.304298	C	-1.944555	-2.125546	-0.468507
C	-1.620898	-0.526771	-0.020103	H	-1.085845	-0.327224	-1.288043
C	-2.409025	-1.571398	0.482663	C	-1.805361	-3.160121	0.449943
C	-2.279308	0.590472	-0.560802	H	-2.554621	-3.937812	0.513617
C	-3.790251	-1.503573	0.475087	C	-1.605432	1.499812	0.824655
H	-1.921134	-2.445062	0.901199	H	-1.646115	0.592961	1.419901
C	-3.656618	0.663669	-0.596363	C	-2.652738	1.828900	0.064039
H	-1.701913	1.406856	-0.977401	H	-2.572209	2.681637	-0.606668
C	-4.426855	-0.389089	-0.079143	C	-3.856046	0.996808	-0.071124
H	-4.401806	-2.302722	0.874504	C	-4.591248	1.043696	-1.263126
H	-4.158662	1.535287	-0.999376	C	-4.251723	0.073440	0.903917
O	-5.764948	-0.394798	-0.136608	C	-5.655645	0.184358	-1.494089
H	-6.143271	0.537050	-0.293438	H	-4.312898	1.760975	-2.028276
O	-6.499297	1.794119	0.271191	C	-5.318219	-0.783418	0.688205
H	-7.119097	1.644137	1.000683	H	-3.723370	0.027902	1.848920
TS(VIN-5OH-•OOH)				C	-6.018738	-0.740701	-0.517319
C	2.112012	1.991551	0.462954	H	-6.218804	0.213761	-2.418302
C	0.858469	1.370587	0.526128	H	-5.604903	-1.496548	1.454347
C	-0.295817	2.164890	0.768405	O	5.914363	-4.421098	-0.985955
				H	5.456295	-5.151288	-1.410851
				O	1.261029	5.427360	1.025850

H	1.829805	5.919600	0.204538	C	-2.371263	1.985401	-0.301883
O	-7.062696	-1.561303	-0.789669	H	-2.439418	2.941101	-0.816826
H	-7.182542	-2.180816	-0.065020	C	-3.538788	1.118837	-0.420970
O	-0.616163	-4.203638	2.179964	C	-4.716091	1.635233	-1.000846
H	0.179956	-4.101405	2.708132	C	-3.523009	-0.236636	-0.038756
O	-3.042323	-2.149073	-1.265776	C	-5.834153	0.851926	-1.171875
H	-3.221828	-1.262348	-1.600260	H	-4.734314	2.675174	-1.308936
O	2.250428	6.301930	-0.918833	C	-4.623732	-1.041286	-0.231062
O	2.530998	5.130877	-1.559607	H	-2.631342	-0.668202	0.400742
H	1.818186	5.038819	-2.207303	C	-5.808072	-0.515448	-0.809612
TS(VIN-12OH•OOH)				H	-6.744550	1.240699	-1.611093
C	2.379257	2.746063	0.166280	H	-4.603836	-2.089557	0.039415
C	1.257176	1.909683	0.189992	O	7.411904	-2.901416	-0.557031
C	-0.016704	2.498936	0.302192	H	7.140977	-3.712081	-0.996028
C	-0.083421	3.889897	0.375639	O	1.000414	6.044638	0.435620
C	1.067054	4.688845	0.347971	H	0.081898	6.315519	0.508314
C	2.333177	4.125989	0.242232	O	-6.850743	-1.269439	-1.042621
C	3.134486	0.693593	-0.014641	H	-7.193852	-1.783238	-0.095887
C	1.780092	0.560616	0.073457	O	0.891164	-3.809756	2.071439
H	-1.052203	4.363830	0.500373	H	1.600289	-3.508123	2.645487
H	3.220607	4.742981	0.227195	O	-1.689641	-2.482759	-1.603965
C	4.030256	-1.502089	-0.787187	H	-1.921757	-1.702953	-2.117148
C	4.227737	-0.263486	-0.170084	O	-7.543349	-2.008720	1.066919
C	5.511741	0.063777	0.283637	O	-6.544770	-1.445750	1.805197
C	6.562965	-0.825292	0.147715	H	-6.940966	-0.638692	2.163441
C	6.348597	-2.064886	-0.452514	TS(VIN-3'OH•OOH)			
C	5.079389	-2.397912	-0.923370	C	1.425134	3.087146	-0.079650
H	3.053977	-1.764048	-1.175751	C	0.433938	2.120777	0.125237
H	5.678479	1.028523	0.746160	C	-0.913001	2.526802	0.184261
H	7.557976	-0.582422	0.498167	C	-1.172369	3.889036	0.043475
H	4.914710	-3.354715	-1.408505	C	-0.149769	4.825943	-0.159824
O	3.510902	2.012265	0.048947	C	1.183338	4.440553	-0.227586
C	1.030607	-0.714068	0.110938	C	2.467122	1.158411	0.053449
C	1.328594	-1.650444	1.099358	C	1.147097	0.862301	0.220423
C	0.031676	-0.982620	-0.826311	H	-2.195707	4.241178	0.127871
C	0.633520	-2.858637	1.138937	H	1.970522	5.165196	-0.380056
H	2.106045	-1.436575	1.825410	C	3.636637	-1.025508	-0.291791
C	-0.676249	-2.182995	-0.751268	C	3.678851	0.342123	0.002238
H	-0.201161	-0.254103	-1.596386	C	4.928063	0.938344	0.220618
C	-0.375917	-3.128381	0.222607	C	6.093367	0.195227	0.164924
H	-0.928566	-4.056960	0.272740	C	6.035006	-1.168868	-0.116749
C	-1.222621	1.665940	0.314537	C	4.801587	-1.775313	-0.347618
H	-1.127873	0.707992	0.812393	H	2.692858	-1.520144	-0.485146

H	4.975974	1.998827	0.432882	C	-0.591106	2.757387	0.007559
H	7.061148	0.649763	0.334416	C	-0.739861	4.139696	0.017744
H	4.749225	-2.833307	-0.583901	C	0.354732	4.998607	-0.173395
O	2.650014	2.506386	-0.121584	C	1.634778	4.502894	-0.383000
C	0.604658	-0.486213	0.483659	C	2.598646	1.102899	-0.591550
C	0.955386	-1.147674	1.663194	C	1.270036	0.907368	-0.353906
C	-0.219064	-1.122198	-0.435134	H	-1.721678	4.560502	0.213016
C	0.509080	-2.453812	1.914510	H	2.475761	5.167610	-0.521936
H	1.593182	-0.642202	2.381970	C	3.529768	-1.078402	-1.365135
C	-0.667987	-2.446243	-0.190580	C	3.721455	0.199821	-0.833568
H	-0.548597	-0.619279	-1.338777	C	5.027267	0.620059	-0.550534
C	-0.278102	-3.112145	0.988782	C	6.107298	-0.216191	-0.768664
H	-0.611685	-4.126090	1.164626	C	5.900336	-1.496275	-1.279867
C	-1.989190	1.544027	0.369405	C	4.608089	-1.922021	-1.582164
H	-1.739479	0.665295	0.954701	H	2.533483	-1.414098	-1.623887
C	-3.214173	1.647041	-0.159933	H	5.187668	1.614780	-0.154303
H	-3.463299	2.529882	-0.745195	H	7.119367	0.098229	-0.548026
C	-4.271880	0.634747	-0.053197	H	4.446113	-2.911736	-1.996897
C	-5.611770	0.997555	-0.235024	O	2.907295	2.441511	-0.614471
C	-3.986232	-0.712989	0.187552	C	0.567713	-0.387175	-0.210349
C	-6.632339	0.065830	-0.146650	C	0.983747	-1.305600	0.747085
H	-5.856433	2.033950	-0.442466	C	-0.549085	-0.673121	-1.005582
C	-4.996889	-1.657131	0.268638	C	0.301495	-2.522560	0.880823
H	-2.957401	-1.040478	0.277607	H	1.836422	-1.108400	1.384417
C	-6.326435	-1.269326	0.108545	C	-1.267806	-1.854986	-0.814370
H	-7.669744	0.345385	-0.279653	H	-0.874998	0.040897	-1.753620
H	-4.748509	-2.701336	0.431220	C	-0.836593	-2.794995	0.113465
O	7.207022	-1.850335	-0.158094	H	-1.386341	-3.718475	0.243395
H	7.036309	-2.771299	-0.372963	C	-1.718866	1.832180	0.190398
O	-0.413987	6.154079	-0.287513	H	-1.532726	0.993119	0.853651
H	-1.361681	6.297691	-0.226817	C	-2.848806	1.860225	-0.521809
O	-7.359756	-2.148596	0.175100	H	-2.988977	2.645460	-1.261655
H	-7.016330	-3.031138	0.337356	C	-3.844161	0.778919	-0.512459
O	0.839467	-3.115621	3.048804	C	-4.615368	0.544913	-1.659194
H	1.401935	-2.561581	3.596865	C	-3.991903	-0.104133	0.563432
O	-1.442155	-3.045220	-1.058761	C	-5.469773	-0.544161	-1.749958
H	-0.818958	-3.243036	-2.028593	H	-4.530524	1.224227	-2.501108
O	0.033114	-3.359292	-2.855333	C	-4.848314	-1.190482	0.487357
O	1.166139	-2.920872	-2.240151	H	-3.436407	0.067281	1.478087
H	1.247415	-1.992176	-2.506733	C	-5.582575	-1.423963	-0.675364
TS(VIN-5'OH-•OH)				H	-6.057853	-0.731518	-2.639465
C	1.756699	3.123755	-0.402790	H	-4.947254	-1.865695	1.331340
C	0.694185	2.234620	-0.224809	O	6.993007	-2.278448	-1.470063
				H	6.719152	-3.133432	-1.812454

O	0.211363	6.351705	-0.150378	C	-3.607512	1.460043	-0.245542
H	-0.709096	6.571237	0.013485	H	-3.748468	2.331554	-0.881924
O	-6.427535	-2.474636	-0.813026	C	-4.656326	0.436981	-0.334457
H	-6.379919	-3.032073	-0.031848	C	-5.838507	0.716977	-1.032003
O	0.779782	-3.412410	1.761351	C	-4.504641	-0.848853	0.198158
H	0.015722	-4.024170	2.097137	C	-6.835575	-0.231501	-1.184278
O	-2.381886	-2.152193	-1.528570	H	-5.975890	1.703039	-1.462964
H	-2.764965	-1.345052	-1.892296	C	-5.489323	-1.811863	0.041491
O	-1.077576	-4.216990	2.910650	H	-3.601998	-1.116016	0.735823
H	-1.457217	-3.335206	3.041848	C	-6.662488	-1.505804	-0.648003
TS(VIN-12'OH-•OOH)				H	-7.750480	-0.012309	-1.719936
C	0.958047	2.901903	0.269308	H	-5.337912	-2.808166	0.444643
C	-0.047094	1.929783	0.341991	O	6.607592	-2.125381	-0.080239
C	-1.391310	2.351313	0.412407	H	7.416545	-1.635332	-0.697030
C	-1.636118	3.719927	0.393450	O	-0.845420	5.996180	0.307337
C	-0.596472	4.661164	0.313816	H	-1.792468	6.146016	0.365348
C	0.733241	4.266849	0.251688	O	-7.660249	-2.406330	-0.834544
C	1.976231	0.957761	0.217261	H	-7.422895	-3.239221	-0.418162
C	0.643072	0.657658	0.310713	O	0.307676	-3.648126	2.596795
H	-2.660330	4.069681	0.479797	H	0.989379	-3.234796	3.133466
H	1.532404	4.992473	0.198664	O	-2.411074	-2.901071	-1.142129
C	3.137052	-1.177660	-0.356183	H	-2.772060	-2.181249	-1.669342
C	3.178989	0.149953	0.122855	O	8.035733	-1.060905	-1.601619
C	4.417143	0.707426	0.483988	O	7.277667	0.047244	-1.840101
C	5.573297	-0.039622	0.412110	H	6.827756	-0.147718	-2.674559
C	5.532838	-1.380830	-0.042201	H₂O₂			
C	4.288360	-1.922113	-0.447496	O	0.000000	0.716572	-0.000180
H	2.195010	-1.602435	-0.678216	H	0.948775	0.876222	0.001440
H	4.451723	1.732454	0.829531	O	-0.000000	-0.716572	-0.000180
H	6.529977	0.375045	0.703196	H	-0.948775	-0.876222	0.001440
H	4.278599	-2.938096	-0.822211	•OOH			
O	2.175913	2.316765	0.204509	O	0.054937	-0.599538	0.000000
C	0.058772	-0.694881	0.437058	H	-0.878985	-0.868258	0.000000
C	0.471545	-1.518157	1.484133	O	0.054937	0.708070	0.000000
C	-0.897602	-1.146218	-0.473206	TS(RES-12OH-•OOH)			
C	-0.063821	-2.799662	1.606349	C	4.685584	-1.197548	-0.128233
H	1.212600	-1.160145	2.191157	C	3.305555	-1.324935	-0.232548
C	-1.446319	-2.419607	-0.316027	C	2.479744	-0.214417	-0.016303
H	-1.222762	-0.504006	-1.284863	C	3.051126	1.012070	0.323024
C	-1.028043	-3.253809	0.714008	C	4.433685	1.123323	0.425695
H	-1.454416	-4.241713	0.825773	C	5.259669	0.026642	0.200220
C	-2.483233	1.370290	0.473360				
H	-2.302232	0.499251	1.093237				

H	2.866377	-2.282877	-0.492438	H	2.465047	-1.908049	-0.179658
H	2.451695	1.887092	0.534376	H	4.491259	1.614165	-1.567400
H	6.338474	0.097239	0.280113	H	6.381669	0.203480	-2.343973
O	4.931617	2.341134	0.761398	H	4.340410	-3.286275	-0.944468
H	5.889817	2.293417	0.811333	O	2.305765	2.119520	-0.731139
O	5.535105	-2.236872	-0.334240	C	0.647406	-0.687013	1.003846
H	5.029277	-3.022633	-0.557136	C	1.151528	-1.097548	2.237131
C	1.030915	-0.393842	-0.156133	C	-0.321583	-1.445589	0.350243
H	0.700291	-1.427342	-0.205836	C	0.686194	-2.285879	2.805876
C	0.124986	0.591787	-0.259371	H	1.915936	-0.506243	2.731526
H	0.471909	1.621309	-0.267971	C	-0.788946	-2.619176	0.943025
C	-1.315707	0.426575	-0.400391	H	-0.722639	-1.109702	-0.600283
C	-2.102321	1.567009	-0.664584	C	-0.284889	-3.047186	2.166555
C	-1.966588	-0.816754	-0.283735	H	-0.649824	-3.958671	2.620704
C	-3.467387	1.480347	-0.812160	C	-1.928031	1.259027	0.863502
H	-1.611455	2.530301	-0.751618	H	-2.079028	0.464828	1.590316
C	-3.328277	-0.922707	-0.444095	C	-2.611775	1.279224	-0.278088
H	-1.394901	-1.706659	-0.052103	H	-2.429713	2.095041	-0.975791
C	-4.113057	0.225395	-0.726749	C	-3.557579	0.245543	-0.726496
H	-4.077759	2.350431	-1.019845	C	-4.247414	0.411067	-1.933733
H	-3.834270	-1.875875	-0.353789	C	-3.768896	-0.944669	-0.020736
O	-5.402605	0.139832	-0.929011	C	-5.113710	-0.555443	-2.418811
H	-5.905224	-0.364303	-0.058899	H	-4.097208	1.321208	-2.504439
O	-5.089020	-0.766506	1.772733	C	-4.629412	-1.924774	-0.497024
H	-5.067955	0.038860	2.309056	H	-3.257716	-1.120112	0.918877
O	-6.265577	-0.682167	1.088736	C	-5.308889	-1.732217	-1.700230
VIN-C1'-OH				H	-5.646497	-0.421817	-3.351785
C	1.208500	2.739670	-0.217988	H	-4.772749	-2.839351	0.071255
C	0.446994	1.825691	0.494729	O	6.543417	-2.336111	-2.132475
C	-0.807476	2.223031	1.229462	H	6.396263	-3.269501	-1.958206
C	-1.152360	3.656051	0.918709	O	-0.661413	5.795372	-0.029553
C	-0.358959	4.486054	0.199774	H	-1.470208	6.014574	0.441072
C	0.873938	4.067580	-0.406230	O	-6.162392	-2.653045	-2.217604
C	2.248990	0.808811	-0.358346	H	-6.226842	-3.402355	-1.619567
C	1.113854	0.582868	0.398204	O	1.144869	-2.745767	3.996631
H	-2.068715	4.022569	1.369471	H	1.811231	-2.143118	4.337543
H	1.474640	4.764819	-0.971032	O	-1.751293	-3.383118	0.366930
C	3.317547	-1.427184	-0.641289	H	-2.104558	-2.924837	-0.404326
C	3.343150	-0.036363	-0.806065	O	-0.591358	2.152815	2.647453
C	4.460795	0.541256	-1.429187	H	-0.321211	1.249092	2.848929
C	5.516669	-0.236803	-1.864522	VIN-C1''-OH			
C	5.480256	-1.619415	-1.687980	C	1.218950	2.983753	-0.072595
C	4.375712	-2.209462	-1.076117	C	0.270051	2.013614	0.270666

C	-1.078379	2.424976	0.375268	O	-0.655042	6.036080	-0.265671
C	-1.363023	3.775469	0.193614	H	-1.597209	6.172398	-0.138465
C	-0.366775	4.716499	-0.103175	O	-7.029835	-2.809833	-0.241424
C	0.956233	4.331254	-0.253090	H	-6.722905	-3.571118	0.257974
C	2.294571	1.072739	-0.026392	O	2.532249	-3.752444	1.070595
C	1.016314	0.756212	0.327200	H	3.230708	-3.292931	1.545474
H	-2.392064	4.106435	0.296870	O	-1.448775	-3.033094	-1.308316
H	1.726423	5.044817	-0.509701	H	-2.159330	-2.395925	-1.439054
C	3.472580	-0.899305	-0.981990	O	-0.268165	-0.349683	2.028695
C	3.511959	0.287145	-0.247630	H	0.322508	0.100127	2.643638
C	4.737103	0.719256	0.270720				
C	5.885228	-0.036078	0.102131	VIN-C2-OH			
C	5.823613	-1.241390	-0.597365	C	1.746128	2.766356	0.218403
C	4.614708	-1.670111	-1.144240	C	0.659120	1.865408	0.743603
H	2.538130	-1.219161	-1.427856	C	-0.701200	2.380766	0.343955
H	4.780219	1.653845	0.817345	C	-0.835766	3.747001	0.107050
H	6.838480	0.283521	0.503408	C	0.265625	4.592201	-0.010150
H	4.568269	-2.597216	-1.706410	C	1.598611	4.077761	-0.040499
O	2.438375	2.420115	-0.243559	C	2.476941	0.710776	-0.088035
C	0.484376	-0.586975	0.808093	C	1.192652	0.524563	0.257016
C	1.578855	-1.558399	1.151844	H	-1.832131	4.170960	0.017847
C	-0.493910	-1.157870	-0.178572	H	2.414454	4.704967	-0.373800
C	1.554310	-2.857156	0.752264	C	3.278670	-1.508744	-0.914190
H	2.375547	-1.192821	1.793072	C	3.547435	-0.207444	-0.478581
C	-0.499195	-2.474668	-0.508840	C	4.880104	0.219845	-0.422940
H	-1.239589	-0.488286	-0.590007	C	5.915824	-0.628590	-0.771894
C	0.515939	-3.357855	-0.062826	C	5.635196	-1.926464	-1.193655
H	0.502920	-4.398351	-0.356168	C	4.312735	-2.361145	-1.267612
C	-2.160478	1.450340	0.584728	H	2.257236	-1.858747	-0.989325
H	-1.969196	0.696207	1.337392	H	5.097596	1.229776	-0.100891
C	-3.258939	1.380331	-0.174662	H	6.948670	-0.307486	-0.727873
H	-3.421276	2.129490	-0.947308	H	4.091132	-3.367485	-1.608459
C	-4.236464	0.282768	-0.129257	O	2.864312	2.046188	-0.046015
C	-5.448458	0.397780	-0.821333	C	0.540577	-0.782152	0.502645
C	-3.974924	-0.926600	0.530119	C	0.921772	-1.508654	1.628664
C	-6.374263	-0.632077	-0.845920	C	-0.434979	-1.288346	-0.358511
H	-5.667762	1.319284	-1.350195	C	0.337113	-2.748969	1.881225
C	-4.891273	-1.968166	0.504521	H	1.667062	-1.095448	2.299542
H	-3.040741	-1.068522	1.063738	C	-1.033593	-2.515524	-0.071713
C	-6.097312	-1.824047	-0.180829	H	-0.739449	-0.717511	-1.229721
H	-7.312863	-0.538976	-1.377442	C	-0.643322	-3.257051	1.037438
H	-4.664894	-2.899638	1.014245	H	-1.109614	-4.209646	1.250749
O	6.974398	-1.950217	-0.720468	C	-1.804872	1.461218	0.380069
H	6.810617	-2.739220	-1.244066	H	-1.632667	0.561648	0.959356

C	-2.966923	1.593690	-0.296246	H	7.070210	-0.019204	0.600865
H	-3.115284	2.473100	-0.918747	H	4.632324	-3.141679	-1.015963
C	-4.024287	0.588739	-0.369697	O	2.832976	2.223141	-0.035250
C	-5.163136	0.839041	-1.150874	C	0.559801	-0.667440	0.248353
C	-3.932828	-0.664581	0.253960	C	0.660924	-1.442398	1.376560
C	-6.163699	-0.104255	-1.307700	C	-0.234934	-1.119690	-0.944048
H	-5.258360	1.798317	-1.648550	C	0.015938	-2.684646	1.469126
C	-4.921687	-1.622470	0.092769	H	1.247725	-1.077054	2.215059
H	-3.077284	-0.907737	0.873277	C	-0.815507	-2.489756	-0.773891
C	-6.044200	-1.346586	-0.688044	H	-1.063925	-0.415930	-1.144018
H	-7.040876	0.094274	-1.910520	C	-0.718958	-3.205327	0.371372
H	-4.813543	-2.591937	0.569062	H	-1.165955	-4.188538	0.442274
O	6.685938	-2.718946	-1.524673	C	-1.826372	1.477345	0.424841
H	6.362508	-3.580037	-1.802469	H	-1.581224	0.572795	0.973919
O	0.149063	5.928688	-0.186738	C	-3.050370	1.617603	-0.096345
H	-0.781822	6.167098	-0.222330	H	-3.287049	2.523278	-0.651410
O	-7.043309	-2.245989	-0.881407	C	-4.116712	0.610470	-0.032470
H	-6.840386	-3.055323	-0.404786	C	-5.431923	0.965864	-0.354688
O	0.678614	-3.503115	2.957492	C	-3.865720	-0.725904	0.300808
H	1.349903	-3.039843	3.465612	C	-6.462488	0.041146	-0.324653
O	-2.023965	-3.037900	-0.844701	H	-5.649338	1.992426	-0.630168
H	-2.380519	-2.347489	-1.413055	C	-4.886066	-1.662233	0.327489
O	0.723517	1.771249	2.185854	H	-2.857996	-1.057602	0.526826
H	0.331935	2.578807	2.537849	C	-6.191554	-1.281293	0.018382
VIN-C2'-OH				H	-7.480417	0.317107	-0.569009
C	1.645121	2.872452	0.042503	H	-4.663643	-2.696187	0.572612
C	0.597845	1.953720	0.152756	O	7.090330	-2.433941	-0.227472
C	-0.719946	2.429310	0.272920	H	6.874635	-3.300841	-0.581254
C	-0.908327	3.809655	0.245038	O	-0.019285	6.047103	0.095554
C	0.167691	4.699055	0.112902	H	-0.956692	6.238895	0.177918
C	1.478174	4.245462	0.013672	O	-7.231436	-2.154874	0.024866
C	2.563654	0.876309	0.009782	H	-6.912635	-3.028329	0.266970
C	1.224882	0.642114	0.135536	O	0.077184	-3.462733	2.577507
H	-1.910025	4.208425	0.373806	H	0.622905	-3.030938	3.240783
H	2.304552	4.937187	-0.069372	O	-1.478132	-2.968525	-1.846473
C	3.614972	-1.308639	-0.565677	H	-1.162595	-2.480906	-2.618120
C	3.725482	-0.006035	-0.069599	O	0.548866	-1.184495	-2.153656
C	4.982411	0.455403	0.341063	H	0.835787	-0.288860	-2.362849
C	6.095063	-0.364843	0.282224	VIN-C3-OH			
C	5.969242	-1.668374	-0.194848	C	2.051130	2.632013	0.558940
C	4.727422	-2.134291	-0.623153	C	0.781000	1.826405	0.480573
H	2.662191	-1.668658	-0.935067	C	-0.464220	2.504164	0.451454
H	5.078661	1.468961	0.709855	C	-0.442967	3.835875	0.108028

C	0.781908	4.494715	-0.306779	O	-6.772489	-2.106715	-0.631250
C	1.988380	3.909063	-0.195696	H	-6.831496	-2.643683	0.163345
C	2.519348	0.478076	0.026880	O	-0.146149	-3.654585	2.576759
C	1.155265	0.479146	0.314569	H	0.621297	-3.412992	3.101841
H	-1.371354	4.399107	0.093352	O	-2.677650	-2.249863	-1.110330
H	2.900038	4.408135	-0.492149	H	-2.943792	-1.428181	-1.539561
C	2.993249	-1.851339	-0.760889	O	2.391608	2.929797	1.891697
C	3.434321	-0.597009	-0.314582	H	2.272485	2.124728	2.409300
C	4.817939	-0.364965	-0.230063				
C	5.727602	-1.354145	-0.549303				
C	5.273034	-2.602424	-0.974917	VIN-C3'-OH			
C	3.903187	-2.843279	-1.084762	C	1.538317	2.909871	0.041092
H	1.936182	-2.050722	-0.875398	C	0.571693	1.897797	0.098668
H	5.164979	0.607426	0.094203	C	-0.786199	2.263661	0.209632
H	6.794615	-1.185160	-0.480527	C	-1.071816	3.629227	0.240173
H	3.549349	-3.807231	-1.436230	C	-0.073697	4.609531	0.160110
O	3.052930	1.718330	0.050615	C	1.267320	4.265961	0.062760
C	0.281855	-0.715968	0.421026	C	2.634939	1.012568	-0.056160
C	0.505110	-1.621095	1.458771	C	1.322920	0.657812	0.035479
C	-0.764940	-0.925834	-0.474626	H	-2.100997	3.944305	0.380134
C	-0.322850	-2.734700	1.592172	H	2.040967	5.019363	0.018563
H	1.326170	-1.458753	2.149792	C	3.885593	-1.037230	-0.731011
C	-1.615432	-2.019459	-0.298284	C	3.870896	0.240921	-0.163936
H	-0.935803	-0.226863	-1.284834	C	5.077836	0.786655	0.291802
C	-1.390110	-2.933923	0.724552	C	6.259342	0.071916	0.207959
H	-2.047793	-3.783364	0.851702	C	6.256796	-1.209951	-0.340191
C	-1.701347	1.729437	0.612256	C	5.066722	-1.759908	-0.812911
H	-1.674271	0.947505	1.364684	H	2.973781	-1.465184	-1.129353
C	-2.747823	1.804114	-0.216966	H	5.079156	1.783716	0.714263
H	-2.718431	2.521438	-1.034397	H	7.196232	0.484783	0.559737
C	-3.858296	0.844789	-0.238579	H	5.065761	-2.748521	-1.260917
C	-4.585019	0.669015	-1.424456	O	2.781316	2.375627	-0.045145
C	-4.163946	0.007836	0.841799	C	0.799844	-0.721604	0.093625
C	-5.552040	-0.318208	-1.546153	C	1.276489	-1.599089	1.107267
H	-4.376059	1.313539	-2.272132	C	-0.129951	-1.154794	-0.795600
C	-5.131659	-0.976768	0.734298	C	0.844830	-2.949912	1.152454
H	-3.640521	0.127926	1.782824	H	1.995824	-1.230292	1.830626
C	-5.823312	-1.153008	-0.464407	C	-0.763041	-2.511467	-0.700074
H	-6.106744	-0.459327	-2.465154	H	-0.520832	-0.493938	-1.562770
H	-5.346818	-1.620476	1.581190	C	-0.082800	-3.415475	0.279638
O	6.205976	-3.538399	-1.274625	H	-0.383644	-4.456223	0.294258
H	5.771302	-4.345874	-1.562062	C	-1.871706	1.273937	0.314349
O	0.693938	5.752197	-0.827665	H	-1.641946	0.343913	0.823594
H	-0.224863	5.951581	-1.020530	C	-3.095130	1.467146	-0.197543
				H	-3.270731	2.368141	-0.782298

C	-4.249651	0.570530	-0.084754	O	2.842217	1.858454	0.103606
C	-5.376974	0.804525	-0.881818	C	0.512014	-0.975335	-0.039910
C	-4.292622	-0.511059	0.801510	C	0.525540	-1.814005	1.070779
C	-6.497502	-0.007454	-0.819155	C	-0.172477	-1.353094	-1.195784
H	-5.370261	1.642721	-1.570787	C	-0.148430	-3.035434	1.019692
C	-5.407387	-1.330410	0.875562	H	1.059295	-1.512195	1.965699
H	-3.441952	-0.723726	1.435740	C	-0.854699	-2.568705	-1.223407
C	-6.515405	-1.082659	0.064428	H	-0.187290	-0.688684	-2.053767
H	-7.367232	0.174391	-1.437587	C	-0.844323	-3.416829	-0.120840
H	-5.426220	-2.160910	1.575183	H	-1.371921	-4.360778	-0.150737
O	7.442038	-1.869810	-0.394061	C	-1.848779	1.265057	0.145070
H	7.312492	-2.727920	-0.806513	H	-1.596788	0.214820	0.192061
O	-0.372670	5.936869	0.198034	C	-3.181484	1.583313	0.128612
H	-1.324233	6.045129	0.270020	H	-3.491284	2.623849	0.104047
O	-7.636143	-1.851332	0.099698	C	-4.261765	0.613784	0.122680
H	-7.528598	-2.540588	0.760119	C	-5.593605	1.059660	0.187956
O	1.361932	-3.806534	2.079734	C	-4.052309	-0.774100	0.036743
H	2.100703	-3.383961	2.524570	C	-6.661433	0.180888	0.177749
O	-0.759251	-3.183504	-1.939744	H	-5.786816	2.125365	0.250932
H	-1.260795	-2.637373	-2.555084	C	-5.114172	-1.661264	0.023443
O	-2.108117	-2.247321	-0.319451	H	-3.048211	-1.177305	-0.029018
H	-2.558243	-3.096085	-0.234147	C	-6.425740	-1.190036	0.095693
VIN-C4'-OH				H	-7.684700	0.530690	0.231042
C	1.667150	2.515236	0.109270	H	-4.923874	-2.727860	-0.050141
C	0.611794	1.651437	0.063125	O	7.071381	-2.823973	-0.027774
C	-0.748986	2.144134	0.108696	H	6.862018	-3.692637	-0.380775
C	-0.880591	3.579869	0.128367	O	0.099890	5.771772	0.173423
C	0.179305	4.413336	0.162320	H	-0.818166	6.047323	0.094633
C	1.626034	3.993029	0.169890	O	-7.504504	-2.016487	0.085854
C	2.559720	0.525448	0.035473	H	-7.205855	-2.927856	0.028382
C	1.207547	0.330373	0.013012	O	-0.165383	-3.895282	2.068974
H	-1.875858	4.012782	0.134495	H	0.341828	-3.520946	2.794243
H	2.090615	4.355154	1.101005	O	-1.567250	-2.976473	-2.304853
C	3.613227	-1.681092	-0.477590	H	-1.534506	-2.295635	-2.982440
C	3.713641	-0.372278	0.002178	O	2.321817	4.540855	-0.940515
C	4.961915	0.082825	0.446673	H	2.183698	5.492834	-0.907679
C	6.070956	-0.743877	0.429127	VIN-C4'-OH			
C	5.953409	-2.051965	-0.036719	C	1.907455	2.851586	0.087889
C	4.721557	-2.515522	-0.492672	C	0.814758	1.981895	0.105595
H	2.668890	-2.051784	-0.855354	C	-0.479233	2.518084	0.237586
H	5.055486	1.100080	0.805195	C	-0.601659	3.905131	0.262575
H	7.038082	-0.398465	0.771671	C	0.519625	4.745891	0.196167
H	4.629913	-3.528799	-0.870972	C	1.808406	4.231548	0.124842

C	2.731514	0.816407	-0.013072	H	1.120444	-3.675693	2.296450
C	1.375415	0.642022	0.030493	O	-2.250388	-2.125302	-1.776884
H	-1.585790	4.343532	0.398467	H	-2.571324	-1.287979	-2.128622
H	2.670639	4.883190	0.110167	C	0.171115	-2.820311	0.889202
C	3.716439	-1.359586	-0.731323	O	-2.170887	-3.244872	0.754406
C	3.857784	-0.104663	-0.131177	H	-2.895182	-3.261957	0.118030
C	5.123129	0.274890	0.336486				
C	6.207465	-0.577569	0.231256				
C	6.048150	-1.833435	-0.351917	C	1.671699	2.644394	0.022154
C	4.799606	-2.219058	-0.836616	C	0.612697	1.710880	0.187673
H	2.756905	-1.659901	-1.133312	C	-0.727689	2.214490	0.390340
H	5.247666	1.252227	0.785526	C	-0.907171	3.552315	0.417771
H	7.187319	-0.292957	0.593012	C	0.180503	4.579208	0.226637
H	4.678115	-3.187763	-1.311113	C	1.544627	3.987483	0.023202
O	3.065305	2.149522	0.033817	C	2.554715	0.632155	-0.123680
C	0.627535	-0.613768	-0.011103	C	1.200201	0.426734	0.098673
C	0.905673	-1.675782	0.891109	H	-1.889361	3.965508	0.625642
C	-0.432662	-0.774457	-0.949795	H	2.378213	4.656897	-0.145863
H	1.725485	-1.562927	1.594998	C	3.502136	-1.578356	-0.788515
C	-1.179849	-1.902977	-0.965523	C	3.677494	-0.265901	-0.330144
H	-0.649206	0.030067	-1.645013	C	4.984172	0.193196	-0.099607
C	-0.987022	-3.054047	-0.028226	C	6.074762	-0.633489	-0.292402
H	-0.805557	-3.975813	-0.604098	C	5.883290	-1.943617	-0.730264
C	-1.634247	1.624547	0.397504	C	4.593147	-2.409516	-0.982358
H	-1.446699	0.746659	1.007019	H	2.509904	-1.948064	-1.012940
C	-2.828358	1.778637	-0.182921	H	5.132313	1.211592	0.236118
H	-2.996439	2.644982	-0.820040	H	7.084682	-0.288021	-0.111935
C	-3.944002	0.826617	-0.089040	H	4.443656	-3.421702	-1.344442
C	-5.172172	1.139569	-0.686432	O	2.844683	1.964523	-0.159110
C	-3.833168	-0.411977	0.557103	C	0.559271	-0.894888	0.289475
C	-6.251639	0.272801	-0.634239	C	1.009533	-1.716057	1.322991
H	-5.281930	2.089641	-1.198942	C	-0.471933	-1.322388	-0.545618
C	-4.905991	-1.287708	0.615337	C	0.433766	-2.971532	1.507030
H	-2.899263	-0.726526	1.008390	H	1.813486	-1.377489	1.968363
C	-6.123639	-0.946820	0.026083	C	-1.058603	-2.570222	-0.326556
H	-7.201150	0.520380	-1.091629	H	-0.824459	-0.682396	-1.347056
H	-4.797514	-2.233806	1.138521	C	-0.604289	-3.403013	0.689046
O	7.143292	-2.633110	-0.426716	H	-1.062381	-4.369764	0.849799
H	6.908172	-3.457905	-0.859713	C	-1.844160	1.263247	0.531192
O	0.397301	6.101175	0.231564	H	-1.677710	0.426798	1.202581
H	-0.532180	6.334049	0.295632	C	-2.972958	1.348226	-0.178072
O	-7.208831	-1.762442	0.057611	H	-3.087004	2.186831	-0.861907
H	-6.998843	-2.554554	0.559381	C	-4.062264	0.362755	-0.193543
O	0.389676	-3.876439	1.703681	C	-5.243369	0.649282	-0.890418

C	-3.954257	-0.894626	0.411581	C	0.758404	-1.433336	1.151461
C	-6.279792	-0.265170	-0.974064	C	-0.661966	-0.772871	-0.676351
H	-5.347604	1.613801	-1.375887	C	0.166738	-2.809934	1.161959
C	-4.979490	-1.824545	0.324446	H	1.548779	-1.242726	1.870011
H	-3.053184	-1.166698	0.949541	C	-1.448841	-1.949930	-0.527908
C	-6.149645	-1.511962	-0.366158	H	-0.907343	-0.057979	-1.452584
H	-7.193381	-0.040070	-1.509616	C	-1.090031	-2.914318	0.352972
H	-4.862454	-2.801053	0.783678	H	-1.677490	-3.821170	0.438752
O	6.986550	-2.713942	-0.900354	C	-1.777375	1.768153	0.565321
H	6.725578	-3.584319	-1.212996	H	-1.609369	0.910895	1.210331
O	-0.072199	5.384995	-0.911320	C	-2.910218	1.842317	-0.139399
H	-0.922139	5.814515	-0.763692	H	-3.036478	2.652131	-0.854893
O	-7.185803	-2.381535	-0.486352	C	-3.941353	0.795203	-0.147616
H	-6.971361	-3.198938	-0.029075	C	-4.779471	0.666234	-1.263780
O	0.838752	-3.817093	2.488702	C	-4.068025	-0.152989	0.875598
H	1.550494	-3.406826	2.987219	C	-5.684913	-0.378247	-1.376360
O	-2.093094	-3.026819	-1.079475	H	-4.706315	1.393003	-2.066054
H	-2.496079	-2.289792	-1.550051	C	-4.972865	-1.197062	0.776176
O	0.128925	5.398693	1.380621	H	-3.453735	-0.075424	1.764807
H	0.807917	6.074108	1.275933	C	-5.780035	-1.320839	-0.354810
VIN-C5'-OH				H	-6.323526	-0.484443	-2.244027
C	1.746585	2.950034	0.058861	H	-5.047921	-1.926371	1.576255
C	0.646045	2.105051	0.212807	O	6.768834	-2.701730	-0.802030
C	-0.626428	2.668073	0.408794	H	6.467817	-3.541828	-1.158186
C	-0.727770	4.054675	0.410998	O	0.307287	6.229789	0.260769
C	0.402734	4.872031	0.245328	H	-0.609183	6.482399	0.396893
C	1.671290	4.332651	0.070343	O	-6.676753	-2.325507	-0.510812
C	2.508543	0.894086	-0.100820	H	-6.612659	-2.931917	0.231730
C	1.167806	0.758290	0.104910	O	1.093526	-3.730690	0.591487
H	-1.697715	4.512368	0.581202	H	1.926883	-3.616922	1.064782
H	2.536361	4.969768	-0.048448	O	-2.554389	-2.136188	-1.306292
C	3.359023	-1.347790	-0.806663	H	-2.976676	-1.284639	-1.471766
C	3.595040	-0.063964	-0.302891	O	-0.045046	-3.149602	2.513859
C	4.912107	0.304127	-0.001253	H	-0.348525	-4.063450	2.527734
C	5.959451	-0.584192	-0.173752	VIN-C6'-OH			
C	5.708136	-1.866779	-0.656486	C	1.526364	2.707737	-0.099165
C	4.404028	-2.243787	-0.974547	C	0.556526	1.720528	-0.025369
H	2.357441	-1.657278	-1.075488	C	-0.820300	2.073534	0.051583
H	5.108435	1.300870	0.373277	C	-1.164478	3.534080	-0.141482
H	6.979475	-0.306921	0.059877	C	0.003387	4.498476	-0.057086
H	4.204132	-3.234774	-1.370524	C	1.292445	4.113502	-0.081023
O	2.874542	2.219639	-0.120099	C	2.617786	0.809492	-0.107887
C	0.418963	-0.511767	0.212319	C	1.298190	0.470410	-0.027159

H	2.104050	4.827184	-0.052438
C	3.886395	-1.268071	-0.662970
C	3.858657	0.041647	-0.174449
C	5.062497	0.625937	0.241011
C	6.252450	-0.077858	0.190599
C	6.262639	-1.389308	-0.280829
C	5.075828	-1.979612	-0.710666
H	2.976510	-1.732649	-1.021691
H	5.056057	1.645288	0.606111
H	7.185793	0.366635	0.511970
H	5.083650	-2.994212	-1.096293
O	2.761210	2.173448	-0.143869
C	0.771428	-0.909006	0.065276
C	1.114708	-1.704615	1.155279
C	-0.068948	-1.412314	-0.929174
C	0.618367	-3.005466	1.244465
H	1.769466	-1.308429	1.924388
C	-0.583472	-2.702077	-0.805756
H	-0.343316	-0.785935	-1.772287
C	-0.237428	-3.508468	0.272401
H	-0.637192	-4.509838	0.359238
C	-1.847895	1.114408	0.165793
H	-1.510384	0.104408	0.355160
C	-3.196098	1.311006	0.019949
H	-3.579209	2.316670	-0.116393
C	-4.181984	0.242614	0.004184
C	-5.548583	0.563807	-0.066181
C	-3.842807	-1.121257	0.017759
C	-6.527891	-0.412161	-0.109547
H	-5.840004	1.608520	-0.085185
C	-4.814121	-2.106132	-0.030641
H	-2.804817	-1.429404	0.060245
C	-6.163923	-1.757286	-0.092068
H	-7.579283	-0.158576	-0.160449
H	-4.520554	-3.151646	-0.030895
O	7.455765	-2.037745	-0.304636
H	7.331284	-2.923377	-0.655709
O	-0.356268	5.793568	-0.005273
H	-1.280213	5.814929	0.281419
O	-7.159083	-2.680983	-0.143051
H	-6.776469	-3.561980	-0.118917
O	0.928673	-3.827340	2.278601
H	1.520329	-3.369286	2.881518
O	-1.458779	-3.222560	-1.706563

H	-1.683196	-2.552147	-2.358186
O	-2.178040	4.009117	0.755236
H	-1.998568	3.621100	1.619364
H	-1.620193	3.671420	-1.135615
VIN-C6'-OH			
C	1.694729	2.895894	-0.022119
C	0.620697	2.008986	0.064979
C	-0.676452	2.517529	0.247988
C	-0.827787	3.899920	0.266752
C	0.274055	4.761864	0.140469
C	1.568286	4.274618	0.006480
C	2.540977	0.873285	-0.153895
C	1.193955	0.680729	-0.037208
H	-1.815117	4.319456	0.435865
H	2.413121	4.945331	-0.061815
C	3.490677	-1.348208	-0.772076
C	3.666083	-0.045111	-0.293892
C	4.960195	0.372202	0.046681
C	6.039031	-0.486072	-0.065415
C	5.847030	-1.788074	-0.525267
C	4.569046	-2.214696	-0.880835
H	2.508241	-1.681687	-1.086463
H	5.110162	1.383622	0.402511
H	7.040827	-0.170887	0.197562
H	4.419065	-3.219748	-1.262786
O	2.859225	2.210592	-0.138660
C	0.487226	-0.606617	-0.010552
C	0.737871	-1.505324	1.162826
C	-0.507850	-0.924106	-0.900566
C	0.272147	-2.907346	0.917114
H	1.807526	-1.503337	1.426637
C	-1.145512	-2.175886	-0.863747
H	-0.790211	-0.207883	-1.666945
C	-0.686079	-3.198532	0.007282
H	-1.098977	-4.196264	-0.070192
C	-1.790278	1.578974	0.439578
H	-1.560849	0.737161	1.086129
C	-2.970495	1.648374	-0.182469
H	-3.168654	2.487216	-0.847254
C	-4.014818	0.616156	-0.122582
C	-5.251922	0.842011	-0.739142
C	-3.805779	-0.631392	0.480952
C	-6.247272	-0.121598	-0.751360

H	-5.434711	1.797907	-1.218769	C	-0.143404	-2.417147	1.971608
C	-4.790589	-1.606601	0.465473	H	1.322984	-0.877785	2.358734
H	-2.856432	-0.859394	0.954329	C	-1.301542	-2.261498	-0.123011
C	-6.017522	-1.355471	-0.147983	H	-0.707958	-0.636220	-1.411854
H	-7.204139	0.056164	-1.225679	C	-1.092528	-2.914921	1.085349
H	-4.599142	-2.573411	0.920574	H	-1.668147	-3.795455	1.337724
O	6.939819	-2.589847	-0.611226	C	-1.751851	1.911806	0.703138
H	6.682550	-3.445480	-0.964537	H	-1.505951	1.031350	1.309900
O	0.124606	6.115043	0.170276	C	-2.428240	1.471863	-0.561554
H	-0.805456	6.327864	0.279440	H	-2.201310	2.012026	-1.474015
O	-7.016527	-2.275236	-0.194924	C	-3.404343	0.444018	-0.597425
H	-6.730790	-3.078273	0.248454	C	-4.005781	0.066634	-1.826146
O	0.722903	-3.864425	1.777262	C	-3.801210	-0.273579	0.558313
H	1.583252	-3.600322	2.118660	C	-4.929422	-0.955668	-1.898960
O	-2.175992	-2.496109	-1.682110	H	-3.727670	0.601958	-2.727823
H	-2.572178	-1.688991	-2.027117	C	-4.731299	-1.292375	0.487175
O	-0.000849	-0.929706	2.264157	H	-3.365733	-0.030496	1.521013
H	0.068535	-1.524593	3.018402	C	-5.297833	-1.647098	-0.738956
VIN-C7'-OH				H	-5.385623	-1.242304	-2.838434
C	1.865658	2.711133	-0.192289	H	-5.007975	-1.835691	1.385101
C	0.726660	1.959554	0.118755	O	6.516860	-3.272595	-0.787530
C	-0.466510	2.646335	0.396931	H	6.146172	-4.147633	-0.928780
C	-0.455768	4.030306	0.335015	O	0.714394	6.104666	-0.044754
C	0.708786	4.744511	0.009576	H	-0.159175	6.430332	0.186376
C	1.902126	4.093104	-0.264477	O	-6.204014	-2.644106	-0.870763
C	2.494193	0.606621	-0.205766	H	-6.328633	-3.081400	-0.024012
C	1.169485	0.576717	0.110051	O	0.021867	-3.089460	3.140738
H	-1.369533	4.563502	0.572486	H	0.702695	-2.654426	3.660841
H	2.801464	4.642927	-0.503800	O	-2.243553	-2.776398	-0.952849
C	3.176450	-1.768345	-0.580876	H	-2.505144	-2.108488	-1.597133
C	3.513748	-0.428398	-0.364844	O	-2.602634	2.775814	1.463715
C	4.870327	-0.080846	-0.313111	H	-3.508669	2.502885	1.297674
C	5.858968	-1.037975	-0.456128	VIN-C7'-OH			
C	5.508710	-2.371563	-0.656988	C	1.586638	2.662240	-0.022661
C	4.164273	-2.731468	-0.721699	C	0.542973	1.807866	0.302960
H	2.137802	-2.064674	-0.652081	C	-0.772494	2.272898	0.281428
H	5.143694	0.955101	-0.159074	C	-0.972067	3.622692	-0.035674
H	6.908594	-0.776075	-0.414947	C	0.100911	4.458795	-0.343947
H	3.887991	-3.767234	-0.892248	C	1.416728	3.990313	-0.352004
O	2.928597	1.895979	-0.393150	C	2.586833	0.723137	0.374178
C	0.377697	-0.628875	0.444005	C	1.117978	0.440081	0.624541
C	0.586491	-1.269721	1.665130	H	-1.975156	4.035986	-0.023647
C	-0.557512	-1.128691	-0.457632	H	2.240993	4.644668	-0.597839

C	3.530272	-1.484661	0.889816	O	0.866201	0.041503	1.974068
C	3.695856	-0.143692	0.475716	H	1.191069	0.745119	2.544260
C	5.004700	0.302397	0.170601				
C	6.083818	-0.549730	0.264276	VIN-C8-OH			
C	5.898669	-1.875284	0.666021	C	1.022163	2.926935	-0.158318
C	4.617141	-2.333104	0.978767	C	0.149521	1.927227	0.271788
H	2.543091	-1.845294	1.149303	C	-1.212858	2.251081	0.526688
H	5.149282	1.328173	-0.143014	C	-1.604952	3.579503	0.229445
H	7.087061	-0.216279	0.029992	C	-0.695281	4.537960	-0.210296
H	4.474991	-3.361545	1.296328	C	0.654338	4.238189	-0.408440
O	2.801205	2.034055	0.008905	C	2.196020	1.071616	-0.074468
C	0.553328	-0.667337	-0.265272	C	0.930500	0.715155	0.299092
C	-0.180782	-1.711660	0.283692	H	-2.625932	3.887730	0.428384
C	0.738535	-0.586540	-1.640731	H	1.350853	4.991854	-0.746886
C	-0.753700	-2.661977	-0.562342	C	3.492990	-1.058251	-0.300255
H	-0.323958	-1.765826	1.356694	C	3.448531	0.339331	-0.243051
C	0.172965	-1.554622	-2.467090	C	4.652359	1.048873	-0.362713
H	1.314536	0.230401	-2.066239	C	5.858509	0.391078	-0.521128
C	-0.583729	-2.595002	-1.935930	C	5.888590	-1.001297	-0.566324
H	-1.031874	-3.333922	-2.586034	C	4.700875	-1.721111	-0.458019
C	-1.870080	1.338440	0.557690	H	2.582932	-1.639305	-0.233220
H	-1.585781	0.436327	1.088474	H	4.632451	2.130367	-0.329374
C	-3.138452	1.485241	0.158507	H	6.790137	0.935104	-0.611161
H	-3.442212	2.393380	-0.357493	H	4.718189	-2.805461	-0.504173
C	-4.180430	0.463645	0.327644	O	2.262899	2.416744	-0.342760
C	-5.528861	0.826328	0.424339	C	0.457265	-0.659807	0.589303
C	-3.864536	-0.898610	0.350489	C	0.709556	-1.239697	1.829830
C	-6.523009	-0.125650	0.577719	C	-0.206300	-1.380706	-0.404252
H	-5.800347	1.876058	0.388209	C	0.308238	-2.554907	2.066768
C	-4.851178	-1.861990	0.492275	H	1.230259	-0.672126	2.593885
H	-2.836368	-1.210355	0.209652	C	-0.572800	-2.704489	-0.158821
C	-6.185393	-1.477318	0.614572	H	-0.408603	-0.920060	-1.365890
H	-7.566299	0.151323	0.661103	C	-0.325588	-3.294411	1.075193
H	-4.583583	-2.914250	0.475068	H	-0.614335	-4.320351	1.260990
O	7.000098	-2.668339	0.737054	C	-2.086766	1.293625	1.082420
H	6.739763	-3.550228	1.015437	H	-1.667281	0.392683	1.514274
O	-0.074854	5.770173	-0.649228	C	-3.568960	1.255355	0.901499
H	-1.011306	5.982499	-0.619009	H	-3.931481	2.169827	0.417859
O	-7.197693	-2.373206	0.752860	C	-3.797553	0.075236	-0.030565
H	-6.837234	-3.263715	0.742651	C	-3.724414	0.238102	-1.412768
O	-1.533982	-3.668204	-0.073426	C	-3.890036	-1.212194	0.494741
H	-1.516500	-3.635234	0.887110	C	-3.709290	-0.861794	-2.258665
O	0.321108	-1.530492	-3.815913	H	-3.641076	1.236523	-1.830644
H	0.857372	-0.772584	-4.063040	C	-3.883238	-2.318707	-0.341056

H	-3.928176	-1.344261	1.569933	C	-1.208411	-2.392278	-0.235958
C	-3.764171	-2.143641	-1.716814	H	-0.915222	-0.392382	-0.958189
H	-3.633894	-0.751247	-3.333479	C	-0.770118	-3.399452	0.617301
H	-3.914524	-3.320387	0.075110	H	-1.248442	-4.369468	0.615728
O	7.098380	-1.598829	-0.720804	C	-1.869016	1.498203	0.411547
H	6.983194	-2.552494	-0.739589	H	-1.812893	0.689208	1.131684
O	-1.070314	5.823898	-0.457930	C	-2.966861	1.645670	-0.340319
H	-2.007756	5.921381	-0.273614	H	-2.991813	2.445528	-1.077596
O	-3.644116	-3.196658	-2.577089	C	-4.132836	0.754719	-0.335647
H	-3.564608	-4.007950	-2.065210	C	-5.278407	1.106990	-1.062135
O	0.525021	-3.174827	3.254734	C	-4.134188	-0.484013	0.318127
H	0.959194	-2.564110	3.856274	C	-6.384126	0.276543	-1.125751
O	-1.166122	-3.483148	-1.103331	H	-5.298648	2.056645	-1.586206
H	-1.352767	-2.957259	-1.888932	C	-5.230517	-1.330347	0.251503
O	-4.182044	1.073881	2.165823	H	-3.264369	-0.807783	0.878847
H	-5.109909	0.871537	2.011438	C	-6.363113	-0.951818	-0.468189
VIN-C8'-•OH				H	-7.269785	0.552503	-1.683921
C	1.753494	2.606779	0.420316	H	-5.198118	-2.294668	0.748503
C	0.630184	1.732966	0.433070	O	6.378220	-2.184650	-2.387849
C	-0.659211	2.313600	0.289131	H	5.961500	-2.837229	-2.956816
C	-0.743913	3.687478	0.060930	O	0.321194	5.829217	-0.202143
C	0.394662	4.492334	0.005226	H	-0.598843	6.086540	-0.306127
C	1.674446	3.957580	0.199778	O	-7.464852	-1.737985	-0.570753
C	2.623859	0.553957	0.871047	H	-7.324084	-2.552261	-0.080328
C	1.126849	0.426268	0.636229	O	0.687132	-4.143423	2.293803
H	-1.723894	4.148436	-0.010141	H	1.413167	-3.834810	2.842353
H	2.549303	4.591970	0.190978	O	-2.251758	-2.691120	-1.055974
C	3.147857	-1.200241	-0.942391	H	-2.608484	-1.878111	-1.429124
C	3.559352	-0.216505	-0.050964	O	2.897863	0.274947	2.218652
C	4.922026	0.101038	0.010205	H	3.851960	0.187572	2.318907
C	5.852195	-0.561490	-0.769323	VIN-C9-•OH			
C	5.427870	-1.561067	-1.644903	C	1.294223	2.934649	-0.169410
C	4.075702	-1.870642	-1.733852	C	0.341265	1.929494	0.042072
H	2.101810	-1.457527	-1.038031	C	-1.005800	2.301412	0.214378
H	5.254127	0.909035	0.654689	C	-1.304382	3.662751	0.159182
H	6.905478	-0.314490	-0.730045	C	-0.322352	4.634000	-0.068061
H	3.739536	-2.637360	-2.424658	C	1.012113	4.285617	-0.237420
O	2.907759	1.954665	0.640163	C	2.396573	1.037227	-0.162778
C	0.453257	-0.865085	0.649059	C	1.095582	0.688916	0.046859
C	0.899814	-1.882739	1.505740	H	-2.325935	3.988229	0.327350
C	-0.596631	-1.142205	-0.243881	H	1.772852	5.036122	-0.399446
C	0.290299	-3.133333	1.476170	C	3.642114	-1.080053	-0.624077
H	1.706128	-1.682008	2.199881	C	3.637622	0.272048	-0.267516

C	4.864284	0.903536	-0.022897
C	6.055939	0.206580	-0.110730
C	6.044779	-1.144996	-0.450573
C	4.833824	-1.783725	-0.710606
H	2.712471	-1.586801	-0.850294
H	4.873759	1.954194	0.237941
H	7.007086	0.687312	0.079357
H	4.823388	-2.831791	-0.992630
O	2.530907	2.396508	-0.293005
C	0.611930	-0.689048	0.287486
C	1.002385	-1.352133	1.449079
C	-0.196217	-1.333895	-0.648719
C	0.599061	-2.669557	1.662590
H	1.634011	-0.843362	2.169672
C	-0.587604	-2.650235	-0.416278
H	-0.512298	-0.811707	-1.545982
C	-0.194945	-3.327573	0.730422
H	-0.499018	-4.352436	0.897813
C	-2.042917	1.285391	0.448678
H	-1.692440	0.321118	0.800038
C	-3.349499	1.447264	0.229641
H	-3.745075	2.380009	-0.167527
C	-4.415049	0.385658	0.446681
C	-5.069971	0.134374	-0.883624
C	-3.848734	-0.878939	1.033135
C	-4.934544	-1.027245	-1.564768
H	-5.639124	0.962937	-1.288446
C	-3.738334	-2.031103	0.326417
H	-3.497175	-0.827890	2.058349
C	-4.225014	-2.115959	-1.001650
H	-5.379593	-1.162795	-2.543451
H	-3.290109	-2.910318	0.780234
O	7.240696	-1.783756	-0.519069
H	7.100270	-2.700380	-0.770607
O	-0.624308	5.959962	-0.116766
H	-1.570357	6.075362	0.001765
O	-4.095595	-3.235948	-1.753277
H	-3.478638	-3.834537	-1.315257
O	0.955251	-3.366553	2.770465
H	1.510781	-2.815253	3.328106
O	-1.372710	-3.335633	-1.296609
H	-1.626654	-2.755354	-2.022827
O	-5.430057	0.941382	1.296411
H	-4.989681	1.272900	2.085551

VIN-C9'-OH

C	1.914183	2.544046	0.265959
C	0.724943	1.820818	0.369665
C	-0.493427	2.527635	0.386474
C	-0.443286	3.911098	0.262739
C	0.776665	4.597997	0.145279
C	1.988912	3.923158	0.152045
C	2.480619	0.424896	0.378989
C	1.120177	0.421757	0.431419
H	-1.371196	4.474263	0.296731
H	2.926425	4.455300	0.073313
C	3.136491	-1.809310	-0.489969
C	3.522129	-0.679492	0.425911
C	4.890274	-0.137491	0.100515
C	5.727938	-0.728321	-0.782087
C	5.313179	-1.852732	-1.534408
C	4.003307	-2.356654	-1.378454
H	2.135640	-2.205885	-0.387209
H	5.204120	0.744729	0.645132
H	6.727371	-0.345163	-0.950416
H	3.680929	-3.192574	-1.993179
O	2.975037	1.702976	0.283044
C	0.219080	-0.750371	0.520054
C	0.381538	-1.687902	1.539144
C	-0.811927	-0.904004	-0.409855
C	-0.490725	-2.773716	1.618290
H	1.204681	-1.584651	2.236834
C	-1.705748	-1.966369	-0.284183
H	-0.930626	-0.186941	-1.213779
C	-1.544779	-2.911248	0.724031
H	-2.234089	-3.740458	0.811148
C	-1.755247	1.785054	0.504901
H	-1.749816	0.972770	1.224005
C	-2.800733	1.922774	-0.315482
H	-2.760590	2.671582	-1.103849
C	-3.934505	0.989236	-0.356111
C	-4.660415	0.842499	-1.545863
C	-4.261613	0.148341	0.714717
C	-5.647335	-0.122912	-1.680712
H	-4.433291	1.489610	-2.386785
C	-5.249356	-0.814497	0.593839
H	-3.738406	0.246870	1.658397
C	-5.939454	-0.963591	-0.609155

H	-6.200036	-0.244338	-2.603673	C	-0.068069	-3.407464	0.536815
H	-5.479318	-1.463547	1.432675	H	-0.448721	-4.412394	0.660642
O	6.203498	-2.381437	-2.404984	C	-1.711081	1.201601	0.488612
H	5.806712	-3.133007	-2.854482	H	-1.426983	0.292269	1.003538
O	0.822405	5.953841	0.036300	C	-2.944160	1.304576	-0.060200
H	-0.071843	6.303800	0.048769	H	-3.212250	2.226676	-0.569988
O	-6.907358	-1.896291	-0.789380	C	-3.933573	0.267215	-0.095427
H	-6.973261	-2.445577	-0.003787	C	-5.265460	0.640052	-0.697823
O	-0.364595	-3.724907	2.581307	C	-3.705927	-1.037261	0.343116
H	0.418778	-3.535856	3.105003	C	-6.259573	-0.478703	-0.734022
O	-2.750321	-2.141824	-1.135895	H	-5.079656	0.978442	-1.732796
H	-2.971967	-1.300993	-1.552439	C	-4.669326	-2.020216	0.247167
O	3.541720	-1.240783	1.764415	H	-2.743967	-1.299839	0.769000
H	3.881391	-0.556738	2.352989	C	-5.968025	-1.716372	-0.290120
VIN-C10'-OH				H	-7.242009	-0.280984	-1.148600
C	1.648327	2.836293	0.063897	H	-4.446656	-3.029894	0.575618
C	0.683123	1.832403	0.197346	O	7.494627	-1.941271	-0.799700
C	-0.664657	2.212799	0.362539	H	7.335045	-2.798775	-1.202698
C	-0.953965	3.577851	0.372328	O	-0.239227	5.878463	0.264167
C	0.046511	4.548465	0.236471	H	-1.184548	5.997523	0.385635
C	1.380848	4.193523	0.078722	O	-6.912582	-2.696244	-0.364174
C	2.720555	0.927295	-0.083149	H	-6.565549	-3.503792	0.021782
C	1.414175	0.580926	0.101369	O	1.457262	-3.797961	2.272478
H	-1.979698	3.894799	0.534162	H	2.154029	-3.359838	2.768444
H	2.152619	4.943508	-0.021936	O	-1.636892	-3.054548	-1.167160
C	3.921049	-1.118346	-0.856250	H	-2.058710	-2.334674	-1.646648
C	3.945821	0.154645	-0.279603	O	-5.744394	1.767680	0.046799
C	5.181937	0.700584	0.088335	H	-6.578383	2.040955	-0.345373
C	6.356080	-0.009308	-0.090995	VIN-C10'-OH			
C	6.315386	-1.285561	-0.649419	C	1.657749	2.751454	-0.066014
C	5.093994	-1.835547	-1.035312	C	0.528259	1.941957	0.102825
H	2.980784	-1.547265	-1.179788	C	-0.720420	2.556908	0.322472
H	5.213001	1.694093	0.517869	C	-0.770851	3.944595	0.316282
H	7.315568	0.403723	0.193084	C	0.385571	4.721252	0.126444
H	5.062258	-2.821093	-1.488913	C	1.630784	4.135615	-0.061463
O	2.877563	2.290394	-0.097446	C	2.354322	0.674338	-0.229521
C	0.895052	-0.797664	0.238171	C	1.001067	0.581530	-0.009491
C	1.432838	-1.634329	1.215152	H	-1.720950	4.437054	0.500411
C	-0.123013	-1.265917	-0.594624	H	2.517712	4.739276	-0.192335
C	0.959725	-2.938840	1.346605	C	3.114950	-1.561691	-0.957864
H	2.222880	-1.266416	1.861546	C	3.381370	-0.305377	-0.439447
C	-0.611022	-2.561494	-0.422976	C	4.767579	0.070905	0.012015
H	-0.545304	-0.616370	-1.354662	C	5.802047	-0.962593	-0.303925

C	5.479453	-2.174799	-0.801434
C	4.123482	-2.496932	-1.133988
H	2.103526	-1.812437	-1.253800
H	5.042256	1.025617	-0.458455
H	6.840165	-0.736241	-0.088863
H	3.892082	-3.471091	-1.551305
O	2.759474	1.991176	-0.249317
C	0.227932	-0.663711	0.181573
C	0.631929	-1.567836	1.164772
C	-0.908729	-0.925310	-0.584221
C	-0.107599	-2.730103	1.373113
H	1.521745	-1.359398	1.751232
C	-1.663764	-2.071087	-0.330548
H	-1.220150	-0.228320	-1.353684
C	-1.261375	-2.982799	0.639023
H	-1.846101	-3.873107	0.828008
C	-1.904996	1.710067	0.519605
H	-1.769531	0.874819	1.199368
C	-3.030550	1.789496	-0.195071
H	-3.125590	2.563871	-0.953333
C	-4.085330	0.766471	-0.159864
C	-4.872613	0.550143	-1.298637
C	-4.275320	-0.084429	0.935526
C	-5.787700	-0.490931	-1.361699
H	-4.751777	1.202832	-2.157001
C	-5.191749	-1.121801	0.887101
H	-3.702631	0.069386	1.842460
C	-5.944661	-1.338203	-0.266855
H	-6.388207	-0.665842	-2.245434
H	-5.317454	-1.775166	1.744406
O	6.465224	-3.094436	-1.009751
H	6.090424	-3.874891	-1.424215
O	0.336929	6.080244	0.133776
H	-0.568120	6.365577	0.281903
O	-6.847700	-2.343769	-0.376910
H	-6.816404	-2.890813	0.412383
O	0.243760	-3.649870	2.310131
H	1.055114	-3.365739	2.739802
O	-2.801105	-2.356187	-1.016286
H	-3.153847	-1.549467	-1.410232
O	4.653326	0.289160	1.430144
H	5.473462	0.690746	1.730153

VIN-C11-•OH

C	2.152193	2.742560	0.049852
C	1.016653	1.948256	0.220571
C	-0.225734	2.574886	0.427113
C	-0.262784	3.963974	0.410140
C	0.901612	4.727416	0.221547
C	2.141618	4.127485	0.045286
C	2.823470	0.654343	-0.089004
C	1.479521	0.575927	0.122711
H	-1.209338	4.466683	0.584739
H	3.035171	4.721038	-0.087524
C	3.567914	-1.614990	-0.804049
C	3.866650	-0.347566	-0.295954
C	5.201350	-0.038858	-0.004459
C	6.205773	-0.971726	-0.192763
C	5.892126	-2.238063	-0.682775
C	4.570239	-2.554577	-0.991357
H	2.547976	-1.865441	-1.067752
H	5.444716	0.946571	0.372427
H	7.239587	-0.742527	0.032280
H	4.326481	-3.533625	-1.391636
O	3.246203	1.962550	-0.124931
C	0.649381	-0.641864	0.252166
C	0.922749	-1.576132	1.251218
C	-0.442188	-0.830081	-0.594303
C	0.096230	-2.689612	1.395878
H	1.772499	-1.428242	1.909946
C	-1.290249	-1.920408	-0.401691
H	-0.655377	-0.106168	-1.372768
C	-1.019336	-2.862352	0.583557
H	-1.676343	-3.709526	0.727808
C	-1.418567	1.739925	0.637689
H	-1.287756	0.919451	1.336427
C	-2.543361	1.808944	-0.077315
H	-2.644038	2.566435	-0.851070
C	-3.595658	0.777746	-0.019686
C	-4.374548	0.559557	-1.119044
C	-3.741234	-0.051902	1.135438
C	-5.395254	-0.529370	-1.204136
H	-4.297520	1.204402	-1.987951
C	-4.686688	-1.090622	1.151064
H	-3.154856	0.147112	2.021205
C	-5.463063	-1.332786	0.058146
H	-5.137301	-1.226655	-2.021662
H	-4.797909	-1.704607	2.039613

O	6.913739	-3.117895	-0.845369	H	-1.856559	0.837860	1.251938
H	6.571427	-3.943276	-1.198483	C	-3.140429	1.710941	-0.149720
O	0.867426	6.088096	0.218647	H	-3.257611	2.489189	-0.900947
H	-0.036826	6.383352	0.350858	C	-4.153443	0.646317	-0.142401
O	-6.404896	-2.299991	-0.027285	C	-4.929821	0.429532	-1.288682
H	-6.452019	-2.789820	0.799612	C	-4.311110	-0.240879	0.928975
O	0.319747	-3.635617	2.346794	C	-5.802061	-0.645232	-1.382809
H	1.114120	-3.407461	2.836712	H	-4.834793	1.110574	-2.128110
O	-2.398506	-2.107738	-1.166351	C	-5.184715	-1.312623	0.849530
H	-2.640135	-1.263689	-1.566085	H	-3.746292	-0.090019	1.841344
O	-6.661077	0.056774	-1.504383	C	-5.926220	-1.527751	-0.312032
H	-7.296534	-0.664101	-1.558696	H	-6.394224	-0.819418	-2.272300
VIN-C11'-OH				H	-5.285636	-1.993622	1.688497
C	1.490099	2.871798	-0.001822	O	6.512934	-2.762853	-1.086549
C	0.403779	2.014008	0.182136	H	6.214544	-3.600971	-1.453821
C	-0.871544	2.570143	0.392045	O	0.020643	6.139528	0.177875
C	-0.985894	3.955083	0.376439	H	-0.896594	6.383154	0.324971
C	0.132142	4.783298	0.180252	O	-6.787752	-2.565579	-0.451829
C	1.401749	4.254184	-0.008471	H	-6.742225	-3.127477	0.326230
C	2.279022	0.827892	-0.150034	O	0.164616	-3.591104	2.361771
C	0.944610	0.670084	0.078344	H	0.940712	-3.288615	2.840383
H	-1.958708	4.403779	0.553938	O	-2.733542	-2.348376	-1.108976
H	2.259413	4.896150	-0.152069	H	-3.095816	-1.545106	-1.501060
C	3.101721	-1.416853	-0.887578	H	6.608862	-0.194708	-0.901418
C	3.379075	-0.115927	-0.369037	O	6.510767	-0.818215	0.989280
C	4.663335	0.268661	-0.115050	H	5.848357	-1.128245	1.614990
C	5.839130	-0.644270	-0.262435	VIN-C12'-OH			
C	5.451554	-1.966885	-0.854949	C	1.998395	2.812439	-0.014647
C	4.154886	-2.317267	-1.113476	C	0.884850	2.003498	0.229210
H	2.088941	-1.699056	-1.136052	C	-0.363492	2.620639	0.443596
H	4.873224	1.261181	0.263495	C	-0.420537	4.013234	0.378433
H	3.938497	-3.297398	-1.528361	C	0.722742	4.785001	0.133691
O	2.624175	2.156789	-0.191946	C	1.965905	4.194791	-0.066999
C	0.199915	-0.599156	0.237997	C	2.702858	0.736329	-0.120096
C	0.570051	-1.498026	1.238129	C	1.369841	0.637930	0.154382
C	-0.892327	-0.882245	-0.582941	H	-1.367618	4.510560	0.565284
C	-0.156214	-2.676145	1.408619	H	2.845170	4.794929	-0.254316
H	1.417488	-1.272960	1.877613	C	3.469692	-1.531542	-0.823094
C	-1.636943	-2.042574	-0.369122	C	3.757347	-0.251299	-0.340765
H	-1.179530	-0.187371	-1.363773	C	5.093207	0.086907	-0.090069
C	-1.265573	-2.949434	0.617774	C	6.110144	-0.829443	-0.291407
H	-1.842550	-3.850610	0.776533	C	5.807834	-2.108676	-0.754444
C	-2.020479	1.672021	0.577145	C	4.484548	-2.454419	-1.023800

H	2.448437	-1.805878	-1.056444	C	-0.936307	2.562370	0.400245
H	5.327758	1.082286	0.265801	C	-1.086965	3.942600	0.385650
H	7.144900	-0.577624	-0.097083	C	0.015476	4.802351	0.237546
H	4.249007	-3.443679	-1.403180	C	1.308531	4.310199	0.100530
O	3.098361	2.048440	-0.214137	C	2.299504	0.907970	-0.026968
C	0.623409	-0.622410	0.380479	C	0.935703	0.721913	0.146509
C	1.042562	-1.476650	1.399538	H	-2.076933	4.364412	0.530514
C	-0.469805	-0.970545	-0.417475	H	2.152486	4.977805	-0.000358
C	0.380383	-2.685915	1.604895	C	3.221454	-1.364554	-0.527300
H	1.893298	-1.201849	2.014552	C	3.398700	0.027484	-0.206398
C	-1.137570	-2.174331	-0.181681	C	4.739531	0.533477	-0.096722
H	-0.797340	-0.310613	-1.213814	C	5.808708	-0.274315	-0.235678
C	-0.711597	-3.037869	0.821948	C	5.698060	-1.742012	-0.540772
H	-1.231615	-3.970299	0.996533	C	4.274050	-2.190768	-0.671825
C	-1.534434	1.786775	0.671367	H	2.220575	-1.746389	-0.678176
H	-1.351771	0.869170	1.215240	H	4.873083	1.584997	0.123064
C	-2.755195	1.983652	0.101493	H	6.819623	0.108174	-0.134609
H	-2.902705	2.861577	-0.523578	H	4.149774	-3.236454	-0.926913
C	-3.793105	1.014060	0.102085	O	2.597683	2.257656	-0.035464
C	-4.889971	1.142350	-0.818925	C	0.209600	-0.557051	0.296225
C	-3.745484	-0.175792	0.917418	C	0.542587	-1.420244	1.340769
C	-5.712527	0.112270	-1.085997	C	-0.840490	-0.875420	-0.565546
H	-5.023938	2.093152	-1.324593	C	-0.177394	-2.601773	1.512078
C	-4.568799	-1.212026	0.691728	H	1.360946	-1.169733	2.008038
H	-3.043327	-0.224642	1.741380	C	-1.582020	-2.037799	-0.350862
C	-5.486148	-1.251113	-0.495491	H	-1.097988	-0.207249	-1.379275
H	-6.522057	0.200026	-1.802825	C	-1.247319	-2.909454	0.679325
H	-4.561798	-2.099433	1.315122	H	-1.818804	-3.814571	0.835671
O	6.841123	-2.971312	-0.930701	C	-2.067108	1.636615	0.548502
H	6.506027	-3.809026	-1.261095	H	-1.903883	0.804827	1.226174
O	0.673456	6.144178	0.090570	C	-3.167718	1.654016	-0.208546
H	-0.228651	6.435328	0.244716	H	-3.280423	2.430409	-0.962418
O	-4.901446	-2.022370	-1.545214	C	-4.159280	0.570042	-0.227429
H	-4.638344	-2.871867	-1.166492	C	-4.898921	0.336636	-1.394550
O	0.754763	-3.559452	2.575105	C	-4.328867	-0.318205	0.841273
H	1.517206	-3.206310	3.041226	C	-5.745630	-0.755876	-1.510994
O	-2.206638	-2.575600	-0.916674	H	-4.794470	1.018464	-2.232227
H	-2.642430	-1.825115	-1.340704	C	-5.177646	-1.407602	0.739488
O	-6.676893	-1.865822	-0.075571	H	-3.793079	-0.154670	1.768864
H	-7.232304	-1.972251	-0.854998	C	-5.881208	-1.639604	-0.442367
VIN-C12'-•OH				H	-6.309034	-0.943603	-2.416247
C	1.436437	2.933485	0.102865	H	-5.288370	-2.089190	1.576699
C	0.364455	2.040989	0.233059	O	6.306392	-2.524065	0.452005
				H	7.257362	-2.434603	0.325089

O	-0.132569	6.152148	0.236643
H	-1.061366	6.372389	0.344541
O	-6.716317	-2.694920	-0.604734
H	-6.680435	-3.256306	0.174259
O	0.107928	-3.484960	2.503304
H	0.889894	-3.189226	2.977223
O	-2.638899	-2.379367	-1.131655
H	-2.998281	-1.591404	-1.555775
O	6.421532	-2.035668	-1.735270
H	6.077794	-1.467482	-2.431410

VIN-C13'-OH

C	2.153945	2.734539	0.050197
C	0.991172	1.974742	0.195461
C	-0.234839	2.642087	0.372207
C	-0.225950	4.031719	0.372517
C	0.966689	4.758363	0.221307
C	2.188718	4.118979	0.059024
C	2.764326	0.628860	-0.089106
C	1.414995	0.588520	0.101238
H	-1.160690	4.563156	0.524315
H	3.103901	4.683285	-0.052222
C	3.458117	-1.661838	-0.789175
C	3.782070	-0.403008	-0.275166
C	5.118784	-0.132222	0.043717
C	6.099966	-1.093332	-0.123743
C	5.760600	-2.350681	-0.619804
C	4.436854	-2.629758	-0.955573
H	2.437026	-1.883645	-1.073385
H	5.382367	0.846105	0.425428
H	7.135030	-0.893296	0.122342
H	4.173579	-3.601927	-1.360174
O	3.226237	1.923123	-0.114640
C	0.573281	-0.619407	0.261912
C	0.858627	-1.517610	1.290230
C	-0.523662	-0.842793	-0.571857
C	0.044099	-2.632403	1.479803
H	1.710966	-1.339895	1.937936
C	-1.356281	-1.937054	-0.337414
H	-0.752648	-0.144347	-1.369118
C	-1.071827	-2.842600	0.677812
H	-1.713374	-3.696806	0.849348
C	-1.460106	1.839889	0.493101
H	-1.388949	0.972339	1.140770

C	-2.549007	1.985633	-0.265142
H	-2.592354	2.793153	-0.992466
C	-3.615542	0.968697	-0.330793
C	-4.273101	0.791022	-1.585462
C	-3.892628	0.129228	0.708737
C	-5.159696	-0.283126	-1.791666
H	-4.068715	1.482229	-2.393649
C	-4.853168	-1.007376	0.602860
H	-3.442019	0.279015	1.682559
C	-5.400225	-1.166198	-0.783554
H	-5.636424	-0.442168	-2.751259
H	-4.332290	-1.944939	0.875501
O	6.759862	-3.259143	-0.760952
H	6.401862	-4.075145	-1.120274
O	0.978107	6.119206	0.235527
H	0.083208	6.443009	0.364567
O	-6.249176	-2.211671	-0.972599
H	-5.954366	-2.957447	-0.437231
O	0.281439	-3.544061	2.458543
H	1.071818	-3.289712	2.942152
O	-2.472852	-2.172770	-1.079146
H	-2.699538	-1.384805	-1.588152
O	-5.912675	-0.785350	1.541709
H	-6.623190	-1.400059	1.335462

VIN-C13'-OH

C	1.069421	3.169458	-0.107071
C	0.164148	2.118745	0.082237
C	-1.186223	2.436798	0.328101
C	-1.543256	3.781841	0.342266
C	-0.603446	4.802102	0.132088
C	0.734525	4.512466	-0.094559
C	2.230953	1.322427	-0.272991
C	0.954191	0.902905	-0.032478
H	-2.572584	4.047315	0.563685
H	1.462415	5.297808	-0.241579
C	3.503437	-0.631844	-1.034191
C	3.484797	0.573108	-0.395487
C	4.644147	1.058216	0.271379
C	5.787585	0.249508	0.378841
C	5.786062	-1.018299	-0.125657
C	4.633759	-1.588232	-0.887196
H	2.635847	-0.973939	-1.586673
H	4.619185	2.035788	0.732956

H	6.664968	0.591500	0.913273	C	0.154613	4.644712	-0.158187
H	4.998038	-1.928085	-1.869536	C	1.473080	4.214386	-0.035876
O	2.319799	2.688061	-0.311081	C	2.652950	0.896709	0.113153
C	0.543873	-0.515592	0.089387	C	1.324779	0.605447	-0.008264
C	1.328095	-1.390574	0.841748	H	-1.909522	4.120749	-0.293281
C	-0.559186	-1.010547	-0.609683	H	2.291090	4.918957	0.017367
C	1.071763	-2.757943	0.808202	C	3.797231	-1.221470	0.769337
H	2.182268	-1.019586	1.395308	C	3.851247	0.069128	0.234155
C	-0.870753	-2.369524	-0.537516	C	5.092755	0.576838	-0.169505
H	-1.169982	-0.345469	-1.210852	C	6.242676	-0.185576	-0.064932
C	-0.044837	-3.255501	0.144607	C	6.171832	-1.477409	0.453031
H	-0.263153	-4.315152	0.151027	C	4.945758	-1.990313	0.873927
C	-2.175728	1.372933	0.545974	H	2.854461	-1.624359	1.117692
H	-1.832835	0.529232	1.134658	H	5.147564	1.581939	-0.568461
C	-3.394606	1.353003	-0.003541	H	7.205649	0.197391	-0.377849
H	-3.705873	2.199378	-0.612609	H	4.891558	-2.989331	1.294679
C	-4.341946	0.232541	0.056584	O	2.871603	2.249583	0.120001
C	-5.641642	0.394182	-0.440556	C	0.782494	-0.763228	-0.185070
C	-3.981951	-1.034135	0.532953	C	-0.152401	-1.297121	0.699861
C	-6.551667	-0.649361	-0.452266	C	1.235543	-1.526232	-1.261909
H	-5.942224	1.362924	-0.825325	C	-0.679253	-2.571788	0.466057
C	-4.879442	-2.091370	0.514154	H	-0.505586	-0.718134	1.545058
H	-2.983601	-1.210841	0.917471	C	0.753630	-2.821209	-1.441292
C	-6.171313	-1.902184	0.024222	H	1.966754	-1.109915	-1.947027
H	-7.557031	-0.521107	-0.832931	C	-0.211462	-3.346298	-0.589977
H	-4.567728	-3.068892	0.868337	H	-0.613526	-4.335672	-0.762679
O	6.838829	-1.841328	0.047495	C	-1.791210	1.401436	-0.174785
H	6.522286	-2.746852	-0.061017	H	-1.498326	0.368457	-0.084223
O	-0.957861	6.115229	0.158782	C	-3.130251	1.663361	-0.234941
H	-1.899079	6.187004	0.335770	H	-3.486748	2.681093	-0.371340
O	-7.092350	-2.898120	-0.021301	C	-4.127177	0.663441	-0.113710
H	-6.710299	-3.704360	0.335639	C	-5.490685	0.988053	-0.238022
O	1.903016	-3.649659	1.410440	C	-3.730469	-0.754657	0.239430
H	2.762909	-3.227721	1.530166	C	-6.478965	0.042186	-0.161412
O	-1.967505	-2.892513	-1.149590	H	-5.757080	2.024498	-0.417461
H	-2.547471	-2.178306	-1.434372	C	-4.856799	-1.735989	0.199833
O	4.247095	-2.785313	-0.148624	H	-2.923975	-1.093848	-0.419859
H	3.631192	-3.292254	-0.689659	C	-6.135800	-1.344100	0.043949
VIN-C14-OH				H	-7.526009	0.293655	-0.266314
C	1.662421	2.847341	0.010109	H	-4.593505	-2.779076	0.345995
C	0.640694	1.889106	-0.057728	O	7.327468	-2.185485	0.530283
C	-0.695706	2.346587	-0.170635	H	7.147946	-3.050433	0.908270
C	-0.898960	3.733686	-0.218155	O	-0.048685	5.989545	-0.206816
				H	-0.988505	6.166687	-0.294089

O	-7.204610	-2.183434	0.047359	C	-3.909335	0.750197	-0.330433
H	-6.896778	-3.084842	0.179141	C	-4.584223	0.508563	-1.533995
O	-1.660442	-3.088373	1.244375	C	-4.204731	-0.074443	0.760891
H	-2.127662	-2.350629	1.671490	C	-5.489257	-0.534597	-1.661922
O	1.175482	-3.613246	-2.462094	H	-4.381889	1.143711	-2.390322
H	1.834046	-3.139118	-2.976493	C	-5.112888	-1.113829	0.647738
O	-3.104989	-0.776391	1.552086	H	-3.719291	0.098629	1.714206
H	-3.773842	-0.497822	2.187198	C	-5.749877	-1.357693	-0.568574
VIN-C14'-•OH				H	-6.003506	-0.729462	-2.594583
C	1.777262	2.808005	0.129504	H	-5.321569	-1.747791	1.503622
C	0.654235	1.988323	0.289270	O	6.694735	-2.918318	-0.766447
C	-0.617437	2.584443	0.408044	H	6.407089	-3.822301	-0.921799
C	-0.687731	3.970037	0.346887	O	0.395612	6.115492	0.144889
C	0.465682	4.758908	0.190361	H	-0.520472	6.390373	0.233577
C	1.729207	4.189833	0.080848	O	-6.638600	-2.367735	-0.742376
C	2.506025	0.727985	0.055760	H	-6.684727	-2.894979	0.059505
C	1.142751	0.633538	0.243131	O	-0.348913	-3.072452	3.064959
H	-1.654706	4.452943	0.450921	H	0.371624	-2.736205	3.604001
H	2.609615	4.804916	-0.040636	O	-2.540927	-2.342592	-1.015222
C	3.148274	-1.660283	-0.466768	H	-2.746620	-1.613516	-1.610344
C	3.539923	-0.236048	-0.133641	O	2.331733	-1.690528	-1.643860
C	4.879748	0.157687	-0.140767	H	2.886619	-1.381241	-2.367701
C	5.900358	-0.744467	-0.352502	TS(VIN-C2-•OH)			
C	5.599177	-2.129418	-0.588482	C	1.742974	2.719138	0.048213
C	4.326721	-2.573341	-0.619403	C	0.656617	1.833592	0.312131
H	2.482983	-2.056008	0.305144	C	-0.671909	2.348378	0.148340
H	5.114880	1.200259	0.032035	C	-0.811259	3.720369	-0.003098
H	6.939138	-0.442335	-0.348341	C	0.304237	4.569539	-0.110656
H	4.100285	-3.617966	-0.808358	C	1.613502	4.076334	-0.108110
O	2.892583	2.055604	0.004302	C	2.554254	0.676888	-0.053875
C	0.311966	-0.572823	0.459091	C	1.225155	0.498617	0.121741
C	0.433529	-1.277067	1.657501	H	-1.806724	4.152807	-0.029137
C	-0.663456	-0.931796	-0.467108	H	2.455358	4.733984	-0.271386
C	-0.424676	-2.346041	1.917213	C	3.587805	-1.589532	0.128111
H	1.181978	-0.978709	2.385167	C	3.681538	-0.237717	-0.218118
C	-1.541384	-1.973901	-0.173207	C	4.896203	0.240594	-0.727411
H	-0.750079	-0.386551	-1.399784	C	5.978397	-0.602938	-0.901653
C	-1.420263	-2.690995	1.012858	C	5.867460	-1.950654	-0.565135
H	-2.102279	-3.501654	1.232057	C	4.669468	-2.438775	-0.046844
C	-1.803122	1.723642	0.531223	H	2.671888	-1.982745	0.549313
H	-1.724291	0.908855	1.244362	H	4.985286	1.287781	-0.985538
C	-2.855827	1.773386	-0.289819	H	6.919318	-0.240752	-1.295797
H	-2.878484	2.526421	-1.074877	H	4.585083	-3.484867	0.230021

O	2.887357	2.022372	-0.089073	C	2.540057	0.507316	0.107786
C	0.497162	-0.780946	0.267140	C	1.190403	0.320755	0.207112
C	0.118897	-1.198683	1.543439	H	-1.803917	4.023149	0.619432
C	0.188816	-1.551353	-0.850572	H	2.446970	4.526110	0.591977
C	-0.564866	-2.404932	1.688817	C	3.529734	-1.637026	-0.693989
H	0.343442	-0.560720	2.392429	C	3.672199	-0.403317	-0.052888
C	-0.494685	-2.757556	-0.683035	C	4.937879	-0.033797	0.418921
H	0.483426	-1.213021	-1.838201	C	6.025441	-0.876941	0.275968
C	-0.871166	-3.192100	0.582188	C	5.866112	-2.112672	-0.348875
H	-1.397514	-4.129430	0.704750	C	4.615148	-2.487617	-0.836658
C	-1.799351	1.426754	0.216992	H	2.567554	-1.929944	-1.095545
H	-1.637674	0.550713	0.833310	H	5.061897	0.927316	0.902241
C	-2.952441	1.561219	-0.450880	H	7.006848	-0.601088	0.640111
H	-3.112888	2.439667	-1.072912	H	4.493149	-3.440931	-1.340897
C	-4.028991	0.565541	-0.448052	O	2.857683	1.839705	0.158355
C	-5.321849	0.923270	-0.848070	C	0.499396	-0.986462	0.246455
C	-3.800755	-0.766439	-0.081380	C	0.871039	-1.927095	1.206173
C	-6.358735	0.005014	-0.852318	C	-0.514891	-1.283119	-0.665119
H	-5.517957	1.945833	-1.153021	C	0.234674	-3.166809	1.240979
C	-4.828455	-1.694752	-0.086132	H	1.659010	-1.691323	1.913867
H	-2.801575	-1.095152	0.184289	C	-1.165522	-2.515114	-0.592126
C	-6.114679	-1.310825	-0.465839	H	-0.807947	-0.549949	-1.409506
H	-7.361204	0.281210	-1.153689	C	-0.789820	-3.465301	0.350360
H	-4.626527	-2.725061	0.190743	H	-1.296148	-4.420065	0.397904
O	6.957237	-2.736533	-0.757776	C	-1.846604	1.289648	0.537266
H	6.756635	-3.634790	-0.481873	H	-1.678661	0.338583	1.028938
O	0.162863	5.908622	-0.244842	C	-3.028104	1.541362	-0.042255
H	-0.771261	6.133601	-0.268652	H	-3.164341	2.489396	-0.557998
O	-7.160389	-2.177518	-0.491533	C	-4.154182	0.606891	-0.130750
H	-6.862176	-3.044362	-0.203800	C	-5.371481	1.041917	-0.671544
O	-0.963577	-2.865353	2.901671	C	-4.053432	-0.738118	0.246858
H	-0.704567	-2.231969	3.576884	C	-6.448840	0.185327	-0.819687
O	-0.825785	-3.553399	-1.732155	H	-5.471002	2.077018	-0.980387
H	-0.541274	-3.134932	-2.548981	C	-5.119885	-1.609031	0.091183
O	0.670771	1.794354	2.270796	H	-3.128649	-1.123503	0.660746
H	0.333007	2.683579	2.448927	C	-6.325201	-1.149584	-0.440060
TS(VIN-C4-•OH)				H	-7.390334	0.523737	-1.233267
C	1.695240	2.521387	0.268534	H	-5.009760	-2.651948	0.371219
C	0.615683	1.648445	0.311799	O	6.963197	-2.903659	-0.459379
C	-0.690804	2.183694	0.472401	H	6.728463	-3.716603	-0.914676
C	-0.826142	3.570189	0.515069	O	0.087954	5.746806	0.408159
C	0.276575	4.418072	0.434349	H	0.784582	6.090263	-0.176103
C	1.596831	3.915428	0.325230	O	-7.402551	-1.955452	-0.617155
				H	-7.191548	-2.843135	-0.315667

O	0.564601	-4.123512	2.145530	C	-3.978721	-0.837433	0.358719
H	1.277845	-3.800709	2.702731	C	-6.345267	-0.209468	-0.955931
O	-2.194402	-2.841969	-1.417270	H	-5.417646	1.660037	-1.408745
H	-2.497586	-2.054262	-1.879587	C	-5.010479	-1.762824	0.315229
O	1.733974	4.924381	-1.514311	H	-3.063721	-1.107840	0.873533
H	2.586062	4.552693	-1.778780	C	-6.201349	-1.450850	-0.340069
TS(VIN-C5-•OH)				H	-7.274992	0.015078	-1.463142
C	1.643208	2.642137	-0.178390	H	-4.882905	-2.734807	0.781234
C	0.597367	1.732894	0.043371	O	7.024578	-2.681556	-0.780943
C	-0.725387	2.229800	0.197624	H	6.780583	-3.556922	-1.093464
C	-0.902854	3.595380	0.114968	O	-0.064062	5.808300	-0.363398
C	0.187546	4.502233	-0.054475	H	-0.321861	6.222292	0.470273
C	1.489450	4.005967	-0.264875	O	-7.244922	-2.315601	-0.417048
C	2.545118	0.645388	-0.201308	H	-7.021548	-3.128744	0.043614
C	1.211390	0.428630	0.035405	O	0.934710	-3.726843	2.590626
H	-1.889988	4.026433	0.233279	H	1.658794	-3.297086	3.053668
H	2.309537	4.687454	-0.439615	O	-2.086125	-3.083739	-0.931671
C	3.533586	-1.564140	-0.803502	H	-2.479421	-2.376319	-1.453098
C	3.689001	-0.247923	-0.357276	O	0.390584	4.972835	1.935501
C	4.980587	0.222604	-0.085006	H	0.179281	4.142969	2.385323
C	6.082351	-0.600383	-0.229526	TS(VIN-C5'-•OH)			
C	5.912315	-1.916061	-0.658769	C	2.015959	2.745046	0.039513
C	4.634534	-2.392843	-0.949768	C	0.871160	1.959751	0.176521
H	2.549040	-1.940059	-1.052254	C	-0.372732	2.582786	0.375391
H	5.111671	1.246071	0.243165	C	-0.398826	3.972138	0.395547
H	7.083567	-0.247569	-0.017869	C	0.774893	4.731280	0.246721
H	4.502933	-3.410526	-1.303015	C	2.014563	4.129715	0.069683
O	2.819090	1.976370	-0.320890	C	2.665526	0.650735	-0.141885
C	0.585330	-0.887381	0.294715	C	1.318586	0.588018	0.049259
C	1.063568	-1.668291	1.346561	H	-1.344675	4.478343	0.563931
C	-0.461777	-1.353406	-0.500876	H	2.912275	4.722334	-0.036113
C	0.500863	-2.920203	1.588992	C	3.388638	-1.644618	-0.793763
H	1.878779	-1.301710	1.961761	C	3.701055	-0.359880	-0.340368
C	-1.036100	-2.594599	-0.221928	C	5.042866	-0.045621	-0.089328
H	-0.836783	-0.746515	-1.318152	C	6.040259	-0.987710	-0.266901
C	-0.553709	-3.387005	0.813091	C	5.713295	-2.270167	-0.703440
H	-1.001668	-4.349670	1.019996	C	4.384101	-2.593584	-0.969631
C	-1.851591	1.300825	0.380299	H	2.363180	-1.904246	-1.024124
H	-1.676325	0.467633	1.052307	H	5.297153	0.951083	0.248037
C	-3.004843	1.391611	-0.289633	H	7.079215	-0.753804	-0.072498
H	-3.139793	2.224183	-0.977216	H	4.128419	-3.586641	-1.325282
C	-4.100291	0.414308	-0.256049	O	3.102598	1.955244	-0.143328
C	-5.302189	0.700291	-0.916472	C	0.445811	-0.600688	0.165833

C	0.576935	-1.460420	1.231598	H	1.996241	4.846946	0.016042
C	-0.583050	-0.802906	-0.774878	C	3.832598	-1.225943	0.374124
C	-0.384150	-2.497055	1.427452	C	3.797140	0.066226	-0.158238
H	1.348142	-1.306603	1.977420	C	4.989680	0.634028	-0.624246
C	-1.491715	-1.852071	-0.624853	C	6.178097	-0.073014	-0.583850
H	-0.683288	-0.118014	-1.609823	C	6.196316	-1.368108	-0.068675
C	-1.363793	-2.733834	0.434264	C	5.019968	-1.939901	0.414390
H	-2.046019	-3.566852	0.545917	H	2.929303	-1.672667	0.770752
C	-1.574763	1.742977	0.509783	H	4.975817	1.641529	-1.020819
H	-1.494519	0.902819	1.197263	H	7.104037	0.356075	-0.944844
C	-2.651914	1.858103	-0.273150	H	5.036031	-2.940409	0.834700
H	-2.682217	2.651469	-1.017505	O	2.710560	2.201956	-0.169427
C	-3.738745	0.870826	-0.327419	C	0.704178	-0.883700	-0.405740
C	-4.528614	0.777743	-1.480920	C	-0.244500	-1.365412	0.497489
C	-3.960740	-0.059702	0.695444	C	1.155521	-1.699649	-1.442481
C	-5.482509	-0.219115	-1.630556	C	-0.752057	-2.655391	0.339079
H	-4.382819	1.496074	-2.281290	H	-0.602336	-0.730743	1.301537
C	-4.916680	-1.053006	0.558970	C	0.665962	-2.999106	-1.562385
H	-3.368146	-0.014164	1.601475	H	1.890811	-1.320401	-2.144522
C	-5.675895	-1.144695	-0.608118	C	-0.293661	-3.481573	-0.680260
H	-6.088194	-0.296380	-2.524608	H	-0.688780	-4.482090	-0.794247
H	-5.076276	-1.767953	1.360930	C	-1.920741	1.117688	-0.389977
O	6.729183	-3.157799	-0.857104	H	-1.704098	0.230579	-0.973291
H	6.376972	-3.997381	-1.163988	C	-3.070960	1.222780	0.290877
O	0.749128	6.091934	0.279710	H	-3.231609	2.116362	0.891928
H	-0.153434	6.388735	0.419644	C	-4.102580	0.184691	0.380406
O	-6.618604	-2.101651	-0.798372	C	-5.309470	0.466864	1.034074
H	-6.632825	-2.692960	-0.041338	C	-3.912686	-1.116212	-0.102541
O	-0.163503	-3.505970	2.307231	C	-6.293719	-0.494406	1.189673
H	0.147897	-3.111340	3.128930	H	-5.473577	1.464801	1.426087
O	-2.501444	-2.072268	-1.507700	C	-4.884030	-2.091654	0.059141
H	-2.798141	-1.231688	-1.876034	H	-2.991259	-1.384042	-0.607258
O	-1.495187	-1.342837	2.628167	C	-6.082277	-1.782938	0.703505
H	-2.297199	-1.880325	2.555567	H	-7.228073	-0.274198	1.690250
TS(VIN-C6-•OH)				H	-4.704213	-3.098112	-0.305638
C	1.476785	2.747865	-0.192354	O	7.386403	-2.019366	-0.055963
C	0.499685	1.741030	-0.261346	H	7.271332	-2.891715	0.330175
C	-0.852750	2.113174	-0.304022	O	-0.466153	5.758541	0.062518
C	-1.146817	3.487969	-0.231524	H	-1.283701	5.744134	0.583737
C	-0.121554	4.464116	-0.097242	O	-7.069073	-2.695707	0.892194
C	1.215402	4.107935	-0.093830	H	-6.805634	-3.535931	0.507536
C	2.555520	0.834264	-0.211641	O	-1.715044	-3.161081	1.154092
C	1.239140	0.489529	-0.279963	H	-2.098099	-2.450793	1.678827
				O	1.080047	-3.839805	-2.544405

H	1.734436	-3.393830	-3.088723	H	-4.116091	0.593498	-2.594006
O	-1.987632	4.102393	1.704105	C	-4.913925	-1.365524	0.634219
H	-1.287517	3.692936	2.234622	H	-3.612748	0.015267	1.624587
H	-2.139737	3.821097	-0.499804	C	-5.492192	-1.750846	-0.576230
TS(VIN-C7-•OH)				H	-5.681787	-1.338840	-2.664907
C	1.803053	2.753403	-0.125537	H	-5.148924	-1.911011	1.542368
C	0.716862	1.898615	0.078442	O	6.921335	-2.840895	-0.705336
C	-0.556876	2.464227	0.259360	H	6.630844	-3.709421	-0.995819
C	-0.675861	3.845731	0.218488	O	0.331373	6.024318	-0.015211
C	0.443345	4.668145	0.010452	H	-0.581493	6.267090	0.159029
C	1.712654	4.134399	-0.169479	O	-6.345425	-2.796580	-0.680541
C	2.600978	0.706652	-0.172899	H	-6.414027	-3.243349	0.167572
C	1.264539	0.555219	0.047561	O	0.504121	-3.492272	2.685583
H	-1.648747	4.282875	0.416757	H	1.256531	-3.125606	3.157458
H	2.571169	4.773129	-0.322815	O	-2.304428	-2.657210	-0.973825
C	3.486298	-1.554733	-0.738096	H	-2.633488	-1.919549	-1.500266
C	3.705154	-0.238573	-0.321076	O	-3.053494	2.703362	1.816439
C	5.018573	0.173527	-0.062554	H	-3.886871	2.642569	1.323039
C	6.079906	-0.704242	-0.195285	TS(VIN-C7'-•OH)			
C	5.846096	-2.018726	-0.594601	C	1.603809	2.764569	0.403500
C	4.545932	-2.439281	-0.869091	C	0.557795	1.839133	0.397340
H	2.483470	-1.888236	-0.974125	C	-0.768537	2.305326	0.385848
H	5.199943	1.195785	0.244573	C	-0.957012	3.688062	0.388065
H	7.097795	-0.394767	0.004910	C	0.120037	4.582420	0.398502
H	4.363405	-3.457446	-1.197978	C	1.439133	4.134778	0.406825
O	2.941829	2.034242	-0.276112	C	2.551645	0.783588	0.349419
C	0.535675	-0.708711	0.296412	C	1.188411	0.527205	0.395005
C	0.894376	-1.501713	1.386052	H	-1.967301	4.083708	0.421229
C	-0.522545	-1.094328	-0.526834	H	2.267324	4.829025	0.416104
C	0.192024	-2.677918	1.643369	C	3.614377	-1.428659	0.655759
H	1.716931	-1.197127	2.024916	C	3.700691	-0.093264	0.249389
C	-1.242926	-2.252556	-0.230474	C	4.917882	0.390539	-0.249674
H	-0.795912	-0.485917	-1.381686	C	6.014240	-0.442883	-0.365985
C	-0.882976	-3.054089	0.846863	C	5.911530	-1.778616	0.023214
H	-1.440548	-3.954033	1.069034	C	4.710616	-2.266255	0.538745
C	-1.719209	1.572643	0.429195	H	2.695437	-1.792377	1.095894
H	-1.624810	0.804362	1.187729	H	4.992997	1.428026	-0.550345
C	-2.705753	1.474638	-0.492577	H	6.959395	-0.085797	-0.754288
H	-2.699955	2.158572	-1.338205	H	4.640649	-3.299784	0.862374
C	-3.715535	0.418459	-0.486598	O	2.806019	2.121593	0.384425
C	-4.336817	0.040975	-1.686500	C	0.532301	-0.751768	-0.001290
C	-4.037724	-0.295087	0.676826	C	-0.045579	-1.618281	0.923955
C	-5.209325	-1.034896	-1.739433	C	0.461498	-1.031094	-1.364244

C	-0.700451	-2.761221	0.466681	C	3.835331	-0.721537	-0.551297
H	0.025621	-1.381050	1.978668	C	3.729521	0.562347	-0.008817
C	-0.187476	-2.187395	-1.799616	C	4.898243	1.215833	0.402083
H	0.907099	-0.348542	-2.080486	C	6.132958	0.600406	0.296633
C	-0.774465	-3.056881	-0.889212	C	6.222626	-0.687361	-0.228711
H	-1.282319	-3.948284	-1.232525	C	5.069765	-1.344140	-0.655970
C	-1.877727	1.348778	0.386006	H	2.949757	-1.233439	-0.906741
H	-1.651452	0.386457	0.829332	H	4.828356	2.217967	0.806071
C	-3.095169	1.548760	-0.131347	H	7.041095	1.097059	0.613699
H	-3.342913	2.508995	-0.579120	H	5.139460	-2.339196	-1.083890
C	-4.148315	0.526164	-0.164384	O	2.484307	2.607042	0.114836
C	-5.492187	0.893880	-0.295006	C	0.693668	-0.621347	0.284874
C	-3.847829	-0.838248	-0.081529	C	1.170565	-1.453221	1.297315
C	-6.503373	-0.053200	-0.306022	C	-0.246893	-1.103266	-0.627143
H	-5.749090	1.944677	-0.378284	C	0.704262	-2.764027	1.388616
C	-4.849148	-1.795092	-0.091938	H	1.900814	-1.075112	2.005502
H	-2.814444	-1.163556	-0.041222	C	-0.741184	-2.401423	-0.491320
C	-6.183980	-1.404828	-0.197919	H	-0.611695	-0.462371	-1.422367
H	-7.544455	0.228922	-0.399101	C	-0.259291	-3.240420	0.507568
H	-4.588870	-2.847656	-0.030135	H	-0.638727	-4.248831	0.604041
O	7.015449	-2.553631	-0.114272	C	-1.993791	1.112599	0.427723
H	6.822096	-3.444317	0.190348	H	-1.712651	0.288927	1.076168
O	-0.067734	5.928149	0.411928	C	-3.090934	0.977032	-0.360069
H	-1.009023	6.119547	0.403044	H	-3.276165	1.720450	-1.128341
O	-7.209273	-2.296406	-0.215202	C	-3.815473	-0.295300	-0.483358
H	-6.856631	-3.187116	-0.141617	C	-4.375799	-0.649151	-1.716081
O	-1.316444	-3.623633	1.319106	C	-3.893297	-1.218770	0.563680
H	-1.197074	-3.309739	2.219887	C	-4.958689	-1.892639	-1.914246
O	-0.279735	-2.513252	-3.113502	H	-4.343758	0.060383	-2.536036
H	0.149444	-1.834154	-3.640492	C	-4.481370	-2.458924	0.380976
O	1.502712	0.143081	2.517718	H	-3.494826	-0.963341	1.538833
H	1.440644	1.079018	2.757093	C	-5.006703	-2.806661	-0.863805
TS(VIN-C8•OH)				H	-5.385067	-2.173902	-2.868788
C	1.206952	3.052022	0.199309	H	-4.526474	-3.165776	1.203065
C	0.325123	1.971532	0.272336	O	7.456940	-1.247525	-0.306318
C	-1.055094	2.233370	0.358601	H	7.387382	-2.122743	-0.696637
C	-1.476243	3.559788	0.335679	O	-0.959692	5.912100	0.253135
C	-0.553448	4.613933	0.256775	H	-1.919224	5.941273	0.293274
C	0.815290	4.380044	0.191990	O	-5.583164	-4.008964	-1.106602
C	2.437274	1.233473	0.111661	H	-5.510412	-4.564202	-0.325810
C	1.154025	0.782861	0.209936	O	1.142310	-3.620652	2.348459
H	-2.539308	3.761554	0.430669	H	1.806924	-3.180103	2.884580
H	1.519727	5.198197	0.137069	O	-1.687976	-2.908721	-1.320830
				H	-2.169752	-2.189806	-1.746535

O	-4.330506	2.223880	0.930131	H	-3.120890	-0.947081	0.744929
H	-3.995069	1.919471	1.787682	C	-6.335891	-1.014884	-0.300543
TS(VIN-C8'-•OH)				H	-7.404926	0.618755	-1.167556
C	1.690138	2.703032	0.089480	H	-5.014898	-2.478809	0.568335
C	0.605047	1.822852	0.220693	O	6.795237	-2.669893	-1.469929
C	-0.688986	2.357542	0.403516	H	6.486841	-3.495813	-1.852144
C	-0.810808	3.741157	0.430582	O	0.176514	5.936650	0.335886
C	0.303479	4.586447	0.293578	H	-0.744538	6.167387	0.481891
C	1.586367	4.079678	0.120709	O	-7.419513	-1.824040	-0.419984
C	2.532706	0.685595	-0.014555	H	-7.206969	-2.695701	-0.075933
C	1.159799	0.504506	0.122396	O	0.399035	-3.812550	2.279813
H	-1.788706	4.179646	0.604184	H	1.083910	-3.457360	2.853126
H	2.440492	4.735000	0.027822	O	-2.235474	-2.670727	-1.423829
C	3.362639	-1.469944	-0.984415	H	-2.527680	-1.895326	-1.912598
C	3.614013	-0.224189	-0.406915	O	2.739967	0.554893	2.155252
C	4.943509	0.175154	-0.213395	H	3.538760	0.015321	2.060404
C	5.992970	-0.649942	-0.573539	TS(VIN-C12-•OH)			
C	5.729842	-1.897989	-1.138325	C	1.967365	2.799080	-0.038202
C	4.412942	-2.302480	-1.344470	C	0.863658	1.987618	0.243285
H	2.345217	-1.791804	-1.166612	C	-0.375219	2.604043	0.494599
H	5.140478	1.146267	0.224698	C	-0.433576	3.995099	0.458550
H	7.023274	-0.351020	-0.428712	C	0.702318	4.770766	0.187328
H	4.206713	-3.267344	-1.796548	C	1.933951	4.181886	-0.073113
O	2.838452	2.015874	-0.099195	C	2.670197	0.723914	-0.166658
C	0.452569	-0.787478	0.218817	C	1.349631	0.622722	0.159338
C	0.785943	-1.681555	1.233828	H	-1.376531	4.488417	0.674696
C	-0.549437	-1.104187	-0.702213	H	2.806259	4.783331	-0.287202
C	0.117758	-2.902777	1.312737	C	3.413299	-1.560783	-0.835328
H	1.536189	-1.389999	1.960415	C	3.718778	-0.263525	-0.412408
C	-1.221089	-2.320778	-0.588981	C	5.064008	0.088621	-0.245314
H	-0.813296	-0.400178	-1.484504	C	6.074393	-0.829311	-0.471770
C	-0.885775	-3.229933	0.408325	C	5.755444	-2.124232	-0.875894
H	-1.413148	-4.170981	0.490449	C	4.421664	-2.484797	-1.060792
C	-1.850881	1.468804	0.529102	H	2.382416	-1.848310	-1.001053
H	-1.691424	0.563231	1.104116	H	5.311457	1.096013	0.064949
C	-3.020449	1.677130	-0.085692	H	7.116562	-0.566467	-0.342489
H	-3.142713	2.582081	-0.677823	H	4.171859	-3.487558	-1.392647
C	-4.154008	0.745083	-0.113749	O	3.058837	2.037257	-0.283370
C	-5.376216	1.156544	-0.660627	C	0.632518	-0.634634	0.481592
C	-4.052599	-0.578562	0.331123	C	1.115913	-1.409055	1.535763
C	-6.459251	0.298347	-0.749114	C	-0.490133	-1.050867	-0.239657
H	-5.476391	2.174520	-1.022180	C	0.485269	-2.610075	1.855742
C	-5.125164	-1.451140	0.236690	H	1.988529	-1.078204	2.089314

C	-1.128732	-2.246353	0.110303	C	4.730054	0.466612	-0.156384
H	-0.867973	-0.453108	-1.062345	C	5.807059	-0.374182	-0.341471
C	-0.634475	-3.029339	1.152393	C	5.601899	-1.734164	-0.687278
H	-1.129229	-3.955378	1.413323	C	4.288091	-2.164547	-0.986343
C	-1.556793	1.763693	0.697481	H	2.221052	-1.663173	-1.041297
H	-1.393462	0.854153	1.262627	H	4.886851	1.495514	0.139714
C	-2.736510	1.967326	0.092549	H	6.823024	-0.027565	-0.196219
H	-2.856659	2.844357	-0.538934	H	4.159841	-3.181466	-1.333143
C	-3.819146	0.993415	0.047768	O	2.609842	2.247006	-0.162413
C	-4.846514	1.175852	-0.902202	C	0.247486	-0.575028	0.210853
C	-3.830090	-0.177169	0.829329	C	0.632229	-1.478770	1.201197
C	-5.795313	0.212388	-1.122279	C	-0.835947	-0.866702	-0.618062
H	-4.866459	2.091156	-1.482696	C	-0.069193	-2.674784	1.350789
C	-4.765856	-1.160992	0.613681	H	1.474962	-1.249027	1.845098
H	-3.084504	-0.325540	1.600798	C	-1.559247	-2.043953	-0.421632
C	-5.711228	-1.020291	-0.429901	H	-1.133616	-0.167139	-1.390675
H	-6.569315	0.346879	-1.869380	C	-1.172332	-2.956503	0.553414
H	-4.774584	-2.076301	1.191973	H	-1.728996	-3.873209	0.694863
O	6.783039	-2.987873	-1.080455	C	-2.024630	1.629608	0.591815
H	6.434978	-3.836873	-1.365515	H	-1.838496	0.786326	1.249085
O	0.652541	6.130791	0.169054	C	-3.147988	1.657493	-0.130483
H	-0.241536	6.419098	0.368442	H	-3.285442	2.447329	-0.866057
O	-4.420546	-1.872466	-1.869564	C	-4.136949	0.570909	-0.140094
H	-4.567194	-2.767091	-1.523799	C	-4.913263	0.359853	-1.287494
O	0.921654	-3.408367	2.865478	C	-4.269430	-0.340576	0.914180
H	1.702151	-3.013767	3.263236	C	-5.760769	-0.732527	-1.399730
O	-2.221114	-2.716954	-0.523261	H	-4.837829	1.059735	-2.113316
H	-2.686224	-2.053825	-1.066495	C	-5.118698	-1.430046	0.816847
O	-6.692457	-1.949561	-0.497022	H	-3.704120	-0.195171	1.827158
H	-7.136187	-1.872501	-1.347545	C	-5.859852	-1.638978	-0.346230
TS(VIN-C12'-•OH)				H	-6.352761	-0.902646	-2.290097
C	1.457199	2.927872	0.034081	H	-5.200497	-2.129716	1.642381
C	0.392252	2.038384	0.199486	O	5.810410	-2.306815	1.273486
C	-0.898550	2.558112	0.420027	H	5.344584	-1.625878	1.778657
C	-1.046898	3.938839	0.428662	O	-0.096135	6.150304	0.268795
C	0.050371	4.799284	0.247232	H	-1.019393	6.369199	0.417990
C	1.333750	4.307075	0.051131	O	-6.697574	-2.692893	-0.503861
C	2.299499	0.906512	-0.149405	H	-6.636658	-3.269750	0.262179
C	0.963850	0.712957	0.072786	O	0.266758	-3.598195	2.288147
H	-2.030249	4.360096	0.614707	H	1.070012	-3.319936	2.736091
H	2.174396	4.973753	-0.079462	O	-2.647217	-2.360988	-1.168398
C	3.220833	-1.317776	-0.813607	H	-3.020546	-1.561344	-1.557174
C	3.419003	0.005261	-0.365527	O	6.631765	-2.529169	-1.076054
				H	7.233329	-2.581351	-0.323548

TS(VIN-C14-•OH)

C	1.657252	2.866546	-0.103856
C	0.645434	1.907517	-0.246190
C	-0.677041	2.360393	-0.426149
C	-0.893162	3.738205	-0.471377
C	0.152502	4.658234	-0.336539
C	1.461314	4.234414	-0.142713
C	2.635204	0.911783	0.063642
C	1.318603	0.622739	-0.144698
H	-1.898163	4.107677	-0.650215
H	2.270584	4.943161	-0.036718
C	3.727251	-1.195223	0.832319
C	3.821179	0.084166	0.276498
C	5.087913	0.581175	-0.054140
C	6.226106	-0.181516	0.141004
C	6.116705	-1.462520	0.678270
C	4.863844	-1.964375	1.027316
H	2.761644	-1.588444	1.125261
H	5.172282	1.578495	-0.467343
H	7.208968	0.193478	-0.114486
H	4.778563	-2.954652	1.463391
O	2.855477	2.266814	0.082169
C	0.767298	-0.740553	-0.326217
C	-0.253357	-1.224665	0.492095
C	1.306091	-1.548535	-1.328347
C	-0.748577	-2.519524	0.285448
H	-0.683576	-0.600884	1.268007
C	0.831949	-2.848174	-1.493671
H	2.100586	-1.165939	-1.960661
C	-0.195073	-3.337106	-0.696869
H	-0.574079	-4.339130	-0.847945
C	-1.784012	1.405812	-0.514782
H	-1.538969	0.444958	-0.950383
C	-3.017260	1.617810	-0.031414
H	-3.255776	2.577419	0.420021
C	-4.069144	0.612071	0.026714
C	-5.389780	0.978524	0.328416
C	-3.791082	-0.769759	-0.114999
C	-6.396594	0.037510	0.412146
H	-5.624304	2.025455	0.484520
C	-4.818707	-1.723324	-0.068292
H	-2.806666	-1.092052	-0.424998
C	-6.113205	-1.325003	0.208022

H	-7.418381	0.319973	0.633573
H	-4.570198	-2.770972	-0.202759
O	7.262460	-2.172040	0.845523
H	7.054935	-3.027063	1.231591
O	-0.060184	6.001361	-0.395703
H	-0.996027	6.169388	-0.530406
O	-7.156857	-2.184695	0.299607
H	-6.850863	-3.081224	0.135366
O	-1.776359	-3.018868	1.004089
H	-2.205037	-2.294068	1.506651
O	1.332638	-3.683332	-2.442996
H	2.036216	-3.232423	-2.917040
O	-3.023828	-0.816778	1.939708
H	-3.900849	-0.879078	2.347286

VIN-C7-•OOH

C	1.814151	2.756609	-0.295888
C	0.712359	1.958392	0.037215
C	-0.519536	2.591348	0.262640
C	-0.588023	3.968940	0.102366
C	0.539761	4.727710	-0.247594
C	1.774918	4.130513	-0.451369
C	2.555991	0.692513	-0.196871
C	1.228830	0.604073	0.097530
H	-1.529726	4.474121	0.286183
H	2.647557	4.715376	-0.706038
C	3.371772	-1.649746	-0.515044
C	3.631453	-0.291801	-0.304145
C	4.965365	0.127071	-0.209180
C	6.006873	-0.778389	-0.303846
C	5.733575	-2.130686	-0.499783
C	4.412854	-2.561122	-0.608480
H	2.353429	-2.001102	-0.621135
H	5.178920	1.177662	-0.059456
H	7.039320	-0.461666	-0.228382
H	4.197059	-3.611499	-0.776686
O	2.924361	1.994288	-0.432688
C	0.494327	-0.642178	0.408428
C	0.716396	-1.297025	1.619369
C	-0.374187	-1.185423	-0.534001
C	0.076498	-2.510281	1.869214
H	1.402463	-0.870895	2.343767
C	-1.021751	-2.390859	-0.260305
H	-0.537051	-0.677144	-1.478235

C	-0.792997	-3.062451	0.934301	C	5.831694	-1.205909	0.062125
H	-1.294522	-3.998583	1.140618	C	5.477850	-2.496143	0.465281
C	-1.758373	1.814858	0.647757	C	4.153601	-2.779343	0.806261
H	-1.482873	0.976100	1.293944	H	2.169067	-2.017964	1.027826
C	-2.508259	1.347876	-0.562614	H	5.150131	0.784330	-0.315116
H	-2.418354	1.963653	-1.451796	H	6.865935	-1.008945	-0.191040
C	-3.331820	0.197379	-0.631175	H	3.881449	-3.780153	1.127031
C	-3.928690	-0.166106	-1.868466	O	2.907622	1.795608	-0.121659
C	-3.584689	-0.653840	0.476240	C	0.298125	-0.586200	-0.313872
C	-4.722929	-1.286956	-1.993613	C	-0.821404	-1.246031	0.181838
H	-3.752873	0.462624	-2.734913	C	0.686683	-0.762528	-1.638655
C	-4.386114	-1.770120	0.352132	C	-1.584440	-2.041917	-0.675258
H	-3.151690	-0.421893	1.440310	H	-1.118089	-1.137135	1.217548
C	-4.958331	-2.100578	-0.879349	C	-0.061652	-1.594982	-2.467613
H	-5.176801	-1.558572	-2.938619	H	1.567323	-0.256559	-2.022425
H	-4.554000	-2.410910	1.212079	C	-1.205815	-2.228952	-1.997391
O	6.790878	-2.978917	-0.582450	H	-1.797475	-2.851904	-2.654499
H	6.471668	-3.874044	-0.723776	C	-1.760428	1.672847	0.647004
O	0.469967	6.078558	-0.393383	H	-1.598297	1.035870	1.510762
H	-0.421412	6.372586	-0.189311	C	-2.882484	1.539131	-0.063537
O	-5.740568	-3.189724	-1.058006	H	-2.993247	2.097325	-0.990262
H	-5.775804	-3.698608	-0.243282	C	-3.922992	0.544677	0.230391
O	0.259733	-3.201464	3.023953	C	-4.746254	0.083734	-0.805016
H	0.876458	-2.722989	3.584362	C	-4.080591	-0.033764	1.494224
O	-1.883545	-2.960926	-1.140043	C	-5.670856	-0.925784	-0.603948
H	-2.194052	-2.293900	-1.763328	H	-4.637600	0.513043	-1.794898
O	-2.553680	2.728074	1.431388	C	-5.005412	-1.048837	1.710075
O	-3.634871	2.003974	1.984465	H	-3.490920	0.323994	2.330557
H	-4.292458	2.030463	1.274997	C	-5.803233	-1.501795	0.657733

VIN-C7'-•OOH

C	1.781674	2.565007	-0.143161	O	6.463283	-3.431141	0.509585
C	0.655551	1.856225	0.244819	H	6.094676	-4.267394	0.806025
C	-0.594018	2.473439	0.245747	O	0.452125	5.801209	-0.918793
C	-0.664541	3.810291	-0.151186	H	-0.454595	6.117443	-0.888846
C	0.490819	4.499988	-0.535708	O	-6.725261	-2.484609	0.805342
C	1.745820	3.888528	-0.535945	H	-6.711886	-2.808892	1.709688
C	2.539665	0.519495	0.250301	O	-2.714963	-2.666629	-0.255397
C	1.062324	0.427494	0.538872	H	-3.036149	-2.240963	0.547680
H	-1.621459	4.322233	-0.133682	O	0.275602	-1.811907	-3.766037
H	2.628805	4.435238	-0.835522	H	1.086653	-1.337027	-3.965309
C	3.189536	-1.791880	0.744302	O	1.485287	0.931715	2.767161
C	3.526412	-0.483940	0.329131	H	0.919602	1.717387	2.769736
C	4.875307	-0.215582	-0.004916	O	0.787368	0.053675	1.907407

VIN-C8--OOH

C	1.107456	2.931962	-0.222511
C	0.256106	1.903174	0.182345
C	-1.125320	2.180932	0.385300
C	-1.554038	3.493717	0.067219
C	-0.664233	4.481019	-0.345888
C	0.702068	4.227375	-0.493483
C	2.343162	1.122079	-0.079958
C	1.078868	0.721198	0.251103
H	-2.593727	3.763663	0.219165
H	1.382832	5.003356	-0.813184
C	3.714816	-0.960929	-0.280866
C	3.625509	0.432963	-0.195418
C	4.811013	1.180795	-0.235610
C	6.043424	0.562538	-0.342374
C	6.118120	-0.827147	-0.414781
C	4.948960	-1.584239	-0.386794
H	2.819606	-1.568637	-0.278048
H	4.755884	2.260304	-0.181396
H	6.961558	1.135410	-0.371019
H	5.001957	-2.666140	-0.456326
O	2.371522	2.466462	-0.357878
C	0.653916	-0.666203	0.556638
C	0.939372	-1.220305	1.801659
C	0.004863	-1.421894	-0.420947
C	0.587018	-2.545650	2.059661
H	1.448737	-0.625216	2.552302
C	-0.315772	-2.753950	-0.153482
H	-0.224449	-0.982129	-1.386307
C	-0.033003	-3.318121	1.085623
H	-0.286722	-4.350090	1.288003
C	-1.982076	1.188046	0.900091
H	-1.547038	0.289033	1.318789
C	-3.455251	1.111492	0.672916
H	-3.863748	2.012977	0.205865
C	-3.640531	-0.085604	-0.241244
C	-3.438665	0.055882	-1.611353
C	-3.808283	-1.358576	0.296182
C	-3.364579	-1.057849	-2.436504
H	-3.299346	1.046181	-2.034096
C	-3.740734	-2.477815	-0.519596
H	-3.974313	-1.466839	1.361248
C	-3.491131	-2.327777	-1.880974

H	-3.190072	-0.966511	-3.501543
H	-3.839039	-3.471769	-0.095397
O	7.351912	-1.384921	-0.515821
H	7.267540	-2.340941	-0.561315
O	-1.073346	5.751316	-0.617052
H	-2.022297	5.814730	-0.483852
O	-3.304634	-3.397413	-2.710468
H	-3.314478	-4.204104	-2.185994
O	0.839615	-3.142102	3.252703
H	1.262061	-2.509696	3.839922
O	-0.889837	-3.567161	-1.077889
H	-1.109969	-3.063555	-1.869452
O	-5.460686	0.783514	1.728587
H	-5.794521	1.507312	2.270766
O	-4.055393	0.922805	1.945340

VIN-C8'-OOH

C	1.609137	2.707093	0.201593
C	0.516008	1.807125	0.314107
C	-0.795318	2.342148	0.213507
C	-0.931459	3.707665	-0.043955
C	0.177521	4.541826	-0.181207
C	1.483633	4.046218	-0.051235
C	2.559695	0.705875	0.692449
C	1.058670	0.520281	0.536411
H	-1.926797	4.138918	-0.078087
H	2.337817	4.702639	-0.139559
C	4.142262	-1.242562	0.327184
C	3.404897	-0.184698	-0.187916
C	3.383535	0.022523	-1.566779
C	4.085461	-0.810051	-2.420745
C	4.822007	-1.871182	-1.896311
C	4.850963	-2.084290	-0.521175
H	4.181508	-1.398768	1.397366
H	2.809856	0.848193	-1.973773
H	4.078187	-0.661166	-3.492867
H	5.431138	-2.905621	-0.112658
O	2.802263	2.078559	0.340921
C	0.451784	-0.801482	0.548094
C	0.955200	-1.788409	1.407031
C	-0.604691	-1.123327	-0.318168
C	0.392525	-3.060727	1.407091
H	1.756943	-1.545339	2.094605
C	-1.168879	-2.394860	-0.282266

H	-0.968677	-0.390689	-1.028831	C	5.117603	0.234782	0.017446
C	-0.676148	-3.372944	0.574769	C	6.199535	-0.623942	-0.061702
H	-1.117583	-4.360176	0.593471	C	6.002459	-1.955006	-0.424299
C	-1.966504	1.484666	0.399992	C	4.718346	-2.411204	-0.716195
H	-1.842986	0.676920	1.113077	H	2.648496	-1.908319	-0.888880
C	-3.104797	1.590019	-0.297207	H	5.270605	1.269892	0.295589
H	-3.198533	2.390408	-1.028431	H	7.205636	-0.286641	0.152630
C	-4.232126	0.653195	-0.239593	H	4.564806	-3.442737	-1.017092
C	-5.434529	0.972896	-0.884541	O	3.013143	2.044599	-0.315353
C	-4.140958	-0.597431	0.384434	C	0.632958	-0.725082	0.235423
C	-6.508179	0.099351	-0.895842	C	0.922840	-1.518630	1.344575
H	-5.525816	1.930646	-1.385853	C	-0.347831	-1.125822	-0.671726
C	-5.204469	-1.486436	0.368659	C	0.232701	-2.715714	1.532397
H	-3.223489	-0.896969	0.878647	H	1.686492	-1.202686	2.047768
C	-6.395554	-1.139969	-0.268421	C	-1.051503	-2.310128	-0.452304
H	-7.438150	0.349232	-1.390565	H	-0.566337	-0.512712	-1.539090
H	-5.101141	-2.458838	0.839481	C	-0.760036	-3.113792	0.643874
O	5.493506	-2.659894	-2.775679	H	-1.305335	-4.033467	0.808782
H	5.951099	-3.354715	-2.295366	C	-1.655714	1.533786	0.378142
O	0.057604	5.869673	-0.416762	H	-1.486616	0.779260	1.137763
H	-0.872849	6.102613	-0.477947	C	-2.607886	1.303870	-0.582914
O	-7.469063	-1.968370	-0.318257	H	-2.637156	1.967185	-1.443438
H	-7.262336	-2.788628	0.137699	C	-3.558622	0.213399	-0.557958
O	0.840773	-4.045222	2.229572	C	-4.344103	-0.046191	-1.698880
H	1.569344	-3.706448	2.756436	C	-3.692860	-0.661866	0.537346
O	-2.220911	-2.742477	-1.071433	C	-5.201253	-1.129437	-1.760037
H	-2.596420	-1.951284	-1.471103	H	-4.263483	0.617585	-2.553434
O	2.838302	0.571927	2.073838	C	-4.559536	-1.738327	0.487715
O	4.205039	0.892161	2.306792	H	-3.115313	-0.495773	1.437167
H	4.200655	1.853146	2.192558	C	-5.309220	-1.986532	-0.662870
TS(VIN-C7-•OOH)				H	-5.796547	-1.334988	-2.640651
C	1.856743	2.746200	-0.231552	H	-4.637560	-2.408456	1.337822
C	0.782518	1.879939	-0.013109	O	7.096685	-2.757356	-0.483103
C	-0.504423	2.425704	0.120091	H	6.831065	-3.640264	-0.753318
C	-0.651689	3.799373	-0.010417	O	0.313833	5.982776	-0.355176
C	0.454403	4.633878	-0.240894	H	-0.607507	6.216293	-0.216899
C	1.739746	4.120526	-0.351549	O	-6.157307	-3.034940	-0.773225
C	2.694532	0.715523	-0.167963	H	-6.108235	-3.574817	0.020506
C	1.355877	0.548191	0.023690	O	0.478355	-3.532922	2.589838
H	-1.637985	4.233149	0.119873	H	1.176449	-3.150894	3.128379
H	2.588453	4.769039	-0.517546	O	-2.031911	-2.735641	-1.290861
C	3.637647	-1.545792	-0.638567	H	-2.358757	-1.989865	-1.806484
C	3.819409	-0.212794	-0.258801	O	-2.670910	2.671111	1.668659
				O	-3.613758	1.874079	2.241747

H	-4.412038	2.026090	1.716571	C	-5.761091	-1.506544	0.426078
TS(VIN-C7'-•OOH)				H	-5.927974	-1.624898	-1.698870
C	1.800734	2.676435	0.108705	H	-5.416906	-1.145472	2.520995
C	0.645054	1.906459	0.190745	O	6.401110	-3.386070	0.149251
C	-0.600993	2.542926	0.242070	H	6.052204	-4.224170	0.464635
C	-0.628573	3.929012	0.121670	O	0.542964	6.024169	-0.114768
C	0.557529	4.670122	-0.004419	H	-0.365967	6.335004	-0.118294
C	1.806680	4.055083	0.007073	O	-6.671749	-2.499866	0.578838
C	2.473803	0.586233	0.153497	H	-6.782153	-2.696256	1.512779
C	1.073240	0.509236	0.254965	O	-2.660731	-2.725951	0.308475
H	-1.582108	4.445319	0.172951	H	-2.980352	-2.138722	1.002360
H	2.715016	4.636919	-0.061014	O	0.123803	-2.502347	-3.459651
C	3.158878	-1.740079	0.594844	H	0.907000	-2.054051	-3.789052
C	3.478026	-0.445307	0.160623	O	1.525858	1.118073	2.847780
C	4.794078	-0.169408	-0.244643	H	0.933861	1.883198	2.831161
C	5.755727	-1.160688	-0.243565	O	0.830837	0.145744	2.172223
C	5.420343	-2.450618	0.171183	TS(VIN-C8-•OOH)			
C	4.121114	-2.733984	0.594874	C	1.791535	2.788074	-0.103625
H	2.161371	-1.948922	0.960832	C	0.778485	1.841924	0.062231
H	5.049800	0.833452	-0.562815	C	-0.553456	2.287407	0.166158
H	6.773038	-0.964273	-0.556977	C	-0.797084	3.655978	0.058617
H	3.869669	-3.732053	0.939004	C	0.252144	4.570823	-0.109521
O	2.907531	1.880303	0.111953	C	1.576616	4.153115	-0.190337
C	0.278766	-0.627413	-0.306461	C	2.766471	0.818531	-0.107180
C	-0.794472	-1.206925	0.363940	C	1.438463	0.551734	0.051229
C	0.602406	-1.053884	-1.595991	H	-1.817035	4.010505	0.176459
C	-1.573043	-2.167401	-0.284174	H	2.379377	4.866408	-0.314187
H	-1.026134	-0.921822	1.381715	C	3.868814	-1.339052	-0.693490
C	-0.155729	-2.048726	-2.208390	C	3.952862	-0.026539	-0.220337
H	1.439109	-0.604270	-2.120739	C	5.210636	0.482771	0.126524
C	-1.255165	-2.601702	-1.564112	C	6.347685	-0.299172	0.026528
H	-1.863057	-3.349076	-2.056056	C	6.247700	-1.612516	-0.429096
C	-1.791365	1.718638	0.513453	C	5.004702	-2.128007	-0.792521
H	-1.707715	1.120009	1.416106	H	2.912068	-1.743471	-0.999519
C	-2.838631	1.535550	-0.290073	H	5.288100	1.504495	0.476478
H	-2.877592	2.046767	-1.248874	H	7.323482	0.085187	0.294882
C	-3.887026	0.539798	-0.018280	H	4.927207	-3.143970	-1.166595
C	-4.528327	-0.102397	-1.084926	O	2.995516	2.171200	-0.190520
C	-4.225264	0.145808	1.279654	C	0.788441	-0.767934	0.205799
C	-5.447348	-1.114950	-0.873973	C	1.173137	-1.619992	1.239860
H	-4.277873	0.183850	-2.100542	C	-0.243060	-1.141732	-0.657626
C	-5.150918	-0.867499	1.505569	C	0.523140	-2.842986	1.401878
H	-3.781641	0.653993	2.128473	H	1.973280	-1.325368	1.911189

C	-0.916415	-2.346121	-0.451355	C	3.274496	-0.269291	-1.512086
H	-0.537484	-0.484908	-1.469081	C	4.659555	-0.147605	-1.359702
C	-0.528886	-3.206979	0.569374	C	5.520669	-0.975696	-2.056012
H	-1.048194	-4.143702	0.721307	C	5.004764	-1.945179	-2.916008
C	-1.628341	1.326990	0.357814	C	3.627072	-2.071596	-3.078895
H	-1.435912	0.510767	1.042997	H	1.698333	-1.329119	-2.523253
C	-2.820468	1.352332	-0.334224	H	5.044050	0.596954	-0.674894
H	-2.889041	2.015871	-1.191197	H	6.594759	-0.896136	-1.947436
C	-3.673687	0.152167	-0.380613	H	3.226023	-2.820411	-3.754309
C	-4.373265	-0.164765	-1.552209	O	2.701512	1.982830	-0.910616
C	-3.778123	-0.723760	0.706651	C	0.327739	-0.779502	-0.340064
C	-5.120345	-1.328328	-1.654065	C	0.979163	-1.823192	0.321409
H	-4.319704	0.510025	-2.399931	C	-0.942199	-0.988487	-0.889869
C	-4.534614	-1.883349	0.618889	C	0.358430	-3.066137	0.424442
H	-3.264880	-0.494243	1.632985	H	1.959388	-1.651568	0.752956
C	-5.197414	-2.197731	-0.566196	C	-1.557112	-2.231478	-0.747851
H	-5.651235	-1.584098	-2.562305	H	-1.444487	-0.189454	-1.424588
H	-4.593035	-2.557685	1.467107	C	-0.911831	-3.277945	-0.098884
O	7.392830	-2.338073	-0.504431	H	-1.393933	-4.241037	0.001786
H	7.194716	-3.214706	-0.844174	C	-1.834984	1.592493	0.537004
O	0.022957	5.909274	-0.188542	H	-1.608761	0.652649	1.028075
H	-0.918972	6.074371	-0.096124	C	-3.096411	1.879156	0.194911
O	-5.935632	-3.323649	-0.719281	H	-3.294835	2.812619	-0.327948
H	-5.860138	-3.868165	0.068883	C	-4.254873	0.996418	0.374070
O	0.862791	-3.716174	2.386053	C	-5.540589	1.473583	0.087314
H	1.595258	-3.353343	2.891158	C	-4.130009	-0.343871	0.760251
O	-1.956946	-2.738595	-1.230882	C	-6.657725	0.662746	0.192326
H	-2.344688	-1.970566	-1.666092	H	-5.662738	2.505381	-0.224678
O	-4.361174	2.013477	1.819263	C	-5.239050	-1.170258	0.855823
H	-5.094990	1.458131	1.517466	H	-3.154247	-0.762026	0.980680
O	-3.914367	2.613935	0.680006	C	-6.510010	-0.668810	0.575591
TS(VIN-C8'-OOH)				H	-7.651013	1.034022	-0.025751
C	1.623817	2.696235	-0.519855	H	-5.112617	-2.211587	1.134541
C	0.535806	1.842342	-0.235541	O	5.893796	-2.736232	-3.569123
C	-0.677558	2.429066	0.202307	H	5.419059	-3.355093	-4.130208
C	-0.730237	3.815362	0.290434	O	0.316590	5.973466	0.071615
C	0.373820	4.622683	-0.027488	H	-0.558060	6.237752	0.368574
C	1.584262	4.070828	-0.435247	O	-7.631457	-1.428728	0.650118
C	2.381526	0.654674	-0.790859	H	-7.397266	-2.320988	0.919404
C	1.009693	0.516411	-0.482647	O	0.950885	-4.113913	1.051456
H	-1.638245	4.283516	0.657802	H	1.827551	-3.849797	1.344284
H	2.441030	4.692249	-0.652307	O	-2.805626	-2.481183	-1.226588
C	2.768197	-1.232820	-2.382300	H	-3.225298	-1.651938	-1.478002
				O	3.137022	0.367146	0.999603

O	2.811147	1.464875	1.746017
H	2.010917	1.201638	2.221821