I. Molecular packing of (I) and (II)

In the crystal structure of (I) (Fig. 1S), molecules related by 2_1 symmetry axis are linked into chains parallel to [100] direction *via* intermolecular C10—H101···O3 hydrogen bond (Table 1). Additionally, the net of C—H···π intermolecular interactions linking the C11—H111 vinyl, C23—H231 methine and C37—H371 methyl bonds with the centroids of benzene rings from quinoline and tosyl groups and pyridine ring, respectively, are observed. There are no classical hydrogen bonds present in the crystal structure of (II) (Fig. 2S). The C22—H221 methine bond is oriented towards the centroid of the pyridine ring of quinoline part of neighbouring molecule related by a 2_1 axis. This interaction connects the C—H···π bonded molecules to the [100] chain.

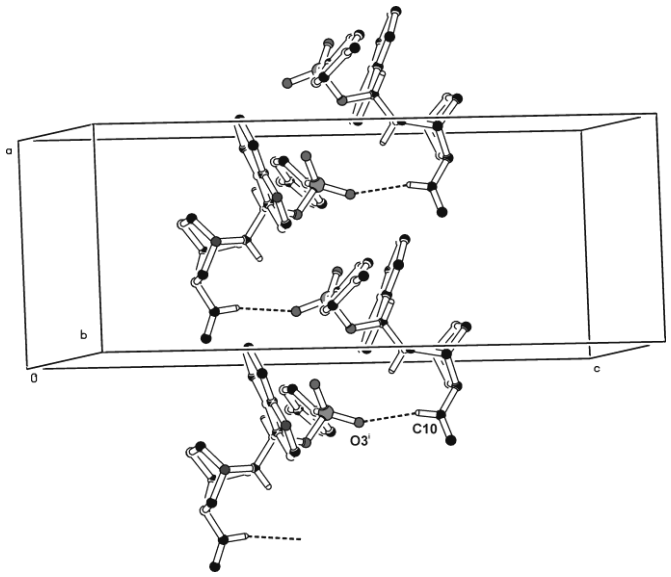

Fig. 1S. The molecular packing of (I), viewed down the *b* axis. Dashed lines indicate intermolecular hydrogen bonds.

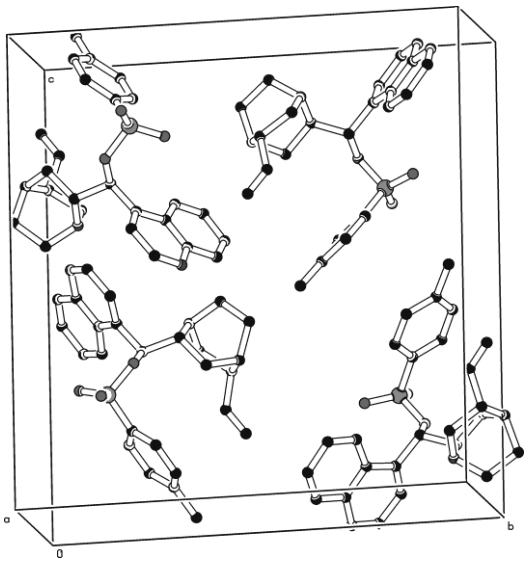

Fig. 2S. The molecular packing of (II), viewed down the *a* axis.

II. Theoretical Calculation

Table 1S. The orthogonal coordinates of molecule (I) obtained after energy minimization and geometry optimization (NWChem package; RHF SCF *ab initio* 6-31G** level).

S	0.63925235	1.78472832	1.29718092
O	0.02276272	0.86494804	0.16591257
O	-0.20992724	1.69939862	2.44236854
O	2.02176100	1.46622920	1.43628523
N	-1.32833859	-2.55881101	0.01941074
N	3.22743609	-2.03278595	-2.30300199
C	-2.41606855	-3.03944098	-0.82753480
H	-2.49135395	-4.11375558	-0.70377467
H	-2.15329000	-2.86024573	-1.86402059
C	-3.77269498	-2.35069492	-0.46474790
H	-4.50529289	-3.11704238	-0.22682401
C	-3.52642662	-1.53105151	0.82455784
H	-4.45781703	-1.08492193	1.15712689
C	-2.98020319	-2.49730126	1.88243893
H	-2.90750749	-2.00152546	2.84587452
H	-3.65628590	-3.33853674	2.00946279
C	-1.58527629	-2.97036372	1.40053533
H	-0.80884077	-2.57125965	2.03929252
H	-1.49290850	-4.04902636	1.44739016
C	-2.46235920	-0.44190886	0.60316337
H	-2.17102457	-0.02382703	1.56155701
H	-2.84575543	0.38222640	0.01282080
C	-1.26098244	-1.10549094	-0.11199686
H	-1.32880658	-0.89425960	-1.17256311
C	0.11203006	-0.57174038	0.32113174
H	0.28797624	-0.78222895	1.36292067
C	-4.33652536	-1.53428668	-1.59877666
H	-3.70370299	-0.75789746	-2.00245405
C	-5.53080231	-1.70831095	-2.13048646
H	-6.20454506	-2.47060438	-1.77582315
H	-5.88117356	-1.09560923	-2.94259440
C	2.38139721	-1.12679830	-2.66093705
H	2.46732198	-0.75027975	-3.66732695
C	1.36752578	-0.61977267	-1.82022729
H	0.70878305	0.14126618	-2.19468004
C	1.24400066	-1.09116158	-0.55034283
C	2.21124451	-2.63195653	1.19938005
H	1.51062328	-2.30525238	1.94161249
C	3.13366444	-3.56697797	1.54075215
H	3.14452889	-3.96930544	2.53800036
C	4.08804987	-4.01328091	0.59640036
H	4.81081176	-4.75702983	0.88138207
C	4.09353201	-3.49685878	-0.65709746
H	4.80862424	-3.80607474	-1.39644689
C	3.14509585	-2.51259136	-1.03894303

C	2.17827730	-2.07576673	-0.10942101
C	0.45259516	3.35211128	0.53043411
C	-0.71621289	4.07442534	0.72350907
H	-1.49366038	3.68085160	1.35059659
C	-0.85238204	5.30497484	0.11454498
H	-1.75518441	5.87058164	0.26488029
C	0.16414749	5.82715460	-0.68331215
C	1.32736877	5.08722039	-0.85410168
H	2.12642334	5.47885254	-1.45770986
C	1.47982641	3.85082724	-0.25062504
H	2.38515482	3.28664028	-0.37275472
C	-0.00831915	7.17171130	-1.34732638
H	-0.77948573	7.12592056	-2.11078134
H	0.90988054	7.49991394	-1.81868124
H	-0.30582964	7.92548133	-0.62569966

Table 2S. The orthogonal coordinates of molecule (II) obtained after energy minimization and geometry optimization (NWChem package; RHF SCF *ab initio* 6-31G** level).

S	0.02106159	1.74647861	1.22764052
O	0.04167049	0.91840169	-0.12080822
O	1.27704344	1.55497786	1.88080634
O	-1.17840323	1.43251609	1.93117453
N	1.06062986	-2.52878474	-0.93000989
N	-4.05968828	-1.61104805	-1.32491272
C	1.88036875	-2.96497293	0.20112010
H	1.73782204	-4.03032049	0.34014362
H	1.52048762	-2.48782868	1.10428722
C	3.38301160	-2.62786337	-0.00955526
H	3.90168845	-3.51449468	-0.36577050
C	3.42310228	-1.57318626	-1.13650715
H	4.42119507	-1.15811532	-1.22820248
C	3.00890135	-2.28314306	-2.43686180
H	3.77759757	-2.98328747	-2.75114477
H	2.89942564	-1.55641625	-3.23800686
C	1.66772585	-3.01760407	-2.16737777
H	0.96711122	-2.87615027	-2.98250177
H	1.82146375	-4.08597809	-2.06408884
C	2.40438100	-0.46038805	-0.83230466
H	2.53606778	0.37586579	-1.51070322
H	2.54688607	-0.06919158	0.16811070
C	0.99286332	-1.07053794	-1.00815321
H	0.63528835	-0.83261396	-2.00328394
C	-0.07077018	-0.52299209	-0.04437108
H	0.14684579	-0.81975706	0.96822407
C	4.05465634	-2.19675941	1.26665083
H	3.65687500	-1.31765436	1.75122714
C	5.07157185	-2.82136853	1.82812375
H	5.50540220	-3.70691708	1.39383039
H	5.50980993	-2.47015589	2.74574933
C	-3.38472783	-0.66041337	-1.87753656
H	-3.85443770	-0.14273761	-2.69818127
C	-2.08923263	-0.27446620	-1.47141269
H	-1.60100785	0.53703656	-1.97738632
C	-1.48301234	-0.92327894	-0.44063351
C	-1.72065403	-2.72356088	1.31183701
H	-0.75137998	-2.51838617	1.71958972
C	-2.47198516	-3.70296496	1.87524285
H	-2.08926074	-4.25548158	2.71471957
C	-3.75894457	-4.00287301	1.36912354
H	-4.34129612	-4.78343386	1.82563455
C	-4.25358449	-3.30428702	0.31792851
H	-5.22793134	-3.50185227	-0.08853592
C	-3.49178646	-2.27069789	-0.28687888
C	-2.20403931	-1.97229721	0.20498387
C	-0.06848769	3.37157532	0.57167963

C	1.09623346	4.08506697	0.34944320
H	2.04760472	3.64932482	0.58903825
C	1.01263733	5.36439263	-0.17072250
H	1.91595095	5.92179921	-0.34359495
C	-0.21883011	5.93716610	-0.46569714
C	-1.37623789	5.19913441	-0.22836262
H	-2.33738121	5.63003762	-0.44674335
C	-1.31041524	3.92169117	0.29048739
H	-2.20418514	3.35946413	0.48568648
C	-0.30848700	7.34419179	-1.00448997
H	0.62658099	7.65367146	-1.45576877
H	-0.53982813	8.04329355	-0.20561482
H	-1.09005182	7.42801092	-1.75137731

Table 3S. The orthogonal coordinates of N-1 protonated molecule (I) obtained after energy minimization and geometry optimization (NWChem package; RHF SCF *ab initio* 6-31G** level).

S	-2.01007345	-1.20123321	0.69917338
O	-0.68231160	-0.30502953	0.74668826
O	-2.39504369	-1.28819421	2.05947529
O	-2.87032373	-0.55693471	-0.25690907
N	-1.89400075	2.18991309	-0.15621332
N	3.92276174	-0.45572884	-1.48686669
C	-2.18289645	3.48880567	-0.85378931
H	-2.11870205	3.31176049	-1.91822461
H	-3.20295221	3.75501240	-0.61489724
C	-1.16842752	4.56136240	-0.36459946
H	-1.74135279	5.41992750	-0.03433735
C	-0.44794585	3.98604478	0.87688098
H	0.18634053	4.74964540	1.30744839
C	-1.52526305	3.55629240	1.87883354
H	-1.08273725	3.30107541	2.83382950
H	-2.22563592	4.36433835	2.05634926
C	-2.24616239	2.32459432	1.30835392
H	-1.95212798	1.41684691	1.80239666
H	-3.32284370	2.40107477	1.35463892
C	0.39054996	2.74164859	0.52906242
H	0.65908992	2.22421976	1.44062641
H	1.31476448	3.00238205	0.03126971
C	-0.43924772	1.84422852	-0.40139628
H	-0.26017105	2.15241676	-1.42223180
C	-0.18869263	0.32227058	-0.43060382
H	-0.74845534	-0.06068855	-1.27138949
C	-0.23962211	5.03575554	-1.45525302
H	0.39716955	4.30242767	-1.92560068
C	-0.15843179	6.28934157	-1.85393344
H	-0.76662481	7.06677377	-1.42341568
H	0.52515143	6.58662212	-2.62830332
C	2.98605995	-0.30815902	-2.35709252
H	3.26213203	-0.36489320	-3.39620785
C	1.63488678	-0.08204792	-2.00587026
H	0.90696238	0.01620810	-2.79247953
C	1.27505505	-0.00159998	-0.69561867
C	2.08125714	-0.16054125	1.71000617
H	1.09623165	-0.02846547	2.10593246
C	3.11978337	-0.33526404	2.56804815
H	2.94195327	-0.32076778	3.62836426
C	4.43277492	-0.54536817	2.08645234
H	5.24003218	-0.68160035	2.78281802
C	4.66466864	-0.57999012	0.75108054
H	5.64600740	-0.74218645	0.34709170
C	3.60200994	-0.40219120	-0.17142325
C	2.28818387	-0.18013239	0.30021875

C	-1.49318444	-2.74730887	0.07302661
C	-1.88005941	-3.14272394	-1.19623037
H	-2.50336842	-2.50873308	-1.79742480
C	-1.46959135	-4.37864835	-1.66679679
H	-1.77349718	-4.69234344	-2.64866083
C	-0.68492314	-5.21657069	-0.88539246
C	-0.31564703	-4.79459490	0.39504613
H	0.28444789	-5.43711700	1.01394684
C	-0.71620632	-3.57242561	0.88257037
H	-0.44181011	-3.26349581	1.87406272
C	-0.24206670	-6.56677589	-1.39017304
H	-0.56992362	-6.73652992	-2.40755952
H	-0.64838968	-7.35721986	-0.76739291
H	0.83941301	-6.64990584	-1.36288486
H	-2.47956849	1.45555033	-0.53062545

Table 4S. The orthogonal coordinates of N-1 protonated molecule (II) obtained after energy minimization and geometry optimization (NWChem package; RHF SCF *ab initio* 6-31G** level).

S	-0.92260777	1.61024331	1.43980774
O	-0.39740161	0.48099389	0.42367504
O	-1.75991538	0.97488421	2.39407953
O	0.26935806	2.27494367	1.89576947
N	2.43885761	0.61549616	0.89208966
N	-1.57792347	-4.50695702	0.34087758
C	3.86216455	0.33324825	1.28279027
H	3.86606096	-0.05794664	2.29063919
H	4.38355765	1.28071910	1.28356085
C	4.45963376	-0.66258051	0.25865718
H	4.38381700	-1.66640860	0.66384214
C	3.58097290	-0.59088675	-1.01404868
H	4.06480836	-1.12310540	-1.82213638
C	3.34933358	0.87595194	-1.39532234
H	4.28442538	1.41684636	-1.46752679
H	2.87011420	0.94555588	-2.36427929
C	2.43502889	1.50099059	-0.33033402
H	2.76714667	2.47511564	-0.00173319
H	1.41479016	1.58205290	-0.65898005
C	2.20307757	-1.21412366	-0.71626612
H	1.50104983	-0.95019154	-1.49631001
H	2.25411049	-2.29508548	-0.68755729
C	1.74115745	-0.70976908	0.66143749
H	2.15489196	-1.36895380	1.41305425
C	0.24053995	-0.65416869	1.01632042
H	0.18628866	-0.53473188	2.08942886
C	5.92162868	-0.38141650	0.02274654
H	6.17367705	0.58306832	-0.38975242
C	6.88884538	-1.23514105	0.29179462
H	7.91788639	-0.99019654	0.10149069
H	6.69443085	-2.20912567	0.70808780
C	-1.03932312	-4.16855104	1.45957546
H	-1.03150430	-4.90217234	2.24741100
C	-0.47033587	-2.89327990	1.68929902
H	-0.05494662	-2.68017587	2.65854952
C	-0.46977725	-1.96055570	0.69945892
C	-1.20546535	-1.42590958	-1.67328572
H	-0.84629003	-0.41955932	-1.61369965
C	-1.80217154	-1.84771893	-2.81864632
H	-1.88849936	-1.17531359	-3.65341965
C	-2.32200202	-3.15826849	-2.92581130
H	-2.79095777	-3.47250434	-3.84040706
C	-2.23308247	-4.00759186	-1.87249304
H	-2.62208869	-5.00741273	-1.91261858
C	-1.61762590	-3.59676868	-0.66249725
C	-1.08320176	-2.29412582	-0.55077201

C	-1.82750819	2.63312866	0.35645975
C	-1.29868493	3.84889564	-0.04673243
H	-0.33521590	4.16588477	0.30420904
C	-2.04358507	4.65424259	-0.88810217
H	-1.64242157	5.60157929	-1.19951519
C	-3.30483381	4.26148628	-1.32411371
C	-3.81385138	3.03415170	-0.89724079
H	-4.78999849	2.72087507	-1.22055598
C	-3.08968814	2.21927539	-0.05471283
H	-3.49554215	1.28464412	0.28508539
C	-4.12752741	5.15903096	-2.21384751
H	-4.70950181	4.58110092	-2.92190497
H	-3.50119054	5.84795662	-2.76678497
H	-4.82018598	5.74420894	-1.61598623
H	1.96573813	1.13344813	1.62081738

Table 5S. The orthogonal coordinates of (I)-H^+-salicylate$^-$-H2O system obtained after energy minimization and geometry optimization (HyperChem package; AM1 level).

S	-2.77969	-3.00960	-0.97282
O	-1.54307	-2.15207	-1.75243
O	-3.90042	-2.51496	-1.60872
O	-2.33039	-4.29256	-1.22349
N	1.43080	-2.31174	-1.74552
N	-2.65995	2.71423	-2.29055
C	2.82246	-2.01458	-2.22601
H	3.46691	-2.89347	-1.94334
H	3.20269	-1.12119	-1.65649
C	2.84427	-1.76583	-3.75034
H	3.45173	-2.59175	-4.22104
C	1.40922	-1.87797	-4.29013
H	1.38842	-1.66342	-5.39042
C	0.92608	-3.29690	-3.99505
H	1.59352	-4.04620	-4.49022
H	-0.11049	-3.44576	-4.39967
C	0.92946	-3.51791	-2.47755
H	-0.11230	-3.75127	-2.11336
H	1.60280	-4.37663	-2.20097
C	0.47657	-0.91033	-3.56314
H	-0.58331	-1.09639	-3.88503
H	0.73707	0.14942	-3.82135
C	0.59578	-1.09443	-2.04214
H	1.16650	-0.21921	-1.59655
C	-0.77227	-1.07353	-1.30208
H	-0.59109	-1.18140	-0.18697
C	3.47952	-0.46302	-4.07885
H	2.78721	0.38284	-4.24520
C	4.79459	-0.29252	-4.19996
H	5.52154	-1.10286	-4.05598
H	5.22399	0.68837	-4.45937
C	-3.03608	1.57482	-2.84046
H	-3.82928	1.62907	-3.61178
C	-2.46328	0.30508	-2.52493
H	-2.84825	-0.60186	-3.01972
C	-1.44602	0.24311	-1.59922
C	-0.03160	1.47792	0.06645
H	0.45546	0.53699	0.38620
C	0.32415	2.66296	0.66480
H	1.08725	2.68030	1.46149
C	-0.29305	3.87475	0.27908
H	0.01449	4.81109	0.77047
C	-1.26561	3.88686	-0.68840
H	-1.75408	4.82962	-0.98148
C	-1.66929	2.66972	-1.32559
C	-1.02967	1.44573	-0.94237
C	-2.70334	-2.60960	0.60400

C	-3.50184	-1.58361	1.14425
H	-4.17762	-1.02324	0.47282
C	-3.46237	-1.27355	2.49510
H	-4.08537	-0.45543	2.90075
C	-2.62569	-1.99494	3.36258
C	-1.83193	-3.02656	2.84155
H	-1.16581	-3.59530	3.50928
C	-1.87077	-3.32280	1.48649
H	-1.24020	-4.13851	1.08772
C	-2.59115	-1.67012	4.80456
H	-2.72000	-0.56638	4.96557
H	-1.62414	-1.98442	5.27033
H	-3.42717	-2.20047	5.33483
H	1.45671	-2.48518	-0.70687
C	2.72251	-1.92551	2.83878
C	3.82400	-2.66624	3.28825
C	4.28151	-2.54758	4.59703
C	3.63779	-1.68459	5.48728
C	2.53970	-0.94145	5.07395
C	2.08618	-1.06011	3.74526
C	2.26998	-2.09330	1.43395
O	2.84776	-2.89550	0.63837
O	1.26787	-1.43051	0.97786
O	1.00716	-0.26696	3.43333
H	4.31745	-3.34795	2.57513
H	5.14729	-3.13576	4.93231
H	3.99802	-1.59328	6.52278
H	1.99883	-0.27319	5.76234
H	0.69806	-0.47253	2.53123
O	4.02478	2.51736	-5.46519
H	3.51337	1.78946	-5.83459
H	3.43111	2.90437	-4.81492
O	-4.15444	1.30404	4.30319
H	-4.12243	1.32342	5.26717
H	-4.37612	2.20956	4.06001
O	0.13076	4.23177	-4.62631
H	-0.59647	4.17355	-3.99872
H	-0.27985	4.57395	-5.42908
O	1.43135	2.05585	-5.23864
H	1.32955	2.77748	-5.87343
H	1.12204	2.43191	-4.40785
O	-1.58797	1.47570	3.89358
H	-2.09733	1.84782	4.62513
H	-2.23057	0.95487	3.39964

O	-3.73644	3.47139	5.61665
H	-2.78511	3.62136	5.61666
H	-3.92088	3.17486	6.51368
O	-2.42497	3.99579	-5.09730
H	-2.88038	4.53102	-4.44086
H	-2.85235	3.13241	-5.03197
O	-0.60760	3.47822	5.45290
H	-0.66918	3.47070	4.49101
H	0.34091	3.45430	5.61856
O	-2.44550	1.11149	-5.74100
H	-2.34156	0.30721	-5.21919
H	-2.18893	0.84505	-6.63183
O	-0.68783	2.71417	-6.61511
H	-1.51480	3.09944	-6.91843
H	-0.85858	2.48737	-5.69097
O	1.12158	2.31001	3.94473
H	0.44825	1.85381	3.42293
H	1.77882	1.62812	4.12160
O	-4.78126	-3.02925	6.92211
H	-4.63644	-3.71940	7.57546
H	-5.73260	-2.89260	6.94153
O	-1.83384	-1.44553	-6.29627
H	-1.65035	-1.15276	-7.19480
H	-0.96460	-1.69172	-5.95485
O	-2.47691	1.59075	6.71248
H	-1.63022	2.05327	6.73929
H	-2.23229	0.65841	6.71704
O	-0.33023	0.48017	5.83498
H	0.00315	1.32452	5.51136
H	-0.45013	-0.03707	5.02926
O	-1.82278	-3.82983	-5.79289
H	-2.42946	-3.36639	-5.20630
H	-2.16689	-3.63285	-6.66939
O	-0.08316	0.20351	-6.64651
H	0.28506	0.90627	-7.19322
H	0.02884	0.53106	-5.74749

Table 6S. The orthogonal coordinates of (II)-H^+-salicylate$^-$-H2O system obtained after energy minimization and geometry optimization (HyperChem package; AM1 level).

S	0.62485	-0.94869	-3.18700
O	0.60166	-0.83952	-1.51387
O	1.71497	-1.76492	-3.46486
O	0.72759	0.35925	-3.63894
N	2.45133	-0.50746	1.60744
N	-0.93134	2.97483	1.21436
C	3.56617	0.48448	1.49828
H	3.72164	0.94211	2.51940
H	3.24273	1.29055	0.78003
C	4.86832	-0.19470	1.02024
H	5.57943	-0.22443	1.89538
C	4.55351	-1.64652	0.62237
H	5.46171	-2.13073	0.18310
C	4.09954	-2.38018	1.88321
H	4.93112	-2.42408	2.63121
H	3.81081	-3.43159	1.62957
C	2.90487	-1.64110	2.48849
H	2.01668	-2.31976	2.63710
H	3.16337	-1.18531	3.49230
C	3.40187	-1.68093	-0.37774
H	3.17809	-2.74030	-0.66516
H	3.69179	-1.13411	-1.31528
C	2.13326	-1.06355	0.24788
H	1.35289	-1.86851	0.42821
C	1.49003	-0.04584	-0.74497
H	2.28322	0.39022	-1.42050
C	5.48681	0.57124	-0.09394
H	4.86135	0.68077	-0.99887
C	6.70992	1.09242	-0.02866
H	7.35363	1.00151	0.85687
H	7.15030	1.65076	-0.86570
C	-1.23620	1.69238	1.23568
H	-2.15535	1.39663	1.78401
C	-0.44829	0.67903	0.60567
H	-0.74687	-0.38074	0.68244
C	0.69235	1.03762	-0.07532
C	2.17174	2.91261	-0.87464
H	2.80515	2.22230	-1.46064
C	2.46980	4.25445	-0.88661
H	3.33693	4.62423	-1.45537
C	1.66264	5.17677	-0.18389
H	1.92867	6.24461	-0.20171
C	0.55572	4.74872	0.50368
H	-0.08494	5.46535	1.04264
C	0.20921	3.35915	0.53055
C	1.05091	2.42192	-0.15536
C	-0.81735	-1.65534	-3.43945

C	-0.90504	-2.99219	-3.86860
H	0.02620	-3.55553	-4.05957
C	-2.13367	-3.61027	-4.04820
H	-2.17780	-4.65654	-4.38822
C	-3.32178	-2.91211	-3.78476
C	-3.25049	-1.57509	-3.36565
H	-4.18334	-1.02418	-3.13908
C	-2.01749	-0.95980	-3.20301
H	-1.97278	0.09323	-2.87179
C	-4.63937	-3.56949	-3.92598
H	-4.53410	-4.66245	-4.13182
H	-5.21241	-3.10226	-4.76670
H	-5.23540	-3.43727	-2.98316
H	1.59797	-0.09122	2.04989
C	-0.96662	-1.20073	4.92115
C	-2.08353	-2.01608	4.70053
C	-2.99145	-2.28519	5.71990
C	-2.78836	-1.74895	6.99373
C	-1.69225	-0.93349	7.24426
C	-0.78186	-0.65486	6.20578
C	-0.01218	-0.94075	3.80857
O	-0.16964	-1.45286	2.65544
O	1.00942	-0.19305	3.99966
O	0.28915	0.13085	6.55459
H	-2.23398	-2.45072	3.69702
H	-3.86631	-2.92109	5.51723
H	-3.49994	-1.97038	7.80326
H	-1.51765	-0.50156	8.23957
H	0.64374	0.56083	5.75283
O	3.74458	0.50081	-2.99035
H	3.13292	0.33617	-3.71867
H	4.26351	1.25136	-3.30152
O	-4.19908	2.26816	4.01878
H	-4.05318	1.39207	4.39406
H	-3.67327	2.26692	3.21276
O	2.68679	2.53475	-3.99168
H	1.85055	2.30748	-3.56729
H	2.46399	3.28198	-4.55732
O	-2.42465	-1.91022	1.43397
H	-2.14058	-1.12303	1.91758
H	-1.66603	-2.50020	1.49622
O	-5.85738	-3.28730	-0.67946
H	-4.92514	-3.10958	-0.51426
H	-6.28627	-3.04474	0.14799

O	-6.21249	2.91283	5.25492
H	-5.38381	2.87824	5.74293
H	-5.97947	3.39060	4.45170
O	-4.94122	-1.58390	1.01406
H	-4.51389	-2.14425	1.67543
H	-4.21342	-1.08305	0.62798
O	-5.98110	-0.99513	-1.85653
H	-5.94240	-1.01103	-0.89469
H	-6.42994	-1.81789	-2.07992
O	-3.87057	0.15104	2.65157
H	-4.80579	0.12533	2.41878
H	-3.74242	-0.64425	3.18505
O	2.67321	-1.09879	6.17617
H	2.23445	-0.79776	6.97791
H	1.94552	-1.26507	5.56318
O	0.51528	2.94396	-5.29809
H	0.80726	2.82152	-6.20803
H	0.28014	2.05370	-5.01375
O	4.43250	0.25198	-5.40527
H	3.98149	-0.46385	-5.86591
H	5.14278	-0.19105	-4.92899
O	4.16589	-2.03764	-4.38260
H	3.96113	-1.66294	-3.51842
H	3.37065	-2.52733	-4.61137
O	-6.15265	0.52502	4.20594
H	-6.42867	0.81777	5.08059
H	-6.15434	1.33376	3.68081
O	3.77101	0.69028	4.65262
H	4.15045	0.13163	5.33869
H	2.82462	0.67590	4.84054
O	-5.44303	-1.82670	3.60481
H	-5.41976	-1.46070	4.49492
H	-6.17345	-1.36449	3.17849
O	2.22331	1.25547	-6.20268
H	2.11400	0.89252	-5.31745
H	3.04766	1.75097	-6.13962