

Supporting Information for:

Towards Routine Organic Structure Determination using Raman Microscopy

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1. Simple computational protocol for modelling the Raman spectrum of organic solids as dimers

- 1- To model an organic molecule containing N_c carbons, we start by creating approximately $\frac{N_c}{4} + 1$ conformers (depending on rigidity) of a single molecule (monomer) in Avogadro and export each set of cartesian atomic coordinates to a .xyz file.
- 2- Then, each monomer geometry is pre-optimized with ORCA at the r²SCAN-3c level of theory in gas phase. An example input file can be used from section 3.1. The optimized monomers are ranked by their final single point energies (SPE), and the two most stable conformers are selected.
- 3- For each of the two pre-optimized monomers, we create, again with Avogadro, at least 8 dimer geometries with various relative positioning by means of rigid transformations. When applicable, we prioritize the hydrogen bonds between molecules followed by π -stacking placements.
- 4- The dimers are optimized with ORCA at the r²SCAN-3c level of theory in gas phase, with the TightOpt command.
- 5- The optimized dimers are again ranked by SPE, and the single most favorable geometry is used to calculate the Raman spectrum at the same level of theory still, with an input file using the commands shown in the example in section 3.2. If an imaginary frequency is found (in an ORCA output file, typically above all the vibration information, near the SPE), a new conformer must be generated. When a spectrum without imaginary frequencies is obtained, the spectral information can be obtained from the output file.
- 6- To extract the spectral data, the tool orca_mapspc is used with the following command:

```
orca_mapspc [OUTPUT FILE NAME] raman -cm -w04 -x00 -x14000 -n4000
```

And the generated .stk file is used for processing with the correlation software.

2. Molecular modelling strategy comparison

	1-DFT	2-DFT	3-DFT	4-DFT	5-DFT	6-DFT	7-DFT	8-DFT	9-DFT	10-DFT	11-DFT	12-DFT
1-Exp	94	49	27	41	56	69	43	33	50	44	55	65
2-Exp	40	79	34	23	53	56	43	22	34	24	31	66
3-Exp	13	16	83	16	48	20	18	20	14	6	13	29
4-Exp	47	25	32	66	44	24	34	31	44	47	40	38
5-Exp	36	32	50	38	62	40	28	35	33	29	34	43
6-Exp	53	58	48	28	59	75	31	20	28	41	38	61
7-Exp	52	52	21	38	49	56	59	46	63	51	65	66
8-Exp	30	25	13	44	30	21	26	54	56	40	34	25
9-Exp	30	24	40	22	42	34	18	41	80	37	38	39
10-Exp	44	35	36	52	48	43	44	29	54	72	54	53
11-Exp	49	27	27	68	48	46	52	55	66	68	73	48
12-Exp	46	53	38	28	51	45	23	13	26	24	23	71

Figure S1. Match scores for the twelve initial compounds, calculated as single molecules (“monomers”), with r^2 SCAN-3c in gas phase. When only one molecule is modelled, several false positives are obtained (in red). An average of 0.4 hours is required to generate the DFT spectra in the final frequency calculation on 16 cores. This figure is also shown in the main article as **Figure 5B**, but is reprinted here for ease of comparison.

	1-DFT	2-DFT	3-DFT	4-DFT	5-DFT	6-DFT	7-DFT	8-DFT	9-DFT	10-DFT	11-DFT	12-DFT
1-Exp	94	53	28	48	54	69	58	44	45	43	56	67
2-Exp	41	89	36	26	52	51	52	24	32	25	33	63
3-Exp	14	16	86	16	47	22	13	16	15	7	16	30
4-Exp	46	30	32	86	42	23	43	54	40	55	40	41
5-Exp	36	34	53	23	81	46	19	23	35	20	18	54
6-Exp	53	55	49	31	57	81	41	21	25	42	39	58
7-Exp	52	67	24	46	45	49	80	52	61	52	66	56
8-Exp	30	27	16	59	28	20	48	78	56	45	35	25
9-Exp	29	36	42	24	40	33	22	45	77	35	41	41
10-Exp	43	43	37	61	43	45	41	37	52	75	53	50
11-Exp	49	44	31	66	44	43	66	65	66	65	75	40
12-Exp	46	51	38	32	52	47	29	22	25	26	23	75

Figure S2. Match scores for the twelve initial compounds, calculated as pairs of molecules (“dimers”), with r^2 SCAN-3c in gas phase. A sizable improvement in spectral correlation can be observed. An average of 3.0 hours is required to generate the DFT spectra in the final frequency calculation on 16 cores. This figure is also shown in the main article as **Figure 5C**, but is reprinted here for ease of comparison.

	1-DFT	2-DFT	3-DFT	4-DFT	5-DFT	6-DFT	7-DFT	8-DFT	9-DFT	10-DFT	11-DFT	12-DFT
1-Exp	94	50	28	50	54	66	56	35	44	53	58	68
2-Exp	41	82	36	28	52	51	52	17	36	37	32	64
3-Exp	14	15	85	20	47	20	19	9	17	13	15	29
4-Exp	46	27	35	78	42	22	45	40	39	64	43	39
5-Exp	36	30	49	28	82	40	24	13	37	27	19	50
6-Exp	52	58	47	36	57	80	42	21	25	52	37	63
7-Exp	51	58	25	45	44	50	77	41	61	55	67	65
8-Exp	31	25	19	50	27	18	45	64	55	39	41	28
9-Exp	30	27	45	27	40	31	26	36	78	36	41	44
10-Exp	43	38	39	63	43	41	51	40	51	81	54	58
11-Exp	49	33	33	69	44	41	68	45	66	59	82	47
12-Exp	45	52	37	35	53	42	29	16	29	36	23	73

Figure S3. Match scores for the twelve initial compounds, calculated as four molecules (“tetramers”), with r^2 SCAN-3c in gas phase. Some correlation scores go down, which we hypothesize is because a complete conformational search for the position of 4 discrete molecules is harder to achieve, or the optimal conformer changes with the number of molecules modeled. An average of 14 hours is required to generate the DFT spectra in the final frequency calculation on 16 cores, which in the context of routine analysis we consider too high for molecules of this size.

3. DFT Data

3.1. ORCA Input file example for pre-optimization

```
# [MOLECULE IDENTIFIER]
!Opt r2SCAN-3c

%pal
  nprocs 16 # Number of cores
end

%maxcore 3000 # Memory allocation per core

*xyz 0 1 # Charge and multiplicity
  [CARTESIAN ATOMIC COORDINATES HERE]
*
```

3.2. ORCA Input file example for final frequency calculation

```
# [MOLECULE IDENTIFIER]
!Opt NumFreq r2SCAN-3c TIGHTOPT

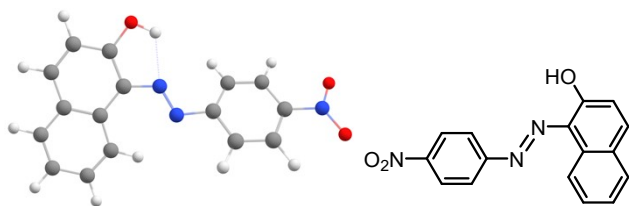
%elprop
  polar 1 # Calculate Raman spectrum
end

%pal
  nprocs 16 # Number of cores
end

%maxcore 3000 # Memory allocation per core

*xyz 0 1 # Charge and multiplicity
  [DIMER CARTESIAN ATOMIC COORDINATES HERE]
*
```

3.3. Optimized atomic coordinates



Main article molecule number: **PR1-enol**

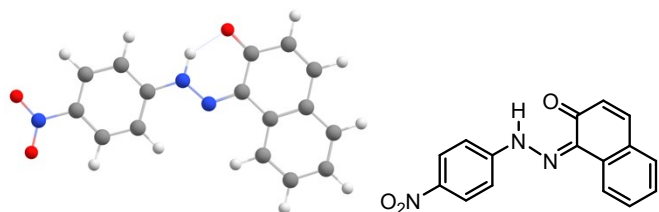
Name: PR1 (Pigment Red #1), enol form

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -2011.9500779559

C	3.40710546377955	-2.74019665988325	0.24975933141068
C	2.45373917678617	-1.74591465514957	0.13989257303273
C	2.83418603508477	-0.39118532590009	0.02363571147449
C	4.23376589228860	-0.08872767828272	0.03204070036504
C	5.17860675403714	-1.12934720557958	0.14266459455293
C	4.77659693244585	-2.44115044586260	0.24842743001514
H	3.08341201184807	-3.77332895814798	0.33874683495552
H	1.40480606901022	-2.00251721127269	0.13913946826118
C	1.91074720880214	0.71214304734943	-0.08636428655890
C	4.67229957495038	1.25912029986993	-0.06648823389195
H	6.23517432639257	-0.87339023597984	0.14526889617247
H	5.51077729768887	-3.23637985545891	0.33322312919138
C	3.79355383883327	2.30033365547036	-0.16516656127435
C	2.41274032129810	2.03215289282406	-0.17665835252368
H	5.74193429919738	1.45400031348476	-0.06082241898973
H	4.12421856842597	3.33068225283790	-0.24021265857454
O	1.58313048869499	3.07732754452983	-0.28668821891926
H	0.68185732972446	2.69163398841909	-0.28169064334013
N	0.53508552183785	0.71115378421091	-0.10142002600821
N	-0.10434158797317	-0.38258094315203	-0.13451842483643
C	-1.49993835936860	-0.23724919558637	-0.07080907323994
C	-2.24838311438980	-1.33517470620516	-0.51914745435471
C	-2.15764869961314	0.88821191171716	0.45444519867185
C	-3.63112767754637	-1.30232455846476	-0.48572967960133
H	-1.72020293274910	-2.20176053384143	-0.90433620940430
C	-3.53869550697343	0.92165672042448	0.50249520459345
H	-1.57595117461085	1.71619616366349	0.84373141292535
C	-4.25948630914698	-0.17095089013262	0.02503939359624
H	-4.22848096552034	-2.13343759082406	-0.84085728447605
H	-4.07067532060077	1.77294450742032	0.91092216318830
N	-5.72898263228212	-0.13237764887981	0.07613249686012
O	-6.33793450934108	-1.10868237876505	-0.34759121959730
O	-6.25548832101060	0.87478959514681	0.53687420632393



Main article molecule number: **PR1-keto**

Name: PR1 (Pigment Red #1), keto form

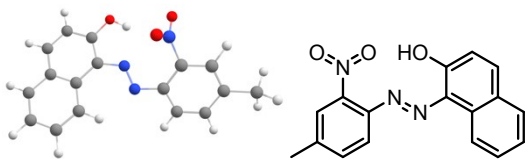
Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -2011.97185737517

C	-3.73803217608272	2.79644582182170	0.00032347321776
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C	-2.70208442824400	1.87812996353103	0.00020631473691
C	-2.96707798080638	0.50079910108170	0.00001604084660
C	-4.31580519830430	0.06783671244378	-0.00005997829635
C	-5.35147324215531	1.01641472920444	0.00004756396960
C	-5.07003125470196	2.36964711762874	0.00024392380673
H	-3.51124080819599	3.85856570369603	0.00048656249223
H	-1.67231783842580	2.21702954936780	0.00028280862156
C	-1.90705773082755	-0.50069329060241	-0.00004814358735
C	-4.60919563535811	-1.33904153206707	-0.00021915955509
H	-6.38154627787650	0.66905879171839	-0.00000754113742
H	-5.87654340415677	3.09624883395094	0.00034285747513
C	-3.64422471092785	-2.28947392720325	-0.00026726844262
C	-2.24389508007566	-1.93761550186375	-0.00018413619433
H	-5.65678639179949	-1.63467344084587	-0.00027985483183
H	-3.87952984996040	-3.34924968299156	-0.00036425291398
O	-1.35306521316088	-2.82213975438781	-0.00011410818222
H	0.04574723450082	-1.91818707071323	0.00020793818606
N	-0.66229253939475	-0.04783741464092	-0.00000673040216
N	0.32023087742480	-0.91107874288996	0.00008827709932
C	1.64178355507320	-0.49160126539721	0.00006080254694
C	1.99641800595804	0.86541208232911	-0.00029193455791
C	2.63349732674631	-1.48446528248458	0.00037553499765
C	3.33207254972606	1.21891625075177	-0.00037423249412
H	1.22156441427697	1.62205507040455	-0.00054356278568
C	3.96845334858188	-1.12785246481931	0.00035384642771
H	2.34723158952584	-2.53250845716271	0.00065275635868
C	4.30542529002805	0.22240127786143	-0.00004353139527
H	3.63616927680979	2.25895190732266	-0.00067891013755
H	4.75177896220903	-1.87614667697618	0.00059997350355
N	5.72105017873793	0.60549161746403	-0.00014384048344
O	6.55403680421188	-0.29536504322336	0.00028289065899
O	5.98631534664387	1.80339701769107	-0.00064737954811



Main article molecule number: **PR3-enol**

Name: PR3 (Pigment Red #3), enol form

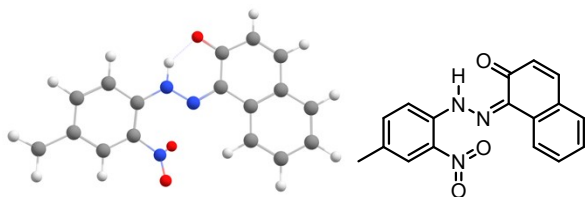
Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1045.254722988221

C	3.83350325769081	-1.98505362799704	-0.63570092924309
C	2.45087629640487	-1.93743441496700	-0.55925016930778
C	1.78574841271945	-0.77914031443440	-0.14226643944239
C	2.58599609985759	0.31382170092944	0.23202822453527
C	3.96608847422412	0.27744290040056	0.14627270169588
C	4.61601872315937	-0.87958414076050	-0.28900661953409
H	4.31798986061189	-2.89568169308996	-0.97801690906195
H	1.84318398687995	-2.78811392789774	-0.85240647302483
H	4.53646381270696	1.15418009004985	0.44174740241884
C	6.11615586863988	-0.93708395868272	-0.33837812761192
H	6.54242919678769	0.02927824414731	-0.62271238772094
H	6.52676311210315	-1.20051403116266	0.64412504349569
H	6.45973204610414	-1.69019800100610	-1.05238443955935
N	2.00115918583744	1.52865693475177	0.82399392018878
O	2.16300611547418	2.58170560613504	0.21426808513699
O	1.45892909728465	1.41079469847102	1.91031819304987
N	0.38633699105749	-0.81127886455383	-0.16127316069530
N	-0.14443462754687	0.33362599723614	-0.27640055984912
C	-1.51202438094917	0.47812651306116	-0.26607940324768
C	-2.53626849360701	-0.51068623950812	-0.02634817264347
C	-1.88599731607449	1.81772993716998	-0.52319345797481
C	-3.90214180508167	-0.08650404078573	-0.08440454415421
C	-2.28320056949519	-1.86705072180694	0.27556855346004
C	-3.23971842236293	2.20498956384680	-0.57328906403872
C	-4.21290773201424	1.27167304158910	-0.36268840860423

C	-4.93906313167526	-1.01420126860226	0.14348799470425
C	-3.32371522849189	-2.74830421329718	0.49834391881261
H	-1.26238089614053	-2.21445995620786	0.33111942212321
H	-3.47113418960621	3.24448191495299	-0.77955453299246
H	-5.25957278974974	1.56356127370292	-0.40122770277314
C	-4.66021439041693	-2.33091375720202	0.42946559268779
H	-5.96767382324791	-0.66580685129226	0.09243382272784
H	-3.09614140515152	-3.78452986181620	0.73203197302411
H	-5.46494896248062	-3.03833735048989	0.60480954165007
O	-0.98232393683036	2.77845712294952	-0.74233063194500
H	-0.09563843662109	2.37594469616683	-0.66187025628678



Main article molecule number: **PR3-keto trans**

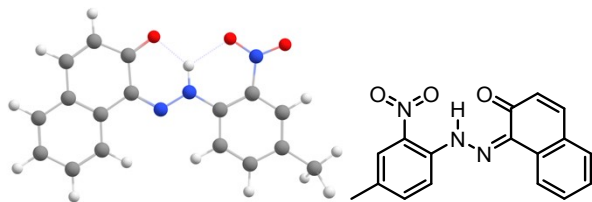
Name: PR3 (Pigment Red #3), keto form, trans isomer

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1045.261171350024

C	4.33900758045149	1.35645583538469	-0.48254878513140
C	3.01107325249910	1.71315065568553	-0.32080733350558
C	2.04119080029894	0.75257769245174	-0.01125763477684
C	2.46981260554732	-0.57194388834995	0.14474286404788
C	3.79195087641887	-0.93387570984655	-0.06081521450732
C	4.75449027902462	0.02556111369653	-0.36979507921816
H	5.06704134870723	2.12573860092076	-0.72579500328095
H	2.69778219386525	2.74390864035771	-0.46248946515902
H	4.06665319711176	-1.97902577320043	0.05105397491924
C	6.19733769237674	-0.35813842164589	-0.53794707199460
H	6.29684266686098	-1.38437148647312	-0.90170461249846
H	6.70342481023207	0.30762006722854	-1.24267524084853
H	6.73120831056124	-0.29299965905760	0.41806729749277
N	1.57160985812879	-1.63452138546651	0.63095604114301
O	1.47271920754376	-2.64062670392027	-0.05822394671940
O	1.04662007416167	-1.45797294688414	1.71888171759069
N	0.71781188541349	1.16321405357968	0.06598363023163
N	-0.25420820908415	0.30254789695397	-0.07164861725648
C	-1.50475127049524	0.73531382153840	-0.01245741327206
C	-2.54885229615939	-0.27055150958097	-0.15698951613713
C	-1.85337209038778	2.15480855617388	0.15820561568819
C	-3.90210626753603	0.14828733835061	-0.15016083624555
C	-2.26374000944177	-1.63783318160445	-0.29067106720453
C	-3.25612957686340	2.49404732660443	0.15376720505921
C	-4.21000189720562	1.54240480026044	0.00625641617452
C	-4.92587992708381	-0.80413075183279	-0.28719636564683
C	-3.28887392014655	-2.55815164505181	-0.42421453746060
H	-1.23177638198006	-1.97138464019052	-0.28104922524743
H	-3.50465460188056	3.54401893718803	0.27406063648838
H	-5.26037721175954	1.82859319667795	0.00748677074509
C	-4.62621778576094	-2.14599324246837	-0.42528489760995
H	-5.95997122924949	-0.46855427598355	-0.28017192375976
H	-3.04762417441399	-3.61228881434270	-0.52470185571960
H	-5.42271542701685	-2.87644624688646	-0.52914197593788
O	-0.96898328621856	3.04019387018229	0.28544644597371
H	0.43493192348037	2.16389187955087	0.17928600358374



Main article molecule number: **PR3-keto cis**

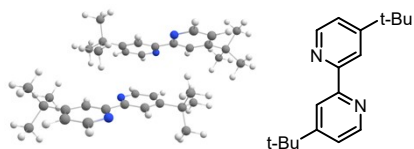
Name: PR3 (Pigment Red #3), keto form, cis isomer

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1045.266450183835

C	3.01991412208171	2.34467060230508	-0.00009811994353
C	1.83213343885746	1.64744792572658	-0.00008171470396
C	1.80807243969198	0.23970745521495	0.00000755375635
C	3.05935668469680	-0.41914667523495	0.00009149100297
C	4.25307001971423	0.30618306126110	0.00007883404872
C	4.26158291960598	1.68980956692127	-0.00001862723550
H	2.98961759203345	3.43196074922949	-0.00017961248501
H	0.88612952286026	2.17313026116152	-0.00014845957119
H	5.17980093617107	-0.25564324369968	0.00014728874195
C	5.54469262951433	2.47030865973733	-0.00001698616720
H	6.41332351635347	1.80786741714484	-0.00022058830518
H	5.61010930632036	3.11728878077405	-0.88206561962011
H	5.61029453635372	3.11697032365326	0.88225426566862
N	3.19000270105766	-1.87818919789268	0.00020145823534
O	4.31798654657478	-2.35666094004175	0.00042329455433
O	2.16051991196726	-2.55559315149844	0.00008071431580
N	0.59311963444391	-0.43117134547303	0.00001456056958
N	-0.52072750222078	0.26373848857767	0.00002797510022
C	-1.68459902940351	-0.35798572713481	0.00002094208747
C	-2.87370569998616	0.49161068317238	0.00003615385967
C	-1.82806590471647	-1.83157339936438	-0.00000802442298
C	-4.15172324574584	-0.11894169704452	0.00003482679803
C	-2.79909682940545	1.89202747869591	0.00005163489910
C	-3.17509040082200	-2.36604432204277	0.00001013245438
C	-4.25645968524830	-1.55469779079431	0.00002511634825
C	-5.30508463096369	0.68100050139109	0.00004745387104
C	-3.94899877083216	2.66338051110569	0.00006331896282
H	-1.82448731711376	2.36675062738588	0.00005579915663
H	-3.26479199299759	-3.44800253872164	0.00000663331033
H	-5.25647390172854	-1.98484165263206	0.00003241970644
C	-5.21051634806085	2.06061954788891	0.00006089545758
H	-6.27879836923448	0.19758095806551	0.00004740707674
H	-3.86720024929273	3.74644239154377	0.00007504116156
H	-6.10850200503577	2.67073264509247	0.00007062326962
O	-0.83368139076971	-2.58209518682397	0.00000204995868
H	0.54571381527935	-1.46553676764977	-0.00000213191755



Main article molecule number: **1**

Name: 4,4'-di-t-butyl-2,2'-bipyridine

Qty of copies of the molecule modelled: 2

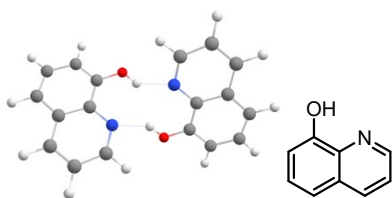
Qty of imaginary frequencies: 0

Final single point energy (Eh): -1619.3857503721

C	3.92732784162321	9.54929003189110	33.20033250623817
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H	3.23886478206480	10.06666608382867	32.52512130362345
H	3.35477505278079	9.17765217834772	34.05860011638485
H	4.33836760226128	8.68622535127841	32.66757412165111
H	3.66067391906175	12.18732150850289	33.86519669525948
N	1.66221558967236	10.88399472457393	30.30723592887676
N	3.25826407758058	14.11667704246955	30.44088013784869
C	0.78769880661516	10.16644801955850	31.01414061764351
H	0.51686280001496	9.19568388192338	30.59868027179347
C	0.23028476703497	10.58797476169592	32.21268291897461
H	-0.47724069015560	9.94163619345103	32.72313302403614
C	0.58972504748557	11.83443735260529	32.73862679798675
C	1.49962168308924	12.58436714969409	32.00010303642293
H	1.83128277635516	13.56392906265622	32.31982152805293
C	2.01089741836792	12.08229302494655	30.79676474228285
C	2.97236807396338	12.88131364925247	29.99378579130219
C	3.52992932016148	12.35446057877475	28.82945644490439
H	3.24524390348592	11.35012362149213	28.53977115173543
C	4.42722054943420	13.10921315157296	28.07386532356833
C	4.70747074394360	14.39417846893961	28.54095283394506
H	5.39430133158687	15.05220062014749	28.02052506101196
C	4.10350369842244	14.84165324854886	29.71274093698780
H	4.32146587006320	15.84344081574485	30.08515501552749
C	-0.01679979480530	12.32123348548710	34.05302904816630
C	-1.53953960507309	12.46774104036031	33.86966429961451
H	-2.00529693160297	11.51702305930308	33.59238020259446
H	-1.76654640339928	13.19721693555262	33.08496398616281
H	-1.99931568760713	12.81077730576584	34.80351952628487
C	0.27027501611497	11.28790035305850	35.15861223674412
H	-0.14811831888520	11.63275351878705	36.11089258533789
H	1.34875841854940	11.14836216350651	35.28642123095721
H	-0.17278644911449	10.31366516142448	34.93173612116314
C	0.55575831853399	13.67341481625121	34.49192834887318
H	0.09538282092344	13.97166677846626	35.43950092731398
H	0.34899629334410	14.46010231286341	33.75894872859575
H	1.63882745485557	13.62194040576363	34.64806361146146
C	5.02163972039393	12.53759167722860	26.78882381054548
C	3.90217091364209	12.46472991926320	25.73226333719658
H	4.29468771452005	12.04867720840374	24.79714967713632
H	3.49474446960929	13.46013047390505	25.52388810912371
H	3.08056277110865	11.82679379307464	26.073173217824501
C	6.16458755787136	13.40629279784976	26.25055744603586
H	5.82255866913780	14.40691717286916	25.96523442849474
H	6.58714559883312	12.93897106302160	25.35455834379075
N	7.90024300123907	8.32220191348973	29.99161919608978
N	7.29340384663029	11.87284822467585	30.22435013451179
C	8.55053166932933	7.47040333900539	29.19667378909623
H	8.47510959182810	6.41546068516544	29.46089934073406
C	9.28516459208564	7.85499802364125	28.08412688501257
H	9.77413649335920	7.09400439637318	27.48314828247010
C	9.37910944567460	9.21333201772829	27.75818411263845
C	8.71911182946275	10.10234407363104	28.59840894942218
H	8.74081101009796	11.17172081239259	28.43439492839077
C	7.98356344573418	9.62540126167030	29.69016131266196
C	7.23713032276790	10.57115519850042	30.55961972301571
C	6.51595941608235	10.11063221390583	31.65979907019074
H	6.52167799228037	9.04579206285336	31.86210583340066
C	5.81459090246707	11.00825719379011	32.46673409651690
C	5.86997488882811	12.35314449955816	32.10179456755662
H	5.33823511723810	13.11929329070660	32.65416360934975
C	6.61791909083039	12.72597158488989	30.98872954288132
H	6.66597700601248	13.77467230172975	30.69831494990771
C	10.16394436862274	9.66511539273860	26.52894461836866
C	11.63308646140573	9.22805574863086	26.67830903899846
H	11.72499028175592	8.14066691538984	26.76057107246909
H	12.08157761781574	9.67392989406880	27.57241891433226
H	12.21200448610129	9.54991560203931	25.80512607213641
C	9.55486223960484	9.00470028792325	25.27725297042235
H	10.10014121228538	9.32430075363432	24.38192762050193
H	8.50398657776576	9.29156911676078	25.16167702046500
H	9.60311170705988	7.91290154468486	25.32900962477180
C	10.11899342739919	11.18562689289432	26.344613139729599
H	10.68529310653122	11.46010083069045	25.44613139729599
H	10.56275059860532	11.71310521832080	27.19318606812434
H	9.09165240172280	11.54412114374681	26.21223511624424
C	5.03919739621977	10.50116424098170	33.67990557968609
C	6.00097504019648	9.74402517297979	34.61492217178948
H	5.45599003479090	9.38012058236544	35.49340525707478
H	6.80794316257197	10.40054975141166	34.95820733535640
H	6.45505321851941	8.88105043427545	34.11931870782682
C	4.39554892624607	11.64543576777819	34.47038340962619
H	5.14366678594258	12.35772166463205	34.83549697453594
H	3.87438734788532	11.23530483316456	35.34193916617919

C	5.57600693212437	11.12671048285094	27.05120428049451
H	6.32807887199777	11.15408471301702	27.84384716315487
H	6.04516040886783	10.73678640539101	26.14035365938110
H	4.79439211467618	10.42167575902082	27.34805175703604
H	6.96774691949400	13.50655939279380	26.99009390932919



Main article molecule number: 2

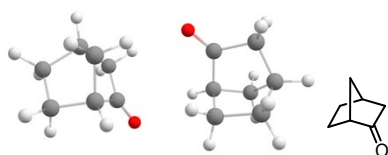
Name: 8-hydroxyquinoline

Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -954.140341993345

N	0.65079015041470	2.14155279026096	0.00933918057436
N	-0.91382388426699	5.14247264676031	-0.06529371049949
C	0.23985400361215	1.00248220887415	-0.51502141308126
C	-0.49856873044556	6.25722333963756	-0.63650285467253
H	-0.83750493653250	0.88108169393396	-0.62261388647117
H	0.57968750519146	6.37430117648051	-0.73994588078942
C	1.11505617117783	-0.02808296811545	-0.90946848499761
C	-1.37033479246985	7.26860590507052	-1.08441764479521
H	0.71366630784736	-0.94007550835690	-1.33951419965126
H	-0.96539586437794	8.16064313711216	-1.55140023479644
C	2.46335215441996	0.14187229662392	-0.72352435589821
C	-2.72023990997119	7.10633821930022	-0.90303257790373
H	3.16958180088935	-0.63696406708152	-1.00120971027284
H	-3.42409470555948	7.87157541968830	-1.22149068762408
C	2.95113088345761	1.34143377558968	-0.15883627444774
C	-3.21275854598142	5.93288981449689	-0.28963960126299
C	4.32262992360076	1.57725750979035	0.08025937213655
C	-4.58631014329348	5.70712325913625	-0.05267723183947
H	5.04868728219456	0.81223974026076	-0.17877054388315
H	-5.31020831918346	6.45929877581343	-0.35212665435626
C	4.71428012773914	2.77090181319444	0.64012273503345
C	-4.98264542506188	4.53930196841603	0.55626976708543
H	5.76674990689308	2.95882887182068	0.83248907306520
H	-6.03675816713264	4.35932346823851	0.74725189243955
C	3.77971150816855	3.76870856646836	0.96208647546734
C	-4.05075691200732	3.55747830364732	0.93087505620887
H	4.10102703878726	4.71261188384605	1.39094862624384
H	-4.37600559394663	2.63353076765527	1.39849319890484
C	2.42939534858011	3.57747770291209	0.73340041131402
C	-2.69842650541020	3.73921985675801	0.70631409220629
C	1.98436093423721	2.33749064484516	0.18235547211837
C	-2.24879959945046	4.95368687135408	0.10441861056113
O	1.57505401220291	4.56413916347064	1.04680708868541
O	-1.84680464138685	2.76845917201198	1.07183201977354
H	0.66883403906593	4.40928931160490	0.68261034920390
H	-0.93722242200208	2.90529246848028	0.70837252622076



Main article molecule number: 3

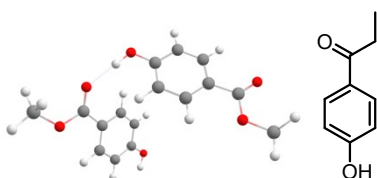
Name: Norcamphor

Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -695.817074433485

C	0.67059079884431	7.76175366788943	0.21176661755461
C	-0.55968131128706	7.59761221878576	1.12133175050621
C	0.90012520504285	6.03964583300230	1.91528593423339
H	0.48017825773172	7.65579475807095	-0.86156766292281
H	1.16453654948527	8.73010652853500	0.36900724224012
C	0.11219059237563	7.24383519135258	2.46583116986971
H	-0.60508066192158	6.95369815697963	3.24086342820773
H	0.75543690926973	8.04348432280138	2.85083223531731
C	-1.24915550854154	6.26567553480214	0.76000986363676
H	-2.21484950363540	6.18017592678499	1.26868689253002
H	-1.43504551009863	6.18133056305818	-0.31581914323657
C	-0.24421809782257	5.19436931859655	1.28012041837435
H	-0.68207594177421	4.55825939801708	2.05455211240283
H	0.12687992588666	4.53249223267731	0.49153229888774
H	-1.22720166890098	8.46339150489338	1.13369488108591
H	1.55194664922275	5.47615565208124	2.58315893243579
C	1.60041087363834	6.65560984441803	0.71999665105638
O	2.65671513707297	6.32310227711151	0.22549897124595
C	4.02962094256689	3.30745845170722	1.24085307738477
C	4.39371444141828	2.76280533049345	-0.15152610077314
C	2.22601462724446	2.13119351949177	0.11015542055905
H	4.67507263455557	2.97568816257922	2.06117646128185
H	4.00032745164621	4.40548001526660	1.23842980793936
C	3.05519000228465	2.94980192791073	-0.89893609832560
H	3.05675593209710	2.50351730397258	-1.89969226075893
H	2.75226229937148	4.00010985424926	-0.96199553105604
C	4.49302032095997	1.22590895614829	-0.06162541536132
H	4.90979081716116	0.80816275263914	-0.98398052653984
H	5.13533614525899	0.90568298818093	0.76533789105770
C	3.00972811678317	0.78654809309990	0.13171650895933
H	2.66658021708217	0.15923282376965	-0.69746382321860
H	2.84319246267696	0.22950557733017	1.05899991670237
H	5.26133911912101	3.24678808969105	-0.60686594443106
H	1.15008588480489	2.02912805249208	-0.04390484575005
C	2.59848045590145	2.80582572814768	1.42099754055485
O	1.91269543447707	2.90663944297211	2.41528132834975



Main article molecule number: 4

Name: Methylparaben

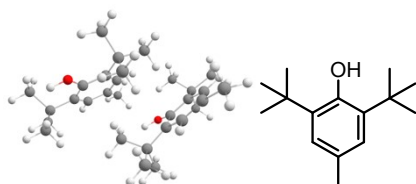
Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1070.537388950418

O	1.84011849141661	1.43325747605527	-1.18070123063178
C	2.81481306307643	-0.55911764425437	-2.08841651479450
C	3.14023754499612	-1.10696134185689	-0.83906479800833
H	2.97608054117070	-0.52560583290643	0.06222127003164
O	4.42452749743008	-4.36356735567636	-1.74987562125362
H	4.52698937143332	-4.78022522767449	-2.61389942791143
C	3.67854103338094	-2.37505388221170	-0.74159738120714
H	3.93151912885327	-2.80588191734635	0.22130742178443
C	3.89790385574062	-3.12130105428406	-1.90207829571823
C	3.58204386430482	-2.58768945024902	-3.15528985786515
H	3.75437227191117	-3.17190985303228	-4.05660132427918
C	3.04690265746999	-1.31430506446831	-3.24474426830727

H	2.79992858193524	-0.90182985104808	-4.21636643098912
C	2.22083622545037	0.78498519051726	-2.14749756640098
O	2.12144125553362	1.26080789555649	-3.40210747864238
C	1.52024457273756	2.56760180042719	-3.52373120943217
H	2.10969063992522	3.30945197560337	-2.97866579158915
H	1.51796312826759	2.78464498209233	-4.59186206063274
H	0.50118484813838	2.55653643624905	-3.12782999479039
H	1.43091295260771	1.05276687298956	0.54521347621047
O	-2.18378547702614	-4.12973213718691	3.38745084552851
C	-1.13280350567082	-2.47837240085718	2.01892988488071
O	-2.54382312772500	-4.15681935119150	1.15691838084187
C	-0.49536102028164	-1.86046880822046	3.10297554652448
H	-0.65294824774053	-2.26748769032066	4.09691111641474
O	1.31920865352240	0.82383222096837	1.49090801969915
C	0.31746397138300	-0.75962074643555	2.91346136742569
H	0.81656223263283	-0.27566916366452	3.74695684120387
C	0.50826645023616	-0.24794612107355	1.62383824558640
C	-0.12993737626411	-0.85366064419272	0.53330939738897
H	0.01339326965723	-0.45055776197518	-0.46520067664770
C	-0.93943652167160	-1.95991968319357	0.73363002700064
H	-1.42999635043072	-2.42694194138087	-0.11316322073686
C	-1.98566413772891	-3.65089329832304	2.28872262656921
C	-3.39032096651093	-5.30091241442103	1.36531732410119
H	-3.75580228652965	-5.57801704538095	0.37560259426339
H	-4.22400483729684	-5.04762530293783	2.02684667884477
H	-2.82321224833464	-6.12339186469486	1.81113208553804



Main article molecule number: 5

Name: BHT

Qty of copies of the molecule modelled: 2

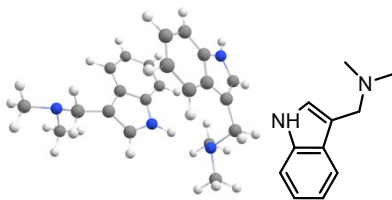
Qty of imaginary frequencies: 0

Final single point energy (Eh): -1322.23997066399

C	-1.46032918050348	1.37493248902218	0.51712037350362
C	-2.35701639261029	0.42831816321459	1.33186730260362
C	-2.92359443148303	-0.69968636398341	0.44412429095265
H	-3.53839052239674	-0.31756981607467	-0.37113645831931
H	-3.54149666159723	-1.36807486785974	1.05590521072291
H	-2.10650386367196	-1.29684019481158	0.02550451513037
C	-3.50784762774561	1.22543317106351	1.97986530983250
H	-4.15429618715078	1.68928915711588	1.23322339180270
H	-3.10722534334127	2.01241938677036	2.62858168378347
H	-4.11831372761655	0.55439864538652	2.59558304047750
C	-1.57487328040454	-0.25588214837473	2.46334502086887
H	-2.24962741635714	-0.93222475918021	2.99901804660901
H	-1.18788941834182	0.46557736683900	3.19170406129916
H	-0.74253387981688	-0.85579019255112	2.07946746408340
C	-1.94572339658167	2.07843587955405	-0.60587371517953
O	-3.26574348723942	1.86972026050584	-0.93115910506778
H	-3.49916113739779	2.43720599160217	-1.67060694755342
C	-1.13139381784841	2.94445738009441	-1.36366242579171
C	-1.65392237879565	3.68173626687853	-2.60991742895566
C	-2.10383498912737	2.67471118184470	-3.69430404165472
H	-2.89289580679236	1.98383729522251	-3.38136366899107
H	-1.25240539434943	2.05686936830061	-3.99735812298564
H	-2.46842028476590	3.21348776444433	-4.57629351927844
C	-2.79395494393365	4.66160171455304	-2.24227064357664
H	-2.43687855129489	5.38459481530439	-1.50201051773052
H	-3.68981544253705	4.19784885927581	-1.81530619732076
H	-3.11476177662074	5.21092597687792	-3.13464196141423
C	-0.56140685136516	4.54263210627155	-3.26546335818807
H	-0.20050177413371	5.32831745435177	-2.59407585550659
H	-0.97852350021005	5.03110766555463	-4.15230536445335
H	0.29237853571774	3.93925064001246	-3.59009073505184

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C	0.18749072209174	3.11802562209917	-0.93482180501531
H	0.84390154288359	3.78991381687430	-1.47609270945601
C	0.70269820395869	2.46463942518583	0.17786886611812
C	2.12751390224489	2.68916130123375	0.61143401695047
H	2.20215682778612	2.76610608149428	1.70095238691928
H	2.53134030149512	3.60917019859793	0.17841386613124
H	2.78196044791984	1.86286414793702	0.30693006229814
C	-0.13084922486469	1.59257506378262	0.87590778550535
H	0.28107729956183	1.06970693252936	1.73114495175361
C	1.63834186701143	-2.37329233613045	1.67863942912801
C	2.71058901890034	-1.89618220882620	2.67043591096426
C	2.52036304159470	-0.40344503893141	3.00303226822220
H	2.61888816859331	0.22169033070767	2.11581408292078
H	3.27472139875739	-0.08758362423461	3.73361642445469
H	1.53126602190022	-0.23376955334333	3.44408604702939
C	4.11745194376089	-2.13495098383150	2.08401278967821
H	4.25730814395584	-3.19746622493520	1.85599041573620
H	4.87813445556976	-1.84124284581595	2.81702386830416
H	4.28211622355826	-1.56210675066195	1.17074881831654
C	2.64122617506832	-2.66455011075237	3.99907833559119
H	3.43558420825281	-2.29995540012892	4.65881984026945
H	2.79472577803687	-3.74028816174566	3.86054608872470
H	1.68756315220471	-2.50965536490804	4.51565418099596
C	1.53859038582006	-1.84681536341115	0.37359785011183
O	2.41017541123448	-0.83286272450259	0.04681324280938
H	2.06859364363139	-0.38322988355568	-0.73397354165609
C	0.61846217343268	-2.34576879754830	-0.57255583321511
C	0.62249096600238	-1.88920295878472	-2.04502454980634
C	0.25018951124997	-0.39791739482120	-2.20428039650304
H	0.92220206403304	0.32626459613547	-1.72693058366767
H	-0.74105587869966	-0.20044150526029	-1.78627565419259
H	0.23463549500200	-0.14014080309130	-3.26968779149586
C	2.00004273539472	-2.18348569723776	-2.68062813220305
H	2.82876153283528	-1.67438957806737	-2.18269723222628
H	1.99617081482977	-1.87600373244182	-3.73280456957604
H	2.20698228223981	-3.25786963844916	-2.63821385637345
C	-0.41380099475106	-2.66113681741021	-2.87879319720629
H	-0.22606229166216	-3.73940567831784	-2.86436060510899
H	-0.35120555767154	-2.32662201701657	-3.91962436568825
H	-1.43660868216307	-2.47594305501492	-2.53352057397283
C	-0.26909090462292	-3.33257825649679	-0.13635631973383
H	-1.00752854074269	-3.73222589560249	-0.82218279243219
C	-0.24771439992353	-3.83728843695658	1.15811672531762
C	-1.26353024092298	-4.85208257967017	1.60867225445867
H	-0.83841602197821	-5.54622980941816	2.34040114307334
H	-1.64434807638741	-5.43708744752738	0.76597456369991
H	-2.12385570370498	-4.36293920142756	2.08326788738688
C	0.72620828837576	-3.36683076283999	2.03341520214989
H	0.75753126116802	-3.78908771149115	3.03153887442543



Main article molecule number: 6

Name: Gramine

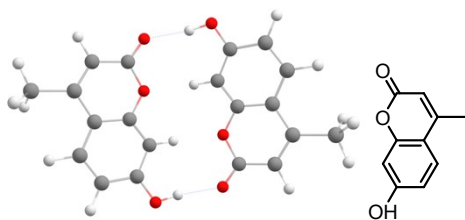
Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1073.92746719103

H	13.04757828433263	24.44665970895246	12.72191219619079
H	14.11782145749662	26.12592564346862	10.71298729657407
H	14.17235202837920	25.71390244271148	16.74412377870799
H	14.87354753037177	26.62788062988737	18.09320453725962
N	13.94118478386574	24.63126479707890	13.14288790456415
N	16.27182189859538	25.68192168494286	16.83545043609470

C	14.33959305683936	24.19520405337746	14.38893090939262
C	15.58554469305796	24.69518597001975	14.67628027919826
C	17.11927137383335	26.24587827935832	13.24618565759556
C	17.15669468105306	26.94981359074009	12.05538475113147
C	16.08179538471734	26.90530365099699	11.14990623709319
C	14.95264541915674	26.14513627669567	11.40742916208035
C	14.92177798364654	25.43832543104135	12.60671717208425
C	15.98203237857461	25.48514611688424	13.54423584309121
C	16.37413251051169	24.51219706701642	15.92868471384551
C	17.34310427956223	25.65997245300085	17.83240927453649
C	14.96650415832547	25.71366391576337	17.49677942860826
H	13.70436038542643	23.54706824582973	14.97873673466268
H	17.94484613648965	26.30909229064219	13.95009436476253
H	18.02073144388463	27.56458412291483	11.82257502513978
H	16.13264635457255	27.48770406895347	10.23510307632499
H	17.43446007407753	24.39258361764607	15.67111219845809
H	16.06481106605488	23.58705823587121	16.45311262874082
H	14.81389581134586	24.84212664922105	18.16221522862821
H	17.26366395270151	26.54113280547870	18.47832973793021
H	18.31749358778276	25.68734173501541	17.33254108829709
H	17.30872885548916	24.75990651834343	18.47580517154903
H	16.08530152993795	27.43152476118932	15.84378960192137
H	13.40622533766367	27.06348272739402	14.99379984104313
H	15.83617683246013	32.12901298181630	15.32479693400909
H	15.95324336921017	33.82775554229995	14.81781679667184
N	15.94636098137521	28.30754890948309	15.32911161846013
N	16.73384970688533	32.44097312186991	13.45278595821554
C	16.96186693882186	29.18950629332214	15.02656868605802
C	16.57447246487224	30.04570970795682	14.02722056465342
C	14.31903223586372	30.13636726943290	12.72062067519740
C	13.09452863247878	29.49650303283189	12.60606294686531
C	12.76739613563774	28.39976283768276	13.42297141127007
C	13.65628825588041	27.91920747137173	14.37297514205563
C	14.88883848126843	28.55905476518927	14.48505685063100
C	15.24125250784031	29.66232304734370	13.66227159885843
C	17.39481296838333	31.12908606627705	13.41437558955358
C	17.54318182412780	33.43171590152757	12.75535871625148
C	16.47392243117136	32.86392995709773	14.82451838168105
H	17.90621188553528	29.14391710935429	15.55473621259908
H	14.56524357615770	30.99417813530045	12.10191378851971
H	12.36881707244236	29.85122128812066	11.87959081604543
H	11.79751281506822	27.92234682564852	13.31122331881759
H	17.58200901421282	30.89592482682608	12.35480812497736
H	18.38803361094766	31.15895967907968	13.91501622431026
H	17.40410815031526	32.97758589127604	15.42010466623900
H	17.02285584194614	34.39589651991339	12.74298431934440
H	17.70473565040327	33.11875603154991	11.71728071888154
H	18.53727217894446	33.58600929698616	13.22506566432404



Main article molecule number: 7

Name: Hymecromone

Qty of copies of the molecule modelled: 2

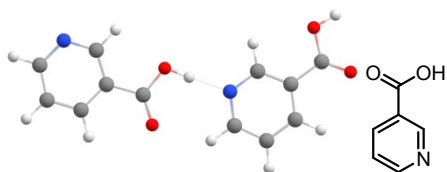
Qty of imaginary frequencies: 0

Final single point energy (Eh): -1222.96523278743

O	-4.37430450465375	1.01608073030708	5.14835164077014
O	-3.09933360318085	0.69442563631339	6.93351621229102
O	-6.54273162797585	1.25616628804854	0.96379634533495
H	-5.65786482343705	1.57637249198308	0.68843242486251
C	-4.19561166316607	0.51262596228369	6.42437302718150
C	-5.32061186019267	-0.15905161196031	7.00677787170265
H	-5.19056673269285	-0.50276187329101	8.02687503987233
C	-6.47662387184019	-0.38431628240616	6.31471207166313
C	-6.57945956244029	0.05997973015200	4.95241878893605
C	-7.67804849215841	-0.16572742598165	4.09621519356632

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H	-8.54819662199110	-0.69293334881926	4.47466461472914
C	-7.66505493751523	0.24602685131665	2.78064499487835
H	-8.50275799088449	0.04696420496985	2.12082987506864
C	-6.53830062934308	0.91752653219358	2.26412093751212
C	-5.46127739910663	1.20436055998523	3.09768235331179
H	-4.59272478598689	1.73174865967788	2.72564533828704
C	-5.48997897663009	0.75615252535484	4.40460712287227
C	-7.62099242204469	-1.10725680940372	6.95494702536887
H	-7.85224769843465	-2.02869612745632	6.40822683391987
H	-8.52546033781446	-0.48850980383313	6.94293180044973
H	-7.39228071801064	-1.36763694742501	7.98993412633128
H	-2.43926960826875	1.59314229062389	4.26267251113515
H	-1.32411209395111	0.89452997578162	6.14836399735342
O	-2.61783181310057	1.71558083906175	1.73735054430718
O	-3.88043318743935	1.86216701594112	-0.07896355796235
C	-2.75984555086976	1.65495807607290	0.36272101868488
O	-0.41091800824267	0.79582244549305	5.80467805334944
C	-1.57305845635266	1.36218266120485	-0.38712249226269
H	-1.68094310998196	1.36865539035428	-1.46597602127240
C	-0.38378152796799	1.06069841865571	0.21369271498735
C	-0.30766170853728	1.02921417454708	1.64795333103249
C	0.82792704043134	0.66544062795097	2.40229872126205
H	1.74873891078988	0.40838761942094	1.88805984366756
C	0.79155254024551	0.60465867207338	3.77919482066862
H	1.66105650654601	0.29965355068902	4.35162600690988
C	-0.39859899904386	0.91803245709730	4.46653493227894
C	-1.51986805782473	1.33367678940380	3.75443428940445
C	-1.46315563727842	1.35996061490907	2.37407095525587
C	0.82678565499766	0.74048288434322	-0.60733668521754
H	1.17924012271219	-0.27591926485636	-0.39761089817065
H	1.64918145790500	1.42398336534234	-0.36763678775840
H	0.61040478473208	0.81818145388082	-1.67431893656339



Main article molecule number: 8

Name: Nicotinic Acid

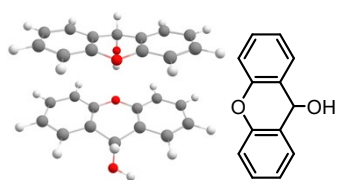
Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -873.592372600774

O	-6.40408672599286	4.78979943938807	-3.52409961964615
C	-1.94603516538560	4.93935672793196	-2.81064106349096
C	-10.55975842706006	4.29349090756707	-4.01326565990257
C	-2.70121798627381	2.38675335386233	-2.19762002989032
C	-1.35568073525728	2.73643216602791	-2.08061037814413
C	-0.97588326894370	4.04224895977972	-2.39469073485245
C	-3.26537663151991	4.50763978864856	-2.90004082454224
C	-0.31534050276336	1.77712225512195	-1.63512863454443
N	-3.63306225439650	3.25488307851278	-2.59811231626288
O	-0.82138101408699	0.54813162275103	-1.37075072813919
O	0.85752867176543	2.04944551639860	-1.51729931888010
C	-8.99006963161404	2.25689392515312	-3.11513543785917
C	-8.39008806968889	3.48285536581119	-3.41762554284825
C	-9.19965785081520	4.52116452861284	-3.87690594944321
C	-11.05966538474811	3.03566633600597	-3.68456010720003
C	-6.92706478165247	3.71695987630341	-3.26587240614441
N	-10.29960951901221	2.02804697002320	-3.24268971797831
O	-6.26473335602791	2.64957880281236	-2.82531960824810
H	-0.07472054442874	-0.00359634171931	-1.08939323759222
H	-5.27994034673856	2.88381138894036	-2.74565543379950
H	-3.03788663463111	1.38021867739383	-1.96203196360244
H	0.06911005761403	4.32386650865486	-2.30596885827758
H	-1.69191399560703	5.96307349355706	-3.06465411691422
H	-4.07239670757573	5.16401272233134	-3.22110558163542
H	-8.38210249819262	1.43007253867767	-2.75495088255193
H	-12.12477072699487	2.82573796548659	-3.78077964191209
H	-11.22725429630601	5.07309385288435	-4.36744935150555

H -8.74659167366554 5.47872957308096 -4.11534285419201



Main article molecule number: 9

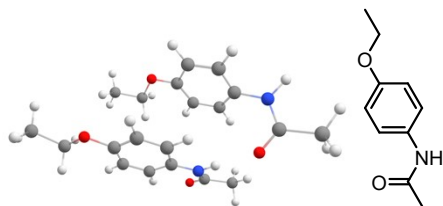
Name: Xanthhydrol

Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1303.46741017142

C	-3.14072364709137	-0.74885613291211	3.48547428933473
C	-1.93214362701649	-0.08227500314548	3.36550087789258
C	-0.74837653223062	-0.81611576513377	3.36093052051621
C	-0.74821376852985	-2.20319820987611	3.48191388333136
C	-1.98252345361588	-2.85255690347608	3.57486679574507
C	-3.17261789696799	-2.14010423708826	3.58318571024214
C	0.53700057623804	-2.96694611173558	3.61228283054632
C	1.71301545801404	-2.14185778602593	3.18786768671134
C	1.60935200350473	-0.76059778411021	3.06285514802684
C	2.71520051693115	0.03312665128705	2.77080346968928
H	2.58936538164514	1.10625726525980	2.66587780199435
C	3.95072514101886	-0.56980213564321	2.60049983443852
C	4.08178954688237	-1.95408734673375	2.71252927154407
C	2.96724370917775	-2.72609630981439	3.00307187238301
H	-4.06509049867697	-0.17965612681586	3.47991477325395
H	-1.88948681217963	0.99695713351908	3.25594606447800
H	-1.99803257002361	-3.93939856883625	3.64380447425146
H	-4.12139903996956	-2.66230415091203	3.65568691075122
H	4.81406562280221	0.04452515927728	2.36402787474326
H	5.05033893588824	-2.42433070980710	2.57472794493896
H	3.05762312590708	-3.80378460720459	3.11404471932091
O	0.41063547243361	-0.09069502301938	3.20661073922659
O	0.77857208388737	-3.33329796818990	4.99374041508418
H	-0.06052302008707	-3.63265530003321	5.36585933775269
H	0.48636496749086	-3.88744112726619	3.00622771090034
C	3.50611814726075	-0.88976343689239	-0.81445397455442
C	2.32166125923629	-1.53133670467691	-0.49496983912349
C	1.17132047100929	-0.77340776262256	-0.28515911824310
C	1.18677564175990	0.61734058261521	-0.37913934724557
C	2.39424215956035	1.23950728792910	-0.70752364724439
C	3.54687454922789	0.50138047581302	-0.92734471222215
C	-0.03965897798572	1.42953597644723	-0.06704061837934
C	-1.26938874826602	0.56384389574359	-0.07097983872326
C	-1.17172092076298	-0.82480010719416	0.00615069188305
C	-2.30560034879031	-1.63195346317988	0.07680557906501
H	-2.18132051497464	-2.70776670108761	0.14591629773869
C	-3.55868030789313	-1.04316826689893	0.06217916610025
C	-3.68504884221929	0.34465061252436	-0.02420622236349
C	-2.54588347503405	1.13217143769836	-0.08766313093585
H	4.40487632033769	-1.47753538394760	-0.97638581304625
H	2.26546237216478	-2.61060702349592	-0.39767563506711
H	2.41384826624517	2.32476598895472	-0.77430115024981
H	4.47511920575090	1.00223004639145	-1.18433863926481
H	-4.44389389220864	-1.67004780323557	0.11777020591264
H	-4.66834673761888	0.80437138730981	-0.04245051462056
H	-2.62753463165588	2.21537796501794	-0.13930456457189
O	0.03313500029724	-1.48361959645228	0.01207635757258
O	0.10170617483927	2.13668555541190	1.18275822223188
H	0.20837808032991	1.46655883840448	1.87576946484687
H	-0.15074392604229	2.23284829785881	-0.80677117659288



Main article molecule number: 10

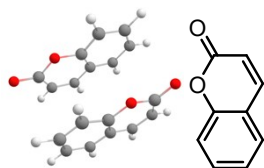
Name: Phenacetin

Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1187.98250256548

C	1.61270133690748	1.22189727766279	-3.25126991339474
C	1.50960448131933	0.72115292497353	-1.94415349021276
C	2.84570832060955	1.41440201891436	-3.84409234332266
H	0.70834572719137	1.48538361083367	-3.79559716533134
C	2.68052996665882	0.40283280381074	-1.25353795278419
N	0.21639616923067	0.57271125437691	-1.41078186703414
C	4.01762699591034	1.10614208577409	-3.14691981503592
H	2.92113858955651	1.81912332909000	-4.84839732523553
C	3.92606557619807	0.59347376553405	-1.85395622152481
H	2.61953941991568	0.01565637004037	-0.24587050643942
C	-0.12916168421283	0.34831740406292	-0.10338106572482
H	-0.54636182399791	0.78361788410559	-2.04840971728661
O	5.18897596079543	1.35153704041753	-3.81085931454523
H	4.81339907002097	0.33470112606159	-1.28765908153843
C	-1.62297579996014	0.29410682983367	0.15271492237174
O	0.67594476485642	0.19463822263810	0.80781942110753
C	6.41111884046577	1.03716747042156	-3.13958277855878
H	-1.86904850742011	1.04705903260002	0.90793421645451
H	-2.23297993005847	0.45091617648337	-0.73992274482510
H	-1.85724790584114	-0.68239704840171	0.58709614628423
C	7.54547240333833	1.41842747512625	-4.06480442542429
H	6.47228997808695	1.59819117942101	-2.19376172289256
H	6.43891193122129	-0.03723044806470	-2.90100663663969
H	7.51400929960003	2.48806824657825	-4.29225725306820
H	8.50557247717177	1.19140879505202	-3.59122705582020
H	7.48049237131065	0.86248518008997	-5.00443832616215
C	4.94624384007090	4.48225093402730	-1.75658889323874
C	3.46352811841813	4.33095670233407	-1.50492777833902
H	5.23736024619814	3.91047862066305	-2.64328811339489
H	5.50505529005464	4.10353688487865	-0.89473371186614
H	5.21381363609940	5.53188997998766	-1.91074113247194
O	2.78272407298702	4.83925286850397	-2.66591733778284
H	3.19963353792027	3.27429068843799	-1.36209508900347
H	3.14888355631827	4.89879046605079	-0.61638612781838
C	1.46425840185400	4.55486604947681	-2.79871264024375
C	0.66450155775858	4.01885113434436	-1.78524124174478
C	0.91019438399468	4.80832851709136	-4.05834186554063
C	-0.66128667226019	3.69928224745437	-2.05143522941416
H	1.06590909370795	3.81832437827423	-0.79889907546489
C	-0.40479386018233	4.46513056196356	-4.32030361920217
H	1.54393305545719	5.23126464476441	-4.83113349394792
C	-1.19331533472304	3.89305471749520	-3.32062774036309
H	-1.27901824704452	3.26906053426934	-1.26950345111353
H	-0.81606944302417	4.61431345043895	-5.31549562931018
N	-2.52866748493699	3.49051268430114	-3.61308055889095
C	-2.98373257543695	2.21239774396156	-3.46585835769084
H	-3.13506916443948	4.15611117914311	-4.06644869147221
C	-4.42182884969503	1.97904264063156	-3.86988371910545
O	-2.29186321216739	1.29701426631723	-3.02719501884311
H	-4.44842694115131	1.15999630796282	-4.59340492180259
H	-4.91360164580876	2.85745518764097	-4.29622942708719
H	-4.98050338884404	1.65217660214911	-2.98787511826311



Main article molecule number: **11**

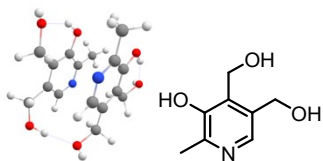
Name: -993.883543951551

Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh):

O	-0.04772284023907	-1.30566853911111	-3.25756047151263
O	-0.15736107692497	-2.06669659384363	-1.16354436938556
H	-0.93822447200873	0.09923796687487	-5.20613071446452
O	0.59988855387132	2.61954693938241	-4.32684820836740
O	0.97546599919684	3.14801677801348	-6.46018792335119
H	-0.90709593780863	2.49530323644956	-2.25969205342262
C	0.57664752742296	-1.22292401360447	-4.46539805463053
C	2.32629629402660	-2.69419752005861	-3.65327325597248
C	-0.01996466089352	-0.42944586336219	-5.43987675198879
C	1.77672047431559	-1.90988508308211	-4.71743731758737
C	2.36407323722935	-1.78981806326278	-5.98740217539219
C	0.46568321323555	-2.05791113695437	-2.19661489441952
C	1.70775696203782	-2.76133805770979	-2.45476687779348
C	0.58553228116340	-0.32328470469758	-6.68316910256057
C	1.77507514157772	-1.00607385275950	-6.96200287584185
H	2.09600772420678	-3.34477151345232	-1.62769778674841
H	0.13426598202597	0.31066253477397	-7.44006648449696
H	2.23537443401457	-0.91310932413631	-7.94033023615861
H	3.25358761214472	-3.23622705791370	-3.82763945584543
H	3.28947921583036	-2.32340498579863	-6.18969042760260
C	0.96748409516065	2.00008545128128	-3.16808886928854
C	3.09084579250067	1.39901168572549	-4.17537169873223
C	0.05134669742920	2.00597442372024	-2.12210981050455
C	2.21460505874525	1.36639801989551	-3.04360329556652
C	2.52634457123879	0.73361318880475	-1.82889358866005
C	1.41542351870460	2.62997108213046	-5.46200464599416
C	2.71665077261337	2.00723159924061	-5.32089237132251
C	0.38246878403898	1.36729775690257	-0.93706406842631
C	1.61988053504923	0.73336817978228	-0.78502956011450
H	3.34960979521482	2.03937657719126	-6.20002806581898
H	-0.33570300555867	1.34644403669069	-0.12375638449687
H	1.85538666695514	0.22508465855306	0.14396738730386
H	4.06329188354133	0.91713757391451	-4.09767681520179
H	3.48856916994161	0.23790462042011	-1.72808877563300



Main article molecule number: **12**

Name: Pyridoxine

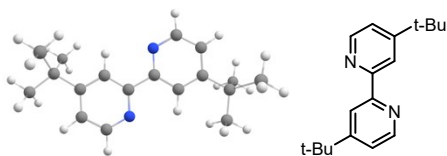
Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1183.58286832443

N	-3.93631146687735	-2.14546602556160	-0.12808367331925
C	-2.89480456905776	-2.57903317796810	-2.69792769316578
C	-2.17537706864446	-1.87333333132334	-1.72927112706991
C	-2.73534589002683	-1.67225326465303	-0.45257446501483
C	-4.62742622507160	-2.82841512093701	-1.05320977226127
C	-4.16878450127788	-3.05550218170964	-2.34271016445823

C	-2.41685729522273	-2.77479192121181	-4.11388904173517
C	-5.04659716811544	-3.75835249488457	-3.35959861023272
C	-1.97002392858908	-0.88809446974912	0.57102467514352
O	-0.95166804422157	-1.32232482632227	-1.93704526003644
O	-0.98294860132456	-2.63189567644792	-4.21190931370637
O	-6.39000294159154	-3.91980525431291	-2.94994890528902
H	-0.65211510329741	-1.61498660385683	-2.81995670152384
H	-0.77077193397982	-2.36337425827883	-5.11171580867473
H	-6.78144141162483	-3.03296713640600	-2.88315481349777
H	-2.91237820795194	-2.03008024292411	-4.75689884474491
H	-2.69258757113692	-3.77851009654802	-4.46623246272930
H	-4.66005548019969	-4.76986540688629	-3.55115339781424
H	-4.99575787219460	-3.21418607834351	-4.31972500542170
H	-1.72137196882646	0.11129735274836	0.19429152459661
H	-2.56153268166979	-0.81180386581214	1.48638742493023
H	-1.01439967945732	-1.37211903552775	0.80242776290396
N	-3.80566567028876	0.29228824088542	-4.41760041135129
C	-4.457221222902759	0.97234469062825	-1.77351135100699
C	-3.24719256871377	1.36686498265429	-2.35157405931082
C	-2.95548043476050	1.00335392387870	-3.68290154543460
C	-4.96998824627867	-0.08283114490070	-3.86931112420285
C	-5.34286298522741	0.22393279539878	-2.57009314532195
C	-4.82472360947212	1.21581226322125	-0.33176591376606
C	-6.65880535053613	-0.24734481690578	-1.99574838387560
C	-1.64423998871607	1.40704370491340	-4.28383341937331
O	-2.28977249299111	2.07886212299779	-1.70793213214913
O	-4.01850560965108	2.25287441139090	0.26356247083320
O	-7.37914511387928	-1.14774350676676	-2.83832898612927
H	-2.64593064752269	2.31235859389564	-0.82861561656893
H	-3.90963259085514	2.05030347988559	1.19831520001000
H	-7.68503018534857	-0.67011442166051	-3.61771297685539
H	-5.88097324228453	1.51399017617642	-0.26041652518190
H	-4.70311632868335	0.27015166461950	0.22082902060915
H	-6.48169952635121	-0.80391394264870	-1.06764794537006
H	-7.29626421202155	0.61586253265966	-1.74198105658625
H	-5.59983578343738	-3.21194977073857	-0.75419907483985
H	-5.61917851434175	-0.68588973733494	-4.50046720114456
H	-1.53555759588429	2.49743444031629	-4.29384520580292
H	-1.58034086939347	1.02861484052830	-5.30585536360294
H	-0.81114759397280	1.01933759382242	-3.68655158045576



Main article molecule number: **1-monomer (Fig. S1)**

Name: 4,4'-di-t-butyl-2,2'-bipyridine

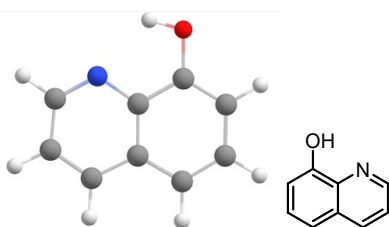
Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -809.684916603281

N	1.88568777204077	11.16674325459677	30.09362165116610
N	3.13137675777119	14.54722965174118	30.31045755615307
C	1.11646144034744	10.33467894347100	30.79752184589665
H	0.96680994578943	9.34270815102191	30.37097169714069
C	0.52049989003213	10.66662319665950	32.00553645771851
H	-0.09195624018654	9.92802184990462	32.51401017886221
C	0.71977082317072	11.94331441436106	32.54457579716895
C	1.52149921372921	12.81150355398342	31.81090385466650
H	1.73495226785471	13.81875320372122	32.14365303362268
C	2.08322538152808	12.39240686113806	30.59902025205684
C	2.94087902690333	13.31428038292739	29.80898853112479
C	3.51075025716888	12.89703223394663	28.60661761069812
H	3.30626370256081	11.88639509291513	28.27259282162241
C	4.31565326423896	13.76659335242277	27.86962098130160
C	4.50571537532551	15.04319808138093	28.39959499219610
H	5.11513879968868	15.78478513143355	27.89562935235732

C	3.89783014667104	15.37622320221315	29.60760455783595
H	4.04101612012284	16.37174442983880	30.02871783862115
C	0.07350399571924	12.33047453915944	33.87283823261480
C	-1.45699171823782	12.21581256846757	33.73836724819395
H	-1.76895746711460	11.19396520080117	33.50156682504579
H	-1.82714974529043	12.87515636343996	32.94615919755229
H	-1.93797607596896	12.50480295345621	34.67971309891372
C	0.56646840695189	11.36870230572828	34.97075560302318
H	0.11748666259253	11.63730862879424	35.93371063421596
H	1.65565221144579	11.42135938332619	35.07208760641943
H	0.29684604939891	10.33103454101757	34.75222136918677
C	0.41970199085348	13.76401971892045	34.28970406032006
H	-0.06555419713981	13.99186632646364	35.24448452222252
H	0.06976062559195	14.49562523769331	33.55389733394048
H	1.49844018158763	13.89765264533583	34.42288810086836
C	4.93819677999229	13.30134351105260	26.55503481350575
C	3.81382567016349	12.89583685964068	25.58290479420128
H	4.24378968044583	12.56294879953289	24.63139558520259
H	3.14870488178647	13.74268705939215	25.38284530151198
H	3.20886707088805	12.07792225428610	25.98481679969767
C	5.78378773609320	14.39506981759877	25.89340767433956
H	5.18476900981330	15.27906081812110	25.64885275983937
H	6.20657816431955	14.01243169517558	24.95870558116443
C	5.84041260322194	12.08352716423535	26.83147624626770
H	6.63870826668293	12.34288209392103	27.53501674431938
H	6.30074588752304	11.73927692583915	25.89837322000671
H	5.27304922583962	11.25026763986406	27.25622743423041
H	6.61847815808323	14.70573596105939	26.53134520298594



Main article molecule number: **2-monomer (Fig. S1)**

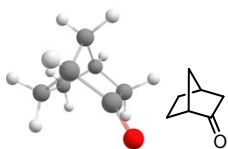
Name: 8-Hydroxyquinoline

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -477.062939536696

N	13.28273251818368	12.89134518786673	6.81453593511704
C	12.88796292487632	11.77263669800358	6.23976153215404
H	11.82874975959226	11.69346873295383	5.99674801425905
C	13.76338037725167	10.70807186846512	5.93812772293519
H	13.37534977168863	9.81223825785397	5.46351165881848
C	15.09534853718796	10.82592476010156	6.25193487010557
H	15.79509237615529	10.02317331343906	6.03206176811675
C	15.56660318346466	12.00606969872075	6.86914579661136
C	16.91428471531573	12.23005566299348	7.23298180543166
H	17.65665884626875	11.46180641193926	7.03703138114179
C	17.26534513916389	13.41912709825106	7.83002420662259
H	18.29992310181257	13.59455866773187	8.11070998894915
C	16.31746452665328	14.42764603867114	8.09250426970810
H	16.61287519601881	15.35922862513564	8.56428849956642
C	14.99740583726187	14.23506891447989	7.74812824599277
C	14.59653284865878	13.01604208042150	7.12778320936030
O	14.06831940262102	15.18354852363401	7.98716160405841
H	13.22673793782474	14.81502245933745	7.65903849105128



Main article molecule number: **3-monomer (Fig. S1)**

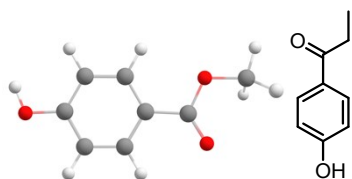
Name: Norcamphor

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -347.90373088891

C	0.51870075833866	1.29505445825362	-0.39453768030950
C	-0.92495754788521	1.03465627530763	0.06874340929238
C	0.16998631877058	-0.86668377367787	0.67221755402151
H	0.63446672574232	1.52602421493894	-1.45873785428489
H	0.98874215009472	2.10681631694529	0.17623588216690
C	-0.68192747819300	0.21885058138186	1.35761727774680
H	-1.60425147289126	-0.18029607841652	1.79359695772752
H	-0.13335838333374	0.77811974679659	2.12405322993522
C	-1.54476652979802	-0.02942049494759	-0.86051306452276
H	-2.61909149340622	-0.12780003296198	-0.67425340420700
H	-1.41548619400753	0.22645172733154	-1.91704818604160
C	-0.78552798816491	-1.33231136760998	-0.46420849389997
H	-1.46987902877844	-2.09086154918258	-0.07089112933918
H	-0.23850489554132	-1.78141582776017	-1.29874451835571
H	-1.52971544171501	1.93794202824448	0.18442672175257
H	0.58922445002852	-1.67139131947136	1.27810791781572
C	1.21922865676530	-0.02172300186194	-0.03658934359973
O	2.35938939397456	-0.32670290330998	-0.29600427589827



Main article molecule number: **4-monomer (Fig. S1)**

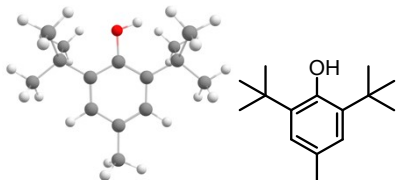
Name: Methylparaben

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -535.260594271769

H	17.90956636744076	9.49520852034183	15.05194227324298
O	14.11359178570963	14.35951895448102	18.15453291883977
C	15.29982396222303	12.88842516475296	16.69508811926987
O	14.01980065765853	14.70933454155191	15.92420649358539
C	15.79538791774179	12.10938325357829	17.74775242469777
H	15.52458070990070	12.37821143059897	18.76380394183927
O	17.75225890092073	9.61646460641000	15.99572165055156
C	16.61171993923992	11.02127791525273	17.50142409149296
H	17.00097942967662	10.41153180217309	18.31024556774631
C	16.94534317713782	10.69673440440707	16.18448806283508
C	16.45865845781015	11.46442350961071	15.12378400008806
H	16.72104077225615	11.20799866636236	14.09942029000077
C	15.64060348039528	12.55382978507080	15.38097209560105
H	15.26257231155943	13.14984960253397	14.55802741244321
C	14.43210409175771	14.03783018266603	17.02828402302531
C	13.16916803118794	15.84030926258792	16.19082516599598
H	13.69105671515362	16.57464225502608	16.81107310584027
H	12.92965405531146	16.26193489754682	15.21401364361216
H	12.25929123691867	15.52216824504740	16.70778971929216



Main article molecule number: **5-monomer (Fig. S1)**

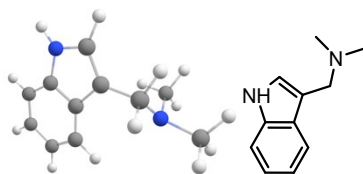
Name: BHT

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -661.112433195317

C	-1.24580697041107	0.16367639212499	-0.00010679246717
C	-1.20445657270553	1.55572807191057	-0.00080453667946
C	-0.00985039341904	2.27259016392019	-0.00075109008396
C	1.18305863314632	1.56310712060862	-0.00051425780852
C	1.22515379757971	0.16510136146893	0.00006135233277
C	-0.00813938501000	-0.51590265040974	0.00038746024206
H	-2.13243026275766	2.11709736619285	-0.00141187601352
H	2.10827114191947	2.12734891388937	-0.00088655887750
C	-2.58478851805513	-0.59012214578974	-0.00016155038682
C	-3.78141274150315	0.37394490401115	-0.00072402829036
H	-3.79673105366340	1.01194586801863	-0.89117998372294
H	-4.70578950382877	-0.21305410654552	-0.00063482976622
H	-3.79699096132860	1.01264937662691	0.88922172453737
C	-2.71039817027253	-1.46186402053977	1.26667841548347
H	-3.69125374659148	-1.95161492115767	1.28178816285126
H	-1.94095836292128	-2.23303220365891	1.30996995030626
H	-2.62777945721709	-0.83942644327613	2.16463068367479
C	-2.70990469511365	-1.46279017430281	-1.26640931562124
H	-1.94047832011909	-2.23401794346405	-1.30877472954036
H	-3.69077836794434	-1.95250209370662	-1.28158382119159
H	-2.62685739877959	-0.84101625296335	-2.16478082688006
C	2.57448960809506	-0.57764373899925	-0.00004335069709
C	2.73615390451046	-1.43536585796644	-1.27751985814350
H	3.71786682973408	-1.92245990438262	-1.27644844771343
H	1.98627383110858	-2.22273776043111	-1.40643084408553
H	2.67057015643334	-0.79517305642866	-2.16300707915255
C	2.73679960853744	-1.43457133322580	1.27788150356787
H	3.71849433208275	-1.92170037172939	1.27658494679014
H	2.67170902593086	-0.79383526282969	2.16301187738396
H	1.98698397041816	-2.22185804060822	1.40770813451686
C	3.76329312852984	0.39813519703836	-0.00062731780060
H	3.76802284799562	1.03578820408186	-0.89038394825499
H	3.76841112603178	1.03639470843287	0.88869193243740
H	4.69505916181898	-0.17718070525539	-0.00064146964117
C	-0.02384654889226	3.77827937431575	0.00100286349741
H	-0.52331892965077	4.17086081663782	0.89444940484081
H	0.99109960509531	4.18508413952823	-0.01999317487595
H	-0.56100126492576	4.17270695685432	-0.86929022927566
O	-0.06978880473339	-1.89015857978773	0.00085911355679
H	0.82390672087584	-2.24243836820282	0.00110139095097



Main article molecule number: **6-monomer (Fig. S1)**

Name: Gramine

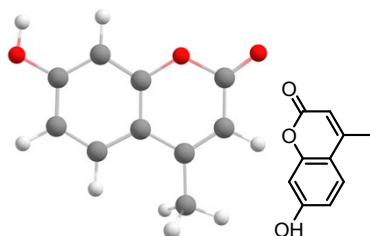
Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -536.954162247783

H	10.59285936876690	14.19369082595759	13.31151605810053
H	10.72981204261871	16.03919265252571	11.16627002253114
H	10.47438549576812	17.42908906350500	16.60786037656080
H	10.74350828643377	18.60775540014236	17.90808065233962
N	11.11166600387260	14.92202888045987	13.76949747693277
N	12.47378915506655	17.64804989739854	17.21522120313990
C	11.56211514764697	14.88203878976847	15.07526006149389
C	12.24476573423588	16.03359673700090	15.36690940371926
C	12.71720151345687	18.10824839887639	13.85654792634735
C	12.50769121969003	18.60222890775338	12.57877405692853
C	11.79821275293730	17.86124628110738	11.61698141210320

C	11.28067657132078	16.60805518367982	11.91038802236325
C	11.49626362108889	16.11346945184651	13.19485609914137
C	12.21328285057136	16.84148334215299	14.17972411980827
C	12.91697029839091	16.36410163433528	16.65724687434695
C	13.24757003500001	17.96946427211195	18.40845282786870
C	11.04647885736318	17.62996806457759	17.51867376036748
H	11.36306528767385	14.02395938469365	15.70350985115468
H	13.24704416033834	18.68801345656849	14.60597342464837
H	12.89191728505301	19.58245647342229	12.31245726226900
H	11.64906614143388	18.27886388916488	10.62563708312026
H	14.00327308961579	16.43863583081911	16.49889609838060
H	12.75639904391386	15.52920438634463	17.37444279345797
H	10.78083120595422	16.85957657331297	18.27232963040199
H	12.94264016609086	18.94751560730103	18.79617108129209
H	14.31396831841748	18.01872305377206	18.16036866867697
H	13.11809834727978	17.22414456140104	19.22044275250493



Main article molecule number: **7-monomer (Fig. S1)**

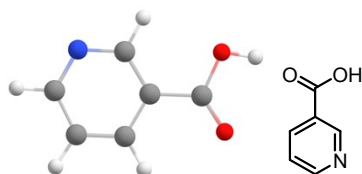
Name: Hymecromone

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -611.466363427428

O	2.15904000166639	4.98358053503154	10.16201776117718
O	1.52962202350872	4.68939004107549	12.28165391202642
O	3.35407198238391	5.74405832116977	5.63455965849819
H	2.62391083365637	6.37052162932369	5.70426546463256
C	2.29672614231088	4.35596432819246	11.41265056857904
C	3.34929524840374	3.374597648885549	11.51709201556346
H	3.44251353947056	2.90028670022390	12.48803996590587
C	4.17133113444605	3.05589277477603	10.48449394972899
C	3.99322740183861	3.72441354800663	9.21975704727955
C	4.77619833438181	3.48604151865611	8.07608055578131
C	4.55516942596771	4.16092387082156	6.89396279683675
H	5.16012787437482	3.97567394109072	6.01325353799980
C	3.52556046251992	5.10970813614529	6.82541104524383
C	2.72884615683932	5.37490420702534	7.93272918589494
H	1.92513862159772	6.10538684615882	7.90343961621565
C	2.96906839015190	4.68265655447368	9.11442863931636
C	5.24919539552224	2.02829425781663	10.64450782912898
H	5.10795789610106	1.20202909064208	9.93819332617419
H	5.57514440932554	2.75305841924532	8.12163853129429
H	6.23526708871745	2.46258533622647	10.44325151396402
H	5.25170963681528	1.62030729504294	11.65688107875857



Main article molecule number: **8-monomer (Fig. S1)**

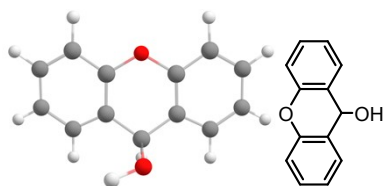
Name: Nicotinic acid

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -436.786352736965

O	7.38050596456261	11.45004572001977	4.54484546818390
C	4.96111726017770	14.89932575258003	4.18785695474100
C	7.62232553976778	15.08140517710174	4.74823406123930
C	7.05504565788738	13.81460162924352	4.57693781661914
C	5.69222280367489	13.72755297283969	4.29030335462650
C	5.61960247036313	16.11270161974874	4.37570814911084
C	7.83928889201111	12.56188872523937	4.68636818380568
N	6.92417580462425	16.21451025657821	4.65105502953557
O	9.14796314470295	12.78587293157785	4.96621562813345
H	9.56830633267468	11.91323568791007	5.01653571989991
H	8.68213185003068	15.18059648157923	4.97231512282394
H	5.07188367534410	17.05177810899120	4.30147839266988
H	3.89862430942547	14.88050502230856	3.96636983338080
H	5.23927329475322	12.75005891428193	4.15498228523006



Main article molecule number: **9-monomer (Fig. S1)**

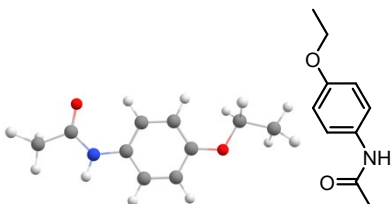
Name: Xanthinol

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -651.722430671294

C	3.54478826820433	-0.99820354766330	-0.11966261171163
C	2.32559935481289	-1.59562997414977	0.16402544649925
C	1.17606394672911	-0.81038690804122	0.20807638815282
C	1.22929354308719	0.56671069832653	-0.01133990766099
C	2.46477975955328	1.14062640922864	-0.31939738218251
C	3.61955180235942	0.37182841203638	-0.37372767831104
C	-0.00121247107381	1.40161426227577	0.18704144451841
C	-1.23595331744550	0.57403097341898	0.00388170030116
C	-1.18120173566896	-0.80412902599834	0.20483913671649
C	-2.32736497139043	-1.59251188916570	0.14746251257621
H	-2.24098114563524	-2.66222993064053	0.30848594449069
C	-3.54769180243458	-0.99185646834371	-0.12307084727032
C	-3.62510405713376	0.38354698940263	-0.34476904273375
C	-2.47262508218134	1.15386169602819	-0.27836913966403
H	4.44207514705633	-1.60868505687596	-0.15810307459528
H	2.24183125787051	-2.66306009568245	0.34134400389428
H	2.51076215039854	2.21055927903382	-0.51496658914321
H	4.57221530993776	0.83277994170774	-0.61408966670233
H	-4.44430757978597	-1.60276261285127	-0.17078276660576
H	-4.58107094215269	0.84931714634219	-0.56166289985447
H	-2.52054598151108	2.22955030409813	-0.42862661720336
O	-0.00183901450828	-1.46553277110829	0.45556755422721
O	-0.05272696337571	1.92030553107120	1.53950311821217
H	0.83674246817270	2.22067918470082	1.76604870312307
H	-0.00250894388470	2.24675545284951	-0.52093372907309



Main article molecule number: **10-monomer (Fig. S1)**

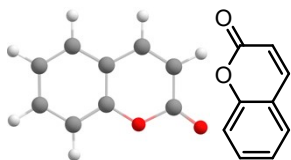
Name: Phenacetin

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -593.979783924289

C	17.74205714886844	12.91407312400948	14.59261173086514
C	16.39405072331122	12.64977126674120	13.95965680654202
H	17.77985507570187	13.92316748360957	15.01269818691488
H	17.92203033972672	12.19502421494327	15.39770904852145
H	18.54169147573750	12.81558136644415	13.85298141208641
O	16.21369633640752	13.61539820748727	12.91931594065203
H	15.58579792643600	12.74646253707105	14.70075524090359
H	16.35051886354021	11.63494217915780	13.53526601877704
C	15.05740922515344	13.56423321221342	12.19649699375934
C	14.02533678619379	12.64937520268952	12.40250465902209
C	14.93268959329149	14.51672245359415	11.18066738362537
C	12.88029744840581	12.67875253508221	11.60794555680787
H	14.08898421397797	11.89810604963173	13.18093145095160
C	13.79780891922145	14.54555626494458	10.39318994978223
H	15.73835748756083	15.22671165220991	11.02393170848223
C	12.75639489145823	13.62863370437497	10.59404928194543
H	12.08496429731820	11.96577631826251	11.77539062376106
H	13.71804935343379	15.29387995312334	9.60707607042250
N	11.63556792613866	13.72871046330153	9.74287837256709
C	10.48908710135239	12.97292966744049	9.73125776779359
H	11.69121618967087	14.45942089548078	9.05119585184063
C	9.48289074874491	13.37026331211415	8.66739161567248
O	10.26714547117619	12.05168683736181	10.50264463354835
H	8.55179080439371	13.65660852049737	9.16493649011610
H	9.80594854775526	14.18880917969942	8.01774594607100
H	9.26673310502335	12.49118239851413	8.05412325856838



Main article molecule number: **11-monomer (Fig. S1)**

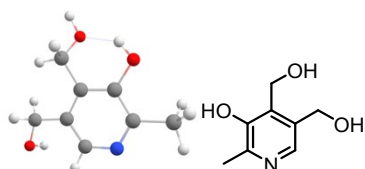
Name: Coumarin

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -496.934305122779

O	11.26467093682450	14.63339543011263	20.83493012569925
O	11.83393017688908	15.33752907975128	18.79539919070798
C	10.41548855206400	13.98174701798808	21.67731737076810
C	8.95999001099150	13.47122112870962	19.80347074821097
C	10.76122724031193	13.93810123077924	23.02444199389168
C	9.23794392663870	13.37742106980483	21.20616790753140
C	8.40585246733131	12.72122541603473	22.12697946029436
C	11.02281877766295	14.74231455425324	19.45876136917057
C	9.80562920459929	14.11842211106650	18.97404060124709
C	9.92061569303537	13.28306208970246	23.91172589073197
C	8.74209949135404	12.67330911165921	23.46760504769515
H	9.62611183798490	14.20807738633700	17.90884348911040
H	10.18452133726485	13.24511558888183	24.96434233247886
H	8.09457975413615	12.16455965929896	24.17424845712779
H	11.67885053458214	14.41619359316512	23.35074099630344
H	8.05291827921928	13.01017018720110	19.41845390924522
H	7.49350977910997	12.25197234525408	21.76790110978564



Main article molecule number: **12-monomer (Fig. S1)**

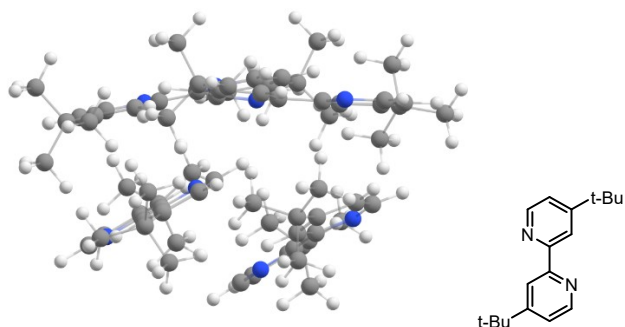
Name: Pyrioxidine

Qty of copies of the molecule modelled: 1

Qty of imaginary frequencies: 0

Final single point energy (Eh): -591.777504554973

N	28.49391257705194	17.36563795917214	21.69068063465522
C	27.61849461937692	16.23863251192103	24.09486816985234
C	28.71567045457061	17.10244718278753	24.04895169607216
C	29.13247748762625	17.65063932213039	22.82369978562905
C	27.42939368913781	16.55428694859214	21.73008699413924
C	26.94131733522420	15.97023417639186	22.89459097170882
C	27.26641288277820	15.56229196712654	25.39006764208153
C	25.71960315790652	15.07406587222670	22.85250373414311
C	30.32030913729839	18.56217130669764	22.77313542317475
O	29.43895850876515	17.42912421823840	25.15555912008028
O	27.21254420769084	16.55363766615432	26.44293392544186
O	25.02517635859085	15.10266368938966	21.61400430866123
H	28.88619607353478	17.24080360780113	25.93545453026885
H	27.11263254498396	16.09314386556500	27.28416941811806
H	24.70851665962274	16.00272836267202	21.47181226776648
H	26.30491361226536	15.04110390848833	25.32087088293760
H	28.04185213082653	14.81399209494814	25.62526222425294
H	26.00922028107950	14.02470399968556	22.99649926860355
H	25.03921043411453	15.33645822918994	23.68012422461359
H	26.94729365087563	16.34712524016666	20.77793427735948
H	30.16983234752582	19.43581649762378	23.41697249922164
H	30.48189951071828	18.88813138109847	21.74461158550829
H	31.22025733843490	18.05630299193248	23.14078241570973



Main article molecule number: **1-tetramer (Fig. S3)**

Name: 4,4'-di-t-butyl-2,2'-bipyridine

Qty of copies of the molecule modelled: 4

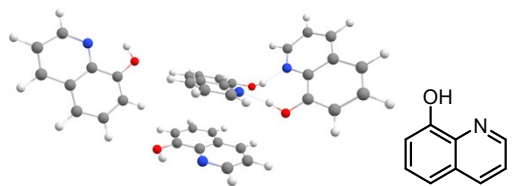
Qty of imaginary frequencies: 0

Final single point energy (Eh): -3238.803750464372

C	-0.44501146663687	-1.86880707826165	4.51364832781682
H	-1.21106191093488	-1.43894509416670	3.85935725044641
H	-0.82567884439991	-1.86481100401742	5.54167402556756
H	-0.29368496003424	-2.91353363918419	4.22695196892942
H	-0.13170253403681	0.89871500348957	4.36038928879017
N	-2.76049176969762	-0.76169659086299	0.37413771377015
N	-0.96114680598033	2.03766938360875	1.77097447530966
C	-3.73053294060553	-1.61361109283190	0.71447277237706
H	-4.02175815289421	-2.33226449584509	-0.05246112142927
C	-4.35166030373144	-1.60852950918879	1.95585220759394
H	-5.13495752419573	-2.33314865924540	2.15723773286191
C	-3.95708945718726	-0.67745797086857	2.92390050045997
C	-2.95363943916612	0.21613959971606	2.56036249159542
H	-2.59048761455896	0.98056114058824	3.23518014854695
C	-2.38469319915864	0.14766749412700	1.28416719831326
C	-1.34570287233019	1.12282268604180	0.86421963352945
C	-0.83505234065985	1.09193224386594	-0.43318702107794

H	-1.19387070450935	0.31700974561814	-1.10030699915116
C	0.10032912009500	2.03867190970264	-0.84681912917476
C	0.48832263097137	2.98699084409294	0.10143066287174
H	1.21219714020134	3.76066895004794	-0.12959317064100
C	-0.06299708828265	2.93789611243234	1.37888192236484
H	0.23937924832027	3.67182094137637	2.12695136200814
C	-4.62332241679728	-0.65954019701283	4.29798897014091
C	-6.11615630571613	-0.32193893623419	4.12097422857344
H	-6.62266291573343	-1.05763500815834	3.48853581258547
H	-6.23966395431864	0.66331088158850	3.65899362013484
H	-6.61643256984848	-0.31133410789572	5.09607679240158
C	-4.48715278163097	-2.04946160905636	4.94801891788937
H	-4.94535255457721	-2.04188759870048	5.94338782103877
H	-3.43363179964081	-2.32887970267566	5.05515878944911
H	-4.982066617440600	-2.82556922617466	4.35661299068018
C	-3.99214827635401	0.37817389455064	5.23287927207558
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C	0.85545111859793	-1.04977674244034	4.44105099513216
C	1.93363601713340	-1.73338462611271	5.30396145743728
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H	2.13463712523716	-2.74954152271193	4.94866508661136
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H	1.48309873065785	0.94539418779258	5.10232893100569
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H	-1.10269961727973	-5.84836225895239	-6.1163266667277
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Main article molecule number: **2-tetramer (Fig. S3)**

Name: 8-Hydroxyquinoline

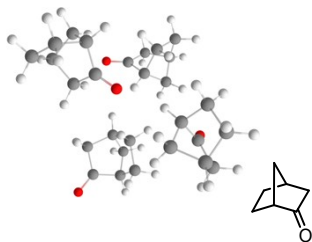
Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1908.29156454211

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N	-2.91380675258471	-1.90905318751997	0.90919987755132
C	5.36343187092662	-5.39505967290430	-3.34511949620321
C	-1.26753113750145	0.85933157272310	-0.92348919699547
C	0.03435380979349	5.74932090668890	-0.33276278825697
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H	-2.24733303682478	1.07216995088924	-1.35096182871165
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H	-4.69050149877722	-1.30396017041801	0.07390446115218
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C	-0.10273911221685	6.90974336068975	-1.11842527267088
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H	5.44510018631850	-7.43004362649255	-4.07627260474625
H	-0.94717877625403	-0.92230812535078	-2.10352540325664
H	0.76047293190188	7.54074060946609	-1.30371366652754
H	-4.73454106485789	0.90238186957111	1.24018443463576
C	3.84149035612612	-7.13100212780408	-2.68103774296902
C	0.67273172997671	-0.52737239596111	-0.74927688236246
C	-1.34106925065824	7.22682609692853	-1.61651308053135
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H	-1.49163926694592	8.12560118173323	-2.20978872671805
H	-2.88518788021129	1.50020717797617	2.78985065038476
C	3.18671038240160	-6.19853342181870	-1.84619932917729
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C	-2.44477712733623	6.38439743161550	-1.35448174959184
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C	-3.75269897208644	6.66805807547019	-1.80475377243695
C	-0.73831222714779	-0.13251529287011	3.33984035945875
H	1.65939078289444	-7.50766505238147	-1.04352098502918
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H	-3.93369723481226	7.56720972321829	-2.38632729067227
H	-0.67632331264076	0.80822338246987	3.87880652506237
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C	2.78552547832670	0.97680248700406	1.91150330311254
C	-4.77551002609833	5.80281715704129	-1.49365420443367
C	0.24572307832154	-1.08466976230276	3.46016491485408
H	0.63569587344321	-5.72831021796236	0.35496333751230
H	3.71991041697149	0.80391246112918	2.43857404859683
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H	2.35026406776554	2.79672046427417	3.01361999975016
H	-5.35169889108319	3.94123544568033	-0.54020731280778
H	0.97262925605682	-3.04732641641851	2.86953147491588
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C	0.82676436031687	2.37386201816384	1.59704763014565
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C	3.71494487174080	-4.87601840922089	-1.83987455681681

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O	-0.95125623120914	-3.71255782108731	1.20905008678223
H	4.37209881288084	-2.65878027385515	-1.64978416084283
H	-0.43993002227618	3.79946973114327	1.20774425668716
H	-2.14830363642629	2.82378976002169	0.32383421489604
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Main article molecule number: **3-tetramer (Fig. S3)**

Name: Norcamphor

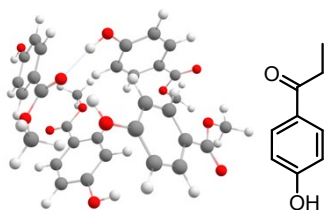
Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1391.6439489357

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H	11.41624887015417	6.08917275930235	6.68157327857100
H	11.34506685773456	6.58290449759749	8.38001642376365
H	14.54066636481506	8.62413681589488	6.54401794164103
H	10.23883774675493	8.26338937327498	6.55889897638633
C	11.57182649126001	9.17534011848294	8.06408216982672
O	10.78975050559014	9.65687681226102	8.85608683025887
C	5.08856749986137	8.34288470025257	7.78143562370430
C	6.22010282336037	7.90121809394663	8.72717620010118
C	7.29736027498771	8.30938558747222	6.76732273410325
H	4.26729170854467	7.62804412371325	7.66050633509249
H	4.65188053594441	9.30142527305724	8.09222478767887
C	7.38518898002386	8.78466846533226	8.23113242404004

H	8.34919119061516	8.55297088515077	8.69440439420557
H	7.19095723894345	9.85778302501546	8.34659951566161
C	6.68924476900480	6.49657417811974	8.29479036439764
H	7.38274660096457	6.07791117290131	9.03094848201135
H	5.85180618534124	5.79825128687073	8.19424122504119
C	7.40877025258644	6.76690478159138	6.93954403284342
H	8.46805519736597	6.49284151914301	6.97696059601148
H	6.96112055567559	6.22482110972371	6.09971530458013
H	5.97591751624425	7.98724148251232	9.78905639864829
H	7.98293101766477	8.73061647993362	6.03318152575752
C	5.83424138727532	8.55764131579649	6.46221618405333
O	5.34084004847201	8.84807257433679	5.39213775776166
C	7.76329649894916	8.67575198351519	2.85643281737985
C	6.80300126406326	7.91809673715792	1.92222883830807
C	7.96825208080341	6.25598604751217	2.94687084221560
H	8.40927693945391	9.41535678190603	2.37078092483061
H	7.20298183589823	9.17293715368905	3.66154645180757
C	6.49307351264124	6.66954427784778	2.77556024293005
H	5.90643541308142	5.91620086851161	2.23836160345766
H	5.99465568536264	6.92177089499230	3.71717024977669
C	7.62583176914650	7.31449079791854	0.76546627336176
H	6.96757880412426	6.90632350659565	-0.00818607026409
H	8.27091547528071	8.06025000591655	0.28948965459911
C	8.43834863999714	6.18210222122711	1.46356704956690
H	8.18286242677939	5.19730275344703	1.05929991389235
H	9.52148007072203	6.30764409350816	1.36922939456791
H	5.93559918894538	8.50304124994775	1.60770517687248
H	8.20907956871739	5.37641161514450	3.54683218012133
C	8.58208731646921	7.54269183279500	3.46722864577060
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Main article molecule number: **4-tetramer (Fig. S3)**

Name: Methylparaben

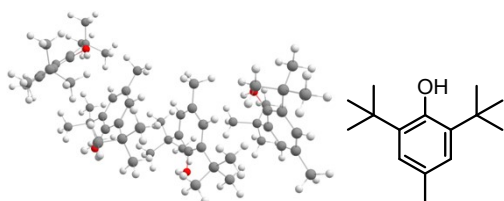
Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

Final single point energy (Eh): -2141.10037416641

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O	-0.22817569039748	-1.94541116792921	-2.24564350324148
C	-0.59519997737067	1.30200198437623	-3.84537031000551
H	-0.46656620657472	1.02762735351184	-4.88813285316328
C	-0.76051316781811	0.63617188993899	-1.53303113006920
H	-0.77274894197659	-0.13018679104377	-0.76931071042750
C	-0.34064381980519	-1.10099021795512	-3.30315615096065
C	-0.02025373601769	-3.32904684607657	-2.58164194016139
H	0.90660141239750	-3.44834108678056	-3.14950655355830
H	0.04920273159717	-3.85317807587376	-1.62751597849715
H	-0.85752161441554	-3.70963945532028	-3.17383399973355
O	3.25216938935806	1.66213179483105	-0.61729143953308
C	3.34105596753012	-0.01633247957198	-2.32640547305653
C	4.05478312408252	-0.95332534518647	-1.56566098872770
H	4.48140337077503	-0.66659032295615	-0.61001965931223
O	3.92119299822855	-3.89425746805147	-3.67022544010739
H	3.54244046907675	-4.02037811905287	-4.54903095544322
C	4.24892278576345	-2.24015505305599	-2.03012565844153
H	4.80617831641486	-2.96916784370430	-1.45135248805778
C	3.72085029471160	-2.61139336130251	-3.26964807982854
C	3.01194541086778	-1.68811584135819	-4.04153839984819
H	2.57609673441794	-1.98167377808033	-4.99345741080854
C	2.83200673954532	-0.39886560803076	-3.57337999180326
H	2.26704885590230	0.31090364921747	-4.16619259438210

C	3.11683678776832	1.33896354657331	-1.79875020010991
H	-1.11972367326873	4.35081786872717	-0.84920424475269
O	-1.07857675356225	4.26799349304298	-1.81559965280299
C	-0.77397512647614	2.62558771928454	-3.48434604822123
H	-0.78812114632910	3.41634791251754	-4.22786174213673
C	-0.93837395685709	2.95614730224899	-2.13493428286722
C	-0.94426161566738	1.95534853237915	-1.16083483135505
H	-1.09717010793981	2.20792312502526	-0.11546703468118
O	2.75268414495011	2.20183463802972	-2.74979729226654
C	2.48461240819920	3.55891423241229	-2.33626243214130
H	1.68020427008720	3.58396321608537	-1.60040340831015
H	3.38808906050959	4.01039451196904	-1.91609506278309
H	2.18155862911023	4.08001960901694	-3.24385896116375
H	3.30723282322993	0.45624695605374	0.78403432378782
O	-1.87690786165807	-2.62716187867581	4.12875587849635
C	-0.20463502671618	-1.90134372465721	2.58456587819053
O	-2.23902127767062	-2.87594744617136	1.91268912574486
C	0.68881615147750	-1.51340839506898	3.59093993638183
H	0.41736517535123	-1.69433324058238	4.62631565430227
O	3.33323801794305	0.06518144614492	1.68305265121170
C	1.88027078080181	-0.88710266802400	3.27334217203953
H	2.57026610480469	-0.56301961672180	4.04610998523015
C	2.19039083408384	-0.61921629853491	1.93477271192868
C	1.32192051882051	-1.03349332124538	0.91893955839157
H	1.56975449747645	-0.84449440622689	-0.12256725736943
C	0.13767024490063	-1.67423772795913	1.24732942876689
H	-0.53511788579800	-1.99224496460371	0.45832659484310
C	-1.49567916738698	-2.49536597617625	2.98193889076116
C	-3.51891269658408	-3.44827102784294	2.23783826794656
H	-3.97339503412564	-3.70834754645848	1.28125706089096
H	-4.13967514821081	-2.72295431887775	2.77213551574238
H	-3.39481865761691	-4.33732447013587	2.86261875901821
O	-2.55449765439269	1.02923175908753	3.49077165403427
C	-3.74613526886984	0.46176422657209	4.07118185618249
H	-4.08570233357019	1.07082437078662	4.91379085023625
H	-3.45603898268035	-0.53600955889010	4.40274446578655
H	-4.54494553154344	0.41374966658550	3.32476260259427
O	-3.71282959796181	2.92987008800056	3.08569158179152
C	-1.40617077546180	2.80644016412730	2.47378573811186
C	-1.37123291300983	4.10772806505318	1.95728075983470
H	-2.27453479097095	4.70907431905977	2.00380242421834
O	2.05778899256412	4.33456488667555	0.77777413669412
H	2.69224950502532	3.61587563787974	0.62635822214900
C	-0.20843752920203	4.61639712582200	1.39492181430973
H	-0.16170251917339	5.63253325771843	1.01159981968889
C	0.94239538062877	3.81802980361652	1.35322093640747
C	0.92471375578097	2.53360217048588	1.89784428920878
H	1.83119509298432	1.93789506457133	1.89441973451019
C	-0.24218663420396	2.03056821142109	2.44678759681631
H	-0.25024639367219	1.02683640455167	2.85711713337961
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Main article molecule number: **5-tetramer (Fig. S3)**

Name: BHT

Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

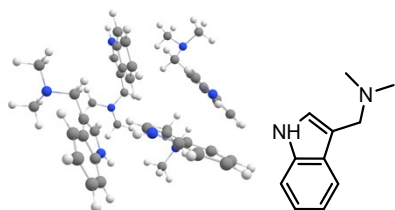
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H	-7.42918339780533	3.79465053066593	-10.80805324596989
H	-7.04682705452542	2.65899549080674	-9.50191224159547

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H	-5.75612501723615	3.62916122587467	-10.22631251262655
C	-8.51458829217383	4.74154939504453	-8.40881757889635
H	-9.19004335099479	4.97285683821538	-9.23401455774088
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C	-6.19620893944857	4.33331684952436	-7.63230953903629
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H	-5.64303223346118	17.31862091989585	-8.89413109266329
C	-6.83258133603596	18.41023766632295	-11.94351387230311
H	-5.81992215190497	18.54262560153948	-12.33851669079979
H	-7.19834882958763	19.39461046354824	-11.63185219362504
H	-7.46005157291256	18.04543180284388	-12.76402773379029
C	-8.35558639603680	16.38088791117733	-9.01282031816362
O	-7.24691835011628	15.72492678770415	-8.52838010349912
H	-7.54787143371463	15.00953276055558	-7.95668007321800
C	-9.60690931543414	16.25644780163790	-8.37328790447829
C	-9.77630468863683	15.51879163502309	-7.02970394496661
C	-9.46261195772687	14.00868722333937	-7.12938186231441
H	-8.41806202157571	13.74249553263191	-7.33488564017620
H	-10.05803786035875	13.53697425878329	-7.91635852603515
H	-9.70539250970746	13.52759779327157	-6.17499592607199
C	-8.89074868161071	16.18998294732614	-5.95620626976532
H	-7.82707226887086	16.18264688115188	-6.20753318689139
H	-9.01636389633877	15.67713019324536	-4.99546506002968
H	-9.18838168911491	17.23590448107030	-5.82826192244611
C	-11.22453314131367	15.60318880155968	-6.51918500094613
H	-11.54693229444262	16.63935605107528	-6.37674625300912
H	-11.28702980761579	15.10006930098933	-5.54878389715940
H	-11.92685137221306	15.10483511586683	-7.19625930934913
C	-10.69248116095198	16.90079089548672	-8.97107265142072
H	-11.67825044003602	16.81493663592172	-8.52838096300068
C	-10.56539873407825	17.66387683075398	-10.12552338172961
C	-11.77143487673356	18.28801426237681	-10.774114171712196
H	-11.51319528362521	19.22144580255628	-11.28373797467312
H	-12.55218491535182	18.50639780237368	-10.03901764167132
H	-12.20699266523664	17.61493842955128	-11.52375305943176
C	-9.29689525554272	17.82280211113546	-10.67413122353622
H	-9.19944179131148	18.44919463887185	-11.55367398580910



Main article molecule number: **6-tetramer (Fig. S3)**

Name: Gramine

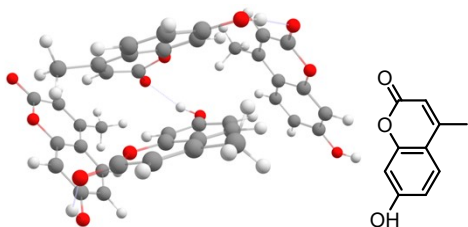
Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

Final single point energy (Eh): -2147.86968350666

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H	-2.81224591500327	-3.81991420161933	-5.73553422090333
N	0.17221754957231	-3.11608470816739	1.60522918252083
N	-3.03223607497139	2.30684465208807	-3.51174167265199
N	-0.71572541112898	1.06315698306302	3.74598403305834
N	2.42239271084893	-2.66978383858388	-1.73698495132613
N	3.03061240656733	0.51821747396324	1.83676589646774
N	1.42765134320265	1.35607528218982	-3.26129868727717
N	-2.71439317422310	4.19288693983983	0.98564781929301
N	-1.24537563836560	-3.42866730275829	-4.39118722280471
C	0.58165481272960	-2.01529592393975	0.88107651630357
C	-1.76852566185816	2.83882456408489	-3.67474612699376
C	-1.54121184966845	1.16755308157501	2.64446104007755
C	1.46816593305269	-2.01996596599636	-2.49680457990581
C	1.18065509370434	-1.10040403787783	1.70597959290922
C	-0.87612563908226	2.17290958097654	-2.87453056083146
C	-1.39062349318885	2.39756635833487	2.05687363233175
C	0.35248818426162	-2.80912714948669	-2.61618646571151
C	1.64023903578545	-1.24713763395849	4.27412024489814
C	-1.29553660160737	0.23316889900119	-1.18912539479263
C	0.19614168320849	4.36162211967253	2.71966189104573
C	-0.15015220077079	-5.13784665739015	-1.55168733201074
C	1.46214131025824	-2.07536143872809	5.37338382010682
C	-2.29735617977474	-0.56293171247789	-0.65903942379396
C	1.18059619685613	4.71305750769646	3.63103500513669
C	0.38943927734434	-6.09084229262555	-0.69889835915187
C	0.84015606593753	-3.33051899592377	5.24772176198646
C	-3.62936494154849	-0.44068696256024	-1.09314765347183
C	1.58149718430974	3.82959410065950	4.64963343747394
C	1.68264833390182	-5.94253619300800	-0.16262018123500
C	0.37770898995466	-3.78467690995712	4.02042737796456
C	-3.99076022229618	0.48835227482166	-2.05902208599848
C	1.00545711191449	2.57435904928807	4.78283541017891
C	2.46429130355458	-4.83649651308731	-0.46376090451240
C	0.54602595800049	-2.94775085838328	2.91952154401802
C	-2.97900167394363	1.29047143564482	-2.58310841925378
C	0.02005639531271	2.22092349602189	3.86293483861458
C	1.91554943220956	-3.87706070706683	-1.31097428662559
C	1.17353130031241	-1.67569790159071	3.02252463704584
C	-1.62821891725467	1.17607496399888	-2.16683616327522
C	-0.39358334271070	3.09405943808302	2.82038040061951
C	0.61208987924121	-4.00335569339554	-1.86294745697190
C	1.69284403326837	0.24483174393377	1.30711010791567
C	0.58383329093888	2.44877384166746	-2.74580075584591
C	-2.08176050124086	2.87694005706394	0.82551140057678
C	-0.90027548659842	-2.45692444442753	-3.34500795524855
C	3.38277869795905	1.91770276006495	1.63132204936846
C	2.83328601939593	1.64453044785300	-2.99071108769287
C	-3.28183059850325	4.61431773785286	-0.28942396098749
C	-2.53376075470016	-3.07870957330073	-4.97837495478563
C	4.01967377043246	-0.36626163937335	1.24162492694370
C	1.21415964746316	1.15089480793966	-4.69162778270704
C	-3.74527337715424	4.16005491164507	2.01808698295193
C	-0.21262702943157	-3.48618546767655	-5.41993356651856
H	-3.86697590445525	2.64966242030814	-3.95407673025637
H	-0.49382840216231	0.19676615616111	4.21353064039266
H	0.39745643795012	-1.96441129425291	-0.18314257475816
H	-1.59733820853685	3.66099668830864	-4.35722864091303
H	-2.17377138720070	0.34205594358569	2.34675563221300
H	1.62395258613535	-1.00867245246547	-2.85666282717567

H	2.15082056020910	-0.29195330787029	4.35752631585317
H	-0.27027579838658	0.14242811973539	-0.84690037715533
H	-0.12802871156178	5.04951466937027	1.94463064021127
H	-1.14034110997105	-5.26161576478266	-1.98029965424049
H	1.82221738122939	-1.75858945946957	6.34812843588975
H	-2.04902670018452	-1.29421949125413	0.10525293138071
H	1.64899937427975	5.69090445999906	3.56508124810582
H	0.72375472555758	-3.95850953012580	6.12601396330074
H	-4.39241477184937	-1.08044609737650	-0.65961121877332
H	2.35382763419776	4.13687424052274	5.34869846397993
H	2.07577737840732	-6.70722705333517	0.50066744884419
H	-5.02278522980535	0.58881179209414	-2.38359037950574
H	1.30844002072005	1.89578265210627	5.57513839093471
H	1.02270921535987	1.03096527735110	1.68056536932349
H	0.81986367783203	3.40755850501261	-3.25441213883001
H	-1.35217132854758	2.96952161847786	0.00717104423072
H	-1.74211281551376	-2.42204543555396	-2.63873160424856
H	1.68083077279221	0.32314242164894	0.19478767116881
H	0.83991878204544	2.58171496171673	-1.68399434109700
H	-2.81499793819019	2.10953624646340	0.50012414982746
H	-0.79889717854334	-1.42899376789866	-3.75490284216778
H	0.16643800505326	0.89643152575622	-4.87881426160057
H	-3.30254226555912	3.87026519673460	2.97597330743516
H	1.83750748715100	0.31998117892723	-5.04173203742824
H	-4.18682678069035	5.15665763423531	2.12815824353210
H	4.10990665123304	-0.21592520195893	0.14069747502236
H	1.46653660194452	2.04806898300315	-5.29305597939823
H	-4.55945994144487	3.44313289383063	1.78282547009600
H	-0.06430649696711	-2.51039186977832	-5.92911429255310
H	4.36586590542064	2.12254210902306	2.06949510085939
H	3.45810616806316	0.81168990297357	-3.33523787631910
H	-3.71023657987223	5.61866050151312	-0.19548423606798
H	2.64682813157853	2.56394406671489	2.12201050207474
H	2.98772537804555	1.76527356723090	-1.91229931332439
H	-2.49684497375517	4.64207716754450	-1.05488231105765
H	-3.30737326206312	-3.07226879869393	-4.20203904744705
H	3.42483561794263	2.19336974334245	0.55543115701414
H	3.18859350437437	2.56526703868186	-3.49551493856298
H	-4.07984800598329	3.92986881555041	-0.64912643454403
H	-2.52809681139872	-2.07852591415320	-5.46013774770574
H	-0.11308627414429	-3.98697319118584	1.18233049935979
H	3.25291454690551	-2.23460792212158	-1.37132025360689
H	-0.09918307920450	-4.75627863572099	3.92389569243539
H	3.45632529517464	-4.71683723399898	-0.03743954828366
H	3.74267043274088	-1.41011988895346	1.42703589052177
H	0.74094370848496	-3.78499837982525	-4.97389122583685
H	5.00360995929468	-0.18360435319827	1.68712451333662
H	-0.48815487917773	-4.22875903040103	-6.17652699731964



Main article molecule number: **7-tetramer (Fig. S3)**

Name: Hymecromone

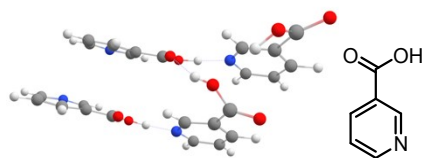
Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

Final single point energy (Eh): -2445.94062319554

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H	-2.81038777850878	0.79657626720604	-4.05107473542904
H	-2.89067716958246	-0.58976564838418	-5.16088485626715
O	0.30921691547521	-2.09110876178714	-1.92672105667610
O	0.94823160498191	-3.22785393940469	-3.71999204928346
O	0.95476253678851	-4.98276863590051	-1.49454788160366
H	1.17592764665139	-4.61572050762967	-2.37352067822172

C	0.14864827682879	-2.42354380146493	-3.26034451767366
C	-0.92762530629654	-1.79035350877299	-3.96205253188562
H	-1.00230510674781	-2.01999750022682	-5.01914147173357
C	-1.81260379397577	-0.95811961037697	-3.34328859766427
C	-1.66472978569689	-0.70635710139884	-1.93639504470097
C	-2.53043037908869	0.09405626294932	-1.16737553907951
C	-2.27437433845126	0.35215892186631	0.16187941439241
H	0.29087210373950	-4.78401861254448	0.97437839730598
C	-1.12226637354838	-0.17245533771440	0.77196480778355
C	-0.28969752133169	-1.03679829721416	0.06531843544729
C	-0.56302904223171	-1.27438727336364	-1.27331086530800
C	-2.91180020500054	-0.29421735732497	-4.11025977222311
H	-3.89283063076697	-0.55389140366069	-3.69649373299050
O	1.17792430654322	1.68690319947795	0.12028723204466
O	1.98075229989981	0.56856757492890	1.86236644141840
O	-1.50394158953107	3.24144755617884	-3.45026783172879
H	-1.97109701606926	3.67395727163917	-2.70641780335304
C	2.07570254463933	0.77801335715267	0.65747446651640
C	2.99710666303722	0.16442654240438	-0.24718988723296
H	3.77657018902607	-0.43419027024221	0.20765497615729
C	2.84658268332278	0.24233301073038	-1.60168585182451
C	1.76002494044176	1.02029923780099	-2.12949857834720
C	1.41514852733954	1.10011686107525	-3.49288906890637
H	1.99965091936980	0.54593468578238	-4.22043340378896
C	0.34023139269276	1.84833239739612	-3.92298687845992
H	0.06968799992566	1.89301636909472	-4.97283068956427
C	-0.43636279150926	2.55898514154515	-2.99056450736150
C	-0.11078228007153	2.51546495329366	-1.63803980881441
H	0.57413137229064	-1.50731049595092	0.52536883818060
H	-0.71427173513815	3.01834564737770	-0.89489773218278
C	0.96059572006772	1.74389055181372	-1.22811888484792
C	3.75348036155158	-0.50846614835690	-2.52219531790826
H	4.17855078665924	0.15815222976950	-3.28065897618748
H	3.18941858925401	-1.28883847533237	-3.05003826533780
H	4.56769921139587	-0.98496963222936	-1.97447626472632
H	-6.37056294758323	2.40857865826606	1.17046254694816
H	-7.56616642042209	1.32865051293173	2.85398761742173
O	4.95622917752440	-2.78599097025933	-0.23723042049938
O	6.85077241221447	-1.71511968607999	0.24330015495551
O	-0.85487522847196	0.20258913998211	2.04448789764089
C	5.79879159431999	-2.12606012350029	0.67377530147026
C	5.29504817104756	-1.98749672929973	2.01554041757994
H	5.94114500041192	-1.44799083870568	2.69938223703745
C	4.08548784962502	-2.47136058626789	2.40728735016243
C	3.26869127379334	-3.16922310251133	1.45002585716775
C	2.01427913277543	-3.74047958418512	1.73492062097772
H	1.62106139665939	-3.68297750556496	2.74506996728698
C	1.26449965877678	-4.35816143945788	0.75622486235711
H	-2.93114642344887	0.98291567413776	0.74997765122664
C	1.74286294659412	-4.40607541226019	-0.56385260107687
C	2.99056755948560	-3.87216206783148	-0.87771481164942
H	3.38227060960547	-3.91347112458932	-1.88893891818214
C	3.73784421808219	-3.27646945690283	0.12712517004345
C	3.58672083725464	-2.25580584204404	3.80159589353314
H	3.35099223677475	-3.20805493844029	4.28985196551594
H	2.67070171489392	-1.65389355138544	3.78064807795613
H	4.32953284227801	-1.73006522309153	4.40427944420304
O	-4.22163139743133	3.46589923087900	0.33766204707684
O	-2.98318924314516	4.33458853379495	-1.28600477981376
C	-3.03255810658093	4.02954449268646	-0.10525281666530
O	-6.91936403856041	1.27677387713747	3.56800387924201
C	-1.98416302636243	4.17591379555639	0.86136193908603
H	-1.09084361099151	4.68724954642521	0.51999872416998
C	-2.06395652134732	3.65353973425702	2.11741189273120
C	-3.28782828847420	3.01678290295353	2.52113066500160
C	-3.50010776920161	2.42594919492168	3.78092486043764
H	-2.69225733650478	2.41544429248121	4.50447764155023
C	-4.70719842921855	1.85312354348584	4.11273786323355
H	-4.86979284961776	1.39604840588861	5.08256173912465
C	-5.75422377144898	1.85219669598552	3.17813252851058
C	-5.58147582008324	2.41149961867767	1.91705863113858
C	-4.35285520372005	2.97864260581985	1.60440811120175
C	-0.89898279120359	3.71662962334972	3.05021003309862
H	-0.54696282203579	2.70149057385930	3.26815945722318
H	-1.17471551028802	4.18763885555213	4.00016919633120
H	-0.07183567176651	4.27358635174571	2.60715110750192
H	0.11582166713647	0.18349201525435	2.18515984169055



Main article molecule number: **8-tetramer (Fig. S3)**

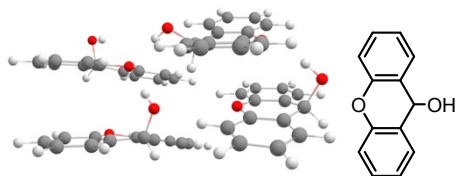
Name: Nicotinic acid

Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1747.20228741639

C	2.08604908674806	-0.16972819730039	-0.42357539944725
N	3.02392817160574	0.66572832365174	0.03664682670201
C	4.15186904256734	0.15505657874037	0.54063498391872
H	4.87785822672570	0.87162875843367	0.92076173270209
C	4.40750555884967	-1.21168960467991	0.57639021808388
H	5.34886503075044	-1.58073229789578	0.97042778556968
C	3.43727306734758	-2.07983422525584	0.10169851864608
H	3.57675160159891	-3.15680371217473	0.10420886814043
C	2.23906401456604	-1.55464829083813	-0.38394678738695
C	1.18419112108381	-2.50699199243203	-0.83817649664833
O	1.43416952239089	-3.64725957275473	-1.15439667226317
O	-0.09024677208545	-2.06298778052759	-0.85553189236326
H	-0.23772020044841	-1.23110705249151	-0.33310378088114
H	1.21002209680369	0.31255115354722	-0.85464831347846
C	0.71279747668751	4.80365535998595	-0.83708779138063
C	1.07194906145850	5.78586828002614	0.08994324157846
H	1.78473144103730	5.55501374426472	0.87815964200647
N	0.56469464333318	7.02130708320577	0.08190122318581
C	-0.32185988412609	7.31675767698716	-0.87443449773216
H	-0.71652449483893	8.33276931571320	-0.86380605439435
C	-0.74181329293737	6.41095623691880	-1.84609996281542
H	-1.46359506692712	6.71050838202128	-2.60003170816336
C	1.24807844153569	3.41767788051793	-0.78095916720478
O	2.25368825831083	3.26991098132141	0.07937295499517
H	2.56461832753219	2.30553776715070	0.05055997585395
O	0.78947044654810	2.51105583232186	-1.45944485679254
C	-0.21846758209377	5.12829403170017	-1.82243176238237
H	-0.51265656315449	4.36973659504706	-2.54176218582421
C	-0.17059317542353	-2.90961542129358	2.00773703503657
H	-1.07216608753344	-2.41985225992443	1.64514161102113
N	0.70044285267571	-2.12780595368303	2.65681596629585
C	1.81805279405305	-2.67794364463558	3.14508111642814
H	2.50739705890857	-2.00362647150927	3.64965711519483
C	2.09767916407257	-4.03356164888755	3.02078771215267
C	1.19796058737125	-4.84217249839252	2.34130365579679
H	1.36733046762484	-5.90710081797559	2.21316949178681
H	3.00898869270479	-4.44199404209312	3.44536905818603
C	0.04855370422794	-4.26815654794508	1.80071764352684
C	-0.92783041460601	-5.12934975743413	1.05563881631064
O	-1.56170941473870	-4.55954294479102	0.01587287067786
H	-1.11220831142073	-3.74584243850006	-0.28213504393025
O	-1.14993945601507	-6.26633573736150	1.39033860967291
C	-0.52827107390030	0.81037258021994	1.52411345018798
O	-0.88231840339310	0.01907747151929	0.64430823997013
O	0.25560674049457	0.48754118143190	2.53340342957447
H	0.44174821516505	-0.52636585157031	2.55259221658751
C	-0.98701656109567	2.21809042975906	1.53381683991412
C	-1.90410182727570	2.65077459619531	0.57514583096391
H	-2.24808573258714	1.95790479395595	-0.18590683070560
C	-2.34422135751557	3.96293175142316	0.62728204279643
H	-3.05770872486995	4.34447325571989	-0.09615791551247
C	-1.84017568901251	4.79713871546396	1.62250658021810
H	-2.15855832987157	5.83745676665419	1.68186680171967
N	-0.94975100162502	4.40266267370855	2.53966592745393
C	-0.53960539626690	3.13479024121537	2.49161745546892
H	0.18179989898281	2.82498032352557	3.24427163098154



Main article molecule number: **9-tetramer (Fig. S3)**

Name: Xanthidrol

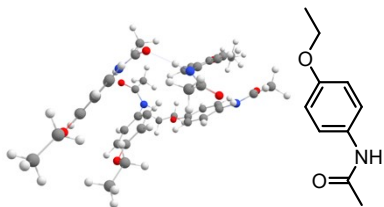
Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

Final single point energy (Eh): -2606.95219290775

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C	-1.24339602276824	-7.62399473114304	2.91365538316070
C	-0.36375810463026	-8.64323709022311	3.26317235243801
C	-0.80367423788139	-9.94016442967315	3.50601422954516
C	-2.16857743373156	-10.20309367582202	3.35978434424925
C	-3.06502165687405	-9.19875565203448	3.02416758211918
C	0.13725110617374	-10.99758919686118	4.00722995536729
C	1.56861873575521	-10.60065069739054	3.81187582192401
C	1.91832427102364	-9.28141753704208	3.55146723767407
C	3.24569606624167	-8.87235180353452	3.47218419574708
H	3.47600989494462	-7.83131943427172	3.26547669935867
C	4.24830287603885	-9.81103156553367	3.65552799970445
C	3.92757292643806	-11.14415058819861	3.91022358666415
C	2.59748004895377	-11.52765738552631	3.98699395350128
H	-3.28567552258983	-7.10856181523951	2.54018037139225
H	-0.85723432161216	-6.62803455284122	2.71960595383804
H	-2.52541158587013	-11.21936437032122	3.52046431749591
H	-4.12201870827119	-9.42238692254298	2.92075551420439
H	5.28615651892162	-9.50013202739538	3.58909469126092
H	4.71513503750951	-11.87764152351343	4.05083326581605
H	2.33282064628857	-12.55855981630365	4.20773245708009
O	0.96927771429654	-8.29110753279854	3.34320229398582
O	-0.02981504588850	-11.20071838938207	5.43046812940516
H	-0.97625265611985	-11.27394583868903	5.60735736444580
H	-0.06251867308968	-11.94832559660340	3.48444203658734
C	4.39291880214412	-10.79276092719839	0.26325985771526
C	3.02056940439351	-10.95303947505163	0.35135279431346
C	2.19247489446361	-9.84496240096821	0.18236830479683
C	2.71580772579707	-8.57598683783193	-0.06121656945586
C	4.10385244927231	-8.44237574511123	-0.15063699253349
C	4.94196828828617	-9.53502500184865	0.00553020542266
C	1.82044832030018	-7.37275707324437	-0.13415734944417
C	0.38528958933585	-7.77418944014115	-0.32039029818594
C	-0.02870019793755	-9.08511600913765	-0.08683085003532
C	-1.36664220520198	-9.45678664183140	-0.20355985225584
H	-1.64541145150231	-10.48750055323605	-0.00962057332149
C	-2.30610841705675	-8.50238105579011	-0.55633278522382
C	-1.91808711440137	-7.18202653173658	-0.79339485386966
C	-0.58252299889816	-6.82922309274303	-0.67347305837576
H	5.04056146407599	-11.65444785157513	0.39544419584150
H	2.57081129745643	-11.92017833961395	0.55113605085302
H	4.51677066123515	-7.45259573675018	-0.33090737821331
H	6.01796064460358	-9.41330722250754	-0.07037635165399
H	-3.34980101189730	-8.78922895921371	-0.64695040957157
H	-2.65488768872287	-6.43388433898615	-1.06945008818973
H	-0.27003859446944	-5.80051773980138	-0.83677518547885
O	0.84296221942625	-10.08668278866520	0.26708432902707
O	1.98124765928047	-6.54420114842190	1.04274041910311
H	1.69679489624030	-7.08203376444604	1.79724319992289
H	2.13436291966083	-6.71681486642927	-0.95651744294713
C	-2.61188967200425	-2.78664352435432	4.99858035327122
C	-1.69488355495439	-2.01328015622914	4.30309880946937
C	-0.49380625279240	-2.58623722021195	3.89814173471092
C	-0.18683033434863	-3.91893892417387	4.16254473389734
C	-1.10984065351302	-4.66478880604710	4.89547224671870
C	-2.31570311522840	-4.11268849854966	5.30835533712668
C	1.06971210584715	-4.53869630606783	3.59510537831923
C	2.08489321493107	-3.47451033223903	3.27388068231157
C	1.68518162786674	-2.15739701718981	3.06658362798893
C	2.58398459470826	-1.16921465352783	2.68016132341598
H	2.22526123739277	-0.15693730397684	2.52132595904502

C	3.91639916095104	-1.50508246094822	2.49416286583535
C	4.34471118970582	-2.81446365200343	2.70646380849739
C	3.43196749429321	-3.78603973005467	3.09365026145521
H	-3.55485455534600	-2.34717065877843	5.30959483563739
H	-1.89453529201933	-0.97324055839069	4.06382282841575
H	-0.87035450342694	-5.69380001138591	5.14763026102423
H	-3.02171009634780	-4.71433290828942	5.87248365171315
H	4.62166991243641	-0.74002539490146	2.18373090769565
H	5.38900310058451	-3.07632887589694	2.56641116185812
H	3.74674965420410	-4.81092389429922	3.26041491098611
O	0.36889906733335	-1.75897460519777	3.20718601610848
O	1.65183876748460	-5.50515263343252	4.47298067351774
H	1.31984879372221	-6.38045856871550	4.23687107474220
H	0.80655686451274	-5.02773786671942	2.63980177526874
C	2.81672749673242	-2.50691969344728	-0.80869629784497
C	1.84745155117400	-3.28654638341556	-0.20026798634255
C	0.60062350174435	-2.72540444415861	0.07212585992347
C	0.31129019704822	-1.39631467524676	-0.22669124328114
C	1.30680313503712	-0.63506787290440	-0.84618578649134
C	2.54639262505344	-1.17857244509347	-1.14465673863281
C	-0.98520278103406	-0.76299772773782	0.19977376232883
C	-1.98138821434731	-1.80514026320077	0.63056179790289
C	-1.59300892453239	-3.12161364158348	0.86878631636820
C	-2.49520892599676	-4.07389936757706	1.34182050219557
H	-2.14553763186286	-5.08893531894666	1.49995893038420
C	-3.80552781880319	-3.70398914564299	1.59142559842031
C	-4.22081297435576	-2.39070607958306	1.36127309483761
C	-3.31163268725277	-1.45937170690212	0.88444765623522
H	3.79424713101875	-2.93413993508137	-1.01208324031434
H	2.03916585535565	-4.31081492766974	0.10570352874515
H	1.09374249364695	0.40732742129386	-1.07081846823439
H	3.30675214462130	-0.57033765641907	-1.62473784958155
H	-4.50846460133485	-4.44033419485842	1.97029893644433
H	-5.24849308108914	-2.10017527651792	1.55560678063617
H	-3.61644302358999	-0.42903410313662	0.71720589149634
O	-0.31116720646941	-3.56734590109285	0.66732352600748
O	-0.76771150172965	0.20594287639332	1.24478949686894
H	-0.38323159608668	-0.28353596221570	1.98890556977434
H	-1.40155309116006	-0.16954721606078	-0.62480575523131



Main article molecule number: **10-tetramer (Fig. S3)**

Name: Phenacetin

Qty of copies of the molecule modelled: 4

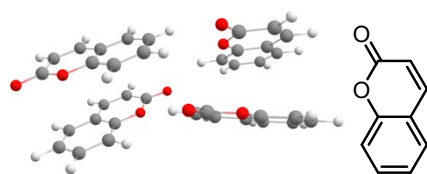
Qty of imaginary frequencies: 0

Final single point energy (Eh): -2375.99581495721

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C	-7.10990460924323	-4.10155437325201	0.75099016158775
H	-8.85666752569692	-4.389397766642934	-0.45288417158600
C	-8.83473592786736	-4.20716702410877	2.93596478940328
N	-10.69981830956513	-4.60454556317742	1.35850235495026
C	-6.59860387903365	-3.95570971201344	2.04384696515711
H	-6.42908455971076	-4.04576143159942	-0.09233872818007
C	-7.46863704839124	-4.00562409001812	3.13268204676560
H	-9.49961310700816	-4.25394351435895	3.78740849837345
C	-11.76930627338321	-4.49902536485619	2.18792703985869
H	-10.91699021565816	-4.73874297099427	0.37328231828283
O	-5.24762952993204	-3.76382572760992	2.13415358443436
H	-7.10535919615034	-3.89869794966299	4.14839612927564
C	-13.07477699337782	-4.99160765450581	1.60642504589341
O	-11.70266834670417	-4.08252676937708	3.35192330303721
C	-4.67282856870896	-3.68817846593644	3.44153157560480

H	-13.89299788888182	-4.36309213345244	1.96460453421253
H	-13.07086837682134	-5.02807296125448	0.51380969656015
H	-13.24592186354779	-6.00566904635643	1.98621099995741
C	-3.17303769284790	-3.58369977442923	3.27576200908901
H	-5.07307064199988	-2.81047261490682	3.97420968292855
H	-4.93998965670949	-4.58739011631972	4.01722543226357
H	-2.90365771317200	-2.68929023674998	2.70691977005874
H	-2.69411425680423	-3.52608157046005	4.25807393582333
H	-2.78310227495174	-4.45928641680557	2.74918484686588
C	-5.06686154353109	-0.16883824476250	2.07317635371195
C	-6.55219321789063	-0.37985045588142	1.88775181458290
H	-4.51979095256705	-1.05174147136965	1.73144158770640
H	-4.84295580699850	-0.00201475618473	3.13173946199929
H	-4.72281589923581	0.70011656143071	1.50483992908452
O	-6.76999153424730	-0.62342100003944	0.49167656061467
H	-6.90526221037251	-1.24595544782524	2.46735680925146
H	-7.12324155211122	0.50760158690891	2.20099408564974
C	-8.03074152640429	-0.91685419609105	0.08337264329421
C	-9.14871741760954	-0.94442125682422	0.92001207444660
C	-8.17156557503749	-1.21547964678890	-1.27698448692358
C	-10.39190359965782	-1.27632089149697	0.39095023729684
H	-9.06704852528367	-0.73611382686489	1.98005326247845
C	-9.41322263712058	-1.54444215176566	-1.79083657640366
H	-7.28951060016435	-1.19137090412300	-1.90901642486468
C	-10.53245390458469	-1.57636314118714	-0.95829000830172
H	-11.26191194691728	-1.29304484981975	1.04122986973274
H	-9.52545611341047	-1.78093816377857	-2.84502080026343
N	-11.82339137824151	-1.87204120264253	-1.50006575708939
C	-12.29076884904851	-3.13159396932191	-1.67825698222712
H	-12.39999833299488	-1.09356315640781	-1.80686770257754
C	-13.68738972962785	-3.22739493046222	-2.25314724173368
O	-11.65128330880547	-4.14603670616760	-1.39051855977558
H	-13.65253358204312	-3.82726421655225	-3.16691389329712
H	-14.13732279491629	-2.25420556927883	-2.46918380322756
H	-14.31998429183730	-3.76151254079956	-1.53716459152977
C	-13.04979947548747	1.63467024493939	0.97438489893417
C	-14.35922959131813	2.00068942415149	1.32016349186604
C	-12.74505464264869	1.22823890942037	-0.30932301916228
H	-12.27062133050900	1.65787646697378	1.73186772767236
C	-15.34435395010125	1.99714471557648	0.33103709546084
N	-14.58772089745495	2.30631523031263	2.67163766659314
C	-13.74992010186482	1.15703715053572	-1.27443362896971
H	-11.72775572982315	0.95497692684968	-0.57301008355003
C	-15.04141745546847	1.56720012649081	-0.96052653935748
H	-16.35177244377419	2.30158251107226	0.57874972985396
C	-15.76027394724420	2.67797376892032	3.26420456866898
H	-13.86519683596981	1.95173047891923	3.29606711756863
O	-13.35736176662063	0.64716936215644	-2.49577431816495
H	-15.83740437917508	1.54482030417595	-1.69604753735096
C	-15.68758488222848	2.76629959558690	4.77593638623035
O	-16.79617808963418	2.94292119642855	2.65967843446759
C	-14.31756360004735	0.64099211732834	-3.55843340779777
H	-16.53431463876088	2.21514702936175	5.19480074009390
H	-14.75409492861363	2.38090226795269	5.19522767688921
H	-15.80792887915745	3.81427364159832	5.06863534949404
C	-13.63061023625217	0.08188378158045	-4.78466336543260
H	-15.18569234357183	0.02529971870089	-3.27490745048688
H	-14.67217717116876	1.66693590455864	-3.73563481302982
H	-13.27134740877804	-0.93588355963903	-4.60092649934509
H	-14.33191042337842	0.05273939886536	-5.62399376646321
H	-12.77606619963989	0.70377827355041	-5.06563169086234
C	-19.77747159185600	0.38681076437676	0.35527512559916
C	-18.75295837216353	0.12855874061432	1.43664467049793
H	-19.33731368192174	0.96875308413573	-0.45990132410798
H	-20.61617884826549	0.95449375940445	0.76964208177505
H	-20.16043955266332	-0.55296902026705	-0.05350541896496
O	-17.68765019425228	-0.63151260291450	0.83938563673517
H	-18.35077785497053	1.06970670802759	1.83726923124412
H	-19.19400704580405	-0.44793737091601	2.26408735428009
C	-16.57171400278109	-0.84705459241079	1.58483185598156
C	-16.44299528968892	-0.50892471274707	2.93386612296388
C	-15.49535669625445	-1.43804930598128	0.91423841771166
C	-15.23030272120826	-0.71540324951172	3.58370183626415
H	-17.26614540534463	-0.06396396990389	3.47973929559411
C	-14.28935156950775	-1.62120437130985	1.56505342021572
H	-15.61198841021594	-1.69294955152756	-0.13423706188166
C	-14.14143412340390	-1.24644996821223	2.90338537145273
H	-15.12363077297221	-0.44061228607494	4.62834770091334
H	-13.44235113995727	-2.03137810025231	1.02118292447192
N	-12.88433741556944	-1.41724945584728	3.54609383095650
C	-12.20308060574670	-0.42562326559347	4.17478461491556
H	-12.46623245787268	-2.34863717089186	3.52700126496250

C	-10.89198441860913	-0.85439193227732	4.79731202205880
O	-12.59421024942108	0.74258443367142	4.25884546295933
H	-10.13883783943508	-0.09408713011302	4.57512032961035
H	-10.55286521745306	-1.83603385148523	4.45395017532319
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Main article molecule number: **11-tetramer (Fig. S3)**

Name: Coumarin

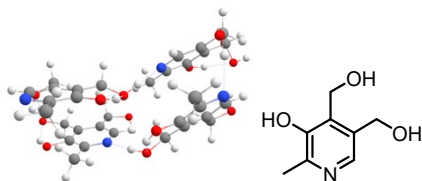
Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1987.78320779229

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O	-0.38017436948922	-2.19478362112380	-1.06633508072037
H	-1.09725583547388	2.12008902286366	-2.65211288538839
O	2.77589416248145	1.98924507241058	-3.76788130790817
O	3.30796897889251	2.08055757279055	-5.93180252188945
C	0.10476500543191	-1.14779021337929	3.24838053162052
C	-2.53240396189601	1.45482270404537	3.00544198185091
C	-0.12135112930784	-0.15037143552916	5.44866184400064
C	-2.11650605170932	0.09940933866618	1.03284712159611
C	-0.10772052611698	-2.15617776599420	2.31438887011444
C	-3.07736739384770	1.66676886602462	4.26800776230870
C	-0.36248676831252	-1.25372636575437	4.56809651344271
C	-2.74766459335310	0.25246001874719	2.31101626524080
C	-1.04965856188414	-2.41923951875119	4.94135686127675
C	-3.53342228029394	-0.73999882007977	2.91636238995546
C	1.04462797736089	1.04922395294888	3.66715026276647
C	-1.19188440903409	2.35805249635416	1.20526033544334
C	0.54543525409854	0.94413365824545	5.02270389595765
C	-1.36555800086029	1.09504239162387	0.51935292891905
C	-0.79484694321692	-3.29349411030613	2.71140805695164
C	-3.84715604962776	0.66691696263330	4.84427209906422
C	-1.26283324904434	-3.43152571013057	4.02362686312664
C	-4.07866494257265	-0.53728366280661	4.17106544095073
H	0.73947275996990	1.79805715169772	5.66138298913958
H	-0.84979746498931	0.99172660463297	-0.42592078940683
H	-0.97008985765604	-4.08199303905051	1.98531152828268
H	-4.27737729973875	0.82770953711782	5.82857017308603
H	-1.79647817224214	-4.32968627529846	4.31806575777632
H	-4.68129815016851	-1.31193782233365	4.63455084383129
H	1.84538344270126	3.02665026170160	-1.60357405571651
H	-0.49198007154340	-0.20761610200019	6.46982452066473
H	-2.22260113393789	-0.83743303328707	0.49049101868118
H	-1.41849843275746	-2.50678549873040	5.96004891042752
H	-3.68942008416146	-1.67607830932752	2.38716663001463
C	-0.36578606211484	0.29471886891478	-3.51126296442060
C	0.50097443944355	-1.74099178247596	-4.50072027643542
C	-0.72020458843723	1.63775559314437	-3.54829821163827
C	0.14354354420068	-0.36331565694886	-4.64159825642623
C	0.29695259645153	0.36956035383203	-5.83027705770879
C	-0.18657847469867	-1.70356056430826	-2.15843734486051
C	0.35188563499909	-2.37940453314260	-3.31813472372545
C	-0.55175277083404	2.33634305762988	-4.73411621284021
C	-0.04456034817383	1.70702294835918	-5.87618931117455
H	0.61533354377830	-3.42143981612780	-3.17783297429080
H	-0.80510884520054	3.39131201889046	-4.76805729372430
H	0.10665054831473	2.27539268529634	-6.78711407590896
H	0.90349837386102	-2.26551718472052	-5.36460971832378
H	0.71089053123385	-0.12575202677902	-6.70459784485584
O	0.77692937484176	-0.03909190330764	2.82647904558383
O	-1.78063446215130	2.46023150068974	2.47329177341446
O	1.66111554593926	1.97201038346254	3.19371417902523
O	-0.59423583915280	3.32071506822731	0.78877973878978

C	2.68886272240977	1.31295437856199	-2.58404316490694
C	3.66669424232699	-0.63854365873608	-3.64335765120076
C	2.16596382690408	1.99610398258243	-1.49082113051423
C	3.11504574717725	-0.02217832486660	-2.47672311291800
C	2.99286246685414	-0.66705179296916	-1.23401407468129
C	3.29149005622926	1.40900129948188	-4.92715757539090
C	3.75747256773854	0.04119746242234	-4.80760398003690
C	2.07143446875303	1.34072709656193	-0.27162131366365
C	2.47897315986018	0.00703707033418	-0.14324380504221
H	4.17649503705383	-0.39245298789831	-5.70858857513693
H	1.68516017602755	1.87087326849296	0.59387641058327
H	2.39306920106005	-0.48442494187134	0.81940091499270
H	0.23333861713023	-2.02772631688853	1.29191771956488
H	-2.88718010133113	2.60759274875760	4.77418737894086
H	4.01596221134924	-1.66695194345274	-3.57419606572852
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Main article molecule number: **12-tetramer (Fig. S3)**

Name: Pyrixodine

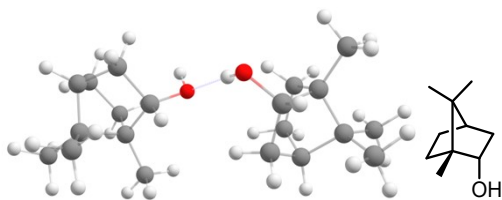
Qty of copies of the molecule modelled: 4

Qty of imaginary frequencies: 0

Final single point energy (Eh): -2367.20657566562

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C	0.78006123610862	1.50799813520581	-2.54876054599901
C	-0.28169030954537	2.39775920660253	-2.35366114885554
C	-1.25844835054274	2.55293441283719	-3.35626413438995
C	-0.13284078426185	1.07967063360606	-4.72753061302894
C	0.85558669845152	0.84268667785810	-3.78504083843757
C	1.77415600721939	1.18742076575421	-1.45836539910358
C	1.97724949862428	-0.13628916109015	-4.06559053681466
C	-2.43092959204328	3.45130084965158	-3.11085812041065
O	-0.46134453820500	3.11199336238227	-1.22201936488371
O	1.83351258873699	2.19278777560951	-0.44806600306789
O	1.92126381394648	-0.74534743449902	-5.34373364011768
H	0.32772209793960	2.92598743392710	-0.65553247945325
H	1.92590055617451	1.73637488874379	0.43310620982293
H	1.21932064760365	-1.41107976070895	-5.35415974994496
H	1.47941648522853	0.22082115834093	-1.01436710389881
H	2.77582525315992	1.05450145502677	-1.89673918367703
H	2.94063515951769	0.39088849666247	-4.03035837171870
H	2.00723291941790	-0.89956811432212	-3.26751600117775
H	-0.08788013223727	0.58961916433818	-5.69655820913568
H	-2.09721358350511	4.47456011723476	-2.90611112435621
H	-2.99403604901875	3.13218444982508	-2.22585489699400
H	-3.09022970703259	3.45402445507809	-3.98118116802838
N	-1.26363769714941	-1.16147111580778	-1.62263589622344
C	-1.23645143344504	-2.40100203766176	-4.10710453874481
C	-0.35529003187024	-2.78774181095365	-3.09221767364881
C	-0.39171478771477	-2.14827091084365	-1.84570084201874
C	-2.10213765327992	-0.77056129828308	-2.59157881642076
C	-2.12738921245930	-1.34857201201528	-3.85473134585089
C	-1.20855283558343	-3.14719770002614	-5.41026116145790
C	-3.07949849372837	-0.81898621982091	-4.91504855868519
C	0.53843064555086	-2.57180012255867	-0.75183483359825
O	0.55553059261454	-3.78902705298914	-3.24155514472093
O	0.16565887940097	-3.17091063352944	-5.87252742539560
O	-3.64662738879161	0.42868224039285	-4.59801809456655
H	0.71114653589056	-3.92390069326296	-4.19200850989163
H	0.20861374210250	-3.62244541458744	-6.72358948103967
H	-2.92914416035289	1.09147811834123	-4.70072112304600
H	-1.84977383057545	-2.67361668557234	-6.15960436969799
H	-1.56238564032760	-4.17916994352448	-5.25468665432757
H	-3.91197068947262	-1.52569646641886	-5.04665129134593

H	-2.54732230335680	-0.77006183371784	-5.88049634725446
H	2.73269046550816	-0.77833895819123	0.69730127728322
H	1.58050044987643	-2.56928001512659	-1.08714252626838
H	0.43913538329080	-1.90912646631571	0.10986937725006
H	0.32798944856736	-3.60016884133919	-0.43569548191001
N	2.15416426148357	0.78495615912565	1.92474433772709
N	-2.65050834853385	2.59120550003258	4.71414373308759
C	2.50599921062175	-0.96627098414649	4.07320003086125
C	-1.67973780956685	0.84322081624155	2.72660075649730
C	2.13721260582967	0.36788993732541	4.26934364165899
C	-2.16257228938186	2.12248026957159	2.41248447275502
C	1.92527398587523	1.21775269907209	3.16399068889376
C	-2.62870136821993	2.97159863705765	3.43931563849680
C	2.55505867305379	-0.47990024739696	1.72616652766555
C	-2.20636062148440	1.36802012702805	5.01964292180131
C	2.72633800273670	-1.39426394181334	2.75263215263718
C	-1.70461457960999	0.46748315112061	4.08278787978361
C	2.70693922101096	-1.92589612932598	5.22919181783557
C	-1.19377662429165	-0.12264069838909	1.67080342605880
C	3.15223520610446	-2.81738699526616	2.45421026812565
C	-1.22275480469283	-0.87864366709818	4.56520544351372
C	1.45576575070015	2.62192000195444	3.37270464242335
C	-3.12849128718911	4.33952147785657	3.09064402368464
O	1.96693013256936	0.92102787401389	5.49998430487915
O	-2.21980344623964	2.62874394041728	1.16274320058881
O	2.02467677591837	-1.55650462367094	6.42731760020135
O	-0.84407763329152	0.53241690754054	0.45837882927010
O	3.49860928649605	-3.04081673640626	1.09462684879618
O	-0.57840956033139	-0.78409803637203	5.85276637508107
H	2.11388183500768	0.20657185822498	6.15935265496479
H	-1.74083393466740	2.01236812328137	0.56394496117012
H	1.06018651588002	-1.57938822123821	6.24531978084356
H	-1.02934559977505	-0.09772305024538	-0.30099132408048
H	4.33205383400171	-2.58899121831155	0.91749558664989
H	-0.21632620254526	0.11412500844942	5.90479172710643
H	3.77383987071710	-1.97322316094914	5.48951861751267
H	-0.31310509722579	-0.66077409397073	2.05867273221466
H	2.40859421898927	-2.94027269426022	4.92739246255108
H	-1.97519291802451	-0.88046245876594	1.48296443866255
H	2.32045945913703	-3.50502724628354	2.66024725966658
H	-2.06348225782330	-1.57223638969583	4.69709829710601
H	3.97936956455786	-3.11371027119275	3.11987266530624
H	-0.52819553954114	-1.33385184121156	3.84652723636437
H	-2.76771575740714	0.05748347514813	-2.36469144563761
H	-2.26242463548587	1.08720158640028	6.07058787373915
H	0.53640955644605	2.63825781721596	3.96917463892983
H	-3.97448232456434	4.28024619976447	2.39663134676437
H	2.20170531210992	3.20442856865107	3.92531467697144
H	-2.35305135972069	4.91908712641935	2.57737222326757
H	1.26457086648749	3.09990981957054	2.41000375693007
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Main article molecule number: 14

Name: (+)-Borneol

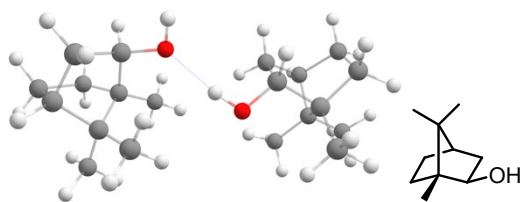
Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -934.027737487291

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C	7.65649321051954	31.36766116624389	11.47197315959708
C	7.43002756524891	32.62838470327893	12.32967848435894

C	6.44269339981910	32.23567350322636	13.44662587763084
C	9.98246368186839	33.02582801031762	12.19113326820860
H	8.13775840708660	31.59258611325870	10.51441918359997
H	6.71040634384473	30.86207944629359	11.24730760193095
H	5.57029788710522	31.71353957272662	13.04093100936392
H	6.89924906527913	30.30398158762947	14.44692357908500
H	10.06588394460707	32.34152233320101	11.34485591637998
C	8.69438417540663	31.30780257375048	13.67896417552949
C	7.30607502957606	31.31630613575802	14.35750388379800
C	8.77507006491868	32.75938936745310	13.09870884231950
C	8.77492924074204	33.85774056812726	14.16703323675632
C	9.82005631691821	30.84067509412919	14.57787279523328
H	6.07818676919420	33.11435920867336	13.98879242920977
H	7.38238004023267	31.70649804244302	15.37814053603473
H	9.92170785229649	34.04224003964940	11.78442123313732
H	10.91443328160982	32.96109940963032	12.76455592065151
H	10.78670803461034	30.87908916800247	14.06189549820201
H	9.88930708095932	31.45413032157741	15.48373188285598
H	9.65062582420213	29.80219816815357	14.88382208631840
H	7.99188340360725	33.74175243244760	14.91887767031668
H	9.73739311942518	33.87894805801076	14.69131021142737
H	7.13125466604429	33.51510610509534	11.75895190428879
H	8.63948776737630	34.83821031865843	13.69459812795904
O	8.10846970018531	29.13955743952584	12.55233732258850
H	7.16150526062860	29.15412027006018	12.76567025055556
H	9.55714352083867	30.35654237305275	11.93145288792804
C	5.04981458756098	28.19227701512389	11.45438212475766
C	5.08135658311395	26.65342619462755	11.65242731037923
C	3.79224152610478	26.18389343553724	10.94999132627492
C	2.61414014366452	26.58289568840383	11.86102290608539
C	4.81308775342076	27.10800089173679	8.75972727445817
H	5.98567142383107	26.21319000636325	11.22211047685279
H	5.08283055084879	26.39220351242298	12.71786539841439
H	2.78207676823199	26.25997023562440	12.89444183357953
H	2.70365503640400	28.66626524465398	12.65821578638097
H	5.80851032958885	27.15286105110331	9.20525797467408
C	3.71206731293107	28.44482880622726	10.71510267656745
C	2.57271521297378	28.13145759976707	11.71102499317823
C	3.66500747819697	27.19374505729930	9.77296847271717
C	2.36034674078584	27.06192426910820	8.98135768967545
C	3.62580013803420	29.81731057732508	10.08075603046844
H	1.67716066357753	26.12227436671456	11.53351143614235
H	1.61397594465266	28.47509926580674	11.30956874338280
H	4.74512285339090	26.16469236758413	8.20577412102291
H	4.73958230992084	27.92032866490067	8.02778625644841
H	4.44635637591382	29.98259251299320	9.37287657909183
H	2.67850074583268	29.95138810080203	9.54665465554755
H	3.69064731646458	30.59623195441455	10.84934151191773
H	1.46145926686149	27.16240800357377	9.59237680978661
H	2.31286967655887	27.82249615834663	8.19385865568348
H	3.79703636982020	25.12767200638795	10.66035689905386
H	2.32011373985843	26.08225499288401	8.49076287046202
O	5.21707354939251	28.95612829236482	12.65904806137662
H	4.68273591282034	28.55718542607142	13.35533818787065
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Main article molecule number: **15**

Name: (+)-Isoborneol

Qty of copies of the molecule modelled: 2

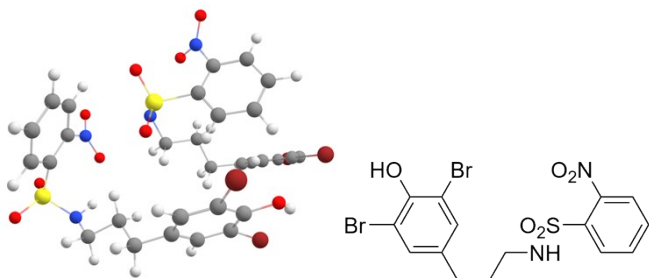
Qty of imaginary frequencies: 0

Final single point energy (Eh): -934.025723151241

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S46

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C	12.77163038304533	30.41922902632165	14.74655140274940
C	14.74426854354847	29.81148691241129	11.50758217962979
H	12.09323337350808	28.99235585761980	11.67722189337511
H	11.18603143326856	28.95347294153969	13.19067742209957
H	11.75013975282783	30.21278062051438	15.08363007314196
H	14.18064217330507	29.00095279351467	11.04788126780018
C	14.34297238916690	28.75876957483163	13.86762419698520
C	13.78056241858907	29.32273411057212	15.19644762822868
C	14.37845927957110	30.04862728063859	12.97696198099962
C	15.31887362841794	31.14126743923477	13.49943303193528
C	15.62823874511635	27.97279403141717	14.02140735184507
H	13.04420778460521	31.40523241510059	15.13575350688941
H	14.57955465131247	30.73110793826987	10.93233263418993
H	15.80694739503671	29.55716003264143	11.41883410634767
H	15.98627735013311	27.60469249121816	13.05639695759752
H	16.40925571587130	28.59215157607495	14.47742652755548
H	15.47251718278322	27.10072398098184	14.66769900963684
H	15.15752243524331	31.40594163531200	14.54614467079378
H	16.36347028348776	30.82744860186197	13.39281346652466
H	12.50112531539080	31.25741218482311	12.69880934497513
H	15.19226425125420	32.05319833701252	12.90392225505944
H	12.70416422819401	27.34116887074482	14.06250390886731
H	13.30999700025211	28.53322491030895	15.79347695713954
H	14.58896032596070	29.73969266048510	15.80581825595058
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H	12.84772625042733	26.60369696757209	11.89140741861217
C	10.58899414491020	25.32625110478326	10.11539372207280
C	10.69723461969735	23.77943599926870	10.00667855981688
C	11.47754424798450	23.56628968179102	8.69291214826218
C	10.52898911910855	23.96169350645390	7.54472377413767
C	13.52167078788849	24.64928182143627	9.84989712231122
H	11.24395998488742	23.38587950946492	10.86944597860780
H	9.71632732165844	23.29175175028178	9.98360426555748
H	9.55157519208377	23.47811434105747	7.64482657917821
H	13.08074821583374	24.48549585378561	10.83258276842633
C	11.38465347192303	25.82851516286760	8.88905159864182
C	10.45087247797282	25.50845066817593	7.69032256851892
C	12.49728855621168	24.73715629454363	8.71346591983448
C	13.29733585091493	24.88196021189543	7.41287043593468
C	11.82060673041962	27.27781786021556	8.95525466328080
H	10.93438896566851	23.66901576988773	6.57148771636447
H	14.21829660803344	23.82645363180356	9.64971882313529
H	14.11304819241019	25.56951321976087	9.91110169654728
H	12.52675476150101	27.45521025131794	9.77142439736641
H	12.30264805918918	27.57386267224062	8.01691262335745
H	10.95867333698926	27.93768137002885	9.11059084876091
H	12.68159695357871	25.01259287830501	6.52106140513255
H	13.97381178749692	25.74149083462595	7.47916064232099
H	11.91329948624096	22.56615629708613	8.59488475985262
H	13.91871820125684	23.99188411721767	7.26001423410646
H	9.54624821349499	25.67016143746765	10.04288459698796
H	9.43158668873754	25.86634166458322	7.87464019538008
H	10.80458343147183	26.02015326243139	6.79035171996834
O	11.13263471759468	25.85535350857861	11.34283821252131
H	10.61526803280558	25.49495036963629	12.07162327401639



Main article molecule number: **16**

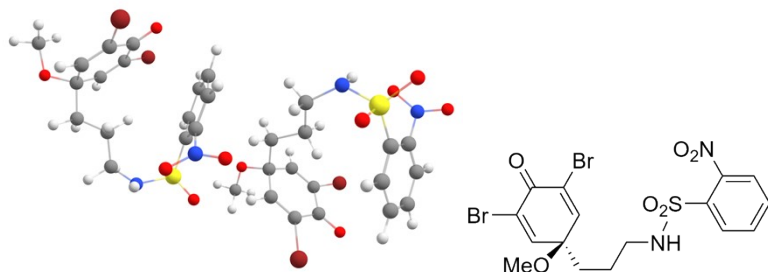
Name: SKS-1-5-2

Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -13223.5757911229

C	-0.85193535931600	0.89378917220941	0.14755668836490
C	-1.95011365619027	0.28843249584645	0.76049482605755
C	-2.58865561143782	0.91227675818816	1.82053837700147
C	-2.17183273498423	2.15398795612077	2.31806267033621
C	-1.08157478479790	2.75254663548603	1.67455884459515
C	-0.42478366573148	2.13367005021288	0.62078365283097
H	-2.32840983683399	-0.66187642130709	0.39489886519853
H	0.42042525827255	2.63353964345575	0.15880511942159
Br	-0.52227149649453	4.48460107447228	2.23544636517167
Br	-4.14344032388674	0.10725190979009	2.59436977091923
O	-2.76004278960910	2.79028961599816	3.35242226614882
H	-3.47434096569497	2.23695576179381	3.71036152175848
C	-0.17567142216637	0.22742316639762	-1.02161800494060
H	-0.94899029676470	-0.15398658855270	-1.70281229057363
H	0.39559576545648	0.97435368822482	-1.58543050131503
C	0.75558339917735	-0.92930253809368	-0.63061005648524
H	0.22370616503645	-1.61305845056852	0.04692501694226
H	1.62341198211515	-0.54491414395319	-0.07913942450915
C	1.19567573044717	-1.69560365612835	-1.87782555961987
H	0.30757489050835	-2.06601527331537	-2.41001243954101
H	1.72007570072836	-1.03643916990736	-2.57980655336517
N	2.06054276583004	-2.84922207657980	-1.59841739511682
H	1.89798535771350	-3.29492553397718	-0.69957682021111
S	3.70872068536175	-2.72676368068678	-1.86608292387087
O	3.86081523311111	-2.12947675609976	-3.19603206145025
O	4.28744277172884	-4.02283635616696	-1.51789223079703
C	4.41977069976195	-1.50578842257409	-0.71306255329534
C	4.81705937474224	-0.28871218770368	-1.25580273267248
C	4.73303865727083	-1.77103073534250	0.62470761462924
C	5.48338324571958	0.65132827373656	-0.47289712612955
H	4.62576253001009	-0.10296983710480	-2.30717549560254
C	5.44437069174048	-0.86294729540931	1.39326486822214
C	5.80341679635549	0.36241785470310	0.84635172572960
H	5.76866622571367	1.60334046419151	-0.90968457319103
H	5.67216136697196	-1.10289929415856	2.42416999597643
H	6.32239385919530	1.08670069674473	1.46523100493627
N	4.27428076290030	-2.98272895417395	1.32606564310109
O	3.13191880079151	-3.37295809849153	1.09432233339937
O	5.02732071938489	-3.48264114250221	2.14133094880801
C	-1.91069575650641	-1.79569622340024	5.24662737421605
C	-2.51146311250706	-2.77795199111612	6.02809507420818
C	-3.39608930927970	-2.41523880849109	7.03454034782552
C	-3.72580489880765	-1.08242728826187	7.30275540859090
C	-3.10762413344023	-0.11344601821799	6.50212906001042
C	-2.21513177718333	-0.45686011015375	5.50394733930567
H	-2.29769012436618	-3.82795003287743	5.85510801000762
H	-1.75931675142337	0.32798363689054	4.90634882325837
Br	-3.55103070504247	1.72167120311072	6.77411180899666
Br	-4.22144266732017	-3.77023570413350	8.10685471811603
O	-4.58894596652364	-0.69631901747691	8.26241505904382
H	-4.92327467950449	-1.48693286471562	8.71520192920816
C	-0.93232765083641	-2.12895912205557	4.15155110791400
H	-0.98426996904607	-3.19656839146858	3.90825278996687
H	-1.22208979068752	-1.58082062370212	3.24285793232336
C	0.50013439433376	-1.73273651668566	4.53472956422333
H	0.88231930523074	-2.40986155052778	5.30999863099922
H	0.47431395105726	-0.73405878593336	4.98109027920243
C	1.43430671389547	-1.72728391144423	3.32651299993275
H	1.54890743826507	-2.73855547758468	2.91679016529931
H	1.02298409037575	-1.10479660523188	2.52224199010134
N	2.79436659245204	-1.23329154844444	3.61349398938235
H	3.21329942492617	-1.63822123703900	4.44891948037749
S	3.0622296205476	0.42394484166146	3.61478386011045
O	2.51324360134662	0.92693153072712	2.34992580317842
O	4.46597068403099	0.62364960488159	3.98394220665998
C	2.06066247441151	1.19652022953566	4.92534348039070
C	0.95374326973953	1.93364032597549	4.51981029604816
C	2.37158270102738	1.15073135665719	6.28627312045301
C	0.14193680947571	2.56580363186843	5.45721211601244
H	0.73979018692425	2.00696179877425	3.45934286895946
C	1.58919536862253	1.80817014446185	7.22557026376812
C	0.45580610061402	2.49636849691616	6.80951700198863
H	-0.73073725585383	3.11581157067835	5.11949795961757
H	1.86979338436921	1.75896054666577	8.27221213449638
H	-0.17728025933572	2.98312189452393	7.54429561100953
N	3.50191181749293	0.36659072450847	6.82305190652509
O	3.62597675991634	-0.78754362141583	6.42783218614082
O	4.19456569496450	0.90174854776606	7.66904848526773



Main article molecule number: 17

Name: SKS-i-2-2

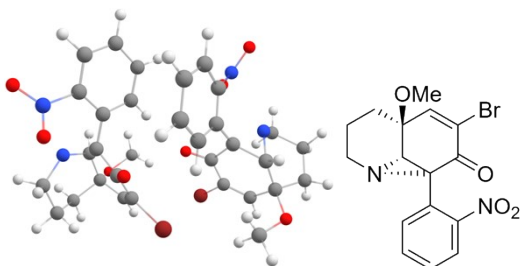
Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -13452.501833357

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C	-1.17445155697410	0.40268312848495	0.53836505052463
C	-2.33627776803058	0.54632188738800	1.17853851053344
C	-3.59067463665019	0.98295962553739	0.50578663244178
C	-3.43646614262081	1.25541571274941	-0.94685345219158
C	-2.27806107607380	1.13112197428844	-1.59713634589055
H	-0.28172931111782	0.05734638096798	1.05523056121315
H	-2.20097275252674	1.30517570219826	-2.66789383038023
Br	-5.02411998904610	1.77239038787763	-1.86245687965390
Br	-2.48918624605881	0.18181779915107	3.04091108215969
O	-4.64761238943339	1.09536870431699	1.09327066185498
C	-0.01307133617409	1.94744606570974	-1.01677352484253
H	0.98147865134253	1.55850175774097	-0.76346110330264
H	0.01366675457345	2.24173593851903	-2.07189507613136
C	-0.36880581675572	3.14659596042534	-0.14606639116751
H	-0.16954780250060	2.92849767946848	0.91134465234597
H	-1.44100803958477	3.35682293955380	-0.22636343426953
C	0.42545393680618	4.38385847346334	-0.57372134254410
H	1.48493024275350	4.11997766959010	-0.70177952864999
H	0.06797651267793	4.75372504060417	-1.54145569471482
N	0.40364463961730	5.50071256767492	0.37932649046737
H	0.75708107300931	5.26405491362952	1.30357211949156
S	-0.98663322337963	6.42394335622353	0.54941254420701
O	-1.45698487746359	6.69915480196818	-0.81072043716221
O	-0.66885040314779	7.48191887765415	1.50700761636929
C	-2.29592155846403	5.41323038303032	1.32383146309914
C	-3.37867562410657	5.06022071309973	0.52220091203087
C	-2.32964490298412	5.06487699649785	2.67588439474721
C	-4.44087114698427	4.33317736920742	1.04887704548823
H	-3.37558007146353	5.36638776308577	-0.51888943544278
C	-3.39981000869957	4.36299407156653	3.21604808406031
C	-4.44747015886405	3.97556501304835	2.39232542179282
H	-5.26002579774709	4.03560314272180	0.40264811229049
H	-3.38796294555251	4.11231534192514	4.27108235886503
H	-5.26324319702566	3.38661685546809	2.79713899027606
N	-1.23060272942238	5.37306114450112	3.61276711861767
O	-0.08476884563208	5.12128353026200	3.25199097263633
O	-1.54219349867098	5.79885524673838	4.70978357812517
O	-0.34239767863638	-0.30687451475766	-1.60817841003065
C	-1.12188789809857	-1.50474588327681	-1.72878095264451
H	-2.01093249202381	-1.34119572565181	-2.35073419948018
H	-0.47534478408355	-2.23138252164851	-2.22206229893806
H	-1.42591491985449	-1.88347479262309	-0.74334651781399
C	4.91322370652267	0.27586415891201	-8.09381473796130
C	4.82510641507354	1.76885081636794	-7.97018325598933
C	5.10516459250134	2.42004666720222	-6.83917284965553
C	5.60994173958686	1.74276674315598	-5.61366194930642
C	5.751337443350526	0.26702325478213	-5.74651168379808
C	5.46318333939948	-0.39420151186077	-6.86876567867309
H	4.48349859053143	2.29861884545215	-8.85696008863692
H	5.60377169201899	-1.47025124686104	-6.94312925858635
Br	6.40964647131374	-0.64033780617986	-4.20917385380023
Br	4.89538240743013	4.30482796760919	-6.70657001351023
O	5.89122925559329	2.34186196004543	-4.59631586358455
C	3.49853239758409	-0.28983685362194	-8.37948164976947
H	3.23641115632588	0.01650283557102	-9.39962462019280
H	3.58389454011000	-1.38429043751512	-8.38619455796837

C	2.43896251255257	0.16938597875638	-7.38156041928825
H	2.17409655031479	1.21891312465478	-7.56462971266810
H	2.84540297630573	0.12422370405652	-6.36454107014639
C	1.17810144105971	-0.69470705113768	-7.46149549775049
H	0.85935703370029	-0.80339934110114	-8.50689279731703
H	1.37380189741442	-1.70265399626738	-7.08001734567820
N	0.01355066818230	-0.15871890273589	-6.74472218063865
H	-0.31154687906776	0.74492493497387	-7.08130968080880
S	-0.02916906367251	-0.17998469426589	-5.07235961925996
O	0.47131616943405	-1.49558071507763	-4.66707150644931
O	-1.35681076461475	0.31700823428938	-4.70010548715612
C	1.16326866830052	1.03159889286249	-4.42186773080853
C	2.27674918862140	0.54492181805818	-3.74240340522002
C	0.97430438292925	2.41131936994743	-4.48691143030869
C	3.20572238776710	1.42356701865079	-3.19740021522296
H	2.39534533515890	-0.52863815498601	-3.63956888146164
C	1.88717273283257	3.29827425881316	-3.93154462819784
C	3.02221677750124	2.79855901581401	-3.30784445848862
H	4.08471821902155	1.03280484511920	-2.69547926175715
H	1.70237133834814	4.36554447345682	-3.99913985807288
H	3.76463577077426	3.48249389605722	-2.91042446515600
N	-0.21573792089237	3.01689127853922	-5.11670310841214
O	-0.44520371858056	2.74466372992258	-6.28941054289351
O	-0.86061841845389	3.78722309567770	-4.42790154834885
O	5.68172806047845	-0.09236701784907	-9.24418238264798
C	7.05207837090086	0.32078594060636	-9.20450338165005
H	7.59039785207681	-0.13553306364739	-8.36310650980642
H	7.49370264131762	-0.02163945137850	-10.14189566282920
H	7.14385077221057	1.41329258213567	-9.13896856896220



Main article molecule number: **18**

Name: SKS-2-1-1b

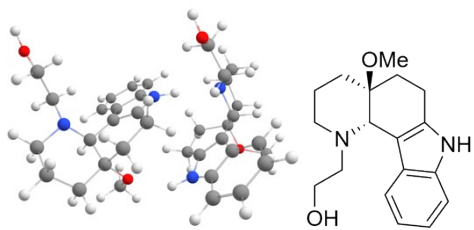
Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -7205.86349706478

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C	1.84586214245310	1.32439820404413	0.81943187319624
C	0.39420844606795	1.07590788359933	0.42422261649091
C	0.80503187036447	-1.43362753822783	0.23439366506722
C	2.26664564555350	-1.15983522001787	0.62312186982083
H	2.89575297401142	-1.92246636020930	0.15079235134698
H	3.76849477046882	0.40807644945869	0.43920229664450
H	0.78069930332005	-1.82015663625455	-0.79266052807498
H	0.35734488782930	-2.20059932662683	0.87406171554512
H	2.41028860742825	-1.26724637859871	1.70340584081285
H	2.62638245921221	0.34288946604927	-0.91240592572093
H	0.00536487745744	1.80729343868783	-0.28661537930365
C	-0.56554131475196	0.45227722601753	1.39547187130762
C	2.09182276237660	1.27082973769317	2.30211064273930
H	3.05993568894320	1.64473651319906	2.62973551073513
C	1.26118736086945	0.67519468834346	3.15797838359238
C	-0.06830099669428	0.13419974264559	2.79085742980855
O	-0.76245059970383	-0.47640510931739	3.57900059656229
N	-0.09731222607907	-0.27159251018968	0.21493034293769
Br	1.76001215414067	0.45063398913881	4.99170774646023
O	2.30559281473710	2.56179306503475	0.29054797557681

C	1.63683676135448	3.71284527993103	0.82082768336870
H	1.64030117140278	3.72045153723041	1.91802131557710
H	2.18519345209109	4.57991119037872	0.44671339797436
H	0.59585991226200	3.77746348876871	0.47409211664527
C	-1.99512543230603	0.89973938334862	1.34554199784264
C	-3.04232323677935	0.13846853515134	0.82712238664864
C	-2.28019820623651	2.21470311498423	1.71938272305834
C	-4.31820093586007	0.66022269310085	0.64493273461397
C	-3.55523342577592	2.74434678064486	1.56841513991944
H	-1.48262150292852	2.82916409005895	2.12887729547476
C	-4.57627563874830	1.96913767243602	1.02530782123558
H	-5.08850948492635	0.03163138369293	0.21192950102061
H	-3.74316507409789	3.77241972219552	1.86428330749731
H	-5.57177862270517	2.38223200731475	0.89397479561694
N	-2.84542863020175	-1.27337733581127	0.45376318270747
O	-3.43045418591478	-1.67380288746111	-0.54502435662651
O	-2.14964151251849	-1.96098795916550	1.18762772505936
C	0.11098826820177	5.32949967462677	8.99207433463277
C	0.27932912993338	4.04923851632933	8.13209015109306
C	-1.06013006985235	3.73009578519800	7.49861419737971
C	-1.07931541015562	6.13371579511497	6.86454909181308
C	-0.76400373977348	6.42283486049194	8.33267226231365
H	-1.71464814951248	6.50159398587635	8.87115982172046
H	1.10827800575990	5.70715176447080	9.24020091144649
H	-1.79808828134997	6.86095613477145	6.47354992331957
H	-0.17338375033693	6.21062933126853	6.25180804462707
H	-0.27689342569516	7.40015568009967	8.40568505055742
H	-0.33911224089222	4.99368595762917	9.93203869297807
H	-1.70676559829888	3.09264050677977	8.10716147279481
C	-1.24689649524085	3.68548684160488	5.99631171414182
C	1.38555529105090	4.26377002889668	7.13867142673639
H	2.34961233804765	4.52264158463926	7.57241238947634
C	1.24786810581547	4.14817467280421	5.81566196961271
C	-0.01647600128428	3.77655614676826	5.13817109516061
O	-0.05787009248045	3.52339063822457	3.94671854454568
N	-1.72353523303933	4.81230683117785	6.81225847015737
Br	2.74223830474327	4.45491027074305	4.66722746176943
O	0.67357666296371	3.03675963199450	9.06150301112830
C	0.92117805155627	1.75569821143633	8.47943167341315
H	1.78066501379334	1.77726656452857	7.79644004053936
H	1.13790060881578	1.08361717813788	9.31206033393637
H	0.04464803477879	1.37886291781626	7.93359018425403
C	-2.34777909961393	2.83556658427920	5.44412266404536
C	-3.57532154703242	3.35833292474638	5.03429027557939
C	-2.20782442364028	1.45077912158799	5.43292445940197
C	-4.64827233128002	2.55039020930321	4.68547007231316
C	-3.25037136460413	0.62409416374106	5.02580098148965
H	-1.26052721483484	1.01134564796155	5.73362959346042
C	-4.47795937574150	1.17221586675012	4.67215292852737
H	-5.58610158441709	3.01096880311156	4.39436041766537
H	-3.09325674710427	-0.44817462613514	4.98641409682265
H	-5.29816947611627	0.53116792839719	4.36480994306588
N	-3.75809118375857	4.80839473853307	4.87296394206846
O	-4.82307625389309	5.29175422341376	5.23071785293401
O	-2.84815394551173	5.42699404263517	4.32937598353314



Main article molecule number: **19**

Name: SKS-4-3b-3

Qty of copies of the molecule modelled: 2

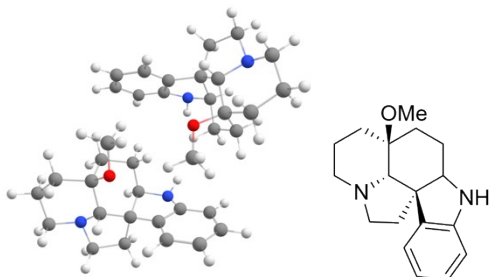
Qty of imaginary frequencies: 0

Final single point energy (Eh): -1920.21246543518

C	-22.11418468397797	-8.95506958918705	-3.55869499148777
C	-20.77833605991088	-8.67533408598246	-4.25036655605066

C	-20.86961208667495	-7.36494883495269	-5.08348996923334
C	-22.60775404045678	-6.49827984276868	-3.60806682053364
C	-22.59542052695710	-7.75437489596320	-2.75083092954668
H	-21.94790967438528	-7.59806308393069	-1.88036160734446
H	-22.86451838260614	-9.18834299877060	-4.32637009724833
H	-23.37616107130831	-6.59816242064323	-4.40512656225415
H	-22.89626088514920	-5.64027671633360	-2.99054362518524
H	-23.60618880267143	-7.93496029790376	-2.36557543682290
H	-22.00887671746670	-9.84569919517547	-2.92793776434146
H	-21.64913011261863	-7.49789020247935	-5.86184262976198
C	-19.63418065541424	-8.57190128316609	-3.23752134393380
H	-19.61460713522309	-9.49640975033470	-2.64935867309614
H	-19.85028589103887	-7.75815607384629	-2.54391458997424
C	-19.54283533697224	-7.13020948140104	-5.72546477591616
C	-18.25818856993362	-8.35136178112627	-3.88899678229504
H	-17.58806832069357	-7.85041327652579	-3.17546937767182
H	-17.80039667316241	-9.31914356730765	-4.13252924810687
C	-18.37908088489037	-7.56700231402785	-5.14531279122179
O	-20.41610266238690	-9.80130508128364	-5.06812742985120
C	-21.06733180955444	-9.95416190940310	-6.32027045246056
H	-20.73011440696326	-9.20517327316485	-7.05128685783745
H	-20.78756969746578	-10.94617231041938	-6.68496476328942
H	-22.16379477942542	-9.91386112744724	-6.24019175869397
N	-21.28818912701956	-6.22477125741621	-4.20388277358203
C	-19.19249863130060	-6.53766372091795	-6.98639240609385
H	-16.37291207075747	-7.15947037395569	-5.60508991283247
N	-17.31034244113823	-7.28891529142642	-5.97196693926662
C	-17.77749981462300	-6.61964876589606	-7.08831206533702
C	-19.91102554763434	-5.94210856101615	-8.03038541163833
H	-20.99504072409677	-5.87531315445372	-7.99022667330609
C	-17.07764514520909	-6.09122017297761	-8.16791247388451
H	-15.99443094573251	-6.15744774415622	-8.22429703959764
C	-17.81584104567454	-5.49116582853269	-9.18081745557221
H	-17.30077099179808	-5.07234412003878	-10.04008086415792
C	-19.21649207605245	-5.42678506151654	-9.11585752496919
H	-19.76427976929091	-4.95996050533959	-9.92910214081885
C	-21.34140520666907	-4.97973973354015	-4.98689452955751
H	-20.36038922565165	-4.81324490207643	-5.44324092667724
H	-22.07398114517961	-5.05402300698180	-5.81469217719730
C	-21.65917683382055	-3.75236505099400	-4.13903385905961
H	-22.74225607429096	-3.65107592258551	-3.97100551639607
H	-21.16553119860879	-3.83810111566410	-3.15636855575149
O	-21.16305252142318	-2.62594623015122	-4.86724947344008
H	-21.43559934409316	-1.82594818952076	-4.40643001350467
C	-16.56857089145154	-4.89817650596681	-2.11596564750669
C	-17.56837098976315	-4.78755062651118	-3.04755046743450
C	-17.41246442768307	-4.30093936674790	-4.43990435561020
H	-17.96094706293725	-3.35829952181614	-4.57312842629923
H	-17.88107186670491	-5.01077346302538	-5.12847040763900
C	-15.92561565487928	-4.08734720608932	-4.80534469984352
H	-15.76664397130265	-4.37062834431218	-5.85309634672830
H	-15.68077827265186	-3.02712838669352	-4.71283332976700
C	-14.91792188718067	-4.85834368548494	-3.94597219584493
C	-13.47855268960000	-4.51748031035501	-4.34377008498868
H	-13.36405254839416	-4.65964093554592	-5.42559054656125
C	-13.06935168993834	-3.10810970203511	-3.92014460384740
H	-13.58341079247193	-2.35512402240579	-4.52887595321408
H	-11.99296321689143	-2.96922672189378	-4.07942779058306
C	-13.40356074073571	-2.88215731600418	-2.45343351897724
H	-13.15804666570684	-1.85374946700802	-2.16580755884554
N	-14.82830322538010	-3.11951218781078	-2.20201644104021
C	-15.20986202247881	-2.64370285254651	-0.86934186705386
C	-15.56735756885707	-1.16521669649214	-0.91920147038169
H	-16.48101107221214	-1.04476373877491	-1.52140398701356
H	-14.76416126955374	-0.58742102007696	-1.40457287538862
O	-15.76302498751379	-0.73099432840978	0.42922318757547
H	-16.07097077193166	0.18021872301247	0.41123501040336
H	-16.08942228031245	-3.19097924616408	-0.52070168076708
H	-14.40852537194972	-2.80247886211820	-0.12217915959993
H	-12.77724769428589	-3.55099828258368	-1.82209759830642
H	-12.80755390909222	-5.23493259523484	-3.85223608601584
O	-15.15665951559712	-6.25888472598450	-4.24165460406804
C	-14.63505013752436	-7.22936547829754	-3.33983164610283
H	-14.75946852771361	-8.19994180405036	-3.83052169691171
H	-13.56550529094694	-7.08496590597455	-3.13478904310066
H	-15.18824496738185	-7.24210148695938	-2.39074709290183
N	-18.75899702042045	-5.23070138862708	-2.51125388612343
H	-19.58182931736405	-5.49198615661776	-3.05777934504621
C	-18.52473471691116	-5.67692176408540	-1.22433136944919
C	-19.40146050035491	-6.21827701817919	-0.28967666141428
H	-20.45879638466477	-6.33667938739520	-0.51084733487882
C	-18.88230130018658	-6.58722677004995	0.94580393960574

H	-19.54198070366229	-7.01375794408661	1.69546163694806
C	-17.52259901616246	-6.40638092908443	1.24402191805662
C	-16.65197940981174	-5.84942855376115	0.31749096894594
H	-15.60471626885951	-5.69760497607368	0.56780870494824
H	-17.15051759757181	-6.69805158724689	2.22171164856228
C	-15.15605259774306	-4.54656103340850	-2.43969341812938
H	-14.47138761401243	-5.18043409116330	-1.83665817905907
C	-17.14538582386250	-5.47972022715267	-0.93978107179929



Main article molecule number: **20**

Name: SKS-5-1-2b

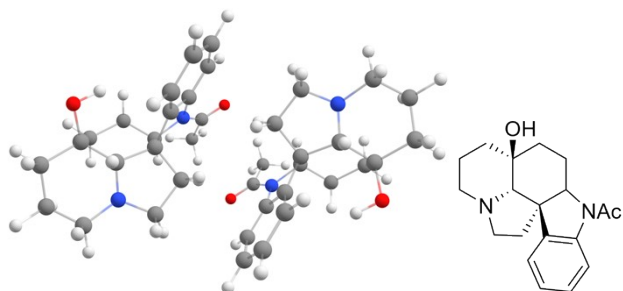
Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1769.78290724427

C	14.30152252368839	5.01364895789819	-0.03086045474253
C	13.00829814012873	5.38059801308495	0.71547421339173
C	12.36496350024472	4.09299382615927	1.24810039585762
C	14.48987881418910	2.89931254220254	1.30625043168652
C	15.23636885370614	4.12128785286855	0.78677641546796
H	15.65134547154734	4.67712668426341	1.63607251211245
H	14.82545449295341	5.92753729344620	-0.33571064431339
H	14.20069870214374	2.24516964134095	0.45334195573514
H	15.13446473322009	2.30408700412866	1.96647369669993
H	16.08239142387596	3.80419108089308	0.16532002044200
H	14.00857099149216	4.48436155405367	-0.94943025570619
H	12.02816798467543	3.50749575707216	0.36271672633232
C	13.25893976840136	6.35811401300754	1.87131659124065
H	13.71187424802155	7.28026193967424	1.48861184057294
H	13.97798697780133	5.90620637606449	2.56429335497193
C	11.18087034111075	4.24722282797955	2.21542904089236
C	11.95530991486508	6.66529304949381	2.60258211600426
H	12.12644982666744	7.41639661975718	3.38711889702391
H	11.23229365703199	7.08120702812815	1.88857582661065
C	11.36316939785837	5.40339124625880	3.23732322562504
O	12.03061450159571	5.91333395865819	-0.19288636074071
C	12.47484808131322	7.00161937883365	-1.00388454390082
H	13.07941369229062	6.65218654243204	-1.85356563518684
H	11.58478101471109	7.50430280685423	-1.38468042560913
H	13.05079272542049	7.74043000851663	-0.43718929322074
N	13.32098910878376	3.32932989456805	2.05559903958642
C	9.80430708438798	4.54999756550170	1.67654383546426
H	9.80673234577148	6.49531335530968	4.17631198442470
N	9.97514469058320	5.61479038697791	3.70734594661503
C	9.12759323717914	5.31626759992039	2.63566092206264
C	9.14309958299678	4.10067333259145	0.54942360236438
H	9.66660982827045	3.51094971724906	-0.19884512579471
C	7.78014529015207	5.63045302266510	2.48377134446303
H	7.24972564803663	6.21290135955889	3.23279911970171
C	7.12366595708707	5.17401995520364	1.339904221098125
H	6.07324225775864	5.41526017658691	1.20058023869284
C	7.79234927217230	4.42337387746878	0.37525419877952
H	7.26389898847183	4.08423992952827	-0.51079386997957
C	12.54401682048467	2.23373410996083	2.63380731850237
H	12.42362615693609	1.40602716400462	1.90558873564648
H	13.05261210370935	1.82572448488371	3.51604471719050
C	11.17667918001220	2.86382053791484	2.95057448993848
H	10.36072207159010	2.24085393657911	2.57446402830891
H	11.01305378030892	3.00481122896258	4.02264803043408
H	12.00061803080988	5.07608896591606	4.06888041675467

C	7.14599109132755	8.58320879858537	-3.06329395466015
C	8.22274432823280	8.74686840667159	-1.97456603831861
C	8.63035973626073	10.22610319859336	-1.88797727242930
C	6.51615654623491	10.99606316329102	-2.83381987212165
C	5.98760986024239	9.57234725096079	-2.93169742777680
H	5.32173256191694	9.47800451416062	-3.79795038001870
H	6.75736675709734	7.55815979324484	-3.05102589045998
H	7.00209342040414	11.28432054735769	-3.79273822682320
H	5.69496375846481	11.70400831296654	-2.66015079693924
H	5.38999281697050	9.34959184872263	-2.03940806536703
H	7.64377552488328	8.73474747015591	-4.03180434840336
H	9.17250419079431	10.46585522992356	-2.83109239186386
C	7.75258594263711	8.24326770934323	-0.60910804963680
H	7.47915405181440	7.18401613527352	-0.67153089423636
H	6.84559172511838	8.79402255456111	-0.33186404064411
C	9.50297919958226	10.65393217685064	-0.69188740339383
C	8.83146391992047	8.45872505196955	0.44582101912564
H	8.52160464848663	8.01490298220522	1.39996868834802
H	9.75636086411441	7.95194304896366	0.13888910024211
C	9.11659647429876	9.94747544449549	0.63631415553610
O	9.43116541702489	8.08222896908138	-2.39415158910614
C	9.36636766743008	6.66113117834001	-2.47404438042023
H	8.51874018499928	6.31440794251564	-3.08062050655852
H	10.28962619697417	6.34120728932241	-2.96388770455441
H	9.31940359034612	6.18683740116879	-1.48346220133337
N	7.45102056392088	11.08343491594114	-1.72486923433298
C	10.99606300438251	10.42622236497867	-0.71587138243154
H	10.40946707100047	9.55999306252193	2.26599085502416
N	10.31850587957297	10.17906979666245	1.47014453542815
C	11.41615201966504	10.21055535500563	0.60536682514458
C	11.92680163810368	10.54732905148279	-1.73040706063516
H	11.60691109751626	10.70790078734532	-2.75688688110945
C	12.76828598176140	10.13046309936530	0.92669587767278
H	13.09317039946908	9.97989955504852	1.95312864464620
C	13.69829346746120	10.25864253704037	-0.10631526146358
H	14.75876329169476	10.19658273680555	0.12374770394111
C	13.28952419844420	10.45352337225131	-1.42422186230585
H	14.02946089869604	10.53885291449963	-2.21400584779232
C	7.98802377547829	12.42375476912784	-1.50197232136483
H	8.30171737767838	12.88916571077714	-2.45893294047113
H	7.22762928821501	13.07348408816203	-1.05136411440520
C	9.20961379634171	12.19207835432366	-0.59999227173328
H	10.07270091168902	12.76458821521939	-0.94973483692969
H	9.02499880188304	12.47838843357098	0.43923849411699
H	8.24229484698687	10.43576785672028	1.08673671943063



Main article molecule number: **21**

Name: SKS-6-2bs-1

Qty of copies of the molecule modelled: 2

Qty of imaginary frequencies: 0

Final single point energy (Eh): -1996.51147290755

C	-15.25463573562393	14.49806279602931	3.82426150526327
C	-15.08341861118351	13.60227767807450	2.59457547137627
C	-15.59615659526143	12.19915427372811	2.93786398595844
C	-17.11824102729275	13.01916934981835	4.64271953996757
C	-16.67317628082852	14.45816437131415	4.39587985609947

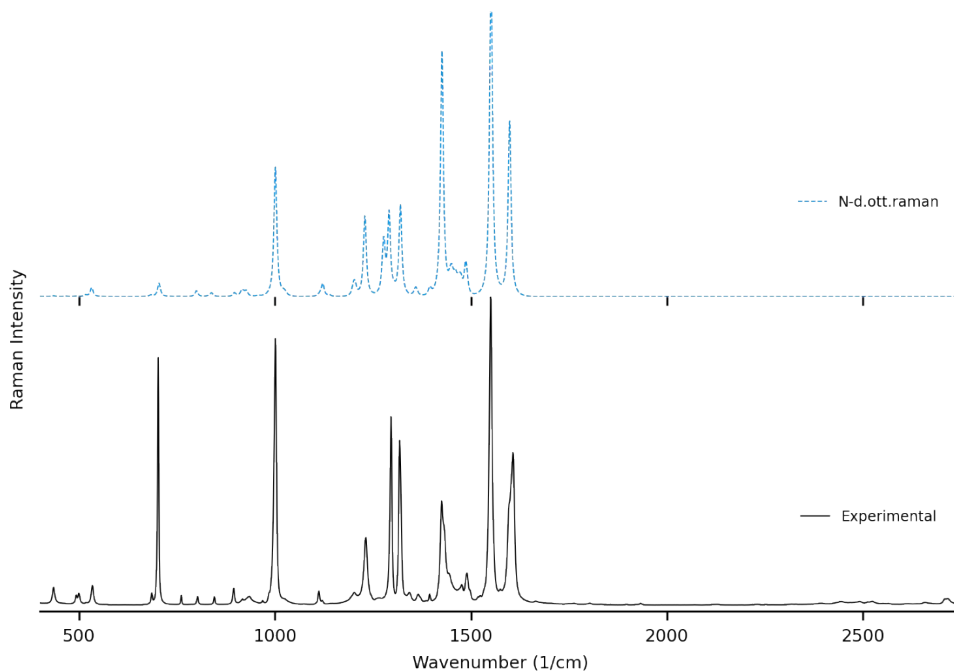
S54

H	-16.70643160159658	15.01945555386329	5.33703109592127
H	-14.96002680354561	15.52231037386198	3.56457777519357
H	-16.51231891195144	12.57641898313809	5.46417628239541
H	-18.16825948213992	12.98977284319437	4.96125792558754
H	-17.38103445509231	14.94111404777342	3.71156137886167
H	-14.54382484798694	14.14164327093533	4.58189883167855
H	-14.91175861973369	11.78095410506606	3.71211314184084
C	-15.81942325652576	14.15438886430660	1.36952824571916
H	-15.39066329267939	15.13298755231405	1.12356268082642
H	-16.87700558566617	14.29989681297379	1.61699595688476
C	-15.70268954851107	11.19951304341702	1.78008845186355
C	-15.69990432277138	13.21104083819817	0.17676280154931
H	-16.20642903024152	13.63352373052539	-0.69922939636358
H	-14.64519844576497	13.09763667343198	-0.10976020762160
C	-16.27969559110652	11.82521782104602	0.48127477979048
O	-13.66813113019455	13.55930023088163	2.35416350828729
N	-16.97676013398068	12.24567431040861	3.41835433439681
C	-14.44602111247630	10.55141870945724	1.25318212567546
N	-15.83002221891694	10.85658726007919	-0.54881627779085
C	-14.60406991723219	10.30628023558798	-0.11705885643281
C	-13.30405799303021	10.12128347331612	1.91026094117597
H	-13.17662089566653	10.29972858659010	2.97469381172091
C	-13.63109048305158	9.64315811032727	-0.85576193341897
H	-13.76917186910539	9.45354758086712	-1.91222856792716
C	-12.48385950827494	9.22298854166000	-0.18161235272934
H	-11.70710392958118	8.70561469503881	-0.73767910379320
C	-12.31553279010101	9.45397711116598	1.18145238482230
H	-11.41074125682435	9.11980530608848	1.67996777235748
C	-17.39694419975190	10.84518454532879	3.52766730434263
H	-17.06733133956997	10.40267676768621	4.48835951925672
H	-18.48945446183394	10.76350451021407	3.48209148468054
C	-16.69058689108369	10.13870626292172	2.35397204755356
H	-16.14778576360532	9.25485972830032	2.70133429654989
H	-17.39155382816112	9.80697381415758	1.58260739943783
H	-17.37107491928097	11.85994826196847	0.52901283697199
H	-13.47657698011701	12.84458785891957	1.73272404145714
C	-16.53935531717891	10.45345216857552	-1.65218805024559
C	-17.84694320664672	11.16570533831619	-1.91038790319337
H	-18.62150787750259	10.77651305019556	-1.23699442623784
H	-17.77553780572079	12.24717665650015	-1.76649850912011
H	-18.14324457263127	10.95296806947592	-2.93826853566328
O	-16.14134327147519	9.54436628694583	-2.37829911901282
C	-16.41390426539246	3.30724280366423	0.69754247298348
C	-17.46274194559311	3.39560585629293	-0.41615941168970
C	-18.35960437100284	4.61810913680028	-0.24142478510740
H	-19.11890132634679	4.65310105930141	-1.03190790872377
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N	-18.39699560254910	7.03275858135429	0.27049794073076
C	-19.06316697346589	7.97003815892777	-0.47792893544507
O	-19.60105895663207	8.94637868473146	0.04120362899855
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H	-19.87442437954136	8.37409142772600	-2.38983789487917
H	-19.25055514907292	6.70833789045808	-2.24827194464931
H	-18.12451288990805	8.07426381203785	-2.40746021834375
C	-18.23252064644770	7.07532349700656	1.67186627746845
C	-19.03924915562144	7.67477309562191	2.63181332678093
H	-19.91925077990275	8.23633623543270	2.34637040883134
C	-18.66338213216343	7.53573746382941	3.96856317109779
H	-19.27989963266778	7.99163274368199	4.73817602953404
C	-17.52087948602883	6.82766030694291	4.33304310671511
H	-17.25414886940696	6.73230040822627	5.38116543096728
C	-16.71830684579507	6.23335328068562	3.35510096817664
H	-15.82257969607615	5.68574116407953	3.63636149087450
C	-17.08365035325775	6.35487860351147	2.02366268032616
H	-17.19386328594764	6.15459737473364	-1.25421326577267
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C	-15.29149471301284	6.94232573077470	0.33601677724597
H	-15.71659745615906	7.70884318282709	-0.31863177488325
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C	-14.49902201933548	2.34098970142624	-0.68189356295628
H	-15.04412794233019	2.29733098876309	-1.63244616335065
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H	-13.18402796220127	3.87462812682703	-1.47453423716811
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H	-13.95156908998736	6.47415634742062	-1.36193772899319
H	-13.27248255638650	6.11795968970761	0.24232886769661
H	-18.06429215928740	2.47919715866950	-0.39642307250412
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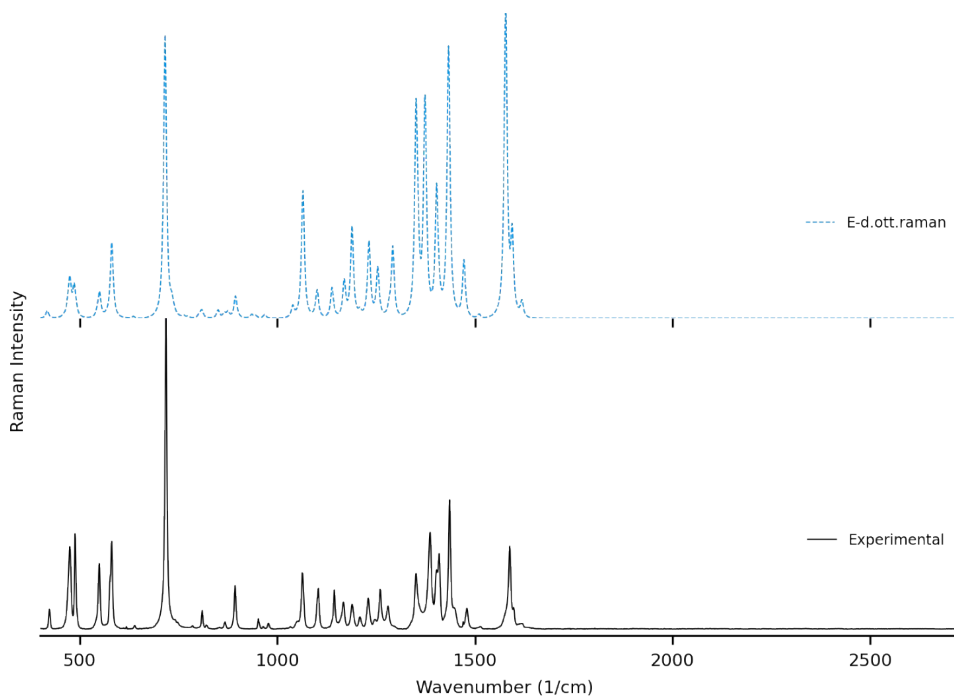
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C	-15.45215333978435	2.13324772313819	0.49699195933119
H	-16.03223981507102	1.20962294276928	0.37958340400422
H	-14.87225875962361	2.03268694517289	1.42431753975661

4. Raman spectra

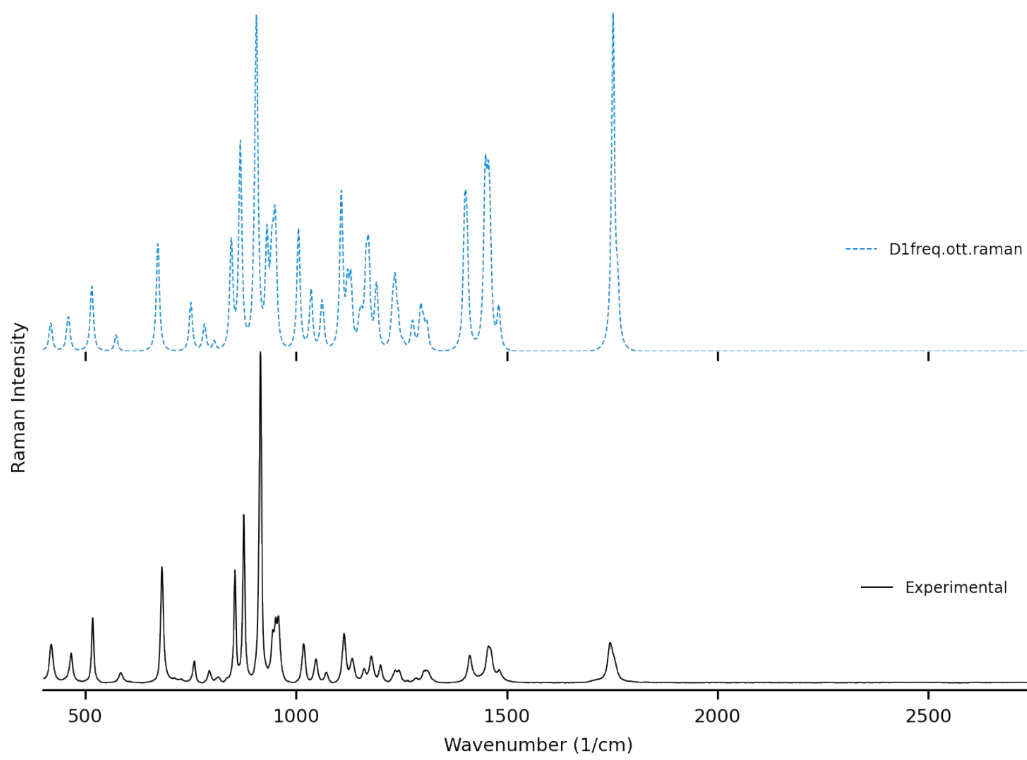
Molecule 1 : 4,4'-di-t-butyl-2,2'-bipyridine



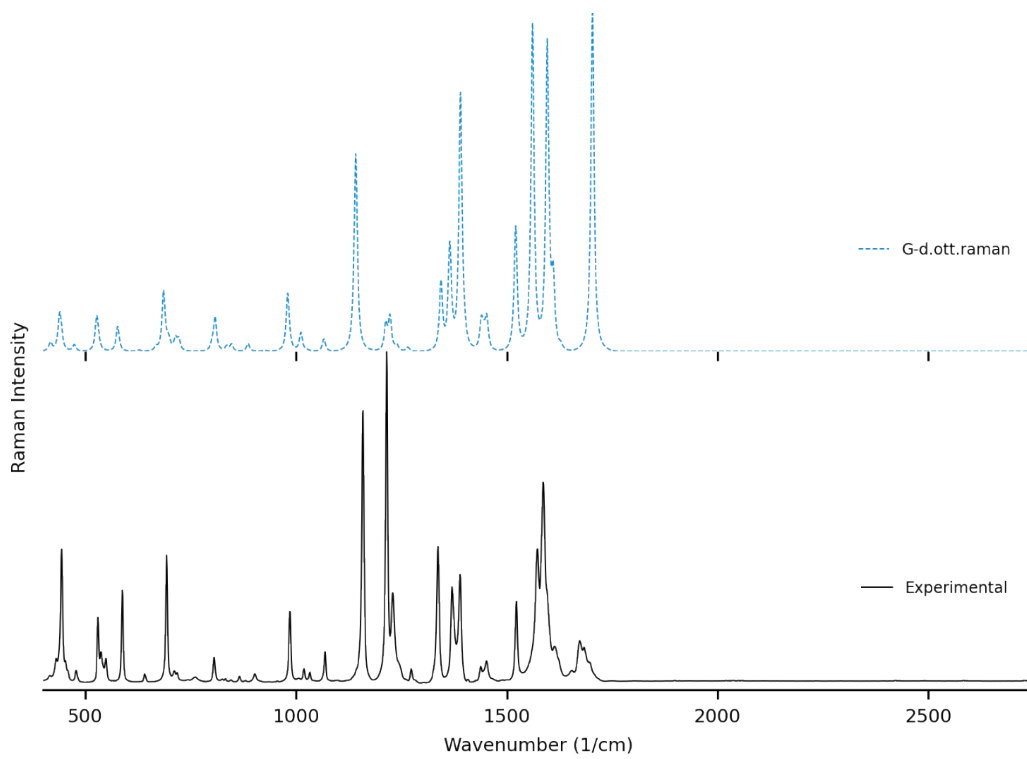
Molecule 2: 8-Hydroxyquinoline



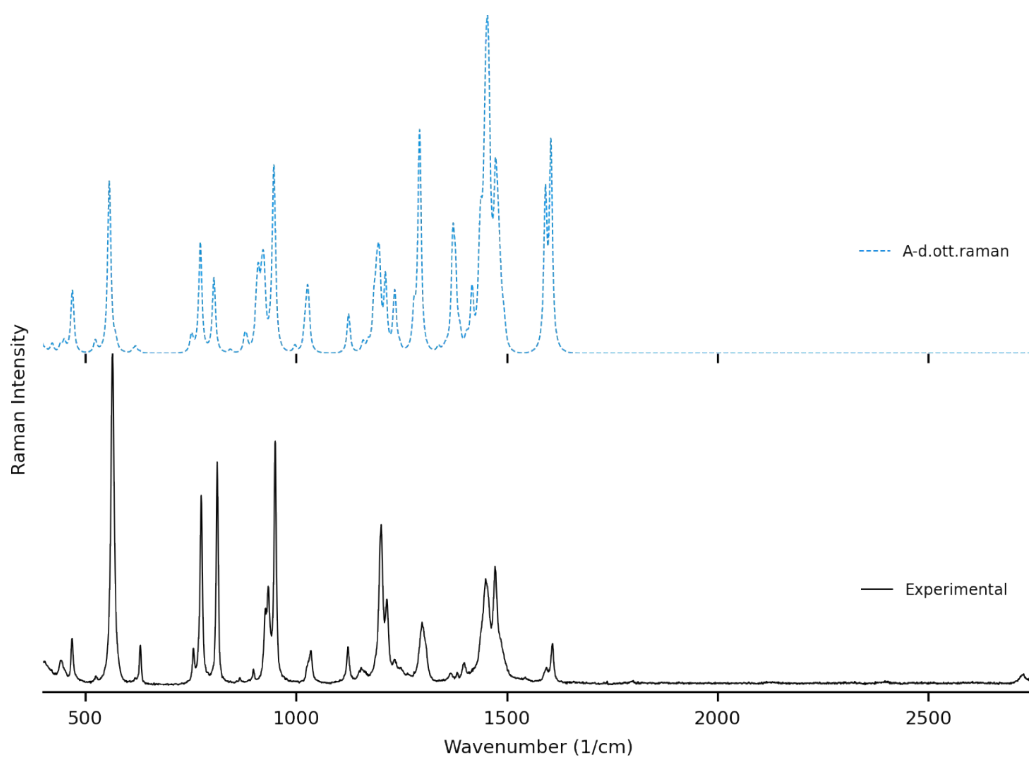
Molecule 3: Norcamphor



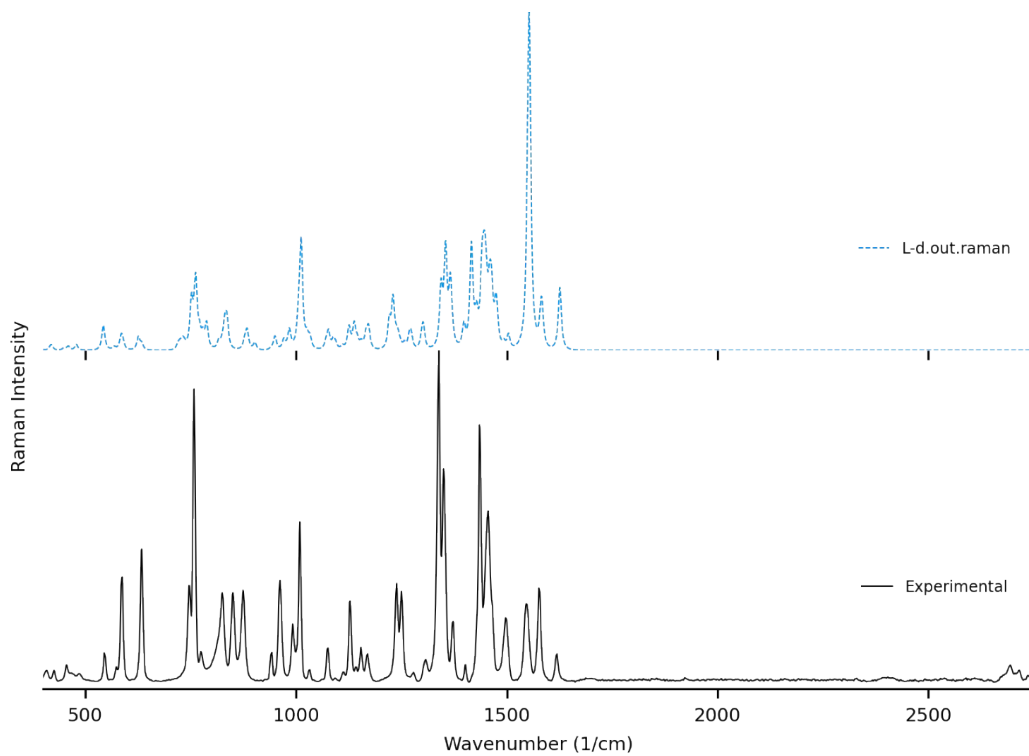
Molecule 4: Methylparaben



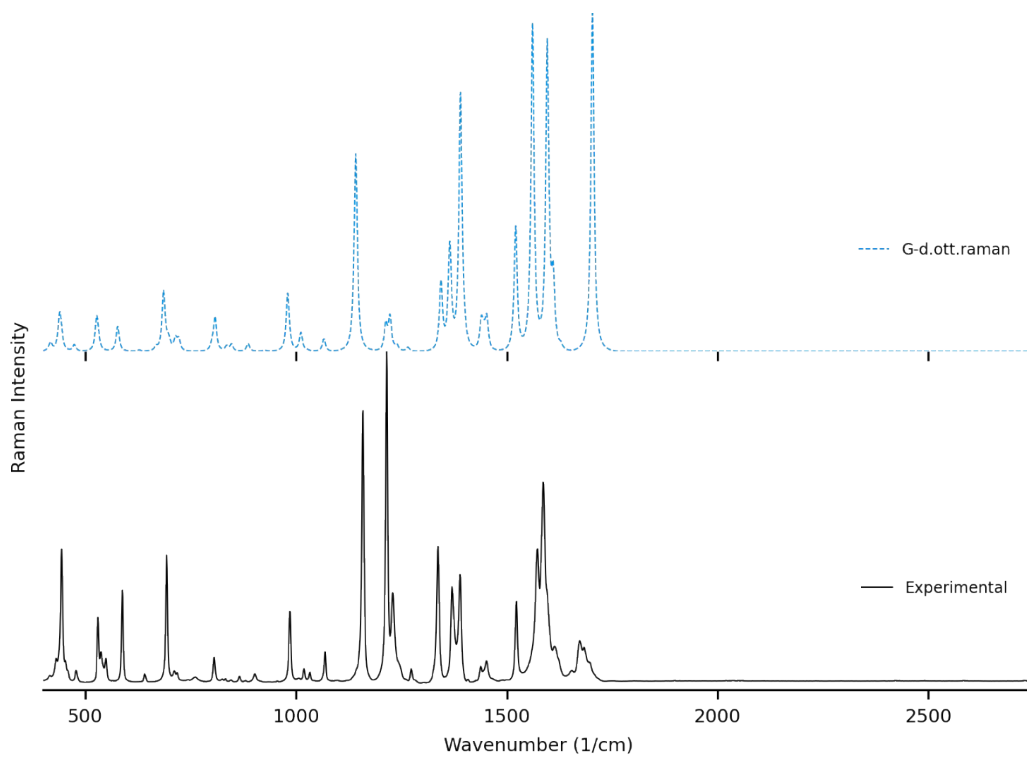
Molecule 5: BHT



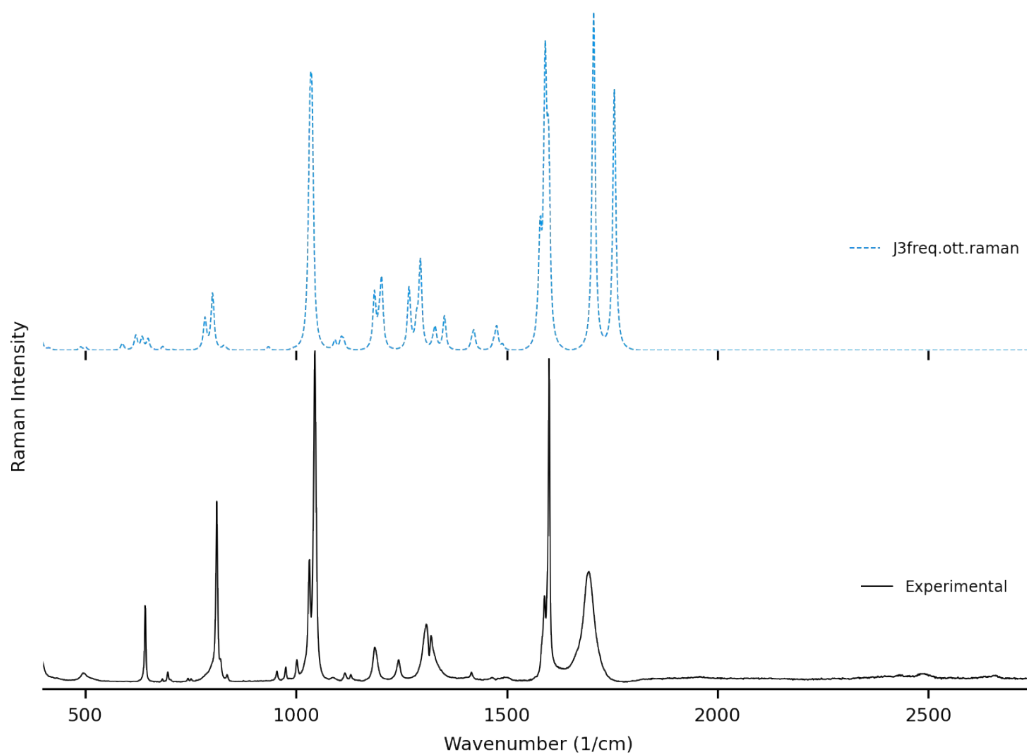
Molecule 6: Gramine



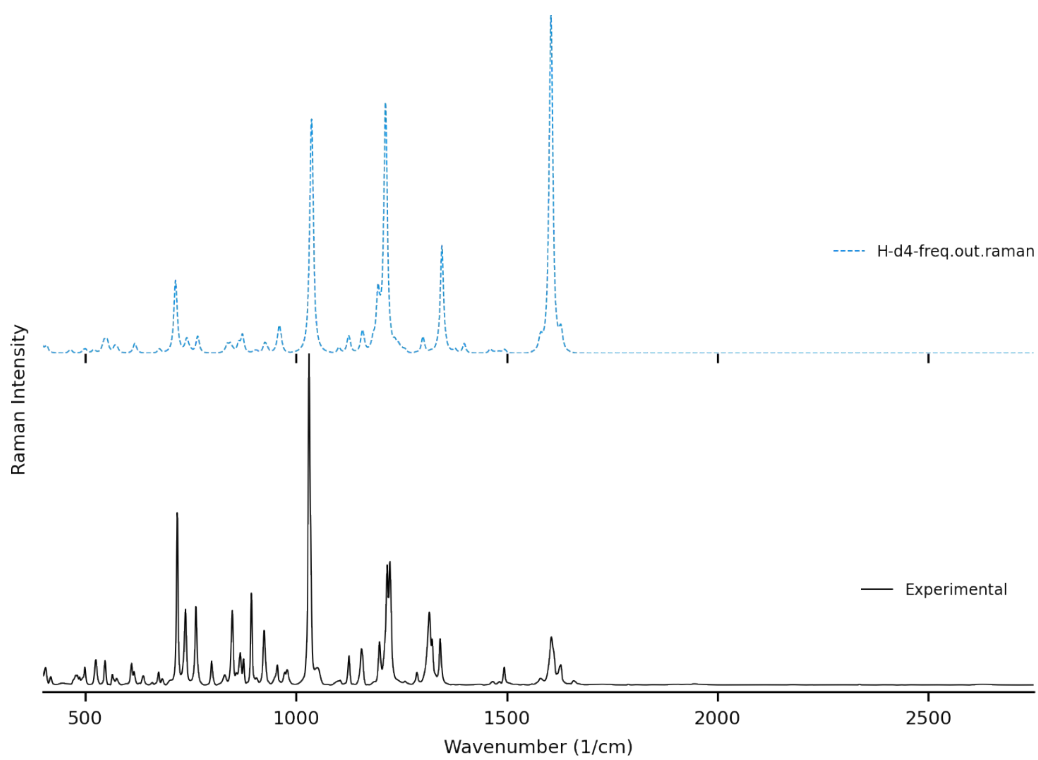
Molecule 7: Hymecromone



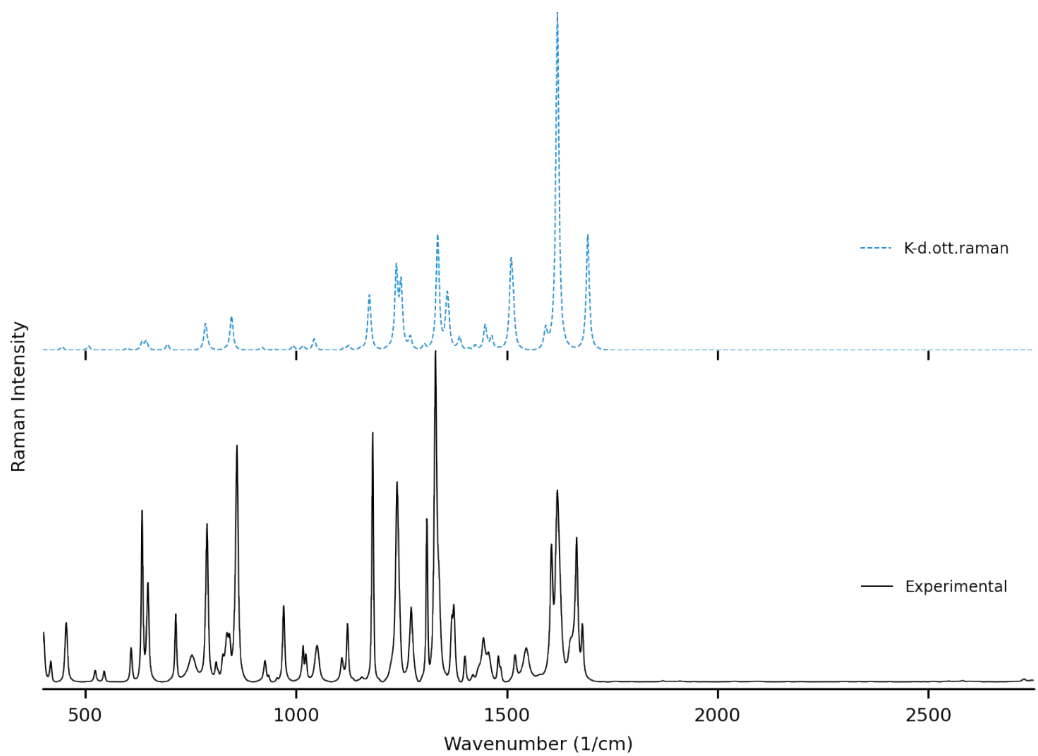
Molecule 8: Nicotinic acid



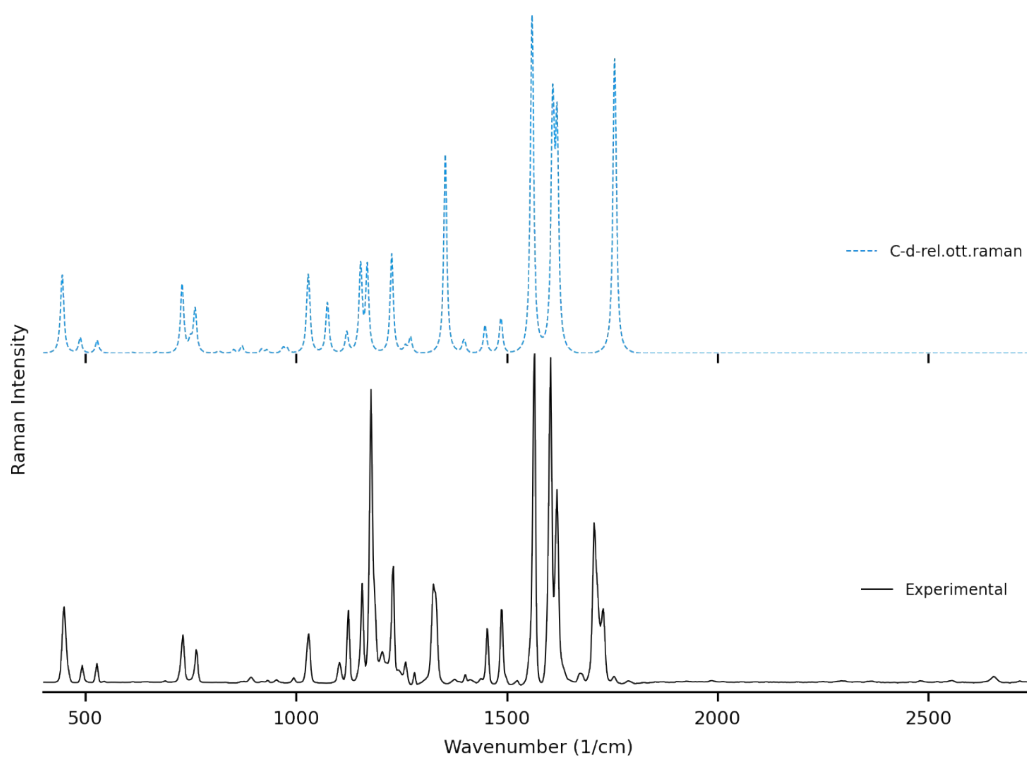
Molecule 9: Xanthinol



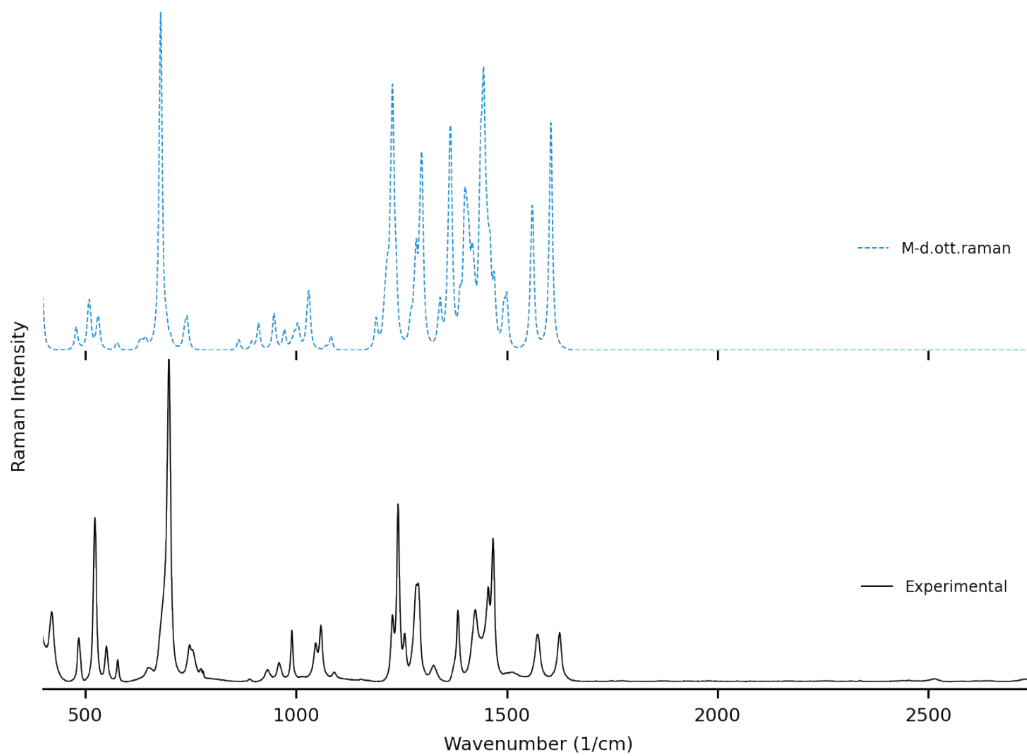
Molecule 10: Phenacetin



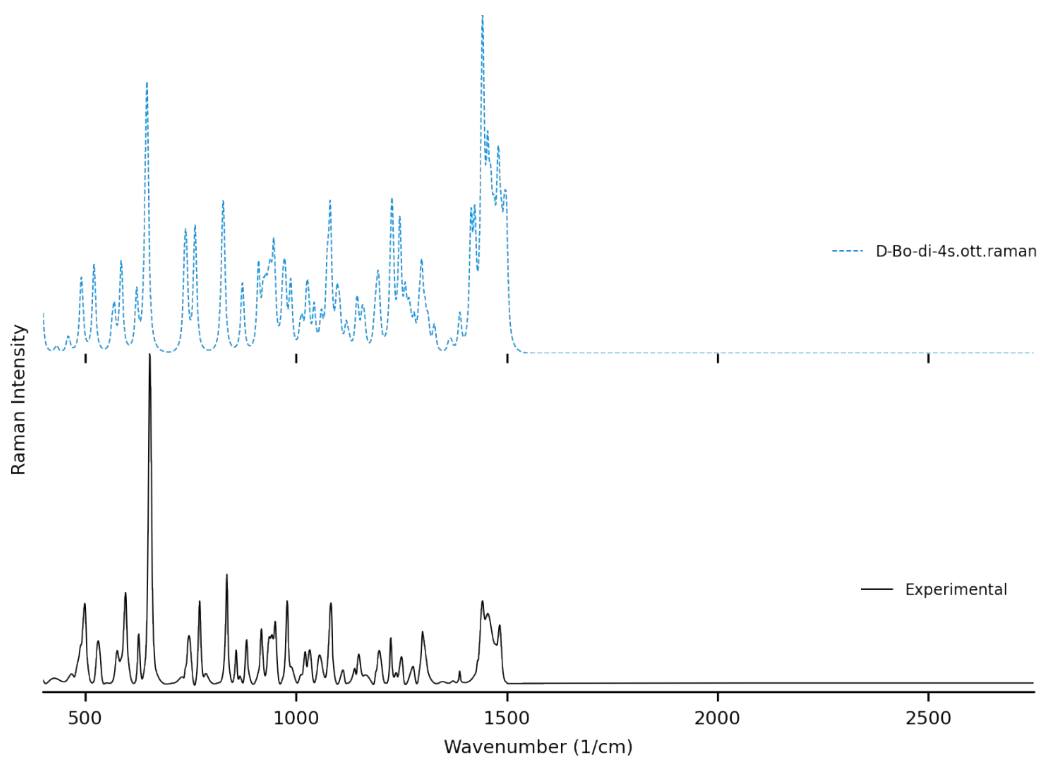
Molecule 11: Coumarin



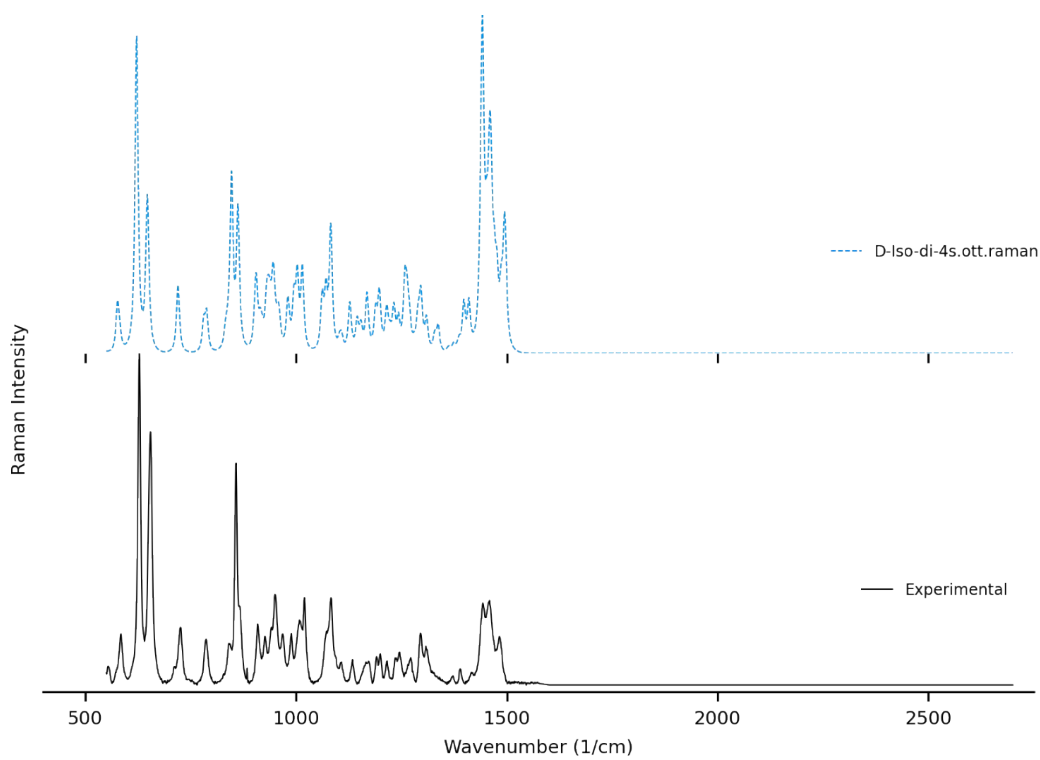
Molecule 12: Pyrioxidine



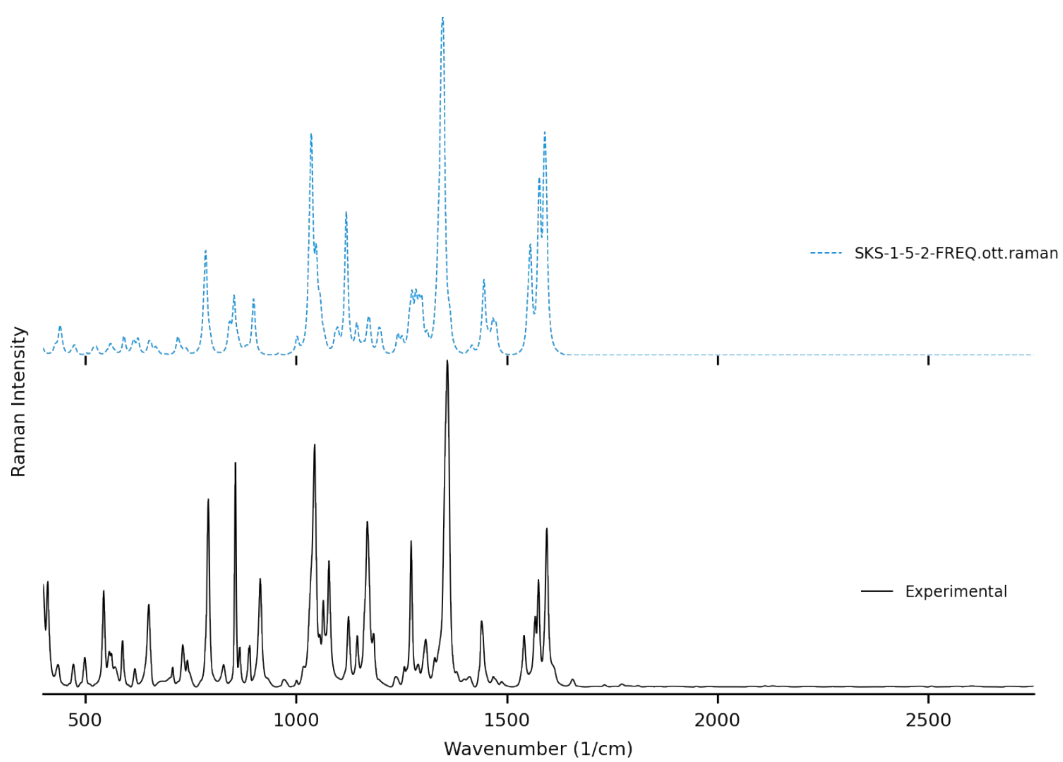
Molecule **14**: (+)-Borneol



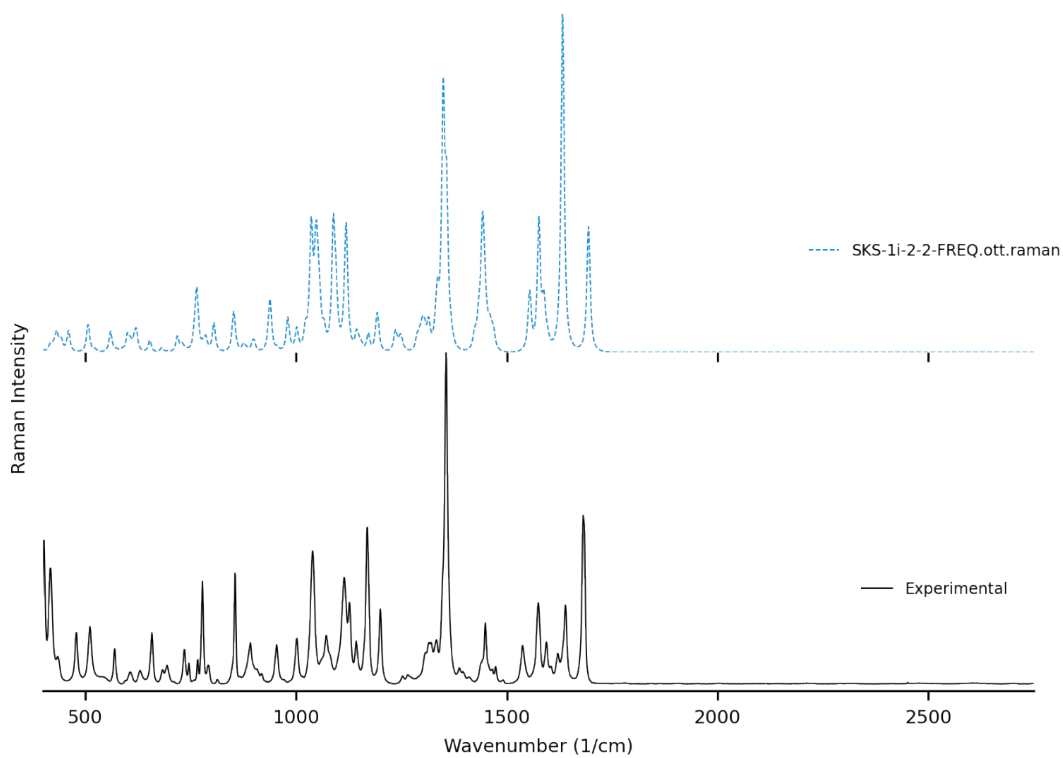
Molecule **15**: (+)-Isoborneol



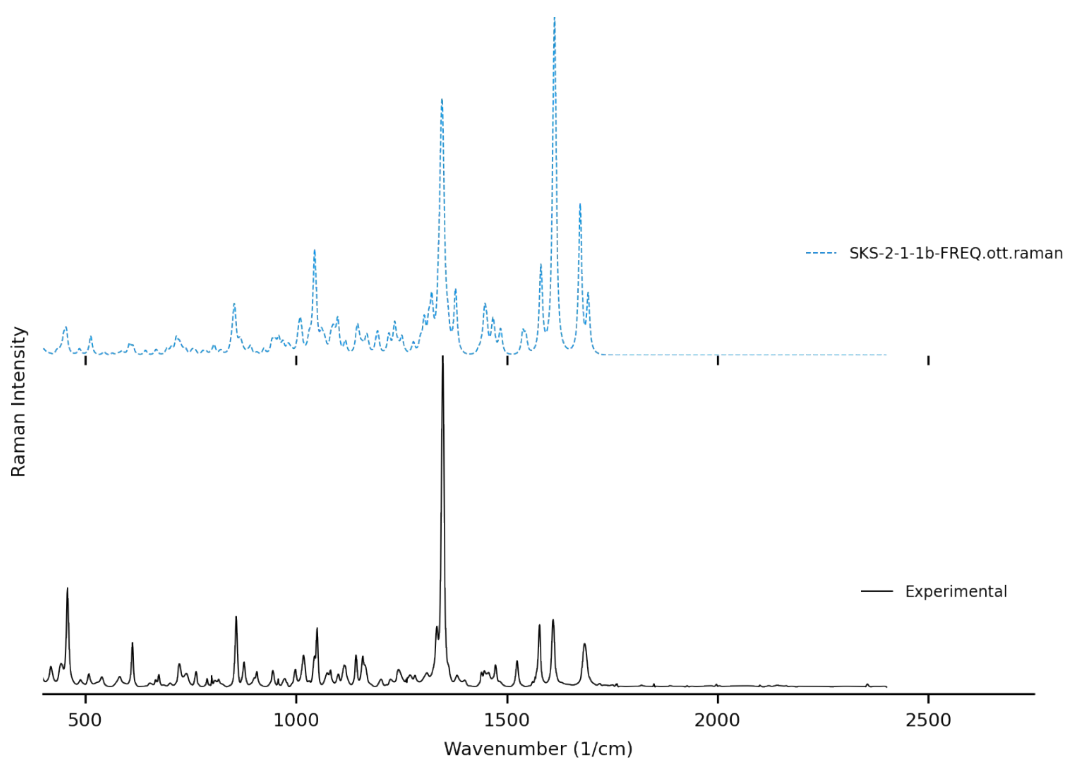
Molecule 16



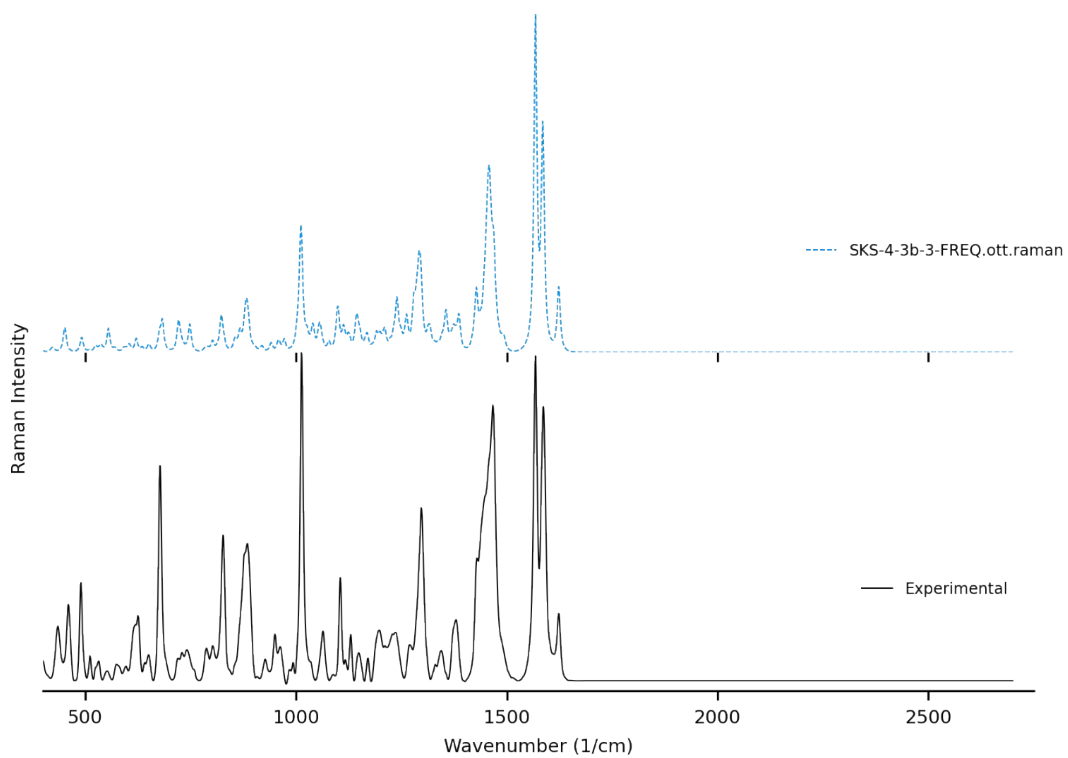
Molecule 17



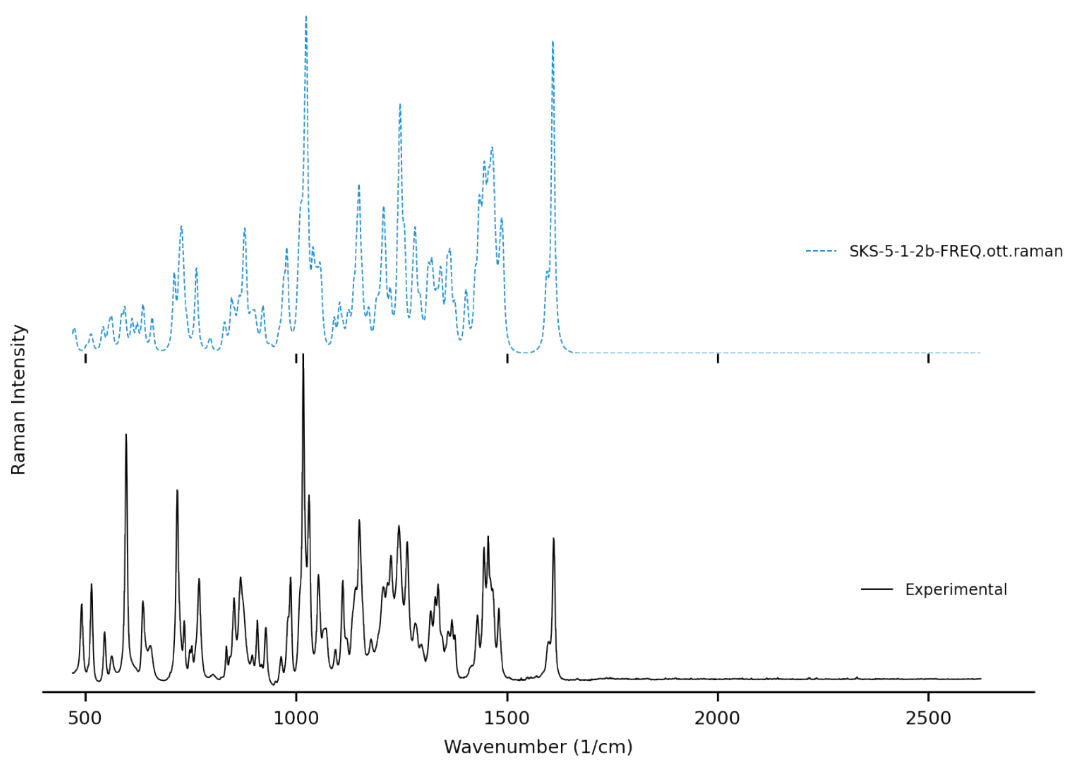
Molecule 18



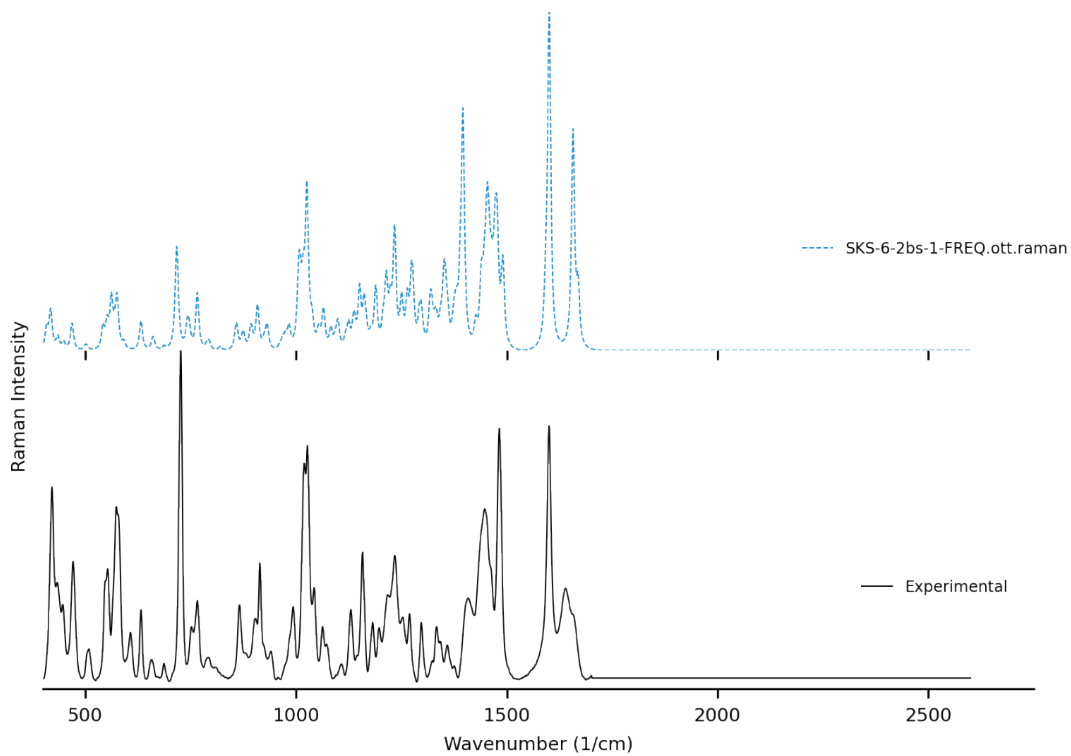
Molecule 19

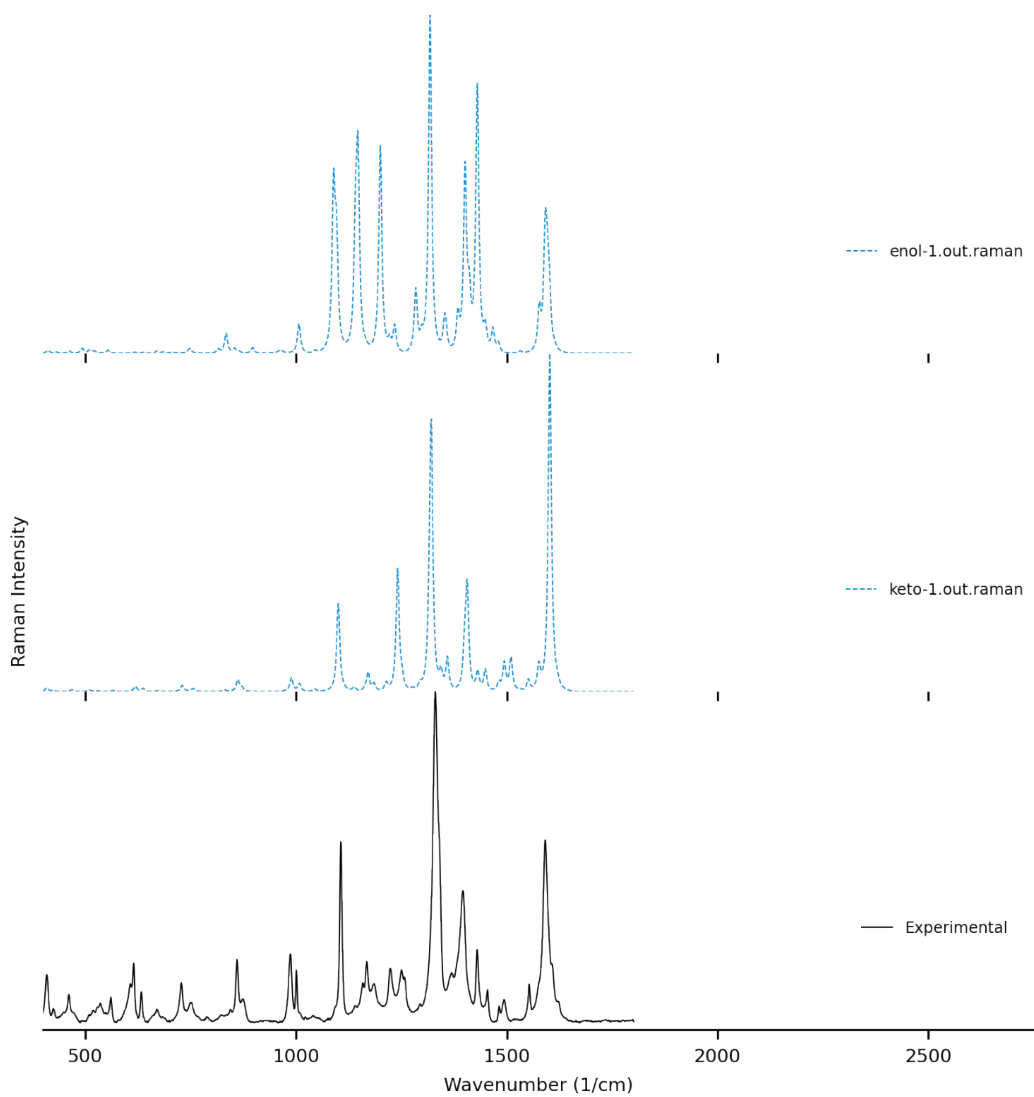


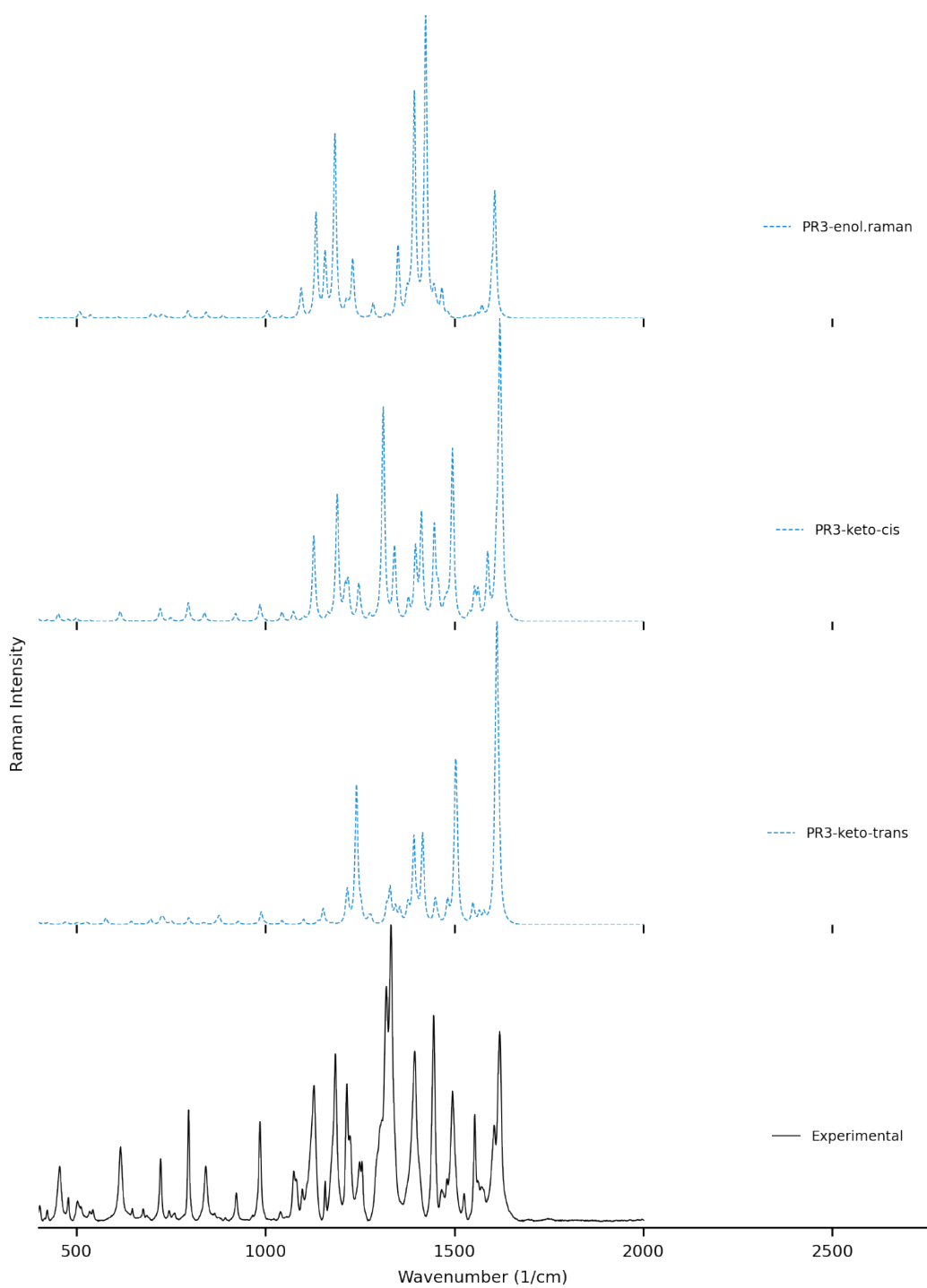
Molecule 20



Molecule 21







5. Materials

The instrument used was a Renishaw inVia microscope (United Kingdom). The following table details the origin of the samples.

Table S1. Suppliers of analyzed powders

Molecule number	Name	Supplier
1	4,4'-di-t-butyl-2,2'-bipyridine	Sigma
2	8-Hydroxyquinoline	EMD (MERCK)
3	Norcamphor	Aldrich
4	Methylparaben	Fisher
5	BHT	Aldrich
6	Gramine	Aldrich
7	Hymecromone	Sigma-Aldrich
8	Nicotinic acid	J.T. Baker
9	Xanthidrol	Anachemia
10	Phenacetin	Anachemia
11	Coumarin	Eastman
12	Pyrixodine	Sigma
13	(+)-Camphor	Aldrich
14	(+)-Borneol	Synthesis
15	(+)-Isoborneol	Synthesis
16	16	Published Synthesis ¹
17	17	Published Synthesis ¹
18	18	Published Synthesis ¹
19	19	Published Synthesis ¹
20	20	Published Synthesis ¹
21	21	Published Synthesis ¹
PR1	PR1	Database ²
PR3	PR3	Database ²

6. Synthesis of Borneol/Isoborneol

To a solution of (+)-Camphor (9.9mg, 0.065mmol) in MeOH (0.5mL) at room temperature is added NaBH₄ (1éq, 2.5mg). The resulting mixture was stirred for 1hour (monitored by TLC). After completion, 1mL of saturated aqueous solution of NH₄Cl was added followed by a dimethyl ether extraction (3x5mL). The organic layers were combined and washed with Brine and dried. Solvent removal in vacuo and column chromatography (8 : 2 Hexane : AcOEt) of the residue afforded the respective alcohols.

Isoborneol/borneol : white solid; m.p. 195,8°C; ¹H NMR (300 MHz, CDCl₃): d=0.81 and 0.84 (2 s, 3H), 0.86 (s, 3H), 0.92 (s, 3H), 1.27–1.38 (m, 3H), 1.62–1.78 (m, 2H), 1.86 (s, 1H), 2.03–2.08 (m, 1H), 2.27–2.36 (m, 1H), 3.43–3.61 (isoborneol) and 3.95–3.97 ppm (borneol) (two m, 1H); ¹³C NMR (75 MHz, CDCl₃): d=11.3, 13.3, 18.6, 20.0, 20.4, 25.8, 27.2, 28.2, 29.6, 33.8, 38.9, 40.3, 45.0, 46.3, 48.9, 49.4, 77.3, 79.8 ppm.

7. Measurement parameters

All the solid powders were placed on a quartz surface and measured using the 50X objective of a Renishaw inVia confocal Raman microscope. Bi-weekly calibration of the wavenumber axis using an internal sample of crystalline silicon ensures proper positioning of the Raman peaks. The 532 nm laser has a maximum power of 50 mW, and the 785 nm laser, of 300 mW.

Table S2. Instrumental parameters for the measurement of Raman spectra

Molecule number	Name	Laser wavelength	Laser intensity	Nb scans	Scan time
1	4,4'-di-t-butyl-2,2'-bipyridine	532 nm	1%	7x	6 m
2	8-Hydroxyquinoline	785 nm	0.50%	4x	2 m
3	Norcamphor	785 nm	0.50%	2x	2 m
4	Methylparaben	785 nm	0.50%	3x	100 s
5	BHT	532 nm	1%	5x	2 m
6	Gramine	532 nm	5%	6x	100 s
7	Hymecromone	785 nm	0.10%	5x	1600 s
8	Nicotinic acid	532 nm	5%	3x	16 s
9	Xanthidrol	785 nm	1%	3x	100 s
10	Phenacetin	785 nm	1%	2x	3 m
11	Coumarin	532 nm	10%	10x	25 s
12	Pyrixodine	785 nm	5%	4x	100 s
13	(+)-Camphor	785 nm	1%	3x	100 s
14	(+)-Borneol	785 nm	1%	2x	100 s
15	(+)-Isoborneol	785 nm	1%	2x	100 s
16	16	785 nm	1%	3x	60 s
17	17	785 nm	1%	8x	100 s
18	18	785 nm	0.05%	20x	800 s
19	19	785 nm	5.00%	14x	2m
20	20	785 nm	0.50%	5x	10 m
21	21	785 nm	5%	35x	100 s

8. SARA Compression function

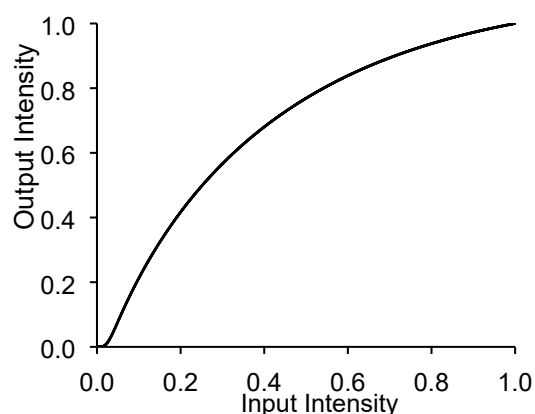


Figure S4. Intensity compression curve used by SARA in the course of its spectral pre-processing.

$$y = 1 - 1.16 (5x + 1.1)^{-0.7(x+1)} + 0.11(46^{-350x^2 - 9.8x - 0.0686})$$

The compression ^(S1) function is implemented in SARA by generating 2000 equally-spaced points along equation (S1) and normalizing each axis with the widely known min-max normalization to ensure that the mapping points are correctly set up from 0 to 1, meaning all spectra have a similar intensity range.

The resulting points shown in **Figure S4** are used by interpolating the spectral input intensity to the corresponding output intensity. The high resolution of the compression curve (2000 points) ensures that no noise is introduced during interpolation.

9. SARA Voigt profile adjustment and DFT functional anharmonic correction

9.1. Voigt Profile adjustment for peak width

Not all DFT software packages which calculate Raman peaks apply peak broadening to generate human-readable spectra. For instance, Gaussian is known to do so, and ORCA has a command line which can generate gaussian-shaped peaks. The SARA software is made with this in mind and will apply an empirically optimized Voigt function to each “datapoint coordinate”-type peak that the ORCA DFT package outputs. The carefully adjusted Voigt profile should generate Raman spectra with strong similarity to those obtained experimentally in most cases. However, in the event that the Raman instrument used produces spectra of drastically different peak width to what the theoretical spectra look like, a variable in the software can be changed to affect the peak width of theoretical spectra.

On line 107 of SARA.py:

```
def gen_from_peaks(data, half_width: int = 60):
```

The numerical value – established at 60 by default - can be changed to a value between 50 and 70. Empirical trial will be necessary to ensure close resemblance between the new peak width and what the chemist sees on their experiment spectra.

9.2. DFT functional anharmonic correction factor of the wavenumbers

Harmonic calculations of molecular frequencies with DFT functionals typically require an anharmonic correction. The amplitude of the scaling factor will change according to the level of theory employed. For this article, r²SCAN-3c had no strongly established correction factor, and 0.98 was used to good effect.

For the chemists who wish to try future levels of theory, the SARA program provides a simple way to change this correction factor.

On line 648 of SARA.py:

```
corrFactor = 0.98 # Anharmonic correction factor, applied on all theoretical frequencies
```

This numerical value can be changed to the appropriate anharmonic correction factor.

10. References

1. Signo K., Canesi S., *Org. Lett.* **2022**, 24, 27, 4939–4942.
2. Fremout, W.; Saverwyns, S., *Journal of Raman spectroscopy*, **2012**, 43.11, 1536-1544.