Supporting Information

Rigid Analogues of Antimitotic Indolobenzazepinones : New Insights into Tubulin Binding via Molecular Modeling

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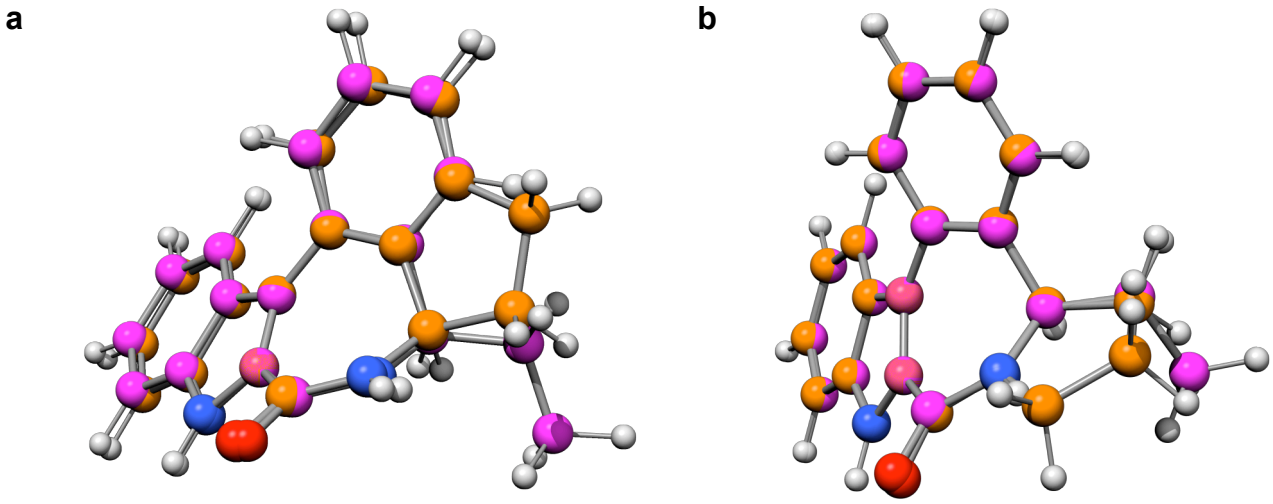

Figure S1. Superposition of the minimized conformations of *aRR*-**4** with *aRR*-**5** (a) and with *aRR*-**6** (b)

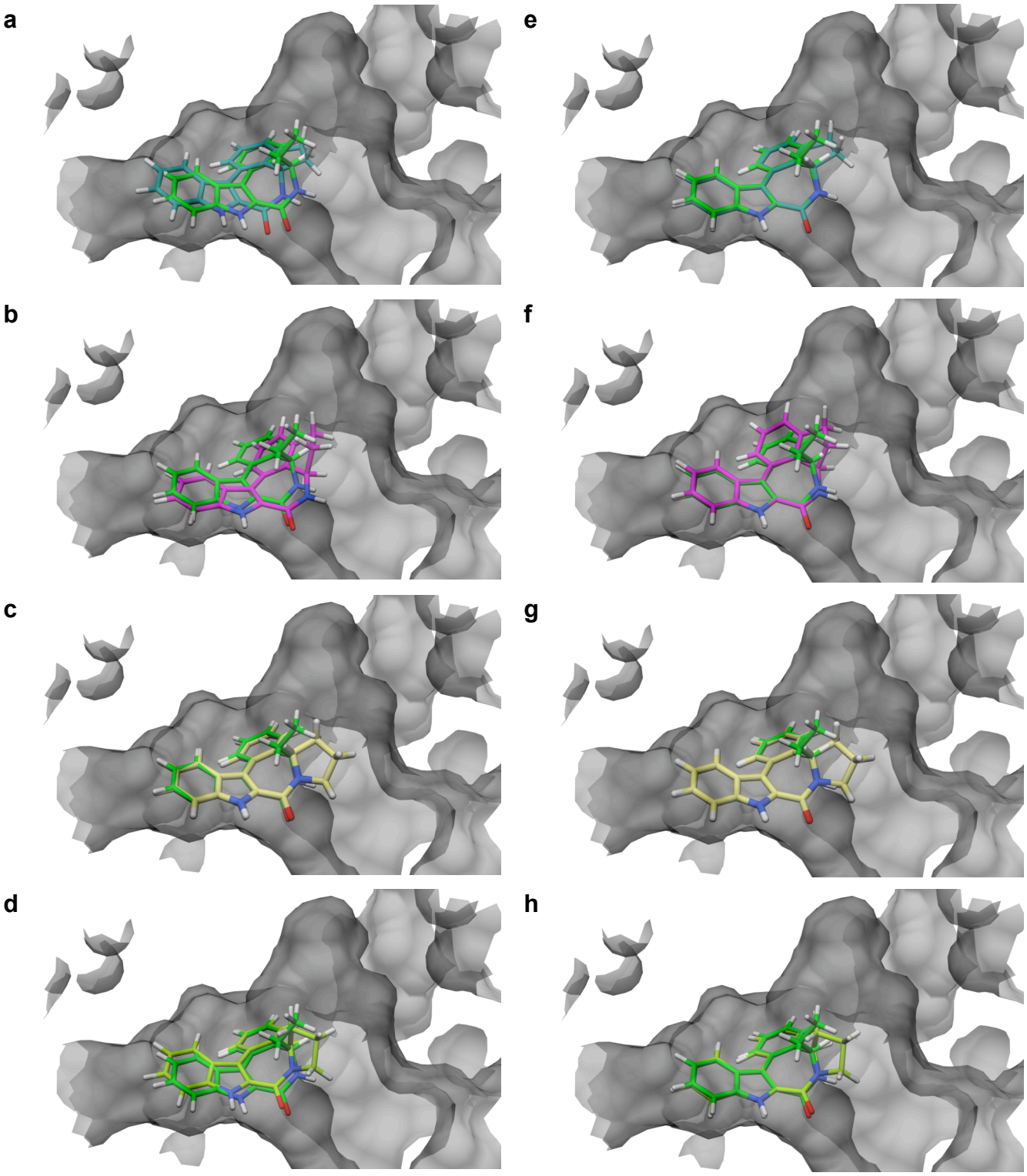

Figure S2. i) Left column : Docked conformations of compounds **5**-*aSS* (a), **5**-*aSR* (b), **6**-*aSS* (c) and **6**-*aSR* (d) in the tubulin binding site, and docked conformation of **4**-*aSR* (green) shown for comparison purposes ; ii) Right column : the same four compounds superimposed on **4**-*aSR* in order to identify potential steric clashes with the protein surface.

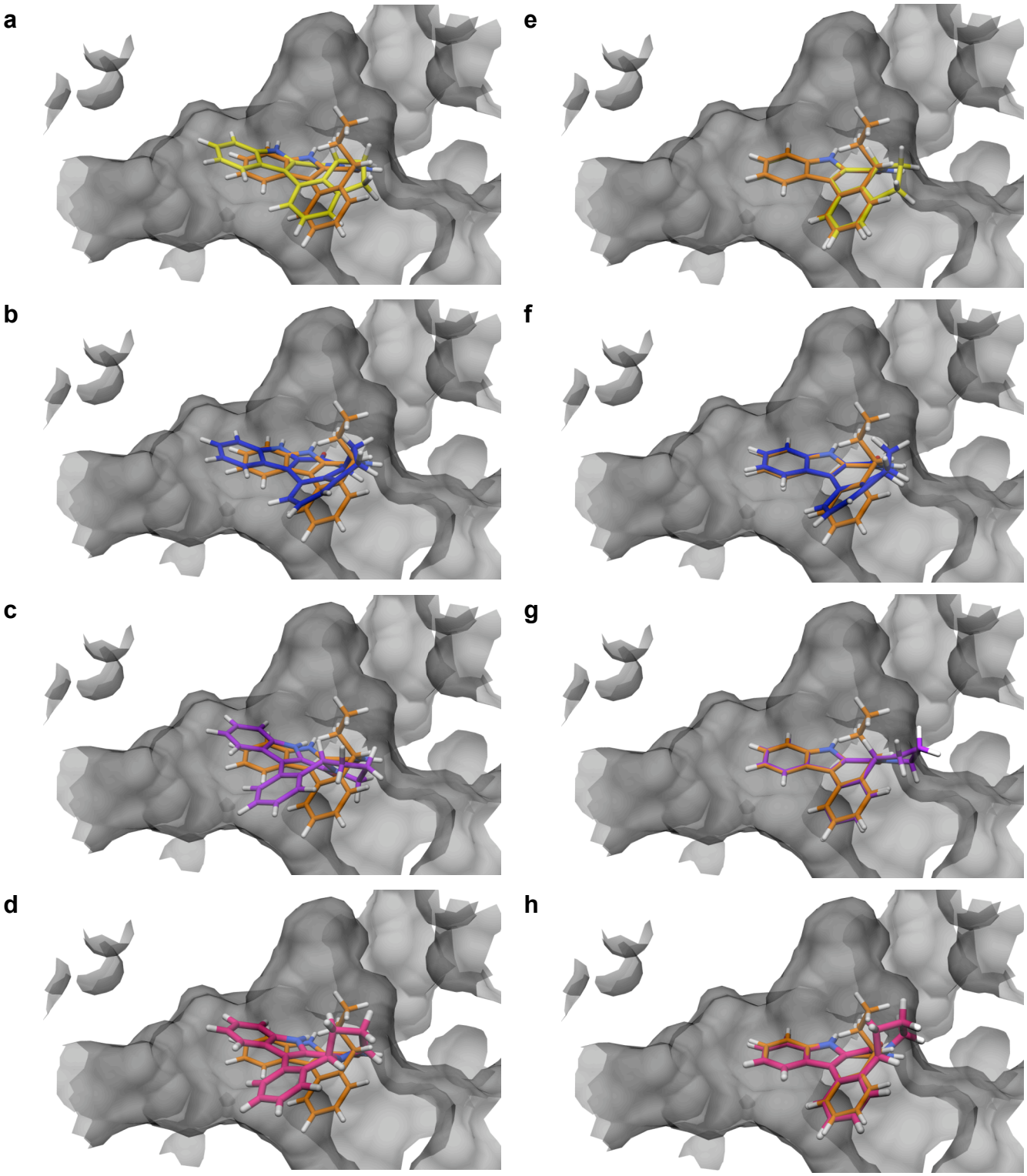

Figure S3. i) Left column : Docked conformations of compounds **5**-*aRR* (a), **5**-*aRS* (b), **6**-*aRR* (c) and **6**-*aRS* (d) in the tubulin binding site, with the docked conformation of **4**-*aRS* as reference (orange) ; ii) Right column : the same compounds superimposed on **4**-*aRS* in order to identify potential steric clashes with the protein surface.

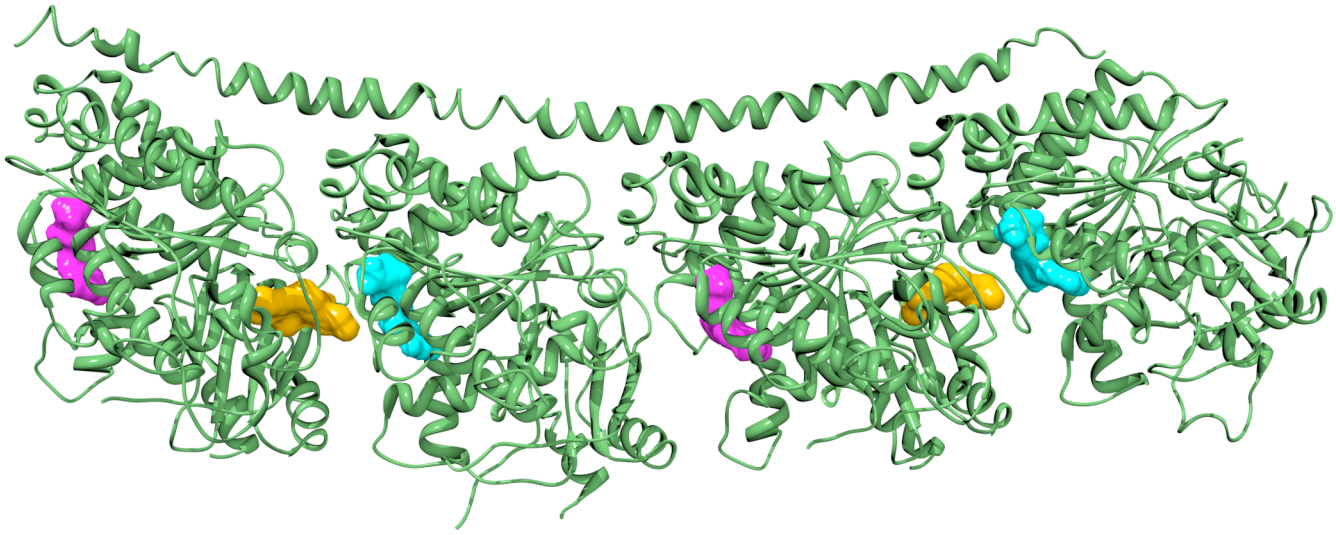

Figure S4. X-ray structure of tubulin (PDB code 1SA0) in a complex with DAMA-colchicine (orange), GDP (magenta) et GTP (cyan)

Theoretical data for compound **5**-*aRR* :

Final Energy in Hartrees: HF = – 873.6395036 (HF/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.571454	-1.784416	0.284644
2	6	0	-3.932638	-1.869472	0.443854
3	6	0	-4.742818	-0.717813	0.392662
4	6	0	-4.197497	0.526346	0.201771
5	6	0	-1.983304	-0.527087	0.060245
6	6	0	-2.808989	0.606180	0.044135
7	7	0	-2.017715	1.699036	-0.114807
8	6	0	-0.712387	1.303625	-0.202538
9	6	0	-0.623202	-0.057201	-0.121633
10	6	0	0.283918	2.380176	-0.414954
11	8	0	-0.090420	3.465814	-0.792319
12	7	0	1.586619	2.112989	-0.183344
13	6	0	2.120857	1.048534	0.658400
14	6	0	1.841187	-0.343125	0.141722
15	6	0	0.606432	-0.863154	-0.237040
16	6	0	3.663972	1.118502	0.663763
17	6	0	2.993530	-1.110018	0.121472
18	6	0	2.962031	-2.415486	-0.341146
19	6	0	1.752686	-2.927788	-0.786730
20	6	0	0.592456	-2.167593	-0.733110
21	6	0	4.159155	-0.339623	0.695804
22	1	0	2.163984	2.914656	-0.315967
23	1	0	-2.300298	2.643280	-0.243470
24	1	0	-1.972062	-2.672218	0.350843
25	1	0	-4.390467	-2.826713	0.617541
26	1	0	-5.806559	-0.817348	0.516817
27	1	0	-4.810842	1.409523	0.179667
28	1	0	1.728421	1.154184	1.669271
29	1	0	3.989111	1.581010	-0.262821
30	1	0	4.045131	1.714846	1.484935
31	1	0	3.853183	-3.018291	-0.364048
32	1	0	1.706713	-3.928667	-1.178542
33	1	0	-0.322278	-2.588995	-1.102903
34	1	0	4.356844	-0.666908	1.713756
35	1	0	5.076534	-0.472564	0.132607

	1	2	3
	A	A	A
Frequencies --	56.2585	82.4238	100.1832
Red. masses --	4.7799	4.0684	6.0807
Frc consts --	0.0089	0.0163	0.0360
IR Inten --	1.8140	0.1685	0.6466
Raman Activ --	2.4979	1.6738	1.9717
Depolar (P) --	0.6626	0.7331	0.7416
Depolar (U) --	0.7970	0.8460	0.8517

Theoretical data for compound **5**-*aSR* :

Final Energy in Hartrees: HF = – 873.6234716 (HF/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.608419	-1.784754	0.240992
2	6	0	3.973659	-1.852035	0.367891
3	6	0	4.777597	-0.704166	0.229329
4	6	0	4.214332	0.521233	-0.011239
5	6	0	1.992024	-0.544613	-0.023117
6	6	0	2.819634	0.583519	-0.117290
7	7	0	2.029299	1.669618	-0.286215
8	6	0	0.716951	1.288220	-0.268950
9	6	0	0.621306	-0.079632	-0.207892
10	6	0	-0.217566	2.423955	-0.048061
11	8	0	0.228589	3.546532	-0.047891
12	7	0	-1.504878	2.184151	0.297893
13	6	0	-2.328634	1.113320	-0.219844
14	6	0	-0.615155	-0.888506	-0.113210
15	6	0	-1.888967	-0.321038	-0.002723
16	6	0	-3.027871	-1.110614	0.088355
17	6	0	-2.952711	-2.489977	-0.002436
18	6	0	-1.715837	-3.059327	-0.248641
19	6	0	-0.578804	-2.269012	-0.330091
20	6	0	-4.280149	-0.265958	0.165364
21	6	0	-3.725563	1.143679	0.412774
22	1	0	-1.990707	3.044632	0.439533
23	1	0	2.297310	2.626249	-0.249881
24	1	0	2.038012	-2.680111	0.379808
25	1	0	4.438801	-2.797280	0.582890
26	1	0	5.845085	-0.791293	0.327178
27	1	0	4.815118	1.408600	-0.102120
28	1	0	-2.433354	1.237481	-1.300903
29	1	0	-3.837065	-3.099399	0.065279
30	1	0	-1.628410	-4.121700	-0.393016
31	1	0	0.348746	-2.746439	-0.563403
32	1	0	-4.959867	-0.590310	0.945897
33	1	0	-4.823751	-0.312851	-0.775973
34	1	0	-3.614600	1.319292	1.478703
35	1	0	-4.350974	1.928718	0.000130

	1	2	3
	A	A	A
Frequencies --	33.4118	82.0824	102.4189
Red. masses --	4.8225	4.2711	7.0762
Frc consts --	0.0032	0.0170	0.0437
IR Inten --	1.4047	0.1879	1.0739
Raman Activ --	0.5736	1.2175	0.8854
Depolar (P) --	0.6829	0.7348	0.7487
Depolar (U) --	0.8116	0.8471	0.8563

Theoretical data for transition state **TS-5**-*aSR*-**5**-*aRR* :

Final Energy in Hartrees: HF = – 873.5958684 (HF / 6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.728075	1.642391	0.452757
2	6	0	-4.102864	1.657608	0.464714
3	6	0	-4.843417	0.496063	0.180447
4	6	0	-4.216677	-0.693873	-0.100985
5	6	0	-2.057810	0.447230	0.147335
6	6	0	-2.820054	-0.701285	-0.109851
7	7	0	-1.957876	-1.741035	-0.323276
8	6	0	-0.676540	-1.281089	-0.199702
9	6	0	-0.663133	0.050882	0.071047
10	6	0	0.484992	-2.207509	-0.327544
11	8	0	0.565561	-2.992033	-1.214521
12	7	0	1.419240	-2.147482	0.740745
13	6	0	2.267011	-0.957868	0.876625
14	6	0	0.556751	0.889981	0.018594
15	6	0	1.830155	0.375147	0.272496
16	6	0	2.971548	1.119811	-0.004480
17	6	0	2.882224	2.419273	-0.469678
18	6	0	1.622525	2.957371	-0.685629
19	6	0	0.483470	2.199492	-0.464424
20	6	0	4.221699	0.307793	0.258724
21	6	0	3.679298	-1.128813	0.306040
22	1	0	0.892241	-2.253198	1.584359
23	1	0	-2.199137	-2.664286	-0.598227
24	1	0	-2.182396	2.535107	0.694490
25	1	0	-4.623372	2.568382	0.700666
26	1	0	-5.917920	0.539546	0.192948
27	1	0	-4.780113	-1.587217	-0.304936
28	1	0	2.360099	-0.803367	1.949326
29	1	0	3.767566	2.993849	-0.679900
30	1	0	1.522610	3.959060	-1.065145
31	1	0	-0.470922	2.617327	-0.719446
32	1	0	4.980437	0.454541	-0.502096
33	1	0	4.663007	0.585461	1.214919
34	1	0	3.608696	-1.540009	-0.696679
35	1	0	4.278557	-1.804936	0.904687

	1	2	3
	A	A	A
Frequencies --	-61.9481	46.3011	94.1083
Red. masses --	5.9251	4.8604	5.1449
Frc consts --	0.0134	0.0061	0.0268
IR Inten --	1.5172	1.8189	1.4449
Raman Activ --	2.2350	1.8818	2.9420
Depolar (P) --	0.5104	0.6148	0.7173
Depolar (U) --	0.6759	0.7615	0.8354

Theoretical data for compound **6**-*aRR* :

Final Energy in Hartrees: HF = – 912.6686034 (HF / 6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.090993	1.307003	0.413456
2	6	0	4.433688	1.044857	0.542885
3	6	0	4.935234	-0.261195	0.384216
4	6	0	4.099441	-1.316416	0.113161
5	6	0	2.213179	0.252798	0.112773
6	6	0	2.733939	-1.042958	-0.014629
7	7	0	1.693629	-1.893067	-0.238570
8	6	0	0.529296	-1.179590	-0.258713
9	6	0	0.777047	0.147706	-0.066455
10	6	0	-0.727932	-1.914288	-0.533862
11	8	0	-0.695670	-2.975925	-1.115686
12	7	0	-1.860851	-1.342846	-0.098502
13	6	0	-1.913474	-0.263902	0.901124
14	6	0	-1.534185	1.076513	0.289397
15	6	0	-0.211228	1.244782	-0.151362
16	6	0	-3.336342	-0.423598	1.458463
17	6	0	-2.430822	2.128008	0.148300
18	6	0	-2.046207	3.334820	-0.415849
19	6	0	-0.745861	3.498516	-0.859662
20	6	0	0.158148	2.458243	-0.730755
21	6	0	-4.141354	-1.003183	0.293285
22	6	0	-3.153982	-1.974093	-0.349671
23	1	0	1.737108	-2.859290	-0.467345
24	1	0	2.723909	2.306152	0.557179
25	1	0	5.113880	1.844735	0.774656
26	1	0	5.991642	-0.435057	0.487517
27	1	0	4.478675	-2.317355	0.007636
28	1	0	-1.191145	-0.475051	1.681676
29	1	0	-3.301509	-1.149176	2.265751
30	1	0	-3.743765	0.489301	1.869956
31	1	0	-3.446652	2.018973	0.477264
32	1	0	-2.760278	4.133313	-0.511614
33	1	0	-0.437152	4.423271	-1.313839
34	1	0	1.154634	2.579083	-1.111309
35	1	0	-5.051296	-1.496473	0.615006
36	1	0	-4.414036	-0.224034	-0.411441
37	1	0	-3.188602	-2.953209	0.119059
38	1	0	-3.306976	-2.110530	-1.411767

	1	2	3
	A	A	A
Frequencies --	59.1014	82.6892	96.3385
Red. masses --	5.1566	4.0363	4.8224
Frc consts --	0.0106	0.0163	0.0264
IR Inten --	1.8625	0.5471	0.1135
Raman Activ --	2.7605	1.5943	3.2462
Depolar (P) --	0.6944	0.7220	0.6596
Depolar (U) --	0.8196	0.8385	0.7949

Theoretical data for compound **6**-*aSR* :

Final Energy in Hartrees: HF = – 912.6473596 (HF / 6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.983524	1.144271	0.597139
2	6	0	-4.281745	0.758552	0.824166
3	6	0	-4.708738	-0.554179	0.540919
4	6	0	-3.839070	-1.494250	0.048874
5	6	0	-2.071698	0.209805	0.075652
6	6	0	-2.514691	-1.097173	-0.170490
7	7	0	-1.451348	-1.823566	-0.599930
8	6	0	-0.336723	-1.028459	-0.624499
9	6	0	-0.661458	0.241495	-0.260401
10	6	0	0.934628	-1.741483	-0.897739
11	8	0	0.857072	-2.860984	-1.347273
12	7	0	2.132011	-1.187761	-0.556398
13	6	0	2.353949	-0.005448	0.291323
14	6	0	0.238645	1.406565	-0.230115
15	6	0	1.608735	1.286276	0.016280
16	6	0	2.393443	2.439219	-0.003515
17	6	0	1.862870	3.686440	-0.278055
18	6	0	0.516698	3.793194	-0.584591
19	6	0	-0.274657	2.660604	-0.573317
20	6	0	3.144675	-2.130439	-0.064123
21	6	0	2.376566	-0.600544	1.707376
22	6	0	3.117941	-1.941354	1.478204
23	1	0	-1.427693	-2.782996	-0.857501
24	1	0	-2.674646	2.144286	0.836774
25	1	0	-4.985052	1.464174	1.228586
26	1	0	-5.733538	-0.824517	0.724248
27	1	0	-4.158587	-2.500883	-0.154341
28	1	0	3.383868	0.245741	0.067804
29	1	0	3.448857	2.356794	0.189818
30	1	0	2.498236	4.553882	-0.281307
31	1	0	0.088435	4.744435	-0.846013
32	1	0	-1.307765	2.742771	-0.851092
33	1	0	4.124213	-1.917454	1.882678
34	1	0	2.597847	-2.764277	1.954984
35	1	0	2.909163	-3.130382	-0.383929
36	1	0	4.107991	-1.854733	-0.477579
37	1	0	2.885115	0.050989	2.409082
38	1	0	1.367250	-0.759215	2.071743

	1	2	3
	A	A	A
Frequencies --	43.8089	75.9148	92.6179
Red. masses --	4.5584	3.9920	4.5953
Frc consts --	0.0052	0.0136	0.0232
IR Inten --	1.6041	0.1916	1.2054
Raman Activ --	3.0481	2.1709	2.3524
Depolar (P) --	0.6804	0.7136	0.7404
Depolar (U) --	0.8098	0.8329	0.8508

Theoretical data for transition state **TS-6**-*aSR*-**6**-*aRR* :

Final Energy in Hartrees: HF = – 912.6429966 (HF / 6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.209255	1.152577	0.429322
2	6	0	-4.530992	0.790550	0.519779
3	6	0	-4.948009	-0.527543	0.259138
4	6	0	-4.033762	-1.495351	-0.062894
5	6	0	-2.239176	0.196021	0.060844
6	6	0	-2.687845	-1.119034	-0.138176
7	7	0	-1.608286	-1.902007	-0.368333
8	6	0	-0.475567	-1.145227	-0.305145
9	6	0	-0.782475	0.167552	-0.095570
10	6	0	0.771342	-1.940870	-0.272686
11	8	0	0.668579	-3.145751	-0.369487
12	7	0	1.952038	-1.365904	0.006886
13	6	0	2.450184	-0.010383	-0.250671
14	6	0	1.558337	1.229714	-0.111044
15	6	0	0.154217	1.318304	-0.110049
16	6	0	3.686978	-0.001180	0.667003
17	6	0	2.291007	2.421570	-0.148823
18	6	0	1.708504	3.671268	-0.189475
19	6	0	0.330328	3.758064	-0.233104
20	6	0	-0.412220	2.597814	-0.205530
21	6	0	4.281985	-1.392391	0.472990
22	6	0	3.069145	-2.294047	0.232693
23	1	0	-1.574349	-2.893383	-0.431180
24	1	0	-2.947596	2.158946	0.683265
25	1	0	-5.259889	1.526703	0.807791
26	1	0	-5.991167	-0.778730	0.332428
27	1	0	-4.330547	-2.513951	-0.239390
28	1	0	2.803388	0.010165	-1.283781
29	1	0	4.398807	0.773142	0.421970
30	1	0	3.359344	0.149359	1.690993
31	1	0	3.361429	2.377147	-0.174081
32	1	0	2.324418	4.552204	-0.215859
33	1	0	-0.164577	4.709847	-0.307465
34	1	0	-1.469313	2.686835	-0.305998
35	1	0	4.936970	-1.398129	-0.392693
36	1	0	4.868066	-1.715934	1.324975
37	1	0	3.199561	-2.948025	-0.620455
38	1	0	2.834199	-2.919271	1.083902

	1	2	3
	A	A	A
Frequencies --	-45.2695	55.0789	64.5995
Red. masses --	3.4149	4.1182	3.8350
Frc consts --	0.0041	0.0074	0.0094
IR Inten --	0.8937	0.5008	0.1079
Raman Activ --	0.4907	0.9488	2.1462
Depolar (P) --	0.6819	0.7412	0.7487
Depolar (U) --	0.8109	0.8514	0.8563

Theoretical data for compound **4**-*aRR* :

Final Energy in Hartrees: HF = – 874.8004089 (HF/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.796793	1.362202	0.675360
2	6	0	4.136249	1.162611	0.906287
3	6	0	4.736126	-0.086799	0.655846
4	6	0	4.001372	-1.149094	0.190747
5	6	0	2.022394	0.301537	0.177023
6	6	0	2.637651	-0.939814	-0.039860
7	7	0	1.681754	-1.815478	-0.456788
8	6	0	0.479242	-1.169787	-0.512005
9	6	0	0.619034	0.138182	-0.151923
10	6	0	-0.699796	-1.927294	-0.988171
11	8	0	-0.561581	-2.905456	-1.684200
12	7	0	-1.900749	-1.464970	-0.593495
13	6	0	-2.126158	-0.524252	0.503978
14	6	0	-1.771801	0.893172	0.075366
15	6	0	-0.428477	1.181410	-0.215036
16	6	0	-3.546372	-0.715622	1.042059
17	6	0	-2.720657	1.900609	-0.046766
18	6	0	-2.366598	3.180538	-0.445450
19	6	0	-1.044562	3.464174	-0.739598
20	6	0	-0.088788	2.469003	-0.628729
21	6	0	-3.769116	-2.081034	1.695516
22	1	0	-2.676790	-1.962034	-0.971066
23	1	0	1.811286	-2.745553	-0.782336
24	1	0	2.351888	2.315938	0.890166
25	1	0	4.737851	1.967236	1.289377
26	1	0	5.787964	-0.211717	0.842658
27	1	0	4.454839	-2.108229	0.014176
28	1	0	-1.443217	-0.790013	1.305528
29	1	0	-4.269217	-0.567003	0.242589
30	1	0	-3.732935	0.057033	1.779975
31	1	0	-3.752458	1.697820	0.168839
32	1	0	-3.120242	3.943013	-0.530784
33	1	0	-0.757595	4.448236	-1.065170
34	1	0	0.928053	2.686202	-0.895761
35	1	0	-4.778916	-2.148151	2.087329
36	1	0	-3.632087	-2.901514	0.999465
37	1	0	-3.082021	-2.232931	2.522734

	1	2	3
	A	A	A
Frequencies --	52.4155	80.6625	98.3238
Red. masses --	4.7386	4.2034	5.7476
Frc consts --	0.0077	0.0161	0.0327
IR Inten --	0.9051	0.5968	0.3558
Raman Activ --	3.6195	2.3291	2.7604
Depolar (P) --	0.7060	0.7488	0.7082
Depolar (U) --	0.8277	0.8563	0.8292

Theoretical data for compound **4**-*aSR* :

Final Energy in Hartrees: HF = – 874.8001742 (HF/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.540266	1.546561	0.622533
2	6	0	-3.890395	1.429692	0.845890
3	6	0	-4.574624	0.235703	0.545045
4	6	0	-3.912712	-0.854690	0.039105
5	6	0	-1.837165	0.456907	0.080137
6	6	0	-2.536425	-0.730669	-0.180950
7	7	0	-1.642576	-1.654563	-0.624705
8	6	0	-0.397324	-1.092558	-0.657576
9	6	0	-0.447463	0.207600	-0.255414
10	6	0	0.718669	-1.949500	-1.110138
11	8	0	0.488991	-2.943662	-1.758981
12	7	0	1.969433	-1.586823	-0.763745
13	6	0	2.386419	-0.662305	0.291960
14	6	0	1.997096	0.776971	-0.006457
15	6	0	0.673746	1.171075	-0.248224
16	6	0	1.997417	-1.113715	1.712643
17	6	0	3.004859	1.734383	-0.032661
18	6	0	2.736513	3.067623	-0.295384
19	6	0	1.434583	3.454805	-0.561110
20	6	0	0.421503	2.512239	-0.542175
21	6	0	2.522895	-2.503112	2.071804
22	1	0	2.659543	-2.215474	-1.110756
23	1	0	-1.829871	-2.568315	-0.968095
24	1	0	-2.034484	2.458274	0.879015
25	1	0	-4.435741	2.257393	1.262532
26	1	0	-5.633094	0.176129	0.726521
27	1	0	-4.429225	-1.773427	-0.175005
28	1	0	3.467562	-0.697631	0.243768
29	1	0	0.921685	-1.080914	1.839145
30	1	0	2.410698	-0.380779	2.400387
31	1	0	4.020994	1.432041	0.153986
32	1	0	3.535651	3.787085	-0.306424
33	1	0	1.206719	4.479832	-0.793590
34	1	0	-0.577487	2.816597	-0.788608
35	1	0	2.278036	-2.744651	3.101134
36	1	0	2.090521	-3.273108	1.441773
37	1	0	3.604599	-2.556114	1.971048

	1	2	3
	A	A	A
Frequencies --	50.6530	73.7464	87.0924
Red. masses --	4.3435	3.8583	3.2548
Frc consts --	0.0066	0.0124	0.0145
IR Inten --	0.7293	0.0649	1.1401
Raman Activ --	3.1283	2.9578	0.8659
Depolar (P) --	0.6870	0.7466	0.7117
Depolar (U) --	0.8145	0.8549	0.8316

Theoretical data for transition state **TS-4**-*aSR*-**4**-*aRR* :

Final Energy in Hartrees: HF = – 874.7735554 (HF/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.970627	1.375211	0.133151
2	6	0	4.329382	1.189047	0.201940
3	6	0	4.894723	-0.097752	0.121673
4	6	0	4.098850	-1.206872	0.002770
5	6	0	2.120144	0.262887	-0.029054
6	6	0	2.714277	-1.008797	-0.053923
7	7	0	1.724951	-1.933195	-0.101997
8	6	0	0.517455	-1.299771	-0.102389
9	6	0	0.676326	0.050376	-0.099659
10	6	0	-0.656160	-2.181624	-0.023315
11	8	0	-0.492115	-3.377445	-0.141676
12	7	0	-1.879734	-1.687735	0.213991
13	6	0	-2.506463	-0.393914	0.480369
14	6	0	-1.716410	0.908971	0.261843
15	6	0	-0.379059	1.089506	-0.128769
16	6	0	-3.792163	-0.381806	-0.390088
17	6	0	-2.485719	2.059726	0.474670
18	6	0	-2.044404	3.331231	0.175360
19	6	0	-0.791365	3.484017	-0.393072
20	6	0	0.015852	2.376403	-0.526350
21	6	0	-4.784918	-1.508996	-0.087492
22	1	0	-2.522631	-2.444055	0.285191
23	1	0	1.806305	-2.923739	-0.112059
24	1	0	2.582127	2.368430	0.234729
25	1	0	4.973945	2.040099	0.329944
26	1	0	5.963147	-0.210295	0.171960
27	1	0	4.516526	-2.197302	-0.033212
28	1	0	-2.809353	-0.401746	1.526030
29	1	0	-3.488088	-0.421568	-1.432034
30	1	0	-4.313455	0.553401	-0.253528
31	1	0	-3.471178	1.958157	0.888621
32	1	0	-2.680542	4.178792	0.356895
33	1	0	-0.438281	4.449864	-0.707330
34	1	0	0.984318	2.500104	-0.962877
35	1	0	-5.712363	-1.328824	-0.620972
36	1	0	-4.433998	-2.486660	-0.400696
37	1	0	-5.021912	-1.555644	0.972794

	1	2	3
	A	A	A
Frequencies --	-77.7639	48.3497	73.3962
Red. masses --	3.5701	4.4888	2.1773
Frc consts --	0.0127	0.0062	0.0069
IR Inten --	0.4427	0.3561	0.1192
Raman Activ --	0.3704	1.3923	0.3214
Depolar (P) --	0.5955	0.6794	0.6101
Depolar (U) --	0.7464	0.8091	0.7578