Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

TD-DFT CALCULATIONS OF UV ABSOPTION BANDS AND THEIR INTENSITIES IN THE SPECTRA OF SOME TETRAHYDROQUINOLINES.

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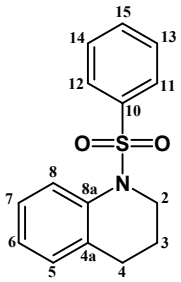
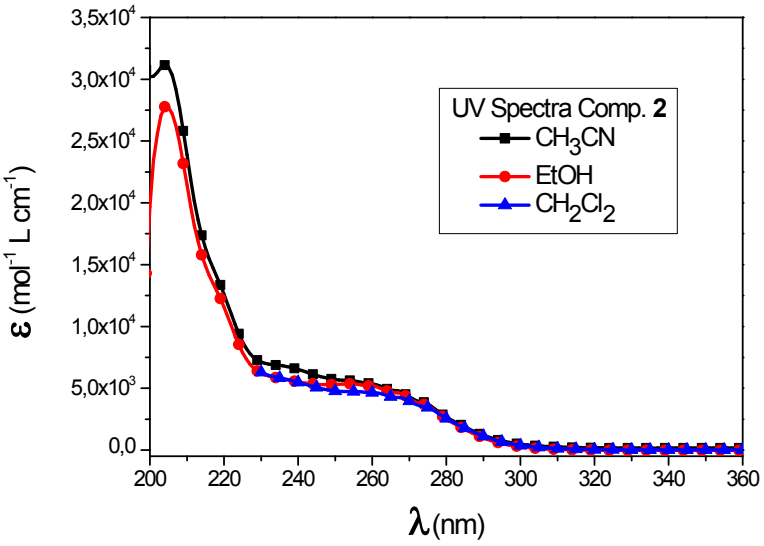
Table of Contents

1-(benzenesulfonyl)-1,2,3,4-tetrahydroquinoline



1-(phenylsulfonyl)-1,2,3,4-tetrahydroquinoline

UV Spectra:



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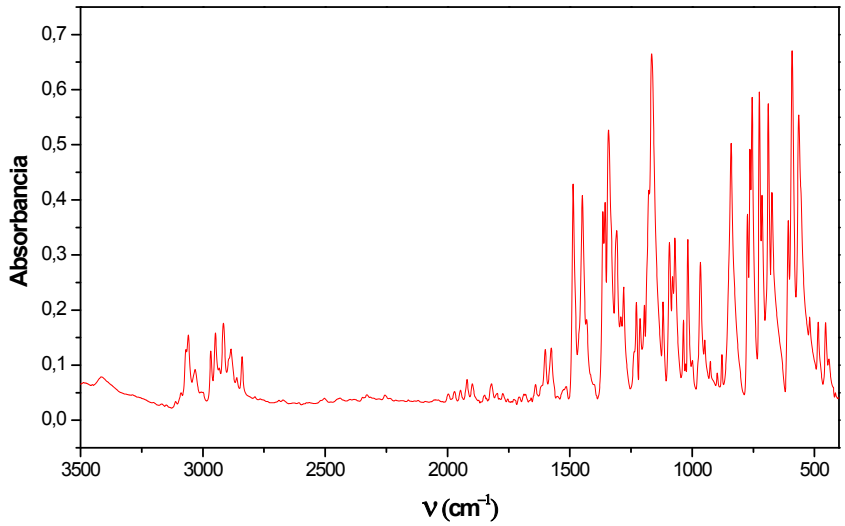
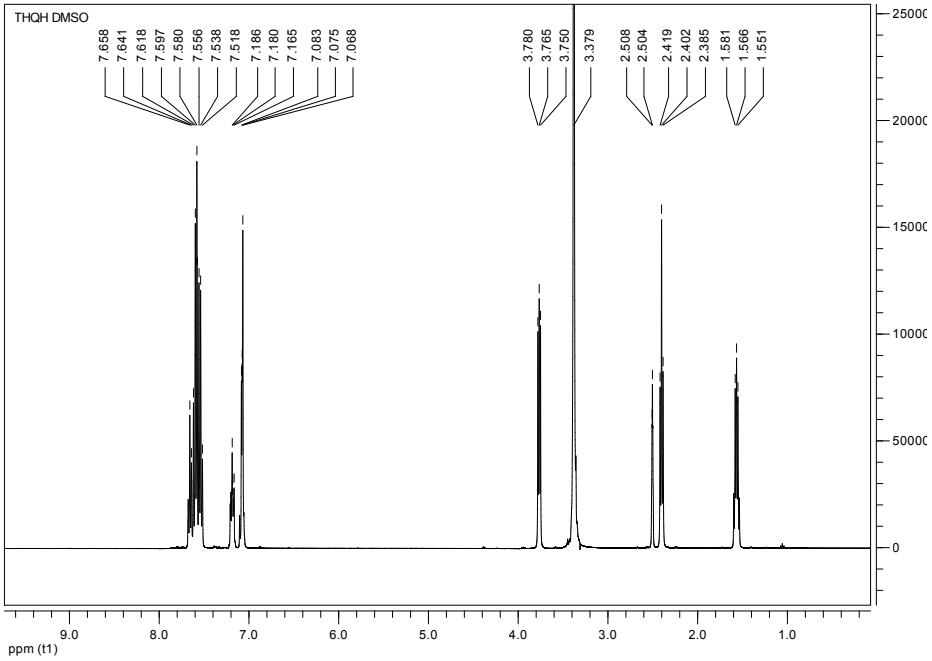
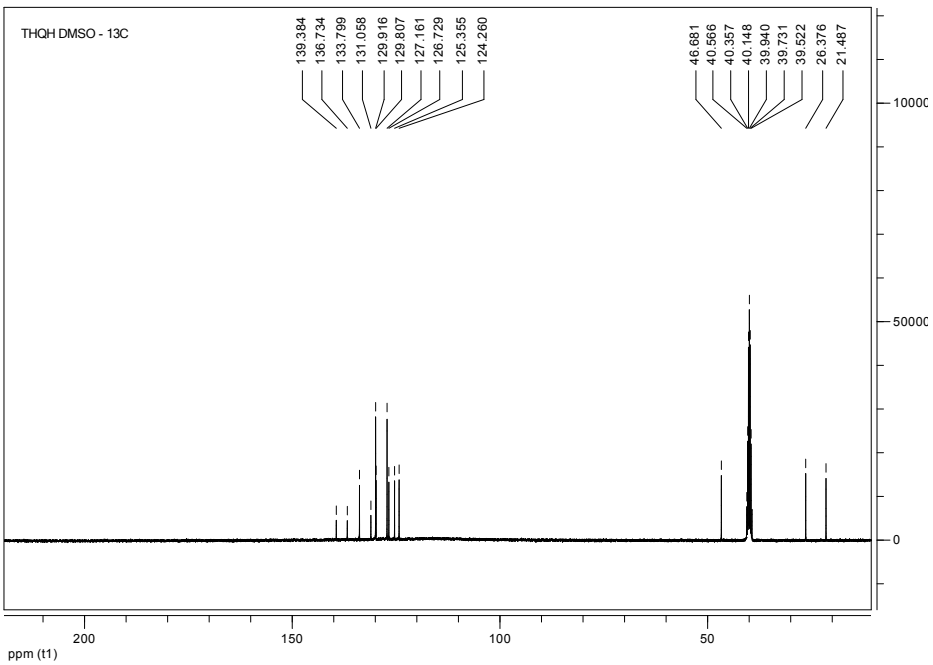
219	14200	220	12800	-	-
237	7190	236	7070	238	6400
258	5790	258	6550	255	5200
271	4350	271	5020	276	3800

IR (υ_{max}/cm^{-1}): 2916, 2840 (CH sp^3), 1342 ($SO_{2\ as}$), 1166 ($SO_{2\ sim}$).
^{1}H NMR: 7.66 (tt,1H, 7.2 and 1.2 Hz, H15); 7.63 (d,1H, 8.0 Hz, H8); 7.59 (dd, 2H, 8.0 and 1.2 Hz, H11 and H12); 7.54 (td, 2H, 8.0 and 1.2 Hz, H13 and H14); 7.19 (ddd, 1H, 8.8, 6.0 and 2.8 Hz, H7); 7.08 (m,2H, H5 and H6); 3,76 (t, 2H, 6.0 Hz, H2); 2.40 (t,2H, 6.6 Hz,H4); 1.57 (quint, 2H, 6.6 Hz, H3).
^{13}C NMR (assigned using HSQC): 139.4 (C10); 136.7 (C8a); 133.8 (C15); 131.05 (C4a); 129.9 (C13 and C14); 129.8 (C5); 127.2 (C11 and C12); 126.7 (C7); 125.3 (C6); 124.3 (C8); 46.7 (C2); 26.4 (C4); 21.9 (C3).
COSY: $^3J_{vec}$:H2-H3; H3-H4. $^3J_{ortho}$: H6-H7; H5-H6; H7-H8; H11/12-H13/14; H13/14-H15. $^4J_{meta}$: H5-H7; H6-H8; H11/12-H15.
HMBC (f_1 =400.16 MHz, f_2 =100.62 MHz) (C→H): C4→H5, H3; C3→H2, H4; C2→H4, H3; C6→H8; C7→H5; C8→H6; C5→H7, H4; C4a→H8, H6, H4, H3; C8a→H7, H5, H2, H4; C10→H13, H14; C11→H15, H13, H14; C12→H15, H13, H14; C13→H11, H12; C14→H11, H12; C15→H11, H12.


Absorbancia
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0,0
3500
3000
2500
2000
1500
1000
500
ν (cm⁻¹)


THQH DMSO
7.658
7.641
7.618
7.597
7.580
7.556
7.538
7.518
7.186
7.180
7.165
7.083
7.075
7.068
3.780
3.765
3.750
3.379
2.508
2.504
2.419
2.402
2.385
1.581
1.566
1.551
25000
20000
15000
10000
5000
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


THQH DMSO - 13C
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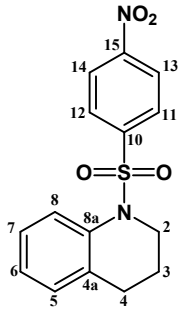
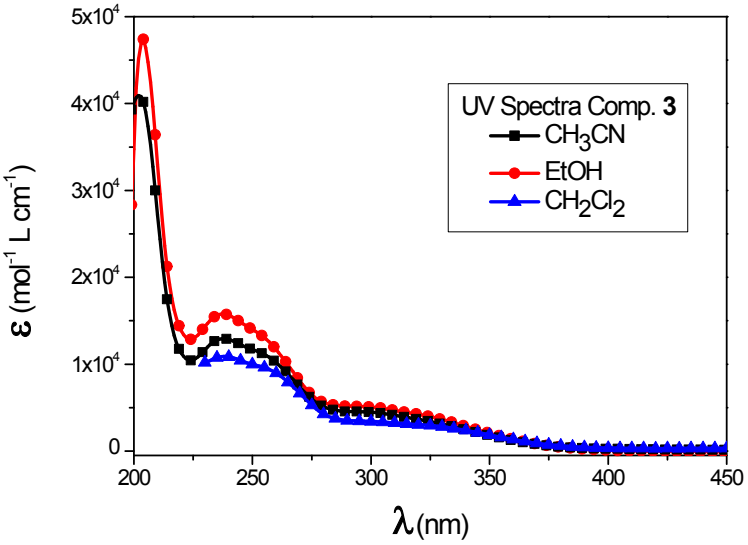
136.734
133.799
131.058
129.916
129.807
127.161
126.729
125.355
124.260
46.681
40.566
40.357
40.148
39.940
39.731
39.522
26.376
21.487
10000
5000
0
200
150
100
50
ppm (t1)

1-(4-nitro-benzenesulfonyl)-1,2,3,4-tetrahydroquinoline



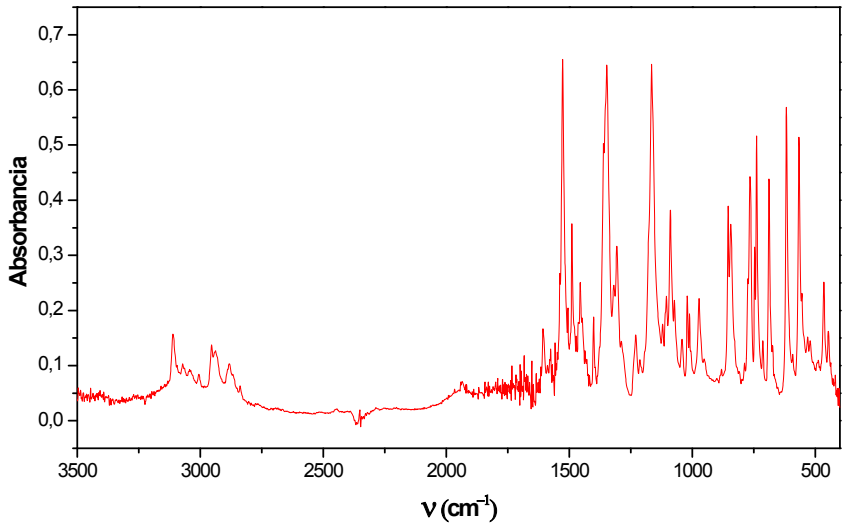
1-(4-nitrophenylsulfonyl)-1,2,3,4-tetrahydroquinoline

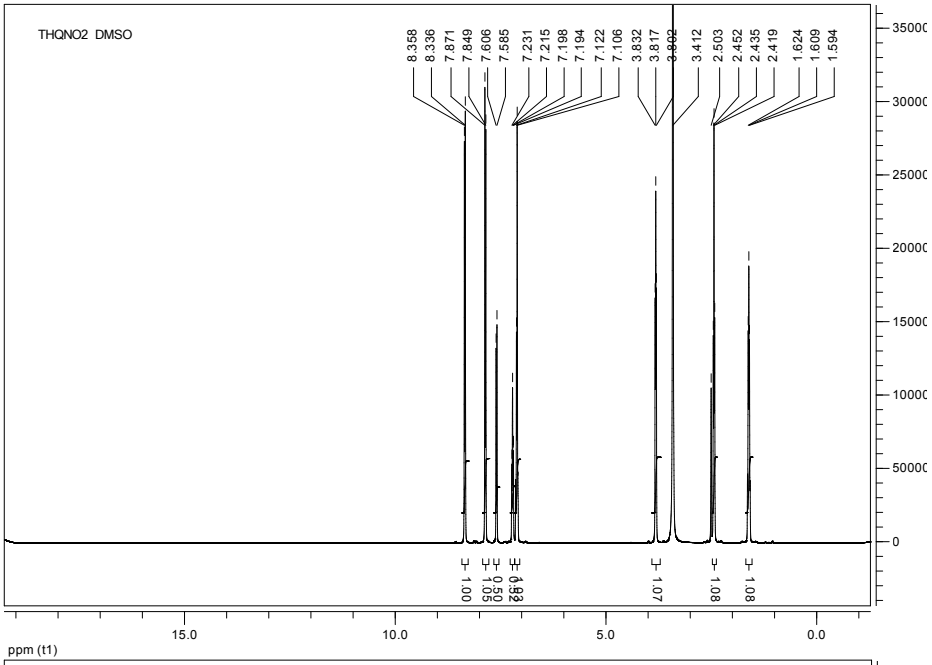
UV Spectra:

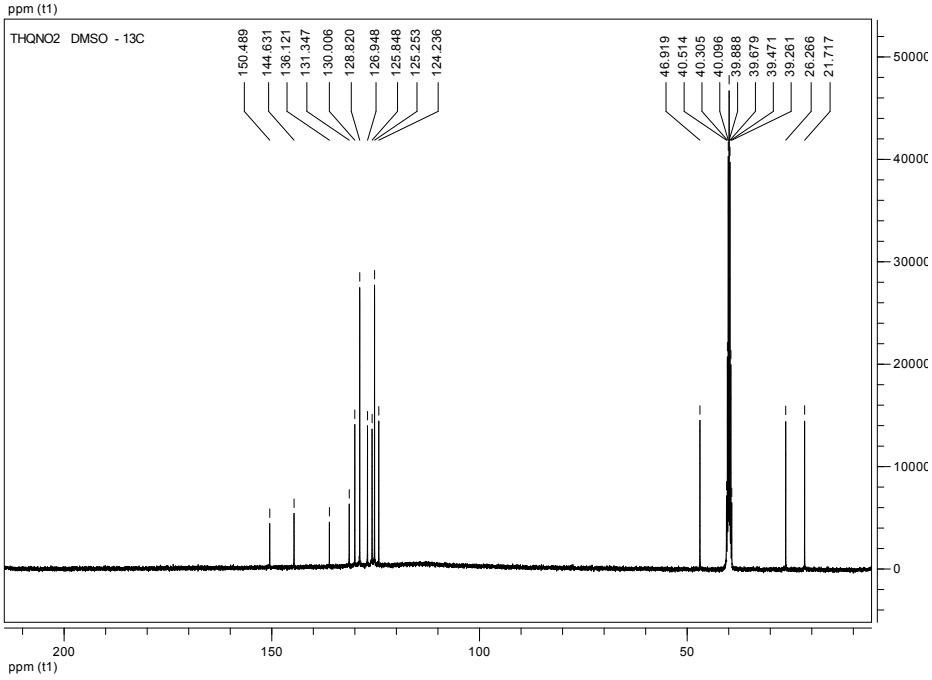


ACN		EtOH		DCM	
λ (nm)	ξ ($M^{-1}cm^{-1}$)	λ (nm)	ξ ($M^{-1}cm^{-1}$)	λ (nm)	ξ ($M^{-1}cm^{-1}$)
202	39000	204	41000	-	-
238	13240	237	15500	238	14500
253	11630	253	14700	255	13300
257	10910	256	13000	260	12400
294	4590	292	5060	294	4580
302	4540	298	4740	297	4800
305	4440	304	4620	304	4690
310	4300	311	4510	309	4460

IR (υ_{max}/cm^{-1}): 2972, 2938 (CH sp^3), 1527 ($NO_{2\ as}$), 1347 ($SO_{2\ as}$), 1306 ($NO_{2\ sim}$), 1165 ($SO_{2\ sim}$).
^{1}H NMR: 8.35 (d, 2H, 8.8 Hz, H13 and H14), 7.86 (d, 2H, 8.8 Hz, H11 and H12); 7.60 (d, 1H, 8.0 Hz, H8); 7.21 (td, 1H, 8.4 and 2.0 Hz, H7); 7.11 (m, 2H, H5 and H6); 3.82 (t, 2H, 6.0 Hz, H2); 2.44(t, 2H, 6.6 Hz, H4); 1.61(quint, 2H, 6.3 Hz, H3).
^{13}C NMR (assigned using HSQC): 150.5 (C15); 144.6 (C10); 136.1 (C8a); 131.3 (C4a); 130.0 (C5); 128.8 (C11 and C12); 126.9 (C7); 125.8 (C6); 125.3 (C13 and C14); 124.3 (C8); 47.0 (C2); 26.3 (C4); 21.7 (C3).
COSY: $^3J_{vec}$:H2-H3; H3-H4. $^3J_{ortho}$: H6-H7; H5-H6; H7-H8; H11/12-H13/14. $^4J_{meta}$: H5-H7; H6-H8.
HMBC (f_1 =400.16 MHz, f_2 =100.62 MHz) (C→H): C4→H5, H3; C3→H2, H4; C2→H4, H3; C6→H8; C7→H5; C8→H6; C5→H7, H4; C4a→H8, H6, H4, H3; C8a→H7, H5, H2, H4; C10→H11, H12, H13, H14; C11→H13, H14; C12→H13, H14; C13→H11, H12; C14→H11, H12; C15→H11, H12.


Absorbancia
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0,0
3500
3000
2500
2000
1500
1000
500
ν (cm⁻¹)


THQNO2 DMSO
8.358
8.336
7.871
7.849
7.606
7.585
7.231
7.215
7.198
7.194
7.122
7.106
3.832
3.817
3.412
2.503
2.452
2.435
2.419
1.624
1.609
1.594
1.00
1.07
1.80
1.08
15.0
10.0
5.0
0.0
ppm (t1)


THQNO2 DMSO - 13C
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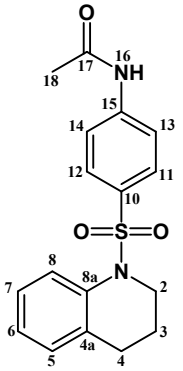
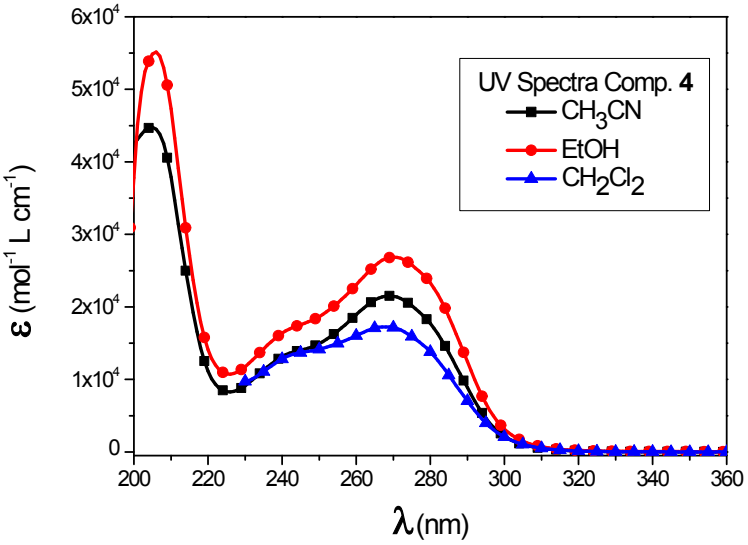
144.631
136.121
131.347
130.006
128.820
126.948
125.848
125.253
124.236
46.919
40.514
40.305
40.096
39.888
39.679
39.471
39.261
26.266
21.717
200
150
100
50
ppm (t1)

1-(4-acetamide-benzenesulfonyl)-1,2,3,4-tetrahydroquinoline



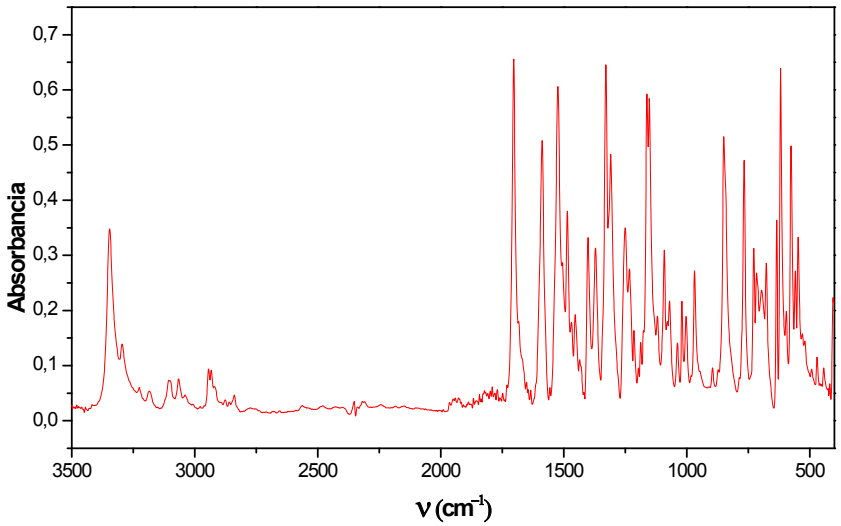
N-(4-(3,4-dihydroquinolin-1(2*H*)-ylsulfonyl)phenyl)acetamide

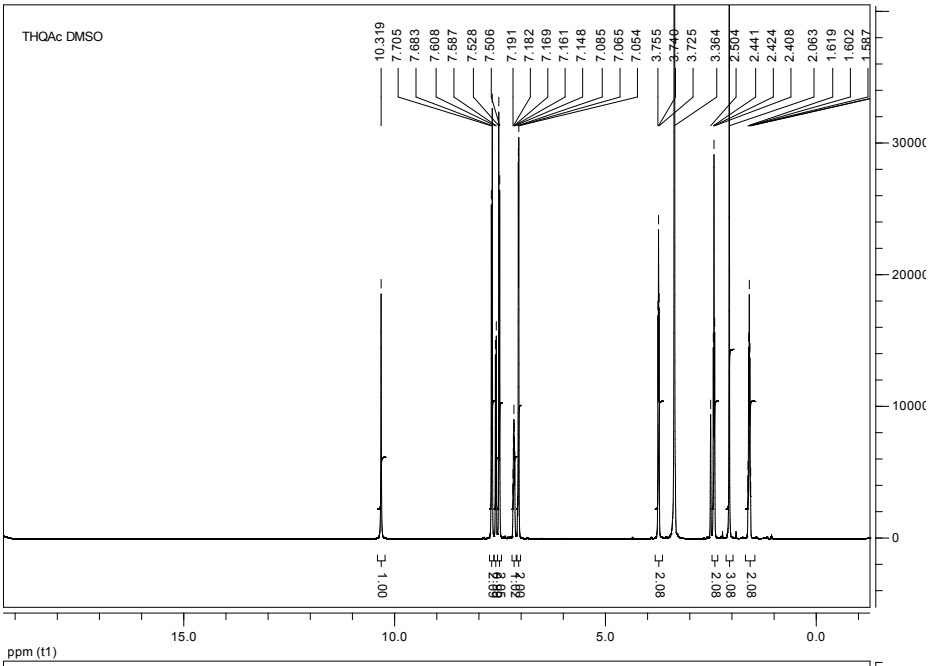
UV Spectra:



ACN		EtOH		DCM	
λ (nm)	ξ ($M^{-1}cm^{-1}$)	λ (nm)	ξ ($M^{-1}cm^{-1}$)	λ (nm)	ξ ($M^{-1}cm^{-1}$)
205	44500	206	51600	-	-
240	13200	240	16500	241	15500
269	21780	270	27200	268	20200

IR (υ_{max}/cm^{-1}): 3346 (NH), 2944, 2839 (CH sp^3), 1704 (CO amide), 1329 ($SO_{2\,as}$), 1309 (CN amide), 1152 ($SO_{2\,sim}$).
^{1}H NMR: 10.32 (s, 1H, H16); 7.69 (d, 2H, 8.8 Hz, H13 and H14); 7.60 (d, 1H, 8.0 Hz, H8); 7.52 (d, 2H, 8.8 Hz, H11 and H12); 7.17 (ddd, 1H, 8.8, 5.2 and 3.6 Hz, H7); 7.07 (m, 2H, H5 and H6); 3.74 (t, 2H, 5.8 Hz, H2); 2.42 (t, 2H, 6.6 Hz, H4); 2.06 (s,3H, H18); 1.59 (quint, 2H, 6.2 Hz, H3).
^{13}C NMR (assigned using HSQC): 169.6 (C17); 143.9 (C15); 136.9(C8a); 132.9 (C10); 131.0 (C4a); 129.7 (C5); 128.8 (C11 and C12); 126.6 (C7); 125.1 (C6); 124.2 (C8); 119.0 (C13 and C14); 46.6 (C2); 26.4 (C4); 24.6 (C18); 21.5 (C3).
COSY: $^3J_{vec}$:H2-H3; H3-H4. $^3J_{ortho}$: H6-H7; H5-H6; H7-H8; H11/12-H13/14. $^4J_{meta}$: H5-H7; H6-H8.
HMBC (f_1 =400.16 MHz, f_2 =100.62 MHz) (C→H): C4→H5, H3; C3→H2, H4; C2→H4, H3; C6→H8; C7→H5; C8→H6; C5→H7, H4; C15→H11, H12; C4a→H8, H6, H4, H3; C8a→H7, H5, H4, H2; C10→H11, H12, H13, H14; C11→H13, H14; C12→H13, H14; C13→H11, H12, H16; C14→H11, H12, H16; C15→H11, H12, H13, H14, H16; C17→H16, H18; C18→H16.


Absorbancia
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0,0
3500
3000
2500
2000
1500
1000
500
ν (cm⁻¹)


THQAc DMSO
10.319
7.705
7.683
7.608
7.587
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7.191
7.182
7.169
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7.085
7.065
7.054
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3.740
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3.364
2.504
2.441
2.424
2.408
2.063
1.619
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1.00
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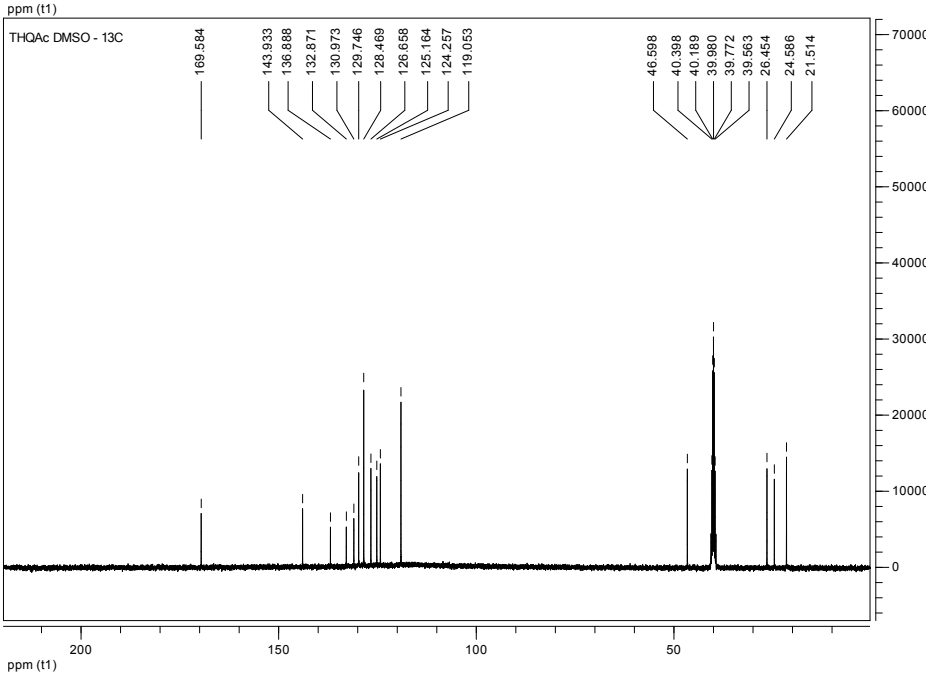
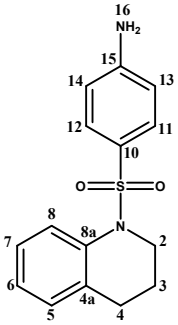
3.08
2.08
15.0
10.0
5.0
0.0
ppm (t1)

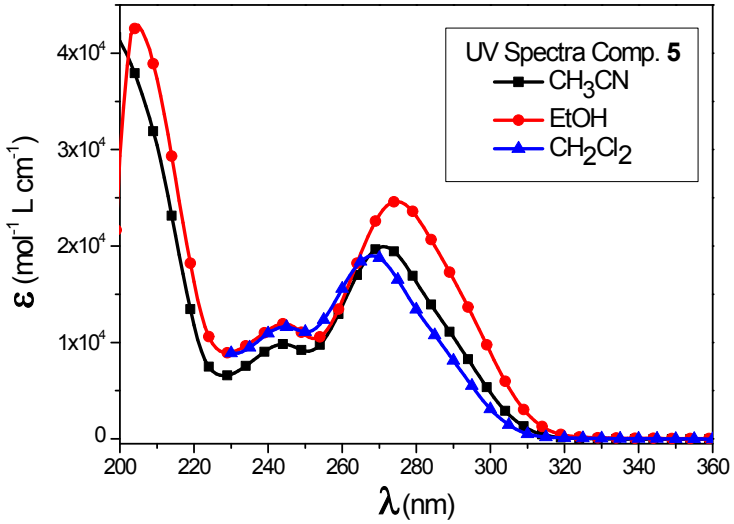

THQAc DMSO - 13C
169.584
143.933
136.888
132.871
130.973
129.746
128.469
126.658
125.164
124.257
119.053
46.598
40.398
40.189
39.980
39.772
39.563
26.454
24.586
21.514
200
150
100
50
ppm (t1)

1-(4-amine-benzenesulfonyl)-1,2,3,4-tetrahydroquinoline



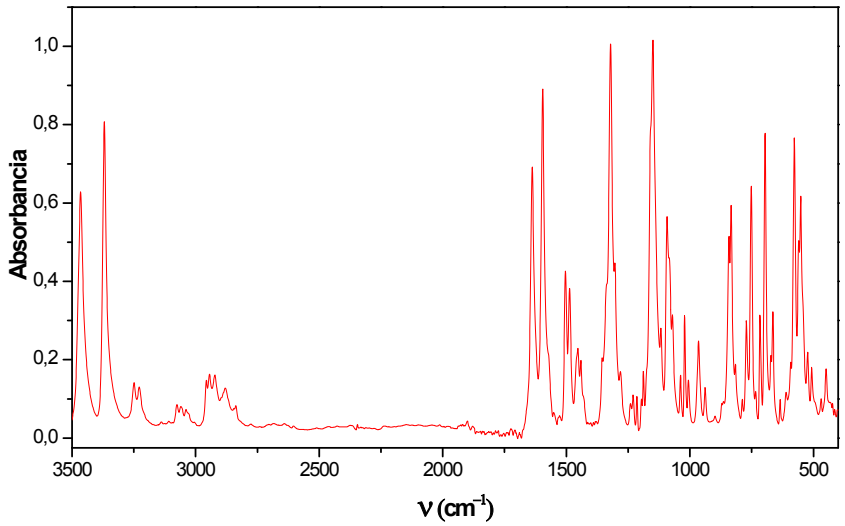
4-(3,4-dihydroquinolin-1(2*H*)-ylsulfonyl)aniline

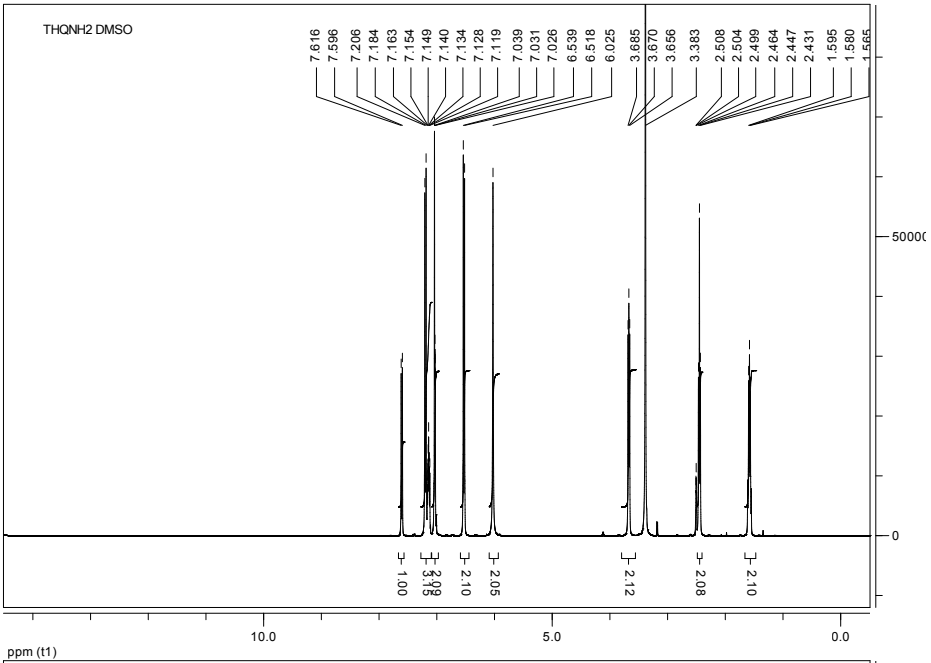
UV Spectra:

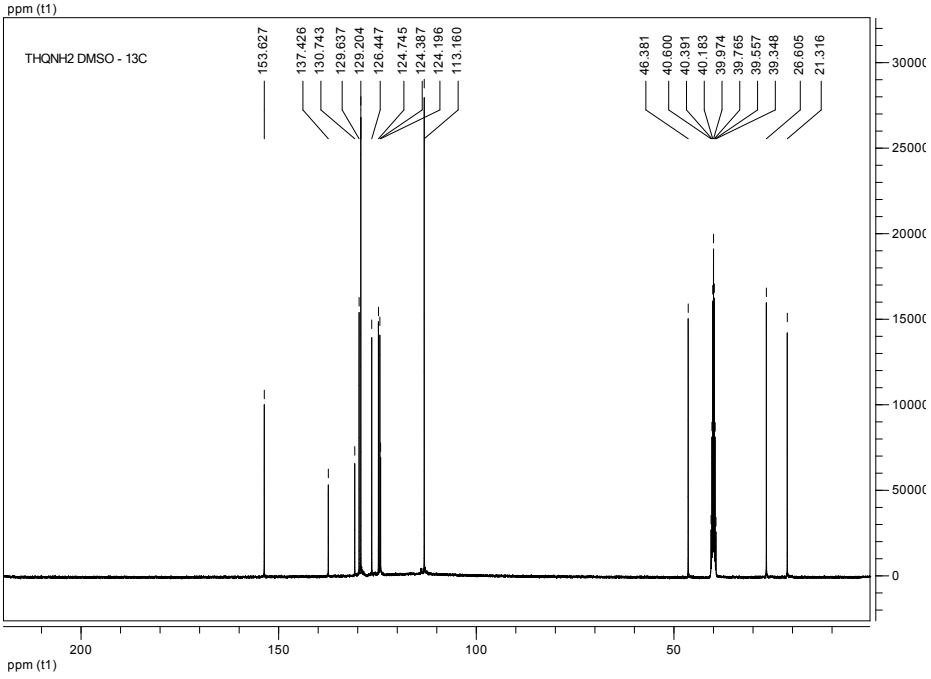


ACN		EtOH		DCM	
λ (nm)	ξ ($M^{-1}cm^{-1}$)	λ (nm)	ξ ($M^{-1}cm^{-1}$)	λ (nm)	ξ ($M^{-1}cm^{-1}$)
199	40400	-	-	-	-
205	37400	204	40800	-	-
212	27500	211	34500	-	-
244	10460	244	11360	245	12600
271	20600	275	23100	268	20400

IR (υ_{max}/cm^{-1}): 3465, 3369 (NH), 2944, 2880 (CH sp^3), 1596 (NH), 1321 ($SO_{2\ as}$), 1150 ($SO_{2\ sim}$).
^{1}H NMR: 7.61 (d, 1H, 8.0 Hz, H8); 7.20 (d, 2H, 8.8 Hz, H11 and H12); 7.14 (ddd, 1H, 9.2, 5.6 and 3.6 Hz, H7); 7.03 (m, 2H, H5 and H6); 6.53 (d, 2H, 8.4 Hz, H13 and H14); 6.02 (s, 1H, H16); 3.67 (t, 2 H, 5.8 Hz, H2); 2.45 (t, 2H, 6.6 Hz, H4); 1.58 (quint, 2H, 6.2 Hz, H3).
^{13}C NMR (assigned using HSQC): 153.6 (C15); 137.4 (C8a); 130.7 (C4a); 129.6 (C5); 129.2 (C11 and C12); 126.4 (C7); 124.7 (C6); 124.2 (C8 and C10); 113.2 (C13 and C14); 46.4 (C2); 26.0 (C4); 21.3 (C3).
COSY: $^3J_{vec}$:H2-H3; H3-H4. $^4J_{meta}$: H5-H7; H6-H8. J with NH_2: H13/14-H16; H11/12-H16.
HMBC (f_1 =400.16 MHz, f_2 =100.62 MHz) (C→H): C4→H5, H3; C3→H2, H4; C2→H4, H3; C6→H8, H7; C7→H5; C8→H6, H7; C5→H7, H4; C4a→H8, H6, H4, H3; C8a→H7, H5, H4, H2; C10→H13, H14; C11→H13, H14; C12→H13, H14; C13→H11, H12, H16; C14→H11, H12, H16; C15→H11, H12.


Absorbancia
1,0
0,8
0,6
0,4
0,2
0,0
3500
3000
2500
2000
1500
1000
500
ν (cm⁻¹)


THQNH2 DMSO
7.616
7.596
7.206
7.184
7.163
7.154
7.149
7.140
7.134
7.128
7.119
7.039
7.031
7.026
6.539
6.518
6.025
3.685
3.670
3.656
3.383
2.508
2.504
2.499
2.464
2.447
2.431
1.595
1.580
1.565
1.00
3.15
3.09
2.10
2.05
2.12
2.08
2.10
10.0
5.0
0.0
ppm (t1)


THQNH2 DMSO - 13C
153.627
137.426
130.743
129.637
129.204
126.447
124.745
124.387
124.196
113.160
46.381
40.600
40.391
40.183
39.974
39.765
39.557
39.348
26.605
21.316
200
150
100
50
ppm (t1)

Theoretical study

Table S1. Total energy, zero-point vibration energy and relative energy of THQ and BSTHQs derivatives conformers, calculated at B3LyP/6-31+G(d,p) theoretical level.

Species		Conformation	B3LyP/6-31+G(d,p)			
			Total Energy (in Hartree)	ΔH (in $kJmol^{-1}$)	$\Delta G^{\neq}$(in $kJmol^{-1}$)	Poblational analysis (%)
Comp.1	**THQ**	---	-404.37715243	---	---	---
Comp. 2	**THQH**	***in***	-1184.01617774	0.000	-133.328	68.6
		out	-1184.01544242	1.930	-135.259	31.4
Comp. 3	**$THQNO_2$**	***in***	-1388.52648087	0.000	-145.961	91.3
		out	-1388.52425824	5.836	-151.796	8.7
Comp. 4	**THQAc**	***in***	-1392.05247788	0.000	-163.199	90.9
		out	-1392.05030682	5.700	-168.900	9.1
Comp. 5	**$THQNH_2$**	***in***	-1239.38845782	0.000	-146.172	88.2
		out	-1239.38655597	4.993	-151.166	11.8

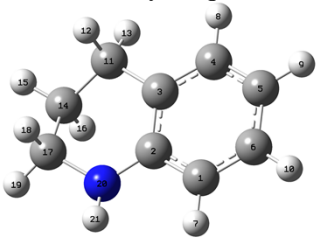
Table S2. Frontier orbital energies (eV) for THQ and BSTHQs derivatives conformers at B3LyP/6-31+G(d,p) theoretical level.

			Occupied MO					Virtual MO						
			H-4	H-3	H-2	H-1	H	L	L+1	L+2	L+3	L+4	L+5	L+6
Comp.1	**THQ**		-9.02	-8.88	-8.11	-6.74	-5.46	-0.41	-0.04	0.21	0.52	0.54	0.92	1.04
Comp. 2	**THQH-ACN**	**In**	-8.33	-7.66	-7.55	-7.00	-6.39	-1.50	-0.95	-0.64	-0.50	-0.07	0.35	0.40
		Out	-8.13	-7.63	-7.55	-6.98	-6.49	-1.50	-0.99	-0.69	-0.62	-0.01	0.28	0.39
Comp. 2	**THQH-EtOH**	**In**	-8.33	-7.66	-7.55	-7.00	-6.39	-1.50	-0.95	-0.64	-0.50	-0.07	0.35	0.39
		Out	-8.13	-7.63	-7.55	-6.98	-6.48	-1.50	-0.98	-0.68	-0.62	-0.01	0.28	0.39
Comp. 2	**THQH-DCM**	**In**	-8.32	-7.66	-7.56	-6.99	-6.37	-1.49	-0.95	-0.63	-0.49	-0.07	0.33	0.38
		Out	-8.11	-7.63	-7.55	-6.97	-6.47	-1.50	-0.98	-0.67	-0.61	-0.01	0.27	0.39
Comp. 3	**THQNO2-ACN**	**In**	-8.59	-8.11	-8.03	-7.00	-6.58	-3.40	-1.42	-1.25	-0.75	-0.61	-0.07	0.31
		Out	-8.49	-8.12	-7.98	-7.03	-6.56	-3.40	-1.43	-1.20	-0.78	-0.66	-0.07	0.25
Comp. 4	**THQAc-ACN**	**In**	-7.74	-7.69	-7.02	-6.90	-6.44	-1.67	-1.11	-0.73	-0.60	-0.14	0.02	0.20
		Out	-7.75	-7.69	-7.03	-6.90	-6.47	-1.67	-1.13	-0.72	-0.64	-0.13	-0.02	0.16
Comp. 5	**THQNH2-ACN**	**In**	-8.09	-7.51	-6.92	-6.56	-6.10	-1.15	-0.86	-0.65	-0.48	-0.03	0.27	0.38
		Out	-7.90	-7.53	-6.96	-6.54	-6.16	-1.15	-0.86	-0.64	-0.56	-0.04	0.22	0.40

Table S3. Lowest energy transition (in eV and nm) for compounds **2-5** in different solvents.

			DCM		ACN		EtOH	
			E (eV)	λ (nm)	E (eV)	λ (nm)	E (eV)	λ (nm)
Comp. 2	**THQH**	**Exp.**	4.49	276	4.58	271	4.58	271
		B3LYP	4.24	293	4.25	292	4.25	292
		CAM-B3LYP	5.10	243	5.12	242	5.11	242
Comp. 3	**THQNO2**	**Exp.**	4.22	294	4.23	293	4.25	292
		B3LYP	2.72	456	2.73	454	2.73	454
		CAM-B3LYP	4.17	297	4.17	297	4.17	297
Comp. 4	**THQAc**	**Exp.**	4.63	268	4.61	269	4.59	270
		B3LYP	4.16	298	4.17	297	4.17	297
		CAM-B3LYP	4.94	251	4.95	251	4.94	251
Comp. 5	**THQNH2**	**Exp.**	4.63	268	4.58	271	4.51	275
		B3LYP	4.38	283	4.38	283	4.38	283
		CAM-B3LYP	4.84	256	4.84	256	4.84	256

1,2,3,4-tetrahydroquinoline (B3LyP/6-31+G(d,p), energy= -404.37715243 a.u.)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.346377	-1.385954	-0.053781
2	6	0	0.115597	-0.697983	-0.022147
3	6	0	0.114398	0.717071	0.037106
4	6	0	1.342413	1.389614	0.046563
5	6	0	2.562776	0.707978	0.013601
6	6	0	2.554493	-0.691531	-0.034134
7	1	0	1.343082	-2.472717	-0.098743
8	1	0	1.336321	2.477266	0.084304
9	1	0	3.499613	1.256802	0.024620
10	1	0	3.489298	-1.245174	-0.057893
11	6	0	-1.197061	1.481449	0.109262
12	1	0	-1.370480	1.805692	1.145338
13	1	0	-1.125524	2.398297	-0.487423
14	6	0	-2.390471	0.634278	-0.355429
15	1	0	-3.332438	1.125563	-0.090720
16	1	0	-2.372965	0.522893	-1.446729
17	6	0	-2.331299	-0.753169	0.284599
18	1	0	-2.414805	-0.656438	1.380327
19	1	0	-3.162859	-1.377018	-0.056182
20	7	0	-1.082861	-1.409143	-0.102708
21	1	0	-1.012556	-2.381676	0.168224

Excitation energies and oscillator strengths:

```
 Excited State   1:      Singlet-A      4.3271 eV  286.53 nm  f=0.0643  <S**2>=0.000
      35 -> 38        -0.14664
      36 -> 37         0.68439
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      4.7138 eV  263.02 nm  f=0.0577  <S**2>=0.000
      36 -> 38         0.57453
      36 -> 39        -0.38890

 Excited State   3:      Singlet-A      5.0138 eV  247.29 nm  f=0.1245  <S**2>=0.000
      35 -> 37         0.13523
      36 -> 38         0.36407
      36 -> 39         0.54141
      36 -> 41         0.21291

 Excited State   4:      Singlet-A      5.2343 eV  236.87 nm  f=0.0056  <S**2>=0.000
      36 -> 40         0.66885
      36 -> 41        -0.18921

 Excited State   5:      Singlet-A      5.3565 eV  231.47 nm  f=0.0321  <S**2>=0.000
      35 -> 37        -0.13147
      36 -> 39        -0.16511
      36 -> 40         0.19370
      36 -> 41         0.63366

 Excited State   6:      Singlet-A      5.6162 eV  220.76 nm  f=0.0286  <S**2>=0.000
      35 -> 38        -0.12087
      36 -> 42         0.67017

 Excited State   7:      Singlet-A      5.7891 eV  214.17 nm  f=0.0007  <S**2>=0.000
      36 -> 43         0.67447
      36 -> 45        -0.16330

 Excited State   8:      Singlet-A      5.8562 eV  211.71 nm  f=0.0165  <S**2>=0.000
```

```
     35 -> 37        -0.20931
     35 -> 38        -0.12287
     36 -> 42        -0.13503
     36 -> 44         0.62348
     36 -> 45         0.15082

Excited State   9:      Singlet-A      5.9643 eV  207.88 nm  f=0.0792  <S**2>=0.000
     35 -> 37        -0.36023
     35 -> 38        -0.12676
     36 -> 43         0.11234
     36 -> 44        -0.28445
     36 -> 45         0.47599

Excited State  10:      Singlet-A      6.0319 eV  205.55 nm  f=0.1947  <S**2>=0.000
     34 -> 37        -0.15787
     35 -> 37        -0.19467
     35 -> 38         0.58773
     35 -> 39        -0.21430
     36 -> 37         0.10096

Excited State  11:      Singlet-A      6.0772 eV  204.01 nm  f=0.2372  <S**2>=0.000
     35 -> 37         0.40665
     35 -> 38         0.11690
     35 -> 39         0.17665
     36 -> 38        -0.11099
     36 -> 43         0.11444
     36 -> 45         0.44218

Excited State  12:      Singlet-A      6.1899 eV  200.30 nm  f=0.1767  <S**2>=0.000
     34 -> 37        -0.15676
     35 -> 37        -0.19679
     35 -> 38         0.11549
     35 -> 39         0.59579
     35 -> 40         0.16956

Excited State  13:      Singlet-A      6.3810 eV  194.30 nm  f=0.0041  <S**2>=0.000
     36 -> 46         0.66420
     36 -> 48        -0.13221
     36 -> 49        -0.12432

Excited State  14:      Singlet-A      6.4618 eV  191.87 nm  f=0.0059  <S**2>=0.000
     35 -> 40         0.12730
     36 -> 47         0.67566

Excited State  15:      Singlet-A      6.5279 eV  189.93 nm  f=0.0104  <S**2>=0.000
     35 -> 39        -0.11371
     35 -> 40         0.54232
     35 -> 41        -0.36834
     36 -> 49         0.16780
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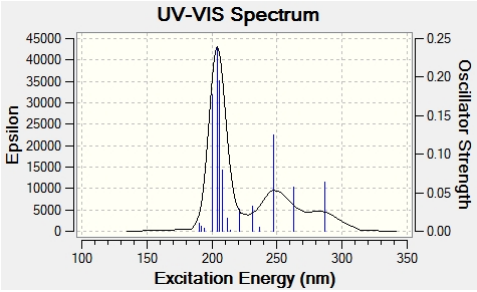
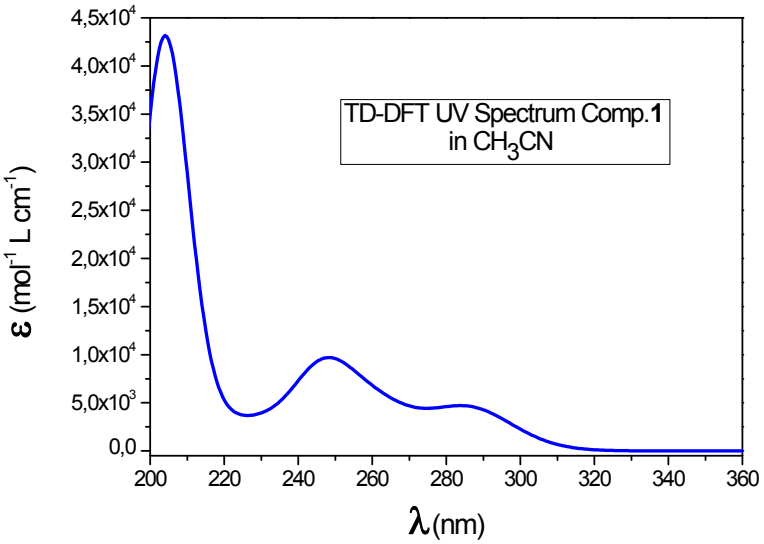
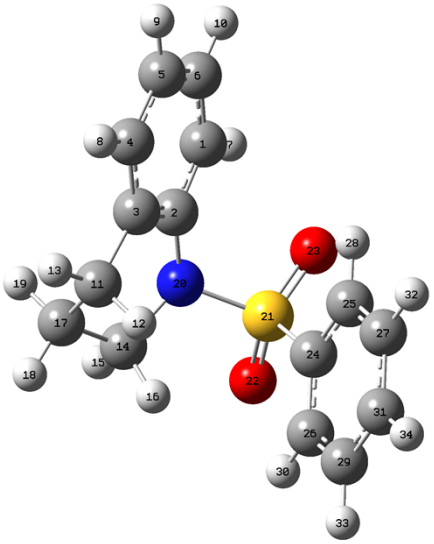




1-(benzenesulfonyl)-1,2,3,4-tetrahydroquinoline *in* conformer (B3LyP/6-31+G(d,p), energy= -1184.01617774 a.u.)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-1.614776	-0.263643	-0.139132
3	6	0	-2.005898	0.625468	0.884165
4	6	0	-3.006852	1.565919	0.614018
5	6	0	-3.606129	1.647177	-0.644913
6	6	0	-3.233232	0.741658	-1.642336
7	1	0	-1.988605	-0.941542	-2.149538
8	1	0	-3.318637	2.239304	1.408389
9	1	0	-4.373022	2.391647	-0.836657
10	1	0	-3.713431	0.769412	-2.615974
11	6	0	-1.420556	0.445471	2.262613
12	1	0	-0.423649	0.902379	2.332971
13	1	0	-2.052289	0.938534	3.007226
14	6	0	-0.348569	-1.700447	1.536361
15	1	0	-0.419518	-2.790452	1.559407
16	1	0	0.671648	-1.426277	1.822718
17	6	0	-1.313301	-1.061361	2.532113
18	1	0	-0.935841	-1.265037	3.539408
19	1	0	-2.306641	-1.518052	2.456570

```
     20          7           0       -0.603006   -1.251122    0.127050
     21         16           0        0.784131   -1.311500   -0.853045
     22          8           0        1.477935   -2.552438   -0.470606
     23          8           0        0.367088   -1.113896   -2.249098
     24          6           0        1.832451    0.074651   -0.394020
     25          6           0        1.552182    1.340535   -0.922662
     26          6           0        2.886055   -0.128333    0.503141
     27          6           0        2.344975    2.422299   -0.535826
     28          1           0        0.742288    1.475205   -1.630632
     29          6           0        3.672140    0.964384    0.878335
     30          1           0        3.096028   -1.121241    0.883868
     31          6           0        3.400732    2.235583    0.363623
     32          1           0        2.141076    3.407966   -0.941955
     33          1           0        4.497496    0.818473    1.567932
     34          1           0        4.015465    3.080643    0.657833
 ---------------------------------------------------------------------

Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      4.2508 eV  291.67 nm  f=0.1759  <S**2>=0.000
      72 -> 73         0.70331
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      4.7620 eV  260.36 nm  f=0.0021  <S**2>=0.000
      71 -> 73         0.35748
      71 -> 75         0.11573
      72 -> 74         0.50949
      72 -> 75         0.13114
      72 -> 76         0.23899

 Excited State   3:      Singlet-A      4.8395 eV  256.19 nm  f=0.0009  <S**2>=0.000
      70 -> 73        -0.13464
      71 -> 73        -0.39264
      72 -> 74         0.44864
      72 -> 75        -0.22082
      72 -> 76        -0.23667

 Excited State   4:      Singlet-A      5.0671 eV  244.68 nm  f=0.0492  <S**2>=0.000
      70 -> 73         0.14829
      71 -> 73        -0.41828
      71 -> 75         0.15531
      71 -> 76        -0.15286
      72 -> 75         0.45337
      72 -> 76         0.16850

 Excited State   5:      Singlet-A      5.2027 eV  238.31 nm  f=0.0474  <S**2>=0.000
      70 -> 73        -0.18931
      71 -> 73        -0.19225
      71 -> 75         0.22683
      72 -> 75        -0.34112
      72 -> 76         0.46487

 Excited State   6:      Singlet-A      5.2442 eV  236.42 nm  f=0.0455  <S**2>=0.000
      69 -> 73         0.22429
      69 -> 74         0.31014
      70 -> 73         0.48007
      70 -> 74        -0.13383
      71 -> 74         0.10430
      72 -> 74         0.14928
      72 -> 75        -0.22511

 Excited State   7:      Singlet-A      5.5279 eV  224.29 nm  f=0.0137  <S**2>=0.000
      71 -> 74         0.68201
      71 -> 75        -0.12093

 Excited State   8:      Singlet-A      5.6317 eV  220.15 nm  f=0.0166  <S**2>=0.000
      69 -> 73         0.14673
      72 -> 77         0.66028

 Excited State   9:      Singlet-A      5.6652 eV  218.85 nm  f=0.0758  <S**2>=0.000
      69 -> 73         0.55618
      70 -> 73        -0.22884
      70 -> 74        -0.21472
      71 -> 75        -0.10365
      72 -> 75         0.11956
      72 -> 77        -0.18814
```

```
Excited State  10:      Singlet-A      5.8711 eV  211.18 nm  f=0.1619  <S**2>=0.000
     68 -> 76        -0.13789
     69 -> 76         0.12765
     71 -> 75         0.52158
     71 -> 76        -0.14804
     72 -> 76        -0.31201

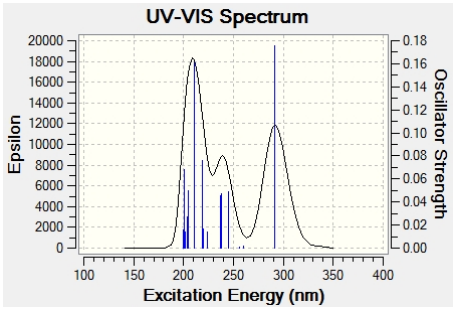
Excited State  11:      Singlet-A      6.0613 eV  204.55 nm  f=0.0498  <S**2>=0.000
     68 -> 73         0.16999
     70 -> 74        -0.11257
     71 -> 75         0.13452
     71 -> 76         0.28895
     72 -> 78         0.46846
     72 -> 79         0.30651
     72 -> 80         0.11833

Excited State  12:      Singlet-A      6.0801 eV  203.92 nm  f=0.0274  <S**2>=0.000
     68 -> 73         0.47354
     69 -> 74        -0.16279
     70 -> 74        -0.17880
     71 -> 76         0.23634
     72 -> 78        -0.32381

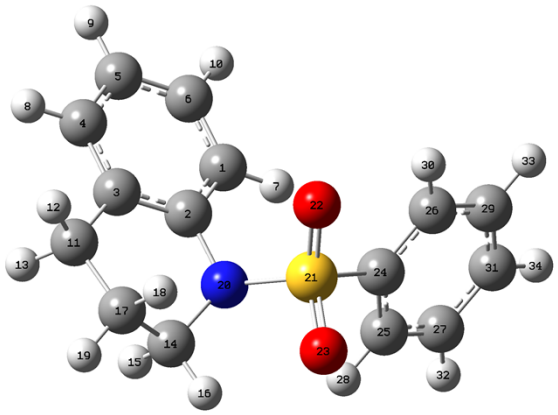
Excited State  13:      Singlet-A      6.1398 eV  201.93 nm  f=0.0144  <S**2>=0.000
     70 -> 75        -0.13299
     71 -> 77        -0.10135
     72 -> 78        -0.24747
     72 -> 79         0.56457
     72 -> 80        -0.23299

Excited State  14:      Singlet-A      6.1679 eV  201.02 nm  f=0.0682  <S**2>=0.000
     68 -> 73        -0.15599
     69 -> 73         0.15011
     69 -> 74        -0.21439
     70 -> 73         0.16702
     70 -> 74         0.28278
     70 -> 75         0.41215
     70 -> 76        -0.13284
     72 -> 78        -0.13404
     72 -> 79         0.19267
     72 -> 80         0.10751

Excited State  15:      Singlet-A      6.1985 eV  200.02 nm  f=0.0154  <S**2>=0.000
     68 -> 73         0.11132
     71 -> 75        -0.11861
     71 -> 77         0.15905
     72 -> 78        -0.16785
     72 -> 79         0.14392
     72 -> 80         0.57737
```



1-(benzenesulfonyl)-1,2,3,4-tetrahydroquinoline *out* conformer (B3LyP/6-31+G(d,p), energy= -1184.01544242 a.u.)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.699032	1.727196	-0.337428
2	6	0	-1.365384	0.491515	-0.312586
3	6	0	-2.759613	0.438858	-0.116334
4	6	0	-3.444132	1.649286	0.077575
5	6	0	-2.780938	2.875484	0.088917
6	6	0	-1.398354	2.912904	-0.123268
7	1	0	0.366568	1.756505	-0.532746
8	1	0	-4.520896	1.618686	0.226850
9	1	0	-3.337289	3.793935	0.250175
10	1	0	-0.868326	3.860402	-0.138496
11	6	0	-3.542205	-0.861142	-0.174782
12	1	0	-4.236038	-0.908844	0.671858
13	1	0	-4.168529	-0.834658	-1.077065
14	6	0	-1.423094	-1.849831	-1.079057
15	1	0	-1.711517	-1.554562	-2.094112
16	1	0	-0.779804	-2.724788	-1.152901
17	6	0	-2.655199	-2.111700	-0.214375
18	1	0	-2.329174	-2.388778	0.795014
19	1	0	-3.217181	-2.961918	-0.615088
20	7	0	-0.620105	-0.721671	-0.541302
21	16	0	0.550057	-1.139652	0.639849
22	8	0	0.155544	-0.659652	1.978281
23	8	0	0.822756	-2.578754	0.456690
24	6	0	2.023713	-0.236164	0.147305
25	6	0	2.556573	-0.444943	-1.129083
26	6	0	2.643106	0.602380	1.075636
27	6	0	3.734505	0.214124	-1.480864
28	1	0	2.059901	-1.100705	-1.836231
29	6	0	3.824806	1.254090	0.709938
30	1	0	2.205970	0.744600	2.057174
31	6	0	4.367425	1.062003	-0.563366
32	1	0	4.157365	0.065659	-2.469303
33	1	0	4.315743	1.910969	1.420818
34	1	0	5.283589	1.572509	-0.843564

Excitation energies and oscillator strengths:

```
 Excited State   1:      Singlet-A      4.2984 eV  288.44 nm  f=0.0233  <S**2>=0.000
      72 -> 73         0.70023
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      4.8106 eV  257.73 nm  f=0.0287  <S**2>=0.000
      71 -> 75        -0.16216
      71 -> 76         0.10363
      72 -> 74         0.61630
      72 -> 75         0.10982
      72 -> 76         0.21509

 Excited State   3:      Singlet-A      4.9051 eV  252.76 nm  f=0.0050  <S**2>=0.000
      71 -> 73         0.65733
```

```
     72 -> 76        -0.20779

Excited State   4:      Singlet-A      4.9957 eV  248.18 nm  f=0.0197  <S**2>=0.000
     69 -> 73        -0.11375
     70 -> 73        -0.10773
     71 -> 73         0.23635
     71 -> 74        -0.19701
     71 -> 75        -0.20875
     72 -> 74        -0.26874
     72 -> 75         0.17828
     72 -> 76         0.45981

Excited State   5:      Singlet-A      5.1407 eV  241.18 nm  f=0.1561  <S**2>=0.000
     69 -> 73        -0.21648
     70 -> 73        -0.14982
     72 -> 75         0.56477
     72 -> 76        -0.21605

Excited State   6:      Singlet-A      5.2407 eV  236.58 nm  f=0.0365  <S**2>=0.000
     69 -> 73         0.30444
     69 -> 74         0.19875
     70 -> 73         0.38003
     70 -> 74        -0.22630
     71 -> 74         0.10775
     72 -> 74        -0.18816
     72 -> 75         0.30404

Excited State   7:      Singlet-A      5.5082 eV  225.09 nm  f=0.1073  <S**2>=0.000
     70 -> 73        -0.17850
     71 -> 74         0.62972
     72 -> 76         0.18485

Excited State   8:      Singlet-A      5.5610 eV  222.95 nm  f=0.0974  <S**2>=0.000
     68 -> 73        -0.14840
     69 -> 73         0.45119
     70 -> 73        -0.41905
     70 -> 74        -0.18104
     71 -> 74        -0.16018
     71 -> 75         0.14876

Excited State   9:      Singlet-A      5.7651 eV  215.06 nm  f=0.0240  <S**2>=0.000
     68 -> 76        -0.11183
     69 -> 74         0.13325
     70 -> 76        -0.10443
     71 -> 75         0.44075
     72 -> 76         0.23161
     72 -> 77        -0.38250
     72 -> 78        -0.12622

Excited State  10:      Singlet-A      5.8391 eV  212.33 nm  f=0.0297  <S**2>=0.000
     68 -> 73        -0.12271
     68 -> 76        -0.10201
     69 -> 74         0.11256
     70 -> 76        -0.10069
     71 -> 75         0.23261
     71 -> 76        -0.18609
     72 -> 76         0.16981
     72 -> 77         0.53601

Excited State  11:      Singlet-A      5.9476 eV  208.46 nm  f=0.1055  <S**2>=0.000
     68 -> 73        -0.34781
     69 -> 75        -0.10031
     70 -> 74         0.26813
     70 -> 75         0.14169
     71 -> 76         0.46537

Excited State  12:      Singlet-A      5.9489 eV  208.41 nm  f=0.0859  <S**2>=0.000
     68 -> 73         0.51960
     69 -> 74        -0.11448
     71 -> 75         0.18254
     71 -> 76         0.32096
     72 -> 77         0.13342

Excited State  13:      Singlet-A      6.1203 eV  202.58 nm  f=0.0036  <S**2>=0.000
     69 -> 74         0.10631
     70 -> 74        -0.10481
     70 -> 75        -0.11124
     72 -> 77        -0.12545
```

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      72 -> 78         0.55517
      72 -> 79         0.28829
      72 -> 80         0.12666

Excited State  14:      Singlet-A      6.1936 eV  200.18 nm  f=0.0816  <S**2>=0.000
      70 -> 74        -0.16261
      70 -> 75        -0.16870
      72 -> 78        -0.35118
      72 -> 79         0.52824

Excited State  15:      Singlet-A      6.2142 eV  199.52 nm  f=0.1796  <S**2>=0.000
      68 -> 73         0.11576
      69 -> 73         0.17657
      69 -> 75         0.27446
      70 -> 74         0.35297
      70 -> 75         0.25938
      70 -> 76         0.15625
      71 -> 76        -0.15227
      71 -> 77         0.14164
      72 -> 79         0.27796
```
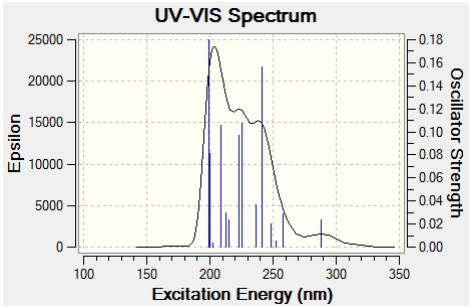
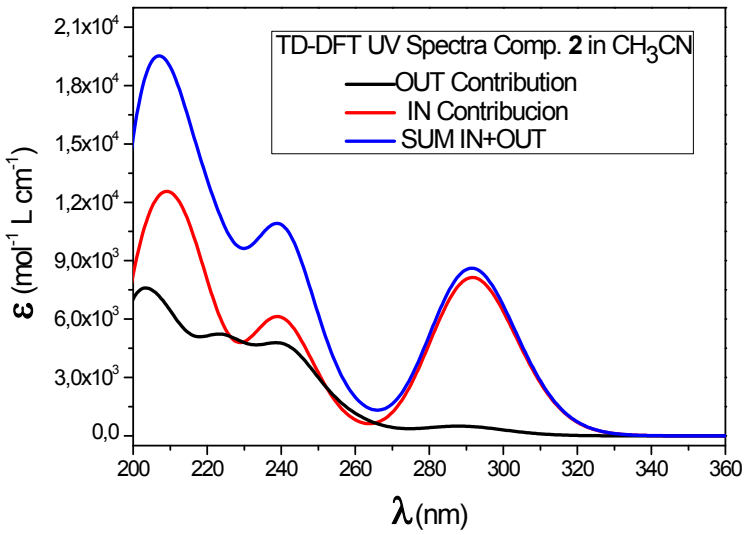
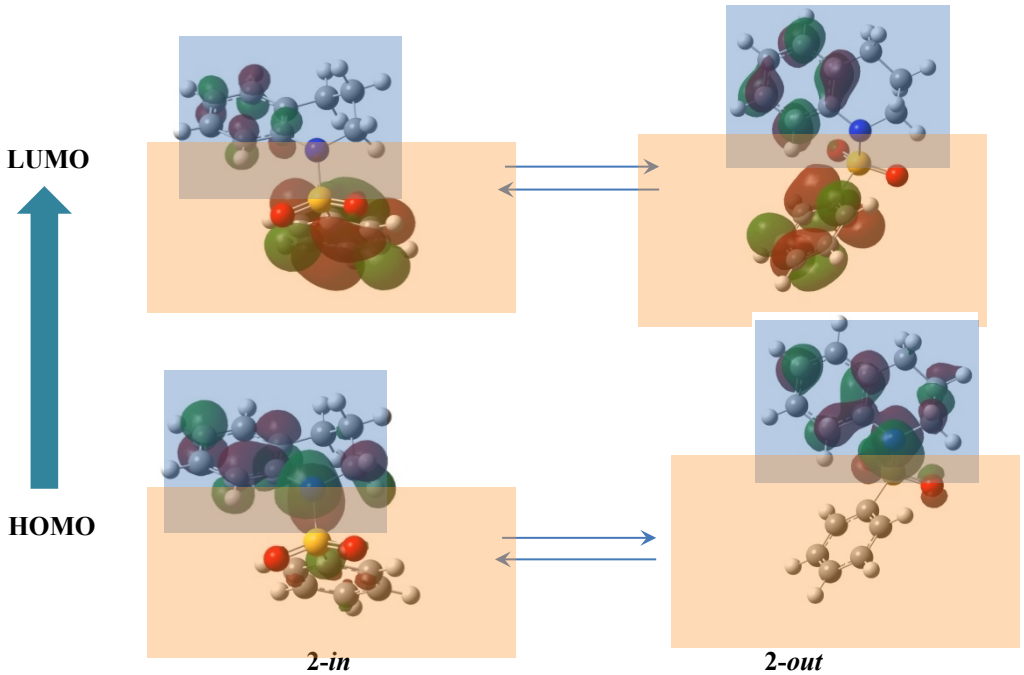
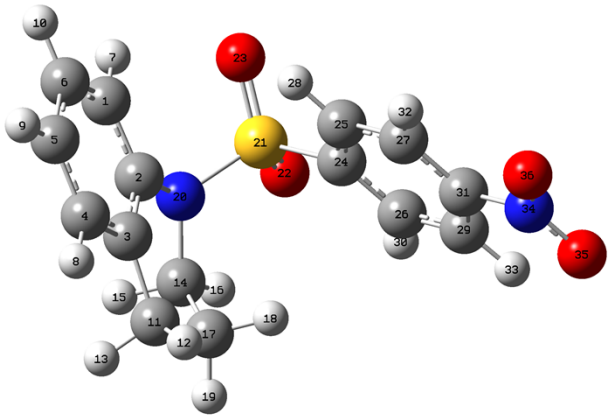







1-(4-nitro-benzenesulfonyl)-1,2,3,4-tetrahydroquinoline *in* conformer (B3LyP/6-31+G(d,p), energy= -1388.52648087 a.u.)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.965356	0.507532	-1.280748
2	6	0	-2.367813	0.245848	-0.034661
3	6	0	-2.300669	1.257054	0.946675
4	6	0	-2.799297	2.528340	0.619844
5	6	0	-3.348437	2.804074	-0.630464
6	6	0	-3.437434	1.782375	-1.582581
7	1	0	-3.052857	-0.292203	-2.003977
8	1	0	-2.750335	3.312231	1.371784
9	1	0	-3.719085	3.799699	-0.855073
10	1	0	-3.888574	1.970875	-2.552052
11	6	0	-1.792033	1.003655	2.354230
12	1	0	-1.110493	1.809054	2.649020
13	1	0	-2.651519	1.070591	3.035117
14	6	0	-1.864966	-1.421951	1.723142
15	1	0	-2.911085	-1.487282	2.042690
16	1	0	-1.425963	-2.412561	1.831432
17	6	0	-1.117112	-0.360497	2.528193
18	1	0	-0.074155	-0.319159	2.197690
19	1	0	-1.105070	-0.646221	3.585021

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     20          7           0       -1.900654   -1.084368    0.275262
     21         16           0       -0.726229   -1.815294   -0.707881
     22          8           0       -0.550604   -3.179615   -0.188645
     23          8           0       -1.126563   -1.612551   -2.106623
     24          6           0        0.844981   -0.948989   -0.494539
     25          6           0        1.044141    0.268473   -1.154929
     26          6           0        1.825528   -1.511160    0.327896
     27          6           0        2.248895    0.944843   -0.980300
     28          1           0        0.281533    0.678288   -1.806221
     29          6           0        3.034801   -0.840764    0.499119
     30          1           0        1.650763   -2.461507    0.817835
     31          6           0        3.221134    0.377076   -0.155546
     32          1           0        2.435667    1.887494   -1.478107
     33          1           0        3.817081   -1.253242    1.123017
     34          7           0        4.497239    1.087460    0.023949
     35          8           0        5.352029    0.571688    0.747948
     36          8           0        4.648824    2.164421   -0.557497
 ---------------------------------------------------------------------

Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      2.7287 eV  454.37 nm  f=0.0640  <S**2>=0.000
      83 -> 84         0.70592
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      3.1577 eV  392.64 nm  f=0.0059  <S**2>=0.000
      82 -> 84         0.70634

 Excited State   3:      Singlet-A      3.7056 eV  334.59 nm  f=0.0000  <S**2>=0.000
      77 -> 84        -0.14619
      78 -> 84         0.67471
      78 -> 86        -0.11421

 Excited State   4:      Singlet-A      3.9854 eV  311.09 nm  f=0.0245  <S**2>=0.000
      80 -> 84         0.53064
      81 -> 84         0.44609

 Excited State   5:      Singlet-A      4.1775 eV  296.79 nm  f=0.2299  <S**2>=0.000
      80 -> 84        -0.44624
      81 -> 84         0.53741

 Excited State   6:      Singlet-A      4.2957 eV  288.63 nm  f=0.0007  <S**2>=0.000
      73 -> 84         0.18162
      75 -> 84         0.66136
      75 -> 86        -0.10700

 Excited State   7:      Singlet-A      4.5471 eV  272.67 nm  f=0.0226  <S**2>=0.000
      83 -> 85         0.69957

 Excited State   8:      Singlet-A      4.6749 eV  265.21 nm  f=0.1257  <S**2>=0.000
      79 -> 84         0.69605

 Excited State   9:      Singlet-A      4.7429 eV  261.41 nm  f=0.0976  <S**2>=0.000
      83 -> 86         0.69405

 Excited State  10:      Singlet-A      4.8612 eV  255.05 nm  f=0.0016  <S**2>=0.000
      77 -> 84         0.13964
      82 -> 85        -0.34020
      82 -> 86        -0.24587
      82 -> 87        -0.11816
      82 -> 88         0.19488
      83 -> 87         0.43383
      83 -> 88         0.23505

 Excited State  11:      Singlet-A      4.8771 eV  254.22 nm  f=0.0026  <S**2>=0.000
      77 -> 84         0.66604
      78 -> 84         0.14404

 Excited State  12:      Singlet-A      5.0736 eV  244.37 nm  f=0.0033  <S**2>=0.000
      82 -> 85         0.60549
      82 -> 86        -0.22487
      82 -> 88         0.12122
      83 -> 87         0.23365

 Excited State  13:      Singlet-A      5.1673 eV  239.94 nm  f=0.0197  <S**2>=0.000
      76 -> 84         0.68816
```

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Excited State  14:      Singlet-A      5.2756 eV  235.01 nm  f=0.0516  <S**2>=0.000
     82 -> 86         0.50485
     82 -> 88         0.14163
     83 -> 87         0.38480
     83 -> 88        -0.23059

Excited State  15:      Singlet-A      5.3515 eV  231.68 nm  f=0.0370  <S**2>=0.000
     82 -> 86         0.34712
     82 -> 87        -0.26737
     83 -> 87        -0.13759
     83 -> 88         0.50976

Excited State  16:      Singlet-A      5.4457 eV  227.67 nm  f=0.0025  <S**2>=0.000
     72 -> 84         0.43021
     73 -> 84         0.52176
     75 -> 84        -0.18175

Excited State  17:      Singlet-A      5.4714 eV  226.60 nm  f=0.0003  <S**2>=0.000
     72 -> 84         0.54618
     73 -> 84        -0.43311

Excited State  18:      Singlet-A      5.7052 eV  217.32 nm  f=0.0035  <S**2>=0.000
     71 -> 84         0.69200

Excited State  19:      Singlet-A      5.7501 eV  215.62 nm  f=0.0065  <S**2>=0.000
     74 -> 84         0.27303
     79 -> 85         0.15895
     80 -> 85        -0.32463
     80 -> 86        -0.26695
     81 -> 85         0.34086
     81 -> 86        -0.28276

Excited State  20:      Singlet-A      5.8129 eV  213.29 nm  f=0.0825  <S**2>=0.000
     82 -> 87        -0.42568
     82 -> 88         0.12454
     83 -> 87        -0.10356
     83 -> 88        -0.21143
     83 -> 89         0.42937
     83 -> 91         0.11982

Excited State  21:      Singlet-A      5.8197 eV  213.04 nm  f=0.0514  <S**2>=0.000
     74 -> 84         0.61612
     80 -> 85         0.13757
     80 -> 86         0.18906
     81 -> 86         0.16106

Excited State  22:      Singlet-A      5.8768 eV  210.97 nm  f=0.0239  <S**2>=0.000
     70 -> 84         0.58750
     82 -> 87         0.11342
     83 -> 89         0.29170

Excited State  23:      Singlet-A      5.8922 eV  210.42 nm  f=0.0756  <S**2>=0.000
     70 -> 84        -0.33761
     82 -> 87         0.17579
     82 -> 88        -0.28773
     83 -> 87         0.12366
     83 -> 88         0.17694
     83 -> 89         0.39445
     83 -> 90         0.10584

Excited State  24:      Singlet-A      5.9547 eV  208.21 nm  f=0.1758  <S**2>=0.000
     81 -> 85         0.14920
     81 -> 86         0.27613
     82 -> 87         0.32176
     82 -> 88         0.43520
     83 -> 89         0.16030
     83 -> 91         0.10023

Excited State  25:      Singlet-A      6.1300 eV  202.26 nm  f=0.1566  <S**2>=0.000
     68 -> 84        -0.13962
     69 -> 84         0.32556
     80 -> 85         0.10947
     80 -> 86        -0.10163
     81 -> 85         0.36171
     81 -> 86         0.30710
     82 -> 87        -0.13112
     82 -> 88        -0.15134
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83 -> 90         0.12074
83 -> 91        -0.14886
```
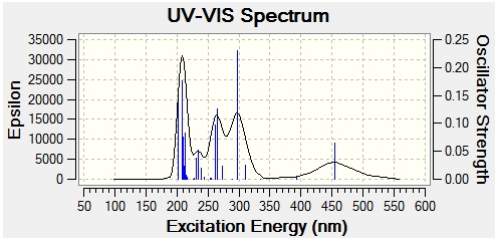
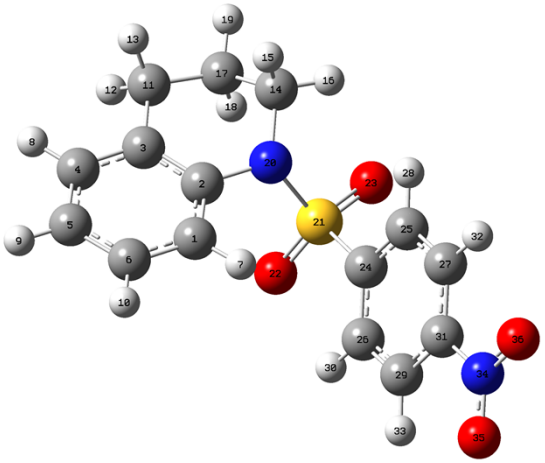



1-(4-nitro-benzenesulfonyl)-1,2,3,4-tetrahydroquinoline *out* conformer (B3LyP/6-31+G(d,p), energy= -1388.52425824 a.u.)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.279290	1.750257	-0.136266
2	6	0	-2.099740	0.622036	-0.290793
3	6	0	-3.501533	0.756410	-0.311303
4	6	0	-4.040935	2.042189	-0.147025
5	6	0	-3.231147	3.161148	0.041326
6	6	0	-1.839889	3.012608	0.043726
7	1	0	-0.201216	1.640054	-0.164134
8	1	0	-5.122088	2.157012	-0.163610
9	1	0	-3.679207	4.141200	0.174245
10	1	0	-1.193093	3.875450	0.169418
11	6	0	-4.429456	-0.417707	-0.568506
12	1	0	-5.251733	-0.399175	0.155207
13	1	0	-4.891246	-0.270276	-1.554359
14	6	0	-2.346508	-1.663477	-1.197664
15	1	0	-2.428974	-1.296805	-2.226688
16	1	0	-1.822385	-2.617068	-1.219257
17	6	0	-3.721565	-1.778071	-0.542765
18	1	0	-3.596253	-2.132203	0.487198
19	1	0	-4.321789	-2.527002	-1.069956
20	7	0	-1.500279	-0.675987	-0.477975
21	16	0	-0.529676	-1.279074	0.782583
22	8	0	-0.911451	-0.695083	2.078958
23	8	0	-0.491677	-2.744463	0.633401
24	6	0	1.127022	-0.672652	0.392741
25	6	0	1.688297	-0.974696	-0.852166
26	6	0	1.836068	0.022658	1.373320
27	6	0	2.988387	-0.562639	-1.127351
28	1	0	1.123427	-1.515724	-1.602622
29	6	0	3.140139	0.436601	1.102534
30	1	0	1.375785	0.243107	2.328848
31	6	0	3.690119	0.136242	-0.142372
32	1	0	3.451126	-0.776466	-2.081974

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     33          1           0        3.716333    0.980520    1.839700
     34          7           0        5.064783    0.574841   -0.432154
     35          8           0        5.674219    1.192325    0.444107
     36          8           0        5.539509    0.302863   -1.537346
 ---------------------------------------------------------------------

Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      2.7016 eV  458.93 nm  f=0.0251  <S**2>=0.000
      83 -> 84         0.70498
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      3.2053 eV  386.81 nm  f=0.0042  <S**2>=0.000
      82 -> 84         0.70581

 Excited State   3:      Singlet-A      3.7069 eV  334.47 nm  f=0.0000  <S**2>=0.000
      78 -> 84         0.68862
      78 -> 86         0.11866

 Excited State   4:      Singlet-A      3.9910 eV  310.66 nm  f=0.0320  <S**2>=0.000
      80 -> 84         0.58068
      81 -> 84         0.38120

 Excited State   5:      Singlet-A      4.1344 eV  299.89 nm  f=0.1903  <S**2>=0.000
      80 -> 84        -0.38016
      81 -> 84         0.58959

 Excited State   6:      Singlet-A      4.2951 eV  288.66 nm  f=0.0005  <S**2>=0.000
      74 -> 84         0.65357
      74 -> 86         0.10663
      75 -> 84         0.20888

 Excited State   7:      Singlet-A      4.5158 eV  274.56 nm  f=0.0241  <S**2>=0.000
      79 -> 84         0.16854
      83 -> 85         0.66812

 Excited State   8:      Singlet-A      4.5683 eV  271.40 nm  f=0.1806  <S**2>=0.000
      79 -> 84         0.67007
      83 -> 85        -0.17681

 Excited State   9:      Singlet-A      4.7594 eV  260.50 nm  f=0.0210  <S**2>=0.000
      83 -> 86         0.67653

 Excited State  10:      Singlet-A      4.9402 eV  250.97 nm  f=0.0116  <S**2>=0.000
      82 -> 85        -0.21308
      82 -> 87        -0.24203
      82 -> 88        -0.20539
      83 -> 86        -0.14517
      83 -> 87        -0.39170
      83 -> 88         0.40270

 Excited State  11:      Singlet-A      5.0030 eV  247.82 nm  f=0.0136  <S**2>=0.000
      76 -> 84         0.28037
      77 -> 84         0.63312

 Excited State  12:      Singlet-A      5.0858 eV  243.78 nm  f=0.0159  <S**2>=0.000
      76 -> 84         0.12099
      82 -> 85         0.60212
      83 -> 87        -0.32290

 Excited State  13:      Singlet-A      5.0918 eV  243.50 nm  f=0.0017  <S**2>=0.000
      76 -> 84         0.62140
      77 -> 84        -0.28557
      82 -> 85        -0.11473

 Excited State  14:      Singlet-A      5.2079 eV  238.07 nm  f=0.1613  <S**2>=0.000
      82 -> 85         0.26538
      82 -> 86         0.11765
      82 -> 87        -0.20779
      83 -> 87         0.40714
      83 -> 88         0.42949

 Excited State  15:      Singlet-A      5.3225 eV  232.94 nm  f=0.0212  <S**2>=0.000
      82 -> 86         0.69244

 Excited State  16:      Singlet-A      5.5065 eV  225.16 nm  f=0.0015  <S**2>=0.000
```

```
     72 -> 84        -0.31385
     74 -> 84        -0.14308
     75 -> 84         0.60910

Excited State  17:      Singlet-A      5.5255 eV  224.39 nm  f=0.0106  <S**2>=0.000
     72 -> 84         0.59965
     74 -> 84        -0.18468
     75 -> 84         0.28666

Excited State  18:      Singlet-A      5.7437 eV  215.86 nm  f=0.0219  <S**2>=0.000
     73 -> 84         0.24191
     79 -> 85         0.16376
     80 -> 85        -0.23617
     80 -> 86         0.28214
     81 -> 85         0.41144
     81 -> 86         0.16775
     82 -> 87         0.15688
     83 -> 88         0.11372
     83 -> 89        -0.10567

Excited State  19:      Singlet-A      5.7807 eV  214.48 nm  f=0.0086  <S**2>=0.000
     70 -> 84         0.40547
     71 -> 84         0.48968
     82 -> 87         0.14931
     83 -> 89        -0.12879

Excited State  20:      Singlet-A      5.7934 eV  214.01 nm  f=0.0624  <S**2>=0.000
     70 -> 84        -0.16619
     71 -> 84        -0.21021
     73 -> 84        -0.19406
     81 -> 86        -0.10757
     81 -> 88        -0.11192
     82 -> 87         0.38109
     83 -> 88         0.21291
     83 -> 89        -0.32205
     83 -> 90         0.11577

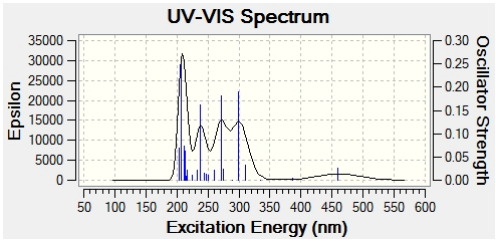
Excited State  21:      Singlet-A      5.8245 eV  212.87 nm  f=0.0553  <S**2>=0.000
     73 -> 84         0.60004
     80 -> 85         0.13313
     80 -> 86        -0.22111
     81 -> 85        -0.11952
     81 -> 86        -0.13161

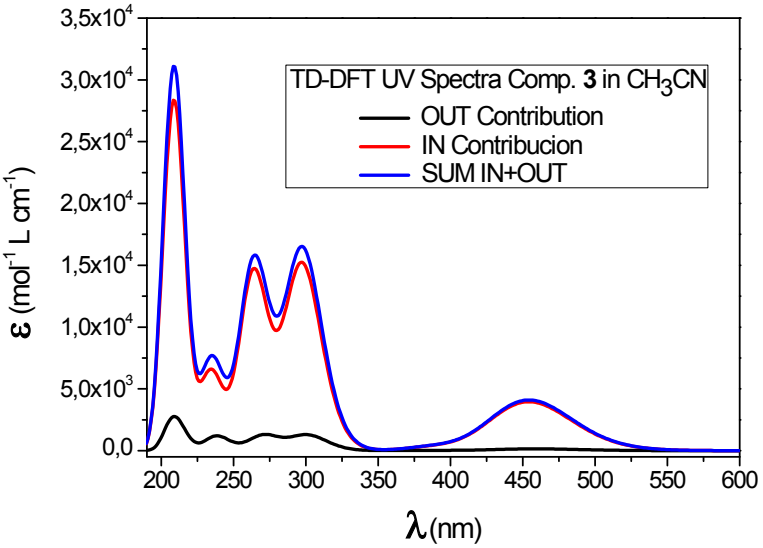
Excited State  22:      Singlet-A      5.8592 eV  211.61 nm  f=0.0044  <S**2>=0.000
     70 -> 84         0.52910
     71 -> 84        -0.42891
     83 -> 89        -0.10892

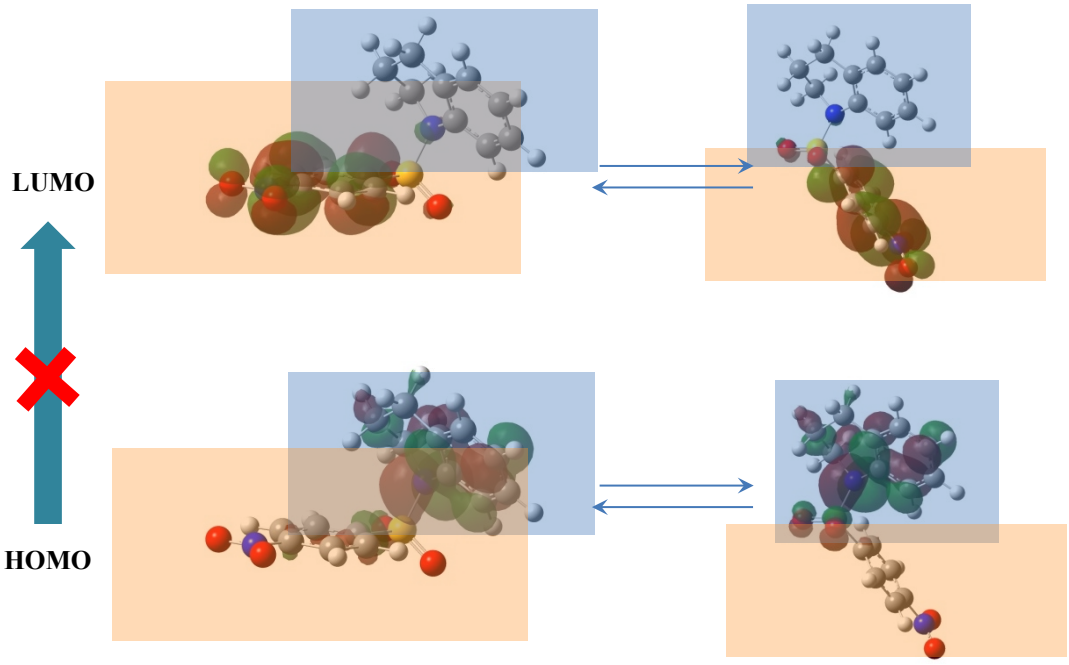
Excited State  23:      Singlet-A      5.8721 eV  211.14 nm  f=0.0734  <S**2>=0.000
     81 -> 86        -0.12731
     81 -> 88        -0.11276
     82 -> 87         0.18291
     82 -> 88         0.24578
     83 -> 88         0.17833
     83 -> 89         0.51997

Excited State  24:      Singlet-A      5.9834 eV  207.21 nm  f=0.2534  <S**2>=0.000
     81 -> 87         0.14842
     81 -> 88         0.11481
     82 -> 87        -0.28621
     82 -> 88         0.51884
     83 -> 89        -0.15966
     83 -> 91         0.15849

Excited State  25:      Singlet-A      6.0783 eV  203.98 nm  f=0.0690  <S**2>=0.000
     79 -> 85        -0.21723
     80 -> 85         0.10609
     81 -> 85         0.45428
     81 -> 86        -0.38662
     82 -> 88        -0.12958
     83 -> 90        -0.10975
     83 -> 91        -0.10188
```



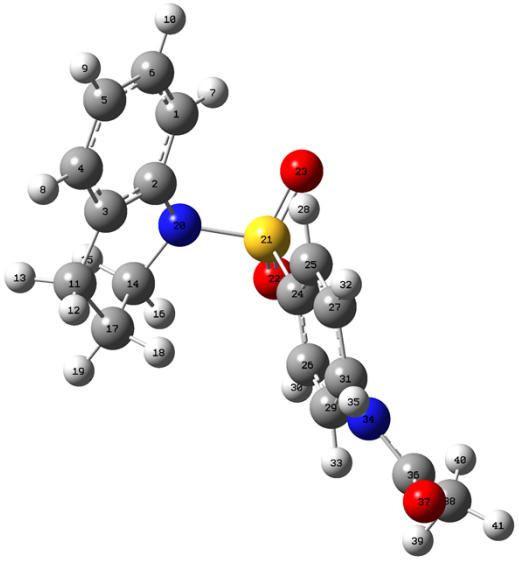




3-*in*
91.3%

3-*out*
8.7%

1-(4-acetamide-benzenesulfonyl)-1,2,3,4-tetrahydroquinoline *in* conformer (B3LyP/6-31+G(d,p), energy= -1392.05247788 a.u.)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.387679	0.414453	-1.288425
2	6	0	-2.772063	0.234694	-0.036126
3	6	0	-2.717625	1.302832	0.884080
4	6	0	-3.248017	2.542619	0.491906
5	6	0	-3.816853	2.735339	-0.765076
6	6	0	-3.891647	1.659232	-1.656716
7	1	0	-3.462822	-0.426629	-1.964706
8	1	0	-3.207792	3.368856	1.197779
9	1	0	-4.212500	3.708184	-1.041178
10	1	0	-4.356400	1.782403	-2.630353
11	6	0	-2.185630	1.142787	2.296554
12	1	0	-1.524750	1.982742	2.537476
13	1	0	-3.038231	1.221984	2.984977
14	6	0	-2.202096	-1.314188	1.802933
15	1	0	-3.239291	-1.388418	2.149508
16	1	0	-1.734542	-2.285211	1.959573
17	6	0	-1.468864	-0.189810	2.533671
18	1	0	-0.433966	-0.138482	2.180476
19	1	0	-1.430221	-0.415096	3.604527
20	7	0	-2.275958	-1.066281	0.339434
21	16	0	-1.071756	-1.810911	-0.614252
22	8	0	-0.871930	-3.145819	-0.025226
23	8	0	-1.501550	-1.697150	-2.016680
24	6	0	0.470122	-0.908326	-0.460168
25	6	0	0.656634	0.269848	-1.193224
26	6	0	1.463988	-1.379942	0.400832
27	6	0	1.854313	0.964968	-1.069480
28	1	0	-0.109380	0.627775	-1.871470
29	6	0	2.657870	-0.672810	0.531228
30	1	0	1.306025	-2.286627	0.973377
31	6	0	2.870317	0.496507	-0.216351
32	1	0	2.013758	1.868909	-1.648972
33	1	0	3.403561	-1.026424	1.231298
34	7	0	4.048417	1.264774	-0.115927
35	1	0	3.937961	2.262261	-0.266482
36	6	0	5.370070	0.903462	0.029893
37	8	0	6.221757	1.794726	0.107879
38	6	0	5.753201	-0.557454	0.062823
39	1	0	5.727249	-0.929385	1.092391
40	1	0	5.099510	-1.184013	-0.546867
41	1	0	6.780274	-0.637043	-0.295772

```
Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      4.1715 eV  297.22 nm  f=0.2971  <S**2>=0.000
      87 -> 88         0.70139
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      4.6484 eV  266.72 nm  f=0.0025  <S**2>=0.000
      83 -> 88        -0.19696
      86 -> 88         0.17549
      87 -> 89         0.62060

 Excited State   3:      Singlet-A      4.6863 eV  264.57 nm  f=0.0624  <S**2>=0.000
      85 -> 88         0.19191
      86 -> 88         0.58048
      87 -> 89        -0.19742
      87 -> 90        -0.15398
      87 -> 91        -0.17980

 Excited State   4:      Singlet-A      4.7949 eV  258.58 nm  f=0.3705  <S**2>=0.000
      85 -> 88         0.54924
      86 -> 88        -0.30179
      87 -> 90        -0.25523

 Excited State   5:      Singlet-A      4.9413 eV  250.91 nm  f=0.0276  <S**2>=0.000
      83 -> 88        -0.17771
      85 -> 88         0.34643
      85 -> 89        -0.12265
      85 -> 91         0.13588
      86 -> 88         0.11539
      86 -> 89         0.30943
      86 -> 90        -0.10398
      87 -> 89        -0.12667
      87 -> 90         0.31780
      87 -> 91         0.22897

 Excited State   6:      Singlet-A      4.9896 eV  248.48 nm  f=0.0060  <S**2>=0.000
      83 -> 88         0.23233
      84 -> 88        -0.13808
      85 -> 88         0.12546
      85 -> 89         0.34988
      86 -> 89        -0.31051
      86 -> 90        -0.16260
      87 -> 89         0.20290
      87 -> 90         0.22473
      87 -> 91         0.21573

 Excited State   7:      Singlet-A      5.0352 eV  246.23 nm  f=0.0059  <S**2>=0.000
      83 -> 88         0.20347
      84 -> 88         0.60431
      84 -> 92         0.15608
      84 -> 93         0.18087

 Excited State   8:      Singlet-A      5.1595 eV  240.30 nm  f=0.0851  <S**2>=0.000
      86 -> 89        -0.17328
      86 -> 90         0.16780
      87 -> 90         0.44744
      87 -> 91        -0.43770

 Excited State   9:      Singlet-A      5.3268 eV  232.76 nm  f=0.0108  <S**2>=0.000
      85 -> 89         0.49673
      86 -> 89         0.44412
      86 -> 90         0.10019
      87 -> 91        -0.16571

 Excited State  10:      Singlet-A      5.6161 eV  220.76 nm  f=0.0748  <S**2>=0.000
      83 -> 88        -0.12486
      85 -> 89         0.11618
      85 -> 90        -0.21742
      85 -> 91        -0.17134
      86 -> 90         0.51548
      87 -> 91         0.25698

 Excited State  11:      Singlet-A      5.7025 eV  217.42 nm  f=0.0308  <S**2>=0.000
      83 -> 88        -0.21639
      85 -> 89         0.13930
      85 -> 90        -0.32078
      85 -> 91         0.15727
```

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     86 -> 89        -0.10095
     86 -> 90        -0.10744
     86 -> 91        -0.25016
     87 -> 92         0.37040
     87 -> 93        -0.14029
     87 -> 94         0.13417

Excited State  12:      Singlet-A      5.7134 eV  217.01 nm  f=0.0623  <S**2>=0.000
     82 -> 88        -0.13102
     83 -> 88         0.30092
     84 -> 88        -0.10624
     85 -> 89        -0.17171
     85 -> 91        -0.12246
     86 -> 89         0.12400
     86 -> 90         0.14264
     86 -> 91         0.11365
     87 -> 92         0.46172
     87 -> 93        -0.13230
     87 -> 94         0.11983

Excited State  13:      Singlet-A      5.7773 eV  214.60 nm  f=0.1106  <S**2>=0.000
     83 -> 88         0.34756
     85 -> 89        -0.14883
     85 -> 90        -0.33090
     85 -> 91         0.21788
     86 -> 89         0.11914
     86 -> 91        -0.27629
     87 -> 91        -0.10032
     87 -> 92        -0.21339

Excited State  14:      Singlet-A      5.8469 eV  212.05 nm  f=0.0266  <S**2>=0.000
     82 -> 88         0.64096
     85 -> 91        -0.19807

Excited State  15:      Singlet-A      5.9293 eV  209.10 nm  f=0.0172  <S**2>=0.000
     84 -> 89         0.11502
     85 -> 91         0.20044
     85 -> 92        -0.10518
     86 -> 90         0.10129
     86 -> 91         0.14642
     87 -> 92         0.19400
     87 -> 93         0.50344
     87 -> 94        -0.19159
     87 -> 96        -0.13419

Excited State  16:      Singlet-A      5.9432 eV  208.62 nm  f=0.1042  <S**2>=0.000
     85 -> 90        -0.36595
     85 -> 91        -0.11079
     86 -> 91         0.40323
     86 -> 92        -0.17922
     87 -> 92        -0.12055
     87 -> 94         0.26403
     87 -> 98         0.10228

Excited State  17:      Singlet-A      5.9594 eV  208.05 nm  f=0.0043  <S**2>=0.000
     83 -> 89         0.16957
     84 -> 89         0.66318

Excited State  18:      Singlet-A      6.0222 eV  205.88 nm  f=0.0699  <S**2>=0.000
     85 -> 92         0.20632
     85 -> 93        -0.13312
     86 -> 91        -0.27451
     86 -> 92        -0.15962
     86 -> 93         0.10618
     87 -> 93         0.32819
     87 -> 94         0.40461

Excited State  19:      Singlet-A      6.0342 eV  205.47 nm  f=0.2770  <S**2>=0.000
     82 -> 88         0.16784
     83 -> 89         0.14264
     85 -> 90         0.17554
     85 -> 91         0.43281
     86 -> 90         0.23690
     87 -> 93        -0.12061
     87 -> 94         0.15928
     87 -> 95        -0.14974
     87 -> 96         0.18253
```
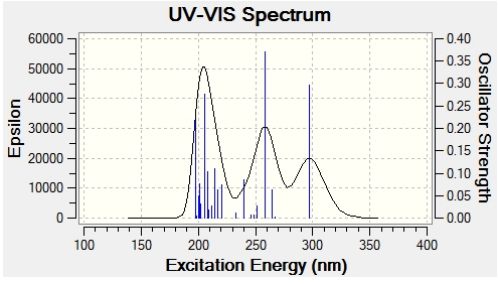
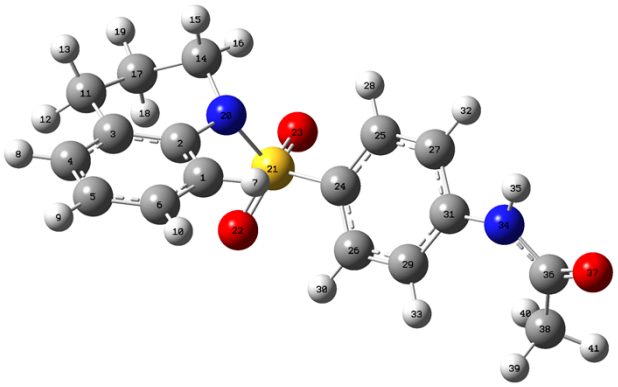

```
Excited State  20:      Singlet-A      6.1242 eV  202.45 nm  f=0.0316  <S**2>=0.000
     84 -> 93         0.10396
     85 -> 92        -0.10486
     86 -> 91         0.11835
     86 -> 92         0.18359
     87 -> 94         0.14254
     87 -> 95         0.50367
     87 -> 96         0.28290

Excited State  21:      Singlet-A      6.1578 eV  201.35 nm  f=0.0766  <S**2>=0.000
     83 -> 89         0.18409
     84 -> 88         0.14371
     84 -> 90         0.10284
     84 -> 92        -0.18872
     84 -> 93        -0.20587
     85 -> 92         0.10826
     86 -> 92        -0.17558
     87 -> 92         0.10344
     87 -> 95         0.39471
     87 -> 96        -0.28250

Excited State  22:      Singlet-A      6.1823 eV  200.55 nm  f=0.0218  <S**2>=0.000
     85 -> 94         0.10420
     86 -> 92         0.42620
     86 -> 93        -0.16300
     87 -> 92        -0.10728
     87 -> 94         0.25114
     87 -> 96        -0.37188
     87 -> 98         0.13776

Excited State  23:      Singlet-A      6.1949 eV  200.14 nm  f=0.0502  <S**2>=0.000
     81 -> 88         0.27118
     84 -> 88        -0.17261
     84 -> 90        -0.12306
     84 -> 91         0.12375
     84 -> 92         0.25397
     84 -> 93         0.25990
     86 -> 92        -0.23955
     87 -> 93        -0.12805
     87 -> 96        -0.25303

Excited State  24:      Singlet-A      6.2508 eV  198.35 nm  f=0.0034  <S**2>=0.000
     80 -> 88         0.14928
     81 -> 88         0.57245
     84 -> 92        -0.10099
     84 -> 93        -0.10318
     85 -> 92         0.18086
     86 -> 94         0.10231
     87 -> 96         0.11040

Excited State  25:      Singlet-A      6.2599 eV  198.06 nm  f=0.2176  <S**2>=0.000
     81 -> 88        -0.16091
     83 -> 89         0.33000
     83 -> 90        -0.13400
     84 -> 92         0.12089
     84 -> 93         0.11857
     85 -> 92         0.35820
     86 -> 93        -0.12495
     86 -> 94         0.18789
     86 -> 95        -0.10364
     87 -> 94        -0.14276
     87 -> 96         0.14496
```



1-(4-acetamide-benzenesulfonyl)-1,2,3,4-tetrahydroquinoline *out* conformer (B3LyP/6-31+G(d,p), energy= -1392.05030682 a.u.)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.527142	1.743802	-0.277014
2	6	0	-2.436640	0.674314	-0.298414
3	6	0	-3.813324	0.907041	-0.110154
4	6	0	-4.232812	2.226312	0.123964
5	6	0	-3.328801	3.285970	0.181657
6	6	0	-1.966503	3.041454	-0.023924
7	1	0	-0.476706	1.556495	-0.466781
8	1	0	-5.293986	2.415878	0.267329
9	1	0	-3.683408	4.294249	0.373283
10	1	0	-1.250661	3.857582	-0.003853
11	6	0	-4.849268	-0.197743	-0.219907
12	1	0	-5.547764	-0.129669	0.621508
13	1	0	-5.445425	-0.008493	-1.123127
14	6	0	-2.972264	-1.574454	-1.151231
15	1	0	-3.178902	-1.187672	-2.155363
16	1	0	-2.524978	-2.561229	-1.256193
17	6	0	-4.243026	-1.604240	-0.303492
18	1	0	-3.995485	-1.981412	0.695692
19	1	0	-4.965489	-2.302168	-0.739768
20	7	0	-1.958157	-0.659735	-0.566291
21	16	0	-0.922787	-1.354223	0.610992
22	8	0	-1.229726	-0.846302	1.962001
23	8	0	-0.956646	-2.811181	0.377258
24	6	0	0.710746	-0.766660	0.169431
25	6	0	1.229613	-1.057999	-1.097118
26	6	0	1.469552	-0.075109	1.113377
27	6	0	2.523259	-0.660080	-1.409356
28	1	0	0.637329	-1.592975	-1.831530
29	6	0	2.762403	0.337470	0.790530
30	1	0	1.048020	0.163006	2.082994
31	6	0	3.306970	0.032475	-0.466007
32	1	0	2.936754	-0.893105	-2.385611
33	1	0	3.323677	0.917028	1.511680
34	7	0	4.597461	0.441070	-0.859541
35	1	0	4.719452	0.625835	-1.849961
36	6	0	5.783394	0.532733	-0.163568
37	8	0	6.784966	0.948491	-0.754859
38	6	0	5.844328	0.100658	1.282568
39	1	0	5.609343	0.946121	1.937652
40	1	0	5.156967	-0.715514	1.512569
41	1	0	6.869076	-0.209447	1.491182

Excitation energies and oscillator strengths:

```
 Excited State   1:      Singlet-A      4.1797 eV  296.63 nm  f=0.0826  <S**2>=0.000
      87 -> 88         0.69809
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      4.6581 eV  266.17 nm  f=0.0084  <S**2>=0.000
      83 -> 88        -0.18627
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     86 -> 88         0.13058
     86 -> 89         0.14058
     87 -> 89         0.63188

Excited State   3:      Singlet-A      4.7162 eV  262.89 nm  f=0.4625  <S**2>=0.000
     86 -> 88         0.67441
     87 -> 89        -0.13430

Excited State   4:      Singlet-A      4.8317 eV  256.61 nm  f=0.1703  <S**2>=0.000
     85 -> 88         0.68647

Excited State   5:      Singlet-A      4.8868 eV  253.71 nm  f=0.0230  <S**2>=0.000
     83 -> 88        -0.22518
     85 -> 90        -0.17206
     85 -> 91         0.14272
     86 -> 88        -0.11477
     86 -> 89         0.37329
     86 -> 90        -0.10717
     87 -> 90         0.26565
     87 -> 91         0.36665

Excited State   6:      Singlet-A      5.0077 eV  247.59 nm  f=0.0081  <S**2>=0.000
     83 -> 88         0.18348
     84 -> 88         0.24505
     85 -> 89         0.27399
     86 -> 89        -0.27384
     86 -> 90        -0.19073
     87 -> 89         0.23900
     87 -> 90         0.10575
     87 -> 91         0.34843

Excited State   7:      Singlet-A      5.0317 eV  246.41 nm  f=0.0075  <S**2>=0.000
     83 -> 88        -0.22623
     84 -> 88         0.57724
     84 -> 92        -0.15246
     84 -> 93        -0.18387
     86 -> 89         0.11578

Excited State   8:      Singlet-A      5.1170 eV  242.30 nm  f=0.1149  <S**2>=0.000
     85 -> 88         0.10716
     86 -> 89        -0.16581
     87 -> 90         0.59357
     87 -> 91        -0.25866

Excited State   9:      Singlet-A      5.3742 eV  230.70 nm  f=0.0514  <S**2>=0.000
     85 -> 89         0.56473
     86 -> 89         0.35333
     87 -> 91        -0.17358

Excited State  10:      Singlet-A      5.5690 eV  222.63 nm  f=0.0296  <S**2>=0.000
     82 -> 88         0.18108
     82 -> 91        -0.10704
     83 -> 88        -0.21893
     85 -> 89         0.18160
     85 -> 91        -0.19301
     86 -> 89        -0.15878
     86 -> 90         0.47006
     87 -> 91         0.23236

Excited State  11:      Singlet-A      5.6996 eV  217.53 nm  f=0.0065  <S**2>=0.000
     82 -> 88         0.63750
     85 -> 90         0.12964
     86 -> 90        -0.21739

Excited State  12:      Singlet-A      5.7280 eV  216.45 nm  f=0.0039  <S**2>=0.000
     85 -> 90         0.40513
     86 -> 91         0.37651
     87 -> 91         0.11955
     87 -> 92        -0.31266
     87 -> 94         0.11355

Excited State  13:      Singlet-A      5.7635 eV  215.12 nm  f=0.0494  <S**2>=0.000
     83 -> 88         0.23477
     85 -> 91        -0.15242
     86 -> 89         0.10609
     86 -> 90         0.12939
     86 -> 91         0.23518
     87 -> 91         0.10715
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     87 -> 92         0.45857
     87 -> 93        -0.18041
     87 -> 94        -0.14883

Excited State  14:      Singlet-A      5.7893 eV  214.16 nm  f=0.1521  <S**2>=0.000
     82 -> 88         0.17180
     83 -> 88         0.39719
     85 -> 89        -0.17458
     86 -> 89         0.20475
     86 -> 90         0.24037
     86 -> 91        -0.22978
     87 -> 92        -0.20924
     87 -> 94         0.12616

Excited State  15:      Singlet-A      5.9145 eV  209.63 nm  f=0.0873  <S**2>=0.000
     82 -> 88         0.11419
     85 -> 90        -0.28618
     85 -> 91         0.12975
     86 -> 90         0.12105
     86 -> 91         0.37114
     87 -> 91        -0.10955
     87 -> 93         0.37205
     87 -> 96        -0.10199

Excited State  16:      Singlet-A      5.9405 eV  208.71 nm  f=0.0923  <S**2>=0.000
     84 -> 89         0.45734
     85 -> 90         0.20186
     85 -> 91         0.11492
     86 -> 91        -0.14087
     86 -> 92         0.15292
     87 -> 92         0.18777
     87 -> 93         0.28841
     87 -> 94         0.14202

Excited State  17:      Singlet-A      5.9585 eV  208.08 nm  f=0.0538  <S**2>=0.000
     83 -> 89        -0.14869
     84 -> 89         0.49177
     85 -> 90        -0.18400
     85 -> 91        -0.11312
     86 -> 91         0.11934
     86 -> 92        -0.11533
     87 -> 92        -0.18677
     87 -> 93        -0.27890
     87 -> 94        -0.13457

Excited State  18:      Singlet-A      5.9830 eV  207.23 nm  f=0.1157  <S**2>=0.000
     82 -> 89        -0.11343
     82 -> 90         0.12745
     85 -> 91         0.34033
     85 -> 92        -0.12537
     86 -> 91         0.18225
     86 -> 92         0.20119
     86 -> 93        -0.16663
     87 -> 93        -0.27484
     87 -> 94         0.34636

Excited State  19:      Singlet-A      6.0346 eV  205.45 nm  f=0.1463  <S**2>=0.000
     82 -> 91        -0.12291
     85 -> 90         0.20170
     85 -> 91         0.39812
     86 -> 90         0.16774
     86 -> 92        -0.18904
     87 -> 94        -0.33437
     87 -> 95        -0.20087

Excited State  20:      Singlet-A      6.1451 eV  201.76 nm  f=0.0343  <S**2>=0.000
     83 -> 89         0.11123
     85 -> 92        -0.14068
     86 -> 92         0.39613
     87 -> 92        -0.15892
     87 -> 94        -0.35098
     87 -> 95         0.30060
     87 -> 96        -0.10094
     87 -> 97         0.11590

Excited State  21:      Singlet-A      6.1638 eV  201.15 nm  f=0.0433  <S**2>=0.000
     82 -> 89        -0.15744
     83 -> 89         0.22285
```
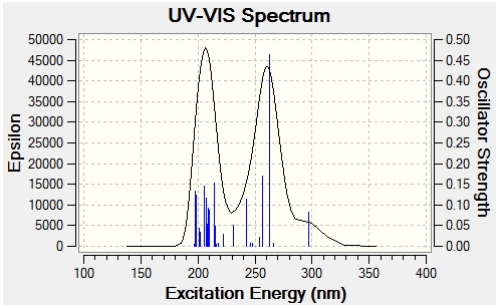
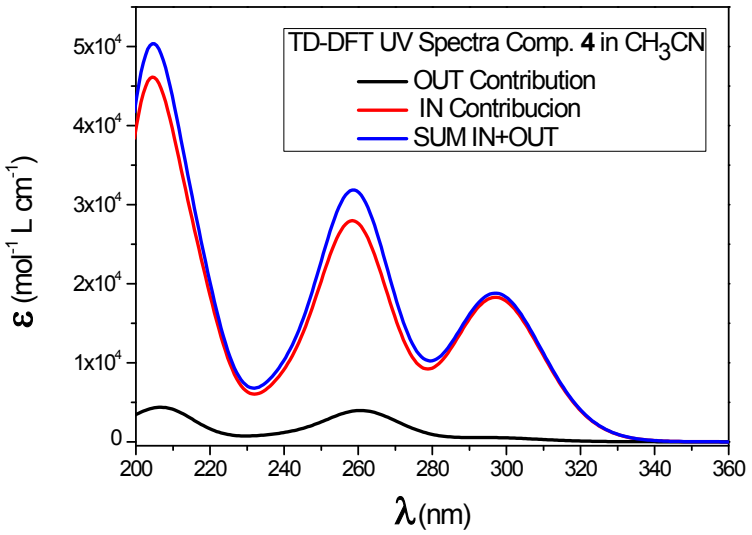
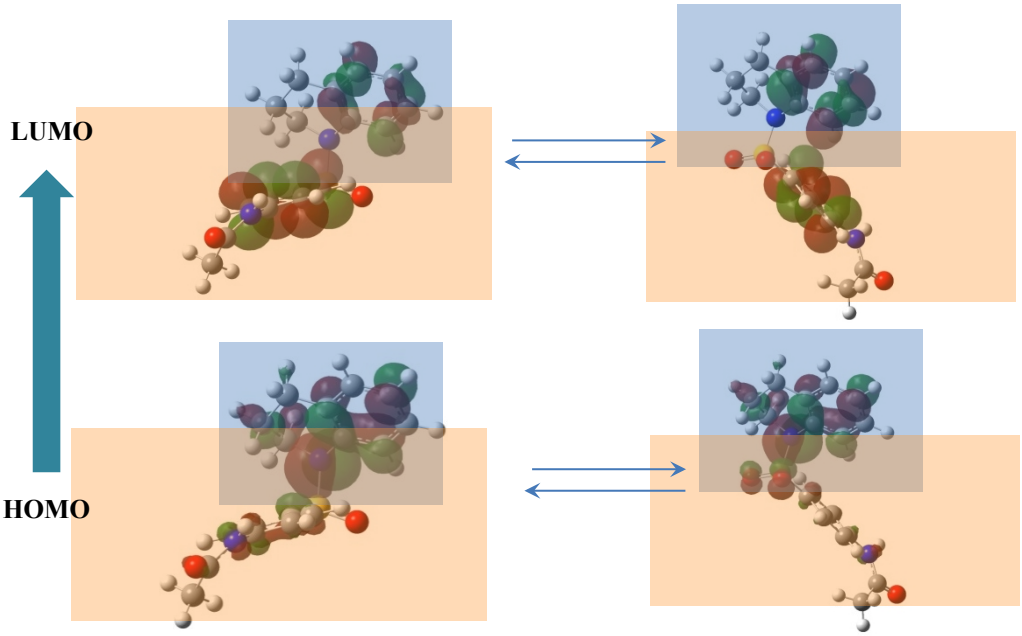

```
      84 -> 93         0.10038
      85 -> 93        -0.14165
      86 -> 92        -0.16701
      86 -> 93         0.26468
      86 -> 94        -0.10286
      87 -> 95         0.37345
      87 -> 96         0.24658

Excited State  22:      Singlet-A      6.1750 eV  200.78 nm  f=0.0149  <S**2>=0.000
      83 -> 89        -0.17775
      84 -> 88        -0.16481
      84 -> 92        -0.24381
      84 -> 93        -0.26108
      85 -> 93         0.10600
      86 -> 92        -0.13391
      86 -> 93        -0.22150
      87 -> 93         0.10188
      87 -> 95         0.37679

Excited State  23:      Singlet-A      6.2359 eV  198.82 nm  f=0.1249  <S**2>=0.000
      81 -> 88        -0.10008
      82 -> 89        -0.28620
      83 -> 89         0.29199
      83 -> 90        -0.10488
      84 -> 88        -0.12142
      84 -> 92        -0.21621
      84 -> 93        -0.22021
      85 -> 91        -0.10745
      85 -> 92         0.14536
      85 -> 94        -0.10546
      86 -> 92         0.19836
      87 -> 95        -0.19019

Excited State  24:      Singlet-A      6.2756 eV  197.57 nm  f=0.1331  <S**2>=0.000
      81 -> 88        -0.17552
      82 -> 89         0.33035
      83 -> 89         0.30498
      83 -> 90        -0.12176
      84 -> 92        -0.12886
      84 -> 93        -0.13027
      85 -> 92        -0.26415
      85 -> 94         0.10391
      86 -> 93         0.13154
      86 -> 94         0.17245
      87 -> 96        -0.14305

Excited State  25:      Singlet-A      6.2938 eV  196.99 nm  f=0.0040  <S**2>=0.000
      81 -> 88         0.32777
      82 -> 89        -0.11819
      83 -> 89        -0.10750
      84 -> 92        -0.10798
      85 -> 92        -0.29824
      85 -> 94         0.10343
      86 -> 93         0.20076
      86 -> 94         0.14861
      87 -> 96         0.29049
      87 -> 97         0.13254
      87 -> 98        -0.16933
```



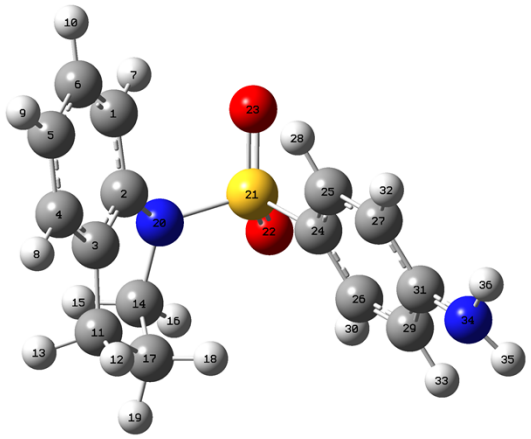




4-*in*
90.9%

4-*out*
9.1%

1-(4-amine-benzenesulfonyl)-1,2,3,4-tetrahydroquinoline *in* conformer (B3LyP/6-31+G(d,p), energy= -1239.38845782 a.u.)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.515614	-0.115210	-1.342016
2	6	0	1.932665	0.041782	-0.070684
3	6	0	2.103241	-0.959382	0.910047
4	6	0	2.823860	-2.113459	0.562001
5	6	0	3.364308	-2.288950	-0.710003
6	6	0	3.212190	-1.276970	-1.664659
7	1	0	2.412025	0.679029	-2.069233
8	1	0	2.956805	-2.886810	1.314922
9	1	0	3.910920	-3.195986	-0.950355
10	1	0	3.648488	-1.383092	-2.653459
11	6	0	1.607899	-0.802075	2.335879
12	1	0	1.127386	-1.730959	2.662598
13	1	0	2.485967	-0.671445	2.983613
14	6	0	1.162398	1.577472	1.701037
15	1	0	2.179499	1.853623	2.003420
16	1	0	0.534492	2.458639	1.823760
17	6	0	0.663753	0.388467	2.521992
18	1	0	-0.351189	0.127221	2.205902
19	1	0	0.609193	0.669846	3.578909
20	7	0	1.236684	1.261646	0.251774
21	16	0	-0.127225	1.714165	-0.688491
22	8	0	-0.558503	3.011997	-0.136670
23	8	0	0.295754	1.641226	-2.097745
24	6	0	-1.449025	0.543775	-0.458495
25	6	0	-1.451732	-0.657209	-1.183310
26	6	0	-2.471767	0.817077	0.460550
27	6	0	-2.469537	-1.580780	-0.985515
28	1	0	-0.672432	-0.861996	-1.908876
29	6	0	-3.491100	-0.105597	0.654425
30	1	0	-2.474134	1.752248	1.009316
31	6	0	-3.507052	-1.324685	-0.060368
32	1	0	-2.472628	-2.506701	-1.553144
33	1	0	-4.287221	0.113086	1.360026
34	7	0	-4.490215	-2.261285	0.171032
35	1	0	-5.341312	-1.952477	0.619653
36	1	0	-4.627853	-2.984717	-0.520797

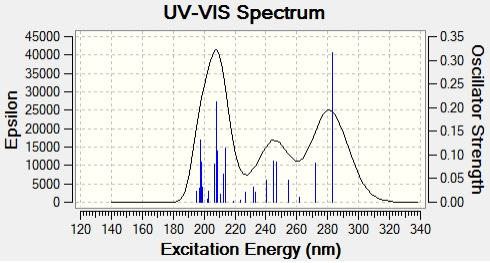
Excitation energies and oscillator strengths:

```
 Excited State   1:      Singlet-A      4.3825 eV  282.91 nm  f=0.3163  <S**2>=0.000
      75 -> 77        -0.15249
      76 -> 77         0.66273
      76 -> 78         0.14632
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      4.5542 eV  272.24 nm  f=0.0817  <S**2>=0.000
      73 -> 77         0.18543
      76 -> 77        -0.12888
```

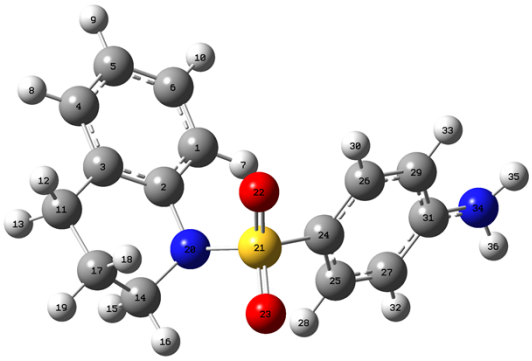
```
     76 -> 78         0.64135

Excited State   3:      Singlet-A      4.7404 eV  261.55 nm  f=0.0099  <S**2>=0.000
     74 -> 77        -0.25608
     74 -> 80        -0.17237
     75 -> 79        -0.25103
     76 -> 79         0.53351
     76 -> 80        -0.15259

Excited State   4:      Singlet-A      4.8686 eV  254.66 nm  f=0.0473  <S**2>=0.000
     75 -> 77         0.60447
     76 -> 77         0.10538
     76 -> 79         0.19618
     76 -> 80         0.27331

Excited State   5:      Singlet-A      5.0182 eV  247.07 nm  f=0.0845  <S**2>=0.000
     74 -> 77        -0.13215
     75 -> 77         0.19049
     75 -> 78         0.45258
     75 -> 79        -0.20371
     76 -> 78        -0.16435
     76 -> 79        -0.14372
     76 -> 80        -0.33794

Excited State   6:      Singlet-A      5.0599 eV  245.03 nm  f=0.0877  <S**2>=0.000
     74 -> 77         0.17654
     75 -> 77        -0.18321
     75 -> 78         0.49530
     75 -> 79         0.15311
     76 -> 79         0.29459
     76 -> 80         0.19382

Excited State   7:      Singlet-A      5.1525 eV  240.63 nm  f=0.0464  <S**2>=0.000
     74 -> 77        -0.34298
     75 -> 78         0.10145
     75 -> 79        -0.29613
     76 -> 79        -0.20799
     76 -> 80         0.44748

Excited State   8:      Singlet-A      5.3228 eV  232.93 nm  f=0.0202  <S**2>=0.000
     74 -> 77        -0.11604
     75 -> 79         0.16512
     75 -> 80         0.14452
     75 -> 81         0.11909
     76 -> 80        -0.11516
     76 -> 81         0.58756
     76 -> 82         0.18213

Excited State   9:      Singlet-A      5.3443 eV  231.99 nm  f=0.0309  <S**2>=0.000
     74 -> 77         0.46786
     74 -> 78        -0.11007
     74 -> 80        -0.21210
     75 -> 79        -0.39527
     76 -> 81         0.20695

Excited State  10:      Singlet-A      5.4648 eV  226.88 nm  f=0.0210  <S**2>=0.000
     74 -> 77         0.12844
     74 -> 78        -0.22451
     74 -> 79        -0.19901
     75 -> 80         0.58093
     76 -> 81        -0.14092

Excited State  11:      Singlet-A      5.5424 eV  223.70 nm  f=0.0053  <S**2>=0.000
     74 -> 78         0.64872
     74 -> 79        -0.15441
     74 -> 80        -0.10799
     75 -> 80         0.16503

Excited State  12:      Singlet-A      5.6648 eV  218.87 nm  f=0.0015  <S**2>=0.000
     74 -> 79         0.13996
     75 -> 81         0.26091
     76 -> 81        -0.21110
     76 -> 82         0.57896

Excited State  13:      Singlet-A      5.8053 eV  213.57 nm  f=0.1137  <S**2>=0.000
     73 -> 77         0.65133
     75 -> 78        -0.10220
     76 -> 78        -0.15332
```

```
Excited State  14:      Singlet-A      5.8344 eV  212.51 nm  f=0.0588  <S**2>=0.000
     72 -> 79         0.10281
     74 -> 79         0.31118
     74 -> 80         0.22919
     75 -> 79        -0.14310
     75 -> 80         0.15192
     75 -> 81         0.16423
     75 -> 82        -0.11309
     76 -> 82        -0.10644
     76 -> 83         0.40413
     76 -> 84         0.18389
     76 -> 85        -0.10703

Excited State  15:      Singlet-A      5.8797 eV  210.87 nm  f=0.0176  <S**2>=0.000
     74 -> 79        -0.15373
     75 -> 81         0.16168
     76 -> 83        -0.14282
     76 -> 84         0.60646
     76 -> 85        -0.11074

Excited State  16:      Singlet-A      5.9346 eV  208.92 nm  f=0.1090  <S**2>=0.000
     72 -> 79        -0.10648
     74 -> 79        -0.27935
     74 -> 80        -0.17449
     75 -> 80        -0.17073
     76 -> 83         0.52278

Excited State  17:      Singlet-A      5.9615 eV  207.98 nm  f=0.2129  <S**2>=0.000
     72 -> 77         0.17252
     72 -> 79         0.10985
     74 -> 79        -0.27891
     74 -> 80         0.44046
     75 -> 79        -0.15379
     75 -> 81        -0.29457
     76 -> 82         0.16088

Excited State  18:      Singlet-A      6.0014 eV  206.59 nm  f=0.0815  <S**2>=0.000
     72 -> 77         0.19143
     74 -> 79        -0.22408
     74 -> 80         0.17969
     75 -> 81         0.47877
     75 -> 82        -0.12154
     76 -> 82        -0.20493
     76 -> 84        -0.19054
     76 -> 86        -0.11537

Excited State  19:      Singlet-A      6.1215 eV  202.54 nm  f=0.0243  <S**2>=0.000
     75 -> 84        -0.22867
     76 -> 84         0.13720
     76 -> 85         0.59455

Excited State  20:      Singlet-A      6.1406 eV  201.91 nm  f=0.0054  <S**2>=0.000
     75 -> 81         0.13819
     75 -> 82         0.39629
     75 -> 84         0.14408
     76 -> 82        -0.13104
     76 -> 86         0.49250

Excited State  21:      Singlet-A      6.2284 eV  199.06 nm  f=0.0311  <S**2>=0.000
     72 -> 77         0.41128
     73 -> 78        -0.18000
     73 -> 79        -0.24172
     73 -> 80        -0.10459
     74 -> 81        -0.32241
     74 -> 82         0.18133
     74 -> 84         0.11302
     75 -> 84         0.10039
     76 -> 85         0.10703

Excited State  22:      Singlet-A      6.2522 eV  198.31 nm  f=0.0839  <S**2>=0.000
     73 -> 78         0.32359
     73 -> 79         0.43864
     73 -> 80         0.18615
     74 -> 81        -0.28953
     74 -> 82         0.15744
     74 -> 84         0.11001
```

```
 Excited State  23:      Singlet-A      6.2696 eV  197.75 nm  f=0.1313  <S**2>=0.000
      72 -> 77         0.43019
      73 -> 79         0.18916
      74 -> 79         0.14160
      74 -> 80        -0.10267
      74 -> 81         0.36263
      74 -> 82        -0.14695
      74 -> 84        -0.12215
      75 -> 82        -0.10016

 Excited State  24:      Singlet-A      6.2944 eV  196.97 nm  f=0.0297  <S**2>=0.000
      72 -> 77        -0.10881
      75 -> 82        -0.20293
      75 -> 83         0.48143
      75 -> 84         0.27937
      76 -> 86         0.18186
      76 -> 87        -0.15399
      76 -> 88        -0.12425
      76 -> 91        -0.11430

 Excited State  25:      Singlet-A      6.3471 eV  195.34 nm  f=0.0234  <S**2>=0.000
      73 -> 78         0.12828
      73 -> 79        -0.15410
      75 -> 82         0.31321
      75 -> 83         0.37833
      75 -> 84        -0.11891
      76 -> 85        -0.11921
      76 -> 86        -0.23199
      76 -> 89        -0.28339
```



1-(4-amine-benzenesulfonyl)-1,2,3,4-tetrahydroquinoline *out* conformer (B3LyP/6-31+G(d,p), energy= -1239.38655597 a.u.)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.718285	1.718861	-0.376031
2	6	0	-1.559181	0.594150	-0.347560
3	6	0	-2.940323	0.746193	-0.111528
4	6	0	-3.432155	2.040765	0.119894
5	6	0	-2.594064	3.154819	0.129028
6	6	0	-1.227768	2.991129	-0.125088
7	1	0	0.333097	1.591300	-0.604548
8	1	0	-4.497295	2.167434	0.299189
9	1	0	-3.003425	4.142451	0.319365

10	1	0	-0.564248	3.850415	-0.145213
11	6	0	-3.910709	-0.420602	-0.170443
12	1	0	-4.575590	-0.388437	0.699970
13	1	0	-4.555573	-0.274083	-1.047815
14	6	0	-1.985820	-1.684856	-1.162543
15	1	0	-2.250126	-1.315112	-2.159769
16	1	0	-1.483956	-2.643439	-1.282354
17	6	0	-3.224681	-1.788874	-0.273589
18	1	0	-2.923555	-2.147951	0.717326
19	1	0	-3.918427	-2.529508	-0.685554
20	7	0	-1.005837	-0.710038	-0.618802
21	16	0	0.062646	-1.344160	0.578296
22	8	0	-0.358450	-0.943171	1.937563
23	8	0	0.170313	-2.787936	0.279518
24	6	0	1.627540	-0.573081	0.240713
25	6	0	2.255642	-0.785743	-0.995012
26	6	0	2.252456	0.192508	1.231529
27	6	0	3.499817	-0.224778	-1.240531
28	1	0	1.773715	-1.382126	-1.762740
29	6	0	3.500941	0.751688	0.986888
30	1	0	1.761224	0.349546	2.185101
31	6	0	4.147472	0.556154	-0.253601
32	1	0	3.983716	-0.386295	-2.199274
33	1	0	3.983261	1.345914	1.757368
34	7	0	5.359847	1.151762	-0.519160
35	1	0	5.910113	1.480443	0.261786
36	1	0	5.906465	0.792788	-1.289251

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 4.4533 eV 278.41 nm f=0.1273 <S**2>=0.000
75 -> 77 0.19508
76 -> 77 0.59764
76 -> 78 -0.26960
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.6036 eV 269.32 nm f=0.0610 <S**2>=0.000
73 -> 77 0.15571
75 -> 77 0.36987
76 -> 77 0.14199
76 -> 78 0.53122
76 -> 80 0.13356

Excited State 3: Singlet-A 4.7819 eV 259.28 nm f=0.3044 <S**2>=0.000
74 -> 79 -0.12618
75 -> 77 0.49227
75 -> 78 -0.14363
75 -> 80 0.11875
76 -> 77 -0.30444
76 -> 78 -0.29207

Excited State 4: Singlet-A 4.8854 eV 253.78 nm f=0.0481 <S**2>=0.000
75 -> 80 -0.11828
76 -> 78 -0.10220
76 -> 79 0.65385

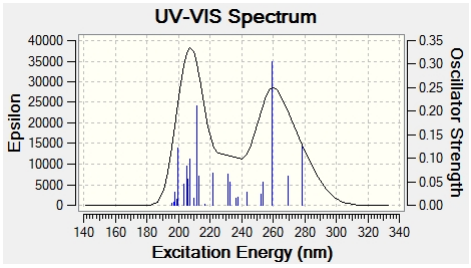
Excited State 5: Singlet-A 4.9105 eV 252.49 nm f=0.0240 <S**2>=0.000
74 -> 79 -0.19070
75 -> 77 -0.24815
75 -> 78 -0.28824
75 -> 80 0.24563
76 -> 80 0.47775

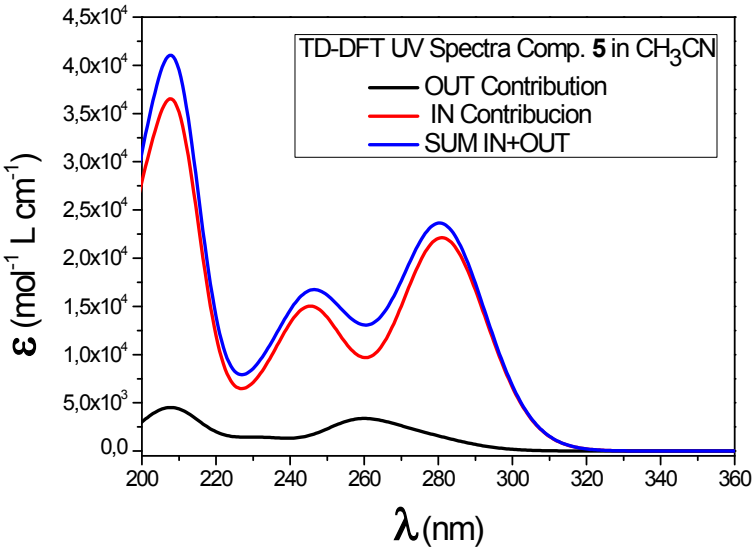
Excited State 6: Singlet-A 5.0922 eV 243.48 nm f=0.0268 <S**2>=0.000
74 -> 77 -0.11016
75 -> 78 0.60087
75 -> 80 0.13389
76 -> 79 0.10054
76 -> 80 0.27173

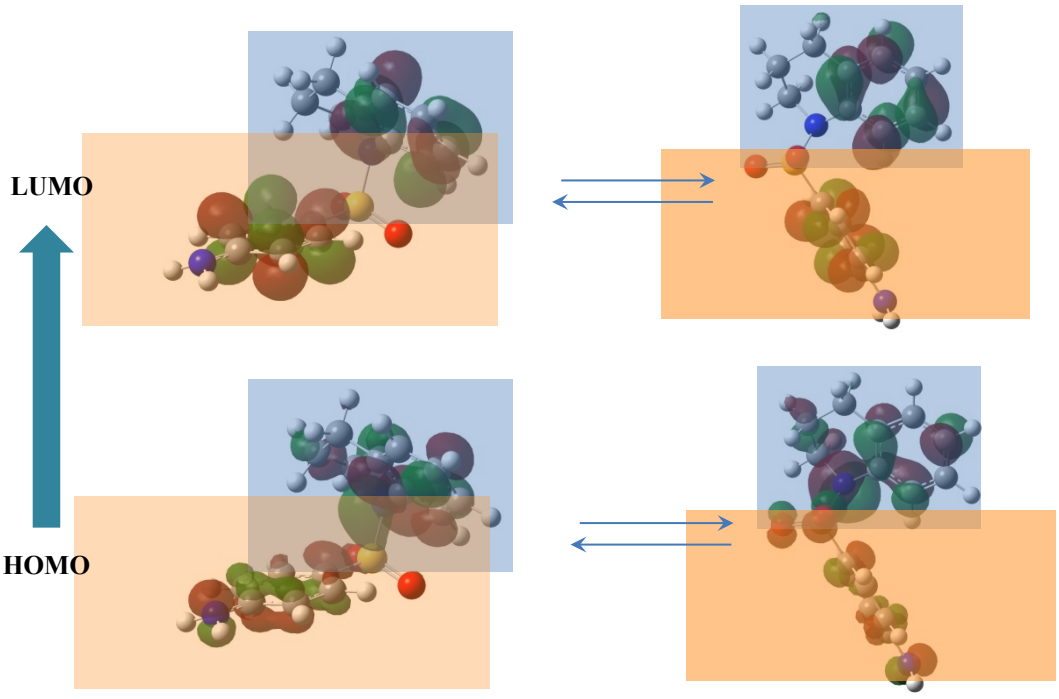
Excited State 7: Singlet-A 5.2134 eV 237.82 nm f=0.0169 <S**2>=0.000
74 -> 77 0.34157
74 -> 78 -0.11357
74 -> 79 0.17198
75 -> 79 0.22285

```
     75 -> 80        -0.33980
     76 -> 79        -0.16937
     76 -> 80         0.35831

Excited State   8:      Singlet-A      5.2451 eV  236.38 nm  f=0.0147  <S**2>=0.000
     74 -> 77         0.40148
     74 -> 78         0.14080
     74 -> 79        -0.12379
     75 -> 79         0.37722
     75 -> 80         0.31793
     76 -> 78         0.10957
     76 -> 80        -0.16215

Excited State   9:      Singlet-A      5.3285 eV  232.68 nm  f=0.0482  <S**2>=0.000
     74 -> 77        -0.27622
     75 -> 79         0.26003
     75 -> 81        -0.11601
     76 -> 81         0.53175
     76 -> 82         0.17398

Excited State  10:      Singlet-A      5.3543 eV  231.56 nm  f=0.0667  <S**2>=0.000
     74 -> 77        -0.31804
     74 -> 78        -0.12720
     74 -> 80         0.10169
     75 -> 79         0.42984
     76 -> 81        -0.37104

Excited State  11:      Singlet-A      5.5868 eV  221.92 nm  f=0.0688  <S**2>=0.000
     74 -> 78         0.63595
     74 -> 79         0.16570
     75 -> 80        -0.19006

Excited State  12:      Singlet-A      5.7181 eV  216.83 nm  f=0.0018  <S**2>=0.000
     75 -> 81        -0.29311
     76 -> 81        -0.22396
     76 -> 82         0.51896
     76 -> 84         0.18586
     76 -> 85         0.13319

Excited State  13:      Singlet-A      5.8158 eV  213.18 nm  f=0.0615  <S**2>=0.000
     72 -> 77        -0.24459
     72 -> 80        -0.18192
     73 -> 77         0.24751
     74 -> 79         0.44288
     75 -> 80         0.29046
     76 -> 82         0.11072
     76 -> 84         0.10743

Excited State  14:      Singlet-A      5.8566 eV  211.70 nm  f=0.2107  <S**2>=0.000
     73 -> 77         0.58065
     73 -> 78         0.10176
     74 -> 79        -0.17927
     74 -> 80        -0.10237
     76 -> 78        -0.13719

Excited State  15:      Singlet-A      5.9118 eV  209.72 nm  f=0.0160  <S**2>=0.000
     72 -> 77         0.14438
     75 -> 81         0.46938
     75 -> 82        -0.17528
     76 -> 82         0.17476
     76 -> 83        -0.35496
     76 -> 84         0.10512

Excited State  16:      Singlet-A      5.9752 eV  207.50 nm  f=0.0992  <S**2>=0.000
     72 -> 79         0.11315
     74 -> 80         0.45566
     75 -> 81         0.12839
     76 -> 83         0.37023
     76 -> 84         0.22775
     76 -> 86         0.11077

Excited State  17:      Singlet-A      6.0097 eV  206.31 nm  f=0.0546  <S**2>=0.000
     74 -> 80        -0.27429
     75 -> 82        -0.17754
     76 -> 82        -0.19049
     76 -> 84         0.52533
     76 -> 85        -0.10071
     76 -> 86         0.10185
```

```
Excited State  18:      Singlet-A      6.0330 eV  205.51 nm  f=0.0831  <S**2>=0.000
     72 -> 79        -0.12327
     73 -> 78        -0.10190
     74 -> 80        -0.30041
     75 -> 81         0.32212
     75 -> 82         0.11774
     76 -> 82         0.24563
     76 -> 83         0.36265
     76 -> 84        -0.12210
     76 -> 85        -0.10040

Excited State  19:      Singlet-A      6.0870 eV  203.69 nm  f=0.0457  <S**2>=0.000
     72 -> 77         0.60355
     74 -> 79         0.20868
     75 -> 80         0.10568
     76 -> 85        -0.14521

Excited State  20:      Singlet-A      6.1001 eV  203.25 nm  f=0.0200  <S**2>=0.000
     72 -> 77         0.11677
     75 -> 82        -0.28405
     76 -> 83         0.17524
     76 -> 85         0.53085
     76 -> 88        -0.11741

Excited State  21:      Singlet-A      6.2099 eV  199.66 nm  f=0.1210  <S**2>=0.000
     73 -> 78         0.50992
     73 -> 79        -0.34936
     73 -> 80        -0.16507
     74 -> 81        -0.15342

Excited State  22:      Singlet-A      6.2327 eV  198.92 nm  f=0.0128  <S**2>=0.000
     74 -> 81         0.17513
     74 -> 82        -0.10020
     75 -> 81         0.11330
     75 -> 82         0.39527
     75 -> 83         0.32187
     76 -> 82        -0.10155
     76 -> 84         0.20408
     76 -> 85         0.17190
     76 -> 86        -0.20734

Excited State  23:      Singlet-A      6.2599 eV  198.06 nm  f=0.0269  <S**2>=0.000
     75 -> 82        -0.32504
     75 -> 83         0.43595
     75 -> 84         0.12709
     76 -> 85        -0.25360
     76 -> 86        -0.24392

Excited State  24:      Singlet-A      6.2967 eV  196.90 nm  f=0.0067  <S**2>=0.000
     72 -> 78         0.16957
     73 -> 79        -0.16146
     74 -> 81         0.38088
     74 -> 82        -0.16543
     74 -> 83        -0.16344
     75 -> 82        -0.12562
     75 -> 84        -0.18790
     75 -> 85         0.11016
     76 -> 86         0.31752
     76 -> 88         0.14948

Excited State  25:      Singlet-A      6.3293 eV  195.89 nm  f=0.0039  <S**2>=0.000
     74 -> 81         0.35310
     74 -> 82        -0.14175
     74 -> 83        -0.11734
     75 -> 83        -0.30606
     75 -> 84         0.24696
     75 -> 85        -0.18325
     76 -> 83         0.14642
     76 -> 86        -0.20843
     76 -> 88        -0.20843
```







5-*in*
88.2%

5-*out*
11.8%

Reference

Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Ioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2010**.