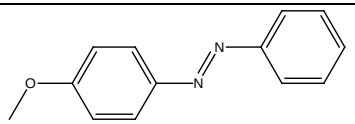
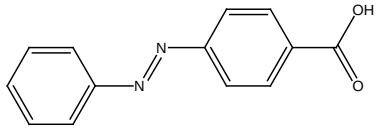
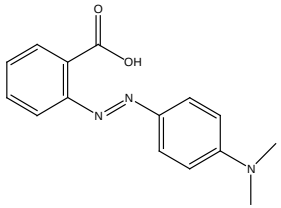
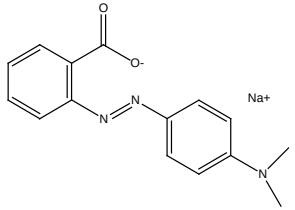
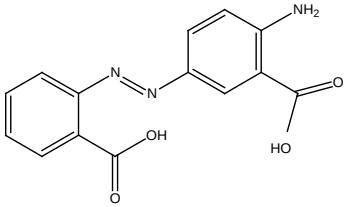
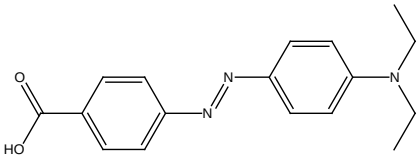
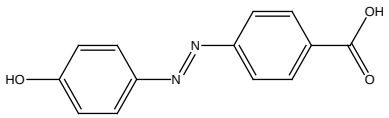
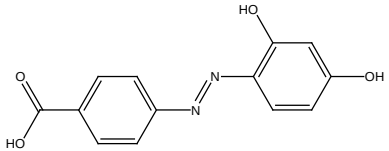
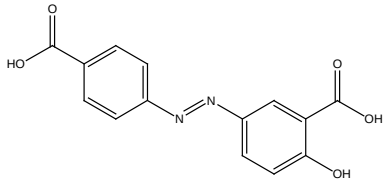
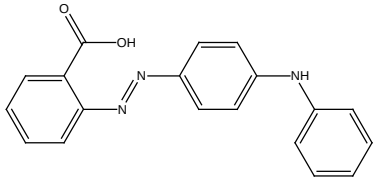
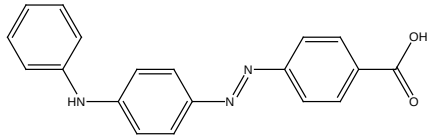
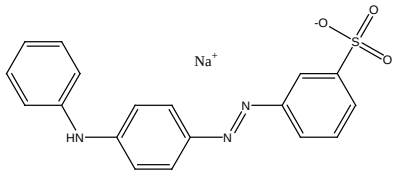
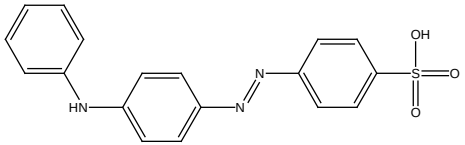
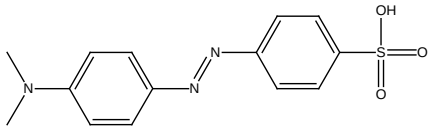
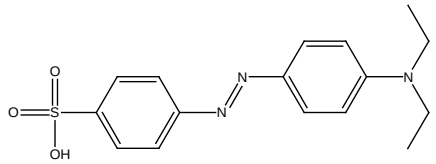
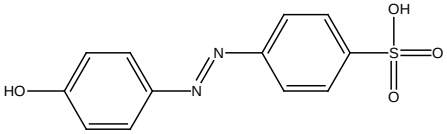
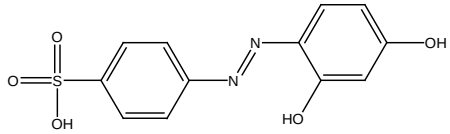
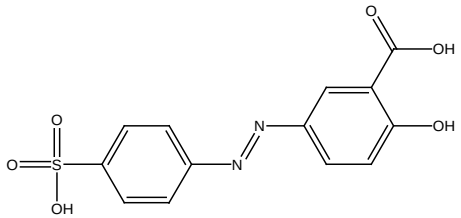
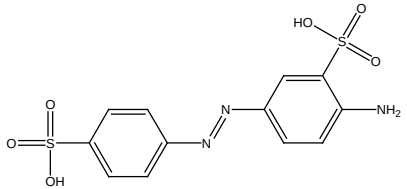
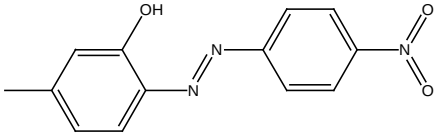
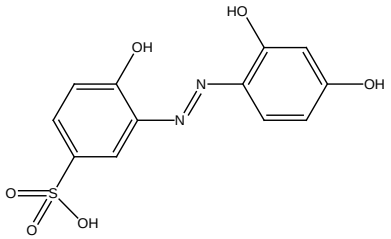
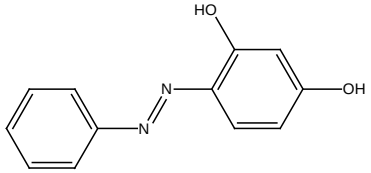
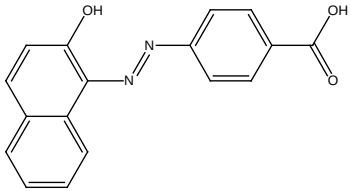
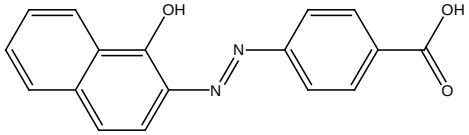
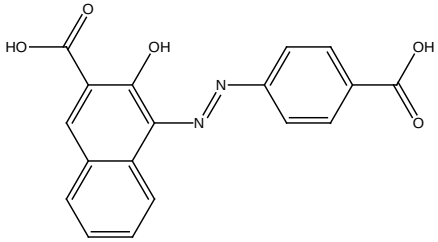
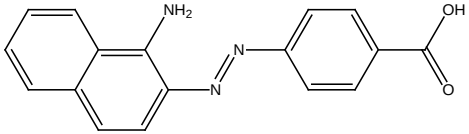
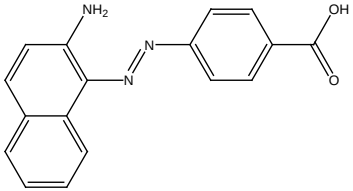
Supplementary Information

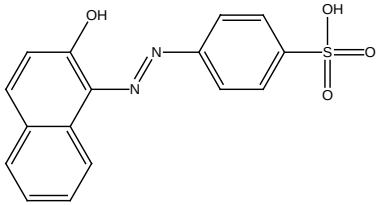
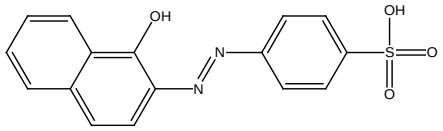
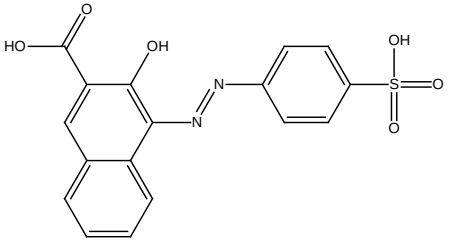
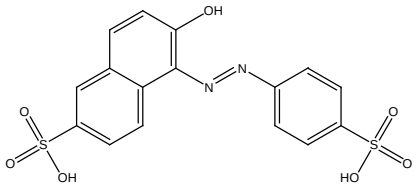
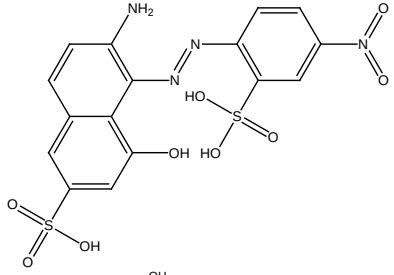
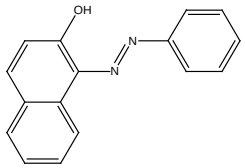
Table S1. Structure of azo-, azo-anilide, diazonium salts derivatives and a*b initio* data for the neutral energy minimized molecules.

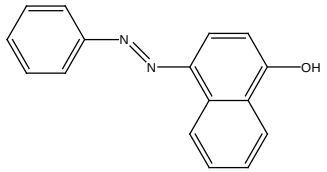
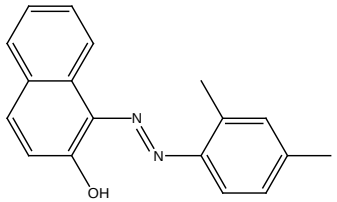
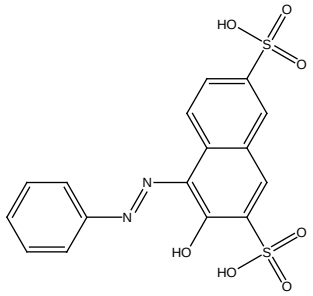
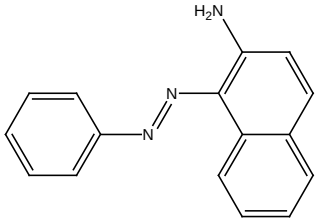
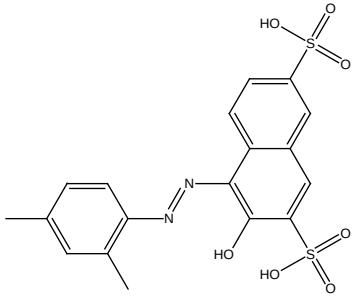
No	CAS	CI	Compound Structure	E(HF/ 3-21G) (a.u.)	ZPE (Hartree/Particle)	Hcorr	Gcorr
1 [a]	2396-60-3			−679.16	0.24	0.26	0.20
2 * [b]				−752.48	0.22	0.24	0.18
3 [b]	493-52-7	13020		−807.20	0.30	0.32	0.25
4 * [b]	845-10-3	13020		−806.61	0.23	0.24	0.18
5 * [a]				−993.77	0.26	0.27	0.21
6 [a]				−962.47	0.36	0.38	0.31

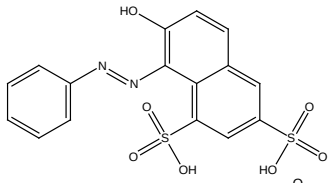
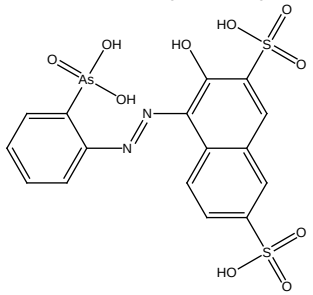
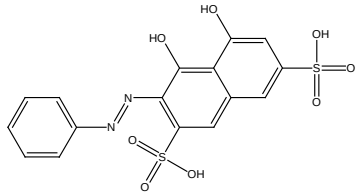
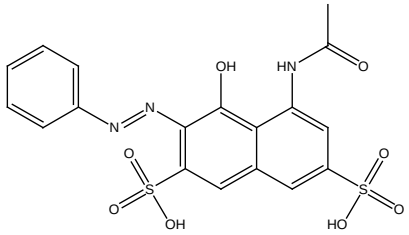
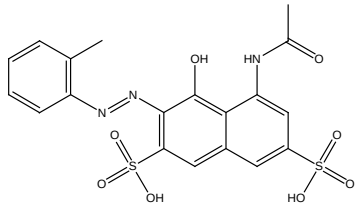
7* [b]				-826.92	0.23	0.24	0.18
8 * [b]				−901.36	0.23	0.25	0.19
9 [b]				−1013.48	0.24	0.26	0.20
10 [c]				−1035.46	0.33	0.35	0.28
11 [c]				−1035.47	0.33	0.35	0.28
12 [a]	587-98-4	13065		−1467.59	0.33	0.35	0.27
13 [c]				−1467.59	0.33	0.35	0.27
14 [b]	547-58-0	13025		−1316.94	0.30	0.32	0.25

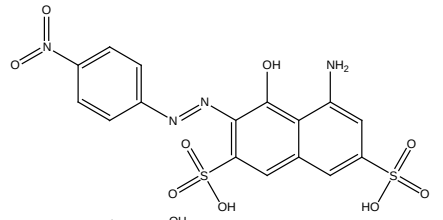
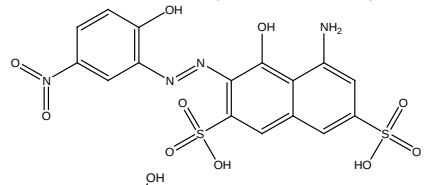
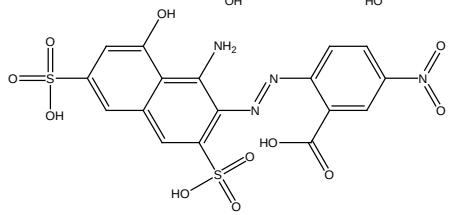
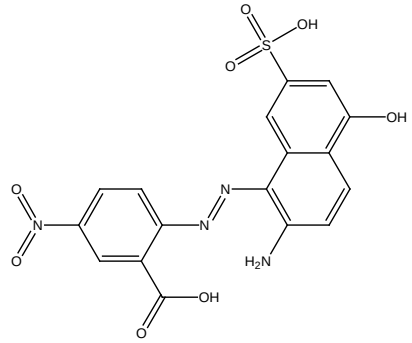
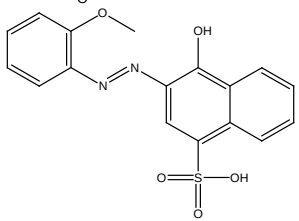
15 [c]				−1394.58	0.36	0.38	0.38
16 [c]				−1259.04	0.22	0.24	0.18
17 [c]	547-57-9			−1333.47	0.23	0.25	0.18
18 [c]				−1445.60	0.24	0.26	0.19
19 [c]	2706-28-7	13015		−1858.02	0.25	0.27	0.20
20 [a]				−881.46	0.24	0.26	0.20
21 [a]				−1407.91	0.23	0.25	0.18

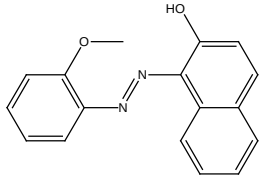
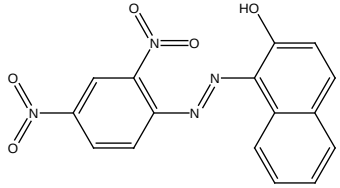
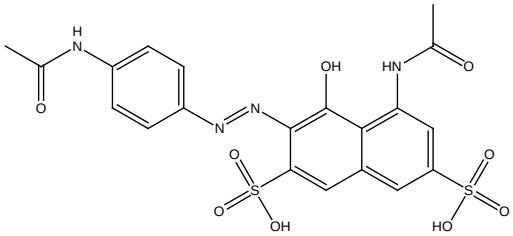
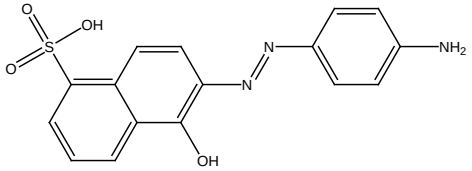
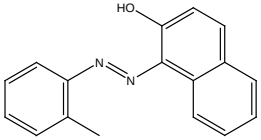
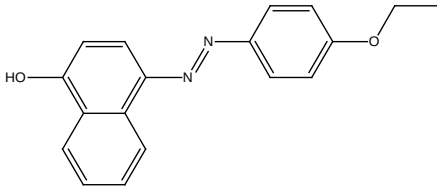
22 [c]	2051-85-6	11920		−714.79	0.22	0.23	0.18
23 [b]				−978.70	0.28	0.28	0.23
24 [c]				−978.73	0.28	0.30	0.23
25 [b]				−1165.29	0.29	0.31	0.24
26[a]				−959.00	0.29	0.31	0.25
27 [c]				−959.01	0.29	0.31	0.25

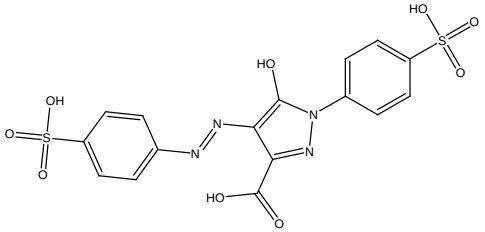
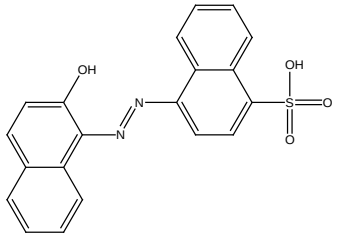
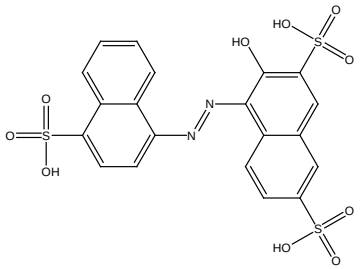
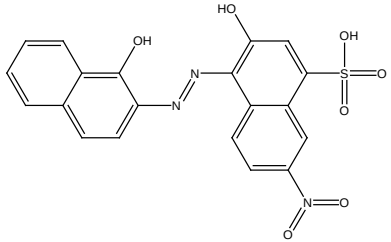
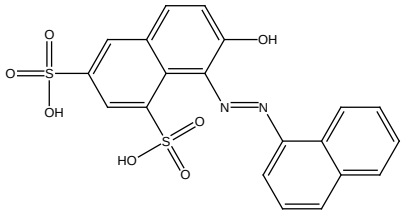
28 [b]	633-96-5	15510		−1410.82	0.28	0.29	0.23
29 [c]				−1410.84	0.28	0.29	0.23
30 [c]				−1597.40	0.29	0.31	0.24
31 [c]	1325-37-7	40000		−2029.51	0.29	0.31	0.23
32 [c]	6441-91-4	17025		−2286.54	0.33	0.36	0.28
33 [c]	842-07-9	12055		−792.13	0.26	0.28	0.22

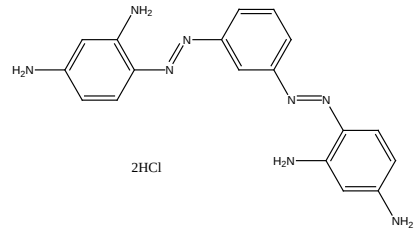
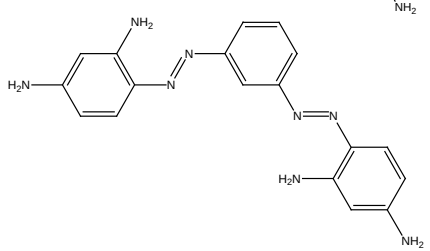
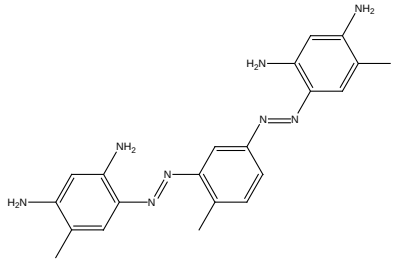
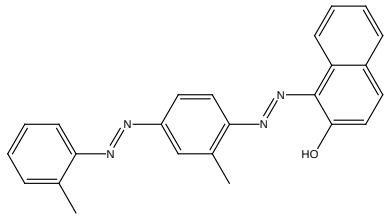
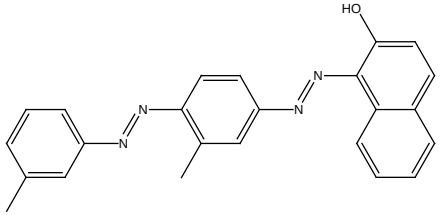
34 [c]				−792.15	0.26	0.28	0.22
35 [c]	3118-97-6	12140		−869.78	0.32	0.32	0.27
36 [c]	5859-00-7	16100		−2029.51	0.29	0.31	0.23
37 [c]	85-84-7	11380		−772.44	0.28	0.29	0.24
38 [a]	3761-53-3	16150		−2107.16	0.35	0.37	0.29

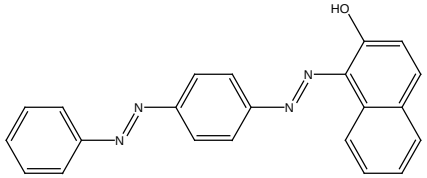
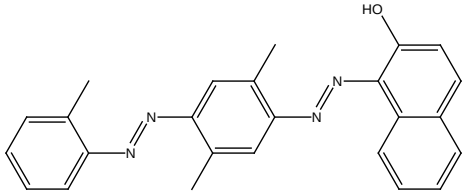
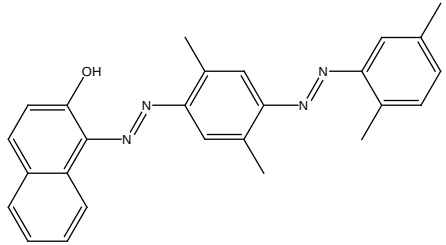
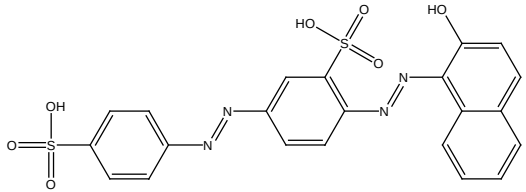
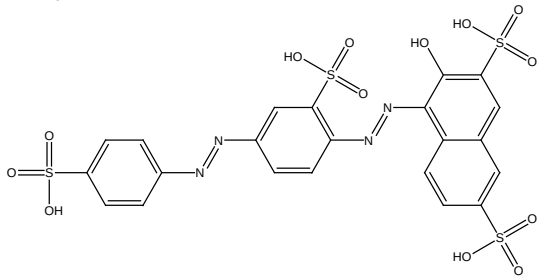
39 [b]	1936-15-8	16230		−2029.50	0.29	0.31	0.24
40 [b]	3688-92-4			-	-	-	-
41 [b]	4197073	16570		−2103.96	0.29	0.32	0.24
42 * [b]	3734-67-6	18050		−2235.20	0.35	0.38	0.29
43 * [b]	6441-93-6	18065		−2274.02	0.38	0.41	0.32

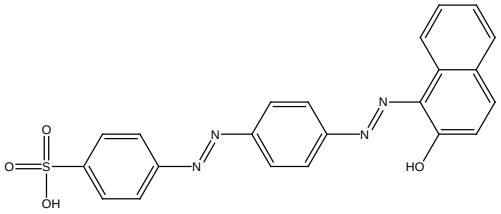
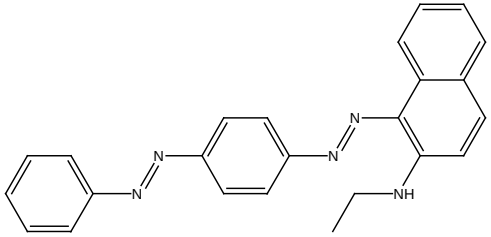
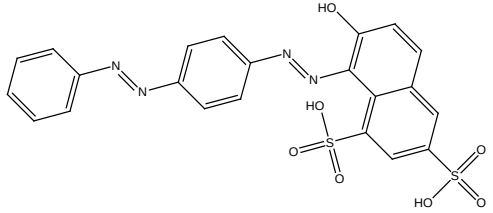
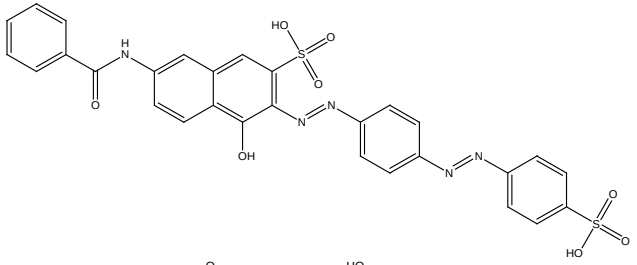
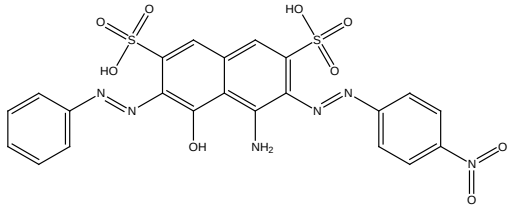
44 [c]				−2286.55	0.31	0.34	0.25
45 [c]				−2360.99	0.31	0.34	0.26
46 [c]				−2473.09	0.33	0.35	0.26
47 [c]				−1854.42	0.31	0.34	0.26
48 [c]	5858-39-4	14070		−1524.08	0.31	0.33	0.26

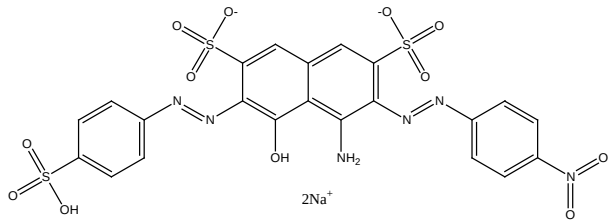
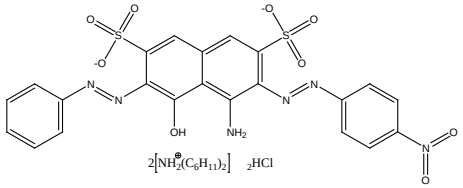
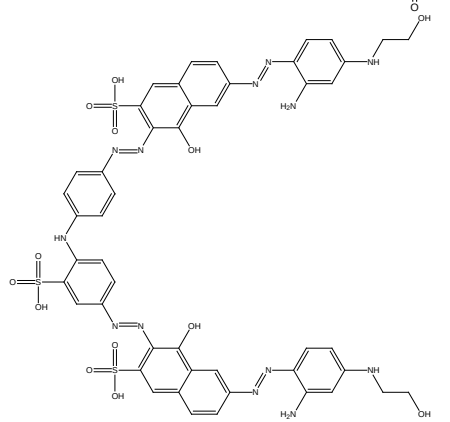
49 [c]	1229-55-6	12150		−905.39	0.30	0.31	0.25
50 [c]	3468-63-1	12075		−1196.70	0.27	0.28	0.22
51 [c]	4321-69-1	18055		−2440.86	0.41	0.44	0.34
52 [c]	5858-51-5	14805		−1466.74	0.32	0.34	0.27
53 [c]	2646-17-5	12100		−830.96	0.29	0.31	0.25
54 [c]	6365-42-8	12010		−944.23	0.33	0.35	0.28

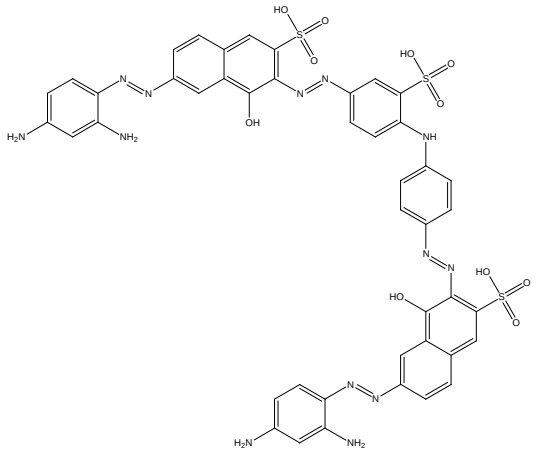
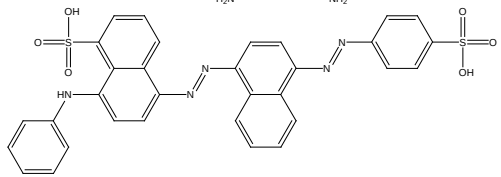
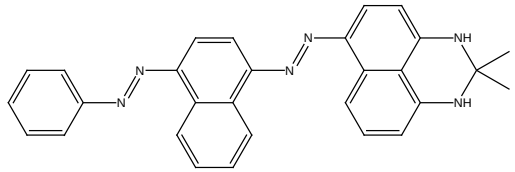
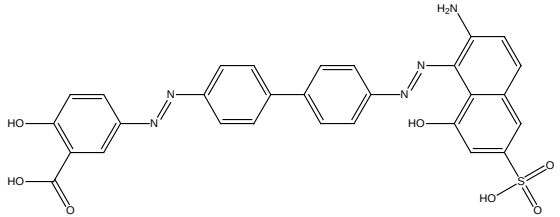
55 *	1934-21-0	19140		−2286.67	0.31	0.34	0.25
56 [b]	1658-56-6	15620		−1562.62	0.33	0.35	0.28
57 * [b]	915-67-3	16185		−2800.00	0.35	0.38	0.29
58 * [a]	1787-61-7	14645		−1839.36	0.33	0.36	0.28
59 [c]	2766-77-0	16250		−2181.30	0.34	0.37	0.29

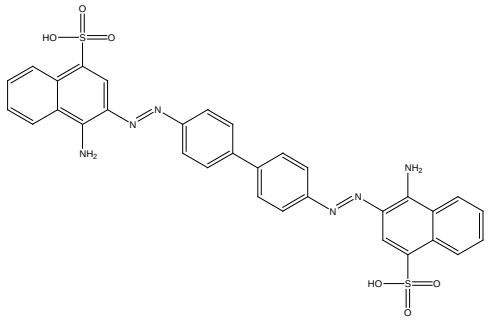
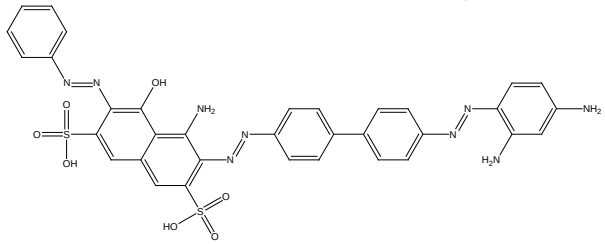
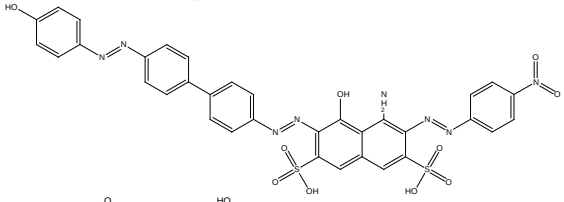
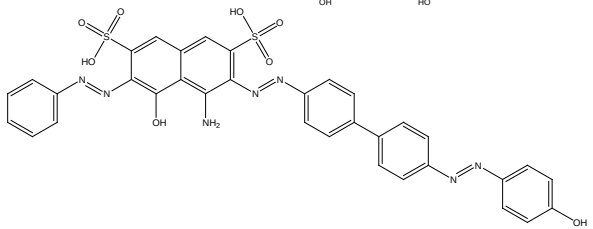
60 [b]	1052-38-6	21000		−1121.31	0.38	0.40	0.32
61 [c]	1052-38-6	21000:1		−1121.31	0.38	0.40	0.32
62 [c]	8005-78-5	21010		−1237.77	0.46	0.49	0.41
63 [b]	85-83-6	26105		−1206.27	0.42	0.44	0.36
64 [b]	3176-79-2	26110		−1206.26	0.42	0.44	0.36

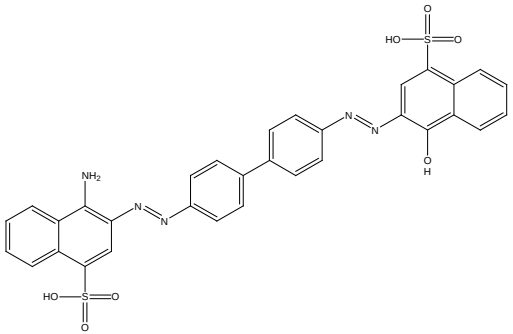
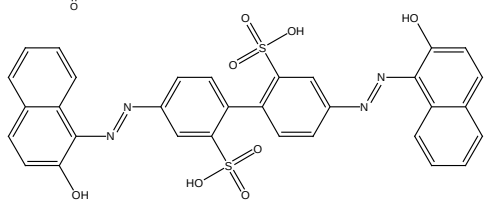
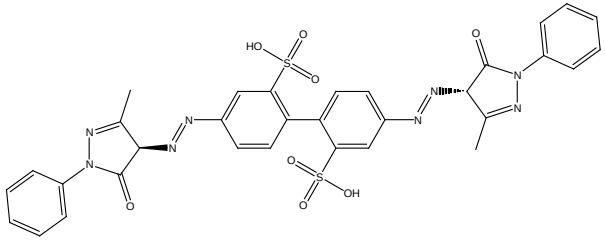
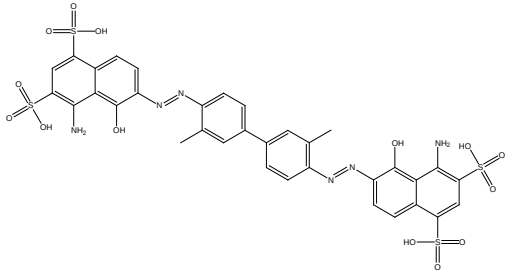
65 [b]	85-86-9	26100		−1128.62	0.36	0.38	0.31
66 [c]	4477-79-6	26120		−1245.09	0.45	0.47	0.39
67 [c]	1320-06-5	26125		−1283.91	0.48	0.50	0.42
68 [b]	4196-99-0	26905		−2366.00	0.39	0.42	0.33
69 [b]	6226-79-5	27195		−3603.37	0.41	0.45	0.34

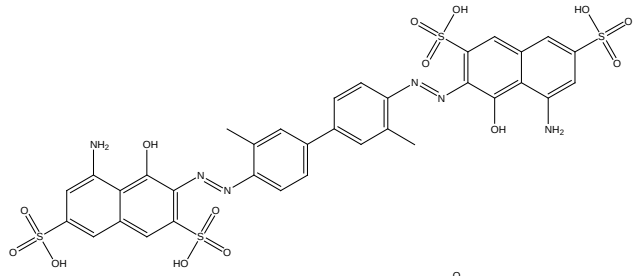
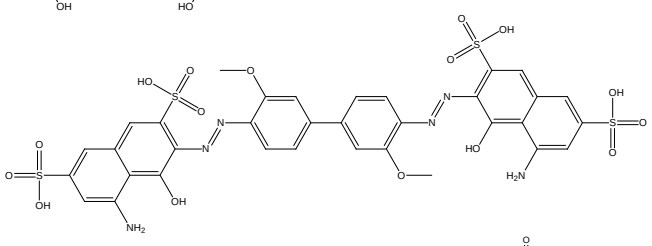
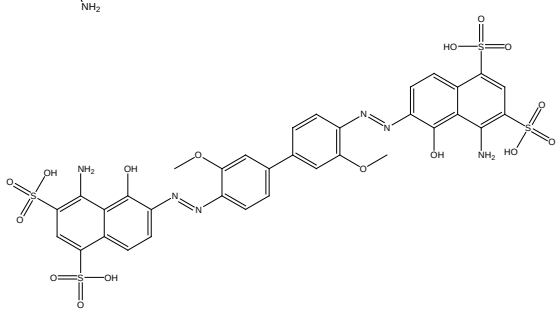
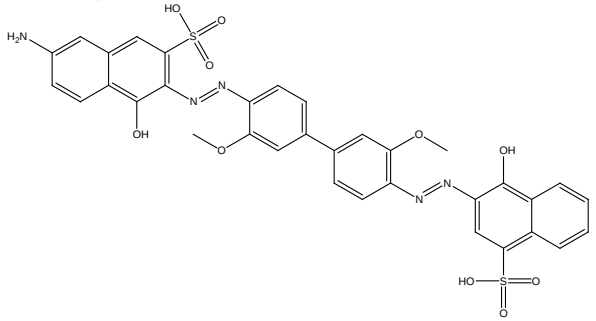
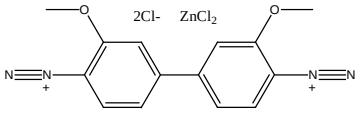
70 [c]	6406-56-0	26900		−1747.31	0.37	0.37	0.31
71 [c]	6368-72-5	26050		−1186.55	0.44	0.46	0.38
72 [c]	5413-75-2	27290		−2365.98	0.39	0.42	0.32
73 [c]	259636	28160		−2761.14	0.51	0.54	0.43
74 * [a]	1064-48-8	20470		−2623.04	0.41	0.44	0.34

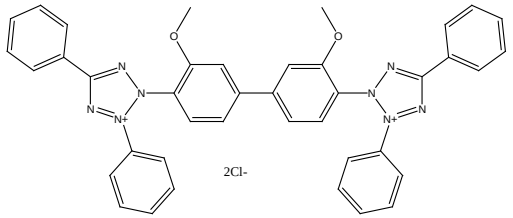
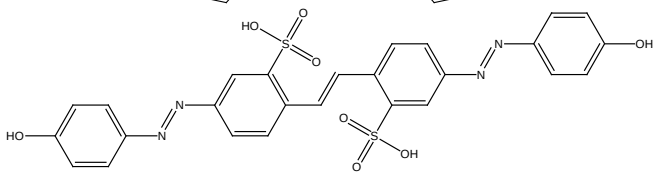
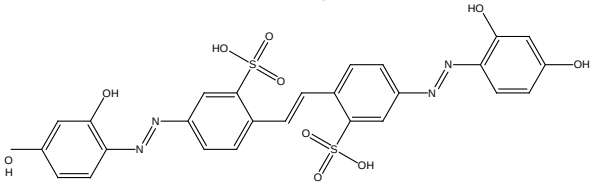
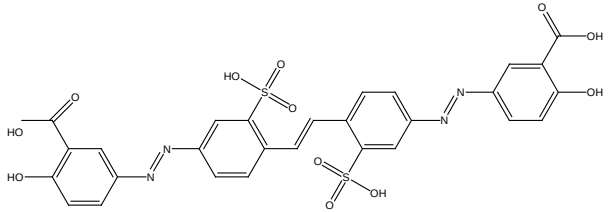
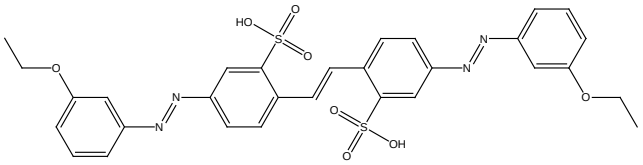
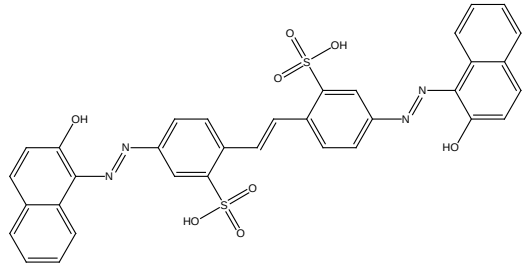
75 [a]				−3241.73	0.42	0.46	0.35
76 [c]		20480		−2623.04	0.41	0.44	0.34
77 [b]	6428-38-2	35440		−4689.99	0.97	1.03	0.85

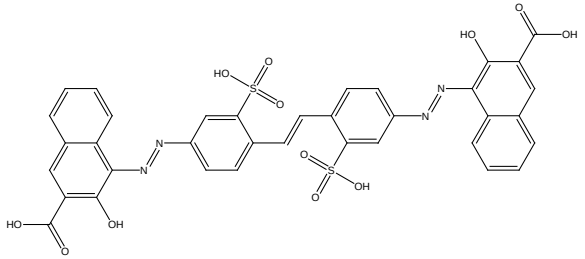
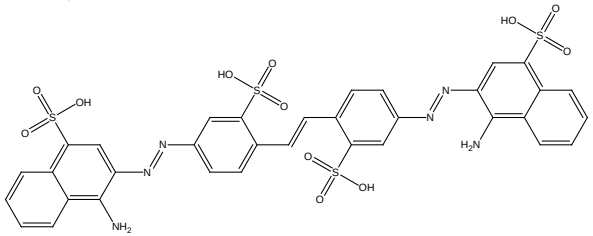
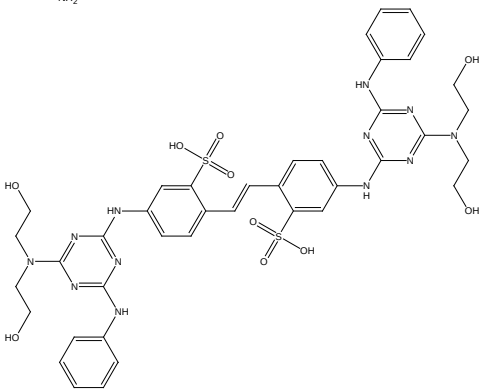
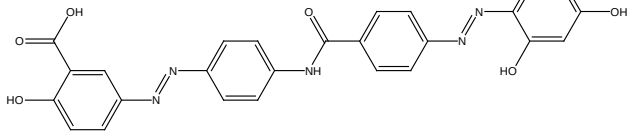
78 [c]	6473-13-8	35435		−4385.86	0.83	0.89	0.73
79 [c]	530-08-9	26360		−2726.35	0.54	0.58	0.47
80 [a]	4197-25-5	26150		−1430.74	0.51	0.54	0.45
81 [b]	2429-84-7	22150		−2291.31	0.50	0.53	0.43

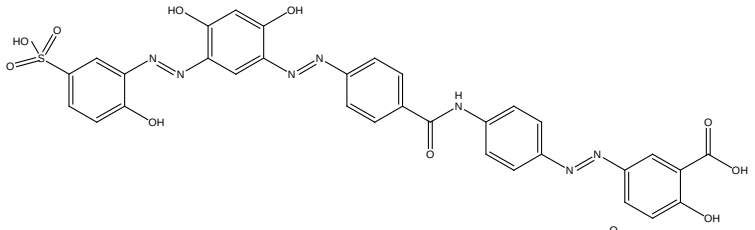
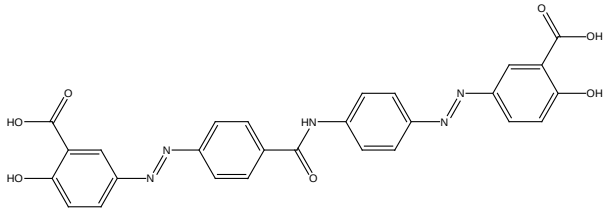
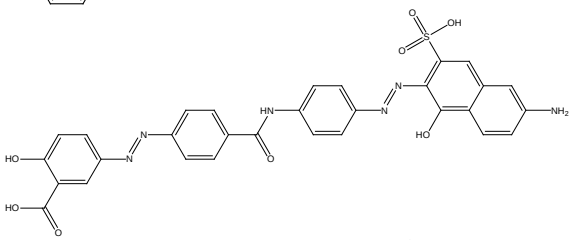
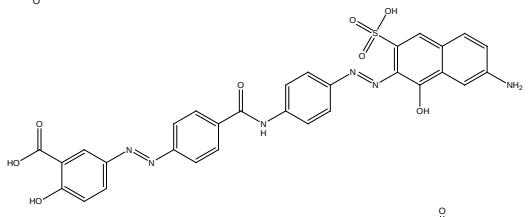
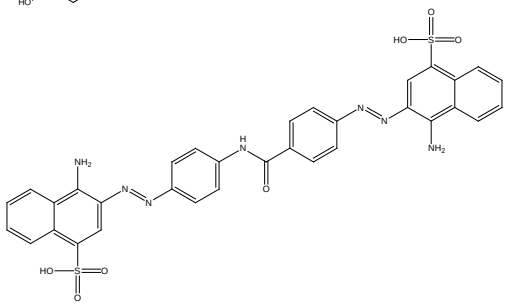
82 * [a]	573-58-0	22120		−2781.10	0.56	0.60	0.48
83 [a]	1937-37-7	30235		−3094.97	0.63	0.67	0.55
84 [c]	4335095	30295		−3262.24	0.60	0.64	0.52
85 [c]	3626-28-6	30280		−3059.95	0.60	0.64	0.52

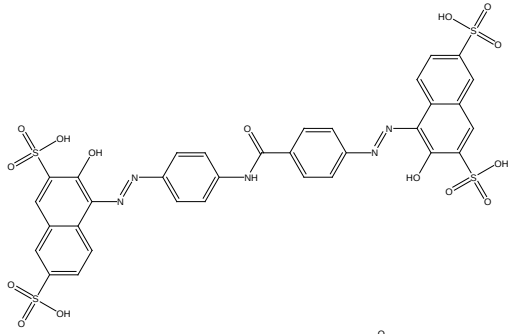
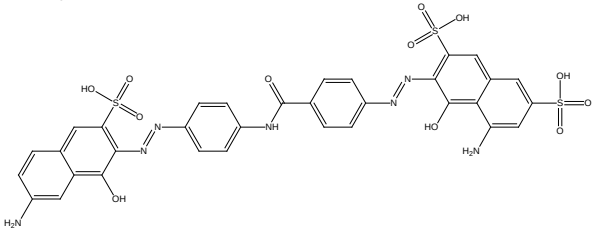
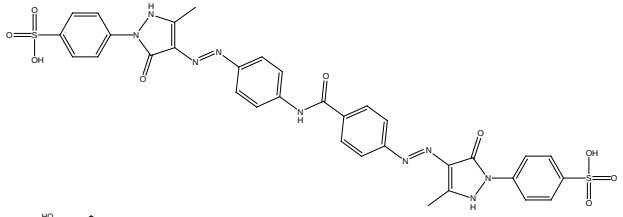
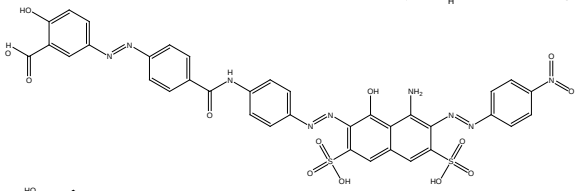
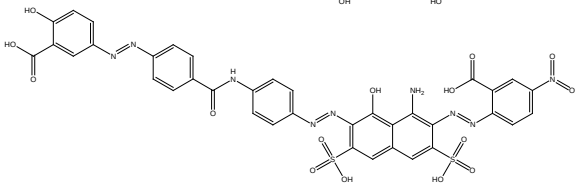
86 [c]	2429-70-1	22145		−2800.82	0.55	0.58	0.47
87 [a]	10169-02-5	22890		−2820.48	0.47	0.57	0.45
88 [c]	6375-55-9	22910		−3039.31	0.60	0.64	0.51
89 [a]	314-13-6	23860		−4245.04	0.66	0.71	0.57

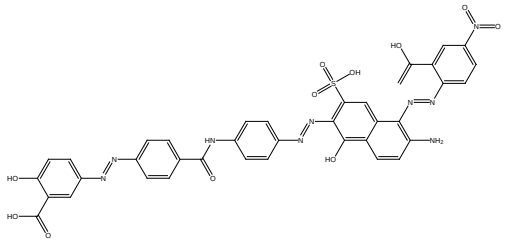
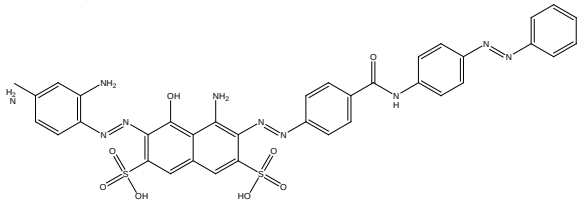
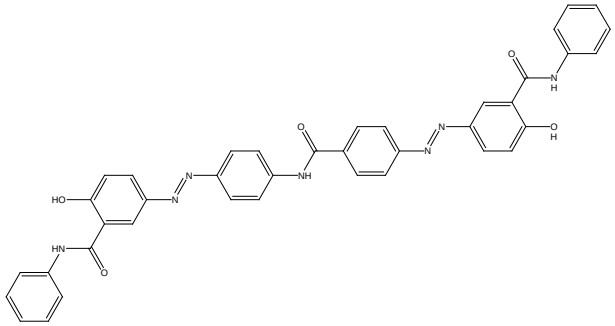
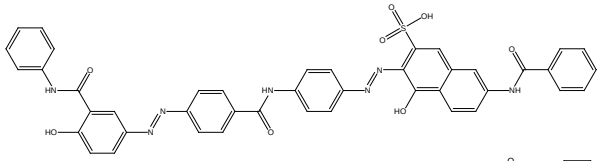
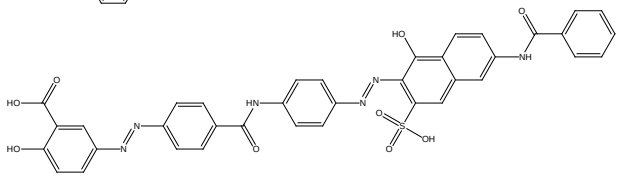
90 [a]	72-57-1	23850		−4245.01	0.65	0.71	0.56
91 [b]	2429-74-5	24400		−4393.88	0.67	0.72	0.57
92 * [b]	2610051	24100		−4393.90	0.67	0.72	0.57
93 [c]	110735-25-6	24175		−3101.77	0.62	0.66	0.54
94 * [a]	14263-94-6			−899.27	0.54	0.27	0.21

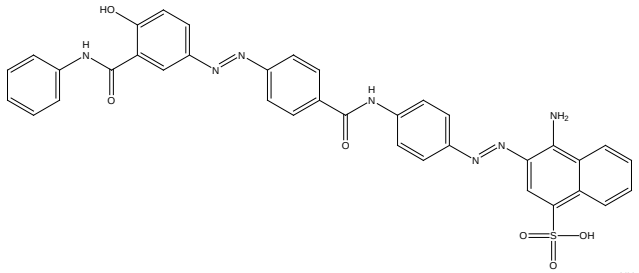
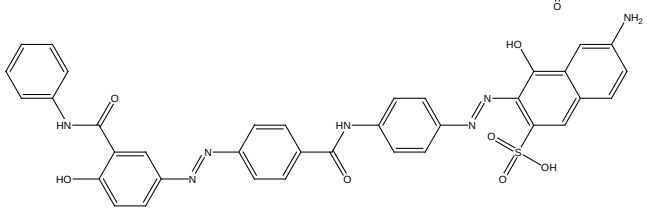
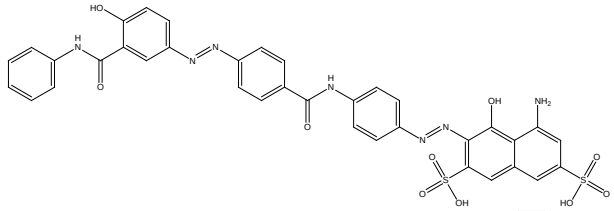
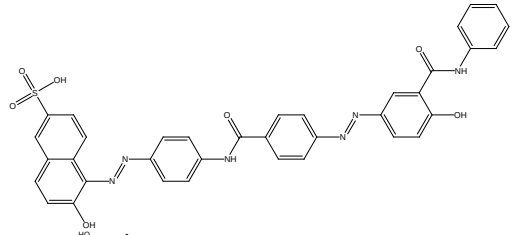
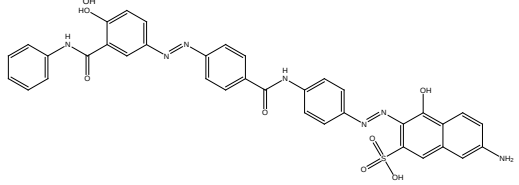
95 [a]	1871-22-3			−2106.49	0.70	0.74	0.62
96 [b]	3051114	24890		−2593.40	0.47	0.50	0.40
97 [b]				−2742.27	0.47	0.51	0.40
98 [b]				−2966.51	0.50	0.54	0.54
99 [c]	2870-32-8			−2748.66	0.59	0.63	0.51
100 * [a]				−2896.96	0.57	0.60	0.49

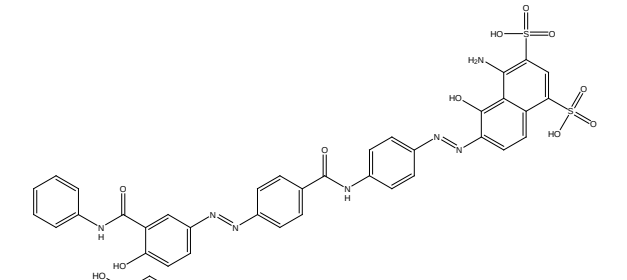
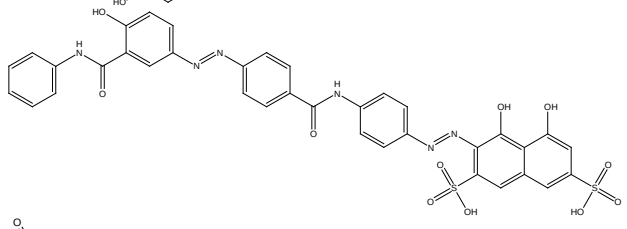
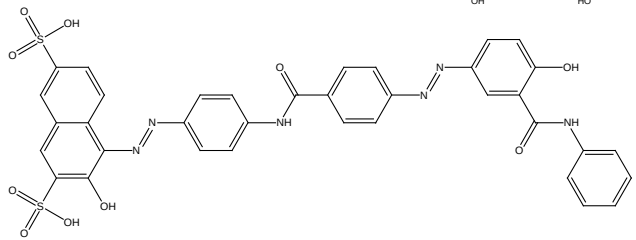
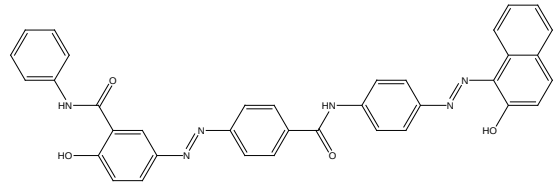
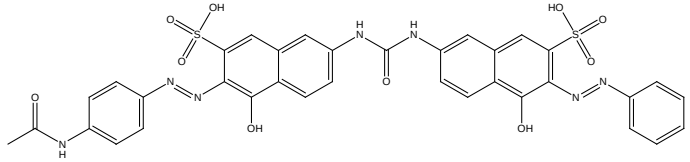
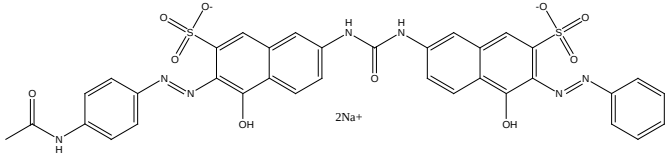
101 [b]				−3270.12	0.60	0.64	0.64
102 [b]				−4094.95	0.62	0.67	0.54
103 * [b]	4404-43-7	40622		−3716.76	0.91	0.97	0.81
104 [a]				−1707.39	0.45	0.48	0.39

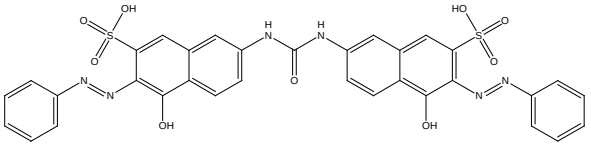
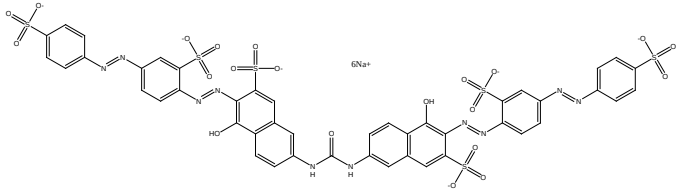
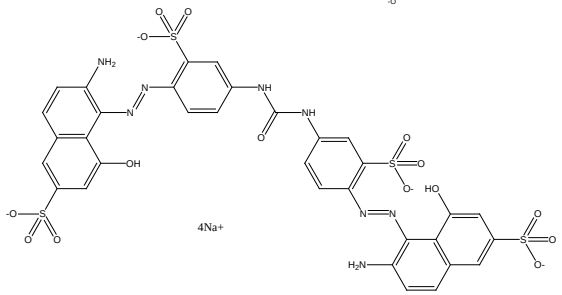
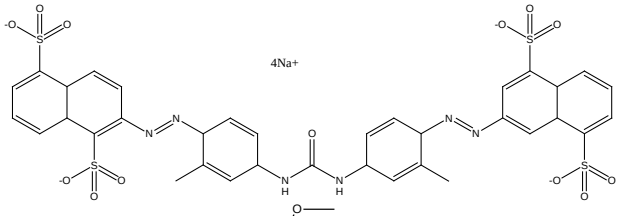
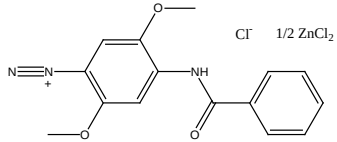
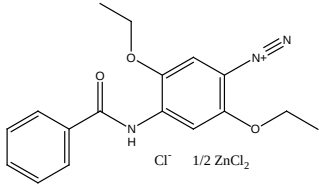
105 [b]		−2717.28	0.58	0.62	0.50
106 [b]		−1819.54	0.47	0.50	0.40
107 [b]		−2458.19	0.53	0.57	0.46
108 [b]		−2458.18	0.53	0.57	0.46
109 [b]		−2947.95	0.59	0.63	0.51

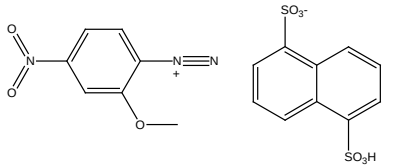
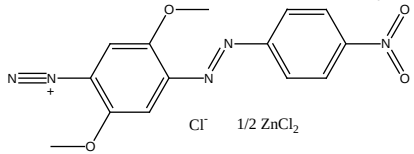
110 [b]		−4224.73	0.59	0.64	0.49
111 [b]		−3715.53	0.61	0.66	0.53
112 [a]		−3206.18	0.63	0.68	0.54
113 [b]		−3615.65	0.65	0.69	0.55
114 [b]		−3802.20	0.66	0.71	0.57

115 [b]		−3147.86	0.67	0.72	0.58
116 [b]		−3261.81	0.66	0.70	0.58
117 [b]		−2236.65	0.67	0.71	0.59
118 [b]		−3007.13	0.73	0.78	0.65
119 [a]		−2798.57	0.63	0.67	0.55

120 [a]		−2592.30	0.63	0.67	0.55
121 [a]		−2666.75	0.63	0.63	0.55
122 [a]		−3285.43	0.65	0.69	0.56
123 [c]		−2611.99	0.61	0.65	0.53
124 [c]		−2666.75	0.63	0.67	0.55

125 [c]				−3285.44	0.65	0.69	0.56
126 [c]				−3305.13	0.63	0.68	0.55
127 [a]				−3230.68	0.63	0.67	0.54
128 * [a]				−1993.30	0.60	0.64	0.53
129 [b]	25188-34-5			−3247.80	0.64	0.69	0.56
130 [c]	3441-14-3	29160		−3247.80	0.64	0.69	0.56

131 [c]	25188-23-2	29150		−3042.13	0.58	0.62	0.50
132 [b]	2610108	35780		−6189.85	0.83	0.90	0.71
133 [c]	2829-43-8			−4388.93	0.64	0.70	0.55
134 [c]	3214-47-9	29025		−4208.22	0.66	0.71	0.56
135 [a]	14726-29-5	37155		−958.48	0.30	0.31	0.25
136 [a]	5486-84-0	37175		−1036.24	0.35	0.37	0.30

137 [a]	49735-71-9	37125		−652.59	0.30	0.15	0.10
138[c]	64071-89-9	37190		−1102.35	0.27	0.29	0.22

C.I. –Colour Index number, E(RHF/3-21G) – predicted SCF energy; ZPE – unscaled zero point correction; Hcorr – thermal correction to the enthalpy; Gcorr – thermal correction to the Gibbs free energy; * Examples of average experimental values, characterizing the reproducibility of the experimental measurements (in parentheses): for compound 2: 3.67 (3.52; 3.82); 4: 3.79 (3.88; 3.70); 5: 4.58 (4.56; 4.67; 4.50); 7: 3.32 (3.35; 3.29); 8: 3.31 (3.40; 3.21); 42: 3.62 (3.71; 3.57; 3.59); 43: 3.63 (3.63; 3.63); 57: 2.33 (2.39; 2.27); 58: 4.13 (4.20; 4.05); 74: 4.33 (4.41; 4.24); 82: 4.49 (4.60; 4.43; 4.44); 92: 3.79 (3.66; 3.92); 94: 4.30 (4.66; 3.93); 100: 4.55 (5.10; 4.20; 4.34); 103: 3.81 (3.86; 3.76); 128: 4.27 (4.14; 4.39); 134: 4.09 (4.20; 4.17; 3.89).

Table S2. Molecular properties of azo-, azo-anilide, diazonium salts derivatives.

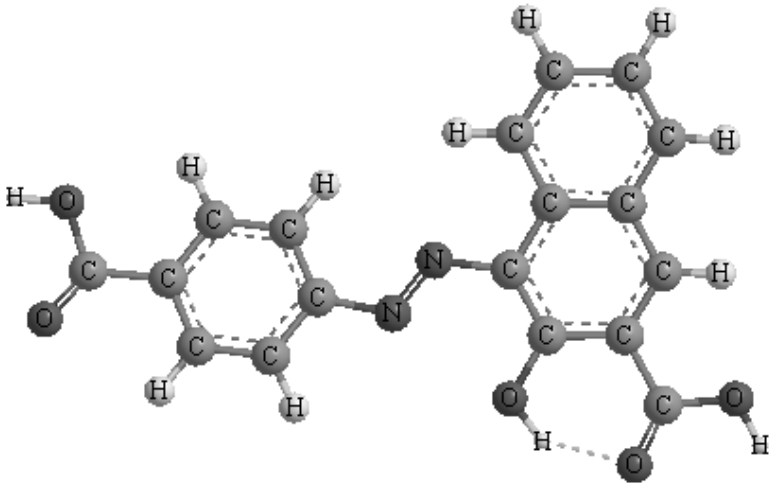
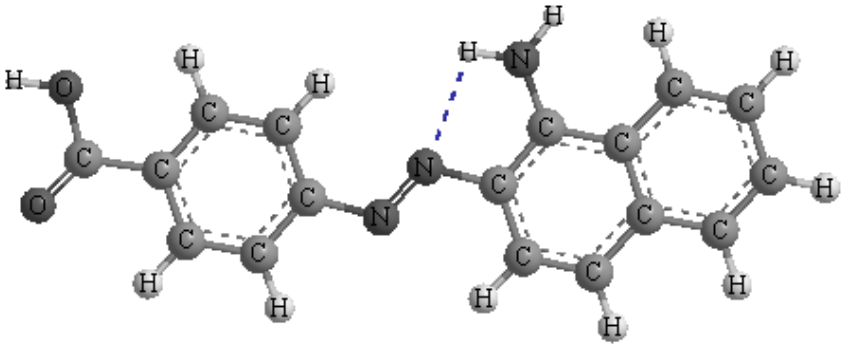
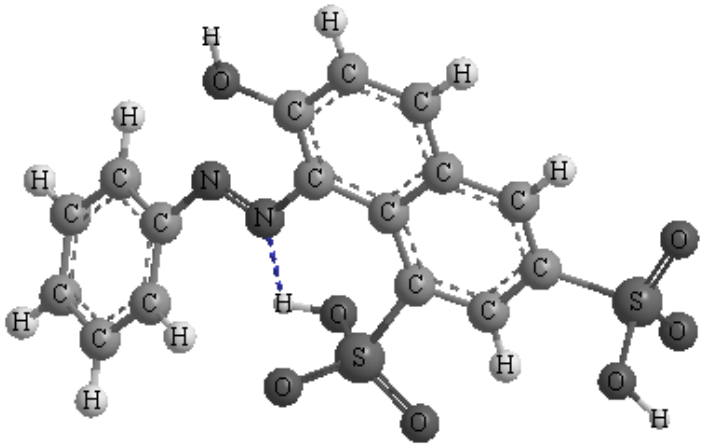
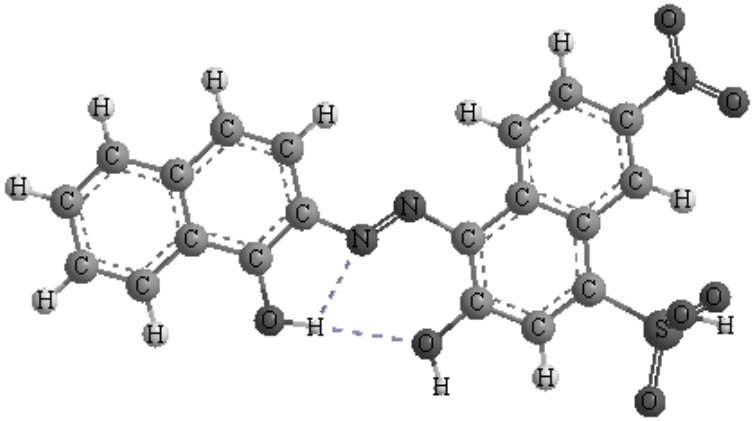
No.	logP	AverPol	logS	HA	HD
1	4.22	23	−4.5	3	0
2	4.04	23	−4.17	4	1
3	3.31	29	−3.49	5	1
4	2.79	24	−3.77	5	1
5	3.52	27	−3.52	7	3
6	3.97	33	−3.97	5	1
7	3.73	24	−3.52	5	2
8	3.43	25	−3.37	6	3
9	4.04	27	−3.62	7	3
10	5.48	34	−4.85	5	2
11	5.48	34	−4.86	5	2
12	3.18	36	−4.68	6	1
13	3.17	36	−4.3	6	2
14	2.61	31	−3.85	6	1
15	3.33	35	−4.18	6	1
16	1.37	27	−3.36	6	2
17	0.89	28	−3.06	7	3
18	1.57	30	−3.35	8	3
19	−0.59	32	−3.65	9	3
20	4.53	26	−3.99	5	1
21	0.49	28	−3	8	4
22	3.77	22	−3.2	4	2
23	4.72	30	−4.43	5	2
24	4.72	30	−4.43	5	2
25	5.03	33	−4.33	7	3
26	4.20	31	−4.47	5	2
27	4.20	30	−4.46	5	2
28	2.19	32	−4.09	6	2
29	2.18	33	−4.04	6	2
30	2.45	36	−3.84	8	3
31	−0.72	38	−4.26	9	3
32	1.01	43	−4.53	11	3
33	5.07	27	−4.67	3	1
34	5.07	27	−4.66	3	1
35	6.09	31	−5.1	3	1
36	−0.01	38	−4.1	9	3
37	4.54	27	−4.83	3	1
38	1.21	42	−4.38	9	3
39	−0.64	38	−4.06	9	3
40	2.61	45	−3.88	10	5
41	−1.04	39	−3.66	10	4
42	−1.39	44	−4.06	10	4
43	−0.77	46	−4.19	10	4
44	0.06	42	−3.89	12	4
45	−0.27	43	−3.64	13	5
46	-2.18	45	−3.9	14	5
47	2.54	39	−4.13	11	4
48	2.08	35	−3.87	7	2

49	4.91	29	−4.72	4	1
50	4.95	31	−5.05	7	1
51	−2.17	50	−3.97	11	5
52	3.14	34	−3.67	7	3
53	5.58	29	−4.91	3	1
54	5.26	32	−4.94	4	1
55	−1.76	42	−3.3	12	4
56	3.32	38	−4.68	6	2
57	−1.98	50	−4.28	12	4
58	2.70	42	−4.38	9	3
59	0.33	44	−4.65	9	3
60	3.47	37		8	4
61	3.47	37	−3.93	8	4
62	5.01	44	−4.35	8	4
63	8.50	43	−5.31	5	1
64	8.50	43	−5.34	5	1
65	7.47	39	−5.17	5	1
66	9.01	45	−5.42	5	1
67	9.52	47	−5.5	5	1
68	1.63	50	−4.75	11	3
69	−3.88	61	−4.54	17	5
70	4.65	45	−4.78	8	2
71	7.60	43	−5.36	5	1
72	1.87	50	−4.74	11	3
73	2.87	64	−4.78	12	4
74	0.78	54	−4.37	14	4
75	−2.47	59	−4.67	17	3
76	0.78	53		14	2
77	6.33	115	−4.63	26	12
78	7.48	104	−4.73	24	10
79	5.02	66	−5.48	11	3
80	8.13	52	−5.37	6	2
81	6.60	60	−4.81	12	5
82	3.57	68	−5.41	12	4
83	5.95	77	−4.81	16	6
84	4.87	78	−4.69	17	5
85	4.98	75	−4.76	15	5
86	4.05	68	−5.18	12	4
87	4.14	65	−5.15	12	4
88	1.32	71	−4.76	14	2
89	−2.69	86	−4.9	20	8
90	1.13	86	−4.86	20	8
91	−0.27	88	−4.72	22	8
92	−4.13	87	−4.74	22	8
93	5.05	75	−4.73	15	5
94	2.98	27		4	0
95	4.51	73	−6.91	6	0
96	3.13	58	−4.62	12	4
97	2.11	60	−4.05	14	6
98	2.73	65	−4.43	16	6
99	3.94	67	−5.51	12	2

100	4.90	70	−5.43	12	4
101	5.42	77	−4.99	16	6
102	−1.87	83	−5.2	18	6
103	−0.54	95	−3.96	22	10
104	7.58	50	−4.69	10	5
105	6.54	70	−4.45	16	7
106	7.88	53	−4.88	11	5
107	6.66	64	−4.64	13	6
108	6.65	64	−4.64	13	6
109	2.89	71	−5.22	13	5
110	−1.16	82	−4.88	19	7
111	2.72	79	−4.48	18	8
112	0.91	77	−4.55	15	5
113	4.32	84	−4.55	20	7
114	3.69	87	−4.57	22	8
115	8.61	83	−4.75	18	7
116	5.39	80	−4.65	17	7
117	9.45	73	−5.34	9	5
118	7.65	86	−5.49	12	6
119	6.87	76	−5.09	13	6
120	6.04	73	−5.29	11	5
121	7.46	74	−5.06	12	6
122	4.65	79	−4.68	15	7
123	6.53	72	−5.16	11	5
124	7.46	74	−5.06	12	6
125	2.86	79	−4.69	15	7
126	3.33	79	−4.55	15	7
127	4.44	78	−4.7	14	6
128	9.35	66	−5.48	8	4
129	3.04	76	−4.56	14	7
130	3.04	76	−4.7	14	5
131	3.89	70	−4.54	13	6
132	9.20	116	−5.12	29	4
133	4.37	83	−4.87	21	6
134	−0.11	82	−5.47	17	2
135	2.59	29		4	1
136	3.30	33		4	1
137	1.32	25	−4.63	6	1
138	3.84	30		7	0

logP - the logarithm of the octanol-water partition coefficient; logS - the logarithm of solubility; AverPol - average polarizability; the number of donor (HD), respectively acceptor (HA) hydrogen bonds.

Table S3. Minimum energy structure of some azo- and azo-anilide derivatives (hydrogen bonds are expressed by dashed line).

No.	Structure
25	
26	
39	
58	

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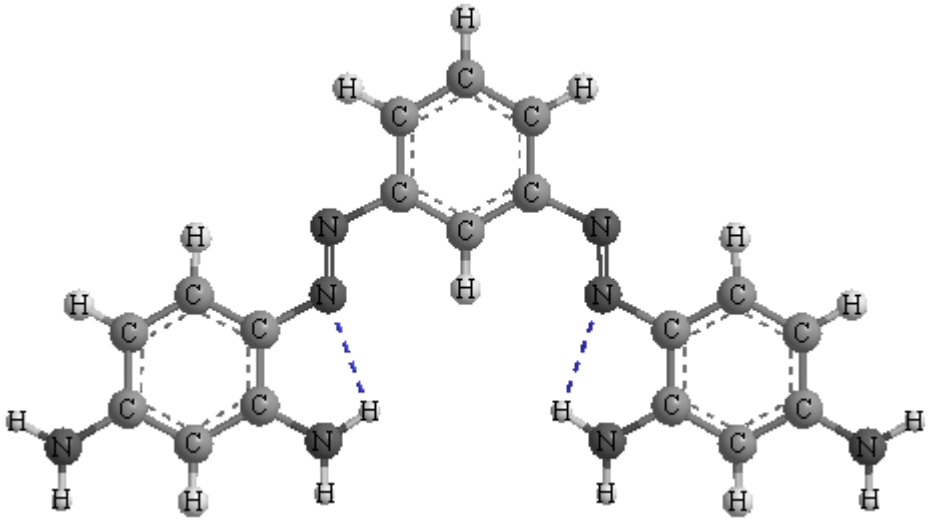

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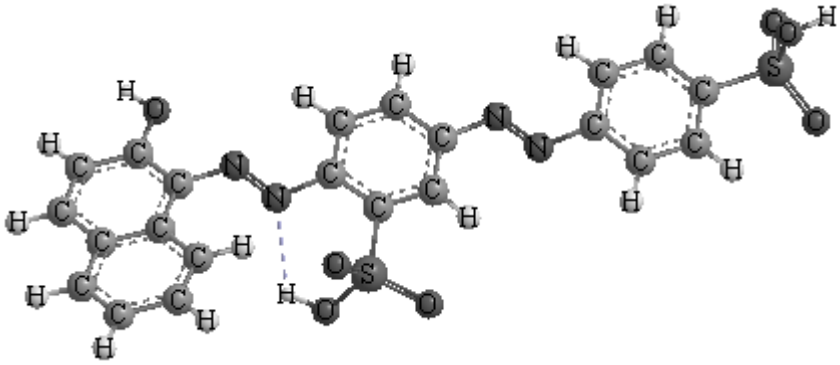

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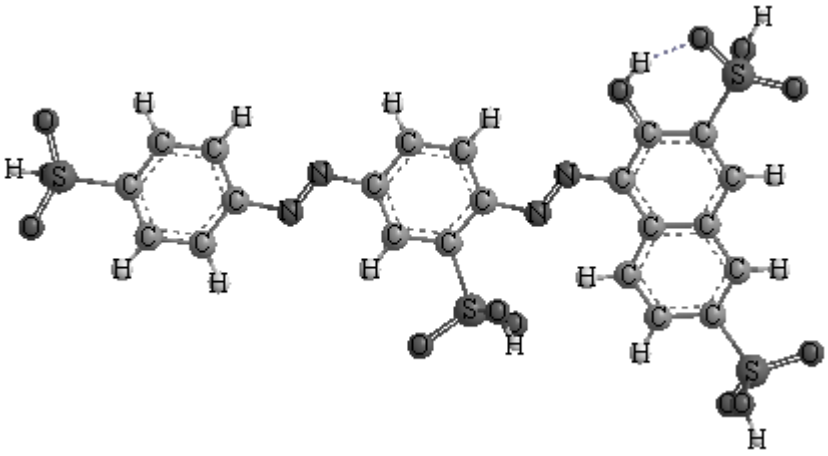

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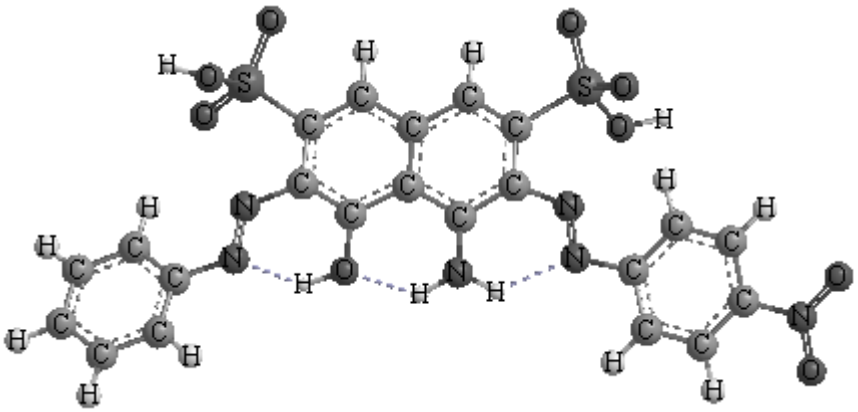

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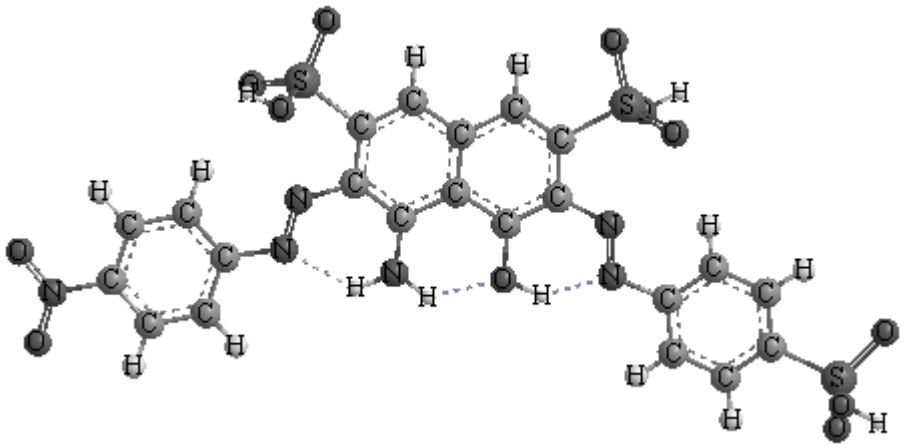

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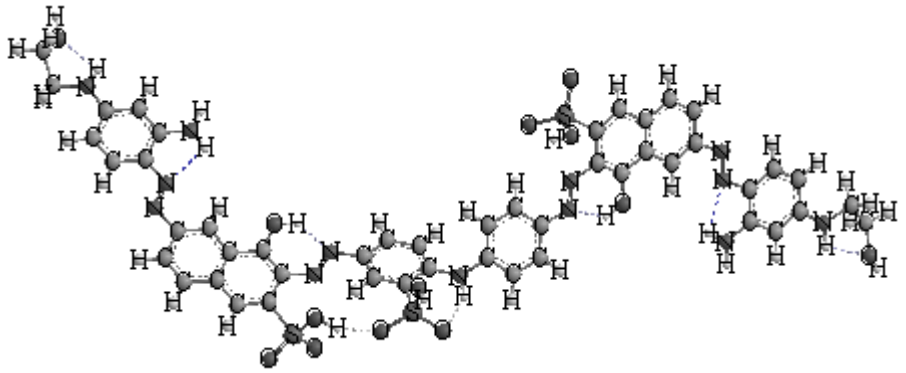

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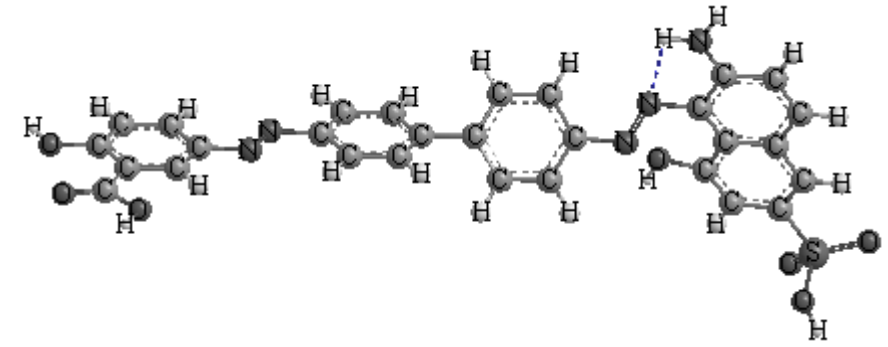

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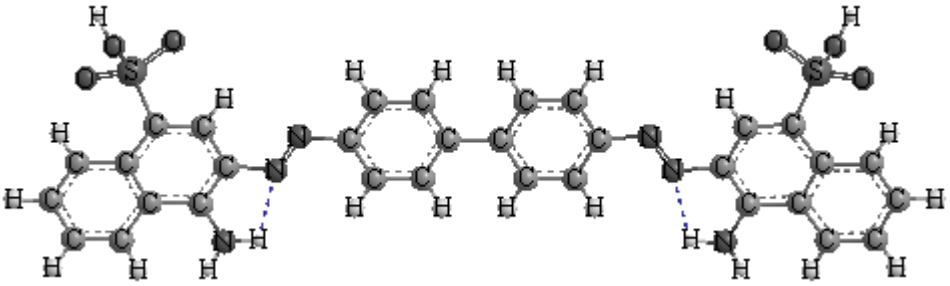

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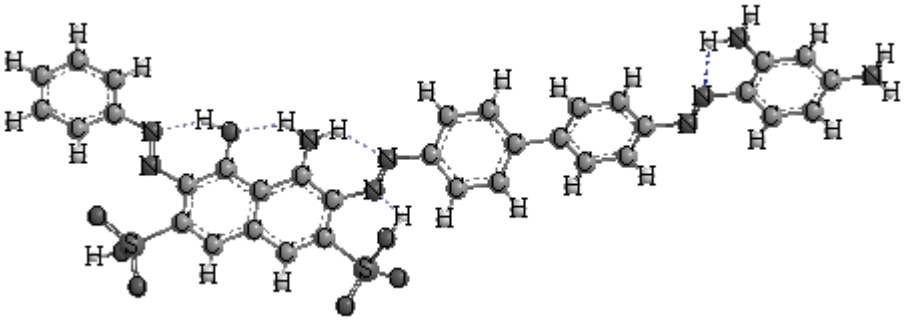

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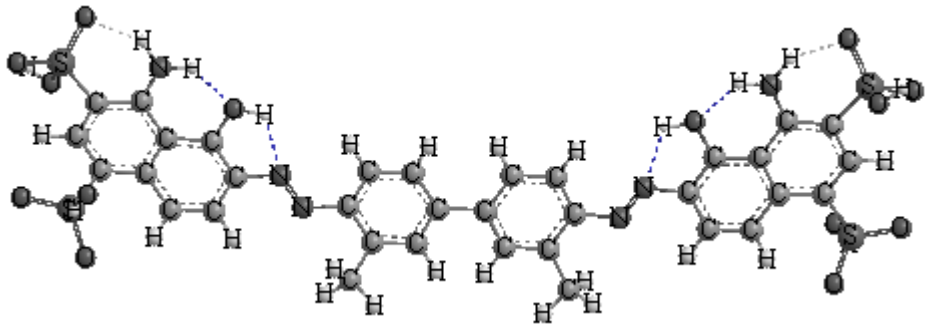

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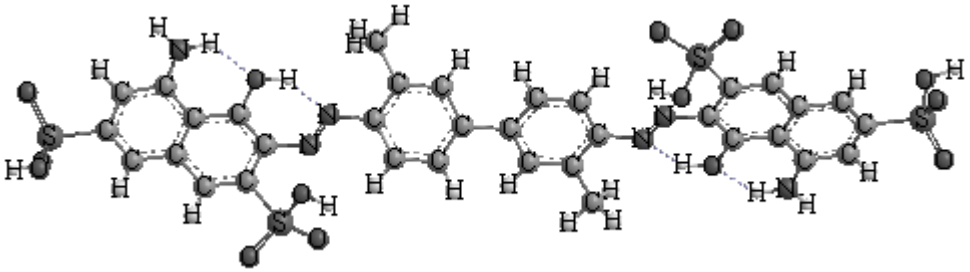

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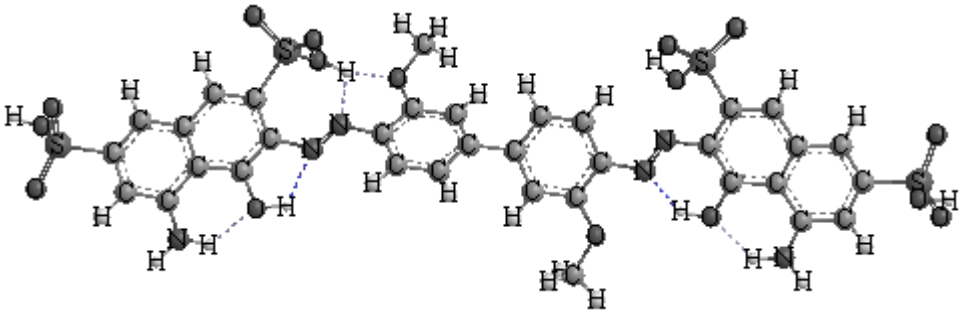

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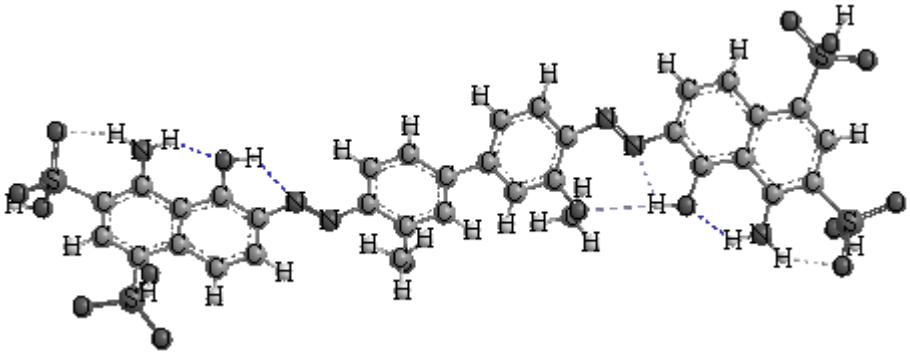

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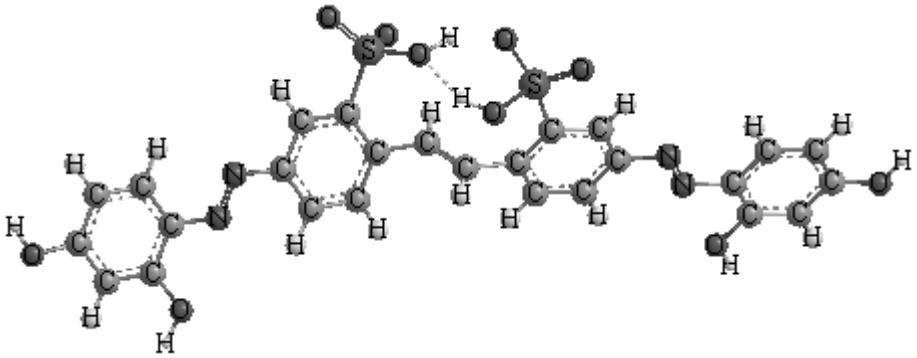

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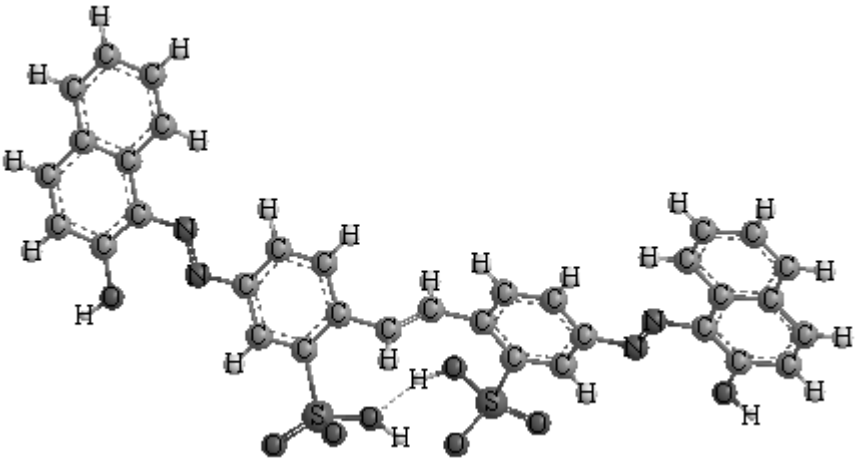

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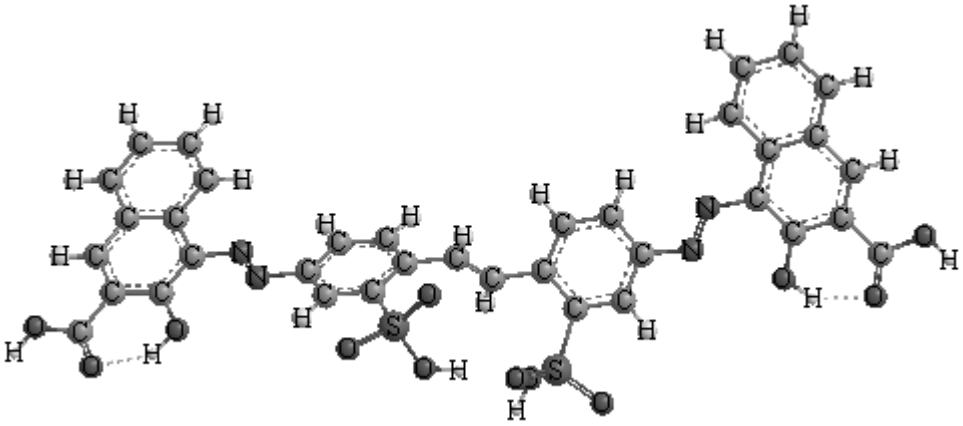

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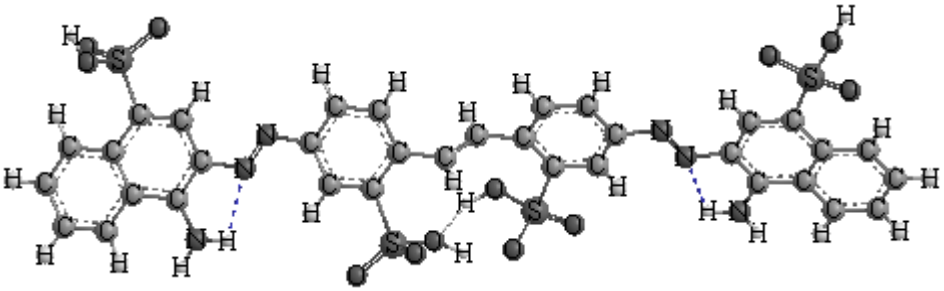

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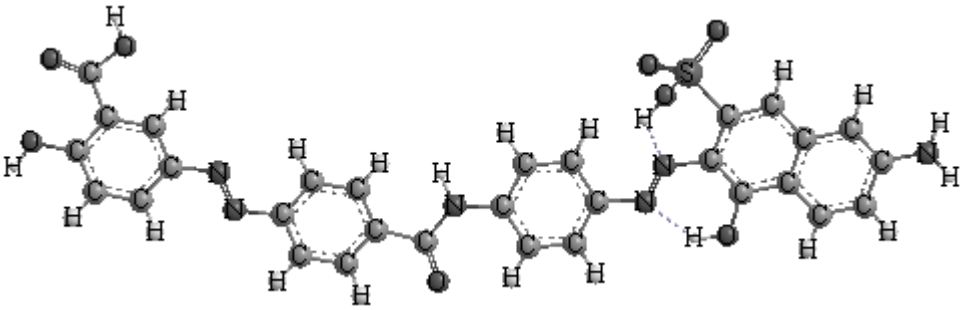

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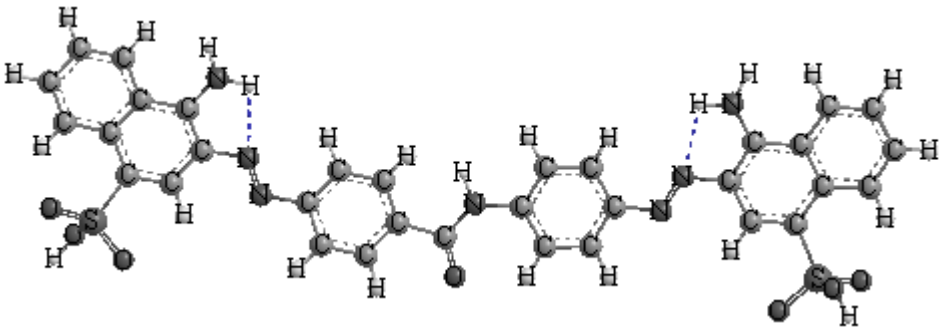

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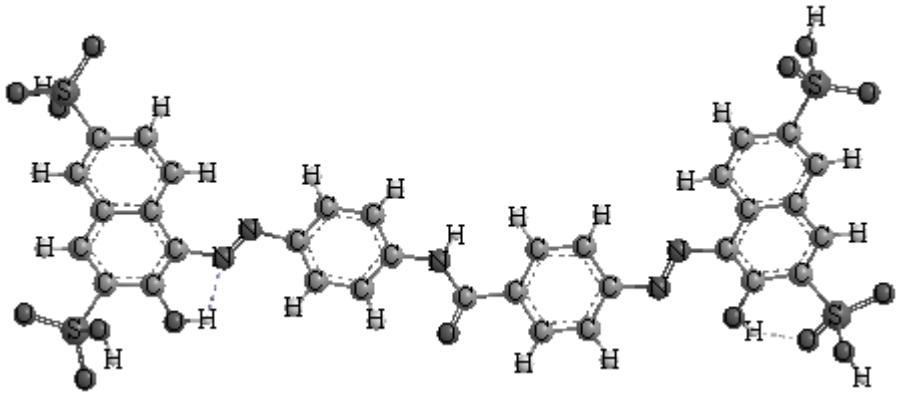

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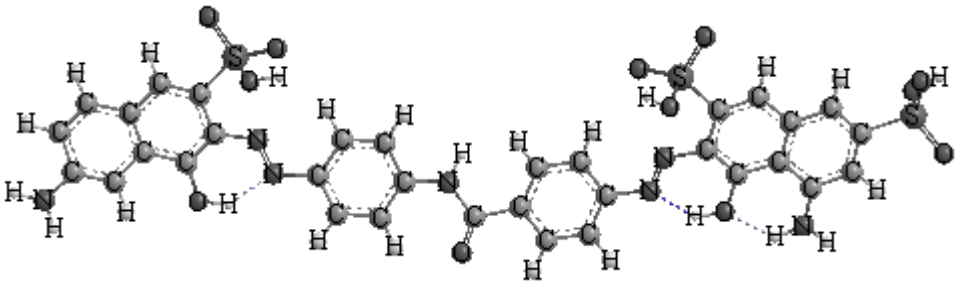

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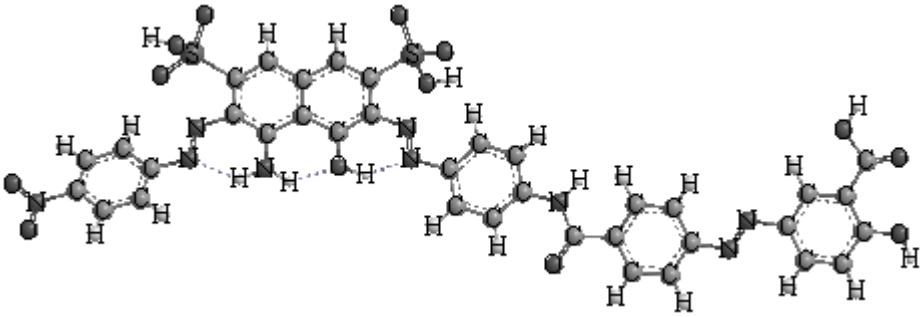

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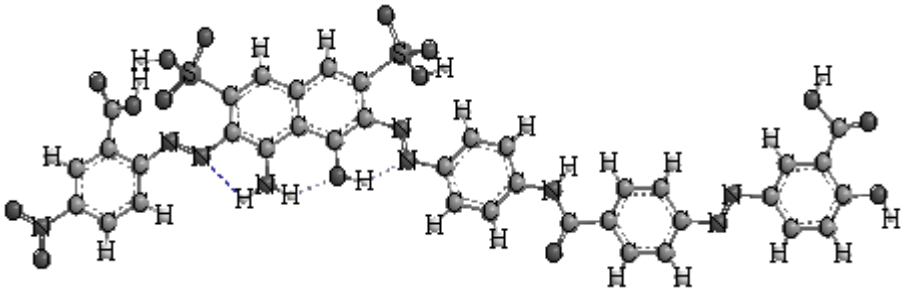

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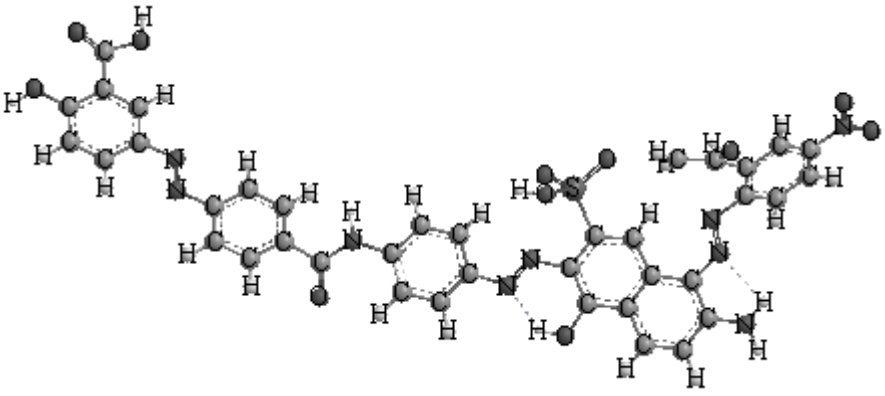

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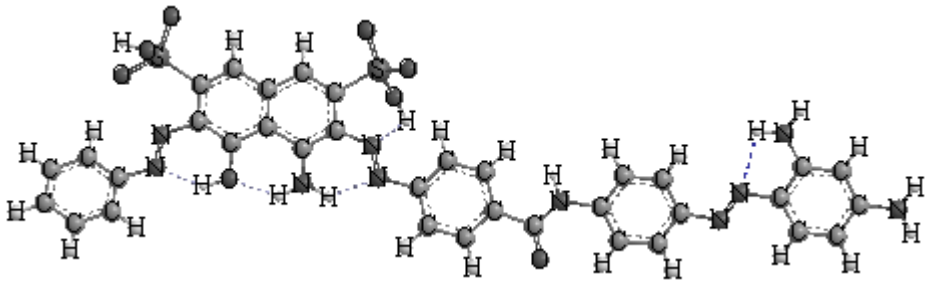

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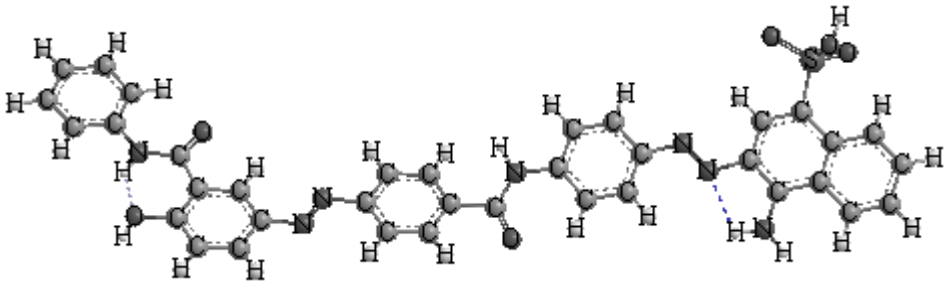

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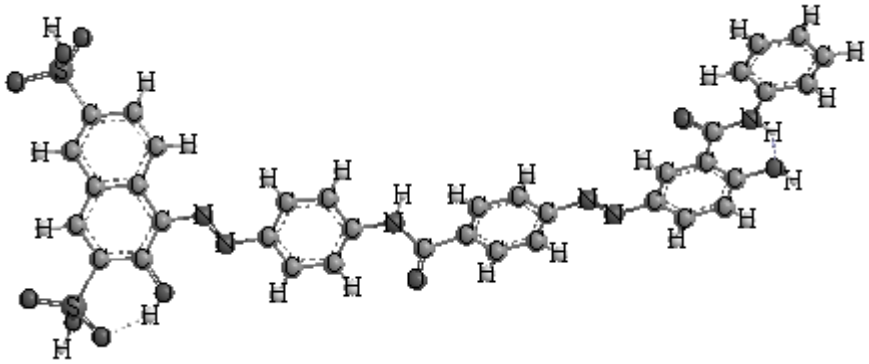

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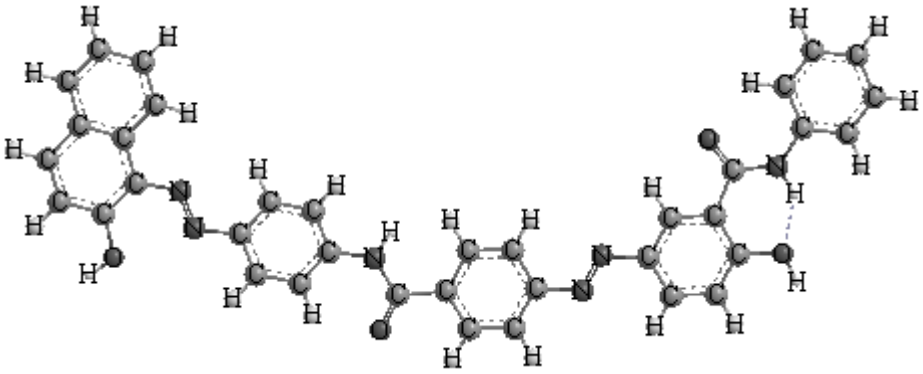

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