

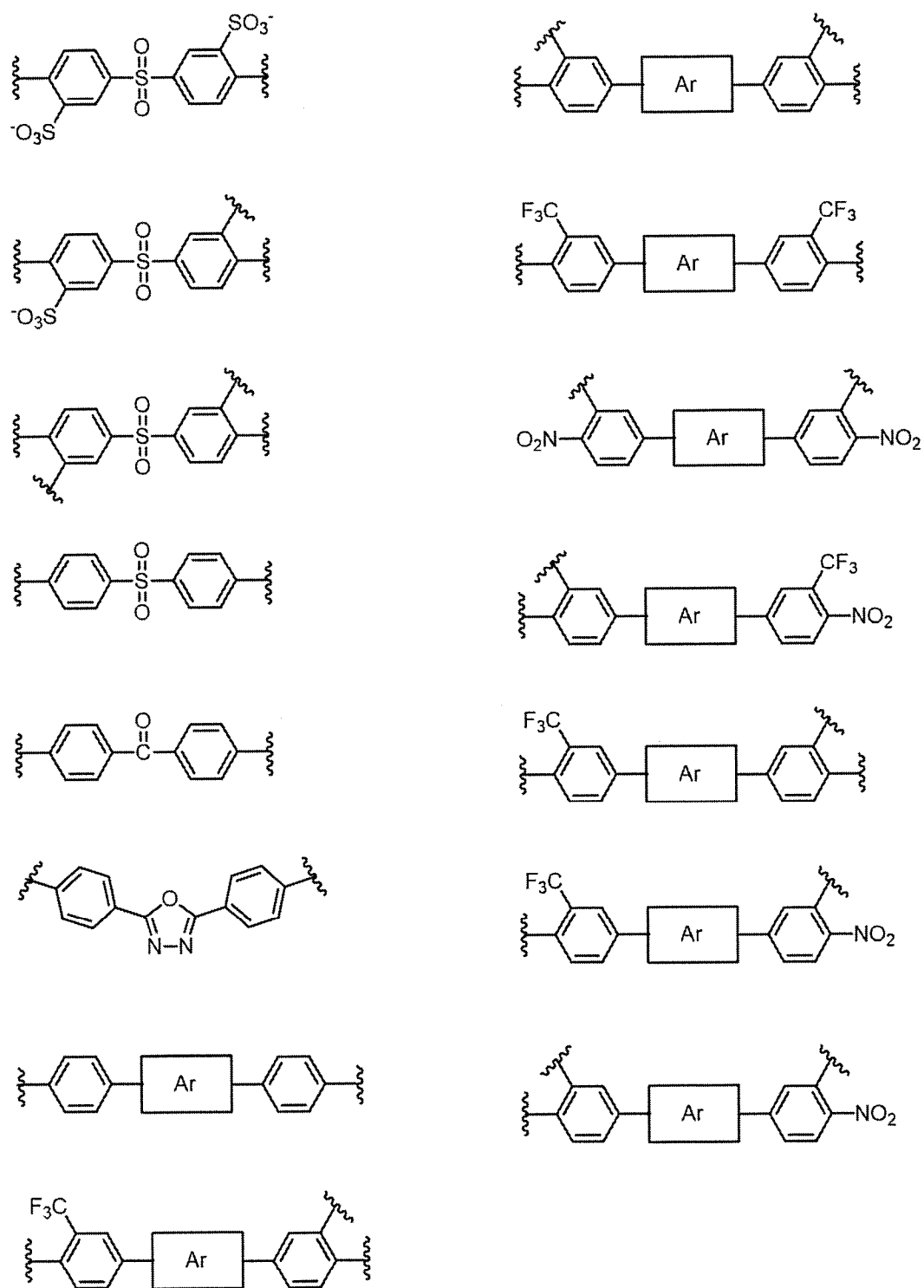
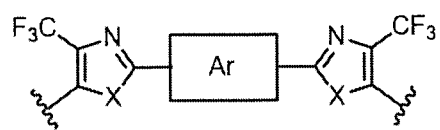
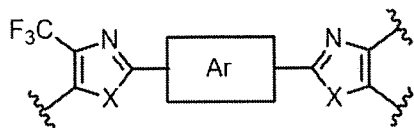


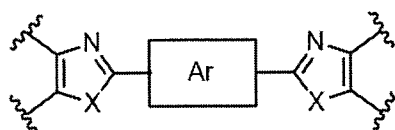
FIG. 1



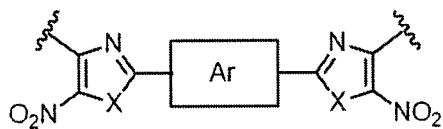
X = O or S



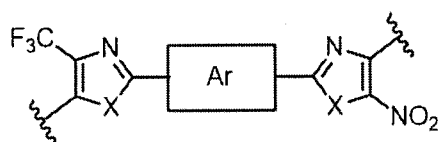
X = O or S



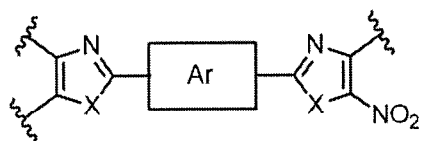
X = O or S



X = O or S



X = O or S



X = O or S

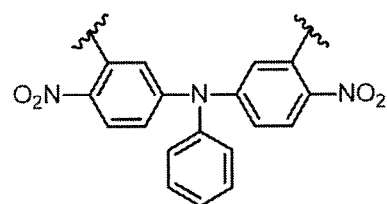
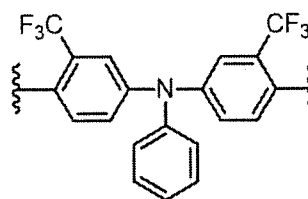
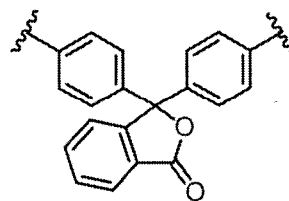
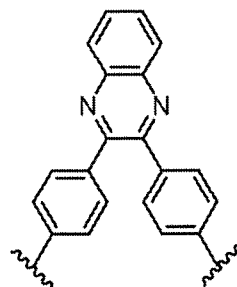
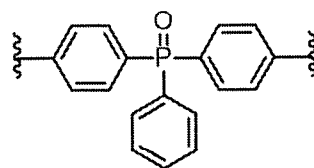
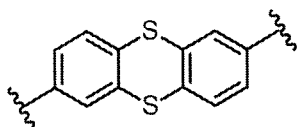


FIG. 2

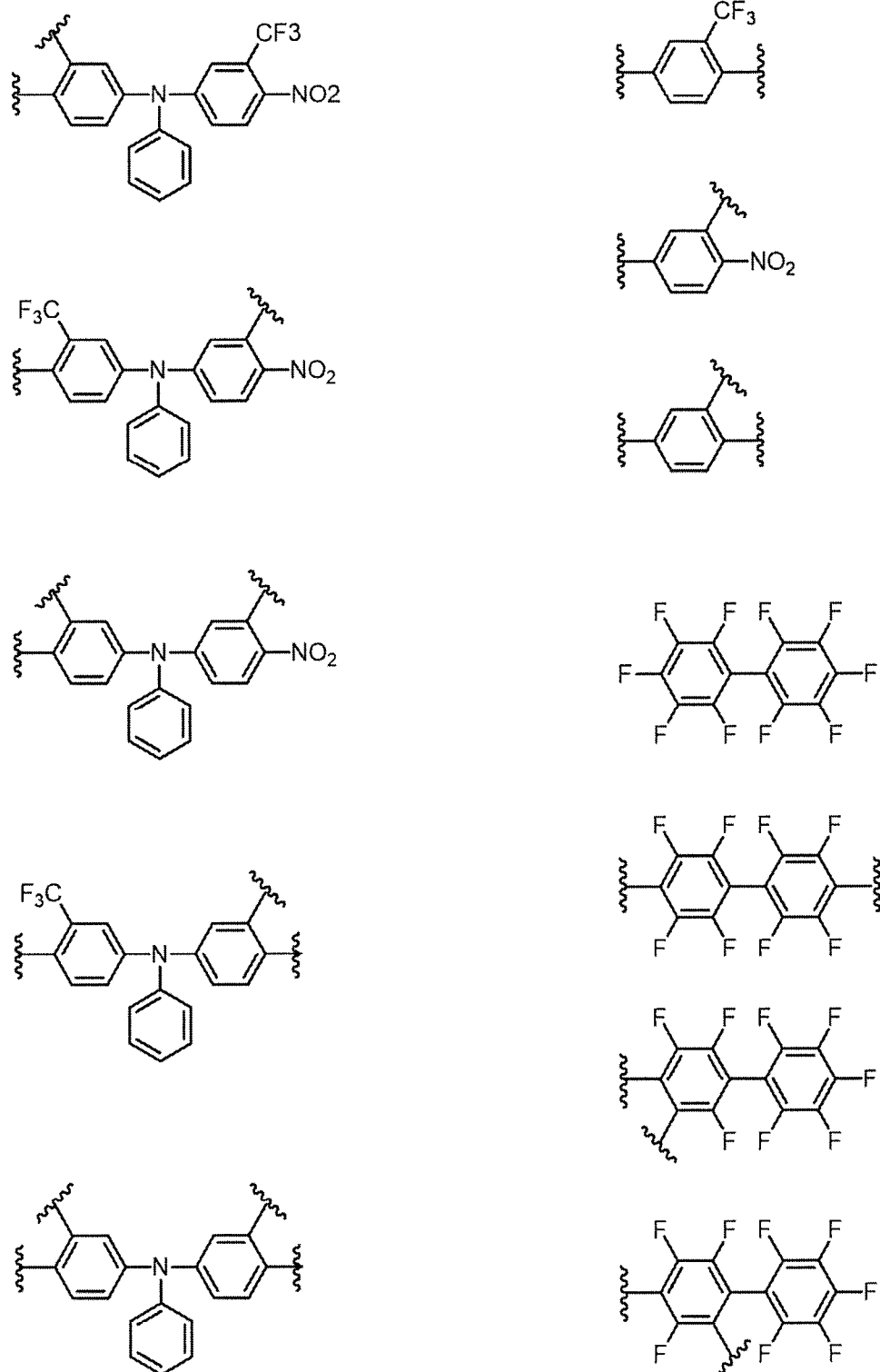


FIG. 3

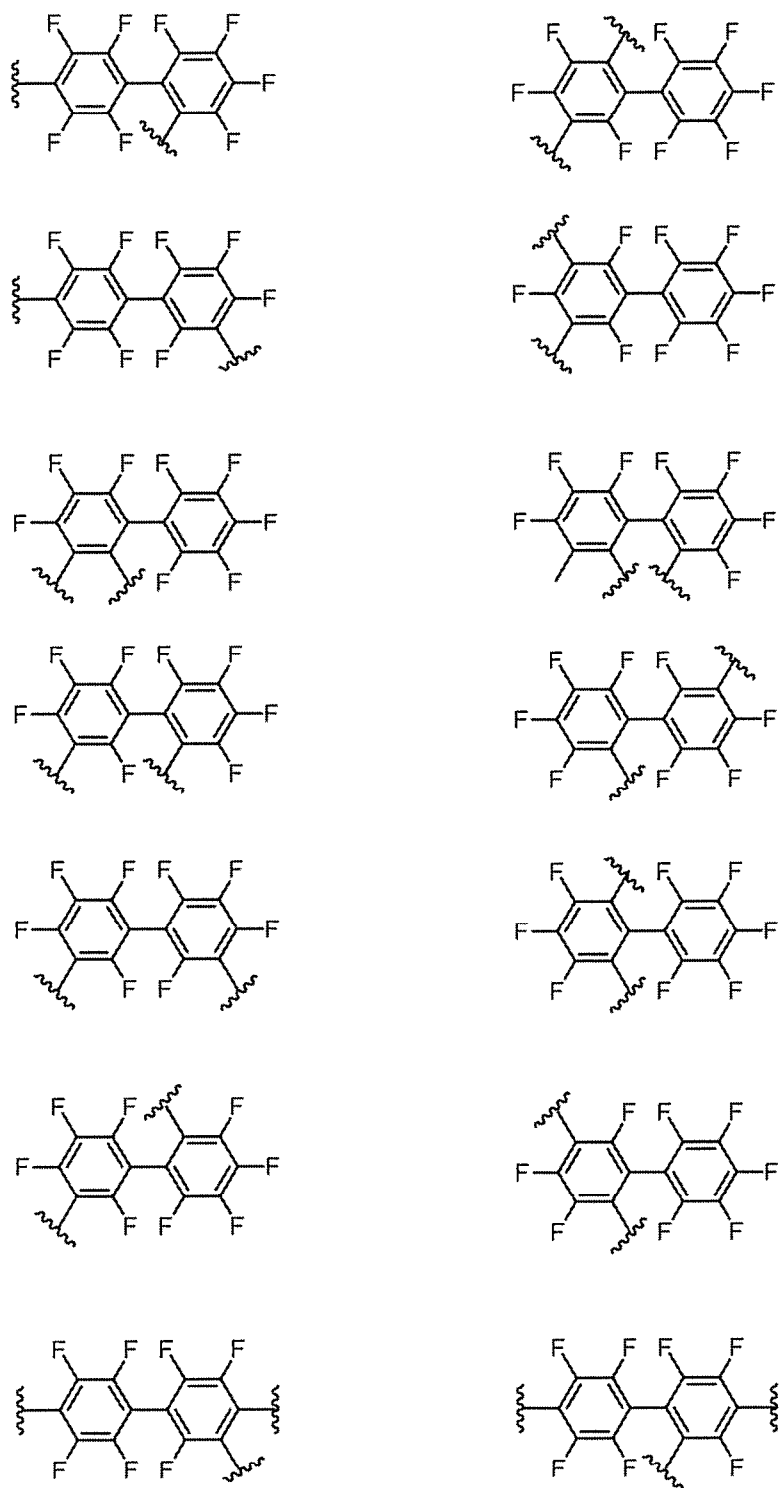


FIG. 4

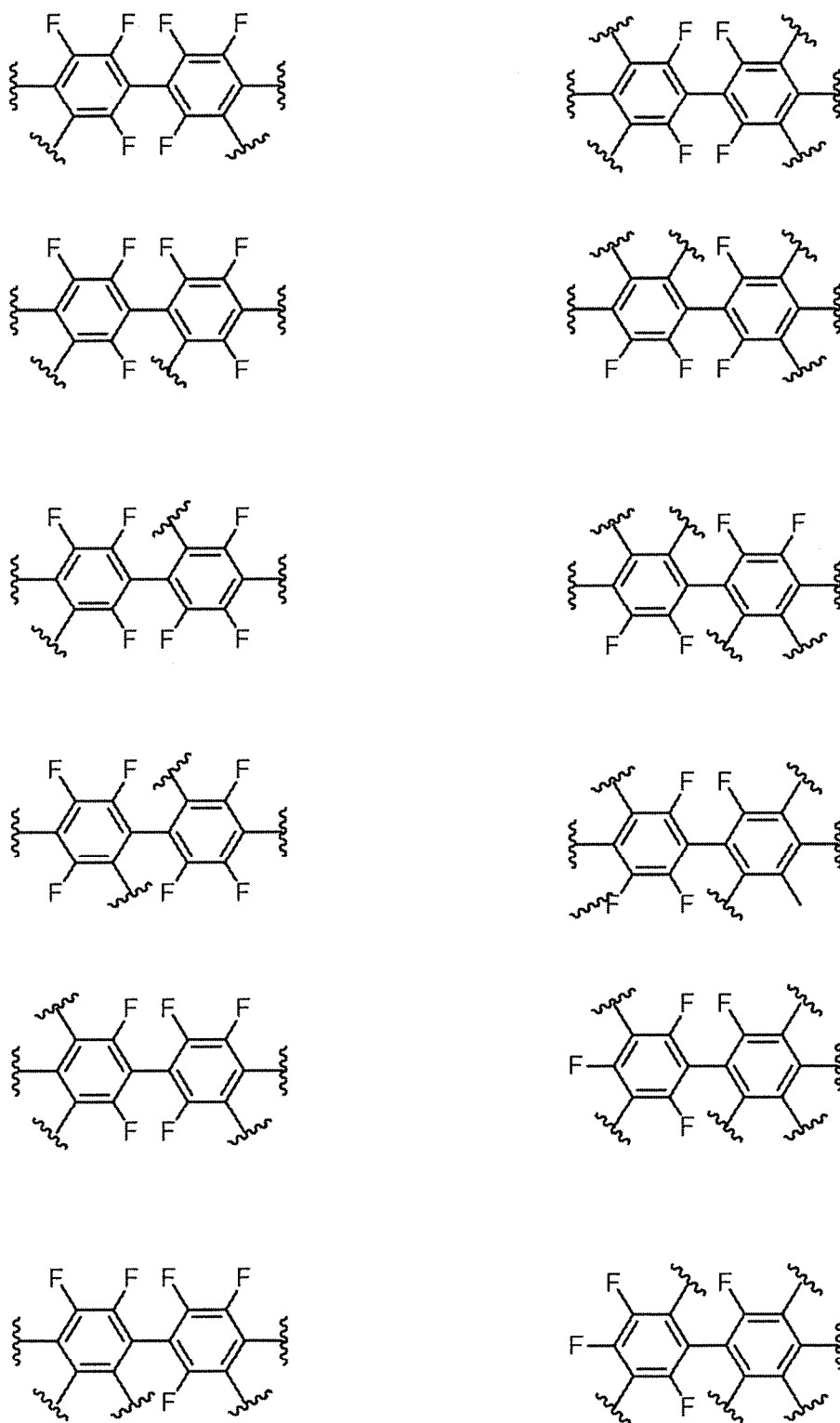


FIG. 5

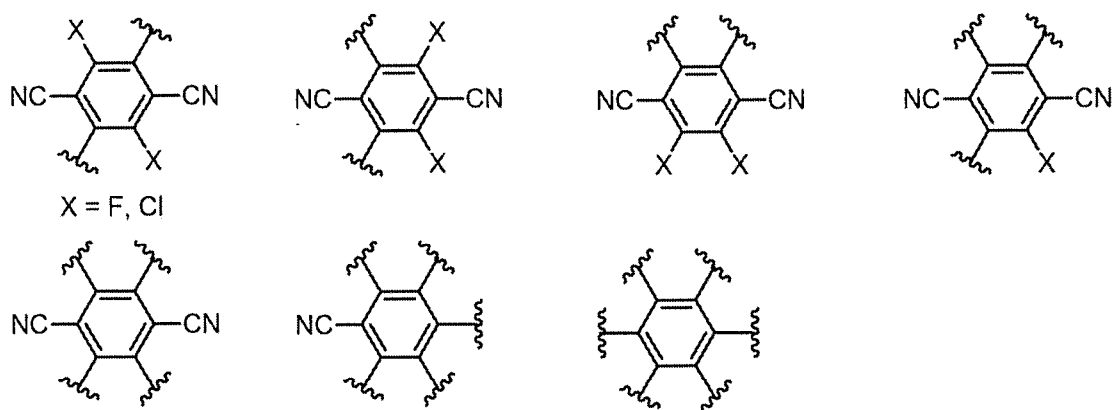


FIG. 6

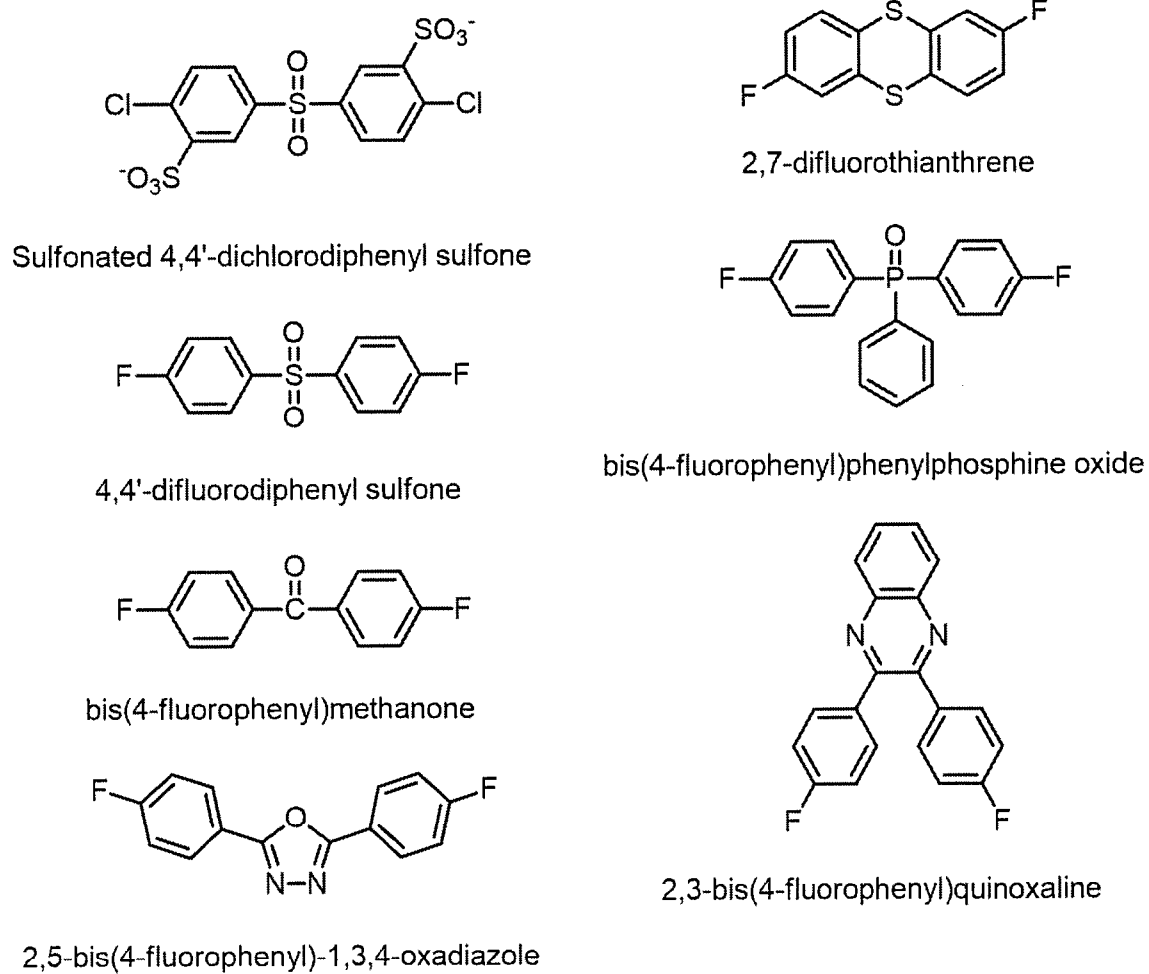


FIG. 7

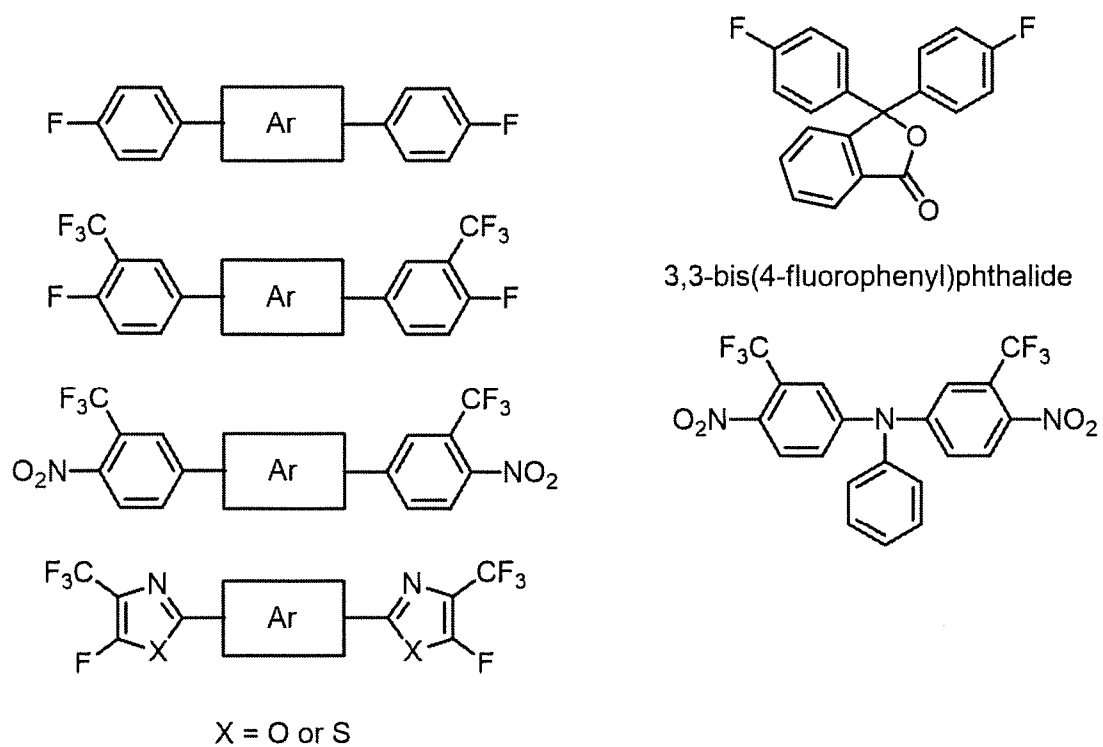


FIG. 8

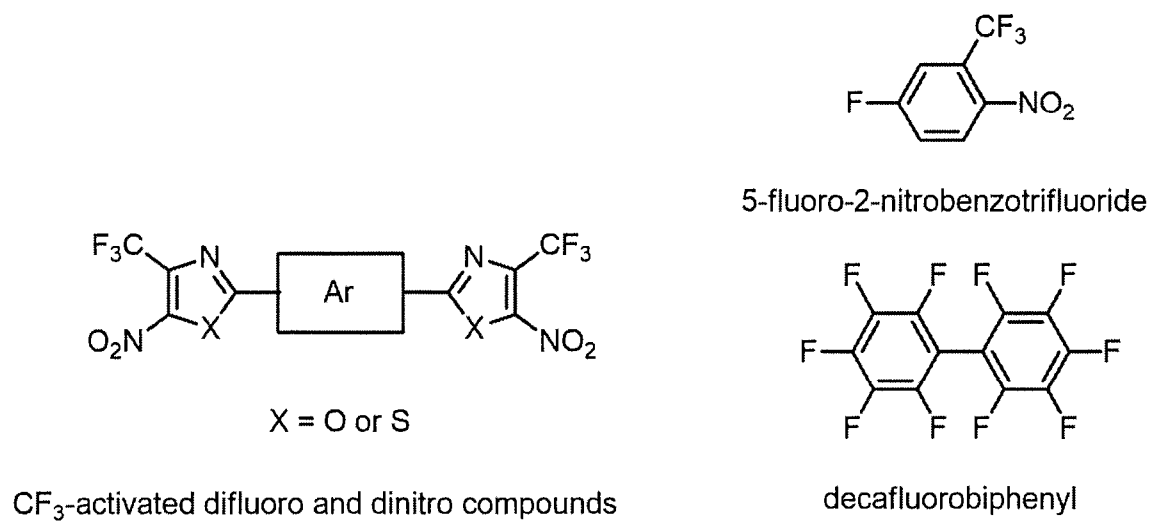


FIG. 9

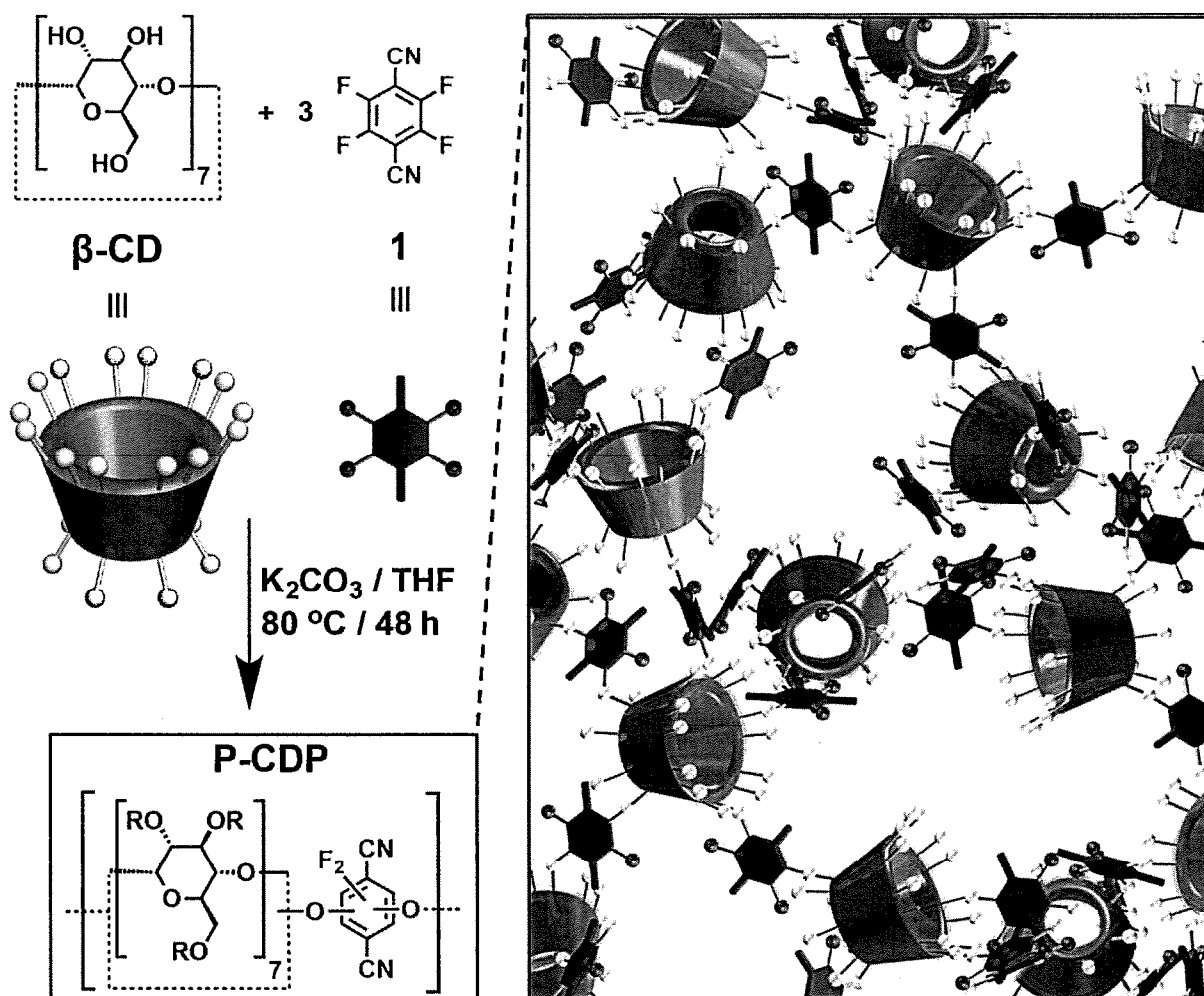


FIG. 10

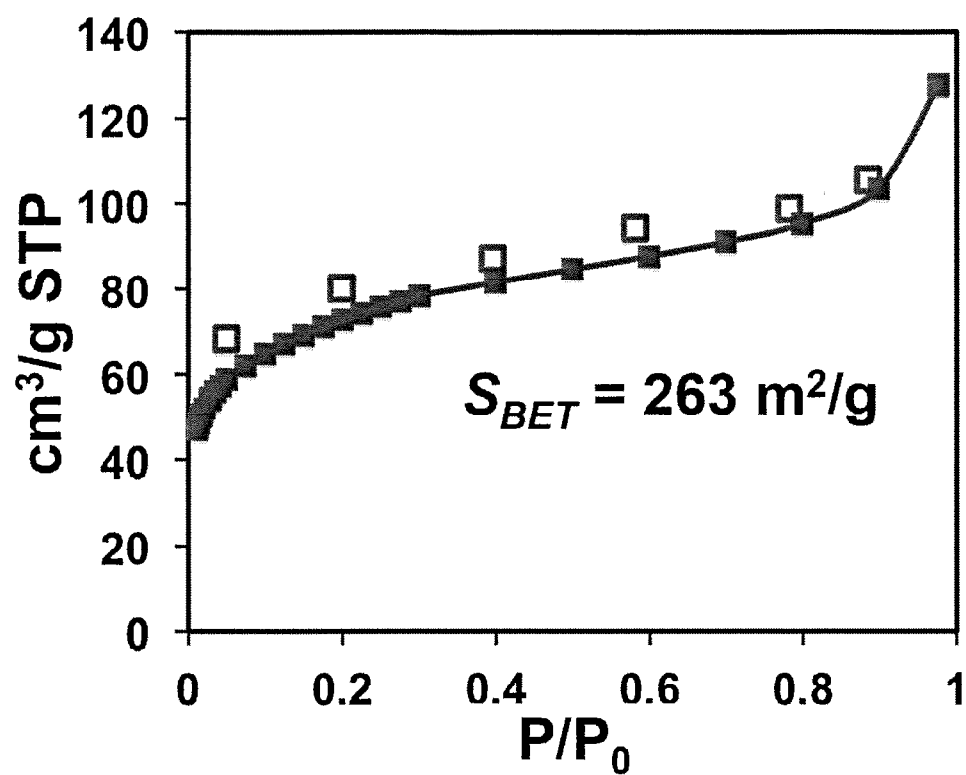


FIG. 11

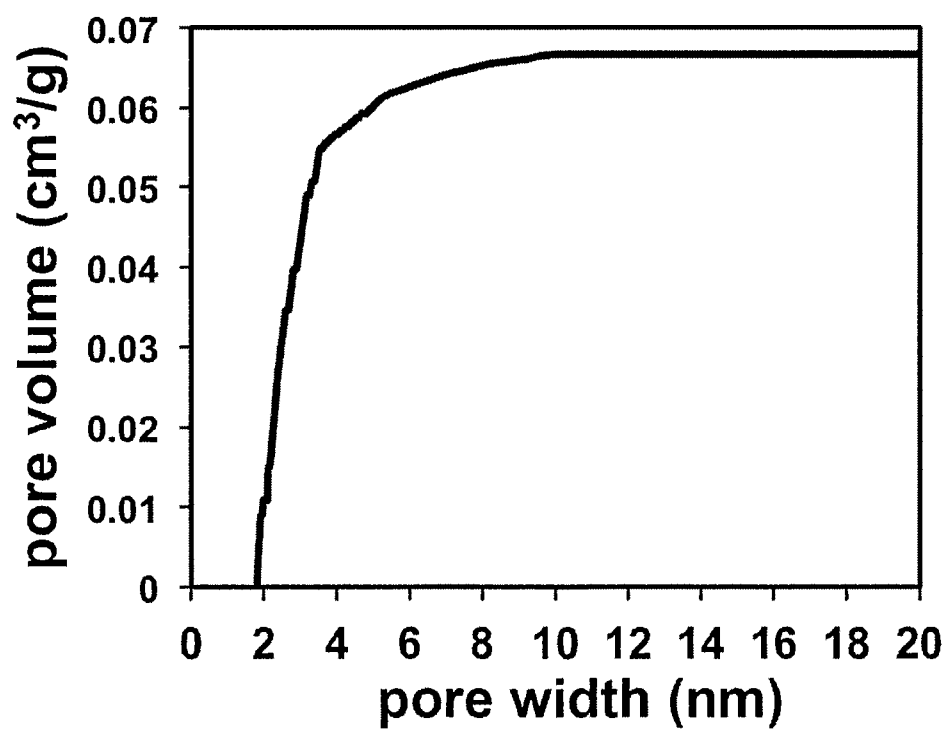


FIG. 12

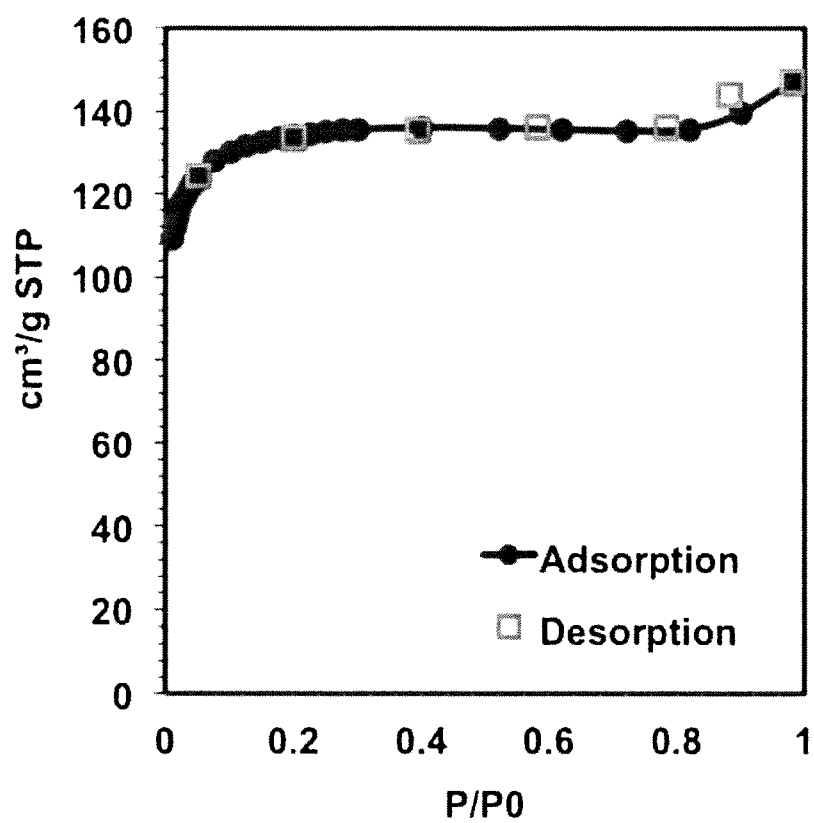


FIG. 13

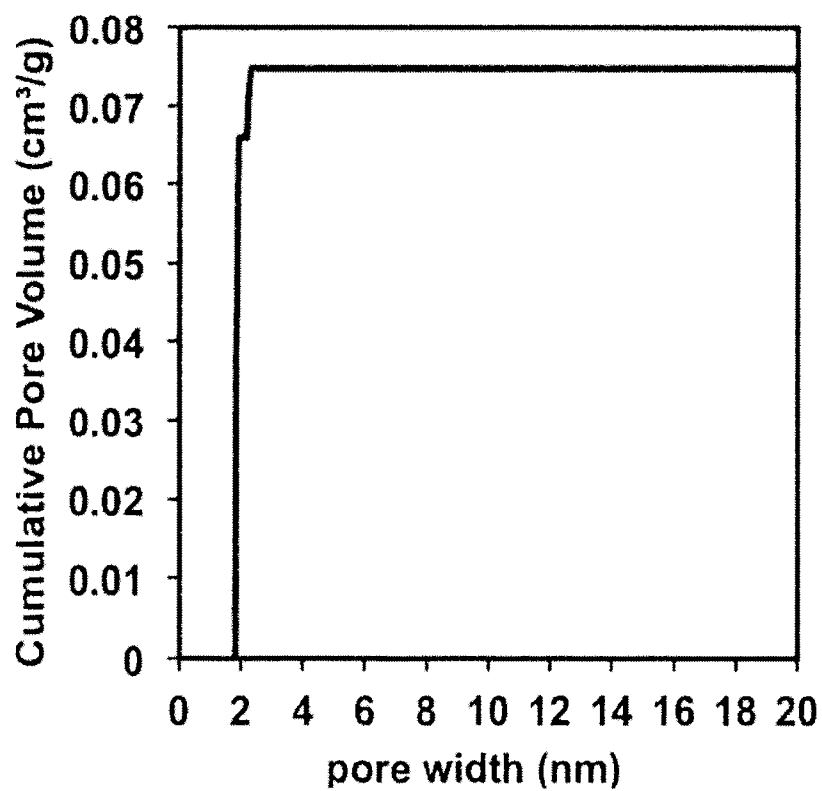


FIG. 14

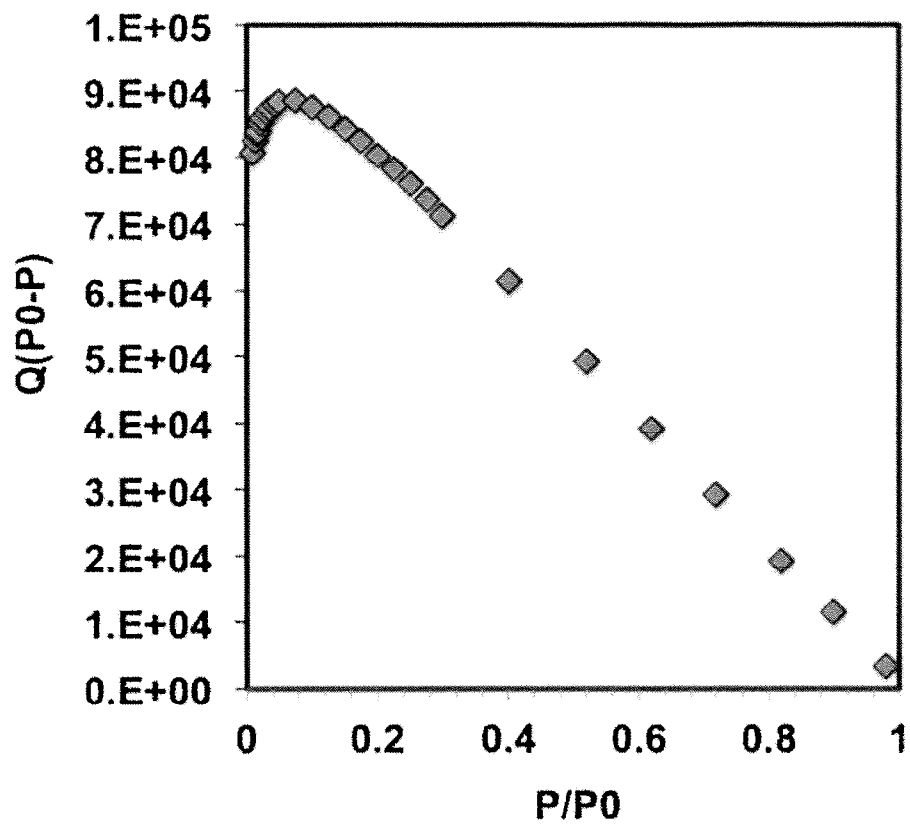


FIG. 15

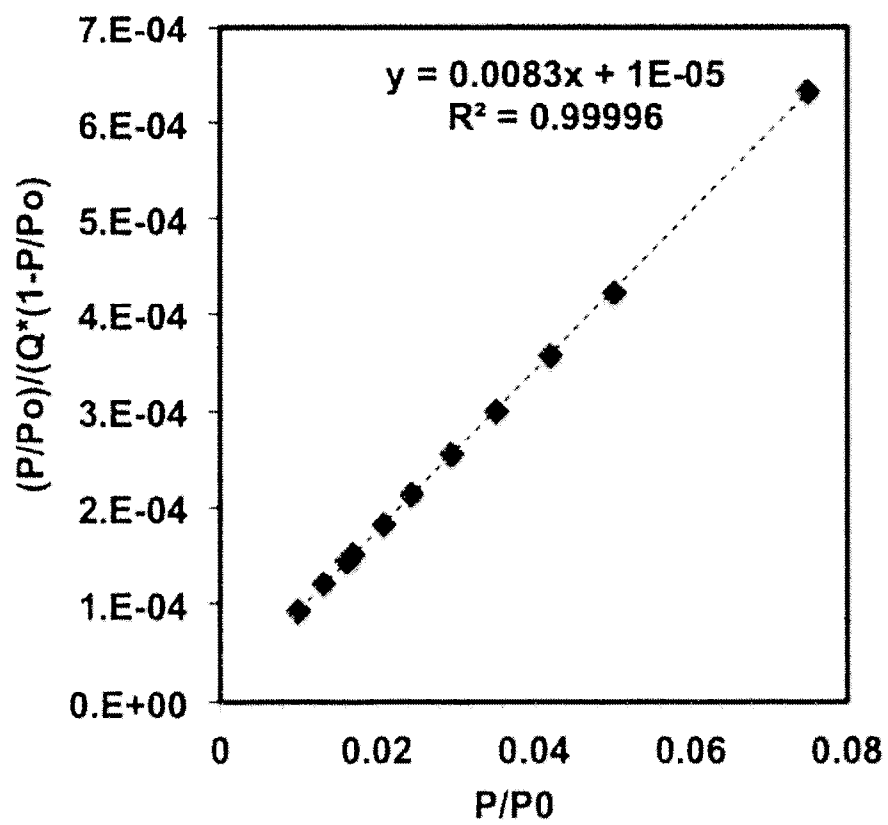


FIG. 16

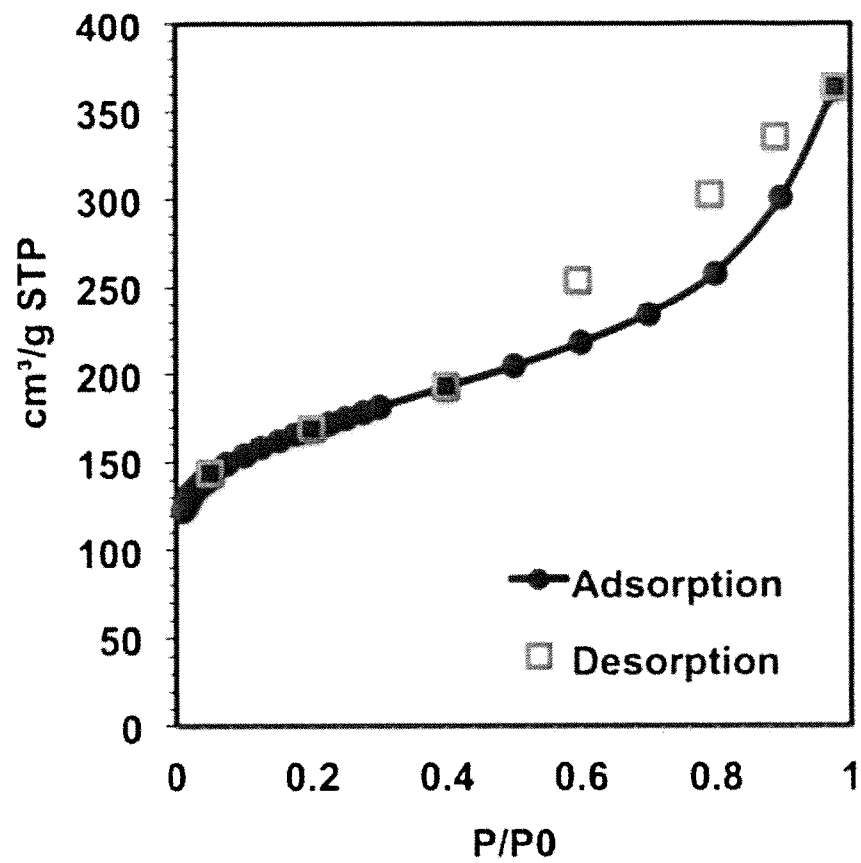


FIG. 17

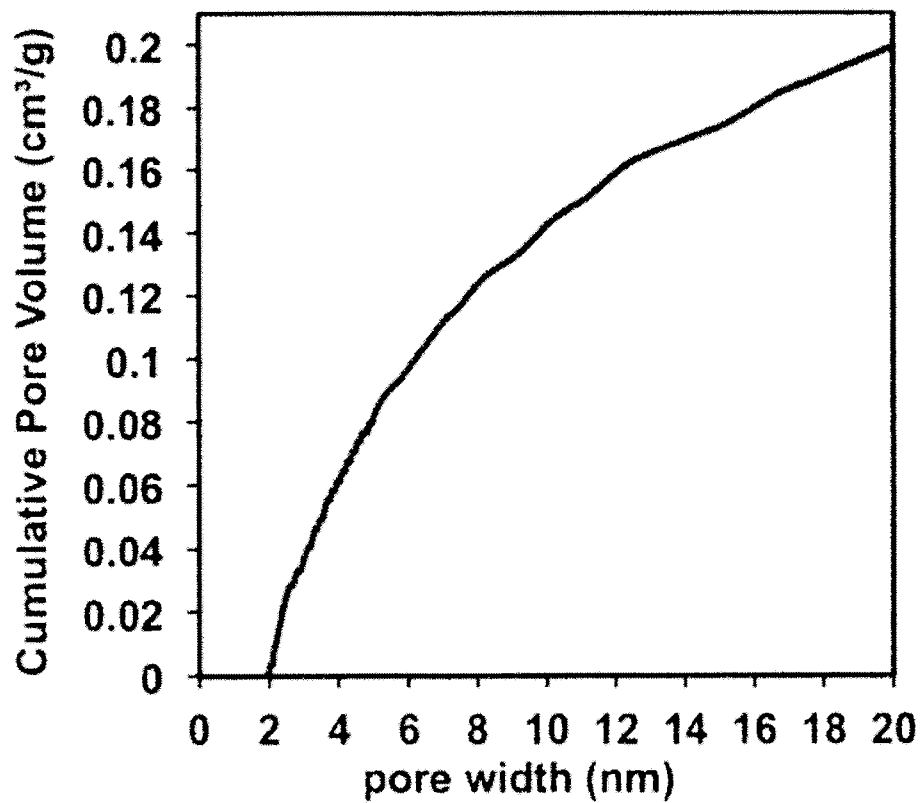


FIG. 18

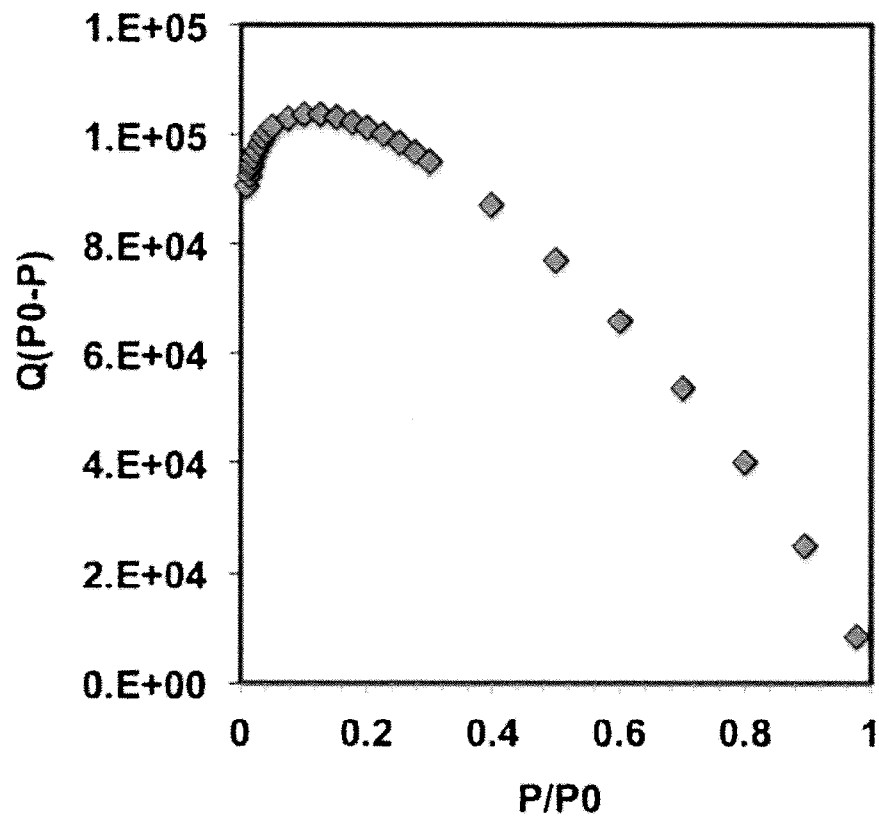


FIG. 19

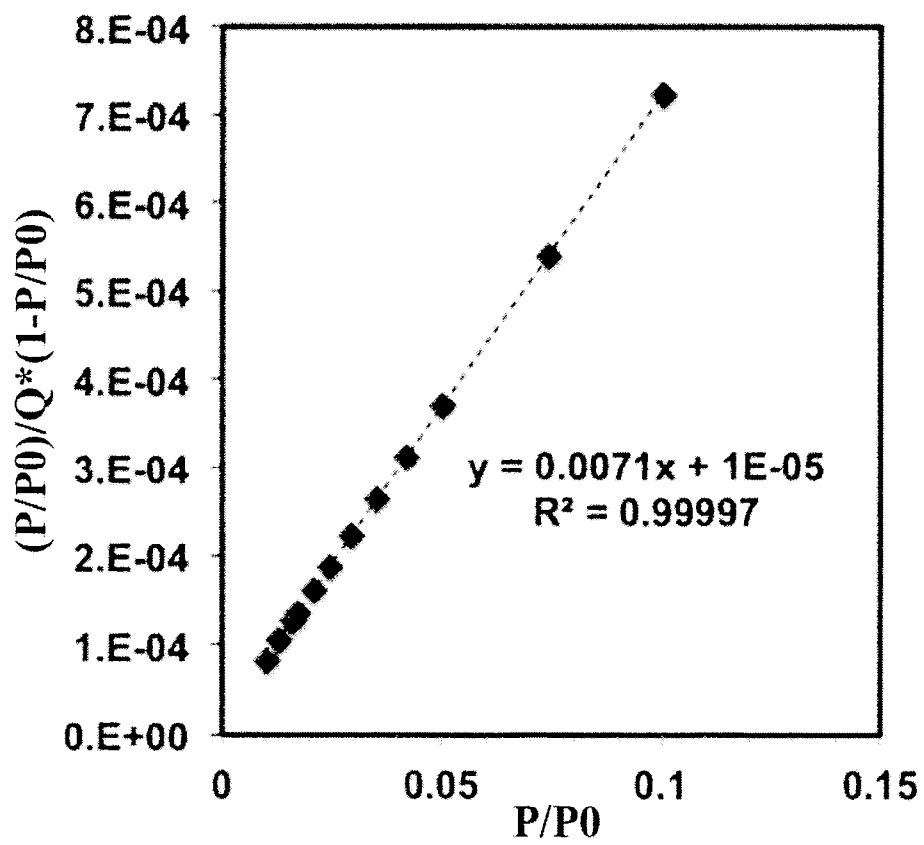


FIG. 20

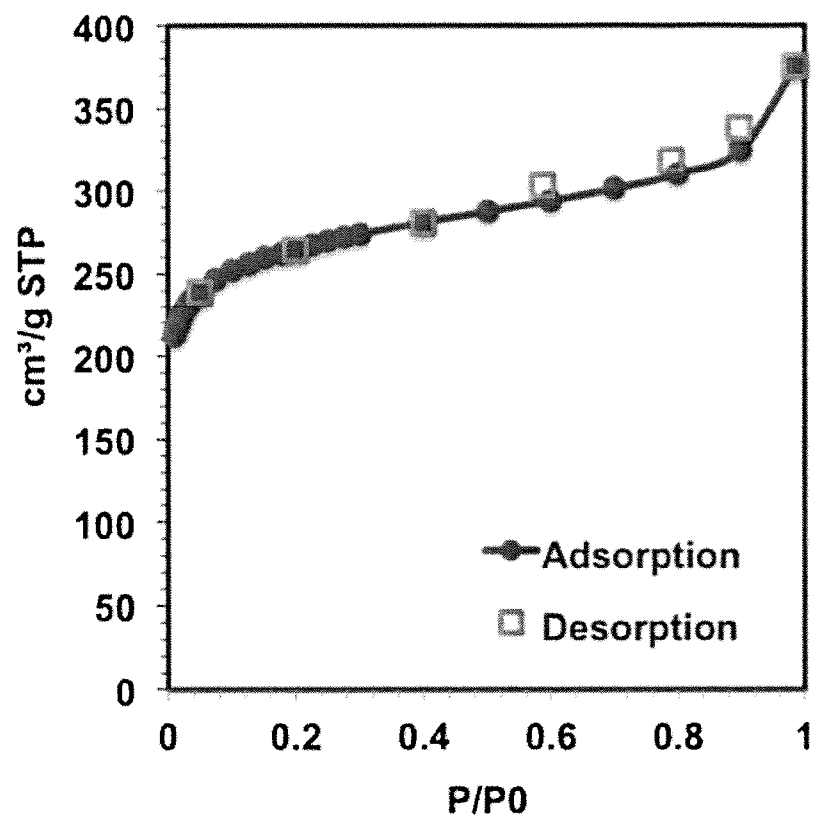


FIG. 21

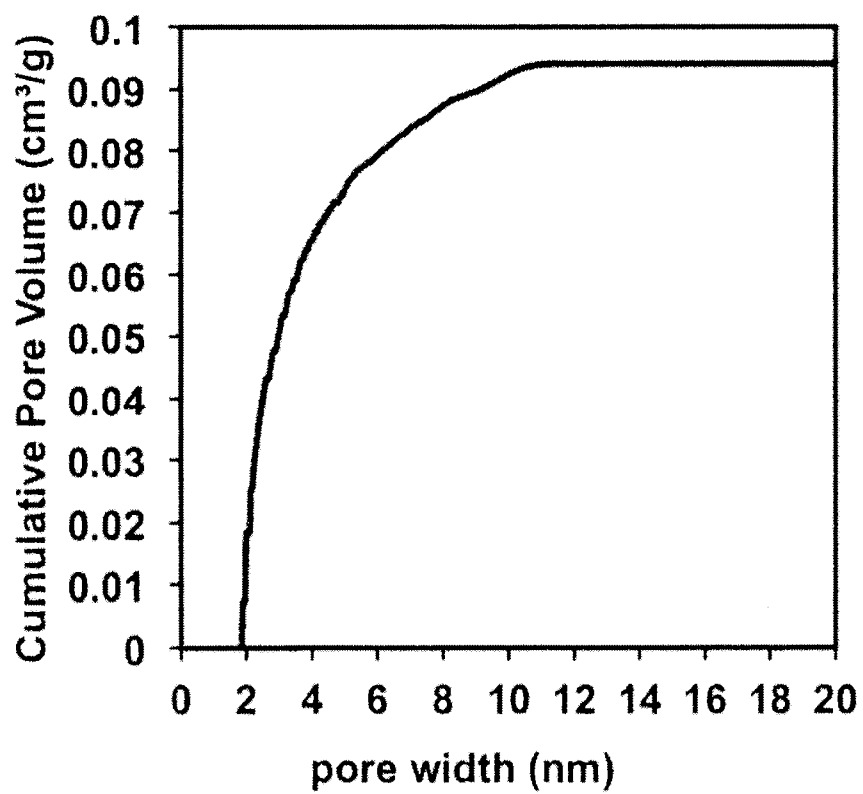


FIG. 22

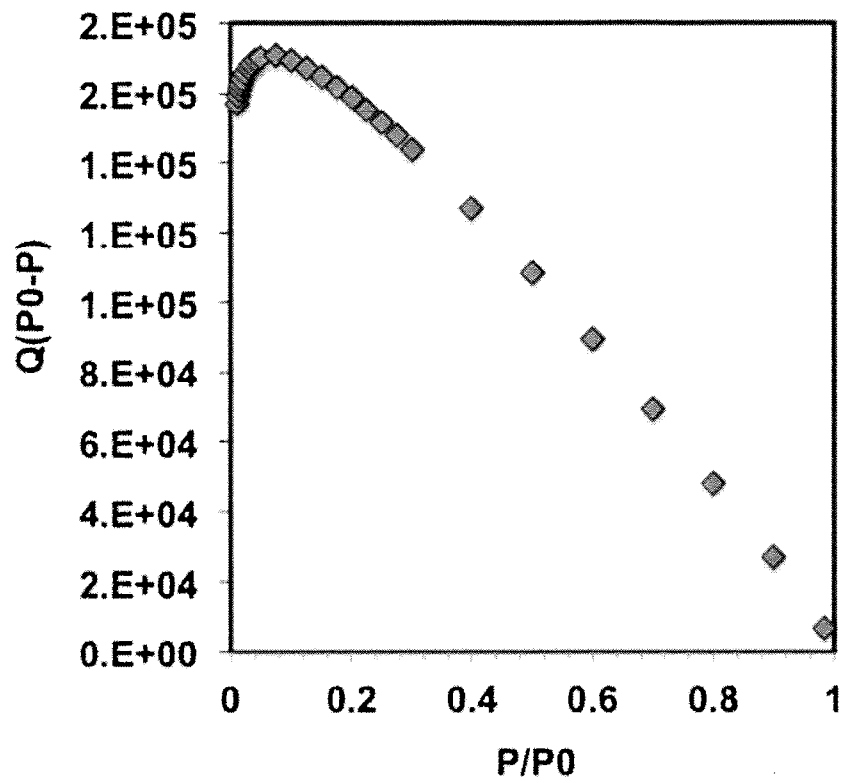


FIG. 23

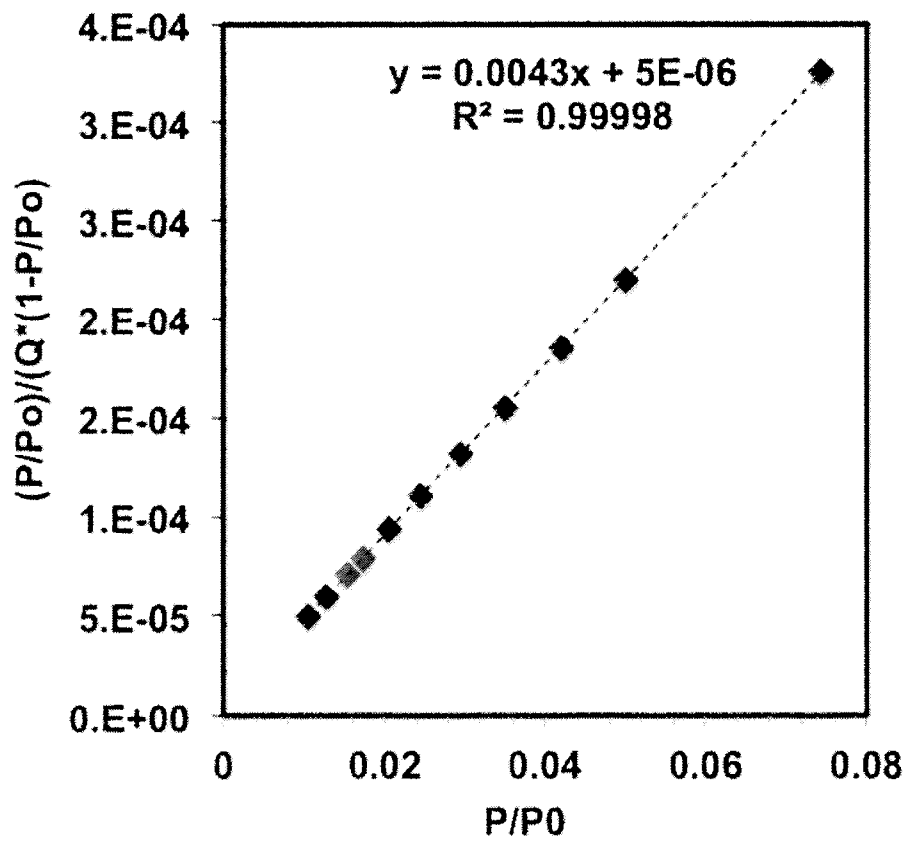


FIG. 24

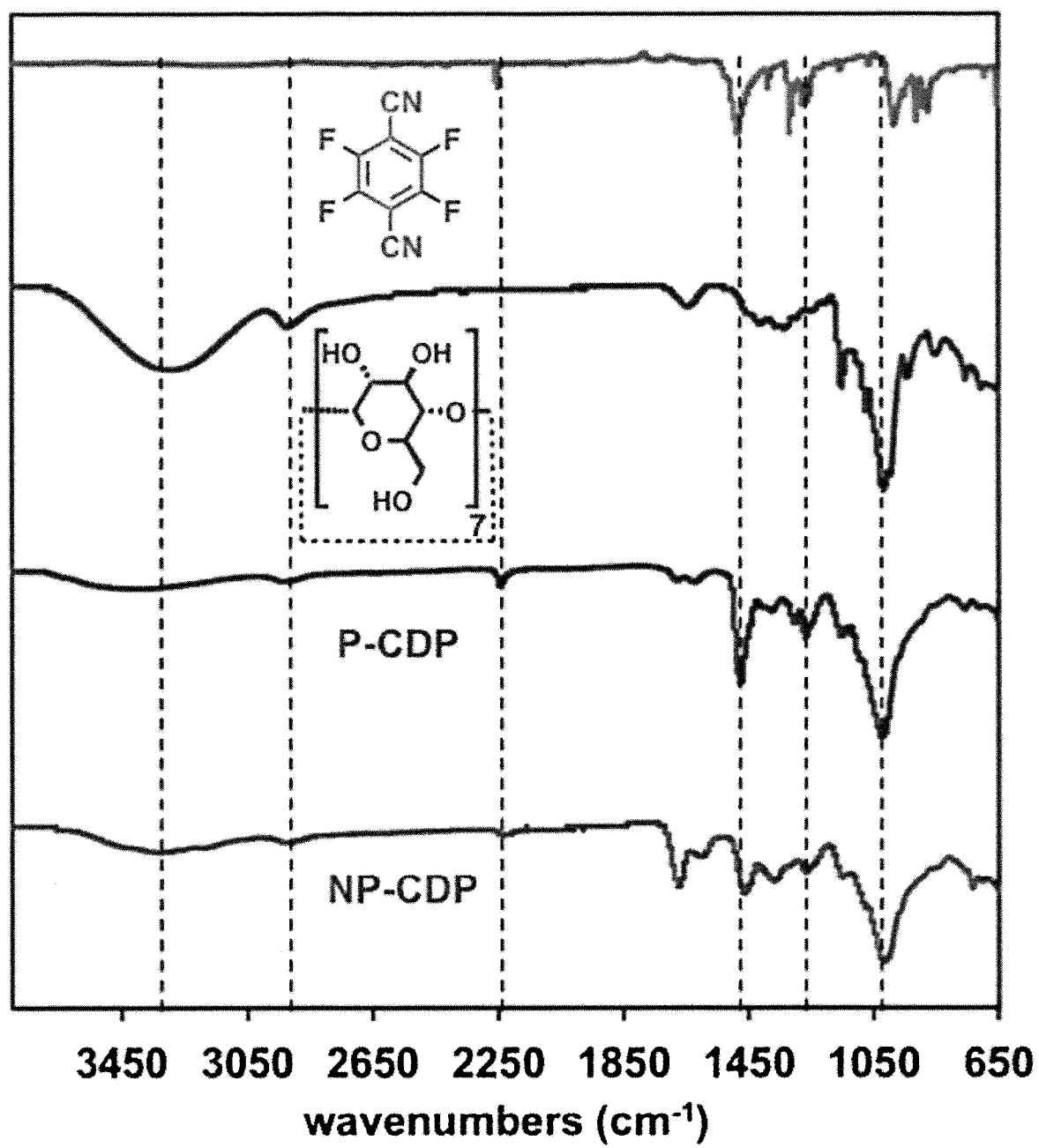


FIG. 25

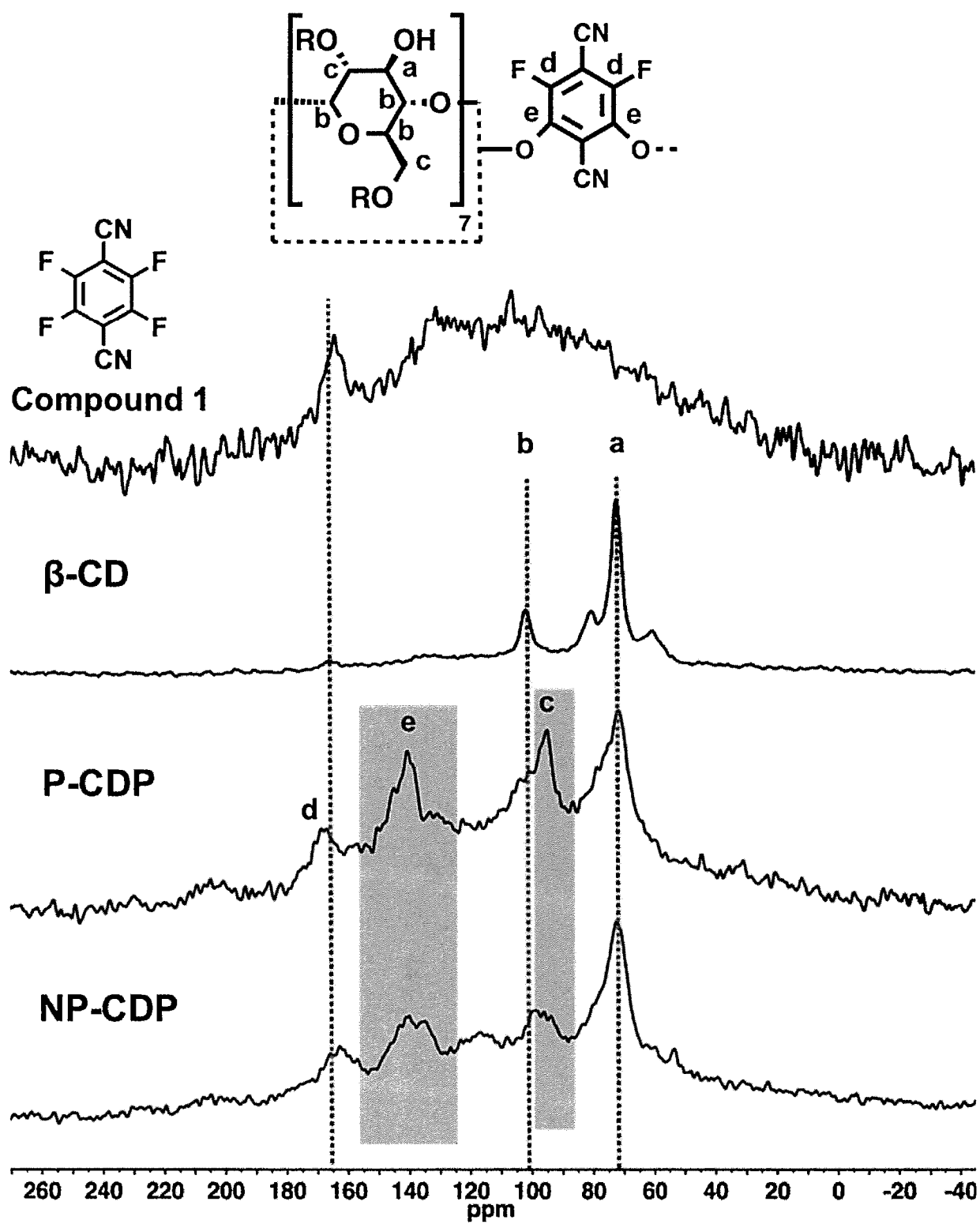


FIG. 26

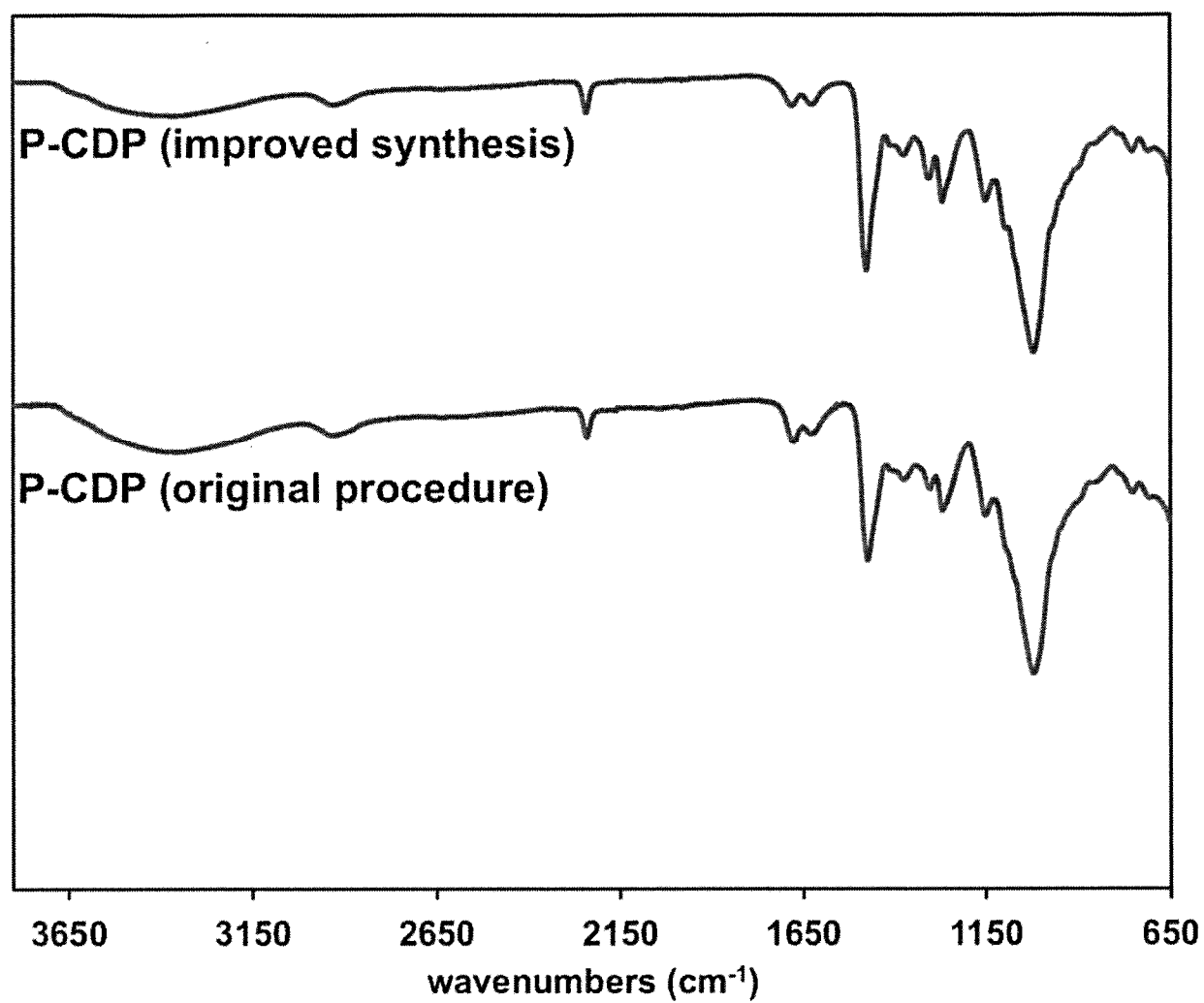


FIG. 27

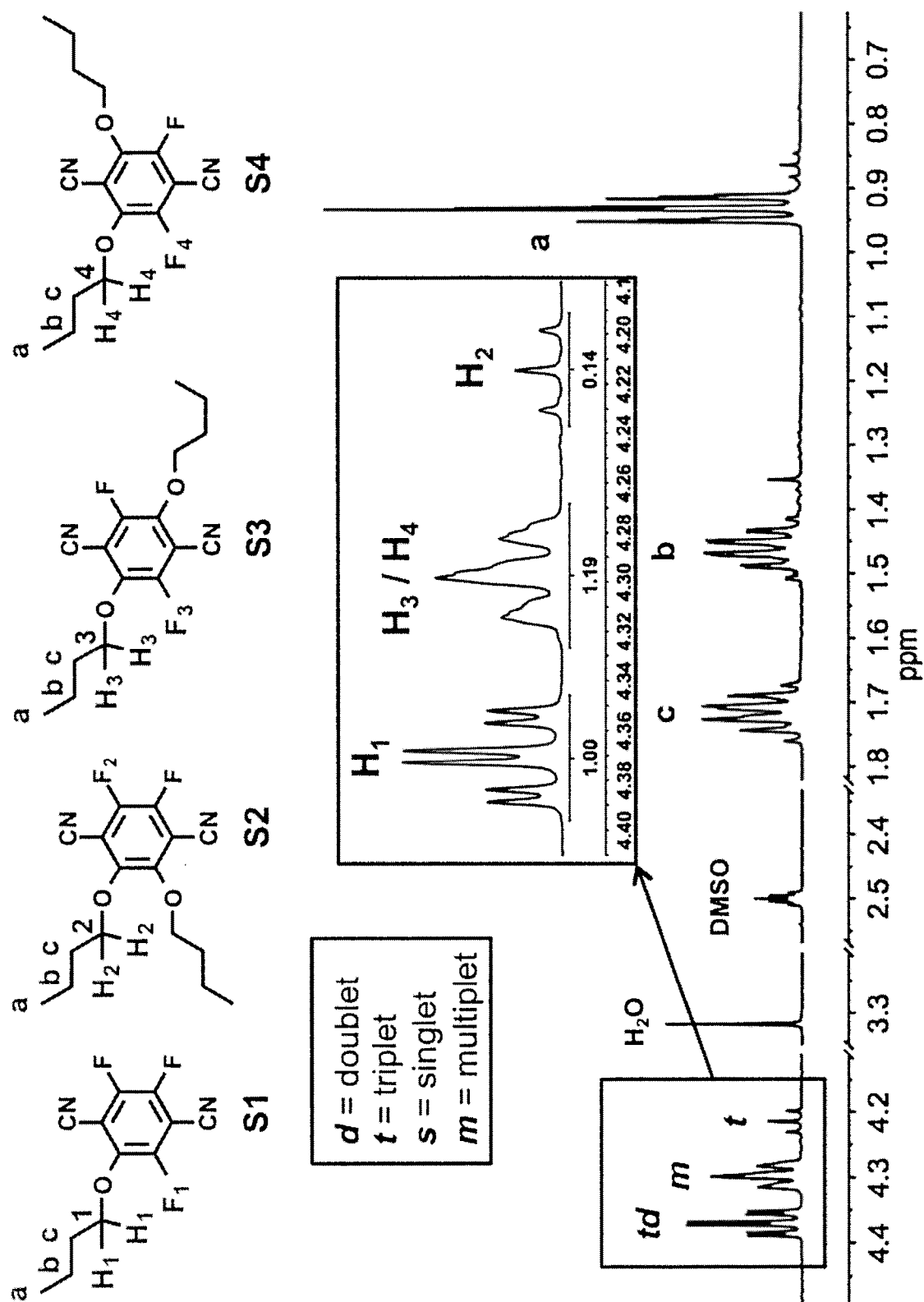


FIG. 28

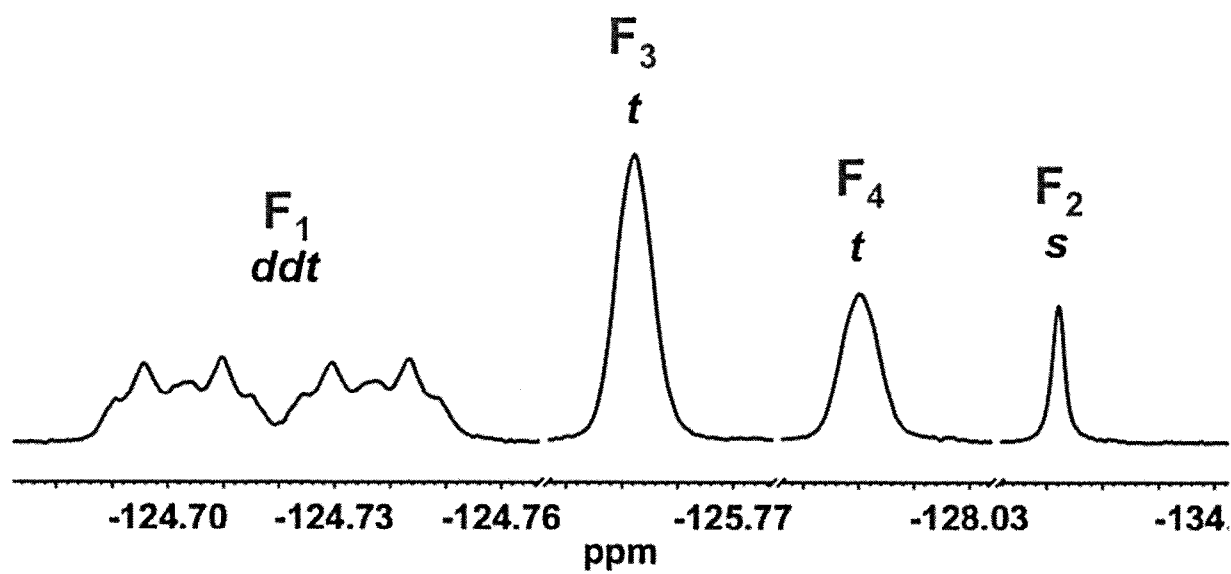


FIG. 29

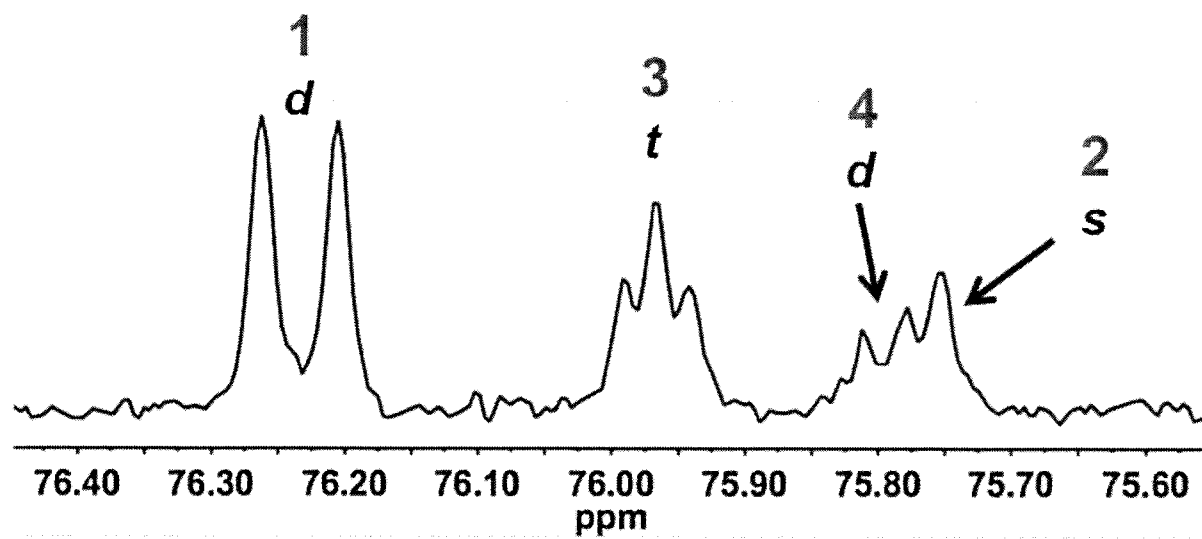


FIG. 30

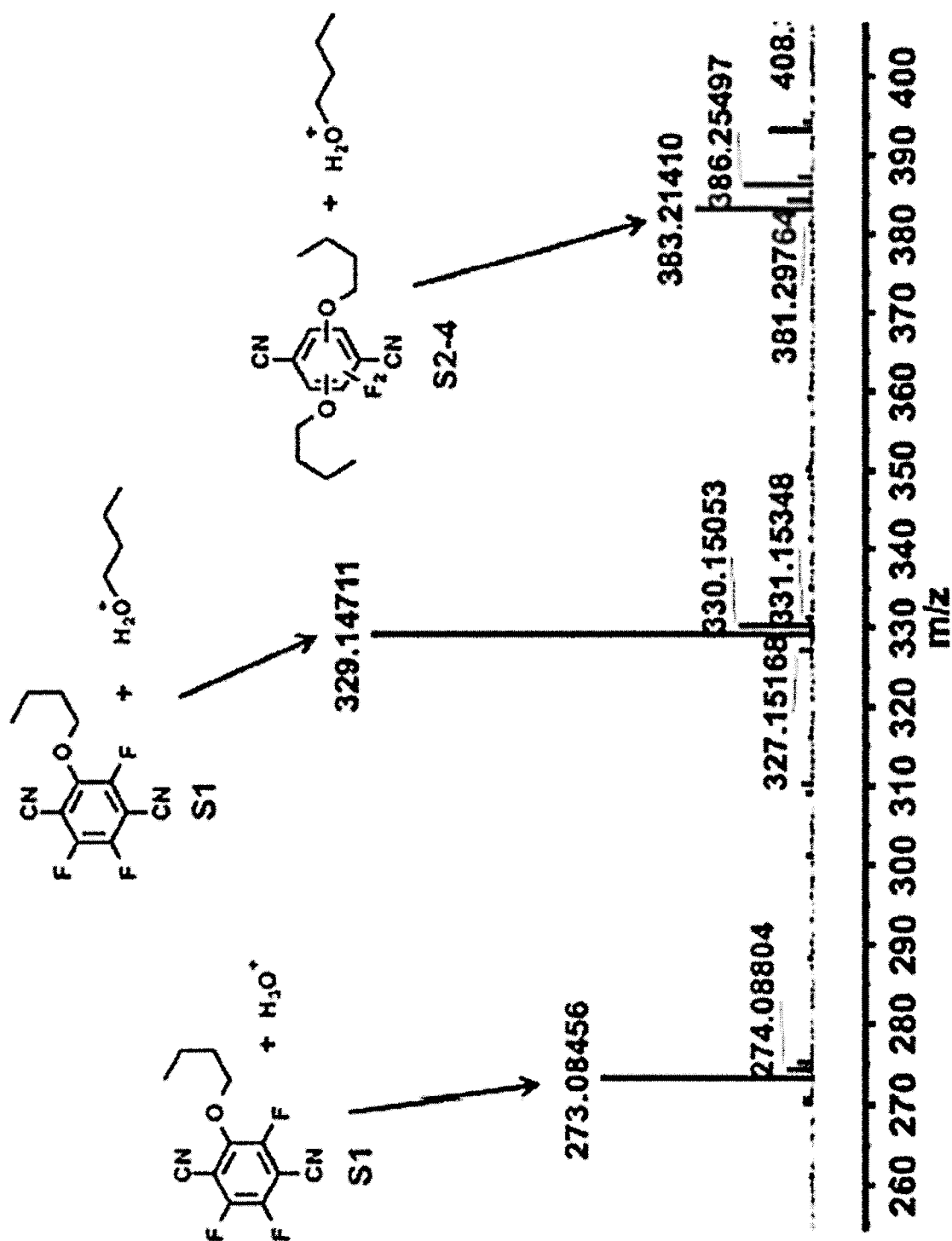


FIG. 31

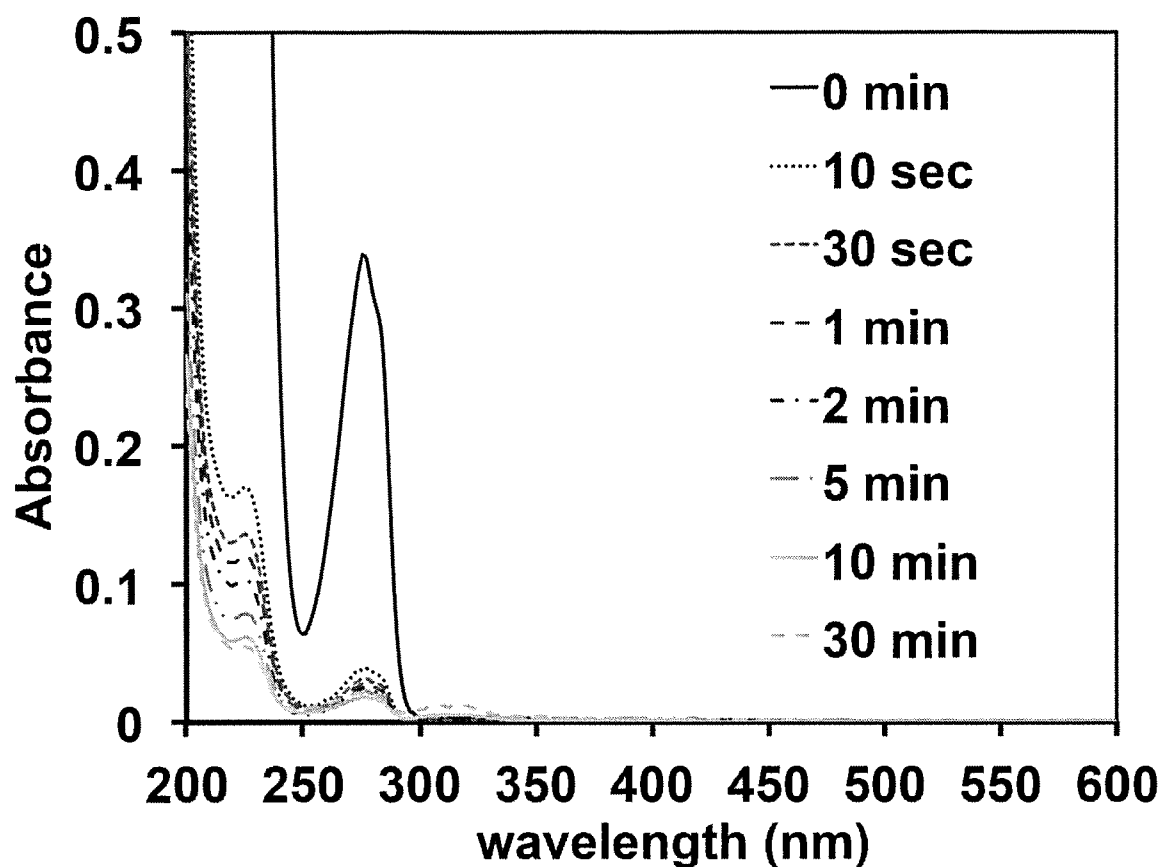


FIG. 32

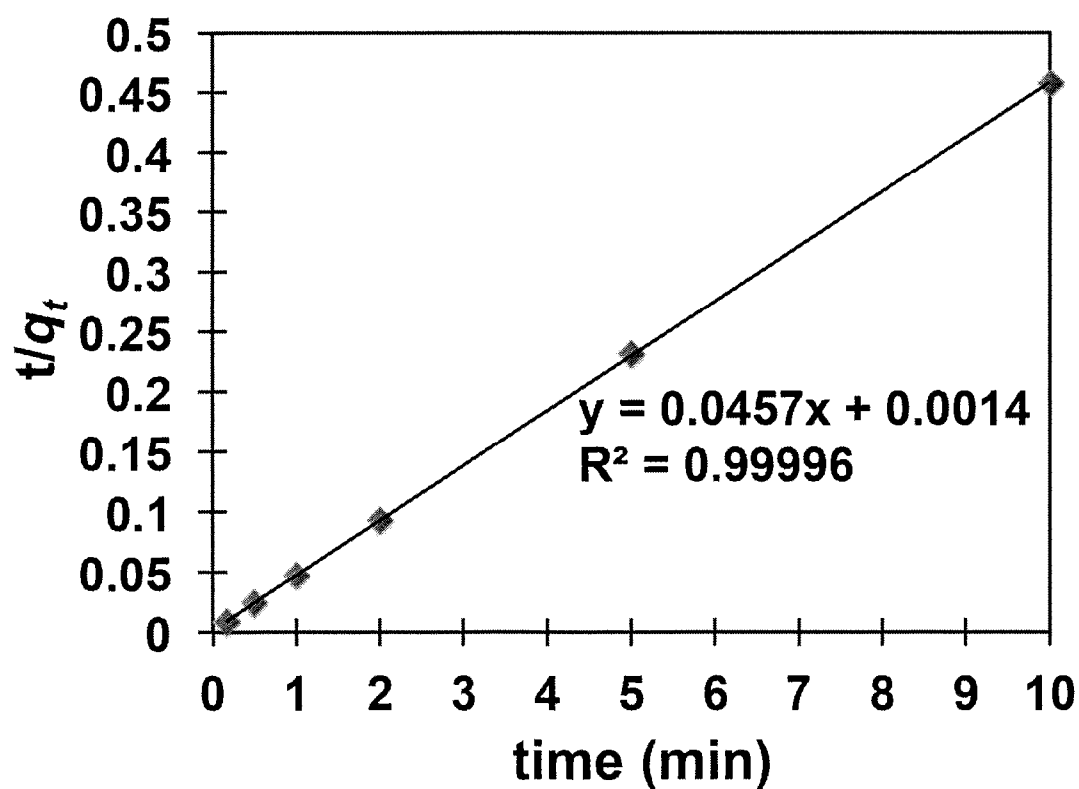


FIG. 33

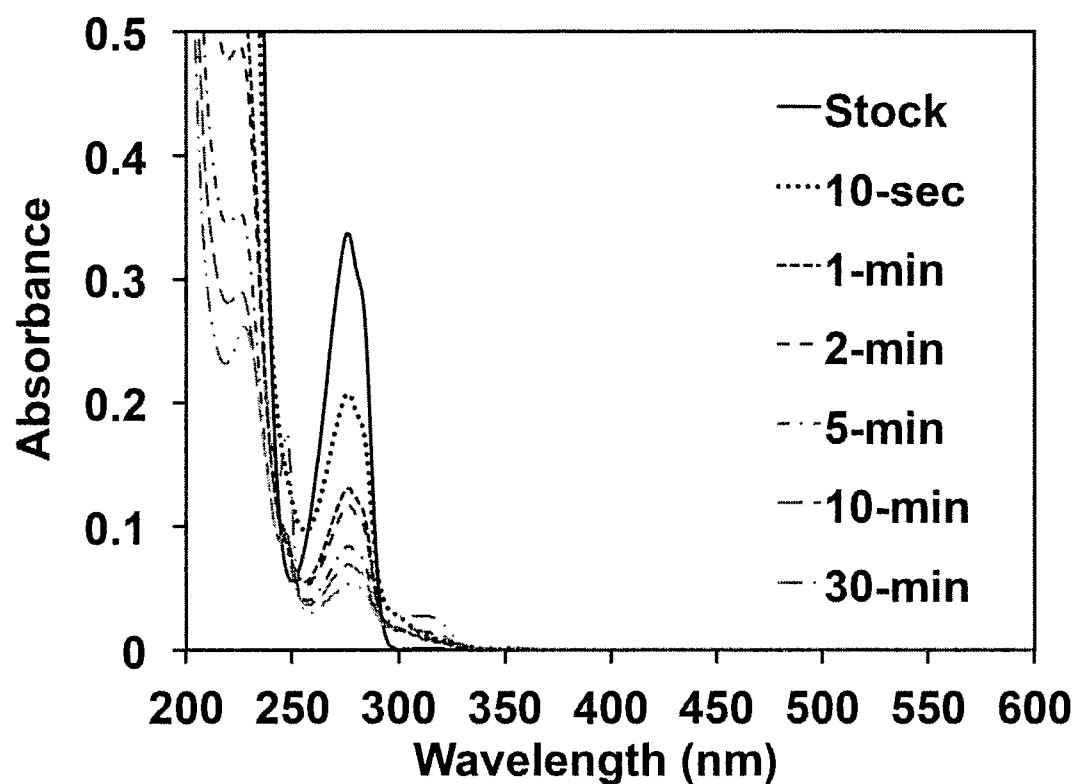


FIG. 34

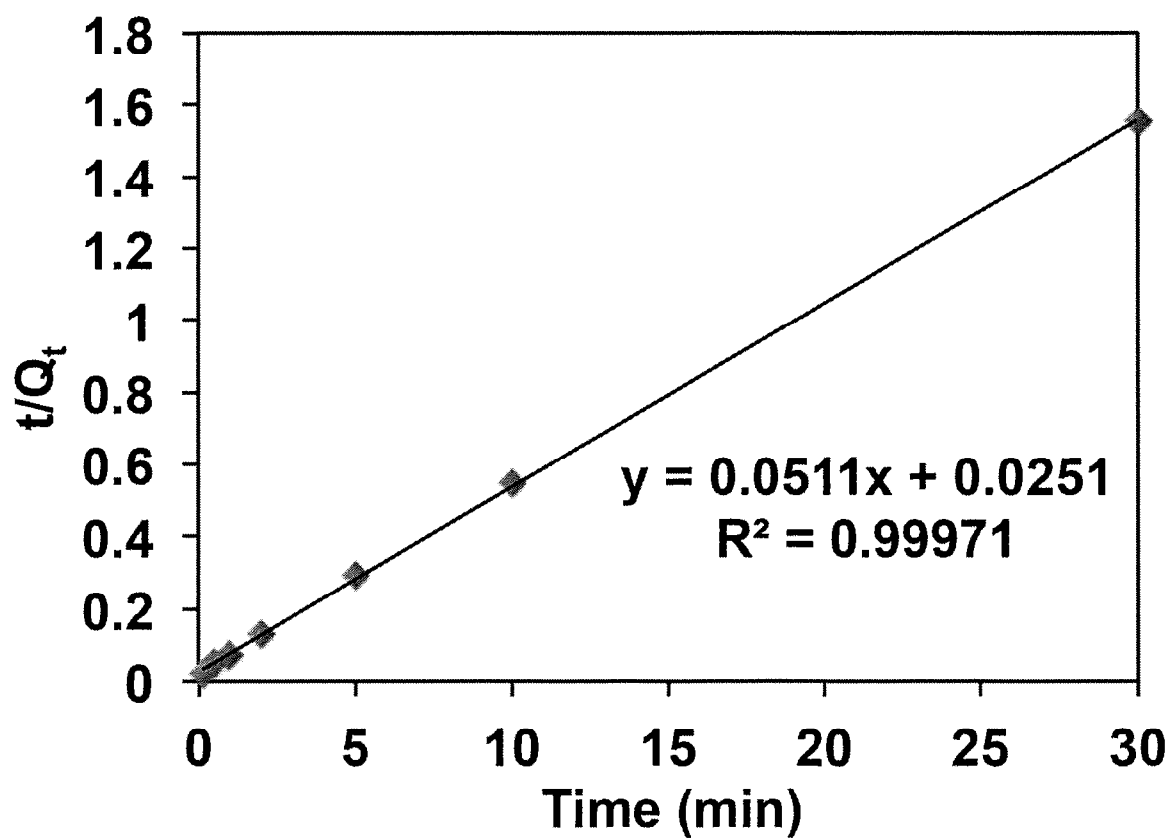


FIG. 35

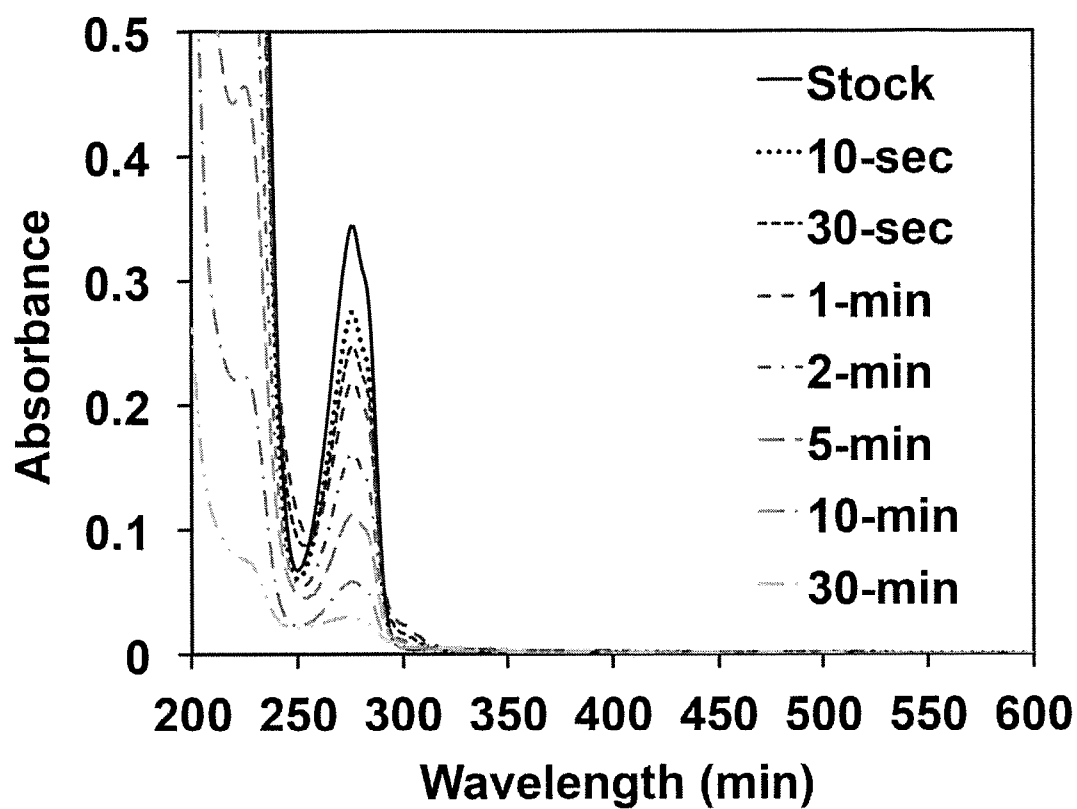


FIG. 36

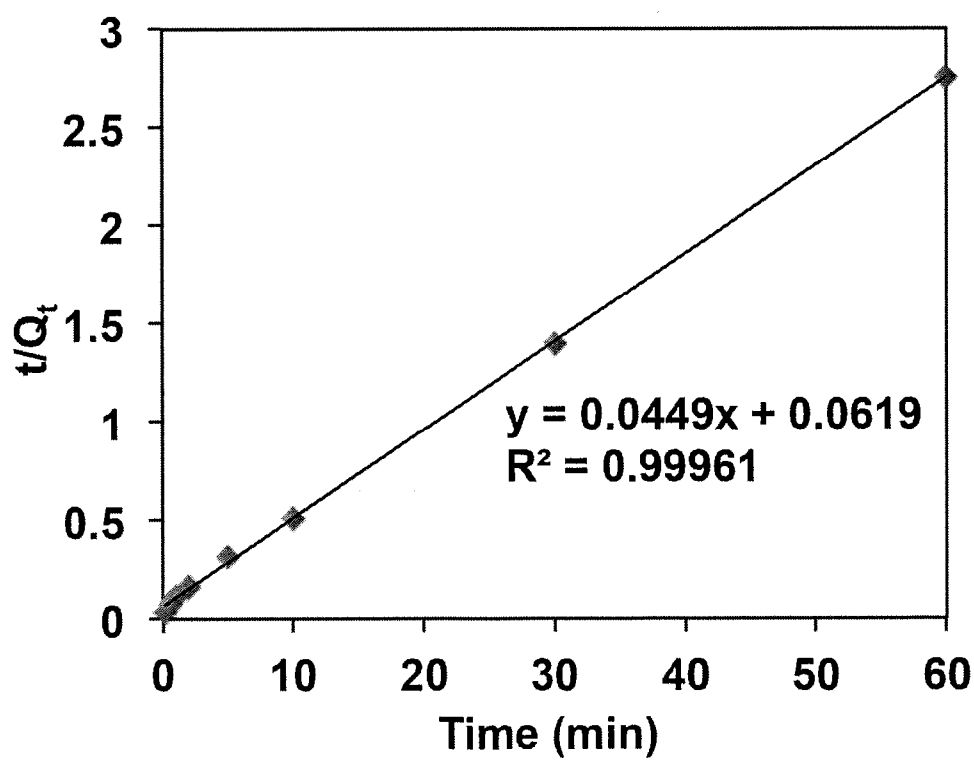


FIG. 37

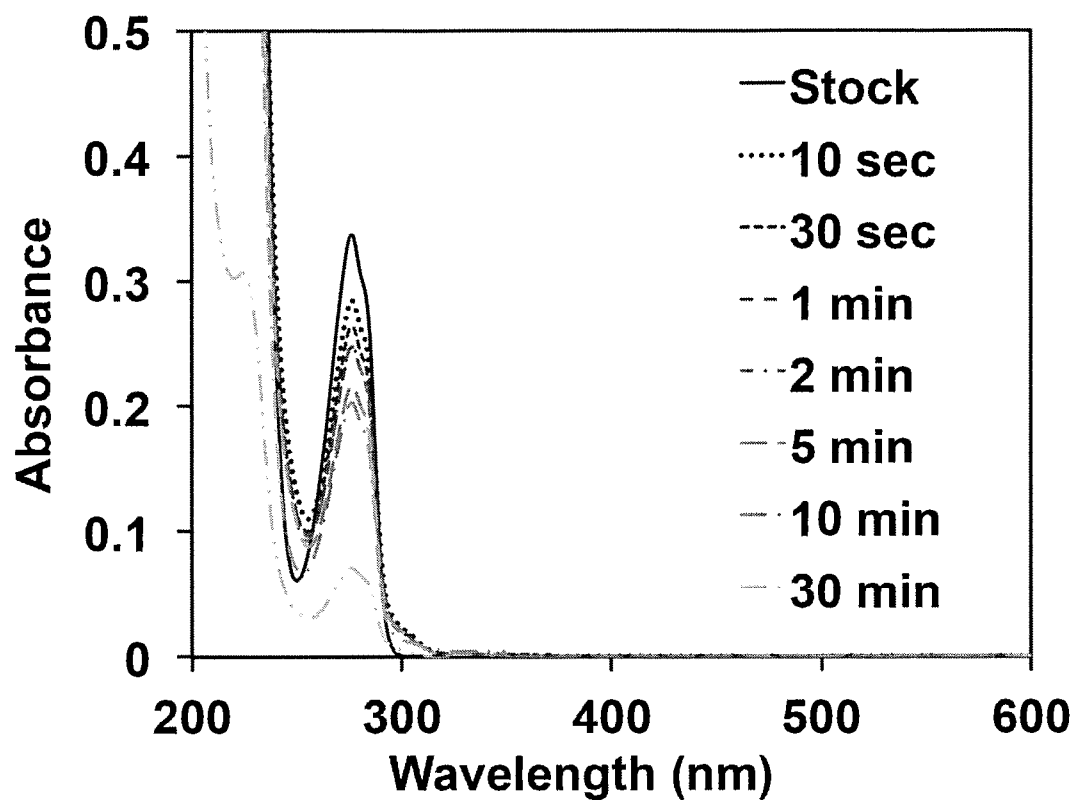


FIG. 38

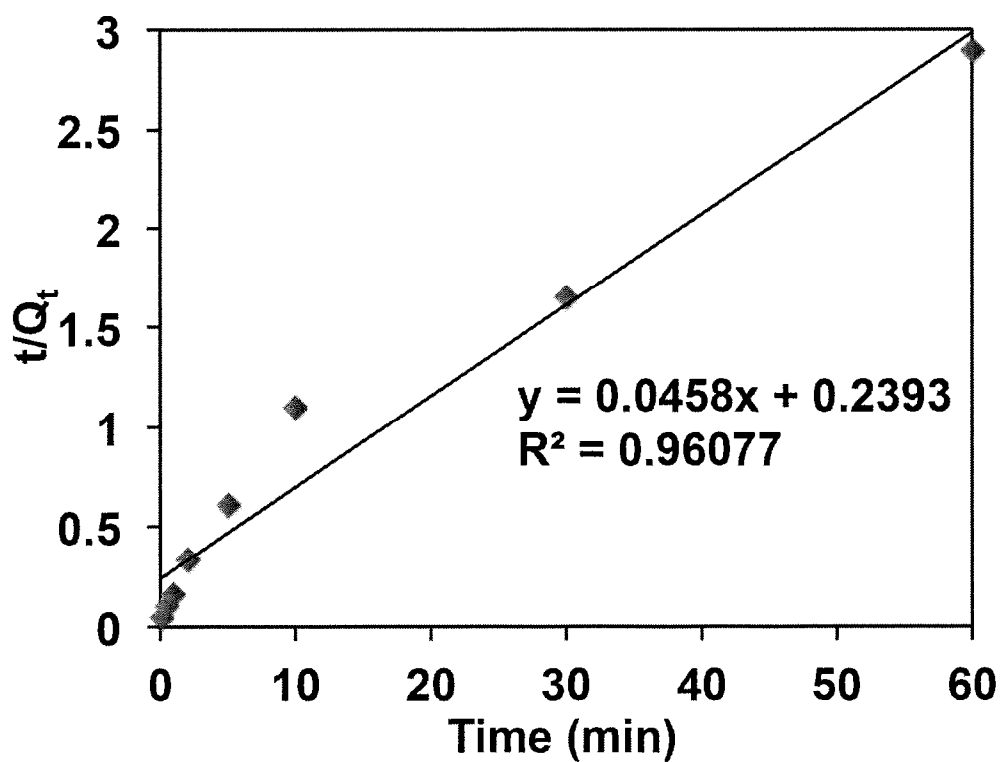


FIG. 39

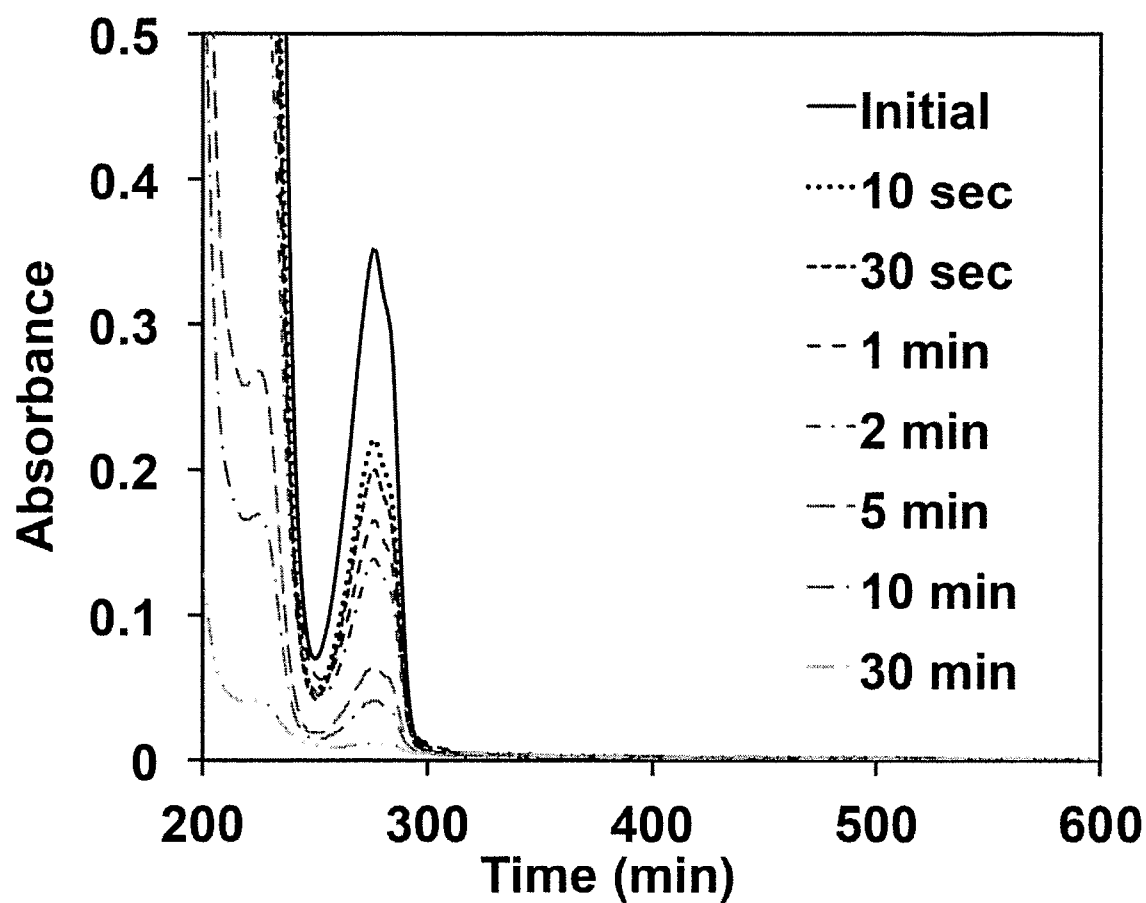


FIG. 40

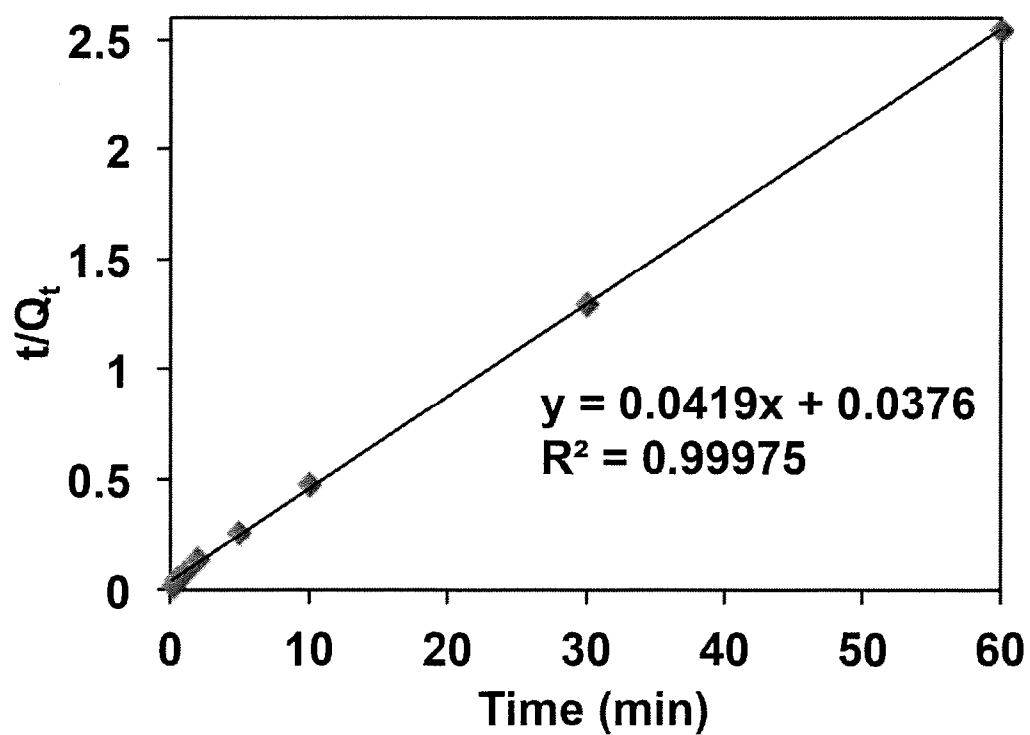


FIG. 41

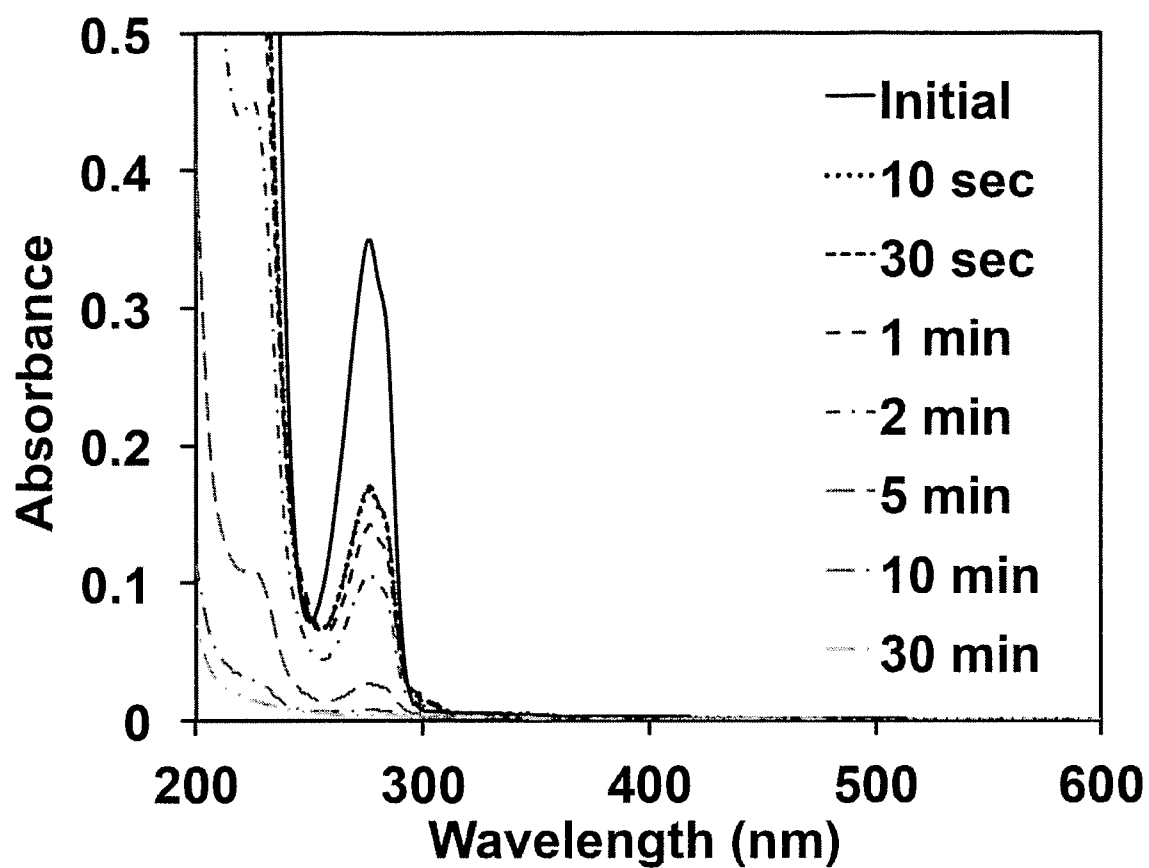


FIG. 42

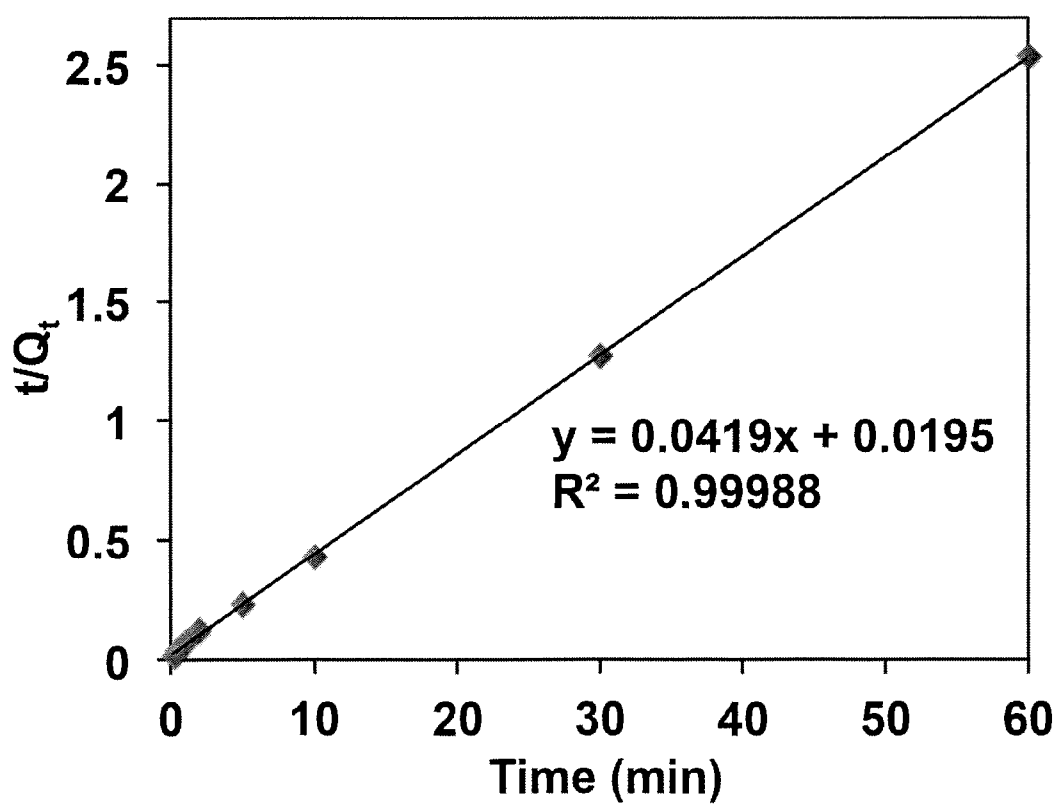


FIG. 43

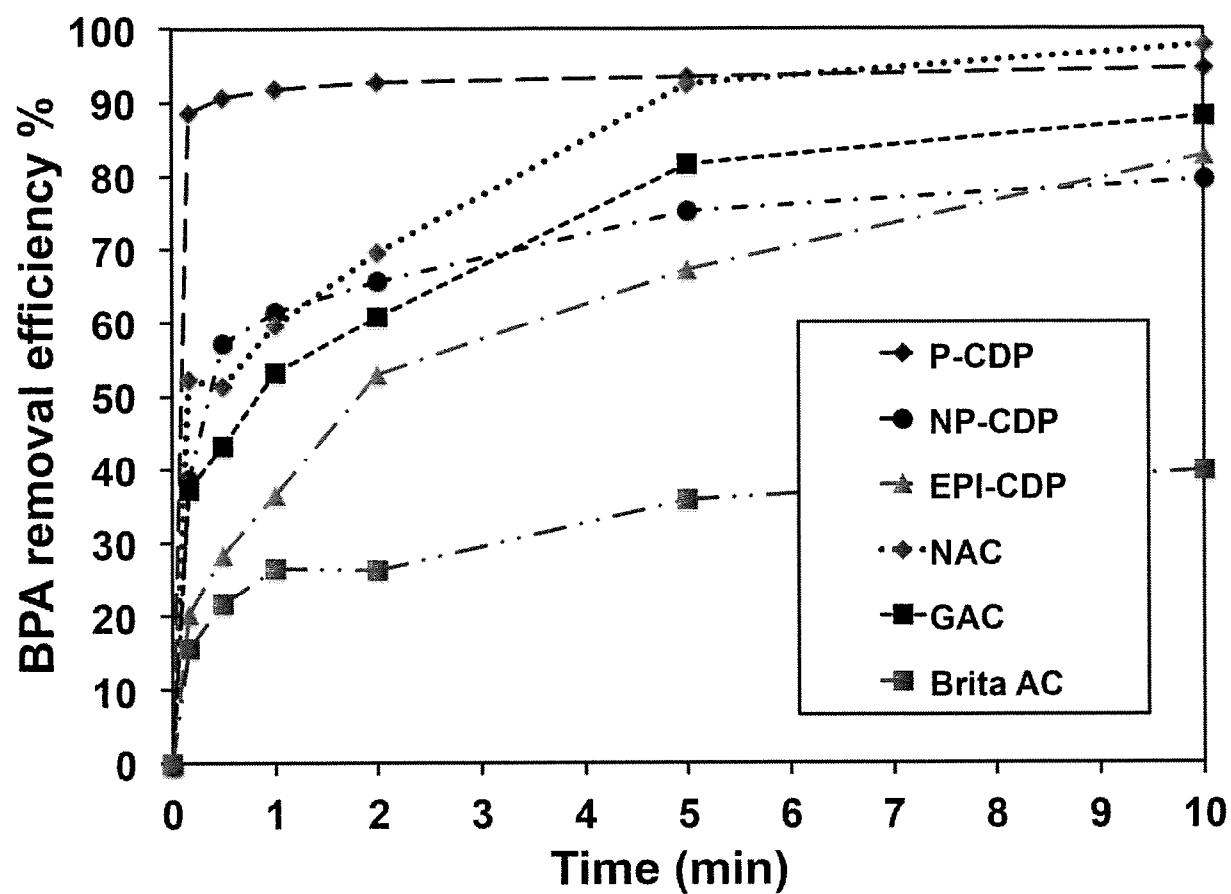


FIG. 44

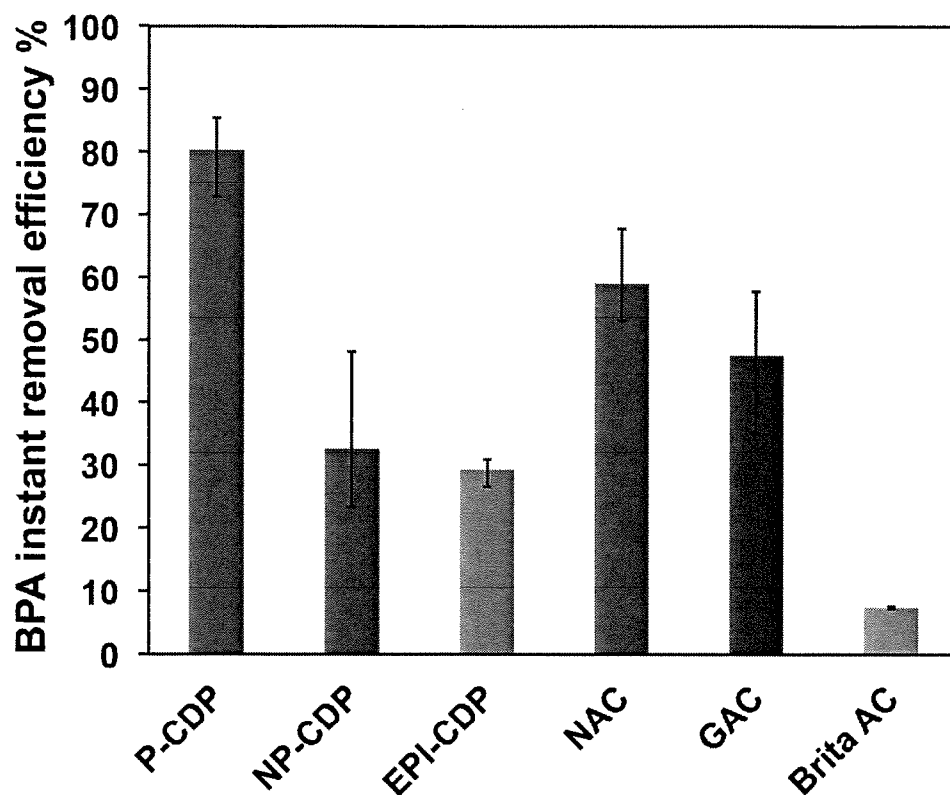


FIG. 45

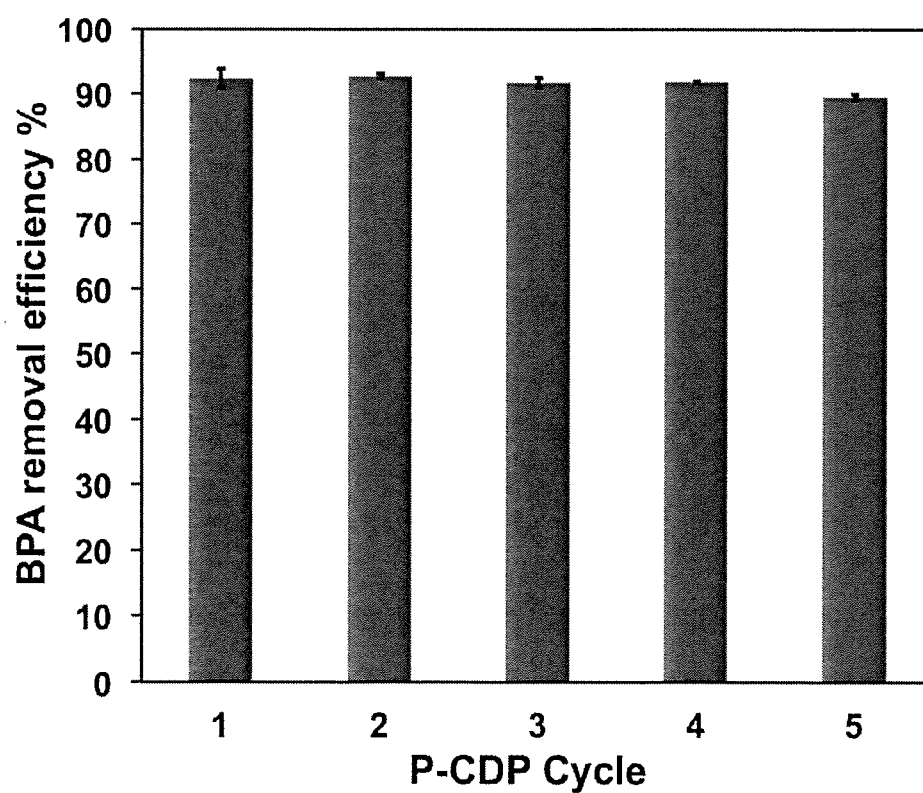


FIG. 46

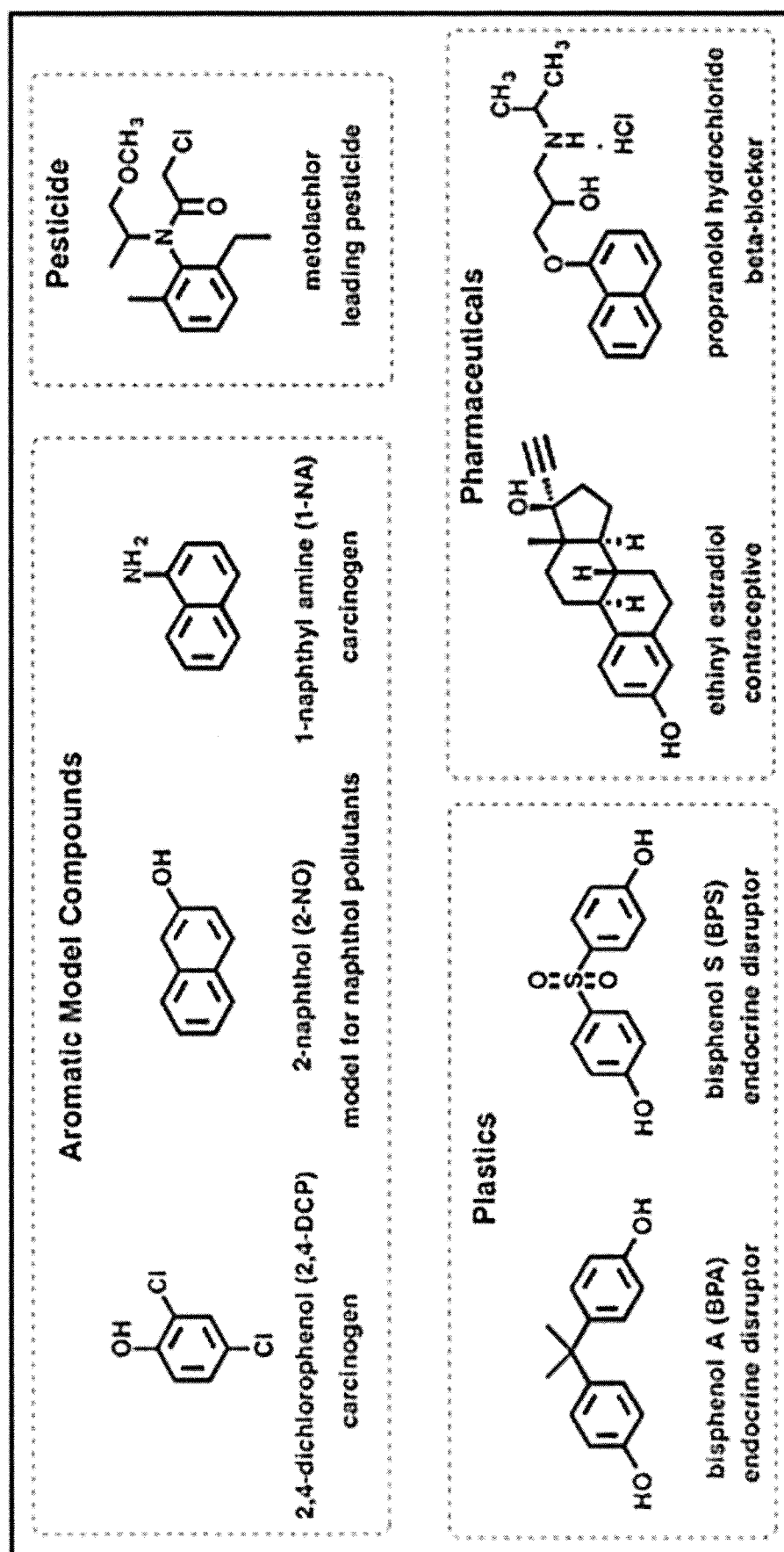


FIG. 47

Pollutant	logK _{ow} ^a	logD ^b	MW (g/mol)	pKa	C _s (g/L) ^c	Min z L (Å) ^d	Max z L (Å) ^e
BPA	3.6	3.6	228.3	9.7	0.12	12.4	8.6
BPS	1.6	1.7	250.3	7.6 ^f	0.38 ^f	12.8	7.0
metolachlor	3.2	3.2	283.8	1.4 ^f	0.53	12.1	9.0
ethinyl estradiol	4.1	3.9	296.4	10.4	0.002	13.9	8.0
propranolol	2.6	1.1	259.3	9.5	0.050 (ref)	15.4	8.3
2-naphthol (2- NO)	2.7	2.9	144.2	9.5	0.76	9.6	4.0
1-naphthyl amine (1-NA)	2.2	2.3	143.2	3.9	1.7	9.5	4.1
2,4- dichlorophenol (DCP)	2.8	3.0	163.0	7.9	4.5	8.8	4.2

^a Log octanol-water partition coefficient. Predicted using KOWWIN v1.67 software implemented in ChemSpider Database.

^b Log distribution coefficient at pH = 7.4. Predicted using ACD/Labs Percepta software implemented in ChemSpider Database.

^c Solubility in water. Experimental values.

^d Minimal molecular z length. Defined as the length of the conformer perpendicular to its minimal projection area. Generated using ChemAxon software implemented in ChemSpider Database.

^e Maximum molecular z length. Defined as the length of the conformer perpendicular to its maximal projection area. Generated using ChemAxon software implemented in ChemSpider Database.

^f Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02, as implemented in the SciFinder CAS Database.

FIG. 48

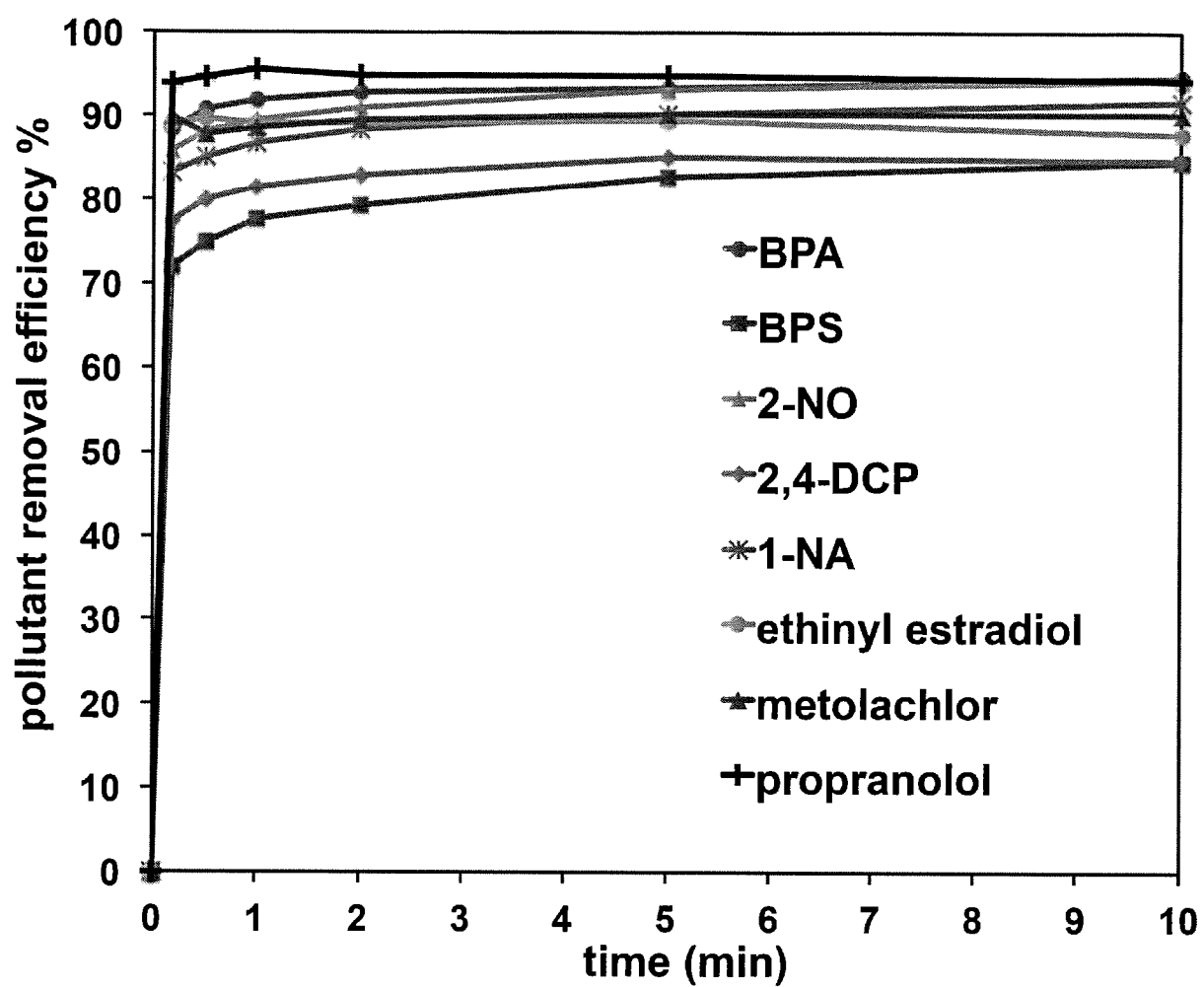


FIG. 49

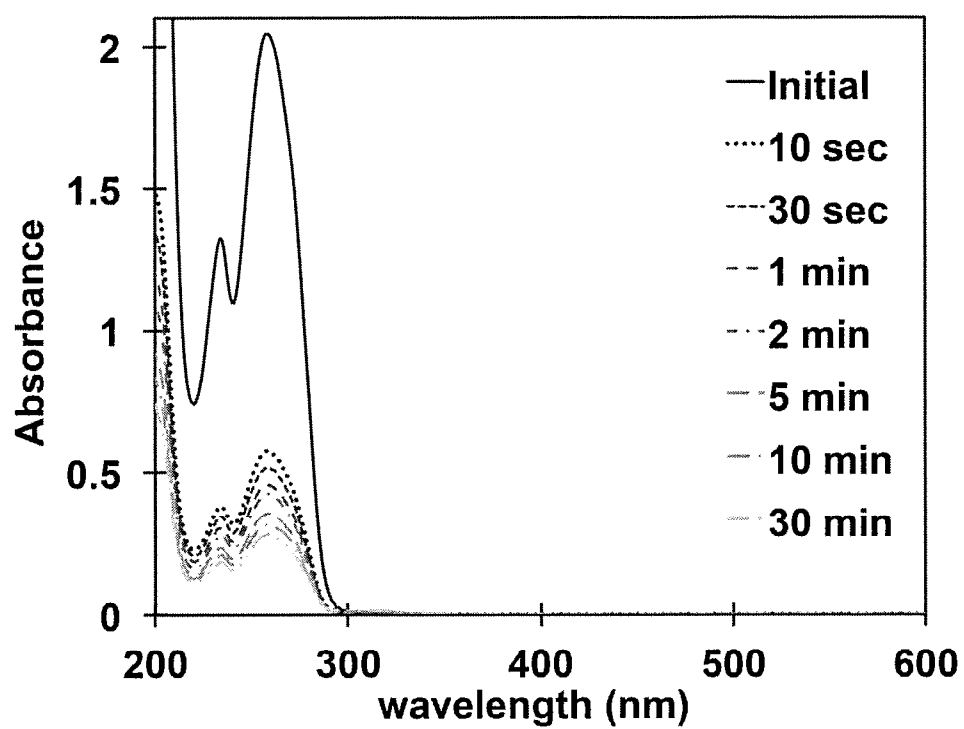


FIG. 50

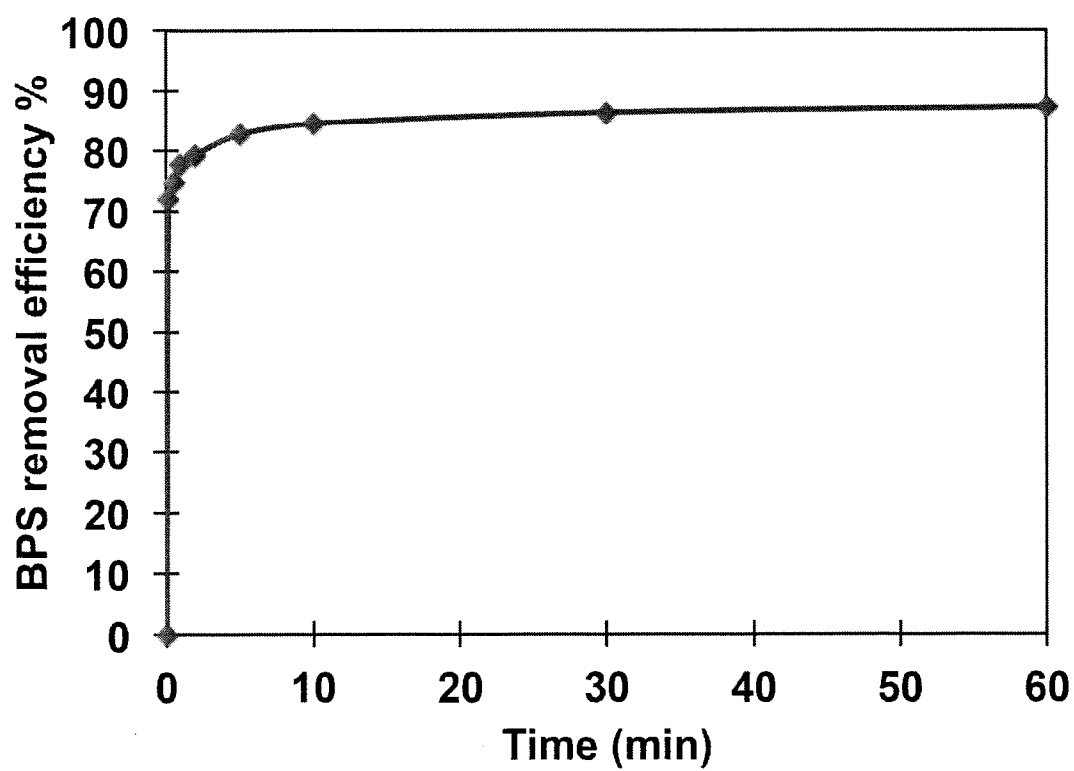


FIG. 51

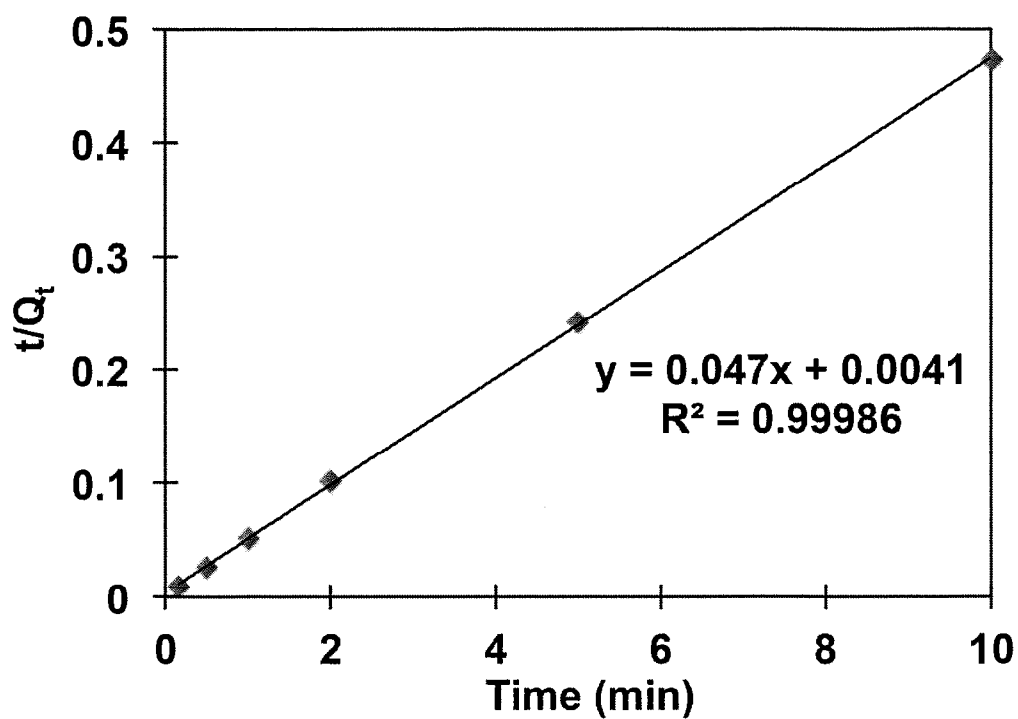


FIG. 52

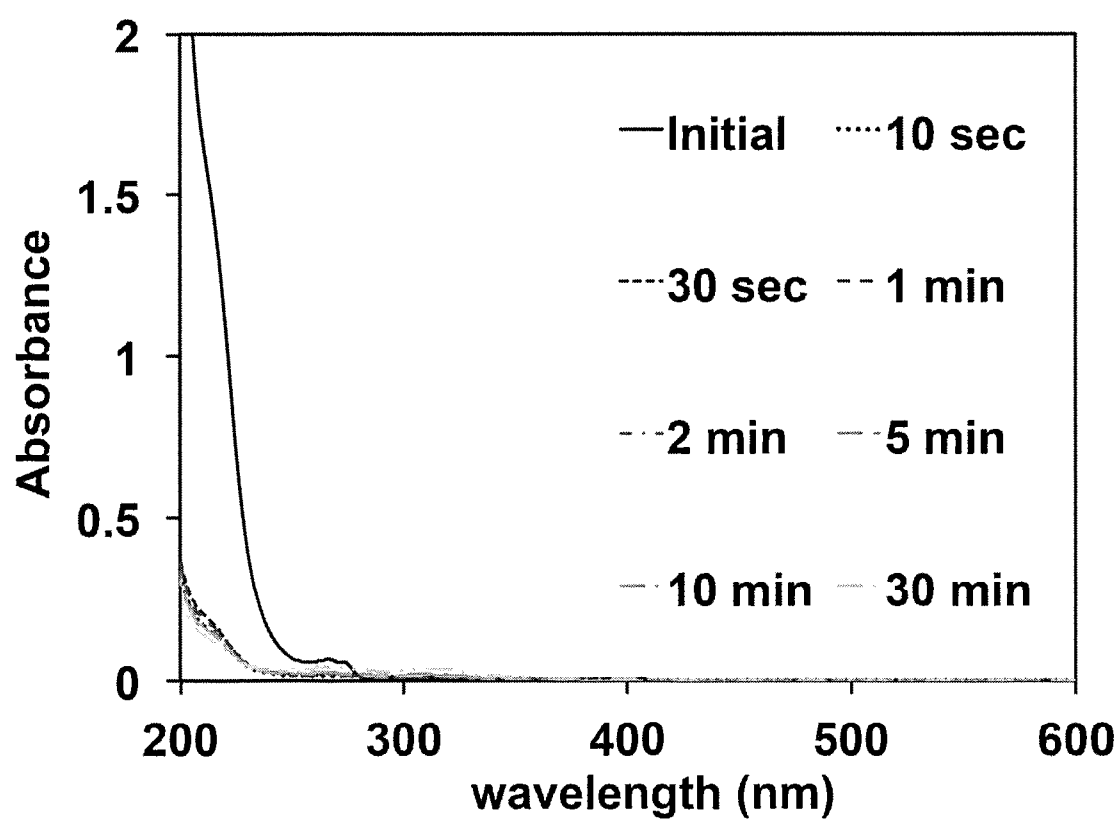


FIG. 53

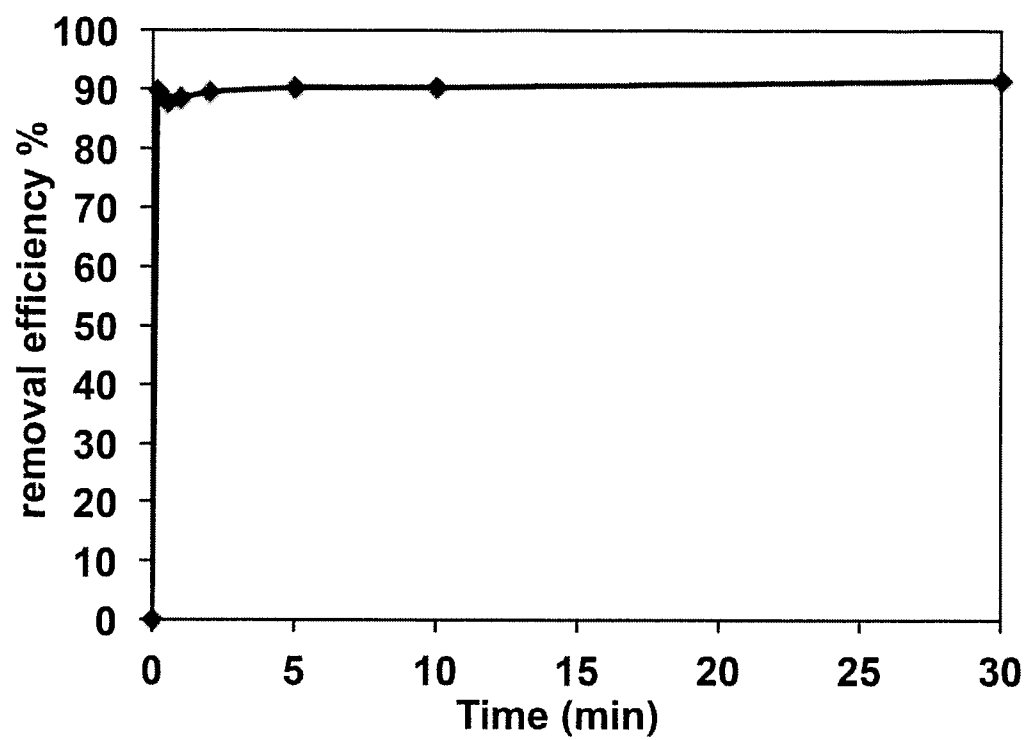


FIG. 54

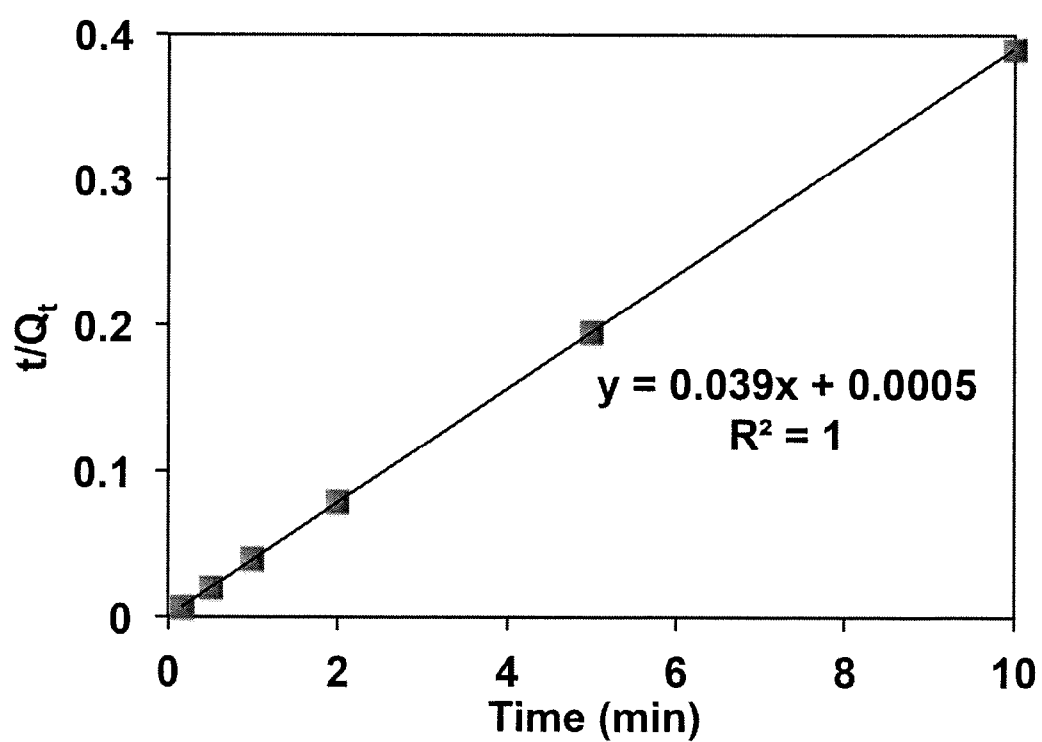


FIG. 55

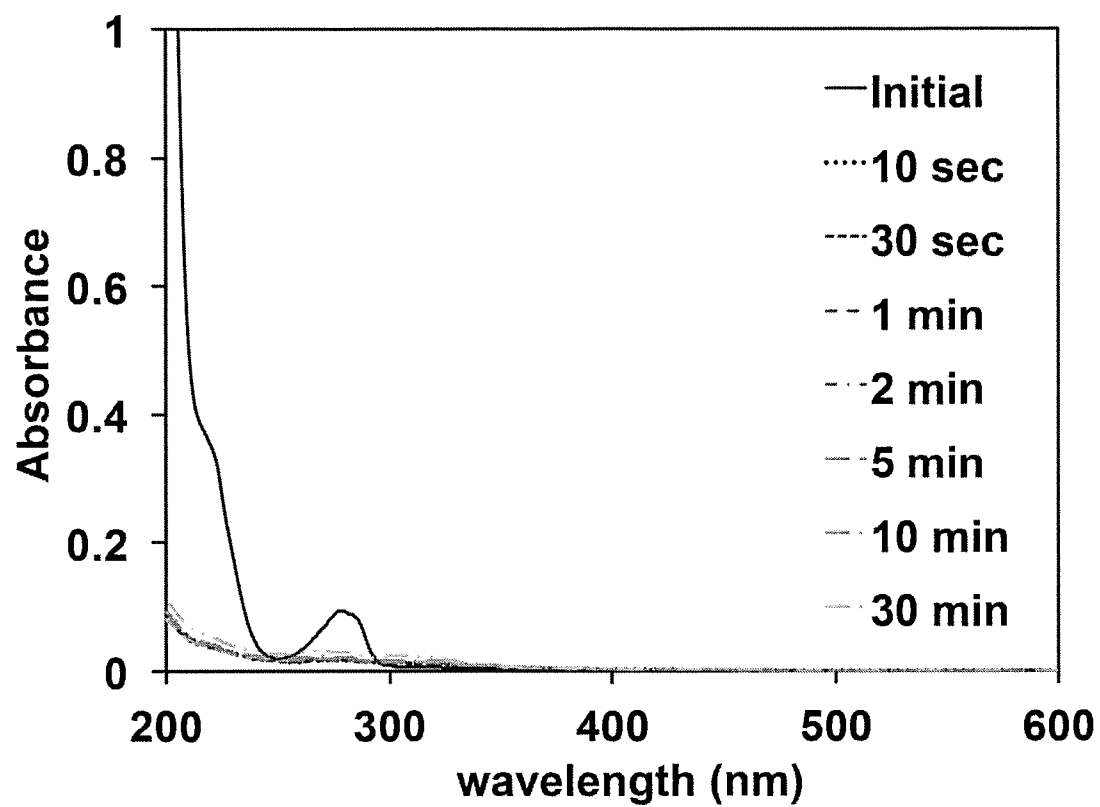


FIG. 56

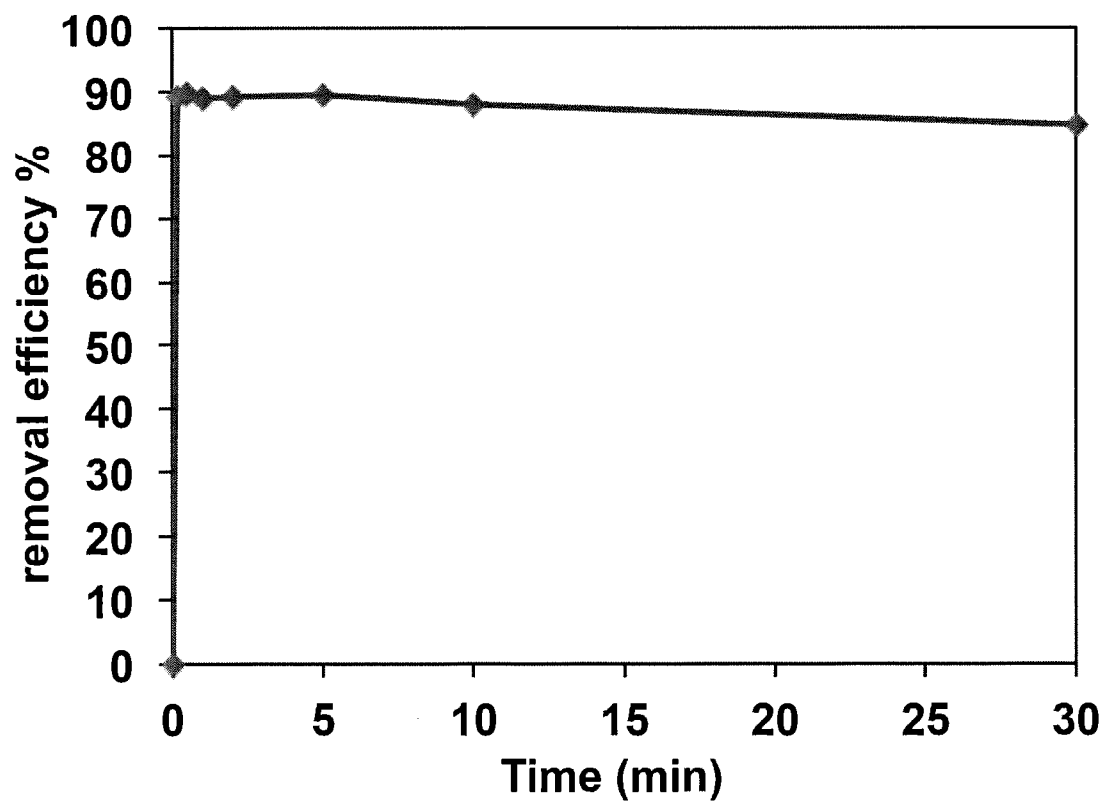


FIG. 57

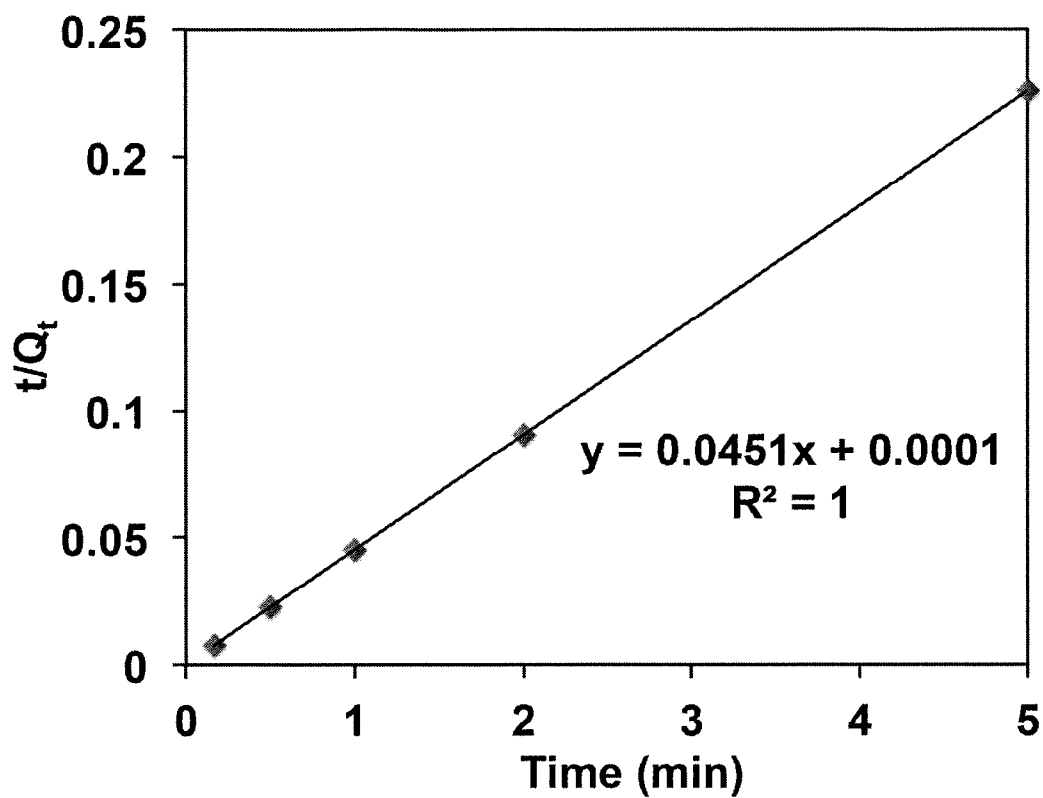


FIG. 58

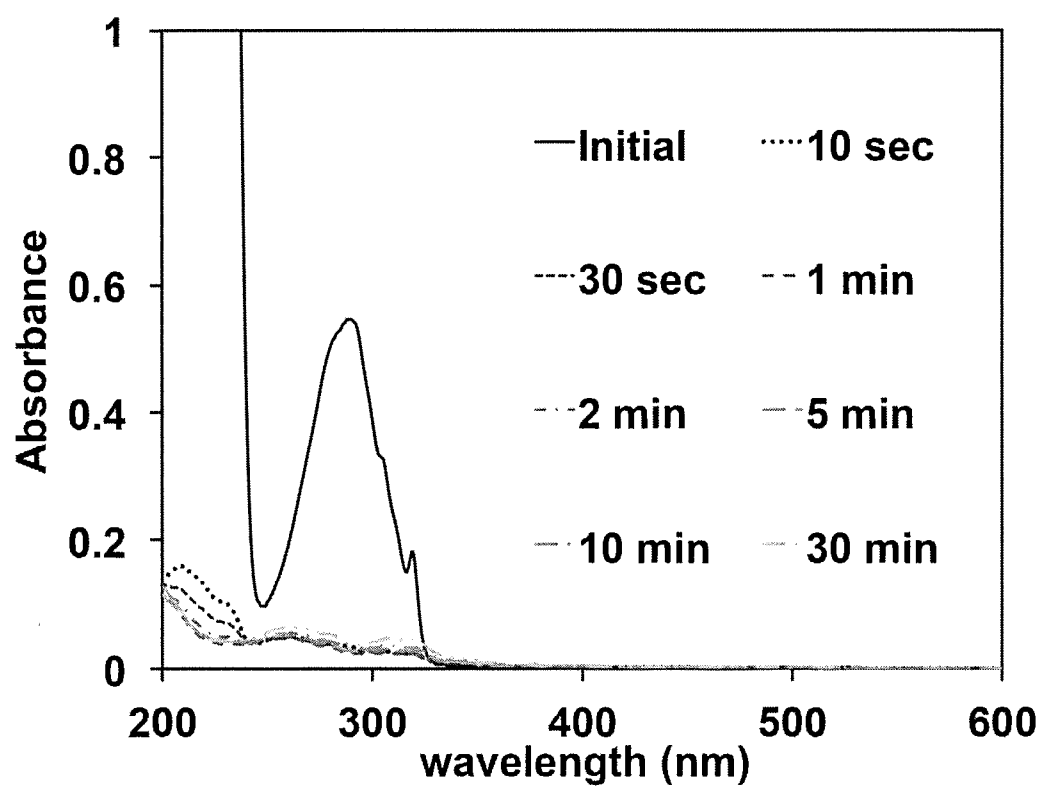


FIG. 59

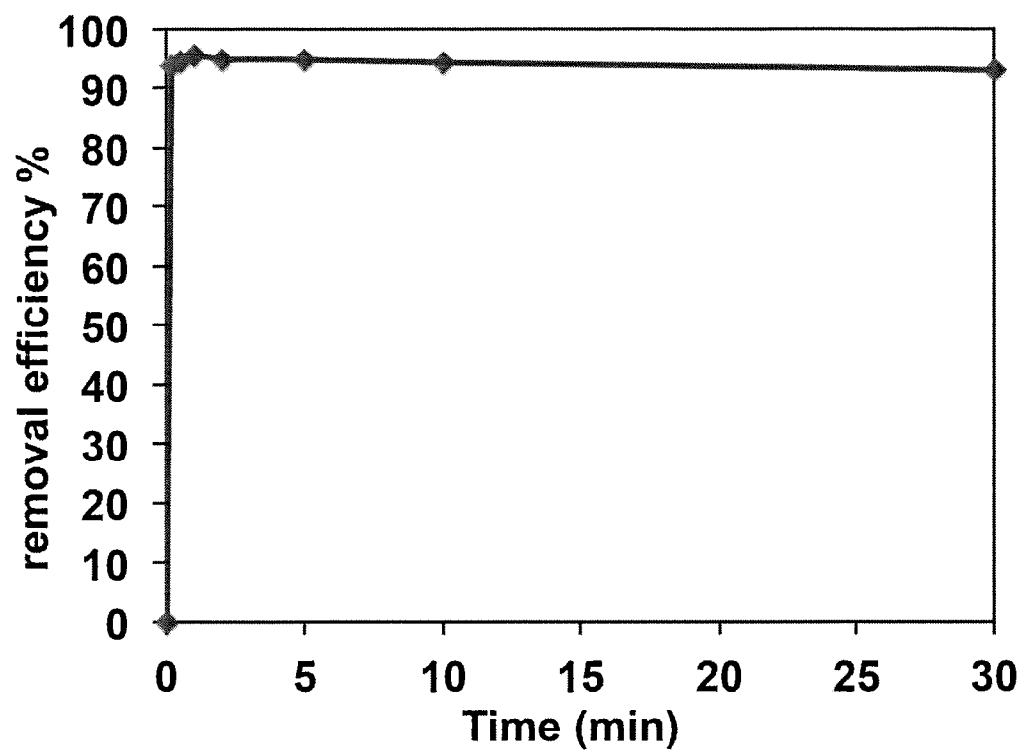


FIG. 60

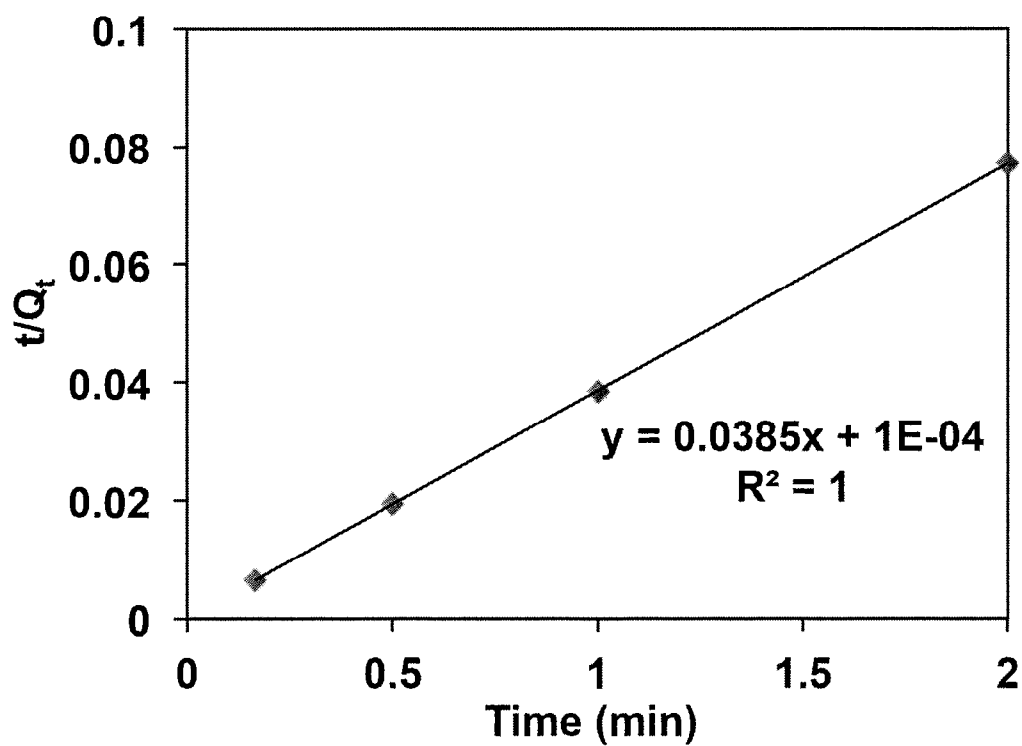


FIG. 61

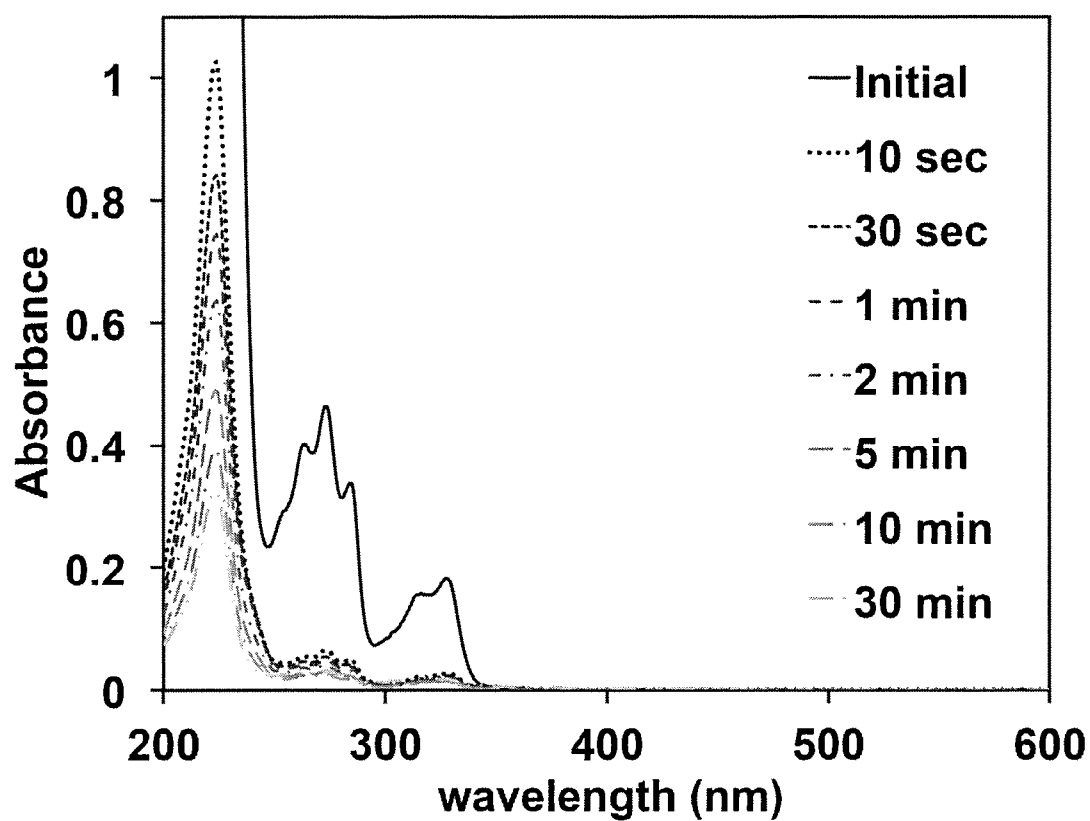


FIG. 62

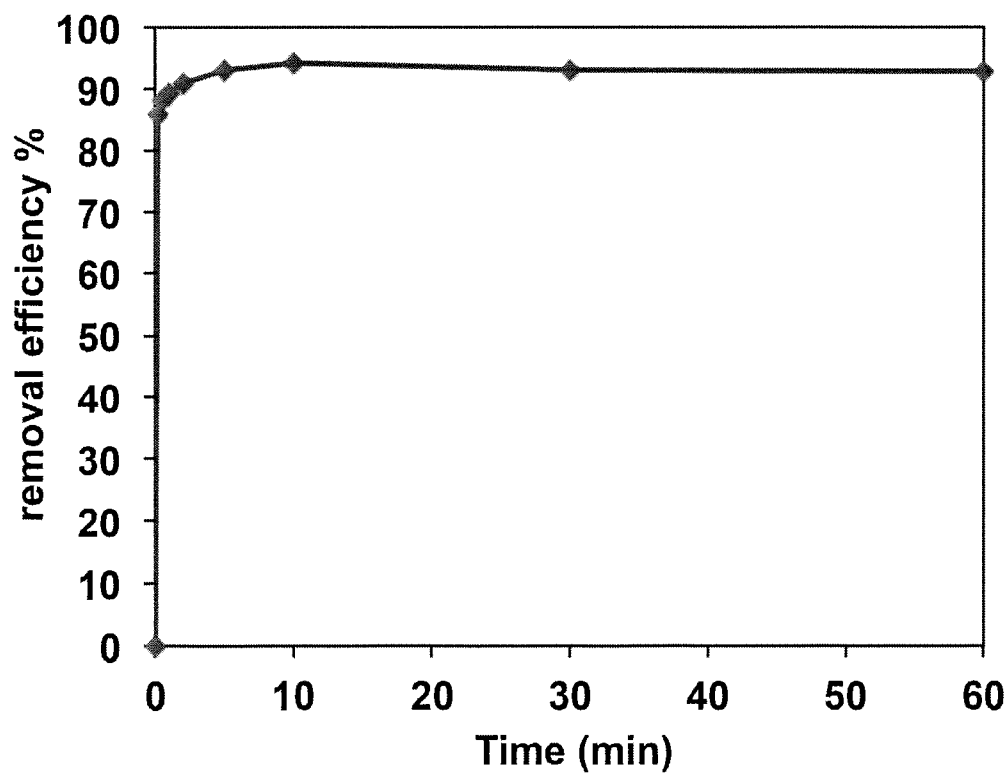


FIG. 63

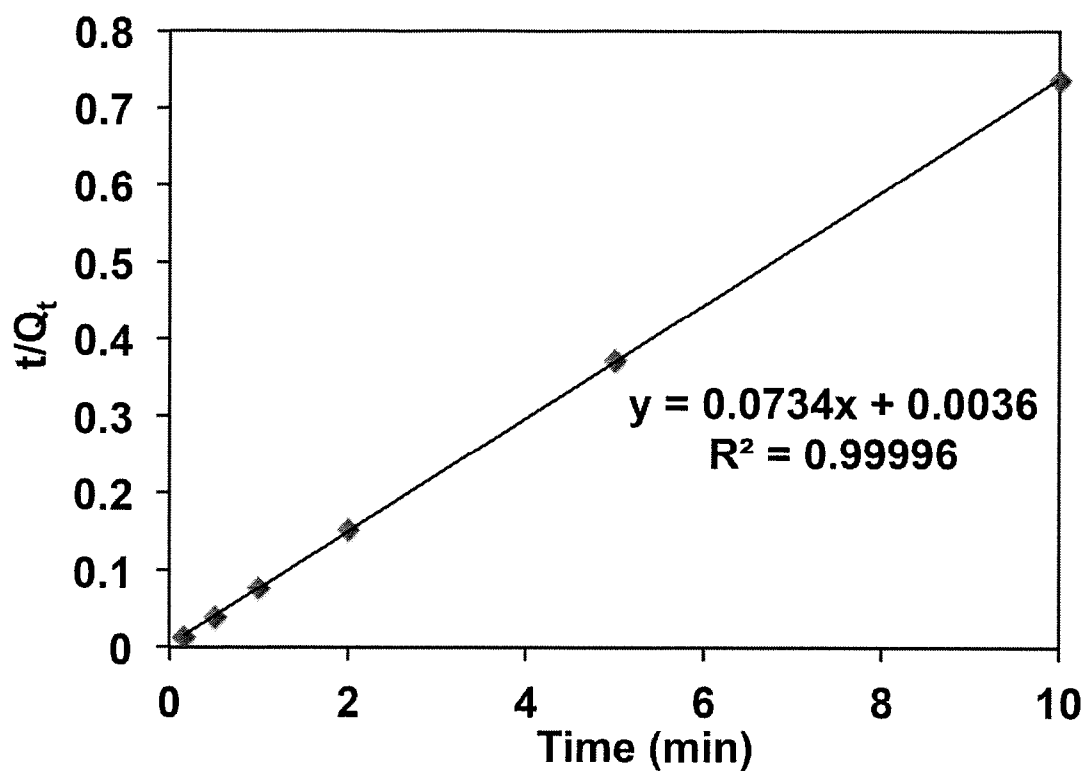


FIG. 64

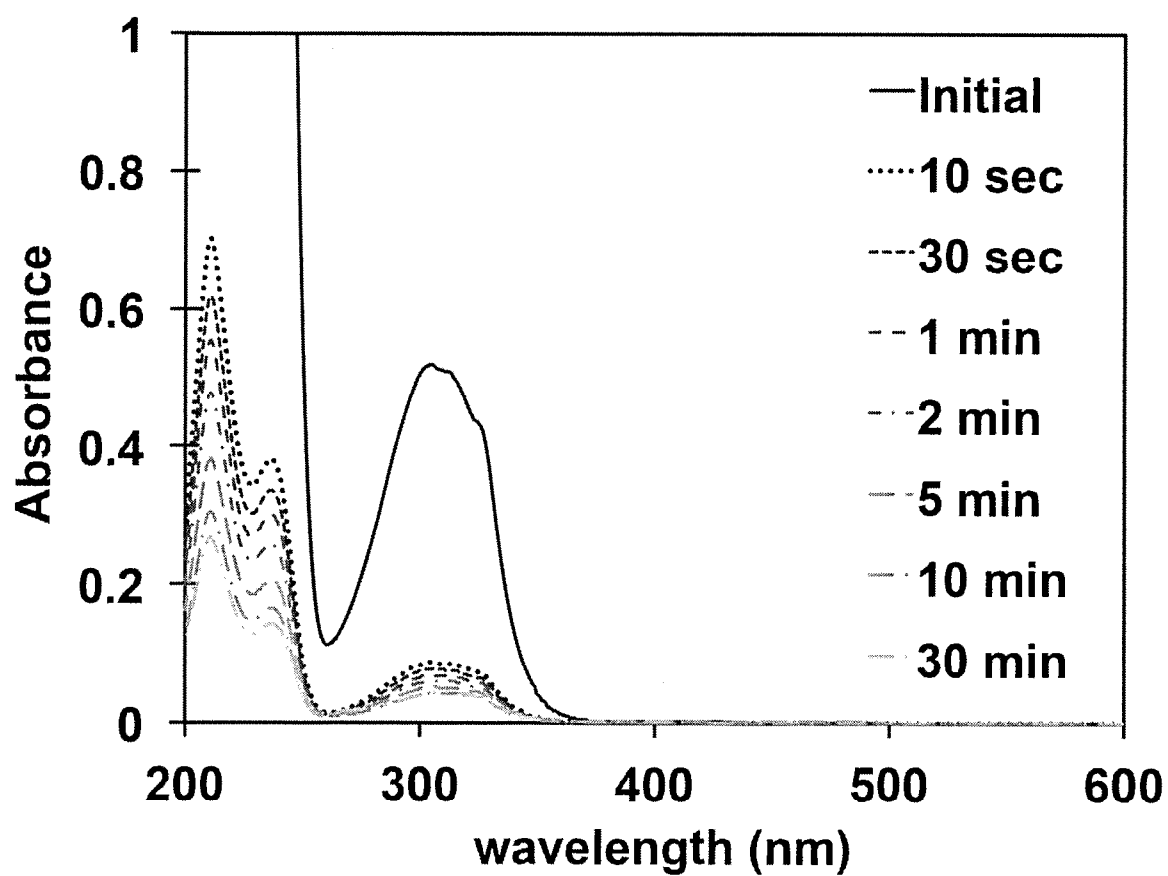


FIG. 65

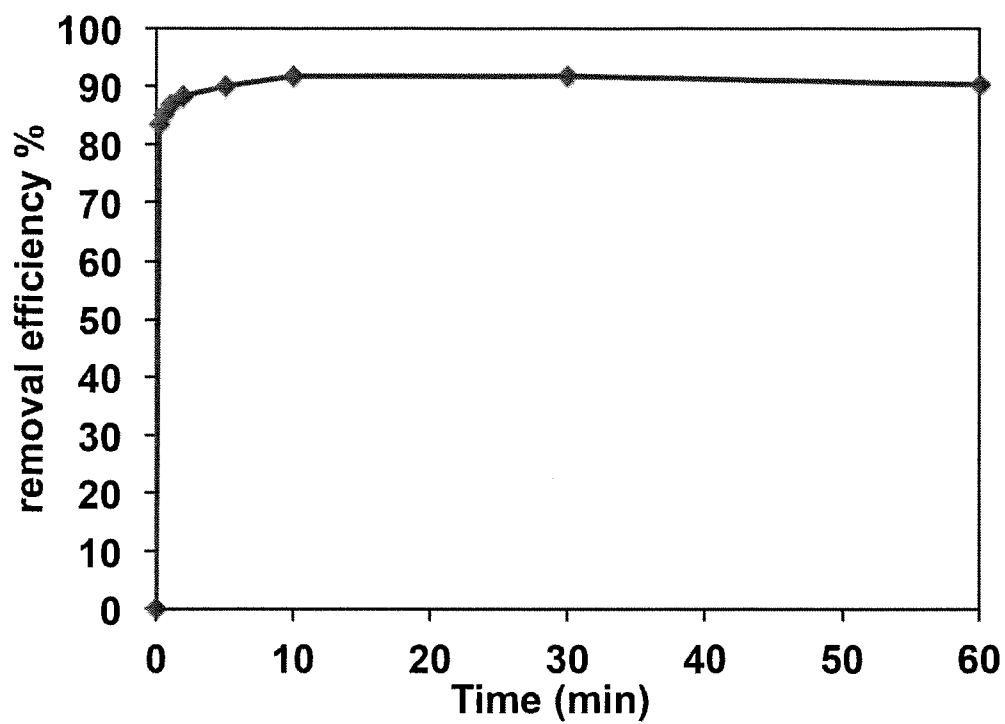


FIG. 66

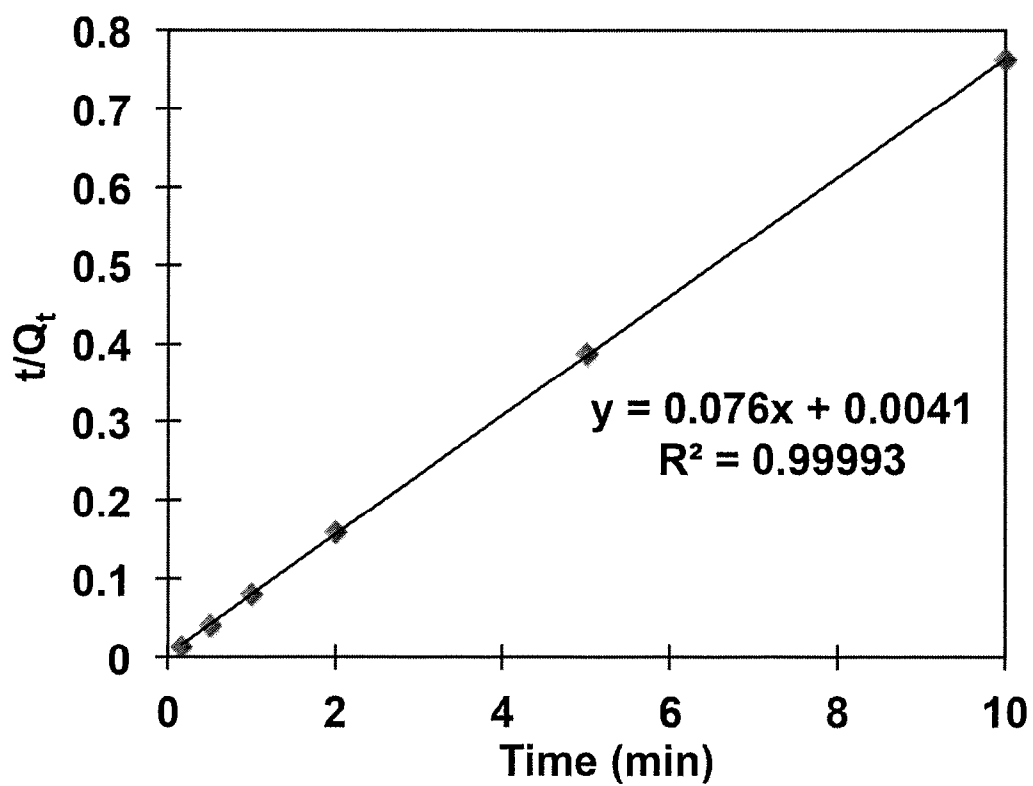


FIG. 67

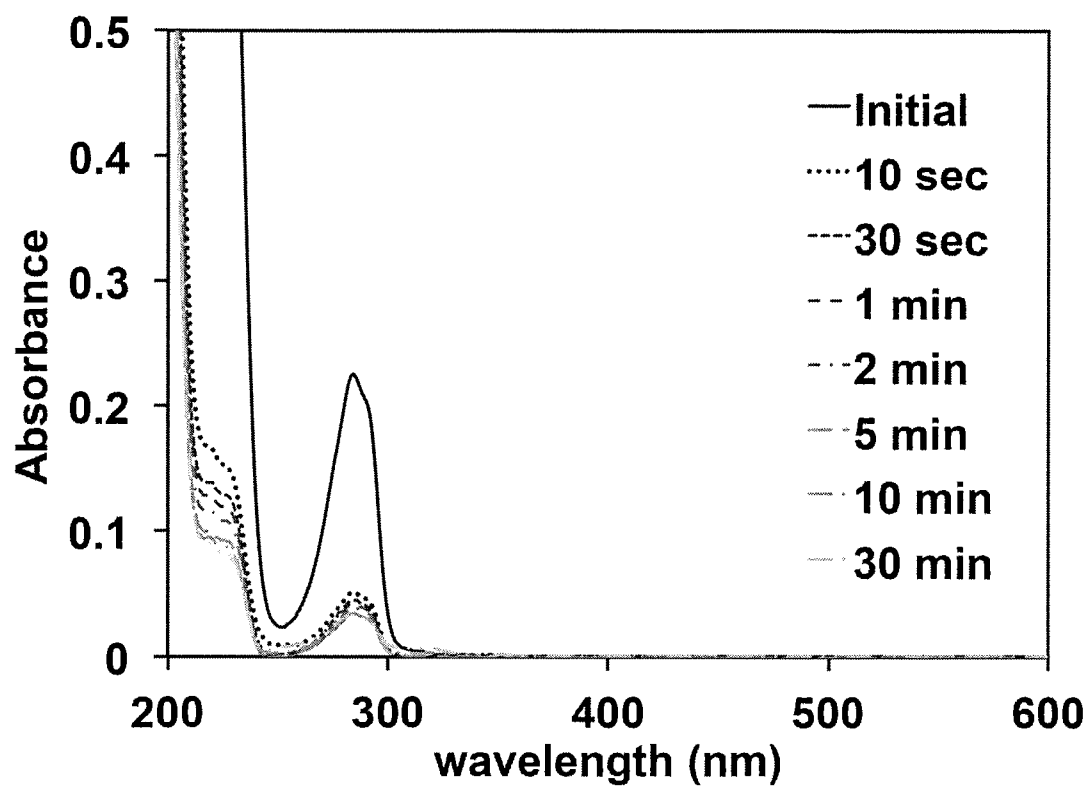


FIG. 68

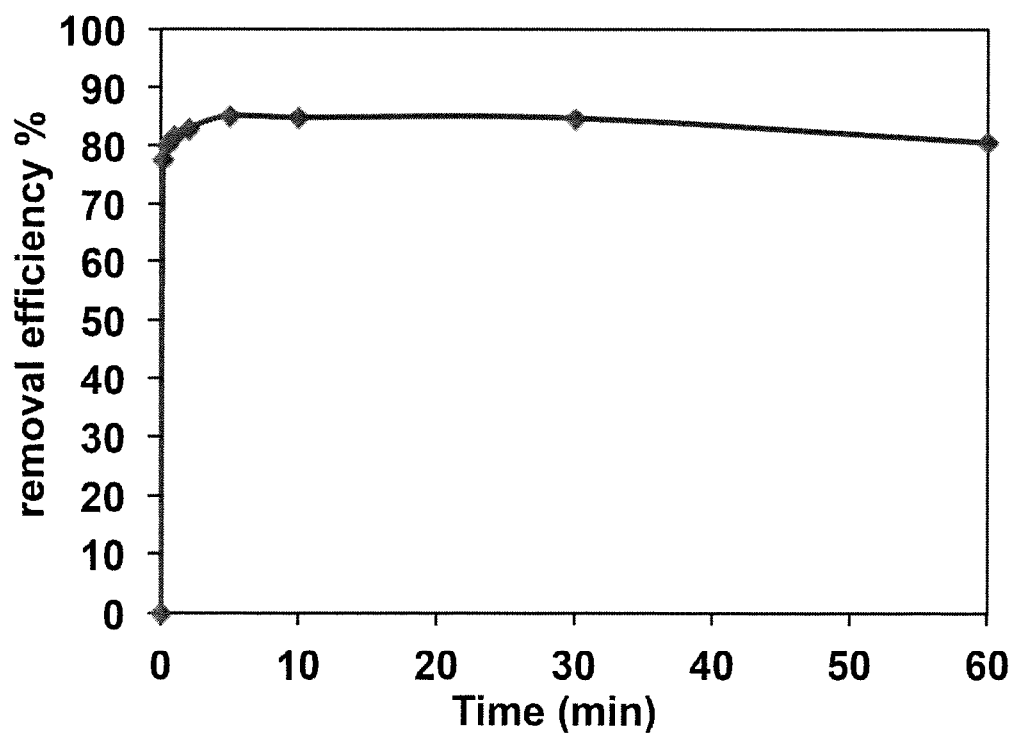


FIG. 69

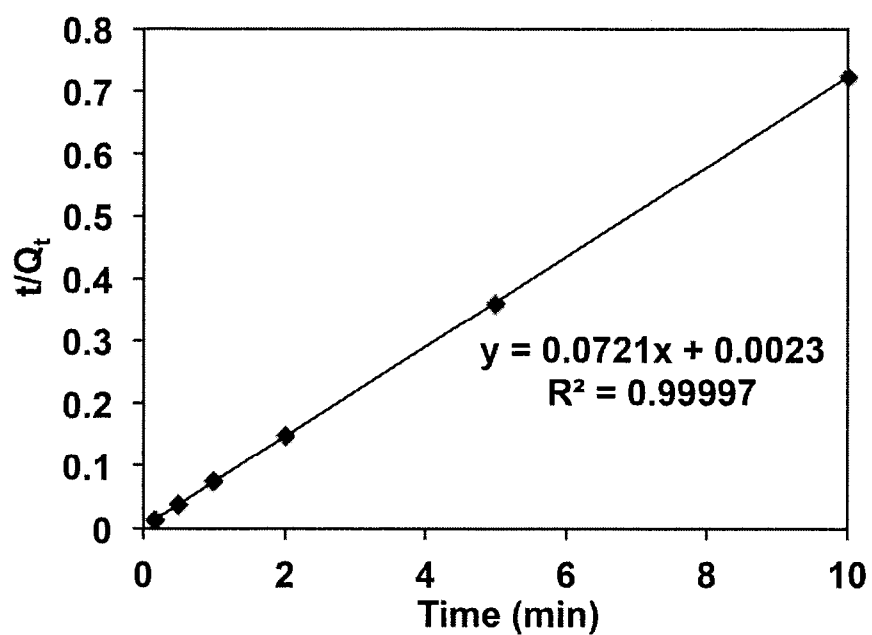


FIG. 70

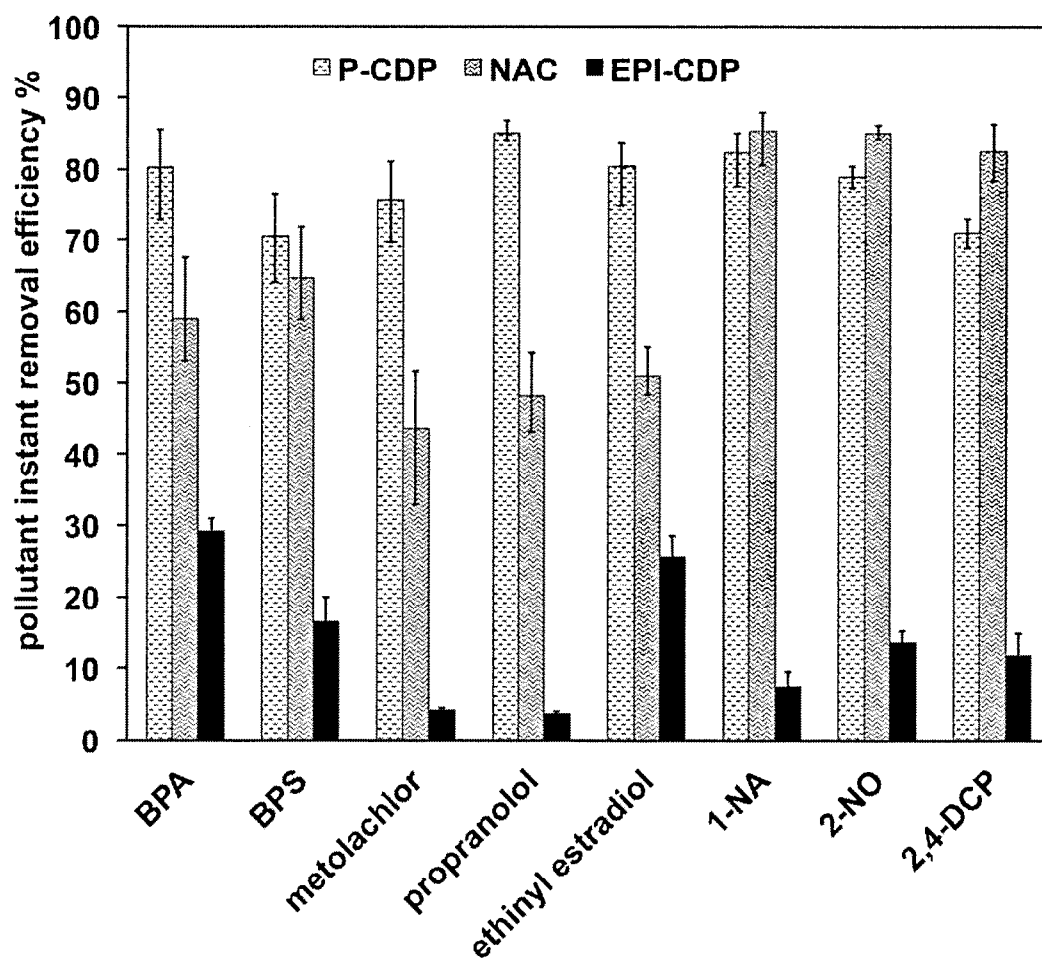


FIG. 71

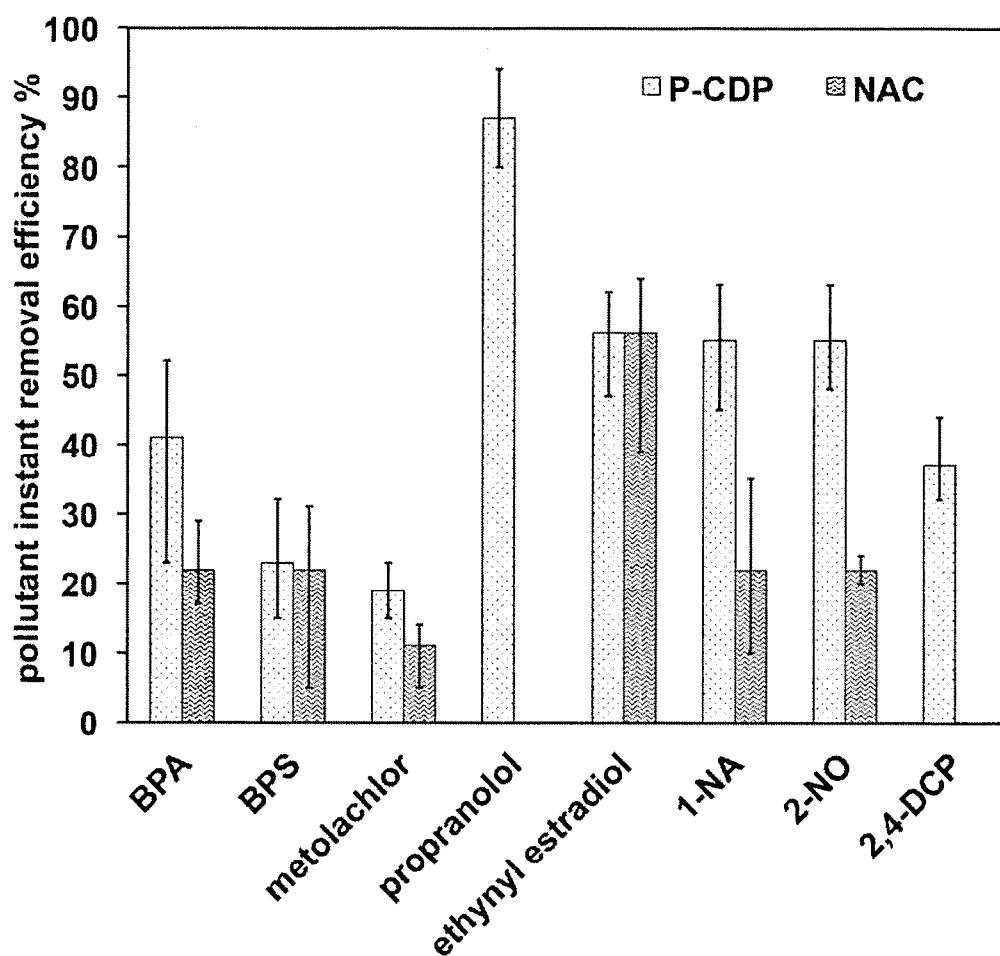


FIG. 72

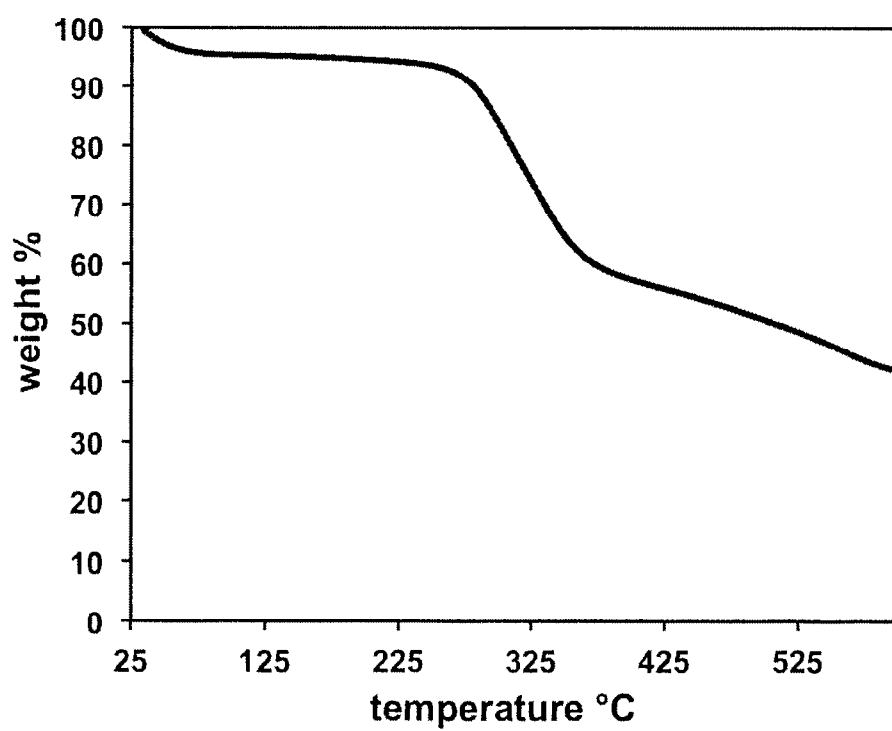


FIG. 73

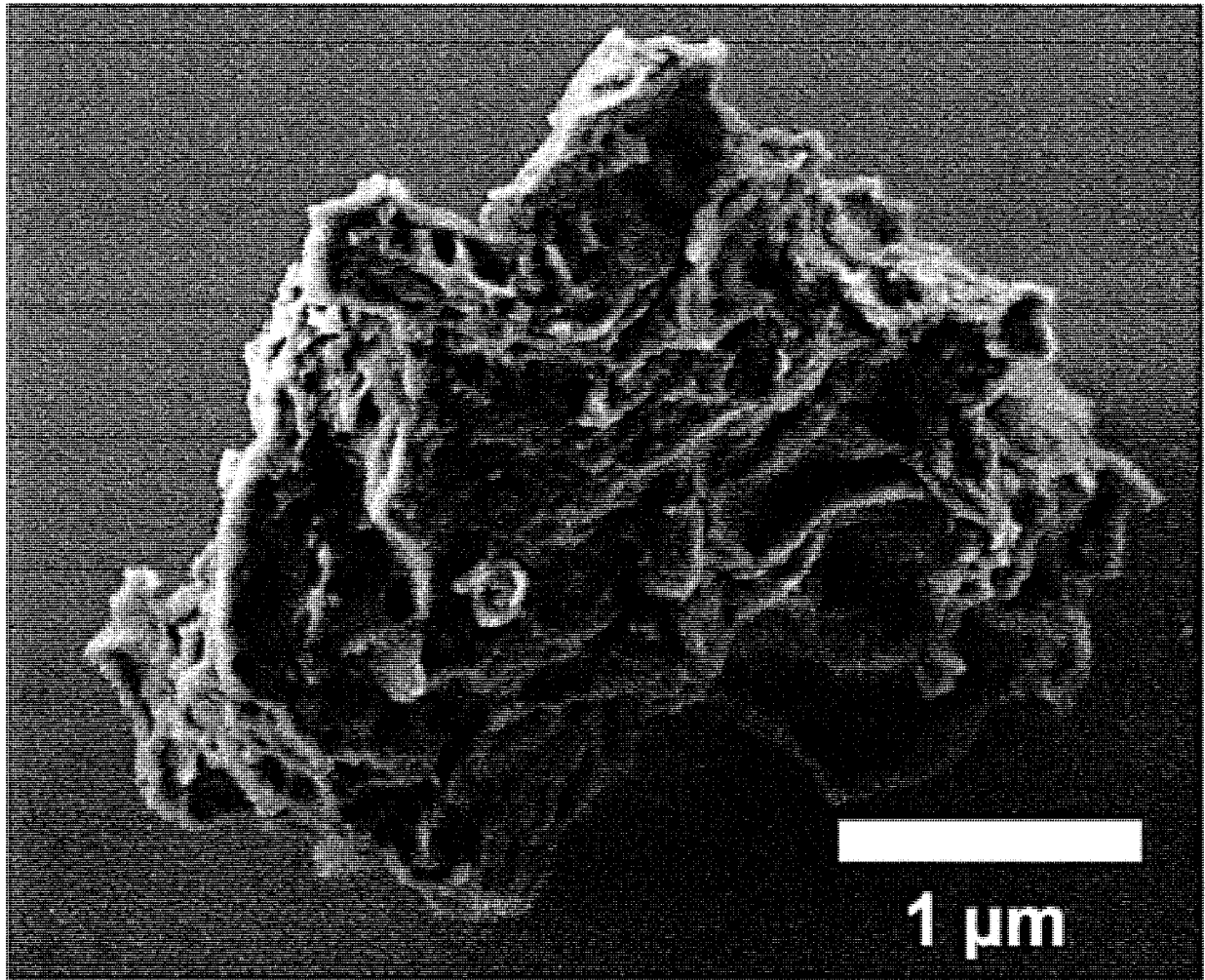


FIG. 74

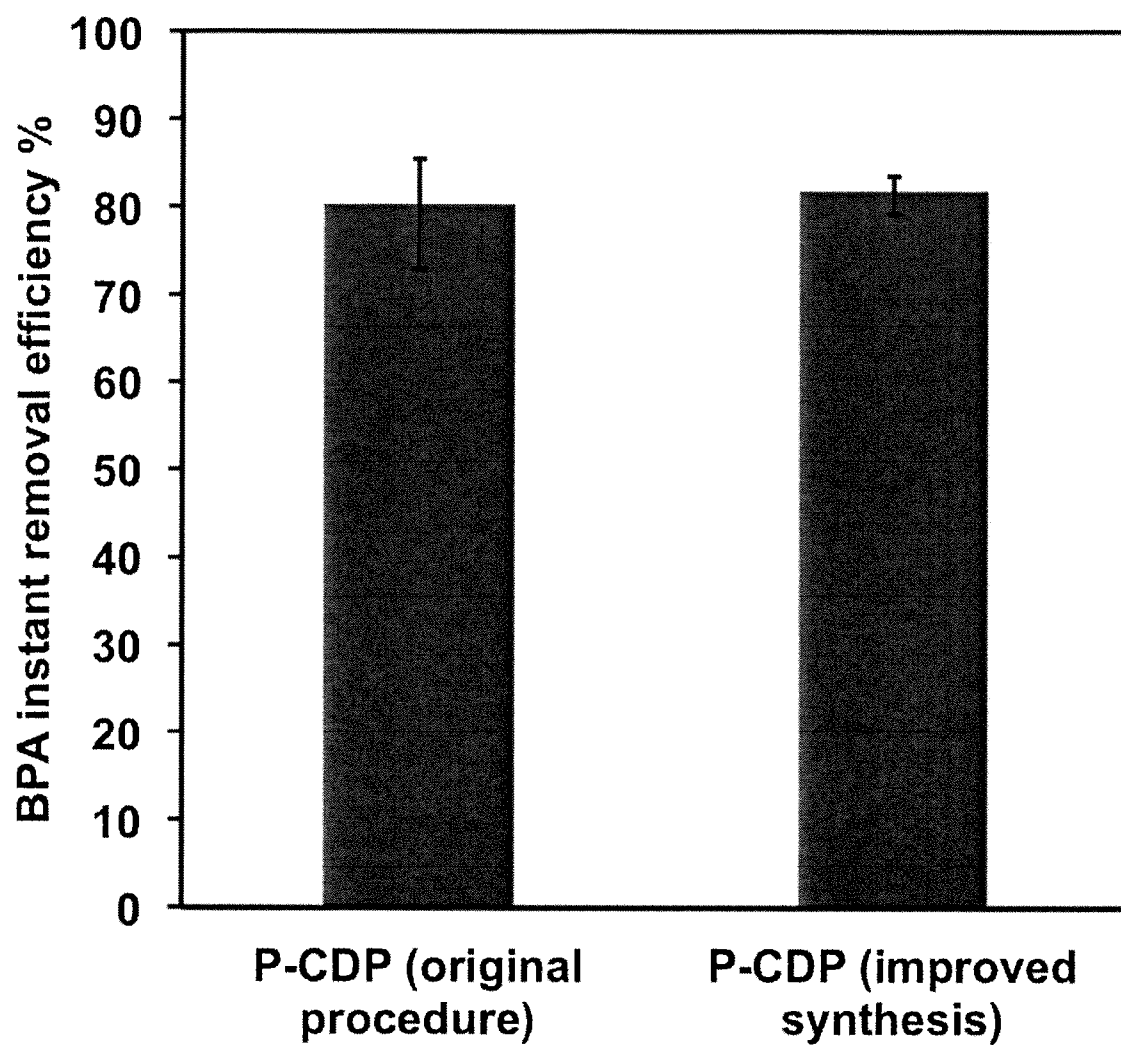


FIG. 75

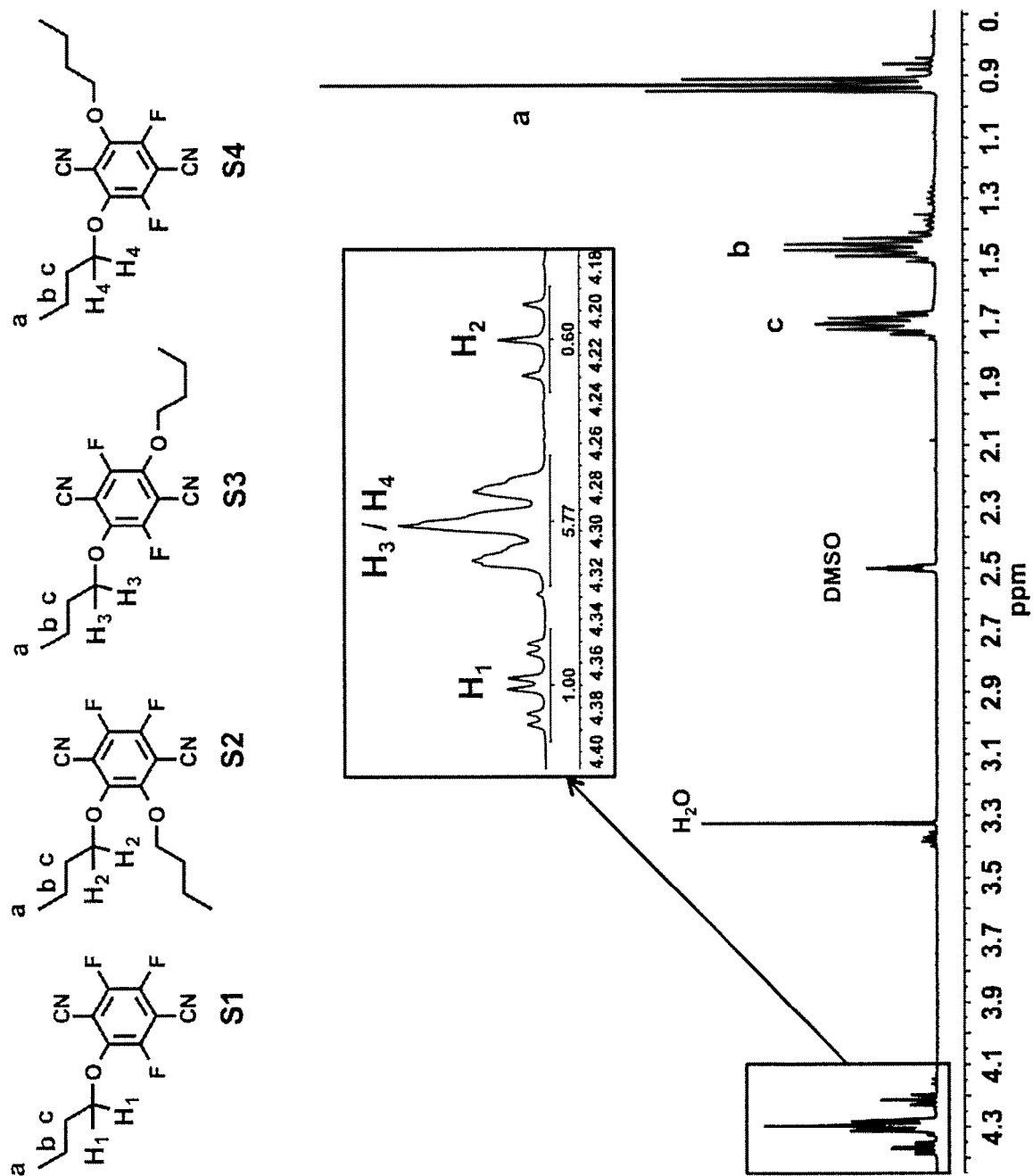


Fig. 76

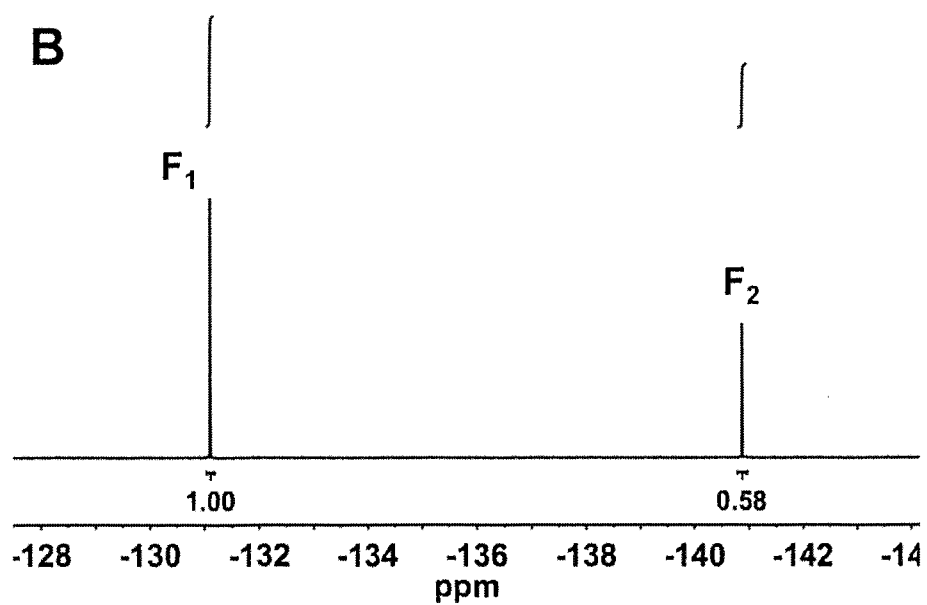
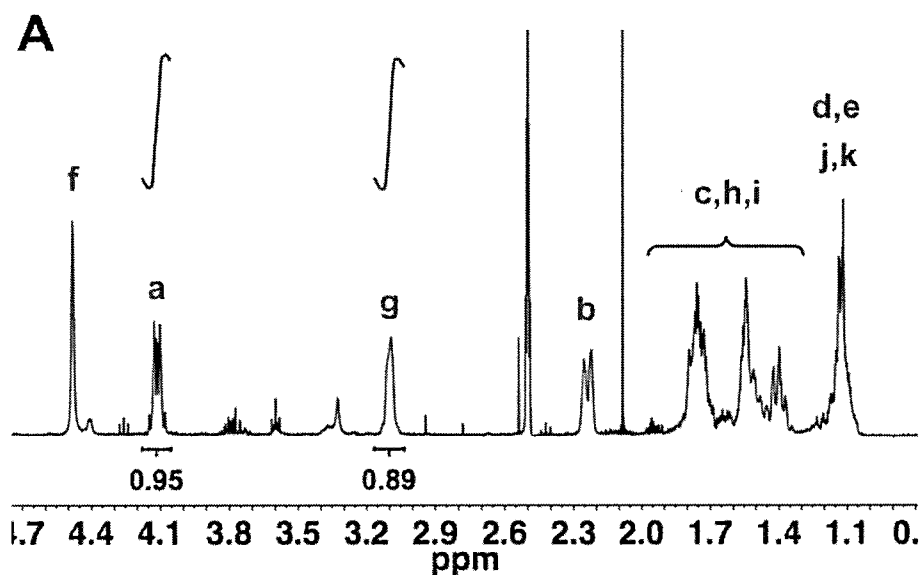
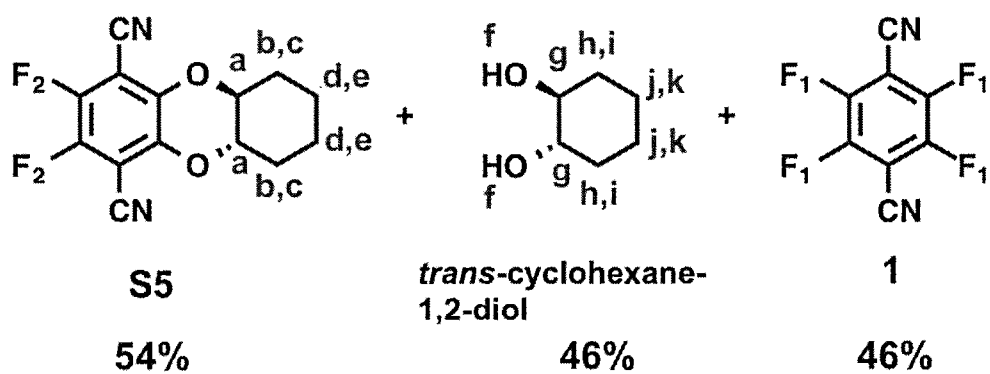


FIG. 77

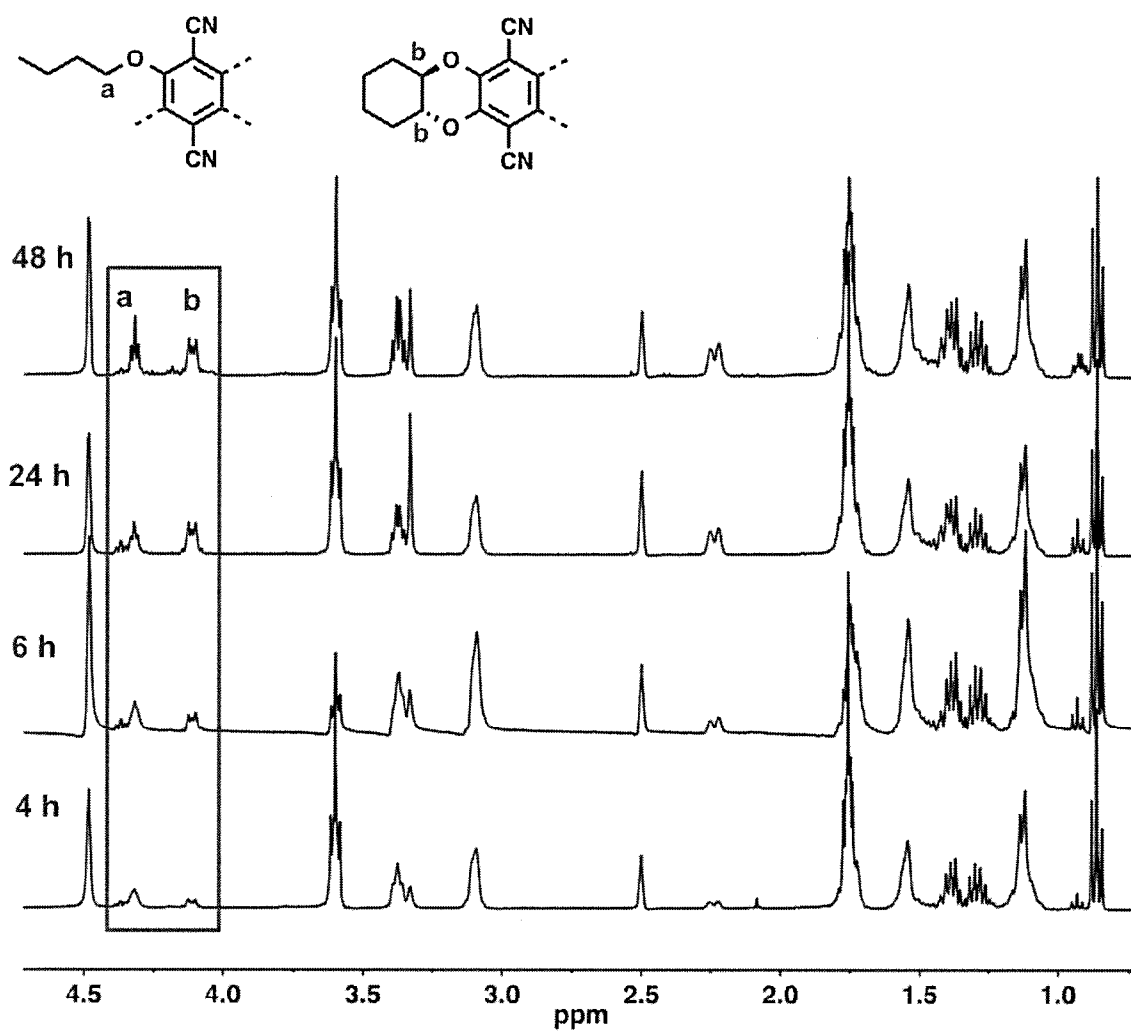


FIG. 78

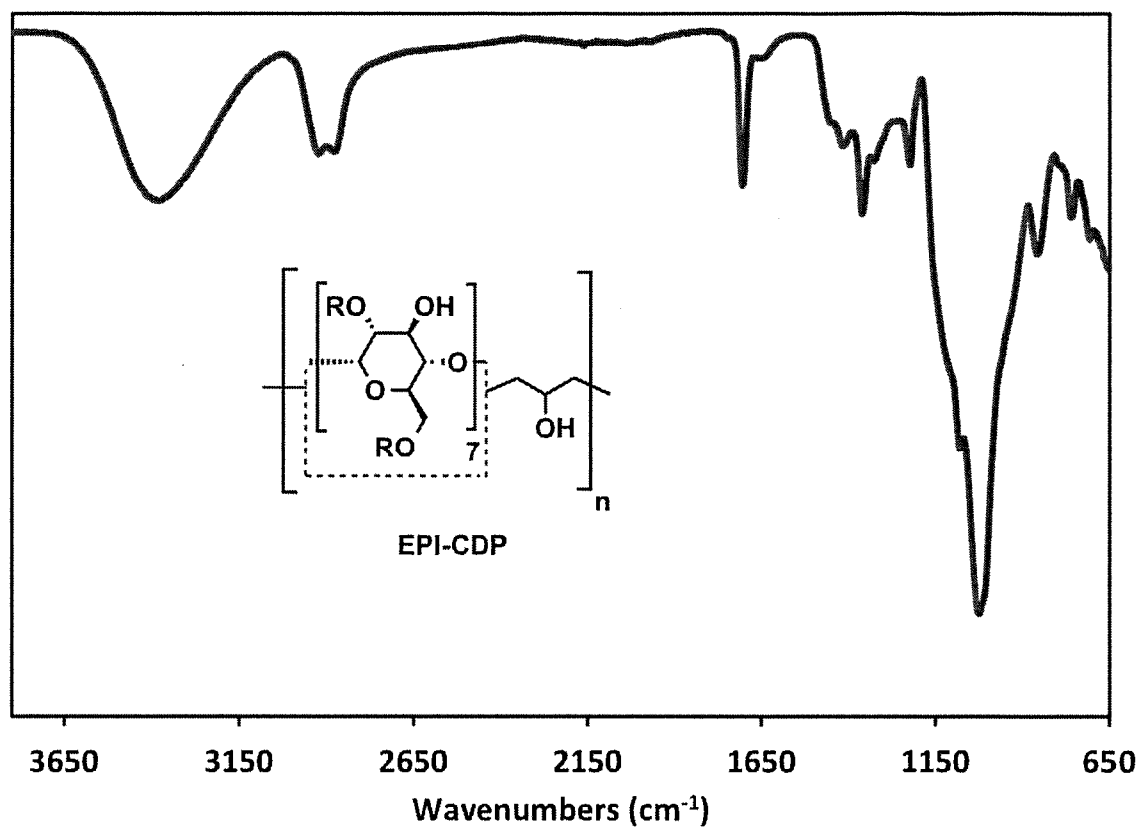


FIG. 79

Compound Name	Supplier	Chemical Formula	pKa	LogK _{ow}	Charge State at pH = 7.4	McGowan Volume
2,4-D	Aldrich	C ₈ H ₆ Cl ₂ O ₃	3.0±0.1	2.50	-	1.38
Abacavir	Aldrich	C ₁₄ H ₁₈ N ₆ O	14.9±0.1	0.39	n	2.09
Acebutolol	Aldrich	C ₁₈ H ₂₈ N ₂ O ₄	13.8±0.2	1.53	+	2.76
Acetaminophen	USP	C ₈ H ₉ NO ₂	9.9±0.1	0.91	n	1.17
Acetochlor	Aldrich	C ₁₄ H ₂₀ ClNO ₂	1.3±0.5	3.50	n	2.14
Albuterol	Aldrich	C ₁₃ H ₂₁ NO ₃	10.0±0.3	0.34	+	1.98
Allopurinol	Aldrich	C ₅ H ₄ N ₄ O	9.2±0.5	0.35	n	0.88
Amphetamine	Aldrich	C ₉ H ₁₃ N	9.9±0.1	1.8	+	1.24
Atenolol	Aldrich	C ₁₄ H ₂₂ N ₂ O ₃	13.9±0.2	0.43	+	2.18
Atenolol Acid	Aldrich	C ₁₄ H ₂₁ N ₁ O ₄	4.4±0.1	-1.24	z	2.14
Atrazine	Aldrich	C ₈ H ₁₄ ClN ₅	2.3±0.1	1.76	n	1.62
Benzotriazole-methyl-1H	Aldrich	C ₇ H ₇ N ₃	8.7±0.4	1.81	n	1.01
Bromacil	Aldrich	C ₉ H ₁₃ BrN ₂ O ₂	8.8±0.4	1.69	z	1.63
Bupropion	Cerillian	C ₁₃ H ₁₈ ClNO		3.27	+	1.94
Caffeine	USP	C ₈ H ₁₀ N ₄ O ₂	0.5±0.7	-0.55	n	1.36
Carbamazepine	Aldrich	C ₁₅ H ₁₂ N ₂ O	13.9±0.2	2.77	n	1.81
Carbaryl	Aldrich	C ₁₂ H ₁₁ NO ₂	12.0±0.5	2.96	n	1.54
Carbofuran	Aldrich	C ₁₂ H ₁₅ NO ₃	12.3±0.5	1.30	n	1.69
Chloridazon	Aldrich	C ₁₀ H ₈ ClN ₃ O ₁	0.7±0.2	1.11	n	1.52
Chloroxylenol	Aldrich	C ₈ H ₉ ClO	9.8±0.2	3.30	n	1.18
Cimetidine	Aldrich	C ₁₀ H ₁₆ N ₆ S	14.1±0.1	-0.29	n	1.96
Clofibric Acid	Aldrich	C ₁₀ H ₁₁ ClO ₃	3.2±0.1	2.90	-	1.54
Codeine	Cerillian	C ₁₈ H ₂₁ NO ₃	13.4±0.2	1.34	+	2.21
Cotinine	Cerillian	C ₁₀ H ₁₂ N ₂ O	4.7±0.1	0.21	n	1.39
DEET	Aldrich	C ₁₂ H ₁₇ NO	-1.4±0.7	2.50	n	1.68
Diazinon	Aldrich	C ₁₂ H ₂₁ N ₂ O ₃ P ₁ S ₁	1.2±0.3	4.19	n	2.31

FIG. 80

Compound Name	Supplier	Chemical Formula	pKa	LogK _{ow}	Charge State at pH = 7.4	McGowan Volume
Diclofenac	Aldrich	C ₁₄ H ₁₁ Cl ₂ N ₁ O ₂	4.2±0.1	4.60	-	2.03
Dimethoate	Aldrich	C ₅ H ₁₂ NO ₃ PS ₂	14.4±0.5	-1.48	n	1.58
Diuron	Aldrich	C ₉ H ₁₀ Cl ₂ N ₂ O ₁	13.6±0.7	2.30	n	1.60
Efavirenz	Aldrich	C ₁₄ H ₉ ClF ₃ NO ₂	10.2±0.4	5.15	n	1.89
Erythromycin	Aldrich	C ₃₇ H ₆₇ N ₁₃ O ₁₃	13.1±0.7	2.60	+	5.77
Estrone	Aldrich	C ₁₈ H ₂₂ O ₂	10.3±0.4	4.31	n	2.16
Famotidine	Aldrich	C ₈ H ₁₅ N ₇ O ₂ S ₃	7.5±0.4	-1.95	+	2.26
Fluconazole	Aldrich	C ₁₃ H ₁₂ F ₂ N ₆ O	11.0±0.3	0.56	n	2.01
Fluoxetine	Aldrich	C ₁₇ H ₁₈ F ₃ NO	10.1±0.1	4.17	+	2.24
Gemfibrozil	Aldrich	C ₁₅ H ₂₂ O ₃	4.8± 0.5	4.39	-	2.12
Hydrocodone	Cerilliant	C ₁₈ H ₂₁ NO ₃	8.5±0.2	1.96	+	2.21
Ibuprofen	Arcos Organics	C ₁₃ H ₁₈ O ₂	4.4±0.1	3.84	-	1.78
Imidacloprid	Aldrich	C ₉ H ₁₀ ClN ₅ O ₂	7.2±0.2	-0.59	z	1.68
Iopromid	Aldrich	C ₁₈ H ₂₄ I ₃ N ₃ O ₈	10.6±0.7	-0.44	z	3.82
Ioxynil	Aldrich	C ₇ H ₃ I ₂ NO	5.0±0.2	3.38	-	1.45
Isoproturon	Aldrich	C ₁₂ H ₁₈ N ₂ O ₁	15.1±0.7	2.57	n	1.78
Ketoprofen	Aldrich	C ₁₆ H ₁₄ O ₃	4.2±0.1	3.61	-	1.98
Linuron	Aldrich	C ₉ H ₁₀ Cl ₂ N ₂ O ₂	12.1±0.7	2.30	n	1.66
Malaoxon	Aldrich	C ₁₀ H ₁₉ O ₇ PS	N.A	0.97	n	2.21
MCPA	Aldrich	C ₉ H ₉ ClO ₃	3.1±0.1	2.41	-	1.39
Mecoprop	Aldrich	C ₁₀ H ₁₁ ClO ₃	3.2±0.1	2.98	-	1.54
Meprobamate	Cerilliant	C ₉ H ₁₈ N ₂ O ₄	13.1±0.5	0.93	n	1.73
Methomyl	Aldrich	C ₅ H ₁₀ N ₂ O ₂ S	13.3±0.5	0.72	n	1.21
Metolachlor	Aldrich	C ₁₅ H ₂₂ ClNO ₂	1.5±0.5	3.45	n	2.28
Metoprolol	Aldrich	C ₁₅ H ₂₅ NO ₃	13.9±0.2	1.76	+	2.26
Metribuzin	Aldrich	C ₈ H ₁₄ N ₄ O ₁ S ₁	-0.2±0.2	1.96	n	1.62
Molinate	Aldrich	C ₉ H ₁₇ NOS	-1.2±0.2	2.34	n	1.55
Morphine	Cerilliant	C ₁₇ H ₁₉ O ₃	9.5±0.4	0.90	+	2.06
Nadolol	Aldrich	C ₁₇ H ₂₇ NO ₄	13.9±0.2	0.87	+	2.49
Naproxen	Aldrich	C ₁₄ H ₁₄ O ₃	4.8±0.3	2.99	-	1.78
Oxcarbazepine	Aldrich	C ₁₅ H ₁₂ N ₂ O ₂	13.7±0.2	1.82	n	1.87
Oxybenzone	Aldrich	C ₁₄ H ₁₂ O ₃	7.6±0.4	3.62	-	1.74
Paraxanthine	Aldrich	C ₇ H ₈ N ₄ O ₂	8.5±0.5	0.09	n	1.22

FIG. 80 (continued)

Compound Name	Supplier	Chemical Formula	pKa	LogK _{ow}	Charge State at pH = 7.4	McGowan Volume
Penciclovir	Aldrich	C ₁₀ H ₁₅ N ₅ O ₃	14.4±0.1	-1.69	n	1.80
Pentoxifylline	Aldrich	C ₁₃ H ₁₈ N ₄ O ₃	0.5±0.7	0.23	n	2.08
PFBA	Aldrich	C ₄ H ₇ F ₇ O ₂	0.4±0.1	2.31	-	0.87
PFOA	Aldrich	C ₈ H ₇ F ₁₅ O ₂	0.5±0.1	5.11	-	1.58
Phenytoin	Aldrich	C ₁₅ H ₁₂ N ₂ O ₂	8.3±0.1	3.40	z	1.87
Progesterone	Aldrich	C ₂₁ H ₃₀ O ₂	N.A	4.15	n	2.62
Prometon	Aldrich	C ₁₀ H ₁₉ N ₅ O	4.4±0.4 1	1.75	n	1.84
Propachlor	Aldrich	C ₁₁ H ₁₄ ClNO	0.3±0.5	2.39	n	1.66
Ranitidine	USP	C ₁₃ H ₂₂ N ₄ O ₃ S	8.4±0.3	0.99	z	2.40
Siduron	Aldrich	C ₁₄ H ₂₀ N ₂ O	12.4±0.4 4	3.27	n	1.95
Simazine	Aldrich	C ₇ H ₁₂ ClN ₅	2.7±0.1	0.63	n	1.48
Sitagliptin	Aldrich	C ₁₆ H ₁₅ F ₆ N ₅ O	7.2±0.1	1.26	+	2.44
Sucralose	Aldrich	C ₁₂ H ₁₉ Cl ₃ O ₈	12.5±0.7 7	-0.47	n	2.42
Sulfamethoxazole	Aldrich	C ₁₀ H ₁₁ N ₃ O ₃ S	5.8±0.5	0.79	-	1.72
Sulfathiazole	Aldrich	C ₉ H ₉ N ₃ O ₂ S ₂	7.2±0.1	0.98	-	1.69
TCEP	Aldrich	C ₆ H ₁₂ Cl ₃ O ₄ P	N.A	2.11	n	1.76
Testosterone	Aldrich	C ₁₉ H ₂₈ O ₂	15.1±0.6 6	3.37	n	2.38
Tramadol	Cerillian t	C ₁₆ H ₂₅ NO ₂	14.5±0.4 4	2.45	+	2.23
Tributyl Phosphate	Aldrich	C ₁₂ H ₂₇ O ₄ P	N.A	4.09	n	2.24
Triclosan	Aldrich	C ₁₂ H ₇ Cl ₃ O ₂	7.8±0.4	4.98	n	1.81
Trimethoprim	Aldrich	C ₁₄ H ₁₈ N ₄ O ₃	7.0±0.1	0.89	+	2.18
Valsartan	USP	C ₂₄ H ₂₉ N ₅ O ₃	3.6±0.1	5.27	-	3.41
Venlafaxine	USP	C ₁₇ H ₂₇ NO ₂	14.8±0.2 2	2.74	+	2.37
Warfarin	Aldrich	C ₁₉ H ₁₆ O ₄	4.5±1.0	3.52	-	2.31

FIG. 80 (continued)

Compound Name	Exact Mass	Ionization Mode	Retention Time, (min)	Limit of Quantification, (ng/l)
2,4-D	219.97	Negative	14.03	10.00
Abacavir	286.15	Positive	9.25	5.00
Acebutolol	336.20	Positive	10.11	5.00
Acetaminophen	151.06	Positive	8.32	10.00
Acetochlor	269.12	Positive	16.20	10.00
Albuterol	239.15	Positive	8.12	5.00
Allopurinol	136.04	Positive	7.35	200.00
Amphetamine	135.10	Positive	9.30	5.00
Atenolol	266.16	Positive	8.16	5.00
Atenolol Acid	267.15	Positive	9.24	5.00
Atrazine	215.09	Positive	13.17	5.00
Benzotriazole-methyl-1H	133.06	Positive	11.12	5.00
Bromacil	260.02	Positive	12.03	10.00
Bupropion	239.11	Positive	10.92	5.00
Caffeine	194.08	Positive	9.44	5.00
Carbamazepine	236.09	Positive	12.55	5.00
Carbaryl	201.08	Positive	12.52	10.00
Carbofuran	221.11	Positive	12.02	5.00
Chloridazon	221.04	Positive	10.62	5.00
Chloroxylenol	156.03	Negative	15.26	200.00
Cimetidine	252.12	Positive	8.31	5.00
Clofibric Acid	214.04	Negative	14.70	10.00
Codeine	299.15	Positive	8.52	10.00
Cotinine	176.09	Positive	6.93	50.00
DEET	191.13	Positive	13.31	5.00
Diazinon	304.10	Positive	17.47	5.00
Diclofenac	295.02	Positive	17.36	10.00
Dimethoate	229.00	Positive	10.52	5.00
Diuron	232.02	Positive	13.88	10.00
Efavirenz	315.03	Positive	17.39	10.00
Erythromycin	733.46	Positive	13.20	200.00
Estrone	270.16	Positive	11.72	5.00
Famotidine	337.04	Positive	8.29	10.00
Fluconazole	306.10	Positive	10.43	50.00
Fluoxetine	309.13	Positive	14.06	10.00
Gemfibrozil	250.16	Positive	19.30	10.00
Hydrocodone	299.15	Positive	8.82	5.00
Ibuprofen	206.13	Positive	17.76	10.00
Imidacloprid	255.05	Positive	10.06	5.00
Iopromid	790.87	Positive	8.43	5.00
Ioxynil	370.83	Negative	14.26	5.00
Isoproturon	206.14	Positive	13.56	5.00
Ketoprofen	254.09	Positive	14.30	10.00

FIG. 81

Compound Name	Exact Mass	Ionization Mode	Retention Time, (min)	Limit of Quantification, (ng/l)
Linuron	248.01	Positive	14.87	10.00
Malaoxon	314.06	Positive	12.06	5.00
MCPA	200.02	Negative	14.37	5.00
Mecoprop	214.04	Negative	15.60	5.00
Meprobamate	218.13	Positive	11.28	10.00
Methomyl	162.05	Positive	9.20	5.00
Metolachlor	283.13	Positive	16.35	5.00
Metoprolol	267.18	Positive	10.23	5.00
Metribuzin	214.09	Positive	11.99	5.00
Molinate	187.10	Positive	15.37	5.00
Morphine	285.14	Positive	7.52	10.00
Nadolol	309.19	Positive	9.40	5.00
Naproxen	230.09	Positive	14.83	5.00
Oxcarbazepine	252.09	Positive	11.61	10.00
Oxybenzone	228.08	Positive	16.72	50.00
Paraxanthine	180.06	Positive	8.78	10.00
Penciclovir	253.12	Positive	8.34	5.00
Pentoxifylline	278.14	Positive	10.54	5.00
PFBA	213.99	Negative	10.70	10.00
PFOA	413.97	Negative	16.99	5.00
Phenytoin	252.09	Positive	12.36	5.00
Progesterone	314.22	Positive	17.29	10.00
Prometon	225.16	Positive	11.62	5.00
Propachlor	211.08	Positive	13.39	5.00
Ranitidine	314.14	Positive	8.24	10.00
Siduron	232.16	Positive	14.84	10.00
Simazine	201.08	Positive	11.92	5.00
Sitagliptin	407.12	Positive	10.42	10.00
Sucralose	396.01	Negative	9.90	5.00
Sulfamethoxazole	253.05	Positive	10.00	10.00
Sulfathiazole	255.01	Positive	8.58	10.00
TCEP	283.95	Positive	12.19	5.00
Testosterone	288.21	Positive	15.40	5.00
Tramadol	263.19	Positive	10.11	5.00
Tributyl Phosphate	266.16	Positive	18.87	5.00
Triclosan	287.95	Negative	19.36	10.00
Trimethoprim	290.14	Positive	9.21	5.00
Valsartan	435.23	Positive	15.60	10.00
Venlafaxine	277.20	Positive	11.28	10.00
Warfarin	308.10	Positive	15.27	5.00

FIG. 81 (continued)

Compound Name	K _{obs} , [g mg ⁻¹ min ⁻¹]		Removal – 5 min, [%]		Removal – 30 min, [%]		Instant Uptake, [%]	
	CCAC	P-CDP	CCAC	P-CDP	CCAC	P-CDP	CCAC	P-CDP
2,4-D	11.0	0.0 (72.9)	43.3 ± 3.4	2.2 ± 5.0	76.8 ± 1.6	4.7 ± 3.0	43.4 ± 4.1	3.7 ± 4.8
Abacavir	14.0	141.8	56.2 ± 2.7	90.4 ± 3.9	88.1 ± 1.9	94.6 ± 0.3	50.8 ± 0.3	98.9 ± 5.2
Acebutolol	1.9	586.88	61.2 ± 4.4	64.1 ± 16.1	97 ± 0.6	82.6 ± 10.1	72.5 ± 0.0	99.9 ± 5.2
Acetaminophen	13.9	0.0 (-772.6)	32.4 ± 7.6	6.8 ± 2.8	56.1 ± 6.9	0.6 ± 1.8	57.8 ± 9.0	0.0 ± 3.9
Acetochlor	13.0	61.9	59.7 ± 4.5	51.7 ± 4.1	90.9 ± 0.8	59.3 ± 2.1	53.5 ± 5.7	66.0 ± 4.5
Albuterol	0 (-1775.1)	151.0	0.0 ± 9.0	74.2 ± 3.9	0.2 ± 6.1	79.2 ± 4.3	23.5 ± 1.9	91.8 ± 10.0
Allopurinol	26.4	37.3	32.9 ± 11.0	1.1 ± 13.1	47.5 ± 4.8	6.3 ± 3.6	53 ± 13.1	0 ± 7.0
Amphetamine	0 (-4485.5)	73712.2	0 ± 7.1	75.5 ± 16.5	0 ± 11.2	72.4 ± 9.9	33.4 ± 0.7	97.1 ± 9.0
Atenolol	5.0	182.8	16.7 ± 8.1	83.3 ± 6.6	45.2 ± 4.3	88.5 ± 2.1	44.4 ± 0.6	97.1 ± 5.8
Atenolol_Acid	16.3	85.7	34.6 ± 1.5	76.4 ± 3.9	57.8 ± 3.6	82.3 ± 2.0	42.3 ± 1.2	94.2 ± 4.8
Atrazine	14.7	177.1	44.6 ± 1.5	17.6 ± 4.8	75.7 ± 1.7	22.2 ± 4.9	43.7 ± 4.8	29.2 ± 6.0
Benzotriazole-methyl-1H	21.0	281.1	60.4 ± 1.8	15.5 ± 2.1	82.9 ± 1.0	18.2 ± 5.0	56.2 ± 4.4	27.1 ± 5.6
Bromacil	16.9	612.7	39.4 ± 2.6	8.7 ± 4.3	64.2 ± 2.8	8.8 ± 6.07	44.7 ± 4.1	6.9 ± 4.4
Bupropion hcl	3.1	5184.7	20.7 ± 2.6	59.6 ± 13.1	67.0 ± 6.4	71.6 ± 4.1	46.6 ± 0.1	99.7 ± 5.8
Caffeine	13.0	207.9	44.7 ± 19.0	0.7 ± 6.7	77.5 ± 3.4	5.5 ± 6.5	61.1 ± 12.1	0.0 ± 6.4
Carbamazepine	13.0	335.1	56.2 ± 5.4	15.1 ± 2.9	86.3 ± 1.4	18.0 ± 3.6	56.3 ± 1.8	26.6 ± 4.7
Carbaryl	16.8	1485.8	49.0 ± 1.8	11.3 ± 3.9	77.2 ± 1.5	12.7 ± 6.3	49.6 ± 1.8	17.7 ± 7
Carbofuran	15.2	0.0 (-980.1)	40.3 ± 1.9	4.8 ± 1.6	67.3 ± 2.2	3.2 ± 5.6	45.3 ± 1.8	4.9 ± 5.5
Chloridazon	14.3	364.9	56.6 ± 5.7	23.9 ± 2.6	86.3 ± 1.6	25.4 ± 2.9	54.7 ± 6.2	29.6 ± 5.9

FIG. 82

Compound Name	K_{obs} , [g mg ⁻¹ min ⁻¹]		Removal – 5 min, [%]		Removal – 30 min, [%]		Instant Uptake, [%]	
Chloroxylenol	10.6	52.8	47.4 ± 4.9	10.1 ± 15.5	77.9 ± 1.0	19 ± 16.4	45.4 ± 7.2	7.5 ± 3.6
Cimetidine	18.7	100.9	58.8 ± 6.9	86.5 ± 5.3	85.5 ± 1.3	92.4 ± 0.5	56.5 ± 0.5	99.8 ± 3.1
Clofibric Acid	16.8	0.0 (-112.9)	36.8 ± 3.1	2.5 ± 5.6	60.4 ± 0.5	4.5 ± 7.3	35.4 ± 1.2	2.3 ± 2.4
Codeine	19.8	1501.2	22.2 ± 6.9	90.6 ± 12.7	59.8 ± 4.2	94.3 ± 1.3	41.2 ± 0.3	100 ± 5.7
Cotinine	17.8	239.3	32.1 ± 9.5	26.8 ± 5.1	50.3 ± 1.7	25.2 ± 4.0	40.6 ± 5.6	42 ± 6.3
DEET	16.8	577.9	39.0 ± 1.1	12.1 ± 2.8	66.7 ± 3.1	13 ± 2.9	42.6 ± 3.2	20.5 ± 4.6
Diazinon	26.3	194.7	72.5 ± 1.4	90.3 ± 5.3	96.8 ± 0.0	94.6 ± 0.9	60.3 ± 0.4	98.4 ± 6.3
Diclofenac	6.4	46.4	48.0 ± 3.7	32.4 ± 4.4	88.1 ± 1.5	40.4 ± 2.8	43.1 ± 3.5	77.8 ± 3.9
Dimethoate	11.1	0.0 (-248.1)	21.5 ± 22.0	7.0 ± 4.4	55.6 ± 8.5	4.9 ± 8.2	50.3 ± 10.2	9.3 ± 9.3
Diuron	21.8	122.4	75.9 ± 2.0	81.6 ± 3.5	96.7 ± 0.3	86.8 ± 1.0	63.6 ± 1.5	93.4 ± 5.6
Efavirenz	25.1	170.6	65.2 ± 4.3	82.0 ± 6.0	95.7 ± 0.4	87.9 ± 1.0	56.8 ± 1.3	95.0 ± 6.4
Erythromycin	14.4	171.9	39.1 ± 8.2	60.6 ± 13.2	92.6 ± 2.8	79.4 ± 3.7	68.4 ± 0.0	100 ± 6.8
Estrone	16.8	67.4	66.2 ± 2.9	55.5 ± 5.3	96.2 ± 0.5	64.9 ± 4.1	61.1 ± 4.2	73.4 ± 3.9
Famotidine	26.1	107.4	74.2 ± 4.0	87.4 ± 6.2	95.5 ± 0.3	93.1 ± 0.7	63.4 ± 0.3	99.3 ± 2.5
Fluconazole	11.8	329.4	43.5 ± 2.4	6.5 ± 4.7	74.3 ± 1.7	7.8 ± 2.7	51.8 ± 3.4	5.7 ± 5.5
Fluoxetine hcl	2563.0	137.0	12.3 ± 37.0	46.8 ± 10.7	71.2 ± 7.7	66.3 ± 6.4	79.2 ± 0.0	100 ± 5.53
Gemfibrozil	8.1	143.0	54.6 ± 4.3	76.1 ± 7.7	93.9 ± 1.3	79.2 ± 5.4	47.7 ± 0.6	97.8 ± 4.2
Hydrocodone	16.7	1506.9	22.2 ± 6.9	89.8 ± 14.8	59.8 ± 4.2	94.1 ± 1.7	40.3 ± 0.3	98.6 ± 5.6
Ibuprofen	2.9	43.7	20.9 ± 4.1	9.1 ± 7.5	62.5 ± 3.9	25.5 ± 10.7	38.2 ± 9.3	48.7 ± 6.6
Imidacloprid	15.1	224.8	56.8 ± 1.6	26.9 ± 3.3	85.8 ± 1.6	29.3 ± 2.6	53.1 ± 3.9	39.4 ± 4.4
Iopromid	5.0	73.9	32.0 ± 10.5	6.9 ± 6.5	72.4 ± 7.7	7.7 ± 7.3	57.5 ± 13.2	1.8 ± 2.4
Ioxynil	6.8	9915.0	47.2 ± 4.7	7.3 ± 4.8	85.9 ± 0.2	8.2 ± 3.4	50.8 ± 3.9	57.5 ± 2.6
Isoproturon	15.3	84.6	55.9 ± 3.4	61.0 ± 4.1	86.1 ± 1.5	67.9 ± 2.1	54.3 ± 4.5	75.1 ± 4.3

FIG. 82 (continued)

Compound Name	K _{obs} , [g mg ⁻¹ min ⁻¹]		Removal – 5 min, [%]		Removal – 30 min, [%]		Instant Uptake, [%]	
Ketoprofen	8.6	268.7	49.8 ± 5.1	23.8 ± 2.9	87.2 ± 1.3	25.3 ± 4.5	43.8 ± 5.1	68.7 ± 4.4
Linuron	24.4	143.3	77.3 ± 3.7	89.0 ± 4.1	97.5 ± 0.1	93.4 ± 0.7	64.3 ± 0.6	97.2 ± 5.0
Malaoxon	12.7	359.4	46.8 ± 1.9	24.4 ± 3.0	78.0 ± 2.2	25.6 ± 3.9	49.3 ± 4.7	44.0 ± 4.8
MCPA	11.9	0.0 (255.6)	43.8 ± 2.6	0.0 ± 4.6	74.8 ± 0.9	1.2 ± 5.6	42.2 ± 2.9	7.6 ± 3.6
Mecoprop	11.2	0.0 (1997.2)	38.8 ± 1.2	0.0 ± 2.3	74.0 ± 1.6	0.0 ± 7.0	40.6 ± 3.8	3.7 ± 2.4
Meprobamate	15.9	0.0 (-405.0)	34.9 ± 4.7	5.1 ± 6.1	57.5 ± 2.2	2.2 ± 4.3	48.1 ± 8.3	3.1 ± 7.7
Methomyl	17.6	0.0 (-98.6)	24.7 ± 7.6	0.0 ± 10.3	47.1 ± 6.3	0.0 ± 11.4	53.9 ± 10.3	0.0 ± 3.7
Metolachlor	11.9	59.5	58.6 ± 2.9	56.7 ± 4.6	91.1 ± 1.2	64.3 ± 2.2	53.6 ± 5.0	71.4 ± 4.2
Metoprolol	1.7	1633.2	40.0 ± 3.9	85.8 ± 20.1	83.3 ± 3.1	91.1 ± 2.8	60.6 ± 0.1	99.7 ± 6.0
Metribuzin	18.8	435.3	36.8 ± 0.9	12.7 ± 3.2	58.9 ± 2.5	13.6 ± 4.5	41.9 ± 3.8	17.8 ± 5.5
Molinate	15.5	212.6	52.7 ± 2.5	32.4 ± 2.8	79.3 ± 1.8	35.9 ± 3.4	51.0 ± 5.7	47.7 ± 4.9
Morphine	3.1	162.1	15.2 ± 13.0	80.5 ± 5.2	41.8 ± 3.0	86.3 ± 2.9	45.3 ± 1.0	96.1 ± 3.0
Nadolol	2.2	197.6	31.1 ± 1.8	85.9 ± 7.8	69.5 ± 5.0	91.4 ± 2.0	56.0 ± 0.3	98.5 ± 4.9
Naproxen	10.5	57.3	52.5 ± 4.0	41.0 ± 6.1	89.2 ± 1.0	51.7 ± 7.0	43.3 ± 2.1	88.9 ± 4.9
Oxcarbazepine	14.5	60.3	59.9 ± 4.5	12.1 ± 11.1	90.3 ± 5.0	20.8 ± 2.6	52.1 ± 1.8	14.6 ± 4.9
Oxybenzone	116.1	927.3	91.5 ± 2.3	94.7 ± 15.4	99.4 ± 0.0	92.8 ± 6.8	76.4 ± 0.2	99.6 ± 5.3
Paraxanthine	15.3	0.0 (60.9)	47.5 ± 8.0	0.1 ± 5.2	71.8 ± 4.7	2.4 ± 7.1	58.2 ± 6.7	5.6 ± 6.0
Penciclovir	16.3	102.7	57.8 ± 6.9	87.4 ± 4.9	88.2 ± 2.9	92.8 ± 0.6	59.1 ± 0.2	98.6 ± 4.2
Pentoxifylline	13.7	1780.0	62.4 ± 6.9	25.6 ± 2.4	94.7 ± 0.4	23.8 ± 3.9	55.9 ± 6.3	33.1 ± 5.3
PFBA	29.0	0.0 (6538.3)	20.5 ± 5.9	0.0 ± 5.3	32.3 ± 4.4	0.3 ± 7.8	28.2 ± 5.4	8.4 ± 7.7
PFOA	9.9	0.0 (-10733.6)	39.0 ± 5.5	0.0 ± 6.3	71.5 ± 1.1	0.0 ± 4.0	35.4 ± 3.1	8.0 ± 4.0

FIG. 82 (continued)

Compound Name	K _{obs} , [g mg ⁻¹ min ⁻¹]		Removal – 5 min, [%]		Removal – 30 min, [%]		Instant Uptake, [%]	
Phenytoin	11.0	244.0	44.4 ± 12.0	19.2 ± 6.2	78.9 ± 2.5	22.1 ± 5.8	47.9 ± 4.7	31.7 ± 5.9
Progesterone	43.7	222.3	84.7 ± 1.7	94.1 ± 3.8	99.3 ± 0.1	97.0 ± 0.1	74.2 ± 0.2	99.3 ± 4.7
Prometon	14.4	179.5	40.4 ± 2.5	91.5 ± 4.0	73.0 ± 1.8	95.1 ± 1.1	42.7 ± 0.5	97.9 ± 3.8
Propachlor	17.0	2055.4	43.6 ± 1.3	14.4 ± 4.0	70.2 ± 1.8	16.0 ± 2.9	45.1 ± 6.7	23.1 ± 4.6
Ranitidine hcl	16.5	9346.4	41.5 ± 4.5	71.2 ± 3.6	84.4 ± 4.2	72.0 ± 0.3	42.2 ± 0.2	99.3 ± 15
Siduron	14.3	73.7	63.2 ± 3.4	62.6 ± 3.2	92.5 ± 0.9	70.2 ± 1.9	55.9 ± 3.8	78.5 ± 4.7
Simazine	18.3	1477.0	68.6 ± 3.7	11.3 ± 3.9	95.0 ± 0.5	12.7 ± 6.3	58.2 ± 3.1	82.6 ± 6.2
Sitagliptin	2.0	1538.2	53.6 ± 3.6	62.6 ± 12.3	93.7 ± 1.2	72.5 ± 2.5	69.0 ± 0.0	99.9 ± 5.4
Sucralose	10.3	114.0	38.6 ± 18	13.9 ± 10.9	74.5 ± 2.7	14.1 ± 10.0	53.9 ± 12.2	10.8 ± 4.1
Sulfamethoxazole	10.0	341.5	35.9 ± 14.0	25.7 ± 3.6	71.1 ± 4.1	26.9 ± 3.8	43.4 ± 5.0	41.7 ± 4.5
Sulfathiazole	10.4	1097.2	50.7 ± 7.7	14.3 ± 4.6	83.2 ± 2.8	15.9 ± 2.7	53.0 ± 2.6	20.9 ± 3.6
TCEP	15.1	240.2	41.2 ± 0.5	10.9 ± 2.7	66.9 ± 2.4	12.8 ± 3.5	48.9 ± 5.4	15.7 ± 6.1
Testosterone	16.5	74.3	71.1 ± 2.9	79.5 ± 4.2	98.4 ± 0.2	86.4 ± 1.3	60.8 ± 2.2	91.2 ± 4.6
Tramadol	5.1	5239.8	11.5 ± 1.8	66.6 ± 12.1	46.5 ± 6.4	81.0 ± 6.7	38.1 ± 0.2	99.4 ± 5.3
Tributyl phosphate	12.1	55.6	60.2 ± 3.1	61.4 ± 5.7	92.6 ± 1.2	70.5 ± 2.1	55.0 ± 3.2	82.5 ± 5.6
Triclosan	264.0	753.4	92 ± 2.3	92.3 ± 7.1	99.5 ± 0.0	95.3 ± 0.8	79.6 ± 0.1	99.7 ± 2.5
Trimethoprim	14.3	898.8	55.5 ± 2.5	95.1 ± 10.5	90.9 ± 1.5	97.9 ± 0.3	65.6 ± 0.0	100 ± 5.3
Valsartan	3.8	87.2	28.5 ± 2.1	12.5 ± 3.1	73.7 ± 0.8	18.0 ± 5.1	27.5 ± 2.6	73.7 ± 3.4
Venlafaxine hcl	5.5	5259.9	13.9 ± 2.5	59.8 ± 17.6	51.8 ± 6.3	72.9 ± 5.2	38.9 ± 0.2	99.4 ± 6.0
Warfarin	6.3	35.5	41.9 ± 4.0	46.5 ± 3.6	84.3 ± 1.7	58.2 ± 2.9	37.9 ± 5.2	73.2 ± 2.1

FIG. 82 (continued)

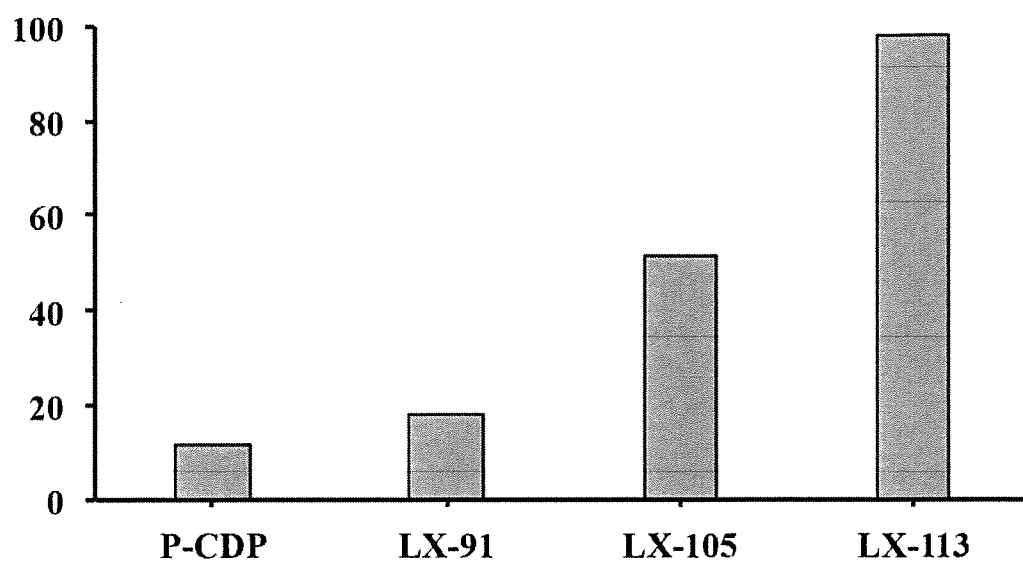


FIG. 83

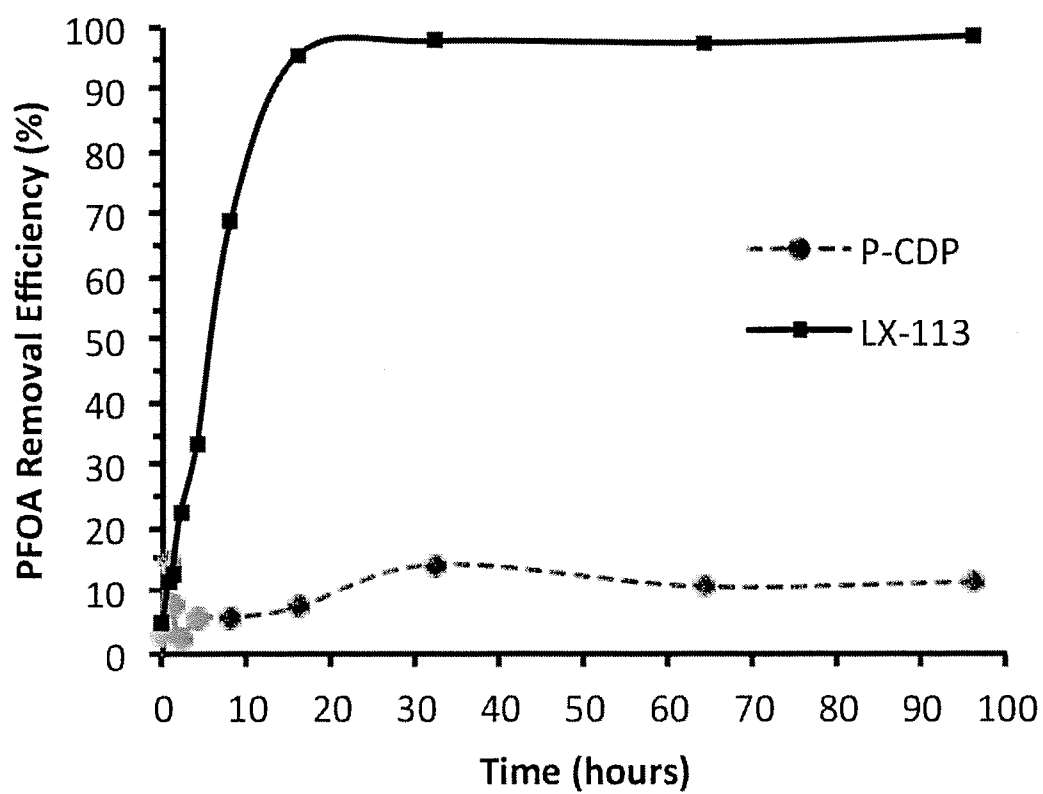


FIG. 84

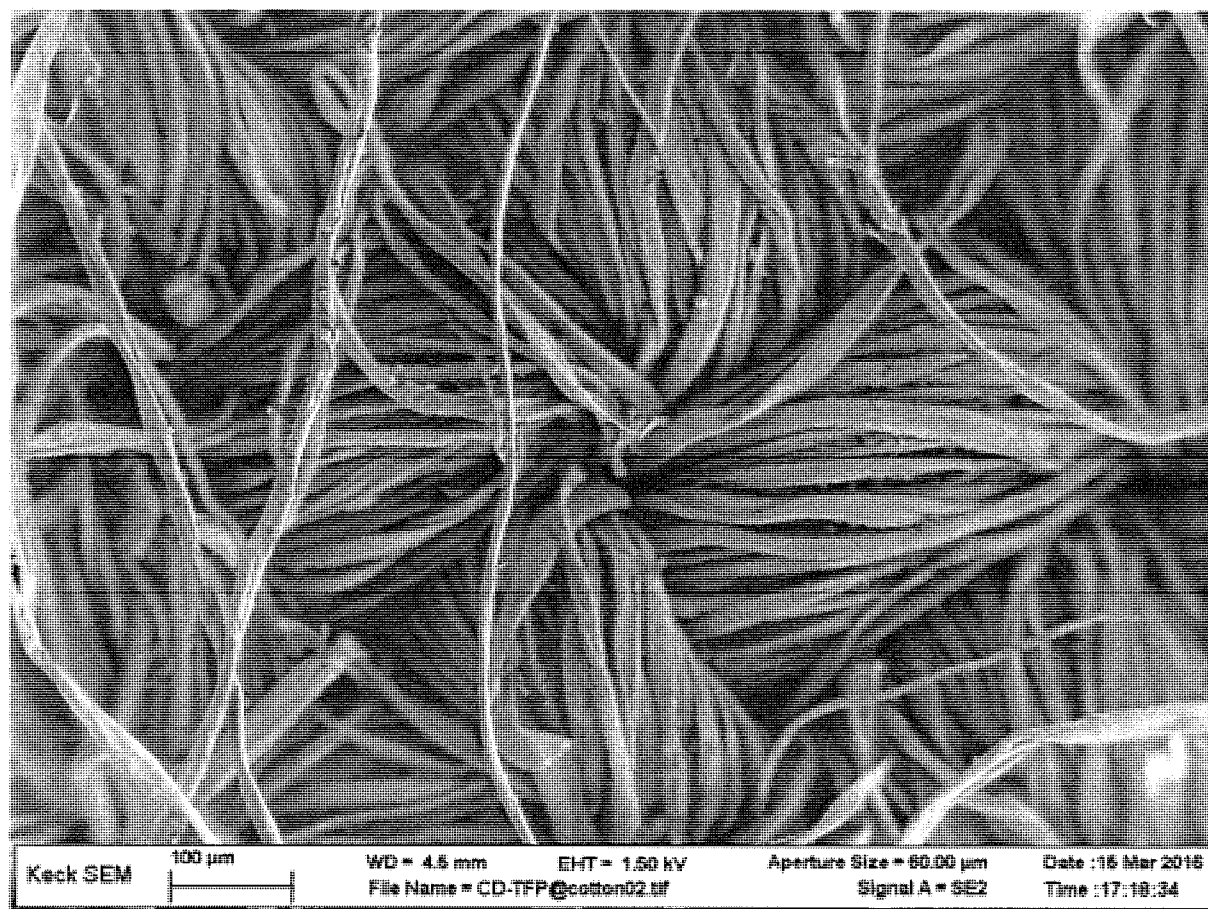


FIG. 85

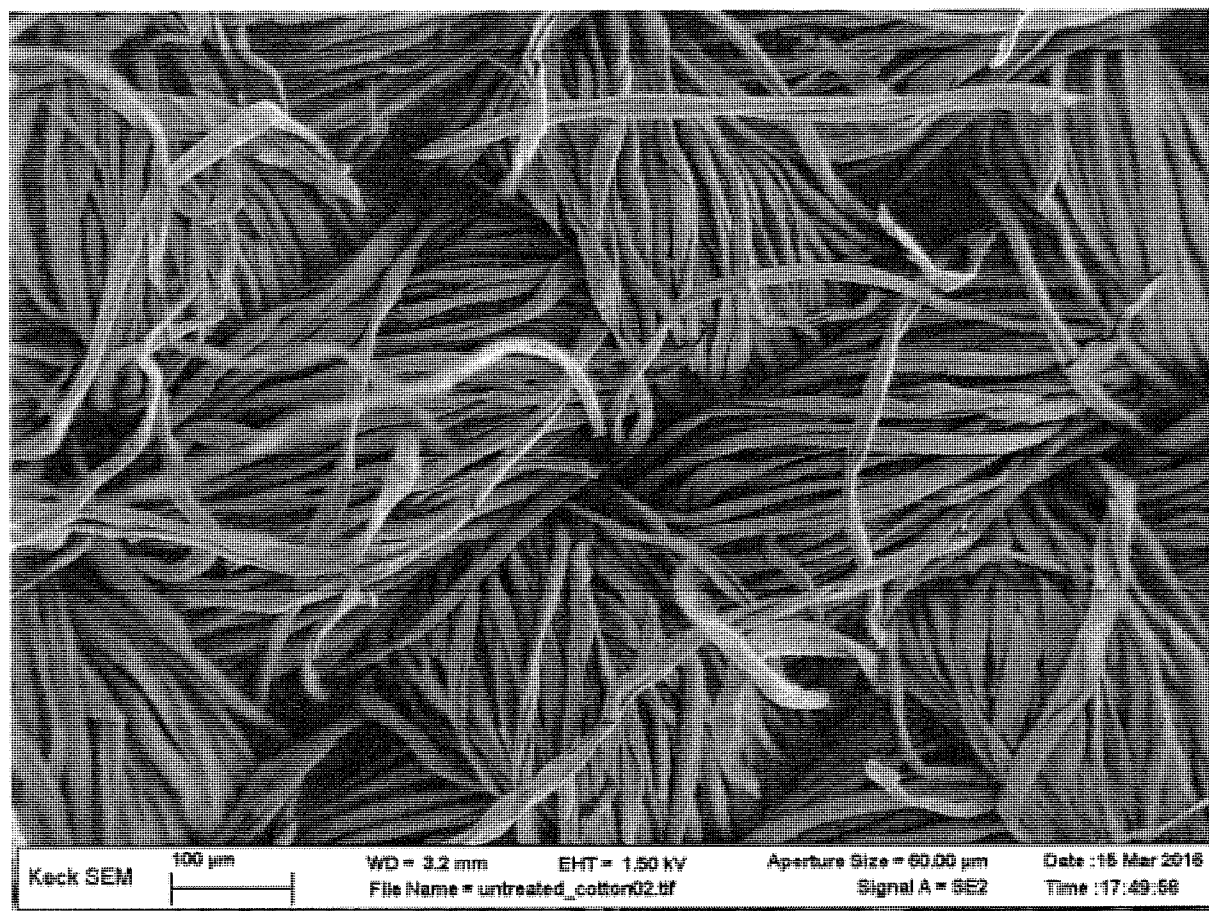


FIG. 86

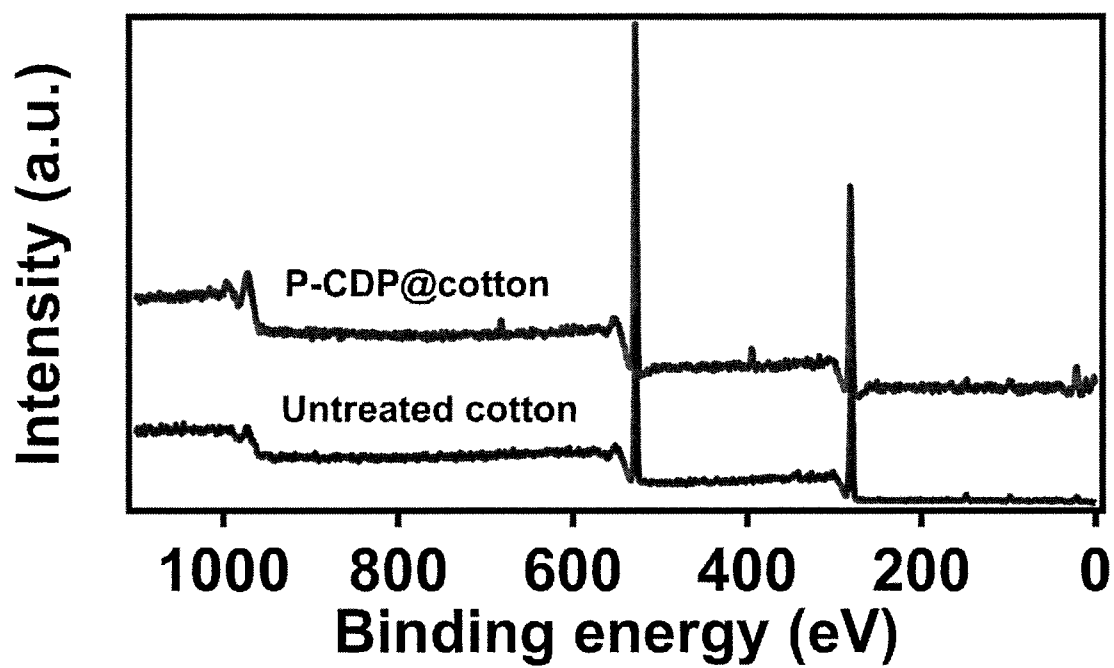


FIG. 87

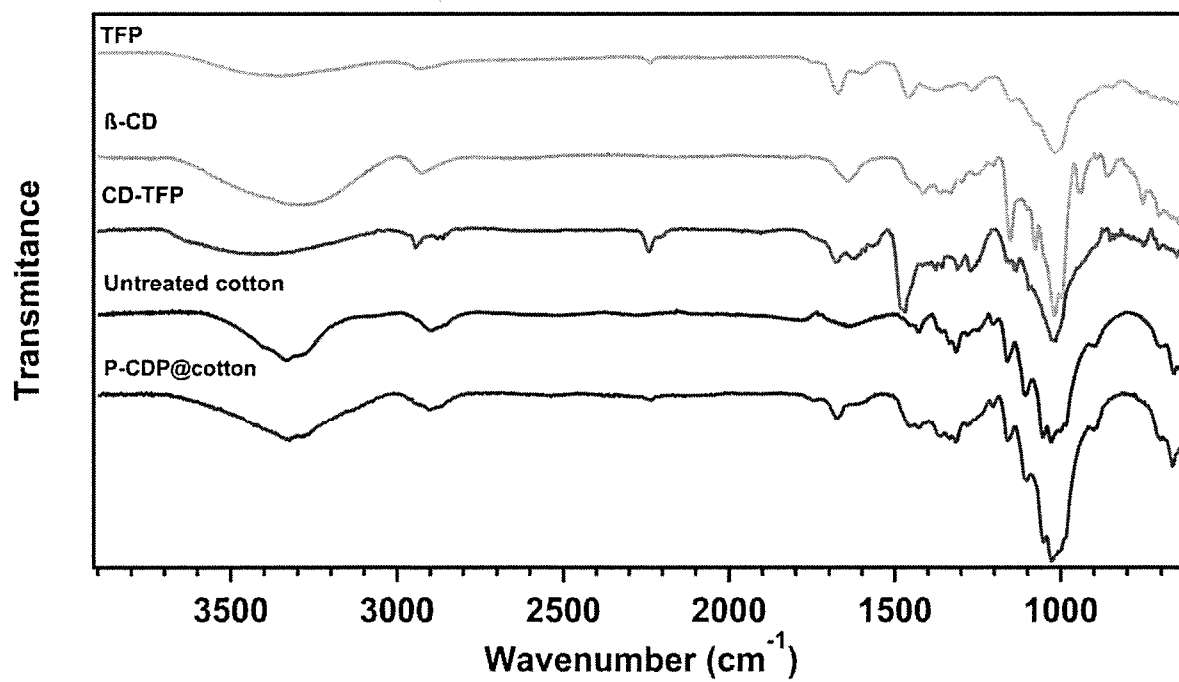


FIG. 88

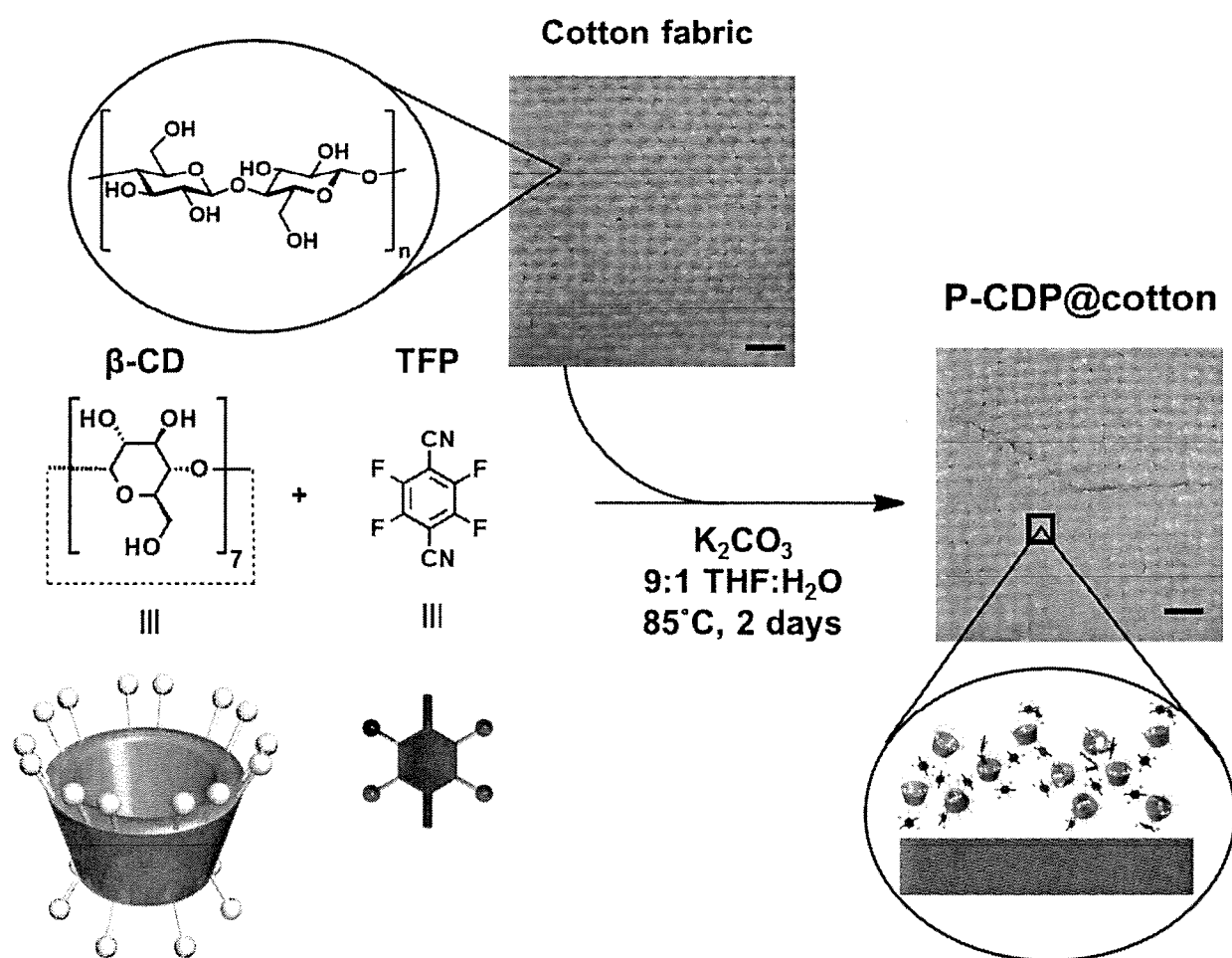


FIG. 89

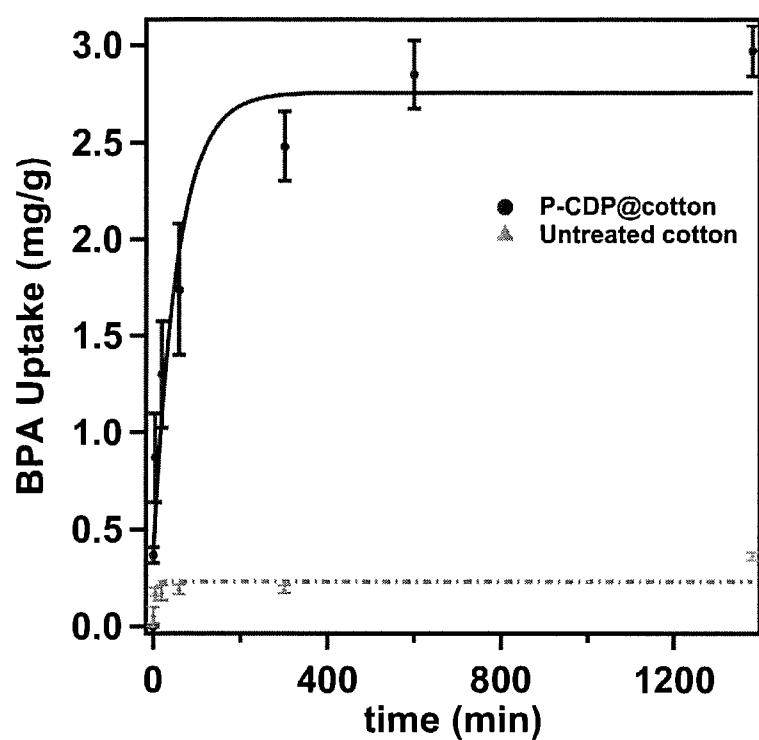


FIG. 90

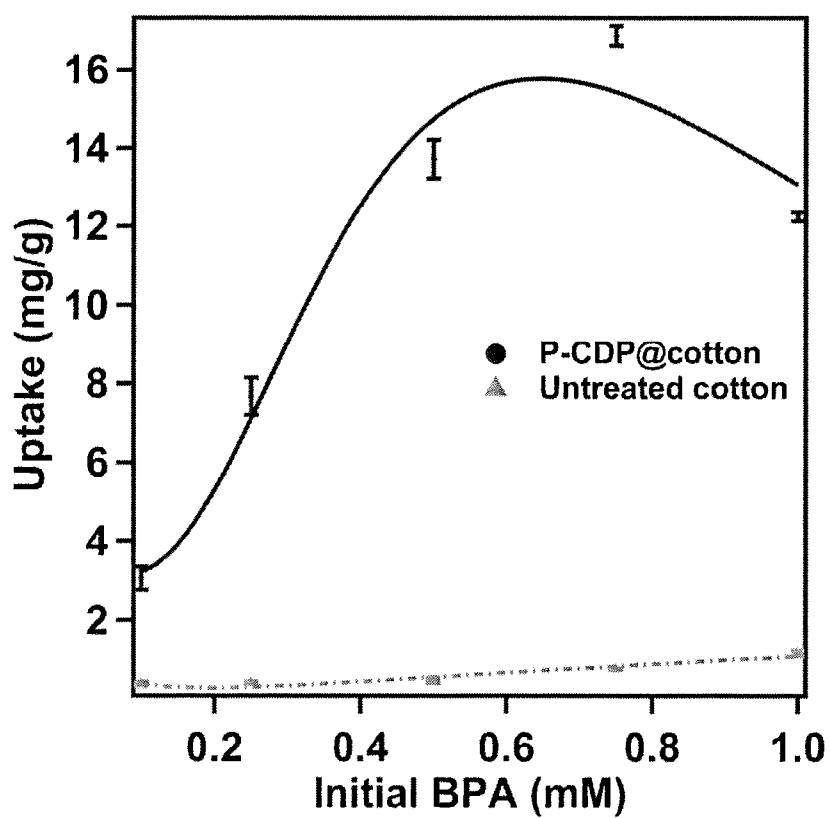


FIG. 91

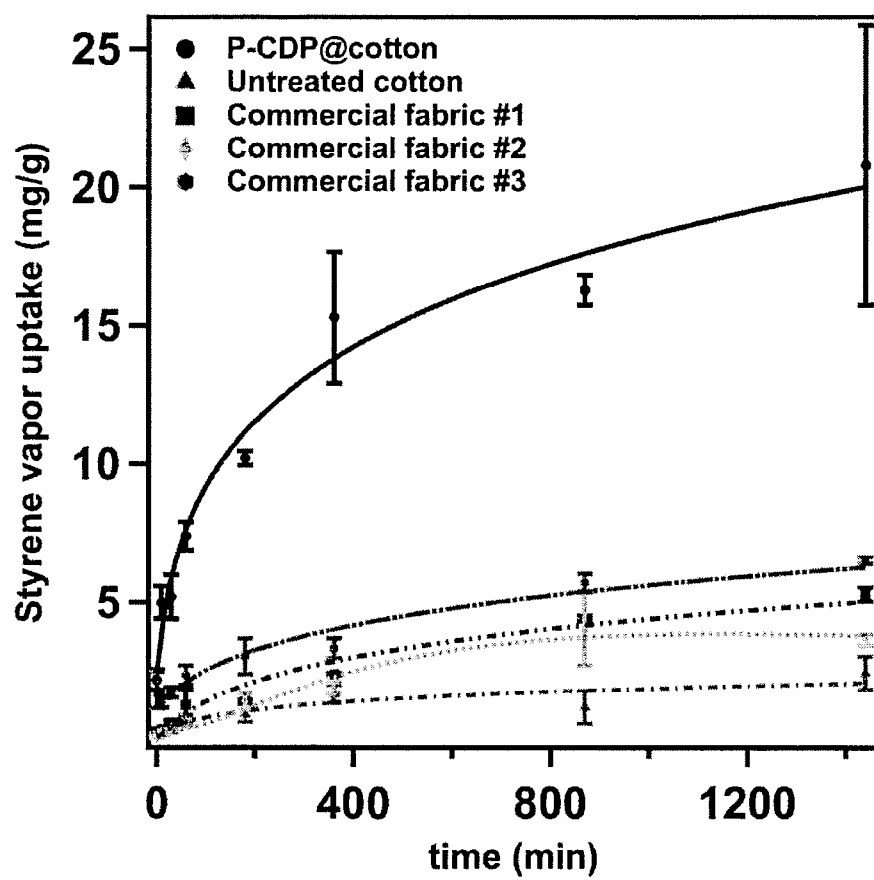


FIG. 92

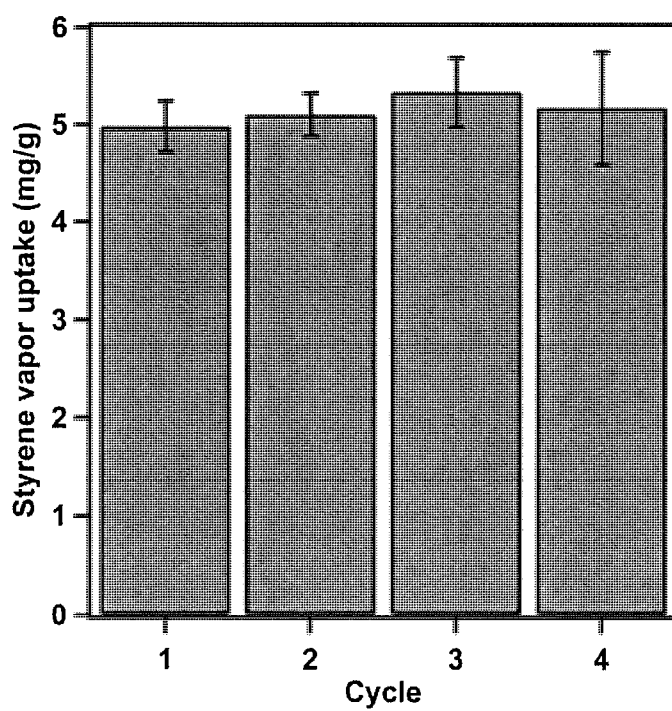


FIG. 93

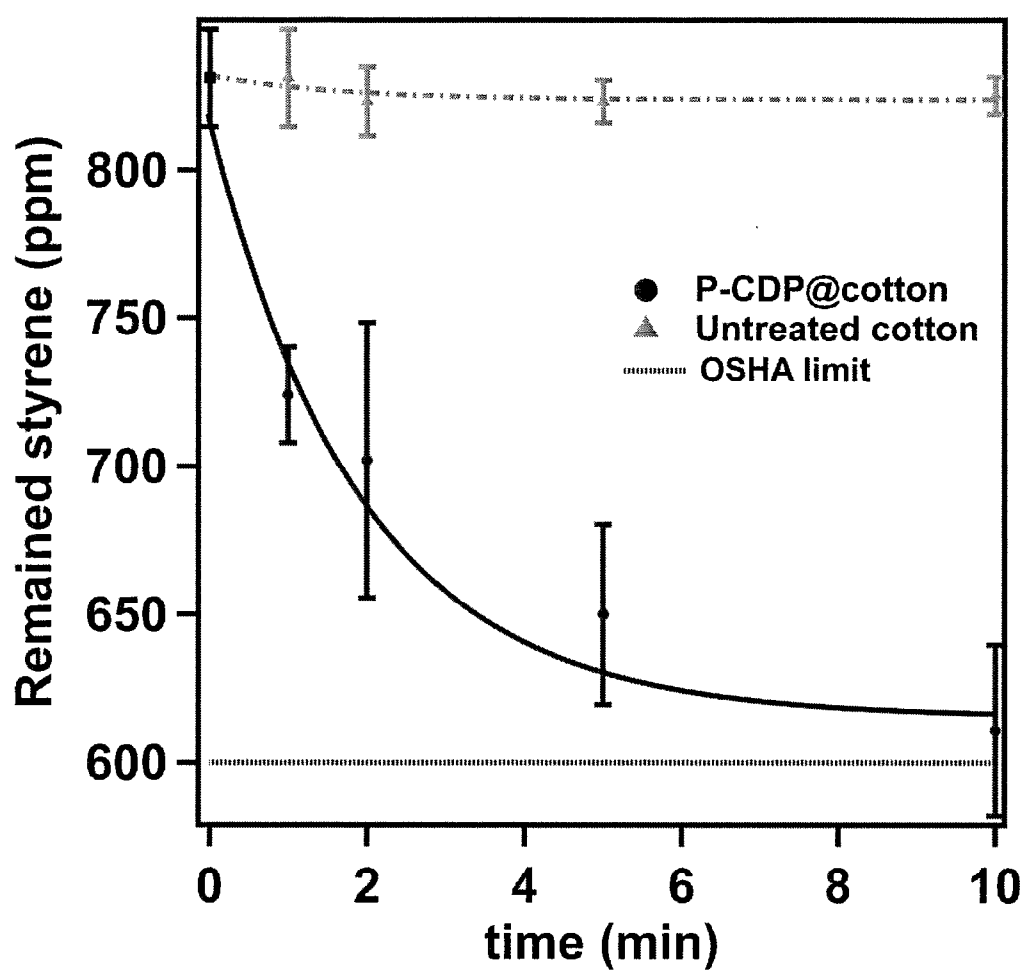


FIG. 94

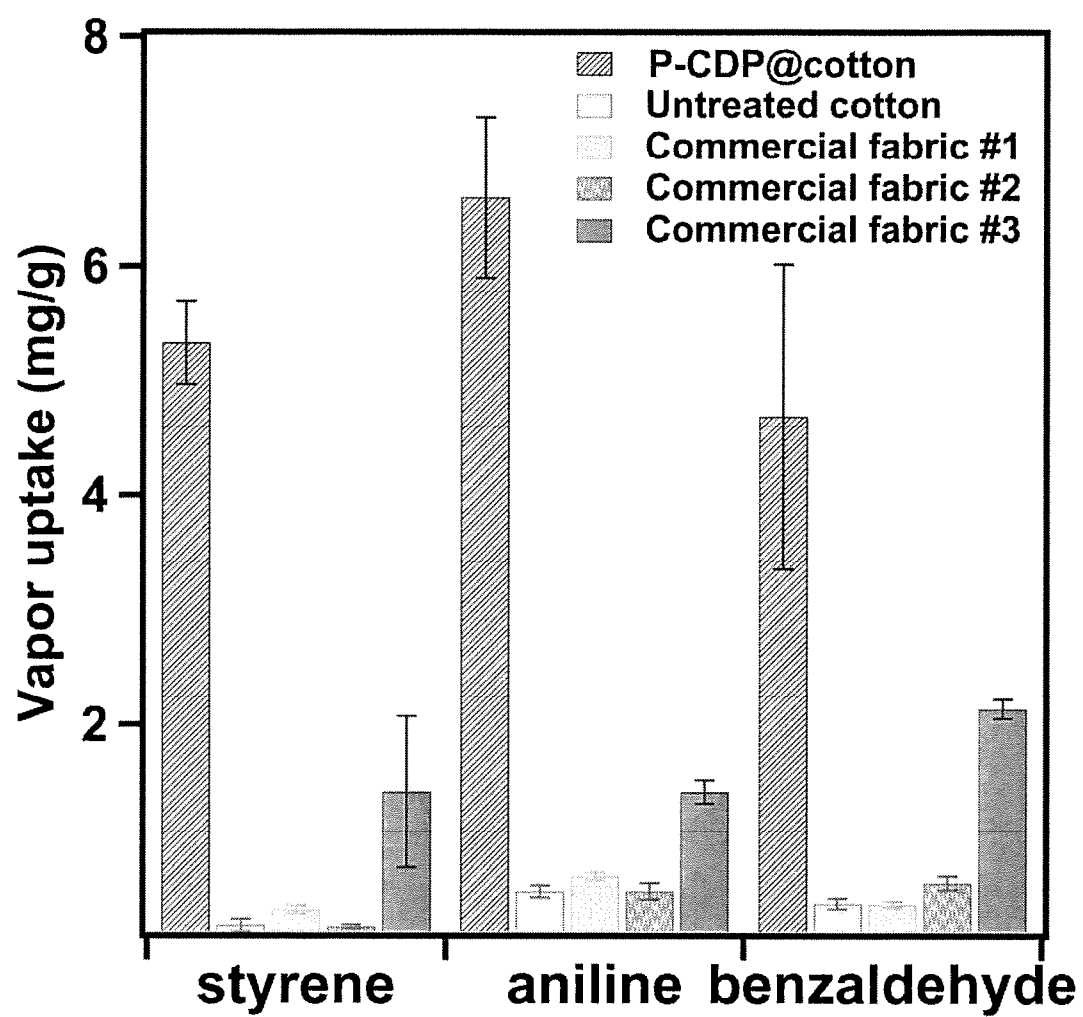


FIG. 95

Compound Name	LogK _∞	α ^H	β ^H	π ^H	R	V	Group
2,4-D	0.45	0.50	0.60	1.24	1.09	1.38	Validation
Abacavir	3.12	0.76	2.85	2.29	1.78	2.09	Training
Acetaminophen	0.72	0.89	0.89	1.32	1.20	1.17	Training
Acetochlor	2.45	0.00	0.70	1.71	1.20	2.14	Training
Albuterol	2.21	1.08	1.90	1.45	1.31	1.98	Validation
Allopurinol	-0.49	0.74	1.07	1.58	1.46	0.88	Training
Atenolol	2.79	0.45	1.72	1.54	1.48	2.18	Training
Atenolol Acid	3.00	0.69	1.54	1.37	1.13	2.14	Validation
Atrazine	1.63	0.65	2.18	1.51	1.22	1.62	Training
Bromacil	1.07	0.35	1.75	1.75	1.36	1.63	Validation
Caffeine	0.68	0.00	1.31	1.00	1.60	1.36	Training
Carbamazepine	1.50	0.46	0.63	1.45	1.76	1.81	Training
Carbaryl	1.38	0.35	0.91	1.55	1.77	1.54	Validation
Carbofuran	1.18	0.35	1.03	1.76	1.25	1.69	Training
Chloridazon	1.76	0.18	1.32	1.76	1.63	1.52	Training
Chloroxylonol	0.68	0.72	0.37	0.96	0.98	1.18	Validation
Cimetidine	2.85	0.59	2.27	2.41	1.43	1.96	Validation
Clofibric Acid	0.64	0.50	0.66	1.11	0.93	1.54	Training
Codeine	2.85	0.26	1.53	2.16	1.91	2.21	Training
Cotinine	1.56	0.00	1.21	1.46	1.15	1.39	Validation
DEET	1.33	0.00	0.84	1.42	0.93	1.68	Training
Diazinon	3.35	0.00	2.56	2.57	1.22	2.31	Training
Diclofenac	2.64	0.59	1.34	2.10	2.06	2.03	Training
Dimethoate	1.01	0.35	2.44	2.41	1.31	1.58	Training
Estrone	2.45	0.55	0.82	1.55	1.54	2.16	Training
Famotidine	3.47	0.73	2.09	2.79	2.50	2.26	Validation
Hydrocodone	2.89	0.00	1.52	2.31	1.74	2.21	Validation
Ibuprofen	1.98	0.59	0.49	0.83	0.75	1.78	Training
Imidacloprid	1.75	0.17	1.53	1.98	1.56	1.68	Training
Ioxynil	1.67	0.50	0.30	1.48	2.07	1.45	Validation
Ketoprofen	2.20	0.59	0.86	1.77	1.53	1.98	Training
Malaoxon	2.20	0.00	2.90	2.51	0.61	2.21	Training
MCPA	0.67	0.50	0.61	1.16	0.96	1.39	Validation

FIG. 96

Compound Name	LogK _∞	α ^H	β ^H	π ^H	R	V	Group
Mecoprop	0.42	0.50	0.63	1.12	0.95	1.54	Training
Meprobamate	0.52	0.91	0.68	0.58	0.48	1.73	Training
Methomyl	0.63	0.35	1.18	1.13	0.94	1.21	Validation
Metolachlor	2.50	0.00	0.72	1.67	1.19	2.28	Training
Metribuzin	1.36	0.00	1.60	1.32	1.15	1.62	Validation
Morphine	2.43	0.55	1.54	2.06	1.99	2.06	Training
Nadolol	2.84	0.70	1.87	1.62	1.51	2.49	Validation
Naproxen	2.56	0.59	0.74	1.40	1.52	1.78	Training
Oxcarbazepine	1.83	0.35	1.00	2.03	2.01	1.87	Training
Paraxanthine	0.08	0.35	2.24	2.17	1.56	1.22	Training
Penciclovir	2.79	1.23	2.84	2.69	2.05	1.80	Training
Pentoxyfylline	1.75	0.00	1.65	1.47	1.73	2.08	Training
PFOA	-0.03	0.83	0.33	-0.10	-0.99	1.58	Validation
Phenytoin	1.67	0.60	2.02	2.19	2.23	1.87	Validation
Progesterone	2.96	0.00	0.89	1.43	1.19	2.62	Training
Propachlor	1.46	0.00	0.52	1.54	1.16	1.66	Training
Ranitidine hcl	2.20	0.20	1.93	1.92	1.54	2.4	Training
Siduron	2.62	0.44	1.20	1.36	1.34	1.95	Training
Simazine	1.38	0.65	2.16	1.55	1.23	1.48	Training
Sulfamethoxazole	1.78	0.61	1.17	2.73	1.82	1.72	Training
Sulfathiazole	1.40	0.61	1.33	2.71	2.17	1.69	Validation
TCEP	1.21	0.00	1.83	1.91	0.51	1.76	Validation
Testosterone	2.99	0.35	0.86	1.28	1.22	2.38	Training
Tributyl_phosphate	2.63	0.00	1.85	1.44	0.13	2.24	Training
Triclosan	2.72	0.41	0.26	1.84	1.81	1.81	Training
Trimethoprim	2.61	0.65	1.84	2.88	1.95	2.18	Validation
Warfarin	2.66	0.35	1.49	2.57	2.10	2.31	Training

FIG. 96 (continued)

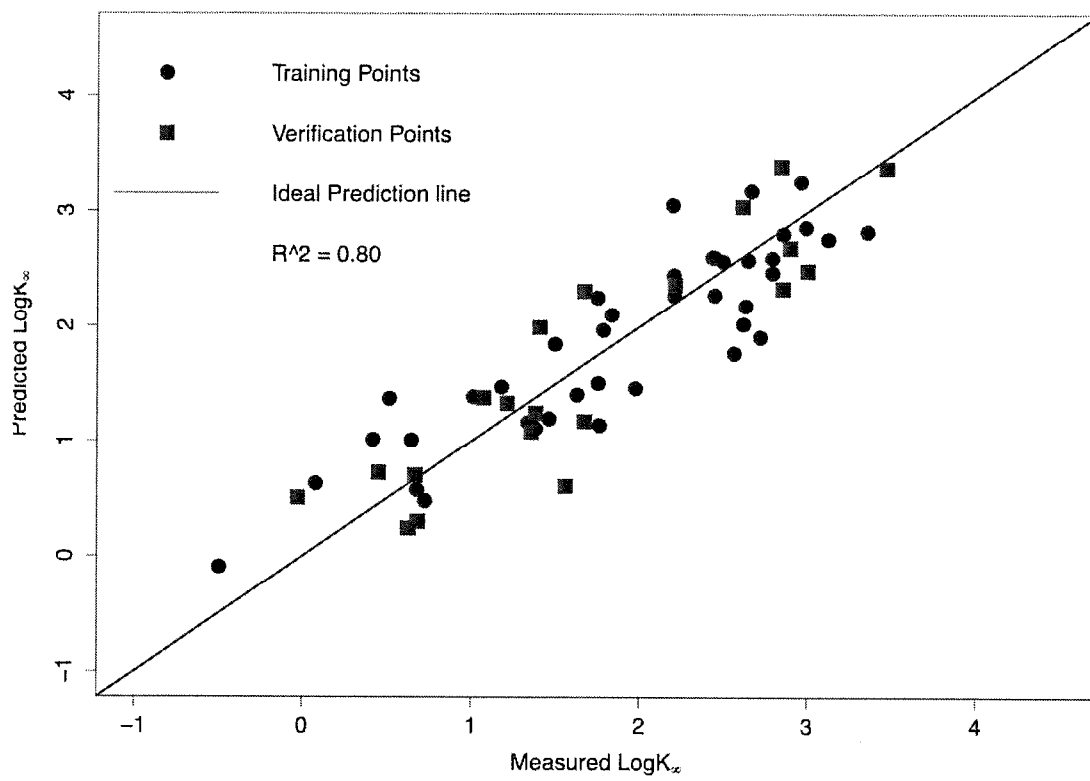


FIG. 97

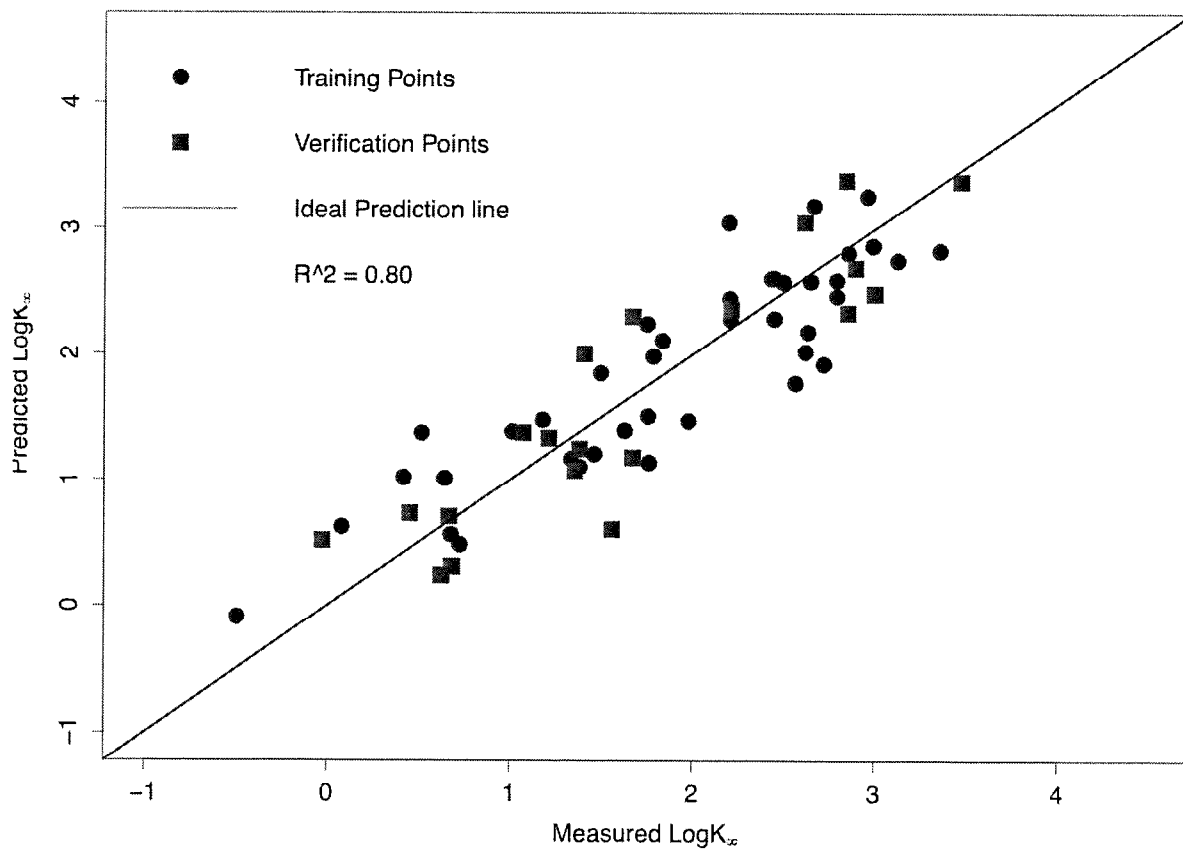


FIG. 98