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APPENDICES

APPENDIX A

DOC, UV-254, SUVA, THMFP AND SPECIFIC THMFP VALUES

Table A-1: DOC, UV-254, SUVA, THMFP and specific THMFP of the effluent water from detention pond collected in June 2004 and those of its DOM fractions

Parameter	Eff[1]. Water from detention pond	DOM fractions					
		HPON	HPOB	HPOA	HPIB	HPIA	HPIN
DOC (mg/L)	6.81±0.2	0.43±0.02	0.27±0.02	2.16±0.04	0.73±0.08	1.86±0.09	1.60±0.10
UV-254 (cm^{-1})	0.208 ±0.004	0.006 ±0.0001	0.010 ±0.001	0.035 ±0.0006	0.015 ±0.0001	0.045 ±0.0002	0.014 ±0.0004
SUVA (L/mg-m)	3.05±0.06	1.47±0.02	3.88±0.37	1.62±0.03	2.05±0.01	2.43±0.01	0.84±0.02
THMFP (µg/L)	625±4	54±2	50±6	306±6	112±2	243±6	178±9
Specific THMFP (µg THMFP/mg DOC)	90±6.7	125±5.2	190±22	142±2.9	153±2.3	130±8.8	112±5.6

Remark: [1]Eff = Effluent

Table A-2: DOC, UV-254, SUVA, THMFP and specific THMFP of industrial estate wastewater and the effluent water from aeration, facultative, oxidation and detention pond collected in September 2004

Parameter	Industrial Estate Wastewater	Eff[1]. Water from aeration ponds	Eff[1]. Water from facultative ponds	Eff[1]. Water from oxidation pond	Eff[1]. Water from detention pond
DOC (mg/L)	14.0±0.2	6.52±0.05	5.96±0.1	5.63±0.1	NA[2]
UV-254 (cm^{-1})	0.182±0.006	0.113±0.002	0.110±0.001	0.109±0.002	NA
SUVA (L/mg-m)	1.28±0.02	1.71±0.01	1.83±0.04	1.94±0.04	NA
THMFP (µg/L)	1245±44	563±33	553±35	491±29	NA
Specific THMFP (µg THMFP/mg DOC)	89±3.2	86±5.1	93±5.8	87±5.2	NA

Remark: [1]Eff = Effluent and [2]NA = Not available

Table A-3: DOC, UV-254, SUVA, THMFP and specific THMFP of industrial estate wastewater and the effluent water from aeration, facultative, oxidation and detention pond collected in October 2004

Parameter	Industrial Estate Wastewater	Eff[1]. Water from aeration ponds	Eff[1]. Water from facultative ponds	Eff[1]. Water from oxidation pond	Eff[1]. Water from detention pond
DOC (mg/L)	12.2±0.07	5.99±0.02	6.07±0.13	6.11±0.02	NA[2]
UV-254 (cm^{-1})	0.143±0.0004	0.112±0.0003	0.108±0.0001	0.106±0.0003	NA
SUVA (L/mg-m)	1.13±0.009	1.90±0.002	1.75±0.034	1.75±0.001	NA
THMFP (µg/L)	1109±39	497±12	435±13	373±21	NA
Specific THMFP (µg THMFP/mg DOC)	91±3.2	83±1.9	72±2.0	61±3.5	NA

Remark: [1]Eff = Effluent and [2]NA = Not available

Table A-4: DOC, UV-254, SUVA, THMFP and specific THMFP of industrial estate wastewater and the effluent water from aeration, facultative, oxidation and detention pond collected in February 2005

Parameter	Industrial Estate Wastewater	Eff[1]. Water from aeration ponds	Eff[1]. Water from facultative ponds	Eff[1]. Water from oxidation pond	Eff[1]. Water from detention pond
DOC (mg/L)	10.3±0.25	5.55±0.02	6.01±0.47	5.60±0.11	6.14±0.29
UV-254 (cm^{-1})	0.163±0.002	0.098±0.0003	0.112±0.007	0.100±0.003	0.112±0.005
SUVA (L/mg-m)	1.58±0.05	1.78±0.01	1.84±0.03	1.75±0.05	1.82±0.07
THMFP (μg/L)	1214±3	530±16	564±11	572±7	588±5
Specific THMFP (μg THMFP/mg DOC)	118±0.3	96±1.4	93±0.5	100±0.7	95±0.6

Remark:[1]Eff = Effluent

Table A-5: DOC, UV-254, SUVA, THMFP and specific THMFP of DOM fractions of industrial estate wastewater collected in February 2005

Parameter	DOM fractions					
	HPON	HPOB	HPOA	HPIB	HPIA	HPIN
DOC (mg/L)	1.51±0.09	0.21±0.02	2.58±0.05	1.72±0.10	1.65±0.10	2.25±0.03
UV-254 (cm^{-1})	0.021 ±0.0004	0.007 ±0.0007	0.029 ±0.0016	0.026 ±0.0015	0.027 ±0.0023	0.019 ±0.0007
SUVA (L/mg-m)	1.36±0.03	3.38±0.33	1.11±0.06	1.51±0.09	1.63±0.14	0.83±0.03
THMFP (μg/L)	141±11	18±5	371±18	115±18	148±8	95±1
Specific THMFP (μg THMFP/mg DOC)	93±8.5	86±14.7	144±5.9	67±9.0	90±4.2	42±0.2

Table A-6: DOC, UV-254, SUVA, THMFP and specific THMFP of DOM fractions of the effluent water from aeration ponds collected in February 2005

Parameter	DOM fractions					
	HPON	HPOB	HPOA	HPIB	HPIA	HPIN
DOC (mg/L)	0.59±0.09	0.12±0.01	1.72±0.03	0.91±0.01	1.14±0.05	1.63±0.05
UV-254 (cm^{-1})	0.011 ±0.0007	0.002 ±0.0007	0.021 ±0.0003	0.012 ±0.0004	0.014 ±0.0011	0.005 ±0.0010
SUVA (L/mg-m)	1.87±0.12	2.02±0.30	1.22±0.02	1.29±0.04	1.23±0.10	0.29±0.06
THMFP (μg/L)	70±6	15±3	218±13	60±4	108±13	66±6
Specific THMFP (μg THMFP/mg DOC)	119±9.0	124±48.2	127±1.6	65±2.6	95±7.8	40±3.9

Table A-7: DOC, UV-254, SUVA, THMFP and specific THMFP of DOM fractions of the effluent water from facultative ponds collected in February 2005

Parameter	DOM fractions					
	HPON	HPOB	HPOA	HPIB	HPIA	HPIN
DOC (mg/L)	0.43±0.03	0.10±0.01	2.80±0.05	0.63±0.04	1.27±0.05	1.24±0.06
UV-254 (cm^{-1})	0.010 ±0.0009	0.002 ±0.0004	0.046 ±0.0002	0.013 ±0.0005	0.023 ±0.0033	0.005 ±0.0005
SUVA (L/mg-m)	2.35±0.20	2.87±0.58	1.63±0.01	2.04±0.07	1.80±0.26	0.41±0.02
THMFP (μg/L)	54±8	10±2	262±15	38±3	171±24	48±4
Specific THMFP (μg THMFP/mg DOC)	125±17.0	142±42.2	93±6.3	60±3.2	141±16.9	39±3.3

Table A-8: DOC, UV-254, SUVA, THMFP and specific THMFP of DOM fractions of the effluent water from oxidation ponds collected in February 2005

Parameter	DOM fractions					
	HPON	HPOB	HPOA	HPIB	HPIA	HPIN
DOC (mg/L)	0.41±0.06	0.10±0.01	2.10±0.05	0.71±0.05	1.46±0.03	1.24±0.05
UV-254 (cm^{-1})	0.009 ±0.0002	0.002 ±0.0008	0.034 ±0.0013	0.012 ±0.0013	0.018 ±0.0002	0.004 ±0.0003
SUVA (L/mg-m)	2.09±0.06	2.08±0.35	1.61±0.06	1.74±0.19	1.23±0.01	0.29±0.02
THMFP (μg/L)	50±8	15±2	244±24	50±6	174±4	59±3
Specific THMFP (μg THMFP/mg DOC)	122±18.3	142±34.2	116±13.9	71±19.4	119±2.4	47±2.0

Table A-9: DOC, UV-254, SUVA, THMFP and specific THMFP of DOM fractions of the effluent water from detention pond collected in February 2005

Parameter	DOM fractions					
	HPON	HPOB	HPOA	HPIB	HPIA	HPIN
DOC (mg/L)	0.45±0.06	0.10±0.03	2.62±0.12	0.74±0.10	1.52±0.07	1.11±0.05
UV-254 (cm^{-1})	0.007 ±0.0044	0.001 ±0.00005	0.043 ±0.0001	0.011 ±0.00005	0.018 ±0.0007	0.003 ±0.0002
SUVA (L/mg-m)	1.64±0.05	1.40±0.05	1.62±0.005	1.48±0.01	1.17±0.04	0.27±0.01
THMFP (μg/L)	45±7	12±1	273±3	48±6	192±6	50±5
Specific THMFP (μg THMFP/mg DOC)	96±8.9	120±4.7	104±0.9	63±4.8	131±1.5	47±3.1

Table A-10: DOC, UV-254, SUVA, THMFP and specific THMFP of industrial estate wastewater and the effluent water from aeration, facultative, oxidation and detention pond collected in July 2005

Parameter	Industrial Estate Wastewater	Eff[1]. Water from aeration ponds	Eff[1]. Water from facultative ponds	Eff[1]. Water from oxidation pond	Eff[1]. Water from detention pond
DOC (mg/L)	14.9±0.7	5.64±0.13	5.78±0.15	5.71±0.25	5.37±0.05
UV-254 (cm^{-1})	0.171±0.002	0.119±0.001	0.120±0.004	0.113±0.002	0.124±0.017
SUVA (L/mg-m)	1.16±0.06	2.09±0.05	2.12±0.07	1.97±0.05	2.31±0.018
THMFP (μg/L)	1351±21	[2]NA	NA	468±3.5	NA
Specific THMFP (μg THMFP/mg DOC)	91±1.4	NA	NA	82±0.6	NA

Remark: [1]Eff = Effluent and [2]NA = Not available

APPENDIX B

INDENTIFICATION OF PYROLYSIS FRAGMANTS, DETAIL OF PYROLYSIS FRAGMENTS AND PYROCHROMATOGRAM OF ALL WATER SAMPLES

Identification of Pyrolysis Fragments

1. Open the data file obtained from the pyrolysis GC/MS using the GC/MS Postrun analysis program. Figure B-1 shows the output of pyrochromatograms of the HPOA fraction of the aeration pond effluent.

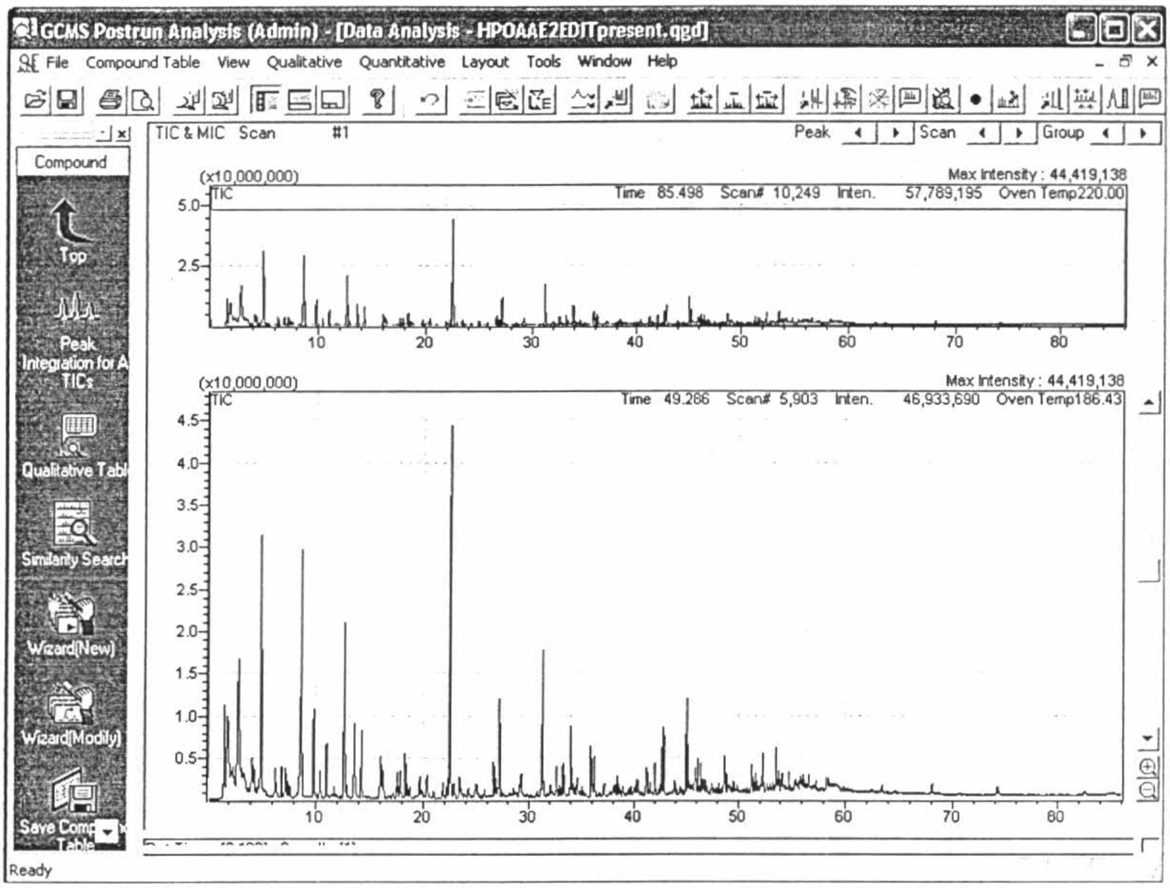

Figure B-1 The output of pyrochromatograms of the HPOA fraction of the aeration pond effluent

2. Integrate the pyrochromatograms of the HPOA fraction of the aeration pond effluent. The result is shown in Figure B-2.

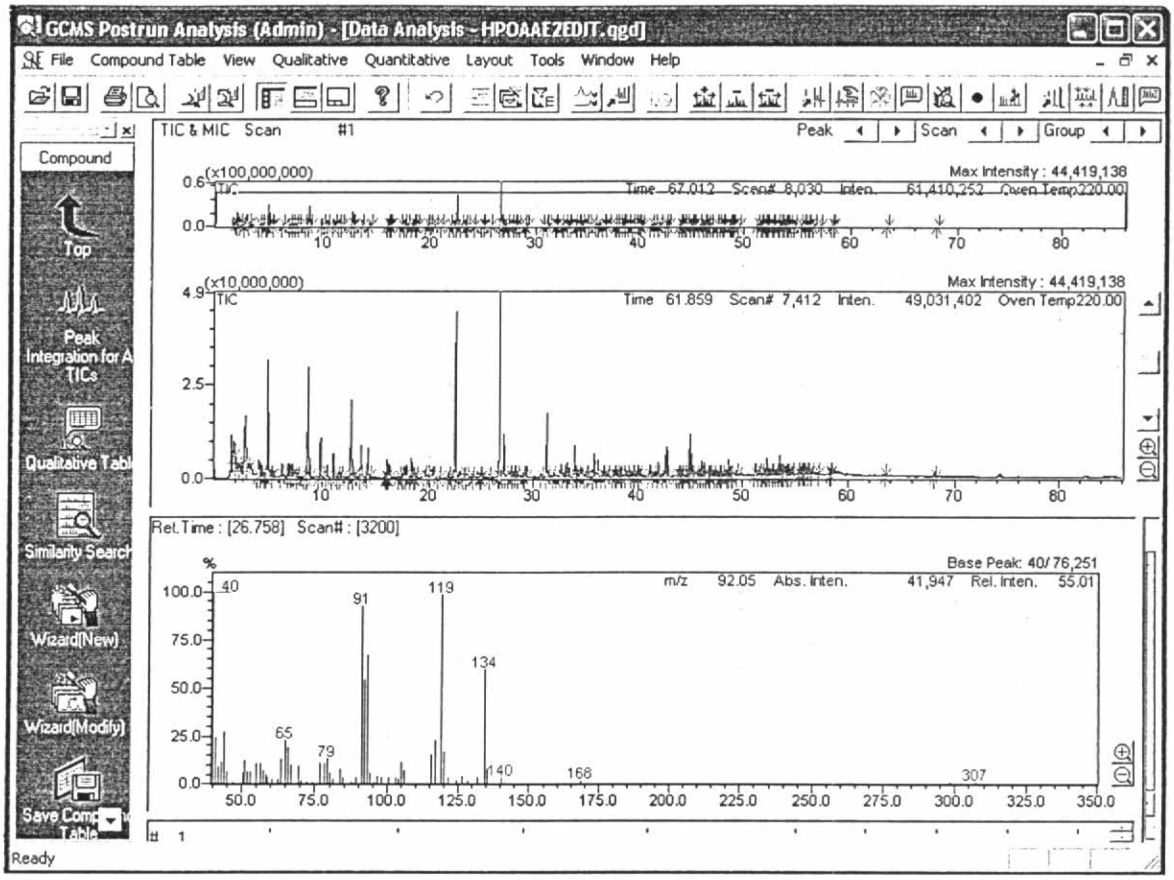

Figure B-2 The output of integrated pyrochromatograms of the HPOA fraction of the aeration pond effluent

3. Open the qualitative table and select the pyrolysis peak (pyrolysis fragment). Figure B-3 shows the outcome of pyrochromatograms of the HPOA fraction of the aeration pond effluent after selecting the pyrolysis peak

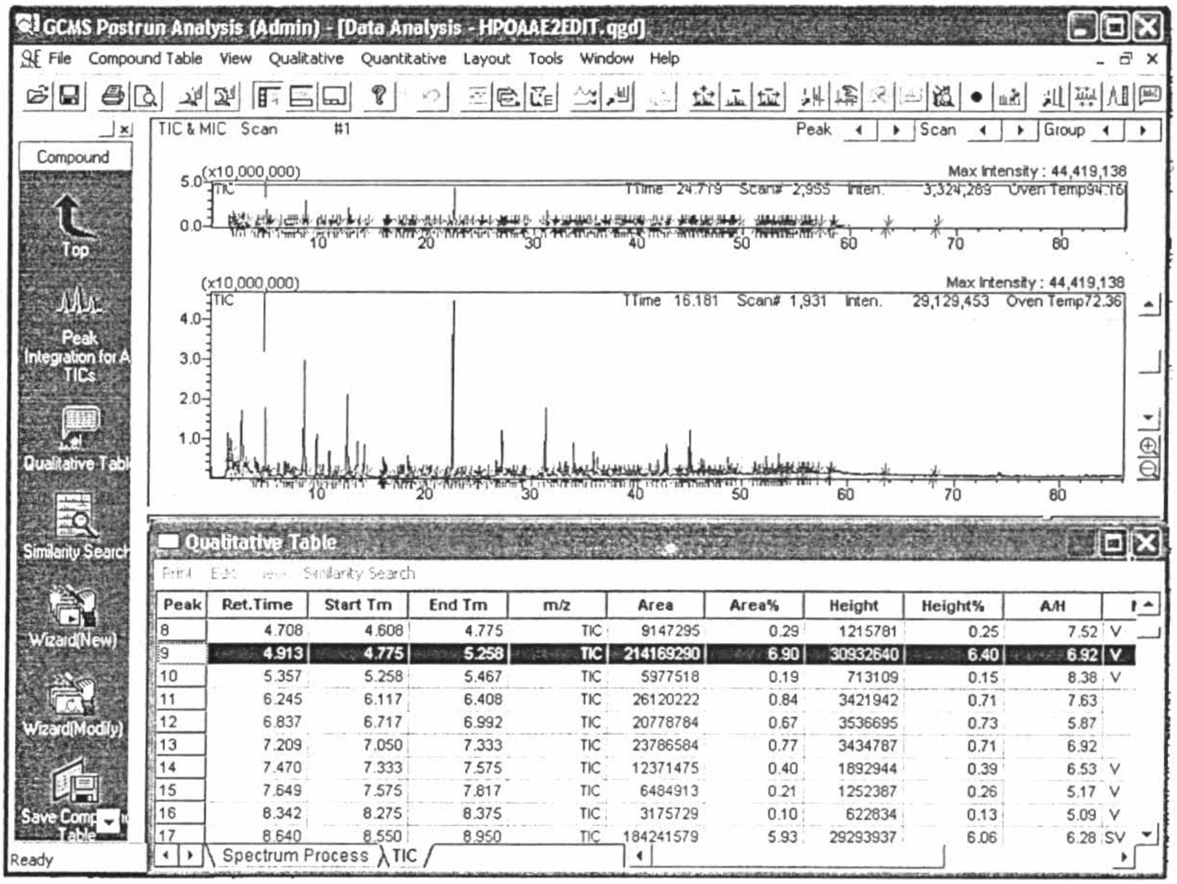

Figure B-3 The outcome of pyrochromatograms of the HPOA fraction of the aeration pond effluent after selecting the pyrolysis peak

4. Choose the similarity search icon. Figure B-4 shows the similarity search results of the selected pyrolysis peak (pyrolysis fragment). As can be seen, the results provide the list of possible compound names with their matching percentage from high to low, molecular weight, mass spectra and chemical structure. When the matching percentage was less than 85%, the pyrolysis fragment was defined as an unknown fragment. In the case of a 85% ≤ matching percentage of a pyrolysis fragment ≤ 90%, the pyrolysis fragment was defined as an acceptable match fragment, whereas, in the case of a matching percentage of a pyrolysis fragment > 90%, the pyrolysis fragment was defined as a satisfactory match fragment

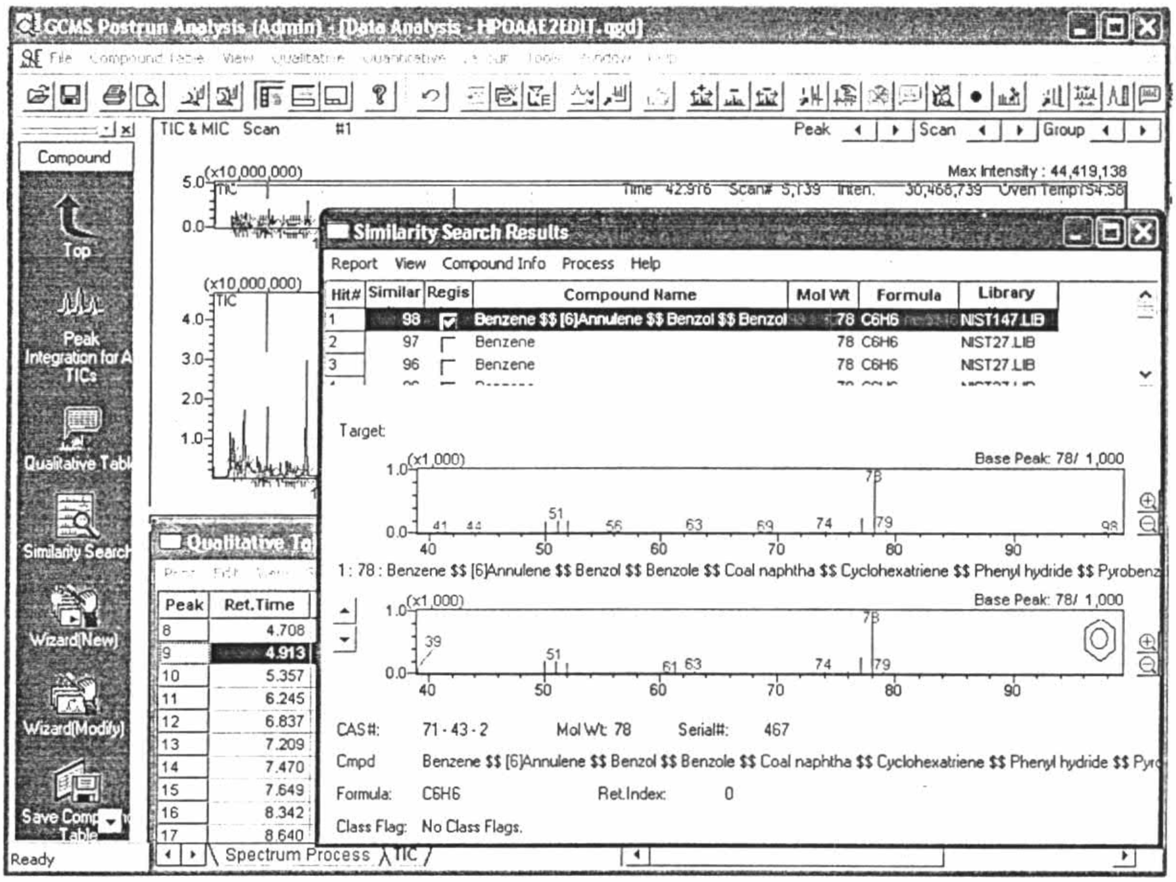

Figure B-4 The similarity search results of the selected pyrolysis peak of the HPOA fraction of the aeration pond effluent

Detail of Pyrolysis Fragment

Table B-1: Average relative ratios of the pyrolysis fragment in influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds

Chemical Classes	Important fragment	Average relative ratio				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AL[3]	*Propene	2.45				
AL	*2-Butene	2.55	1.70			
AL	*1-Pentene	2.47	4.19			1.79
AL	*1,3-Pentadiene	0.29				
AL	1-Pentene, 4-methyl				4.82	3.04
AL	*1-Hexene	3.48	4.28			
AL	Cyclohexene	0.73	0.56			
AL	2,4-Hexadiyne					5.61
AL	*1-Heptene	3.52	5.03	2.93	3.62	
AL	*___1-Octene___	2.38	2.40	1.86	3.10	1.60
AL	1,3-Octadiene					0.10
AL	*___1-Nonene___	2.16	2.57	2.68	2.51	1.42
AL	*___1-Decene___	2.06	2.01	1.33	2.11	1.03
AL	5-Decyne					0.11
AL	*___1-Undecene___	1.85	1.72	1.21	1.84	0.75
AL	1,4 Undecadiene	0.20	0.26			0.12
AL	*1-Dodecene	1.81	1.76	0.79		0.62
AL	2-Dodecene	0.20			1.52	
AL	3-Dodecene	0.51				
AL	6-Dodecyne	0.37	0.43			0.11
AL	Undecene, 5-methyl-	0.19				
AL	2,4-Dodecadiene, (E,Z)	0.22				
AL	2-Butyl-1-decene	0.23				
AL	*1-Tridecene	2.04	1.70		1.58	0.79
AL	*Z-1,6 Tridecadiene	0.44	0.38			0.14
AL	*___1-Tetradecene___	1.95	2.05	0.67	1.86	0.81
AL	*Cyclotetradecane	0.12				
AL	*7-Tetradecyne	0.28				
AL	*___1-Pentadecene___	2.02	2.25	0.81	2.14	1.45
AL	*3-Hexadecene	0.14				
AL	Cyclopentene,1-hexy		0.39			
AL	3-Hexadecyne	0.37				0.27
AL	Cyclopentene, 1-octyl	0.38	0.53			0.38
AL	Cyclohexene, 3-nonyl	0.19				0.17
AL	Cyclotetradecane		0.79			
AL	*1-Heptadecene	0.51	0.89			0.46
AL	*Cyclohexadecane	0.55				
AL	*1-Nonadecene		0.99			0.29
AL	10-Methyl-octadec-1-ene	0.26				
AL	Octadecane, 2-methyl			1.43		
AL	*9-Eicosene, (E)	0.69				

Table B-1: Average relative ratios of the pyrolysis fragment in influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AL	*Nonadecane, 2-methyl			2.73		
AL	*Eicosane			2.82	3.01	
AL	*Eicosane 10 methyl			2.74	4.00	
AL	*Tricosane			2.21		
AR[4]	***Toluene***	1.00	1.00	1.00	1.00	1.00
AR	*p-Xylene	0.54				
AR	***Styrene***	0.53	0.72	0.81	0.80	0.40
AR	*Benzene, propyl	0.13				0.11
AR	*Benzene, butyl					
AR	*Benzene, pentyl-					0.11
AR	*Naphthalene	0.13	0.19			0.19
AR	*Benzene, heptyl					0.10
AR	*Benzene, octyl-					0.20
AR	*Benzene, nonyl	0.11	0.23			0.29
PN[5]	*Phenol	0.34		1.93	0.89	0.45
PN	*Phenol, 4-methyl	0.41			0.23	
PN	.alpha.,.alpha.'-Dihydroxy-m-diisopropylbenzene			2.46		
PN	Benzeneethanol, .alpha.-methyl-3-(1-methylethyl)			7.08		
PN	*Phenol, 4-(1,1,3,3-tetramethylbutyl)	0.29				
ON[6]	Ethylamine				1.47	
ON	*Acetronitrile			0.82		
ON	*Isobutyronitrile			2.12		
ON	Butanenitrile	0.13	0.25	0.51		
ON	***Butanenitrile, 2-methyl***	0.10	0.62	0.40	0.26	0.15
ON	***Butanenitrile, 3-methyl***	0.23	0.46	0.85	0.42	0.34
ON	*Pyrrole	0.33		1.27	0.75	0.19
ON	1H-Pyrazole, 3-methyl			0.87		
ON	*1H-Pyrrole, 2-methyl			0.38		
ON	*1H-Pyrrole, 3-methyl			0.37		
ON	*Pentanenitrile, 4-methyl	0.23		0.68		0.13
ON	*Acetamide			4.20		
ON	*Benzonitrile			2.31		0.46
ON	Octanenitrile		0.32	0.31		
ON	Benzenepropanenitrile		0.19			
ON	Nonanenitrile		0.23			
ON	*Indole	0.49				
ON	*Decanenitrile		0.42			
ON	*Undecanenitrile		0.42			
ON	*Dodecanenitrile		2.16	0.62		
ON	*Tridecanenitrile		1.89		0.91	
ON	Tetradecanenitrile			0.74		0.20

Table B-1: Average relative ratios of the pyrolysis fragment in influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
ON	*Pentadecanenitrile		8.48		1.34	
ON	Hexadecanenitrile		0.47	1.82	1.53	0.40
ON	****Heptadecanenitrile***	0.57	2.01	1.25	1.42	0.59
ON	Octadecanenitrile		4.61			
AH[7]	*Acetaldehyde					2.80
AH	*Furfural			0.66		
AH	Heptanal					0.15
AH	Benzaldehyde					0.29
AH	*Octanal					0.12
AH	Nonanal					0.11
AH	Decanal			0.39		0.18
AH	*E-14-Hexadecenal					0.43
AH	E-15-Heptadecenal					0.33
AH	Octadecanal					0.55
KT[8]	*2-Pentadecanone	0.21				
KT	*2-Hexadecanone	0.11				
KT	*2-Heptadecanone	0.31				
AC[9]	*1-Hexanol, 2-ethyl	1.21	3.28		1.53	
AC	1-Decanol, 2-methyl	0.15				
AC	2-Methyl-1-undecanol	0.18				
AC	3-Dodecen-1-ol	0.24				
AC	* 1-Octanol, 2-butyl	0.13				
AC	*1-Decanol, 2-hexyl	0.53				
AC	*9-Tetradecen-1-ol	0.27	1.12			0.44
AC	1-Hexadecanol, 2-methyl	0.45				
CA[10]	Acetic acid					1.81
CA	*Tetradecanoic acid			4.18		0.66
CA	*n-Hexadecanoic acid					2.75
OT[11]	****Cyclotrisiloxane, hexamethyl***	0.82	1.39	3.77	1.38	0.20
OT	Cyclotetrasiloxane, octamethyl		0.79			
OT	Silane, tetramethyl-			9.84		
	Sum of relative ratio of AL	37.64	36.88	24.21	32.11	21.06
	Sum of relative ratio of AR	2.44	2.14	1.81	1.80	2.41
	Sum of relative ratio of PN	1.04	0.00	11.46	1.12	0.45
	Sum of relative ratio of ON	2.08	22.53	19.52	8.08	2.46
	Sum of relative ratio of AH and KT	0.63	0.00	1.05	0.00	4.97
	Sum of relative ratio of OT	3.98	6.58	17.79	2.91	5.86
	Total unknown	6.19	17.62	21.44	9.6	7.13
	Sum of relative ratio	53.99	85.75	97.28	55.62	44.34

Remark: [1]Inf = Influent and [2]Eff. = Effluent, [3]AL= aliphatic hydrocarbon, [4]AR = aromatic hydrocarbon, [5]PN =phenol, [6]ON = organic nitrogen, [7]AH = aldehydes, [8]KT = ketones, [9]AC = alcohol, [10]CA = carboxylic acids and [12]OT = others. The pyrolysis fragments that have a average relative ratio more than 0.2 were identified as the major pyrolysis fragments in the samples, Common fragments = Italic bold letter.

Table B-2: Average relative ratio of the pyrolysis fragment in HPON of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds

Chemical Classes	Important fragment	Average relative ratio of HPON				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AL3	****Propene***	1.03	2.31	0.83	0.21	0.63
AL	****2-Butene***	0.62	1.08	0.95	0.30	0.50
AL	*1-Pentene	0.95	0.66	0.44		0.98
AL	*1,3-Cyclopentadiene					0.88
AL	Cyclobutane			1.28		
AL	*1-Hexene	0.89			0.32	1.32
AL	Cyclohexene					0.12
AL	2,4-Hexadiyne		1.73			
AL	*1-Heptene	1.74				
AL	*1,3-Pentadiene, 2,4-dimethyl				0.11	
AL	2,4-Hexadiene, 2-methyl	0.12	0.16			
AL	1,3,5-Heptatriene					0.13
AL	****1-Octene***	0.49	0.34	0.28	0.26	1.24
AL	****1-Nonene***					1.34
AL	****1-Decene***	0.32	0.39	0.38	0.33	1.13
AL	****1-Undecene***	0.28	0.34	0.24	0.47	0.89
AL	2,6-Octadiene, 2,7-dimethyl			0.16		
AL	1,4 Undecadiene					0.12
AL	*1-Dodecene		0.36	0.24		0.75
AL	2-Dodecene	0.26				
AL	6-Dodecyne					0.20
AL	2,4-Dodecadiene, (E,Z)					0.11
AL	*1-Tridecene					0.84
AL	*Z-1,6 Tridecadiene					0.19
AL	*1-Tetradecene					0.89
AL	2,6-Octadiene, 4-methy			0.10		
AL	*7-Tetradecyne					0.22
AL	*1-Pentadecene	0.42				1.04
AL	3-Hexadecyne					0.29
AL	*1-Heptadecene					0.55
AR[4]	*Benzene			1.42	0.88	2.60
AR	****Toluene***	1.00	1.00	1.00	1.00	1.00
AR	*Ethylbenzene	0.94	0.82	0.67	0.65	
AR	****p-Xylene***	0.61	0.31	0.31	0.30	0.24
AR	Benzene, 1,3-dimethy			0.12		
AR	o-xylene		0.24		0.12	0.13
AR	****Styrene***	0.47	0.48	0.28	0.27	0.29
AR	****Benzene, (1-methylethyl)***	0.25	0.22	0.17	0.16	0.10
AR	****Benzene, propyl***	0.58	0.33	0.20	0.28	0.15
AR	Benzene, 1-ethyl-2-methyl					0.10
AR	****.alpha.-Methylstyrene***	0.60	0.43	0.32	0.38	0.22

Table B-2: Average relative ratio of the pyrolysis fragment in HPON of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPON				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AR	*Benzene, 1-ethenyl-2-methyl		0.10			
AR	*Indane	0.16				
AR	*Benzene, butyl	0.82	0.23			
AR	*Benzene, (1-methylenepropyl)	0.31				
AR	*Indene		0.22			
AR	*Benzene, (2-methyl-1-propenyl)	0.11				
AR	*Benzene, 1-ethenyl-3-ethyl	0.15	0.14			
AR	*Benzene, (1-methylenebutyl)	0.39	0.25			
AR	****Benzene, pentyl***	0.76	0.30	0.13	0.14	0.10
AR	Benzene, (1-methylpentyl)	0.36	0.14			
AR	****Naphthalene***	0.11	0.23	0.15	0.13	0.11
AR	*Benzene, (1-methylenepentyl)	0.67	0.15			
AR	*Benzene, hexyl	1.03				
AR	Benzene, (1-methylhexyl)	0.27				
AR	Benzene, (3-methyl-1-methylenepentyl)	0.55				
AR	Hex-1-enylbenzene	0.20				
AR	Naphthalene, 1-methyl	0.26	0.27			
AR	Naphthalene, 2-methyl		0.32		0.17	
AR	*Benzene, heptyl	0.73				0.11
AR	*Benzene, (1-methylheptyl)	0.19				
AR	*Biphenyl	0.36	0.50	0.13		0.17
AR	Benzene, (1-methylenepentyl)	0.65				
AR	Benzene, 2-heptenyl	0.21				
AR	*Indole	0.70	0.70			
AR	*Benzene, octyl-	0.58				0.26
AR	*Benzene, (1-butylhexyl)	1.74				
AR	*Benzene, (1-propylheptyl)	1.36				
AR	*Benzene, (1-ethyloctyl)	1.12				
AR	*Benzene, nonyl	0.43				0.28
AR	*Benzene, (1-methylnonyl)	0.51				
AR	Naphthalene, 2-(1-methylethyl)		0.37			
AR	Naphthalene, 2-methyl-1-propyl		0.95	0.63	0.42	0.19
AR	*Benzene, (1-pentylhexyl)	1.96	0.52	0.14	0.21	
AR	Benzene, (1-butylheptyl)	3.48	0.89	0.34	0.47	
AR	*Benzene, (1-propyloctyl)	2.43	0.77	0.27	0.33	
AR	*Benzene, (1-ethylnonyl)	1.67	1.30	0.56	0.69	
AR	*Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis	0.50				
AR	Benzene, (1-methyldecyl)	0.53	1.34		0.52	
AR	****Benzene, (1-pentylheptyl)***	2.54	1.24	0.26	0.47	0.10
AR	****Benzene, (1-butyloctyl)***	2.08	1.09	0.26	0.52	0.32
AR	****Benzene, (1-propylnonyl)***	1.24	1.29	0.89	0.51	0.31

Table B-2: Average relative ratio of the pyrolysis fragment in HPON of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPON				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AR	Benzene, (1-pentyloctyl)	1.20	1.31		0.66	0.62
AR	Benzene, (1-butylnonyl)	0.82			0.70	0.32
AR	Benzene, (1-propyldecyl)	0.42			0.56	0.33
PN[5]	***Phenol***	0.47	1.76	0.86	0.89	0.36
PN	***Phenol, 2-methyl***	0.15	0.77	0.27	0.39	0.11
PN	Phenol, 2,5-dimethyl-		0.13			
PN	***Phenol, 4-methyl***	0.40	0.53	0.24	0.34	0.23
PN	*Phenol, 2-ethyl		0.14			
PN	***Phenol, 2,4-dimethyl***	0.21	0.47	0.14	0.27	0.18
PN	*Phenol, 4-ethyl	0.11	0.34		0.17	
PN	*Phenol, 4-(1-methylethyl)		2.19	0.59	0.71	
PN	*Phenol, 2-methyl-5-(1-methylethyl)		0.36			
PN	Phenol, p-tert-butyl		0.31			
PN	*Phenol, 4-(1-methylpropyl)		0.59	0.29	0.32	
PN	p-Isopropenylphenol		2.55			
PN	2-Allyl-4-methylphenol			0.26		
PN	Phenol, 2-methyl-6-(2-propenyl)		0.75			
PN	Phenol, 2-(2-methyl-2-propenyl)				0.36	
PN	.alpha.,.alpha.'-Dihydroxy-m-diisopropylbenzene		0.56			
PN	***Phenol, 4-(1,1,3,3-tetramethylbutyl)***	1.03	3.68	0.79	0.78	0.38
PN	*Phenol, 4-(1-methyl-1-phenylethyl)	1.54	3.62	0.57		
ON[6]	*Acetronitrile	0.35				0.82
ON	2-Propenenitrile					0.74
ON	*Butanenitrile, 2-methyl-	0.12				
ON	*Butanenitrile, 3-methyl	0.17	0.16	0.19		0.29
ON	***Pyrrole***	0.98	0.26	0.30	0.24	0.33
ON	1H-Pyrazole, 3-methyl-	0.15		0.17	0.16	
ON	*1H-Pyrrole, 2-methyl-	0.15				
ON	*1H-Pyrrole, 3-methyl-	0.30				
ON	*Pentanenitrile, 4-methyl	0.11				0.13
ON	*Acetamide	0.13	0.34	0.15	0.38	
ON	1H-Pyrrole, 3-ethyl	0.26				
ON	*Aniline			1.08	0.71	0.63
ON	*Pyridine, 3-methyl	0.14	0.70			
ON	*Benzonitrile		0.32	0.24		
ON	*2H-Benzotriazole, 2-methyl		0.58	0.21	0.31	0.10
ON	6-Quinoxalinamine		0.22			0.50
ON	*Pentanedinitrile					0.36
ON	*Pentanedinitrile, 2-methy					0.18
ON	Benzenepropanenitrile	0.14				0.10
ON	*1H-Pyrrole-2-carbonitrile	0.26				

Table B-2: Average relative ratio of the pyrolysis fragment in HPON of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPON				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
ON	1H-Benzotriazole, 1-ethenyl-		0.77		0.33	
ON	*1H-Benzotriazole, 1-methyl		3.10	1.02	1.33	
ON	*Undecanenitrile	0.91				
ON	*Dodecanenitrile	1.34				
ON	*Benzonitrile, 2-hydroxy		0.89			
ON	Dodecanamide		1.93			
ON	*Heptadecanenitrile			0.11		0.25
AH7	*Butanal, 2-methylene-				0.45	0.12
AH	*2-Pentenal, (E)	0.15	1.30	0.42		
KT8	Acetone	0.71				
KT	*2-Butanone	0.49				
KT	*2-Pentanone	0.18				
KT	*2-Propanone, 1-hydroxy				0.13	
KT	2,3-Hexanedione			0.22	0.14	
KT	3-Penten-2-one, (E)-			0.14		
KT	*Cyclopentanone					0.11
KT	*2-Cyclopenten-1-one, 2-methyl-				0.21	
KT	*2-Octanone	0.15				
KT	*Methanone, dicyclopropyl-				0.72	
KT	2-Cyclopenten-1-one, 3,4-dimethyl	0.29				
KT	Acetophenone			0.18		0.1
KT	2-Cyclohexen-1-one, 3,5,5-trimethyl			0.17		0.12
KT	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	0.18		0.23	0.26	0.12
KT	*2-Heptadecanone					0.23
AC[9]	2-Hexen-1-ol, (E)		0.27			0.16
AC	*1-Hexanol, 2-ethyl	0.57				1.63
AC	*Cyclopentanol		0.44			
AC	3-Dodecen-1-ol					0.25
AC	* 1-Octanol, 2-butyl		0.53	0.29	0.51	
AC	*9-Tetradecen-1-ol					0.23
AC	1-Naphthalenol		1.00			
CA[10]	*Tetradecanoic acid		1.16			
CA	*n-Hexadecanoic acid		1.61			

Table B-2: Average relative ratio of the pyrolysis fragment in HPON of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPON				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
ES[11]	2-Propenoic acid, 2-methyl ester		7.40	6.20	4.43	1.92
ES	2-Propenoic acid, 2-methyl-, oxiranylmethyl ester		1.84		0.50	
ES	2-Propenoic acid, 2-methyl-, 2-ethyl-2-[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl ester		8.48	2.50	3.02	
OT[12]	****Cyclotrisiloxane, hexamethyl***	1.17	1.99	1.48	0.91	1.28
OT	Cyclotetrasiloxane, octamethyl-	0.34	0.75	0.33	0.26	
OT	Benzofuran, 2,3-dihydro-2-methyl			0.71		
	Sum of relative ratio of AL	7.11	7.37	4.90	2.01	14.34
	Sum of relative ratio of AR	38.06	18.47	8.27	10.55	8.06
	Sum of relative ratio of PN	3.91	18.75	4.01	4.23	1.26
	Sum of relative ratio of ON	5.51	9.28	3.44	3.45	4.42
	Sum of relative ratio of AH and KT	2.16	1.30	1.35	1.91	0.79
	Sum of relative ratio of OT	2.07	27.57	11.51	9.62	5.47
	Total unknown	10.3	16.37	7.54	7.9	6.44
	Sum of relative ratio	69.14	99.12	41.01	39.68	40.77

Remark: [1]Inf = Influent and [2]Eff. = Effluent, [3]AL= aliphatic hydrocarbon, [4]AR = aromatic hydrocarbon, [5]PN =phenol, [6]ON = organic nitrogen, [7]AH = aldehydes, [8]KT = ketones, [9]AC = alcohol, [10]CA = carboxylic acids , [11]ES = Ester and [12]OT = others, Common fragments = Italic bold letter.

Table B-3: Average relative ratio of the pyrolysis fragment in the HPOB fraction of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds

Chemical Classes	Important fragment	Average relative ratio of HPOB				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AL[3]	*1-Pentene	0.63				
AL	*1-Hexene	0.60				
AL	2,4-Hexadiene	1.10	1.48		2.95	
AL	2,4-Hexadiyne					0.78
AL	*1-Heptene	0.98				
AL	Hexane, 2-methyl-4-methylene	0.25				
AL	*1-Octene	0.36		0.52	0.57	0.36
AL	*1-Nonene	0.36		0.68	0.82	0.41
AL	*1-Decene	0.34		0.60	1.23	0.29
AL	*1-Undecene	0.25		0.31	0.57	0.15
AL	*1-Dodecene	0.20		0.32	0.59	0.16
AL	*1-Tridecene	0.25			0.49	0.15
AL	*1-Tetradecene			0.29	0.54	0.20
AL	*1-Pentadecene	0.38		0.28	0.51	
AL	3-Hexadecyne					0.14
AL	*1-Heptadecene	0.52				
AL	*1-Nonadecene	0.13	0.33		0.39	
AL	*Nonadecane, 2-methyl		0.56			
AL	*Eicosane	0.27	1.39			
AL	*Eicosane, 2-methyl-	0.28				
AL	Heneicosane		0.42			
AR[4]	*Benzene			3.71		
AR	****Toluene***	1.00	1.00	1.00	1.00	1.00
AR	*Ethylbenzene					
AR	****p-Xylene***	0.12	0.13	0.30	0.12	0.12
AR	Benzene, 1,3-dimethy					
AR	****Styrene***	0.22	0.26	1.23	0.63	0.27
AR	*.alpha.-Methylstyrene			0.30		
AR	**Naphthalene*	0.10	0.24	0.16	0.18	0.10
AR	Naphthalene, 1-methyl		0.12			
AR	*Biphenyl		0.15			
PN[5]	****Phenol***	0.57	1.51	0.77	1.93	0.94
PN	*Phenol, 2-methyl	0.10	0.31		0.45	0.23
PN	*Phenol, 4-methyl	0.40	0.53		0.32	
ON[6]	Ethylamine			1.56		
ON	*Acetronitrile	0.66	0.58	1.31		
ON	*Pyridine	0.20				
ON	*Butanenitrile, 3-methyl	0.15		0.35	0.21	0.16
ON	*Pyrrole	0.49		0.45		

Table B-3: Average relative ratio of the pyrolysis fragment in the HPOB fraction of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPOB				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
ON	*1H-Pyrrole, 3-methyl	0.22		0.20		
ON	*Pentanenitrile, 4-methyl	0.14				
ON	*Acetamide	0.89				
ON	1H-Pyrrole, 3-ethyl	0.21				
ON	*Benzonitrile		0.19		0.26	
ON	Benzenepropanenitrile		0.16			
ON	1H-Pyrrole-2-carbonitrile		0.13			
ON	*Indole	0.17				
ON	1H-Indole, 2,3-dimethy	0.10				
ON	1H-Indole, 1,2,3-trimethyl-	0.25				
ON	*1H-Isoindole-1,3(2H)-dione		0.49			
ON	*1H-Benzotriazole		1.62		1.63	
ON	*Tridecanenitrile			0.20		
ON	*Pentadecanenitrile			0.28		
ON	*Heptadecanenitrile	0.23	0.35	0.93	0.25	
AH[7]	Butanal, 3-methyl			0.11		
AH	****Furfural***	0.46	1.34	0.46	0.20	0.31
AH	*Octanal		3.17	0.78		
AH	*2-Furancarboxaldehyde, 5-methyl	1.29			0.62	0.51
AH	*E-14-Hexadecenal	0.17				0.22
AH	E-15-Heptadecenal				0.42	0.19
KT[8]	*2,3-Butanedione			1.27		
KT	****Cyclopentanone***	0.12	0.17	0.38	0.86	0.24
KT	*2-Cyclopenten-1-one	0.29			0.36	0.13
KT	*2-Cyclopenten-1-one, 2-methyl-		0.16			
KT	*Ethanone, 1-(2-furanyl)		0.44			
KT	Cycloheptanone				0.18	
KT	1H-Isoindole-1,3(2H)-dione			0.16		
KT	*2-Heptadecanone	0.13				
AC[9]	*1-Butanol			0.90		
AC	*1-Hexanol, 2-ethyl	0.32				
CA[10]	*Formic acid		0.61			
CA	*Acetic acid		3.30		1.70	1.58
CA	*Propanoic acid		0.26			0.16
CA	*Hexanoic acid				0.18	
CA	*Benzoic Acid		0.60		0.42	0.52
CA	Nonanoic acid				0.15	
CA	*n-Decanoic acid				0.29	
CA	*1,2-Benzenedicarboxylic acid		0.25			
CA	*Benzoylformic acid					0.20
CA	Dodecanoic acid		0.38	0.21	0.62	0.36

Table B-3: Average relative ratio of the pyrolysis fragment in the HPOB fraction of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPOB				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
CA	*Tetradecanoic acid		1.92	2.63	2.11	4.73
CA	*Pentadecanoic acid		0.83	1.27	0.51	3.60
CA	*n-Hexadecanoic acid		3.64	6.81	6.42	7.25
CA	*Heptadecanoic acid					22.44
OT	*Methane, chloro	1.33				
OT[11]	****Cyclotrisiloxane, hexamethyl***	0.46	5.49	0.34	0.52	0.81
OT	Cyclotetrasiloxane, octamethyl	0.12	0.43			
OT	*Dodecane, 1-chloro-					0.15
OT	*Phthalic anhydride				0.82	0.11
OT	Tetradecane, 1-chloro					0.20
	Sum of relative ratio of AL	6.90	4.19	3.00	8.67	2.65
	Sum of relative ratio of AR	1.44	1.90	6.69	1.93	1.49
	Sum of relative ratio of PN	1.07	2.36	0.77	2.71	1.17
	Sum of relative ratio of ON	3.70	3.52	5.28	2.35	0.16
	Sum of relative ratio of AH and KT	2.46	5.29	3.17	2.65	1.61
	Sum of relative ratio of OT	2.24	17.12	12.15	13.75	42.12
	Total unknown	1.33	7.31	7.35	7.80	5.61
	Sum of relative ratio	19.14	42.29	38.42	37.75	50.07

Remark: [1]Inf = Influent and [2]Eff. = Effluent, [3]AL= aliphatic hydrocarbon, [4]AR = aromatic hydrocarbon, [5]PN =phenol, [6]ON = organic nitrogen, [7]AH = aldehydes, [8]KT = ketones, [9]AC = alcohol, [10]CA = carboxylic acids , [11]ES = Ester and [12]OT = others, Common fragments = italic bold letter.

Table B-4: Average relative ratios of the pyrolysis fragment in HPOA of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds

Chemical Classes	Important fragment	Average relative ratio of HPOA				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AL[3]	****Propene***	0.51	0.36	0.56	0.24	0.30
AL	****2-Butene***	0.62	0.22	0.24	0.28	0.18
AL	*1-Pentene	0.53			0.53	0.28
AL	****1,3-Cyclopentadiene***	1.01	0.86	2.81	0.96	1.10
AL	*1-Hexene	0.40			0.32	0.38
AL	*1,3,5-Hexatriene, (Z)	0.51	0.30	0.70		
AL	****1,3-Cyclohexadiene***	0.43	0.23	0.50	0.14	0.21
AL	*Cyclopentene, 3-ethenyl	0.14	0.11	0.10		0.11
AL	1,3,5-Heptatriene,			0.10		
AL	*1,3-Cyclopentadiene, 5,5-dimethy	0.16	0.13			0.11
AL	*1,3,5-Hexatriene, 3-methyl-, (Z)	0.10	0.10			
AL	*1-Octene	0.27		0.10	0.50	0.29
AL	*Cyclopentene, 3-ethylidene-1-methyl	0.10				
AL	*1-Nonene				0.60	0.26
AL	*1-Decene	0.36			0.43	0.21
AL	Cyclobutane, 3-hexyl-1,1,2-trimethyl		0.10			
AL	*1-Undecene	0.19			0.25	0.10
AL	1,4 Undecadiene				0.11	
AL	*1-Dodecene	0.25	0.10		0.38	0.19
AL	6-Dodecyne	0.10			0.13	
AL	2,4-Dodecadiene, (E,Z)				0.11	
AL	*1-Tridecene	0.30			0.10	0.22
AL	*6-Tridecene, (E)				0.10	
AL	*Z-1,6 Tridecadiene	0.10				
AL	*Benzocycloheptatriene		0.20			
AL	*1-Tetradecene	0.30			0.59	0.20
AL	*7-Tetradecyne	0.10			0.24	0.17
AL	*1-Pentadecene	0.34			0.08	
AL	3-Hexadecyne	0.10			0.14	0.10
AL	Cyclopentene, 1-octyl				0.10	
AL	*1-Heptadecene	0.10			0.62	0.11
AL	*1-Nonadecene	0.10			0.23	0.16
AL	*Tridecane 7-hexyl				0.12	
AL	*9-Eicosene, (E)				0.21	0.11
AL	*Eicosane		0.10	0.11	0.30	0.17
AL	*Eicosane, 2-methyl-			0.12	0.17	
AL	Heneicosane		0.10			0.34
AL	*Eicosane 10 methy					0.19
AR[4]	****Benzene***	1.52	1.52	3.13	2.35	2.18
AR	****Toluene***	1.00	1.00	1.00	1.00	1.00
AR	*Ethylbenzene	0.53	0.35	0.16		0.10

Table B-4: Average relative ratios of the pyrolysis fragment in HPOA of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPOA				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AR	*Styrene	0.12	0.19		0.10	0.10
AR	*Benzene, (1-methylethyl)	0.13	0.11			
AR	*Benzene, propyl	0.17	0.10			
AR	Benzene, 1-ethyl-2-methyl	0.10	0.10			
AR	*.alpha.-Methylstyrene	0.10	0.10			
AR	Benzene, 1-ethyl-3-methyl	0.10	0.10			
AR	Benzene, 1,2,3-trimethyl		0.17			
AR	*Benzene, 1-ethenyl-4-methy		0.13			
AR	Benzene, 1-ethyl-4-methyl		0.10			
AR	*Benzene, 1-ethenyl-2-methyl	0.17				
AR	*Benzene, butyl	0.26	0.13			
AR	***Indene***	0.26	0.45	0.26	0.41	0.30
AR	*Benzene, (1-methylenebutyl)		0.12			
AR	*Benzene, pentyl	0.14	0.12		0.10	
AR	*1H-Indene, 1-methyl	0.10	0.12			
AR	*1H-Indene, 2-methy	0.10	0.10			
AR	Benzene, (1-methylpentyl)		0.10			
AR	*Naphthalene	0.10	0.16	0.10	0.11	
AR	*Benzene, (1-methylenepentyl)		0.10			
AR	Naphthalene, 1-methyl	0.12	0.11	0.10		
AR	Naphthalene, 2-methyl	0.10	0.16		0.11	
AR	*Benzene, heptyl				0.10	
AR	*Biphenyl	0.14	0.27		0.19	0.10
AR	*Naphthalene, 1-ethyl		0.12			
AR	Naphthalene, 1,3-dimethyl		0.11			
AR	*Benzene, octyl-	0.10			0.22	0.10
AR	1,1'-Biphenyl, 4-methyl		0.12	0.11		
AR	*Benzene, nonyl				0.14	0.10
AR	Fluorene		0.10	0.11	0.12	0.10
AR	*Benzene, decyl				0.16	
AR	Benzene, (1-methyldecyl)		0.10			
AR	*Benzene, (1-pentylheptyl)		0.10		0.10	
AR	*Benzene, (1-butyloctyl)				0.10	
AR	*Benzene, (1-propylnonyl)		0.10			
AR	Benzene, (1-ethyldecyl)		0.11			
AR	*Benzene, undecyl-				0.10	
AR	Benzene, (1-methylundecyl)		0.10		0.10	
AR	9H-Fluorene, 2-methyl		0.11			
AR	Benzene, (1-pentyloctyl)		0.10		0.10	

Table B-4: Average relative ratios of the pyrolysis fragment in HPOA of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPOA				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AR	Benzene, tetradecyl				0.10	
AR	Benzene, (1-methyldodecyl)		0.10			
PN[5]	*Phenol	0.13	0.45	0.28	0.12	
PN	*Phenol, 2-methyl	0.10	0.28	0.24		
PN	*Phenol, 4-methyl	0.10	0.18	0.12	0.11	
PN	*Phenol, 2-ethyl	0.10				
PN	*Phenol, 2,4-dimethyl		0.10	0.11		
PN	*Phenol, 4-ethyl		0.10			
PN	*Phenol, 4-(1-methylethyl)		0.28	0.17		
PN	*1-Naphthalenol		0.13	0.11		
ON[6]	*Acetronitrile		0.10			
ON	*Isobutyronitrile	0.12	0.14		0.10	0.12
ON	*Butanenitrile, 2-methyl-	0.10	0.10		0.10	0.10
ON	*Butanenitrile, 3-methyl	0.24	0.26	0.10	0.15	0.22
ON	***Pyrrole***	0.26	0.80	0.50	0.43	0.48
ON	*1H-Pyrrole, 2-methyl	0.11	0.13	0.10		0.10
ON	*1H-Pyrrole, 3-methyl	0.10	0.22	0.13		0.10
ON	*Pentanenitrile, 4-methyl	0.10				
ON	*1H-Pyrrole, 2,3-dimethyl-	0.10	0.10			
ON	*Pyridine, 3-methyl					0.10
ON	***Indole***	0.16	0.15	0.10	0.22	0.13
ON	*Pentadecanenitrile				0.15	
ON	*Heptadecanenitrile	0.10			0.17	
AH[7]	*E-14-Hexadecenal	0.11				0.11
KT[8]	***Methyl Isobutyl Ketone***	0.27	0.43	0.27	0.21	0.35
KT	*Cyclopentanone, 2-methyl		0.15			
KT	*Cyclopentanone, 2,5-dimethyl		0.10			
KT	*Cyclopentanone, 2,4,4-trimethyl-	0.82	1.47	0.98	0.47	0.75
KT	***2-Cyclopenten-1-one,2 3,4-dimethyl***	0.10				
KT	*2-Pentadecanone				0.10	
KT	*2-Heptadecanone	0.10			0.15	
AC[9]	*1-Hexanol, 2-ethyl	0.18				0.20
AC	*1-Octanol, 2-butyl				0.56	
AC	*2-Hexyl-1-octanol		0.10			
AC	1-Decanol, 2-methyl				1.27	
AC	*2-Ethyl-1-dodecanol					0.35
AC	*1-Decanol, 2-ethyl				0.30	
AC	*1-Decanol, 2-hexyl				0.36	0.14
AC	*9-Tetradecen-1-ol	0.10			0.10	
CA[10]	Heptanoic acid, anhydride		0.11			
CA	Dodecanoic acid				0.30	

Table B-4: Average relative ratios of the pyrolysis fragment in HPOA of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPOA				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
ES[11]	Allyl heptanoate			0.18		
OT[12]	Cyclotetrasiloxane, octamethyl	0.10				
OT	Silane, tetramethyl-					0.14
	Sum of relative ratio of AL	7.12	2.92	5.34	7.95	5.47
	Sum of relative ratio of AR	5.33	7.17	4.97	5.64	4.07
	Sum of relative ratio of PN	0.42	1.52	1.03	0.23	0.00
	Sum of relative ratio of ON	1.40	2.01	0.93	1.32	1.34
	Sum of relative ratio of AH and KT	1.40	2.15	1.25	0.93	1.21
	Sum of relative ratio of OT	0.38	0.21	0.18	2.87	0.82
	Total unknown	0.99	1.31	0.85	2.86	1.58
	Sum of relative ratio	17.04	17.27	14.54	21.80	14.49

Remark: [1]Inf = Influent and [2]Eff. = Effluent, [3]AL= aliphatic hydrocarbon, [4]AR = aromatic hydrocarbon, [5]PN =phenol, [6]ON = organic nitrogen, [7]AH = aldehydes, [8]KT = ketones, [9]AC = alcohol, [10]CA = carboxylic acids, and [12]OT = others, Common fragments = Italic bold letter.

Table B-5: Average relative ratios of the pyrolysis fragment in HPIB of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds

Chemical Classes	Important fragment	Average relative ratio of HPIB				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AL[3]	*Propene					1.07
AL	*2-Butene		0.43			
AL	*1-Pentene					1.20
AL	*1,3-Cyclopentadiene	2.02		0.65		
AL	*1,3-Pentadiene					0.54
AL	*1-Hexene		0.46	0.97		1.25
AL	*1,3,5-Hexatriene, (Z)		1.99			
AL	2,4-Hexadiene			4.37		
AL	2,4-Hexadiyne	3.89			7.44	3.83
AL	***1-Octene***	0.71	0.41	1.02	1.70	0.46
AL	***1-Nonene***	0.80	0.43	1.04	1.63	0.40
AL	***1-Decene***	0.65	0.40	0.90	1.11	0.28
AL	*1-Undecene	0.79	0.35	0.78		0.23
AL	*2-Undecene				1.03	
AL	***1-Dodecene***	0.51	0.28	0.61	0.81	0.26
AL	Cyclododecene, (E)	0.16				
AL	*1-Tridecene	0.64	0.32	0.50	0.78	
AL	***1-Tetradecene***	0.58	0.24	0.60	0.73	0.22
AL	*7-Tetradecyne	0.27	0.17			0.10
AL	*1-Pentadecene	0.91		1.15		0.31
AL	*1-Nonadecene		0.22			
AR[4]	***Toluene***	1.00	1.00	1.00	1.00	1.00
AR	*p-Xylene		0.11			
AR	o-xylene		0.11			
AR	***Styrene***	0.20	0.14	0.37	0.29	0.24
AR	*Benzene, octyl-	0.16				
AR	*Benzene, (1-butyloctyl)					0.13
AR	Benzene, (1-ethyldecyl)					0.11
PN[5]	*Phenol	0.14	0.56			0.11
ON[6]	*Acetronitrile	4.50				2.52
ON	1,2-Propanediamine				5.35	
ON	*2-Propenenitrile	2.51				0.94
ON	*Isobutyronitrile					1.25
ON	*2-Propenenitrile, 2-methyl-	0.26				
ON	Butanenitrile					0.22
ON	*2-Methyl-2-butenenitrile	0.19				
ON	*Butanenitrile, 2-methyl-	0.10	0.20	0.27		0.46
ON	2-Pentenenitrile	0.10				
ON	***Pyrrole***	0.18	0.19	0.51	0.52	0.27
ON	***Butanenitrile, 3-methyl***	0.33	0.25	0.60	0.35	1.69
ON	*2,4-Pentadienenitrile	0.22				0.30

Table B-5: Average relative ratios of the pyrolysis fragment in HPIB of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPIB				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
ON	*Pyridine, 3-methyl					0.39
ON	*Benzonitrile	0.30				
ON	*Benzonitrile, 2-methyl	0.15				
ON	*Indole					0.12
AH[7]	*Acetaldehyde			1.17		
AH	*E-14-Hexadecenal		0.12			
KT[8]	*Cyclopentanone			0.19		
KT	*Cyclopentanone, 2,4,4-trimethyl-		0.52			
AC[9]	*1-Hexanol, 2-ethyl					0.96
AC	*1-Decanol, 2-methyl		0.54			
AC	*1-Decanol, 2-ethyl				0.91	
AC	*9-Tetradecen-1-ol		0.14			
	Sum of relative ratio of AL	11.93	5.71	12.61	15.23	10.14
	Sum of relative ratio of AR	1.36	1.36	1.37	1.29	1.49
	Sum of relative ratio of PN	0.14	0.56	0.00	0.00	0.11
	Sum of relative ratio of ON	8.84	0.64	1.38	6.22	8.16
	Sum of relative ratio of AH and KT	0.00	0.64	1.37	0.00	0.00
	Sum of relative ratio of OT	0.00	0.67	0.00	0.91	0.96
	Total unknown	2.04	1.57	2.29	2.53	1.59
	Sum of relative ratio	24.31	11.14	19.01	26.18	22.46

Remark: [1]Inf = Influent and [2]Eff. = Effluent, [3]AL= aliphatic hydrocarbon, [4]AR = aromatic hydrocarbon, [5]PN =phenol, [6]ON = organic nitrogen, [7]AH = aldehydes, [8]KT = ketones and [9]AC = alcohol, Common fragment = Italic bold letter

Table B-6: Average relative ratios of the pyrolysis fragment in HPIA of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds

Chemical Classes	Important fragment	Average relative ratio of HPIA				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AL[3]	*Propene	1.78	2.21			2.16
AL	*2-Butene	0.97	2.05			
AL	*1-Pentene	1.31	2.26			
AL	Cyclopentene			2.26		
AL	*1-Hexene	3.44	3.02			5.02
AL	2,4-Hexadiene	0.61	3.91	4.35		
AL	*1-Heptene	3.52			6.09	5.64
AL	***1-Octene***	1.86	1.34	1.87	2.60	2.22
AL	***1-Nonene***	1.75	1.16	2.13	2.19	1.61
AL	***1-Decene***	1.20	0.93	2.96	2.03	1.21
AL	***1-Undecene***	1.06	0.85	2.58	1.06	0.98
AL	1,4 Undecadiene		0.14			
AL	*1-Dodecene	0.96	0.75	2.43	0.87	0.77
AL	Cyclododecene, (E)				0.19	
AL	6-Dodecyne	0.20				
AL	Undecane, 2,10-dimethyl			4.05		
AL	2,4-Dodecadiene, (E,Z)		0.21			
AL	***1-Tridecene***	0.86	0.75	17.18	0.90	0.77
AL	*Z-1,6 Tridecadiene	0.22	0.14			
AL	Tridecane, 3-methyl			1.97		
AL	***1-Tetradecene***	0.93	0.82	1.49	0.86	0.82
AL	*Dodecane, 2,6,11-trimethyl			2.51		
AL	*7-Tetradecyne	0.20	0.25			
AL	Tetradecane, 2-methyl-			6.29		
AL	***1-Pentadecene***	1.00	1.12	12.20	1.00	0.84
AL	3-Hexadecyne		0.16			
AL	Cyclopentene, 1-octyl	0.31		1.41		
AL	Cyclohexene, 3-nonyl	0.14				
AL	Cyclotetradecane				0.44	
AL	*1-Heptadecene	0.55	0.43	3.51	0.36	
AL	*1-Nonadecene		0.48			
AL	10-Methyl-octadec-1-ene	0.69				
AL	*Nonadecane, 2-methyl	1.28				
AL	*Eicosane	1.85				
AL	*Eicosane 10 methy	1.26				
AL	*Tricosane	0.95				
AR[4]	***Toluene***	1.00	1.00	1.00	1.00	1.00
AR	o-xylene	0.19				
AR	***Styrene***	0.30	0.22	1.07	0.53	2.07
AR	*Naphthalene		0.16			
AR	*Biphenyl		0.16			

Table B-6: Average relative ratios of the pyrolysis fragment in HPIA of influent wastewater and effluent water from the aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPIA				
		Inf.[1] wastewater	Eff.[2] Water from aeration ponds	Eff. Water from facultative ponds	Eff. Water from oxidation ponds	Eff. Water from detention pond
AR	Benzene, (1-methyldecyl)	0.27				
PN[5]	*Phenol	0.16				
PN	*Benzenemethanol, .alpha.,.alpha.-dimethyl-	0.55				
PN	*Phenol, 4-methyl	0.19				
ON[6]	*1,2-Propanediamine				2.51	
ON	*Butanenitrile, 2-methyl-	0.16				
ON	*Butanenitrile, 3-methyl	0.42	0.49			0.43
ON	*Pyrrole	0.21	0.30			0.23
ON	*Pentanenitrile, 4-methyl	0.29	0.33			0.29
ON	*Indole	0.53	0.34			
ON	*Tridecanenitrile		0.30			
ON	Tetradecanenitrile	0.49	0.52			
ON	*Pentadecanenitrile				0.33	
ON	Hexadecanenitrile		0.37			0.40
ON	Dodecanamide					
ON	*Heptadecanenitrile	0.94				
AH[7]	*Acetaldehyde					2.37
AH	*Furfural				0.47	
AH	*E-14-Hexadecenal	0.42				0.27
AH	E-15-Heptadecenal	0.50				
KT[8]	*Cyclopentanone			0.99	0.89	
KT	*2-Heptadecanone	0.48			0.48	
AC[9]	*1-Hexanol, 2-ethyl	1.99		1.29	1.17	0.62
AC	*1-Octanol, 2-butyl			4.12		
AC	10-Undecen-1-ol	0.19		0.69		
AC	*1-Decanol, 2-hexyl			1.33		
AC	*9-Tetradecen-1-ol	0.18		2.47		
OT[12]	*Cyclotrisiloxane, hexamethyl				1.97	
	Sum of relative ratio of AL	28.91	22.99	69.20	18.58	22.03
	Sum of relative ratio of AR	1.76	1.54	2.07	1.53	3.07
	Sum of relative ratio of PN	0.90	0.00	0.00	0.00	0.00
	Sum of relative ratio of ON	3.04	2.66	0.00	2.84	1.35
	Sum of relative ratio of AH and KT	1.40	0.00	0.99	1.84	2.64
	Sum of relative ratio of OT	2.36	0.00	9.91	3.14	0.62
	Total unknown	7.12	7.82	19.01	8.57	1.32
	Sum of relative ratio	45.49	35.00	101.18	36.50	31.03

Remark: [1]Inf = Influent and [2]Eff. = Effluent, [3]AL= aliphatic hydrocarbon, [4]AR = aromatic hydrocarbon, [5]PN =phenol, [6]ON = organic nitrogen, [7]AH = aldehydes, [8]KT = ketones [9]AC = alcohol and [12]OT = others
Common fragments = Italic bold letter

Table B-7: Average relative ratio of the pyrolysis fragment in HPIN of influent wastewater, and effluent water from aeration, facultative, oxidation and detention ponds

Chemical Classes	Important fragment	Average relative ratio of HPIN				
		Inf.[1] wastewater	Eff.[2] Water after aeration ponds	Eff. Water after facultative ponds	Eff. Water after oxidation ponds	Eff. Water after detention pond
AL[3]	*Propene	1.72	0.61			
AL	*2-Butene	2.80	0.73	4.81		1.37
AL	*1-Pentene	1.52				1.08
AL	*1-Hexene	3.44				2.95
AL	2,4-Hexadiene		2.39	3.28		
AL	*1-Heptene	5.44				4.33
AL	1-Pentene, 2,4,4-trimethyl				0.12	
AL	***1-Octene***	1.31	0.67	1.26	0.45	0.95
AL	*Cyclopentene, 3-ethylidene-1-methyl				0.53	
AL	*1-Nonene	1.33	0.78	1.66		1.14
AL	***1-Decene***	1.29	0.51	1.46	0.34	1.14
AL	***1-Undecene***	1.08	0.38	1.29	0.30	0.92
AL	1,4 Undecadiene	0.17				
AL	***1-Dodecene***	0.83	0.42	1.74	0.24	0.83
AL	6-Dodecyne	0.26				0.17
AL	***1-Tridecene***	0.74	0.46	2.07	0.23	1.10
AL	*Z-1,6 Tridecadiene	0.22				
AL	***1-Tetradecene***	0.69	0.35	1.78	0.18	0.69
AL	*1-Pentadecene		0.44		0.18	1.17
AL	3-Hexadecyne	1.00				
AL	*1-Heptadecene	0.63		3.79	0.11	
AL	*1-Nonadecene		0.43	6.98		
AL	*Tridecane 7-hexyl		0.87		0.25	
AL	Octadecane, 2-methyl	1.06				1.15
AL	*9-Eicosene, (E)		1.78		0.74	
AL	*Nonadecane, 2-methyl	2.49		16.90		2.80
AL	*Nonadecane, 9-methyl		3.25			
AL	*Eicosane	3.58		27.80	1.58	5.85
AL	*Eicosane, 2-methyl-		3.35		2.71	
AL	Heneicosane	3.45		26.17		6.75
AL	*Eicosane 10 methy		2.69		2.90	
AL	*Tricosane	2.21				4.73
AL	*Tetracosane				1.93	
AR[4]	*Benzene				3.04	
AR	***Toluene***	1.00	1.00	1.00	1.00	1.00
AR	***p-Xylene***	0.28	0.40	0.49	0.15	0.20
AR	o-xylene		0.23			0.49
AR	***Styrene***	0.29	0.25	0.59	0.26	0.36
AR	*Indene		0.25			
AR	*Naphthalene	0.14	0.13			0.15
AR	*Benzene, hexyl			0.87		

Table B-7: Average relative ratio of the pyrolysis fragment in HPIN of influent wastewater, and effluent water from aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPIN				
		Inf.[1] wastewater	Eff.[2] Water after aeration ponds	Eff. Water after facultative ponds	Eff. Water after oxidation ponds	Eff. Water after detention pond
AR	*Benzene, (1-butyloctyl)	0.13				
AR	*Benzene, undecyl-			0.90		
PN[5]	*Phenol	1.06		2.63	0.71	1.87
PN	*Phenol, 2-methyl	0.31		0.93	0.16	0.32
PN	*Phenol, 4-methyl	0.45		0.75	0.18	0.49
PN	Phenol, p-tert-butyl			1.22		
PN	*Phenol, 4-(1,1,3,3-tetramethylbutyl)	0.72		7.70	0.86	1.70
ON[6]	*Acetronitrile (SI:85)			2.07		
ON	*Butanenitrile, 3-methyl	0.20	0.35		0.11	0.12
ON	****Pyrrole***	0.79	0.58	1.18	0.46	0.45
ON	*1H-Pyrrole, 2-methyl	0.24	0.21	0.39		0.24
ON	*1H-Pyrrole, 3-methyl	0.39	0.25	0.32		0.20
ON	*Pentanenitrile, 4-methyl	0.23				0.54
ON	*Acetamide	0.76		3.34		0.64
ON	1H-Pyrrole, 3-ethyl	0.45	0.19			
ON	Caprolactam			3.97		1.12
ON	*Benzonitrile, 2-hydroxy					0.56
ON	Tetradecanenitrile					0.19
ON	*Heptadecanenitrile	0.41				0.64
AH[7]	*Acetaldehyde				0.65	
AH	*2-Pentenal, (E)	0.33				
AH	Butanedia					0.17
AH	*Furfural					0.94
AH	*2-Furancarboxaldehyde, 5-methyl					0.48
AH	*E-14-Hexadecenal	0.32				0.32
KT[8]	Acetone		1.70			
KT	*2-Butanone	3.51	0.84			
KT	*2-Butanone, 3-methyl-			0.60		0.34
KT	*2,3-Butanedione					0.23
KT	*2-Pentanone				0.12	
KT	*2,3-Pentanedione			0.56		
KT	*2-Propanone, 1-hydroxy	0.40				0.34
KT	2,3-Pentanedione, 4-methy					0.33
KT	*Cyclopentanone	0.50		0.49	0.25	0.22
KT	*Cyclopentanone, 2-methyl		0.17			
KT	*2-Cyclopenten-1-one	2.22		3.91	0.66	0.81
KT	*2-Cyclopenten-1-one, 2-methyl-	1.13		1.67	0.33	0.52
KT	*Ethanone, 1-(2-furanyl)	0.28				
KT	2-Cyclopenten-1-one, 2,3-dimethyl-	0.20				
KT	*Butyrolactone	0.26		0.71		0.24
KT	2-Cyclopenten-1-one,2 3,4-dimethyl	0.17				

Table B-7: Average relative ratio of the pyrolysis fragment in HPIN of influent wastewater, and effluent water from aeration, facultative, oxidation and detention ponds *(continued)*

Chemical Classes	Important fragment	Average relative ratio of HPIN				
		Inf.[1] wastewater	Eff.[2] Water after aeration ponds	Eff. Water after facultative ponds	Eff. Water after oxidation ponds	Eff. Water after detention pond
AC[9]	*2-Propanol, 2-methyl					1.88
AC	*1-Hexanol, 2-ethyl	1.57	0.25	4.41	0.66	
AC	* 1-Octanol, 2-butyl			8.94		
CA[10]	*Acetic acid					0.72
CA	*Benzoic Acid					0.24
CA	Isopropyl Myristate					0.34
OT[12]	*Cyclotrisiloxane, hexamethyl	1.26			0.90	1.37
OT	Cyclotetrasiloxane, octamethyl				0.13	
	Sum of relative ratio of AL	37.29	20.10	100.97	12.76	39.14
	Sum of relative ratio of AR	1.84	2.26	3.85	4.45	2.20
	Sum of relative ratio of PN	2.54	0.00	13.24	1.90	4.38
	Sum of relative ratio of ON	3.47	1.57	11.27	0.57	4.71
	Sum of relative ratio of AH and KT	9.31	2.72	7.93	2.00	4.94
	Sum of relative ratio of OT	2.83	0.25	13.35	1.69	4.54
	Total unknown	12.42	4.32	48.76	5.16	15.74
	Sum of relative ratio	69.69	31.22	199.36	28.53	75.64

Remark: [1]Inf = Influent and [2]Eff. = Effluent, [3]AL= aliphatic hydrocarbon, [4]AR = aromatic hydrocarbon, [5]PN =phenol, [6]ON = organic nitrogen, [7]AH = aldehydes, [8]KT = ketones, [9]AC = alcohol, [10]CA = carboxylic acids , and [12]OT = others, Common fragment = Italic bold letter

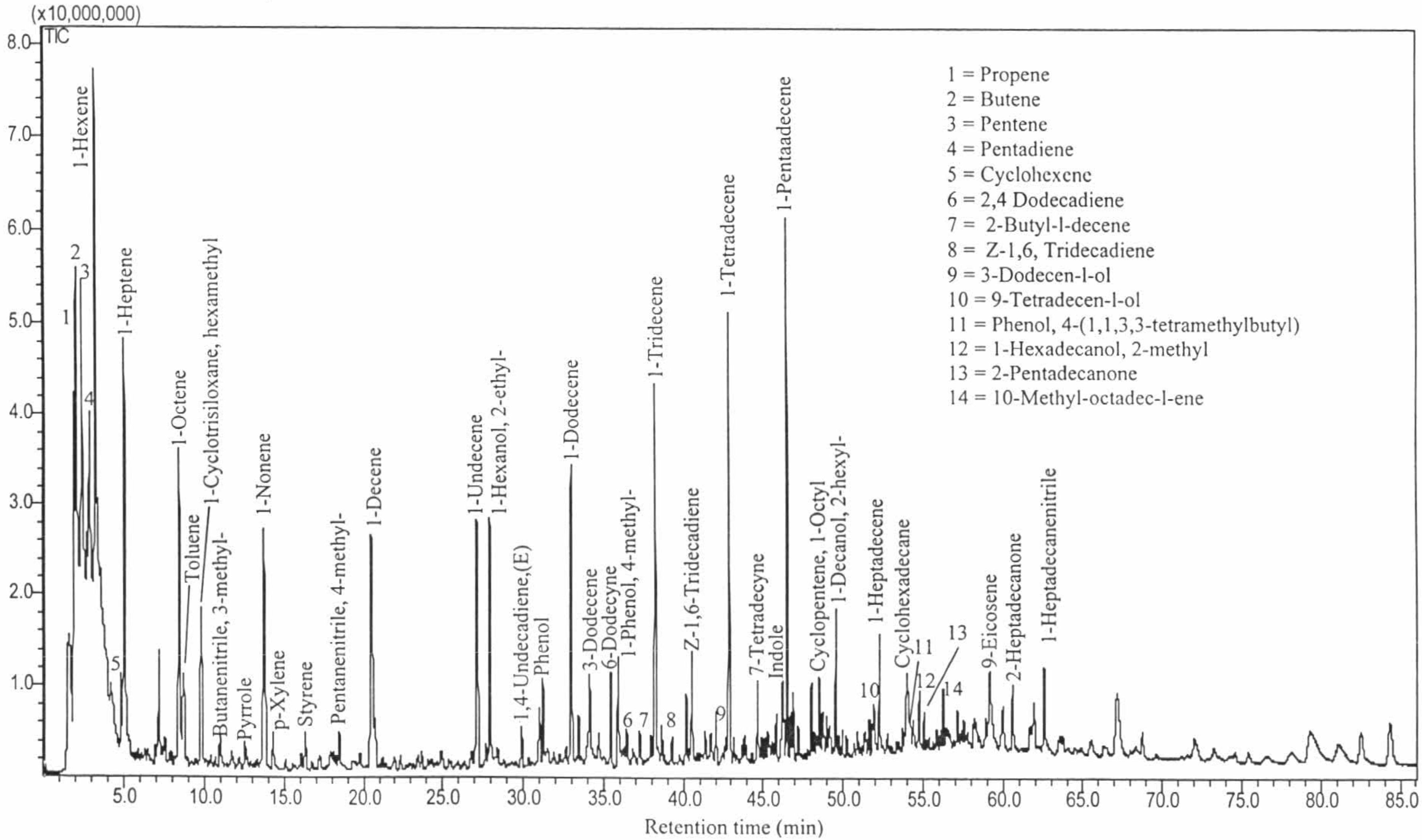

Figure B-5: Pyrochromatogram of major fragments of influent wastewater

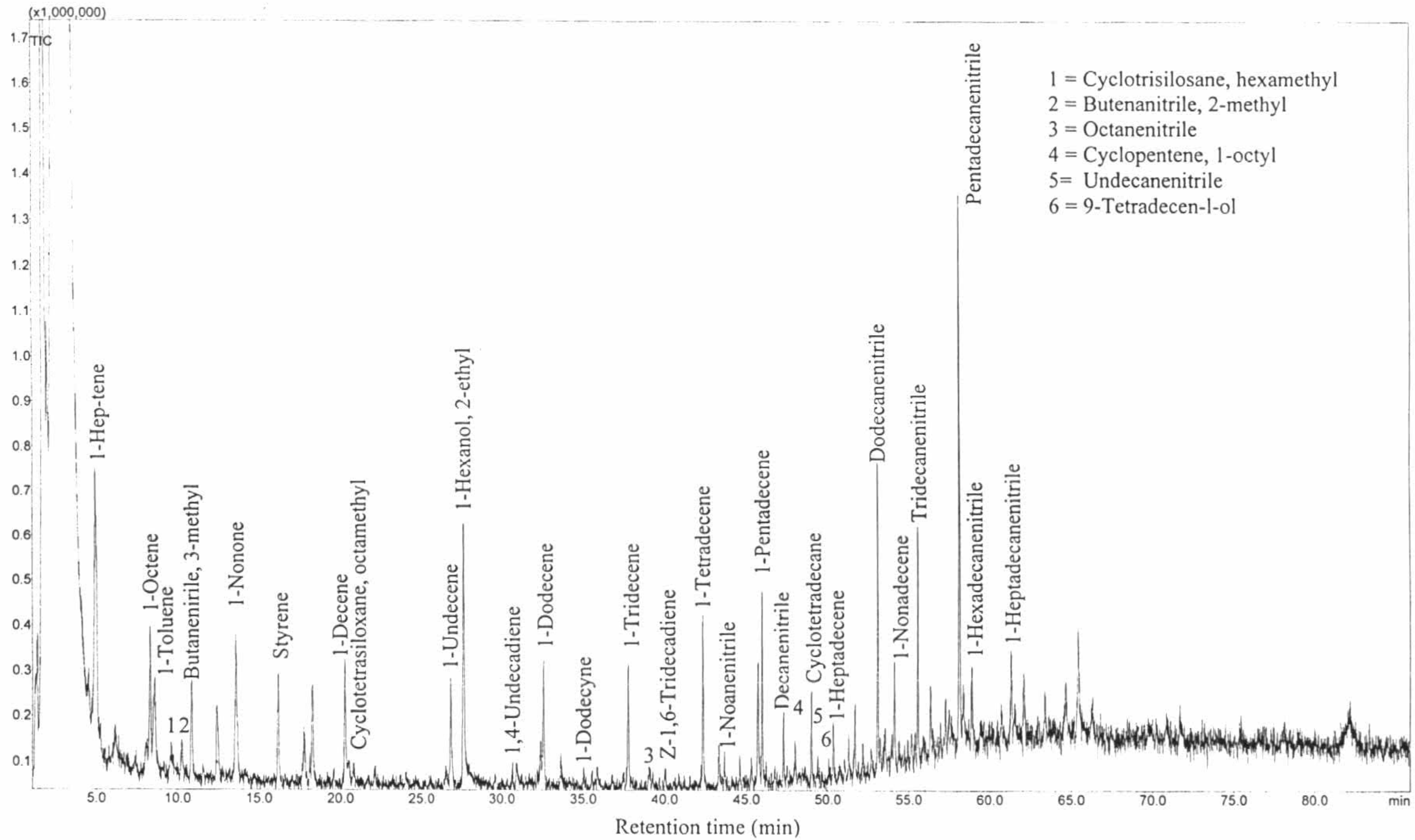

Figure B-6: Pyrochromatogram of major fragments of the aeration pond effluent

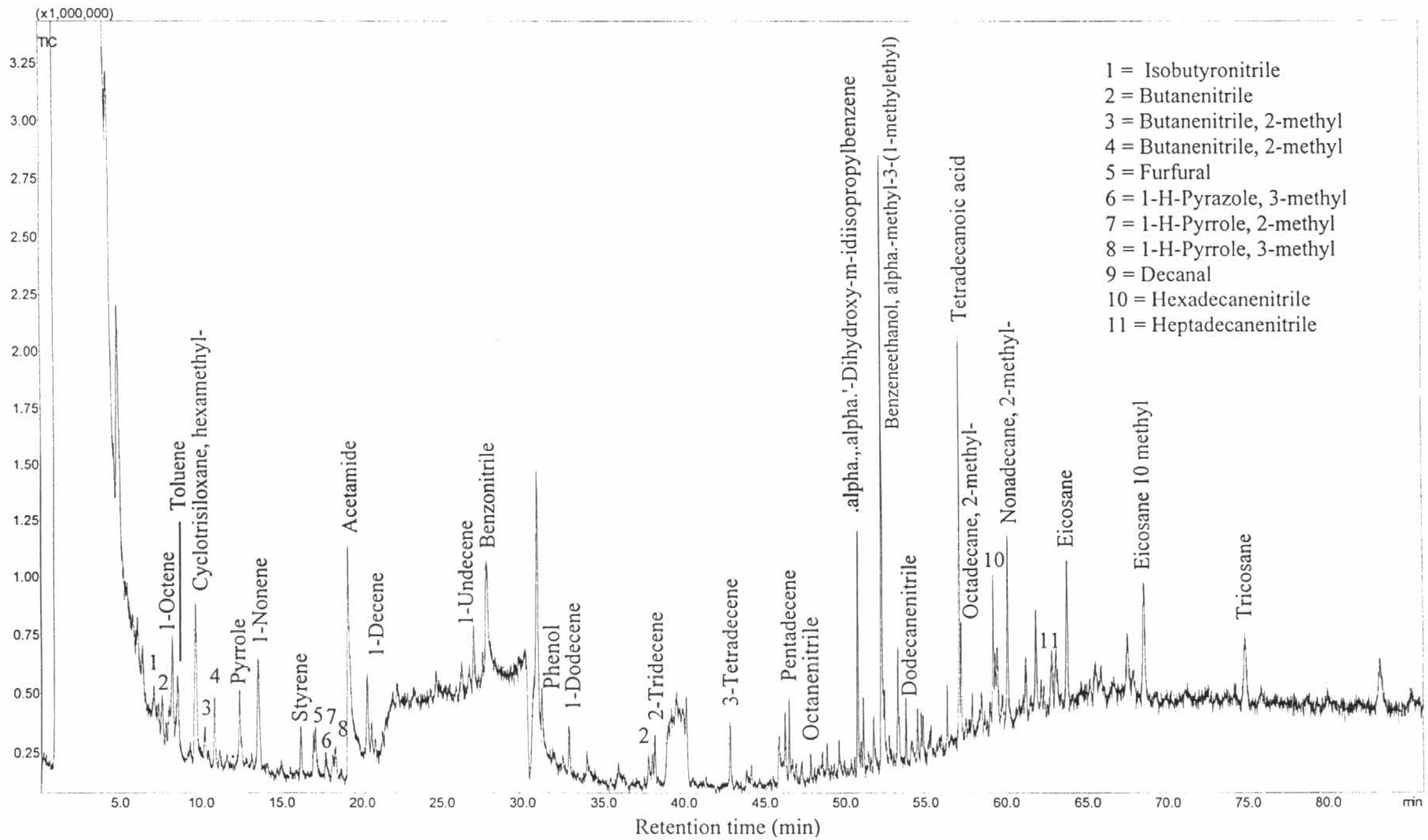

Figure B-7: Pyrochromatogram of major fragments of the facultative pond effluent

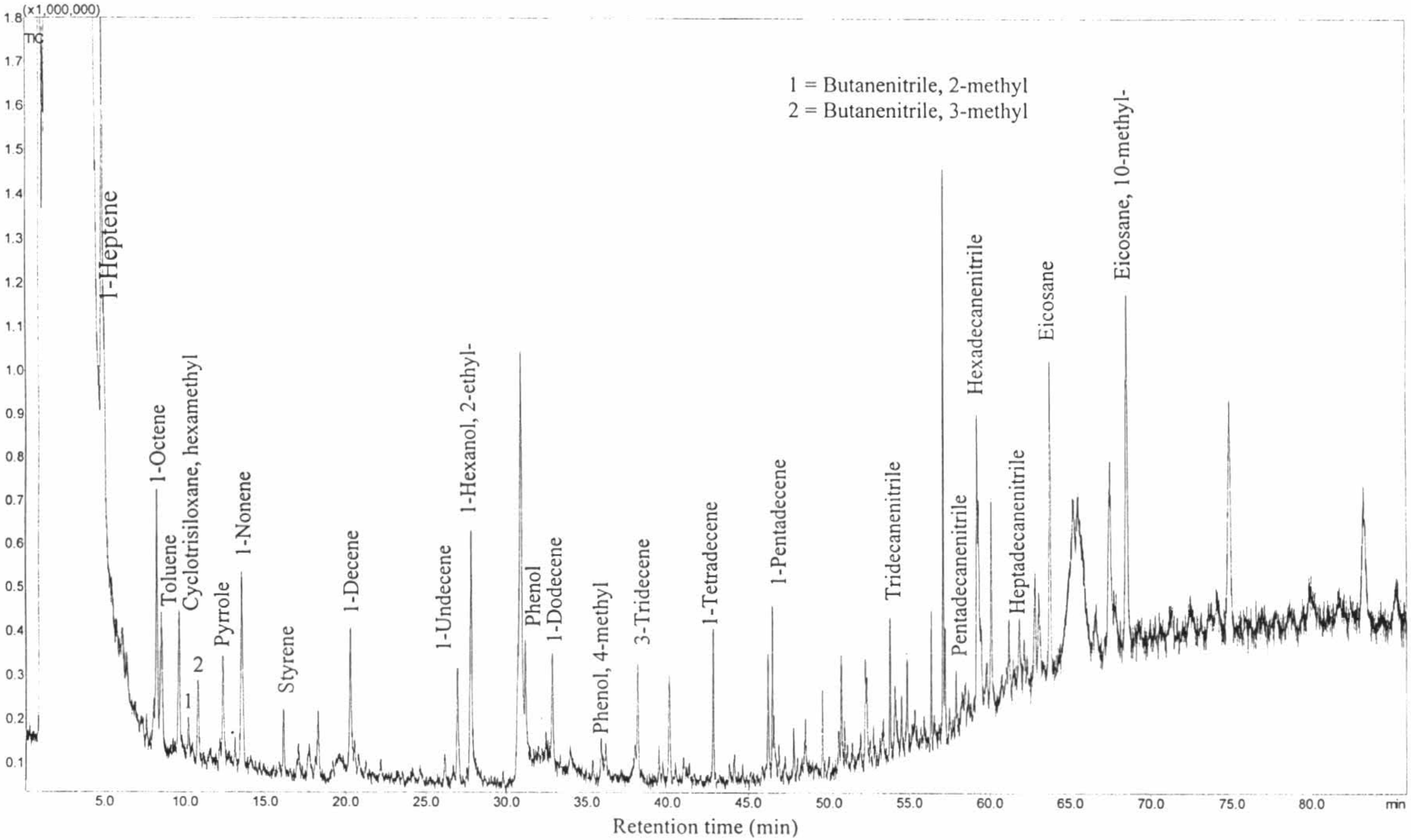

Figure B-8: Pyrochromatogram of major fragments of the oxidation pond effluent

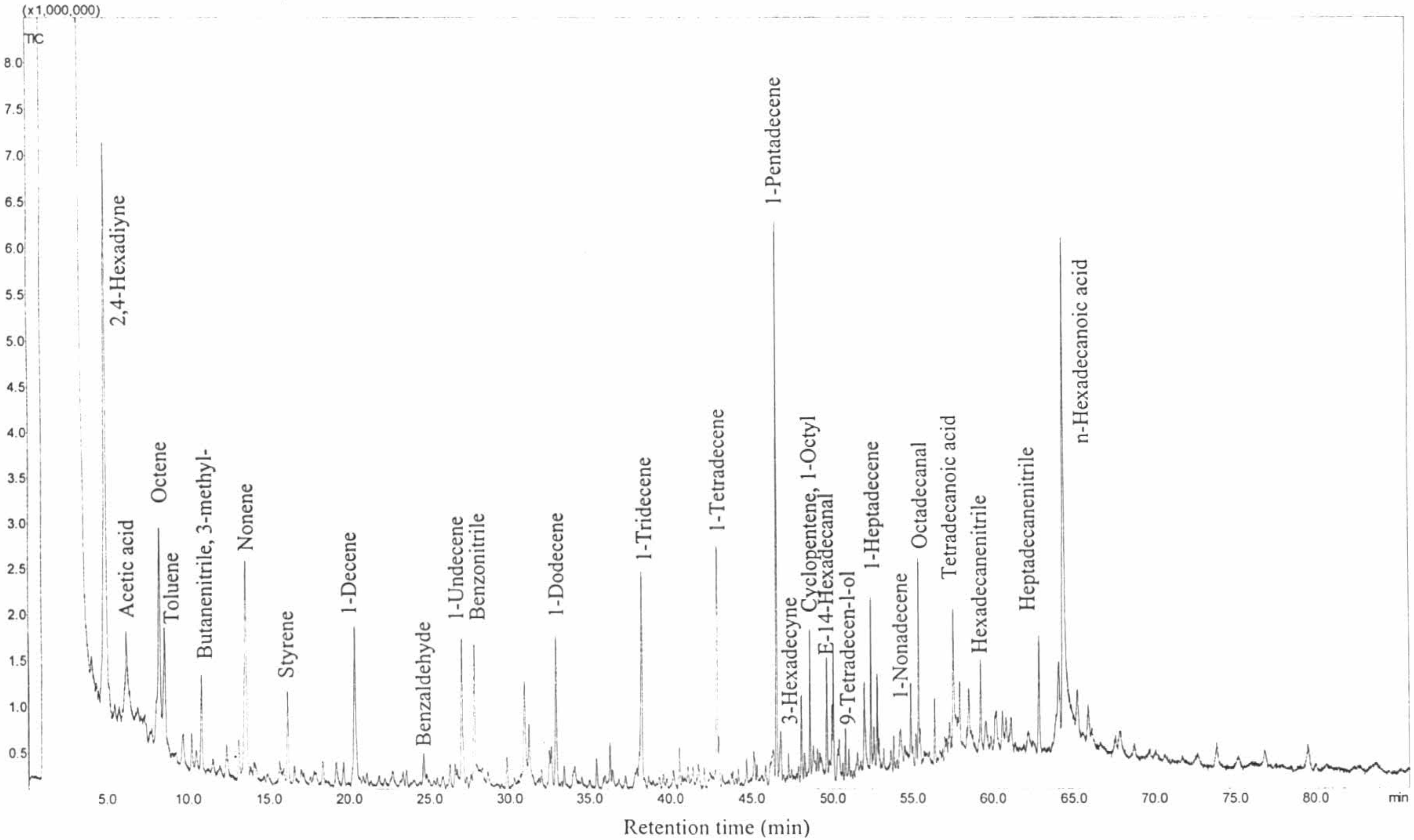

Figure B-9: Pyrochromatogram of major fragments of the detention pond effluent

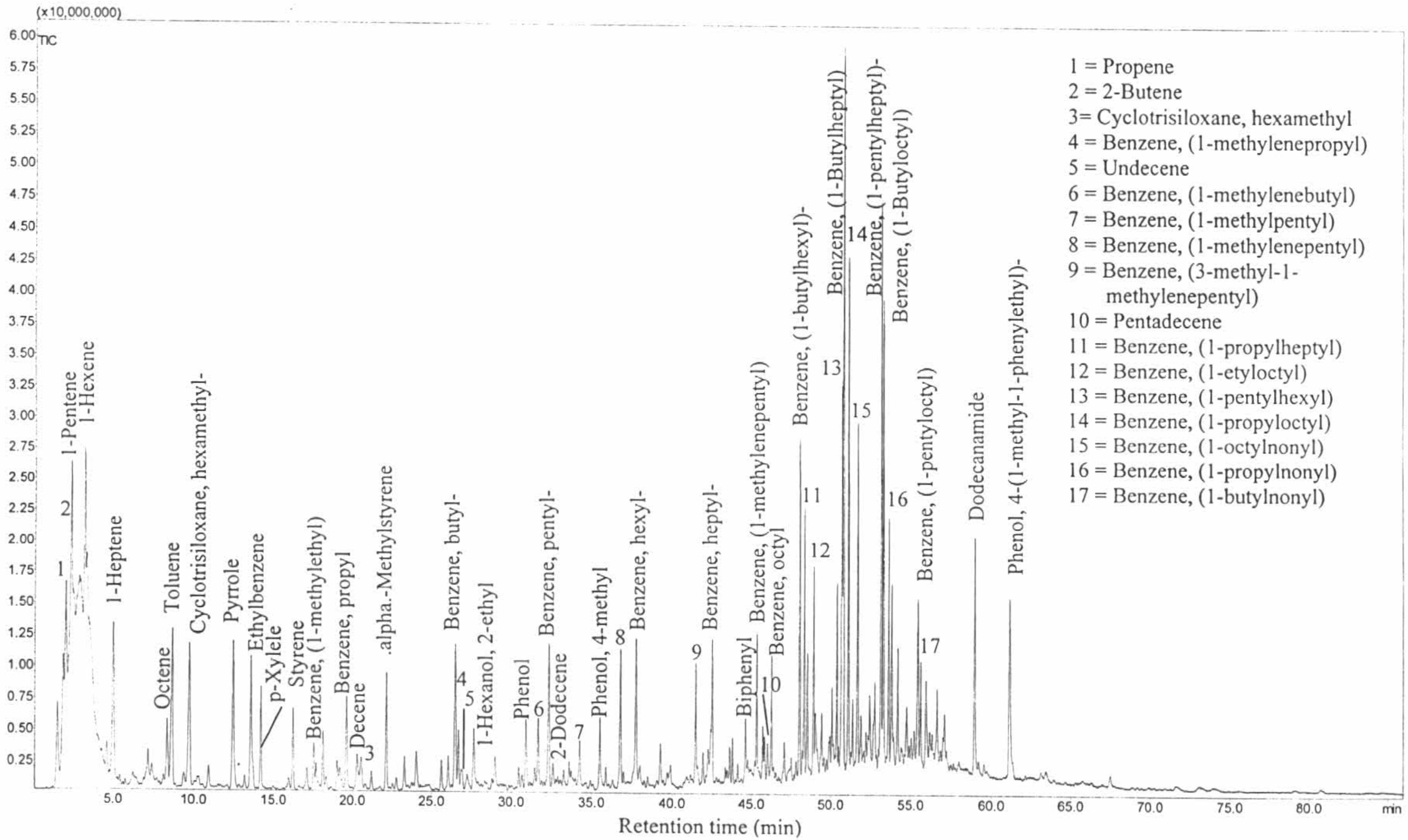

Figure B-10: Pyrochromatogram of major fragments of the HPON of influent wastewater

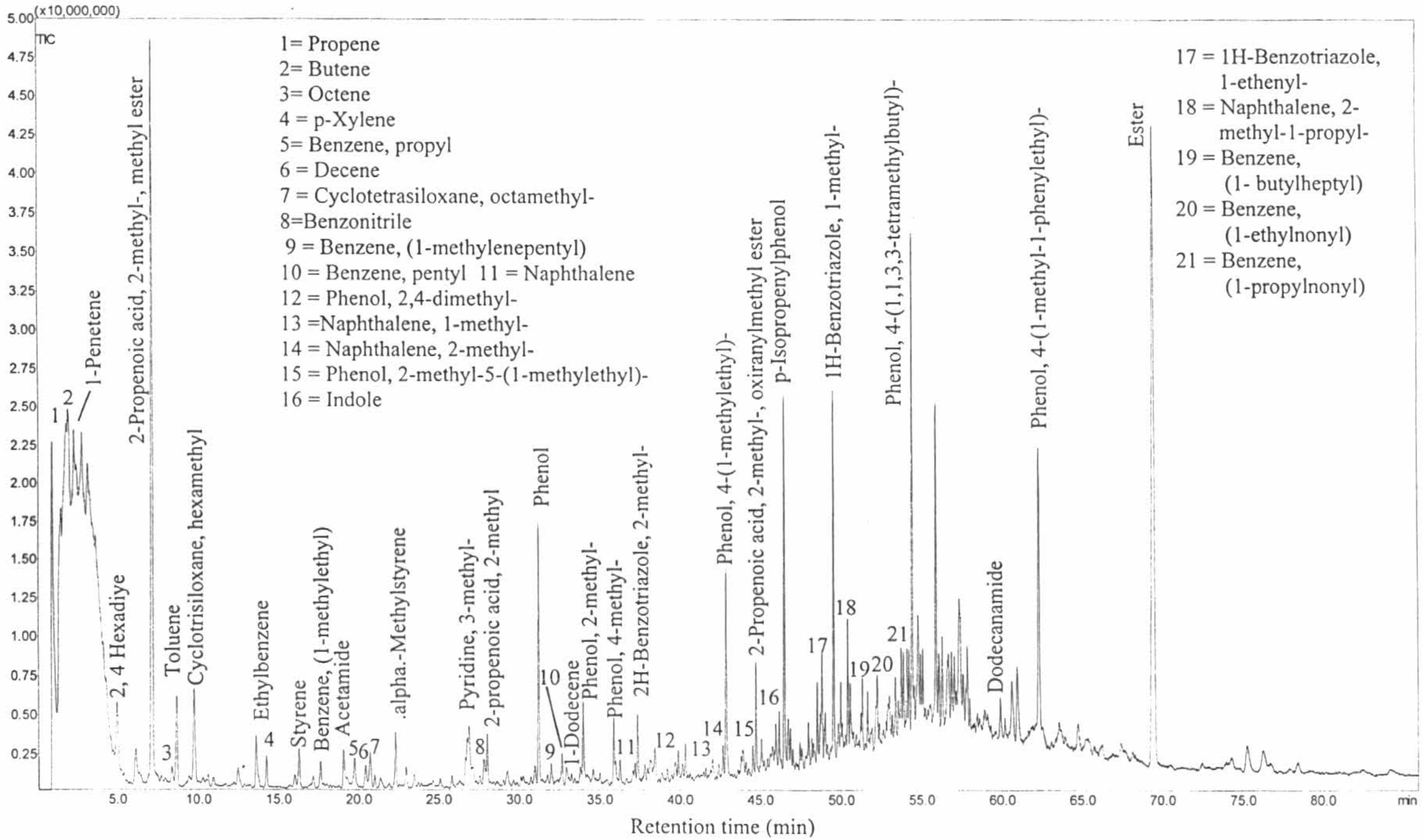

Figure B-11: Pyrochromatogram of major fragments of the HPON of the aeration pond effluent

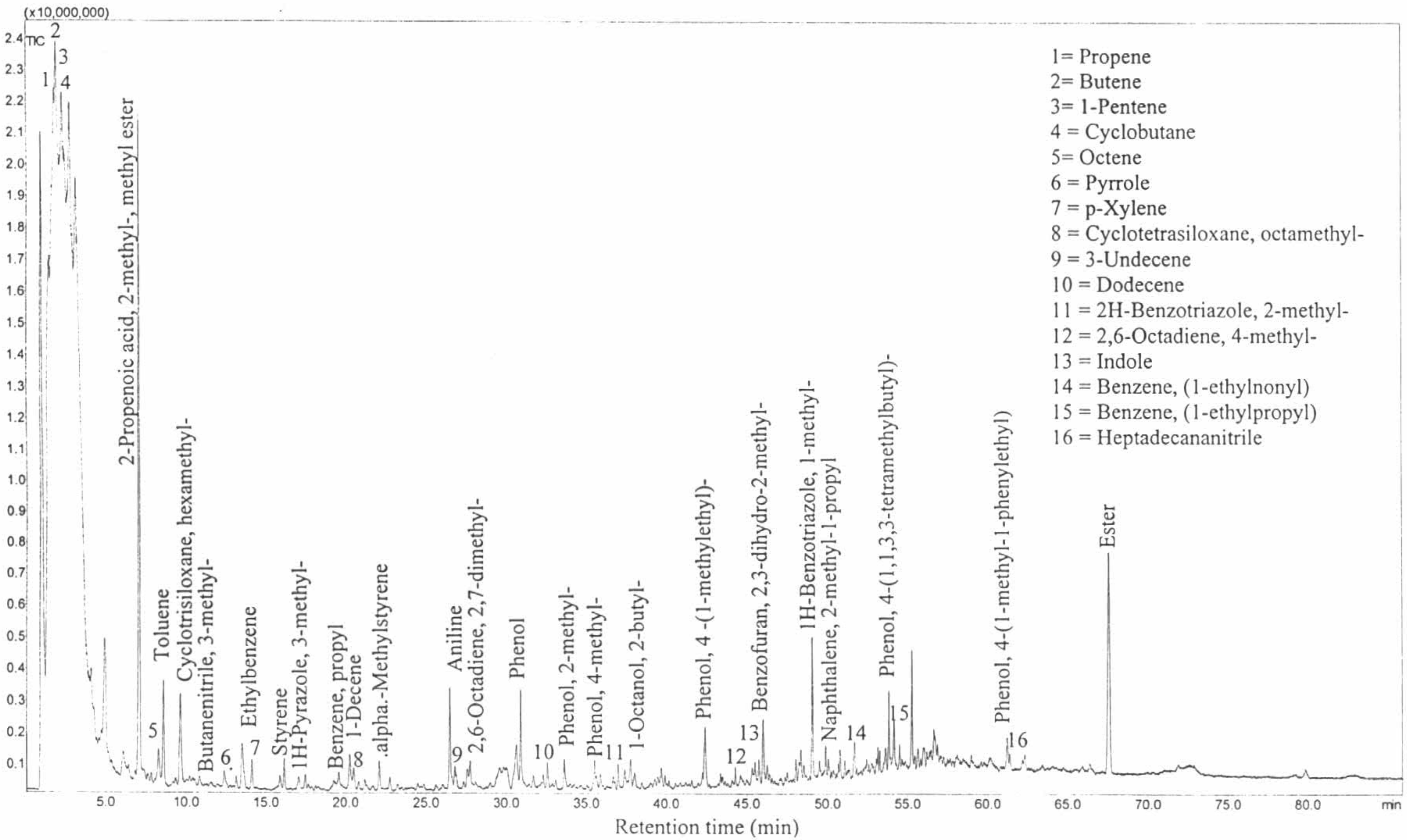

Figure B-12: Pyrochromatogram of major fragments of the HPON of the facultative pond effluent

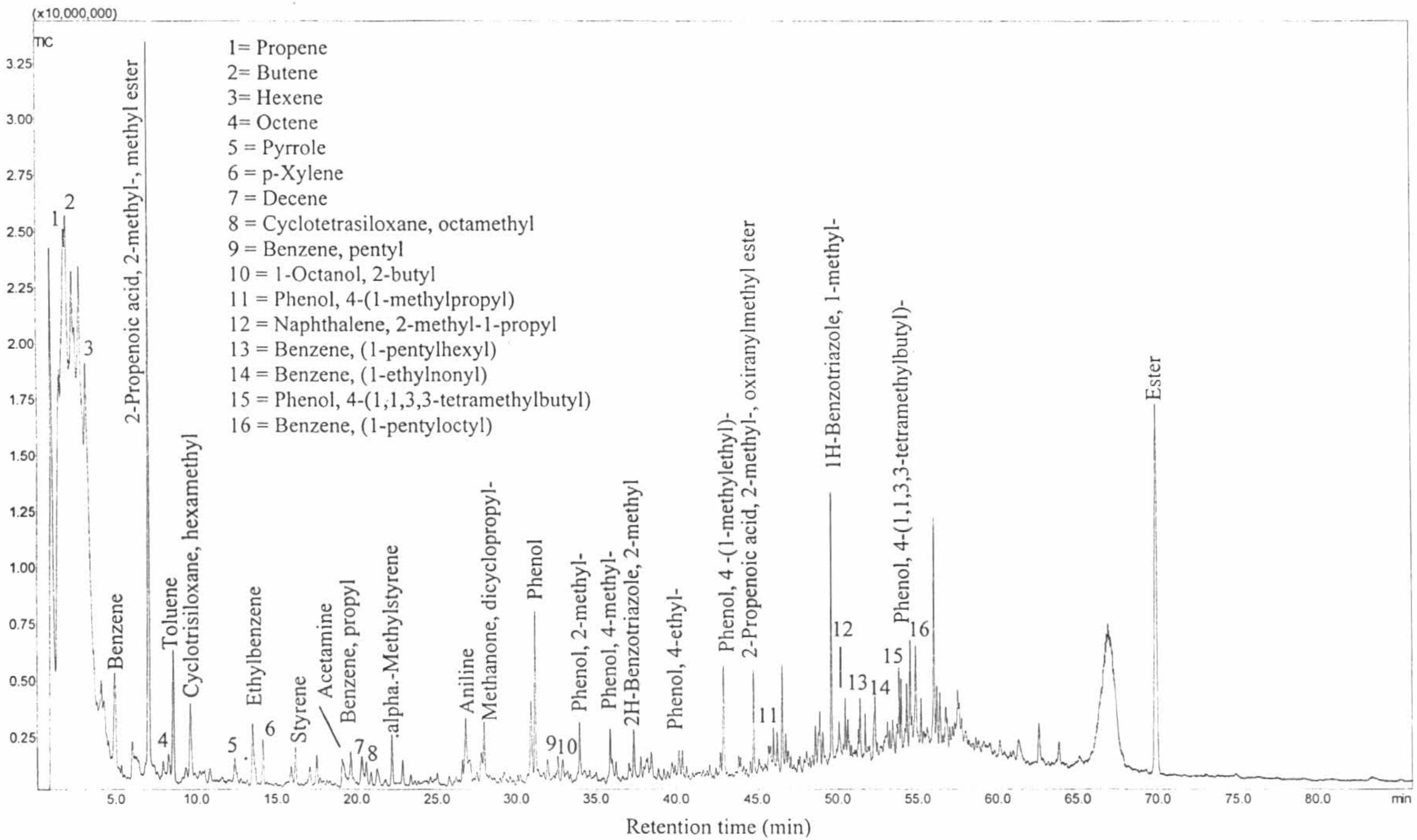

Figure B-13: Pyrochromatogram of major fragments of the HPON of the oxidation pond effluent

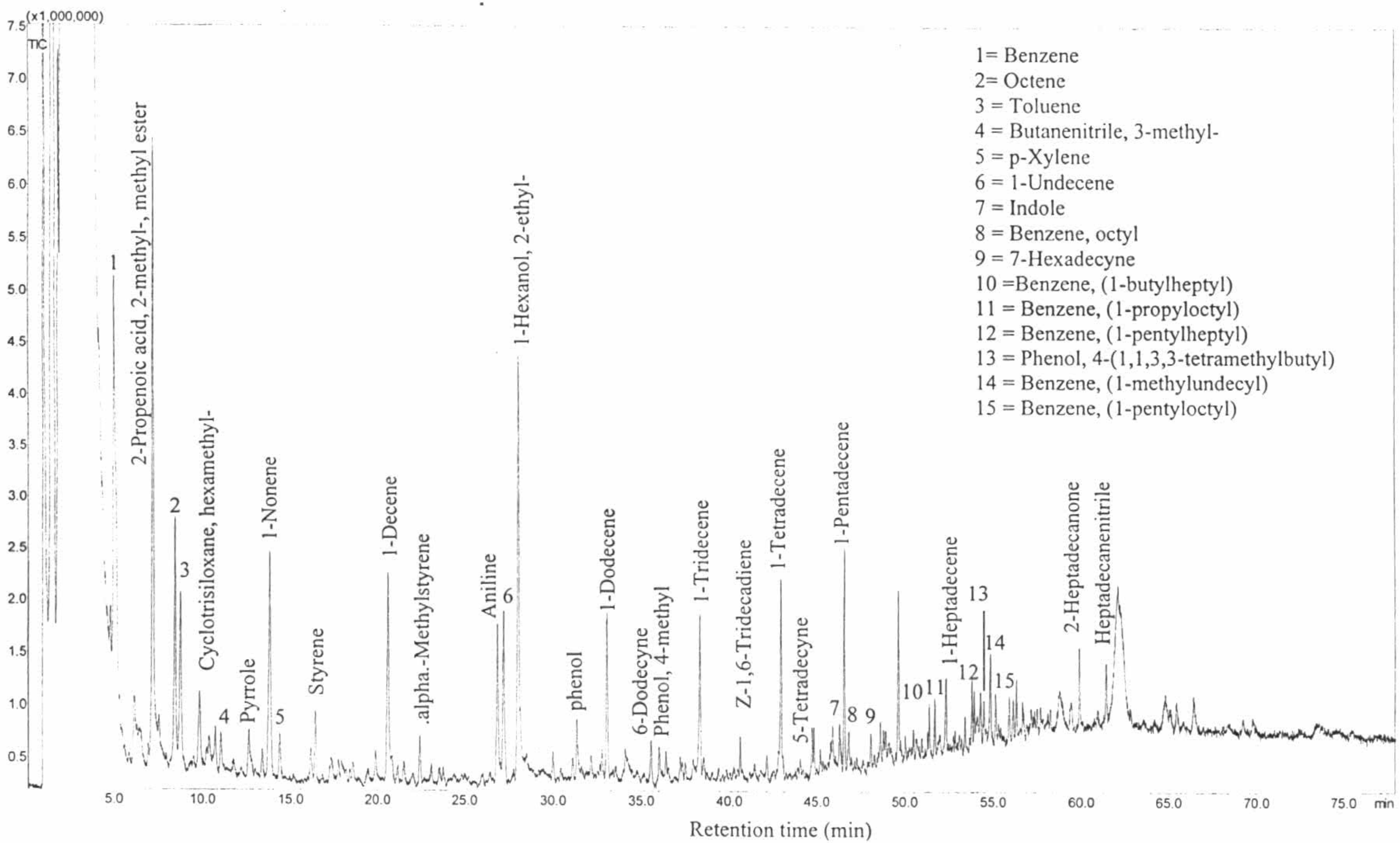

Figure B-14: Pyrochromatogram of major fragments of the HPON of the detention pond effluent

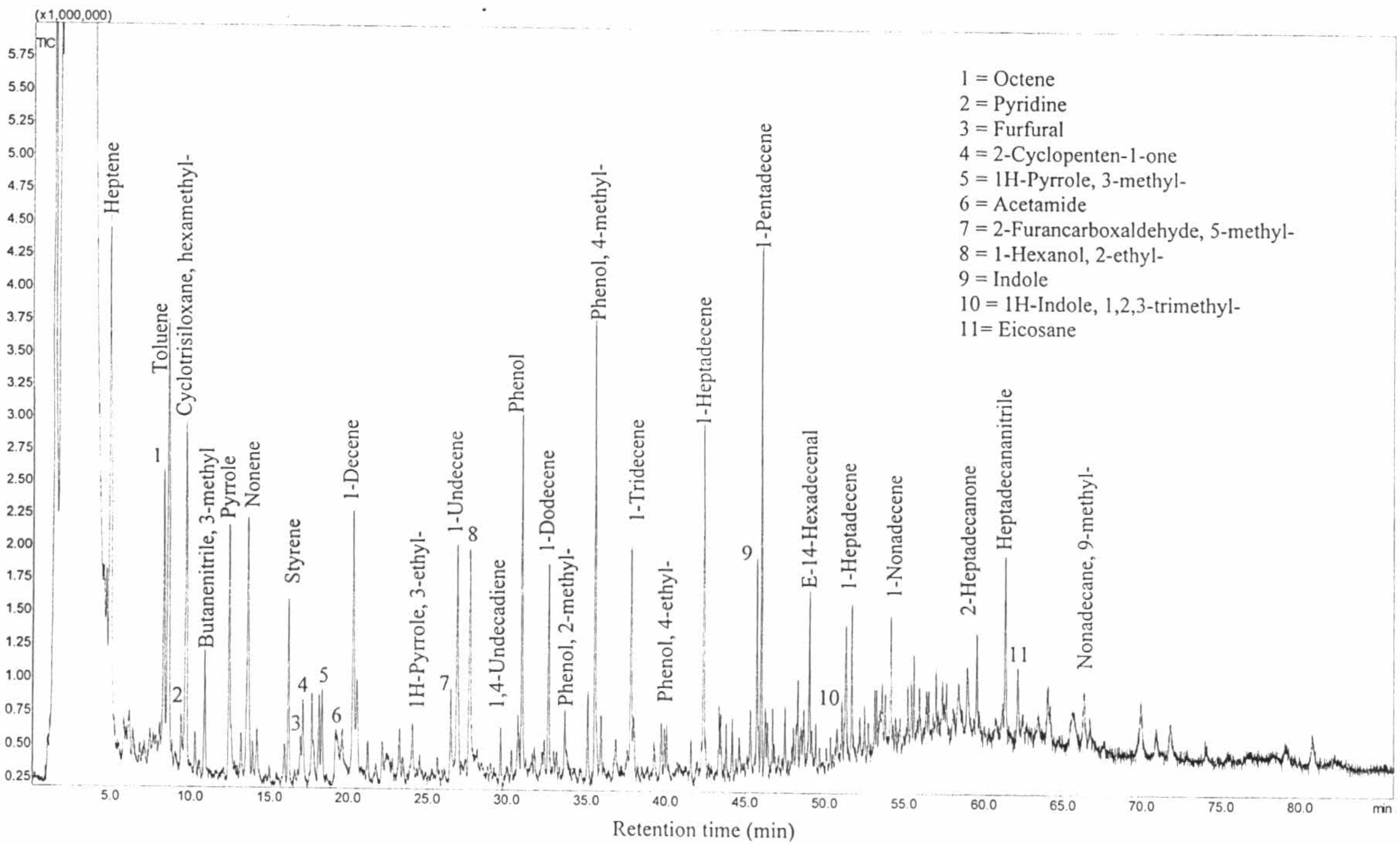

Figure B-15: Pyrochromatogram of major fragments of the HPOB of influent wastewater

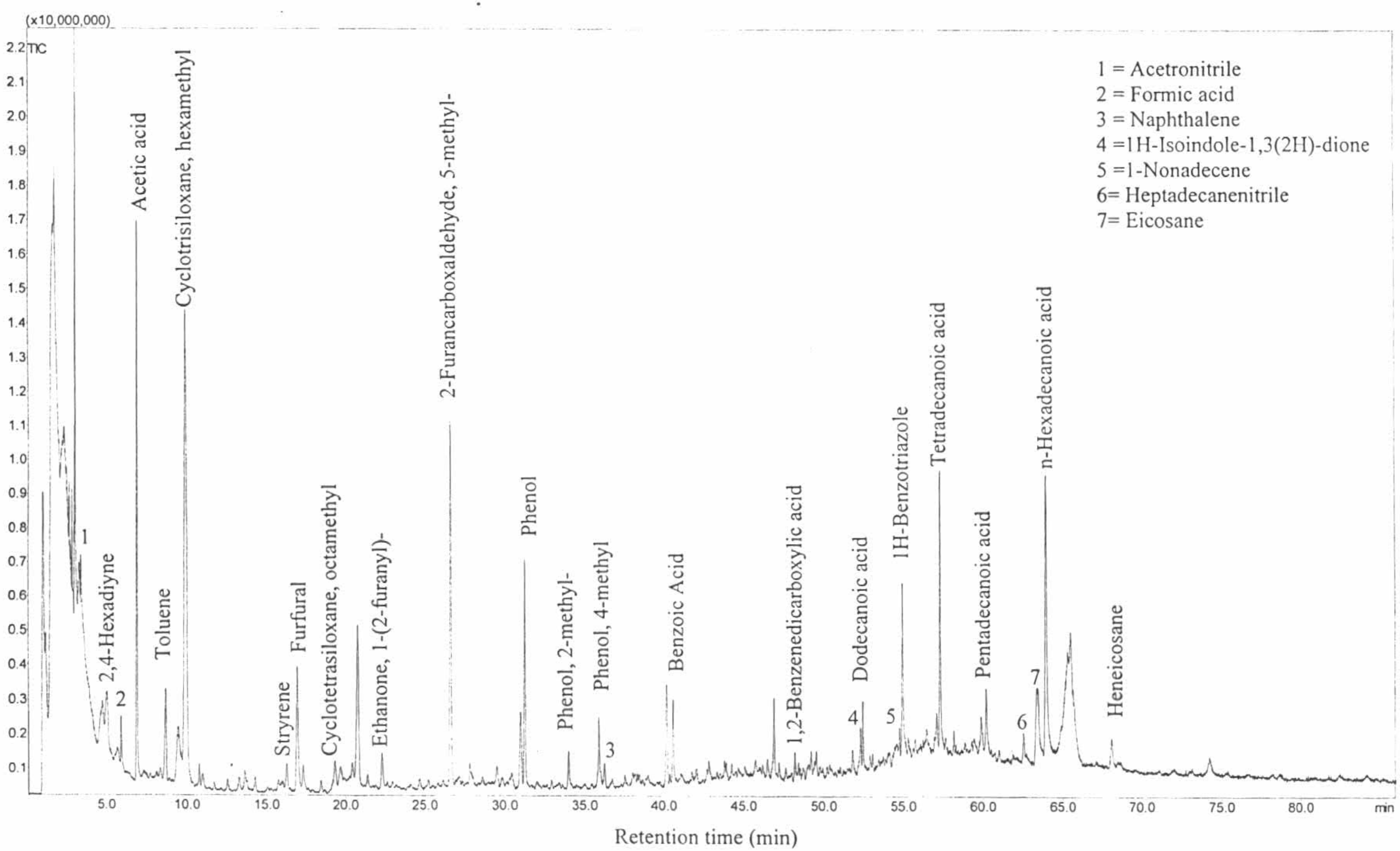

Figure B-16: Pyrochromatogram of major fragments of the HPOB of the aeration pond effluent

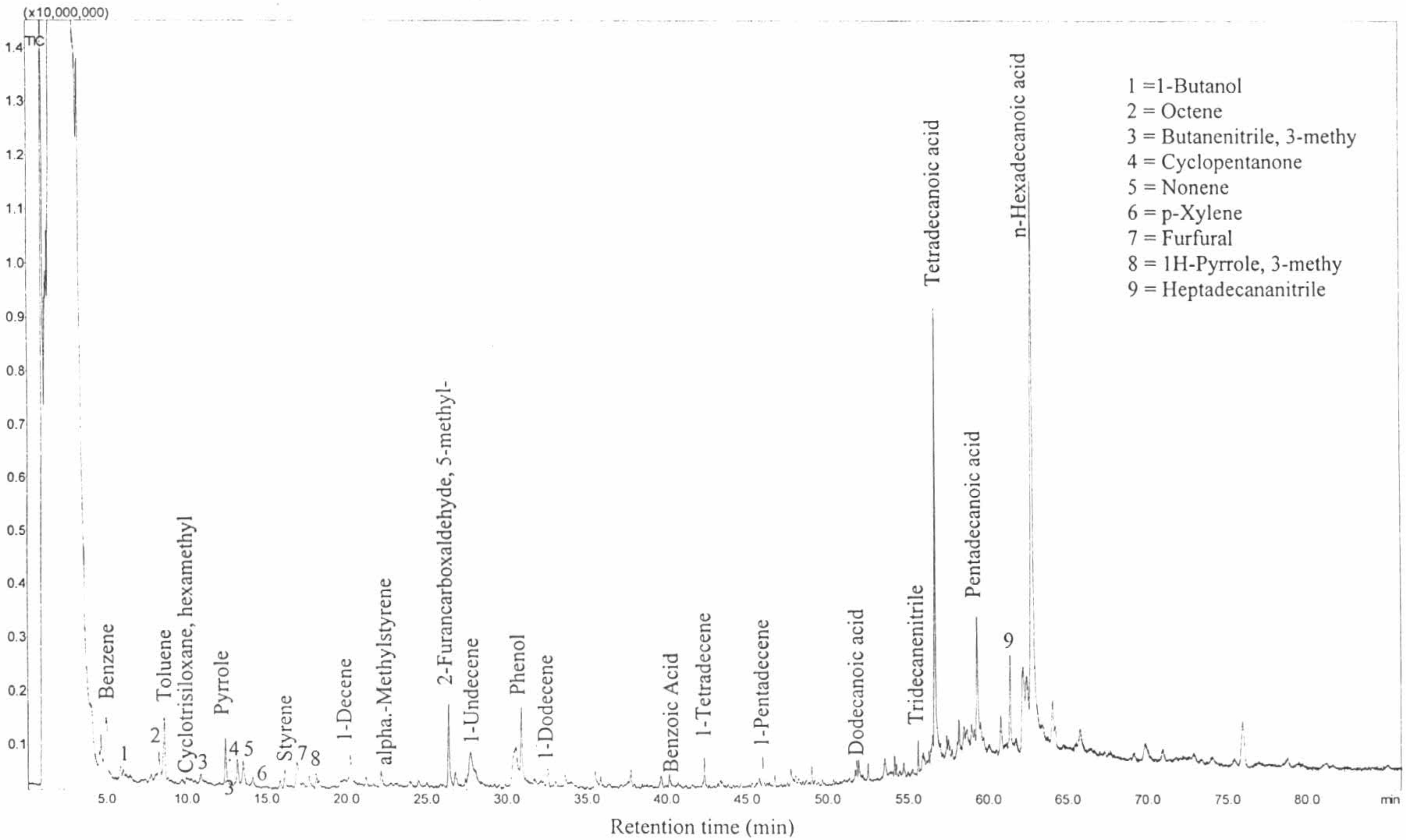

Figure B-17: Pyrochromatogram of major fragments of the HPOB of the facultative pond effluent

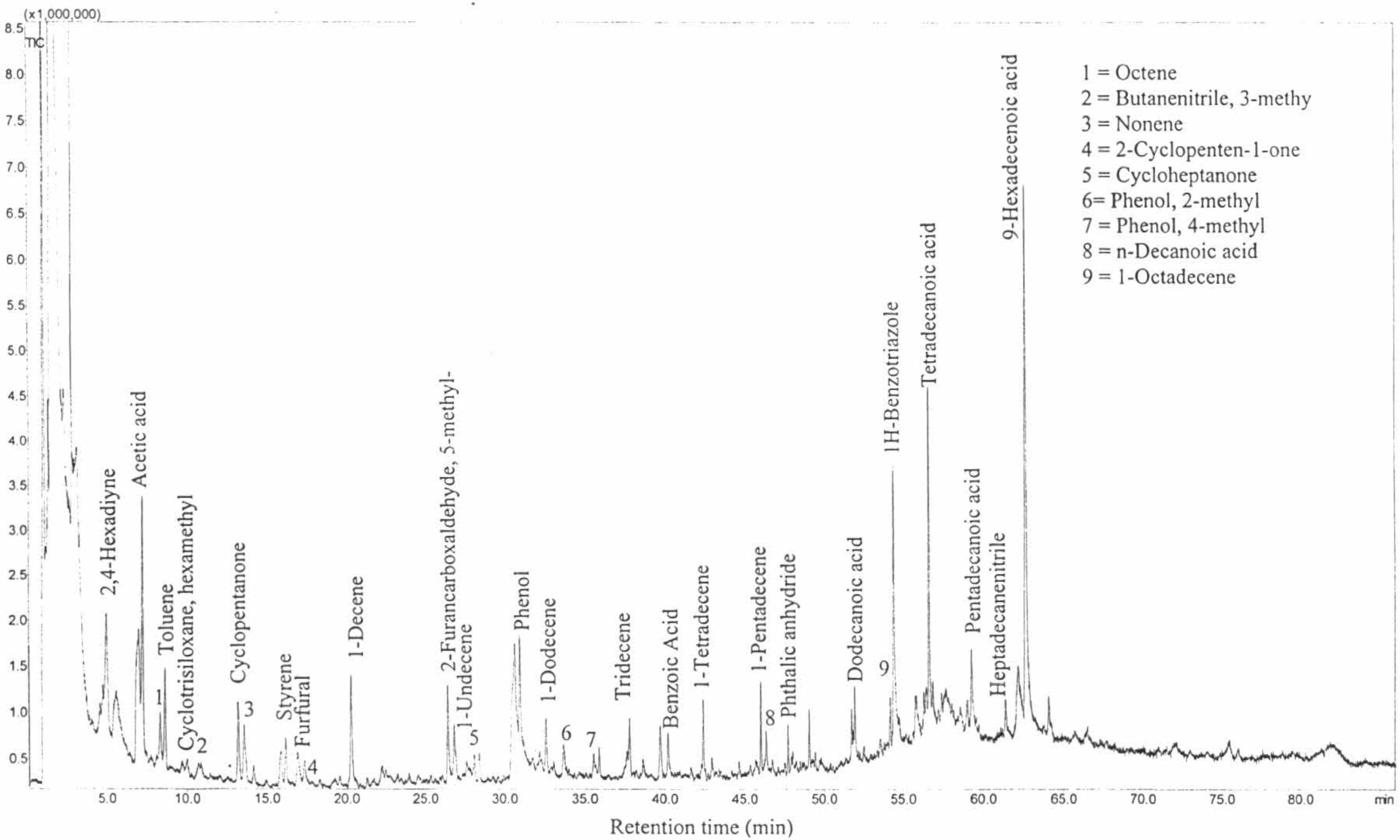

Figure B-18: Pyrochromatogram of major fragments of the HPOB of the oxidation pond effluent

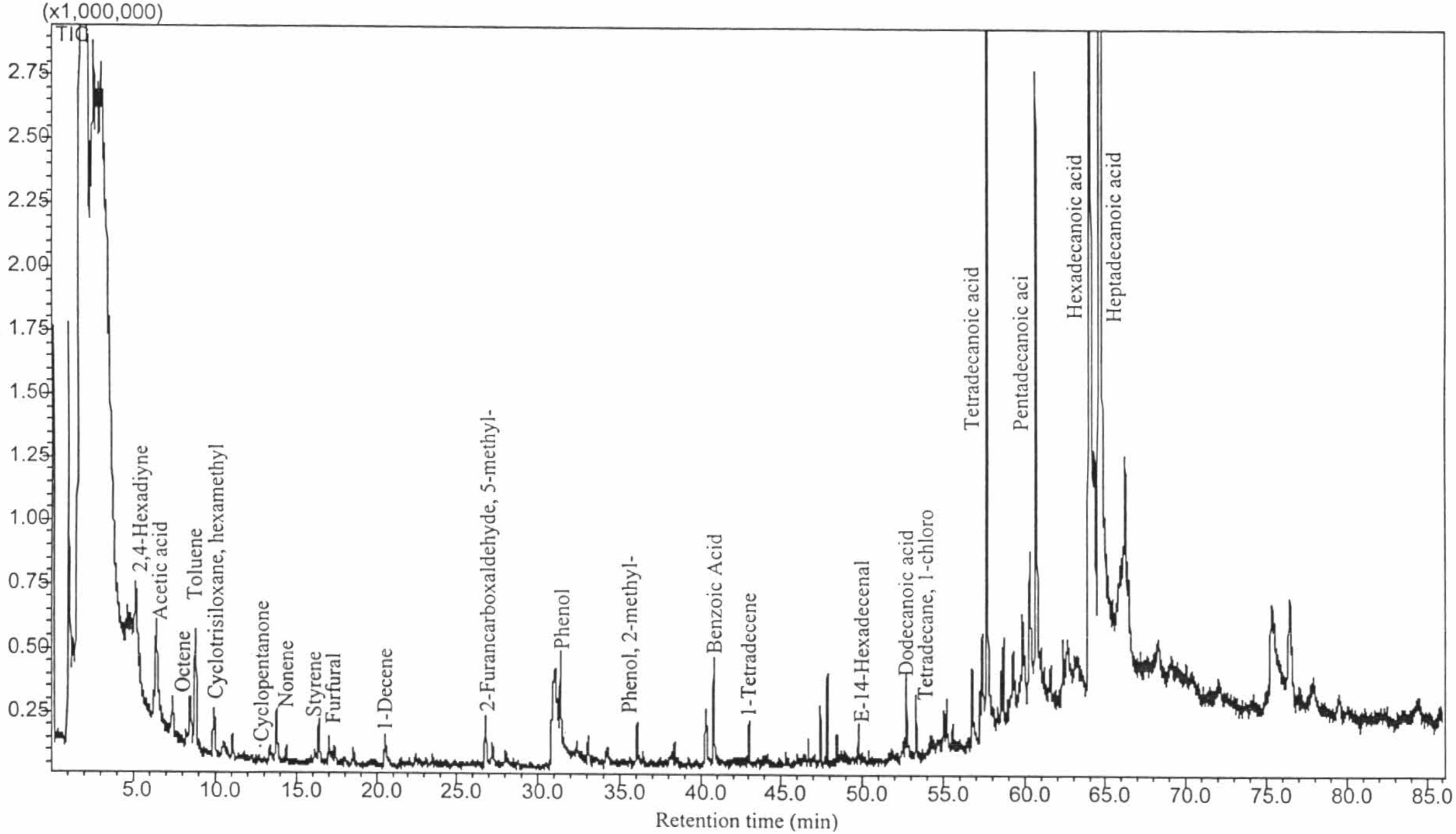

Figure B-19: Pyrochromatogram of major fragments of the HPOB of the detention pond effluent

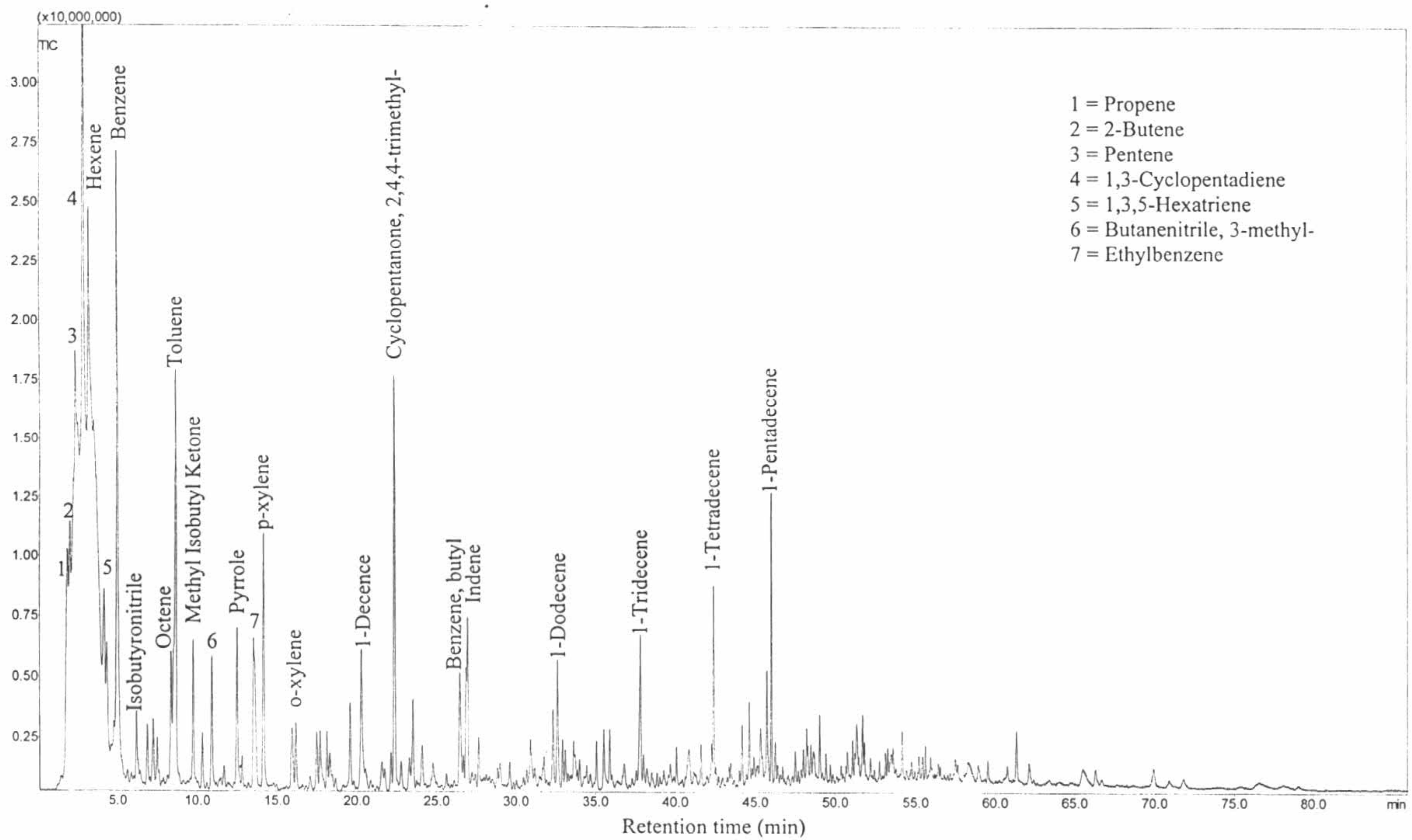

Figure B-20: Pyrochromatogram of major fragments of the HPOA of influent wastewater

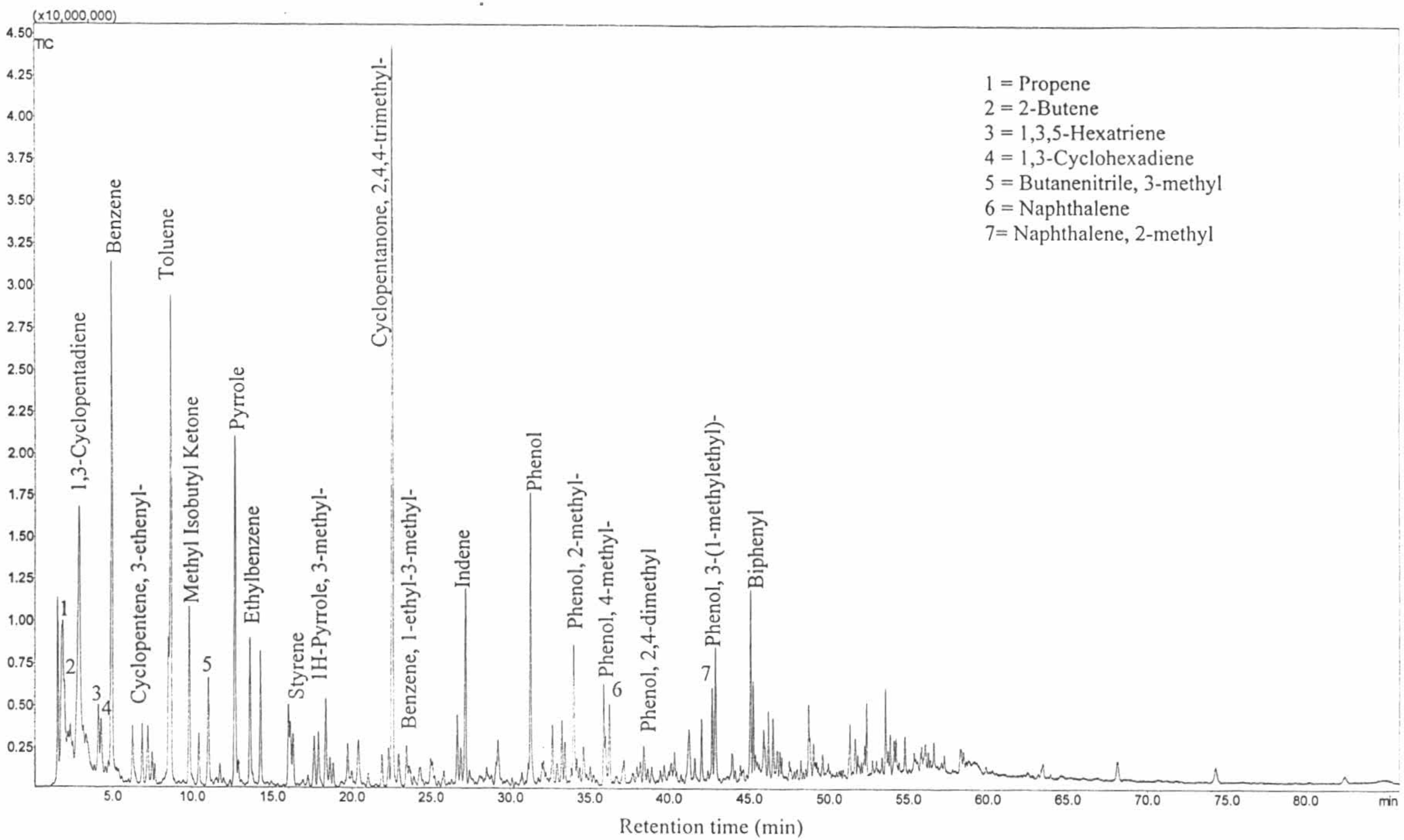

Figure B-21: Pyrochromatogram of major fragments of the HPOA of the aeration pond effluent

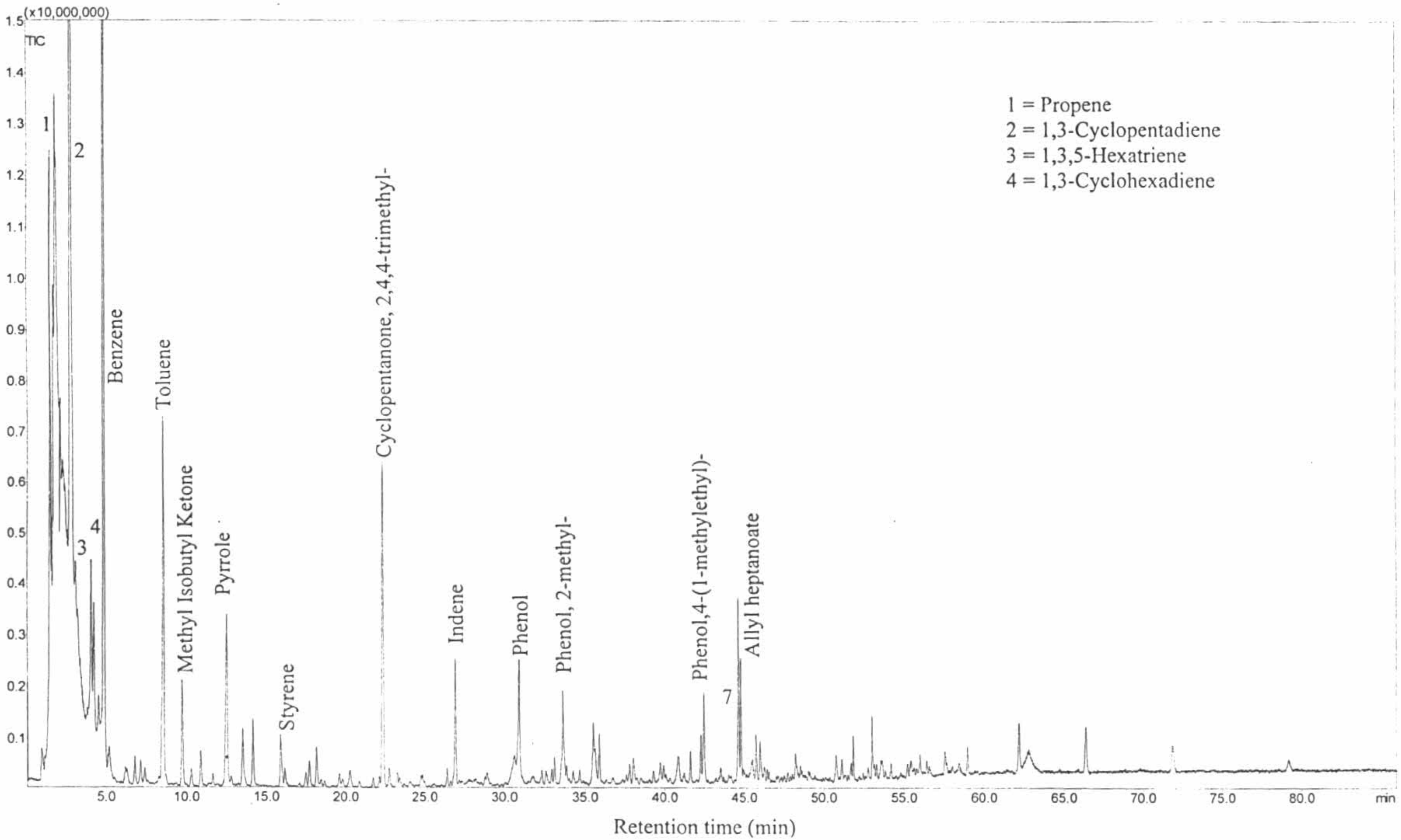

Figure B-22: Pyrochromatogram of major fragments of the HPOA of the facultative pond effluent

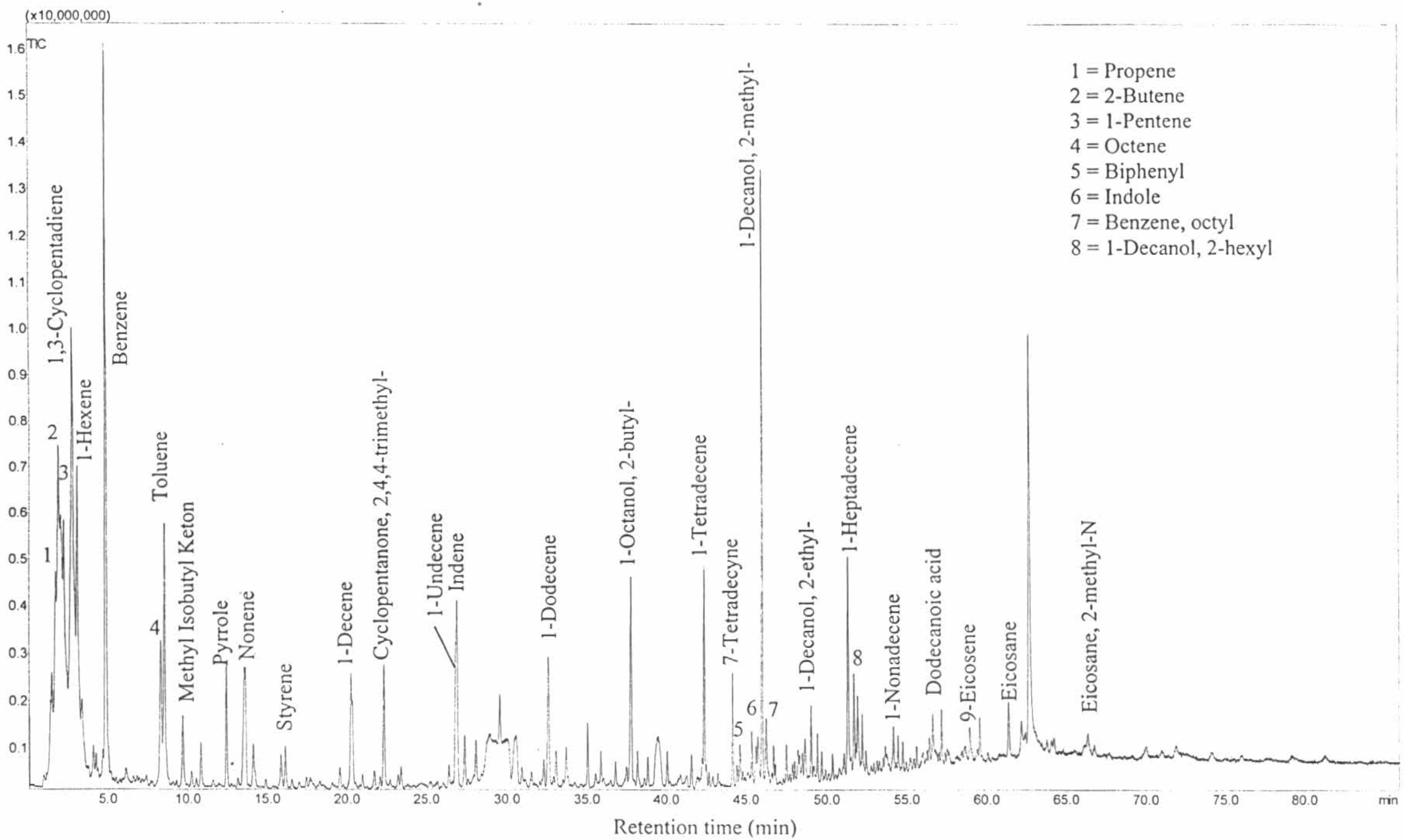

Figure B-23: Pyrochromatogram of major fragments of the HPOA of the oxidation pond effluent

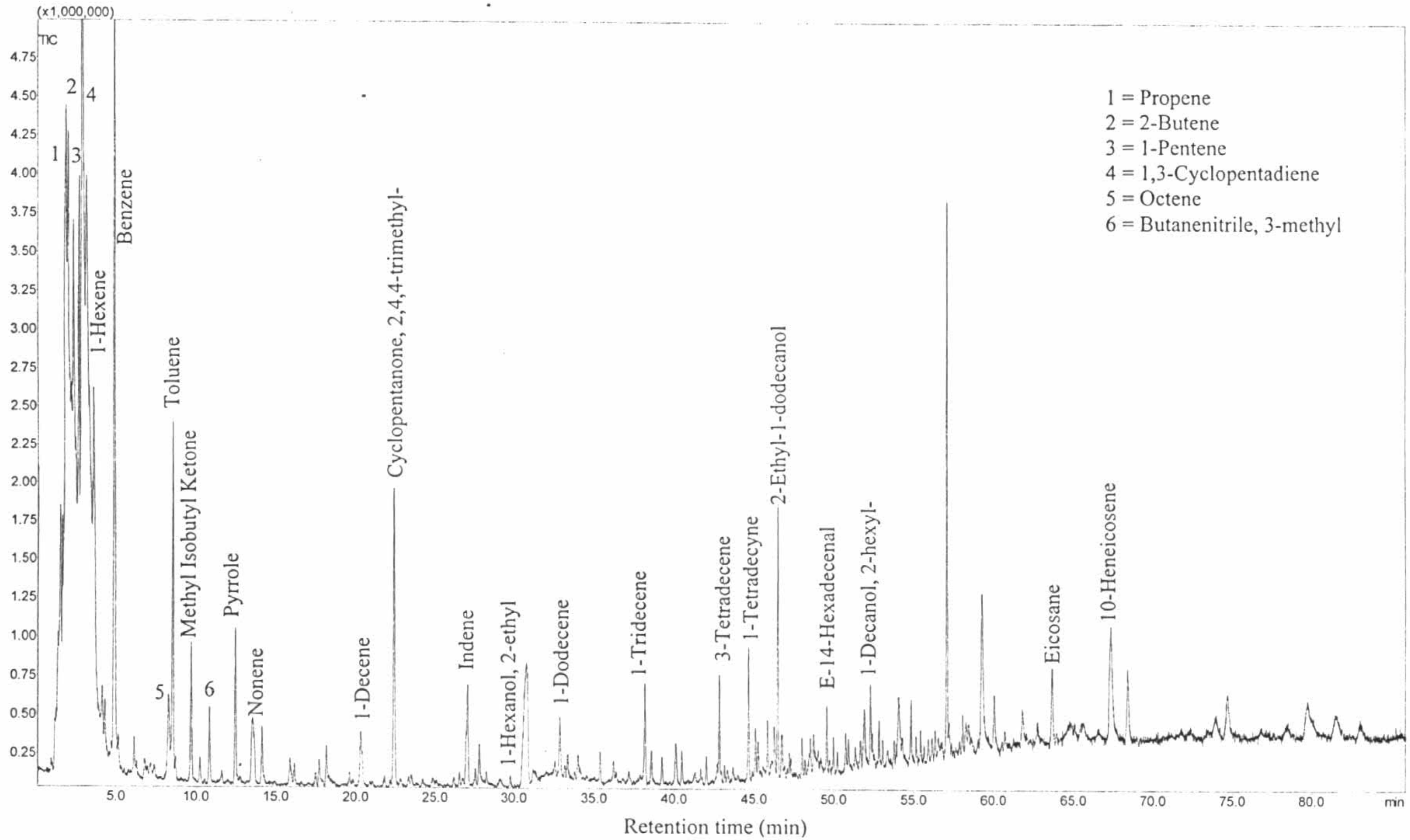

Figure B-24: Pyrochromatogram of major fragments of the HPOA of the detention pond effluent

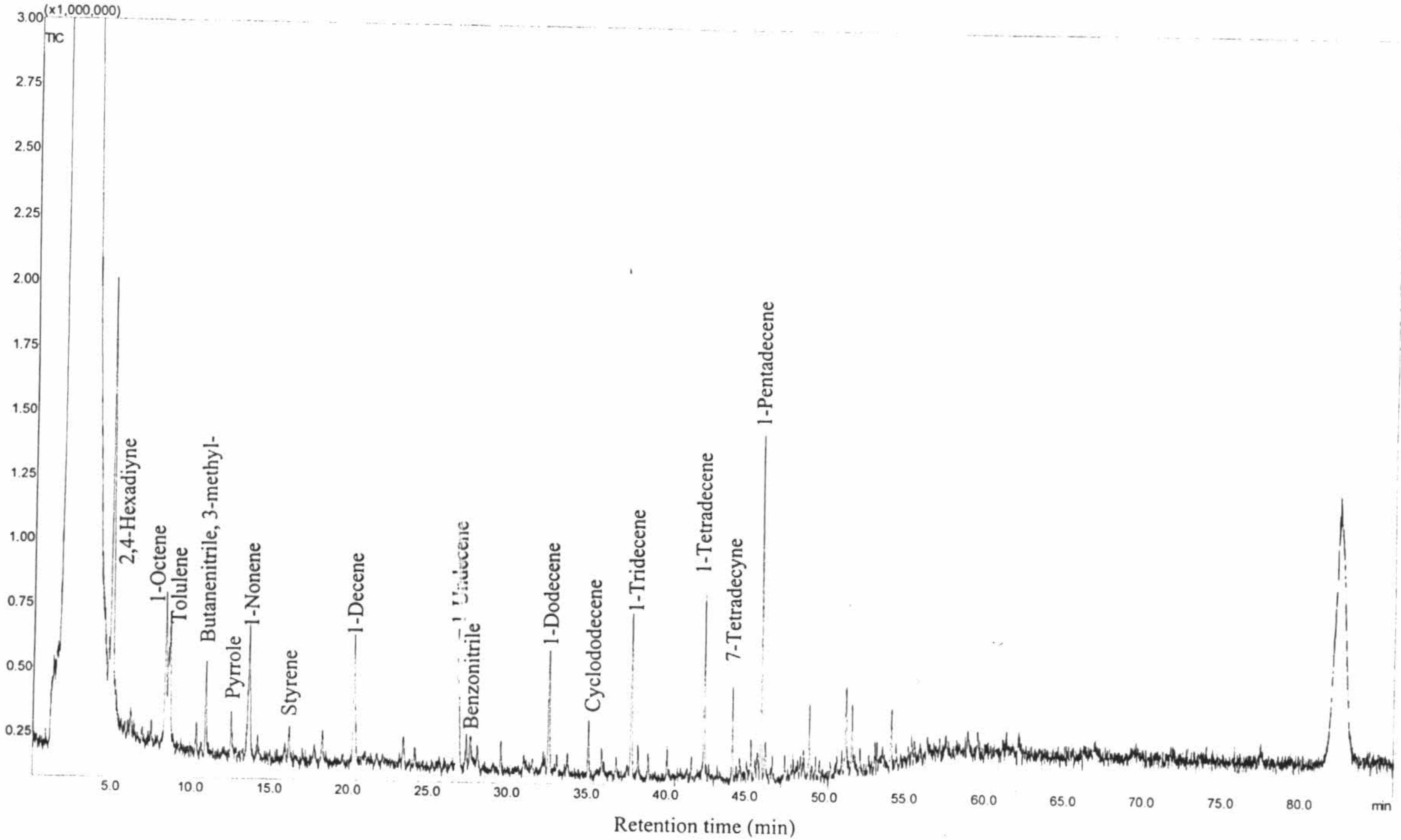

Figure B-25: Pyrochromatogram of major fragments of the HPIB of influent wastewater

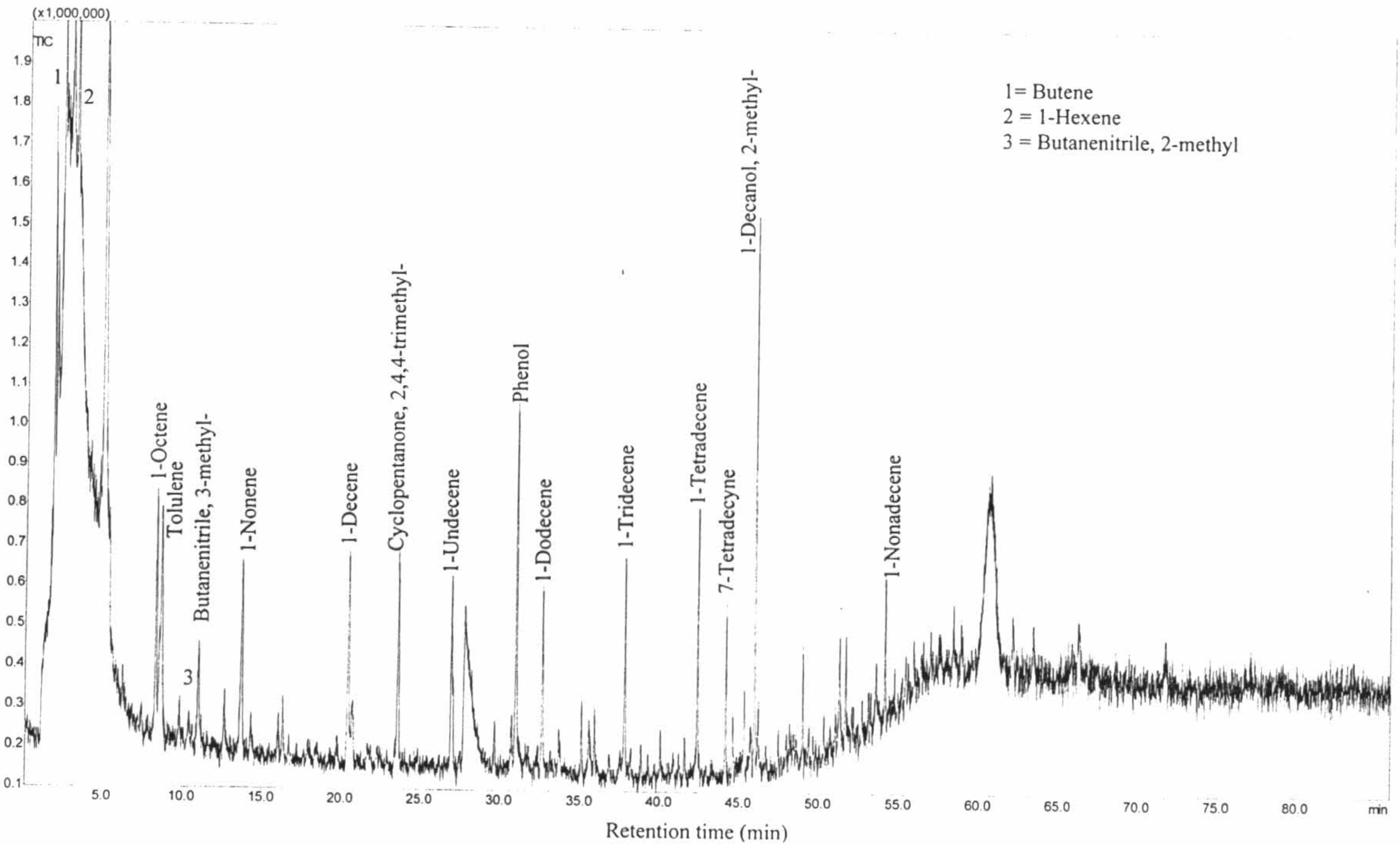

Figure B-26: Pyrochromatogram of major fragments of the HPIB of the aeration pond effluent

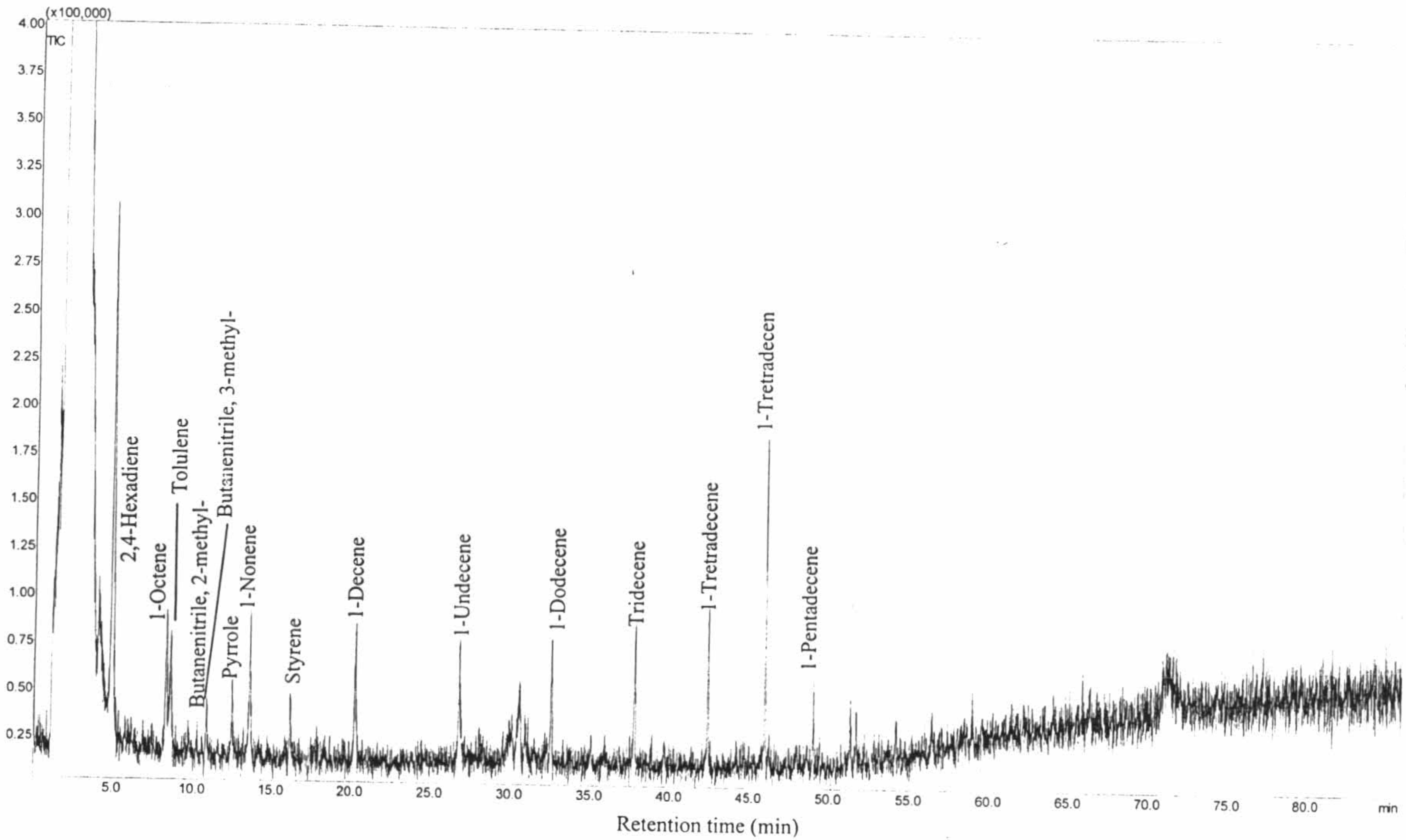

Figure B-27: Pyrochromatogram of major fragments of the HPIB of the facultative pond effluent

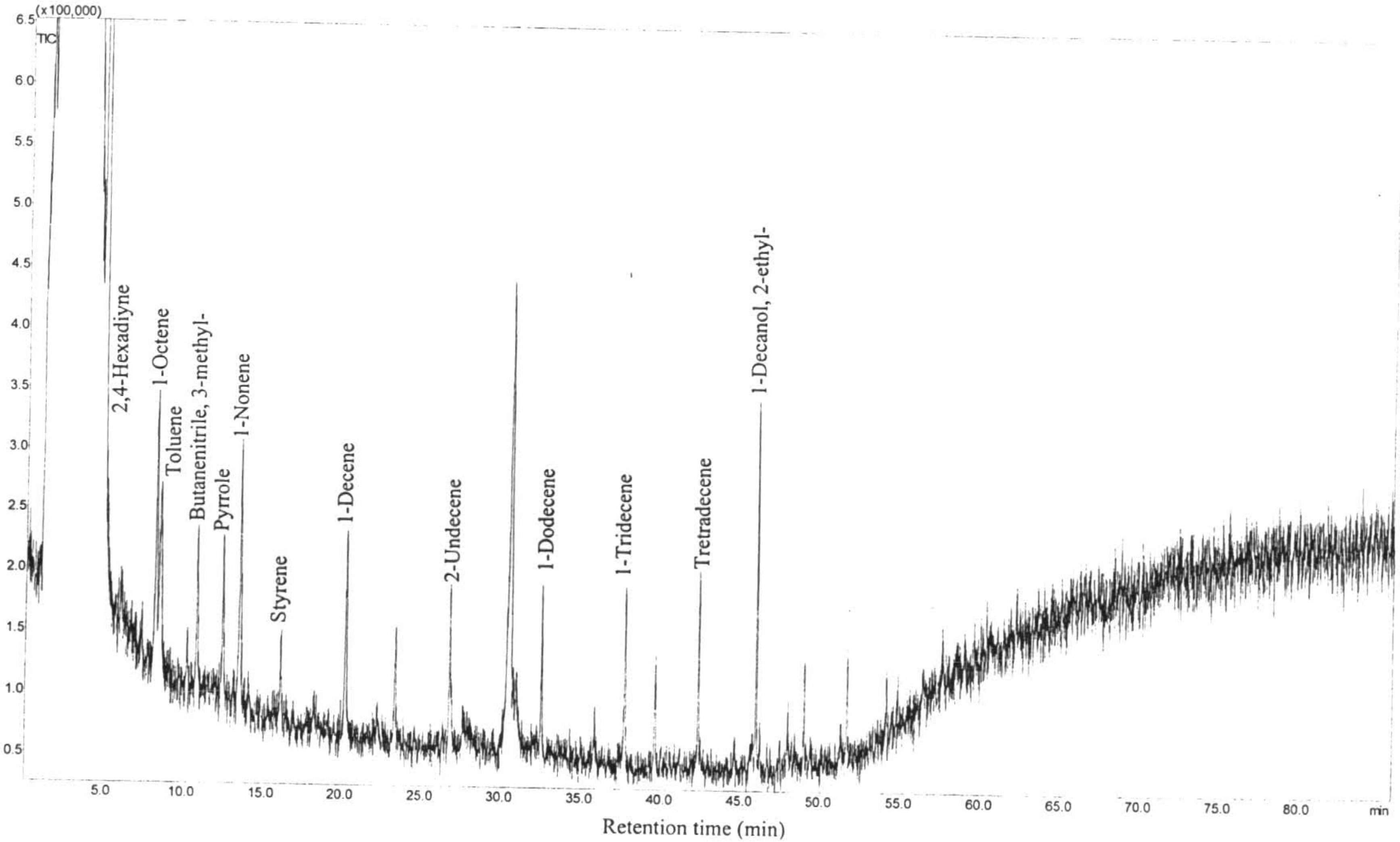

Figure B-28: Pyrochromatogram of major fragments of the HPIB of the oxidation pond effluent

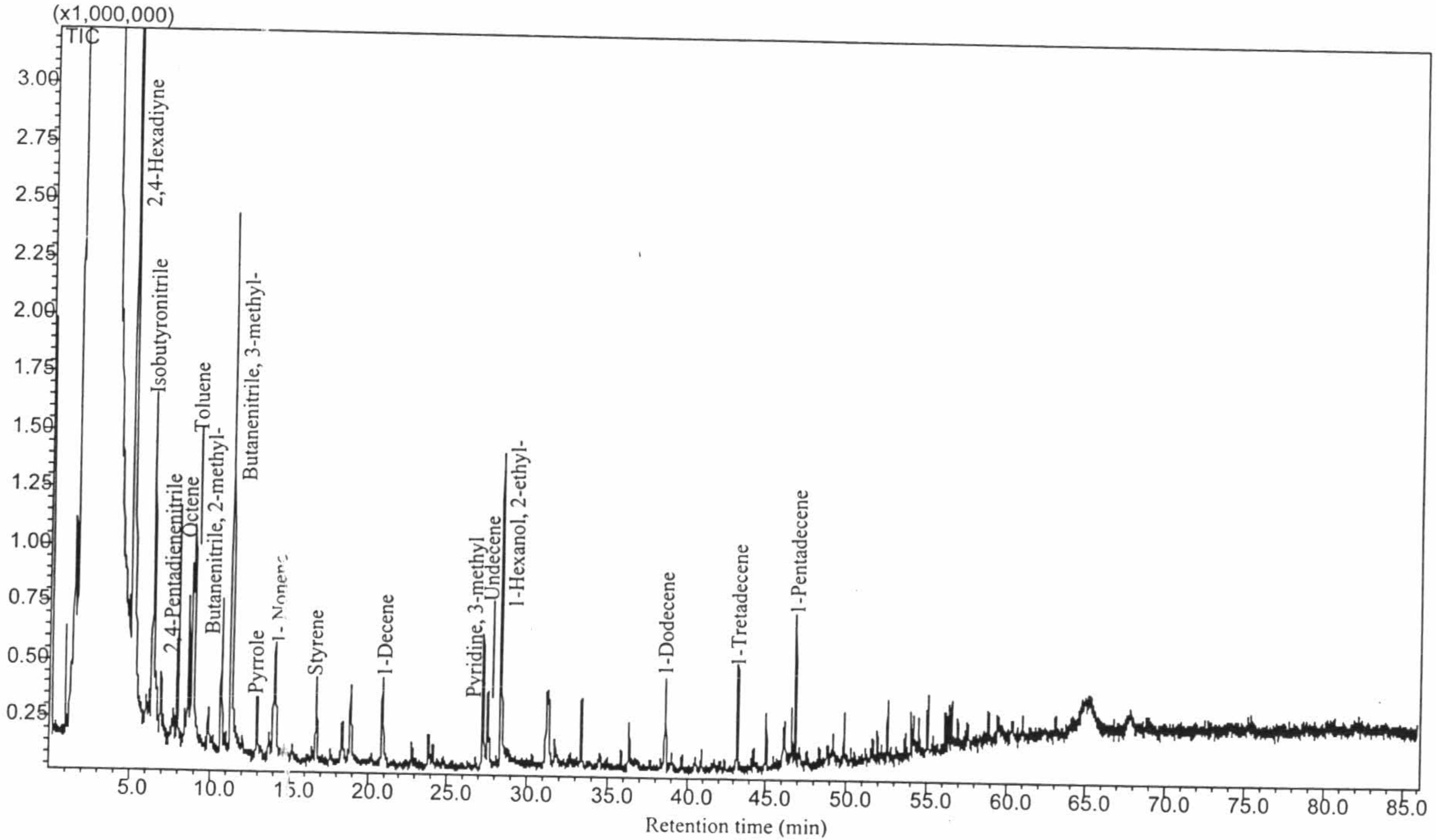

Figure B-29: Pyrochromatogram of major fragments of the HPIB of the detention pond effluent

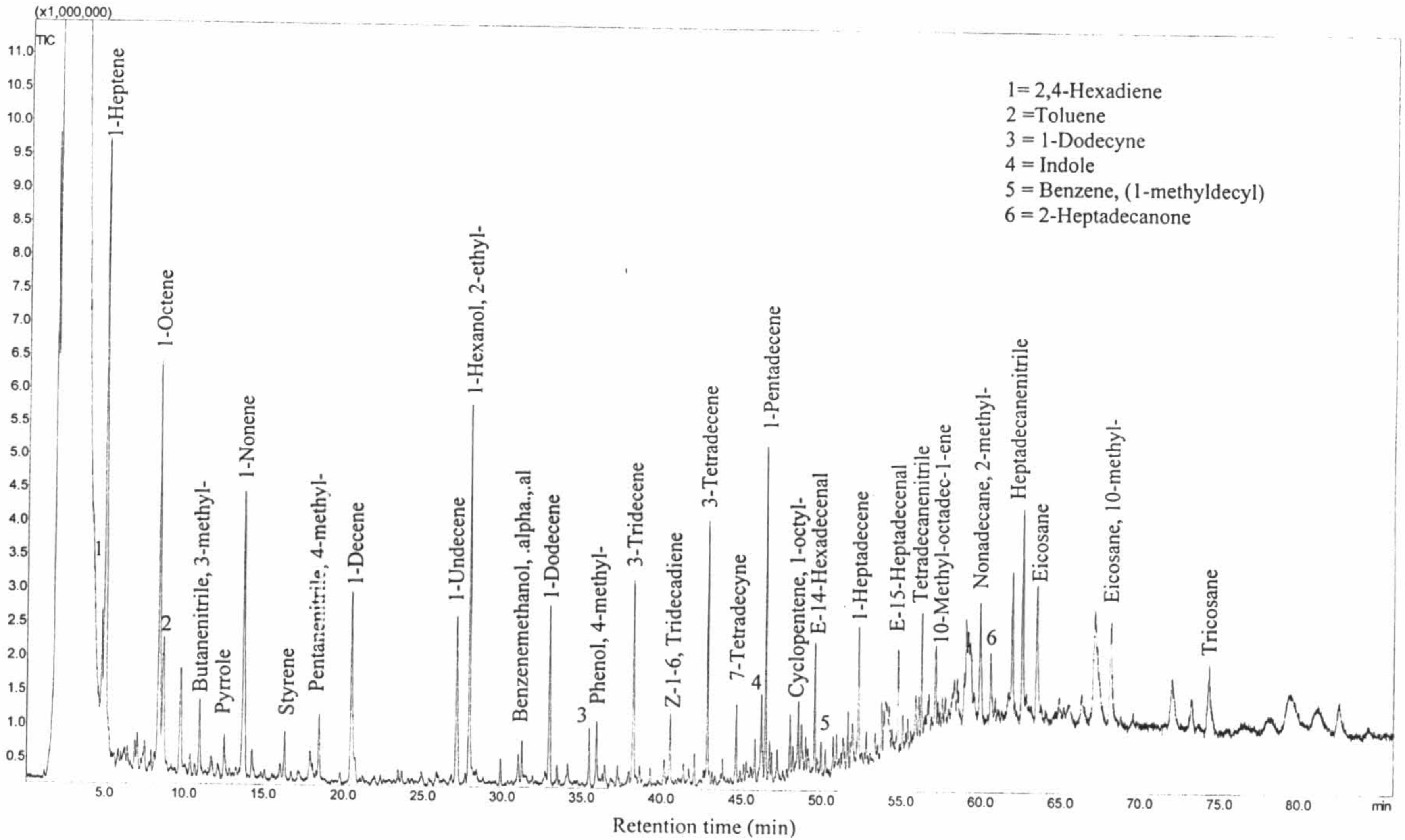

Figure B-30: Pyrochromatogram of major fragments of the HPIA of influent wastewater

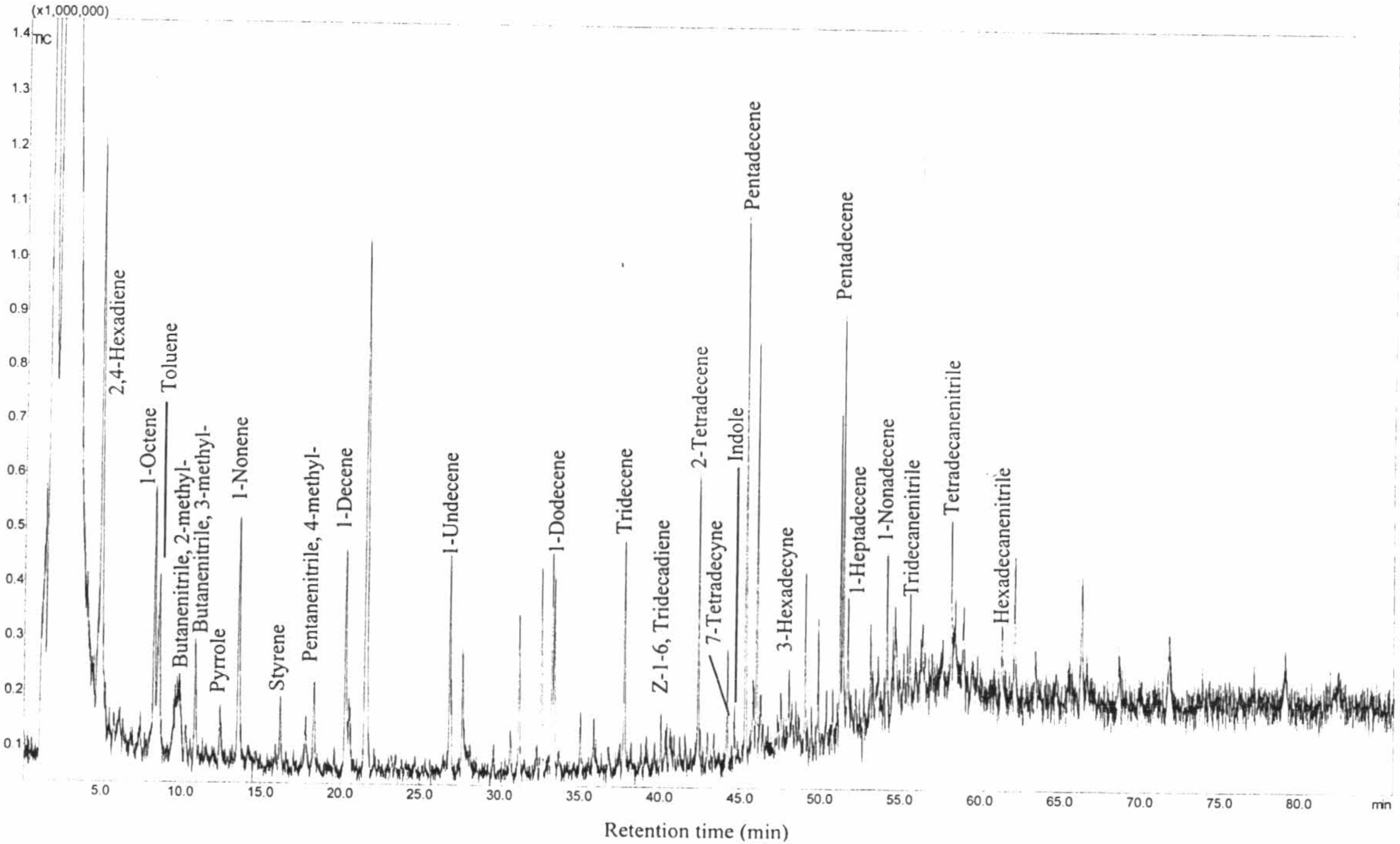

Figure B-31: Pyrochromatogram of major fragments of the HPIA of the aeration pond effluent

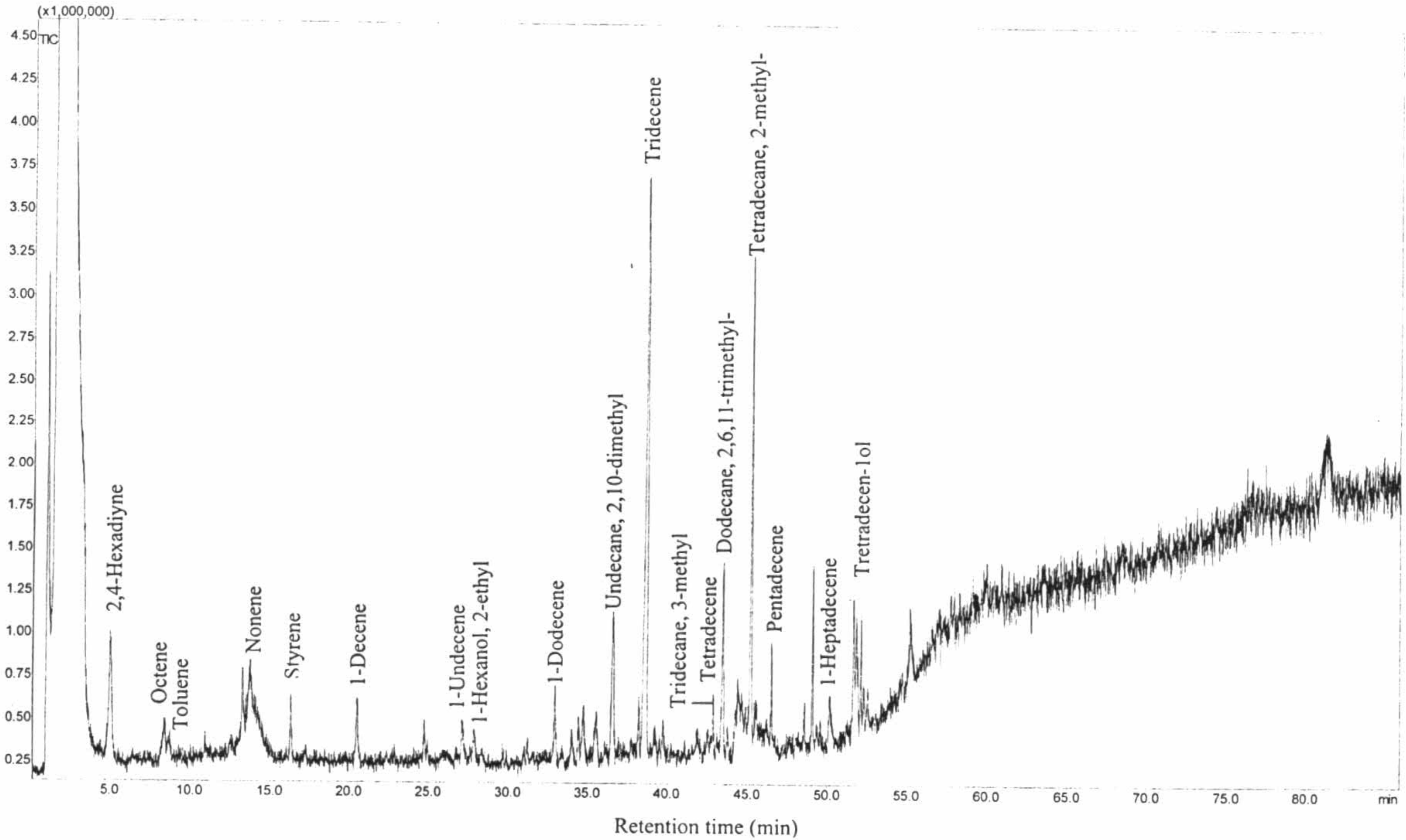

Figure B-32: Pyrochromatogram of major fragments of the HPIA of the facultative pond effluent

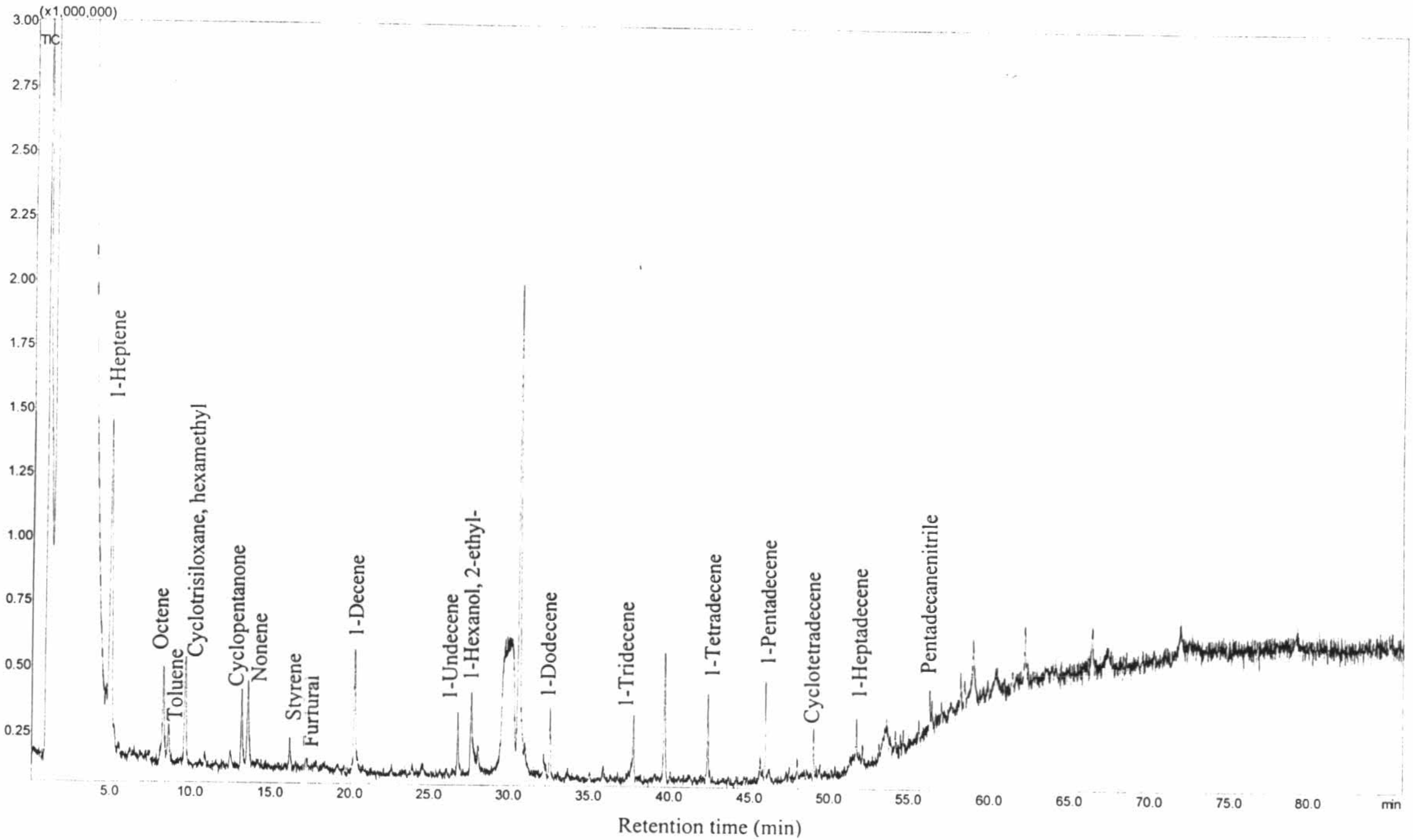

Figure B-33: Pyrochromatogram of major fragments of the HPIA of the oxidation pond effluent

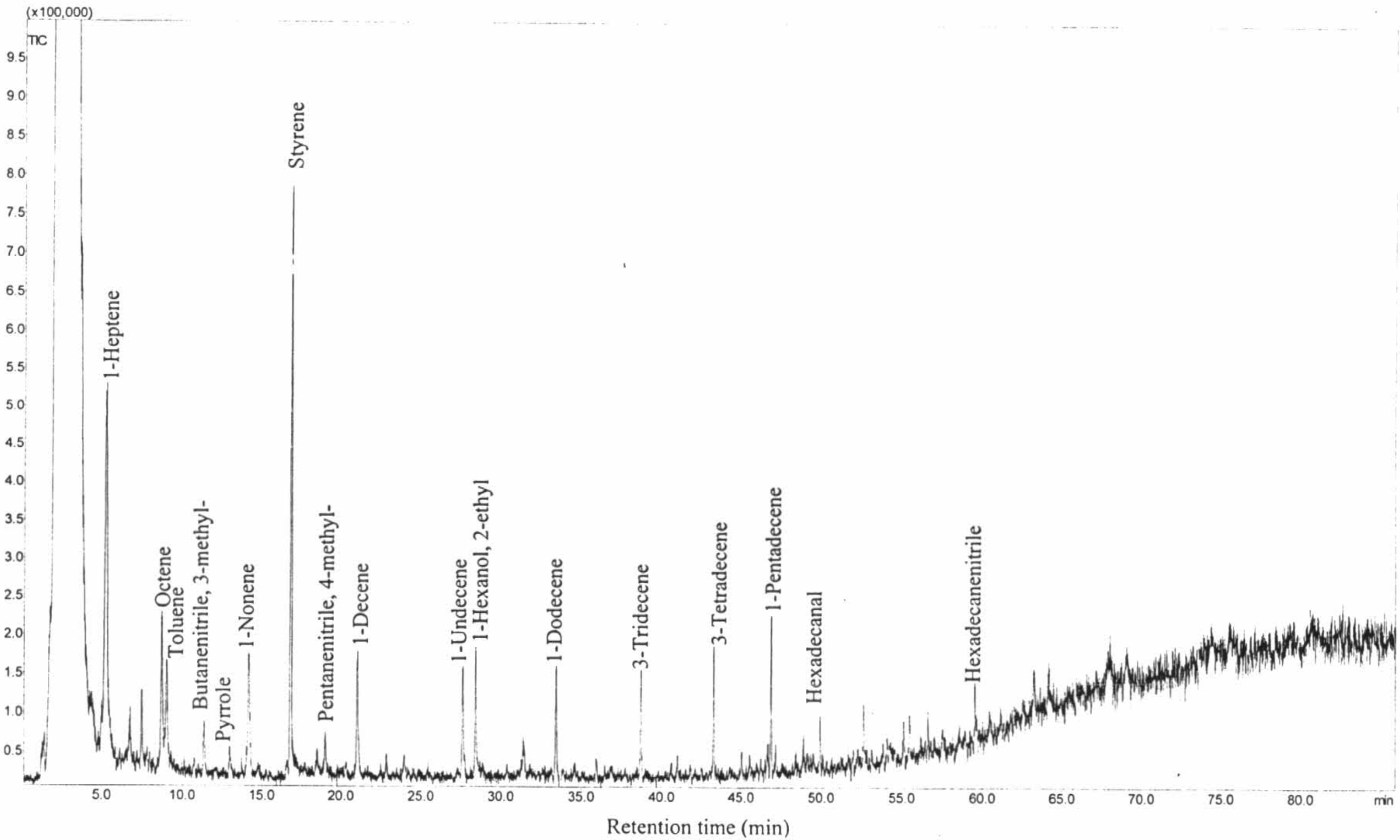

Figure B-34: Pyrochromatogram of major fragments of the HPIA of the detention pond effluent

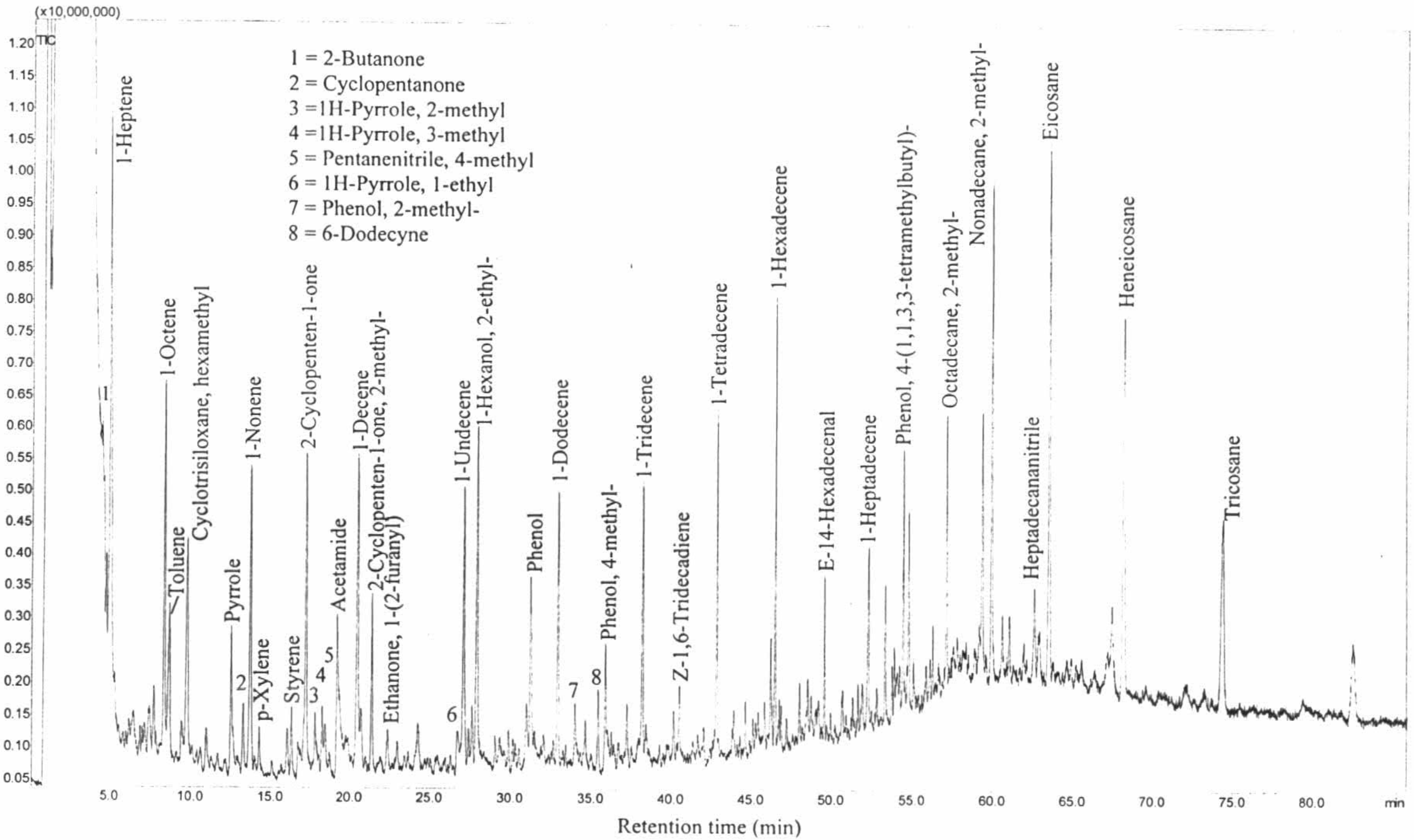

Figure B-35: Pyrochromatogram of major fragments of the HPIN of influent wastewater

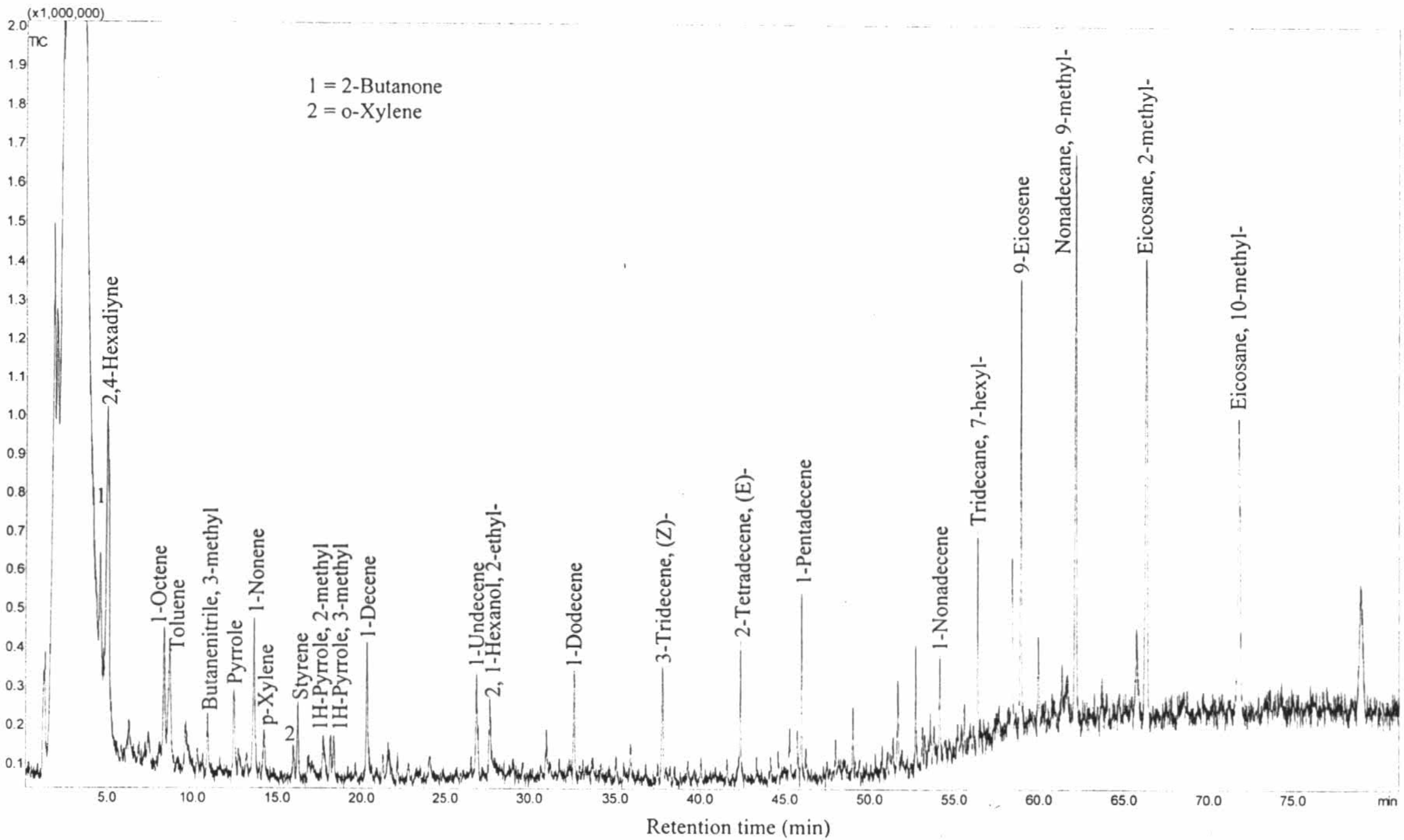

Figure B-36: Pyrochromatogram of major fragments of the HPIN of the aeration pond effluent

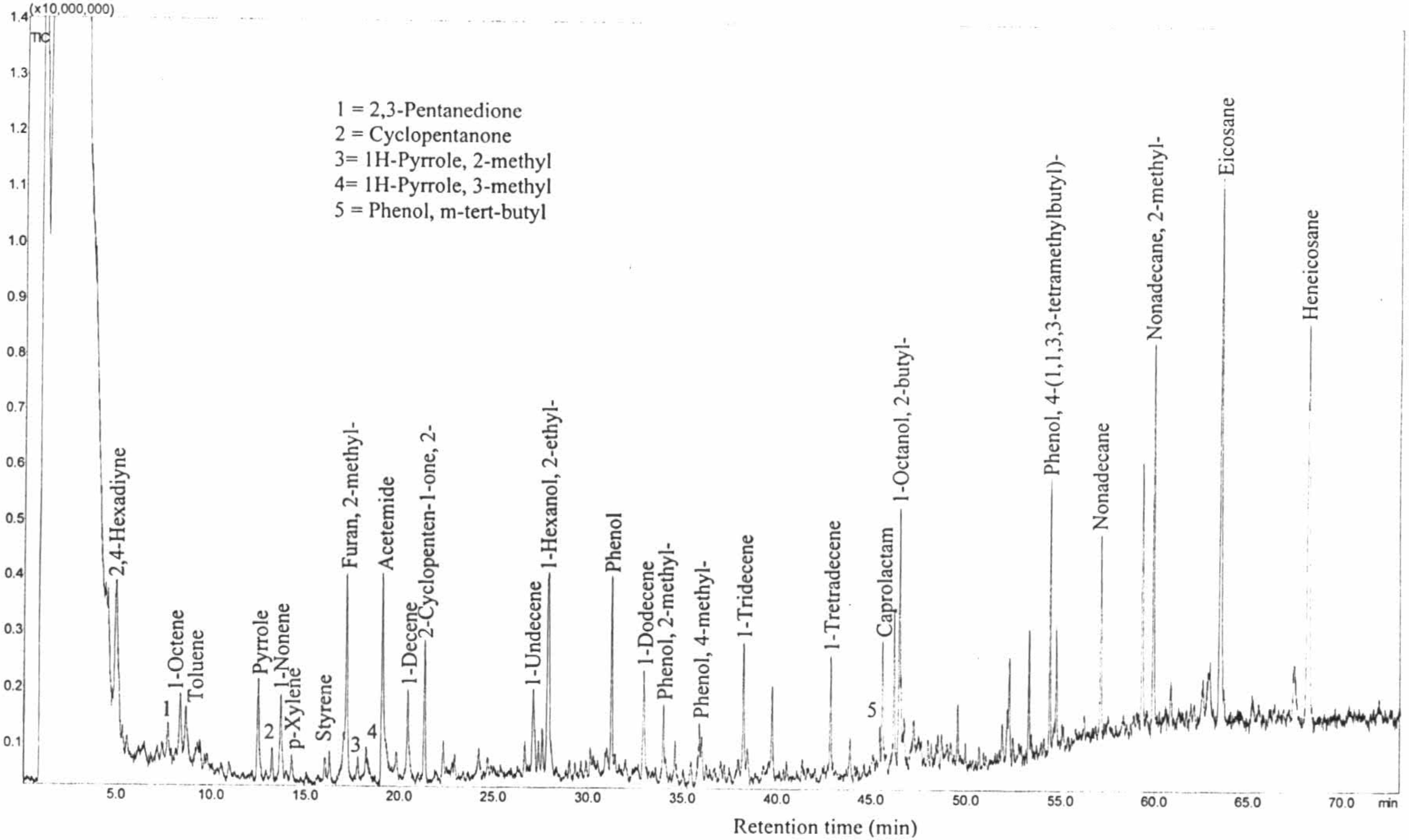

Figure B-37: Pyrochromatogram of major fragments of the HPIN of the facultative pond effluent

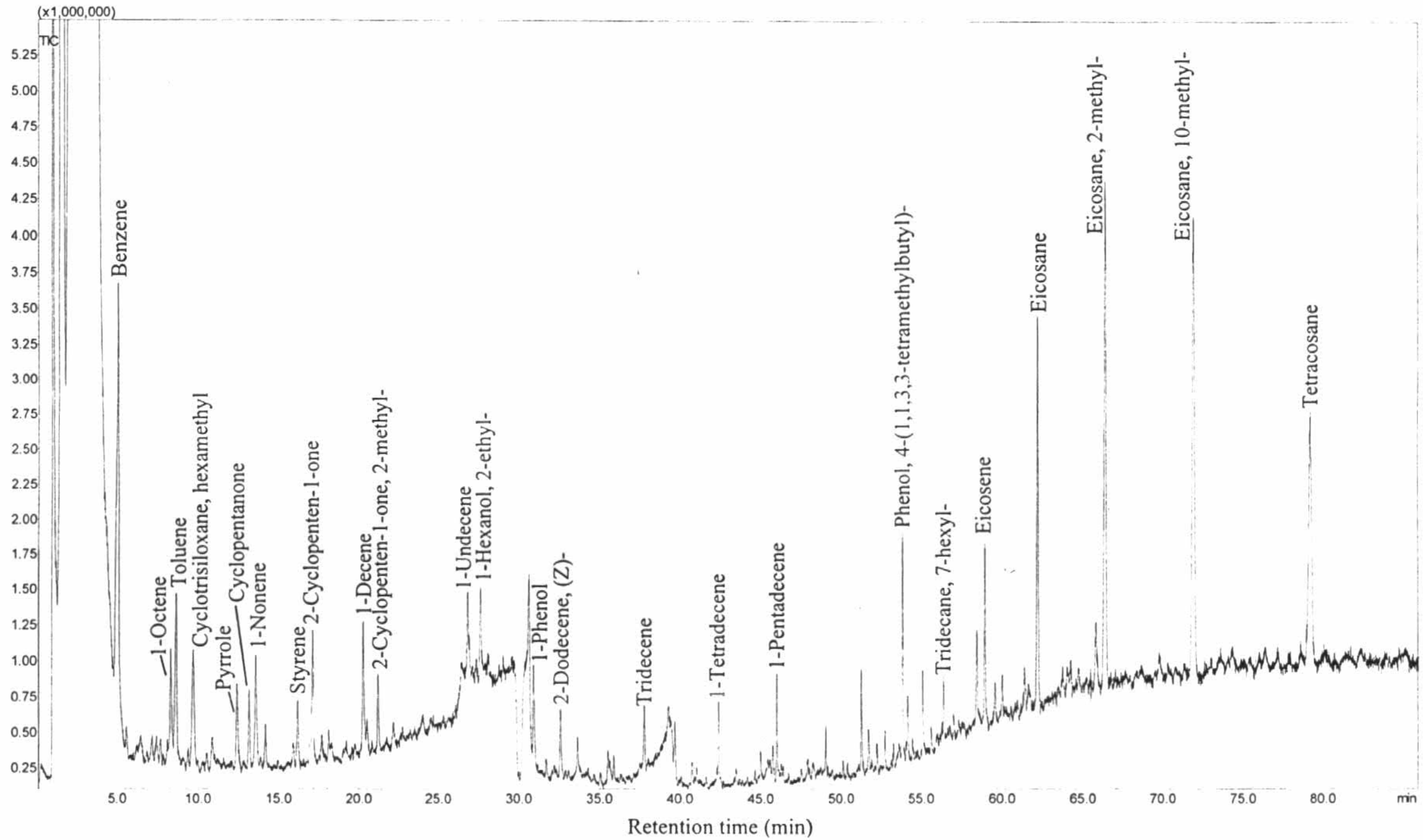

Figure B-38: Pyrochromatogram of major fragments of the HPIN of the oxidation pond effluent

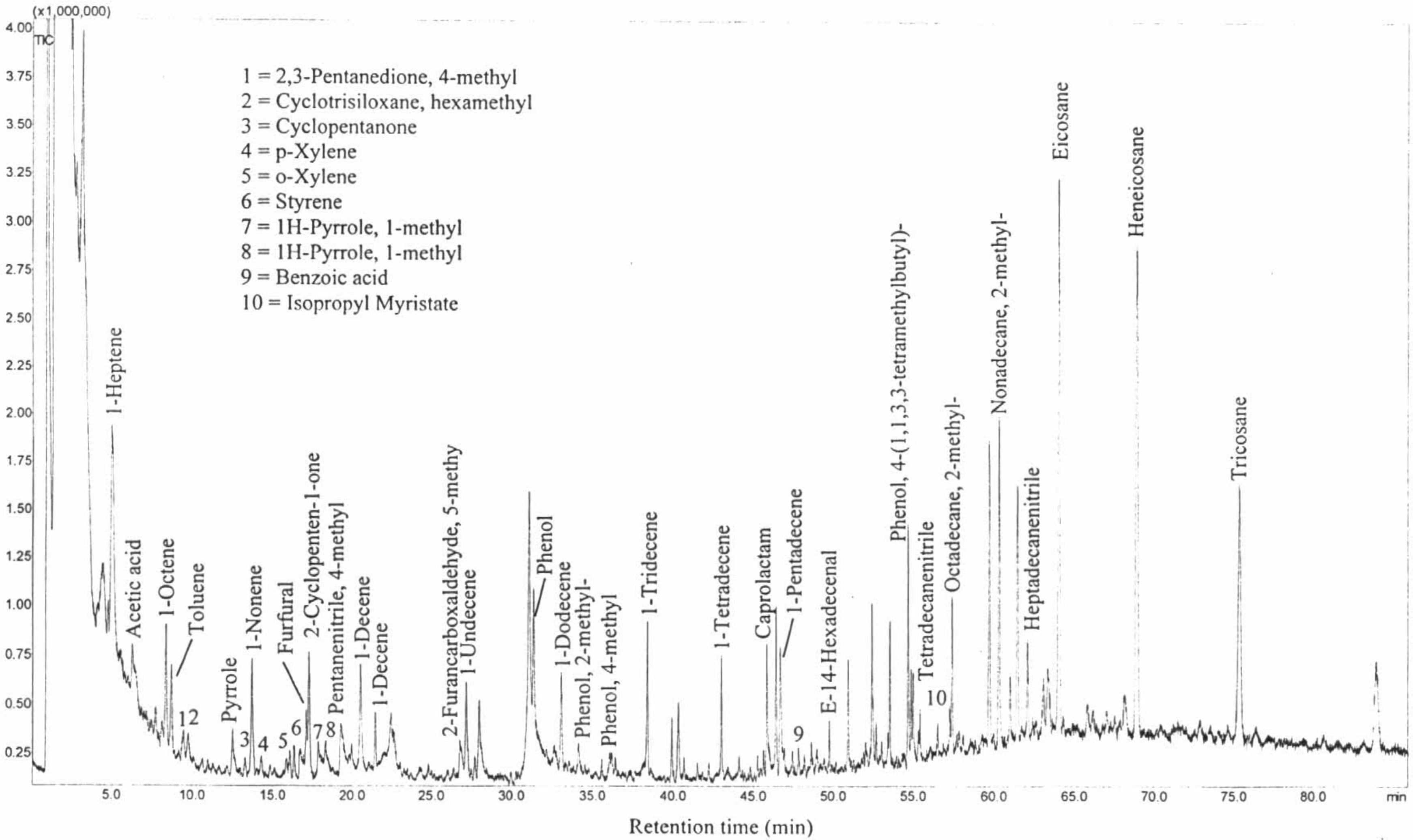

Figure B-39: Pyrochromatogram of major fragments of the HPIN of the detention pond effluent

APPENDIX C

ADVANTAGES, DISADVANTAGES AND LIMITATIONS OF DOM CHARACTERIZATION USING RESIN FRACTIONATION, PYROLYSIS GC/MS AND SPECTROFLUOROMETRY

Advantages, Disadvantages, and Limitations of DOM characterization Using Resin Fractionation, Pyrolysis GC/MS and Spectrofluorometry

The resin fractionation, pyrolysis gas chromatography mass spectrometer (GC/MS) and spectrofluorometry methods were utilized to characterize the dissolved organic matter (DOM) in industrial estate wastewater and effluent water from the aeration, facultative, oxidation and detention ponds of the Northern-Region Industrial Estate, Lamphun province, Thailand. The advantages, disadvantages and limitations using these three techniques to characterize DOM have been summarized according to the sample preparation, analytical and data interpretation processes of each technique.

Resin Fractionation

Resin fractionation of DOM in water is a technique that concentrates and categorizes the DOM in water into structurally more specific and physiochemically more analogous subgroups (Marhaba *et al.* 2003). It could be used to identify the major DOM fractions in water. By conducting trihalomethane formation potential (THMFP) tests on DOM fractions, the ability of each DOM fraction for reacting with chlorine to form carcinogenic substances such as trihalomethane (THMs) and haloacetic acids (HAAs) can be determined. The major THMs and HAAs precursors and the active DOM fractions that form THMs and HAAs can be determined. Sample fractionation provides opportunities to identify the complex positions of DOM fractions, especially the complex positions of the major DOM fractions and major THMs and HAAs precursors, by using other techniques such as pyrolysis GC/MS and spectrofluorometry analysis.

Nevertheless, resin fractionation also has disadvantages:

1. It consumes acetone, hexane and methanol in the resin preparation process and an acid and base solution in the sample preparation, resin preparation and elution processes.
2. It is time consuming and labor intensive.

The process has some limitations. The fractionation and isolation of organic matter only exhibits a good recovery of organic matter when the sample containes a low level of inorganic salt or salinity. A desalting step before fractionation might be need prior to fractionation, even when the organic matter is only present in a small quantity (Leenheer, 2000). Specific conductance in a water sample should not exceed 2,000 μmhos/cm, as above this level the concentration of inorganic ionic salts would exceed the capacity of ion exchange resins. The nature of organic fractions is based on the operational definition. Finally, colloid clay could foul resin adsorbents.

Pyrolysis GC/MS Analysis

Pyrolysis is a method that thermally cleaves an organic molecule into volatile fragments, which are then separated by gas chromatography and identified by mass spectroscopy (MS). Pyrolysis GC/MS yields a reproducible fragmentation pattern or fingerprint, which is highly characteristic of the parent organic matter.

One advantage of the pyrolysis approach is that the natural biopolymers that represent the bulk of DOM precursors is able to be clearly identified because they yield very specific fragments with few interferences among the biopolymers (Leenheer and Croue, 2003). Saiz-Jimenez, (1994) proposed several advantages of pyrolysis GC/MS. First, it requires a small sample amount; only a few hundred micrograms of organic carbon was enough for analysis. Furthermore, an elaborate sample preparation such as derivatization and extraction is not required. Finally, it is capable to providing detailed molecular weight information. Since it does not require solvents for the extraction of the target chemical from a solid or liquid matrix, the target organic matter being studied is not partially oxidized or modified. The organic matrices in the environment that are composed of material too large to be volatilized at 300 °C can be analyzed by GC/MS, since, pyrolysis will thermally extract intact molecules or crack large molecules into fragments that can be separated and identified by GC/MS (White *et al.*, 2004). By using freeze-drying to concentrate DOM, there is the possibility of a high concentration factor, convenient for small sample volumes, easy operation, and a high recovery of DOC and UV-254.

While there are many advantages to utilizing pyrolysis GC/MS, there are also some disadvantages. After the freeze-drying process, a considerably high concentration of inorganic salts may be observed in the samples. It is also inconvenient to use with larger volumes (low DOC concentration) and takes longer in time. In addition, the overall effect in the DOM structure remains uncertain; while data interpretation can be time consuming and complicated. Finally, it is difficult to make quantitative and provide the indirect information.

Pyrolysis' limitations are listed as follows:

1. In the sample preparation process, when a sample contains a low level of DOM, it is very difficult to receive a uniform fine powder after the freeze-drying process. The concentration of DOM with membranes or an evaporation technique is required.
2. Since, the pyrolysis technique is a destructive technique, fragments of the organic molecule can become involved with side reactions that form new compounds such as ring structures.
3. Pyrolysis results, especially of humic substances, are highly dependent on the temperature selected (Salz-Jimenez, 1994).
4. The library spectrum for some unknown compounds is still limited.
5. The specific biopolymer types of specific water sources such as wastewater and treated wastewater have not been widely established.

Spectrofluorometry Analysis

A fluorescent excitation-emission matrix (FEEM) is obtained by spectrofluorometry. An FEEM can provide information on the putative origin of fluorescent organic matter of DOM in water. It has the advantage of its simplicity due to its minimal sample amount, pretreatment, and analysis time requirements. It can be an alternative that allows for on-line processing and control at reduced operating costs. A fluorescence spectrophotometer can scan the entire usable band in a short period of time (in minutes) without sample pretreatment (Marhaba and Pu, 2000). However, conclusive results from past research established that it is difficult to quantify the level of fluorescent organic matter such as tyrosine-like, tryptophan-like, and humic and fulvic acids-like substances using FEEM analysis.

The limitations for spectrofluorometry analysis are as follows:

1. Since not every compound fluoresces, water samples that contain high levels of non-fluoresced compounds cannot be analyzed by this technique.
2. The fluorescent peak positions of target compounds have not been widely determined. The major putative origins of DOM in water have been at present classified into three groups: tyrosine-like, tryptophan-like, and humic and fulvic acids-like substances.
3. The metal-binding and subsequent fluorescent quenching could occur in water samples that have high pH values
4. The DOC level is significantly important to determining the fluorescent peaks in an FEEM. In the case of low DOC concentrations, the fluorescent peaks cannot be detected (under scale). The concentration of DOM with a membrane and evaporation technique, therefore, may be required. In the case of high DOC concentrations, the florescent intensity will be higher than the detection limit of spectrofluorometry (over scale) and the dilution of water samples using Milli-Q water would be required.

Finally the overall integration and application of DOM characterization by using resin fractionation, pyrolysis GC/MS and spectrofluorometry analysis is tabulated in Table C-1.

Table C-1: The overall integration and application of DOM characterization by using the resin fractionation, pyrolysis GC/MS and spectrofluorometry techniques

Techniques	Provided information			Applicability in water and wastewater treatment
	Mass	Physical chemical structure	Disinfection by-products (DBPs) /reactivity	
Resin fractionation	Yes (By conducting the DOC test	Chemical	Yes (By conducting the DOC and THMFP test)	To monitor the major DOM fractions, major DBPs precursors and highly reactive DOM fractions that form DBPs.
Spectrofluorometry analysis	Only, tyrosine-like, tryptophan-like and humic and fulvic acids-like substances	Moderate both chemical and physical	Indirect	Online, easy monitoring, useful for checking alterations/additions of new substances, useful for checking the major DOM fractions, major DBPs precursors and highly reactive DOM fractions that form DBPs.
Pyrolysis GC/MS	Low	Chemical	Indirect	Identification of chemical class of DOM in unfractionated water and in the major DOM fractions, major DBPs precursors and highly reactive DOM fractions that form DBPs.

APPENDIX D
PUBLICATIONS

Peer Reviewed International Journals/Books

1. Musikavong C. and Wattanachira S. (2007) Reduction of Dissolved Organic Matter in Terms of DOC, UV-254, SUVA and THMFP in Industrial Estate Wastewater Treated by Stabilization Ponds. Environmental Monitoring and Assessment (Accepted: January 22, 2007)
2. Janhom T., Musikavong C., Wattanachira S., and Furumai H. (2006) Reactivity and Sensitivity of DOM Fractions to Form THMs in Raw Water Supply and Treated Wastewater Used for Reclaimed Water of The Northern-Region Industrial Estate, Thailand. Southeast Asian Water Environment 2: Book published by International Water Association (IWA). London, UK. (In press)

International Symposium/Conference Proceedings

1. Musikavong C., Wattanachira S., Nakajima F., and Furumai H. (2006) Three-Dimensional Fluorescent Spectroscopy Analysis for Evaluation of Organic Matter Removal from Industrial Estate Wastewater by Stabilization Ponds. The seventh IWA Specialist Conference on Waste Stabilization Ponds: Advances in Pond Technology and Management. September 25-27, AIT, Bangkok, Thailand
2. Musikavong C., Wattanachira S. and Pavasant P. (2006) Relationships between Dissolved Organic Matter Surrogates and Area of Excitation Spectrum of Fluorescent Excitation-Emission Matrix in Industrial Estate Wastewater. The proceeding of international conference on hazardous waste management for a sustainable future. January 10-12, Bangkok, Thailand.
3. Janhom T., Musikavong C., Wattanachira S., and Furumai H. (2005) Reactivity and Sensitivity of DOM Fractions to Form THMs in Raw Water Supply and in Treated Industrial Used for Reclaimed Water of the Northern-Region Industrial Estate. The proceeding of the third international symposium on Southeast Asian Water Environment. pp. 201-208, December 6-9, AIT, Bangkok, Thailand.
4. Musikavong C., Wattanachira S. and Pavasant P. (2004) Dissolved Organic Matter in Treated Industrial Estate Wastewater Characterized by Resin Fractionation and Excitation-Emission Fluorescent Spectra. The proceeding of the second international symposium on Southeast Asian Water Environment. pp. 158-165, December 1-3, Hanoi, Vietnam.

National Symposium/Conference Proceedings

1. Musikavong C., Wattanachira S. and Pavasant P. (2005) Application of Excitation-Emission Fluorescence Spectra to Quantify Trihalomethane Formation Potential of Wastewater and Treated Wastewater. The proceeding of the fourth National Environmental Conferences. pp. 564-571, January 19-21, Chonburi, Thailand.

BIOGRAPHY

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