Electronic Supplementary Material (ESI) for RSC Advances.

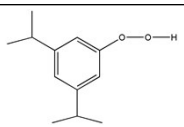
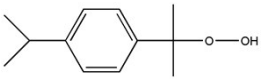
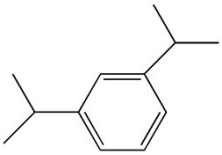
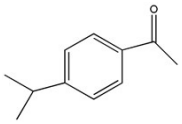
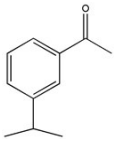
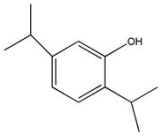
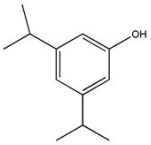
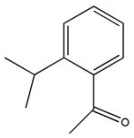
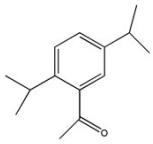
Supporting Information

1. Key additives analysis data

1) Diisopropylbenzene hydroperoxide

The mass spectrometry result of diisopropylbenzene hydroperoxide using GC-MS and micro OTOF as shown table S1.

Table S1. Diisopropylbenzene hydroperoxide analysis data

#	Molecular structure	Relative molecular weight	Relative content (%)
1		194	35.12
2		194	17.89
3		161	1.42
4		178	0.74
5		178	1.00
6		162	5.25
7		162	4.52
8		162	2.65
9		204	2.35

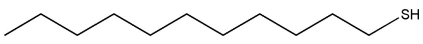
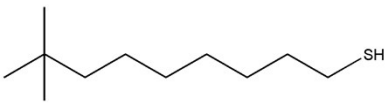
2) Tert-Dodecyl Mercaptan

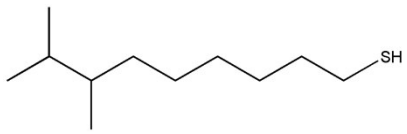
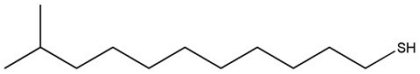
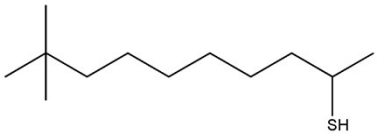
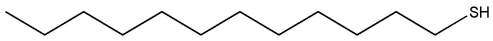
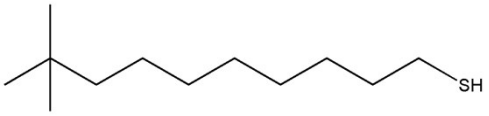
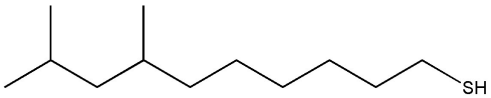
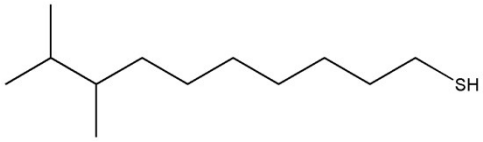
The mass spectrometry result of tert-Dodecyl Mercaptan using GC-MS and micro OTOF as shown table S2. Its content is 90.03% when retention time in 10.759-11.842min. and it contains about 20 main components, more branched chains and a small amount of primary mercaptan. The partial isomer structure of aliphatic mercaptan of C10 and C11 is shown in Table S3

Table S2. Tert-Dodecyl Mercaptan analysis data

#	Retention time (min)	Mass fraction (%)	Carbon number
1	9.897	2.21	C10
2	10.473	7.78	C11
3	10.759	4.83	C12
4	10.850	5.01	C12
5	10.922	5.40	C12
6	10.987	3.07	C12
7	11.035	7.11	C12
8	11.127	8.42	C12
9	11.228	14.89	C12
10	11.293	9.44	C12
11	11.375	11.52	C12
12	11.478	11.97	C12
13	11.652	4.24	C12
14	11.842	3.91	C12

Table S3. Tert-Dodecyl Mercaptan Isomers

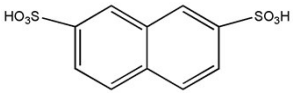
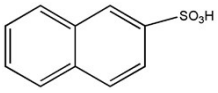
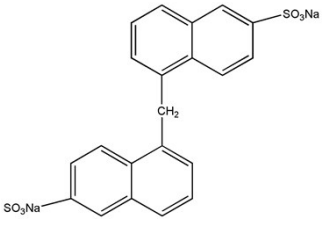
#	Molecular structure	Carbon number
1		C11
2		C11

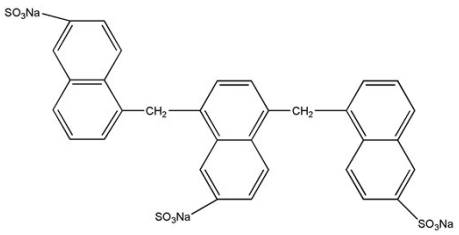
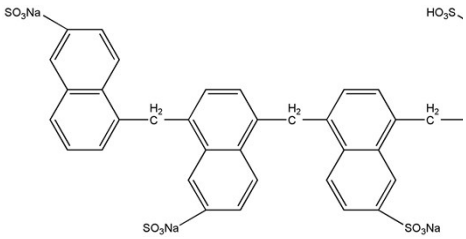
3		C11
4		C12
5		C12
6		C12
7		C12
8		C12
9		C12

3) β- Naphthalenesulfonic acidformaldehyde condensate (Dispersing Agent DN)

The solid content of Dispersing Agent DN is 44.0~46.0%(wt.), and its analysis data as shown S4 using HPLC-MS combined with INFRARED spectroscopy was used for analysis.

Table S4. Dispersing Agent DN analysis data

#	Name	Content (%)	Molecular structure
1	Di-sulfonic acid	49.84	
2	Mono-sulfonic acid	25.41	
3	dimer of mono-sulfonic acid	15.47	

4	Trimer of mono-sulfonic acid	5.74	
5	Tetramer of mono-sulfonic acid	3.54	
	Total	50.16	

4) Dodecylbenzene sulfonate

Table S5. Dodecylbenzene sulfonate analysis data

#	Composition	Mass fraction (%)
1	Decylbenzenesulfonic acid	35.6~35.8
2	Undecylbenzenesulfonic acid	23.5~23.7
3	Dodecylbenzenesulfonic acid	21.7~21.9
4	Tridecylbenzenesulphonic acid	18.7~18.9

2. Thermodynamic property

Table S6. Modified binary interaction parameters of polymer NRTL

Component i	water	water	BD
Component j	AN	BD	AN
a_{ij}	6.726	3.589	6.666
a_{ji}	-0.0436	-0.00852	-0.398
b_{ij}	1513.5	862.345	1343
b_{ji}	1469.7	702.17	1430
c_{ij}	0.325	0.28	0.3

3. Mooney viscosity experimental data

Table S2. Experimental data of NBR Mooney viscosity

Code	Mn	Mw	Degree of Branching *10^6	MV
1	86760	178856	0.692384	52.3
2	85680	201705	1.213287	52.5
3	71590	242270	3.217078	58
4	94930	226234	1.155977	55.1
5	101300	313546	1.560297	61.7
6	88750	203479	1.426622	51.1
7	79920	215661	1.984999	51.1
8	81600	344589	2.764819	62.1
9	91680	324715	1.901948	61.8
10	82460	315372	2.127494	60.8
11	72950	195582	2.012828	49.2
12	95050	352401	1.997343	63.5
13	88360	252386	1.490157	57
14	90890	302968	1.863836	60
15	98250	339111	1.714705	63.5
16	91940	339935	2.037649	62.5
17	90220	317363	2.089022	60.4
18	100800	345828	2.225611	61.8
19	93990	307337	1.979322	59.6
20	107500	503023	2.233061	73
21	78743	222851	2.139162	51.6
22	72104	321363	3.022166	60.8
23	70639	191272	2.629015	49.2
24	71812	316481	3.235933	61.8
25	78313	219394	2.383084	51.1
26	81916	344901	2.545379	62.1
27	82470	350808	2.716938	62.5
28	85136	364558	2.708322	63.5
29	72417	253365	3.047483	56.5
30	69529	245523	3.112646	56.1
31	71543	265513	3.028053	56.9
32	72141	235901	2.893686	54.1
33	75970	188050	2.002547	48
34	73521	196447	2.293545	48.8
35	81306	218172	2.049	51.1
36	86588	289891	2.120747	58
37	79213	209932	1.84206	51

38	80584	228462	2.310662	51.9
39	94388	302949	1.796672	60
40	81988	202828	1.635224	50.7
41	91177	304752	2.050487	59.3
42	89333	284132	1.920785	58
43	71263	313053	3.258374	61.7
44	82394	360209	2.865841	63.5
45	59409	204657	3.408884	55
46	91583	274984	2.255185	56
47	86536	273416	2.450744	56
48	86723	272632	2.493182	56
49	75999	265885	2.950953	57
50	74568	238079	2.934761	55
51	87643	275898	2.503737	56.3
52	97800	247648	1.440569	55.7
53	101773	287005	1.998039	57.1
54	93139	243817	1.911513	53.5
55	79499	226498	2.018647	52.3
56	77744	233686	2.343166	52.5
57	73066	271534	3.083794	58
58	102569	294809	1.994467	57.8

Table S3. Results of Kramer correlation

Code	Mn	Mw	MV	$\log(\sqrt{M_n \cdot M_w})$	$\log(MV)$
1	86760	178856	52.3	5.095	1.719
2	85680	201705	52.5	5.119	1.72
3	71590	242270	58	5.12	1.763
4	94930	226234	55.1	5.166	1.741
5	101300	313546	61.7	5.251	1.79
6	88750	203479	51.1	5.128	1.708
7	79920	215661	51.1	5.118	1.708
8	81600	344589	62.1	5.224	1.793
9	91680	324715	61.8	5.237	1.791
10	82460	315372	60.8	5.208	1.784
11	72950	195582	49.2	5.077	1.692
12	95050	352401	63.5	5.262	1.803
13	88360	252386	57	5.174	1.756
14	90890	302968	60	5.22	1.778
15	98250	339111	63.5	5.261	1.803
16	91940	339935	62.5	5.247	1.796
17	90220	317363	60.4	5.228	1.781

18	100800	345828	61.8	5.271	1.791
19	93990	307337	59.6	5.23	1.775
20	107500	503023	73	5.366	1.863
21	78743	222851	51.6	5.122	1.713
22	72104	321363	60.8	5.182	1.784
23	70639	191272	49.2	5.065	1.692
24	71812	316481	61.8	5.178	1.791
25	78313	219394	51.1	5.118	1.708
26	81916	344901	62.1	5.226	1.793
27	82470	350808	62.5	5.231	1.796
28	85136	364558	63.5	5.246	1.803
29	72417	253365	56.5	5.132	1.752
30	69529	245523	56.1	5.116	1.749
31	71543	265513	56.9	5.139	1.755
32	72141	235901	54.1	5.115	1.733
33	75970	188050	48	5.077	1.681
34	73521	196447	48.8	5.08	1.688
35	81306	218172	51.1	5.124	1.708
36	86588	289891	58	5.2	1.763
37	79213	209932	51	5.11	1.708
38	80584	228462	51.9	5.133	1.715
39	94388	302949	60	5.228	1.778
40	81988	202828	50.7	5.11	1.705
41	91177	304752	59.3	5.222	1.773
42	89333	284132	58	5.202	1.763
43	71263	313053	61.7	5.174	1.79
44	82394	360209	63.5	5.236	1.803
45	59409	204657	55	5.042	1.74
46	91583	274984	56	5.201	1.748
47	86536	273416	56	5.187	1.748
48	86723	272632	56	5.187	1.748
49	75999	265885	57	5.153	1.756
50	74568	238079	55	5.125	1.74
51	87643	275898	56.3	5.192	1.751
52	97800	247648	55.7	5.192	1.746
53	101773	287005	57.1	5.233	1.757
54	93139	243817	53.5	5.178	1.728
55	79499	226498	52.3	5.128	1.719
56	77744	233686	52.5	5.13	1.72
57	73066	271534	58	5.149	1.763
58	102569	294809	57.8	5.24	1.762

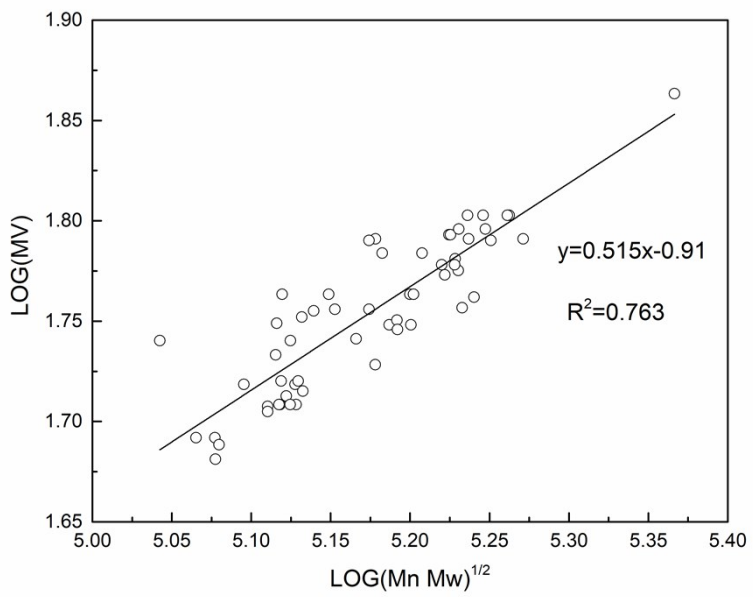


Figure S1. The fitting results of Kramer correlation

4. GPC-MALLS-Viscometer introduction

The volume exclusion chromatography / gel permeation chromatograph (SEC/GPC) combined with the multi angle laser light scattering (MALLS) three detector system (GPC-MALLS-Viscometer) can make full use of the advantages of both, which can separate molecules of different sizes and molecular weights by SEC/GPC, and determine the absolute molecular weight and molecular size of polymers by MALLS. Therefore, the data of Mn, MW, PDI, intrinsic viscosity, rotation radius (Rg) of polymer can be obtained by GPC-MALLS-Viscometer, thus a series of useful information such as polymer configuration, branching degree can be obtained, which provides reliable basis for the analysis and research of polymer microstructure.

GPC-MALLS-Viscometer can also be used in the detection of branching degree. The combination of MALLS and GPC is the only method to determine the branching coefficient. This method does not need many hypotheses and "virtual factors", because the molecular weight obtained by MALLS is absolute, and the branching ratio can also be calculated. While the combination of light scattering detector and GPC can not only distinguish different groups, but also measure the distribution of different groups. Based on these advantages, GPC-MALLS-Viscometer was used to determine Rg of polymers with different molecular weights. And the average degree of branching of polymers could be obtained by calculation.

Rg of branched polymers is smaller than that of linear molecules with the same molecular

weight, which is the base point for determining the degree of branching by the properties of polymer solution. The branching factor can then be calculated according to the both ratios.

$$g_M = \left(R^2\right)_b / \left(R^2\right)_l$$

Branching factor is a parameter related to branching degree and molecular weight, which represents the reduction of the random coil after branching.

According to Zimm-stockmayer theory, the relationship between g_M and the number of branching points B_W is discussed：

$$g_M = \frac{3B_W - 2}{{B_W}^2}$$

Therefore, as long as the branching factor is calculated, the number of branching points can be calculated, and the calculation formula of branching degree is as follows:

$$\overline{\lambda} = B_W / M_W$$

$\overline{\lambda}$ denotes the average branching degree of the sample.