Supporting Information

Multi-Objective Synthesis Optimization and Kinetics of a Sustainable Terpolymer

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1. GitHub Repositories

The data and software that support the findings of this study are openly available in GitHub Repositories.

1.2. Terpolymer NMR, DSC and GPC Data

All data, including NMR spectra, DSC trace and GPC trace of all terpolymer samples synthesized are included in the GitHub repository: https://github.com/TanJinDa-94/April-2024-Terpolymer. Tables summarizing the terpolymer details are also included in the SI in the subsequent sections.

1.3. Bayesian Optimization Code

The code for carrying out random initial Sobol sampling, and Bayesian Optimization can be found in: https://github.com/andrelowky/Styrene-Terpolymer-Optimization

1.4. Ternary Reactivity Ratio Calculation

The code and theory for calculating the ternary reactivity ratios can be found in: https://github.com/LiQianxiao/Generalized-Mayo-Lewis-Calculator.

2. Experimental Methods

Prior to terpolymer synthesis, all monomers, namely Styrene, Myrcene, and DBI, were first passed through basic Al_2O_3 for inhibitor removal before being transferred into the reactor. AIBN was used as the radical initiator according to the calculated molar ratio. To quantify the monomer conversion, 1.6 mL of DMF was added to a 20 mL Biotage sealable microwave reaction vial as an internal standard. The individual monomers were added to the reaction vial according to the calculated molar ratio and the reaction vial was sealed with a rubber septum. Subsequently, the reaction mixture was degassed for 30 minutes in an ice bath to remove any dissolved gases and to create an inert atmosphere within the sealed tube. At this stage, a small aliquot of the reaction mixture was extracted for ^{1}H NMR analysis, serving as the baseline for monomer calculations. The sealed tubes were then transferred to a heating element, and the temperature was set to the suggested reaction temperature. The reactions were allowed to proceed for the specified reaction time. Once the reactions were completed, another small aliquot of the reaction mixture was taken for ^{1}H NMR analysis to determine the monomer conversion after the reaction. To isolate the terpolymer, the reaction mixture was immediately added dropwise into an excess amount of methanol (>100 mL) under stirring, leading to precipitation of the polymer. Careful decantation was performed to remove the excess methanol, and the precipitated polymer was subsequently dissolved in a minimal amount of DCM. To further purify the terpolymer, the dissolved polymer in DCM was added dropwise into an excess amount of methanol (>100 mL) while stirring for a second precipitation. Again, the excess methanol was carefully decanted, and the precipitated polymer was dissolved in DCM.

The DCM solvent was then removed by evaporation using a rotary evaporator, leaving behind the purified terpolymer. The terpolymer was subsequently dried overnight in a vacuum oven set at 50 degrees Celsius to remove any residual solvent or moisture. For further analysis, small samples of the terpolymer were taken. One sample was dissolved in deuterated methylene chloride for ^{1}H NMR analysis, allowing for the quantification of monomer incorporation within the terpolymer. A second sample was used for differential scanning calorimetry (DSC) analysis to determine the glass transition temperature (T_g) of the terpolymer. A third sample was diluted in THF and used for Gel Permeation Chromatography (GPC) analysis. Gel permeation chromatography (GPC) was conducted on a Viscotek TDAmax, which consists of three components. The GPCmax integrated solvent and sample delivery module, the TDA 302 Triple Detector Array, and the OmniSEC software. The TDA 302 incorporates RI and, Light Scattering detectors and viscometer. Only RI detector was used. 2 columns: 2 x PLgel 10 μm Mixed-B (500 to 10,000,000) and 1 guard column (10 μm) were applied in sequence for separation. THF was used as the eluent at 1.0 mL/min with column and detector temperature at 40 ^{o}C. The apparent molecular weight and dispersity (M_w/M_n) were determined with the conventional linear calibration based on polystyrene standards with calibration range of 580 to 3,000,000 Da. The thermal transitions of the samples are measured using Differential Scanning Calorimeter (TA Instruments, DSC Q100). The sample is crimped in the hermetic aluminium pan, and subjected to a heat-cool-heat profile under nitrogen atmosphere with the flow rate of 50ml/min. Sample is first ramped to 150 ^{o}C with the ramp rate of 20^{o}C/min, followed by a cool cycle to -80 ^{o}C and then heated to 100 ^{o}C at the rate of 10 ^{o}C/min. The first heat cycle was to remove any thermal history inherent to the received samples. The glass transition of the sample is show as a step from the heat flow traces due to the change in the heat capacity. The glass transition reported is the inflection point of the step, determined from the second heat cycle.

2.1. Synthesis of Terpolymers and Copolymers for Characterization

Styrene (1.04 g, 10.0 mmol), Myrcene (1.36 g, 10.0 mmol), DBI (2.42 g, 10.0 mmol), and azobisisobutyronitrile (AIBN) (0.05 g, 0.30 mmol, 1.0 mmol with respect to 30.0 mmol of monomers) were taken in a Schlenk tube. The reaction mixture was purged with nitrogen for 10 minutes by keeping the contents at 0°C. Vacuum was applied carefully for 2-3 minutes, followed by filling with nitrogen by gently turning the knob for three repeats. The contents were then placed in an oil bath and heated to 80°C, maintaining that temperature for 4 hours.

The viscous reaction mixture was precipitated by adding dropwise to methanol (200 mL). The precipitated polymer was dried and analysed using NMR, GPC, and DSC measurements.

For kinetic studies, 0.8 mL of DMF was added as an internal standard to determine the conversion. Samples were taken every 30 minutes and analysed by ^{1}H NMR. The conversion of Styrene, Myrcene and DBI was calculated and tabulated below using the ^{1}H NMR.

2.2. Kinetic Data for Terpolymer Synthesis

Time (min)	Conversion (%)			
	Styrene	Myrcene	DBI	Overall
0	0	0	0	0.00
30	9.30	13.19	13.83	12.18
60	17.44	32.97	27.66	26.20
90	23.26	42.86	37.23	34.69
120	30.23	51.65	45.74	42.80
150	36.05	59.34	50.00	48.71
180	37.21	62.64	53.19	51.29
210	38.37	67.03	58.51	54.98
240	38.37	67.03	58.51	54.98

Table S1. Summary of Kinetic Data for Terpolymer Synthesis. *The individual conversion of monomers Styrene, Myrcene and DBI, as well as the overall conversion of all monomers. ^{1}H NMR peaks at 6.75 ppm, 6.41 ppm, 5.71 ppm were used for calculating conversion of Styrene, Myrcene and DBI respectively against DMF (8.03 ppm) as an internal standard.*

2.3. Analytical Data Collected for Validating the Terpolymer Formation

The copolymers Styrene/Myrcene, Myrcene/DBI and DBI/Styrene were synthesized under identical conditions used for terpolymer synthesis. The consolidated Mn, Mn, PDI and T_g values for the terpolymer, copolymers and homopolymers are given in the table below. The copolymerization of pairwise combinations of styrene, myrcene, and DBI as well as homopolymerisation of individual monomers under identical conditions also provided for reference and comparison:

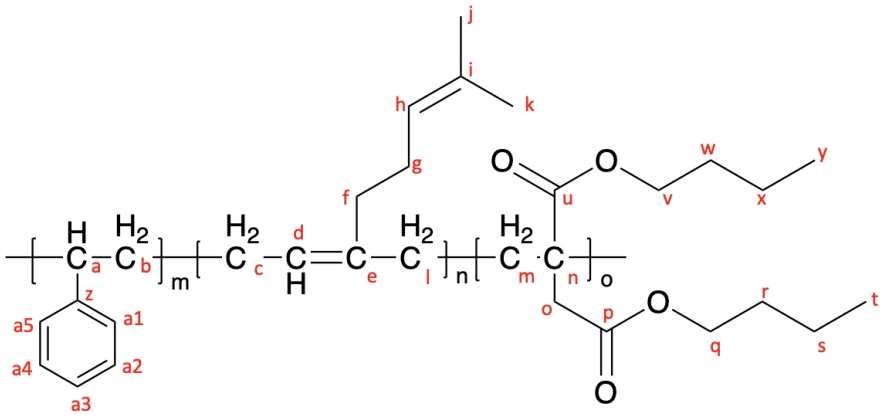
S. No.	Monomer feed (mol %)			Molecular Weight Distribution (MWD)			T_g (^{o}C)	Overall Conversion (%)
	Styrene	Myrcene	DBI	Mn	Mw	PDI		

1	33.33	33.33	33.33	14150	25700	1.82	-17.5	51.3
2	50	50	0	4700	10400	2.21	n.d.*	25.4
3	50	0	50	15600	26600	1.71	36.2	69.7
4	0	50	50	17600	30800	1.75	-31.8	48.4
5	100	0	0	12500	27060	2.14	91.8	65.4
6	0	100	0	6160	10440	1.65	-61.9	16.4
7	0	0	100	13650	22400	1.61	-8.6	30.2

Table S2. Summary of Kinetic Data for Terpolymer Synthesis. *The individual conversion of monomers Styrene, Myrcene and DBI, as well as the overall conversion of all monomers. * No polymer isolated upon precipitation with methanol. Only milky emulsion formed. No attempts were made to change the precipitation methods; Reaction temperature = 80 °C; AIBN = 1 mol % with respect to total monomer concentration; Neat conditions*

2.4. ^{1}H, ^{13}C and ^{2}D NMR data for Synthesized Terpolymer

The carbons of the terpolymer are labelled as shown in the figure below for easier assignment of respective protons and carbon signals:



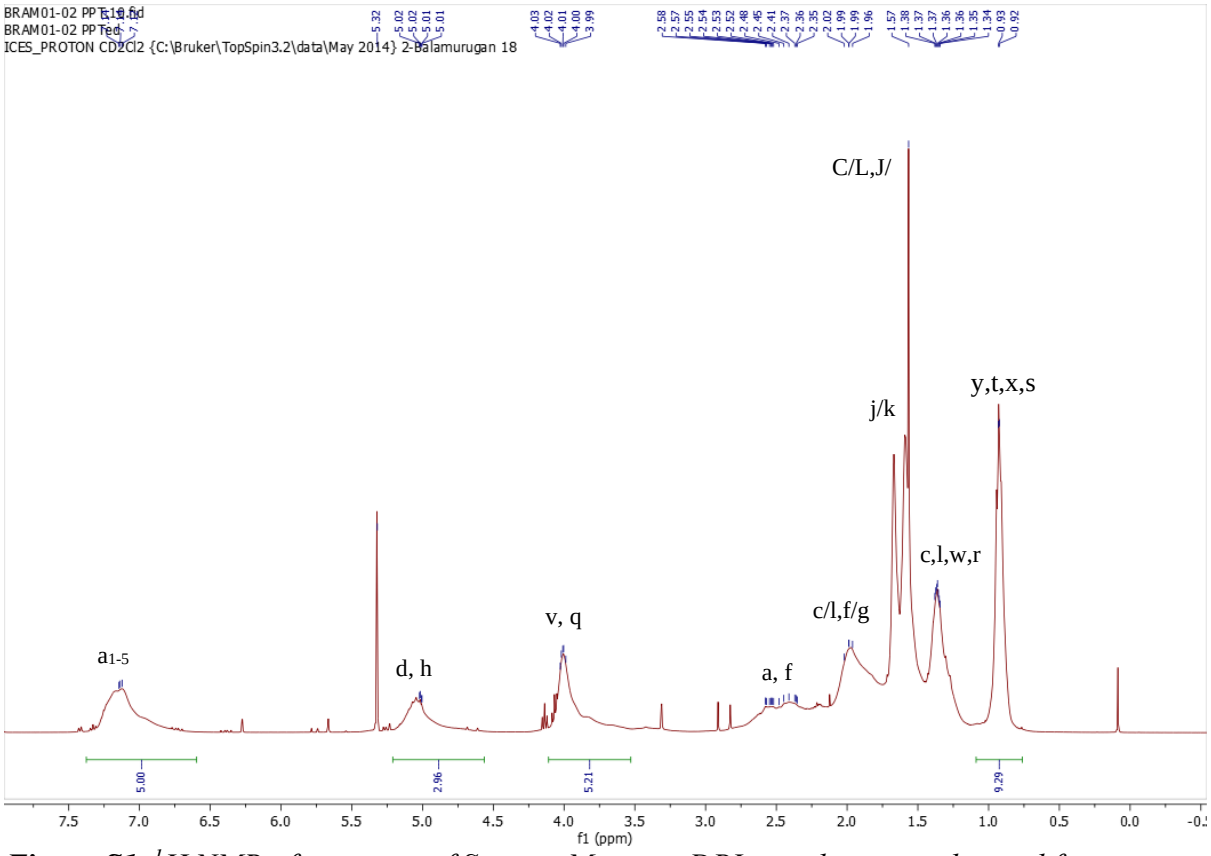


Figure S1. *^{1}H NMR of spectrum of Styrene-Myrcene-DBI terpolymer synthesized from an equimolar feed ratio of all monomers. Peaks assigned based on HSQC spectrum and literature data on myrcene/DBI copolymers.[1] The broad peaks observed at 7.2 ppm, 5.0 ppm and 4.0 ppm are respectively assigned to the protons of styrene, myrcene and DBI. The ratio of styrene, myrcene and DBI are calculated as ratio of 27.4:36.3:36.3.*

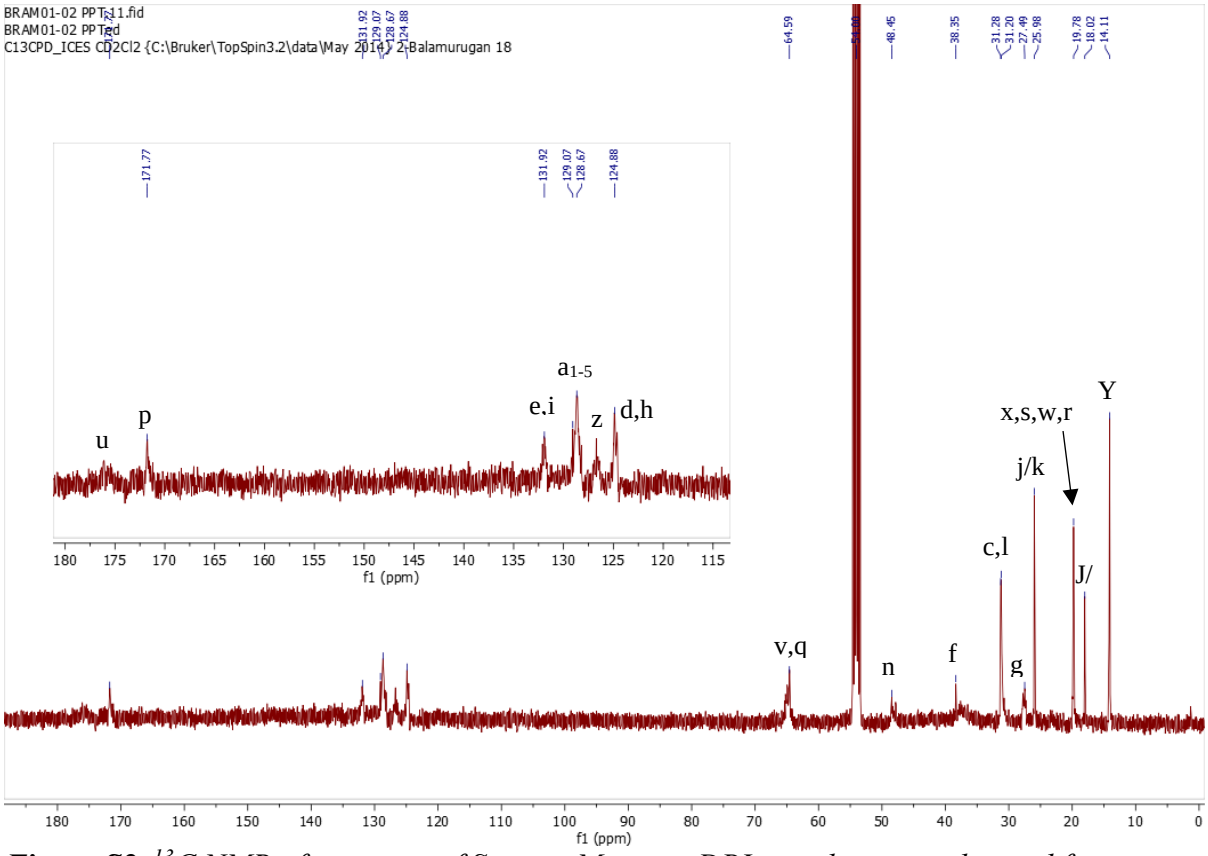


Figure S2. *^{13}C NMR of spectrum of Styrene-Myrcene-DBI terpolymer synthesized from an equimolar feed ratio of all monomers. Peaks assigned based on HSQC spectrum and literature on data on myrcene/DBI copolymers.[1]*

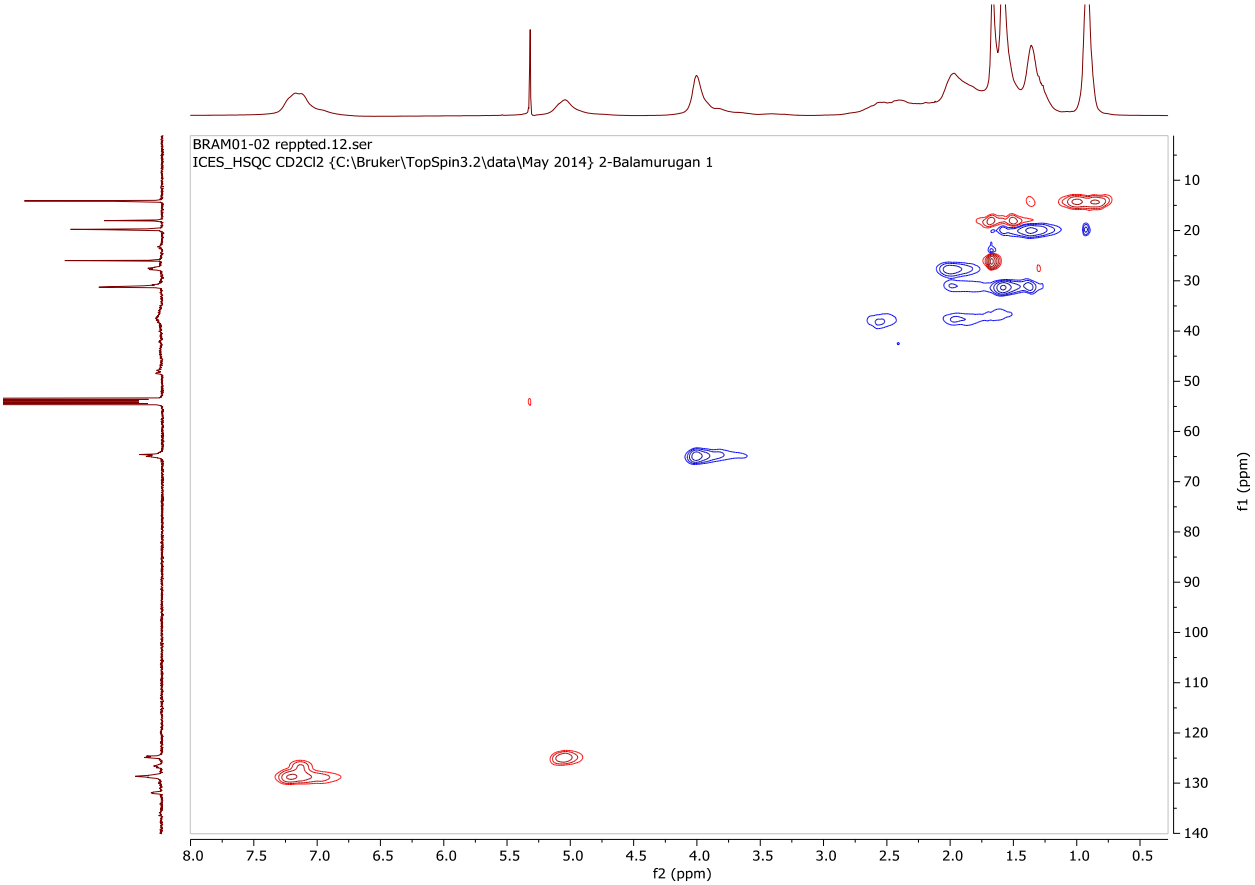


Figure S3. *Heteronuclear Single Quantum Coherence (HSQC) spectrum Styrene-Myrcene-DBI terpolymer synthesized from an equimolar feed ratio of all monomers. Red shows proton-carbon cross peaks of CH and CH_3 groups. Blue shows proton-carbon cross peaks of CH_2 groups. The cross peaks in HSQC spectrum provide potential connection points in the terpolymer.*

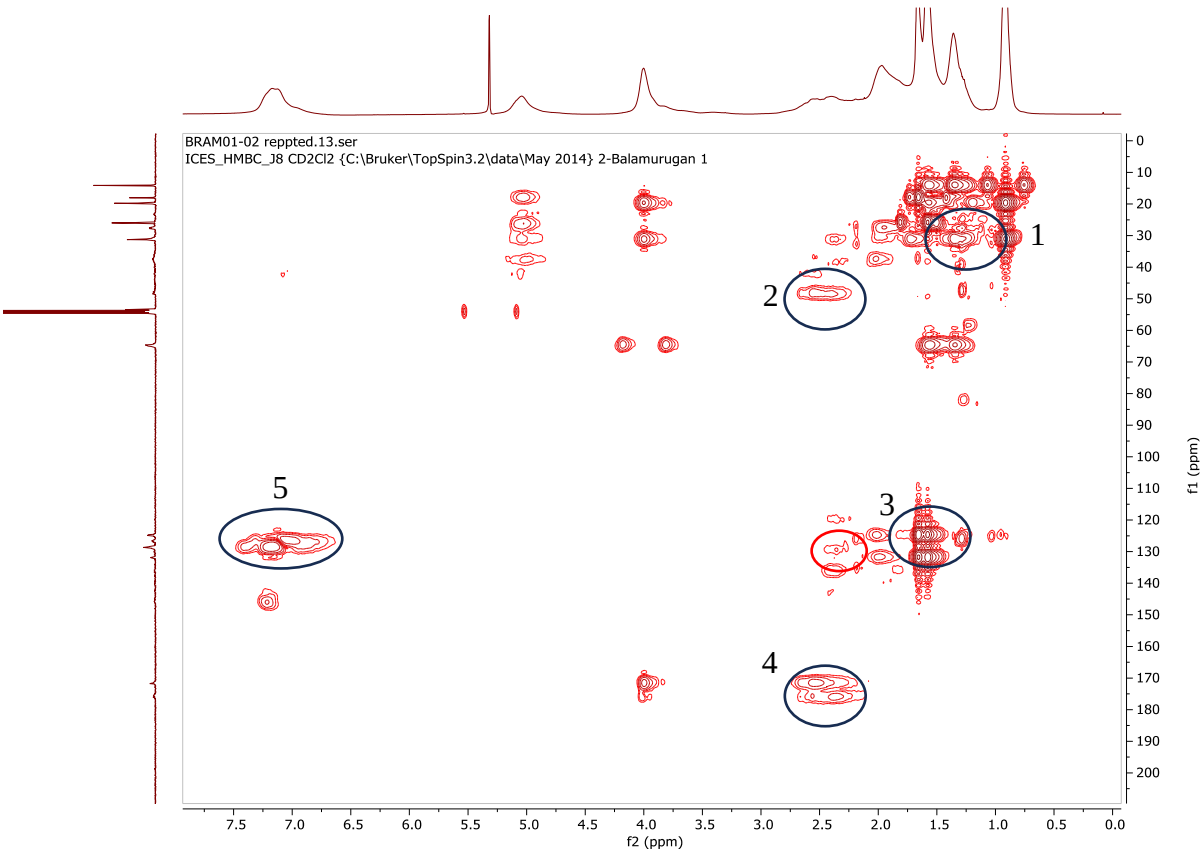
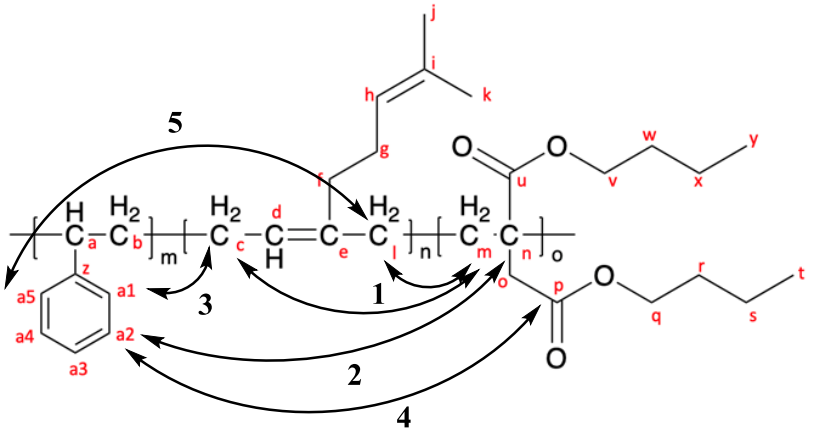


Figure S4. *Heteronuclear Multiple Bond Correlation (HMBC) spectrum Styrene-Myrcene-DBI terpolymer synthesized from an equimolar feed ratio of all monomers.*

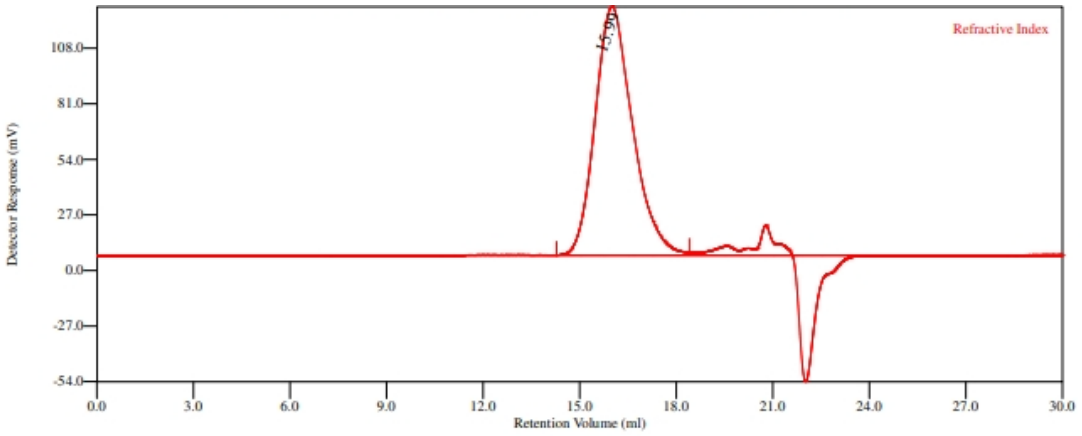


HMBC spectra provides the C-H correlation over 2 to 4 bonds depending upon the orientation of protons with respect to the carbon atom. This 2D NMR method helps to establish the connectivity of different monomer in the terpolymer system. The key correlations were identified and indicated in the Figure S4.

Point 1: Connection between myrcene proton ‘c/l’ and dibutyl itaconate carbon ‘m’.
Point 2: Connection between styrene proton a and dibutyl itaconate carbon ‘n’.
Point 3: Styrene aromatic ring carbon with myrcene proton ‘c/l’ connectivity and Styrene aromatic ring carbon with dibutyl itaconate carbon m connectivity.
Point 4: Connection between Styrene proton ‘a’ and dibutyl itaconate carbon ‘u/p’.
Point 5: Connection between styrene aromatic protons and myrcene carbon ‘l’.

All the above carbon-proton correlations confirms the formation of terpolymers and the propagation of monomers in the polymer chain.

2.5. GPC Studies of Terpolymer and Copolymers



Conventional Calibration - Homopolymers : Results

Peak RV - (ml)	15.990
Mn - (Daltons)	14,148
Mw - (Daltons)	25,704
Mz - (Daltons)	40,520
Mp - (Daltons)	23,107
Mw / Mn	1.817
Percent Above Mw: 0	100.000
Percent Below Mw: 0	0.000
Mw 10.0% Low	4,795
Mw 10.0% High	69,564
Wt Fr (Peak)	1.000
RI Area - (mvml)	163.27
UV Area - (mvml)	0.00

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Calculation Operator	admin : Administrator
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System	THF
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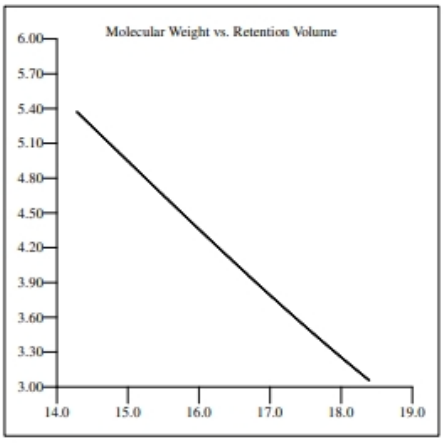
Inj Volume - (ul)	100.0
Volume Increment - (ml)	0.00333
Detector Temp. - (deg C)	40.0
Column Temp. - (deg C)	40.0
OmniSEC Build Number	406



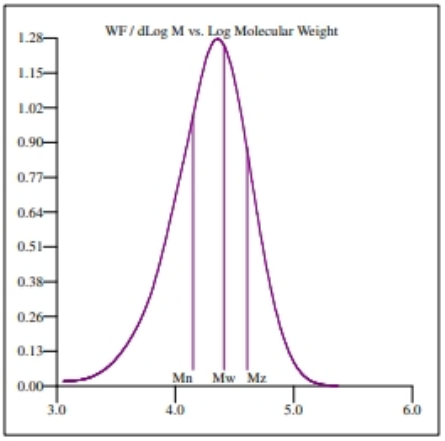
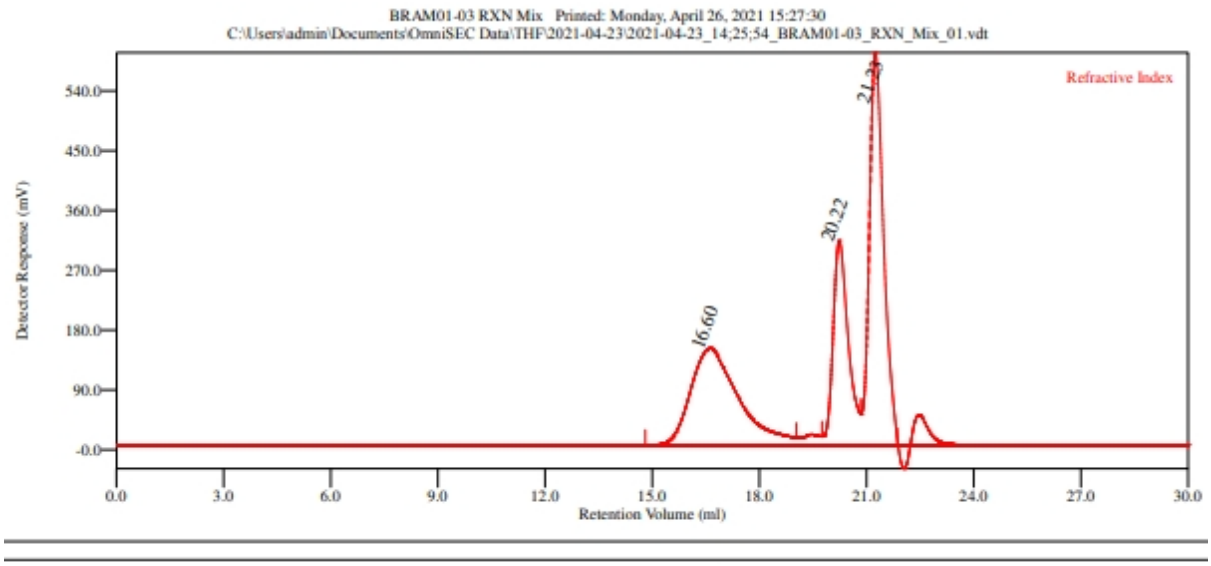


Figure S5. *GPC trace and molecular weight statistics of Styrene-Myrcene-DBI terpolymer synthesized from an equimolar feed ratio of all monomers.*



Conventional Calibration - Homopolymers : Results

Peak RV - (ml)	16.600	20.223	21.233
Mn - (Daltons)	4,721	166	79
Mw - (Daltons)	10,428	172	80
Mz - (Daltons)	17,503	177	81
Mp - (Daltons)	10,325	179	82
Mw / Mn	2.209	1.033	1.015
Percent Above Mw: 0	100.000	100.000	100.000
Percent Below Mw: 0	0.000	0.000	0.000
Mw 10.0% Low	1,309	121	63
Mw 10.0% High	29,450	227	97
Wt Fr (Peak)	0.346	0.234	0.419
RI Area - (mvml)	225.36	152.67	273.06
UV Area - (mvml)	0.00	0.00	0.00

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Inj Volume - (ul)	100.0
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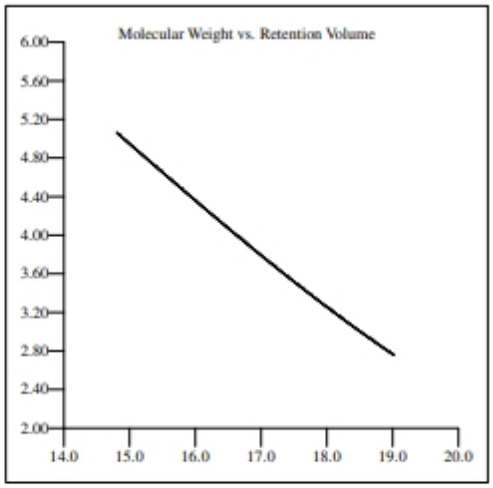
Column Temp. - (deg C)	40.0
OmniSEC Build Number	406



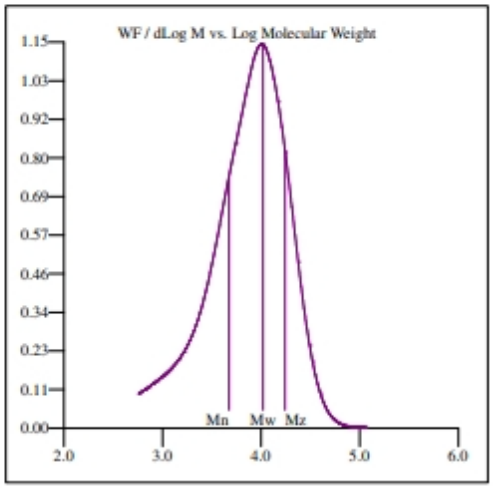
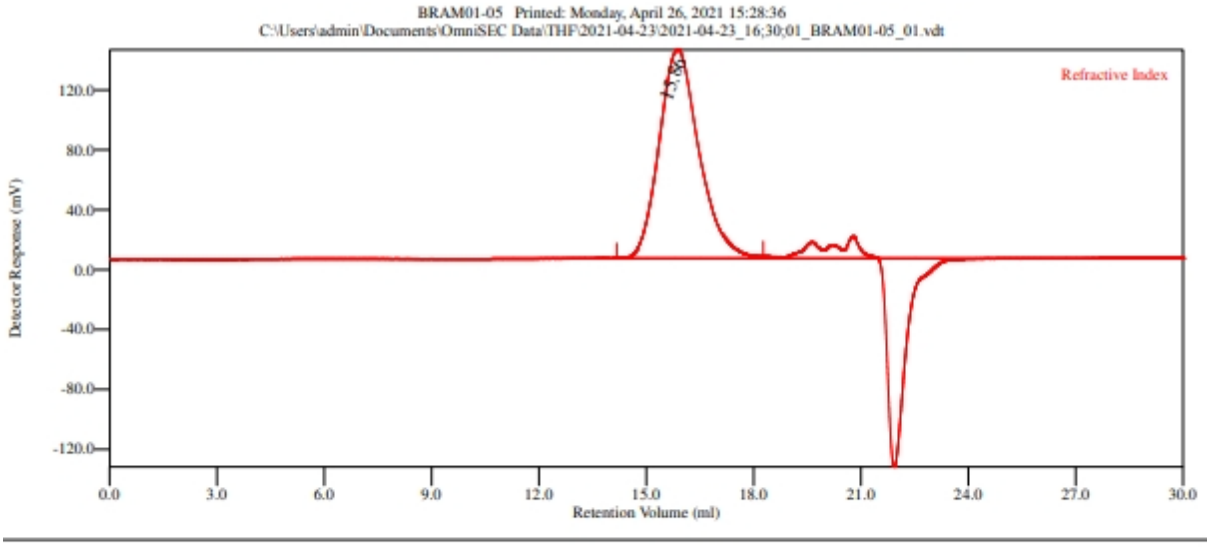


Figure S6. *GPC trace and molecular weight statistics Styrene-Myrcene copolymer synthesized from an equimolar feed ratio of both monomers.*



Conventional Calibration - Homopolymers : Results

Peak RV - (ml)	15.860
Mn - (Daltons)	17,598
Mw - (Daltons)	30,853
Mz - (Daltons)	47,396
Mp - (Daltons)	27,571
Mw / Mn	1.753
Percent Above Mw: 0	100.000
Percent Below Mw: 0	0.000
Mw 10.0% Low	6,137
Mw 10.0% High	81,603
Wt Fr (Peak)	1.000
RI Area - (mvml)	181.15
UV Area - (mvml)	0.00

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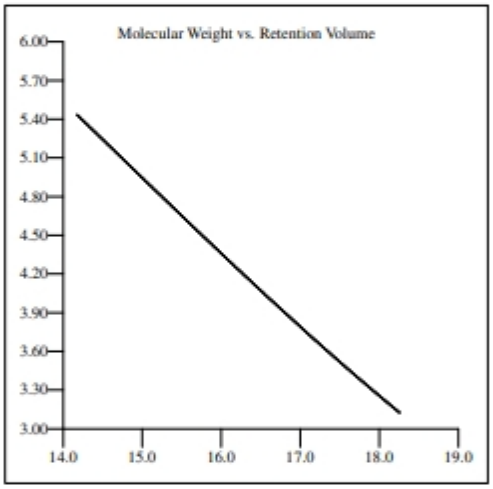
OmniSEC Build Number	406



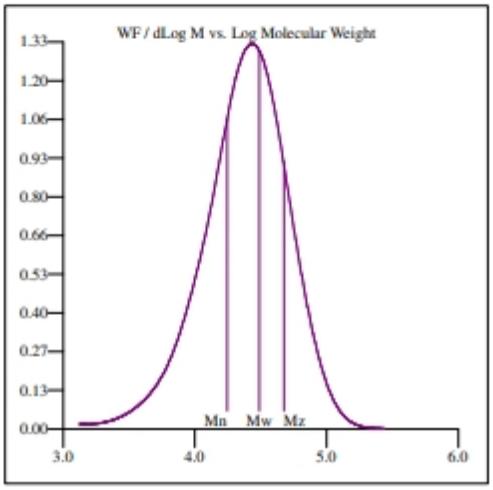
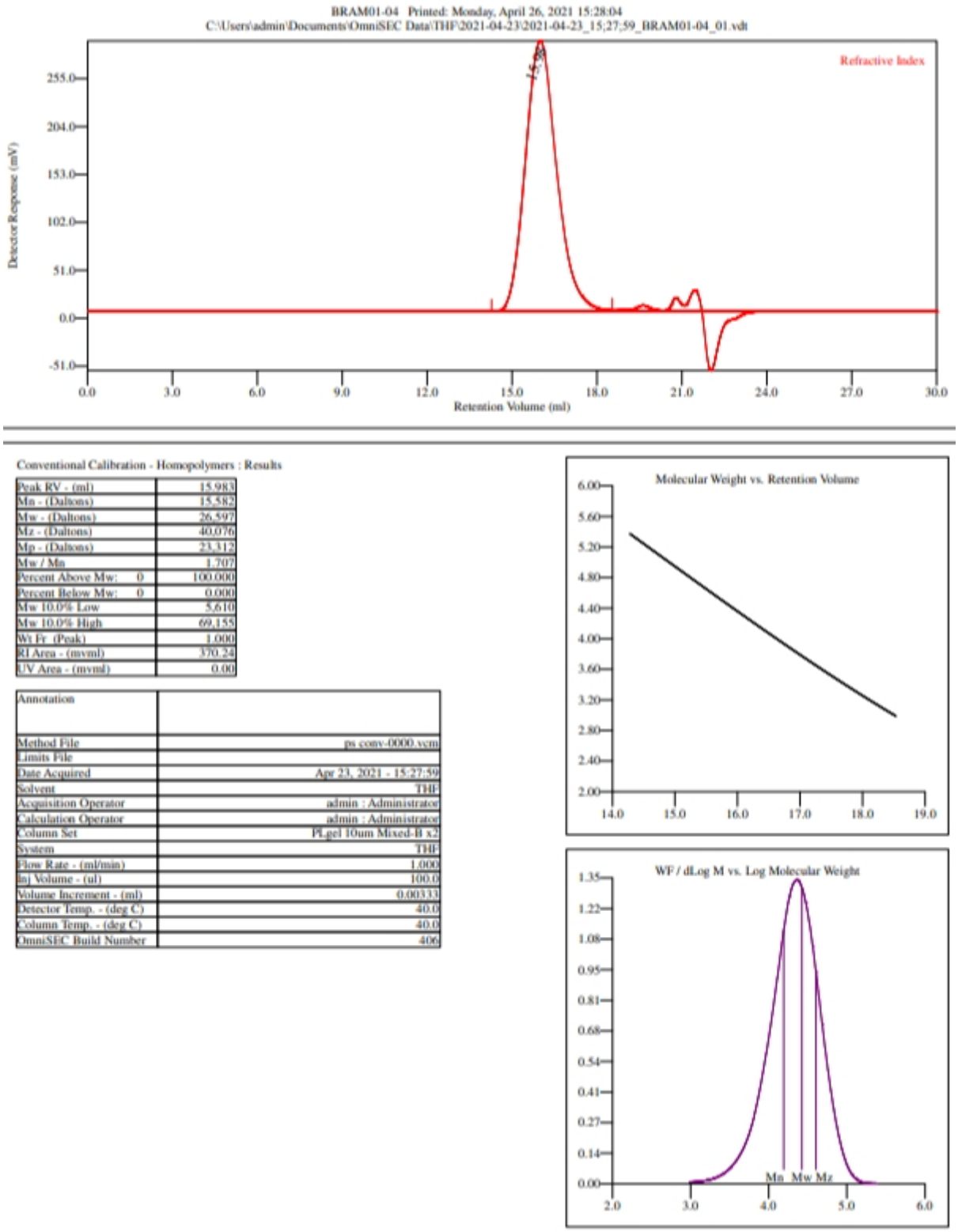


Figure S7. *GPC trace and molecular weight statistics of Myrcene-DBI copolymer synthesized from an equimolar feed ratio of both monomers.*



Peak RV - (ml)	15.983
Mn - (Daltons)	15,582
Mw - (Daltons)	26,597
Mz - (Daltons)	40,076
Mp - (Daltons)	23,312
Mw / Mn	1.707
Percent Above Mw: 0	100.000
Percent Below Mw: 0	0.000
Mw 10.0% Low	5,610
Mw 10.0% High	69,155
Wt Fr (Peak)	1.000
RI Area - (mvml)	370.24
UV Area - (mvml)	0.00

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Inj Volume - (ul)	100.0
Volume Increment - (ml)	0.00333
Detector Temp. - (deg C)	40.0
Column Temp. - (deg C)	40.0
OmniSEC Build Number	406

Figure S8. *GPC trace and molecular weight statistics of Styrene-DBI copolymer synthesized from an equimolar feed ratio of both monomers.*

2.6. DSC Study of Terpolymer and Copolymers

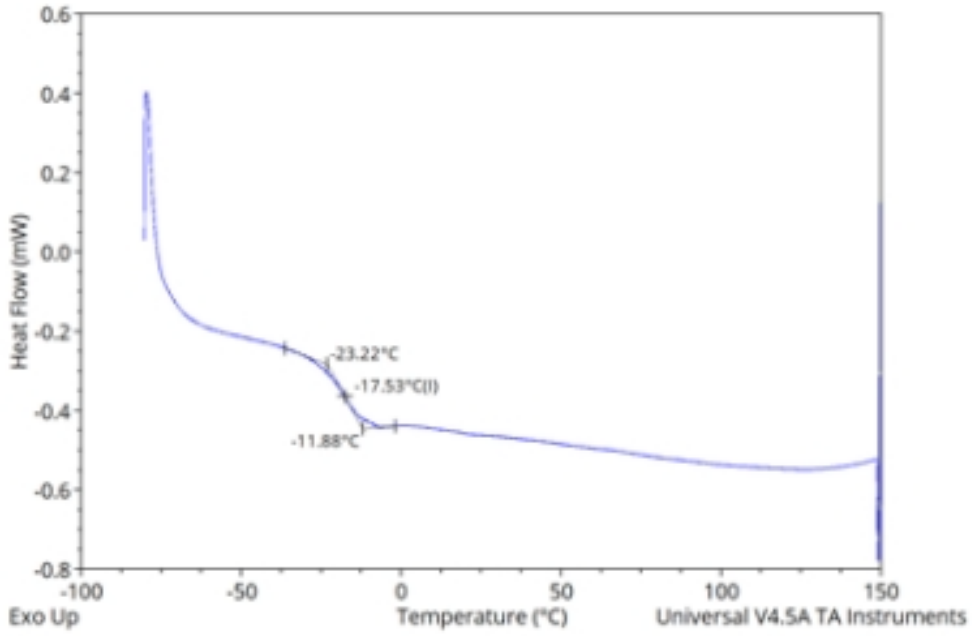

Figure S9. *DSC trace of Styrene-Myrcene-DBI terpolymer synthesized from an equimolar feed ratio of all monomers.*

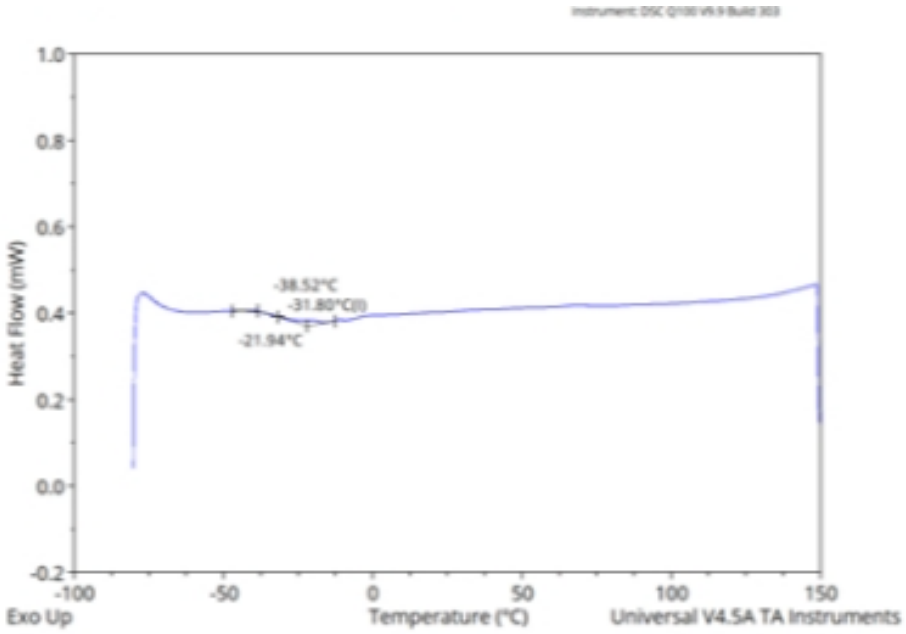

Figure S10. *DSC trace of Myrcene-DBI copolymer synthesized from an equimolar feed ratio of both monomers.*

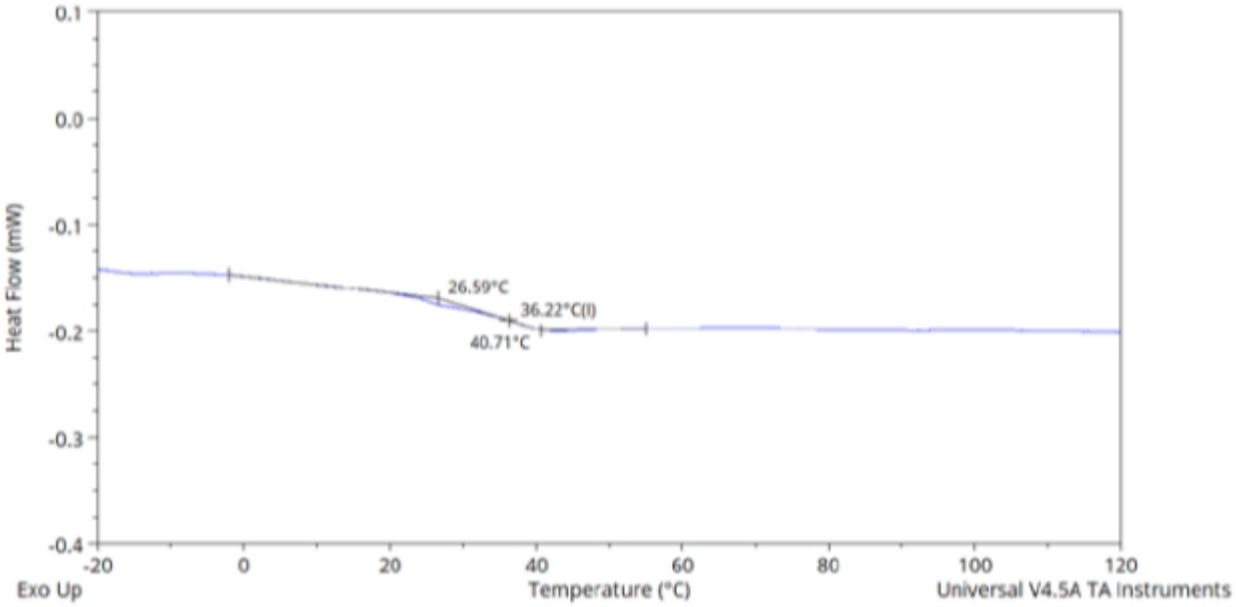

Figure S11. *DSC of trace styrene-DBI synthesized from an equimolar feed ratio of both monomers.*

3. Terpolymer Data

Section 3 of the SI collates all terpolymer data collected during the optimization phase of the study into tables for easy reference.

3.1. Summary of all Initial Monomer Feed and Experimental Conditions

The following table summarizes the initial monomer feed as well as the experimental conditions for all 89 terpolymerization reactions:

Sample	Styrene (mol %)	Myrcene (mol %)	DBI (mol %)	Temperature (deg C)	AIBN (mol %)	Time (min)
TP1	42.73801586	20.02767454	37.2343096	78.20206641	1.747083294	464.7929061
TP2	35.41030328	63.6148099	0.974886826	72.7083501	4.089130719	128.993385
TP3	38.60700538	31.17194849	30.22104613	66.87686549	2.992601157	91.9906235
TP4	70.54610542	21.69995774	7.753936842	71.4947115	0.604480811	147.9513405
TP5	32.48398115	47.60626268	19.90975617	62.35325967	4.337931681	268.6935466
TP6	2.182697747	47.83389803	49.98340422	60.88769149	0.19288254	227.4049233
TP7	26.22740608	3.214398767	70.55819515	73.61556432	1.308429724	298.860031
TP8	46.49326751	8.374224161	45.13250833	65.42451532	3.355735608	41.45221997
TP9	27.88490174	56.71202248	15.40307578	69.48533947	0.953465846	351.2404299
TP10	27.25628652	28.33509964	44.40861384	64.01912763	2.527522335	381.235779
TP11	26.06063833	39.62502573	34.31433594	78.69318778	4.944339734	438.3929144
TP12	7.098782633	50.40500367	42.4962137	75.71289142	2.373224705	198.2150931
TP13	10.60184533	33.86874378	55.5294109	69.39126459	0.052966075	82.47584277
TP15	35.8188977	10.30606915	53.87503315	69.78814675	4.931485061	126.9982419

TP16	8.897586562	79.66920034	11.4332131	62.63016272	0.554273422	103.7671546
TP17	11.47785769	34.96801287	53.55412944	69.19186878	0.183775705	96.18152409
TP18	60.81574484	29.07018509	10.11407007	62.44137826	2.638214752	93.77736336
TP19	46.2983347	25.28283109	28.41883421	66.11488454	1.397929295	130.014941
TP21	11.47674418	34.96718482	53.556071	69.1921489	0.183633695	96.17398632
TP22	25.45468545	38.28227249	36.26304206	65.94123052	1.801658837	168.9413281
TP23	8.982768751	51.05871264	39.95851861	65.3124427	1.895371988	146.4087538
TP24	29.06880553	53.62424803	17.30694644	73.41140816	1.579158518	459.0569256
TP8R	46.49326751	8.374224161	45.13250833	65.42451532	3.355735608	41.45221997
TP36	33.33333333	33.33333333	33.33333333	80	0.01	480
TP7R	26.22740608	3.214398767	70.55819515	73.61556432	1.308429724	298.860031
TP8R2	46.49326751	8.374224161	45.13250833	65.42451532	3.355735608	41.45221997
TP19R	46.2983347	25.28283109	28.41883421	66.11488454	1.397929295	130.014941
TP37	18.12316921	19.26501801	62.61181278	67.44276766	4.815959786	235.3127
TP38	25.14868723	39.37080947	35.4805033	76.59507267	2.8102189	275.5266796
TP39	10.86318351	17.70569035	71.43112615	79.85894956	4.180993366	61.41768945
TP40	39.45242733	13.79182026	46.75575241	78.88989398	3.259604853	67.17073191
TP41	53.26989082	37.90370204	8.826407144	63.31619902	2.443876164	468.9708083
TP42	21.18401635	41.81146592	37.00451772	79.14344935	4.480730916	101.1794941
TP43	45.92123815	15.96822134	38.11054052	64.99688625	0.17073896	420.9300958
TP44	43.57105898	31.1980986	25.23084242	63.11794959	3.676245341	413.2140345
TP45	16.44603056	51.07171976	32.48224969	74.02085358	1.338144354	309.9427094
TP46	21.27810249	56.85350662	21.8683909	61.23197081	2.891953246	427.6562615
TP47	24.10943711	33.56737234	42.32319055	71.55372437	4.36878218	124.1342939
TP48	42.09829844	34.19577757	23.705924	79.78168452	3.246879501	253.7180608
TP49	48.13747583	5.723735705	46.13878846	73.84444682	3.322489937	320.7434185
TP50	15.13946797	67.42498117	17.43555086	68.20733514	4.72127865	284.7395267
TP51	29.13833597	36.94205397	33.91961006	72.63426246	1.06295214	101.0330373
TP52	10.85130644	82.24716741	6.90152615	74.66291416	1.177787323	381.3599159
TP53	38.49997968	22.23280833	39.26721199	71.3788862	4.89668709	254.9074672
TP54	76.77141637	6.938258409	16.29032522	78.63732886	4.924731168	476.7142603
TP55	41.61300467	35.47299944	22.91399588	65.60943099	3.328266065	437.4132239
TP56	66.29151461	29.48351928	4.224966109	63.29045104	0.568458684	306.5135858
TP57	11.38441771	34.66858803	53.94699427	74.38026248	2.941242176	236.8223333
TP58	45.56709951	15.19988425	39.23301625	74.88685403	4.280840078	278.2288157
TP59	9.327477083	42.13040084	48.54212208	62.41298638	1.986792736	64.08790961
TP60	12.8614924	16.52165833	70.61684927	67.34149171	0.916999484	239.2189879
TP61	5	5	90	75	0.1	240
TP62	25	5	70	75	0.1	240
TP15R	39.45242733	13.79182026	46.75575241	78.88989398	3.259604853	67.17073191
TP40R	35.8188977	10.30606915	53.87503315	69.78814675	4.931485061	126.9982419
TP63	35	5	60	65	0.5	120
TP64	15	5	80	70	1	150

TP65	45	10	45	75	1.5	180
TP66	55	10	35	80	2	210
TP67	65	15	20	80	0.5	210
TP68	75	15	10	75	1	180
TP69	85	10	5	70	1.5	150
TP70	75	10	15	65	2	120
TP71	5.817141484	23.1362894	76.04656911	73.90267832	0.197124157	126.705955
TP72	12.83839619	12.39139086	79.77021295	61.93194153	1.326026083	451.484819
TP73	10.65426715	46.19647251	48.14926034	61.1626867	4.990837835	471.5999767
TP74	9.300917322	24.52262302	71.17645966	62.4424886	3.421079327	393.9568051
TP75	5.62468005	15.43253995	83.94278	78.55379838	2.303679732	154.2801145
TP76	6.349994515	35.91835297	62.73165252	66.29308401	3.835560643	321.844105
TP77	5.944150323	37.10532729	61.95052238	62.77099773	4.046350235	255.2977864
TP78	5.230837181	36.26025807	63.50890475	62.39960153	4.530969336	226.0671558
TP79	5.003776938	43.98955644	56.00666662	70.45411795	2.549919195	477.0084104
TP80	6.487648311	34.5316656	63.98068609	67.73694405	4.423989223	433.396232
TP81	5.831153061	17.86471581	81.30413113	75.39229061	1.155122591	436.9574186
TP82	13.44786123	5.446357864	86.1057809	74.74092945	0.199034634	316.8225859
TP83	56.42840275	6.949994835	41.62160242	78.79616918	1.58940528	72.88348692
TP84	71.54026422	5.152875867	28.30685991	76.74227383	3.284804993	118.9623407
TP85	75.42799063	5.413338045	24.15867132	66.48887699	2.242041561	128.3132982
TP86	57.90887713	6.361677752	40.72944512	76.66119302	3.627537844	148.7356632
TP87	78.47067379	5.778520622	20.75080558	64.46776135	1.028713885	161.550922
TP88	66.35836766	8.368602335	30.27303001	64.02569858	0.839720853	221.0160857
TP89	26.24842565	7.377925195	71.37364915	79.93979141	4.394749329	313.2887613
TP90	42.27469457	9.140924935	53.58438049	60.37135404	1.18009823	458.1411079
TP91	8.158884051	48.64524014	48.19587581	79.75569913	0.727789595	73.30421844
TP92	10.85451018	14.82696653	79.31852329	78.0952397	2.343185423	461.632338
TP93	33.14663048	5.111834884	66.74153463	70.62249478	0.090641677	190.4096881
TP94	30.23066151	6.35008313	68.41925536	61.59787608	0.698512969	406.7679498
TP49R	48.13747583	5.723735705	46.13878846	73.84444682	3.322489937	320.7434185
TP58R	45.56709951	15.19988425	39.23301625	74.88685403	4.280840078	278.2288157

Table S3. Summary of all Initial Monomer Feed and Experimental Conditions. *Summary of all initial monomer feed ratios, reaction temperature, amount of AIBN and reaction time. R stands for a repeat of the experiment of a given condition.*

3.2. Summary of ^{1}H Integration Values for Reaction Mixture Prior to Reaction

The following table summarizes the initial ^{1}H integration values for each monomer as well as the overall ^{1}H integration values for all 89 terpolymerization reactions before the reaction starts:

Sample	0 min Myrcene Integration	0 min DBI Integration	0 min Styrene Integration	0 min Overall Integration

TP1	0.557	1.133	1.17	2.86
TP2	1.687	0.027	1.033	2.747
TP3	0.833	0.936	1.173	2.942
TP4	0.606	0.271	2.109	2.986
TP5	1.342	0.719	0.977	3.038
TP6	1.404	1.643	0.065	3.112
TP7	0.12	2.212	0.772	3.104
TP8	0.225	1.388	1.356	2.969
TP9	1.59	0.539	0.826	2.955
TP10	0.815	1.47	0.647	2.932
TP11	1.066	1.083	0.554	2.703
TP12	1.401	1.396	0.224	3.021
TP13	0.896	1.631	0.319	2.846
TP15	0.314	1.668	1.061	3.043
TP16	2.174	0.435	0.314	2.923
TP17	0.974	1.712	0.402	3.088
TP18	0.79	0.323	1.84	2.953
TP19	0.727	0.977	1.497	3.201
TP21	1.018	1.748	0.38	3.146
TP22	1.14	1.239	0.774	3.153
TP23	1.406	1.28	0.274	2.96
TP24	1.459	0.552	0.841	2.852
TP8R	0.218	1.303	1.31	2.831
TP36	0.94	1.064	0.996	3
TP7R	0.109	2.255	0.793	3.157
TP8R2	0.231	1.402	1.37	3.003
TP19R	0.704	0.942	1.459	3.105
TP37	0.605	2.011	0.516	3.132
TP38	1.15	1.157	0.742	3.049
TP39	0.505	2.32	0.338	3.163
TP40	0.384	1.495	1.201	3.08
TP41	1.105	0.312	1.757	3.174
TP42	1.187	1.26	0.711	3.158
TP43	0.487	1.269	1.478	3.234
TP44	0.925	0.863	1.449	3.237
TP45	1.551	1.112	0.502	3.165
TP46	1.409	0.614	0.603	2.626
TP47	0.876	1.29	0.722	2.888
TP48	0.902	0.699	1.146	2.747
TP49	0.149	1.421	1.424	2.994
TP50	1.907	0.615	0.463	2.985
TP51	1.012	1.066	0.871	2.949
TP52	2.355	0.284	0.332	2.971

TP53	0.659	1.235	1.115	3.009
TP54	0.165	0.506	2.275	2.946
TP55	0.889	0.683	1.131	2.703
TP56	0.838	0.146	2.042	3.026
TP57	0.999	1.83	0.408	3.237
TP58	0.484	1.301	1.397	3.182
TP59	1.154	1.519	0.276	2.949
TP60	0.476	2.081	0.379	2.936
TP61	0.142	2.722	0.156	3.02
TP62	0.138	2.054	0.707	2.899
TP15R	0.281	1.659	1.039	2.979
TP40R	0.369	1.483	1.17	3.022
TP63	0.142	1.941	1.074	3.157
TP64	0.159	2.654	0.481	3.294
TP65	0.255	1.45	1.353	3.058
TP66	0.245	1.087	1.618	2.95
TP67	0.414	0.628	2.03	3.072
TP68	0.401	0.306	2.291	2.998
TP69	0.277	0.157	2.759	3.193
TP70	0.351	0.604	3.098	4.053
TP71	0.696	2.449	0.186	3.331
TP72	0.349	2.487	0.385	3.221
TP73	1.238	1.537	0.297	3.072
TP74	0.711	2.154	0.27	3.135
TP75	0.467	2.681	0.172	3.32
TP76	1.014	2.08	0.174	3.268
TP77	1.012	2.068	0.167	3.247
TP78	1.064	1.99	0.168	3.222
TP79	1.231	1.827	0.122	3.18
TP80	0.905	1.983	0.168	3.056
TP81	0.473	2.545	0.165	3.183
TP82	0.167	2.728	0.386	3.281
TP83	0.158	1.288	1.635	3.081
TP84	0.107	0.897	2.133	3.137
TP85	0.136	0.735	2.29	3.161
TP86	0.161	1.23	1.734	3.125
TP87	0.135	0.612	2.281	3.028
TP88	0.214	0.953	1.924	3.091
TP89	0.279	3.422	1.143	4.844
TP90	0.223	1.674	1.225	3.122
TP91	1.274	1.498	0.272	3.044
TP92	0.427	2.429	0.309	3.165
TP93	0.176	3.058	1.433	4.667

TP94	0.175	2.214	0.88	3.269
TP49R	0.139	1.451	1.414	3.004
TP58R	0.404	1.207	1.334	2.945

Table S4. Summary of ^{1}H Integration Values for Reaction Mixture Prior to Reaction. *Summary of all initial monomer and overall ^{1}H integration values before the reaction starts. R stands for a repeat of the experiment of a given condition.*

3.3. Summary of ^{1}H Integration Values for Reaction Mixture After Reaction Prior to Precipitation

The following table summarizes the initial ^{1}H integration values for each monomer as well as the overall ^{1}H integration values for all 89 terpolymerization reactions after reaction reaction time has elapsed and prior to precipitation in MeOH:

Sample	Pre-Precipitation Myrcene Integration	Pre-Precipitation DBI Integration	Pre-Precipitation Styrene Integration	Pre-Precipitation Overall Integration
TP1	0.005	0.231	0.32	0.556
TP2	1.304	0.013	0.898	2.215
TP3	0.673	0.817	1.04	2.53
TP4	0.5	0.222	1.905	2.627
TP5	0.932	0.539	0.855	2.326
TP6	1.297	1.576	0.038	2.911
TP7	0	1.046	0.079	1.125
TP8	0.176	1.299	1.23	2.705
TP9	1.134	0.334	0.686	2.154
TP10	0.346	0.896	0.423	1.665
TP11	0.051	0.125	0.155	0.331
TP12	0.727	0.812	0.164	1.703
TP13	0.799	1.504	0.29	2.593
TP15	0.078	0.928	0.485	1.491
TP16	2.126	0.424	0.302	2.852
TP17	0.866	1.646	0.366	2.878
TP18	0.697	0.281	1.73	2.708
TP19	0.556	0.787	1.309	2.652
TP21	0.928	1.682	0.36	2.97
TP22	0.873	1.019	0.667	2.559
TP23	1.124	1.048	0.229	2.401
TP24	0.647	0.172	0.558	1.377
TP8R	0.169	1.196	1.167	2.532
TP36	0.778	0.939	0.937	2.654
TP7R	0	1.078	0.143	1.221
TP8R2	0.176	1.31	1.237	2.723
TP19R	0.549	0.807	1.289	2.645

TP37	0.151	1.199	0.253	1.603
TP38	0.252	0.352	0.364	0.968
TP39	0.144	1.582	0.177	1.903
TP40	0.134	0.848	0.693	1.675
TP41	0.638	0.137	1.327	2.102
TP42	0.379	0.556	0.402	1.337
TP43	0.339	1.051	1.234	2.624
TP44	0.407	0.411	0.97	1.788
TP45	0.774	0.571	0.348	1.693
TP46	1.031	0.418	0.506	1.955
TP47	0.417	0.826	0.49	1.733
TP48	0.126	0.106	0.461	0.693
TP49	0	0.217	0.132	0.349
TP50	1.147	0.304	0.341	1.792
TP51	0.734	0.822	0.717	2.273
TP52	1.664	0.141	0.276	2.081
TP53	0.104	0.436	0.493	1.033
TP54	0	0	0.056	0.056
TP55	0.336	0.26	0.709	1.305
TP56	0.669	0.101	1.784	2.554
TP57	0.232	0.894	0.176	1.302
TP58	0.003	0.211	0.225	0.439
TP59	1.044	1.397	0.251	2.692
TP60	0.268	1.732	0.268	2.268
TP61	0.023	2.414	0.07	2.507
TP62	0.058	1.864	0.528	2.45
TP15R	0.141	0.925	0.592	1.658
TP40R	0.119	0.764	0.616	1.499
TP63	0.079	1.855	0.925	2.859
TP64	0.055	2.078	0.229	2.362
TP65	0.033	0.731	0.597	1.361
TP66	0.012	0.238	0.438	0.688
TP67	0.161	0.295	1.259	1.715
TP68	0.219	0.143	1.57	1.932
TP69	0.205	0.083	1.961	2.249
TP70	0.26	0.455	2.537	3.252
TP71	0.475	2.28	0.154	2.909
TP72	0.149	1.891	0.191	2.231
TP73	0.532	0.897	0.174	1.603
TP74	0.182	1.419	0.115	1.716
TP75	0.079	1.709	0.069	1.857
TP76	0.365	1.214	0.095	1.674
TP77	0.534	1.443	0.113	2.09

TP78	0.594	1.582	0.115	2.291
TP79	0.242	0.787	0.027	1.056
TP80	0.105	0.963	0.043	1.111
TP81	0.031	1.417	0.03	1.478
TP82	0	2.302	0.202	2.504
TP83	0	0.856	1.02	1.876
TP84	0	0.217	0.648	0.865
TP85	0	0.492	1.588	2.08
TP86	0	0.357	0.446	0.803
TP87	0	0.343	1.538	1.881
TP88	0.125	0.732	1.535	2.392
TP89	0	0.811	0	0.811
TP90	0.057	1.132	0.728	1.917
TP91	0.943	1.293	0.229	2.465
TP92	0	0.871	0	0.871
TP93	0.154	2.657	1.083	3.894
TP94	0	1.391	0.33	1.721
TP49R	0	0.317	0.173	0.49
TP58R	0	0.162	0.242	0.404

Table S5. Summary of 1H Integration Values for Reaction Mixture After Reaction Prior to Precipitation. *Summary of all initial monomer and overall ^{1}H integration values after the reaction time has elapsed, prior to precipitation in MeOH. R stands for a repeat of the experiment of a given condition.*

3.4. Summary of Monomer Conversion Values for All Samples

The following table summarizes the monomer conversion values for each monomer as well as the overall conversion for all 89 terpolymerization reactions:

Sample	Myrcene Conversion (%)	DBI Conversion (%)	Styrene Conversion (%)	Overall Conversion (%)
TP1	99.10233393	79.61165049	72.64957265	80.55944056
TP2	22.70302312	51.85185185	13.06873185	19.36658173
TP3	19.20768307	12.71367521	11.33844842	14.00407886
TP4	17.49174917	18.08118081	9.672830725	12.02277294
TP5	30.5514158	25.03477051	12.48720573	23.43647136
TP6	7.621082621	4.077906269	41.53846154	6.458868895
TP7	100	52.7124774	89.76683938	63.7564433
TP8	21.77777778	6.412103746	9.292035398	8.891882789
TP9	28.67924528	38.03339518	16.94915254	27.10659898
TP10	57.54601227	39.04761905	34.62132921	43.21282401
TP11	95.21575985	88.45798707	72.02166065	87.75434702
TP12	48.10849393	41.83381089	26.78571429	43.62793777
TP13	10.82589286	7.786633967	9.090909091	8.889669712

TP15	75.15923567	44.36450839	54.28840716	51.00230036
TP16	2.207911684	2.528735632	3.821656051	2.42901129
TP17	11.08829569	3.855140187	8.955223881	6.800518135
TP18	11.7721519	13.00309598	5.97826087	8.296647477
TP19	23.5213205	19.44728762	12.55845023	17.15089035
TP21	8.84086444	3.775743707	5.263157895	5.594405594
TP22	23.42105263	17.75625504	13.82428941	18.83920076
TP23	20.056899	18.125	16.42335766	18.88513514
TP24	55.65455792	68.84057971	33.65041617	51.71809257
TP8R	22.47706422	8.21181888	10.91603053	10.561639
TP36	17.23404255	11.7481203	5.923694779	11.53333333
TP7R	100	52.19512195	81.96721311	61.32404181
TP8R2	23.80952381	6.562054208	9.708029197	9.324009324
TP19R	22.01704545	14.33121019	11.65181631	14.81481481
TP37	75.04132231	40.37792143	50.96899225	48.81864623
TP38	78.08695652	69.57649092	50.94339623	68.25188586
TP39	71.48514851	31.81034483	47.63313609	39.83559911
TP40	65.10416667	43.27759197	42.29808493	45.61688312
TP41	42.26244344	56.08974359	24.47353443	33.77441714
TP42	68.07076664	55.87301587	43.45991561	57.6630779
TP43	30.39014374	17.17888101	16.50879567	18.86209029
TP44	56	52.37543453	33.05728088	44.76367006
TP45	50.0967118	48.65107914	30.67729084	46.50868878
TP46	26.82753726	31.9218241	16.08623549	25.5521706
TP47	52.39726027	35.96899225	32.13296399	39.99307479
TP48	86.03104213	84.83547926	59.77312391	74.77247907
TP49	100	84.72906404	90.73033708	88.34335337
TP50	39.85317252	50.56910569	26.34989201	39.96649916
TP51	27.47035573	22.88930582	17.68082664	22.92302475
TP52	29.3418259	50.35211268	16.86746988	29.95624369
TP53	84.2185129	64.69635628	55.78475336	65.66965769
TP54	100	100	97.53846154	98.09911745
TP55	62.20472441	61.93265007	37.31211317	51.72031077
TP56	20.16706444	30.82191781	12.63467189	15.59814937
TP57	76.77677678	51.14754098	56.8627451	59.77757183
TP58	99.38016529	83.78170638	83.8940587	86.20364551
TP59	9.532062392	8.031599737	9.057971014	8.714818583
TP60	43.69747899	16.77078328	29.28759894	22.7520436
TP61	83.8028169	11.3152094	55.12820513	16.98675497
TP62	57.97101449	9.250243427	25.31824611	15.48809934
TP15R	49.82206406	44.24352019	43.02213667	44.34373951
TP40R	67.75067751	48.48280512	47.35042735	50.39708802
TP63	44.36619718	4.430705822	13.87337058	9.439341147

TP64	65.40880503	21.70308968	52.39085239	28.29386764
TP65	87.05882353	49.5862069	55.87583149	55.49378679
TP66	95.10204082	78.1048758	72.92954265	76.6779661
TP67	61.11111111	53.02547771	37.98029557	44.17317708
TP68	45.38653367	53.26797386	31.47097337	35.55703803
TP69	25.99277978	47.13375796	28.92352302	29.56467272
TP70	25.92592593	24.66887417	18.10845707	19.76313842
TP71	31.75287356	6.900775827	17.20430108	12.66886821
TP72	57.30659026	23.964616	50.38961039	30.73579634
TP73	57.02746365	41.63955758	41.41414141	47.81901042
TP74	74.40225035	34.12256267	57.40740741	45.26315789
TP75	83.08351178	36.25512868	59.88372093	44.06626506
TP76	64.00394477	41.63461538	45.40229885	48.77600979
TP77	47.23320158	30.22243714	32.33532934	35.6328919
TP78	44.17293233	20.50251256	31.54761905	28.89509621
TP79	80.34118603	56.92391899	77.86885246	66.79245283
TP80	88.39779006	51.43721634	74.4047619	63.64528796
TP81	93.44608879	44.32220039	81.81818182	53.56581841
TP82	100	15.61583578	47.66839378	23.68180433
TP83	100	33.54037267	37.6146789	39.11067835
TP84	100	75.80824972	69.62025316	72.4258846
TP85	100	33.06122449	30.65502183	34.1980386
TP86	100	70.97560976	74.27912341	74.304
TP87	100	43.95424837	32.5734327	37.87978864
TP88	41.58878505	23.18992655	20.21829522	22.61404076
TP89	100	76.30040912	100	83.25763832
TP90	74.43946188	32.37753883	40.57142857	38.59705317
TP91	25.9811617	13.68491322	15.80882353	19.02102497
TP92	100	64.14162207	100	72.48025276
TP93	12.5	13.11314585	24.42428472	16.56310264
TP94	100	37.17253839	62.5	47.35393087
TP49R	100	78.15299793	87.76520509	83.68841545
TP58R	100	86.57829329	81.85907046	86.28183362

Table S6. Summary of Monomer Conversion. *Summary of monomer and overall conversion for all 89 terpolymerization reactions. R stands for a repeat of the experiment of a given condition.*

3.5. Summary of Monomer ^{1}H Integration Values for Terpolymer Samples

The following table summarizes the ^{1}H integration values for each monomer functional group peak in the terpolymer sample for all 89 terpolymerization reactions:

Sample	Sty Integration	Myr Integration	DBI Integration
TP1	1	0.138	0.557

TP2	1	1.142	0.039
TP3	1	0.501	0.869
TP4	1	0.167	0.116
TP5	1	0.889	0.895
TP6	1	22.855	40.372
TP7	1	0.014	1.065
TP8	1	0.036	0.499
TP9	1	1.325	1.09
TP10	1	0.755	1.813
TP11	1	0.885	1.562
TP12	1	4.377	7.056
TP13	1	1.957	4.306
TP15	1	0.062	0.674
TP16	1	4.872	2.891
TP17	1	1.72	3.667
TP18	1	0.269	0.221
TP19	1	0.274	0.626
TP21	1	1.901	4.077
TP22	1	1.002	1.599
TP23	1	3.583	5.406
TP24	1	1.054	0.863
TP8R	1	0.045	0.5
TP36	1	0.633	1.133
TP7R	1	0.019	1.02
TP8R2	1	0.058	0.515
TP19R	1	0.299	0.616
TP37	1	0.532	2.15
TP38	1	0.873	1.474
TP39	1	0.789	3.369
TP40	1	0.177	0.784
TP41	1	0.38	0.223
TP42	1	0.953	1.663
TP43	1	0.216	0.678
TP44	1	0.411	0.652
TP45	1	2.035	2.783
TP46	1	1.632	1.602
TP47	1	0.72	1.58
TP48	1	0.328	0.509
TP49	1	0.043	0.533
TP50	1	2.609	2.033
TP51	1	0.734	1.264
TP52	1	4.853	1.635
TP53	1	0.313	0.851

TP54	1	0.01	0.124
TP55	1	0.493	0.681
TP56	1	0.275	0.095
TP57	1	1.449	3.401
TP58	1	0.152	0.611
TP59	1	3.157	5.806
TP60	1	0.695	2.74
TP61	1	0.306	4.135
TP62	1	0.093	1.12
TP15R	1	0.053	0.668
TP40R	1	0.195	0.762
TP63	1	0.04	0.661
TP64	1	0.059	1.52
TP65	1	0.068	0.626
TP66	1	0.068	0.506
TP67	1	0.036	0.241
TP68	1	0.062	0.122
TP69	1	0.05	0.057
TP70	1	0.034	0.175
TP71	1	2.683	8.821
TP72	1	0.373	2.297
TP73	1	2.62	4.956
TP74	1	1.427	4.643
TP75	1	1.225	6.966
TP76	1	3.452	8.906
TP77	1	4.205	9.987
TP78	1	4.083	9.64
TP79	1	5.559	12.093
TP80	1	3.032	8.427
TP81	1	1.138	6.527
TP82	1	0.162	1.989
TP83	1	0.035	0.423
TP84	1	0.183	0.346
TP85	1	0.091	0.271
TP86	1	0.131	0.498
TP87	1	0.086	0.235
TP88	1	0.194	0.49
TP89	1	0.271	1.1
TP90	1	0.164	0.711
TP91	1	2.228	3.065
TP92	1	0.619	2.692
TP93	1	0.184	0.745
TP94	1	0.276	0.91

TP49R	1	0.021	0.496
TP58R	1	0.182	0.59

Table S7. Summary of Monomer 1H Integration Values for Terpolymer Samples. *Summary of monomer ^{1}H integration values for each monomer functional group peak in the terpolymer sample for all 89 terpolymerization reactions. The ^{1}H integration is standardized to 1. R stands for a repeat of the experiment of a given condition.*

3.6. Summary of ^{1}H Protons per Integration for Terpolymer Samples

The following table summarizes the ^{1}H integration values per proton for each monomer functional group peak in the terpolymer sample for all 89 terpolymerization reactions:

Sample	Sty Proton Per Integration	Myr Proton Per Integration	DBI Proton Per Integration
TP1	0.2	0.069	0.1393
TP2	0.2	0.571	0.0098
TP3	0.2	0.2505	0.2173
TP4	0.2	0.0835	0.029
TP5	0.2	0.4445	0.2238
TP6	0.2	11.428	10.093
TP7	0.2	0.007	0.2663
TP8	0.2	0.018	0.1248
TP9	0.2	0.6625	0.2725
TP10	0.2	0.3775	0.4533
TP11	0.2	0.4425	0.3905
TP12	0.2	2.1885	1.764
TP13	0.2	0.9785	1.0765
TP15	0.2	0.031	0.1685
TP16	0.2	2.436	0.7228
TP17	0.2	0.86	0.9168
TP18	0.2	0.1345	0.0553
TP19	0.2	0.137	0.1565
TP21	0.2	0.9505	1.0193
TP22	0.2	0.501	0.3998
TP23	0.2	1.7915	1.3515
TP24	0.2	0.527	0.2158
TP8R	0.2	0.0225	0.125
TP36	0.2	0.3165	0.2833
TP7R	0.2	0.0095	0.255
TP8R2	0.2	0.029	0.1288
TP19R	0.2	0.1495	0.154
TP37	0.2	0.266	0.5375
TP38	0.2	0.4365	0.3685
TP39	0.2	0.3945	0.8423
TP40	0.2	0.0885	0.196

TP41	0.2	0.19	0.0558
TP42	0.2	0.4765	0.4158
TP43	0.2	0.108	0.1695
TP44	0.2	0.2055	0.163
TP45	0.2	1.0175	0.6958
TP46	0.2	0.816	0.4005
TP47	0.2	0.36	0.395
TP48	0.2	0.164	0.1273
TP49	0.2	0.0215	0.1333
TP50	0.2	1.3045	0.5083
TP51	0.2	0.367	0.316
TP52	0.2	2.4265	0.4088
TP53	0.2	0.1565	0.2128
TP54	0.2	0.005	0.031
TP55	0.2	0.2465	0.1703
TP56	0.2	0.1375	0.0238
TP57	0.2	0.7245	0.8503
TP58	0.2	0.076	0.1528
TP59	0.2	1.5785	1.4515
TP60	0.2	0.3475	0.685
TP61	0.2	0.153	1.0338
TP62	0.2	0.0465	0.28
TP15R	0.2	0.0265	0.167
TP40R	0.2	0.0975	0.1905
TP63	0.2	0.02	0.1653
TP64	0.2	0.0295	0.38
TP65	0.2	0.034	0.1565
TP66	0.2	0.034	0.1265
TP67	0.2	0.018	0.0603
TP68	0.2	0.031	0.0305
TP69	0.2	0.025	0.0143
TP70	0.2	0.017	0.0438
TP71	0.2	1.3415	2.2053
TP72	0.2	0.1865	0.5743
TP73	0.2	1.31	1.239
TP74	0.2	0.7135	1.1608
TP75	0.2	0.6125	1.7415
TP76	0.2	1.726	2.2265
TP77	0.2	2.1025	2.4968
TP78	0.2	2.0415	2.41
TP79	0.2	2.7795	3.0233
TP80	0.2	1.516	2.1068
TP81	0.2	0.569	1.6318

TP82	0.2	0.081	0.4973
TP83	0.2	0.0175	0.1058
TP84	0.2	0.0915	0.0865
TP85	0.2	0.0455	0.0678
TP86	0.2	0.0655	0.1245
TP87	0.2	0.043	0.0588
TP88	0.2	0.097	0.1225
TP89	0.2	0.1355	0.275
TP90	0.2	0.082	0.1778
TP91	0.2	1.114	0.7663
TP92	0.2	0.3095	0.673
TP93	0.2	0.092	0.1863
TP94	0.2	0.138	0.2275
TP49R	0.2	0.0105	0.124
TP58R	0.2	0.091	0.1475

Table S8. Summary of Monomer 1H Integration Values per proton for Terpolymer Samples. *Summary of monomer ^{1}H integration values for each monomer normalized against the number of protons in the terpolymer sample for all 89 terpolymerization reactions. The ^{1}H integration for Styrene is standardized to 0.2 as there are 5 protons in the phenyl ring of styrene. R stands for a repeat of the experiment of a given condition.*

3.7. Summary of Monomer Incorporation in All Terpolymer Samples

The following table summarizes the percentage monomer incorporation each monomer in the terpolymer sample for all 89 terpolymerization reactions:

Sample	Sty Incorporation (mol%)	Myr Incorporation (mol%)	DBI Incorporation (mol%)
TP1	48.99	16.901	34.109
TP2	25.616	73.135	1.2488
TP3	29.951	37.514	32.535
TP4	64	26.72	9.28
TP5	23.035	51.195	25.77
TP6	0.9208	52.612	46.468
TP7	42.261	1.4791	56.26
TP8	58.352	5.2516	36.397
TP9	17.621	58.37	24.009
TP10	19.403	36.624	43.973
TP11	19.361	42.836	37.803
TP12	4.8164	52.703	42.48
TP13	8.8692	43.392	47.738
TP15	50.063	7.7597	42.178
TP16	5.9546	72.527	21.518
TP17	10.118	43.506	46.377
TP18	51.315	34.509	14.176

TP19	40.527	27.761	31.712
TP21	9.2177	43.807	46.975
TP22	18.169	45.514	36.316
TP23	5.9827	53.59	40.428
TP24	21.215	55.9	22.885
TP8R	57.554	6.4748	35.971
TP36	25.008	39.575	35.417
TP7R	43.057	2.0452	54.898
TP8R2	55.905	8.1062	35.989
TP19R	39.722	29.692	30.586
TP37	19.93	26.507	53.563
TP38	19.9	43.433	36.667
TP39	13.92	27.458	58.622
TP40	41.28	18.266	40.454
TP41	44.868	42.625	12.507
TP42	18.311	43.626	38.064
TP43	41.885	22.618	35.497
TP44	35.18	36.148	28.672
TP45	10.453	53.182	36.365
TP46	14.119	57.607	28.274
TP47	20.942	37.696	41.361
TP48	40.712	33.384	25.903
TP49	56.378	6.0606	37.562
TP50	9.9367	64.812	25.252
TP51	22.65	41.563	35.787
TP52	6.5892	79.944	13.467
TP53	35.134	27.492	37.374
TP54	84.746	2.1186	13.136
TP55	32.428	39.968	27.604
TP56	55.363	38.062	6.5744
TP57	11.269	40.823	47.908
TP58	46.647	17.726	35.627
TP59	6.192	48.87	44.938
TP60	16.227	28.195	55.578
TP61	14.422	11.033	74.545
TP62	37.987	8.8319	53.181
TP15R	50.826	6.7344	42.44
TP40R	40.984	19.98	39.037
TP63	51.914	5.1914	42.894
TP64	32.814	4.84	62.346
TP65	51.216	8.7068	40.077
TP66	55.479	9.4313	35.09
TP67	71.878	6.469	21.653

TP68	76.482	11.855	11.663
TP69	83.595	10.449	5.9561
TP70	76.702	6.5197	16.779
TP71	5.338	35.804	58.858
TP72	20.817	19.412	59.771
TP73	7.2754	47.654	45.071
TP74	9.642	34.398	55.96
TP75	7.8309	23.982	68.187
TP76	4.8164	41.565	53.618
TP77	4.1673	43.809	52.024
TP78	4.2997	43.889	51.811
TP79	3.3318	46.304	50.364
TP80	5.2318	39.657	55.111
TP81	8.3307	23.701	67.968
TP82	25.699	10.408	63.893
TP83	61.872	5.4138	32.715
TP84	52.91	24.206	22.884
TP85	63.847	14.525	21.628
TP86	51.282	16.795	31.923
TP87	66.28	14.25	19.47
TP88	47.676	23.123	29.201
TP89	32.76	22.195	45.045
TP90	43.502	17.836	38.662
TP91	9.6142	53.551	36.835
TP92	16.913	26.173	56.913
TP93	41.819	19.237	38.944
TP94	35.367	24.403	40.23
TP49R	59.791	3.139	37.07
TP58R	45.61	20.753	33.637

Table S9. Summary of Percentage Monomer Incorporation in All Terpolymer Samples. *Summary of percentage monomer incorporation into the final terpolymer. R stands for a repeat of the experiment of a given condition.*

3.8. Summary of Molecular Weight Statistics for All Terpolymer Samples

The following table summarizes the molecular weight (MW) information for all 89 terpolymer samples:

Sample	Mn	Mw	Mz	Mp	PDI	MW 10% Low	MW 10% High	Asymmetry Factor
TP1	13523	23270	35694	20559	1.7208	4924	61576	1.3028
TP2	4797	6534	8880	5329	1.3621	2202	15305	0.8377
TP3	17188	25585	36212	22248	1.4885	6980	62372	1.1245

TP4	19075	32779	49704	29968	1.7184	6685	85315	1.434
TP5	10715	17308	25805	16280	1.6153	4061	44265	1.3882
TP6	64280	113998	175664	102814	1.7735	22201	301545	1.4245
TP7	13005	20490	30448	17271	1.5755	5025	52750	1.1057
TP8	25143	37117	52887	30717	1.4762	10530	91579	0.98
TP9	12936	22012	34806	17860	1.7016	4753	60315	1.0877
TP10	20491	32635	48599	27724	1.5927	7846	84084	1.1377
TP11	7760	12031	17691	9821	1.5504	3062	30563	1.0266
TP12	12356	20523	31822	17743	1.661	4606	54593	1.1999
TP13	47208	78583	114682	76836	1.6646	16572	195608	1.6416
TP15	11445	16882	23430	16077	1.4751	4563	39997	1.3818
TP16	20375	31731	45542	28597	1.5573	7692	78098	1.307
TP17	37131	58983	84007	57937	1.5885	13749	142692	1.5958
TP18	12377	18265	25339	17877	1.4757	4918	43062	1.4681
TP19	19589	29834	42253	26922	1.523	7578	72519	1.2793
TP21	44067	69716	98994	68249	1.582	16312	168550	1.5831
TP22	17468	26321	37631	22783	1.5068	6927	64752	1.1398
TP23	16377	24354	34597	20723	1.4871	6612	59628	1.0809
TP24	10863	16511	23635	15753	1.5199	4244	40512	1.3885
TP8R	16401	23735	32953	20856	1.4472	6836	56618	1.1169
TP36	56187	95959	145044	83174	1.7079	20005	249983	1.2949
TP7R	12442	19285	27453	17159	1.55	4827	47196	1.2535
TP8R2	18425	26756	37114	23894	1.4522	7589	63752	1.1687
TP19R	17648	27034	38345	24176	1.5318	6871	65766	1.2571
TP37	12573	19741	28965	17209	1.5701	4844	49934	1.19
TP38	8443	14507	22631	12630	1.7182	3101	39036	1.2445
TP39	9401	13609	19113	12078	1.4476	3931	32846	1.122
TP40	9118	15157	22514	14160	1.6623	3366	38703	1.4288
TP41	9085	15285	23549	14154	1.6824	3301	40379	1.3887
TP42	6543	10328	15390	8360	1.5785	2556	26586	1.0243
TP43	31613	61729	111989	40567	1.9526	11169	191622	0.8308
TP44	10966	18801	28497	17436	1.7145	3861	49013	1.4587
TP45	13658	23263	35850	20184	1.7033	4888	61764	1.2679
TP46	12404	20532	31452	18493	1.6553	4503	53730	1.3245
TP47	10286	16478	24365	15450	1.602	3891	41804	1.3853
TP48	6739	11128	16974	9182	1.6513	2524	29222	1.1155
TP49	12094	19530	28874	17537	1.6149	4481	49592	1.3126
TP50	6506	10170	15228	8244	1.5632	2560	26276	1.0089
TP51	17209	27387	40091	24153	1.5914	6438	68977	1.26
TP52	7940	13039	20046	11037	1.6422	2964	34544	1.1523
TP53	8636	14181	21906	11516	1.6421	3237	37905	1.0653
TP54	7080	11862	18040	10274	1.6754	2584	30967	1.251
TP55	10205	17194	25973	16363	1.6849	3632	44515	1.504

TP56	19658	31011	44585	27757	1.5775	7395	76714	1.3011
TP57	12181	19232	28415	17117	1.5789	4648	48973	1.2401
TP58	8349	13740	20978	12254	1.6457	3100	36159	1.2702
TP59	22988	36332	54004	31583	1.5805	8803	92703	1.1864
TP60	27903	44869	66321	39054	1.608	10434	113623	1.2359
TP61	24034	31506	40968	27466	1.3109	11133	69558	0.9718
TP62	28755	47543	72025	40131	1.6534	10607	123842	1.1808
TP15R	11692	18534	27614	15750	1.5852	4486	47720	1.1329
TP40R	9339	14995	22236	14146	1.6056	3447	38095	1.4253
TP63	34907	58040	89909	51405	1.6627	13037	153986	1.2505
TP64	19866	29029	40915	24356	1.4612	8222	70786	1.0179
TP65	14294	24758	38516	21095	1.7321	5123	66502	1.2326
TP66	11921	19993	30234	18179	1.6771	4238	52098	1.3831
TP67	17109	31459	49576	28157	1.8387	5689	85282	1.4432
TP68	12132	21626	33086	20078	1.7826	4084	56665	1.5349
TP69	11768	20740	31251	19633	1.7624	3988	53371	1.5938
TP70	16118	28127	42170	26190	1.7451	5542	72107	1.5334
TP71	36211	60224	90386	56831	1.6631	13190	154462	1.4608
TP72	22253	36518	54867	31033	1.641	8360	94657	1.1761
TP73	14627	23966	35879	21274	1.6385	5340	61669	1.2988
TP74	17858	28882	42937	25425	1.6173	6663	74192	1.2505
TP75	11483	16873	23713	15118	1.4694	4628	40676	1.196
TP76	14512	23473	35020	20350	1.6175	5406	60460	1.2173
TP77	15921	25753	38549	22510	1.6175	5929	66477	1.232
TP78	17908	28718	42120	26057	1.6036	6632	72367	1.3396
TP79	15391	25286	38211	22111	1.6429	5630	65814	1.2541
TP80	13128	20461	30199	17631	1.5586	5065	52189	1.1494
TP81	15489	23861	35048	19499	1.5405	6096	60769	1.0229
TP82	19136	28686	42353	22116	1.4991	7966	73729	0.848
TP83	15184	25974	39302	23089	1.7106	5440	67664	1.3445
TP84	9726	16895	25384	16463	1.7371	3349	43332	1.6455
TP85	17594	29812	44119	27921	1.6944	6151	75490	1.5209
TP86	10712	17690	26033	16597	1.6514	3884	44538	1.4713
TP87	17987	31303	47146	28784	1.7403	6230	80645	1.4855
TP88	29612	49638	73707	45159	1.6763	10569	126158	1.4136
TP89	10017	17007	24250	17263	1.6978	3340	40856	1.9067
TP90	29436	51572	79133	45775	1.752	10508	135851	1.3528
TP91	20265	33305	48614	30784	1.6435	7316	83164	1.4459
TP92	12125	18436	25832	17205	1.5205	4600	43969	1.4059
TP93	26557	44472	66606	38292	1.6746	9677	114333	1.2574
TP94	23284	37205	54011	32185	1.5979	8860	92859	1.2174
TP49R	13666	22683	33757	20301	1.6598	4972	58672	1.3256
TP58R	9959	16107	23519	15305	1.6173	3613	40283	1.4918

Table S10. Summary of Molecular Weight Information for Terpolymer Samples. *Summary of Molecular Weight (MW) information for all 89 terpolymer samples. Results are derived from the GPC trace. R stands for a repeat of the experiment of a given condition.*

3.9. Summary of T_g and Negative Styrene Incorporation for All Terpolymer Samples

The following table summarizes the T_g (Deg C) and the Negative Styrene Incoporation (mol %) for all 89 terpolymer samples:

Sample	T_g (Deg C)	Negative Sty Incorporation (mol%)
TP1	-6.73	-48.9896
TP2	-43.13	-25.6164
TP3	-17.33	-29.9513
TP4	7.76	-64
TP5	-32.22	-23.0348
TP6	-42.53	-0.92079
TP7	12.76	-42.261
TP8	13.64	-58.3516
TP9	-38.71	-17.6211
TP10	-24.74	-19.4033
TP11	-30.65	-19.3611
TP12	-41.71	-4.81638
TP13	-32.17	-8.86918
TP15	5.64	-50.0626
TP16	-48.03	-5.9546
TP17	-35.89	-10.1176
TP18	-7.84	-51.3149
TP19	-15.4	-40.5268
TP21	-35.01	-9.21765
TP22	-32.59	-18.1694
TP23	-44.99	-5.98265
TP24	-39.05	-21.2145
TP8R	5.61	-57.554
TP36	-24.21	-25.0078
TP7R	9.14	-43.0571
TP8R2	6.19	-55.905
TP19R	-19.35	-39.7219
TP37	-23.22	-19.9302
TP38	-38.83	-19.9005
TP39	-27.69	-13.9203
TP40	-2.68	-41.2797
TP41	-24.9	-44.8682
TP42	-31.85	-18.3108

TP43	-0.87	-41.8848
TP44	-19.54	-35.1803
TP45	-43.1	-10.4534
TP46	-40.51	-14.1193
TP47	-29.2	-20.9424
TP48	-23.45	-40.7125
TP49	22.03	-56.3777
TP50	-46.52	-9.93665
TP51	-28.06	-22.6501
TP52	-56.36	-6.58924
TP53	-14.22	-35.1339
TP54	45.94	-84.7458
TP55	-24.34	-32.4281
TP56	-5.06	-55.3633
TP57	-31.78	-11.2692
TP58	3.82	-46.6472
TP59	-37.23	-6.19195
TP60	-23.98	-16.2272
TP61	-4.89	-14.4222
TP62	5.99	-37.9867
TP15R	4.77	-50.8259
TP40R	-2.37	-40.9836
TP63	20.84	-51.9143
TP64	3.79	-32.8138
TP65	12.97	-51.2164
TP66	22.62	-55.4785
TP67	13.73	-71.8778
TP68	18.9	-76.4818
TP69	34.91	-83.5946
TP70	31.43	-76.7018
TP71	-31.32	-5.33796
TP72	-16.07	-20.8171
TP73	-42.72	-7.27537
TP74	-36.25	-9.64204
TP75	-27.71	-7.83085
TP76	-39.84	-4.81638
TP77	-40.76	-4.16732
TP78	-39.65	-4.29969
TP79	-38.26	-3.33181
TP80	-38.93	-5.23184
TP81	-25.71	-8.33073
TP82	-1.94	-25.6987
TP83	15.65	-61.8716

TP84	25.91	-52.9101
TP85	11.34	-63.8468
TP86	24.82	-51.2821
TP87	33.48	-66.28
TP88	24.58	-47.6758
TP89	-0.78	-32.76
TP90	11.34	-43.5019
TP91	-42.98	-9.61423
TP92	-16.86	-16.9133
TP93	-19.71	-41.8191
TP94	6.22	-35.3669
TP49R	21.57	-59.7907
TP58R	2.85	-45.61

Table S11. Summary of T_g and Negative Styrene Incorporation for all Terpolymer Samples.

Summary of the glass transition temperature as determined by the DSC analysis, and the negative styrene incorporation as determined by NMR analysis for all 89 terpolymer samples.

3.10. Relationships Between Terpolymer Variables

In this section, we plot different terpolymer variables collected during the experiments in order to visualise the relationships between them:

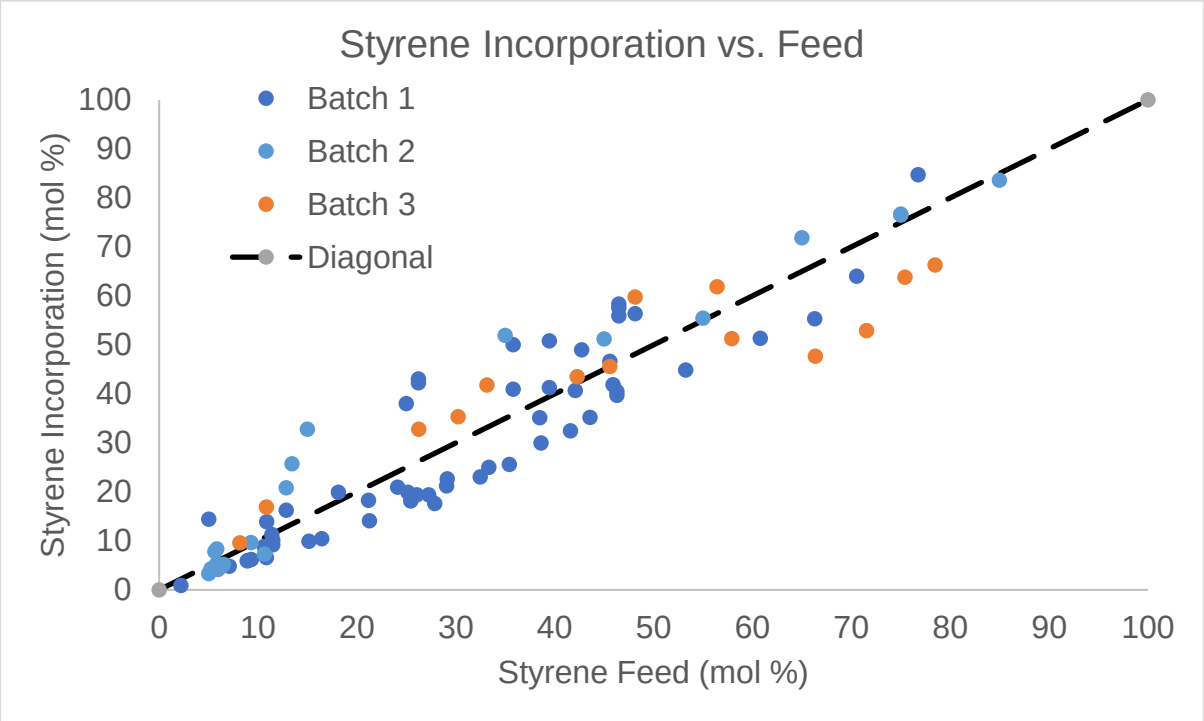

Figure S12. *Styrene Incorporation plotted against Styrene Feed.*

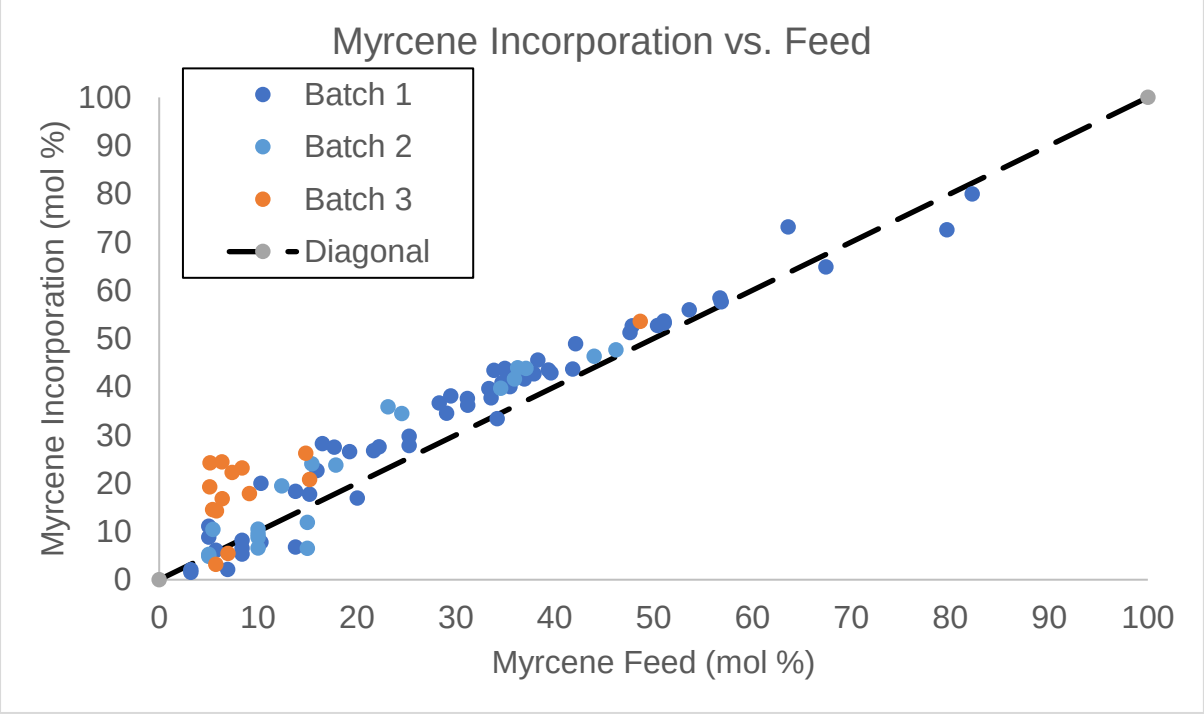

Figure S13. *Myrcene Incorporation plotted against Myrcene Feed.*

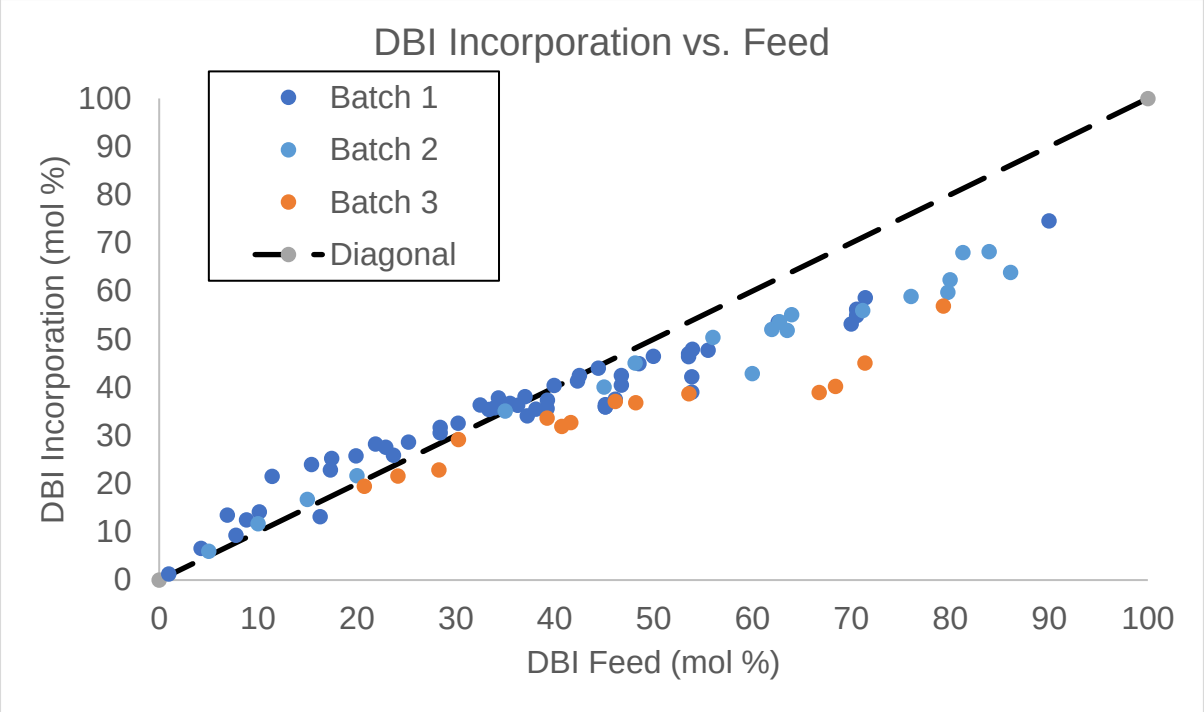

Figure S14. *DBI Incorporation plotted against DBI Feed.*

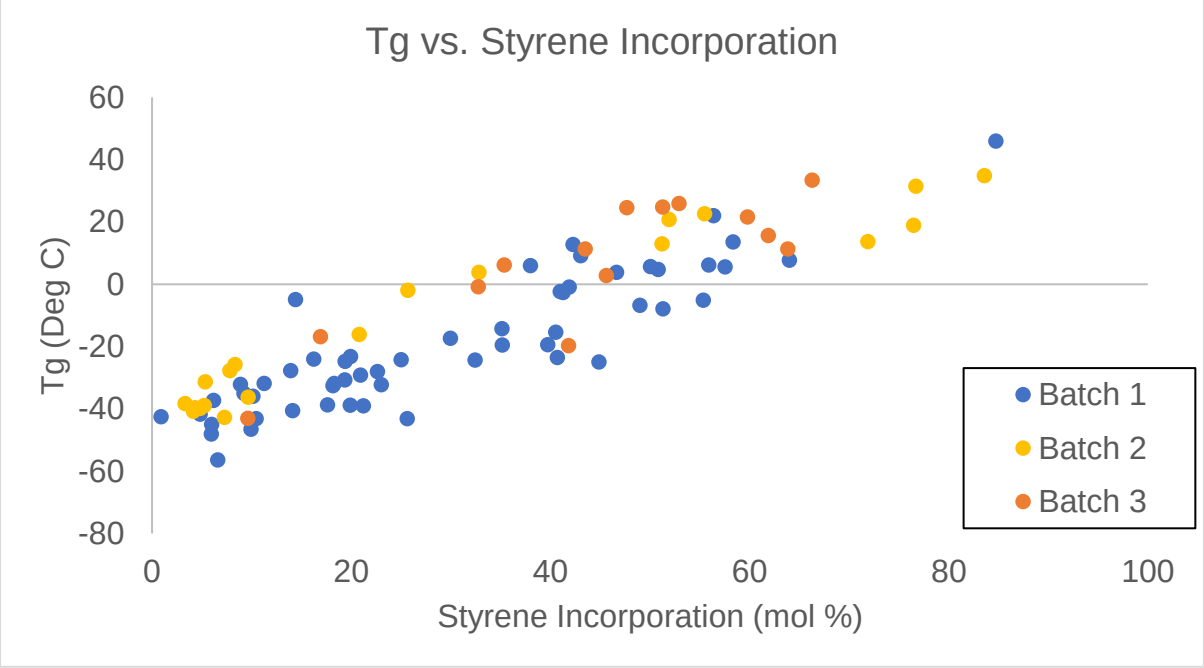

Figure S15. *Tg plotted against Styrene Incorporation.*

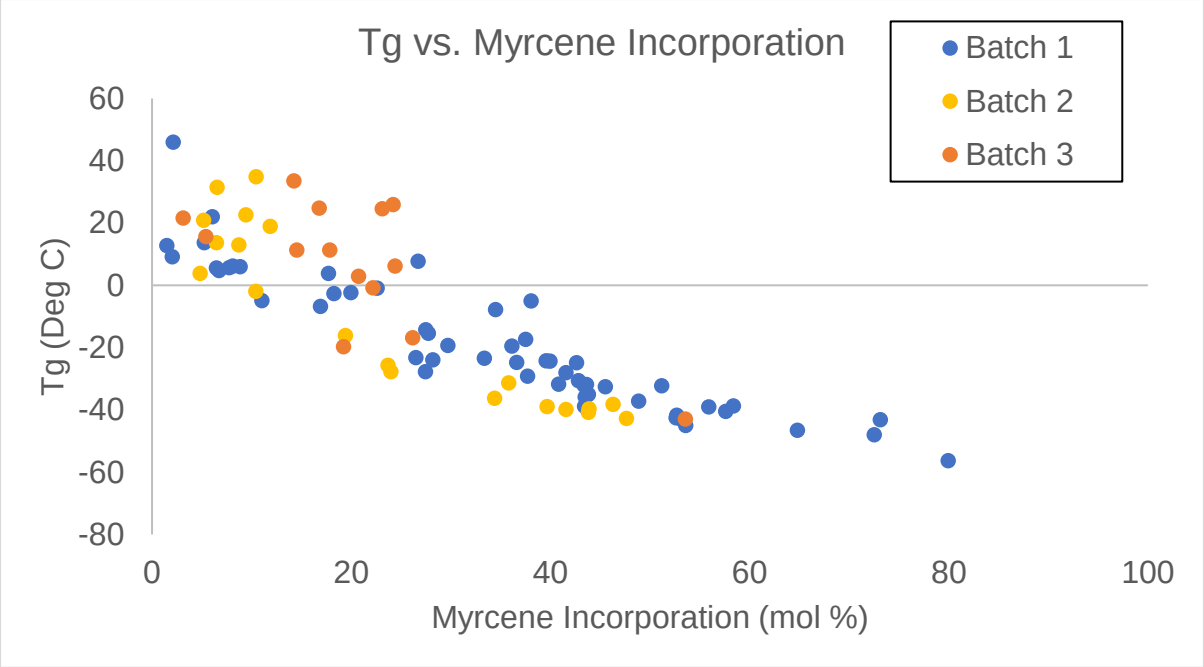

Figure S16. *Tg plotted against Myrcene Incorporation.*

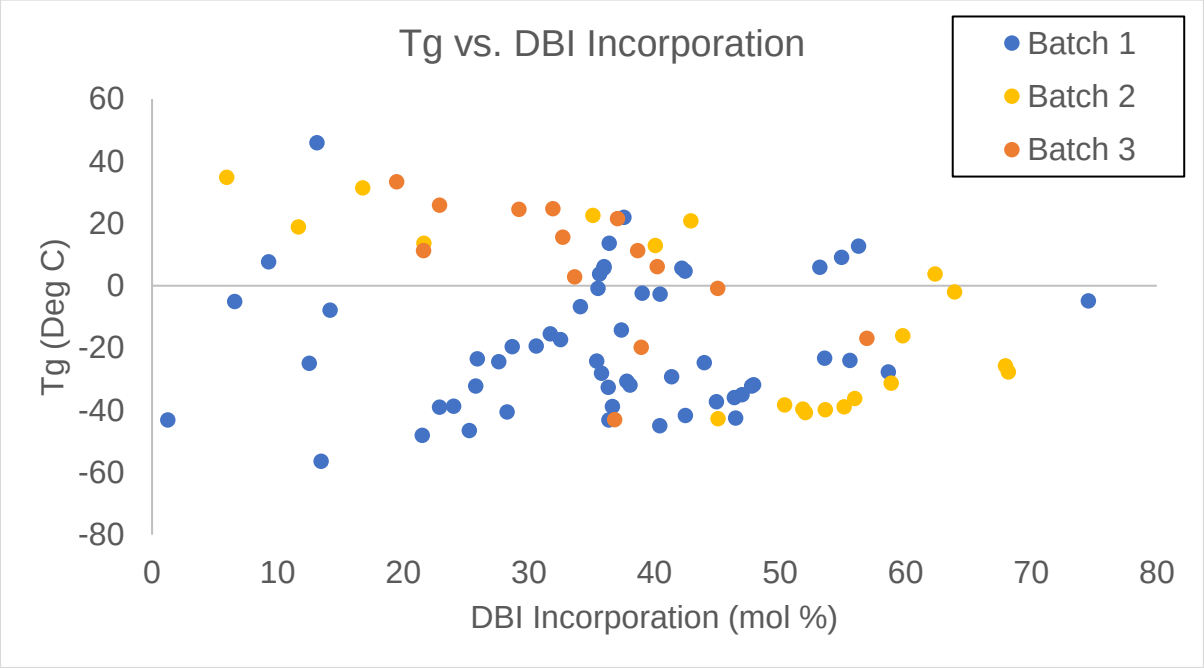

Figure S17. *Tg plotted against DBI Incorporation.*

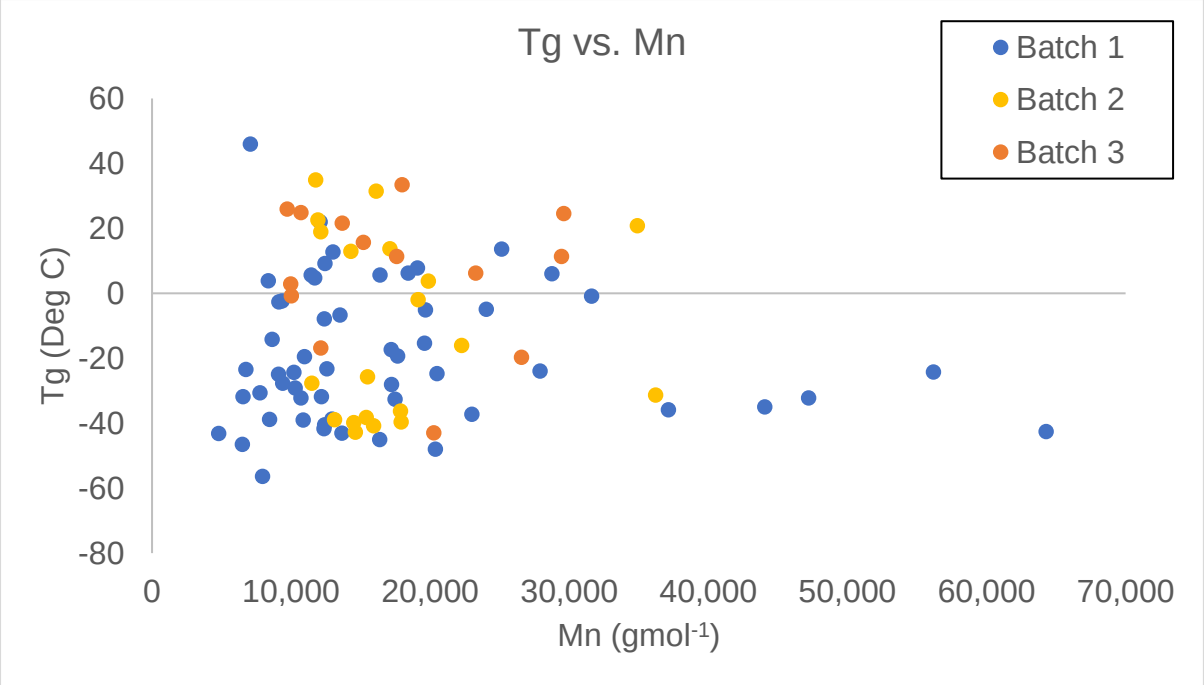

Figure S18. *Tg plotted against Mn.*

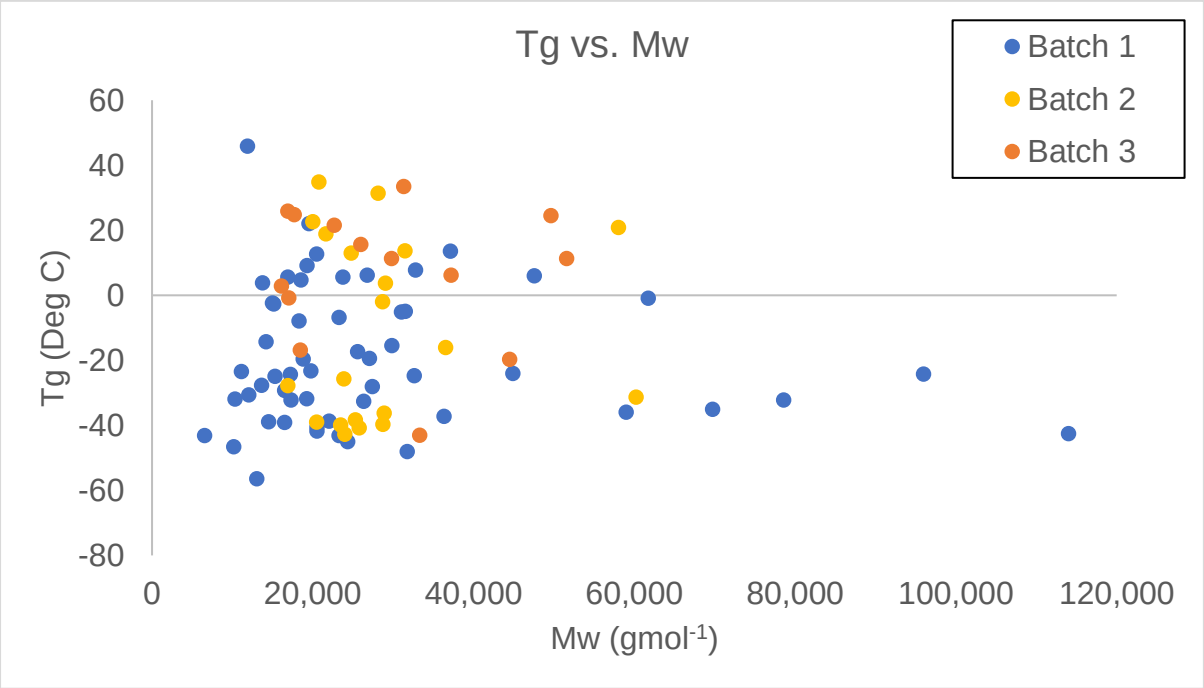

Figure S19. *Tg plotted against Mw.*

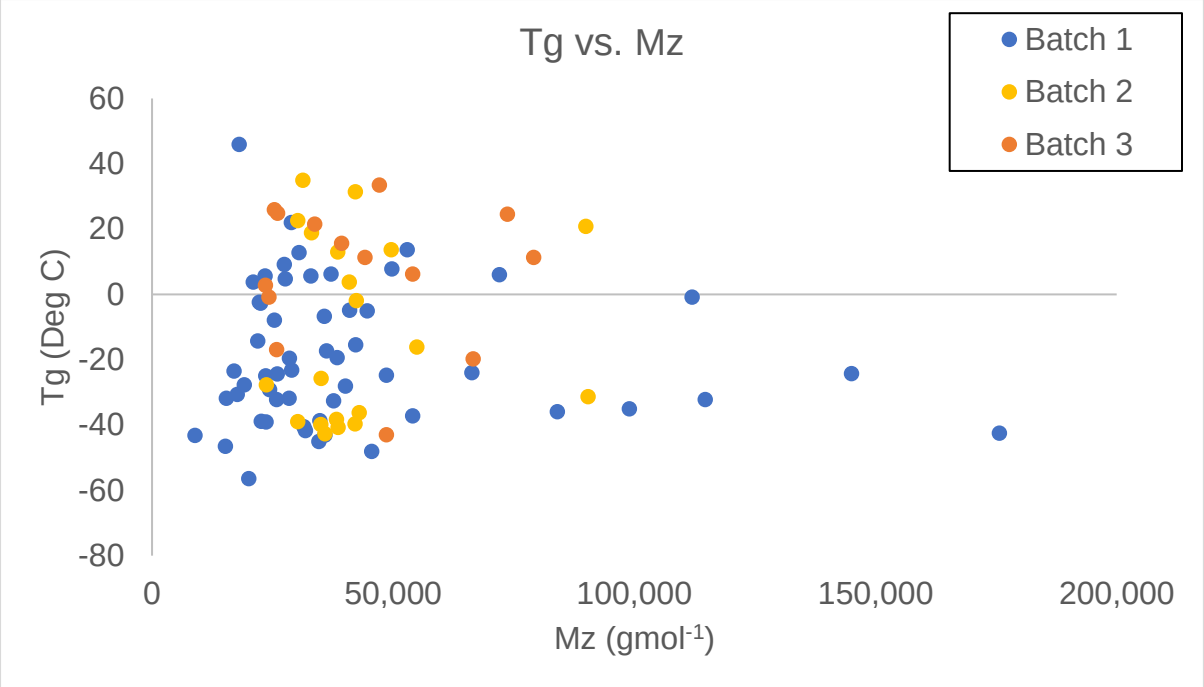

Figure S20. *Tg plotted against Mz.*

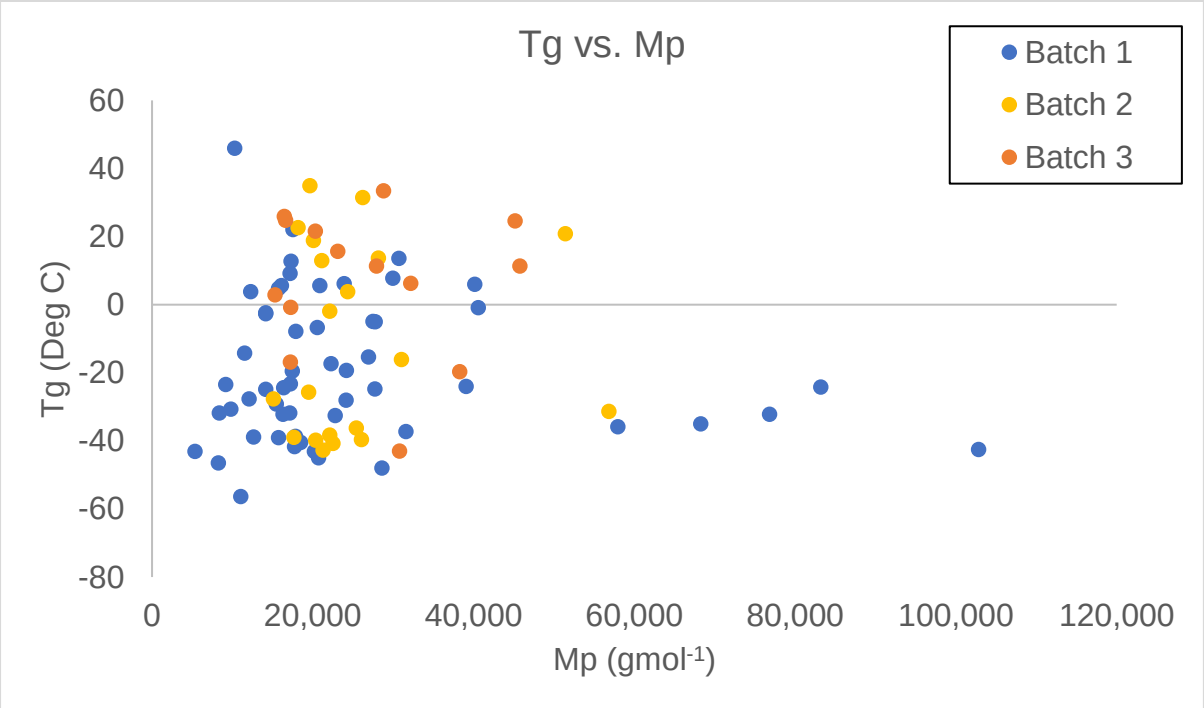

Figure S21. *Tg plotted against Mp.*

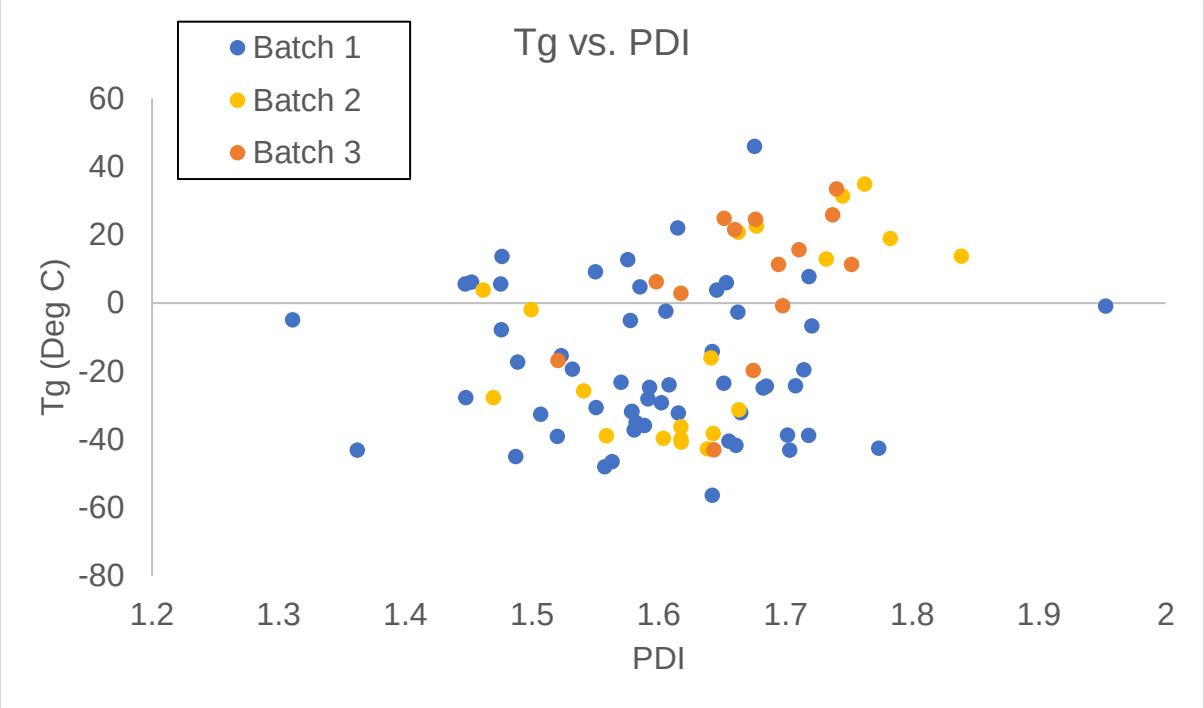

Figure S22. *Tg plotted against PDI.*

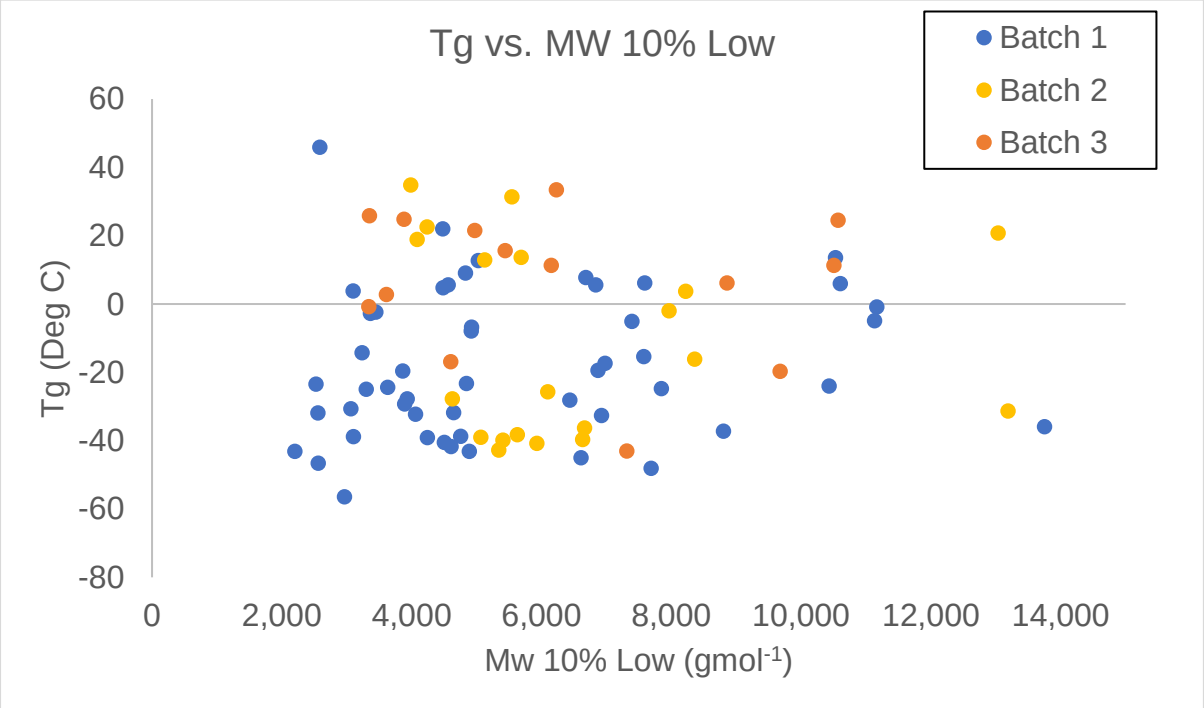

Figure S23. *Tg plotted against MW 10% Low.*

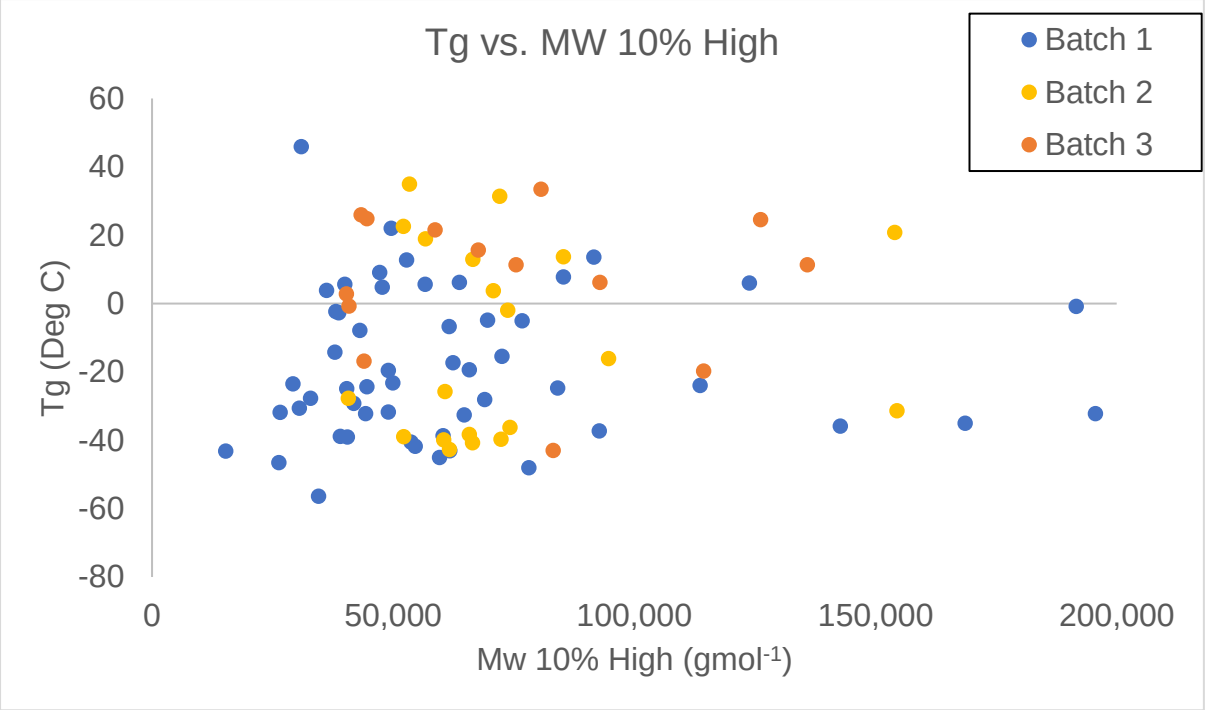

Figure S24. *Tg plotted against MW 10% High.*

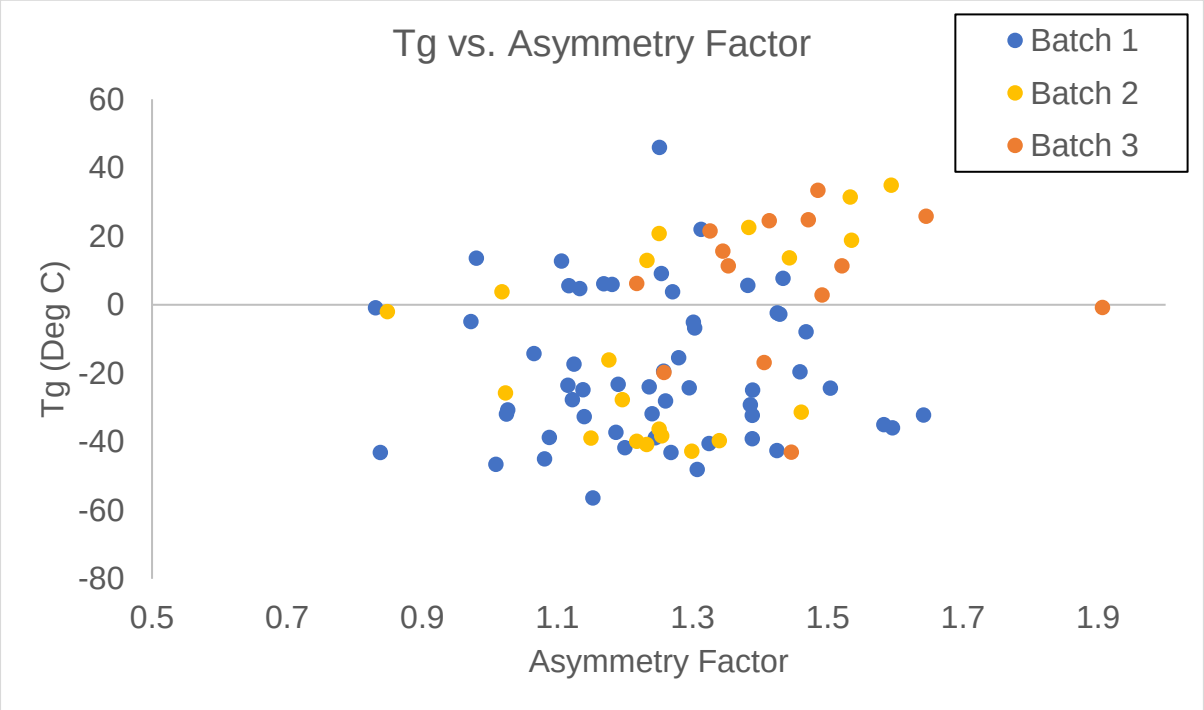

Figure S25. *Tg plotted against Asymmetry Factor.*

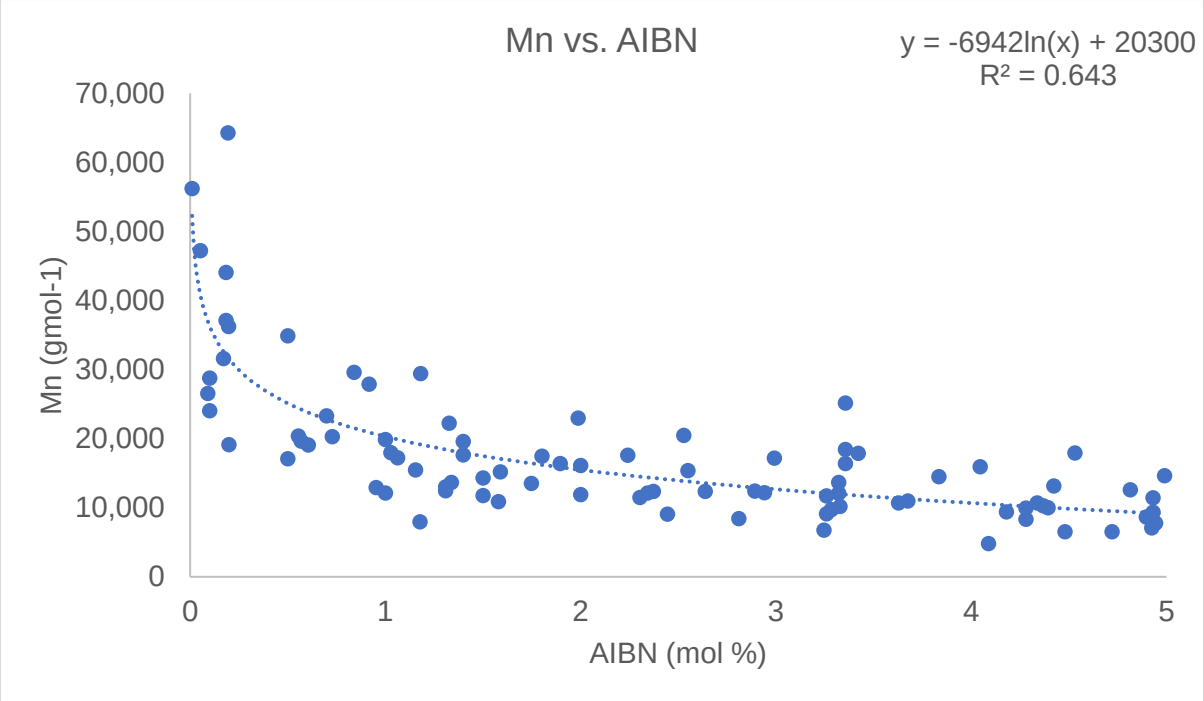

Figure S26. *Mn plotted against AIBN (mol %).*

Reference

1. Sarkar, P.; Bhowmick, A. K. Green Approach toward Sustainable Polymer: Synthesis and Characterization of Poly(Myrcene-Co-Dibutyl Itaconate). *ACS Sustain. Chem. Eng*. **2016**, *4* (4), 2129–2141. https://doi.org/10.1021/acssuschemeng.5b01591.