

SUPPORTING INFORMATION

MANGANESE TRIACETATE AS AN EFFICIENT CATALYST FOR BISPEROXIDATION OF STYRENES

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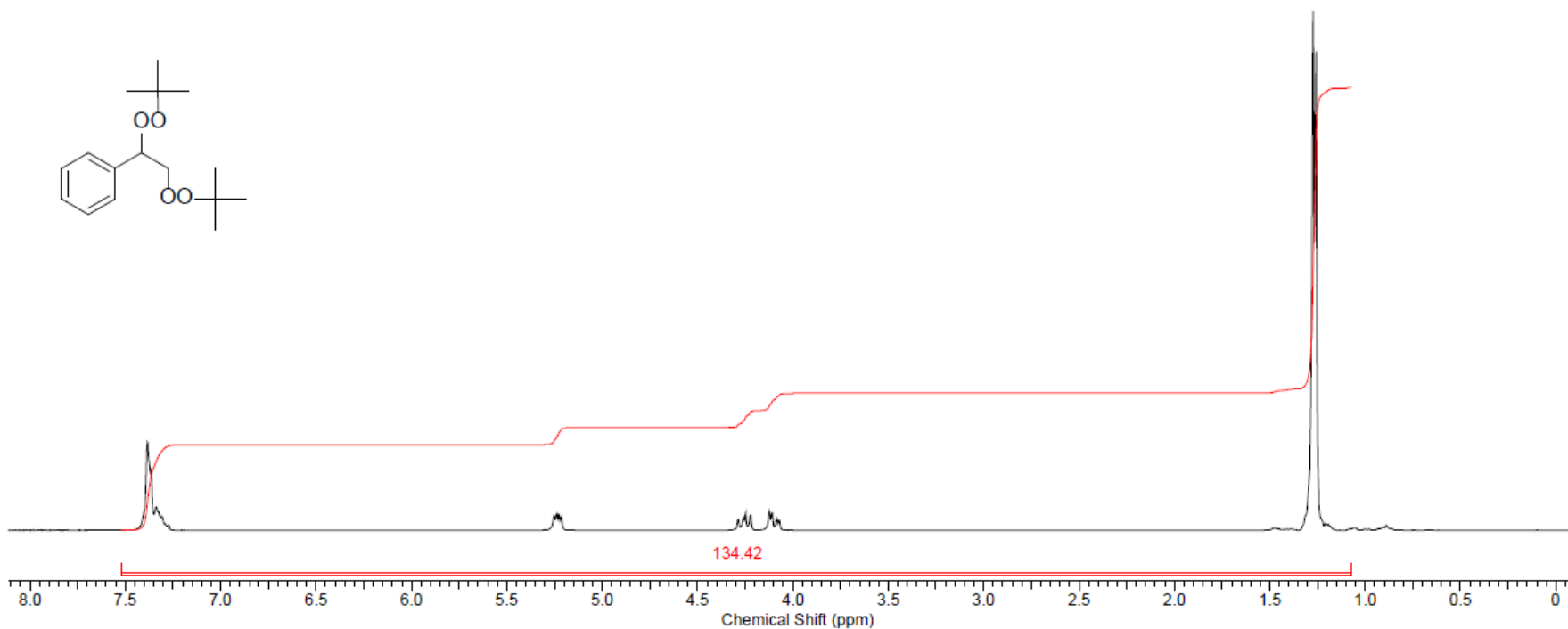
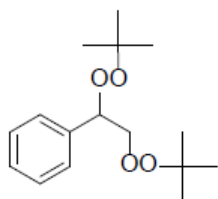
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NMR spectra of 1,2-bis-*tert*-butyl peroxides

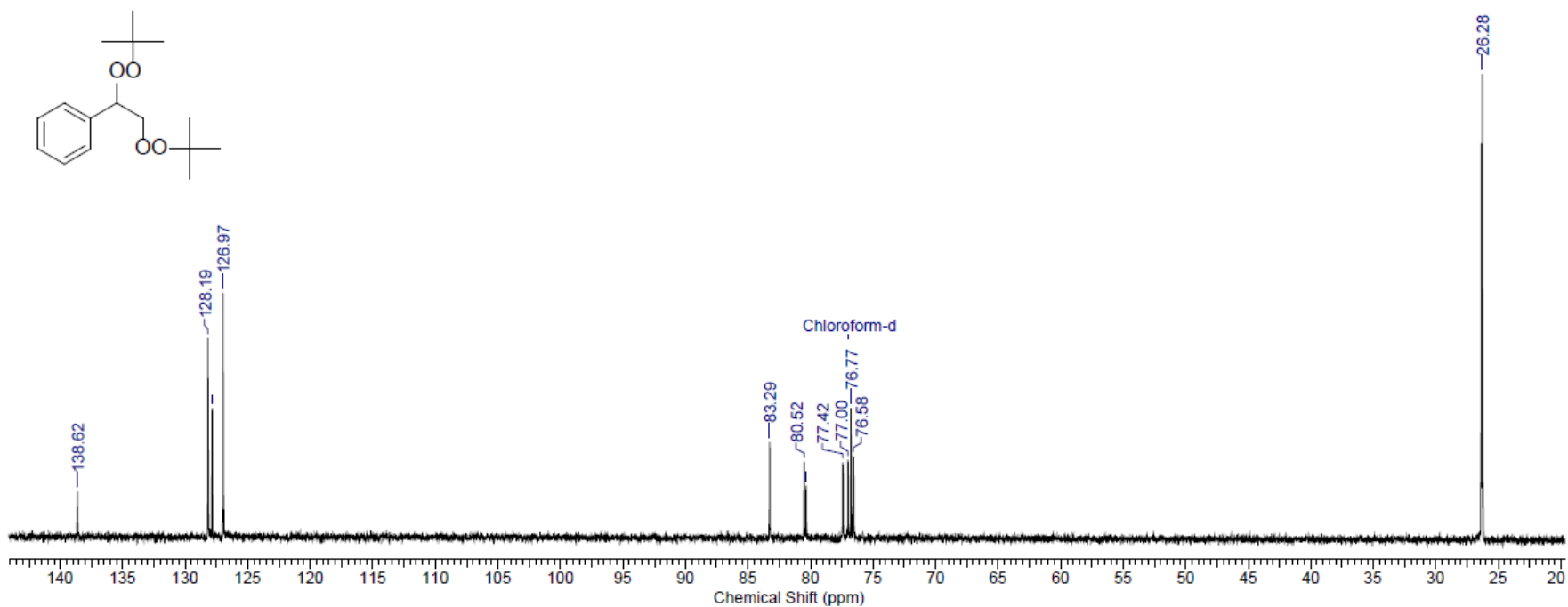
[1,2-Bis(*tert*-butylperoxy)ethyl]benzene, 2a

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Points Count	8192	Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	6009.62
Temperature (degree C)	27.000						



[1,2-Bis(*tert*-butylperoxy)ethyl]benzene, 2a

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File Name					
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Temperature (degree C)	28.200	Sweep Width (Hz)	18115.94		

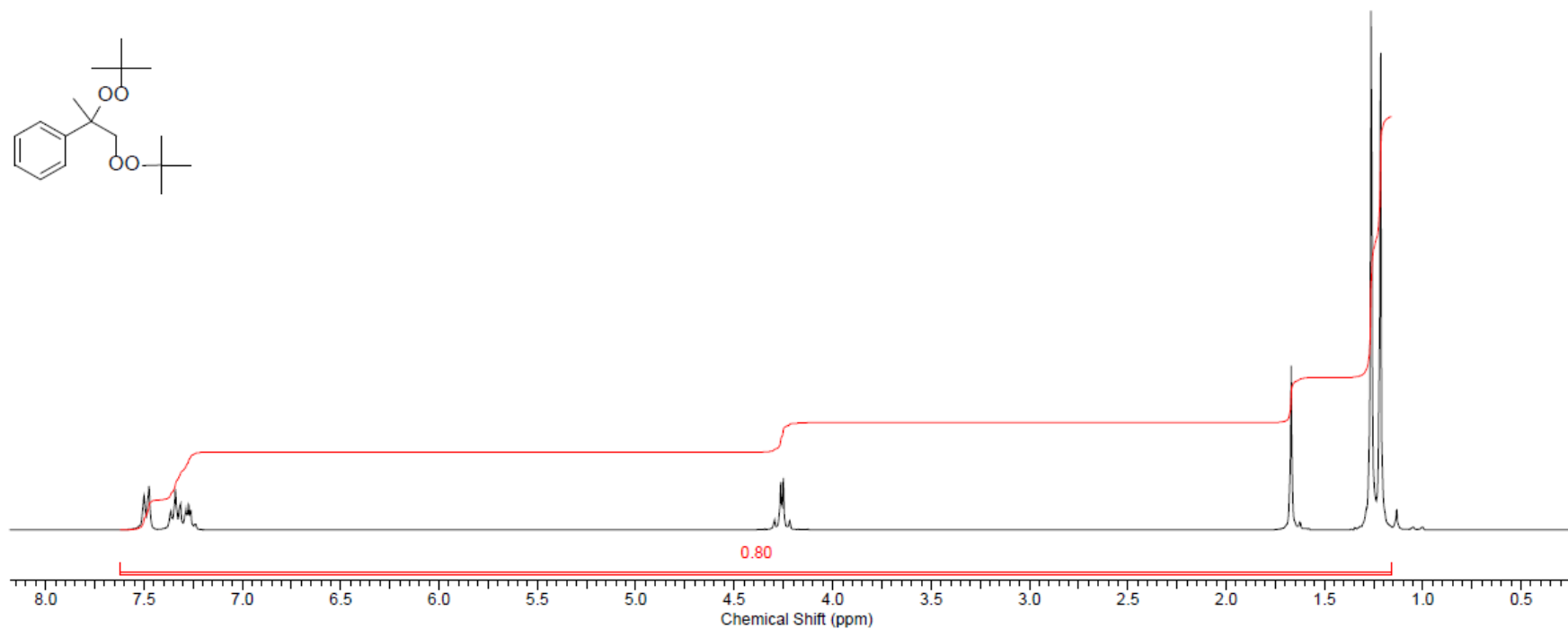
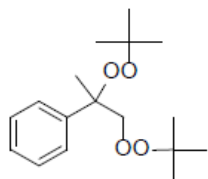


No.	(ppm)	(Hz)	Height
1	26.28	1983.5	1.0000
2	26.37	1990.1	0.8546
3	76.58	5779.6	0.1941
4	76.77	5794.0	0.2950
5	77.00	5811.7	0.1864
6	77.42	5843.7	0.1813
7	80.36	6064.9	0.1318
8	80.52	6077.0	0.1818
9	83.29	6286.0	0.2238
10	126.97	9583.5	0.5385
11	127.85	9649.8	0.2951
12	128.19	9675.2	0.4435
13	138.62	10462.6	0.1193

No.	Annotation	(ppm)
1	Chloroform-d	77.00

[1,2-Bis(*tert*-butylperoxy)-1-methylethyl]benzene, 2b

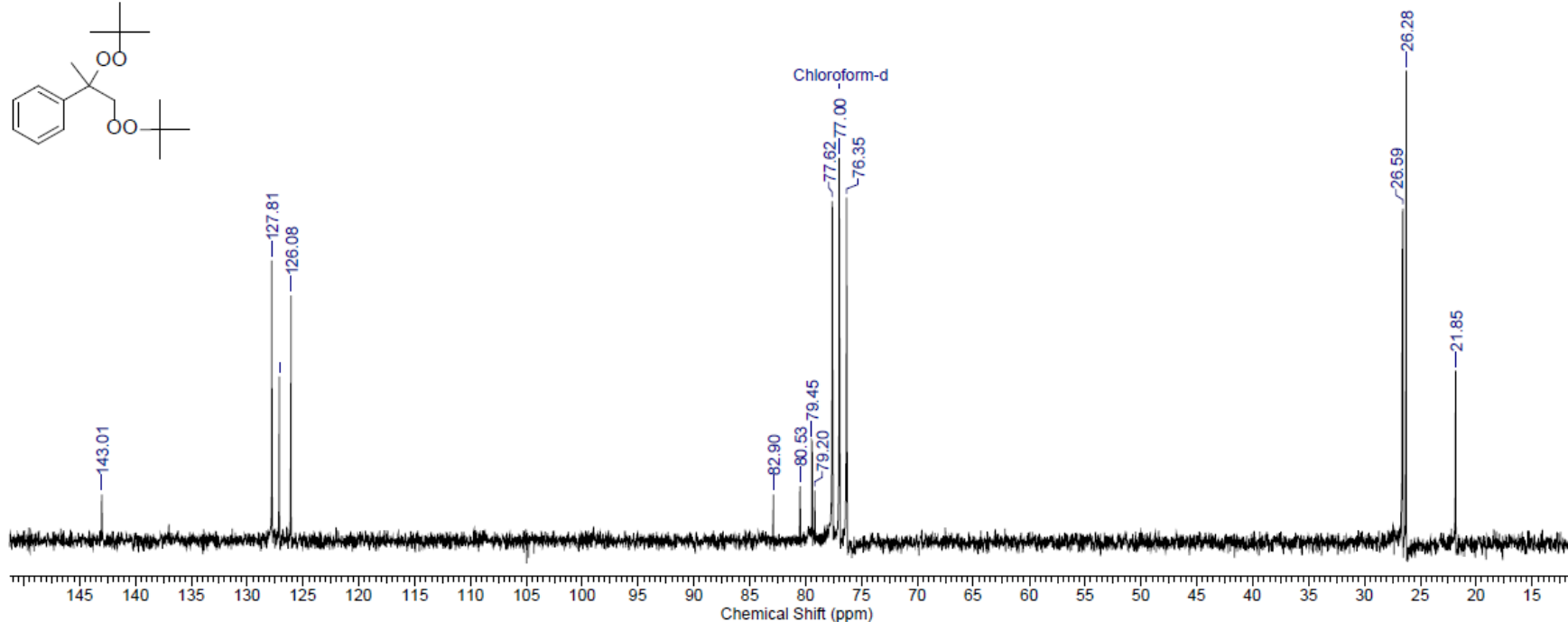
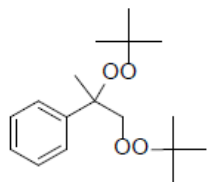
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Points Count	8192	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Temperature (degree C)	24.800			Original Points Count	8124
				Sweep Width (Hz)	7500.00



No.	(ppm)	Value	Absolute Value
1	[1.16 .. 7.62]	0.796	1.57952e+9

[1,2-Bis(*tert*-butylperoxy)-1-methylethyl]benzene, 2b

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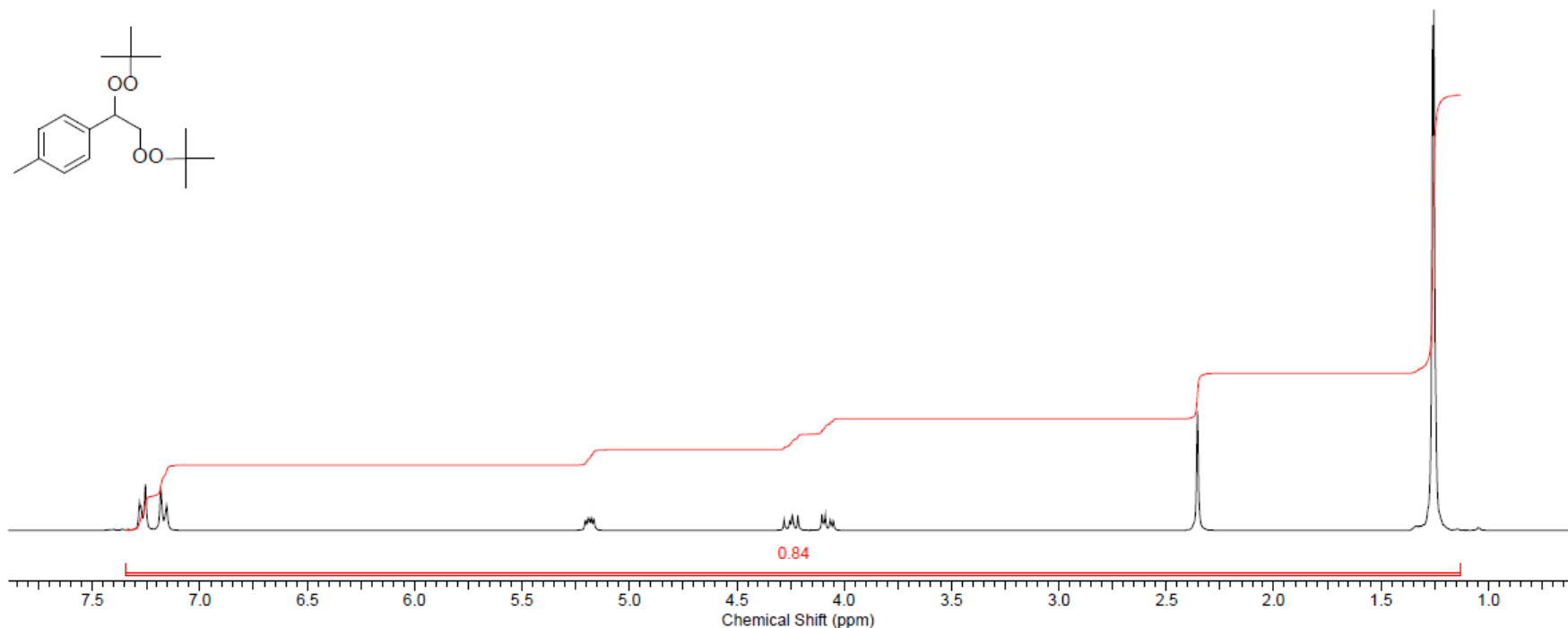
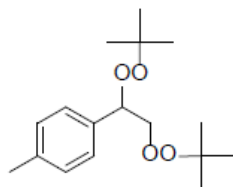


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	21.85	1099.6	0.3610	8	79.45	3998.4	0.2123
2	26.28	1322.5	1.0000	9	80.53	4052.4	0.1150
3	26.59	1338.1	0.7070	10	82.90	4171.6	0.0975
4	76.35	3842.3	0.7299	11	126.08	6345.0	0.5209
5	77.00	3874.9	0.8136	12	127.13	6397.5	0.3486
6	77.62	3906.1	0.7217	13	127.81	6431.6	0.5956
7	79.20	3985.6	0.1062	14	143.01	7196.8	0.0975

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-methylbenzene, 2c

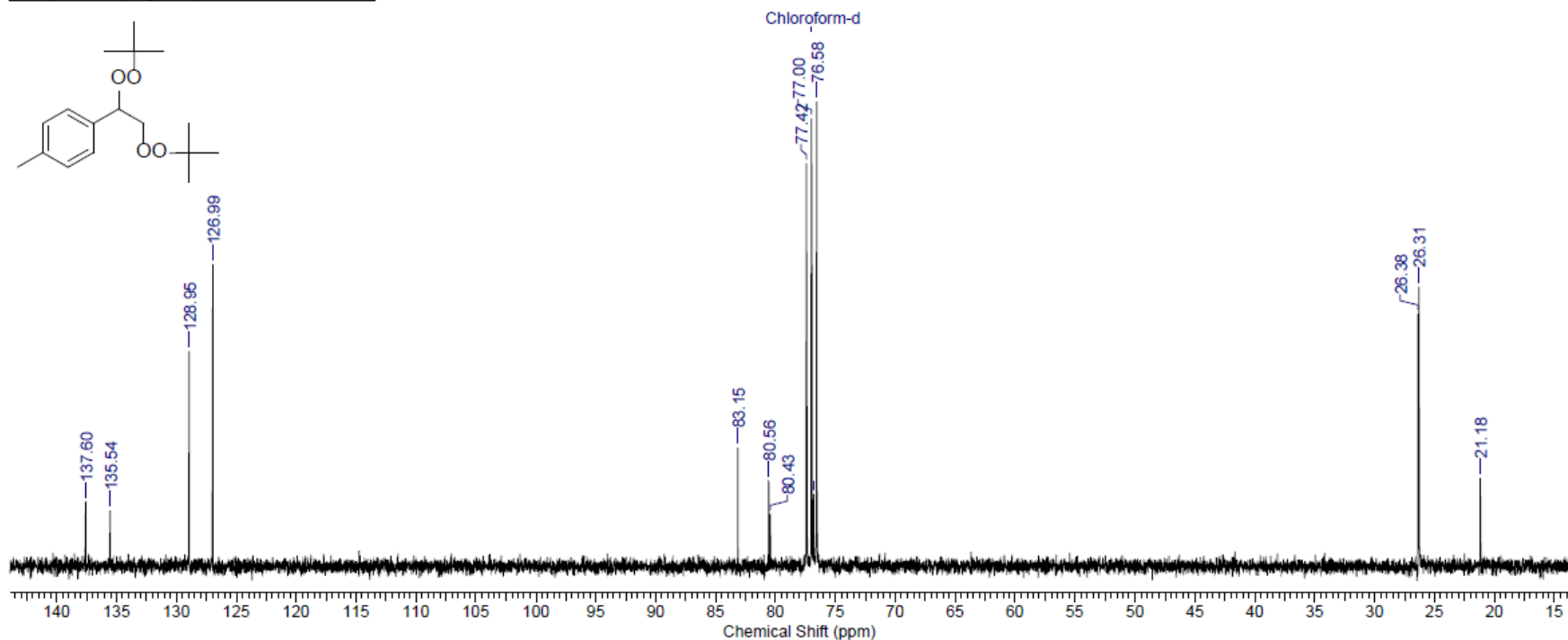
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Points Count	8192	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Temperature (degree C)	27.000	Sweep Width (Hz)	6009.62		



No.	(ppm)	Value	Absolute Value
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1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-methylbenzene, 2c

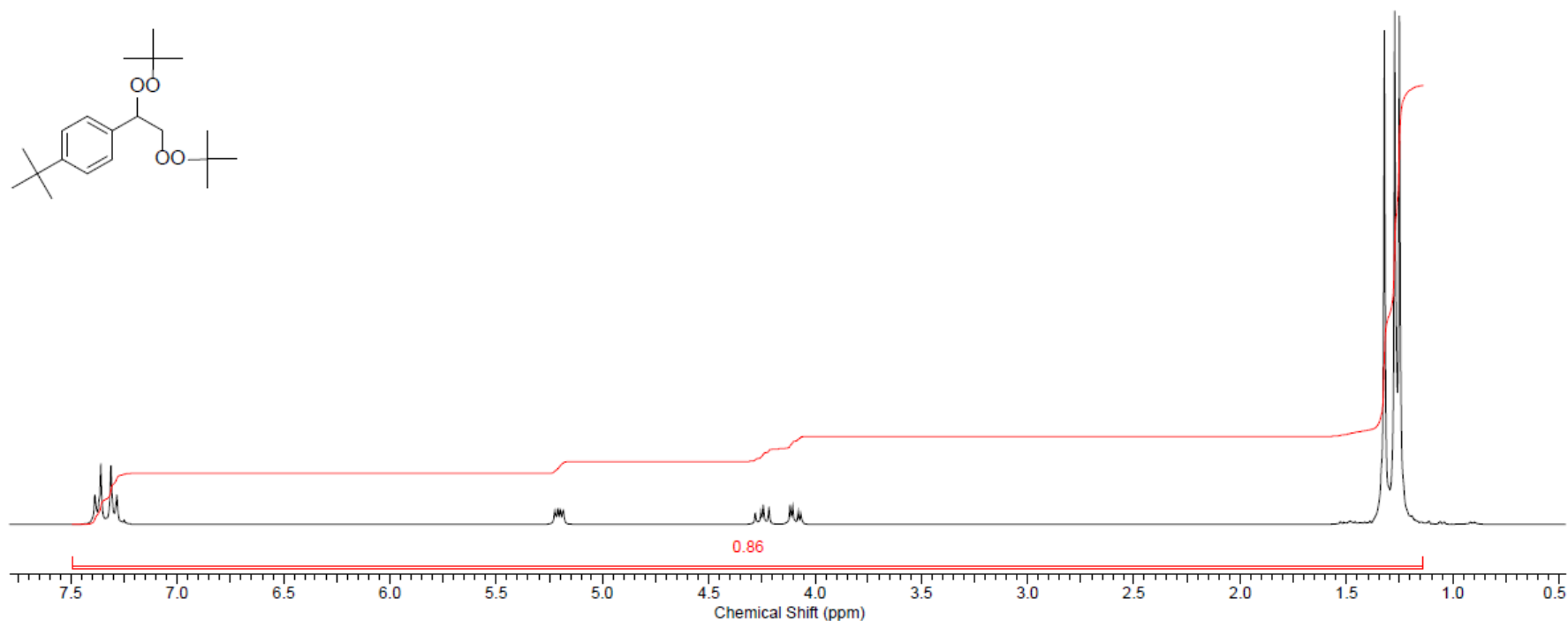
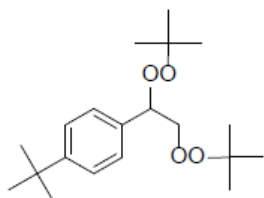
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Points Count	16384	Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D
Temperature (degree C)	24.600	Sweep Width (Hz)	18115.94		



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)
1	21.18	1598.6	0.2140	8	80.43	6070.4	0.1380	1	Chloroform-d	77.00
2	26.31	1985.7	0.6135	9	80.56	6080.4	0.2082			
3	26.38	1991.2	0.5565	10	83.15	6276.1	0.2773			
4	76.58	5779.6	1.0000	11	126.99	9584.6	0.6598			
5	76.81	5797.3	0.1804	12	128.95	9732.7	0.4788			
6	77.00	5811.7	0.9659	13	135.54	10230.3	0.1463			
7	77.42	5843.7	0.8717	14	137.60	10385.1	0.1644			

1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-*tert*-butylbenzene, 2d

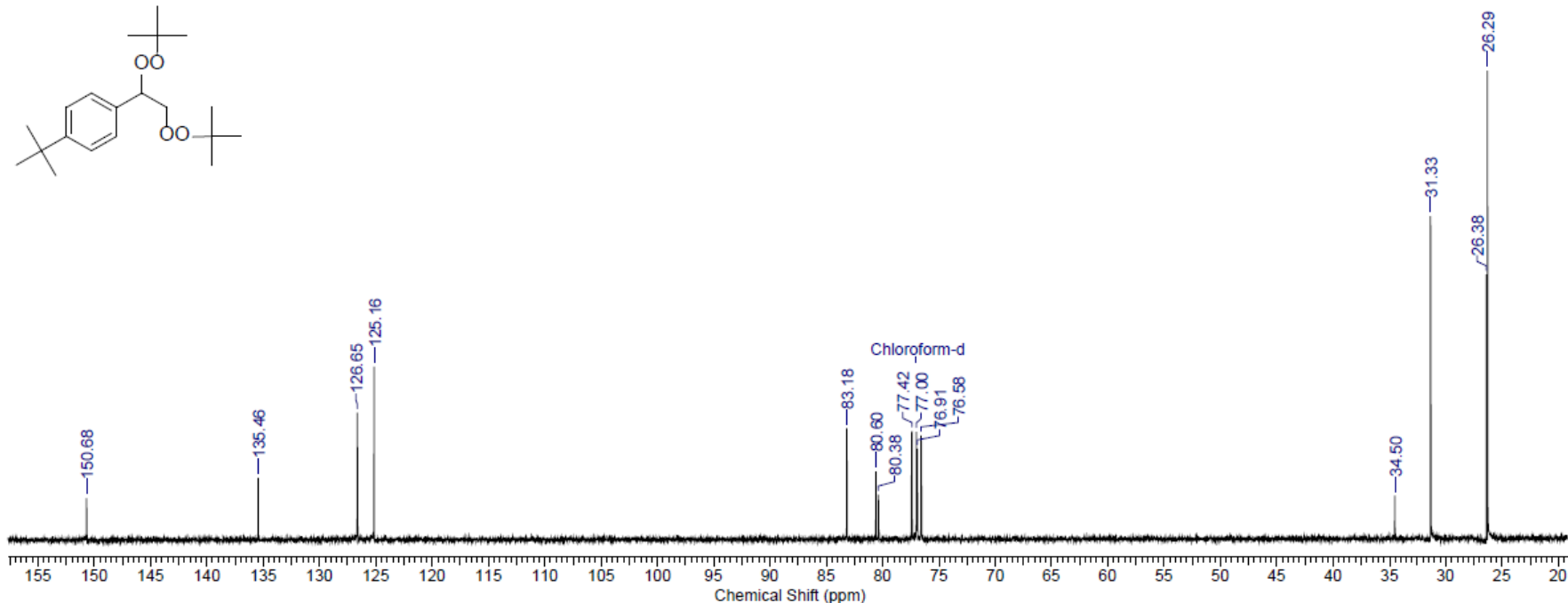
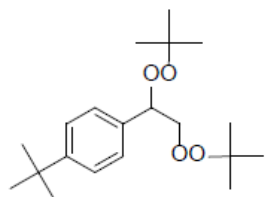
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Temperature (degree C)	24.600			Original Points Count	8124
				Sweep Width (Hz)	6009.62



No.	(ppm)	Value	Absolute Value
1	[1.14 .. 7.49]	0.856	1.66265e+9

1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-*tert*-butylbenzene, 2d

Acquisition Time (sec)	0.9006	Date	06 May 2013 09:40:16		
File Name					
Frequency (MHz)	75.48	Nucleus	13C	Number of Transients	212
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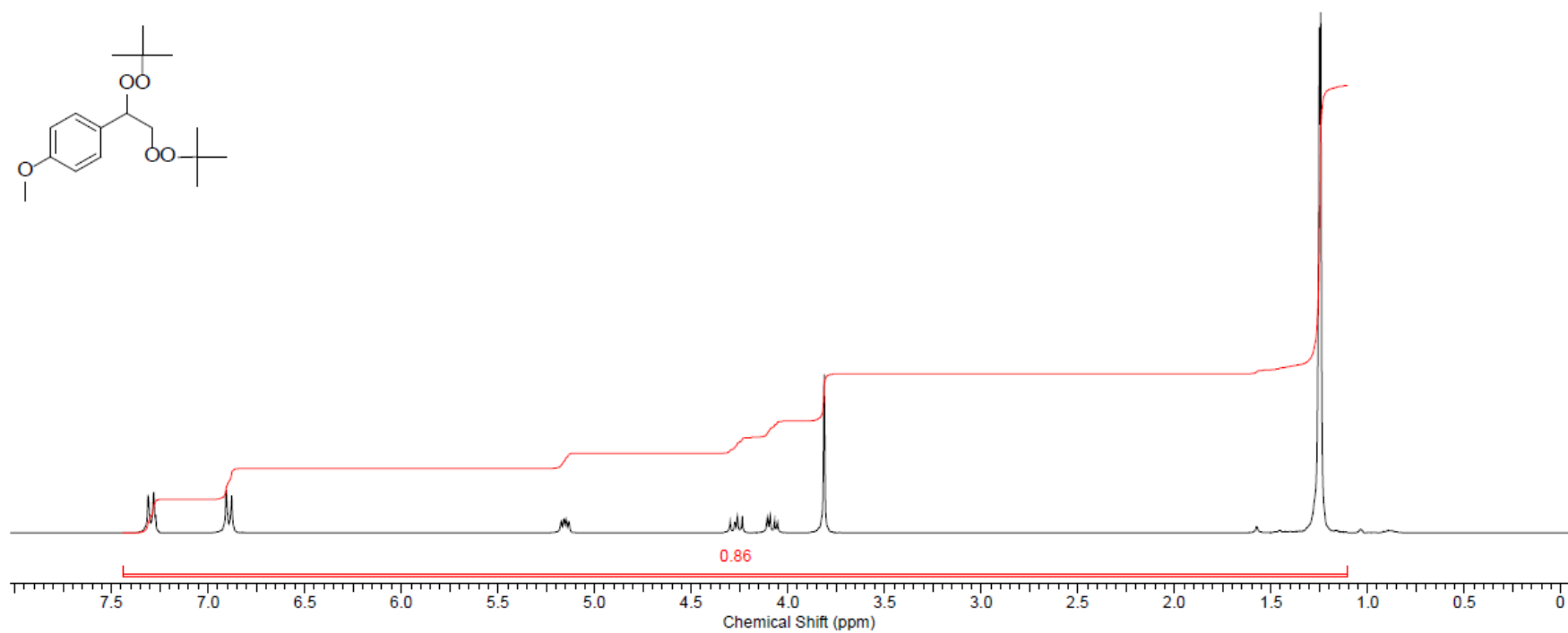
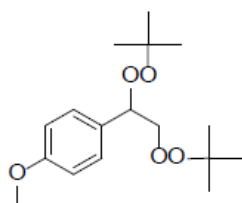


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	26.29	1984.6	1.0000	9	80.38	6067.1	0.0886
2	26.38	1991.2	0.5626	10	80.60	6083.7	0.1383
3	31.33	2364.9	0.6875	11	83.18	6278.3	0.2314
4	34.50	2603.8	0.0867	12	125.16	9446.3	0.3642
5	76.58	5779.6	0.2156	13	126.65	9559.1	0.2649
6	76.91	5805.0	0.1876	14	135.46	10223.7	0.1254
7	77.00	5811.7	0.2238	15	150.68	11372.6	0.0810
8	77.42	5843.7	0.2256				

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-methoxybenzene, 2e

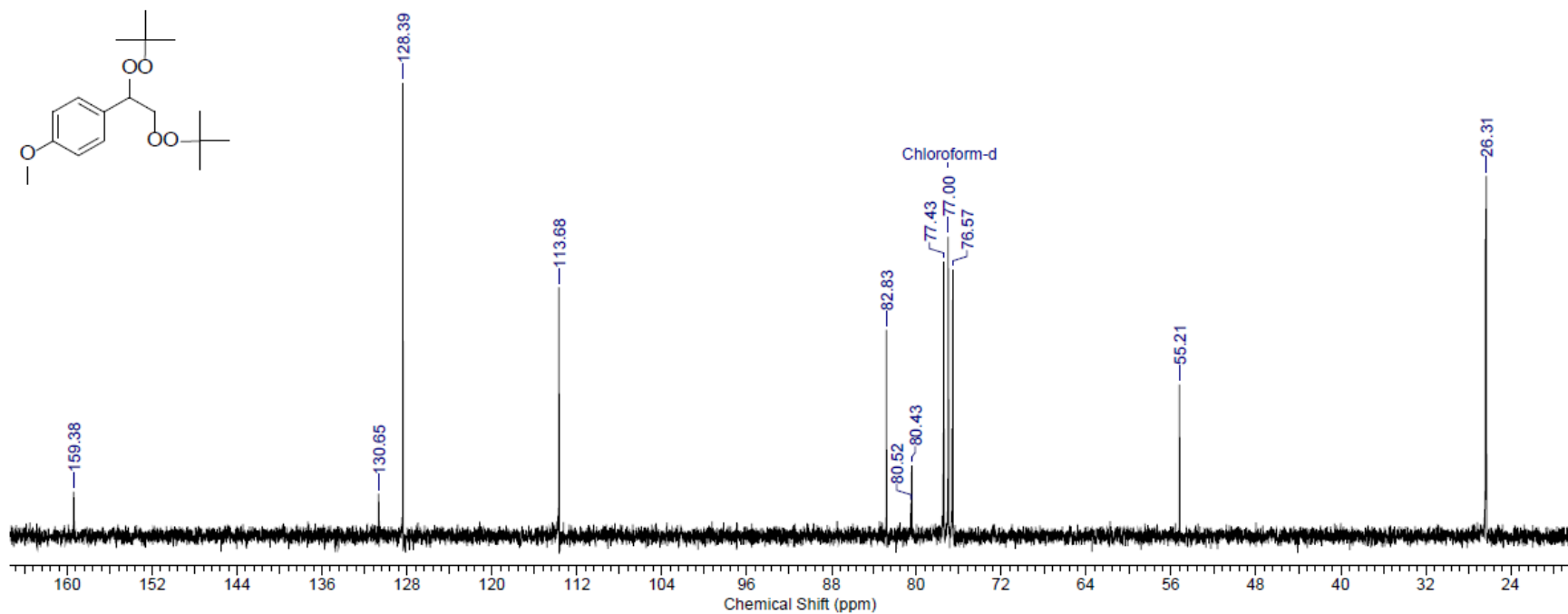
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Points Count	8192	Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	7500.00
Temperature (degree C)	26.200						



No.	(ppm)	Value	Absolute Value
1	[1.10 .. 7.44]	0.859	1.97518e+9

1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-methoxybenzene, 2e

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Temperature (degree C)	27.000	Original Points Count	16308	Sweep Width (Hz)	18867.92



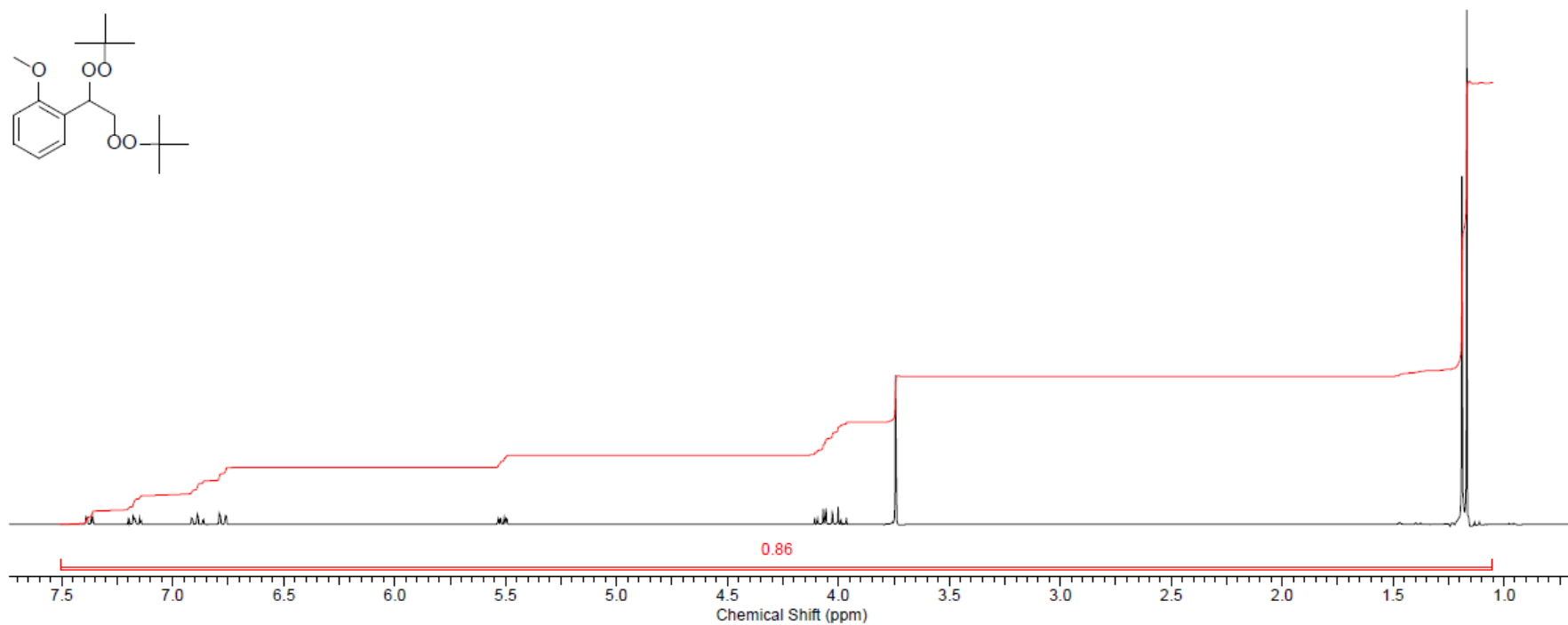
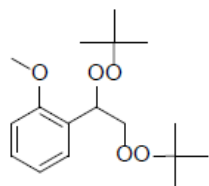
No.	(ppm)	(Hz)	Height
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3	55.21	4167.0	0.3348
4	76.57	5779.4	0.5879
5	76.65	5785.1	0.2376
6	77.00	5811.6	0.6600
7	77.43	5843.9	0.6050

No.	(ppm)	(Hz)	Height
8	80.43	6070.8	0.1545
9	80.52	6077.7	0.0716
10	82.83	6251.6	0.4547
11	113.68	8580.3	0.5491
12	128.39	9690.5	1.0000
13	130.65	9860.9	0.0936
14	159.38	12029.5	0.0979

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[1,2-Bis(*tert*-butylperoxy)ethyl]-2-methoxybenzene, 2f

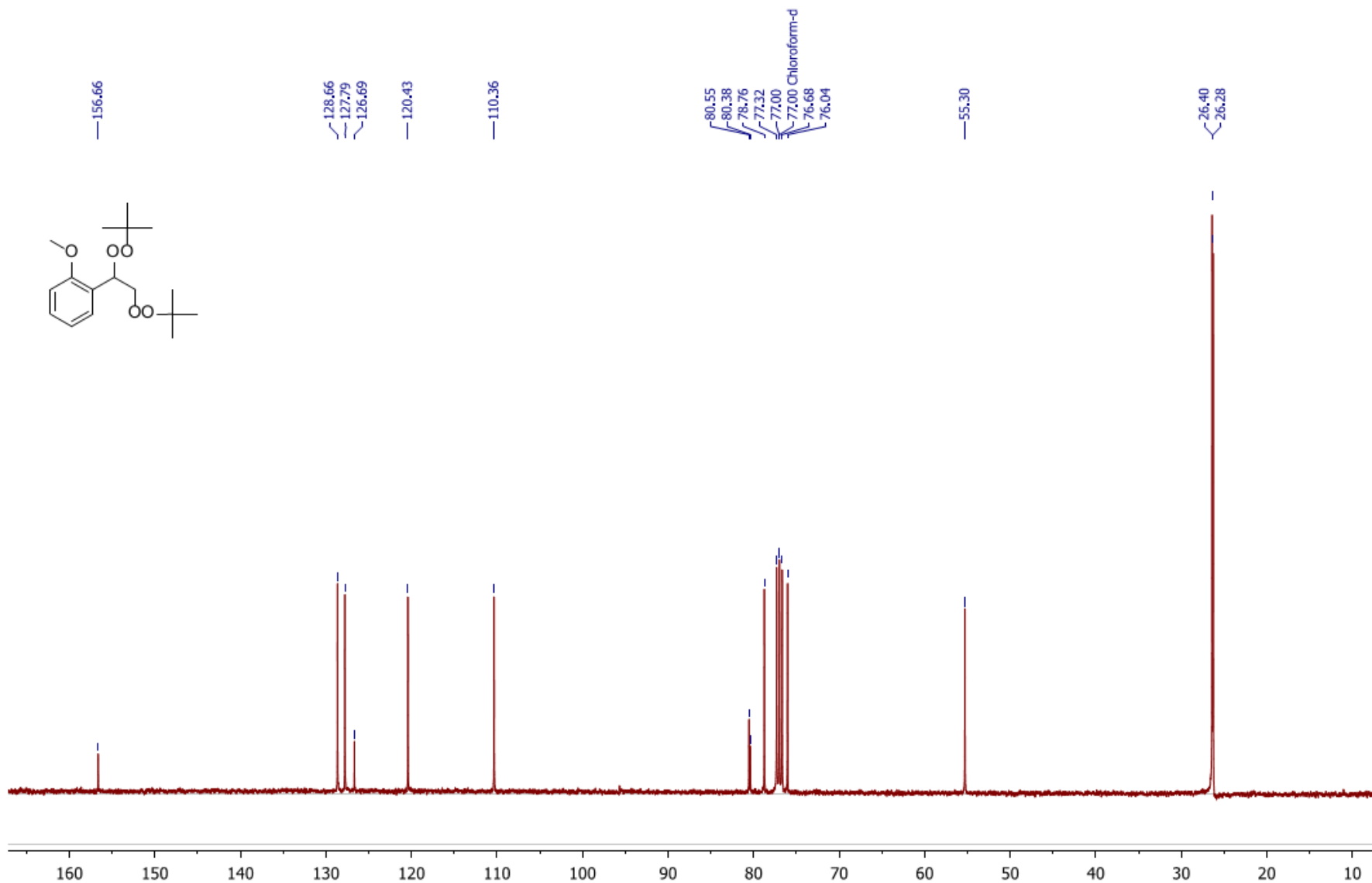
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Temperature (degree C)	30.100	Sweep Width (Hz)	6009.62		



No.	(ppm)	Value	Absolute Value
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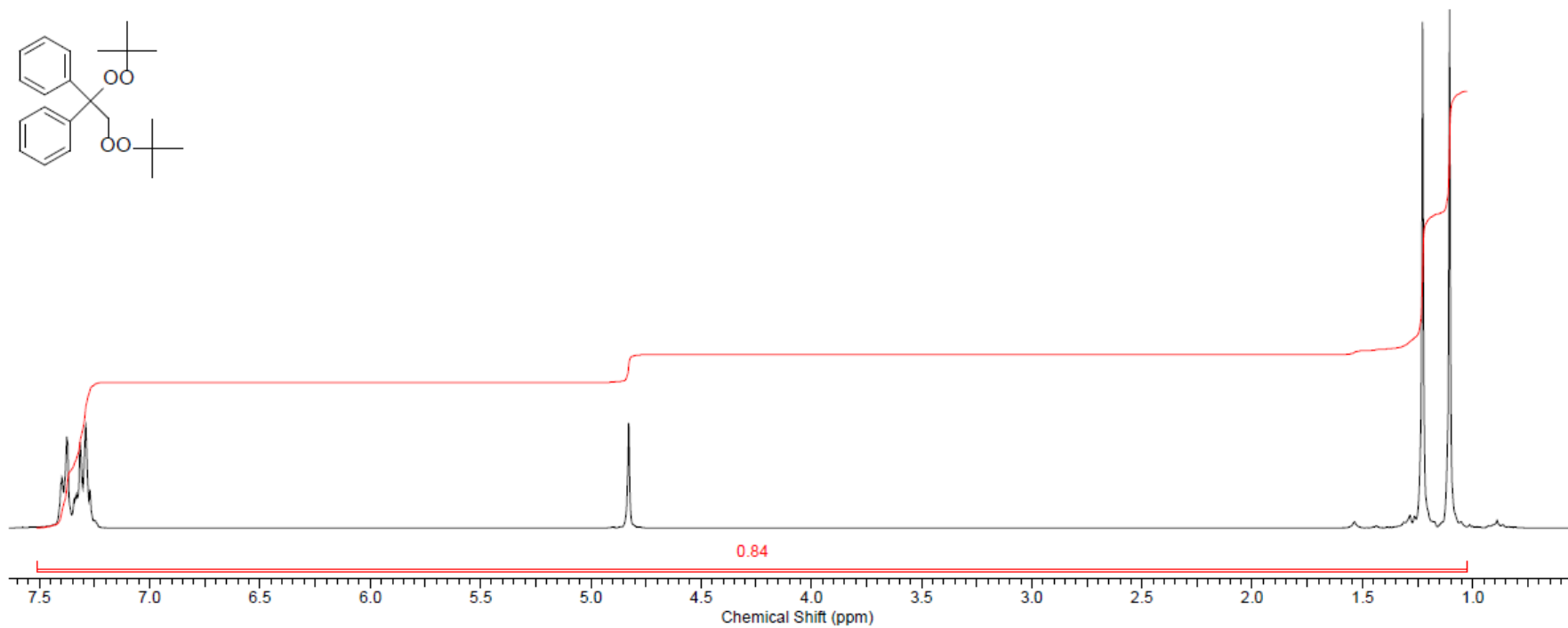
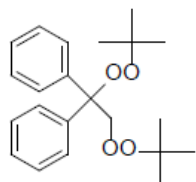
1-[1,2-Bis(*tert*-butylperoxy)ethyl]-2-methoxybenzene, 2f

^{13}C NMR (101 MHz, CDCl_3) δ 156.66, 128.66, 127.79, 126.69, 120.43, 110.36, 80.55, 80.38, 78.76, 77.32, 77.00, 77.00, 76.68, 76.04, 55.30, 26.40, 26.28.



[1,2-Bis(*tert*-butylperoxy)-1-phenylethyl]benzene, 2g

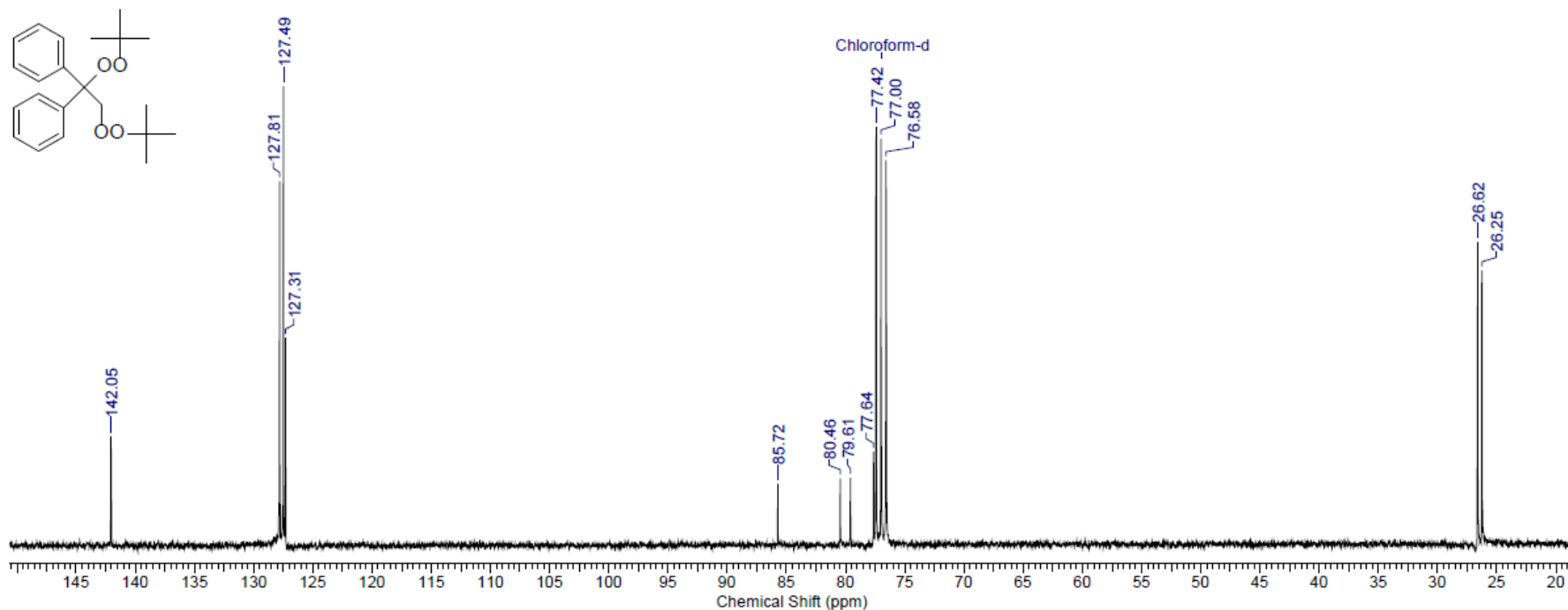
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Points Count	8192	Pulse Sequence	zg	Solvent	CHLOROFORM-D	Sweep Width (Hz)	6009.62
Temperature (degree C)	27.000						



No.	(ppm)	Value	Absolute Value
1	[1.03 .. 7.51]	0.842	2.14884e+9

[1,2-Bis(*tert*-butylperoxy)-1-phenylethyl]benzene, 2g

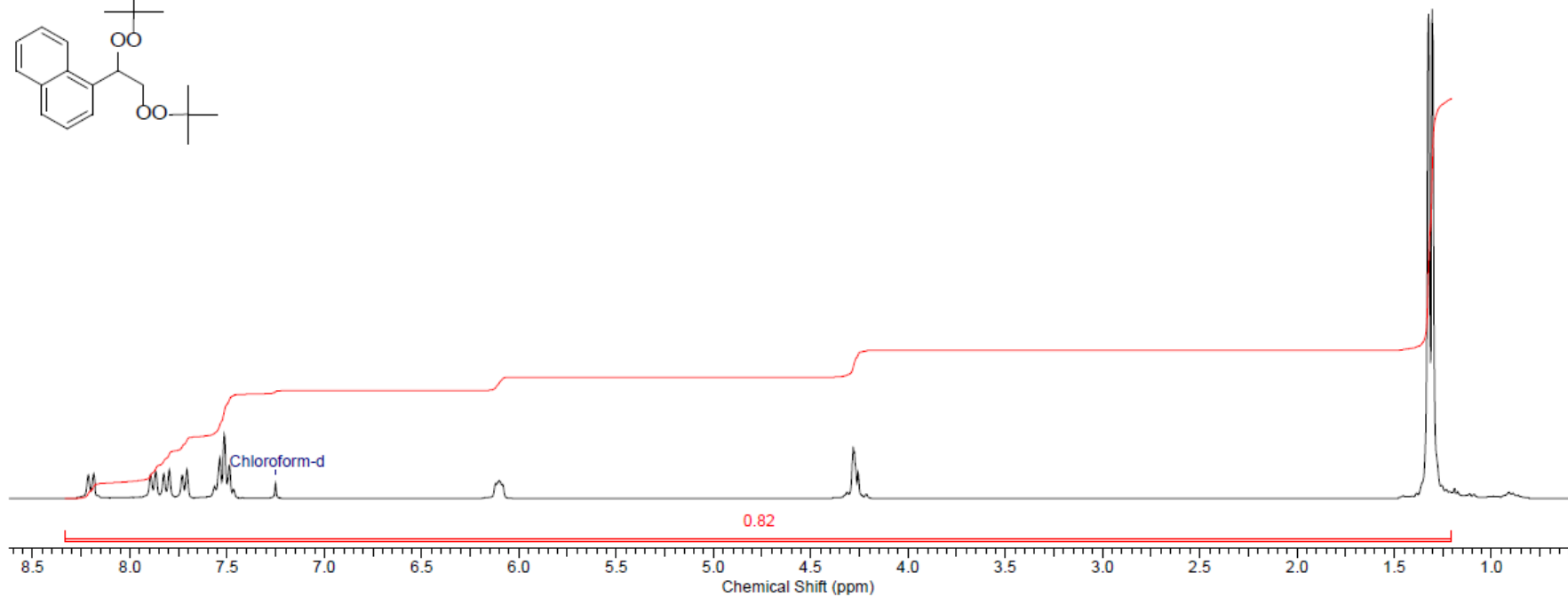
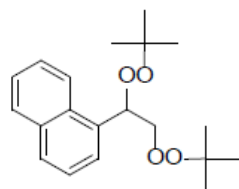
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Temperature (degree C)	27.200	Sweep Width (Hz)	18115.94		



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)
1	26.25	1981.2	0.5887	8	80.46	6072.6	0.1252	1	Chloroform-d	77.00
2	26.62	2008.9	0.6534	9	85.72	6469.6	0.1135			
3	76.58	5779.6	0.8341	10	127.31	9608.9	0.4389			
4	77.00	5811.7	0.8834	11	127.49	9622.2	1.0000			
5	77.42	5843.7	0.9089	12	127.81	9646.5	0.7877			
6	77.64	5860.3	0.1845	13	142.05	10721.3	0.2187			
7	79.61	6008.5	0.1257							

1-[1,2-Bis(*tert*-butylperoxy)ethyl]naphthalene, 2h

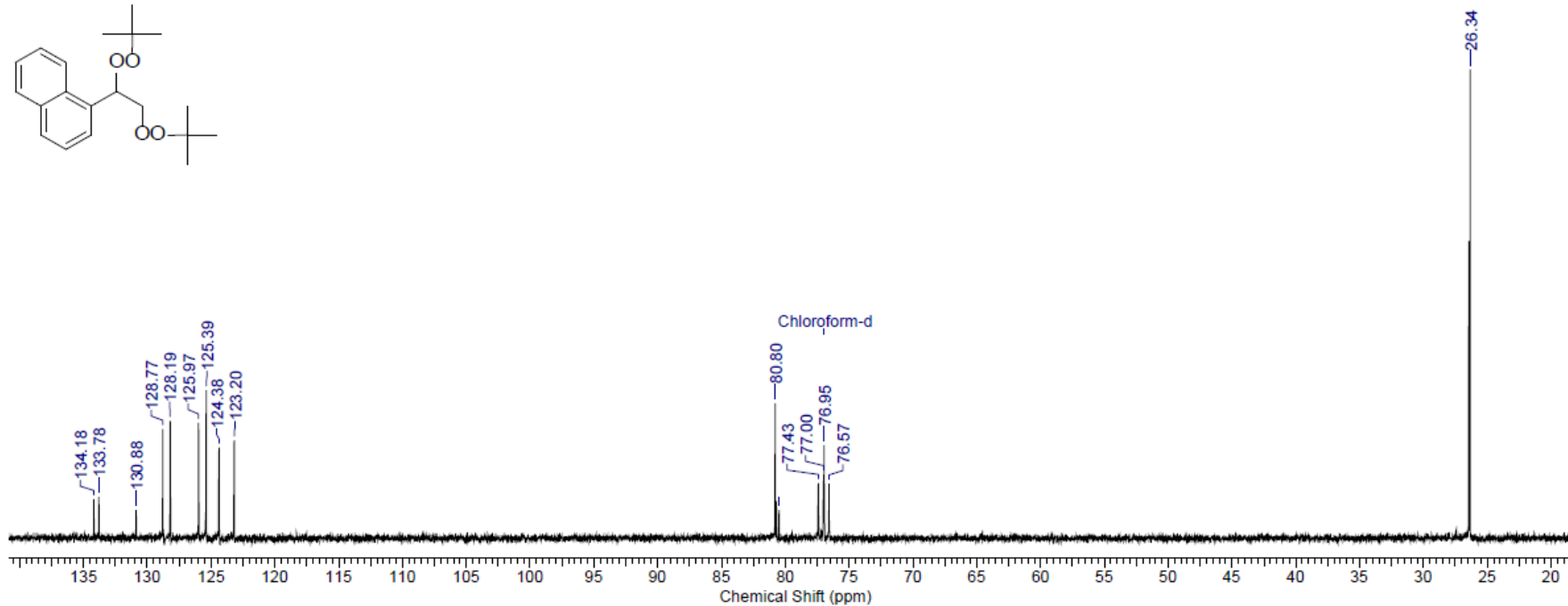
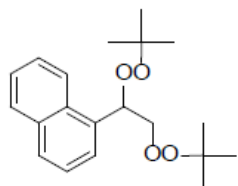
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Points Count	8192	Pulse Sequence	zg	Solvent	CHLOROFORM-D
Temperature (degree C)	27.200			Original Points Count	8124
				Sweep Width (Hz)	6009.62



No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.20 .. 8.33]	0.817	1.43951e+9

1-[1,2-Bis(*tert*-butylperoxy)ethyl]naphthalene, 2h

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Temperature (degree C)	27.700	Original Points Count	16308	Sweep Width (Hz)	18867.92

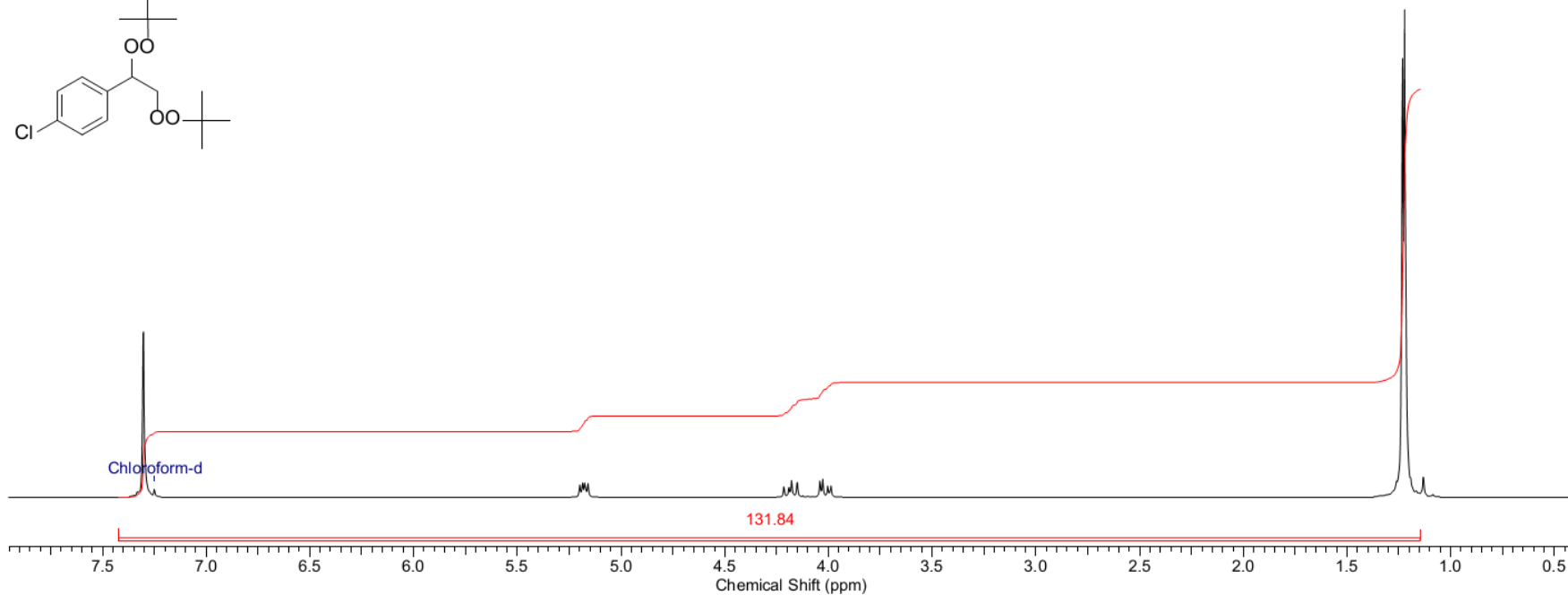
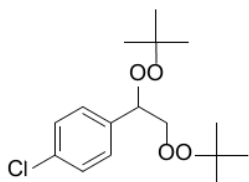


No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	26.34	1988.1	1.0000	10	123.20	9298.9	0.2093
2	26.45	1996.1	0.6347	11	124.38	9387.6	0.1935
3	76.57	5779.4	0.1167	12	125.39	9463.6	0.3162
4	76.95	5808.2	0.1984	13	125.97	9507.4	0.2464
5	77.00	5811.6	0.1367	14	128.19	9675.5	0.2504
6	77.43	5843.9	0.1174	15	128.77	9719.3	0.2326
7	80.49	6075.4	0.0608	16	130.88	9878.2	0.0607
8	80.69	6090.3	0.0795	17	133.78	10097.0	0.0888
9	80.80	6098.4	0.2881	18	134.18	10127.0	0.0831

No.	Annotation	(ppm)
1	Chloroform-d	77.00

1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-chlorobenzene, 2i

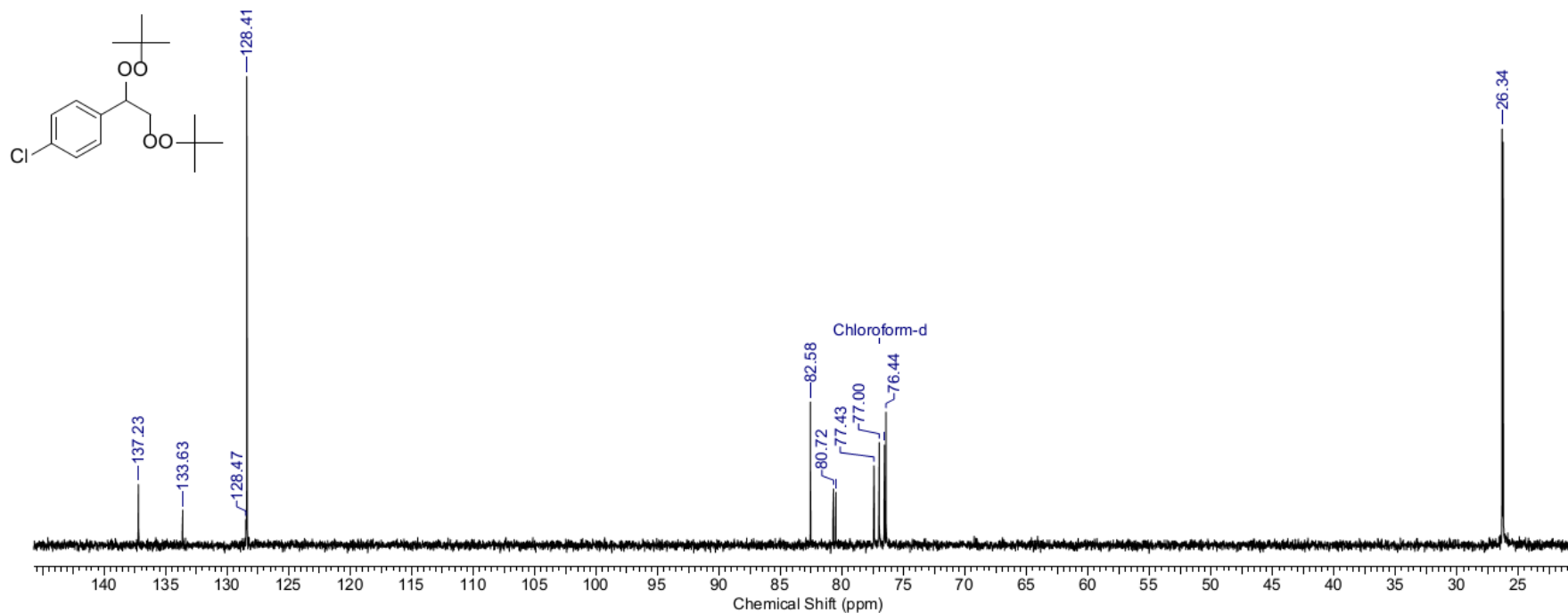
Acquisition Time (sec)	1.3518	Comment	Avance-300, 1H CDCl3	Date	05 Jul 2014 09:42:24
File Name				Frequency (MHz)	300.13
Nucleus	1H	Number of Transients	1	Original Points Count	8124
Pulse Sequence	zg	Solvent	CHLOROFORM-D	Points Count	8192
Temperature (degree C)	24.400			Sweep Width (Hz)	6009.62



No.	Annotation	(ppm)	No.	(ppm)	Value	Absolute Value
1	Chloroform-d	7.25	1	[1.15 .. 7.42]	131.836	1.45295e+9

1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-chlorobenzene, 2i

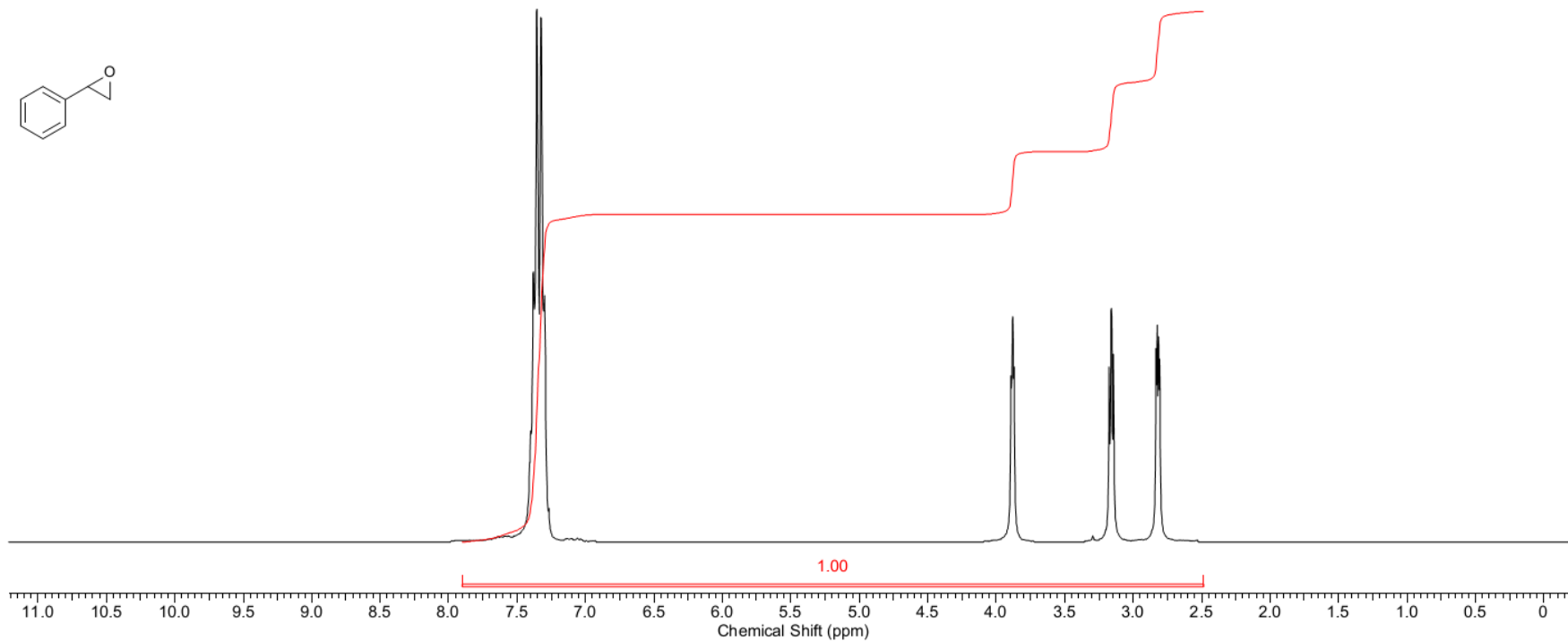
Acquisition Time (sec)	0.8643	Comment	adil.cdcl3.c13	Date	05 Jul 2014 09:46:40
File Name				Frequency (MHz)	75.48
Nucleus	13C	Number of Transients	115	Original Points Count	16308
Pulse Sequence	zgpg60base	Solvent	CHLOROFORM-D	Sweep Width (Hz)	18867.92
				Temperature (degree C)	25.000



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)
1	26.26	1982.3	0.8604	8	80.72	6092.6	0.1206	1	Chloroform-d	77.00
2	26.34	1988.1	0.8882	9	82.58	6233.1	0.3051			
3	76.44	5769.0	0.2835	10	128.41	9691.6	1.0000			
4	76.57	5779.4	0.2135	11	128.47	9696.2	0.0543			
5	77.00	5811.6	0.2189	12	133.63	10085.5	0.0751			
6	77.43	5843.9	0.1698	13	137.23	10357.3	0.1296			
7	80.52	6077.7	0.1131							

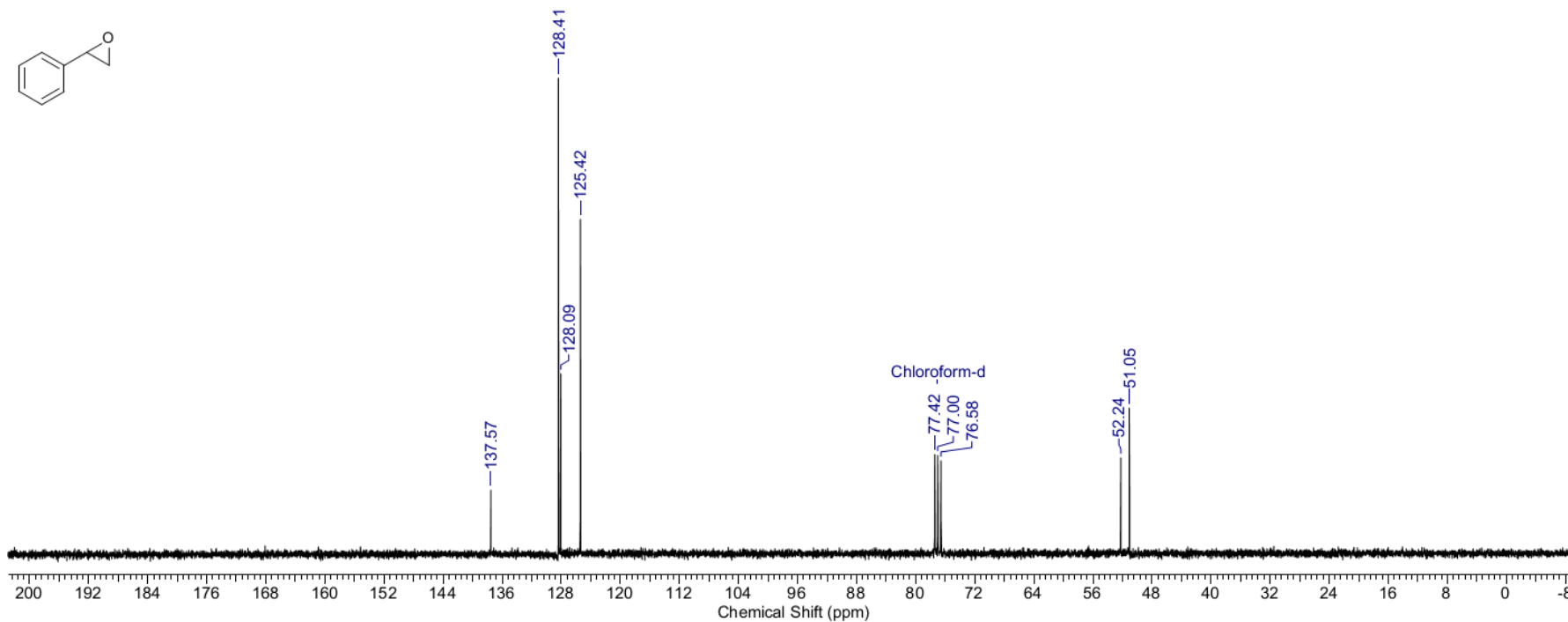
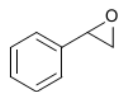
2-Phenyloxirane

Acquisition Time (sec) 1.3518	Date			Frequency (MHz) 300.13
File Name				Points Count 8192
Nucleus 1H	Number of Transients 1	Original Points Count 8124	Temperature (degree C) 28.200	
Pulse Sequence zq	Solvent CHLOROFORM-D	Sweep Width (Hz) 6009.62		



2-Phenyloxirane

Acquisition Time (sec) 0.9006	Date			Frequency (MHz) 75.48
File Name	Number of Transients 108	Original Points Count 16316	Points Count 16384	
Nucleus 13C	Solvent CHLOROFORM-D	Sweep Width (Hz) 18115.94	Temperature (degree C) 28.200	
Pulse Sequence zgpg30				



No.	(ppm)	Height
1	51.05	0.3078
2	52.24	0.2033
3	76.58	0.1969
4	77.00	0.2086
5	77.42	0.2103
6	125.42	0.7030
7	128.09	0.3792
8	128.41	1.0000
9	137.57	0.1358

No.	Annotation	(ppm)
1	Chloroform-d	77.00

HRMS of 1,2-bis-*tert*-butyl peroxides

[1,2-Bis(*tert*-butylperoxy)ethyl]benzene, 2a

Display Report

Analysis Info

Analysis Name D:\Data\Kolotyrkina\2013\Sharipov\0515_006.d
Method tune_low.m
Sample Name /TERN
Comment C16H26O4 mw 282 calibrant added

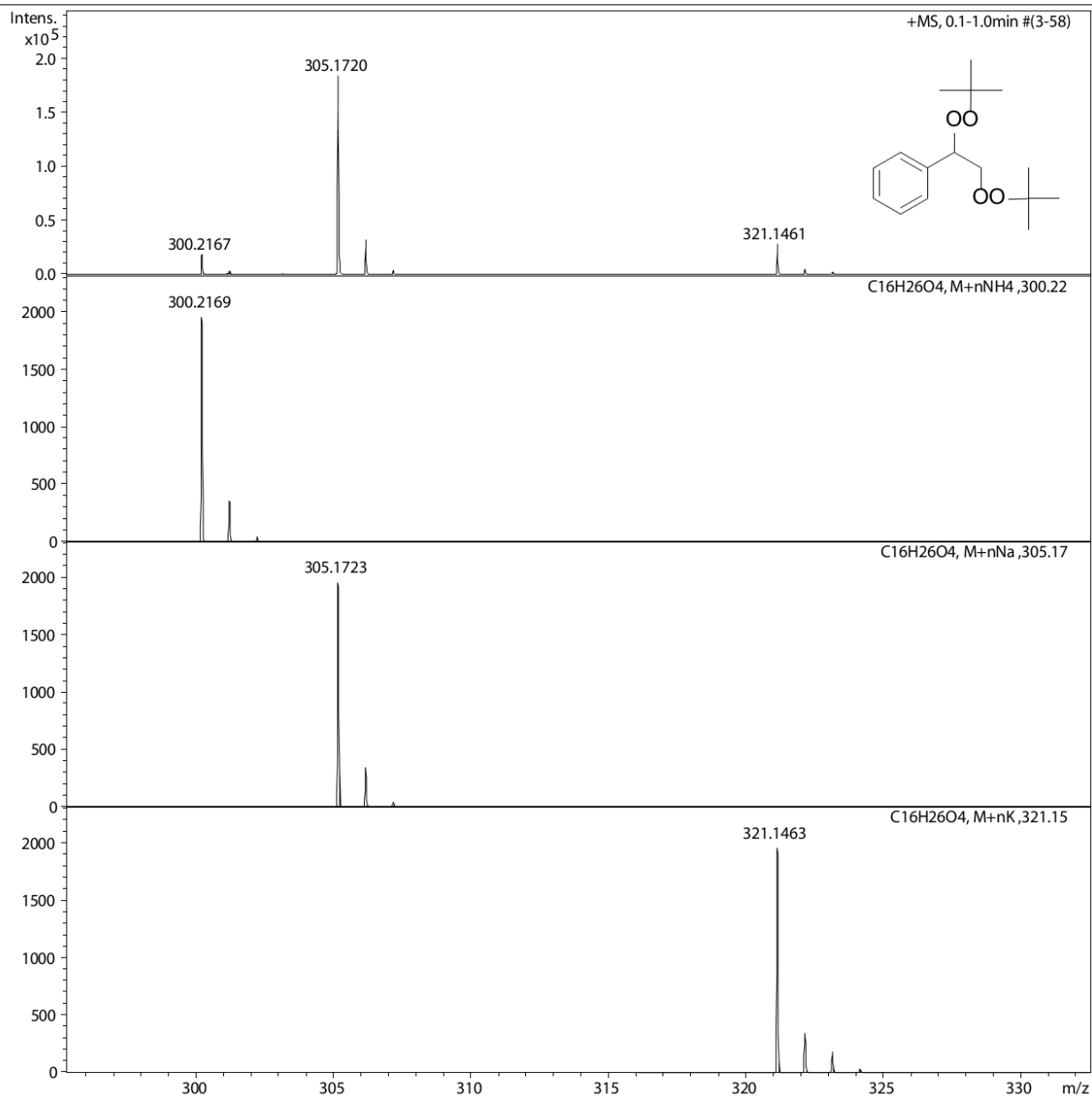
Acquisition Date 16.04.2013 17:47:25

Operator BDAL@DE

Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



[1,2-Bis(*tert*-butylperoxy)-1-methylethyl]benzene, 2b

Display Report

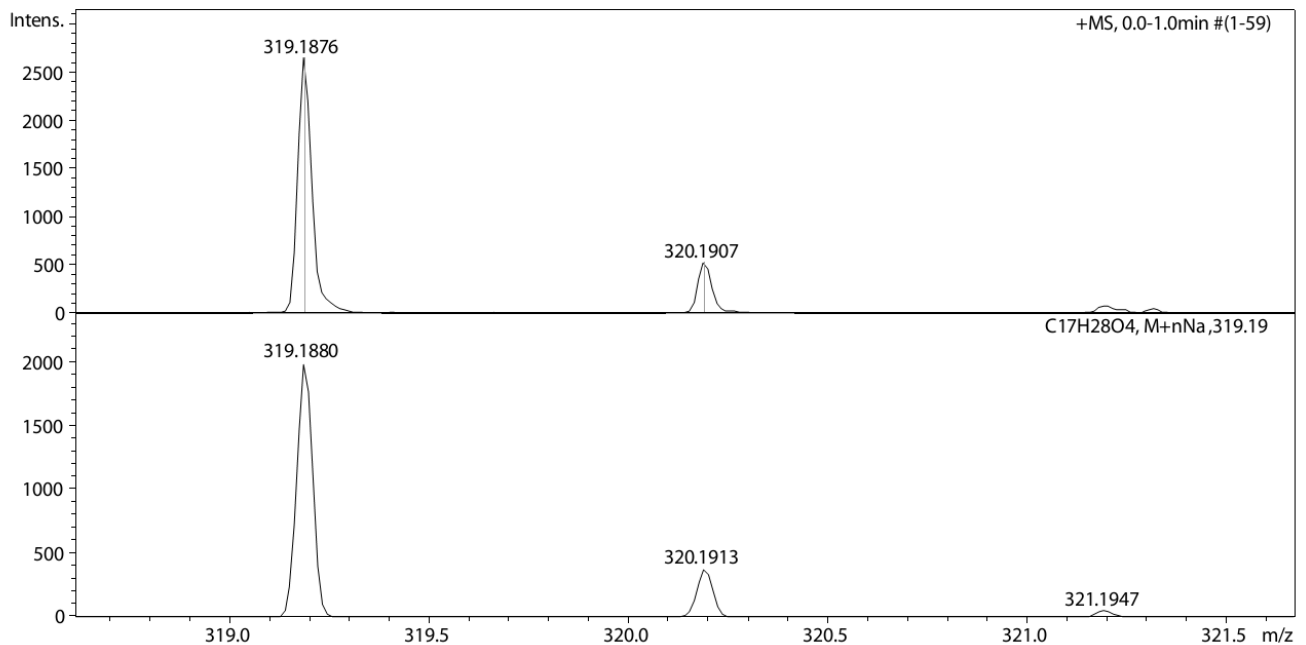
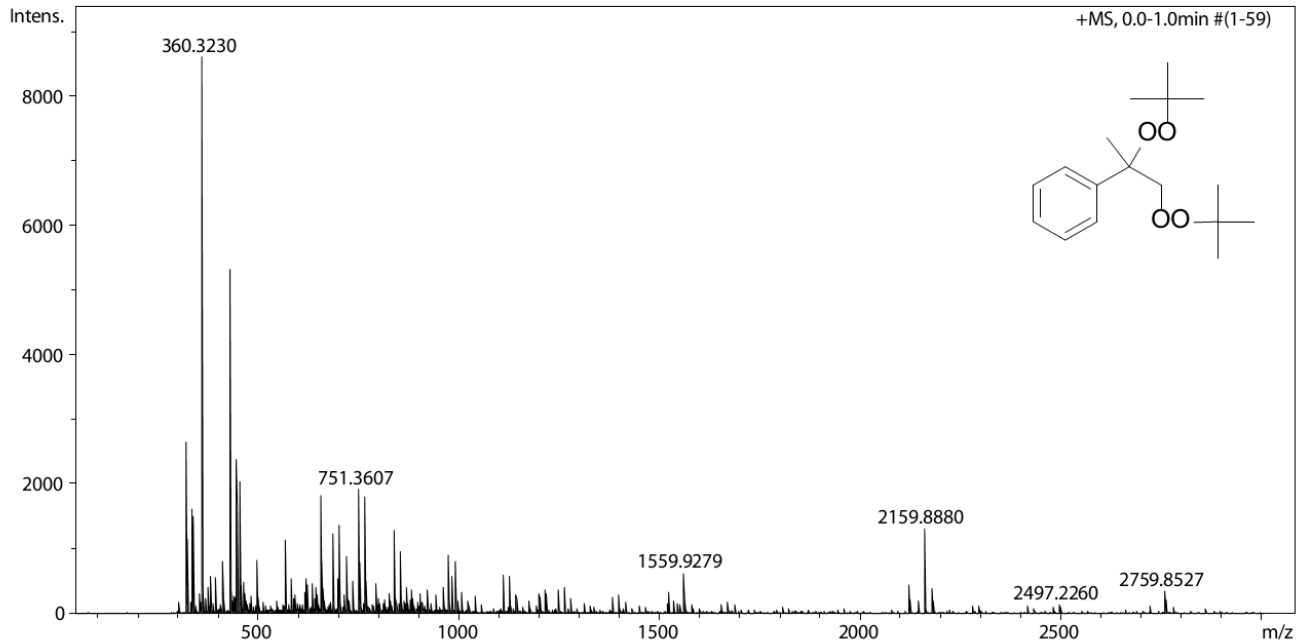
Analysis Info

Analysis Name D:\Data\Chizhov\Nikishin\Terentiev\Sha ripov\m-235_&clb.d
Method tune_wide.m
Sample Name /TERN M-235
Comment CH3CN 100 %, dil. 200, calibrant added

Acquisition Date 28.07.2014 16:26:33
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-methylbenzene, 2c

Display Report

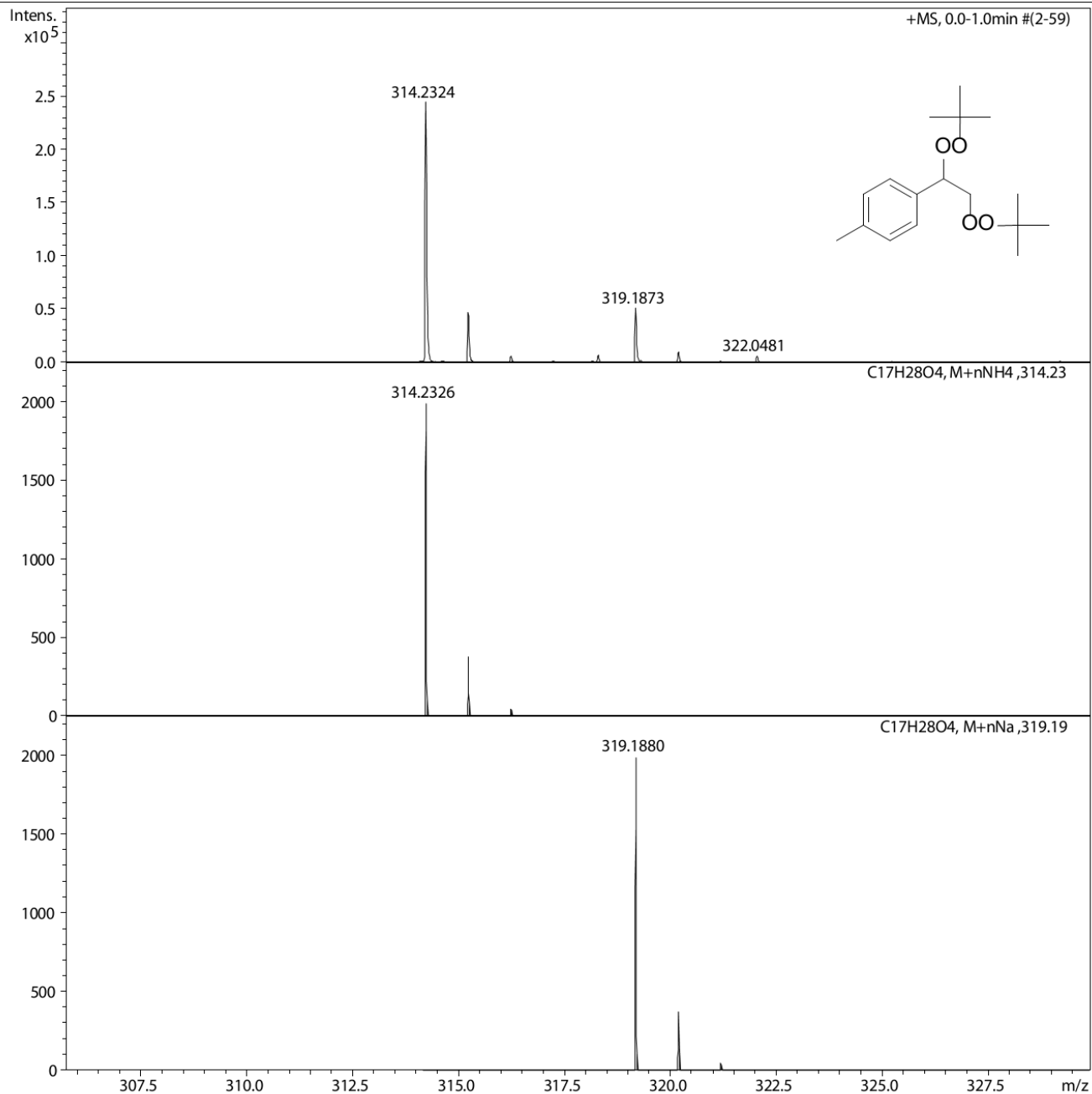
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2014\Sharipov\0129_030.d
Method tune_low.m
Sample Name /TERN M-240
Comment C17H28O4 mw 296 calibrant added

Acquisition Date 29.01.2014 17:38:51
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-*tert*-butylbenzene, 2d

Display Report

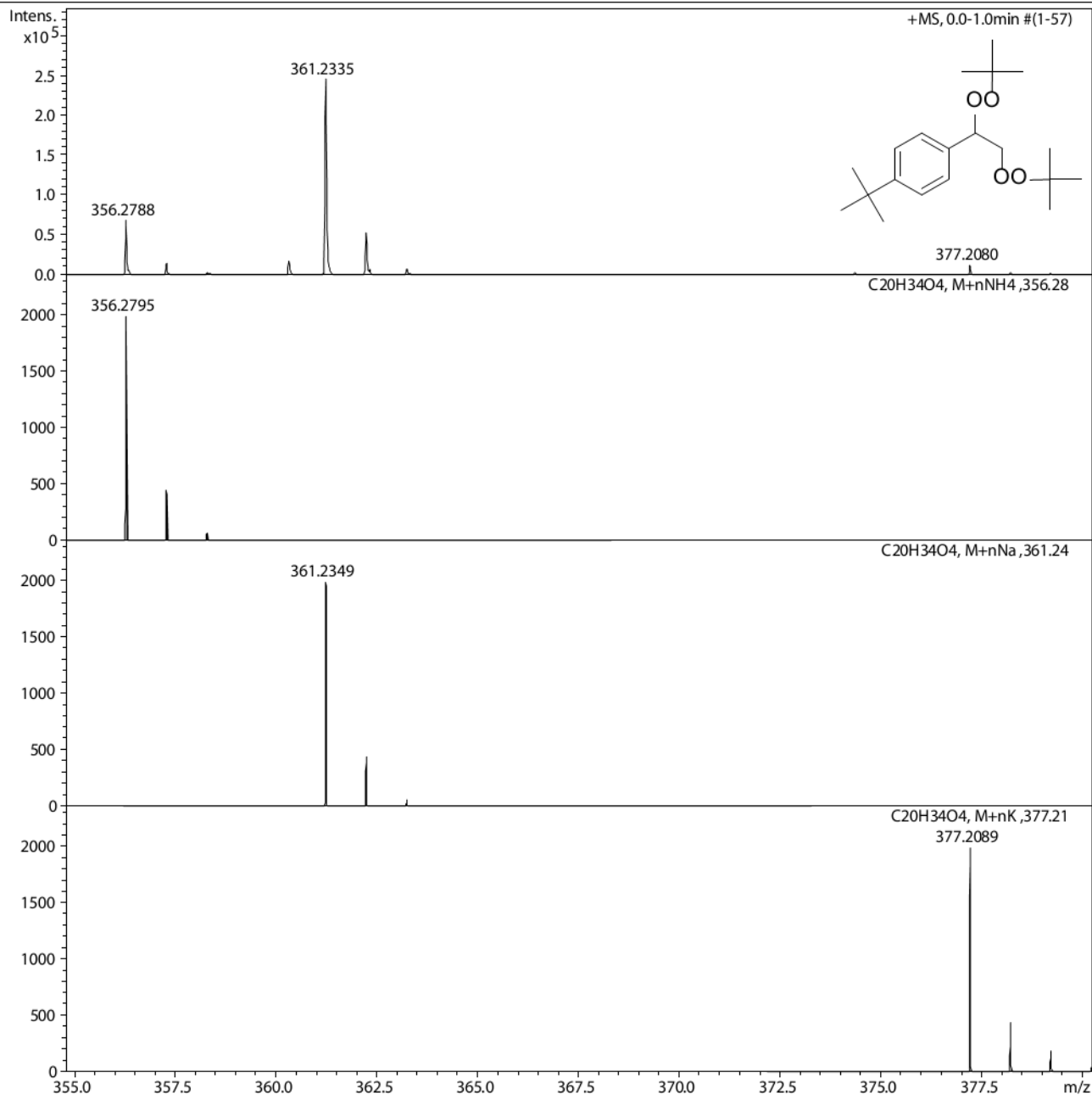
Analysis Info

Analysis Name D:\Data\Kolotyrykina\2014\Sharipov\0116_002.d
 Method tune_low.m
 Sample Name /TERN M-226
 Comment C20H34O4 mw 338 in CH3CN calibrant added

Acquisition Date 06.05.2013 15:14:37
 Operator BDAL@DE
 Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-methoxybenzene, 2e

Display Report

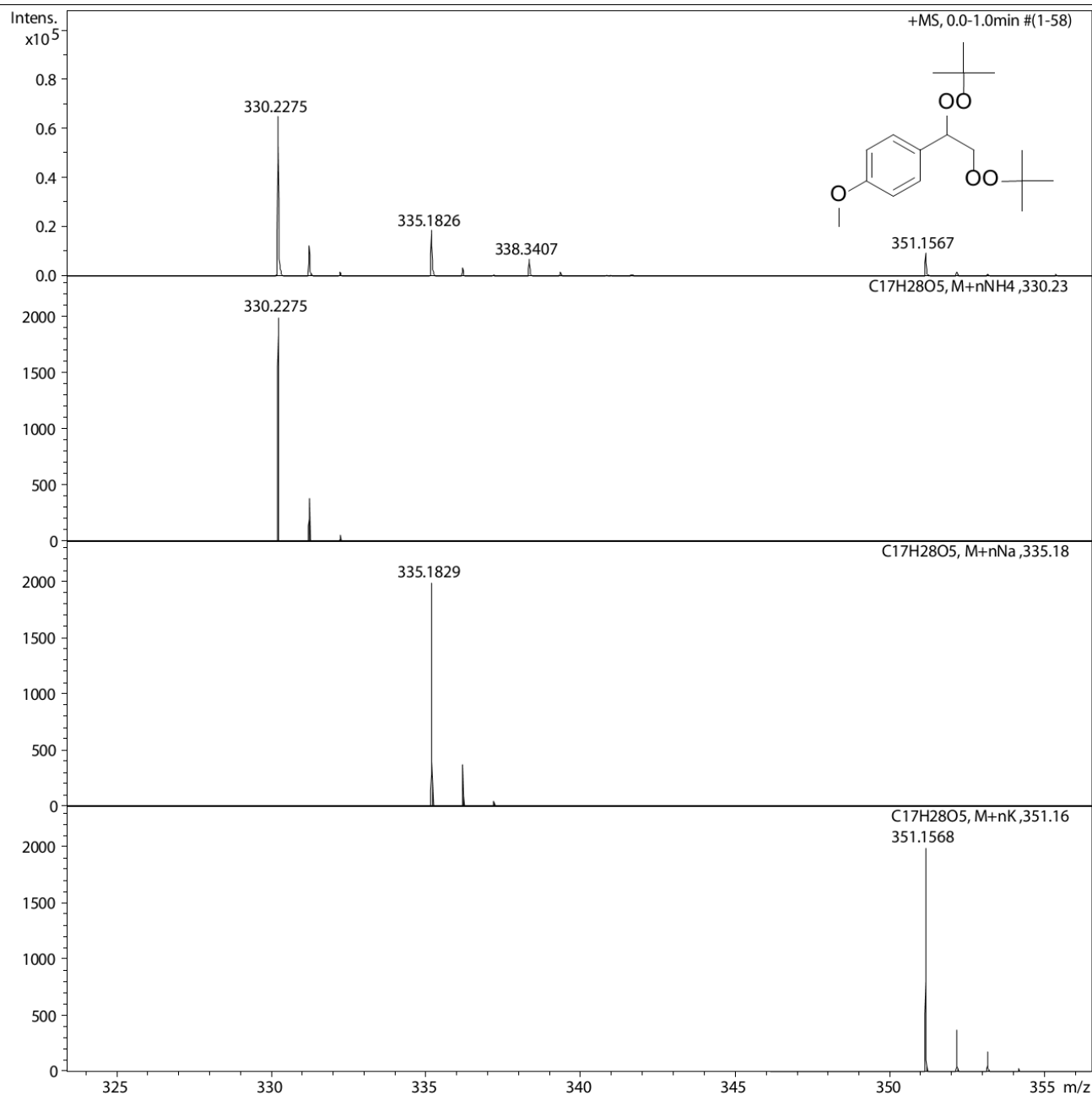
Analysis Info

Analysis Name D:\Data\Kolotyrykina\2014\Sharipov\0305 010.d
 Method tune_low.m
 Sample Name /TERN M-256
 Comment C17H28O5 mw 312 calibrant added

Acquisition Date 05.03.2014 13:56:13
 Operator BDAL@DE
 Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



1-[1,2-Bis(*tert*-butylperoxy)ethyl]-2-methoxybenzene, 2f

Display Report

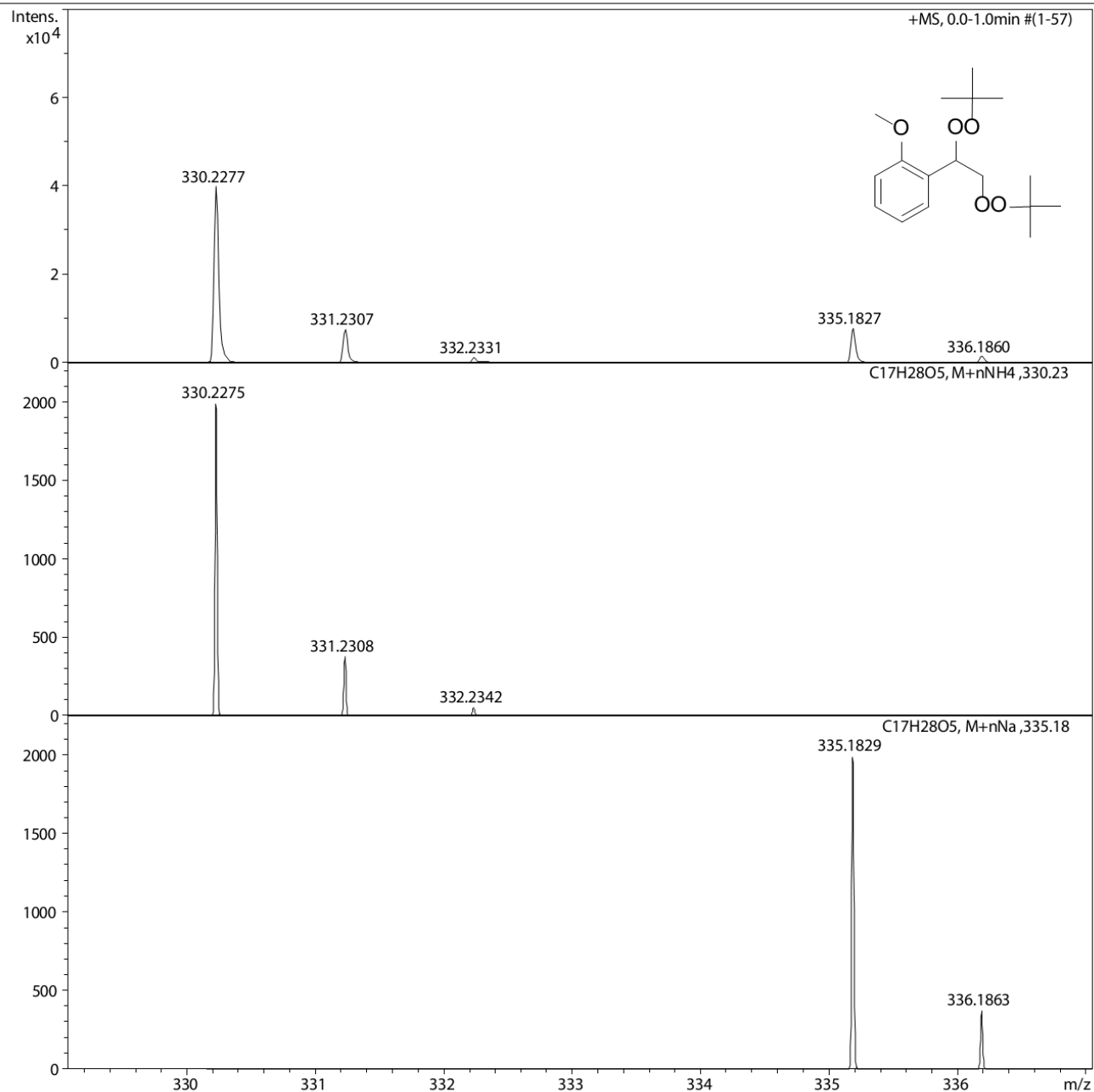
Analysis Info

Analysis Name D:\Data\Kolotyrykina\2014\Sharipov\0305_009.d
 Method tune_low.m
 Sample Name /TERN M-255
 Comment C17H28O5 mw 312 calibrant added

Acquisition Date 05.03.2014 13:45:00
 Operator BDAL@DE
 Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



[1,2-Bis(*tert*-butylperoxy)-1-phenylethyl]benzene, 2g

Display Report

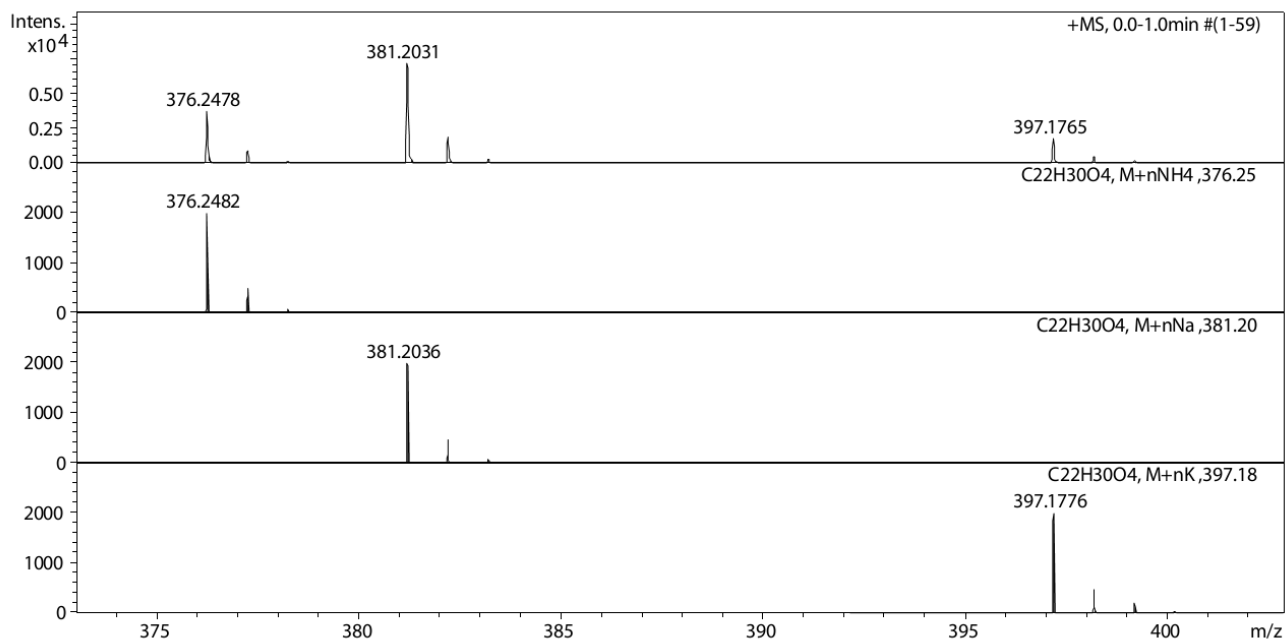
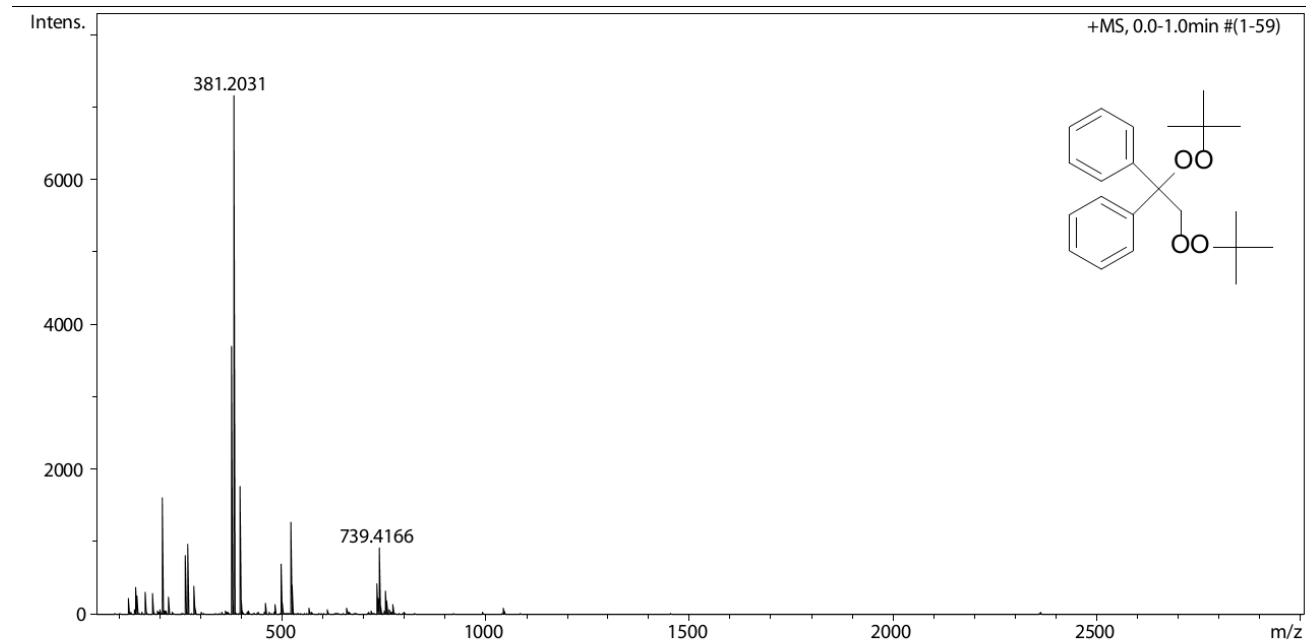
Analysis Info

Analysis Name D:\Data\Chizhov\Nikishin\Terentiev\Sha ripov\m-259_low.d
Method tune_low.m
Sample Name /TERN M-259
Comment CH3CN 10 %, dil. 200, no calibrant added

Acquisition Date 07.04.2014 12:39:28
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



1-[1,2-Bis(*tert*-butylperoxy)ethyl]naphthalene, 2h

Display Report

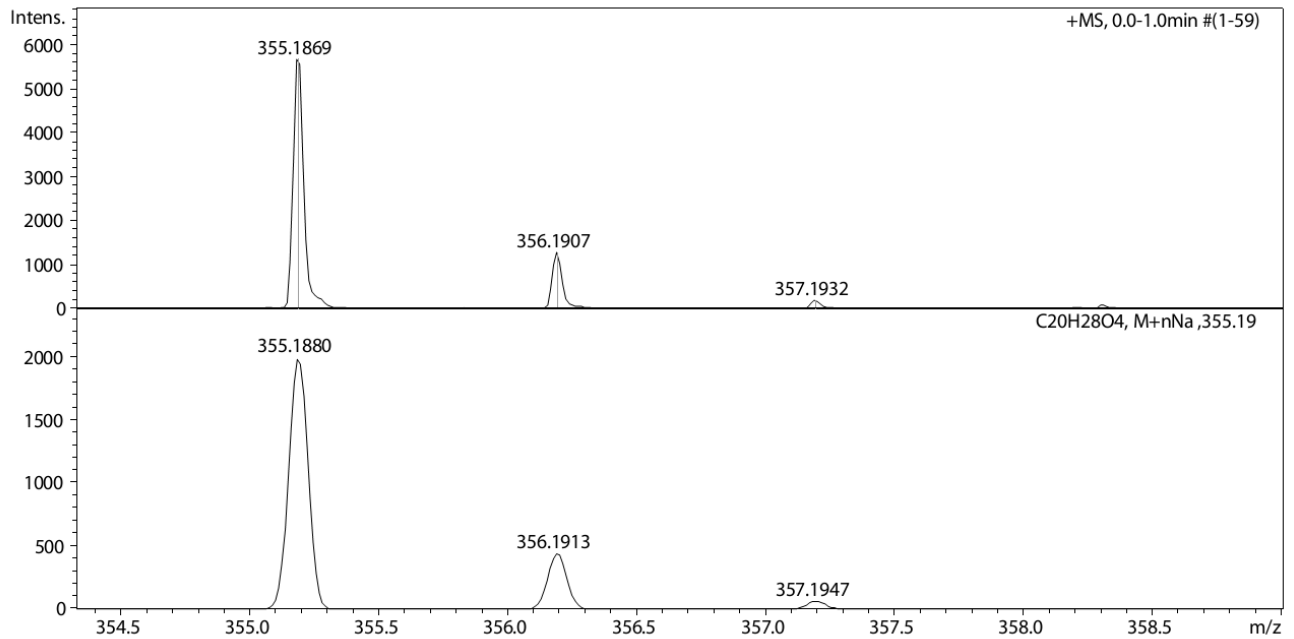
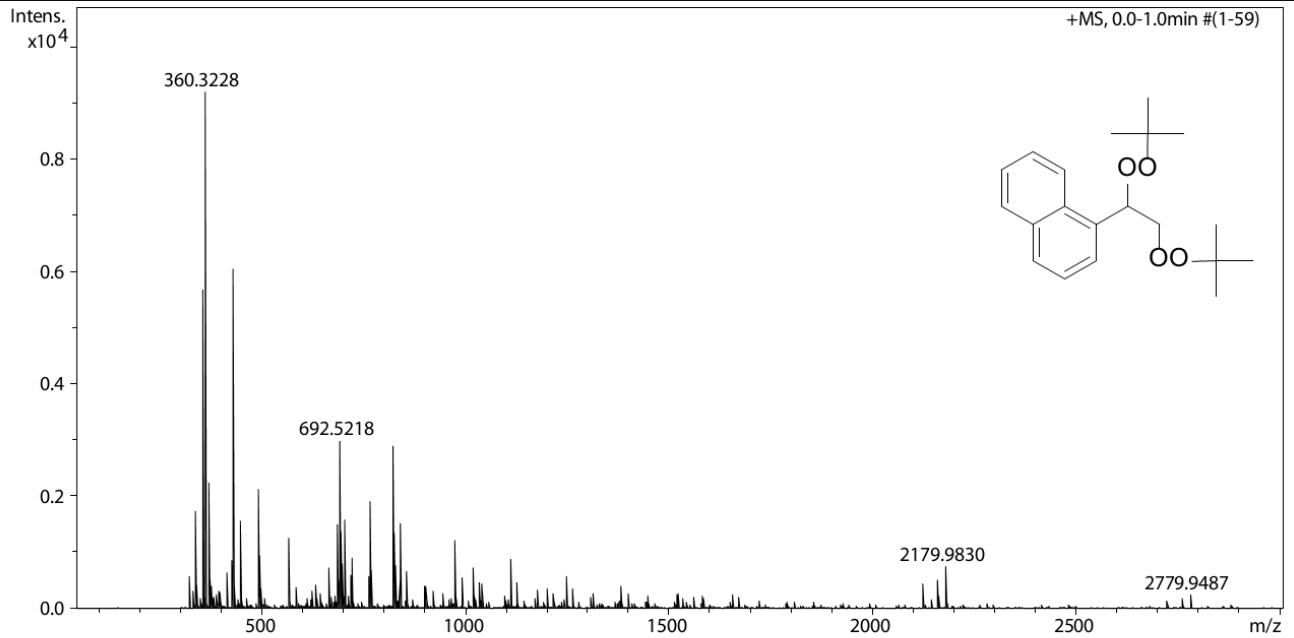
Analysis Info

Analysis Name D:\Data\Chizhov\Nikishin\Terentiev\Sha ripov\m287_&clb.d
Method tune_wide.m
Sample Name /TERN M-287
Comment CH3CN 100 %, dil. 200, calibrant added

Acquisition Date 09.06.2014 17:38:34
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



1-[1,2-Bis(*tert*-butylperoxy)ethyl]-4-chlorobenzene, 2i

Display Report

Analysis Info

Analysis Name D:\Data\Kolotyrykina\2014\Sharipov\0707_018.d
 Method tune_low.m
 Sample Name /TERN M-295
 Comment C16H25ClO4 mw 316 calibrant added

Acquisition Date 07.07.2014 17:00:33
 Operator BDAL@DE
 Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

