Supplementary Material

Cytotoxic Alkylynols of the Sponge *Cribrochalina vasculum*: Structure, Synthetic Analogs and SAR Studies

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Table of Content

Figure S1. ^{1}H NMR spectrum of (3*R*)-18-methylnonadec-(4*E*)-en-1-yn-3-ol (**1**) in $CDCl_3$.

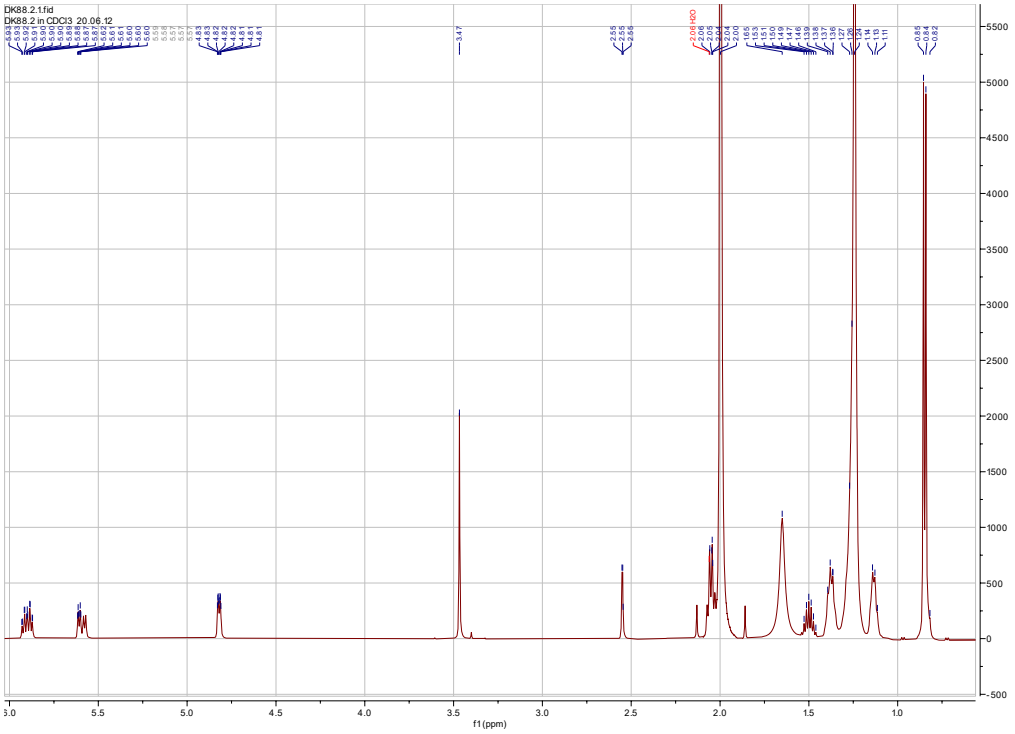


Figure S2. ^{13}C NMR spectrum of (3*R*)-18-methylnonadec-(4*E*)-en-1-yn-3-ol (**1**) in $CDCl_3$.

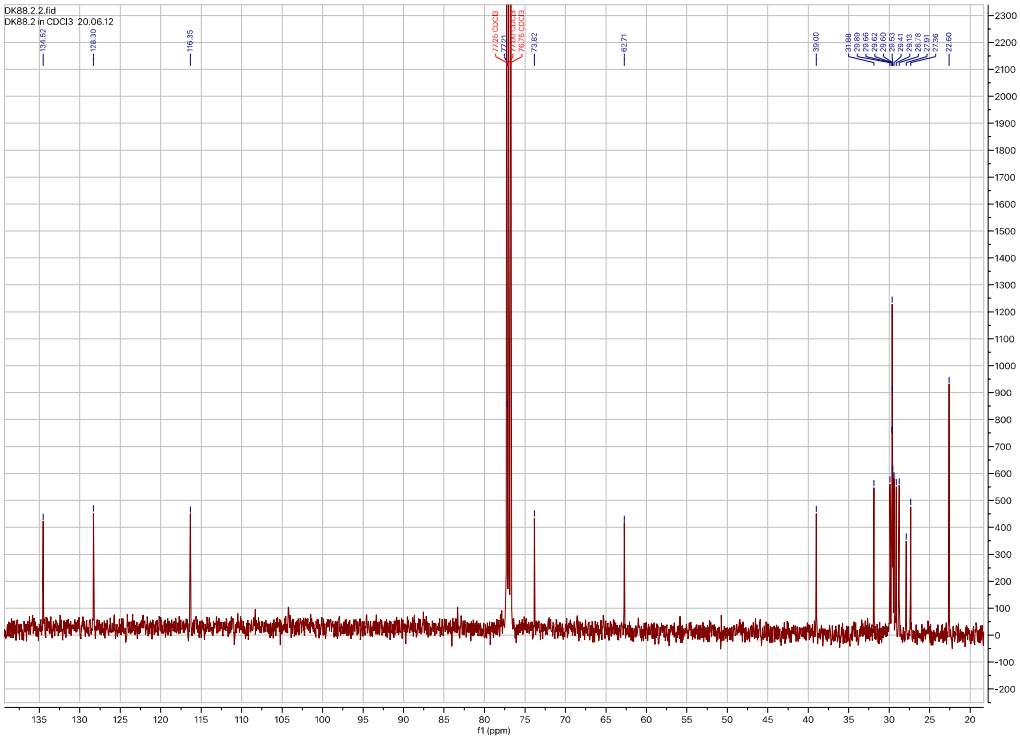


Figure S3. HSQC spectrum of (3*R*)-18-methylnonadec-(4*E*)-en-1-yn-3-ol (**1**) in $CDCl_3$.

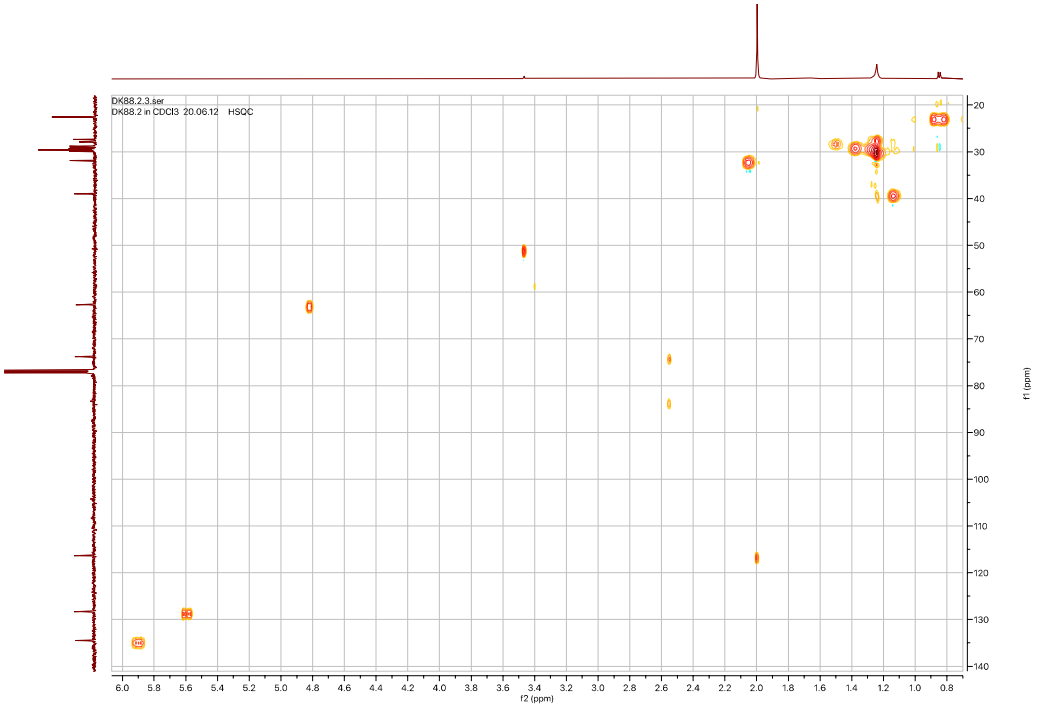


Figure S4. HMBC spectrum of (3*R*)-18-methylnonadec-(4*E*)-en-1-yn-3-ol (**1**) in $CDCl_3$.

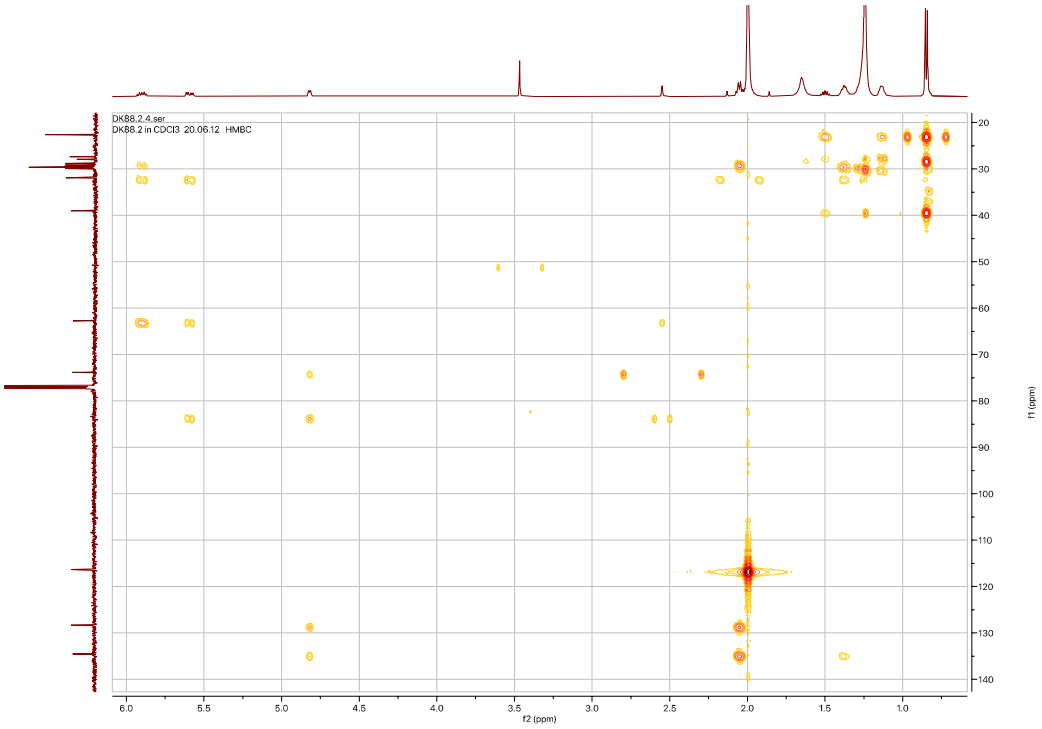


Figure S5. COSY spectrum of (3*R*)-18-methylnonadec-(4*E*)-en-1-yn-3-ol (**1**) in $CDCl_3$.

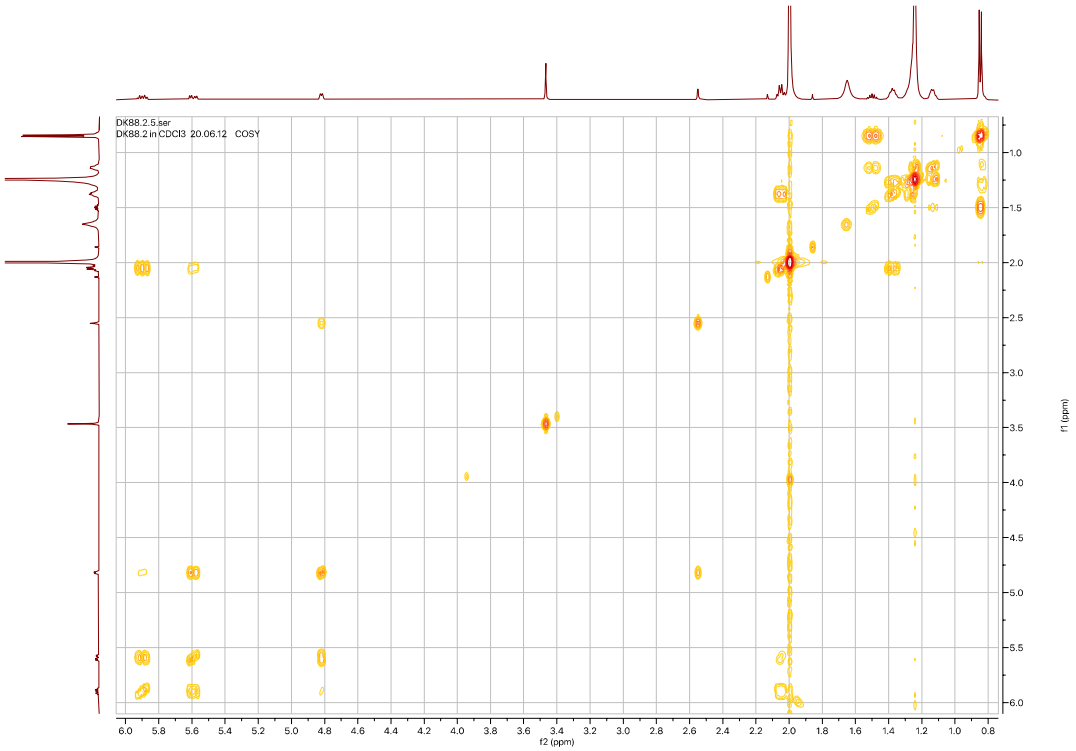


Figure S6. DEPT spectrum of (3*R*)-18-methylnonadec-(4*E*)-en-1-yn-3-ol (**1**) in $CDCl_3$.

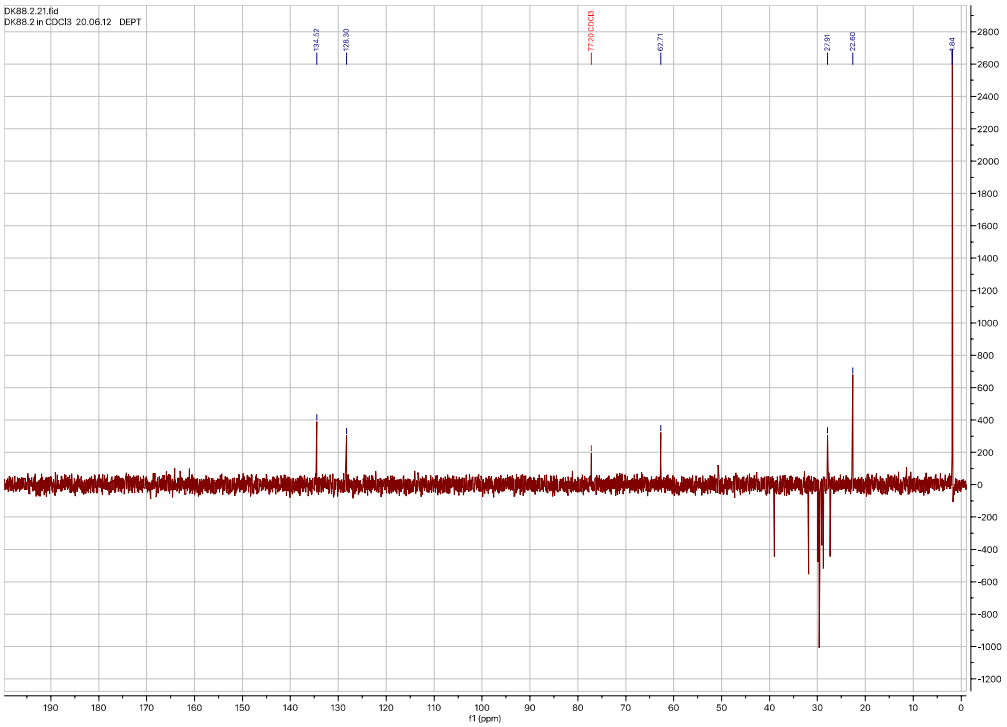


Table S1. NMR data of (3*R*)-18-methylnonadec-(4*E*)-en-1-yn-3-ol (**1**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.8[d] CH	2.55 d (2.1)	3
2	83.3[e] qC	-	1, 3, 4
3	62.7 CH	4.82 d (6.0)	1, 4, 5
4	128.3 CH	5.59 dd (15.2, 6.0)	3, 6
5	134.5 CH	5.90 dt (15.2, 7.0)	3, 6, 7
6	31.9 CH_2	2.05 q (7.0)	4, 5, 7, 8
7	28.8 CH_2	1.38 m	5, 6, 8
8-15	~29.6[f] 8 × CH_2	1.22 – 1.26 brm	
16	27.4 CH_2	1.24 m	15, 17
17	39.0 CH_2	1.13 m	16, 18, 19, 20
18	27.9 CH	1.50 qqt (6.5, 6.5, 6.5)	17, 19, 20
19	22.6 CH_3	0.85 d (6.5)	17, 18, 20
20	22.6 CH_3	0.85 d (6.5)	17, 18, 19

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 250.0 Hz; [e] ^2J = 49.0 Hz; [f]Exact ^{13}C chemical shifts 29.13, 29.41, 29.62 (× 4), 29.66, 29.89 ppm.

Figure S7. GCMS spectrum of (3*R*)-18-methylnonadec-(4*E*)-en-1-yn-3-ol (**1**).

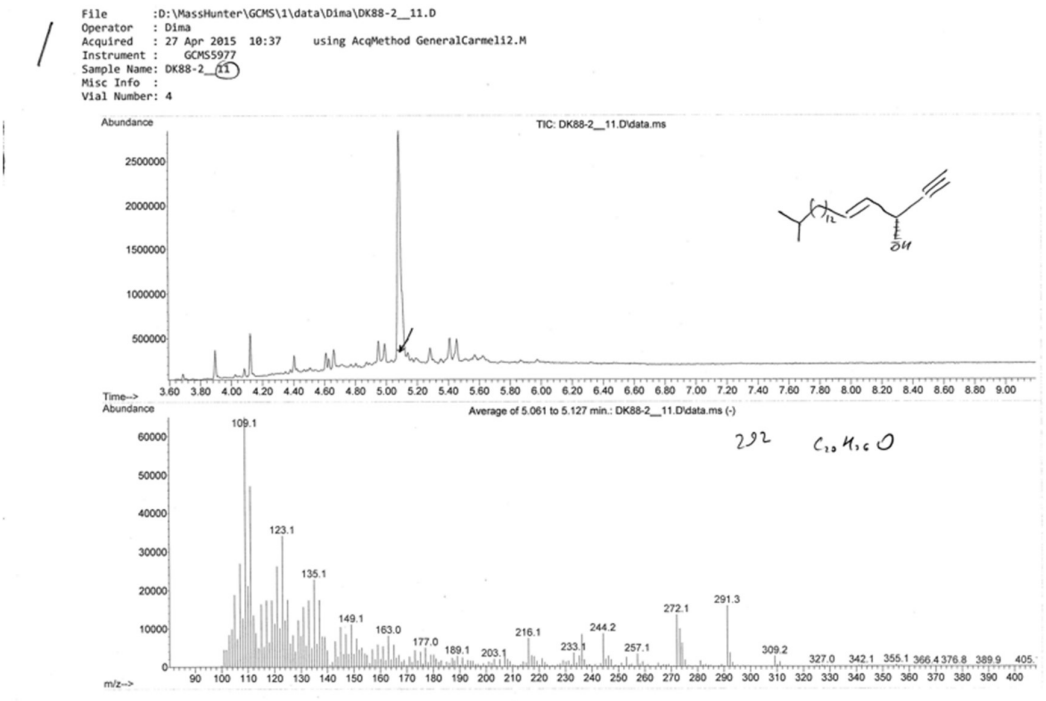


Figure S8. HRMS spectrum of (3*R*)-18-methylnonadec-(4*E*)-en-1-yn-3-ol (**1**).

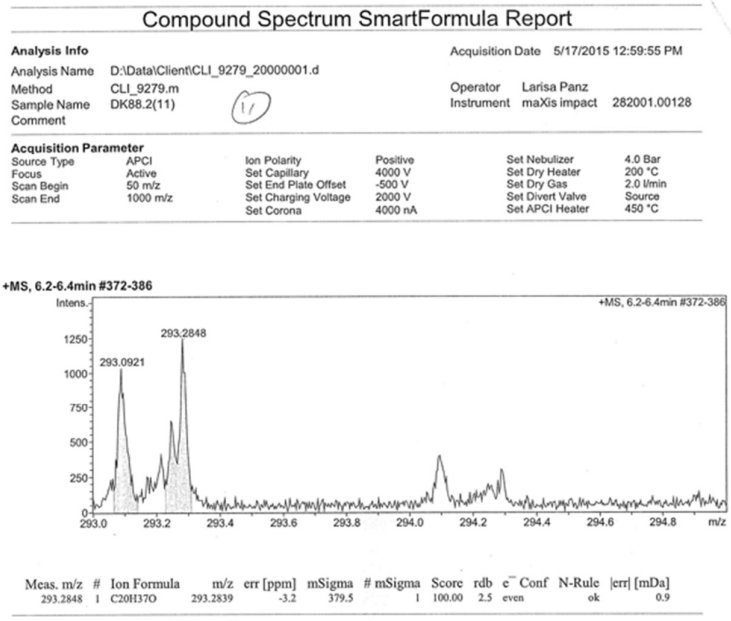


Figure S9. ^{1}H NMR spectrum of (3*R*)-14-methylnonadec-(4*E*)-en-1-yn-3-ol (**2**) in $CDCl_3$

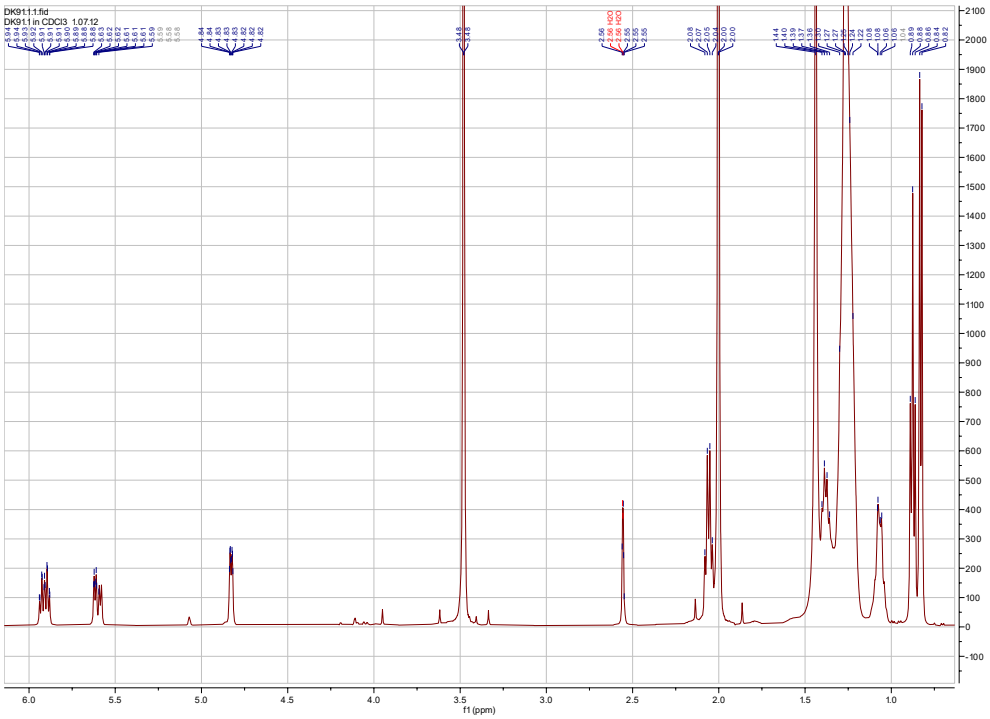


Figure S10. ^{13}C NMR spectrum of (3*R*)-14-methylnonadec-(4*E*)-en-1-yn-3-ol (**2**) in $CDCl_3$

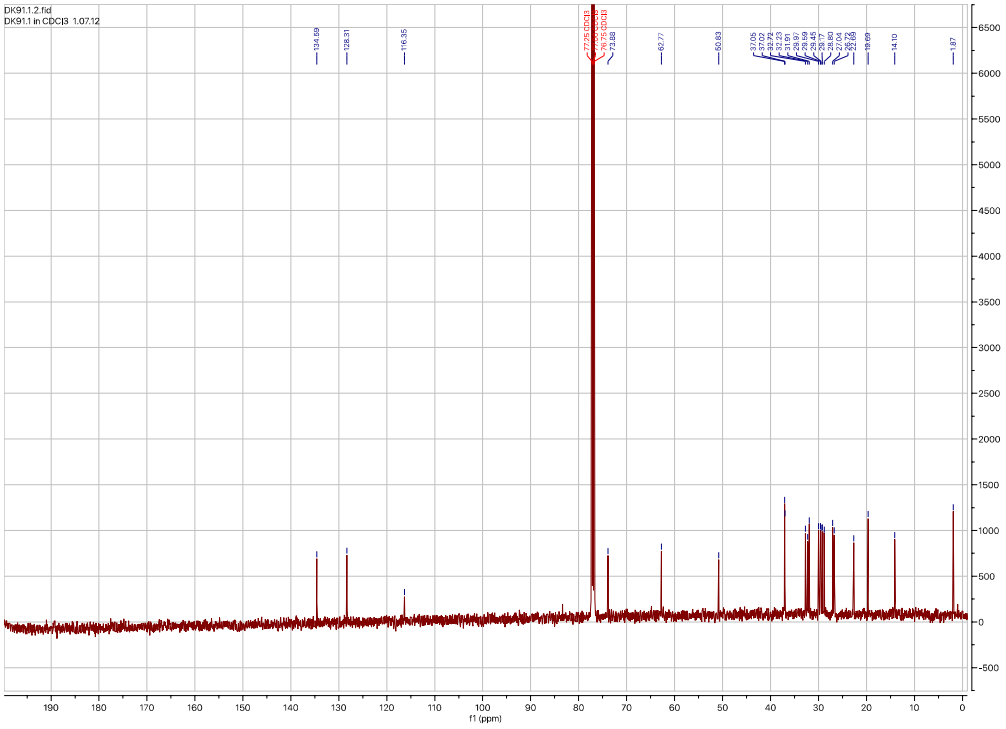


Figure S11. HSQC spectrum of (3*R*)-14-methylnonadec-(4*E*)-en-1-yn-3-ol (**2**) in $CDCl_3$

Figure S12. HMBC spectrum of (3*R*)-14-methylnonadec-(4*E*)-en-1-yn-3-ol (**2**) in $CDCl_3$

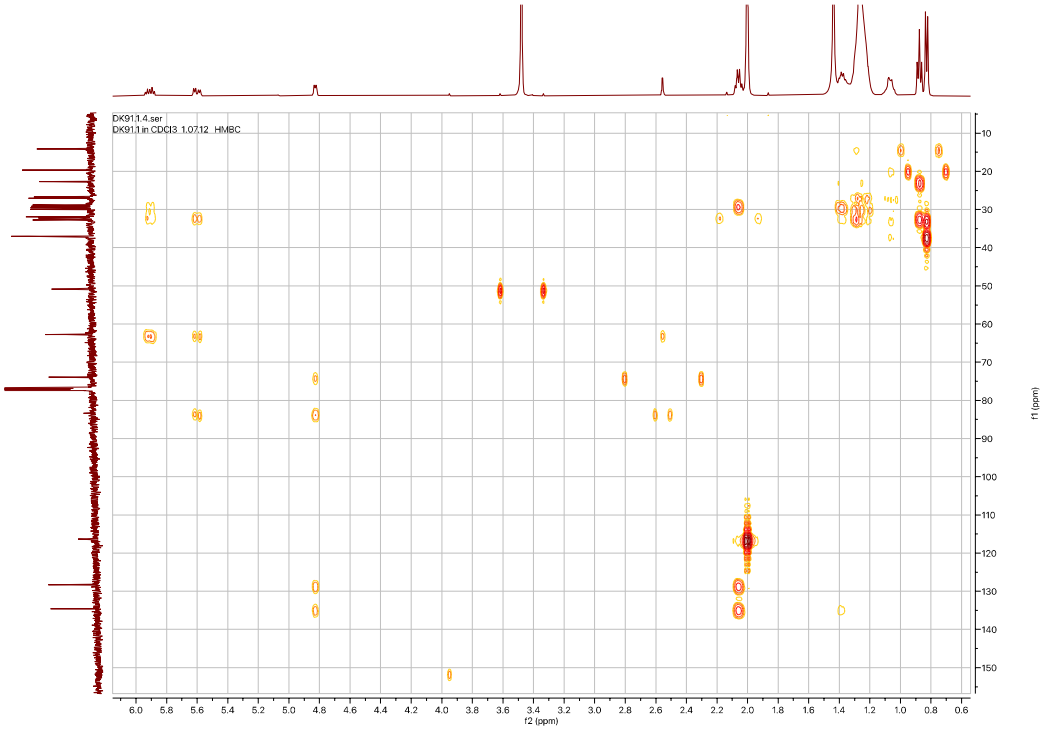


Figure S13. COSY spectrum of (3*R*)-14-methylnonadec-(4*E*)-en-1-yn-3-ol (**2**) in $CDCl_3$

Table S2. NMR data of (3*R*)-14-methylnonadec-(4*E*)-en-1-yn-3-ol (**2**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.9[d] CH	2.55 d (2.0)	3
2	83.4[e] qC	-	1, 3, 4
3	62.8 CH	4.82 d (5.7)	1, 4, 5
4	128.3 CH	5.60 dd (15.0, 5.7)	3, 6
5	134.5 CH	5.90 dt (15.0, 7.0)	3, 6, 7
6	31.9 CH_2	2.06 q (7.0)	4, 5, 7, 8
7	28.8 CH_2	1.36 m	5, 6, 8
8-11	~29.6[f] 4 × CH_2	1.21 – 1.31 brm	
12	27.0 CH_2	1.23 m	11, 13a, 13b
13a	37.0 CH_2	1.25 m	12, 14, 15a, 15b, 21
b		1.06 m	
14	32.7 CH	1.37 m	13a, 13b, 15a, 15a, 21
15a	37.0 CH_2	1.25 m	13a, 13b, 14, 16, 21
b		1.06 m	
16	26.7 CH_2	1.24 m	15a, 15b, 17
17	32.2 CH_2	1.24 m	16, 18a, 18b, 19
18a	22.7 CH_2	1.30 m	17, 19
b		1.24 m	
19	14.1 CH_3	0.87 t (7.0)	18a, 18b
20	19.7 CH_3	0.83 d (7.0)	13b, 15b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 250.0 Hz; [e] ^2J = 48.8 Hz; [f]Exact ^{13}C chemical shifts 29.17, 29.45, 29.59, 29.97 ppm.

Figure S14. GCMS spectrum of (3*R*)-14-methylnonadec-(4*E*)-en-1-yn-3-ol (**2**)

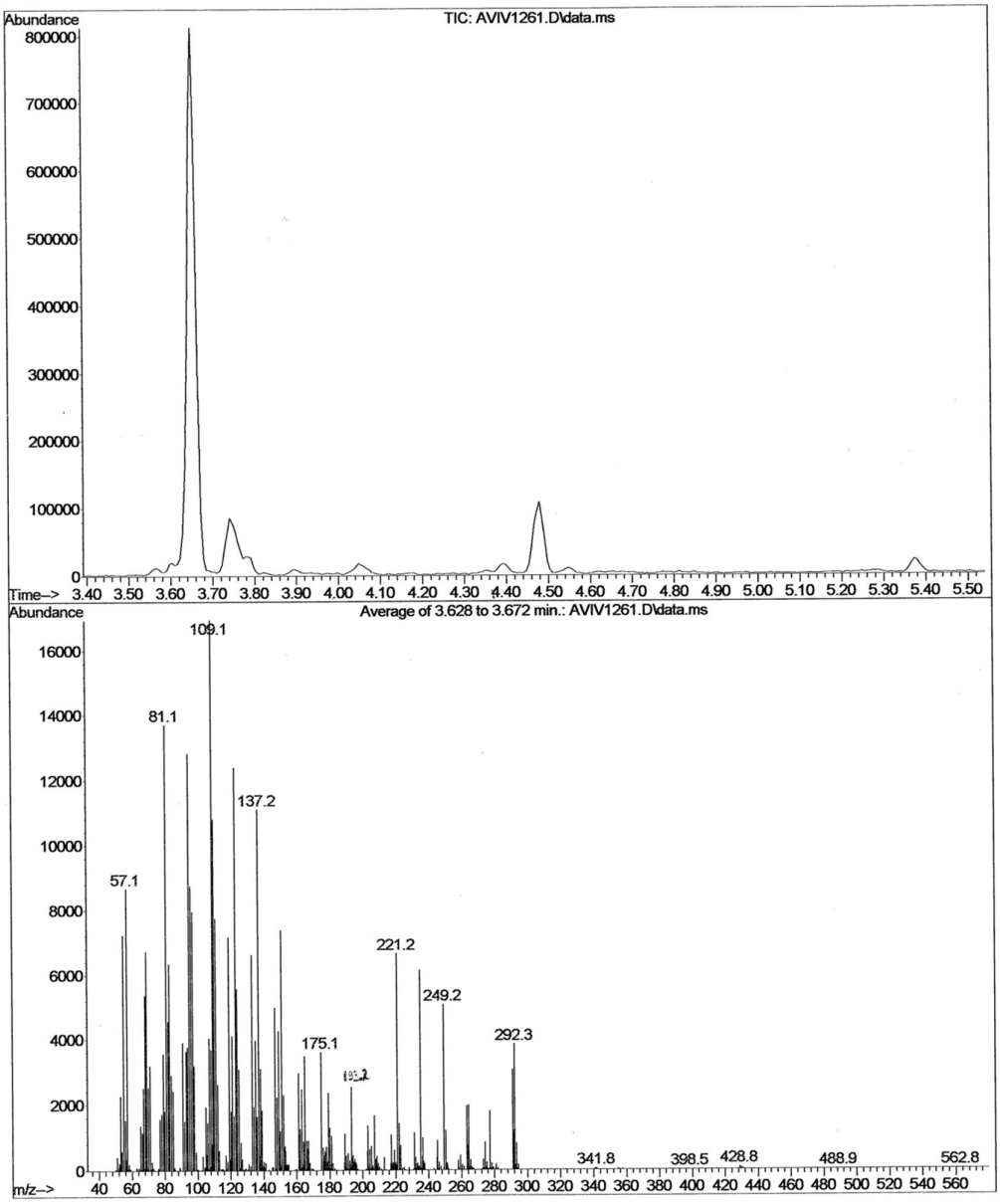
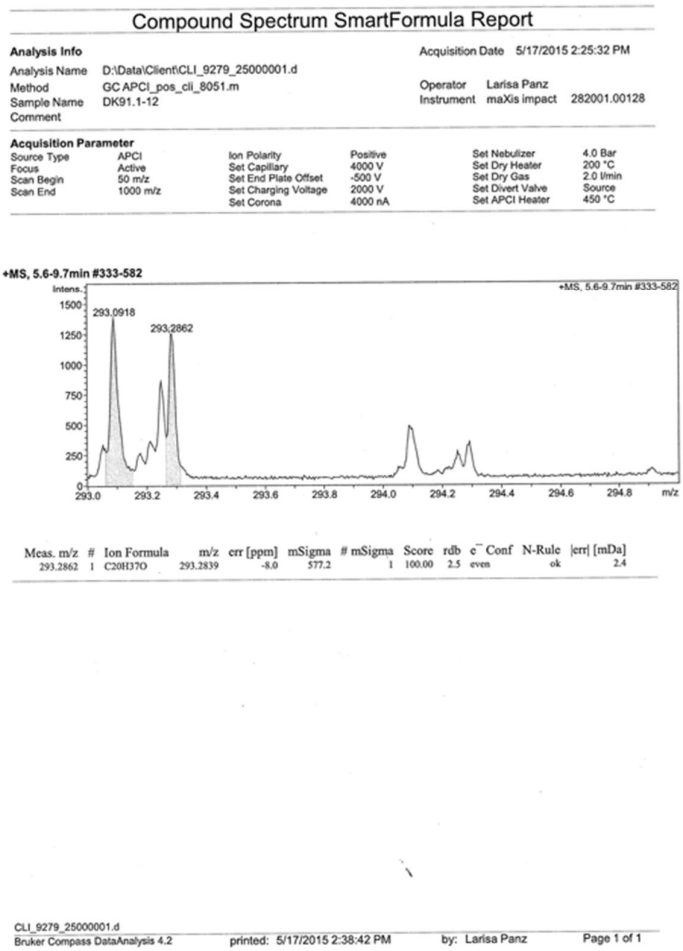


Figure S15. HRMS spectrum of (3*R*)-14-methylnonadec-(4*E*)-en-1-yn-3-ol (**2**)



Compound Spectrum SmartFormula Report

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Sample Name	DK91.1-12	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

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Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
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+MS, 5.6-9.7min #333-582

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
293.2862	1	C20H37O	293.2839	-8.0	577.2	1	100.00	2.5	even	ok	2.4

Figure S16. ^{1}H NMR spectrum of 14-methylnonadec-(4*E*)-en-1-yn-3-one (**3**) in $CDCl_3$

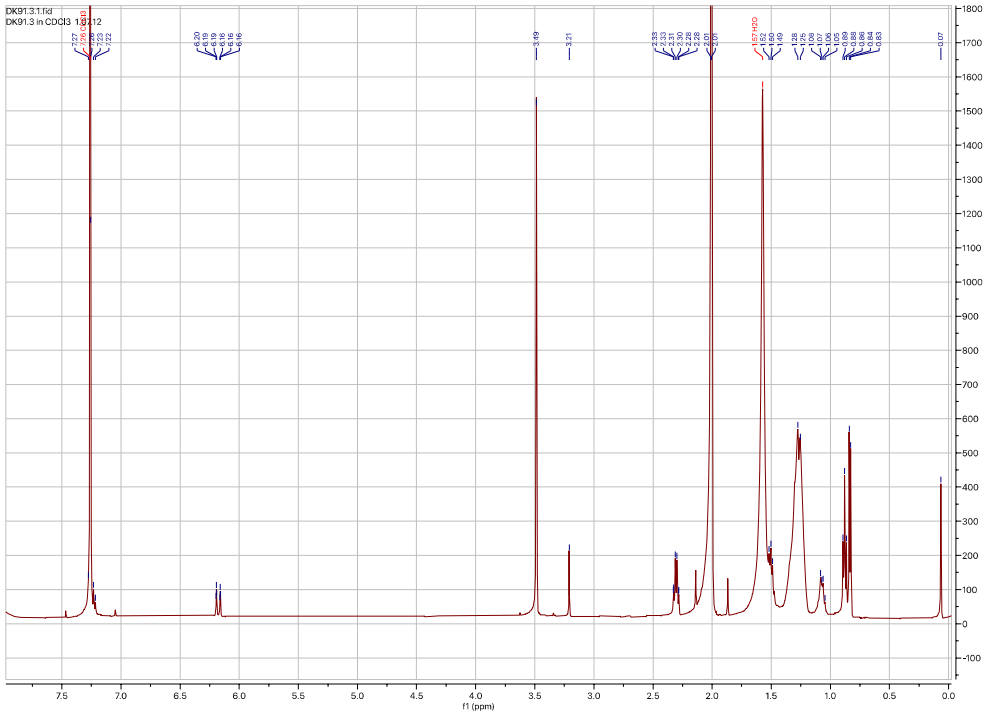


Figure S17. ^{13}C NMR spectrum of 14-methylnonadec-(4*E*)-en-1-yn-3-one (**3**) in $CDCl_3$

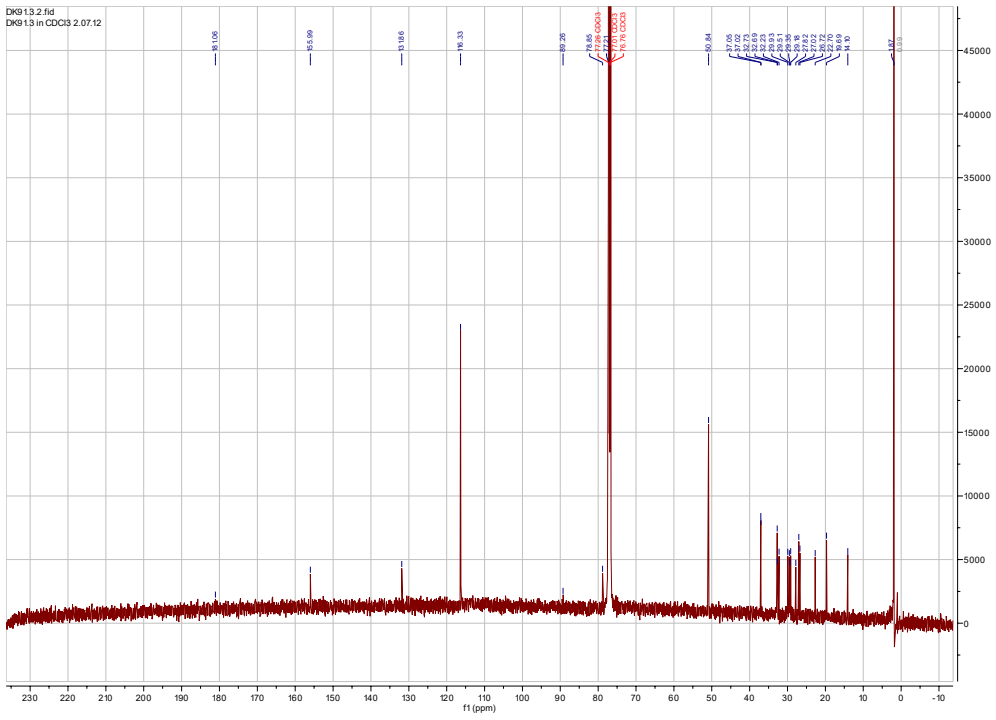
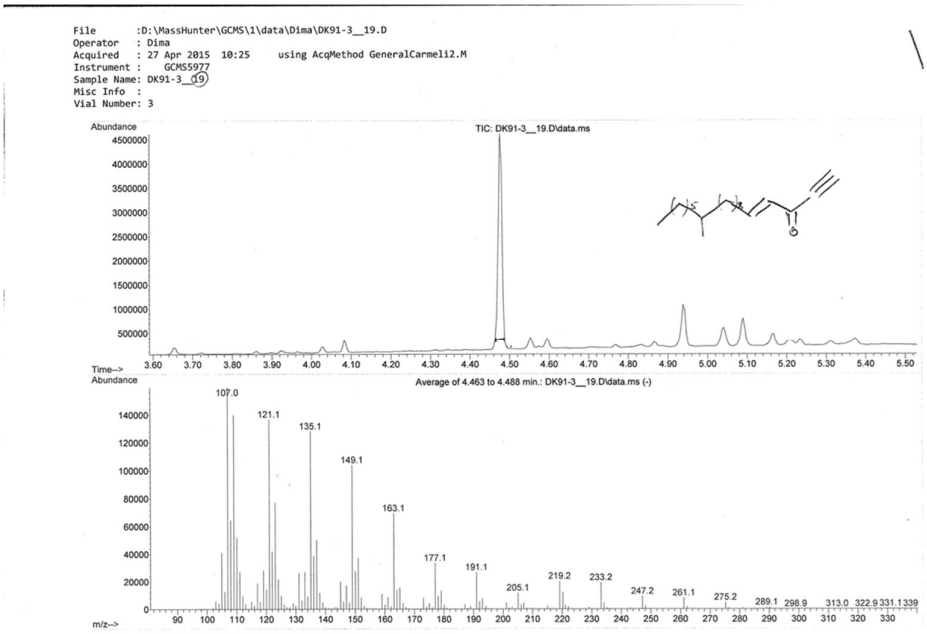


Table S3. NMR data of 14-methylnonadec-(4*E*)-en-1-yn-3-one (**3**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	78.8[d] CH	3.20 s	-
2	79.8[e] qC	-	1, 4
3	177.9 qC	-	1, 4, 5
4	131.9 CH	6.17 d (16.0)	6
5	156.0 CH	7.23 dt (16.0, 7.0)	6, 7
6	32.7 CH_2	2.30 q (7.0)	4, 5, 7, 8
7	27.8 CH_2	1.50 tt (7.0, 7.0)	5, 6, 8
8	29.2 CH_2	1.30 m	
9-11	~29.6[f] 3 × CH_2	1.23 – 1.31 brm	
12	27.0 CH_2	1.23 m	11, 13a, 13b
13a	37.0 CH_2	1.26 m	12, 14, 15a, 15b, 21
b		1.07 m	
14	32.7 CH	1.37 m	13a, 13b, 15a, 15a, 21
15a	37.0 CH_2	1.26 m	13a, 13b, 14, 16, 21
b		1.07 m	
16	26.7 CH_2	1.25 m	15a, 15b, 17
17	32.2 CH_2	1.25 m	16, 18a, 18b, 19
18a	22.7 CH_2	1.31 m	17, 19
b		1.25 m	
19	14.1 CH_3	0.88 t (7.0)	18a, 18b
20	19.7 CH_3	0.83 d (7.0)	13b, 15b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 252.0 Hz [e] ^2J = 48.0 Hz; [f]Exact ^{13}C chemical shifts 29.34, 29.51, 29.92 ppm.

Figure S18. EIMS and fragmentation pattern of 14-methylnonadec-(4*E*)-en-1-yn-3-one (**3**).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Misc Info :
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Abundance
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Time-->
Abundance
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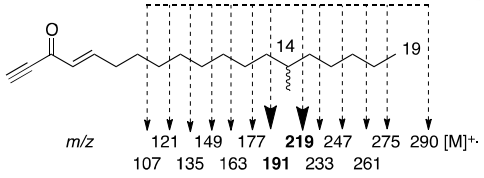
m/z-->


O
14
19
m/z
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107 135 163 191 233 261

Figure S19. HRCIMS and fragmentation pattern of 14-methylnonadec-(4*E*)-en-1-yn-3-one (**3**)

Compound Spectrum SmartFormula Report

Analysis Info

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Method	CLI_9279.m	Operator	Larisa Panz
Sample Name	DK-91-3(19)	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

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Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

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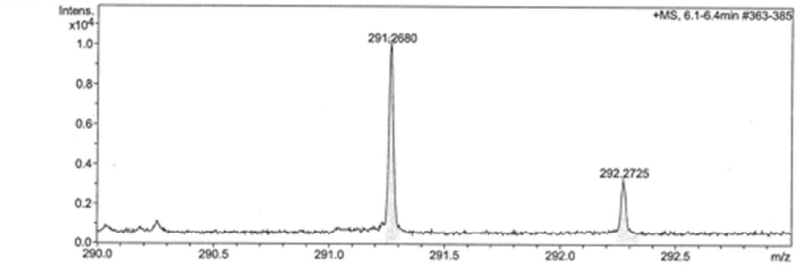


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
291.2680	1	C20H35O	291.2682	0.8	572.8	1	100.00	3.5	even	ok	0.2
	2	C13H35N6O	291.2867	64.2	580.9	2	0.00	-0.5	even	ok	18.7

CLI_9279_2.d
Bruker Compass DataAnalysis 4.2 printed: 5/17/2015 9:06:36 AM by: Larisa Panz Page 1 of 1

Figure S20. ^{1}H NMR spectrum of (3*R*)-13,18-dimethylnonadec-(4*E*)-en-1-yn-3-ol (**4**) in $CDCl_3$

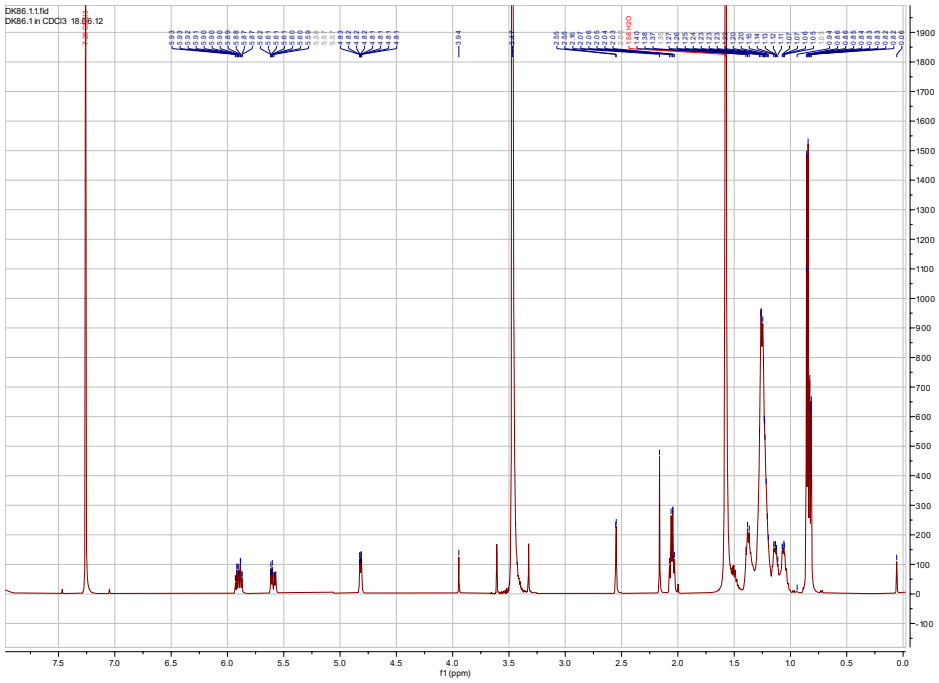


Figure S21. ^{13}C NMR spectrum of (3*R*)-13,18-dimethylnonadec-(4*E*)-en-1-yn-3-ol (**4**) in $CDCl_3$

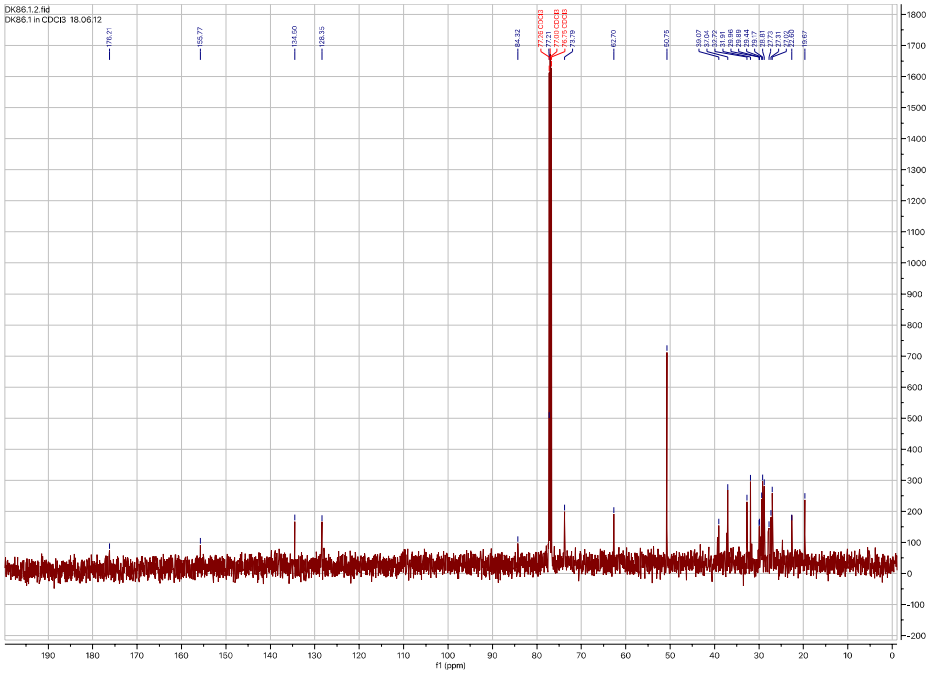


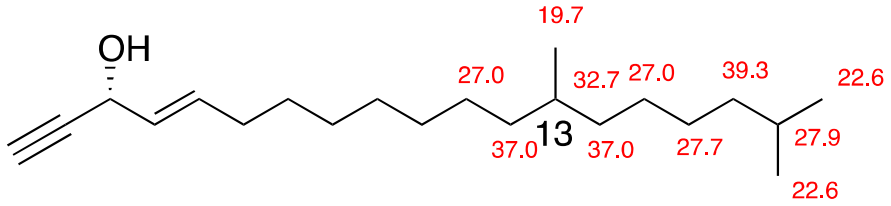
Table S4. NMR data of (3*R*)-13,18-dimethylnonadec-(4*E*)-en-1-yn-3-ol (**4**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.8[d] CH	2.56 d (2.5)	3
2	83.3[e] qC	-	1, 3, 4
3	62.7 CH	4.82 brd (6.0)	1, 4, 5
4	128.3 CH	5.59 dd (15.0, 6.0)	3, 6
5	134.5 CH	5.90 dt (15.0, 7.5)	3, 6, 7
6	31.9 CH_2	2.05 q (7.0)	4, 5, 7, 8
7	28.8 CH_2	1.40 m	5, 6, 8
8-10	~29.6[f] 3 × CH_2	1.23 – 1.26 brm	
11	27.0 CH_2	1.25 m	10, 12a, 12b
12a	37.0 CH_2	1.26 m	11, 13, 14a, 14b, 21
b		1.07 m	
13	32.7 CH	1.35 m	12a, 12b, 14a, 14b, 21
14a	37.0 CH_2	1.26 m	12a, 12b, 13, 15, 21
b		1.07 m	
15	27.0 CH_2	1.25 m	14a, 14b, 16
16	27.7 CH_2	1.25 m	15, 17
17	39.3 CH_2	1.15 m	16, 18, 19, 20
18	27.9 CH	1.51 m	17, 19, 20
19	22.6 CH_3	0.86 d (7.0)	17, 18, 20
20	22.6 CH_3	0.86 d (7.0)	17, 18, 19
21	19.7 CH_3	0.82 d (6.5)	12b, 14b

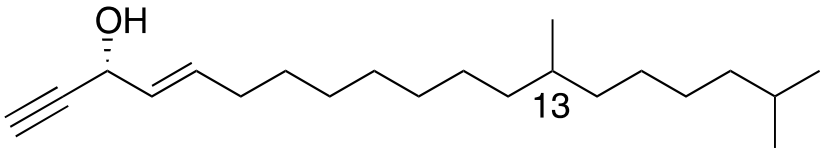
[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 250.0 Hz; [e] ^2J = 49.0 Hz; [f]Exact ^{13}C chemical shifts 29.16, 29.44, 29.45 ppm.

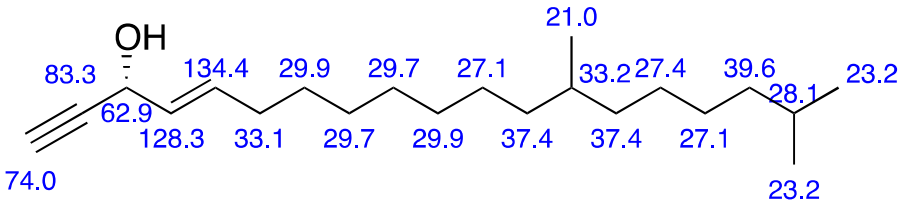
Figure S22. Measured and calculated ^{13}C NMR data of (3*R*)-13,18-dimethylnonadec-(4*E*)-en-1-yn-3-ol (**4**).

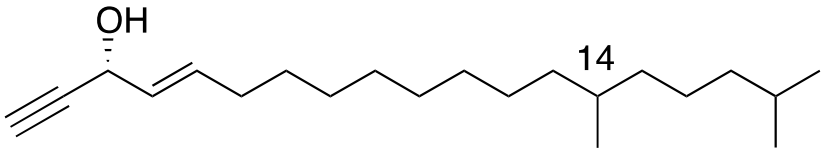
Measured



Calculated







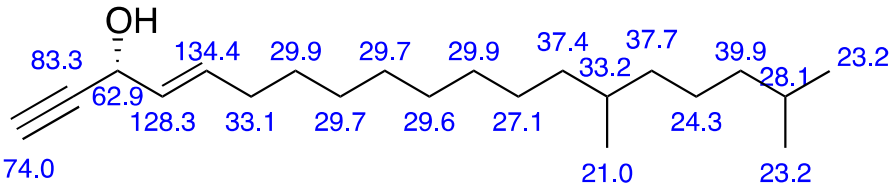
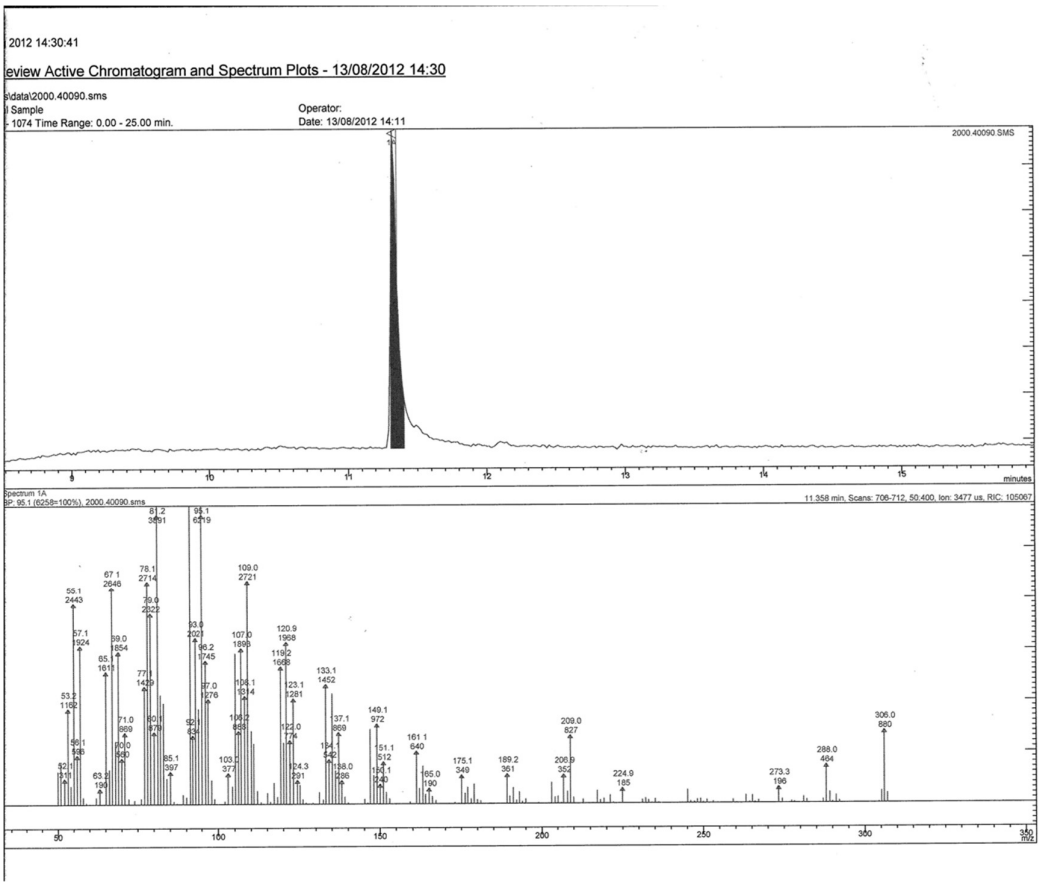


Figure S23. EIMS and fragmentation pattern of (3*R*)-13,18-dimethylnonadec-(4*E*)-en-1-yn-3-ol (**4**).



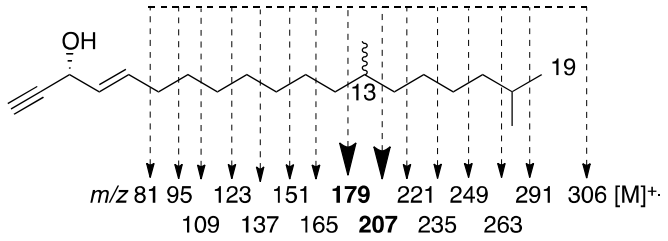
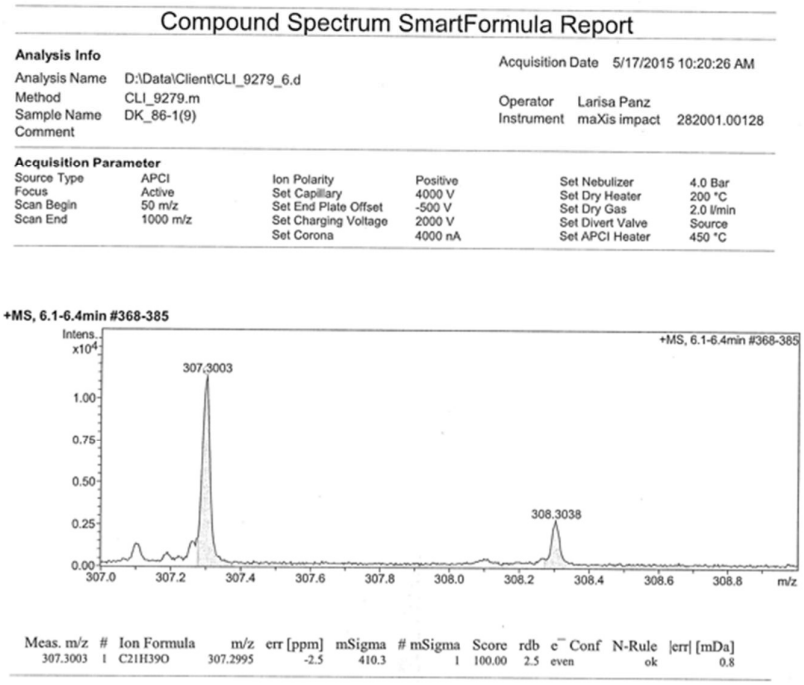


Figure S24. HRMS and fragmentation pattern of (3*R*)-13,18-dimethylnonadec-(4*E*)-en-1-yn-3-ol (**4**)



Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Client\CLI_9279_6.d	Acquisition Date	5/17/2015 10:20:26 AM
Method	CLI_9279.m		
Sample Name	DK_86-1(9)	Operator	Larisa Panz
Comment		Instrument	maXis impact 282001.00128

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 6.1-6.4min #368-385

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
307.3003	1	C21H39O	307.2995	-2.5	410.3	1	100.00	2.5	even	ok	0.8

Figure S25. ^{1}H NMR spectrum of (3*R*)-14-methylicos-(4*E*)-en-1-yn-3-ol (**5**) in $CDCl_3$.

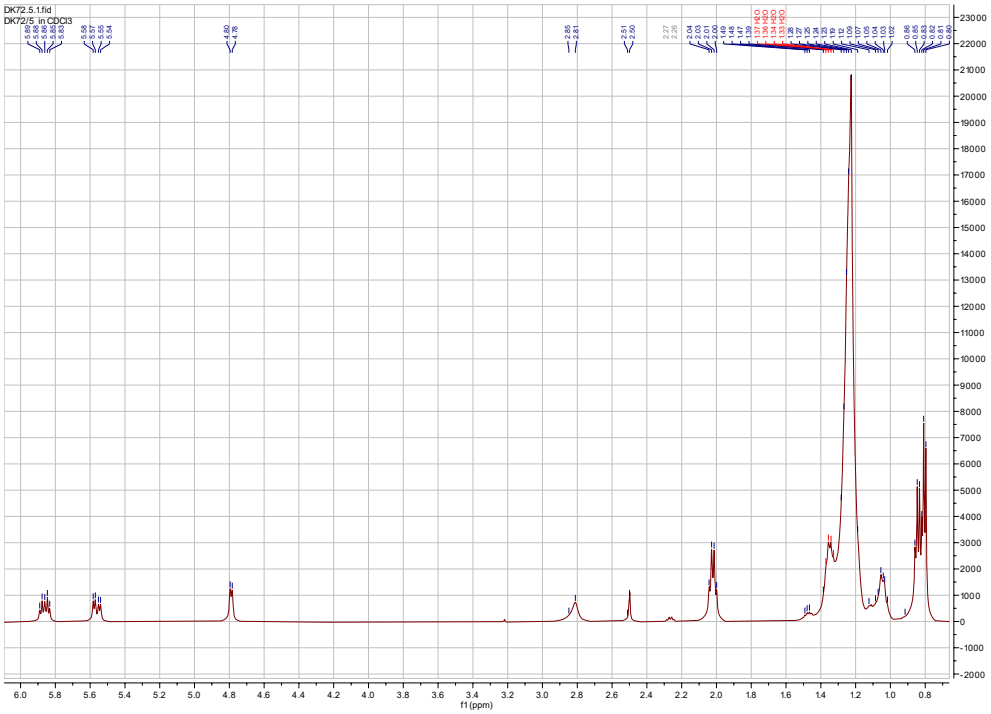


Figure S26. ^{13}C NMR spectrum of (3*R*)-14-methylicos-(4*E*)-en-1-yn-3-ol (**5**) in $CDCl_3$.

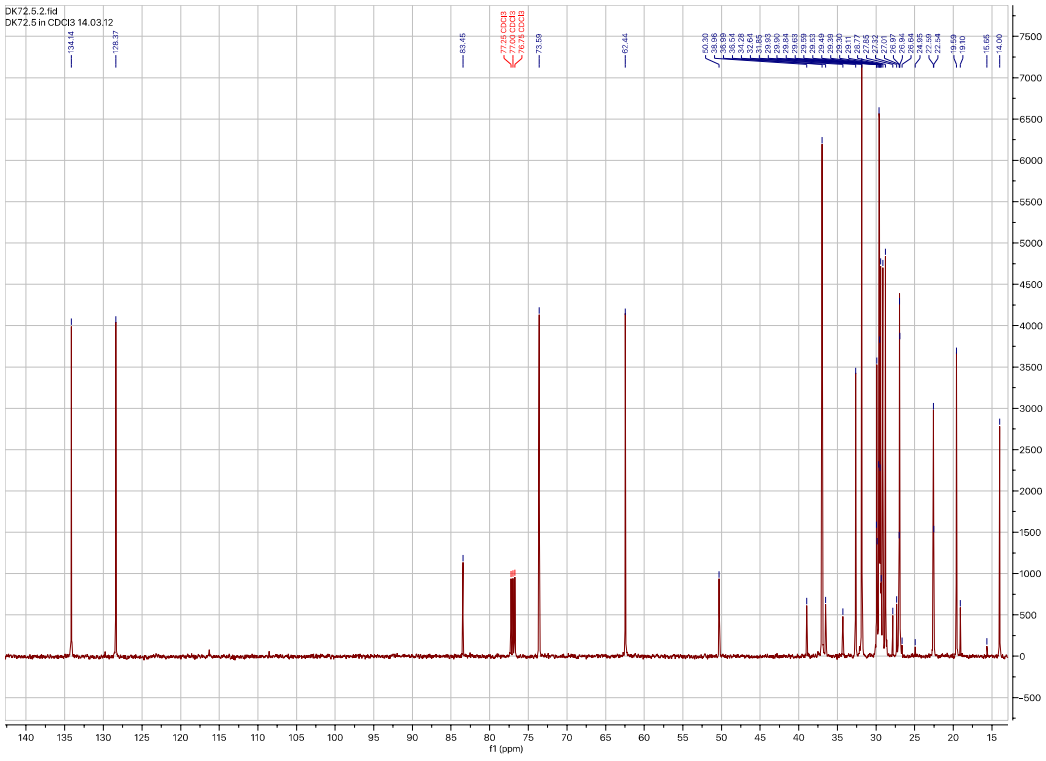


Figure S27. HSQC spectrum of (3*R*)-14-methylicos-(4*E*)-en-1-yn-3-ol (**5**) in $CDCl_3$.

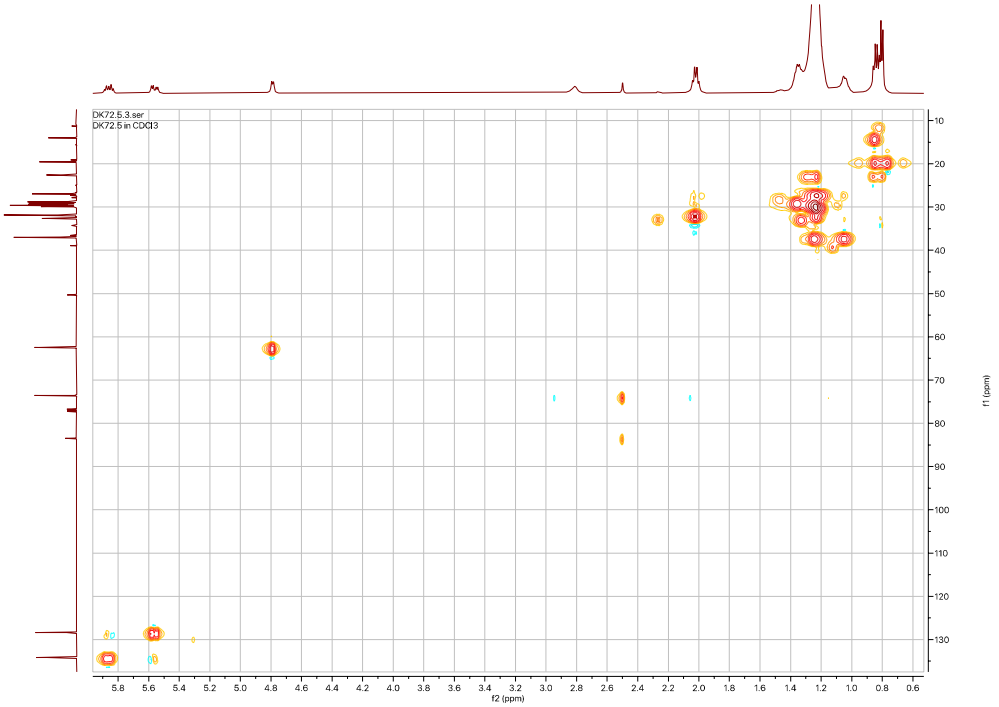


Figure S28. HMBC spectrum of (3*R*)-14-methylicos-(4*E*)-en-1-yn-3-ol (**5**) in $CDCl_3$.

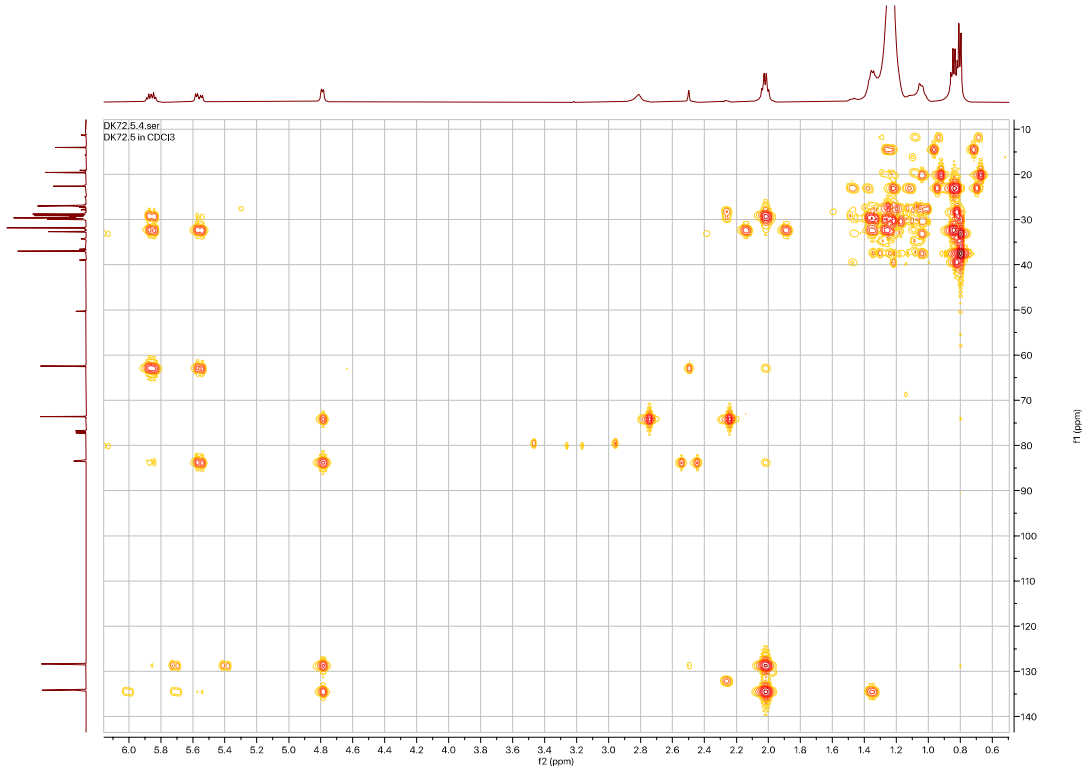


Figure S29. COSY spectrum of (3*R*)-14-methylicos-(4*E*)-en-1-yn-3-ol (**5**) in $CDCl_3$.

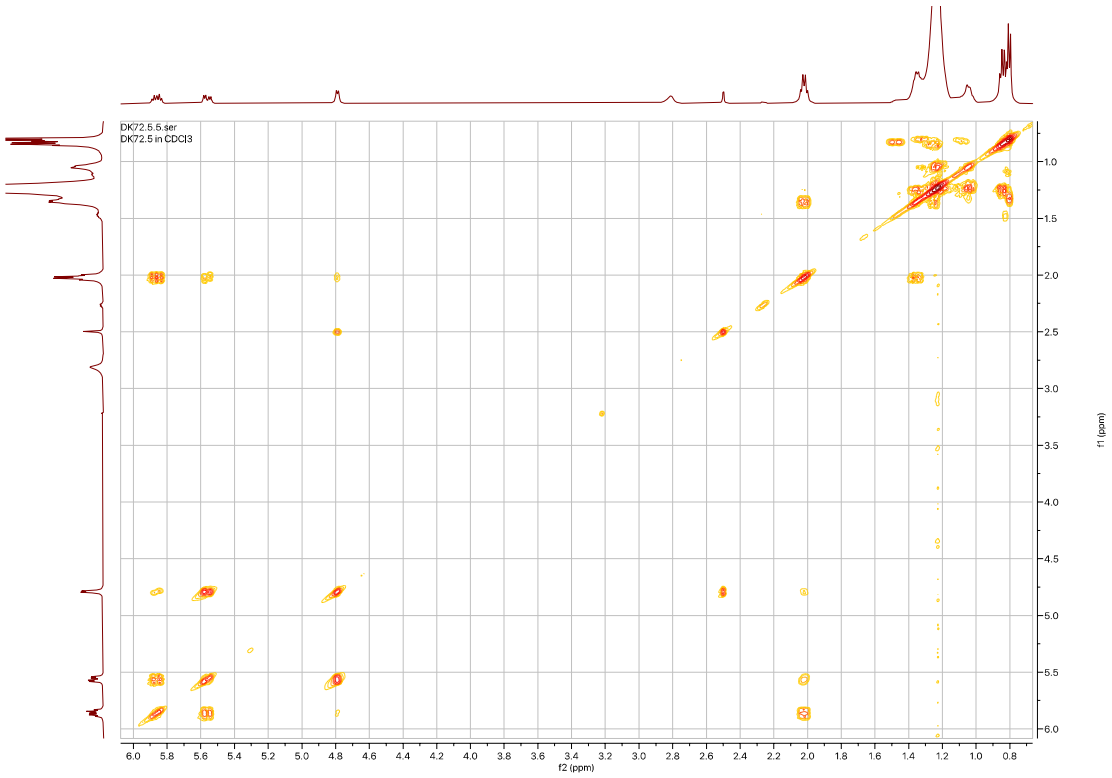
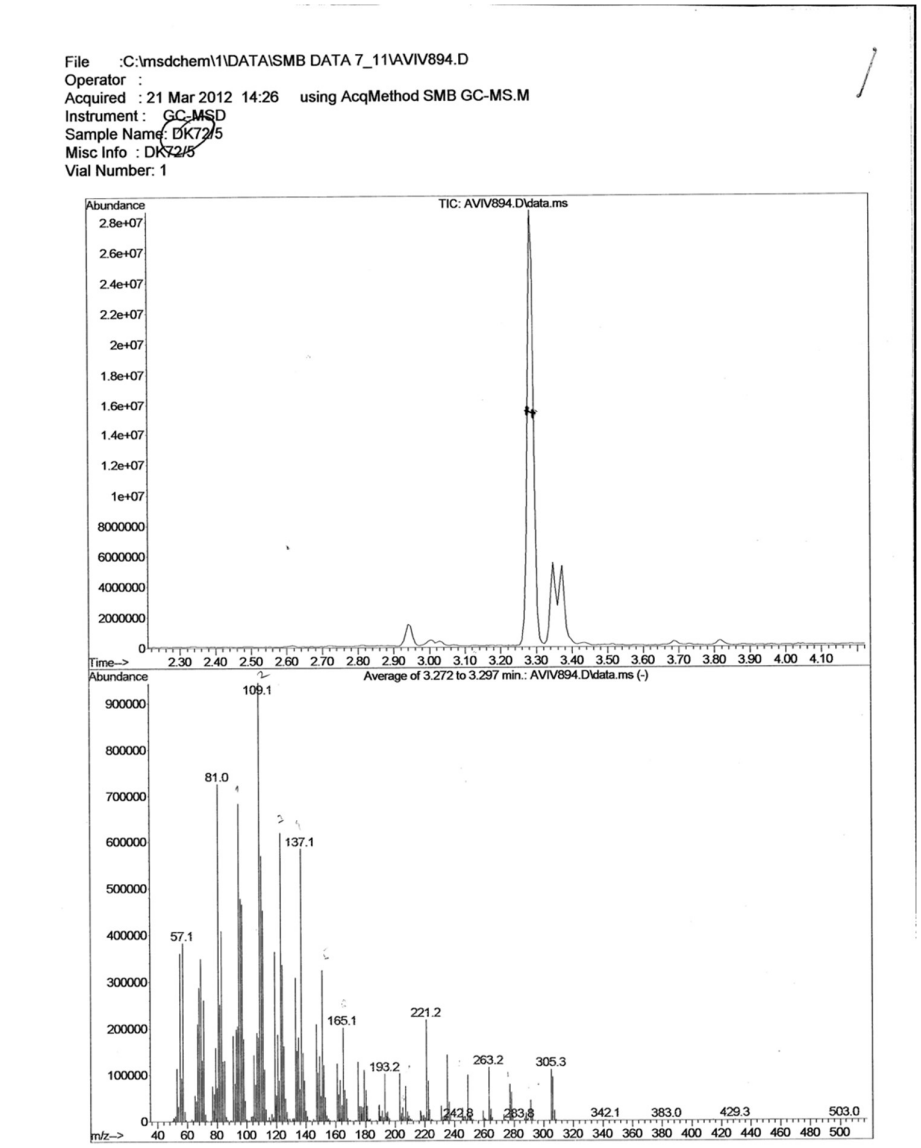


Table S5. NMR data of (3*R*)-14-methylicos-(4*E*)-en-1-yn-3-ol (**5**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.8[d] CH	2.50 d (2.1)	3
2	83.4[e] qC	-	1, 3, 4
3	62.6 CH	4.79 d (6.0)	1, 4, 5
4	128.4 CH	5.56 dd (15.0, 6.0)	3, 6
5	134.3 CH	5.85 dt (15.0, 6.8)	3, 6, 7
6	31.9 CH_2	2.02 q (6.8)	4, 5, 7, 8
7	28.8 CH_2	1.36 m	5, 6, 8
8-11	~29.6[f] 4 × CH_2	1.21 – 1.26 brm	
12	27.0 CH_2	1.23 m	11, 13a, 13b
13a	37.0 CH_2	1.25 m	12, 14, 15a, 15b, 21
b		1.08 m	
14	32.7 CH	1.34 m	13a, 13b, 15a, 15a, 21
15a	37.0 CH_2	1.25 m	13a, 13b, 14, 16, 21
b		1.08 m	
16	27.0 CH_2	1.23 m	15a, 15b, 17
17	~29.6[f] CH_2	1.21 – 1.26 brm	
18	31.9 CH_2	1.23 m	17, 19a, 19b, 20
19a	22.6 CH_2	1.29 m	18, 20
b		1.23 m	
20	14.0 CH_3	0.87 t (6.6)	19a, 19b
21	19.6 CH_3	0.83 d (6.6)	13b, 15b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 250.0 Hz; [e] ^2J = 48.8 Hz; [f]Exact ^{13}C chemical shifts 29.15, 29.43, 29.57, 29.63, 29.95 ppm.

Figure S30. EIMS and fragmentation pattern of (3*R*)-14-methylicos-(4*E*)-en-1-yn-3-ol (**5**).



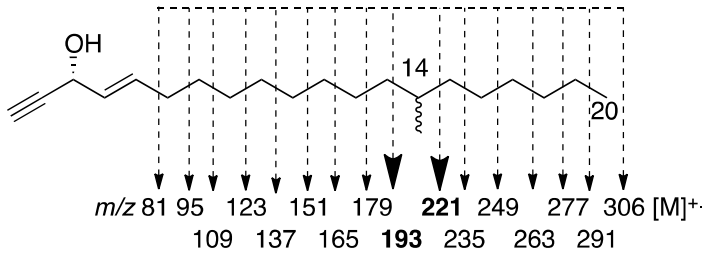


Figure S31. HRMS and fragmentation pattern of (3*R*)-14-methylicos-(4*E*)-en-1-yn-3-ol (**5**).

Compound Spectrum SmartFormula Report

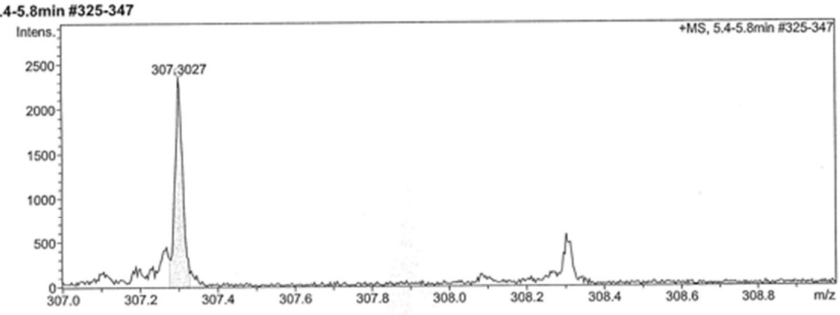
Analysis Info

Analysis Name	D:\Data\Client\CLI_9279_21000001.d	Acquisition Date	5/17/2015 1:19:29 PM
Method	GC APCI_pos_cli_8051.m	Operator	Larisa Panz
Sample Name	DK107.1(7)	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 5.4-5.8min #325-347



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
307.3027	1	C21H39O	307.2995	-10.1	175.1	1	100.00	2.5	even	ok	3.1

Figure S32. ^{1}H NMR spectrum of 14-methylicos-(4*E*)-en-1-yn-3-one (**6**) in $CDCl_3$.

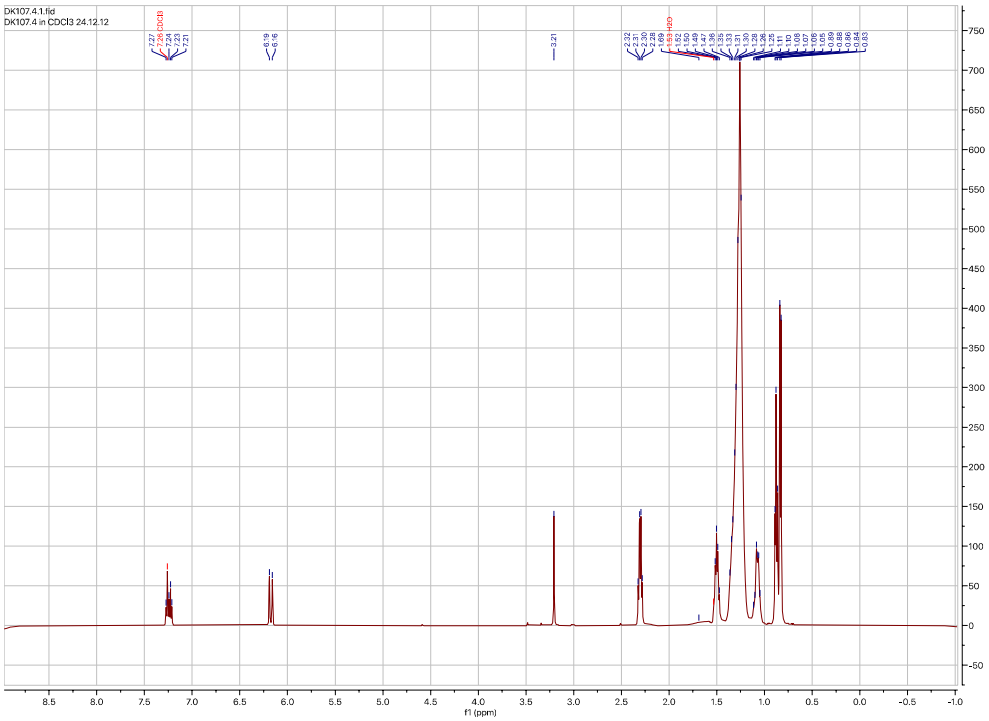


Figure S33. ^{13}C NMR spectrum of 14-methylicos-(4*E*)-en-1-yn-3-one (**6**) in $CDCl_3$.

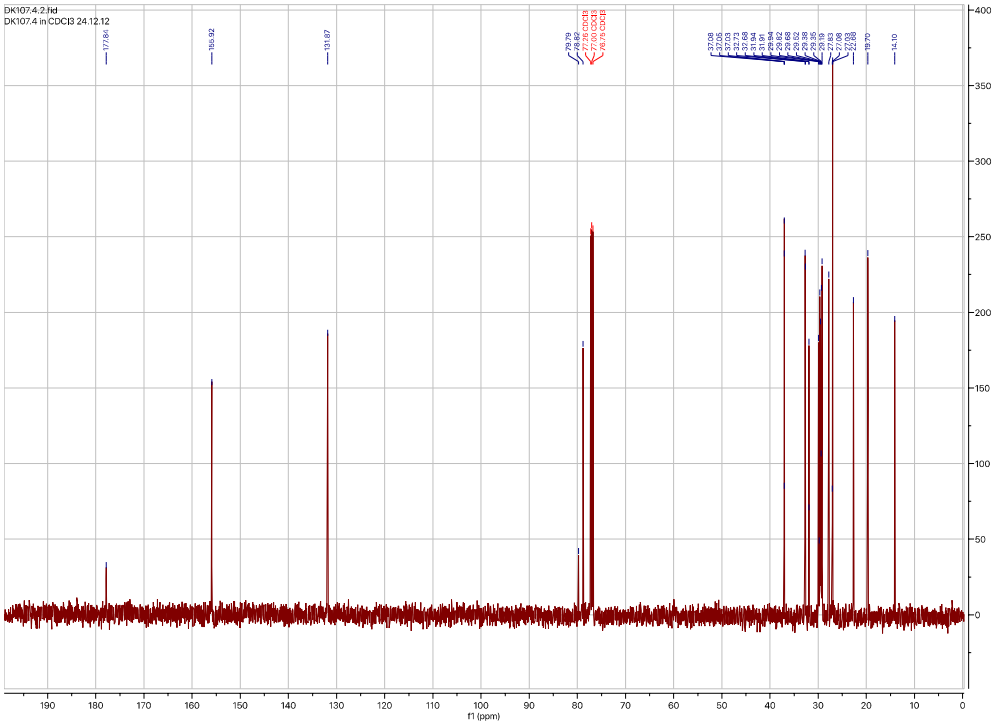
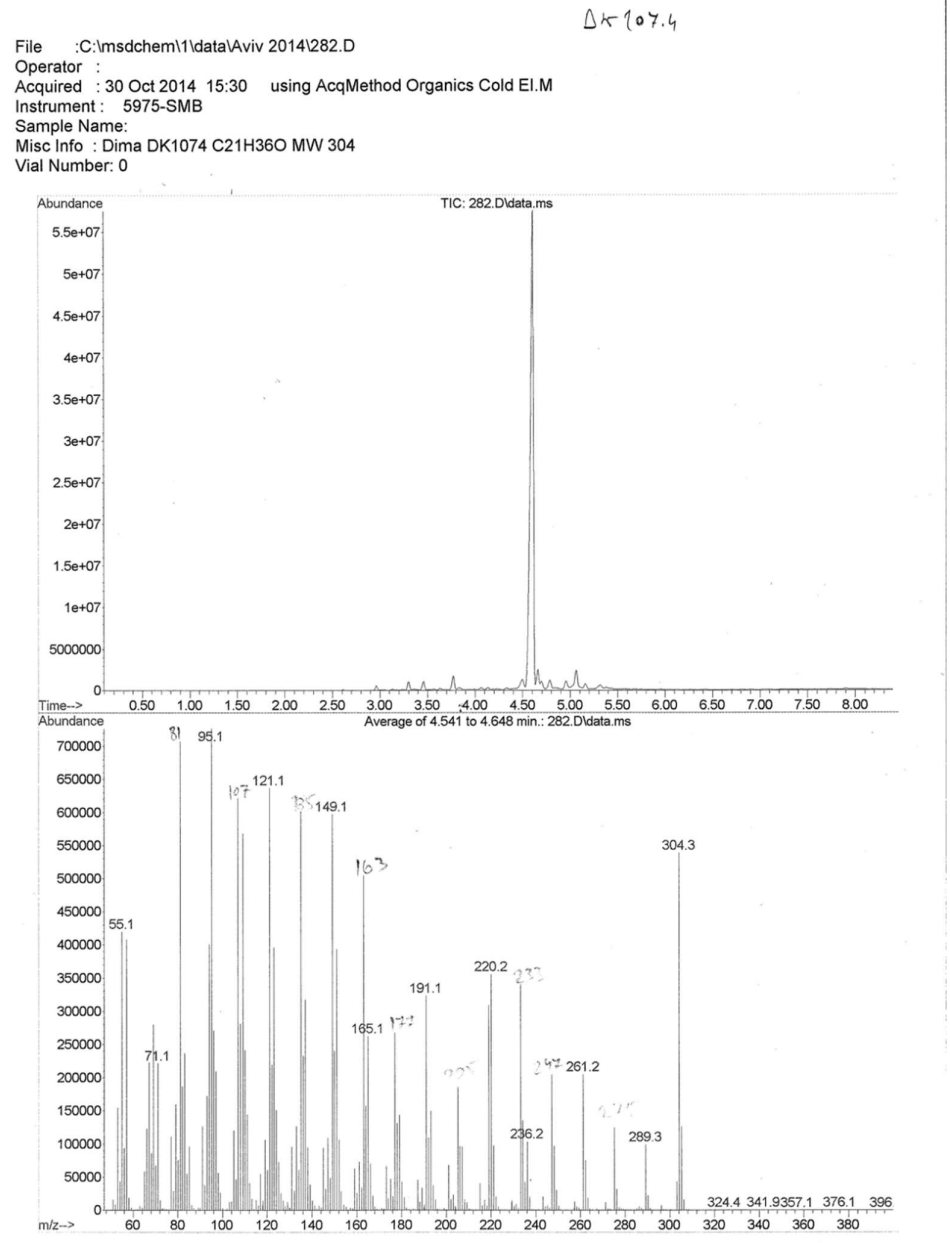


Table S6. NMR data of 14-methylicos-(4*E*)-en-1-yn-3-one (**6**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	78.8[d] CH	3.21 s	-
2	79.8[e] qC	-	1, 4
3	177.8 qC	-	1, 4, 5
4	131.9 CH	6.17 d (16.0)	6
5	155.9 CH	7.24 dt (16.0, 7.0)	6, 7
6	32.7 CH_2	2.30 q (7.0)	4, 5, 7, 8
7	27.8 CH_2	1.50 tt (7.0, 7.0)	5, 6, 8
8	29.2 CH_2	1.30 m	
9-11	~29.6[f] 3 × CH_2	1.23 – 1.31 brm	
12	27.0 CH_2	1.23 m	11, 13a, 13b
13a	37.1 CH_2	1.26 m	12, 14, 15a, 15b, 21
b		1.07 m	
14	32.7 CH	1.37 m	13a, 13b, 15a, 15a, 21
15a	37.1 CH_2	1.26 m	13a, 13b, 14, 16, 21
b		1.07 m	
16	27.0 CH_2	1.25 m	15a, 15b, 17
17	29.9 CH_2	1.26 m	
18	31.9 CH_2	1.25 m	17, 19a, 19b, 20
19a	22.7 CH_2	1.31 m	18, 20
b		1.25 m	
20	14.1 CH_3	0.88 t (6.5)	19a, 19b
21	19.7 CH_3	0.83 d (6.5)	13b, 15b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 253.5 Hz; [e] ^2J = 48.0 Hz; [f]Exact ^{13}C chemical shifts 29.34, 29.51, 29.67ppm.

Figure S34. EIMS and fragmentation pattern of 14-methylicos-(4*E*)-en-1-yn-3-one (**6**)



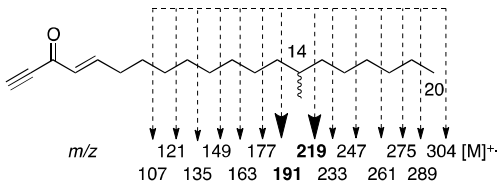


Figure S35. HRCIMS and fragmentation pattern of 14-methylicos-(4*E*)-en-1-yn-3-one (**6**)

Compound Spectrum SmartFormula Report

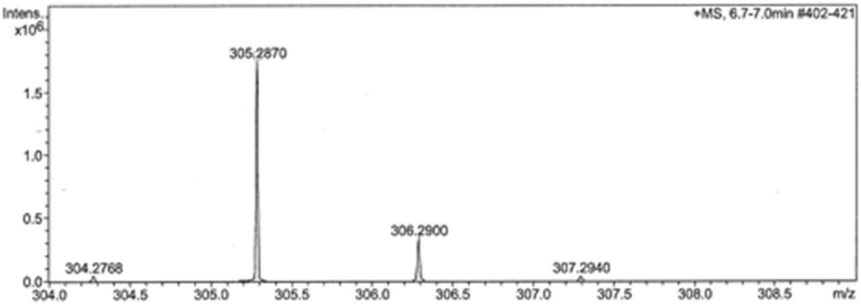
Analysis Info

Analysis Name	D:\Data\Client\CLI_9279_9.d	Acquisition Date	5/17/2015 11:06:37 AM
Method	CLI_9279.m		
Sample Name	DK_107.4(20)	Operator	Larisa Panz
Comment		Instrument	maXis impact 282001.00128

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 6.7-7.0min #402-421



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
305.2870	1	C14H37N6O	305.3023	50.2	10.0	1	0.00	-0.5	even	ok	15.3
	2	C21H37O	305.2839	-10.2	22.2	2	100.00	3.5	even	ok	3.1

CLI_9279_9.d
Bruker Compass DataAnalysis 4.2 printed: 5/17/2015 11:16:57 AM by: Larisa Panz Page 1 of 1

Figure S36. ^{1}H NMR spectrum of (3*R*)-14-methylicos-1-yn-3-ol (**7**) in $CDCl_3$

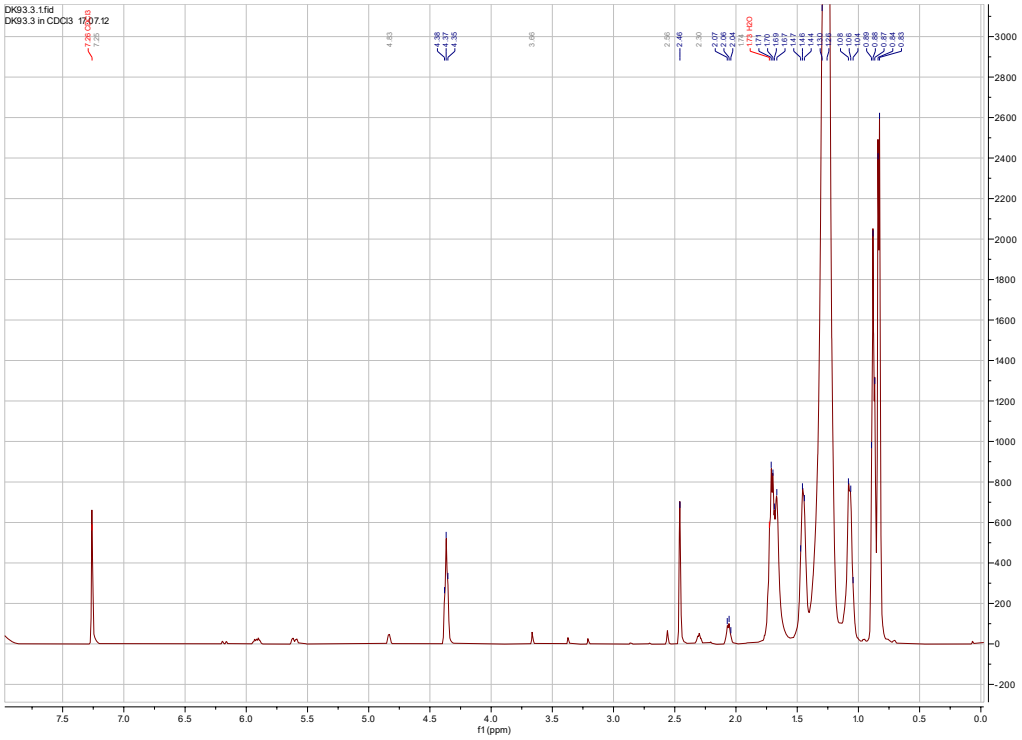


Figure S35. ^{13}C NMR spectrum of (3*R*)-14-methylicos-1-yn-3-ol (**7**) in $CDCl_3$

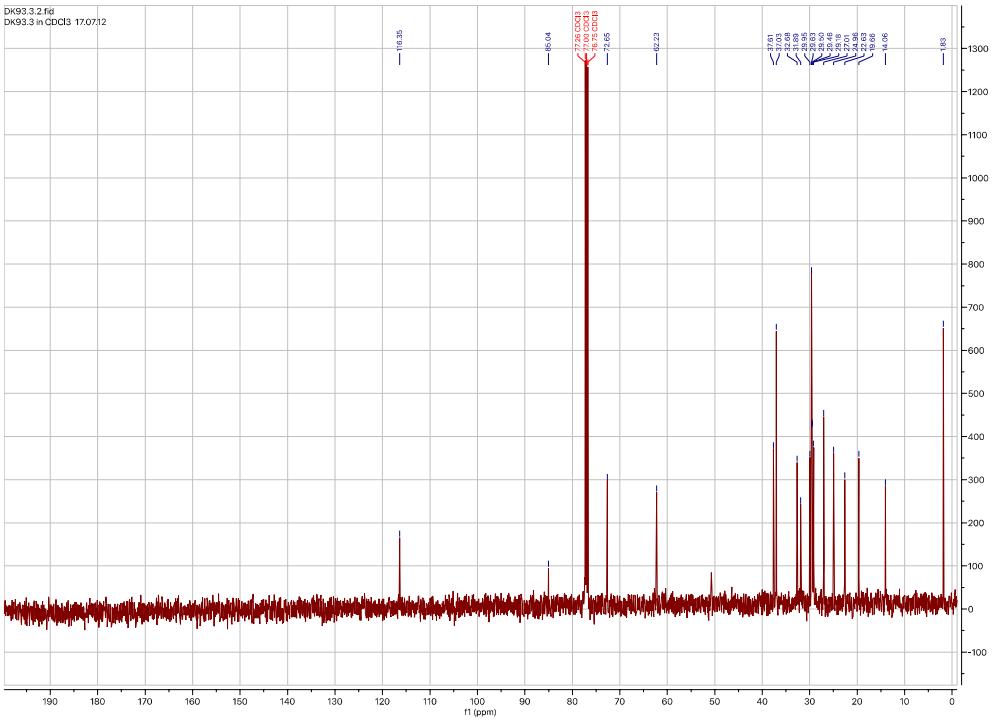


Figure S38. HSQC spectrum of (3*R*)-14-methylicos-1-yn-3-ol (**7**) in $CDCl_3$

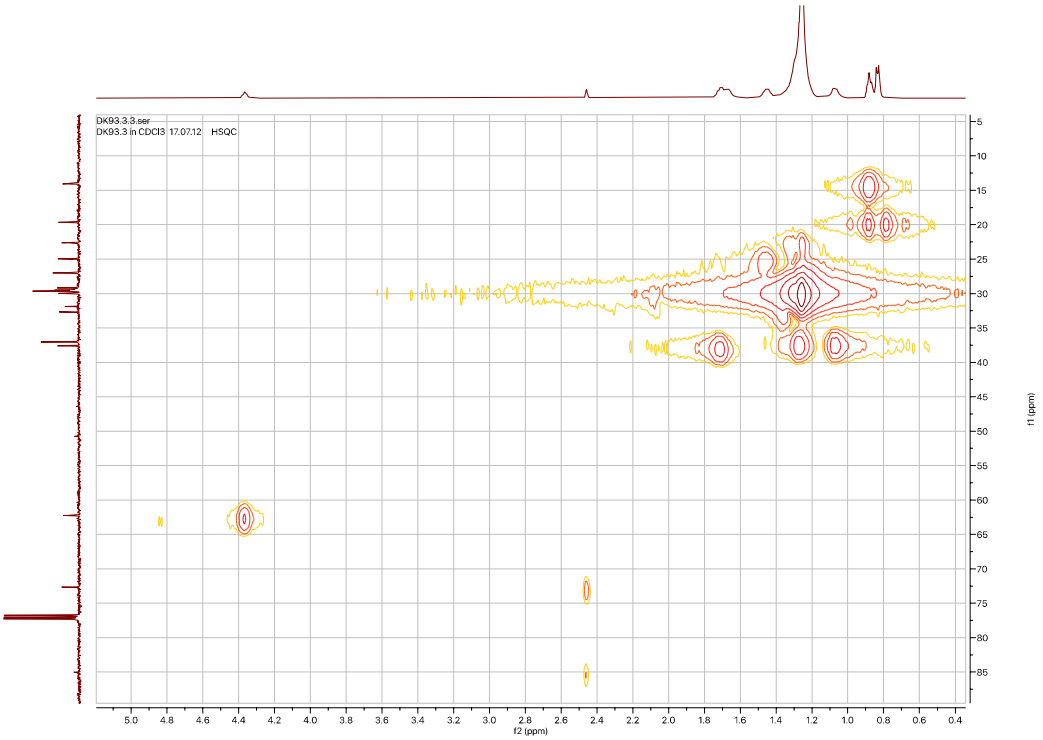


Figure S39. HMBC spectrum of (3*R*)-14-methylicos-1-yn-3-ol (**7**) in $CDCl_3$

Figure S40. COSY spectrum of (3*R*)-14-methylicos-1-yn-3-ol (**7**) in $CDCl_3$

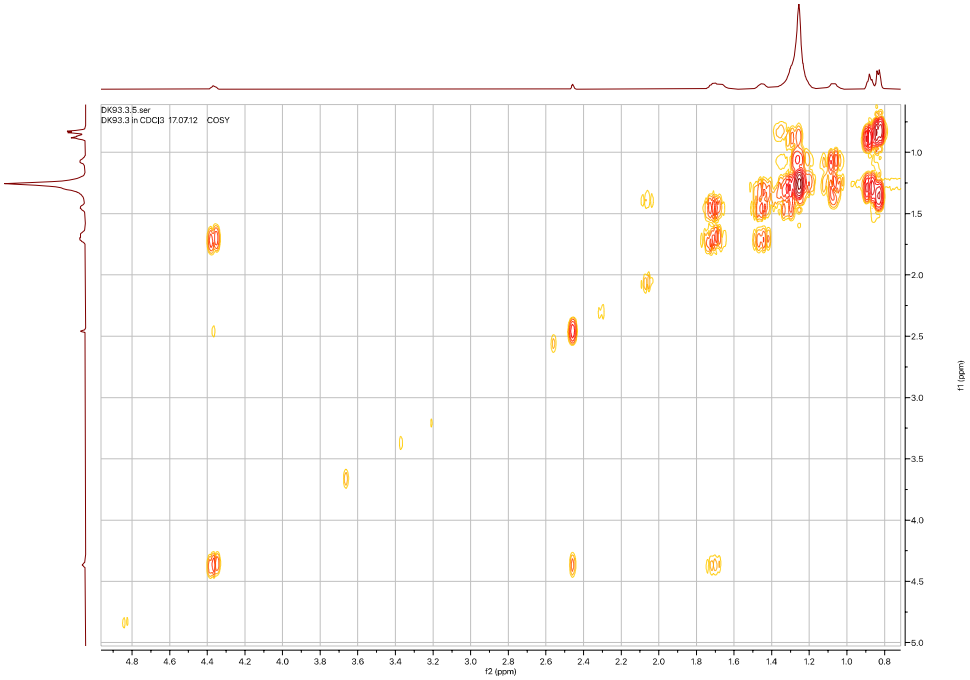


Figure S41. DEPT spectrum of (3*R*)-14-methylicos-1-yn-3-ol (**7**) in $CDCl_3$

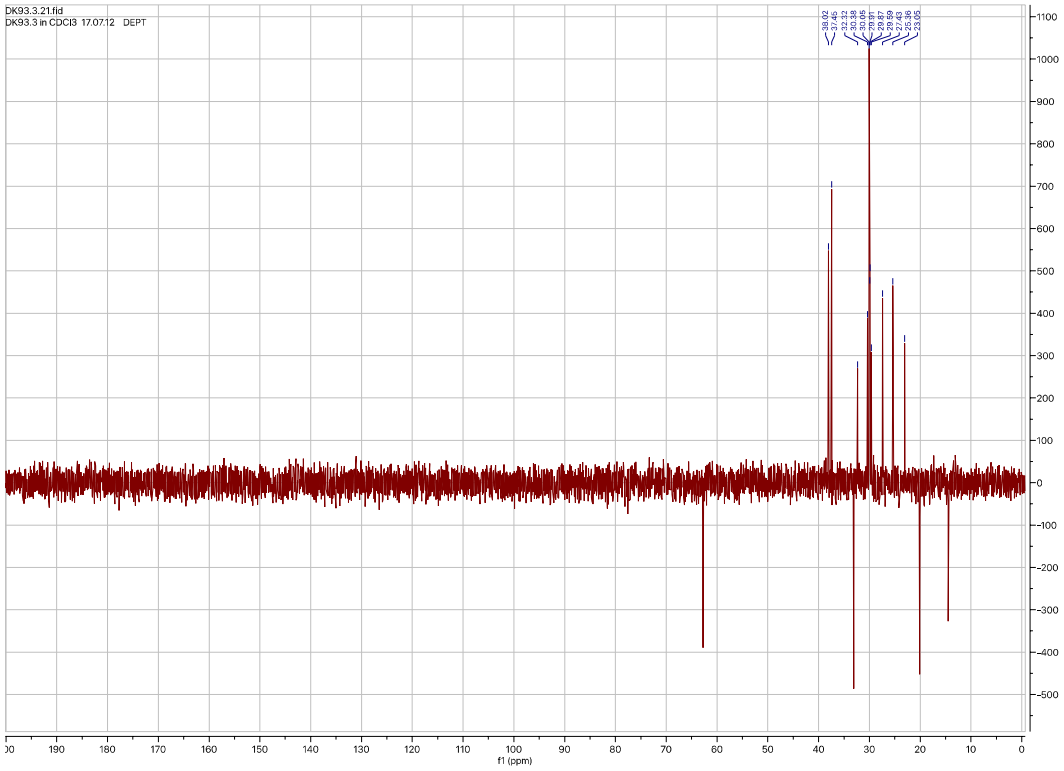
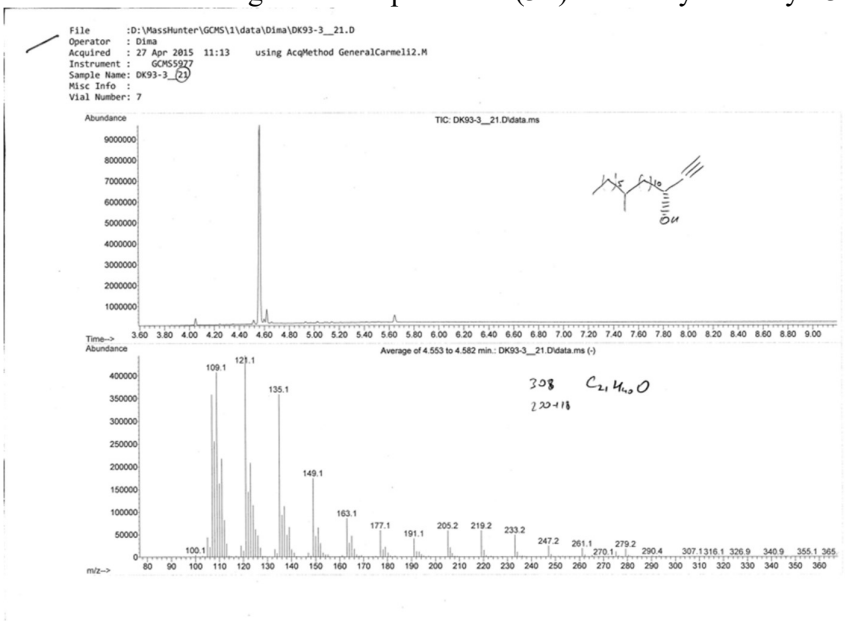


Table S7. NMR data of (3*R*)-14-methylicos-1-yn-3-ol (**7**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	72.6[d] CH	2.46 d (2.0)	3
2	85.0[e] qC	-	1, 3, 4
3	62.2 CH	4.36 td (6.5, 2.0)	1, 4
4	37.6 CH_2	1.71 m	3, 6
5	25.0 CH_2	1.45 m	3, 4, 6, 7
6	29.2 CH_2	1.26 m	4, 5
7-11	~29.5[f] 5 × CH_2	1.22 – 1.31 brm	
12	27.0 CH_2	1.23 m	11, 13a, 13b
13a	37.0 CH_2	1.25 m	12, 14, 15a, 15b, 21
b		1.07 m	
14	32.6 CH	1.34 m	13a, 13b, 15a, 15a, 21
15a	37.0 CH_2	1.25 m	13a, 13b, 14, 16, 21
b		1.07 m	
16	27.0 CH_2	1.23 m	15a, 15b, 17
17	30.0 CH_2	1.24 m	
18	31.9 CH_2	1.23 m	17, 19a, 19b, 20
19a	22.6 CH_2	1.29 m	18, 20
b		1.23 m	
20	14.1 CH_3	0.87 t (7.0)	19a, 19b
21	19.6 CH_3	0.83 d (7.0)	13b, 15b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 251.0 Hz; [e] ^2J = 46.0 Hz; [f]Exact ^{13}C chemical shifts 29.46, 29.50, 29.58, 29.63 (× 2) ppm.

Figure S42. EIMS and fragmentation pattern of (3*R*)-14-methylicos-1-yn-3-ol (**7**)



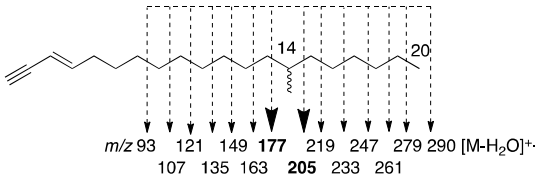


Figure S43. HRMS and fragmentation pattern of (3*R*)-14-methylicos-1-yn-3-ol (**7**)

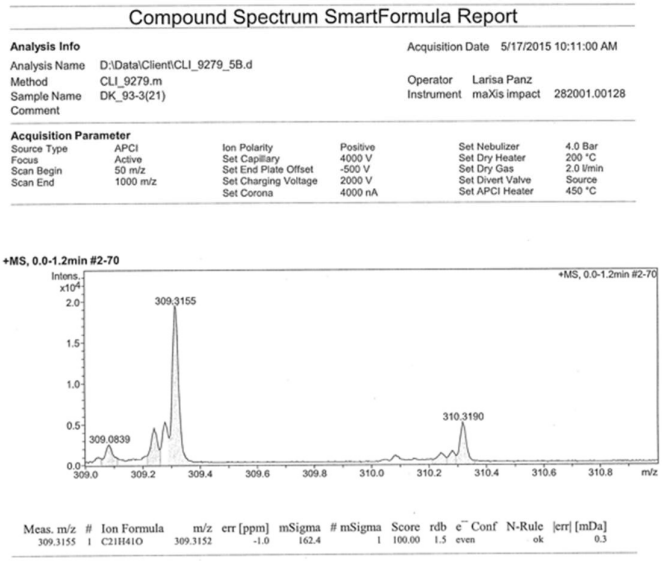


Figure S44. ^{1}H NMR spectrum of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**) in $CDCl_3$.

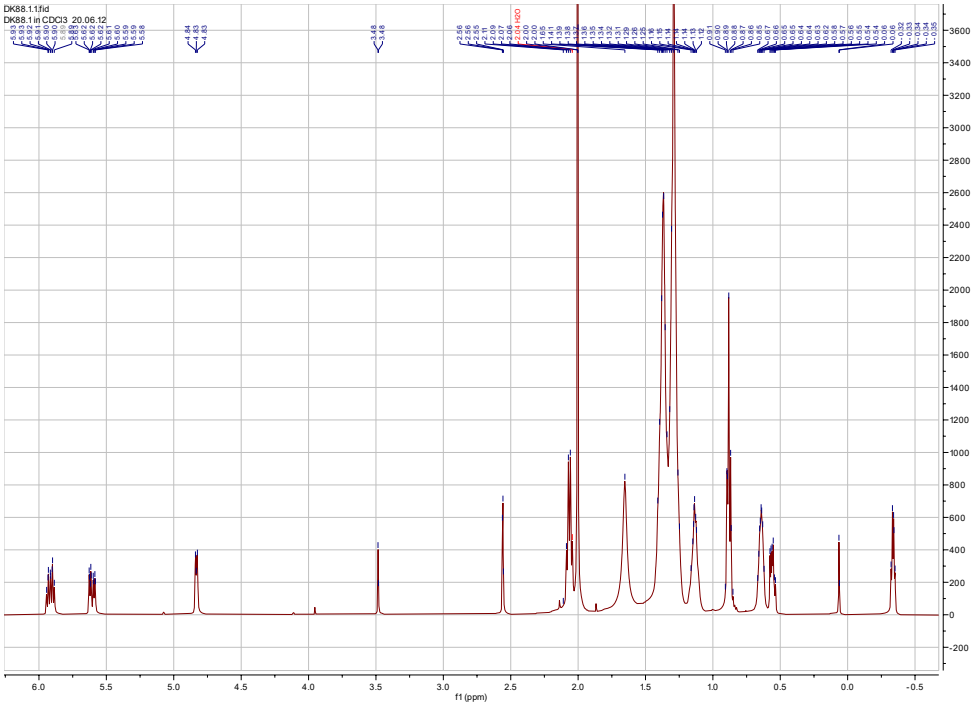


Figure S45. ^{13}C NMR spectrum of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**) in $CDCl_3$.

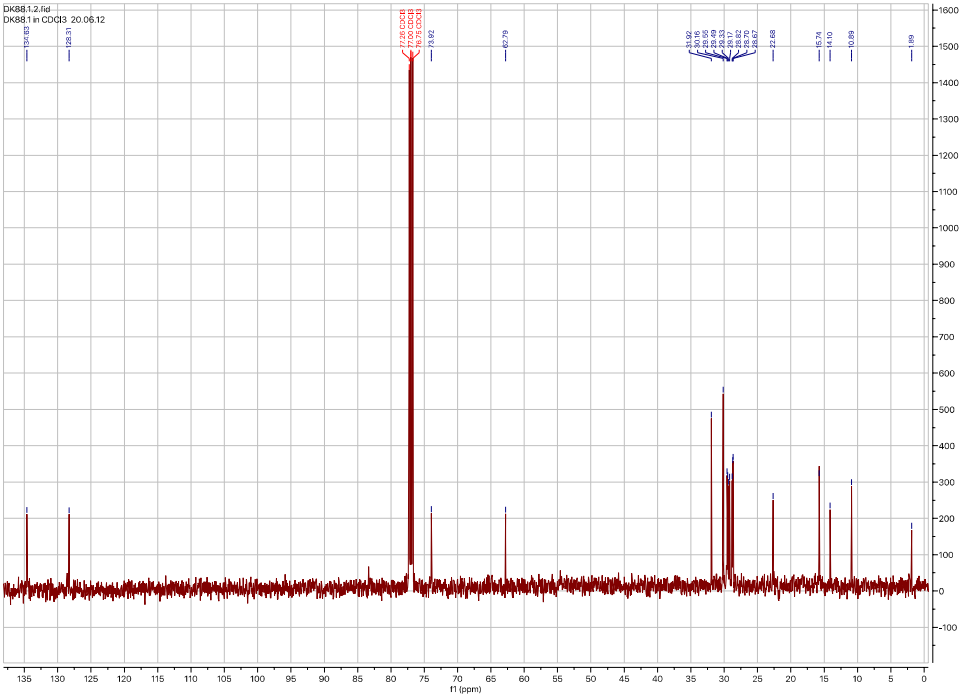


Figure S46. HSQC spectrum of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**) in $CDCl_3$.

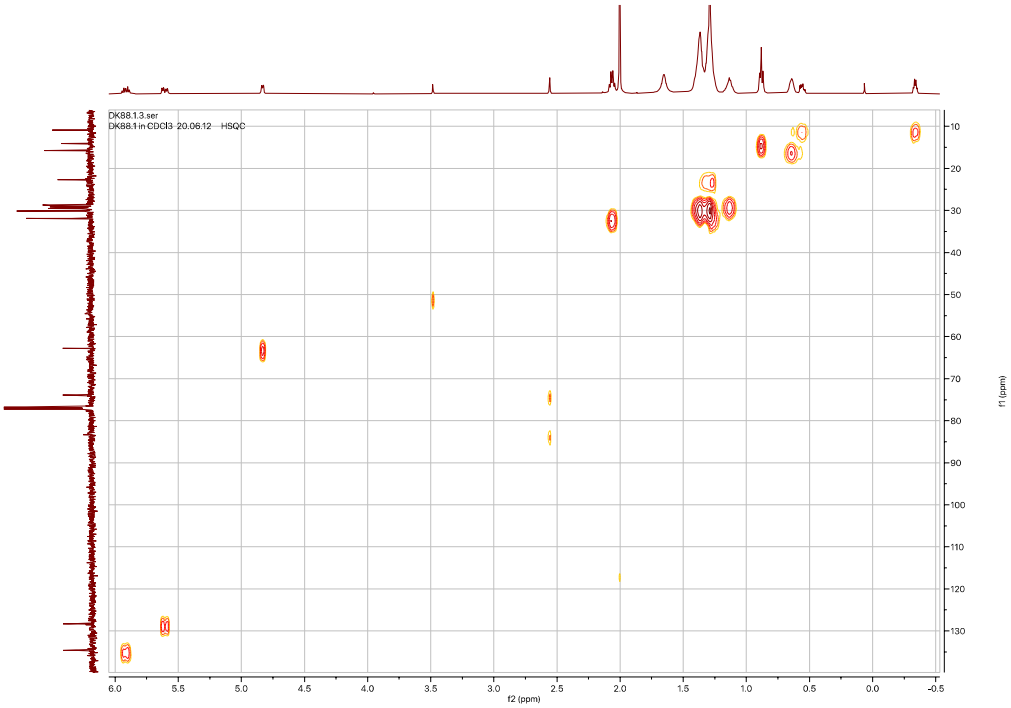


Figure S47. HMBC spectrum of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**) in $CDCl_3$.

Figure S48. COSY spectrum of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**) in $CDCl_3$.

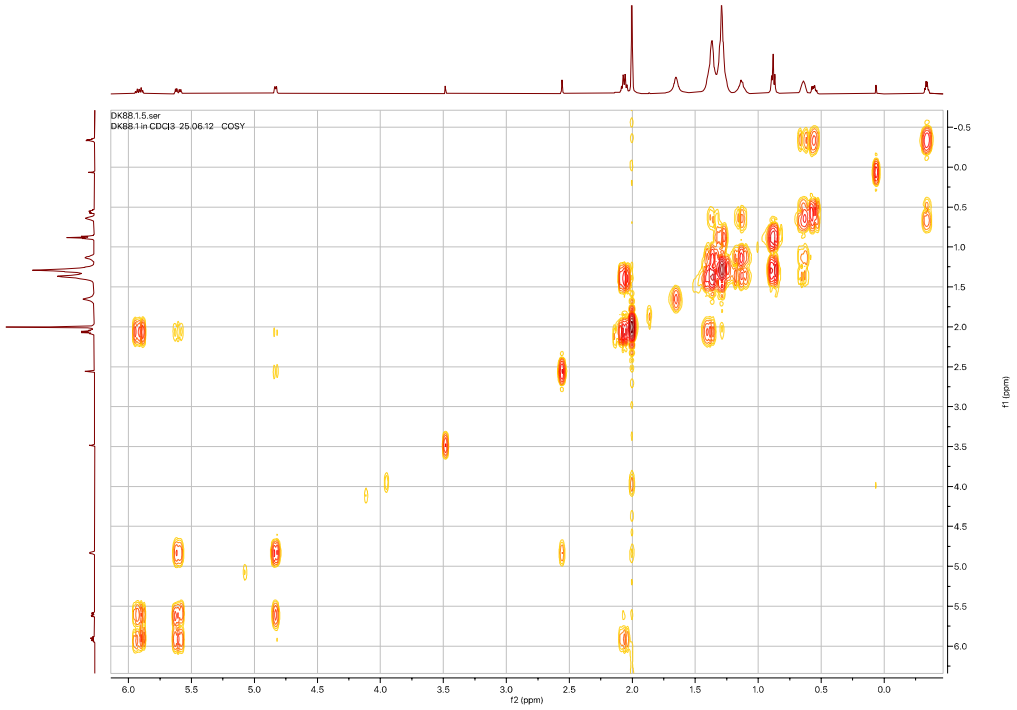


Figure S49. DEPT spectrum of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**) in $CDCl_3$.

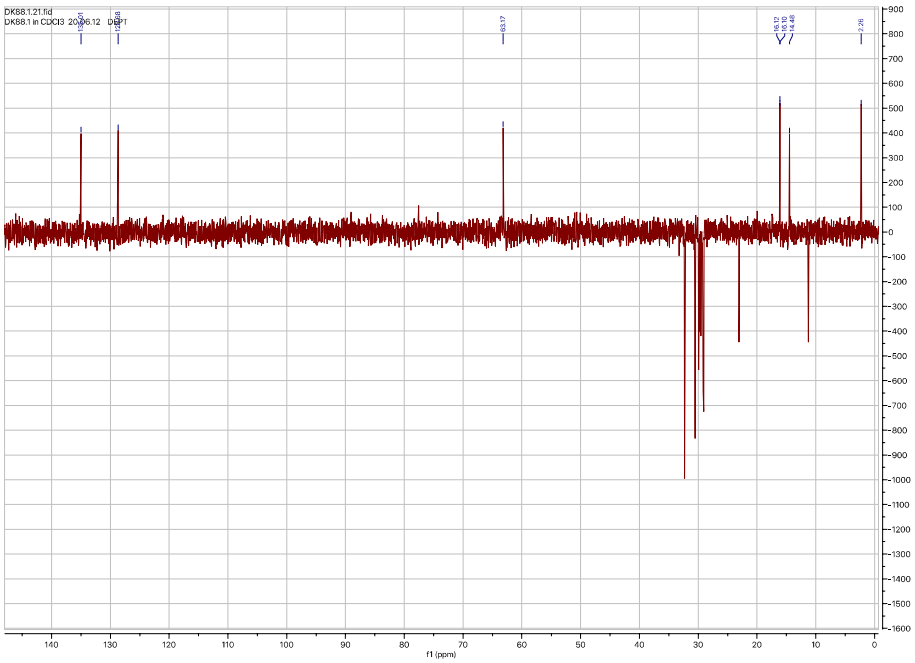


Table S8. NMR data of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.9[d] CH	2.56 d (2.1)	3
2	83.3[e] qC	-	1, 3, 4
3	62.8 CH	4.83 brd (5.7)	1, 4
4	128.3 CH	5.60 dd (15.2, 5.7)	3, 6
5	134.6 CH	5.91 dt (15.2, 7.0)	3, 4, 6, 7
6	31.9 CH_2	2.06 q (7.0)	4, 5, 7, 8
7	28.8 CH_2	1.36 m	5, 6, 8
8-10	~29.6[f] 3 × CH_2	1.24 – 1.32 brm	
11	30.2 CH_2	1.35 m	10, 12a, 12b,
12a	28.7 CH_2	1.35 m	11, 13a, 13b
b		1.13 m	
13	15.7 CH	0.64 m	11, 12a, 12b, 14, 15a, 15b, 21a, 21b
14	15.7 CH	0.64 m	11, 12a, 12b, 14, 15a, 15b, 21a, 21b
15a	28.7 CH_2	1.35 m	13a, 13b, 14, 16, 21a, 21b
b		1.13 m	
16	30.2 CH_2	1.35 m	15a, 15b, 17
17	~29.6[f] CH_2	1.24 – 1.32 brm	
18	31.9 CH_2	1.26 m	17, 19
19	22.7 CH_2	1.31 m	18, 20
20	14.1 CH_3	0.88 t (6.8)	18, 19
21a	10.9 CH_2	-0.55 td (8.2, 4.0)	11, 12a, 12b, 13, 14, 15a, 15b, 16
b		-0.33 td (4.9, 4.0)	

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 251.3 Hz; [e] ^2J = 48.9 Hz; [f]Exact ^{13}C chemical shifts 29.17, 29.33, 29.49, 29.55 ppm.

Figure S50. Measured and calculated ^{13}C NMR data of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**)

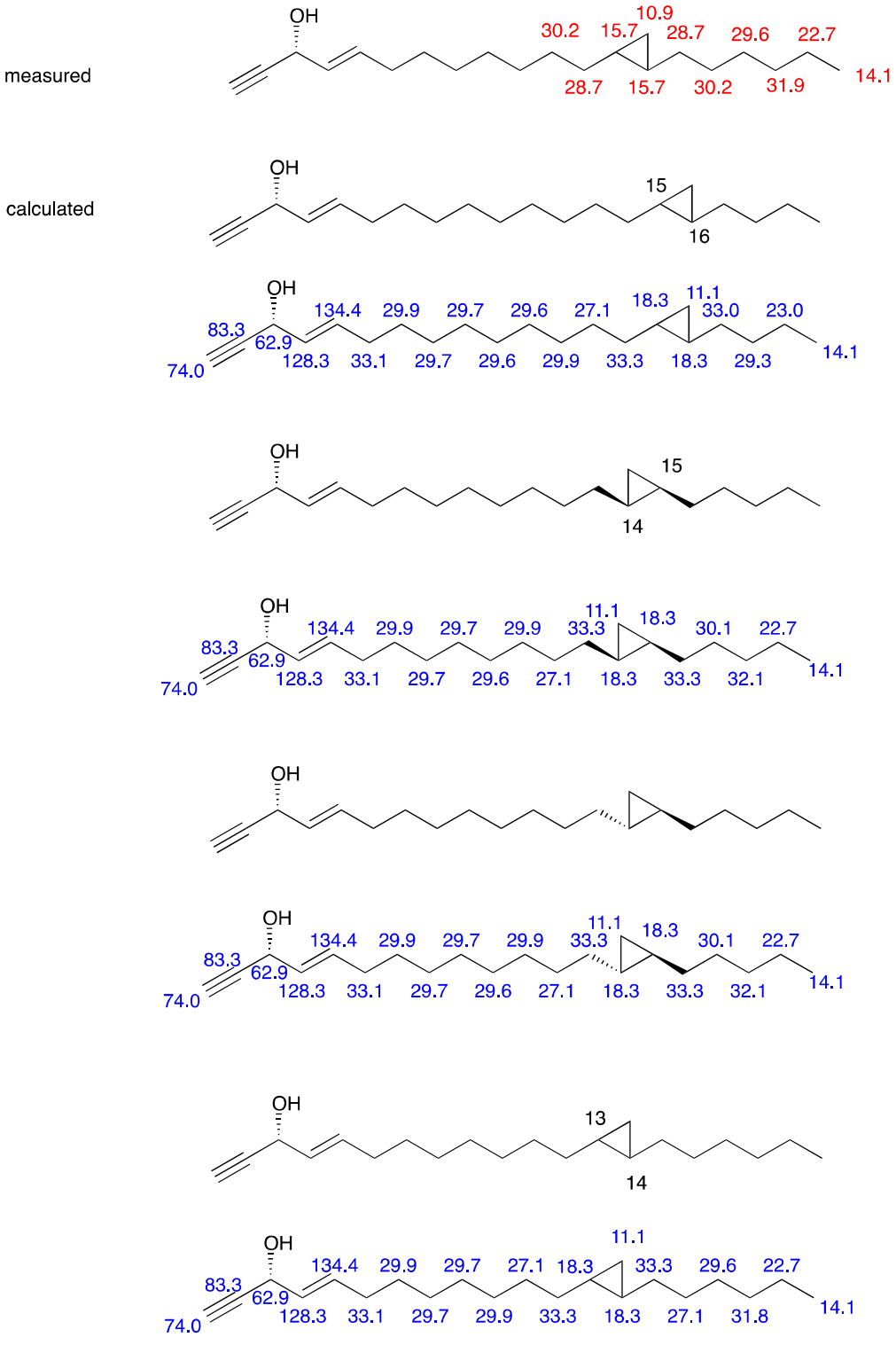


Figure S51. EIMS of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**).

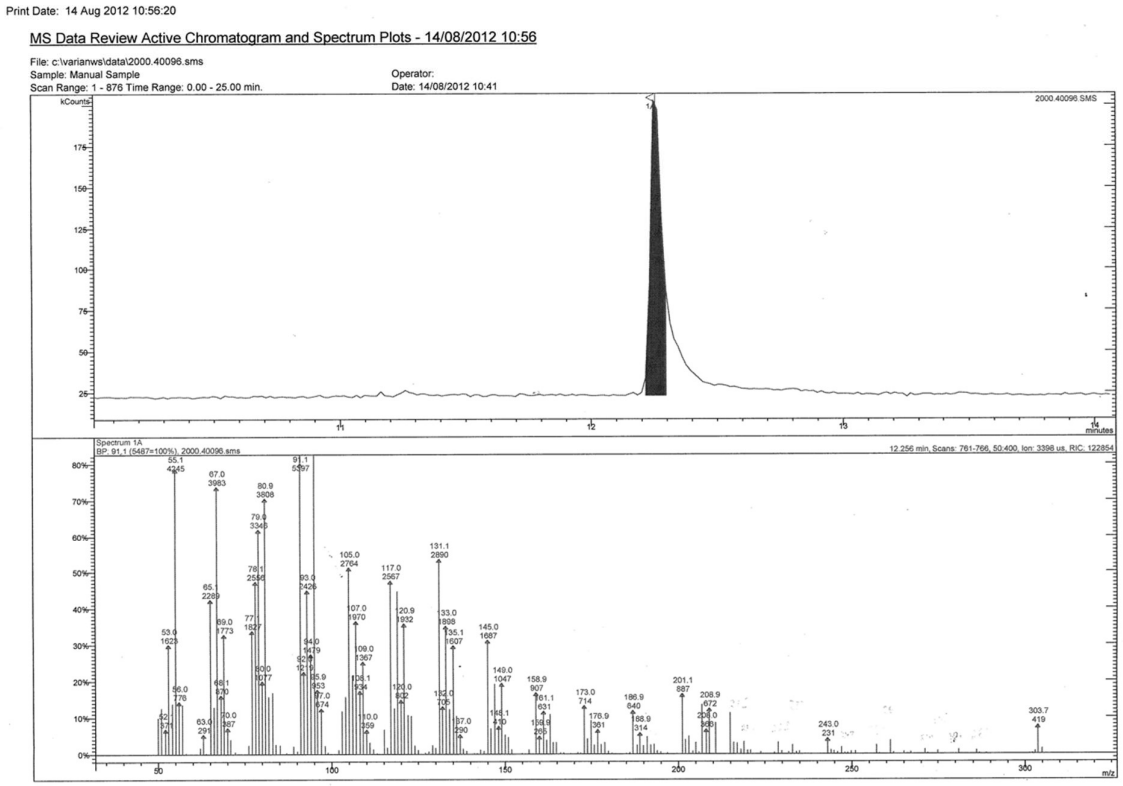


Figure S52. HRMS of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**).

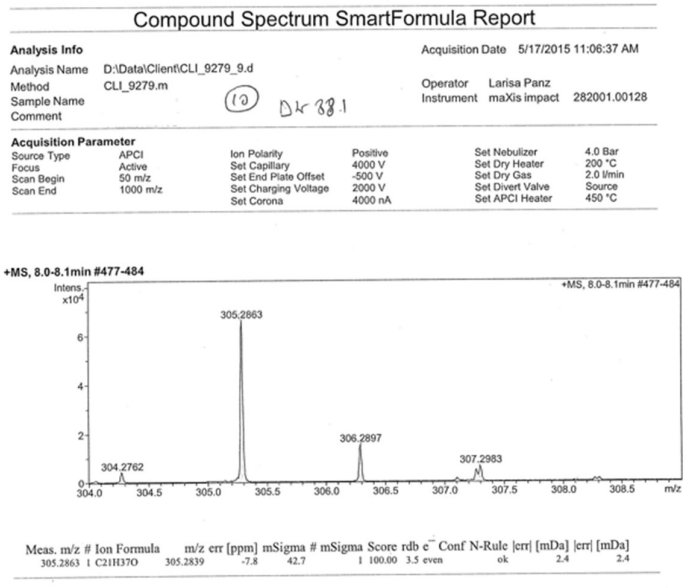


Figure S53a. Proposed fragmentation pattern of the EIMS parent ion of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**).

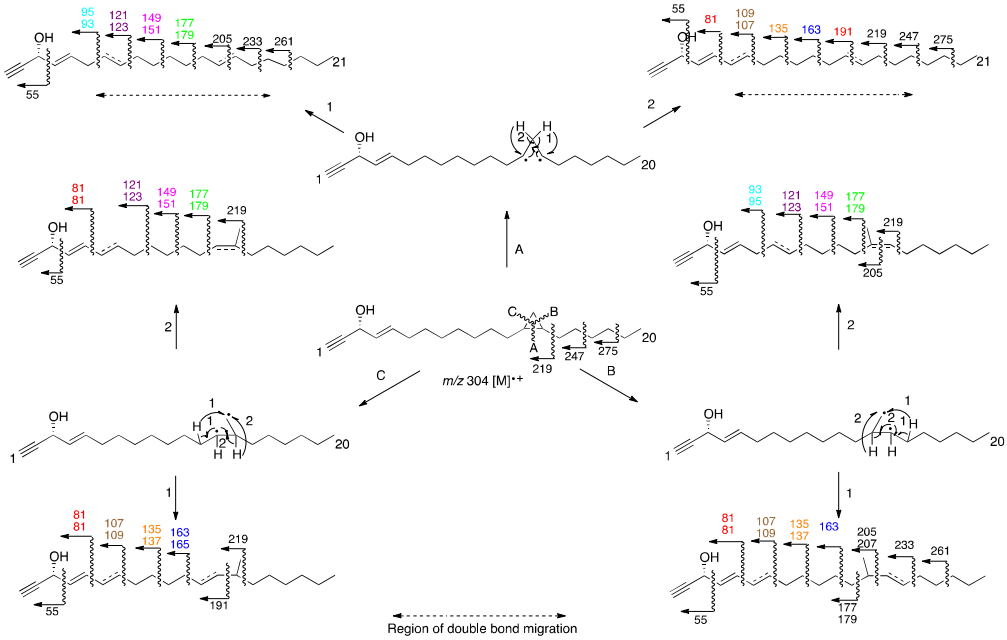


Figure S53b. Proposed fragmentation pattern of the EIMS water elimination product ion of (3*R*,*E*)-12-*cis*-(2-hexylcyclopropyl)dodec-4-en-1-yn-3-ol (**8**).

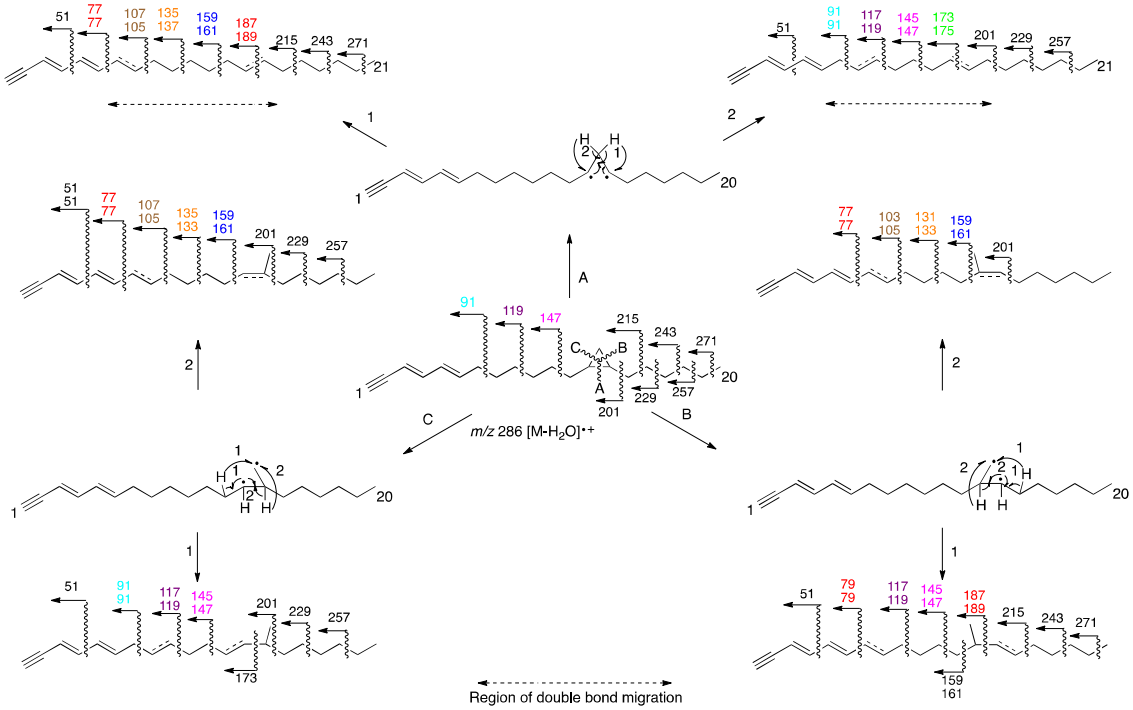


Figure S54. ^{1}H NMR spectrum of (3*R*)-13-methylhenicos-(4*E*)-en-1-yn-3-ol (**9**) in $CDCl_3$

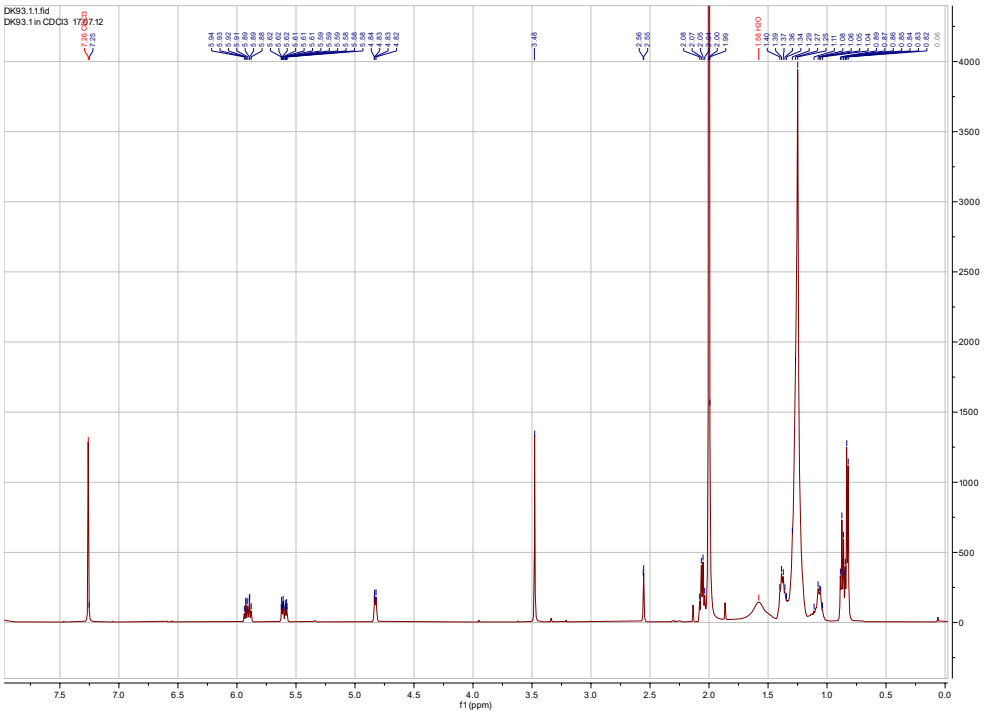


Figure S55. ^{13}C NMR spectrum of (3*R*)-13-methylhenicos-(4*E*)-en-1-yn-3-ol (**9**) in $CDCl_3$

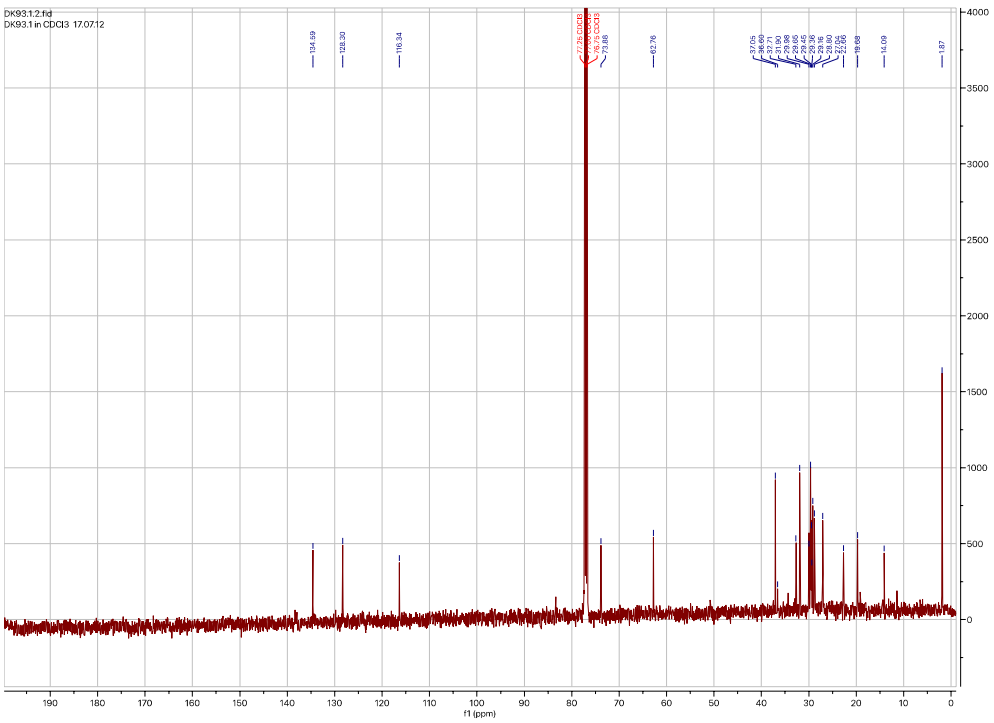


Table S9. NMR data of (3*R*)-13-methylhenicos-(4*E*)-en-1-yn-3-ol (**9**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.9[d] CH	2.55 d (2.5)	3
2	83.3[e] qC	-	1, 3, 4
3	62.8 CH	4.82 brd (6.0)	1, 4, 5
4	128.3 CH	5.60 dd (16.0, 6.0)	6
5	134.6 CH	5.91 dt (16.0, 7.5)	3, 6, 7
6	31.9 CH_2	2.05 q (7.5)	4, 5, 7, 8
7	28.8 CH_2	1.36 m	5, 6, 8
8-11	~29.6[f] 4 × CH_2	1.21 – 1.30 brm	
12	27.0 CH_2	1.23 m	11, 13a, 13b
13a	37.1 CH_2	1.25 m	12, 14, 15a, 15b, 21
b		1.07 m	
14	32.7 CH	1.37 m	13a, 13b, 15a, 15a, 22
15a	37.1 CH_2	1.25 m	13a, 13b, 14, 16, 22
b		1.07 m	
16	27.0 CH_2	1.23 m	15a, 15b, 17
17-18	~29.6[f] 2 × CH_2	1.21 – 1.30 brm	
19	31.9 CH_2	1.23 m	18, 20a, 20b, 21
20a	22.7 CH_2	1.29 m	19, 21
b		1.23 m	
21	14.1 CH_3	0.87 t (6.5)	19a, 19b
22	19.7 CH_3	0.83 d (6.5)	13b, 15b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 250.5 Hz; [e] ^2J = 48.8 Hz; [f]Exact ^{13}C chemical shifts 29.16, 29.44, 29.66 (× 3), 29.96 ppm.

Figure S56. EIMS and fragmentation pattern of (3*R*)-13-methylhenicos-(4*E*)-en-1-yn-3-ol (**9**)

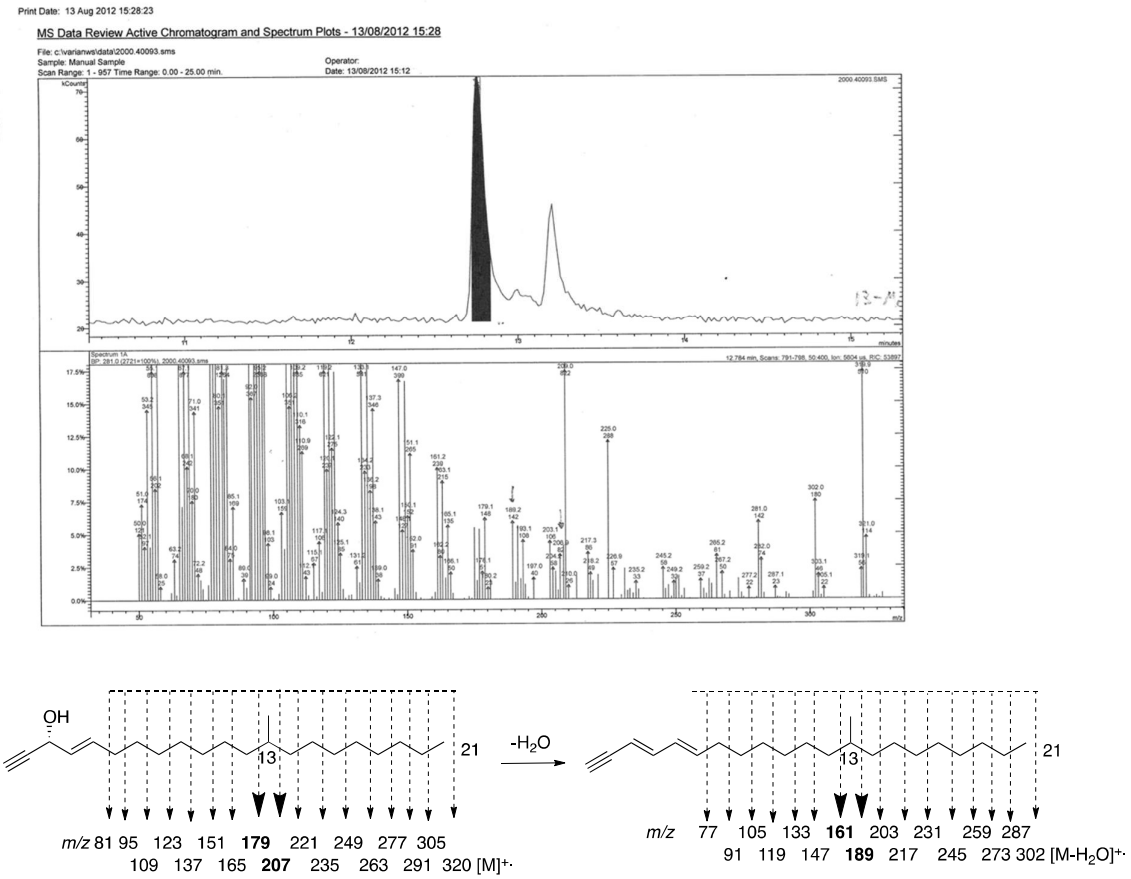


Figure S57. HRMS of (3*R*)-13-methylhenicos-(4*E*)-en-1-yn-3-ol (**9**)

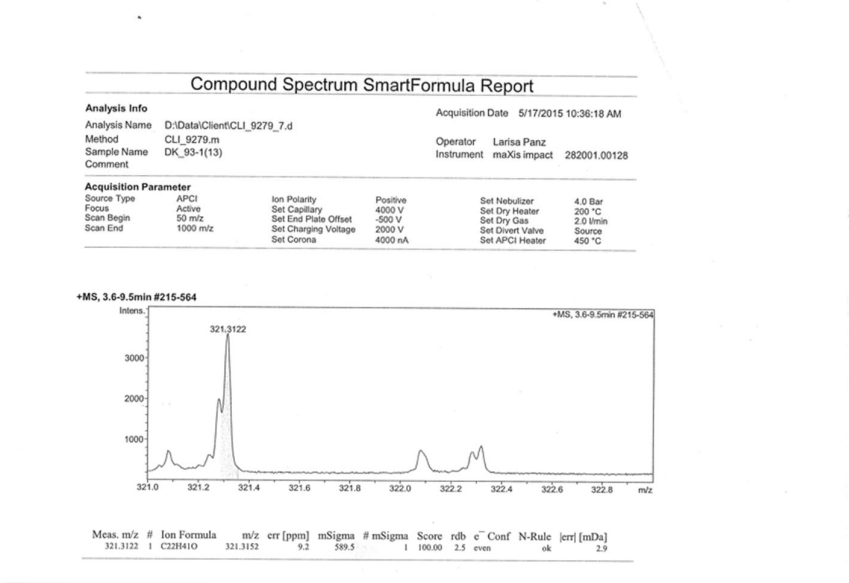


Figure S58. ^{1}H NMR spectrum of docos-(4*E*,15*Z*)-dien-1-yn-3-one (**10**) in $CDCl_3$

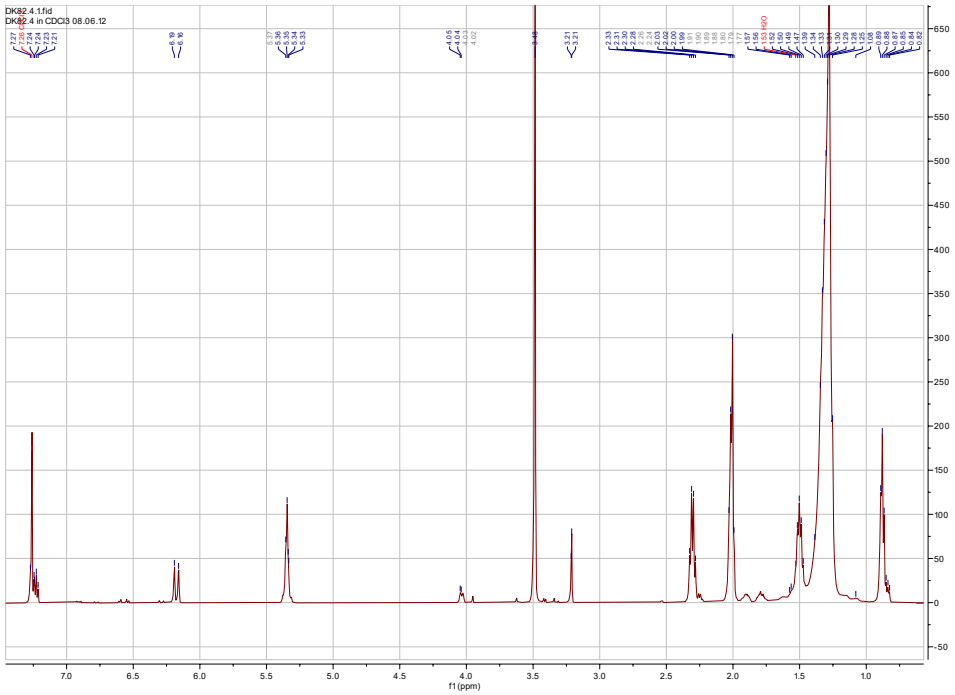


Figure S59. ^{13}C NMR spectrum of docos-(4*E*,15*Z*)-dien-1-yn-3-one (**10**) in $CDCl_3$

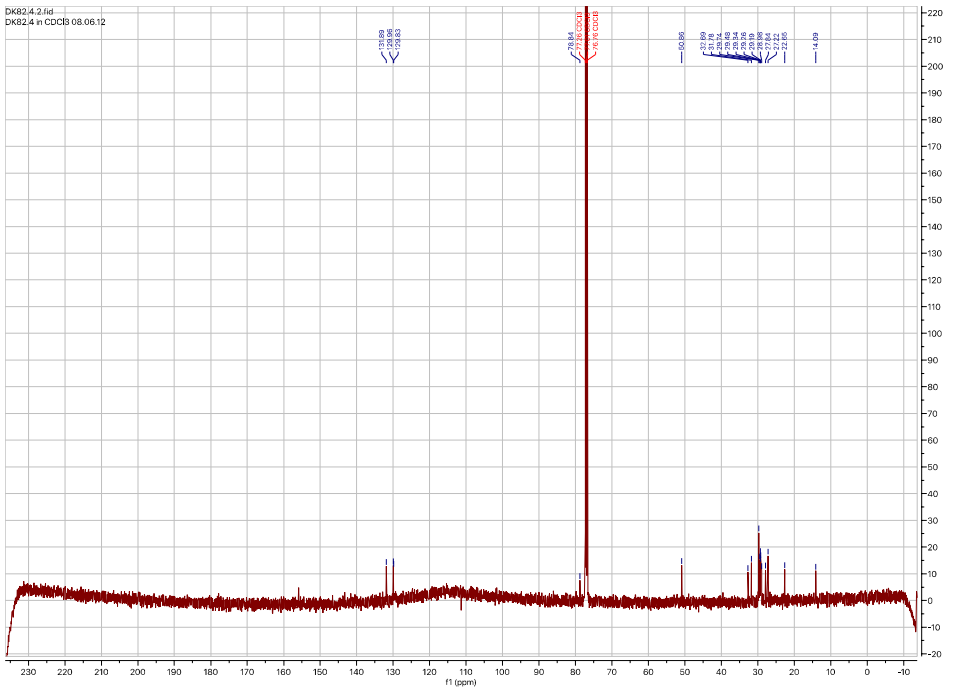


Figure S60. HSQC spectrum of docos-(4*E*,15*Z*)-dien-1-yn-3-one (**10**) in $CDCl_3$

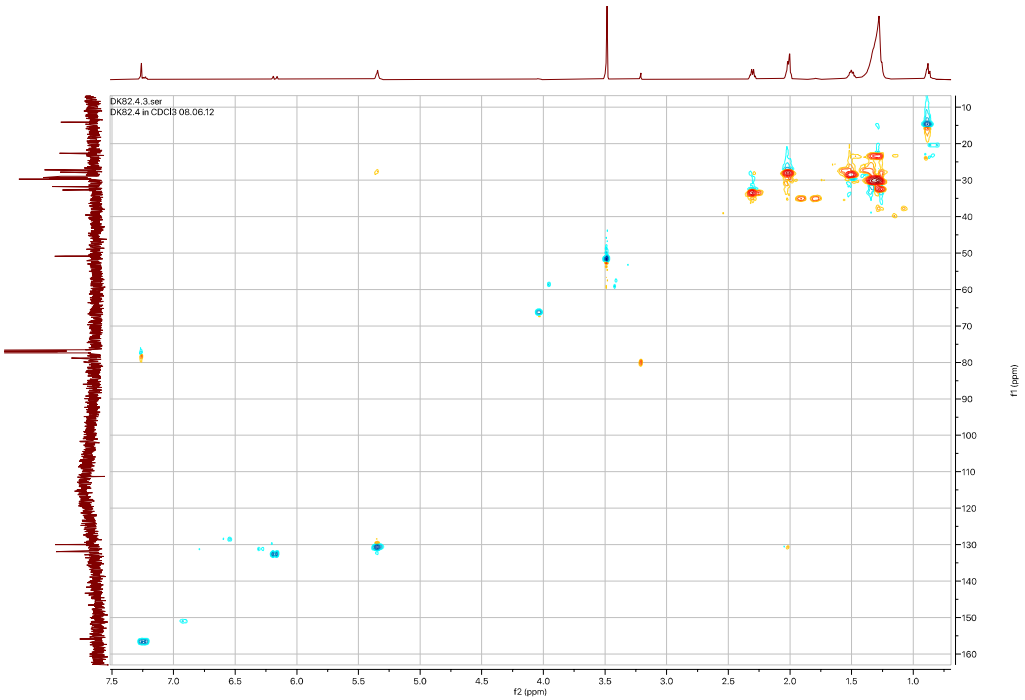


Figure S61. HMBC spectrum of docos-(4*E*,15*Z*)-dien-1-yn-3-one (**10**) in $CDCl_3$

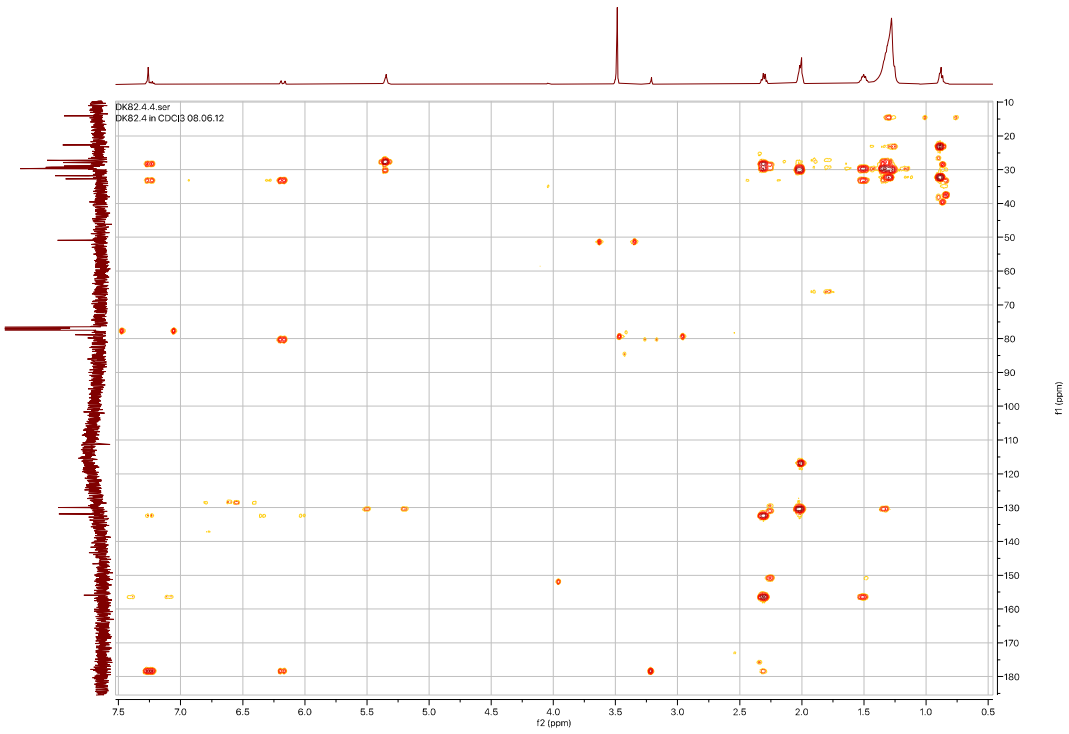


Figure S62. COSY spectrum of docos-(4*E*,15*Z*)-dien-1-yn-3-one (**10**) in $CDCl_3$

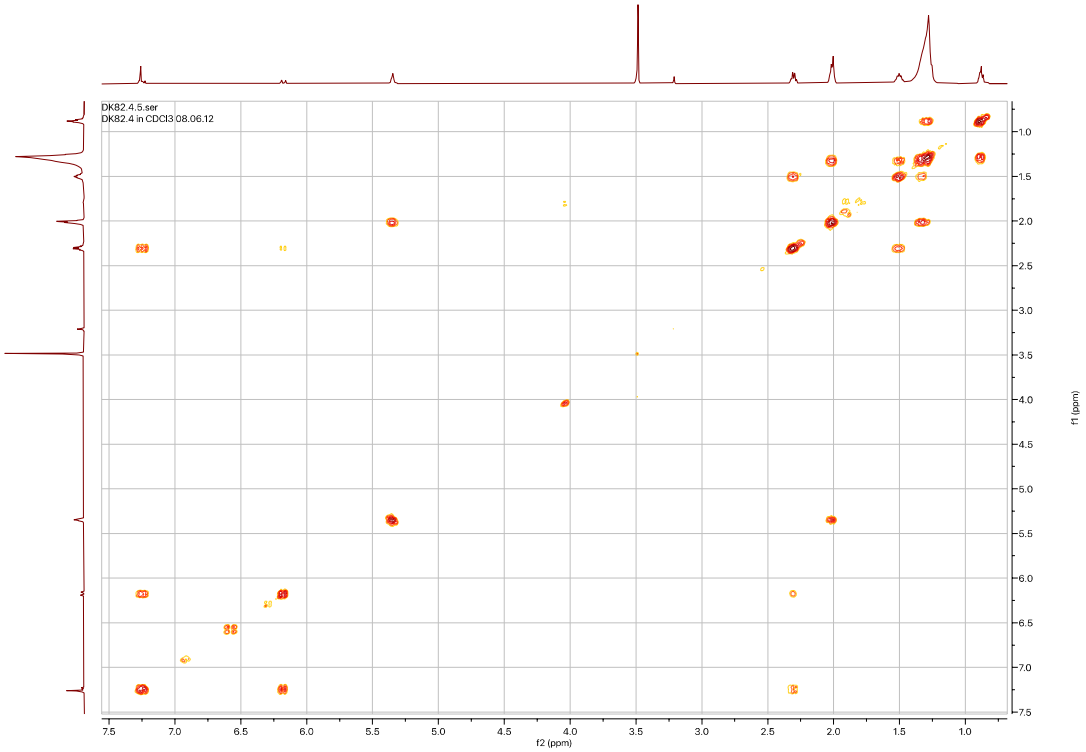


Table S10. NMR data of docos-(4*E*,15*Z*)-dien-1-yn-3-one (**10**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	78.8[d] CH	3.20 s	-
2	79.8[e] qC	-	1, 4
3	177.9 qC	-	1, 4, 5
4	131.9 CH	6.17 d (16.0)	6
5	155.9 CH	7.23 dt (16.0, 7.0)	6, 7
6	32.7 CH_2	2.30 q (7.0)	4, 5, 7, 8
7	27.8 CH_2	1.50 tt (7.0, 7.0)	5, 6, 8
8	29.2 CH_2	1.30 m	
9-13	~29.6[f] 5 × CH_2	1.23 – 1.35 brm	
14	27.2 CH_2	2.02 m	13, 15
15	129.8 CH	5.35 m	13, 14
16	129.9 CH	5.35 m	17, 18
17	27.2 CH_2	2.02 m	16, 18
18-19	29.6[f] 2 × CH_2	1.23 – 1.35 brm	
20	31.8 CH_2	1.27 m	19, 21a, 21b, 22
21a	22.6 CH_2	1.31 m	20, 22
b		1.27 m	
22	14.1 CH_3	0.88 t (6.7)	20, 21a, 21b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 254.6 Hz; [e] ^2J = 47.6 Hz; [f]Exact ^{13}C chemical shifts 29.25, 29.33, 29.47, 29.73 (× 4) ppm.

Figure S63. EIMS and fragmentation pattern of docos-(4*E*,15*Z*)-dien-1-yn-3-one (**10**)

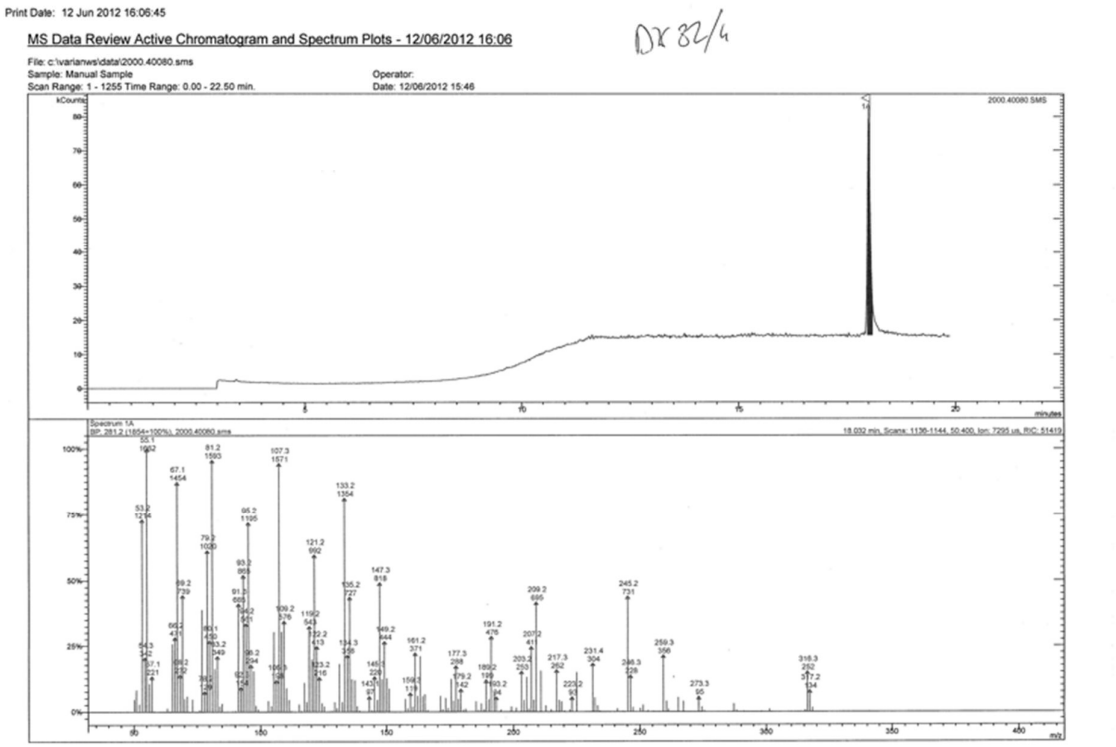


Figure S64. LCMS chromatogram and mass spectrum of the periodate-permanganate oxidation products of docos-(4*E*,15*Z*)-dien-1-yn-3-one (**10**). 2 Minutes gradient from 100% solvent A (95% H_2O, 5% ACN, 0.1% FA) to 100% of solvent B (99.9% ACN, 0.1% FA) and then isocratic elution in 100% of solvent B for 2 more minutes.

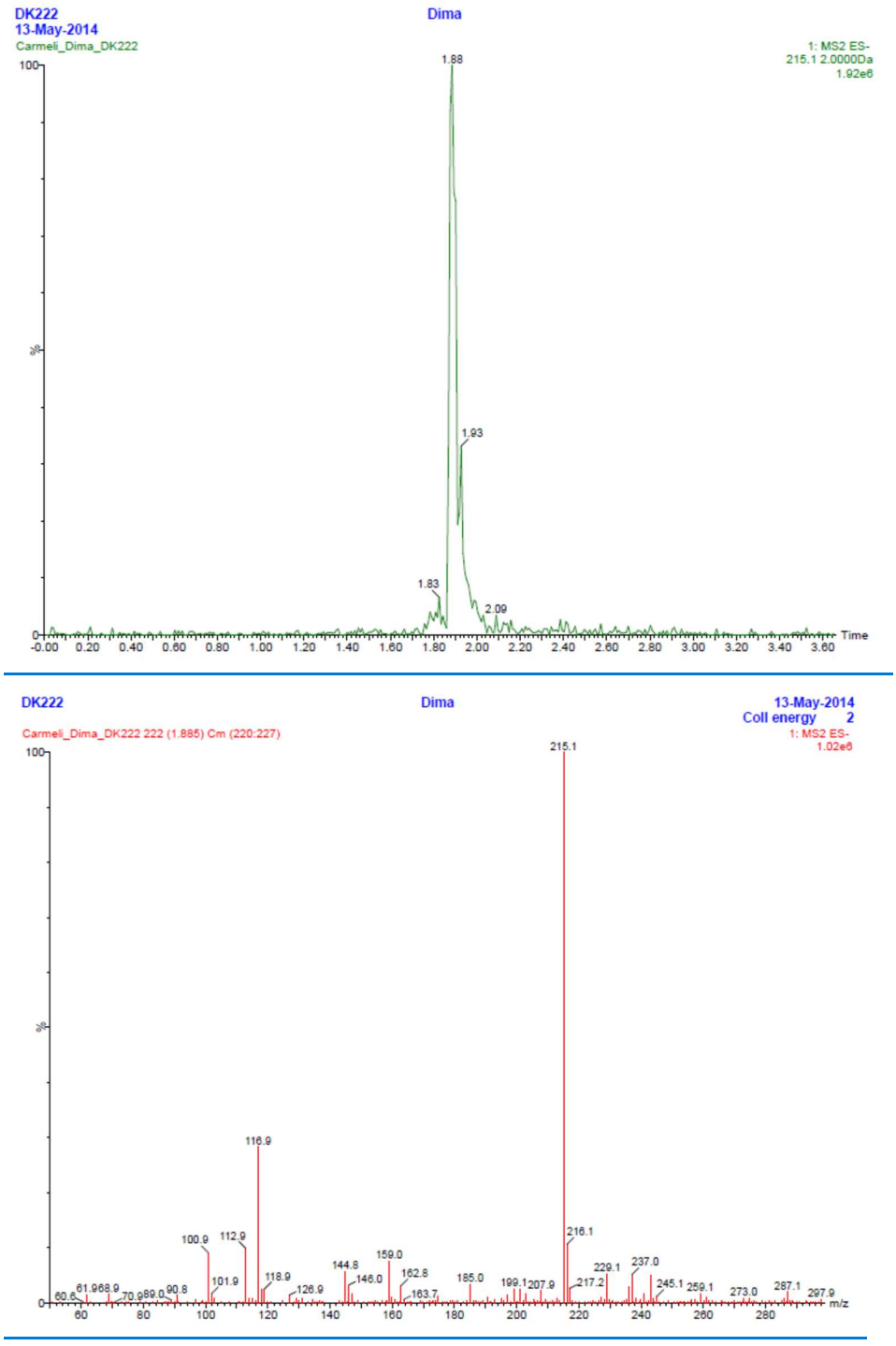


Figure S65. ^{1}H NMR spectrum of (3*R*)-docos-(15*Z*)- en-1-yn-3-ol (**11**) in $CDCl_3$

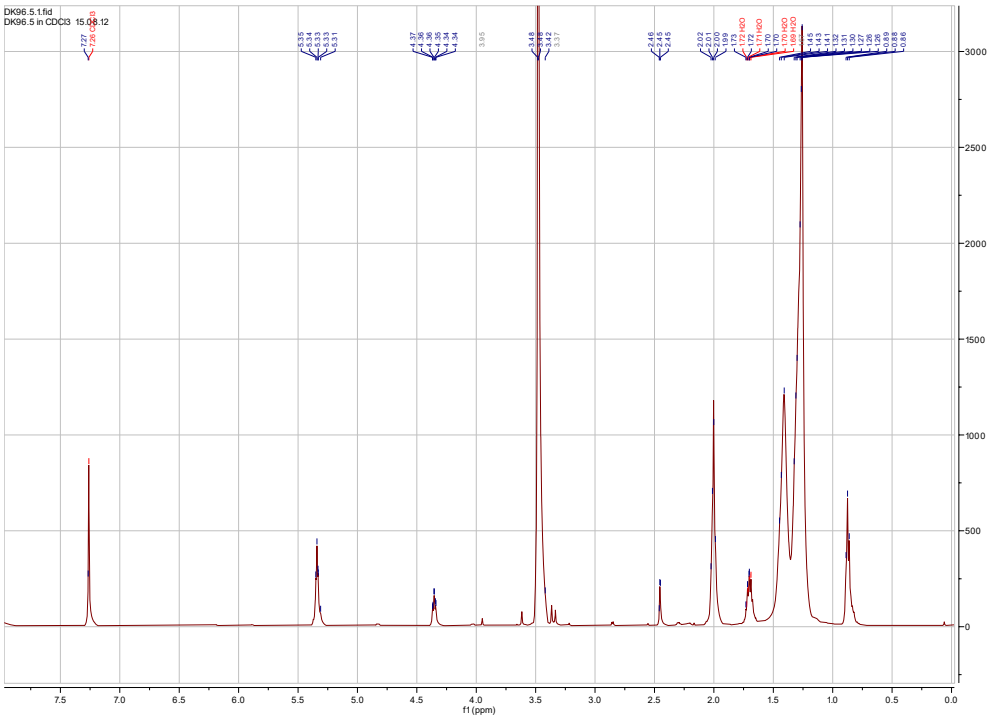


Figure S66. ^{13}C NMR spectrum of (3*R*)-docos-(15*Z*)- en-1-yn-3-ol (**11**) in $CDCl_3$

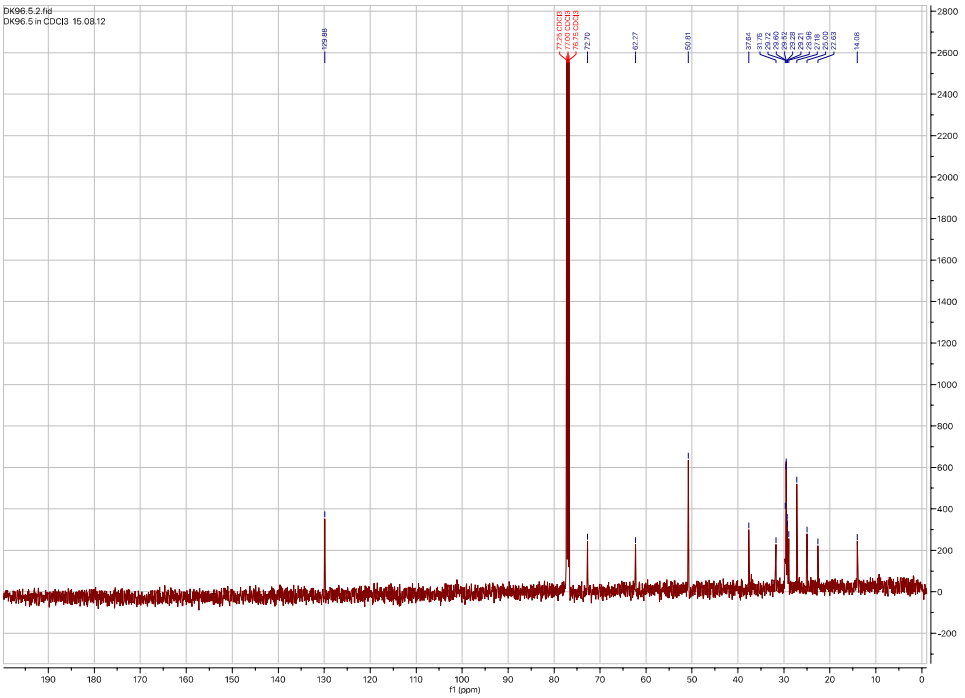


Table S11. NMR data of (3*R*)-docos-(15*Z*)- en-1-yn-3-ol (**11**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	72.6[d] CH	2.45 d (2.0)	3
2	85.0[e] qC	-	1, 3, 4
3	62.3 CH	4.36 td (6.5, 2.0)	1, 4
4	37.6 CH_2	1.70 m	3, 6
5	25.0 CH_2	1.41 m	3, 4, 6
6	29.0 CH_2	1.26 m	4, 5
7-13	~29.6[f] 7 × CH_2	1.22 – 1.31 brm	
14	27.2 CH_2	2.01 m	13, 15
15	129.9 CH	5.34 t (4.5)	13, 14
16	129.9 CH	5.34 t (4.5)	17, 18
17	27.2 CH_2	2.01 m	16, 18
18-19	29.6[f] 2 × CH_2	1.22 – 1.31 brm	
20	31.8 CH_2	1.25 m	19, 21a, 21b, 22
21a	22.6 CH_2	1.33 m	20, 22
b		1.28 m	
22	14.1 CH_3	0.87 t (7.0)	20, 21a, 21b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 251.0 Hz; [e] ^2J = 46.0 Hz; [f]Exact ^{13}C chemical shifts 29.21, 29.49, 29.52 (× 3), 29.60 (× 2), 29.72, 29.74 ppm.

Figure S67. EIMS of (3*R*)-docos-(15*Z*)- en-1-yn-3-ol (**11**)

Print Date: 14 Aug 2012 11:41:52

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MS Data Review Active Chromatogram and Spectrum Plots - 14/08/2012 11:41

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Date: 14/08/2012 11:22

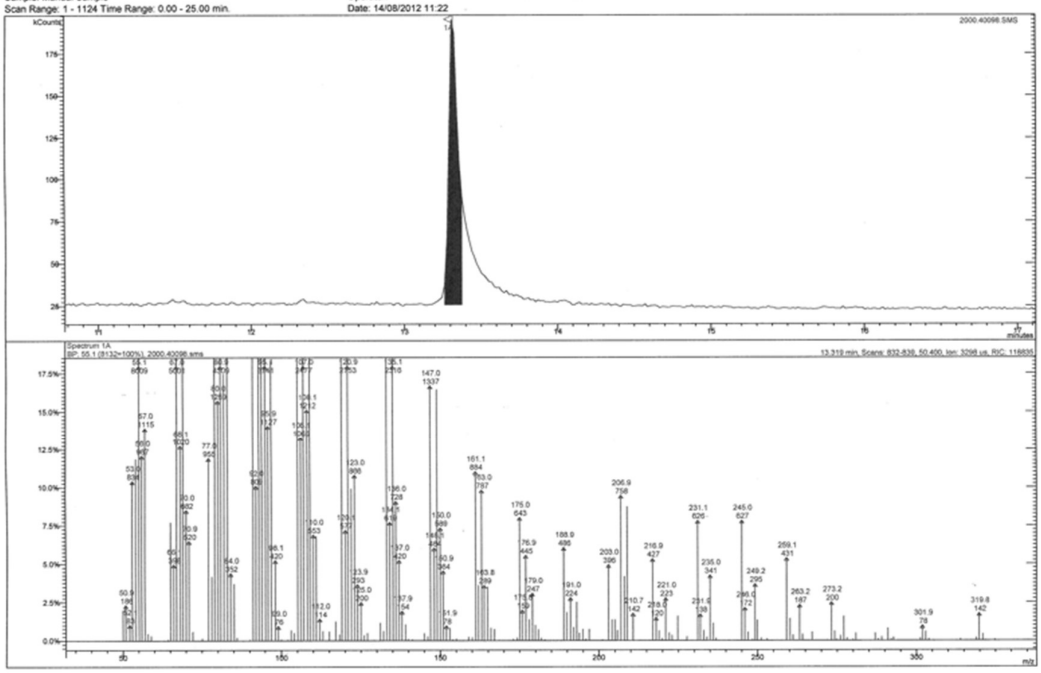


Figure S68. ^{1}H NMR spectrum of (3*R*)-tetracos-(4*E*,15*Z*)-dien-1-yn-3-ol (**12**) in $CDCl_3$

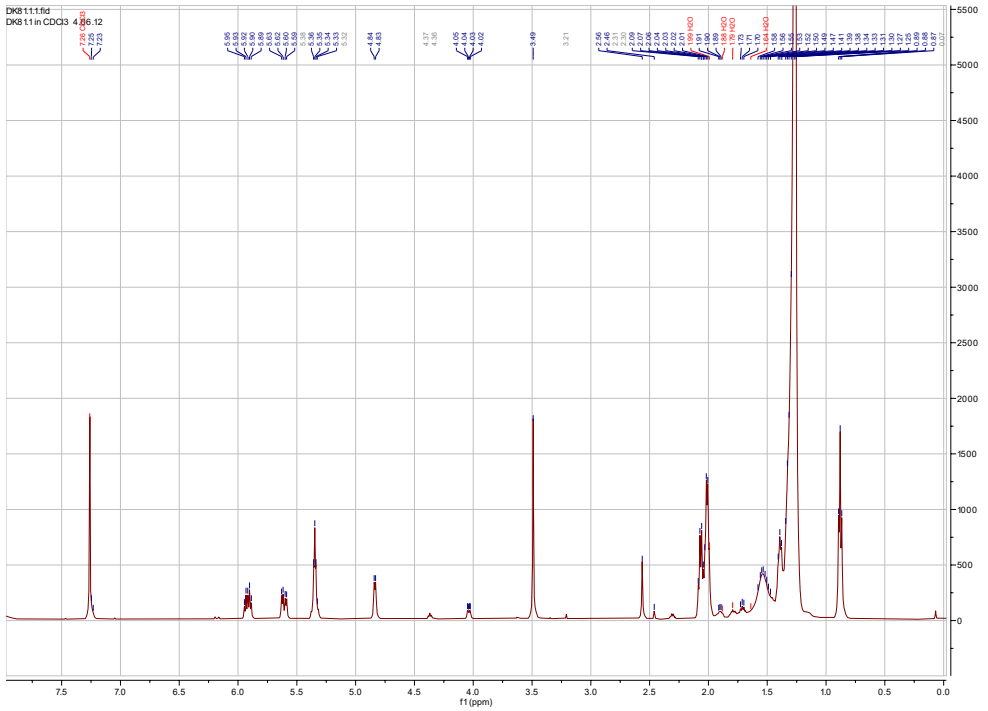


Figure S69. ^{13}C NMR spectrum of (3*R*)-tetracos-(4*E*,15*Z*)-dien-1-yn-3-ol (**12**) in $CDCl_3$

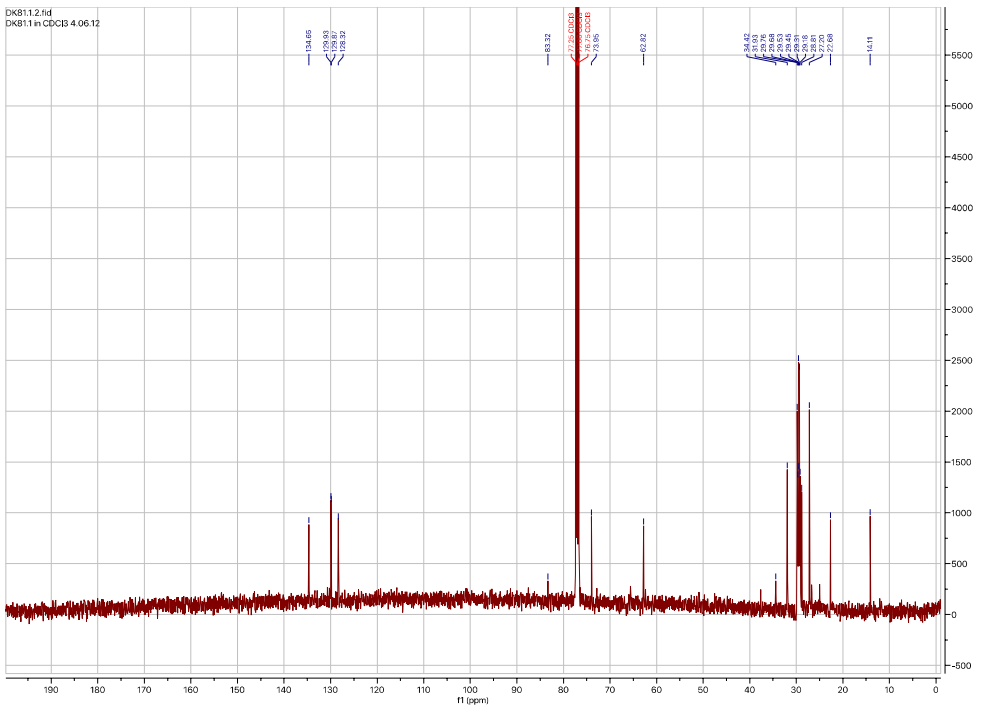


Figure S70. HSQC spectrum of (3*R*)-tetracos-(4*E*,15*Z*)-dien-1-yn-3-ol (**12**) in $CDCl_3$

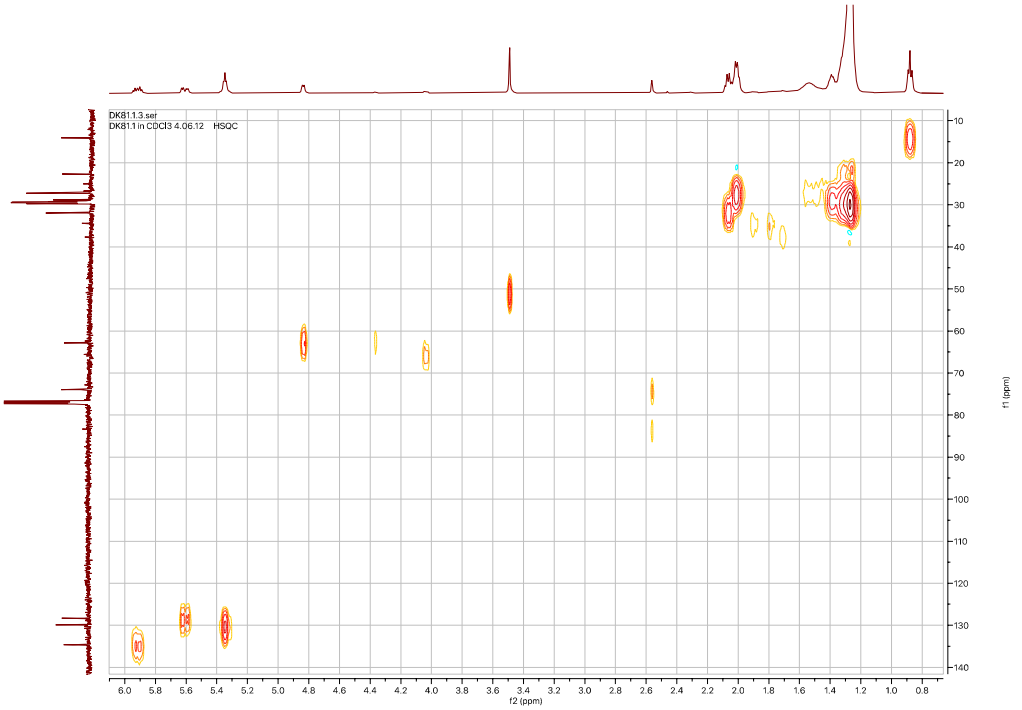


Figure S71. HMBC spectrum of (3*R*)-tetracos-(4*E*,15*Z*)-dien-1-yn-3-ol (**12**) in $CDCl_3$

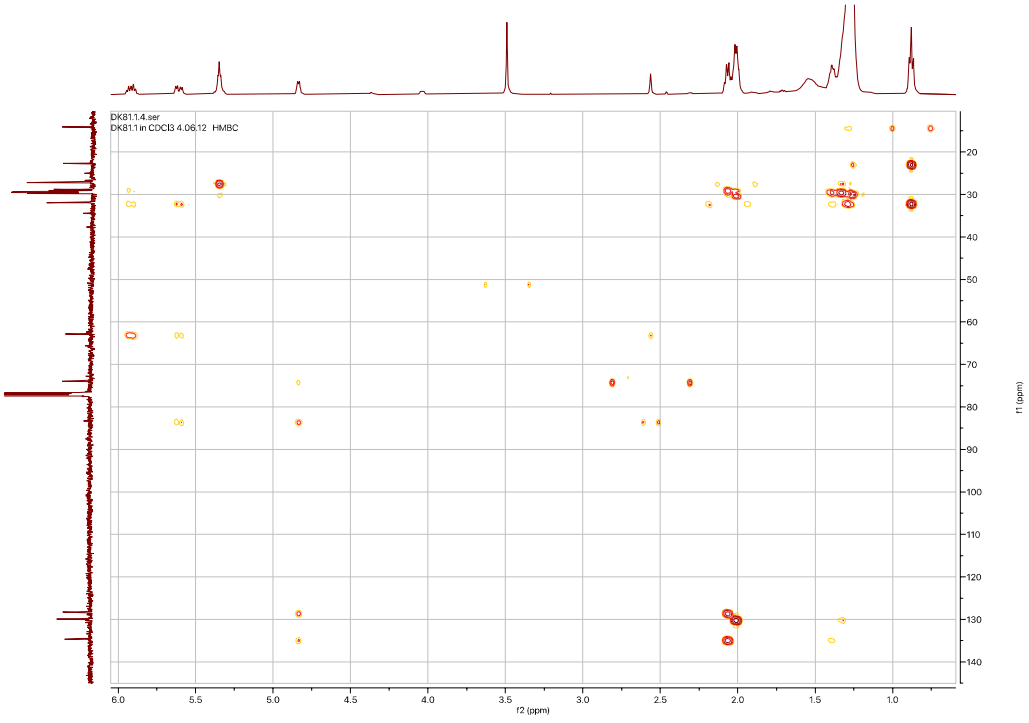


Figure S72. COSY spectrum of (3*R*)-tetracos-(4*E*,15*Z*)-dien-1-yn-3-ol (**12**) in $CDCl_3$

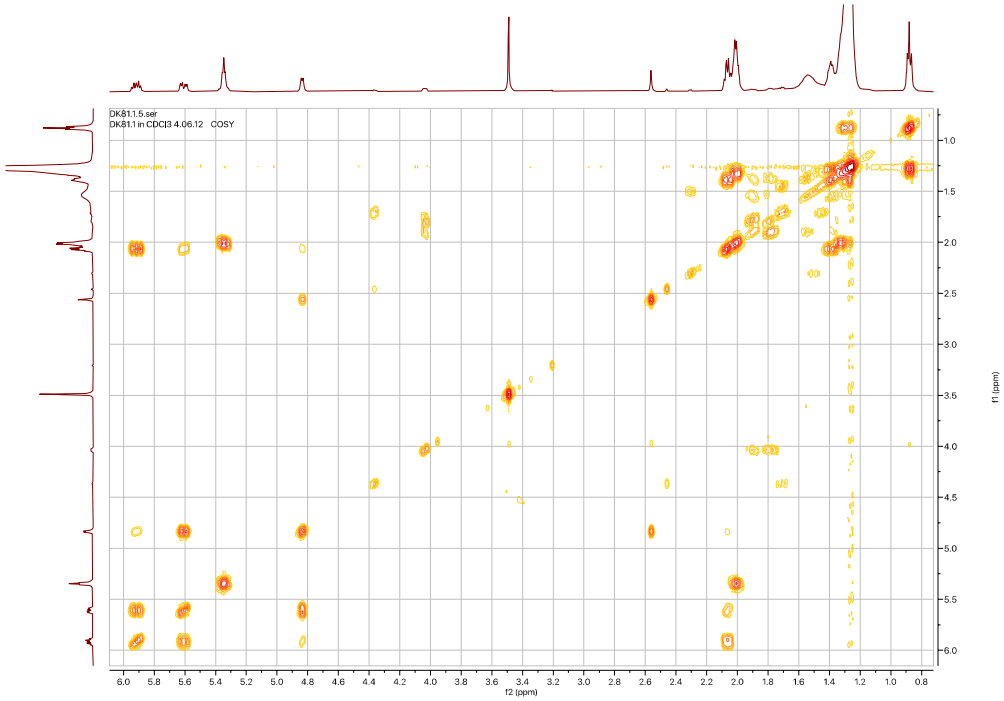


Figure S73. DEPT spectrum of (3*R*)-tetracos-(4*E*,15*Z*)-dien-1-yn-3-ol (**12**) in $CDCl_3$

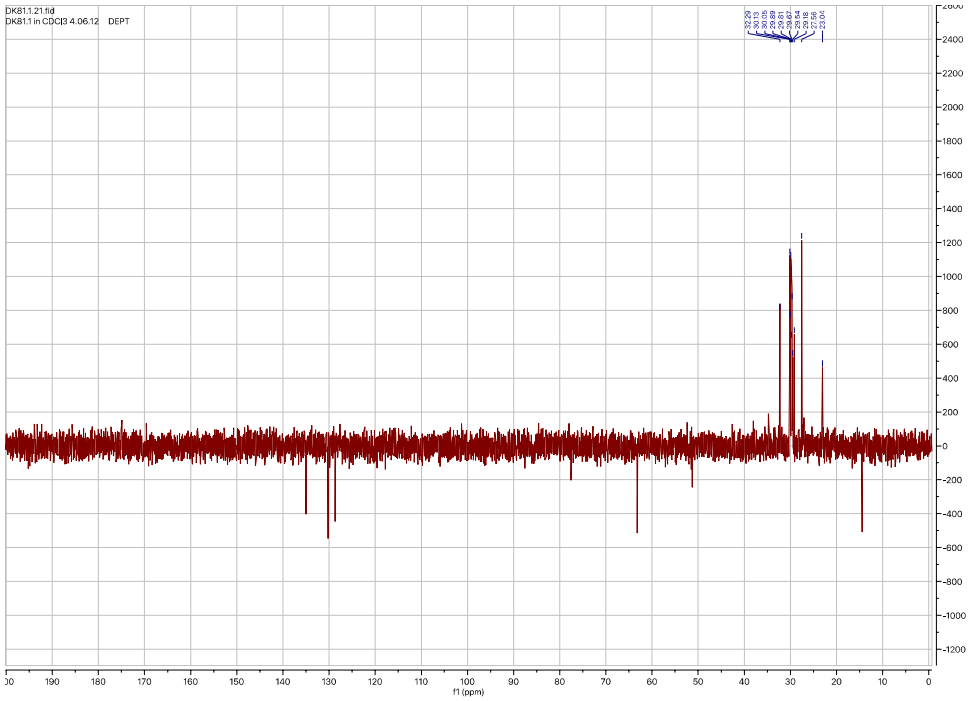


Table S12. NMR data of (3*R*)-tetracos-(4*E*,15*Z*)-dien-1-yn-3-ol (**12**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.9[d] CH	2.56 brs	3
2	83.4[e] qC	-	1, 3, 4
3	62.8 CH	4.83 brd (6.0)	1, 4, 5
4	128.3 CH	5.60 dd (15.3, 6.0)	3, 6
5	134.6 CH	5.91 dt (15.3, 7.1)	3, 6, 7
6	31.9 CH_2	2.06 q (7.1)	4, 5, 7, 8
7	28.8 CH_2	1.38 m	5, 6, 8
8-13	~29.6[f] 6 × CH_2	1.22 – 1.32 brm	
14	27.2 CH_2	2.01 m	13, 15
15	129.9 CH	5.34 t (5.0)	13, 14
16	129.9 CH	5.34 t (5.0)	17, 18
17	27.2 CH_2	2.01 m	16, 18
18-21	29.6[f] 4 × CH_2	1.22 – 1.32 brm	
22	31.9 CH_2	1.25 m	21, 23a, 23b, 24
23a	22.7 CH_2	1.32 m	22, 24
b		1.28 m	
24	14.1 CH_3	0.88 t (6.7)	22, 21a, 21b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 251.5 Hz; [e] ^2J = 49.4 Hz; [f]Exact ^{13}C chemical shifts 29.18, 29.31 (× 2), 29.45, 29.52 (× 4), 29.68, 29.76 ppm.

Figure S74. EIGCMS spectrum of (3*R*)-tetracos-(4*E*,15*Z*)-dien-1-yn-3-ol (**12**)

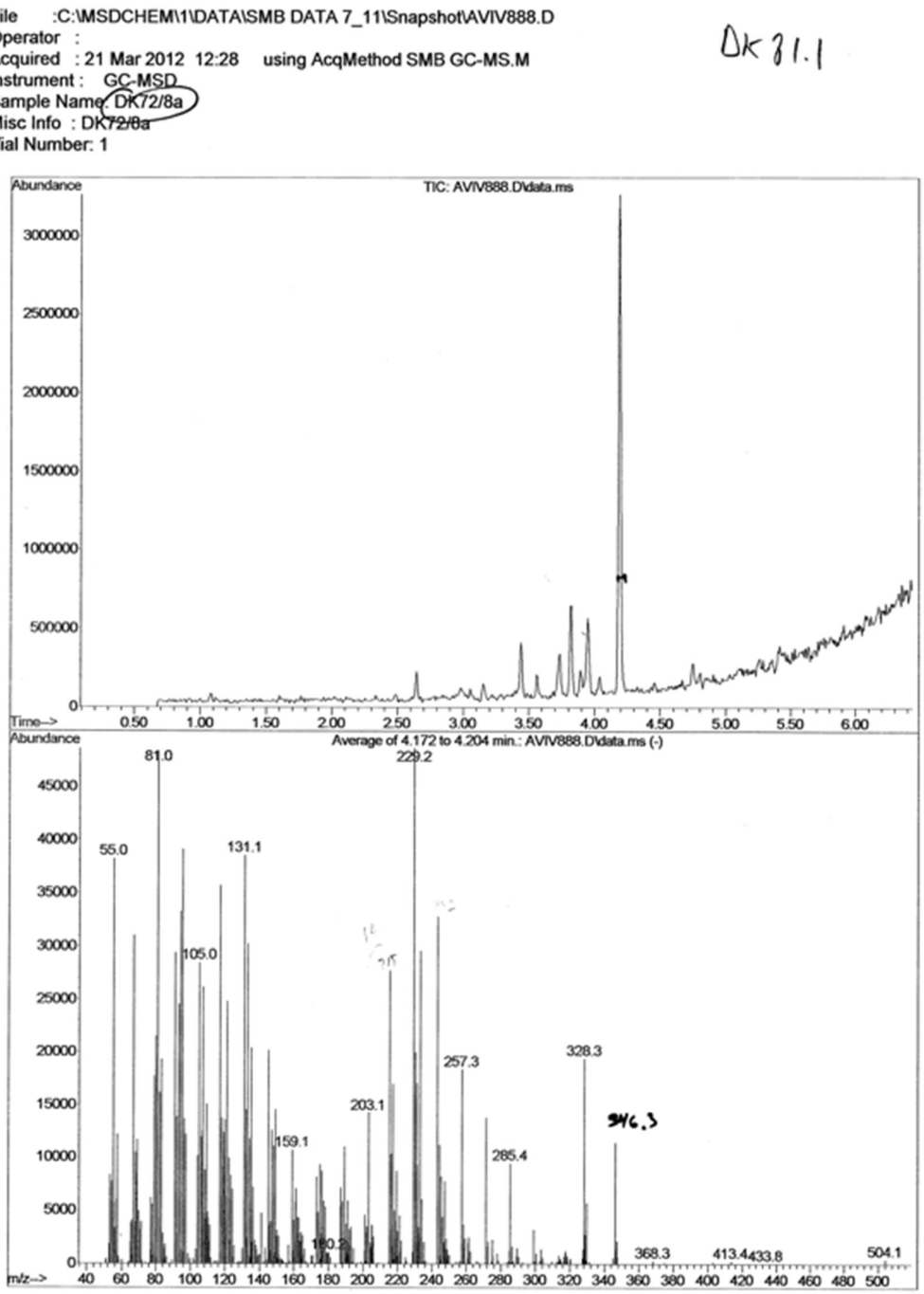
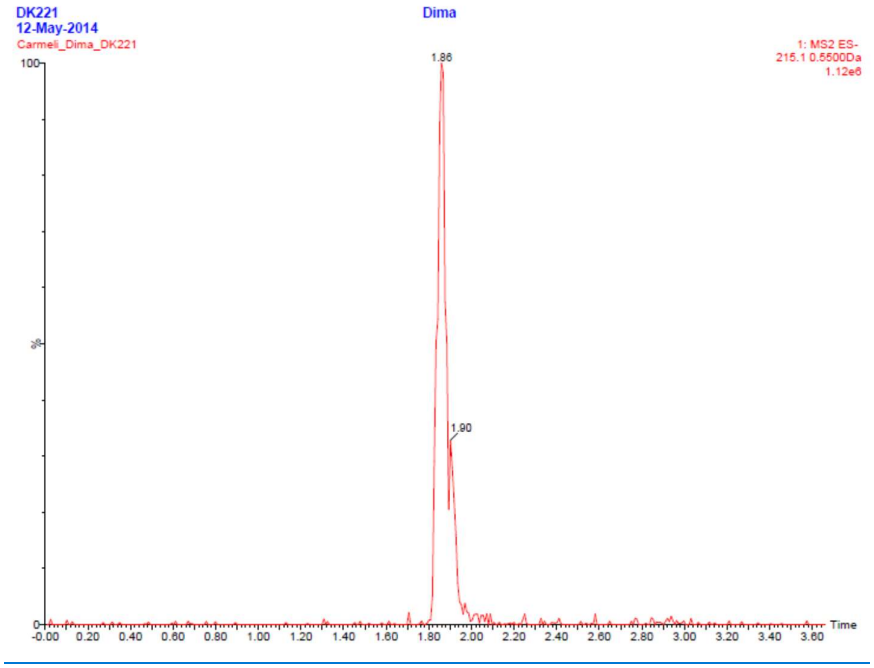


Figure S75. LCMS chromatogram and mass spectrum of the periodate-permanganate oxidation products of (3*R*)-tetracos-(4*E*,15*Z*)-dien-1-yn-3-ol (**12**). 2 Minutes gradient from 100% solvent A (95% H_2O, 5% ACN, 0.1% FA) to 100% of solvent B (99.9% ACN, 0.1% FA) and then isocratic elution in 100% of solvent B for 2 more minutes.



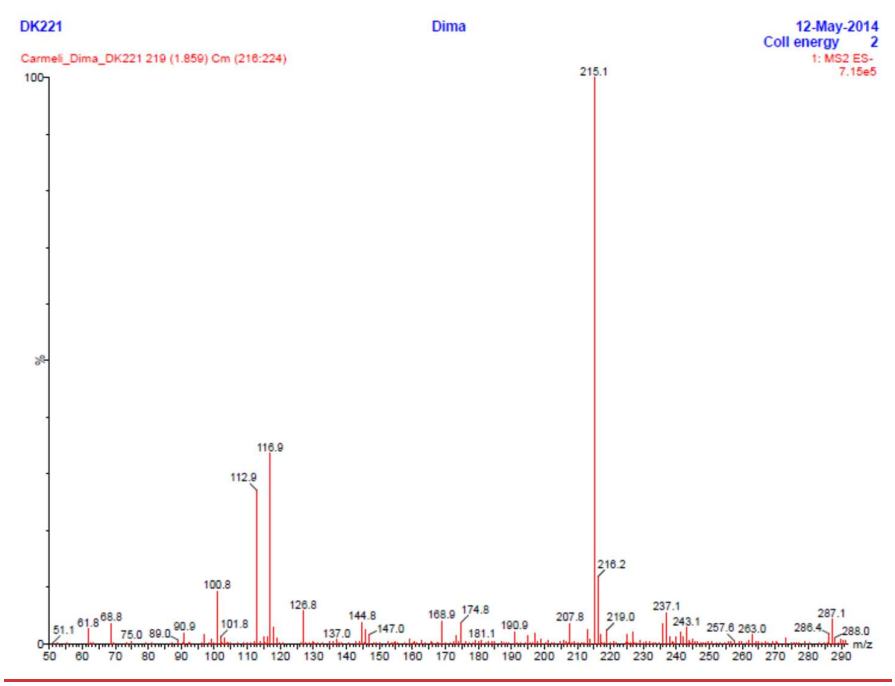


Figure S76. ^{1}H NMR spectrum of (5*S*)-icos-(3*Z*)-en-1-yn-5-ol (**13**) in $CDCl_3$

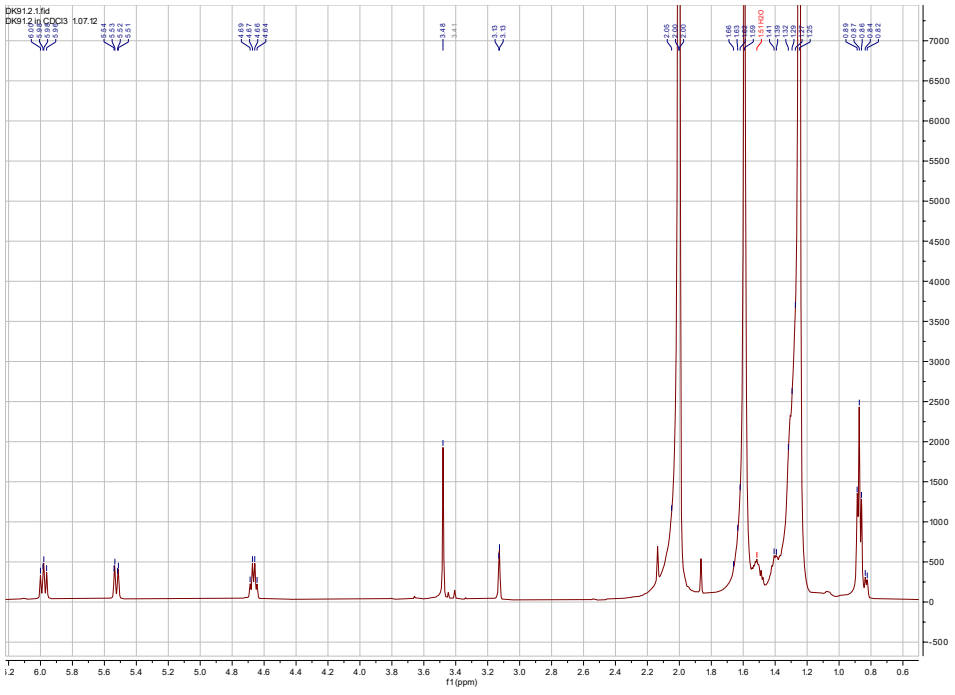


Figure S77. ^{13}C NMR spectrum of (5*S*)-icos-(3*Z*)-en-1-yn-5-ol (**13**) in $CDCl_3$

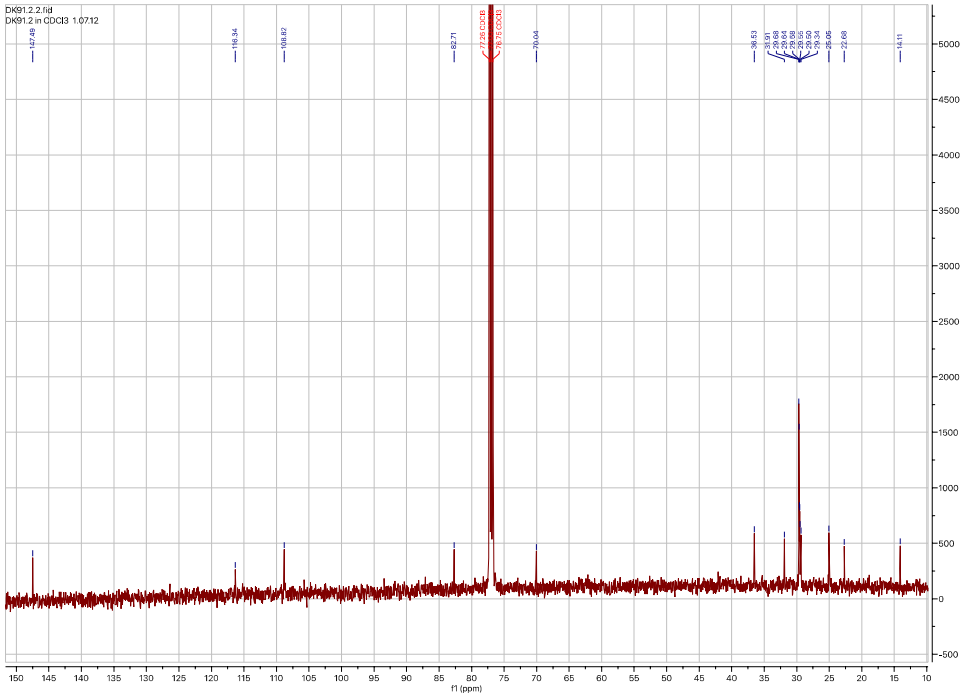


Figure S78. HSQC spectrum of (5*S*)-icos-(3*Z*)-en-1-yn-5-ol (**13**) in $CDCl_3$

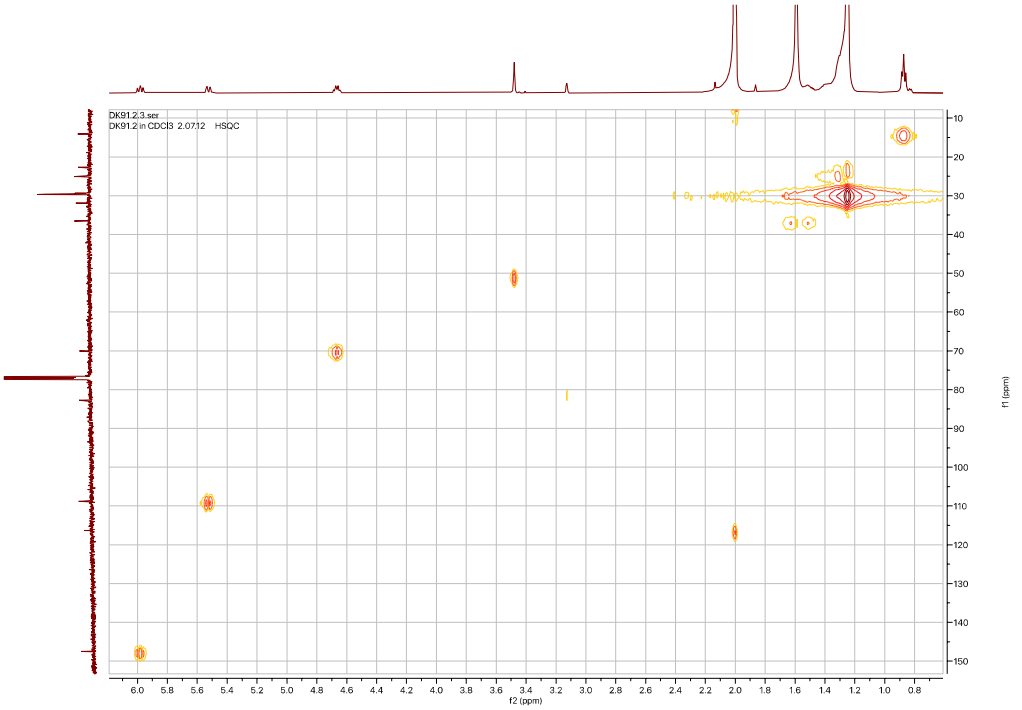


Figure S79. HMBC spectrum of (5*S*)-icos-(3*Z*)-en-1-yn-5-ol (**13**) in $CDCl_3$

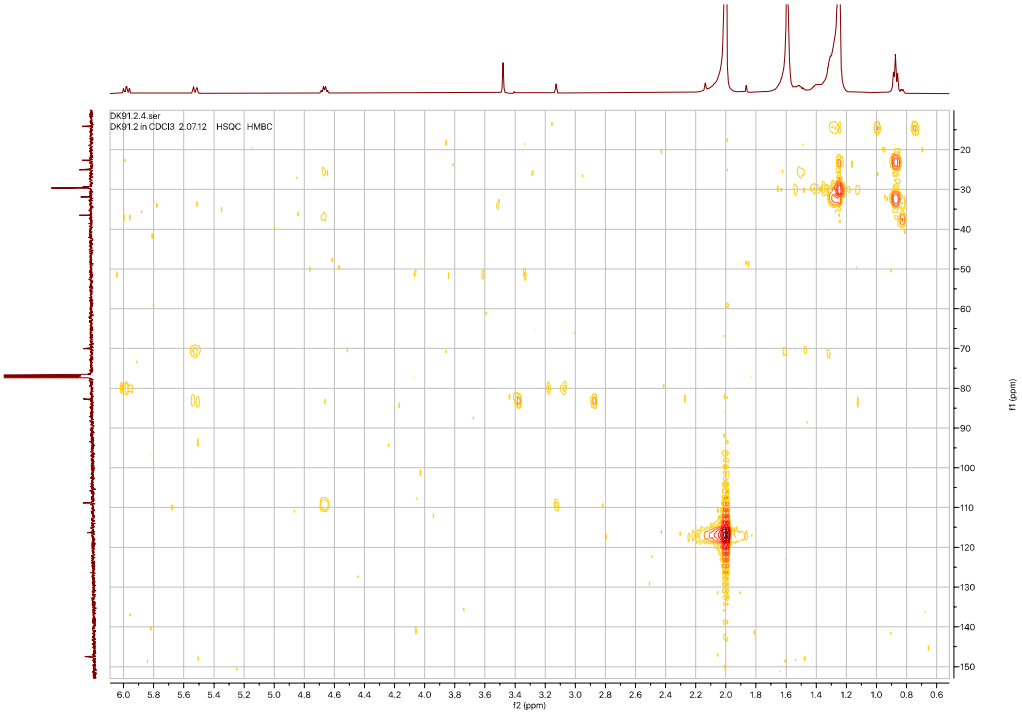


Figure S80. COSY spectrum of (5*S*)-icos-(3*Z*)-en-1-yn-5-ol (**13**) in $CDCl_3$

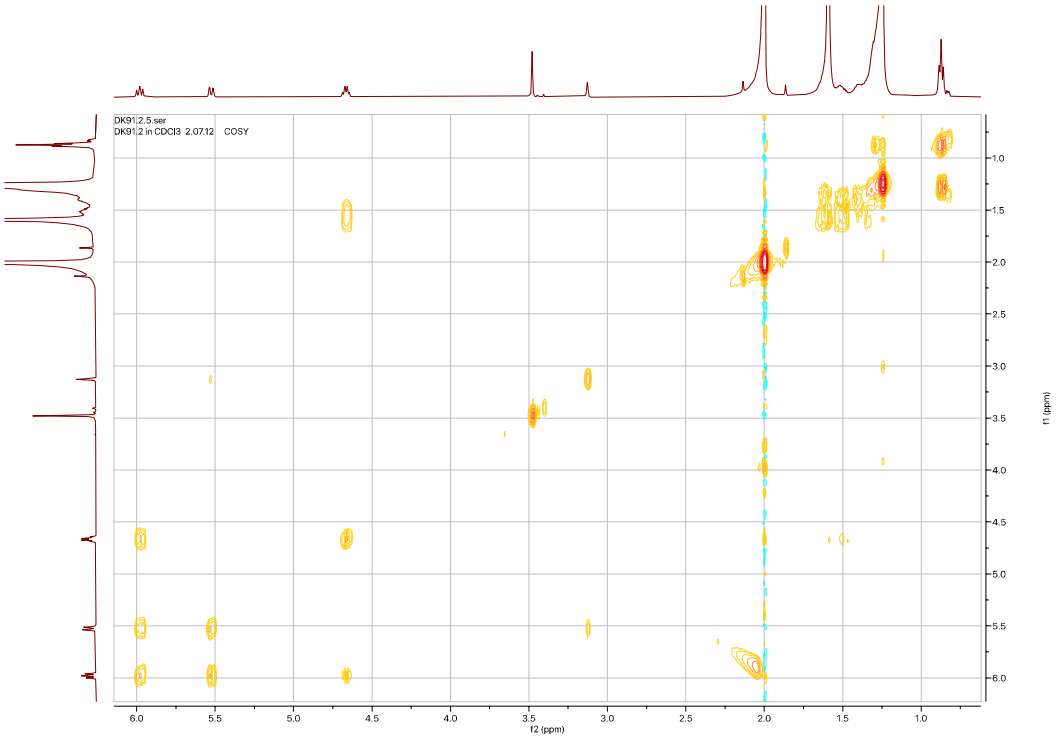


Figure S81. DEPT spectrum of (5*S*)-icos-(3*Z*)-en-1-yn-5-ol (**13**) in $CDCl_3$

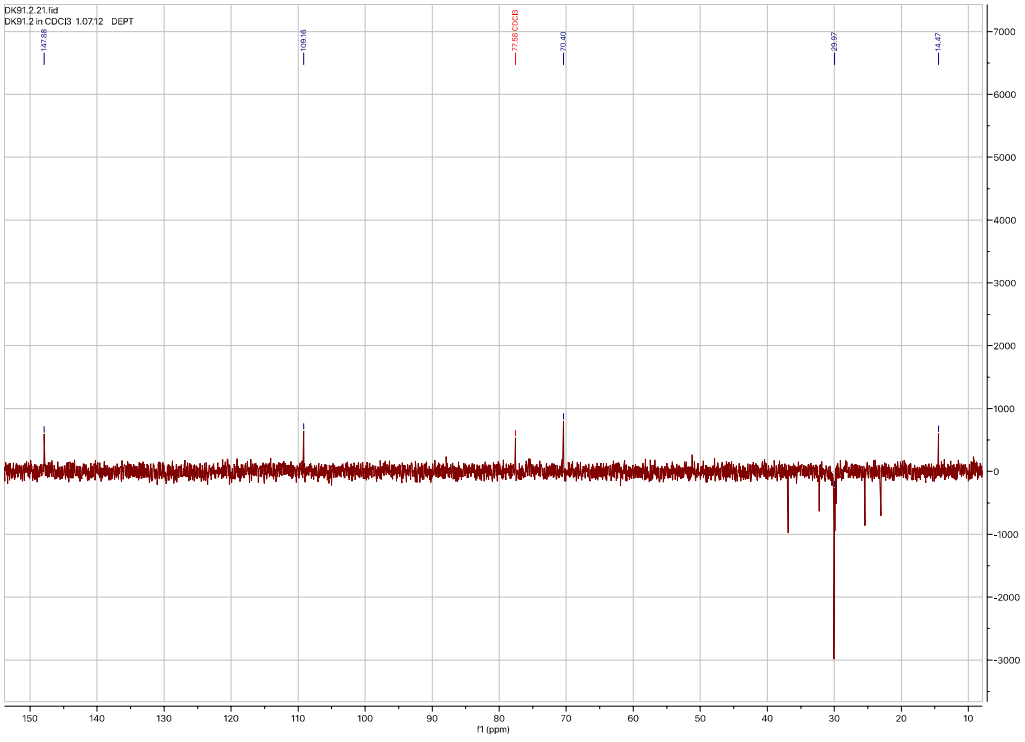


Table S13. NMR data of (5*S*)-icos-(3*Z*)-en-1-yn-5-ol (**13**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	82.7[d] CH	3.13 d (1.5)	3
2	79.5[e] qC	-	1, 4
3	108.8 CH	5.52 dd (11.0, 1.5)	1, 4, 5
4	147.5 CH	5.98 dd (11.0, 8.9)	1, 3, 5, 6a, 6b
5	70.0 CH	4.67 dt (8.9, 8.5)	3, 4, 6a, 6b, 7a, 7b
6a	36.5 CH_2	1.61 m	4, 5, 7a, 7b, 8
b		1.52 m	
7a	28.8 CH_2	1.41 m	5, 6a, 6b, 8
b		1.32 m	
8-17	~29.6[f] 10 × CH_2	1.23 – 1.35 brm	
18	31.9 CH_2	1.26 m	17, 19a, 19b, 20
19a	22.7 CH_2	1.31 m	18, 20
b		1.26 m	
20	14.1 CH_3	0.88 t (7.0)	18, 19a, 19b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 252.0 Hz; [e] ^2J = 49.1 Hz; [f]Exact ^{13}C chemical shifts 29.34, 29.50, 29.54, 29.54, 29.65 (× 3), 29.67 (× 3) ppm.

Figure S82. EIGCMS spectrum of (5*S*)-icos-(3*Z*)-en-1-yn-5-ol (**13**)

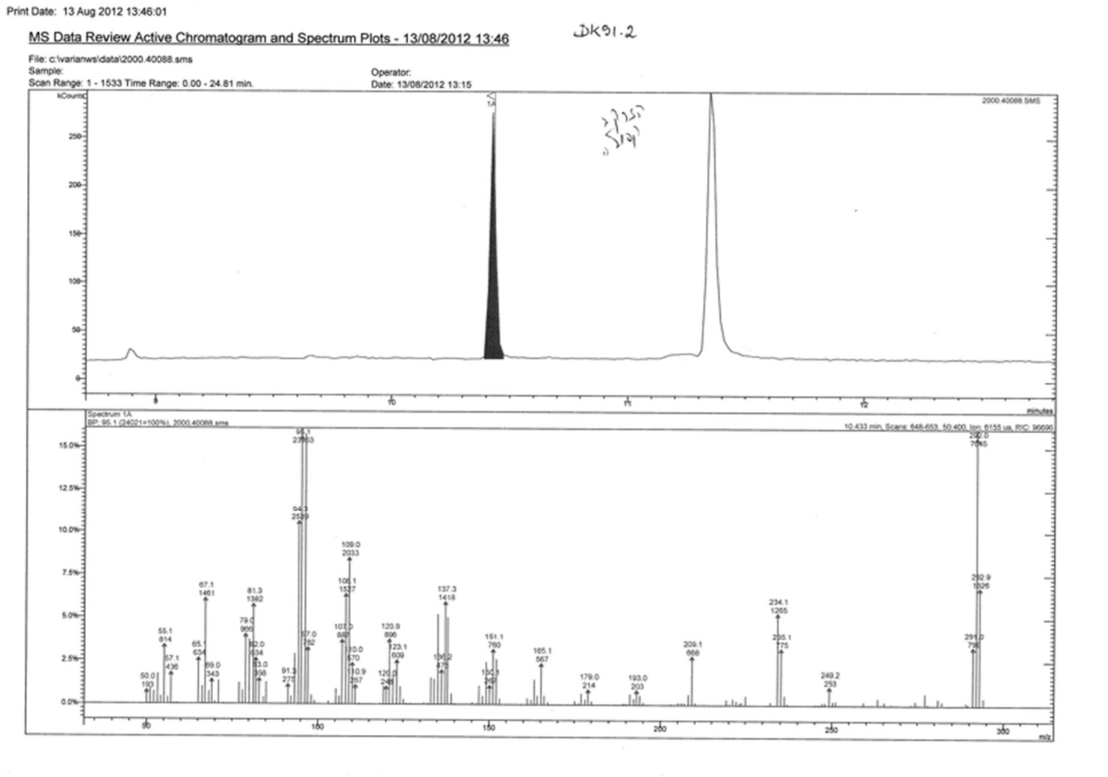


Figure S83. HRCIMS spectrum of (5*S*)-icos-(3*Z*)-en-1-yn-5-ol (**13**)

Compound Spectrum SmartFormula Report

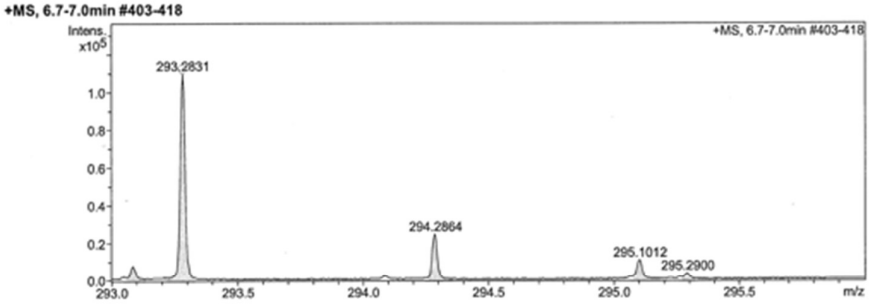
Analysis Info

Analysis Name	D:\Data\Eichen\Acq000004.d	Acquisition Date	5/17/2015 8:28:47 AM
Method	GC APCI_pos_Na_Formate.m	Operator	Larisa Panz
Sample Name	dk-91-2(17)	Instrument	maXis impact 282001.00128
Comment	uNI		

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 6.7-7.0min #403-418



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
293.2831	1	C20H37O	293.2839	2.8	9.4	1	100.00	2.5	even	ok	0.8

Figure S84. ^{1}H NMR spectrum of (5*S*)-14-methylicos-(3*Z*)-en-1-yn-5-ol (**14**) in $CDCl_3$

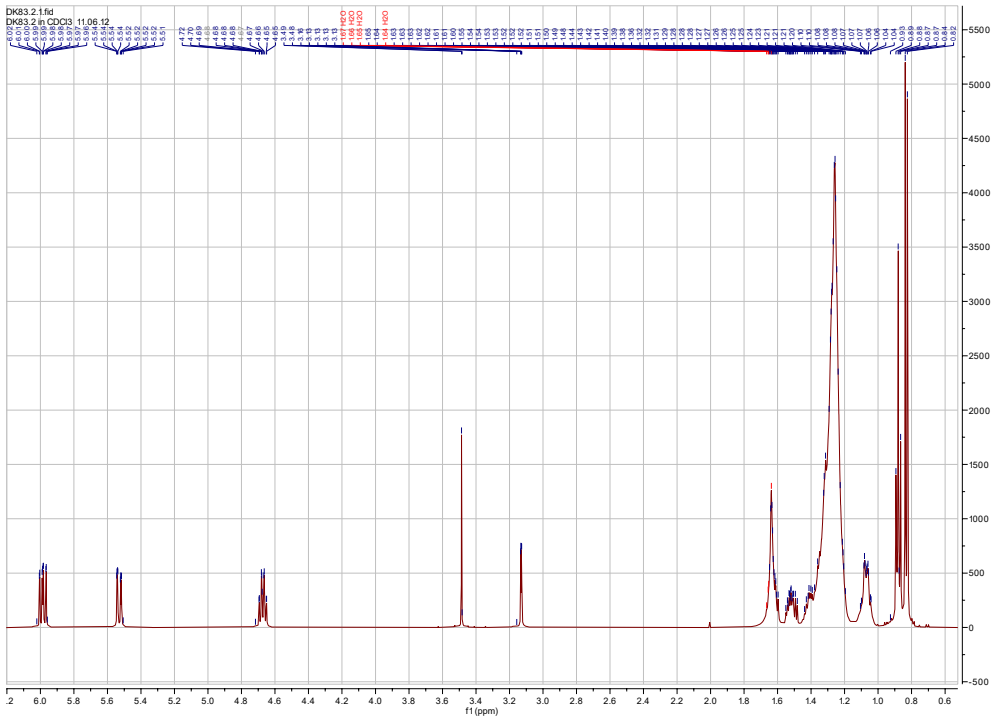


Figure S85. ^{13}C NMR spectrum of (5*S*)-14-methylicos-(3*Z*)-en-1-yn-5-ol (**14**) in $CDCl_3$

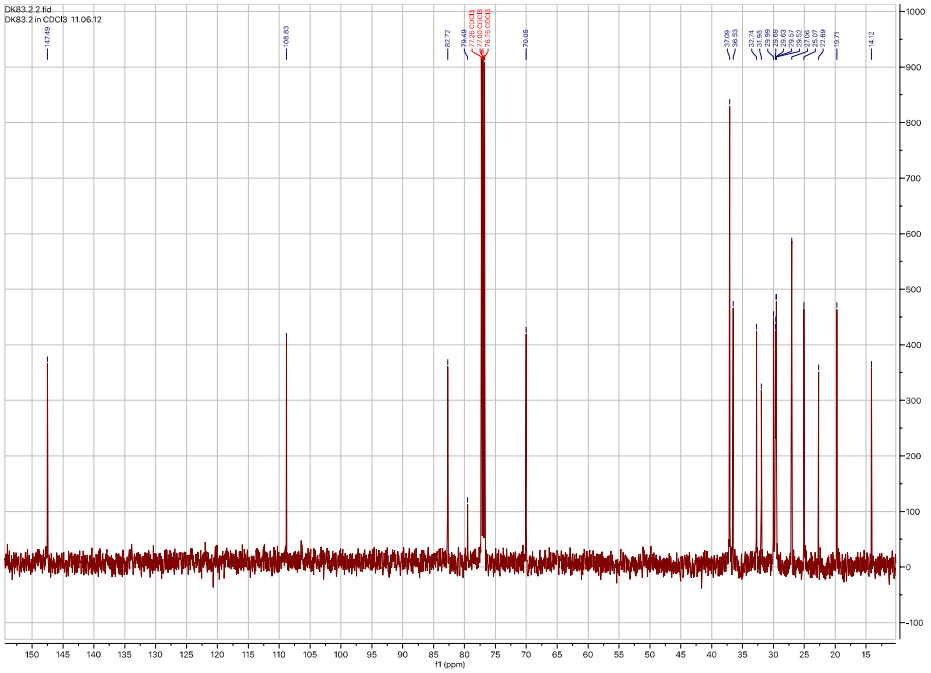


Figure S86. HSQC spectrum of (5*S*)-14-methylicos-(3*Z*)-en-1-yn-5-ol (**14**) in $CDCl_3$

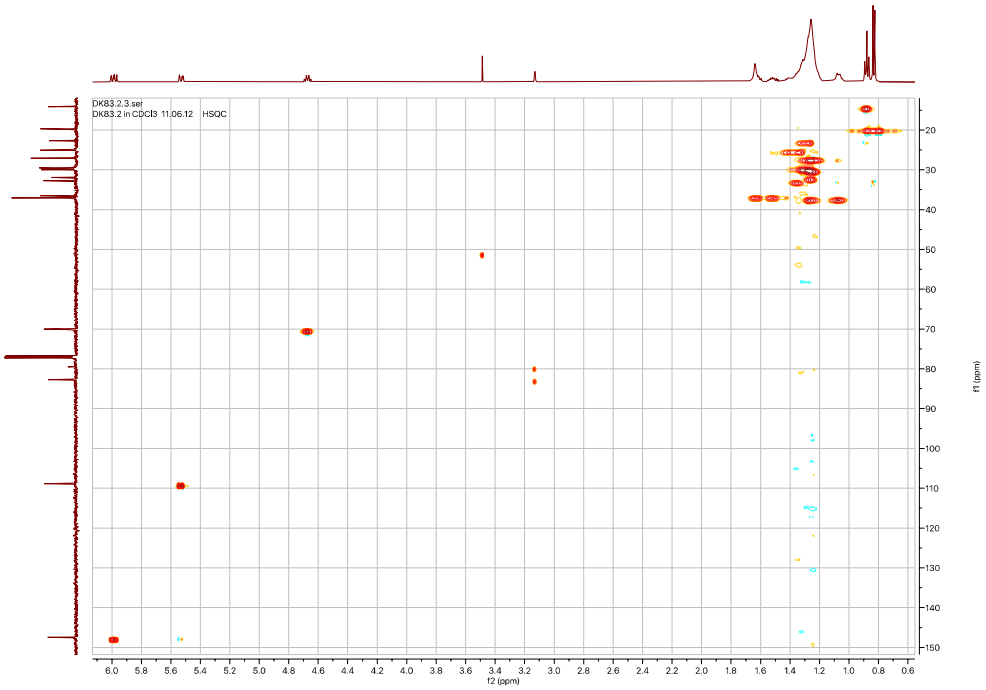


Figure S87. HMBC spectrum of (5*S*)-14-methylicos-(3*Z*)-en-1-yn-5-ol (**14**) in $CDCl_3$

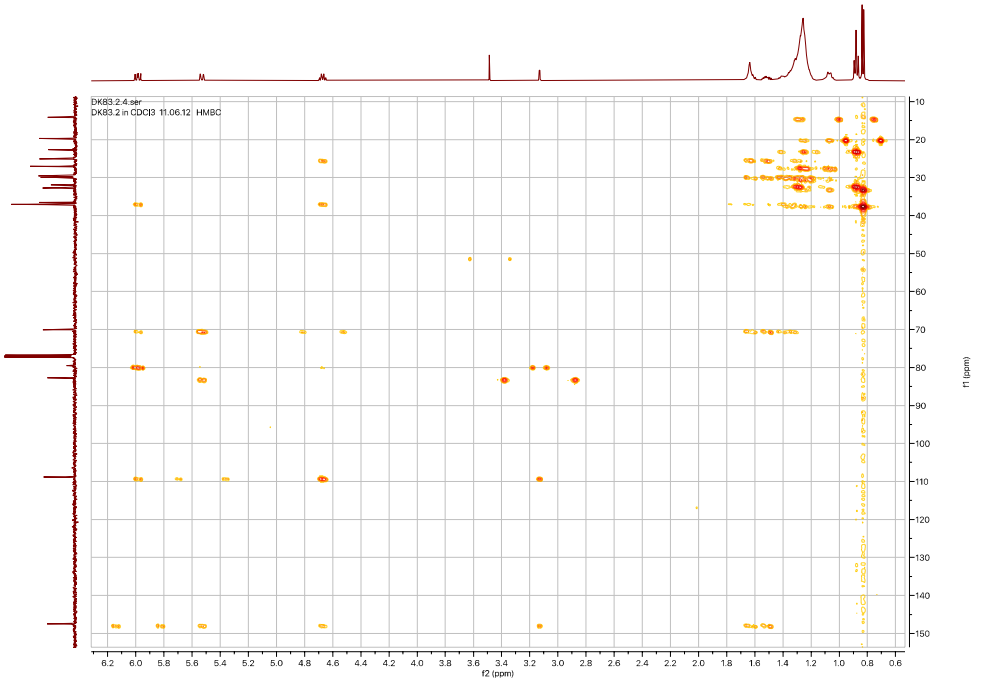


Figure S88. COSY spectrum of (5*S*)-14-methylicos-(3*Z*)-en-1-yn-5-ol (**14**) in $CDCl_3$

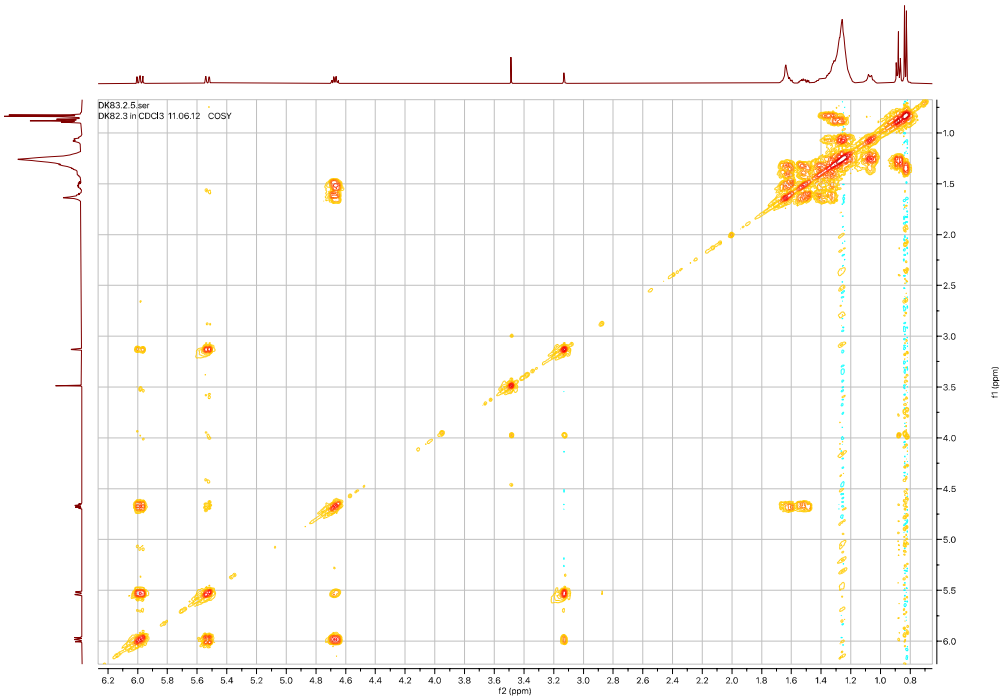


Figure S89. DEPT spectrum of (5*S*)-14-methylicos-(3*Z*)-en-1-yn-5-ol (**14**) in $CDCl_3$

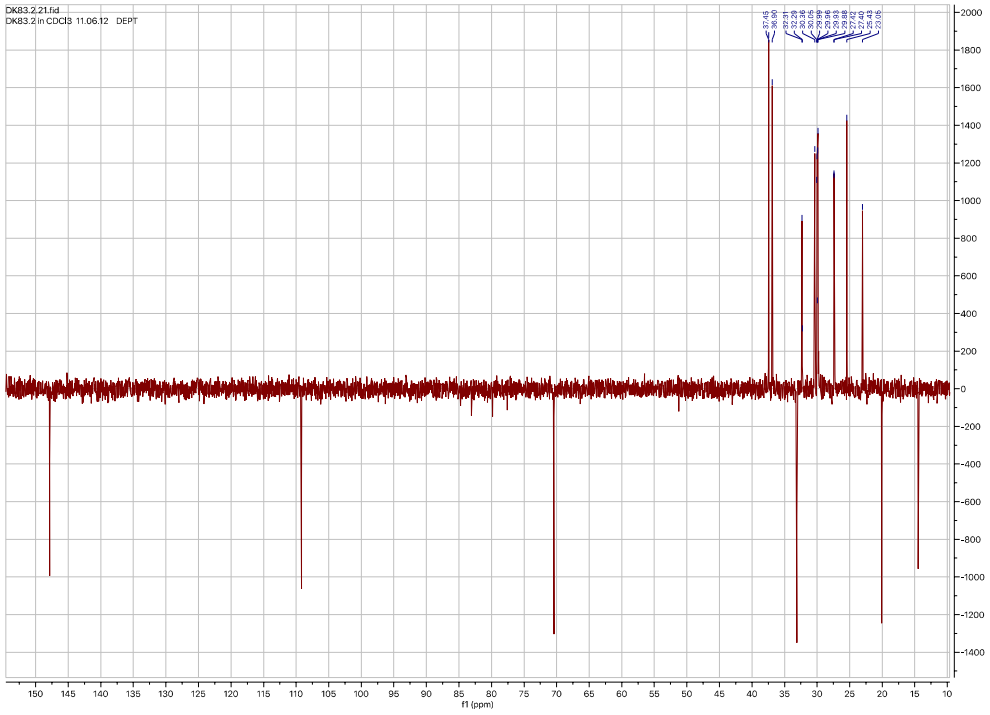
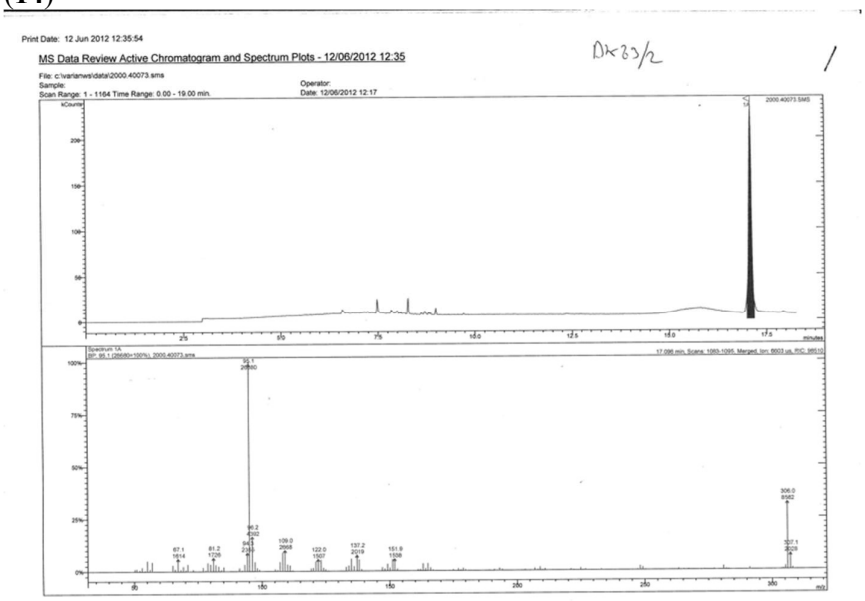


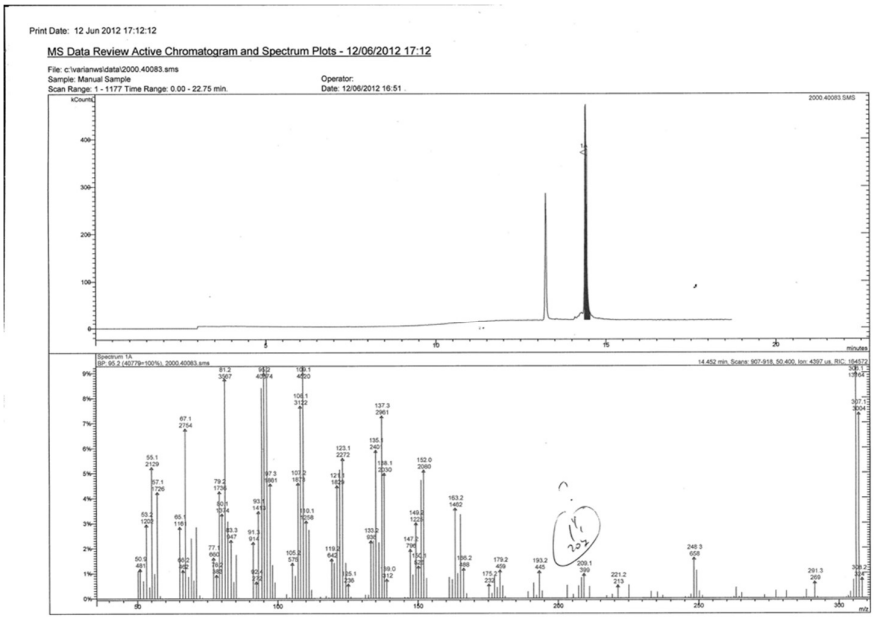
Table S14. NMR data of (5*S*)-14-methylicos-(3*Z*)-en-1-yn-5-ol (**14**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	82.7[d] CH	3.13 dd (3.5, 1.0)	3
2	79.5[e] qC	-	1, 4
3	108.8 CH	5.53 dd (11.0, 3.5, 1.0)	1, 4, 5
4	147.5 CH	5.98 ddd (11.0, 8.0, 1.0)	1, 3, 5, 6a, 6b
5	70.0 CH	4.67 qd (8.0, 1.0)	3, 4, 6a, 6b, 7a, 7b
6a	36.5 CH_2	1.62 m	4, 5, 7a, 7b, 8
b		1.52 m	
7a	25.1 CH_2	1.41 m	5, 6a, 6b, 8
b		1.32 m	
8-11	~29.6[f] 4 × CH_2	1.21 – 1.33 brm	
12	27.1 CH_2	1.26 m	11, 13a, 13b
13a	37.1 CH_2	1.26 m	12, 14, 15a, 15b, 21
b		1.07 m	
14	32.7 CH	1.35 m	13a, 13b, 15a, 15a, 21
15a	37.1 CH_2	1.26 m	13a, 13b, 14, 16, 21
b		1.07 m	
16	27.1 CH_2	1.26 m	15a, 15b, 17
17	~29.6[f] CH_2	1.21 – 1.33 brm	
18	32.3 CH_2	1.26 m	17, 19a, 19b, 20
19a	22.7 CH_2	1.31 m	18, 20
b		1.26 m	
20	14.1 CH_3	0.88 t (7.0)	18, 19a, 19b
21	19.7 CH_3	0.83 d (6.5)	13b, 15b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 252.0 Hz; [e] ^2J = 49.1 Hz; [f]Exact ^{13}C chemical shifts 29.52, 29.56, 29.63, 29.67, 29.99 ppm.

Figure S90. EIGCMS spectrum and fragmentation of (5*S*)-14-methylicos-(3*Z*)-en-1-yn-5-ol (**14**)





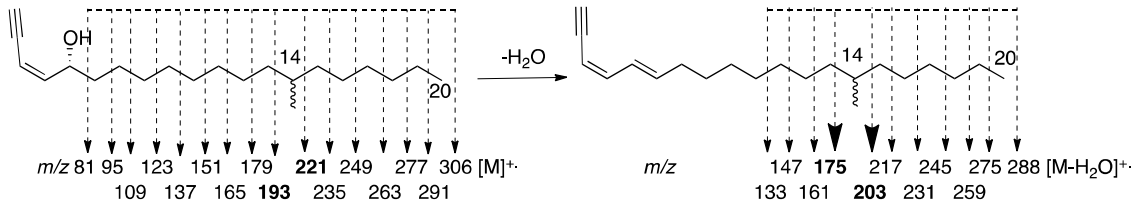


Figure S91. HRCIMS spectrum of (5*S*)-14-methylicos-(3*Z*)-en-1-yn-5-ol (**14**)

Compound Spectrum SmartFormula Report

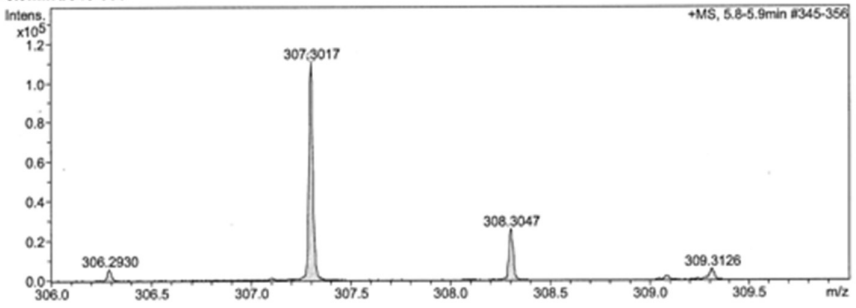
Analysis Info

Analysis Name	D:\Data\Client\CLI_9279_8.d	Acquisition Date	5/17/2015 10:53:27 AM
Method	CLI_9279.m	Operator	Larisa Panz
Sample Name	DK_83-2(14)	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 5.8-5.9min #345-356



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
307.3017	1	C21H39O	307.2995	-6.9	12.7	1	100.00	2.5	even	ok	2.1

Figure S92. ^{1}H NMR spectrum of (5*S*)-18-methylicos-(3*Z*)-en-1-yn-5-ol (**15**) and (5*S*)-19-methylicos-(3*Z*)-en-1-yn-5-ol (**16**) in $CDCl_3$

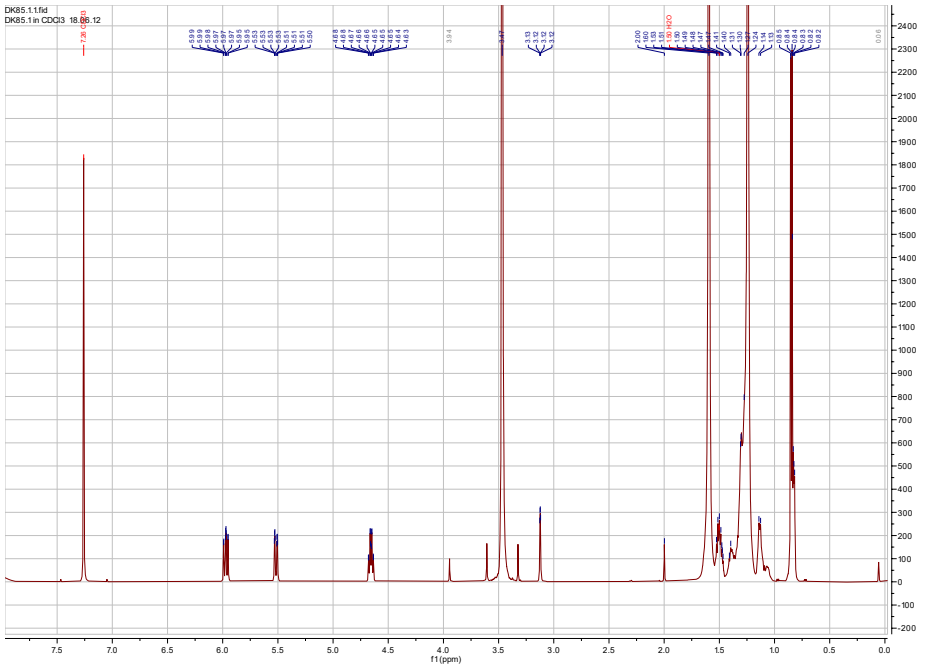


Figure S93. ^{13}C NMR spectrum of (5*S*)-18-methylicos-(3*Z*)-en-1-yn-5-ol (**15**) and (5*S*)-19-methylicos-(3*Z*)-en-1-yn-5-ol (**16**) in $CDCl_3$

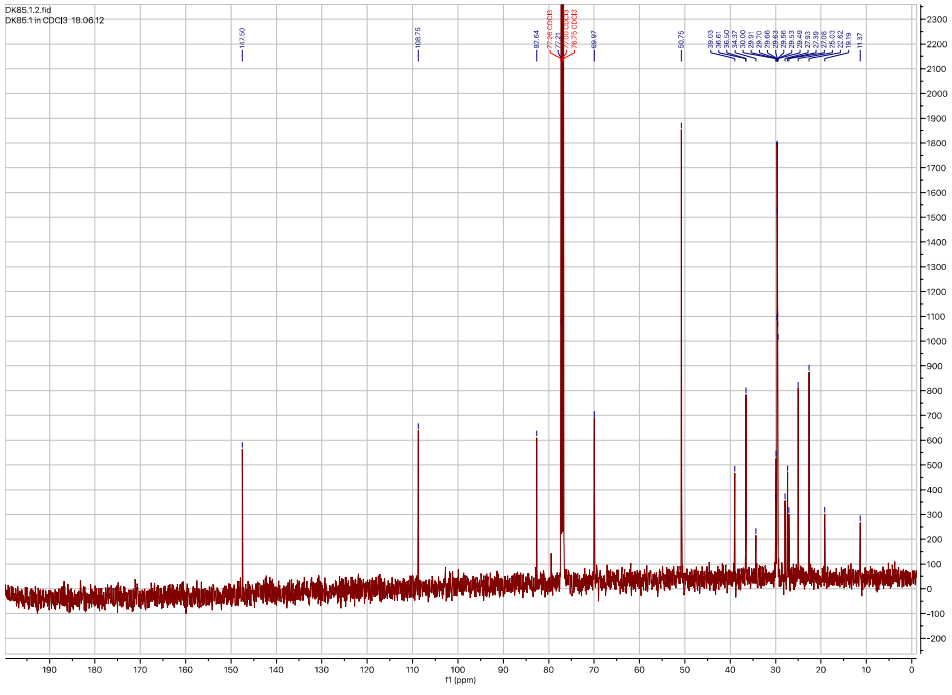


Figure S94. HSQC spectrum of (5*S*)-18-methylicos-(3*Z*)-en-1-yn-5-ol (**15**) and (5*S*)-19-methylicos-(3*Z*)-en-1-yn-5-ol (**16**) in $CDCl_3$

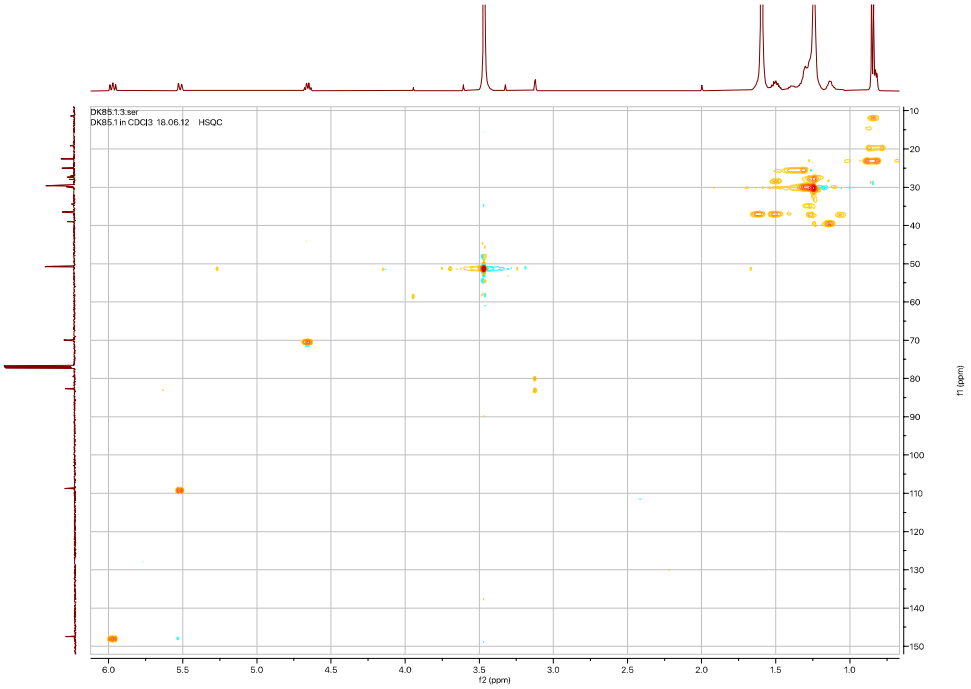


Figure S95. HMBC spectrum of (5*S*)-18-methylicos-(3*Z*)-en-1-yn-5-ol (**15**) and (5*S*)-19-methylicos-(3*Z*)-en-1-yn-5-ol (**16**) in $CDCl_3$

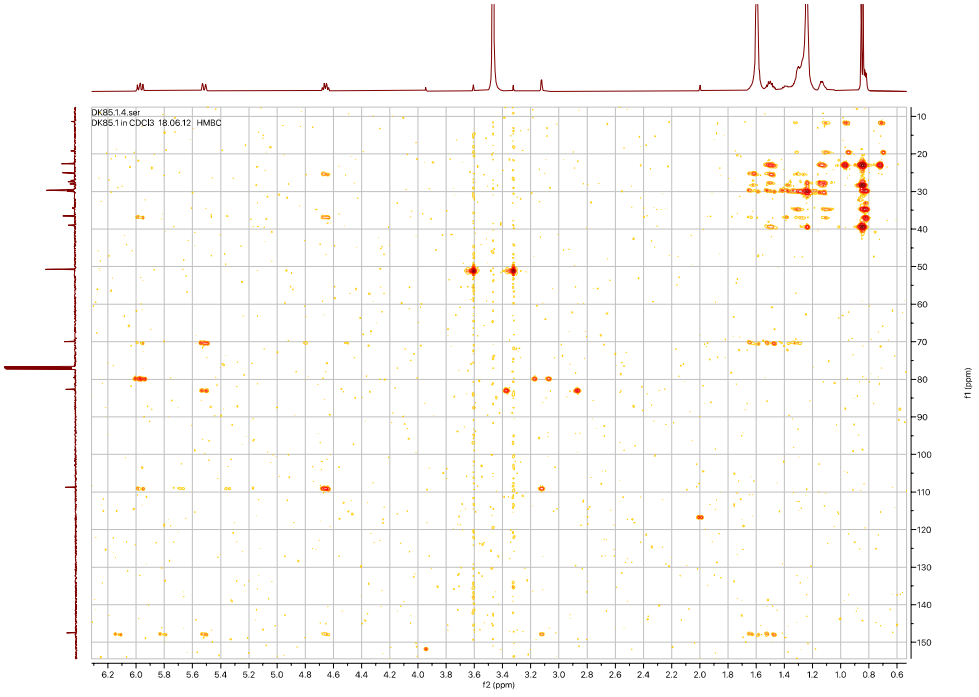


Figure S96. COSY spectrum of (5*S*)-18-methylicos-(3*Z*)-en-1-yn-5-ol (**15**) and (5*S*)-19-methylicos-(3*Z*)-en-1-yn-5-ol (**16**) in $CDCl_3$

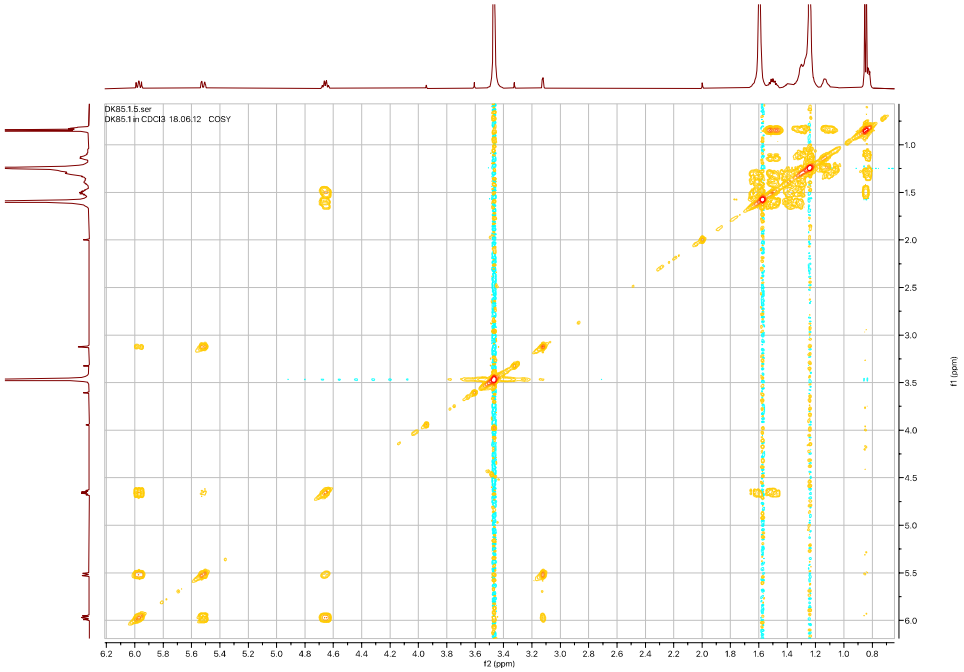


Figure S97. DEPT spectrum of (5*S*)-18-methylicos-(3*Z*)-en-1-yn-5-ol (**15**) and (5*S*)-19-methylicos-(3*Z*)-en-1-yn-5-ol (**16**) in $CDCl_3$

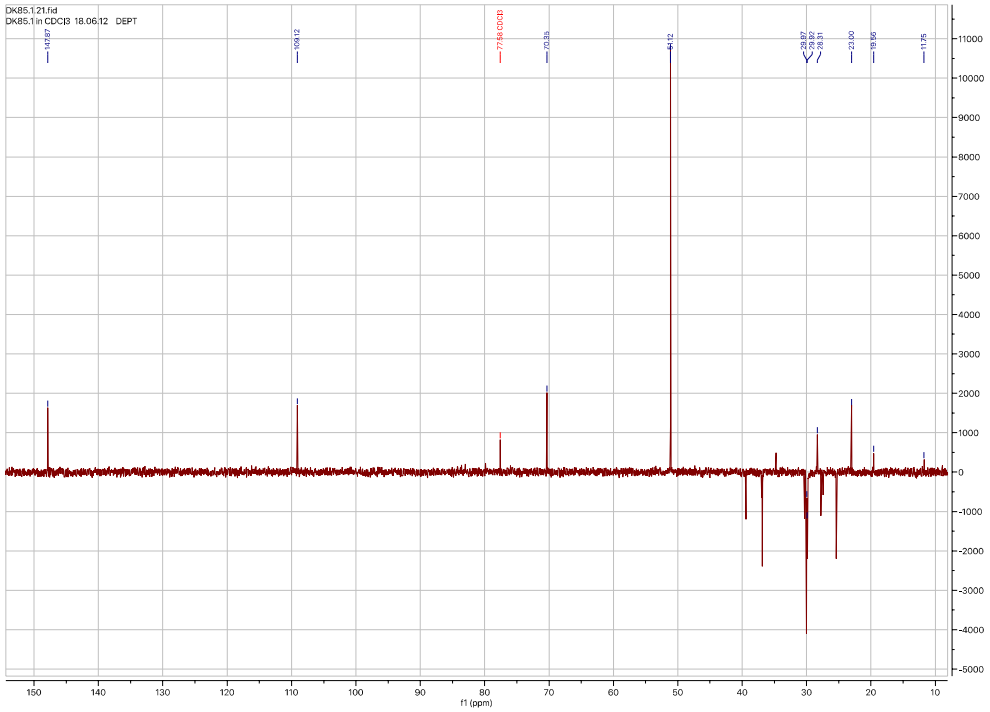


Table S15. NMR data of (5*S*)-18-methylicos-(3*Z*)-en-1-yn-5-ol (**15**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	82.6[d] CH	3.13 d (2.0)	3
2	79.6[e] qC	-	1, 4
3	108.7 CH	5.52 dd (11.0, 2.0)	1, 4, 5
4	147.5 CH	5.97 dd (11.0, 8.0)	1, 3, 5, 6a, 6b
5	70.0 CH	4.65 q (8.0)	3, 4, 6a, 6b, 7a, 7b
6a	36.5 CH_2	1.62 m	4, 5, 7a, 7b, 8
b		1.52 m	
7a	25.0 CH_2	1.39 m	5, 6a, 6b, 8
b		1.32 m	
8-15	~29.6[f] 8 × CH_2	1.22 – 1.30 brm	
16	27.1 CH_2	1.24 m	15, 17a, 17b
17a	36.6 CH_2	1.06 m	16, 18, 21
b		1.26 m	
18	34.4 CH	1.28 m	17a, 17b, 19a, 19b, 20, 21
19a	22.6 CH_2	1.31 m	20, 21
b		1.10 m	
20	11.4 CH_3	0.84 m	19a, 19b
21	19.2 CH_3	0.83 d (6.2)	17a, 17b, 18, 19a, 19b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 251.5 Hz; [e] ^2J = 50.6 Hz; [f]Exact ^{13}C chemical shifts 29.53, 29.56, 29.66 (× 3), 29.70, 29.91, 30.00 ppm.

Table S16. NMR data of (5*S*)-19-methylicos-(3*Z*)-en-1-yn-5-ol (**16**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	82.6[d] CH	3.13 d (2.0)	3
2	79.6[e] qC	-	1, 4
3	108.7 CH	5.52 dd (10.5, 2.0)	1, 4, 5
4	147.5 CH	5.97 dd (10.5, 8.0)	1, 3, 5, 6a, 6b
5	70.0 CH	4.65 q (8.0)	3, 4, 6a, 6b, 7a, 7b
6a	36.5 CH_2	1.62 m	4, 5, 7a, 7b, 8
b		1.52 m	
7a	25.0 CH_2	1.39 m	5, 6a, 6b, 8
b		1.32 m	
8-16	~29.6[f] 9 × CH_2	1.22 – 1.30 brm	
17	27.4 CH_2	1.24 m	16, 18
18	39.0 CH_2	1.13 m	17, 19, 20, 21
19	27.9 CH	1.50 m	18, 20, 21
20	22.6 CH_3	0.85 d (6.5)	18, 19, 21
21	22.6 CH_3	0.85 d (6.5)	18, 19, 20

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 251.5 Hz; [e] ^2J = 50.6 Hz; [f]Exact ^{13}C chemical shifts 29.49, 29.53, 29.56, 29.66 (× 6) ppm.

Figure S98. EIGCMS spectrum of (5*S*)-18-methylicos-(3*Z*)-en-1-yn-5-ol (**15**)

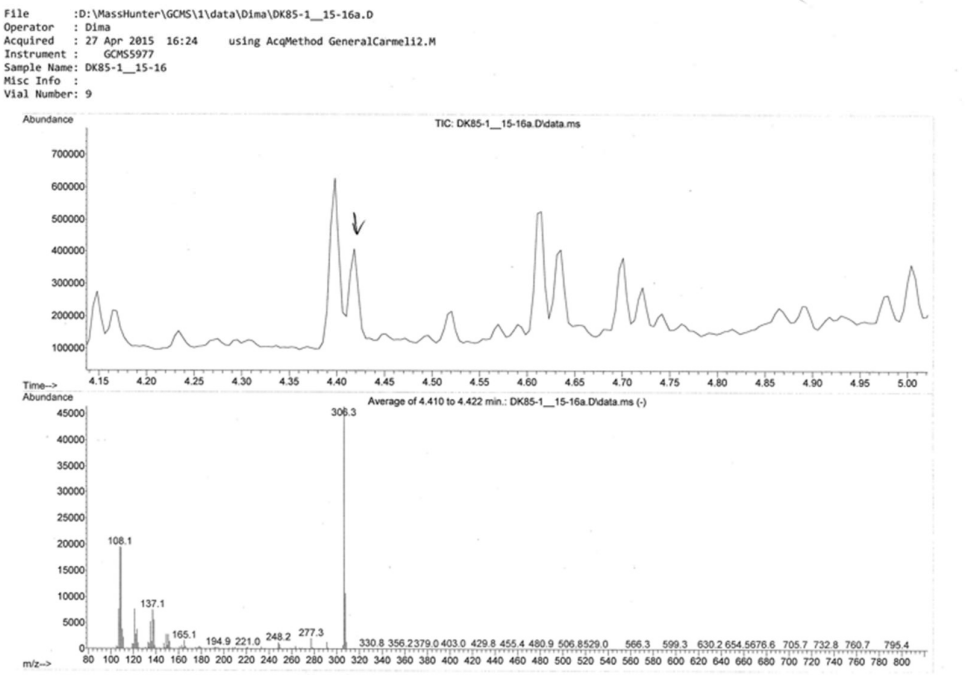


Figure S99. EIGCMS spectrum of (5*S*)-19-methylicos-(3*Z*)-en-1-yn-5-ol (**16**)

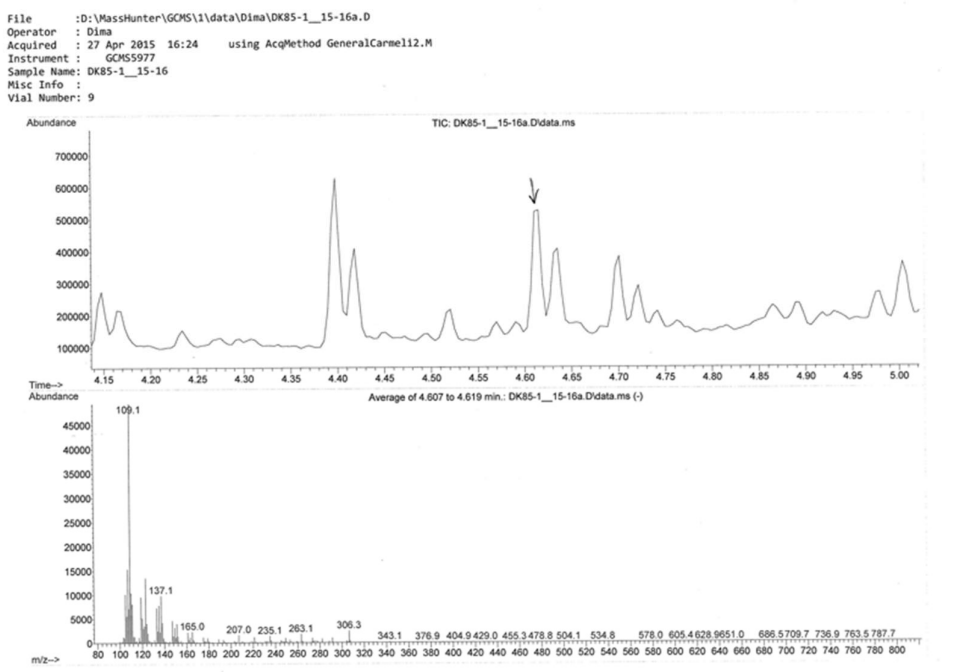


Figure S100. HRCIMS spectrum of (5*S*)-18-methylicos-(3*Z*)-en-1-yn-5-ol (**15**)

Compound Spectrum SmartFormula Report

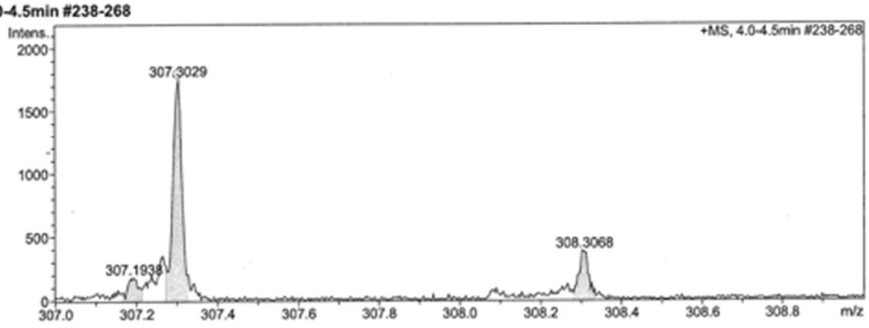
Analysis Info

Analysis Name	D:\Data\Client\CLI_9279_22000001.d	Acquisition Date	5/17/2015 1:38:53 PM
Method	GC APCI_pos_cli_8051.m	Operator	Larisa Panz
Sample Name	DK85.1(15+16) 15	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 4.0-4.5min #238-268



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
307.3029	1	C21H39O	307.2995	-10.9	106.6	1	100.00	2.5	even	ok	3.3

Figure S101. HRCIMS spectrum of (5*S*)-19-methylicos-(3*Z*)-en-1-yn-5-ol (**16**)

Compound Spectrum SmartFormula Report

Analysis Info

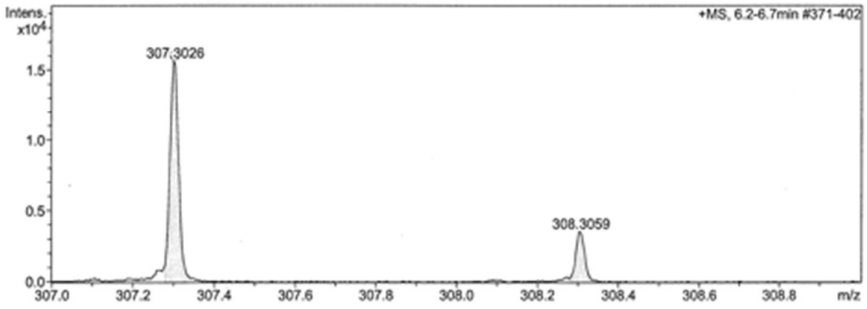
Acquisition Date 5/17/2015 1:38:53 PM

Analysis Name	D:\Data\Client\CLI_9279_22000001.d		
Method	GC APCI_pos_cli_8051.m	Operator	Larisa Panz
Sample Name	DK85.1(15+16)	Instrument	maXis impact 282001.00128
Comment	16		

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 6.2-6.7min #371-402



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
307.3026	1	C21H39O	307.2995	-9.9	27.5	1	100.00	2.5	even	ok	3.0

CLI_9279_22000001.d
Bruker Compass DataAnalysis 4.2 printed: 5/17/2015 1:49:56 PM by: Larisa Panz Page 1 of 1

Figure S102. ^{1}H NMR spectrum of 14-methyldocos-(3*Z*)-en-1-yn-5,6-diol (**17**) in $CDCl_3$

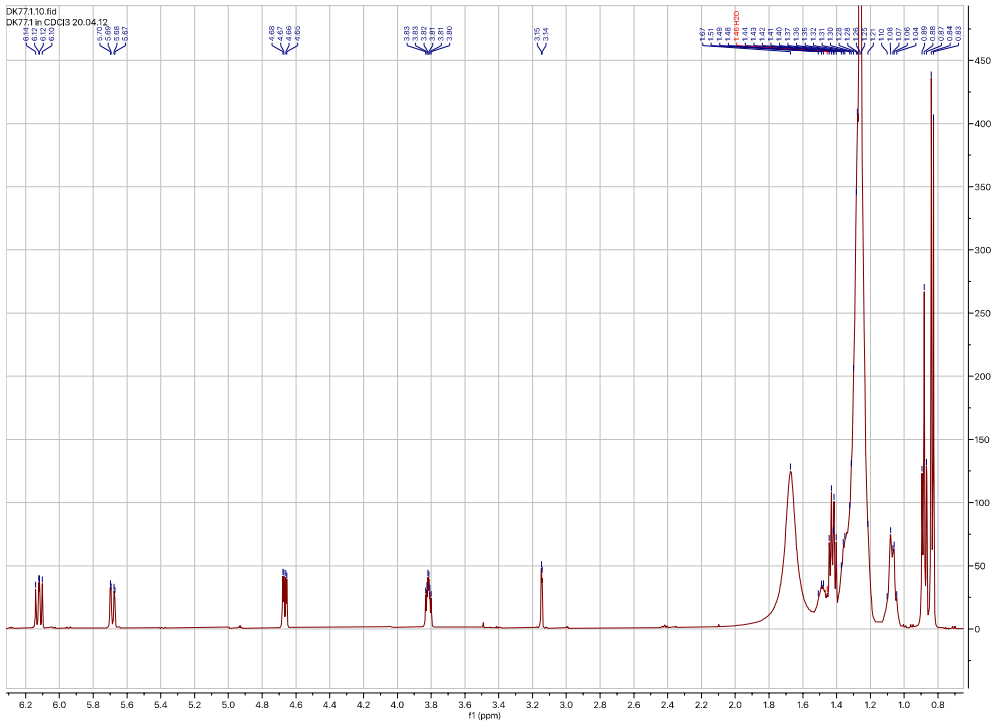


Figure S103. ^{13}C NMR spectrum of 14-methyldocos-(3*Z*)-en-1-yn-5,6-diol (**17**) in $CDCl_3$

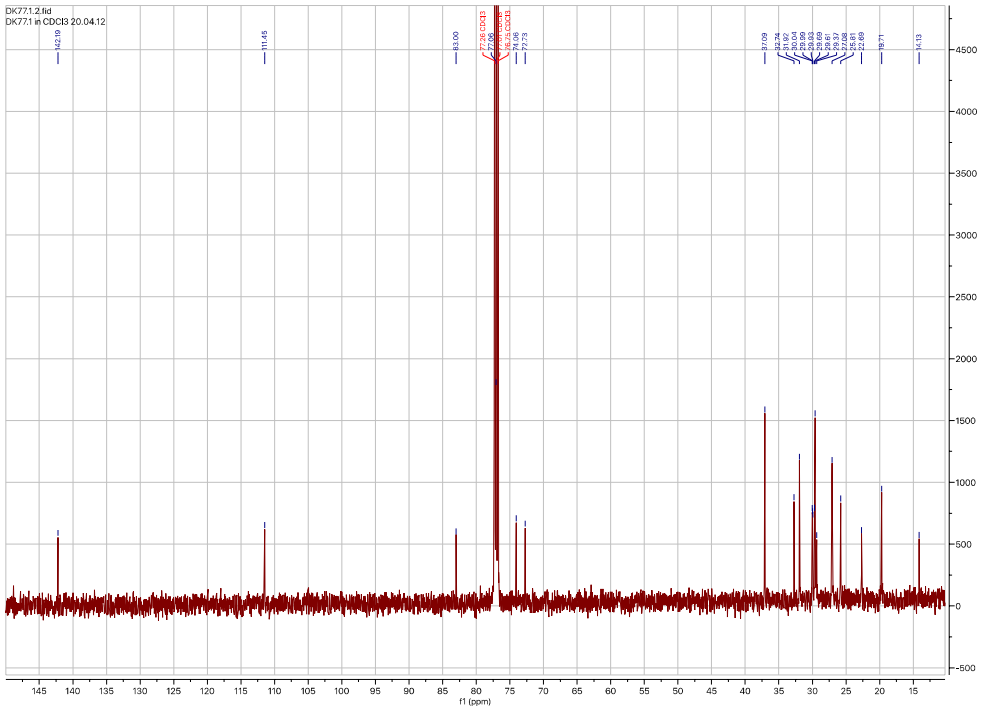


Figure S104. HSQC spectrum of 14-methyldocos-(3*Z*)-en-1-yn-5,6-diol (**17**) in $CDCl_3$

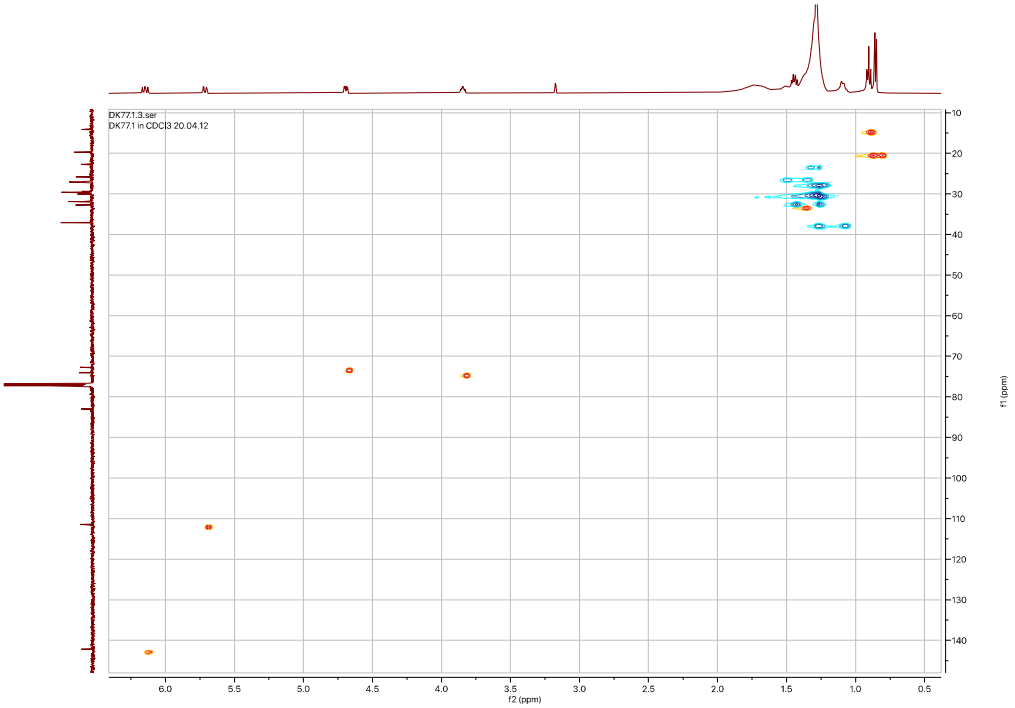


Figure S105. HMBC spectrum of 14-methyldocos-(3*Z*)-en-1-yn-5,6-diol (**17**) in $CDCl_3$

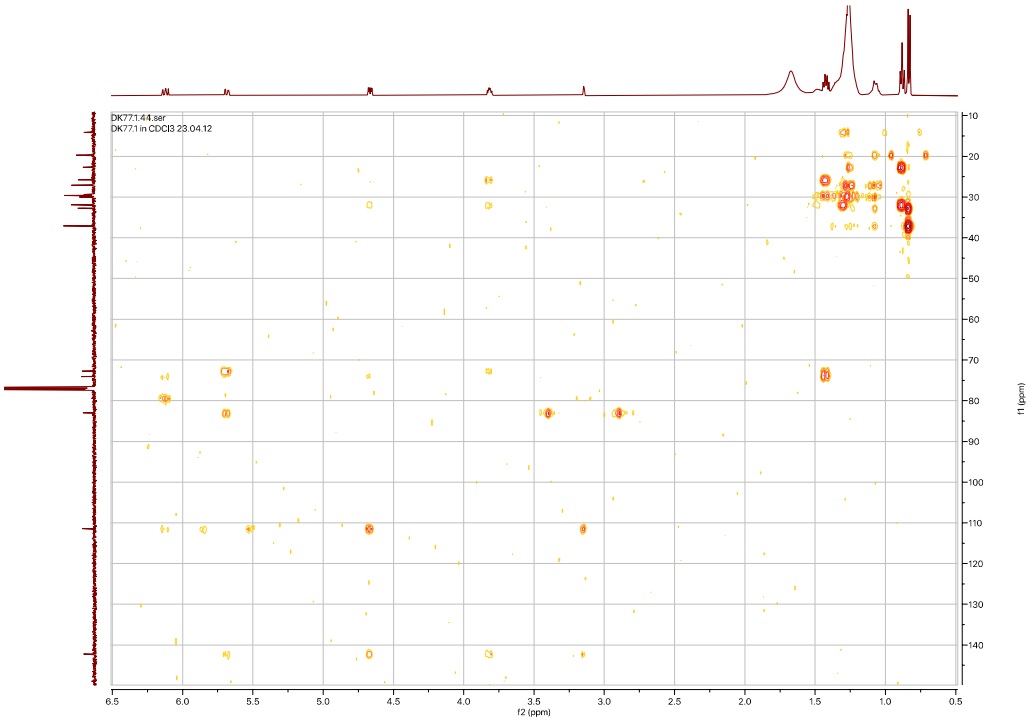


Figure S106. COSY spectrum of 14-methyldocos-(3*Z*)-en-1-yn-5,6-diol (**17**) in $CDCl_3$

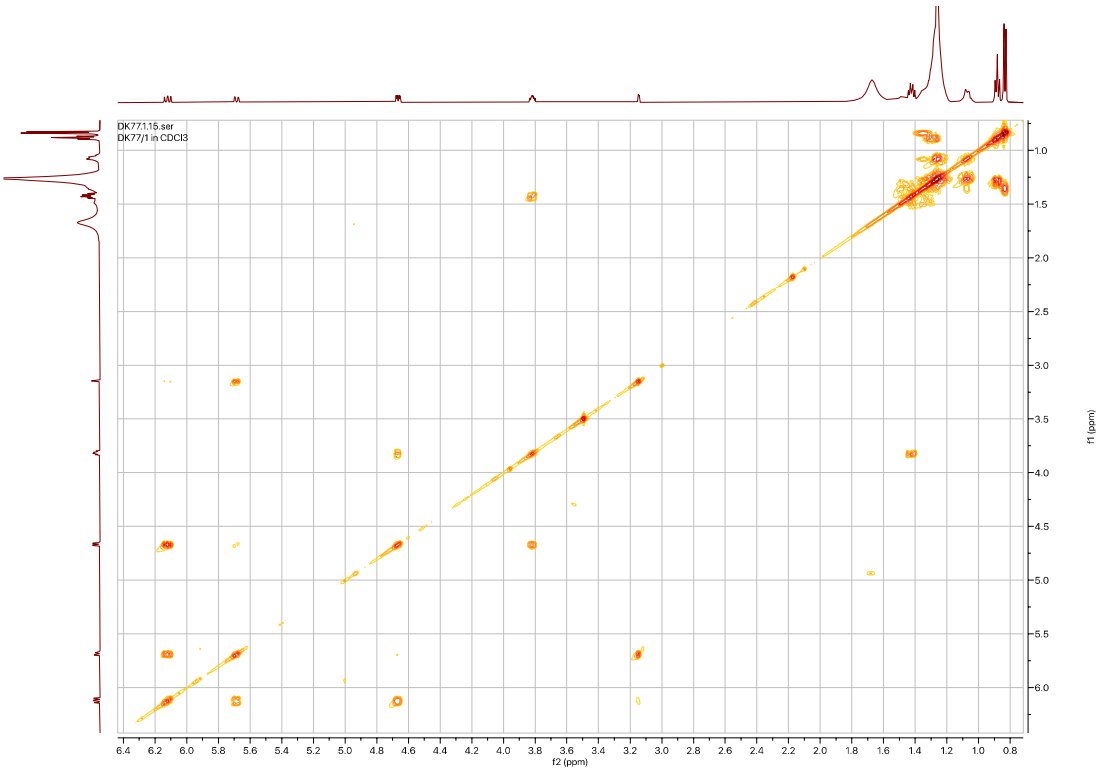


Table S17. NMR data of 14-methyldocos-(3*Z*)-en-1-yn-5,6-diol (**17**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	83.0[d] CH	3.16 d (1.5)	3
2	79.3[e] qC	-	1, 4
3	111.4 CH	5.68 dd (11.0, 1.5)	1, 4, 5
4	147.5 CH	6.12 dd (11.0, 9.0)	1, 3, 5, 6
5	72.7 CH	4.68 dd (9.0,3.0)	3, 6, 7
6	74.1 CH	3.82 td (6.5, 3.0)	4, 5, 7
7	31.9 CH_2	1.43 q (6.5)	5, 6, 8a, 8b
8a	25.8 CH_2	1.49 m	6, 7
b		1.34 m	
9	29.4 CH_2	1.28 m	7
10-11	~29.6[f] 2 × CH_2	1.24 – 1.28 brm	
12	27.1 CH_2	1.25 m	11, 13a, 13b
13a	37.1 CH_2	1.26 m	14, 15a, 15b, 23
b		1.06 m	
14	32.7 CH	1.35 m	13a, 13b, 15a, 15b, 23
15a	37.1 CH_2	1.26 m	13a, 13b, 14, 23
b		1.06 m	
16	27.1 CH_2	1.25 m	15a, 15b, 17
17-19	~29.6[f] 3 × CH_2	1.24 – 1.28 brm	
20	31.9 CH	1.25 m	19, 21a, 21b, 22
21a	22.7 CH_2	1.32 m	20, 22
b		1.26 m	
22	14.1 CH_3	0.84 t (6.5)	21a, 21b
23	19.7 CH_3	0.83 d (6.5)	13a, 13b, 14, 15a, 15b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 250.5 Hz; [e] ^2J = 45.0 Hz; [f]Exact ^{13}C chemical shifts 29.61, 29.69, 29.93, 29.98, 30.03 ppm.

Figure S107. EIMS and fragmentation pattern of 14-methyldocos-(3*Z*)-en-1-yn-5,6-diol (**17**)

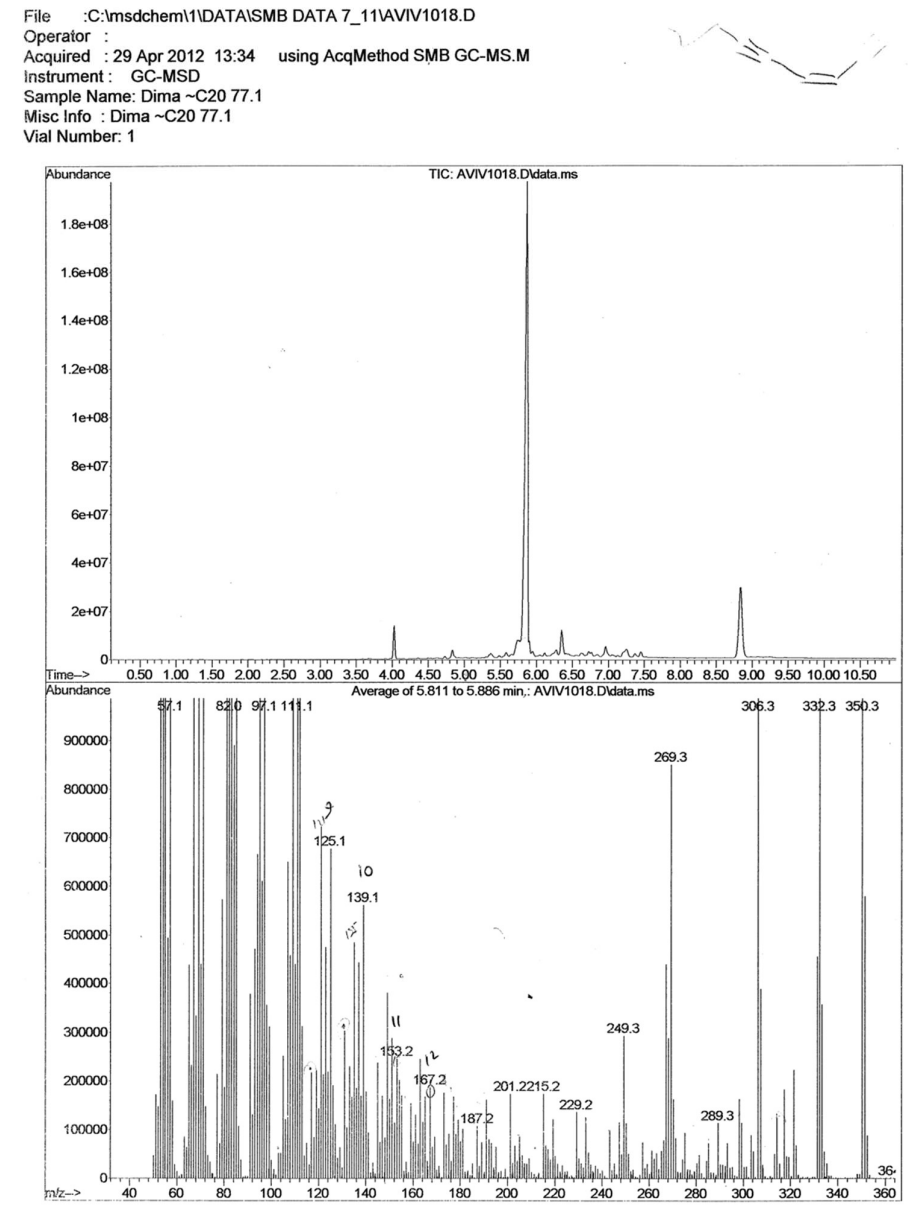


Figure S108. ^{1}H NMR spectrum of (3*R*)-icos-(4*E*)-en-1-yn-3-ol (**18**) in $CDCl_3$

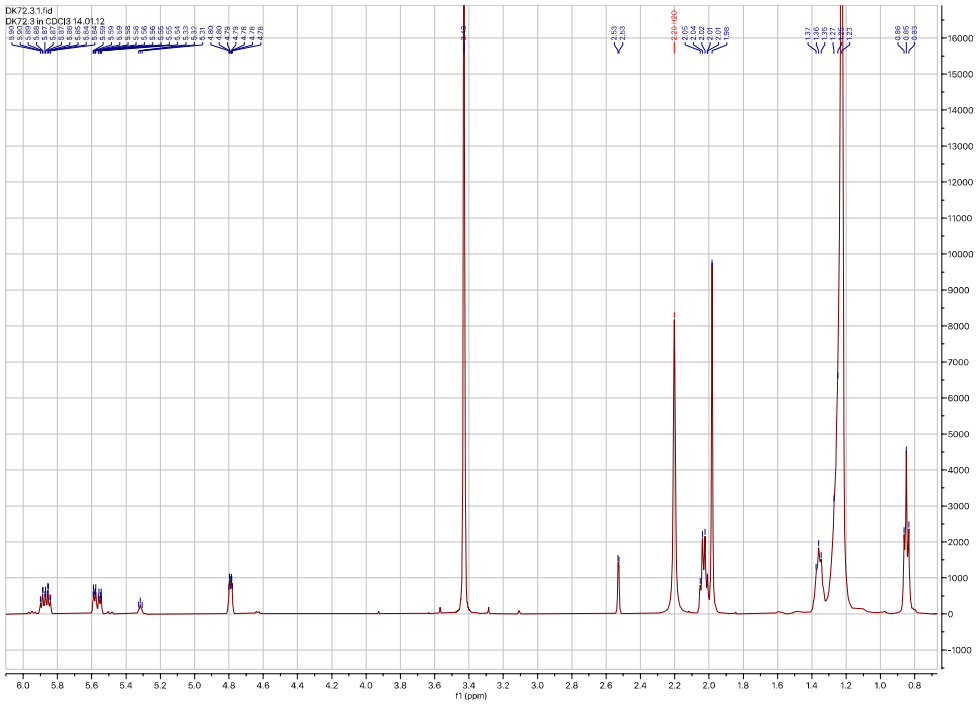


Figure S109. ^{13}C NMR spectrum of(3*R*)-icos-(4*E*)-en-1-yn-3-ol (**18**) in $CDCl_3$

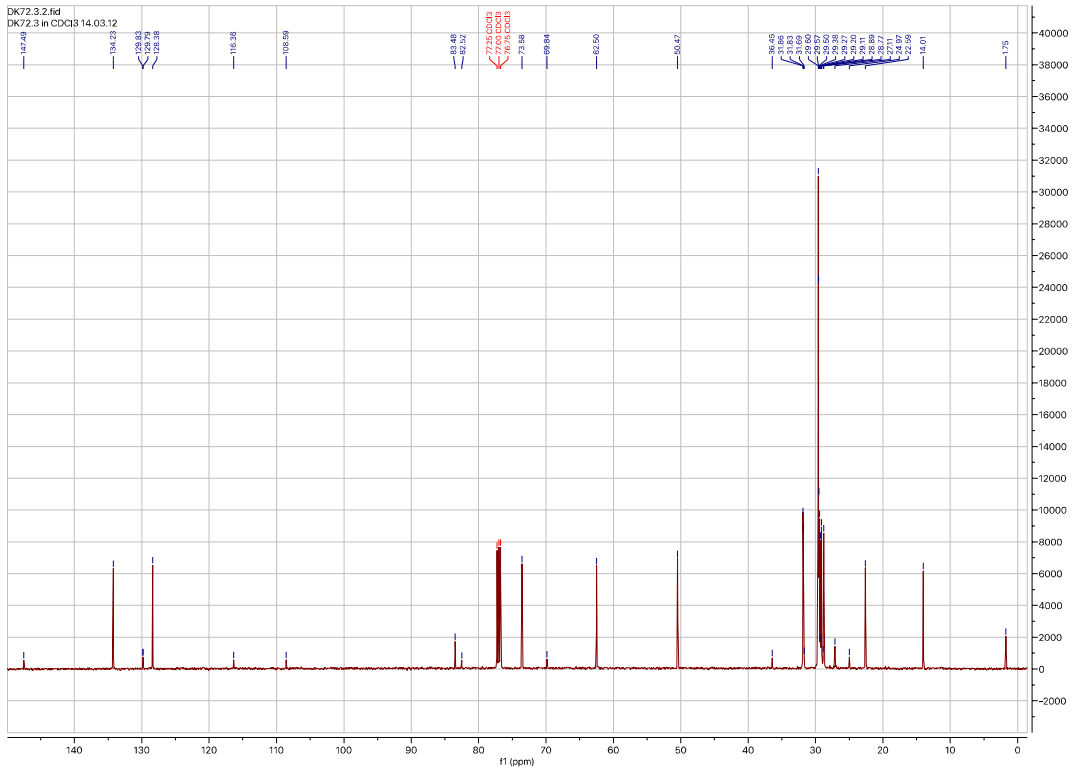


Figure S110. HSQC spectrum of(3*R*)-icos-(4*E*)-en-1-yn-3-ol (**18**) in $CDCl_3$.

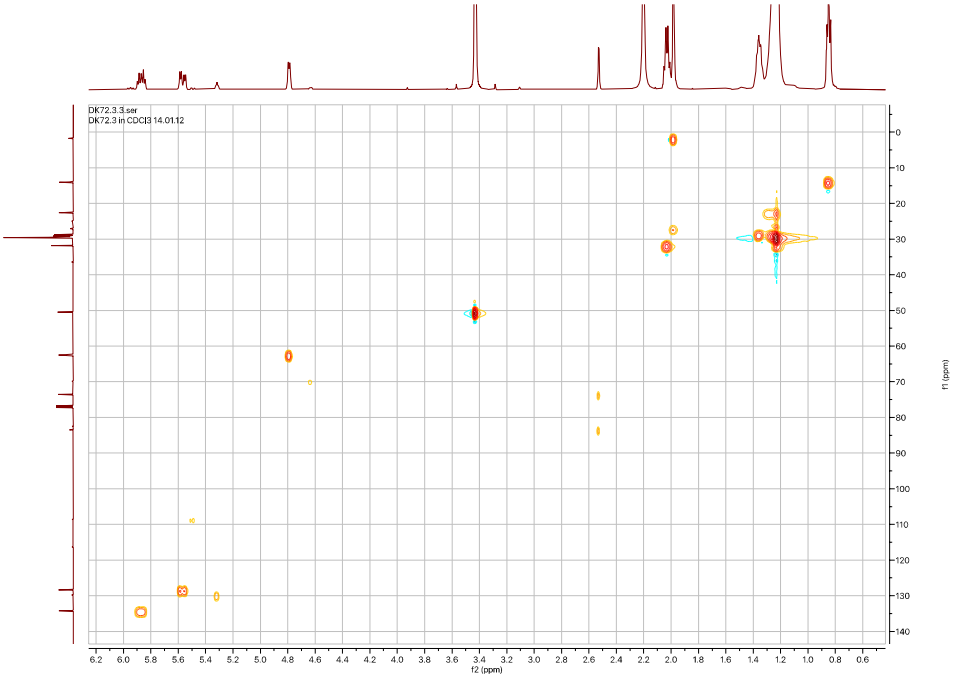


Figure S111. HMBC spectrum of(3*R*)-icos-(4*E*)-en-1-yn-3-ol (**18**) in $CDCl_3$.

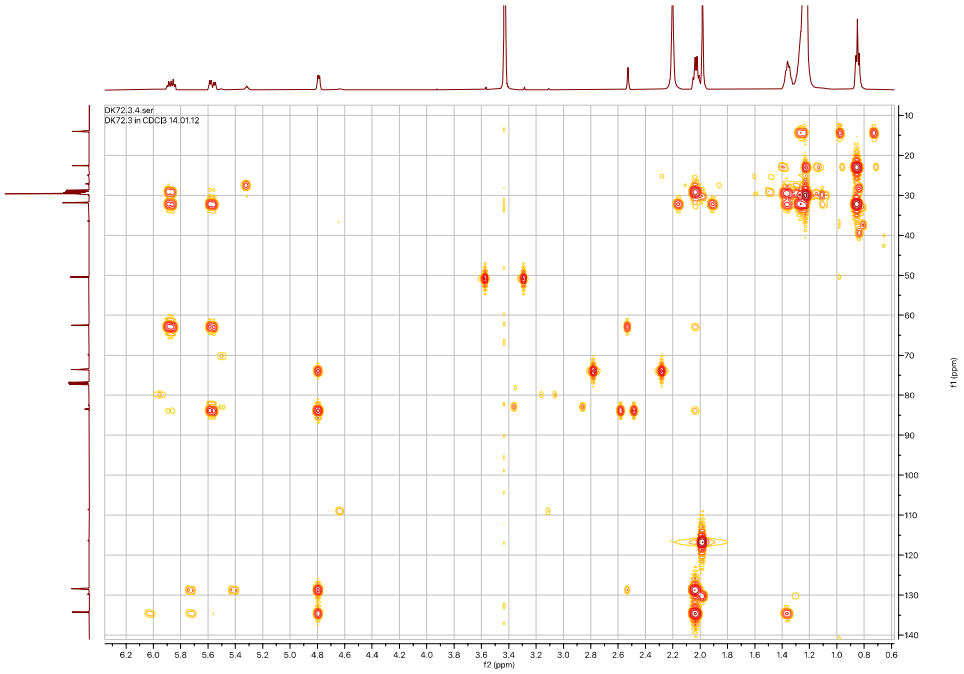


Figure S112. COSY spectrum of(3*R*)-icos-(4*E*)-en-1-yn-3-ol (**18**) in $CDCl_3$.

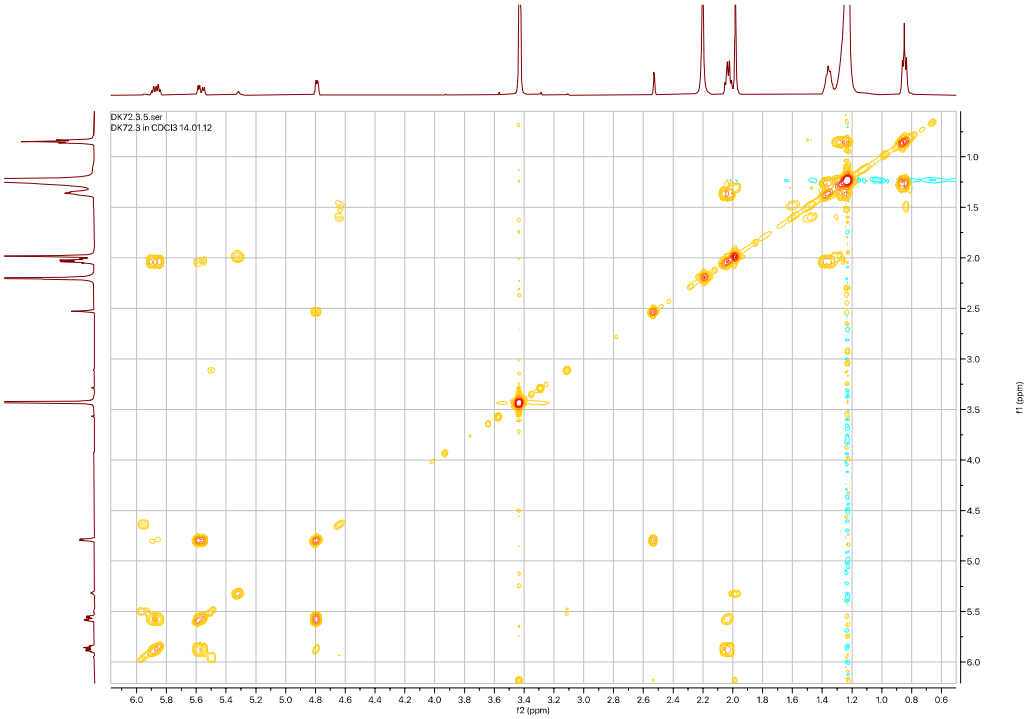


Figure S113. DEPT spectrum of(3*R*)-icos-(4*E*)-en-1-yn-3-ol (**18**) in $CDCl_3$.

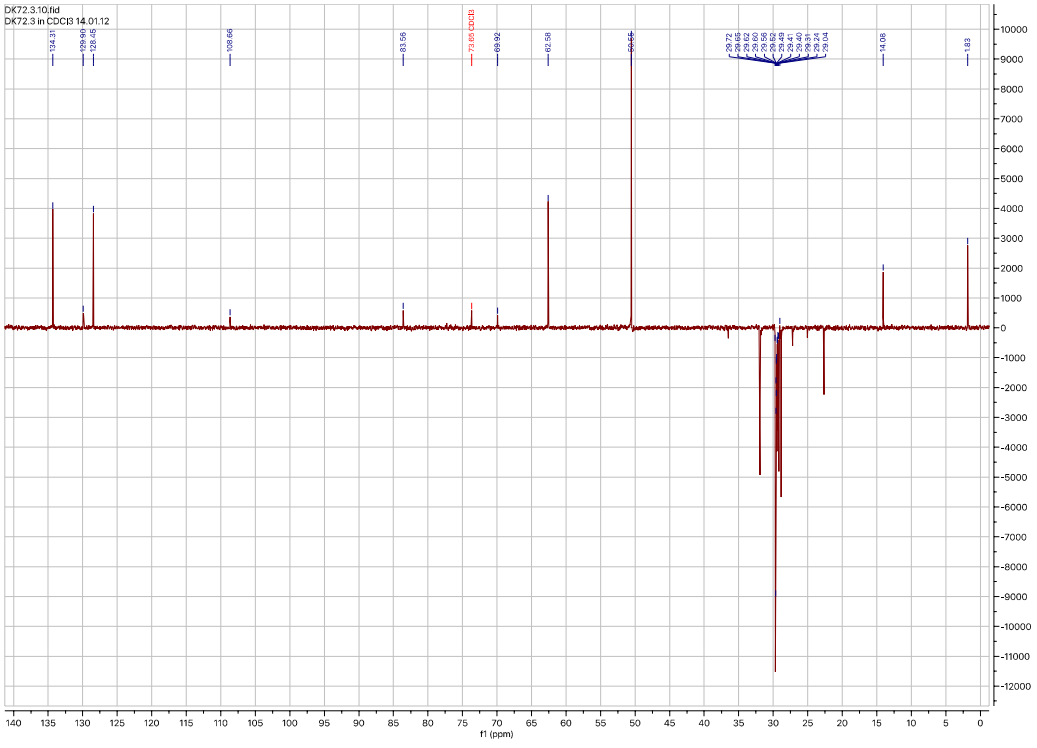


Table S18. NMR data of (3*R*)-icos-(4*E*)-en-1-yn-3-ol (**18**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.6[d] CH	2.53 d (2.0)	3
2	83.5[e] qC	-	1, 3, 4
3	62.5 CH	4.79 d (6.0)	1, 4, 5
4	128.4 CH	5.56 dd (15.5, 6.0)	3, 6
5	134.5 CH	5.87 dt (15.5, 7.0)	3, 6, 7
6	31.9 CH_2	2.03 q (7.0)	5, 7, 8
7	28.8 CH_2	1.36 m	5, 6, 8
8-17	~29.6[f] 10 × CH_2	1.21 – 1.28 brm	
18	31.8 CH	1.23 m	17, 19a, 19b, 20
19a	22.6 CH_2	1.36 m	18, 20
b		1.26 m	
20	14.0 CH_3	0.85 t (7.0)	18, 19b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 250.0 Hz; [e] ^2J = 48.4 Hz; [f]Exact ^{13}C chemical shifts 29.10, 29.26, 29.38 , 29.59 (× 6), 29.50 ppm.

Figure S114. EIGCMS spectrum of (3*R*)-icos-(4*E*)-en-1-yn-3-ol (**18**)

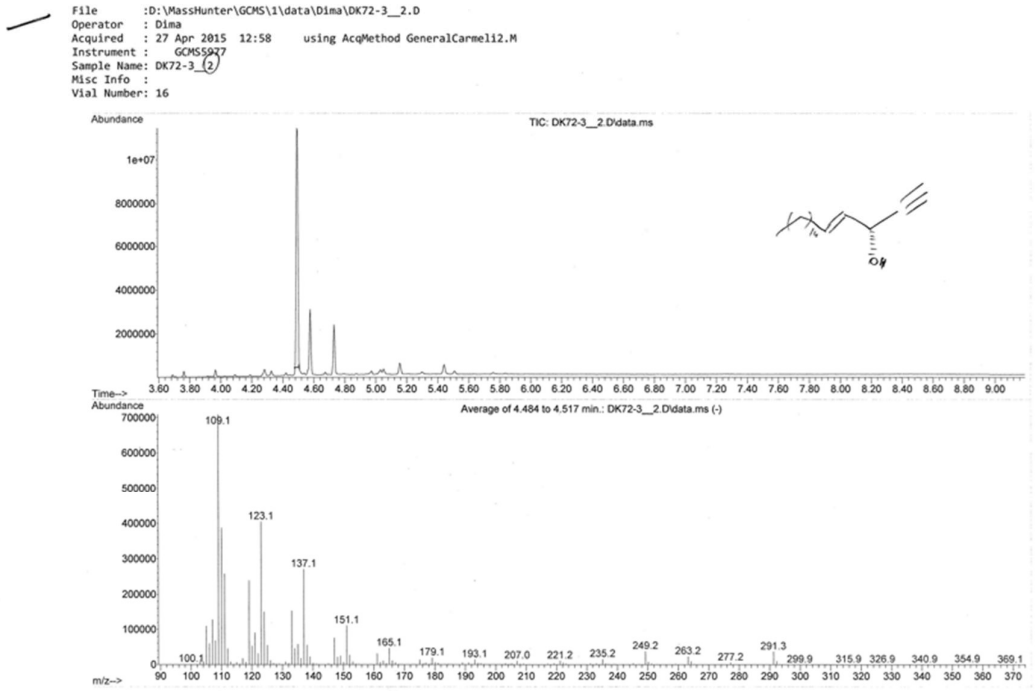


Figure S115. HRCIMS spectrum of (3*R*)-icos-(4*E*)-en-1-yn-3-ol (**18**)

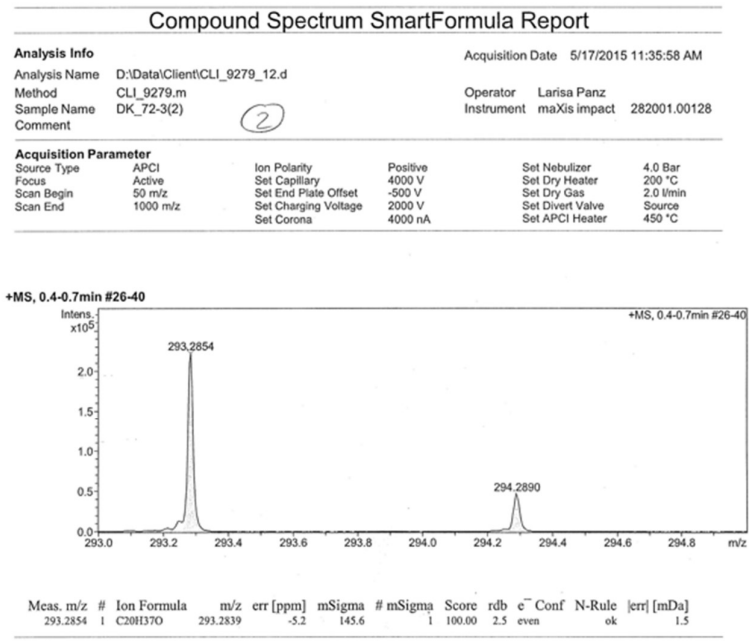


Figure S116. ^{1}H NMR spectrum of (3*R*)-19-methylicos-(4*E*)-en-1-yn-3-ol (**19**) in $CDCl_3$

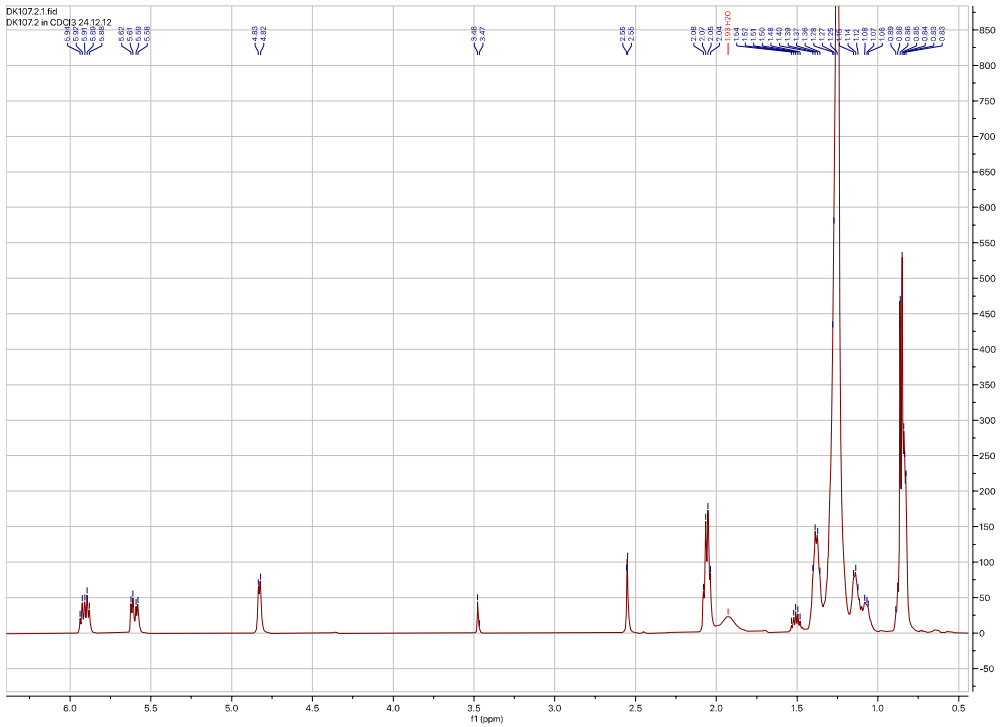


Figure S117. ^{13}C NMR spectrum of (3*R*)-19-methylicos-(4*E*)-en-1-yn-3-ol (**19**) in $CDCl_3$

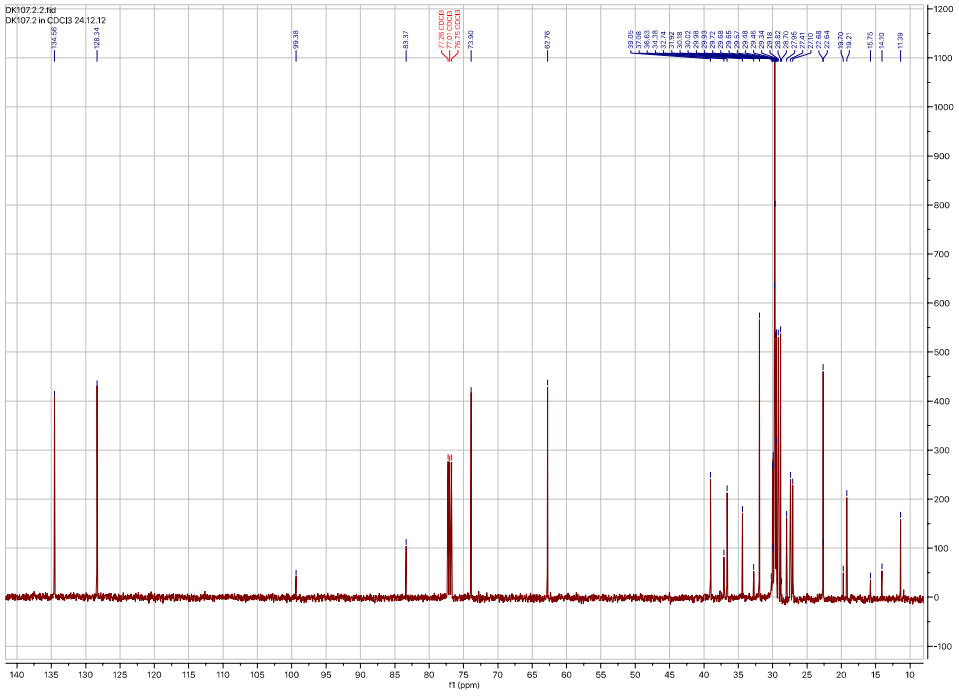


Table S19. NMR data of (3*R*)-19-methylicos-(4*E*)-en-1-yn-3-ol (**19**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.9[d] CH	2.55 d (2.0)	3
2	83.4[e] qC	-	1, 3, 4
3	62.8 CH	4.82 d (6.0)	1, 4, 5
4	128.3 CH	5.59 dd (15.0, 6.0)	3, 6
5	134.6 CH	5.90 dt (15.0, 7.0)	3, 6, 7
6	31.9 CH_2	2.05 q (7.0)	4, 5, 7, 8
7	28.8 CH_2	1.38 m	5, 6, 8
8-16	~29.6[f] 9 × CH_2	1.22 – 1.31 brm	
17	27.4 CH_2	1.24 m	16, 18
18	39.0 CH_2	1.14 m	17, 19, 20, 21
19	27.9 CH	1.50 qqt (6.0, 6.0, 6.0)	18, 20, 21
20	22.6 CH_3	0.85 d (6.0)	18, 19, 21
21	22.6 CH_3	0.85 d (6.0)	18, 19, 20

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 250.0 Hz; [e] ^2J = 49.0 Hz; [f]Exact ^{13}C chemical shifts 29.45, 29.57, 29.67 (× 6), 29.71 ppm.

Figure S118. HRCIMS spectrum of (3*R*)-19-methylicos-(4*E*)-en-1-yn-3-ol (**19**)

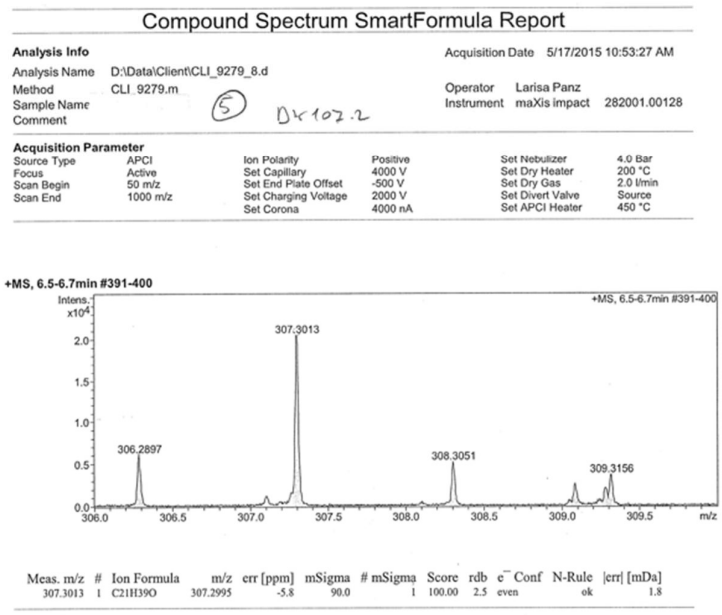


Figure S119. ^{1}H NMR spectrum of (3*R*)-henicos-(4*E*)-en-1-yn-3-ol (**20**) in $CDCl_3$

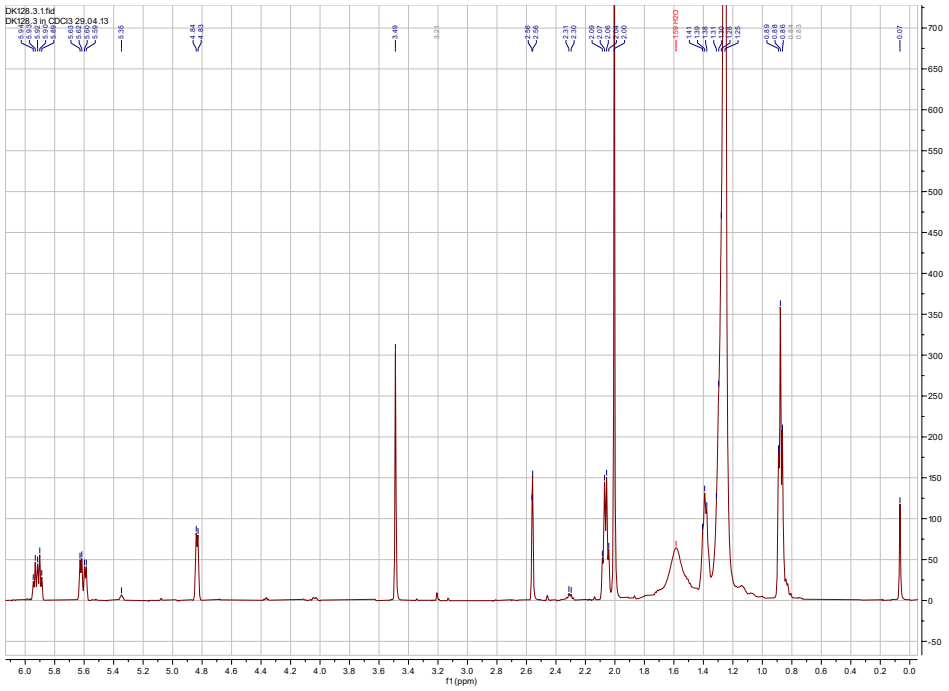


Table S20. NMR data of (3*R*)-henicos-(4*E*)-en-1-yn-3-ol (**20**) in $CDCl_3$.[a]

Position	δ_H, mult. *J* (Hz)	δ_H, mult. *J* (Hz) published[b]
1	2.56 s	2.54 d 12.0)
2	-	-
3	4.83 d (6.0)	4.82 d (5.5)
4	5.61 dd (15.0, 6.0)	5.58 ddt (15.0, 5.5, 1.0)
5	5.90 dt (15.0, 7.0)	5.90 dtd (15.0, 7.0, 1.0)
6	2.07 q (7.0)	2.04 q (7.0)
7	1.39 m	1.23 - 1.36 m
8-18	1.23 – 1.30 brm	1.23 – 1.36 m
19	1.25 m	1.23 – 1.36 m
20a	1.39 m	1.23 – 1.36 m
b	1.28 m	1.23 – 1.36 m
21	0.88 t (6.5)	0.86 t (7.0)

[a]500.13 MHz for ^{1}H and 125.76 MHz for ^{13}C; [b]Hallock. Y. F.; Cardelina II, J. H.; Balaschak, M. S.; Alexander, M. R.; Prather, T.R.; Shoemaker, R. H.; Boyd, M. R. *J. Nat. Prod.* **1995**, *58*, 1801-1807.

Figure S120. CIGCMS spectrum of (3*R*)-henicos-(4*E*)-en-1-yn-3-ol (**20**)

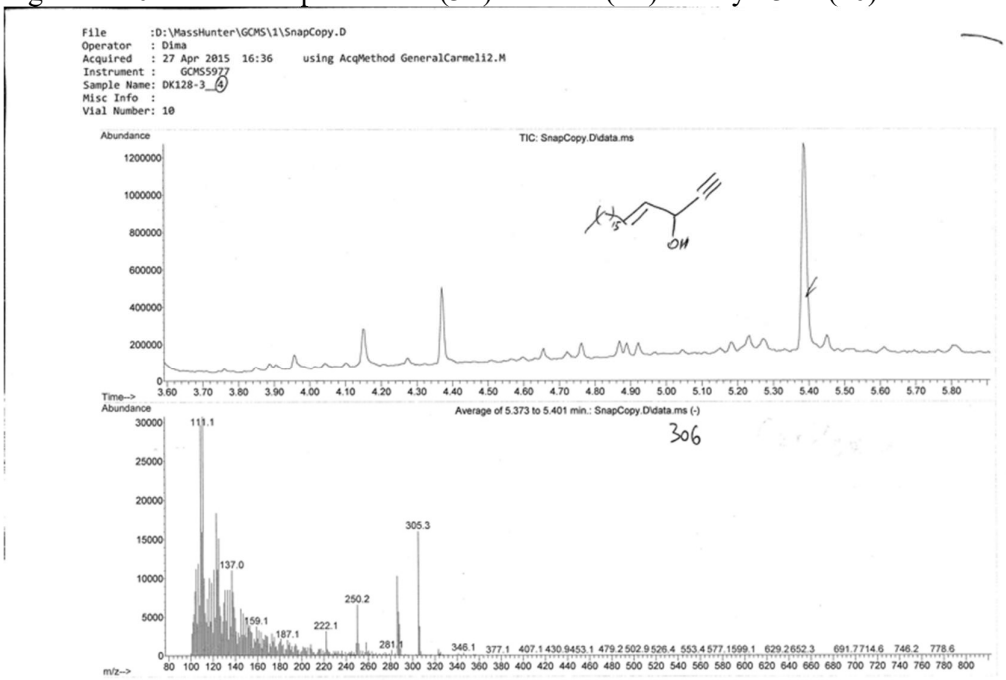


Figure S121. HRCIMS of (3*R*)-henicos-(4*E*)-en-1-yn-3-ol (**20**)

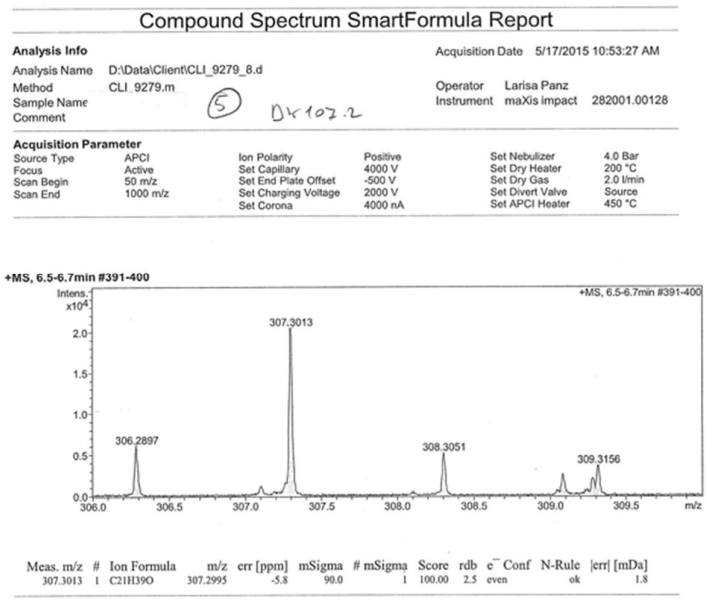


Figure S122. ^{1}H NMR spectrum of (3*R*)-docos-(4*E*,15*Z*)-dien-1-yn-3-ol (**21**) in $CDCl_3$

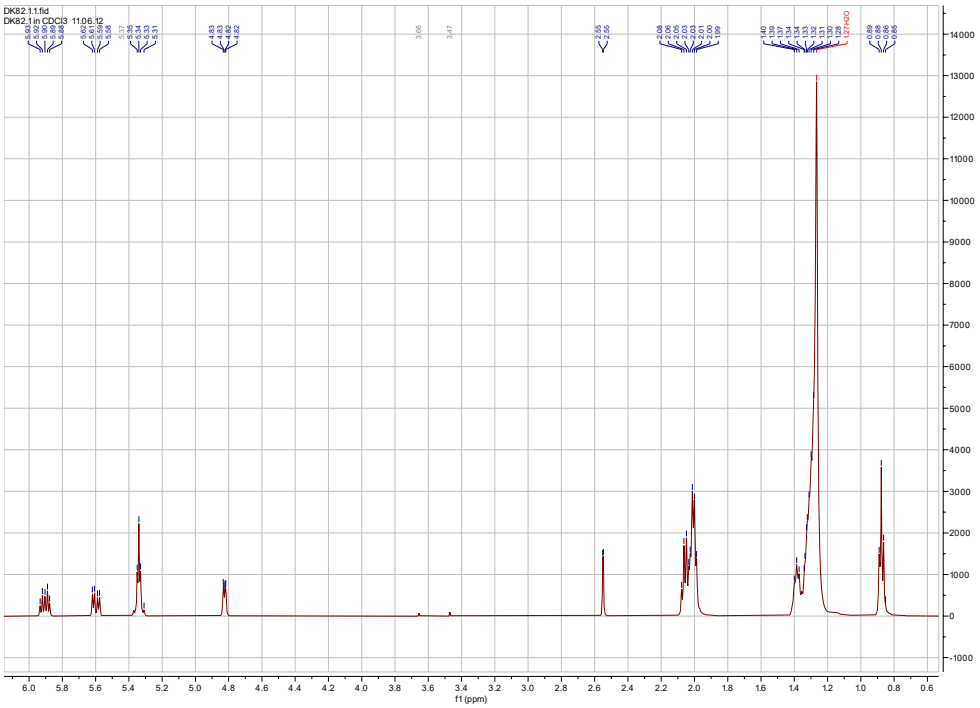


Figure S123. ^{13}C NMR spectrum of (3*R*)-docos-(4*E*,15*Z*)-dien-1-yn-3-ol (**21**) in $CDCl_3$

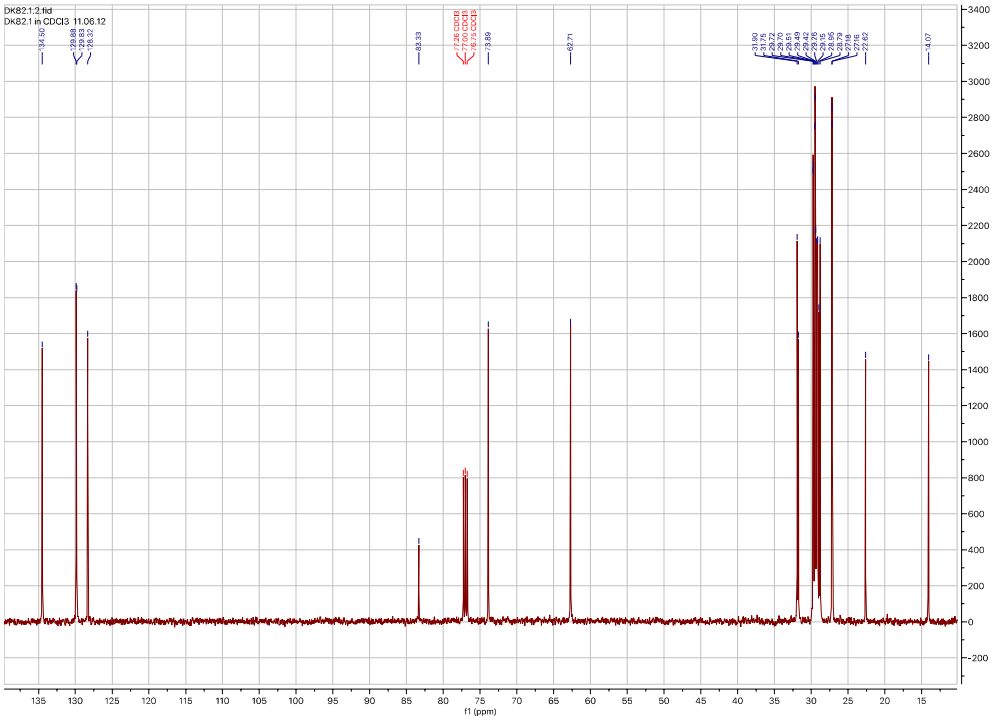


Table S21. NMR data of (3*R*)-docos-(4*E*,15*Z*)-dien-1-yn-3-ol (**21**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.9[d] CH	2.55 d (2.5)	3
2	83.3[e] qC	-	1, 3, 4
3	62.7 CH	4.82 brd (6.0)	1, 4, 5
4	128.3 CH	5.60 dd (15.0, 6.0)	3, 6
5	134.5 CH	5.91 dt (15.0, 7.5)	3, 6, 7
6	31.9 CH_2	2.05 q (7.5)	4, 5, 7, 8
7	28.8 CH_2	1.38 m	5, 6, 8
8-13	~29.6[f] 6 × CH_2	1.22 – 1.30 brm	
14	27.2 CH_2	2.01 q (5.5)	13, 15
15	129.8 CH	5.34 t (5.5)	13, 14
16	129.9 CH	5.34 t (5.5)	17, 18
17	27.2 CH_2	2.01 m	16, 18
18-19	29.6[f] 2 × CH_2	1.22 – 1.30 brm	
20	31.7 CH_2	1.25 m	19, 21a, 21b, 22
21a	22.6 CH_2	1.32 m	22, 24
b		1.27 m	
22	14.1 CH_3	0.88 t (6.7)	20, 21a, 21b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 252.0 Hz; [e] ^2J = 49.0 Hz; [f]Exact ^{13}C chemical shifts 28.95, 29.15, 29.25, 29.42, 29.49 (× 2), 29.70, 29.72 ppm.

Figure S124. EIGCMS spectrum of (3*R*)-docos-(4*E*,15*Z*)-dien-1-yn-3-ol (**21**)

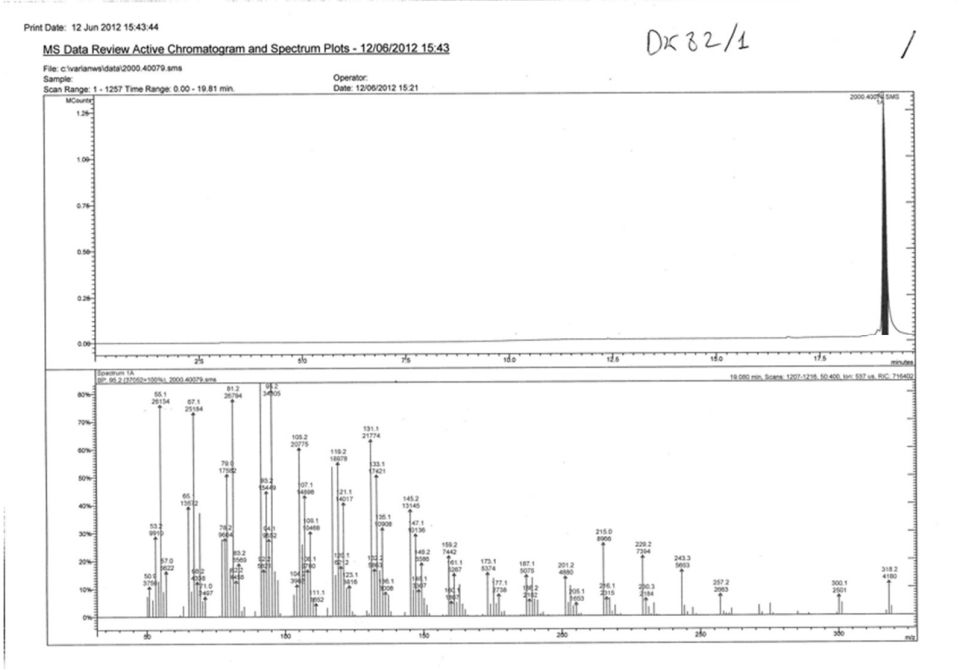


Figure S125. ^{1}H NMR spectrum of (3*R*)-21-methyldocos-(4*E*,15*Z*)-dien-1-yn-3-ol (**22**) in $CDCl_3$

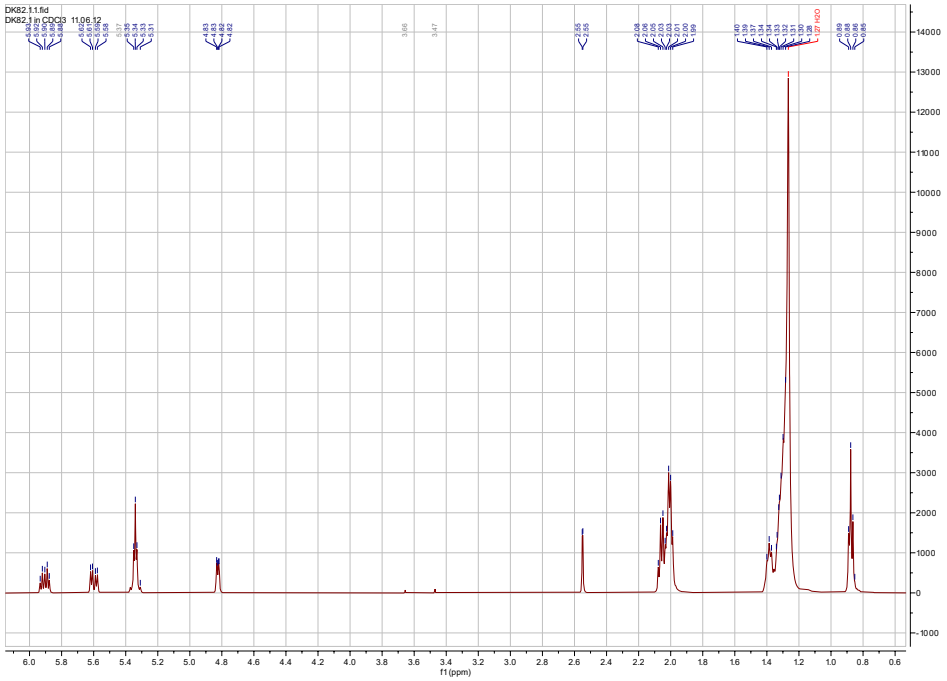


Figure S126. ^{13}C NMR spectrum of (3*R*)-21-methyldocos-(4*E*,15*Z*)-dien-1-yn-3-ol (**22**) in $CDCl_3$

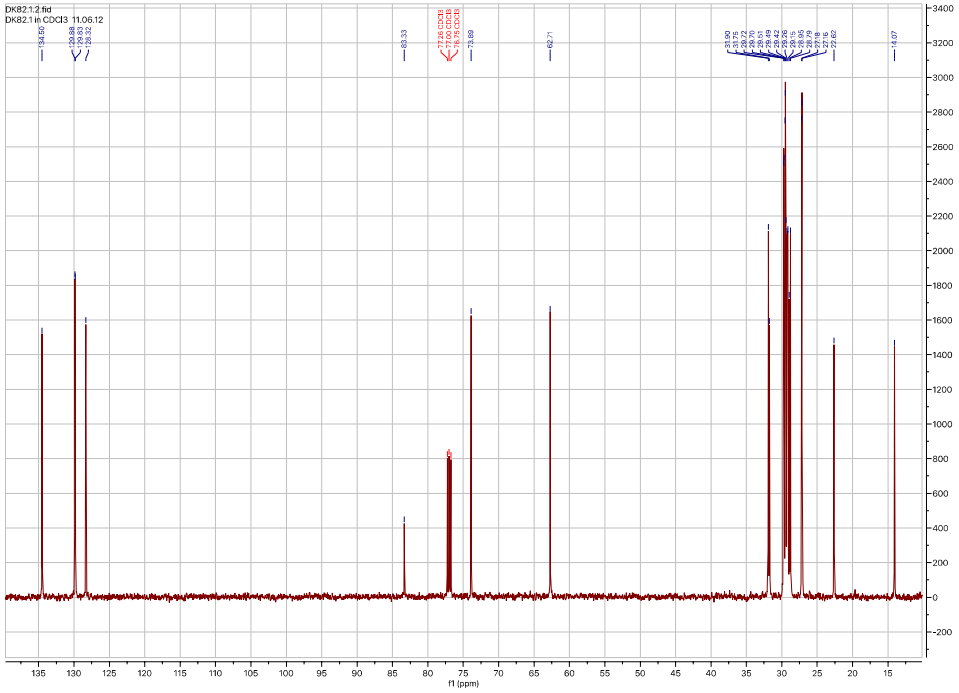


Table S22. NMR data of (3*R*)-21-methyldocos-(4*E*,15*Z*)-dien-1-yn-3-ol (**22**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.9[d] CH	2.56 s	3
2	83.3[e] qC	-	1, 3, 4
3	62.8 CH	4.83 brd (6.0)	1, 4, 5
4	128.3 CH	5.61 dd (15.0, 6.0)	3, 6
5	134.6 CH	5.91 dt (15.0, 7.0)	3, 6, 7
6	31.9 CH_2	2.06 q (7.0)	4, 5, 7, 8
7	28.8 CH_2	1.39 m	5, 6, 8
8-13	~29.6[f] 6 × CH_2	1.24 – 1.32 brm	
14	27.2 CH_2	2.01 m	13, 15
15	129.9 CH	5.34 t (4.0)	13, 14
16	129.9 CH	5.34 t (4.0)	17, 18
17	27.2 CH_2	2.01 m	16, 18
18	30.0 CH_2	1.31 m	
19	27.2 CH_2	1.28 m	18,20
20	39.3 CH_2	1.17 m	19, 21, 22, 23
21	28.0 CH		20, 22, 23
22	22.6 CH_3	0.85 d (6.5)	20, 21, 23
23	22.6 CH_3	0.85 d (6.5)	20, 21, 22

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 251.0 Hz; [e] ^2J = 49.5 Hz; [f]Exact ^{13}C chemical shifts 29.17, 29.29, 29.44, 29.53 (× 2), 29.73 ppm.

Figure S127. EIMS spectrum of (3*R*)-21-methyldocos-(4*E*,15*Z*)-dien-1-yn-3-ol (**22**)

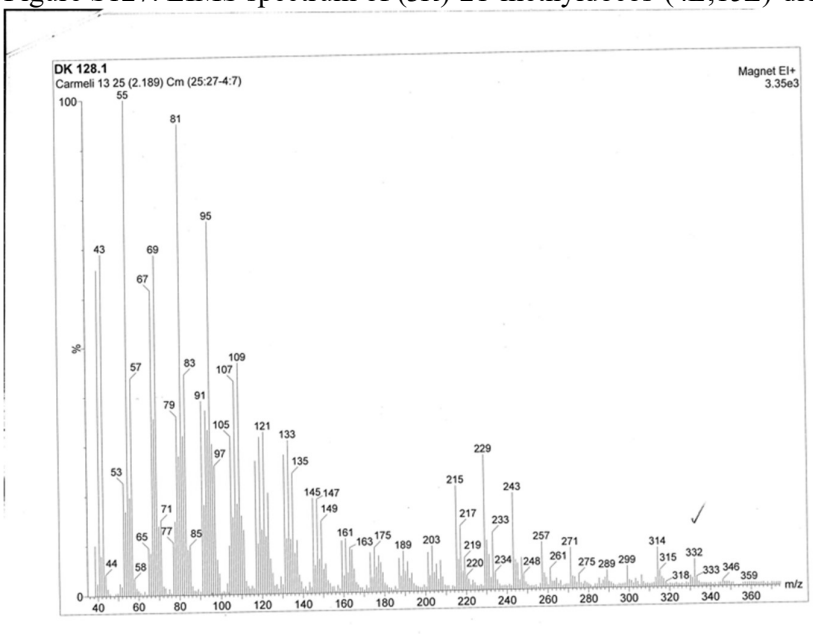


Figure S128. ^{1}H NMR spectrum of (3*R*)-14-methyldocos-1-yn-3-ol (**23**) in $CDCl_3$

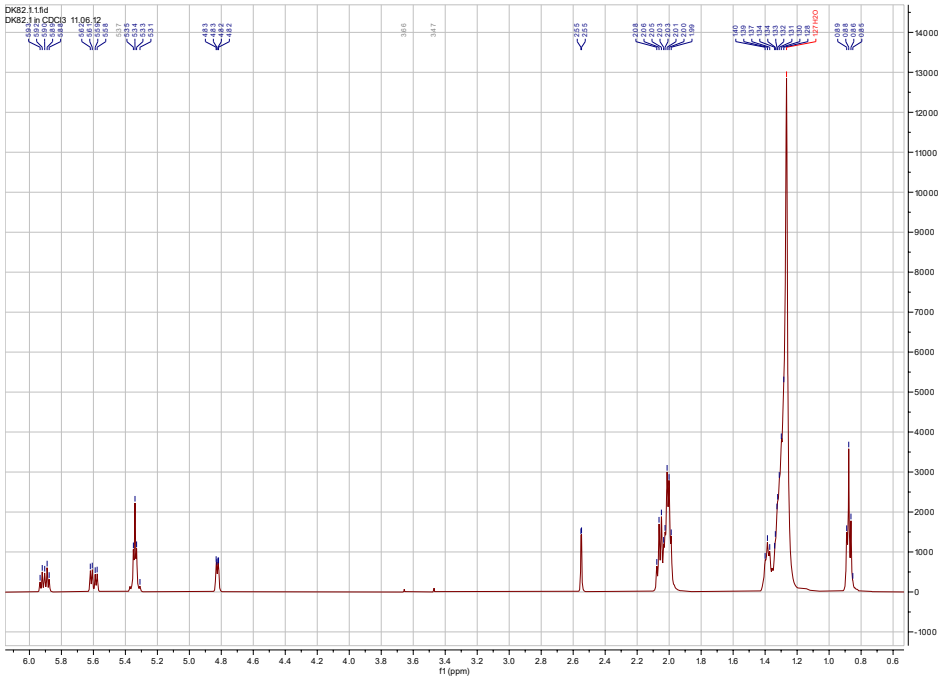


Figure S129. ^{13}C NMR spectrum of (3*R*)-14-methyldocos-1-yn-3-ol (**23**) in $CDCl_3$

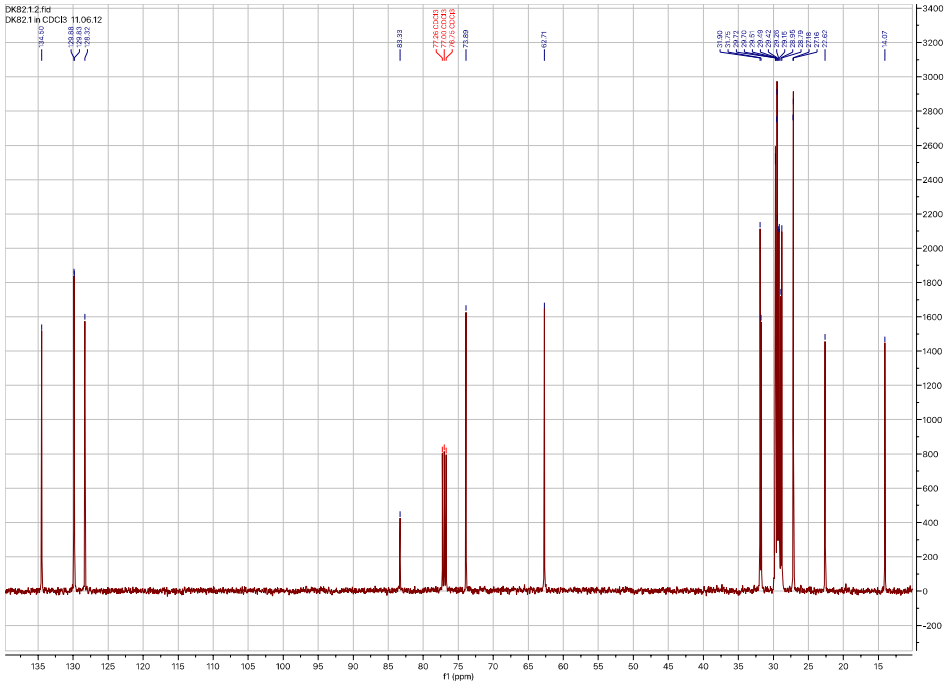


Table S23. NMR data of (3*R*)-14-methyldocos-1-yn-3-ol (**23**) in $CDCl_3$.[a]

Position	δ_C, mult.[b]	δ_H, mult. *J* (Hz)	LR H-C Correlations[c]
1	73.9[d] CH	2.55 d (2.0)	3
2	83.4[e] qC	-	1, 3, 4
3	62.8 CH	4.82 brd (5.5)	1, 4, 5
4	128.3 CH	5.60 dd (15.3, 6.0)	3, 6
5	134.5 CH	5.90 dt (15.3, 7.0)	3, 6, 7
6	31.9 CH_2	2.06 q (7.0)	4, 5, 7, 8
7	28.8 CH_2	1.38 m	5, 6, 8
8-11	~29.5[f] 4 × CH_2	1.23 – 1.26 brm	
12	27.1 CH_2	1.24 m	11, 13a, 13b
13a	37.1 CH_2	1.26 m	12, 14, 15a, 15b, 23
b		1.06 m	
14	32.7 CH	1.34 m	13a, 13b, 15a, 15a, 23
15a	37.1 CH_2	1.26 m	13a, 13b, 14, 16, 23
b		1.06 m	
16	27.0 CH_2	1.23 m	15a, 15b, 17
17-19	~29.5[f] 3 × CH_2	1.23 – 1.26 brm	
20	31.9 CH_2	1.24 m	19, 21a, 21b, 22
21a	22.7 CH_2	1.31 m	20, 22
b		1.25 m	
22	14.1 CH_3	0.87 t (6.7)	21a, 21b
23	19.7 CH_3	0.83 d (6.5)	13b, 15b

[a]500.13 MHz for ^1H and 125.76 MHz for ^{13}C; [b]Multiplicity and assignment from HSQC experiment; [c]Determined from HMBC experiment; [d] ^1J = 250.5 Hz; [e] ^2J = 48.3 Hz; [f]Exact ^{13}C chemical shifts 29.17, 29.34, 29.46, 29.60, 29.67, 29.98, 30.00 ppm.

Figure S130. EIMS of (3*R*)-14-methyldocos-1-yn-3-ol (**23**)

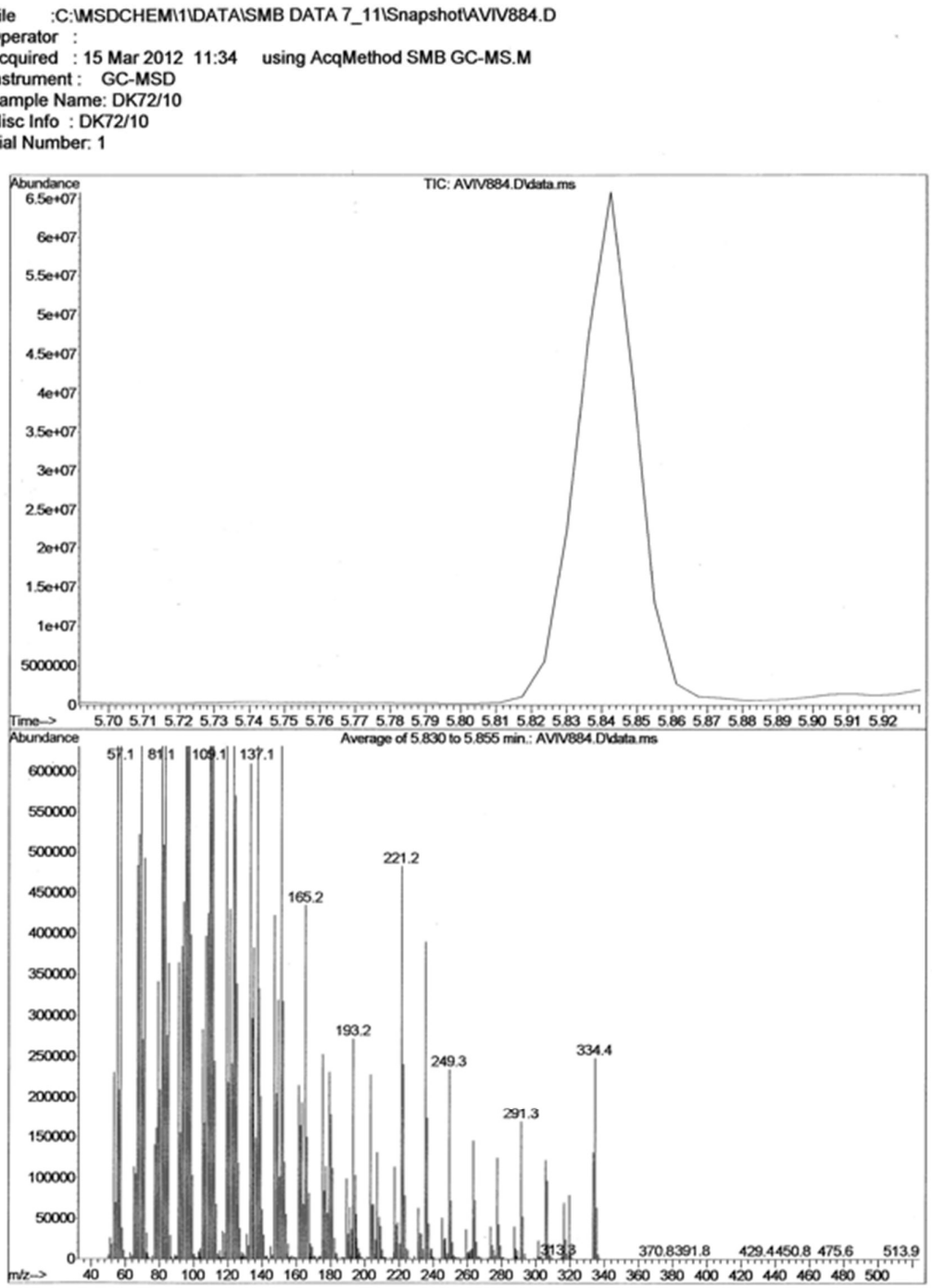


Figure S131. ^{1}H NMR spectrum of (4*E*,6*E*)-docosa-4,6-dien-1-yn-3-ol (***rac*-27**) in $CDCl_3$

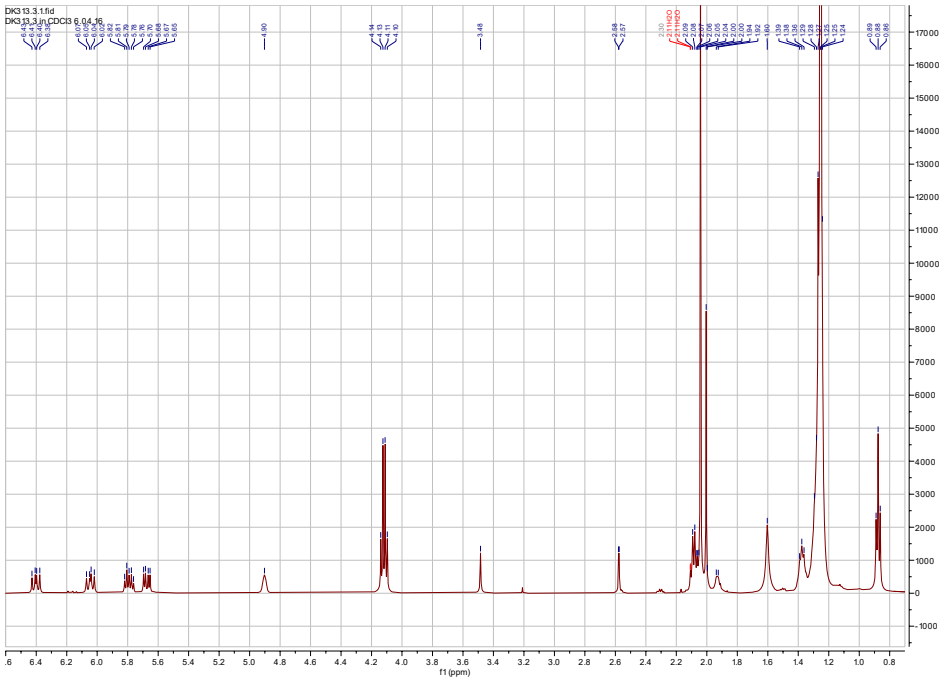


Figure S132. ^{13}C NMR spectrum of (4*E*,6*E*)-docosa-4,6-dien-1-yn-3-ol (***rac*-27**) in $CDCl_3$

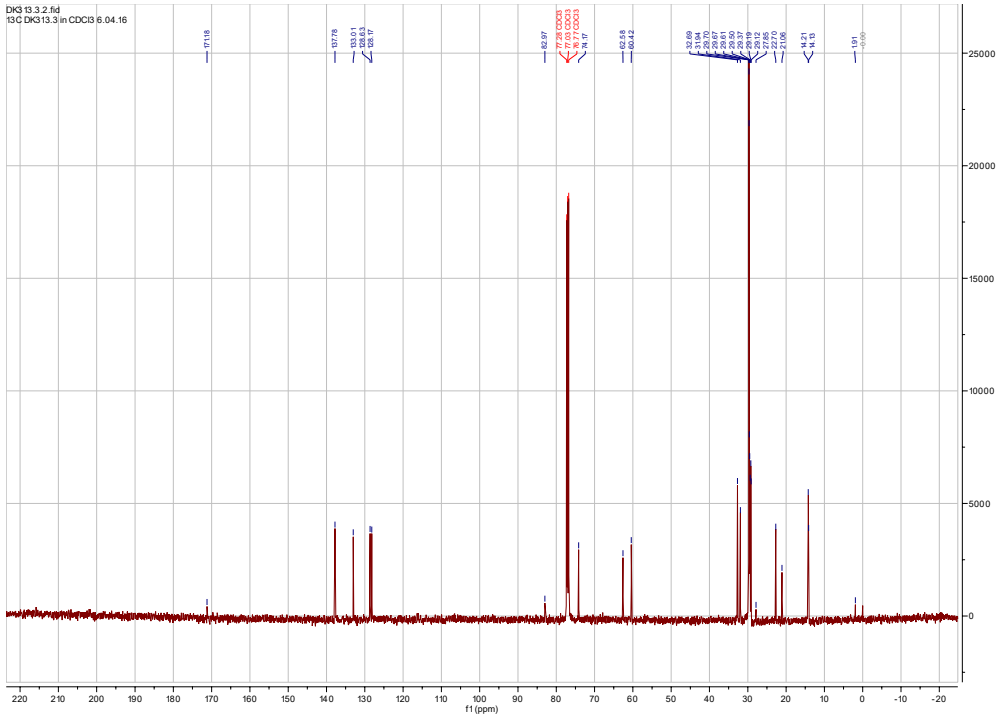
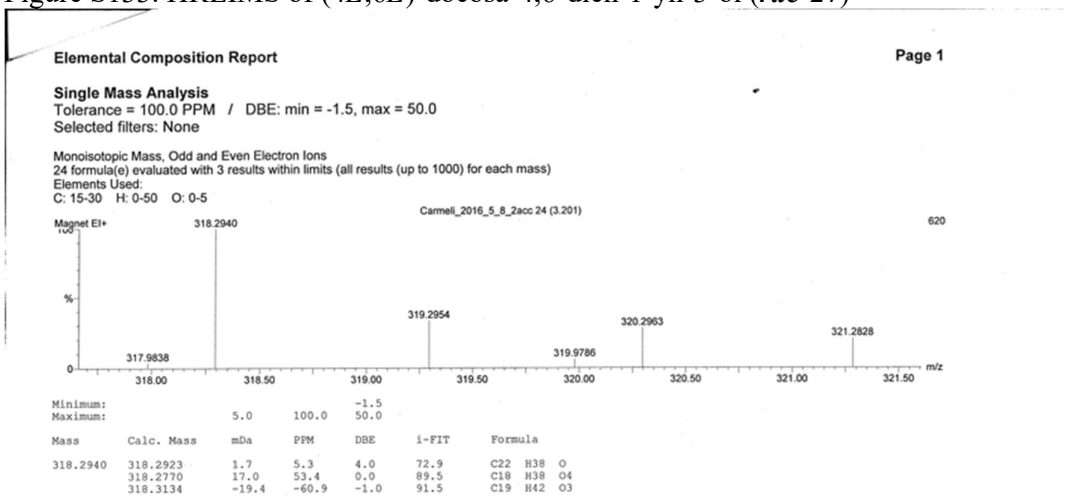


Figure S133. HREIMS of (4*E*,6*E*)-docosa-4,6-dien-1-yn-3-ol (***rac*-27**)



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
24 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-30 H: 0-50 O: 0-5

Carmeli_2016_5_8_2acc 24 (3.201)

Minimum:				-1.5		
Maximum:		5.0	100.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
318.2940	318.2923	1.7	5.3	4.0	72.9	C22 H38 O
	318.2770	17.0	53.4	0.0	89.5	C18 H38 O4
	318.3134	-19.4	-60.9	-1.0	91.5	C19 H42 O3

Figure S134. ^{1}H NMR spectrum of (*S*)-((*R*)-icos-(4*E*)-en-1-yn-3-yl-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (**(*S,R*)-29**) in $CDCl_3$

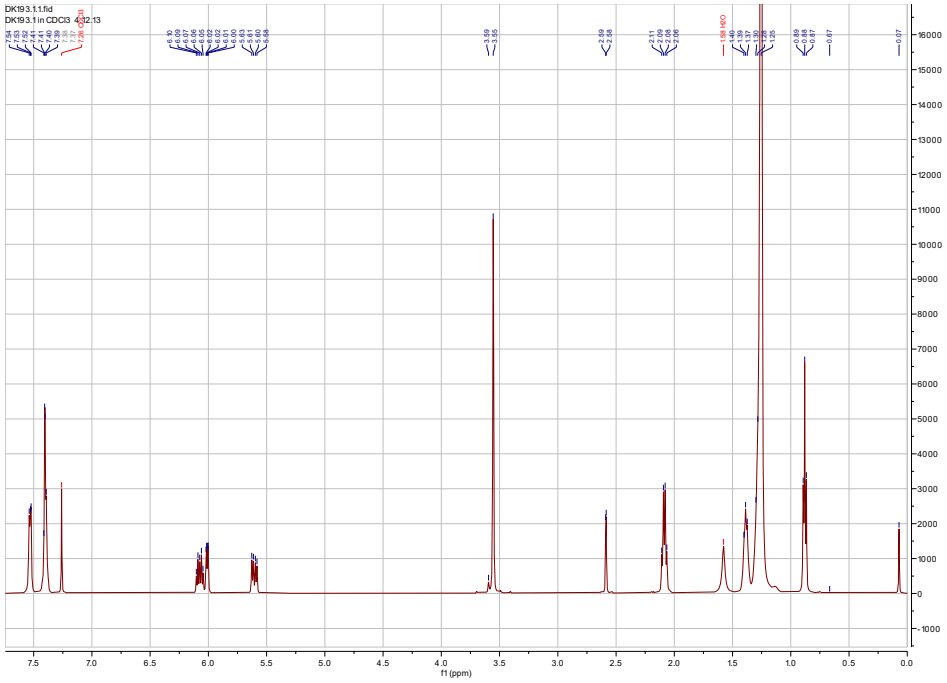


Figure S135. ^{1}H NMR spectrum of (*S*)-((*S*)-icos-(4*E*)-en-1-yn-3-yl-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (**(*S,S*)-29**) in $CDCl_3$

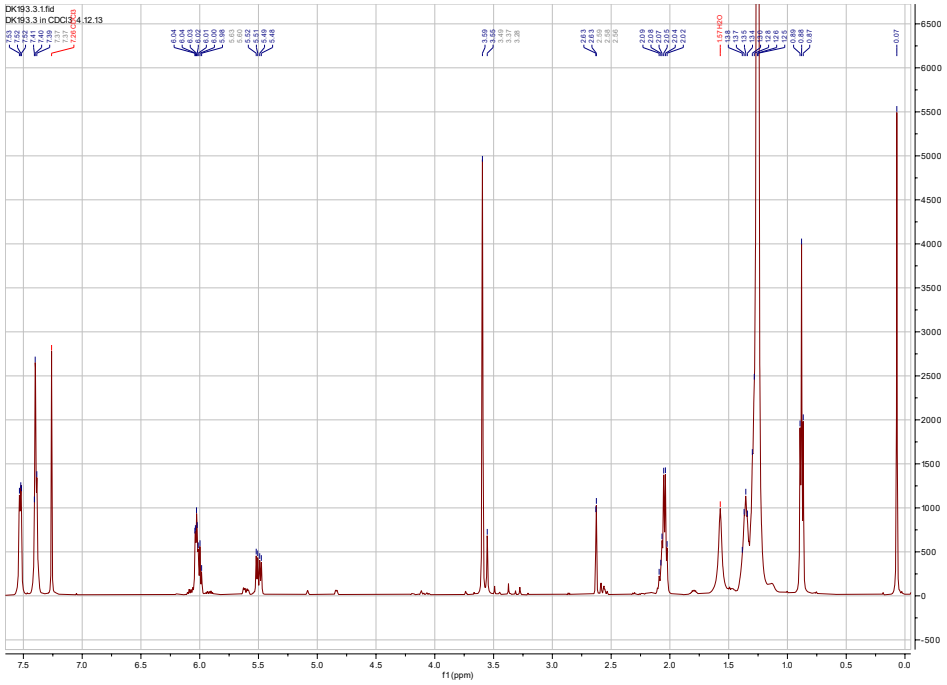


Figure S136. ^{1}H NMR spectrum of dodec-1-yn-3-ol (***rac*-31**) in $CDCl_3$

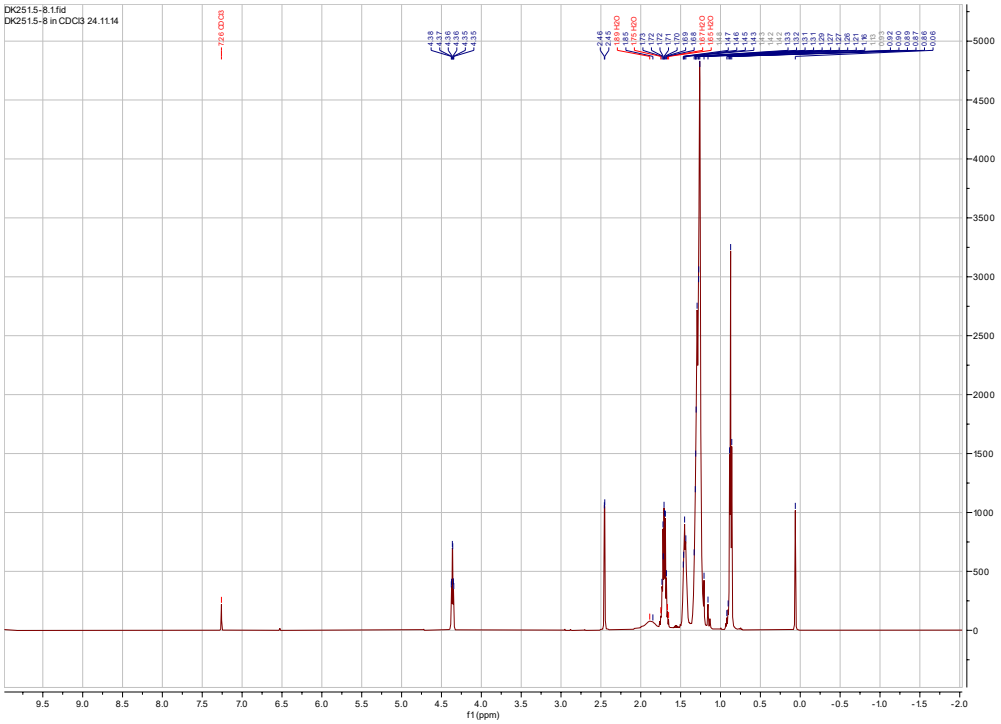


Figure S137. ^{13}C NMR spectrum of dodec-1-yn-3-ol (***rac*-31**) in $CDCl_3$

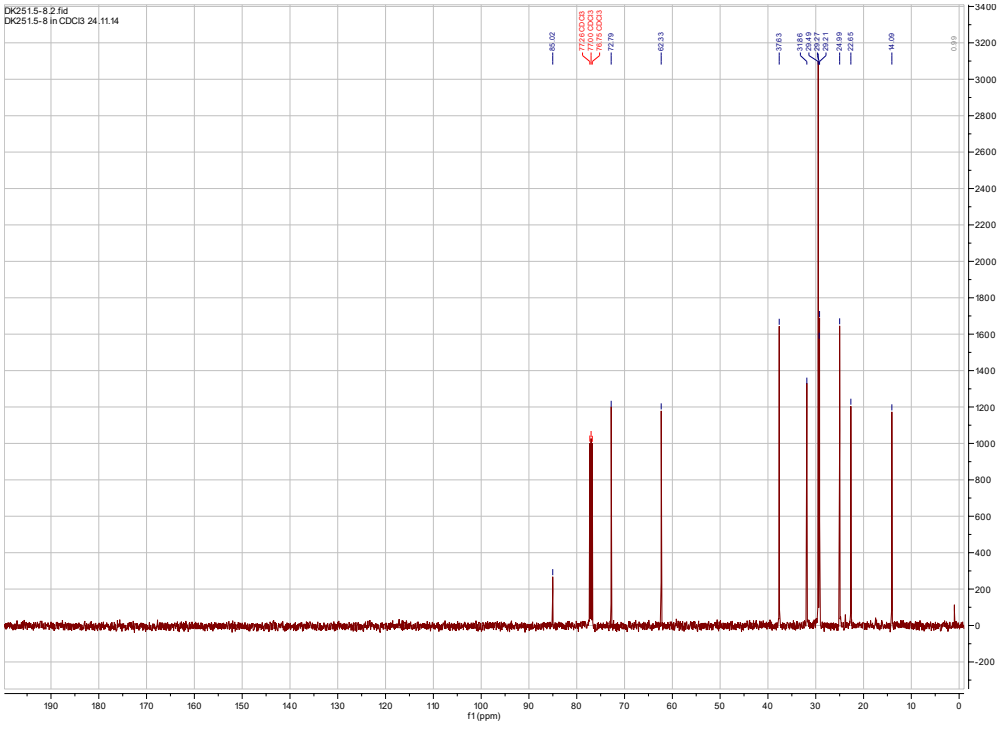
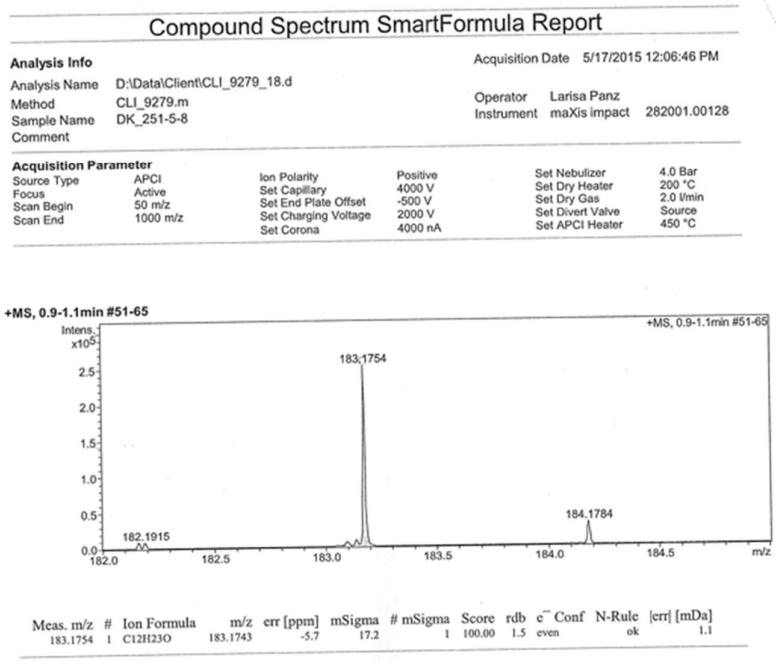


Figure S138. HRCIMS of dodec-1-yn-3-ol (***rac*-31**)



Compound Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Client\CLI_9279_18.d	Acquisition Date	5/17/2015 12:06:46 PM
Method	CLI_9279.m	Operator	Larisa Panz
Sample Name	DK_251-5-8	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 0.9-1.1min #51-65

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
183.1754	1	C12H23O	183.1743	-5.7	17.2	1	100.00	1.5	even	ok	1.1

Figure S139. ^{1}H NMR spectrum of octadec-1-yn-3-ol (***rac*-32**) in $CDCl_3$

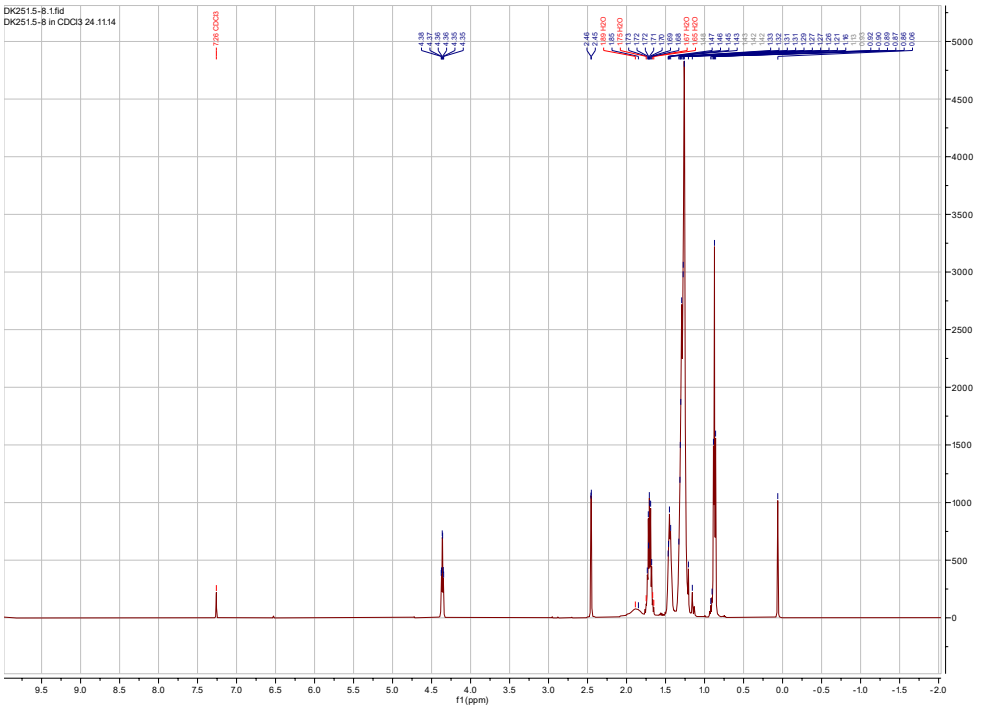


Figure S140. ^{13}C NMR spectrum of octadec-1-yn-3-ol (***rac*-32**) in $CDCl_3$

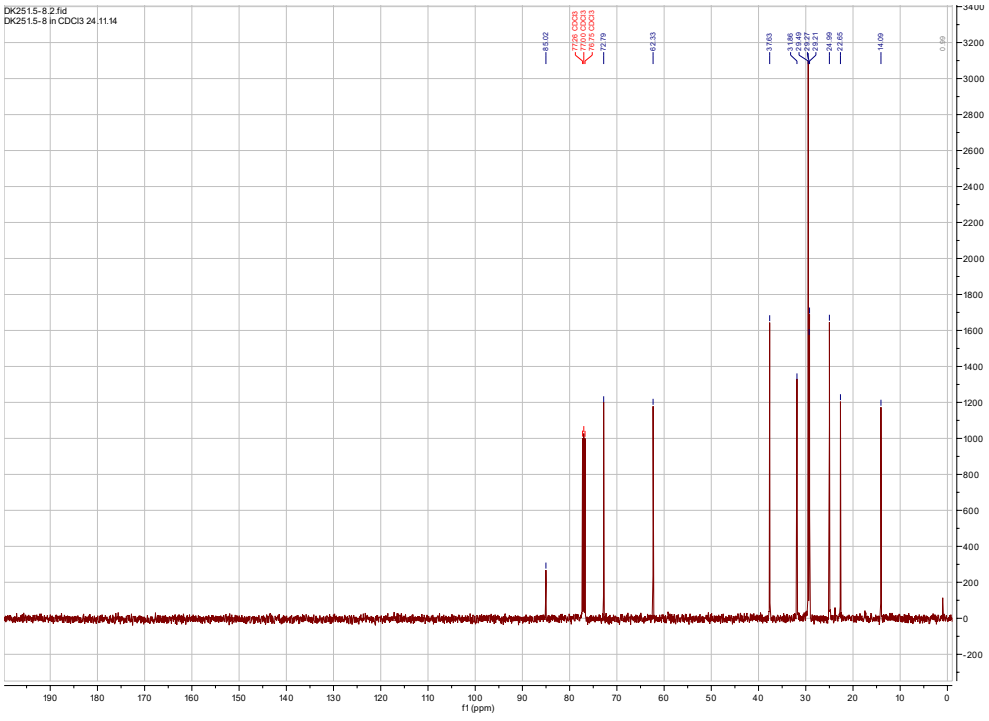


Figure S141. CIGCMS of octadec-1-yn-3-ol (***rac*-32**)

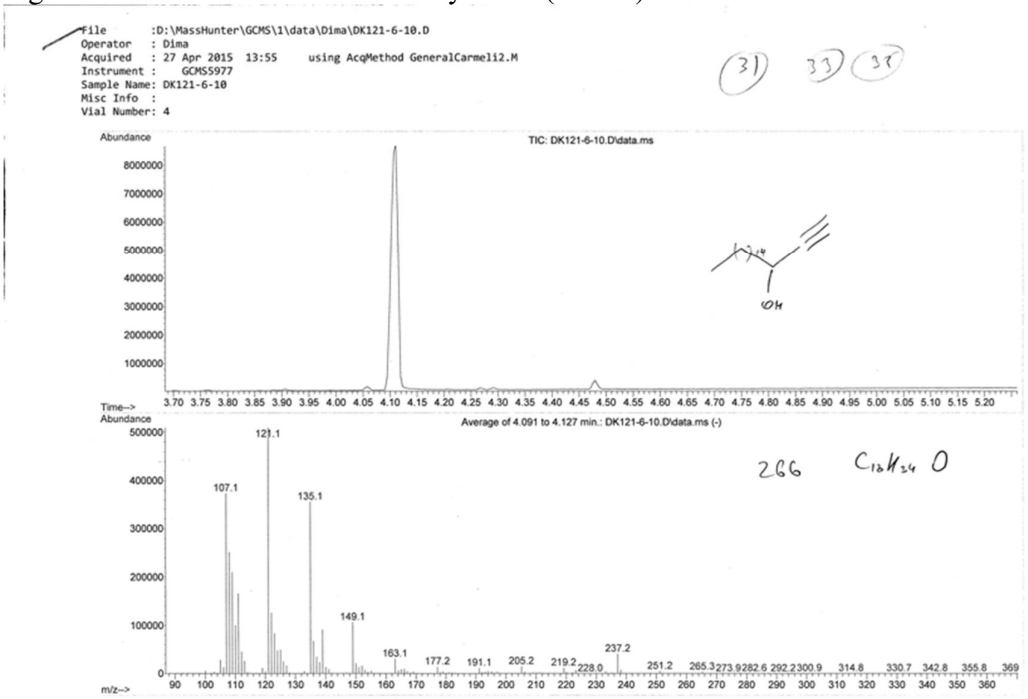


Figure S142. HRCIMS of octadec-1-yn-3-ol (***rac*-32**)

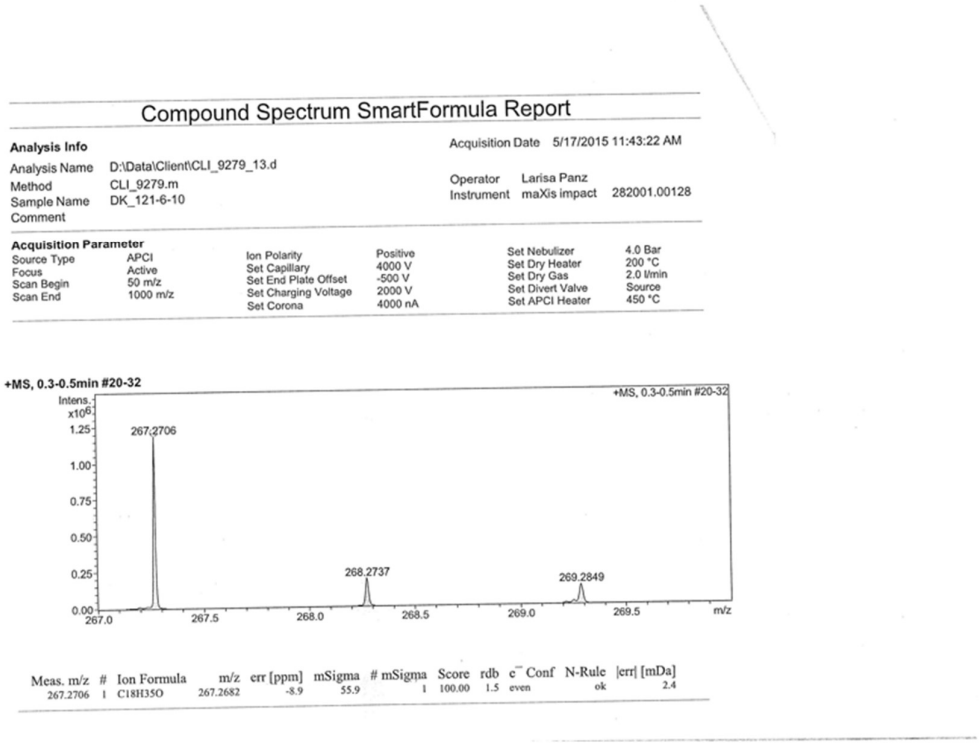


Figure S143. ^{1}H NMR spectrum of octadec-1-yn-3-ol (***R*-32**) in $CDCl_3$

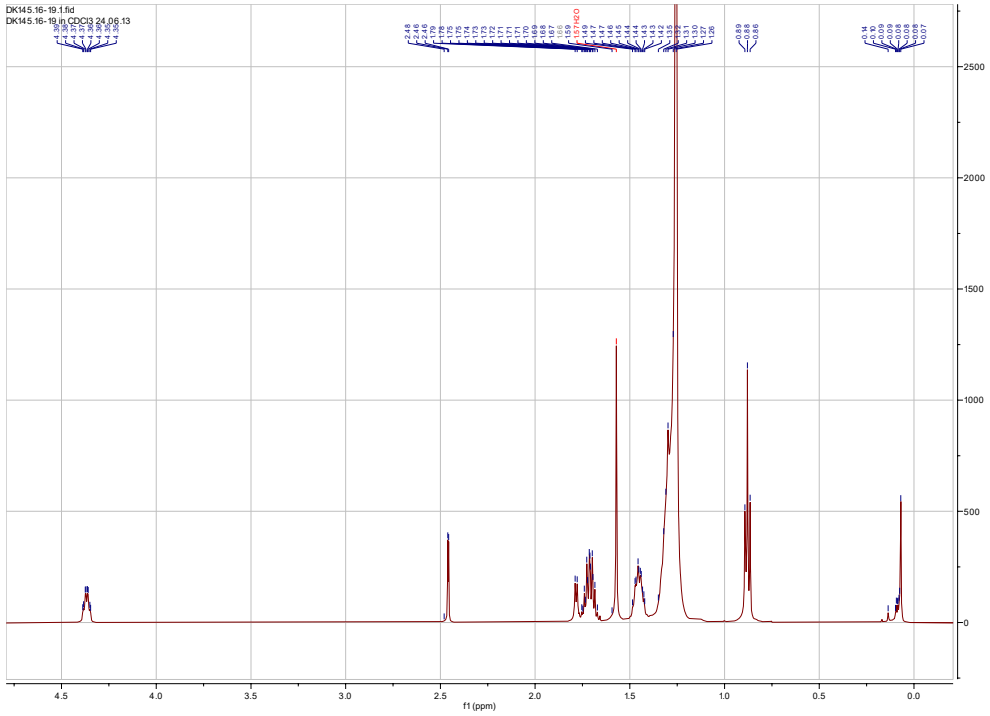


Figure S144. ^{1}H NMR spectrum of octadec-1-yn-3-ol (***S*-32**) in $CDCl_3$

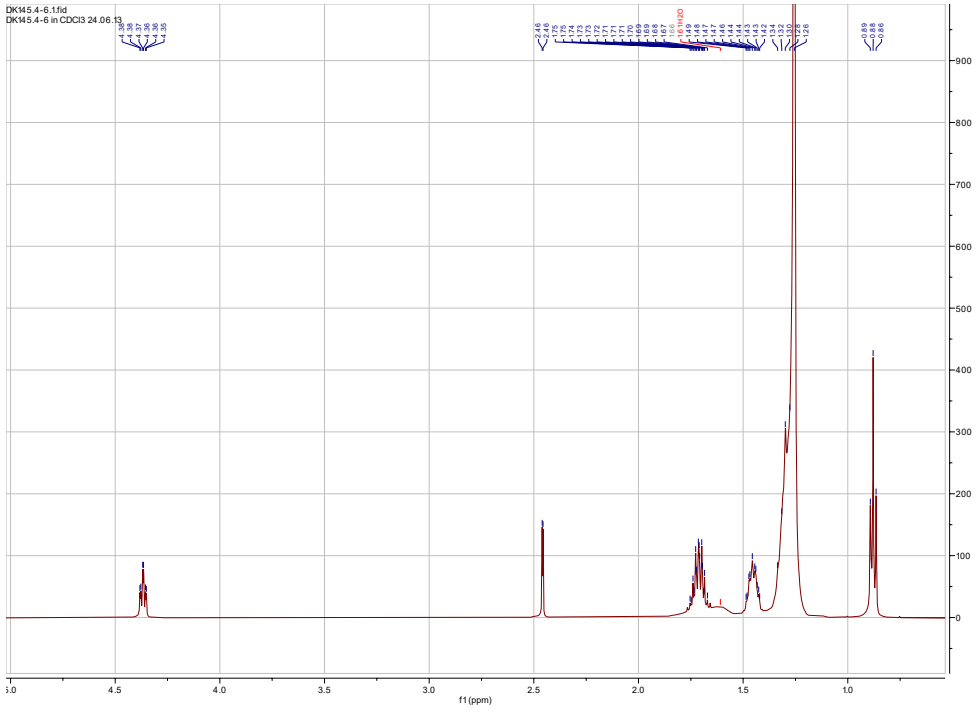


Figure S145. ^{1}H NMR spectrum of icos-1-yn-3-ol (***rac*-33**) in $CDCl_3$

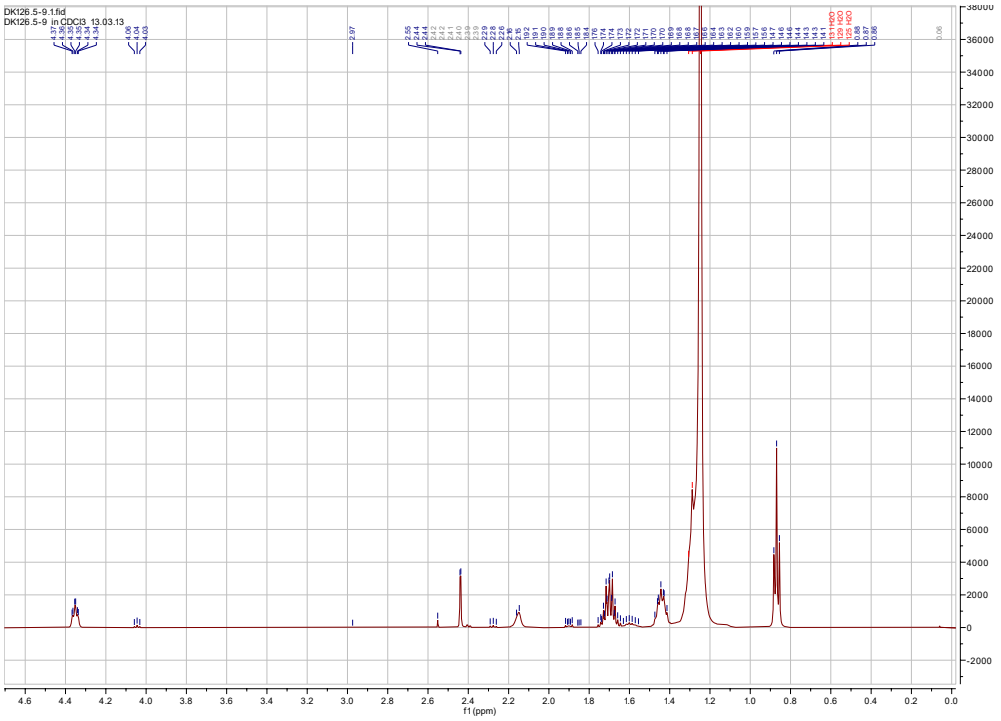


Figure S146. ^{13}C NMR spectrum of icos-1-yn-3-ol (***rac*-33**) in $CDCl_3$

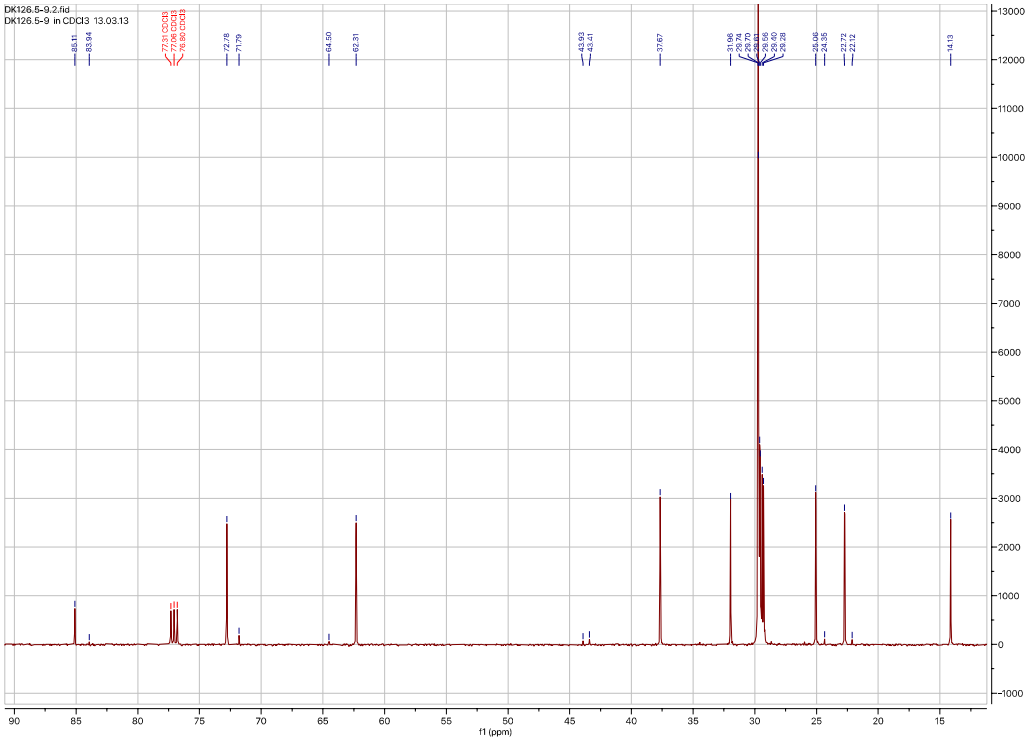


Figure S147. CIGCMS of icos-1-yn-3-ol (***rac*-33**)

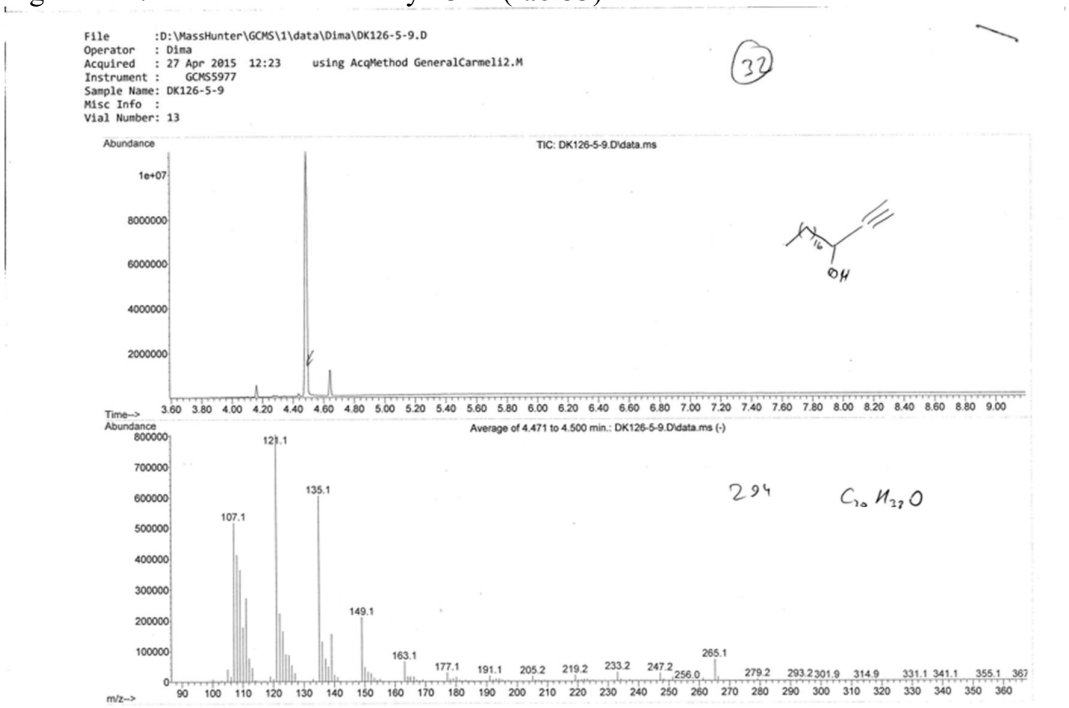


Figure S148. HRCIMS of icosc-1-yn-3-ol (***rac*-33**)

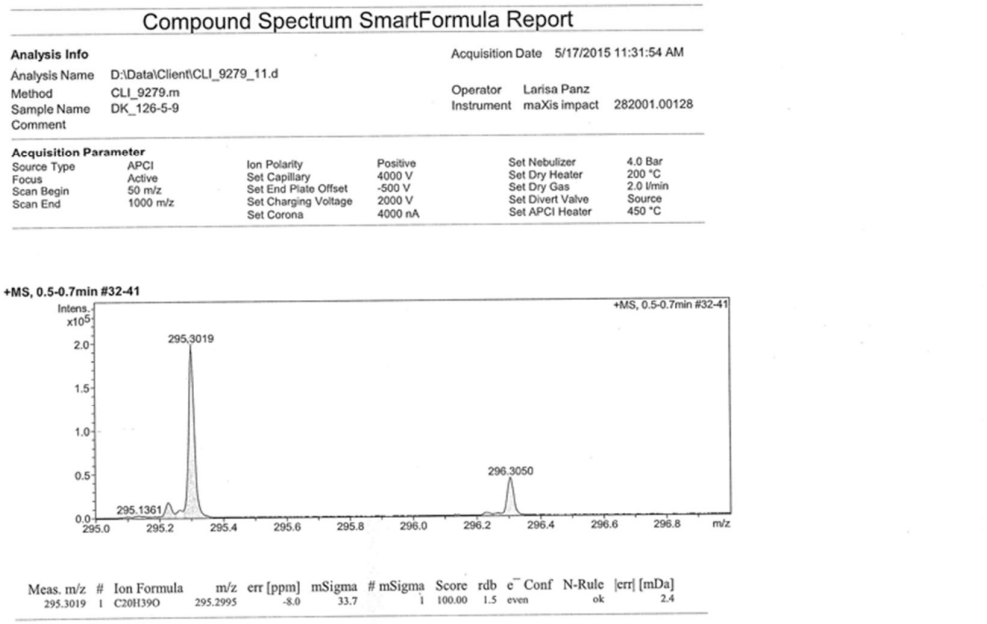


Figure S149. ^{1}H NMR spectrum of (*R*)-((*S*)-octadec-1-yn-3-yl)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (**(*R,S*)-34**) in $CDCl_3$

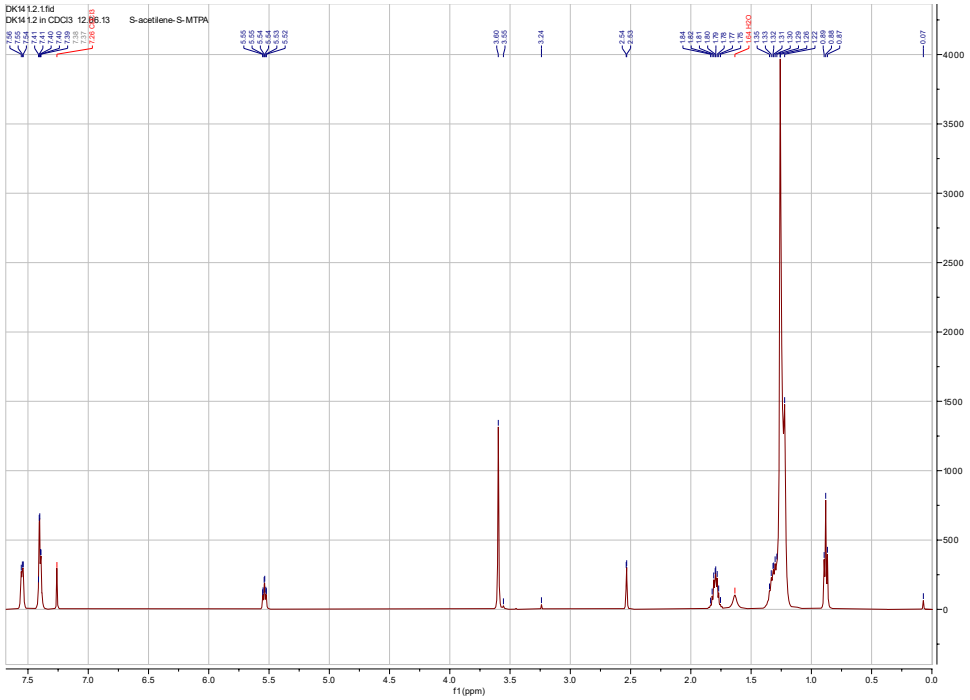


Figure S150. ^{13}C NMR spectrum of (*R*)-((*S*)-octadec-1-yn-3-yl)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (**(*R,S*)-34**) in $CDCl_3$

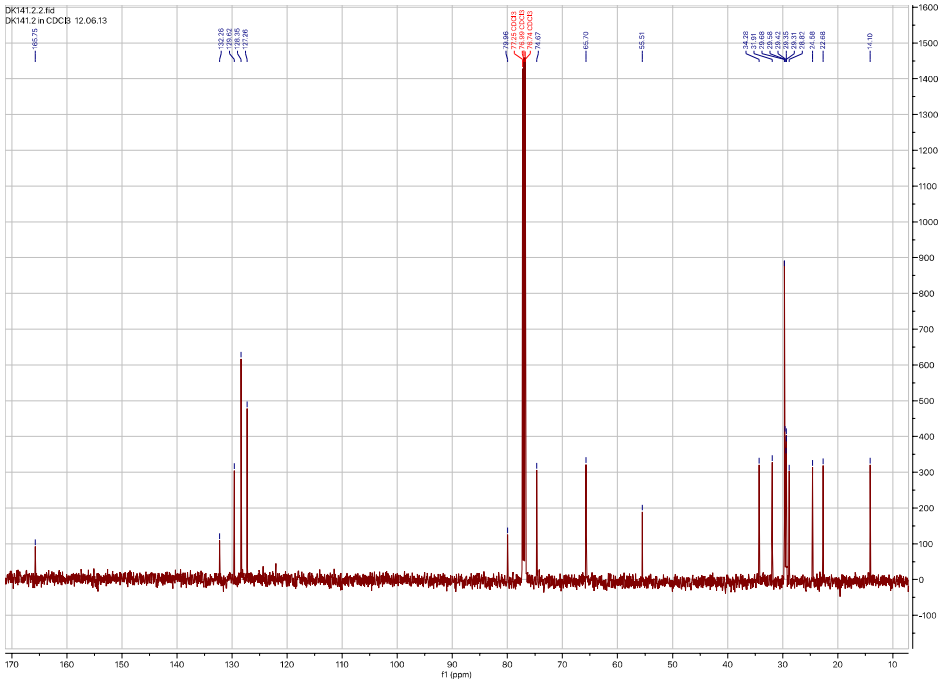


Figure S151. ^{1}H NMR spectrum of (*R*)-((*R*)-octadec-1-yn-3-yl)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (**(*R,R*)-34**) in $CDCl_3$

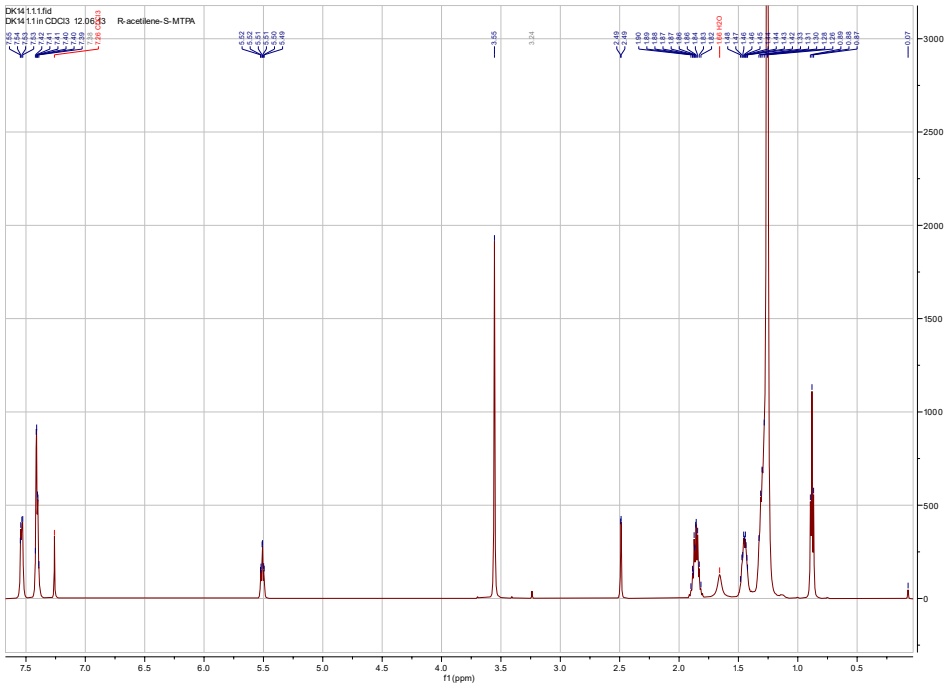


Figure S152. ^{13}C NMR spectrum of (*R*)-((*R*)-octadec-1-yn-3-yl)-3,3,3-trifluoro-2-methoxy-2-phenylpropanoate (**(*R,R*)-34**) in $CDCl_3$

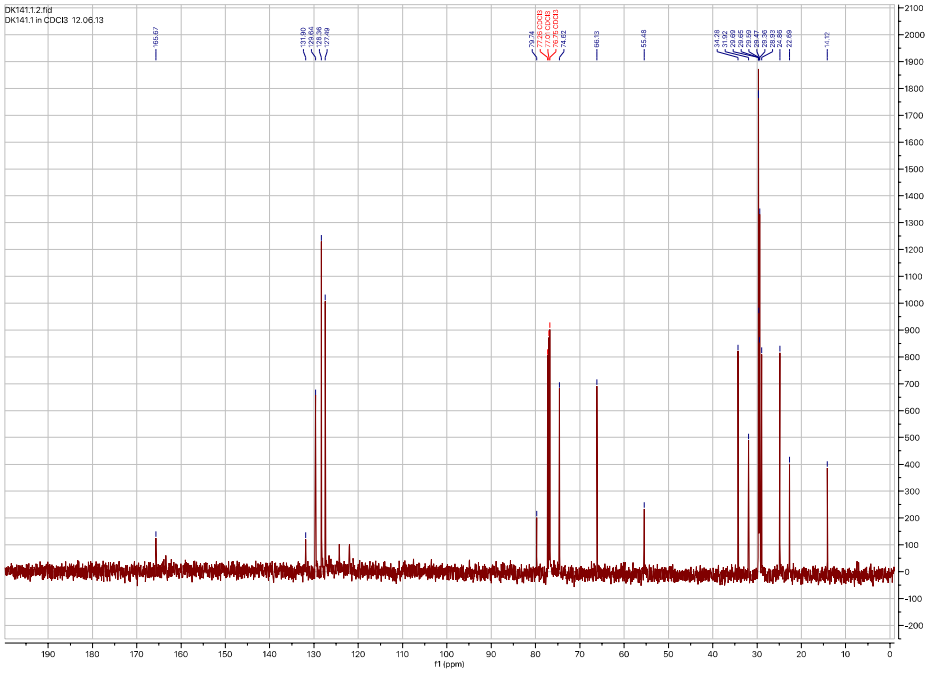


Figure S153. ^{1}H NMR spectrum of octadec-1-yn-3-yl 4-methylbenzenesulfonate (***rac*-35**) in $CDCl_3$

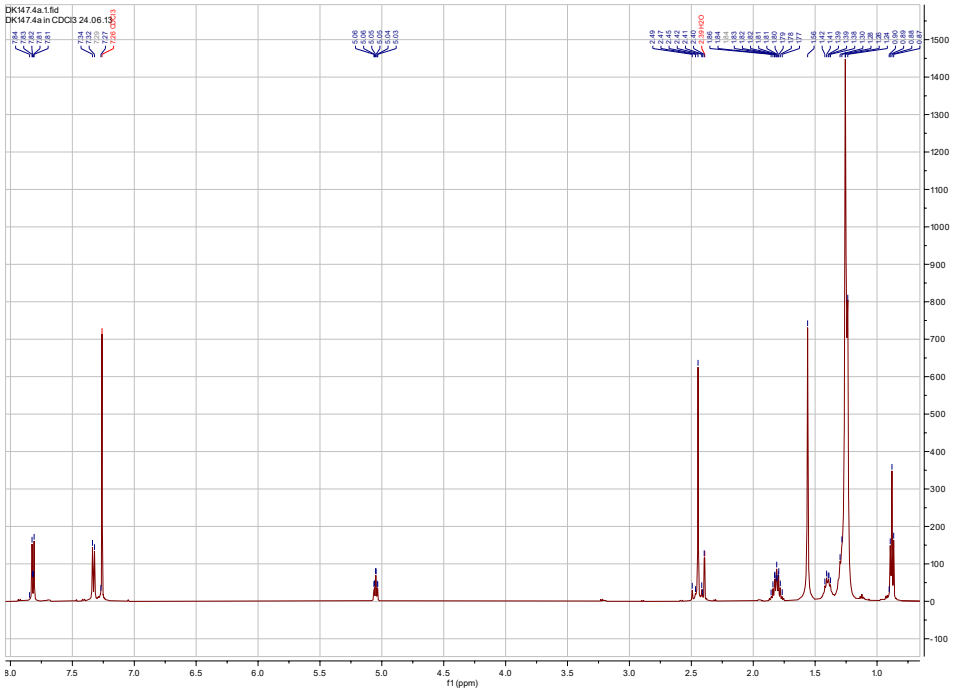


Figure S154. ^{13}C NMR spectrum of octadec-1-yn-3-yl 4-methylbenzenesulfonate (***rac*-35**) in $CDCl_3$

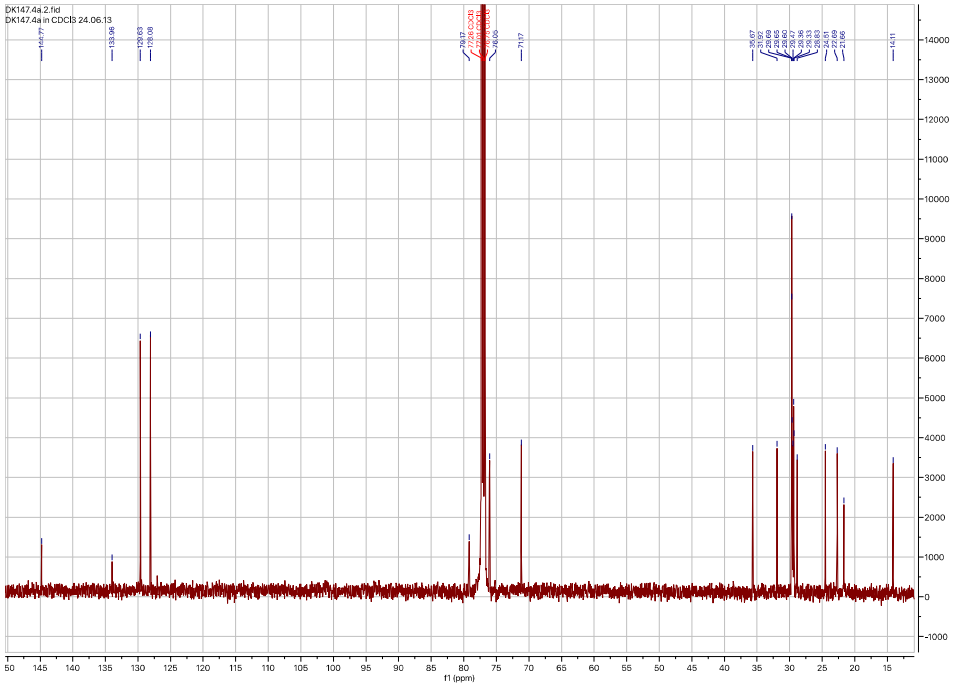


Figure S155. ESIMS of octadec-1-yn-3-yl 4-methylbenzenesulfonate (***rac*-35**)

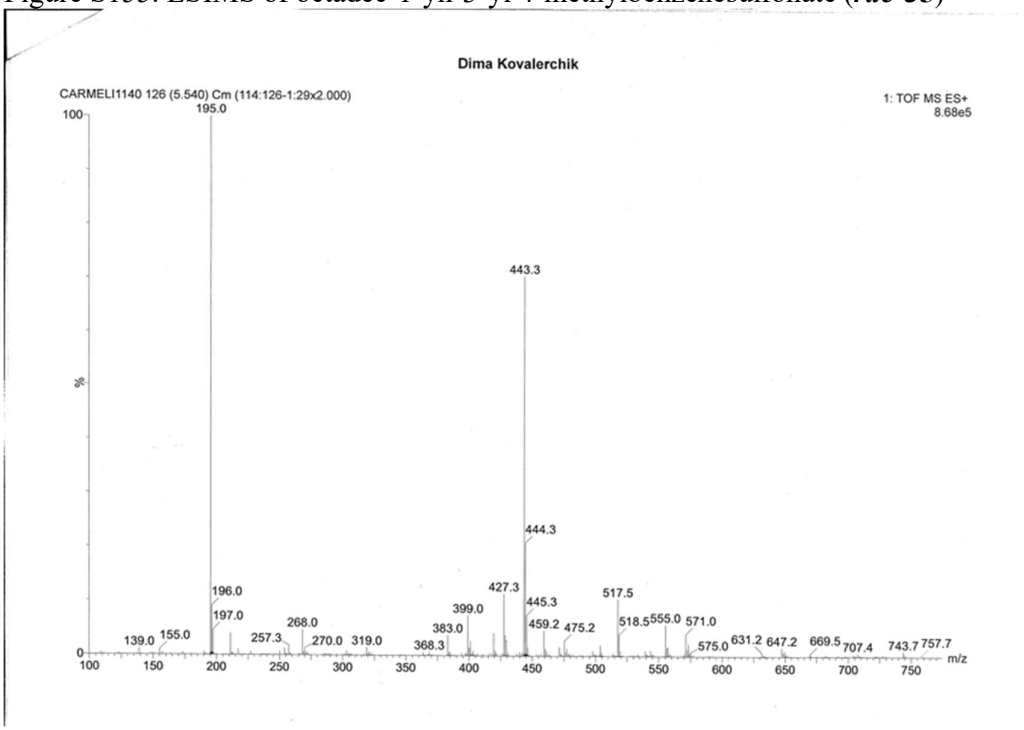


Figure S156. HRESIMS of octadec-1-yn-3-yl 4-methylbenzenesulfonate (***rac*-35**)

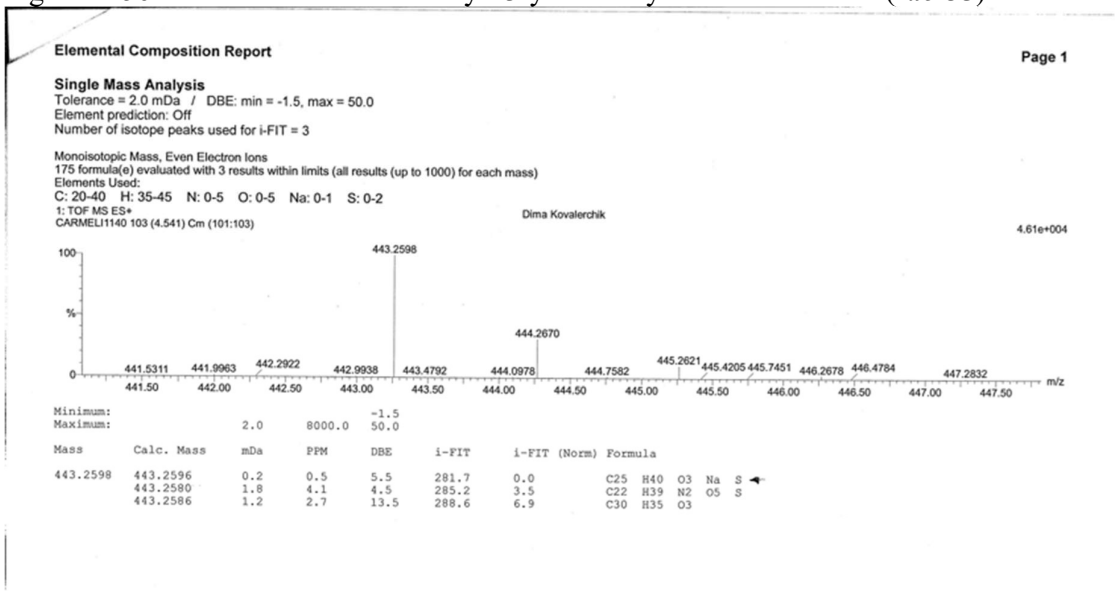


Figure S157. ^{1}H NMR spectrum of 3-chlorooctadec-1-yne (***rac*-36**) in $CDCl_3$

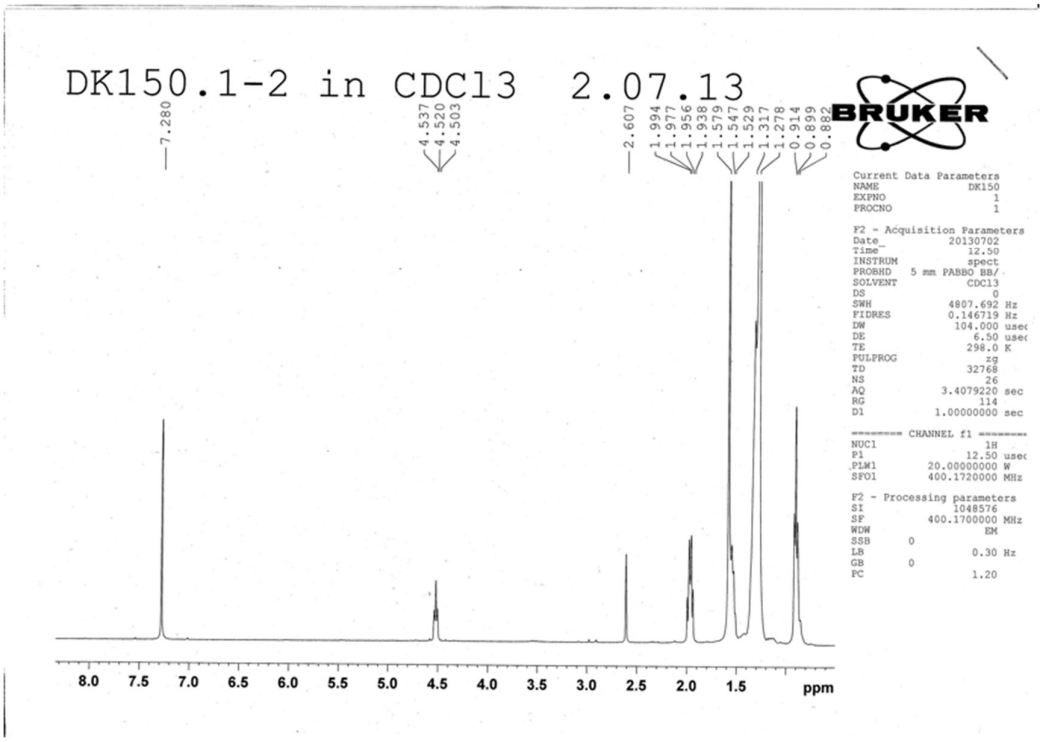


Figure S158. ^{1}H NMR spectrum of 3-chlorooctadec-1-yne (***rac*-36**) in $CDCl_3$

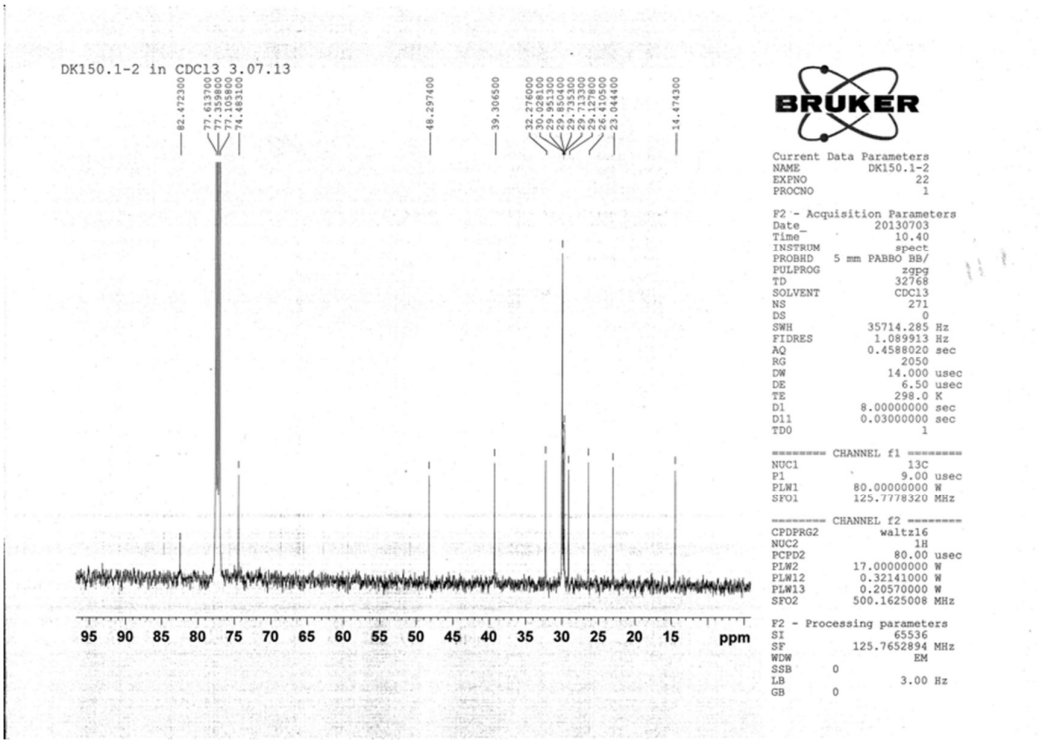


Figure S159. SMBEIMS of 3-chlorooctadec-1-yne (***rac*-36**)

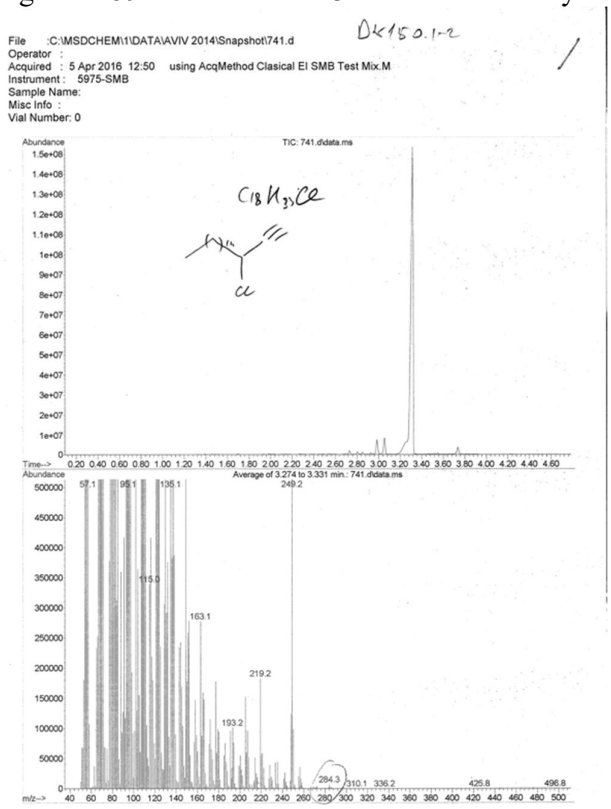


Figure S160. HRESIMS of 3-chlorooctadec-1-yne (***rac*-36**)

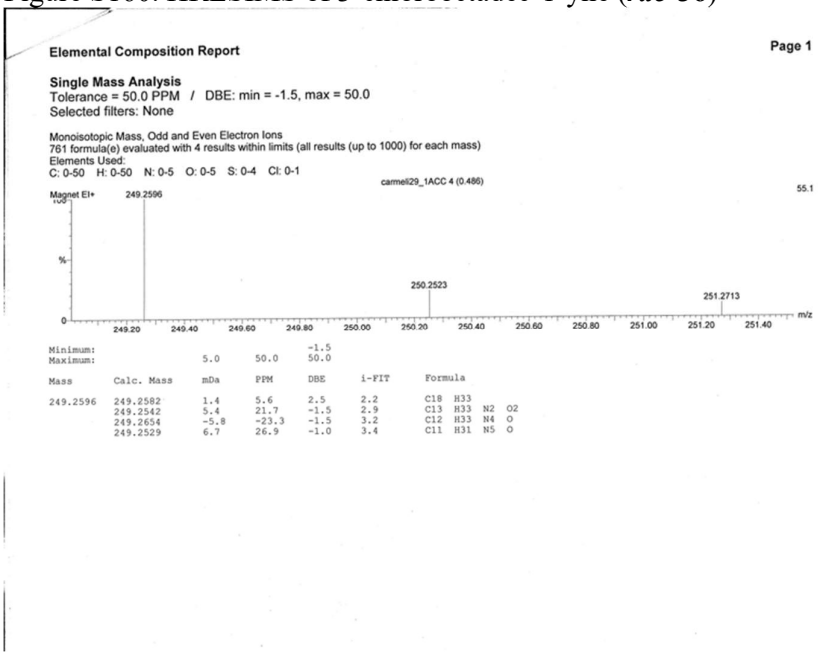


Figure S161. ^{1}H NMR spectrum of octadec-1-yn-3-amine (***rac*-37**) in $CDCl_3$

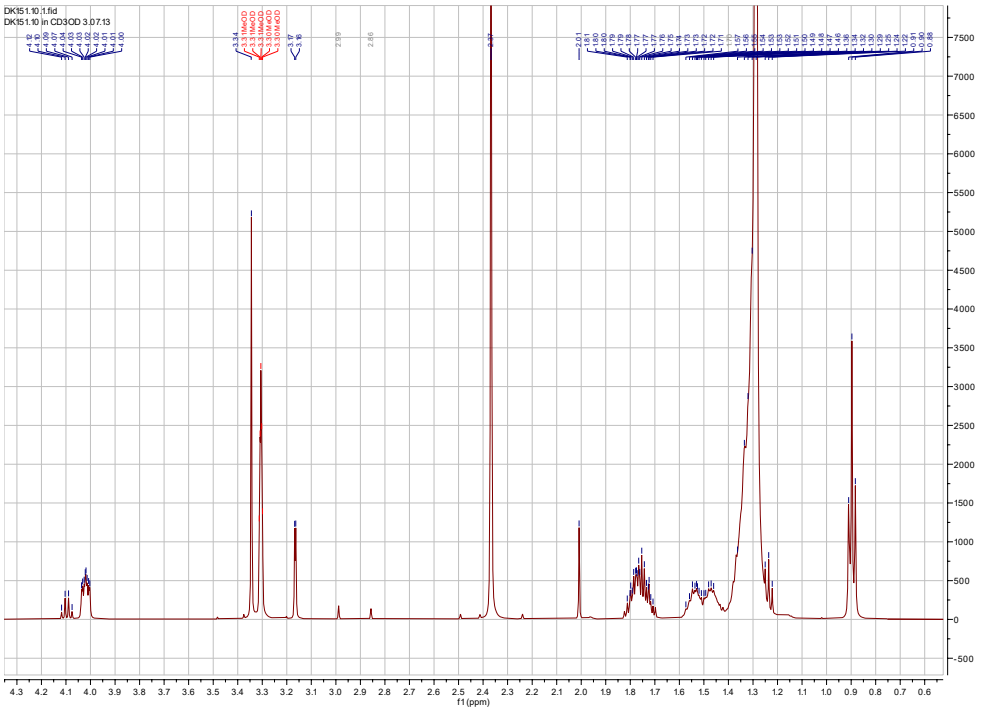


Figure S162. ^{13}C NMR spectrum of octadec-1-yn-3-amine (***rac*-37**) in $CDCl_3$

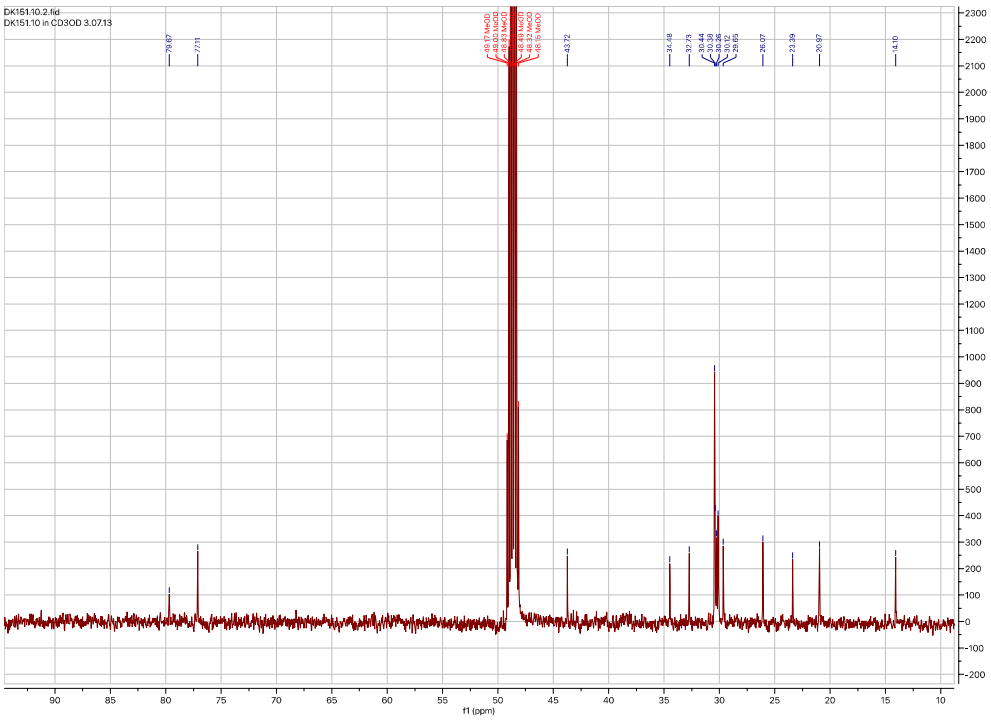


Figure S163. ESIMS of octadec-1-yn-3-amine (***rac*-37**)

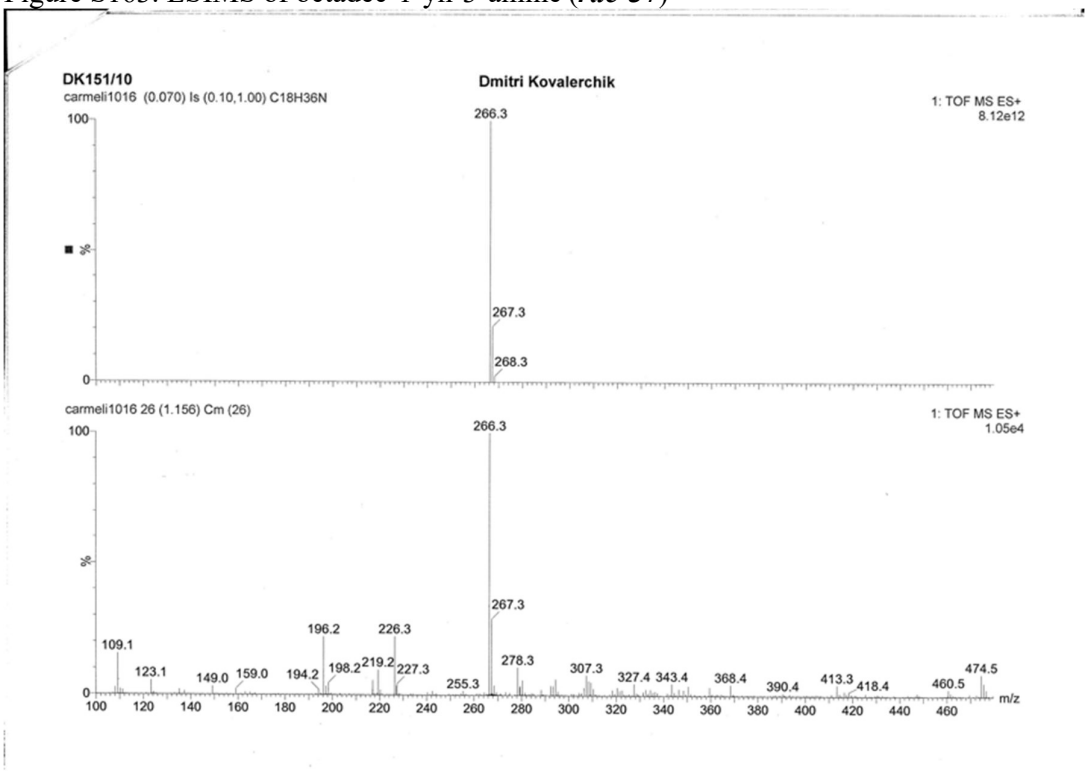


Figure S164. HRESIMS of octadec-1-yn-3-amine (***rac*-37**)

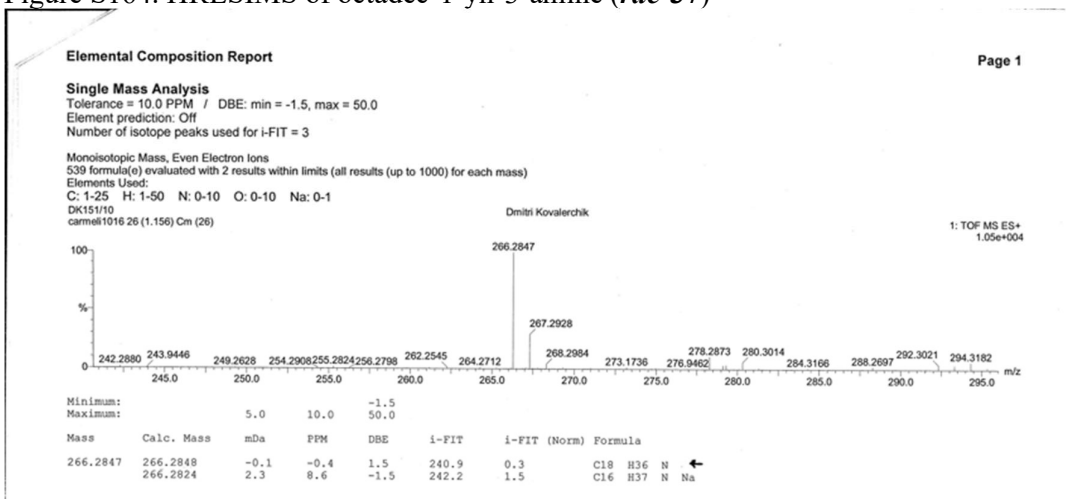


Figure S165. ^{1}H NMR spectrum of 3-methoxyoctadec-1-yne (***rac*-38**) in $CDCl_3$

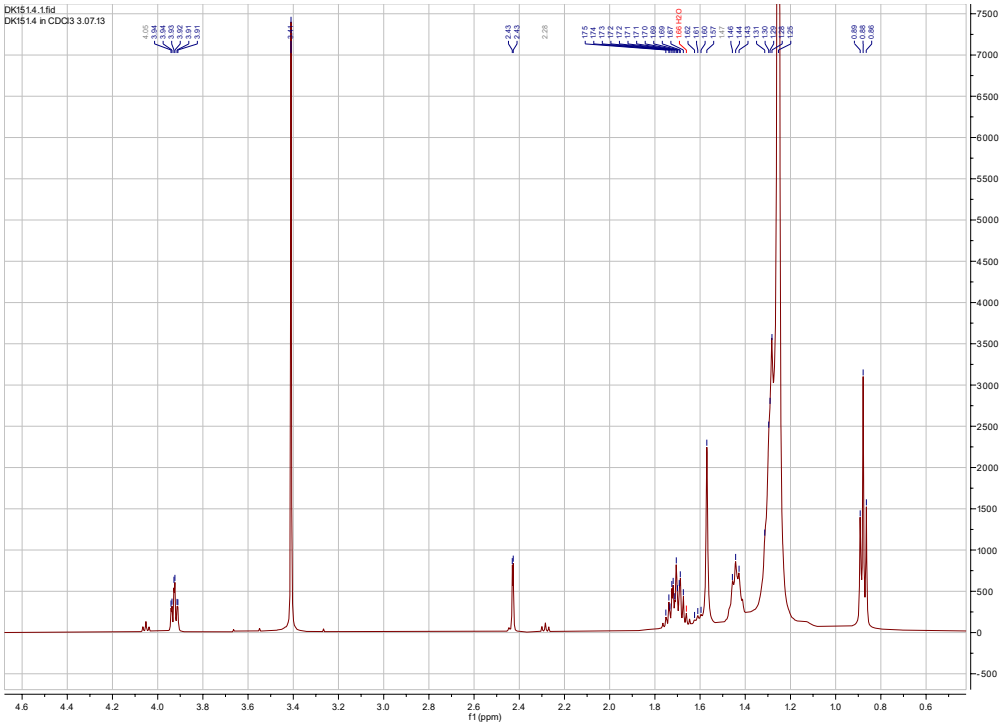


Figure S166. ^{1}H NMR spectrum of 3-methoxyoctadec-1-yne (***rac*-38**) in $CDCl_3$

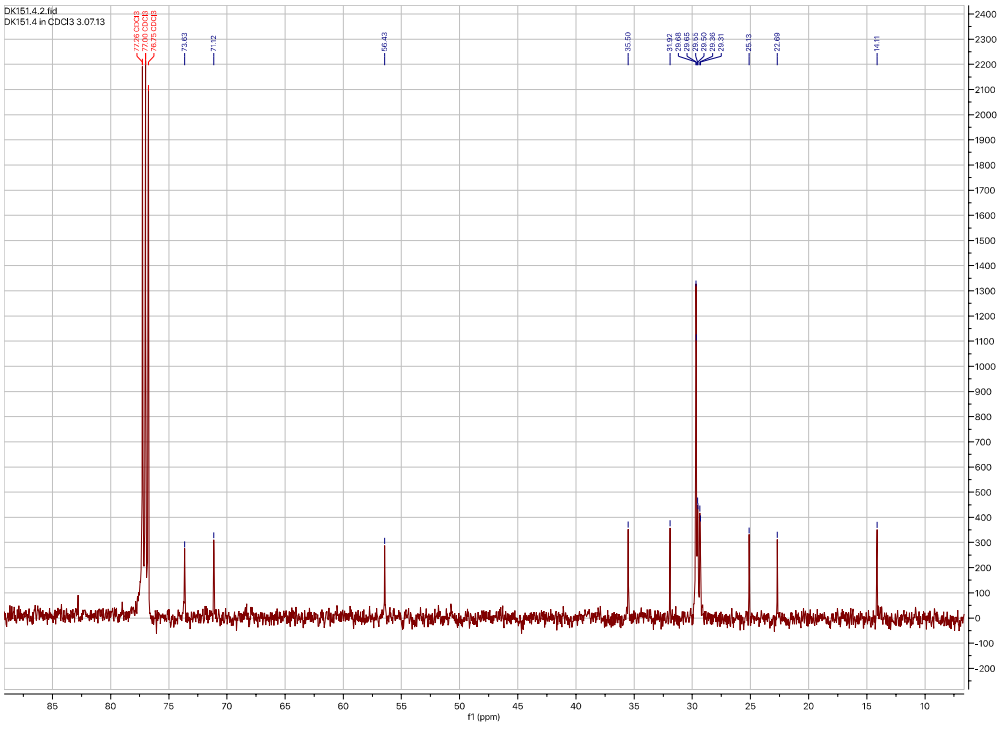


Figure S167. EIGCMS of 3-methoxyoctadec-1-yne (***rac*-38**)

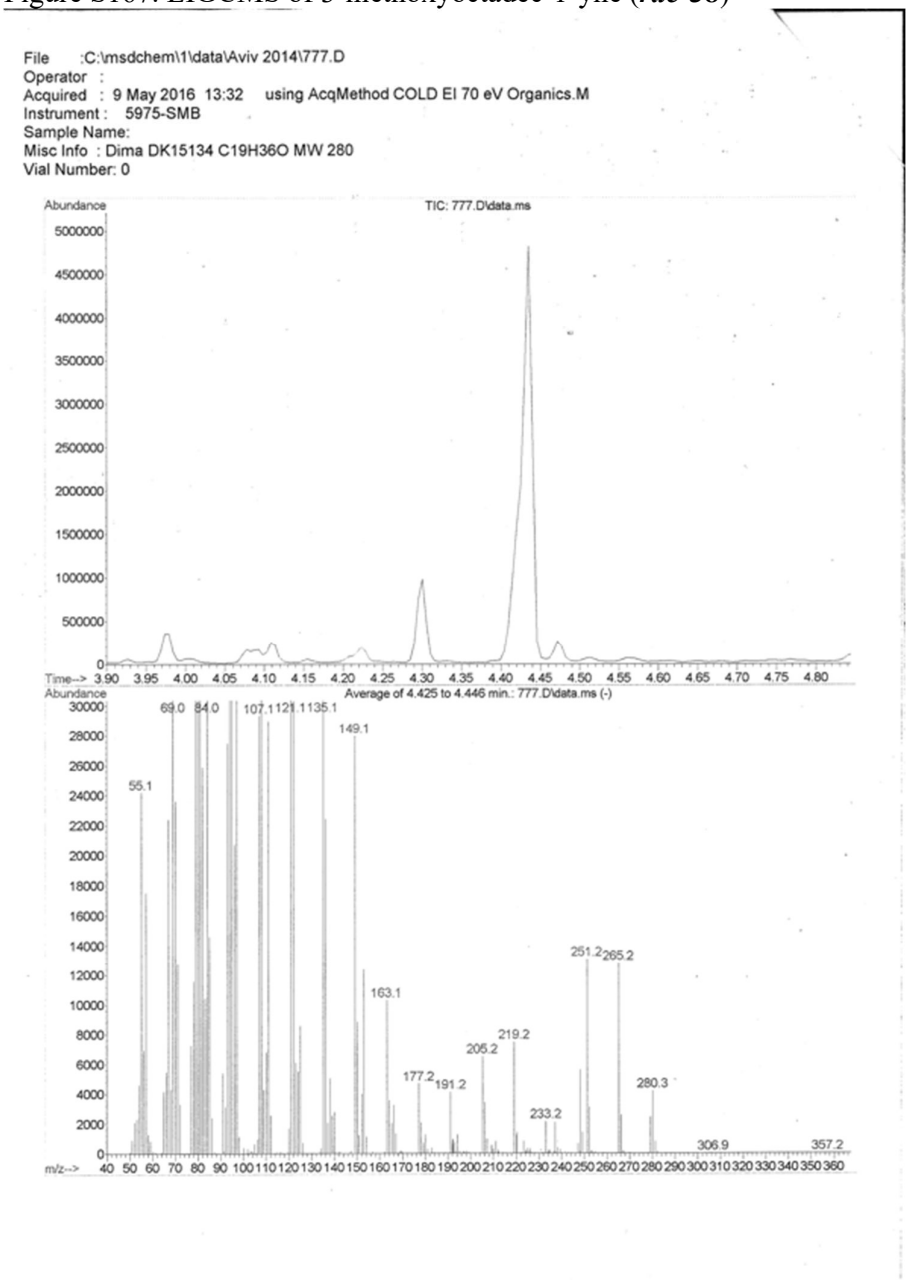


Figure S168. ^{1}H NMR spectrum of *S*-octadec-1-yn-3-yl ethanethioate (***rac*-39**) in $CDCl_3$

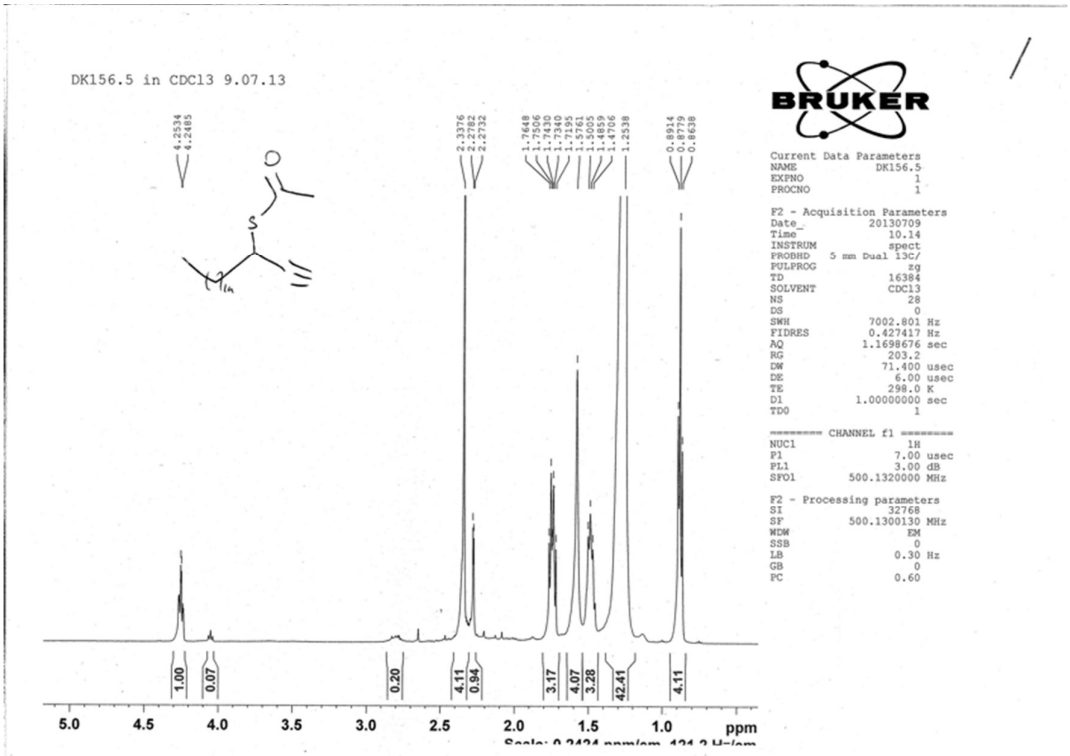


Figure S169. ^{13}C NMR spectrum of *S*-octadec-1-yn-3-yl ethanethioate (***rac*-39**) in $CDCl_3$

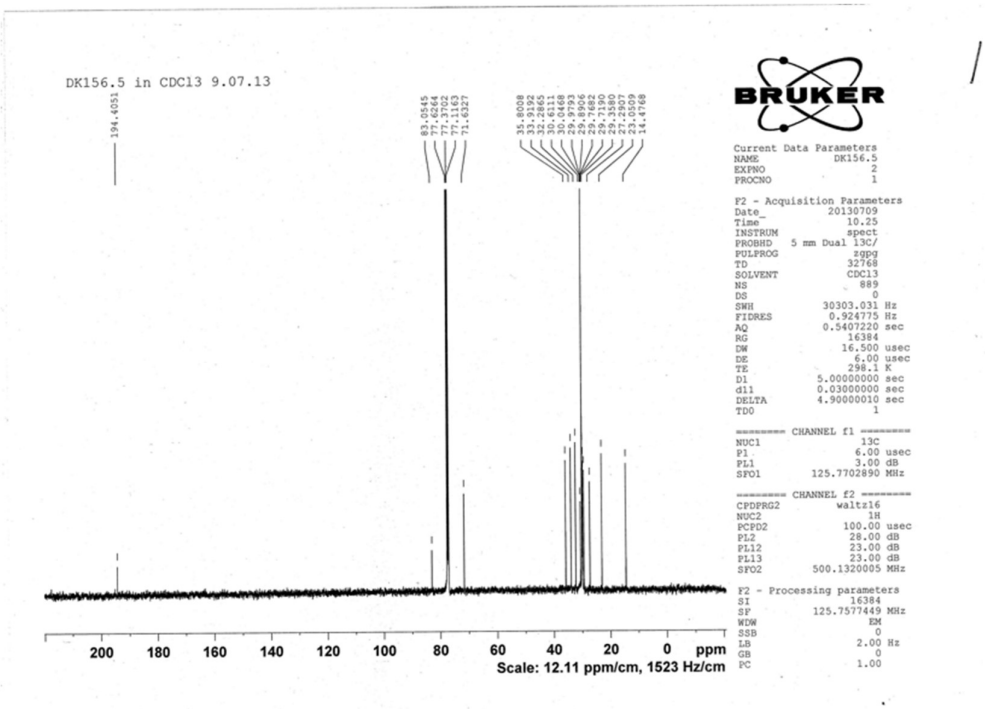


Figure S170. ESIMS of *S*-octadec-1-yn-3-yl ethanethioate (***rac*-39**)

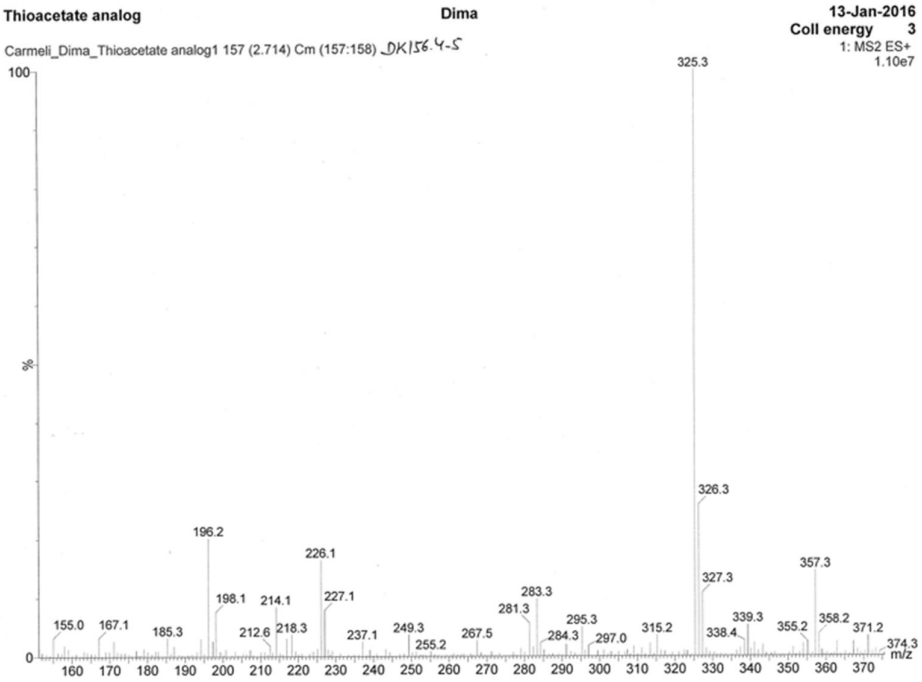


Figure S171. ^{1}H NMR spectrum of octadec-1-yn-3-thiol (***rac*-40**) in $CDCl_3$

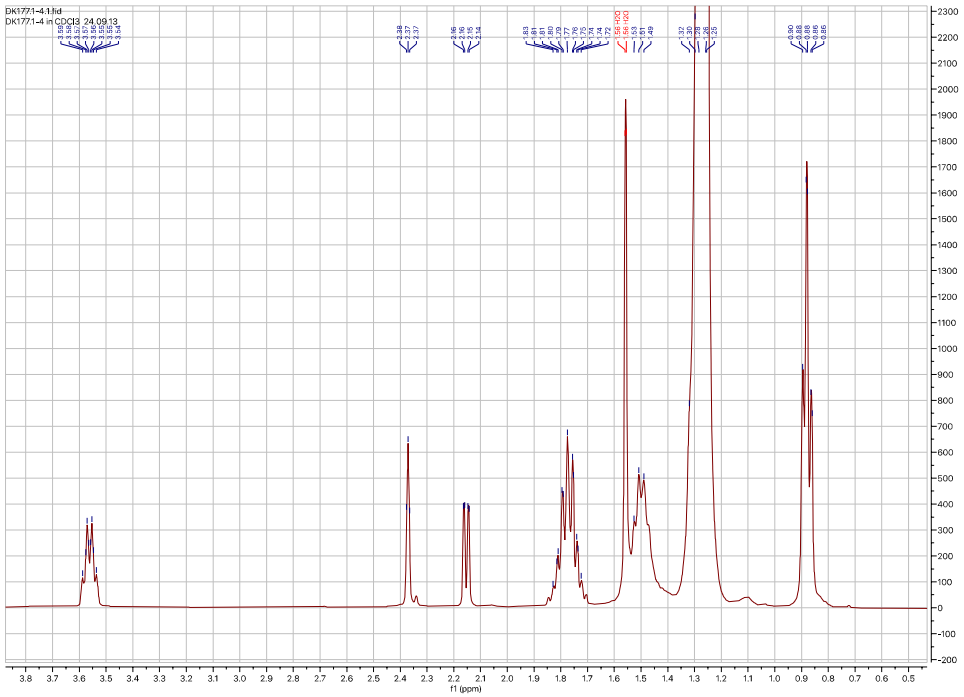


Figure S172. ^{13}C NMR spectrum of octadec-1-yn-3-thiol (***rac*-40**) in $CDCl_3$

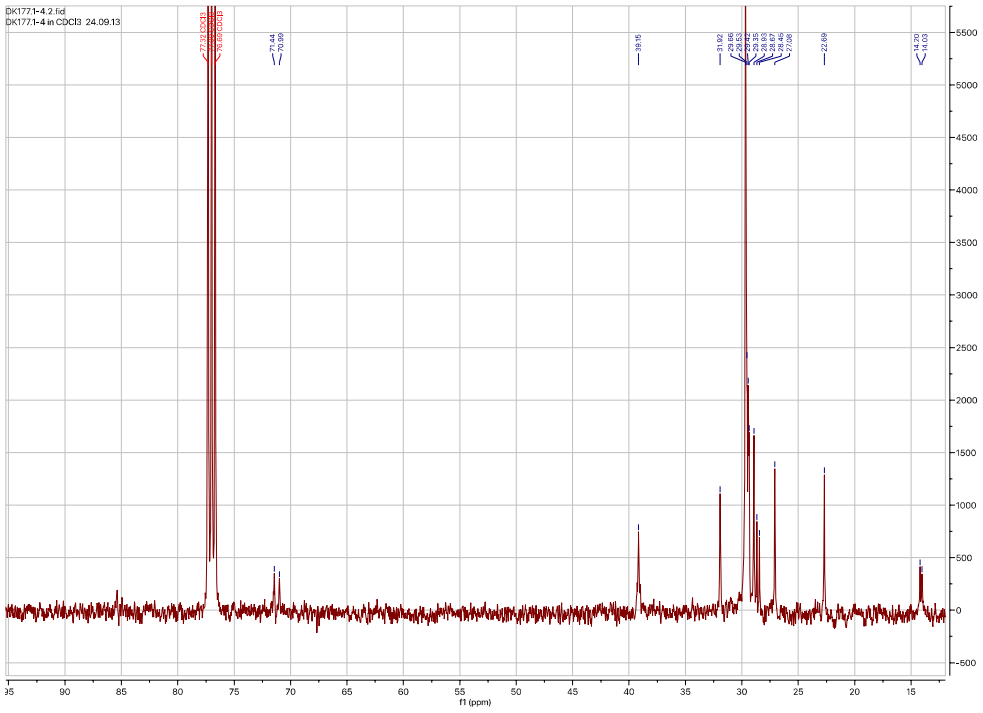


Figure S173. ^{1}H NMR spectrum of 3-methylnonadec-1-yn-3-ol (***rac*-41**) in $CDCl_3$

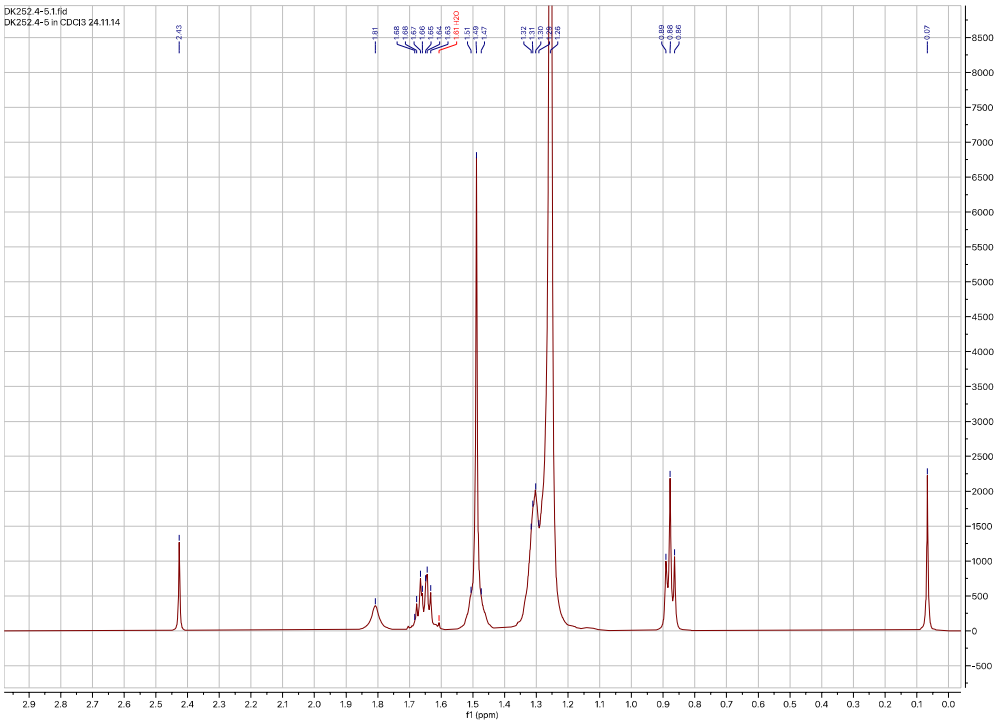


Figure S174. ^{13}C NMR spectrum of 3-methylnonadec-1-yn-3-ol (***rac*-41**) in $CDCl_3$

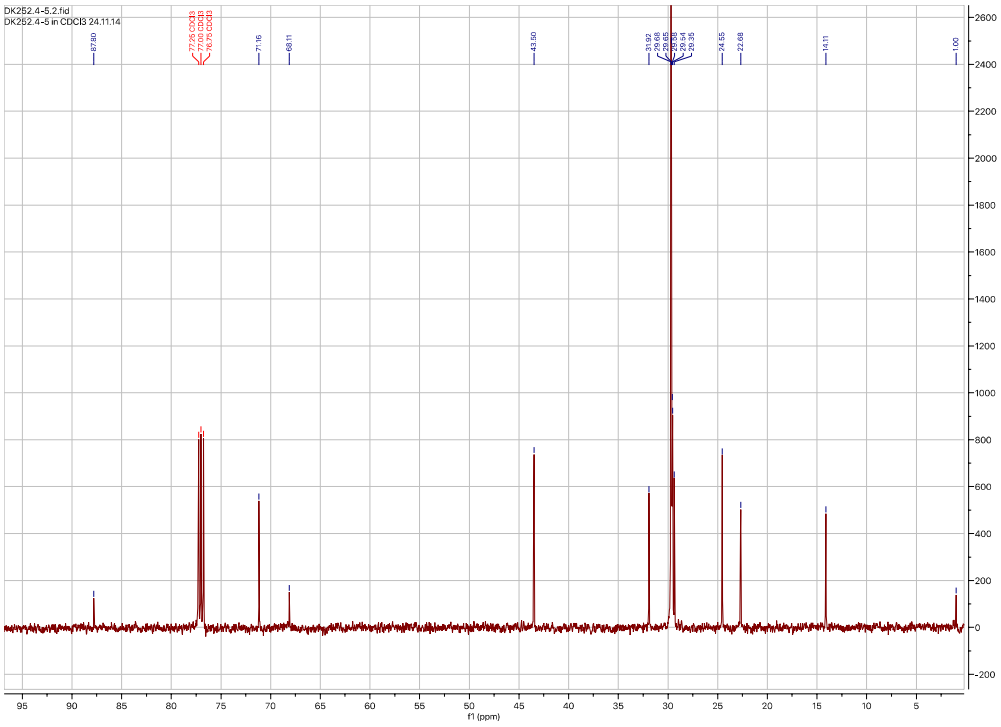


Figure S175. HRCIMS of 3-methylnonadec-1-yn-3-ol (***rac*-41**)

Compound Spectrum SmartFormula Report

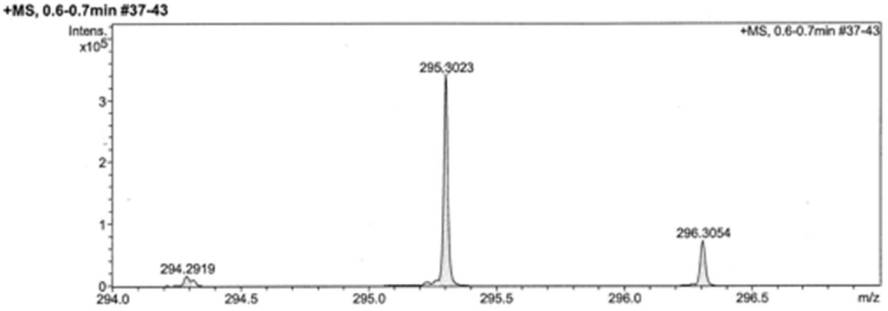
Analysis Info

Analysis Name	D:\Data\Client\CLI_9279_16.d	Acquisition Date	5/17/2015 11:57:03 AM
Method	CLI_9279.m	Operator	Larisa Panz
Sample Name	DK_252-4-7	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 0.6-0.7min #37-43



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
295.3023	1	C20H39O	295.2995	-9.2	18.0	1	100.00	1.5	even	ok	2.7 ←
	2	C18H35N2O	295.2744	-94.4	20.1	2	0.00	2.5	even	ok	27.9

Figure S176. ^{1}H NMR spectrum of henicos-2-yn-4-ol (***rac*-42**) in $CDCl_3$

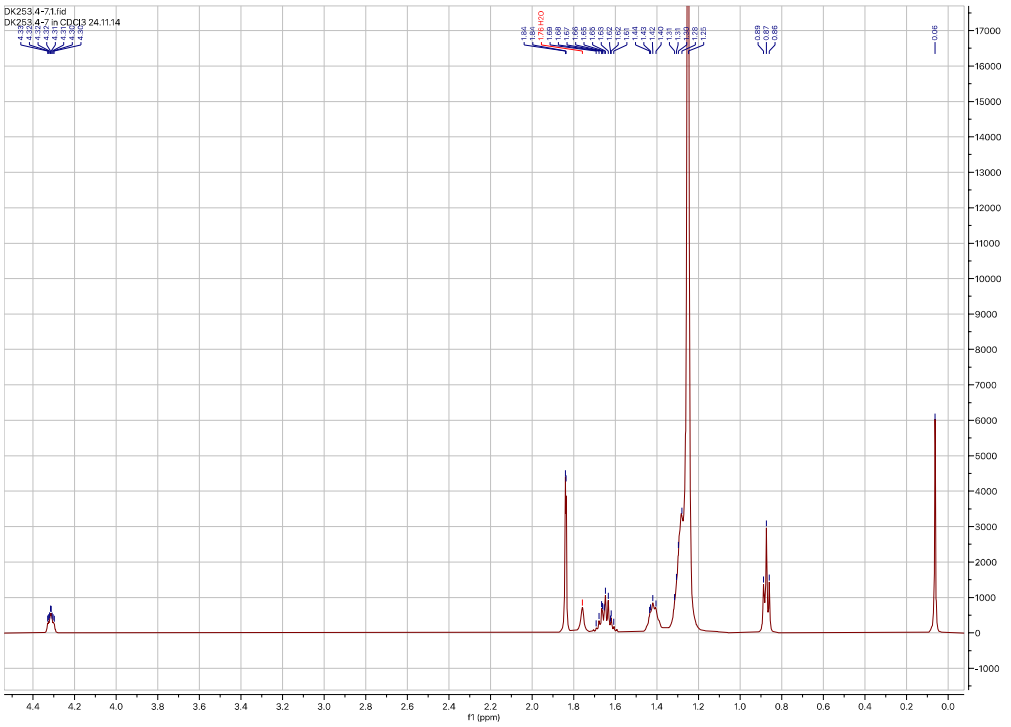


Figure S177. ^{13}C NMR spectrum of henicos-2-yn-4-ol (***rac*-42**) in $CDCl_3$

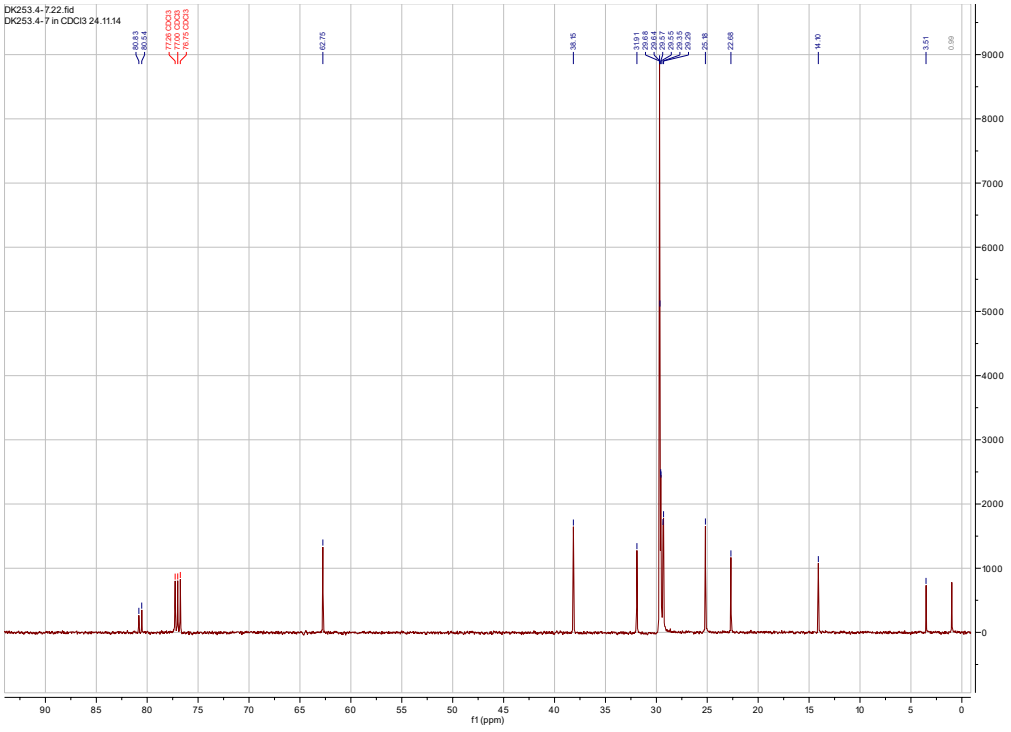


Figure S178. HRCIMS of henicos-2-yn-4-ol (***rac*-42**)

Compound Spectrum SmartFormula Report

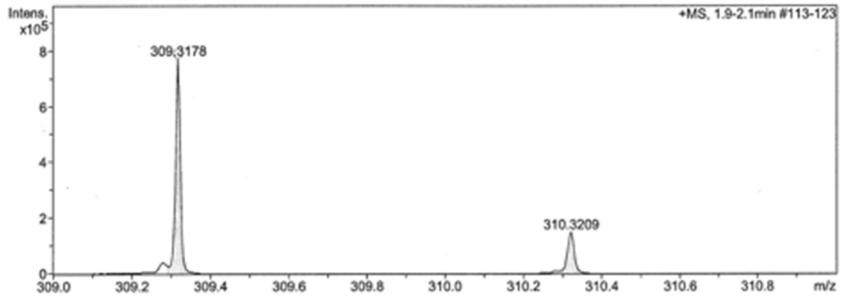
Analysis Info

Analysis Name	D:\Data\Client\CLI_9279_15.d	Acquisition Date	5/17/2015 11:51:17 AM
Method	CLI_9279.m	Operator	Larisa Panz
Sample Name	DK_253-4-7	Instrument	maXis impact 282001.00128
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

+MS, 1.9-2.1min #113-123



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	|err| [mDa]
309.3178	1	C19H37N2O	309.2900	-89.7	17.8	1	0.00	2.5	even	ok	27.8
	2	C21H41O	309.3152	-8.4	24.4	2	100.00	1.5	even	ok	2.6

CLI_9279_15.d
Bruker Compass DataAnalysis 4.2 printed: 5/17/2015 11:55:30 AM by: Larisa Panz Page 1 of 1

Figure S179. ^{1}H NMR spectrum of 1-(3-tetradecylphenyl)prop-2-yn-1-ol (***rac*-45**) in $CDCl_3$

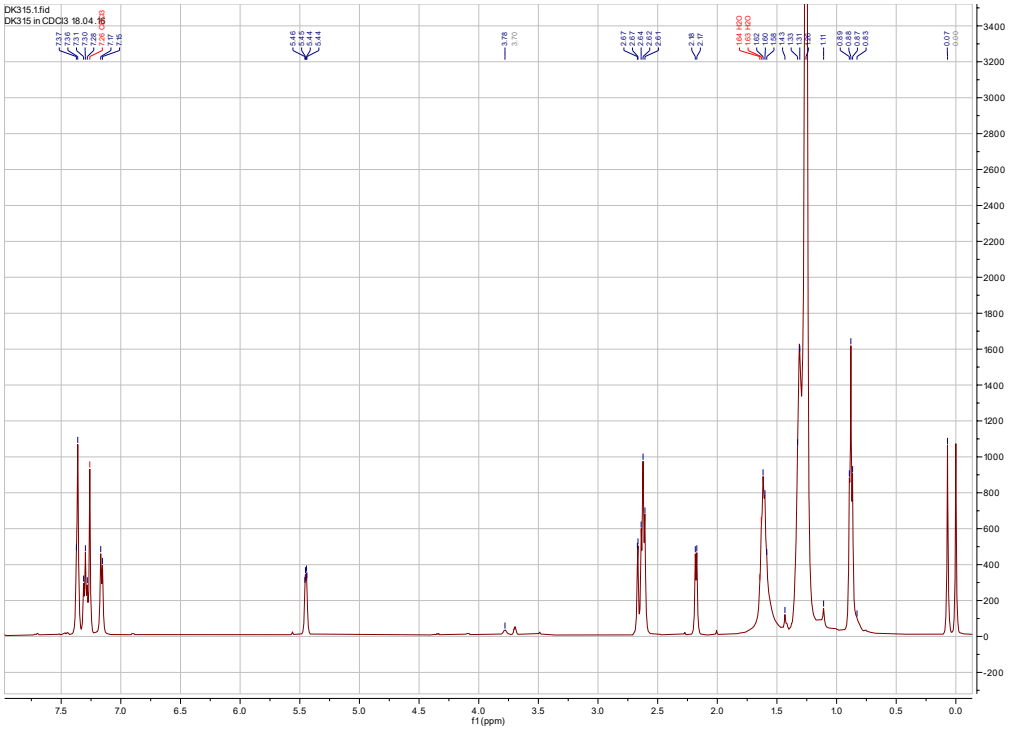


Figure S180. ^{13}C NMR spectrum of 1-(3-tetradecylphenyl)prop-2-yn-1-ol (***rac*-45**) in $CDCl_3$

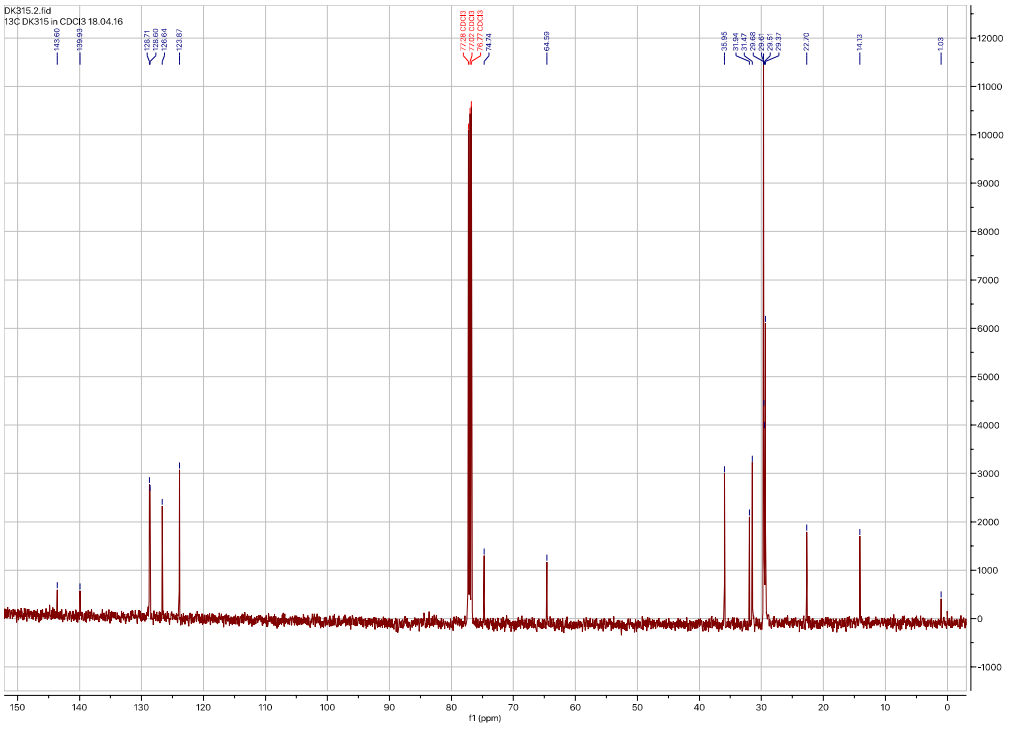
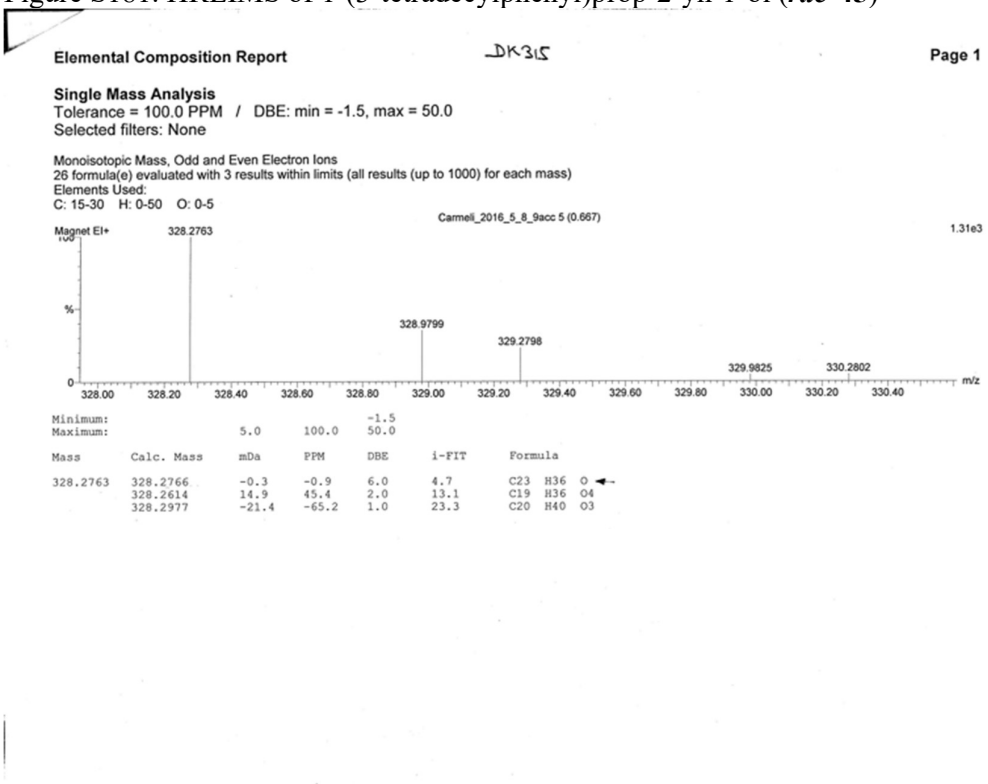


Figure S181. HREIMS of 1-(3-tetradecylphenyl)prop-2-yn-1-ol (***rac*-45**)



Elemental Composition Report DK315 **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
26 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-30 H: 0-50 O: 0-5

Carmeli_2016_5_8_9acc 5 (0.667)

Minimum:				-1.5		
Maximum:		5.0	100.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
328.2763	328.2766	-0.3	-0.9	6.0	4.7	C23 H36 O ◄
	328.2614	14.9	45.4	2.0	13.1	C19 H36 O4
	328.2977	-21.4	-65.2	1.0	23.3	C20 H40 O3

Figure S182. ^{1}H NMR spectrum of 1-(2-tetradecylphenyl)prop-2-yn-1-ol (***rac*-48**) in $CDCl_3$

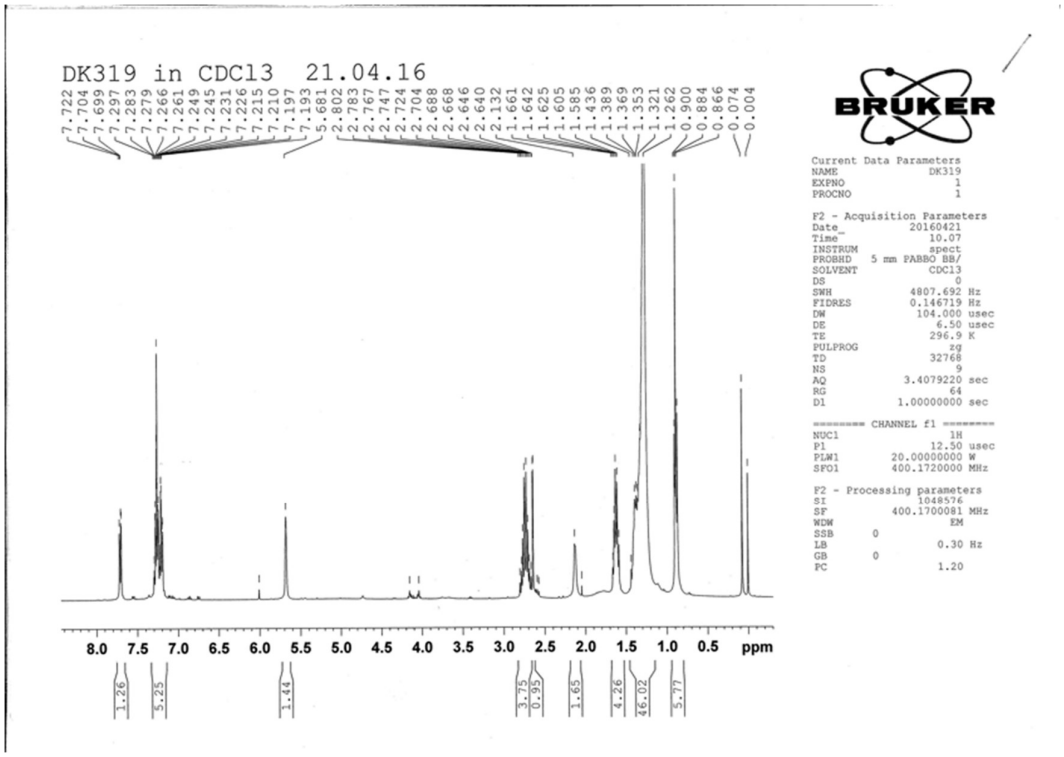


Figure S183. ^{13}C NMR spectrum of 1-(2-tetradecylphenyl)prop-2-yn-1-ol (***rac*-48**) in $CDCl_3$

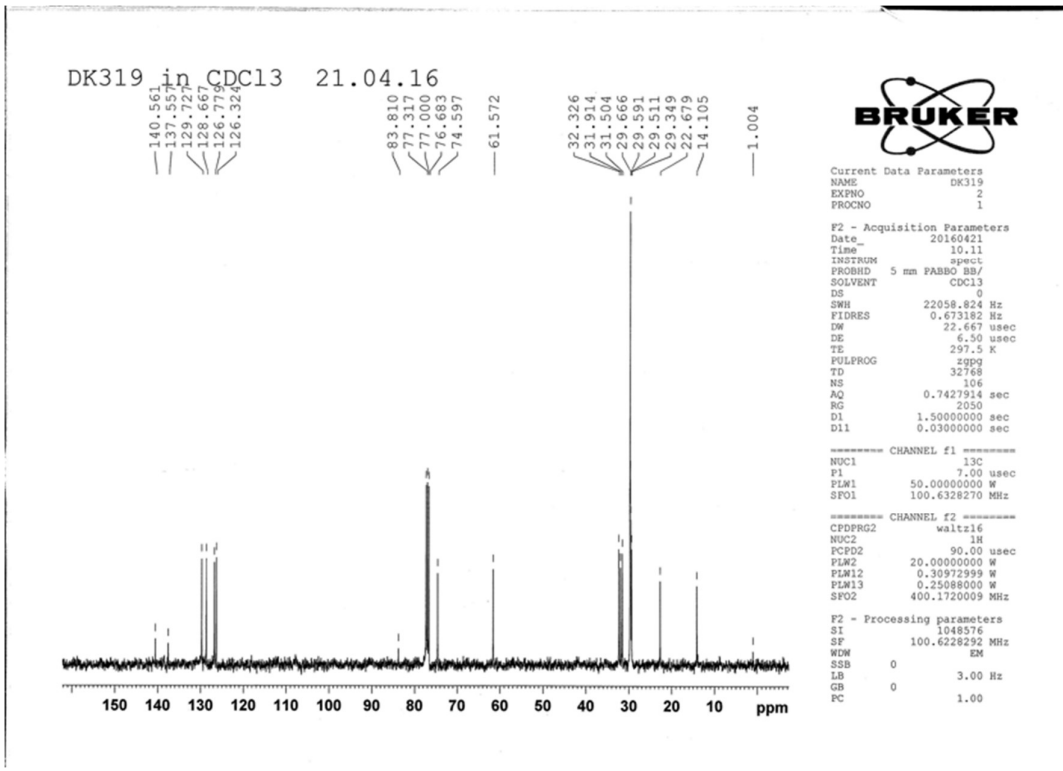
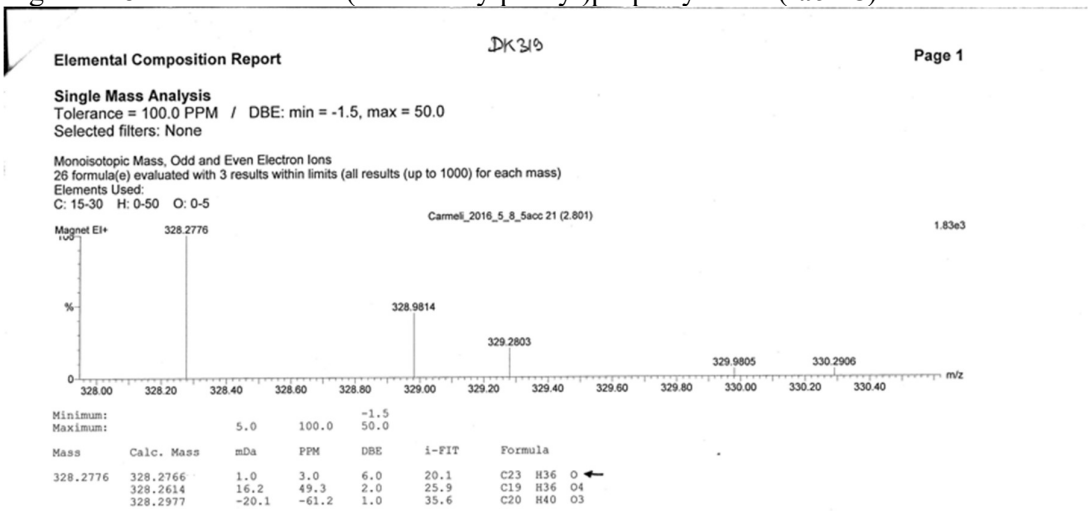


Figure S184. HREIMS of 1-(2-tetradecylphenyl)prop-2-yn-1-ol (***rac*-48**)



DK316

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
26 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 15-30 H: 0-50 O: 0-5

Minimum:				-1.5		
Maximum:		5.0	100.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
328.2776	328.2766	1.0	3.0	6.0	20.1	C23 H36 O ←
	328.2614	16.2	49.3	2.0	25.9	C19 H36 O4
	328.2977	-20.1	-61.2	1.0	35.6	C20 H40 O3

Figure S185. ^{1}H NMR spectrum of 1-phenylprop-2-yn-1-ol (***rac*-49**) in $CDCl_3$

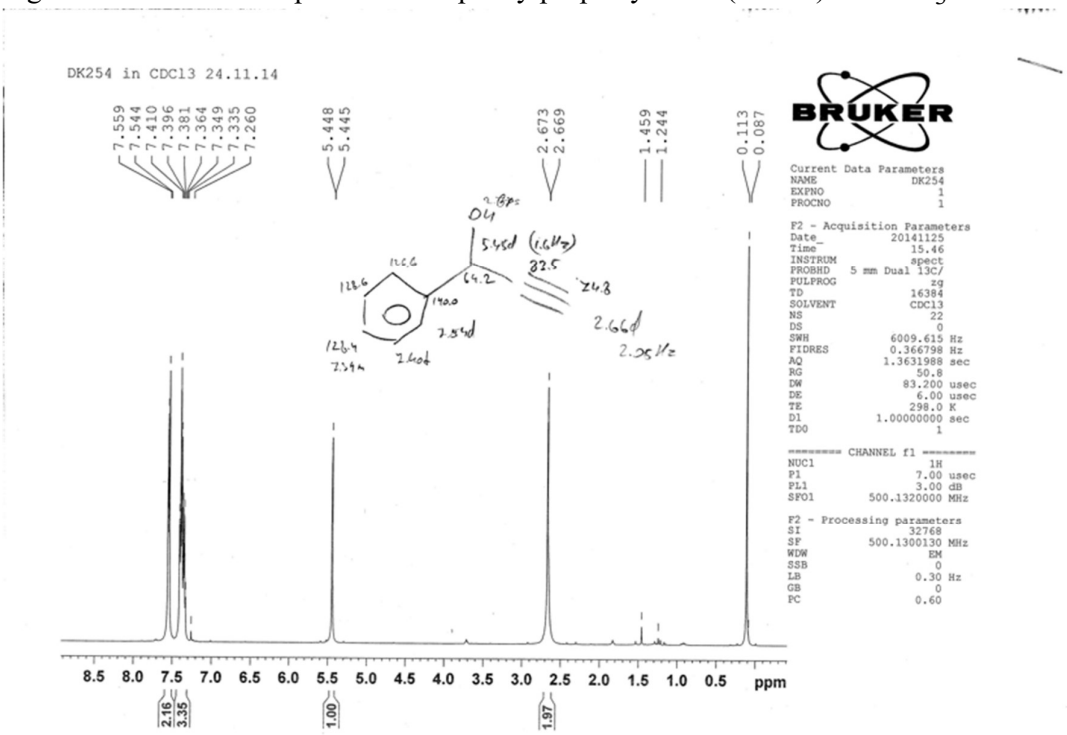


Figure S186. ^{13}C NMR spectrum of 1-phenylprop-2-yn-1-ol (***rac*-49**) in $CDCl_3$

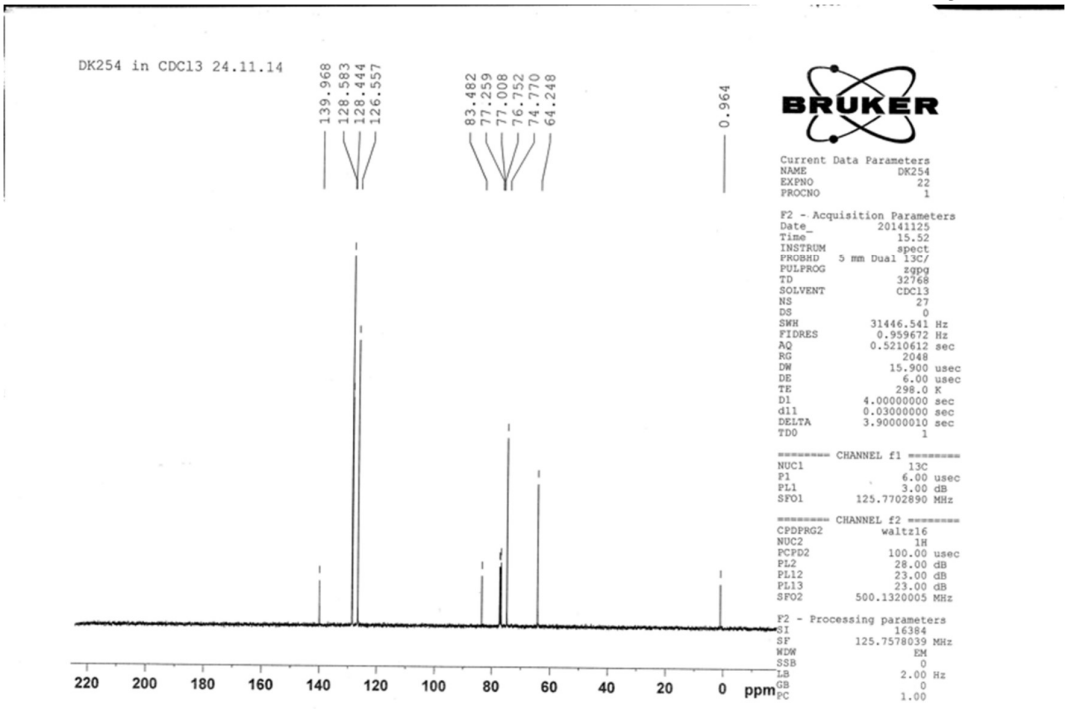
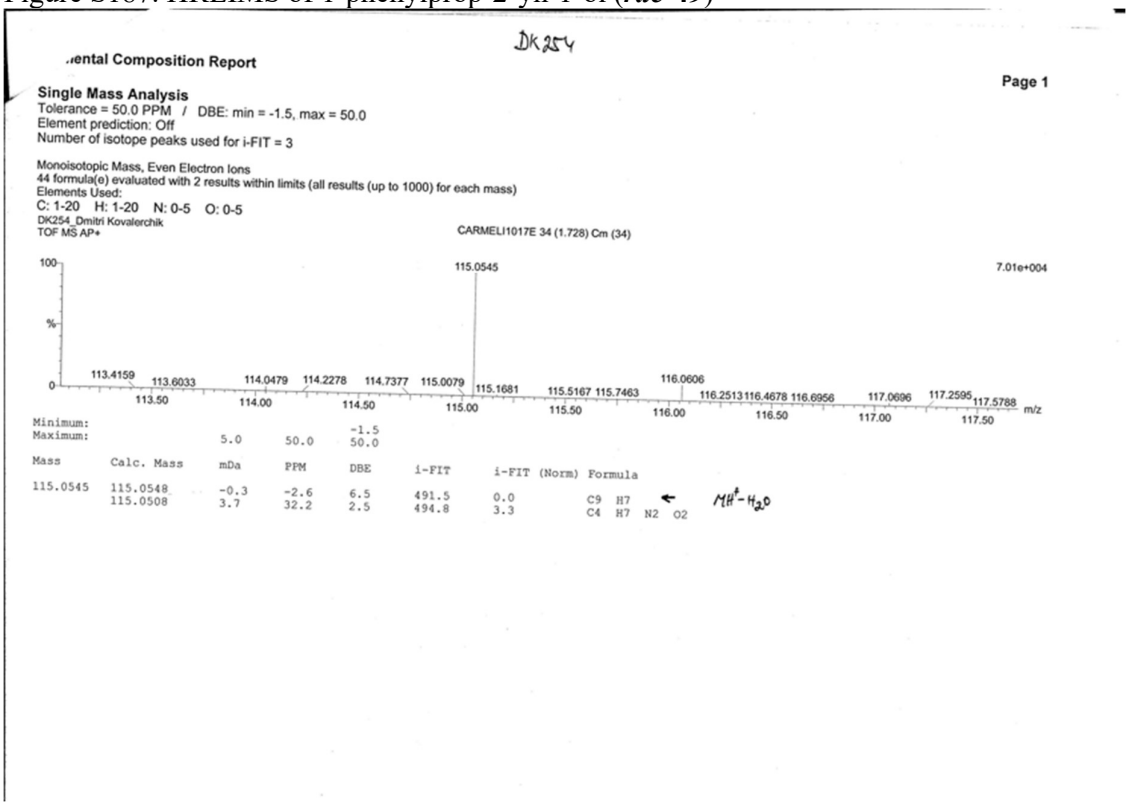


Figure S187. HREIMS of 1-phenylprop-2-yn-1-ol (***rac*-49**)



DK254

...ental Composition Report

Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
44 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-20 H: 1-20 N: 0-5 O: 0-5

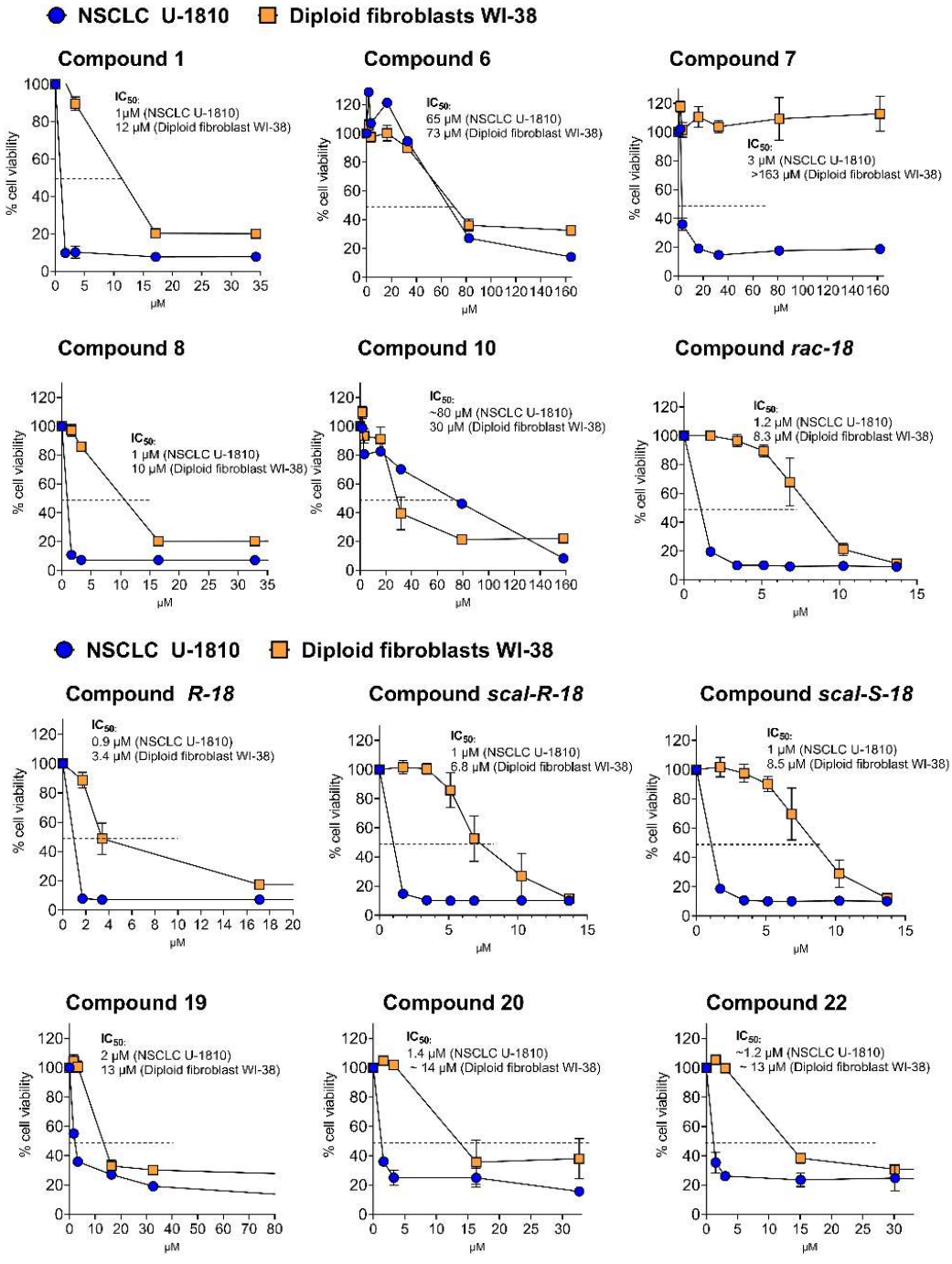
DK254_Dmitri Kovalerchik
TOF MS AP+

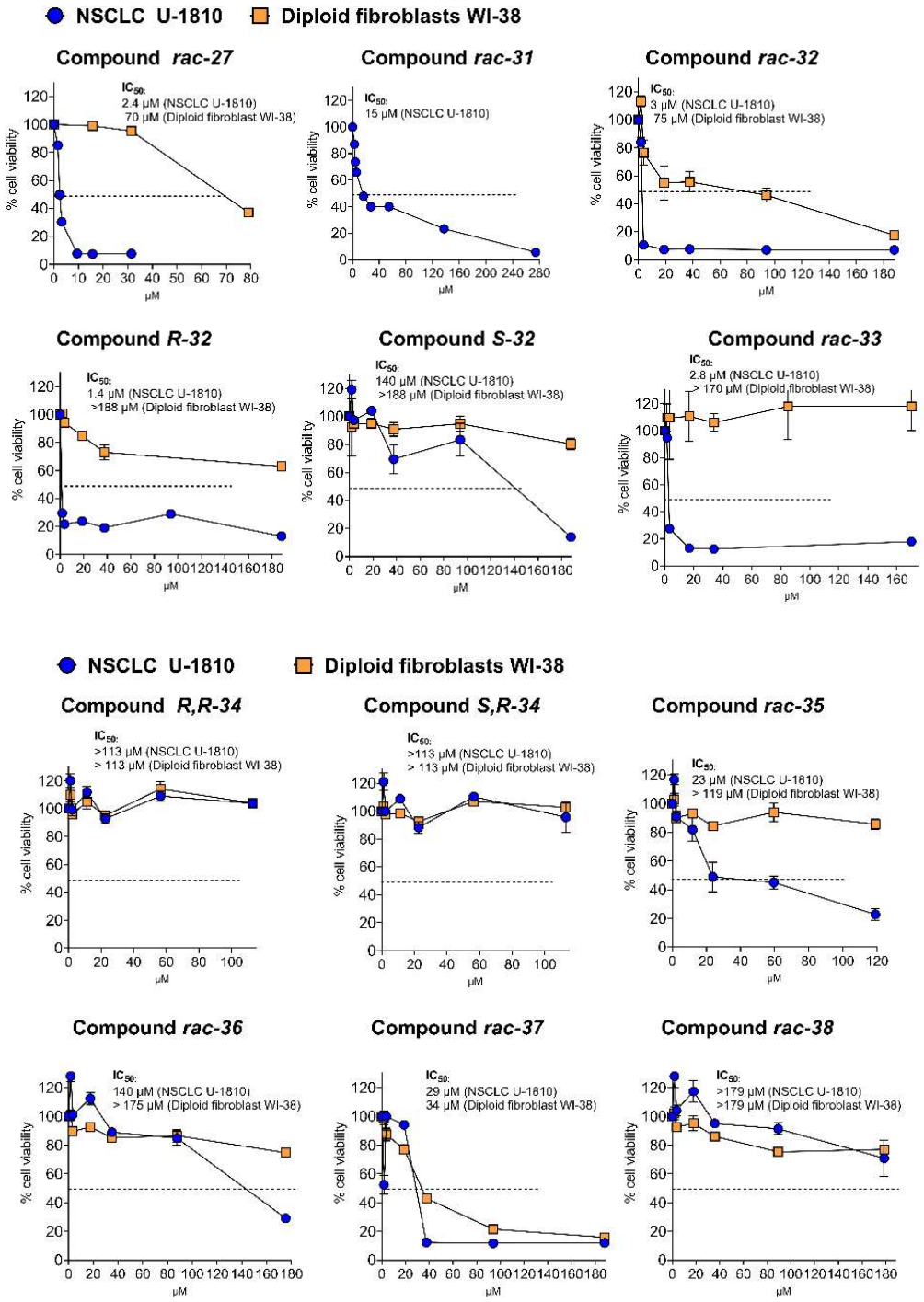
CARMELI1017E 34 (1.728) Cm (34)

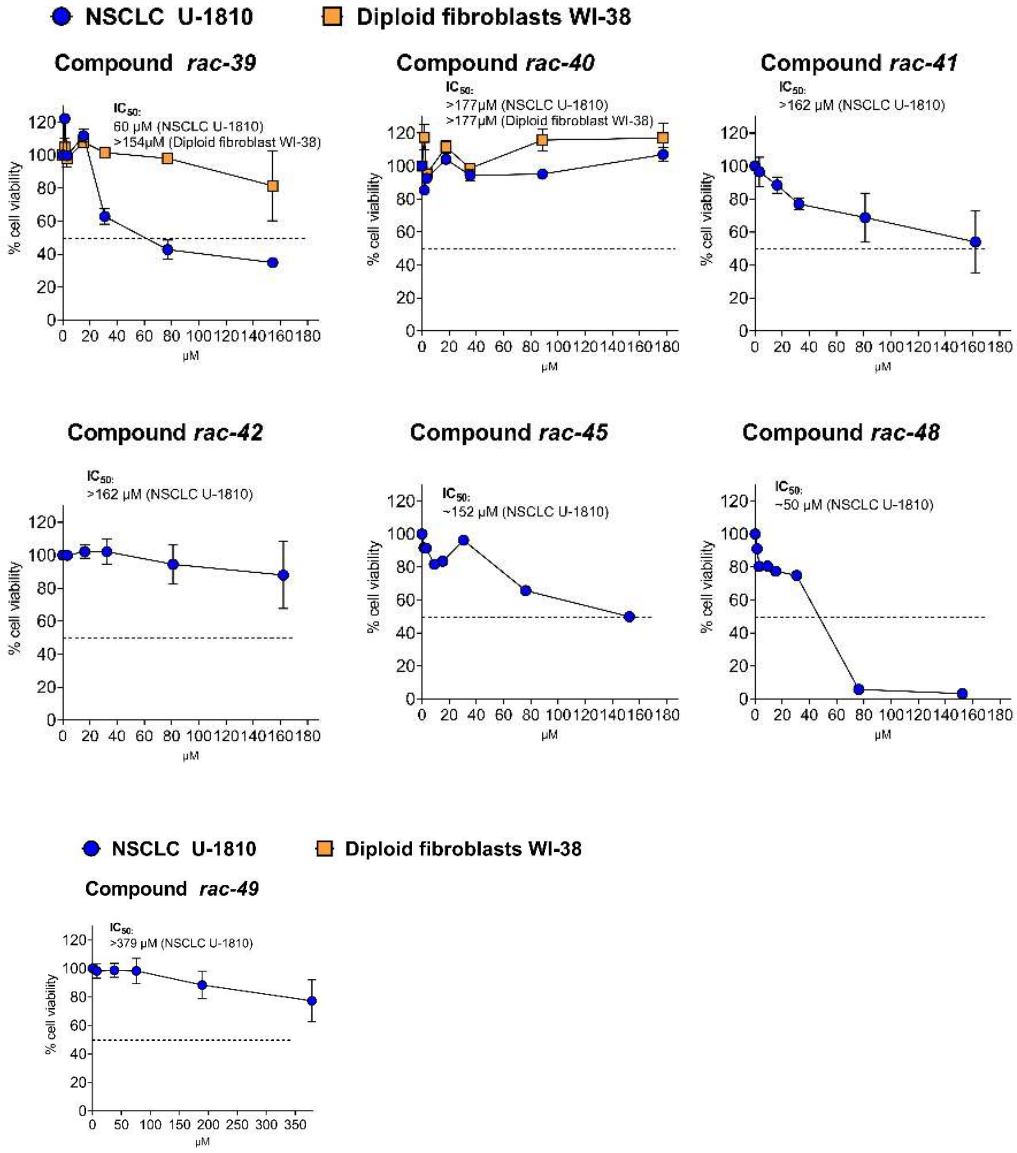
7.01e+004

Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
115.0545	115.0548	-0.3	-2.6	6.5	491.5	0.0	C9 H7	← MH^+-H_2O
	115.0508	3.7	32.2	2.5	494.8	3.3	C4 H7 N2 O2	

Figure S188. Dose response curves of the compounds described in Table 1 obtained from screening of NSCLC U-1810 cells or diploid fibroblast WI-38 cells are presented. The IC_{50} values were deduced from the cell viability curves.




NSCLC U-1810
Diploid fibroblasts WI-38
Compound rac-27
IC50:
2.4 µM (NSCLC U-1810)
70 µM (Diploid fibroblast WI-38)
Compound rac-31
IC50:
15 µM (NSCLC U-1810)
Compound rac-32
IC50:
3 µM (NSCLC U-1810)
75 µM (Diploid fibroblast WI-38)
Compound R-32
IC50:
1.4 µM (NSCLC U-1810)
>188 µM (Diploid fibroblast WI-38)
Compound S-32
IC50:
140 µM (NSCLC U-1810)
>188 µM (Diploid fibroblast WI-38)
Compound rac-33
IC50:
2.8 µM (NSCLC U-1810)
> 170 µM (Diploid fibroblast WI-38)
% cell viability
µM
NSCLC U-1810
Diploid fibroblasts WI-38
Compound R,R-34
IC50:
>113 µM (NSCLC U-1810)
> 113 µM (Diploid fibroblast WI-38)
Compound S,R-34
IC50:
>113 µM (NSCLC U-1810)
> 113 µM (Diploid fibroblast WI-38)
Compound rac-35
IC50:
23 µM (NSCLC U-1810)
> 119 µM (Diploid fibroblast WI-38)
Compound rac-36
IC50:
140 µM (NSCLC U-1810)
> 175 µM (Diploid fibroblast WI-38)
Compound rac-37
IC50:
29 µM (NSCLC U-1810)
34 µM (Diploid fibroblast WI-38)
Compound rac-38
IC50:
>179 µM (NSCLC U-1810)
>179 µM (Diploid fibroblast WI-38)
% cell viability
µM


NSCLC U-1810
Diploid fibroblasts WI-38
Compound rac-39
IC50:
60 µM (NSCLC U-1810)
>154µM (Diploid fibroblast WI-38)
Compound rac-40
IC50:
>177µM (NSCLC U-1810)
>177µM (Diploid fibroblast WI-38)
Compound rac-41
IC50:
>162 µM (NSCLC U-1810)
Compound rac-42
IC50:
>162 µM (NSCLC U-1810)
Compound rac-45
IC50:
~152 µM (NSCLC U-1810)
Compound rac-48
IC50:
~50 µM (NSCLC U-1810)
% cell viability
µM

NSCLC U-1810
Diploid fibroblasts WI-38
Compound rac-49
IC50:
>379 µM (NSCLC U-1810)
% cell viability
µM