5,6-Diphenyl-1,3,4,7-tetra-*p*-tolyl-1,3,3a,7a-tetrahydropentaleno[1,2-c]furan

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Supplementary Materials

Table S1. Crystal data and experimental details for **3** [CCDC 2341418] (ic21784).

	Crystal data	
Empirical formula	$C_{50}H_{42}O$	
Formula weight	658.83	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 16.4711(10) Å	α= 90°.
	b = 9.1373(6) Å	β= 106.575(3)°.
	c = 25.0870(15) Å	γ = 90°.
Volume	3618.7(4) $Å^3$	
Z	4	
F(000)	1400	
Density (calculated)	1.209 Mg/m^3	
Wavelength	1.54178 Å	
Cell parameters reflections used	9817	
Theta range for Cell parameters	2.88 to 77.91°.	
Absorption coefficient	0.534 mm^{-1}	
Temperature	100(2) K	
Crystal size	0.350 x 0.080 x 0.020 mm^3	
	Data collection	
Diffractometer	Bruker AXS D8 VENTURE, PhotonIII_C28	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8115	
No. of measured reflections	77656	
No. of independent reflections	7628 [R(int) = 0.0644]	
No. of observed [I>2_igma(I)]	6196	
Completeness to theta = 67.679°	99.8 %	
Theta range for data collection	2.877 to 78.600°.	
	Refinement	
Final R indices [I>2sigma(I)]	R1 = 0.0487, wR2 = 0.1259	
R indices (all data)	R1 = 0.0616, wR2 = 0.1365	
Goodness-of-fit on F^2	1.051	
No. of reflections	7628	
No. of parameters	465	
No. of restraints	0	
Largest diff. peak and hole	0.369 and -0.274 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5312(1)	5827(1)	4442(1)	24(1)
C(1)	5515(1)	6731(2)	4034(1)	23(1)
C(2)	5926(1)	8122(2)	4358(1)	22(1)
C(3)	6882(1)	8068(2)	4624(1)	23(1)
C(4)	7061(1)	8123(2)	5186(1)	23(1)
C(5)	7779(1)	8285(2)	5690(1)	24(1)
C(6)	7430(1)	8578(2)	6113(1)	24(1)
C(7)	6485(1)	8577(2)	5904(1)	23(1)
C(8)	6286(1)	8280(2)	5351(1)	22(1)
C(9)	5522(1)	8196(2)	4850(1)	22(1)
C(10)	5015(1)	6751(2)	4811(1)	23(1)
C(11)	6057(1)	5869(2)	3756(1)	24(1)
C(12)	6074(1)	6256(2)	3221(1)	28(1)
C(13)	6605(1)	5537(2)	2969(1)	30(1)
C(14)	7121(1)	4391(2)	3232(1)	28(1)
C(15)	7091(1)	3994(2)	3763(1)	27(1)
C(16)	6571(1)	4730(2)	4025(1)	25(1)
C(17)	7675(1)	3588(2)	2944(1)	39(1)
C(18)	7484(1)	8140(2)	4286(1)	24(1)
C(19)	7433(1)	9297(2)	3915(1)	28(1)
C(20)	8039(1)	9455(2)	3630(1)	32(1)
C(21)	8696(1)	8455(2)	3691(1)	30(1)
C(22)	8728(1)	7277(2)	4049(1)	30(1)
C(23)	8139(1)	7128(2)	4347(1)	28(1)
C(24)	9356(1)	8658(2)	3387(1)	39(1)
C(25)	8691(1)	8048(2)	5746(1)	26(1)
C(26)	9108(1)	8744(2)	5406(1)	30(1)
C(27)	9947(1)	8432(2)	5446(1)	35(1)
C(28)	10392(1)	7419(2)	5830(1)	38(1)
C(29)	9993(1)	6743(2)	6180(1)	36(1)
C(30)	9155(1)	7055(2)	6142(1)	31(1)

C(31)	7898(1)	8942(2)	6695(1)	25(1)
C(32)	8522(1)	10025(2)	6802(1)	32(1)
C(33)	8942(1)	10434(2)	7344(1)	38(1)
C(34)	8744(1)	9778(2)	7787(1)	34(1)
C(35)	8127(1)	8703(2)	7689(1)	32(1)
C(36)	7708(1)	8277(2)	7149(1)	28(1)
C(37)	5920(1)	8911(2)	6252(1)	23(1)
C(38)	6063(1)	10145(2)	6599(1)	26(1)
C(39)	5574(1)	10405(2)	6956(1)	28(1)
C(40)	4924(1)	9458(2)	6979(1)	28(1)
C(41)	4766(1)	8247(2)	6626(1)	27(1)
C(42)	5254(1)	7977(2)	6267(1)	25(1)
C(43)	4404(1)	9722(2)	7379(1)	39(1)
C(44)	4056(1)	6902(2)	4638(1)	23(1)
C(45)	3667(1)	7939(2)	4890(1)	26(1)
C(46)	2791(1)	7954(2)	4793(1)	31(1)
C(47)	2282(1)	6929(2)	4442(1)	36(1)
C(48)	2671(1)	5918(2)	4182(1)	38(1)
C(49)	3546(1)	5892(2)	4278(1)	29(1)
C(50)	1335(1)	6899(2)	4362(1)	55(1)

Table S3. Bond lengths [Å] and angles [°] for **3** (ic21784).

O(1)-C(1)	1.4274(17)	C(21)-C(22)	1.393(2)
O(1)-C(10)	1.4362(17)	C(21)-C(24)	1.507(2)
C(1)-C(11)	1.504(2)	C(22)-C(23)	1.391(2)
C(1)-C(2)	1.555(2)	C(25)-C(26)	1.394(2)
C(2)-C(3)	1.527(2)	C(25)-C(30)	1.399(2)
C(2)-C(9)	1.5623(19)	C(26)-C(27)	1.386(2)
C(3)-C(4)	1.356(2)	C(27)-C(28)	1.385(3)
C(3)-C(18)	1.478(2)	C(28)-C(29)	1.383(2)
C(4)-C(8)	1.457(2)	C(29)-C(30)	1.386(2)
C(4)-C(5)	1.473(2)	C(31)-C(32)	1.396(2)
C(5)-C(6)	1.370(2)	C(31)-C(36)	1.401(2)
C(5)-C(25)	1.483(2)	C(32)-C(33)	1.390(2)
C(6)-C(31)	1.482(2)	C(33)-C(34)	1.381(3)
C(6)-C(7)	1.495(2)	C(34)-C(35)	1.384(3)
C(7)-C(8)	1.357(2)	C(35)-C(36)	1.390(2)
C(7)-C(37)	1.478(2)	C(37)-C(42)	1.399(2)
C(8)-C(9)	1.506(2)	C(37)-C(38)	1.402(2)
C(9)-C(10)	1.550(2)	C(38)-C(39)	1.386(2)
C(10)-C(44)	1.521(2)	C(39)-C(40)	1.391(2)
C(11)-C(16)	1.389(2)	C(40)-C(41)	1.394(2)
C(11)-C(12)	1.395(2)	C(40)-C(43)	1.512(2)
C(12)-C(13)	1.383(2)	C(41)-C(42)	1.390(2)
C(13)-C(14)	1.391(2)	C(44)-C(45)	1.393(2)
C(14)-C(15)	1.394(2)	C(44)-C(49)	1.393(2)
C(14)-C(17)	1.508(2)	C(45)-C(46)	1.393(2)
C(15)-C(16)	1.392(2)	C(46)-C(47)	1.391(2)
C(18)-C(19)	1.395(2)	C(47)-C(48)	1.389(3)
C(18)-C(23)	1.396(2)	C(47)-C(50)	1.514(2)
C(19)-C(20)	1.392(2)	C(48)-C(49)	1.392(2)
C(20)-C(21)	1.391(2)		

C(1)-O(1)-C(10)	108.31(11)	C(11)-C(1)-C(2)	116.30(12)
O(1)-C(1)-C(11)	108.78(12)	C(3)-C(2)-C(1)	116.25(12)
O(1)-C(1)-C(2)	104.79(11)	C(3)-C(2)-C(9)	105.92(11)

C(1)-C(2)-C(9)	103.16(11)	C(19)-C(18)-C(3)	119.64(14)
C(4)-C(3)-C(18)	127.76(14)	C(23)-C(18)-C(3)	122.13(14)
C(4)-C(3)-C(2)	110.13(13)	C(20)-C(19)-C(18)	120.47(15)
C(18)-C(3)-C(2)	121.66(12)	C(21)-C(20)-C(19)	121.61(15)
C(3)-C(4)-C(8)	110.61(13)	C(20)-C(21)-C(22)	117.70(15)
C(3)-C(4)-C(5)	141.15(14)	C(20)-C(21)-C(24)	120.93(16)
C(8)-C(4)-C(5)	107.49(12)	C(22)-C(21)-C(24)	121.36(16)
C(6)-C(5)-C(4)	105.80(13)	C(23)-C(22)-C(21)	121.15(16)
C(6)-C(5)-C(25)	126.28(13)	C(22)-C(23)-C(18)	120.87(15)
C(4)-C(5)-C(25)	127.69(13)	C(26)-C(25)-C(30)	117.71(14)
C(5)-C(6)-C(31)	126.31(14)	C(26)-C(25)-C(5)	122.52(14)
C(5)-C(6)-C(7)	110.68(13)	C(30)-C(25)-C(5)	119.74(14)
C(31)-C(6)-C(7)	122.92(13)	C(27)-C(26)-C(25)	121.15(15)
C(8)-C(7)-C(37)	129.47(14)	C(28)-C(27)-C(26)	120.46(16)
C(8)-C(7)-C(6)	106.43(13)	C(29)-C(28)-C(27)	119.15(16)
C(37)-C(7)-C(6)	124.05(13)	C(28)-C(29)-C(30)	120.54(16)
C(7)-C(8)-C(4)	109.55(13)	C(29)-C(30)-C(25)	120.96(15)
C(7)-C(8)-C(9)	139.77(14)	C(32)-C(31)-C(36)	118.34(14)
C(4)-C(8)-C(9)	110.38(12)	C(32)-C(31)-C(6)	119.70(14)
C(8)-C(9)-C(10)	113.77(12)	C(36)-C(31)-C(6)	121.90(14)
C(8)-C(9)-C(2)	102.68(12)	C(33)-C(32)-C(31)	120.79(16)
C(10)-C(9)-C(2)	104.84(11)	C(34)-C(33)-C(32)	120.26(17)
O(1)-C(10)-C(44)	112.72(11)	C(33)-C(34)-C(35)	119.73(15)
O(1)-C(10)-C(9)	105.40(11)	C(34)-C(35)-C(36)	120.48(15)
C(44)-C(10)-C(9)	115.94(12)	C(35)-C(36)-C(31)	120.39(15)
C(16)-C(11)-C(12)	118.74(14)	C(42)-C(37)-C(38)	117.88(14)
C(16)-C(11)-C(1)	121.79(13)	C(42)-C(37)-C(7)	121.36(14)
C(12)-C(11)-C(1)	119.42(14)	C(38)-C(37)-C(7)	120.70(14)
C(13)-C(12)-C(11)	120.52(15)	C(39)-C(38)-C(37)	120.91(14)
C(12)-C(13)-C(14)	121.38(14)	C(38)-C(39)-C(40)	121.10(15)
C(13)-C(14)-C(15)	117.83(14)	C(39)-C(40)-C(41)	118.27(14)
C(13)-C(14)-C(17)	120.61(14)	C(39)-C(40)-C(43)	121.08(15)
C(15)-C(14)-C(17)	121.54(15)	C(41)-C(40)-C(43)	120.65(15)
C(16)-C(15)-C(14)	121.21(15)	C(42)-C(41)-C(40)	121.02(15)
C(11)-C(16)-C(15)	120.29(14)	C(41)-C(42)-C(37)	120.79(14)
C(19)-C(18)-C(23)	118.14(14)	C(45)-C(44)-C(49)	118.33(14)

C(45)-C(44)-C(10)	120.53(13)	C(48)-C(47)-C(50)	121.45(17)
C(49)-C(44)-C(10)	120.65(14)	C(46)-C(47)-C(50)	120.54(17)
C(44)-C(45)-C(46)	121.00(15)	C(47)-C(48)-C(49)	121.56(16)
C(47)-C(46)-C(45)	120.80(16)	C(48)-C(49)-C(44)	120.29(16)
C(48)-C(47)-C(46)	117.98(15)		

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3** (ic21784). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	32(1)	23(1)	21(1)	-1(1)	10(1)	-2(1)
C(1)	26(1)	25(1)	18(1)	1(1)	5(1)	-2(1)
C(2)	25(1)	23(1)	17(1)	1(1)	4(1)	0(1)
C(3)	26(1)	21(1)	21(1)	0(1)	5(1)	-2(1)
C(4)	25(1)	23(1)	22(1)	0(1)	7(1)	-2(1)
C(5)	27(1)	26(1)	19(1)	2(1)	4(1)	-2(1)
C(6)	26(1)	24(1)	20(1)	1(1)	4(1)	-2(1)
C(7)	26(1)	23(1)	20(1)	-1(1)	5(1)	-2(1)
C(8)	26(1)	21(1)	21(1)	0(1)	6(1)	-2(1)
C(9)	26(1)	23(1)	17(1)	0(1)	4(1)	-1(1)
C(10)	27(1)	24(1)	17(1)	-1(1)	5(1)	-1(1)
C(11)	26(1)	24(1)	20(1)	-3(1)	5(1)	-4(1)
C(12)	33(1)	30(1)	20(1)	1(1)	4(1)	0(1)
C(13)	36(1)	34(1)	20(1)	1(1)	8(1)	-1(1)
C(14)	27(1)	34(1)	23(1)	-4(1)	7(1)	-3(1)
C(15)	28(1)	27(1)	24(1)	0(1)	4(1)	-1(1)
C(16)	29(1)	28(1)	19(1)	1(1)	6(1)	-3(1)
C(17)	38(1)	50(1)	32(1)	2(1)	15(1)	8(1)
C(18)	26(1)	28(1)	18(1)	-3(1)	5(1)	-4(1)
C(19)	31(1)	32(1)	21(1)	1(1)	7(1)	-1(1)
C(20)	35(1)	38(1)	22(1)	4(1)	9(1)	-4(1)
C(21)	30(1)	41(1)	20(1)	-4(1)	6(1)	-6(1)
C(22)	29(1)	35(1)	26(1)	-3(1)	6(1)	-1(1)
C(23)	30(1)	29(1)	23(1)	0(1)	6(1)	-2(1)
C(24)	34(1)	57(1)	28(1)	2(1)	12(1)	-3(1)
C(25)	27(1)	29(1)	19(1)	-4(1)	4(1)	-2(1)
C(26)	29(1)	34(1)	25(1)	3(1)	5(1)	-3(1)
C(27)	30(1)	45(1)	31(1)	5(1)	10(1)	-5(1)
C(28)	26(1)	54(1)	33(1)	4(1)	7(1)	3(1)
C(29)	30(1)	47(1)	30(1)	10(1)	4(1)	5(1)
C(30)	30(1)	40(1)	22(1)	5(1)	6(1)	-2(1)

C(31)	24(1)	31(1)	20(1)	-1(1)	4(1)	2(1)
C(32)	32(1)	42(1)	22(1)	-4(1)	7(1)	-7(1)
C(33)	34(1)	46(1)	28(1)	-10(1)	3(1)	-8(1)
C(34)	35(1)	42(1)	20(1)	-6(1)	-1(1)	6(1)
C(35)	39(1)	36(1)	19(1)	4(1)	5(1)	10(1)
C(36)	31(1)	28(1)	23(1)	1(1)	6(1)	2(1)
C(37)	24(1)	28(1)	16(1)	2(1)	3(1)	1(1)
C(38)	27(1)	27(1)	21(1)	0(1)	3(1)	-1(1)
C(39)	30(1)	29(1)	21(1)	-3(1)	3(1)	3(1)
C(40)	30(1)	35(1)	18(1)	2(1)	5(1)	3(1)
C(41)	26(1)	32(1)	22(1)	2(1)	6(1)	-2(1)
C(42)	27(1)	28(1)	18(1)	-1(1)	4(1)	-2(1)
C(43)	45(1)	46(1)	30(1)	-4(1)	18(1)	-1(1)
C(44)	27(1)	24(1)	18(1)	3(1)	4(1)	-2(1)
C(45)	28(1)	25(1)	24(1)	1(1)	5(1)	-2(1)
C(46)	29(1)	28(1)	35(1)	3(1)	9(1)	2(1)
C(47)	25(1)	32(1)	45(1)	4(1)	3(1)	0(1)
C(48)	31(1)	35(1)	40(1)	-4(1)	-2(1)	-5(1)
C(49)	30(1)	30(1)	25(1)	-2(1)	1(1)	0(1)
C(50)	26(1)	45(1)	86(2)	-4(1)	4(1)	-1(1)

Table S5 Selected bond distances (Å), bond angles (deg) and torsional angle (deg).

Bond distance		**Bond Angle**		**Torsional angle**	
O1-C2	1.4274(17)	O1-C1-C2	104.79(11)	C2-C3-C4-C8	2.45(17)
O1-C10	1.4362(17)	C1-C2-C9	103.16(11)	C9-C8-C4-C3	5.09(18)
C1-C2	1.555(2)	C2-C9-C10	104.84(11)	C8-C9-C2-C3	3.71(14)
C2-C3	1.527(2)	C9-C10-O1	105.40(11)	C1-C2-C9-C10	7.17(14)
C3-C4	1.356(2)	C7-C8-C9	139.77(14)	C4-C5-C6-C7	1.43(17)
C4-C5	1.473(2)	C3-C4-C5	141.15(14)	C7-C8-C4-C5	2.38(17)
C5-C6	1.370(2)			O1-C10-C9-C2	14.63(14)
C6-C7	1.495(2)			O1-C1-C2-C9	26.83(14)
C7-C8	1.357(2)				
C8-C9	1.506(2)				
C9-C10	1.550(2)				

Figure S1. ^{1}H NMR spectrum of compound **3** in $CDCl_3$

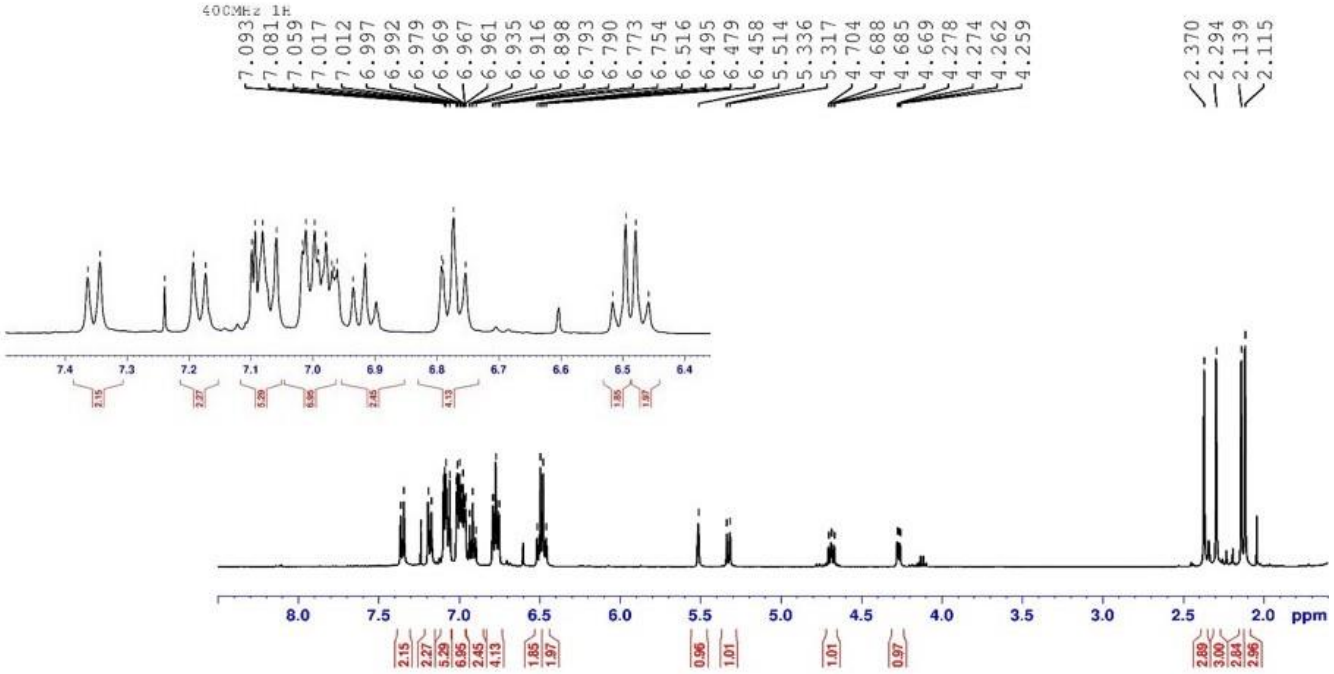

Figure S2. ^{13}C NMR spectrum of compound **3** in $CDCl_3$

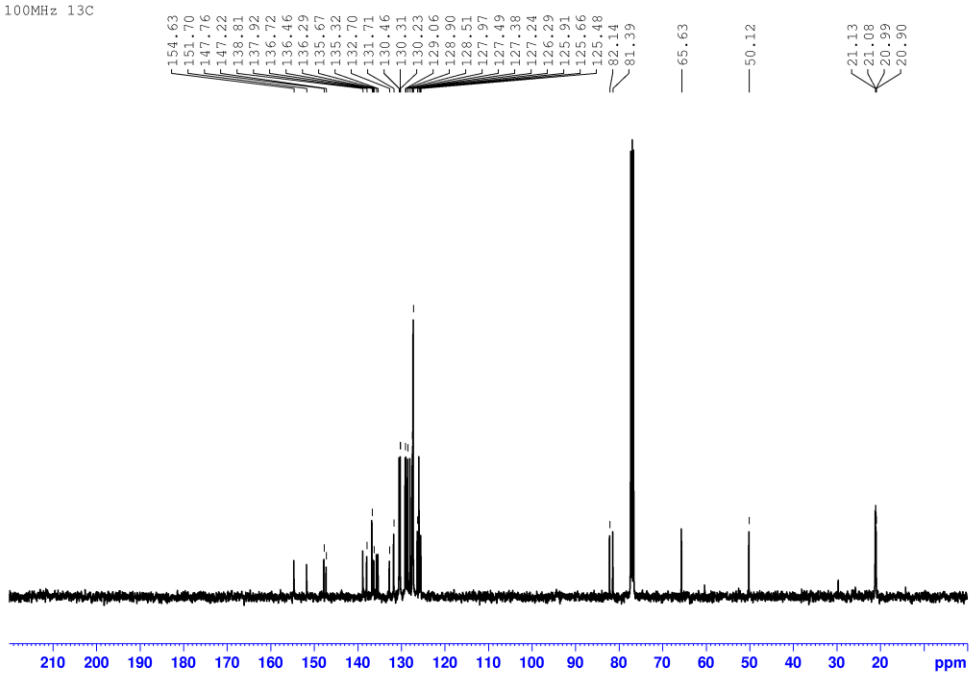

Figure S3. Mass spectrum of **3**

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\fish\data\2022q4(datas)\20221205\221205_UN1_pw_1-40_01_51646.d	Acquisition Date	12/5/2022 10:45:39 AM
Method	tune_wide_pos_LCMS_with lock mass_220107-3.m	Operator	Bruker microTOF-Q II
Sample Name	221205_UN1_pw	Instrument / Ser#	micrOTOF-Q 228888.10183
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.9 l/min
Scan End	3000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

+MS, 0.2min #13