

Electronic Supporting Information (ESI)

SITE-SELECTIVE UNIDIRECTIONAL BENZYLIC sp^3 C-H OXIDATION OF DODECAHYDROTRIPHENYLENE WITH $RuCl_3 - NaIO_4$: FORMATION OF BENZYLIC KETONES

Gaurang Bhatt,^a Pradeep T Deota,^{*a} Deepak Upadhyay^b and Prafulla K. Jha^c

^aApplied Chemistry Department, Faculty of Technology & Engineering, The Maharaja Sayajirao University of Baroda, Vadodara-390 001, Gujarat, India

^bDepartment of Applied Physics, Faculty of Technology & Engineering, The Maharaja Sayajirao University of Baroda, Vadodara-390 001, Gujarat, India

^cDepartment of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390 001, Gujarat, India

*Corresponding authors' e-mail: ptdeota-appchem@msubaroda.ac.in or deotapt@yahoo.com (Prof P T Deota).

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SECTION 1 EXPERIMENTAL PROCEDURES WITH SPECTRAL DATA

Experimental Procedures:

General Information

All the chemicals were purchased from Sigma Aldrich, Spectrochem and SD Fine-Chem Limited. Gift samples of RuCl_3 were received from Hindustan Platinum Pvt. Ltd, Navi Mumbai and Heraeus Pvt Ltd, Jaipur. All solvents were distilled prior to use and stored on oven dried molecular sieves. All the compounds were purified by column chromatography using Acme silica gel (60-120 mesh). Thin Layer Chromatography was performed on silica gel aluminium plates. The spots were visualized under UV light or with iodine vapour. IR spectra were recorded on a SHIMADZU FTIR-245068 spectrophotometer over KBr pellets. Bruker Avance 600 MHz NMR was used to record ^1H & ^{13}C NMR spectra. HRMS data of final compounds were recorded in XEVO G2-XS QTOF Mass Spectrometer from IIT Ropar.

Typical procedure for the synthesis of dodecahydrotriphenylene (3)

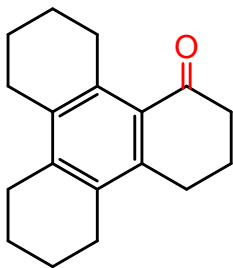
Compound **3** was prepared following the literature procedure ¹ as follows. A mixture of ZrCl_4 (46.40 mmol, 10.8 g) and cyclohexanone (1160.00 mmol, 120.0 mL) was taken in a round-bottomed flask (250 mL) equipped with a condenser. The reaction mixture was refluxed for 10 h after which the reaction mixture became semisolid. Chloroform was added to the reaction mixture and then it was filtered to remove the inorganic material. The filtrate was concentrated under reduced pressure and ethanol was added to the residue and then it was filtered and washed with ethanol several times. The precipitate was collected and dried to give a white powder (56.83 g, 62%). The white powder was further purified by recrystallization with $\text{CHCl}_3/\text{EtOH}$, mp 231 °C.¹

General procedure of RuCl_3 - NaIO_4 oxidation

A solution of ruthenium trichloride (125.0 mg, 0.60 mmol) in a mixture of acetonitrile and carbon tetrachloride (50.0 mL each) was added to a stirred mixture of sodium

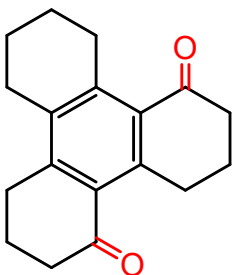
metaperiodate (80.2 g, 375.00 mmol) in distilled water (100.0 mL). To this mixture, dodecahydrotriphenylene **3** (5.0 g, 20.83 mmol) was added and the reaction mixture was left at room temperature with vortex stirring for 30 h. After completion of reaction (TLC), the reaction mixture was filtered, and the filtrate was extracted with ethyl acetate (3 x 60 mL). The combined organic extracts were washed with water (50 mL) and brine (50 mL), dried over anhydrous sodium sulphate. Removal of solvent under reduced pressure furnished a dark brown thick liquid which was chromatographed on a column of silica gel using light petroleum and ethyl acetate.

3,4,5,6,7,8,9,10,11,12-decahydrotriphenylen-1(2H)-one (**4**)



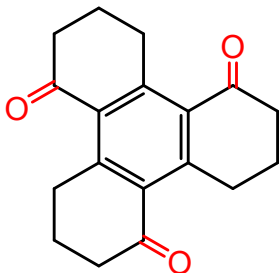
White solid; 1.05 g, 19%, mp 225 °C², IR (KBr cm⁻¹): 2918, 2857, 1674; ¹H NMR (600 MHz, CDCl₃) δ 3.13 (t, *J* = 6.0 Hz, 1H), 2.78 (t, *J* = 5.9 Hz, 1H), 2.59 (dd, *J* = 14.3, 7.5 Hz, 4H), 2.08 (dd, *J* = 12.8, 6.5 Hz, 1H), 1.84 – 1.66 (m, 4H); ¹³C NMR (151 MHz, CDCl₃) δ 201.21, 141.37, 141.16, 137.13, 134.53, 132.23, 129.63, 41.00, 29.70, 27.69, 27.35, 27.24, 26.91, 23.10, 22.77, 22.70, 22.66, 22.53; HRMS (EI): *m/z* calculated for C₁₈H₂₃O: 255.1749, found 255.1748.

3,4,7,8,9,10,11,12-octahydrotriphenylene-1,5(2H,6H)-dione (**5**)



Light yellow solid; 0.52 g, 10%, mp 215 °C, IR (KBr, cm^{-1}): 2934, 2863, 1684; ^1H NMR (600 MHz, CDCl_3) δ 3.29 (t, $J = 6.0$ Hz, 2H), 3.16 (t, $J = 6.2$ Hz, 2H), 2.83 (q, $J = 5.9$ Hz, 3H), 2.63 (dt, $J = 14.3, 6.1$ Hz, 7H), 2.15 – 2.08 (m, 3H), 2.00 – 1.94 (m, 2H), 1.81 (dd, $J = 11.5, 5.6$ Hz, 2H); ^{13}C NMR (151 MHz, CDCl_3) δ 200.98, 200.64, 148.11, 144.95, 134.33, 131.79, 129.67, 40.71, 40.51, 30.36, 29.40, 29.18, 27.62, 27.47, 22.76, 22.61, 22.43, 22.07; HRMS (ESI): m/z calculated for $\text{C}_{18}\text{H}_{21}\text{O}_2$: 269.1542, found 269.1521.

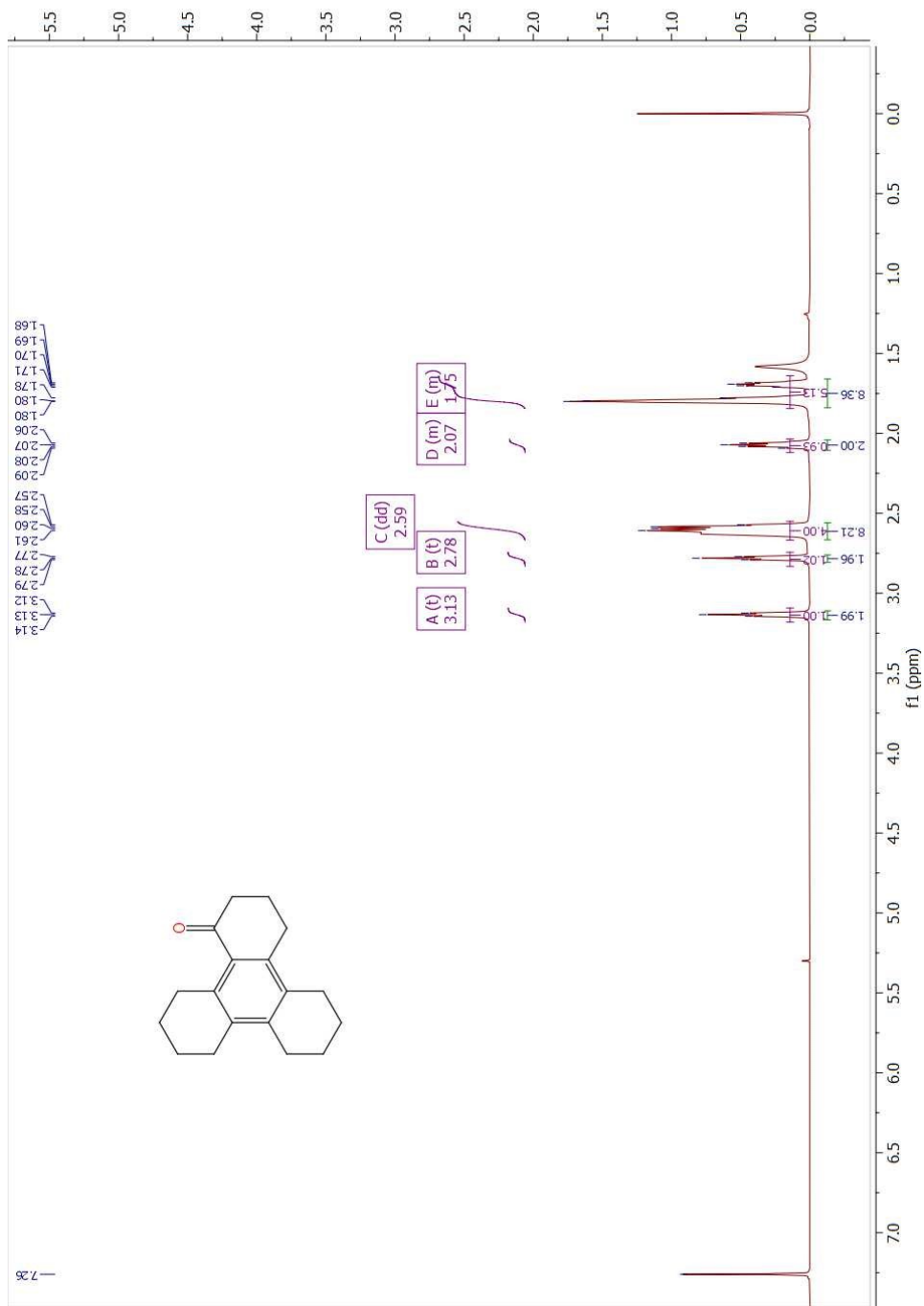
3,4,7,8,11,12-hexahydrotriphenylene-1,5,9(2H,6H,10H)-trione (6)



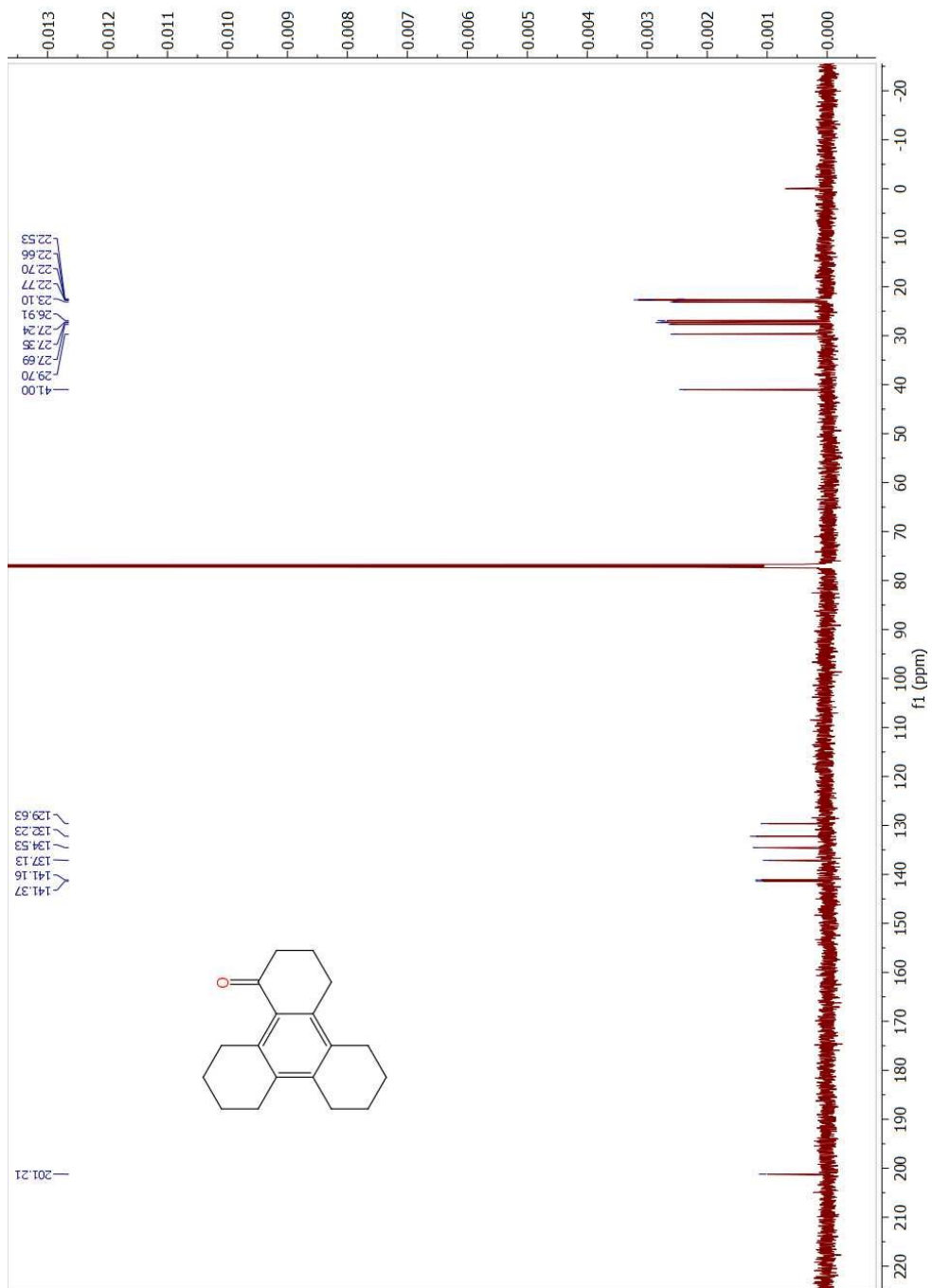
Pale yellow solid; 0.46 g, 8%, mp 210 °C, IR (KBr, cm^{-1}): 2868, 1690; ^1H NMR (600 MHz, CDCl_3) δ 3.33 (t, $J = 6.1$ Hz, 1H), 2.68 (t, $J = 6.8$ Hz, 1H), 2.05 – 1.99 (m, 1H); ^{13}C NMR (151 MHz, CDCl_3) δ 200.12, 151.60, 131.79, 40.32, 29.81, 22.44; HRMS (ESI): m/z calculated for $\text{C}_{18}\text{H}_{19}\text{O}_3$: 283.1334, found 283.1320.

SECTION 2 ^1H , ^{13}C NMR AND HRMS SPECTRA

^1H NMR of 3,4,5,6,7,8,9,10,11,12-decahydrotriphenylen-1(2H)-one (4)



¹³C NMR of 3,4,5,6,7,8,9,10,11,12-decahydrotriphenylen-1(2H)-one (4)



41.00
29.70
27.69
27.35
27.24
26.91
23.10
22.77
22.70
22.66
22.53

141.37
141.16
137.13
134.53
132.23
129.63

201.21

HRMS of 3,4,5,6,7,8,9,10,11,12-decahydrotriphenylen-1(2H)-one (4)

Monoisotopic Mass, Even Electron Ions

72 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 11-25 H: 10-30 N: 0-2 O: 0-8 Na: 0-1

Sample Name : GB026

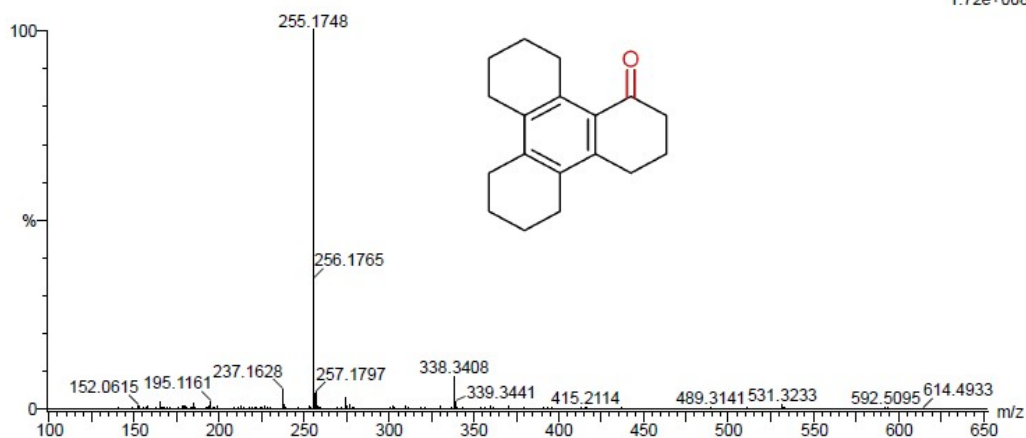
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020320-GB026 93 (0.883)

IITRPR

XEVO G2-XS QTOF

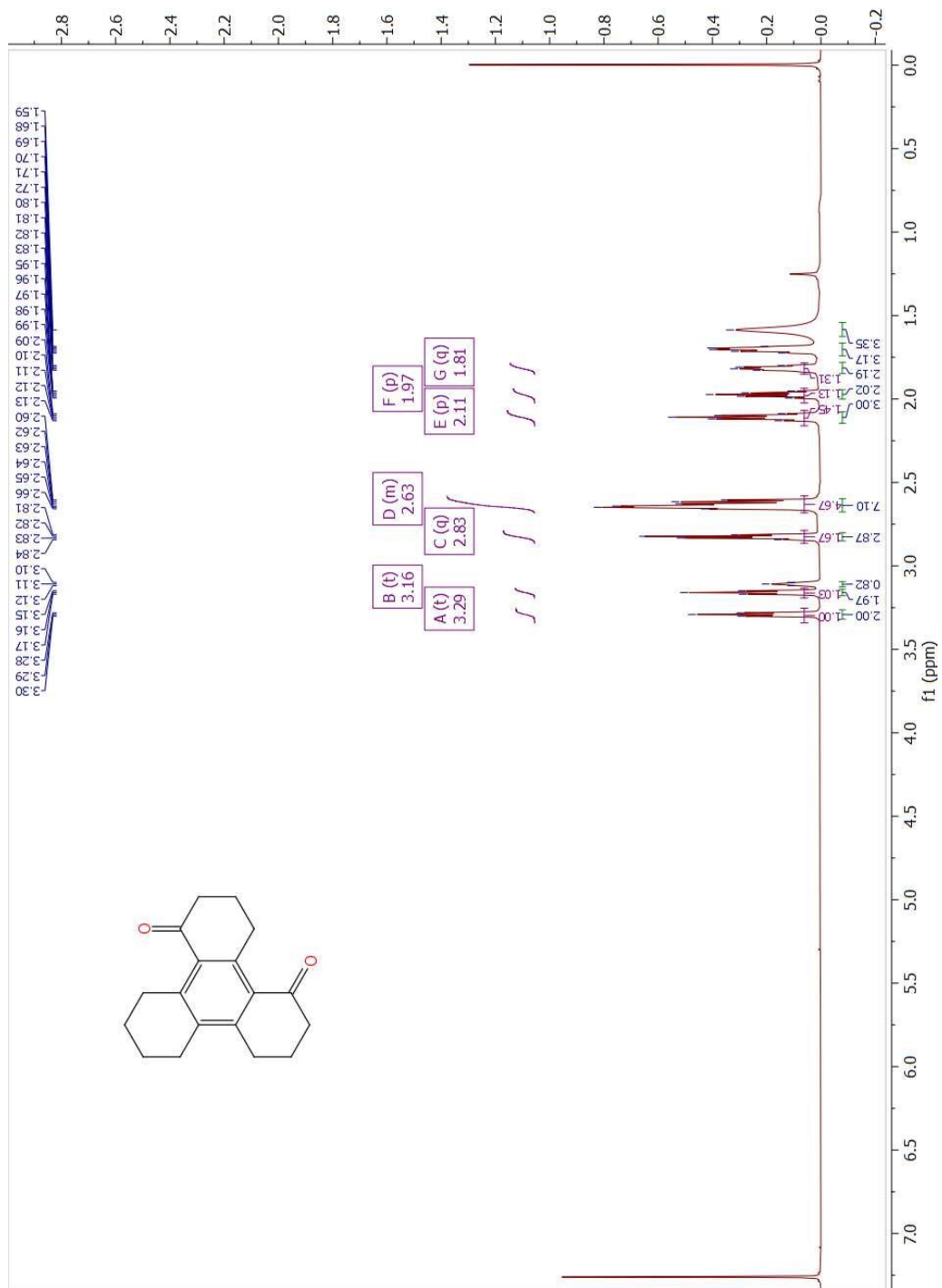
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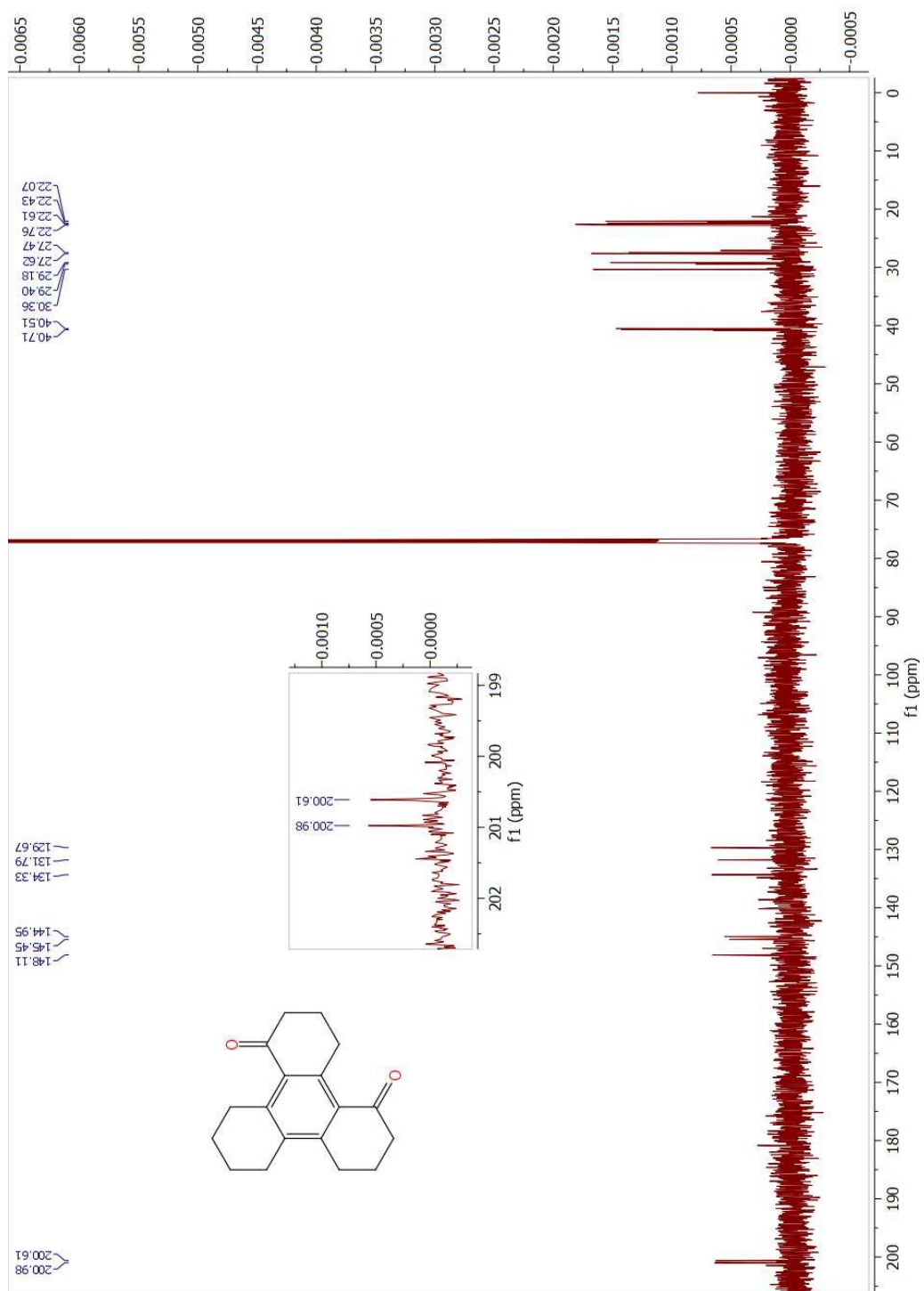
Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
255.1748	255.1749	-0.1	-0.4	7.5	2329.6	n/a	n/a	C18 H23 O

¹H NMR of 3,4,7,8,9,10,11,12-octahydrotriphenylene-1,5(2H,6H)-dione (5)



^{13}C NMR of 3,4,7,8,9,10,11,12-octahydrotriphenylene-1,5(2H,6H)-dione (5)



HRMS of 3,4,7,8,9,10,11,12-octahydrotriphenylene-1,5(2H,6H)-dione (5)

Monoisotopic Mass, Even Electron Ions

9 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 11-25 H: 10-30 O: 0-4

Sample Name : GB027

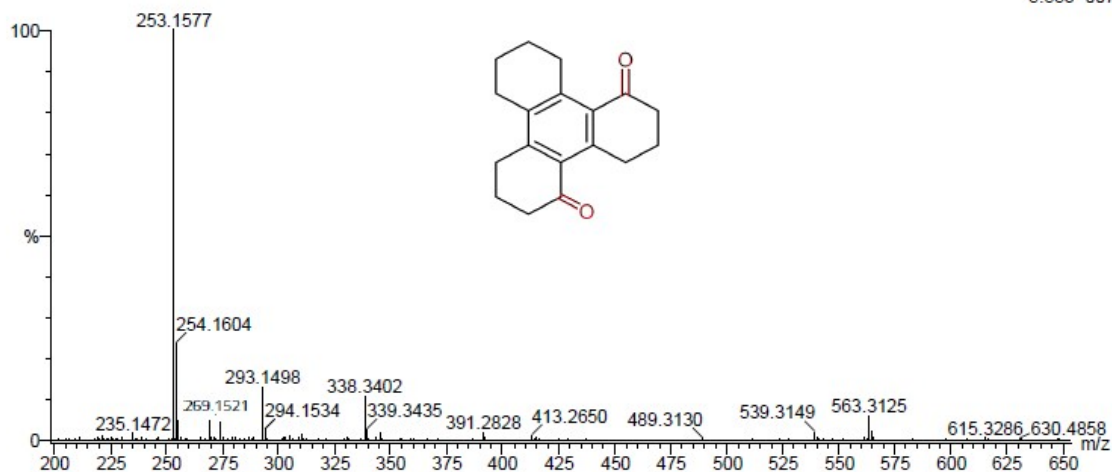
Test Name : HRMS-1

020320-GB027 23 (0.237)

IITRPR

XEVO G2-XS QTOF

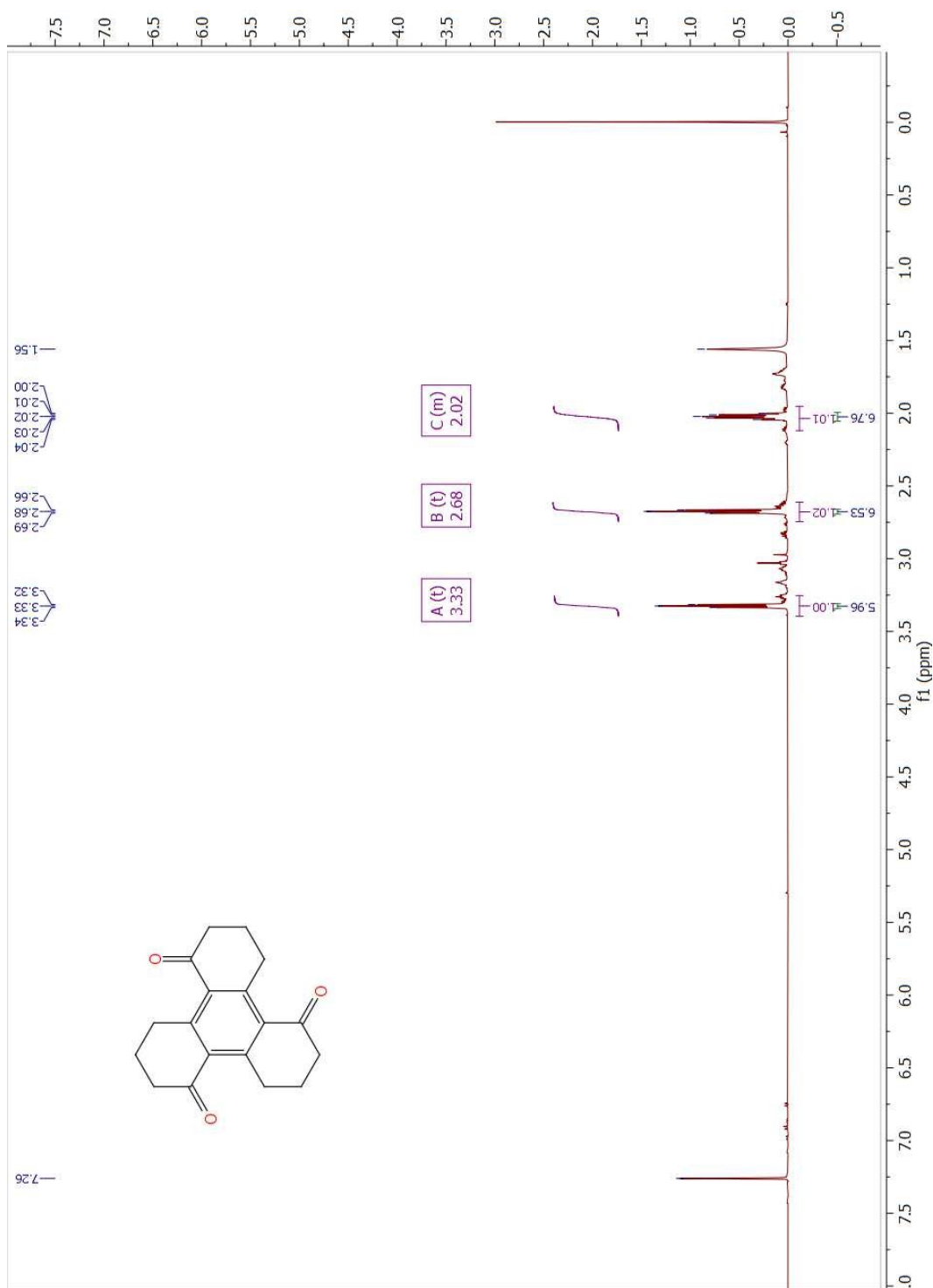
1: TOF MS ES+
5.55e+007



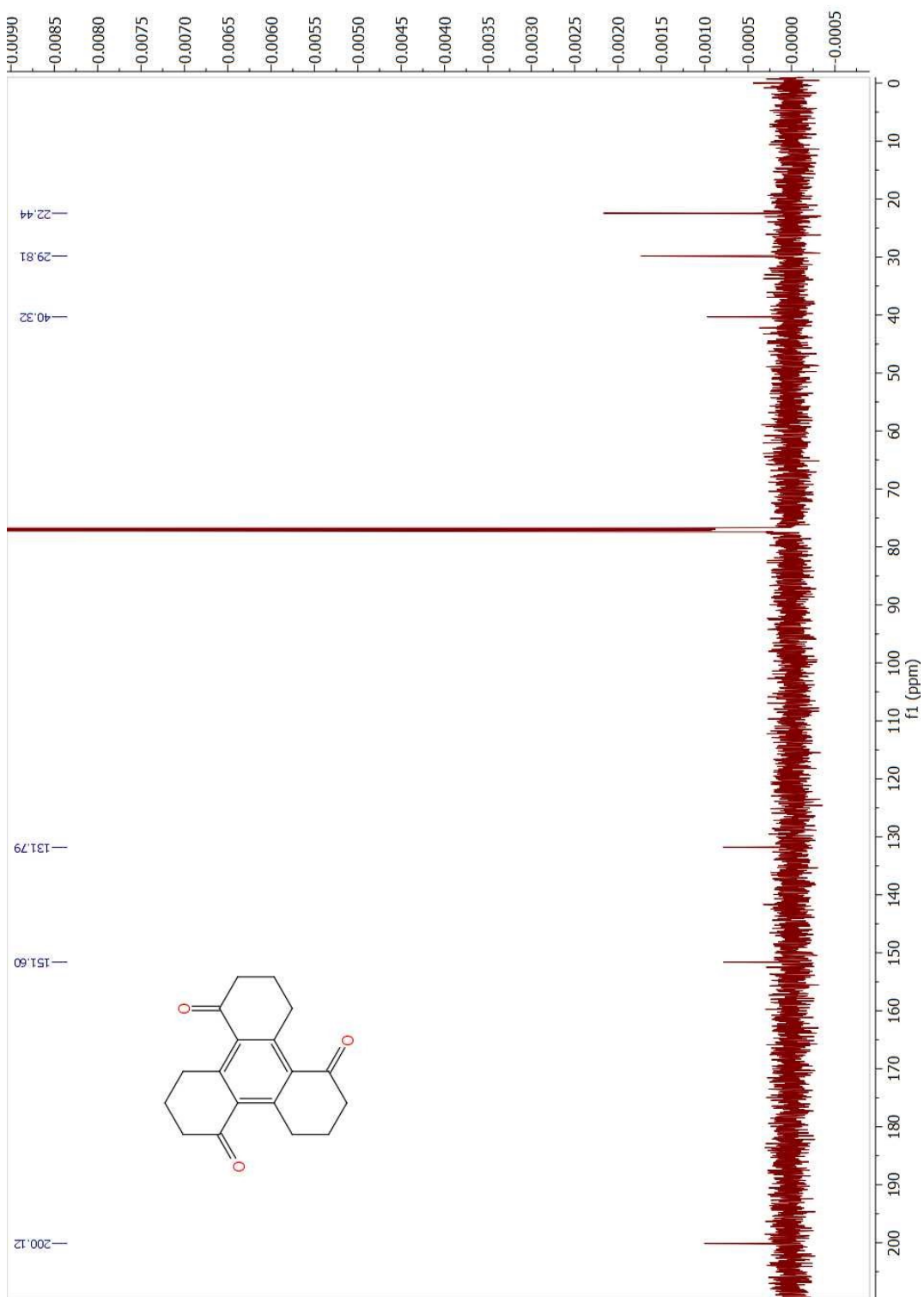
Minimum: -1.5
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
269.1521	269.1542	-2.1	-7.8	8.5	1519.8	n/a	n/a	C18 H21 O2

¹H NMR of 3,4,7,8,11,12-hexahydrotriphenylene-1,5,9(2H,6H,10H)-trione (6)



^{13}C NMR of 3,4,7,8,11,12-hexahydrotriphenylene-1,5,9(2H,6H,10H)-trione (6)



HRMS of 3,4,7,8,11,12-hexahydrotriphenylene-1,5,9(2H,6H,10H)-trione (6)

Monoisotopic Mass, Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

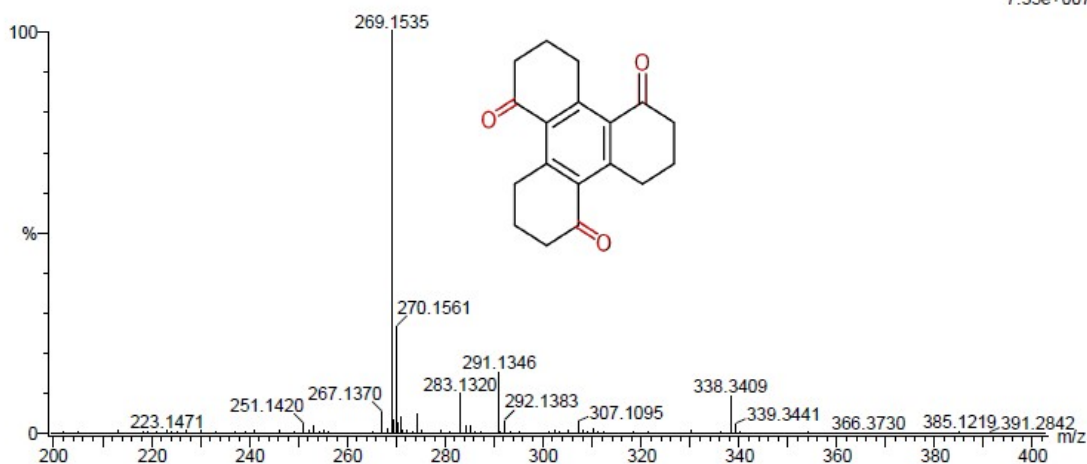
C: 11-25 H: 10-30 O: 0-4

Sample Name : GB028
Test Name : HRMS-1
020320-GB028 21 (0.220)

IITRPR

XEVO G2-XS QTOF

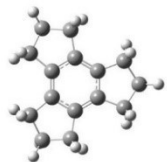
1: TOF MS ES+
7.35e+007



Minimum: -1.5
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
283.1320	283.1334	-1.4	-4.9	9.5	1622.7	n/a	n/a	C18 H19 O3

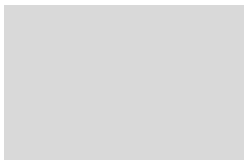
SECTION 3 OPTIMIZED ATOMIC COORDINATES OF COMPOUNDS IN
ANGSTROM (Å)



Compound 1

C	-0.41011300	1.33955300	-0.07648900
C	0.94764000	1.03178000	-0.07642300
C	1.36541600	-0.31483900	-0.07703300
C	0.41987400	-1.33671400	-0.07729000
C	-0.95529400	-1.02504000	-0.07748900
C	-1.36772400	0.30465100	-0.07736900
C	-2.77308800	0.87624500	-0.08960200
C	-2.56173200	2.36966500	0.29580800
C	-1.08886700	2.69651500	-0.08778200
C	2.14504100	1.96351300	-0.08799200
C	3.33337000	1.03365800	0.29509400
C	2.87990200	-0.40519000	-0.08906300
C	0.62758000	-2.83964700	-0.08869100
C	-0.77136800	-3.40286400	0.29724800
C	-1.79071200	-2.29157200	-0.08887300
H	-3.44895300	0.36447100	0.59947700
H	-3.21781400	0.78948500	-1.08815000
H	-3.27717500	3.03214500	-0.19217000
H	-2.68820900	2.48566300	1.37491600
H	-0.63194000	3.40920100	0.60275500
H	-1.03550300	3.14781900	-1.08570600
H	2.04012700	2.80343500	0.60271000
H	2.29100600	2.39389700	-1.08590200
H	4.26408600	1.32263400	-0.19391500
H	3.49853200	1.08447700	1.37400900
H	3.26881400	-1.15771700	0.60088000
H	3.24372800	-0.67646900	-1.08727000
H	1.40877500	-3.16868900	0.60047900
H	0.92495800	-3.18198900	-1.08708300
H	-0.98706000	-4.35469200	-0.18894200
H	-0.80889500	-3.56822000	1.37668100
H	-2.63749600	-2.25149800	0.60022500

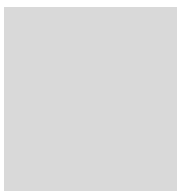
H	-2.20653000	-2.47223900	-1.08731000
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Compound 2

C	-0.58502600	-1.53909100	0.15107100
C	-1.69806200	-0.57869100	0.78317400
C	-1.52600100	0.77667700	0.02509700
O	-0.24542500	0.68316200	-0.68189400
C	0.07384700	-0.69567000	-1.00236800
C	-1.59958200	2.07665200	0.83195200
C	-3.12144400	2.33298400	0.98910500
C	-3.74016200	1.86341200	-0.35131000
C	-2.69905100	0.96317800	-0.96892300
O	-2.70587500	0.54250400	-2.13462900
C	0.30313900	-1.96335800	1.33435200
C	0.08564500	-0.90332800	2.43106400
C	-1.41254600	-0.57558500	2.29590500
C	1.57735700	-0.81435600	-1.25947700
C	2.49421000	0.02474600	-0.35829100
C	3.97149700	-0.09036700	-0.80107500
O	-3.02975000	-1.08047600	0.50653700
O	-1.22618500	-2.70835700	-0.41220100
O	-0.57237600	-1.10010600	-2.24358500
C	4.91233600	0.69878400	0.08106800
O	5.80816600	0.22248300	0.76311800
O	4.70263300	2.07552700	0.10609700
H	-1.06480100	2.02842900	1.77702200
H	-1.13960900	2.86519000	0.23109700
H	-3.33607300	3.37830000	1.20444400
H	-3.51816200	1.73811600	1.81270000
H	-4.67395400	1.31429000	-0.22968000
H	-3.93717100	2.68982900	-1.03844300
H	-0.08068600	-2.92754500	1.67181800
H	1.34485000	-2.11229000	1.06004500
H	0.69539200	-0.01518600	2.24547600
H	0.34328000	-1.27482800	3.42260800
H	-2.00915700	-1.38615900	2.71904400

H	-1.71283900	0.34080300	2.79984700
H	1.71835600	-0.50669900	-2.29646700
H	1.84679100	-1.87267300	-1.21394700
H	2.41925100	-0.28068000	0.68584300
H	2.15809600	1.06200900	-0.40097700
H	4.07060500	0.25462400	-1.83595200
H	4.29934700	-1.12767900	-0.76980000
H	-2.91353600	-1.99124700	0.14641700
H	-1.21611800	-2.58172400	-1.39207300
H	-1.33607500	-0.49386700	-2.44060400
H	3.97577300	2.36517600	-0.47401900



Compound 3

C	-1.22839100	0.69637700	0.02980500
C	-0.00429900	1.41209300	0.02106400
C	1.21427400	0.71372300	-0.01483900
C	1.22128600	-0.70168900	0.01485200
C	0.00968400	-1.41208100	-0.02103200
C	-1.22145400	-0.70853800	-0.02983100
C	-2.52536200	-1.49986900	-0.08305700
C	-3.76421400	-0.65834800	-0.41849300
C	-3.77051000	0.62104800	0.41848100
C	-2.54003300	1.47477000	0.08304200
C	-0.03600700	2.93823700	0.02766800
C	1.31980200	3.60523700	0.30108500
C	2.42025100	2.92198500	-0.51308700
C	2.54678100	1.45454400	-0.08357400
C	2.56108600	-1.42923700	0.08361000
C	2.44919000	-2.89787100	0.51302000
C	1.35553800	-3.59194700	-0.30114700
C	-0.00680900	-2.93846500	-0.02758200
H	-2.43854300	-2.30411200	-0.81696200
H	-2.68440200	-2.00121700	0.88103200
H	-3.75587600	-0.39465700	-1.48190800
H	-4.66813200	-1.24820000	-0.24582100

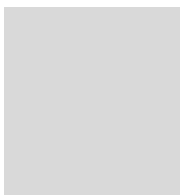
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H	-3.75955300	0.35744400	1.48189500
H	-2.70403700	1.97455700	-0.88102800
H	-2.46112600	2.27979000	0.81697300
H	-0.75601100	3.29156600	0.76946000
H	-0.41807800	3.29172100	-0.93933200
H	1.25836300	4.67117200	0.06709300
H	1.56196100	3.52881300	1.36692000
H	3.37954600	3.42971500	-0.38345000
H	2.17249700	2.97706300	-1.57884700
H	3.21853300	0.93496800	-0.77086900
H	3.04005500	1.41669600	0.89703300
H	3.22757200	-0.90299900	0.77096000
H	3.05400200	-1.38639500	-0.89696800
H	3.41349000	-3.39599800	0.38327900
H	2.20207300	-2.95550600	1.57879400
H	1.30471300	-4.65845900	-0.06722700
H	1.59687100	-3.51305300	-1.36699000
H	-0.72337600	-3.29892600	-0.76926400
H	-0.38520700	-3.29572200	0.93948000



Compound 4

C	-0.52106800	1.35639000	-0.06217600
C	-1.51423700	0.34278500	-0.05671300
C	-1.14647200	-1.01189700	0.02423400
C	0.21846000	-1.36644800	0.00838200
C	1.21637700	-0.36010500	0.00608000
C	0.84289000	1.01836300	0.01471400
C	1.89780300	2.11360200	0.14026300
C	1.33509000	3.48207100	0.54139700
C	0.14245700	3.83272400	-0.34621100
C	-0.97976000	2.81122200	-0.12672200
C	-2.98209000	0.75098100	-0.11084200
C	-3.96471800	-0.40336600	-0.35157000

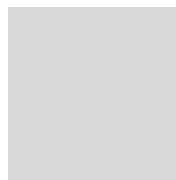
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C	-2.19901400	-2.11213700	0.12960700
C	0.57883100	-2.84754700	0.01002900
C	2.00824900	-3.14219000	-0.45161400
C	2.98195700	-2.21934400	0.28368800
C	2.64965000	-0.76785200	0.00126600
O	3.58649400	0.02746500	-0.23216200
H	2.66099200	1.80247900	0.85128900
H	2.43769800	2.20438600	-0.80644000
H	1.01799300	3.46801600	1.59057000
H	2.12416400	4.23339400	0.45964000
H	-0.23176900	4.83858400	-0.14004400
H	0.45876300	3.82022500	-1.39480100
H	-1.51003100	3.05866400	0.80210500
H	-1.72053900	2.92373800	-0.92222900
H	-3.12450200	1.50481500	-0.88806700
H	-3.24241800	1.25296900	0.83018100
H	-4.98328700	-0.06515900	-0.14691600
H	-3.93649700	-0.70141700	-1.40533600
H	-4.32244100	-2.40984300	0.41514800
H	-3.59771100	-1.30503200	1.57436900
H	-1.87305200	-2.85980100	0.85618100
H	-2.27511700	-2.64235400	-0.82887700
H	-0.12442700	-3.39729700	-0.61731100
H	0.44648500	-3.24534300	1.02579000
H	2.25408600	-4.19095500	-0.27163400
H	2.09247100	-2.97536800	-1.52988100
H	4.01875100	-2.38155800	-0.00617600
H	2.90821300	-2.39541700	1.36438300



Compound 5

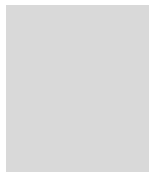
C	-0.41806600	-1.50391300	-0.04876600
C	0.95659500	-1.17812700	-0.04507100
C	1.37804100	0.17155500	0.06052600
C	0.41406000	1.21743200	0.00466100

C	-0.96333300	0.88411600	-0.01104000
C	-1.38339200	-0.48136100	0.03350400
C	-2.85444700	-0.84112900	0.20193500
C	-3.09653400	-2.28557800	0.65154000
C	-2.32201800	-3.23870800	-0.25621600
C	-0.81709900	-2.97768000	-0.11441300
C	1.98345200	-2.29713300	-0.12373100
C	3.34170600	-1.82750800	-0.65016900
C	3.83396400	-0.66315700	0.20109700
C	2.82154100	0.46334300	0.29862100
C	0.86361900	2.67271500	-0.04214200
C	-0.20257100	3.64425700	-0.55007800
C	-1.51787600	3.39610600	0.18911000
C	-1.97879700	1.98156700	-0.06932200
O	-3.18016500	1.77244400	-0.34216600
O	3.23636200	1.59440800	0.63511400
H	-3.31737200	-0.14756800	0.90184800
H	-3.37932200	-0.65757000	-0.73912000
H	-2.77253100	-2.42043700	1.68965700
H	-4.16810800	-2.49503500	0.62400100
H	-2.53487400	-4.28412200	-0.02146500
H	-2.63365300	-3.07641700	-1.29342100
H	-0.45043800	-3.48461300	0.78649600
H	-0.29948200	-3.45557100	-0.95004700
H	1.60875800	-3.10000800	-0.75633000
H	2.11499800	-2.74137900	0.87260600
H	4.05824000	-2.65122400	-0.63494800
H	3.23977800	-1.51195300	-1.69300400
H	4.76439300	-0.22989900	-0.16656600
H	4.03723200	-1.00935500	1.22250000
H	1.76540600	2.75717100	-0.64353000
H	1.18344900	2.97116200	0.96109200
H	0.13774800	4.67122200	-0.40478800
H	-0.35730100	3.50960700	-1.62543500
H	-2.31688000	4.06763200	-0.12003100
H	-1.36268700	3.53275900	1.26662700



Compound 6

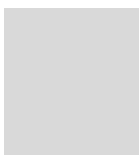
C	1.25928700	0.66426100	-0.00260100
C	0.05698200	1.42258800	-0.04784400
C	-1.18763800	0.75982400	0.08586200
C	-1.25433800	-0.66054100	0.05550700
C	-0.05344200	-1.41012000	-0.02018500
C	1.20994200	-0.75245100	0.01951100
C	2.49683000	-1.56353000	0.09252000
C	3.71643800	-0.77701000	0.57483700
C	3.82643800	0.53365200	-0.20681200
C	2.58624800	1.35715100	0.03579100
C	0.07729600	2.92669200	-0.27121000
C	-1.22950500	3.44288500	-0.87918300
C	-2.39372700	3.05959500	0.02465300
C	-2.41375300	1.57884800	0.33865800
C	-2.60446000	-1.36478900	0.08083000
C	-2.58224700	-2.79385000	-0.46399300
C	-1.43965700	-3.57580100	0.18669600
C	-0.12899100	-2.90168900	-0.13501900
O	0.84049800	-3.59283100	-0.51138100
O	-3.44151900	1.08763300	0.85146300
O	2.69508100	2.57471100	0.29082800
H	2.34293500	-2.43851300	0.71952500
H	2.69786900	-1.97973800	-0.89908200
H	3.63063700	-0.55871200	1.64389400
H	4.61520600	-1.38232400	0.44616400
H	4.68756700	1.13368000	0.08109800
H	3.91178000	0.31439500	-1.27829000
H	0.92073600	3.18896300	-0.90338200
H	0.27845000	3.43916700	0.67503700
H	-1.17592500	4.52547500	-1.00639200
H	-1.36992800	3.01121700	-1.87533600
H	-3.36710500	3.31683600	-0.39600500
H	-2.32204200	3.59578900	0.97883900
H	-3.33981700	-0.77002400	-0.45498900
H	-2.96650600	-1.37062500	1.11356600
H	-3.54220800	-3.27480200	-0.26873900
H	-2.44681800	-2.78434100	-1.55009500
H	-1.37727400	-4.60693600	-0.15576000
H	-1.58027000	-3.58990200	1.27456500



Compound 7

C	0.58015400	-1.47329400	0.07604800
C	-0.83163500	-1.34694700	0.05152300
C	-1.44417700	-0.07681300	-0.01564500
C	-0.62066100	1.07991300	0.03764400
C	0.79991800	0.94649000	0.02199300
C	1.40775600	-0.33198900	0.01348100
C	2.92272600	-0.48472200	-0.09083900
C	3.37515600	-1.88005300	-0.53462100
C	2.69503600	-2.93745600	0.33333200
C	1.17536300	-2.87600400	0.13426000
C	-1.66493600	-2.62461700	0.08297500
C	-3.17100800	-2.41692500	0.27843800
C	-3.64487900	-1.26077900	-0.59907500
C	-2.95859500	0.03720300	-0.15965200
C	-1.22459900	2.43868700	0.17841100
C	-0.32390500	3.65840400	0.16908500
C	0.99441000	3.42048000	-0.57049400
C	1.64198500	2.17849300	-0.01257100
O	2.82277000	2.20895200	0.38835100
O	-2.44809100	2.62210700	0.35561600
H	3.32276300	0.26840500	-0.76800000
H	3.37414900	-0.24748300	0.87597700
H	3.11816300	-2.04597100	-1.58695200
H	4.46275700	-1.94719500	-0.45945500
H	3.05204600	-3.94272800	0.09804100
H	2.94221000	-2.75130300	1.38375700
H	0.91450200	-3.40283400	-0.79249300
H	0.68963600	-3.44176800	0.93268200
H	-1.29115200	-3.28082500	0.87190400
H	-1.49861900	-3.17307100	-0.85318700
H	-3.70047000	-3.34395900	0.04667500
H	-3.38293500	-2.18370600	1.32719600
H	-4.72768400	-1.13213500	-0.53612100
H	-3.41149500	-1.47720300	-1.64780900
H	-3.19556600	0.83802600	-0.85725000
H	-3.38772800	0.37421600	0.78808100
H	-0.89439700	4.48366700	-0.25508900

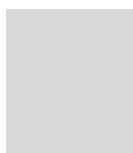
H	-0.11667700	3.92508600	1.21154800
H	1.68405700	4.25440900	-0.45840600
H	0.80036900	3.27747900	-1.63859400



Compound 8

C	0.70574200	1.16050400	0.03554400
C	1.40850000	-0.08038800	0.02354600
C	0.70363900	-1.30857700	-0.00648200
C	-0.70363400	-1.30857900	0.00648000
C	-1.40849800	-0.08039200	-0.02354400
C	-0.70574400	1.16050100	-0.03554500
C	-1.47548800	2.47472700	-0.14632400
C	-0.60943600	3.69798800	-0.45873100
C	0.60942200	3.69799300	0.45871700
C	1.47548000	2.47473300	0.14632000
C	2.90635100	-0.12093300	0.04216600
C	3.57537200	-1.43990500	0.36207200
C	2.90421300	-2.56272000	-0.43260500
C	1.42779500	-2.65089500	-0.03955200
C	-1.42778800	-2.65089900	0.03954400
C	-2.90420700	-2.56272900	0.43259800
C	-3.57537000	-1.43991000	-0.36207000
C	-2.90635000	-0.12094000	-0.04215600
O	-3.61757900	0.87294600	0.21012100
O	3.61758200	0.87295600	-0.21009600
H	-2.25977800	2.37055900	-0.89533000
H	-2.01903400	2.64571800	0.78605600
H	-0.27803500	3.67658900	-1.50292200
H	-1.20945400	4.60232300	-0.33442600
H	1.20943600	4.60232900	0.33440800
H	0.27802000	3.67660000	1.50290900
H	2.01902800	2.64572300	-0.78605900
H	2.25976700	2.37057300	0.89532900
H	4.63490900	-1.33658400	0.13564500
H	3.47980300	-1.64189500	1.43601600
H	3.39922000	-3.51860100	-0.25077500
H	2.99574400	-2.35559000	-1.50311500

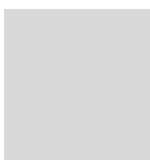
H	0.91272500	-3.32786300	-0.72293400
H	1.35572600	-3.11700400	0.95250500
H	-0.91271600	-3.32786800	0.72292400
H	-1.35571800	-3.11700300	-0.95251400
H	-3.39921100	-3.51861000	0.25076100
H	-2.99573800	-2.35560700	1.50310900
H	-4.63490500	-1.33659300	-0.13564000
H	-3.47980200	-1.64189300	-1.43601600



Compound 9

C	0.26074300	-1.42557600	0.02208300
C	1.50857700	-0.75307300	-0.01271500
C	1.54273000	0.65263400	0.05504500
C	0.33573000	1.39868900	0.01998700
C	-0.89629900	0.72578800	0.01020100
C	-0.92594500	-0.68271900	0.10063200
C	-2.17407200	-1.40847300	0.48903300
C	-2.38202800	-2.80618200	-0.05962300
C	-1.13064900	-3.37789300	-0.74396500
C	0.14740600	-2.94276500	0.00020400
C	2.79395300	-1.56994000	-0.08475100
C	4.05633700	-0.74176300	-0.36462300
C	4.06433500	0.51666700	0.50573300
C	2.86546400	1.40459200	0.14627900
C	0.38741100	2.92210600	0.02387900
C	-0.90870900	3.60553800	-0.44231500
C	-2.14965700	2.94024300	0.18346700
C	-2.15993300	1.48876200	-0.22400000
O	-3.12187200	0.98163400	-0.82658600
O	-2.95948600	-0.92986200	1.32503500
H	-3.22897300	-2.76432200	-0.75062900
H	-2.69964700	-3.43409000	0.77692900
H	-1.19056500	-4.46719300	-0.78905900
H	-1.06927300	-3.01860500	-1.77472600
H	0.12977400	-3.33994500	1.02326500
H	1.01712600	-3.38718700	-0.48089100
H	2.69470200	-2.33810300	-0.85533300
H	2.92393800	-2.11408700	0.85894700

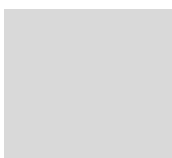
H	4.94296700	-1.35328000	-0.18286400
H	4.08335100	-0.45080600	-1.42025700
H	4.99120400	1.07983000	0.37570500
H	4.01181500	0.23012600	1.56145000
H	2.77451500	2.20744700	0.88188500
H	3.06735300	1.90207700	-0.81132700
H	1.21592200	3.27240800	-0.59407400
H	0.61601100	3.25456200	1.04542800
H	-0.87736500	4.66722500	-0.18974100
H	-0.98630700	3.54158200	-1.53187100
H	-3.07479600	3.40426800	-0.15312600
H	-2.10325600	3.01410000	1.27539700



Compound 10

C	-0.25724400	-1.51517300	0.07854500
C	1.11903400	-1.19983000	0.03341900
C	1.53303000	0.15797000	0.09151600
C	0.57104900	1.21174000	0.01390800
C	-0.79399600	0.87126300	0.00306200
C	-1.19262500	-0.47306900	0.13732500
C	-2.59510200	-0.84236600	0.52406900
C	-3.18967100	-2.07991200	-0.11053100
C	-2.11984000	-3.00369000	-0.72431200
C	-0.80198000	-2.93664300	0.07750000
C	2.14731300	-2.31697300	-0.04445600
C	3.48292500	-1.85141600	-0.63159700
C	3.99808900	-0.66077700	0.17086400
C	2.98306000	0.46144700	0.27907600
C	0.97722700	2.67939000	-0.04588600
C	-0.11088900	3.61966400	-0.58607600
C	-1.48159500	3.32966800	0.05232200
C	-1.84234300	1.90526500	-0.26109100
O	-2.91646600	1.59365000	-0.80603100
O	-3.18232700	-0.22630900	1.42720600
O	3.39166400	1.60409900	0.57658500
H	-3.90640600	-1.74980400	-0.86827600
H	-3.76714300	-2.59111400	0.66263700
H	-2.48754800	-4.03066700	-0.75921400
H	-1.91050500	-2.70461600	-1.75451700

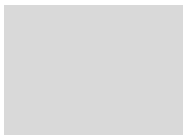
H	-0.97921600	-3.27717400	1.10513800
H	-0.08229800	-3.63155600	-0.35027400
H	1.75450600	-3.13792900	-0.64358900
H	2.31743400	-2.73150100	0.95788400
H	4.20619000	-2.66892400	-0.61977200
H	3.34144800	-1.56451100	-1.67797600
H	4.91115700	-0.23270300	-0.24351100
H	4.24315200	-0.97851900	1.19228100
H	1.88636800	2.79336800	-0.63102100
H	1.26685700	2.99079900	0.96281800
H	0.18311200	4.65399300	-0.39943200
H	-0.19429800	3.50667700	-1.67161600
H	-2.26405000	3.98338700	-0.32808700
H	-1.42038400	3.45992300	1.13851000



Compound 11

C	-0.13047800	-1.57644800	0.00418400
C	1.23245400	-1.18954400	-0.02372800
C	1.58320500	0.17660600	0.03566400
C	0.54977000	1.16405400	-0.03286600
C	-0.80168300	0.76091100	-0.03925000
C	-1.13775000	-0.59813500	0.06931800
C	-2.52522800	-0.99796400	0.44599900
C	-2.99389900	-2.39567300	0.09905100
C	-1.93817800	-3.21338900	-0.65163400
C	-0.55306400	-3.03602600	-0.00389300
C	2.29514600	-2.28258400	-0.08703800
C	3.72290000	-1.77412700	-0.32115100
C	3.98427500	-0.55694200	0.56481600
C	3.04279600	0.58730000	0.17242900
C	0.85188800	2.62522700	-0.11433900
C	-0.28678600	3.63850600	-0.07581400
C	-1.63854800	3.09523100	0.42523100
C	-1.87091300	1.78777900	-0.27318600
O	-2.78798900	1.59751700	-1.08493400
O	-3.24491600	-0.23469300	1.11537700
O	2.01305400	3.06681300	-0.23930600
H	-3.91858200	-2.30089600	-0.47530400

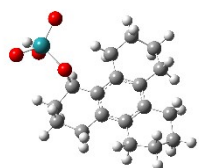
H	-3.26991500	-2.88568900	1.03846800
H	-2.21454400	-4.26927700	-0.66404100
H	-1.88354200	-2.88528800	-1.69332500
H	-0.57535000	-3.42405400	1.02306100
H	0.17798500	-3.64139200	-0.53667000
H	2.03490700	-2.98963100	-0.87844800
H	2.26831600	-2.85931400	0.84560600
H	4.43452300	-2.57808400	-0.12098900
H	3.85046300	-1.49043200	-1.37105300
H	5.01783600	-0.21635400	0.47458900
H	3.83124900	-0.82943300	1.61499400
H	3.12000700	1.40105500	0.89156200
H	3.37756000	1.03435400	-0.76820200
H	0.05706700	4.48388400	0.51994800
H	-0.40694700	4.01238700	-1.09824200
H	-2.45086000	3.78329300	0.20118200
H	-1.60679600	2.92906700	1.50501200



Compound 12

C	-1.07681800	-1.48790500	-0.66533200
C	-1.71496300	-1.00525600	0.70117600
C	-1.95401900	0.52522600	0.45401300
O	-0.73011100	0.89662900	-0.30866200
C	-0.36478900	-0.18028200	-1.22001500
C	1.15879500	-0.13685500	-1.42940700
C	2.02520100	0.29522500	-0.23545800
C	3.52015900	0.30798200	-0.59712800
C	4.40258500	0.76956800	0.58518100
O	-2.91786600	-1.72844900	0.99580400
O	-2.18004900	-1.86354900	-1.54378200
O	-1.00829400	0.07179200	-2.50697900
C	-2.00167200	1.42120100	1.70738800
C	-2.10854600	2.92179100	1.37220000
C	-3.31093400	3.22856400	0.46611500
C	-3.27496800	2.34537900	-0.80676300
C	-3.19060500	0.89072500	-0.40571300
O	-4.10471700	0.09508700	-0.66908600
C	-0.25626200	-2.78759400	-0.55852000

C	0.58582300	-2.99171300	0.70883600
C	-0.25207300	-2.68601200	1.95808300
C	-0.79120000	-1.25025600	1.90864400
C	5.86572300	0.90503800	0.22659300
O	6.50982000	1.94265000	0.27321900
O	6.49550600	-0.26281400	-0.19698800
H	1.34603600	0.57413100	-2.24091200
H	1.47979500	-1.10835100	-1.80913500
H	1.87001100	-0.36583500	0.61744600
H	1.71532100	1.29049100	0.08504200
H	3.68929900	0.97352400	-1.44887100
H	3.82094200	-0.69352600	-0.92592300
H	4.29895200	0.06408900	1.41674000
H	4.07110400	1.74327700	0.94022700
H	-3.47890300	-1.71692500	0.19315700
H	-2.28127800	-1.19759500	-2.25095800
H	-0.72332700	0.92889200	-2.86620500
H	-1.11084700	1.24515700	2.30617700
H	-2.86390000	1.10320400	2.30230900
H	-2.18462000	3.49051300	2.30227300
H	-1.18744700	3.23982700	0.87789300
H	-3.32029700	4.28220200	0.17996600
H	-4.24327000	3.03696400	1.00637400
H	-4.16710400	2.48192000	-1.41553600
H	-2.39673100	2.61204300	-1.39782300
H	0.33795700	-2.90916300	-1.46709300
H	-1.01351100	-3.57202000	-0.59170000
H	0.93855800	-4.02627200	0.73008600
H	1.48161800	-2.36394000	0.70167200
H	0.34586700	-2.81995400	2.86334000
H	-1.09360700	-3.37896100	2.01912800
H	-1.37184700	-1.04081700	2.80746500
H	0.04642400	-0.55019000	1.88703300
H	5.91188000	-1.04242900	-0.18971700



Intermediate Ru(VI) species

C	-3.31102700	0.27417900	-0.11594200
C	-2.86454500	-1.06772100	-0.06362600
C	-1.51230300	-1.35197000	0.27528000
C	-0.61771300	-0.28476600	0.52431100
C	-1.04551000	1.06849100	0.40748700
C	-2.39852000	1.34680400	0.11477300
C	-0.03230600	2.19837500	0.61097000
C	-0.49965900	3.55474200	0.05279000
C	-1.92478100	3.85294800	0.54245200
C	-2.90513400	2.78823100	0.01319000
C	-1.07325800	-2.81082900	0.41127700
C	0.44455200	-3.02388100	0.56584400
C	1.04327500	-1.97307700	1.51099900
C	0.81789800	-0.56946500	0.93799400
C	-4.77054300	0.60223400	-0.43916300
C	-5.73298200	-0.59457900	-0.32626600
C	-5.13354900	-1.81762800	-1.03491600
C	-3.81904100	-2.23057800	-0.34666800
O	1.60969500	-0.44846800	-0.33911000
Ru	3.45208600	-0.00589200	-0.46678300
O	3.50718500	0.29123000	1.43480400
O	4.34408800	-1.43649500	-0.84465600
O	3.58554200	1.52977000	-1.25061400
H	0.91930800	1.93029400	0.14147700
H	0.17359400	2.31391500	1.68869400
H	-0.48516700	3.53076900	-1.04718800
H	0.19842300	4.34209900	0.36752400
H	-1.93321900	3.85369200	1.64340500
H	-2.25585700	4.84920600	0.21869700
H	-3.85638800	2.88805600	0.55228100
H	-3.14001600	3.00788500	-1.04167000
H	-1.42290700	-3.38683600	-0.45516200
H	-1.59153500	-3.24659300	1.28226700
H	0.93551400	-2.93606100	-0.41214800
H	0.63923600	-4.03804500	0.93818900
H	0.56214700	-2.02496400	2.49976000
H	2.11764000	-2.13090400	1.66263200
H	1.20091500	0.18413400	1.62940900
H	-5.12470400	1.40535000	0.21943600
H	-4.82583000	1.01374300	-1.46110000
H	-5.90469700	-0.83755300	0.73353100
H	-6.70710300	-0.32554900	-0.75703900
H	-5.83493700	-2.66312100	-1.02738500
H	-4.94048100	-1.56699200	-2.08909900

H	-3.31447100	-2.98072500	-0.96899200
H	-4.05555300	-2.74327100	0.60105100
H	4.39308700	0.56336700	1.77178000

SECTION 4 REFERENCES ASSOCIATED WITH SI

1. J. Wei, X. Jia, J. Yu, X. Shi, C. Zhang and Z. Chen, *Chemical Communications*, 2009, 4714-4716.
2. M. Farina and G. Audisio, *Tetrahedron*, 1970, **26**, 1827-1837.