Electronic Supplementary Material (ESI) for Analyst.

Supplementary Information

Application of cup-shaped trilactams for selective extraction of volatile compounds by gas chromatography-mass spectrometry

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Supplementary figures and Table

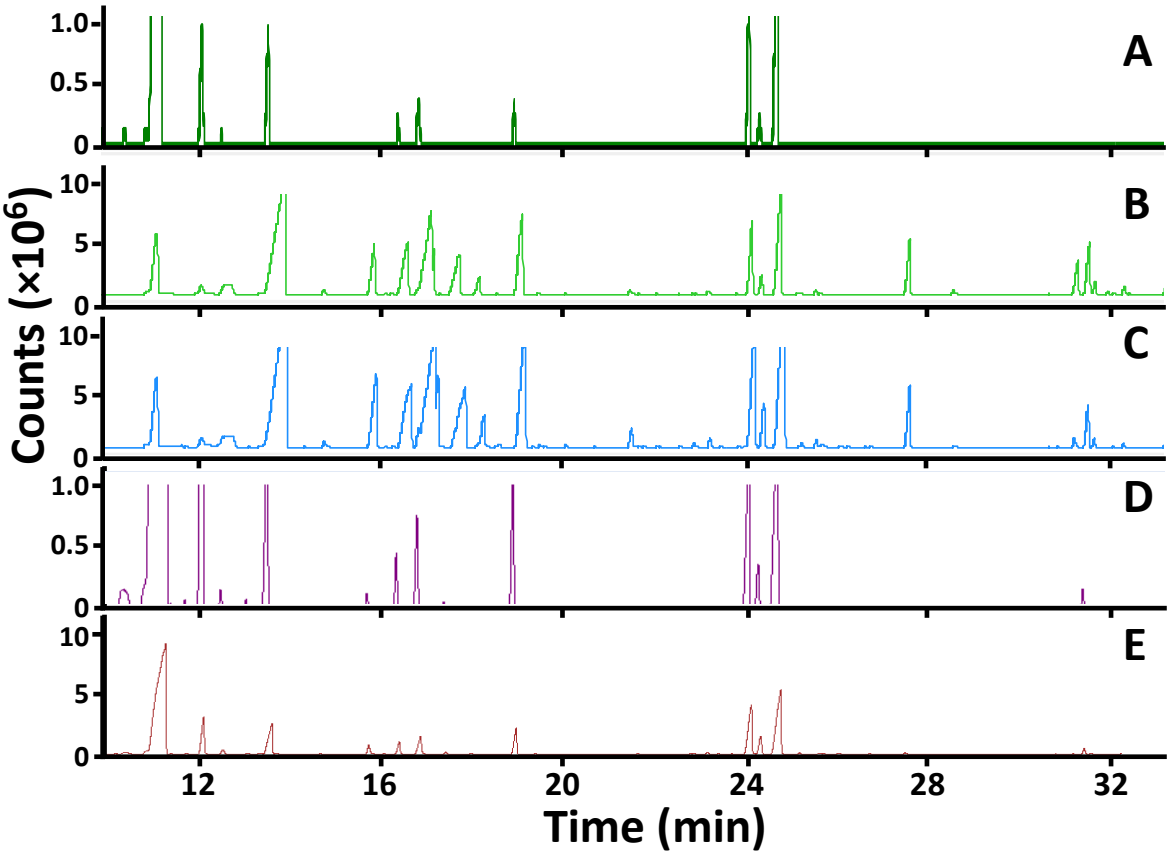


Fig. S1. GC–qMS total ion chromatogram of (A) volatile compounds present in a perfume solution with 3 days extraction in MeOH (control sample) with the insert of the corresponding chromatograms of different extracts obtained by using (B) (+)-**1**, (C) (–)-**1** and (D) achiral 2-piperidinone, and (E) result obtained with the same condition as (B) except that extraction time was 5 h. The identified compounds are listed in Table S1.

Table S1. Compound profiles of retention index from literature (I_{Lit}), average peak area (counts·s) with n = 3, enrichment factor (EF) analyzed with GC–MS with the potential compounds showing significant chiral recognition highlighted in bold and italic. The average match score for the compounds is 841.

No.	Compound name	I_{Lit}	Peak area in Control	Perfume-(–)-1		Perfume-(+)-1		Perfume-(2-Piperidinone)	
				Peak area	EF	Peak area	EF	Peak area	EF
1	Camphene	952	$(9.2\pm4.0)\times10^4$	0±0	-[a]	0±0	-	0±0	-
2	Sabinene	974	$(22\pm7.2)\times10^5$	$(9.1\pm3.9)\times10^4$	-	$(1.6\pm1.2)\times10^5$	-	0±0	-
3	3-Carene	1011	$(3.0\pm1.6)\times10^5$	$(2.0\pm1.8)\times10^4$	-	$(3.4\pm1.7)\times10^4$	-	0±0	-
4	Sylvestrene	1027	$(11\pm1.2)\times10^7$	$(2.5\pm1.1)\times10^7$	-	$(2.8\pm0.34)\times10^7$	-	0±0	-
5	7-Octen-2-ol, 2,6-dimethyl-	1064	$(13\pm9.1)\times10^5$	$(8.0\pm4.5)\times10^6$	6.1	$(1.7\pm0.73)\times10^7$	13	$(6.6\pm0.8)\times10^4$	1.5
6	Linalool	1099	$(1.8\pm1.3)\times10^7$	$(8.0\pm4.5)\times10^7$	4.5	$(1.2\pm0.18)\times10^8$	6.5	$(7.1\pm0.8)\times10^5$	1.1
7	***l-menthol (LMT)***	***1175***	$\boldsymbol{(5.0\pm4.4)\times10^5}$	***0±0***	***-***	$\boldsymbol{(2.7\pm1.2)\times10^7}$	***54***	0±0	-
8	Linalyl formate	1215	0±0	$(5.2\pm0.017)\times10^7$	NA[b]	$(6.2\pm2.9)\times10^7$	NA	0±0	-
9	Citronellol	1228	$(3.1\pm2.6)\times10^5$	$(5.4\pm4.1)\times10^6$	17	$(6.7\pm2.4)\times10^6$	22	$(0.3\pm0.3)\times10^4$	0.2
10	Carvone	1242	$(0.20\pm0.20)\times10^4$	$(4.3\pm3.7)\times10^5$	22×10	$(7.3\pm2.9)\times10^5$	37×10	0±0	-
11	Linalyl acetate	1257	$(5.6\pm4.5)\times10^6$	$(2.9\pm2.0)\times10^7$	-	$(4.5\pm1.5)\times10^7$	8	$(2.7\pm1.2)\times10^5$	1.3
12	***δ-EIemene***	***1338***	$\boldsymbol{(4.4\pm1.9)\times10^4}$	$\boldsymbol{(1.3\pm0.68)\times10^5}$	***-***	$\boldsymbol{(4.1\pm1.8)\times10^5}$	***9.3***	$(0.3\pm0.3)\times10^4$	0.6
13	*α*-Terpinyl acetate	1350	$(3.9\pm3.4)\times10^4$	$(2.3\pm1.7)\times10^5$	-	$(4.4\pm2.1)\times10^5$	11	0±0	-
14	***Ylangene***	***1372***	$\boldsymbol{(1.7\pm1.2)\times10^4}$	***0±0***	***-***	$\boldsymbol{(7.4\pm6.1)\times10^5}$	***44***	$(0.6\pm0.3)\times10^4$	22
15	***Copaene***	***1376***	$\boldsymbol{(5.3\pm2.7)\times10^4}$	***0±0***	***-***	$\boldsymbol{(1.5\pm0.67)\times10^5}$	***2.8***	$(0.6\pm0.5)\times10^4$	0.5
16	*β*-Funebrene	1414	$(8.0\pm3.1)\times10^6$	$(2.2\pm1.6)\times10^7$	-	$(3.7\pm1.7)\times10^7$	4.6	0±0	-
17	*cis*-Thujopsene	1429	$(1.6\pm0.63)\times10^7$	$(4.0\pm2.9)\times10^7$	-	$(6.6\pm2.9)\times10^7$	4.1	$(1.6\pm0.3)\times10^6$	0.5
18	Cyclamal	1466	$(3.3\pm2.9)\times10^4$	$(6.9\pm6.0)\times10^5$	21	$(1.0\pm0.41)\times10^6$	32	0±0	-
20	*γ*-Himachalene	1477	0±0	$(1.9\pm1.6)\times10^5$	NA	$(3.4\pm0.0)\times10^5$	NA	0±0	-
21	*α*-Curcumene	1483	$(1.0\pm0.80)\times10^4$	$(0.60\pm0.50)\times10^4$	-	$(1.2\pm1.0)\times10^5$	-	0±0	-
21	Lilial	1533	$(3.8\pm3.3)\times10^5$	$(7.0\pm5.6)\times10^6$	19	$(1.3\pm0.47)\times10^7$	33	0±0	-
22	***Kharismal (KRM)***	***1649***	***0±0***	$\boldsymbol{(9.5\pm8.3)\times10^5}$	***NA***	$\boldsymbol{(5.0\pm3.2)\times10^6}$	***NA***	0±0	-
23	*β*-Acorenol	1649	$(5.5\pm4.8)\times10^4$	0±0	-	$(1.5\pm0.59)\times10^5$	-	0±0	-

[a]Insignificant enrichment effect.

[b]Enrichment factor was very high and could not be calculated due to the compounds not detected in control.

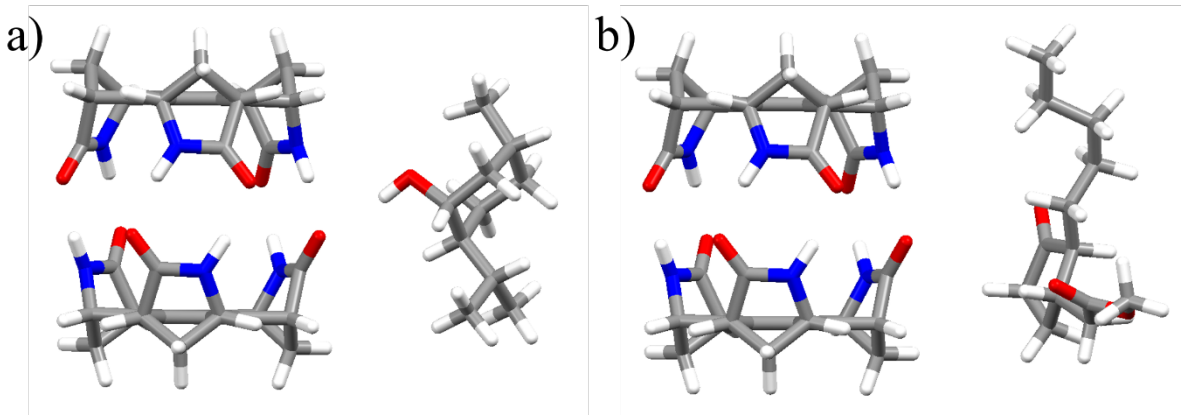


Figure S2. MD simulation displayed the initial molecular complex of (–)-**1**$_{dimer}$ and selected enrich compounds a) LMT and b) KRM. C, grey; N, Blue; O, red; H, white.

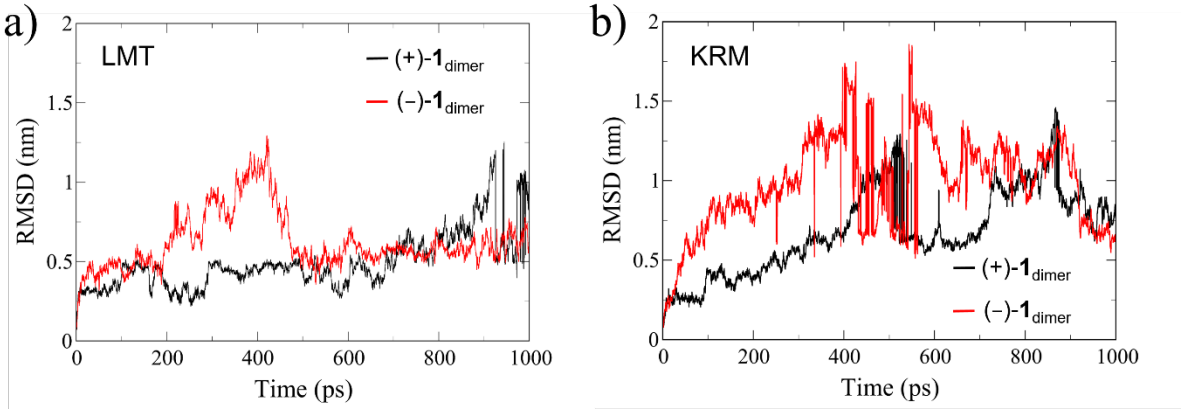
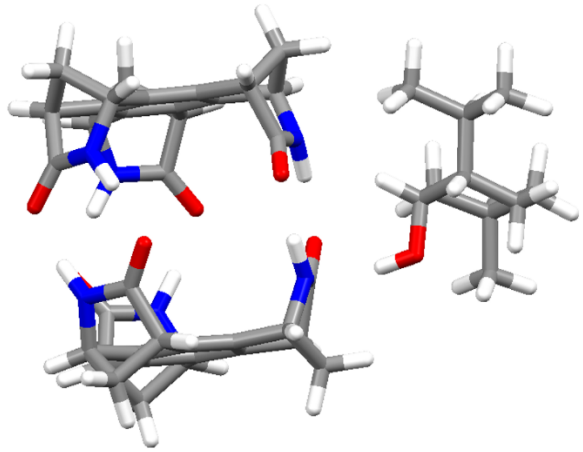


Figure S3. Root mean squared deviation (RMSD) measured the changes in movement of the selected enrich compounds a) LMT and b) KRM from their corresponding initial complexes structures; (+)-**1**$_{dimer}$ (black color) and (–)-**1**$_{dimer}$ (red color).

Cartesian coordinates of optimized complex structures

a) (+)-**1**$_{dimer}$-LMT



	X	Y	Z
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C	-2.46720000	-3.33142200	-2.42630000
C	-1.86592500	-3.26002200	-1.02203800
C	-3.74880200	-4.15438100	-2.12968800
H	-4.41640100	-4.21362500	-2.99380100
H	-3.54256900	-5.15208900	-1.73382000
H	-5.19144000	-3.30220100	-0.55326800
H	-1.81890100	-3.65766400	-3.23772000
C	-1.45890500	-2.95950000	1.73437200
C	-1.60526400	-2.74214800	3.23967300
C	-3.69708000	-2.73700700	2.41000500
C	-2.78676400	-2.97415200	1.20390900
C	-2.92330300	-3.53288600	3.49414300
H	-3.33687600	-3.38560900	4.49570000
H	-2.83179400	-4.59844200	3.26852000
H	-0.73325700	-2.93083400	3.86253300
H	-4.76097300	-2.93140000	2.28605300
C	1.13215700	-3.03916200	1.06704000
C	0.79869300	-3.31828900	-1.14334800
C	1.57200800	-4.06130300	-0.01343400
H	1.19287000	-5.07000200	0.16647500

H	2.65588500	-4.07977700	-0.15943400
C	-0.38422700	-3.08730800	0.89174300
C	-0.59244600	-3.25040500	-0.51320800
H	1.53335700	-3.14594700	2.07323200
H	0.87136300	-3.67093600	-2.17002300
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H	-3.93509200	-0.52758400	2.56818100
N	1.62107000	-1.79417100	0.40930700
H	1.60280800	-0.87433600	0.87731000
N	-3.09801900	-2.01906900	-2.71145000
H	-2.60036000	-1.22468600	-3.13568900
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C	-1.97755800	3.44150400	2.49715400
C	-1.52364800	3.32811900	1.04142900
C	-3.21776100	4.35772400	2.32303900
H	-3.79136800	4.46498100	3.24791600
H	-2.97821600	5.33802200	1.90301600
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C	-1.72261400	2.81806900	-3.22434300
C	-3.00048000	3.70054100	-3.34834100
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H	-3.52099300	3.58775200	-4.30348000
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C	-1.41193400	3.01751300	-1.74134100
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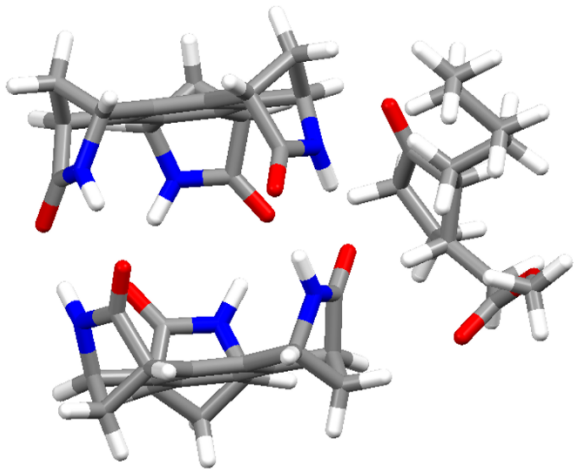
H	-0.90623200	2.94845000	-3.93193800
N	-2.67274200	2.17934700	2.85067800
H	-2.19566200	1.34882500	3.22646300
N	-3.60414900	1.56884900	-2.70621500
H	-4.12439300	0.77019500	-2.31898000
N	1.70673100	1.65647200	-0.72716700
H	1.64734600	0.74933200	-1.20472300
C	1.57520400	1.74845700	0.62500600
C	-3.79227300	2.07039600	2.08328400
C	-2.37616100	1.41416500	-3.27309700
O	1.71406100	0.84892400	1.45583900
O	-1.86204700	0.37510800	-3.68967600
O	-4.55430800	1.10703200	1.99213700
C	6.23266000	0.00628900	0.92834900
C	4.87351600	-0.37179000	0.30981800
C	4.87401800	-0.22088400	-1.22043500
C	6.00971500	-0.98122500	-1.94161200
C	7.36768400	-0.68688900	-1.26547200
C	7.32518000	-0.86397400	0.26309100
H	3.90105100	-0.53362500	-1.61554800
H	4.08655300	0.26415600	0.72684700
H	6.16857600	-0.27042400	1.99049600
H	6.05826700	-0.58947000	-2.96796900
H	8.14121500	-1.33856200	-1.69261600
H	7.67053000	0.34129600	-1.50515300

H	7.11130900	-1.91064300	0.50386900
H	8.30966700	-0.64603100	0.69016900
H	4.96076900	0.85177600	-1.44466600
C	5.73543600	-2.49166500	-2.05696500
H	4.76717400	-2.67005100	-2.54066300
H	6.50904900	-2.97747400	-2.66431600
H	5.70681400	-2.96966900	-1.07552900
O	4.59800600	-1.72851200	0.71591000
H	3.64745200	-1.87227500	0.58224700
C	6.53639300	1.53084400	0.87808100
H	6.74578700	1.81688500	-0.16145400
C	5.35118300	2.38858400	1.35839200
H	5.64487700	3.44220900	1.43271800
H	4.49891700	2.33023900	0.67605800
H	5.00484200	2.06439100	2.34761200
C	7.78425100	1.87242200	1.71145800
H	7.99920900	2.94624700	1.66772700
H	7.62826600	1.60564400	2.76465900
H	8.67607300	1.34460100	1.36175400

Absolute energy = –2638.29736632 a.u.

b) (+)-**1**$_{dimer}$-KRM



	X	Y	Z
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C	-1.08406300	-3.51380300	-2.20298100
C	-1.35305800	-3.32253200	-0.71126000
C	-2.30228900	-4.39378600	-2.58917200
H	-2.38518700	-4.54282700	-3.66950200
H	-2.32812600	-5.35254600	-2.06507200
H	-4.38942000	-3.54102600	-2.13153700
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C	-2.52436500	-2.85485800	1.78837600
C	-3.47596900	-2.56574100	2.94895200
C	-4.77208000	-2.73036700	1.11713400
C	-3.34640600	-2.97777400	0.62397400
C	-4.70225100	-3.41827400	2.50630200
H	-5.59972000	-3.24143900	3.10576000
H	-4.48085400	-4.48727400	2.45100300
H	-3.08362400	-2.66857400	3.95872300
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C	0.01866200	-2.78778400	2.64124200
C	0.94662500	-3.18303800	0.62904900
C	1.01111600	-3.82113900	2.04642400
H	0.63435100	-4.84696500	2.06693800
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C	-1.16051600	-2.95454100	1.67870600
C	-0.56312300	-3.19603400	0.40190700
H	-0.19164000	-2.82082000	3.70889900
H	1.59617300	-3.56695700	-0.15226000
N	-4.85399900	-1.31784600	1.56491700
H	-5.09165500	-0.53409800	0.94191900
N	0.72899400	-1.54250500	2.25274700
H	0.49527200	-0.61221400	2.62582200
N	-1.47765200	-2.26201500	-2.89599000
H	-0.84616900	-1.45755500	-3.00928400
C	-2.81983700	-2.08474000	-2.73673400
C	-4.02071100	-1.15125500	2.62929800
C	1.22520900	-1.70872300	0.99814300

O	-3.48872800	-1.09778800	-3.04462000
O	1.72857300	-0.84699100	0.27205300
O	-3.71639900	-0.09908700	3.19228500
C	-0.96793000	3.33971900	0.87279000
C	-0.04098100	3.43417900	2.08472200
C	1.29473000	3.03245500	0.31370400
C	-0.12174200	3.09357200	-0.25357000
C	1.19354200	4.11355300	1.42146100
H	2.07921500	4.14017000	2.06204700
H	0.97340700	5.11099400	1.03282700
H	-0.45498100	3.84216600	3.00474500
H	2.12146700	3.07835100	-0.39186800
C	-2.89984800	3.22406100	-0.59130900
C	-4.41427100	3.31469400	-0.40323800
C	-3.52328000	3.54934600	1.64944200
C	-2.32832200	3.39241700	0.70869800
C	-4.47815100	4.36888600	0.74174800
H	-5.47445300	4.48358600	1.17812500
H	-4.07165500	5.34061300	0.44986000
H	-5.02520800	3.44707700	-1.29394000
H	-3.32896400	3.91291700	2.65704000
C	-2.31890900	2.69068300	-3.15169100
C	-0.08321300	2.59714700	-2.87419200
C	-1.08080600	3.39612300	-3.76758200
H	-1.05294700	4.47169100	-3.57591900
H	-0.97356600	3.19379400	-4.83720000
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N	1.36351300	1.82697600	1.18026800
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C	0.50479000	1.99202300	2.22465900
C	-4.75469500	2.03879800	0.40588100
C	-0.58768500	1.16279100	-3.16288900
O	0.18231900	1.15471900	3.06930700
O	0.07687800	0.12053200	-3.14003100
O	-5.30537400	1.02164600	-0.01811500
C	3.33375100	0.23801000	-3.66327900
C	4.57496000	0.24562900	-1.50675100
C	4.17001500	-1.19737100	-1.89403000
C	4.02251000	-1.11680800	-3.42962100
H	2.24051300	0.14397300	-3.63147000
H	3.59607500	0.74146400	-4.59922600
H	5.60685100	0.39375600	-1.87667700
H	3.18617100	-1.39808800	-1.45427900
H	5.01655500	-1.13570800	-3.89790300
H	3.45303400	-1.96062600	-3.83167500
C	3.72176200	1.08552500	-2.46243000
O	3.37089900	2.23840500	-2.27268700
C	5.14044400	-2.30858200	-1.44897200
H	4.89907400	-3.22406900	-1.99995300
H	6.17461500	-2.02772500	-1.67226700
O	5.98592000	-2.12414800	0.76922100
C	5.85378000	-2.30117200	2.19393300
H	6.71024900	-1.78901400	2.63087600
H	4.91899700	-1.85433800	2.54245800
H	5.86272800	-3.36407500	2.44840200
C	4.99081500	-2.64140600	0.01826000
O	4.06780900	-3.27988300	0.48992200
C	4.49879600	0.67931600	-0.03321200
H	4.11477600	-0.14382000	0.57575900
H	3.75954100	1.47785900	0.04553700
C	5.83280200	1.17630900	0.53898000

H	6.59123600	0.39478500	0.40480800
H	6.16835000	2.04832700	-0.04096600
C	5.75915500	1.55443900	2.02642900
H	6.76633800	1.81863400	2.37903300
H	5.45251000	0.67223800	2.60747500
C	4.79992700	2.71100000	2.34248000
H	3.78049200	2.42831900	2.05937000
H	5.06759600	3.57829100	1.72188100
C	4.81499700	3.10880500	3.82250400
H	4.12027400	3.93201400	4.02497300
H	4.52048800	2.26444400	4.45732100
H	5.81483200	3.43039500	4.13883000

Absolute energy = –2904.29842881 a.u.