

# Supplementary materials

Molecularly imprinted polymers for selective extraction of oblongifolin

C from *Garcinia yunnanensis* Hu

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## Part 1. Experimental section

### 1. Method of validation of the HPLC and UHPLC analyses

#### 1.1 Apparatus and analytical conditions

##### 1.1.1 Apparatus

HPLC experiments were implemented using a Waters 2535 Series High-performance Liquid Chromatographic instrument. UHPLC analysis was performed on a Waters ACQUITY UPLC H-class system equipped with a quaternary solvent manager, a sample manager-FTN, and a PDA detector (Waters Corp., Massachusetts, USA) connected to a reversed-phase column (Waters Acquity UPLC BEH Shield RP C18, 100 mm × 2.1 mm, i.d., 1.7 μm).

##### 1.1.2 Analytical conditions and method of validation of the HPLC analysis

The analytical column used was a Shim-pack VP-ODS column (4.6 × 250 mm, 4.5 μm, Shimadzu, Tokyo, Japan). The mobile phase consisted of 0.1% formic acid (A)-acetonitrile (B) in a gradient elution in which (B)% was 70, 100, 100, 70, and 70 at 0, 15, 35, 50, and 60 min, respectively, at a flow rate of 1.0 mL min<sup>-1</sup>. The detection wavelength was at 327 nm and the injection volume was 10 μL. The method of validation of the HPLC analysis was described in Table S1.

##### 1.1.3 Analytical conditions and method of validation of the UHPLC analysis

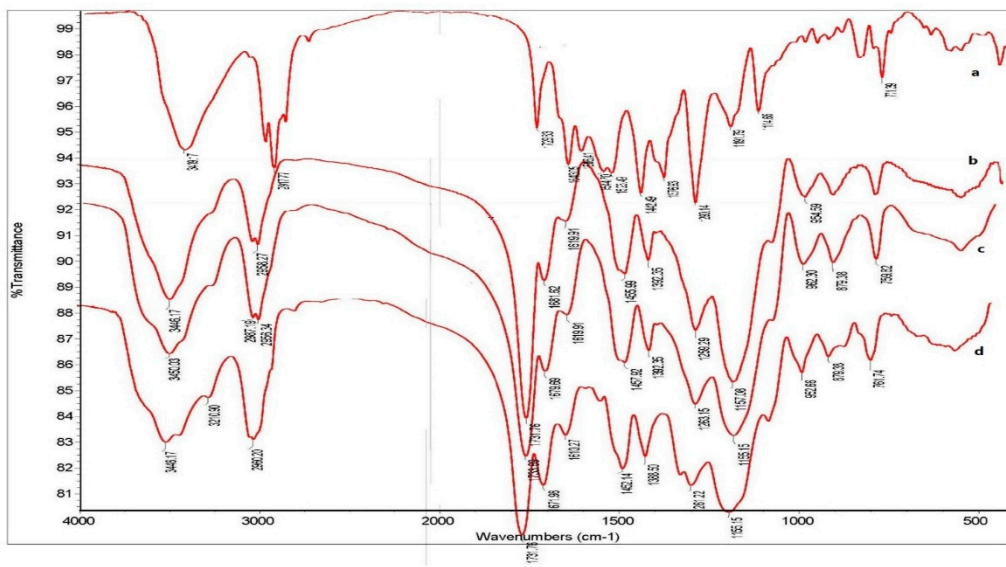
A gradient program was used at a flow rate of 0.4 mL min<sup>-1</sup> by combining solvent A (0.1% formic acid) and solvent B (acetonitrile) as follows: 75–85% B (10 min), 85-100% B (3 min), 100-75% B (2 min) and 75% B (3 min). The column temperature was maintained at 40 °C. The injection volume was 5 μL, and the detection wavelength was set at 327 nm. The method of validation of the UHPLC analysis was described in Table S1.

**Table S1.** Standard curves, LOD, LOQs, linear ranges and Rt of the HPLC and UHPLC analyses

Entry	standard curve	LOD ( $\mu\text{g mL}^{-1}$ )	LOQ ( $\mu\text{g mL}^{-1}$ )	Linear range ( $\mu\text{g mL}^{-1}$ )	Retention time (min)	Precision (RSD%)
HPLC(OC)	$y=7.9274x-27.431$ ( $R^2=0.9995$ )	2.0	6.0	6.0-200	40.808	3.00
HPLC(GK)	$y=8.4102x-18.473$ ( $R^2=0.9996$ )	1.5	5.0	5.0-200	35.617	3.73
UHPLC(OC)	$y=21.077x-15.706$ ( $R^2=0.9998$ )	0.08	0.40	0.48-200	8.531	0.88

## Part 2. Figures and Tables

**Figure S1.** FTIR spectra of OC, NIPs, leached MIPs, and unleached MIPs



**Fig. S1.** FTIR spectra of OC (a), NIPs (b), leached MIPs, (c) and unleached MIPs (d)

**Figure S2.** <sup>1</sup>H NMR in DMSO-*d* of OC and OC + AM.

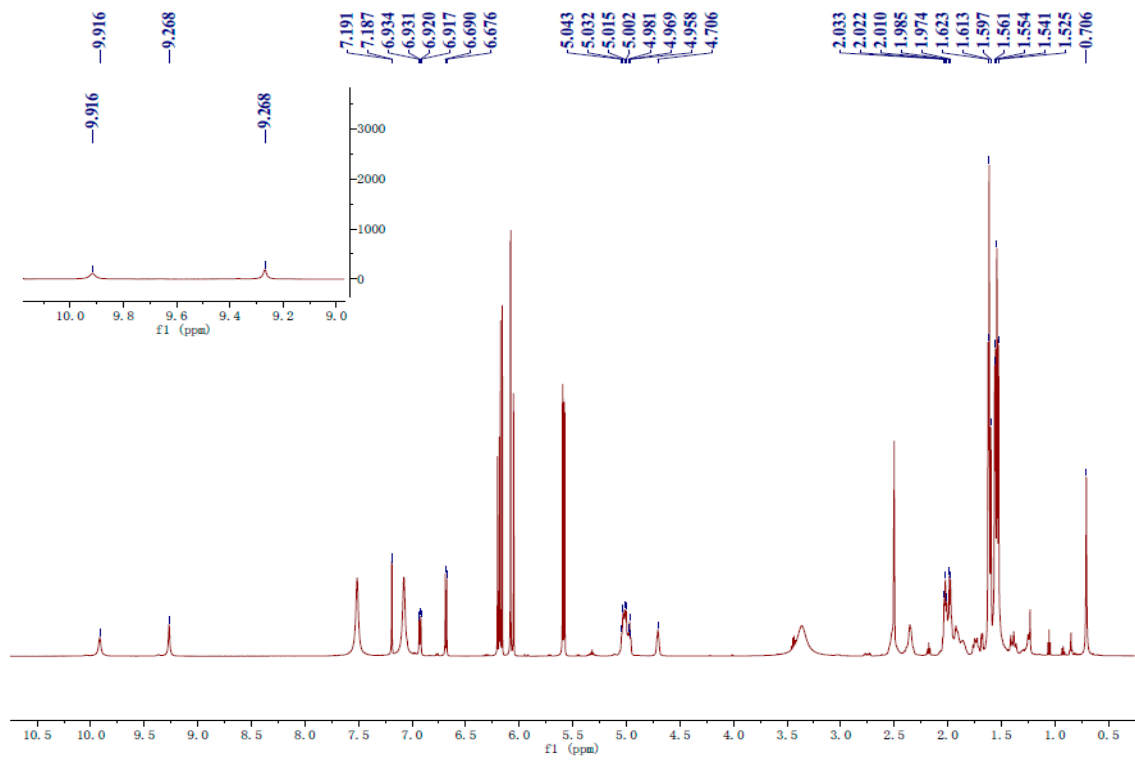
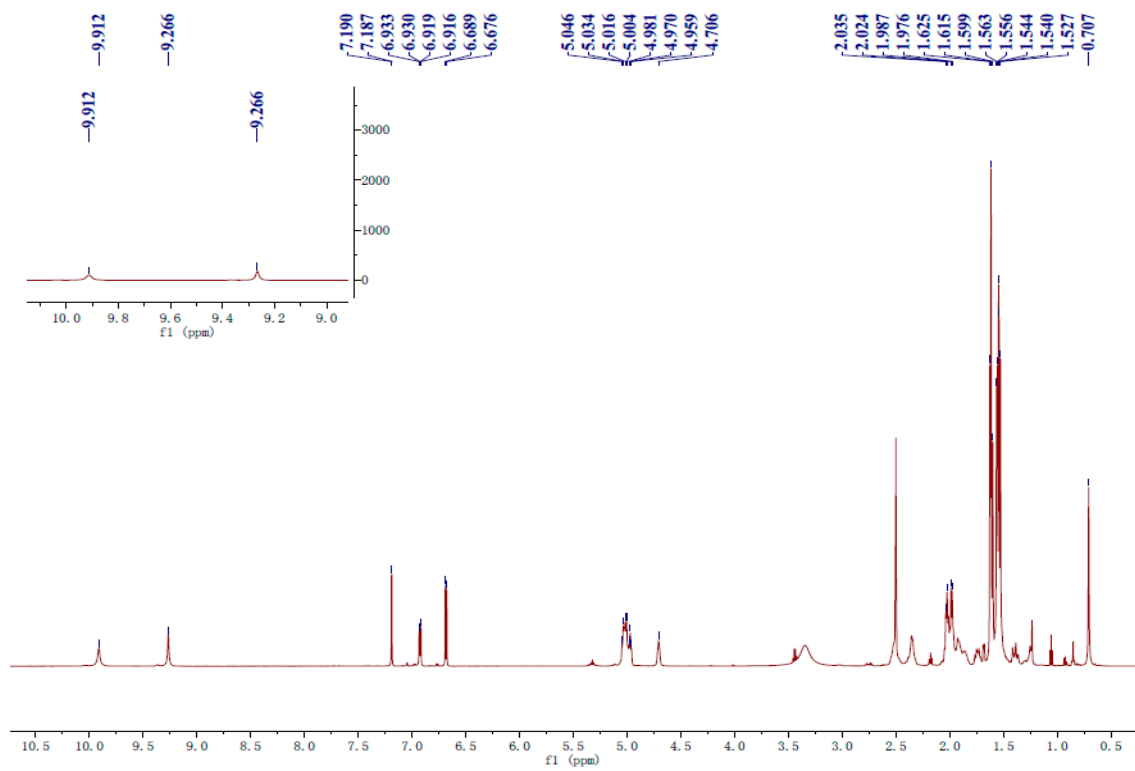
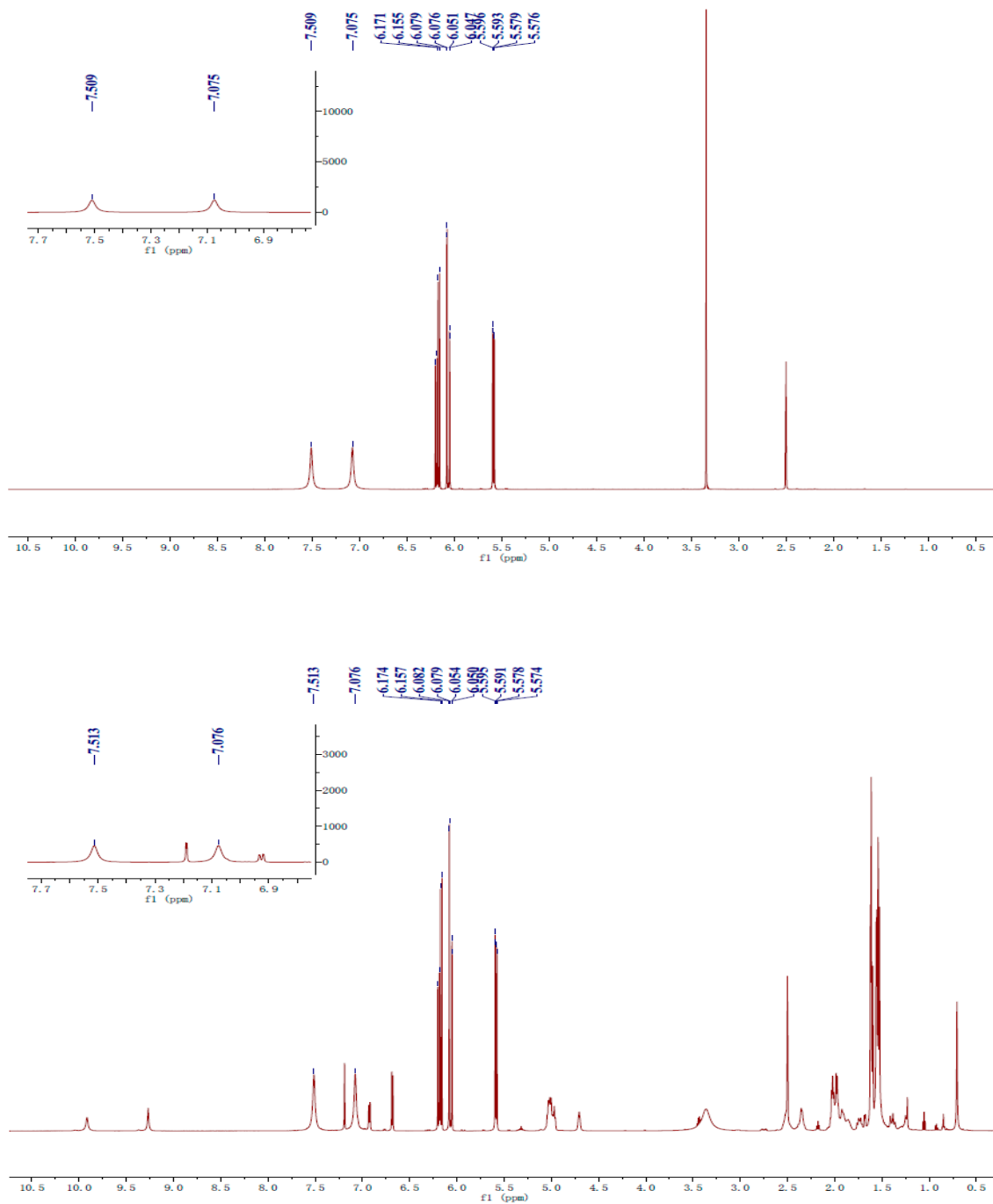


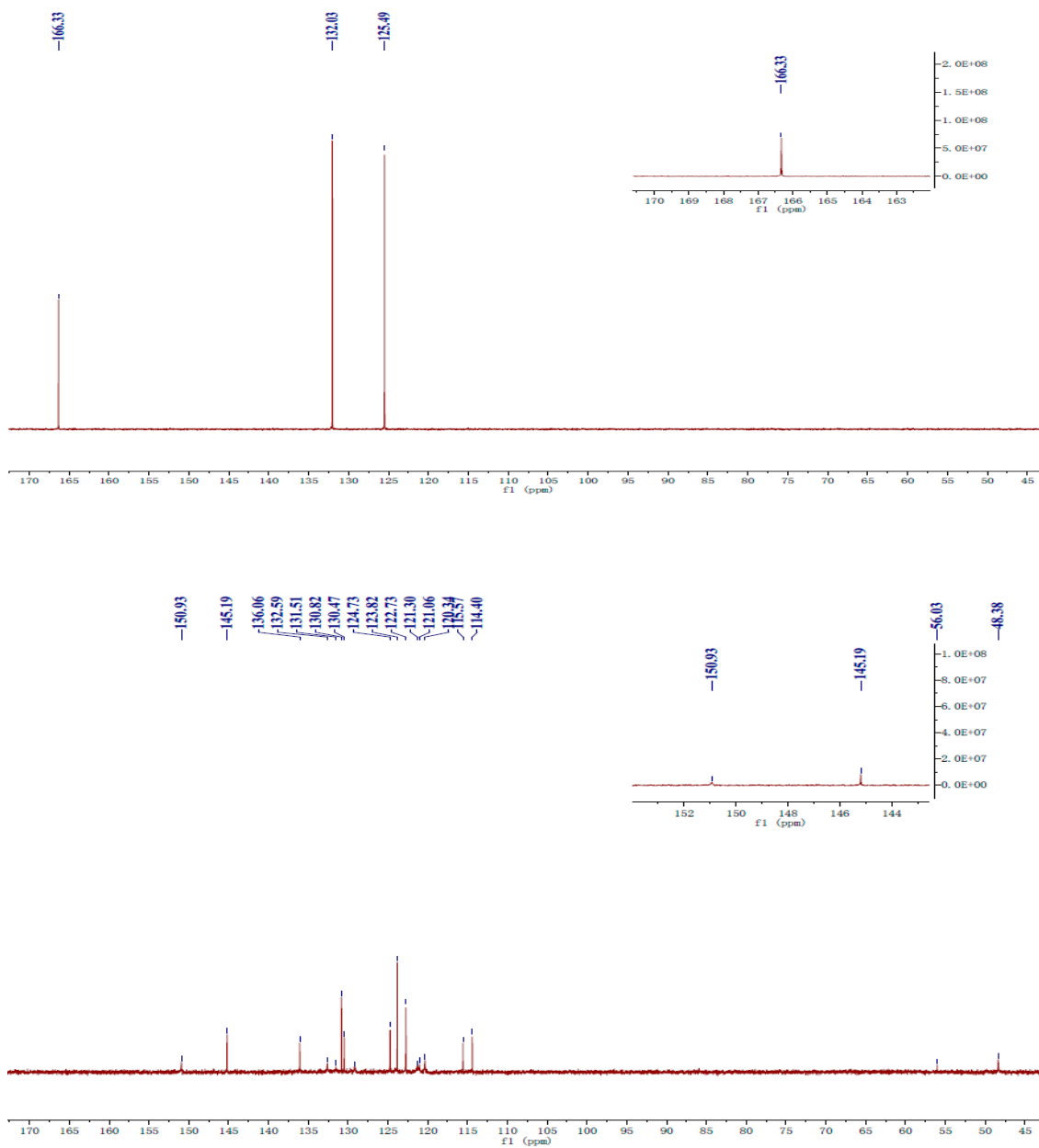
Fig. S2. <sup>1</sup>H NMR in DMSO-*d* of OC (top) and OC + AM (bottom).

**Figure S3.**  $^1\text{H}$  NMR in  $\text{DMSO-}d$  of AM and OC + AM.

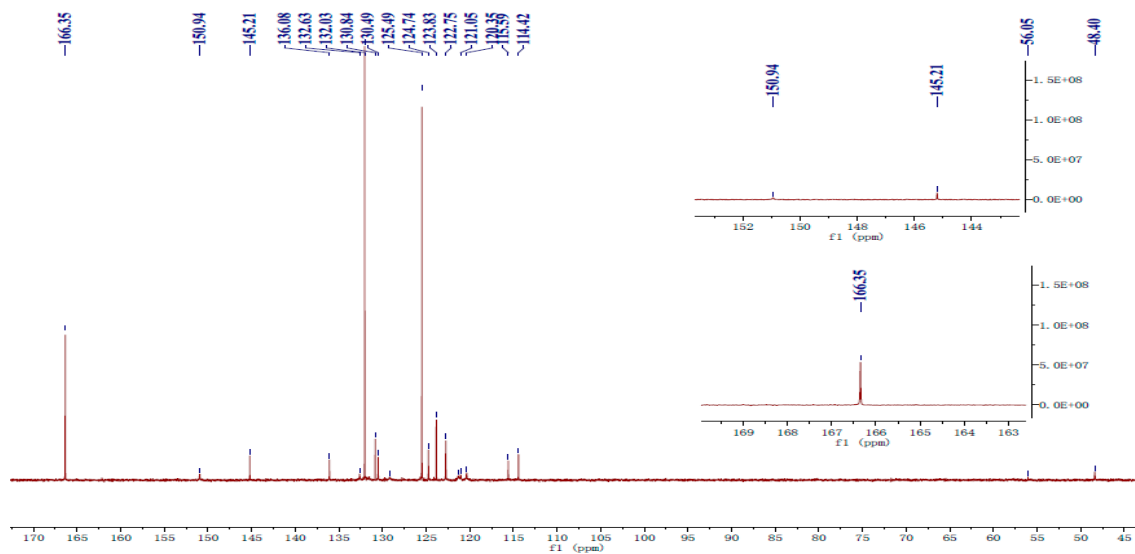


**Fig. S3.**  $^1\text{H}$  NMR in  $\text{DMSO-}d$  of AM (top) and OC + AM (bottom).

**Figure S4.**  $^{13}\text{C}$  NMR in  $\text{DMSO-}d$  of OC, AM and OC + AM.

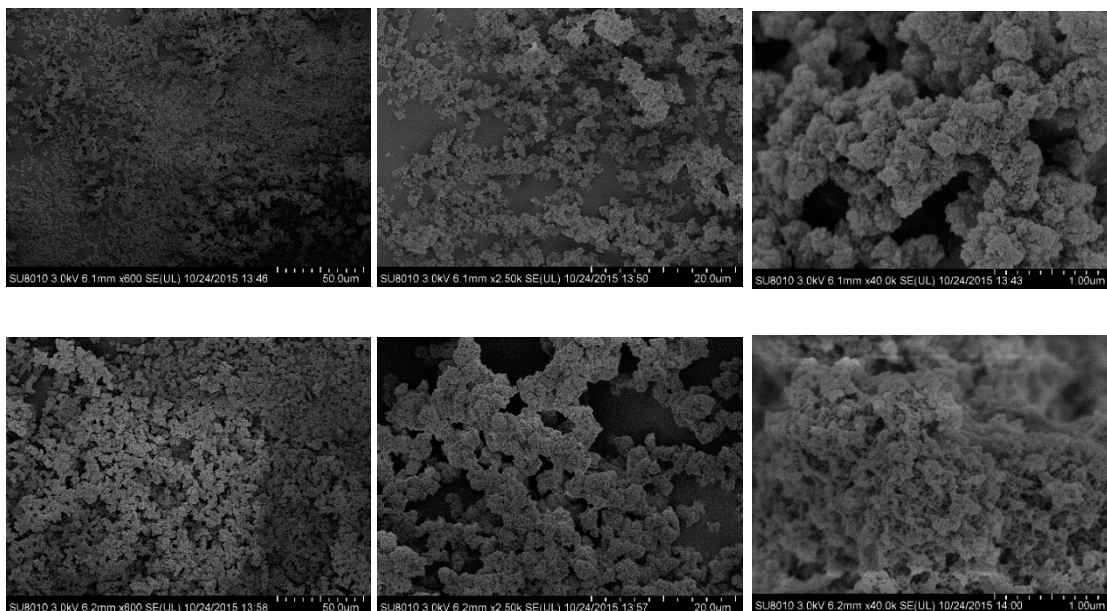






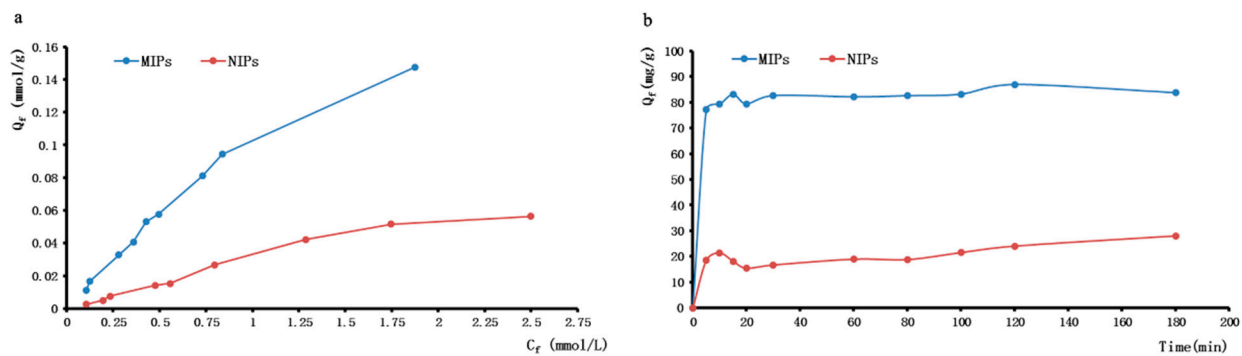
**Fig. S4.**  $^{13}\text{C}$  NMR in  $\text{DMSO-}d_6$  of OC (top), AM (middle) and OC + AM (bottom).

**Figure S5.** SEM images of MIPs C and NIPs C.



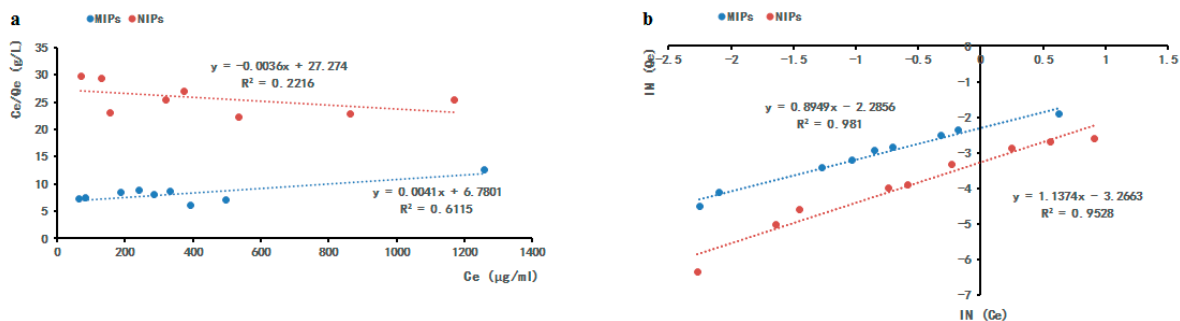
**Fig. S5.** SEM images of MIPs C (top) and NIPs C (bottom) at magnifications of 600 $\times$ , 2500 $\times$ , and 40,000 $\times$  from left to right.

**Figure S6.** Evaluation of the adsorption properties



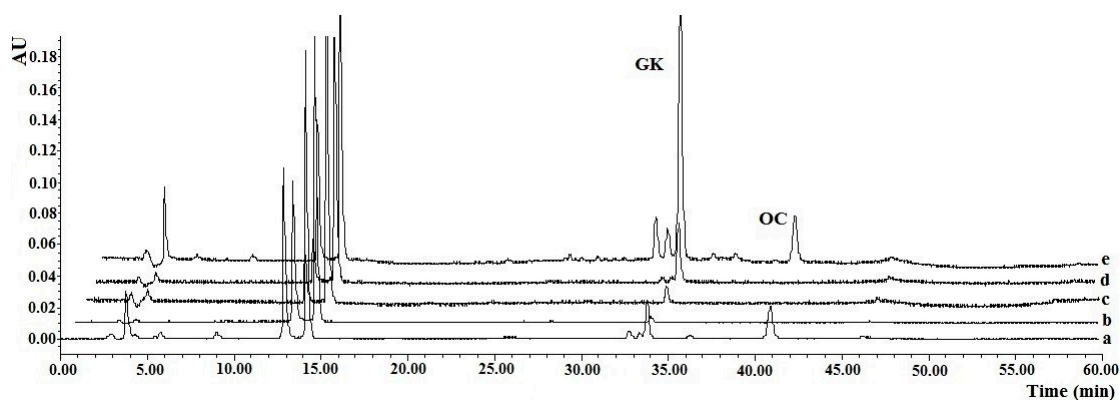
**Fig. S6.** Evaluation of the adsorption properties. a. The adsorption isotherms of OC on MIPs and NIPs. b. Dynamic adsorption isotherms of MIPs and NIPs for OC.

**Figure S7.** Langmuir and Freundlich isotherm for adsorption of OC on MIPs and NIPs.



**Fig. S7.** Langmuir and Freundlich isotherm for adsorption of OC on MIPs and NIPs. a. Langmuir isotherm for adsorption of OC on MIPs and NIP. b. Freundlich isotherm for adsorption of OC on MIPs and NIPs

**Figure S8.** Chromatograms for elution solvent selection.



**Fig. S8.** Chromatograms for elution solvent selection. a Chromatograms of fruit extracts solutions. b Chromatogram of elution solutions from the OC-MISPE column of methanol-water (35:65, v/v). c Chromatogram of elution solutions from the OC-MISPE column of methanol-water (40:60, v/v). d Chromatogram of elution solutions from the OC-MISPE column of methanol-water (50:50, v/v). e Chromatogram of elution solutions from the OC-MISPE column of methanol-water (60:40, v/v).

**Table S2.** Binding rates of different loading solvents on the static adsorption

**Table S2.** Binding rates of different loading solvents on the static adsorption

solvent	binding rate	RSD <sup>[a]</sup> (%)
70% MeOH:H <sub>2</sub> O	56.6%	0.8%
80% MeOH:H <sub>2</sub> O	32.0%	2.2%
90% MeOH:H <sub>2</sub> O	18.0%	1.8%
MeOH	7.9%	3.9%
70% EtOH:H <sub>2</sub> O	25.6%	1.5%
80% EtOH:H <sub>2</sub> O	19.4%	4.1%
EtOH	20.3%	1.5%
MeCN	21.4%	0.9%

[a]. Tests were performed in triplicate (n = 3).

**Table S3.** Solution efficiency of different volumes of the loading solution of methanol-water (80:20, v/v)**Table S3.** Solution efficiency of different volumes of the loading solution of methanol-water (80:20, v/v)

solvent volume (mL)	solution efficiency <sup>[a]</sup>		RSD <sup>[b]</sup> (%)	
	GK	OC	GK	OC
2	17.4%	16.1%	1.5%	1.8%
3	47.3%	36.4%	0.7%	0.9%
4	94.5%	84.8%	4.5%	4.0%
5	101.0%	99.7%	2.9%	4.9%

[a]. Solution efficiency = the amount of dissolved OC or GK / the amount of total OC or GK in fruit extracts. [b]. Tests were performed in triplicate (n = 3) with 1g of extracts.

**Table S4.** Binding rates of different loading amount of extracts**Table S4.** Binding rates of different loading amount of extracts

loading amount of extracts (g)	binding rates		RSD <sup>[a]</sup> (%)	
	GK	OC	GK	OC
1g	58.4%	76.9%	2.8%	2.5%
3g	33.8%	63.6%	4.6%	4.4%
5g	14.1%	57.8%	2.8%	3.5%

[a]. Tests were performed in triplicate (n = 3).

**Table S5.** The lifetime of MIPs**Table S5.** The lifetime of MIPs

entry	reused times of MIPs	relative binding rate <sup>[a]</sup> (%)	RSD <sup>[c]</sup> (%)
1	5	88.05	4.10

2	10	77.17	4.73
3	20	70.28	4.59
4 <sup>[b]</sup>	21	92.58	4.89

[a]. Relative binding rate (%) = xth binding rate / 1st binding rate × 100.

[b]. Acid activation after 20 times of MIPs.

[c]. Tests were performed in triplicate (n = 3).

**Table S6.** Purification of OC and GK in *G. yunnanensis* Hu fruit extracts

**Table S6.** Purification of OC and GK in *G. yunnanensis* Hu fruit extracts

entry <sup>[a]</sup>	loading amount of extracts (g)	purified amount of OC (mg)	recovery (%)	purified amount of GK (mg)	recovery (%)
1 <sup>[b]</sup>	1	22.3	61.7	9.2	32.1
2 <sup>[b]</sup>	3	52.0	48.0	21.6	25.1
3 <sup>[c]</sup>	5	140.5	77.7	46.5	32.4
4 <sup>[d]</sup>	12000	5000		3000	

[a]. Tests were repeated twice (n = 2).

[b]. 250 mg polymers for each test.

[c]. 2 g polymers for each test.

[d.] from the J. Agric. Food Chem. 2008, 56, 11144–11150.

### Part 3. Cartesian coordinates of the computed structures:

1	<b>Acrylamide (AM) in the DMSO</b>	60	C -8.680943534 -1.862596855 -6.075824532
2	Energy = -247.118065481278 a.u.	61	C -9.029907199 -1.024628238 -4.887976489
3	O 0.521819367 1.325799372 0.001847414	62	C -8.297552571 0.000413580 -4.429949041
4	N 1.626415015 -0.619098538 -0.001580827	63	C -8.744967798 0.788287832 -3.241871478
5	C 0.462421251 0.094091494 0.000821088	64	C -7.005156218 0.432740314 -5.033485507
6	C -0.811879963 -0.652398004 0.001871991	65	H -5.707462991 0.282857711 -2.067234859
7	C -1.980987800 -0.010347528 -0.001497633	66	H -7.265840736 -1.615724702 -2.478091809
8	H -0.740611271 -1.741839130 0.005995244	67	H -4.076407521 -4.427010900 -1.692538464
9	H 1.652948939 -1.624979695 -0.003801869	68	H -9.229529957 -7.246828302 -5.354422184
10	H 2.521136118 -0.156021635 -0.001531100	69	H -10.202795015 -6.235976826 -6.415048149
11	H -2.939485980 -0.518203269 -0.000698151	70	H -7.208151772 -5.867333850 -5.720942440
12	H -2.071451529 1.071858363 -0.005558309	71	H -7.814464319 -6.240962800 -1.992978361
13		72	H -10.166865075 -4.294208945 -7.650457200
14	<b>Oblongifolin C (OC) in the DMSO</b>	73	H -9.146689999 -3.068576847 -8.412008265
15	Energy = -2122.94081692631 a.u.	74	H -8.971138133 -4.758730092 -8.852746755
16	C -4.023308460 -1.005639202 -1.689190683	75	H -6.733147680 -4.013587846 -8.584807045
17	C -5.356586326 -0.745635988 -1.992555367	76	H -6.608707379 -2.738771674 -7.375624766
18	C -6.222048904 -1.815883930 -2.216254848	77	H -8.788783681 -7.024671311 -8.077788806
19	C -5.758733035 -3.127549098 -2.126433552	78	H -7.286963379 -6.189664159 -8.438983400
20	C -4.427335759 -3.398512102 -1.791127870	79	H -7.461221745 -8.393827492 -6.274437508
21	C -3.562172890 -2.334758827 -1.587494521	80	H -5.908418439 -10.191983819 -6.560001556
22	C -6.665499539 -4.270067101 -2.366184458	81	H -4.906151564 -10.264920198 -8.006547474
23	C -7.569552593 -4.315859885 -3.492300739	82	H -6.103865789 -7.714545083 -9.816996481
24	C -8.555580534 -5.285287834 -3.535825481	83	H -4.988865640 -6.785592929 -8.802820948
25	C -9.684976486 -5.278506963 -4.528561169	84	H -4.523159031 -8.381484041 -9.390705500
26	C -9.803459895 -3.893009667 -5.159864798	85	H -11.837173921 -5.620531760 -4.551222315
27	C -8.495395000 -3.343167314 -5.684669336	86	H -10.940707755 -6.763534363 -3.547160273
28	C -7.414133906 -3.379746608 -4.601464006	87	H -11.337740760 -3.750720449 -2.899078987
29	C -8.094429729 -4.267401814 -6.900931708	88	H -12.536859864 -4.488984942 0.266488469
30	C -9.346356143 -6.202020535 -5.710625669	89	H -11.670807465 -3.223250472 -0.615626745
31	C -8.063261909 -5.755109666 -6.436645715	90	H -10.789448953 -4.312277948 0.461337529
32	O -8.590158253 -6.303943658 -2.716209041	91	H -10.323267843 -7.106657675 -1.267826107
33	C -9.151741630 -4.086763676 -8.004715717	92	H -12.071484437 -7.271714716 -1.470316064
34	C -6.726298174 -3.836831048 -7.489990130	93	H -11.403642194 -6.813384660 0.098491109
35	C -7.824219757 -6.716270539 -7.623404923	94	H -3.444736427 -9.968982126 -6.031451366
36	C -7.066243007 -7.919765188 -7.172236028	95	H -3.347167289 -8.530424876 -7.054518333
37	C -5.969813855 -8.398665212 -7.775260632	96	H -5.344942925 -8.654699940 -4.706310796
38	C -5.243424416 -9.581526599 -7.202423844	97	H -5.333355190 -6.792922545 -3.244141000
39	C -5.370153238 -7.800122659 -9.003120696	98	H -4.641914002 -5.326208932 -3.948840922
40	O -6.456802110 -2.650243109 -4.693658681	99	H -3.676483492 -6.323320175 -2.840932138
41	O -10.866379587 -3.348284194 -5.296833178	100	H -2.026296134 -7.268618964 -5.940937332
42	C -10.991643201 -5.690805159 -3.831381695	101	H -3.007796865 -5.837233538 -6.285327963
43	C -11.252103666 -4.809329349 -2.654194163	102	H -2.078076932 -5.936506858 -4.783951394
44	C -11.376549689 -5.233663408 -1.388921400	103	H -5.422540575 -4.362150389 -5.809136631
45	C -11.606451149 -4.265954847 -0.275872194	104	H -5.514414761 -5.615101948 -7.041049016
46	C -11.292705916 -6.665755383 -0.983794724	105	H -4.180720058 -4.253618982 -8.637143328
47	C -4.029342283 -9.095211182 -6.386507831	106	H -1.186406962 -3.132409978 -7.291744570
48	C -4.466008896 -8.269382524 -5.221770661	107	H -2.051806531 -1.666673313 -7.764119727
49	C -3.879302137 -7.133922870 -4.822345569	108	H -2.107144835 -3.098222672 -8.798807473
50	C -4.411373397 -6.363506453 -3.658643078	109	H -4.325680869 -2.339722817 -5.315361003
51	C -2.689225741 -6.524808733 -5.481798109	110	H -2.572386948 -2.106735751 -5.295170375
52	C -5.475063936 -4.511932696 -6.904673129	111	H -3.262765379 -3.682234624 -4.891824568
53	C -4.257227792 -3.979092027 -7.587146487	112	H -1.997451866 -3.432701595 -1.131194023
54	C -3.313958259 -3.233503331 -6.995011805	113	H -2.284208450 -0.210508842 -1.263510534
55	C -2.114875098 -2.764297320 -7.753461666	114	H -7.754261988 -1.497743871 -6.570884298
56	C -3.361930934 -2.817203628 -5.564619255	115	H -9.485784848 -1.768853553 -6.836076502
57	O -2.243342524 -2.477483346 -1.291293855	116	H -9.964850554 -1.302174420 -4.403415364
58	O -3.217162508 0.064921236 -1.497567841	117	H -9.671522666 0.404989534 -2.793783744
59	O -6.649398160 -5.202117970 -1.551872832	118	H -8.924526498 1.840508435 -3.505743113

1	H	-7.981655470	0.786218231	-2.449035906	63	C	1.30468213	4.55122608	-1.14519631
2	H	-7.105917064	0.663813499	-6.102651502	64	C	2.27843237	5.07927945	-0.14080446
3	H	-6.577998059	1.319081149	-4.549260935	65	C	3.58981046	5.26057939	-0.35073736
4	H	-6.251945040	-0.373469106	-4.950860243	66	C	4.47468075	5.76399486	0.74365296
5					67	C	4.28790678	4.96834026	-1.63373458
6					68	H	6.87182945	2.24338970	-1.11925998
7	<b>OC-AM complex in the DMSO</b>				69	H	4.94013083	2.44519942	0.43560538
8	Energy = -2370.06266710 a.u. #Cluster: 1				70	H	3.70270540	-1.57282608	-0.56504900
9	O	3.31328274	-3.15294742	-2.50336738	71	H	-1.61103482	0.31499967	0.64327949
10	N	3.31907402	-1.62903197	-4.14384646	72	H	-2.33172627	1.84746749	0.17735455
11	C	2.65737647	-2.50608560	-3.33345416	73	H	0.15059153	0.50545093	-1.08445058
12	C	1.20093069	-2.65241476	-3.49837087	74	H	1.62444496	-0.07934709	2.65649327
13	C	0.52254398	-3.57898480	-2.81940938	75	H	-1.96649065	3.71981827	-0.97400632
14	H	0.71826732	-1.97324222	-4.20426850	76	H	-1.14228655	4.45508515	-2.35114448
15	H	2.84760754	-1.01719951	-4.79295024	77	H	-2.20567628	3.07404757	-2.59181679
16	H	4.30776582	-1.46678057	-4.02347271	78	H	-0.39237555	2.46223949	-3.90556947
17	H	-0.54809186	-3.72308780	-2.91440072	79	H	1.08244182	3.21567658	-3.31601739
18	H	0.98307844	-4.26817329	-2.11641177	80	H	-2.75905398	1.02805148	-2.00022277
19	C	6.35982492	0.23691379	-1.72011127	81	H	-1.49995839	0.54141035	-3.11656361
20	C	6.18163387	1.40942331	-0.99275474	82	H	-1.04490928	-1.54585018	-1.85514110
21	C	5.10049183	1.51648416	-0.11591226	83	H	-3.89112376	-3.32442440	-0.40432109
22	C	4.21967440	0.45003880	0.02990328	84	H	-2.30562377	-3.51275587	-1.14891624
23	C	4.39659773	-0.73819706	-0.68360393	85	H	-4.06180196	0.37305272	-0.57990422
24	C	5.46670173	-0.84500512	-1.56200935	86	H	-4.99919812	-0.96029856	-1.26326622
25	C	3.06212585	0.51966312	0.94893177	87	H	-4.54098206	-0.98388152	0.44209282
26	C	1.91067553	1.34657263	0.67122890	88	H	-1.29202760	1.33746170	3.14131161
27	C	0.79454191	1.25927974	1.48080642	89	H	-0.58281709	2.95398444	3.24030640
28	C	-0.45880819	2.06059248	1.25622768	90	H	-2.50478884	3.96679870	2.07435515
29	C	-0.05036975	3.37266936	0.58725959	91	H	-5.54568061	2.48495098	1.39631606
30	C	0.73653266	3.18943218	-0.69704731	92	H	-4.88167531	4.02049485	1.96249345
31	C	1.93456852	2.26227035	-0.46928156	93	H	-5.66473182	2.92051164	3.10382363
32	C	-0.26018327	2.54193683	-1.73403813	94	H	-3.29902322	0.18045797	2.15181145
33	C	-1.35469898	1.32212203	0.24906610	95	H	-4.85583866	0.48194737	2.92424923
34	C	-0.73919577	1.18206581	-1.15326955	96	H	-3.36700925	0.63882623	3.85906668
35	O	0.71641869	0.45324349	2.50967531	97	H	-2.77021859	-2.26049822	1.64374296
36	C	-1.45279482	3.49769699	-1.91513889	98	H	-2.36195977	-3.95426451	1.37292181
37	C	0.39266625	2.36700914	-3.12670167	99	H	-0.58557441	-1.50118090	0.99651358
38	C	-1.79331245	0.48923099	-2.04778924	100	H	1.75748260	-1.92368314	0.85261992
39	C	-1.91560658	-0.93326998	-1.61354936	101	H	2.03570087	-3.12248327	-0.42451272
40	C	-2.94036634	-1.45425604	-0.92640142	102	H	2.27860163	-3.55949972	1.27311711
41	C	-2.87910189	-2.87631623	-0.44586713	103	H	-0.38023123	-5.36414205	1.41648101
42	C	-4.18393527	-0.71853603	-0.56385250	104	H	-0.75120533	-5.10834760	-0.28888552
43	O	2.87353221	2.31278131	-1.22551450	105	H	0.91110878	-5.43897788	0.21183102
44	O	-0.36419084	4.44102372	1.03724988	106	H	1.94232785	0.89886651	-2.62208391
45	C	-1.19907546	2.29730162	2.58640458	107	H	0.47939665	0.18475429	-3.30505454
46	C	-2.53903403	2.91774890	2.36530688	108	H	1.07148467	0.81197828	-5.55569430
47	C	-3.70599298	2.26917259	2.48741350	109	H	4.43248825	0.91553108	-6.51880016
48	C	-5.00194906	2.96133048	2.22670835	110	H	3.81375486	2.55594704	-6.72069095
49	C	-3.81611426	0.83209493	2.87251263	111	H	2.80635243	1.17379671	-7.16218465
50	C	-2.22791156	-2.93677206	0.95214490	112	H	3.57213417	2.87046621	-3.46119157
51	C	-0.78273367	-2.56560151	0.88280786	113	H	4.94907117	2.20516694	-4.35990016
52	C	0.21367894	-3.43574531	0.66964872	114	H	4.07823418	1.22054361	-3.17199561
53	C	1.63350938	-2.98307525	0.59375763	115	H	4.87163223	-2.57020001	-2.28737790
54	C	-0.00432719	-4.90074113	0.49174295	116	H	7.91812939	0.88936344	-2.71577401
55	C	1.15720042	1.05841670	-3.38728326	117	H	1.77845708	4.43992082	-2.14520925
56	C	1.74947612	1.11127204	-4.75972551	118	H	0.47727747	5.27934638	-1.28293670
57	C	3.00139124	1.51395125	-5.02380057	119	H	1.83479333	5.31900795	0.82496903
58	C	3.52910108	1.53653099	-6.41987415	120	H	3.94439170	5.91658393	1.69283573
59	C	3.95185580	1.96858277	-3.97261290	121	H	4.94009327	6.72310813	0.47534078
60	O	5.70046573	-1.96828003	-2.28019593	122	H	5.29464849	5.05708166	0.94373541
61	O	7.37116549	0.05953619	-2.60151043	123	H	3.69763591	5.26005629	-2.51243741
62	O	3.07862103	-0.20297260	1.95217122	124	H	5.26044554	5.46911073	-1.71621460

1	H	4.47635755	3.88165593	-1.72526042	63	H	6.84825182	0.41612428	-1.71839764
2					64	H	5.61100077	1.09770145	0.32806933
3	Energy = -2370.05841892 a.u. #Cluster: 2								
4	O	7.28733257	4.44008637	0.75450532	65	H	2.13924811	-1.11131146	-1.01490173
5	N	5.24454221	3.56847813	1.04867026	66	H	-1.45840143	0.34242941	1.03274378
6	C	6.28624168	3.93645570	0.24257320	67	H	-2.25422477	1.81423176	0.50965657
7	C	6.15716700	3.67213922	-1.20446670	68	H	0.26051734	0.52588313	-0.75181840
8	C	7.14212402	3.97066662	-2.05142775	69	H	1.81273734	0.14887988	2.95644878
9	H	5.21132116	3.22787019	-1.53214538	70	H	-1.99666186	3.64777369	-0.68583014
10	H	4.38413655	3.21809665	0.65916449	71	H	-1.27512260	4.35267964	-2.13359289
11	H	5.24724411	3.77416681	2.03371618	72	H	-2.27785861	2.91487636	-2.25818070
12	H	7.08408291	3.79449034	-3.11983453	73	H	-0.52338619	2.18230959	-3.60761652
13	H	8.08398943	4.41254652	-1.74473811	74	H	0.81127584	3.25194558	-3.21764829
14	C	5.19999955	-0.74567056	-2.48449927	75	H	-2.64180887	0.92876537	-1.74332712
15	C	5.82300904	0.08005356	-1.55926331	76	H	-1.33515677	0.27560814	-2.72005937
16	C	5.11906543	0.46898360	-0.41631549	77	H	-1.02870310	-1.65591695	-1.21239688
17	C	3.80542521	0.05704521	-0.23509340	78	H	-4.01587475	-3.13738271	0.29907865
18	C	3.16782420	-0.78060732	-1.15757624	79	H	-2.42411840	-3.48140254	-0.37570661
19	C	3.87392667	-1.18889301	-2.28136688	80	H	-4.04185748	0.49537763	-0.41445171
20	C	3.03586475	0.46274729	0.96492129	81	H	-5.02614202	-0.94707443	-0.68722147
21	C	1.95846187	1.42612119	0.84345822	82	H	-4.44691455	-0.56330534	0.93720041
22	C	0.91255114	1.39652561	1.74041428	83	H	-1.10496582	1.50728908	3.48080849
23	C	-0.36442442	2.16190286	1.53227040	84	H	-0.47766324	3.15826169	3.46706188
24	C	-0.01929798	3.45746071	0.79666288	85	H	-2.47886021	4.00236207	2.29033966
25	C	0.73613197	3.24970516	-0.50813268	86	H	-5.44390157	2.34788788	1.78833376
26	C	1.99347969	2.42384948	-0.22302938	87	H	-4.86109201	3.94029715	2.28219073
27	C	-0.26925133	2.51179911	-1.47334912	88	H	-5.56462165	2.84544658	3.47911991
28	C	-1.25308101	1.33785905	0.58214233	89	H	-2.99345720	0.21112919	2.71261305
29	C	-0.66181766	1.15488875	-0.82598622	90	H	-4.61580056	0.44399830	3.36839237
30	O	0.90673446	0.65107435	2.82105314	91	H	-3.20444190	0.79376415	4.36928875
31	C	-1.51531128	3.40388679	-1.63829446	92	H	-2.91201179	-1.97302887	2.28100321
32	C	0.31467991	2.31555138	-2.89102029	93	H	-2.56078878	-3.69573100	2.16177776
33	C	-1.68880844	0.36925552	-1.67182262	94	H	-0.64764834	-1.41313068	1.95561952
34	C	-1.87590699	-0.98573145	-1.07485159	95	H	1.65280553	-1.85330255	1.50817722
35	C	-2.94784571	-1.38302565	-0.37248697	96	H	1.94462621	-3.08709205	0.26937043
36	C	-2.97873898	-2.75089838	0.24757597	97	H	2.05246166	-3.50574091	1.98104197
37	C	-4.16310855	-0.55727978	-0.12597704	98	H	-1.16581064	-5.08643460	1.19839295
38	O	3.01727999	2.64915452	-0.82772636	99	H	-0.33743642	-4.70091646	-0.31325063
39	O	-0.34699896	4.53412674	1.21333455	100	H	0.57095824	-5.37251451	1.04672162
40	C	-1.07685397	2.43561998	2.86853661	101	H	2.09826480	1.17923983	-2.31988589
41	C	-2.45209329	2.97524183	2.65174422	102	H	0.77754665	0.17607793	-2.92092922
42	C	-3.58043453	2.28079969	2.85640001	103	H	1.26723239	0.70353034	-5.21647910
43	C	-4.91725596	2.88772890	2.59074626	104	H	4.55875218	1.28941813	-6.18927428
44	C	-3.60437781	0.87188780	3.34605307	105	H	3.70377240	2.79674268	-6.53723302
45	C	-2.37157415	-2.72013970	1.66530858	106	H	2.92579951	1.24214595	-6.86102514
46	C	-0.90778788	-2.42126271	1.63783370	107	H	3.29550650	3.18288839	-3.14244395
47	C	0.04026461	-3.28628143	1.25225261	108	H	4.71643134	3.03065091	-4.19701987
48	C	1.48481013	-2.90630591	1.25251604	109	H	4.31281642	1.75127061	-3.03678430
49	C	-0.23543094	-4.67432285	0.78348173	110	H	3.75756459	-2.13101605	-3.98946950
50	C	1.29090915	1.14669719	-3.07757479	111	H	6.66481193	-0.73905869	-3.79320238
51	C	1.86839718	1.19435304	-4.45640344	112	H	1.64556213	4.44882128	-2.07203521
52	C	3.03341751	1.78314382	-4.75951165	113	H	0.31535615	5.26863012	-1.23220728
53	C	3.57182293	1.77528811	-6.15189171	114	H	1.94889730	5.22434383	0.89783713
54	C	3.88389421	2.47547294	-3.75051942	115	H	3.84736288	6.55758131	1.40509721
55	O	3.24560821	-2.03143826	-3.13635938	116	H	4.05059842	7.84079970	0.20383563
56	O	5.79762134	-1.20267466	-3.61206958	117	H	5.14679194	6.45459929	0.21306340
57	O	3.25563266	-0.09372808	2.03749534	118	H	2.69309313	6.50874827	-2.64837253
58	C	1.19597737	4.60936137	-1.06623250	119	H	4.35380478	6.91953157	-2.21347493
59	C	2.16049492	5.31123255	-0.16594449	120	H	3.90373340	5.23044569	-2.46230244
60	C	3.20014971	6.03604693	-0.60246185	121				
61	C	4.09687316	6.75197562	0.35306884	122	Energy = -2370.05569446 a.u. #Cluster: 3			
62	C	3.55312447	6.18786170	-2.04370044	123	O	2.12715531	-0.51913071	4.32482056
					124	N	3.98950290	-1.30034589	3.35371148



1	C	2.84890112	-1.49177298	4.07354222	63	H	0.28759196	0.81682206	-0.52450000
2	C	2.53834859	-2.84524379	4.57088389	64	H	1.44343412	0.66204023	3.30285437
3	C	1.27375572	-3.21024319	4.78686983	65	H	-2.22680584	3.71081498	-0.92101888
4	H	3.38711746	-3.50858380	4.74213341	66	H	-1.44386347	4.34937456	-2.36854055
5	H	4.58641081	-2.05494182	3.06068346	67	H	-2.30246595	2.81802179	-2.43373702
6	H	4.21249057	-0.38118135	2.99557756	68	H	-0.35628644	2.21737057	-3.57816465
7	H	0.98893521	-4.19130807	5.14946387	69	H	0.90254124	3.35076944	-3.11136647
8	H	0.42323368	-2.55802862	4.60802831	70	H	-2.57503246	0.84777698	-1.69988954
9	C	4.81531719	-0.99506328	-1.63873145	71	H	-1.16041977	0.31275871	-2.59235960
10	C	5.59923119	-0.07911585	-0.94999934	72	H	-0.70581029	-1.51477548	-1.01361104
11	C	5.01527272	0.68689215	0.06157509	73	H	-3.51045890	-3.12050987	0.79805746
12	C	3.66328387	0.54110791	0.35422460	74	H	-2.02491672	-3.46252341	-0.08103236
13	C	2.86357193	-0.37514703	-0.33871679	75	H	-4.11634249	-0.48337479	1.10119384
14	C	3.44356942	-1.14964493	-1.33407024	76	H	-3.99454651	0.27898541	-0.48683218
15	C	3.05429303	1.37053032	1.41875197	77	H	-4.77961249	-1.29405475	-0.32093343
16	C	1.79486796	2.05027776	1.12306470	78	H	-1.40877137	1.97825923	3.53135525
17	C	0.69201868	1.91541737	1.91269106	79	H	-0.98212626	3.68594331	3.38878978
18	C	-0.63778367	2.54307378	1.56546165	80	H	-2.99625081	4.15293233	2.01741028
19	C	-0.37133305	3.80884191	0.75357106	81	H	-5.71771896	2.12649292	1.60415050
20	C	0.49548412	3.59265562	-0.47667734	82	H	-5.35653583	3.81789050	1.95948177
21	C	1.80157912	2.91161519	-0.06081581	83	H	-5.98980531	2.76265440	3.22855600
22	C	-0.34628680	2.68042552	-1.45157152	84	H	-3.00681695	0.44647105	2.98018157
23	C	-1.38642522	1.58024083	0.62782627	85	H	-4.73473895	0.47001649	3.34180595
24	C	-0.67757157	1.35040369	-0.71782549	86	H	-3.58744375	1.16482829	4.48815074
25	O	0.60992460	1.19158276	3.00442767	87	H	-2.06436748	-1.62072109	2.40242008
26	C	-1.64442800	3.43043296	-1.80463707	88	H	-1.90737971	-3.36958425	2.54151222
27	C	0.39405562	2.42043049	-2.78594316	89	H	0.11269074	-1.38498178	1.44269850
28	C	-1.56675133	0.41075101	-1.56451470	90	H	2.39667367	-2.27118184	1.36100731
29	C	-1.61834350	-0.92649810	-0.90258217	91	H	2.19901947	-3.41256588	0.02796338
30	C	-2.63747185	-1.39085465	-0.16758826	92	H	2.66210117	-3.99607621	1.63264211
31	C	-2.51455549	-2.70065448	0.55805487	93	H	0.06916647	-5.13832396	2.66152813
32	C	-3.93450841	-0.68597753	0.03469846	94	H	-0.85217946	-5.05109003	1.15606782
33	O	2.82485451	3.11502676	-0.66992173	95	H	0.83009032	-5.58358044	1.13007379
34	O	-0.84585376	4.87010870	1.05673365	96	H	2.16616114	1.40889211	-1.99036815
35	C	-1.45487794	2.84441334	2.83490666	97	H	0.93187620	0.30152745	-2.58694904
36	C	-2.87025700	3.18686067	2.50425998	98	H	1.50022709	0.73652884	-4.90998372
37	C	-3.92051134	2.39174160	2.75252217	99	H	4.87934978	0.97457529	-5.67568292
38	C	-5.30363656	2.80061674	2.36994270	100	H	4.20034789	2.53501556	-6.15131419
39	C	-3.81071102	1.05917784	3.41459935	101	H	3.29729233	1.04580810	-6.45696918
40	C	-1.70497624	-2.51831739	1.86029047	102	H	3.60715717	3.18117965	-2.86041831
41	C	-0.24418625	-2.40479527	1.56603324	103	H	5.08532995	2.78305170	-3.75922468
42	C	0.57980283	-3.45359651	1.43512816	104	H	4.44318269	1.66771608	-2.54427102
43	C	2.02453758	-3.27184730	1.10800643	105	H	3.11366313	-2.45217141	-2.75199742
44	C	0.13858074	-4.86971598	1.59614779	106	H	6.22298261	-1.57114118	-2.88400123
45	C	1.41853339	1.27690577	-2.79729451	107	H	1.38472143	4.78825530	-2.06098936
46	C	2.08984429	1.21320914	-4.13150923	108	H	-0.06672470	5.51549562	-1.34955686
47	C	3.32004220	1.68327158	-4.37915665	109	H	1.21926262	5.99899394	0.78951563
48	C	3.94421693	1.55238692	-5.72955808	110	H	3.11574229	7.24448218	1.47439300
49	C	4.15966688	2.36215841	-3.35235366	111	H	3.95022701	8.04410767	0.13664451
50	O	2.64581982	-2.04069760	-1.97045119	112	H	4.61447400	6.56260439	0.83277418
51	O	5.28610478	-1.80132862	-2.61919438	113	H	3.05448138	6.35847379	-2.59665581
52	O	3.57828800	1.45524614	2.51452388	114	H	4.61707382	6.45856074	-1.78052200
53	C	0.85971712	4.95630923	-1.09518578	115	H	3.77522348	4.90598622	-1.88572640
54	C	1.69204590	5.78062086	-0.16642162	116				
55	C	2.91777978	6.24494538	-0.44673552	117		Energy = -2370.05003075 a.u. #Cluster: 4		
56	C	3.67572852	7.06189573	0.54769527	118	O	-2.43279420	8.69987674	1.50152544
57	C	3.62647526	5.99023916	-1.73333404	119	N	-0.89342013	7.21709283	0.82474599
58	H	6.65485865	0.03792271	-1.19423844	120	C	-1.85542779	7.62951737	1.70087599
59	H	5.62407600	1.40699907	0.61336436	121	C	-2.13793257	6.76324707	2.86539580
60	H	1.80177281	-0.49118579	-0.11570657	122	C	-3.33241181	6.77254619	3.45583397
61	H	-1.53583843	0.60595613	1.14204984	123	H	-1.31575123	6.12313140	3.19873943
62	H	-2.41524762	1.95773293	0.45108040	124	H	-0.43102061	6.32483841	0.93504807

1	H	-0.67061390	7.75012815	0.00063356	63	H	-0.62646723	2.50886549	-3.31979800
2	H	-3.57855704	6.15527757	4.31254374	64	H	0.87296950	3.28956312	-2.84069586
3	H	-4.15935801	7.39612512	3.13201867	65	H	-2.96482508	1.39217804	-1.32913592
4	C	5.99867916	0.30085280	-1.95402730	66	H	-1.80068359	0.73270876	-2.46964113
5	C	6.04704544	1.29361114	-0.98283446	67	H	-1.59221013	-1.37173321	-1.21515176
6	C	5.05699385	1.32637481	0.00034679	68	H	-4.49619595	-2.68484994	0.63317598
7	C	4.04506577	0.37003617	0.00031978	69	H	-3.13884525	-3.13355218	-0.39804504
8	C	3.98660380	-0.63385127	-0.96981895	70	H	-4.32368476	0.94136720	0.01395133
9	C	4.96783559	-0.66162311	-1.95333313	71	H	-5.42943835	-0.43674982	-0.00311405
10	C	2.98883048	0.39927175	1.03902428	72	H	-4.49359508	-0.06997175	1.45042246
11	C	1.89194997	1.33681043	0.96670675	73	H	-0.97190607	1.38671135	3.78555528
12	C	0.84665686	1.24772028	1.86481259	74	H	-0.24233886	2.99561903	3.82271261
13	C	-0.36579545	2.13675291	1.82329571	75	H	-2.27771192	4.03373693	2.87607525
14	C	0.02083112	3.45547880	1.15889574	76	H	-5.38300804	2.61211061	2.59429038
15	C	0.69310054	3.30231807	-0.19049721	77	H	-4.64314567	4.13093174	3.11106066
16	C	1.90602228	2.37692997	-0.06206891	78	H	-5.30730850	3.01576786	4.31228368
17	C	-0.38228985	2.67927106	-1.16442655	79	H	-2.96040546	0.26908198	3.21360925
18	C	-1.40909750	1.50593915	0.88520355	80	H	-4.54363172	0.55427701	3.94148720
19	C	-0.91018423	1.34700313	-0.55917085	81	H	-3.07906804	0.79000494	4.89830283
20	O	0.79881697	0.35119102	2.81926329	82	H	-2.92903632	-1.93912661	2.44663166
21	C	-1.53331360	3.69247892	-1.30283498	83	H	-2.69817214	-3.63637330	2.02450140
22	C	0.19922178	2.44783611	-2.58057263	84	H	-0.75691644	-1.38942170	1.74262123
23	C	-2.06689328	0.74626437	-1.39223388	85	H	1.37235088	-1.78926991	0.77999990
24	C	-2.34298198	-0.63918317	-0.91225681	86	H	1.22471891	-2.62602416	-0.77698607
25	C	-3.35935624	-1.00279194	-0.11857886	87	H	1.79508966	-3.49995456	0.65169491
26	C	-3.45058811	-2.41516763	0.38696691	88	H	-1.57476179	-4.89878260	0.58652523
27	C	-4.44456600	-0.09706206	0.35109364	89	H	-1.12290661	-4.28500229	-1.00624076
28	O	2.85165761	2.53192481	-0.79503572	90	H	0.06271958	-5.15525921	-0.02495667
29	O	-0.24003721	4.51264098	1.66852158	91	H	1.78250855	1.00160662	-2.09924954
30	C	-0.93755559	2.35287709	3.23679071	92	H	0.28105242	0.25948242	-2.65720929
31	C	-2.28772750	2.98791498	3.18454365	93	H	0.82507859	0.60726448	-4.93872455
32	C	-3.43646858	2.35899023	3.46892984	94	H	4.07203439	0.99012330	-6.07650980
33	C	-4.74592087	3.06798857	3.36802681	95	H	3.30687765	2.54139452	-6.43455069
34	C	-3.51319348	0.93188008	3.89607146	96	H	2.41001293	1.03683139	-6.67686769
35	C	-2.56521240	-2.60417479	1.63772193	97	H	3.07722651	3.19775296	-3.18839876
36	C	-1.12666162	-2.33165304	1.34008481	98	H	4.48618861	2.69068007	-4.13903297
37	C	-0.32887544	-3.12671203	0.61424543	99	H	3.86846820	1.67817716	-2.82465985
38	C	1.08086528	-2.73662390	0.30914157	100	H	5.54971673	-1.51379882	-3.61390319
39	C	-0.75786602	-4.42642539	0.02339727	101	H	7.53869977	0.95337687	-2.98355990
40	C	0.95160982	1.12739785	-2.82168082	102	H	1.66910881	4.54381062	-1.68604527
41	C	1.47680444	1.09934852	-4.22207837	103	H	0.38330487	5.38029404	-0.81237967
42	C	2.64965110	1.62823417	-4.59849124	104	H	1.83246493	5.44267086	1.27872574
43	C	3.12213666	1.54272637	-6.01268816	105	H	3.93165283	6.22397799	1.99775720
44	C	3.56766531	2.33233236	-3.66227366	106	H	4.84420012	7.03271185	0.71709916
45	O	4.88749296	-1.65189541	-2.87839430	107	H	5.26828708	5.38664831	1.20115614
46	O	6.91781196	0.17046884	-2.94297383	108	H	3.51491649	5.67189132	-2.16721976
47	O	3.03961539	-0.43260627	1.94997009	109	H	5.12301246	5.72326447	-1.43683350
48	C	1.22318167	4.66911074	-0.67340243	110	H	4.24388976	4.19190771	-1.52364916
49	C	2.22033999	5.24346668	0.28084741	111				
50	C	3.50075940	5.51216630	-0.01208667	112		Energy = -2370.04927123 a.u. #Cluster: 5		
51	C	4.42018645	6.06707061	1.02711734	113	O	4.32771805	-3.35106866	-4.60243917
52	C	4.12545770	5.27711908	-1.34386624	114	N	4.16219000	-1.28829331	-5.47291734
53	H	6.83937754	2.04206474	-0.99526160	115	C	4.70892738	-2.54086395	-5.45753981
54	H	5.06893710	2.11622679	0.75396600	116	C	5.68190254	-2.89563703	-6.50688357
55	H	3.19066439	-1.37747372	-0.97356123	117	C	6.48448102	-3.95116302	-6.36265172
56	H	-1.72231962	0.51702884	1.28472113	118	H	5.70701883	-2.24995996	-7.38712671
57	H	-2.33857417	2.11421648	0.90171480	119	H	4.51115237	-0.56000565	-6.07411190
58	H	-0.06911737	0.60831447	-0.56009990	120	H	3.56655408	-0.97811571	-4.71736055
59	H	1.66664276	-0.25603176	2.82874317	121	H	7.21886450	-4.24696981	-7.10395229
60	H	-1.96867963	3.96815295	-0.33674610	122	H	6.47368613	-4.59983032	-5.49158704
61	H	-1.20778797	4.61585393	-1.79723957	123	C	5.13912844	-0.84293014	-2.09345907
62	H	-2.35118690	3.29171011	-1.91539389	124	C	5.73977498	0.17653502	-1.36714595

1	C	5.07400098	0.70978143	-0.25967099	63	H	-3.49151172	-3.55444967	-0.17038471
2	C	3.82491756	0.21798827	0.09245052	64	H	-1.74983157	-3.63831628	-0.42980349
3	C	3.20465889	-0.80330728	-0.63505670	65	H	-3.77828944	-0.01664397	0.12992677
4	C	3.86811769	-1.34341878	-1.73069838	66	H	-4.23820156	-0.57993693	-1.48147080
5	C	3.08044800	0.75289585	1.25636690	67	H	-4.67365971	-1.52278740	-0.05382263
6	C	1.94191889	1.61920125	1.00477655	68	H	-1.34766147	1.54023372	3.34781467
7	C	0.84550861	1.57436470	1.82642112	69	H	-0.88085289	3.24330072	3.31633476
8	C	-0.47348739	2.18829641	1.45382926	70	H	-2.82216428	3.84322506	1.91805004
9	C	-0.17154019	3.47940349	0.69090164	71	H	-5.54489663	1.88652898	1.17765531
10	C	0.72173281	3.29208420	-0.52455369	72	H	-5.17202297	3.54237074	1.66505903
11	C	1.99315784	2.52689249	-0.14332799	73	H	-5.88947286	2.41902702	2.82586035
12	C	-0.13738948	2.45732201	-1.55290330	74	H	-2.99066915	0.03711746	2.45678953
13	C	-1.18250017	1.24757464	0.46134091	75	H	-4.70200750	0.11139581	2.87777775
14	C	-0.47584585	1.08999603	-0.89672081	76	H	-3.48666279	0.64229344	4.04277073
15	O	0.82538024	0.93749194	2.98124282	77	H	-3.08736385	-2.24290153	1.98419048
16	C	-1.42899533	3.24409729	-1.84786242	78	H	-2.47395370	-3.89476239	2.00694764
17	C	0.58491167	2.27665676	-2.90865853	79	H	-0.91752532	-1.36241103	2.21794506
18	C	-1.38531054	0.21782714	-1.79138065	80	H	1.47474446	-1.43071413	2.25563583
19	C	-1.48748294	-1.14923897	-1.20066732	81	H	2.26386779	-2.70248404	1.30669882
20	C	-2.58031944	-1.64778241	-0.60691938	82	H	1.90405676	-2.96601335	3.01422128
21	C	-2.54528515	-3.01014863	0.02070870	83	H	-0.69398683	-5.04974400	1.38996125
22	C	-3.87477190	-0.91492296	-0.49895950	84	H	0.43491336	-4.51470244	0.14035550
23	O	3.02030039	2.70562725	-0.75062599	85	H	1.04446194	-5.08231448	1.70069451
24	O	-0.64447438	4.53272293	1.02115879	86	H	2.35191939	1.16317557	-2.22632061
25	C	-1.34412981	2.44255355	2.69736633	87	H	1.08777694	0.14102207	-2.90739331
26	C	-2.73472858	2.83478794	2.32025651	88	H	1.69101489	0.69615698	-5.17281552
27	C	-3.80572884	2.03627440	2.43284854	89	H	4.99214644	1.65151922	-6.04008248
28	C	-5.15895453	2.49883348	2.00723744	90	H	3.91936309	3.00849081	-6.35946739
29	C	-3.74760846	0.64676915	2.97263734	91	H	3.38655655	1.37435409	-6.74745893
30	C	-2.31149549	-2.89975417	1.54115417	92	H	3.52285479	3.32911593	-3.05750251
31	C	-0.94349713	-2.39003786	1.86007682	93	H	5.03690614	3.08684523	-3.94989511
32	C	0.18651521	-3.09852148	1.72973240	94	H	4.47670641	1.88655293	-2.77392939
33	C	1.51351845	-2.51392284	2.08909359	95	H	3.73850775	-2.66841784	-3.20592528
34	C	0.24298793	-4.50013741	1.22539837	96	H	6.55605727	-0.95822819	-3.44657447
35	C	1.59183247	1.12062750	-3.03148619	97	H	1.74899818	4.52771857	-1.99052947
36	C	2.23776272	1.19859219	-4.37898741	98	H	0.26082228	5.25680642	-1.36184341
37	C	3.37411545	1.86609346	-4.62605648	99	H	1.37229091	5.67272137	0.86524128
38	C	3.93820721	1.96569052	-6.00488510	100	H	3.24229098	6.76933046	1.79207322
39	C	4.14577683	2.57618253	-3.56982987	101	H	4.21235177	7.59762768	0.56836731
40	O	3.23331974	-2.33101799	-2.38827091	102	H	4.77854679	6.07459261	1.26246982
41	O	5.71448379	-1.42355121	-3.17588465	103	H	3.52046070	5.82596474	-2.31497311
42	O	3.34278025	0.36930683	2.39025515	104	H	4.98323493	6.14133118	-1.37841187
43	C	1.15549692	4.66980001	-1.06088201	105	H	4.30394932	4.50813885	-1.42868621
44	C	1.93056791	5.43983486	-0.04034607	106				
45	C	3.19991100	5.84767372	-0.17795170	107				
46	C	3.88087496	6.60776584	0.91366872	108	<b>OC-(AM)<sub>2</sub> complex in the DMSO</b>			
47	C	4.04043464	5.58110169	-1.37882811	109				
48	H	6.71701295	0.56027550	-1.66026896	110	Energy = -2617.19089169 a.u. #Cluster: 1			
49	H	5.53024349	1.52240743	0.30792969	111	O	1.63711575	-3.12024551	-3.36866533
50	H	2.21564358	-1.17763459	-0.36895826	112	N	3.24858928	-1.83164599	-4.23107298
51	H	-1.31031095	0.24553743	0.92575201	113	C	1.94883085	-2.24356049	-4.18456443
52	H	-2.21891946	1.61268734	0.29513266	114	C	0.98117244	-1.65726483	-5.12948227
53	H	0.48310904	0.53337860	-0.74171925	115	C	-0.32682596	-1.70729372	-4.87210188
54	H	1.75245928	0.55004609	3.22696251	116	H	1.39243819	-1.19421103	-6.02726247
55	H	-2.02527632	3.43816471	-0.95048911	117	H	3.55880773	-1.05782687	-4.79632609
56	H	-1.21657708	4.21378019	-2.31399076	118	H	3.92252776	-2.20175401	-3.57824320
57	H	-2.07982541	2.69922938	-2.54351148	119	H	-1.08142407	-1.29191046	-5.53050742
58	H	-0.17911010	2.14338784	-3.70393230	120	H	-0.74313641	-2.16564245	-3.97728796
59	H	1.10088228	3.22178394	-3.17390106	121	O	2.74477077	-0.07923545	4.27611446
60	H	-2.37841656	0.69228711	-1.91093224	122	N	4.78686011	-0.60127979	3.51187216
61	H	-0.97334788	0.15713009	-2.82048623	123	C	3.68405584	-0.88454057	4.25766895
62	H	-0.56523170	-1.72860662	-1.24965864	124	C	3.67683161	-2.11868055	5.06656213

1	C	2.63811706	-2.41301718	5.85051831	63	H	-1.96365328	3.33708933	-1.39020349
2	H	4.55586360	-2.76100682	4.98716864	64	H	-1.11348792	4.13256972	-2.71964988
3	H	5.55155644	-1.24728835	3.39539294	65	H	-1.79490278	2.53190586	-2.94587794
4	H	4.82347542	0.23987175	2.95508083	66	H	0.30294959	2.21772880	-3.90601586
5	H	2.58754959	-3.30632756	6.46313530	67	H	1.45256276	3.36124712	-3.22830603
6	H	1.75727050	-1.78300636	5.94059221	68	H	-1.97578893	0.58642734	-2.26163069
7	C	4.59978912	-1.83368930	-1.08712877	69	H	-0.46643357	0.17300933	-3.05453195
8	C	5.52373146	-0.84948346	-0.75320649	70	H	-0.01574058	-1.63816099	-1.33965096
9	C	5.11388476	0.22484038	0.03604918	71	H	-2.80101775	-3.86807471	-1.07033773
10	C	3.79076195	0.31548736	0.46188455	72	H	-1.06840235	-3.68430989	-0.78821837
11	C	2.85945029	-0.67693449	0.13625333	73	H	-4.26147343	-1.86408285	-0.82481008
12	C	3.26620456	-1.76472145	-0.62297376	74	H	-3.56274180	-0.24574113	-0.89238188
13	C	3.37293044	1.49275465	1.25563589	75	H	-3.76056735	-1.18548361	-2.37615121
14	C	2.05098744	2.05383516	0.94368995	76	H	-1.33652143	1.45917249	3.04953917
15	C	0.92546269	1.76842274	1.64624707	77	H	-1.01302362	3.19666771	3.08863655
16	C	-0.44482067	2.23822917	1.21635679	78	H	-2.95670236	3.69993155	1.69670322
17	C	-0.26480670	3.56026461	0.47254904	79	H	-5.45479554	1.50790320	0.63510681
18	C	0.70495621	3.49462439	-0.69743709	80	H	-5.20253245	3.18302525	1.13199343
19	C	2.04486652	2.93328098	-0.22550130	81	H	-5.89276068	2.01835527	2.26729537
20	C	0.05571114	2.53476800	-1.76623973	82	H	-3.34168492	-0.27272156	1.45904579
21	C	-1.01368659	1.24112680	0.19289487	83	H	-4.55856919	-0.09946481	2.72408894
22	C	-0.20258205	1.14987419	-1.10836395	84	H	-2.85534012	0.16683496	3.10263412
23	O	0.86431675	1.02326390	2.73138903	85	H	-3.25071620	-2.68697849	1.16286254
24	C	-1.27136071	3.16845266	-2.22162192	86	H	-2.43898110	-4.24577611	1.29731733
25	C	0.95068556	2.39331540	-3.02244814	87	H	-1.38008860	-1.55046929	2.03756350
26	C	-0.95822896	0.19802595	-2.05930444	88	H	0.82834379	-1.37188963	2.90732254
27	C	-0.99615098	-1.17852895	-1.48402348	89	H	2.02933377	-2.33397114	2.02359804
28	C	-2.11722621	-1.82962692	-1.14775710	90	H	1.37009852	-2.92447382	3.55277839
29	C	-2.05258130	-3.21572857	-0.57852535	91	H	-0.42409973	-5.11255703	1.16703492
30	C	-3.48664488	-1.25878582	-1.31318112	92	H	0.98795073	-4.34828547	0.42082657
31	O	3.07301195	3.21753190	-0.79353351	93	H	1.09417221	-4.98784632	2.06602706
32	O	-0.86628197	4.55403884	0.77907998	94	H	2.68834036	1.41370858	-2.11246842
33	C	-1.38377669	2.38191098	2.42855958	95	H	1.56148793	0.29053527	-2.87145571
34	C	-2.78614138	2.66795312	2.00253217	96	H	2.19610108	1.12519899	-5.15583686
35	C	-3.77543163	1.76461502	1.95634596	97	H	5.63553535	0.76802116	-5.66925203
36	C	-5.13816550	2.14243243	1.47667148	98	H	5.25988319	2.47212970	-5.93075563
37	C	-3.62517984	0.33026427	2.33449692	99	H	4.15147899	1.22648103	-6.51232811
38	C	-2.29458591	-3.20343829	0.94392396	100	H	4.52711977	2.61569320	-2.53528449
39	C	-1.16559032	-2.55333852	1.67522787	101	H	5.97348248	2.22691512	-3.47842214
40	C	0.03496747	-3.11307092	1.87623970	102	H	5.14552791	0.96084461	-2.56641592
41	C	1.10899290	-2.39562517	2.62501175	103	H	2.20719441	-2.93017785	-1.80364324
42	C	0.43242992	-4.45724108	1.36953540	104	H	5.86789837	-2.90291053	-2.14657194
43	C	2.02386107	1.29351421	-2.99015601	105	H	1.51061555	4.85540069	-2.19414075
44	C	2.79710324	1.31676683	-4.26840029	106	H	-0.01431834	5.40405231	-1.48136649
45	C	4.11414178	1.54642370	-4.36055068	107	H	1.16138435	5.89722223	0.70528516
46	C	4.81257904	1.49898616	-5.67949543	108	H	2.92548972	7.27930238	1.49915707
47	C	4.98350532	1.85320500	-3.19023170	109	H	3.83443220	8.12270838	0.23817398
48	O	2.38895959	-2.77559280	-0.82036593	110	H	4.48180480	6.64316637	0.95587922
49	O	4.89926204	-2.88538124	-1.88274560	111	H	3.14321659	6.62743184	-2.56202949
50	O	4.09767746	1.96631858	2.10555367	112	H	4.66375782	6.60193144	-1.66315212
51	C	0.95412777	4.91747084	-1.23355247	113	H	3.79510685	5.09290768	-1.96991889
52	C	1.68792584	5.75549524	-0.23689157	114				
53	C	2.89069407	6.30898072	-0.44613762	115		Energy = -2617.19029291 a.u. #Cluster: 2		
54	C	3.55458281	7.12745644	0.61212149	116	O	3.91751048	-2.97997872	-3.97688241
55	C	3.66172562	6.15876224	-1.71373884	117	N	2.37406496	-2.26268273	-5.41842872
56	H	6.55409676	-0.91877605	-1.10230559	118	C	3.67065468	-2.45437681	-5.08368946
57	H	5.83415563	1.00232481	0.30784682	119	C	4.73185164	-2.09435058	-6.03667524
58	H	1.82065515	-0.62134241	0.47323764	120	C	5.98887120	-1.89868781	-5.63512280
59	H	-1.08320900	0.23119008	0.65461255	121	H	4.42856887	-1.99885595	-7.08339063
60	H	-2.06418185	1.51363991	-0.04110585	122	H	2.08939754	-1.79725735	-6.26746251
61	H	0.79016546	0.68897056	-0.87213338	123	H	1.62788871	-2.49552252	-4.77760033
62	H	1.74728696	0.68000355	3.12725237	124	H	6.79442337	-1.63546491	-6.31471105

1	H	6.31964887	-1.98245843	-4.60453911	63	H	1.92163218	-0.47804912	-0.00731794
2	O	2.11437968	-0.37102537	4.44479856	64	H	-1.34593939	0.45141057	0.92491383
3	N	4.05456532	-1.13740941	3.62754783	65	H	-2.22513536	1.73888095	0.12107656
4	C	2.87520849	-1.33267170	4.28109856	66	H	0.58505965	0.67714022	-0.61378720
5	C	2.56868375	-2.67316485	4.81378342	67	H	1.42861804	0.71474423	3.32521132
6	C	1.30332767	-3.04471327	5.01498902	68	H	-1.99336916	3.46279471	-1.26978815
7	H	3.41932637	-3.32313390	5.02272673	69	H	-1.13422457	4.09128430	-2.67853218
8	H	4.68914637	-1.88602038	3.40667305	70	H	-1.93550999	2.53030789	-2.75828520
9	H	4.27691881	-0.22729144	3.24726449	71	H	0.08779476	1.94830825	-3.74730817
10	H	1.02025274	-4.01740490	5.40053618	72	H	1.26406766	3.15540703	-3.25430015
11	H	0.45042199	-2.40665213	4.80041571	73	H	-2.17441439	0.56427609	-2.00910805
12	C	4.99101811	-1.21076316	-1.30265283	74	H	-0.67535335	0.04125165	-2.75656436
13	C	5.78289832	-0.33714631	-0.55761612	75	H	-0.29670047	-1.70243993	-1.06561143
14	C	5.18329270	0.49397087	0.38628965	76	H	-3.21129567	-3.35957799	0.50874340
15	C	3.80288326	0.45890932	0.56975048	77	H	-1.62550383	-3.66324890	-0.19128799
16	C	3.00307663	-0.42717992	-0.15595309	78	H	-3.66493794	0.01196466	-0.86939555
17	C	3.59655700	-1.26870533	-1.09048871	79	H	-4.41277803	-1.58672816	-0.82918637
18	C	3.16548606	1.38562530	1.52945309	80	H	-3.95935793	-0.78518391	0.67845619
19	C	1.90954288	2.01716454	1.11896735	81	H	-1.49598434	1.90952682	3.24486861
20	C	0.75286660	1.87629585	1.82299834	82	H	-1.08717482	3.62181047	3.09627338
21	C	-0.56351465	2.44036863	1.34153659	83	H	-2.98062859	4.01985357	1.54686114
22	C	-0.26572391	3.68570566	0.50884283	84	H	-5.61532066	1.92875583	0.93269523
23	C	0.69795175	3.45108699	-0.64404274	85	H	-5.31882550	3.63387885	1.28087076
24	C	1.98382348	2.82175526	-0.10248280	86	H	-6.04430796	2.59248151	2.51159290
25	C	-0.04669694	2.48456541	-1.64474722	87	H	-3.02707857	0.31978371	2.54854721
26	C	-1.19787406	1.41345092	0.38739769	88	H	-4.77268930	0.33925457	2.80978052
27	C	-0.38279838	1.16688345	-0.89367215	89	H	-3.69725151	1.06227614	4.00768086
28	O	0.60482556	1.19716245	2.93774071	90	H	-2.01005482	-1.75651138	2.21236930
29	C	-1.34237514	3.18105952	-2.10362992	91	H	-1.79916116	-3.49297155	2.42325363
30	C	0.78244054	2.21291689	-2.92242253	92	H	0.24754516	-1.45507561	1.47783867
31	C	-1.16938499	0.16651032	-1.77084340	93	H	2.55308162	-2.23602915	1.61150966
32	C	-1.23665009	-1.14616218	-1.06264981	94	H	2.54759724	-3.48350330	0.36312311
33	C	-2.30566160	-1.62329947	-0.41188077	95	H	2.86161176	-3.92116435	2.05121915
34	C	-2.21202582	-2.90529831	0.36586538	96	H	0.11024624	-5.14048378	2.80157375
35	C	-3.63940882	-0.96054266	-0.35976687	97	H	-0.48536190	-5.18278986	1.13898366
36	O	3.04455931	3.01954030	-0.64592499	98	H	1.18531833	-5.63141910	1.48767795
37	O	-0.78014607	4.74621226	0.74123930	99	H	2.55880079	1.31299888	-2.00648833
38	C	-1.49482741	2.75799035	2.52532406	100	H	1.41001251	0.12804182	-2.62534752
39	C	-2.88072574	3.06560979	2.06214899	101	H	1.98929993	0.66860475	-4.97132306
40	C	-3.93402908	2.25385713	2.23096947	102	H	5.42748594	0.75657227	-5.63479644
41	C	-5.28439705	2.62674222	1.71739346	103	H	4.77772127	2.34472613	-6.05527748
42	C	-3.85768490	0.93543067	2.92536778	104	H	3.95870117	0.88532371	-6.43562703
43	C	-1.55799246	-2.65230941	1.74167146	105	H	4.18814611	2.71886092	-2.62850798
44	C	-0.07983538	-2.48462671	1.60081154	106	H	5.62921295	2.46817896	-3.62942152
45	C	0.79275906	-3.50178769	1.59344587	107	H	5.04685771	1.17851192	-2.56784147
46	C	2.25519368	-3.27193412	1.40561492	108	H	3.13139935	-2.46788393	-2.59084160
47	C	0.38703017	-4.92840936	1.75783636	109	H	5.03729212	-2.38891089	-2.89350167
48	C	1.85932087	1.12047448	-2.84285507	110	H	1.65492833	4.61210054	-2.21420848
49	C	2.58507214	1.05708750	-4.14827513	111	H	0.15414462	5.33348179	-1.61063305
50	C	3.85482132	1.44157407	-4.33390536	112	H	1.30569776	5.91346187	0.57886398
51	C	4.50195570	1.34955098	-5.67721724	113	H	3.14045494	7.22881063	1.31527128
52	C	4.72385358	1.98086384	-3.24993551	114	H	4.07496597	7.95876156	0.00419991
53	O	2.76455261	-2.13022658	-1.71775655	115	H	4.67644327	6.50998126	0.81723332
54	O	5.64465161	-1.98929801	-2.19108016	116	H	3.36962884	6.25476561	-2.69513465
55	O	3.65744271	1.59368178	2.62277540	117	H	4.87428124	6.25473984	-1.77043697
56	C	1.07356722	4.80058373	-1.28499966	118	H	3.95172429	4.75655462	-1.95541168
57	C	1.83831332	5.66856576	-0.33838749	119				
58	C	3.07379432	6.13698284	-0.56380317	120		Energy = -2617.18523403 a.u. #Cluster: 3		
59	C	3.76450347	6.99896276	0.44151437	121	O	2.40036463	-0.41659912	4.14001992
60	C	3.85702047	5.84567396	-1.79890448	122	N	4.28094065	-1.14737801	3.16242426
61	H	6.85892641	-0.30993090	-0.72541452	123	C	3.16303787	-1.36352724	3.90920664
62	H	5.79768608	1.18296007	0.97014052	124	C	2.92525014	-2.70875469	4.46537431

1	C	1.68866467	-3.09982911	4.77753177	63	C	2.94840332	6.25850791	-0.71369674
2	H	3.80146879	-3.34512944	4.59727349	64	C	3.79276345	7.04714844	0.23268708
3	H	4.90438130	-1.88617552	2.88353632	65	C	3.53885067	6.04245363	-2.06616038
4	H	4.45314804	-0.23419598	2.76294642	66	H	6.54210113	-0.41092041	-1.39049376
5	H	1.45614454	-4.07667853	5.18611337	67	H	5.68050541	1.07238211	0.41257933
6	H	0.81070054	-2.47453910	4.64021703	68	H	1.66524196	-0.38640980	-0.28786135
7	O	7.46567975	3.86225909	0.94419220	69	H	-1.47481113	0.61521819	1.06014915
8	N	5.22680627	3.74566347	0.95806396	70	H	-2.36623159	1.97354463	0.39772203
9	C	6.42063384	3.76461981	0.29807294	71	H	0.31802087	0.84324023	-0.64427491
10	C	6.38205564	3.67583444	-1.17599201	72	H	1.58927881	0.66918250	3.13714689
11	C	7.45801886	3.31058609	-1.87242894	73	H	-2.21636153	3.73139330	-0.96411425
12	H	5.42440679	3.91315748	-1.64692954	74	H	-1.48056702	4.36706720	-2.43733579
13	H	4.35412238	3.62454586	0.46344241	75	H	-2.33599961	2.83264966	-2.47087043
14	H	5.17858055	3.75135898	1.96328460	76	H	-0.41581561	2.22230293	-3.66961438
15	H	7.46941794	3.22493203	-2.95325304	77	H	0.82309347	3.39663945	-3.25445916
16	H	8.41209587	3.06391257	-1.41874452	78	H	-2.56577904	0.85175584	-1.76352413
17	C	4.59384862	-1.22437788	-1.82976198	79	H	-1.16125826	0.32127052	-2.67583020
18	C	5.47986346	-0.40172883	-1.14610497	80	H	-0.66929283	-1.49524646	-1.09605983
19	C	4.98931146	0.43116046	-0.13930426	81	H	-3.43785886	-3.12832172	0.73303410
20	C	3.62856276	0.45182776	0.15439485	82	H	-1.93157562	-3.43888514	-0.13232498
21	C	2.73167394	-0.38120202	-0.52379764	83	H	-3.95671316	0.28492510	-0.51549082
22	C	3.21528711	-1.22300369	-1.51573958	84	H	-4.73290313	-1.29301306	-0.35501477
23	C	3.12728794	1.37145382	1.19853606	85	H	-4.06113199	-0.48974043	1.06771281
24	C	1.86079935	2.06683257	0.95418959	86	H	-1.26810066	1.96253045	3.45573086
25	C	0.78007522	1.91333594	1.77142346	87	H	-0.84591121	3.67125356	3.31623406
26	C	-0.55903488	2.54625109	1.47217393	88	H	-2.90086433	4.15282466	2.01387456
27	C	-0.31687181	3.82033787	0.66607340	89	H	-5.63122438	2.12788713	1.65338184
28	C	0.51153436	3.61603966	-0.59485554	90	H	-5.26212836	3.81520141	2.01983480
29	C	1.83389631	2.95718867	-0.20279218	91	H	-5.85762588	2.74292271	3.29316595
30	C	-0.35021943	2.70401576	-1.54941344	92	H	-2.87995662	0.43533519	2.93104261
31	C	-1.33475677	1.59217229	0.54781374	93	H	-4.59692423	0.45105599	3.34197694
32	C	-0.65602849	1.36946998	-0.81410987	94	H	-3.41792495	1.13436672	4.46347647
33	O	0.72919327	1.16360998	2.84622850	95	H	-2.04753280	-1.59623432	2.35693157
34	C	-1.66075921	3.44946110	-1.86437389	96	H	-1.85437503	-3.34136271	2.49979896
35	C	0.35427162	2.45417589	-2.90432374	97	H	0.13616806	-1.31466754	1.41828414
36	C	-1.55281650	0.42163267	-1.64242624	98	H	2.43003002	-2.13895134	1.32948137
37	C	-1.58461261	-0.91323932	-0.97363956	99	H	2.28999651	-3.35788508	0.05845702
38	C	-2.58931584	-1.38108695	-0.22126613	100	H	2.74254666	-3.83793105	1.70096393
39	C	-2.44770579	-2.68732705	0.50727138	101	H	0.10453093	-5.03949735	2.67599434
40	C	-3.88769130	-0.68353637	-0.00178953	102	H	-0.71927872	-5.01363895	1.11253544
41	O	2.85287736	3.21425291	-0.80606645	103	H	0.97400687	-5.50272936	1.20913935
42	O	-0.77049504	4.88209690	0.99643512	104	H	2.17922971	1.50488496	-2.15636246
43	C	-1.33601461	2.83512038	2.76900509	105	H	0.96069366	0.35404669	-2.70368618
44	C	-2.76050413	3.18060909	2.48436468	106	H	1.37856424	0.90055456	-5.07294896
45	C	-3.80248848	2.38129968	2.75314957	107	H	4.74295457	0.84455127	-5.94320993
46	C	-5.19645538	2.79290942	2.41570069	108	H	4.19866597	2.48032136	-6.33089289
47	C	-3.67213740	1.04106959	3.39561870	109	H	3.15037400	1.09608129	-6.66432151
48	C	-1.66119278	-2.48607680	1.82081592	110	H	3.75342593	2.94869876	-2.91852791
49	C	-0.19930624	-2.34101313	1.54669440	111	H	5.13983370	2.62113655	-3.97910922
50	C	0.64946046	-3.37244601	1.43899117	112	H	4.56763139	1.38461746	-2.85024632
51	C	2.09359264	-3.16334175	1.12596761	113	H	2.73549636	-2.50972863	-2.90515300
52	C	0.23629514	-4.79602128	1.61062298	114	H	5.92122831	-1.96381001	-3.07775782
53	C	1.41163076	1.34248715	-2.93785694	115	H	1.28833461	4.83282773	-2.22360363
54	C	2.03607922	1.27998053	-4.29444006	116	H	-0.09628354	5.55875236	-1.39204021
55	C	3.29873547	1.63735539	-4.56438222	117	H	1.36028693	5.97735658	0.65788784
56	C	3.86485198	1.50803734	-5.94030235	118	H	3.28126693	7.27963172	1.17623801
57	C	4.23816481	2.17739195	-3.54107850	119	H	4.11085449	8.00264318	-0.20781106
58	O	2.31720054	-2.02286369	-2.13931429	120	H	4.70853970	6.49396838	0.49310376
59	O	4.96351588	-2.08015767	-2.80959663	121	H	2.99375678	6.60519400	-2.83746297
60	O	3.74781138	1.53957455	2.23112683	122	H	4.59068905	6.34900771	-2.12946642
61	C	0.84112218	4.98742178	-1.21739709	123	H	3.49229496	4.97846713	-2.35477430
62	C	1.75046802	5.78685813	-0.34052946	124				

1 Energy = -2617.18418481 a.u. #Cluster: 4

2	O	3.11593190	-3.05596938	-2.67544990	63	O	5.55818894	-1.98990280	-2.45106232
3	N	3.13879355	-1.42133714	-4.20554250	64	O	7.31072703	-0.01828915	-2.67384892
4	C	2.46461428	-2.32887881	-3.44017846	65	O	3.14117992	-0.42177614	1.99016837
5	C	1.00013578	-2.41131990	-3.57559277	66	C	1.49850862	4.57055351	-0.78965637
6	C	0.30197415	-3.34631713	-2.92902414	67	C	2.47370388	5.05022855	0.23650628
7	H	0.52788647	-1.67784278	-4.23261472	68	C	3.79090763	5.20210434	0.03814178
8	H	2.67480348	-0.74789402	-4.79647912	69	C	4.68047828	5.65668403	1.14945354
9	H	4.13556609	-1.30356069	-4.10094209	70	C	4.48692986	4.92536074	-1.24932010
10	H	-0.77540035	-3.44462005	-3.00486873	71	H	6.95338421	2.06752816	-1.01867386
11	H	0.75133913	-4.08875863	-2.27467961	72	H	5.07981692	2.23278770	0.60958293
12	O	-2.17857077	8.65135465	1.27760941	73	H	3.63158303	-1.63985611	-0.64731810
13	N	-0.65089163	7.13685243	0.64569714	74	H	-1.55105694	0.37085077	0.86795001
14	C	-1.63009416	7.56911982	1.49301355	75	H	-2.22457490	1.95625256	0.52312742
15	C	-1.96385067	6.70924807	2.64863139	76	H	0.15556002	0.59983034	-0.91080539
16	C	-3.17737033	6.73623353	3.19831658	77	H	1.71406644	-0.28322186	2.74376582
17	H	-1.16224901	6.05856618	3.01038043	78	H	-1.80943437	3.88575414	-0.49527799
18	H	-0.21506557	6.23267304	0.76559228	79	H	-1.02256119	4.67139054	-1.87011469
19	H	-0.39544560	7.66372231	-0.17293420	80	H	-2.15511530	3.35272051	-2.13298887
20	H	-3.46072407	6.12408647	4.04734953	81	H	-0.43873823	2.73780621	-3.57598411
21	H	-3.98419222	7.37049982	2.84595484	82	H	1.07859252	3.42874720	-3.02339287
22	C	6.33397356	0.13564682	-1.74991776	83	H	-2.75917802	1.29286354	-1.68521080
23	C	6.23052494	1.25635227	-0.93200826	84	H	-1.55954133	0.82565381	-2.87355911
24	C	5.18141728	1.34316511	-0.01498497	85	H	-1.15020590	-1.35117111	-1.75769320
25	C	4.25735165	0.30790916	0.07901824	86	H	-4.02017506	-3.10218067	-0.31867067
26	C	4.35923425	-0.82960730	-0.72572388	87	H	-2.47099417	-3.30649224	-1.13306616
27	C	5.39754003	-0.91548942	-1.64379371	88	H	-4.04094475	0.60282645	-0.26361363
28	C	3.12845729	0.36169956	1.03386200	89	H	-5.05604049	-0.64873785	-0.98936807
29	C	2.00466554	1.24895464	0.84028766	90	H	-4.53970885	-0.79364010	0.69361661
30	C	0.91129347	1.16037167	1.68025078	91	H	-1.14822357	1.23687964	3.39540301
31	C	-0.30812366	2.02964737	1.54229224	92	H	-0.32288180	2.78941799	3.58554714
32	C	0.14589432	3.35732388	0.93881600	93	H	-2.18469858	4.01734140	2.54613735
33	C	0.87473220	3.22045582	-0.38337566	94	H	-5.31670284	2.85161419	1.80637629
34	C	2.03428435	2.22702982	-0.24642585	95	H	-4.54555459	4.26795651	2.52816246
35	C	-0.19477746	2.68818277	-1.41412083	96	H	-5.41452501	3.11563554	3.55039774
36	C	-1.26776691	1.38983068	0.52620962	97	H	-3.23105673	0.30204430	2.40356825
37	C	-0.70760634	1.31327414	-0.90381162	98	H	-4.78249651	0.66191355	3.16168976
38	O	0.82611759	0.29650290	2.65993667	99	H	-3.30865276	0.65872780	4.13371637
39	C	-1.35112523	3.70332523	-1.47271924	100	H	-2.78520035	-2.21919523	1.74822029
40	C	0.38311568	2.58303142	-2.84535739	101	H	-2.45551855	-3.90660411	1.35571302
41	C	-1.81910650	0.71966234	-1.79993061	102	H	-0.59436005	-1.50602859	1.07808165
42	C	-1.98631729	-0.72094739	-1.44862078	103	H	1.72210222	-2.00694270	0.81312092
43	C	-3.00892350	-1.24269117	-0.75889819	104	H	1.90447116	-3.11826364	-0.55661995
44	C	-2.99189174	-2.69381702	-0.37038950	105	H	2.19026780	-3.68785604	1.09464874
45	C	-4.20758727	-0.48203671	-0.30758068	106	H	-0.52792780	-5.39509487	1.21462730
46	O	2.95355426	2.28190833	-1.02646357	107	H	-0.95954296	-5.00107626	-0.44975964
47	O	-0.09181930	4.40650034	1.47507086	108	H	0.70775120	-5.42929698	-0.04907333
48	C	-0.99928360	2.22382868	2.90555562	109	H	1.90561395	1.04413175	-2.49030767
49	C	-2.29338978	2.95376385	2.76101473	110	H	0.40369227	0.41768926	-3.17273987
50	C	-3.50476789	2.38971970	2.86460086	111	H	0.94352563	1.19403678	-5.39398259
51	C	-4.74554203	3.19874839	2.68139129	112	H	4.27607734	1.24967081	-6.45751944
52	C	-3.72057637	0.94231010	3.15279098	113	H	3.71073971	2.92068198	-6.51930893
53	C	-2.29531940	-2.86973698	0.99555956	114	H	2.64094154	1.60928759	-7.02575974
54	C	-0.83945808	-2.55069138	0.89626371	115	H	3.58792944	3.00129124	-3.24027183
55	C	0.11174127	-3.44077378	0.58258549	116	H	4.90778229	2.35155662	-4.23012354
56	C	1.54535225	-3.03887186	0.48393607	117	H	4.03512420	1.31680069	-3.08712101
57	C	-0.17275342	-4.87948073	0.30950161	118	H	4.70402557	-2.55530402	-2.47231749
58	C	1.10353361	1.27680383	-3.21772005	119	H	7.88923587	0.79483281	-2.74553244
59	C	1.65641569	1.40893050	-4.60106455	120	H	1.99078339	4.45615120	-1.78258448
60	C	2.91429044	1.78483194	-4.87620908	121	H	0.70461684	5.32843541	-0.94776737
61	C	3.39916567	1.89190782	-6.28390362	122	H	2.03430059	5.27840616	1.20691508
62	C	3.91409502	2.12531696	-3.82740411	123	H	4.14147977	5.83476648	2.08941494
					124	H	5.20129024	6.59030408	0.89301237

1	H	5.45753090	4.90601145	1.36207360	63	C	1.57006259	1.08090352	-3.32281412
2	H	3.94188181	5.32492691	-2.11524811	64	C	2.23559395	1.14132687	-4.66163688
3	H	5.50164822	5.34079326	-1.28722481	65	C	3.45170396	1.66501988	-4.87127565
4	H	4.58104327	3.83458689	-1.40885861	66	C	4.01582941	1.77980945	-6.24934186
5					67	C	4.31090056	2.19604118	-3.77820923
6	Energy = -2617.18369056 a.u. #Cluster: 5								
7	O	6.91860257	-1.50416804	-5.06324194	68	O	5.06427146	-2.21819031	-2.51897606
8	N	4.69975731	-1.41149749	-5.37675073	69	O	7.18898754	-0.50332656	-2.59373189
9	C	5.97786479	-1.23101766	-5.81798405	70	O	3.00910899	-0.25751379	2.06873208
10	C	6.18451212	-0.76830121	-7.20379053	71	C	1.51595748	4.57029020	-1.07505571
11	C	7.31298227	-0.14921306	-7.55275918	72	C	2.39214203	5.10439141	0.01237677
12	H	5.37387033	-0.96519014	-7.90790414	73	C	3.71289794	5.31046318	-0.08630886
13	H	3.89707063	-1.09274628	-5.89320719	74	C	4.49354145	5.82325318	1.08056834
14	H	4.53040379	-1.70722969	-4.42871686	75	C	4.51886578	5.03849592	-1.30950112
15	H	7.51105228	0.20767860	-8.55758078	76	H	7.10629880	1.47173162	-0.95200058
16	H	8.12681930	0.05235500	-6.86233399	77	H	5.26945338	1.91005719	0.67885981
17	O	2.74951002	-3.25596679	-3.29836681	78	H	3.14504707	-1.56503541	-0.75408806
18	N	1.37326810	-3.45768336	-1.54230202	79	H	-1.55651119	0.33902942	0.44456526
19	C	1.59377643	-3.21092892	-2.86518955	80	H	-2.23185545	1.87894268	-0.06481873
20	C	0.44172442	-2.092129631	-3.73150379	81	H	0.32438814	0.52188703	-1.14426922
21	C	0.56757137	-2.06211551	-4.76013907	82	H	1.49604638	-0.07394513	2.72217490
22	H	-0.49365663	-3.41144366	-3.49484824	83	H	-1.75459087	3.76083238	-1.19360087
23	H	0.45668001	-3.44000565	-1.12314331	84	H	-0.80038106	4.49645189	-2.48515020
24	H	2.11916690	-3.77263343	-0.94002467	85	H	-1.85108864	3.12976209	-2.83123322
25	H	-0.24944591	-1.81319066	-5.42927586	86	H	0.05287817	2.46510889	-3.97213008
26	H	1.49444356	-1.55760245	-5.01544698	87	H	1.46557692	3.23979899	-3.27057834
27	C	6.15563811	-0.28734784	-1.75397084	88	H	-2.50479449	1.10101942	-2.25751264
28	C	6.24597994	0.80530396	-0.89538281	89	H	-1.17315305	0.65248693	-3.30390805
29	C	5.21786765	1.04262579	0.01833726	90	H	-0.81352963	-1.47889508	-2.12061375
30	C	4.11901894	0.19178009	0.06340359	91	H	-3.73485641	-3.33420672	-1.04675003
31	C	4.01134852	-0.90910620	-0.79080236	92	H	-2.05517709	-3.46178921	-1.54731667
32	C	5.04019295	-1.15006258	-1.68966182	93	H	-3.88124749	0.38466067	-0.88006227
33	C	3.01911608	0.40927169	1.03116264	94	H	-4.76971783	-0.84947575	-1.78053980
34	C	1.93034596	1.31029231	0.73093747	95	H	-4.48095496	-1.05359230	-0.05069803
35	C	0.77282094	1.26246580	1.47993690	96	H	-1.42890880	1.35181792	2.97638405
36	C	-0.45142449	2.07521378	1.16215429	97	H	-0.73944157	2.97262290	3.12711932
37	C	0.01801672	3.38728334	0.53334744	98	H	-2.57124947	3.97135228	1.81545033
38	C	0.91079809	3.20728539	-0.68097704	99	H	-5.53336179	2.45615179	0.88125417
39	C	2.07970125	2.27133769	-0.36172438	100	H	-4.93084224	3.99912785	1.49476630
40	C	0.00226076	2.57009050	-1.80072748	101	H	-5.79418007	2.89398216	2.57210816
41	C	-1.26597297	1.34723900	0.07944887	102	H	-3.34339642	0.17479330	1.80133337
42	C	-0.54480542	1.21540896	-1.27228092	103	H	-4.95206946	0.46215534	2.46339048
43	O	0.62195444	0.47987729	2.52115931	104	H	-3.53355491	0.62229308	3.50132483
44	C	-1.15871887	3.53990820	-2.08534655	105	H	-2.97207319	-2.40039574	1.21592521
45	C	0.77239528	2.38433446	-3.13039199	106	H	-2.49859080	-4.06731201	0.89263637
46	C	-1.53838650	0.56107571	-2.25981212	107	H	-0.62660587	-1.66409243	0.33809378
47	C	-1.69289584	-0.87624724	-1.89452654	108	H	1.56746757	-2.51522009	2.71613924
48	C	-2.76155686	-1.42596271	-1.30338690	109	H	1.64489604	-1.98151532	1.03331031
49	C	-2.73645479	-2.87306208	-0.90244935	110	H	2.14297591	-3.62628978	1.47700195
50	C	-4.02219223	-0.69982556	-0.98567556	111	H	-1.15801945	-4.54773712	2.83644795
51	O	3.10239914	2.35489293	-0.99670847	112	H	-0.57680983	-5.40090280	1.40365710
52	O	-0.33236213	4.45446284	0.95823556	113	H	0.53492583	-5.03253972	2.72542935
53	C	-1.29750952	2.31076837	2.42761164	114	H	2.31556232	0.94273493	-2.51514505
54	C	-2.61998963	2.92060317	2.09817679	115	H	0.90294959	0.19857451	-3.26809184
55	C	-3.78630560	2.25957984	2.11842445	116	H	1.63226037	0.76603609	-5.48403845
56	C	-5.06287056	2.93947825	1.75140528	117	H	5.05053724	1.41355242	-6.30398007
57	C	-3.91372503	0.81957616	2.48690910	118	H	4.04000739	2.83270995	-6.57108508
58	C	-2.31250187	-3.02178283	0.57214598	119	H	3.43261256	1.23469593	-7.00300769
59	C	-0.89145359	-2.62192664	0.78683609	120	H	3.81135402	3.02194731	-3.24342443
60	C	0.00367755	-3.32937667	1.49033345	121	H	5.28087541	2.56623878	-4.12748779
61	C	1.40095380	-2.83738115	1.67436112	122	H	4.50740320	1.43336017	-3.00521171
62	C	-0.30690791	-4.63217082	2.14432443	123	H	4.15720811	-2.66577668	-2.61203525
					124	H	6.91323099	-0.97541835	-3.44974655



1	H	2.07878443	4.45892048	-2.02761554	63	C	-2.43416455	-2.99894187	0.57712143
2	H	0.70292206	5.29684464	-1.28795719	64	C	-1.10511386	-2.54853142	1.09008476
3	H	1.86501250	5.32909803	0.93860182	65	C	0.04562046	-3.21539719	0.92538033
4	H	3.87645450	5.99248608	1.97263031	66	C	1.32308244	-2.70048612	1.50554569
5	H	4.99068931	6.77519248	0.84670916	67	C	0.17157266	-4.49862638	0.17834511
6	H	5.2858809	5.11054691	1.36715727	68	C	1.56329230	1.83875871	-3.24428974
7	H	4.02353429	5.38983731	-2.22443962	69	C	2.03386363	2.08249898	-4.64227840
8	H	5.51231564	5.50232822	-1.28073512	70	C	3.24790453	2.53471041	-4.98182586
9	H	4.67363040	3.94918511	-1.42813481	71	C	3.62322304	2.71853809	-6.41739574
10					72	C	4.32472748	2.87232338	-4.01085982
11	Energy = -2617.18309061 a.u. #Cluster: 6								
12	O	7.40029491	-2.88026930	-3.74922401	73	O	3.99822477	-2.38077442	-2.68262921
13	N	5.66200883	-4.12897515	-4.40351280	74	O	5.89993073	-0.67114289	-3.69178117
14	C	7.00126952	-3.89394818	-4.34324099	75	O	3.33679153	0.04881160	2.04482604
15	C	7.92479940	-4.86923020	-4.94964162	76	C	1.26334563	4.91007180	-0.67119716
16	C	9.23429703	-4.62224373	-5.01357005	77	C	2.15637772	5.44634229	0.40070267
17	H	7.47925199	-5.78794639	-5.33730994	78	C	3.42398323	5.83913154	0.21111345
18	H	5.26098736	-4.87917311	-4.94579367	79	C	4.24415712	6.35773843	1.34683103
19	H	5.01031486	-3.47449387	-3.99973019	80	C	4.12105742	5.78934237	-1.10597032
20	H	9.94994071	-5.31018436	-5.45070124	81	H	6.52649641	1.33529227	-2.15324472
21	H	9.69409073	-3.71408357	-4.63490225	82	H	5.26963383	1.98689831	-0.09502405
22	O	1.79646184	-2.14894714	-4.04077772	83	H	2.71445722	-1.47426056	-0.55919685
23	N	3.12405603	-0.79652439	-5.25336662	84	H	-1.22627871	0.24716041	0.59251872
24	C	1.89336887	-1.29130150	-4.93226781	85	H	-2.15766423	1.69071004	0.22045367
25	C	0.71697450	-0.81591284	-5.68295273	86	H	0.52122156	0.81861032	-1.04362274
26	C	-0.51120732	-0.96931656	-5.18529913	87	H	1.83309623	0.16512036	2.90327929
27	H	0.90991559	-0.34418898	-6.64767437	88	H	-1.96609542	3.71521952	-0.63403753
28	H	3.24271550	-0.02890758	-5.89558011	89	H	-1.19621875	4.73236917	-1.85416456
29	H	3.94478219	-1.04685389	-4.72067458	90	H	-2.08689244	3.29284021	-2.33325545
30	H	-1.40753831	-0.63492343	-5.69516997	91	H	-0.26133133	2.90887352	-3.64996208
31	H	-0.71526789	-1.44172631	-4.22716146	92	H	1.02612670	3.91789491	-3.01329781
32	C	5.31676903	-0.41338443	-2.49637064	93	H	-2.36112319	1.18671771	-2.10805806
33	C	5.69928150	0.72457937	-1.79264624	94	H	-0.97963742	0.81597111	-3.12405214
34	C	4.99554576	1.08007971	-0.64022188	95	H	-0.53167975	-1.30561821	-1.85983721
35	C	3.93102309	0.29604089	-0.20922438	96	H	-3.46847772	-3.32178788	-1.31494765
36	C	3.55255124	-0.86284235	-0.89323315	97	H	-1.71058869	-3.33806476	-1.44915879
37	C	4.26247134	-1.22264193	-2.03029899	98	H	-3.79229768	0.21139178	-0.47121920
38	C	3.13200038	0.64294775	0.98882140	99	H	-4.28184011	-0.30623897	-2.08942423
39	C	2.01252717	1.55694822	0.86518662	100	H	-4.65224872	-1.31196850	-0.68542485
40	C	0.92135860	1.40297058	1.68726945	101	H	-1.29918311	1.13231553	3.16950628
41	C	-0.39282811	2.08279296	1.42615779	102	H	-0.77021403	2.79485969	3.45101261
42	C	-0.05974922	3.47880332	0.89588524	103	H	-2.68195100	3.71490564	2.20179919
43	C	0.79926107	3.47571295	-0.35768022	104	H	-5.46543678	2.01922136	1.08481812
44	C	2.05472343	2.62229874	-0.13782587	105	H	-5.03064606	3.54888356	1.85239287
45	C	-0.11143839	2.85705011	-1.48516365	106	H	-5.80059362	2.27113393	2.80049490
46	C	-1.11506443	1.31489119	0.30280408	107	H	-3.10669114	-0.12747635	1.86323894
47	C	-0.43811400	1.39520276	-1.07667012	108	H	-4.72916478	-0.03803330	2.54667301
48	O	0.90576813	0.61164070	2.73803049	109	H	-3.32407111	0.16510191	3.59484700
49	C	-1.40387041	3.69306339	-1.57308305	110	H	-3.25413796	-2.44520836	1.07784506
50	C	0.54305122	2.92787341	-2.88327872	111	H	-2.60790673	-4.06611687	0.83035955
51	C	-1.36865083	0.69636976	-2.09133048	112	H	-1.12823587	-1.60334251	1.62899088
52	C	-1.46619822	-0.75372930	-1.75101805	113	H	1.31106040	-1.61452935	1.66000349
53	C	-2.57543733	-1.36031378	-1.30835744	114	H	2.18915179	-2.93692776	0.87077464
54	C	-2.55245278	-2.81657210	-0.94928625	115	H	1.51880400	-3.16341723	2.48583336
55	C	-3.88337065	-0.66569549	-1.12885559	116	H	-0.77177168	-5.05926906	0.12901242
56	O	3.06586318	2.86406330	-0.75059565	117	H	0.48458296	-4.31208150	-0.86175836
57	O	-0.46782625	4.47469305	1.42851533	118	H	0.92103838	-5.16790287	0.62311269
58	C	-1.25960690	2.13870919	2.69699404	119	H	2.40888125	1.82442873	-2.52993179
59	C	-2.63244454	2.64481404	2.39883771	120	H	1.11015601	0.82817280	-3.17658975
60	C	-3.73099184	1.87787180	2.34676394	121	H	1.28402872	1.86717585	-5.40274475
61	C	-5.06159082	2.46220012	2.00830772	122	H	4.54869090	2.17695801	-6.66405390
62	C	-3.72657734	0.40755340	2.59910473	123	H	3.80708712	3.77820312	-6.64796817
					124	H	2.85078633	2.37222587	-7.11589918

1	H	3.94097460	3.03877118	-2.98971498	63	C	-1.31632804	2.53007651	2.34473500
2	H	4.87314234	3.77791681	-4.29910797	64	C	-2.69748806	2.84512150	1.87335662
3	H	5.05876810	2.05325971	-3.94314890	65	C	-3.73140822	1.99311596	1.92419281
4	H	3.06349920	-2.35398238	-3.12616573	66	C	-5.07605162	2.38443022	1.40929457
5	H	6.38782008	-1.56582468	-3.69429434	67	C	-3.63809714	0.61069666	2.47787267
6	H	1.77670628	4.91746697	-1.65846607	68	C	-1.61811097	-3.61092380	0.98904513
7	H	0.38142162	5.57618973	-0.78602209	69	C	-0.80639650	-2.64034929	1.78371389
8	H	1.69341056	5.50741273	1.38373812	70	C	0.51066264	-2.74294266	2.00867669
9	H	3.69349639	6.39570026	2.29587994	71	C	1.21777281	-1.75942082	2.88352843
10	H	4.61299129	7.37376895	1.14635590	72	C	1.37500890	-3.81204133	1.43518554
11	H	5.12844173	5.72339899	1.51363315	73	C	1.91231358	1.21489374	-3.22991737
12	H	3.60535974	6.39397952	-1.86468618	74	C	2.51860835	1.24188510	-4.59563917
13	H	5.15730226	6.14457720	-1.05827566	75	C	3.76032501	1.65751451	-4.87776891
14	H	4.15314359	4.75297269	-1.48973720	76	C	4.28753823	1.61405104	-6.27467658
15					77	C	4.71666701	2.17516232	-3.85993131
16	Energy = -2617.18285680 a.u. #Cluster: 7								
17	O	1.72360968	-3.10070621	-4.02797081	78	O	2.83834745	-2.92533733	-1.60261525
18	N	3.16453647	-1.75777153	-5.08954057	79	O	5.15926398	-2.34234706	-2.92609865
19	C	1.89672031	-2.21049224	-4.86940742	80	O	3.56671879	0.80395653	2.29795198
20	C	0.8793407	-1.64976281	-5.66326734	81	C	1.19139776	4.73616480	-1.42619027
21	C	-0.44666048	-1.61619723	-5.15964983	82	C	1.99703673	5.56410917	-0.47830353
22	H	1.03777825	-1.27505048	-6.65658989	83	C	3.19527305	6.09343667	-0.76272527
23	H	3.36410083	-0.96855688	-5.68216145	84	C	3.92125763	6.93415502	0.23534389
24	H	3.92662950	-2.07009941	-4.50515655	85	C	3.89646309	5.90212106	-2.06510443
25	H	-1.29856422	-1.21045529	-5.69379296	86	H	6.47595637	-0.18947695	-2.00501407
26	H	-0.70051689	-1.99117369	-4.17038471	87	H	5.60443420	1.29019796	-0.20444927
27	O	7.49138440	4.13426124	1.13303799	88	H	2.05211794	-1.16696197	0.09719127
28	N	5.28283777	3.75347474	1.11335926	89	H	-0.95041724	0.22621018	0.71480895
29	C	6.48906386	3.84219619	0.47888425	90	H	-1.99765346	1.44921797	0.00453203
30	C	6.51780887	3.56002846	-0.97062558	91	H	0.82220178	0.61166925	-0.93135365
31	C	7.66307852	3.29980327	-1.60116156	92	H	1.93531108	1.04341504	3.16069307
32	H	5.55188401	3.57953227	-1.48462283	93	H	-1.91957971	3.27420457	-1.27988025
33	H	4.43583534	3.55891178	0.60260522	94	H	-1.16044801	4.07107182	-2.66033517
34	H	5.18643346	3.96881218	2.09257779	95	H	-1.89118943	2.48055414	-2.84543108
35	H	7.72458481	3.08920697	-2.66333776	96	H	0.05922371	2.03277631	-3.96900550
36	H	8.62890085	3.27364174	-1.10708150	97	H	1.22515029	3.24748595	-3.48358312
37	C	4.76105704	-1.49589460	-1.94635917	98	H	-2.05074241	0.37370912	-2.03041680
38	C	5.50976762	-0.39656092	-1.54326385	99	H	-0.65699179	0.16748659	-3.07341924
39	C	5.01654508	0.43112658	-0.53178366	100	H	0.26074227	-1.65379246	-1.60419592
40	C	3.78496249	0.15880301	0.04629374	101	H	-1.99929202	-4.21451453	-1.06916225
41	C	3.02197669	-0.94423928	-0.35483368	102	H	-0.33194833	-3.71980936	-0.75917718
42	C	3.51950535	-1.78673006	-1.33840792	103	H	-3.26761733	-0.88120362	-0.12138541
43	C	3.21820776	0.98089680	1.14061266	104	H	-3.54937143	-1.26868181	-1.82351741
44	C	2.09246083	1.84949585	0.82288785	105	H	-3.81143294	-2.49547083	-0.58259555
45	C	0.98658629	1.81784437	1.63448427	106	H	-1.31483872	1.64726404	3.02152961
46	C	-0.36131772	2.28283158	1.16441521	107	H	-0.92923599	3.36958358	2.96533665
47	C	-0.10707301	3.55593538	0.35358542	108	H	-2.81081942	3.84519168	1.45686555
48	C	0.83298696	3.36376894	-0.82903505	109	H	-5.36557783	1.76250223	0.54787566
49	C	2.13134570	2.70211138	-0.35984676	110	H	-5.12472664	3.42988253	1.07640100
50	C	0.05200999	2.43616811	-1.83240576	111	H	-5.85674867	2.25195428	2.17281864
51	C	-0.93002272	1.21460686	0.20675154	112	H	-2.80757551	0.04366366	2.03340384
52	C	-0.17976631	1.07200854	-1.12983339	113	H	-4.55004550	0.02162998	2.30924463
53	O	0.99131998	1.32337665	2.85507531	114	H	-3.46759596	0.62634834	3.56631273
54	C	-1.29667401	3.10284122	-2.16388128	115	H	-2.69683046	-3.48162216	1.21268083
55	C	0.79918188	2.27039455	-3.17499405	116	H	-1.38059938	-4.65318198	1.29183985
56	C	-0.97996934	0.09187363	-2.01398762	117	H	-1.37894005	-1.81093824	2.19328817
57	C	-0.76916699	-1.30140013	-1.52431025	118	H	0.55965445	-0.95243364	3.23336236
58	C	-1.72485751	-2.08552072	-1.00897622	119	H	2.07558439	-1.30258279	2.37132014
59	C	-1.38749176	-3.46517059	-0.52642469	120	H	1.61684173	-2.25215085	3.78433340
60	C	-3.15164299	-1.66970533	-0.87989408	121	H	0.83884507	-4.76167691	1.30081225
61	O	3.18069306	2.93850293	-0.91648854	122	H	1.74561388	-3.51540981	0.43743786
62	O	-0.61917808	4.60430355	0.63375540	123	H	2.25715126	-4.02055958	2.05448474
					124	H	2.67201204	1.38955670	-2.44384094

1	H	1.50922518	0.20156280	-3.02426995	63	C	-2.73056456	-1.05995340	0.04189682
2	H	1.84687596	0.90121078	-5.38286753	64	C	-2.67009154	-2.42557052	0.66543721
3	H	5.20442020	1.00828850	-6.33714776	65	C	-3.96077326	-0.28254519	0.36147793
4	H	4.55134422	2.62001918	-6.63411834	66	O	3.02753417	3.08891495	-0.42297816
5	H	3.57437566	1.19898419	-6.99841640	67	O	-0.41640501	4.94167830	1.61615276
6	H	4.19832503	2.67907726	-3.02624276	68	C	-1.08605373	2.84346369	3.26590230
7	H	5.42905876	2.89528434	-4.28247885	69	C	-2.48032868	3.32356757	3.03209286
8	H	5.30617122	1.35472819	-3.42214802	70	C	-3.58419329	2.60267404	3.27234136
9	H	2.53063528	-2.97405594	-2.56660662	71	C	-4.94073042	3.15582424	2.98745858
10	H	6.06677121	-2.11020970	-3.28465342	72	C	-3.56314221	1.21889770	3.82906422
11	H	1.73441997	4.58531803	-2.38575267	73	C	-1.77321446	-2.40312944	1.92222644
12	H	0.62244782	5.28522308	-1.69557094	74	C	-0.32781134	-2.37472386	1.54337327
13	H	1.52399917	5.73478993	0.48736974	75	C	0.40121810	-3.46729232	1.27695033
14	H	3.34252746	7.11179676	1.15191260	76	C	1.83375941	-3.36673176	0.87075102
15	H	4.17963341	7.91877295	-0.18071780	77	C	-0.14047088	-4.85524644	1.35596769
16	H	4.86567069	6.45880789	0.54060707	78	C	1.37440181	1.53357812	-2.62055692
17	H	3.40626769	6.46705389	-2.87126992	79	C	1.98202198	1.54598963	-3.98624748
18	H	4.94493870	6.22581844	-2.03896644	80	C	3.22112675	1.97996101	-4.25465829
19	H	3.89240068	4.84212508	-2.37052499	81	C	3.77809268	1.93074863	-5.63949345
20					82	C	4.13567791	2.53790351	-3.21910945
21	Energy = -2617.17782765 a.u. #Cluster: 8				83	O	2.36862682	-1.91864591	-2.13231713
22	O	2.29414297	-0.89169157	4.28575594	84	O	4.97193827	-1.78434031	-2.94215276
23	N	4.04054547	-1.72947613	3.15802018	85	O	3.80381073	1.10300605	2.55708696
24	C	2.92651947	-1.89178575	3.92461791	86	C	1.18985518	5.06552063	-0.64326356
25	C	2.53943640	-3.25296823	4.34093745	87	C	2.04213131	5.82181482	0.32365476
26	C	1.26109905	-3.54533296	4.58438767	88	C	3.28855189	6.24591030	0.07088029
27	H	3.34521786	-3.98272348	4.43067648	89	C	4.06367855	7.00192907	1.09950790
28	H	4.56174018	-2.50114305	2.77722801	90	C	4.00255498	6.00845234	-1.21561474
29	H	4.31472190	-0.80457636	2.85464664	91	H	6.55019904	-0.16727747	-1.46546083
30	H	0.92101137	-4.52789621	4.89117570	92	H	5.73234241	1.09628200	0.51935504
31	H	0.45289514	-2.82574280	4.48555074	93	H	1.75176058	-0.48994443	-0.09981642
32	O	-3.05021013	8.78762645	0.82530223	94	H	-1.40927841	0.74285712	1.42735213
33	N	-1.27164401	7.47242119	0.45965492	95	H	-2.22754160	2.19842515	0.88912184
34	C	-2.37142529	7.82510452	1.18759208	96	H	0.33252518	0.95910070	-0.32470264
35	C	-2.67449087	7.03264587	2.39857284	97	H	1.65772073	0.41405038	3.40538282
36	C	-3.91835851	6.94433728	2.86819700	98	H	-1.98383686	4.03859484	-0.34101092
37	H	-1.82437412	6.53080500	2.87063600	99	H	-1.24730235	4.73291455	-1.79079229
38	H	-0.72133265	6.65887107	0.70095391	100	H	-2.21544203	3.27336956	-1.90526299
39	H	-1.02692014	7.95705935	-0.38777232	101	H	-0.39135244	2.61610258	-3.21732698
40	H	-4.18260183	6.37801274	3.75423103	102	H	0.95473039	3.64857197	-2.76528907
41	H	-4.77206058	7.43002532	2.40700914	103	H	-2.57638233	1.27543073	-1.33176157
42	C	4.62053129	-1.04169374	-1.86594410	104	H	-1.24983734	0.70819663	-2.33394346
43	C	5.50699542	-0.24091777	-1.15855981	105	H	-0.85694672	-1.25735857	-0.91397881
44	C	5.04229426	0.46679851	-0.04743675	106	H	-3.68051884	-2.78579312	0.93946345
45	C	3.70495530	0.37972798	0.32446869	107	H	-2.28136053	-3.17203105	-0.05603147
46	C	2.80245299	-0.42084623	-0.38551799	108	H	-3.96936470	0.72405905	-0.07822845
47	C	3.26383726	-1.13866647	-1.48031322	109	H	-4.86339481	-0.79683337	-0.00117661
48	C	3.21993624	1.15295283	1.48996647	110	H	-4.08225321	-0.15616230	1.44797725
49	C	2.00444631	1.94735503	1.32414735	111	H	-1.08022045	1.92532871	3.89273064
50	C	0.93710092	1.83096978	2.16421034	112	H	-0.52107222	3.60071607	3.85489161
51	C	-0.35554027	2.57838052	1.93692637	113	H	-2.54338506	4.33338771	2.62587866
52	C	-0.03616680	3.87819340	1.20340874	114	H	-5.44427162	2.57878137	2.19646049
53	C	0.74625939	3.69937368	-0.08591805	115	H	-4.92001928	4.20213932	2.65387780
54	C	2.01782805	2.90016260	0.21372634	116	H	-5.59034003	3.11108435	3.87358844
55	C	-0.21758313	2.92756876	-1.07082235	117	H	-2.83707267	0.57566066	3.31007444
56	C	-1.21954002	1.74146573	0.97711881	118	H	-4.53794149	0.71744165	3.76141100
57	C	-0.60137975	1.56908538	-0.42067449	119	H	-3.28233488	1.22221920	4.89413834
58	O	0.85416061	1.02996186	3.19989079	120	H	-2.02918809	-1.52588738	2.54957015
59	C	-1.47702321	3.79053524	-1.27904941	121	H	-2.00042536	-3.28706157	2.55223439
60	C	0.41892522	2.72516390	-2.46620684	122	H	0.10107657	-1.37768897	1.47766980
61	C	-1.59807792	0.75925551	-1.28149321	123	H	2.29992132	-2.42299811	1.18031343
62	C	-1.71681154	-0.61593561	-0.71281296	124	H	1.93151519	-3.42431310	-0.22653982

1	H	2.44136952	-4.18002395	1.28981446	63	O	1.01646800	0.10560355	2.87452362
2	H	-0.16157470	-5.20692170	2.39895296	64	C	-1.29112199	3.70434379	-0.99650952
3	H	-1.16906457	-4.92484926	0.97471142	65	C	0.33889500	2.54648442	-2.45461671
4	H	0.46021374	-5.57633653	0.78646753	66	C	-1.84870272	0.74487383	-1.31959710
5	H	2.16323344	1.55644555	-1.84318455	67	C	-2.16129995	-0.64269186	-0.86718847
6	H	0.84133832	0.57197528	-2.46570463	68	C	-3.22919790	-1.00226436	-0.14263103
7	H	1.33643613	1.15911939	-4.77006547	69	C	-3.37766178	-2.42086870	0.32847933
8	H	4.67824221	1.29861406	-5.67797225	70	C	-4.32990328	-0.08415248	0.26397034
9	H	4.07459287	2.93007822	-5.98951664	71	O	3.17424044	2.43879734	-0.54997712
10	H	3.07128412	1.52574594	-6.37482797	72	O	0.21457806	4.32717470	1.94664405
11	H	3.65644106	3.36263202	-2.66476952	73	C	-0.66665182	2.12058564	3.37060660
12	H	5.07675809	2.91752857	-3.63116684	74	C	-1.92455239	2.92386352	3.37215087
13	H	4.39231344	1.78079714	-2.45937036	75	C	-3.15613510	2.41509971	3.51838710
14	H	2.75831223	-2.29188119	-2.97398615	76	C	-4.36037944	3.29525657	3.47434814
15	H	5.90437824	-1.59113548	-3.24886712	77	C	-3.43145271	0.96389331	3.72180397
16	H	1.73235326	4.89887957	-1.60220709	78	C	-2.61091242	-2.63453788	1.65053205
17	H	0.30389702	5.67509675	-0.91772906	79	C	-1.13467395	-2.50753778	1.45672852
18	H	1.57463762	6.02680464	1.28545047	80	C	-0.36235951	-3.42316119	0.85606119
19	H	3.50216190	7.16867805	2.02850005	81	C	1.10434622	-3.20469232	0.67655841
20	H	4.37022194	7.98984977	0.72550236	82	C	-0.87087310	-4.70987568	0.30047266
21	H	4.98535062	6.46579507	1.37249668	83	C	1.15454873	1.29365841	-2.80298829
22	H	3.45735736	6.43285128	-2.07094943	84	C	1.67436160	1.40351290	-4.20103035
23	H	5.01250691	6.43609290	-1.23428213	85	C	2.85477534	1.95278500	-4.51946354
24	H	4.10899622	4.92599099	-1.40894867	86	C	3.33304712	2.00467929	-5.93285310
25					87	C	3.77728036	2.54559891	-3.51129145
26		Energy = -2617.17737629 a.u. #Cluster: 9			88	O	3.39892834	-1.86029210	-3.48981017
27	O	-1.59182352	8.54328232	0.65821503	89	O	5.92854777	-0.89772210	-3.79690155
28	N	0.11055308	7.18086287	1.18198053	90	O	3.19009737	-0.77040849	1.86007042
29	C	-1.22397868	7.43228348	1.04066342	91	C	1.54062281	4.53758797	-0.47306605
30	C	-2.16108228	6.33980494	1.38005764	92	C	2.51110061	5.12735338	0.49756898
31	C	-3.31991157	6.19790347	0.73857920	93	C	3.15472817	6.28149562	0.26833599
32	H	-1.83815827	5.66844175	2.18023162	94	C	4.11327407	6.84507154	1.26186399
33	H	0.45410573	6.26408055	1.43802181	95	C	2.98679649	7.06564247	-0.98831857
34	H	0.80454346	7.86626417	0.93374582	96	H	6.90105790	0.46779211	-1.67593908
35	H	-4.03172953	5.40994780	0.95816586	97	H	5.62291906	0.79653743	0.43150082
36	H	-3.65162071	6.85503226	-0.05900821	98	H	2.23421894	-1.28618135	-1.27649686
37	O	7.21433708	4.88555245	0.46916869	99	H	-1.49152386	0.39202679	1.33856685
38	N	5.63900701	3.36088448	0.93011947	100	H	-2.08173211	2.01999100	1.04594680
39	C	6.21479160	4.27218014	0.09134899	101	H	0.15190704	0.55799675	-0.52484384
40	C	5.60415278	4.45742497	-1.24143412	102	H	1.85704491	-0.52823590	2.85595128
41	C	6.31448292	4.91802985	-2.26965600	103	H	-1.65225512	3.94305526	0.00907399
42	H	4.54291106	4.19605933	-1.31848497	104	H	-0.98320169	4.64554612	-1.46880542
43	H	4.81068760	2.85345457	0.66369734	105	H	-2.15918474	3.34822291	-1.56714540
44	H	5.98290641	3.21365530	1.86375596	106	H	-0.53949757	2.58574774	-3.13340744
45	H	5.90047779	5.06948952	-3.25983073	107	H	0.93164533	3.44538985	-2.71731032
46	H	7.36537197	5.17736389	-2.20544330	108	H	-2.73069835	1.41113101	-1.25428266
47	C	5.30114478	-0.62375661	-2.62659754	109	H	-1.57398338	0.74082366	-2.39538993
48	C	5.88700250	0.07726801	-1.58162870	110	H	-1.40142123	-1.37983925	-1.13288426
49	C	5.15804987	0.27388974	-0.40602178	111	H	-4.44440209	-2.68207142	0.47352836
50	C	3.85480728	-0.19713738	-0.30915808	112	H	-3.00269490	-3.13210415	-0.43531621
51	C	3.25438653	-0.91011939	-1.35253750	113	H	-4.04410361	0.97577213	0.23503944
52	C	3.98765334	-1.13022178	-2.51125892	114	H	-5.20126786	-0.20020983	-0.39942427
53	C	3.05995531	0.01690040	0.92331451	115	H	-4.68031306	-0.29059393	1.28593808
54	C	2.07644117	1.07792136	0.99119201	116	H	-0.83140261	1.11921544	3.82650861
55	C	1.07147775	1.01817052	1.93651382	117	H	0.09574483	2.61103083	4.01716632
56	C	-0.10298878	1.95867457	1.94764679	118	H	-1.77011384	3.99407805	3.23632564
57	C	0.35370869	3.29109527	1.35535042	119	H	-4.99763331	3.04803857	2.61076744
58	C	0.97764284	3.17699592	-0.02686161	120	H	-4.11487244	4.36296435	3.39694362
59	C	2.16367126	2.20963256	0.07523538	121	H	-4.98439802	3.17285363	4.37203627
60	C	-0.15545726	2.66268341	-0.99451202	122	H	-3.05365217	0.35807922	2.88417306
61	C	-1.16517101	1.39542998	0.98747499	123	H	-4.50291014	0.73989419	3.81457010
62	C	-0.68391652	1.30017239	-0.46919207	124	H	-2.94748729	0.58255407	4.63464094

1	H	-2.97063840	-1.90742075	2.40604607	63	C	0.98973670	3.34127509	-0.13197123
2	H	-2.86731756	-3.63354412	2.06244672	64	C	2.21674640	2.46781649	0.15594321
3	H	-0.70958403	-1.57906481	1.83379293	65	C	0.03748145	2.65000211	-1.18578984
4	H	1.44182511	-2.22854145	1.04521230	66	C	-1.01737584	1.34983352	0.76089569
5	H	1.38613599	-3.27446484	-0.38522094	67	C	-0.36328482	1.25674646	-0.62872603
6	H	1.69060664	-3.96760133	1.21117622	68	O	1.02845038	0.71643709	3.18394640
7	H	-1.78007809	-5.06163924	0.80771244	69	C	-1.21165210	3.53722249	-1.35636973
8	H	-1.12436009	-4.59982943	-0.76593988	70	C	0.68987575	2.53957709	-2.58269060
9	H	-0.12969513	-5.51777991	0.37174795	71	C	-1.35039516	0.51303332	-1.55617250
10	H	1.99420895	1.15612447	-2.09334175	72	C	-1.52765653	-0.88443636	-1.06243418
11	H	0.53155001	0.38113236	-2.70529214	73	C	-2.63825295	-1.35537954	-0.47927329
12	H	1.01805797	0.99162283	-4.96226097	74	C	-2.67971835	-2.76050699	0.04504970
13	H	4.27857397	1.45254592	-6.04702849	75	C	-3.88063749	-0.55247677	-0.28922028
14	H	3.52645192	3.03850526	-6.25383692	76	O	3.24350214	2.63579508	-0.45578845
15	H	2.62053813	1.57034170	-6.64564248	77	O	-0.23170787	4.54020902	1.56358729
16	H	3.27918049	3.33215585	-2.92395189	78	C	-1.04375805	2.38269709	3.07960895
17	H	4.68106147	2.97923985	-3.95417324	79	C	-2.39991058	2.92451697	2.76939314
18	H	4.10709241	1.79083656	-2.77544182	80	C	-3.53663876	2.21682626	2.82807929
19	H	3.92677919	-1.81994501	-4.33795540	81	C	-4.84620675	2.83694108	2.47048046
20	H	6.76715101	-0.36306941	-3.90684389	82	C	-3.59845998	0.78369822	3.23648372
21	H	2.03958819	4.41516343	-1.46443120	83	C	-2.39745821	-2.78134389	1.56107324
22	H	0.70905957	5.25237236	-0.65582320	84	C	-0.98951789	-2.38999472	1.87354988
23	H	2.67720167	4.56643262	1.41363691	85	C	0.08570538	-3.15826052	1.65101036
24	H	4.15173145	6.26920384	2.19668776	86	C	1.45867730	-2.69344193	2.01251694
25	H	3.85928016	7.88089512	1.53060430	87	C	0.03330498	-4.51514898	1.03597224
26	H	5.13672065	6.86008452	0.85522346	88	C	1.63776941	1.35471562	-2.83061072
27	H	1.93115134	7.17933004	-1.27398115	89	C	2.25500708	1.51989367	-4.18335421
28	H	3.41124822	8.07644750	-0.92051178	90	C	3.43394259	2.12063067	-4.40038759
29	H	3.49069922	6.56585193	-1.83142619	91	C	3.97320605	2.30686125	-5.78030556
30					92	C	4.28350111	2.66635511	-3.30689146
31	Energy = -2617.17102767 a.u. #Cluster: 10				93	O	3.01770992	-2.27302195	-2.50609812
32	O	3.97743664	-3.16619449	-4.83488173	94	O	5.52968511	-1.48022029	-3.31848047
33	N	3.77279656	-1.02720300	-5.48036754	95	O	3.48234350	0.02488670	2.46089312
34	C	4.30248226	-2.27823835	-5.63408310	96	C	1.50791065	4.71434565	-0.59934744
35	C	5.18814751	-2.53011108	-6.78486307	97	C	2.29485815	5.41381873	0.46106033
36	C	5.98751015	-3.59772665	-6.80773511	98	C	3.58068915	5.77664861	0.35061543
37	H	5.15275508	-1.80129210	-7.59713946	99	C	4.27499102	6.47536008	1.47394435
38	H	4.07056757	-0.24419571	-6.03611776	100	C	4.42233468	5.52174551	-0.85181016
39	H	3.23695000	-0.79451053	-4.65519346	101	H	6.72726449	0.29656288	-1.69097290
40	H	6.65958790	-3.82137867	-7.62922287	102	H	5.68135605	1.17707176	0.39192292
41	H	6.03605956	-4.32952341	-6.00655525	103	H	2.15472826	-1.21547269	-0.36534862
42	O	-2.83019904	8.40398901	0.69131102	104	H	-1.19383034	0.32421391	1.15227212
43	N	-1.04077387	7.08564475	0.39685547	105	H	-2.03360870	1.78870704	0.65952008
44	C	-2.16563968	7.44298739	1.08283832	106	H	0.56370907	0.63379709	-0.55142032
45	C	-2.51273544	6.65675033	2.28598212	107	H	1.93301111	0.24879424	3.36815974
46	C	-3.77463916	6.55877583	2.70261621	108	H	-1.75777514	3.69325392	-0.42058436
47	H	-1.67843305	6.16777658	2.79764423	109	H	-0.95878266	4.52481169	-1.76026636
48	H	-0.49987060	6.27375573	0.66225507	110	H	-1.92536175	3.08881083	-2.06007510
49	H	-0.76452264	7.56604744	-0.44331881	111	H	-0.11409332	2.49487757	-3.34841902
50	H	-4.07021727	5.99662214	3.58150637	112	H	1.23334145	3.47949008	-2.80773104
51	H	-4.61281591	7.03181218	2.20119584	113	H	-2.31270935	1.05759399	-1.61249335
52	C	5.03629538	-0.95141110	-2.17109621	114	H	-0.96864194	0.50132370	-2.59871986
53	C	5.73453661	-0.03954234	-1.39103358	115	H	-0.64563545	-1.51515743	-1.17579084
54	C	5.14719508	0.44837961	-0.22009265	116	H	-3.66617698	-3.22447533	-0.15479937
55	C	3.87717762	0.02050330	0.14044598	117	H	-1.94184750	-3.40400449	-0.47631037
56	C	3.15933174	-0.89221764	-0.63988771	118	H	-3.69858432	0.33614310	0.33376514
57	C	3.74491960	-1.38889225	-1.79846653	119	H	-4.28192290	-0.19312885	-1.24844173
58	C	3.21313767	0.51270528	1.36979286	120	H	-4.68369756	-1.11824697	0.20169396
59	C	2.13286690	1.47402844	1.22736170	121	H	-1.11318639	1.43064306	3.64932738
60	C	1.06090981	1.43818361	2.08106168	122	H	-0.50272602	3.08559858	3.75292396
61	C	-0.22099774	2.16618084	1.79684861	123	H	-2.40284751	3.97180912	2.46580096
62	C	0.15172793	3.48836231	1.12593903	124	H	-5.28517708	2.35088275	1.58539843

1	H	-4.76879892	3.90816699	2.24006579	63	C	6.87507106	1.93058697	-3.05241606
2	H	-5.57840117	2.73324495	3.28464562	64	H	4.96787859	2.01791756	-2.09982788
3	H	-2.90057122	0.16066791	2.65727441	65	H	4.63599484	2.94904071	0.02521797
4	H	-4.59657663	0.34451653	3.10472827	66	H	5.85582264	3.72904263	0.94866273
5	H	-3.33313415	0.65734857	4.29792291	67	H	6.57097773	1.38235254	-3.93879077
6	H	-3.11350001	-2.10927763	2.07606808	68	H	7.93371308	2.16630460	-3.04172335
7	H	-2.61537682	-3.79584101	1.95730675	69	C	5.67953682	-0.91574112	-1.12275473
8	H	-0.88412750	-1.39871551	2.31049926	70	C	6.14911024	-0.44553391	0.10333801
9	H	1.49764512	-1.62836388	2.27023264	71	C	5.26072755	0.18434786	0.96995492
10	H	2.17197137	-2.86198481	1.19178396	72	C	3.91913618	0.34568743	0.61515920
11	H	1.84433303	-3.24725963	2.88280131	73	C	3.43070180	-0.17770703	-0.58544641
12	H	-0.93488139	-5.01272795	1.18498310	74	C	4.31158530	-0.80848144	-1.45353113
13	H	0.19691445	-4.45443814	-0.05211267	75	C	3.02102575	1.05249196	1.54486704
14	H	0.80469427	-5.18561691	1.43931830	76	C	1.83590616	1.76442367	1.08734537
15	H	2.41623514	1.29174687	-2.04509451	77	C	0.72770415	1.79868948	1.90045797
16	H	1.08965470	0.39218382	-2.77683288	78	C	-0.55224277	2.49242327	1.49781664
17	H	1.64971430	1.14419206	-5.00475011	79	C	-0.16124743	3.67264468	0.60903823
18	H	4.98347153	1.88330105	-5.88430933	80	C	0.62987474	3.27656897	-0.62747074
19	H	4.06568060	3.37770318	-6.02234290	81	C	1.86711273	2.48176235	-0.18439621
20	H	3.34056720	1.86590023	-6.56174969	82	C	-0.37417441	2.43522657	-1.50358406
21	H	3.74221425	3.43121100	-2.72490745	83	C	-1.36901179	1.49806240	0.65564066
22	H	5.21447085	3.12020004	-3.66341999	84	C	-0.73278021	1.15487669	-0.70296429
23	H	4.55781517	1.88717082	-2.57465885	85	O	0.60636134	1.21380541	3.06059628
24	H	3.47724724	-2.59035770	-3.35863466	86	C	-1.64050426	3.28571393	-1.74052472
25	H	6.39953764	-1.06281336	-3.57819138	87	C	0.17001963	2.10784473	-2.91103526
26	H	2.12350050	4.56945600	-1.51691015	88	C	-1.70422450	0.21890045	-1.45852815
27	H	0.66114119	5.35518433	-0.92242284	89	C	-1.73620681	-1.09132979	-0.74425660
28	H	1.74030916	5.63522215	1.37195855	90	C	-2.69781930	-1.50636666	0.09081349
29	H	3.62999453	6.63607115	2.34812509	91	C	-2.51591777	-2.77562041	0.87467956
30	H	4.64908025	7.46181944	1.16283766	92	C	-3.97534491	-0.78646150	0.35062230
31	H	5.14690699	5.89917729	1.81915499	93	O	2.86741147	2.50898503	-0.86644613
32	H	3.94764128	5.88553322	-1.77398613	94	O	-0.46760115	4.80282014	0.87475302
33	H	5.41186908	5.99143605	-0.79383635	95	C	-1.34492944	2.95786633	2.73302557
34	H	4.58962895	4.43690549	-0.98339536	96	C	-2.70010164	3.45662317	2.35324130
35					97	C	-3.84557242	2.81016525	2.61227691
36	<b>OC-(AM)<sub>3</sub> complex in the DMSO</b>				98	C	-5.15981660	3.36909383	2.18056337
37					99	C	-3.91284371	1.50598076	3.33368028
38	Energy = -2864.31633933 a.u. #Cluster: 1				100	C	-1.62290459	-2.51403486	2.10771309
39	O	5.69461325	-0.86587626	-4.38940979	101	C	-0.21760264	-2.22292056	1.69086400
40	N	4.90749701	-1.63318248	-6.33039621	102	C	0.71355397	-3.15935143	1.46421374
41	C	5.94359639	-1.39152147	-5.48987109	103	C	2.08304420	-2.79315302	0.99683082
42	C	7.31973542	-1.69645090	-5.91493106	104	C	0.47048228	-4.61916797	1.64922939
43	C	8.36230640	-1.24659371	-5.21400754	105	C	1.20861511	0.98408685	-3.02972871
44	H	7.43031922	-2.29742987	-6.81976022	106	C	1.42532216	0.69946497	-4.48261776
45	H	5.00807629	-2.14252989	-7.19579118	107	C	2.45245647	1.15995862	-5.20829376
46	H	3.95903127	-1.43743337	-6.04583441	108	C	2.55296505	0.86580126	-6.67066546
47	H	9.39354563	-1.44250372	-5.48907595	109	C	3.56363011	1.98591483	-4.65742344
48	H	8.26829722	-0.64487479	-4.31380248	110	O	3.78915762	-1.35535973	-2.57933617
49	O	1.78247565	-0.56146057	4.59879041	111	O	6.58001286	-1.49579098	-1.94585171
50	N	3.61312926	-1.57217630	3.78668256	112	O	3.26175823	1.01300231	2.74699476
51	C	2.41759354	-1.60983511	4.44105829	113	C	1.13582297	4.53278962	-1.35930082
52	C	1.94827689	-2.89900682	4.98627826	114	C	2.09698028	5.32448525	-0.53322595
53	C	0.64452729	-3.17237809	5.03986137	115	C	3.32204817	5.68805069	-0.93818914
54	H	2.71883416	-3.59199407	5.32652700	116	C	4.20875475	6.51059068	-0.06246082
55	H	4.13105256	-2.40200127	3.55365379	117	C	3.89997248	5.31216773	-2.26071213
56	H	3.92023222	-0.70520993	3.36178990	118	H	7.20091163	-0.55999957	0.35970873
57	H	0.24397209	-4.10263795	5.42581878	119	H	5.62336296	0.57427297	1.92542910
58	H	-0.12493027	-2.48818872	4.69259930	120	H	2.37611223	-0.09918150	-0.85389423
59	O	7.66584099	3.39045473	-0.73906934	121	H	-1.53135881	0.56419429	1.23717565
60	N	5.60390999	3.22164239	0.11941513	122	H	-2.39230033	1.90043411	0.49803969
61	C	6.50582024	2.99733086	-0.88036451	123	H	0.21209960	0.58090132	-0.52650885
62	C	6.03326502	2.26969786	-2.07607448	124	H	1.41036630	0.65065076	3.41371527

1	H	-2.12768621	3.60927933	-0.81536244	63	H	8.33250543	-4.53579575	-6.86037543
2	H	-1.42068411	4.18825555	-2.32329265	64	O	3.57702780	-1.99472127	-5.48467476
3	H	-2.39536370	2.72294724	-2.30457973	65	N	4.61265004	-0.03056997	-5.74722651
4	H	-0.69135822	1.84879772	-3.56519062	66	C	3.69173880	-0.95114381	-6.14326500
5	H	0.59101300	3.02641959	-3.36818054	67	C	2.88961762	-0.68397566	-7.35259189
6	H	-2.70655303	0.67978519	-1.54191780	68	C	1.57506399	-0.90044976	-7.35980874
7	H	-1.37125616	0.07368181	-2.50680670	69	H	3.44140537	-0.31310382	-8.21919675
8	H	-0.84337936	-1.70081857	-0.89936302	70	H	4.72518378	0.86012018	-6.19918075
9	H	-3.48898010	-3.18828375	1.20339474	71	H	5.13142374	-0.18602977	-4.89358729
10	H	-2.05994593	-3.56732792	0.24729237	72	H	0.94651078	-0.71930694	-8.22510923
11	H	-4.01172242	0.21531950	-0.09774315	73	H	1.01931825	-1.27261860	-6.50484502
12	H	-4.83210789	-1.34813992	-0.05247761	74	O	7.65849342	3.64468481	-1.13065055
13	H	-4.15816970	-0.66253787	1.42854577	75	N	5.80244439	3.27062205	0.06654862
14	H	-1.41714064	2.12887277	3.47121780	76	C	6.49262648	3.24407134	-1.11108415
15	H	-0.77958858	3.76190270	3.25546944	77	C	5.79752924	2.70549555	-2.29928035
16	H	-2.69673171	4.40757937	1.82267042	78	C	6.36108069	2.75230711	-3.50614664
17	H	-5.63699621	2.72072140	1.42929383	79	H	4.80872365	2.26754612	-2.12553418
18	H	-5.07940200	4.36830560	1.73191303	80	H	4.82883700	3.00707158	0.11037105
19	H	-5.86340728	3.44840778	3.02213818	81	H	6.20512813	3.65317341	0.90350827
20	H	-3.19963820	0.77286100	2.92818295	82	H	5.88612111	2.36986086	-4.40078925
21	H	-4.90720743	1.04240920	3.28311861	83	H	7.34119534	3.17660733	-3.69622459
22	H	-3.67458417	1.62809271	4.40220779	84	C	4.99393416	-0.82826018	-2.14525321
23	H	-2.03815975	-1.67057756	2.69552068	85	C	5.77063750	-0.34091260	-1.10372384
24	H	-1.66596256	-3.39208418	2.78343650	86	C	5.13597923	0.15244648	0.04037670
25	H	0.00019771	-1.16563593	1.55326647	87	C	3.74880733	0.16764622	0.11202590
26	H	2.32522621	-1.73783541	1.17545982	88	C	2.95835746	-0.37141987	-0.91168761
27	H	2.18445389	-2.97082569	-0.08575104	89	C	3.58273102	-0.88682607	-2.03731966
28	H	2.86029700	-3.39294488	1.49073904	90	C	3.05329613	0.71422961	1.29392543
29	H	0.46202129	-4.88225817	2.71836700	91	C	1.92334029	1.61453482	1.09038035
30	H	-0.49890595	-4.93399575	1.23739662	92	C	0.83882688	1.53719949	1.92750068
31	H	1.23724606	-5.24261608	1.17154884	93	C	-0.47029933	2.20703384	1.61745414
32	H	2.15896662	1.27089126	-2.53556551	94	C	-0.11940553	3.54912581	0.96979068
33	H	0.86557979	0.06248787	-2.51823970	95	C	0.71543029	3.42501467	-0.29740218
34	H	0.65116920	0.08472729	-4.93725795	96	C	1.96532587	2.58503120	-0.00066419
35	H	3.59309915	0.73169962	-6.99840111	97	C	-0.24063413	2.73867884	-1.34474052
36	H	2.14452070	1.69790744	-7.26439988	98	C	-1.21126502	1.35057888	0.57376417
37	H	2.00056048	-0.03619281	-6.96504715	99	C	-0.55474122	1.31318943	-0.81756825
38	H	3.27947316	2.51987595	-3.73771010	100	O	0.81818426	0.82969695	3.03864722
39	H	3.91918286	2.73720833	-5.37450233	101	C	-1.53495451	3.57471781	-1.43565890
40	H	4.42430811	1.34030641	-4.41026478	102	C	0.33340880	2.71340560	-2.77802371
41	H	4.37779086	-1.17729578	-3.38009766	103	C	-1.48494057	0.52054712	-1.76133089
42	H	6.34377763	-1.34026306	-2.92156343	104	C	-1.60751356	-0.88101082	-1.26271199
43	H	1.60131180	4.22292294	-2.32179733	105	C	-2.69357409	-1.40547547	-0.67994209
44	H	0.27549884	5.17956040	-1.63712912	106	C	-2.66625380	-2.81546760	-0.16442115
45	H	1.72063497	5.61933164	0.44429920	107	C	-3.98510243	-0.68613617	-0.49168258
46	H	3.76065517	6.73771830	0.91415256	108	O	2.98267964	2.78128955	-0.62623798
47	H	4.45551988	7.47225338	-0.53598189	109	O	-0.48764718	4.59475279	1.42966715
48	H	5.16292913	5.99876785	0.13251753	110	C	-1.32237812	2.38742459	2.88617527
49	H	3.29596578	5.69563398	-3.09509332	111	C	-2.68174392	2.91219706	2.56055547
50	H	4.92053178	5.68707436	-2.40694052	112	C	-3.80446373	2.17969275	2.58404779
51	H	3.94051017	4.21404395	-2.36971587	113	C	-5.12094657	2.77741120	2.21560123
52					114	C	-3.84032011	0.73491465	2.95388397
53		Energy = -2864.31412389 a.u. #Cluster: 2			115	C	-2.27149691	-2.84696735	1.32609555
54	O	7.66384226	-2.57399849	-3.64451079	116	C	-0.87348909	-2.37049700	1.55323515
55	N	6.22497483	-3.48401558	-5.12107540	117	C	0.23285210	-3.04638407	1.21421962
56	C	7.41458879	-3.47412282	-4.46804602	118	C	1.59327740	-2.49497682	1.49110279
57	C	8.39527931	-4.54869952	-4.71990570	119	C	0.22984619	-4.37330433	0.53528113
58	C	8.74072283	-4.94551893	-5.94311276	120	C	1.44765326	1.70526176	-3.09028105
59	H	8.83402020	-4.96933693	-3.80955966	121	C	1.80438119	1.81150870	-4.53998112
60	H	5.98467402	-4.19120460	-5.80058232	122	C	2.56357730	2.78307833	-5.06422237
61	H	5.53682991	-2.75400601	-4.98236331	123	C	2.84613450	2.84533048	-6.53005235
62	H	9.47730567	-5.72067007	-6.12977288	124	C	3.15563595	3.89426150	-4.26634503

1	O	2.79680500	-1.45003969	-2.97471988	63	H	5.13659752	6.01014679	1.14672324
2	O	5.49379056	-1.22448797	-3.32705399	64	H	3.28959834	6.39270618	-2.12397211
3	O	3.35004785	0.33865749	2.42176211	65	H	4.90579164	6.43591091	-1.41805549
4	C	1.19978312	4.81607265	-0.74452359	66	H	4.11323262	4.88033157	-1.70870392
5	C	2.11434339	5.43670242	0.26178896	67				
6	C	3.32829570	5.93275306	-0.01500289	68	Energy = -2864.31254030 a.u. #Cluster: 3			
7	C	4.17442151	6.53680979	1.05704682	69	O	3.62575018	-2.73807806	-4.18681940
8	C	3.93912066	5.91813090	-1.37511623	70	N	2.06781348	-1.81652203	-5.49018109
9	H	6.85668098	-0.33218770	-1.18346605	71	C	3.36379098	-2.10769753	-5.23370033
10	H	5.73575145	0.53785048	0.86723739	72	C	4.40329317	-1.72865564	-6.20311102
11	H	1.87080516	-0.40207471	-0.83702353	73	C	5.68420029	-1.62957696	-5.84390731
12	H	-1.32245755	0.31208887	0.95592953	74	H	4.06323616	-1.53574153	-7.22481763
13	H	-2.25524670	1.71973899	0.47709204	75	H	1.77579882	-1.26476714	-6.28340022
14	H	0.40954308	0.74788850	-0.74976414	76	H	1.33736609	-2.05840899	-4.83491367
15	H	1.74489250	0.43098738	3.26507547	77	H	6.47501326	-1.35536656	-6.53634848
16	H	-2.06662107	3.65760062	-0.48243782	78	H	6.05085280	-1.81074764	-4.83828035
17	H	-1.33538023	4.59468523	-1.78538298	79	O	2.23152848	-0.77047821	4.52507493
18	H	-2.24540689	3.13205842	-2.14573352	80	N	4.08629578	-1.60675728	3.58532497
19	H	-0.50310113	2.52212382	-3.48526548	81	C	2.91439242	-1.76783423	4.25991120
20	H	0.68814848	3.72997350	-3.04468258	82	C	2.52238152	-3.12111118	4.69615952
21	H	-2.46823440	1.02067396	-1.84880417	83	C	1.23498594	-3.42974576	4.85914450
22	H	-1.07421590	0.51689280	-2.79331015	84	H	3.33150626	-3.83213858	4.86833482
23	H	-0.69724188	-1.47293864	-1.37099163	85	H	4.65619713	-2.38019114	3.28451637
24	H	-3.65486151	-3.29908790	-0.29430802	86	H	4.36563602	-0.68766526	3.26958168
25	H	-1.95718542	-3.43747623	-0.74759757	87	H	0.89026302	-4.40771617	5.17496909
26	H	-3.86468228	0.40359165	-0.42328836	88	H	0.42366188	-2.72982000	4.67908998
27	H	-4.66885905	-0.88158493	-1.33182779	89	O	-2.77662760	8.76768696	0.42784848
28	H	-4.50715987	-1.00387539	0.42249484	90	N	-1.02236420	7.39357123	0.17731498
29	H	-1.38704342	1.42222337	3.43545046	91	C	-2.17045086	7.76678974	0.81438417
30	H	-0.80607176	3.08418649	3.58408141	92	C	-2.61331968	6.94765778	1.96318209
31	H	-2.70043600	3.96407863	2.27854656	93	C	-3.90023162	6.87677603	2.30104200
32	H	-5.54545760	2.28227556	1.32830967	94	H	-1.82711518	6.41007718	2.50217053
33	H	-5.06014334	3.84898275	1.98274037	95	H	-0.52855652	6.54977172	0.43722611
34	H	-5.85753433	2.66424185	3.02469719	96	H	-0.68375529	7.89326170	-0.62781720
35	H	-3.23366685	0.12724428	2.26463447	97	H	-4.26620278	6.29024954	3.13622788
36	H	-4.85452991	0.31369292	2.93425766	98	H	-4.69151636	7.39739241	1.77202399
37	H	-3.44488198	0.56278863	3.96685471	99	C	4.90035108	-1.27643642	-1.41556025
38	H	-2.99042056	-2.23490842	1.90775426	100	C	5.76800678	-0.51885678	-0.62914235
39	H	-2.39408525	-3.88202562	1.71060691	101	C	5.25309839	0.24990895	0.41271820
40	H	-0.80448282	-1.39557601	2.03293477	102	C	3.88113795	0.26966771	0.65207056
41	H	1.56868758	-1.49512772	1.94045274	103	C	3.00533369	-0.50169158	-0.11580208
42	H	2.19048691	-2.42876218	0.56817819	104	C	3.51418449	-1.28222452	-1.14796460
43	H	2.15166406	-3.14303311	2.18378868	105	C	3.33213175	1.13732951	1.71567310
44	H	1.08313427	-4.99792561	0.83332495	106	C	2.11315582	1.88683291	1.40484402
45	H	-0.68021017	-4.95364192	0.74053218	107	C	0.97380900	1.77210596	2.14205802
46	H	0.28931394	-4.24998076	-0.55830364	108	C	-0.31206360	2.46310493	1.75332961
47	H	2.34270194	1.88723743	-2.46206225	109	C	0.05163692	3.74397229	1.00692358
48	H	1.12860895	0.67003256	-2.85299641	110	C	0.95094975	3.53601279	-0.19963754
49	H	1.38698136	1.02591660	-5.16494792	111	C	2.20591644	2.78183031	0.25013970
50	H	3.92157551	2.94030560	-6.73912052	112	C	0.09599146	2.70668165	-1.23579899
51	H	2.36501939	3.72492812	-6.98445869	113	C	-1.04946609	1.55690242	0.75214160
52	H	2.48014966	1.96836398	-7.07946067	114	C	-0.29904501	1.35778922	-0.57557149
53	H	3.26792000	3.62828866	-3.20162532	115	O	0.81298011	1.02121360	3.20669871
54	H	2.51719908	4.78952671	-4.30807679	116	C	-1.16707933	3.52382150	-1.57236700
55	H	4.14649992	4.19163899	-4.63540586	117	C	0.84442642	2.48514065	-2.57058034
56	H	3.29581542	-1.66134856	-3.82645472	118	C	-1.18104246	0.48023208	-1.49244940
57	H	6.43945664	-1.63417874	-3.29713458	119	C	-1.30565943	-0.87721612	-0.88355794
58	H	1.70089358	4.72129853	-1.73335707	120	C	-2.37778733	-1.33872162	-0.22673796
59	H	0.32832229	5.48541308	-0.91158484	121	C	-2.33587404	-2.68123440	0.44647187
60	H	1.71506989	5.47751548	1.27354655	122	C	-3.66548902	-0.60491125	-0.07198104
61	H	3.70090447	6.50959810	2.04753025	123	O	3.26395228	2.96092483	-0.30569130
62	H	4.40615444	7.58976260	0.83938981	124	O	-0.36950542	4.81588150	1.35205051



1	C	-1.18228932	2.75550344	2.98902280	63	H	1.36977251	0.35518324	-2.46487881
2	C	-2.54337946	3.22601169	2.59505007	64	H	1.90585963	1.05325656	-4.77923266
3	C	-3.66496622	2.50313593	2.71914687	65	H	5.32142485	1.03772531	-5.55075224
4	C	-4.98287509	3.04765110	2.27878330	66	H	4.74249250	2.68553724	-5.81844715
5	C	-3.70083198	1.12470887	3.28833045	67	H	3.73838792	1.30966754	-6.28584351
6	C	-1.60446750	-2.57890726	1.80266727	68	H	4.27759112	2.84014602	-2.38197929
7	C	-0.12604827	-2.49898213	1.60020611	69	H	5.68186747	2.54181712	-3.42175917
8	C	0.67209672	-3.56727671	1.46664829	70	H	5.02128877	1.24173214	-2.41983295
9	C	2.13689123	-3.41922147	1.22291958	71	H	2.92486725	-2.31228272	-2.72841041
10	C	0.17694474	-4.97314301	1.53847842	72	H	4.81841076	-2.30230078	-3.10732604
11	C	1.86444679	1.33805011	-2.61840053	73	H	2.01458901	4.70457709	-1.68674494
12	C	2.54484761	1.34680485	-3.94940854	74	H	0.53559029	5.47806834	-1.11679434
13	C	3.82501992	1.68862116	-4.14694922	75	H	1.66288649	5.90973270	1.15243794
14	C	4.42685718	1.67693953	-5.51404657	76	H	3.52160307	7.12631084	1.96201263
15	C	4.74869126	2.10137080	-3.05263809	77	H	4.49294967	7.88424965	0.69391812
16	O	2.61139307	-2.03742837	-1.81325502	78	H	5.04217129	6.38460636	1.44932555
17	O	5.47443267	-2.00009699	-2.40019463	79	H	3.77764433	6.33254907	-2.08168060
18	O	3.86104824	1.20620287	2.80939566	80	H	5.26708147	6.22267803	-1.13895981
19	C	1.41099510	4.89094841	-0.76888606	81	H	4.28747232	4.77581981	-1.41285107
20	C	2.19100697	5.68653821	0.22690279	82				
21	C	3.44497316	6.12067228	0.03604549	83		Energy = -2864.31167291 a.u. #Cluster: 4		
22	C	4.14936089	6.91580761	1.08574966	84	O	5.51919910	-3.52407657	-4.01347691
23	C	4.23434460	5.85813907	-1.20113535	85	N	3.38613524	-4.12030225	-3.62486151
24	H	6.83652769	-0.53106359	-0.84130815	86	C	4.52410290	-4.15220552	-4.38461036
25	H	5.92700378	0.84869961	1.02970863	87	C	4.54420871	-5.02472125	-5.57647690
26	H	1.92946527	-0.50908102	0.07447033	88	C	5.20319653	-4.65039332	-6.67274664
27	H	-1.24389375	0.56792766	1.22161715	89	H	3.99141224	-5.96199589	-5.49976938
28	H	-2.06083260	1.96957777	0.55355662	90	H	2.52165745	-4.52764227	-3.94651864
29	H	0.64355993	0.78722035	-0.37365182	91	H	3.29998514	-3.43525977	-2.88658254
30	H	1.61137882	0.44926936	3.52405649	92	H	5.24585018	-5.24520534	-7.57741454
31	H	-1.75478133	3.78796893	-0.68738886	93	H	5.74570225	-3.71254748	-6.75171950
32	H	-0.92368096	4.45484659	-2.09818872	94	O	3.94955090	-1.57920656	-5.32008483
33	H	-1.83809464	2.96310131	-2.23567870	95	N	1.74767476	-1.25679361	-5.60259176
34	H	0.09641402	2.31211636	-3.37320371	96	C	3.01822855	-1.32540777	-6.09841424
35	H	1.35586474	3.42353840	-2.86642392	97	C	3.23724438	-1.13464309	-7.54243831
36	H	-2.16629419	0.95675068	-1.65724430	98	C	4.47714882	-1.02726425	-8.02355825
37	H	-0.73291555	0.40217720	-2.50474020	99	H	2.34837813	-1.08722430	-8.17270477
38	H	-0.40352052	-1.48720340	-0.96797252	100	H	0.95497842	-0.98249886	-6.15710597
39	H	-3.35605392	-3.08063342	0.60487005	101	H	1.59156117	-1.34608541	-4.61024513
40	H	-1.82754549	-3.42864584	-0.19543589	102	H	4.69965745	-0.88483453	-9.07482932
41	H	-3.63134026	0.42392295	-0.45442187	103	H	5.36409838	-1.07476094	-7.39649614
42	H	-4.47925230	-1.11740873	-0.60701256	104	O	7.38103982	4.58368148	0.95060569
43	H	-3.96886268	-0.54245215	0.98374050	105	N	5.25027846	3.92537843	1.17270557
44	H	-1.24284398	1.85046399	3.63193188	106	C	6.37504118	4.11111255	0.41887882
45	H	-0.68509177	3.52761681	3.61861894	107	C	6.32276976	3.69447974	-0.99727317
46	H	-2.56485001	4.23072260	2.17214837	108	C	7.27531032	4.05440794	-1.85704805
47	H	-5.39044699	2.46320419	1.43936444	109	H	5.46135695	3.08316140	-1.28803165
48	H	-4.92895111	4.09183435	1.94239452	110	H	4.38698607	3.61472694	0.75274588
49	H	-5.72896134	3.00518648	3.08540546	111	H	5.20242038	4.23731246	2.12787190
50	H	-2.93637655	0.47393352	2.83792238	112	H	7.27250350	3.77026628	-2.90360449
51	H	-4.66853550	0.62732140	3.13936754	113	H	8.13202124	4.66059707	-1.58475296
52	H	-3.51340071	1.13535560	4.37352950	114	C	5.30541580	-0.57255348	-2.04535810
53	H	-1.97103719	-1.69375081	2.35992369	115	C	6.00300147	0.14873183	-1.07888108
54	H	-1.87260726	-3.45158287	2.43192200	116	C	5.30749500	0.69021308	0.00306303
55	H	0.26667102	-1.48675124	1.54288020	117	C	3.92965701	0.53175890	0.09511210
56	H	2.51848876	-2.43108611	1.50951541	118	C	3.21558098	-0.17930598	-0.87496027
57	H	2.36360899	-3.54611359	0.15057773	119	C	3.90540468	-0.73077480	-1.94575504
58	H	2.72509538	-4.16806522	1.76970881	120	C	3.16551291	1.05152804	1.24730471
59	H	-0.03031515	-5.26306389	2.57971185	121	C	1.97445484	1.85490487	0.99720780
60	H	-0.75807717	-5.11198226	0.97715343	122	C	0.86929540	1.69134210	1.79404350
61	H	0.89859544	-5.69810493	1.14030179	123	C	-0.48167840	2.23337828	1.42150821
62	H	2.59895368	1.42540727	-1.79480633	124	C	-0.23823365	3.57724932	0.72897059

1	C	0.65502994	3.48984537	-0.50070060	63	H	-5.21961398	3.42424103	1.58599290
2	C	1.97148797	2.80783511	-0.11069547	64	H	-5.92780943	2.22345070	2.67382355
3	C	-0.17548656	2.65894167	-1.55256888	65	H	-3.05341455	-0.08331274	2.09856160
4	C	-1.10383160	1.27325141	0.38956973	66	H	-4.70244816	-0.02422472	2.72069002
5	C	-0.38712547	1.23661186	-0.96710503	67	H	-3.35139925	0.40850440	3.77117571
6	O	0.86708382	0.99580435	2.91269204	68	H	-2.08268580	-2.48422634	1.80099894
7	C	-1.53865527	3.35215116	-1.75311537	69	H	-1.39643606	-4.10292337	1.66449497
8	C	0.48631365	2.62133709	-2.94799155	70	H	0.05159865	-1.49791273	1.76004742
9	C	-1.17602057	0.30639451	-1.90630209	71	H	2.44084230	-1.52582704	1.68995889
10	C	-1.06944858	-1.09315535	-1.39789555	72	H	3.06155410	-2.49443861	0.34308138
11	C	-2.04783176	-1.77307597	-0.78652200	73	H	3.10555398	-3.13312192	1.99163407
12	C	-1.78863194	-3.15136885	-0.25060526	74	H	0.34527922	-5.16178730	0.82364199
13	C	-3.43366335	-1.26484063	-0.57957303	75	H	1.16901764	-4.50885076	-0.59387599
14	O	3.00406114	3.10966796	-0.66659243	76	H	2.11054856	-5.09145234	0.78395709
15	O	-0.72673384	4.59765003	1.12960184	77	H	2.46006447	1.86263630	-2.38234099
16	C	-1.38745468	2.38073232	2.65647491	78	H	1.36641258	0.61179643	-2.96764188
17	C	-2.78067346	2.75374789	2.27071641	79	H	1.47955247	1.57095319	-5.30329465
18	C	-3.82745653	1.91664019	2.30278308	80	H	4.69378180	1.50605488	-6.44545050
19	C	-5.18471704	2.36527736	1.87516974	81	H	4.32766309	3.23762058	-6.49719249
20	C	-3.73430771	0.49412526	2.74240975	82	H	3.10310387	2.05676863	-6.97302269
21	C	-1.34800847	-3.08358565	1.22579828	83	H	4.05242328	3.02451670	-2.93877079
22	C	0.02629776	-2.51612406	1.37767321	84	H	5.27089024	3.17749777	-4.21890028
23	C	1.15756164	-3.16937216	1.07828453	85	H	4.98401304	1.60488266	-3.45413978
24	C	2.49756942	-2.54472619	1.28805743	86	H	3.59091210	-1.45731119	-3.78493457
25	C	1.19825668	-4.54602891	0.50668596	87	H	5.60448004	-1.88912956	-3.49951375
26	C	1.67123320	1.66675649	-3.13434298	88	H	1.54613364	4.81207675	-1.97244286
27	C	2.20133260	1.80878717	-4.52464707	89	H	0.06270189	5.45435689	-1.24457746
28	C	3.45077981	2.18074227	-4.83179609	90	H	1.31587032	5.80461637	0.95650913
29	C	3.90750249	2.25246113	-6.25266289	91	H	3.14686515	7.10593746	1.71953424
30	C	4.48940237	2.52053996	-3.81789567	92	H	3.84640200	8.09096376	0.42862865
31	O	3.18604501	-1.44505247	-2.82992883	93	H	4.68517281	6.63924632	0.98656851
32	O	6.02010581	-1.06671178	-3.07510445	94	H	3.11011158	6.54857285	-2.40234441
33	O	3.45707241	0.71308607	2.38767068	95	H	4.67259207	6.61554071	-1.58339184
34	C	0.99815786	4.90227517	-1.00734865	96	H	3.86617774	5.05740127	-1.82353464
35	C	1.79218654	5.68826119	-0.01509326	97				
36	C	2.98302026	6.24827240	-0.27101091	98		Energy = -2864.30912391 a.u. #Cluster: 5		
37	C	3.69112017	7.05584870	0.76682172	99	O	2.37681153	-1.06116203	3.74919359
38	C	3.69407282	6.12000024	-1.57564689	100	N	4.46382934	-1.51701677	3.05401123
39	H	7.08112114	0.27449466	-1.17125423	101	C	3.30884235	-1.86863906	3.68351807
40	H	5.85081692	1.23491719	0.77722645	102	C	3.19077525	-3.22714411	4.25217542
41	H	2.13553764	-0.31864052	-0.80617603	103	C	2.00485368	-3.83454538	4.30096055
42	H	-1.14552040	0.24592483	0.81217476	104	H	4.11196291	-3.68336896	4.61645599
43	H	-2.16843663	1.54995903	0.23227805	105	H	5.29839563	-2.07866115	3.08410155
44	H	0.63273374	0.77497812	-0.82561447	106	H	4.57266690	-0.57731302	2.69625928
45	H	1.81367218	0.67440519	3.17465464	107	H	1.85711878	-4.82845474	4.70644695
46	H	-2.11217640	3.45841182	-0.82701067	108	H	1.08866652	-3.38369847	3.92609648
47	H	-1.42597473	4.35478841	-2.18294691	109	O	-2.70075253	9.01648570	0.81544020
48	H	-2.17361615	2.78334567	-2.44475089	110	N	-0.97220953	7.62247646	0.50552283
49	H	-0.28983591	2.35957869	-3.69924584	111	C	-2.12196074	7.98072614	1.14818558
50	H	0.80665455	3.64495481	-3.23091358	112	C	-2.59980335	7.10169824	2.23700890
51	H	-2.22649518	0.64381949	-1.99132186	113	C	-3.89099220	7.05057688	2.56189051
52	H	-0.77962596	0.36167629	-2.94152632	114	H	-1.83535982	6.50596304	2.74424597
53	H	-0.08211065	-1.53974320	-1.52566607	115	H	-0.49815581	6.75542153	0.71997239
54	H	-2.69443071	-3.78304497	-0.33918050	116	H	-0.60760894	8.16540186	-0.25921798
55	H	-1.01117028	-3.67097312	-0.84653633	117	H	-4.28275917	6.42372076	3.35499395
56	H	-3.49372117	-0.16826250	-0.56822176	118	H	-4.66069237	7.63028464	2.06283455
57	H	-4.10085542	-1.61355421	-1.38283492	119	O	7.59658249	3.93263422	1.04622672
58	H	-3.86668002	-1.61794959	0.36763274	120	N	5.37784541	3.71324074	1.26212108
59	H	-1.37541941	1.43740670	3.24625782	121	C	6.51288441	3.70274994	0.50475447
60	H	-0.96445989	3.15418970	3.33637872	122	C	6.36931477	3.39880482	-0.93296236
61	H	-2.89266206	3.78422199	1.93601466	123	C	7.43381293	3.30697218	-1.72997793
62	H	-5.53727192	1.78620467	1.00750139	124	H	5.34667667	3.25444949	-1.29554902

1	H	4.47115990	3.55751524	0.85071127	63	H	-2.30754709	3.23383368	-1.93850238
2	H	5.40134744	3.92364803	2.24607209	64	H	-0.51401260	2.55943636	-3.30241011
3	H	7.36821381	3.08489460	-2.78943013	65	H	0.80957729	3.64493474	-2.91513350
4	H	8.45389880	3.44381718	-1.38720065	66	H	-2.62137175	1.23131364	-1.37454539
5	C	4.56337038	-1.10170125	-1.99687058	67	H	-1.30705755	0.66940445	-2.39571620
6	C	5.48514253	-0.35663682	-1.27277238	68	H	-0.86315909	-1.27663580	-0.96186914
7	C	5.04442750	0.37670207	-0.16992935	69	H	-3.66699595	-2.85196962	0.86728374
8	C	3.69655000	0.37726638	0.17733480	70	H	-2.24040371	-3.20186880	-0.10381386
9	C	2.76311574	-0.37688012	-0.54193320	71	H	-3.96606515	0.68991639	-0.05328211
10	C	3.19900390	-1.12153616	-1.62965116	72	H	-4.86354586	-0.83125138	-0.05390795
11	C	3.24249108	1.19226159	1.32494603	73	H	-4.10178029	-0.25428524	1.43186322
12	C	2.01143493	1.97055449	1.17016231	74	H	-1.00828143	1.92767162	3.81417341
13	C	0.95990200	1.83439683	2.02892495	75	H	-0.45516451	3.60414116	3.75858290
14	C	-0.33997973	2.57954875	1.83831144	76	H	-2.51218078	4.33256185	2.59020659
15	C	-0.04001852	3.87977147	1.09689869	77	H	-5.41945382	2.55003907	2.22400030
16	C	0.70290144	3.69870232	-0.21795420	78	H	-4.88949561	4.17911393	2.65106701
17	C	1.99259309	2.92871322	0.07033642	79	H	-5.51965125	3.09695734	3.89999142
18	C	-0.27885800	2.91347834	-1.16994731	80	H	-2.78919571	0.56221756	3.23102959
19	C	-1.22478949	1.73511259	0.90450540	81	H	-4.46551507	0.70460861	3.76638589
20	C	-0.63381679	1.55548520	-0.50361814	82	H	-3.15390566	1.19565551	4.84074883
21	O	0.90749496	1.01932045	3.05427776	83	H	-2.09293972	-1.59779008	2.53620908
22	C	-1.55053025	3.76571087	-1.34785456	84	H	-1.99050262	-3.35698617	2.49347254
23	C	0.31776426	2.70859196	-2.58185532	85	H	0.06625720	-1.33977941	1.56304431
24	C	-1.63654599	0.72648082	-1.33734976	86	H	2.29347796	-2.28400475	1.25340479
25	C	-1.73009631	-0.64584522	-0.75699060	87	H	1.99739191	-3.20725335	-0.22676529
26	C	-2.73230780	-1.10048775	0.00659835	88	H	2.50007110	-4.03685489	1.25370361
27	C	-2.65760767	-2.47092689	0.61791408	89	H	-0.05074245	-5.23922207	2.22143605
28	C	-3.96525209	-0.33446868	0.34269396	90	H	-1.08617490	-4.88779961	0.83341336
29	O	2.99975590	3.15877553	-0.56318251	91	H	0.56451600	-5.46022908	0.57963369
30	O	-0.38917910	4.94663932	1.52604812	92	H	2.13483770	1.62807971	-2.01431524
31	C	-1.03419126	2.84475669	3.18601468	93	H	0.82222888	0.57283027	-2.53425343
32	C	-2.43553609	3.32050669	2.98767638	94	H	1.11800107	1.20013712	-4.89200649
33	C	-3.52962452	2.59092212	3.24637320	95	H	4.42137194	1.14322763	-5.99652585
34	C	-4.89577265	3.13622886	2.99506601	96	H	3.86298518	2.79633698	-6.27681828
35	C	-3.48698594	1.20271568	3.79078078	97	H	2.78390233	1.43180826	-6.59303147
36	C	-1.78730664	-2.44695387	1.89269219	98	H	3.66993175	3.10906853	-2.81830976
37	C	-0.33608063	-2.35062150	1.54938404	99	H	4.97428119	2.81739923	-3.98663554
38	C	0.43492663	-3.39958577	1.23132723	100	H	4.46199950	1.53030233	-2.88345157
39	C	1.87195701	-3.22290359	0.86819998	101	H	2.65005586	-2.26123727	-3.11904477
40	C	-0.05618012	-4.80845650	1.20853158	102	H	5.83444015	-1.72493038	-3.36059511
41	C	1.30873256	1.54876647	-2.74751199	103	H	1.59264033	4.90161771	-1.79035946
42	C	1.83543287	1.53420584	-4.14637119	104	H	0.21322230	5.67792639	-1.01265070
43	C	3.08240741	1.88445264	-4.48851673	105	H	1.64917708	5.97680065	1.12129020
44	C	3.55043340	1.80980563	-5.90453564	106	H	3.57604810	7.21942843	1.69335975
45	C	4.09883177	2.36238120	-3.50846902	107	H	4.37647439	8.02033930	0.33479139
46	O	2.26887745	-1.85223403	-2.29068600	108	H	5.00783284	6.49142682	0.95658484
47	O	4.88638144	-1.85997761	-3.07071675	109	H	3.25980220	6.63536620	-2.36444949
48	O	3.86896053	1.21464275	2.36719536	110	H	4.86875054	6.45577930	-1.65798414
49	C	1.11385243	5.06589400	-0.79767114	111	H	3.84044918	5.03511934	-1.87941115
50	C	2.03019296	5.81578863	0.11422328	112				
51	C	3.23517543	6.28528291	-0.23956112	113		Energy = -2864.30515561 a.u. #Cluster: 6		
52	C	4.07982607	7.03956579	0.73398060	114	O	6.69924489	-1.44641826	-5.23081375
53	C	3.83250391	6.10072686	-1.59305877	115	N	4.48152792	-1.19328749	-5.44988406
54	H	6.53659169	-0.34918359	-1.55965364	116	C	5.75319024	-1.05307887	-5.92321350
55	H	5.76264091	0.95643473	0.41434678	117	C	5.94276370	-0.48718684	-7.27281604
56	H	1.70781576	-0.39594450	-0.26376750	118	C	7.08290234	0.12148638	-7.60124312
57	H	-1.40313671	0.73878018	1.36495238	119	H	5.10889548	-0.60109699	-7.96818793
58	H	-2.23483864	2.19055625	0.83522771	120	H	3.68460562	-0.78029302	-5.90497365
59	H	0.30901133	0.95700592	-0.42185123	121	H	4.32555973	-1.55717214	-4.52346596
60	H	1.70087758	0.36876840	3.19288701	122	H	7.26901048	0.55105727	-8.57955229
61	H	-2.02465814	4.02854753	-0.39677107	123	H	7.91927537	0.24137413	-6.91885501
62	H	-1.34456853	4.70099926	-1.88256013	124	O	2.48510870	-3.09876391	-3.45668879

1	N	1.16044739	-3.37236565	-1.67128967	63	O	3.10575973	-0.55652485	2.12257116
2	C	1.34888586	-3.02910911	-2.97756050	64	C	1.79152055	4.56321971	-0.63803253
3	C	0.18726904	-2.58981364	-3.77194197	65	C	2.65907459	5.05117612	0.47674785
4	C	0.32612582	-1.68155856	-4.73842931	66	C	3.98567172	5.22847797	0.39957078
5	H	-0.76791304	-3.06300285	-3.53747013	67	C	4.76005078	5.70491119	1.58547524
6	H	0.26203239	-3.33938988	-1.21563494	68	C	4.79962516	4.96537384	-0.82022596
7	H	1.90862767	-3.77253087	-1.12475236	69	H	7.20766319	1.14993045	-0.89823968
8	H	-0.49794045	-1.33573825	-5.35381112	70	H	5.45467391	1.56508182	0.82859241
9	H	1.27166388	-1.21199987	-4.99190999	71	H	3.06125213	-1.63463738	-0.80729820
10	O	-2.21254542	8.56177588	0.93717697	72	H	-1.45594162	0.40381408	0.72424430
11	N	-0.58289526	7.08400171	0.50478538	73	H	-2.06511162	2.00755987	0.34500222
12	C	-1.64316044	7.51462994	1.24956819	74	H	0.38269655	0.60379787	-0.91517669
13	C	-2.03539961	6.69808181	2.41793705	75	H	1.63035255	-0.33935396	2.84261347
14	C	-3.28794399	6.70586249	2.87263279	76	H	-1.52684835	3.93619123	-0.65212568
15	H	-1.24289249	6.09508107	2.87087340	77	H	-0.59416111	4.71011531	-1.94172618
16	H	-0.12709416	6.20344775	0.70131606	78	H	-1.72522062	3.42086833	-2.31925704
17	H	-0.28571963	7.57997042	-0.31922109	79	H	0.09245757	2.72989554	-3.59019550
18	H	-3.61534925	6.12468449	3.72761691	80	H	1.55456299	3.42614052	-2.91182595
19	H	-4.08609344	7.29213934	2.42887000	81	H	-2.44426248	1.39853988	-1.89324052
20	C	6.11871360	-0.47208764	-1.80615379	82	H	-1.16886855	0.94416286	-3.00599824
21	C	6.30712608	0.53703036	-0.86540173	83	H	-0.89516185	-1.27163715	-1.96298770
22	C	5.32542770	0.76156529	0.10119836	84	H	-3.88903669	-3.02876734	-0.90514252
23	C	4.17454463	-0.01848034	0.11598337	85	H	-2.24094009	-3.21868692	-1.48512256
24	C	3.96788032	-1.03473817	-0.82109405	86	H	-3.82081259	0.67191524	-0.51925550
25	C	4.95097378	-1.26480962	-1.77241024	87	H	-4.79878386	-0.44905600	-1.47324059
26	C	3.12300341	0.18664700	1.13848200	88	H	-4.48160305	-0.78250729	0.23172016
27	C	2.08090667	1.16985776	0.94825541	89	H	-1.21708396	1.23396441	3.29892908
28	C	0.94748526	1.12830239	1.73350053	90	H	-0.40685656	2.78531179	3.55327921
29	C	-0.23659570	2.02778483	1.51665856	91	H	-2.18590137	4.01580384	2.38263281
30	C	0.28338027	3.35235856	0.96109020	92	H	-5.26702274	2.82345186	1.40413050
31	C	1.12399389	3.21632797	-0.29377314	93	H	-4.53631903	4.25460055	2.13957197
32	C	2.25328084	2.20521635	-0.06979960	94	H	-5.46895370	3.12613364	3.13259540
33	C	0.14098678	2.70596575	-1.41709634	95	H	-3.24228940	0.30079826	2.10177744
34	C	-1.12443436	1.41876913	0.41749639	96	H	-4.82043487	0.65707130	2.80263821
35	C	-0.454445810	1.34497102	-0.96451229	97	H	-3.38646996	0.63086943	3.83211292
36	O	0.78335847	0.27751267	2.71715317	98	H	-2.97623562	-2.27297785	1.37274000
37	C	-0.98049236	3.74854088	-1.58219548	99	H	-2.63048644	-3.94545566	0.93614334
38	C	0.84617098	2.58108575	-2.78800363	100	H	-0.63185862	-1.62711041	0.45994496
39	C	-1.50992088	0.80824344	-1.95842537	101	H	1.61338831	-2.80640581	2.63287961
40	C	-1.73417474	-0.63840381	-1.67610175	102	H	1.64678086	-2.13993212	0.99761475
41	C	-2.81599783	-1.16568837	-1.08852716	103	H	2.06172721	-3.84236575	1.28074798
42	C	-2.86032517	-2.63419062	-0.77706739	104	H	-1.20355256	-4.68453057	2.74153478
43	C	-4.02561304	-0.39376276	-0.69072478	105	H	-0.78996019	-5.43333010	1.19630949
44	O	3.27018767	2.29464603	-0.71369365	106	H	0.43671383	-5.26984716	2.45621450
45	O	0.00183957	4.40130292	1.47630932	107	H	2.35266606	1.05037609	-2.31198893
46	C	-1.02992459	2.22126790	2.82276507	108	H	0.90045074	0.40910731	-3.08288854
47	C	-2.30967413	2.95063219	2.58059865	109	H	1.60080550	1.12101256	-5.26992982
48	C	-3.52378424	2.38272642	2.58145607	110	H	5.01838772	1.68689892	-6.12465297
49	C	-4.74848180	3.18935109	2.30373433	111	H	4.07921170	3.17371013	-6.24627647
50	C	-3.75787180	0.93268281	2.84047371	112	H	3.37771197	1.65103822	-6.79301591
51	C	-2.38738027	-2.89735206	0.66640048	113	H	3.92904487	3.12409611	-2.92924204
52	C	-0.93480511	-2.60388474	0.83789080	114	H	5.35583750	2.64812996	-3.86959840
53	C	-0.05266168	-3.42320340	1.42710442	115	H	4.53937204	1.48770344	-2.80754442
54	C	1.37971313	-3.03110609	1.57837597	116	H	3.94500330	-2.64478598	-2.77963112
55	C	-0.41205781	-4.75956182	1.98089612	117	H	6.77721202	-1.06068117	-3.57898578
56	C	1.59641193	1.27074790	-3.09044010	118	H	2.38023955	4.44253170	-1.57622689
57	C	2.23638960	1.40737241	-4.43598463	119	H	1.02076547	5.32353685	-0.87879722
58	C	3.46785726	1.89878248	-4.63408011	120	H	2.12816179	5.26901273	1.40246704
59	C	4.00608719	2.09994701	-6.01264637	121	H	4.13301852	5.87699289	2.47026069
60	C	4.37252520	2.30904713	-3.52570520	122	H	5.28335618	6.64808046	1.37251178
61	O	4.88029608	-2.25919555	-2.68607889	123	H	5.52757612	4.97020503	1.87404279
62	O	7.10970068	-0.68270687	-2.69670940	124	H	4.36157084	5.42196761	-1.71839434

1	H	5.82873295	5.33617399	-0.73874368	63	C	-3.46141617	2.11848125	2.78178258
2	H	4.86340136	3.87793595	-1.01281019	64	C	-4.73570989	2.85851486	2.54409442
3					65	C	-3.60226983	0.64224852	2.93849732
4	Energy = -2864.30426101 a.u. #Cluster: 7								
5	O	7.50290474	-2.77772643	-3.97790477	66	C	-2.75390926	-2.71990891	0.78836864
6	N	5.76461012	-3.96881852	-4.73170638	67	C	-1.34160880	-2.42323412	1.17525118
7	C	7.10325570	-3.73296376	-4.66164578	68	C	-0.28171332	-3.17237330	0.84181872
8	C	8.02556887	-4.64117979	-5.36614442	69	C	1.09622121	-2.80034431	1.28451494
9	C	9.33220388	-4.37818379	-5.42441781	70	C	-0.35756129	-4.41540402	0.02291938
10	H	7.58147211	-5.52481261	-5.82969645	71	C	1.51480418	1.91722089	-3.07289600
11	H	5.36173759	-4.66612364	-5.33929568	72	C	1.94231520	2.20855416	-4.47578770
12	H	5.11404715	-3.36035210	-4.26057596	73	C	3.16043683	2.63280410	-4.83708161
13	H	10.04681315	-5.01749886	-5.93150275	74	C	3.49304049	2.87626487	-6.27395178
14	H	9.79042666	-3.50414233	-4.97095087	75	C	4.28010564	2.87833743	-3.88712691
15	O	1.85061922	-2.12329100	-4.02033183	76	O	4.13384956	-2.39359683	-2.81131898
16	N	3.09294281	-0.65936929	-5.19296165	77	O	5.99055877	-0.58975724	-3.73109437
17	C	1.88803272	-1.19648869	-4.84461277	78	O	3.38830092	-0.29578016	2.02779330
18	C	0.66532962	-0.67898962	-5.48580242	79	C	1.58415635	4.84356749	-0.38506729
19	C	-0.52160852	-0.82084093	-4.89407241	80	C	2.48806356	5.33256676	0.69952960
20	H	0.79163285	-0.18605631	-6.45102439	81	C	3.77628870	5.66103566	0.52549639
21	H	3.16741346	0.15388074	-5.78429209	82	C	4.60496758	6.13965152	1.67241959
22	H	3.94522531	-0.93842157	-4.72889182	83	C	4.48794250	5.57750313	-0.78153596
23	H	-1.44873250	-0.45579810	-5.32206835	84	H	6.61651146	1.31446735	-2.06718061
24	H	-0.65874464	-1.31353658	-3.93502528	85	H	5.37252860	1.81663368	0.03871457
25	O	-2.41778983	8.54221014	1.61744873	86	H	2.85263706	-1.63743478	-0.62316285
26	N	-0.70818869	7.18429133	1.10726662	87	H	-1.19309034	0.32812817	0.83873616
27	C	-1.81587613	7.49116618	1.84393612	88	H	-2.02604217	1.85430088	0.58568035
28	C	-2.21942955	6.53986046	2.90139472	89	H	0.50186065	0.84594863	-0.87323272
29	C	-3.48784745	6.45299819	3.30032082	90	H	1.96869750	-0.12550766	2.93448077
30	H	-1.42080624	5.92176706	3.32182131	91	H	-1.72725476	3.89301352	-0.17306516
31	H	-0.22196269	6.30648230	1.23120743	92	H	-0.95839433	4.91300646	-1.39520494
32	H	-0.39871165	7.77692452	0.35467754	93	H	-1.98171904	3.56870453	-1.87807991
33	H	-3.82418144	5.77198326	4.07422455	94	H	-0.27636311	3.08647261	-3.32798243
34	H	-4.29145336	7.05404905	2.88729005	95	H	1.09378383	4.01073315	-2.74049521
35	C	5.42274538	-0.42250049	-2.51311520	96	H	-2.37597098	1.52197953	-1.79204594
36	C	5.79952591	0.67171776	-1.74003722	97	H	-1.07769598	1.01066092	-2.85699701
37	C	5.10014619	0.94575409	-0.56316127	98	H	-0.84798972	-1.17145716	-1.64031671
38	C	4.04112442	0.12919876	-0.17935929	99	H	-4.01606840	-2.82000439	-0.98576680
39	C	3.67833696	-0.99469999	-0.92713106	100	H	-2.30133206	-3.06276220	-1.31470890
40	C	4.38570686	-1.27516511	-2.08803814	101	H	-3.83807476	0.75383018	-0.21411244
41	C	3.23066928	0.40607648	1.02852789	102	H	-4.53499599	0.16209218	-1.72660022
42	C	2.16302555	1.38548664	0.98731301	103	H	-4.84953812	-0.68911285	-0.20972775
43	C	1.09771351	1.25849510	1.85097885	104	H	-1.07350489	1.08570730	3.43454850
44	C	-0.16972732	2.05105311	1.69861802	105	H	-0.37040655	2.67134915	3.77903939
45	C	0.24087178	3.44184358	1.21513817	106	H	-2.23709335	3.84684645	2.70018635
46	C	1.02327867	3.44097340	-0.08517608	107	H	-5.23669215	2.50044494	1.63142288
47	C	2.22545317	2.49373376	0.03465886	108	H	-4.59173639	3.94087041	2.42487733
48	C	0.00317764	2.94622277	-1.18071978	109	H	-5.44558694	2.71593689	3.37215117
49	C	-1.01302660	1.39666260	0.58848098	110	H	-3.19038229	0.10736817	2.06791794
50	C	-0.41006539	1.49288469	-0.82313664	111	H	-4.64828737	0.32135243	3.03618005
51	O	1.06820849	0.40623294	2.84944030	112	H	-3.07112096	0.26680738	3.82613799
52	C	-1.22501535	3.87912672	-1.14564038	113	H	-3.46002788	-2.11361558	1.39116257
53	C	0.57365977	3.03966414	-2.61297961	114	H	-3.00710931	-3.77632064	1.01938628
54	C	-1.44675330	0.91984035	-1.81370204	115	H	-1.21915051	-1.51762503	1.76649552
55	C	-1.70593817	-0.51454851	-1.49317359	116	H	1.18217421	-1.74339729	1.56490545
56	C	-2.86513328	-0.99618106	-1.02499520	117	H	1.84192327	-2.99842638	0.50093926
57	C	-3.00620346	-2.45640389	-0.70973603	118	H	1.39748870	-3.39309036	2.16286071
58	C	-4.07483734	-0.15901646	-0.77986592	119	H	-1.34189083	-4.90045405	0.07385434
59	O	3.21956139	2.70605707	-0.61626339	120	H	-0.16732163	-4.19241224	-1.03935318
60	O	-0.05819014	4.43319180	1.82561430	121	H	0.38629998	-5.16331537	0.33117374
61	C	-0.95997248	2.11073799	3.01889341	122	H	2.38689698	1.81886119	-2.39888507
62	C	-2.28792296	2.76480349	2.82549414	123	H	1.00697544	0.93155111	-3.03531068
					124	H	1.15806900	2.05753296	-5.21646311

1	H	4.40250574	2.33526664	-6.57547495	63	C	0.02413732	2.52411545	-1.11017061
2	H	3.68545071	3.94327685	-6.46105267	64	C	-1.00231500	1.25684108	0.85640867
3	H	2.69324166	2.57352882	-6.96197452	65	C	-0.39971421	1.13929883	-0.55413337
4	H	3.92750565	3.10714062	-2.86703349	66	O	1.09378765	0.43334524	3.13832024
5	H	4.91879495	3.71343912	-4.20056144	67	C	-1.19596052	3.46313850	-1.19769592
6	H	4.92414521	1.98765942	-3.80382180	68	C	0.58367417	2.41788792	-2.54587596
7	H	3.17518379	-2.37509384	-3.19981995	69	C	-1.43205296	0.42348797	-1.45261022
8	H	6.48330704	-1.47839253	-3.80636697	70	C	-1.65092970	-0.95898496	-0.93373221
9	H	2.12227880	4.80903272	-1.36100602	71	C	-2.75084235	-1.38214248	-0.29692592
10	H	0.75494636	5.56395710	-0.54064775	72	C	-2.81945058	-2.78095453	0.24437360
11	H	2.02372785	5.41680349	1.68036804	73	C	-3.96778407	-0.55305476	-0.06734996
12	H	4.04372309	6.20412205	2.61402418	74	O	3.30526197	2.45102788	-0.43956077
13	H	5.02427110	7.13726707	1.47742220	75	O	0.07996524	4.39044120	1.72252214
14	H	5.45588444	5.46445282	1.85126155	76	C	-0.86252944	2.24140138	3.19083196
15	H	4.00463141	6.19655416	-1.55047506	77	C	-2.16923385	2.92771010	2.96881645
16	H	5.53593657	5.89506228	-0.72271289	78	C	-3.36647417	2.32704743	3.02259912
17	H	4.48765947	4.53891368	-1.16015876	79	C	-4.62043657	3.08978030	2.75321664
18					80	C	-3.55165196	0.88013359	3.33236657
19	Energy = -2864.29981188 a.u. #Cluster: 8								
20	O	3.72196426	-3.02959489	-5.22221384	81	C	-2.34048345	-2.82088008	1.70993322
21	N	3.99670223	-0.89344684	-5.85733614	82	C	-0.87863264	-2.53531617	1.83074979
22	C	4.28554387	-2.22351693	-5.97437514	83	C	0.09711987	-3.38553712	1.48303128
23	C	5.20677271	-2.65153013	-7.04337066	84	C	1.53686461	-3.02546741	1.65133366
24	C	5.76695807	-3.86168406	-7.01532536	85	C	-0.13955651	-4.73739627	0.90084955
25	H	5.40057211	-1.92857020	-7.83842998	86	C	1.55620144	1.26629101	-2.84198126
26	H	4.50639999	-0.18928760	-6.36684539	87	C	2.12822537	1.47936773	-4.20807529
27	H	3.44250239	-0.55366390	-5.08364702	88	C	3.30132469	2.08515899	-4.44113043
28	H	6.45361843	-4.21812187	-7.77549904	89	C	3.78274190	2.34606488	-5.83002501
29	H	5.58623688	-4.58927072	-6.22940324	90	C	4.20081296	2.56435581	-3.35533086
30	O	-1.61127957	8.49774636	0.06639659	91	O	2.82902039	-2.17100601	-2.85534356
31	N	0.06398636	7.20462797	0.81251809	92	O	5.40394652	-1.51697473	-3.59175968
32	C	-1.25817582	7.42478989	0.55627248	93	O	3.48686178	-0.33650030	2.32229416
33	C	-2.20627916	6.34638828	0.91374075	94	C	1.60081249	4.50692945	-0.59575548
34	C	-3.24610276	6.05192957	0.13576506	95	C	2.50393559	5.17677287	0.38825447
35	H	-1.98809724	5.81711052	1.84513892	96	C	3.24910776	6.24648717	0.07371811
36	H	0.39319107	6.31098602	1.15594013	97	C	4.13771663	6.89770846	1.07879492
37	H	0.76895515	7.87440762	0.55534166	98	C	3.25966146	6.84863828	-1.29009341
38	H	-3.95995175	5.26852220	0.36407721	99	H	6.74159264	-0.02731164	-1.79451670
39	H	-3.46956374	6.56601435	-0.79307840	100	H	5.77293011	0.70205496	0.37808098
40	O	7.30989826	4.46259103	1.30535216	101	H	2.04429567	-1.25850802	-0.62272146
41	N	5.48157211	3.18400336	1.52084667	102	H	-1.22882036	0.24080370	1.24768261
42	C	6.36510494	3.89499022	0.75638687	103	H	-1.99271430	1.75748424	0.79743996
43	C	6.14711926	3.90664990	-0.70453831	104	H	0.51021336	0.48880789	-0.51154285
44	C	6.63839948	4.88379760	-1.46542828	105	H	1.98132837	-0.08397803	3.28210591
45	H	5.54500339	3.08680521	-1.10755728	106	H	-1.64813797	3.67435644	-0.22327976
46	H	4.66461006	2.76377146	1.11143356	107	H	-0.93671772	4.42654657	-1.65358657
47	H	5.53487169	3.19038359	2.52588698	108	H	-1.98791258	3.02833933	-1.82199069
48	H	6.49115188	4.93493355	-2.53822715	109	H	-0.26962028	2.33451346	-3.25333358
49	H	7.22276251	5.71092057	-1.07752009	110	H	1.07251247	3.37540715	-2.81874199
50	C	4.95031340	-1.06416306	-2.39714334	111	H	-2.37303879	1.00405870	-1.50338073
51	C	5.71969367	-0.30153981	-1.52930778	112	H	-1.06767736	0.38078232	-2.50097265
52	C	5.16955462	0.11139076	-0.31255737	113	H	-0.79974242	-1.62714393	-1.07305995
53	C	3.85991645	-0.22538625	-0.00100626	114	H	-3.85325222	-3.17524971	0.18264259
54	C	3.07396092	-0.99485176	-0.86553773	115	H	-2.20378622	-3.47416676	-0.36441549
55	C	3.62345644	-1.42552438	-2.06771728	116	H	-3.75317327	0.52315354	-0.02084921
56	C	3.22268477	0.21417901	1.26149456	117	H	-4.69991391	-0.69953258	-0.87641334
57	C	2.18235594	1.22682507	1.18591715	118	H	-4.47689915	-0.81410751	-0.87169239
58	C	1.13272238	1.20212811	2.07254228	119	H	-1.00294726	1.27121850	3.71633337
59	C	-0.11701364	2.01154122	1.86465807	120	H	-0.22726568	2.85092913	3.87279407
60	C	0.31269428	3.32796958	1.21360301	121	H	-2.08166093	3.99025012	2.74275161
61	C	1.05678631	3.15719596	-0.10284275	122	H	-5.11067039	2.72864590	1.83524156
62	C	2.26736613	2.25345245	0.15101847	123	H	-4.45313565	4.16744214	2.62374473
					124	H	-5.34998110	2.97306616	3.56806282

1	H	-3.03687443	0.23958601	2.59996869	63	H	-0.48112815	6.58934101	0.57717796
2	H	-4.60648450	0.57358834	3.33107679	64	H	-0.52706950	7.95713654	-0.46506613
3	H	-3.14694610	0.62131604	4.32327077	65	H	-4.51999068	6.22765328	2.80383610
4	H	-2.92984261	-2.09793945	2.30936219	66	H	-4.79193401	7.37457706	1.43277782
5	H	-2.57796679	-3.81642712	2.14196242	67	O	7.86047382	3.25790122	-0.59185982
6	H	-0.64394720	-1.55209811	2.23427642	68	N	5.85056174	3.31785811	0.39319998
7	H	1.68634276	-1.98860495	1.97449304	69	C	6.66318020	2.97062505	-0.64795910
8	H	2.09741493	-3.16514310	0.71444221	70	C	6.05112246	2.24852425	-1.78301549
9	H	2.01927060	-3.66626328	2.40582697	71	C	6.76960133	1.92285616	-2.85740219
10	H	-1.10085183	-5.17033359	1.21061991	72	H	4.99007109	1.99806170	-1.68270187
11	H	-0.15174952	-4.68922492	-0.20002588	73	H	4.85953750	3.13128345	0.37180797
12	H	0.64238536	-5.45636256	1.18157103	74	H	6.19970629	3.83425505	1.18140398
13	H	2.35800290	1.21120638	-2.08084957	75	H	6.36415360	1.39303362	-3.70926740
14	H	1.03814468	0.28706211	-2.79087732	76	H	7.82268621	2.15907501	-2.96970209
15	H	1.49282358	1.13848578	-5.02189008	77	C	5.04643949	-1.33227553	-1.31328816
16	H	4.81976208	2.00963758	-5.97682148	78	C	5.84919127	-0.75774094	-0.33474660
17	H	3.77866859	3.42694551	-6.04466399	79	C	5.26275712	0.05450843	0.63530757
18	H	3.16416852	1.87168572	-6.60298006	80	C	3.88990226	0.29174709	0.61324301
19	H	3.67952029	3.26450279	-2.68023570	81	C	3.07434975	-0.29994766	-0.35753434
20	H	5.09606969	3.07431439	-3.72969771	82	C	3.64839936	-1.11571285	-1.32390967
21	H	4.53747283	1.72894932	-2.71754154	83	C	3.28742540	1.15835127	1.64383461
22	H	3.26428497	-2.44369032	-3.73616271	84	C	2.04926383	1.87511753	1.33242747
23	H	6.30215878	-1.14060405	-3.81819092	85	C	0.94556115	1.75502705	2.12840362
24	H	2.15643156	4.34246220	-1.55119680	86	C	-0.36083576	2.43970096	1.80107985
25	H	0.76110075	5.18407505	-0.86272956	87	C	-0.02555846	3.72843049	1.05397986
26	H	2.53352426	4.74738031	1.38581942	88	C	0.80125527	3.52435299	-0.20607634
27	H	4.07641836	6.43275945	2.07208809	89	C	2.06823740	2.74700648	0.16479224
28	H	3.89421922	7.96314420	1.20391583	90	C	-0.13620888	2.73108373	-1.19530833
29	H	5.19157512	6.84392627	0.76528211	91	C	-1.13679076	1.52935815	0.83406573
30	H	2.24465657	7.06173417	-1.65592638	92	C	-0.46996015	1.36252194	-0.54215657
31	H	3.82378763	7.78934173	-1.33877172	93	O	0.84267086	1.00652188	3.19687806
32	H	3.72234758	6.16297941	-2.01803081	94	C	-1.42468579	3.55502217	-1.39537403
33					95	C	0.48098573	2.55908735	-2.60083336
34	<b>OC-(AM)<sub>4</sub> complex in the DMSO</b>				96	C	-1.39817829	0.49034113	-1.41772502
35					97	C	-1.47146412	-0.87490432	-0.81831885
36	Energy = -3111.43796223 a.u. #Cluster: 1				98	C	-2.48979086	-1.35243380	-0.09077050
37	O	3.93064285	-2.74749999	-4.39620286	99	C	-2.37742223	-2.69325992	0.57794032
38	N	4.46730677	-0.61147785	-4.80674914	100	C	-3.77343227	-0.63760471	0.15449043
39	C	4.68934159	-1.95129742	-4.96431186	101	O	3.08393490	2.90670632	-0.47741015
40	C	5.79935281	-2.38208945	-5.83222358	102	O	-0.40623208	4.80078541	1.44054008
41	C	6.15025735	-3.66762714	-5.90039690	103	C	-1.17526556	2.72476706	3.07622890
42	H	6.30964935	-1.60150646	-6.40035311	104	C	-2.56133769	3.16967424	2.74456924
43	H	5.04455450	0.09090762	-5.23071250	105	C	-3.66266395	2.43082755	2.93844861
44	H	3.72635289	-0.27740742	-4.20539866	106	C	-5.01072324	2.94204407	2.55386187
45	H	6.96292440	-4.03220477	-6.51954769	107	C	-3.64517362	1.06443423	3.53670937
46	H	5.65459278	-4.45525348	-5.34014413	108	C	-1.57421518	-2.56959385	1.89107138
47	O	2.29788589	-0.77644790	4.44480437	109	C	-0.11958930	-2.37514538	1.60917220
48	N	4.22696091	-1.49650794	3.55612514	110	C	0.74944266	-3.37490503	1.40724702
49	C	3.04936958	-1.72855801	4.19873815	111	C	2.18399989	-3.10423040	1.09662502
50	C	2.73043136	-3.10297988	4.62923447	112	C	0.37329602	-4.81722323	1.46959568
51	C	1.46087083	-3.49316772	4.75199562	113	C	1.54515494	1.46685553	-2.77923588
52	H	3.57823342	-3.75923485	4.83171692	114	C	2.00186227	1.45827361	-4.20372692
53	H	4.84744628	-2.23504941	3.26916933	115	C	2.91181603	2.29924009	-4.71510805
54	H	4.45207862	-0.56412531	3.23354849	116	C	3.30546574	2.23173018	-6.15480486
55	H	1.16984921	-4.49031080	5.06290123	117	C	3.58192315	3.37797569	-3.93691934
56	H	0.61308344	-2.84667475	4.54115669	118	O	2.81076853	-1.67135884	-2.21964761
57	O	-2.75379983	8.76897267	0.33748563	119	O	5.52722807	-2.12040216	-2.30038880
58	N	-0.95464875	7.43179914	0.27936165	120	O	3.79357443	1.25371729	2.74837225
59	C	-2.18137222	7.76919659	0.77477684	121	C	1.26310513	4.87787998	-0.77740892
60	C	-2.74749723	6.91493914	1.84073820	122	C	2.10809400	5.63478400	0.19572206
61	C	-4.06390931	6.83656601	2.03140239	123	C	3.34515437	6.08525213	-0.05750277
62	H	-2.02541593	6.36152709	2.44800526	124	C	4.11975733	6.82297519	0.98459402





1	C	-3.56359570	-0.87107730	-0.97982901	63	H	0.85061127	-4.22856029	0.23065795
2	O	3.24667150	3.21824453	-0.62995943	64	H	1.06259538	-4.98711878	1.81405468
3	O	-0.45875840	4.66123485	1.28270419	65	H	2.64213794	1.57727951	-2.07225931
4	C	-1.06803225	2.41721478	2.78247618	66	H	1.44372693	0.55267382	-2.86049596
5	C	-2.46560204	2.82247130	2.44924782	67	H	1.97983647	1.64859984	-5.09767309
6	C	-3.52063680	1.99658247	2.41721324	68	H	5.34504161	1.05289347	-5.85687855
7	C	-4.87384914	2.49748548	2.03268079	69	H	5.12544127	2.80412583	-5.86419547
8	C	-3.45539820	0.53881930	2.72236396	70	H	3.87572138	1.75634981	-6.54320872
9	C	-2.32517176	-3.00324963	1.06074920	71	H	4.59973667	2.59182832	-2.48075458
10	C	-1.12373206	-2.45117683	1.75669777	72	H	5.93807482	2.07968961	-3.52309581
11	C	0.06120128	-3.07113652	1.84014130	73	H	4.95499975	0.87242055	-2.68815813
12	C	1.20731470	-2.45714159	2.57404830	74	H	1.96745375	-2.76815610	-2.08082297
13	C	0.36801373	-4.38743213	1.21185802	75	H	5.59506151	-2.91583071	-2.60615900
14	C	1.93104333	1.54922711	-2.92010655	76	H	1.74790749	4.98068708	-1.84661678
15	C	2.63870349	1.66366385	-4.23095315	77	H	0.29246088	5.59198679	-1.06316605
16	C	3.96659293	1.77777300	-4.37020540	78	H	1.60841435	5.86402096	1.12518343
17	C	4.59740439	1.84940782	-5.72127538	79	H	3.49022227	7.09597225	1.88853704
18	C	4.91241223	1.83454882	-3.22067373	80	H	4.39573534	7.95568687	0.63575552
19	O	2.19534251	-2.70194460	-1.09720156	81	H	4.96223367	6.38455275	1.21699827
20	O	4.64112939	-2.86031369	-2.29623707	82	H	3.42084637	6.76165696	-2.20022888
21	O	4.32415426	1.65451958	2.13375472	83	H	4.98861513	6.54768628	-1.41863980
22	C	1.22961605	5.03367199	-0.86206188	84	H	3.98503301	5.13645961	-1.79835081
23	C	2.06192075	5.76548083	0.14043669	85				
24	C	3.27963035	6.26780829	-0.10963440	86		Energy = -3111.43031752 a.u. #Cluster: 3		
25	C	4.05922808	6.96022376	0.95907766	87	O	5.98820480	-3.22434260	-4.56109367
26	C	3.95538196	6.17846941	-1.43605197	88	N	3.92552495	-4.08985574	-4.34363896
27	H	6.45941958	-1.09001276	-1.41205042	89	C	5.07601962	-3.89084652	-5.05796655
28	H	5.92587013	0.73067916	0.20029945	90	C	5.21969793	-4.57805600	-6.35766222
29	H	1.82256784	-0.64076694	0.40050689	91	C	5.98617885	-4.05594900	-7.31527703
30	H	-0.97950874	0.36238346	0.86995952	92	H	4.66341322	-5.50826706	-6.47950904
31	H	-1.93428851	1.73382126	0.32214705	93	H	3.11270769	-4.52386036	-4.75334072
32	H	0.81529183	0.83130464	-0.75084825	94	H	3.74864635	-3.53329829	-3.51866935
33	H	2.00715456	0.52381578	3.21172994	95	H	6.11973115	-4.51219958	-8.28908119
34	H	-1.80832087	3.65755715	-0.85623300	96	H	6.53514155	-3.12602896	-7.19984209
35	H	-1.02980274	4.48628127	-2.21156711	97	O	4.09506554	-1.34877153	-5.54085382
36	H	-1.82732035	2.94414650	-2.46371311	98	N	1.86876553	-1.15543677	-5.74624083
37	H	0.16203647	2.56106928	-3.63094417	99	C	3.12482821	-1.11851176	-6.27863999
38	H	1.39693305	3.64052074	-3.00436458	100	C	3.28805918	-0.84433946	-7.71706778
39	H	-2.03521099	0.94946579	-1.95324089	101	C	4.50433526	-0.64836210	-8.22945562
40	H	-0.60141692	0.52019818	-2.86917102	102	H	2.37784340	-0.81280116	-8.31736013
41	H	-0.13242773	-1.42068914	-1.31851913	103	H	1.04461293	-0.90398792	-6.26510392
42	H	-2.99078418	-3.52592150	-0.94871553	104	H	1.74517817	-1.29324569	-4.75347942
43	H	-1.23638935	-3.43390838	-0.77347859	105	H	4.68457975	-0.44303971	-9.27839095
44	H	-3.55629724	0.10468938	-0.47301701	106	H	5.41302953	-0.67952659	-7.63311334
45	H	-3.90325544	-0.69279164	-2.01113371	107	O	-1.68264213	8.61245986	0.50522588
46	H	-4.33576810	-1.47783336	-0.48905977	108	N	0.01188743	7.28638219	1.14078368
47	H	-1.05118722	1.45470689	3.34030567	109	C	-1.31697354	7.51735192	0.93321554
48	H	-0.61048938	3.16231872	3.47111168	110	C	-2.25500995	6.42218522	1.26387755
49	H	-2.57409150	3.87924419	2.20220043	111	C	-3.33415183	6.18626439	0.52006903
50	H	-5.28645239	1.92359760	1.18923186	112	H	-1.99701492	5.82957604	2.14584434
51	H	-4.87402407	3.55323307	1.72988879	113	H	0.35108522	6.37878114	1.43460027
52	H	-5.58939938	2.39966714	2.86240502	114	H	0.70944782	7.96995950	0.89894083
53	H	-3.18974996	-0.03917073	1.82193641	115	H	-4.04215487	5.39234490	0.72940899
54	H	-4.41578253	0.14028973	3.07780037	116	H	-3.59849194	6.76296536	-0.35998590
55	H	-2.70691076	0.29661324	3.49101491	117	O	7.10608321	4.98878795	0.98480631
56	H	-3.23937409	-2.45821847	1.37090703	118	N	5.51908093	3.46633874	1.42592598
57	H	-2.49755904	-4.05766032	1.36315570	119	C	6.22699397	4.24384572	0.55129442
58	H	-1.27173176	-1.47064188	2.20342824	120	C	5.92197537	4.10152306	-0.88822947
59	H	0.98508775	-1.45244844	2.95776439	121	C	6.11847785	5.11246615	-1.73301201
60	H	2.09198438	-2.37663729	1.92411996	122	H	5.50604408	3.13689749	-1.19709164
61	H	1.50239260	-3.07106962	3.43742701	123	H	4.74092521	2.91200338	1.10757727
62	H	-0.52604067	-4.99894979	1.03534019	124	H	5.62575173	3.56822295	2.42071875

1	H	5.89728590	5.05701374	-2.79274534	63	H	1.05765023	3.66269901	-2.62843477
2	H	6.51160007	6.07735081	-1.43348381	64	H	-2.42318209	1.20207708	-1.37364713
3	C	5.43474070	-0.62105373	-2.18392238	65	H	-1.13522493	0.71590424	-2.46269772
4	C	6.09223831	0.01661629	-1.13479864	66	H	-0.74989734	-1.39844308	-1.24195574
5	C	5.38414501	0.32441613	0.02787746	67	H	-3.66704210	-3.14684063	0.11589442
6	C	4.03097222	0.02158947	0.11603483	68	H	-2.08706219	-3.35646248	-0.63589888
7	C	3.35257201	-0.60519414	-0.93358371	69	H	-3.74169130	0.54965419	0.04982442
8	C	4.06099952	-0.93307997	-2.08318351	70	H	-4.69470304	-0.72959429	-0.71044248
9	C	3.24891675	0.32986309	1.33300947	71	H	-4.28141364	-0.83392195	1.00405059
10	C	2.18405716	1.31456586	1.26586792	72	H	-0.99607100	1.23218906	3.80027731
11	C	1.12268591	1.23383673	2.13891236	73	H	-0.21022122	2.79806475	4.03038878
12	C	-0.12208400	2.06242804	1.98096174	74	H	-2.06930714	4.00156637	2.97152535
13	C	0.31069295	3.40863219	1.39619512	75	H	-5.10241448	2.81983708	2.03734071
14	C	1.04906645	3.30199552	0.07102127	76	H	-4.44451597	4.19938785	2.92556863
15	C	2.25629052	2.37680612	0.26705243	77	H	-5.34397545	2.94224225	3.78249001
16	C	0.00296357	2.73309559	-0.96025900	78	H	-2.98692237	0.26214159	2.72386457
17	C	-1.01952598	1.36614096	0.94259816	79	H	-4.59954665	0.56256908	3.37049781
18	C	-0.42382224	1.32269706	-0.47516171	80	H	-3.20061881	0.58969594	4.44776530
19	O	1.07242418	0.39730620	3.14906021	81	H	-2.50258779	-2.17436725	2.19224304
20	C	-1.21422957	3.67944251	-0.98638376	82	H	-2.18985431	-3.88171222	1.87995220
21	C	0.55079983	2.70229150	-2.40403568	83	H	-0.23985687	-1.62180868	1.86105882
22	C	-1.46190450	0.65441690	-1.40344369	84	H	2.05318041	-2.09171286	1.38885574
23	C	-1.61202768	-0.77467870	-0.99940129	85	H	2.25618296	-3.07821637	-0.07012899
24	C	-2.65882361	-1.29144656	-0.34300851	86	H	2.42964959	-3.81015017	1.52885783
25	C	-2.64146035	-2.72900988	0.09101537	87	H	-0.86242773	-5.17372783	0.70708495
26	C	-3.89232428	-0.53773936	0.01887139	88	H	-0.03368663	-4.64464979	-0.75972112
27	O	3.27881033	2.58604863	-0.34552847	89	H	0.86529958	-5.48744382	0.50715426
28	O	0.08017663	4.44471830	1.95840928	90	H	2.36261736	1.50917319	-2.07897446
29	C	-0.85493662	2.22744222	3.32410637	91	H	0.99060618	0.56985955	-2.66128183
30	C	-2.16005670	2.93035507	3.15063131	92	H	1.19179967	1.47699277	-4.92629996
31	C	-3.35999478	2.33432966	3.19415540	93	H	4.33599860	1.58349724	-6.23949376
32	C	-4.61314754	3.11547596	2.97912862	94	H	3.91006223	3.30247122	-6.22313629
33	C	-3.54932164	0.87623638	3.44309304	95	H	2.70183208	2.09414846	-6.67019866
34	C	-1.99508971	-2.86187346	1.48562050	96	H	3.81920798	3.01910566	-2.67482388
35	C	-0.52645087	-2.58672923	1.44763978	97	H	4.97547157	3.21303719	-4.00797523
36	C	0.39370674	-3.42258351	0.94709672	98	H	4.76290681	1.63158171	-3.23857595
37	C	1.84652641	-3.07615063	0.95212431	99	H	3.76945627	-1.43408311	-4.00094766
38	C	0.07621777	-4.74331207	0.33240710	100	H	5.83487967	-1.67549154	-3.82082175
39	C	1.49691493	1.55070385	-2.76842897	101	H	2.18325159	4.53965994	-1.30571556
40	C	1.94472668	1.73093764	-4.18402477	102	H	0.77029182	5.35507155	-0.62096844
41	C	3.15707966	2.17015502	-4.54674215	103	H	2.53317881	4.80462665	1.63530948
42	C	3.53575643	2.29707131	-5.98641804	104	H	3.95115279	6.54218914	2.45977443
43	C	4.22894711	2.53479904	-3.57780782	105	H	3.85715940	8.09246507	1.61459945
44	O	3.39019891	-1.58750286	-3.04663821	106	H	5.12552550	6.92941983	1.19859239
45	O	6.15923299	-0.87319029	-3.29308411	107	H	2.15499303	7.28632113	-1.25518176
46	O	3.44285809	-0.30556545	2.36575386	108	H	3.68135250	8.08605495	-0.86415501
47	C	1.60406168	4.66952412	-0.35786135	109	H	3.68895014	6.50475112	-1.65290436
48	C	2.48384032	5.30196554	0.67049224	110				
49	C	3.18928998	6.41726657	0.43140864					
50	C	4.06351603	7.02131637	1.47762230					
51	C	3.17664199	7.11133834	-0.88791385					
52	H	7.14974601	0.26272860	-1.22782850					
53	H	5.90047562	0.80165672	0.86242355					
54	H	2.28953477	-0.83520654	-0.87500753					
55	H	-1.24760943	0.33130540	1.27907839					
56	H	-2.00830454	1.87239687	0.91741313					
57	H	0.48456477	0.66824238	-0.46898127					
58	H	1.96074982	-0.14101323	3.25800294					
59	H	-1.65731717	3.84160507	0.00142671					
60	H	-0.95642974	4.66366629	-1.39638095					
61	H	-2.01351062	3.27799242	-1.62330018					
62	H	-0.30949362	2.67487764	-3.10732344					